wwPDB EM Validation Summary Report

Nov 15, 2022 – 12:15 PM JST

PDB ID	:	6L35
EMDB ID	:	EMD-0821
Title	:	PSI-LHCI Supercomplex from Physcometrella patens
Authors	:	Zhao, L.; Yan, Q.J.; Qin, X.C.
Deposited on	:	2019-10-09
Resolution	:	3.23 Å(reported)

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:

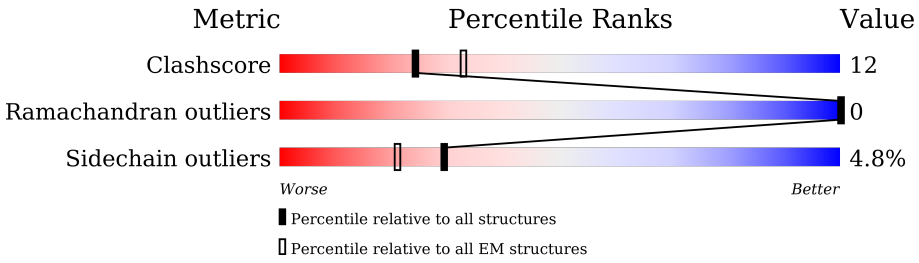
EMDB validation analysis	:	0.0.1.dev43
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.2

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 3.23 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	742	77% 22%
2	B	733	77% 22%
3	C	80	6% 70% 25% 5%
4	D	141	6% 83% 16%
5	E	62	13% 71% 27%
6	F	159	9% 74% 24%
7	G	98	24% 68% 28%
8	H	90	93% 79% 20%

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Mol	Chain	Length	Quality of chain
9	I	34	15% 68% 32%
10	J	41	10% 78% 22%
11	K	79	46% 65% 30% 5%
12	L	159	32% 73% 26%
13	M	29	10% 72% 24%
14	2	210	14% 77% 20%
15	6	192	27% 69% 29%
16	3	213	21% 71% 28%
17	5	205	26% 63% 34%

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
18	CLA	2	602	X	-	-	-
18	CLA	2	603	X	-	-	-
18	CLA	2	604	X	-	-	-
18	CLA	2	609	X	-	-	-
18	CLA	2	610	X	-	-	-
18	CLA	2	611	X	-	-	-
18	CLA	2	612	X	-	-	-
18	CLA	2	613	X	-	-	-
18	CLA	2	614	X	-	-	-
18	CLA	3	602	X	-	-	-
18	CLA	3	603	X	-	-	-
18	CLA	3	604	X	-	-	-
18	CLA	3	606	X	-	-	-
18	CLA	3	607	X	-	-	-
18	CLA	3	609	X	-	-	-
18	CLA	3	610	X	-	-	-
18	CLA	3	611	X	-	-	-
18	CLA	3	612	X	-	-	-
18	CLA	3	613	X	-	-	-
18	CLA	3	614	X	-	-	-
18	CLA	3	615	X	-	-	-
18	CLA	3	617	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
18	CLA	5	601	X	-	-	-
18	CLA	5	602	X	-	-	-
18	CLA	5	603	X	-	-	-
18	CLA	5	604	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	6	602	X	-	-	-
18	CLA	6	603	X	-	-	-
18	CLA	6	604	X	-	-	-
18	CLA	6	606	X	-	-	-
18	CLA	6	608	X	-	-	-
18	CLA	6	609	X	-	-	-
18	CLA	6	610	X	-	-	-
18	CLA	6	611	X	-	-	-
18	CLA	6	612	X	-	-	-
18	CLA	6	613	X	-	-	-
18	CLA	6	614	X	-	-	-
18	CLA	6	616	X	-	-	-
18	CLA	A	801	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	-	-	-
18	CLA	A	819	X	-	-	-
18	CLA	A	820	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
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	842	X	-	-	-
18	CLA	A	843	X	-	-	-
18	CLA	A	845	X	-	-	-
18	CLA	A	854	X	-	-	-
18	CLA	B	802	X	-	-	-
18	CLA	B	803	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	-	-	-
18	CLA	B	818	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
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	F	301	X	-	-	-
18	CLA	F	303	X	-	-	-
18	CLA	F	304	X	-	-	-
18	CLA	F	305	X	-	-	-
18	CLA	G	201	X	-	-	-
18	CLA	G	203	X	-	-	-
18	CLA	G	204	X	-	-	-
18	CLA	J	101	X	-	-	-
18	CLA	K	201	X	-	-	-
18	CLA	K	203	X	-	-	-
18	CLA	K	204	X	-	-	-
18	CLA	K	206	X	-	-	-
18	CLA	L	302	X	-	-	-
18	CLA	L	303	X	-	-	-
18	CLA	L	304	X	-	-	-
22	SF4	C	101	-	-	X	-
22	SF4	C	102	-	-	X	-
25	CHL	2	601	X	-	-	-
25	CHL	2	606	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
25	CHL	2	607	X	-	-	-
25	CHL	2	608	X	-	-	-
25	CHL	2	616	X	-	-	-
25	CHL	3	608	X	-	-	-
25	CHL	5	606	X	-	-	-
25	CHL	5	607	X	-	-	-
25	CHL	5	608	X	-	-	-
25	CHL	5	615	X	-	-	-
25	CHL	6	601	X	-	-	-
25	CHL	6	607	X	-	-	-
27	XAT	2	620	-	-	X	-
27	XAT	5	620	-	-	X	-

2 Entry composition (i)

There are 27 unique types of molecules in this entry. The entry contains 34822 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	S		
1	A	742	5837	3827	993	998	19	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	S		
2	B	733	5849	3839	996	998	16	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	C	80	595	365	103	116	11	0	0

- Molecule 4 is a protein called Predicted protein PsaD.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	D	141	1104	707	196	198	3	0	0

- Molecule 5 is a protein called PsaE.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
5	E	62	487	309	87	91	0	0

- Molecule 6 is a protein called PSI-F.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	F	159	1226	793	209	221	3	0	0

- Molecule 7 is a protein called Predicted protein PsaG.

Mol	Chain	Residues	Atoms				AltConf	Trace
7	G	98	Total	C	N	O	0	0
			749	483	128	138		

- Molecule 8 is a protein called PsaH photosystem I reaction center subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	H	90	Total	C	N	O	S	0	0
			693	445	117	130	1		

- Molecule 9 is a protein called Photosystem I reaction center subunit VIII.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	I	34	Total	C	N	O	S	0	0
			266	181	35	48	2		

- Molecule 10 is a protein called Photosystem I reaction center subunit IX.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	J	41	Total	C	N	O	S	0	0
			325	222	48	54	1		

- Molecule 11 is a protein called PsaK.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	K	79	Total	C	N	O	S	0	0
			550	346	96	105	3		

- Molecule 12 is a protein called PSI subunit V.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	L	159	Total	C	N	O	S	0	0
			1189	781	192	214	2		

- Molecule 13 is a protein called Photosystem I reaction center subunit XII.

Mol	Chain	Residues	Atoms				AltConf	Trace
13	M	29	Total	C	N	O	0	0
			214	141	34	39		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
14	2	206	Total	C	N	O	S	0	0
			1595	1039	267	285	4		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
15	6	192	Total	C	N	O	S	0	0
			1473	961	247	264	1		

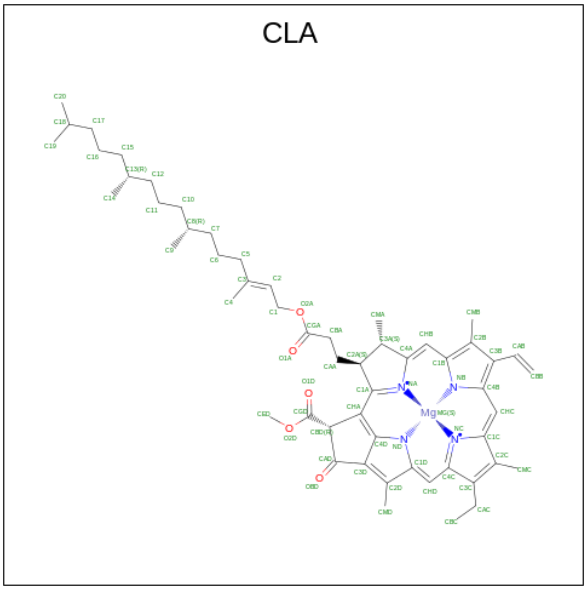
- Molecule 16 is a protein called Chlorophyll a-b binding protein, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	3	213	Total	C	N	O	S	0	0
			1644	1076	265	296	7		

- Molecule 17 is a protein called Chlorophyll a-b binding protein, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	5	202	Total	C	N	O	S	0	0
			1566	1020	258	282	6		

- Molecule 18 is CHLOROPHYLL A (three-letter code: CLA) (formula: $C_{55}H_{72}MgN_4O_5$).



Mol	Chain	Residues	Atoms					AltConf
18	A	1	Total	C	Mg	N	O	0
			2421	1977	45	180	219	

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Mol	Chain	Residues	Atoms					AltConf
18	A	1	Total 2421	C 1977	Mg 45	N 180	O 219	0
18	A	1	Total 2421	C 1977	Mg 45	N 180	O 219	0
18	A	1	Total 2421	C 1977	Mg 45	N 180	O 219	0
18	A	1	Total 2421	C 1977	Mg 45	N 180	O 219	0
18	A	1	Total 2421	C 1977	Mg 45	N 180	O 219	0
18	A	1	Total 2421	C 1977	Mg 45	N 180	O 219	0
18	A	1	Total 2421	C 1977	Mg 45	N 180	O 219	0
18	A	1	Total 2421	C 1977	Mg 45	N 180	O 219	0
18	A	1	Total 2421	C 1977	Mg 45	N 180	O 219	0
18	A	1	Total 2421	C 1977	Mg 45	N 180	O 219	0
18	A	1	Total 2421	C 1977	Mg 45	N 180	O 219	0
18	A	1	Total 2421	C 1977	Mg 45	N 180	O 219	0
18	A	1	Total 2421	C 1977	Mg 45	N 180	O 219	0
18	A	1	Total 2421	C 1977	Mg 45	N 180	O 219	0
18	A	1	Total 2421	C 1977	Mg 45	N 180	O 219	0
18	A	1	Total 2421	C 1977	Mg 45	N 180	O 219	0
18	A	1	Total 2421	C 1977	Mg 45	N 180	O 219	0
18	A	1	Total 2421	C 1977	Mg 45	N 180	O 219	0
18	A	1	Total 2421	C 1977	Mg 45	N 180	O 219	0
18	A	1	Total 2421	C 1977	Mg 45	N 180	O 219	0
18	A	1	Total 2421	C 1977	Mg 45	N 180	O 219	0

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Mol	Chain	Residues	Atoms					AltConf
18	A	1	Total 2421	C 1977	Mg 45	N 180	O 219	0
18	A	1	Total 2421	C 1977	Mg 45	N 180	O 219	0
18	A	1	Total 2421	C 1977	Mg 45	N 180	O 219	0
18	A	1	Total 2421	C 1977	Mg 45	N 180	O 219	0
18	A	1	Total 2421	C 1977	Mg 45	N 180	O 219	0
18	A	1	Total 2421	C 1977	Mg 45	N 180	O 219	0
18	A	1	Total 2421	C 1977	Mg 45	N 180	O 219	0
18	A	1	Total 2421	C 1977	Mg 45	N 180	O 219	0
18	A	1	Total 2421	C 1977	Mg 45	N 180	O 219	0
18	A	1	Total 2421	C 1977	Mg 45	N 180	O 219	0
18	A	1	Total 2421	C 1977	Mg 45	N 180	O 219	0
18	A	1	Total 2421	C 1977	Mg 45	N 180	O 219	0
18	A	1	Total 2421	C 1977	Mg 45	N 180	O 219	0
18	A	1	Total 2421	C 1977	Mg 45	N 180	O 219	0
18	A	1	Total 2421	C 1977	Mg 45	N 180	O 219	0
18	A	1	Total 2421	C 1977	Mg 45	N 180	O 219	0
18	A	1	Total 2421	C 1977	Mg 45	N 180	O 219	0
18	A	1	Total 2421	C 1977	Mg 45	N 180	O 219	0
18	A	1	Total 2421	C 1977	Mg 45	N 180	O 219	0
18	A	1	Total 2421	C 1977	Mg 45	N 180	O 219	0
18	A	1	Total 2421	C 1977	Mg 45	N 180	O 219	0

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Mol	Chain	Residues	Atoms					AltConf
18	A	1	Total 2421	C 1977	Mg 45	N 180	O 219	0
18	A	1	Total 2421	C 1977	Mg 45	N 180	O 219	0
18	B	1	Total 2093	C 1697	Mg 40	N 160	O 196	0
18	B	1	Total 2093	C 1697	Mg 40	N 160	O 196	0
18	B	1	Total 2093	C 1697	Mg 40	N 160	O 196	0
18	B	1	Total 2093	C 1697	Mg 40	N 160	O 196	0
18	B	1	Total 2093	C 1697	Mg 40	N 160	O 196	0
18	B	1	Total 2093	C 1697	Mg 40	N 160	O 196	0
18	B	1	Total 2093	C 1697	Mg 40	N 160	O 196	0
18	B	1	Total 2093	C 1697	Mg 40	N 160	O 196	0
18	B	1	Total 2093	C 1697	Mg 40	N 160	O 196	0
18	B	1	Total 2093	C 1697	Mg 40	N 160	O 196	0
18	B	1	Total 2093	C 1697	Mg 40	N 160	O 196	0
18	B	1	Total 2093	C 1697	Mg 40	N 160	O 196	0
18	B	1	Total 2093	C 1697	Mg 40	N 160	O 196	0
18	B	1	Total 2093	C 1697	Mg 40	N 160	O 196	0
18	B	1	Total 2093	C 1697	Mg 40	N 160	O 196	0
18	B	1	Total 2093	C 1697	Mg 40	N 160	O 196	0
18	B	1	Total 2093	C 1697	Mg 40	N 160	O 196	0
18	B	1	Total 2093	C 1697	Mg 40	N 160	O 196	0
18	B	1	Total 2093	C 1697	Mg 40	N 160	O 196	0

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Mol	Chain	Residues	Atoms	AltConf
18	B	1	Total C Mg N O 2093 1697 40 160 196	0
18	B	1	Total C Mg N O 2093 1697 40 160 196	0
18	B	1	Total C Mg N O 2093 1697 40 160 196	0
18	B	1	Total C Mg N O 2093 1697 40 160 196	0
18	B	1	Total C Mg N O 2093 1697 40 160 196	0
18	B	1	Total C Mg N O 2093 1697 40 160 196	0
18	B	1	Total C Mg N O 2093 1697 40 160 196	0
18	B	1	Total C Mg N O 2093 1697 40 160 196	0
18	B	1	Total C Mg N O 2093 1697 40 160 196	0
18	B	1	Total C Mg N O 2093 1697 40 160 196	0
18	B	1	Total C Mg N O 2093 1697 40 160 196	0
18	B	1	Total C Mg N O 2093 1697 40 160 196	0
18	B	1	Total C Mg N O 2093 1697 40 160 196	0
18	B	1	Total C Mg N O 2093 1697 40 160 196	0
18	B	1	Total C Mg N O 2093 1697 40 160 196	0
18	B	1	Total C Mg N O 2093 1697 40 160 196	0
18	B	1	Total C Mg N O 2093 1697 40 160 196	0
18	B	1	Total C Mg N O 2093 1697 40 160 196	0
18	B	1	Total C Mg N O 2093 1697 40 160 196	0
18	B	1	Total C Mg N O 2093 1697 40 160 196	0
18	B	1	Total C Mg N O 2093 1697 40 160 196	0

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Mol	Chain	Residues	Atoms	AltConf
18	F	1	Total C Mg N O 176 138 4 16 18	0
18	F	1	Total C Mg N O 176 138 4 16 18	0
18	F	1	Total C Mg N O 176 138 4 16 18	0
18	F	1	Total C Mg N O 176 138 4 16 18	0
18	G	1	Total C Mg N O 139 109 3 12 15	0
18	G	1	Total C Mg N O 139 109 3 12 15	0
18	G	1	Total C Mg N O 139 109 3 12 15	0
18	J	1	Total C Mg N O 42 34 1 4 3	0
18	K	1	Total C Mg N O 180 140 4 16 20	0
18	K	1	Total C Mg N O 180 140 4 16 20	0
18	K	1	Total C Mg N O 180 140 4 16 20	0
18	K	1	Total C Mg N O 180 140 4 16 20	0
18	L	1	Total C Mg N O 132 104 3 12 13	0
18	L	1	Total C Mg N O 132 104 3 12 13	0
18	L	1	Total C Mg N O 132 104 3 12 13	0
18	2	1	Total C Mg N O 410 326 9 36 39	0
18	2	1	Total C Mg N O 410 326 9 36 39	0
18	2	1	Total C Mg N O 410 326 9 36 39	0
18	2	1	Total C Mg N O 410 326 9 36 39	0
18	2	1	Total C Mg N O 410 326 9 36 39	0
18	2	1	Total C Mg N O 410 326 9 36 39	0

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Mol	Chain	Residues	Atoms					AltConf
18	2	1	Total 410	C 326	Mg 9	N 36	O 39	0
18	2	1	Total 410	C 326	Mg 9	N 36	O 39	0
18	2	1	Total 410	C 326	Mg 9	N 36	O 39	0
18	6	1	Total 525	C 413	Mg 12	N 48	O 52	0
18	6	1	Total 525	C 413	Mg 12	N 48	O 52	0
18	6	1	Total 525	C 413	Mg 12	N 48	O 52	0
18	6	1	Total 525	C 413	Mg 12	N 48	O 52	0
18	6	1	Total 525	C 413	Mg 12	N 48	O 52	0
18	6	1	Total 525	C 413	Mg 12	N 48	O 52	0
18	6	1	Total 525	C 413	Mg 12	N 48	O 52	0
18	6	1	Total 525	C 413	Mg 12	N 48	O 52	0
18	6	1	Total 525	C 413	Mg 12	N 48	O 52	0
18	6	1	Total 525	C 413	Mg 12	N 48	O 52	0
18	6	1	Total 525	C 413	Mg 12	N 48	O 52	0
18	6	1	Total 525	C 413	Mg 12	N 48	O 52	0
18	3	1	Total 577	C 465	Mg 13	N 52	O 47	0
18	3	1	Total 577	C 465	Mg 13	N 52	O 47	0
18	3	1	Total 577	C 465	Mg 13	N 52	O 47	0
18	3	1	Total 577	C 465	Mg 13	N 52	O 47	0
18	3	1	Total 577	C 465	Mg 13	N 52	O 47	0
18	3	1	Total 577	C 465	Mg 13	N 52	O 47	0

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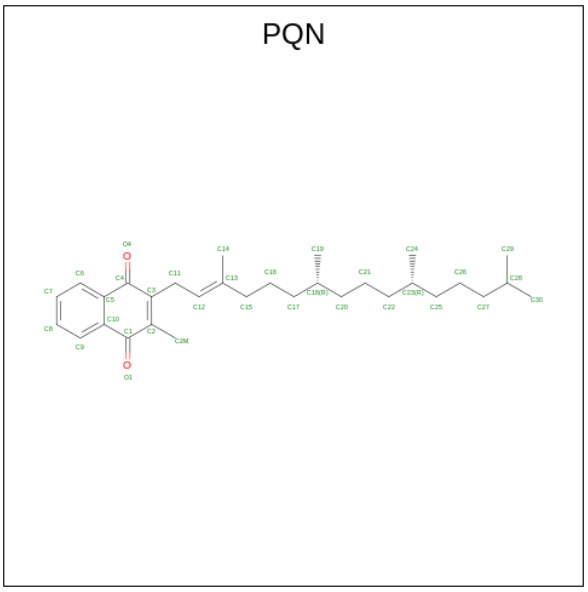
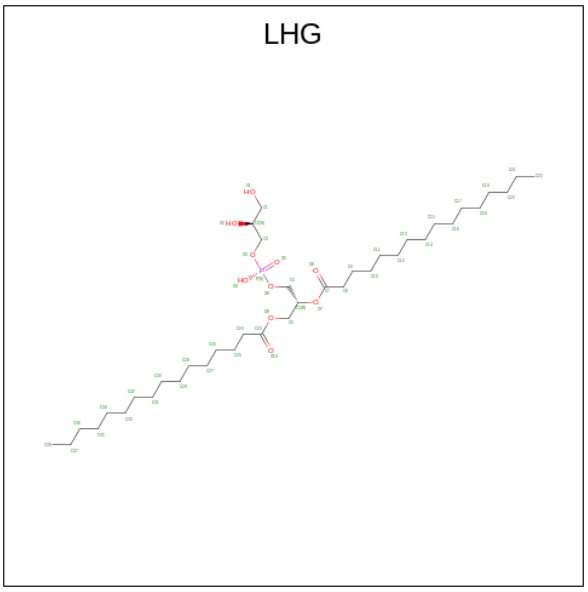
Mol	Chain	Residues	Atoms	AltConf
18	3	1	Total C Mg N O 577 465 13 52 47	0
18	3	1	Total C Mg N O 577 465 13 52 47	0
18	3	1	Total C Mg N O 577 465 13 52 47	0
18	3	1	Total C Mg N O 577 465 13 52 47	0
18	3	1	Total C Mg N O 577 465 13 52 47	0
18	3	1	Total C Mg N O 577 465 13 52 47	0
18	3	1	Total C Mg N O 577 465 13 52 47	0
18	5	1	Total C Mg N O 445 351 10 40 44	0
18	5	1	Total C Mg N O 445 351 10 40 44	0
18	5	1	Total C Mg N O 445 351 10 40 44	0
18	5	1	Total C Mg N O 445 351 10 40 44	0
18	5	1	Total C Mg N O 445 351 10 40 44	0
18	5	1	Total C Mg N O 445 351 10 40 44	0
18	5	1	Total C Mg N O 445 351 10 40 44	0
18	5	1	Total C Mg N O 445 351 10 40 44	0
18	5	1	Total C Mg N O 445 351 10 40 44	0
18	5	1	Total C Mg N O 445 351 10 40 44	0

- Molecule 19 is PHYLLOQUINONE (three-letter code: PQN) (formula: $C_{31}H_{46}O_2$).



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 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (three-letter code: LHG) (formula: $C_{38}H_{75}O_{10}P$).



Mol	Chain	Residues	Atoms				AltConf
20	A	1	Total	C	O	P	0
			76	54	20	2	

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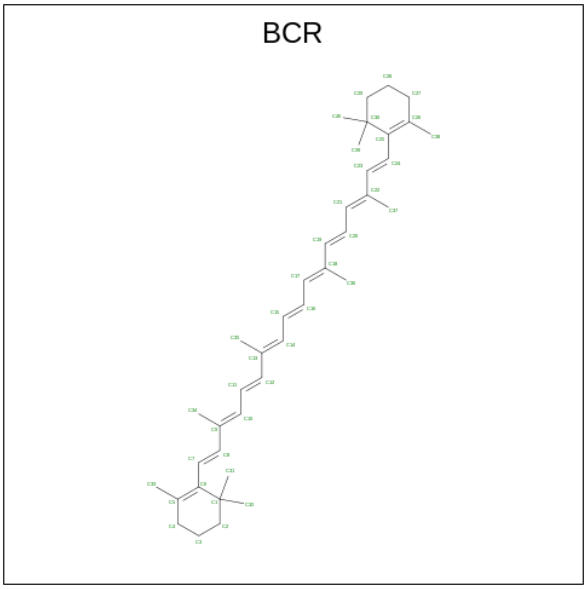
Mol	Chain	Residues	Atoms				AltConf
20	A	1	Total	C	O	P	0
			76	54	20	2	
20	B	1	Total	C	O	P	0
			23	12	10	1	
20	2	1	Total	C	O	P	0
			35	24	10	1	
20	6	1	Total	C	O	P	0
			28	17	10	1	
20	5	1	Total	C	O	P	0
			37	26	10	1	

- Molecule 21 is BETA-CAROTENE (three-letter code: BCR) (formula: $C_{40}H_{56}$).



Mol	Chain	Residues	Atoms		AltConf
21	A	1	Total	C	0
			240	240	
21	A	1	Total	C	0
			240	240	
21	A	1	Total	C	0
			240	240	
21	A	1	Total	C	0
			240	240	
21	A	1	Total	C	0
			240	240	
21	A	1	Total	C	0
			240	240	

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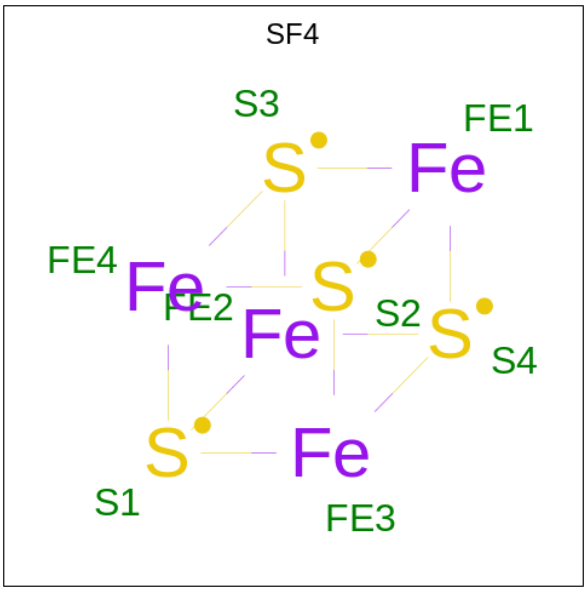
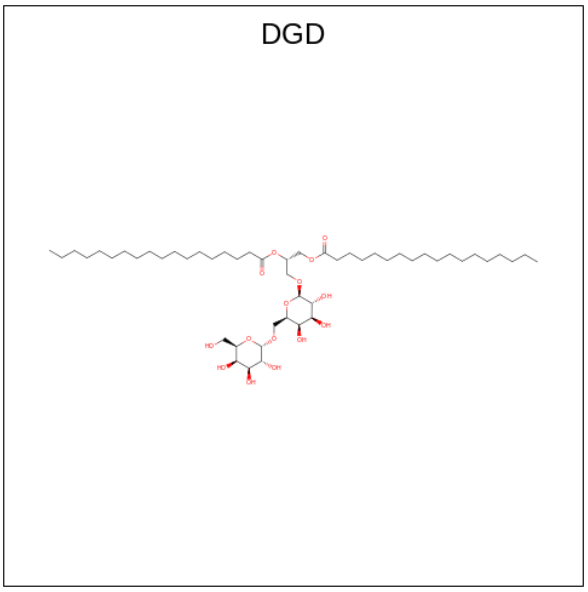
Mol	Chain	Residues	Atoms	AltConf
21	B	1	Total C 280 280	0
21	B	1	Total C 280 280	0
21	B	1	Total C 280 280	0
21	B	1	Total C 280 280	0
21	B	1	Total C 280 280	0
21	B	1	Total C 280 280	0
21	B	1	Total C 280 280	0
21	F	1	Total C 40 40	0
21	G	1	Total C 40 40	0
21	I	1	Total C 40 40	0
21	J	1	Total C 80 80	0
21	J	1	Total C 80 80	0
21	K	1	Total C 80 80	0
21	K	1	Total C 80 80	0
21	L	1	Total C 80 80	0
21	L	1	Total C 80 80	0
21	2	1	Total C 40 40	0
21	3	1	Total C 80 80	0
21	3	1	Total C 80 80	0
21	5	1	Total C 40 40	0

- Molecule 22 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe_4S_4).



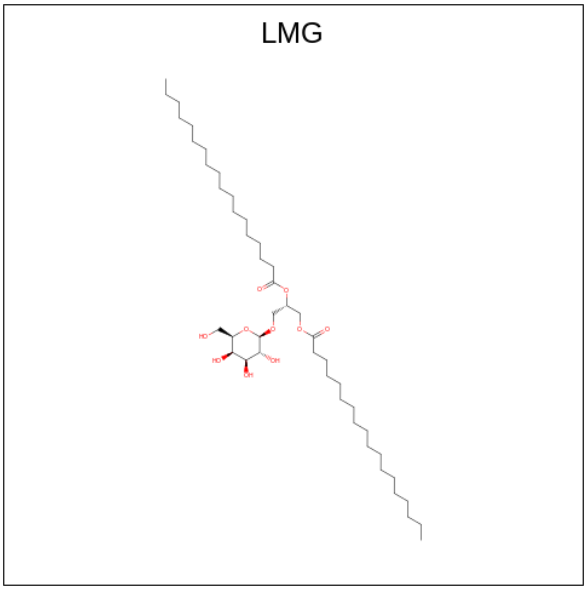
Mol	Chain	Residues	Atoms	AltConf
22	A	1	Total Fe S 8 4 4	0
22	C	1	Total Fe S 16 8 8	0
22	C	1	Total Fe S 16 8 8	0

- Molecule 23 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (three-letter code: DGD) (formula: $C_{51}H_{96}O_{15}$).



