wwPDB EM Validation Summary Report

Jul 2, 2023 – 12:31 AM JST

PDB ID	:	7WZN
EMDB ID	:	EMD-32907
Title	:	PSI-LHCI from Chlamydomonas reinhardtii with bound ferredoxin
Authors	:	Kurisu, G.; Gerle, C.; Mitsuoka, K.; Kawamoto, A.; Tanaka, H.
Deposited on	:	2022-02-18
Resolution	:	4.90 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:

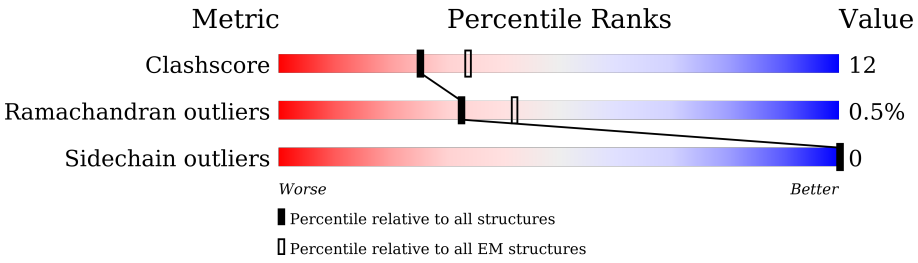
EMDB validation analysis	:	0.0.1.dev50
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.33

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 4.90 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 <=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	91% 7% •
2	B	735	91% 8%
3	C	81	75% 23% •
4	D	196	62% 11% • 27%
5	E	97	51% 12% 37%
6	F	227	67% 6% 27%
7	J	41	88% 7% 5%
8	1	224	78% 9% 13%

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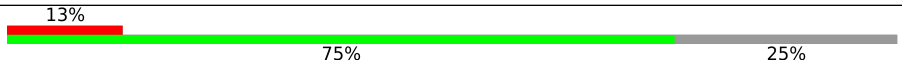
Mol	Chain	Length	Quality of chain
9	3	298	
10	7	241	
11	8	243	
12	Z	228	
13	4	264	
14	5	257	
15	6	257	
16	G	126	

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
17	CL0	A	801	X	-	-	-
18	CLA	1	602	X	-	-	-
18	CLA	1	603	X	-	-	-
18	CLA	1	604	X	-	-	-
18	CLA	1	605	X	-	-	-
18	CLA	1	607	X	-	-	-
18	CLA	1	608	X	-	-	-
18	CLA	1	609	X	-	-	-
18	CLA	1	610	X	-	-	-
18	CLA	1	611	X	-	-	-
18	CLA	1	612	X	-	-	-
18	CLA	1	613	X	-	-	-
18	CLA	1	614	X	-	-	-
18	CLA	3	301	X	-	-	-
18	CLA	3	302	X	-	-	-
18	CLA	3	303	X	-	-	-
18	CLA	3	304	X	-	-	-
18	CLA	3	305	X	-	-	-
18	CLA	3	307	X	-	-	-
18	CLA	3	308	X	-	-	-
18	CLA	3	309	X	-	-	-
18	CLA	3	310	X	-	-	-
18	CLA	3	311	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
18	CLA	3	312	X	-	-	-
18	CLA	3	313	X	-	-	-
18	CLA	3	314	X	-	-	-
18	CLA	4	601	X	-	-	-
18	CLA	4	602	X	-	-	-
18	CLA	4	603	X	-	-	-
18	CLA	4	606	X	-	-	-
18	CLA	4	607	X	-	-	-
18	CLA	4	608	X	-	-	-
18	CLA	4	609	X	-	-	-
18	CLA	4	610	X	-	-	-
18	CLA	4	611	X	-	-	-
18	CLA	4	612	X	-	-	-
18	CLA	5	601	X	-	-	-
18	CLA	5	602	X	-	-	-
18	CLA	5	603	X	-	-	-
18	CLA	5	604	X	-	-	-
18	CLA	5	605	X	-	-	-
18	CLA	5	608	X	-	-	-
18	CLA	5	609	X	-	-	-
18	CLA	5	610	X	-	-	-
18	CLA	5	611	X	-	-	-
18	CLA	5	612	X	-	-	-
18	CLA	5	613	X	-	-	-
18	CLA	5	614	X	-	-	-
18	CLA	5	615	X	-	-	-
18	CLA	5	617	X	-	-	-
18	CLA	6	301	X	-	-	-
18	CLA	6	302	X	-	-	-
18	CLA	6	303	X	-	-	-
18	CLA	6	304	X	-	-	-
18	CLA	6	308	X	-	-	-
18	CLA	6	309	X	-	-	-
18	CLA	6	310	X	-	-	-
18	CLA	6	311	X	-	-	-
18	CLA	6	312	X	-	-	-
18	CLA	6	313	X	-	-	-
18	CLA	6	314	X	-	-	-
18	CLA	6	315	X	-	-	-
18	CLA	6	317	X	-	-	-
18	CLA	7	601	X	-	-	-
18	CLA	7	602	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
18	CLA	7	603	X	-	-	-
18	CLA	7	604	X	-	-	-
18	CLA	7	605	X	-	-	-
18	CLA	7	607	X	-	-	-
18	CLA	7	608	X	-	-	-
18	CLA	7	609	X	-	-	-
18	CLA	7	610	X	-	-	-
18	CLA	7	611	X	-	-	-
18	CLA	7	612	X	-	-	-
18	CLA	7	613	X	-	-	-
18	CLA	7	614	X	-	-	-
18	CLA	8	601	X	-	-	-
18	CLA	8	602	X	-	-	-
18	CLA	8	603	X	-	-	-
18	CLA	8	604	X	-	-	-
18	CLA	8	605	X	-	-	-
18	CLA	8	607	X	-	-	-
18	CLA	8	608	X	-	-	-
18	CLA	8	609	X	-	-	-
18	CLA	8	610	X	-	-	-
18	CLA	8	611	X	-	-	-
18	CLA	8	612	X	-	-	-
18	CLA	8	613	X	-	-	-
18	CLA	8	614	X	-	-	-
18	CLA	8	615	X	-	-	-
18	CLA	A	802	X	-	-	-
18	CLA	A	803	X	-	-	-
18	CLA	A	804	X	-	-	-
18	CLA	A	805	X	-	-	-
18	CLA	A	806	X	-	-	-
18	CLA	A	807	X	-	-	-
18	CLA	A	808	X	-	-	-
18	CLA	A	809	X	-	-	-
18	CLA	A	810	X	-	-	-
18	CLA	A	811	X	-	-	-
18	CLA	A	812	X	-	-	-
18	CLA	A	813	X	-	-	-
18	CLA	A	814	X	-	-	-
18	CLA	A	815	X	-	-	-
18	CLA	A	816	X	-	-	-
18	CLA	A	817	X	-	-	-
18	CLA	A	818	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
18	CLA	A	819	X	-	-	-
18	CLA	A	820	X	-	-	-
18	CLA	A	821	X	-	-	-
18	CLA	A	822	X	-	-	-
18	CLA	A	823	X	-	-	-
18	CLA	A	824	X	-	-	-
18	CLA	A	825	X	-	-	-
18	CLA	A	826	X	-	-	-
18	CLA	A	827	X	-	-	-
18	CLA	A	828	X	-	-	-
18	CLA	A	829	X	-	-	-
18	CLA	A	830	X	-	-	-
18	CLA	A	831	X	-	-	-
18	CLA	A	832	X	-	-	-
18	CLA	A	833	X	-	-	-
18	CLA	A	834	X	-	-	-
18	CLA	A	835	X	-	-	-
18	CLA	A	836	X	-	-	-
18	CLA	A	837	X	-	-	-
18	CLA	A	838	X	-	-	-
18	CLA	A	839	X	-	-	-
18	CLA	A	840	X	-	-	-
18	CLA	A	841	X	-	-	-
18	CLA	A	843	X	-	-	-
18	CLA	A	844	X	-	-	-
18	CLA	A	845	X	-	-	-
18	CLA	B	801	X	-	-	-
18	CLA	B	802	X	-	-	-
18	CLA	B	804	X	-	-	-
18	CLA	B	805	X	-	-	-
18	CLA	B	806	X	-	-	-
18	CLA	B	807	X	-	-	-
18	CLA	B	808	X	-	-	-
18	CLA	B	809	X	-	-	-
18	CLA	B	810	X	-	-	-
18	CLA	B	811	X	-	-	-
18	CLA	B	812	X	-	-	-
18	CLA	B	813	X	-	-	-
18	CLA	B	814	X	-	-	-
18	CLA	B	815	X	-	-	-
18	CLA	B	816	X	-	-	-
18	CLA	B	817	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
18	CLA	B	818	X	-	-	-
18	CLA	B	819	X	-	-	-
18	CLA	B	820	X	-	-	-
18	CLA	B	821	X	-	-	-
18	CLA	B	822	X	-	-	-
18	CLA	B	823	X	-	-	-
18	CLA	B	824	X	-	-	-
18	CLA	B	825	X	-	-	-
18	CLA	B	826	X	-	-	-
18	CLA	B	827	X	-	-	-
18	CLA	B	828	X	-	-	-
18	CLA	B	829	X	-	-	-
18	CLA	B	830	X	-	-	-
18	CLA	B	831	X	-	-	-
18	CLA	B	832	X	-	-	-
18	CLA	B	833	X	-	-	-
18	CLA	B	834	X	-	-	-
18	CLA	B	835	X	-	-	-
18	CLA	B	836	X	-	-	-
18	CLA	B	837	X	-	-	-
18	CLA	B	838	X	-	-	-
18	CLA	B	839	X	-	-	-
18	CLA	B	840	X	-	-	-
18	CLA	B	841	X	-	-	-
18	CLA	B	842	X	-	-	-
18	CLA	B	843	X	-	-	-
18	CLA	F	301	X	-	-	-
18	CLA	F	302	X	-	-	-
18	CLA	J	101	X	-	-	-
18	CLA	Z	602	X	-	-	-
18	CLA	Z	603	X	-	-	-
18	CLA	Z	604	X	-	-	-
18	CLA	Z	606	X	-	-	-
18	CLA	Z	607	X	-	-	-
18	CLA	Z	608	X	-	-	-
18	CLA	Z	609	X	-	-	-
18	CLA	Z	610	X	-	-	-
18	CLA	Z	611	X	-	-	-
18	CLA	Z	612	X	-	-	-
18	CLA	Z	613	X	-	-	-
20	SF4	C	101	-	-	X	-
21	CHL	1	601	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
21	CHL	1	606	X	-	-	-
21	CHL	3	306	X	-	-	-
21	CHL	4	604	X	-	-	-
21	CHL	4	605	X	-	-	-
21	CHL	5	606	X	-	-	-
21	CHL	5	607	X	-	-	-
21	CHL	5	616	X	-	-	-
21	CHL	6	305	X	-	-	-
21	CHL	6	306	X	-	-	-
21	CHL	6	307	X	-	-	-
21	CHL	6	316	X	-	-	-
21	CHL	7	606	X	-	-	-
21	CHL	8	606	X	-	-	-
21	CHL	Z	601	X	-	-	-
21	CHL	Z	605	X	-	-	-

2 Entry composition (i)

There are 22 unique types of molecules in this entry. The entry contains 27190 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
			Total	C	N	O		
1	A	738	3628	2151	739	738	0	0

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

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
2	B	732	3601	2136	733	732	0	0

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

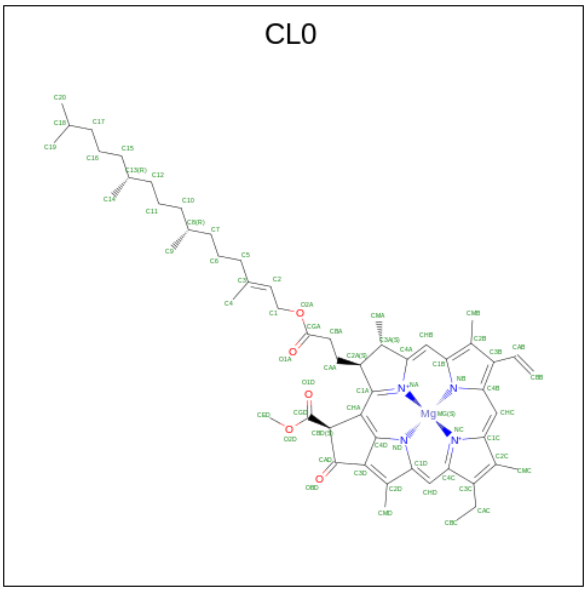
- Molecule 15 is a protein called Chlorophyll a-b binding protein, chloroplastic.

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

- Molecule 16 is a protein called Ferredoxin, chloroplastic.

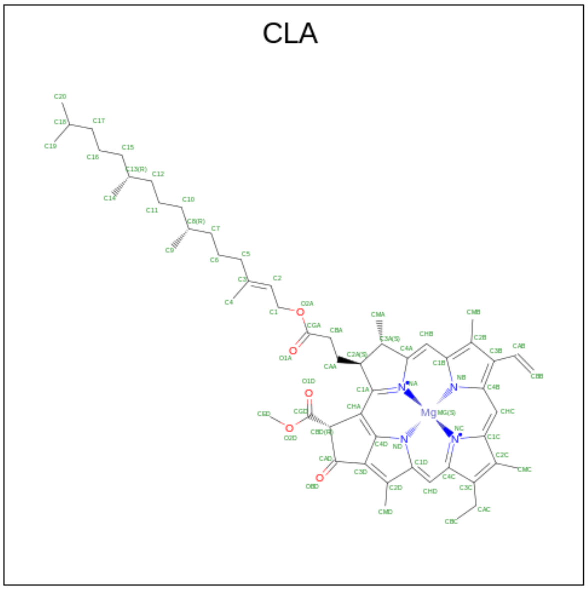
Mol	Chain	Residues	Atoms				AltConf	Trace
16	G	95	Total 493	C 293	N 100	O 100	5	0

- Molecule 17 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
17	A	1	Total 42	C 34	Mg 1	N 4	O 3	0

- Molecule 18 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
18	A	1	Total C Mg N O 42 34 1 4 3	0
18	A	1	Total C Mg N O 42 34 1 4 3	0
18	A	1	Total C Mg N O 42 34 1 4 3	0
18	A	1	Total C Mg N O 42 34 1 4 3	0
18	A	1	Total C Mg N O 42 34 1 4 3	0
18	A	1	Total C Mg N O 42 34 1 4 3	0
18	A	1	Total C Mg N O 42 34 1 4 3	0
18	A	1	Total C Mg N O 42 34 1 4 3	0
18	A	1	Total C Mg N O 42 34 1 4 3	0
18	A	1	Total C Mg N O 43 35 1 4 3	0
18	A	1	Total C Mg N O 42 34 1 4 3	0
18	A	1	Total C Mg N O 42 34 1 4 3	0
18	A	1	Total C Mg N O 42 34 1 4 3	0
18	A	1	Total C Mg N O 42 34 1 4 3	0

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Mol	Chain	Residues	Atoms					AltConf
18	A	1	Total 42	C 34	Mg 1	N 4	O 3	0
18	A	1	Total 47	C 37	Mg 1	N 4	O 5	0
18	A	1	Total 42	C 34	Mg 1	N 4	O 3	0
18	A	1	Total 42	C 34	Mg 1	N 4	O 3	0
18	A	1	Total 42	C 34	Mg 1	N 4	O 3	0
18	A	1	Total 42	C 34	Mg 1	N 4	O 3	0
18	A	1	Total 42	C 34	Mg 1	N 4	O 3	0
18	A	1	Total 51	C 41	Mg 1	N 4	O 5	0
18	A	1	Total 42	C 34	Mg 1	N 4	O 3	0
18	A	1	Total 42	C 34	Mg 1	N 4	O 3	0
18	A	1	Total 42	C 34	Mg 1	N 4	O 3	0
18	A	1	Total 42	C 34	Mg 1	N 4	O 3	0
18	A	1	Total 42	C 34	Mg 1	N 4	O 3	0
18	A	1	Total 42	C 34	Mg 1	N 4	O 3	0
18	A	1	Total 42	C 34	Mg 1	N 4	O 3	0
18	A	1	Total 42	C 34	Mg 1	N 4	O 3	0
18	A	1	Total 42	C 34	Mg 1	N 4	O 3	0
18	A	1	Total 42	C 34	Mg 1	N 4	O 3	0
18	A	1	Total 42	C 34	Mg 1	N 4	O 3	0
18	A	1	Total 42	C 34	Mg 1	N 4	O 3	0
18	A	1	Total 42	C 34	Mg 1	N 4	O 3	0

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Mol	Chain	Residues	Atoms					AltConf
18	A	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
18	A	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
18	A	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
18	A	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
18	A	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
18	A	1	Total	C	Mg	N	O	0
			52	42	1	4	5	
18	A	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
18	A	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
18	B	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
18	B	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
18	B	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
18	B	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
18	B	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
18	B	1	Total	C	Mg	N	O	0
			50	42	1	4	3	
18	B	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
18	B	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
18	B	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
18	B	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
18	B	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
18	B	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
18	B	1	Total	C	Mg	N	O	0
			42	34	1	4	3	

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Mol	Chain	Residues	Atoms					AltConf
18	B	1	Total 42	C 34	Mg 1	N 4	O 3	0
18	B	1	Total 42	C 34	Mg 1	N 4	O 3	0
18	B	1	Total 42	C 34	Mg 1	N 4	O 3	0
18	B	1	Total 42	C 34	Mg 1	N 4	O 3	0
18	B	1	Total 42	C 34	Mg 1	N 4	O 3	0
18	B	1	Total 42	C 34	Mg 1	N 4	O 3	0
18	B	1	Total 42	C 34	Mg 1	N 4	O 3	0
18	B	1	Total 45	C 35	Mg 1	N 4	O 5	0
18	B	1	Total 42	C 34	Mg 1	N 4	O 3	0
18	B	1	Total 42	C 34	Mg 1	N 4	O 3	0
18	B	1	Total 42	C 34	Mg 1	N 4	O 3	0
18	B	1	Total 42	C 34	Mg 1	N 4	O 3	0
18	B	1	Total 42	C 34	Mg 1	N 4	O 3	0
18	B	1	Total 42	C 34	Mg 1	N 4	O 3	0
18	B	1	Total 42	C 34	Mg 1	N 4	O 3	0
18	B	1	Total 45	C 35	Mg 1	N 4	O 5	0
18	B	1	Total 42	C 34	Mg 1	N 4	O 3	0
18	B	1	Total 42	C 34	Mg 1	N 4	O 3	0
18	B	1	Total 42	C 34	Mg 1	N 4	O 3	0
18	B	1	Total 39	C 31	Mg 1	N 4	O 3	0
18	B	1	Total 42	C 34	Mg 1	N 4	O 3	0

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Mol	Chain	Residues	Atoms	AltConf
18	B	1	Total C Mg N O 42 34 1 4 3	0
18	B	1	Total C Mg N O 42 34 1 4 3	0
18	B	1	Total C Mg N O 43 35 1 4 3	0
18	B	1	Total C Mg N O 42 34 1 4 3	0
18	B	1	Total C Mg N O 42 34 1 4 3	0
18	B	1	Total C Mg N O 42 34 1 4 3	0
18	B	1	Total C Mg N O 42 34 1 4 3	0
18	B	1	Total C Mg N O 42 34 1 4 3	0
18	F	1	Total C Mg N O 45 35 1 4 5	0
18	F	1	Total C Mg N O 65 55 1 4 5	0
18	J	1	Total C Mg N O 42 34 1 4 3	0
18	1	1	Total C Mg N O 42 34 1 4 3	0
18	1	1	Total C Mg N O 42 34 1 4 3	0
18	1	1	Total C Mg N O 42 34 1 4 3	0
18	1	1	Total C Mg N O 42 34 1 4 3	0
18	1	1	Total C Mg N O 42 34 1 4 3	0
18	1	1	Total C Mg N O 42 34 1 4 3	0
18	1	1	Total C Mg N O 42 34 1 4 3	0
18	1	1	Total C Mg N O 42 34 1 4 3	0
18	1	1	Total C Mg N O 42 34 1 4 3	0
18	1	1	Total C Mg N O 46 36 1 4 5	0

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Mol	Chain	Residues	Atoms					AltConf
18	1	1	Total 42	C 34	Mg 1	N 4	O 3	0
18	1	1	Total 46	C 36	Mg 1	N 4	O 5	0
18	3	1	Total 42	C 34	Mg 1	N 4	O 3	0
18	3	1	Total 42	C 34	Mg 1	N 4	O 3	0
18	3	1	Total 42	C 34	Mg 1	N 4	O 3	0
18	3	1	Total 42	C 34	Mg 1	N 4	O 3	0
18	3	1	Total 42	C 34	Mg 1	N 4	O 3	0
18	3	1	Total 42	C 34	Mg 1	N 4	O 3	0
18	3	1	Total 42	C 34	Mg 1	N 4	O 3	0
18	3	1	Total 41	C 33	Mg 1	N 4	O 3	0
18	3	1	Total 46	C 36	Mg 1	N 4	O 5	0
18	3	1	Total 45	C 35	Mg 1	N 4	O 5	0
18	3	1	Total 45	C 35	Mg 1	N 4	O 5	0
18	3	1	Total 46	C 36	Mg 1	N 4	O 5	0
18	3	1	Total 42	C 34	Mg 1	N 4	O 3	0
18	7	1	Total 42	C 34	Mg 1	N 4	O 3	0
18	7	1	Total 42	C 34	Mg 1	N 4	O 3	0
18	7	1	Total 46	C 36	Mg 1	N 4	O 5	0
18	7	1	Total 43	C 35	Mg 1	N 4	O 3	0
18	7	1	Total 42	C 34	Mg 1	N 4	O 3	0
18	7	1	Total 42	C 34	Mg 1	N 4	O 3	0

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Mol	Chain	Residues	Atoms					AltConf
18	7	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
18	7	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
18	7	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
18	7	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
18	7	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
18	7	1	Total	C	Mg	N	O	0
			43	35	1	4	3	
18	7	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
18	8	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
18	8	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
18	8	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
18	8	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
18	8	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
18	8	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
18	8	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
18	8	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
18	8	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
18	8	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
18	8	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
18	8	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
18	8	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
18	8	1	Total	C	Mg	N	O	0
			42	34	1	4	3	

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Mol	Chain	Residues	Atoms					AltConf
18	Z	1	Total 42	C 34	Mg 1	N 4	O 3	0
18	Z	1	Total 42	C 34	Mg 1	N 4	O 3	0
18	Z	1	Total 43	C 35	Mg 1	N 4	O 3	0
18	Z	1	Total 42	C 34	Mg 1	N 4	O 3	0
18	Z	1	Total 42	C 34	Mg 1	N 4	O 3	0
18	Z	1	Total 42	C 34	Mg 1	N 4	O 3	0
18	Z	1	Total 42	C 34	Mg 1	N 4	O 3	0
18	Z	1	Total 42	C 34	Mg 1	N 4	O 3	0
18	Z	1	Total 45	C 35	Mg 1	N 4	O 5	0
18	Z	1	Total 42	C 34	Mg 1	N 4	O 3	0
18	Z	1	Total 42	C 34	Mg 1	N 4	O 3	0
18	4	1	Total 42	C 34	Mg 1	N 4	O 3	0
18	4	1	Total 42	C 34	Mg 1	N 4	O 3	0
18	4	1	Total 46	C 36	Mg 1	N 4	O 5	0
18	4	1	Total 42	C 34	Mg 1	N 4	O 3	0
18	4	1	Total 42	C 34	Mg 1	N 4	O 3	0
18	4	1	Total 42	C 34	Mg 1	N 4	O 3	0
18	4	1	Total 42	C 34	Mg 1	N 4	O 3	0
18	4	1	Total 42	C 34	Mg 1	N 4	O 3	0
18	4	1	Total 42	C 34	Mg 1	N 4	O 3	0
18	4	1	Total 41	C 33	Mg 1	N 4	O 3	0

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Mol	Chain	Residues	Atoms					AltConf
18	5	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
18	5	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
18	5	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
18	5	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
18	5	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
18	5	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
18	5	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
18	5	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
18	5	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
18	5	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
18	5	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
18	5	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
18	5	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
18	5	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
18	6	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
18	6	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
18	6	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
18	6	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
18	6	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
18	6	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
18	6	1	Total	C	Mg	N	O	0
			42	34	1	4	3	

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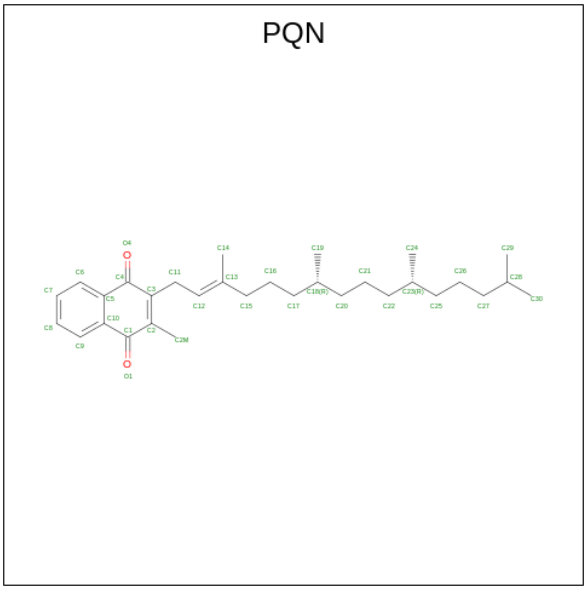
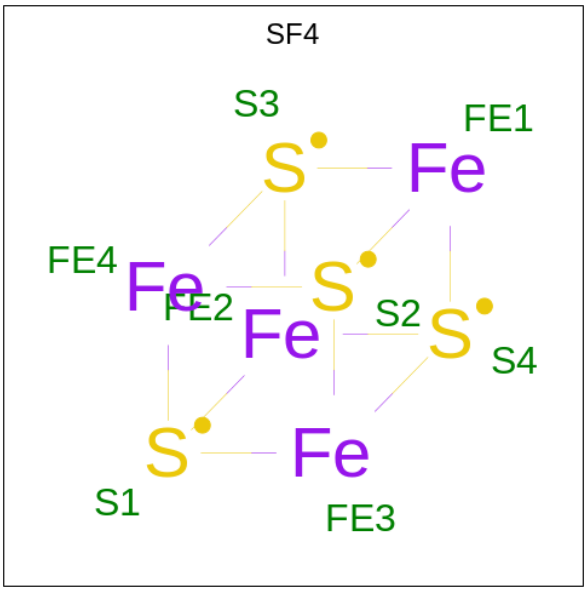
Mol	Chain	Residues	Atoms					AltConf
18	6	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
18	6	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
18	6	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
18	6	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
18	6	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
18	6	1	Total	C	Mg	N	O	0
			45	35	1	4	5	

- Molecule 19 is PHYLLOQUINONE (three-letter code: PQN) (formula: $C_{31}H_{46}O_2$) (labeled as "Ligand of Interest" by depositor).



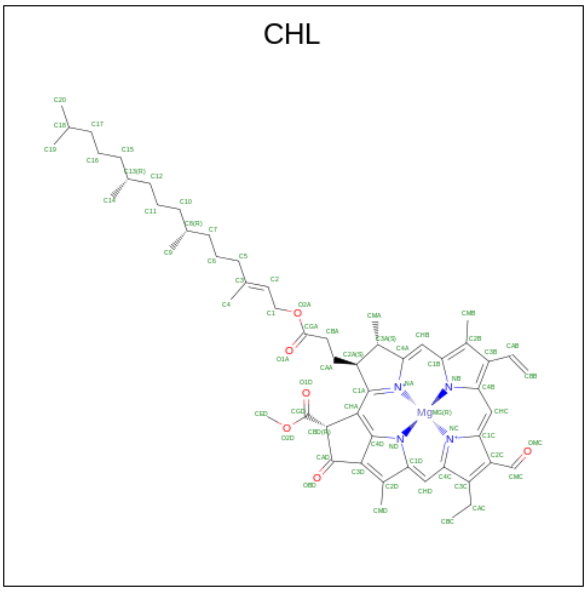
Mol	Chain	Residues	Atoms			AltConf
19	A	1	Total	C	O	0
			33	31	2	
19	B	1	Total	C	O	0
			33	31	2	

- Molecule 20 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe_4S_4) (labeled as "Ligand of Interest" by depositor).



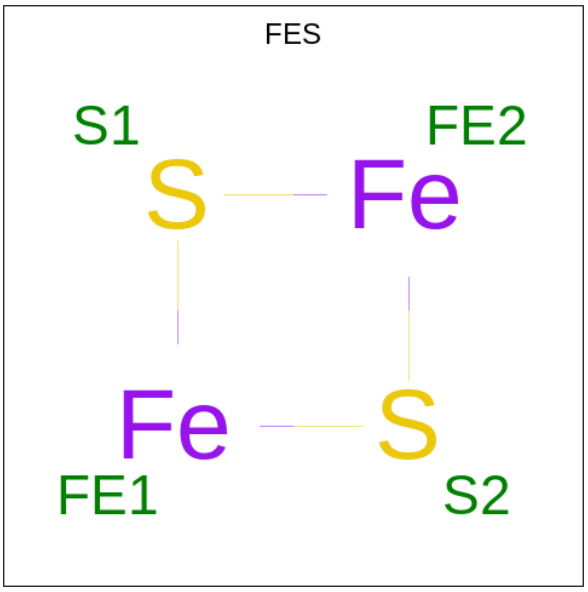
Mol	Chain	Residues	Atoms	AltConf
20	B	1	Total Fe S 8 4 4	0
20	C	1	Total Fe S 8 4 4	0
20	C	1	Total Fe S 8 4 4	0

- Molecule 21 is CHLOROPHYLL B (three-letter code: CHL) (formula: $C_{55}H_{70}MgN_4O_6$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
21	1	1	Total	C	Mg	N	O	0
			53	42	1	4	6	
21	1	1	Total	C	Mg	N	O	0
			43	34	1	4	4	
21	3	1	Total	C	Mg	N	O	0
			43	34	1	4	4	
21	7	1	Total	C	Mg	N	O	0
			43	34	1	4	4	
21	8	1	Total	C	Mg	N	O	0
			43	34	1	4	4	
21	Z	1	Total	C	Mg	N	O	0
			43	34	1	4	4	
21	Z	1	Total	C	Mg	N	O	0
			43	34	1	4	4	
21	4	1	Total	C	Mg	N	O	0
			43	34	1	4	4	
21	4	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
21	5	1	Total	C	Mg	N	O	0
			43	34	1	4	4	
21	5	1	Total	C	Mg	N	O	0
			43	34	1	4	4	
21	5	1	Total	C	Mg	N	O	0
			43	34	1	4	4	
21	6	1	Total	C	Mg	N	O	0
			43	34	1	4	4	
21	6	1	Total	C	Mg	N	O	0
			43	34	1	4	4	
21	6	1	Total	C	Mg	N	O	0
			43	34	1	4	4	
21	6	1	Total	C	Mg	N	O	0
			43	34	1	4	4	

- Molecule 22 is FE2/S2 (INORGANIC) CLUSTER (three-letter code: FES) (formula: Fe_2S_2) (labeled as "Ligand of Interest" by depositor).

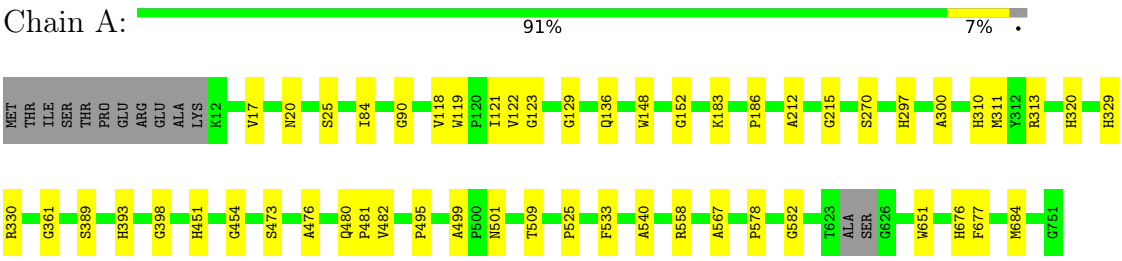


Mol	Chain	Residues	Atoms			AltConf
			Total	Fe	S	
22	G	1	4	2	2	0

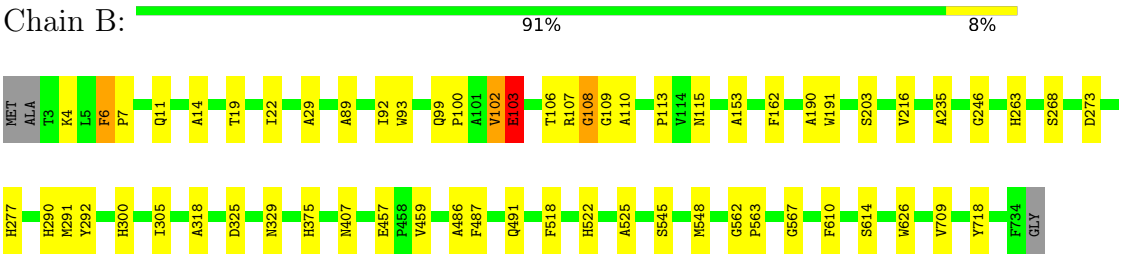
3 Residue-property plots (i)

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

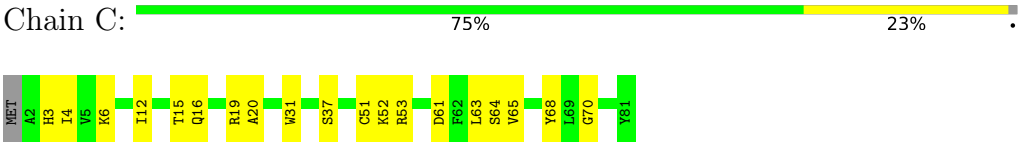
• Molecule 1: Photosystem I P700 chlorophyll a apoprotein A1



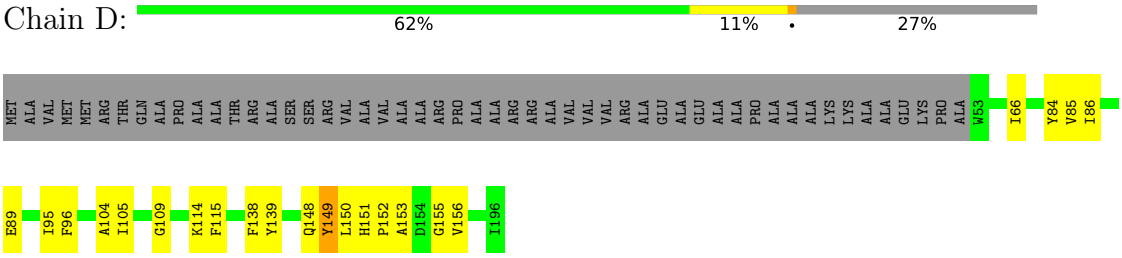
• Molecule 2: Photosystem I P700 chlorophyll a apoprotein A2



• Molecule 3: Photosystem I iron-sulfur center

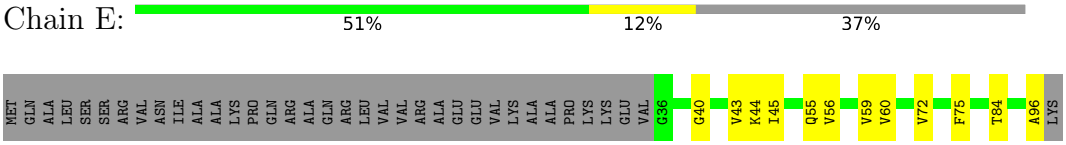


• Molecule 4: Photosystem I reaction center subunit II, chloroplastic



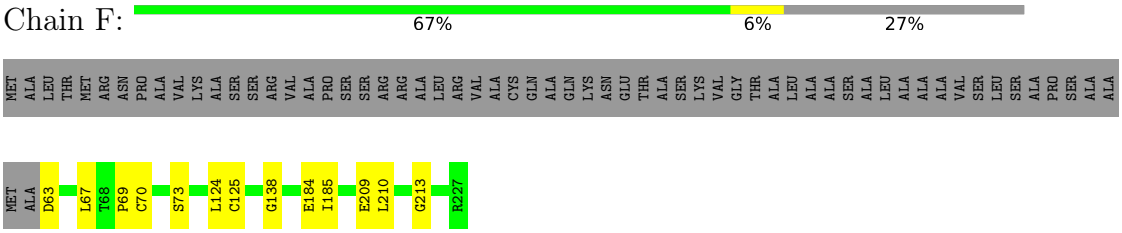
• Molecule 5: Photosystem I reaction center subunit IV, chloroplastic

Chain E:



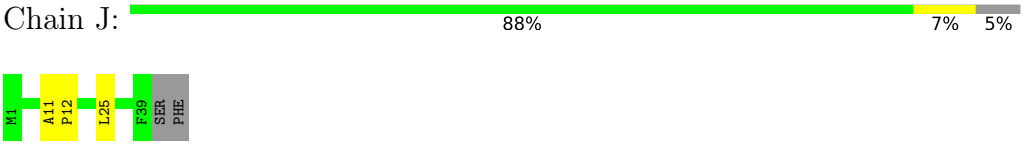
• Molecule 6: Photosystem I reaction center subunit III, chloroplastic

Chain F:



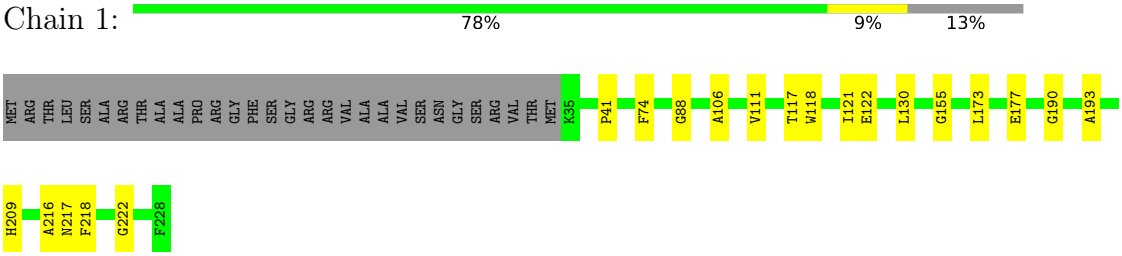
• Molecule 7: Photosystem I reaction center subunit IX

Chain J:



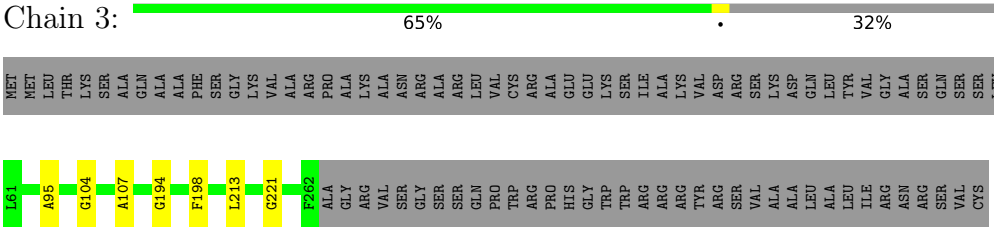
• Molecule 8: Chlorophyll a-b binding protein, chloroplastic

Chain 1:



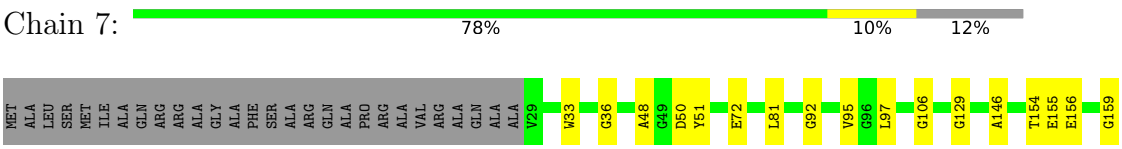
• Molecule 9: Chlorophyll a-b binding protein, chloroplastic

Chain 3:



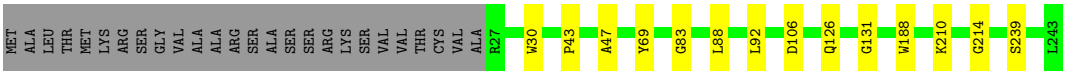
• Molecule 10: Chlorophyll a-b binding protein, chloroplastic

Chain 7:



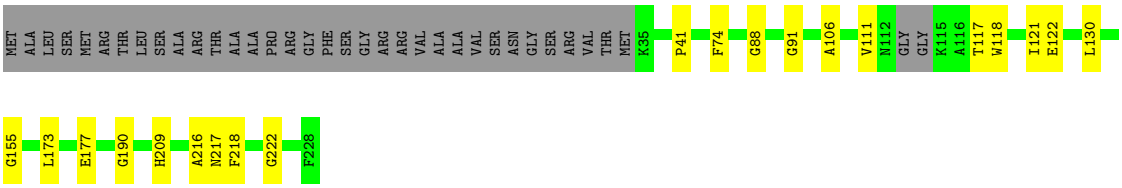
• Molecule 11: Chlorophyll a-b binding protein, chloroplastic

Chain 8:



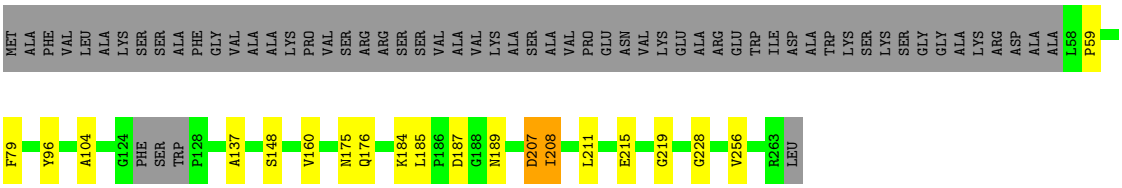
• Molecule 12: Chlorophyll a-b binding protein, chloroplastic

Chain Z:



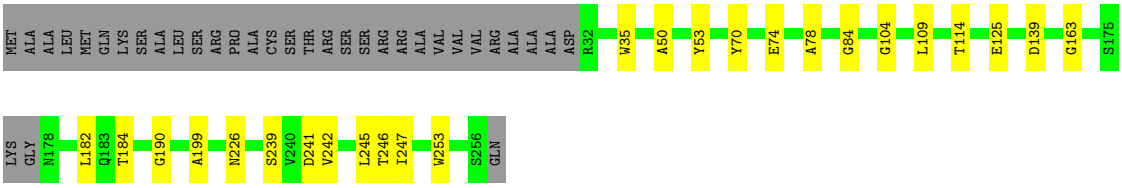
• Molecule 13: Chlorophyll a-b binding protein, chloroplastic

Chain 4:



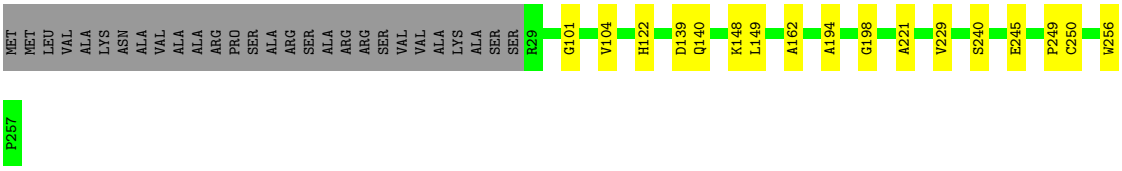
• Molecule 14: Chlorophyll a-b binding protein, chloroplastic

Chain 5:

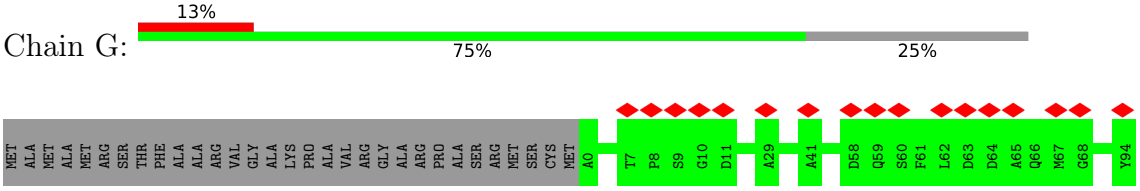


• Molecule 15: Chlorophyll a-b binding protein, chloroplastic

Chain 6:



• Molecule 16: Ferredoxin, chloroplastic



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	48941	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 ($e^-/Å^2$)	91	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	3.579	Depositor
Minimum map value	-0.699	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.125	Depositor
Recommended contour level	0.3	Depositor
Map size (Å)	431.2, 431.2, 431.2	wwPDB
Map dimensions	392, 392, 392	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	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: FES, PQN, CHL, SF4, CLA, 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	0.33	0/3628	0.48	0/5034
2	B	0.34	0/3602	0.59	3/5001 (0.1%)
3	C	0.35	0/394	0.55	0/547
4	D	0.37	0/705	0.52	0/977
5	E	0.30	0/299	0.48	0/414
6	F	0.31	0/809	0.44	0/1122
7	J	0.31	0/193	0.46	0/268
8	1	0.32	0/941	0.47	0/1299
9	3	0.33	0/984	0.46	0/1361
10	7	0.34	0/1032	0.48	1/1427 (0.1%)
11	8	0.33	0/1058	0.46	0/1464
12	Z	0.33	0/932	0.47	0/1286
13	4	0.32	0/990	0.52	0/1369
14	5	0.32	0/1089	0.47	0/1507
15	6	0.34	0/1121	0.47	0/1554
16	G	0.40	0/492	0.65	0/683
All	All	0.34	0/18269	0.51	4/25313 (0.0%)

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
4	D	0	1
13	4	0	2
All	All	0	3

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	103	GLU	N-CA-CB	14.49	136.68	110.60
2	B	102	VAL	N-CA-C	-10.71	82.08	111.00
2	B	102	VAL	CB-CA-C	-8.29	95.65	111.40
10	7	36	GLY	C-N-CA	-5.14	108.84	121.70

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
13	4	207	ASP	Peptide
13	4	208	ILE	Peptide
4	D	149	TYR	Mainchain

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3628	0	1728	56	0
2	B	3601	0	1713	75	0
3	C	395	0	178	14	0
4	D	706	0	316	11	0
5	E	300	0	135	6	0
6	F	810	0	404	10	0
7	J	194	0	87	4	0
8	1	942	0	489	19	0
9	3	985	0	480	7	0
10	7	1033	0	498	18	0
11	8	1059	0	527	15	0
12	Z	934	0	482	20	0
13	4	992	0	471	17	0
14	5	1091	0	504	19	0
15	6	1122	0	524	16	0
16	G	493	0	239	0	0
17	A	42	0	31	9	0
18	1	512	0	376	24	0
18	3	559	0	409	20	0
18	4	423	0	310	10	0
18	5	613	0	458	20	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
18	6	566	0	415	24	0
18	7	565	0	419	24	0
18	8	599	0	440	22	0
18	A	1831	0	1361	79	0
18	B	1782	0	1314	79	0
18	F	110	0	105	12	0
18	J	42	0	31	2	0
18	Z	466	0	345	25	0
19	A	33	0	46	6	0
19	B	33	0	46	5	0
20	B	8	0	0	1	0
20	C	16	0	0	3	0
21	1	96	0	70	5	0
21	3	43	0	29	0	0
21	4	89	0	59	5	0
21	5	129	0	87	4	0
21	6	172	0	116	3	0
21	7	43	0	29	1	0
21	8	43	0	29	3	0
21	Z	86	0	58	3	0
22	G	4	0	0	0	0
All	All	27190	0	15358	490	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 12.

The worst 5 of 490 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)
2:B:102:VAL:CA	2:B:106:THR:CB	1.79	1.59
2:B:103:GLU:N	2:B:106:THR:CB	1.71	1.51
2:B:102:VAL:C	2:B:106:THR:CB	1.97	1.32
2:B:103:GLU:CA	2:B:107:ARG:H	1.46	1.25
2:B:103:GLU:C	2:B:107:ARG:H	1.44	1.12

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%)	670 (91%)	63 (9%)	1 (0%)	51 85
2	B	730/735 (99%)	656 (90%)	68 (9%)	6 (1%)	19 60
3	C	78/81 (96%)	64 (82%)	12 (15%)	2 (3%)	5 34
4	D	142/196 (72%)	120 (84%)	16 (11%)	6 (4%)	3 24
5	E	59/97 (61%)	55 (93%)	4 (7%)	0	100 100
6	F	163/227 (72%)	154 (94%)	9 (6%)	0	100 100
7	J	37/41 (90%)	32 (86%)	5 (14%)	0	100 100
8	1	192/224 (86%)	175 (91%)	17 (9%)	0	100 100
9	3	200/298 (67%)	182 (91%)	18 (9%)	0	100 100
10	7	210/241 (87%)	193 (92%)	17 (8%)	0	100 100
11	8	215/243 (88%)	192 (89%)	23 (11%)	0	100 100
12	Z	188/228 (82%)	172 (92%)	16 (8%)	0	100 100
13	4	199/264 (75%)	175 (88%)	22 (11%)	2 (1%)	15 54
14	5	219/257 (85%)	194 (89%)	25 (11%)	0	100 100
15	6	227/257 (88%)	205 (90%)	22 (10%)	0	100 100
16	G	98/126 (78%)	93 (95%)	5 (5%)	0	100 100
All	All	3691/4266 (86%)	3332 (90%)	342 (9%)	17 (0%)	32 68

5 of 17 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	6	PHE
2	B	7	PRO
2	B	103	GLU
3	C	64	SER
4	D	149	TYR

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

211 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	$\#\|Z\|>2$
18	CLA	3	304	-	42,50,73	2.66	10 (23%)	48,85,113	1.58	9 (18%)
18	CLA	Z	604	-	43,51,73	2.80	9 (20%)	49,86,113	1.55	8 (16%)
21	CHL	6	306	-	43,51,74	2.48	10 (23%)	45,86,114	1.95	8 (17%)
18	CLA	A	845	-	42,50,73	2.85	9 (21%)	48,85,113	1.46	9 (18%)
18	CLA	B	823	-	42,50,73	2.97	9 (21%)	48,85,113	1.58	7 (14%)
18	CLA	B	815	-	42,50,73	2.85	9 (21%)	48,85,113	1.94	12 (25%)
18	CLA	Z	602	-	42,50,73	2.85	8 (19%)	48,85,113	1.51	8 (16%)
21	CHL	8	606	-	43,51,74	2.51	9 (20%)	45,86,114	2.17	10 (22%)
18	CLA	A	809	-	42,50,73	2.76	11 (26%)	48,85,113	1.45	7 (14%)
18	CLA	A	836	1	42,50,73	2.88	10 (23%)	48,85,113	1.55	7 (14%)
18	CLA	A	807	-	42,50,73	2.79	10 (23%)	48,85,113	1.59	9 (18%)
18	CLA	A	841	-	42,50,73	2.72	11 (26%)	48,85,113	1.49	9 (18%)
18	CLA	F	301	-	45,53,73	2.66	8 (17%)	52,89,113	1.52	7 (13%)
18	CLA	1	612	-	46,54,73	2.59	9 (19%)	53,90,113	1.41	8 (15%)
18	CLA	B	827	-	42,50,73	2.69	9 (21%)	48,85,113	1.86	11 (22%)
18	CLA	A	810	-	42,50,73	2.82	10 (23%)	48,85,113	1.48	7 (14%)
18	CLA	8	608	-	42,50,73	2.81	9 (21%)	48,85,113	1.65	10 (20%)
18	CLA	Z	613	-	42,50,73	2.85	9 (21%)	48,85,113	1.55	7 (14%)
18	CLA	6	309	-	45,53,73	2.77	9 (20%)	52,89,113	1.47	8 (15%)
18	CLA	6	312	-	45,53,73	2.72	11 (24%)	52,89,113	1.37	8 (15%)
18	CLA	A	812	-	42,50,73	2.78	11 (26%)	48,85,113	1.57	9 (18%)
18	CLA	A	826	-	42,50,73	2.85	10 (23%)	48,85,113	1.72	7 (14%)
18	CLA	A	818	-	42,50,73	2.72	10 (23%)	48,85,113	1.51	8 (16%)
18	CLA	A	806	-	42,50,73	2.76	10 (23%)	48,85,113	1.59	8 (16%)
18	CLA	8	612	-	46,54,73	2.73	11 (23%)	53,90,113	1.46	9 (16%)
18	CLA	4	601	13	42,50,73	2.89	8 (19%)	48,85,113	1.86	9 (18%)
18	CLA	6	311	-	45,53,73	2.70	10 (22%)	52,89,113	1.48	9 (17%)
18	CLA	A	815	-	42,50,73	2.78	9 (21%)	48,85,113	1.48	7 (14%)
18	CLA	B	838	-	43,51,73	2.63	9 (20%)	49,86,113	1.46	8 (16%)
18	CLA	4	608	-	42,50,73	2.78	7 (16%)	48,85,113	1.95	11 (22%)
18	CLA	A	821	-	42,50,73	2.76	10 (23%)	48,85,113	1.45	8 (16%)
18	CLA	7	613	-	43,51,73	2.71	9 (20%)	49,86,113	1.63	8 (16%)
21	CHL	1	601	8	53,61,74	2.22	10 (18%)	57,98,114	1.51	6 (10%)
18	CLA	Z	612	-	42,50,73	2.84	9 (21%)	48,85,113	1.61	9 (18%)
18	CLA	B	831	-	42,50,73	2.82	10 (23%)	48,85,113	1.56	9 (18%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
18	CLA	A	803	-	42,50,73	2.95	12 (28%)	48,85,113	1.77	9 (18%)
18	CLA	A	814	-	42,50,73	2.79	9 (21%)	48,85,113	1.57	7 (14%)
18	CLA	B	817	-	42,50,73	2.80	8 (19%)	48,85,113	1.63	9 (18%)
18	CLA	A	817	-	47,55,73	2.62	11 (23%)	54,91,113	1.47	8 (14%)
18	CLA	B	828	-	42,50,73	2.69	10 (23%)	48,85,113	1.49	7 (14%)
18	CLA	4	612	-	41,49,73	2.81	8 (19%)	47,84,113	1.32	6 (12%)
18	CLA	3	313	-	46,54,73	2.59	8 (17%)	53,90,113	1.47	9 (16%)
18	CLA	A	816	-	42,50,73	2.78	10 (23%)	48,85,113	1.47	7 (14%)
18	CLA	3	302	-	42,50,73	2.84	10 (23%)	48,85,113	1.53	7 (14%)
18	CLA	B	809	-	42,50,73	2.80	9 (21%)	48,85,113	1.58	9 (18%)
18	CLA	B	836	-	42,50,73	2.75	9 (21%)	48,85,113	1.64	9 (18%)
18	CLA	3	310	-	46,54,73	2.64	10 (21%)	53,90,113	1.45	7 (13%)
19	PQN	A	842	-	34,34,34	0.24	0	42,45,45	0.35	0
18	CLA	7	611	-	42,50,73	2.81	10 (23%)	48,85,113	1.50	8 (16%)
18	CLA	B	835	-	42,50,73	2.85	8 (19%)	48,85,113	1.79	9 (18%)
18	CLA	B	826	-	42,50,73	2.79	10 (23%)	48,85,113	1.48	8 (16%)
18	CLA	B	812	-	42,50,73	2.75	10 (23%)	48,85,113	1.97	12 (25%)
18	CLA	7	614	10	42,50,73	2.72	9 (21%)	48,85,113	2.22	10 (20%)
18	CLA	8	611	-	42,50,73	2.80	10 (23%)	48,85,113	1.78	8 (16%)
18	CLA	A	823	-	51,59,73	2.45	9 (17%)	59,96,113	1.70	12 (20%)
21	CHL	5	616	-	43,51,74	2.54	11 (25%)	45,86,114	1.73	7 (15%)
21	CHL	4	604	-	43,51,74	2.60	11 (25%)	45,86,114	2.09	14 (31%)
18	CLA	6	308	-	42,50,73	2.75	8 (19%)	48,85,113	1.56	8 (16%)
18	CLA	5	617	-	46,54,73	2.44	9 (19%)	53,90,113	1.63	9 (16%)
18	CLA	A	813	-	42,50,73	2.79	10 (23%)	48,85,113	1.49	8 (16%)
18	CLA	3	314	-	42,50,73	2.68	10 (23%)	48,85,113	1.45	8 (16%)
18	CLA	A	808	-	42,50,73	2.98	10 (23%)	48,85,113	1.69	9 (18%)
18	CLA	8	602	-	42,50,73	2.78	8 (19%)	48,85,113	1.44	8 (16%)
18	CLA	6	314	15	46,54,73	2.68	9 (19%)	53,90,113	1.49	10 (18%)
21	CHL	6	307	-	43,51,74	2.48	10 (23%)	45,86,114	1.71	8 (17%)
18	CLA	A	831	-	42,50,73	2.77	8 (19%)	48,85,113	1.67	9 (18%)
21	CHL	1	606	-	43,51,74	2.57	11 (25%)	45,86,114	1.89	9 (20%)
21	CHL	4	605	-	46,54,74	2.32	11 (23%)	49,90,114	2.38	11 (22%)
18	CLA	B	829	-	42,50,73	2.57	9 (21%)	48,85,113	1.53	8 (16%)
18	CLA	7	605	-	42,50,73	2.80	10 (23%)	48,85,113	1.63	9 (18%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
18	CLA	5	601	14	42,50,73	2.76	8 (19%)	48,85,113	1.42	7 (14%)
18	CLA	B	816	-	42,50,73	2.82	9 (21%)	48,85,113	1.55	7 (14%)
18	CLA	7	608	-	50,58,73	2.52	10 (20%)	58,95,113	1.49	10 (17%)
18	CLA	A	819	-	42,50,73	2.74	8 (19%)	48,85,113	1.69	7 (14%)
18	CLA	A	802	-	42,50,73	2.65	10 (23%)	48,85,113	1.87	10 (20%)
18	CLA	8	605	-	42,50,73	2.84	9 (21%)	48,85,113	1.48	8 (16%)
18	CLA	5	608	-	42,50,73	2.84	9 (21%)	48,85,113	1.41	6 (12%)
18	CLA	A	843	-	52,60,73	2.60	8 (15%)	60,97,113	1.32	9 (15%)
21	CHL	Z	605	-	43,51,74	2.56	11 (25%)	45,86,114	1.88	9 (20%)
18	CLA	A	837	-	42,50,73	2.77	10 (23%)	48,85,113	1.53	9 (18%)
20	SF4	C	102	3	0,12,12	-	-	-		
18	CLA	A	832	-	42,50,73	2.67	9 (21%)	48,85,113	1.55	8 (16%)
18	CLA	5	609	-	42,50,73	2.71	9 (21%)	48,85,113	1.51	10 (20%)
18	CLA	A	835	-	42,50,73	2.89	9 (21%)	48,85,113	1.55	10 (20%)
18	CLA	B	818	-	42,50,73	2.78	9 (21%)	48,85,113	1.58	8 (16%)
18	CLA	B	801	-	42,50,73	2.65	9 (21%)	48,85,113	1.58	10 (20%)
18	CLA	B	840	-	42,50,73	2.64	9 (21%)	48,85,113	1.55	9 (18%)
18	CLA	3	303	-	42,50,73	2.70	10 (23%)	48,85,113	1.52	8 (16%)
18	CLA	8	604	-	42,50,73	2.80	8 (19%)	48,85,113	1.46	8 (16%)
18	CLA	8	614	-	42,50,73	2.79	8 (19%)	48,85,113	1.73	9 (18%)
18	CLA	8	601	11	42,50,73	2.77	9 (21%)	48,85,113	1.46	8 (16%)
18	CLA	1	610	-	42,50,73	2.62	8 (19%)	48,85,113	1.69	9 (18%)
18	CLA	3	312	-	45,53,73	2.74	8 (17%)	52,89,113	1.50	8 (15%)
18	CLA	1	611	-	42,50,73	2.85	10 (23%)	48,85,113	1.56	9 (18%)
18	CLA	A	820	-	42,50,73	2.63	10 (23%)	48,85,113	1.58	9 (18%)
18	CLA	3	309	-	41,49,73	2.78	9 (21%)	47,84,113	2.02	11 (23%)
18	CLA	5	612	-	42,50,73	2.69	10 (23%)	48,85,113	1.50	8 (16%)
18	CLA	Z	606	-	42,50,73	2.75	9 (21%)	48,85,113	1.50	7 (14%)
18	CLA	A	834	-	42,50,73	2.83	10 (23%)	48,85,113	2.02	12 (25%)
18	CLA	7	609	-	45,53,73	2.71	9 (20%)	52,89,113	1.44	8 (15%)
18	CLA	B	811	-	42,50,73	2.60	10 (23%)	48,85,113	1.56	8 (16%)
18	CLA	B	837	-	42,50,73	2.70	9 (21%)	48,85,113	1.45	8 (16%)
18	CLA	A	833	-	42,50,73	2.91	10 (23%)	48,85,113	1.47	7 (14%)
19	PQN	B	844	-	34,34,34	0.24	0	42,45,45	0.37	0
18	CLA	B	802	-	46,54,73	2.59	10 (21%)	53,90,113	1.44	7 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
18	CLA	8	615	-	42,50,73	2.81	11 (26%)	48,85,113	1.49	7 (14%)
18	CLA	A	824	-	42,50,73	2.65	12 (28%)	48,85,113	1.73	9 (18%)
18	CLA	3	305	9	42,50,73	2.72	9 (21%)	48,85,113	2.17	13 (27%)
18	CLA	Z	610	-	42,50,73	2.85	10 (23%)	48,85,113	1.55	9 (18%)
18	CLA	Z	611	-	45,53,73	2.62	9 (20%)	52,89,113	1.43	8 (15%)
18	CLA	B	832	-	42,50,73	2.81	8 (19%)	48,85,113	1.52	7 (14%)
18	CLA	4	609	-	42,50,73	2.87	7 (16%)	48,85,113	1.51	7 (14%)
18	CLA	B	822	-	45,53,73	2.56	9 (20%)	52,89,113	1.60	8 (15%)
18	CLA	5	611	-	42,50,73	2.73	10 (23%)	48,85,113	1.65	10 (20%)
18	CLA	8	610	-	46,54,73	2.33	7 (15%)	53,90,113	1.64	10 (18%)
18	CLA	1	607	-	42,50,73	2.75	8 (19%)	48,85,113	1.50	8 (16%)
18	CLA	A	829	-	42,50,73	2.63	10 (23%)	48,85,113	1.56	8 (16%)
18	CLA	1	614	-	46,54,73	2.73	9 (19%)	53,90,113	1.45	7 (13%)
18	CLA	Z	609	-	42,50,73	2.63	8 (19%)	48,85,113	1.70	9 (18%)
18	CLA	4	610	-	42,50,73	2.77	10 (23%)	48,85,113	1.53	8 (16%)
18	CLA	5	604	-	42,50,73	2.80	8 (19%)	48,85,113	1.57	9 (18%)
18	CLA	7	607	-	42,50,73	2.78	11 (26%)	48,85,113	1.52	9 (18%)
22	FES	G	101	-	0,4,4	-	-	-		
18	CLA	B	805	-	42,50,73	2.70	9 (21%)	48,85,113	1.73	9 (18%)
18	CLA	3	308	-	42,50,73	2.75	10 (23%)	48,85,113	1.47	9 (18%)
18	CLA	1	605	-	42,50,73	2.83	9 (21%)	48,85,113	1.58	8 (16%)
18	CLA	6	313	-	42,50,73	2.75	9 (21%)	48,85,113	1.67	10 (20%)
21	CHL	3	306	-	43,51,74	2.49	12 (27%)	45,86,114	1.88	7 (15%)
18	CLA	3	301	-	42,50,73	2.71	9 (21%)	48,85,113	1.62	9 (18%)
18	CLA	B	808	-	42,50,73	2.67	11 (26%)	48,85,113	1.60	8 (16%)
18	CLA	5	602	-	42,50,73	2.79	10 (23%)	48,85,113	1.60	8 (16%)
18	CLA	4	602	-	42,50,73	2.89	10 (23%)	48,85,113	1.59	10 (20%)
20	SF4	B	803	-	0,12,12	-	-	-		
18	CLA	B	824	-	42,50,73	2.81	8 (19%)	48,85,113	1.55	7 (14%)
18	CLA	8	607	-	42,50,73	2.80	10 (23%)	48,85,113	1.57	9 (18%)
18	CLA	8	609	-	42,50,73	2.82	9 (21%)	48,85,113	1.57	8 (16%)
18	CLA	B	834	-	38,46,73	4.73	12 (31%)	37,77,113	1.75	8 (21%)
21	CHL	5	606	-	43,51,74	2.54	8 (18%)	45,86,114	2.67	11 (24%)
18	CLA	B	825	-	42,50,73	2.87	9 (21%)	48,85,113	1.47	7 (14%)
18	CLA	A	804	-	42,50,73	2.75	10 (23%)	48,85,113	1.58	8 (16%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
18	CLA	6	315	-	42,50,73	2.66	8 (19%)	48,85,113	1.73	9 (18%)
18	CLA	7	603	-	46,54,73	2.64	9 (19%)	53,90,113	1.46	6 (11%)
18	CLA	B	821	-	42,50,73	2.71	8 (19%)	48,85,113	1.45	8 (16%)
21	CHL	6	305	-	43,51,74	2.48	10 (23%)	45,86,114	1.84	9 (20%)
18	CLA	5	613	-	42,50,73	2.79	9 (21%)	48,85,113	1.63	8 (16%)
18	CLA	A	828	-	42,50,73	2.65	11 (26%)	48,85,113	1.46	8 (16%)
18	CLA	3	311	-	45,53,73	2.70	11 (24%)	52,89,113	1.39	9 (17%)
18	CLA	6	304	-	42,50,73	2.86	9 (21%)	48,85,113	1.50	10 (20%)
18	CLA	4	606	-	42,50,73	2.82	8 (19%)	48,85,113	1.49	7 (14%)
18	CLA	1	602	-	42,50,73	2.84	9 (21%)	48,85,113	1.51	8 (16%)
18	CLA	A	844	-	42,50,73	2.56	8 (19%)	48,85,113	1.47	8 (16%)
18	CLA	A	827	-	42,50,73	2.57	7 (16%)	48,85,113	1.87	12 (25%)
18	CLA	B	814	-	42,50,73	2.90	8 (19%)	48,85,113	1.45	6 (12%)
18	CLA	1	604	-	42,50,73	2.82	9 (21%)	48,85,113	1.45	9 (18%)
18	CLA	5	605	-	42,50,73	2.84	9 (21%)	48,85,113	1.53	8 (16%)
21	CHL	6	316	-	43,51,74	2.55	9 (20%)	45,86,114	1.74	6 (13%)
18	CLA	Z	603	-	42,50,73	2.82	8 (19%)	48,85,113	1.45	9 (18%)
18	CLA	1	613	-	42,50,73	2.83	9 (21%)	48,85,113	1.61	9 (18%)
18	CLA	6	302	-	42,50,73	2.68	9 (21%)	48,85,113	1.63	9 (18%)
18	CLA	A	822	-	42,50,73	2.84	10 (23%)	48,85,113	1.65	10 (20%)
18	CLA	B	819	-	42,50,73	2.80	10 (23%)	48,85,113	1.86	10 (20%)
18	CLA	A	805	-	42,50,73	2.76	10 (23%)	48,85,113	1.64	8 (16%)
18	CLA	8	603	-	45,53,73	2.69	8 (17%)	52,89,113	1.51	8 (15%)
18	CLA	A	838	-	42,50,73	2.58	9 (21%)	48,85,113	1.66	9 (18%)
18	CLA	A	811	-	43,51,73	2.68	9 (20%)	49,86,113	1.51	7 (14%)
18	CLA	B	843	-	42,50,73	2.69	10 (23%)	48,85,113	1.60	8 (16%)
18	CLA	7	610	-	41,49,73	2.91	9 (21%)	47,84,113	2.15	11 (23%)
20	SF4	C	101	3	0,12,12	-	-	-		
18	CLA	B	839	-	42,50,73	2.62	8 (19%)	48,85,113	1.51	7 (14%)
18	CLA	5	610	-	55,63,73	2.14	8 (14%)	64,101,113	1.36	7 (10%)
18	CLA	B	804	-	42,50,73	2.76	10 (23%)	48,85,113	1.86	10 (20%)
18	CLA	4	611	-	42,50,73	2.70	8 (19%)	48,85,113	1.48	8 (16%)
18	CLA	B	830	-	45,53,73	2.60	8 (17%)	52,89,113	1.37	8 (15%)
18	CLA	A	825	-	42,50,73	2.77	9 (21%)	48,85,113	1.81	11 (22%)
18	CLA	6	301	-	42,50,73	2.96	9 (21%)	48,85,113	1.43	9 (18%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
18	CLA	B	813	-	41,49,73	2.71	9 (21%)	51,84,113	1.53	9 (17%)
18	CLA	7	612	-	45,53,73	2.76	11 (24%)	52,89,113	1.44	8 (15%)
18	CLA	4	603	-	46,54,73	2.69	11 (23%)	53,90,113	1.45	7 (13%)
18	CLA	Z	608	-	42,50,73	2.85	9 (21%)	48,85,113	1.46	7 (14%)
21	CHL	7	606	-	43,51,74	2.54	9 (20%)	45,86,114	1.93	6 (13%)
18	CLA	1	608	-	42,50,73	2.70	8 (19%)	48,85,113	1.95	12 (25%)
18	CLA	B	820	-	42,50,73	2.58	7 (16%)	48,85,113	1.87	11 (22%)
18	CLA	B	842	-	42,50,73	2.71	11 (26%)	48,85,113	1.71	8 (16%)
18	CLA	6	303	-	46,54,73	2.65	9 (19%)	53,90,113	1.39	6 (11%)
18	CLA	B	841	-	42,50,73	2.73	9 (21%)	48,85,113	1.72	10 (20%)
18	CLA	3	307	-	42,50,73	2.74	9 (21%)	48,85,113	1.81	8 (16%)
18	CLA	6	310	-	42,50,73	2.27	7 (16%)	48,85,113	2.17	7 (14%)
18	CLA	1	603	-	42,50,73	2.83	10 (23%)	48,85,113	1.48	7 (14%)
18	CLA	A	840	-	42,50,73	2.81	11 (26%)	48,85,113	1.71	7 (14%)
18	CLA	B	833	-	42,50,73	2.75	9 (21%)	48,85,113	1.44	8 (16%)
18	CLA	F	302	-	65,73,73	2.16	9 (13%)	76,113,113	1.25	9 (11%)
18	CLA	4	607	-	42,50,73	2.86	9 (21%)	48,85,113	1.58	9 (18%)
18	CLA	5	614	14	42,50,73	2.65	8 (19%)	48,85,113	1.49	10 (20%)
18	CLA	A	830	-	42,50,73	2.77	10 (23%)	48,85,113	1.46	7 (14%)
21	CHL	Z	601	12	43,51,74	2.45	10 (23%)	45,86,114	1.69	7 (15%)
21	CHL	5	607	-	43,51,74	2.45	10 (23%)	45,86,114	1.87	10 (22%)
18	CLA	1	609	-	42,50,73	2.86	9 (21%)	48,85,113	1.46	7 (14%)
18	CLA	J	101	-	42,50,73	2.82	8 (19%)	48,85,113	1.55	9 (18%)
18	CLA	8	613	-	42,50,73	2.72	10 (23%)	48,85,113	1.55	7 (14%)
18	CLA	Z	607	-	42,50,73	2.70	8 (19%)	48,85,113	1.95	12 (25%)
18	CLA	B	807	-	49,57,73	2.59	10 (20%)	55,92,113	1.57	11 (20%)
18	CLA	5	615	-	46,54,73	2.55	7 (15%)	53,90,113	2.04	11 (20%)
18	CLA	5	603	-	46,54,73	2.68	10 (21%)	53,90,113	1.39	8 (15%)
18	CLA	B	810	-	42,50,73	2.60	9 (21%)	48,85,113	1.50	7 (14%)
18	CLA	7	604	-	43,51,73	2.98	9 (20%)	49,86,113	1.64	11 (22%)
17	CL0	A	801	-	42,50,73	2.66	10 (23%)	48,85,113	1.59	8 (16%)
18	CLA	7	601	10	42,50,73	2.76	9 (21%)	48,85,113	1.56	8 (16%)
18	CLA	B	806	-	45,53,73	2.76	10 (22%)	52,89,113	1.86	8 (15%)
18	CLA	7	602	-	42,50,73	2.77	11 (26%)	48,85,113	1.58	9 (18%)
18	CLA	A	839	-	42,50,73	2.73	11 (26%)	48,85,113	1.57	9 (18%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
18	CLA	6	317	-	45,53,73	2.72	10 (22%)	52,89,113	1.41	8 (15%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
18	CLA	3	304	-	1/1/10/20	1/10/88/115	-
18	CLA	Z	604	-	1/1/10/20	4/11/89/115	-
21	CHL	6	306	-	3/3/15/26	0/12/110/137	-
18	CLA	A	845	-	1/1/10/20	2/10/88/115	-
18	CLA	B	823	-	1/1/10/20	2/10/88/115	-
18	CLA	B	815	-	1/1/10/20	5/10/88/115	-
18	CLA	Z	602	-	1/1/10/20	2/10/88/115	-
21	CHL	8	606	-	3/3/15/26	1/12/110/137	-
18	CLA	A	809	-	1/1/10/20	0/10/88/115	-
18	CLA	A	836	1	1/1/10/20	3/10/88/115	-
18	CLA	A	807	-	1/1/10/20	2/10/88/115	-
18	CLA	A	841	-	1/1/10/20	1/10/88/115	-
18	CLA	F	301	-	1/1/11/20	2/13/91/115	-
18	CLA	1	612	-	1/1/11/20	3/15/93/115	-
18	CLA	B	827	-	1/1/10/20	1/10/88/115	-
18	CLA	A	810	-	1/1/10/20	0/10/88/115	-
18	CLA	8	608	-	1/1/10/20	0/10/88/115	-
18	CLA	Z	613	-	1/1/10/20	2/10/88/115	-
18	CLA	6	309	-	1/1/11/20	3/13/91/115	-
18	CLA	6	312	-	1/1/11/20	5/13/91/115	-
18	CLA	A	812	-	1/1/10/20	1/10/88/115	-
18	CLA	A	826	-	1/1/10/20	1/10/88/115	-
18	CLA	A	818	-	1/1/10/20	2/10/88/115	-
18	CLA	A	806	-	1/1/10/20	4/10/88/115	-
18	CLA	8	612	-	1/1/11/20	4/15/93/115	-
18	CLA	4	601	13	1/1/10/20	2/10/88/115	-
18	CLA	6	311	-	1/1/11/20	6/13/91/115	-
18	CLA	A	815	-	1/1/10/20	0/10/88/115	-
18	CLA	B	838	-	1/1/10/20	2/11/89/115	-
18	CLA	4	608	-	1/1/10/20	2/10/88/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
18	CLA	A	821	-	1/1/10/20	2/10/88/115	-
18	CLA	7	613	-	1/1/10/20	3/11/89/115	-
21	CHL	1	601	8	3/3/17/26	4/24/122/137	-
18	CLA	Z	612	-	1/1/10/20	3/10/88/115	-
18	CLA	B	831	-	1/1/10/20	2/10/88/115	-
18	CLA	A	803	-	1/1/10/20	6/10/88/115	-
18	CLA	A	814	-	1/1/10/20	2/10/88/115	-
18	CLA	B	817	-	1/1/10/20	3/10/88/115	-
18	CLA	A	817	-	1/1/11/20	4/16/94/115	-
18	CLA	B	828	-	1/1/10/20	4/10/88/115	-
18	CLA	4	612	-	1/1/10/20	0/8/86/115	-
18	CLA	3	313	-	1/1/11/20	3/15/93/115	-
18	CLA	A	816	-	1/1/10/20	1/10/88/115	-
18	CLA	3	302	-	1/1/10/20	1/10/88/115	-
18	CLA	B	809	-	1/1/10/20	2/10/88/115	-
18	CLA	B	836	-	1/1/10/20	1/10/88/115	-
18	CLA	3	310	-	1/1/11/20	5/15/93/115	-
19	PQN	A	842	-	-	7/23/43/43	0/2/2/2
18	CLA	7	611	-	1/1/10/20	0/10/88/115	-
18	CLA	B	835	-	1/1/10/20	1/10/88/115	-
18	CLA	B	826	-	1/1/10/20	1/10/88/115	-
18	CLA	B	812	-	1/1/10/20	4/10/88/115	-
18	CLA	7	614	10	1/1/10/20	3/10/88/115	-
18	CLA	8	611	-	1/1/10/20	2/10/88/115	-
18	CLA	A	823	-	1/1/12/20	4/21/99/115	-
21	CHL	5	616	-	3/3/15/26	2/12/110/137	-
21	CHL	4	604	-	3/3/15/26	1/12/110/137	-
18	CLA	6	308	-	1/1/10/20	0/10/88/115	-
18	CLA	5	617	-	1/1/11/20	8/15/93/115	-
18	CLA	A	813	-	1/1/10/20	7/10/88/115	-
18	CLA	3	314	-	1/1/10/20	0/10/88/115	-
18	CLA	A	808	-	1/1/10/20	2/10/88/115	-
18	CLA	8	602	-	1/1/10/20	2/10/88/115	-
18	CLA	6	314	15	1/1/11/20	2/15/93/115	-
21	CHL	6	307	-	3/3/15/26	2/12/110/137	-
18	CLA	A	831	-	1/1/10/20	3/10/88/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
21	CHL	1	606	-	3/3/15/26	3/12/110/137	-
21	CHL	4	605	-	3/3/16/26	4/15/113/137	-
18	CLA	B	829	-	1/1/10/20	4/10/88/115	-
18	CLA	7	605	-	1/1/10/20	1/10/88/115	-
18	CLA	5	601	14	1/1/10/20	2/10/88/115	-
18	CLA	B	816	-	1/1/10/20	2/10/88/115	-
18	CLA	7	608	-	1/1/12/20	3/19/97/115	-
18	CLA	A	819	-	1/1/10/20	2/10/88/115	-
18	CLA	A	802	-	1/1/10/20	4/10/88/115	-
18	CLA	8	605	-	1/1/10/20	2/10/88/115	-
18	CLA	5	608	-	1/1/10/20	2/10/88/115	-
18	CLA	A	843	-	1/1/12/20	7/22/100/115	-
21	CHL	Z	605	-	3/3/15/26	3/12/110/137	-
18	CLA	A	837	-	1/1/10/20	1/10/88/115	-
20	SF4	C	102	3	-	-	0/6/5/5
18	CLA	A	832	-	1/1/10/20	0/10/88/115	-
18	CLA	5	609	-	1/1/10/20	1/10/88/115	-
18	CLA	A	835	-	1/1/10/20	1/10/88/115	-
18	CLA	B	818	-	1/1/10/20	1/10/88/115	-
18	CLA	B	801	-	1/1/10/20	2/10/88/115	-
18	CLA	B	840	-	1/1/10/20	2/10/88/115	-
18	CLA	3	303	-	1/1/10/20	0/10/88/115	-
18	CLA	8	604	-	1/1/10/20	0/10/88/115	-
18	CLA	8	614	-	1/1/10/20	0/10/88/115	-
18	CLA	8	601	11	1/1/10/20	5/10/88/115	-
18	CLA	1	610	-	1/1/10/20	1/10/88/115	-
18	CLA	3	312	-	1/1/11/20	2/13/91/115	-
18	CLA	1	611	-	1/1/10/20	2/10/88/115	-
18	CLA	A	820	-	1/1/10/20	3/10/88/115	-
18	CLA	3	309	-	1/1/10/20	2/8/86/115	-
18	CLA	5	612	-	1/1/10/20	2/10/88/115	-
18	CLA	Z	606	-	1/1/10/20	0/10/88/115	-
18	CLA	A	834	-	1/1/10/20	3/10/88/115	-
18	CLA	7	609	-	1/1/11/20	0/13/91/115	-
18	CLA	B	811	-	1/1/10/20	2/10/88/115	-
18	CLA	B	837	-	1/1/10/20	0/10/88/115	-
18	CLA	A	833	-	1/1/10/20	2/10/88/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
19	PQN	B	844	-	-	5/23/43/43	0/2/2/2
18	CLA	B	802	-	1/1/11/20	1/15/93/115	-
18	CLA	8	615	-	1/1/10/20	2/10/88/115	-
18	CLA	A	824	-	1/1/10/20	4/10/88/115	-
18	CLA	3	305	9	1/1/10/20	1/10/88/115	-
18	CLA	Z	610	-	1/1/10/20	2/10/88/115	-
18	CLA	Z	611	-	1/1/11/20	4/13/91/115	-
18	CLA	B	832	-	1/1/10/20	2/10/88/115	-
18	CLA	4	609	-	1/1/10/20	3/10/88/115	-
18	CLA	B	822	-	1/1/11/20	4/13/91/115	-
18	CLA	5	611	-	1/1/10/20	3/10/88/115	-
18	CLA	8	610	-	1/1/11/20	1/15/93/115	-
18	CLA	1	607	-	1/1/10/20	0/10/88/115	-
18	CLA	A	829	-	1/1/10/20	0/10/88/115	-
18	CLA	1	614	-	1/1/11/20	3/15/93/115	-
18	CLA	Z	609	-	1/1/10/20	1/10/88/115	-
18	CLA	4	610	-	1/1/10/20	2/10/88/115	-
18	CLA	5	604	-	1/1/10/20	1/10/88/115	-
18	CLA	7	607	-	1/1/10/20	2/10/88/115	-
22	FES	G	101	-	-	-	0/1/1/1
18	CLA	B	805	-	1/1/10/20	2/10/88/115	-
18	CLA	3	308	-	1/1/10/20	1/10/88/115	-
18	CLA	1	605	-	1/1/10/20	3/10/88/115	-
18	CLA	6	313	-	1/1/10/20	3/10/88/115	-
21	CHL	3	306	-	3/3/15/26	1/12/110/137	-
18	CLA	3	301	-	1/1/10/20	2/10/88/115	-
18	CLA	B	808	-	1/1/10/20	0/10/88/115	-
18	CLA	5	602	-	1/1/10/20	4/10/88/115	-
18	CLA	4	602	-	1/1/10/20	1/10/88/115	-
20	SF4	B	803	-	-	-	0/6/5/5
18	CLA	B	824	-	1/1/10/20	2/10/88/115	-
18	CLA	8	607	-	1/1/10/20	1/10/88/115	-
18	CLA	8	609	-	1/1/10/20	2/10/88/115	-
18	CLA	B	834	-	1/1/10/20	2/10/85/115	-
21	CHL	5	606	-	3/3/15/26	3/12/110/137	-
18	CLA	B	825	-	1/1/10/20	3/10/88/115	-
18	CLA	A	804	-	1/1/10/20	3/10/88/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
18	CLA	6	315	-	1/1/10/20	2/10/88/115	-
18	CLA	7	603	-	1/1/11/20	2/15/93/115	-
18	CLA	B	821	-	1/1/10/20	1/10/88/115	-
21	CHL	6	305	-	3/3/15/26	0/12/110/137	-
18	CLA	5	613	-	1/1/10/20	1/10/88/115	-
18	CLA	A	828	-	1/1/10/20	0/10/88/115	-
18	CLA	3	311	-	1/1/11/20	2/13/91/115	-
18	CLA	6	304	-	1/1/10/20	2/10/88/115	-
18	CLA	4	606	-	1/1/10/20	3/10/88/115	-
18	CLA	1	602	-	1/1/10/20	2/10/88/115	-
18	CLA	A	844	-	1/1/10/20	6/10/88/115	-
18	CLA	A	827	-	1/1/10/20	1/10/88/115	-
18	CLA	B	814	-	1/1/10/20	0/10/88/115	-
18	CLA	1	604	-	1/1/10/20	1/10/88/115	-
18	CLA	5	605	-	1/1/10/20	0/10/88/115	-
21	CHL	6	316	-	3/3/15/26	2/12/110/137	-
18	CLA	Z	603	-	1/1/10/20	1/10/88/115	-
18	CLA	1	613	-	1/1/10/20	3/10/88/115	-
18	CLA	6	302	-	1/1/10/20	3/10/88/115	-
18	CLA	A	822	-	1/1/10/20	5/10/88/115	-
18	CLA	B	819	-	1/1/10/20	2/10/88/115	-
18	CLA	A	805	-	1/1/10/20	2/10/88/115	-
18	CLA	8	603	-	1/1/11/20	0/13/91/115	-
18	CLA	A	838	-	1/1/10/20	2/10/88/115	-
18	CLA	A	811	-	1/1/10/20	1/11/89/115	-
18	CLA	B	843	-	1/1/10/20	3/10/88/115	-
18	CLA	7	610	-	1/1/10/20	2/8/86/115	-
20	SF4	C	101	3	-	-	0/6/5/5
18	CLA	B	839	-	1/1/10/20	3/10/88/115	-
18	CLA	5	610	-	1/1/13/20	4/25/103/115	-
18	CLA	B	804	-	1/1/10/20	1/10/88/115	-
18	CLA	4	611	-	1/1/10/20	2/10/88/115	-
18	CLA	B	830	-	1/1/11/20	4/13/91/115	-
18	CLA	A	825	-	1/1/10/20	2/10/88/115	-
18	CLA	6	301	-	1/1/10/20	4/10/88/115	-
18	CLA	B	813	-	1/1/10/20	1/10/86/115	-
18	CLA	7	612	-	1/1/11/20	4/13/91/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
18	CLA	4	603	-	1/1/11/20	4/15/93/115	-
18	CLA	Z	608	-	1/1/10/20	2/10/88/115	-
21	CHL	7	606	-	3/3/15/26	1/12/110/137	-
18	CLA	1	608	-	1/1/10/20	2/10/88/115	-
18	CLA	B	820	-	1/1/10/20	2/10/88/115	-
18	CLA	B	842	-	1/1/10/20	1/10/88/115	-
18	CLA	6	303	-	1/1/11/20	4/15/93/115	-
18	CLA	B	841	-	1/1/10/20	1/10/88/115	-
18	CLA	3	307	-	1/1/10/20	1/10/88/115	-
18	CLA	6	310	-	1/1/10/20	2/10/88/115	-
18	CLA	1	603	-	1/1/10/20	2/10/88/115	-
18	CLA	A	840	-	1/1/10/20	2/10/88/115	-
18	CLA	B	833	-	1/1/10/20	3/10/88/115	-
18	CLA	F	302	-	1/1/15/20	5/37/115/115	-
18	CLA	4	607	-	1/1/10/20	1/10/88/115	-
18	CLA	5	614	14	1/1/10/20	1/10/88/115	-
18	CLA	A	830	-	1/1/10/20	1/10/88/115	-
21	CHL	Z	601	12	3/3/15/26	1/12/110/137	-
21	CHL	5	607	-	3/3/15/26	2/12/110/137	-
18	CLA	1	609	-	1/1/10/20	2/10/88/115	-
18	CLA	J	101	-	1/1/10/20	4/10/88/115	-
18	CLA	8	613	-	1/1/10/20	1/10/88/115	-
18	CLA	Z	607	-	1/1/10/20	2/10/88/115	-
18	CLA	B	807	-	1/1/11/20	4/15/93/115	-
18	CLA	5	615	-	1/1/11/20	3/15/93/115	-
18	CLA	5	603	-	1/1/11/20	4/15/93/115	-
18	CLA	B	810	-	1/1/10/20	2/10/88/115	-
18	CLA	7	604	-	1/1/10/20	2/11/89/115	-
17	CL0	A	801	-	3/3/15/25	2/10/108/135	-
18	CLA	7	601	10	1/1/10/20	5/10/88/115	-
18	CLA	B	806	-	1/1/11/20	4/13/91/115	-
18	CLA	7	602	-	1/1/10/20	2/10/88/115	-
18	CLA	A	839	-	1/1/10/20	2/10/88/115	-
18	CLA	6	317	-	1/1/11/20	2/13/91/115	-

The worst 5 of 1910 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	B	834	CLA	C4C-NC	22.91	1.47	1.30
18	7	604	CLA	C4B-NB	15.66	1.49	1.35
18	B	823	CLA	C4B-NB	15.01	1.48	1.35
18	6	301	CLA	C4B-NB	14.68	1.48	1.35
18	A	833	CLA	C4B-NB	14.61	1.48	1.35

The worst 5 of 1748 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	5	606	CHL	C4A-NA-C1A	-12.99	100.87	106.71
21	4	605	CHL	C4A-NA-C1A	-12.67	101.01	106.71
18	7	614	CLA	C4A-NA-C1A	-10.95	101.78	106.71
18	7	610	CLA	C4A-NA-C1A	-10.06	102.18	106.71
18	A	834	CLA	C4A-NA-C1A	-9.90	102.26	106.71

5 of 239 chirality outliers are listed below:

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

5 of 458 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
18	A	802	CLA	C1A-C2A-CAA-CBA
18	A	802	CLA	C3A-C2A-CAA-CBA
18	A	802	CLA	CHA-CBD-CGD-O1D
18	A	802	CLA	CHA-CBD-CGD-O2D
18	A	803	CLA	C1A-C2A-CAA-CBA

There are no ring outliers.

177 monomers are involved in 352 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
18	3	304	CLA	2	0
18	Z	604	CLA	4	0
21	6	306	CHL	1	0
18	A	845	CLA	11	0
18	B	823	CLA	3	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
18	B	815	CLA	4	0
18	Z	602	CLA	1	0
21	8	606	CHL	3	0
18	A	809	CLA	3	0
18	A	836	CLA	4	0
18	A	807	CLA	3	0
18	A	841	CLA	2	0
18	F	301	CLA	1	0
18	1	612	CLA	6	0
18	B	827	CLA	1	0
18	8	608	CLA	5	0
18	6	309	CLA	2	0
18	6	312	CLA	4	0
18	A	812	CLA	3	0
18	A	826	CLA	1	0
18	A	818	CLA	2	0
18	A	806	CLA	3	0
18	8	612	CLA	4	0
18	6	311	CLA	1	0
18	A	815	CLA	3	0
18	7	613	CLA	2	0
21	1	601	CHL	3	0
18	Z	612	CLA	4	0
18	B	831	CLA	2	0
18	A	803	CLA	2	0
18	A	814	CLA	3	0
18	B	817	CLA	2	0
18	A	817	CLA	4	0
18	3	313	CLA	5	0
18	A	816	CLA	2	0
18	3	302	CLA	3	0
18	B	809	CLA	2	0
18	B	836	CLA	1	0
19	A	842	PQN	6	0
18	B	835	CLA	3	0
18	B	826	CLA	3	0
18	B	812	CLA	1	0
18	7	614	CLA	1	0
18	8	611	CLA	1	0
18	A	823	CLA	3	0
21	5	616	CHL	1	0
21	4	604	CHL	4	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
18	6	308	CLA	1	0
18	A	813	CLA	3	0
18	3	314	CLA	3	0
18	A	808	CLA	3	0
18	8	602	CLA	1	0
18	6	314	CLA	1	0
21	6	307	CHL	1	0
21	1	606	CHL	2	0
21	4	605	CHL	1	0
18	B	829	CLA	3	0
18	7	605	CLA	4	0
18	5	601	CLA	1	0
18	B	816	CLA	4	0
18	7	608	CLA	3	0
18	A	819	CLA	1	0
18	A	802	CLA	3	0
18	8	605	CLA	3	0
18	5	608	CLA	1	0
18	A	843	CLA	7	0
21	Z	605	CHL	2	0
18	A	837	CLA	1	0
20	C	102	SF4	1	0
18	5	609	CLA	1	0
18	A	835	CLA	5	0
18	B	818	CLA	1	0
18	B	801	CLA	1	0
18	B	840	CLA	2	0
18	3	303	CLA	4	0
18	8	604	CLA	1	0
18	8	614	CLA	1	0
18	8	601	CLA	2	0
18	3	312	CLA	2	0
18	1	611	CLA	1	0
18	A	820	CLA	1	0
18	5	612	CLA	3	0
18	A	834	CLA	2	0
18	7	609	CLA	1	0
18	B	811	CLA	4	0
18	B	837	CLA	2	0
18	A	833	CLA	1	0
19	B	844	PQN	5	0
18	B	802	CLA	5	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
18	8	615	CLA	2	0
18	A	824	CLA	1	0
18	3	305	CLA	2	0
18	Z	610	CLA	1	0
18	Z	611	CLA	5	0
18	B	832	CLA	3	0
18	B	822	CLA	2	0
18	5	611	CLA	5	0
18	1	614	CLA	1	0
18	4	610	CLA	4	0
18	5	604	CLA	1	0
18	B	805	CLA	1	0
18	3	308	CLA	2	0
18	1	605	CLA	4	0
18	6	313	CLA	3	0
18	B	808	CLA	3	0
18	5	602	CLA	2	0
18	4	602	CLA	2	0
20	B	803	SF4	1	0
18	B	824	CLA	4	0
18	8	609	CLA	2	0
18	B	834	CLA	3	0
21	5	606	CHL	1	0
18	B	825	CLA	3	0
18	A	804	CLA	1	0
18	6	315	CLA	1	0
18	7	603	CLA	1	0
18	B	821	CLA	2	0
21	6	305	CHL	2	0
18	5	613	CLA	3	0
18	A	828	CLA	2	0
18	3	311	CLA	2	0
18	6	304	CLA	1	0
18	4	606	CLA	1	0
18	1	602	CLA	1	0
18	A	844	CLA	5	0
18	A	827	CLA	3	0
18	B	814	CLA	6	0
18	1	604	CLA	4	0
18	5	605	CLA	2	0
18	Z	603	CLA	6	0
18	1	613	CLA	3	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
18	A	822	CLA	3	0
18	B	819	CLA	2	0
18	A	805	CLA	2	0
18	8	603	CLA	2	0
18	A	838	CLA	4	0
18	A	811	CLA	1	0
18	B	843	CLA	4	0
20	C	101	SF4	2	0
18	B	839	CLA	2	0
18	5	610	CLA	4	0
18	B	804	CLA	7	0
18	4	611	CLA	3	0
18	B	830	CLA	3	0
18	A	825	CLA	1	0
18	6	301	CLA	13	0
18	B	813	CLA	2	0
18	7	612	CLA	4	0
18	4	603	CLA	2	0
18	Z	608	CLA	4	0
21	7	606	CHL	1	0
18	1	608	CLA	2	0
18	B	842	CLA	6	0
18	B	841	CLA	2	0
18	3	307	CLA	5	0
18	1	603	CLA	2	0
18	B	833	CLA	2	0
18	F	302	CLA	11	0
18	4	607	CLA	2	0
18	5	614	CLA	2	0
18	A	830	CLA	2	0
21	Z	601	CHL	1	0
21	5	607	CHL	3	0
18	1	609	CLA	4	0
18	J	101	CLA	2	0
18	8	613	CLA	3	0
18	Z	607	CLA	2	0
18	B	807	CLA	1	0
18	5	615	CLA	1	0
18	B	810	CLA	3	0
18	7	604	CLA	7	0
17	A	801	CL0	9	0
18	7	601	CLA	2	0

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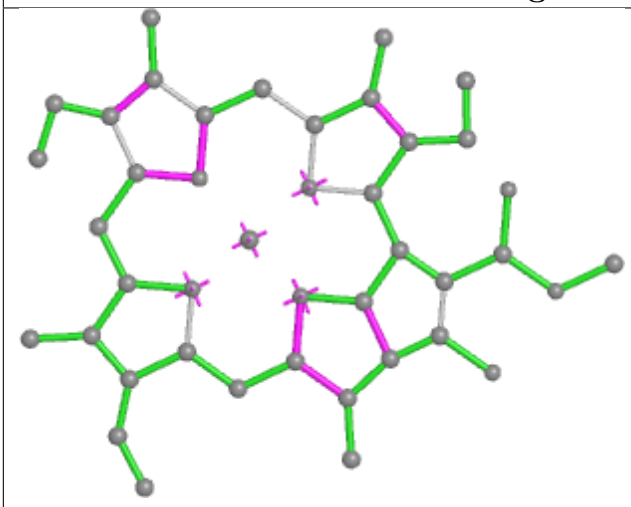
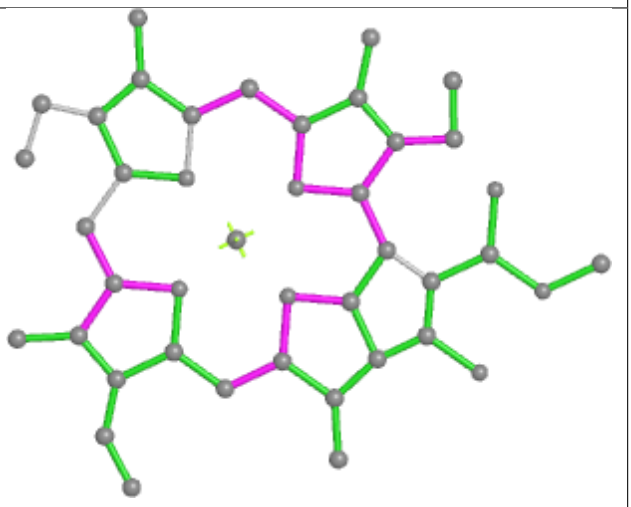
Mol	Chain	Res	Type	Clashes	Symm-Clashes
18	B	806	CLA	3	0
18	7	602	CLA	3	0
18	A	839	CLA	1	0
18	6	317	CLA	2	0

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 then 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.

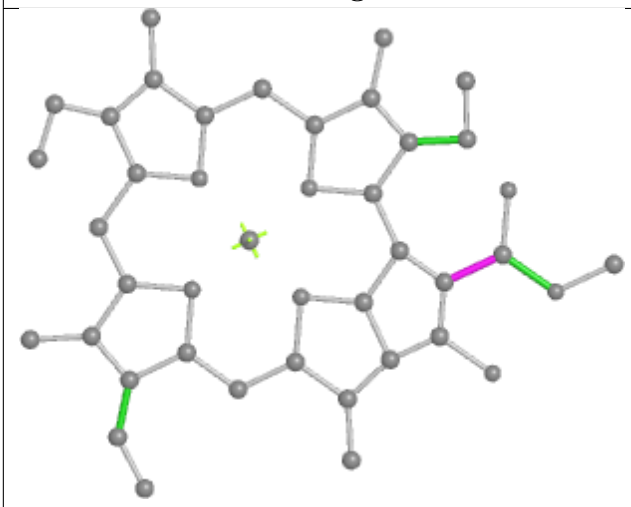
Ligand CLA 3 304



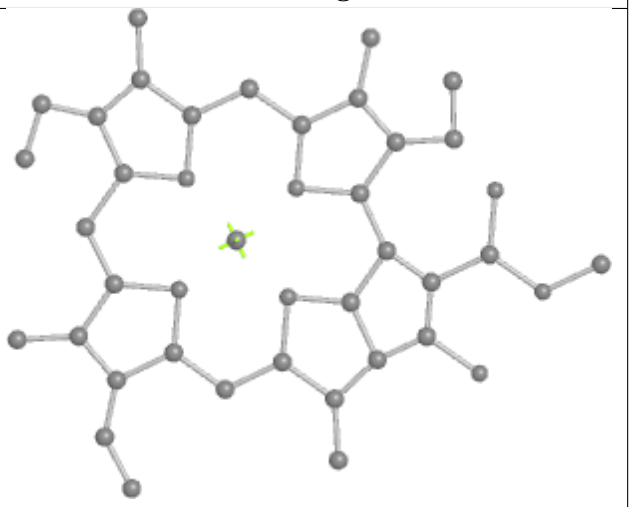
Bond lengths



Bond angles

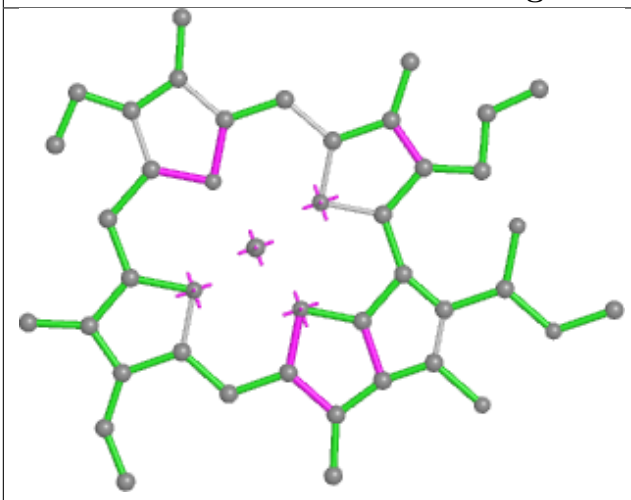


Torsions

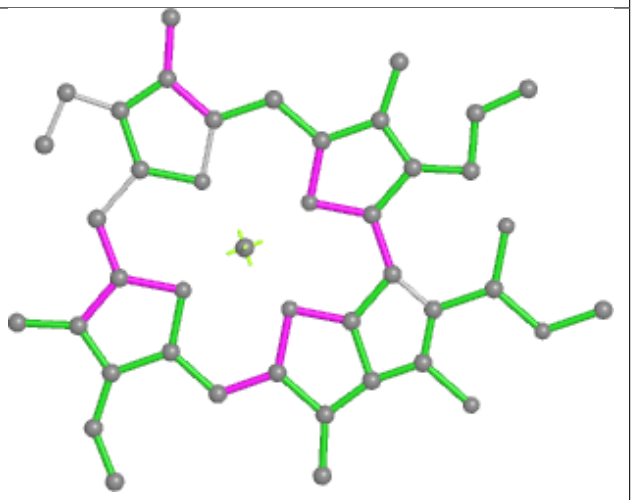


Rings

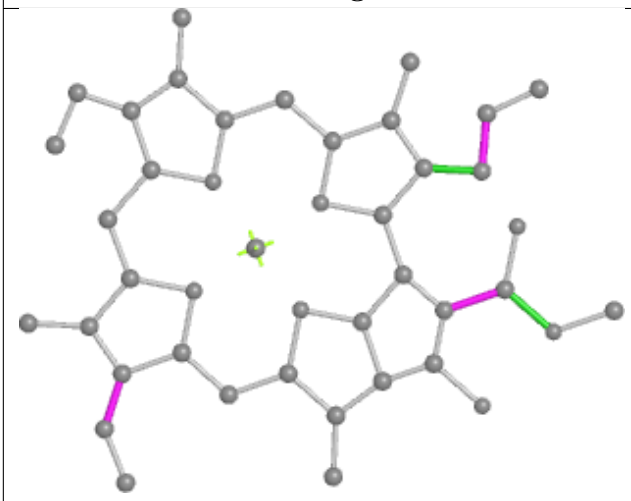
Ligand CLA Z 604



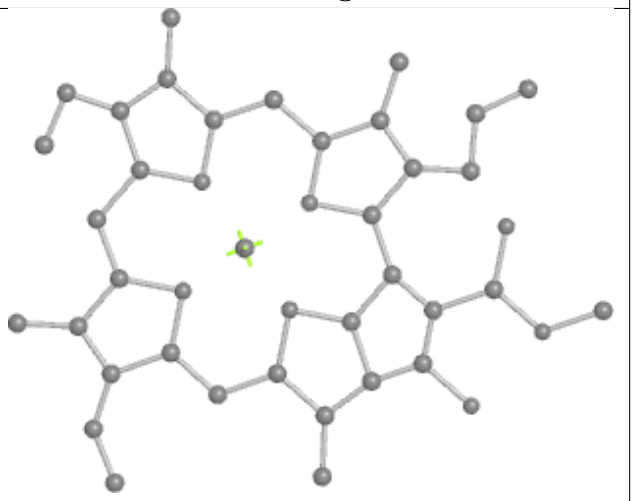
Bond lengths



Bond angles

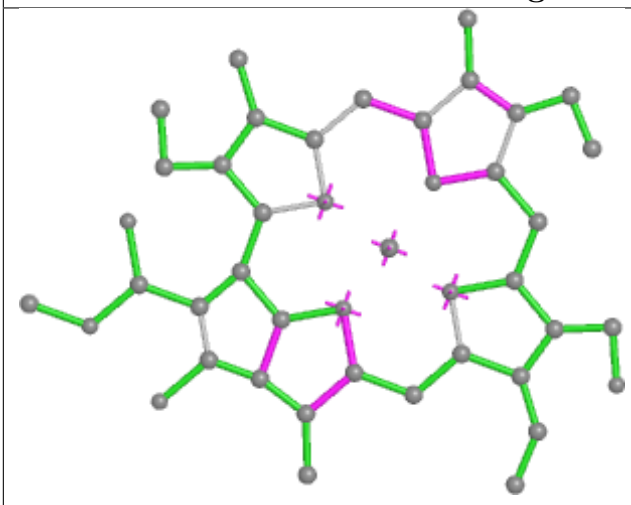


Torsions

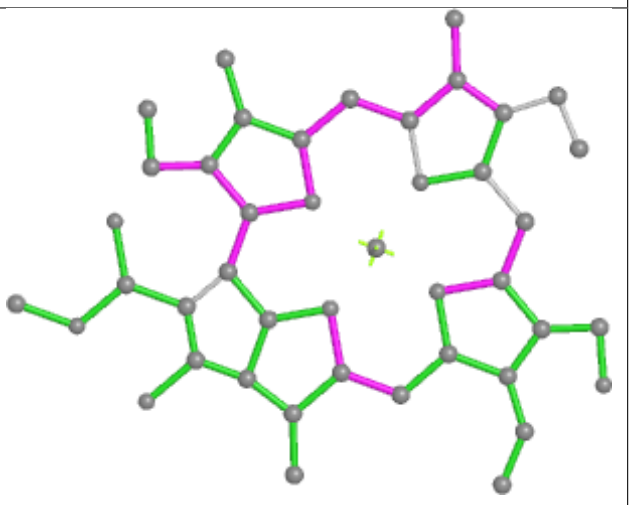


Rings

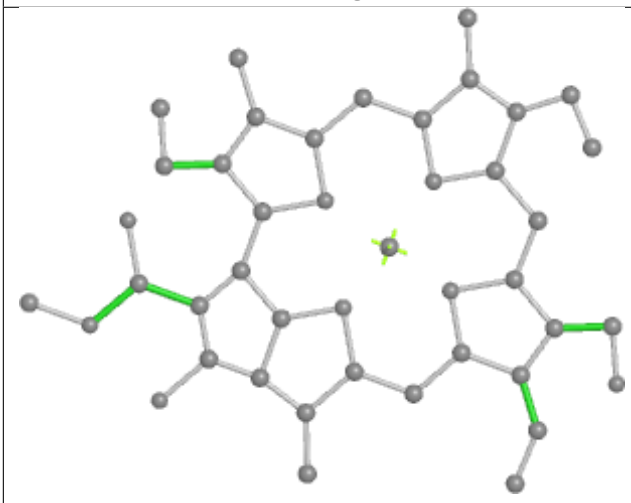
Ligand CHL 6 306



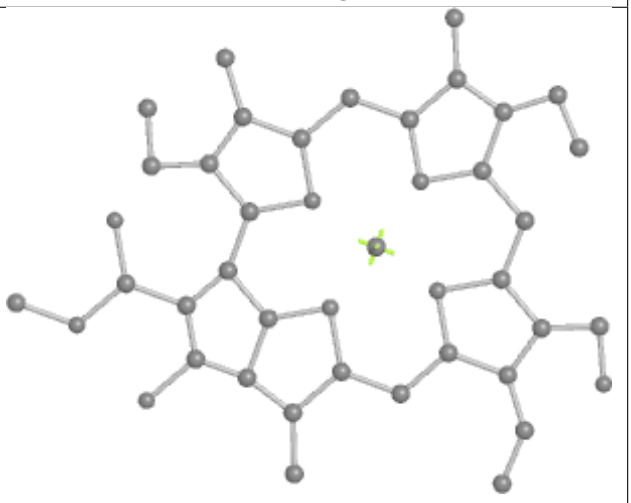
Bond lengths



Bond angles

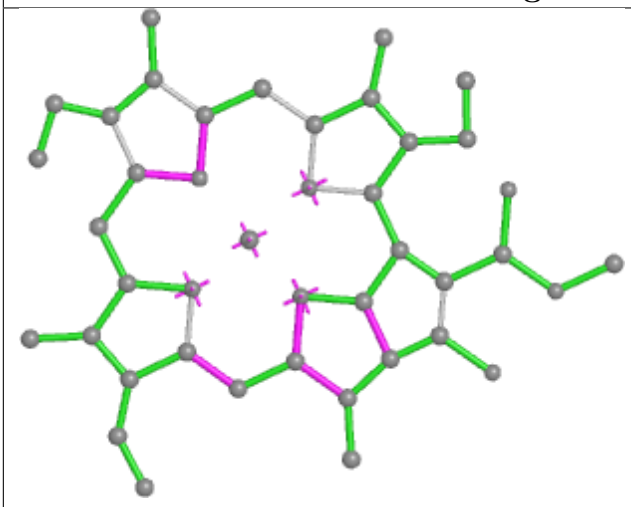


Torsions

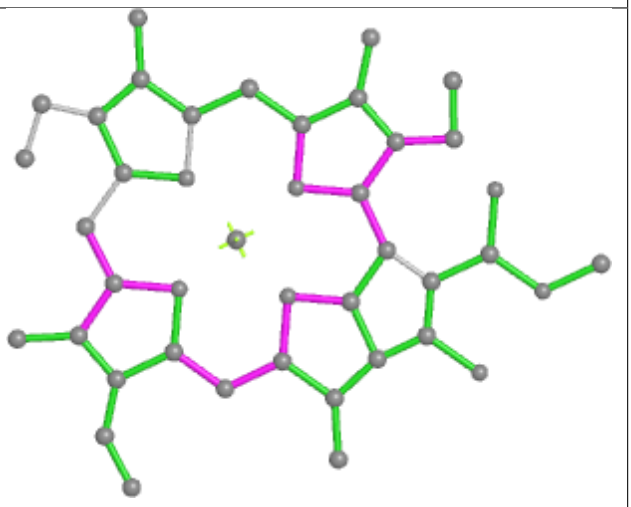


Rings

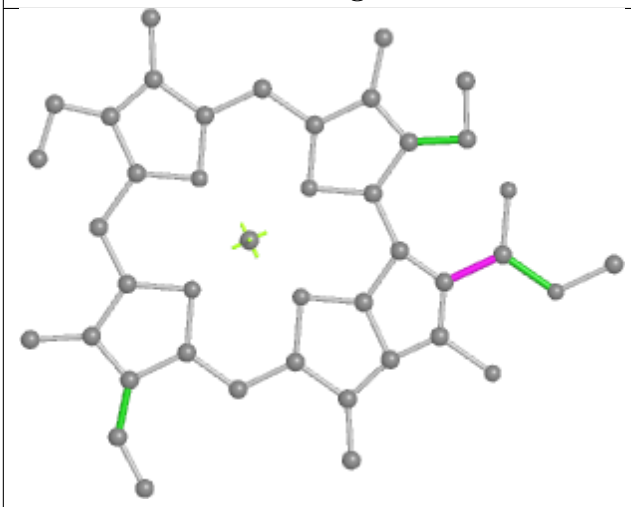
Ligand CLA A 845



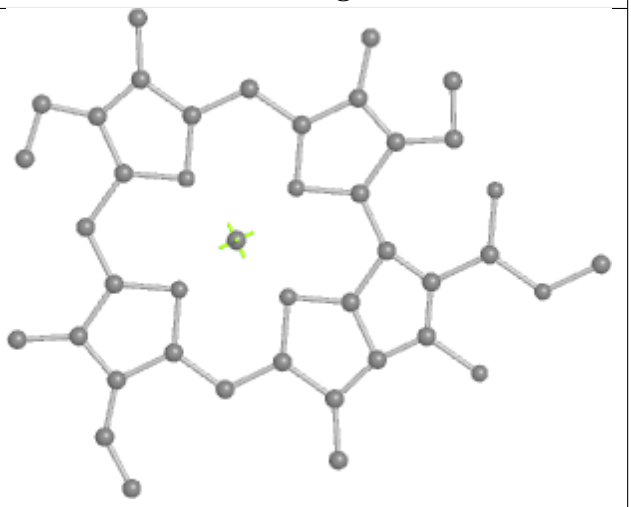
Bond lengths



Bond angles

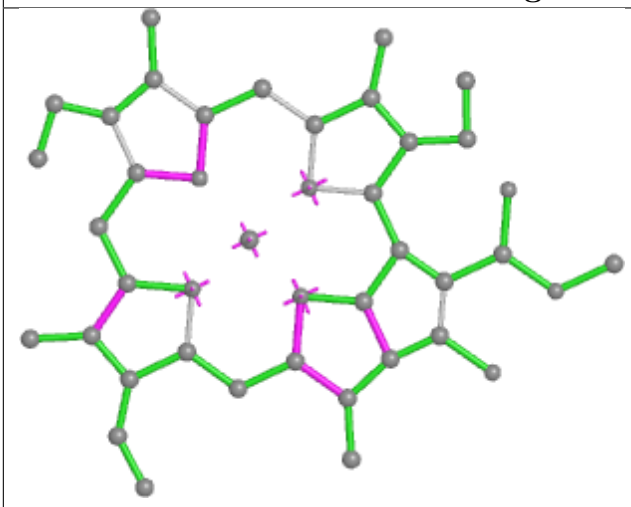


Torsions

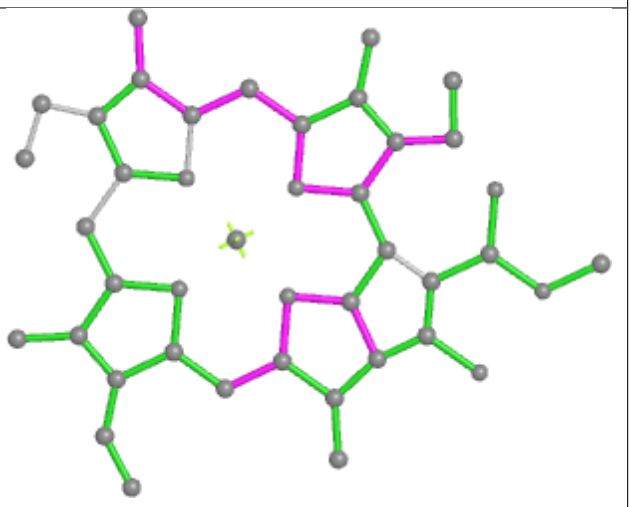


Rings

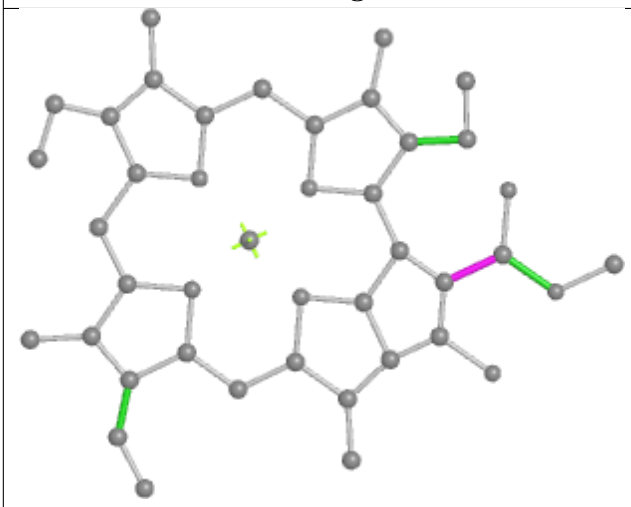
Ligand CLA B 823



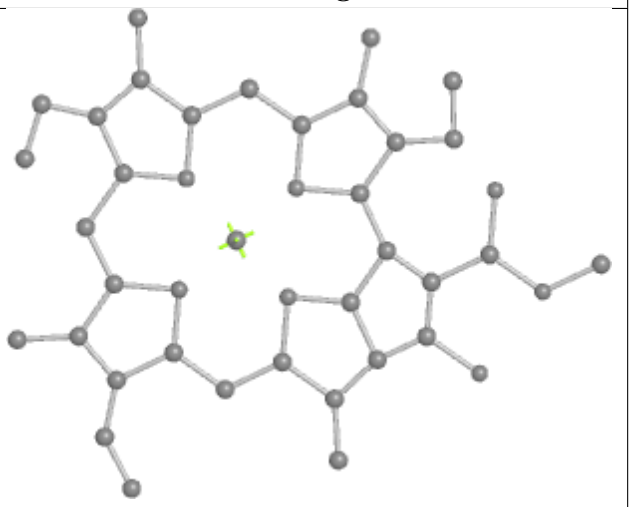
Bond lengths



Bond angles

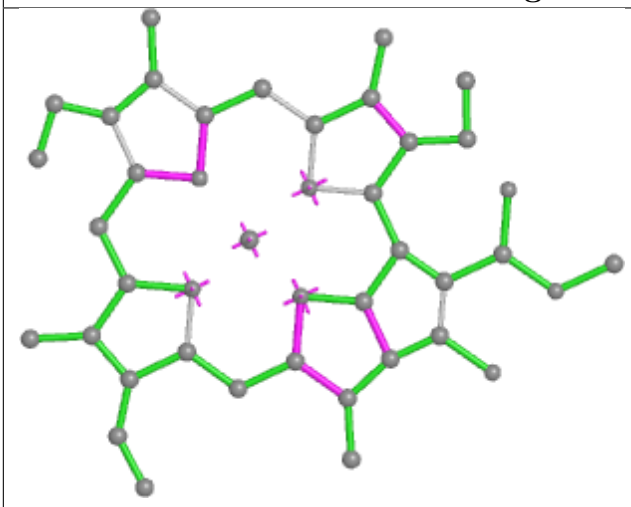


Torsions

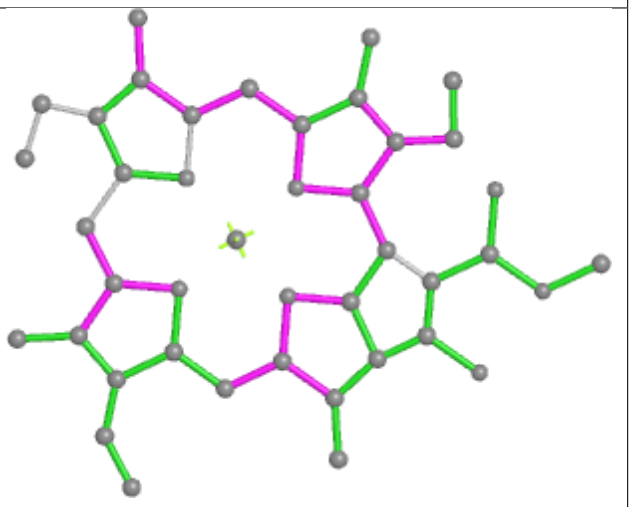


Rings

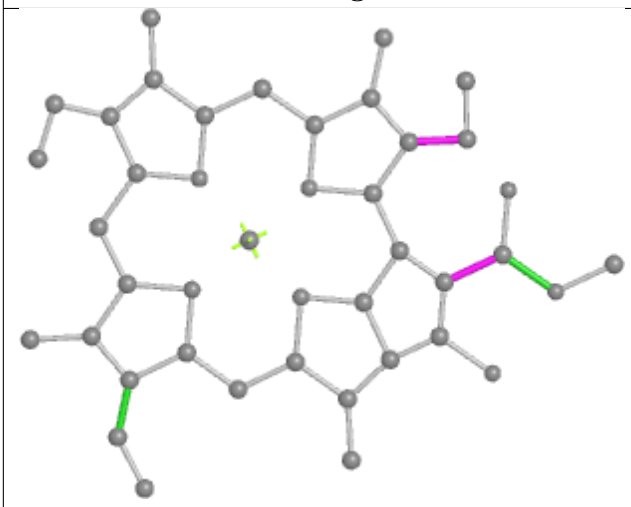
Ligand CLA B 815



Bond lengths



Bond angles



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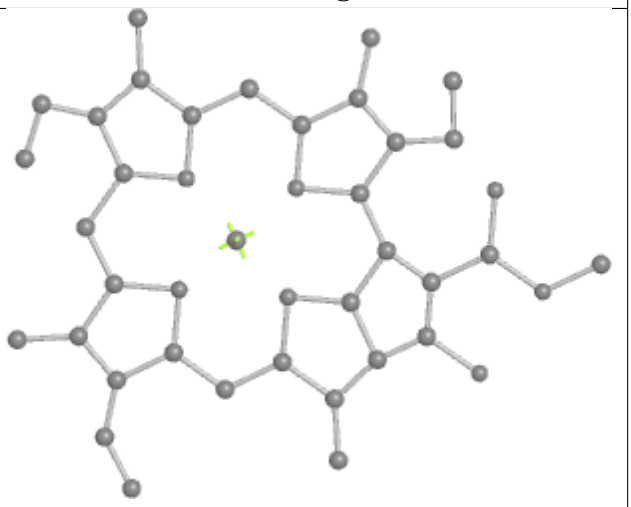
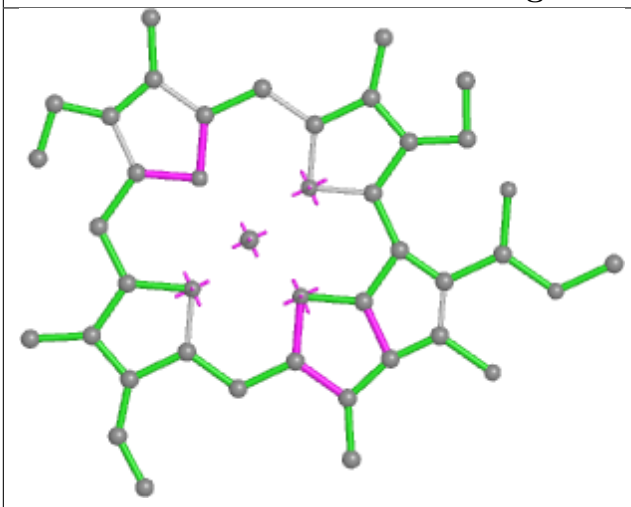
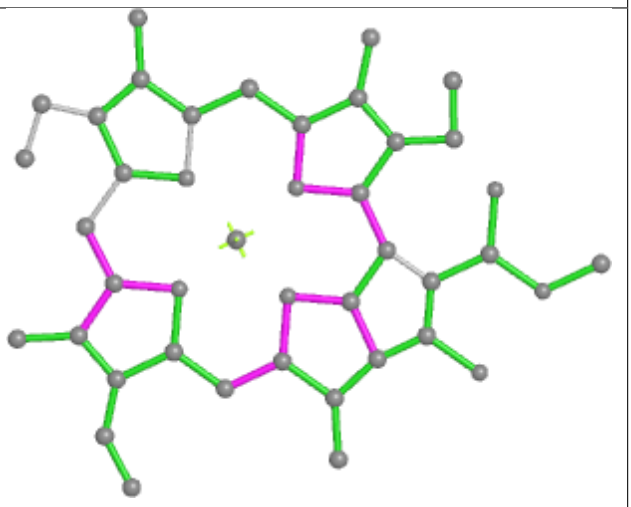