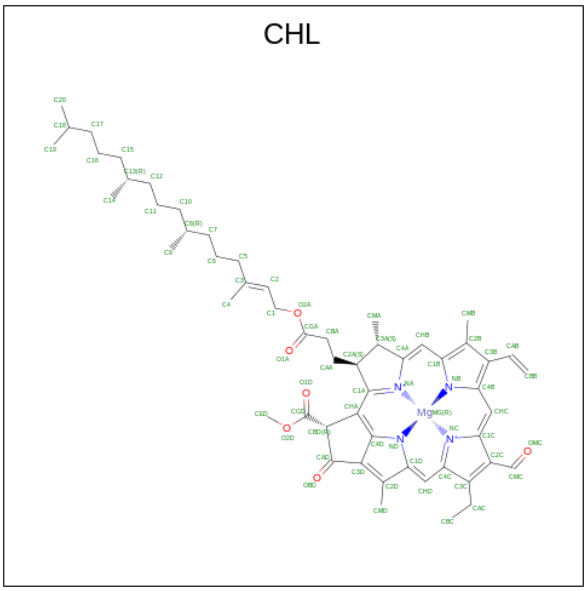
Mol	Chain	Residues	Atoms			AltConf
23	B	1	Total	C	O	0
			66	51	15	

- Molecule 24 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (three-letter code: LMG) (formula: $C_{45}H_{86}O_{10}$).



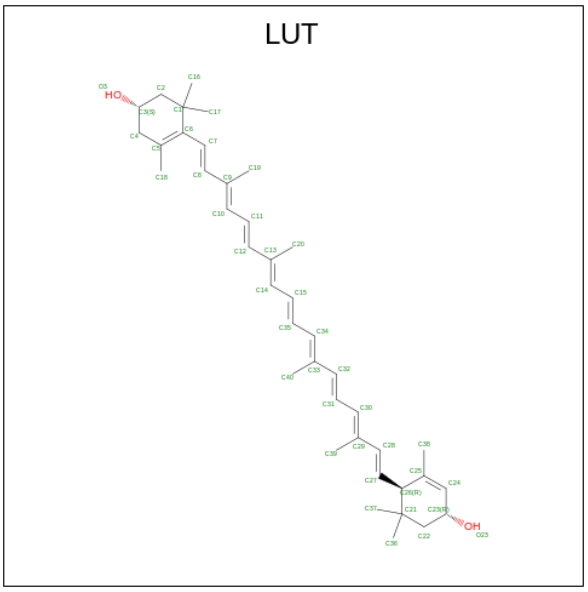
Mol	Chain	Residues	Atoms			AltConf
24	J	1	Total	C	O	0
			30	20	10	
24	2	1	Total	C	O	0
			26	14	12	
24	2	1	Total	C	O	0
			26	14	12	

- Molecule 25 is CHLOROPHYLL B (three-letter code: CHL) (formula: $C_{55}H_{70}MgN_4O_6$).



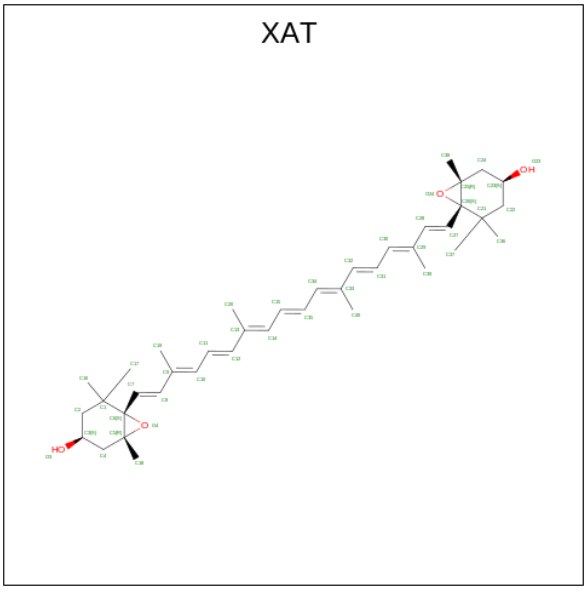
Mol	Chain	Residues	Atoms					AltConf
25	2	1	Total	C	Mg	N	O	0
			221	170	5	20	26	
25	2	1	Total	C	Mg	N	O	0
			221	170	5	20	26	
25	2	1	Total	C	Mg	N	O	0
			221	170	5	20	26	
25	2	1	Total	C	Mg	N	O	0
			221	170	5	20	26	
25	2	1	Total	C	Mg	N	O	0
			221	170	5	20	26	
25	6	1	Total	C	Mg	N	O	0
			86	66	2	8	10	
25	6	1	Total	C	Mg	N	O	0
			86	66	2	8	10	
25	3	1	Total	C	Mg	N	O	0
			40	32	1	4	3	
25	5	1	Total	C	Mg	N	O	0
			178	140	4	16	18	
25	5	1	Total	C	Mg	N	O	0
			178	140	4	16	18	
25	5	1	Total	C	Mg	N	O	0
			178	140	4	16	18	
25	5	1	Total	C	Mg	N	O	0
			178	140	4	16	18	

- Molecule 26 is (3R,3'R,6S)-4,5-DIDEHYDRO-5,6-DIHYDRO-BETA,BETA-CAROTENE-3 ,3'-DIOL (three-letter code: LUT) (formula: $C_{40}H_{56}O_2$).



Mol	Chain	Residues	Atoms			AltConf
26	2	1	Total	C	O	0
			42	40	2	
26	6	1	Total	C	O	0
			42	40	2	
26	3	1	Total	C	O	0
			42	40	2	
26	5	1	Total	C	O	0
			42	40	2	

- Molecule 27 is (3S,5R,6S,3'S,5'R,6'S)-5,6,5',6'-DIEPOXY-5,6,5',6'- TETRAHYDRO-BETA ,BETA-CAROTENE-3,3'-DIOL (three-letter code: XAT) (formula: $C_{40}H_{56}O_4$).



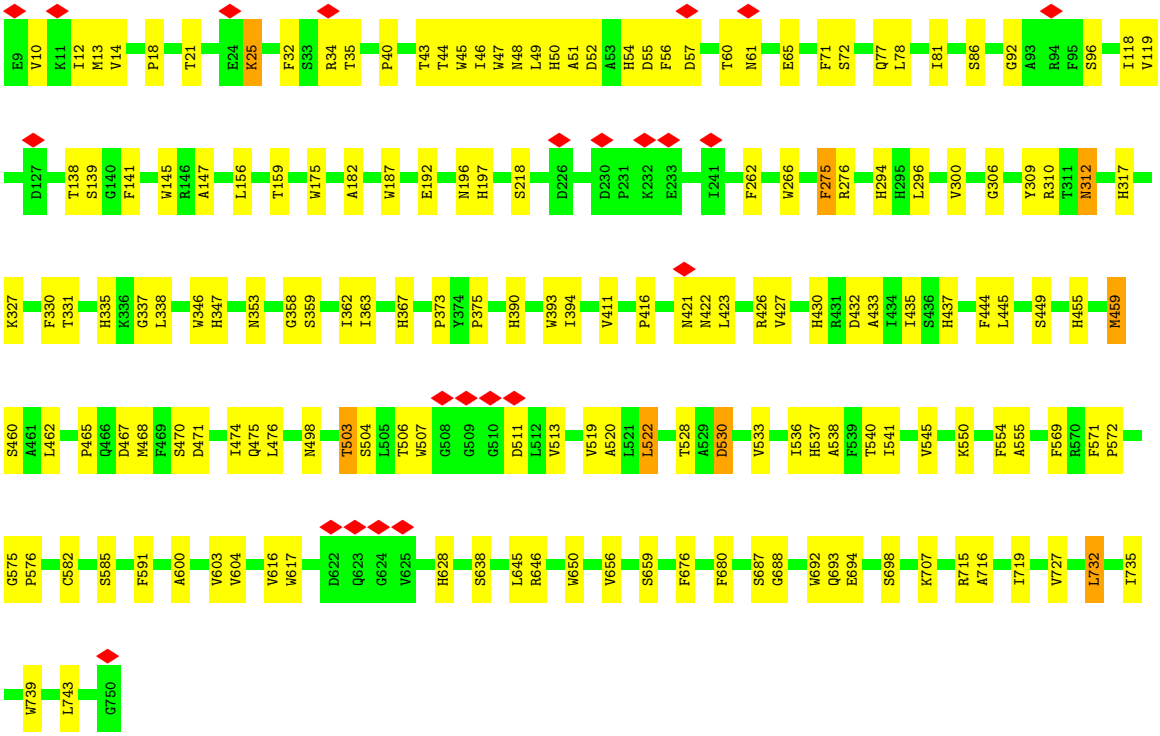
Mol	Chain	Residues	Atoms			AltConf
27	2	1	Total	C	O	0
			44	40	4	
27	6	1	Total	C	O	0
			44	40	4	
27	3	1	Total	C	O	0
			44	40	4	
27	5	1	Total	C	O	0
			44	40	4	

3 Residue-property plots (i)

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

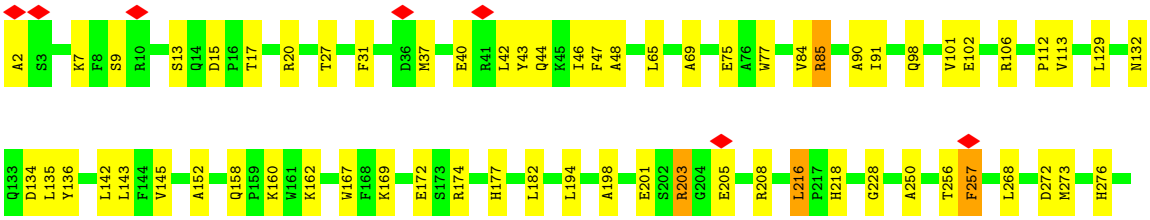
• Molecule 1: Photosystem I P700 chlorophyll a apoprotein A1

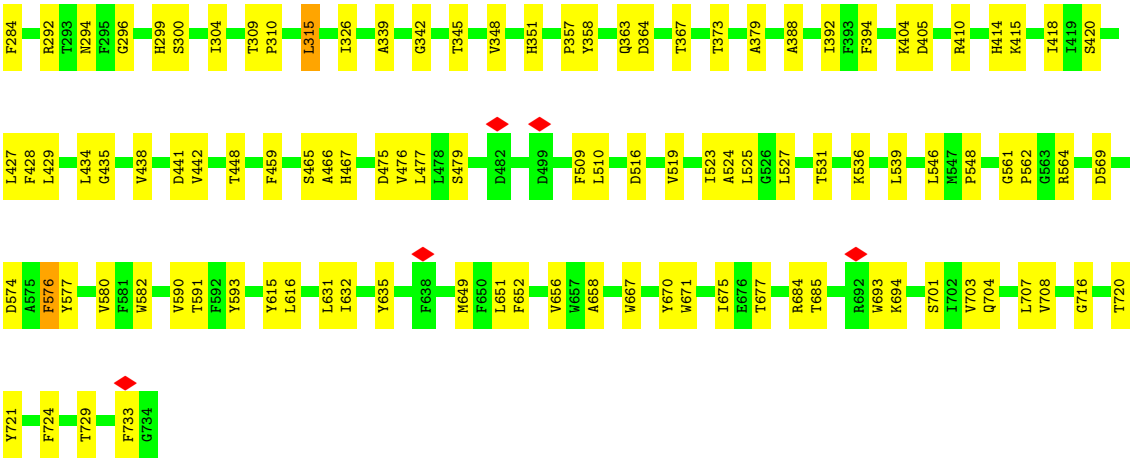
Chain A:



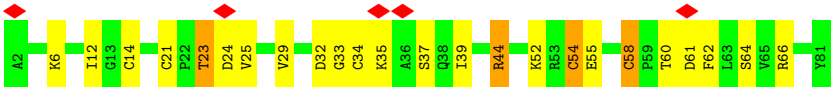
• Molecule 2: Photosystem I P700 chlorophyll a apoprotein A2

Chain B:

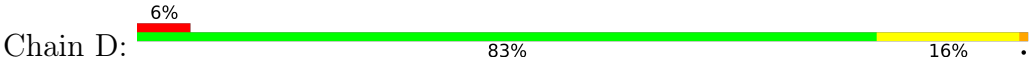




• Molecule 3: Photosystem I iron-sulfur center

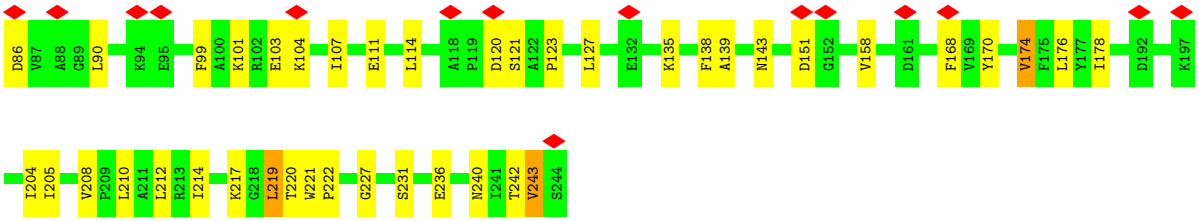


• Molecule 4: Predicted protein PsaD



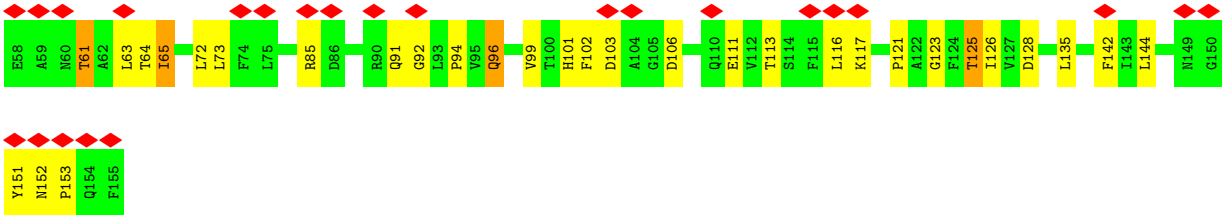
• Molecule 5: PsaE

• Molecule 6: PSI-F



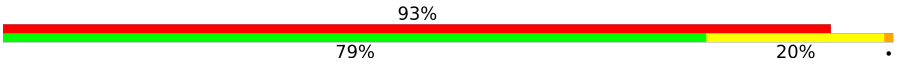
• Molecule 7: Predicted protein PsaG

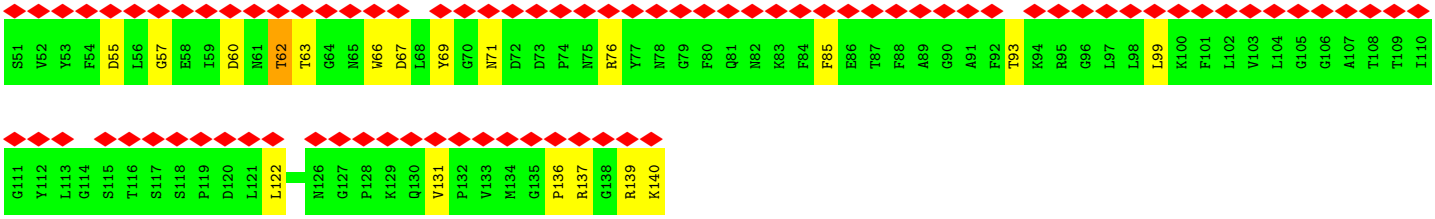
Chain G:



• Molecule 8: PsaH photosystem I reaction center subunit

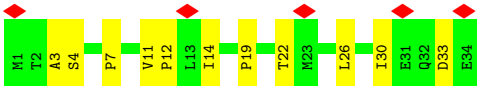
Chain H:





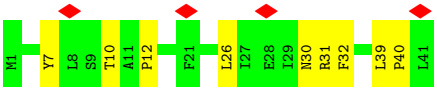
• Molecule 9: Photosystem I reaction center subunit VIII

Chain I:



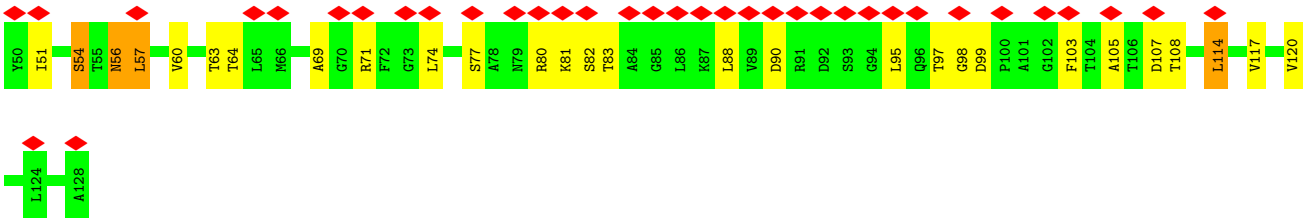
• Molecule 10: Photosystem I reaction center subunit IX

Chain J:



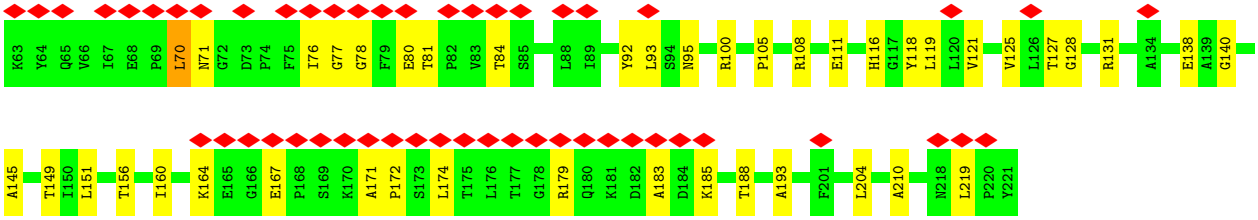
• Molecule 11: PsaK

Chain K:

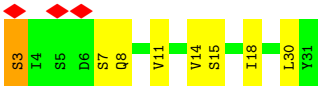


• Molecule 12: PSI subunit V

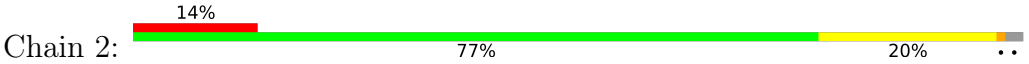
Chain L:

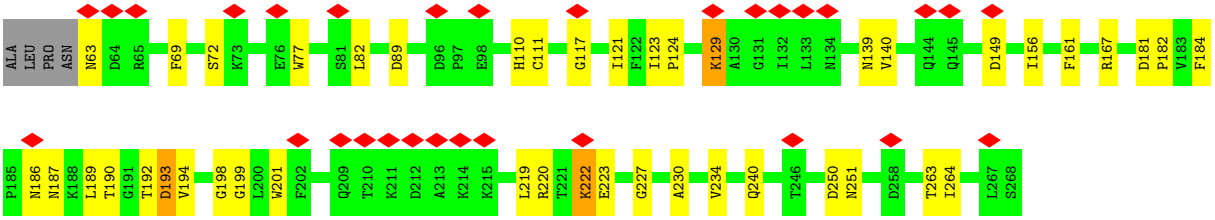


• Molecule 13: Photosystem I reaction center subunit XII

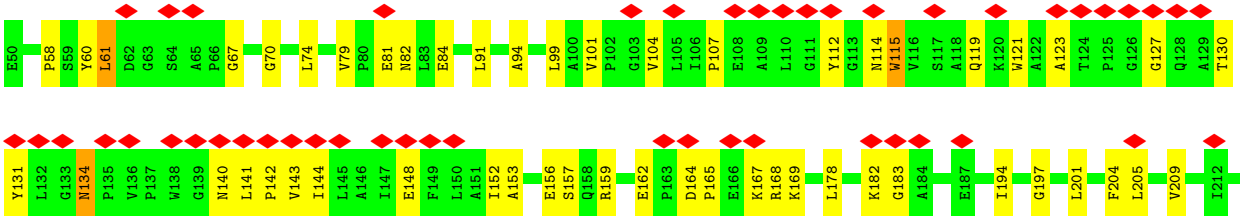


• Molecule 14: Chlorophyll a-b binding protein, chloroplastic

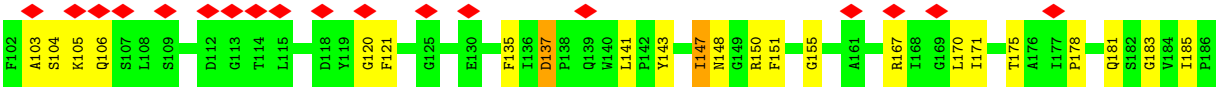


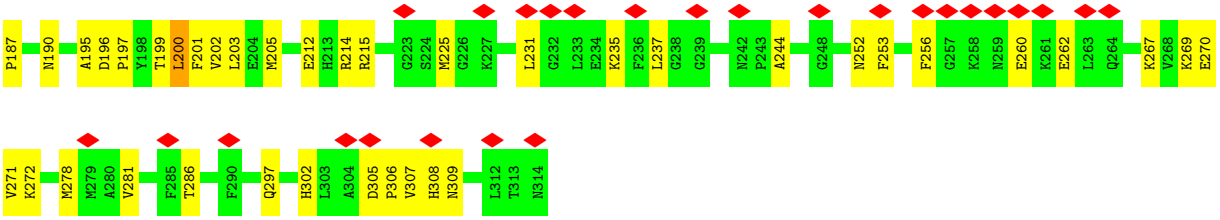


• Molecule 15: Chlorophyll a-b binding protein, chloroplastic



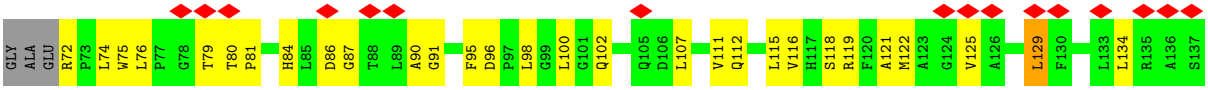
• Molecule 16: Chlorophyll a-b binding protein, chloroplastic

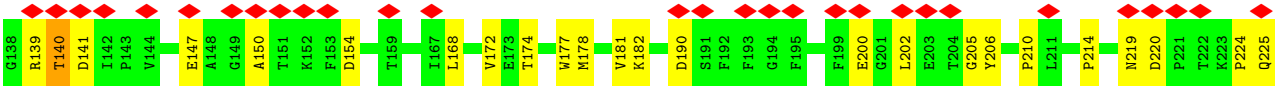




• Molecule 17: Chlorophyll a-b binding protein, chloroplastic

Chain 5:





4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	70288	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	50	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.162	Depositor
Minimum map value	-0.053	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.004	Depositor
Recommended contour level	0.03	Depositor
Map size (Å)	407.424, 407.424, 407.424	wwPDB
Map dimensions	384, 384, 384	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.061, 1.061, 1.061	Depositor

5 Model quality

5.1 Standard geometry

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

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	0.26	0/6032	0.40	0/8227
2	B	0.26	0/6063	0.41	0/8274
3	C	0.27	0/605	0.45	0/821
4	D	0.26	0/1132	0.45	0/1532
5	E	0.27	0/498	0.44	0/677
6	F	0.26	0/1251	0.43	0/1692
7	G	0.25	0/767	0.46	0/1046
8	H	0.25	0/710	0.42	0/961
9	I	0.27	0/273	0.45	0/373
10	J	0.26	0/334	0.39	0/457
11	K	0.26	0/556	0.51	0/752
12	L	0.26	0/1222	0.42	0/1671
13	M	0.24	0/215	0.37	0/290
14	2	0.26	0/1646	0.41	0/2252
15	6	0.26	0/1522	0.40	0/2081
16	3	0.27	0/1695	0.43	0/2302
17	5	0.26	0/1614	0.45	0/2201
All	All	0.26	0/26135	0.42	0/35609

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen

atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5837	0	5725	120	0
2	B	5849	0	5623	133	0
3	C	595	0	576	25	0
4	D	1104	0	1112	15	0
5	E	487	0	480	11	0
6	F	1226	0	1269	27	0
7	G	749	0	729	20	0
8	H	693	0	672	16	0
9	I	266	0	274	7	0
10	J	325	0	341	9	0
11	K	550	0	566	15	0
12	L	1189	0	1200	29	0
13	M	214	0	236	6	0
14	2	1595	0	1561	35	0
15	6	1473	0	1446	43	0
16	3	1644	0	1598	62	0
17	5	1566	0	1531	62	0
18	2	410	0	310	12	0
18	3	577	0	422	21	0
18	5	445	0	318	20	0
18	6	525	0	355	4	0
18	A	2421	0	2229	103	0
18	B	2093	0	1861	77	0
18	F	176	0	128	5	0
18	G	139	0	102	4	0
18	J	42	0	31	1	0
18	K	180	0	126	4	0
18	L	132	0	97	7	0
19	A	33	0	46	1	0
19	B	33	0	46	5	0
20	2	35	0	40	3	0
20	5	37	0	44	5	0
20	6	28	0	26	1	0
20	A	76	0	98	3	0
20	B	23	0	16	1	0
21	2	40	0	56	5	0
21	3	80	0	112	8	0
21	5	40	0	56	2	0
21	A	240	0	336	14	0
21	B	280	0	392	16	0
21	F	40	0	56	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
21	G	40	0	56	3	0
21	I	40	0	56	2	0
21	J	80	0	110	6	0
21	K	80	0	112	5	0
21	L	80	0	112	2	0
22	A	8	0	0	0	0
22	C	16	0	0	11	0
23	B	66	0	96	4	0
24	2	26	0	22	0	0
24	J	30	0	30	1	0
25	2	221	0	143	16	0
25	3	40	0	23	1	0
25	5	178	0	116	18	0
25	6	86	0	52	8	0
26	2	42	0	56	2	0
26	3	42	0	55	1	0
26	5	42	0	56	2	0
26	6	42	0	56	3	0
27	2	44	0	56	24	0
27	3	44	0	56	17	0
27	5	44	0	56	31	0
27	6	44	0	56	13	0
All	All	34822	0	33617	814	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 814 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:2:121:ILE:HD11	27:2:620:XAT:C17	1.25	1.61
3:C:21:CYS:SG	22:C:101:SF4:FE2	1.20	1.34
3:C:14:CYS:SG	22:C:102:SF4:S4	2.29	1.29
14:2:121:ILE:CD1	27:2:620:XAT:H173	1.68	1.22
3:C:21:CYS:SG	22:C:101:SF4:S1	2.38	1.20

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	740/742 (100%)	700 (95%)	40 (5%)	0	100	100
2	B	731/733 (100%)	696 (95%)	35 (5%)	0	100	100
3	C	78/80 (98%)	68 (87%)	10 (13%)	0	100	100
4	D	139/141 (99%)	133 (96%)	6 (4%)	0	100	100
5	E	60/62 (97%)	56 (93%)	4 (7%)	0	100	100
6	F	157/159 (99%)	149 (95%)	8 (5%)	0	100	100
7	G	96/98 (98%)	90 (94%)	6 (6%)	0	100	100
8	H	88/90 (98%)	84 (96%)	4 (4%)	0	100	100
9	I	32/34 (94%)	29 (91%)	3 (9%)	0	100	100
10	J	39/41 (95%)	39 (100%)	0	0	100	100
11	K	77/79 (98%)	66 (86%)	11 (14%)	0	100	100
12	L	157/159 (99%)	146 (93%)	11 (7%)	0	100	100
13	M	27/29 (93%)	27 (100%)	0	0	100	100
14	2	204/210 (97%)	192 (94%)	12 (6%)	0	100	100
15	6	190/192 (99%)	170 (90%)	20 (10%)	0	100	100
16	3	211/213 (99%)	195 (92%)	16 (8%)	0	100	100
17	5	200/205 (98%)	173 (86%)	27 (14%)	0	100	100
All	All	3226/3267 (99%)	3013 (93%)	213 (7%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains (i)

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	603/603 (100%)	580 (96%)	23 (4%)	33 65
2	B	595/595 (100%)	580 (98%)	15 (2%)	47 74
3	C	67/67 (100%)	63 (94%)	4 (6%)	19 52
4	D	115/115 (100%)	111 (96%)	4 (4%)	36 67
5	E	52/52 (100%)	49 (94%)	3 (6%)	20 53
6	F	128/129 (99%)	123 (96%)	5 (4%)	32 65
7	G	78/78 (100%)	68 (87%)	10 (13%)	4 19
8	H	72/73 (99%)	66 (92%)	6 (8%)	11 38
9	I	30/30 (100%)	29 (97%)	1 (3%)	38 68
10	J	35/35 (100%)	35 (100%)	0	100 100
11	K	56/57 (98%)	46 (82%)	10 (18%)	2 8
12	L	121/122 (99%)	114 (94%)	7 (6%)	20 53
13	M	24/24 (100%)	23 (96%)	1 (4%)	30 62
14	2	164/167 (98%)	153 (93%)	11 (7%)	16 47
15	6	148/148 (100%)	140 (95%)	8 (5%)	22 55
16	3	166/166 (100%)	158 (95%)	8 (5%)	25 59
17	5	162/164 (99%)	152 (94%)	10 (6%)	18 51
All	All	2616/2625 (100%)	2490 (95%)	126 (5%)	29 59

5 of 126 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
7	G	72	LEU
16	3	147	ILE
11	K	54	SER
16	3	137	ASP
17	5	168	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 43 such sidechains are listed below:

Mol	Chain	Res	Type
8	H	130	GLN
14	2	261	HIS

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Mol	Chain	Res	Type
10	J	2	GLN
14	2	186	ASN
15	6	226	HIS

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

205 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	A	834	-	65,73,73	1.49	6 (9%)	76,113,113	1.35	7 (9%)
18	CLA	B	812	-	45,53,73	1.77	5 (11%)	52,89,113	1.63	7 (13%)
18	CLA	5	602	-	45,53,73	1.82	6 (13%)	52,89,113	1.52	8 (15%)
18	CLA	B	823	-	45,53,73	1.76	7 (15%)	52,89,113	1.61	6 (11%)
18	CLA	5	611	-	38,45,73	2.93	9 (23%)	41,76,113	1.45	8 (19%)
18	CLA	5	612	-	44,52,73	1.82	6 (13%)	51,88,113	1.59	7 (13%)
18	CLA	3	613	-	53,62,73	1.66	6 (11%)	61,100,113	1.46	8 (13%)
18	CLA	6	609	-	40,48,73	1.91	7 (17%)	50,83,113	1.70	10 (20%)
25	CHL	2	616	-	46,54,74	2.34	15 (32%)	49,90,114	2.78	18 (36%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
18	CLA	6	606	-	39,48,73	1.87	6 (15%)	45,82,113	1.75	9 (20%)
19	PQN	A	844	-	34,34,34	0.39	0	42,45,45	0.47	0
18	CLA	3	615	-	37,44,73	1.95	6 (16%)	42,77,113	1.59	6 (14%)
18	CLA	A	813	-	54,62,73	1.60	6 (11%)	62,99,113	1.48	6 (9%)
18	CLA	A	832	-	41,49,73	1.81	6 (14%)	47,84,113	1.71	9 (19%)
18	CLA	B	840	-	65,73,73	1.48	6 (9%)	76,113,113	1.40	6 (7%)
18	CLA	3	604	-	41,50,73	1.92	7 (17%)	51,86,113	1.63	9 (17%)
18	CLA	6	611	20	37,46,73	2.01	7 (18%)	46,81,113	1.70	9 (19%)
21	BCR	B	847	-	41,41,41	1.14	2 (4%)	56,56,56	1.23	6 (10%)
18	CLA	B	803	-	65,73,73	1.47	7 (10%)	76,113,113	1.42	7 (9%)
18	CLA	2	612	-	41,49,73	1.87	6 (14%)	47,84,113	1.62	7 (14%)
18	CLA	B	819	-	45,53,73	1.78	6 (13%)	52,89,113	1.61	8 (15%)
18	CLA	3	612	-	43,51,73	1.83	5 (11%)	49,86,113	1.56	6 (12%)
18	CLA	B	821	-	46,54,73	1.75	5 (10%)	53,90,113	1.54	7 (13%)
18	CLA	3	611	-	39,48,73	1.90	6 (15%)	44,83,113	1.68	8 (18%)
18	CLA	A	837	1	45,53,73	1.79	5 (11%)	52,89,113	1.59	9 (17%)
18	CLA	2	609	14	55,63,73	1.60	6 (10%)	64,101,113	1.47	8 (12%)
18	CLA	B	838	-	47,55,73	1.72	6 (12%)	54,91,113	1.57	8 (14%)
18	CLA	B	828	-	65,73,73	1.49	7 (10%)	76,113,113	1.31	8 (10%)
18	CLA	B	817	-	45,53,73	1.77	6 (13%)	52,89,113	1.58	6 (11%)
18	CLA	2	613	14	45,53,73	1.79	5 (11%)	52,89,113	1.55	7 (13%)
18	CLA	3	606	-	40,49,73	1.87	6 (15%)	45,84,113	1.61	6 (13%)
18	CLA	A	826	-	65,73,73	1.46	6 (9%)	76,113,113	1.43	7 (9%)
21	BCR	I	101	-	41,41,41	1.13	2 (4%)	56,56,56	1.19	4 (7%)
18	CLA	A	819	-	45,53,73	1.77	7 (15%)	52,89,113	1.62	7 (13%)
18	CLA	B	822	-	55,63,73	1.60	6 (10%)	64,101,113	1.49	8 (12%)
21	BCR	3	620	-	41,41,41	1.12	2 (4%)	56,56,56	1.25	6 (10%)
25	CHL	3	608	-	39,48,74	2.42	15 (38%)	44,83,114	2.74	19 (43%)
18	CLA	B	807	-	65,73,73	1.47	6 (9%)	76,113,113	1.41	9 (11%)
18	CLA	A	825	-	55,63,73	1.62	6 (10%)	64,101,113	1.42	8 (12%)
21	BCR	L	301	-	41,41,41	1.15	2 (4%)	56,56,56	1.22	6 (10%)
18	CLA	B	829	-	45,53,73	1.81	6 (13%)	52,89,113	1.64	7 (13%)
18	CLA	A	833	-	45,53,73	1.78	5 (11%)	52,89,113	1.63	7 (13%)
18	CLA	B	810	-	46,54,73	1.74	6 (13%)	53,90,113	1.53	6 (11%)
18	CLA	K	204	-	44,52,73	1.84	6 (13%)	55,88,113	1.65	8 (14%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
18	CLA	K	206	11	45,53,73	1.80	6 (13%)	52,89,113	1.54	7 (13%)
18	CLA	6	610	15	42,51,73	1.83	6 (14%)	48,87,113	1.61	7 (14%)
18	CLA	B	836	-	60,68,73	1.52	6 (10%)	70,107,113	1.44	7 (10%)
18	CLA	B	830	-	45,53,73	1.78	6 (13%)	52,89,113	1.62	7 (13%)
18	CLA	A	824	-	51,59,73	1.68	6 (11%)	59,96,113	1.52	6 (10%)
25	CHL	5	615	17	43,51,74	2.31	15 (34%)	45,86,114	2.89	20 (44%)
18	CLA	K	203	-	45,53,73	1.79	6 (13%)	52,89,113	1.57	7 (13%)
21	BCR	B	848	-	41,41,41	1.14	2 (4%)	56,56,56	1.24	7 (12%)
18	CLA	3	602	16	60,68,73	1.54	5 (8%)	70,107,113	1.42	8 (11%)
21	BCR	A	851	-	41,41,41	1.18	2 (4%)	56,56,56	1.26	9 (16%)
18	CLA	2	614	-	42,50,73	1.82	6 (14%)	48,85,113	1.59	7 (14%)
20	LHG	A	847	18	26,26,48	0.83	1 (3%)	29,32,54	1.35	3 (10%)
21	BCR	B	843	-	41,41,41	1.17	2 (4%)	56,56,56	1.22	7 (12%)
18	CLA	2	610	14	45,53,73	1.72	7 (15%)	52,89,113	1.59	6 (11%)
26	LUT	6	617	-	42,43,43	7.20	25 (59%)	51,60,60	3.87	19 (37%)
18	CLA	B	832	-	45,53,73	1.76	6 (13%)	52,89,113	1.62	9 (17%)
21	BCR	3	622	-	41,41,41	1.11	2 (4%)	56,56,56	1.28	6 (10%)
18	CLA	3	610	-	41,49,73	1.82	7 (17%)	47,84,113	1.67	8 (17%)
18	CLA	5	601	17	45,53,73	1.79	5 (11%)	52,89,113	1.56	7 (13%)
25	CHL	2	606	14	46,54,74	2.28	15 (32%)	49,90,114	2.87	18 (36%)
20	LHG	A	846	-	48,48,48	0.64	1 (2%)	51,54,54	1.27	6 (11%)
18	CLA	B	805	-	65,73,73	1.49	6 (9%)	76,113,113	1.38	8 (10%)
21	BCR	A	849	-	41,41,41	1.17	2 (4%)	56,56,56	1.21	6 (10%)
18	CLA	A	835	-	65,73,73	1.48	7 (10%)	76,113,113	1.42	9 (11%)
21	BCR	A	848	-	41,41,41	1.13	2 (4%)	56,56,56	1.28	4 (7%)
18	CLA	G	203	-	50,58,73	1.70	6 (12%)	58,95,113	1.51	8 (13%)
18	CLA	B	804	-	45,53,73	1.76	6 (13%)	52,89,113	1.64	7 (13%)
18	CLA	A	841	-	65,73,73	1.48	7 (10%)	76,113,113	1.38	9 (11%)
20	LHG	2	622	18,14	34,34,48	0.72	0	37,40,54	1.27	4 (10%)
18	CLA	F	303	-	45,53,73	1.78	5 (11%)	52,89,113	1.55	8 (15%)
18	CLA	B	837	-	46,54,73	1.75	7 (15%)	53,90,113	1.57	8 (15%)
26	LUT	5	619	-	42,43,43	7.28	26 (61%)	51,60,60	3.85	19 (37%)
18	CLA	A	842	-	43,52,73	1.81	6 (13%)	49,88,113	1.56	7 (14%)
18	CLA	A	814	-	65,73,73	1.45	7 (10%)	76,113,113	1.43	8 (10%)
18	CLA	A	801	-	65,73,73	1.46	6 (9%)	76,113,113	1.33	7 (9%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
18	CLA	5	614	-	43,51,73	1.81	6 (13%)	49,86,113	1.59	7 (14%)
25	CHL	2	607	-	43,51,74	2.37	15 (34%)	45,86,114	2.85	20 (44%)
18	CLA	5	603	-	43,52,73	1.82	6 (13%)	49,88,113	1.57	6 (12%)
26	LUT	2	619	-	42,43,43	7.18	25 (59%)	51,60,60	4.12	21 (41%)
21	BCR	F	302	-	41,41,41	1.12	2 (4%)	56,56,56	1.21	6 (10%)
18	CLA	A	816	-	42,50,73	1.78	6 (14%)	48,85,113	1.69	7 (14%)
18	CLA	3	609	-	45,53,73	1.75	6 (13%)	52,89,113	1.61	6 (11%)
18	CLA	F	301	-	45,53,73	1.77	6 (13%)	52,89,113	1.56	6 (11%)
18	CLA	5	610	-	55,63,73	1.61	6 (10%)	64,101,113	1.45	8 (12%)
18	CLA	A	815	-	45,53,73	1.77	6 (13%)	52,89,113	1.57	8 (15%)
25	CHL	6	601	15	44,53,74	2.38	16 (36%)	46,89,114	2.73	17 (36%)
18	CLA	A	854	-	65,73,73	1.46	6 (9%)	76,113,113	1.38	9 (11%)
18	CLA	B	816	-	53,62,73	1.64	6 (11%)	61,100,113	1.42	6 (9%)
18	CLA	A	831	-	65,73,73	1.49	6 (9%)	76,113,113	1.44	7 (9%)
18	CLA	B	827	-	45,53,73	1.76	7 (15%)	52,89,113	1.61	8 (15%)
18	CLA	L	304	-	42,50,73	1.80	6 (14%)	48,85,113	1.67	7 (14%)
18	CLA	6	616	15	43,51,73	1.91	6 (13%)	54,87,113	1.66	8 (14%)
21	BCR	5	621	-	41,41,41	1.16	2 (4%)	56,56,56	1.24	5 (8%)
20	LHG	5	622	-	36,36,48	0.72	1 (2%)	39,42,54	1.25	4 (10%)
26	LUT	3	618	16	42,43,43	7.26	24 (57%)	51,60,60	3.85	22 (43%)
18	CLA	A	809	1	45,53,73	1.73	6 (13%)	52,89,113	1.65	8 (15%)
18	CLA	A	802	-	45,53,73	1.75	6 (13%)	52,89,113	1.63	6 (11%)
18	CLA	A	827	-	65,73,73	1.47	6 (9%)	76,113,113	1.38	8 (10%)
18	CLA	A	838	-	51,59,73	1.68	5 (9%)	59,96,113	1.48	8 (13%)
18	CLA	3	607	16	39,48,73	1.93	7 (17%)	48,83,113	1.67	9 (18%)
24	LMG	2	617	-	13,13,55	1.01	0	18,18,63	1.55	4 (22%)
18	CLA	B	809	-	65,73,73	1.47	6 (9%)	76,113,113	1.37	8 (10%)
18	CLA	B	825	-	65,73,73	1.46	7 (10%)	76,113,113	1.39	8 (10%)
21	BCR	A	852	-	41,41,41	1.16	2 (4%)	56,56,56	1.18	6 (10%)
21	BCR	G	205	-	41,41,41	1.13	2 (4%)	56,56,56	1.23	6 (10%)
18	CLA	6	604	-	49,57,73	1.70	6 (12%)	55,93,113	1.53	8 (14%)
18	CLA	6	614	-	37,46,73	2.00	6 (16%)	46,81,113	1.69	11 (23%)
25	CHL	2	601	14	45,53,74	2.33	15 (33%)	52,89,114	2.80	21 (40%)
22	SF4	C	101	3	0,12,12	-	-	-		
21	BCR	2	621	-	41,41,41	1.15	2 (4%)	56,56,56	1.22	6 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
18	CLA	6	603	-	55,63,73	1.61	6 (10%)	64,101,113	1.49	8 (12%)
21	BCR	K	207	-	41,41,41	1.15	2 (4%)	56,56,56	1.32	6 (10%)
18	CLA	B	833	-	45,53,73	1.77	6 (13%)	52,89,113	1.65	9 (17%)
18	CLA	5	613	17	45,53,73	1.78	6 (13%)	52,89,113	1.63	7 (13%)
18	CLA	B	815	-	60,68,73	1.55	7 (11%)	70,107,113	1.39	7 (10%)
18	CLA	A	818	-	65,73,73	1.47	7 (10%)	76,113,113	1.43	8 (10%)
18	CLA	6	608	-	43,52,73	1.83	6 (13%)	49,88,113	1.56	6 (12%)
25	CHL	5	607	-	43,51,74	2.44	15 (34%)	45,86,114	2.84	20 (44%)
18	CLA	B	835	-	45,53,73	1.79	6 (13%)	52,89,113	1.57	7 (13%)
18	CLA	B	841	20	65,73,73	1.49	6 (9%)	76,113,113	1.35	9 (11%)
18	CLA	L	303	-	45,53,73	1.77	6 (13%)	52,89,113	1.58	7 (13%)
18	CLA	A	804	-	65,73,73	1.46	7 (10%)	76,113,113	1.43	9 (11%)
18	CLA	A	808	-	45,53,73	1.76	6 (13%)	52,89,113	1.63	8 (15%)
18	CLA	A	839	-	65,73,73	1.45	5 (7%)	76,113,113	1.41	8 (10%)
18	CLA	B	818	-	45,53,73	1.79	6 (13%)	52,89,113	1.55	7 (13%)
18	CLA	A	812	-	65,73,73	1.50	6 (9%)	76,113,113	1.36	8 (10%)
18	CLA	J	101	-	42,50,73	1.83	6 (14%)	48,85,113	1.57	6 (12%)
18	CLA	2	604	-	50,58,73	1.65	6 (12%)	58,95,113	1.64	8 (13%)
21	BCR	B	801	-	41,41,41	1.14	2 (4%)	56,56,56	1.17	4 (7%)
18	CLA	G	204	7	43,52,73	1.83	6 (13%)	49,88,113	1.56	7 (14%)
21	BCR	J	102	-	41,41,41	1.17	2 (4%)	56,56,56	1.27	6 (10%)
18	CLA	A	823	1	44,52,73	1.78	6 (13%)	51,88,113	1.66	6 (11%)
18	CLA	B	826	-	65,73,73	1.46	7 (10%)	76,113,113	1.41	8 (10%)
18	CLA	B	808	-	50,58,73	1.67	7 (14%)	58,95,113	1.55	9 (15%)
18	CLA	B	814	-	43,52,73	1.81	6 (13%)	49,88,113	1.61	7 (14%)
18	CLA	2	603	-	45,53,73	1.78	6 (13%)	52,89,113	1.57	6 (11%)
18	CLA	3	614	-	39,48,73	1.89	6 (15%)	44,83,113	1.62	7 (15%)
18	CLA	3	603	-	55,63,73	1.63	7 (12%)	64,101,113	1.43	6 (9%)
21	BCR	K	202	-	41,41,41	1.14	2 (4%)	56,56,56	1.28	6 (10%)
27	XAT	5	620	-	39,47,47	1.03	3 (7%)	54,74,74	2.76	21 (38%)
18	CLA	A	829	-	65,73,73	1.45	7 (10%)	76,113,113	1.42	9 (11%)
18	CLA	A	805	-	55,63,73	1.56	7 (12%)	64,101,113	1.56	8 (12%)
24	LMG	2	618	-	13,13,55	1.07	0	18,18,63	1.54	4 (22%)
18	CLA	A	811	-	45,53,73	1.77	6 (13%)	52,89,113	1.62	7 (13%)
25	CHL	5	608	-	51,59,74	2.16	16 (31%)	55,96,114	2.69	20 (36%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
18	CLA	A	806	-	65,73,73	1.47	7 (10%)	76,113,113	1.40	7 (9%)
18	CLA	F	305	-	45,53,73	1.78	6 (13%)	52,89,113	1.57	6 (11%)
18	CLA	A	803	-	65,73,73	1.49	6 (9%)	76,113,113	1.36	7 (9%)
18	CLA	5	604	-	43,51,73	1.78	5 (11%)	48,86,113	1.66	7 (14%)
21	BCR	B	844	-	41,41,41	1.10	2 (4%)	56,56,56	1.18	4 (7%)
18	CLA	B	834	-	45,53,73	1.80	6 (13%)	52,89,113	1.57	7 (13%)
18	CLA	F	304	-	41,49,73	1.83	6 (14%)	47,84,113	1.67	7 (14%)
27	XAT	2	620	-	39,47,47	1.01	2 (5%)	54,74,74	3.14	22 (40%)
18	CLA	B	811	-	54,62,73	1.68	7 (12%)	67,100,113	1.48	9 (13%)
23	DGD	B	850	-	67,67,67	0.86	2 (2%)	81,81,81	1.44	11 (13%)
18	CLA	B	806	2	65,73,73	1.47	6 (9%)	76,113,113	1.39	8 (10%)
21	BCR	J	103	2	41,41,41	1.15	3 (7%)	56,56,56	1.30	7 (12%)
18	CLA	A	820	-	45,53,73	1.78	6 (13%)	52,89,113	1.60	7 (13%)
18	CLA	A	840	-	45,53,73	1.79	6 (13%)	52,89,113	1.55	6 (11%)
18	CLA	B	831	-	49,57,73	1.69	6 (12%)	55,93,113	1.53	6 (10%)
18	CLA	A	821	-	44,52,73	1.81	6 (13%)	51,88,113	1.58	7 (13%)
18	CLA	2	611	20	41,50,73	1.85	6 (14%)	49,85,113	1.60	6 (12%)
18	CLA	3	617	-	39,48,73	1.88	6 (15%)	44,83,113	1.69	8 (18%)
18	CLA	G	201	-	45,53,73	1.80	5 (11%)	52,89,113	1.56	7 (13%)
18	CLA	A	828	-	46,54,73	1.73	7 (15%)	53,90,113	1.53	6 (11%)
18	CLA	A	817	-	39,48,73	1.86	6 (15%)	44,83,113	1.68	8 (18%)
18	CLA	B	802	-	53,61,73	1.63	7 (13%)	61,98,113	1.42	8 (13%)
21	BCR	B	845	-	41,41,41	1.16	2 (4%)	56,56,56	1.22	5 (8%)
18	CLA	6	602	-	45,53,73	1.76	6 (13%)	52,89,113	1.62	7 (13%)
27	XAT	6	619	-	39,47,47	0.98	2 (5%)	54,74,74	3.10	21 (38%)
19	PQN	B	842	-	34,34,34	0.40	0	42,45,45	0.45	0
24	LMG	J	104	-	30,30,55	0.94	0	38,38,63	1.27	5 (13%)
21	BCR	L	305	-	41,41,41	1.12	2 (4%)	56,56,56	1.28	9 (16%)
25	CHL	2	608	-	40,49,74	2.43	16 (40%)	41,84,114	2.87	18 (43%)
18	CLA	A	822	-	43,51,73	1.87	7 (16%)	54,87,113	1.65	8 (14%)
21	BCR	B	846	-	41,41,41	1.16	2 (4%)	56,56,56	1.23	6 (10%)
25	CHL	5	606	-	41,49,74	2.24	13 (31%)	48,84,114	2.95	19 (39%)
18	CLA	A	807	1	43,52,73	1.80	6 (13%)	49,88,113	1.57	6 (12%)
21	BCR	A	856	-	41,41,41	1.15	2 (4%)	56,56,56	1.33	7 (12%)
18	CLA	L	302	-	45,53,73	1.78	6 (13%)	52,89,113	1.61	7 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
22	SF4	C	102	3	0,12,12	-	-	-		
20	LHG	6	620	18,15	27,27,48	0.80	1 (3%)	30,33,54	1.25	2 (6%)
20	LHG	B	851	18	22,22,48	0.83	0	25,28,54	1.20	1 (4%)
18	CLA	6	613	15	45,53,73	1.79	6 (13%)	52,89,113	1.56	7 (13%)
18	CLA	A	843	-	65,73,73	1.50	7 (10%)	76,113,113	1.37	9 (11%)
18	CLA	5	609	17	43,51,73	1.79	6 (13%)	48,86,113	1.64	6 (12%)
18	CLA	K	201	11	46,54,73	1.84	7 (15%)	53,90,113	1.46	4 (7%)
18	CLA	A	810	1	45,53,73	1.79	6 (13%)	52,89,113	1.59	7 (13%)
18	CLA	2	602	-	45,53,73	1.77	6 (13%)	52,89,113	1.59	7 (13%)
18	CLA	A	836	-	50,58,73	1.69	6 (12%)	58,95,113	1.54	7 (12%)
22	SF4	A	853	1,2	0,12,12	-	-	-		
18	CLA	A	830	-	65,73,73	1.46	6 (9%)	76,113,113	1.40	6 (7%)
21	BCR	A	850	-	41,41,41	1.15	2 (4%)	56,56,56	1.20	6 (10%)
18	CLA	B	813	-	65,73,73	1.45	7 (10%)	76,113,113	1.47	10 (13%)
18	CLA	6	612	-	45,53,73	1.79	6 (13%)	52,89,113	1.57	7 (13%)
25	CHL	6	607	15	40,49,74	2.53	16 (40%)	41,84,114	2.84	19 (46%)
27	XAT	3	619	-	39,47,47	0.98	2 (5%)	54,74,74	2.74	20 (37%)
18	CLA	A	845	20	52,60,73	1.66	5 (9%)	60,97,113	1.52	8 (13%)
18	CLA	B	820	-	43,51,73	1.77	6 (13%)	49,86,113	1.64	6 (12%)
18	CLA	B	824	-	45,53,73	1.79	6 (13%)	52,89,113	1.59	8 (15%)
18	CLA	B	839	-	40,49,73	1.86	6 (15%)	45,84,113	1.61	6 (13%)