Rings

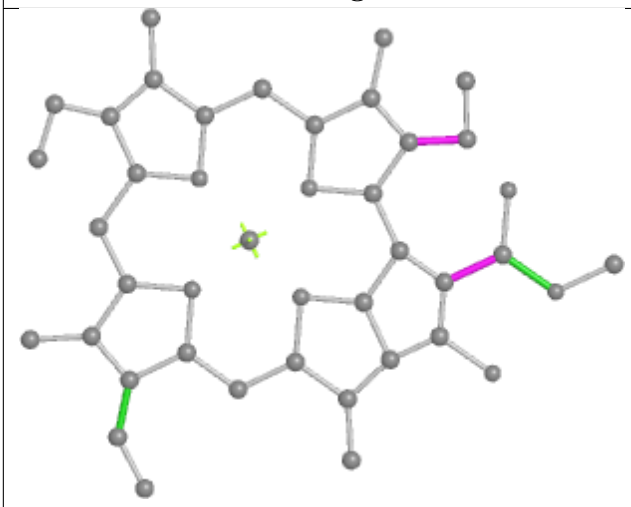
Ligand CLA Z 602



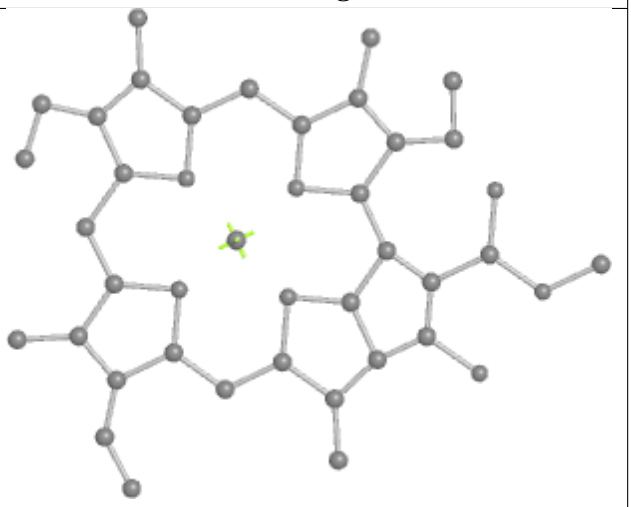
Bond lengths



Bond angles

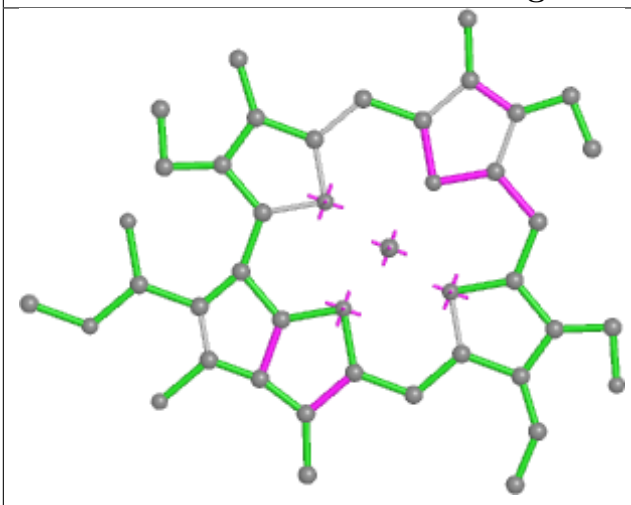


Torsions

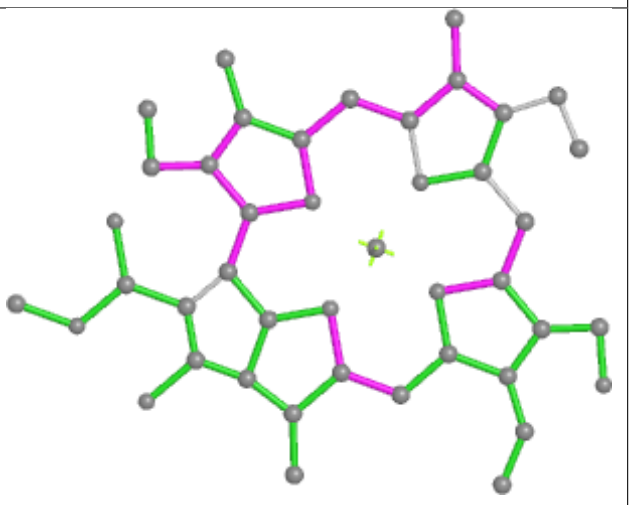


Rings

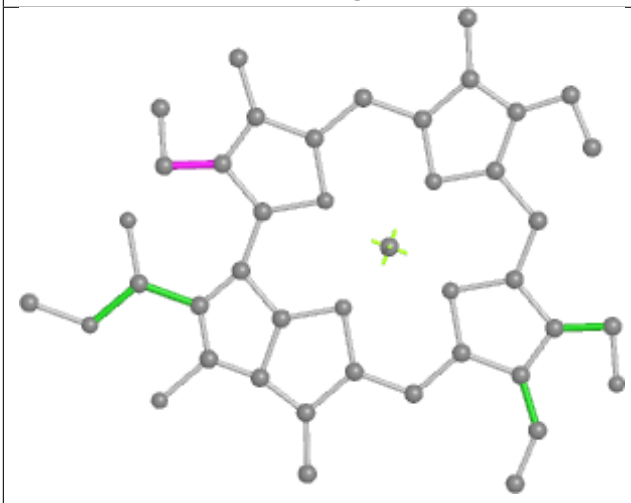
Ligand CHL 8 606



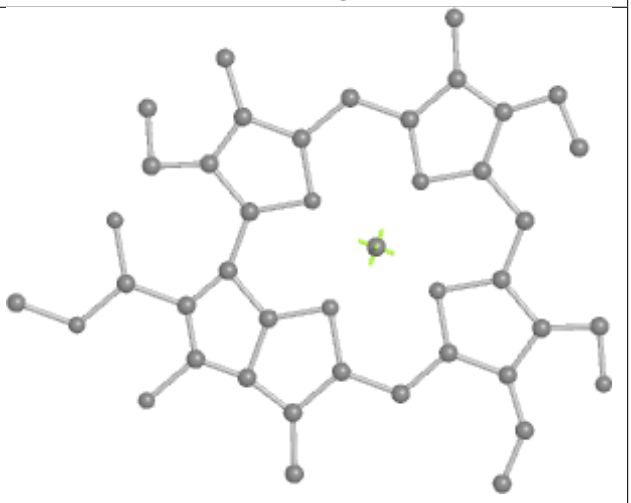
Bond lengths



Bond angles

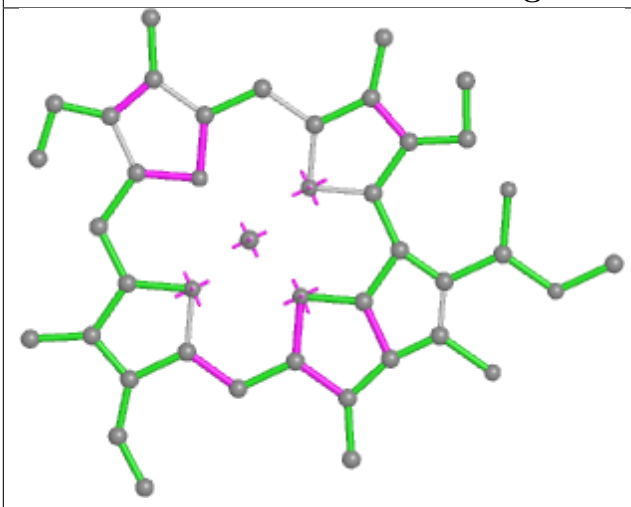


Torsions

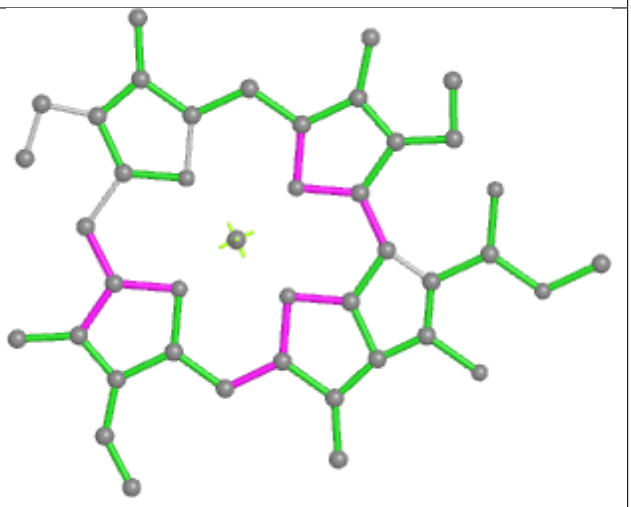


Rings

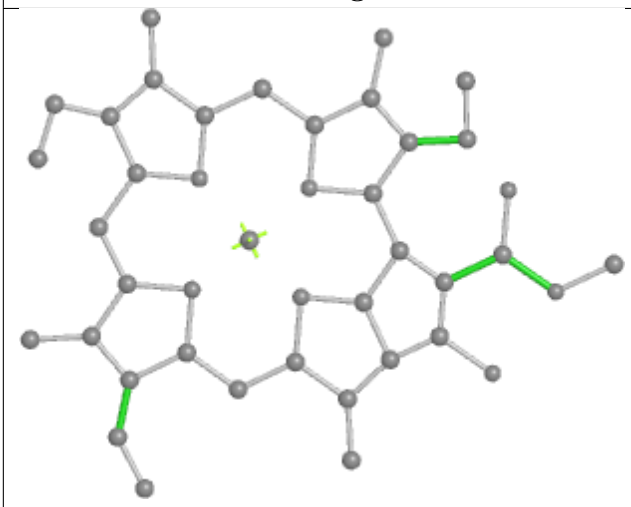
Ligand CLA A 809



Bond lengths



Bond angles



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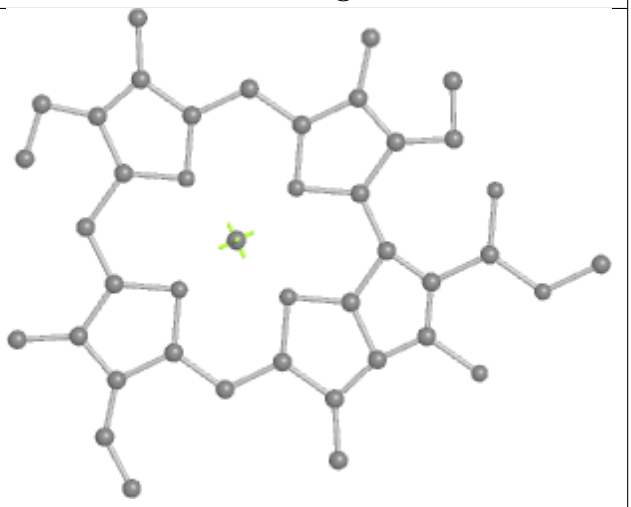
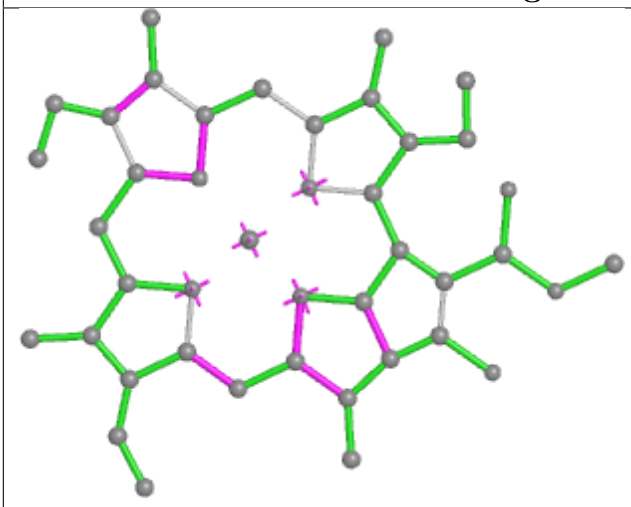
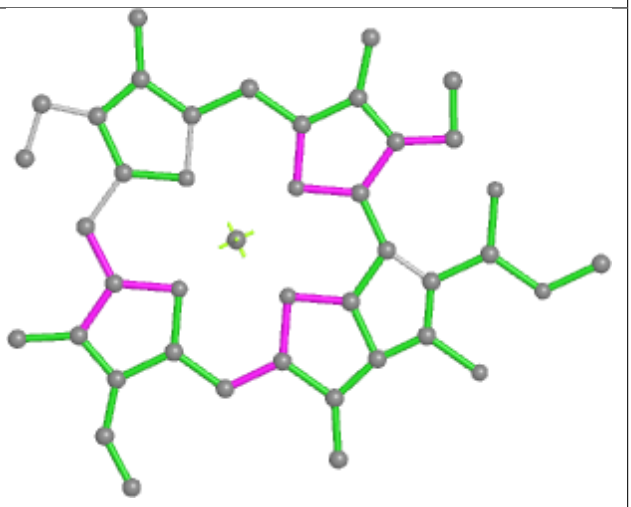


Rings

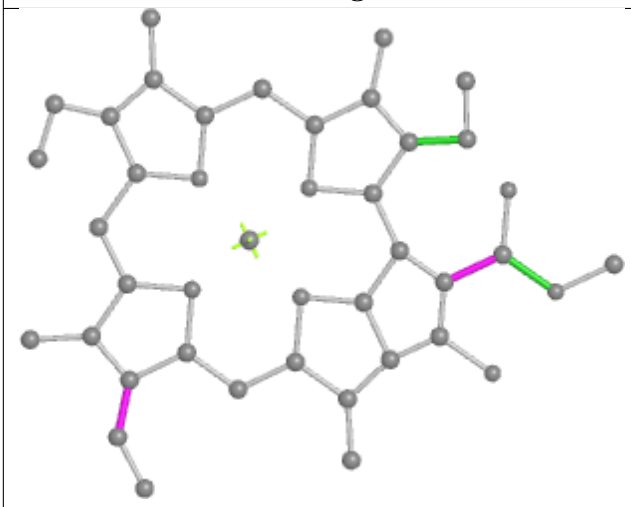
Ligand CLA A 836



Bond lengths



Bond angles



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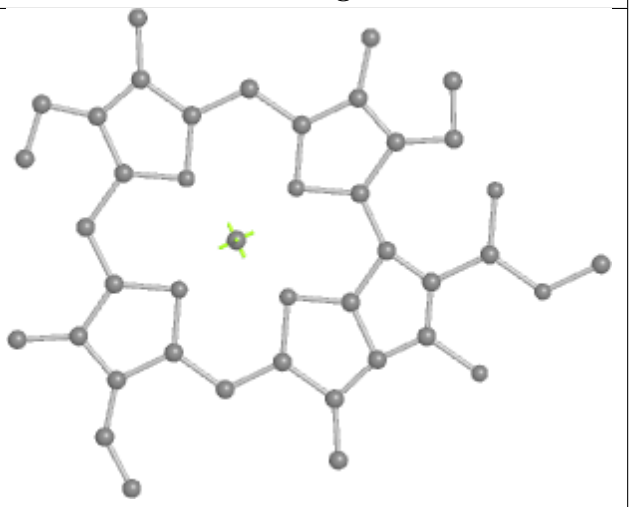
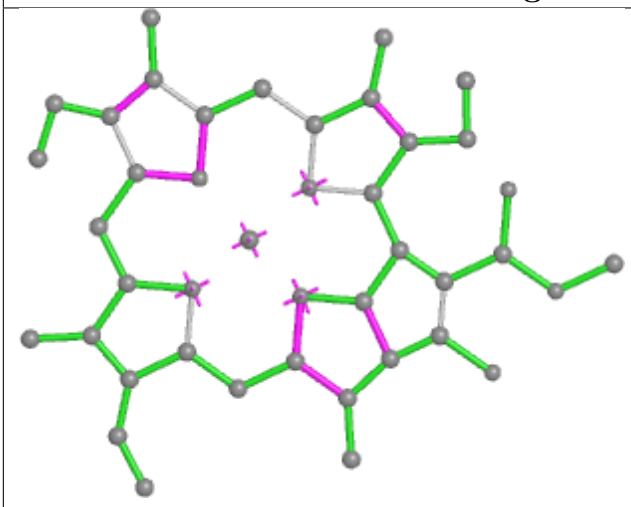
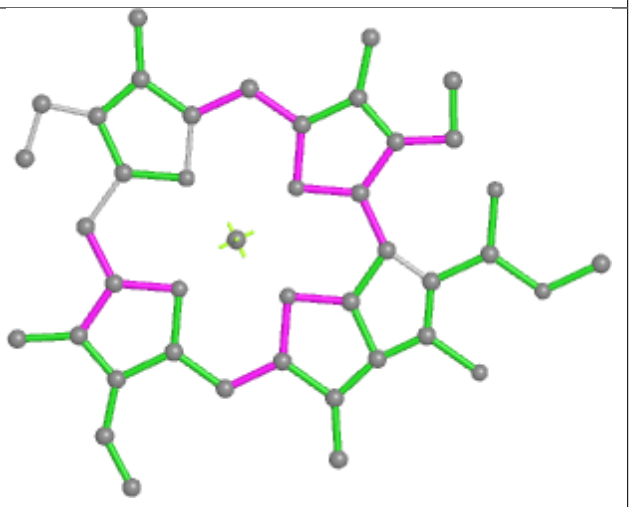


Rings

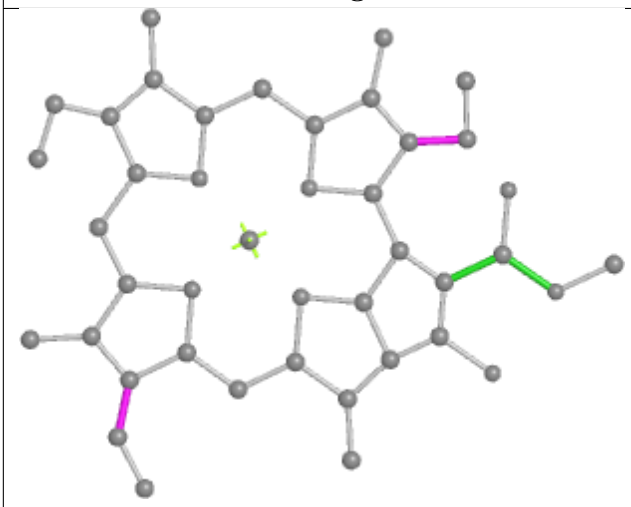
Ligand CLA A 807



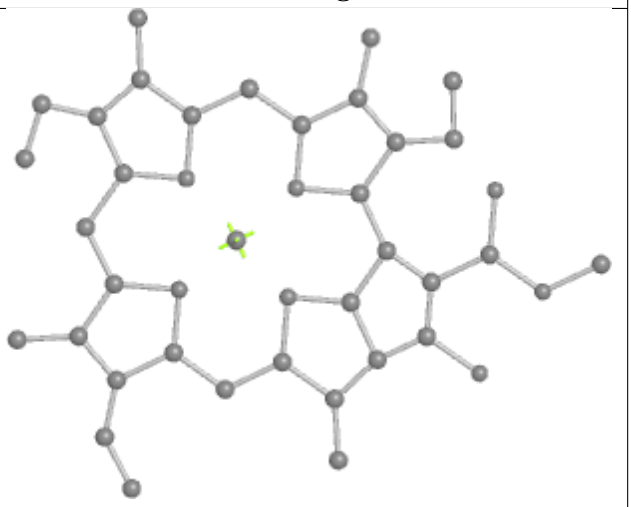
Bond lengths



Bond angles

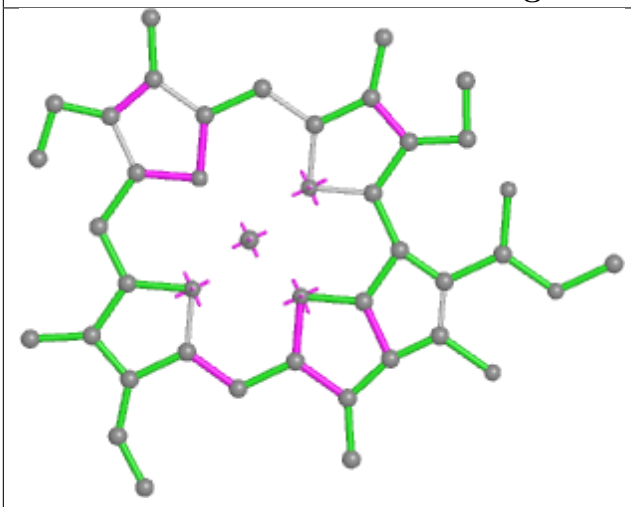


Torsions

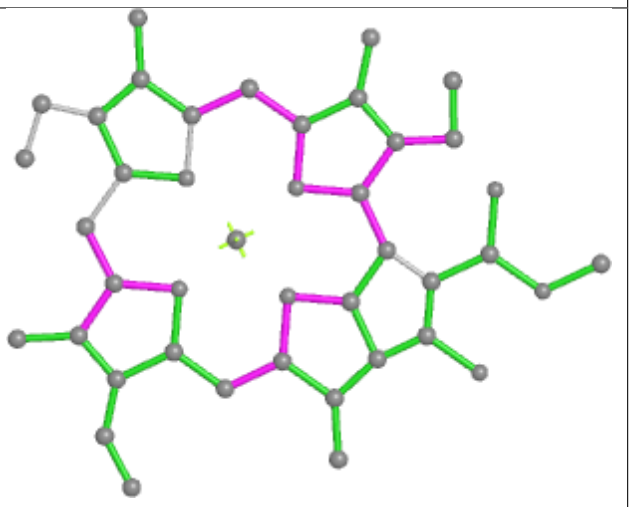


Rings

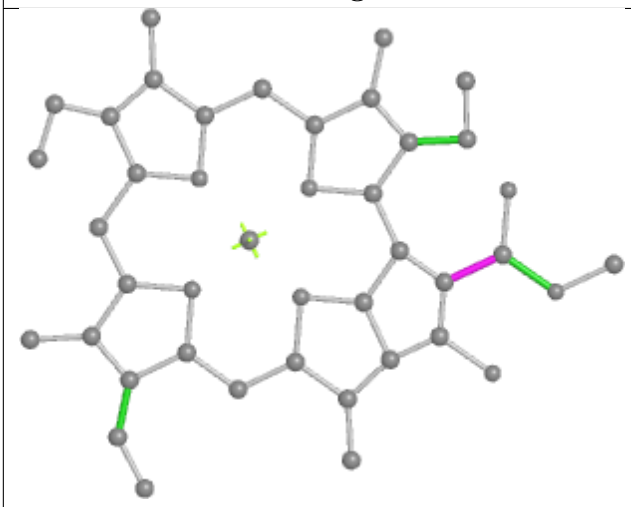
Ligand CLA A 841



Bond lengths



Bond angles



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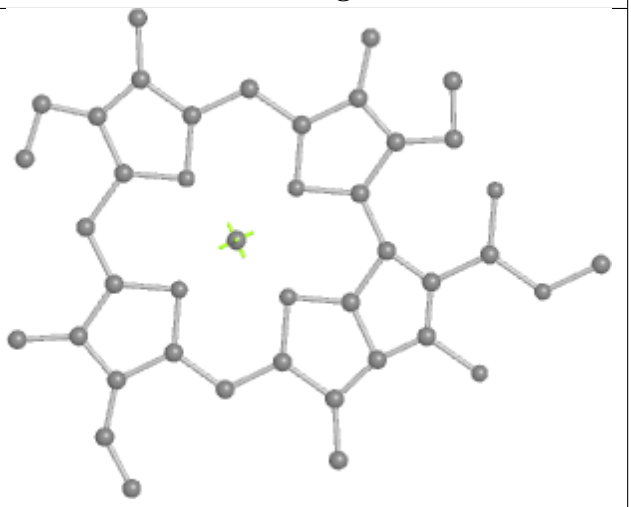
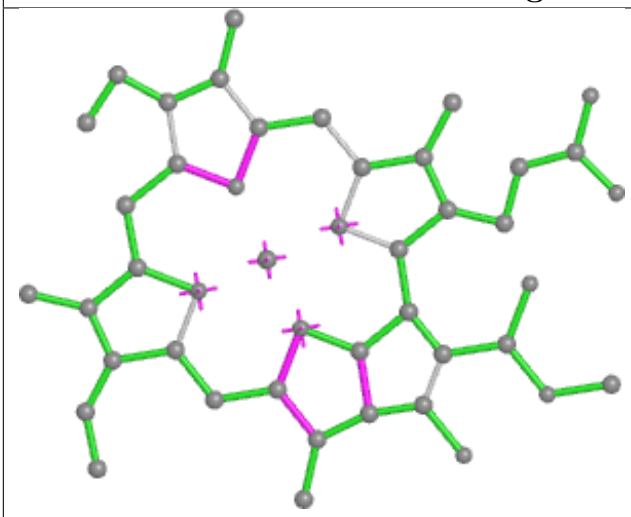
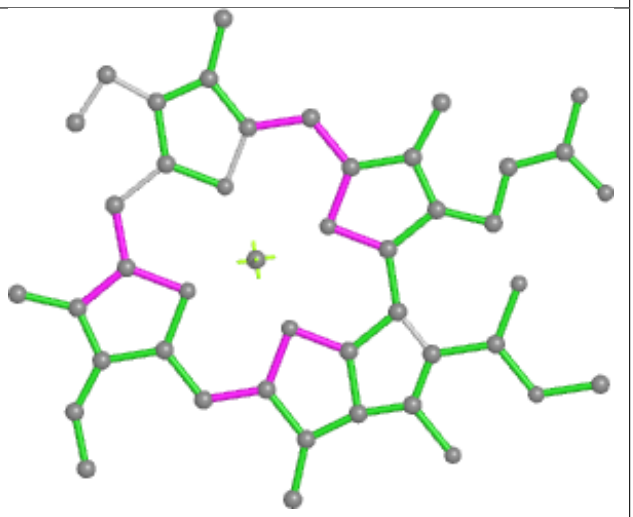


Rings

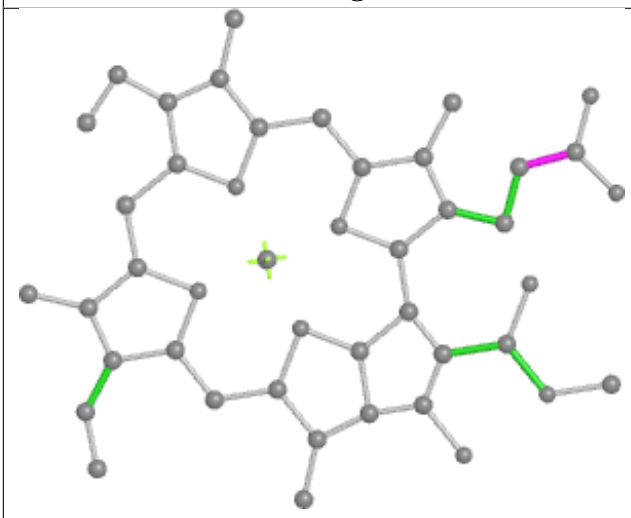
Ligand CLA F 301



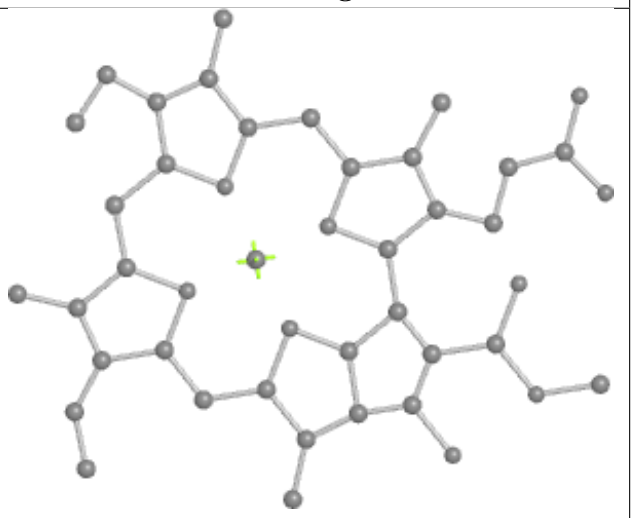
Bond lengths



Bond angles

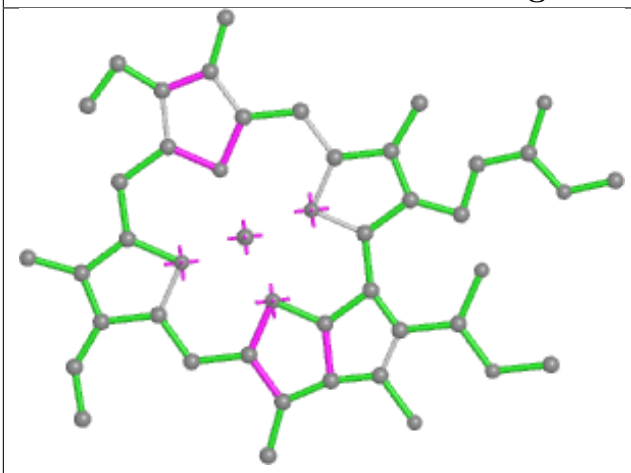


Torsions

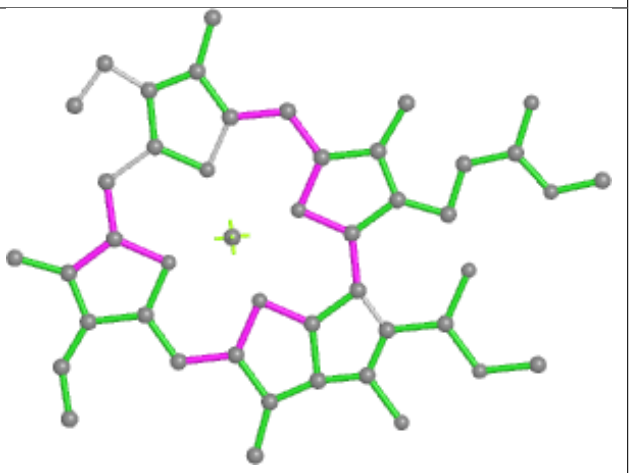


Rings

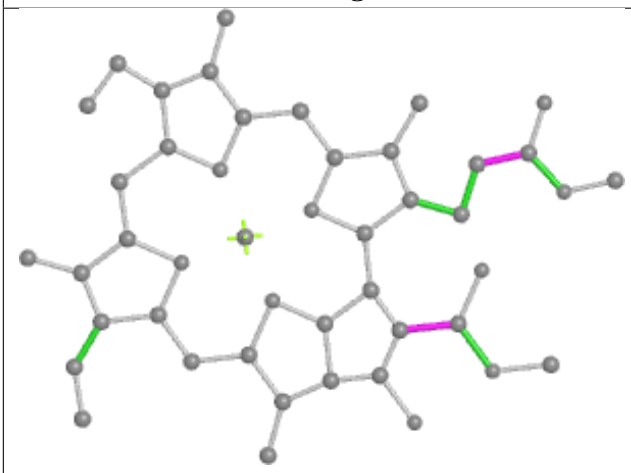
Ligand CLA 1 612



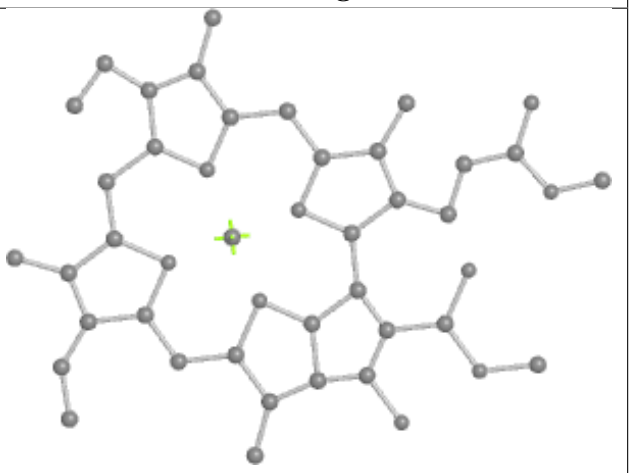
Bond lengths



Bond angles

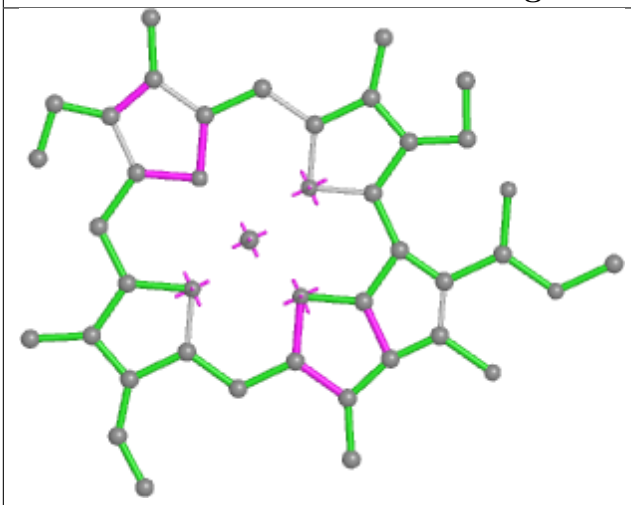


Torsions

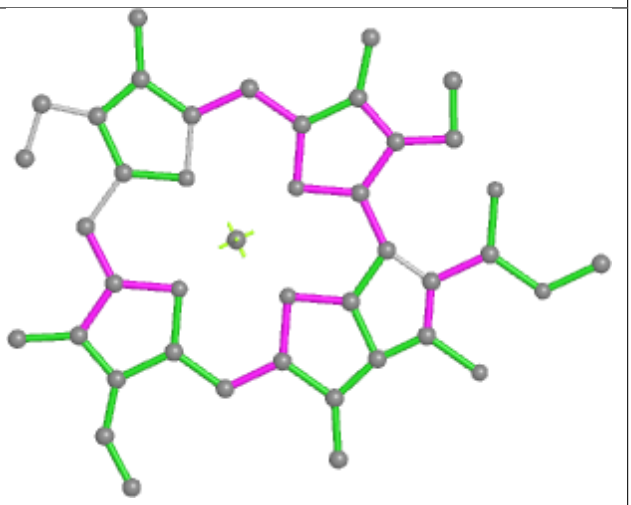


Rings

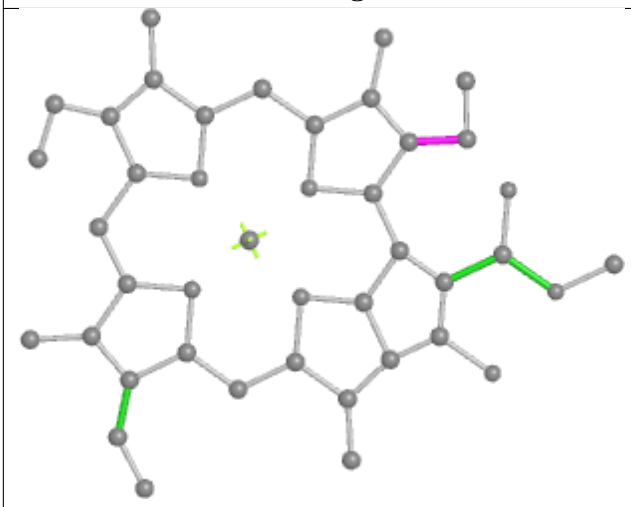
Ligand CLA B 827



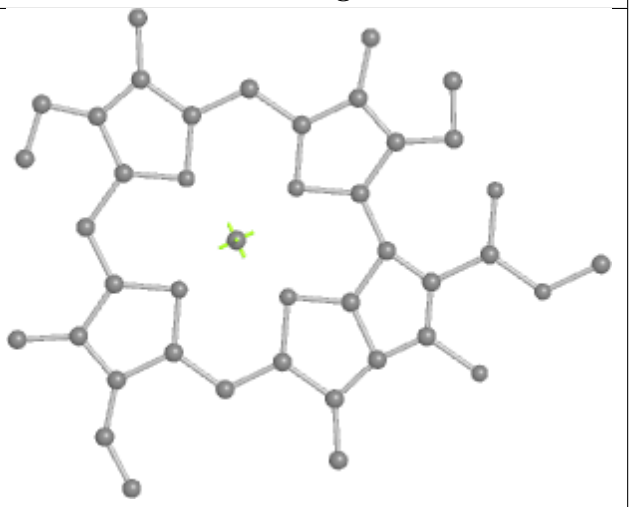
Bond lengths



Bond angles

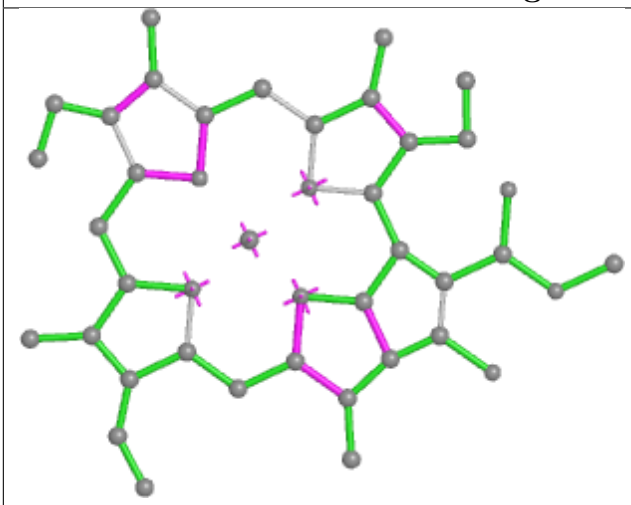


Torsions

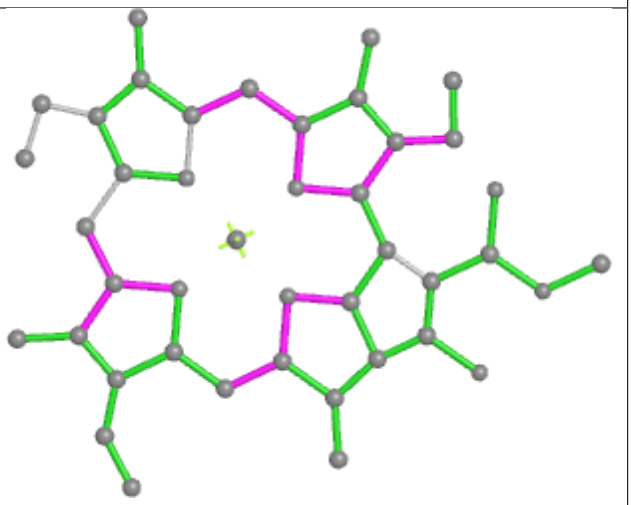


Rings

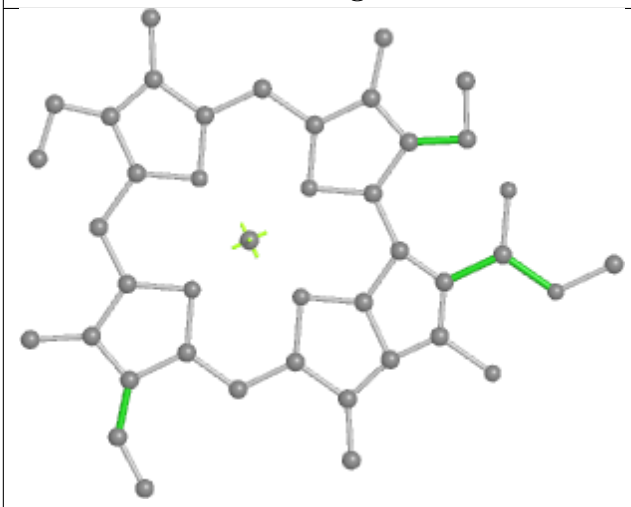
Ligand CLA A 810



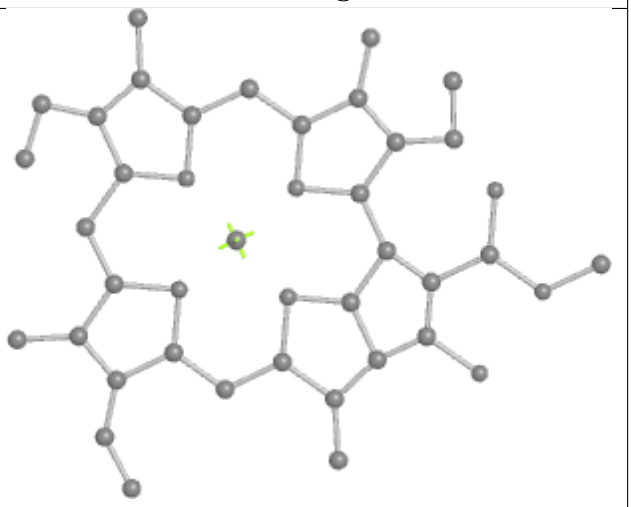
Bond lengths



Bond angles

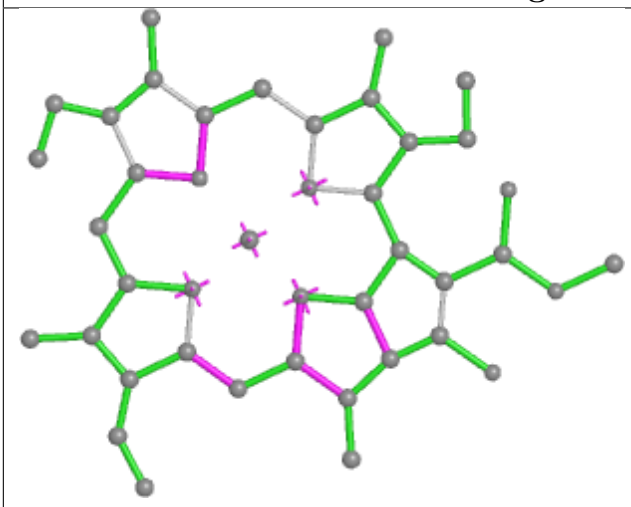


Torsions

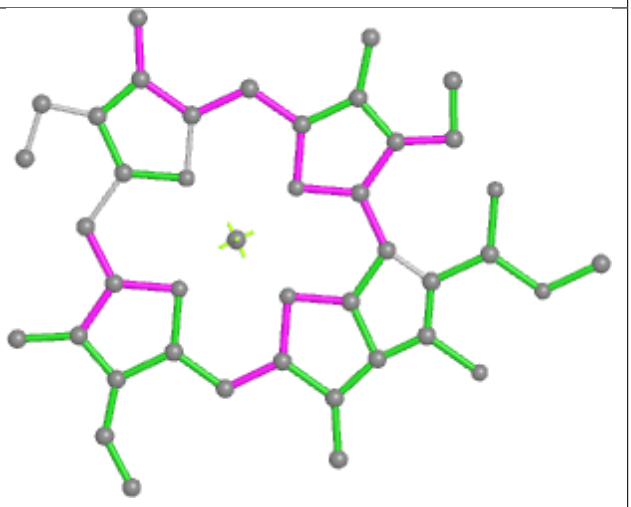


Rings

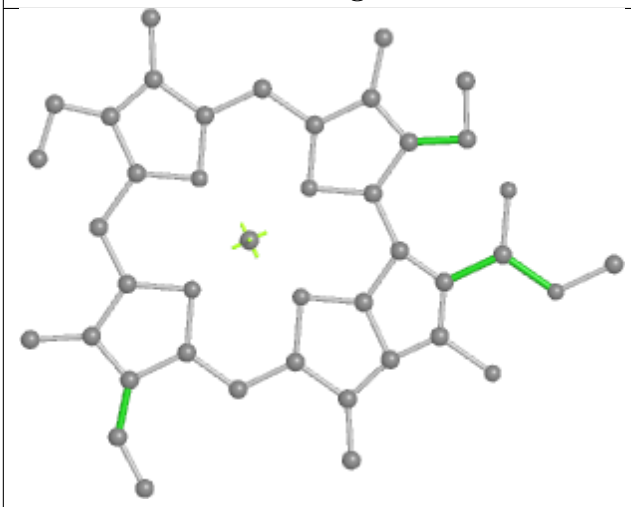
Ligand CLA 8 608



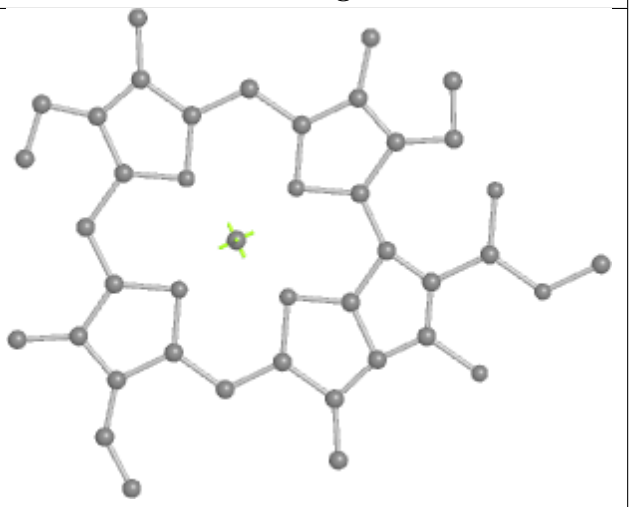
Bond lengths



Bond angles

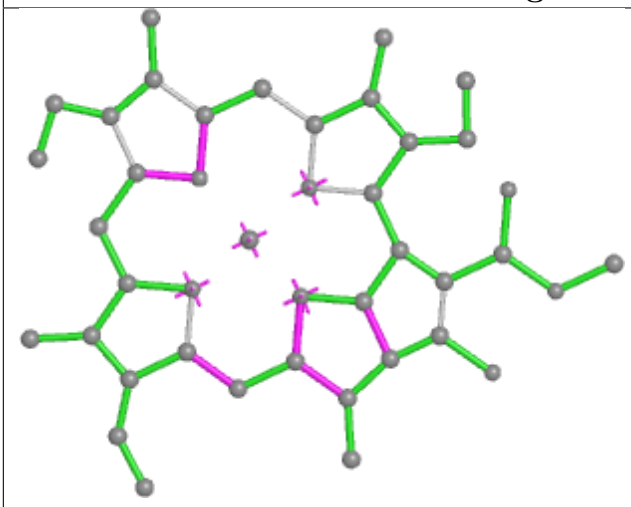


Torsions

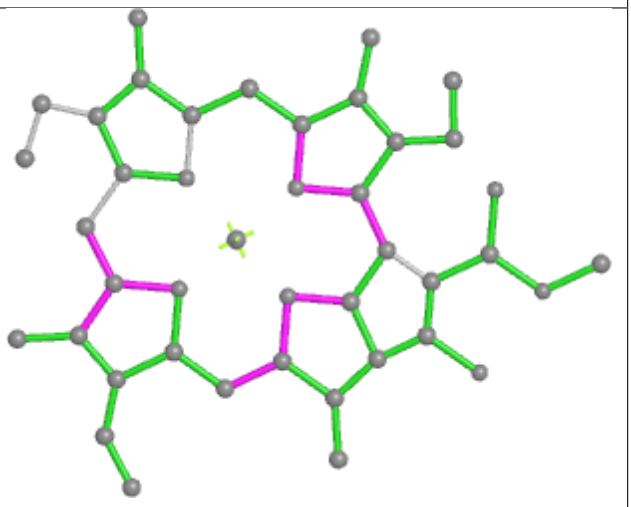


Rings

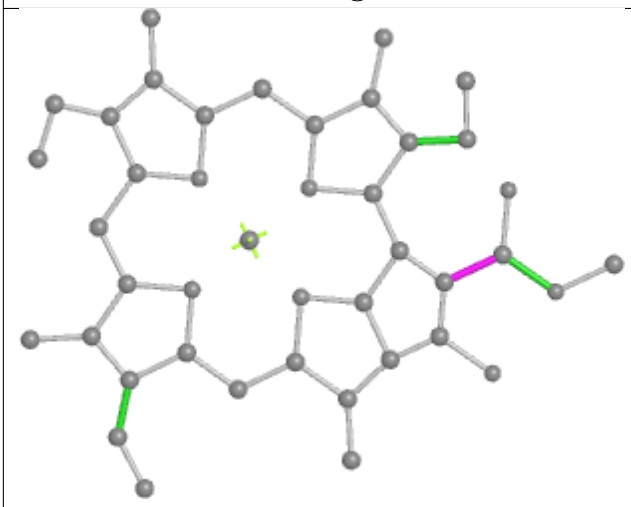
Ligand CLA Z 613



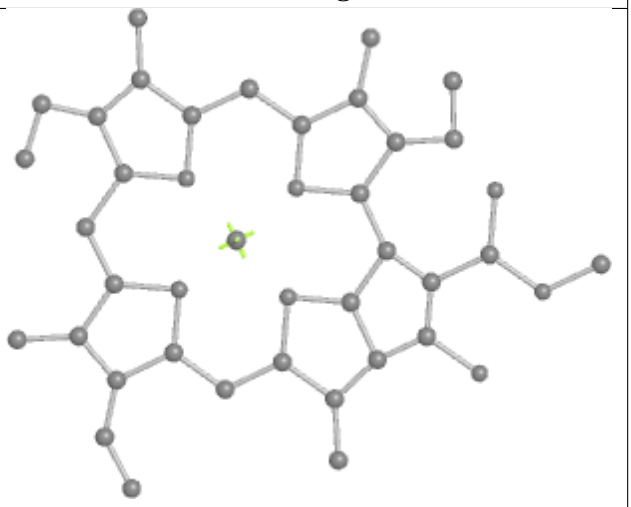
Bond lengths



Bond angles

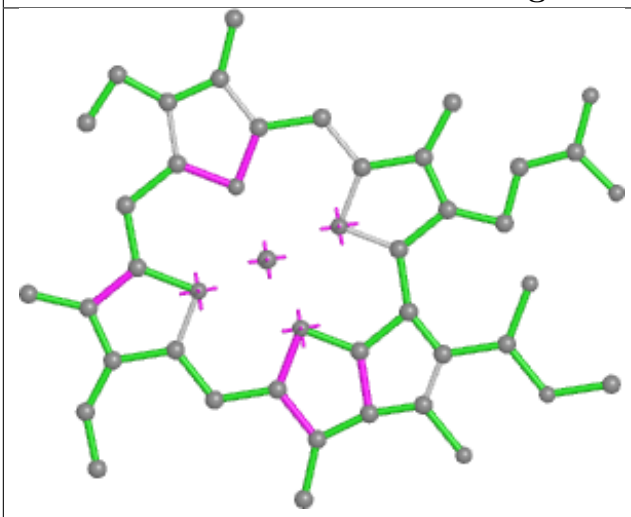


Torsions

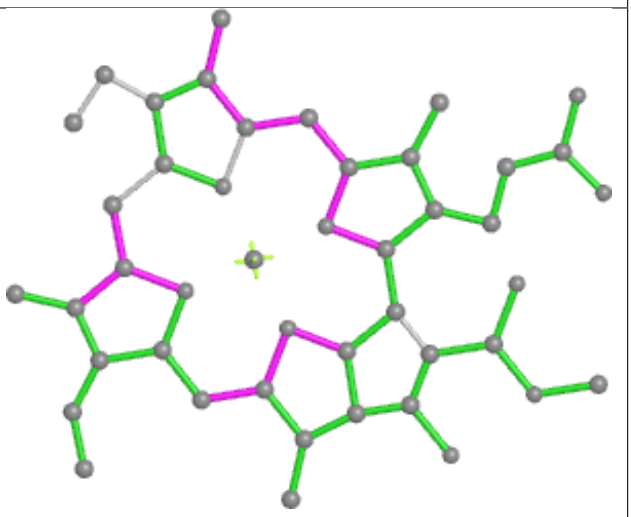


Rings

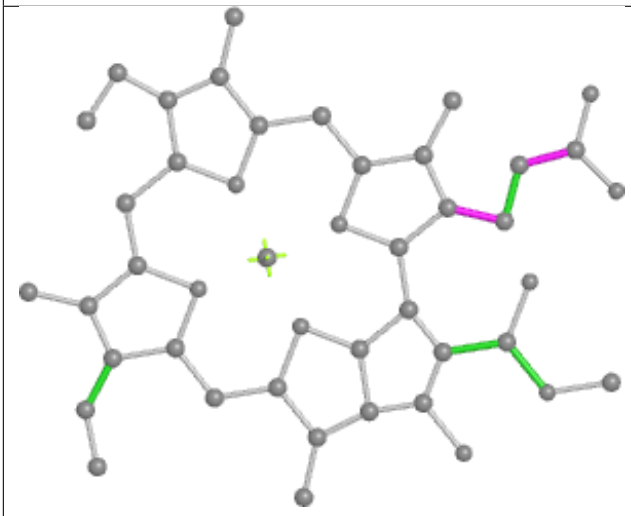
Ligand CLA 6 309



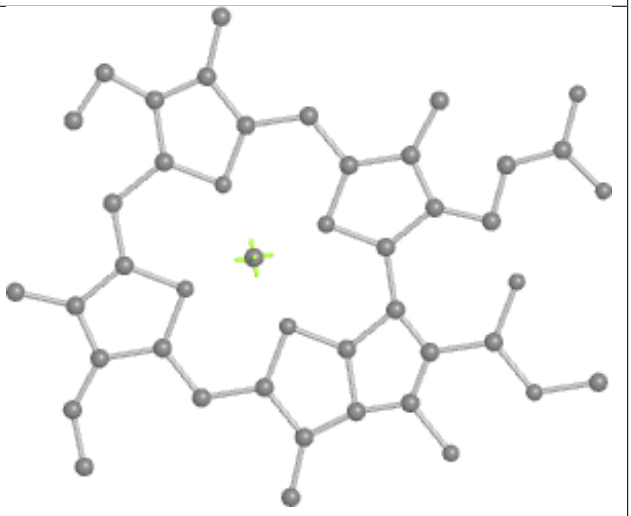
Bond lengths



Bond angles

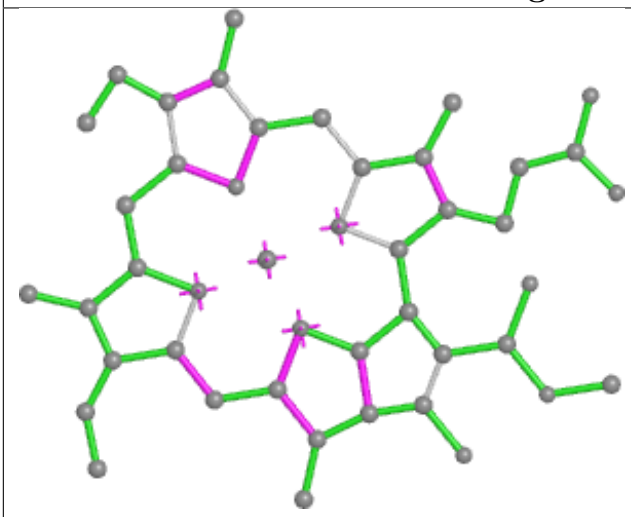


Torsions

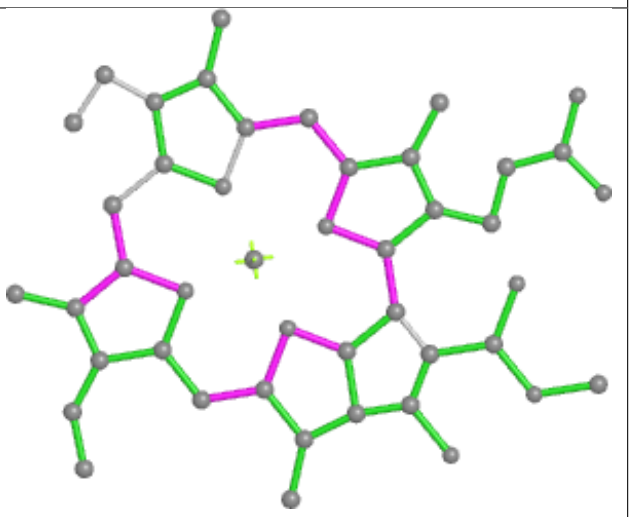


Rings

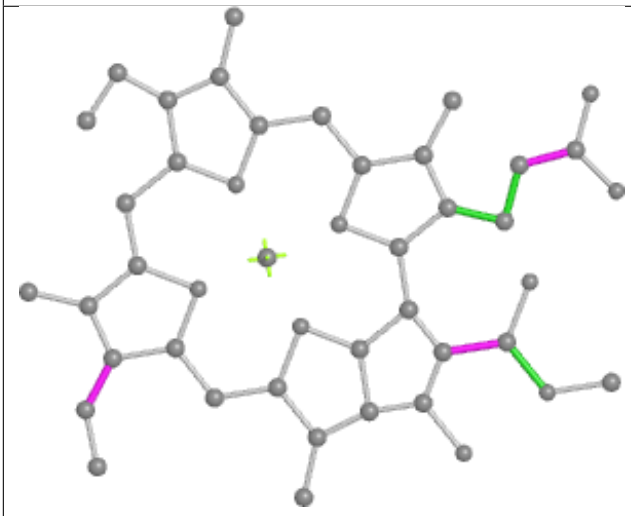
Ligand CLA 6 312



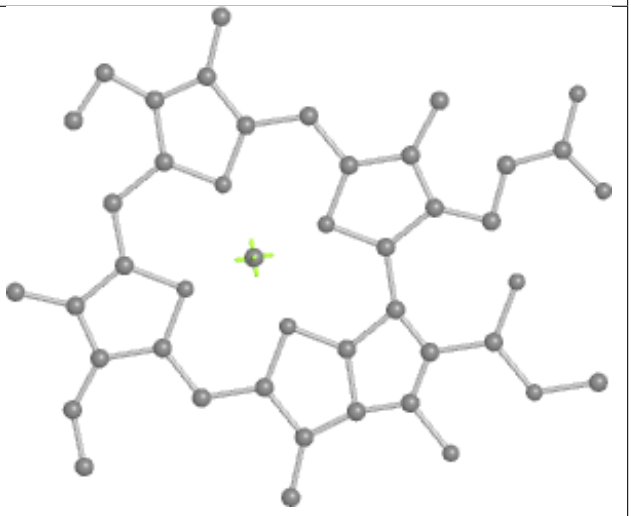
Bond lengths



Bond angles

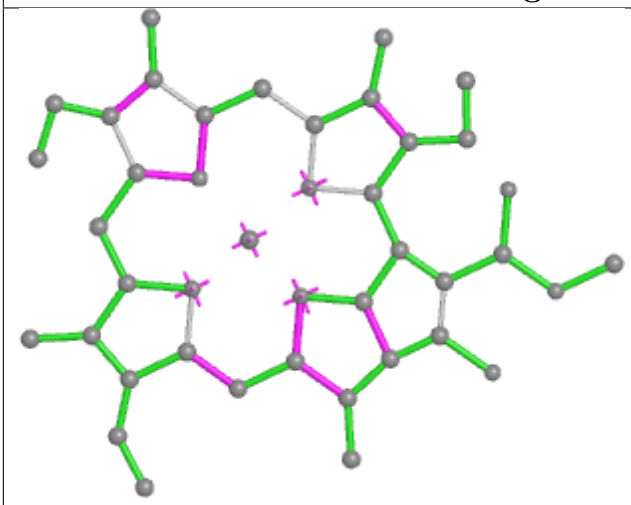


Torsions

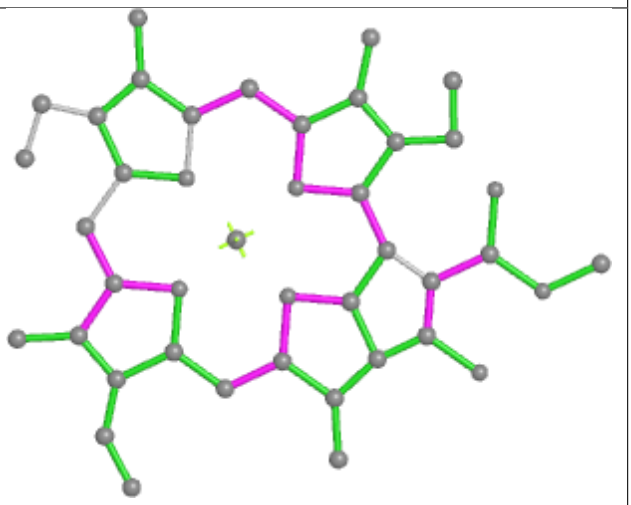


Rings

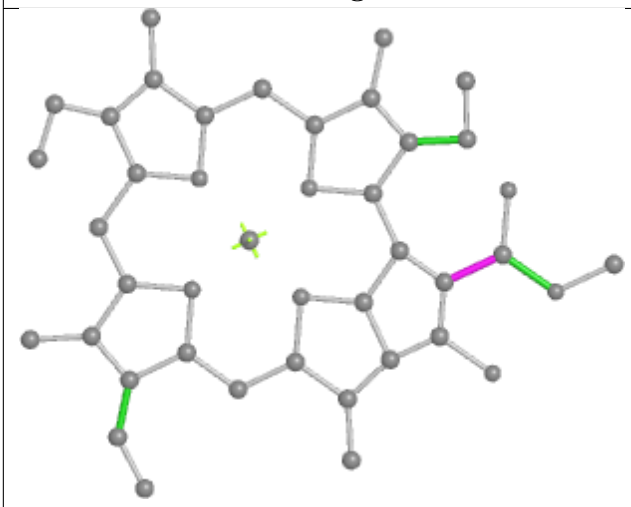
Ligand CLA A 812



Bond lengths



Bond angles



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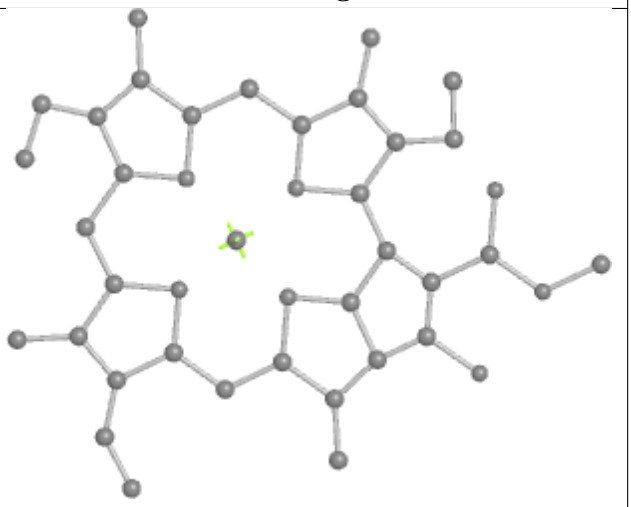
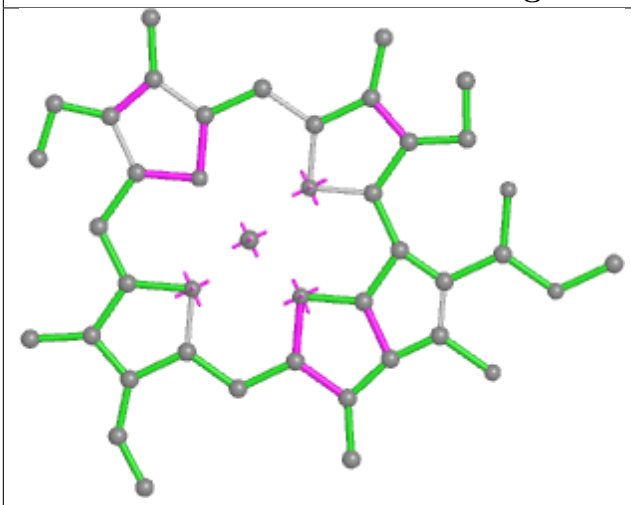


Rings

Ligand CLA A 826



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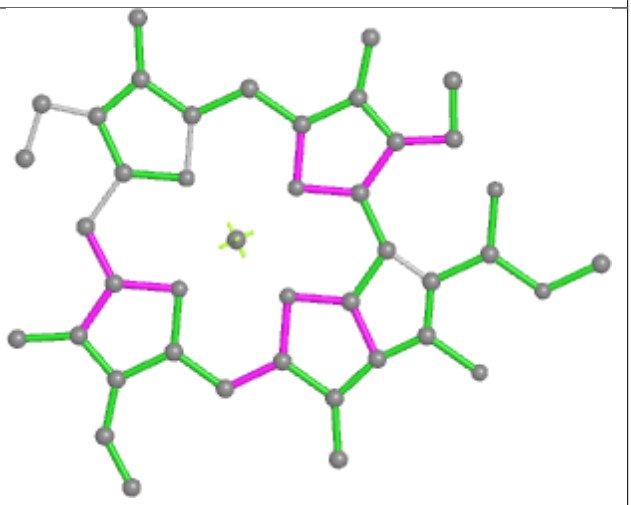
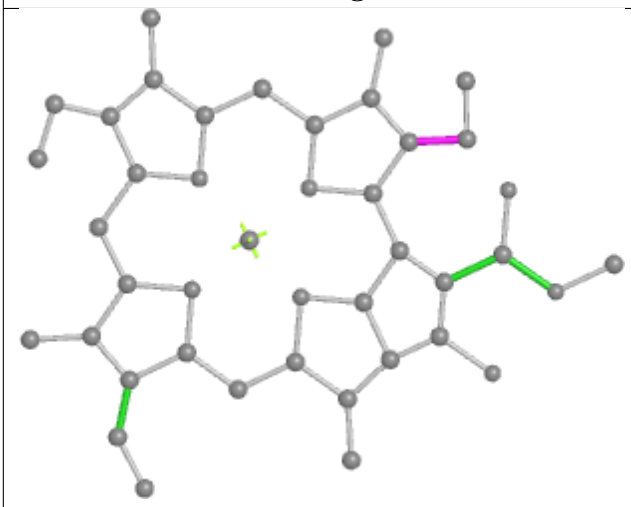
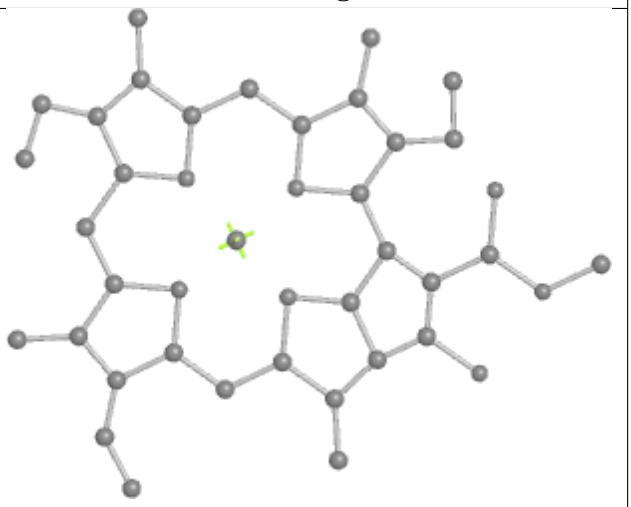


Bond angles

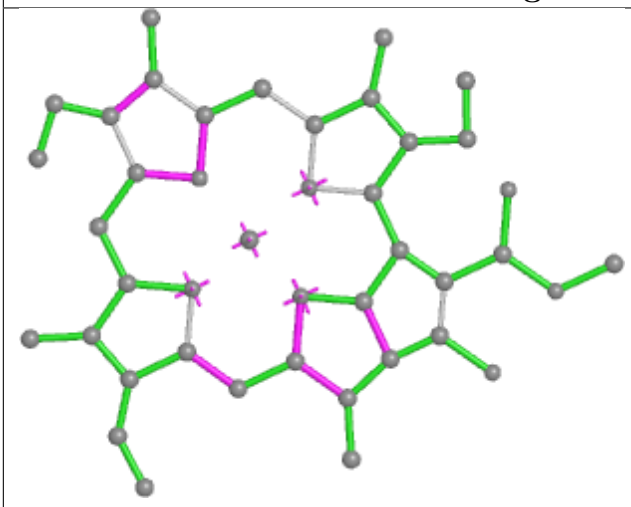


Torsions

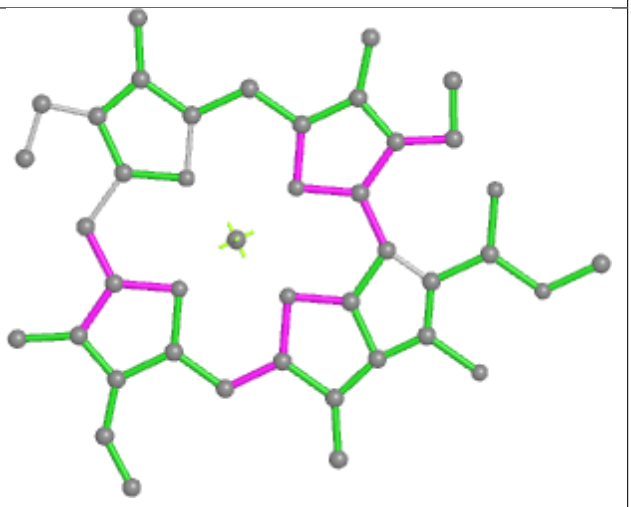


Rings

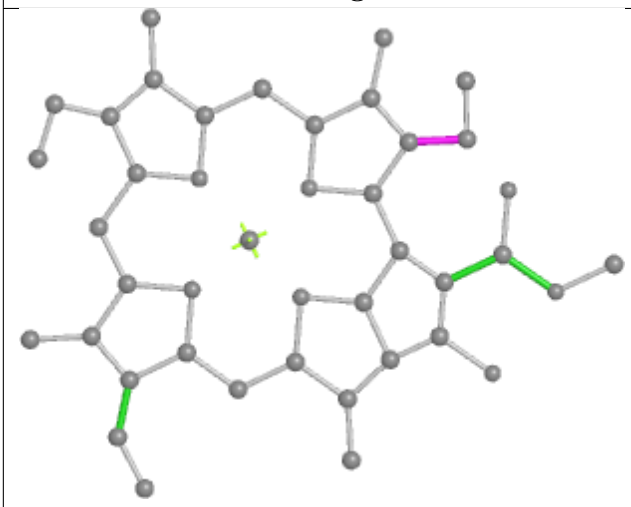
Ligand CLA A 818



Bond lengths



Bond angles



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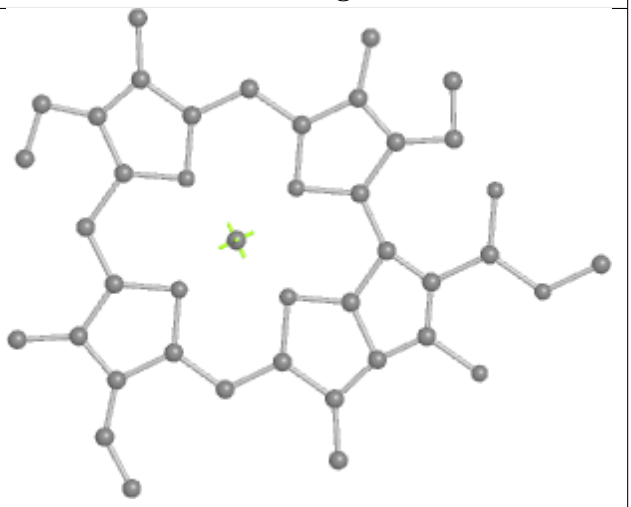
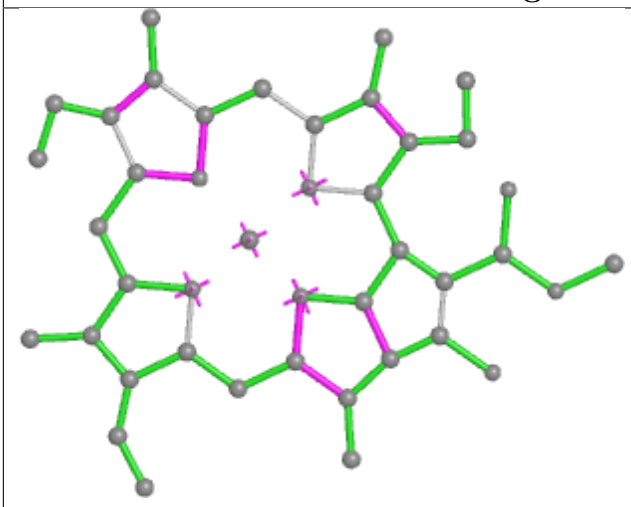


Rings

Ligand CLA A 806



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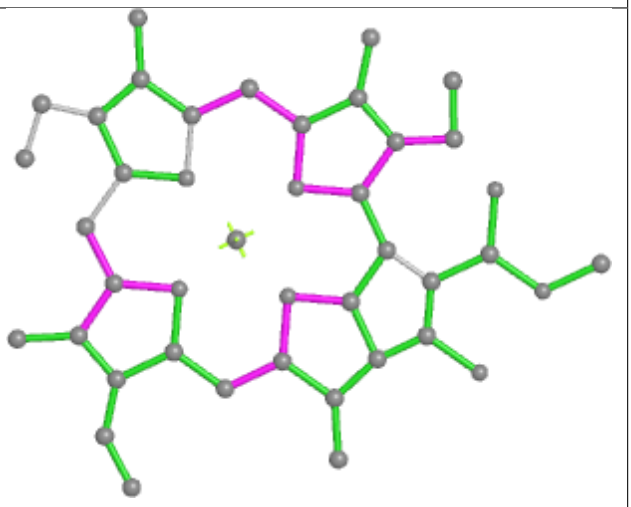
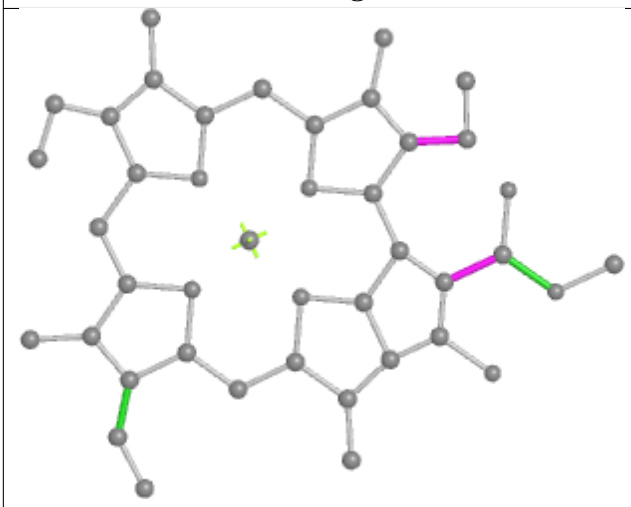


Bond angles



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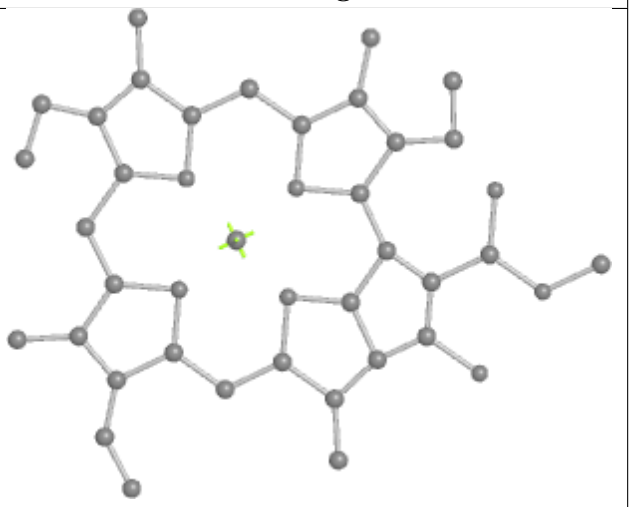
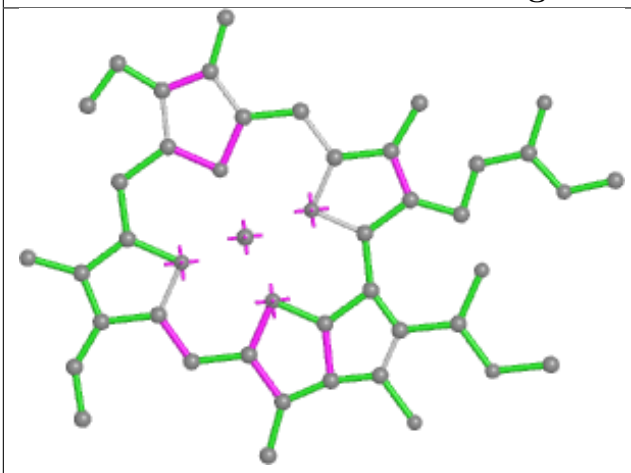


Rings

Ligand CLA 8 612



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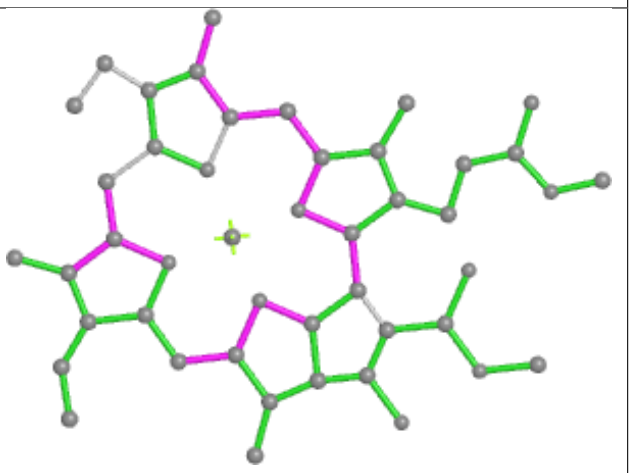
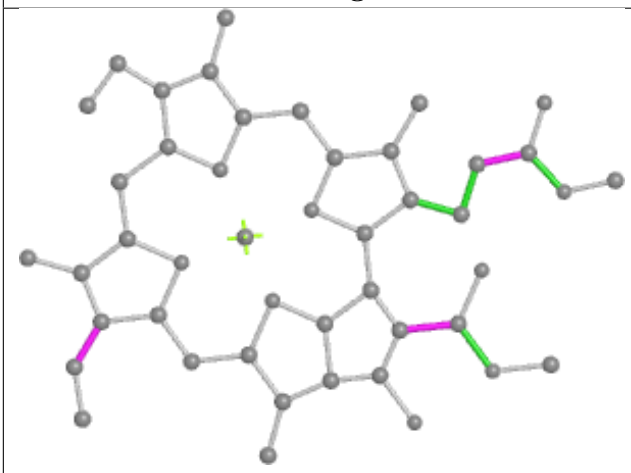
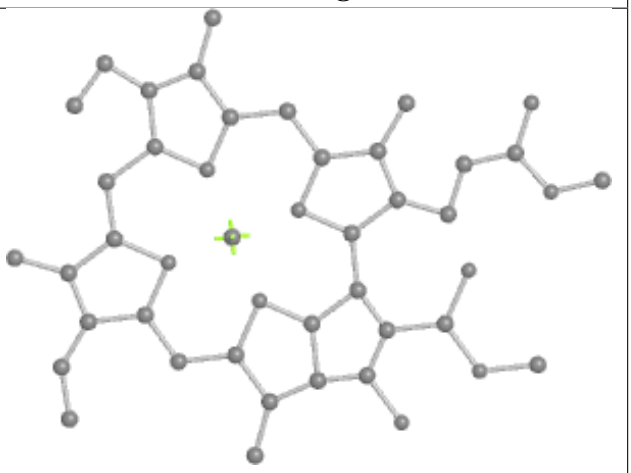


Bond angles

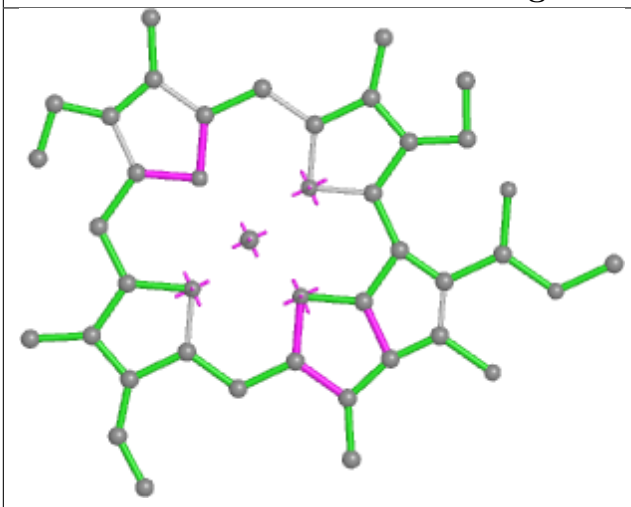


Torsions



Rings

Ligand CLA 4 601



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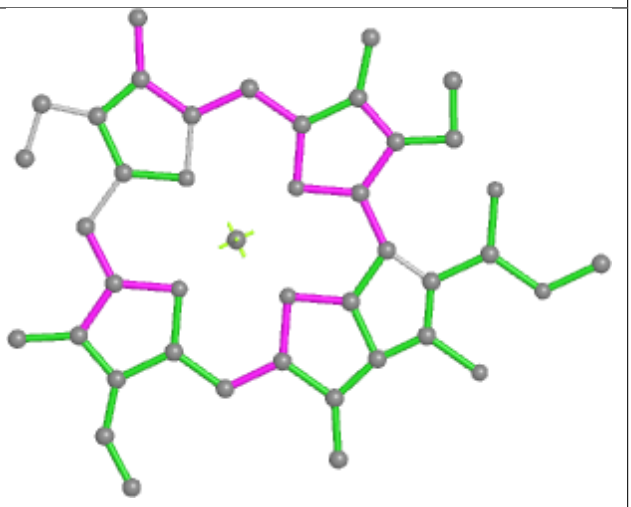
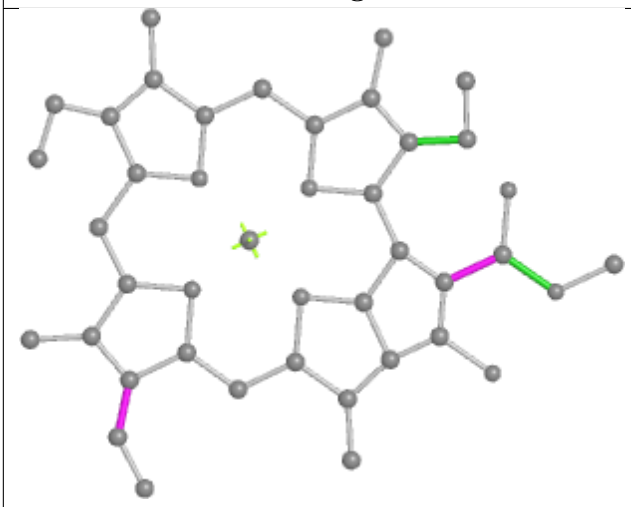


Bond angles



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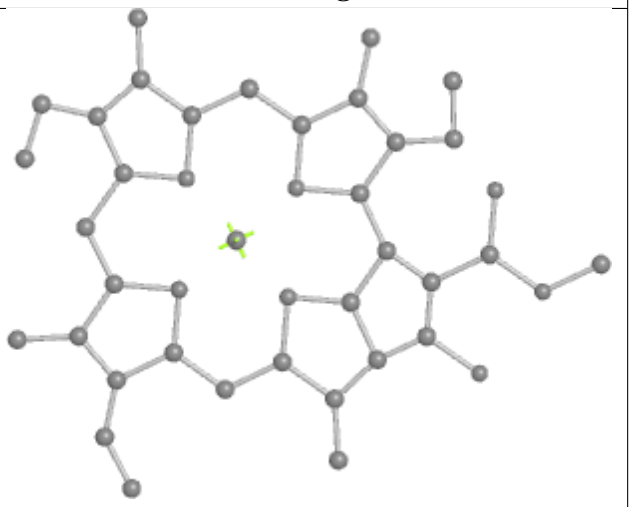
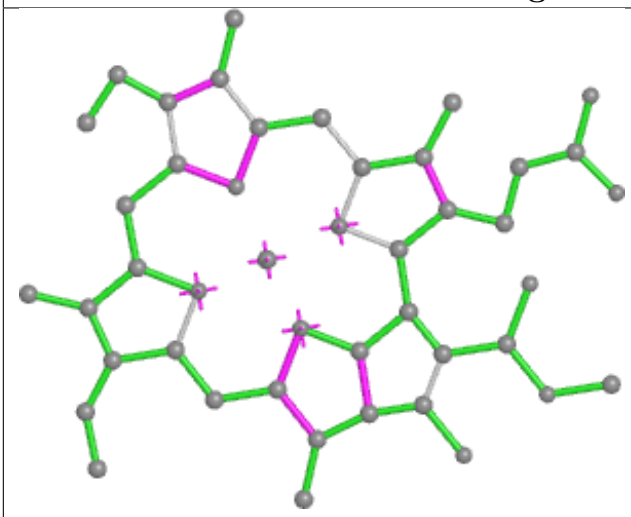
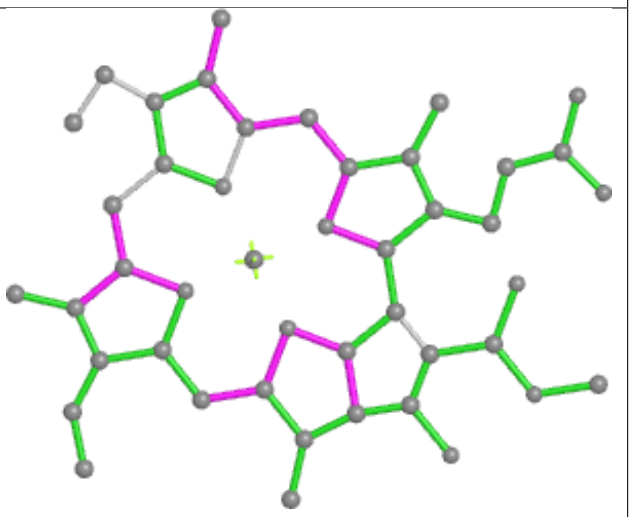


Rings

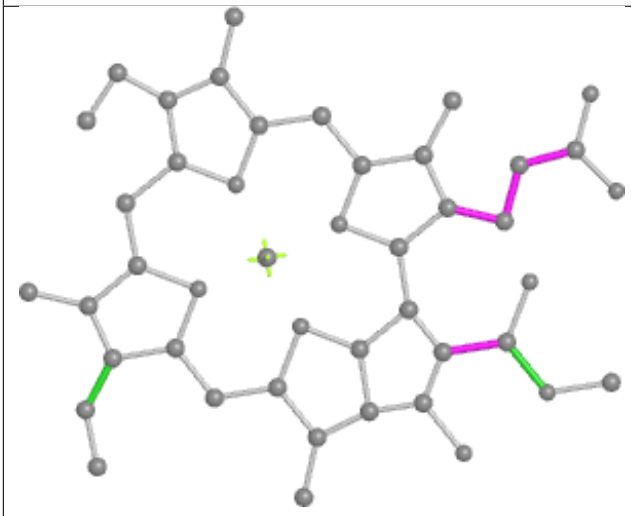
Ligand CLA 6 311



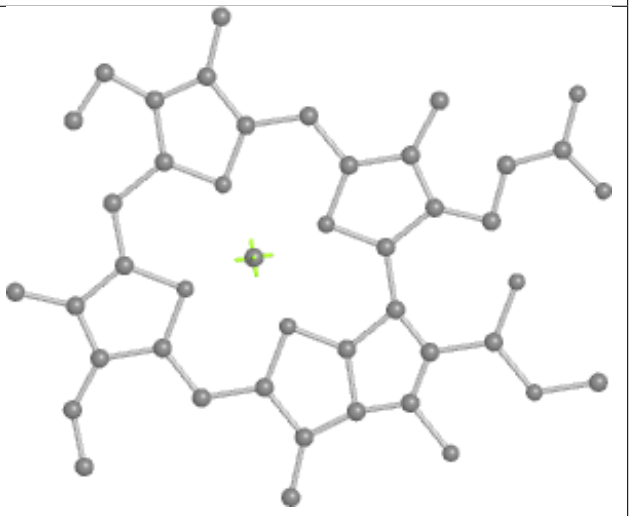
Bond lengths



Bond angles

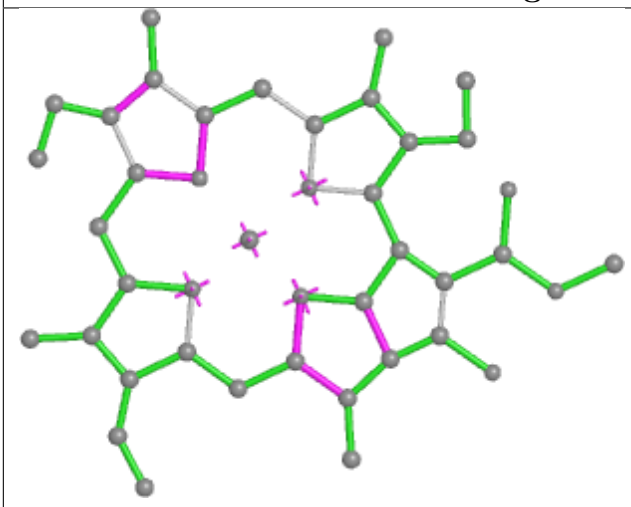


Torsions

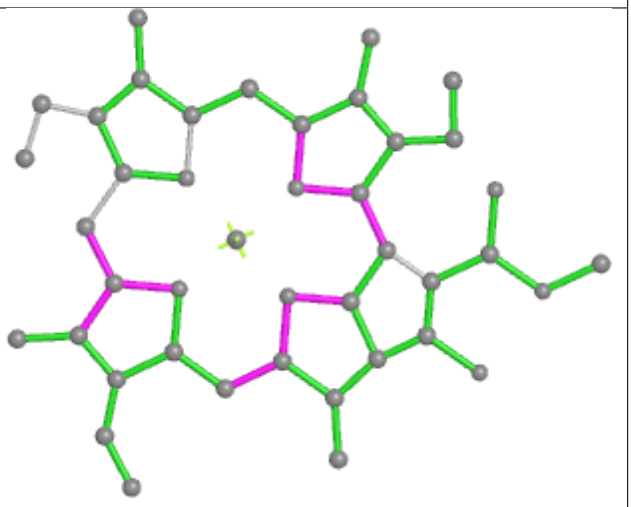


Rings

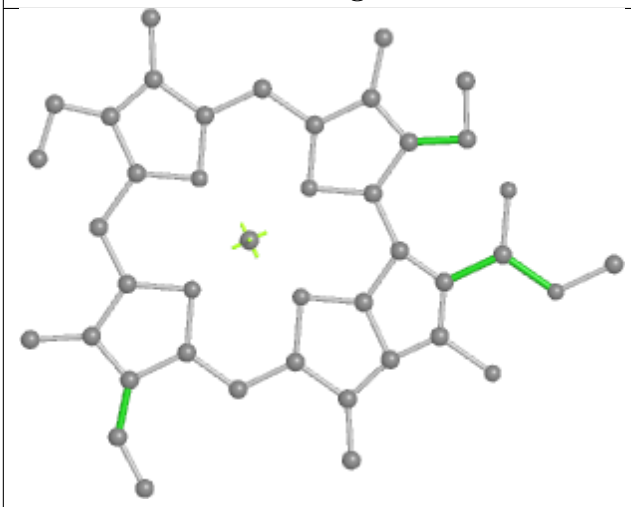
Ligand CLA A 815



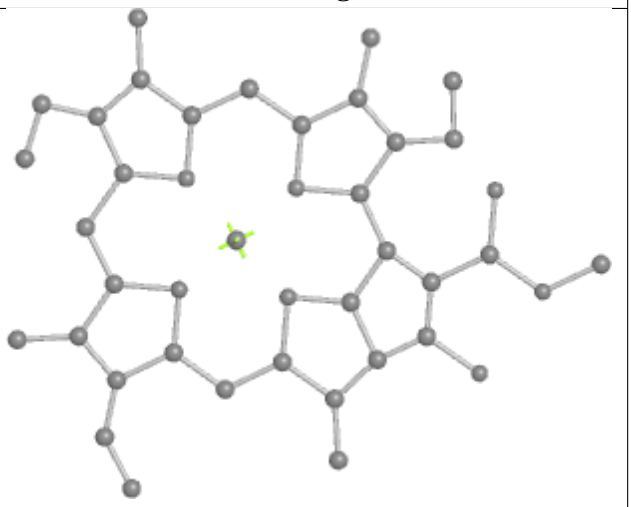
Bond lengths



Bond angles

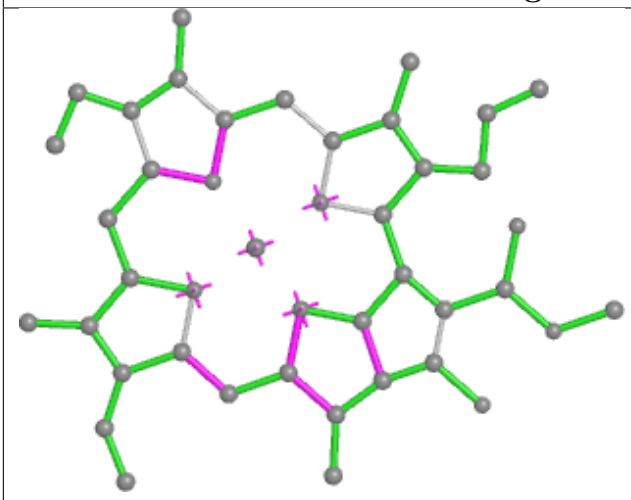


Torsions



Rings

Ligand CLA B 838



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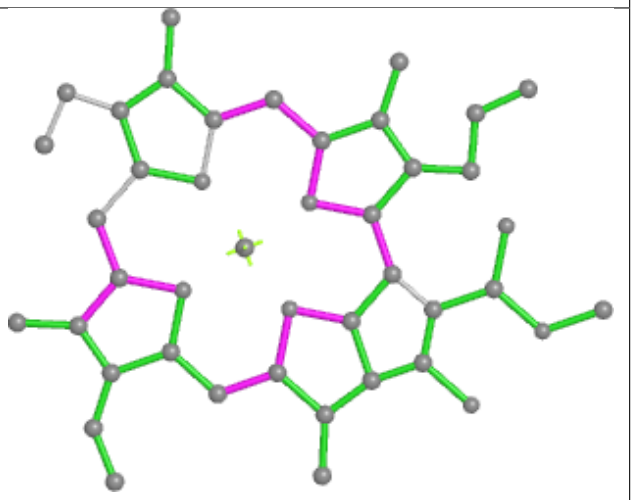
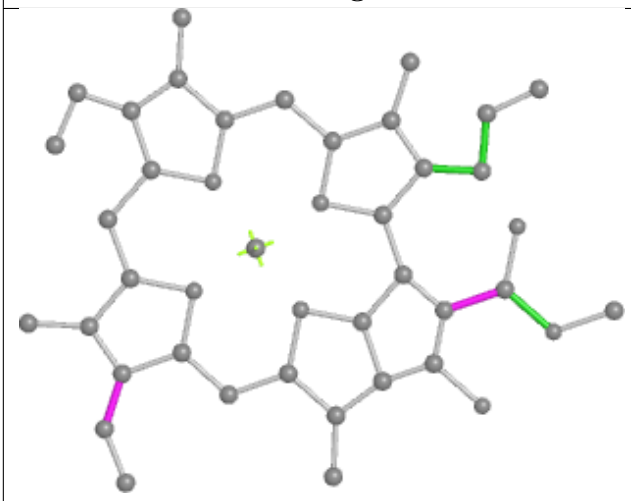
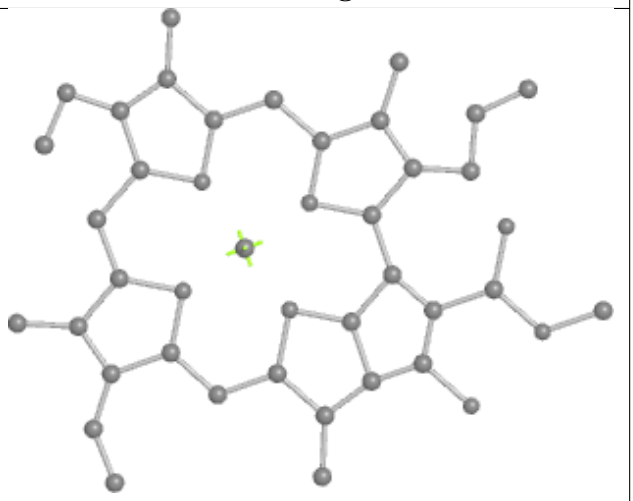


Bond angles

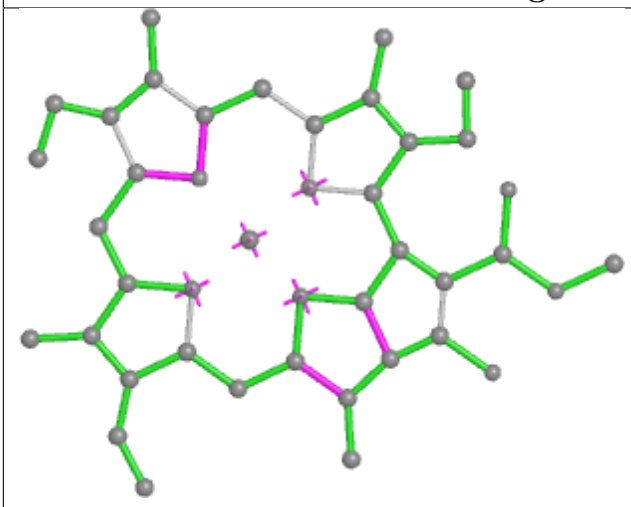


Torsions

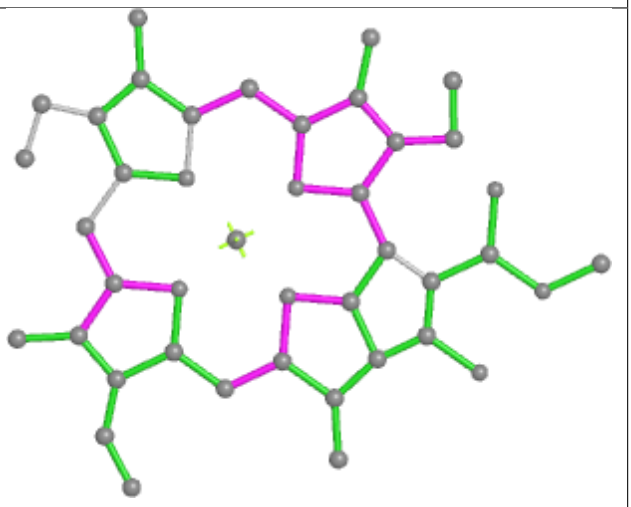


Rings

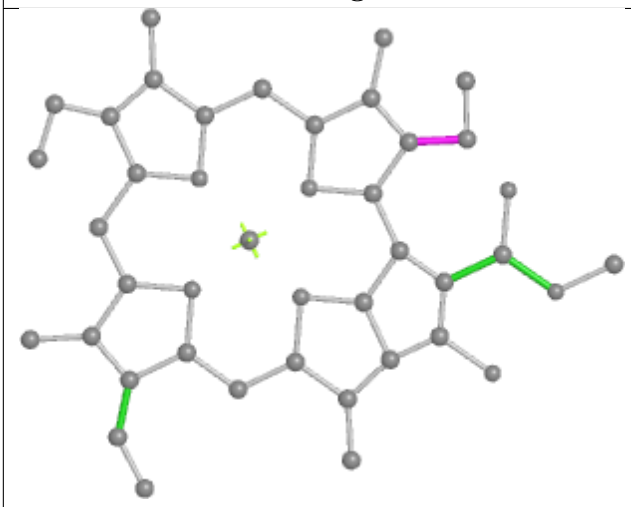
Ligand CLA 4 608



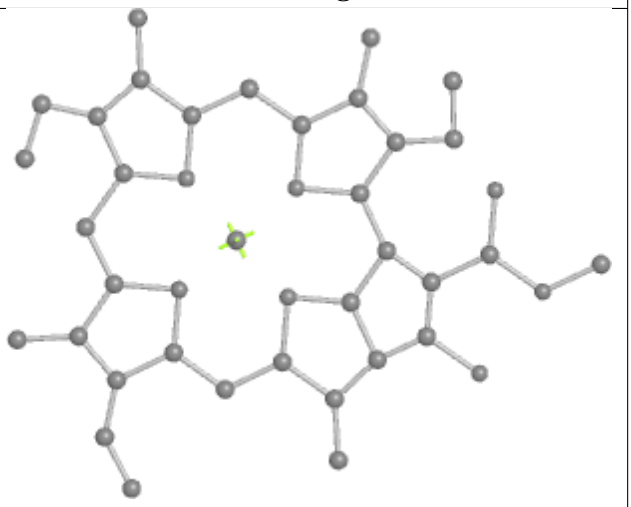
Bond lengths



Bond angles

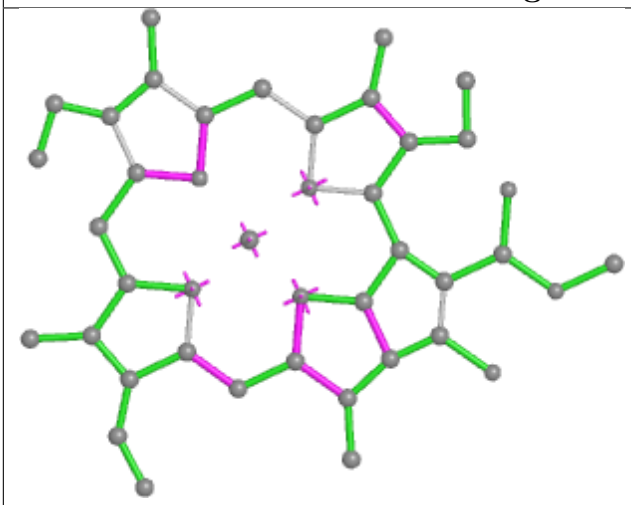


Torsions

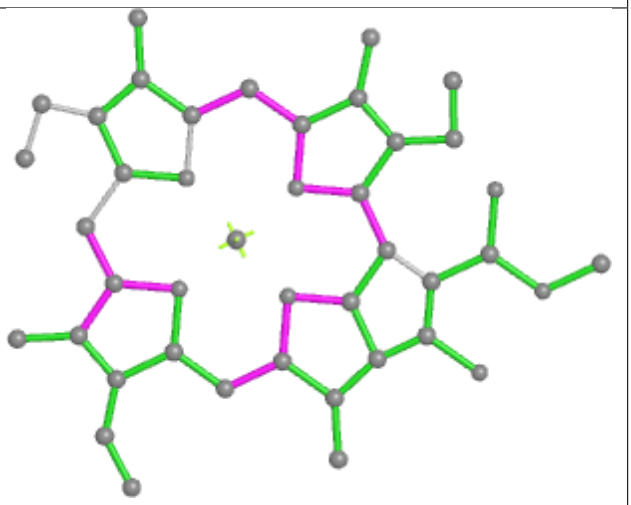


Rings

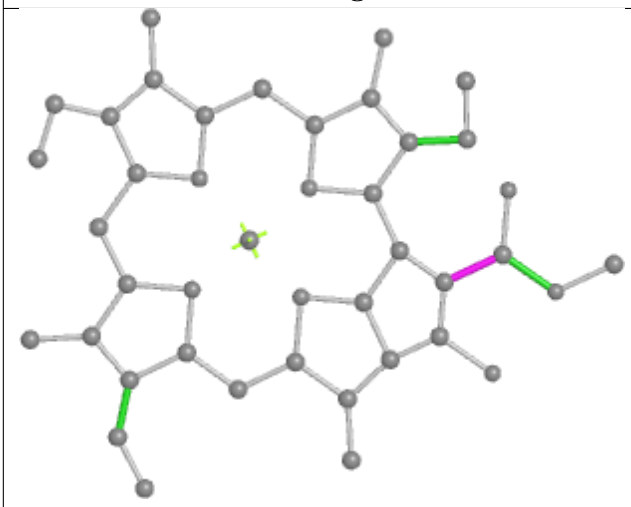
Ligand CLA A 821



Bond lengths



Bond angles



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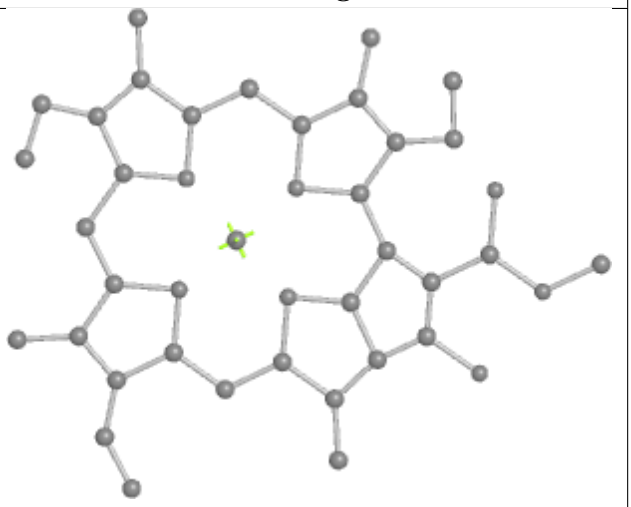
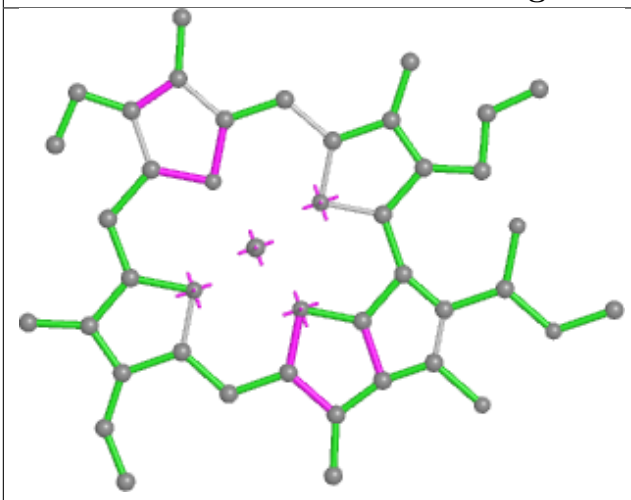
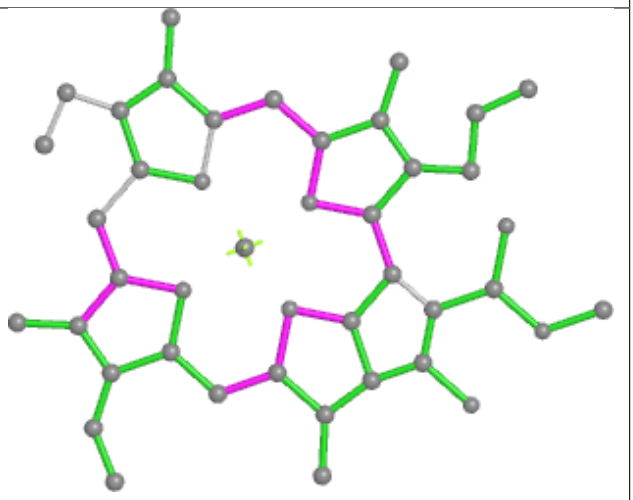


Rings

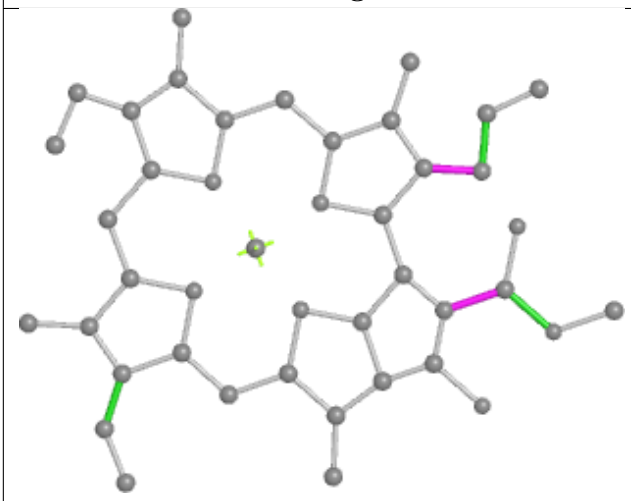
Ligand CLA 7 613



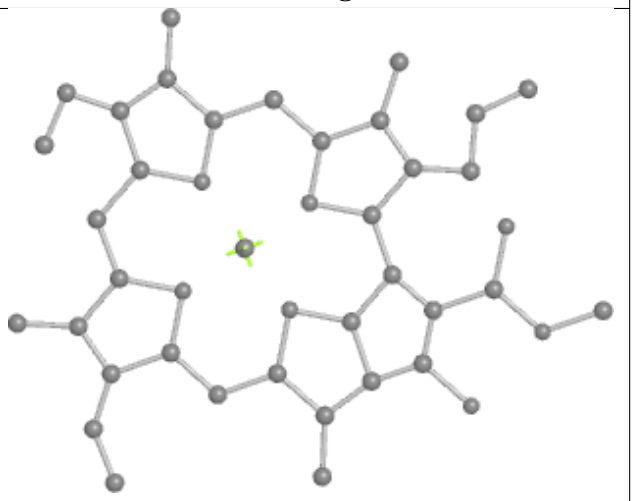
Bond lengths



Bond angles

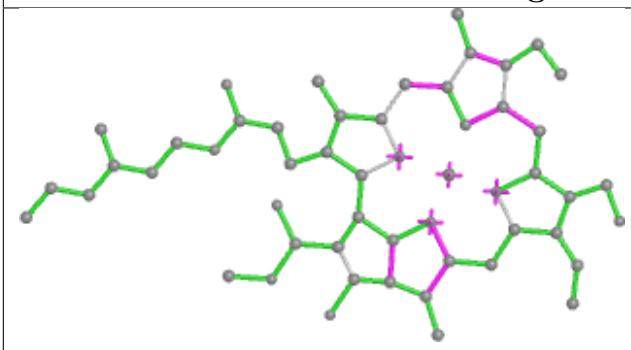


Torsions

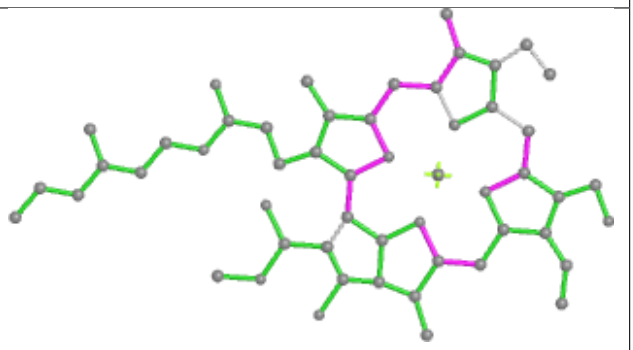


Rings

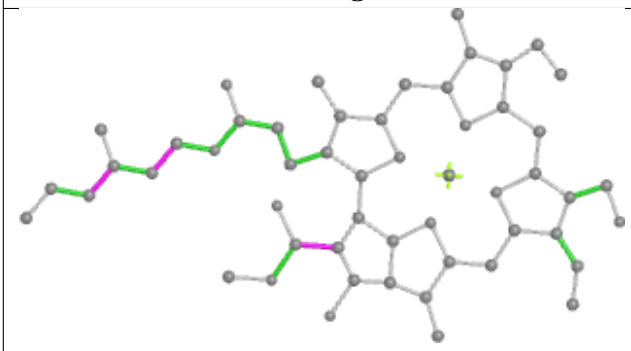
Ligand CHL 1 601



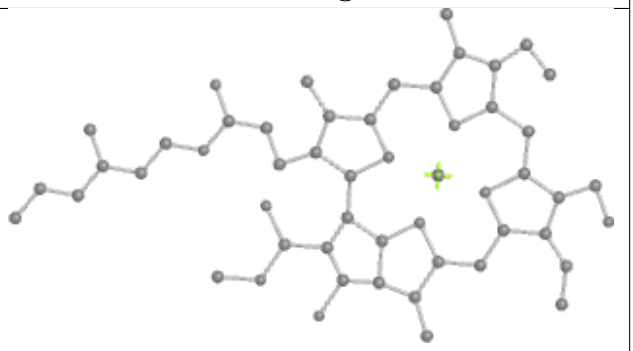
Bond lengths



Bond angles

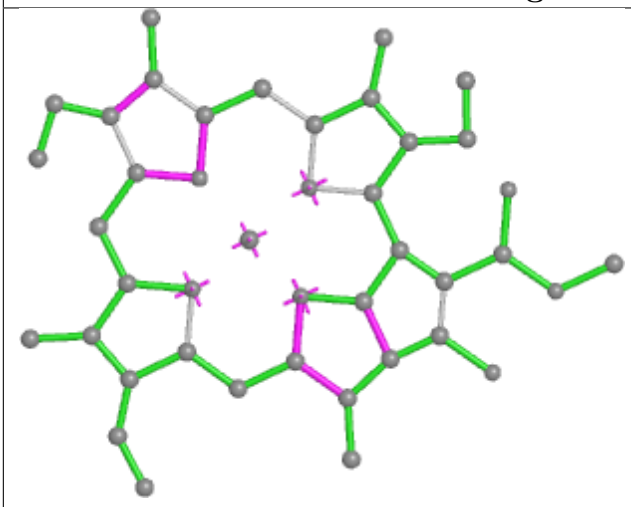


Torsions

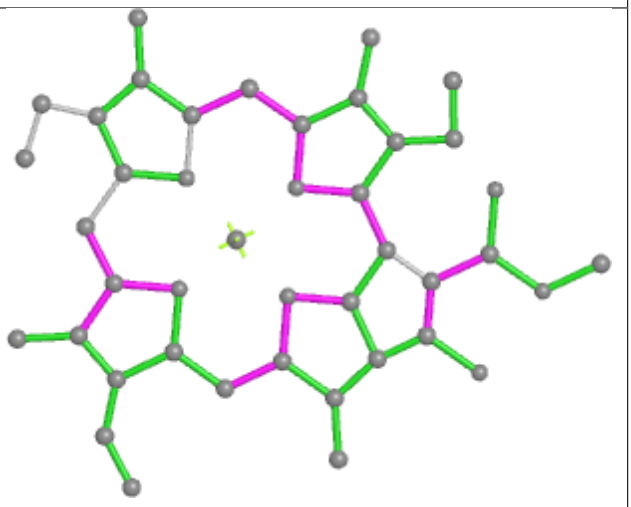


Rings

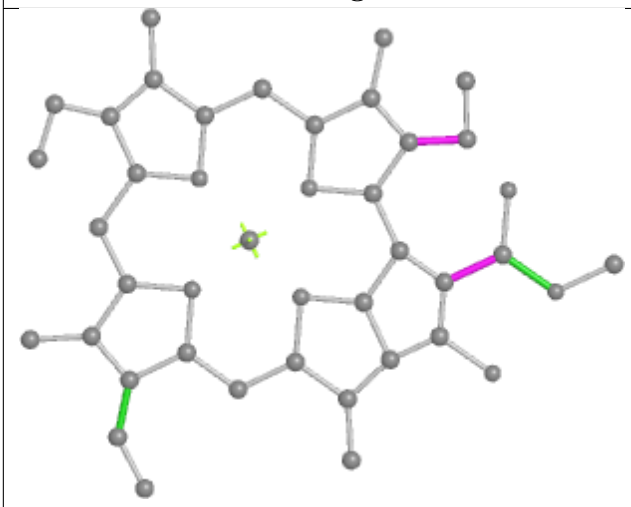
Ligand CLA Z 612



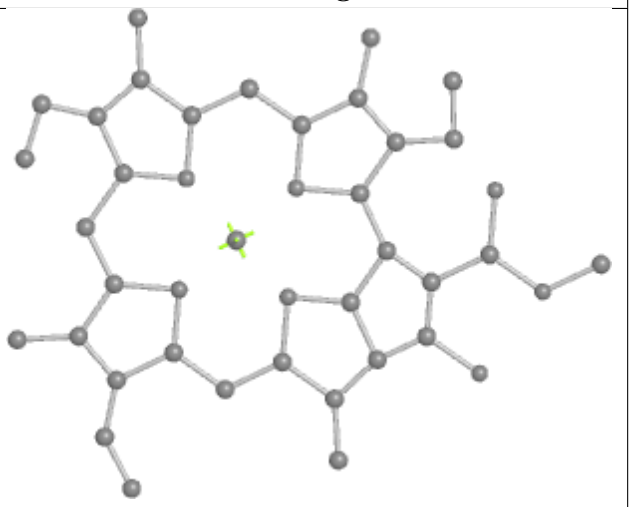
Bond lengths



Bond angles

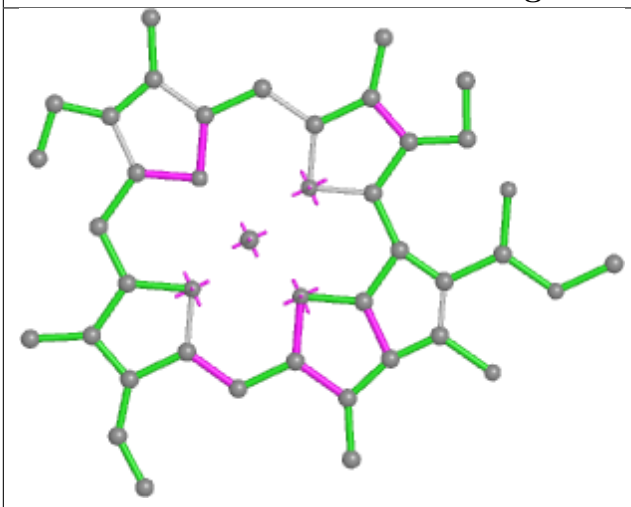


Torsions

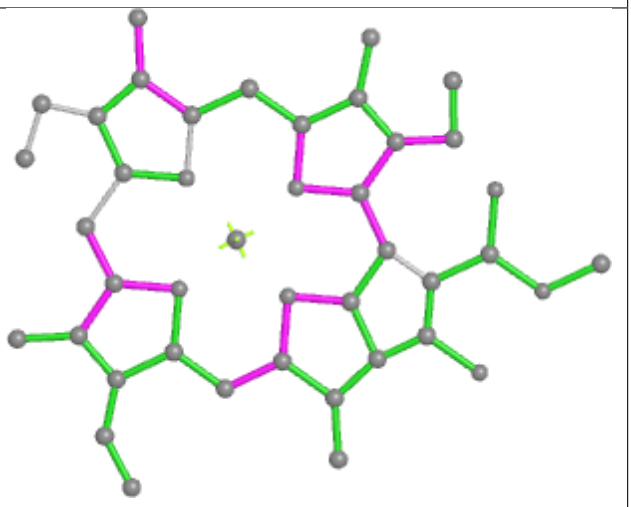


Rings

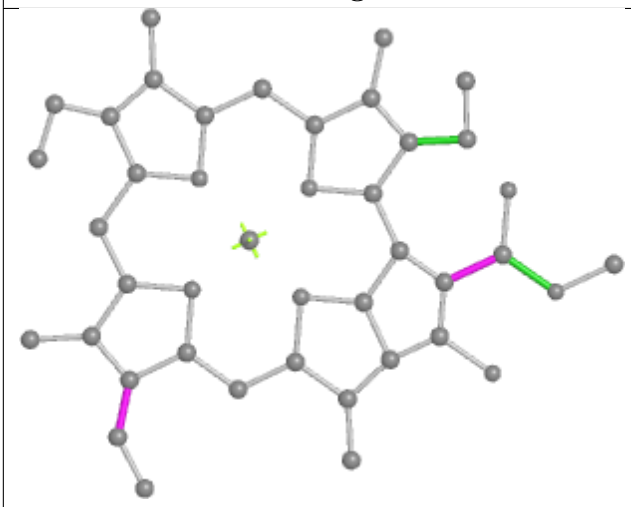
Ligand CLA B 831



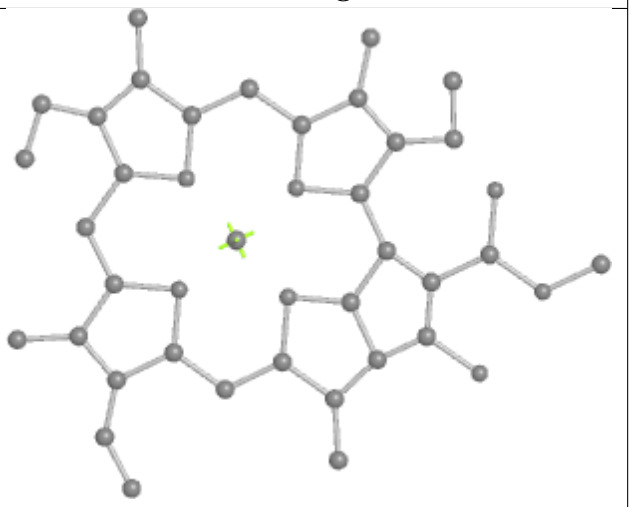
Bond lengths



Bond angles

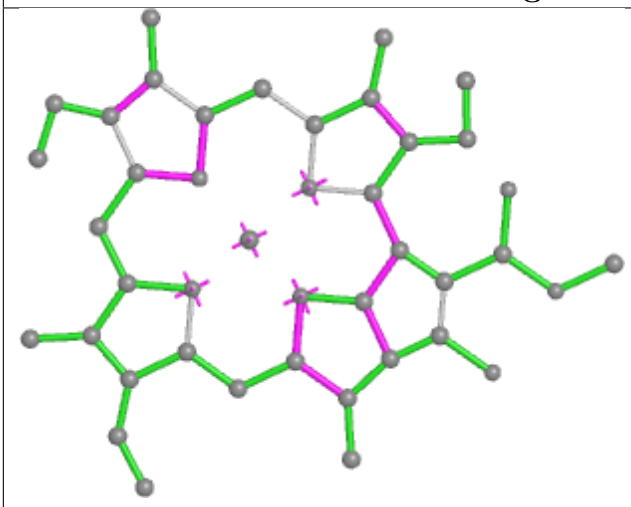


Torsions

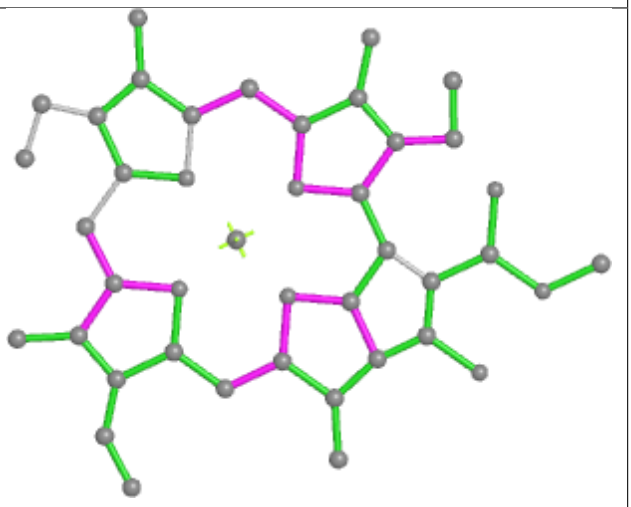


Rings

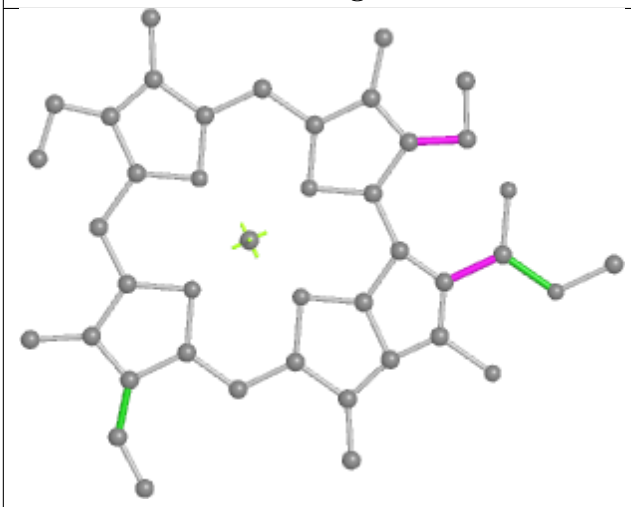
Ligand CLA A 803



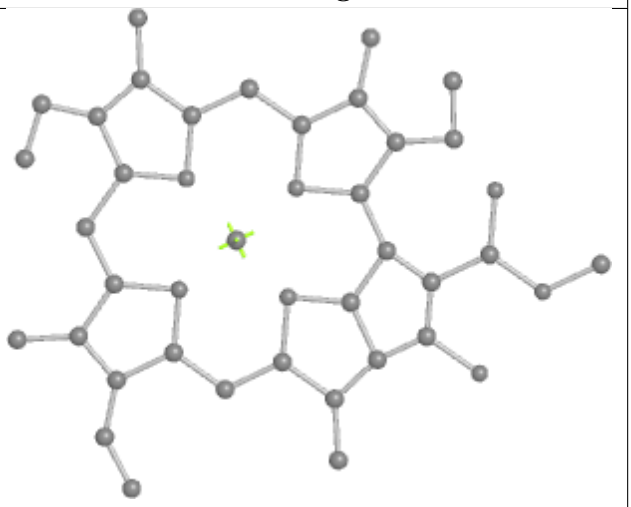
Bond lengths



Bond angles

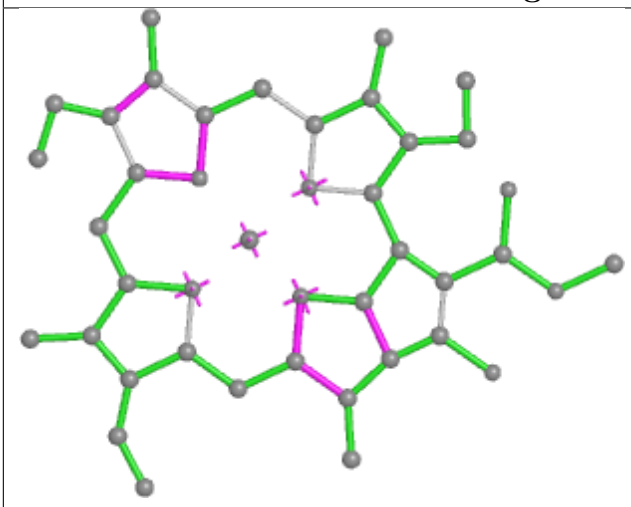


Torsions

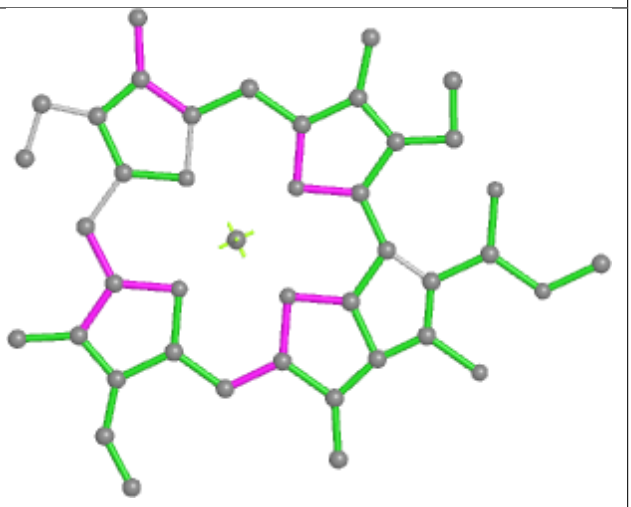


Rings

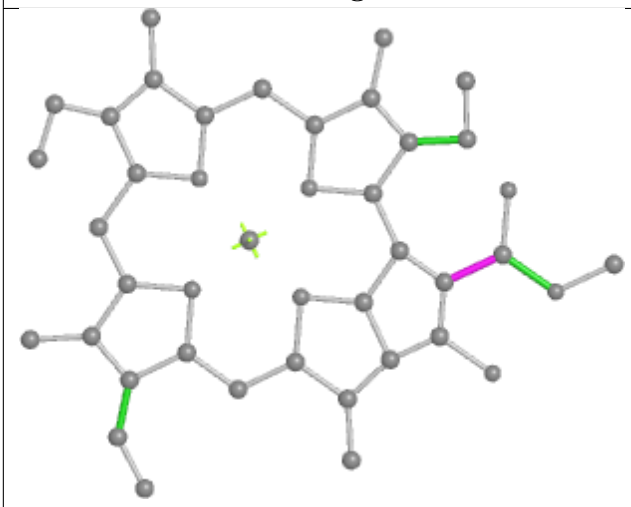
Ligand CLA A 814



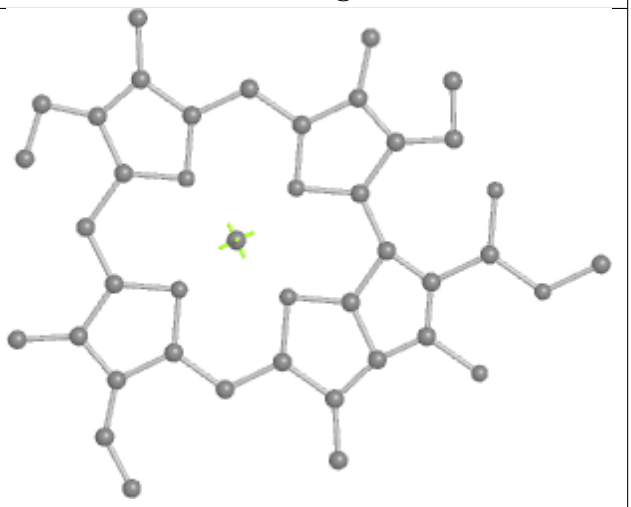
Bond lengths



Bond angles

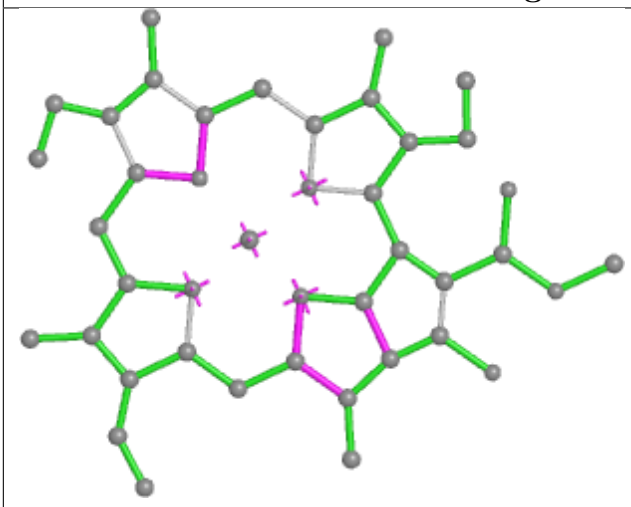


Torsions

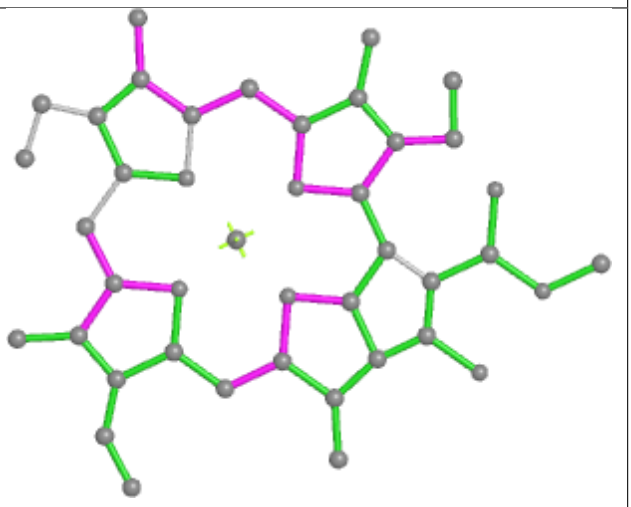


Rings

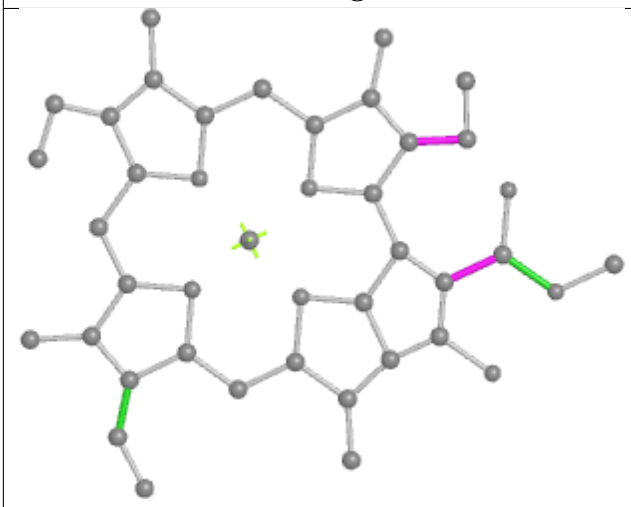
Ligand CLA B 817



Bond lengths



Bond angles



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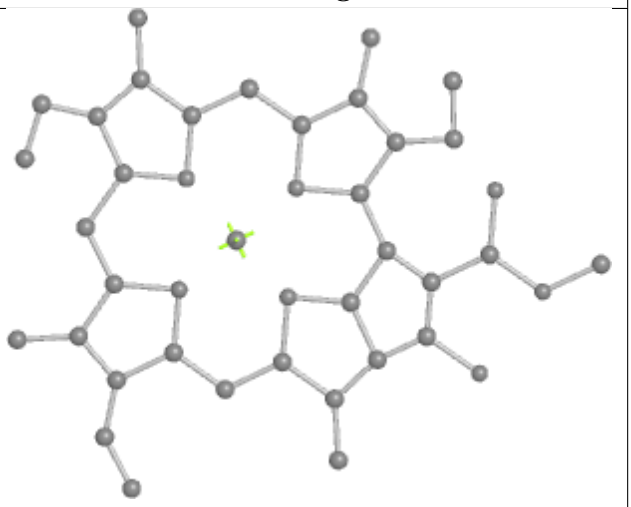
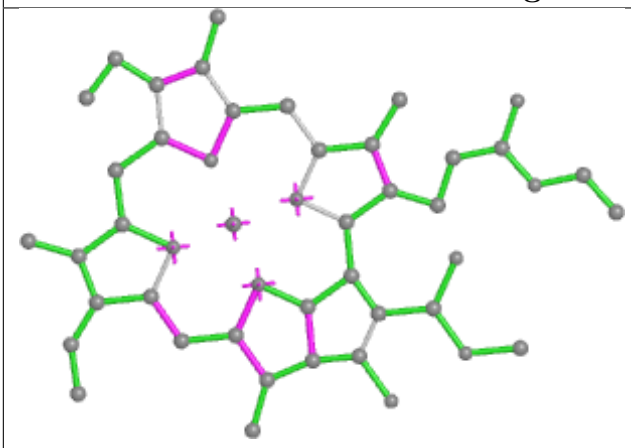


Rings

Ligand CLA A 817



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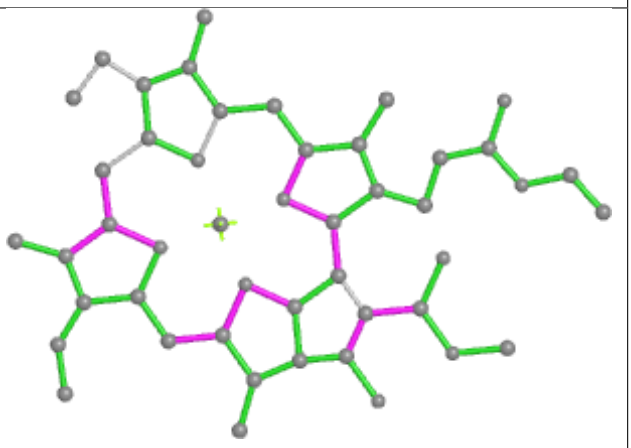
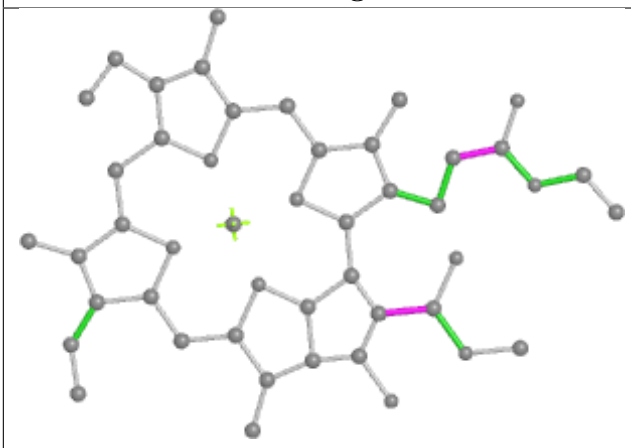
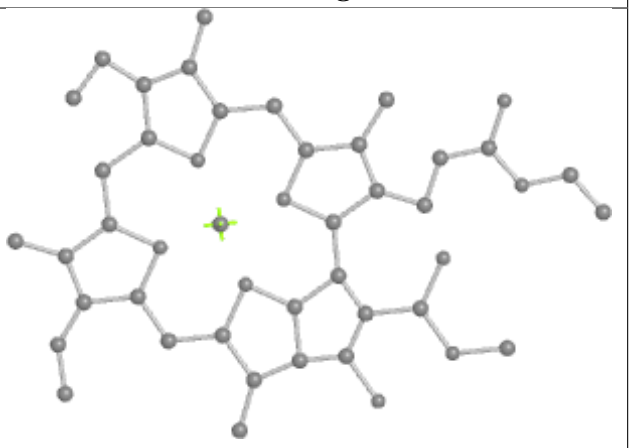


Bond angles

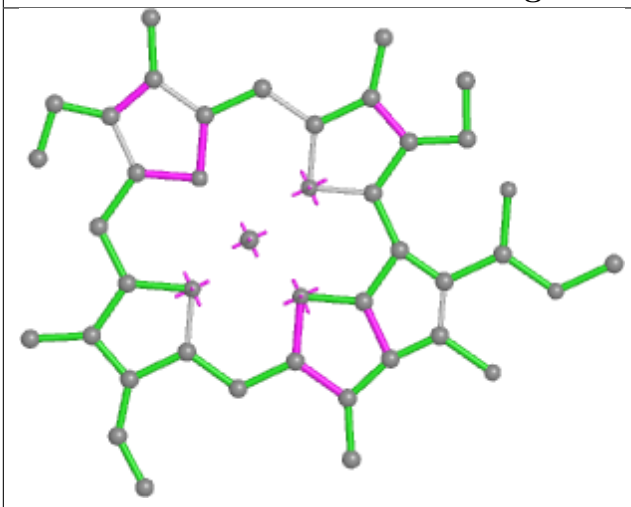


Torsions

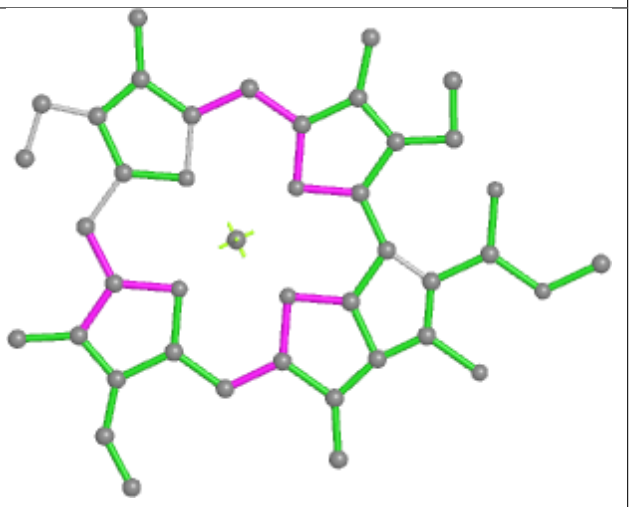


Rings

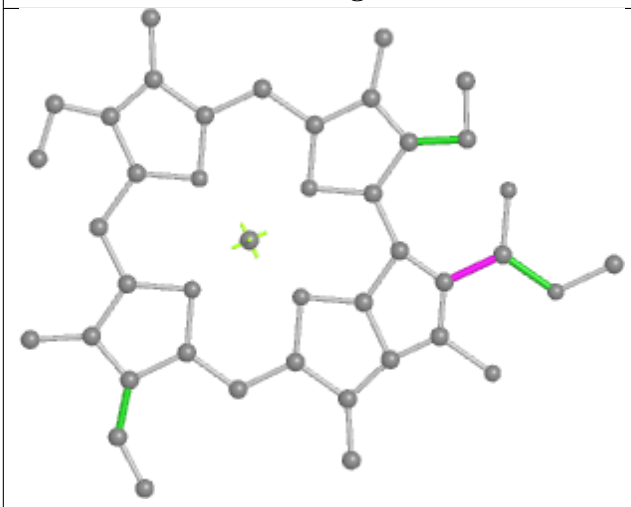
Ligand CLA B 828



Bond lengths



Bond angles



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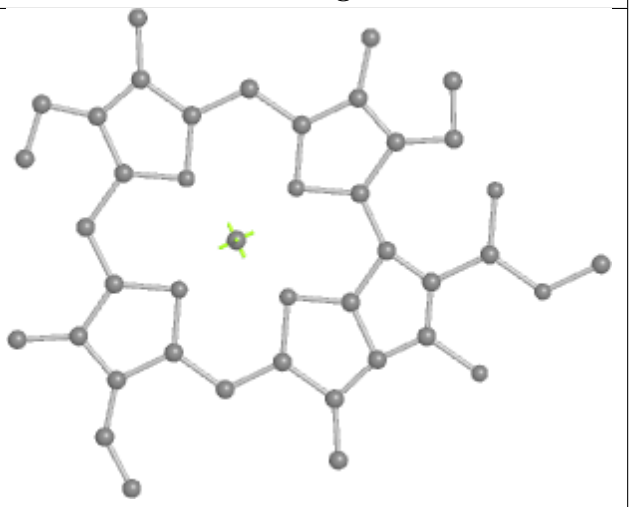
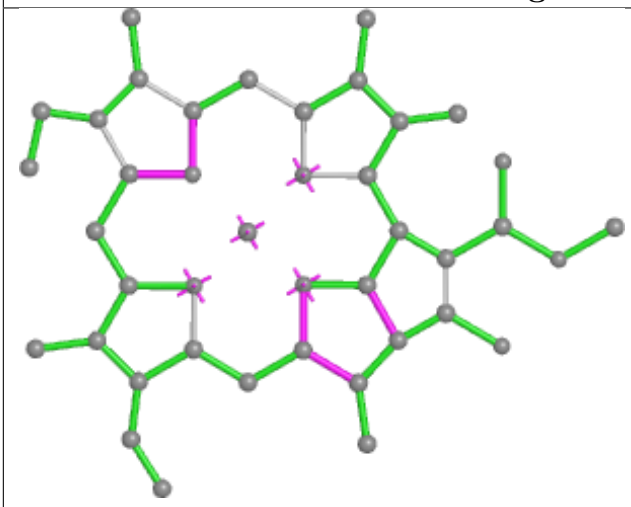
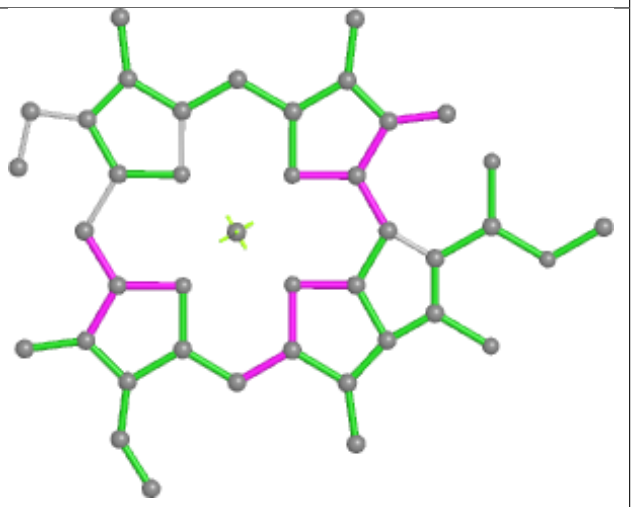


Rings

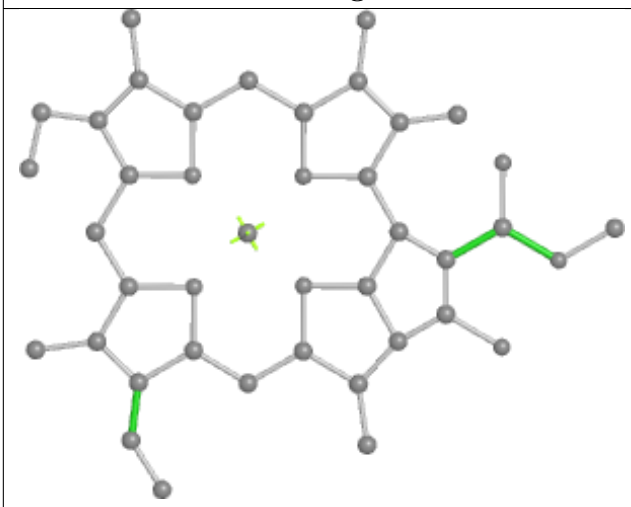
Ligand CLA 4 612



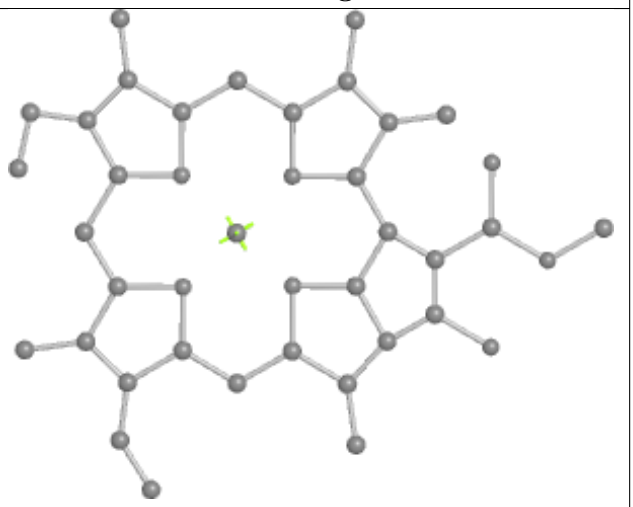
Bond lengths



Bond angles

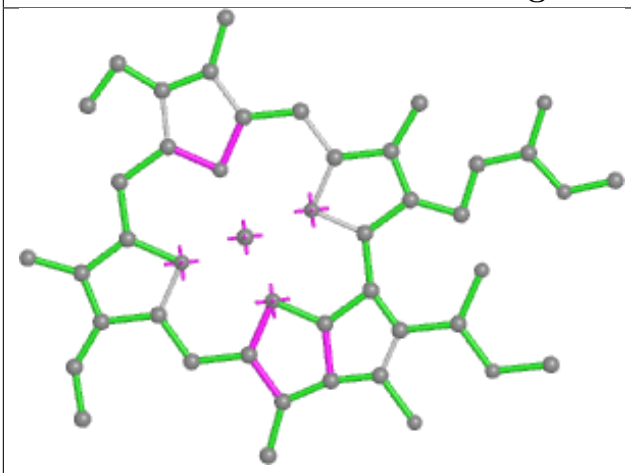


Torsions

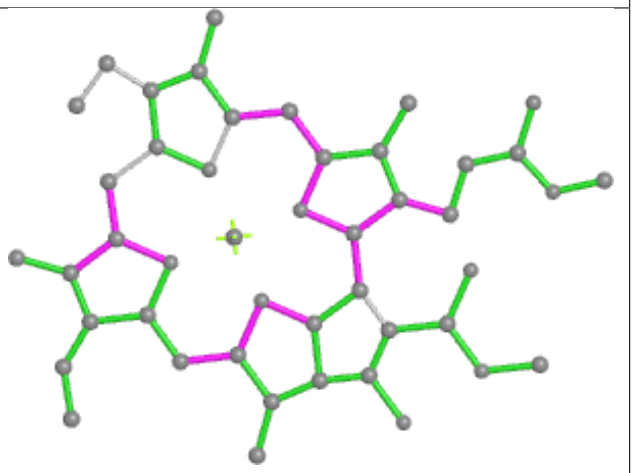


Rings

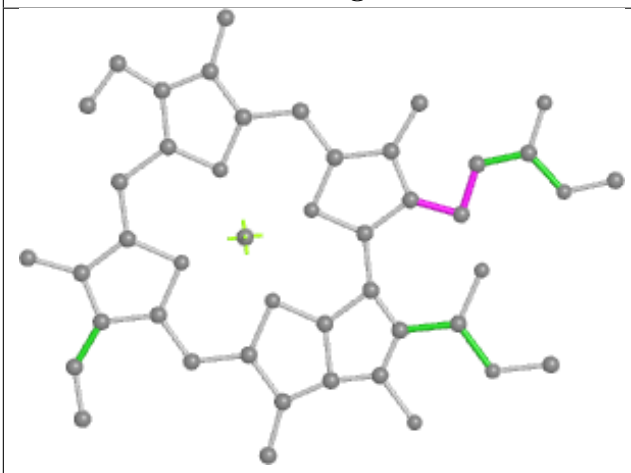
Ligand CLA 3 313



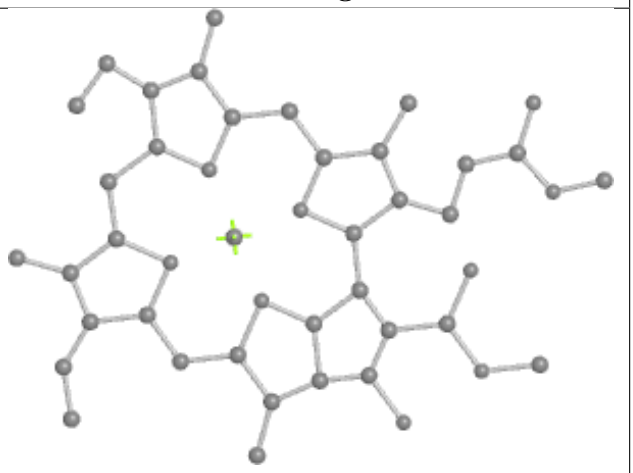
Bond lengths



Bond angles

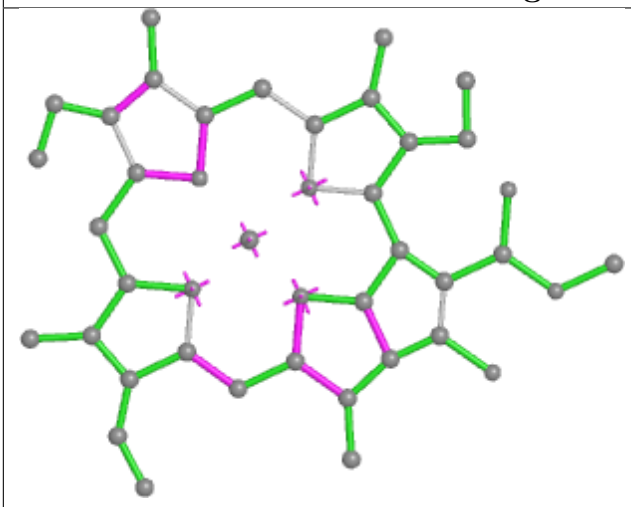


Torsions

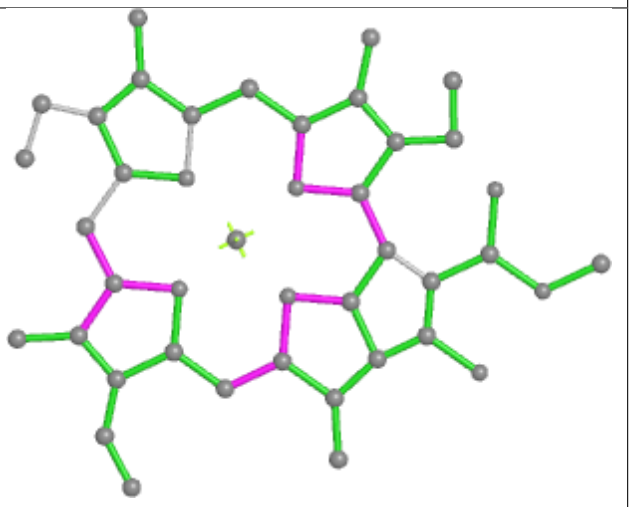


Rings

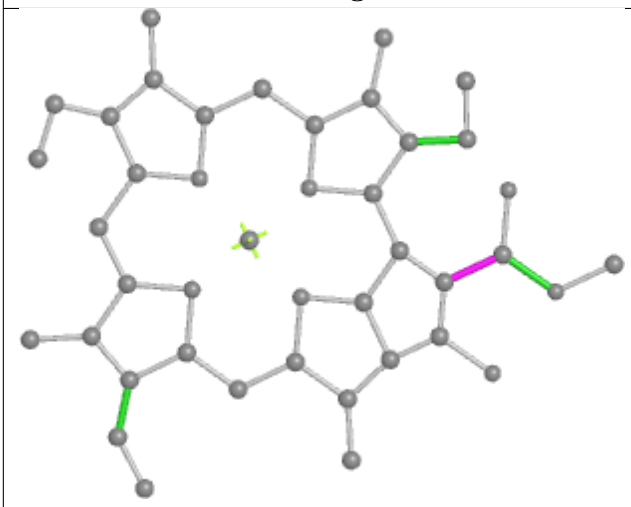
Ligand CLA A 816



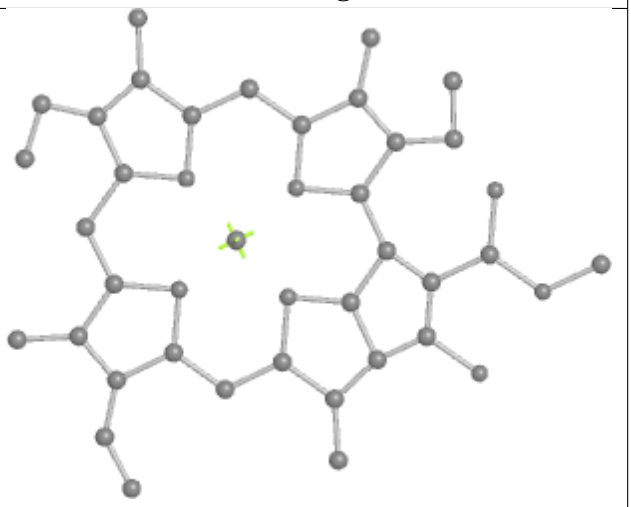
Bond lengths



Bond angles

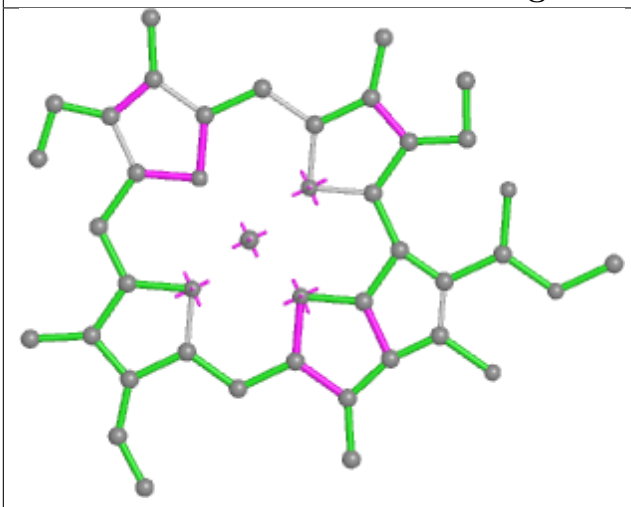


Torsions

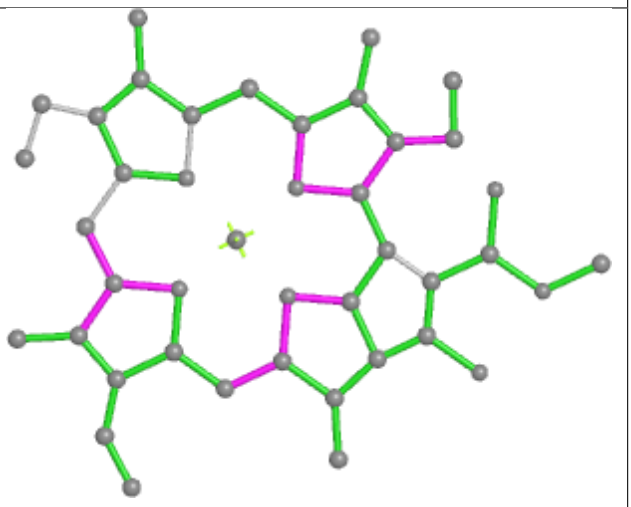


Rings

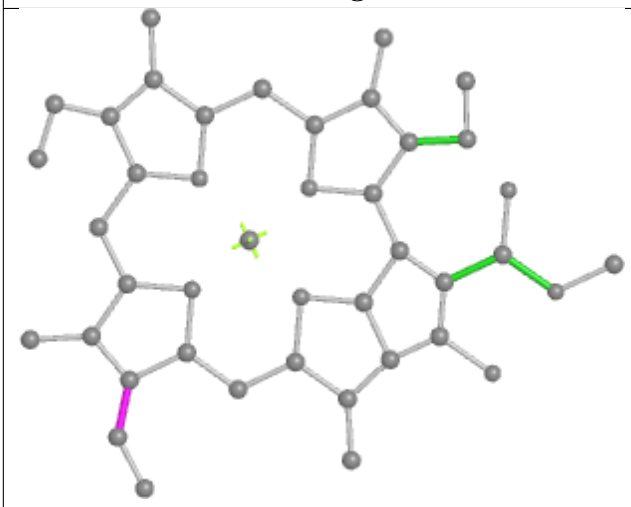
Ligand CLA 3 302



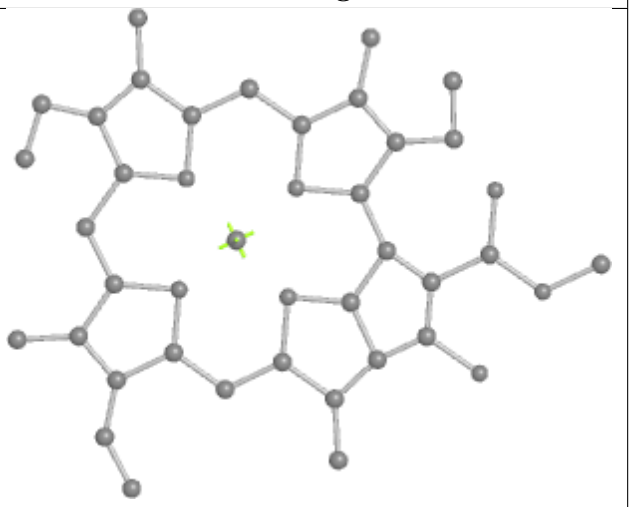
Bond lengths



Bond angles

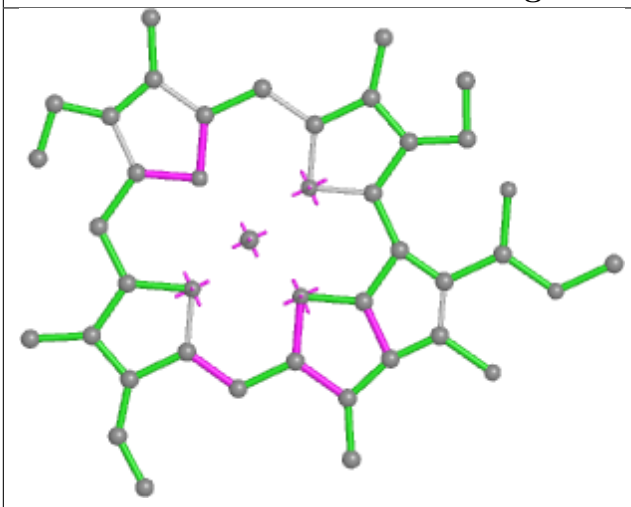


Torsions

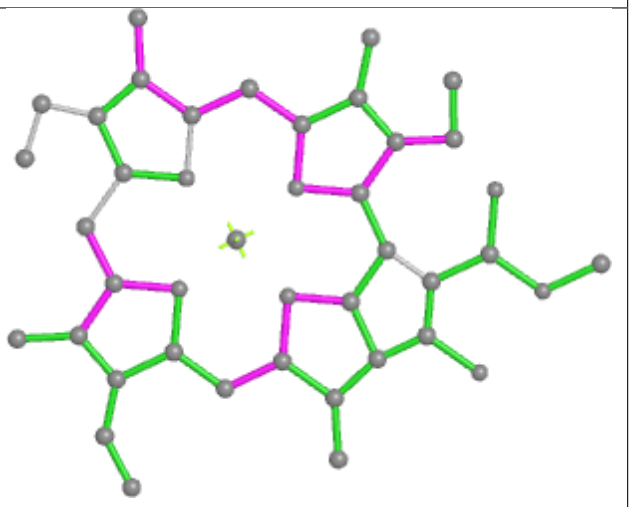


Rings

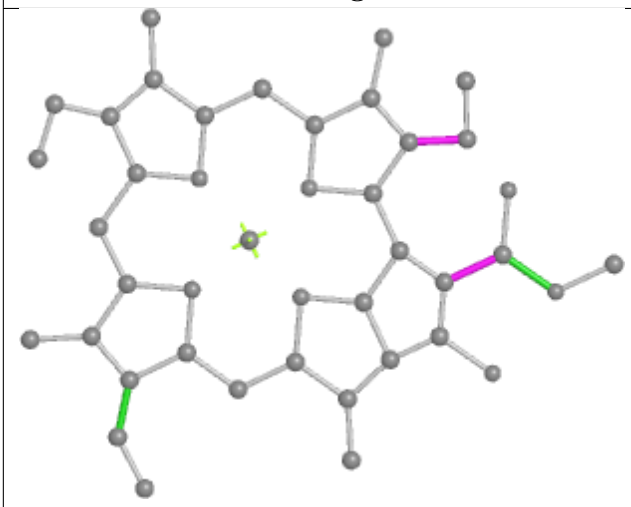
Ligand CLA B 809



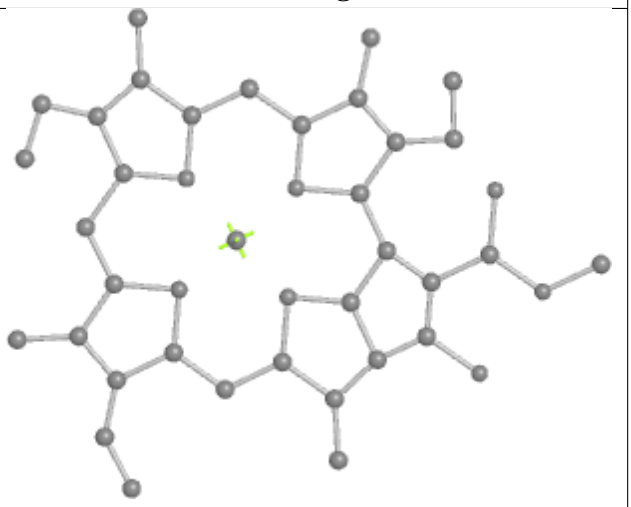
Bond lengths



Bond angles

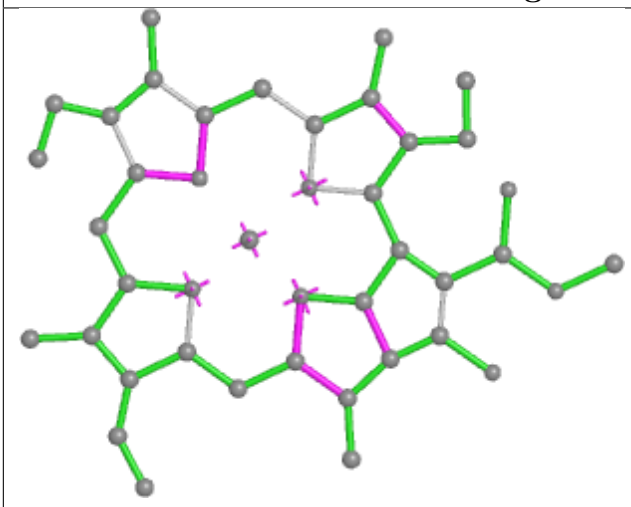


Torsions

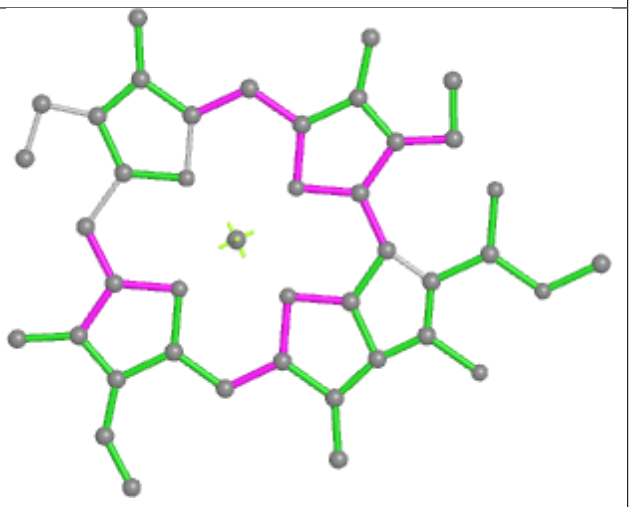


Rings

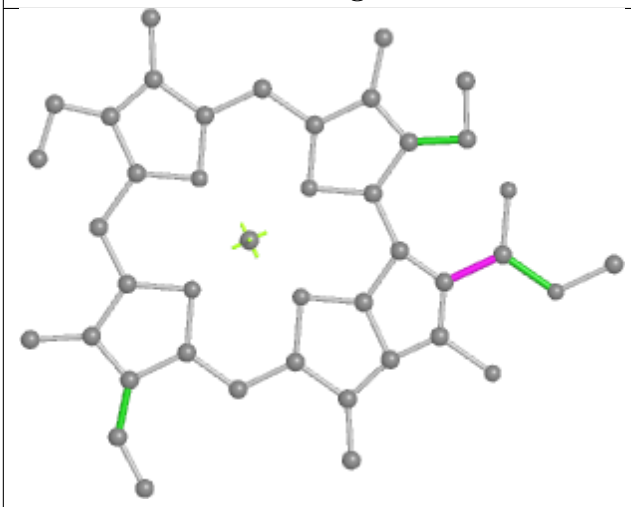
Ligand CLA B 836



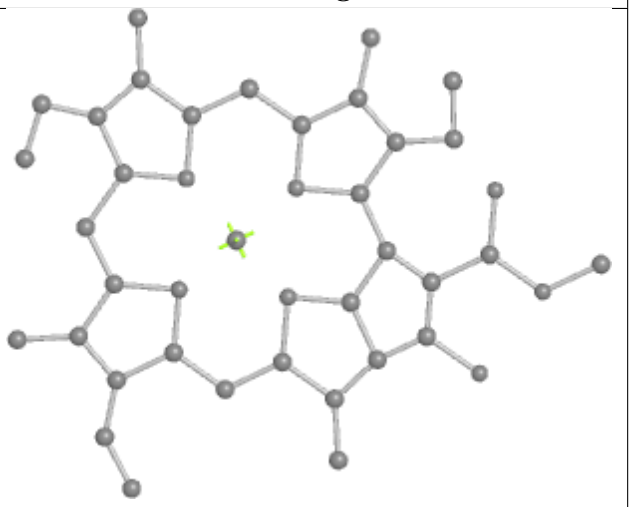
Bond lengths



Bond angles

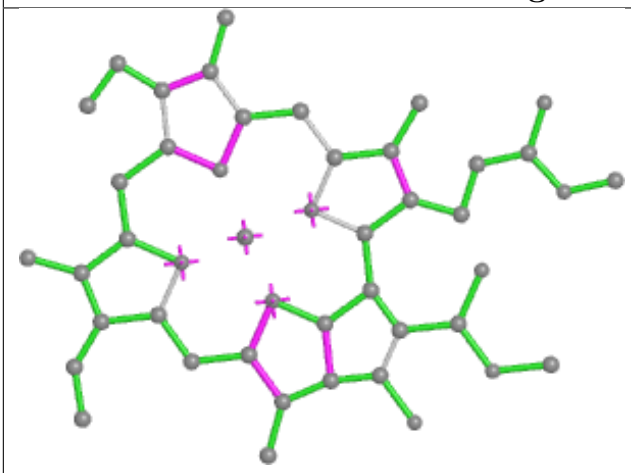


Torsions

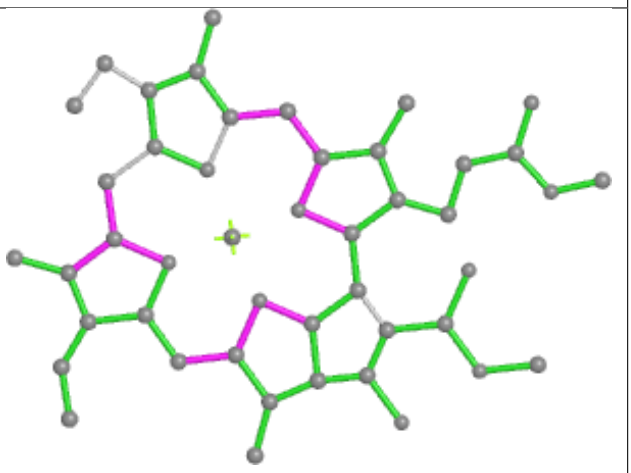


Rings

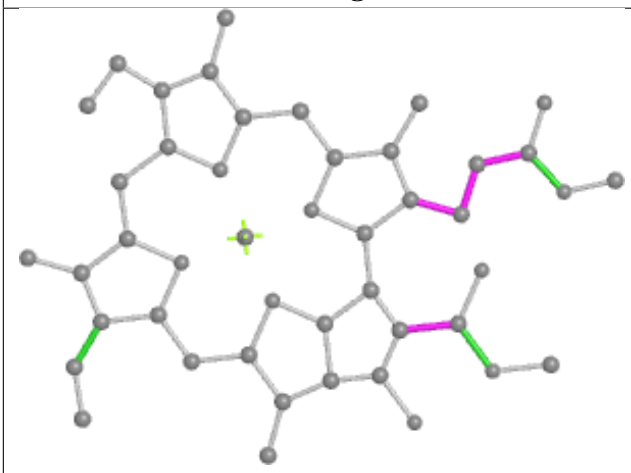
Ligand CLA 3 310



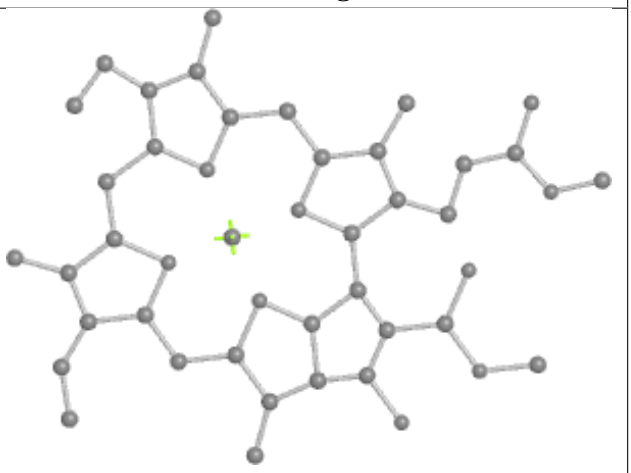
Bond lengths



Bond angles

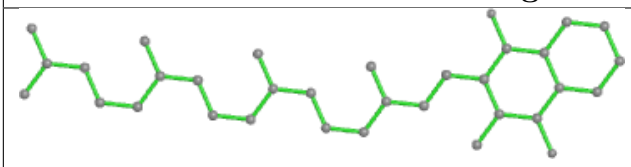


Torsions

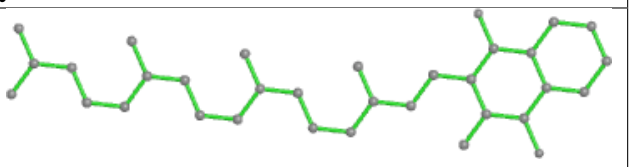


Rings

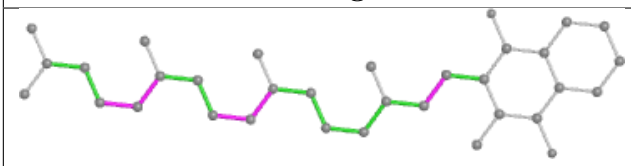
Ligand PQN A 842



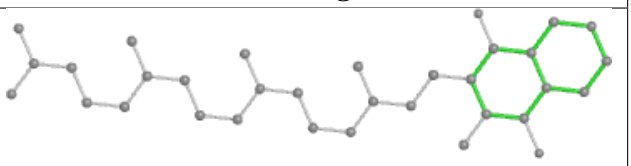
Bond lengths



Bond angles

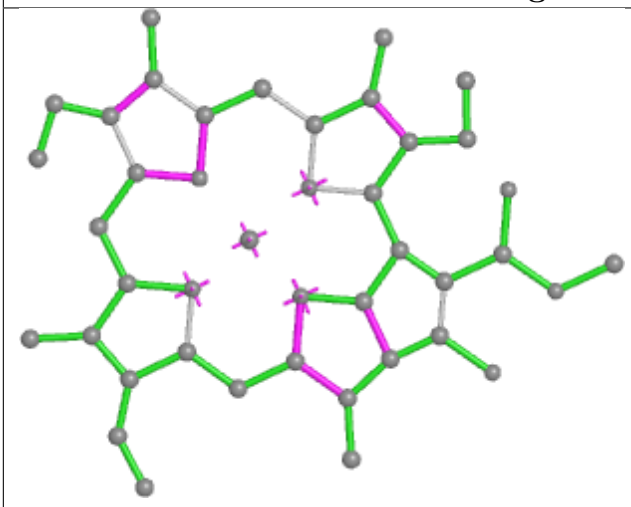


Torsions

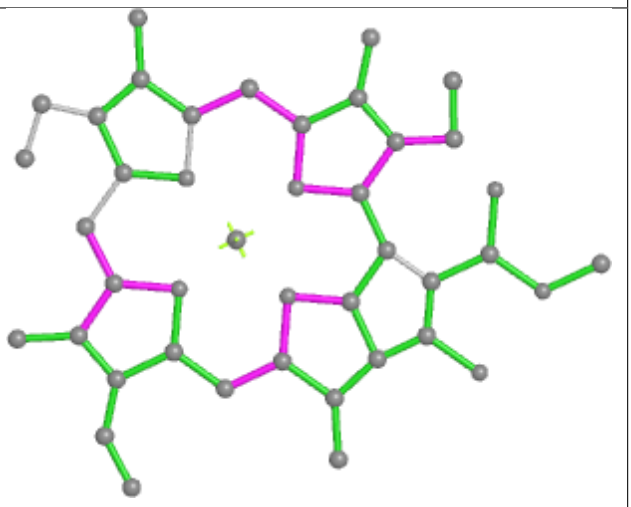


Rings

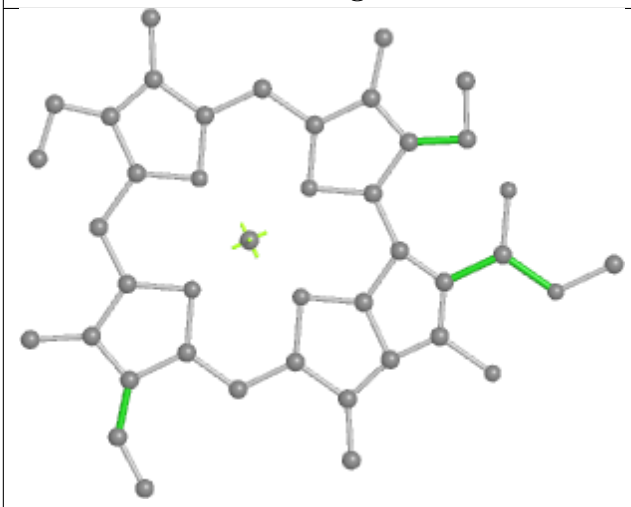
Ligand CLA 7 611



Bond lengths



Bond angles



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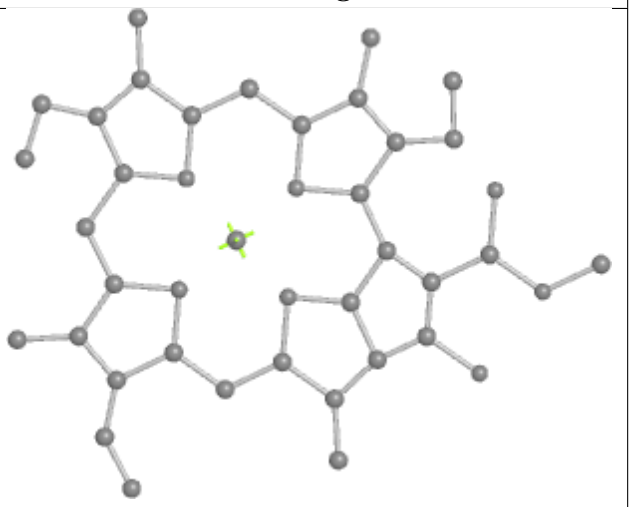
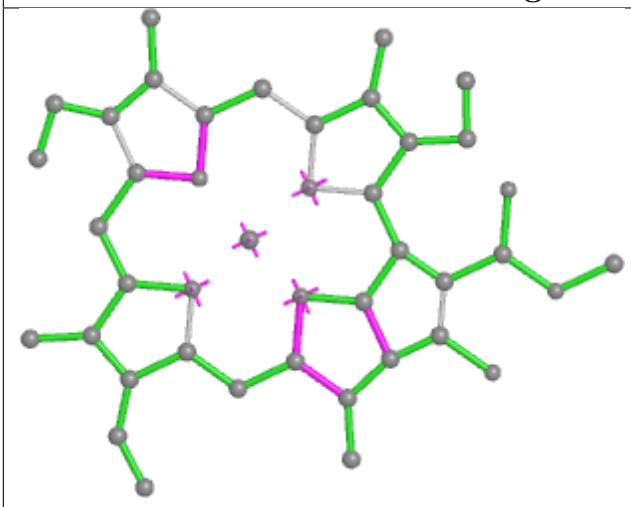
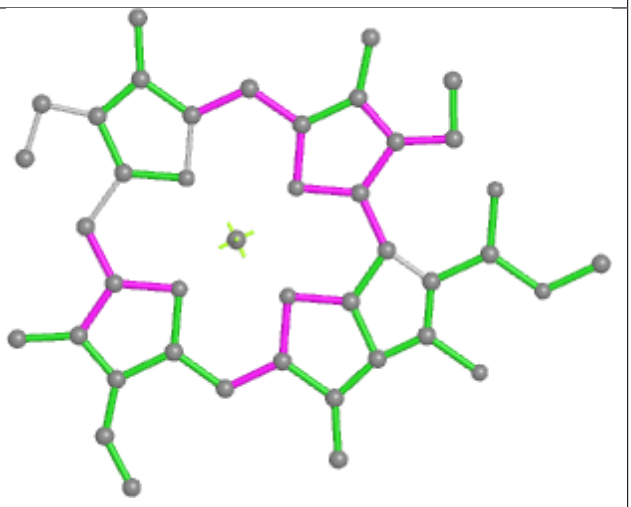


Rings

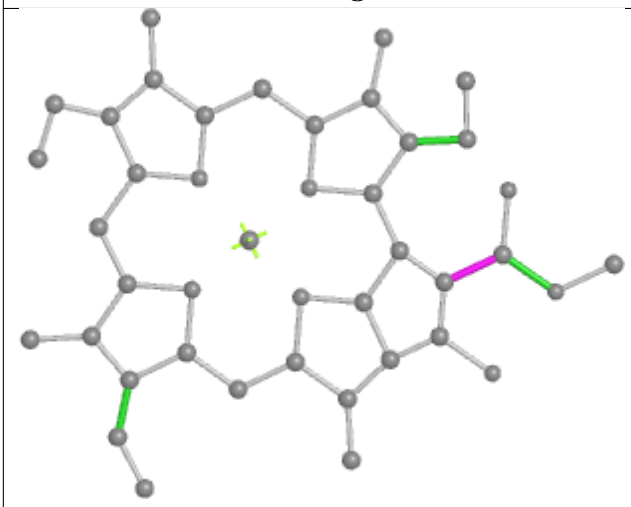
Ligand CLA B 835



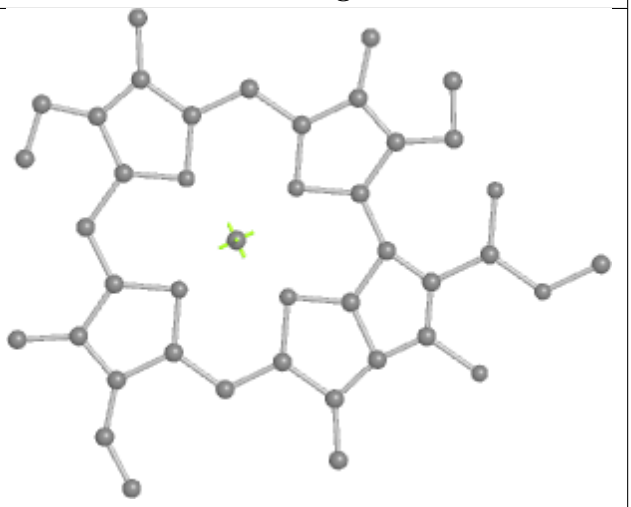
Bond lengths



Bond angles

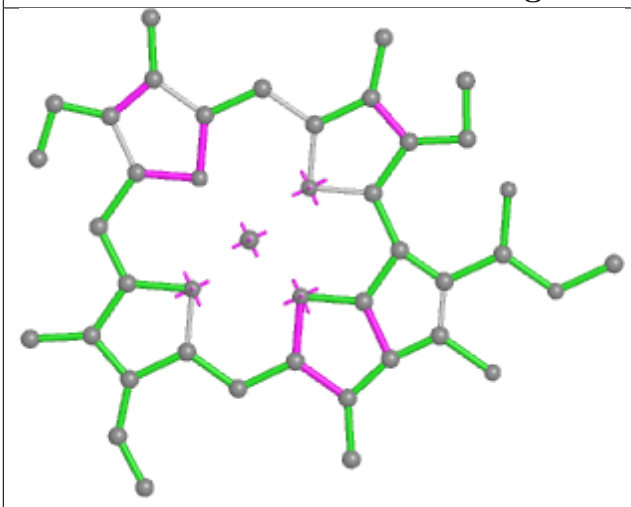


Torsions

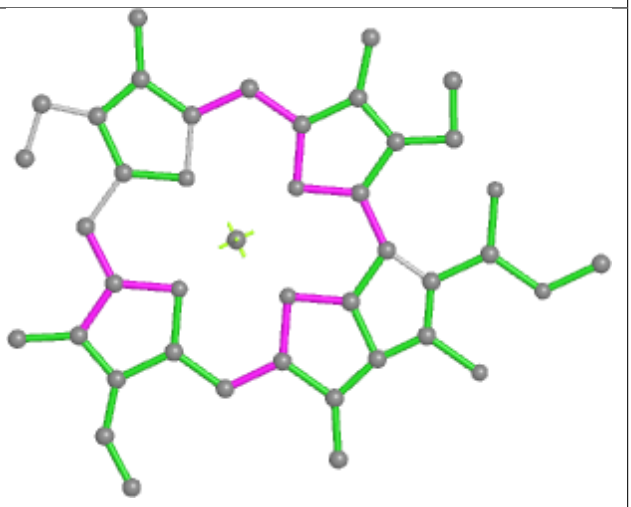


Rings

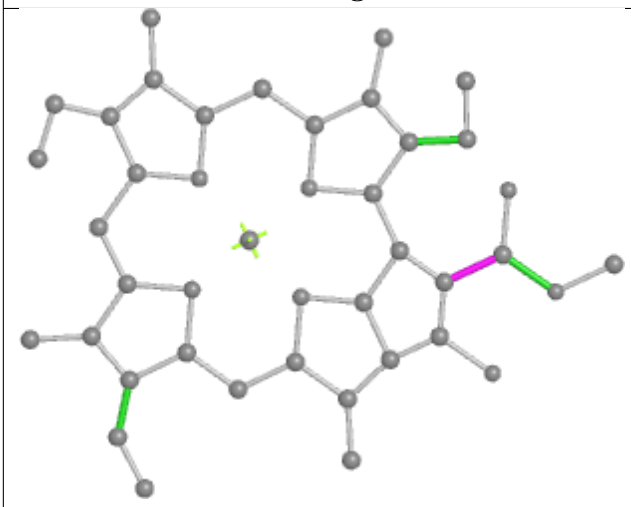
Ligand CLA B 826



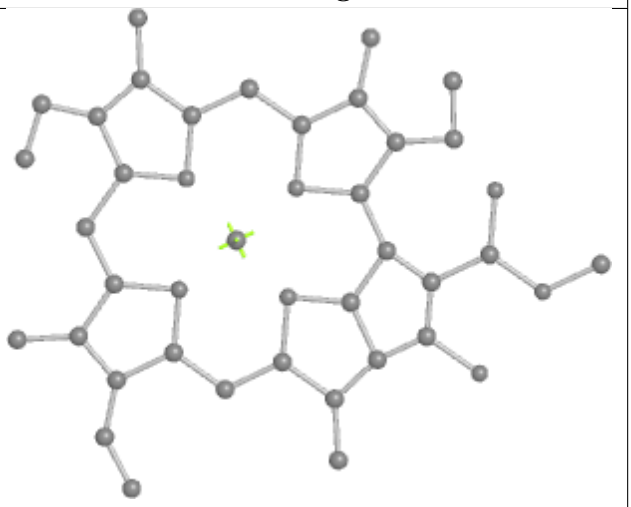
Bond lengths



Bond angles

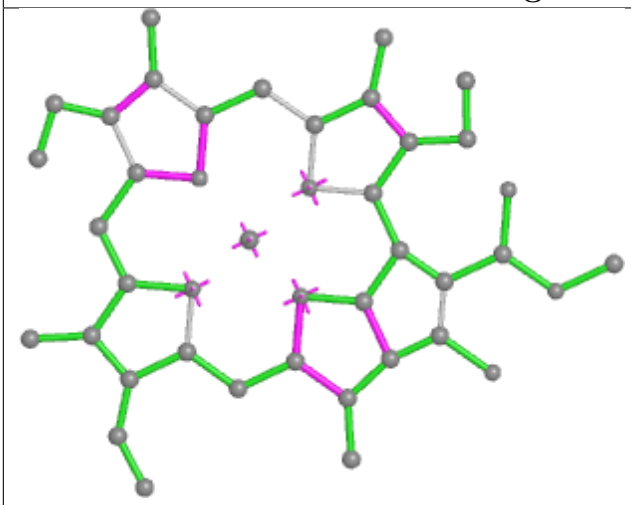


Torsions

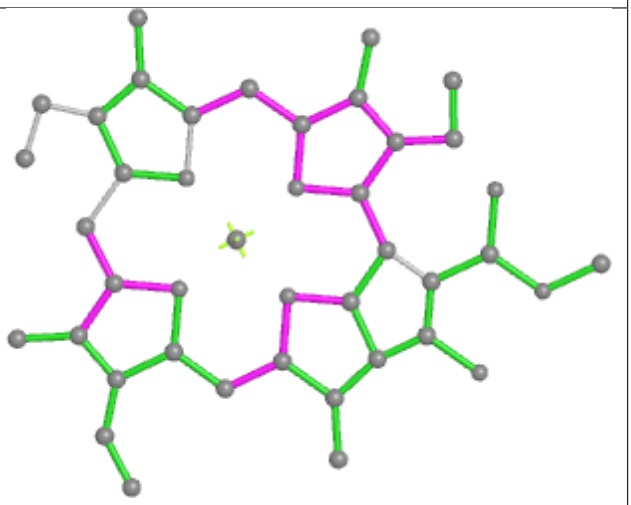


Rings

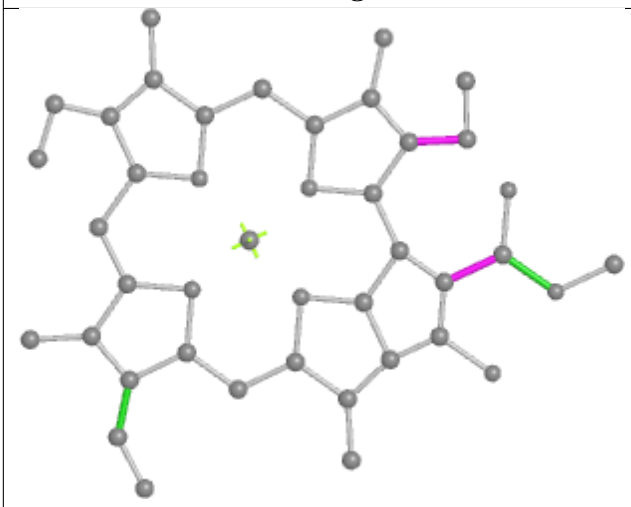
Ligand CLA B 812



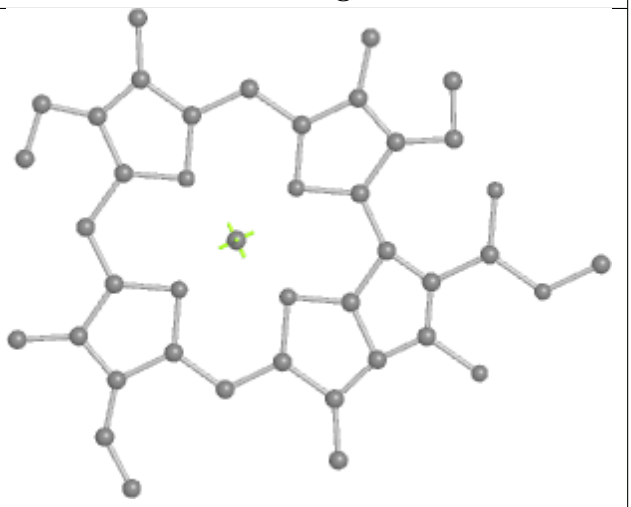
Bond lengths



Bond angles

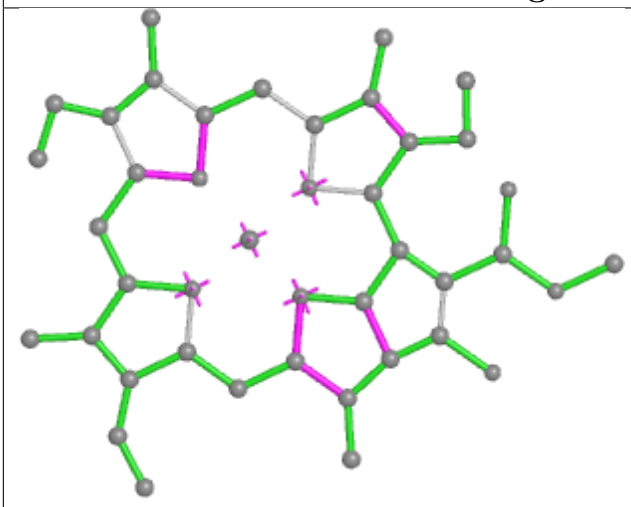


Torsions

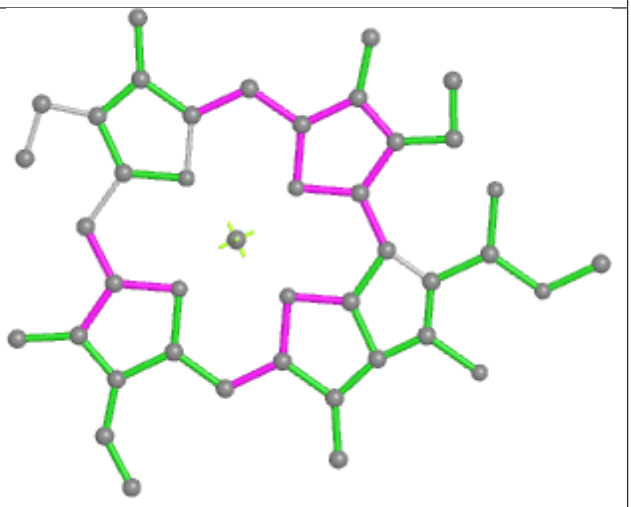


Rings

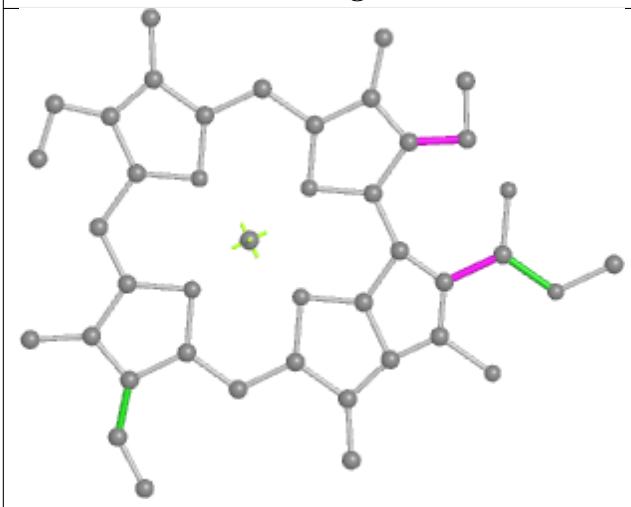
Ligand CLA 7 614



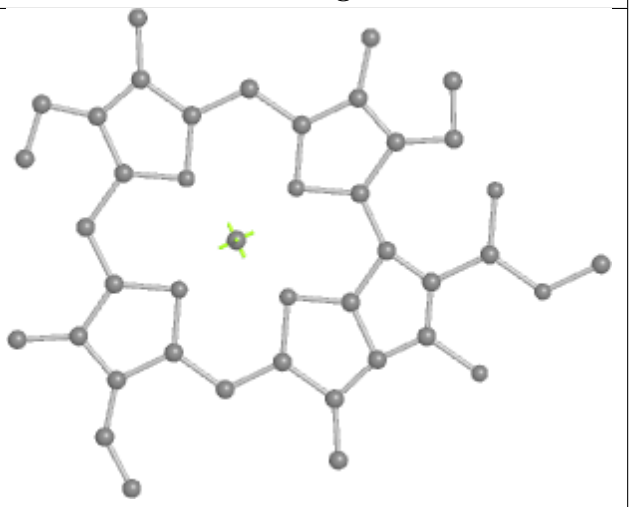
Bond lengths



Bond angles

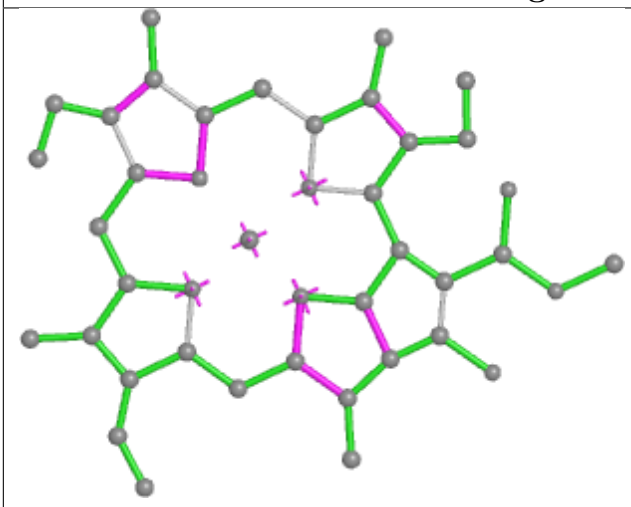


Torsions



Rings

Ligand CLA 8 611



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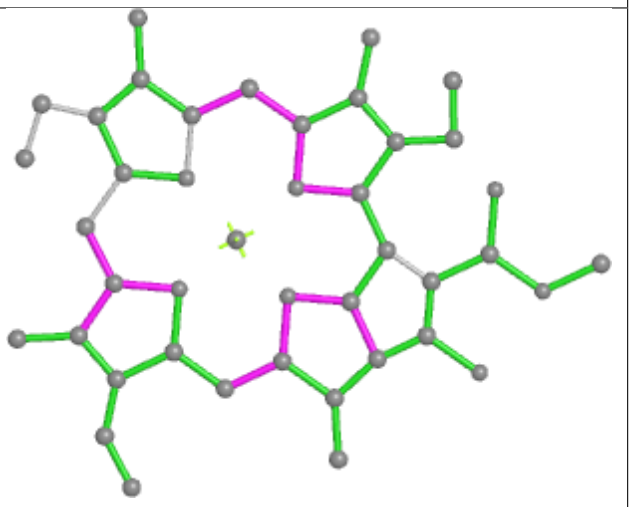
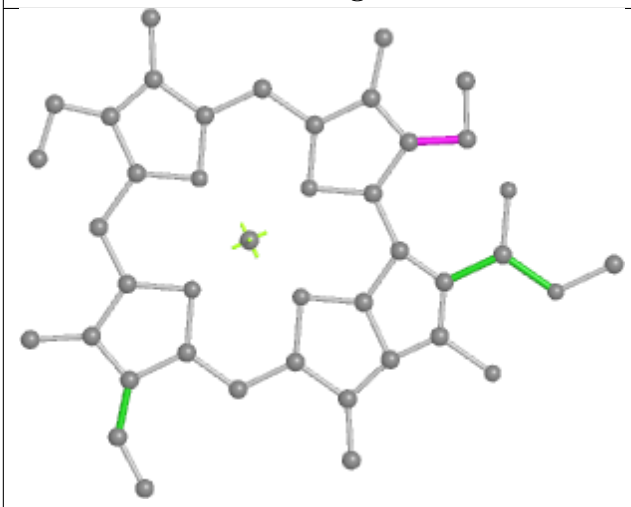


Bond angles



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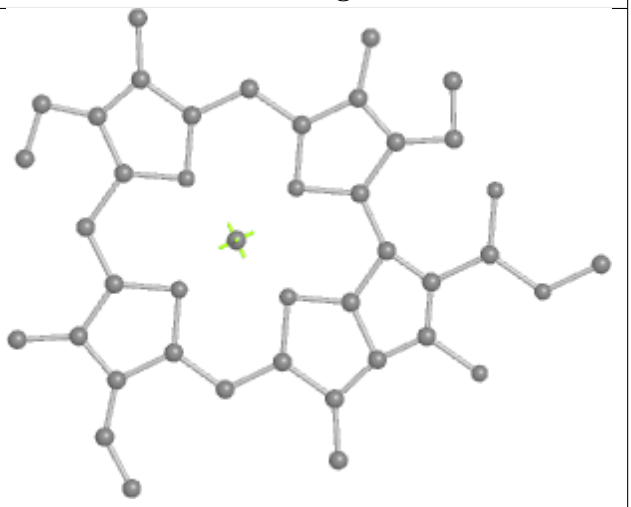
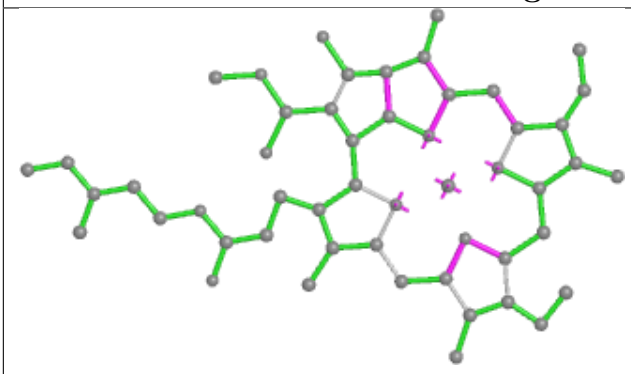


Rings

Ligand CLA A 823



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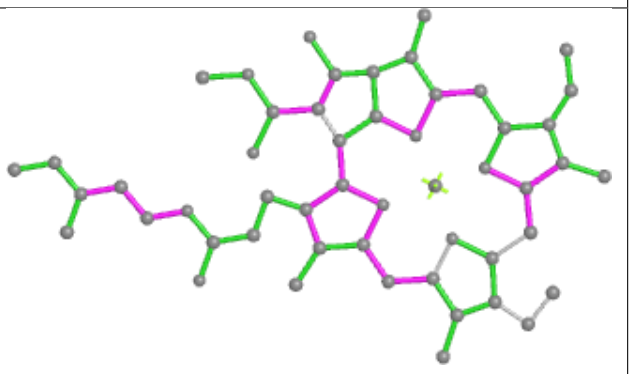
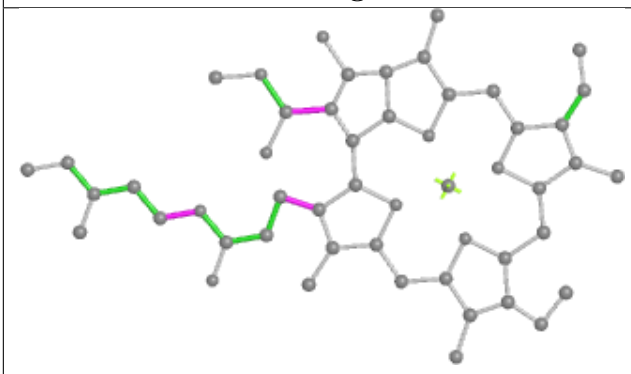
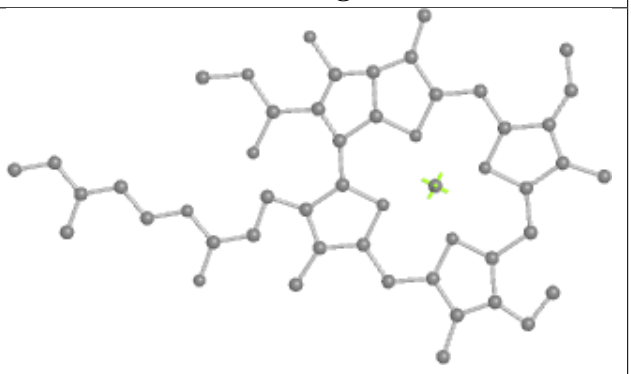


Bond angles

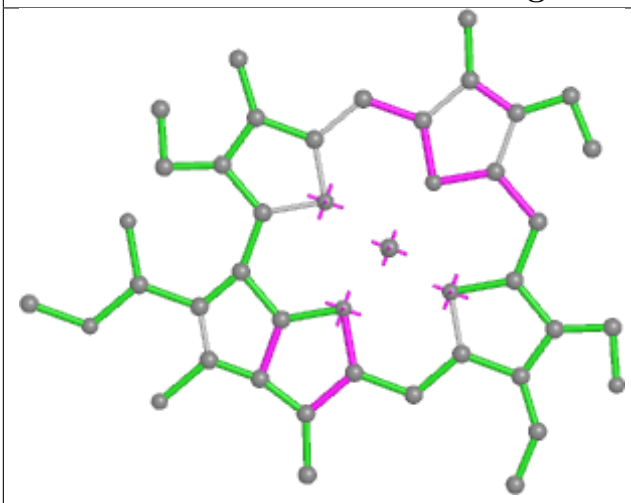


Torsions

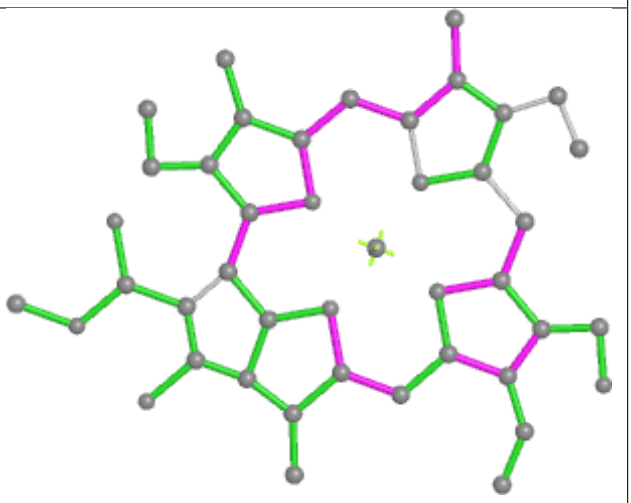


Rings

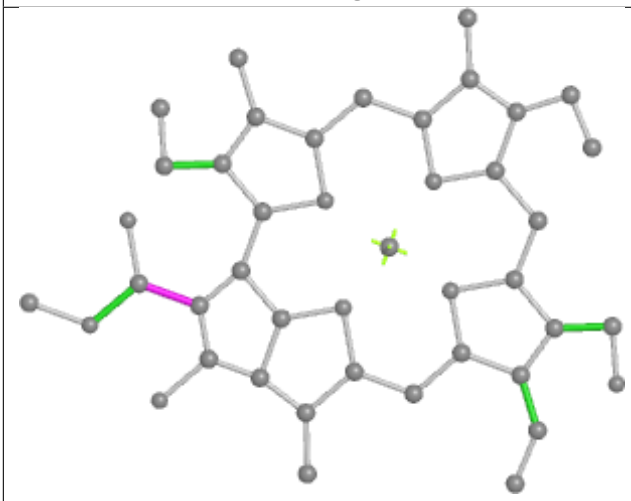
Ligand CHL 5 616



Bond lengths



Bond angles



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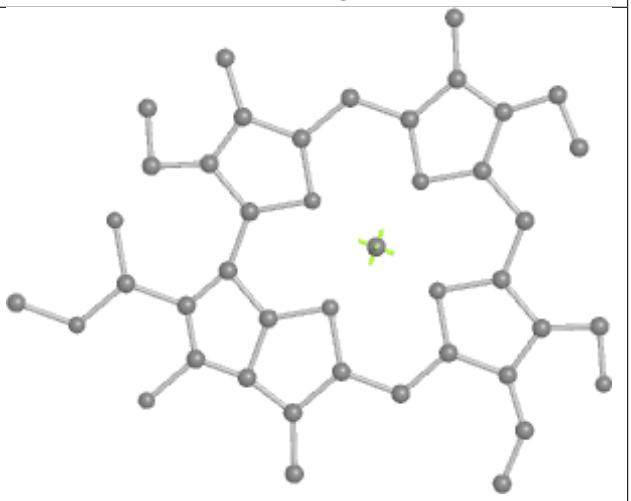
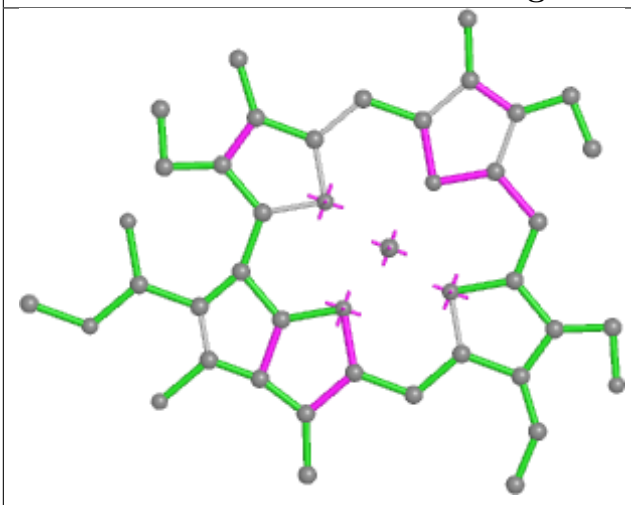
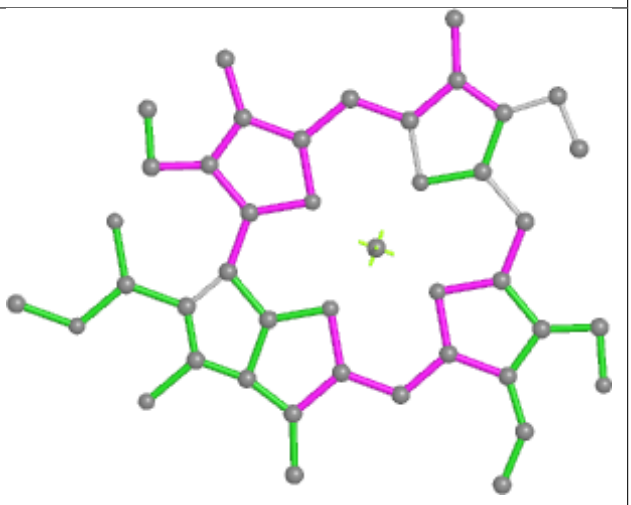


Rings

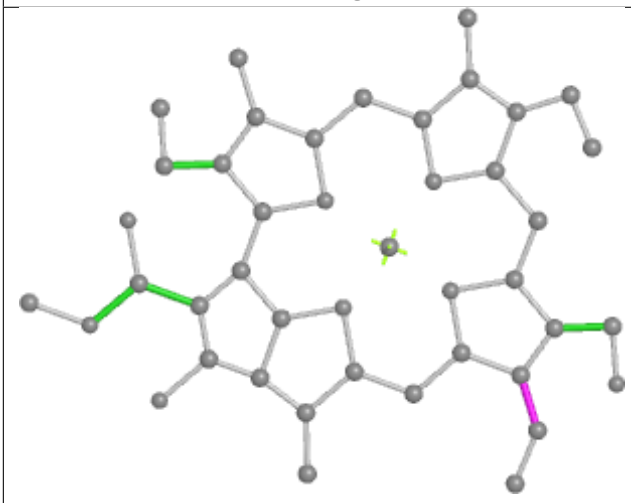
Ligand CHL 4 604



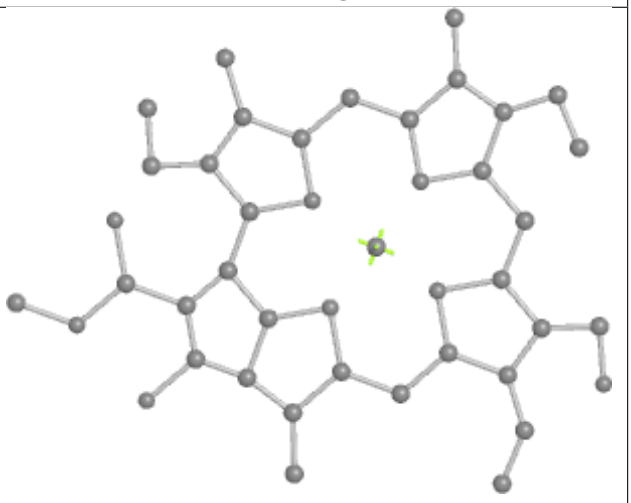
Bond lengths



Bond angles

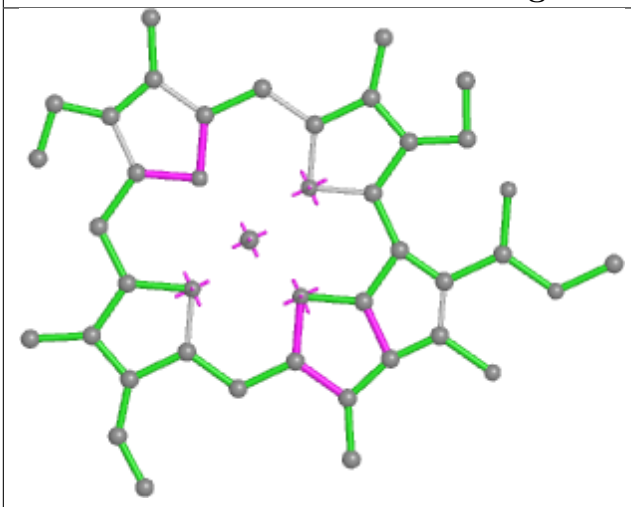


Torsions

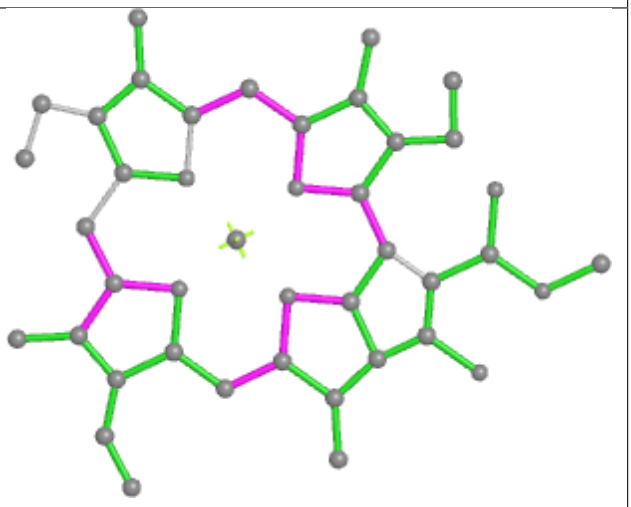


Rings

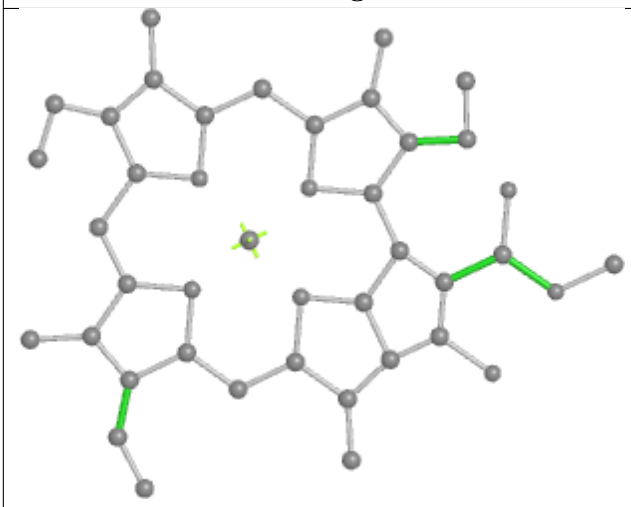
Ligand CLA 6 308



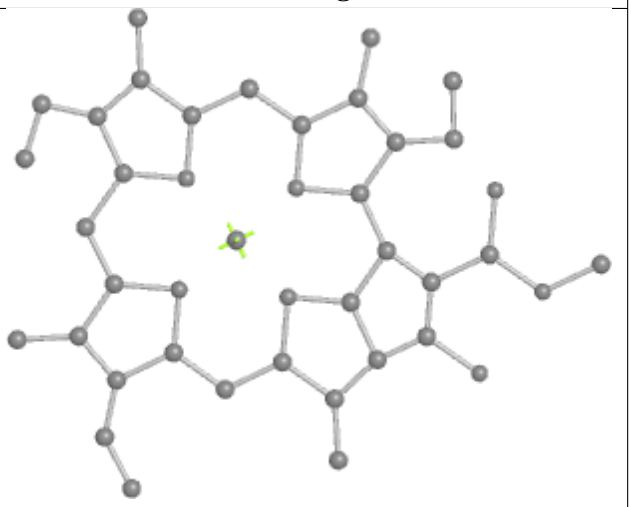
Bond lengths



Bond angles

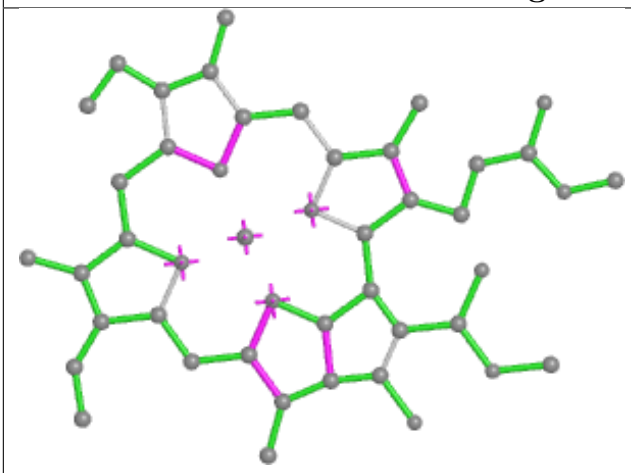


Torsions

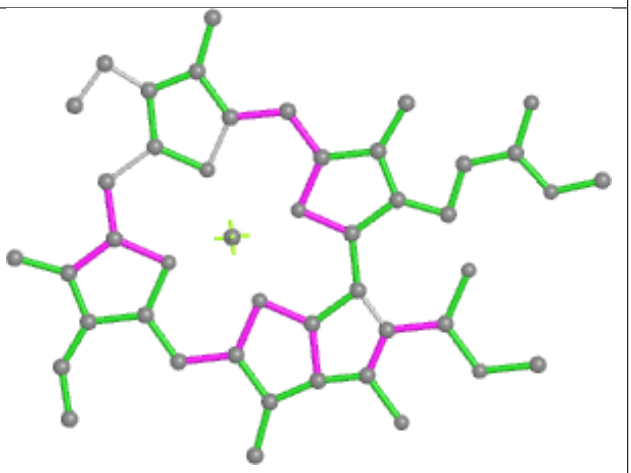


Rings

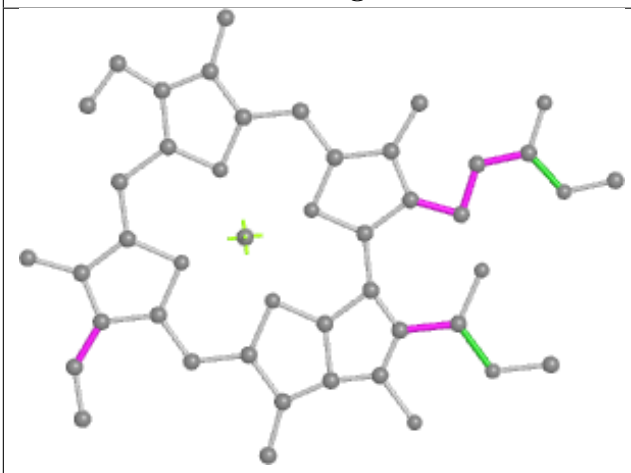
Ligand CLA 5 617



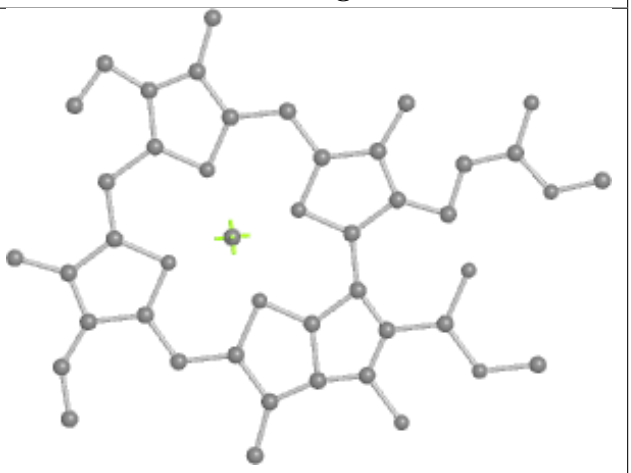
Bond lengths



Bond angles

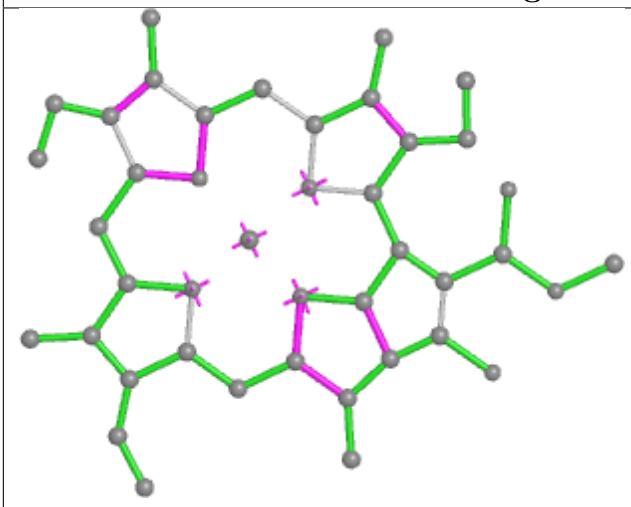


Torsions

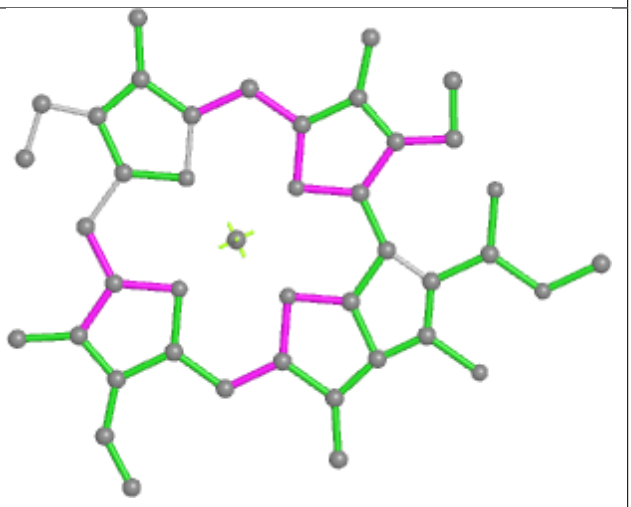


Rings

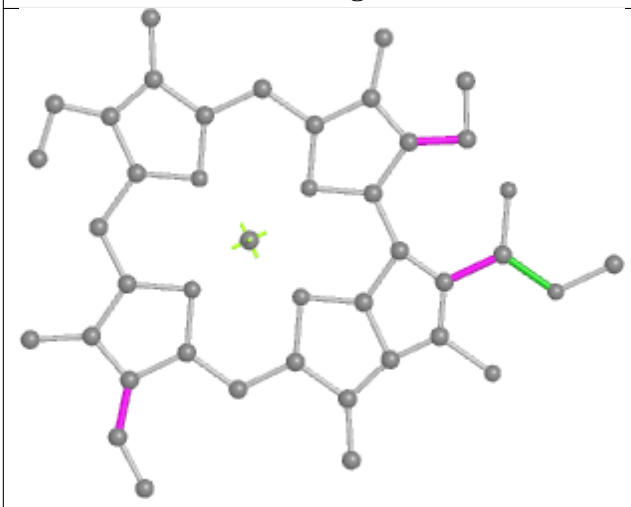
Ligand CLA A 813



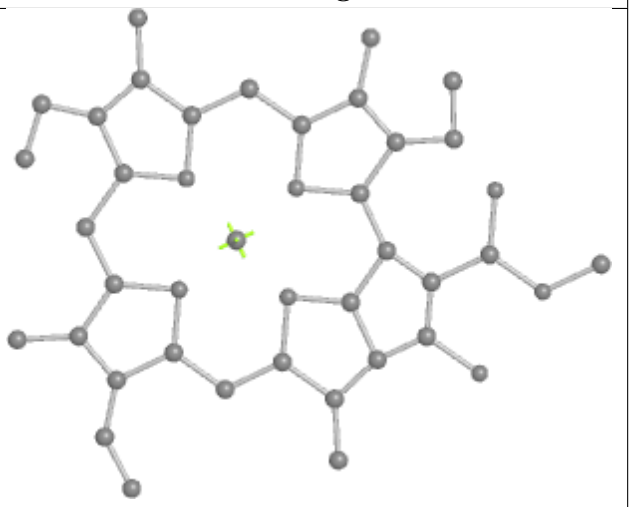
Bond lengths



Bond angles

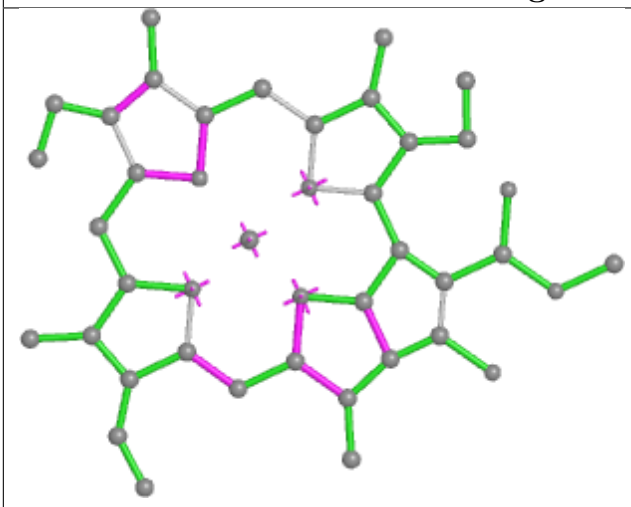


Torsions



Rings

Ligand CLA 3 314



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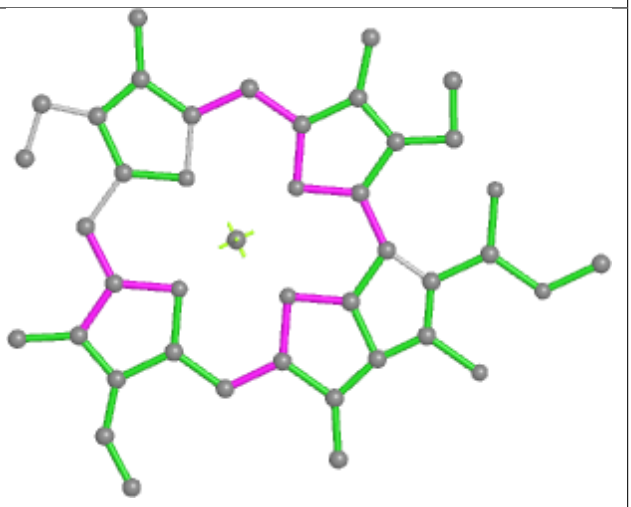
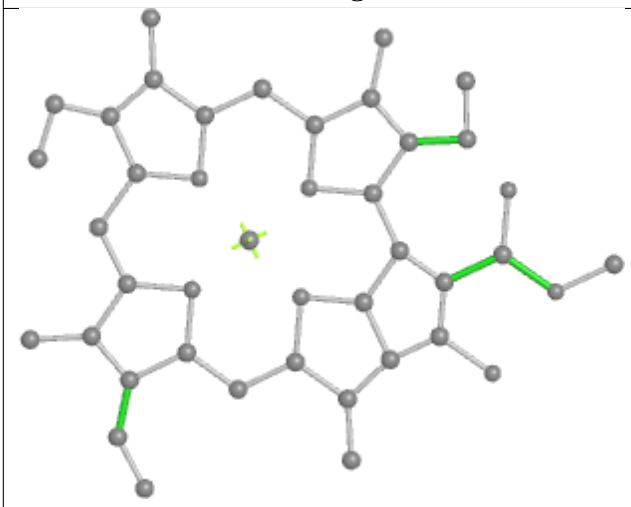
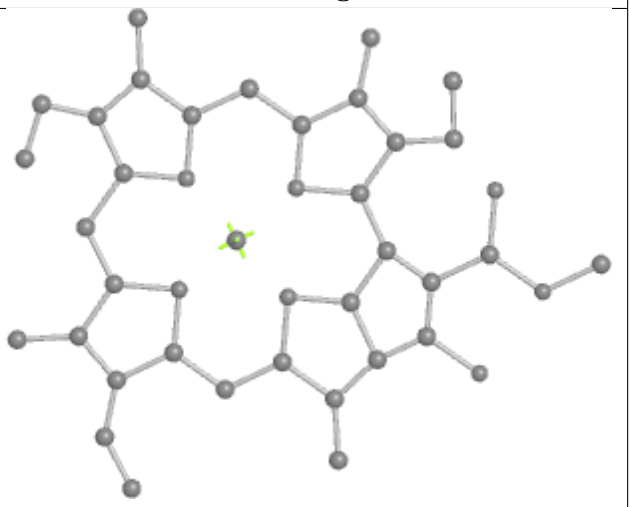


Bond angles

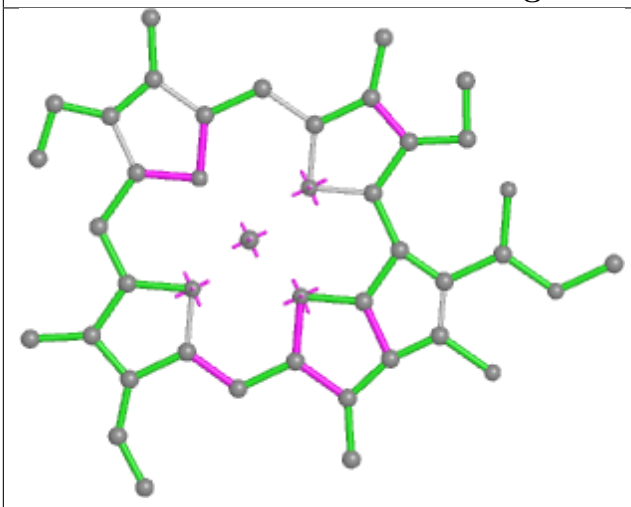


Torsions

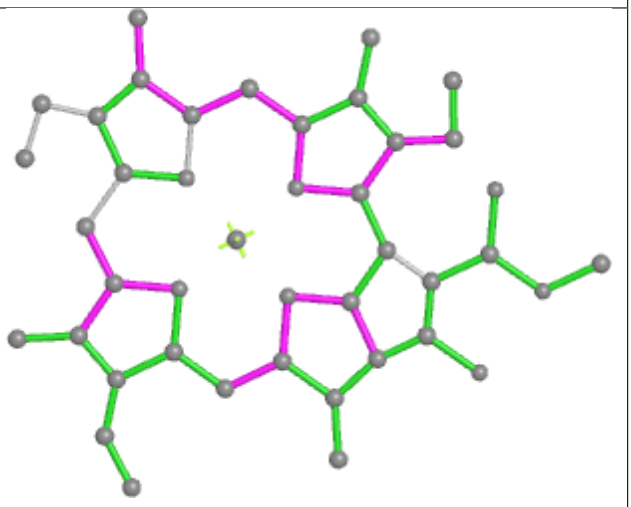


Rings

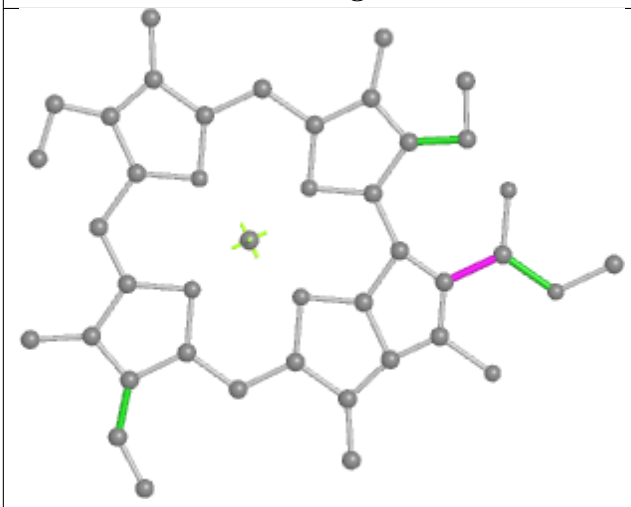
Ligand CLA A 808



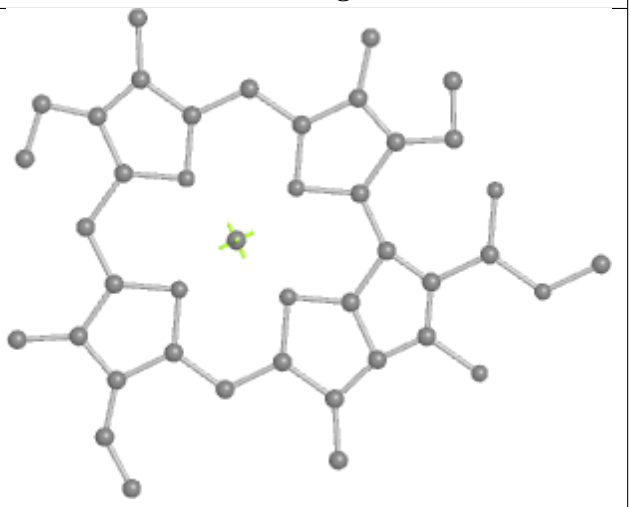
Bond lengths



Bond angles

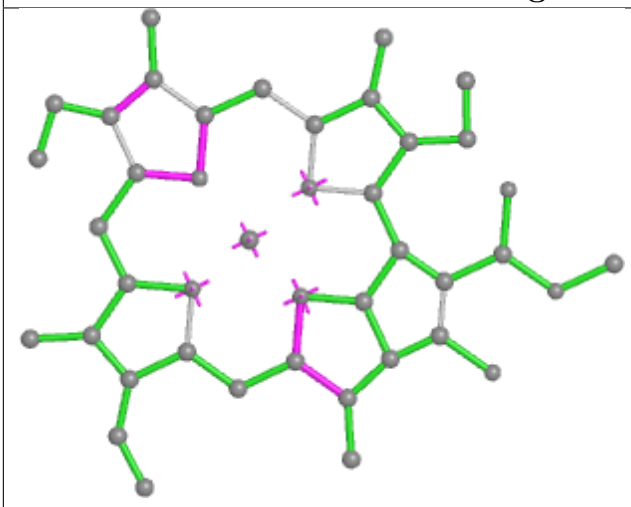


Torsions

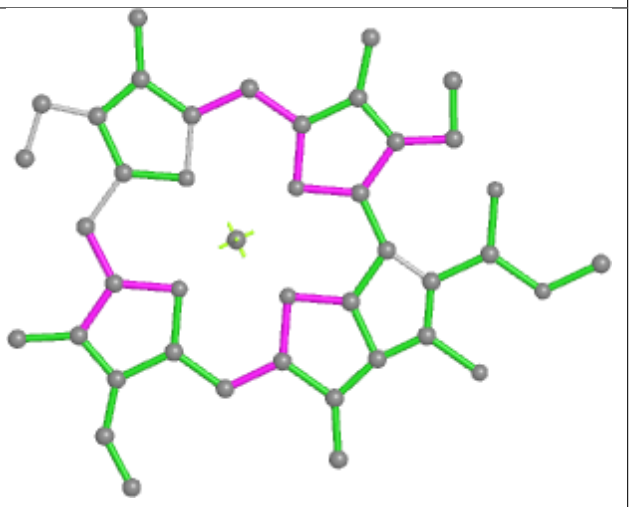


Rings

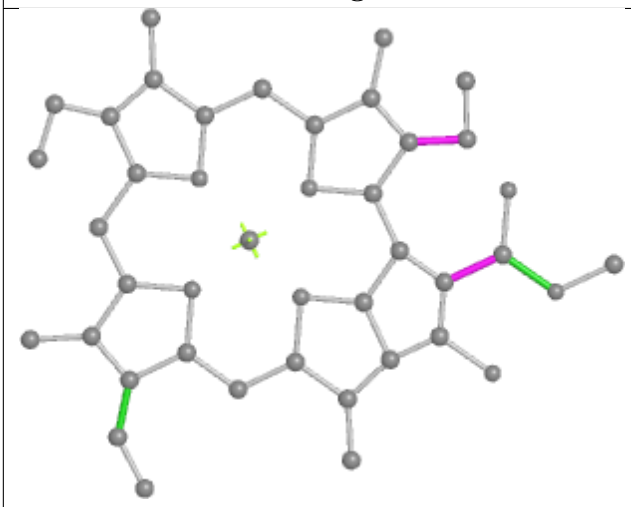
Ligand CLA 8 602



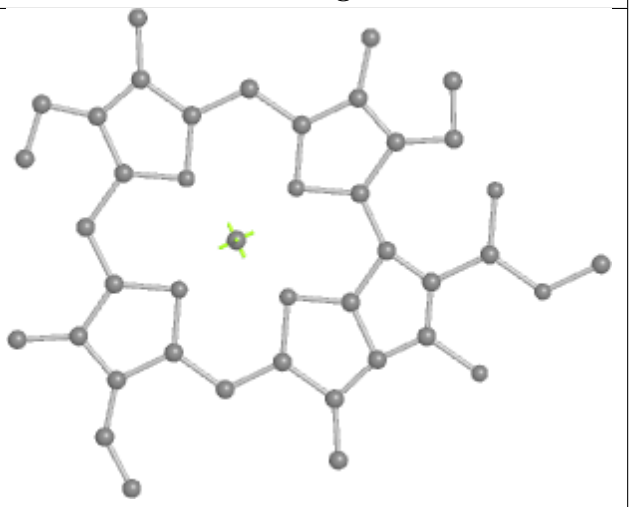
Bond lengths



Bond angles

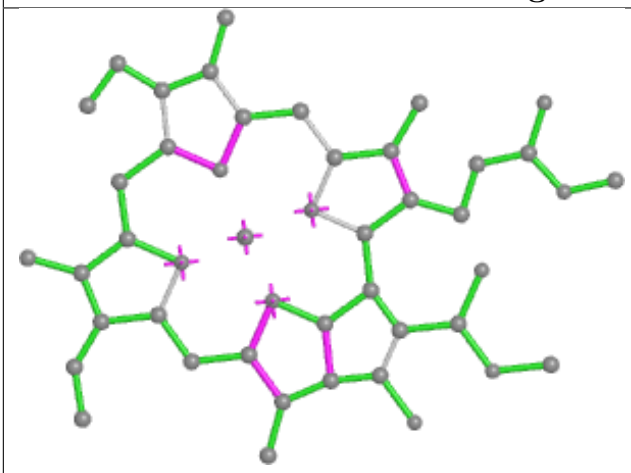


Torsions

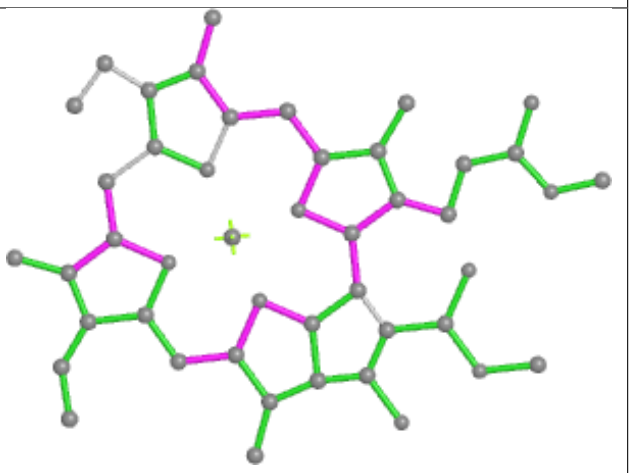


Rings

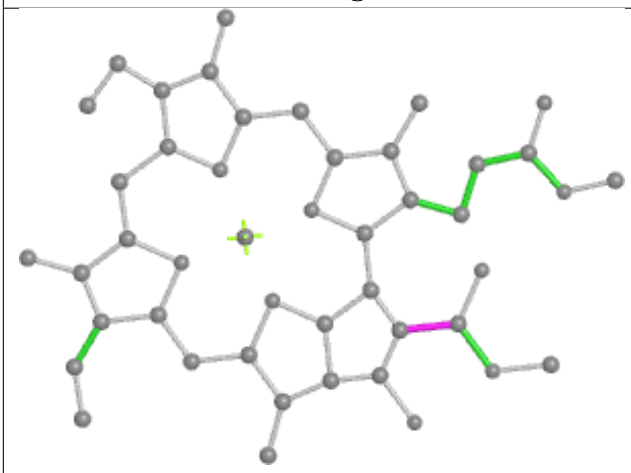
Ligand CLA 6 314



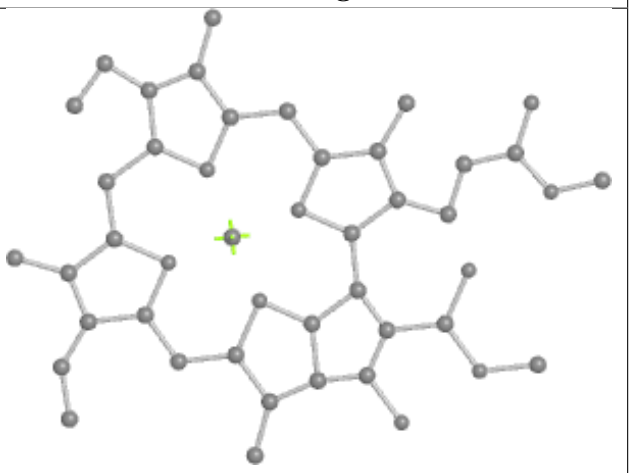
Bond lengths



Bond angles

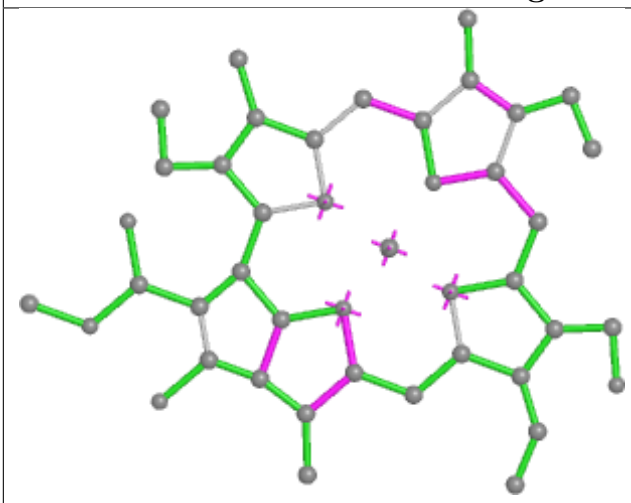


Torsions

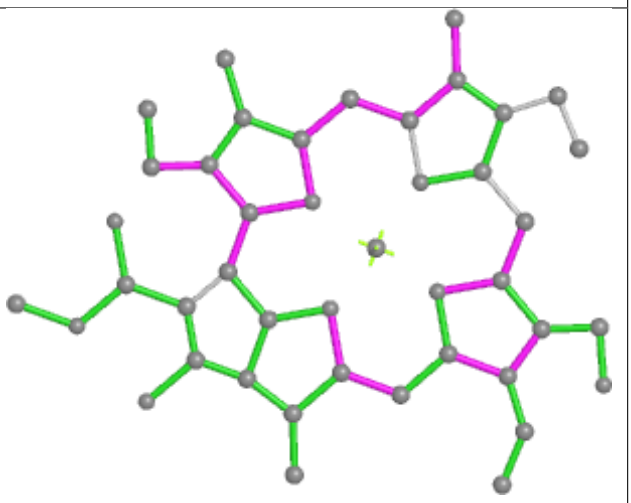


Rings

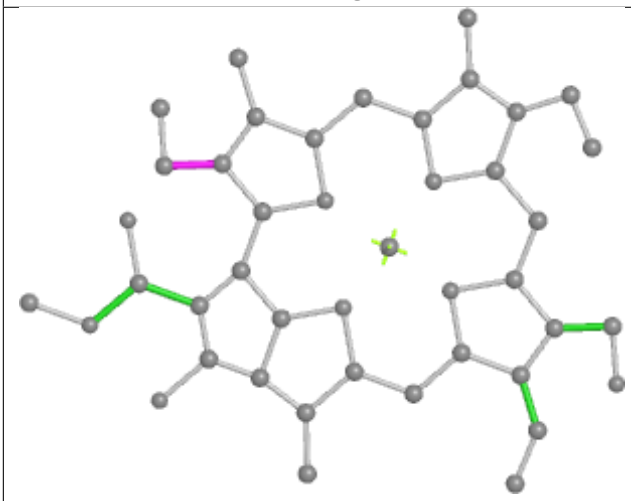
Ligand CHL 6 307



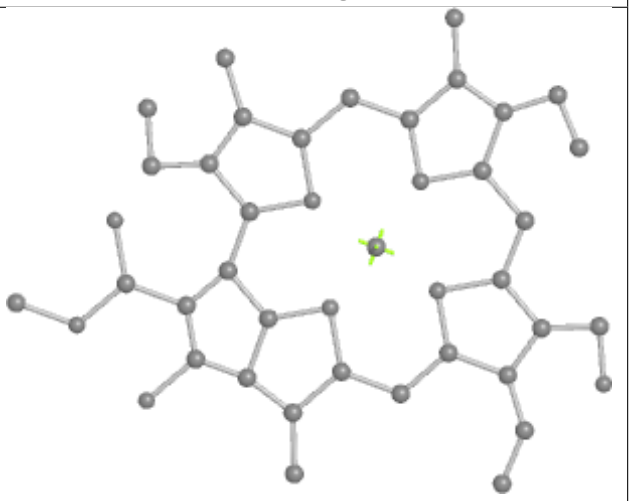
Bond lengths



Bond angles

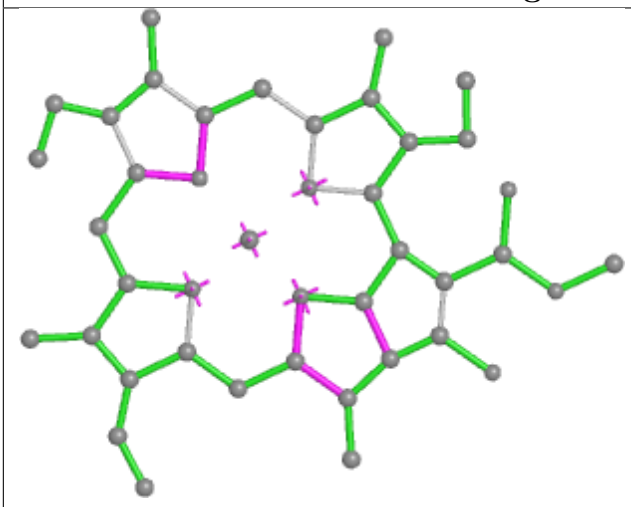


Torsions



Rings

Ligand CLA A 831



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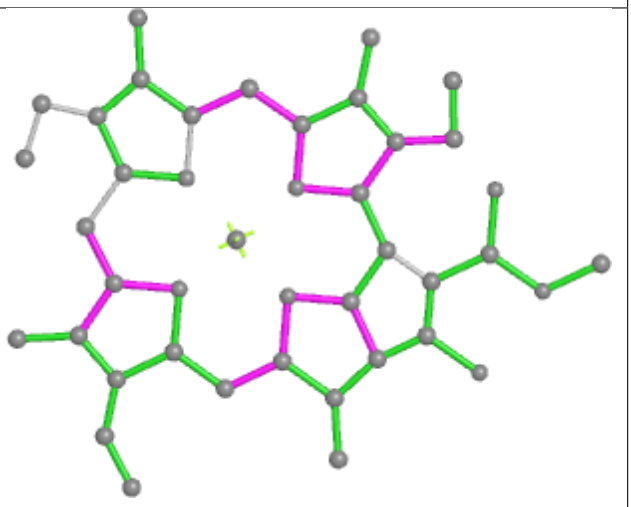
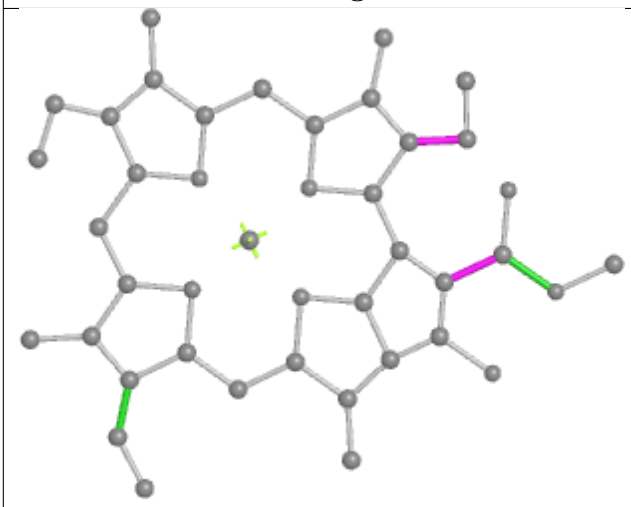


Bond angles



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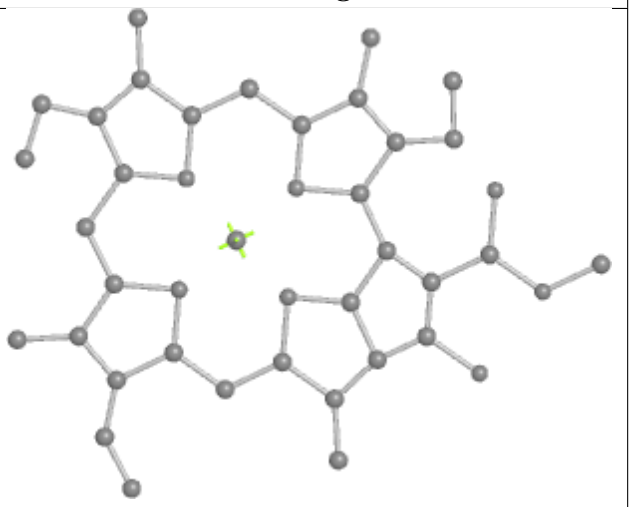
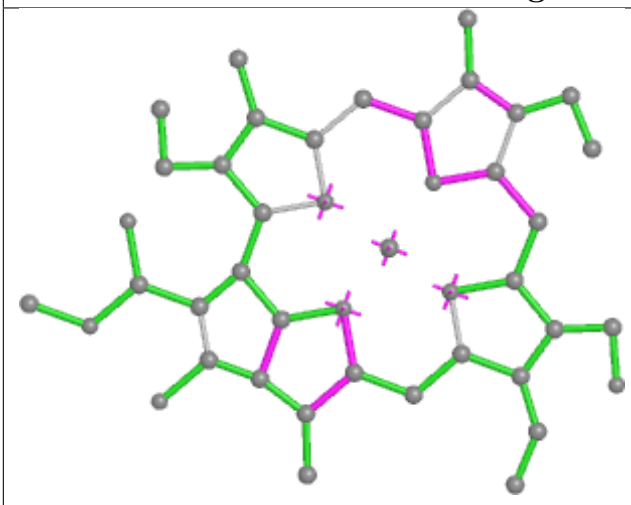


Rings

Ligand CHL 1 606



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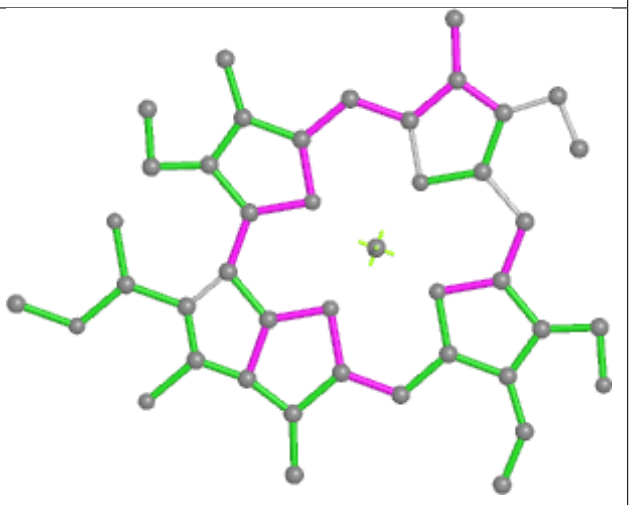

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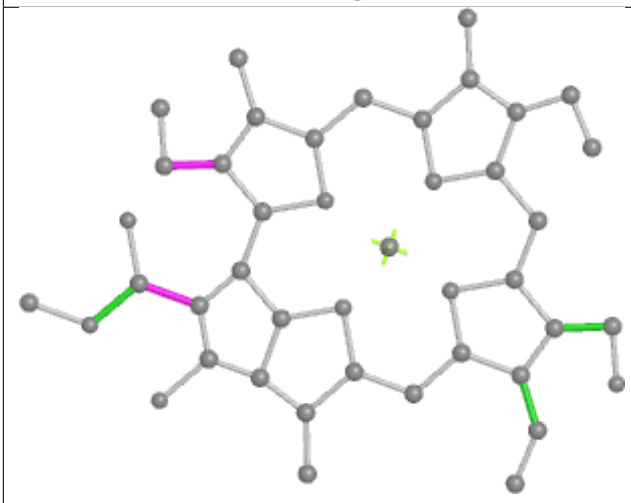

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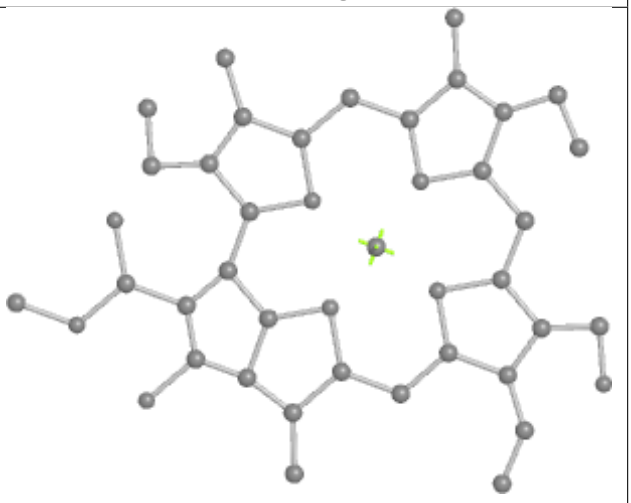
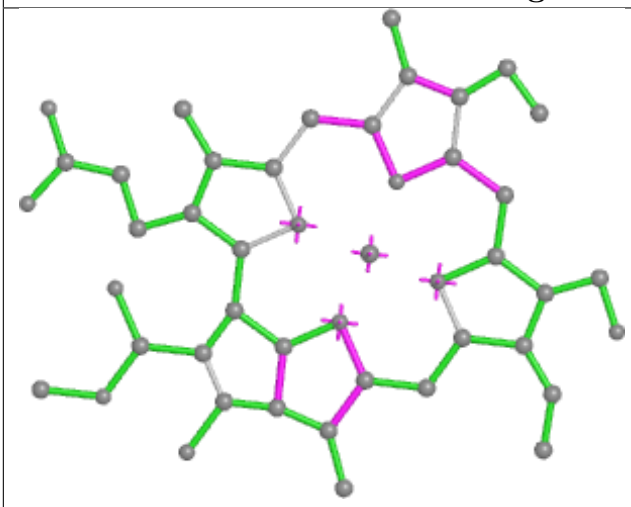