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	A	834	-	1/1/15/20	12/37/115/115	-
18	CLA	B	812	-	1/1/11/20	3/13/91/115	-
18	CLA	5	602	-	1/1/11/20	3/13/91/115	-
18	CLA	B	823	-	1/1/11/20	5/13/91/115	-
18	CLA	5	611	-	1/1/7/20	5/10/70/115	-
18	CLA	5	612	-	1/1/11/20	5/11/89/115	-
18	CLA	3	613	-	1/1/13/20	7/23/101/115	-
18	CLA	6	609	-	1/1/10/20	3/8/84/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
25	CHL	2	616	-	3/3/16/26	6/15/113/137	-
18	CLA	6	606	-	1/1/9/20	3/8/82/115	-
19	PQN	A	844	-	-	8/23/43/43	0/2/2/2
18	CLA	3	615	-	1/1/8/20	0/0/74/115	-
18	CLA	A	813	-	1/1/12/20	3/24/102/115	-
18	CLA	A	832	-	1/1/10/20	6/8/86/115	-
18	CLA	B	840	-	1/1/15/20	12/37/115/115	-
18	CLA	3	604	-	1/1/11/20	0/9/85/115	-
18	CLA	6	611	20	1/1/10/20	1/4/80/115	-
21	BCR	B	847	-	-	2/29/63/63	0/2/2/2
18	CLA	B	803	-	1/1/15/20	10/37/115/115	-
18	CLA	2	612	-	1/1/10/20	0/8/86/115	-
18	CLA	B	819	-	1/1/11/20	3/13/91/115	-
18	CLA	3	612	-	1/1/10/20	2/11/89/115	-
18	CLA	B	821	-	1/1/11/20	7/15/93/115	-
18	CLA	3	611	-	1/1/10/20	2/6/84/115	-
18	CLA	A	837	1	1/1/11/20	2/13/91/115	-
18	CLA	2	609	14	1/1/13/20	11/25/103/115	-
18	CLA	B	838	-	1/1/11/20	2/16/94/115	-
18	CLA	B	828	-	1/1/15/20	10/37/115/115	-
18	CLA	B	817	-	1/1/11/20	2/13/91/115	-
18	CLA	2	613	14	1/1/11/20	6/13/91/115	-
18	CLA	3	606	-	1/1/10/20	0/8/86/115	-
18	CLA	A	826	-	1/1/15/20	12/37/115/115	-
21	BCR	I	101	-	-	5/29/63/63	0/2/2/2
18	CLA	A	819	-	1/1/11/20	6/13/91/115	-
18	CLA	B	822	-	1/1/13/20	8/25/103/115	-
25	CHL	3	608	-	3/3/15/26	2/6/104/137	-
21	BCR	3	620	-	-	9/29/63/63	0/2/2/2
18	CLA	B	807	-	1/1/15/20	12/37/115/115	-
18	CLA	A	825	-	1/1/13/20	9/25/103/115	-
21	BCR	L	301	-	-	10/29/63/63	0/2/2/2
18	CLA	B	829	-	1/1/11/20	0/13/91/115	-
18	CLA	A	833	-	1/1/11/20	7/13/91/115	-
18	CLA	B	810	-	1/1/11/20	9/15/93/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
18	CLA	K	204	-	1/1/11/20	5/13/89/115	-
18	CLA	K	206	11	1/1/11/20	5/13/91/115	-
18	CLA	6	610	15	1/1/11/20	1/9/87/115	-
18	CLA	B	836	-	1/1/14/20	7/31/109/115	-
18	CLA	B	830	-	1/1/11/20	1/13/91/115	-
18	CLA	A	824	-	1/1/12/20	9/21/99/115	-
25	CHL	5	615	17	3/3/15/26	3/12/110/137	-
18	CLA	K	203	-	1/1/11/20	4/13/91/115	-
21	BCR	B	848	-	-	13/29/63/63	0/2/2/2
18	CLA	3	602	16	1/1/14/20	9/31/109/115	-
21	BCR	A	851	-	-	9/29/63/63	0/2/2/2
18	CLA	2	614	-	1/1/10/20	2/10/88/115	-
20	LHG	A	847	18	-	19/31/31/53	-
21	BCR	B	843	-	-	9/29/63/63	0/2/2/2
18	CLA	2	610	14	1/1/11/20	4/13/91/115	-
26	LUT	6	617	-	-	12/29/67/67	0/2/2/2
18	CLA	B	832	-	1/1/11/20	6/13/91/115	-
21	BCR	3	622	-	-	10/29/63/63	0/2/2/2
18	CLA	3	610	-	1/1/10/20	3/8/86/115	-
18	CLA	5	601	17	1/1/11/20	2/13/91/115	-
25	CHL	2	606	14	3/3/16/26	5/15/113/137	-
20	LHG	A	846	-	-	24/53/53/53	-
18	CLA	B	805	-	1/1/15/20	11/37/115/115	-
21	BCR	A	849	-	-	8/29/63/63	0/2/2/2
18	CLA	A	835	-	1/1/15/20	7/37/115/115	-
21	BCR	A	848	-	-	6/29/63/63	0/2/2/2
18	CLA	G	203	-	1/1/12/20	7/19/97/115	-
18	CLA	B	804	-	1/1/11/20	5/13/91/115	-
18	CLA	A	841	-	1/1/15/20	13/37/115/115	-
20	LHG	2	622	18,14	-	23/39/39/53	-
18	CLA	F	303	-	1/1/11/20	4/13/91/115	-
18	CLA	B	837	-	1/1/11/20	4/15/93/115	-
26	LUT	5	619	-	-	8/29/67/67	0/2/2/2
18	CLA	A	842	-	1/1/11/20	3/11/89/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
18	CLA	A	814	-	1/1/15/20	16/37/115/115	-
18	CLA	A	801	-	1/1/15/20	7/37/115/115	-
18	CLA	5	614	-	1/1/10/20	7/11/89/115	-
25	CHL	2	607	-	3/3/15/26	3/12/110/137	-
18	CLA	5	603	-	1/1/11/20	4/11/89/115	-
26	LUT	2	619	-	-	7/29/67/67	0/2/2/2
21	BCR	F	302	-	-	14/29/63/63	0/2/2/2
18	CLA	A	816	-	1/1/10/20	4/10/88/115	-
18	CLA	3	609	-	1/1/11/20	1/13/91/115	-
18	CLA	F	301	-	1/1/11/20	3/13/91/115	-
18	CLA	5	610	-	1/1/13/20	3/25/103/115	-
18	CLA	A	815	-	1/1/11/20	5/13/91/115	-
25	CHL	6	601	15	3/3/16/26	3/13/111/137	-
18	CLA	A	854	-	1/1/15/20	15/37/115/115	-
18	CLA	B	816	-	1/1/13/20	3/23/101/115	-
18	CLA	A	831	-	1/1/15/20	14/37/115/115	-
18	CLA	B	827	-	1/1/11/20	5/13/91/115	-
18	CLA	L	304	-	1/1/10/20	2/10/88/115	-
18	CLA	6	616	15	1/1/11/20	4/11/87/115	-
21	BCR	5	621	-	-	9/29/63/63	0/2/2/2
20	LHG	5	622	-	-	19/41/41/53	-
26	LUT	3	618	16	-	7/29/67/67	0/2/2/2
18	CLA	A	809	1	1/1/11/20	5/13/91/115	-
18	CLA	A	802	-	1/1/11/20	7/13/91/115	-
18	CLA	A	827	-	1/1/15/20	12/37/115/115	-
18	CLA	A	838	-	1/1/12/20	3/21/99/115	-
18	CLA	3	607	16	1/1/10/20	1/8/84/115	-
24	LMG	2	617	-	-	4/4/24/70	0/1/1/1
18	CLA	B	809	-	1/1/15/20	9/37/115/115	-
18	CLA	B	825	-	1/1/15/20	11/37/115/115	-
21	BCR	A	852	-	-	11/29/63/63	0/2/2/2
21	BCR	G	205	-	-	5/29/63/63	0/2/2/2
18	CLA	6	604	-	1/1/11/20	8/18/96/115	-
18	CLA	6	614	-	1/1/10/20	2/4/80/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
25	CHL	2	601	14	3/3/16/26	8/15/111/137	-
22	SF4	C	101	3	-	-	0/6/5/5
21	BCR	2	621	-	-	8/29/63/63	0/2/2/2
18	CLA	6	603	-	1/1/13/20	13/25/103/115	-
21	BCR	K	207	-	-	11/29/63/63	0/2/2/2
18	CLA	B	833	-	1/1/11/20	8/13/91/115	-
18	CLA	5	613	17	1/1/11/20	5/13/91/115	-
18	CLA	B	815	-	1/1/14/20	11/31/109/115	-
18	CLA	A	818	-	1/1/15/20	18/37/115/115	-
18	CLA	6	608	-	1/1/11/20	3/11/89/115	-
25	CHL	5	607	-	3/3/15/26	4/12/110/137	-
18	CLA	B	835	-	1/1/11/20	8/13/91/115	-
18	CLA	B	841	20	1/1/15/20	14/37/115/115	-
18	CLA	L	303	-	1/1/11/20	0/13/91/115	-
18	CLA	A	804	-	1/1/15/20	9/37/115/115	-
18	CLA	A	808	-	1/1/11/20	3/13/91/115	-
18	CLA	A	839	-	1/1/15/20	15/37/115/115	-
18	CLA	B	818	-	1/1/11/20	2/13/91/115	-
18	CLA	A	812	-	1/1/15/20	11/37/115/115	-
18	CLA	J	101	-	1/1/10/20	5/10/88/115	-
18	CLA	2	604	-	1/1/12/20	7/19/97/115	-
21	BCR	B	801	-	-	7/29/63/63	0/2/2/2
18	CLA	G	204	7	1/1/11/20	4/11/89/115	-
21	BCR	J	102	-	-	9/29/63/63	0/2/2/2
18	CLA	A	823	1	1/1/11/20	5/11/89/115	-
18	CLA	B	826	-	1/1/15/20	12/37/115/115	-
18	CLA	B	808	-	1/1/12/20	2/19/97/115	-
18	CLA	B	814	-	1/1/11/20	1/11/89/115	-
18	CLA	2	603	-	1/1/11/20	5/13/91/115	-
18	CLA	3	614	-	1/1/10/20	1/6/84/115	-
18	CLA	3	603	-	1/1/13/20	6/25/103/115	-
21	BCR	K	202	-	-	8/29/63/63	0/2/2/2
27	XAT	5	620	-	-	3/31/93/93	0/4/4/4
18	CLA	A	829	-	1/1/15/20	20/37/115/115	-
18	CLA	A	805	-	1/1/13/20	10/25/103/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
25	CHL	5	608	-	3/3/17/26	8/21/119/137	-
18	CLA	A	811	-	1/1/11/20	2/13/91/115	-
24	LMG	2	618	-	-	2/4/24/70	0/1/1/1
18	CLA	A	806	-	1/1/15/20	14/37/115/115	-
18	CLA	F	305	-	1/1/11/20	5/13/91/115	-
18	CLA	A	803	-	1/1/15/20	7/37/115/115	-
18	CLA	5	604	-	1/1/10/20	5/9/88/115	-
21	BCR	B	844	-	-	6/29/63/63	0/2/2/2
18	CLA	B	834	-	1/1/11/20	5/13/91/115	-
18	CLA	F	304	-	1/1/10/20	2/8/86/115	-
27	XAT	2	620	-	-	3/31/93/93	0/4/4/4
18	CLA	B	811	-	1/1/13/20	9/25/101/115	-
23	DGD	B	850	-	-	29/55/95/95	0/2/2/2
18	CLA	B	806	2	1/1/15/20	19/37/115/115	-
21	BCR	J	103	2	-	23/29/63/63	0/2/2/2
18	CLA	A	820	-	1/1/11/20	4/13/91/115	-
18	CLA	A	840	-	1/1/11/20	4/13/91/115	-
18	CLA	B	831	-	1/1/11/20	7/18/96/115	-
18	CLA	A	821	-	1/1/11/20	6/11/89/115	-
18	CLA	2	611	20	1/1/10/20	0/7/85/115	-
18	CLA	3	617	-	1/1/10/20	2/6/84/115	-
18	CLA	G	201	-	1/1/11/20	5/13/91/115	-
18	CLA	A	828	-	1/1/11/20	7/15/93/115	-
18	CLA	A	817	-	1/1/10/20	0/6/84/115	-
18	CLA	B	802	-	1/1/12/20	3/23/101/115	-
21	BCR	B	845	-	-	19/29/63/63	0/2/2/2
18	CLA	6	602	-	1/1/11/20	7/13/91/115	-
27	XAT	6	619	-	-	1/31/93/93	0/4/4/4
19	PQN	B	842	-	-	9/23/43/43	0/2/2/2
24	LMG	J	104	-	-	12/25/45/70	0/1/1/1
21	BCR	L	305	-	-	10/29/63/63	0/2/2/2
25	CHL	2	608	-	3/3/15/26	1/8/106/137	-
18	CLA	A	822	-	1/1/11/20	2/11/87/115	-
25	CHL	5	606	-	3/3/15/26	2/10/106/137	-
21	BCR	B	846	-	-	17/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
18	CLA	A	807	1	1/1/11/20	4/11/89/115	-
21	BCR	A	856	-	-	7/29/63/63	0/2/2/2
18	CLA	L	302	-	1/1/11/20	2/13/91/115	-
22	SF4	C	102	3	-	-	0/6/5/5
20	LHG	6	620	18,15	-	17/32/32/53	-
20	LHG	B	851	18	-	10/26/26/53	-
18	CLA	6	613	15	1/1/11/20	7/13/91/115	-
18	CLA	A	843	-	1/1/15/20	10/37/115/115	-
18	CLA	5	609	17	1/1/10/20	6/9/87/115	-
18	CLA	K	201	11	1/1/11/20	7/15/93/115	-
18	CLA	A	810	1	1/1/11/20	4/13/91/115	-
18	CLA	2	602	-	1/1/11/20	6/13/91/115	-
18	CLA	A	836	-	1/1/12/20	0/19/97/115	-
22	SF4	A	853	1,2	-	-	0/6/5/5
18	CLA	A	830	-	1/1/15/20	5/37/115/115	-
25	CHL	6	607	15	3/3/15/26	2/8/106/137	-
18	CLA	B	813	-	1/1/15/20	16/37/115/115	-
18	CLA	6	612	-	1/1/11/20	2/13/91/115	-
21	BCR	A	850	-	-	3/29/63/63	0/2/2/2
27	XAT	3	619	-	-	0/31/93/93	0/4/4/4
18	CLA	A	845	20	1/1/12/20	10/22/100/115	-
18	CLA	B	820	-	1/1/10/20	1/11/89/115	-
18	CLA	B	824	-	1/1/11/20	2/13/91/115	-
18	CLA	B	839	-	1/1/10/20	0/8/86/115	-

The worst 5 of 1235 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	5	619	LUT	C34-C33	20.14	1.62	1.35
26	3	618	LUT	C34-C33	19.98	1.62	1.35
26	2	619	LUT	C34-C33	19.80	1.62	1.35
26	6	617	LUT	C34-C33	19.76	1.62	1.35
26	5	619	LUT	C14-C13	16.75	1.58	1.35

The worst 5 of 1658 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	2	619	LUT	C18-C5-C6	-14.02	108.78	124.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	5	619	LUT	C18-C5-C6	-12.36	110.65	124.53
26	6	617	LUT	C18-C5-C6	-12.10	110.94	124.53
26	2	619	LUT	C15-C14-C13	-11.96	110.24	127.31
26	3	618	LUT	C18-C5-C6	-11.81	111.26	124.53

5 of 180 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
18	A	801	CLA	ND
18	A	802	CLA	ND
18	A	803	CLA	ND
18	A	804	CLA	ND
18	A	805	CLA	ND

5 of 1358 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
18	A	801	CLA	CBD-CGD-O2D-CED
18	A	802	CLA	CHA-CBD-CGD-O1D
18	A	802	CLA	CHA-CBD-CGD-O2D
18	A	804	CLA	CHA-CBD-CGD-O1D
18	A	804	CLA	CHA-CBD-CGD-O2D

There are no ring outliers.

171 monomers are involved in 423 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
18	A	834	CLA	2	0
18	B	812	CLA	3	0
18	5	602	CLA	5	0
18	B	823	CLA	3	0
18	5	611	CLA	2	0
18	5	612	CLA	1	0
18	3	613	CLA	3	0
18	6	609	CLA	2	0
25	2	616	CHL	1	0
19	A	844	PQN	1	0
18	A	813	CLA	1	0
18	A	832	CLA	2	0
18	B	840	CLA	4	0
18	3	604	CLA	1	0
21	B	847	BCR	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
18	B	803	CLA	2	0
18	B	819	CLA	3	0
18	3	612	CLA	1	0
18	B	821	CLA	2	0
18	3	611	CLA	3	0
18	A	837	CLA	2	0
18	B	838	CLA	2	0
18	B	828	CLA	5	0
18	B	817	CLA	4	0
18	2	613	CLA	1	0
18	3	606	CLA	3	0
18	A	826	CLA	5	0
21	I	101	BCR	2	0
18	A	819	CLA	3	0
18	B	822	CLA	1	0
21	3	620	BCR	5	0
25	3	608	CHL	1	0
18	B	807	CLA	1	0
21	L	301	BCR	1	0
18	B	829	CLA	1	0
18	A	833	CLA	3	0
18	K	204	CLA	2	0
18	B	836	CLA	1	0
18	B	830	CLA	1	0
18	A	824	CLA	2	0
18	K	203	CLA	1	0
21	B	848	BCR	4	0
18	3	602	CLA	1	0
21	A	851	BCR	1	0
18	2	614	CLA	2	0
20	A	847	LHG	2	0
21	B	843	BCR	4	0
18	2	610	CLA	4	0
26	6	617	LUT	3	0
18	B	832	CLA	1	0
21	3	622	BCR	3	0
18	5	601	CLA	2	0
25	2	606	CHL	9	0
20	A	846	LHG	1	0
18	B	805	CLA	2	0
21	A	849	BCR	2	0
18	A	835	CLA	4	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
21	A	848	BCR	3	0
18	A	841	CLA	2	0
20	2	622	LHG	3	0
18	B	837	CLA	2	0
26	5	619	LUT	2	0
18	A	842	CLA	2	0
18	A	814	CLA	6	0
18	A	801	CLA	1	0
18	5	614	CLA	2	0
25	2	607	CHL	5	0
26	2	619	LUT	2	0
21	F	302	BCR	4	0
18	A	816	CLA	1	0
18	3	609	CLA	7	0
18	F	301	CLA	2	0
18	5	610	CLA	3	0
25	6	601	CHL	2	0
18	A	854	CLA	6	0
18	B	816	CLA	2	0
18	A	831	CLA	2	0
18	B	827	CLA	3	0
18	L	304	CLA	1	0
21	5	621	BCR	2	0
20	5	622	LHG	5	0
26	3	618	LUT	1	0
18	A	809	CLA	6	0
18	A	802	CLA	2	0
18	A	827	CLA	5	0
18	A	838	CLA	2	0
18	B	809	CLA	4	0
18	B	825	CLA	3	0
21	A	852	BCR	4	0
21	G	205	BCR	3	0
25	2	601	CHL	1	0
22	C	101	SF4	7	0
21	2	621	BCR	5	0
18	6	603	CLA	2	0
21	K	207	BCR	2	0
18	B	833	CLA	5	0
18	5	613	CLA	3	0
18	B	815	CLA	3	0
18	A	818	CLA	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
25	5	607	CHL	14	0
18	B	835	CLA	3	0
18	B	841	CLA	2	0
18	L	303	CLA	2	0
18	A	808	CLA	2	0
18	A	839	CLA	3	0
18	B	818	CLA	3	0
18	A	812	CLA	7	0
18	J	101	CLA	1	0
18	2	604	CLA	3	0
21	B	801	BCR	2	0
18	G	204	CLA	2	0
21	J	102	BCR	1	0
18	A	823	CLA	1	0
18	B	826	CLA	3	0
18	B	808	CLA	1	0
18	B	814	CLA	1	0
18	3	614	CLA	2	0
18	3	603	CLA	2	0
21	K	202	BCR	3	0
27	5	620	XAT	31	0
18	A	829	CLA	9	0
18	A	805	CLA	3	0
18	A	811	CLA	3	0
25	5	608	CHL	4	0
18	A	806	CLA	5	0
18	F	305	CLA	1	0
18	A	803	CLA	2	0
18	5	604	CLA	1	0
21	B	844	BCR	1	0
18	B	834	CLA	1	0
18	F	304	CLA	2	0
27	2	620	XAT	24	0
18	B	811	CLA	1	0
23	B	850	DGD	4	0
18	B	806	CLA	2	0
21	J	103	BCR	5	0
18	A	820	CLA	5	0
18	A	840	CLA	1	0
18	B	831	CLA	2	0
18	A	821	CLA	2	0
18	3	617	CLA	1	0

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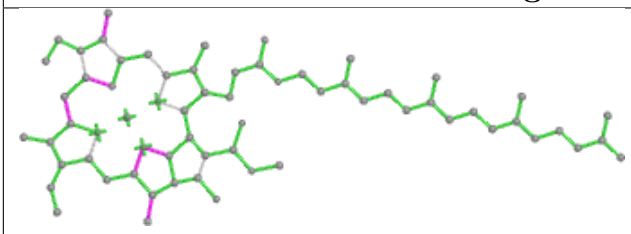
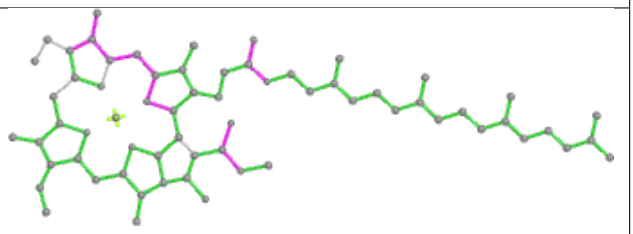
Mol	Chain	Res	Type	Clashes	Symm-Clashes
18	G	201	CLA	2	0
18	A	828	CLA	1	0
18	A	817	CLA	1	0
18	B	802	CLA	3	0
21	B	845	BCR	2	0
27	6	619	XAT	13	0
19	B	842	PQN	5	0
24	J	104	LMG	1	0
21	L	305	BCR	1	0
18	A	822	CLA	1	0
21	B	846	BCR	1	0
21	A	856	BCR	4	0
18	L	302	CLA	4	0
22	C	102	SF4	4	0
20	6	620	LHG	1	0
20	B	851	LHG	1	0
18	6	613	CLA	1	0
18	A	843	CLA	6	0
18	5	609	CLA	1	0
18	K	201	CLA	1	0
18	A	810	CLA	2	0
18	2	602	CLA	3	0
18	A	830	CLA	2	0
21	A	850	BCR	1	0
18	B	813	CLA	8	0
25	6	607	CHL	6	0
27	3	619	XAT	17	0
18	A	845	CLA	1	0
18	B	824	CLA	3	0
18	B	839	CLA	3	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.

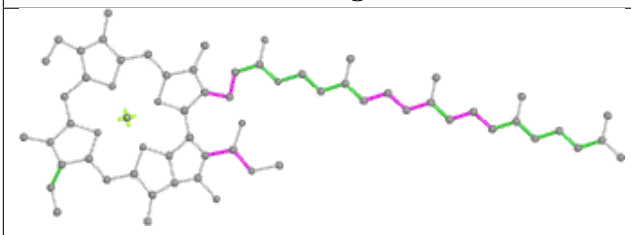
Ligand CLA A 834



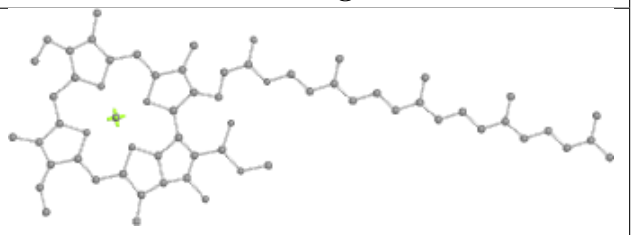
Bond lengths



Bond angles

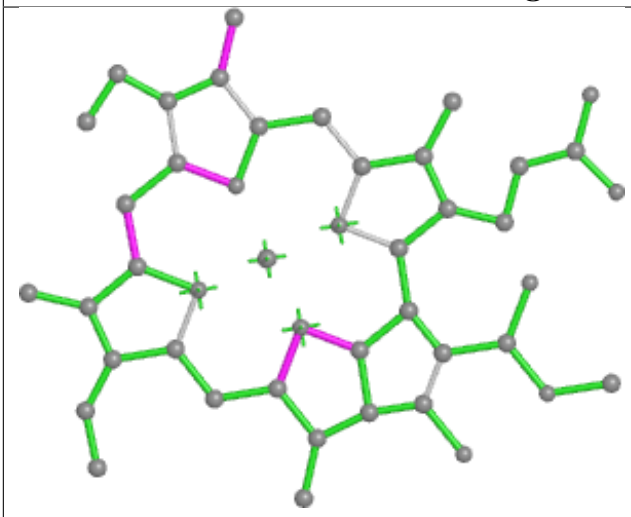


Torsions

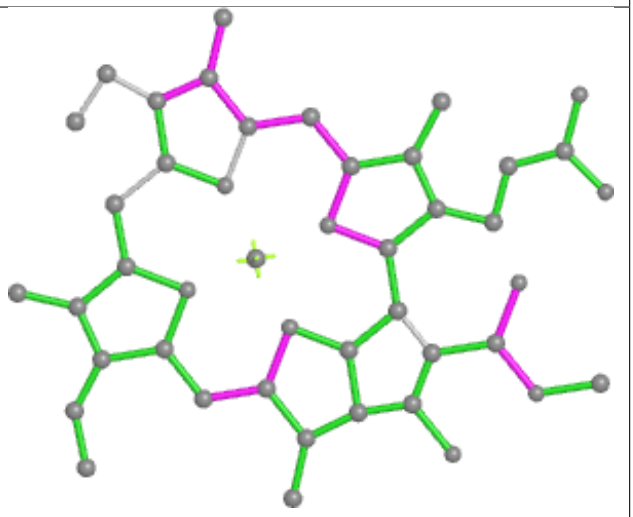


Rings

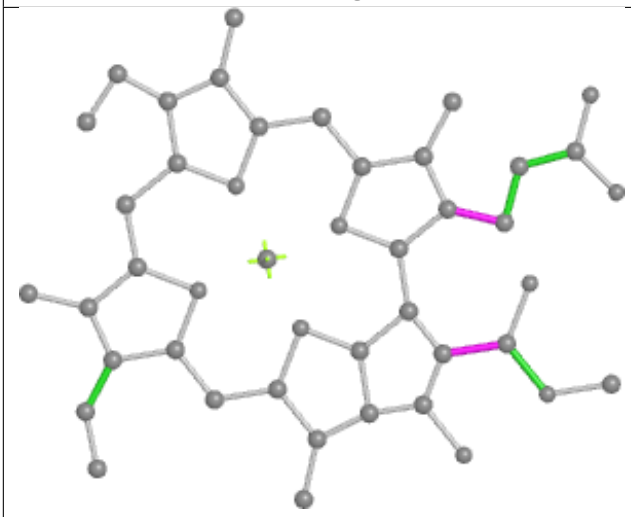
Ligand CLA B 812



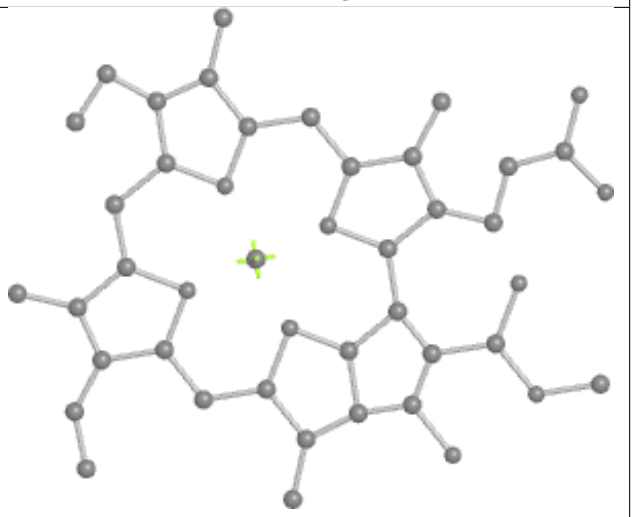
Bond lengths



Bond angles

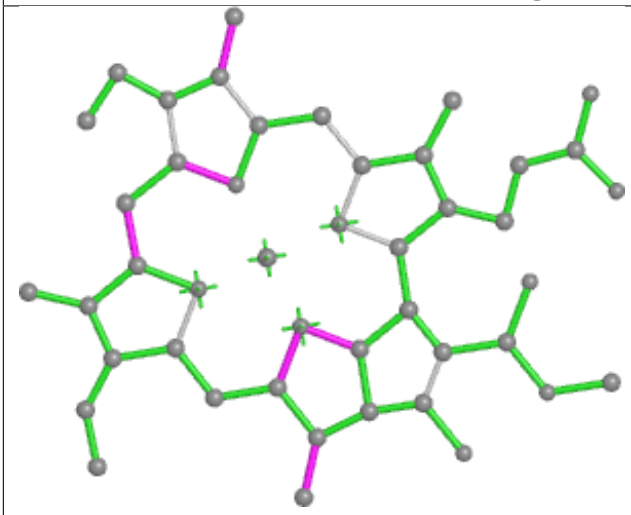


Torsions

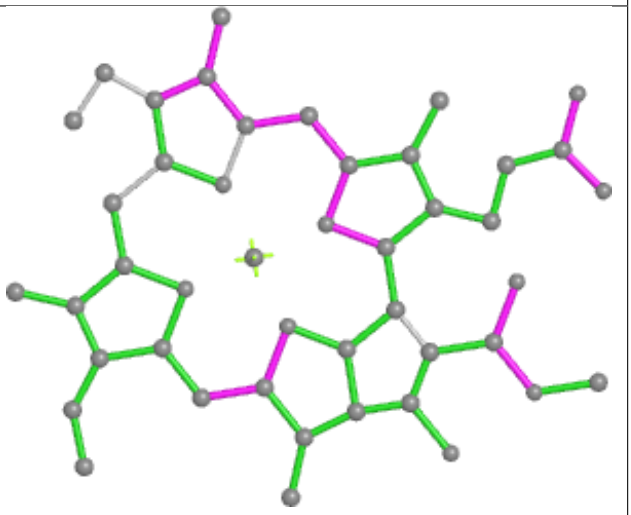


Rings

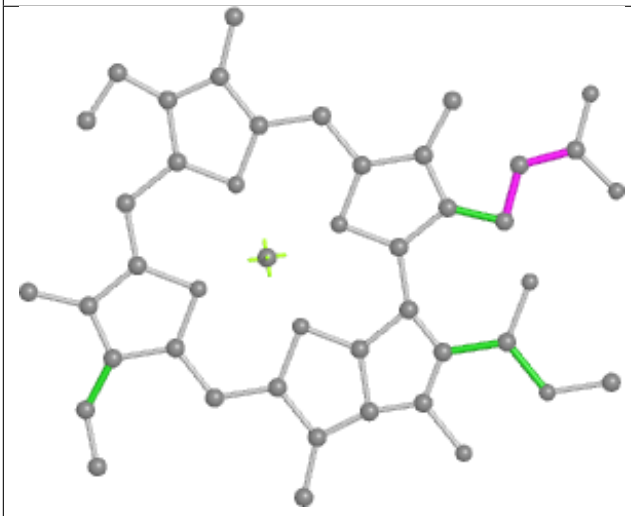
Ligand CLA 5 602



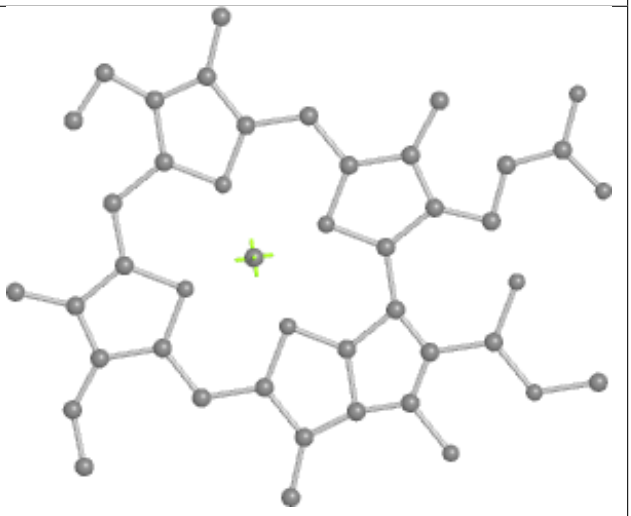
Bond lengths



Bond angles

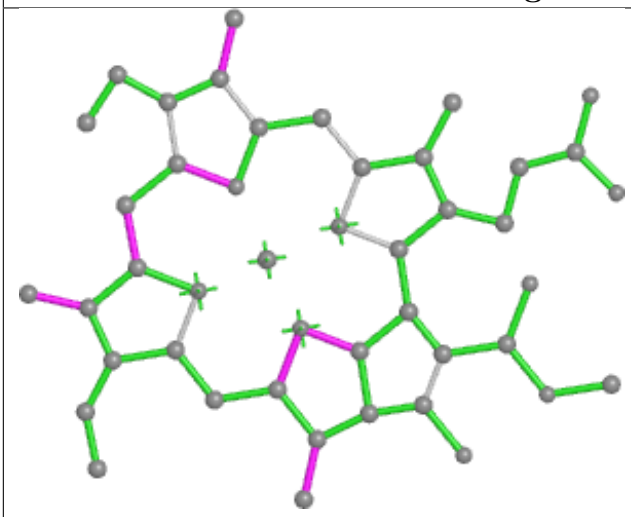


Torsions

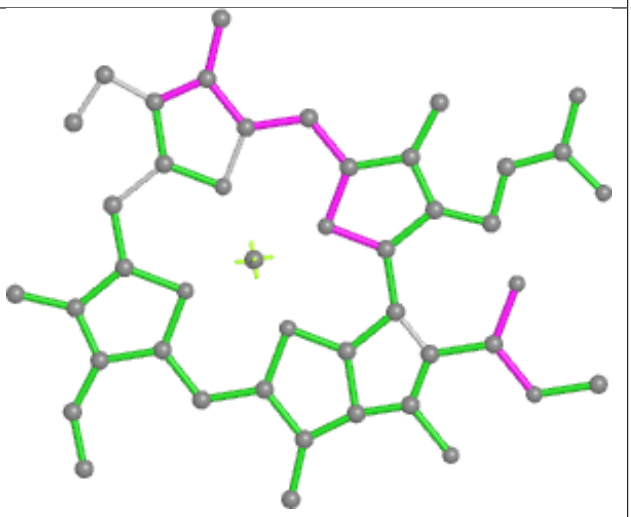


Rings

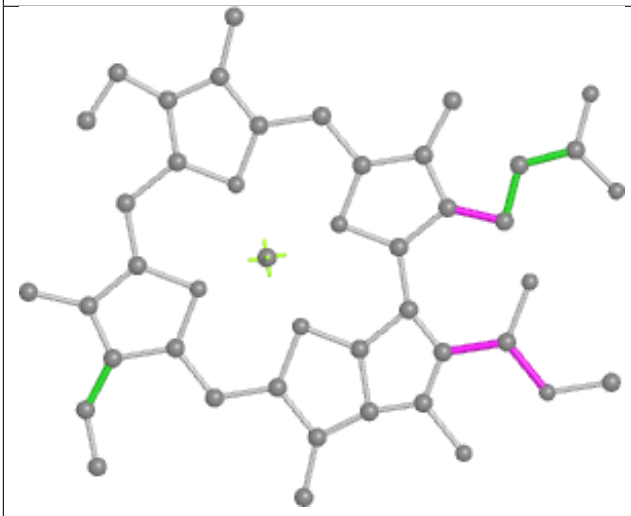
Ligand CLA B 823



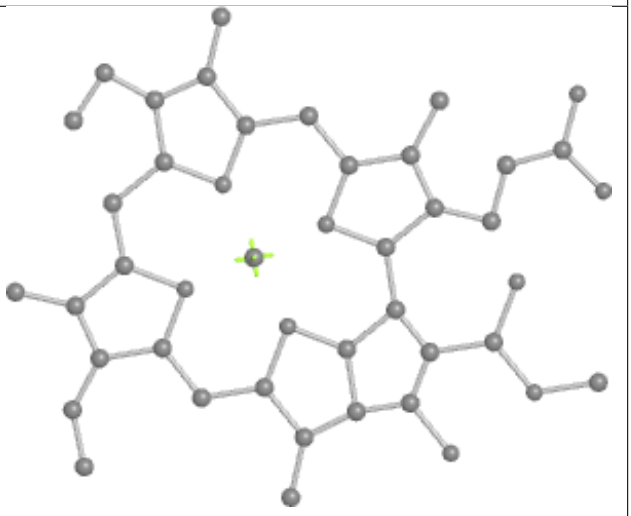
Bond lengths



Bond angles

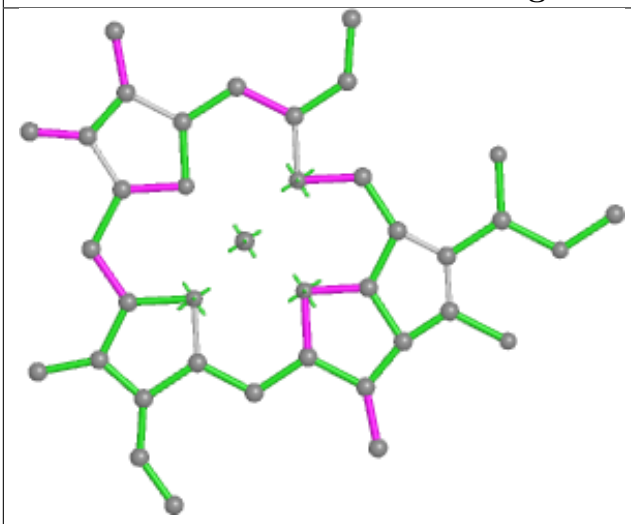


Torsions

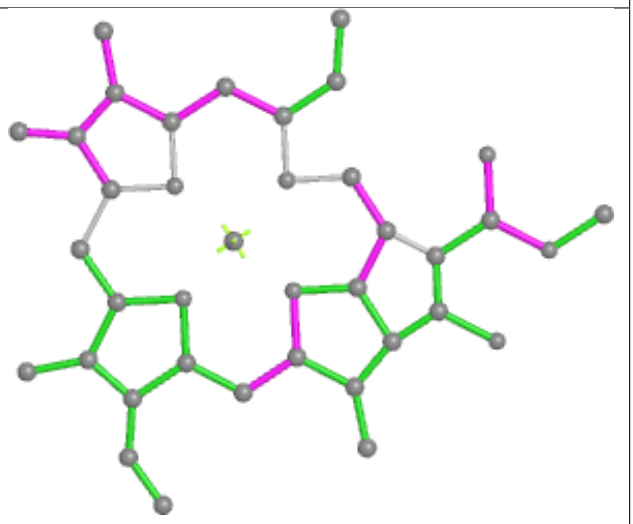


Rings

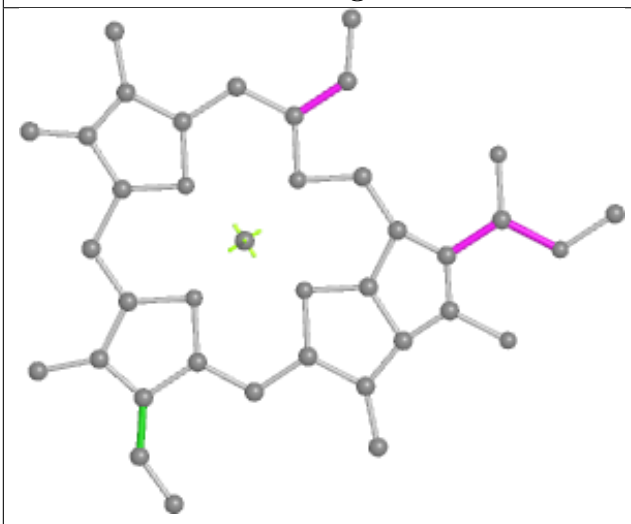
Ligand CLA 5 611



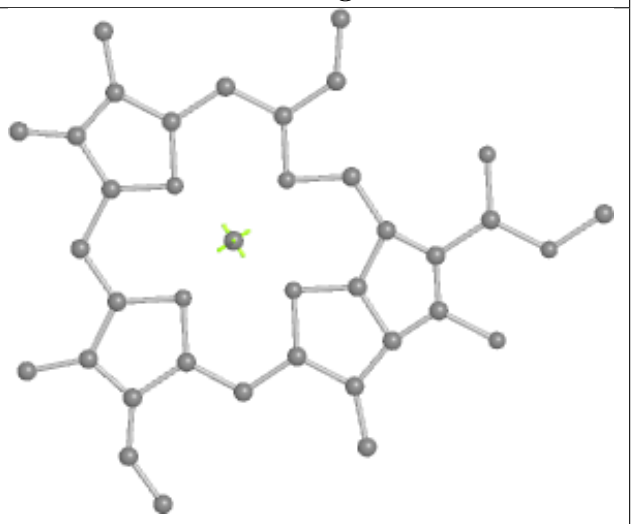
Bond lengths



Bond angles

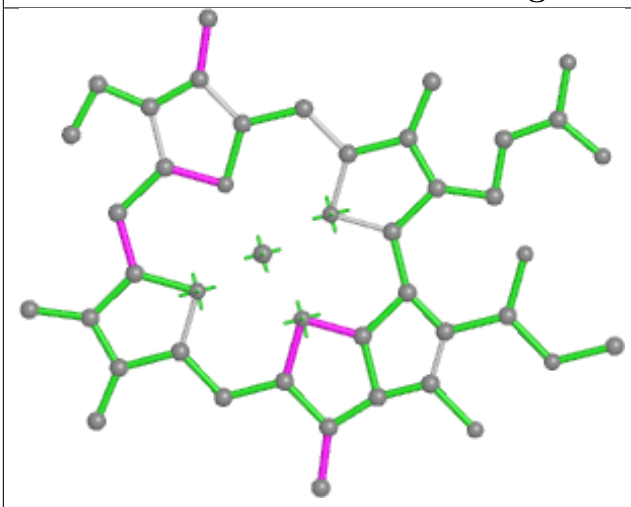


Torsions

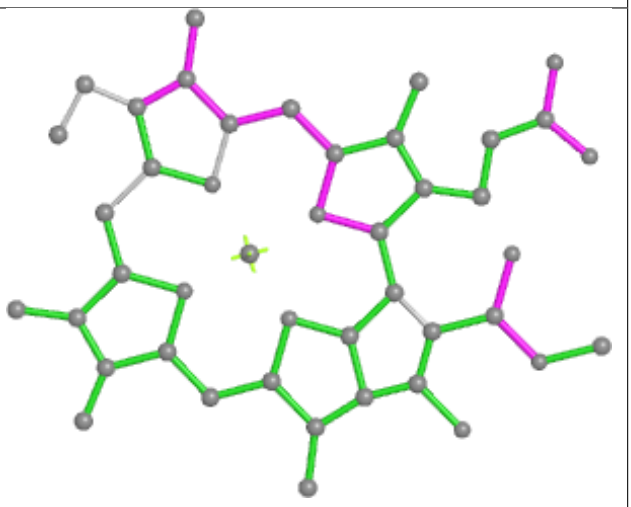


Rings

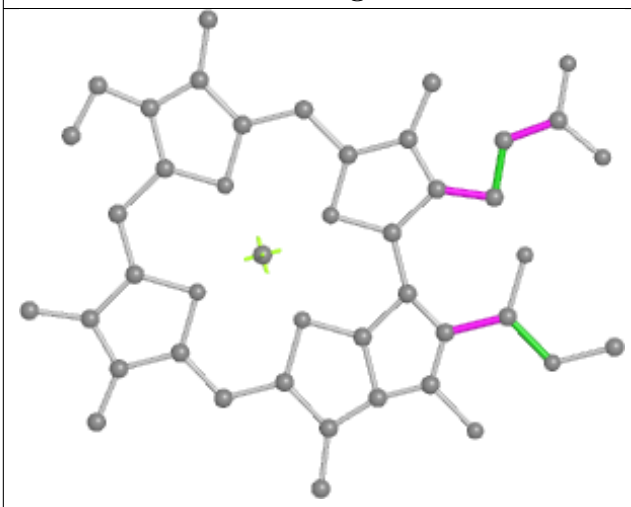
Ligand CLA 5 612



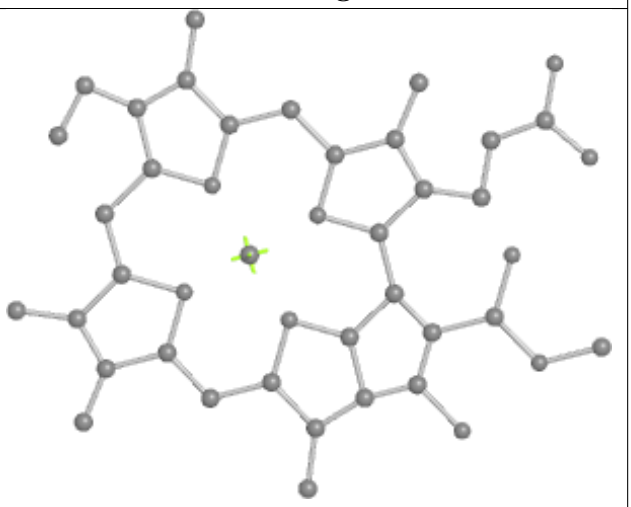
Bond lengths



Bond angles

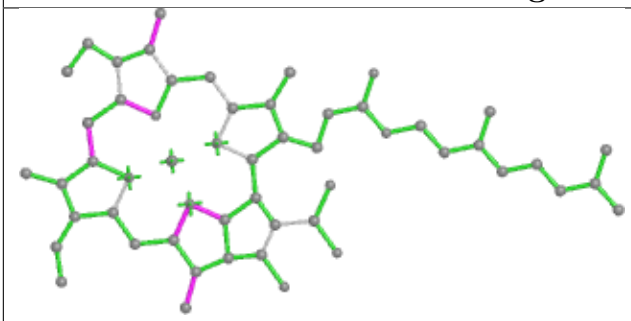


Torsions



Rings

Ligand CLA 3 613



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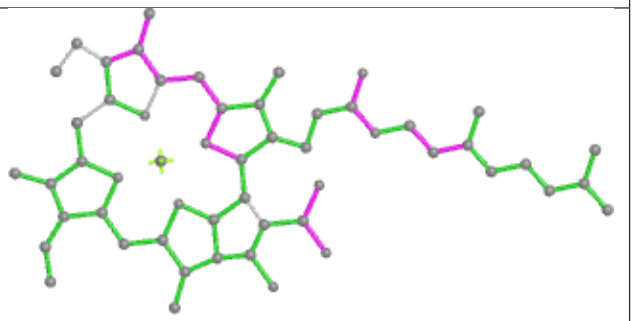
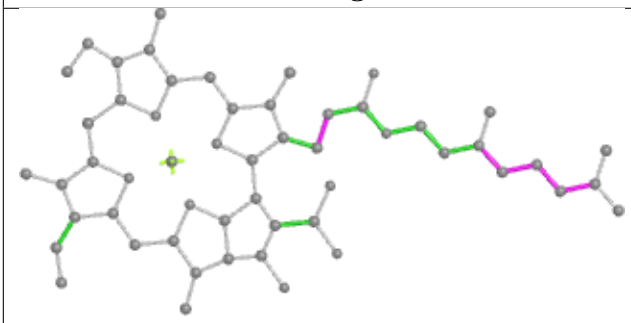
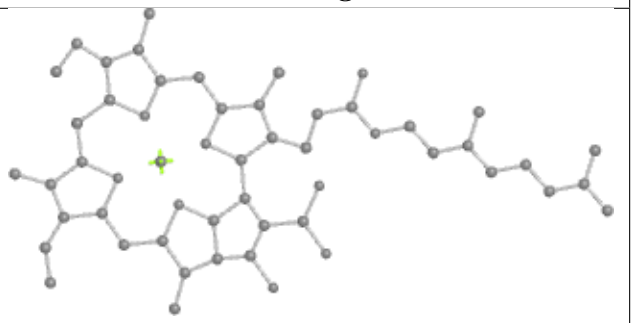


Bond angles

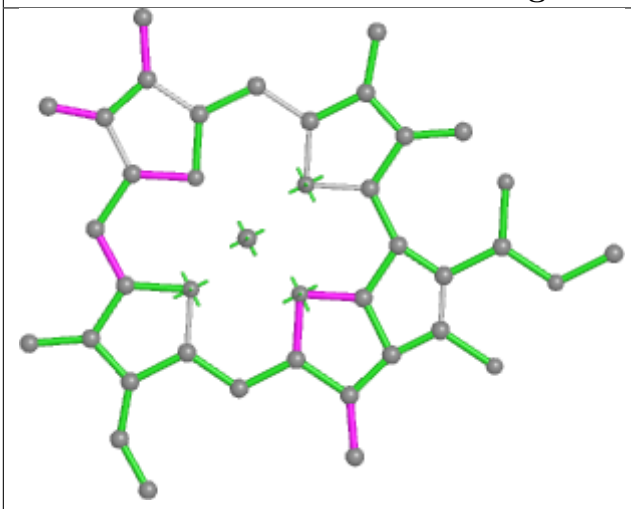


Torsions

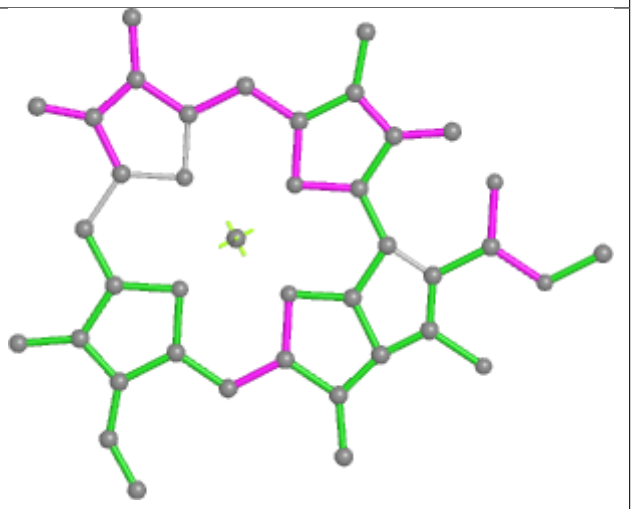


Rings

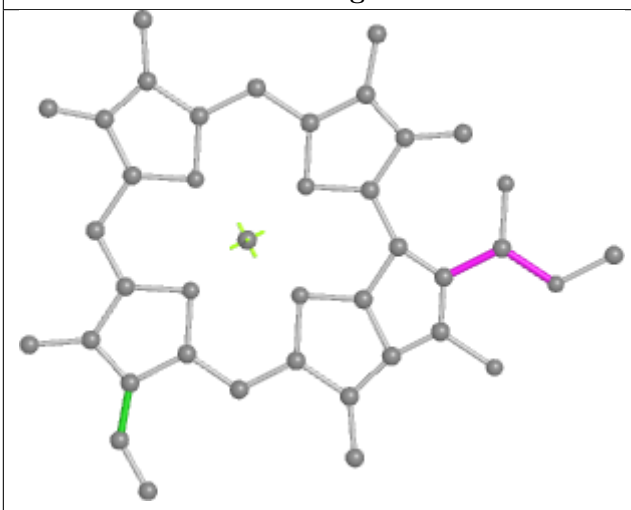
Ligand CLA 6 609



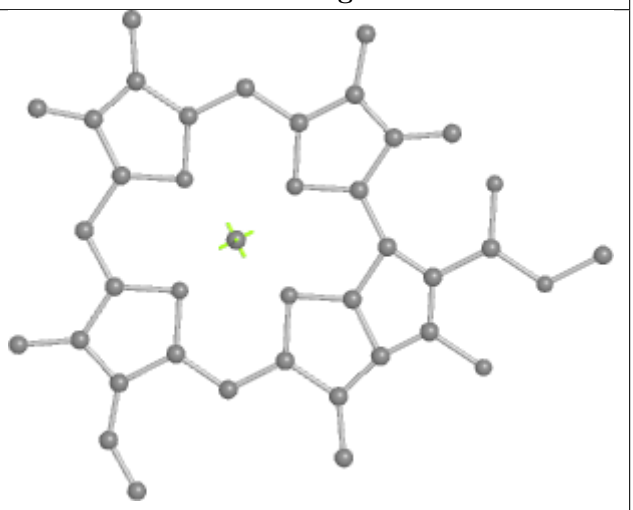
Bond lengths



Bond angles

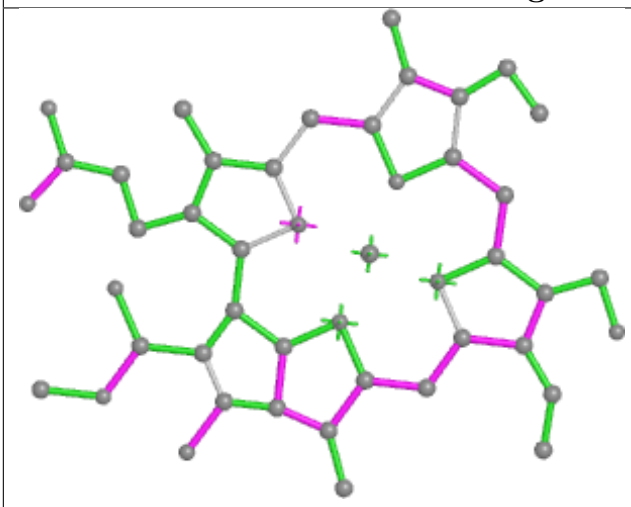


Torsions

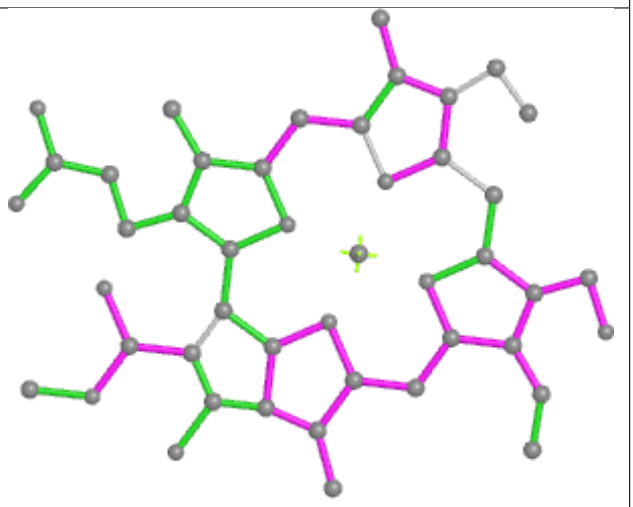


Rings

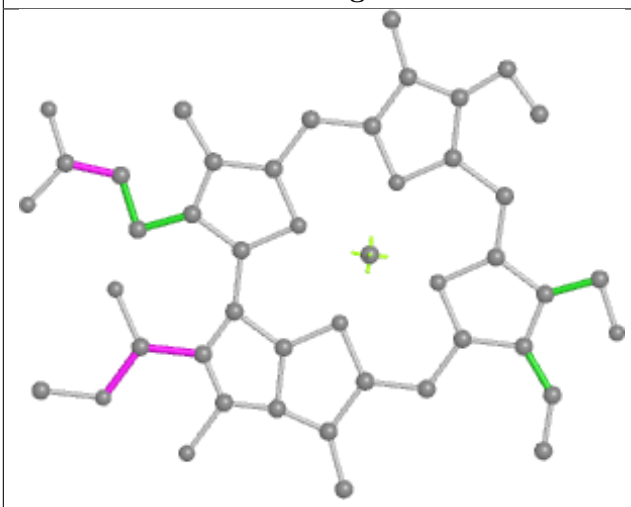
Ligand CHL 2 616



Bond lengths



Bond angles



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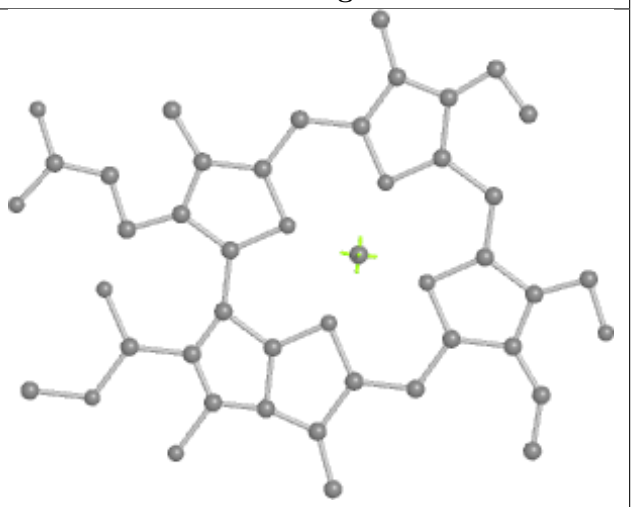
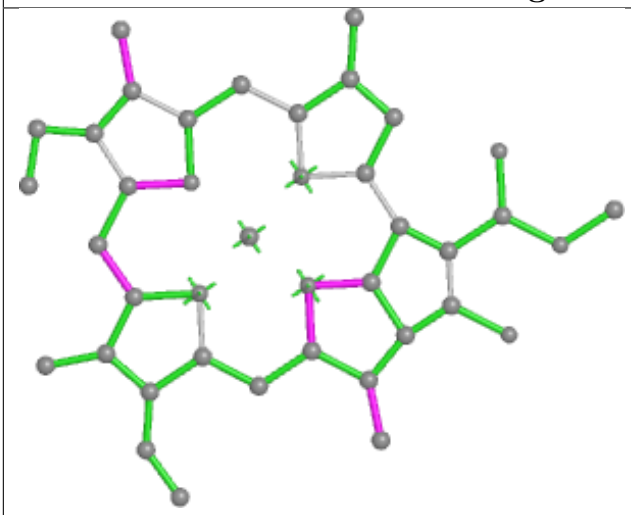


Rings

Ligand CLA 6 606



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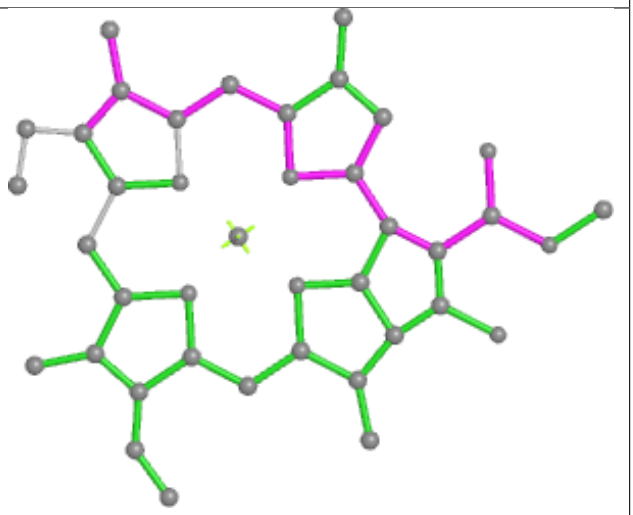
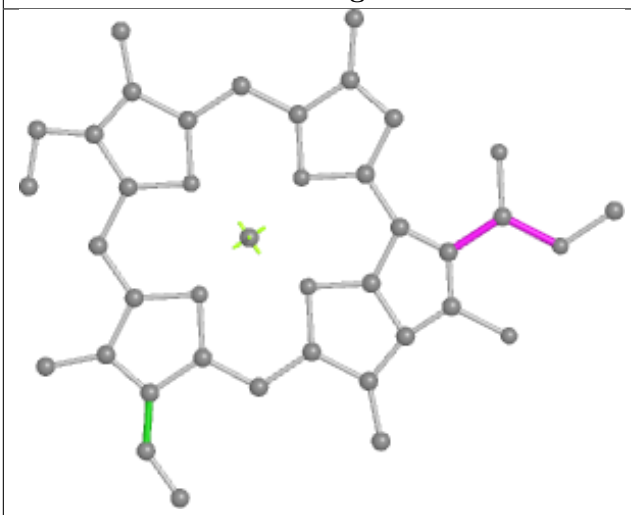