Rings

Ligand CHL 4 605



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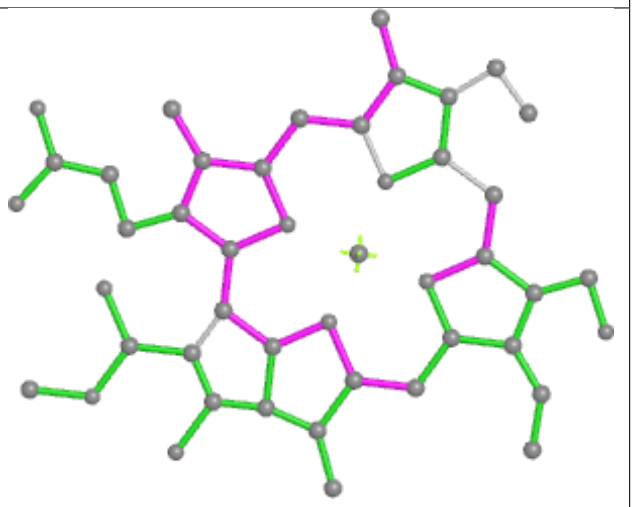
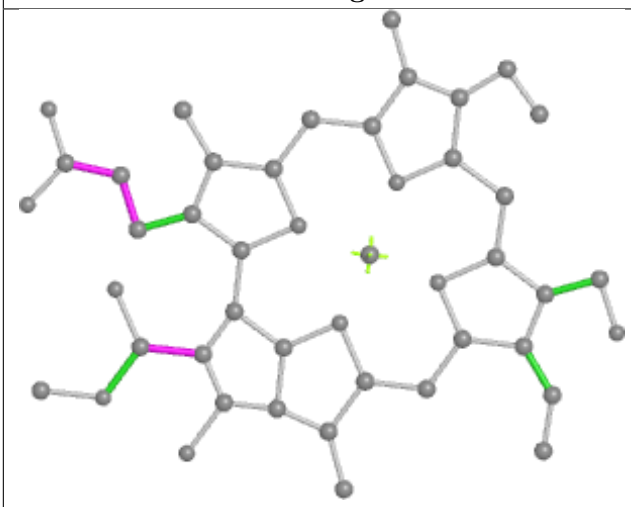


Bond angles



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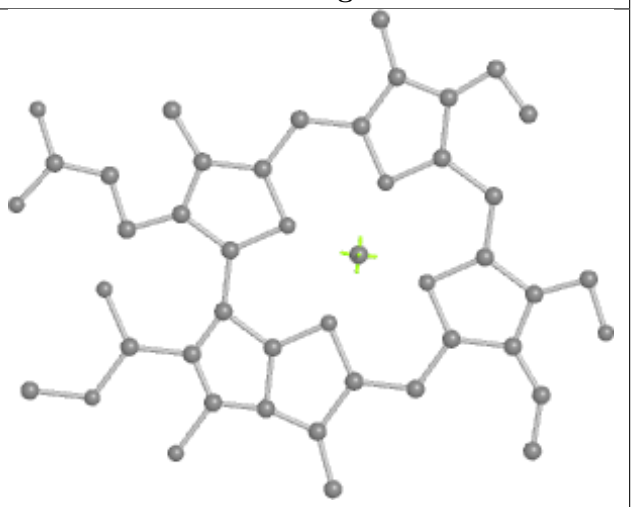
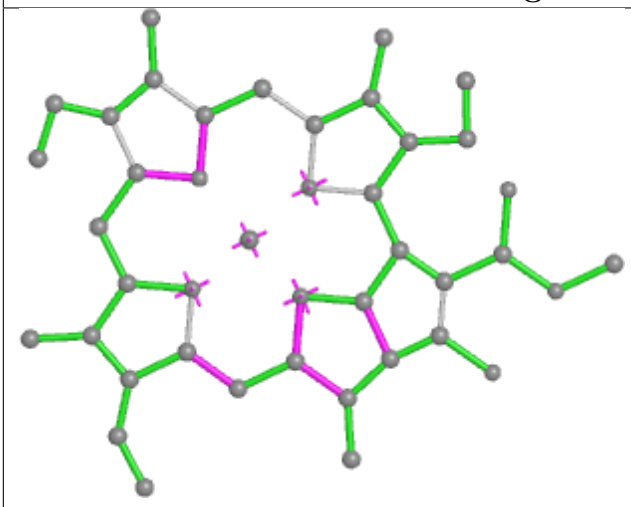


Rings

Ligand CLA B 829



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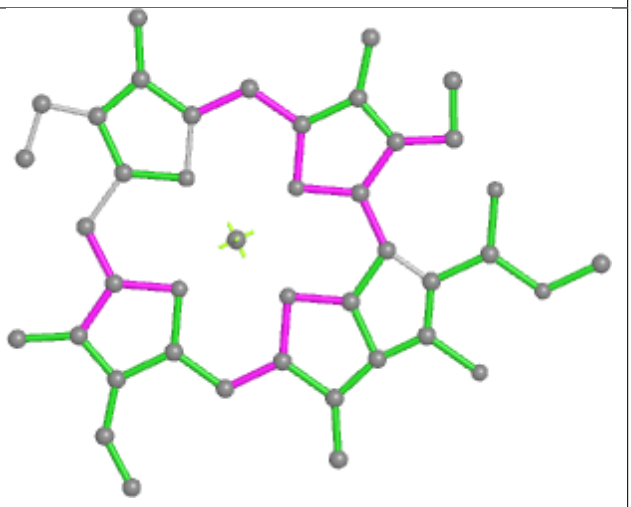
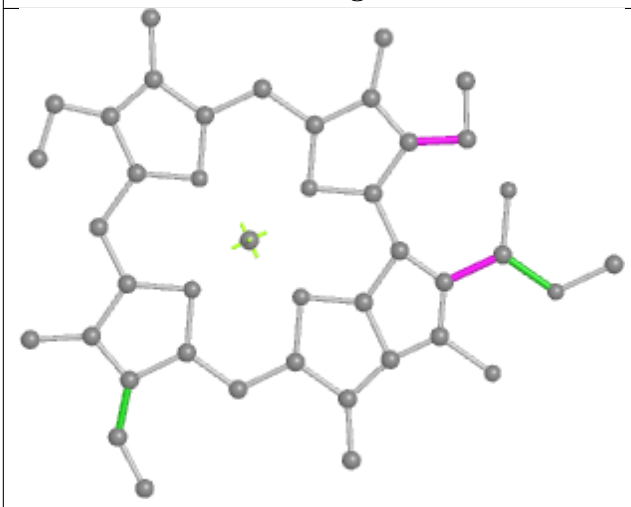


Bond angles



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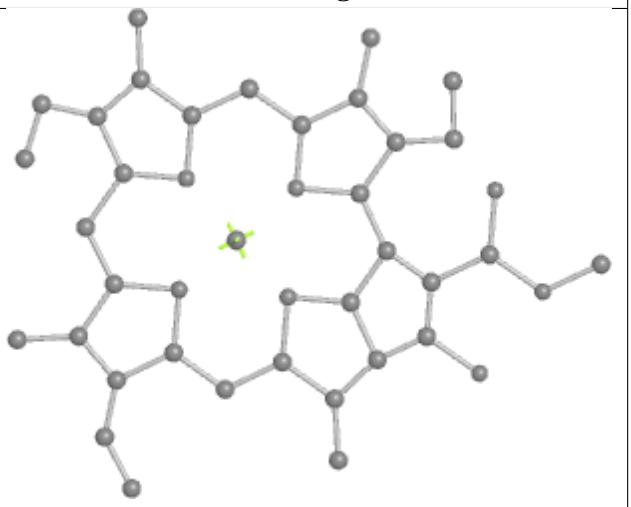
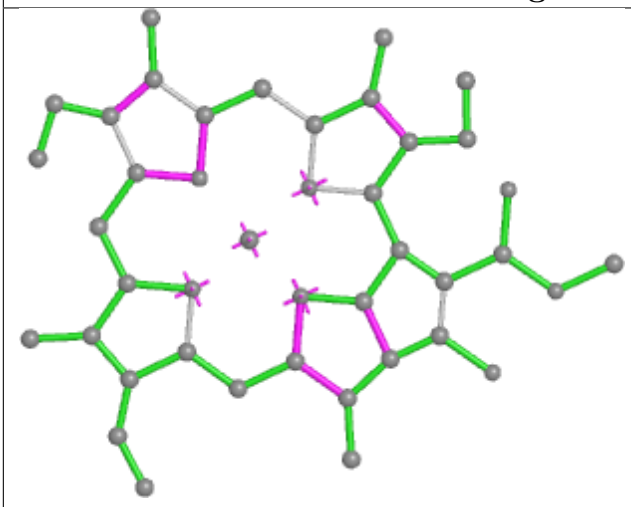


Rings

Ligand CLA 7 605



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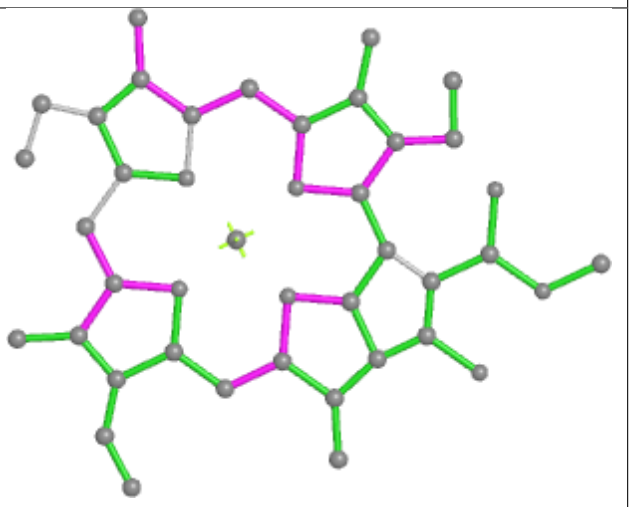
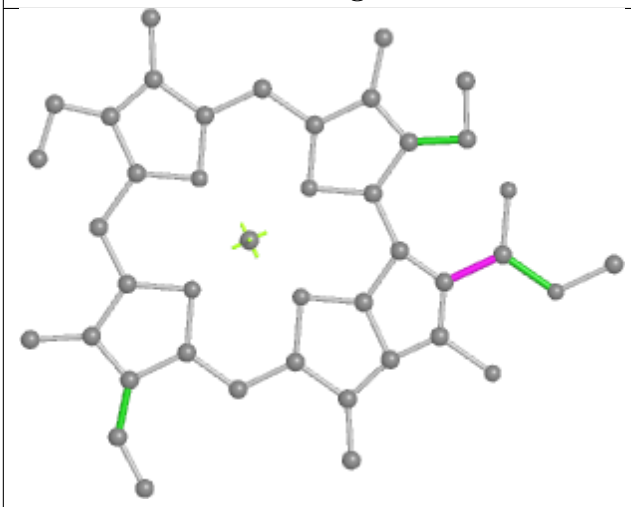


Bond angles



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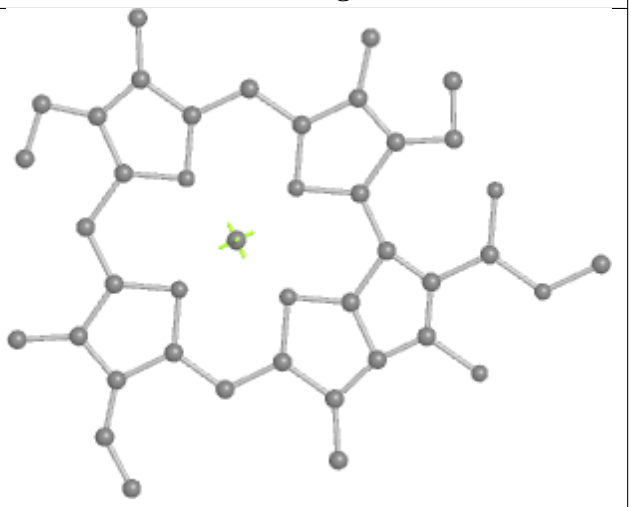
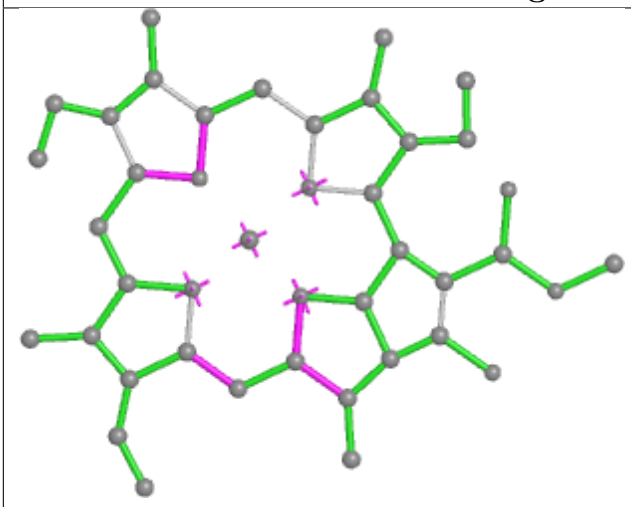


Rings

Ligand CLA 5 601



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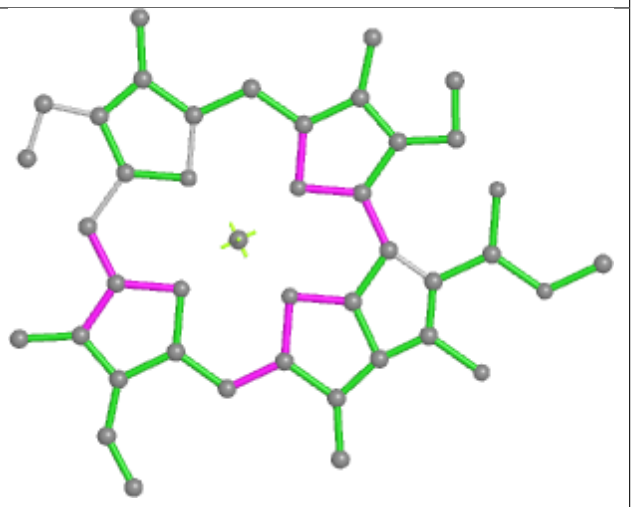
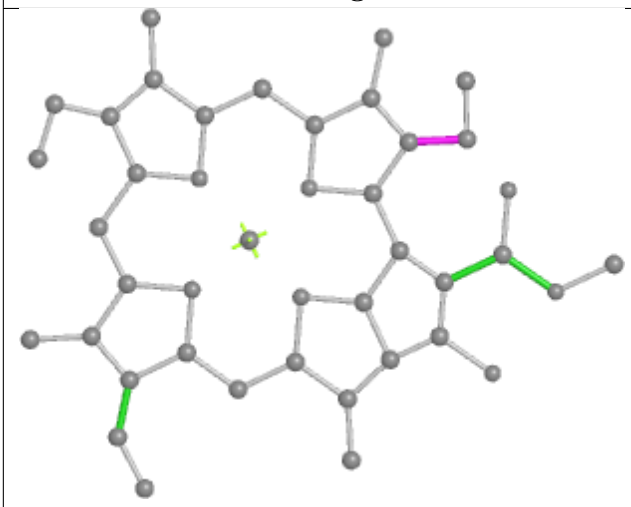


Bond angles



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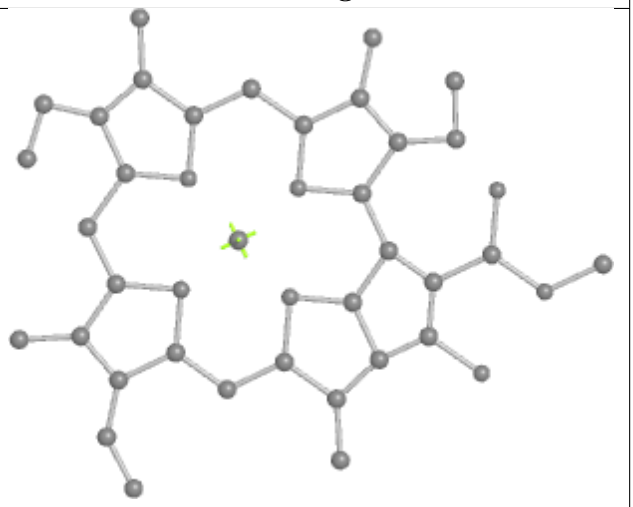
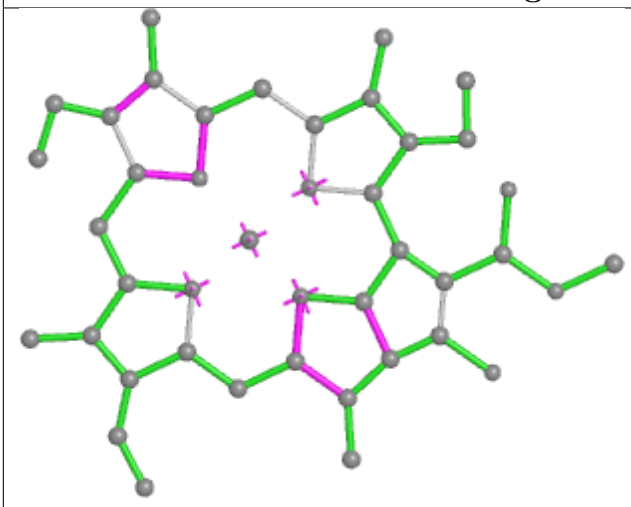
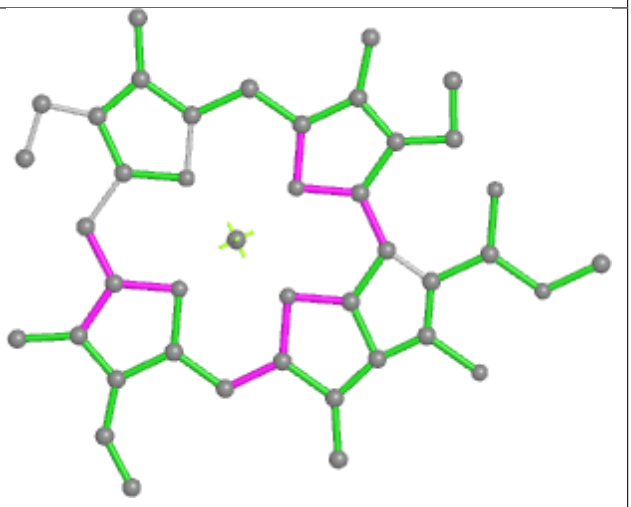


Rings

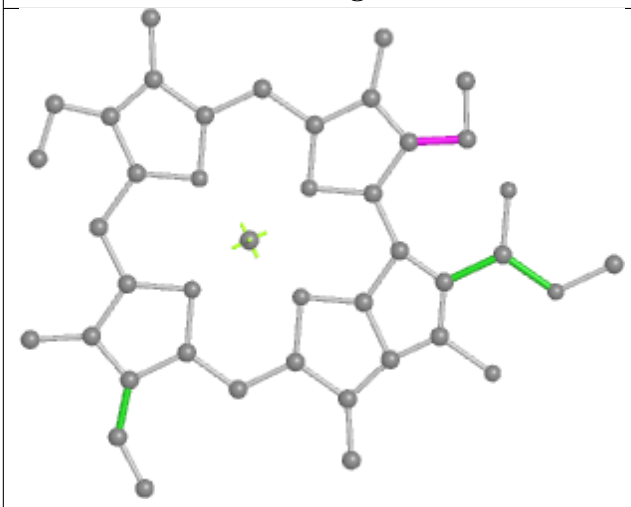
Ligand CLA B 816



Bond lengths



Bond angles



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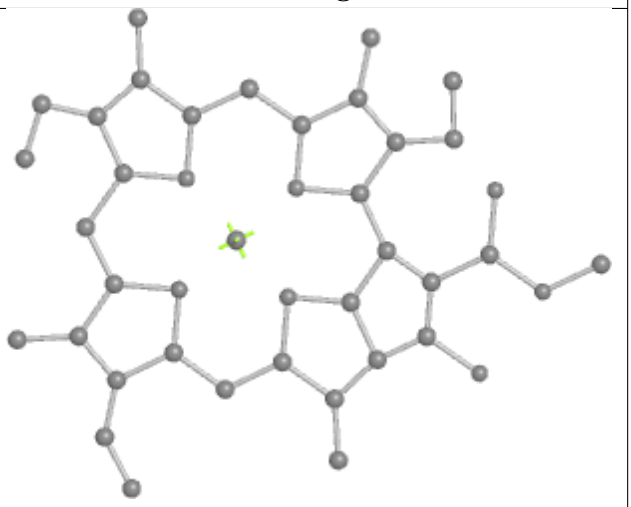
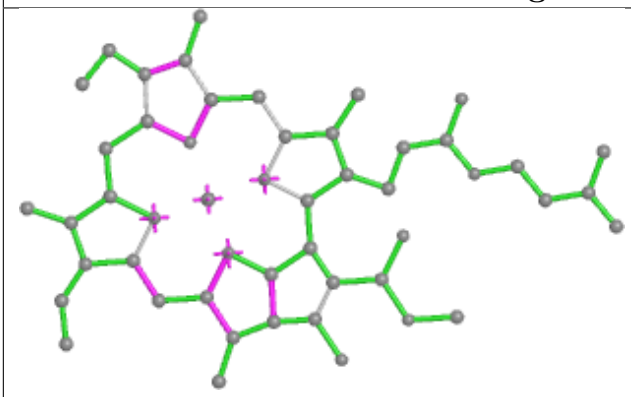


Rings

Ligand CLA 7 608



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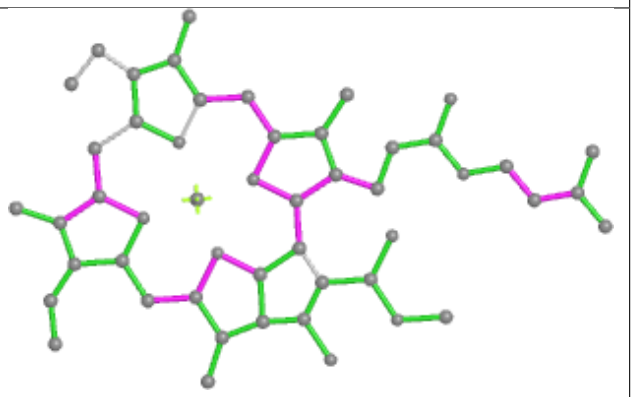
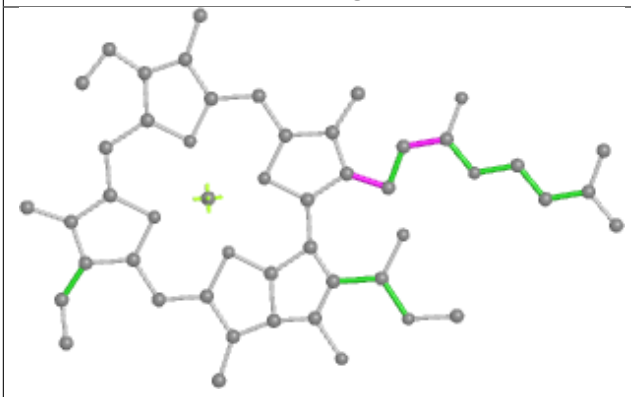


Bond angles



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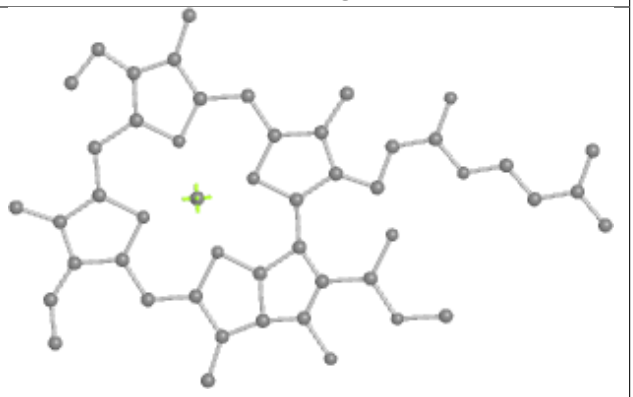
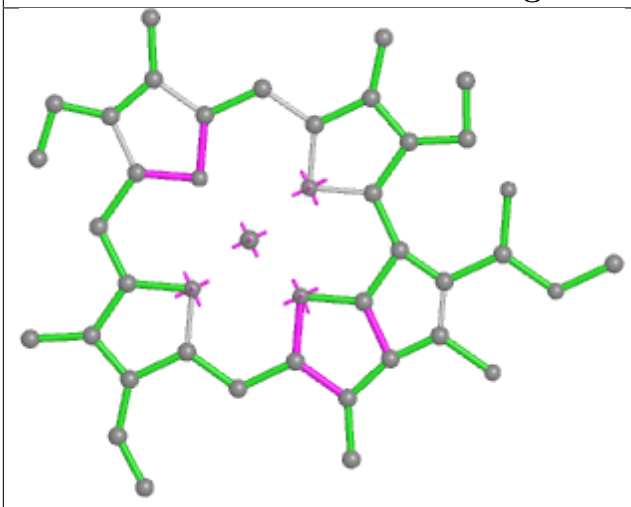
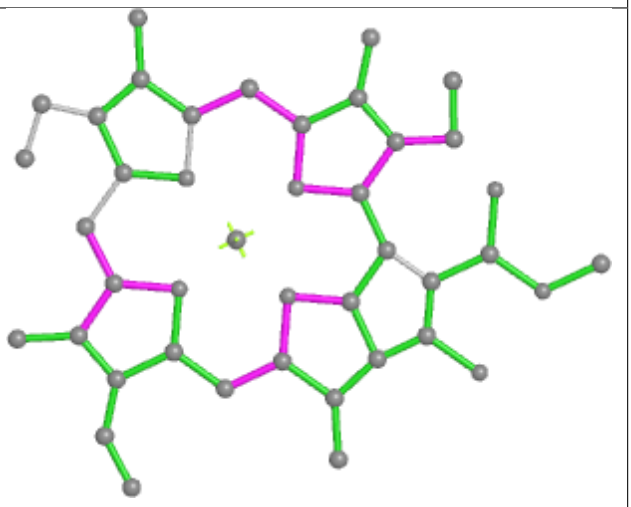


Rings

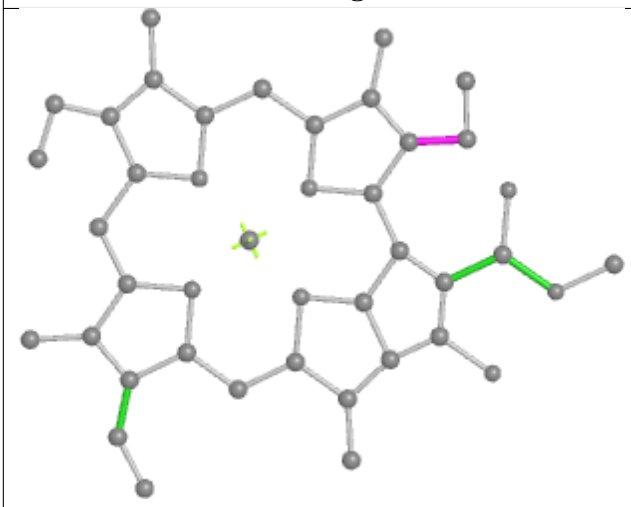
Ligand CLA A 819



Bond lengths



Bond angles



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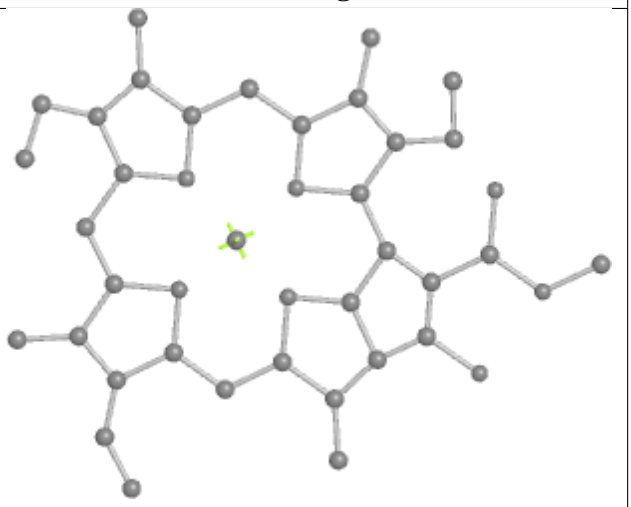
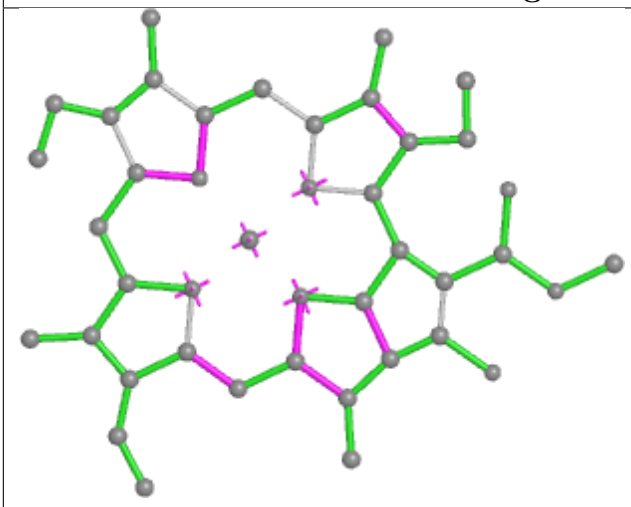


Rings

Ligand CLA A 802



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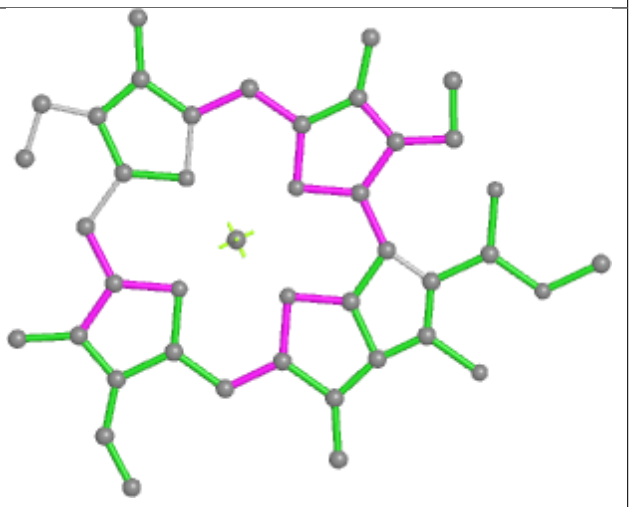
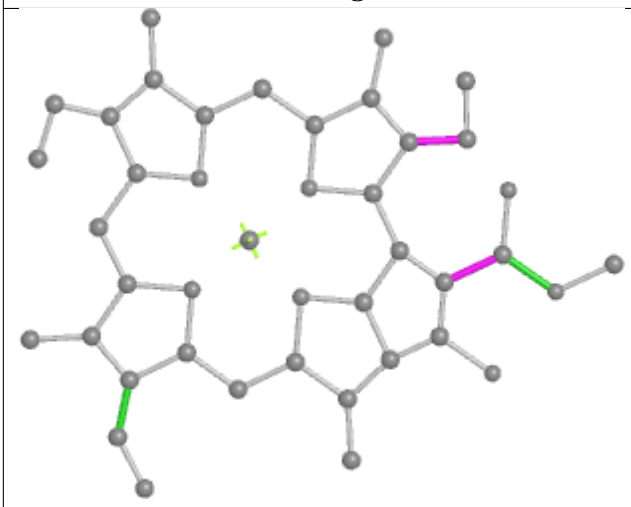
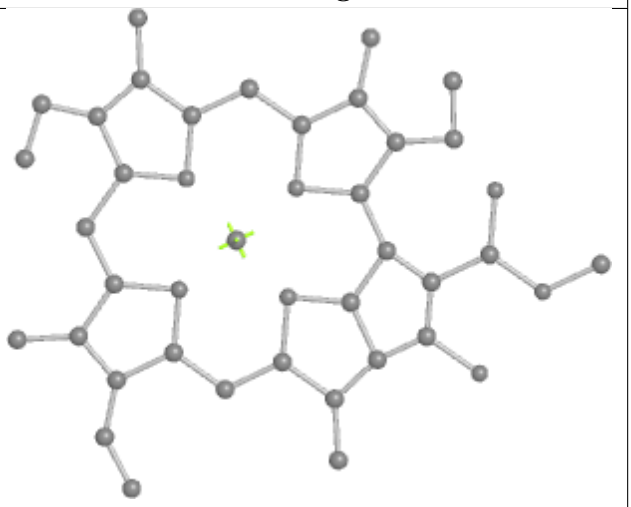


Bond angles

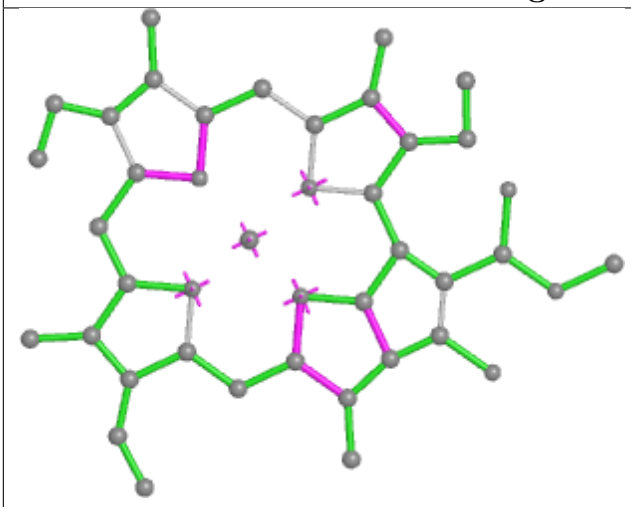


Torsions



Rings

Ligand CLA 8 605



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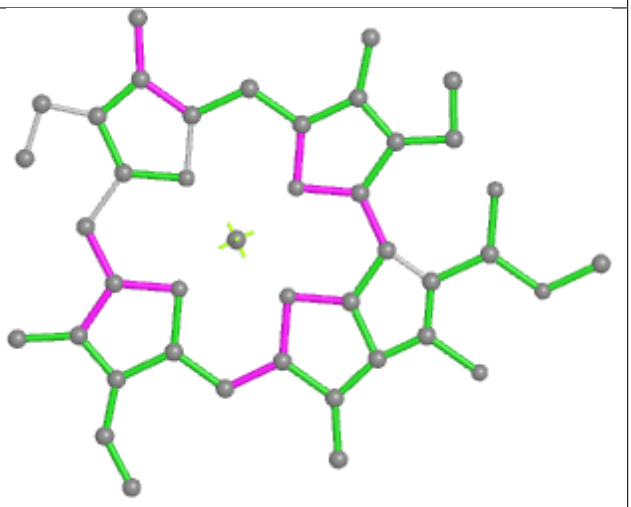
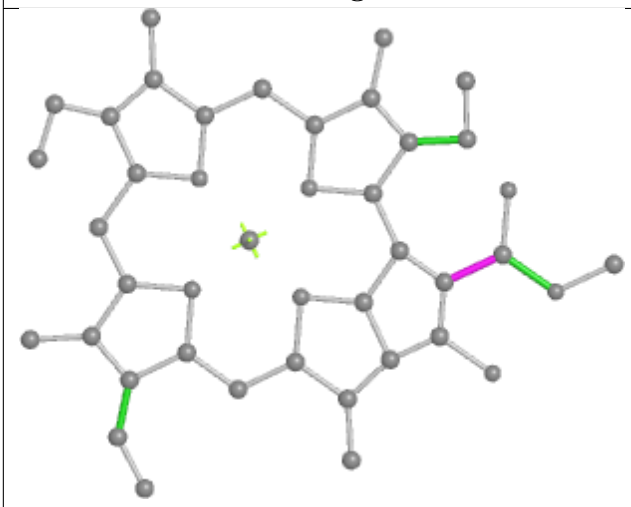


Bond angles



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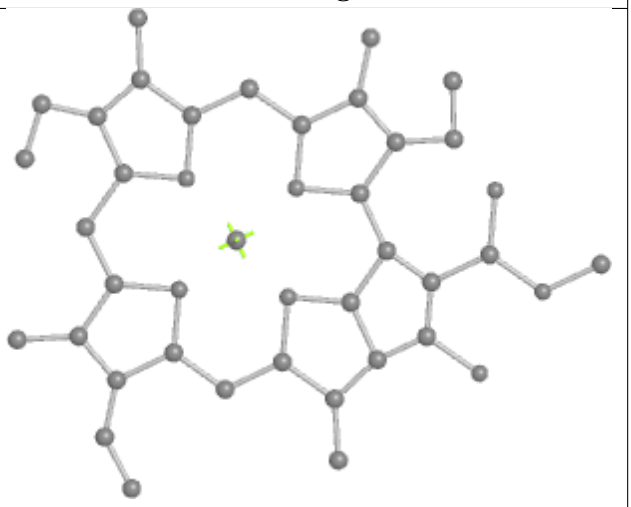
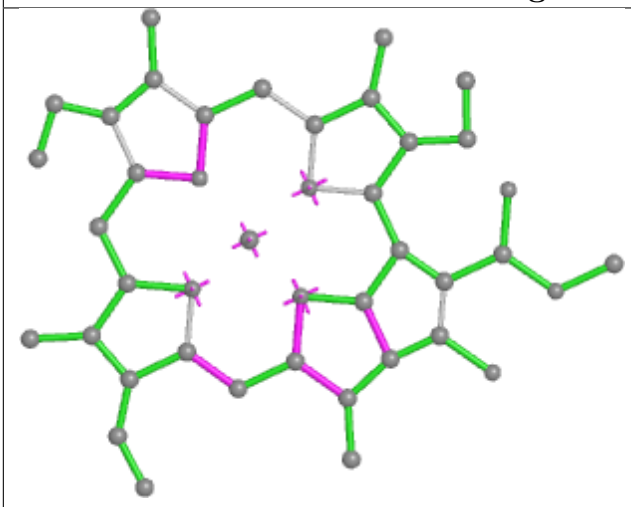
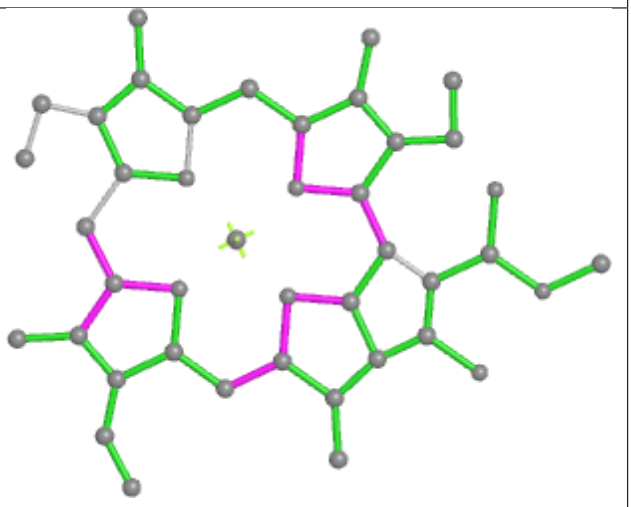


Rings

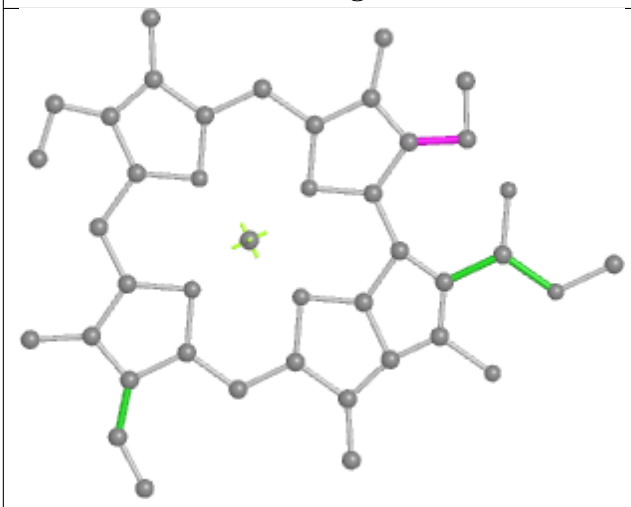
Ligand CLA 5 608



Bond lengths



Bond angles



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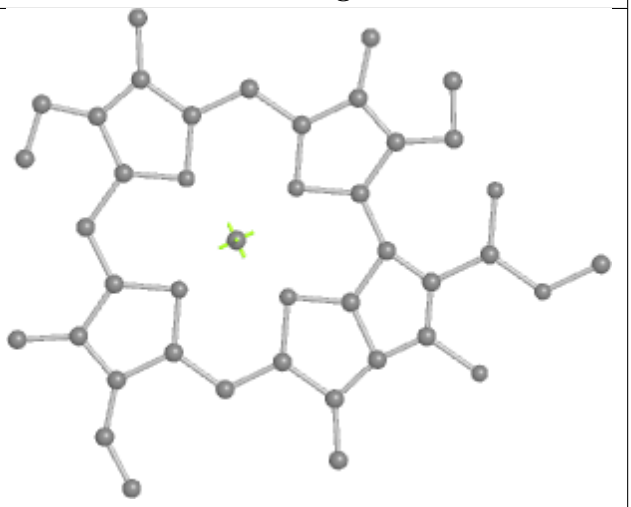
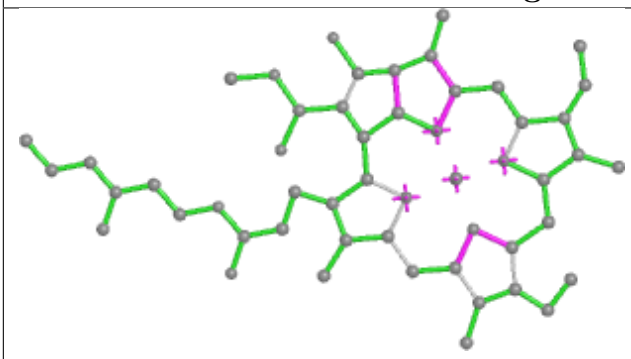
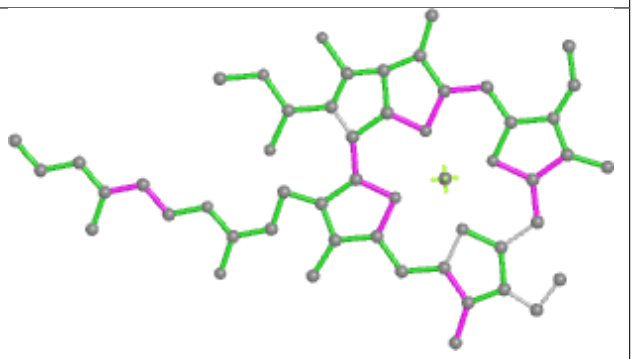
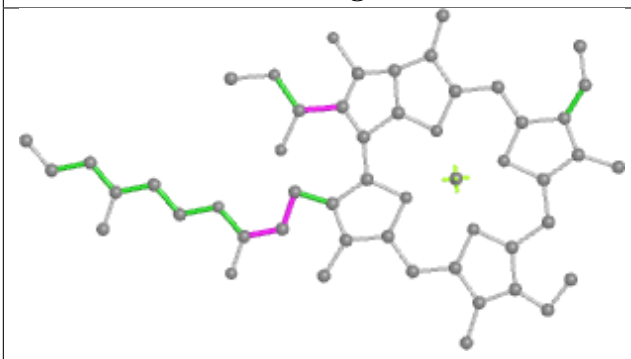
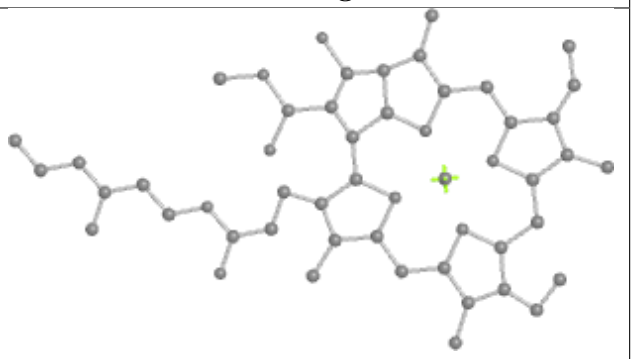
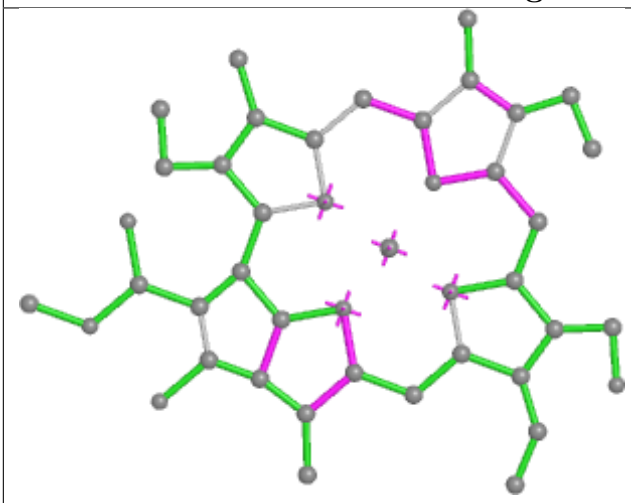


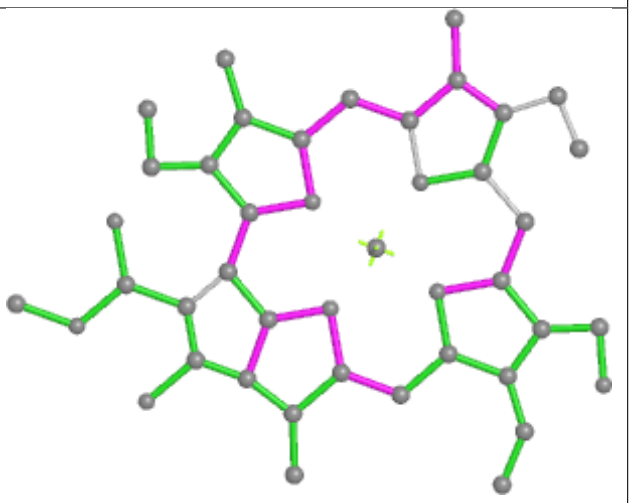
Rings

Ligand CLA A 843	
	
Bond lengths	**Bond angles**
	
Torsions	**Rings**

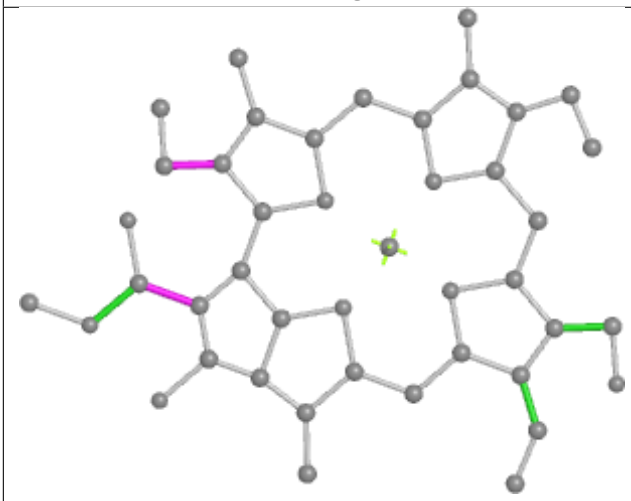
Ligand CHL Z 605



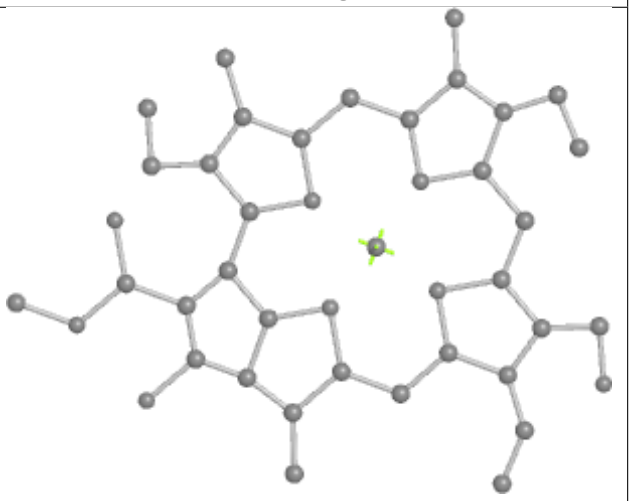
Bond lengths



Bond angles

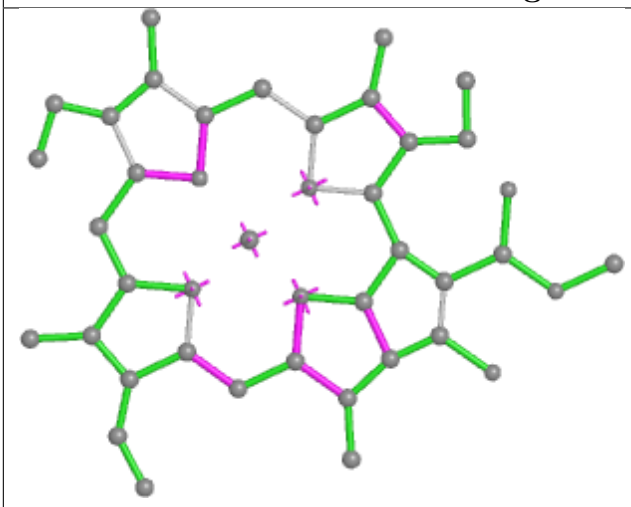


Torsions

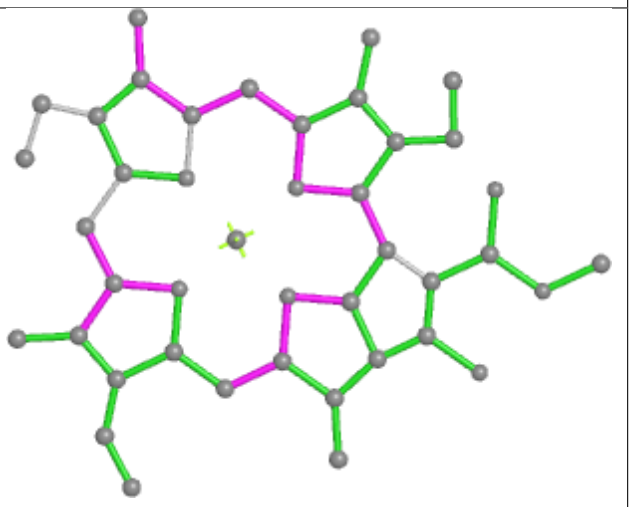


Rings

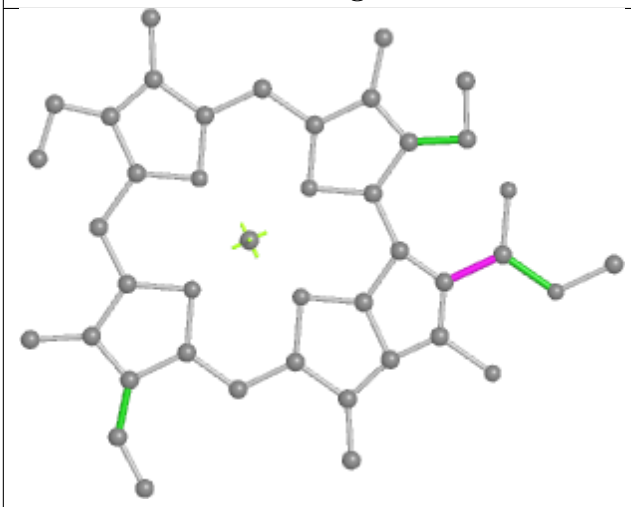
Ligand CLA A 837



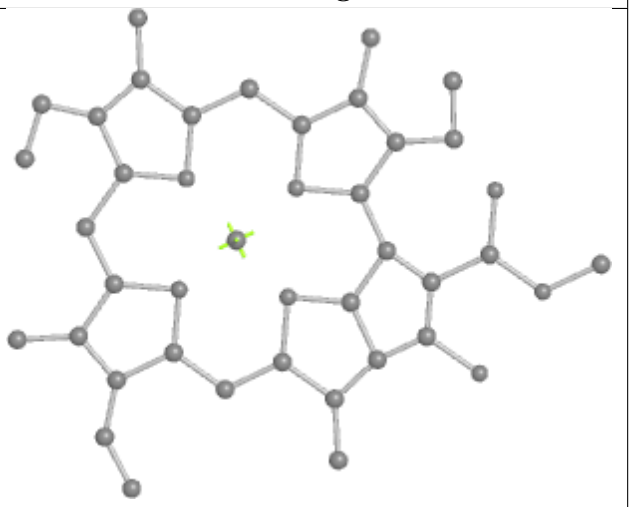
Bond lengths



Bond angles

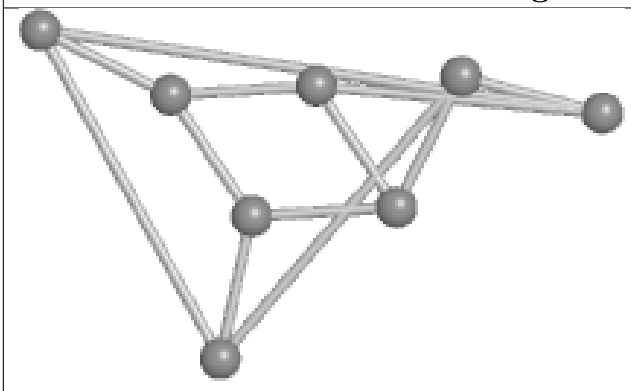


Torsions



Rings

Ligand SF4 C 102



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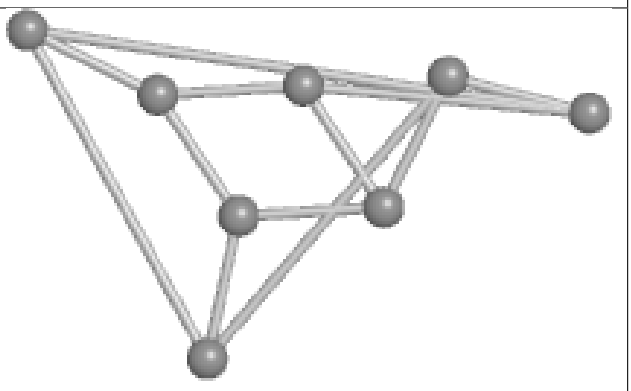

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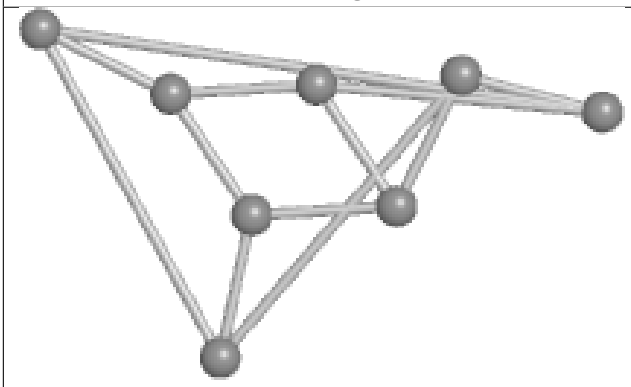

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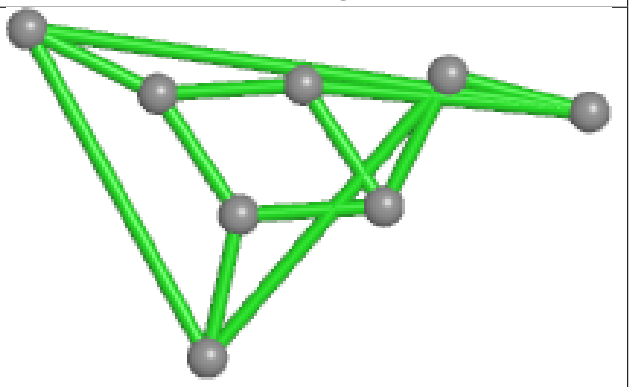
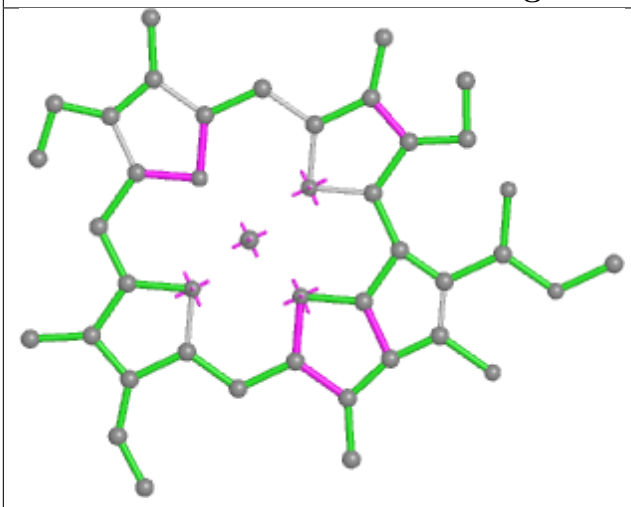


Rings

Ligand CLA A 832



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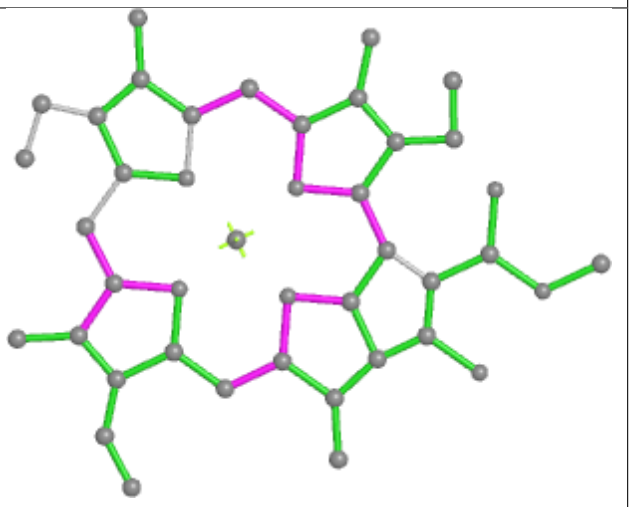
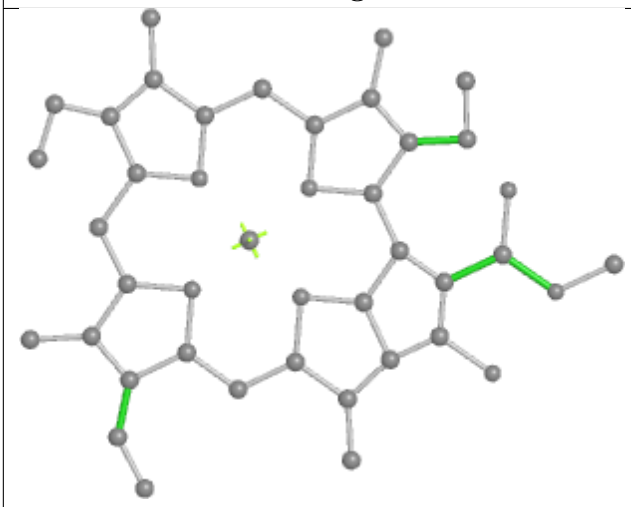


Bond angles



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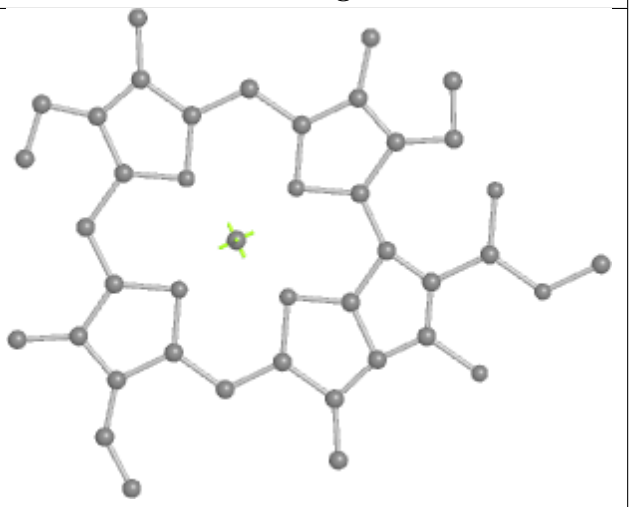
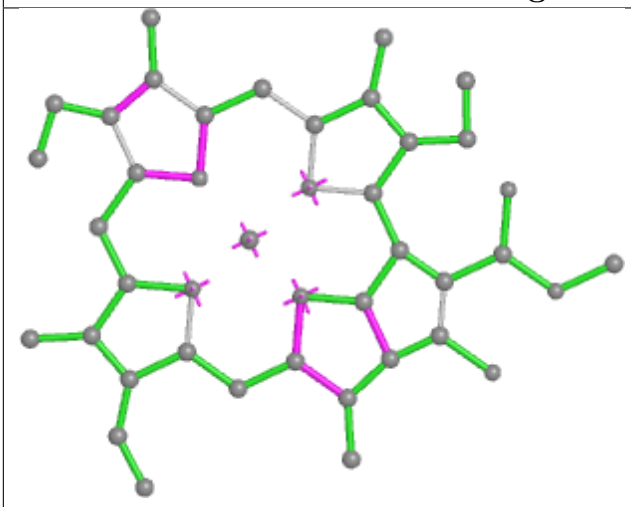


Rings

Ligand CLA 5 609



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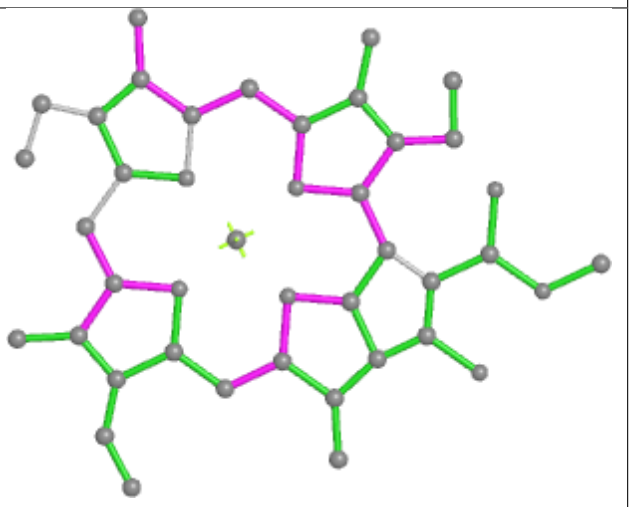
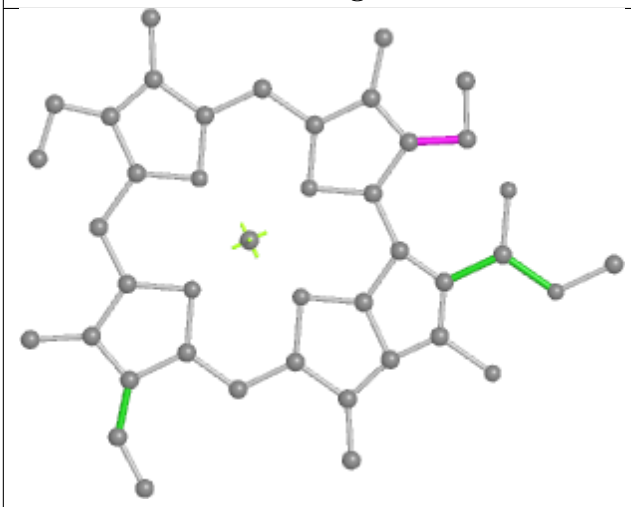


Bond angles



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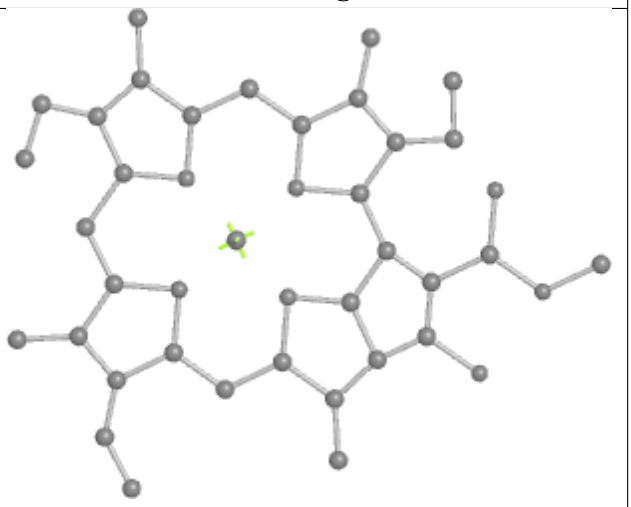
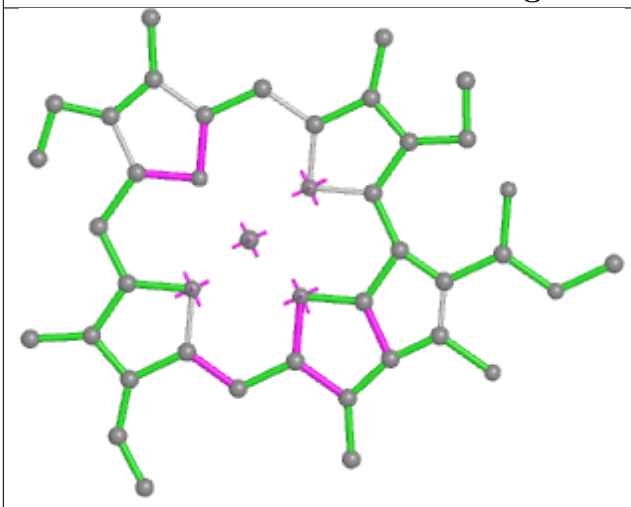
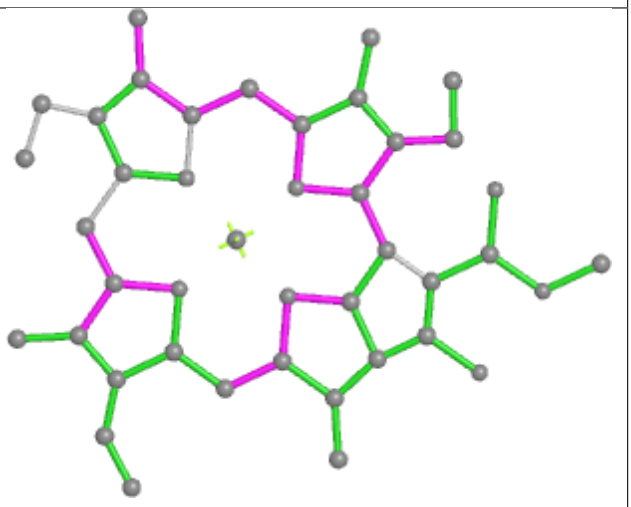


Rings

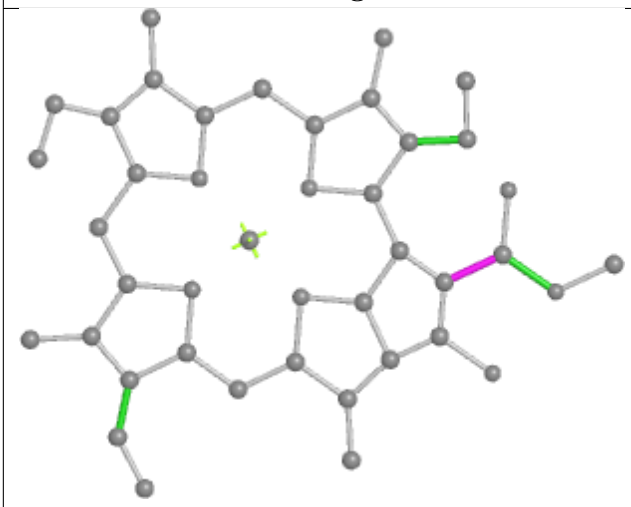
Ligand CLA A 835



Bond lengths



Bond angles



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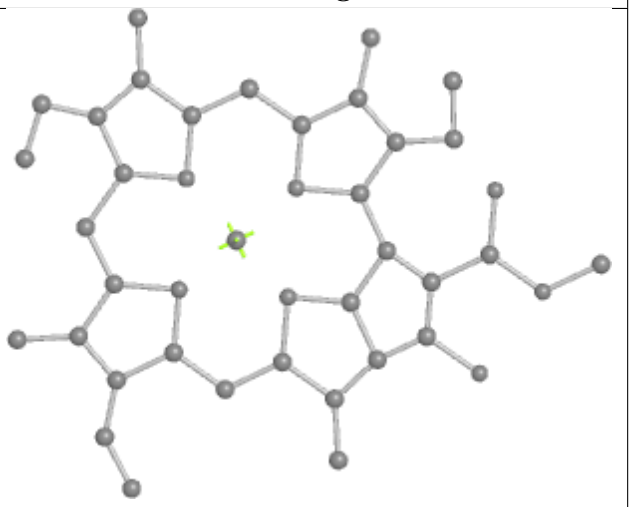
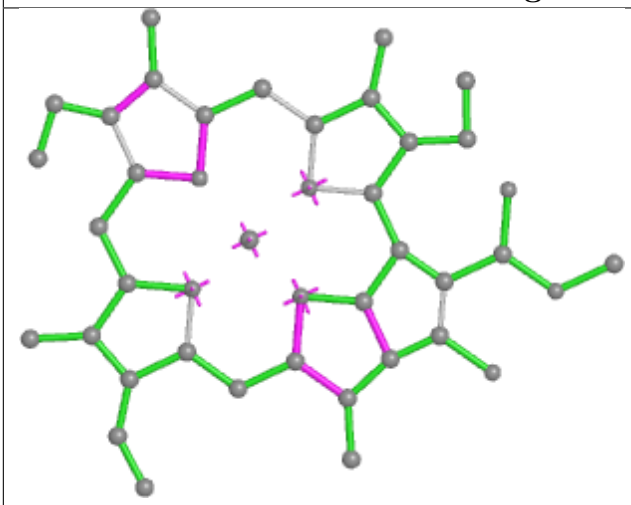


Rings

Ligand CLA B 818



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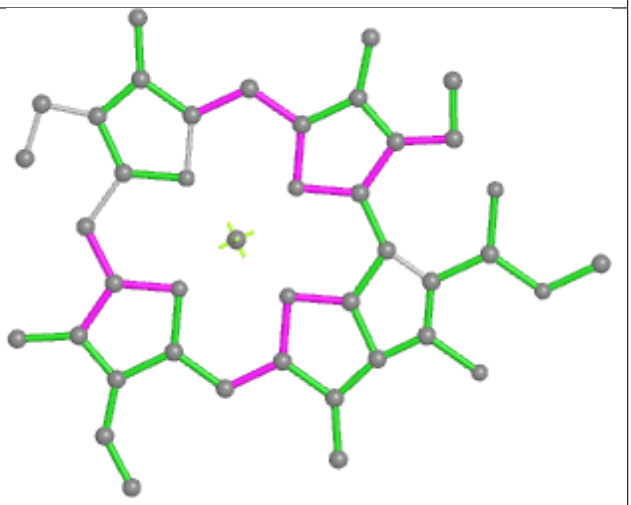
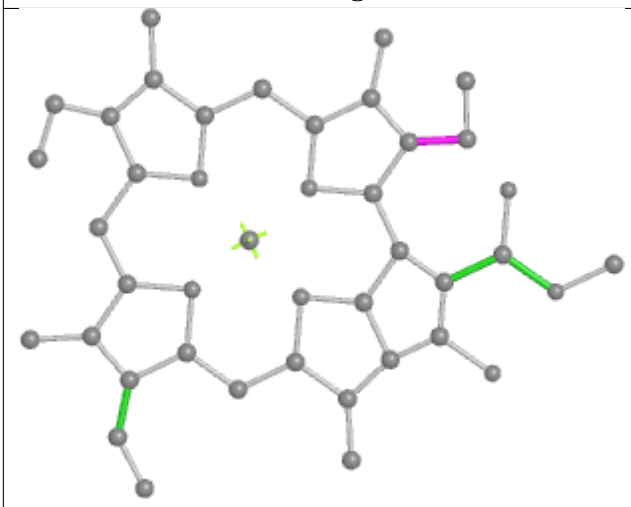


Bond angles



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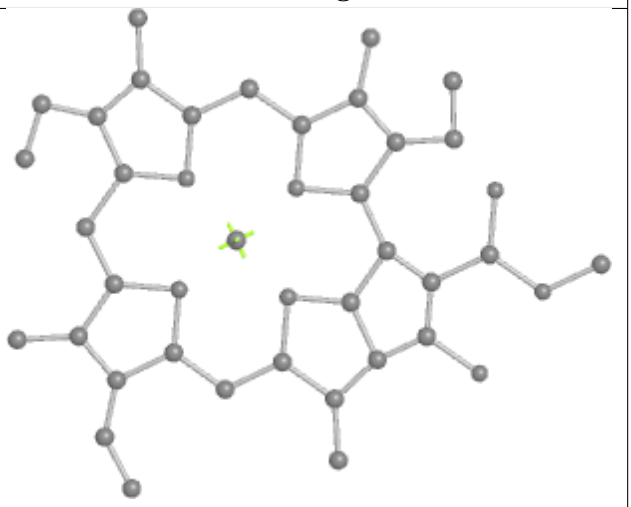
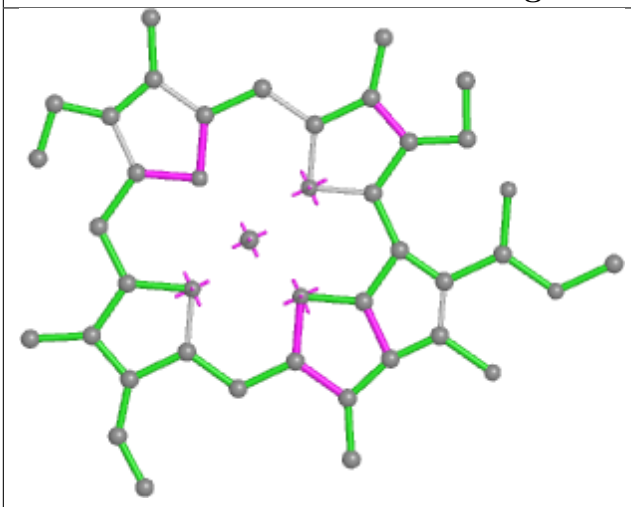
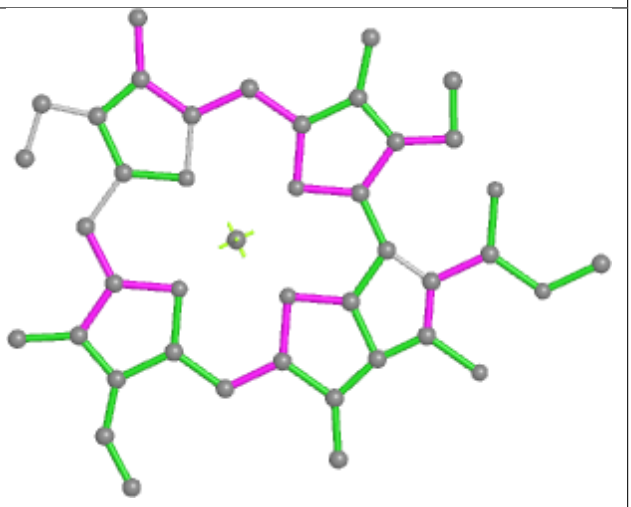


Rings

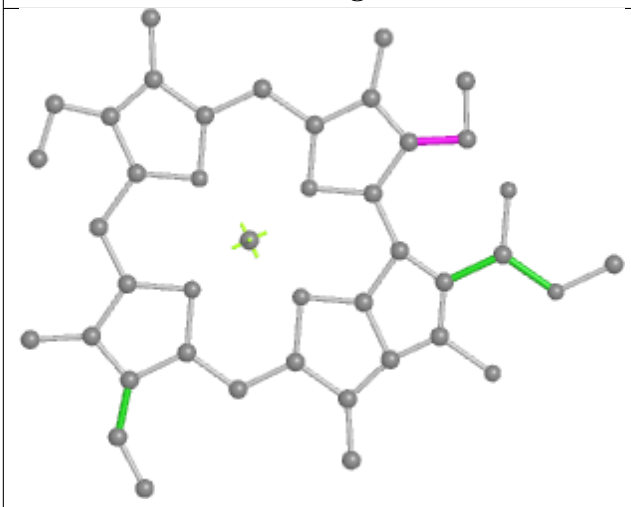
Ligand CLA B 801



Bond lengths



Bond angles



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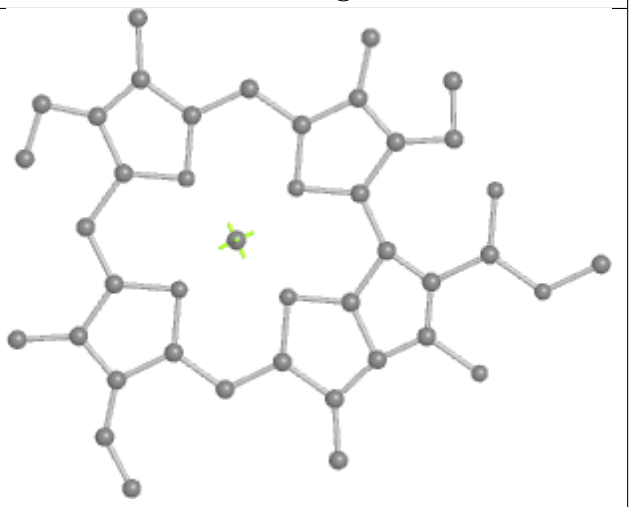
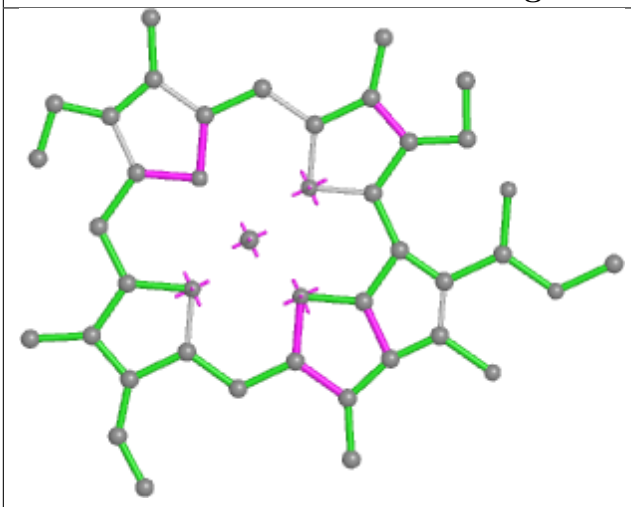


Rings

Ligand CLA B 840



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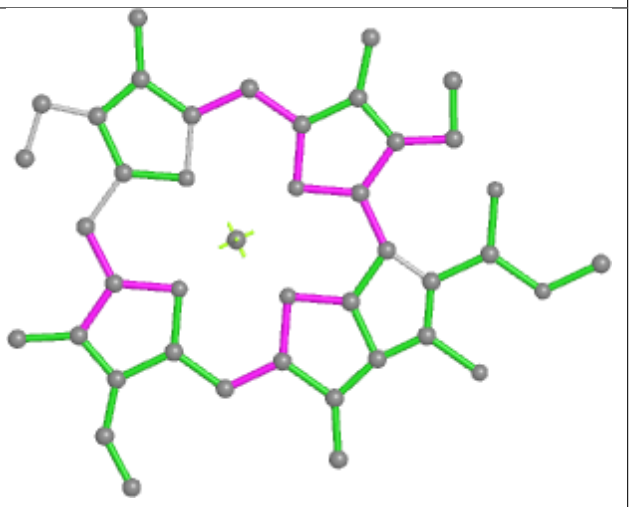
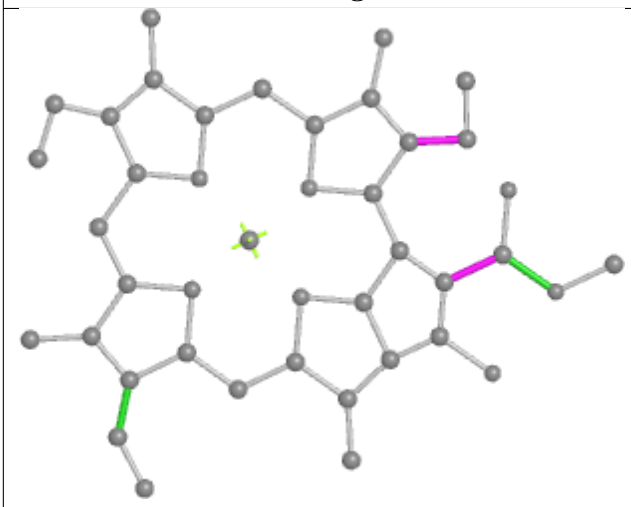


Bond angles



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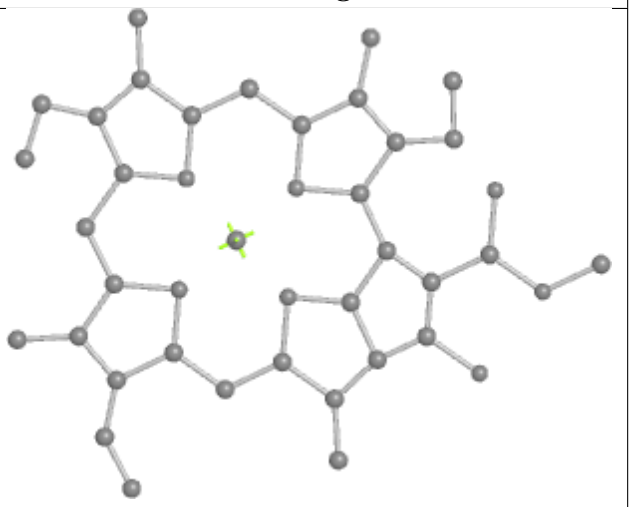
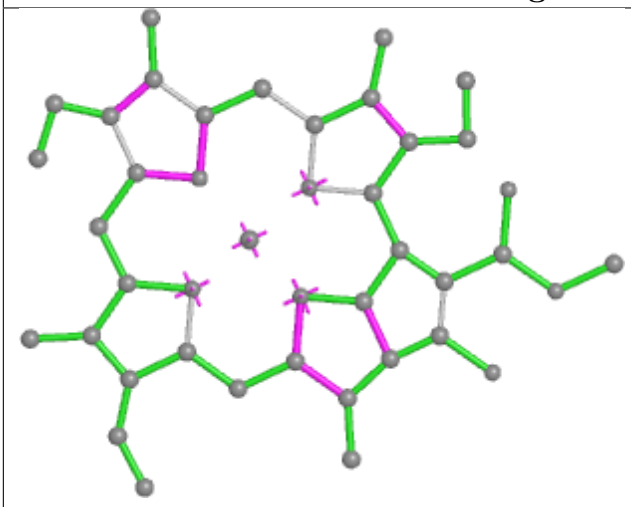
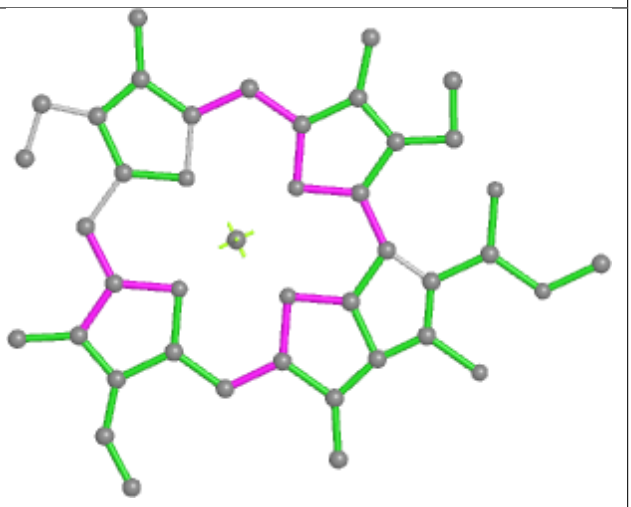


Rings

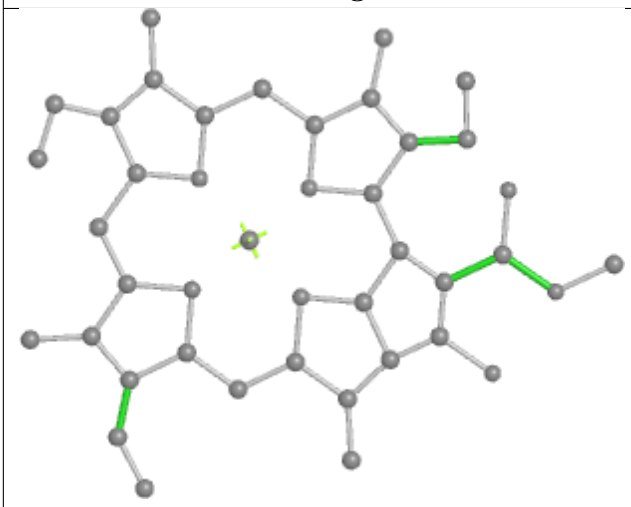
Ligand CLA 3 303



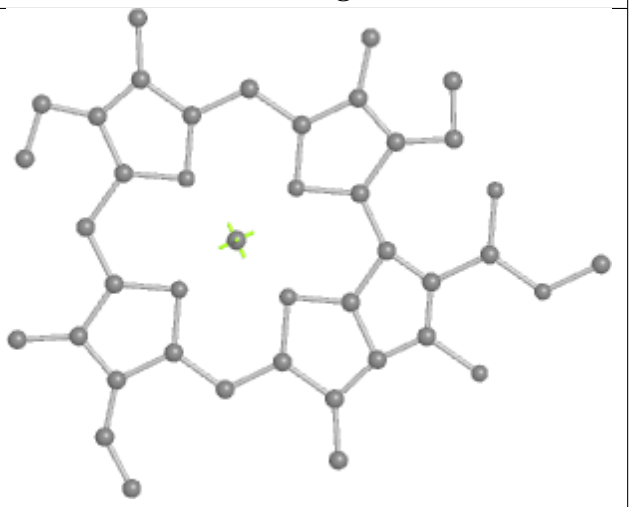
Bond lengths



Bond angles

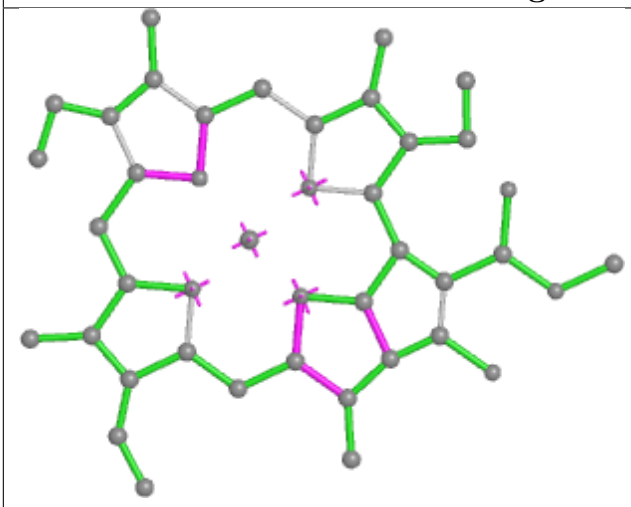


Torsions

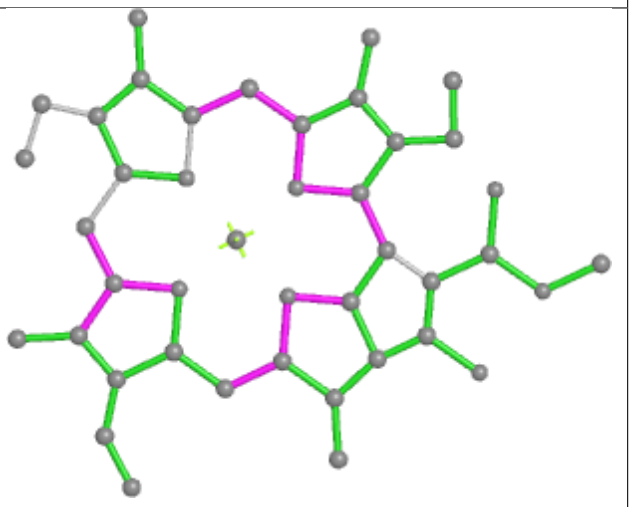


Rings

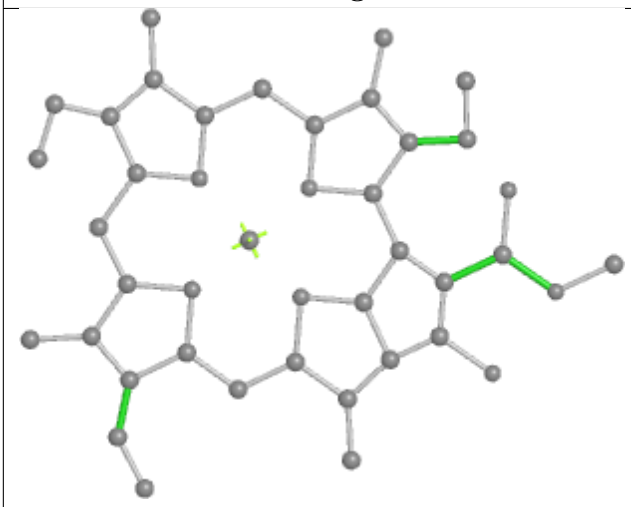
Ligand CLA 8 604



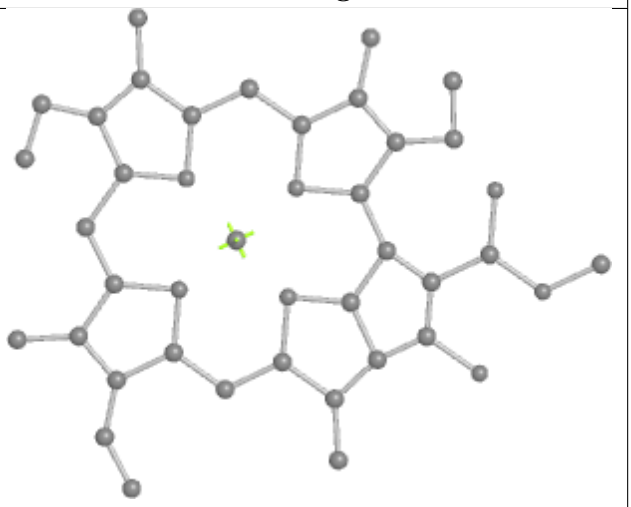
Bond lengths



Bond angles

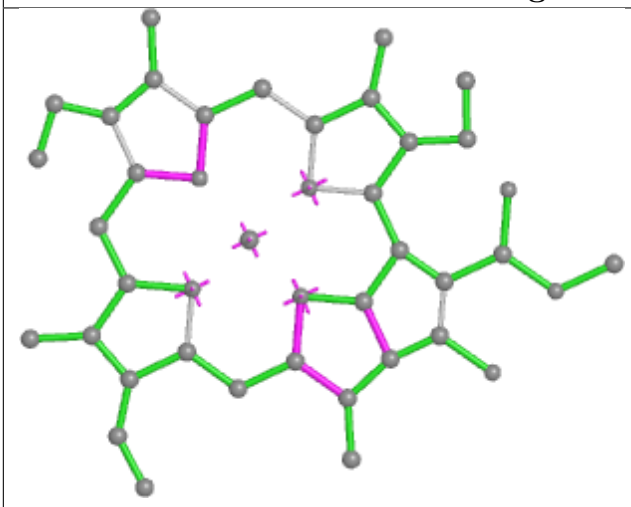


Torsions



Rings

Ligand CLA 8 614



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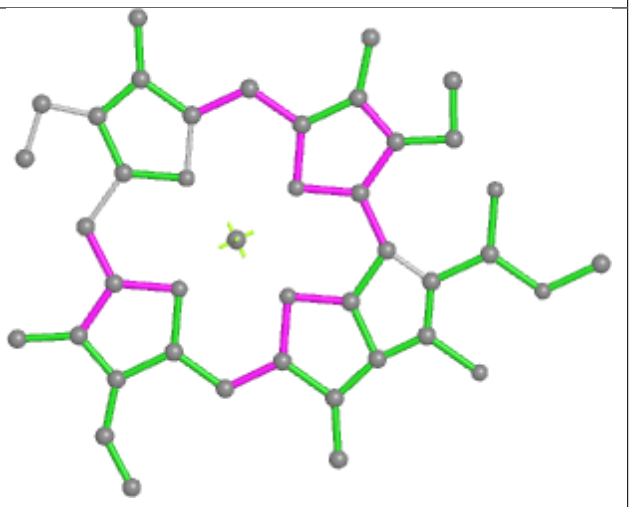
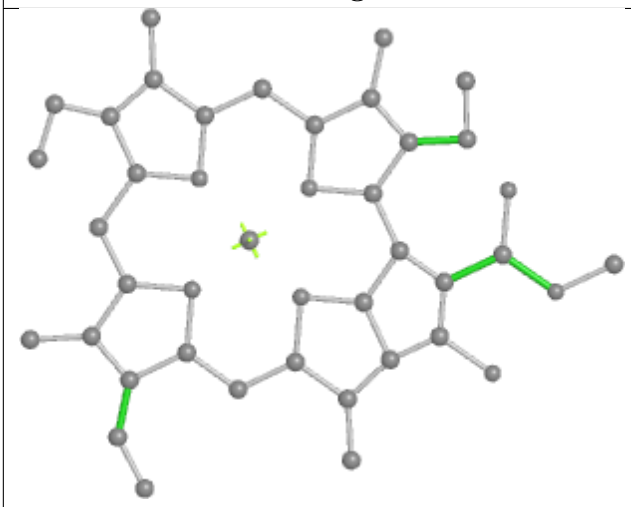
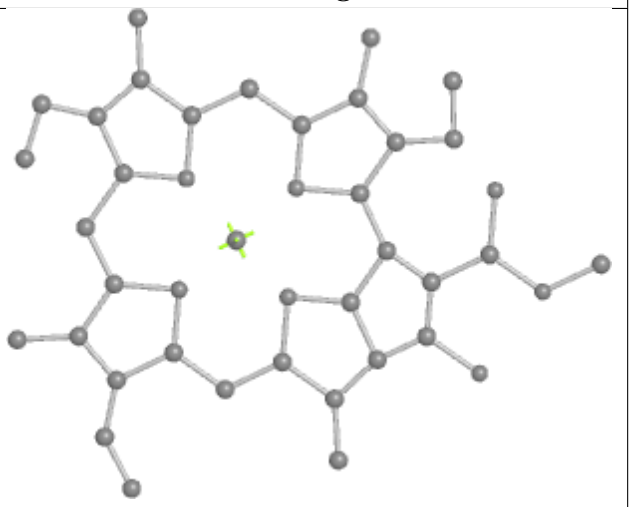


Bond angles

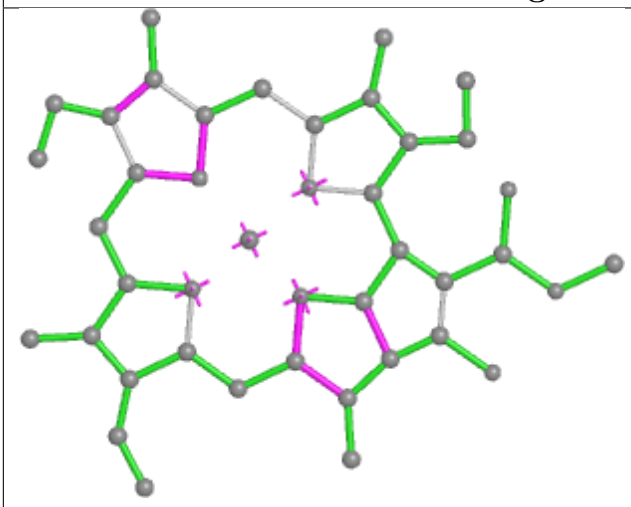


Torsions



Rings

Ligand CLA 8 601



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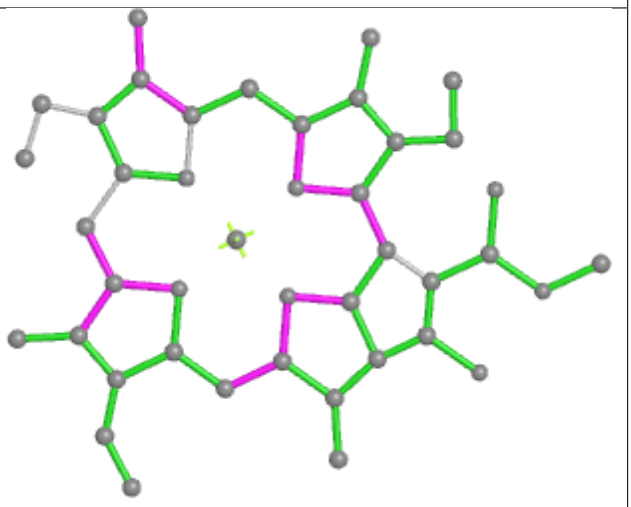
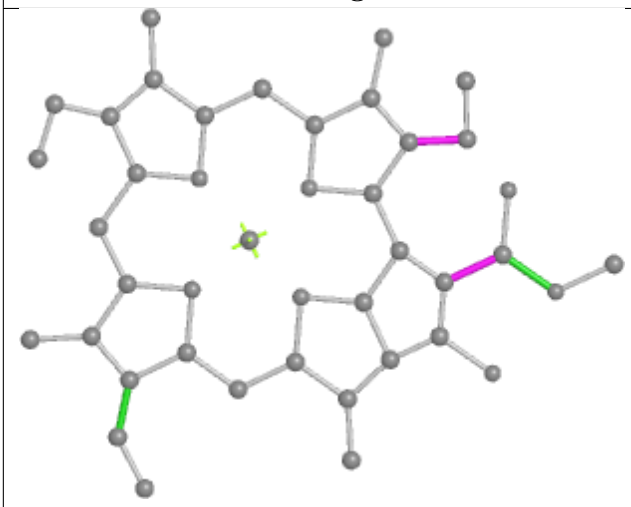


Bond angles



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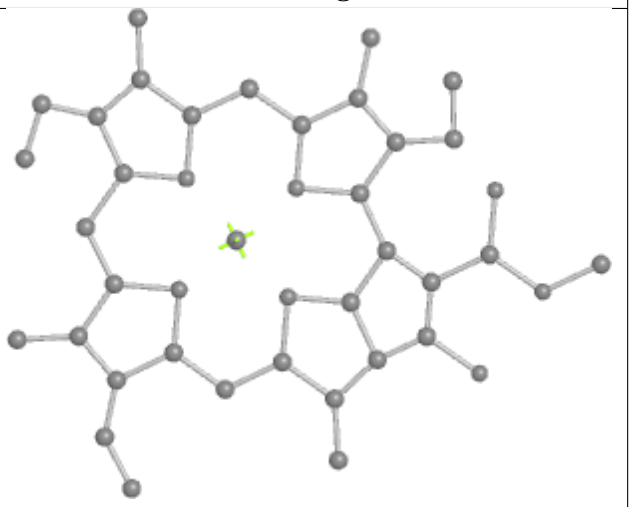
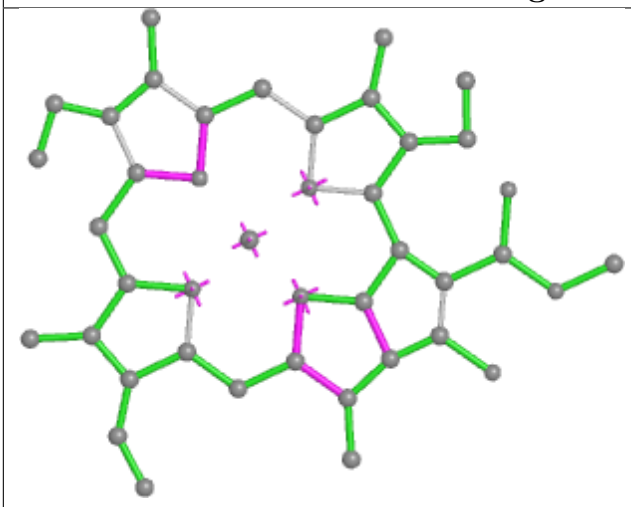
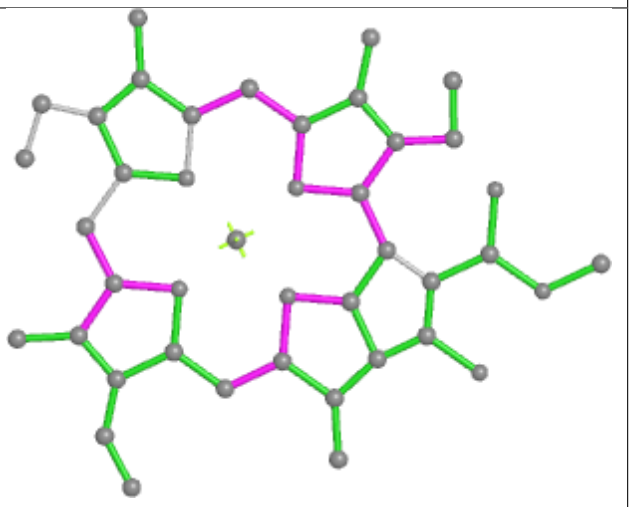


Rings

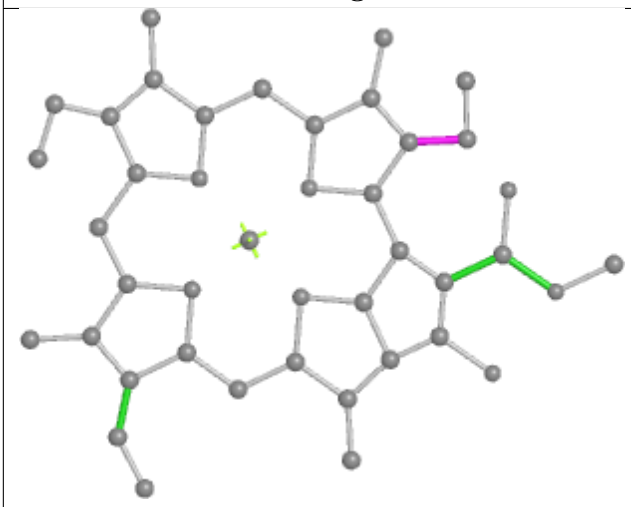
Ligand CLA 1 610



Bond lengths



Bond angles



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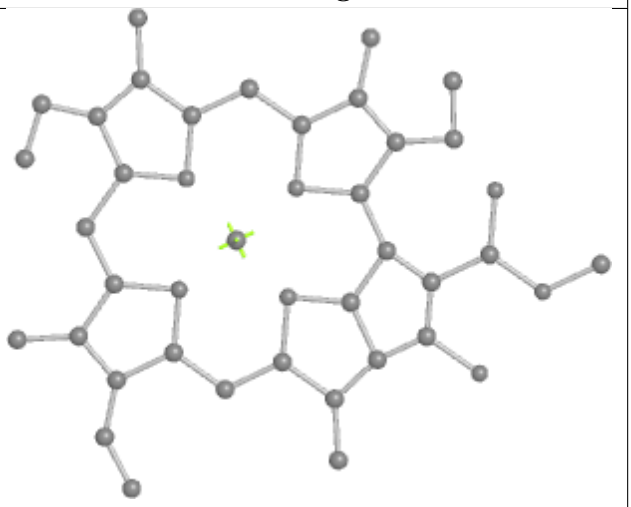
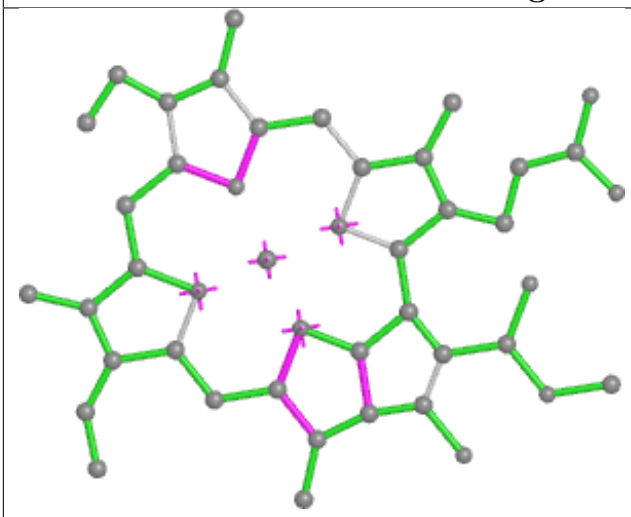
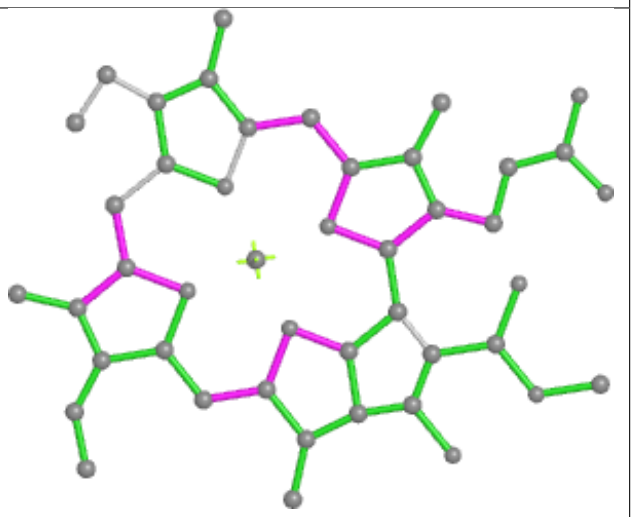


Rings

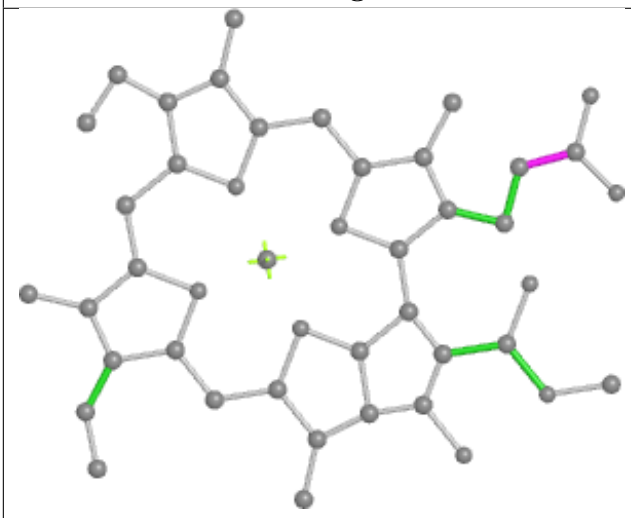
Ligand CLA 3 312



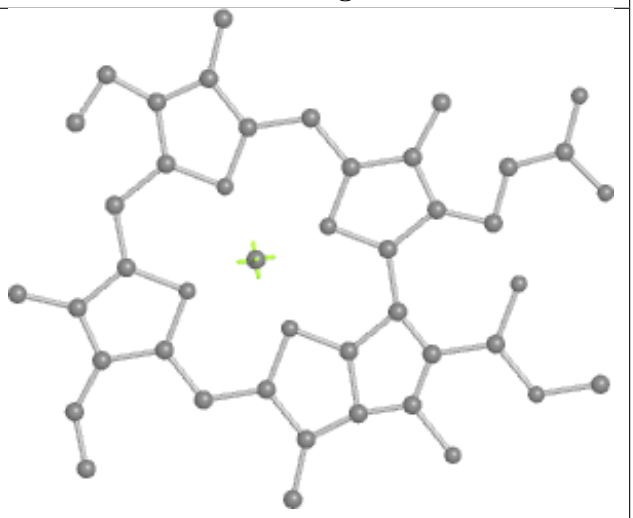
Bond lengths



Bond angles

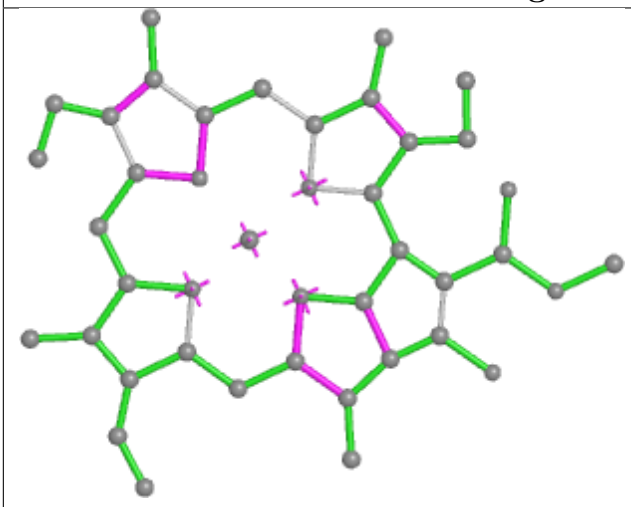


Torsions



Rings

Ligand CLA 1 611



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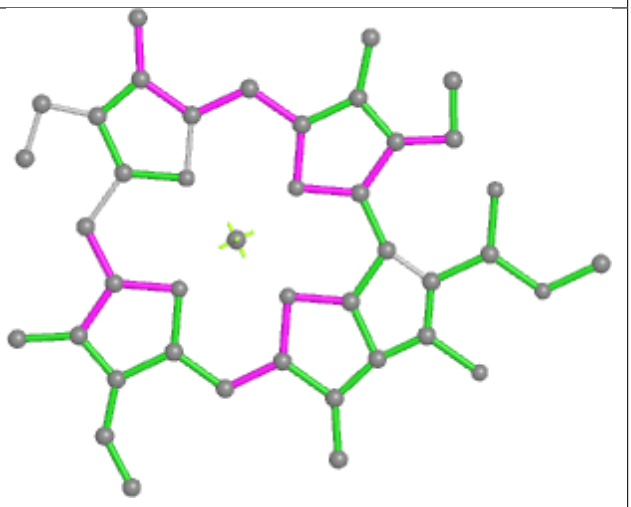
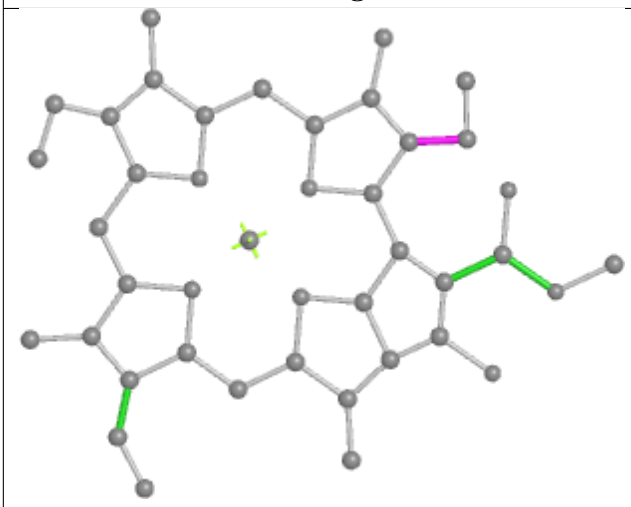


Bond angles



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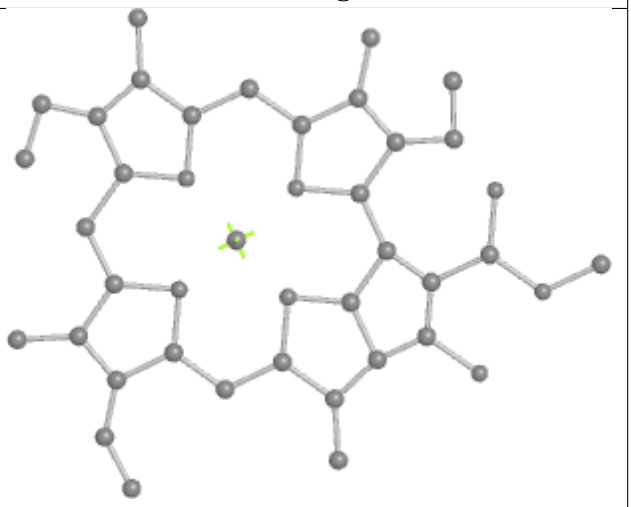
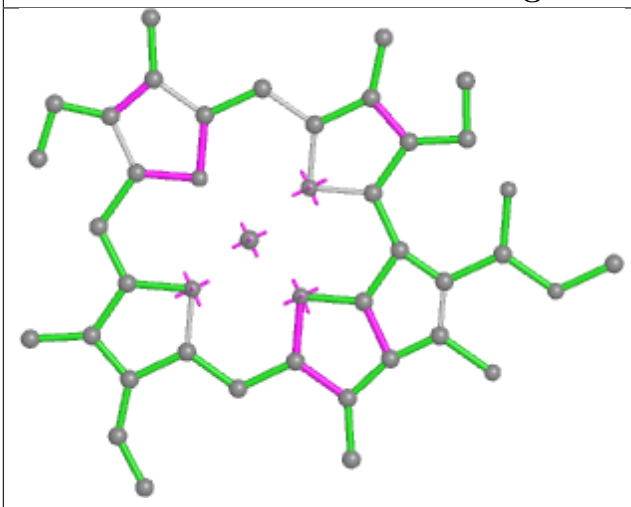
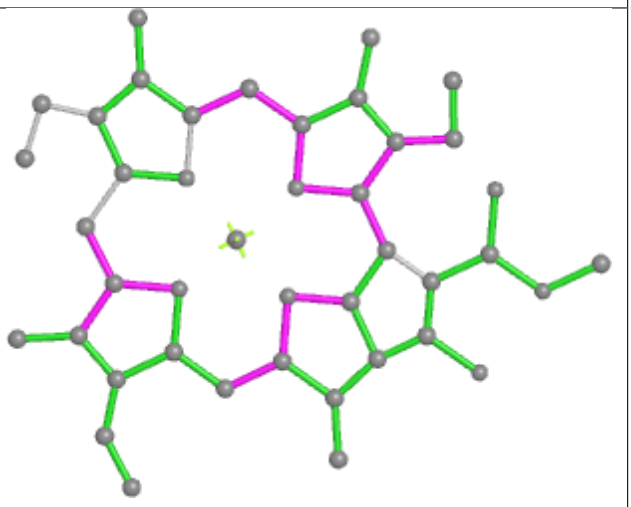


Rings

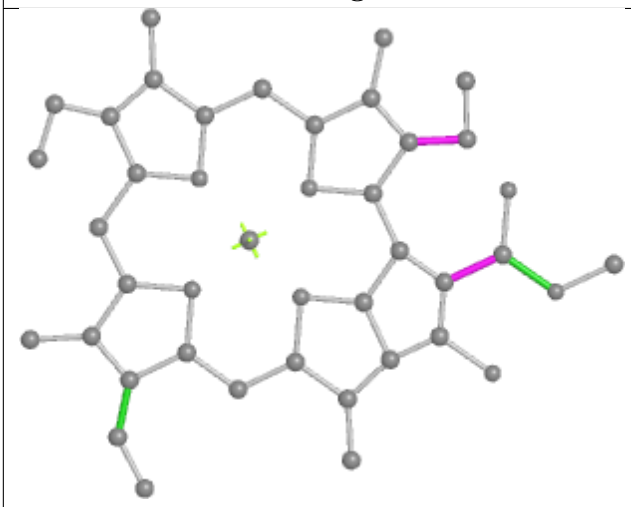
Ligand CLA A 820



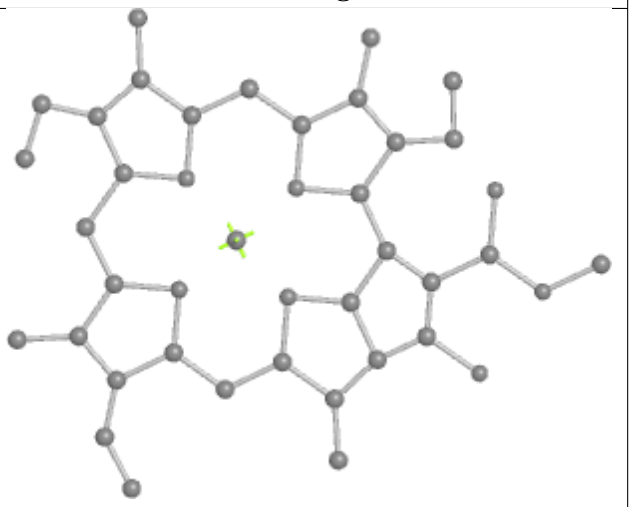
Bond lengths



Bond angles

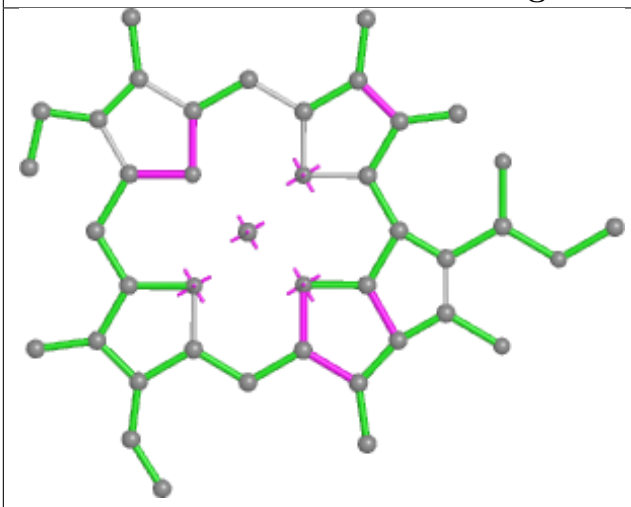


Torsions

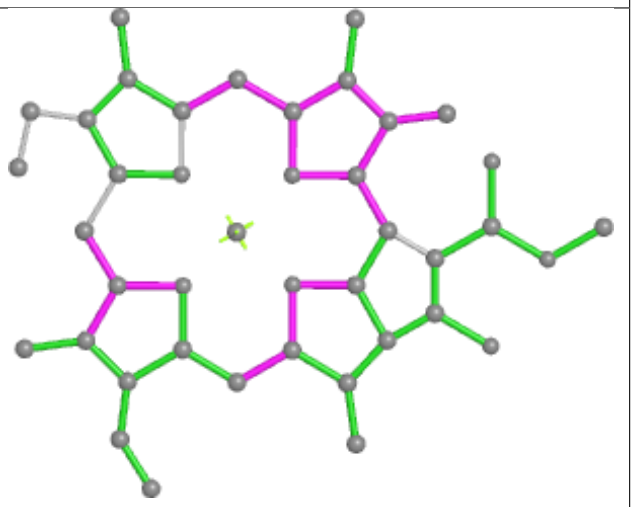


Rings

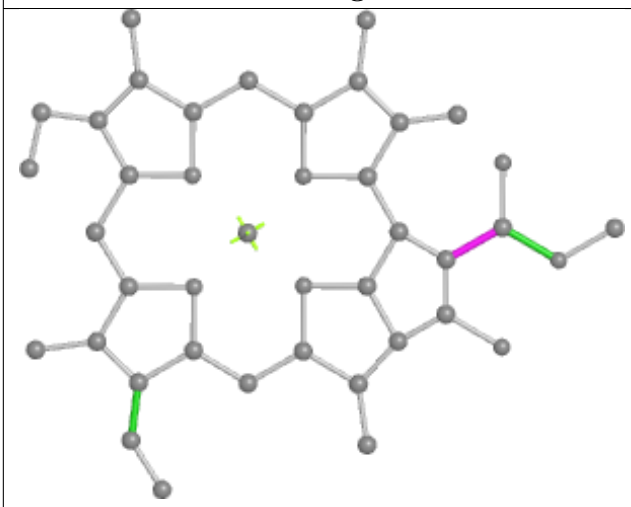
Ligand CLA 3 309



Bond lengths



Bond angles



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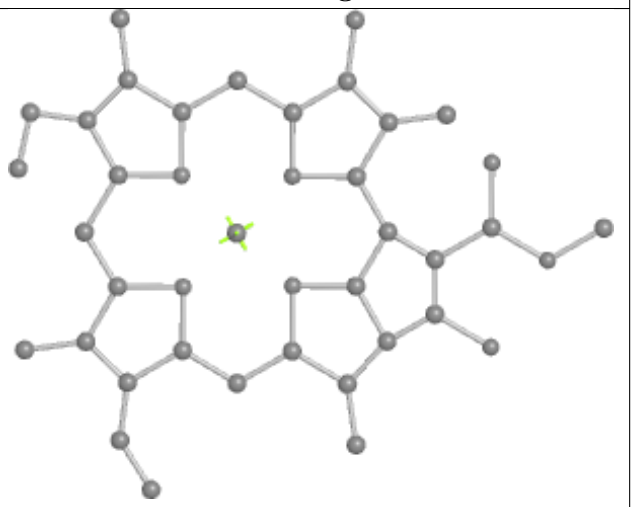
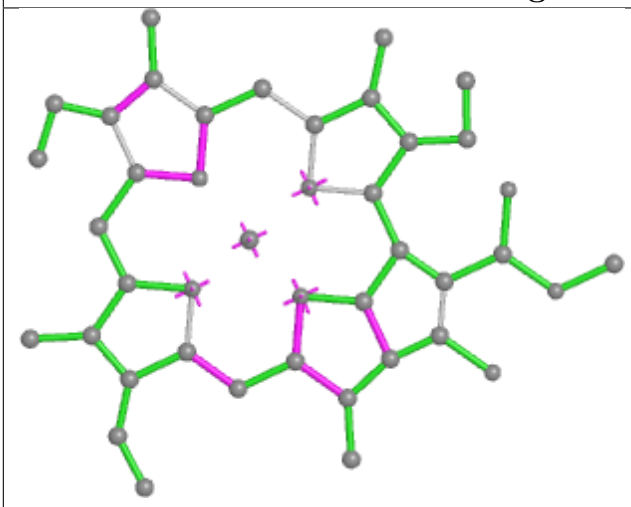


Rings

Ligand CLA 5 612



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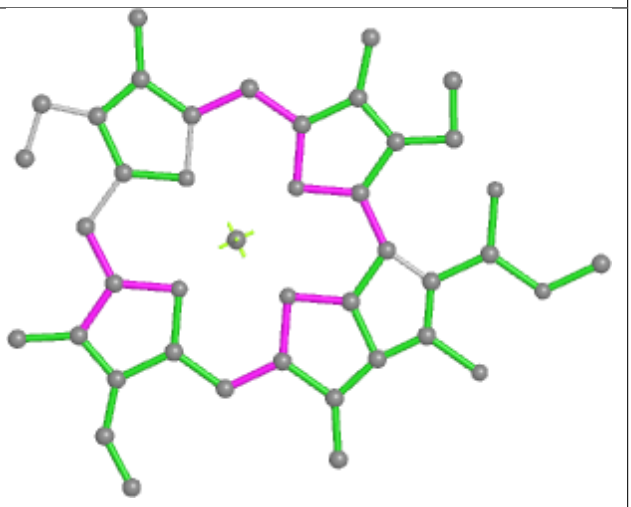
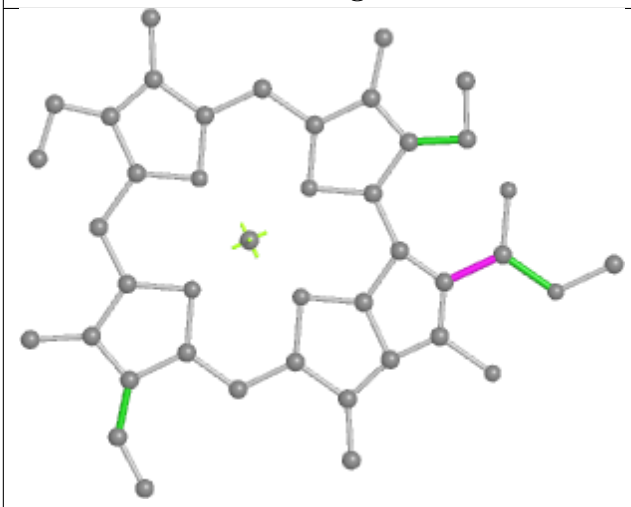


Bond angles



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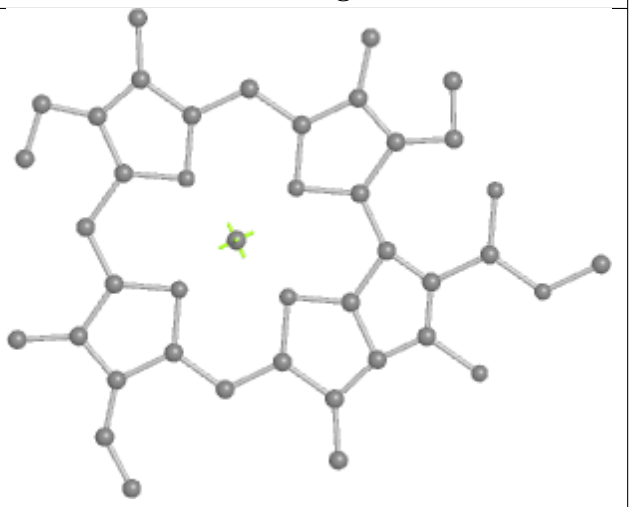
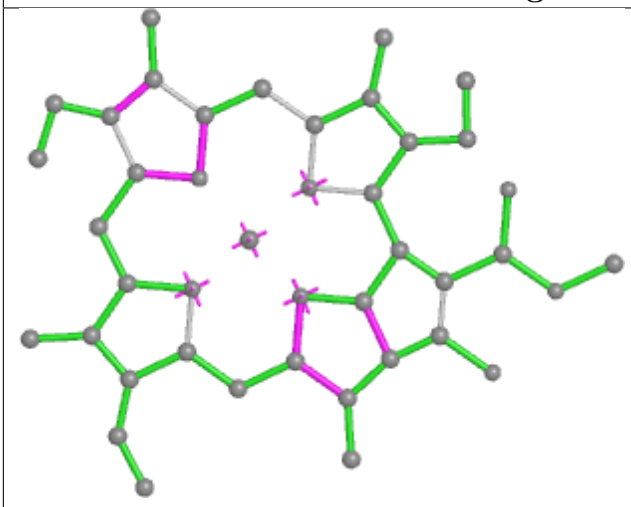