Bond angles



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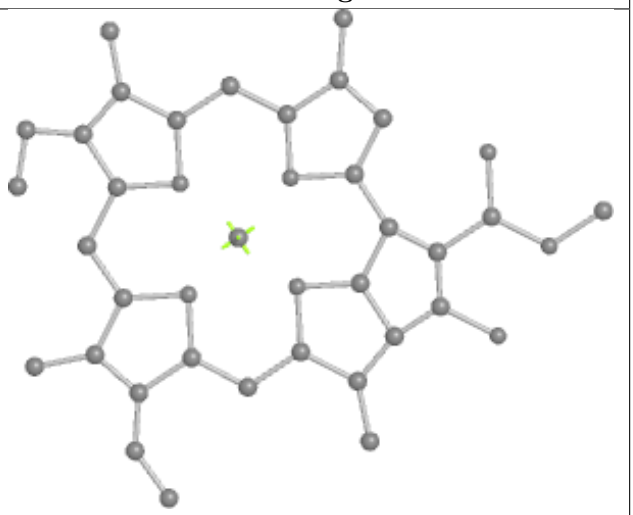
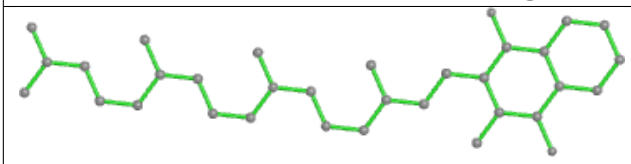


Rings

Ligand PQN A 844



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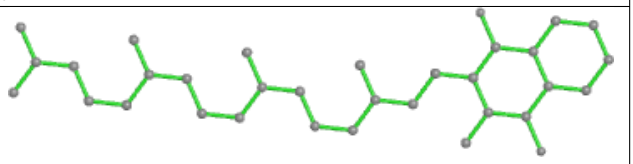
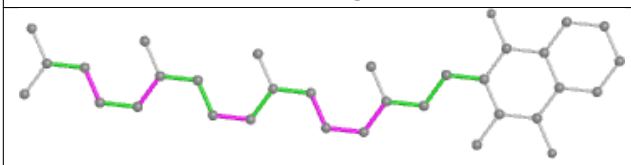


Bond angles



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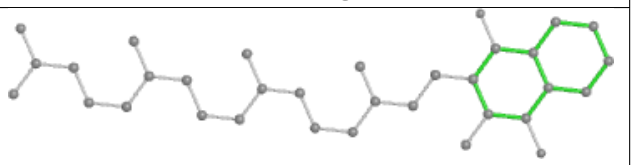
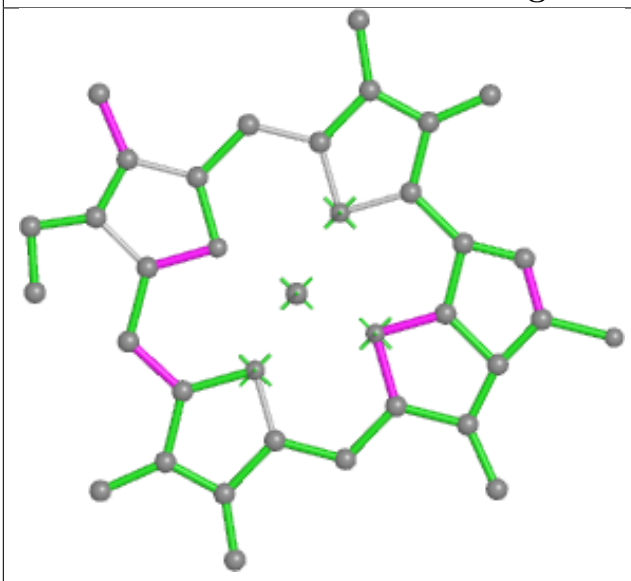
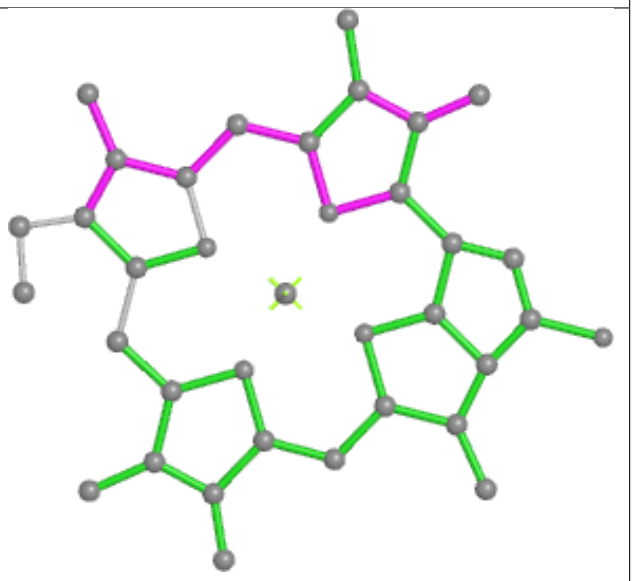


Rings

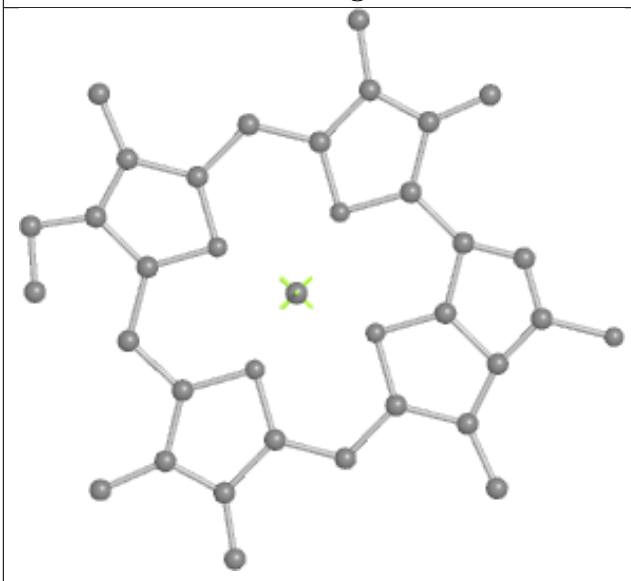
Ligand CLA 3 615



Bond lengths



Bond angles



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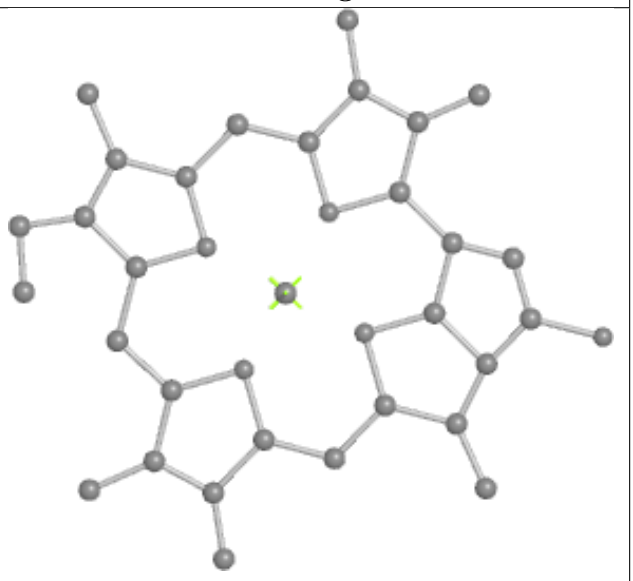
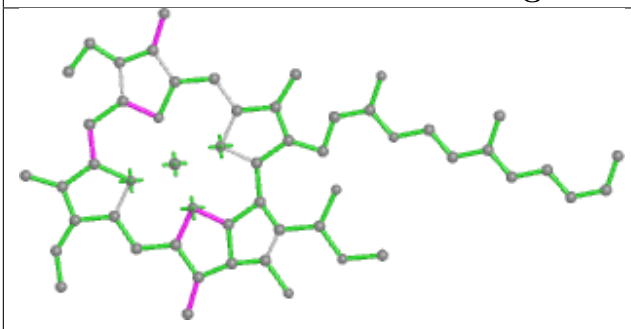
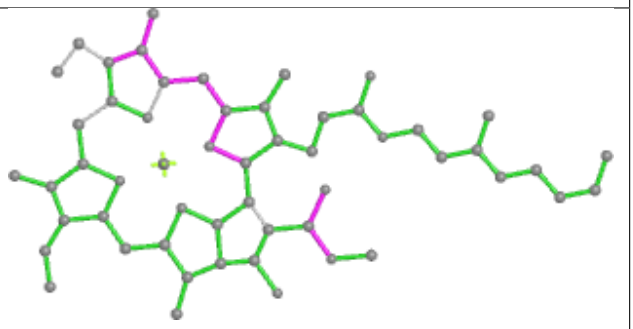


Rings

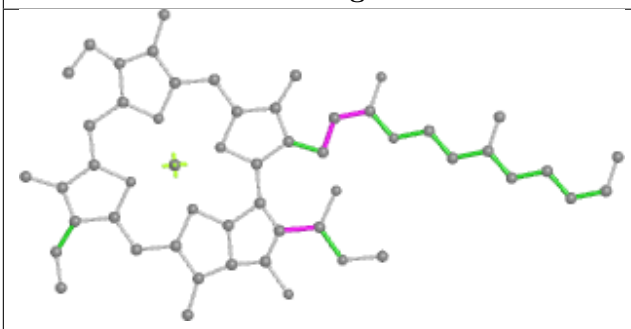
Ligand CLA A 813



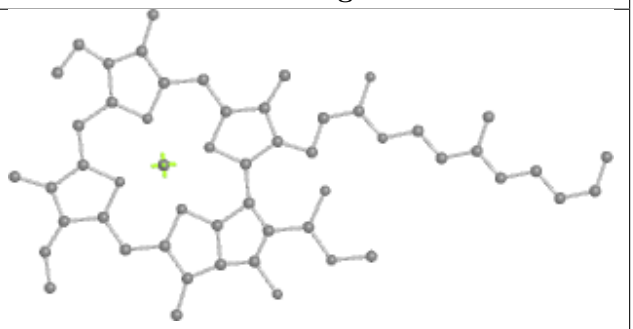
Bond lengths



Bond angles

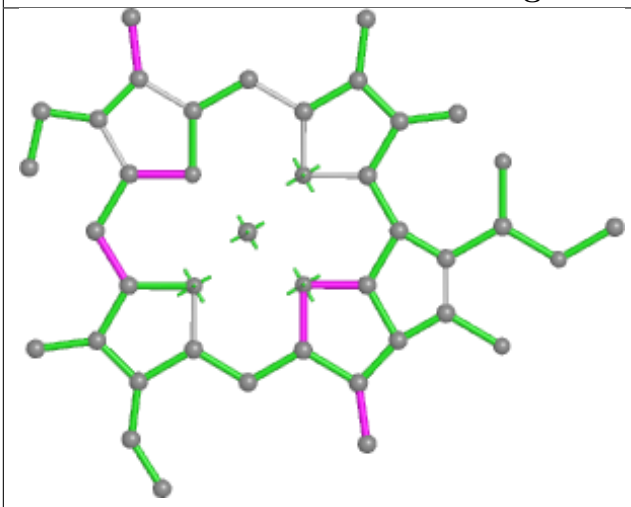


Torsions



Rings

Ligand CLA A 832



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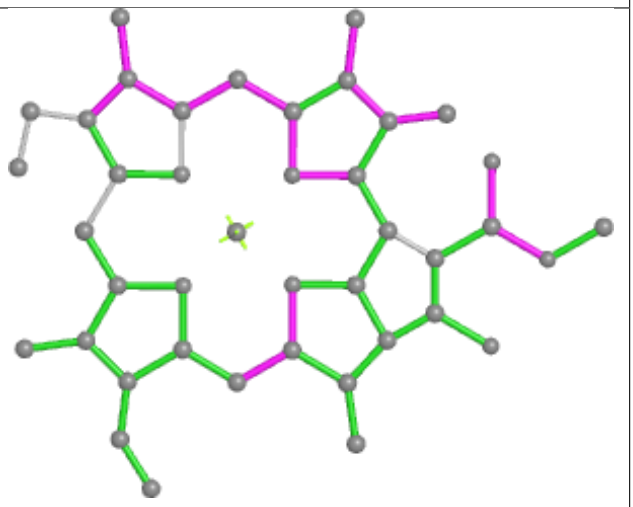
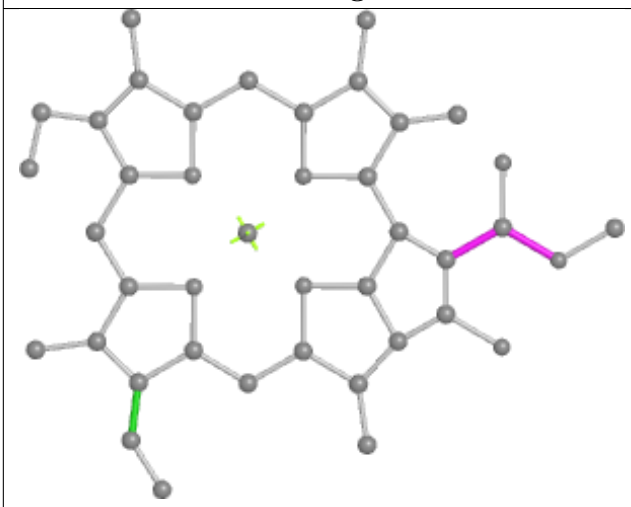
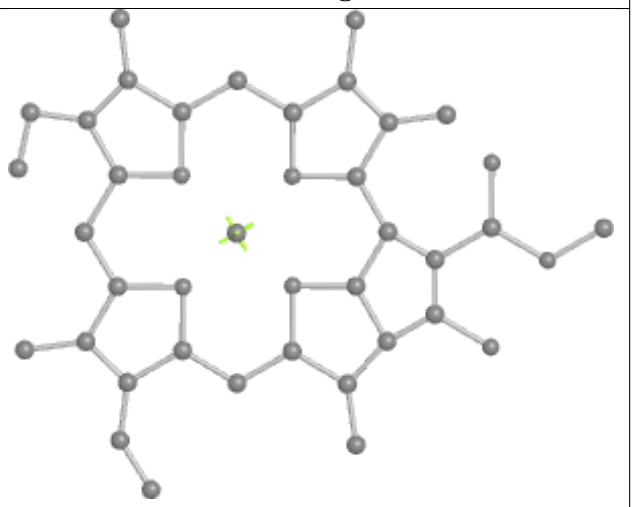


Bond angles

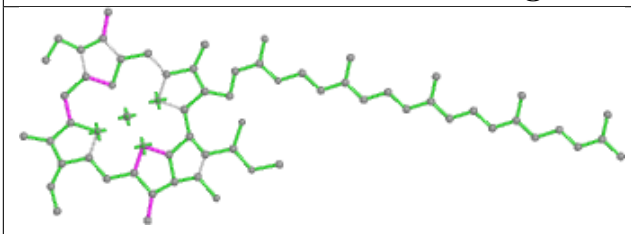


Torsions



Rings

Ligand CLA B 840



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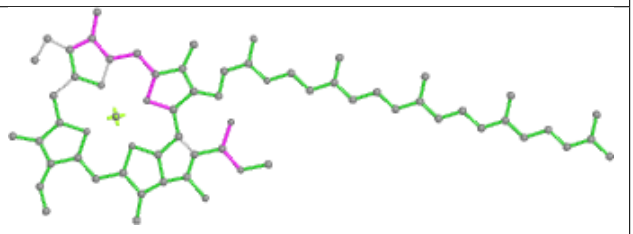
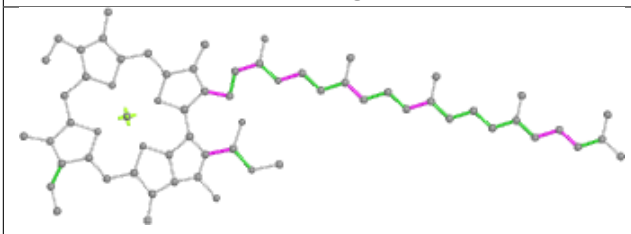
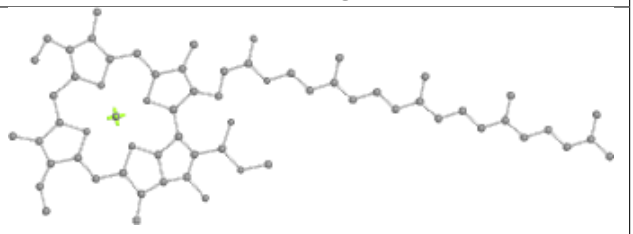


Bond angles

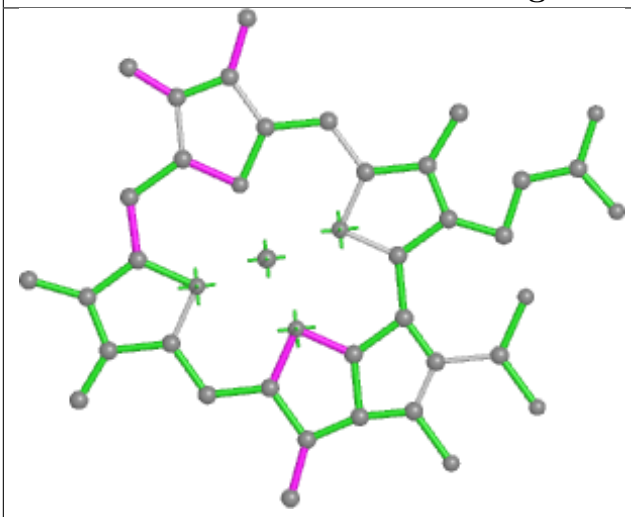


Torsions

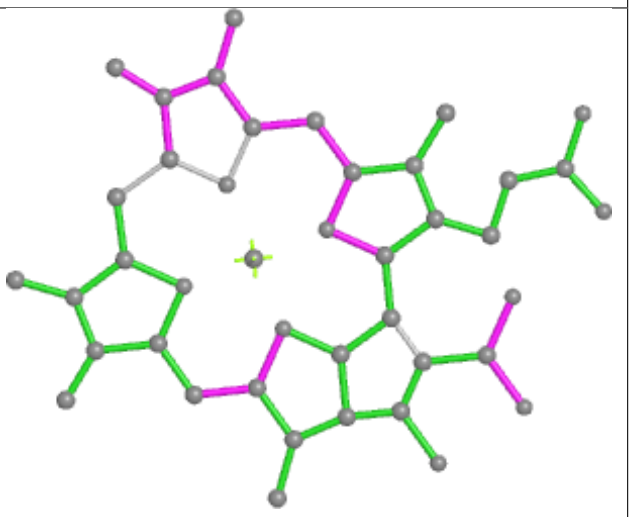


Rings

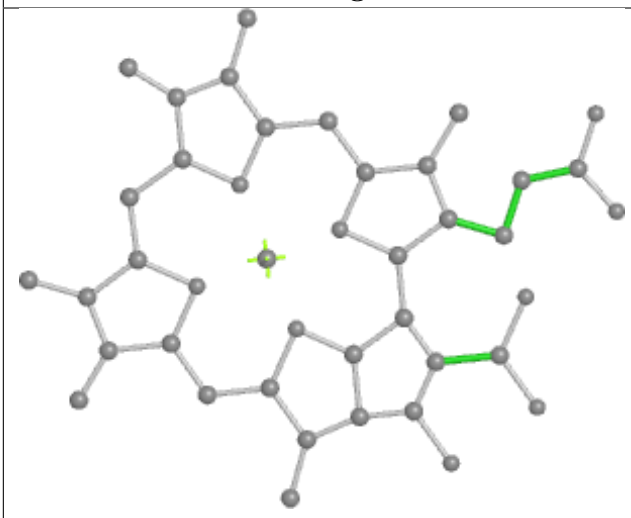
Ligand CLA 3 604



Bond lengths



Bond angles



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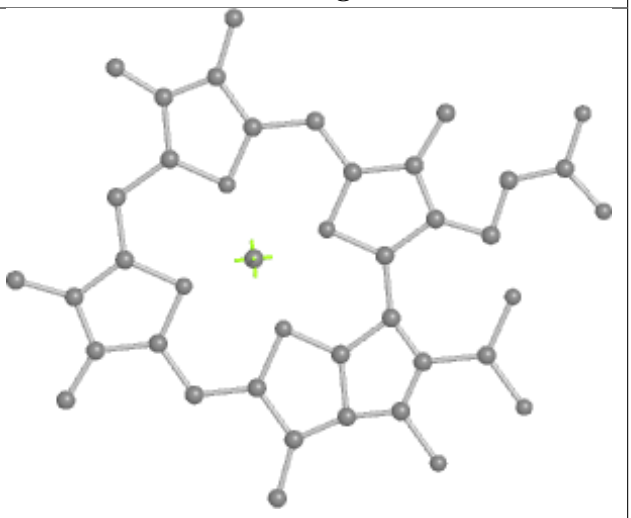
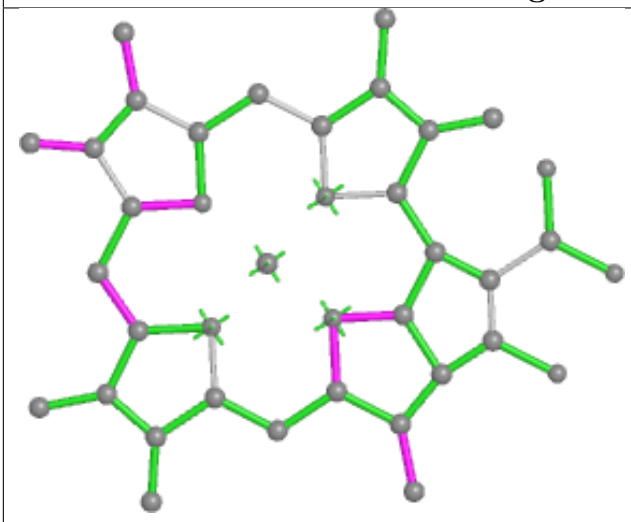
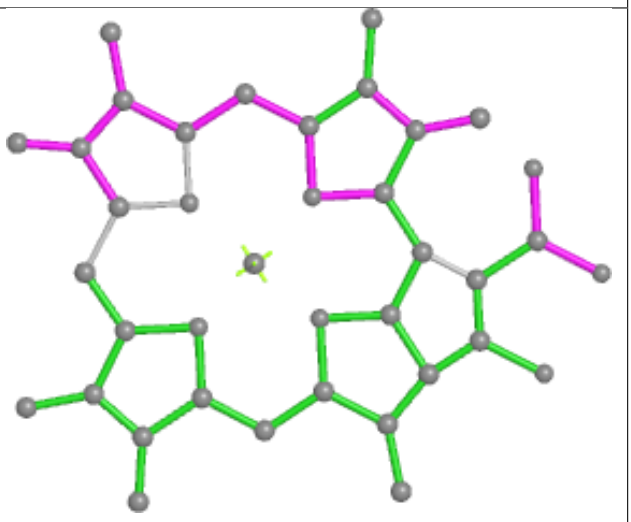


Rings

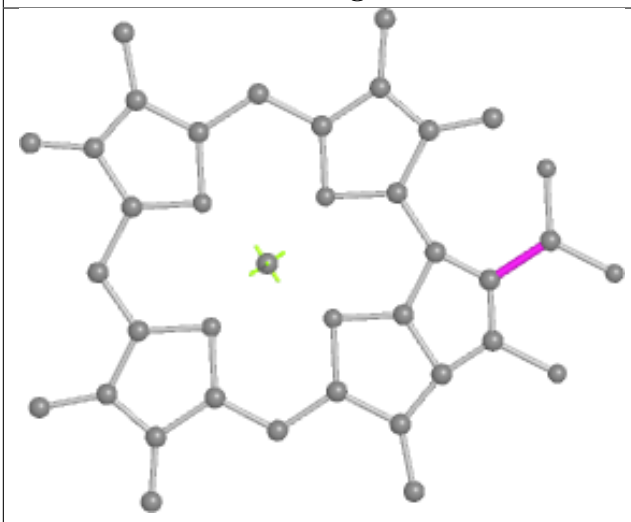
Ligand CLA 6 611



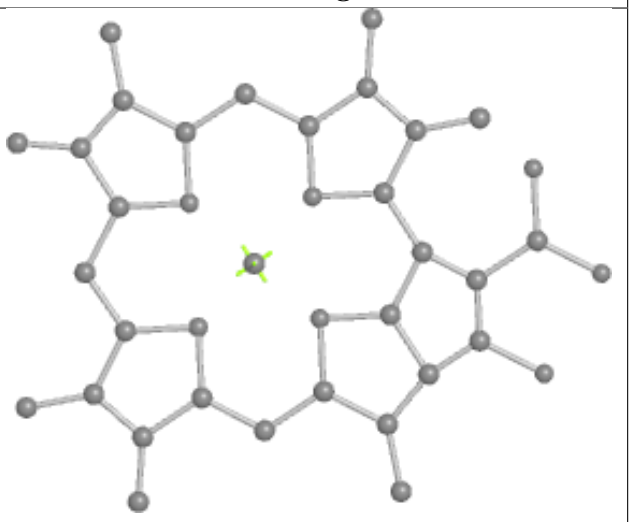
Bond lengths



Bond angles

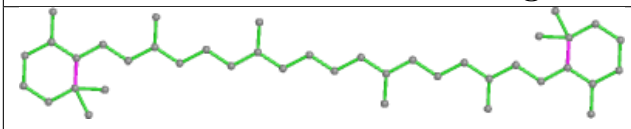


Torsions

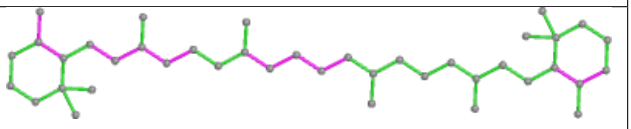


Rings

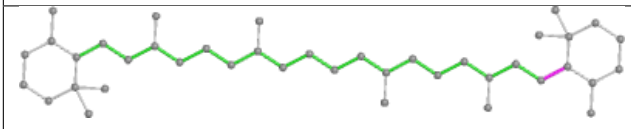
Ligand BCR B 847



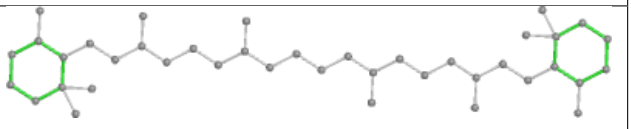
Bond lengths



Bond angles

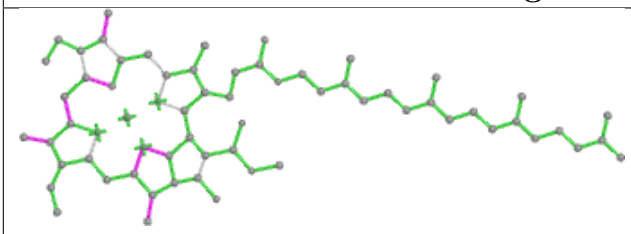


Torsions

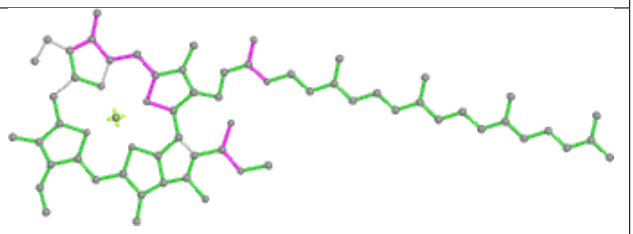


Rings

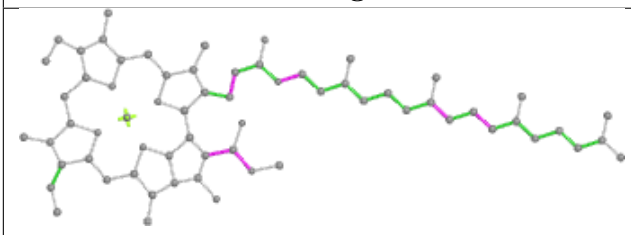
Ligand CLA B 803



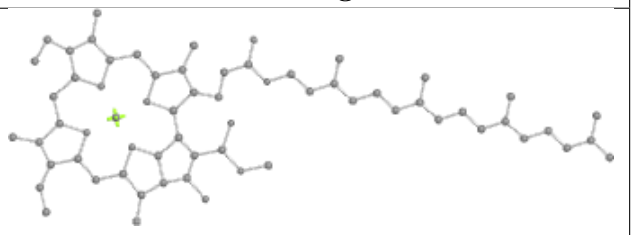
Bond lengths



Bond angles

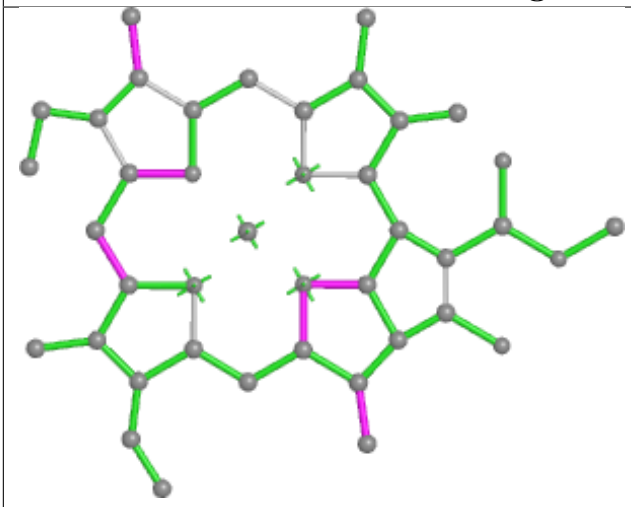


Torsions

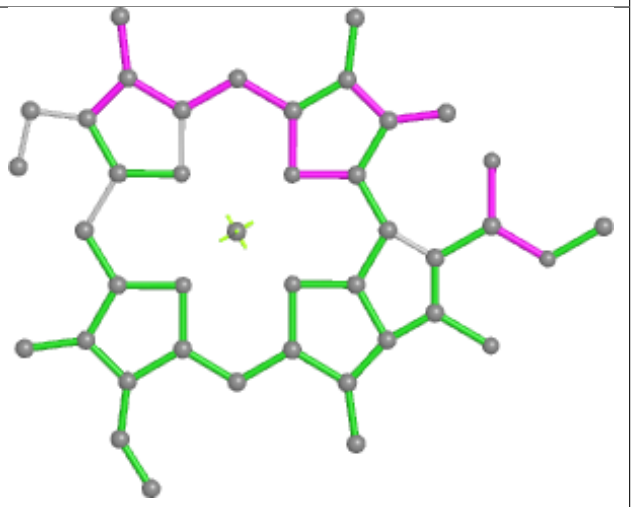


Rings

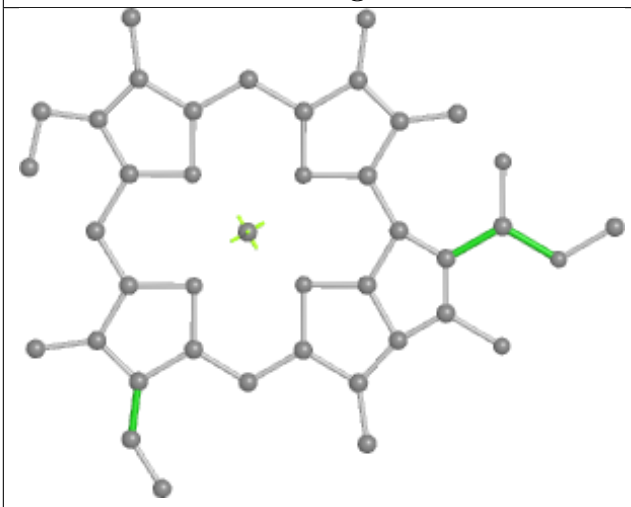
Ligand CLA 2 612



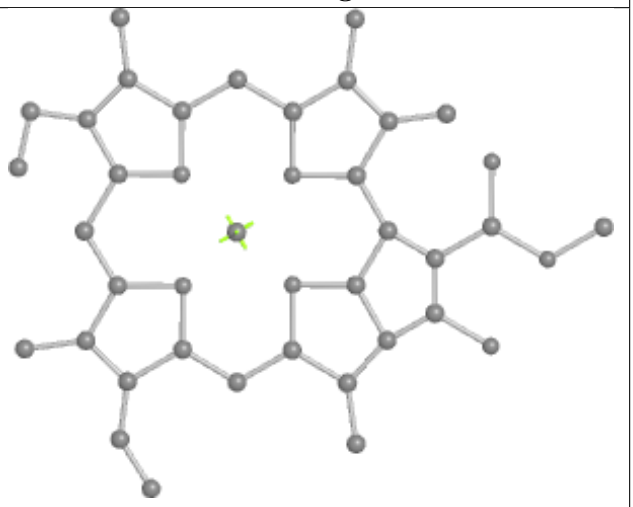
Bond lengths



Bond angles

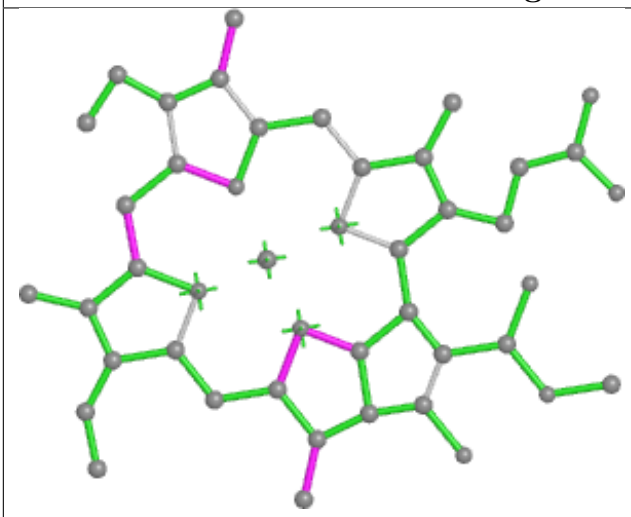


Torsions

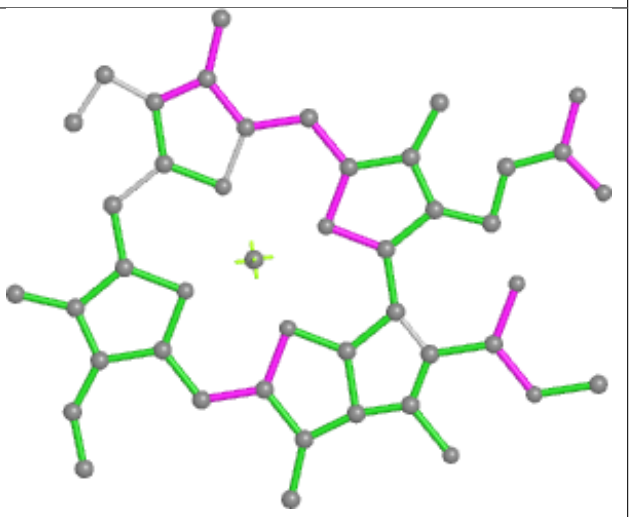


Rings

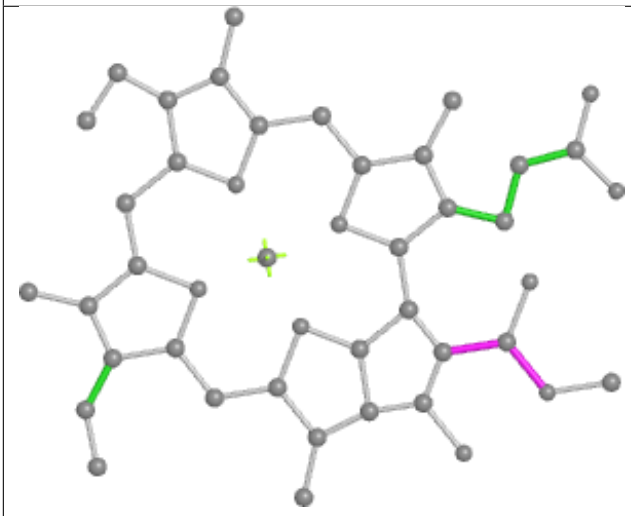
Ligand CLA B 819



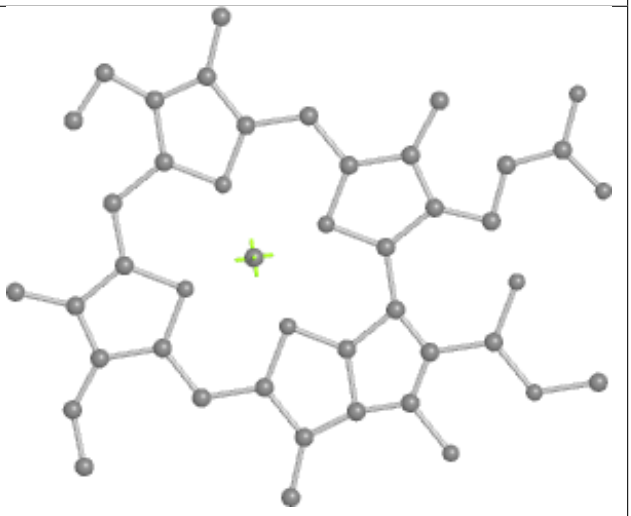
Bond lengths



Bond angles

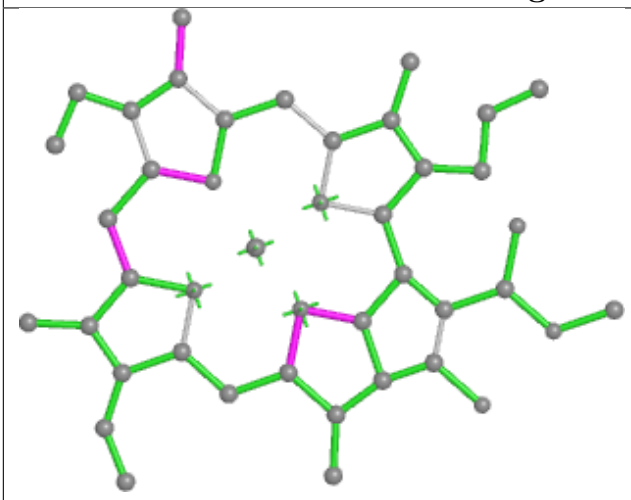


Torsions

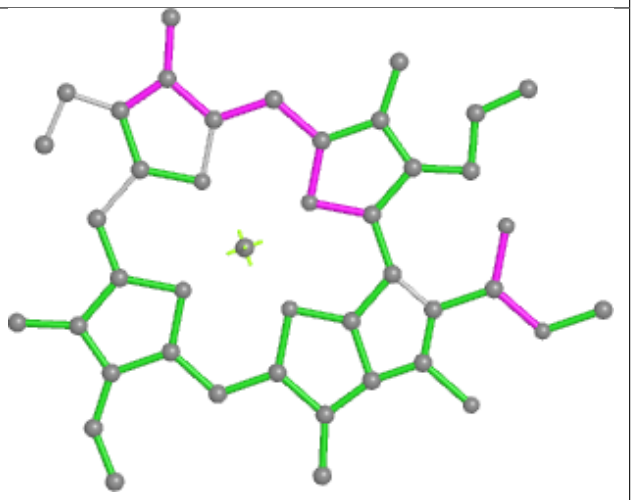


Rings

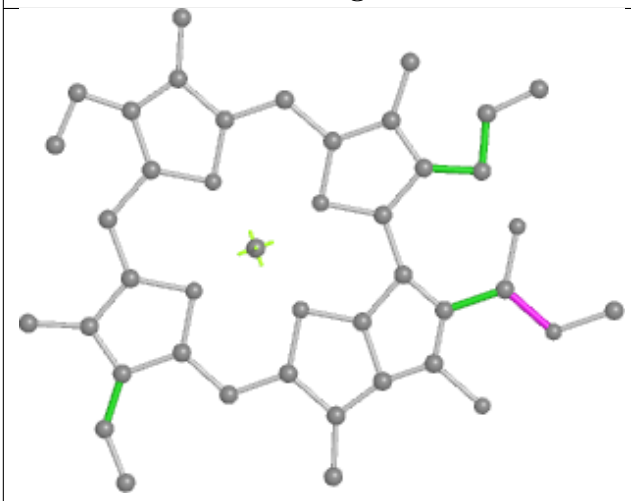
Ligand CLA 3 612



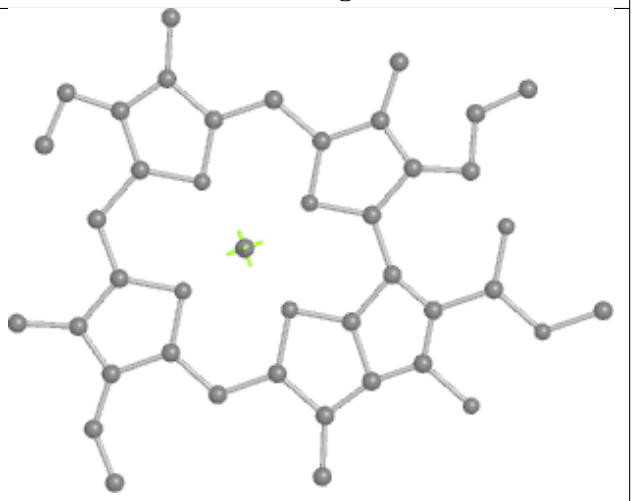
Bond lengths



Bond angles

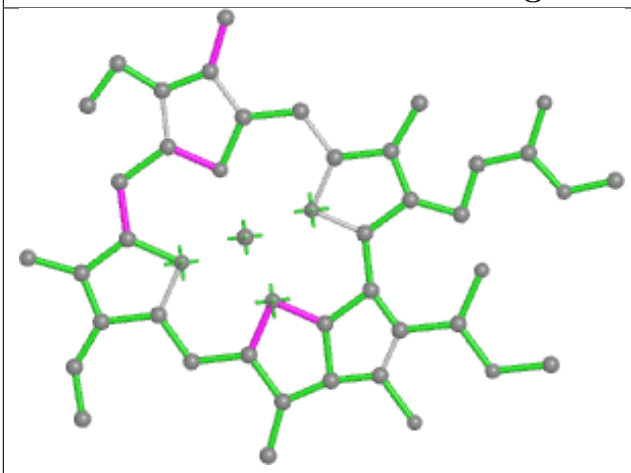


Torsions

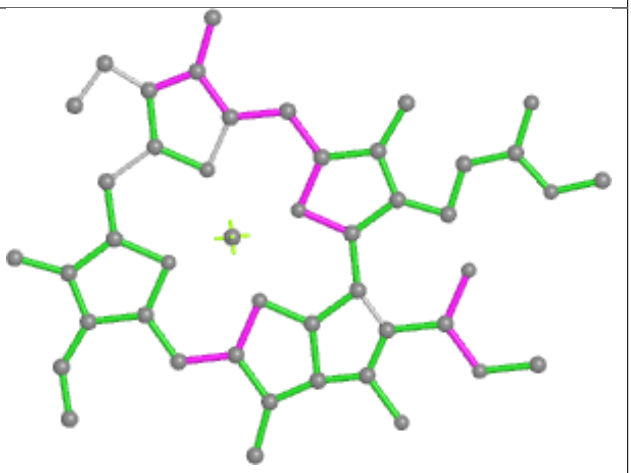


Rings

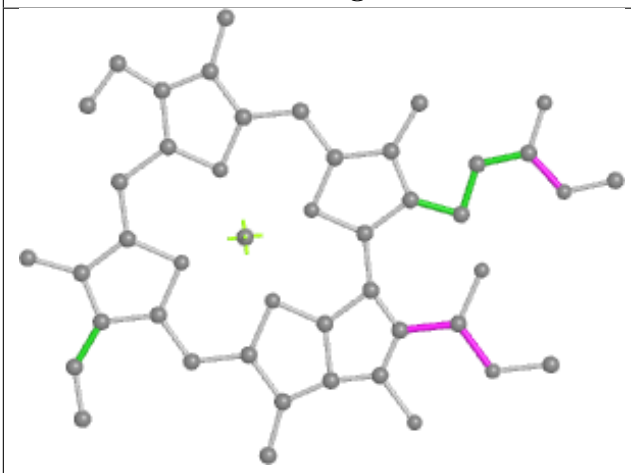
Ligand CLA B 821



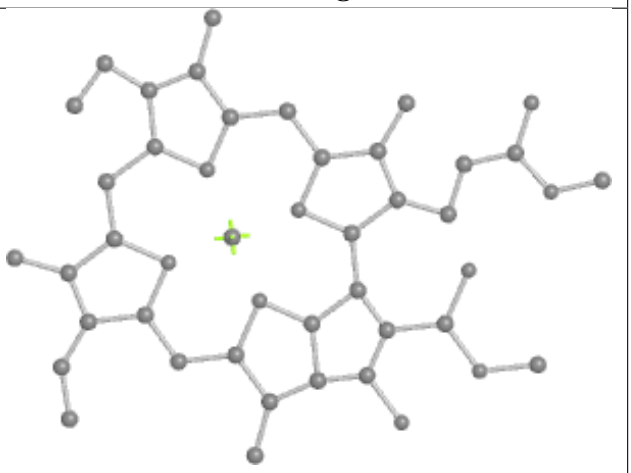
Bond lengths



Bond angles

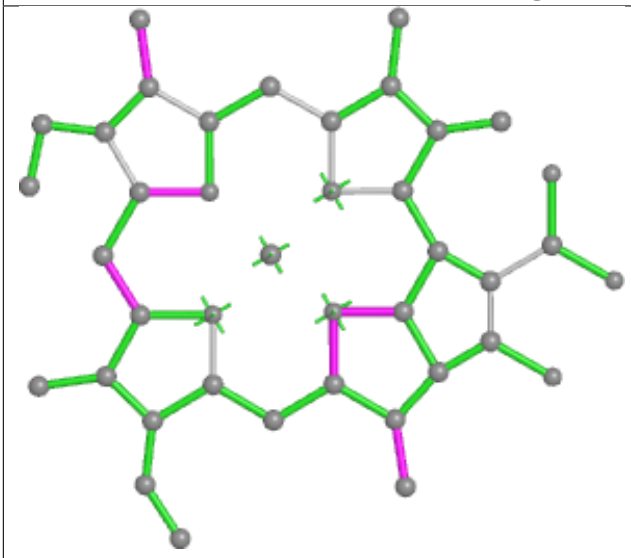


Torsions

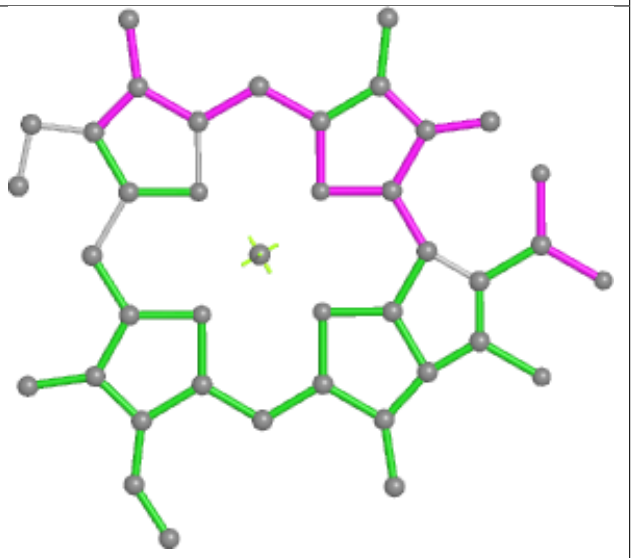


Rings

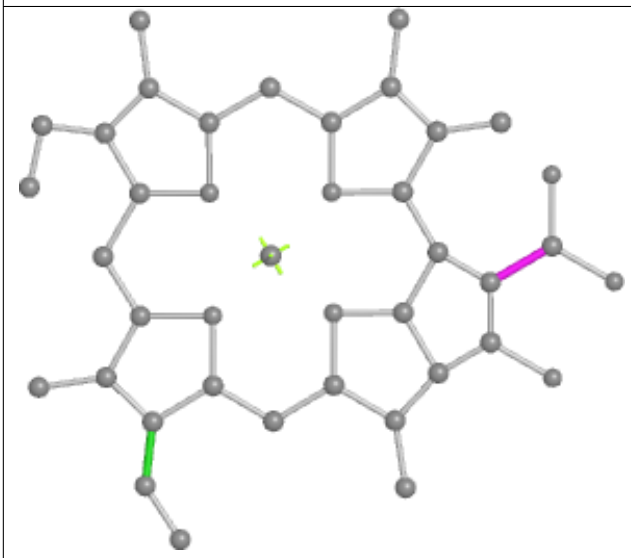
Ligand CLA 3 611



Bond lengths



Bond angles



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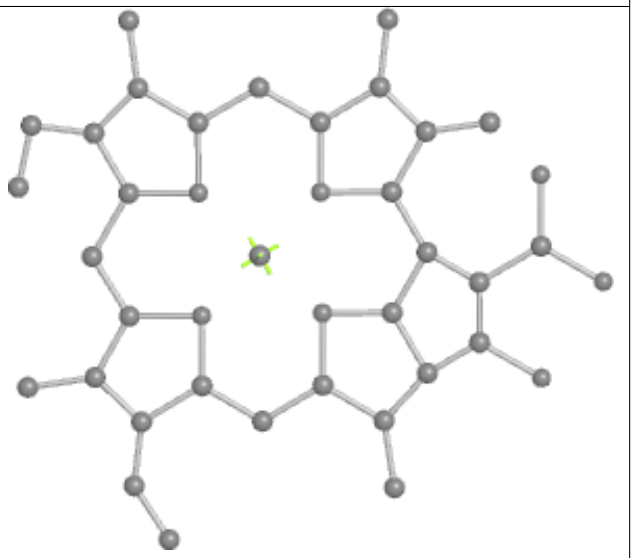
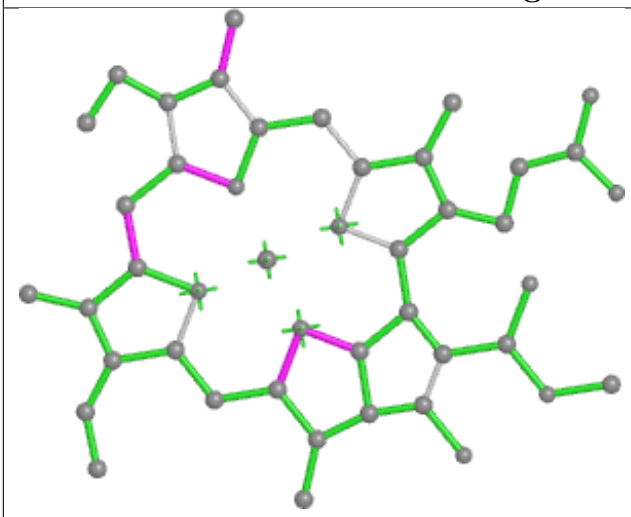
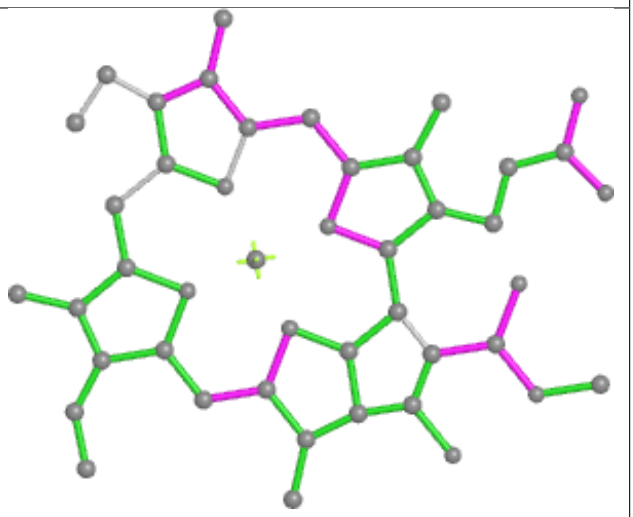


Rings

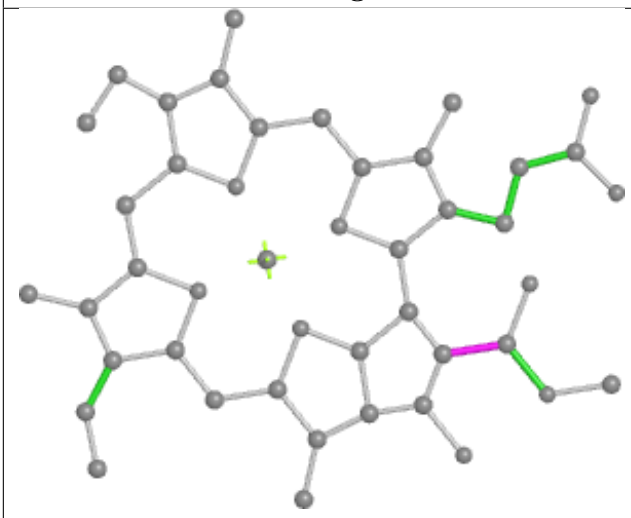
Ligand CLA A 837



Bond lengths



Bond angles



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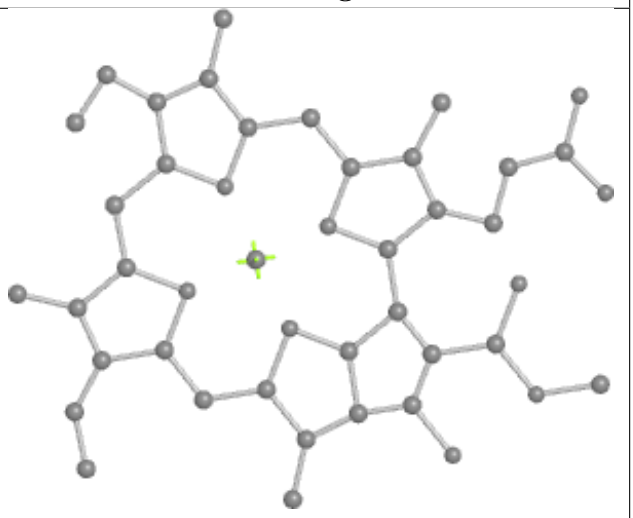
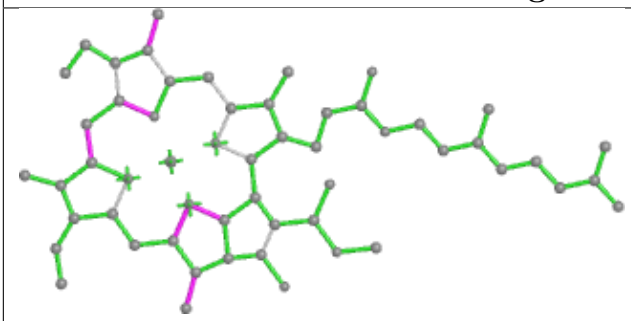