Rings

Ligand CLA Z 606



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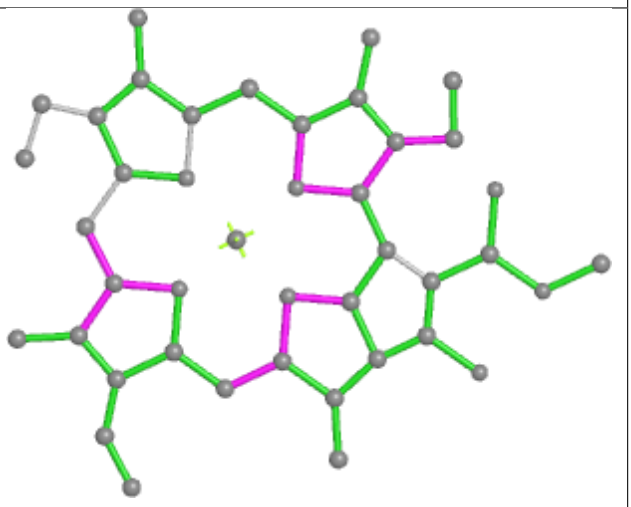
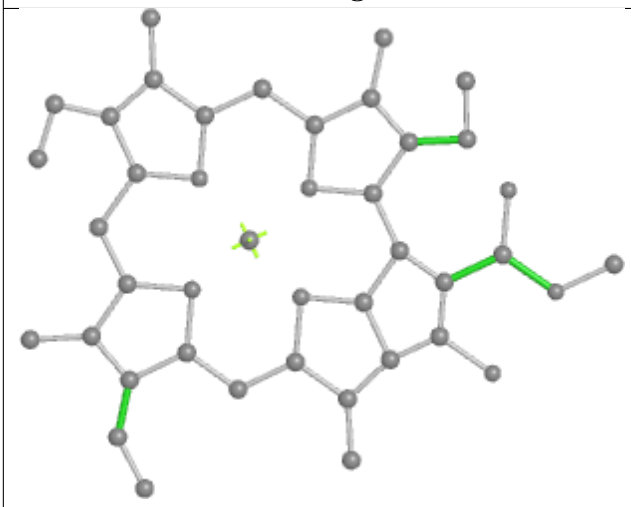


Bond angles



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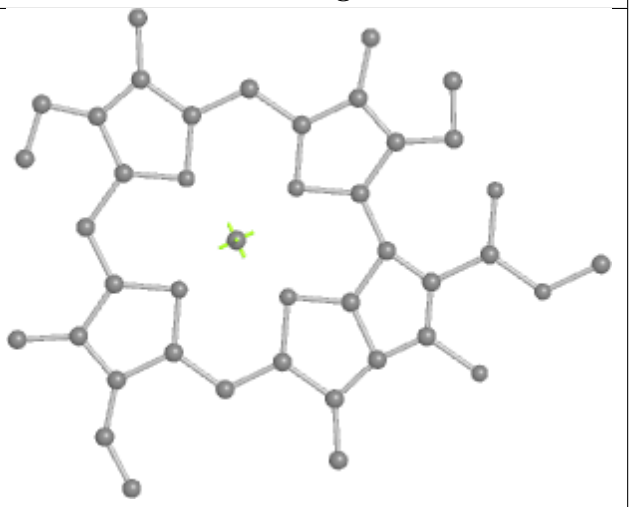
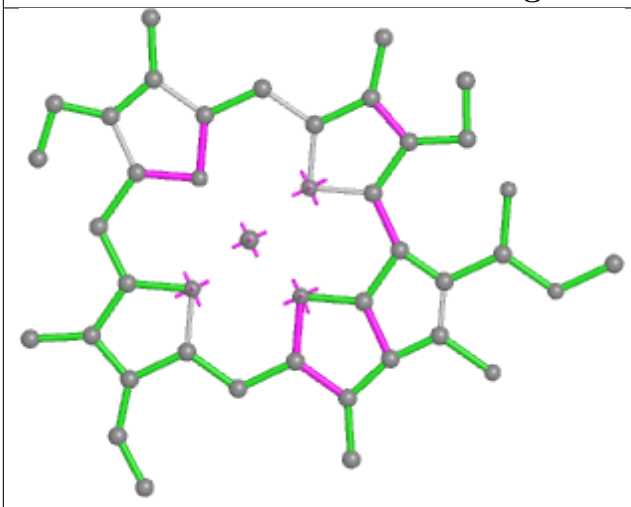


Rings

Ligand CLA A 834



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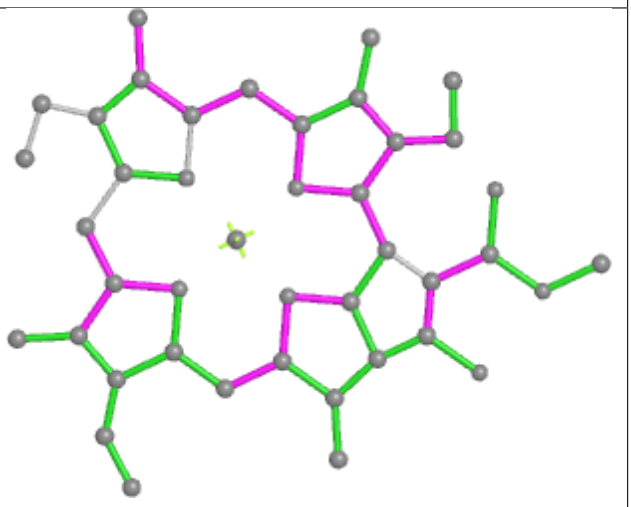
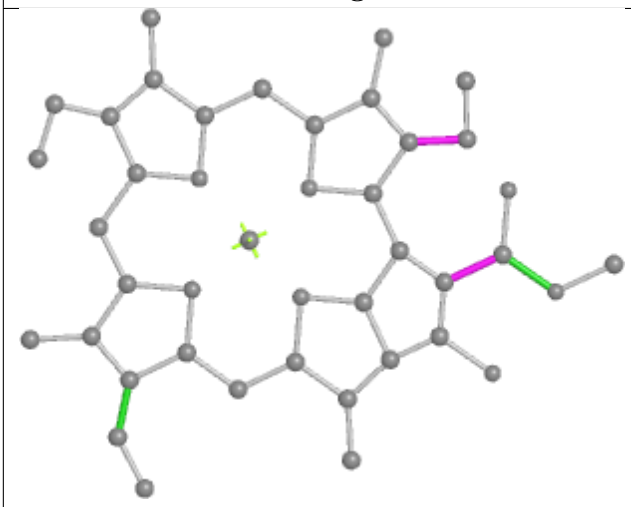


Bond angles



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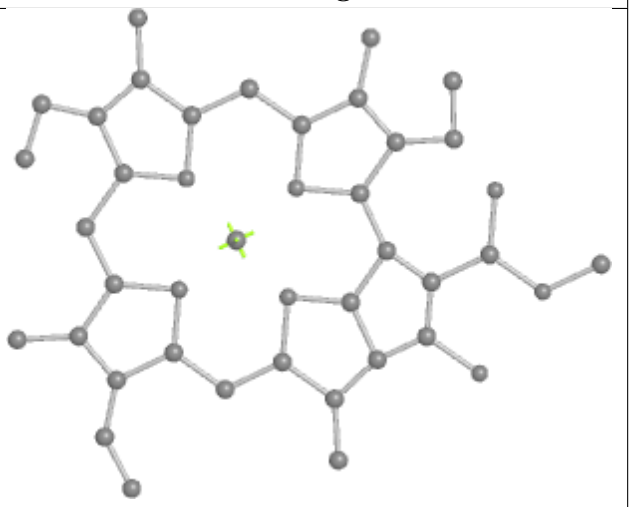
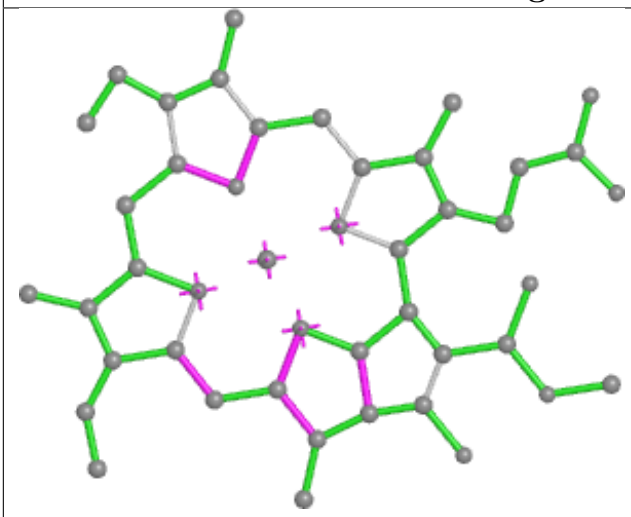


Rings

Ligand CLA 7 609



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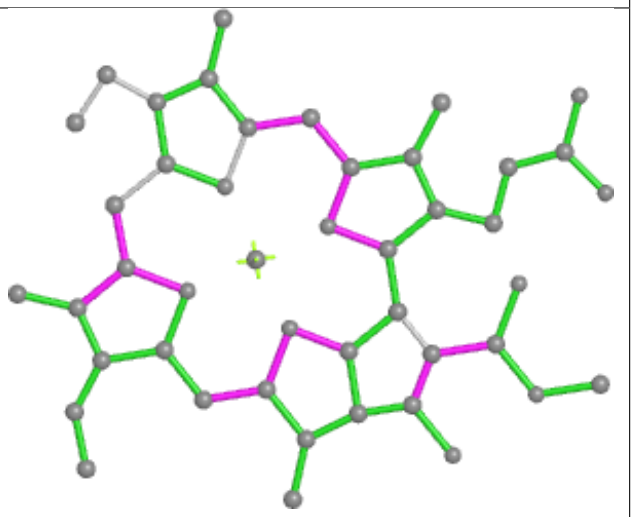
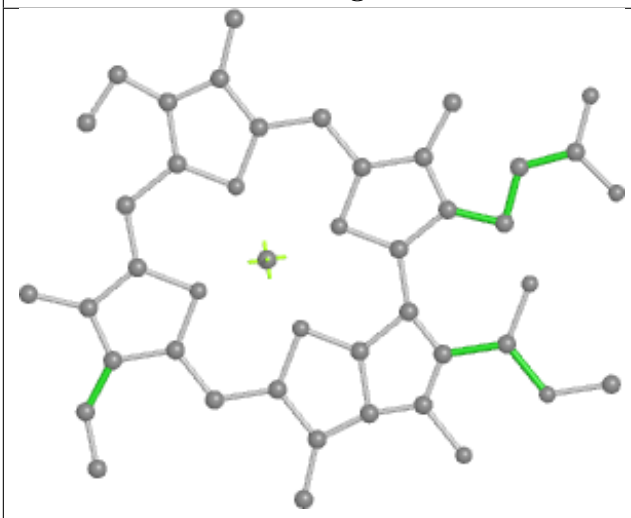
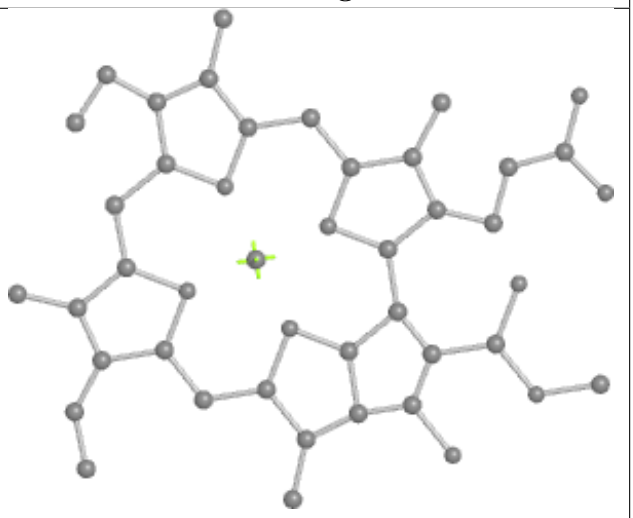


Bond angles

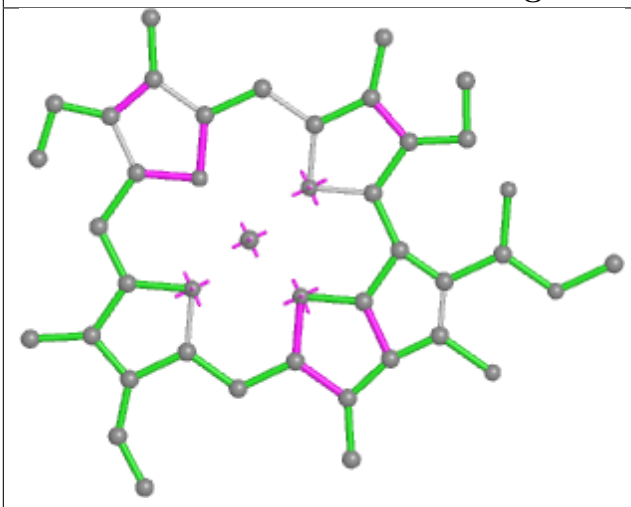


Torsions

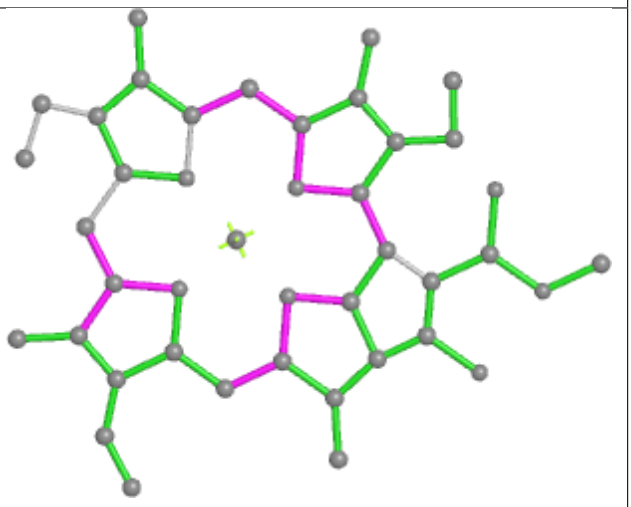


Rings

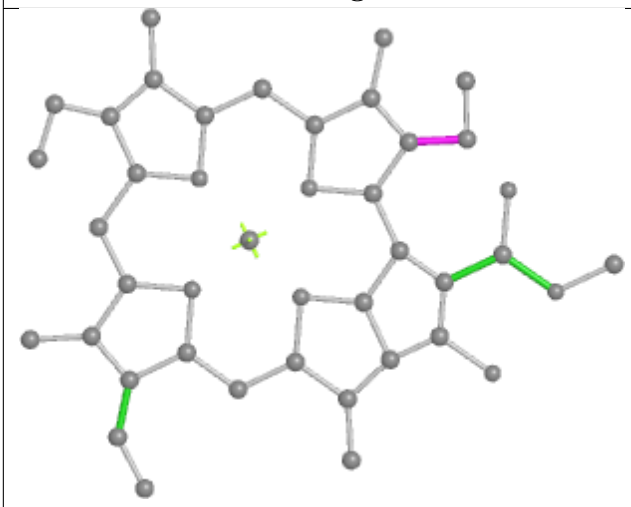
Ligand CLA B 811



Bond lengths



Bond angles



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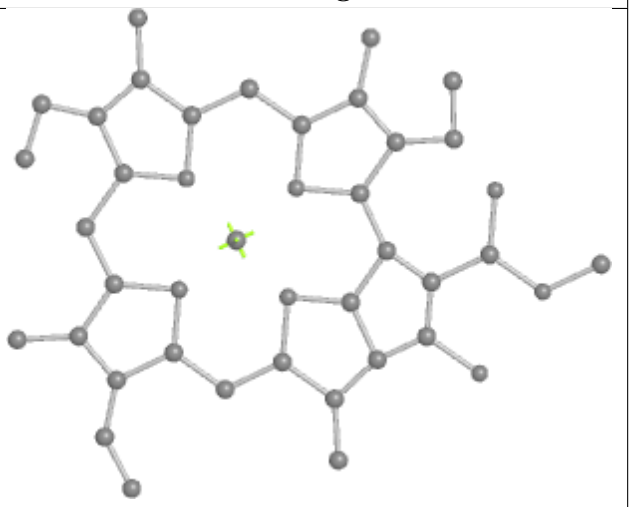
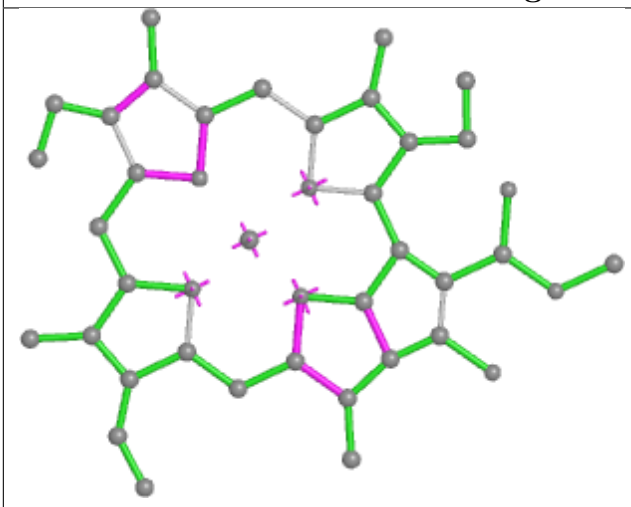


Rings

Ligand CLA B 837



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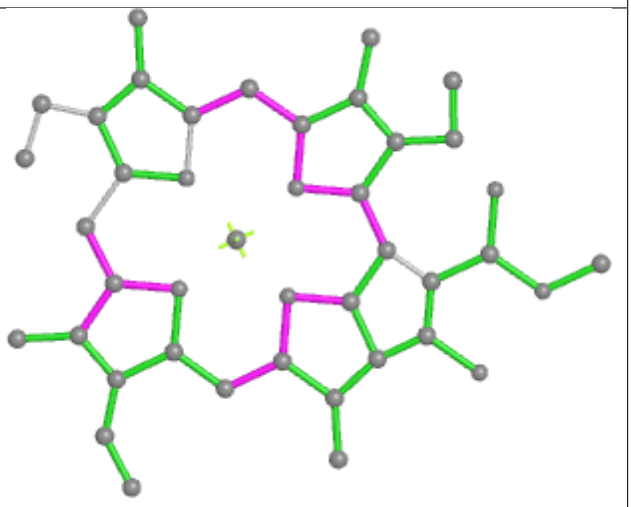
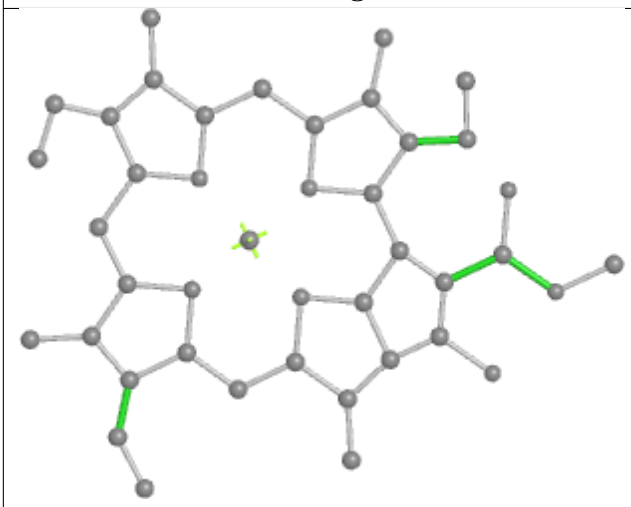
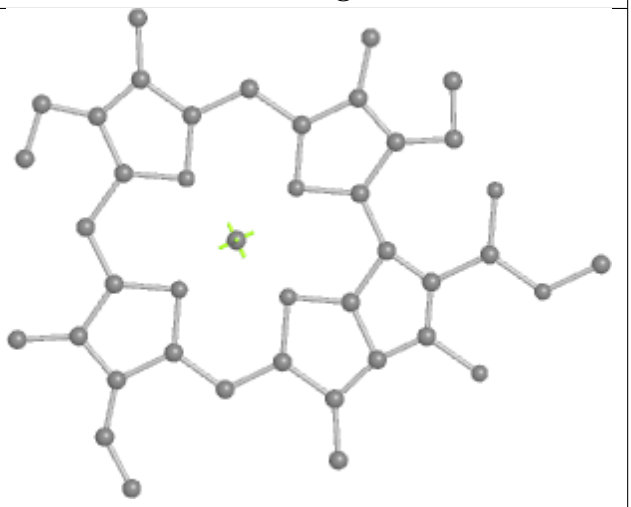


Bond angles

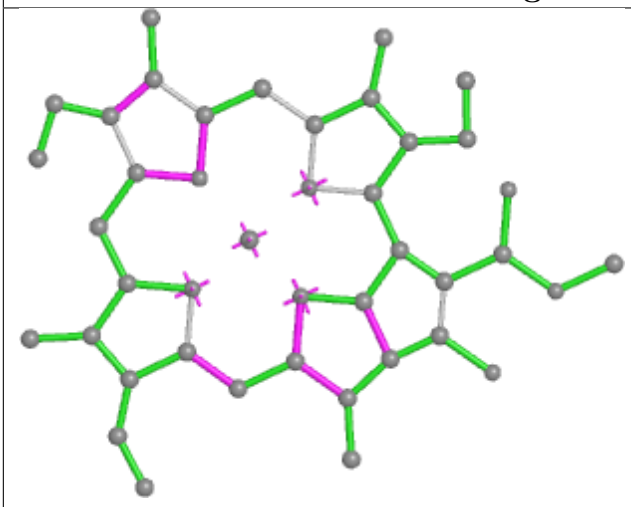


Torsions

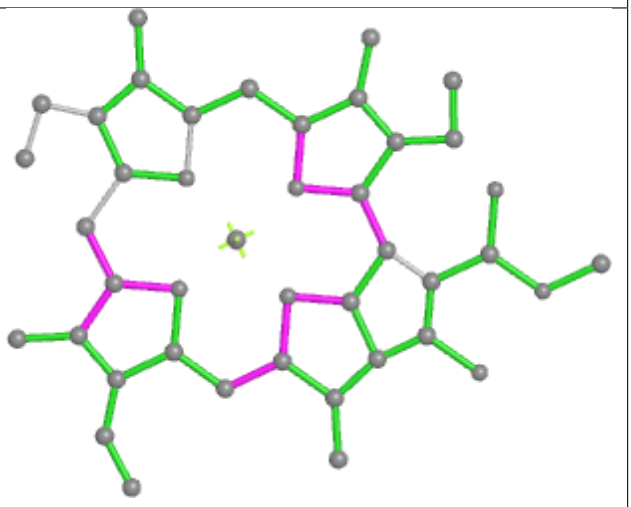


Rings

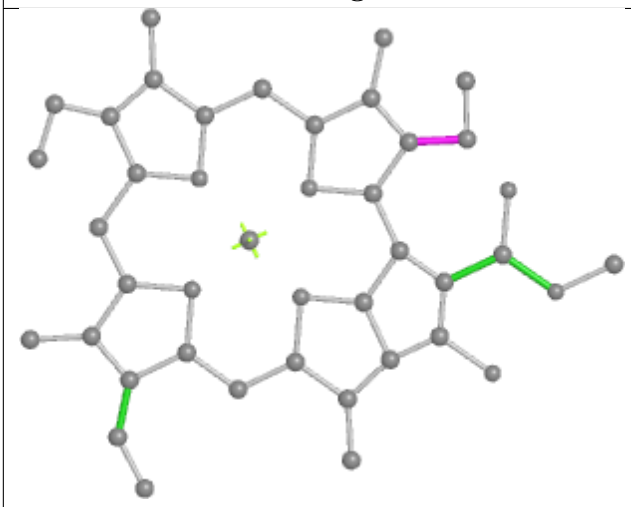
Ligand CLA A 833



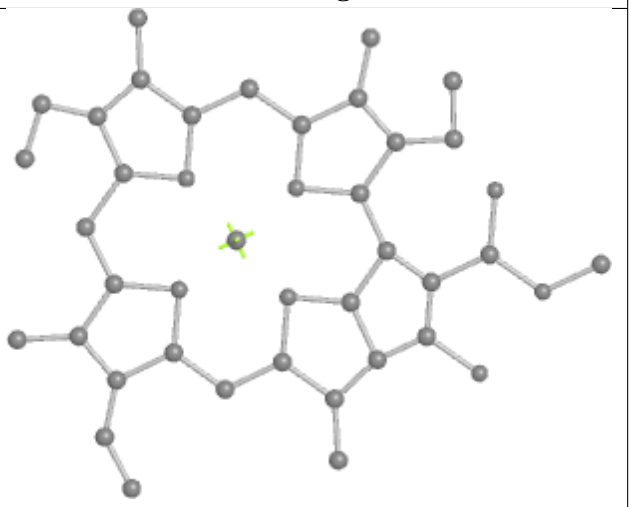
Bond lengths



Bond angles

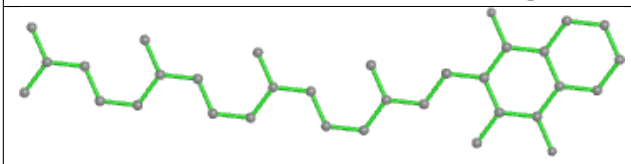


Torsions

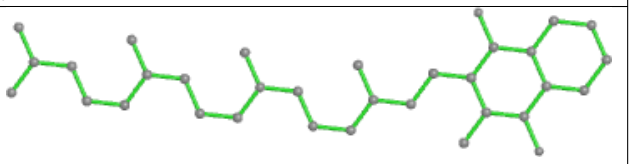


Rings

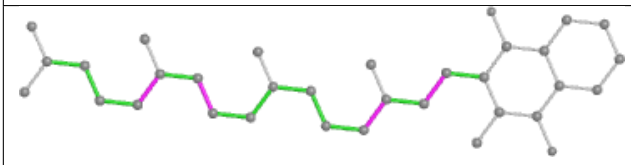
Ligand PQN B 844



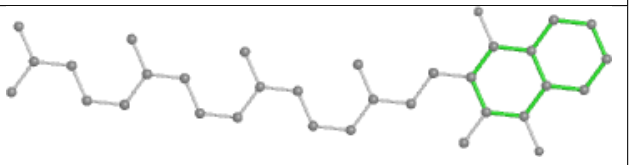
Bond lengths



Bond angles

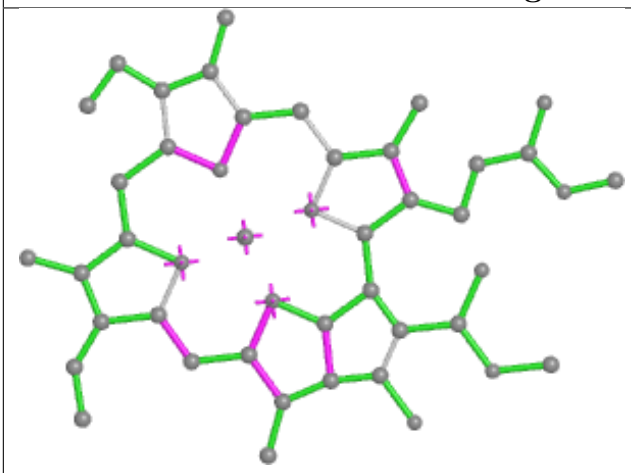


Torsions

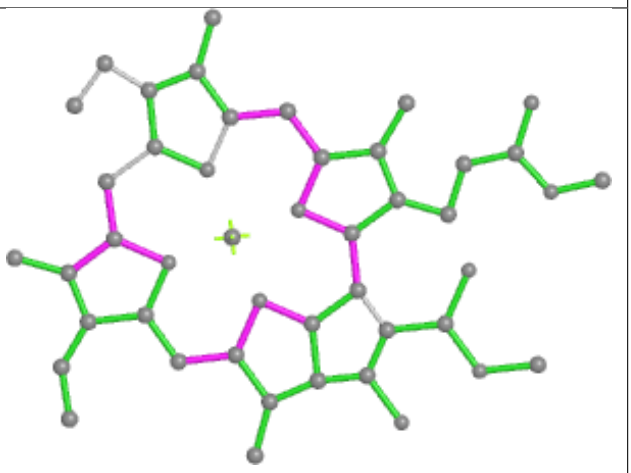


Rings

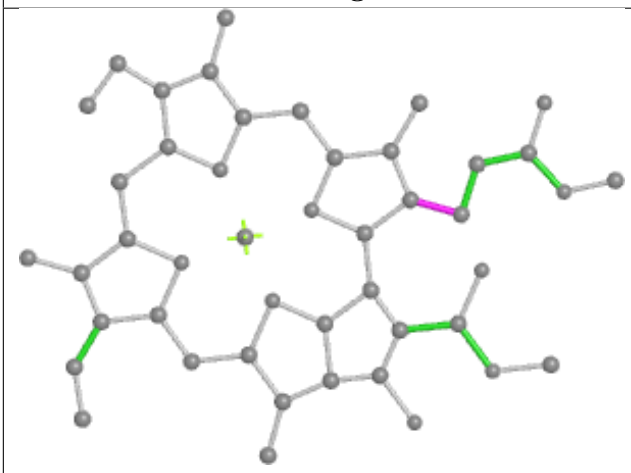
Ligand CLA B 802



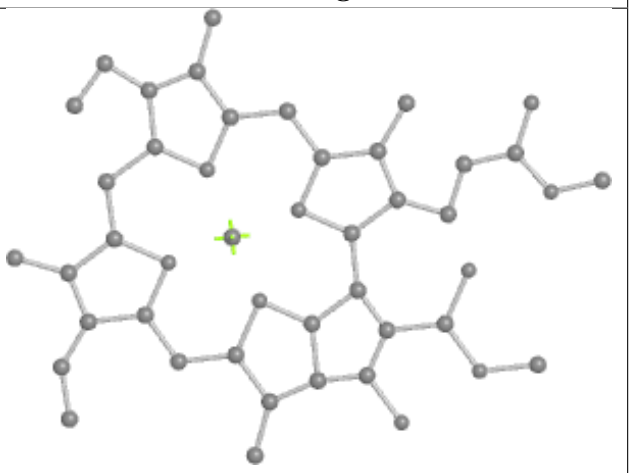
Bond lengths



Bond angles

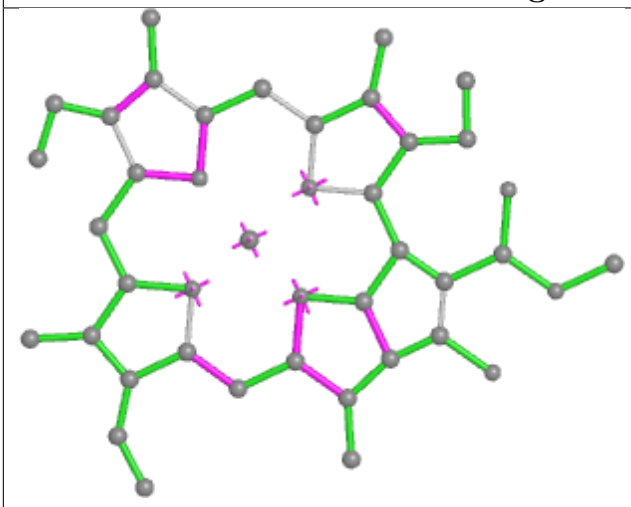


Torsions



Rings

Ligand CLA 8 615



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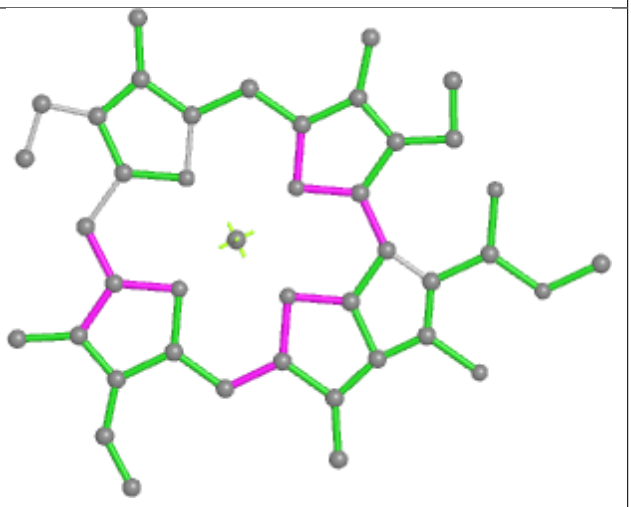
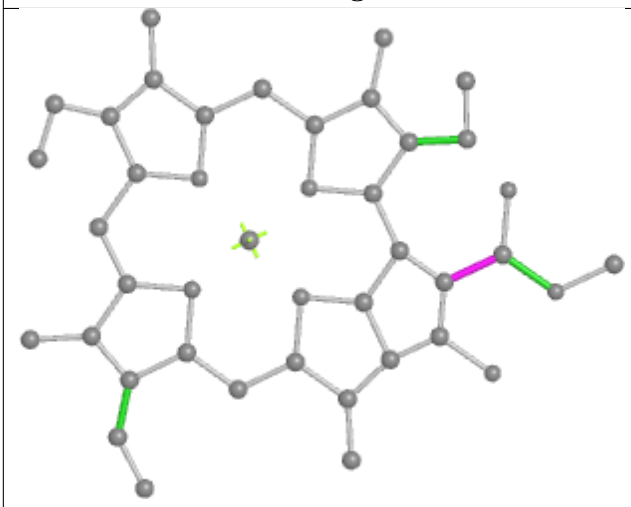
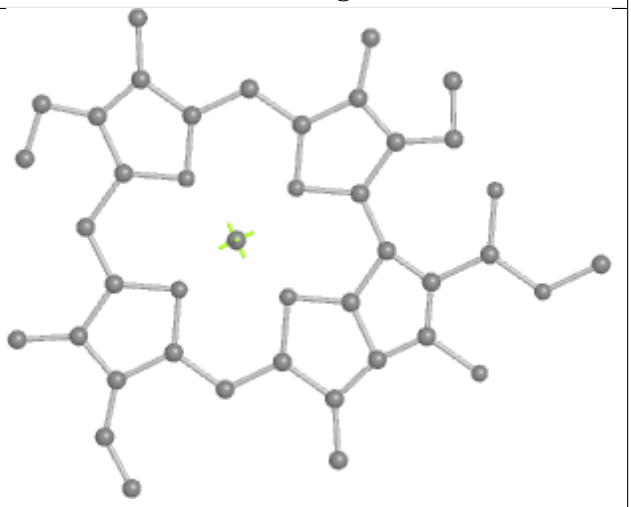


Bond angles

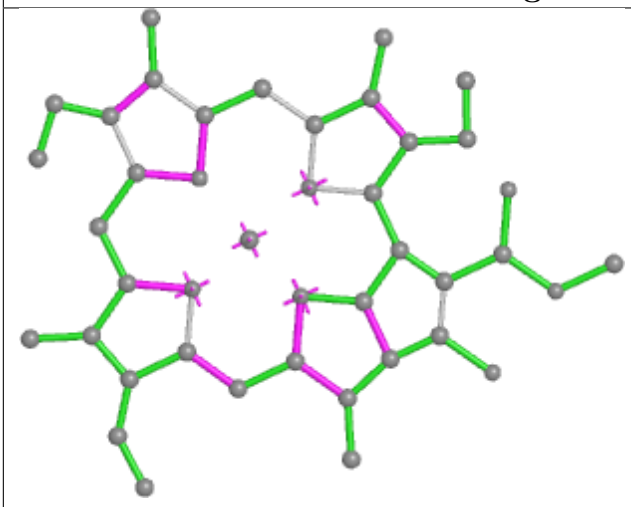


Torsions

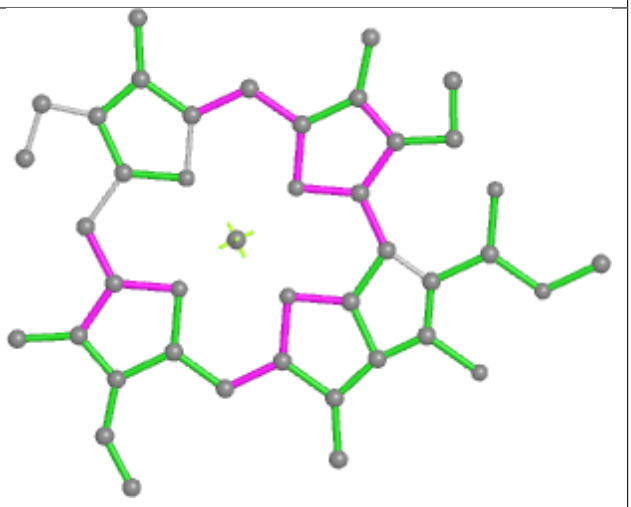


Rings

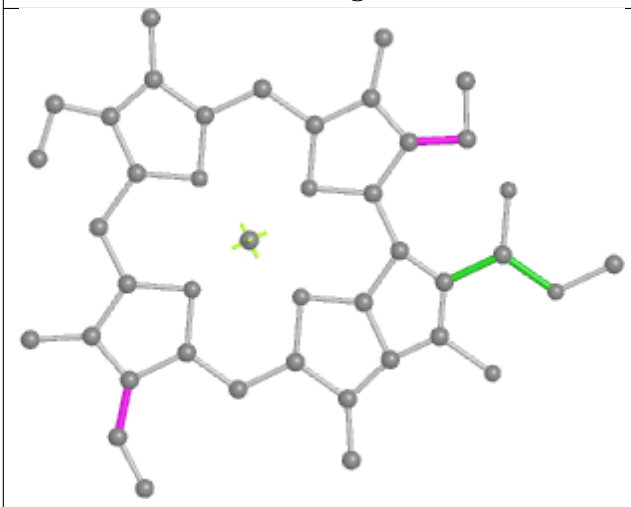
Ligand CLA A 824



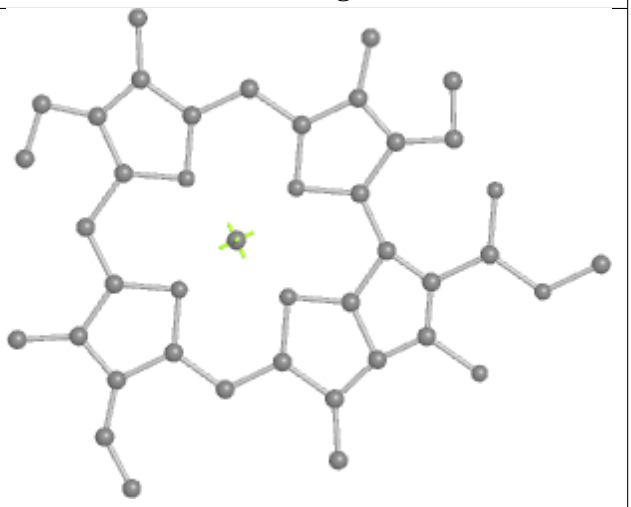
Bond lengths



Bond angles

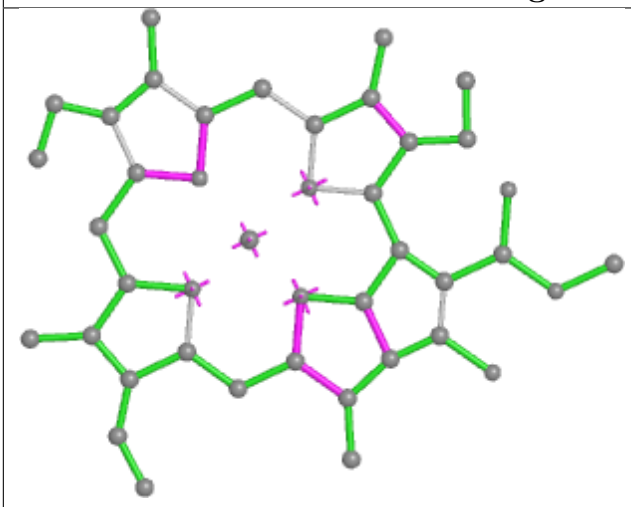


Torsions

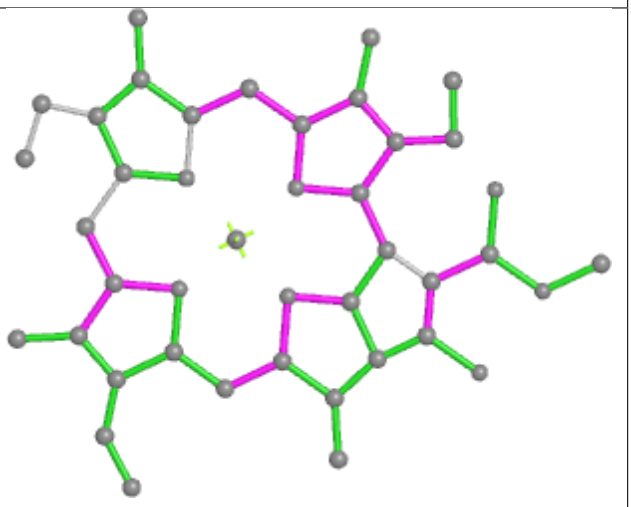


Rings

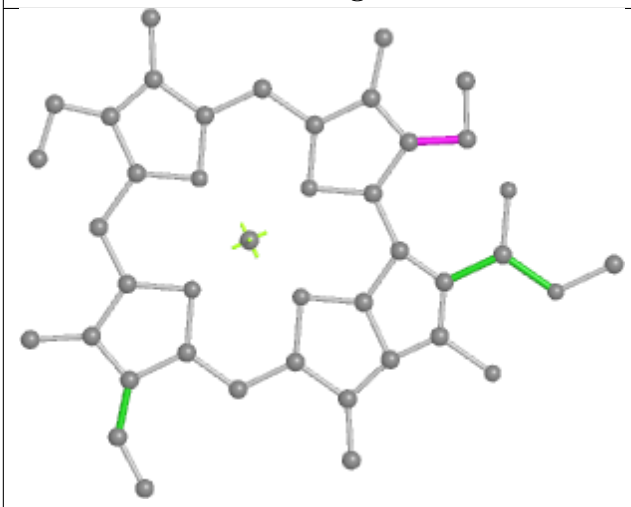
Ligand CLA 3 305



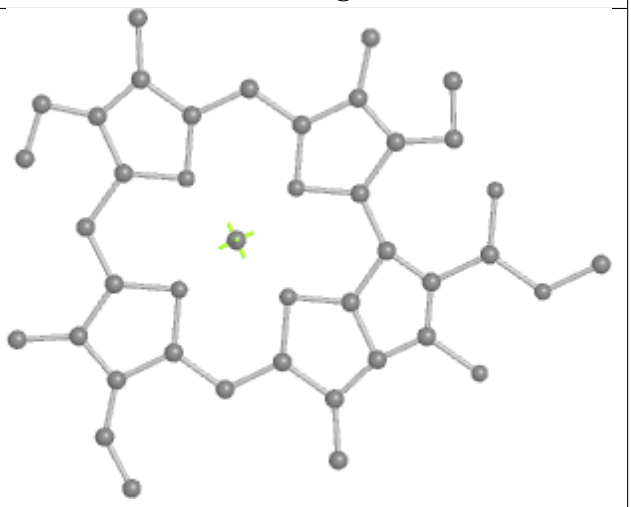
Bond lengths



Bond angles

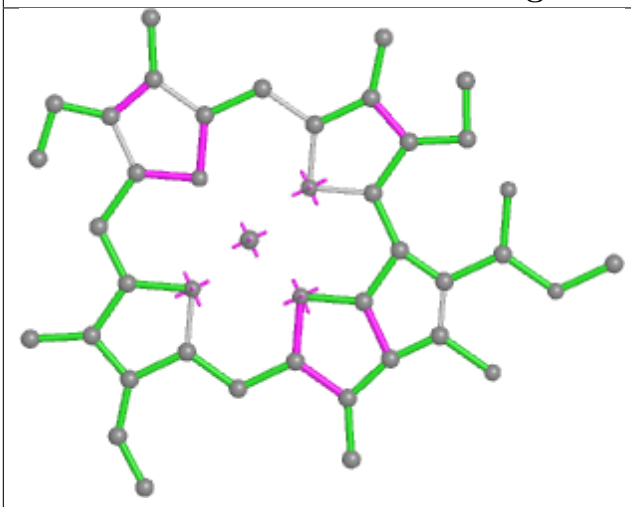


Torsions

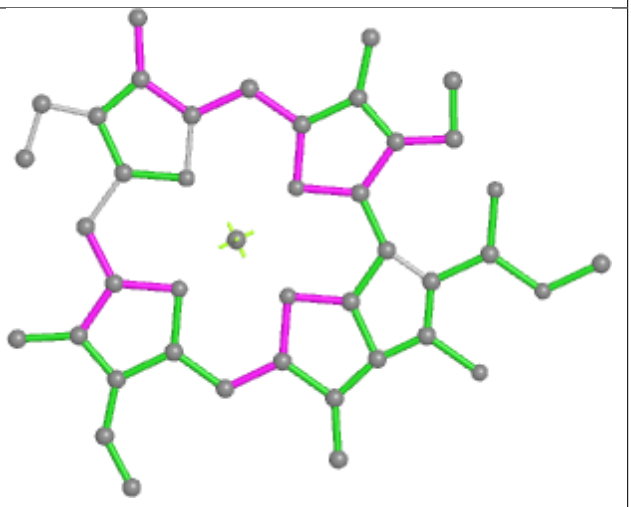


Rings

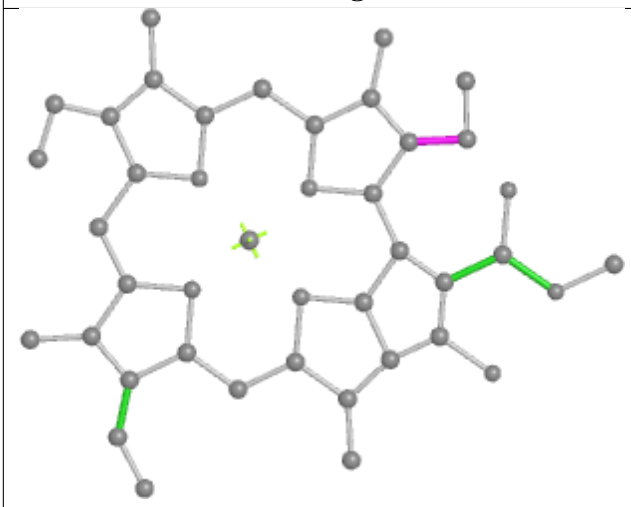
Ligand CLA Z 610



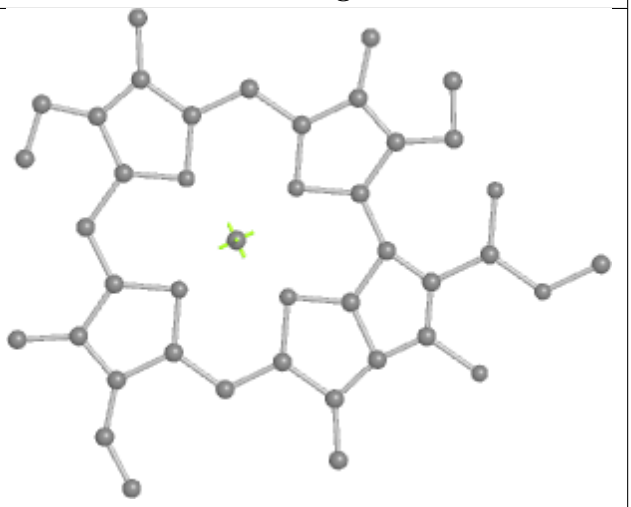
Bond lengths



Bond angles

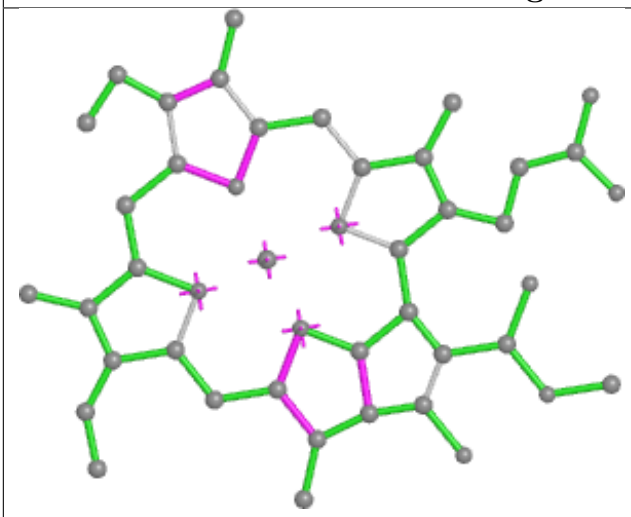


Torsions

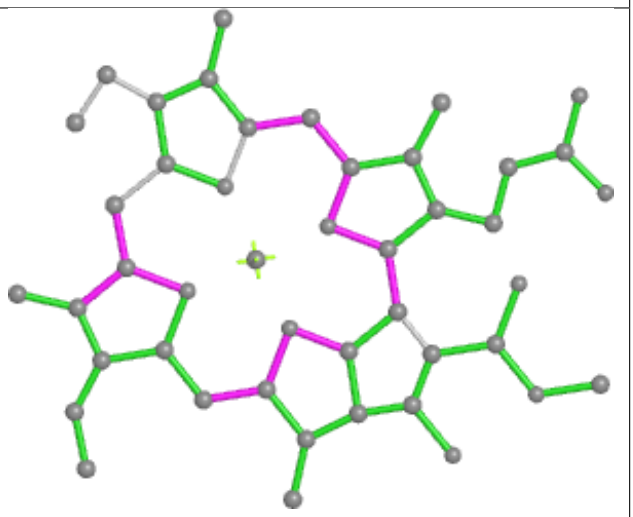


Rings

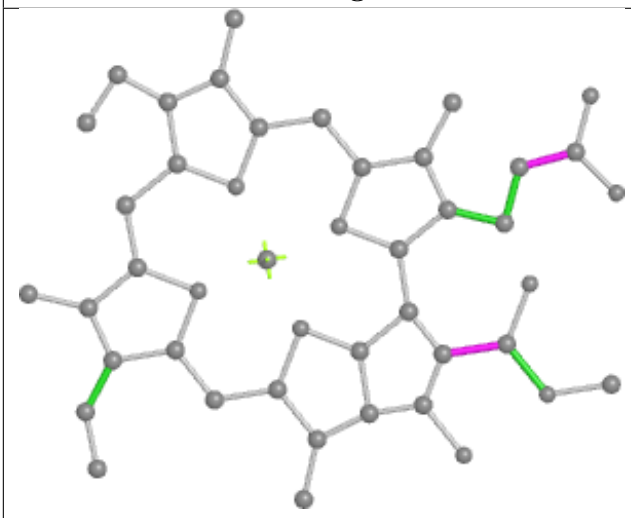
Ligand CLA Z 611



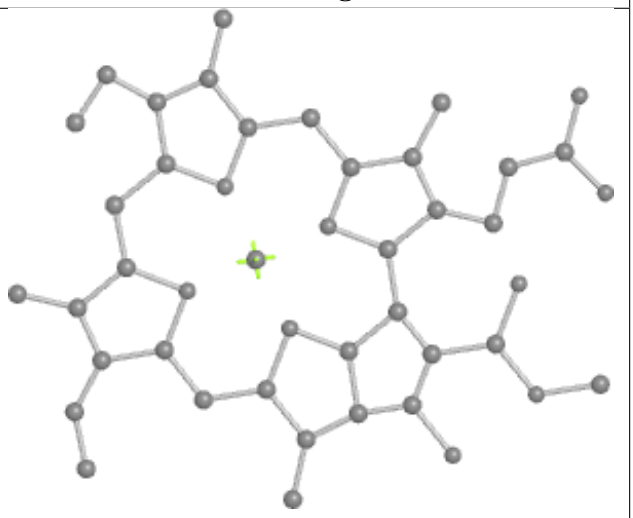
Bond lengths



Bond angles

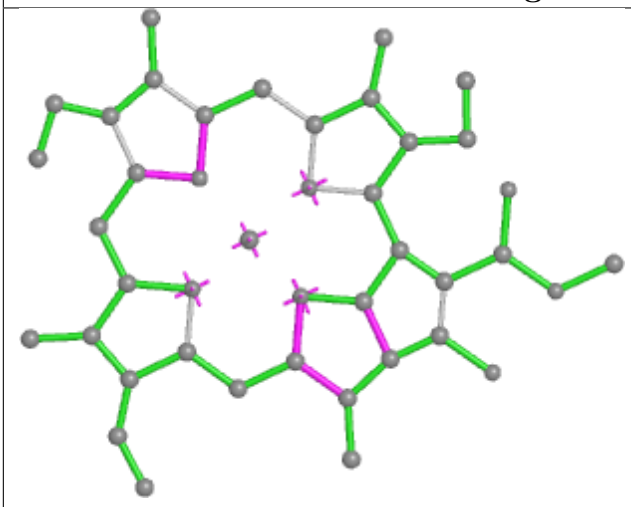


Torsions



Rings

Ligand CLA B 832



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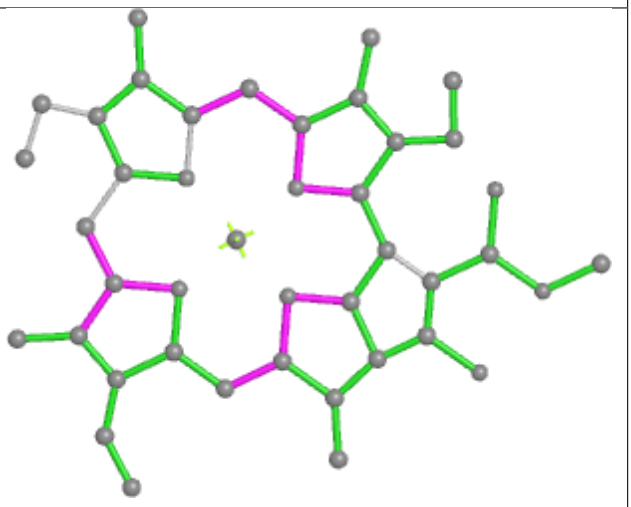

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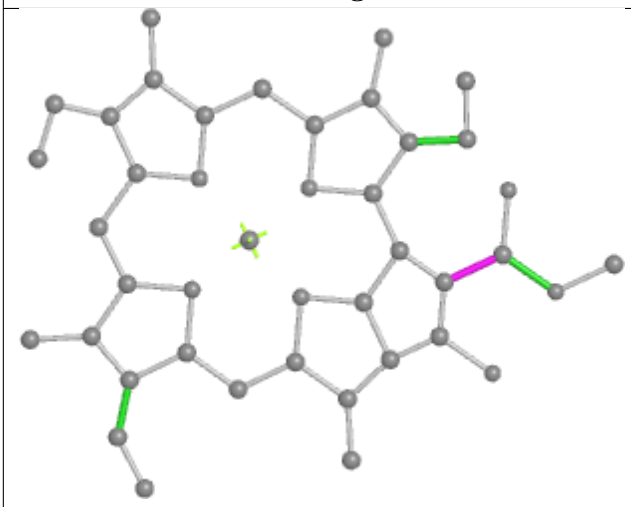

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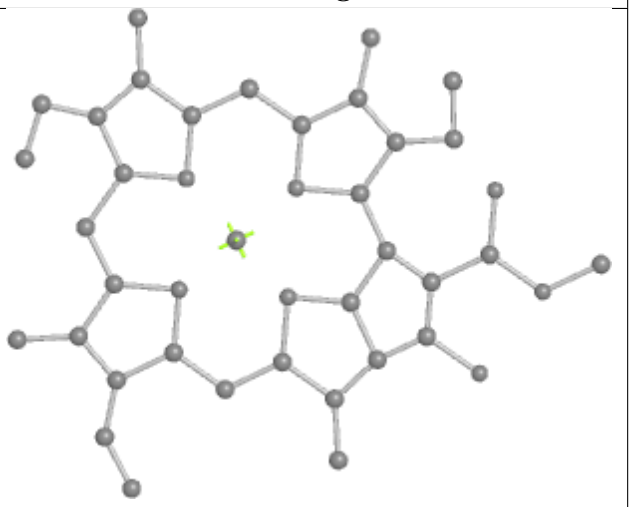
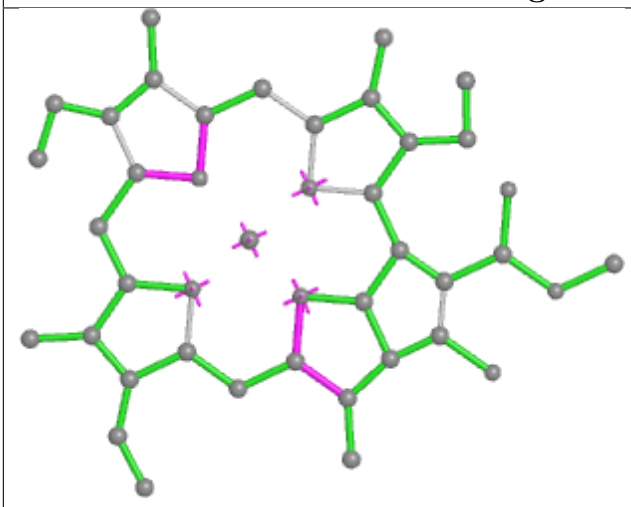


Rings

Ligand CLA 4 609



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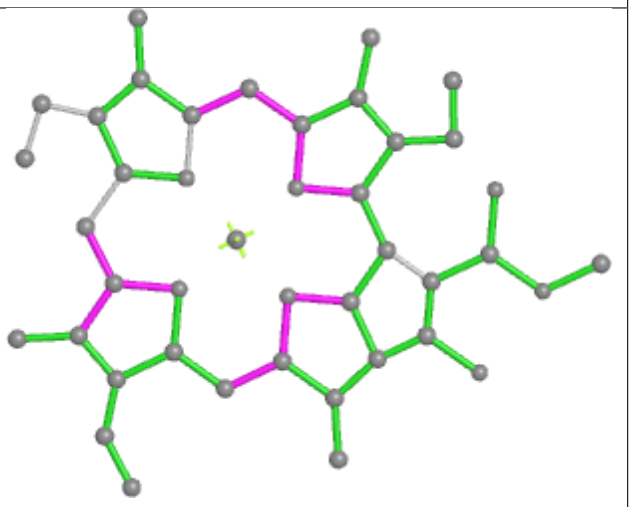

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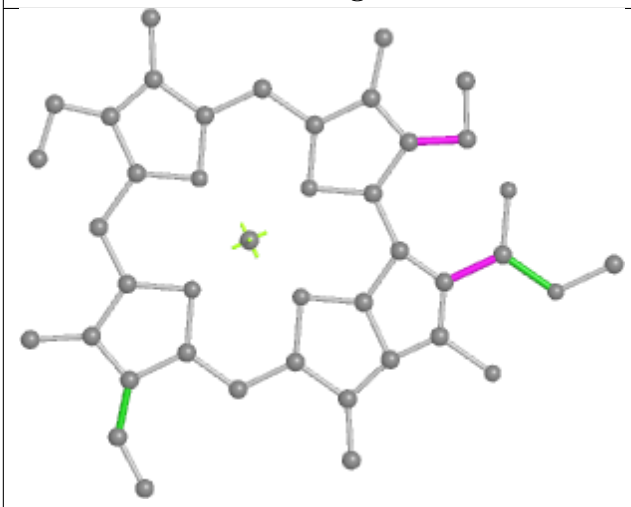

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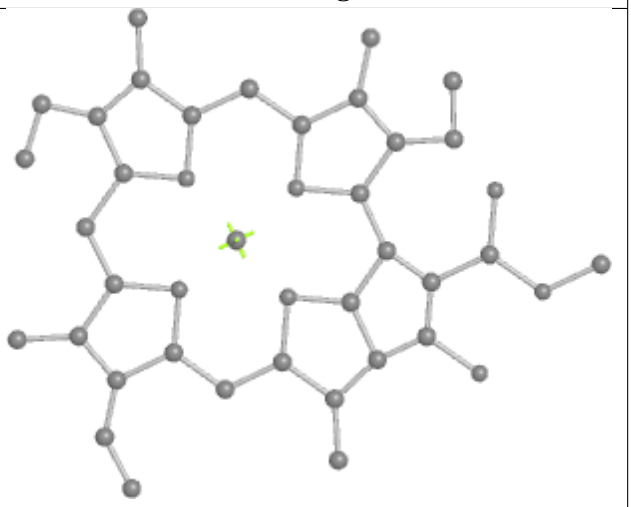
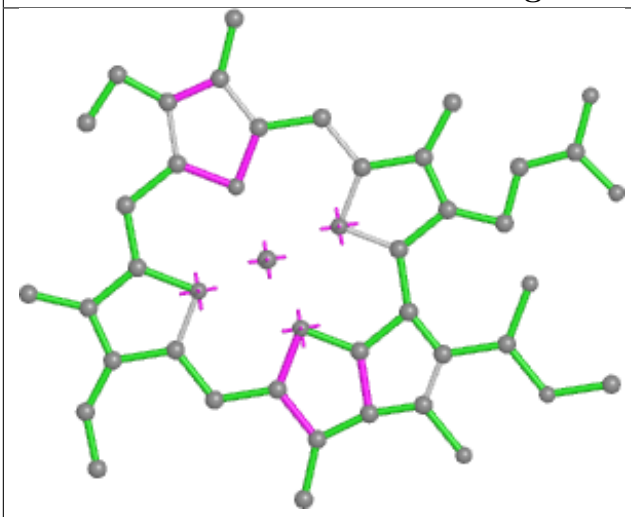


Rings

Ligand CLA B 822



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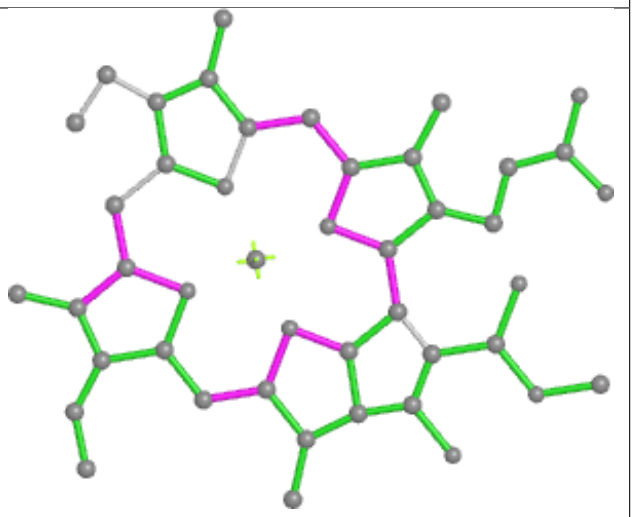
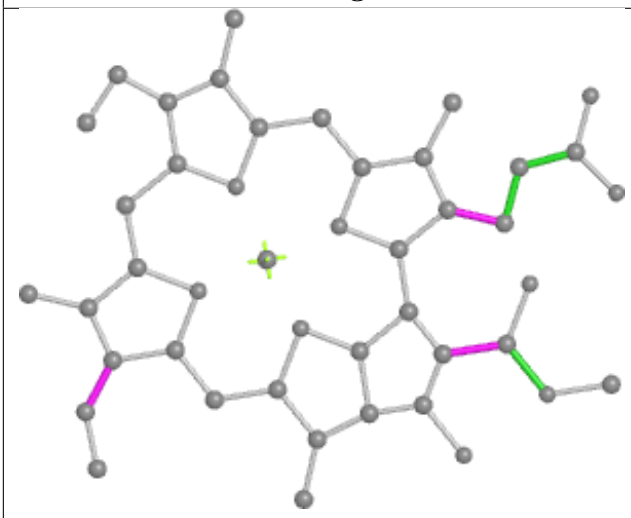


Bond angles



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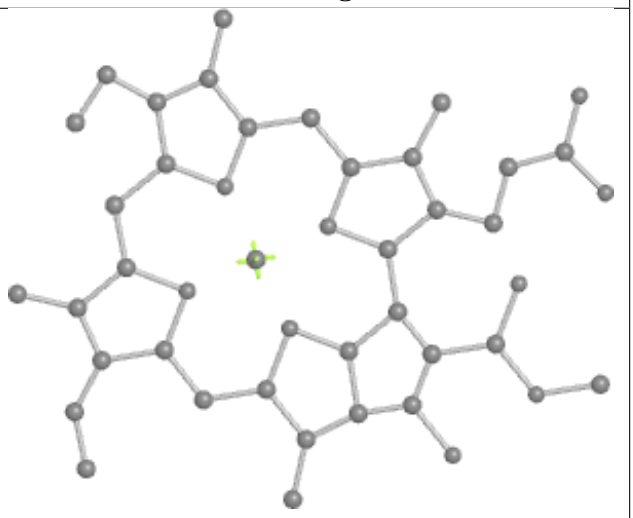
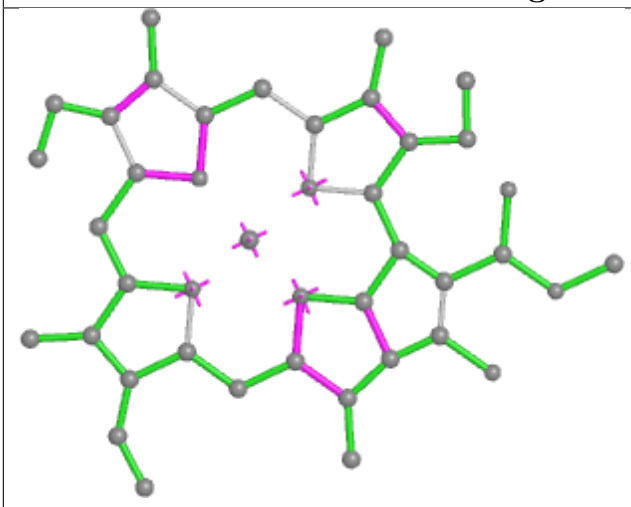


Rings

Ligand CLA 5 611



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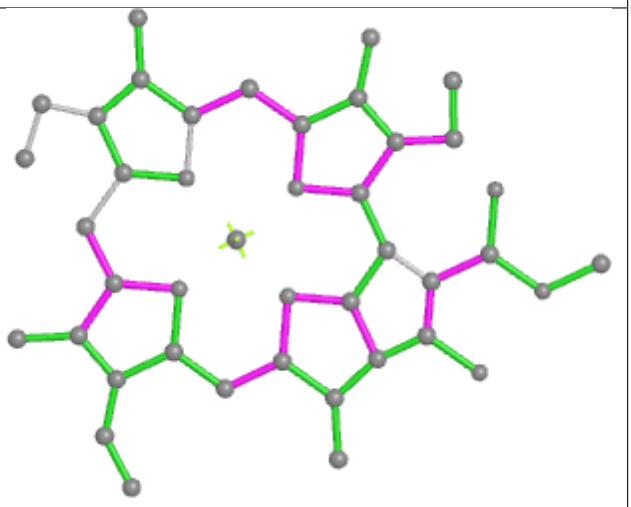
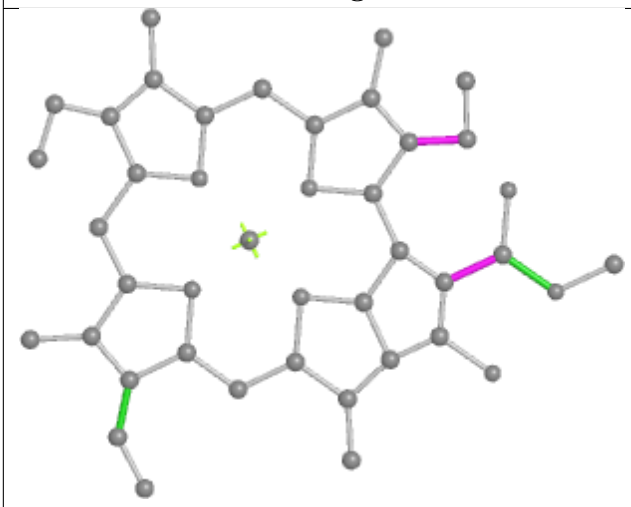


Bond angles



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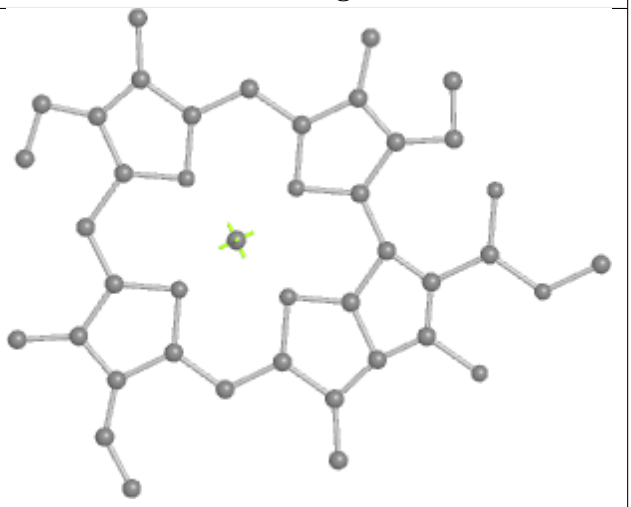
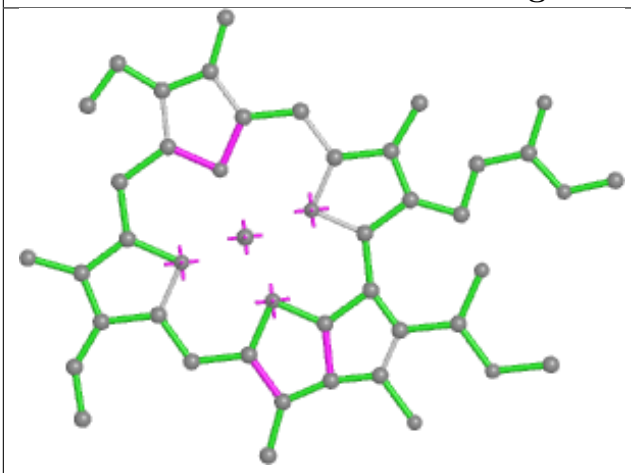


Rings

Ligand CLA 8 610



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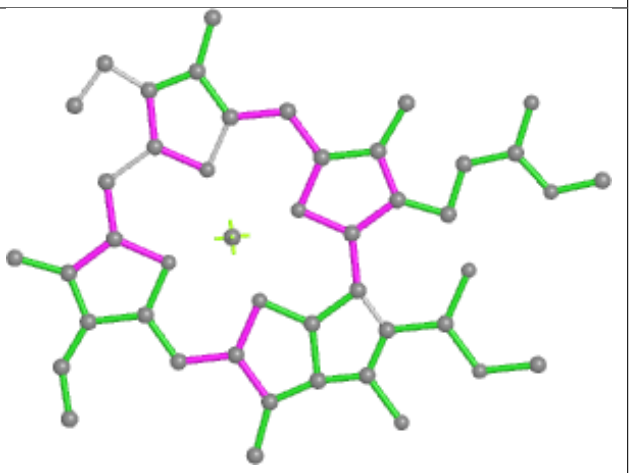

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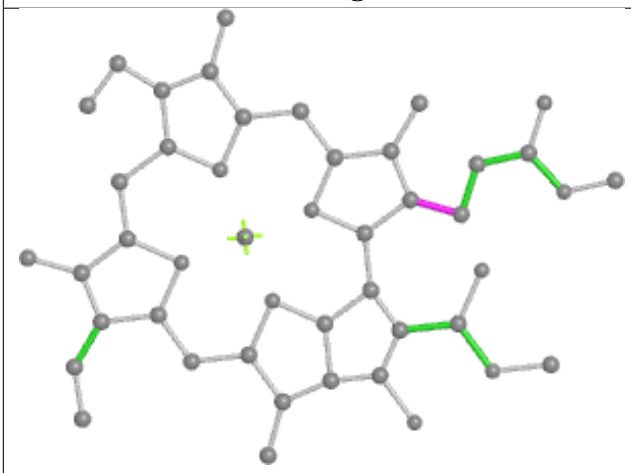

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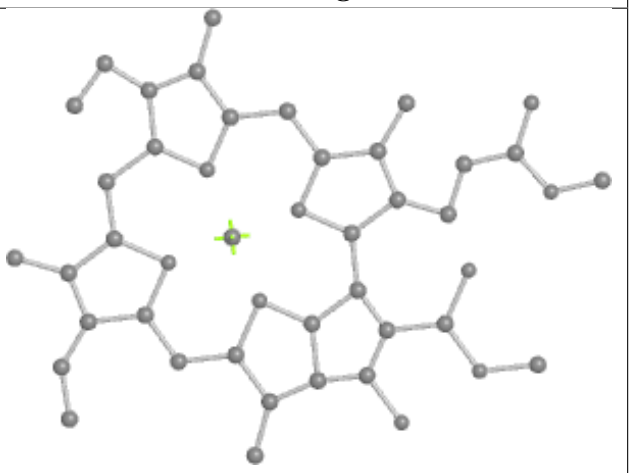
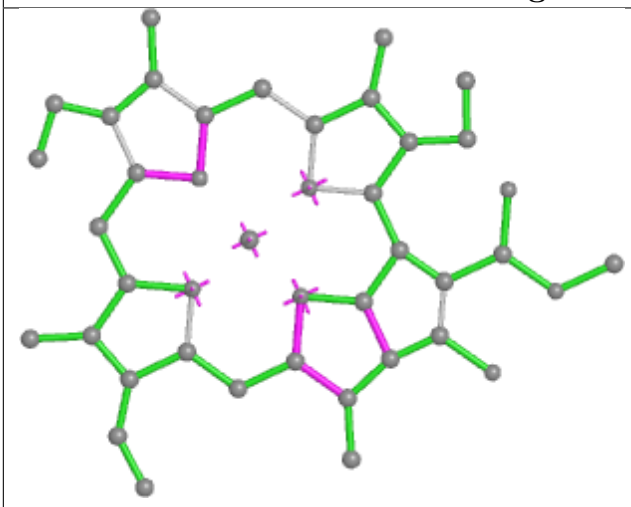


Rings

Ligand CLA 1 607



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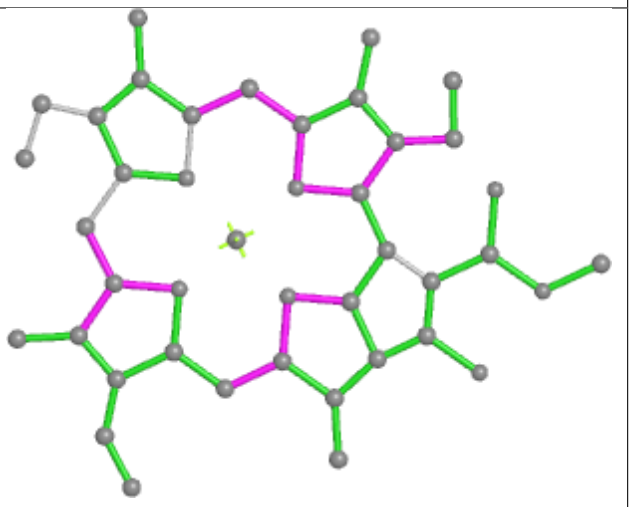

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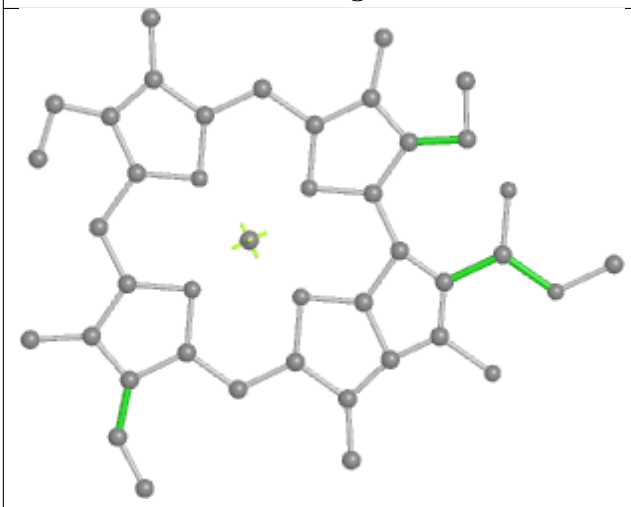

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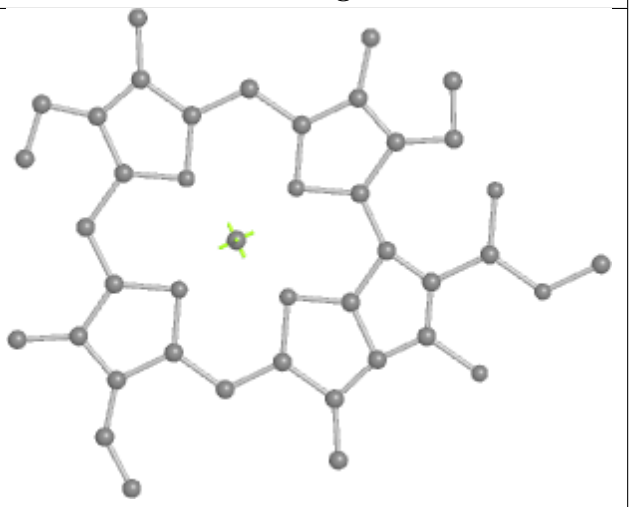
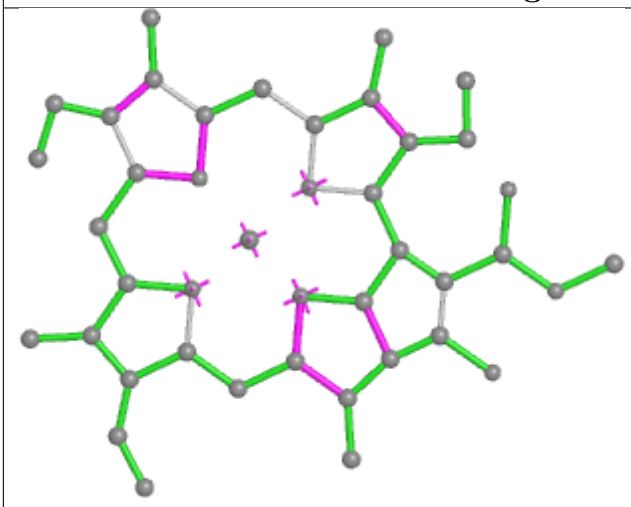


Rings

Ligand CLA A 829



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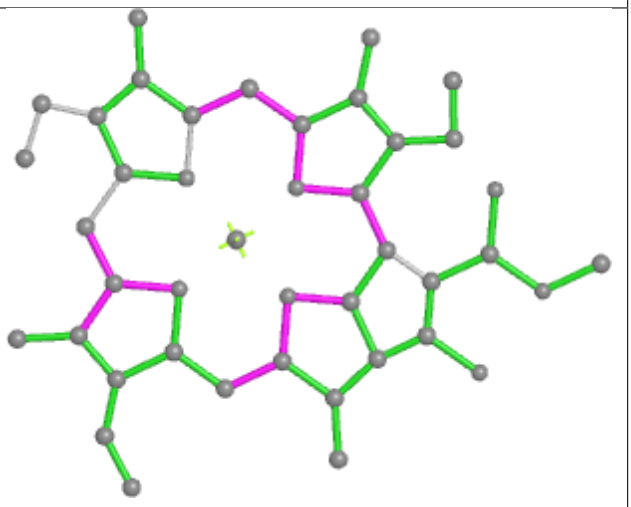

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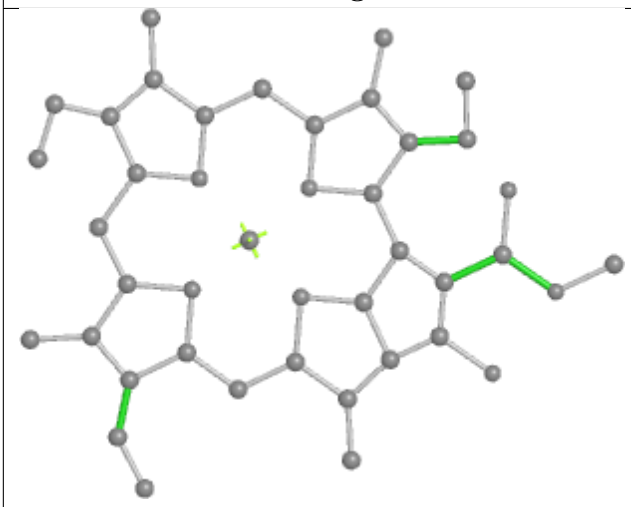

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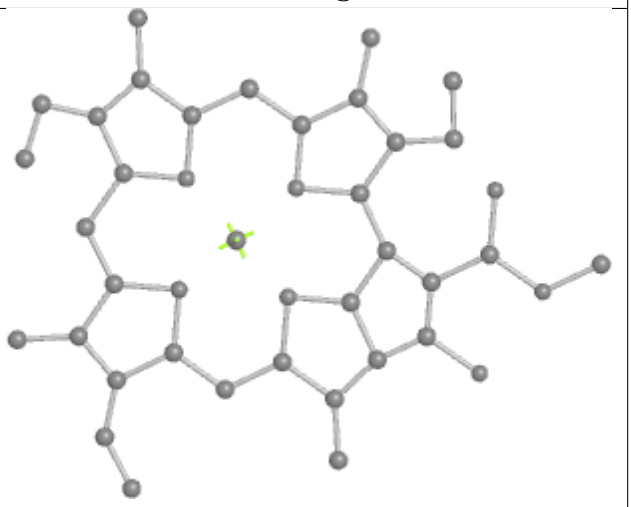
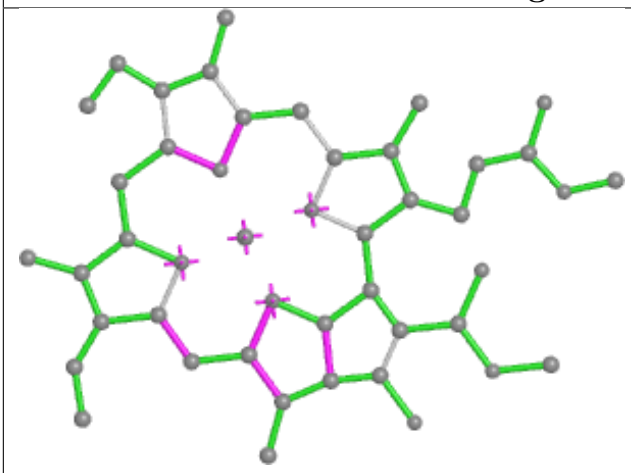


Rings

Ligand CLA 1 614



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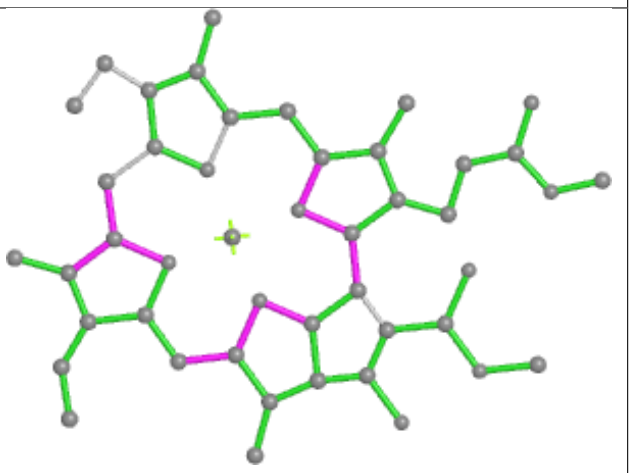
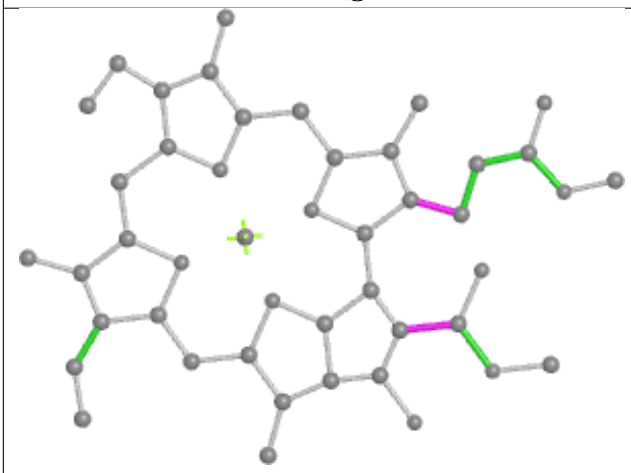


Bond angles



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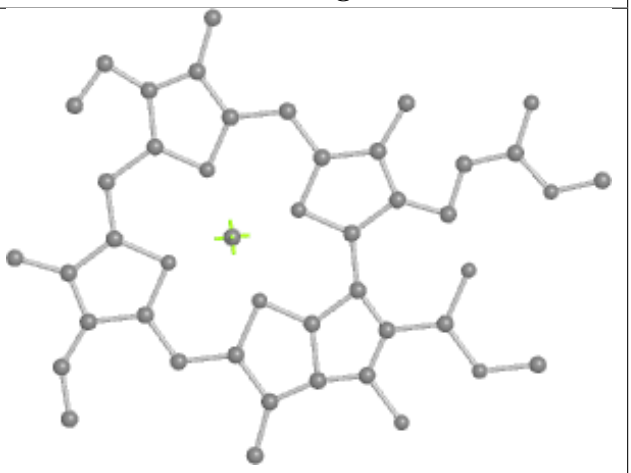
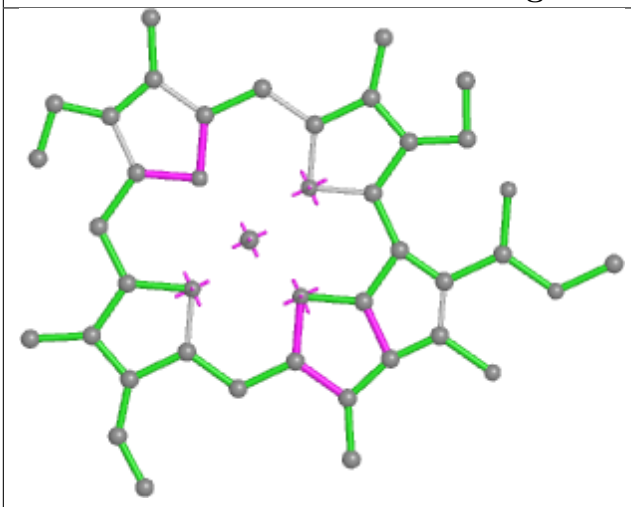


Rings

Ligand CLA Z 609



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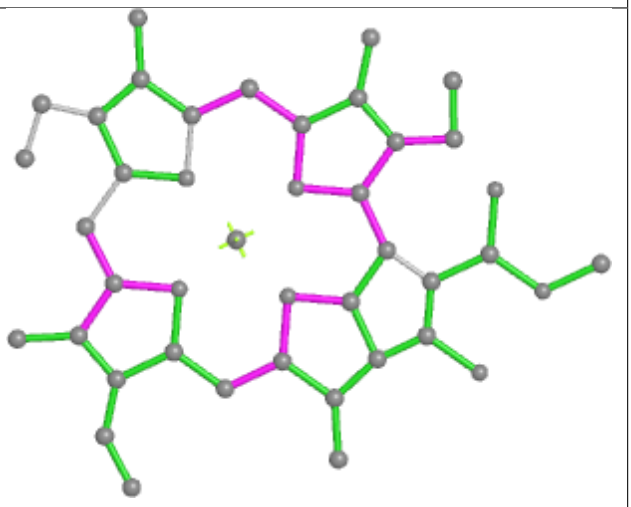

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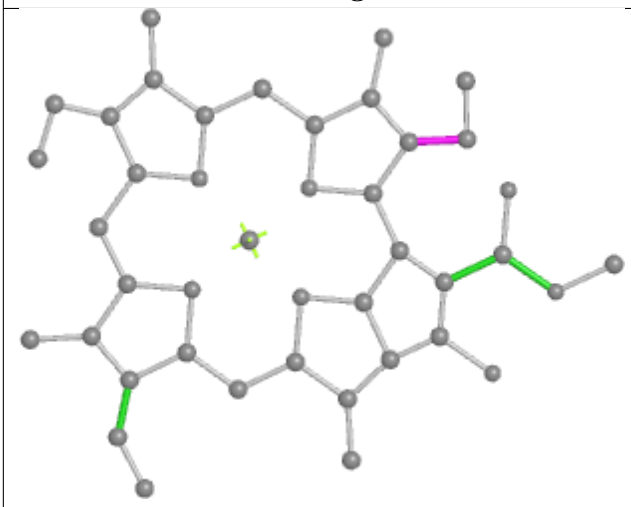

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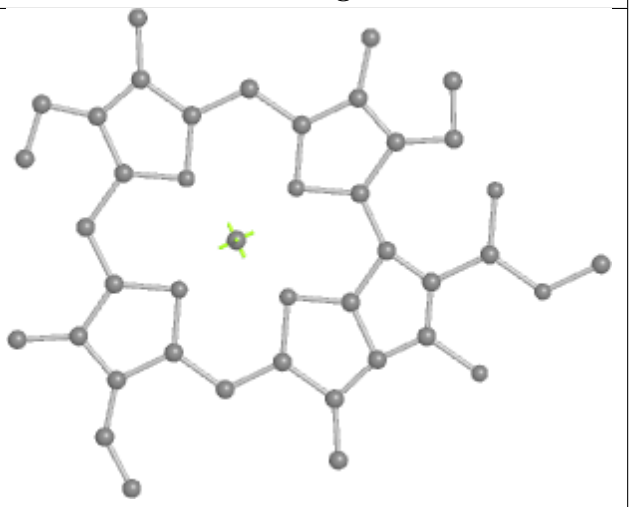
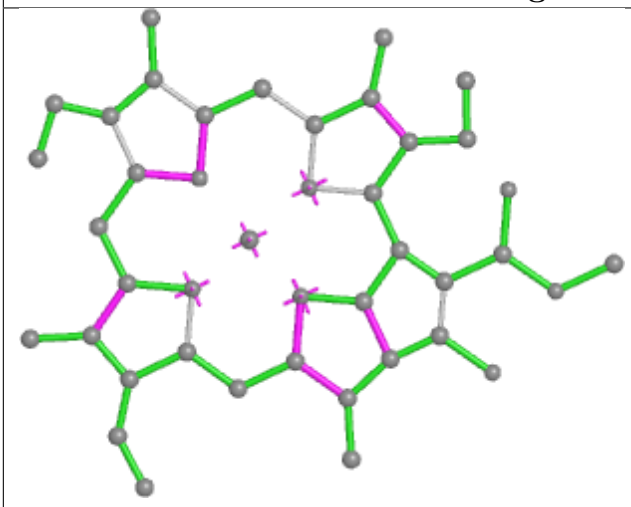


Rings

Ligand CLA 4 610



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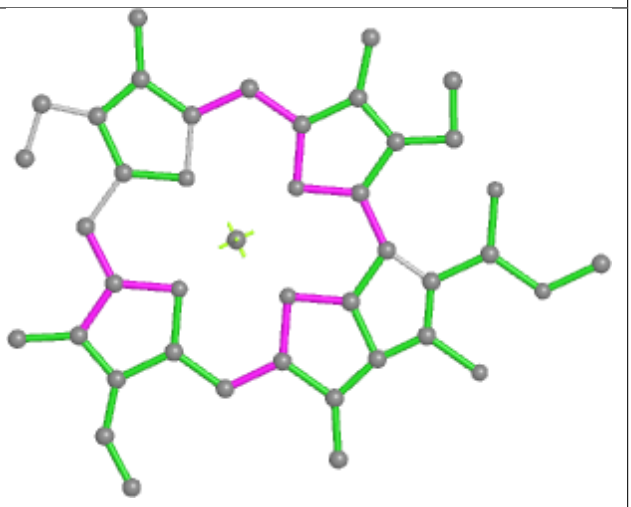

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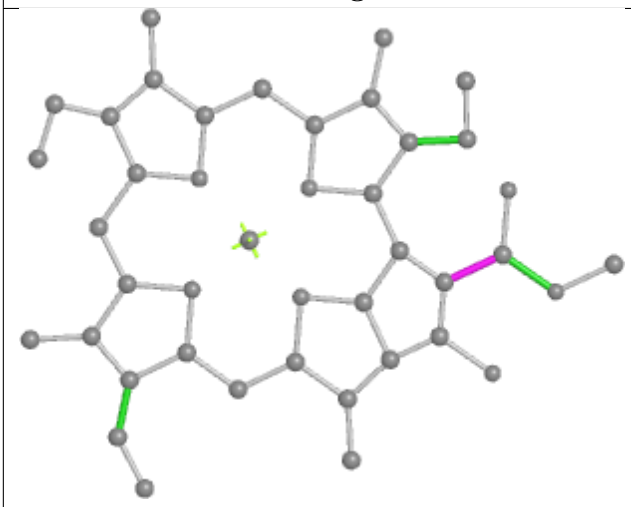

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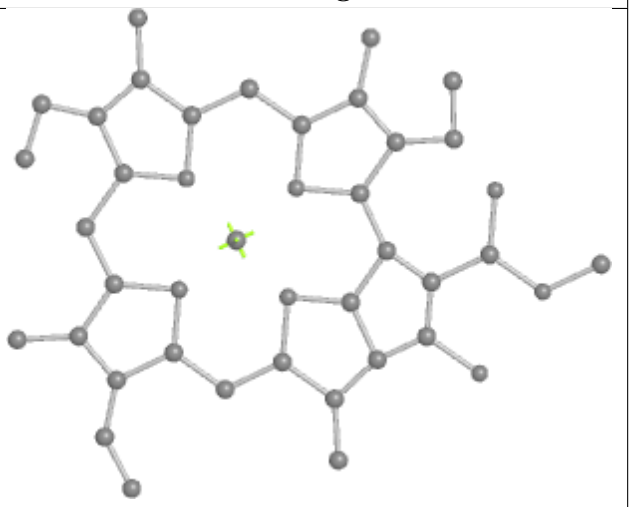
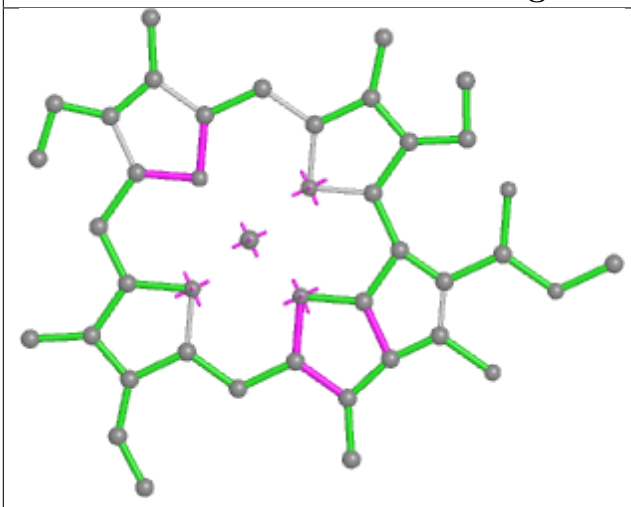


Rings

Ligand CLA 5 604



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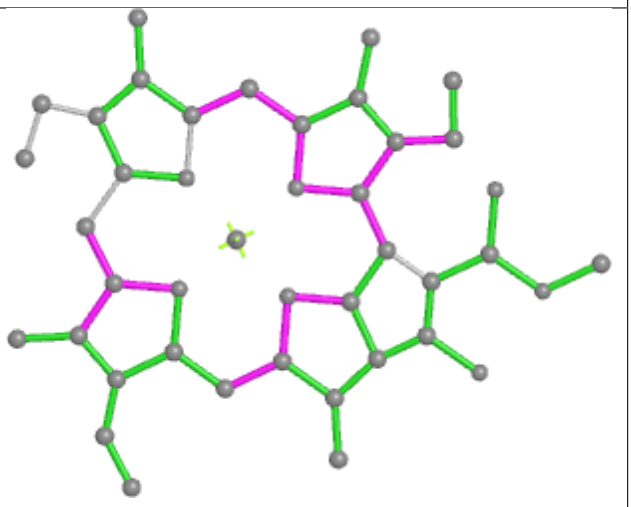

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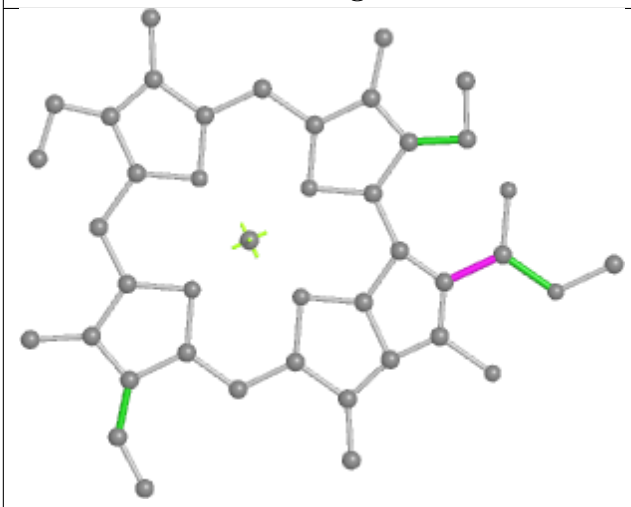

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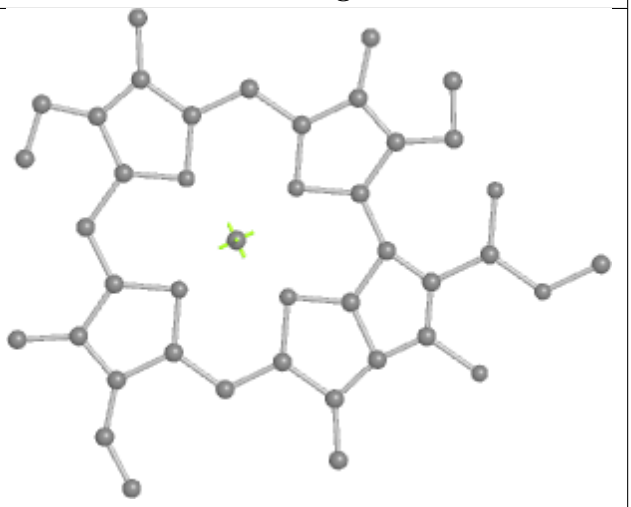
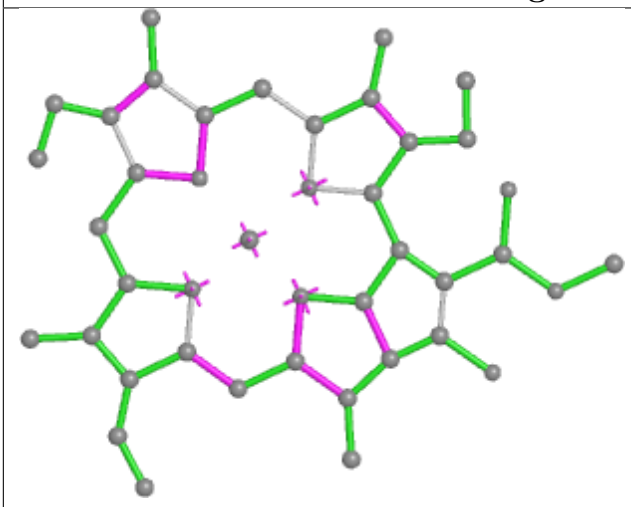
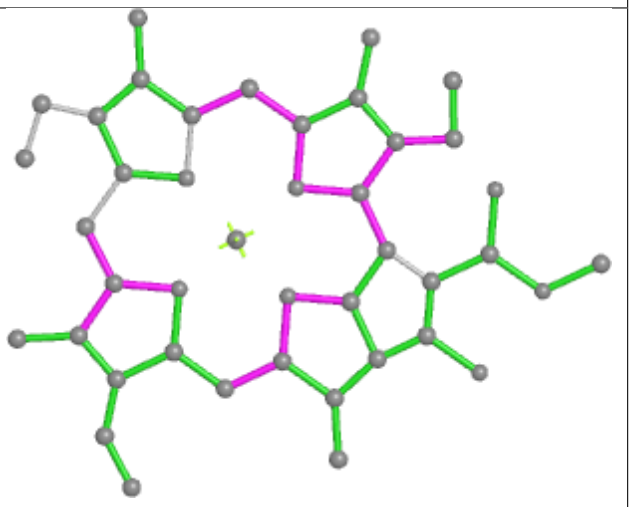


Rings

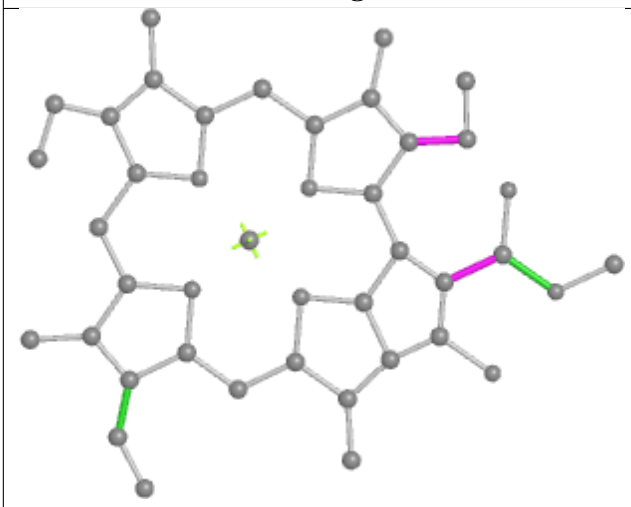
Ligand CLA 7 607



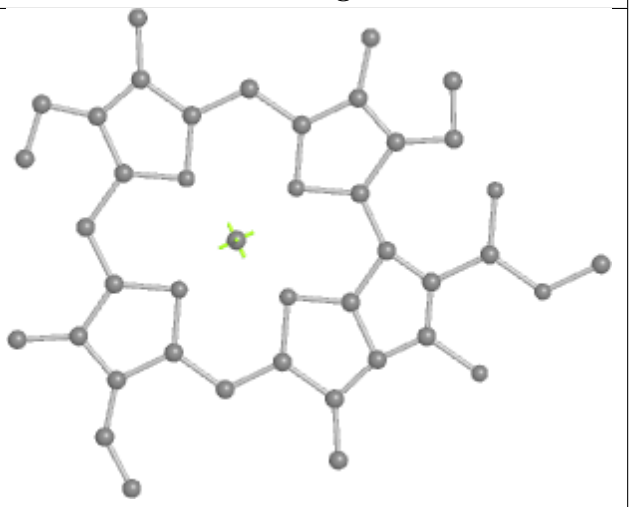
Bond lengths



Bond angles

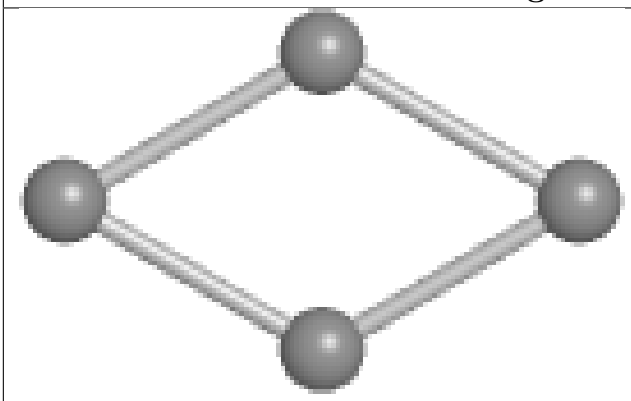


Torsions

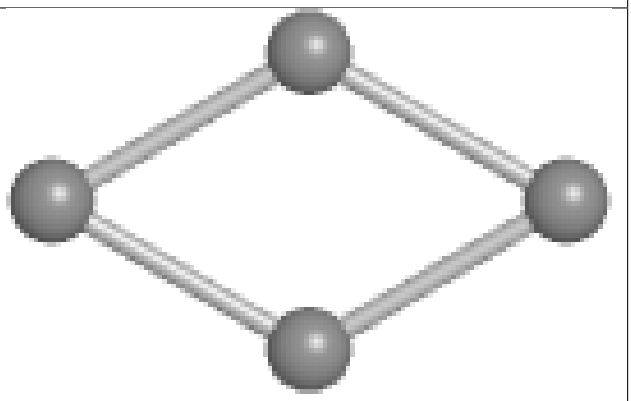


Rings

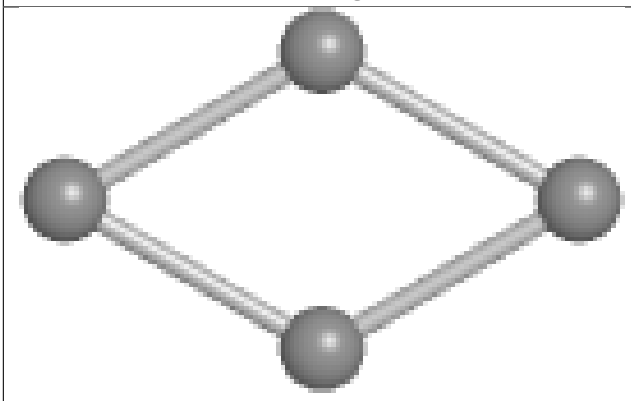
Ligand FES G 101



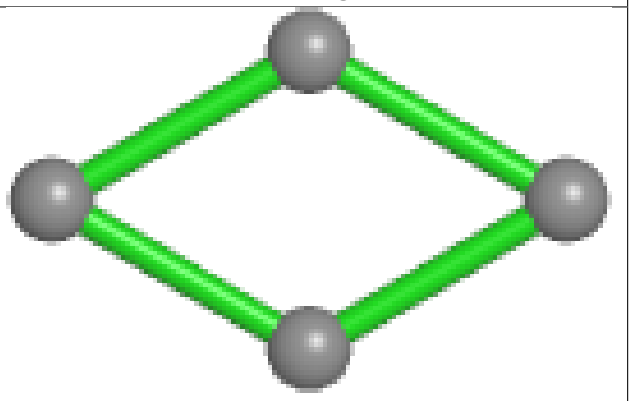
Bond lengths



Bond angles

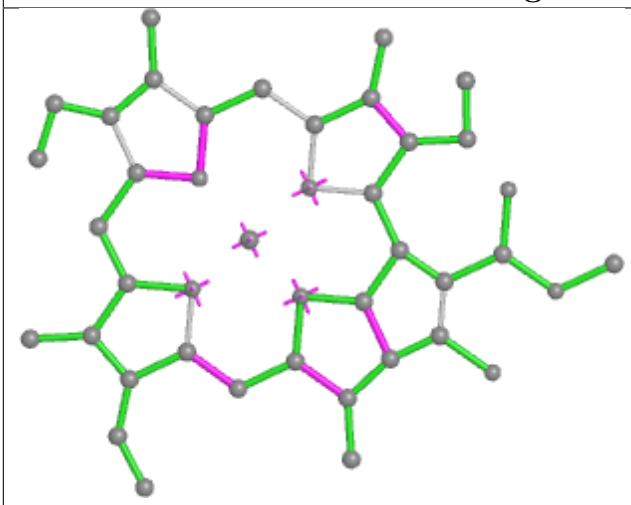


Torsions

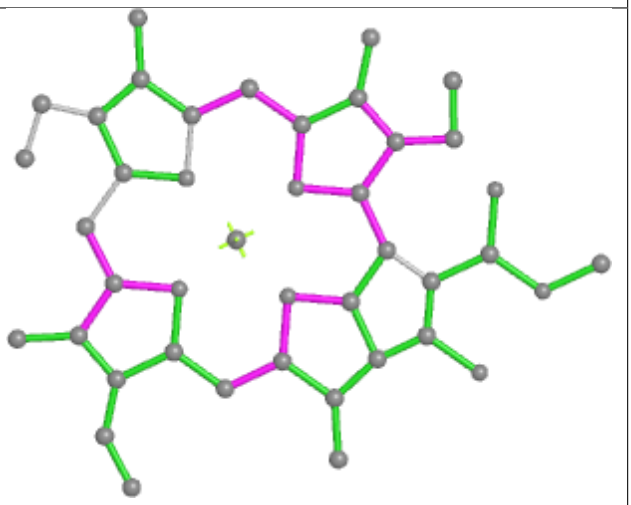


Rings

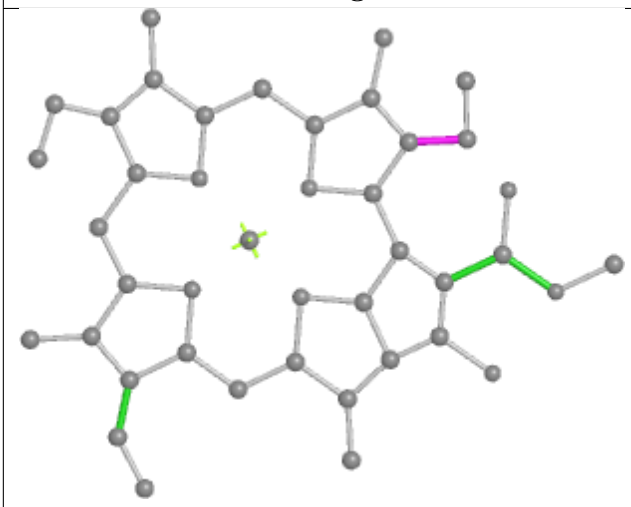
Ligand CLA B 805



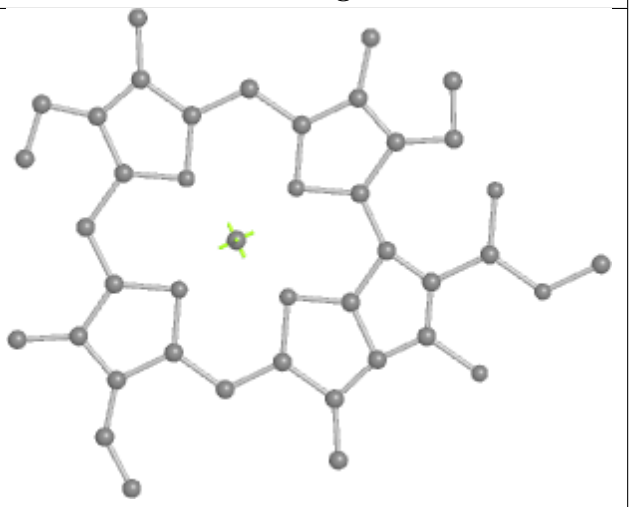
Bond lengths



Bond angles

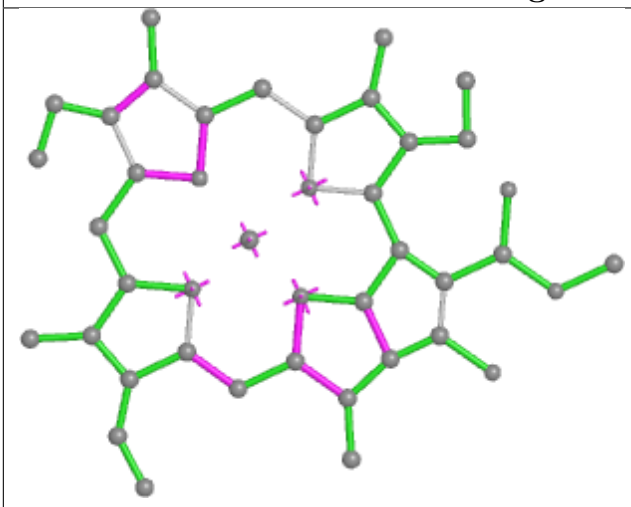


Torsions

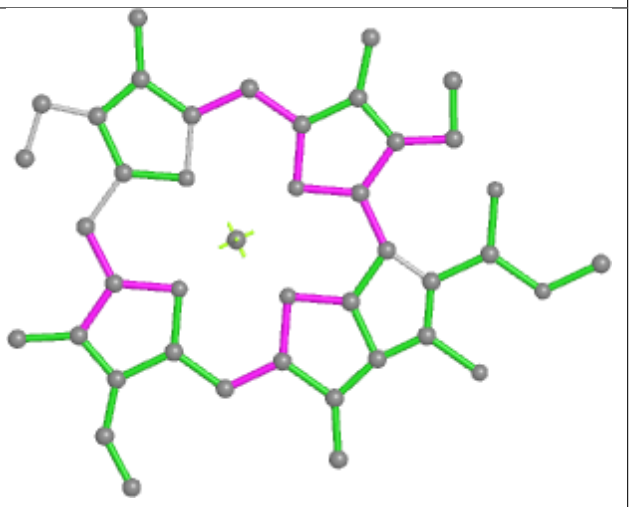


Rings

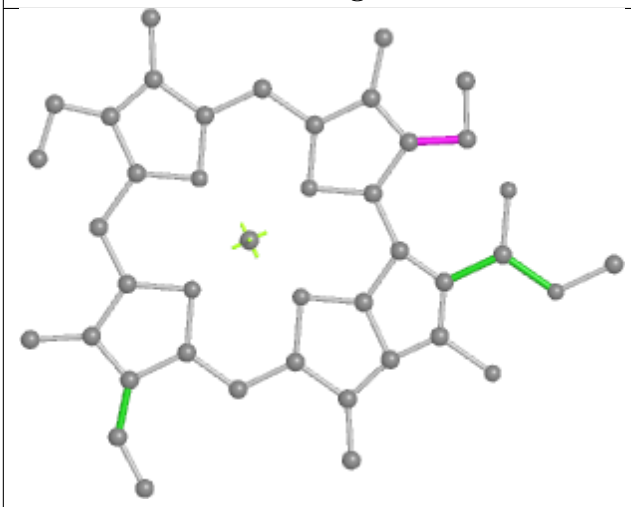
Ligand CLA 3 308



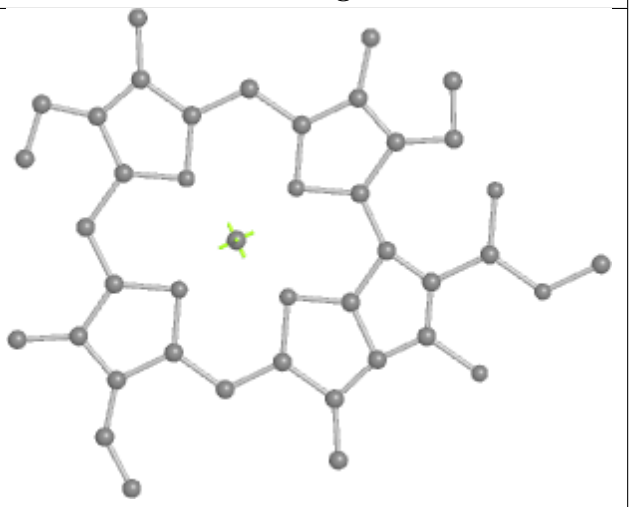
Bond lengths



Bond angles

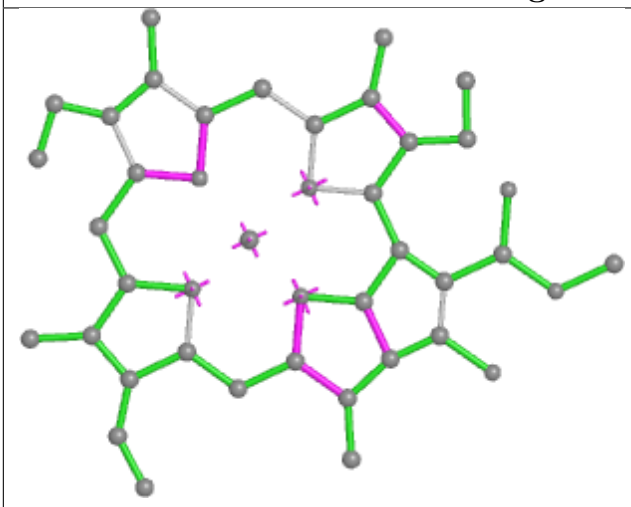


Torsions



Rings

Ligand CLA 1 605



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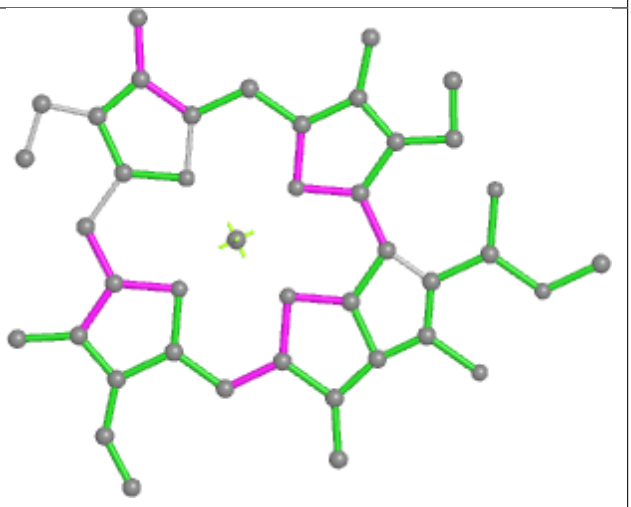
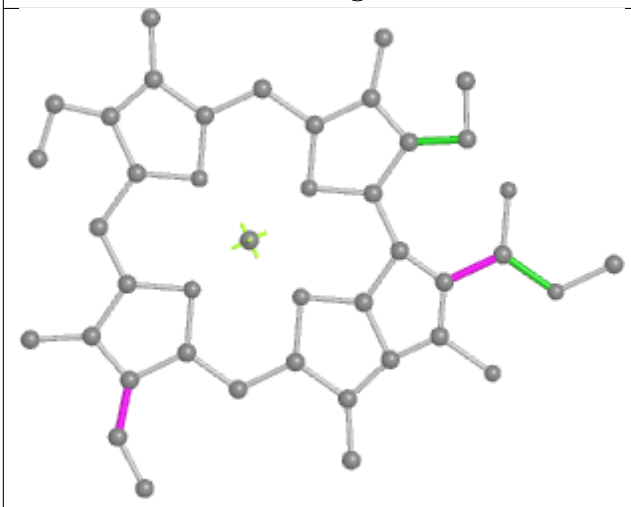


Bond angles



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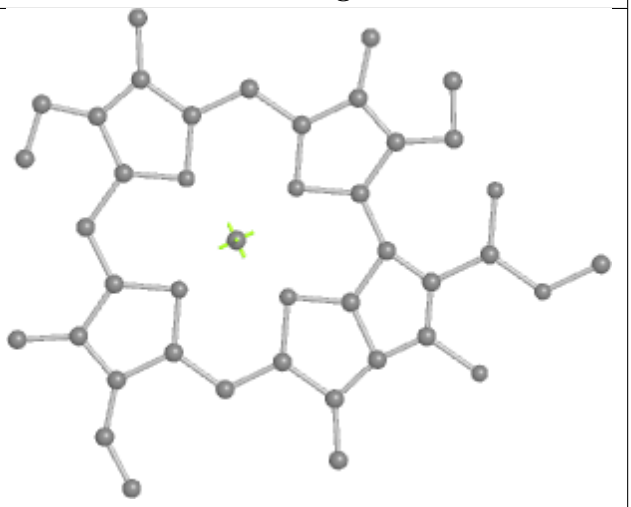
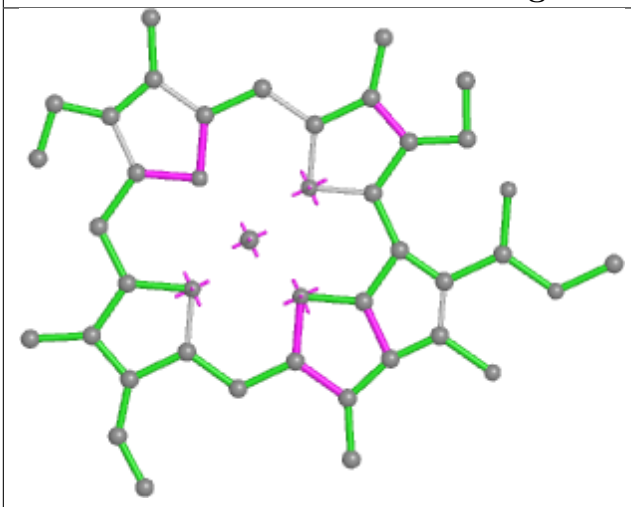


Rings

Ligand CLA 6 313



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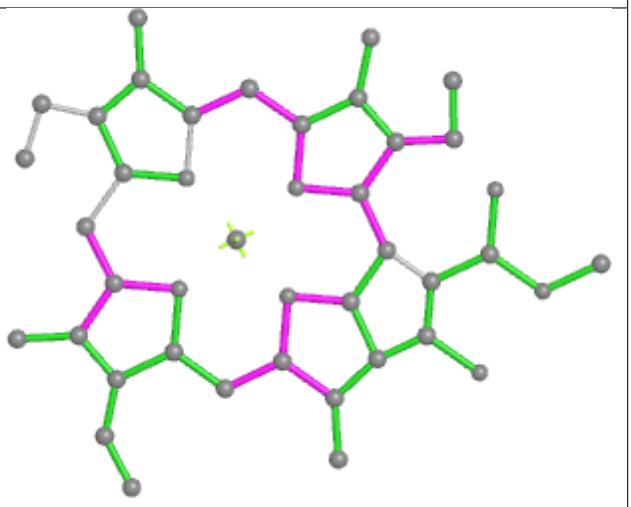
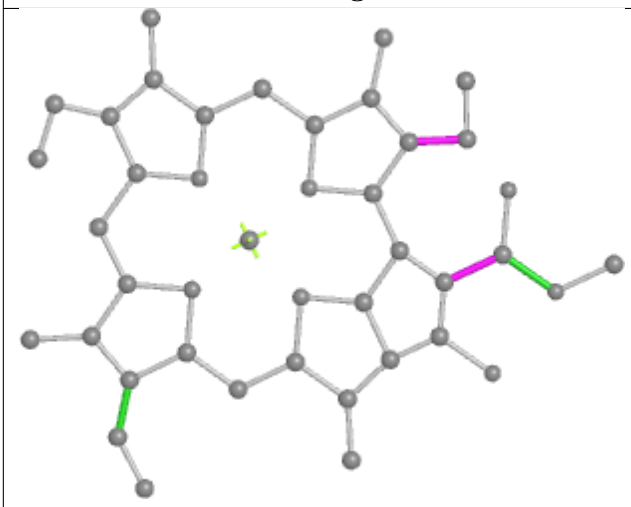
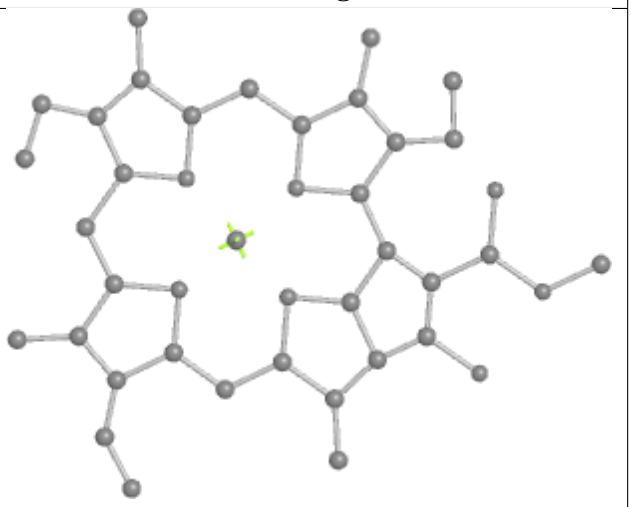


Bond angles

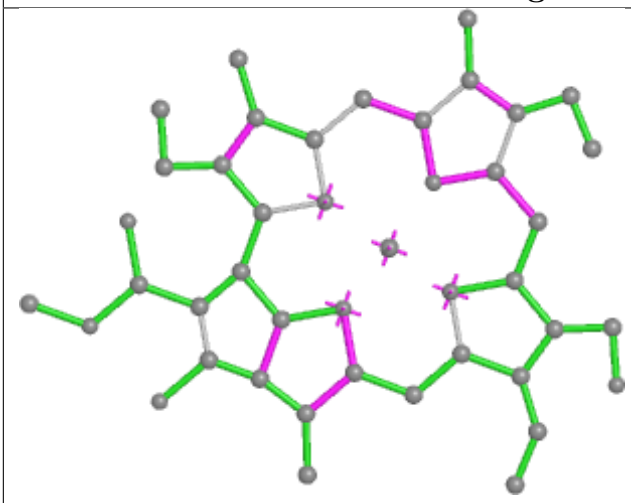


Torsions



Rings

Ligand CHL 3 306



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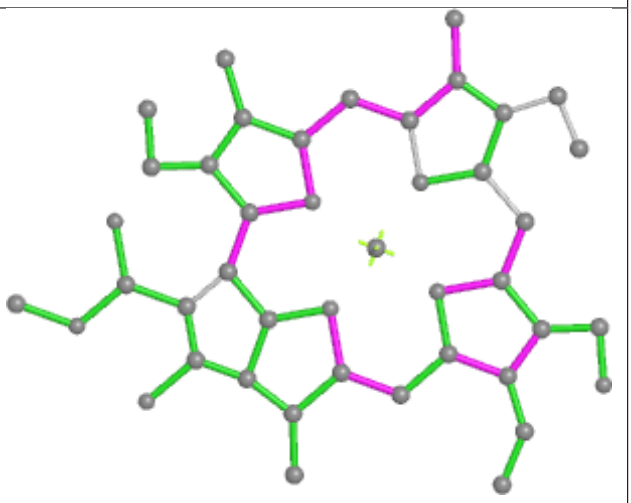
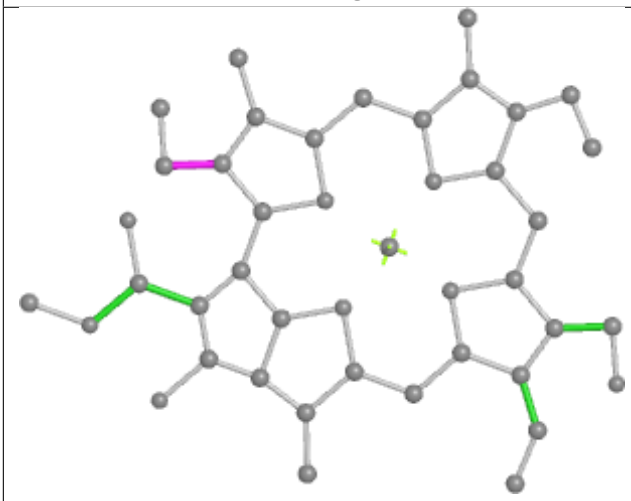


Bond angles



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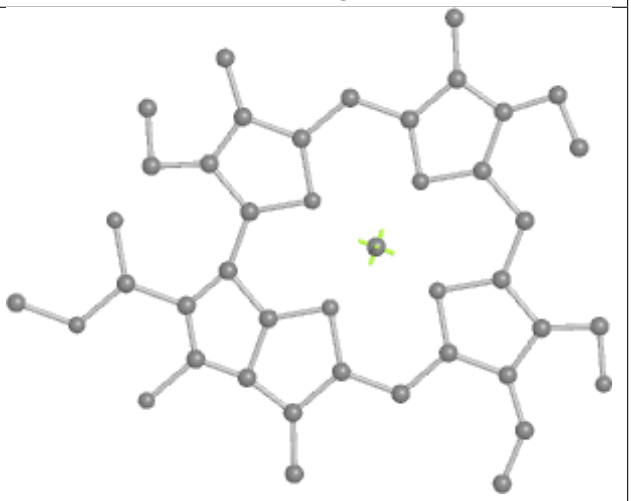
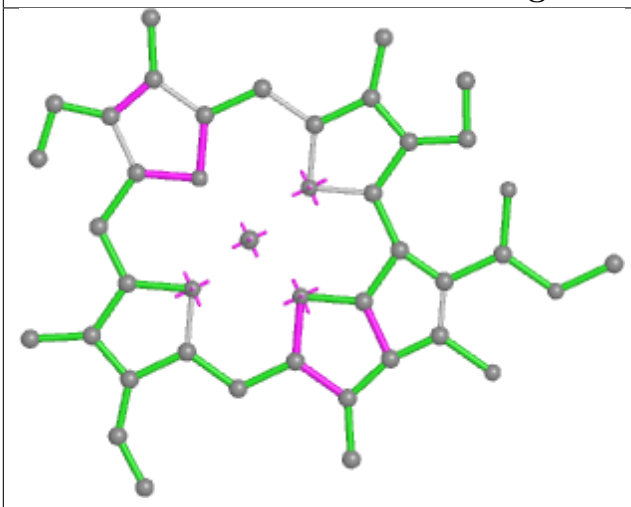


Rings

Ligand CLA 3 301



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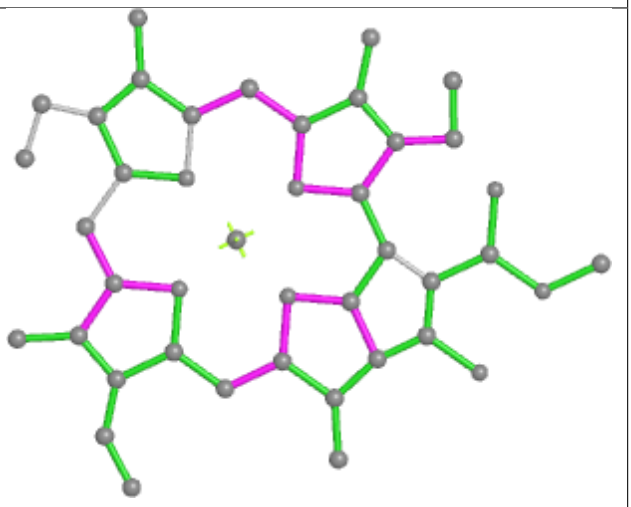

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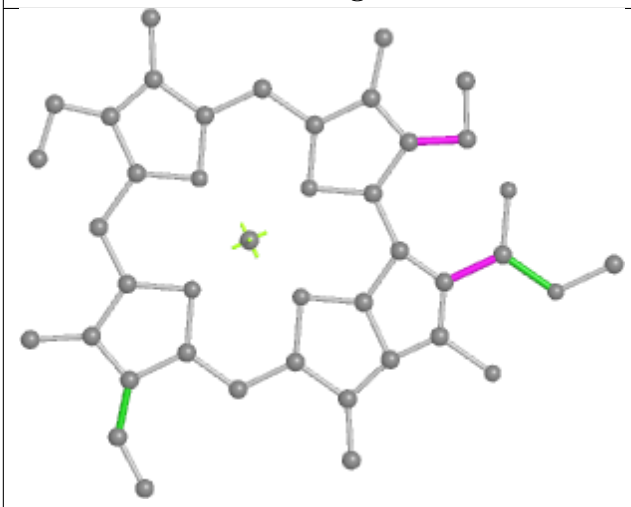

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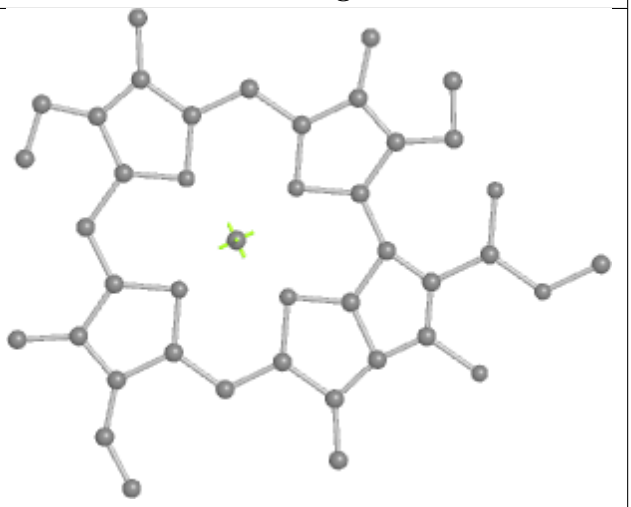
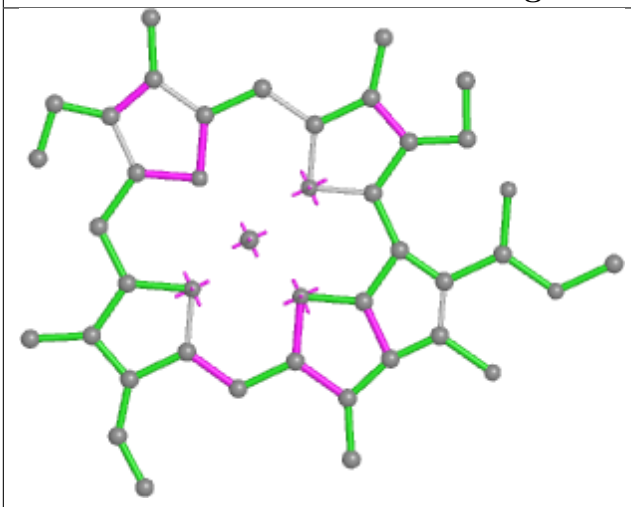


Rings

Ligand CLA B 808



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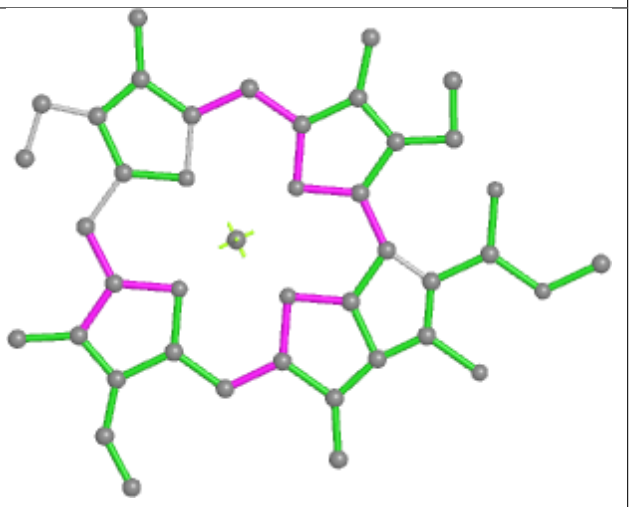
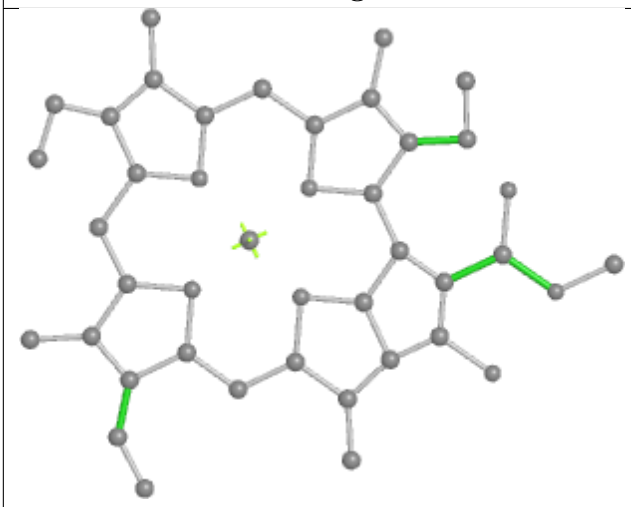


Bond angles



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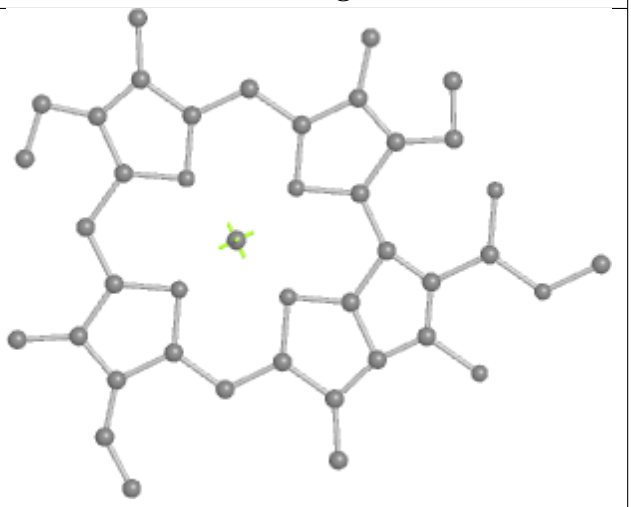
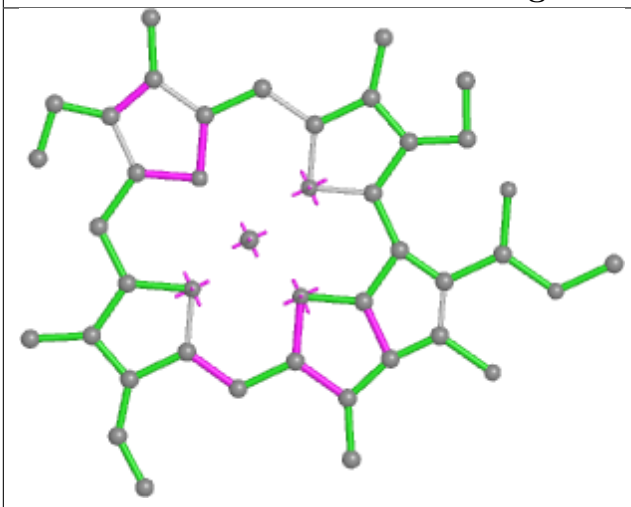


Rings

Ligand CLA 5 602



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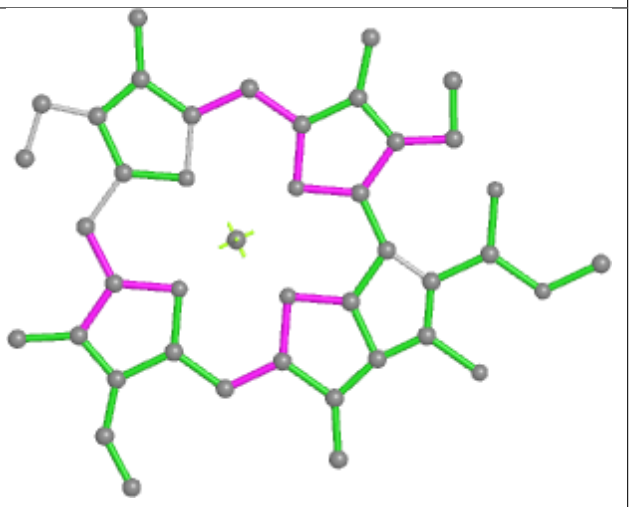
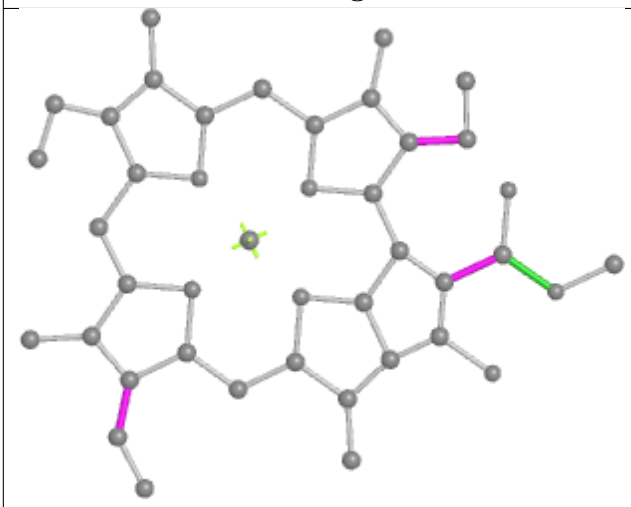


Bond angles



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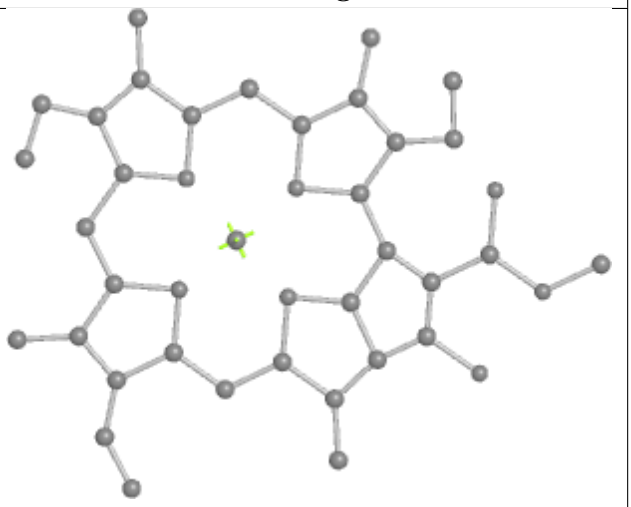
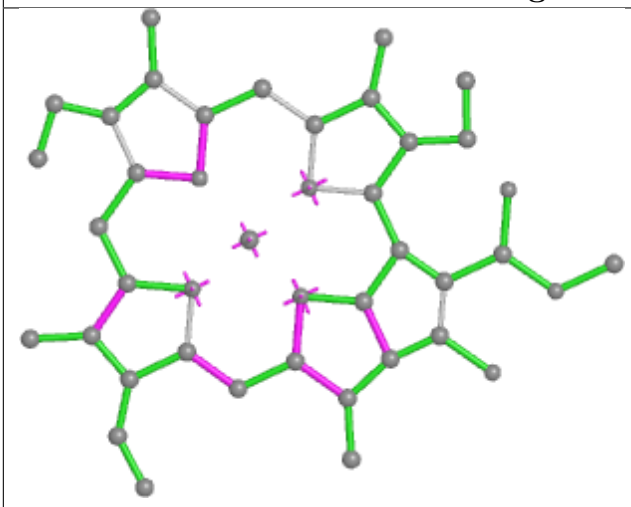
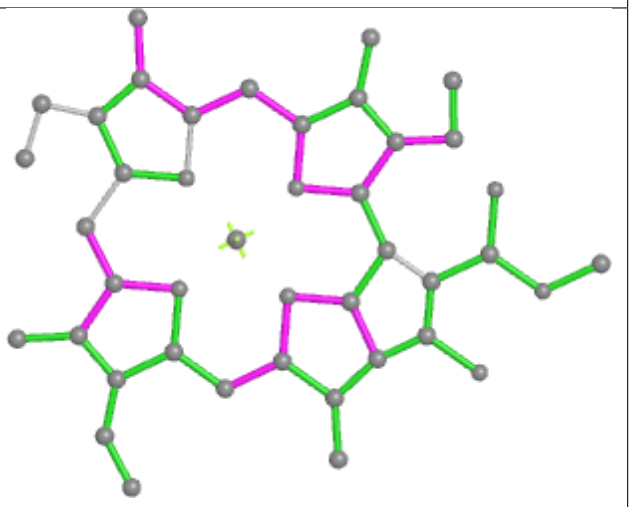


Rings

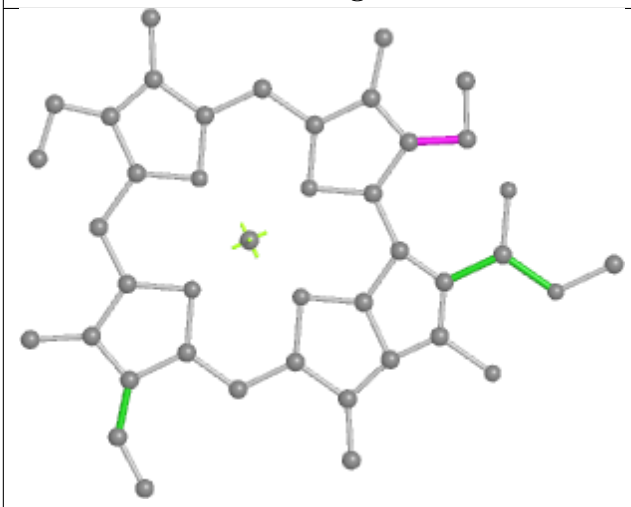
Ligand CLA 4 602



Bond lengths



Bond angles



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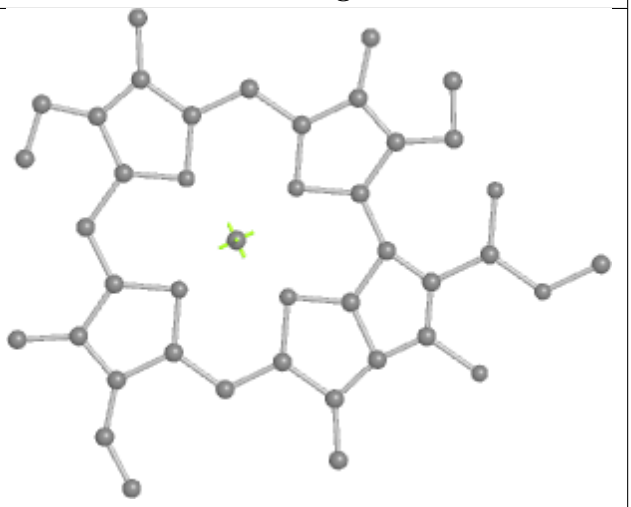
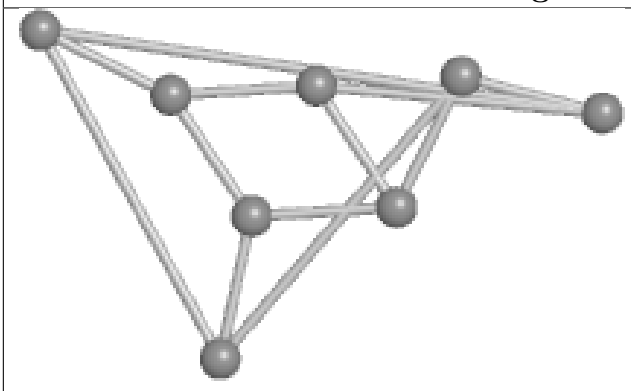
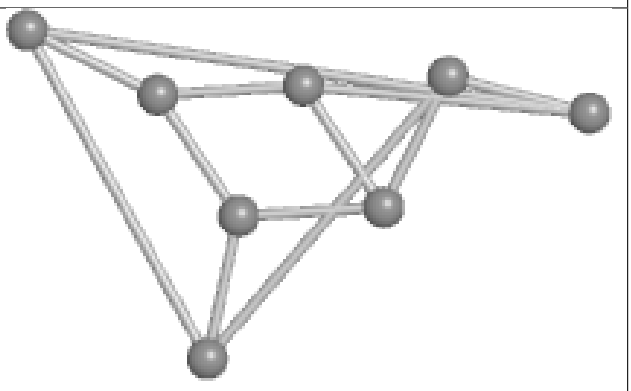


Rings

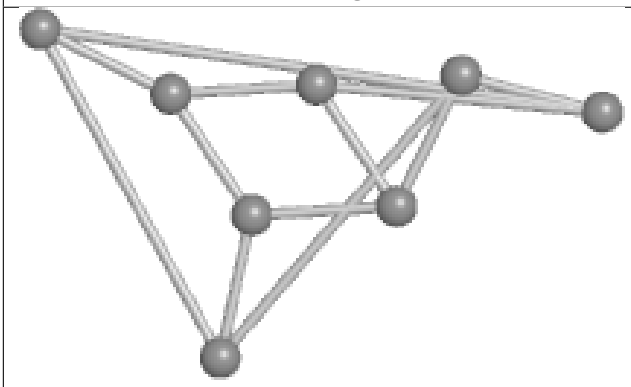
Ligand SF4 B 803



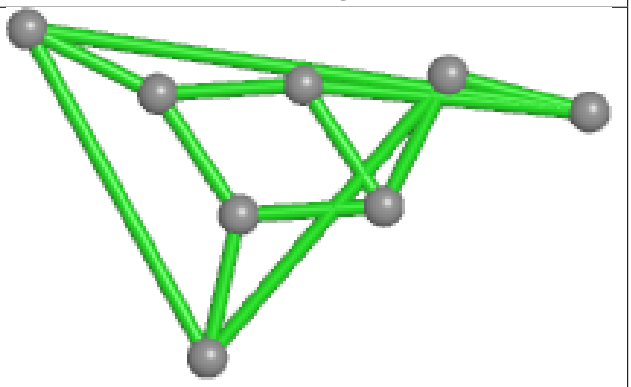
Bond lengths



Bond angles

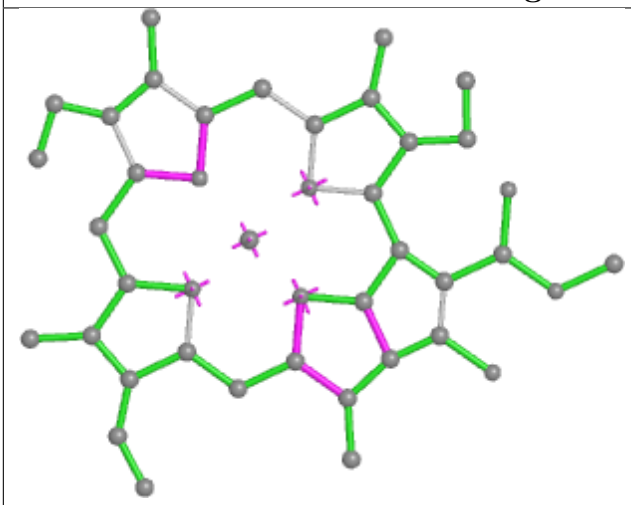


Torsions

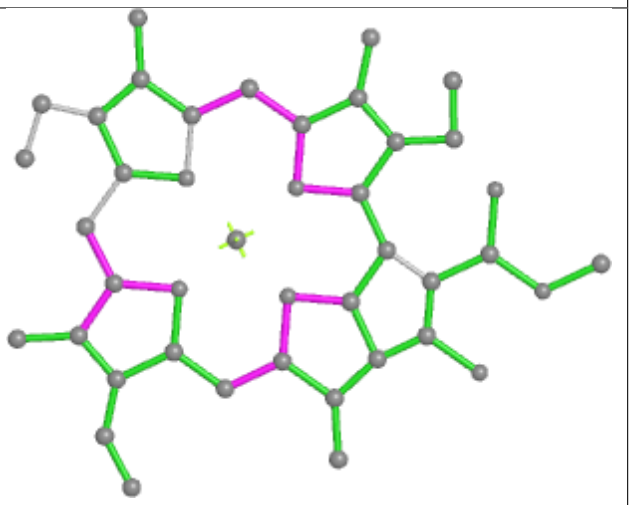


Rings

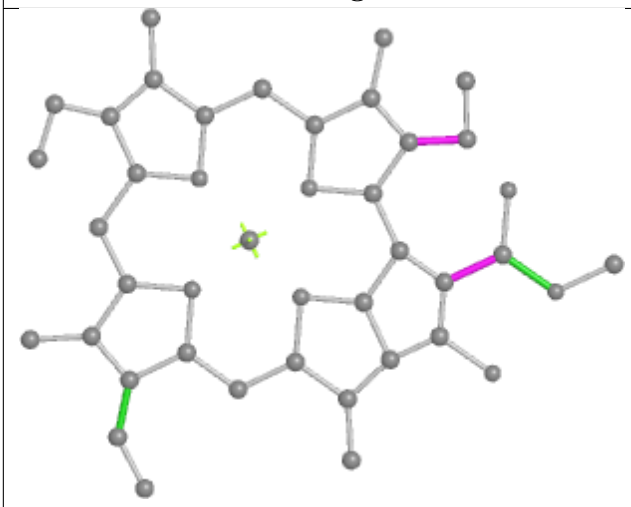
Ligand CLA B 824



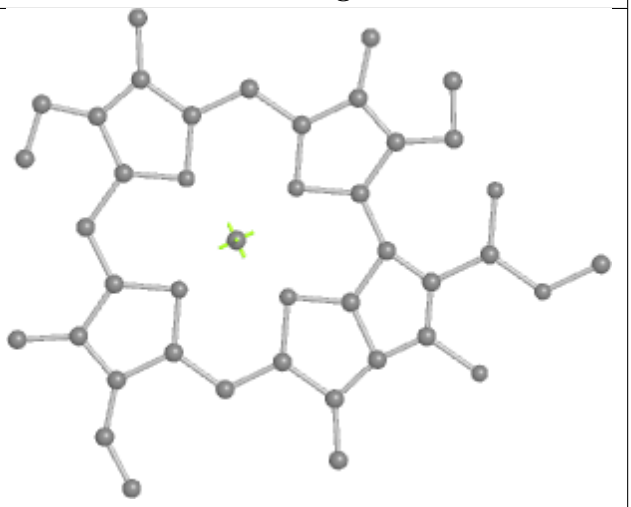
Bond lengths



Bond angles

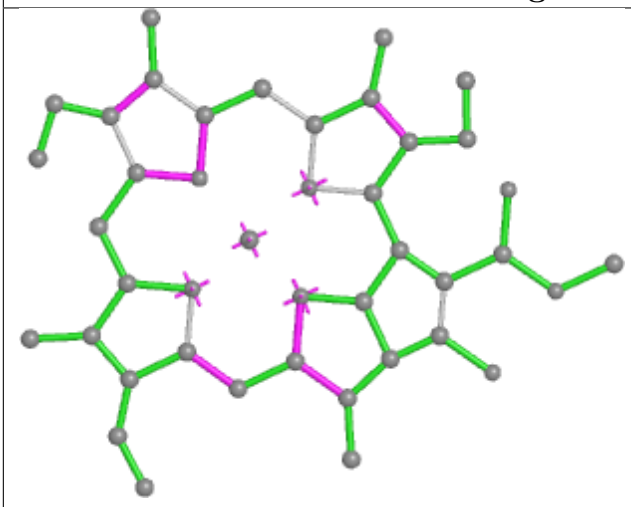


Torsions



Rings

Ligand CLA 8 607



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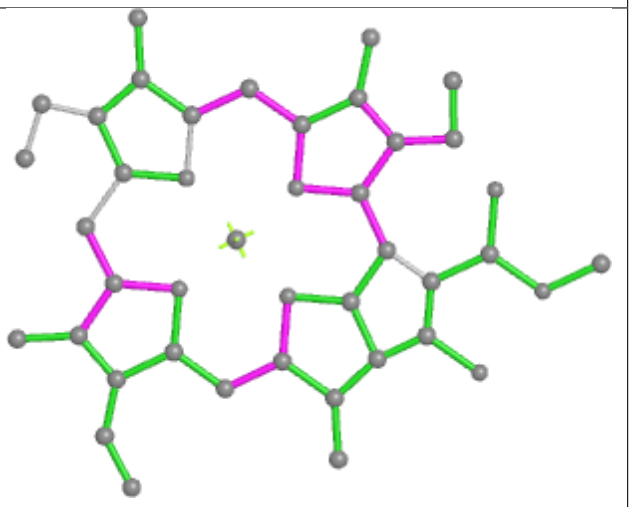
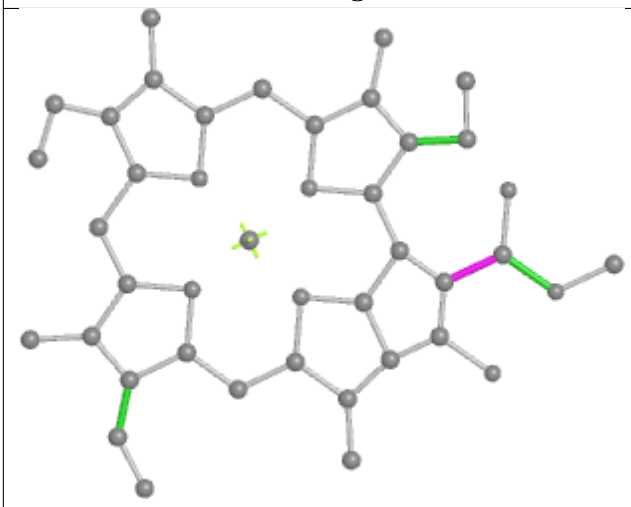


Bond angles



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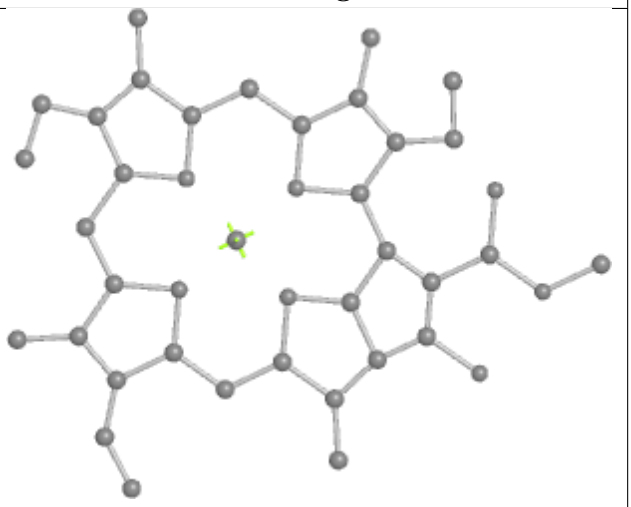

Rings

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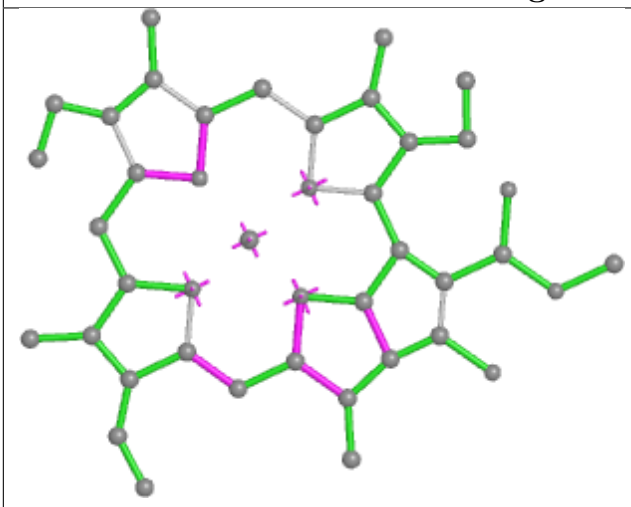

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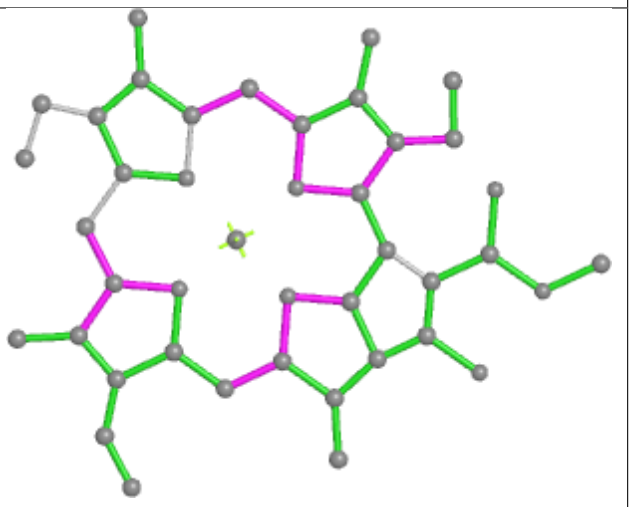
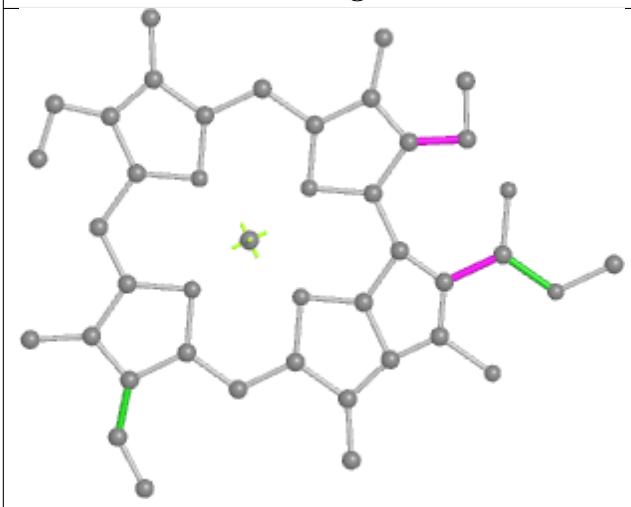


Bond angles



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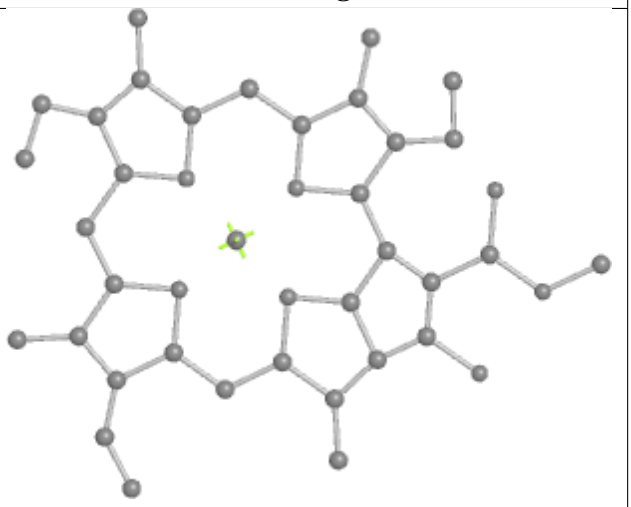
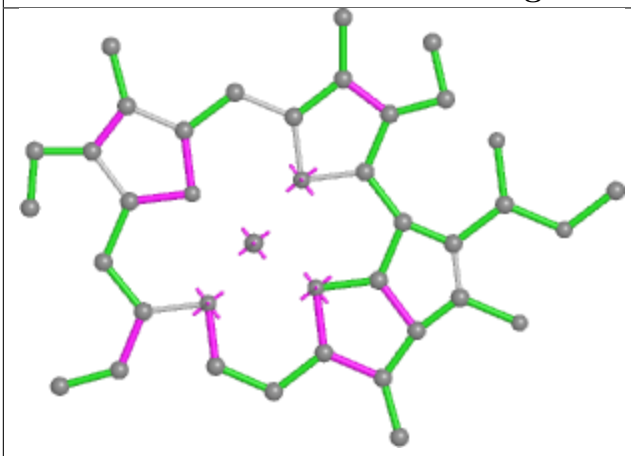
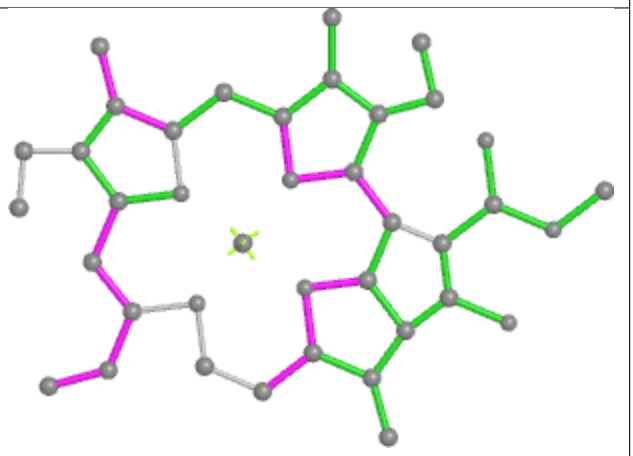


Rings

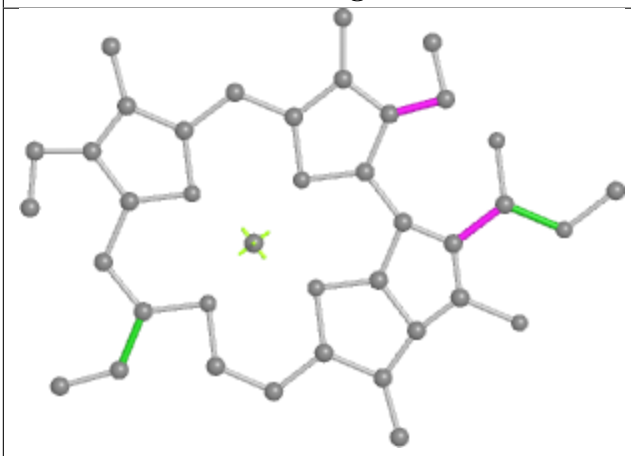
Ligand CLA B 834



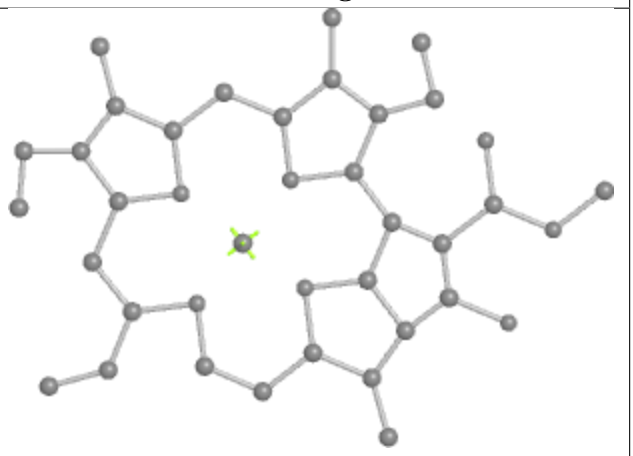
Bond lengths



Bond angles

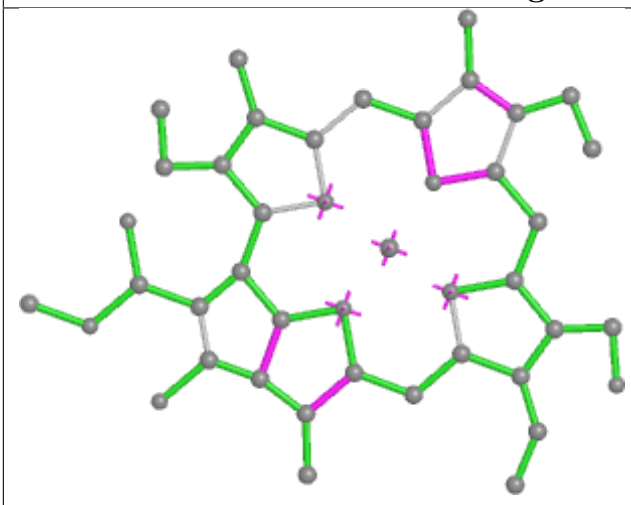


Torsions

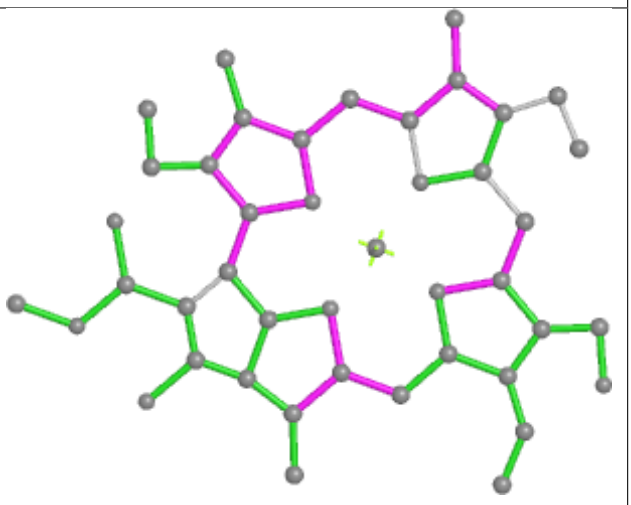


Rings

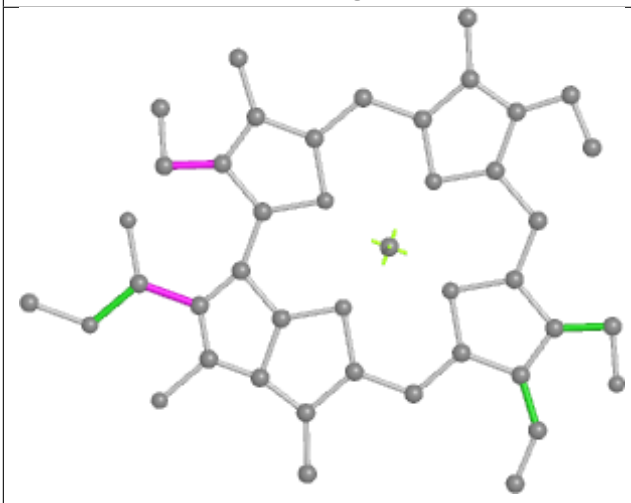
Ligand CHL 5 606



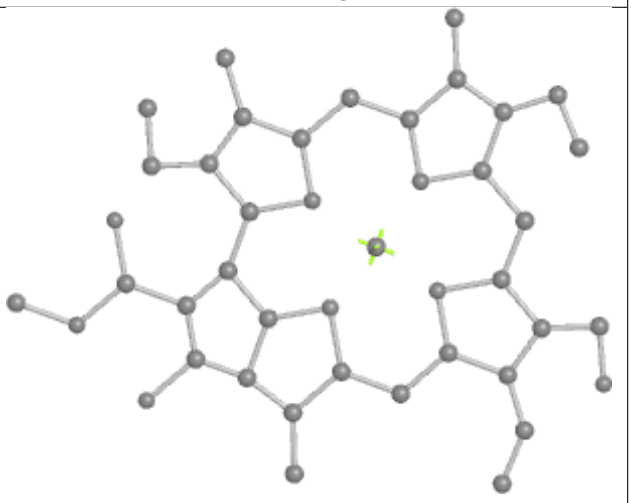
Bond lengths



Bond angles

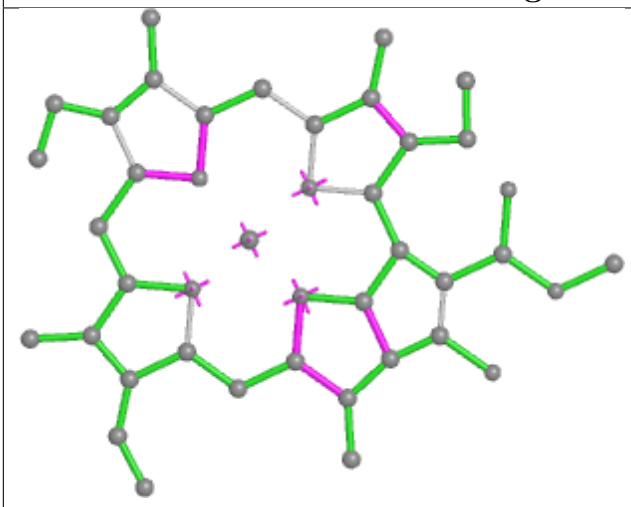


Torsions

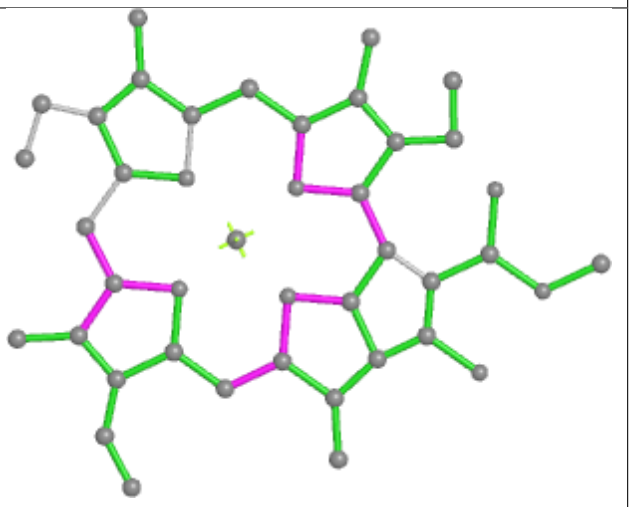


Rings

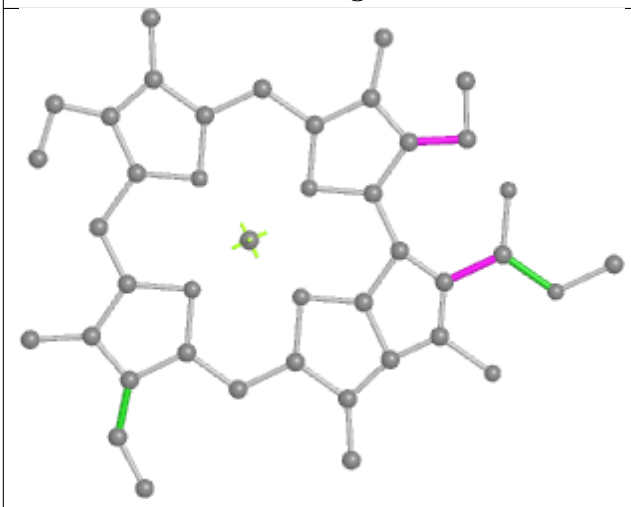
Ligand CLA B 825



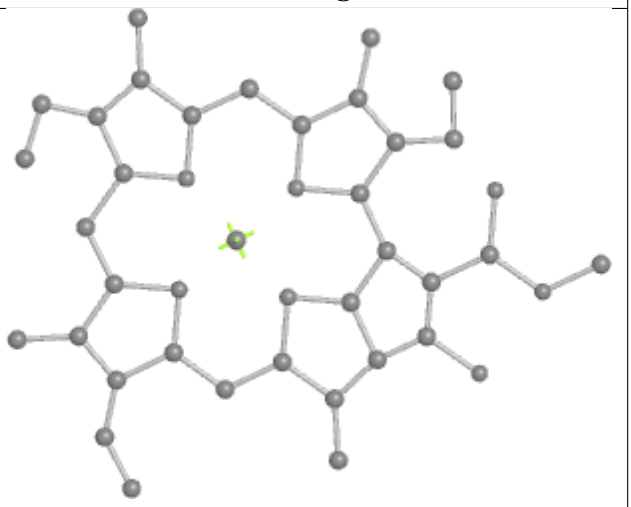
Bond lengths



Bond angles

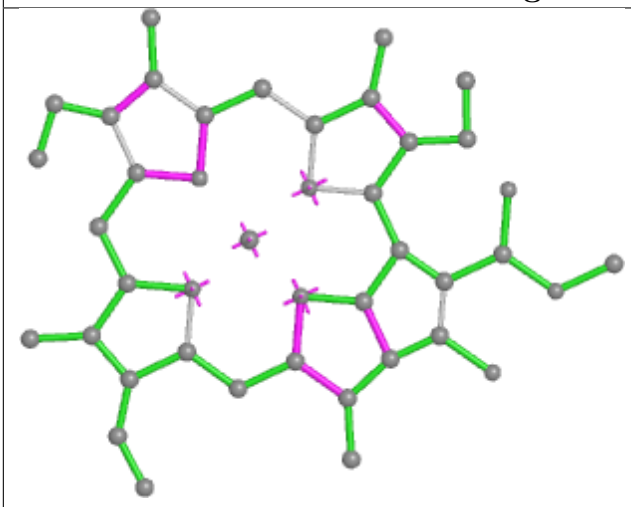


Torsions

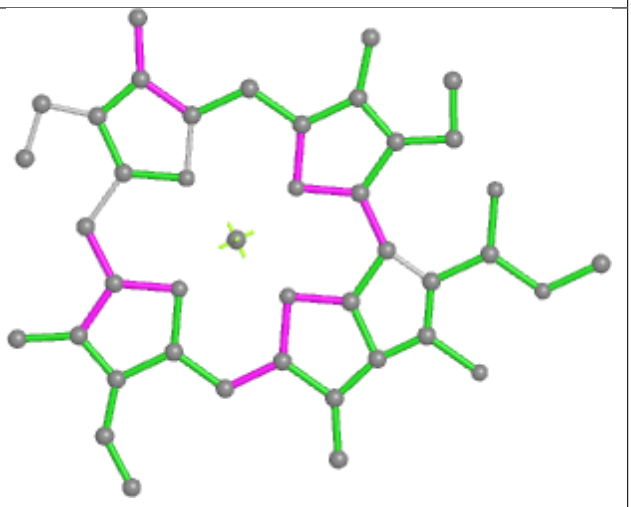


Rings

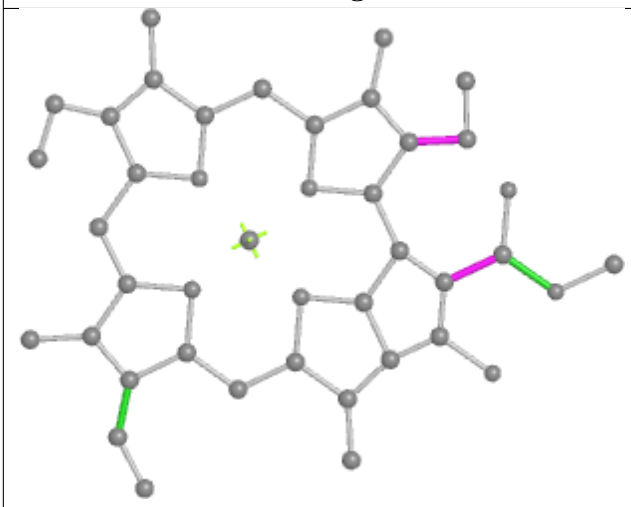
Ligand CLA A 804



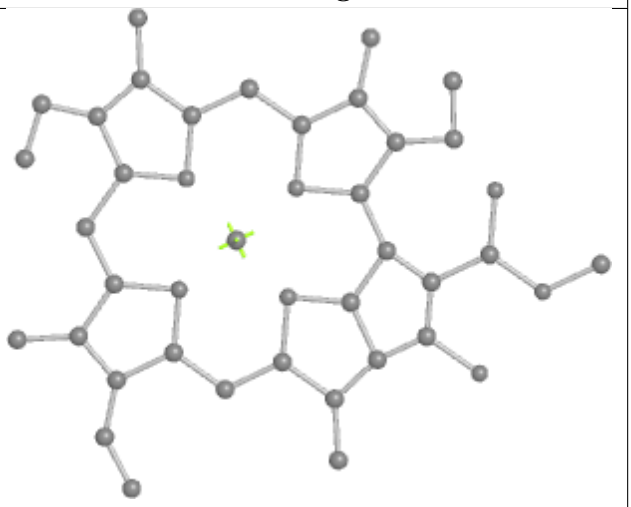
Bond lengths



Bond angles

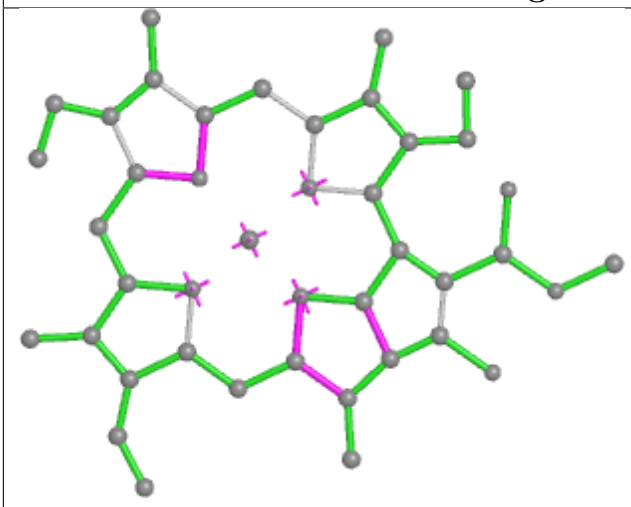


Torsions

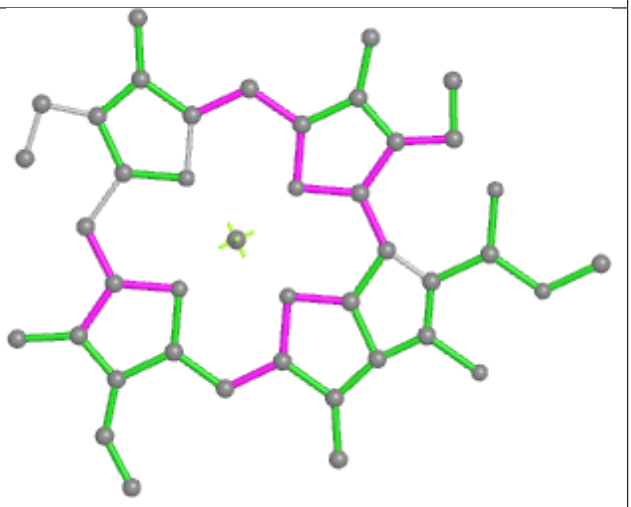


Rings

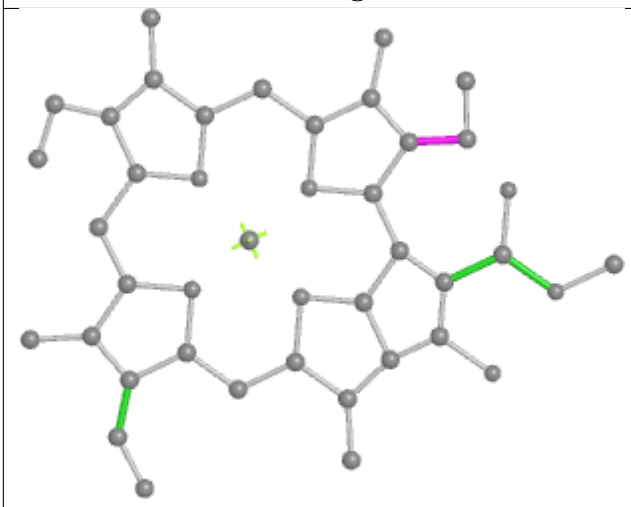
Ligand CLA 6 315



Bond lengths



Bond angles



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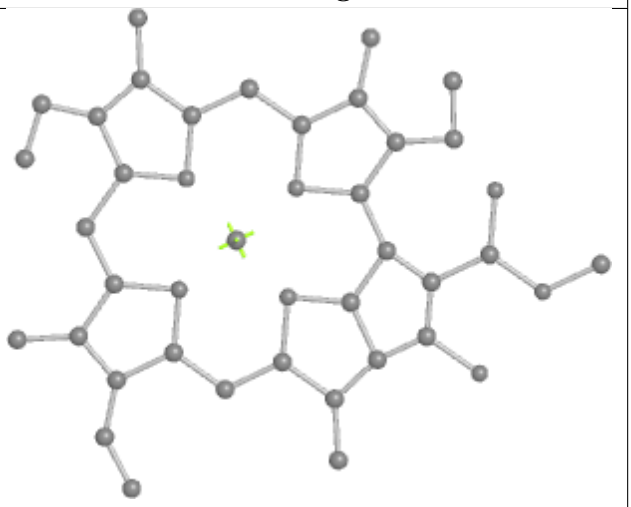
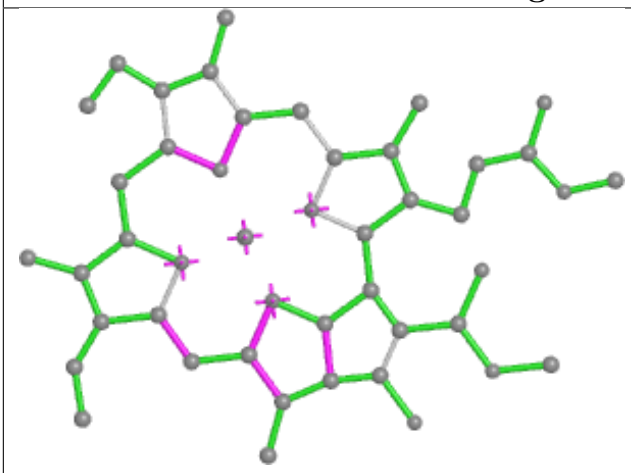


Rings

Ligand CLA 7 603



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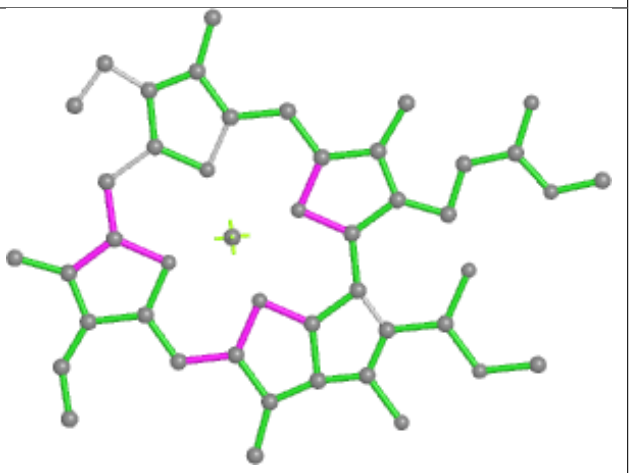
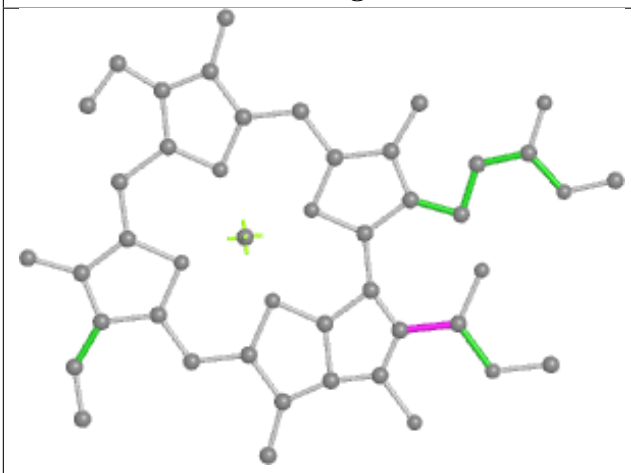
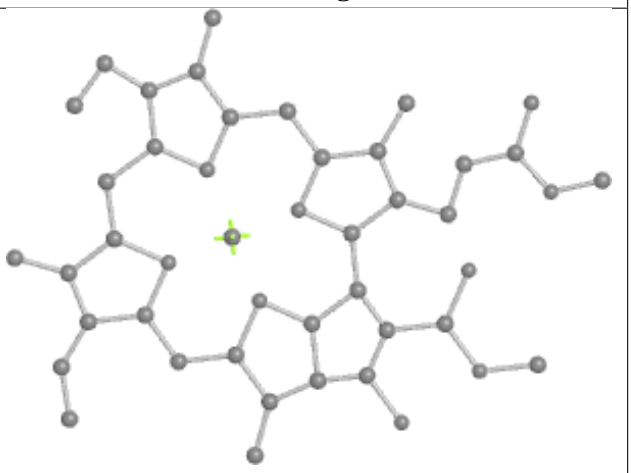


Bond angles

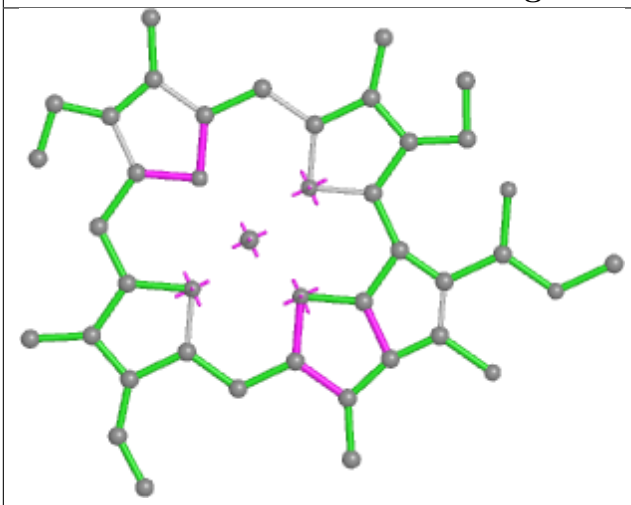


Torsions

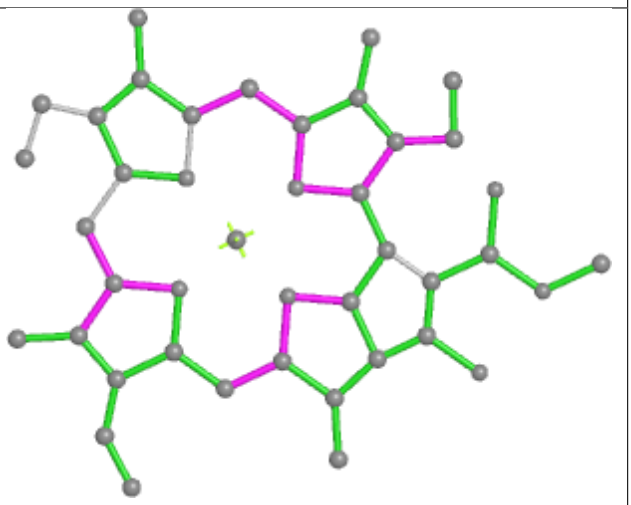


Rings

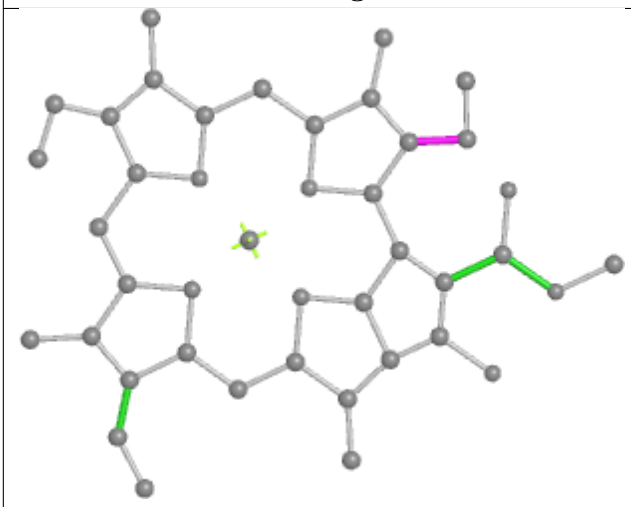
Ligand CLA B 821



Bond lengths



Bond angles



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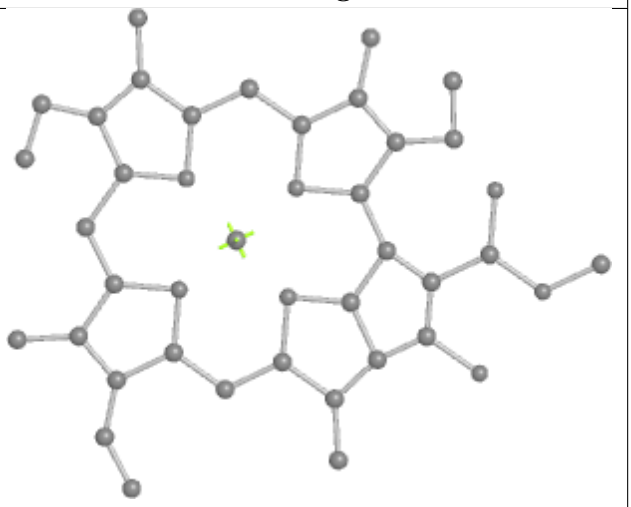
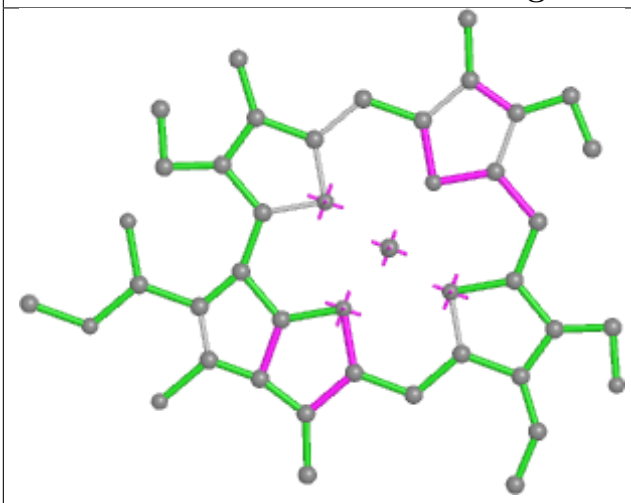


Rings

Ligand CHL 6 305



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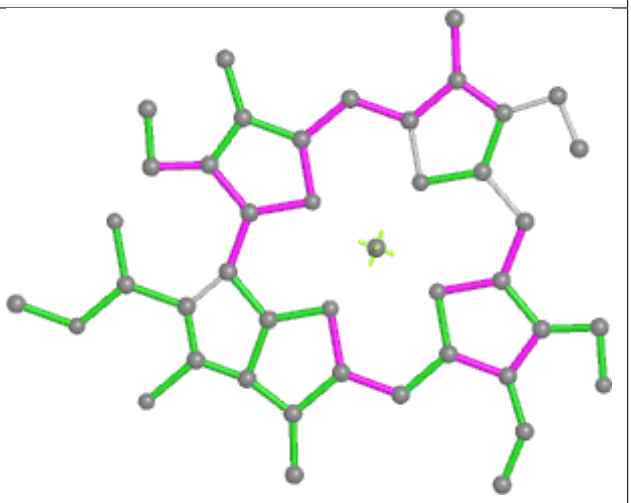
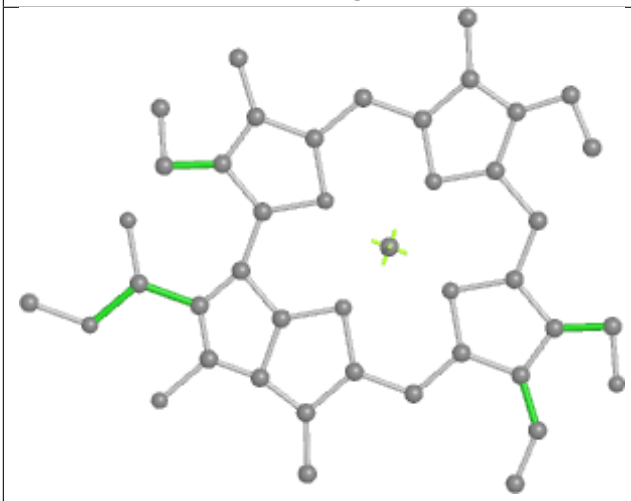


Bond angles



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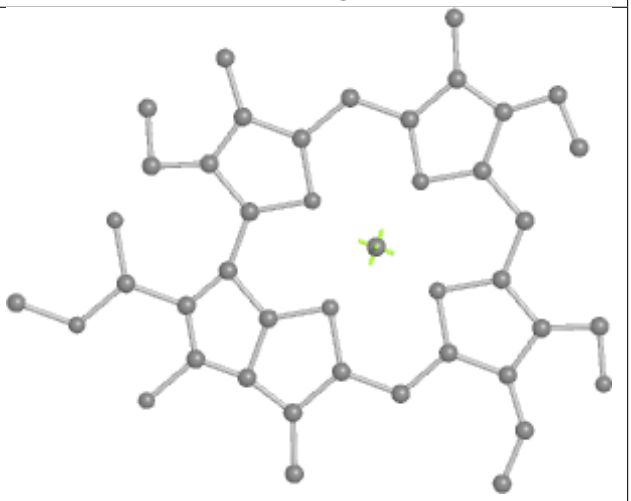
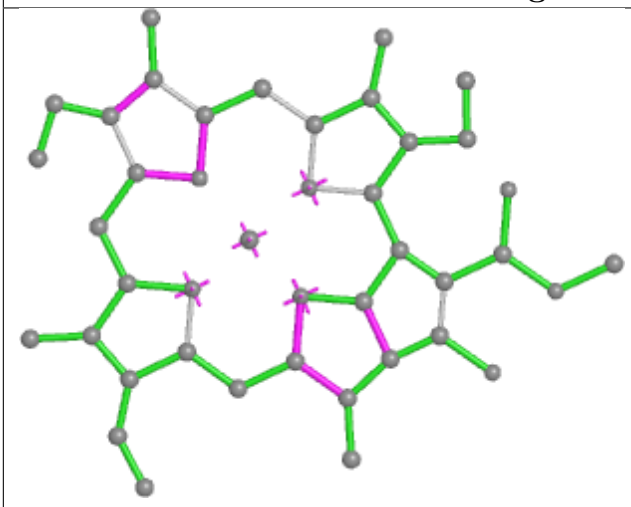


Rings

Ligand CLA 5 613



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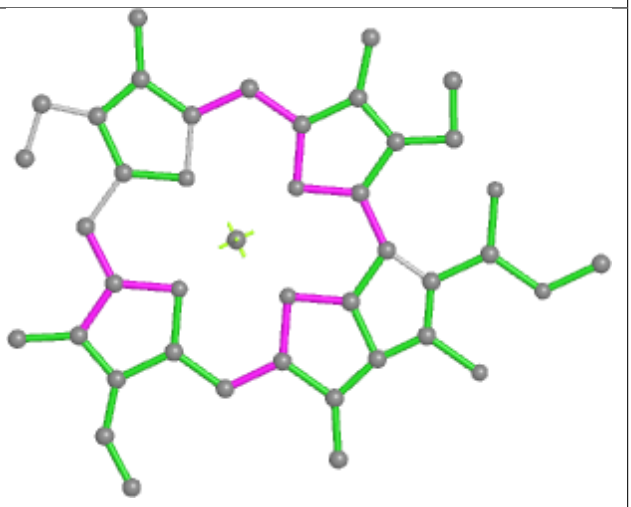
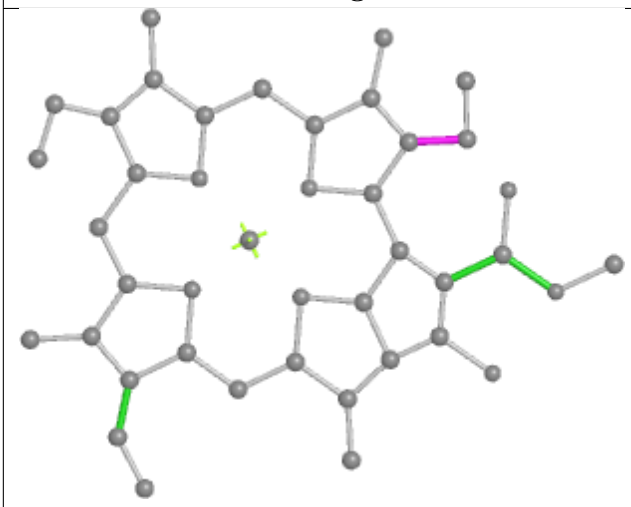


Bond angles



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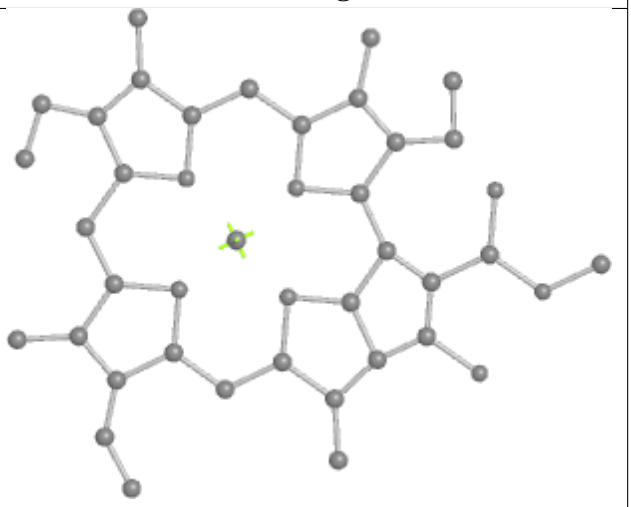
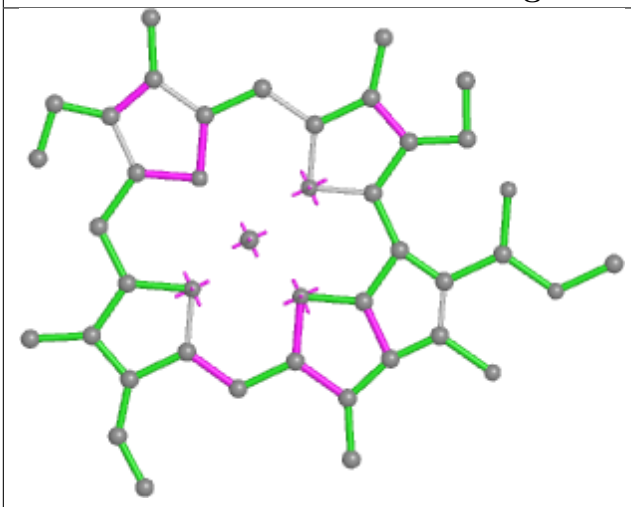
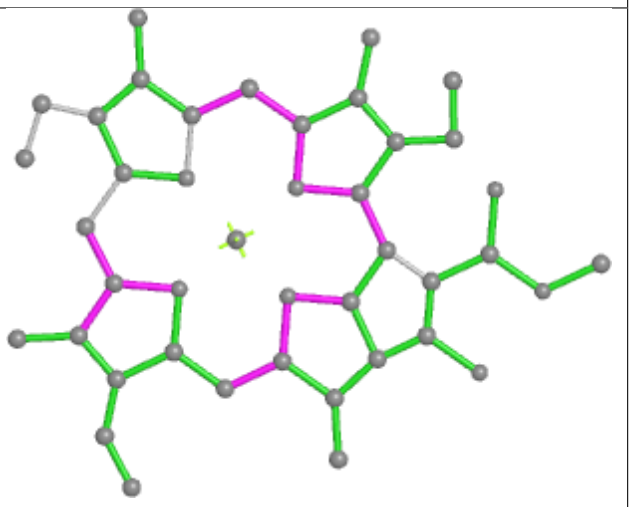


Rings

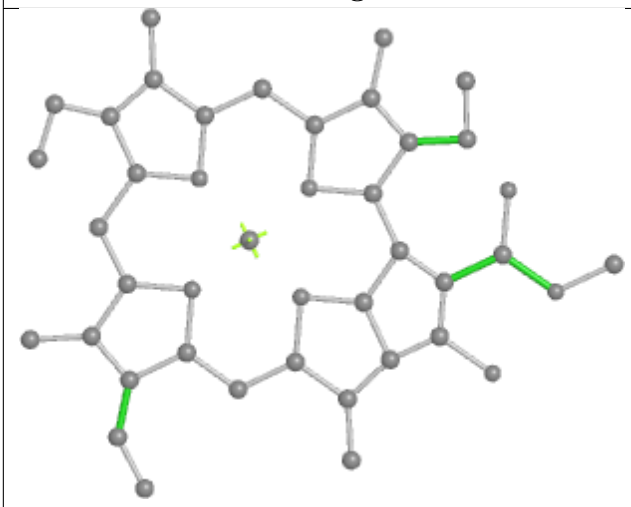
Ligand CLA A 828



Bond lengths



Bond angles



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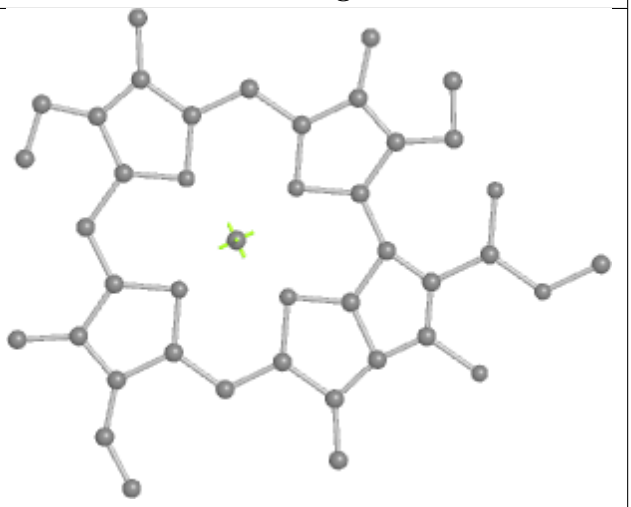
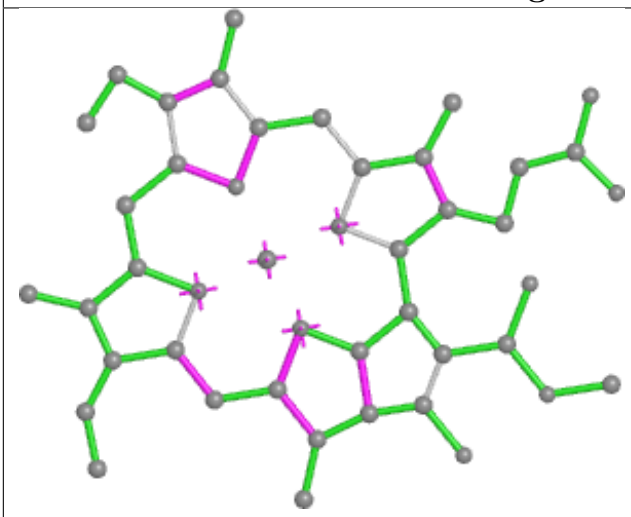


Rings

Ligand CLA 3 311



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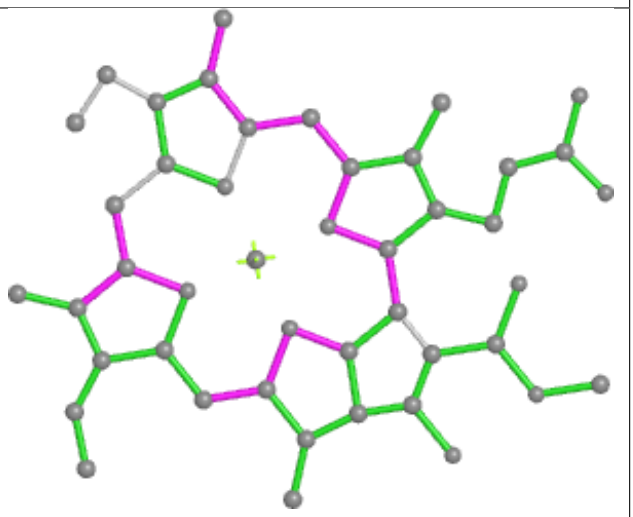
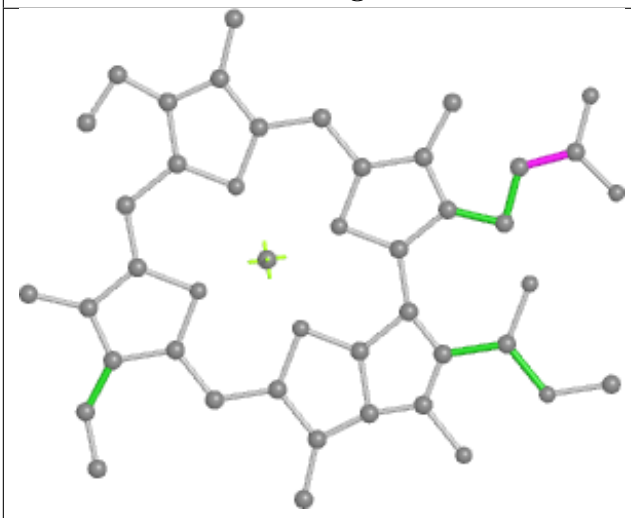


Bond angles



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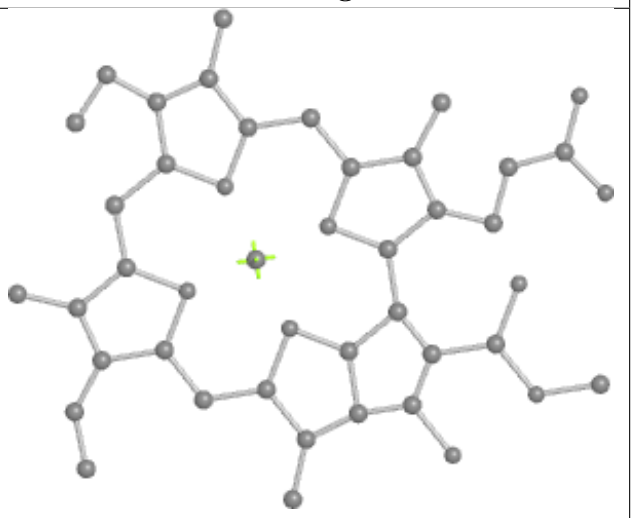
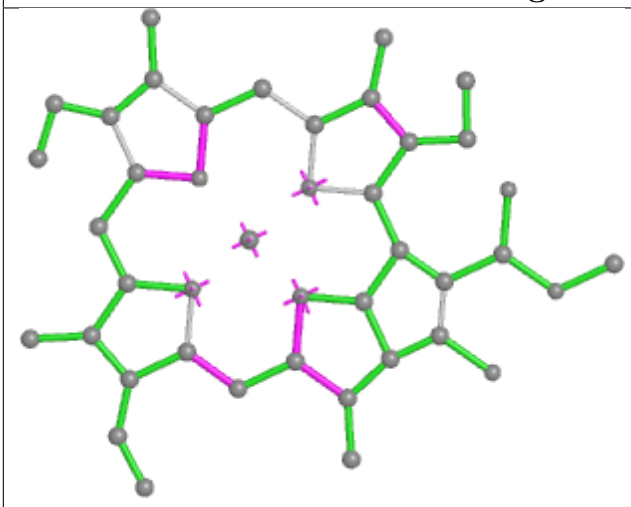
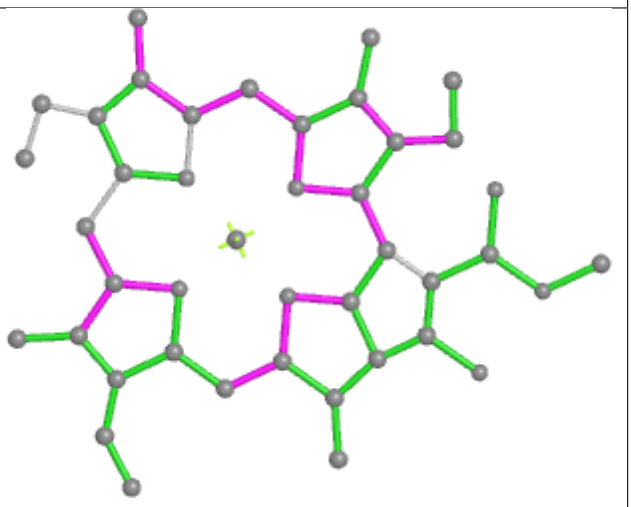


Rings

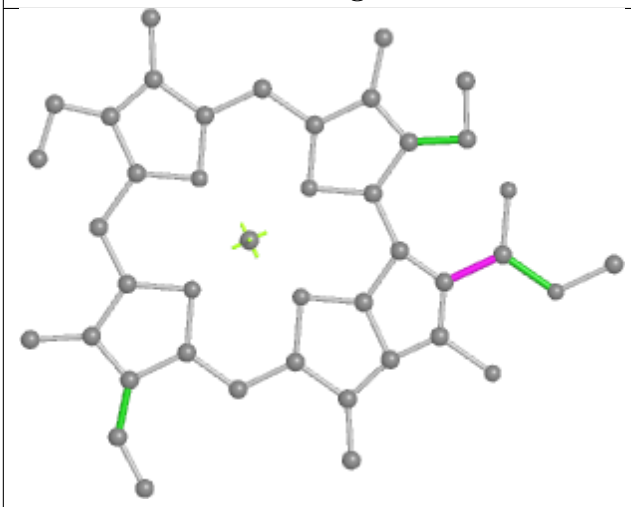
Ligand CLA 6 304



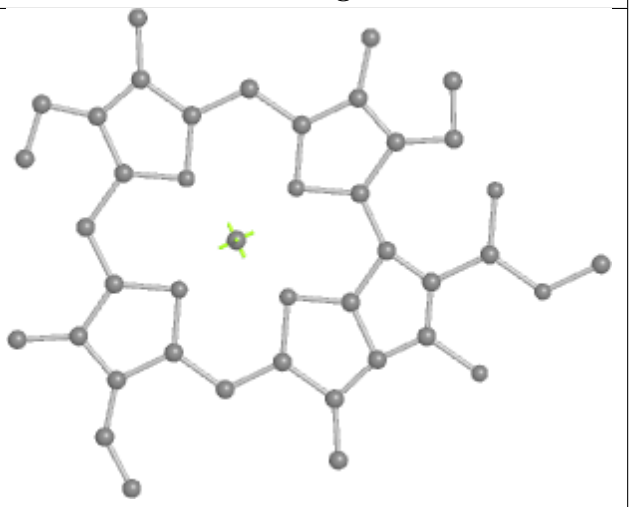
Bond lengths



Bond angles

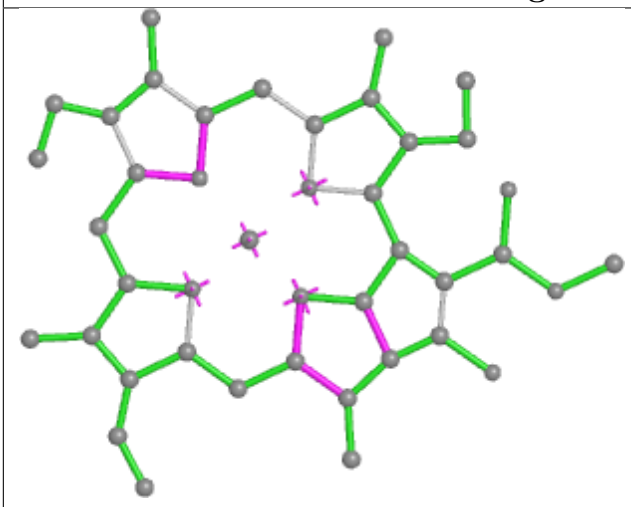


Torsions

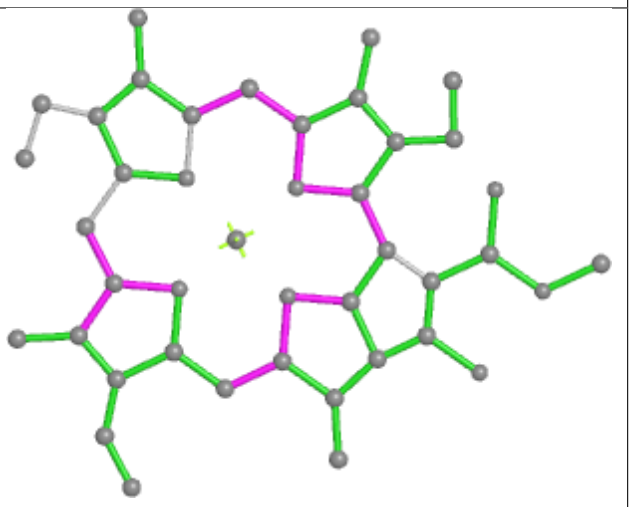


Rings

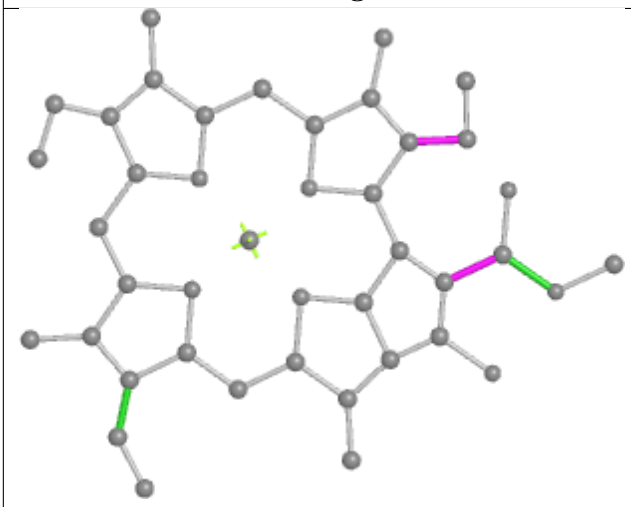
Ligand CLA 4 606



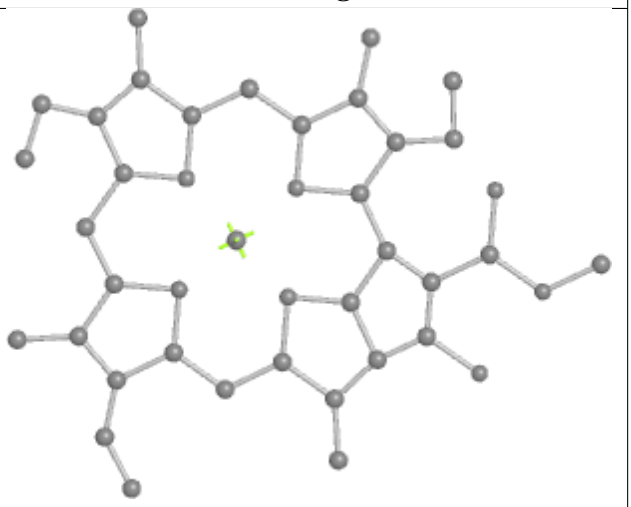
Bond lengths



Bond angles

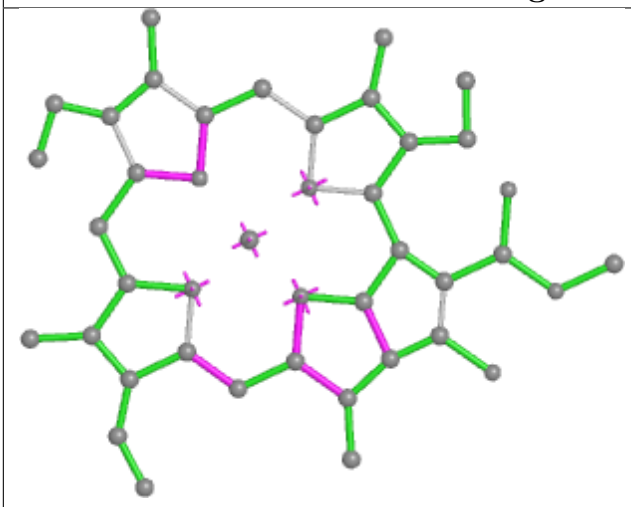


Torsions



Rings

Ligand CLA 1 602



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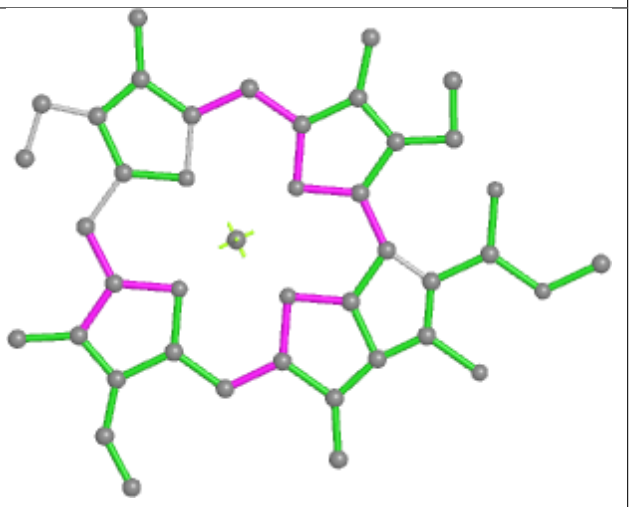
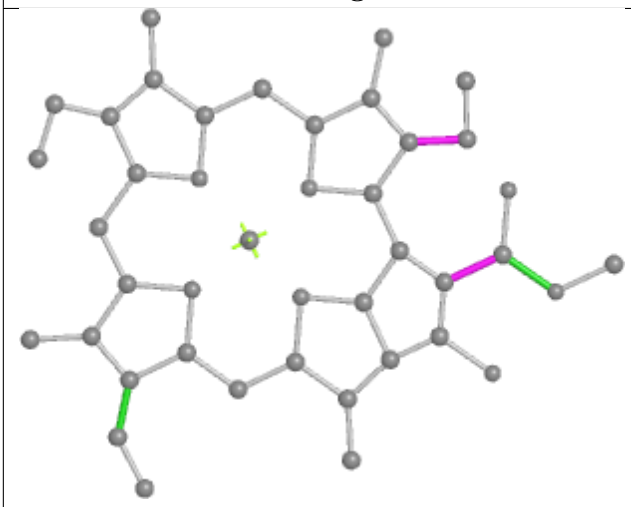
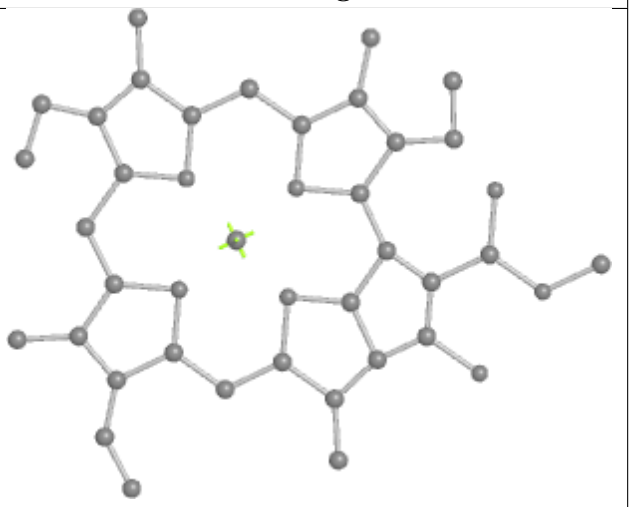


Bond angles

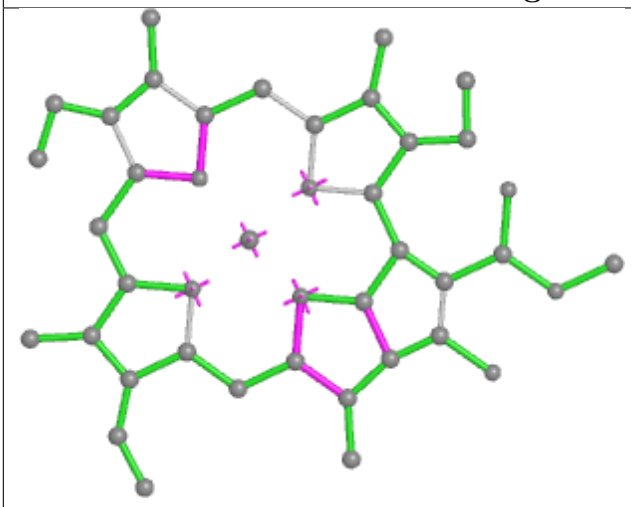


Torsions



Rings

Ligand CLA A 844



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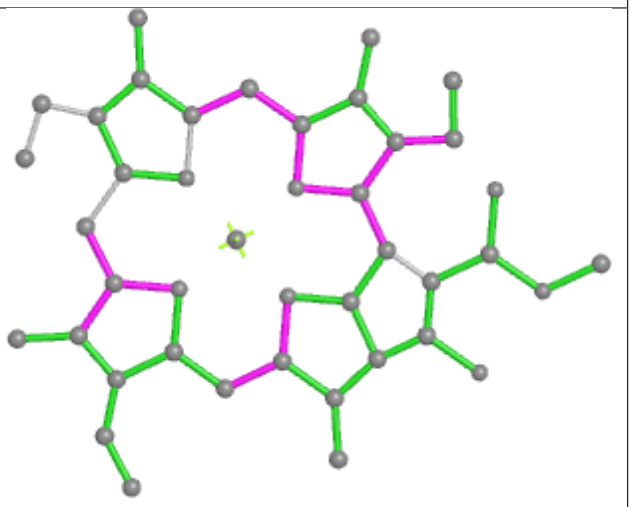
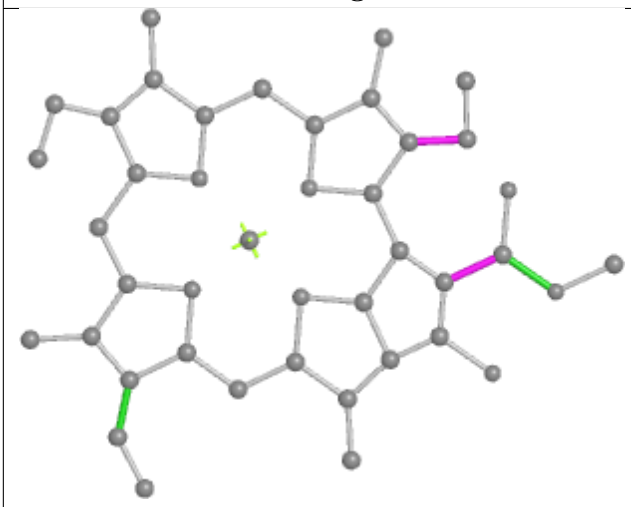
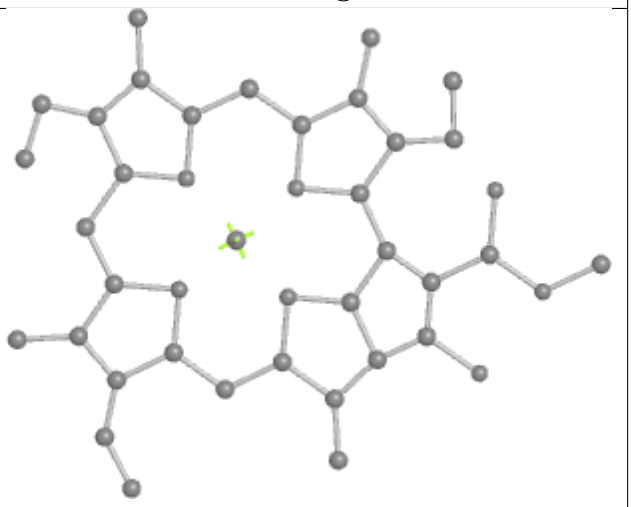


Bond angles

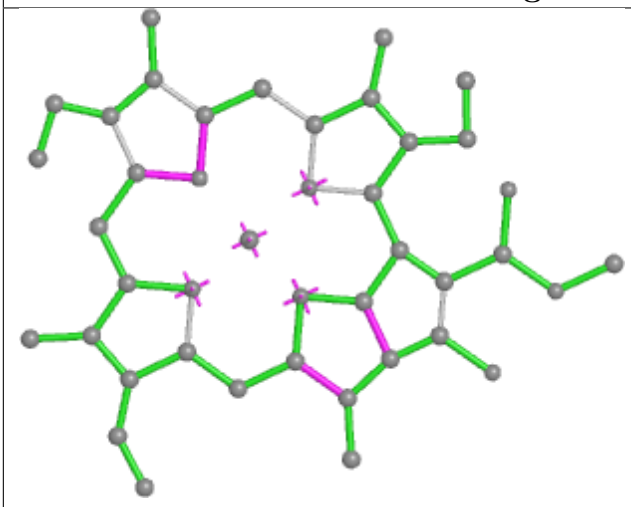


Torsions

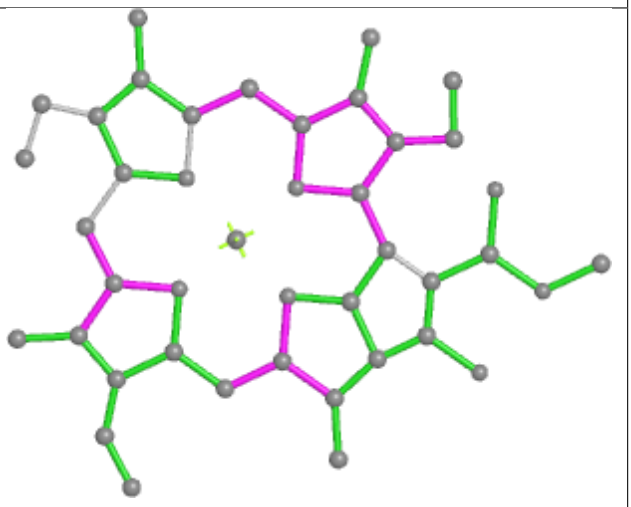


Rings

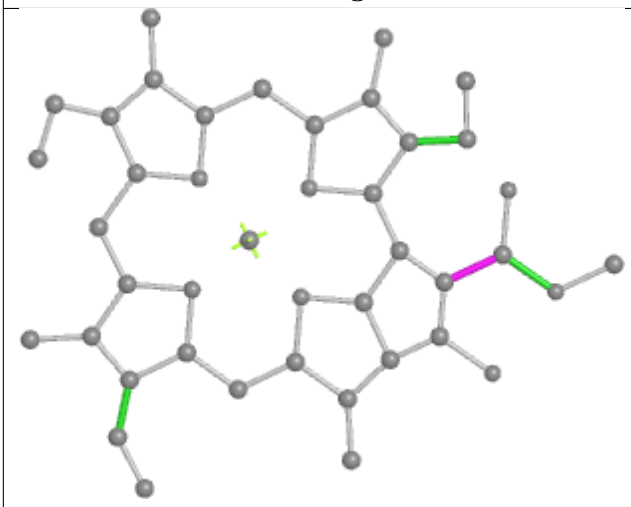
Ligand CLA A 827



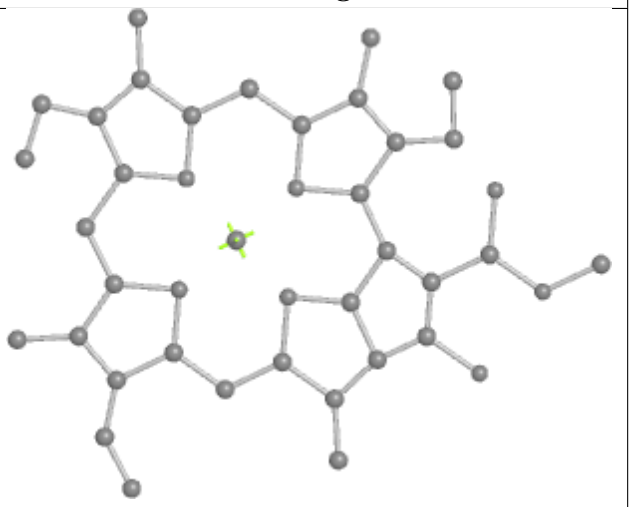
Bond lengths



Bond angles

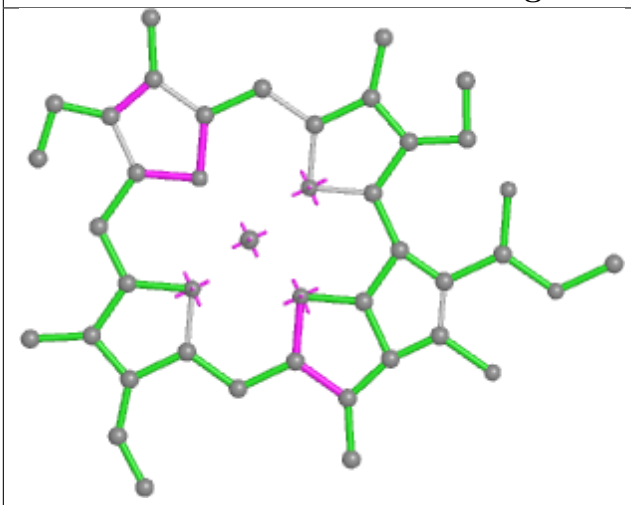


Torsions

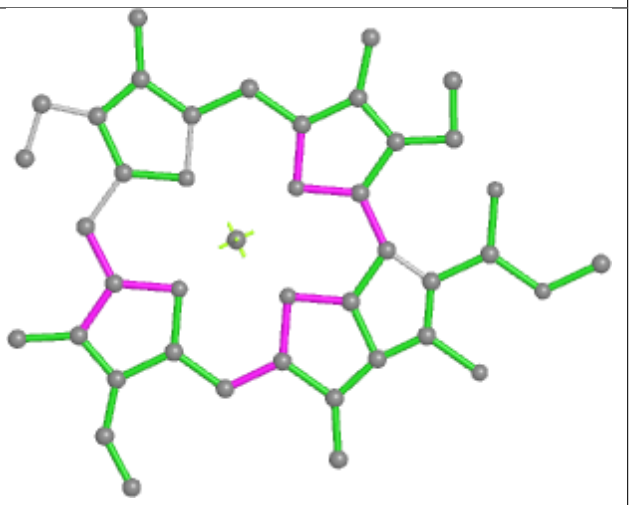


Rings

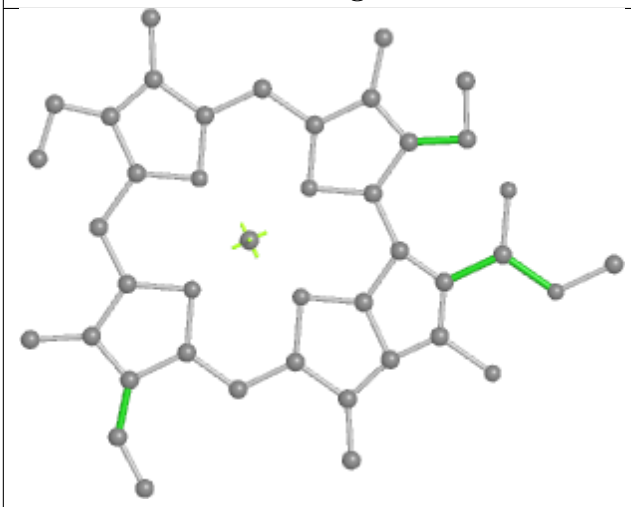
Ligand CLA B 814



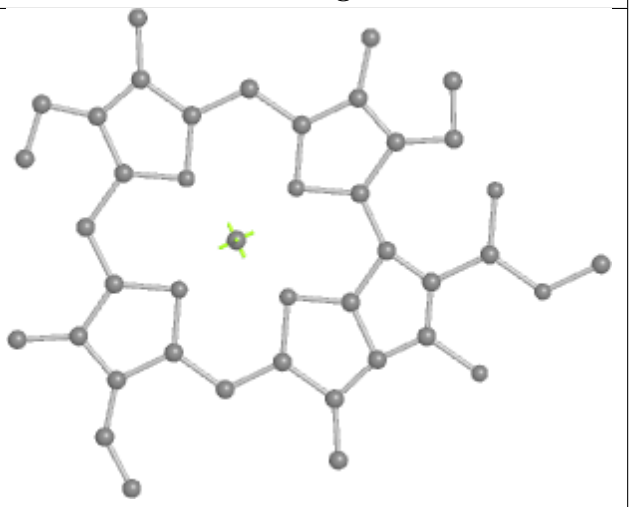
Bond lengths



Bond angles

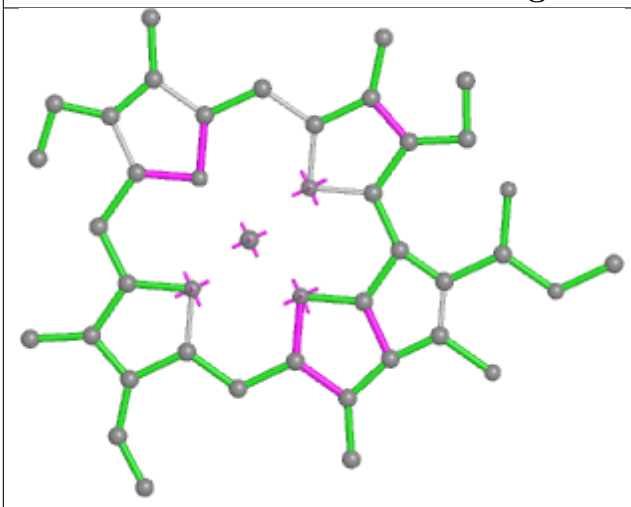


Torsions

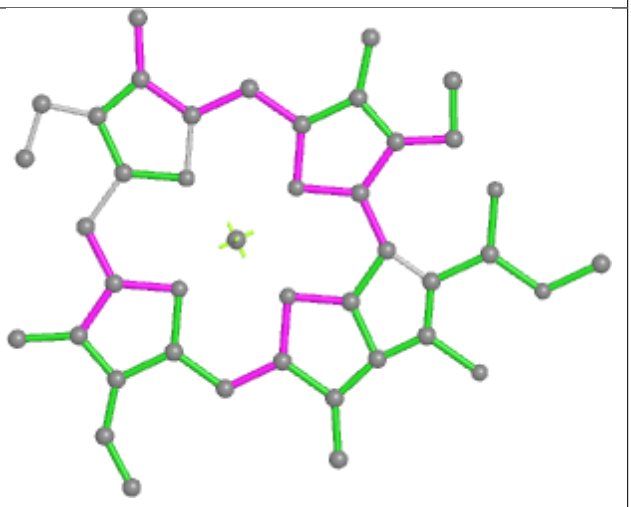


Rings

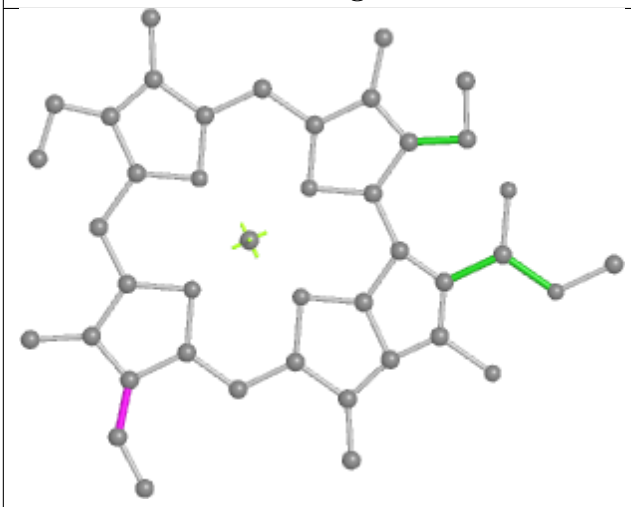
Ligand CLA 1 604



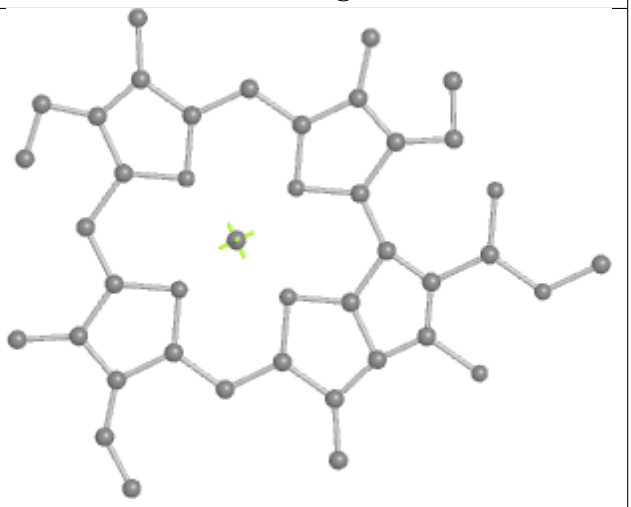
Bond lengths



Bond angles

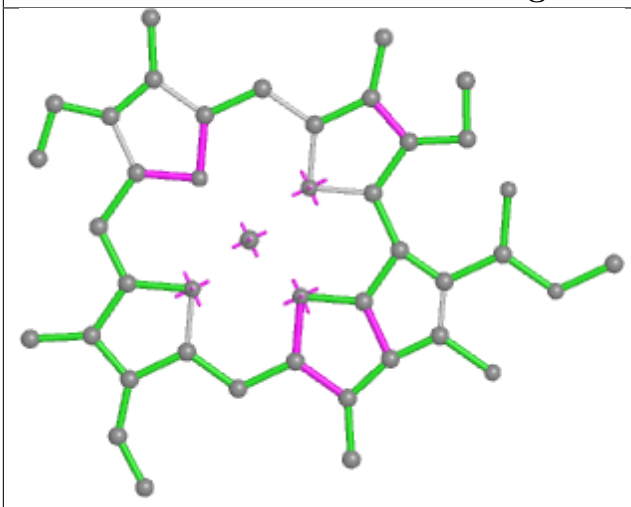


Torsions

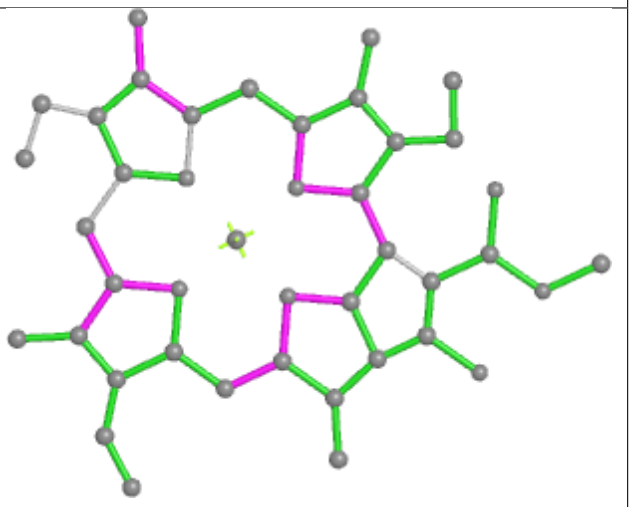


Rings

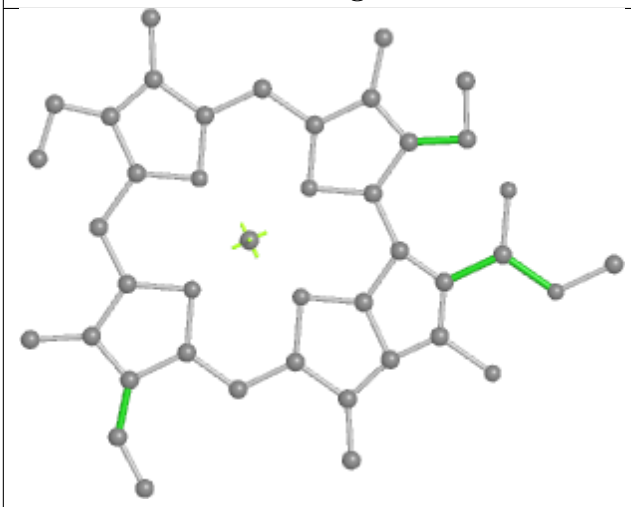
Ligand CLA 5 605



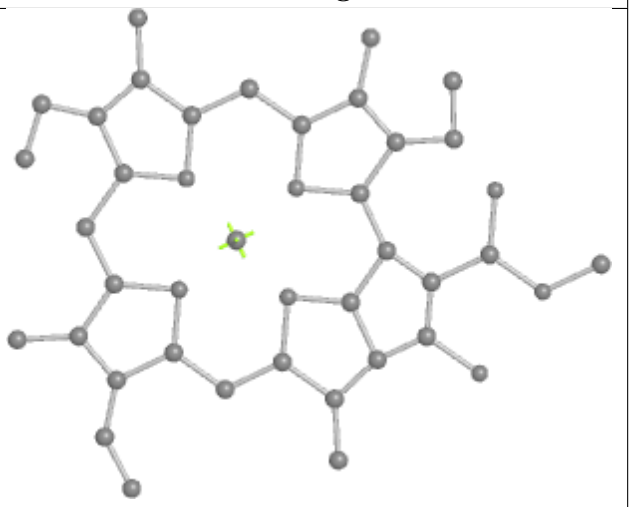
Bond lengths



Bond angles

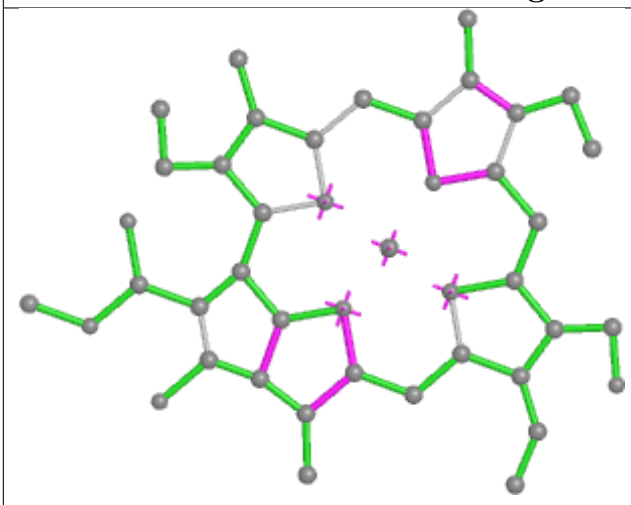


Torsions



Rings

Ligand CHL 6 316



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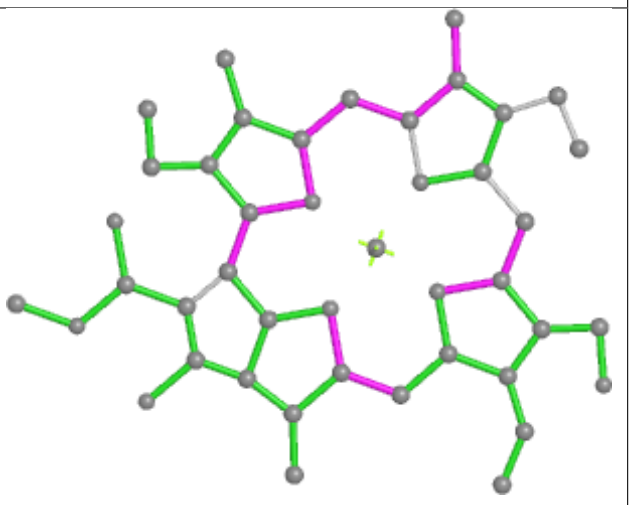
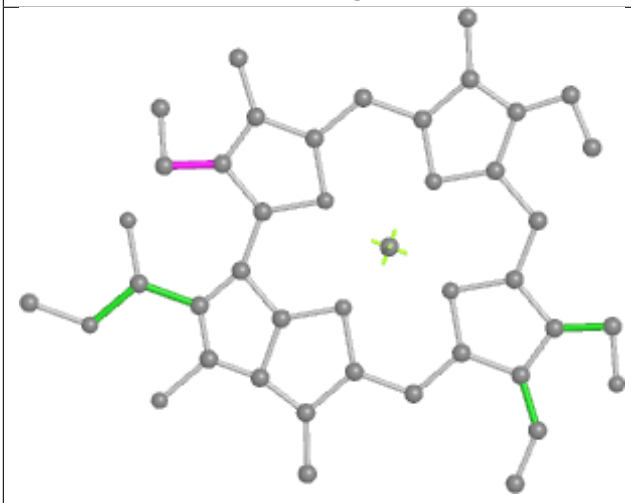


Bond angles



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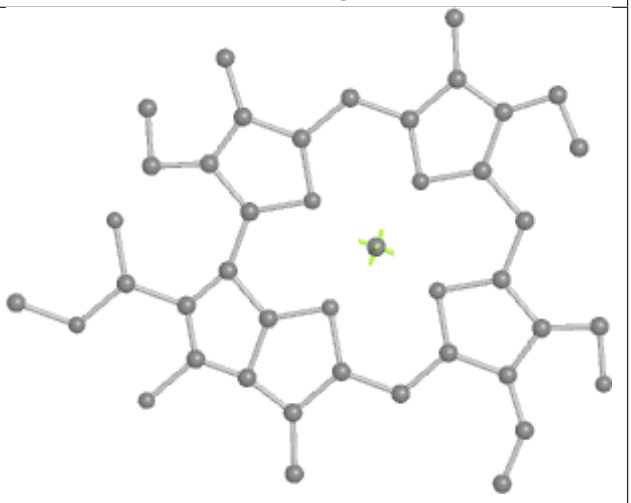
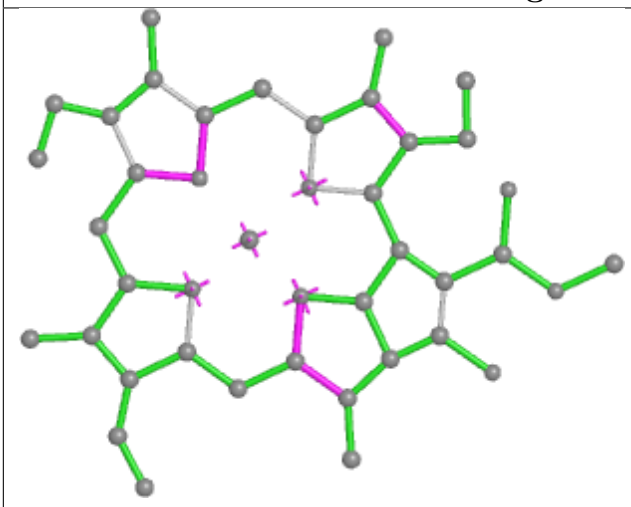


Rings

Ligand CLA Z 603



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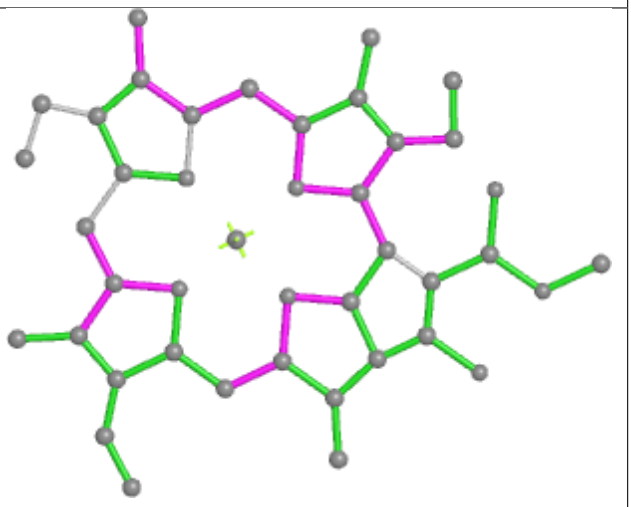
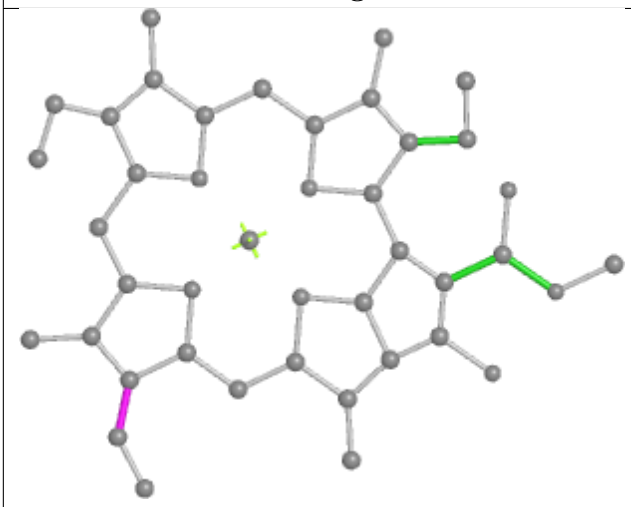
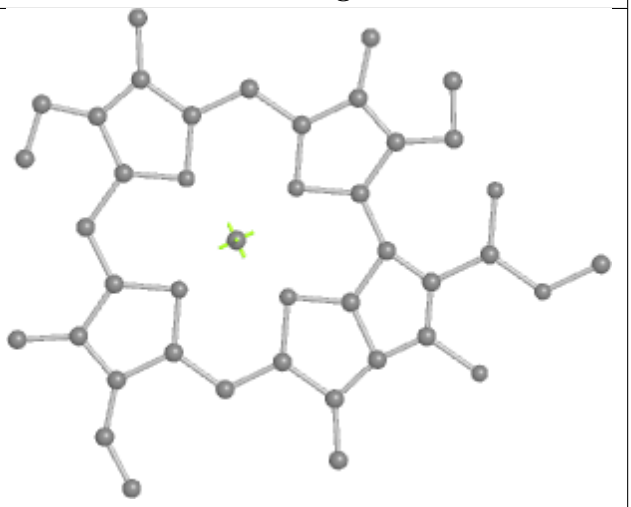


Bond angles

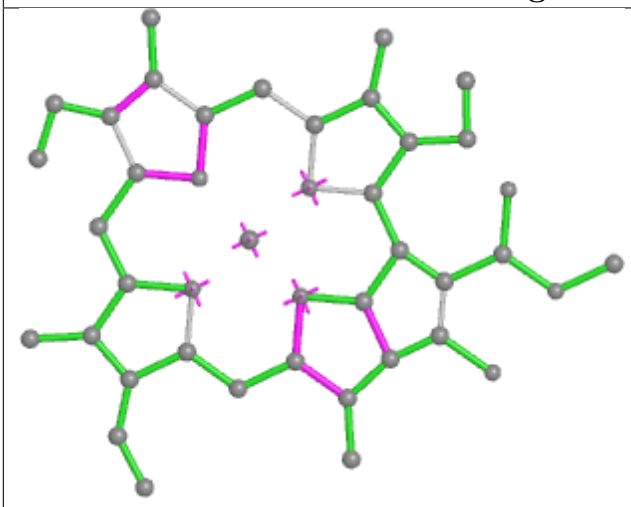


Torsions



Rings

Ligand CLA 1 613



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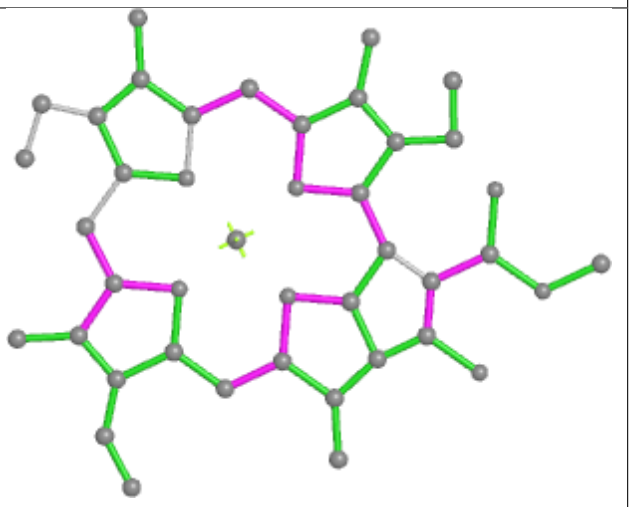
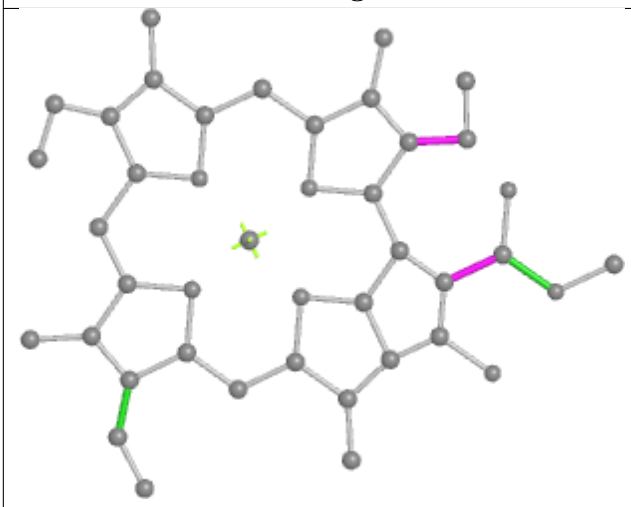


Bond angles



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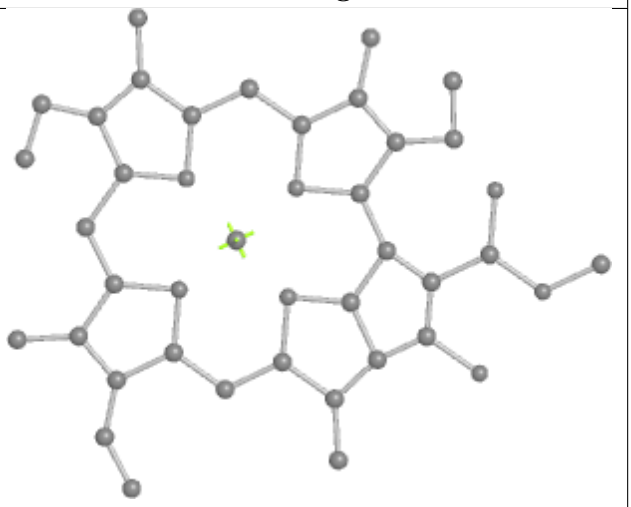
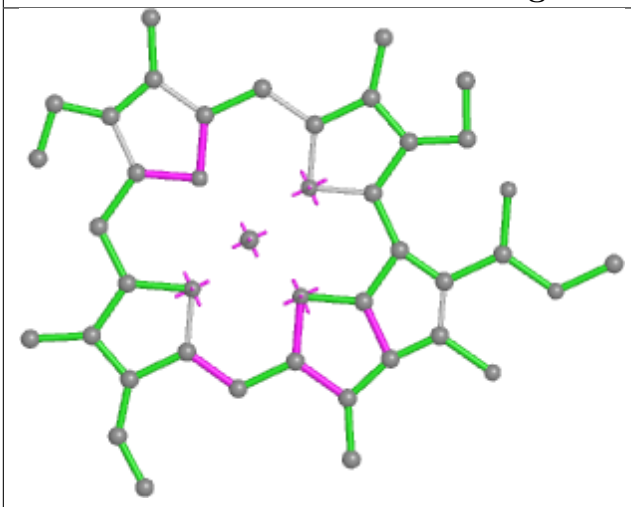


Rings

Ligand CLA 6 302



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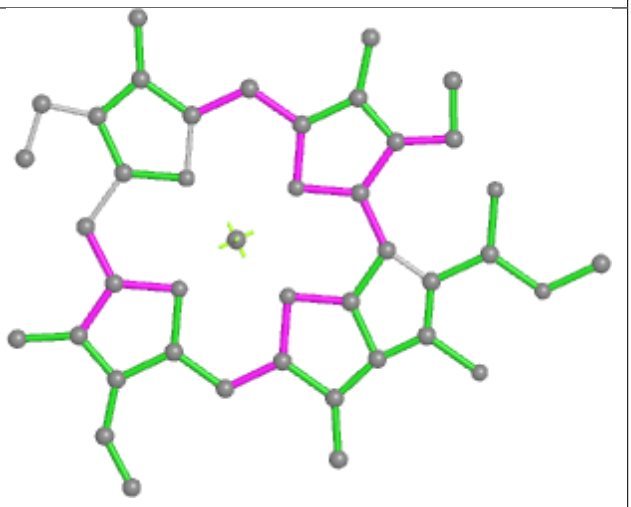
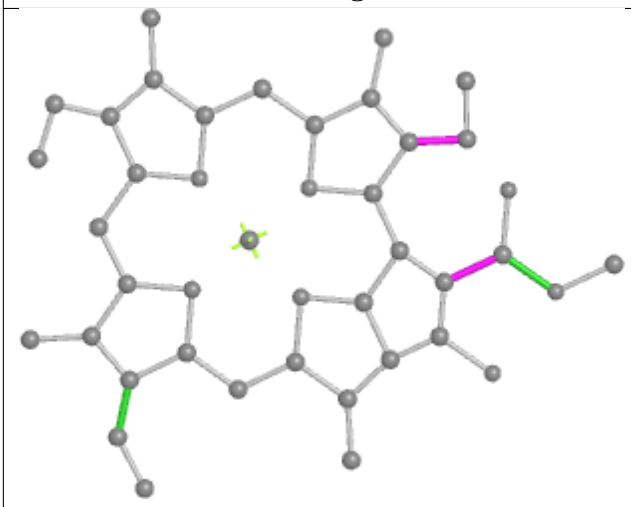


Bond angles



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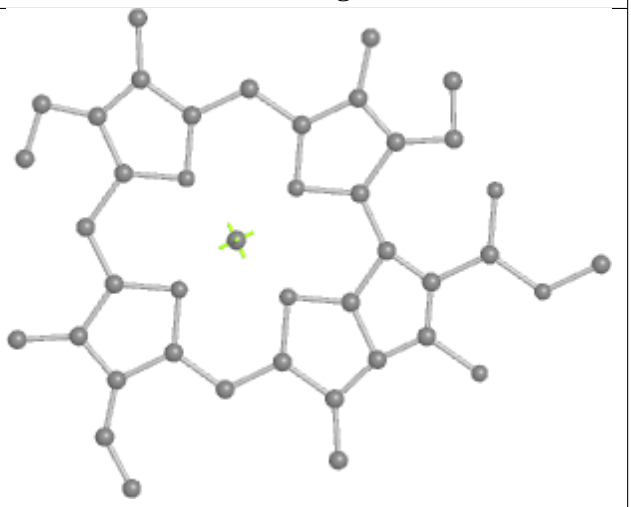
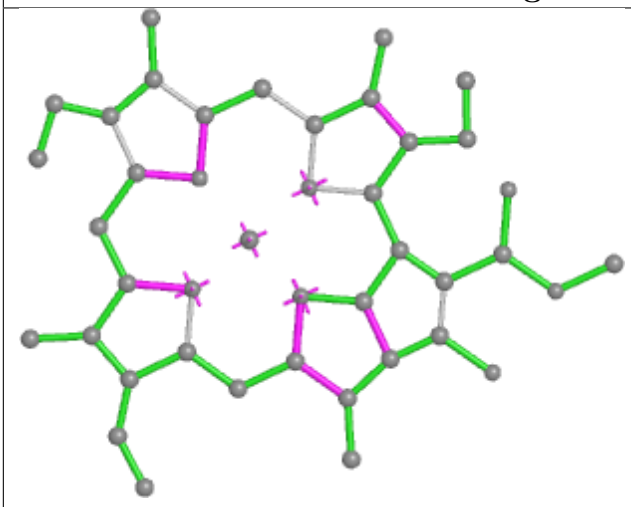


Rings

Ligand CLA A 822



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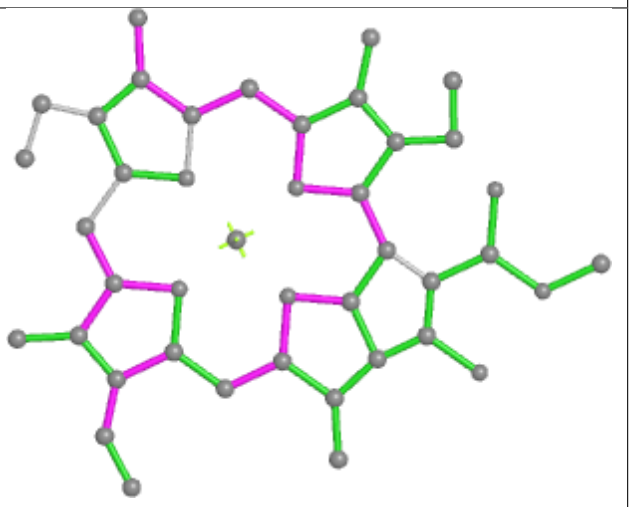
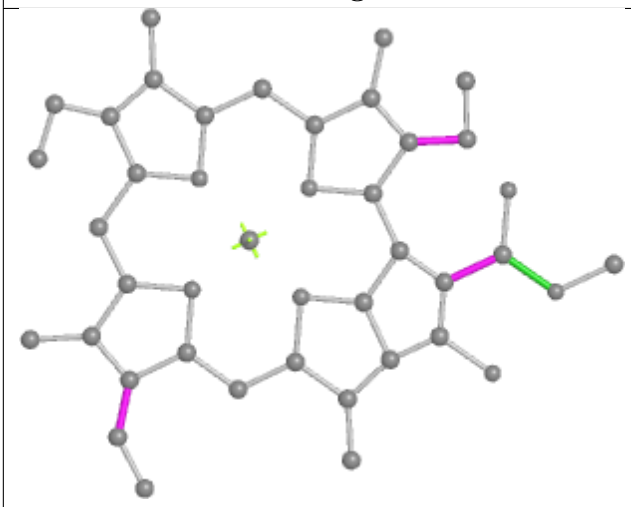


Bond angles



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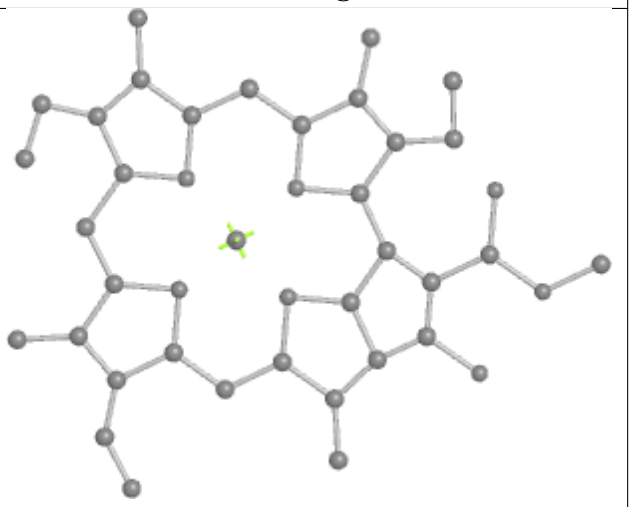
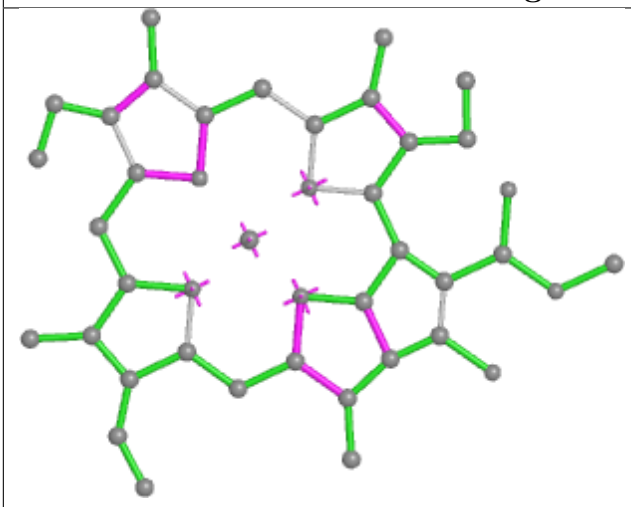
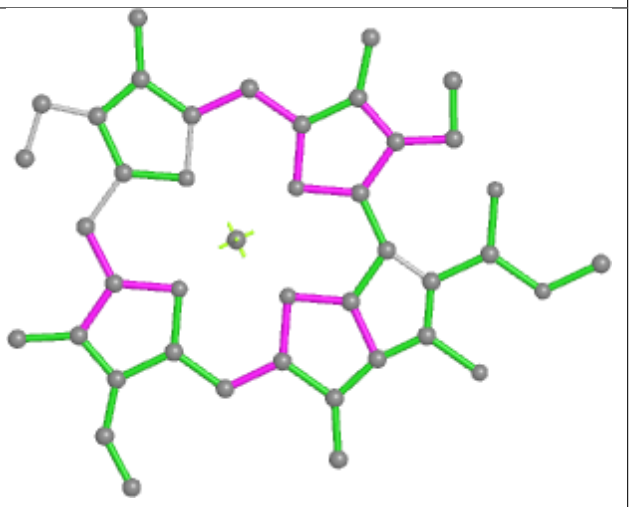


Rings

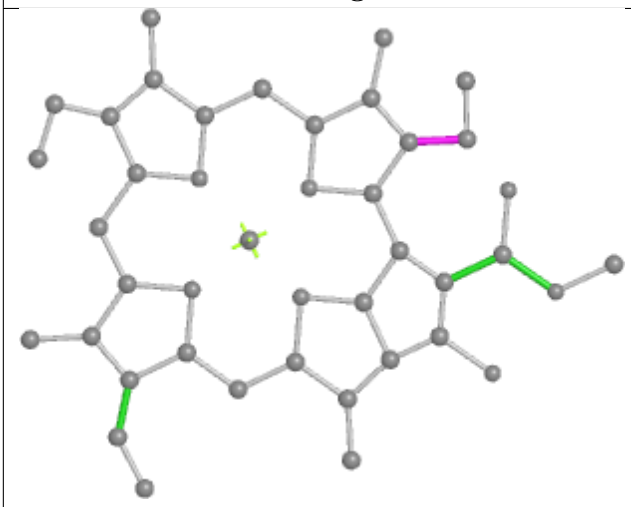
Ligand CLA B 819



Bond lengths



Bond angles



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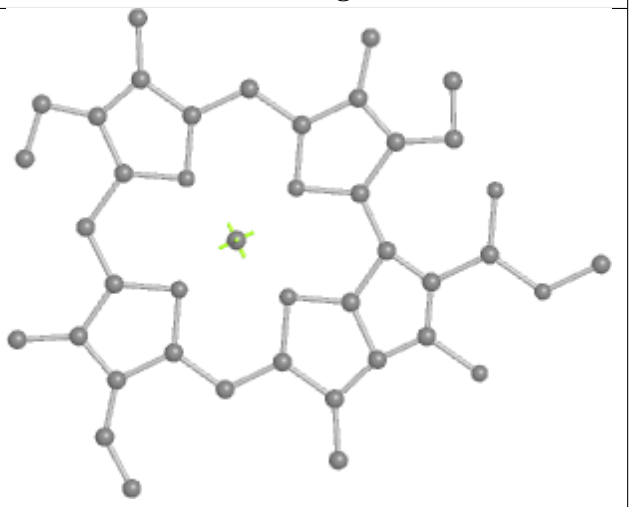
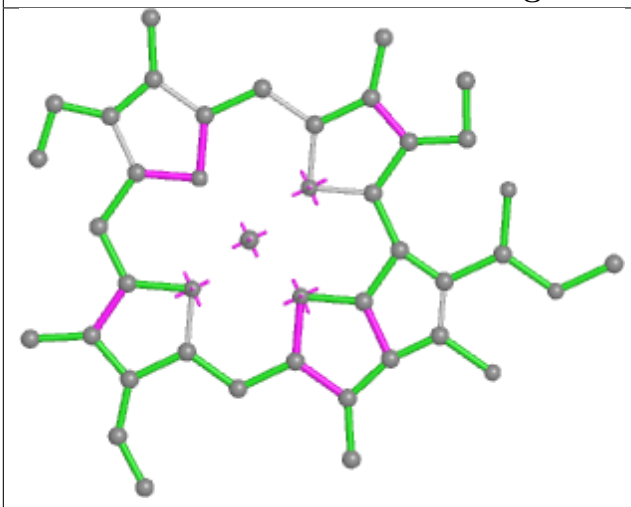
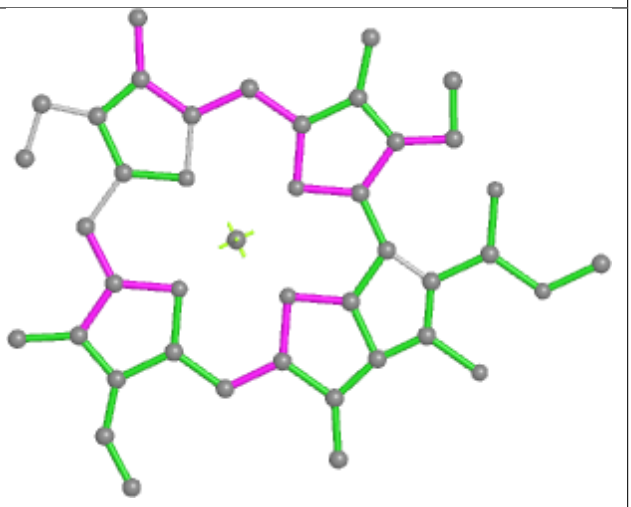


Rings

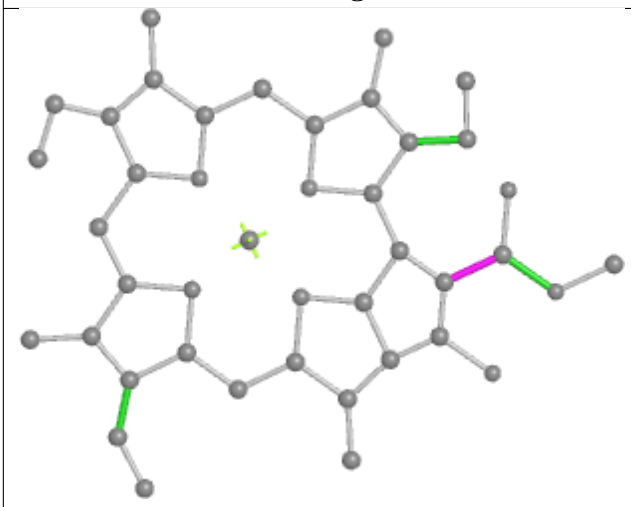
Ligand CLA A 805



Bond lengths



Bond angles



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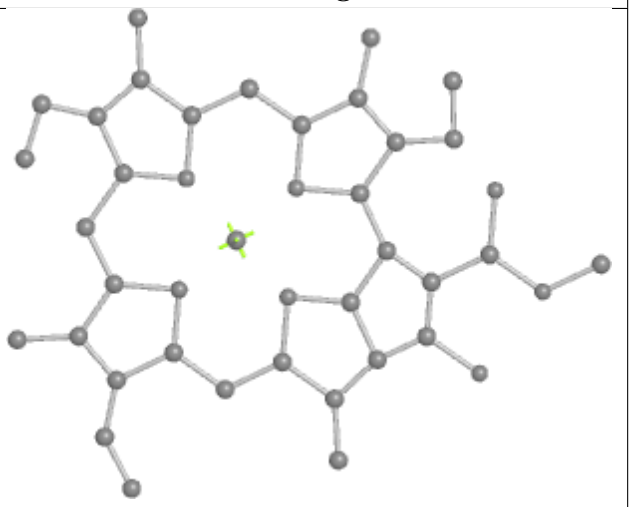
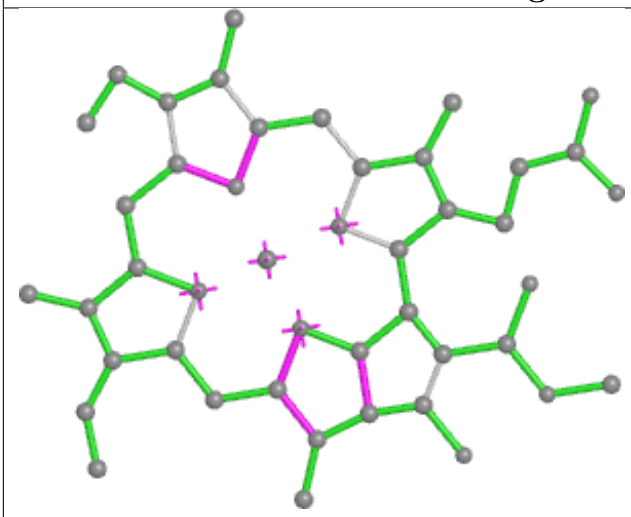
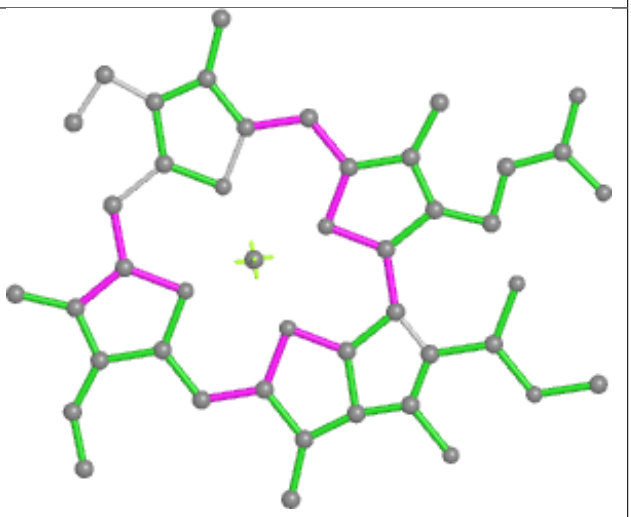


Rings

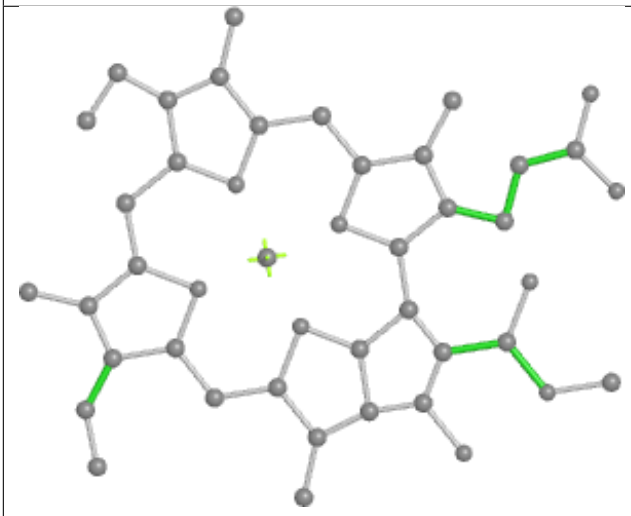
Ligand CLA 8 603



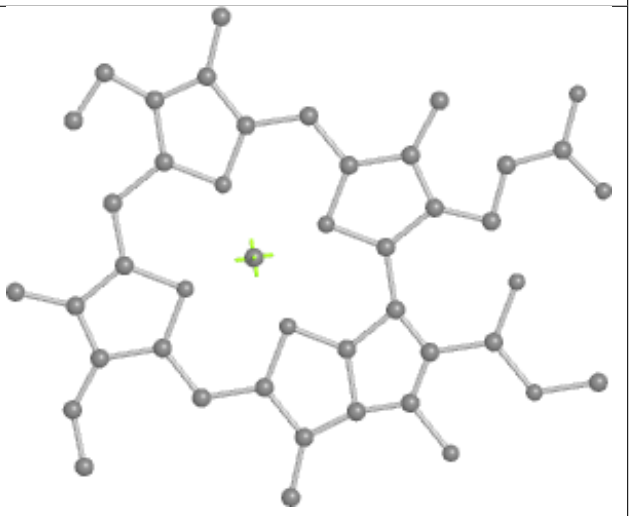
Bond lengths



Bond angles

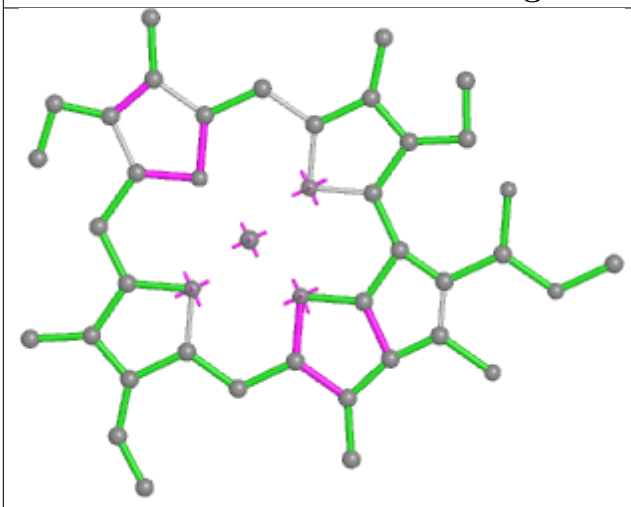


Torsions

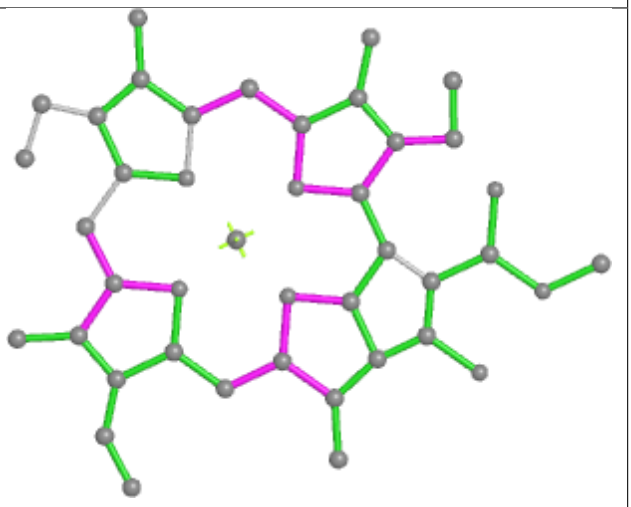


Rings

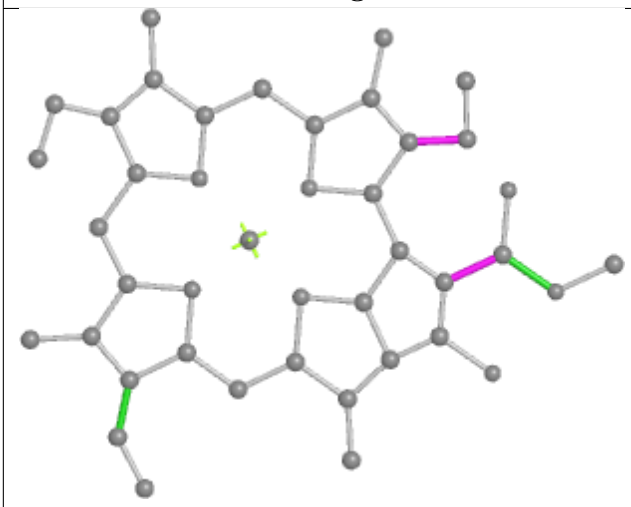
Ligand CLA A 838



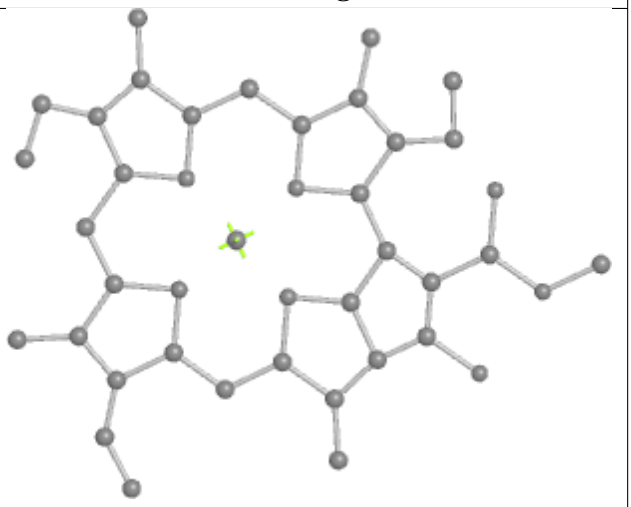
Bond lengths



Bond angles

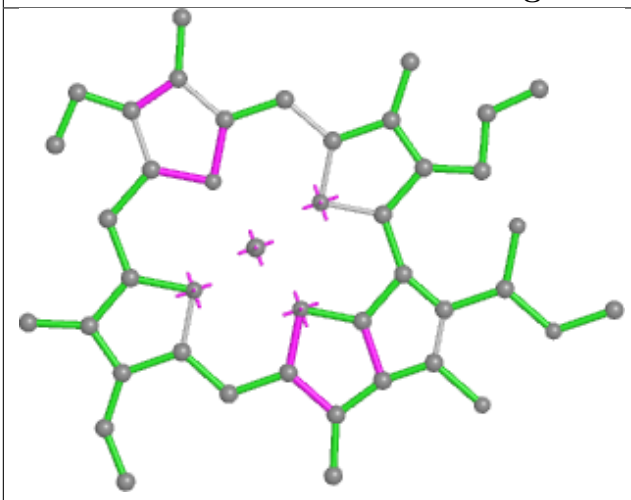


Torsions

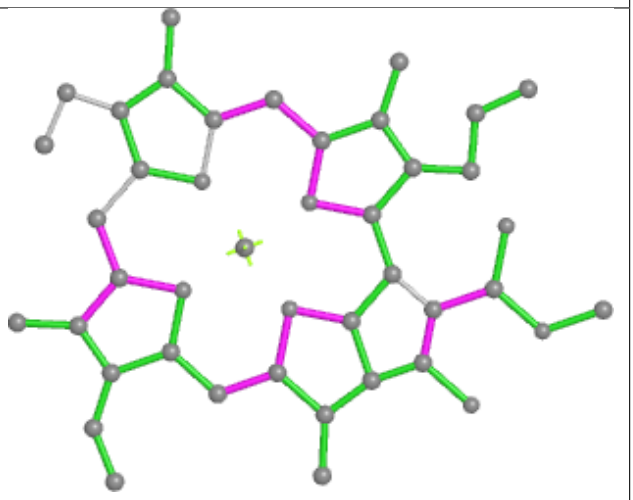


Rings

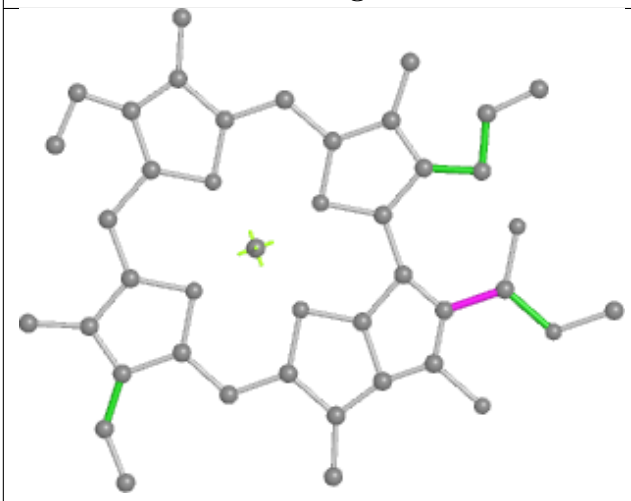
Ligand CLA A 811



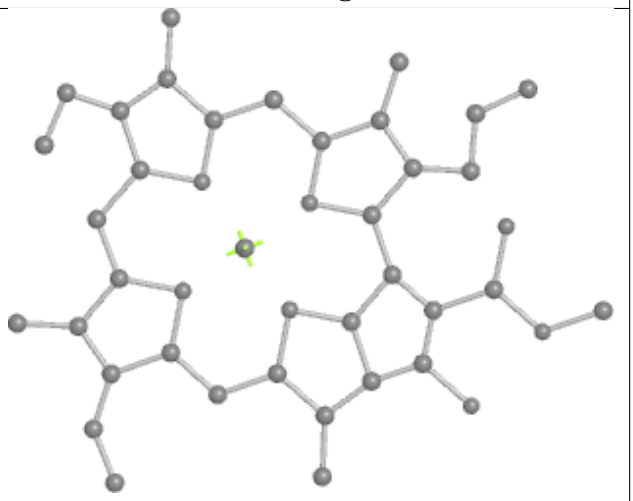
Bond lengths



Bond angles

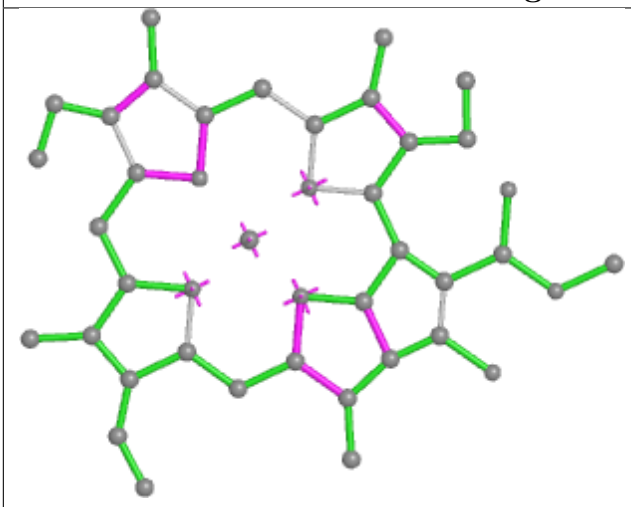


Torsions

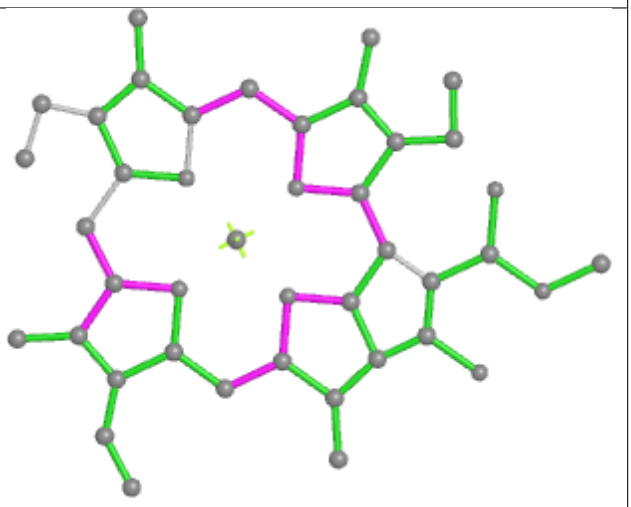


Rings

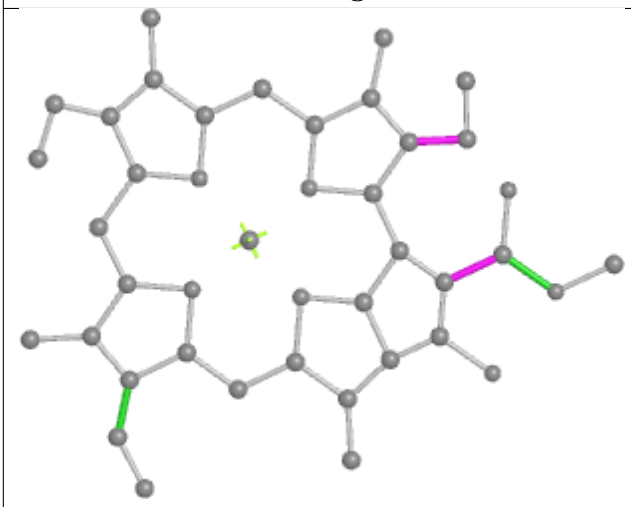
Ligand CLA B 843



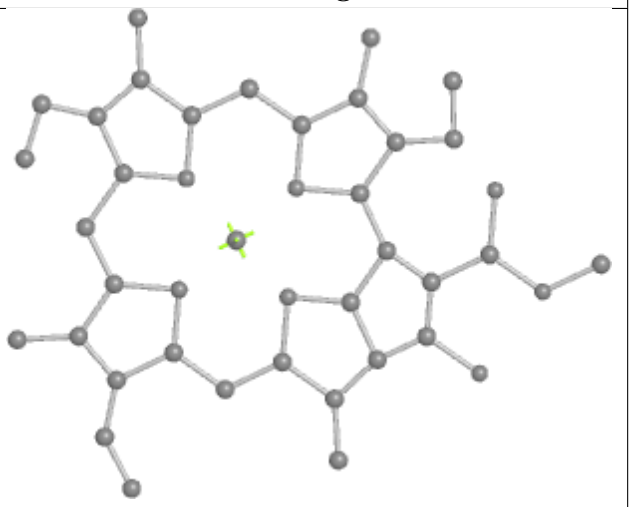
Bond lengths



Bond angles

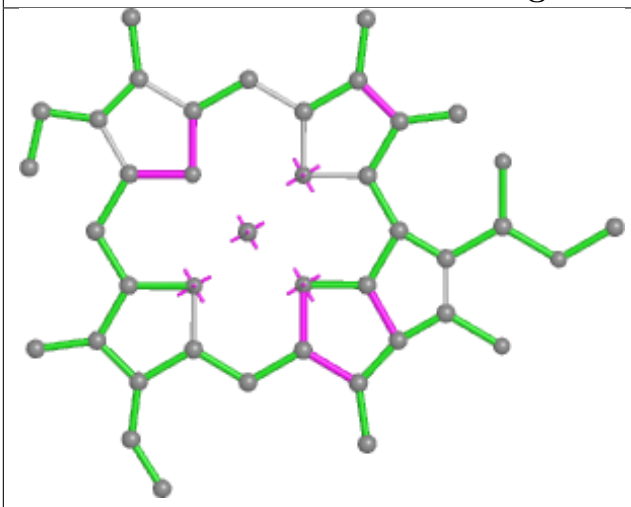


Torsions

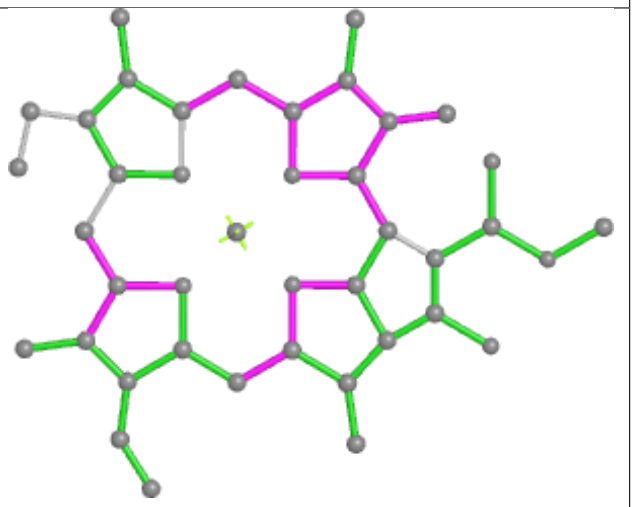


Rings

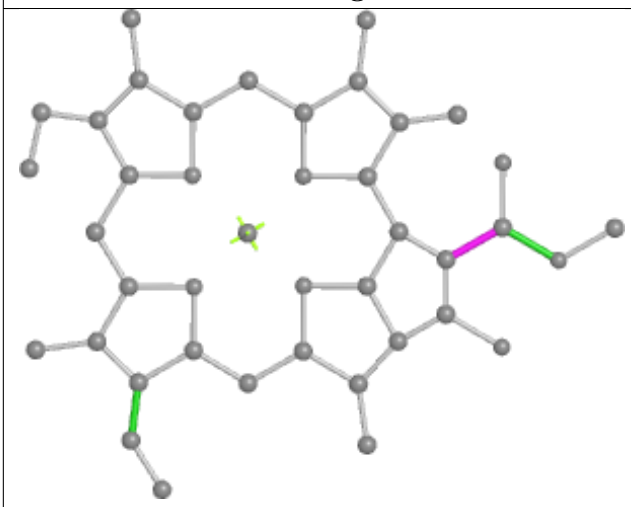
Ligand CLA 7 610



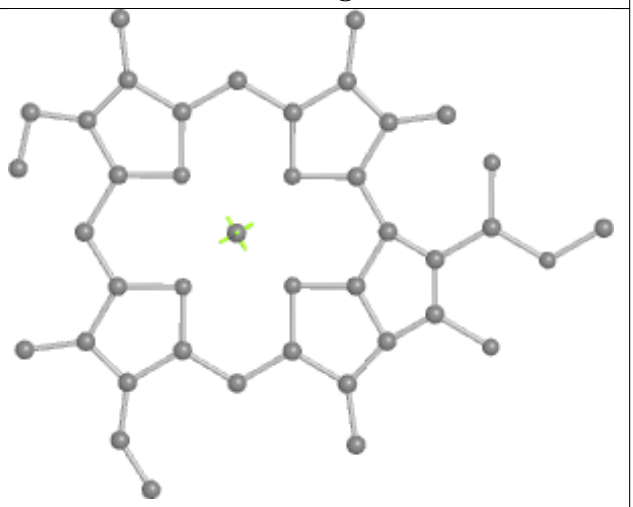
Bond lengths



Bond angles

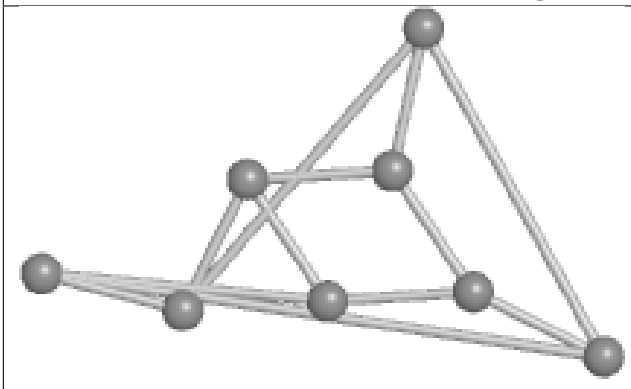


Torsions

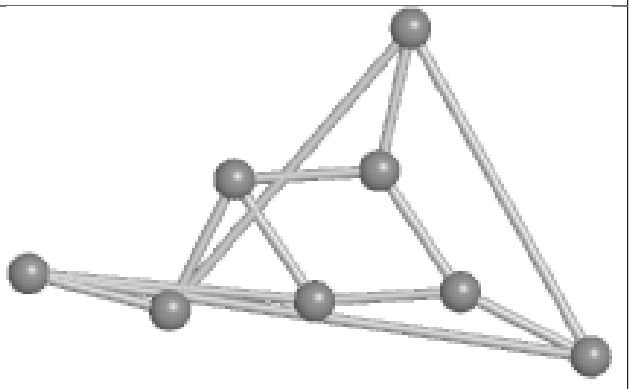


Rings

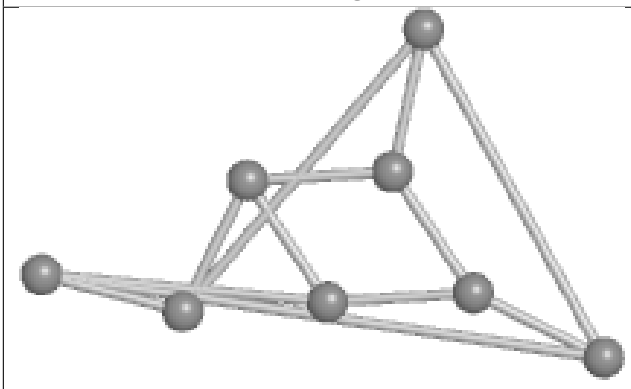
Ligand SF4 C 101



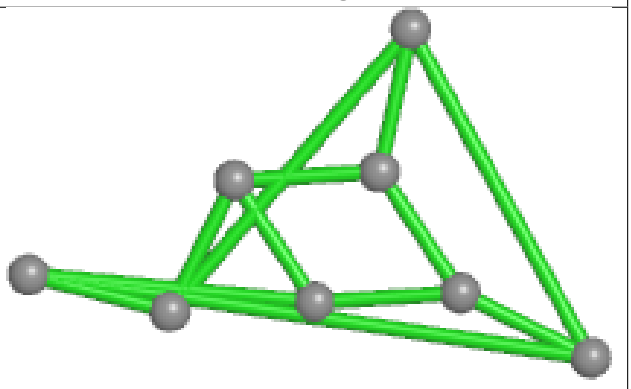
Bond lengths



Bond angles

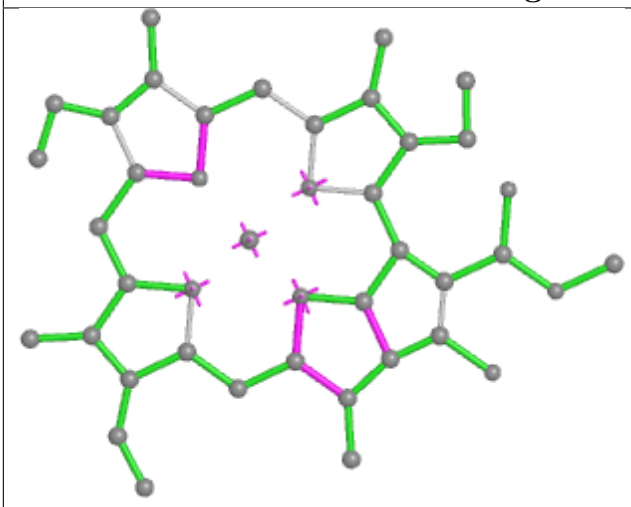


Torsions

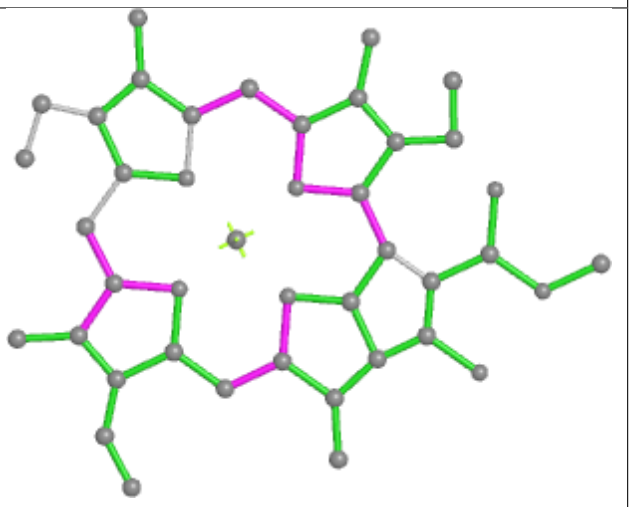


Rings

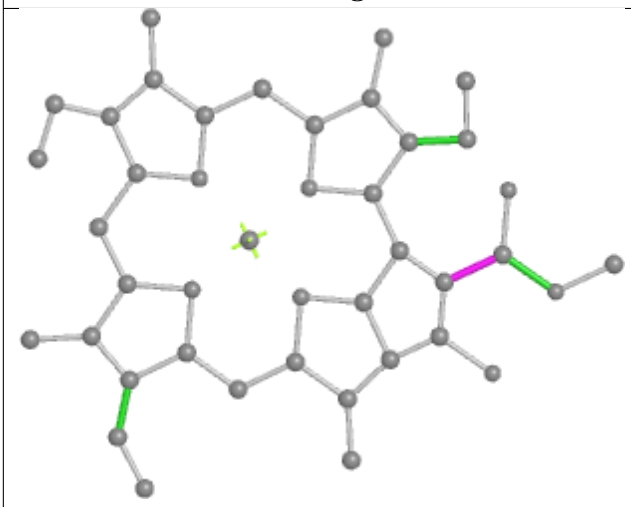
Ligand CLA B 839



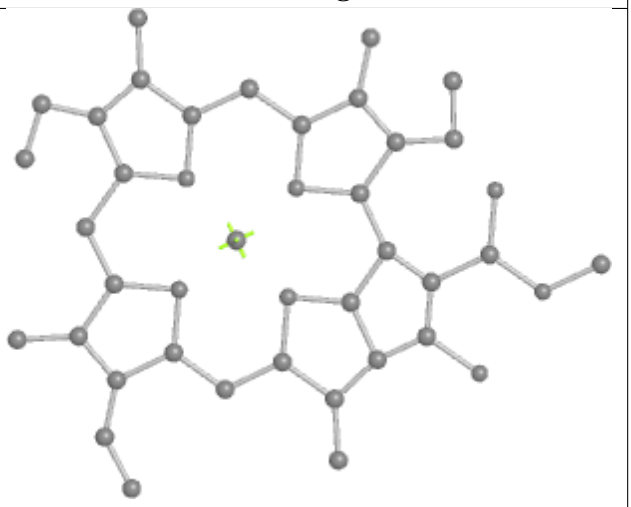
Bond lengths



Bond angles

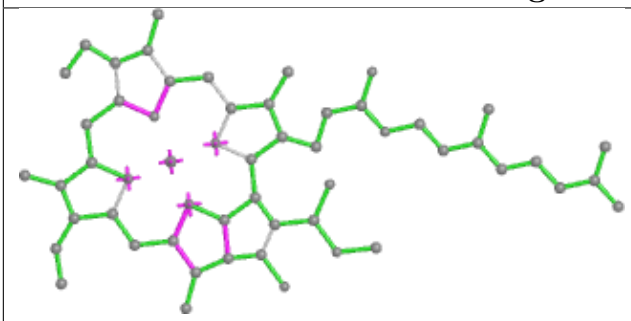


Torsions

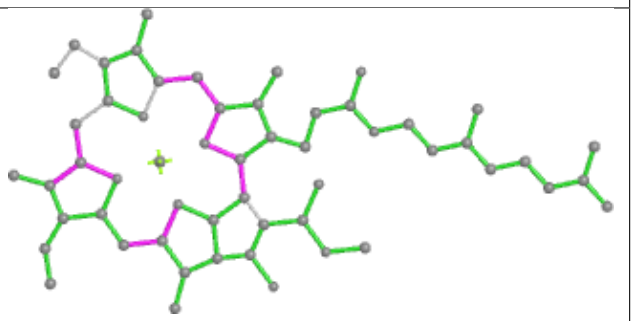


Rings

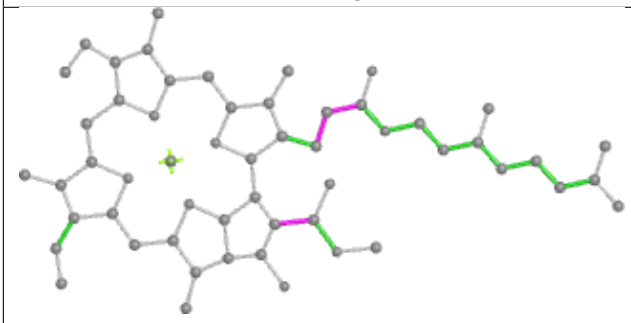
Ligand CLA 5 610



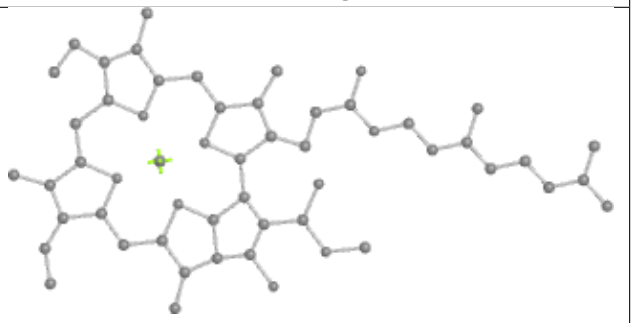
Bond lengths



Bond angles

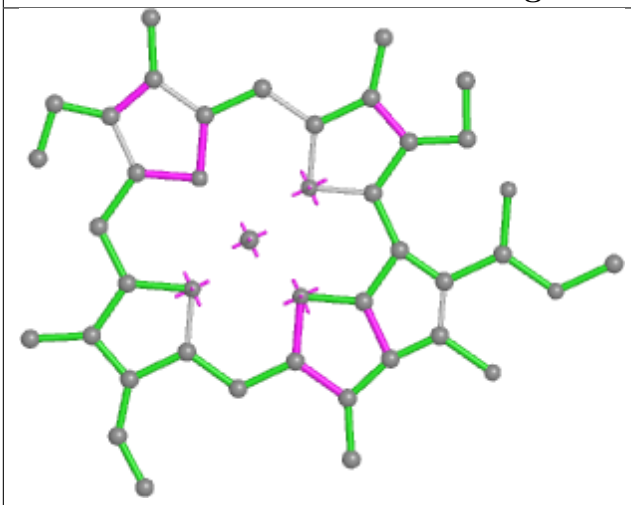


Torsions

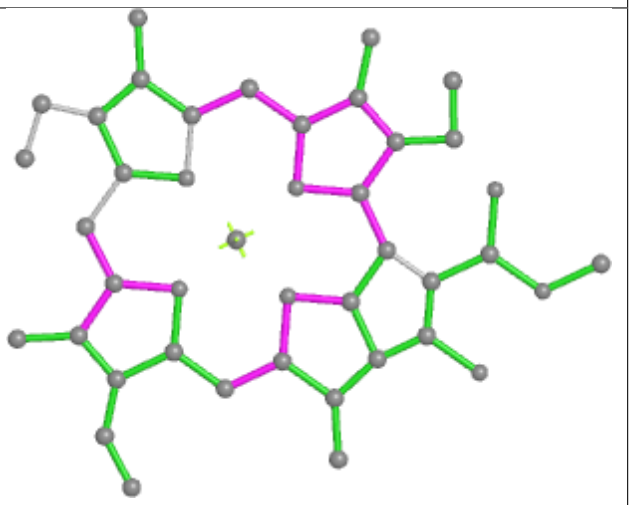


Rings

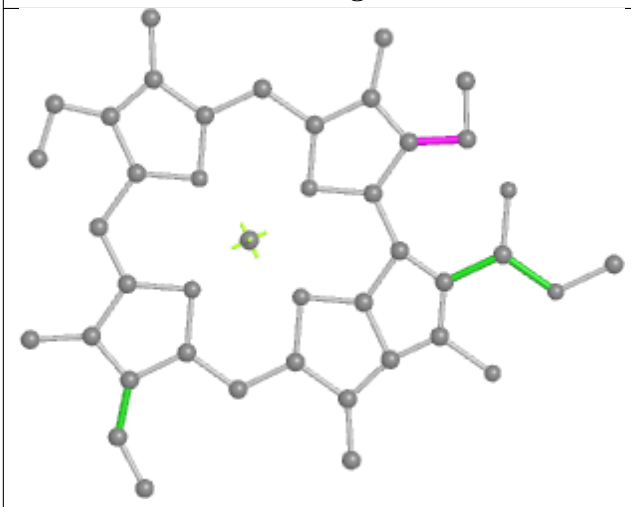
Ligand CLA B 804



Bond lengths



Bond angles



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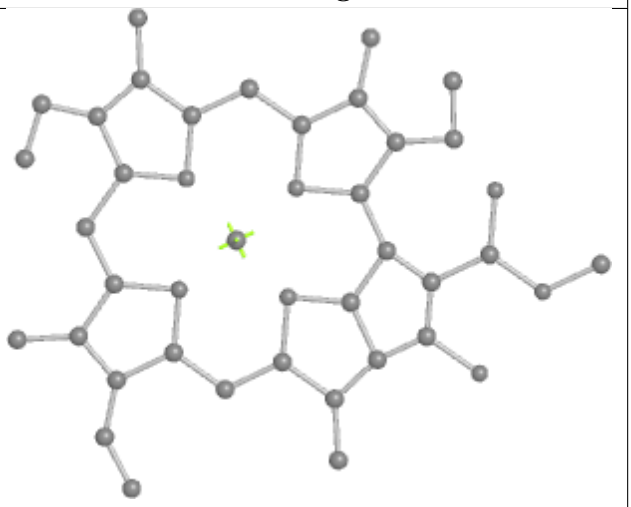
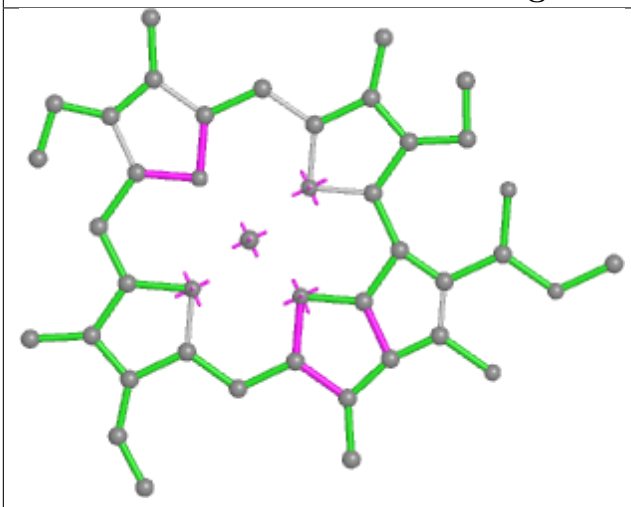


Rings

Ligand CLA 4 611



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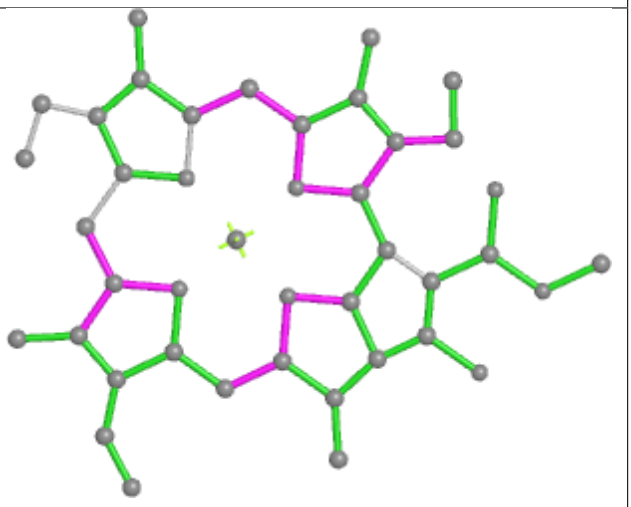
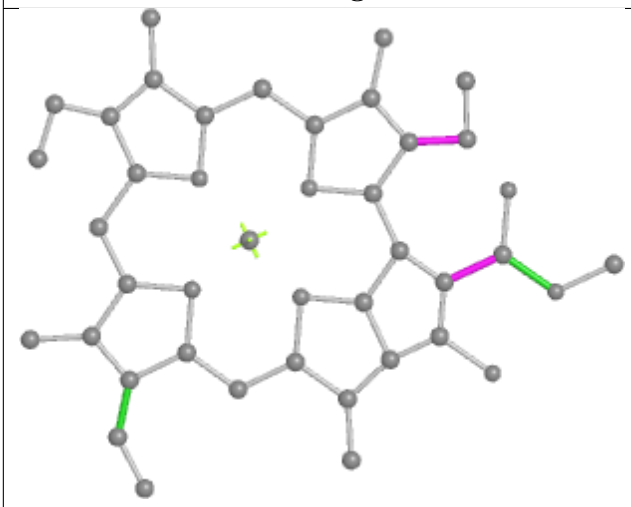


Bond angles



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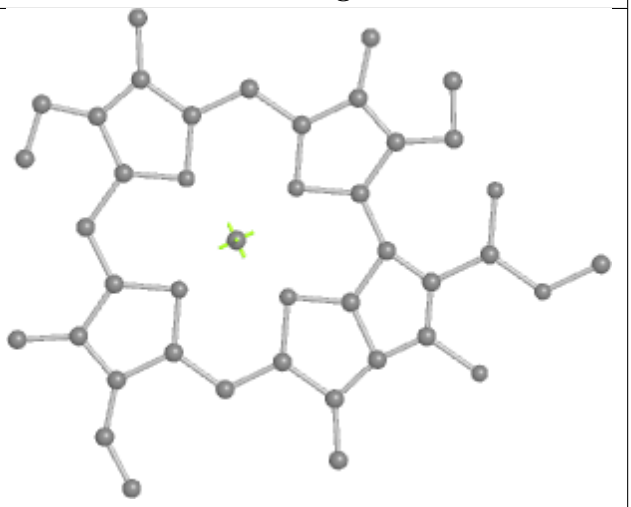
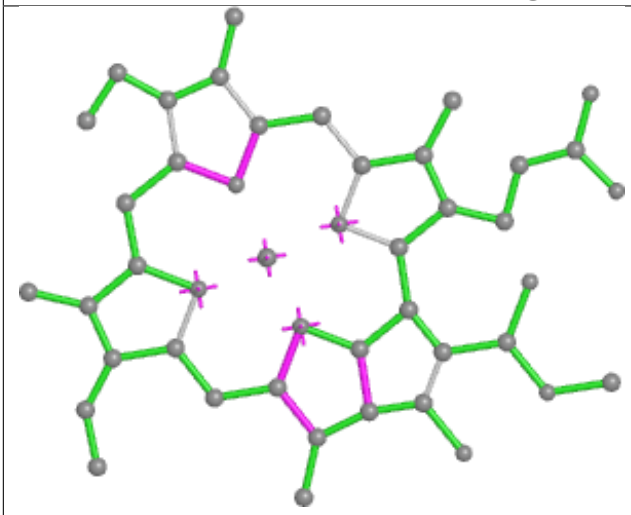


Rings

Ligand CLA B 830



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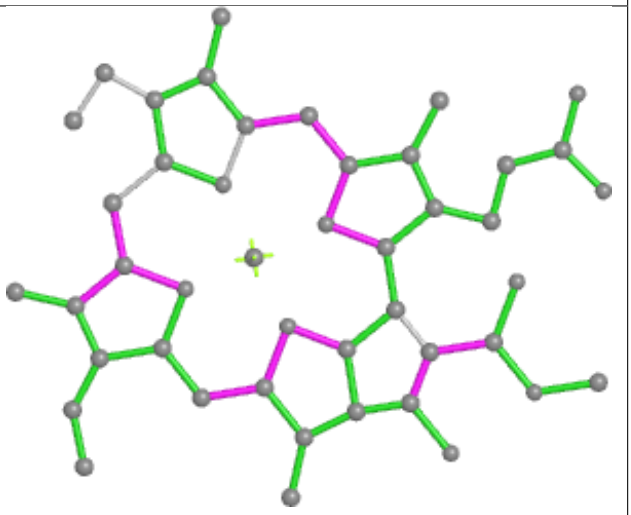
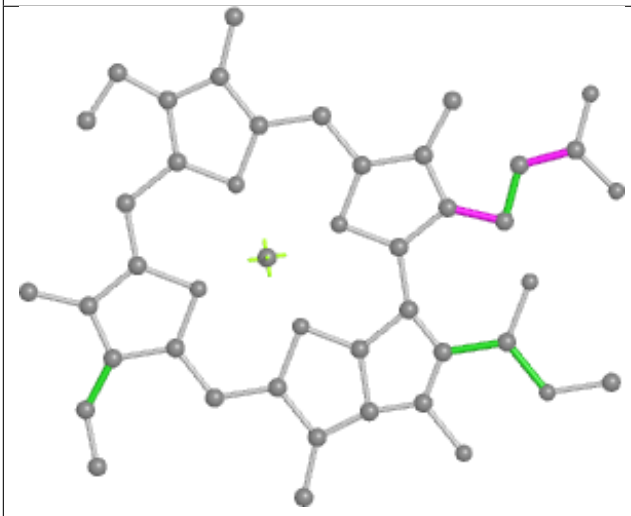


Bond angles



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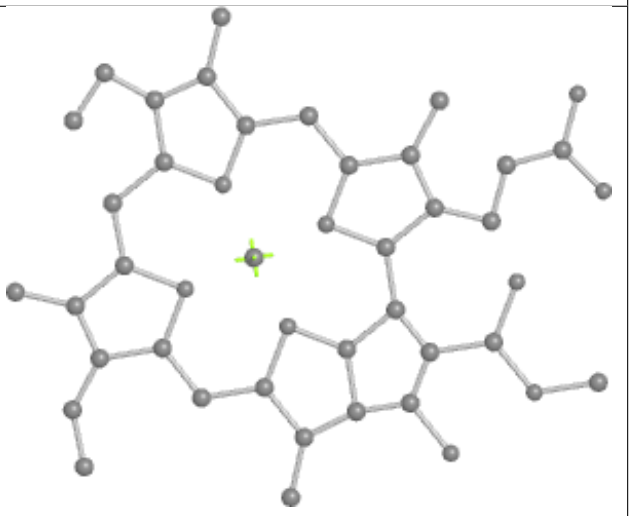
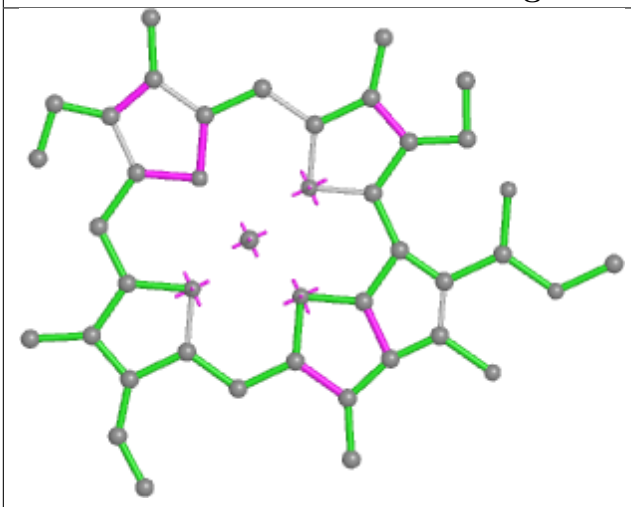


Rings

Ligand CLA A 825



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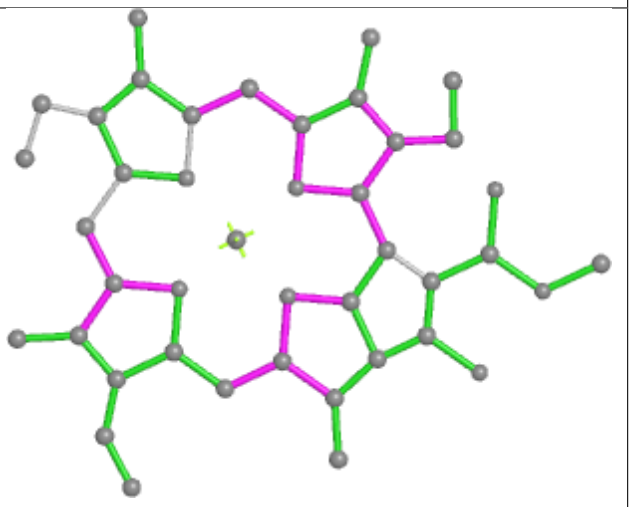
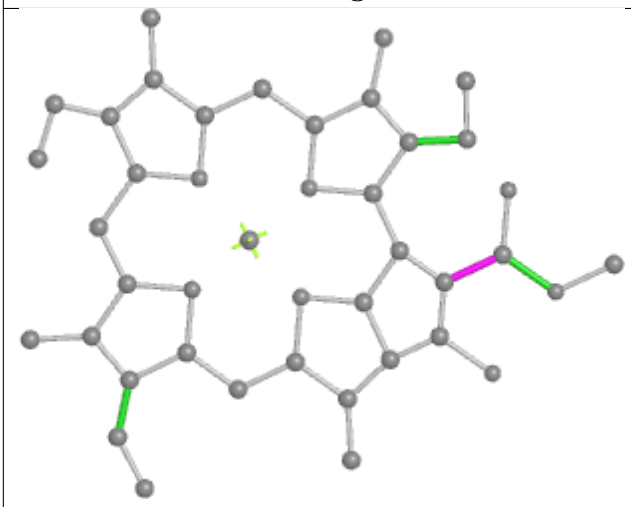


Bond angles



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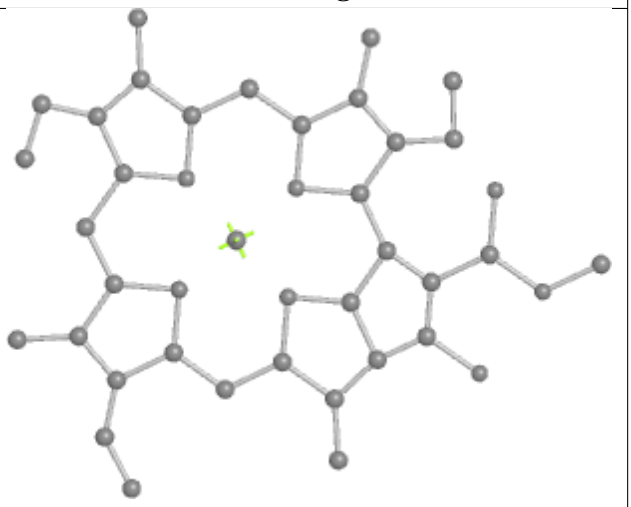
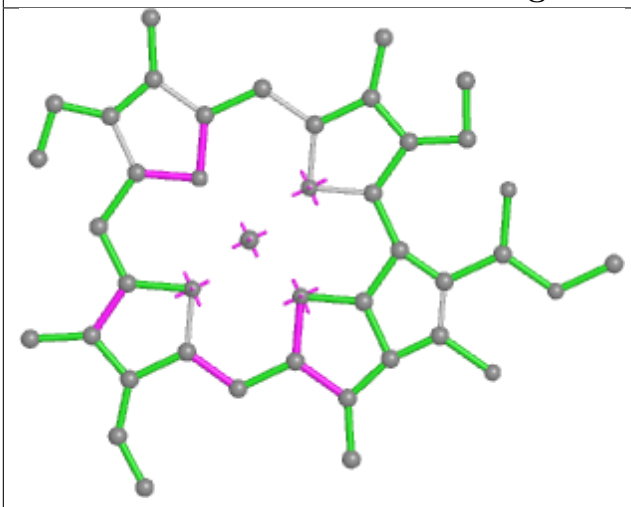


Rings

Ligand CLA 6 301



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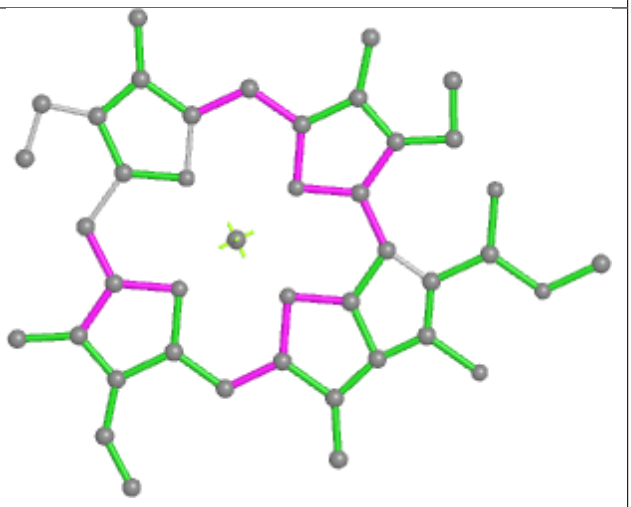
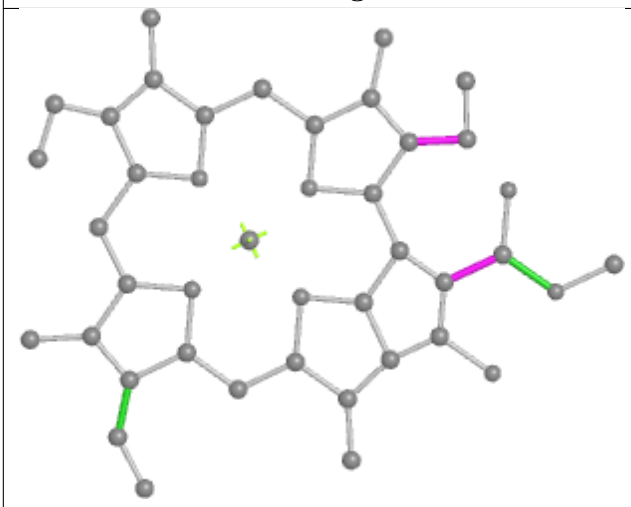


Bond angles



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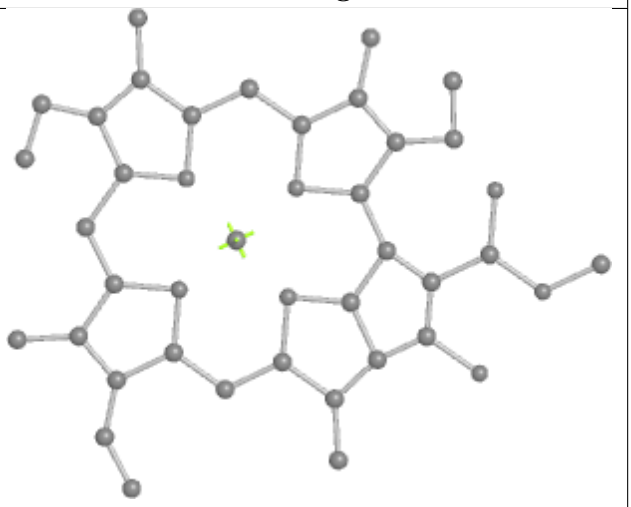
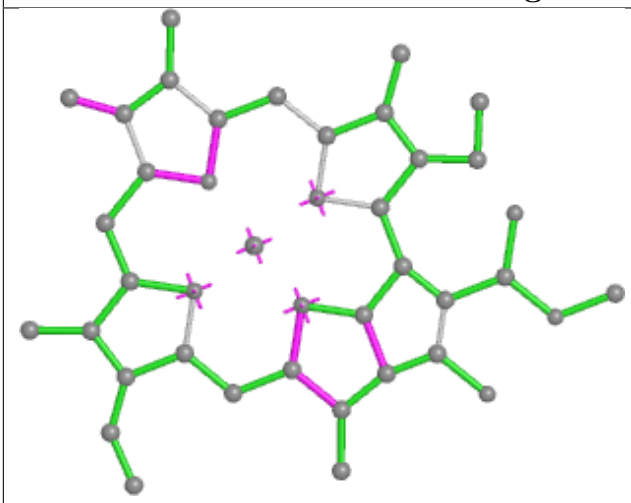


Rings

Ligand CLA B 813



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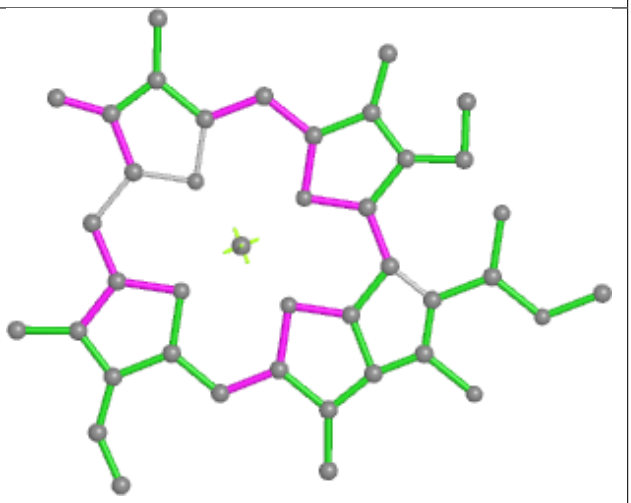
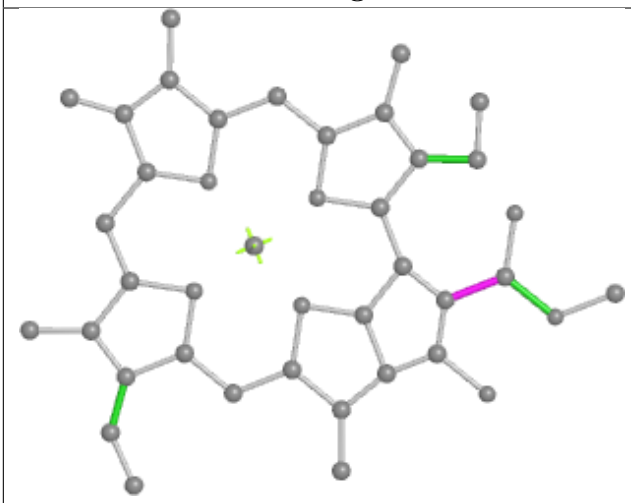


Bond angles



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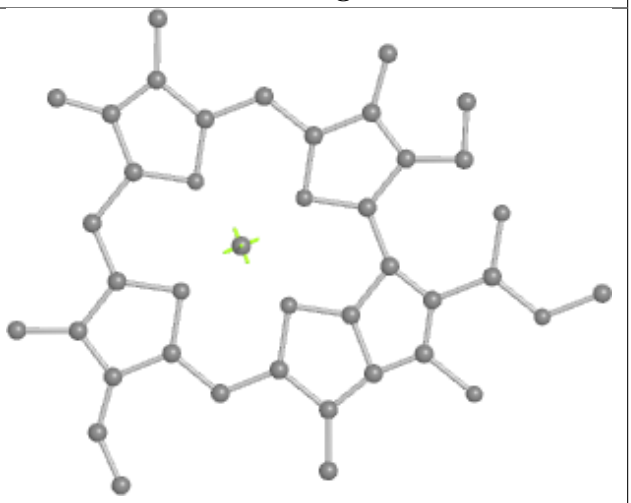
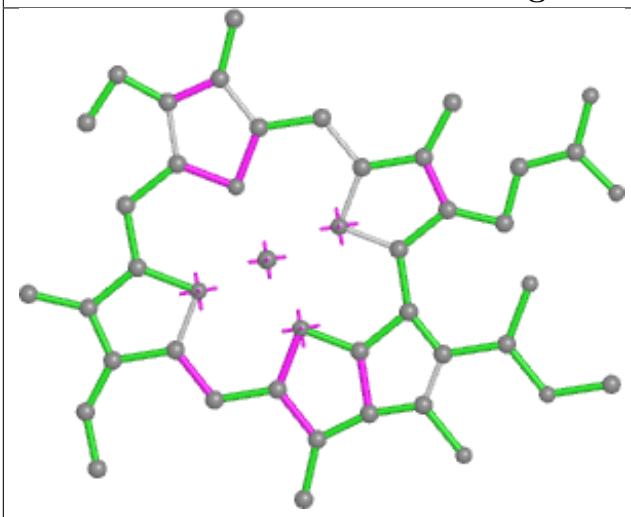


Rings

Ligand CLA 7 612



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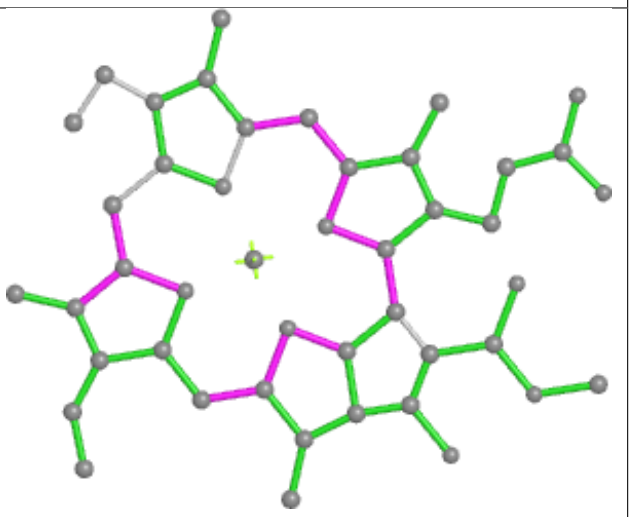
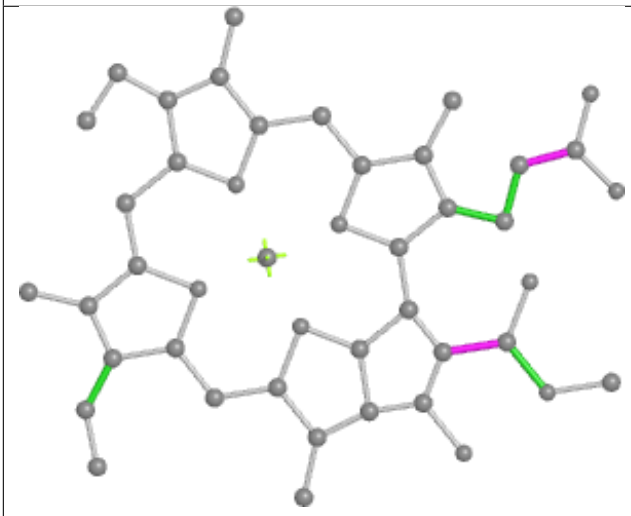


Bond angles



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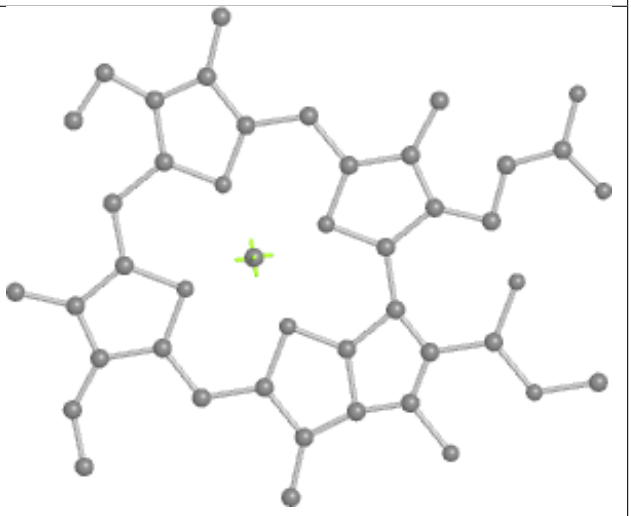
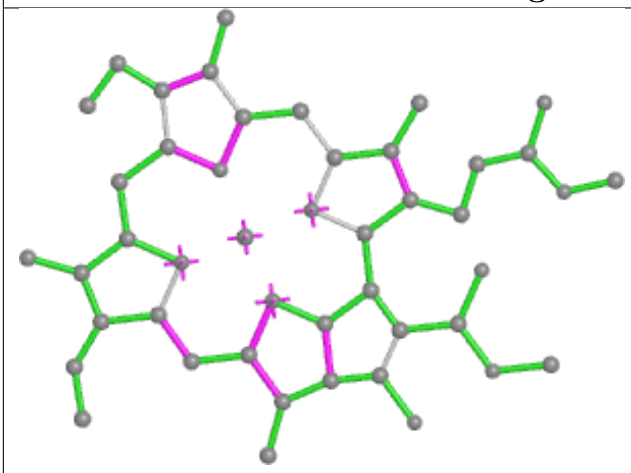
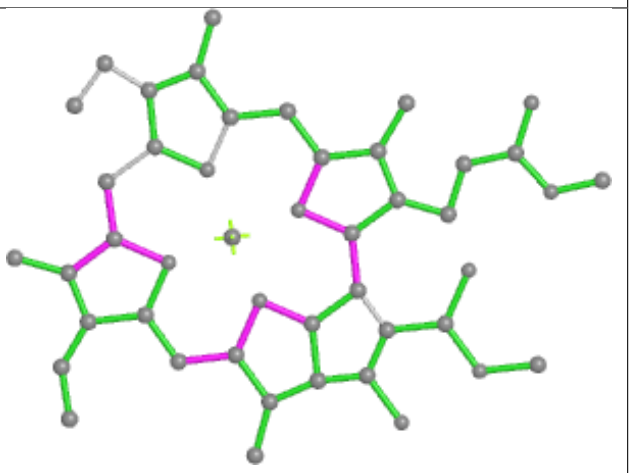


Rings

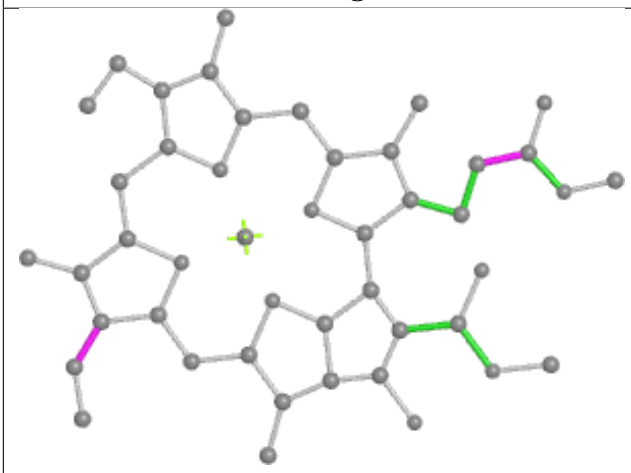
Ligand CLA 4 603



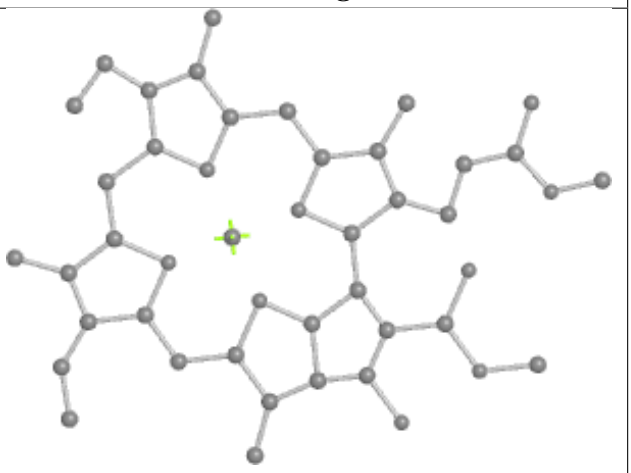
Bond lengths



Bond angles

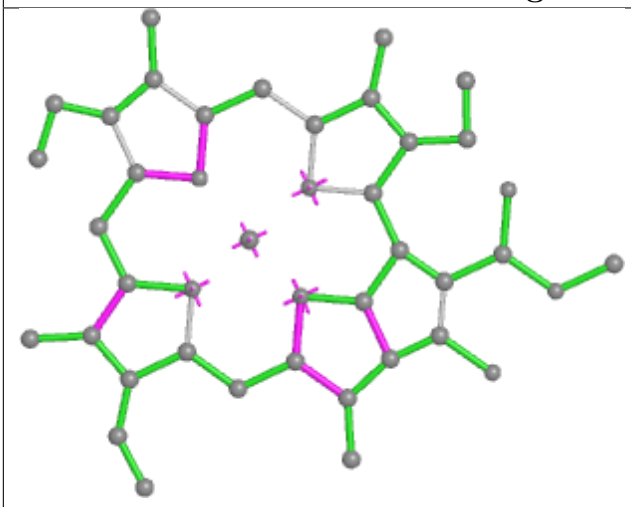


Torsions



Rings

Ligand CLA Z 608



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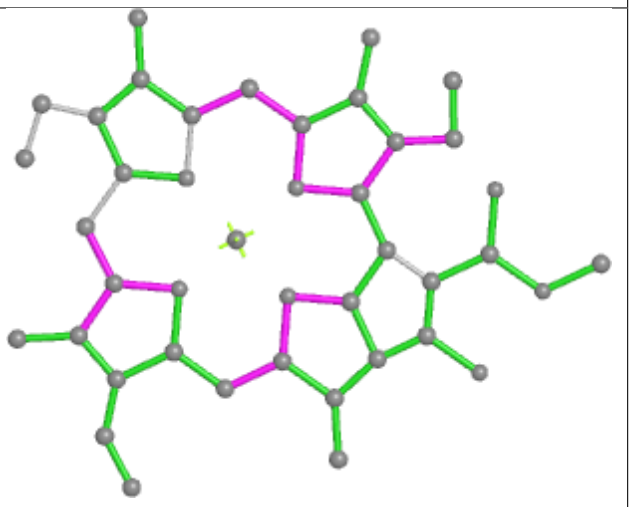
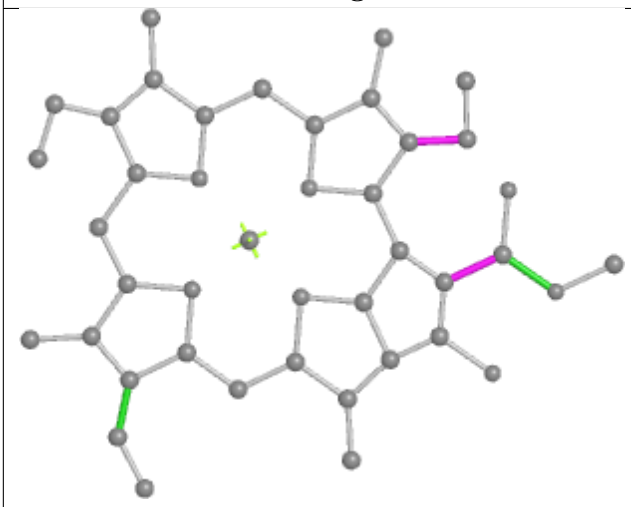
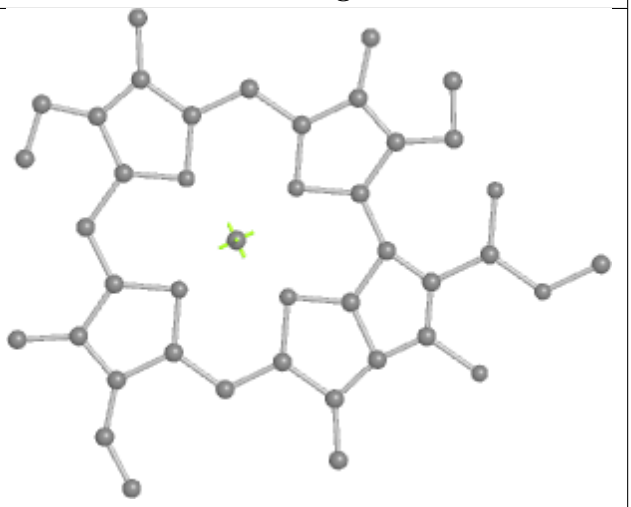


Bond angles

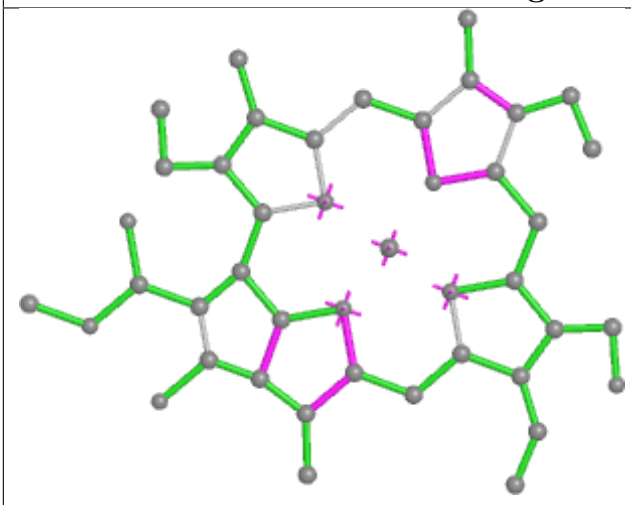


Torsions



Rings

Ligand CHL 7 606



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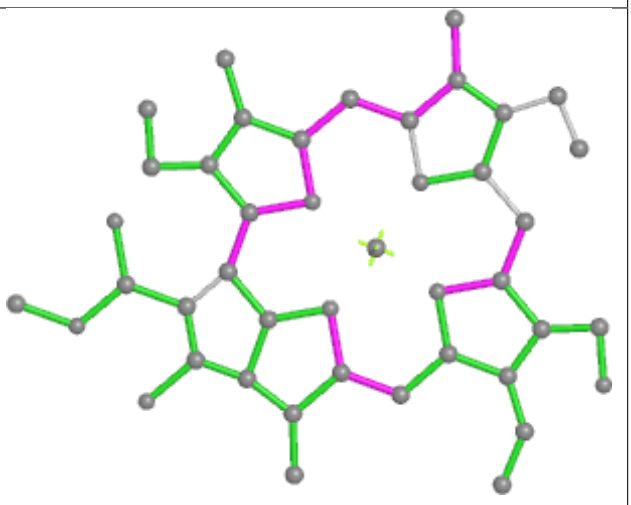
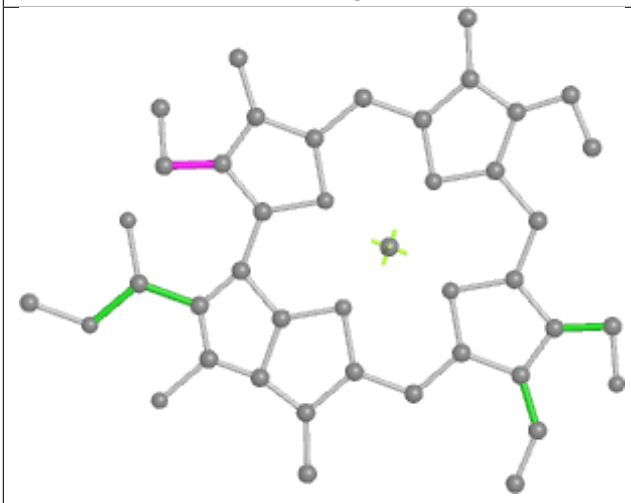


Bond angles



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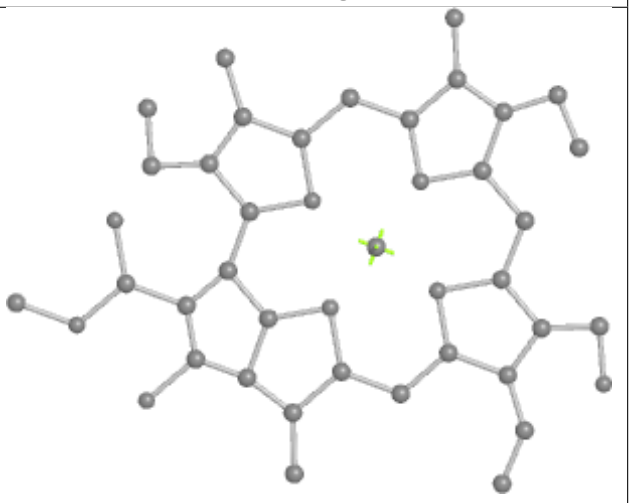
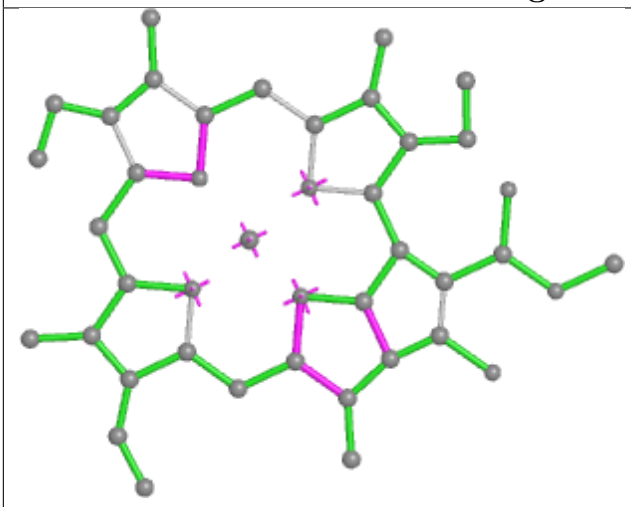


Rings

Ligand CLA 1 608



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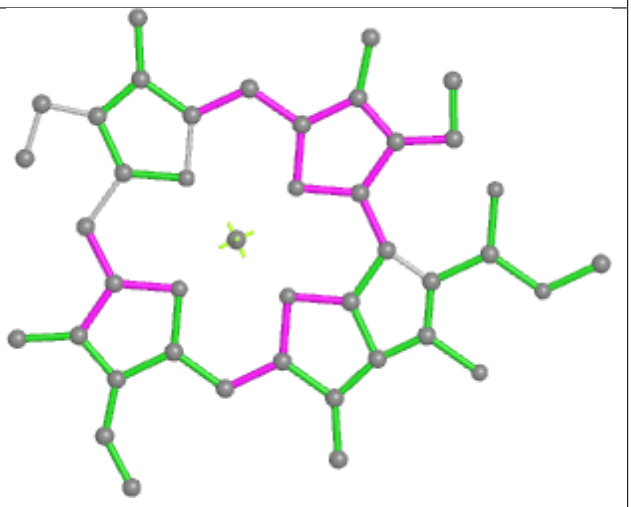
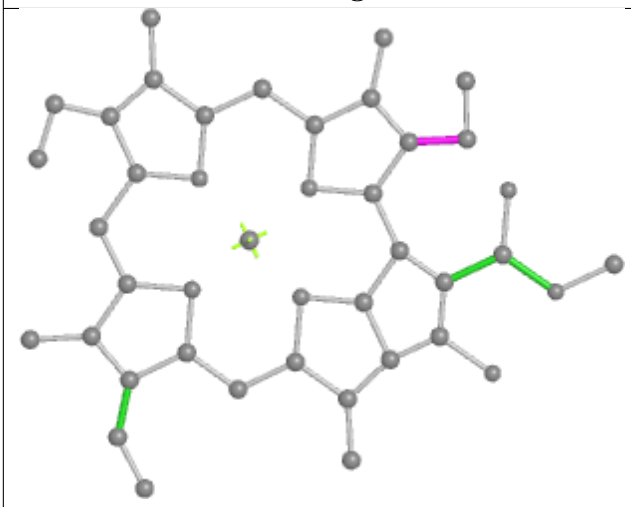


Bond angles



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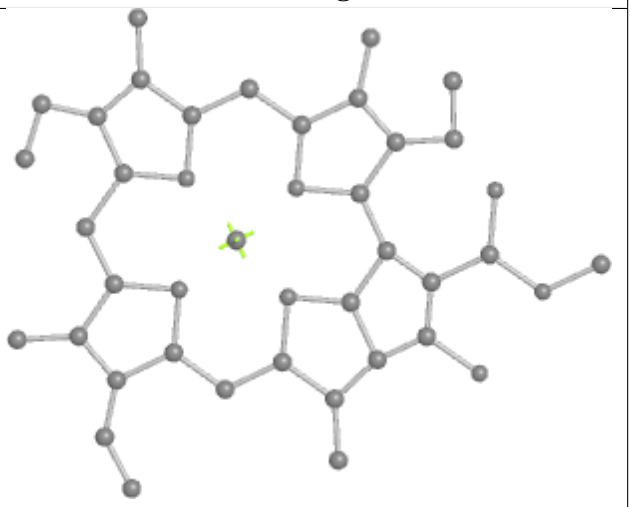
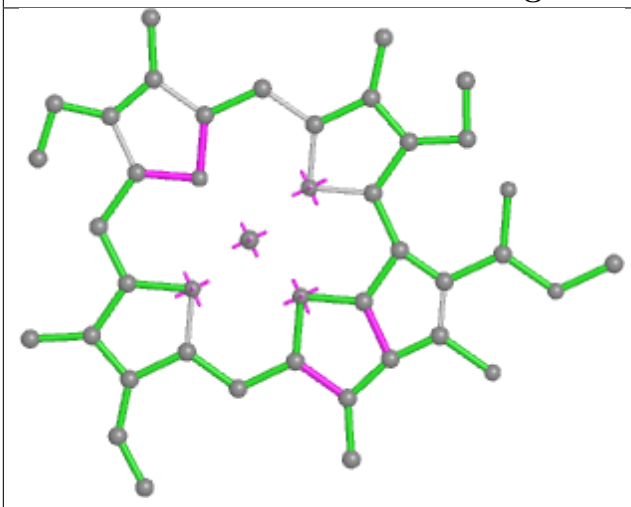
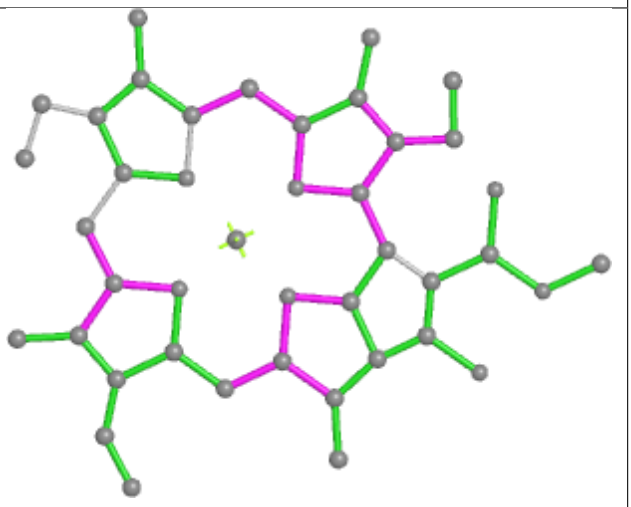


Rings

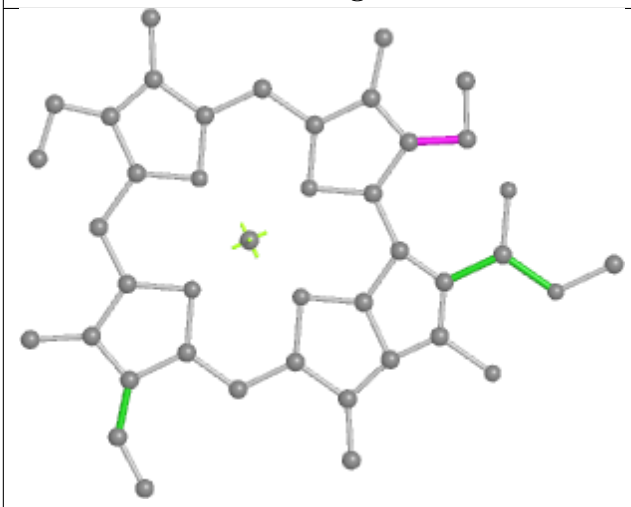
Ligand CLA B 820



Bond lengths



Bond angles



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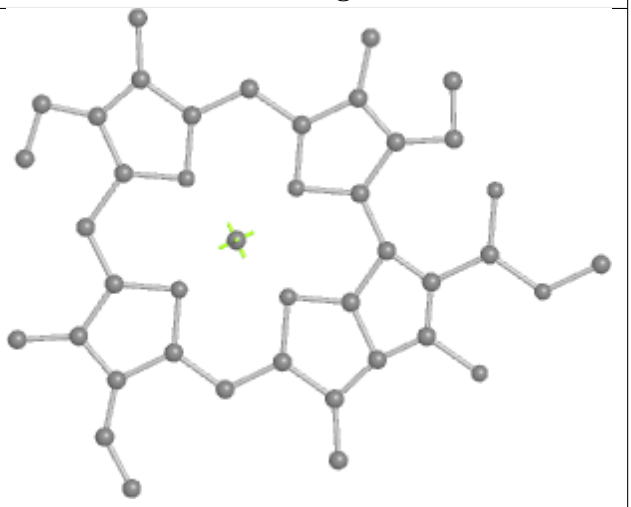
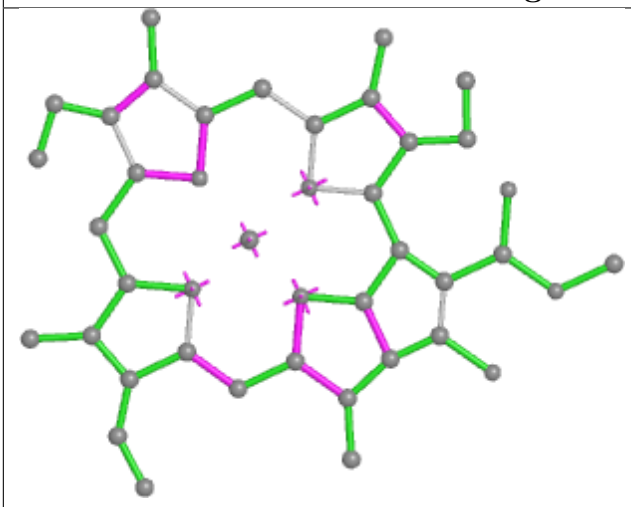
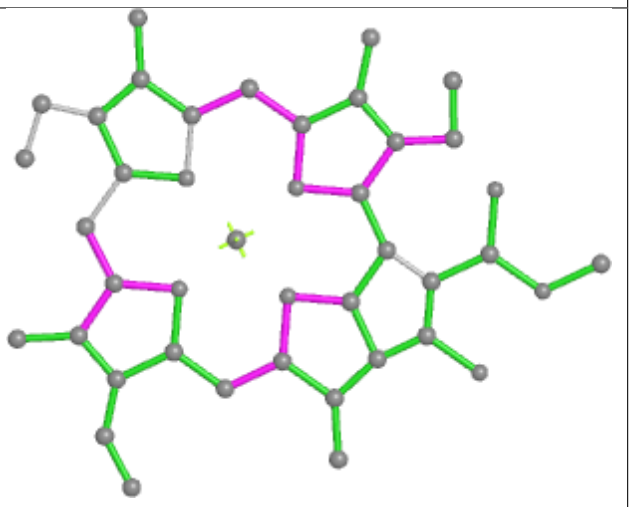


Rings

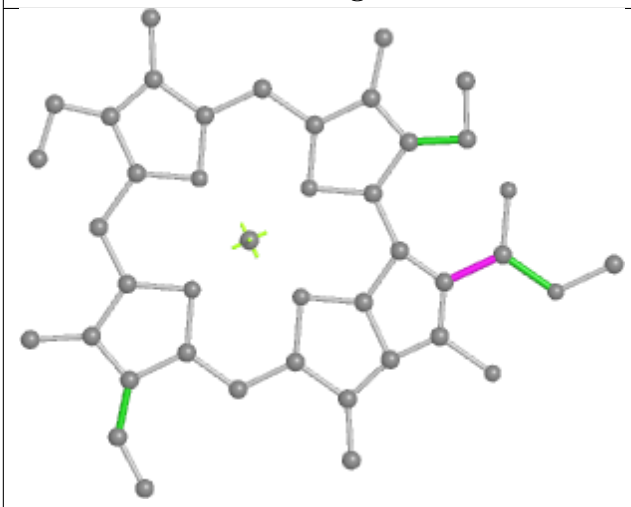
Ligand CLA B 842



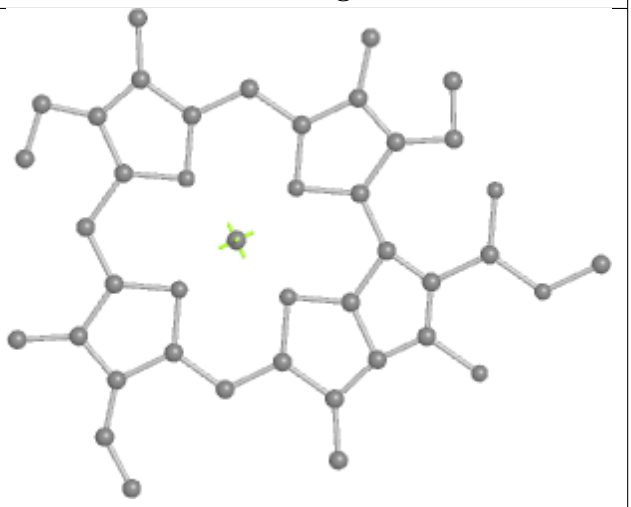
Bond lengths



Bond angles

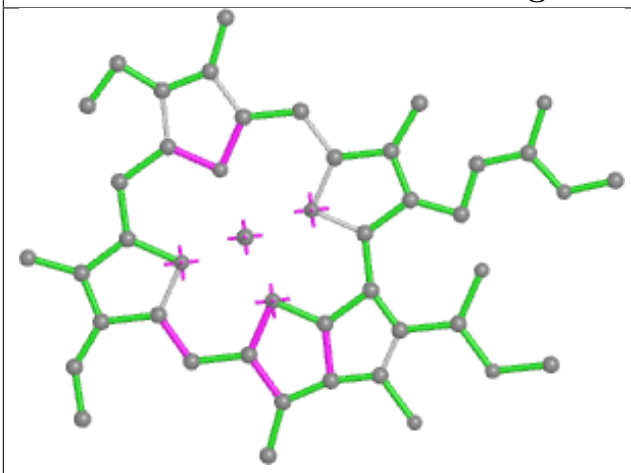


Torsions

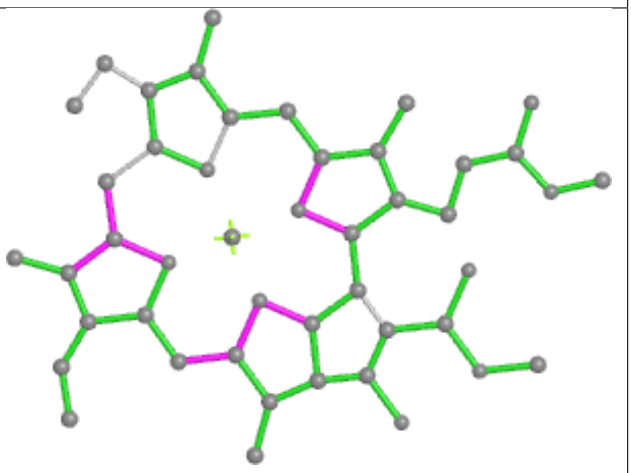


Rings

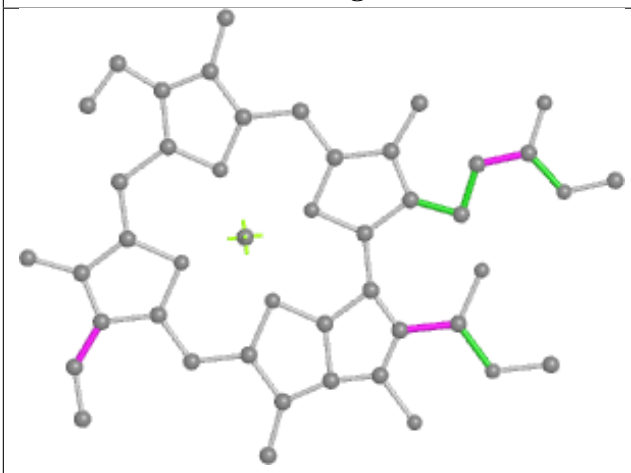
Ligand CLA 6 303



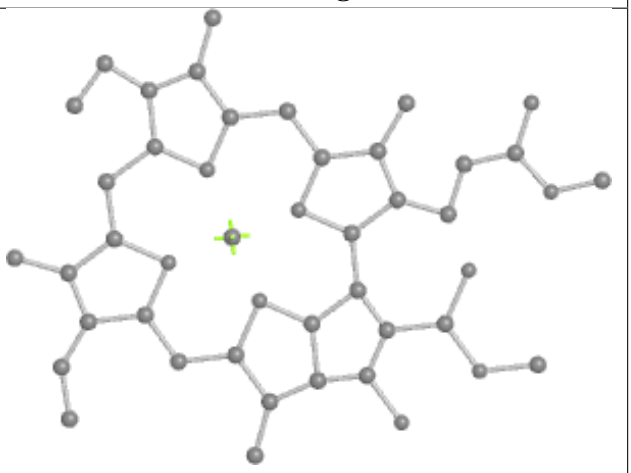
Bond lengths



Bond angles

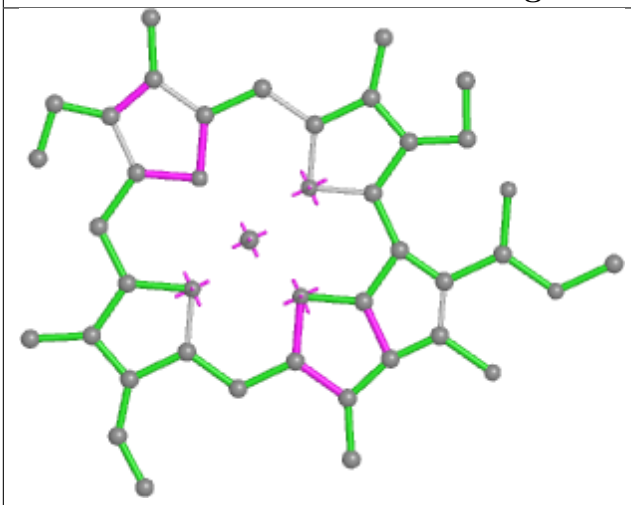


Torsions

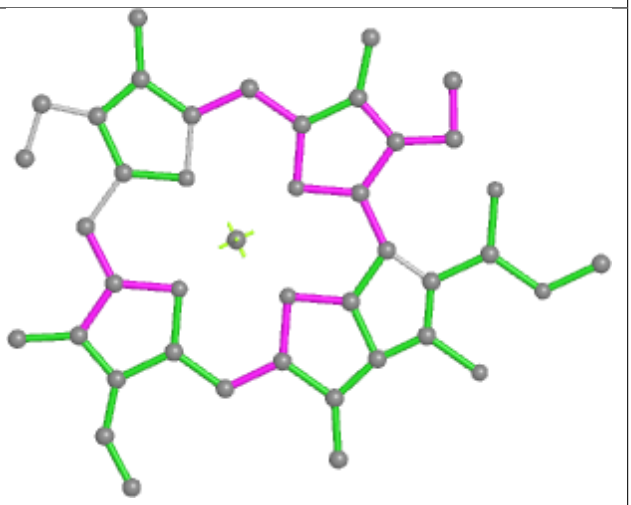


Rings

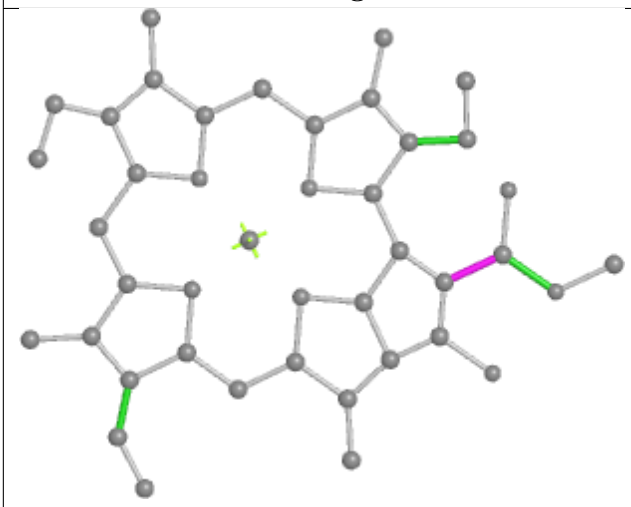
Ligand CLA B 841



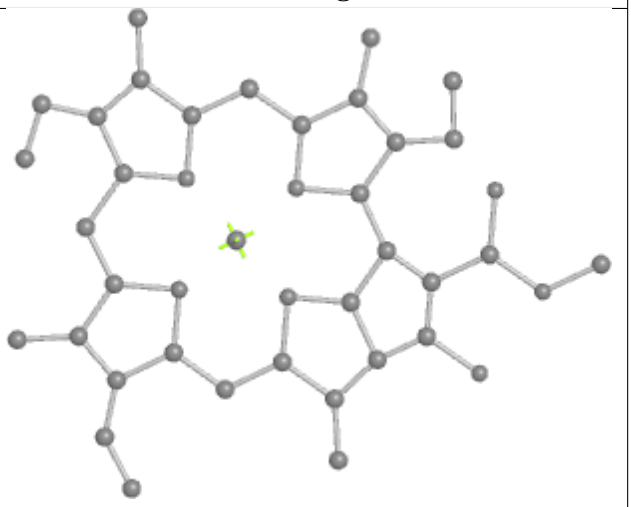
Bond lengths



Bond angles

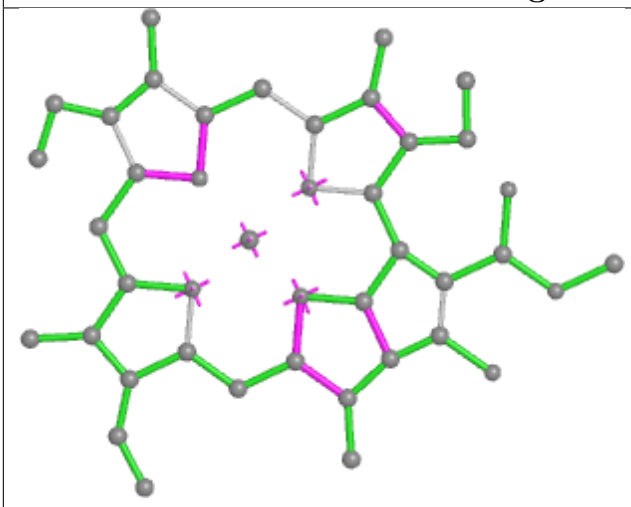


Torsions



Rings

Ligand CLA 3 307



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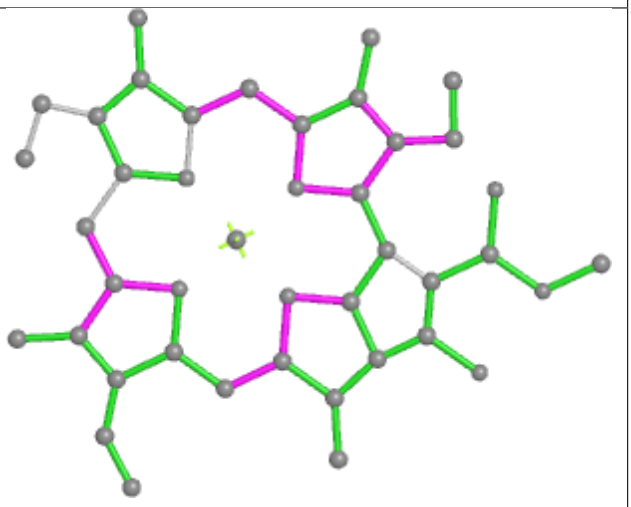
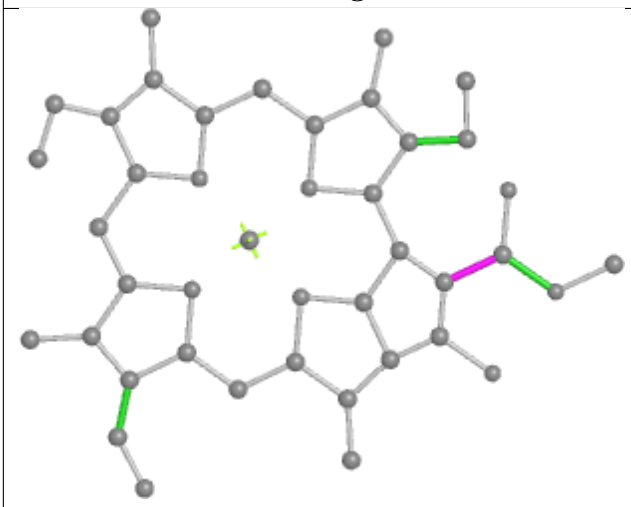


Bond angles



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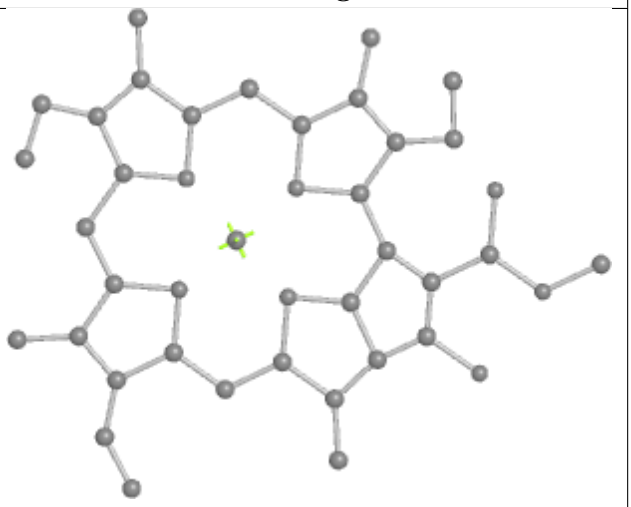
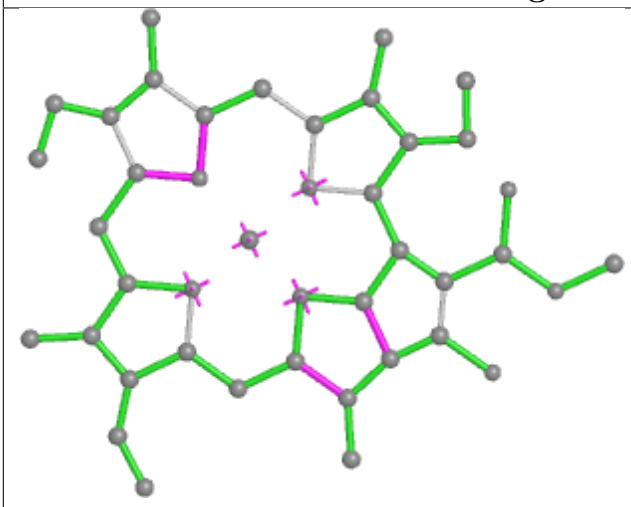


Rings

Ligand CLA 6 310



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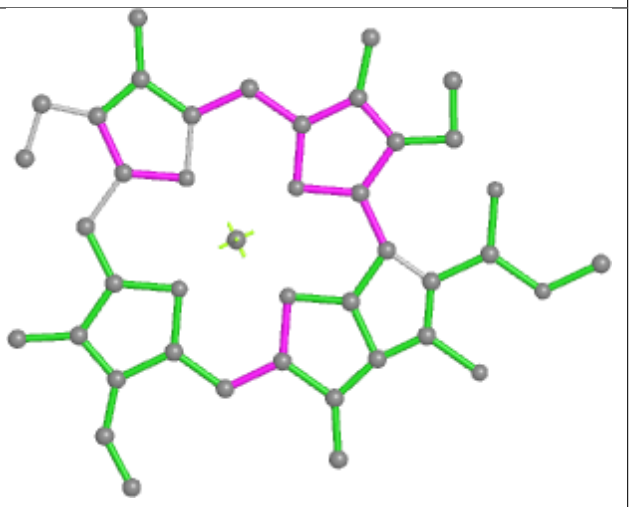
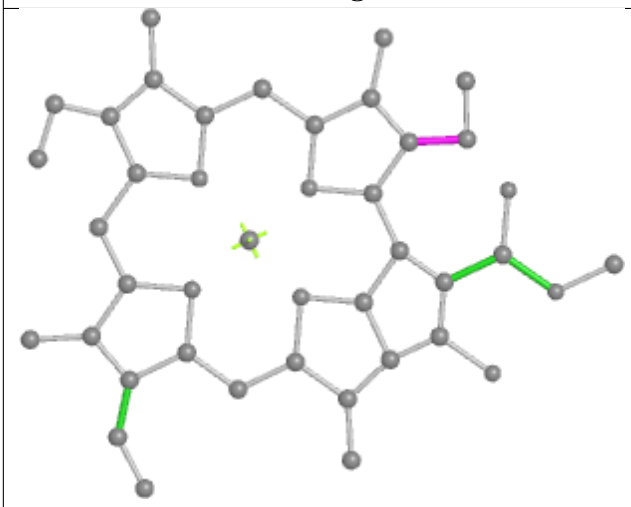


Bond angles



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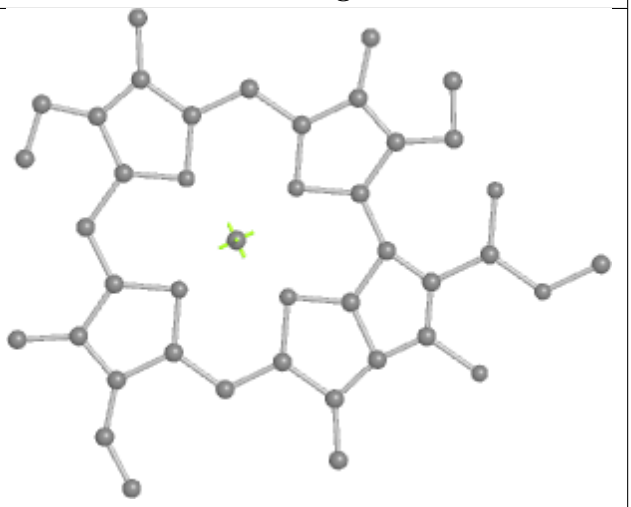
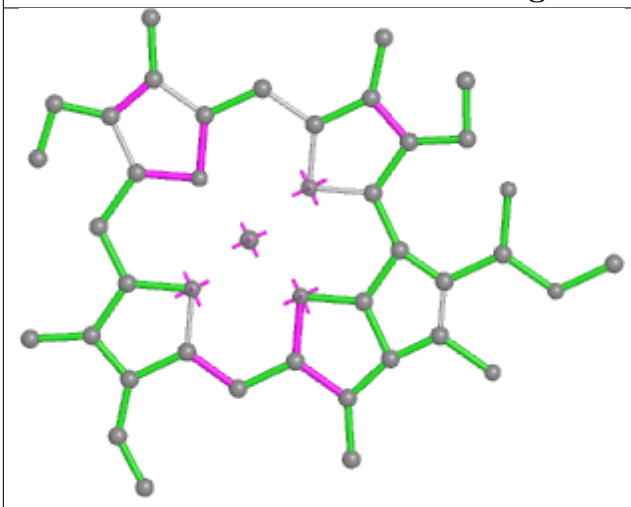


Rings

Ligand CLA 1 603



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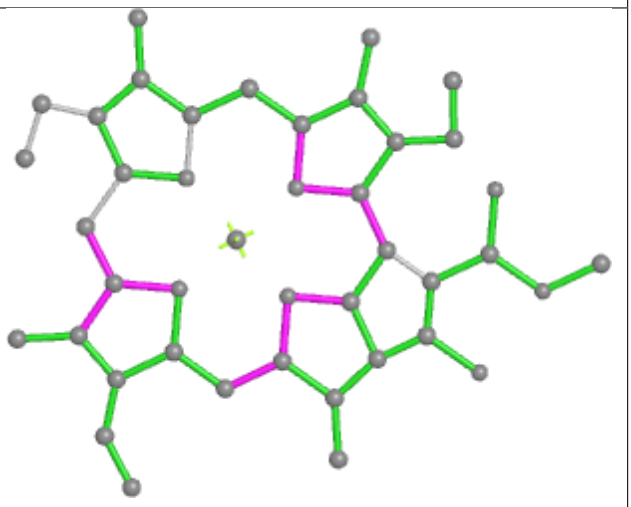
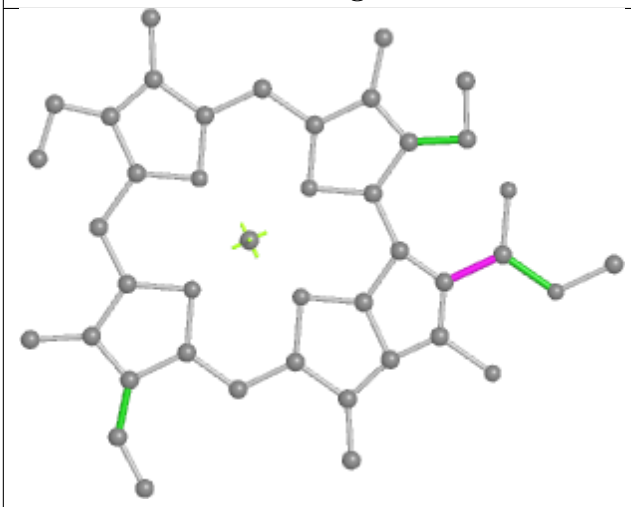


Bond angles



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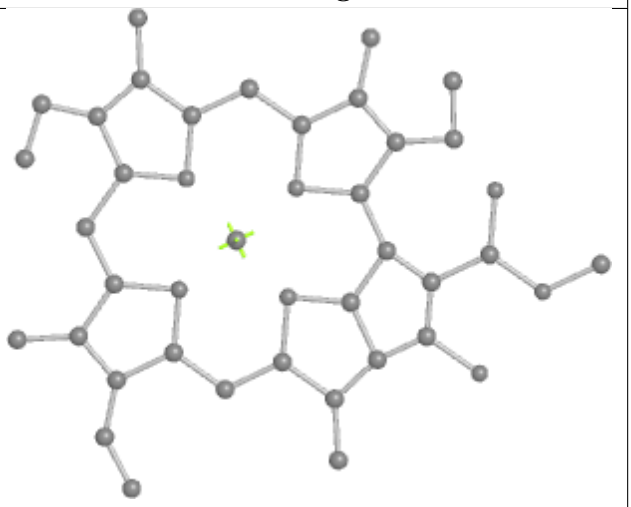
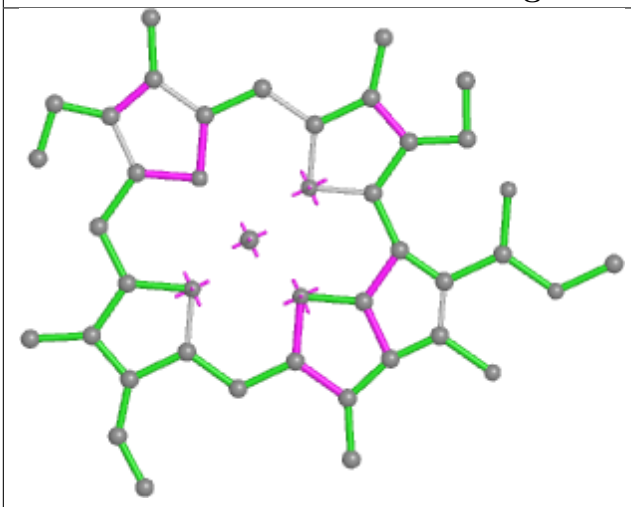


Rings

Ligand CLA A 840



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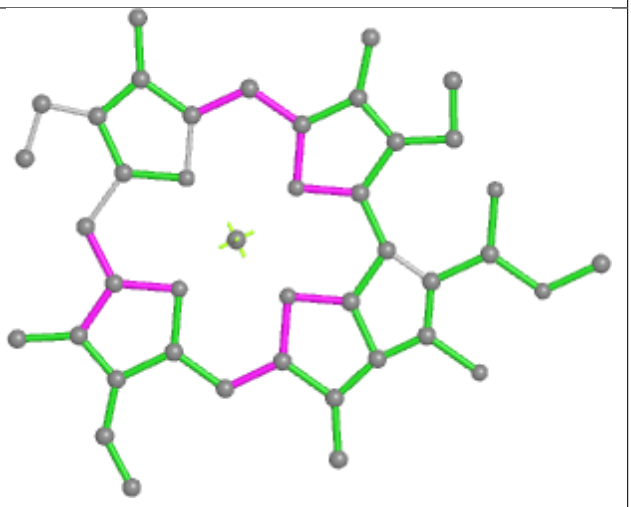
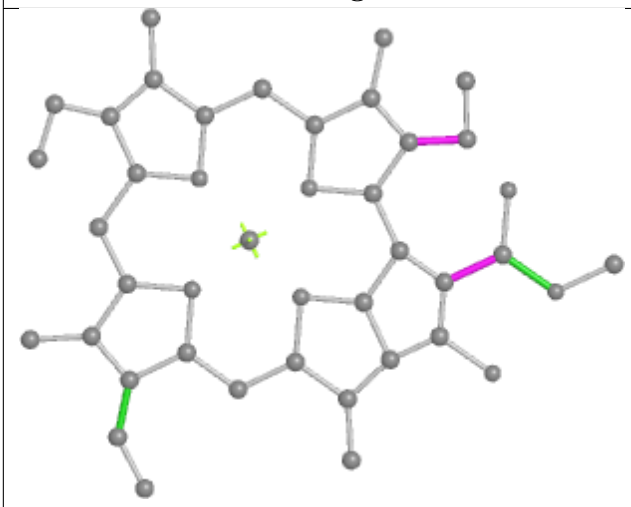


Bond angles



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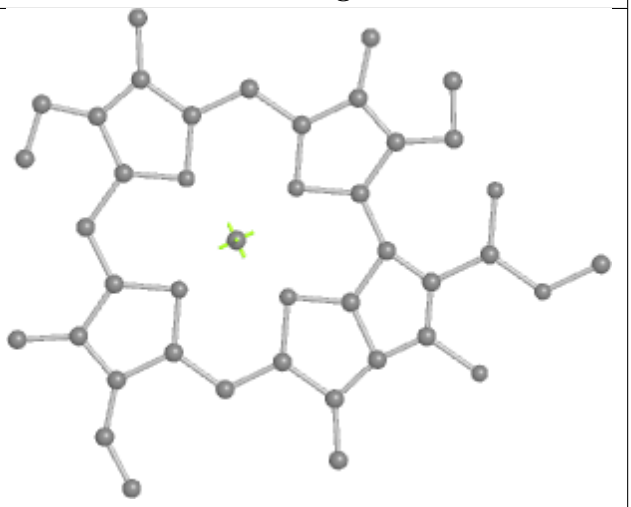
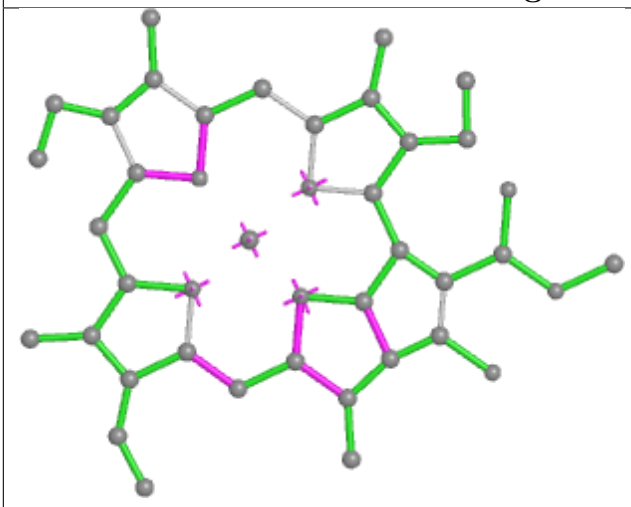


Rings

Ligand CLA B 833



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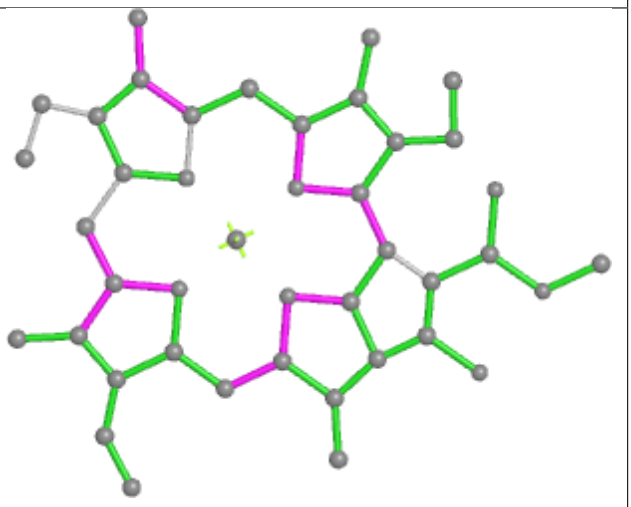
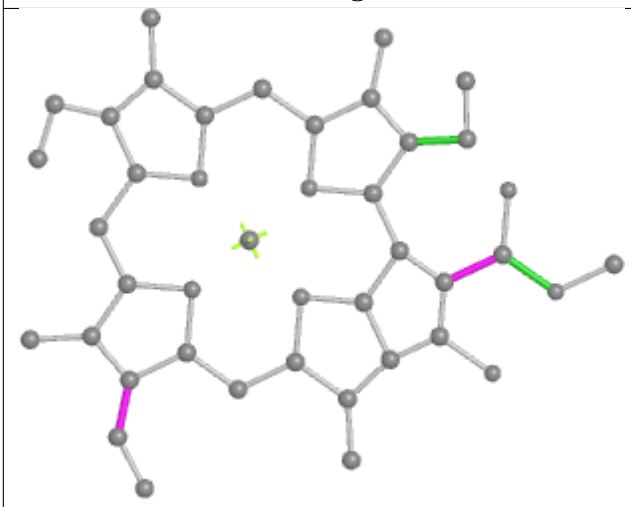


Bond angles



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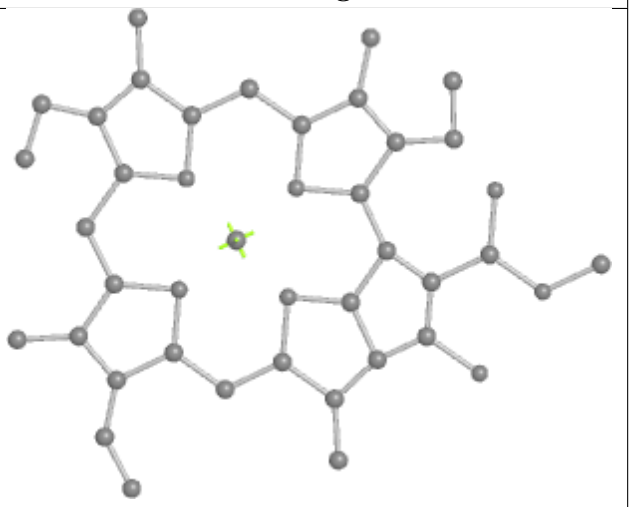
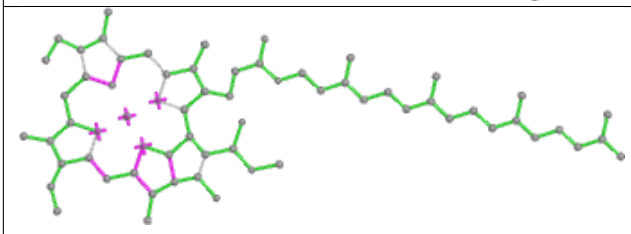


Rings

Ligand CLA F 302



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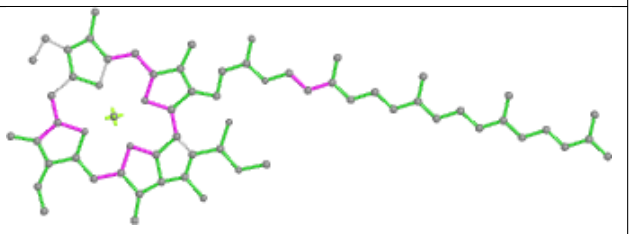
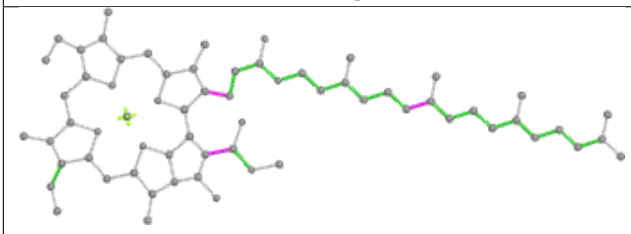


Bond angles



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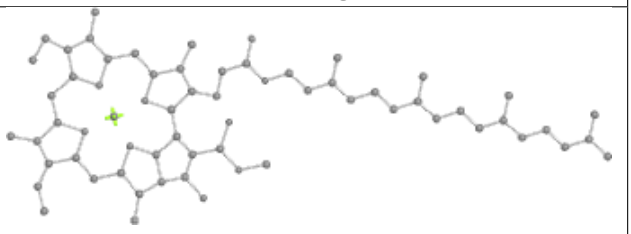
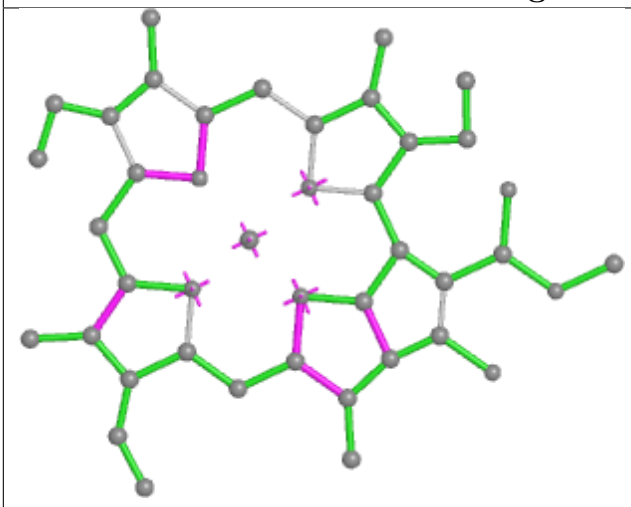


Rings

Ligand CLA 4 607



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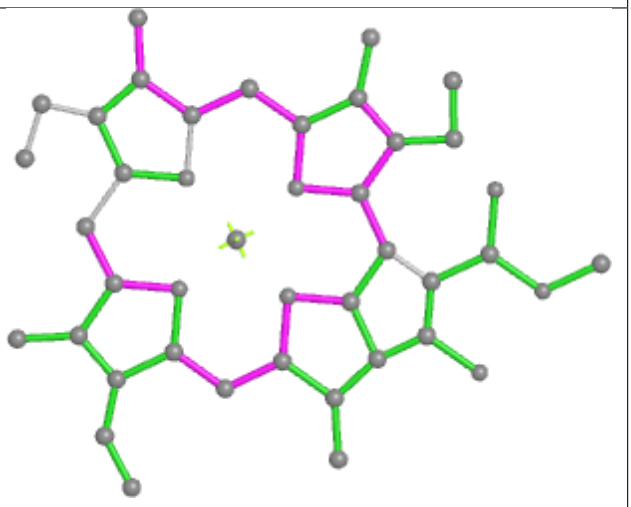
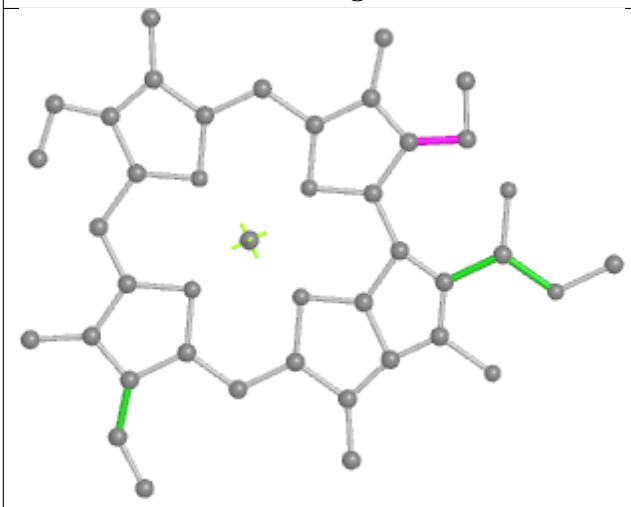


Bond angles



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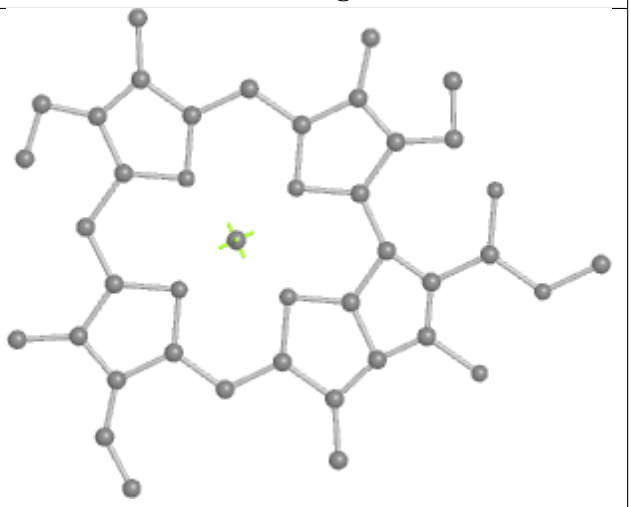
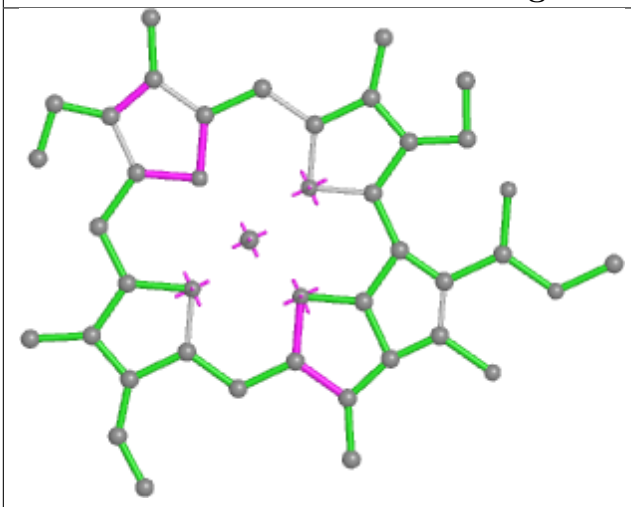


Rings

Ligand CLA 5 614



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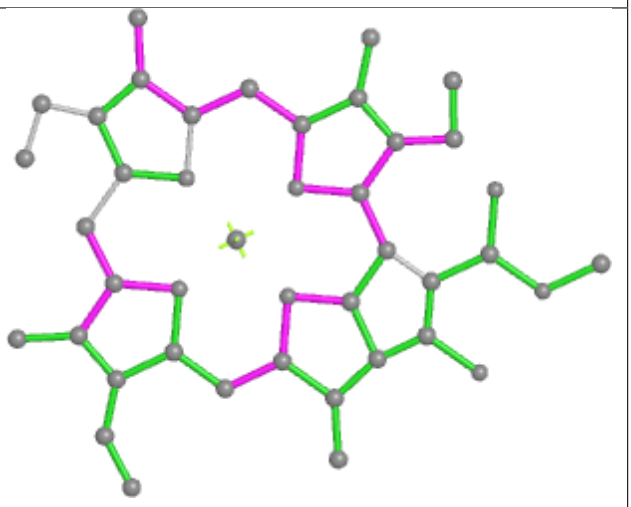
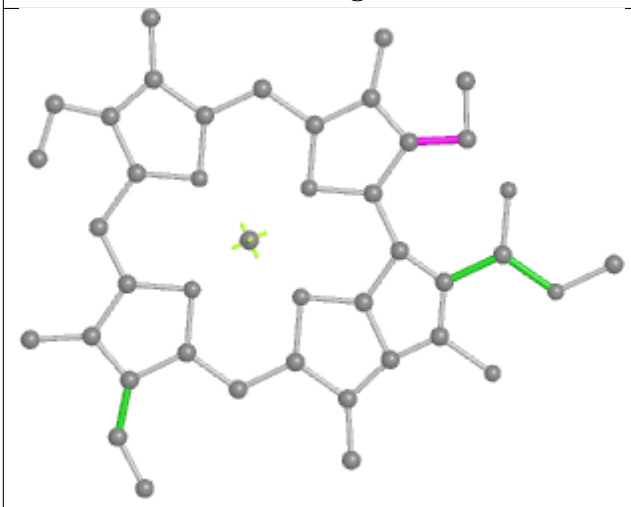


Bond angles



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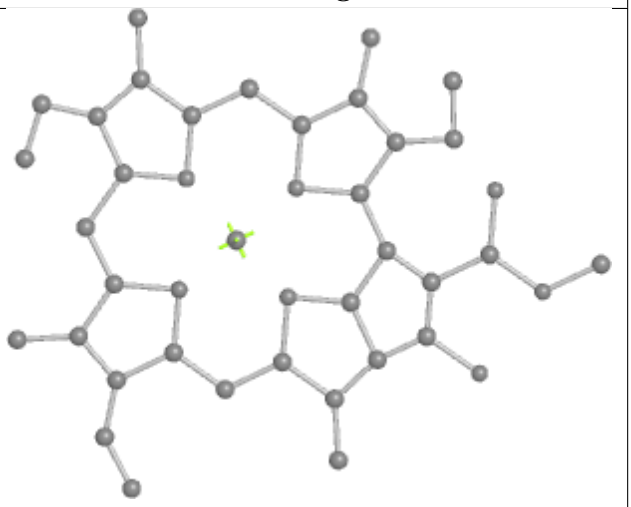
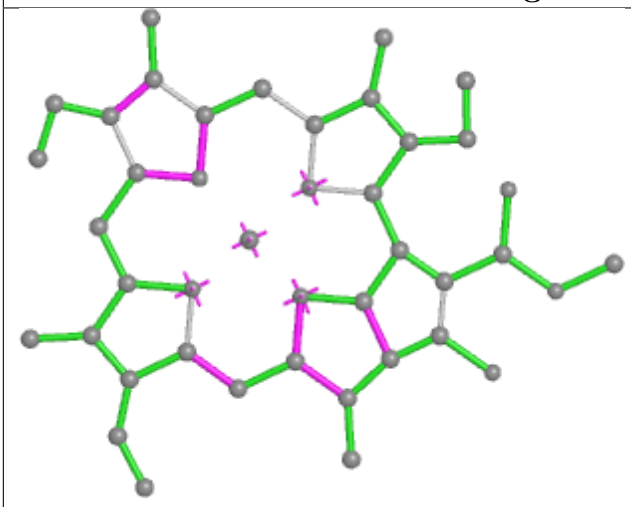


Rings

Ligand CLA A 830



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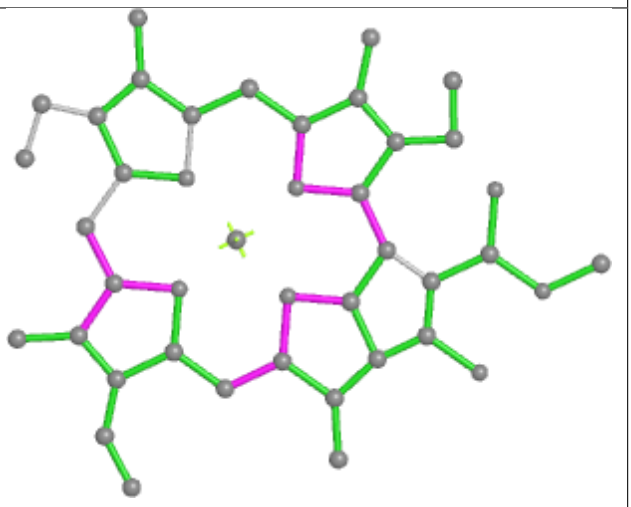
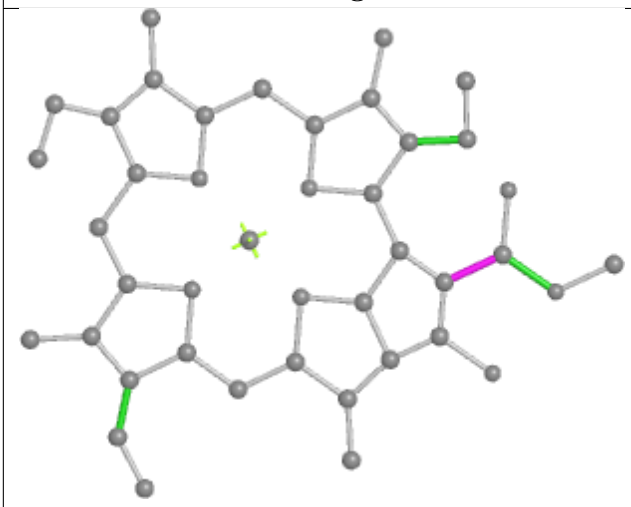
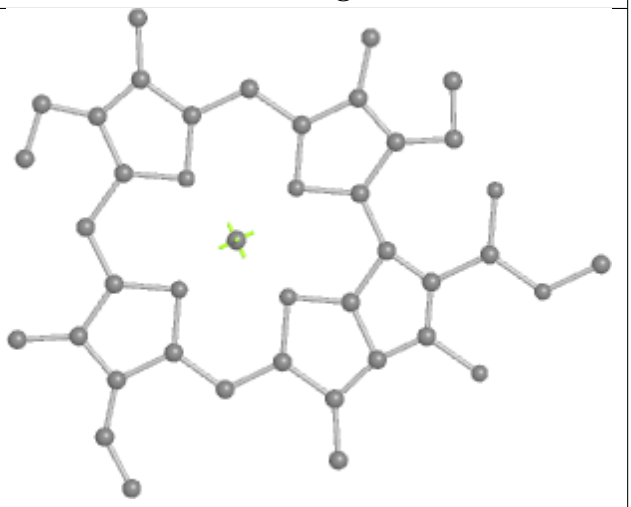


Bond angles

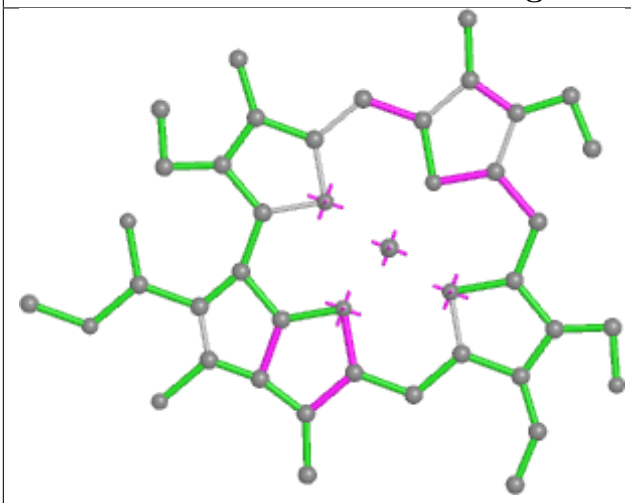


Torsions



Rings

Ligand CHL Z 601



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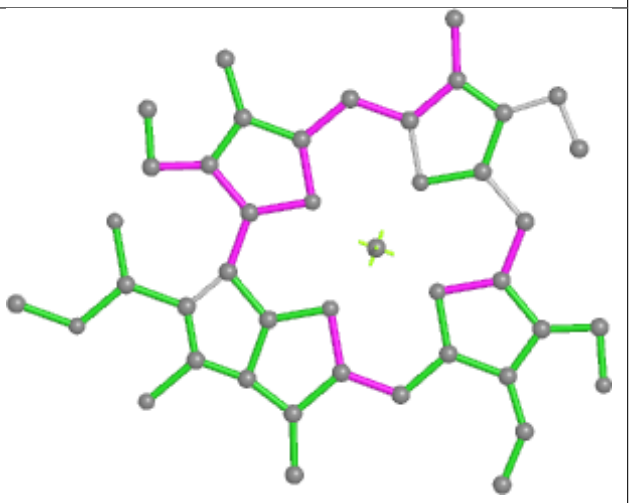
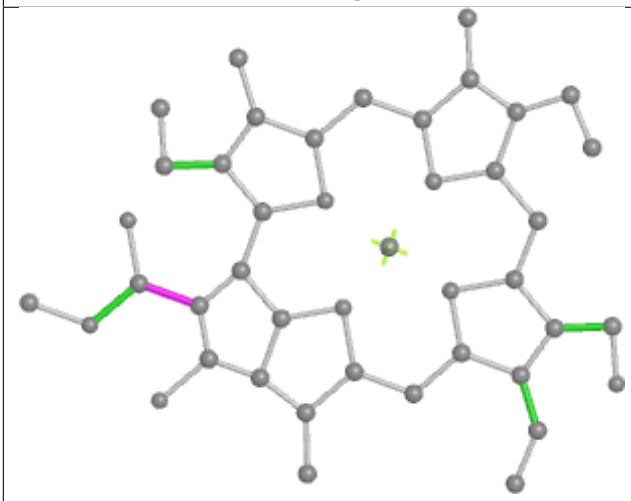


Bond angles



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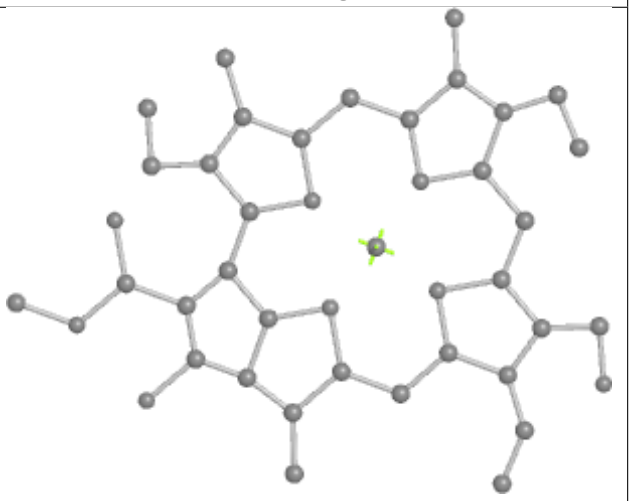
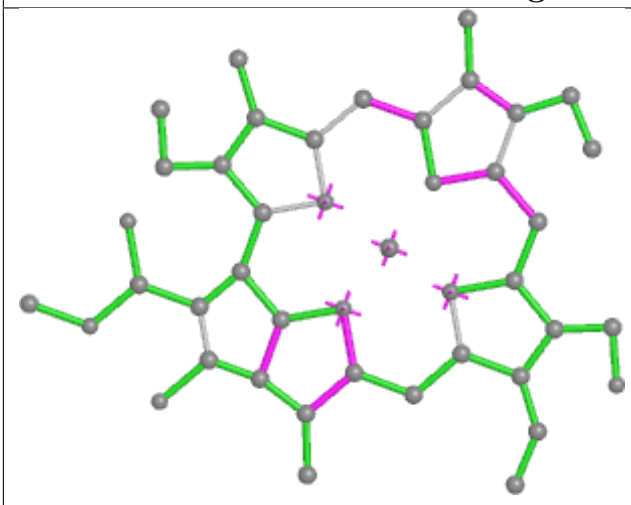


Rings

Ligand CHL 5 607



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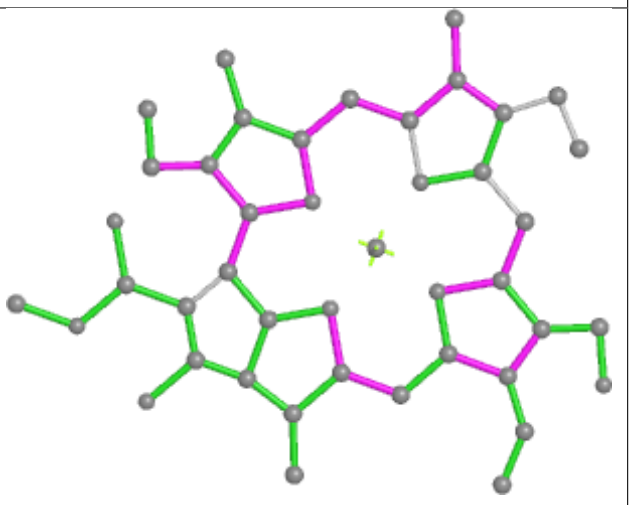
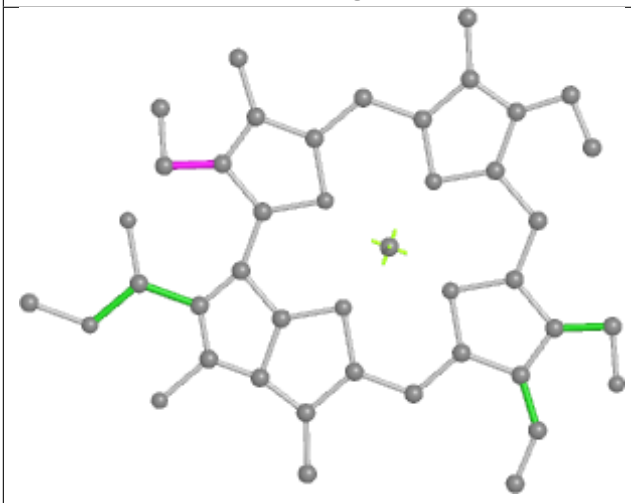


Bond angles



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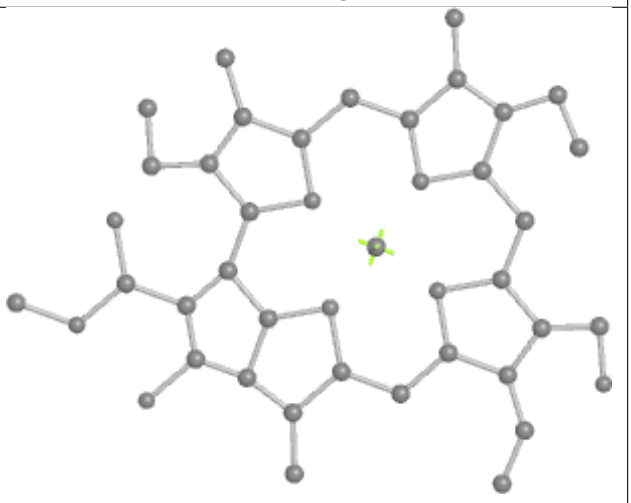
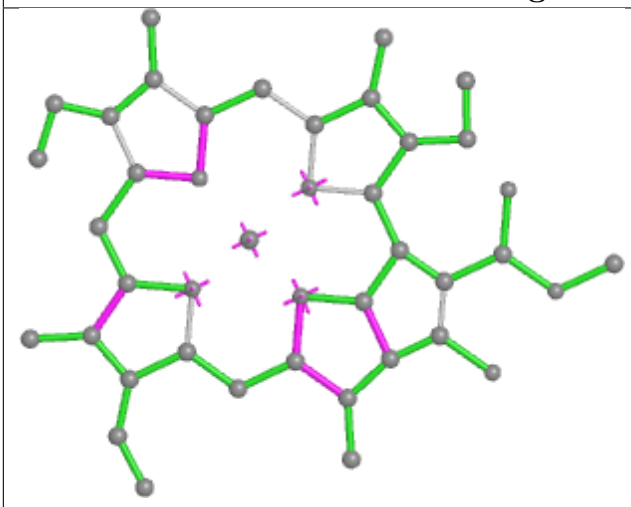
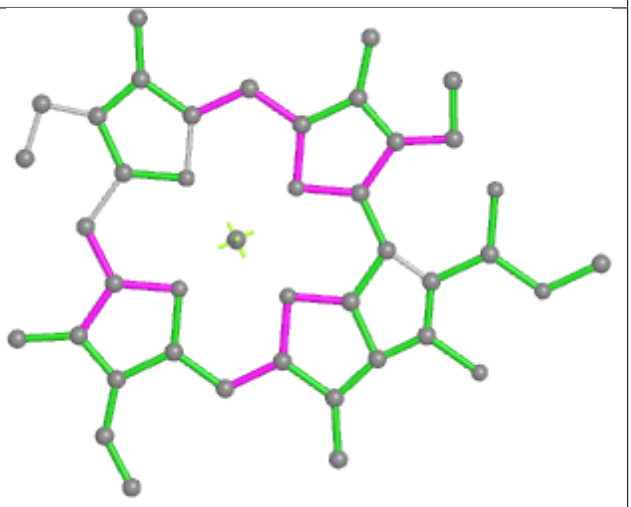


Rings

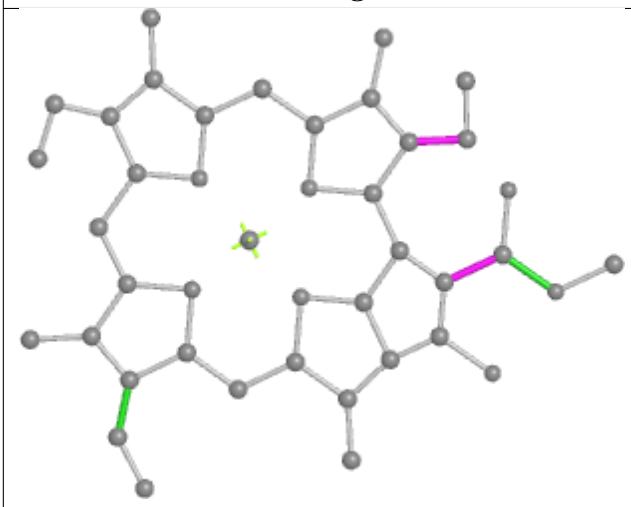
Ligand CLA 1 609



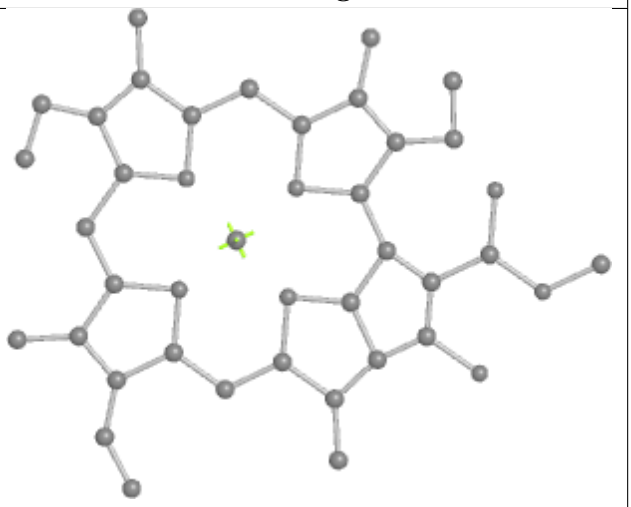
Bond lengths



Bond angles

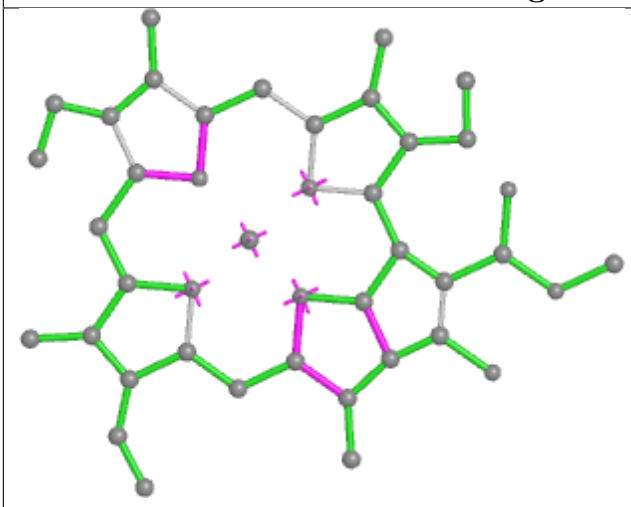


Torsions

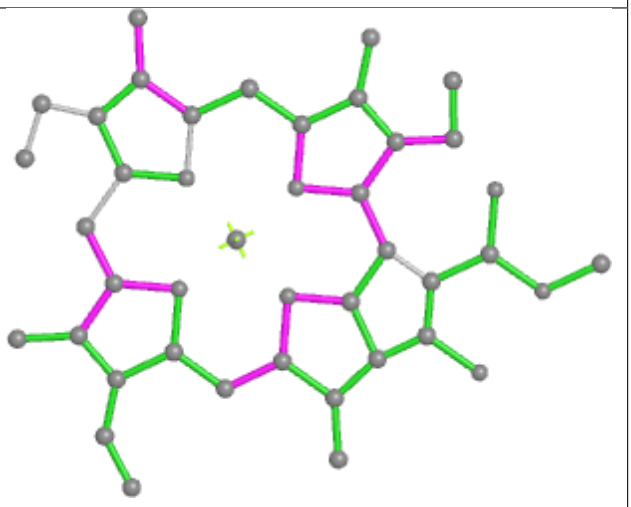


Rings

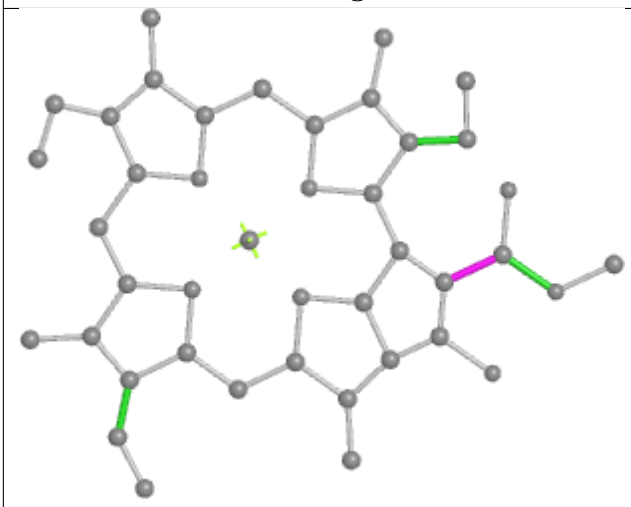
Ligand CLA J 101



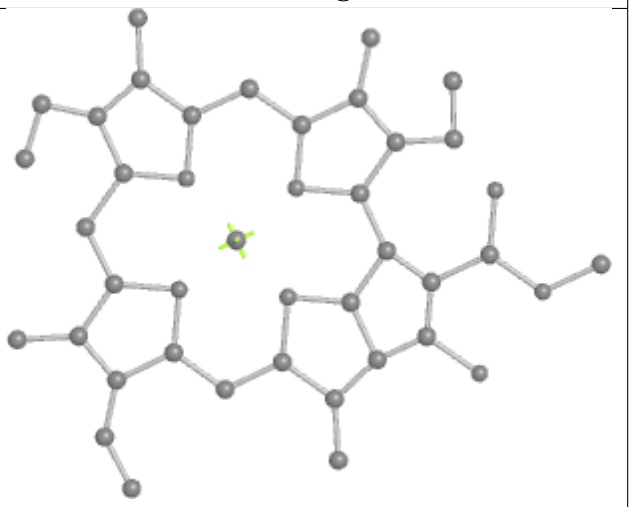
Bond lengths



Bond angles

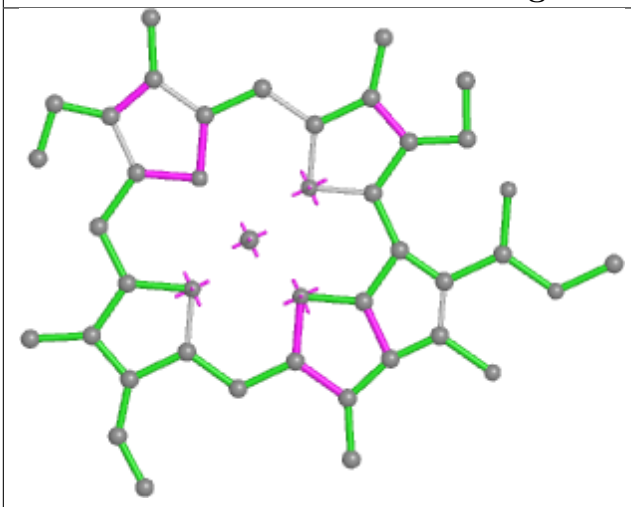


Torsions

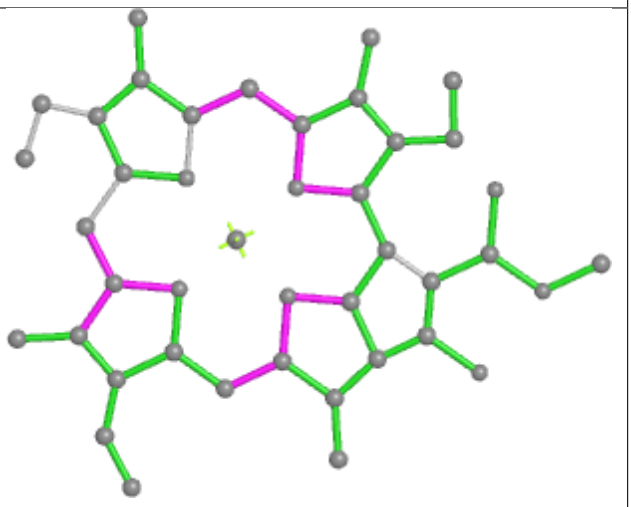


Rings

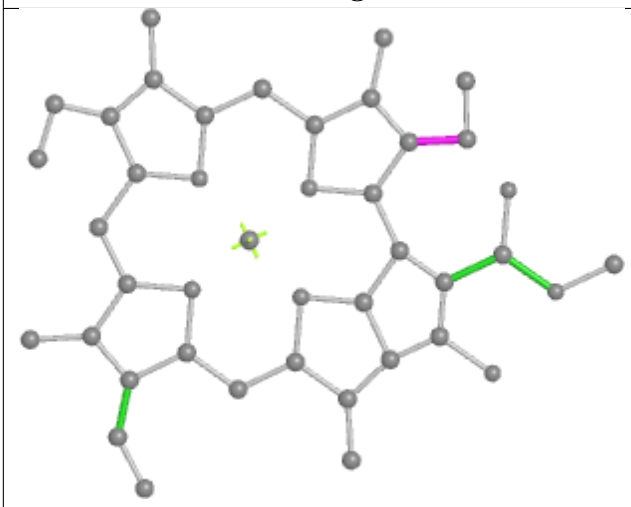
Ligand CLA 8 613



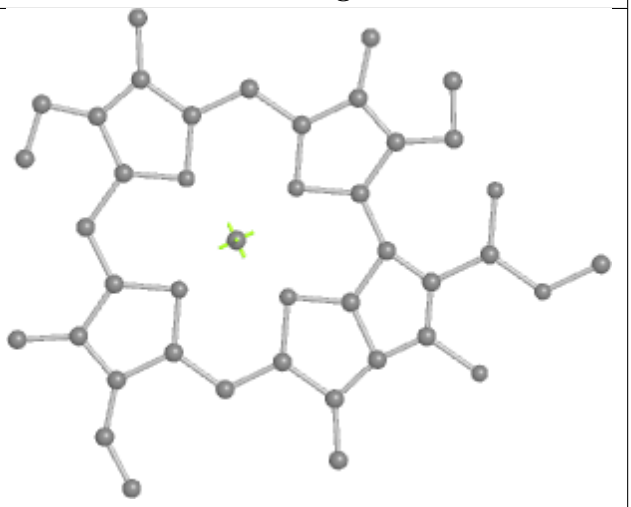
Bond lengths



Bond angles

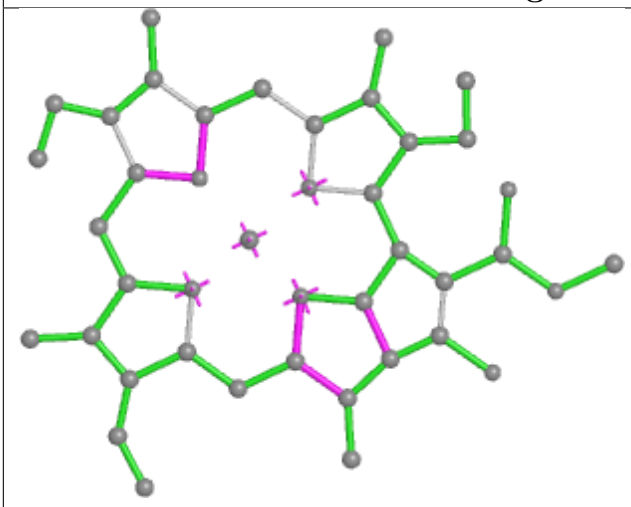


Torsions

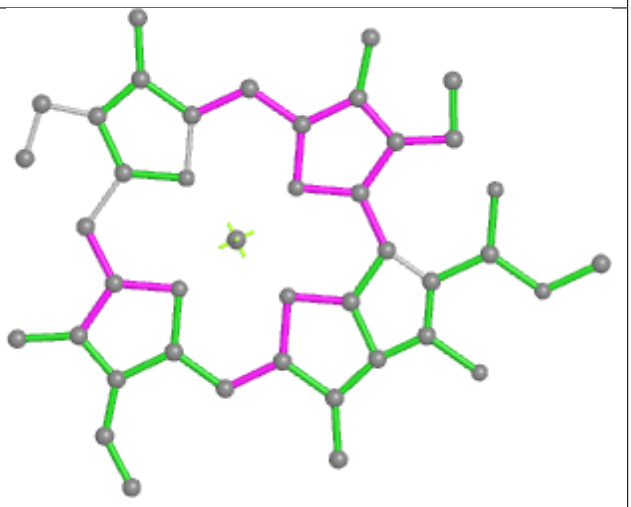


Rings

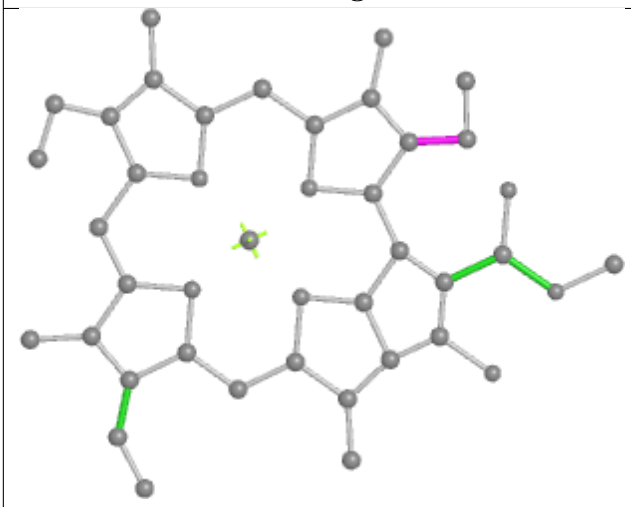
Ligand CLA Z 607



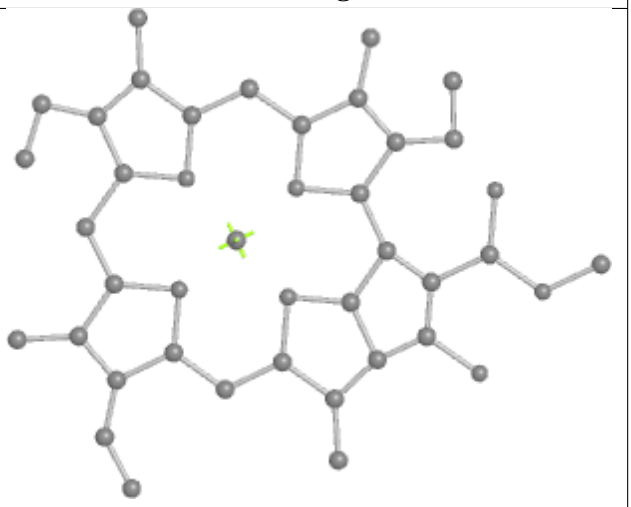
Bond lengths



Bond angles

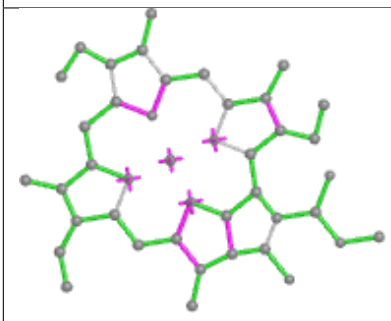
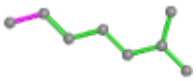


Torsions

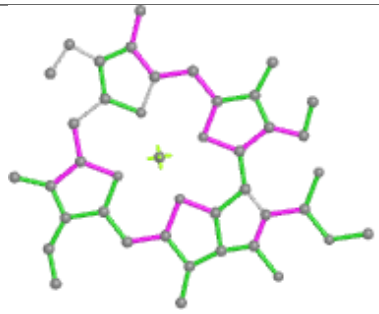
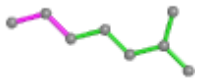


Rings

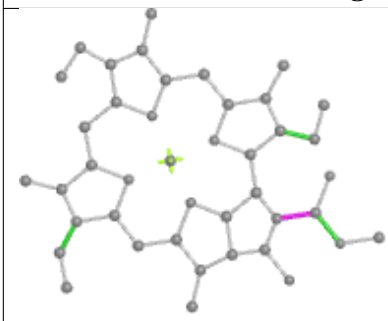
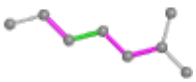
Ligand CLA B 807

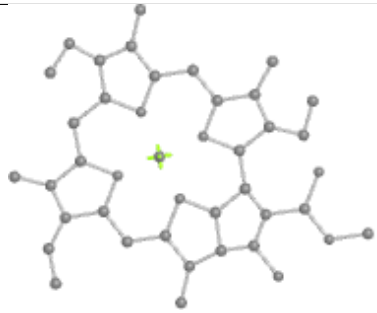
Bond lengths

Bond angles

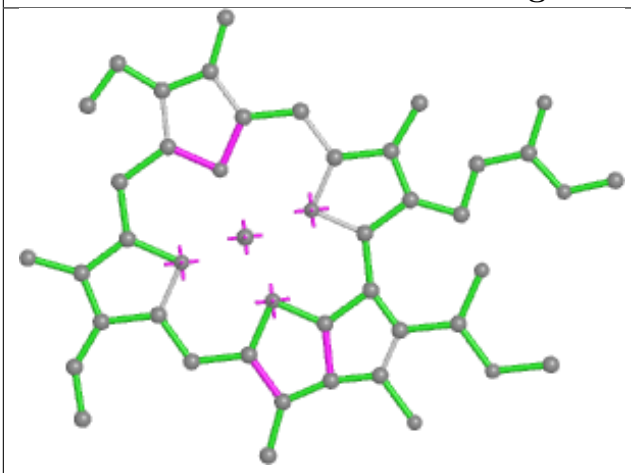



Torsions

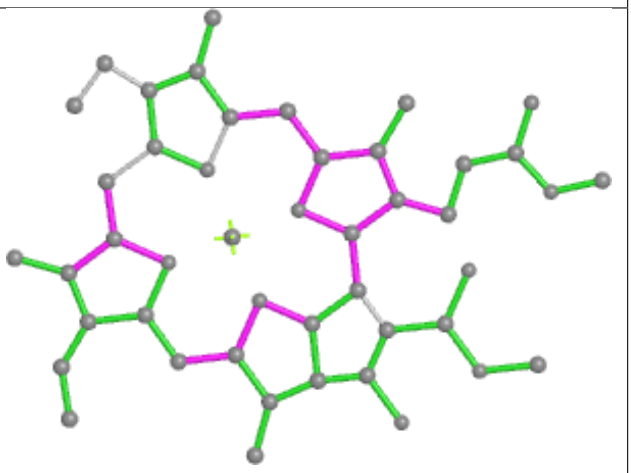



Rings

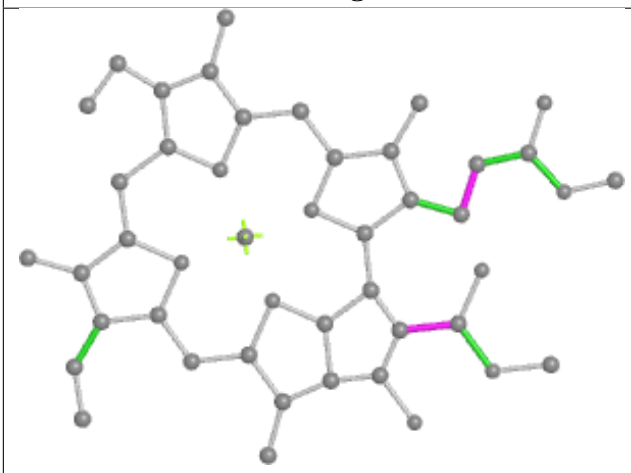
Ligand CLA 5 615



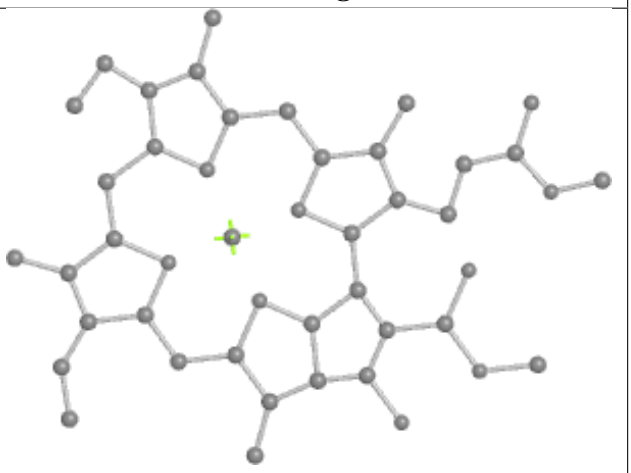
Bond lengths



Bond angles

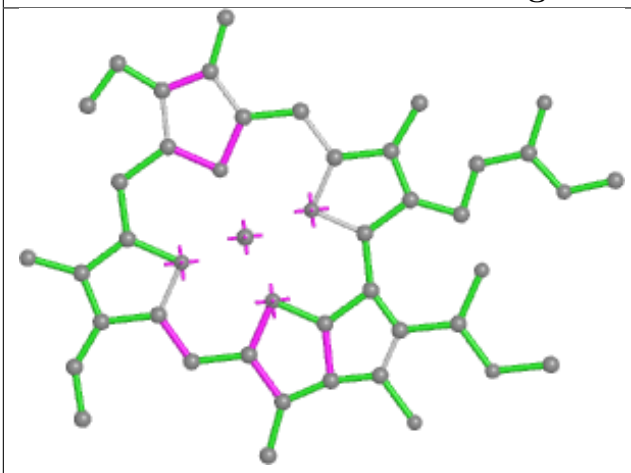


Torsions

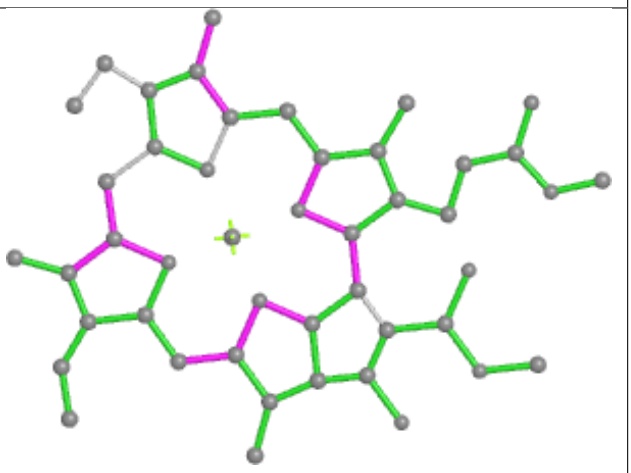


Rings

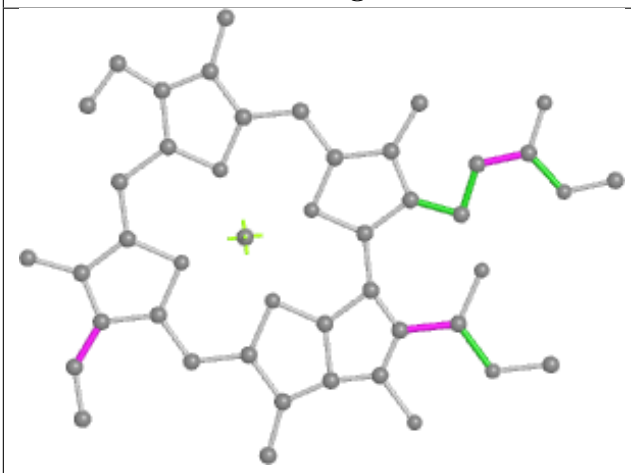
Ligand CLA 5 603



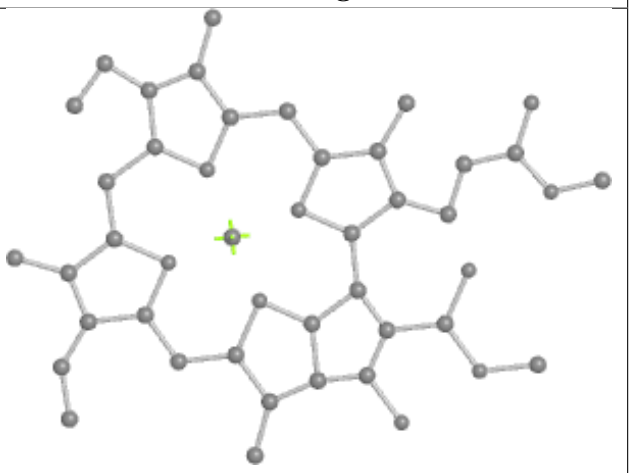
Bond lengths



Bond angles

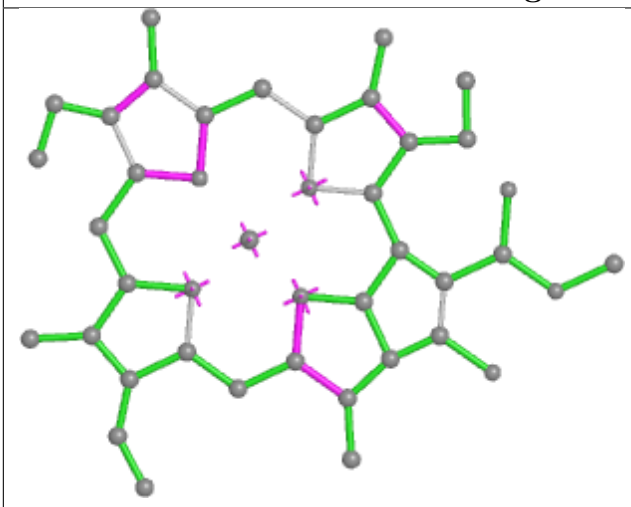


Torsions

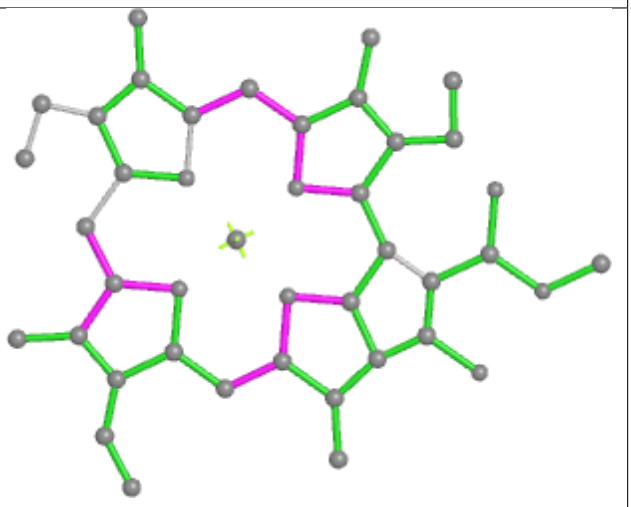


Rings

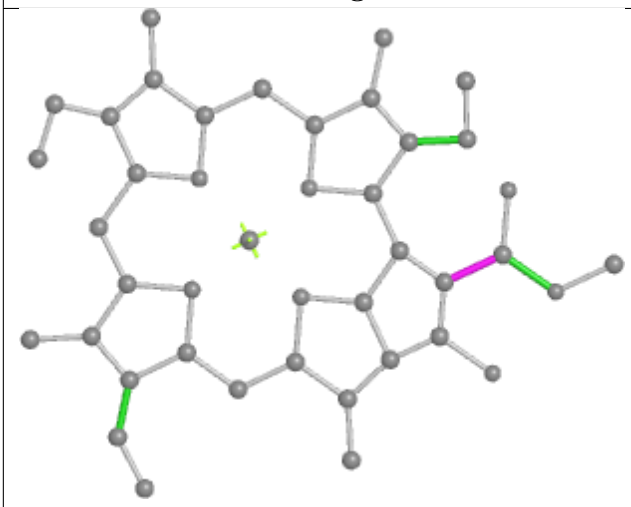
Ligand CLA B 810



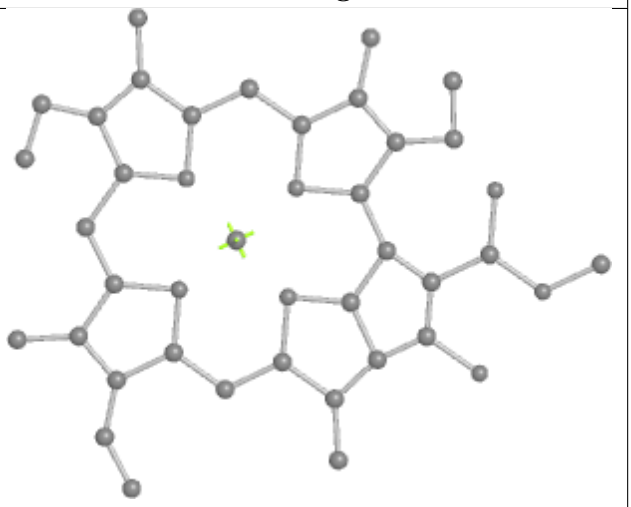
Bond lengths



Bond angles

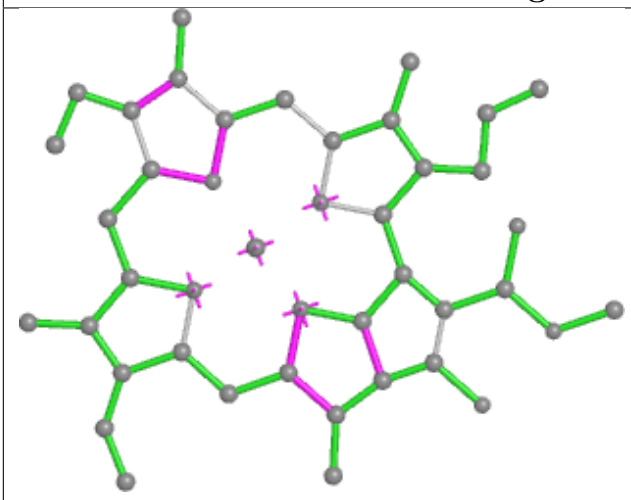


Torsions

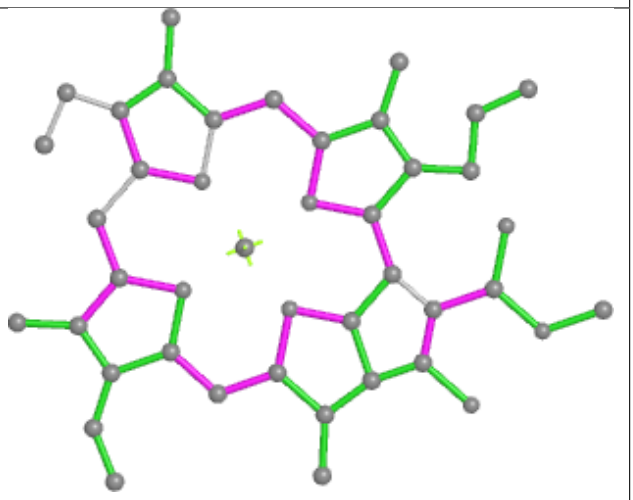


Rings

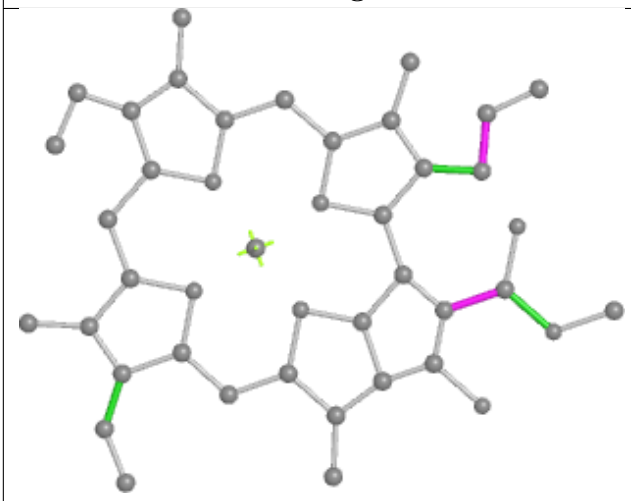
Ligand CLA 7 604



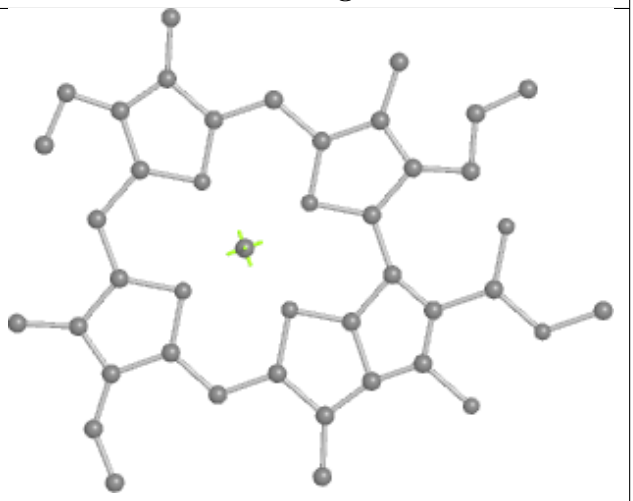
Bond lengths



Bond angles

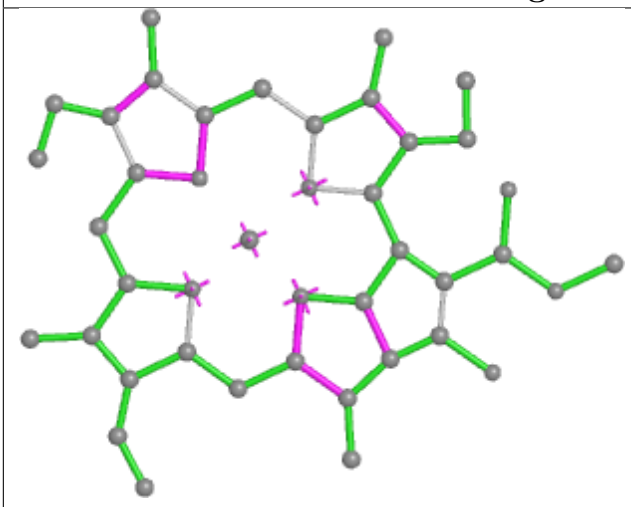


Torsions

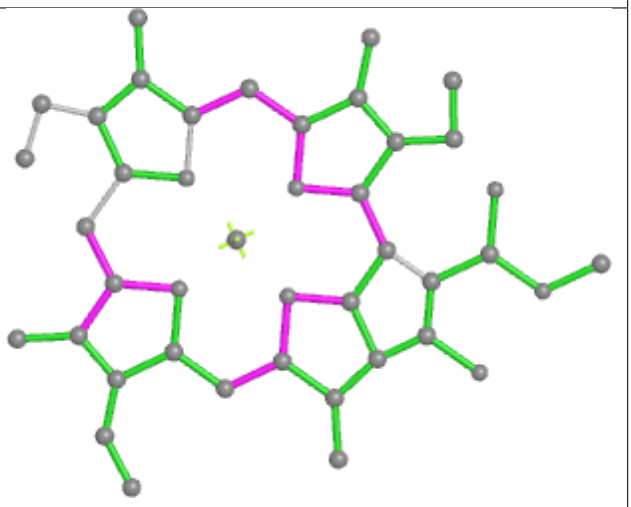


Rings

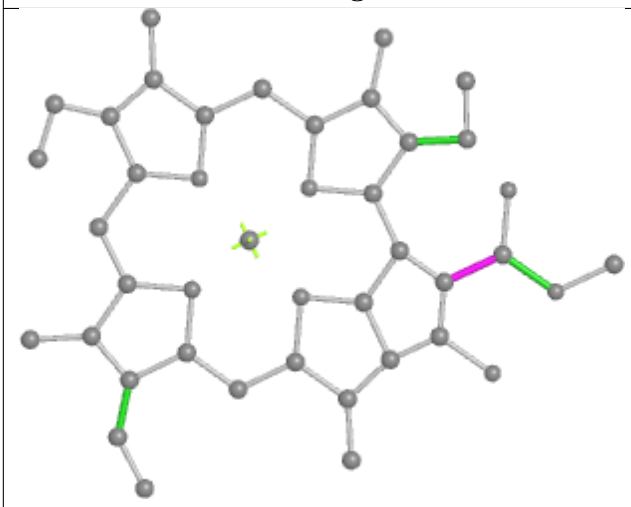
Ligand CL0 A 801



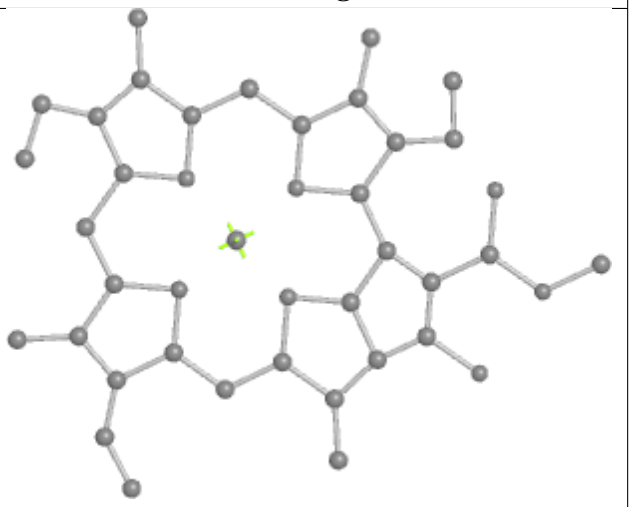
Bond lengths



Bond angles

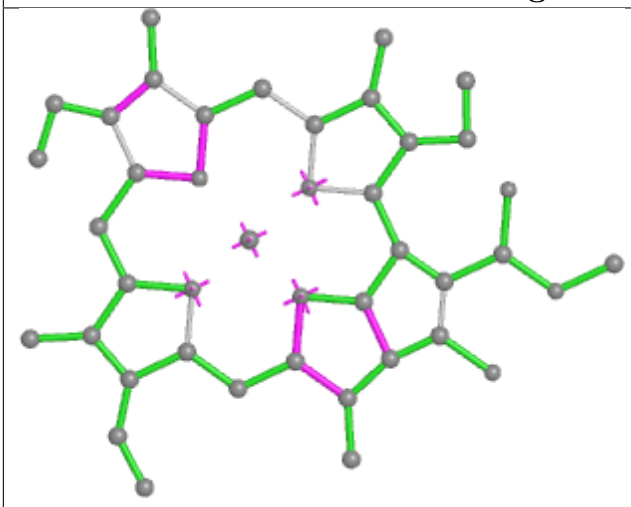


Torsions

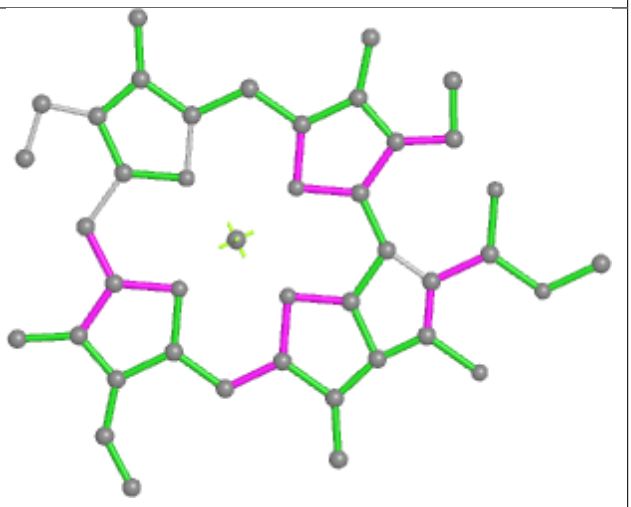


Rings

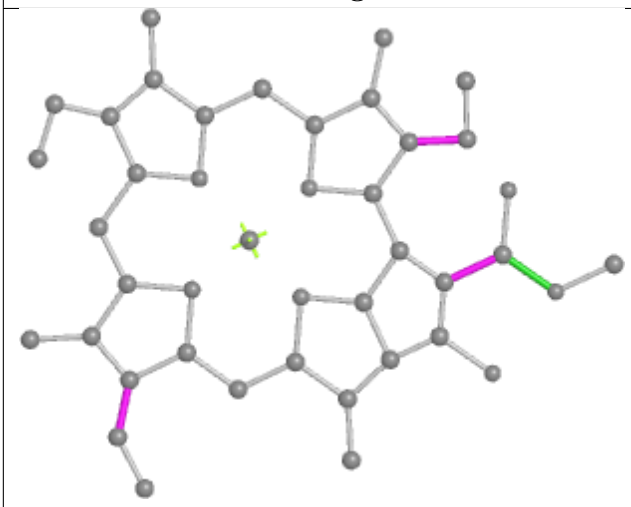
Ligand CLA 7 601



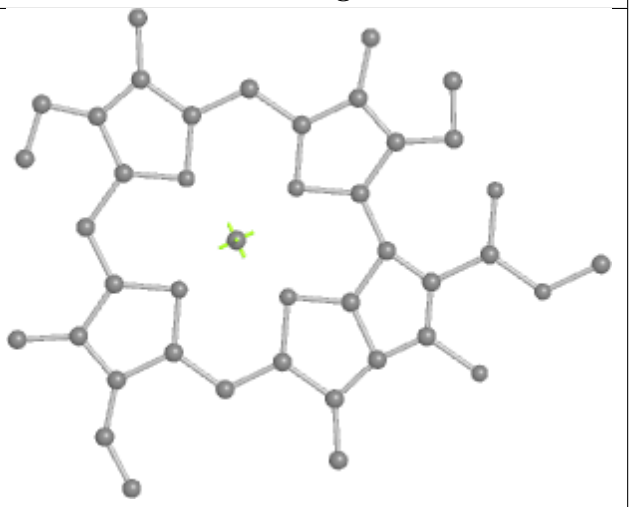
Bond lengths



Bond angles

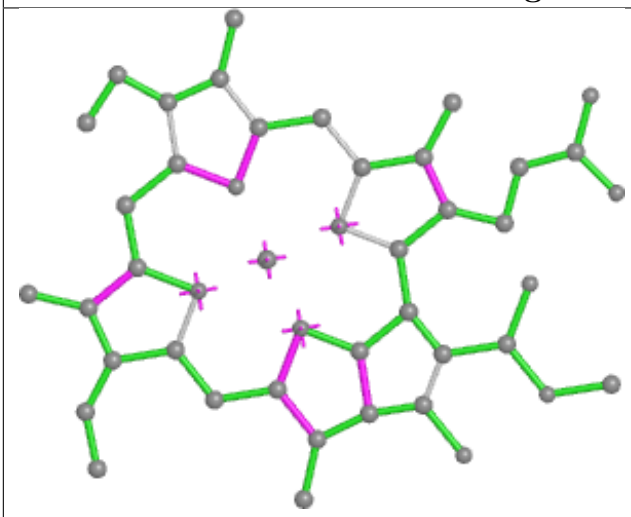


Torsions

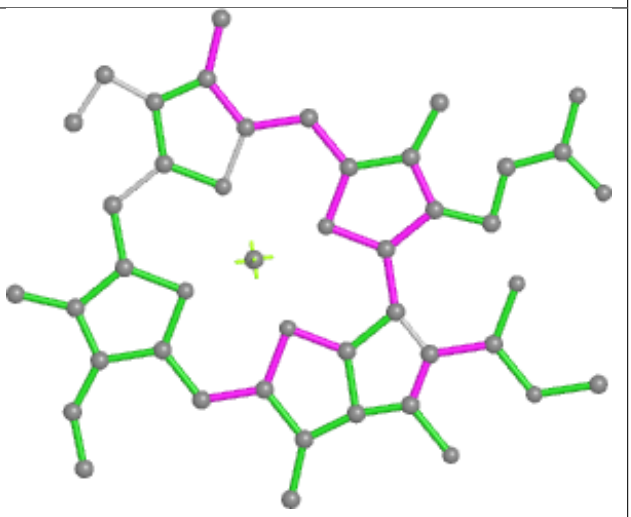


Rings

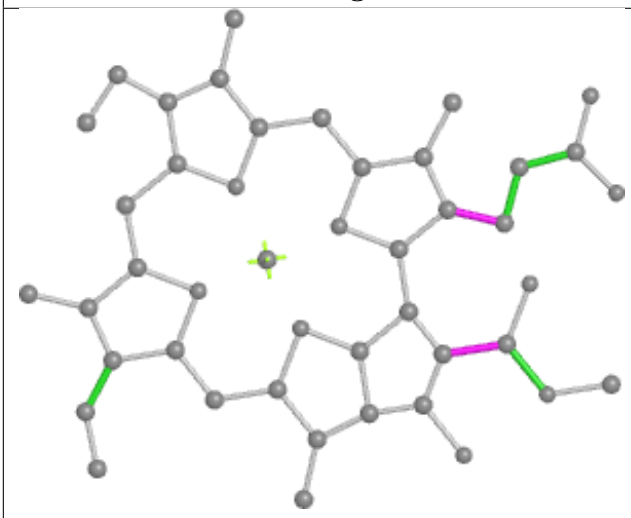
Ligand CLA B 806



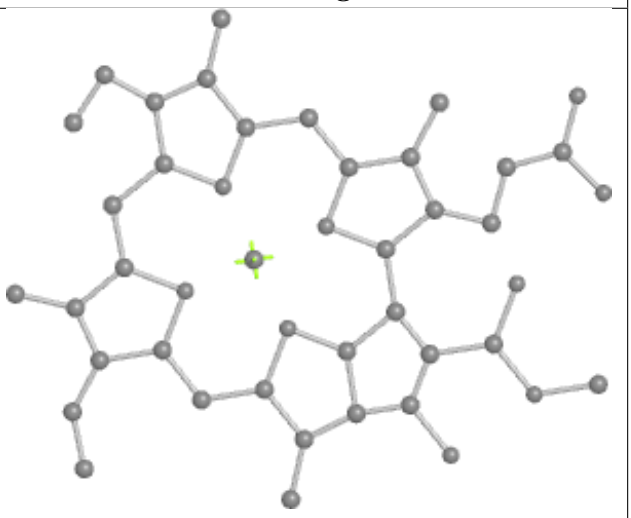
Bond lengths



Bond angles

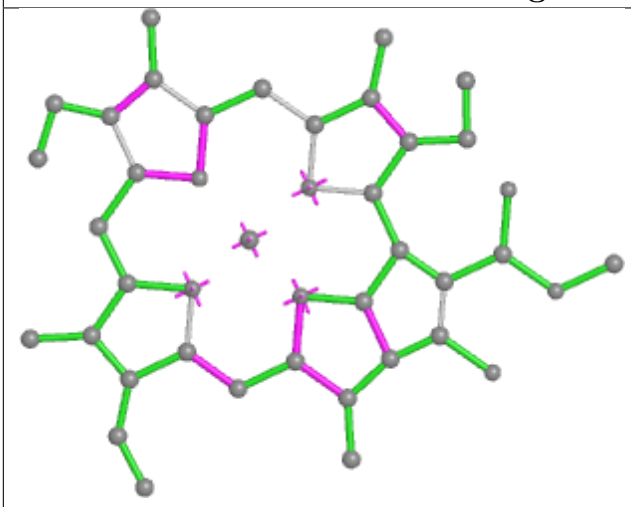


Torsions

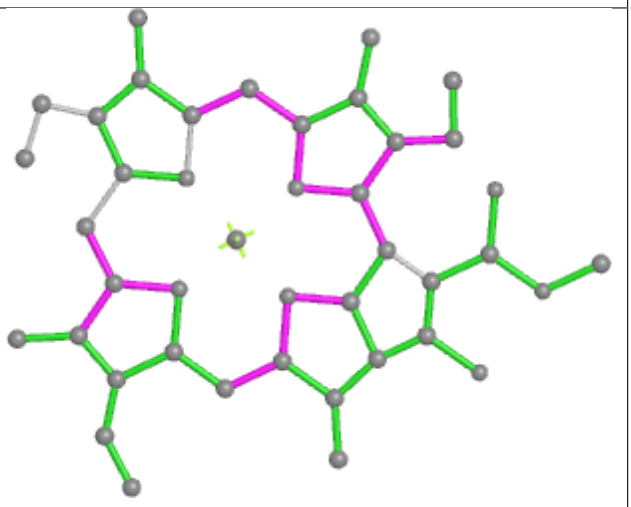


Rings

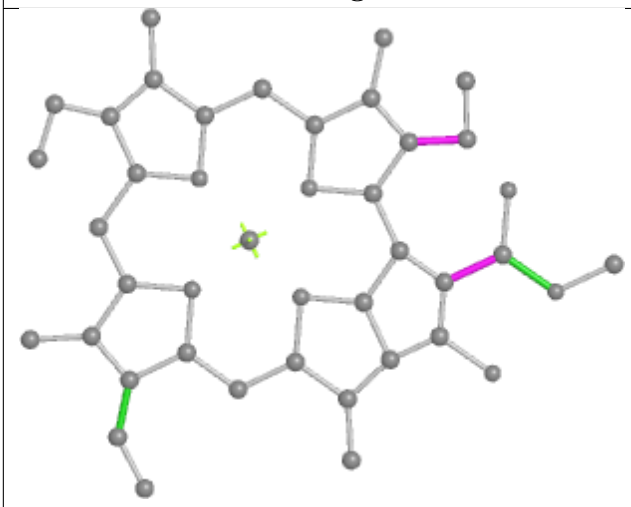
Ligand CLA 7 602



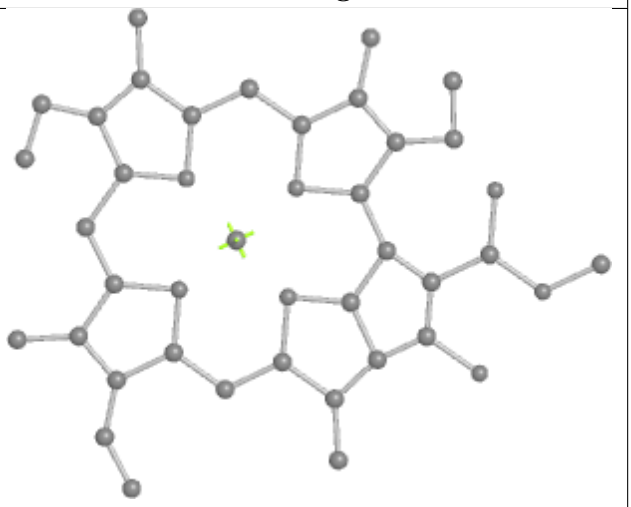
Bond lengths



Bond angles

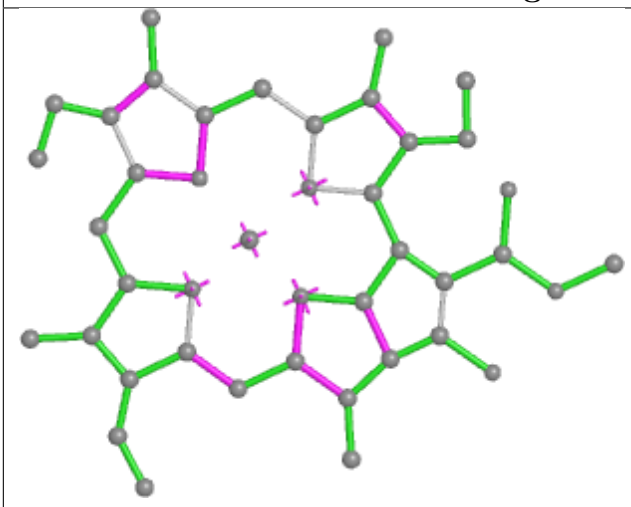


Torsions

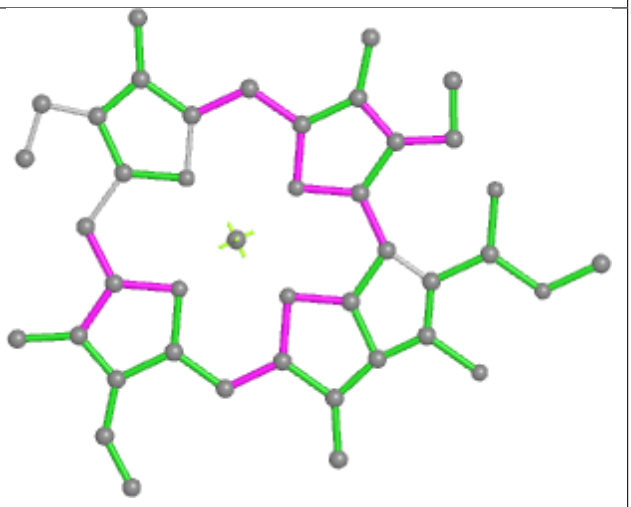


Rings

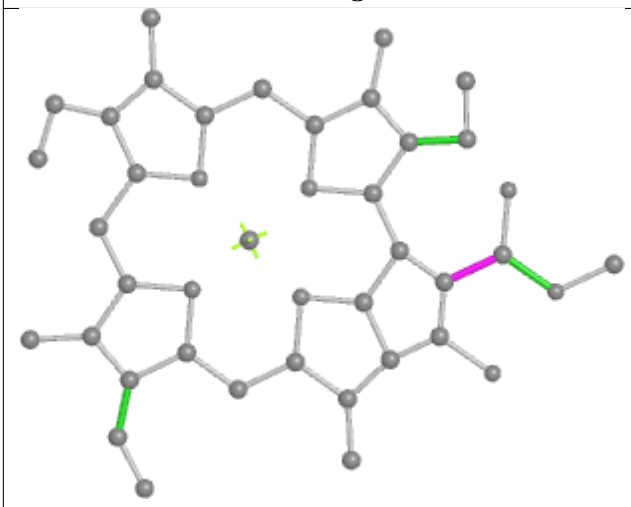
Ligand CLA A 839



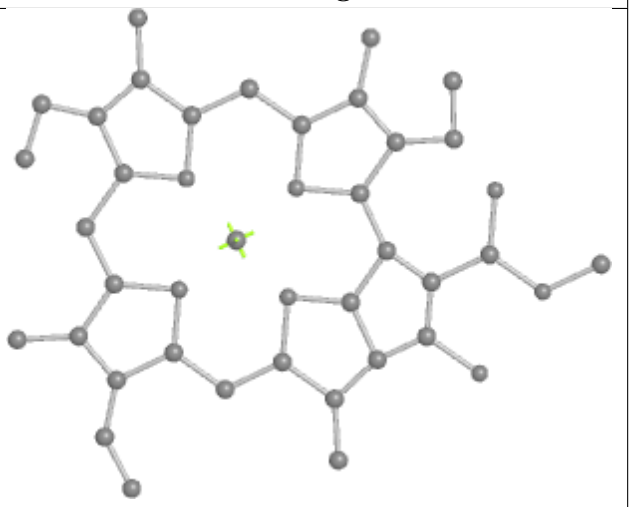
Bond lengths



Bond angles

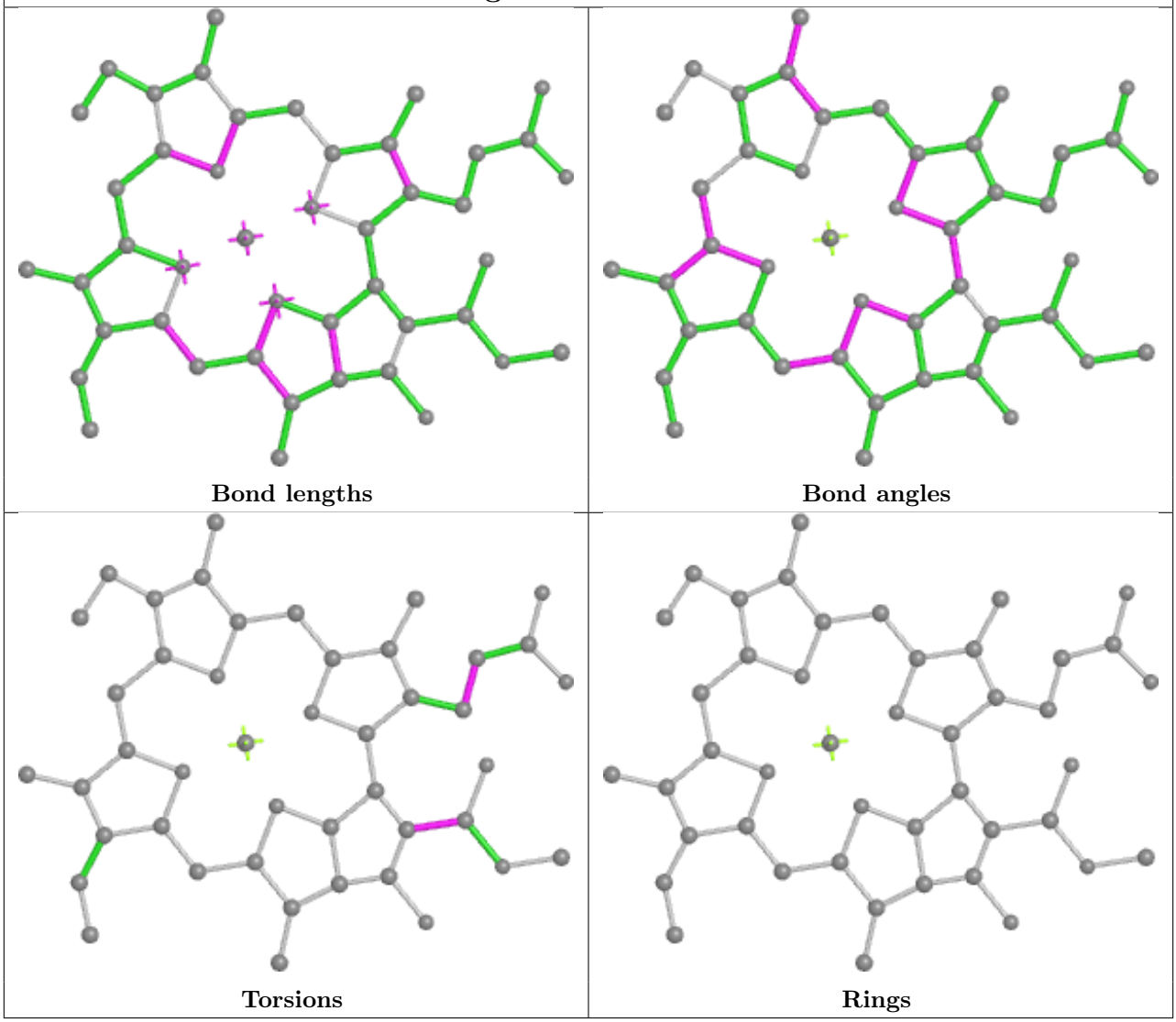


Torsions



Rings

Ligand CLA 6 317



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.

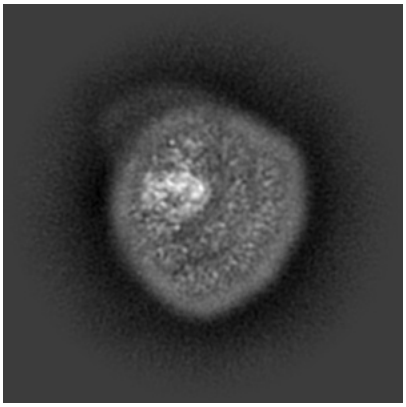
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-32907. These allow visual inspection of the internal detail of the map and identification of artifacts.

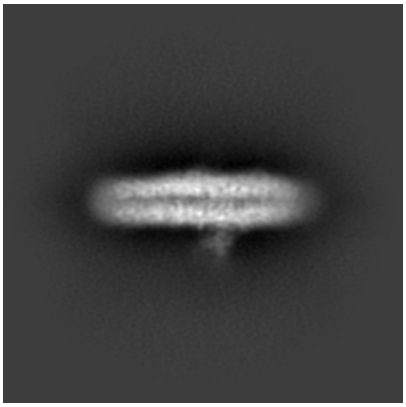
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

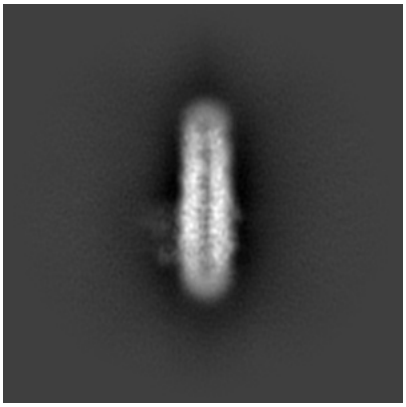
6.1.1 Primary map



X



Y

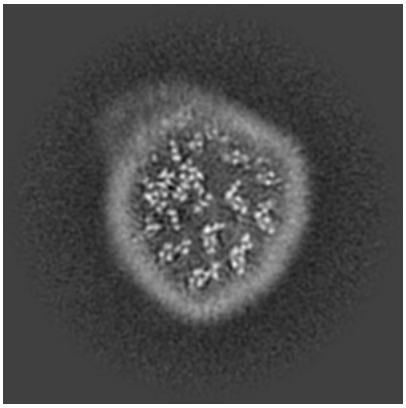


Z

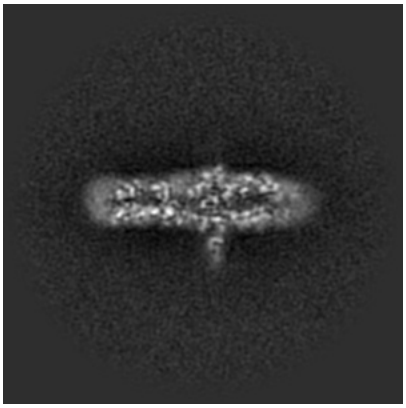
The images above show the map projected in three orthogonal directions.

6.2 Central slices

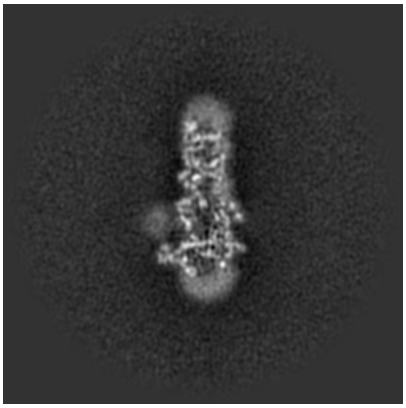
6.2.1 Primary map



X Index: 196



Y Index: 196

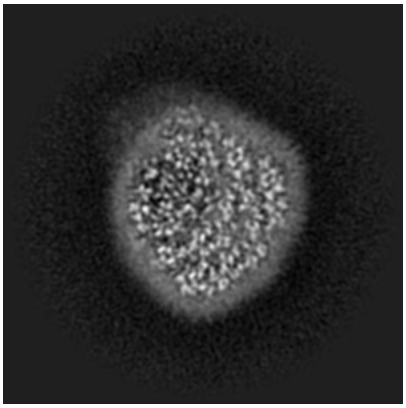


Z Index: 196

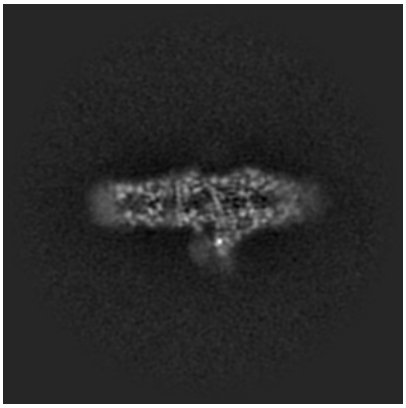
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

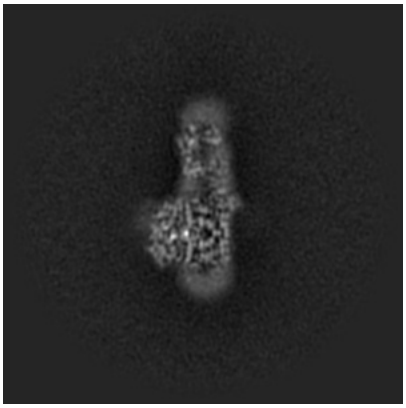
6.3.1 Primary map



X Index: 186



Y Index: 172

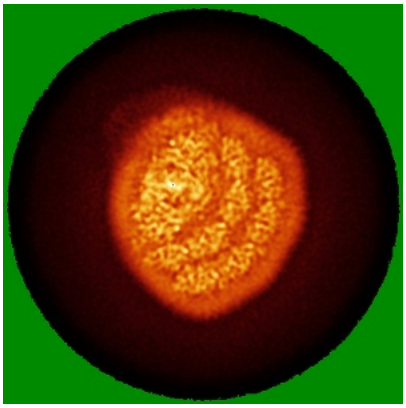


Z Index: 214

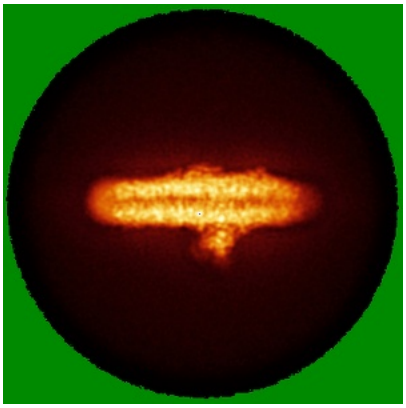
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) (i)

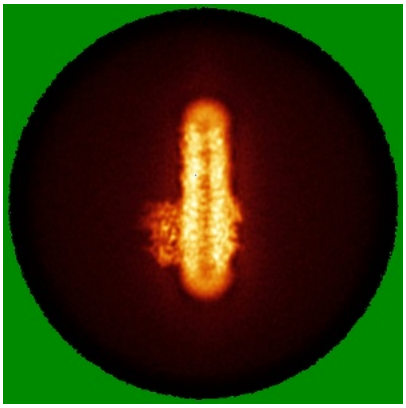
6.4.1 Primary map



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

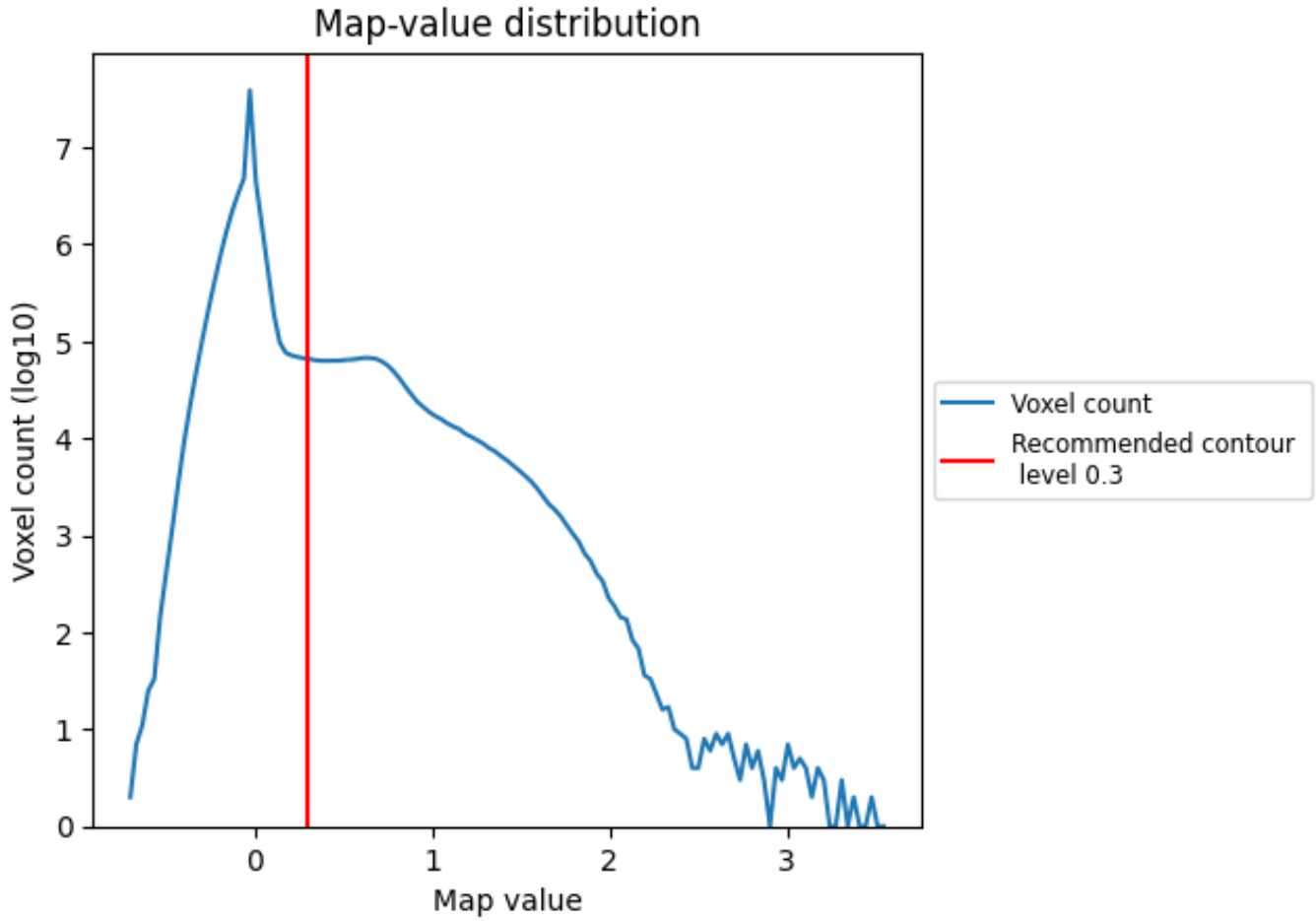
6.6 Mask visualisation (i)

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

7 Map analysis

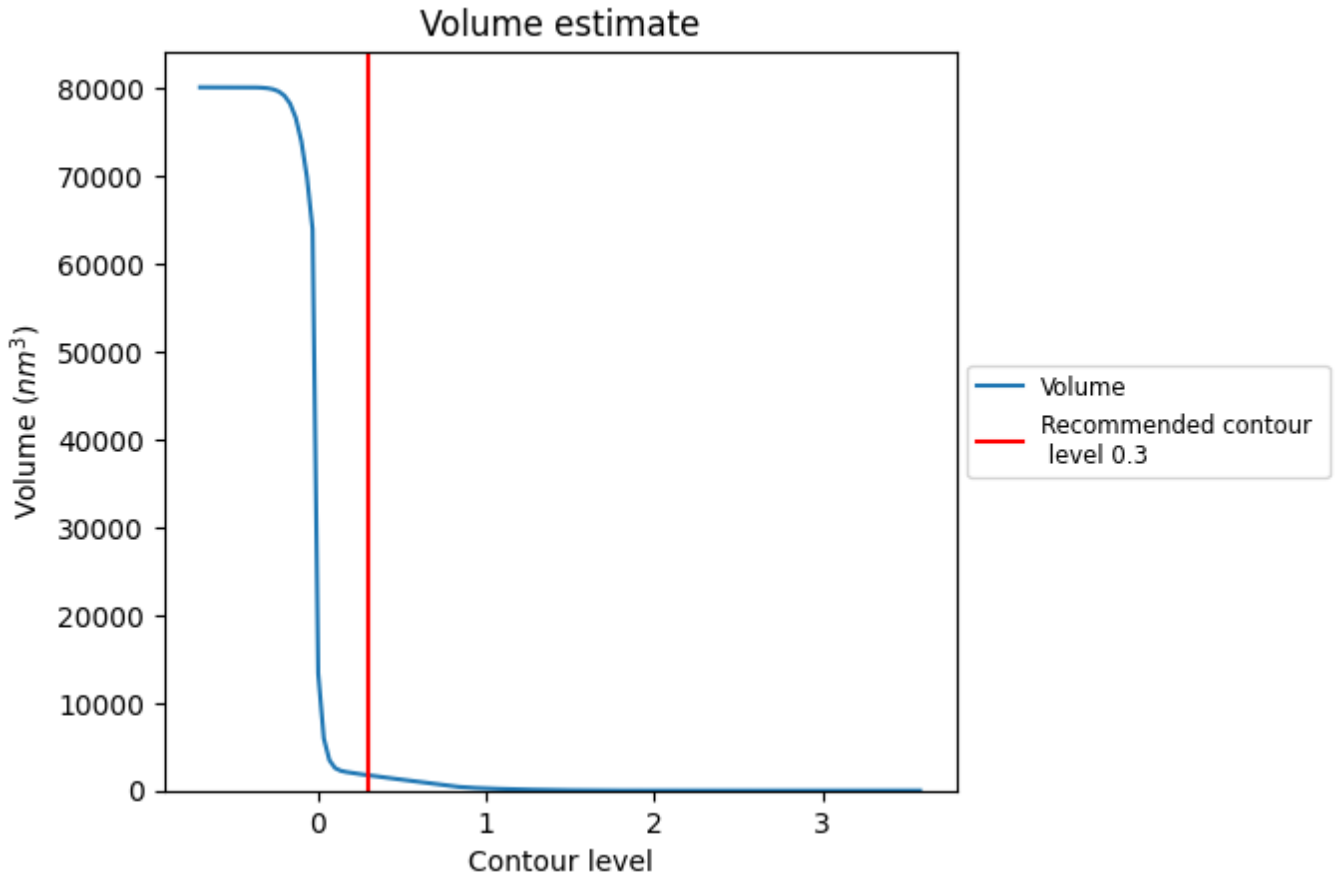
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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.

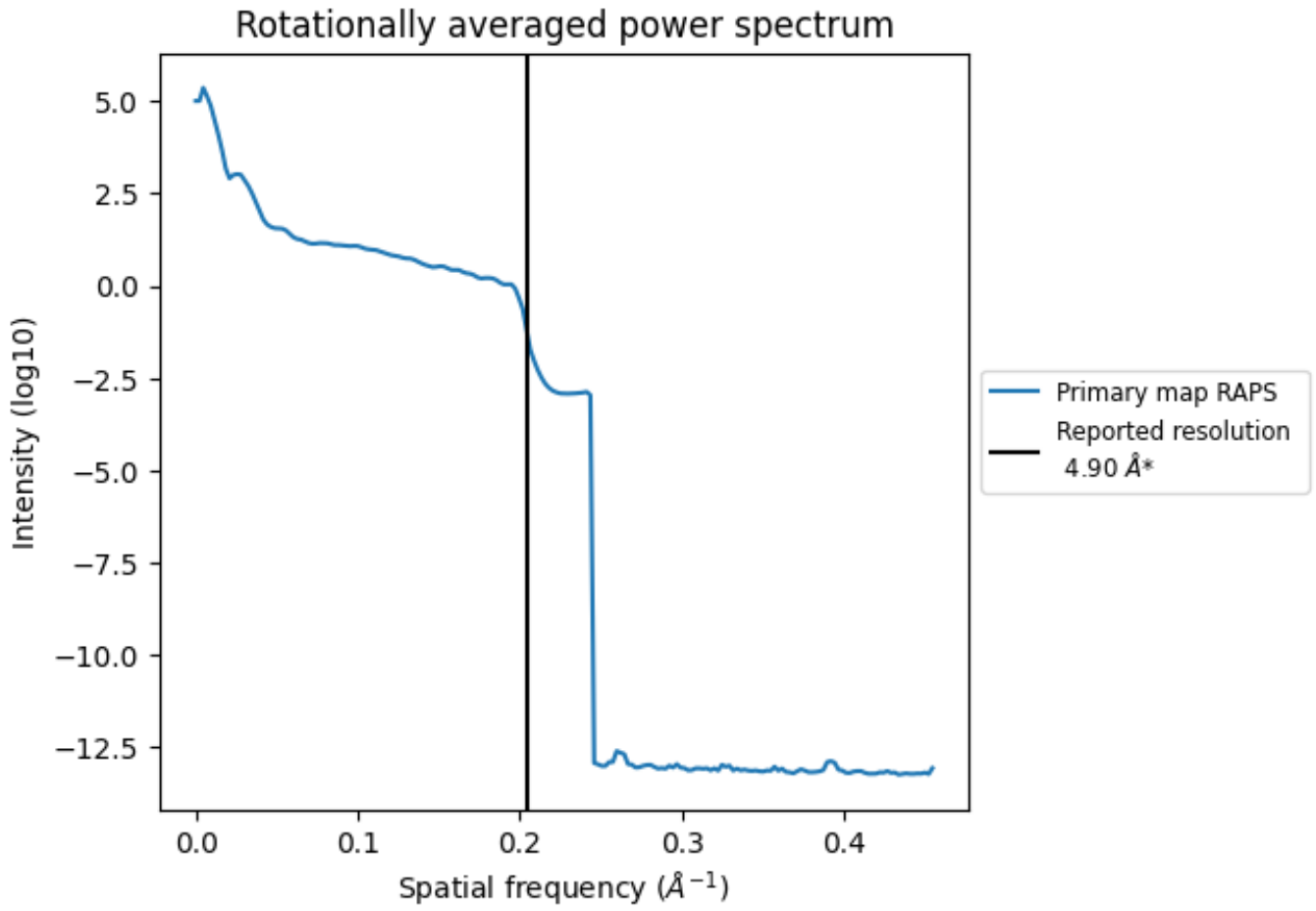
7.2 Volume estimate (i)



The volume at the recommended contour level is 1747 nm^3; this corresponds to an approximate mass of 1578 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 (i)

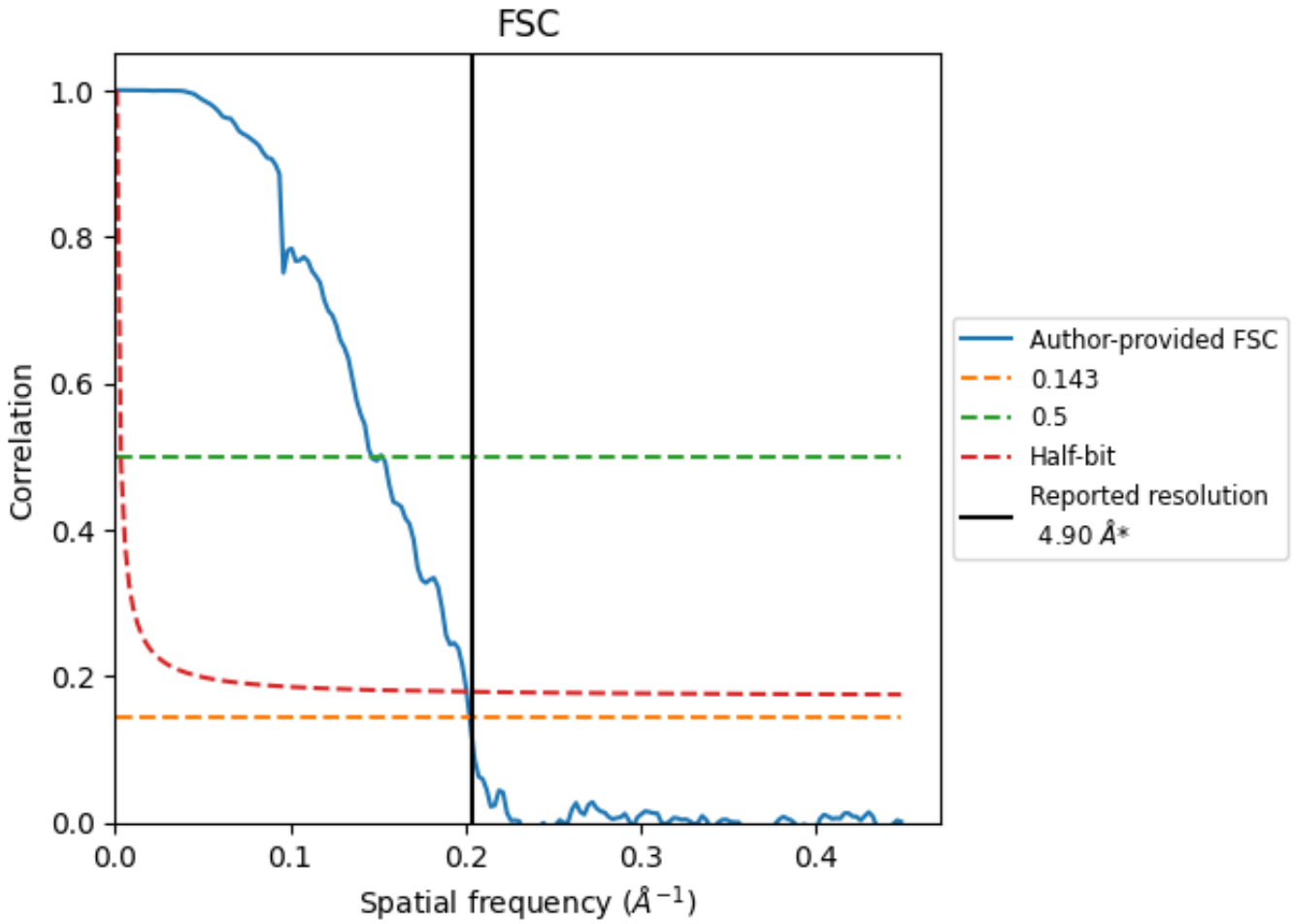


*Reported resolution corresponds to spatial frequency of 0.204 $Å^{-1}$

8 Fourier-Shell correlation

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



*Reported resolution corresponds to spatial frequency of 0.204 Å^{-1}

8.2 Resolution estimates (i)

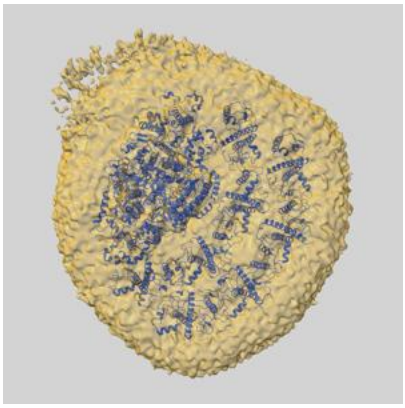
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.90	-	-
Author-provided FSC curve	4.94	6.82	4.98
Unmasked-calculated*	-	-	-

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

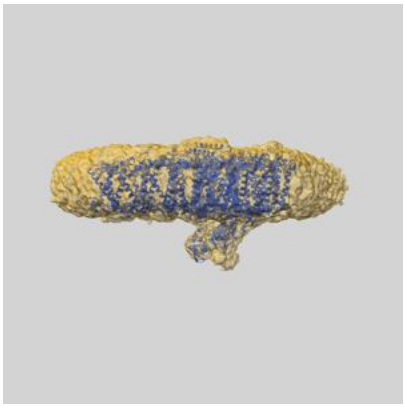
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-32907 and PDB model 7WZN. Per-residue inclusion information can be found in section 3 on page 25.

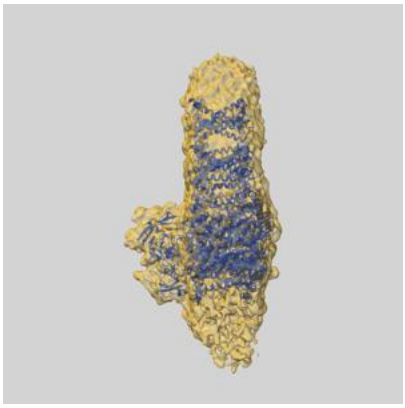
9.1 Map-model overlay



X



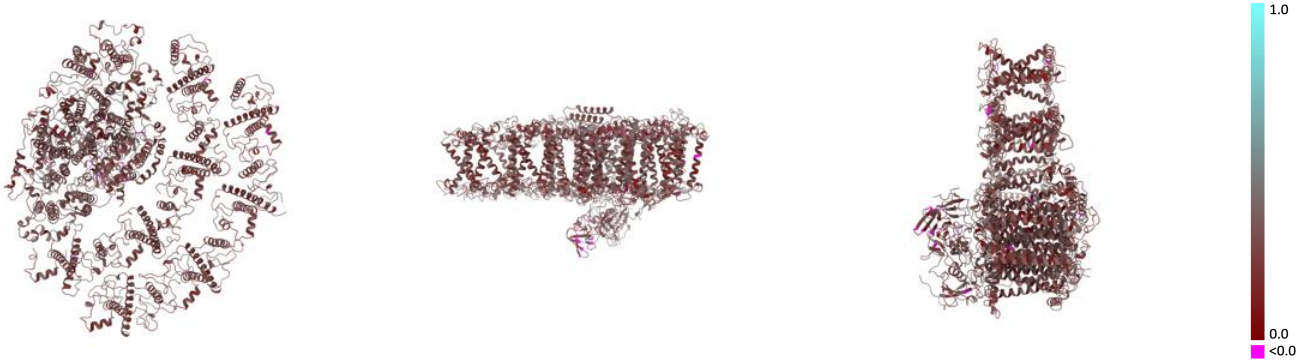
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.3 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model (i)

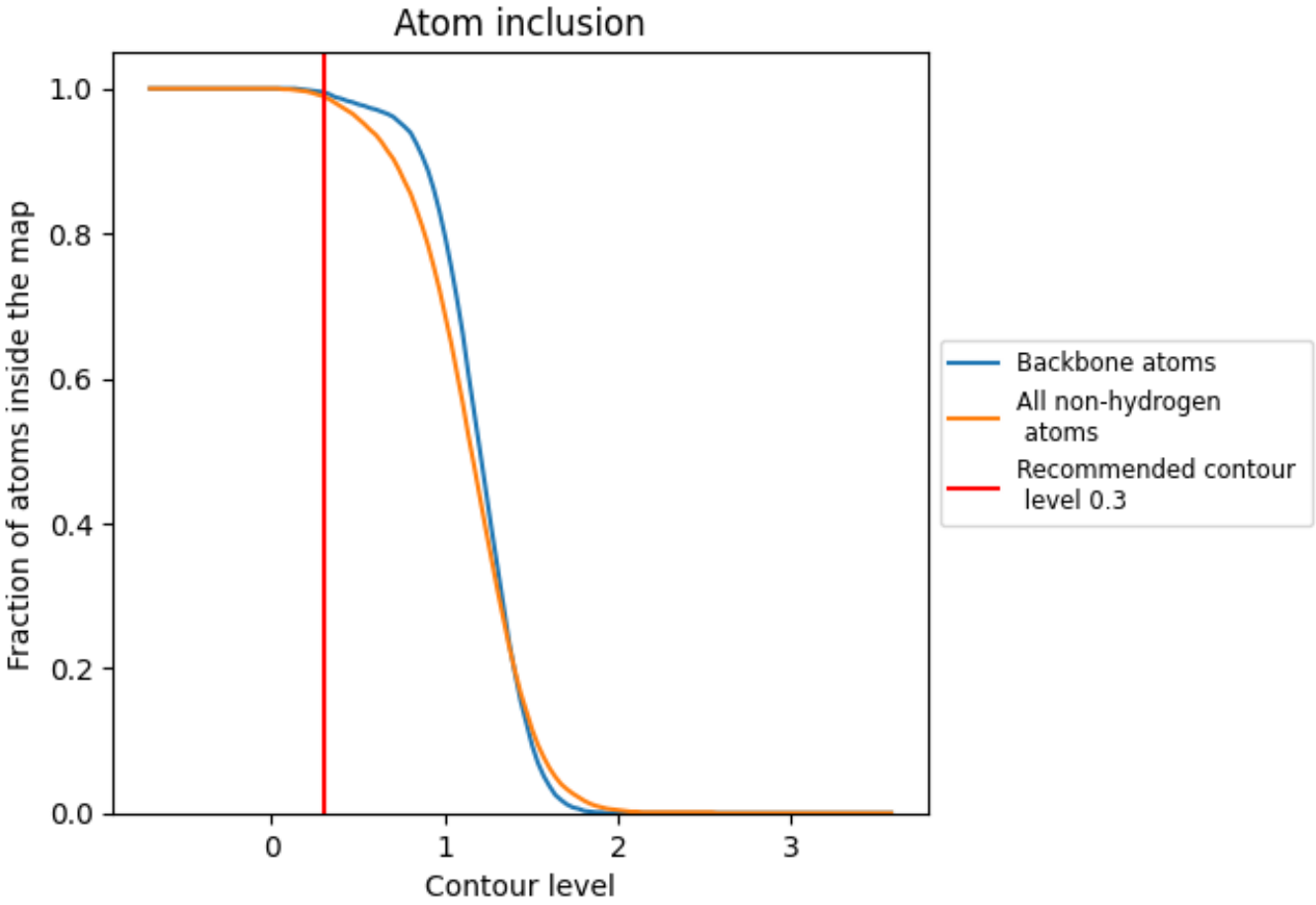


The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.3).

9.4 Atom inclusion (i)



At the recommended contour level, 100% of all backbone atoms, 99% 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 (0.3) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.9890	0.2950
1	0.9930	0.2740
3	0.9970	0.3020
4	0.9920	0.2710
5	0.9970	0.2920
6	0.9960	0.2900
7	0.9930	0.3080
8	0.9960	0.2980
A	0.9920	0.3100
B	0.9890	0.2970
C	1.0000	0.3050
D	1.0000	0.3520
E	1.0000	0.3480
F	0.9960	0.2970
G	0.7650	0.1610
J	1.0000	0.2920
Z	0.9990	0.2560