Rings

Ligand CLA 2 609



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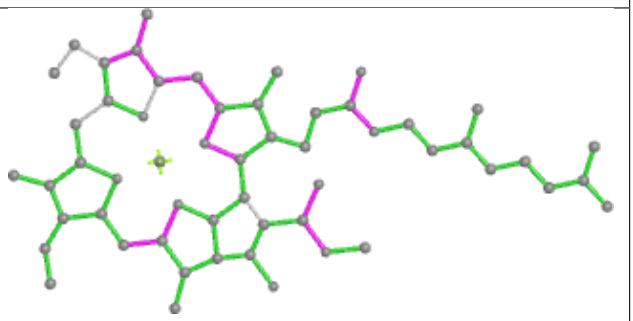
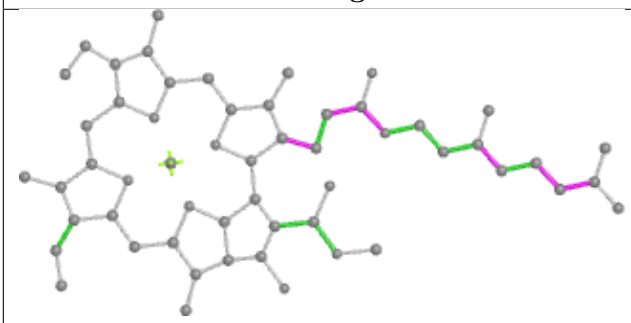
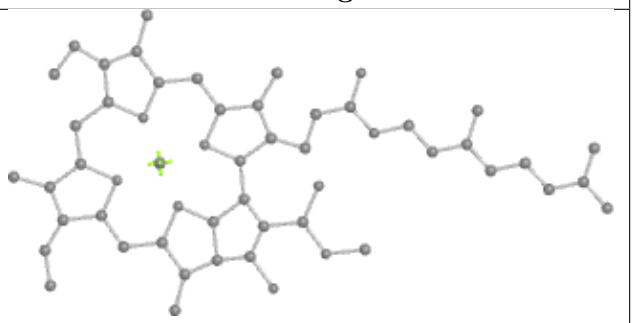


Bond angles

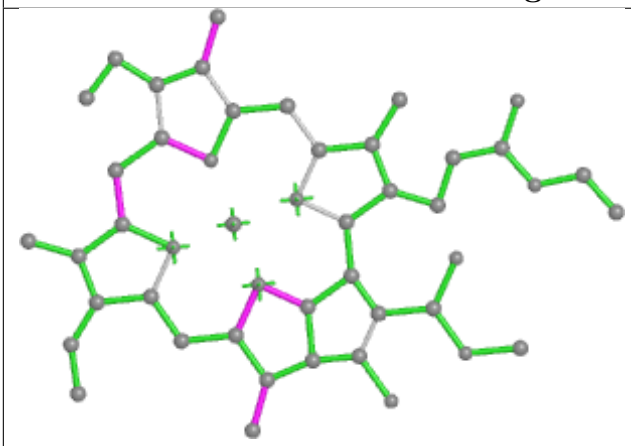


Torsions

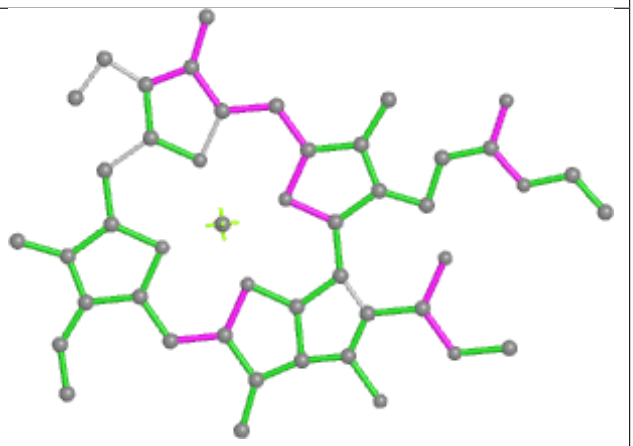


Rings

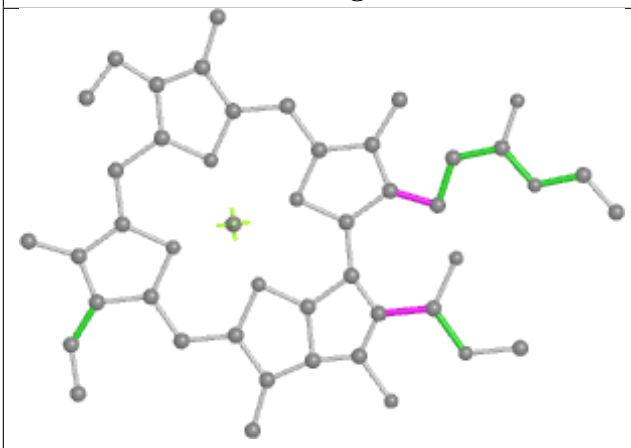
Ligand CLA B 838



Bond lengths



Bond angles



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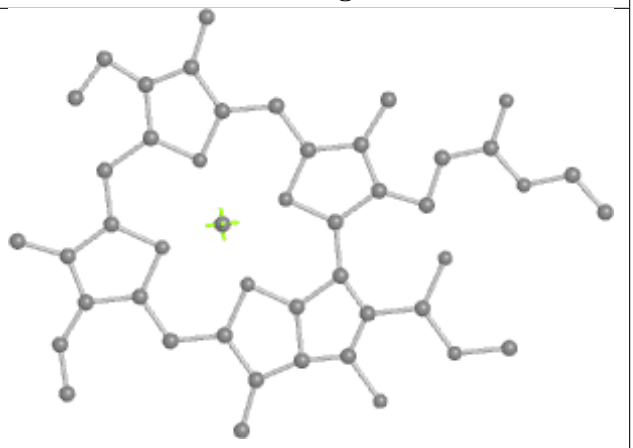
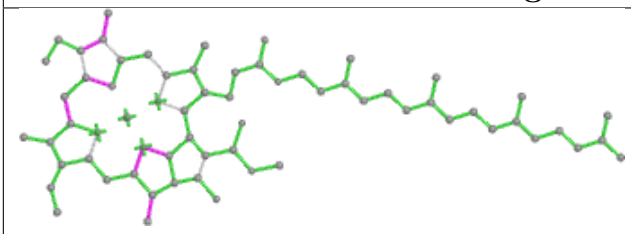
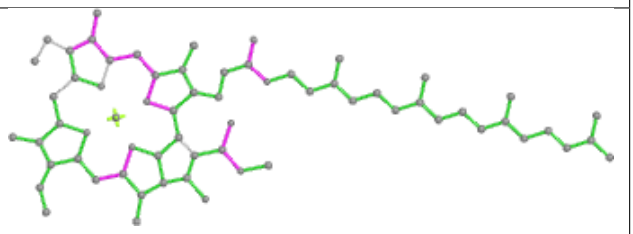


Rings

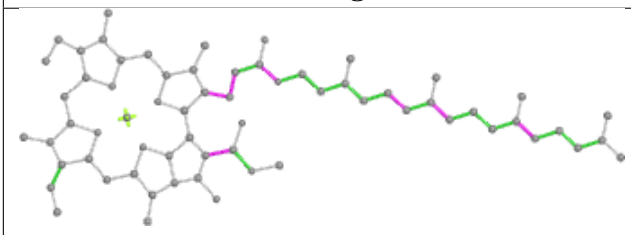
Ligand CLA B 828



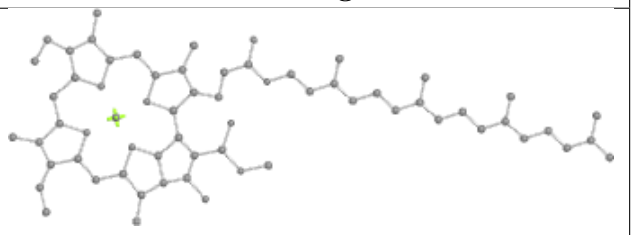
Bond lengths



Bond angles

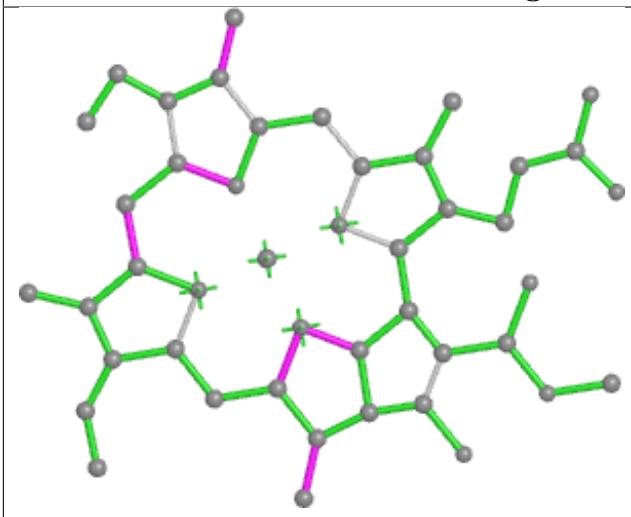


Torsions

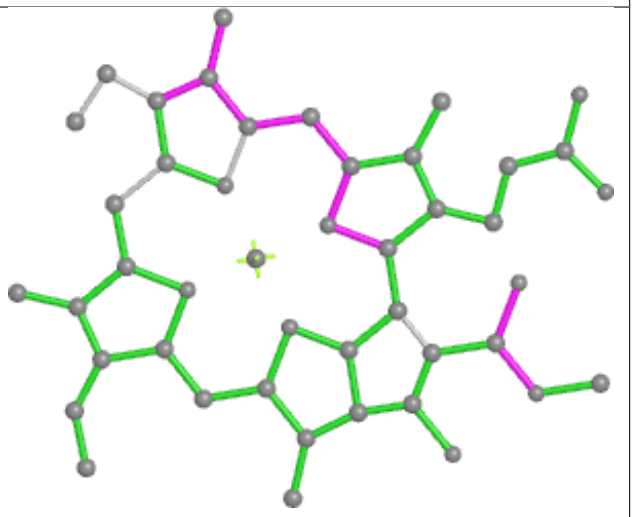


Rings

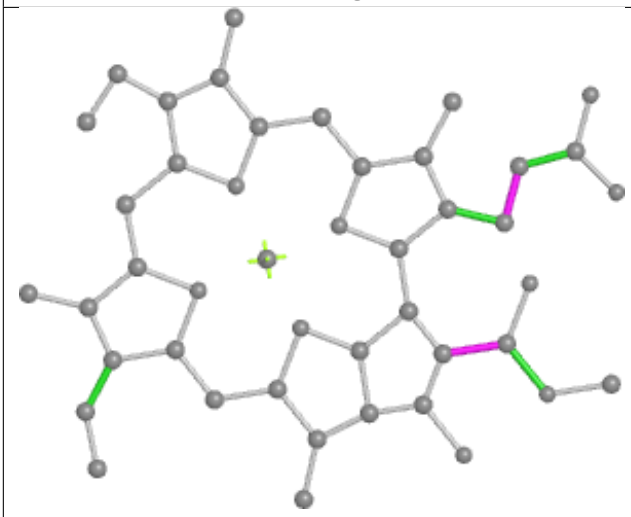
Ligand CLA B 817



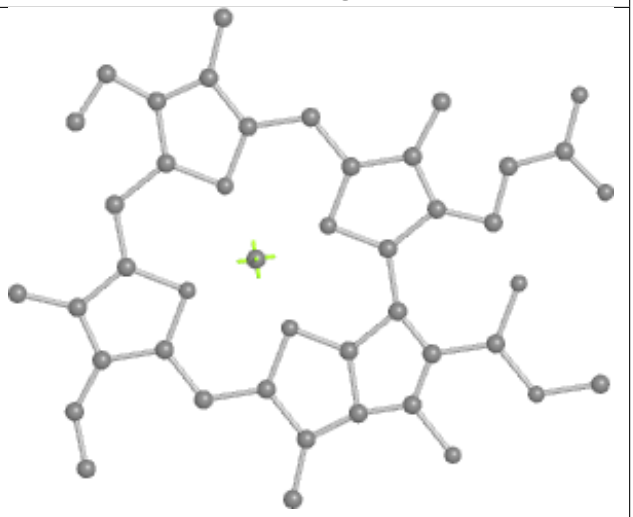
Bond lengths



Bond angles

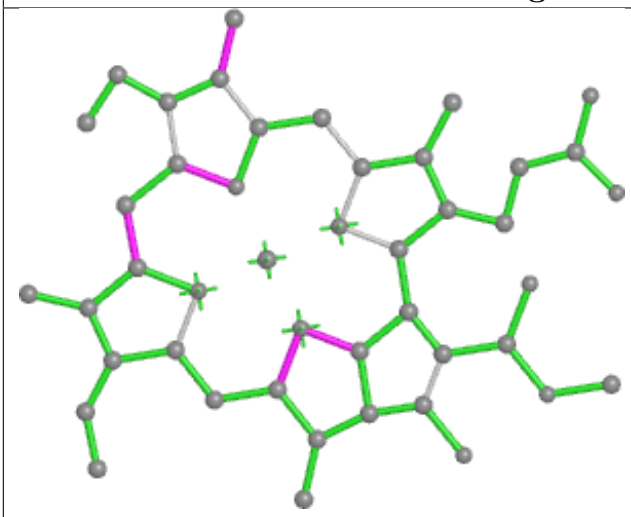


Torsions

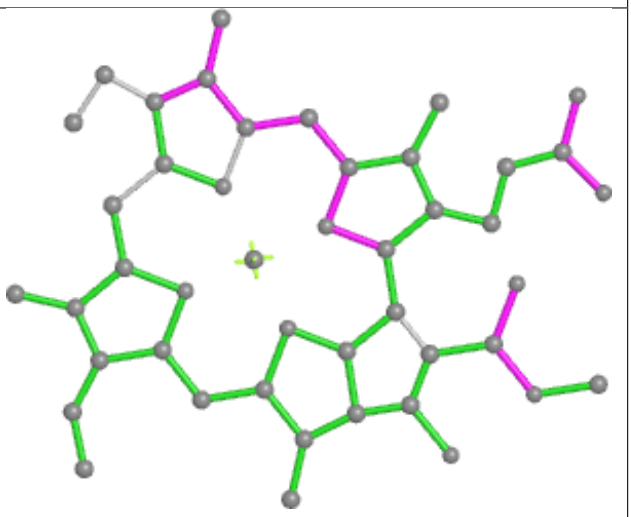


Rings

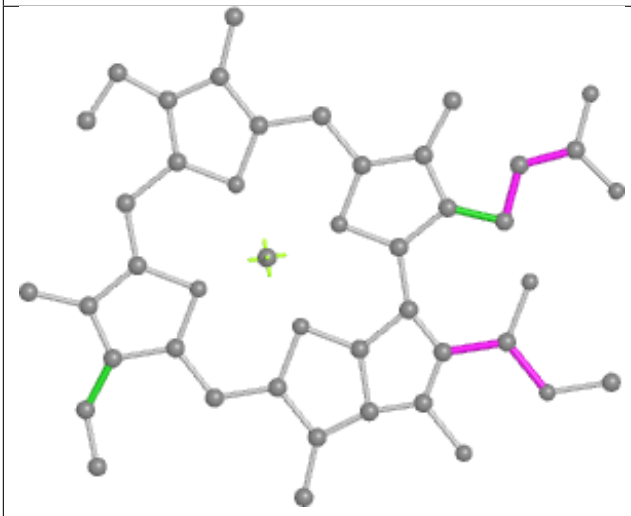
Ligand CLA 2 613



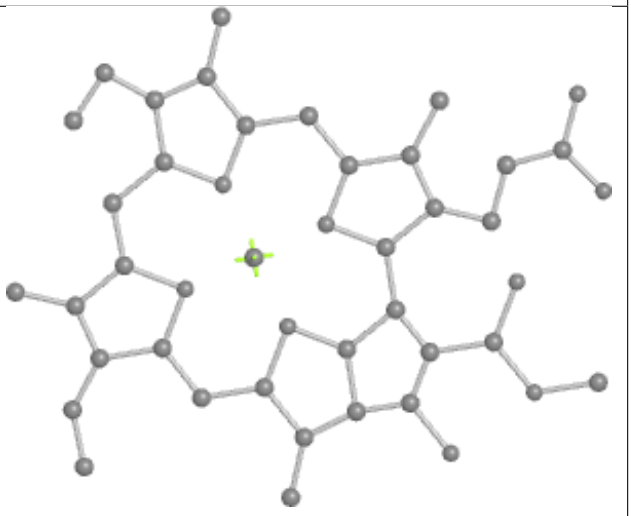
Bond lengths



Bond angles

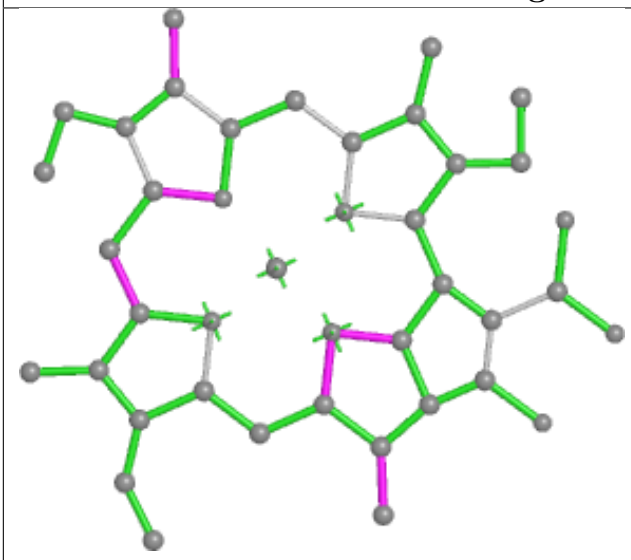


Torsions



Rings

Ligand CLA 3 606



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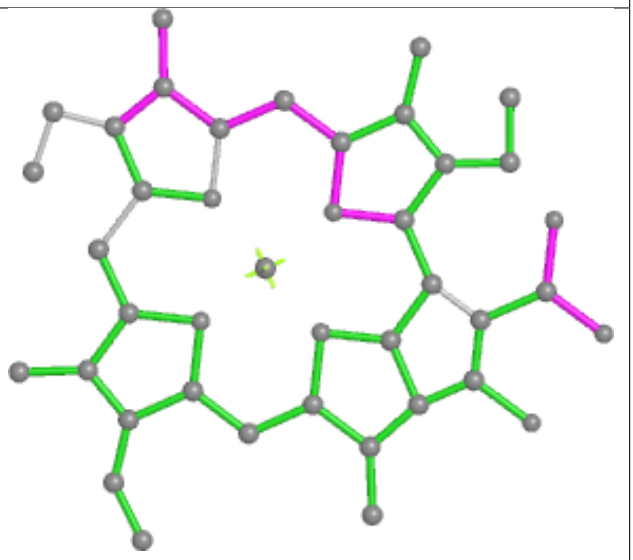
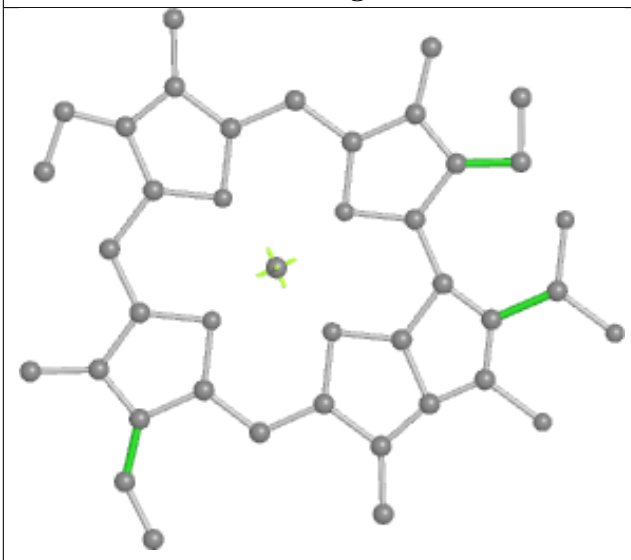
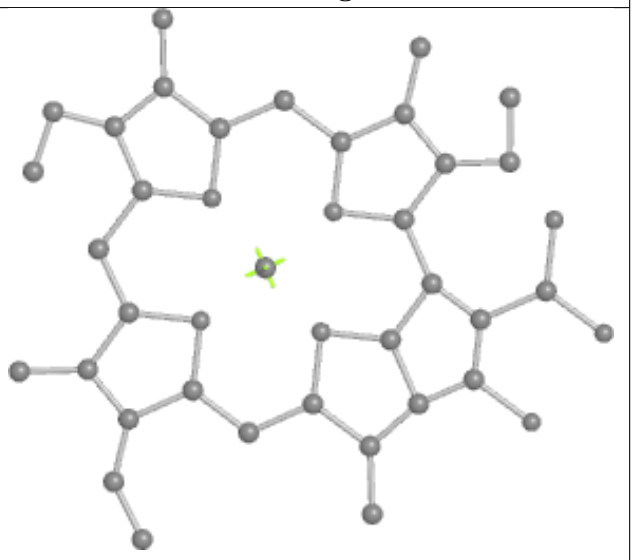


Bond angles

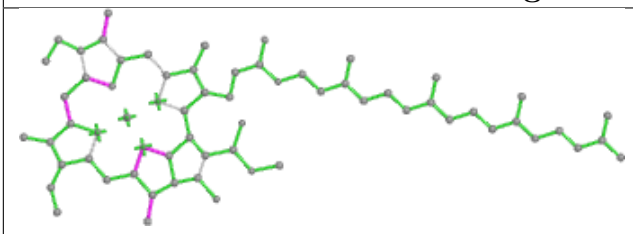


Torsions

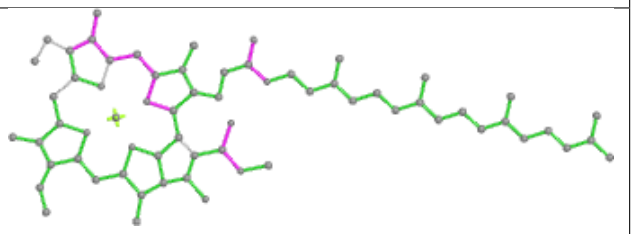


Rings

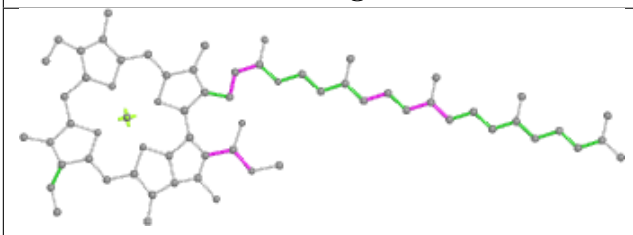
Ligand CLA A 826



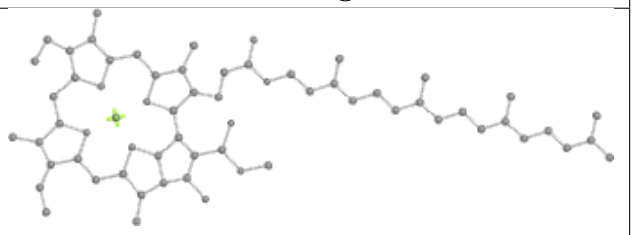
Bond lengths



Bond angles

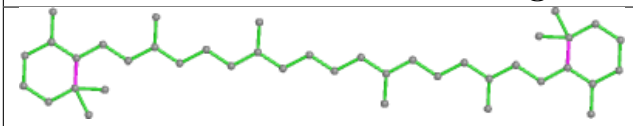


Torsions

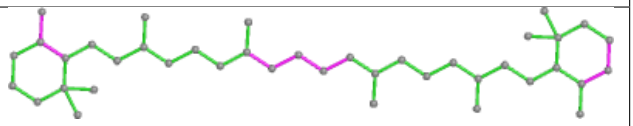


Rings

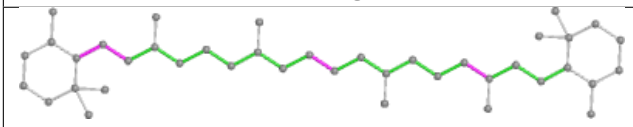
Ligand BCR I 101



Bond lengths



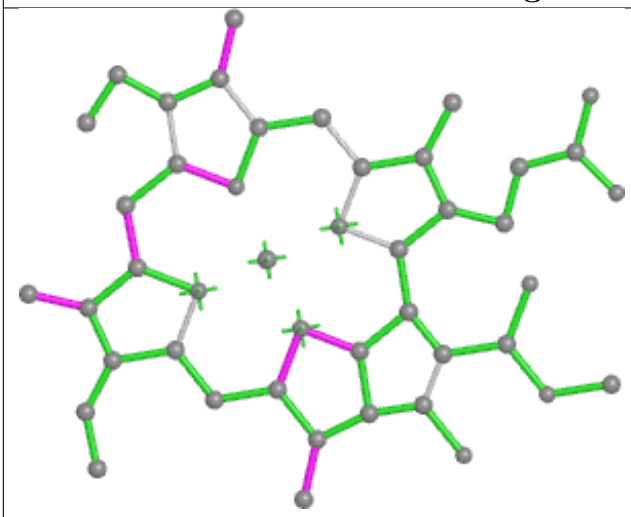
Bond angles



Torsions

Rings

Ligand CLA A 819



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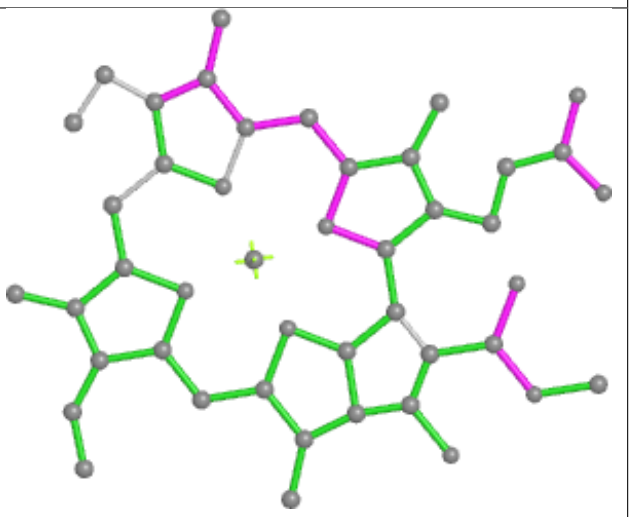
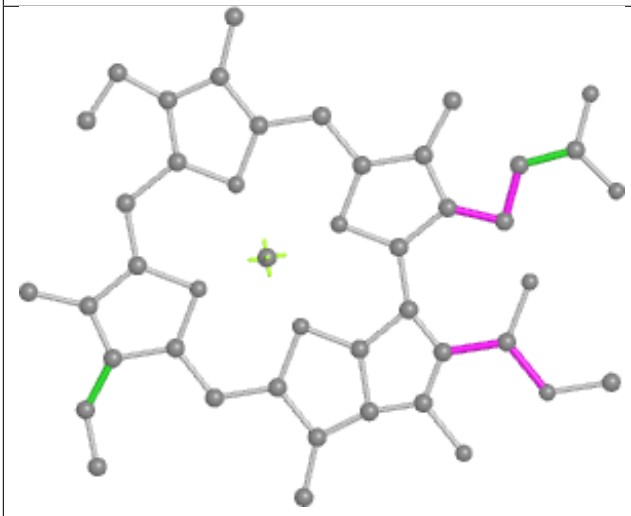
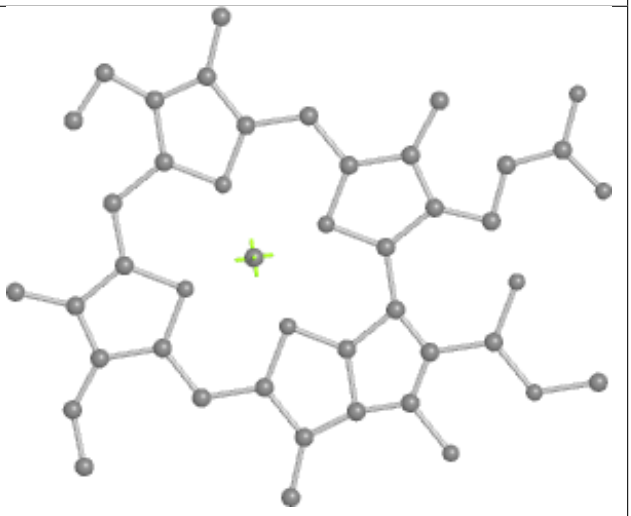


Bond angles

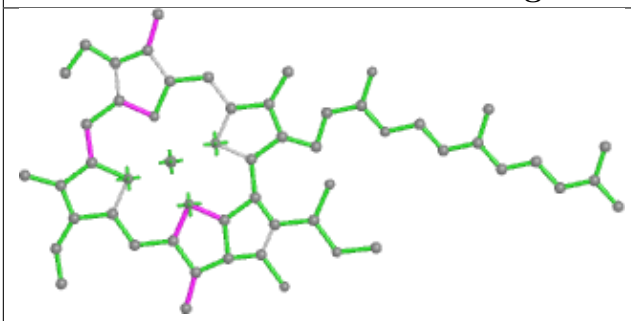


Torsions

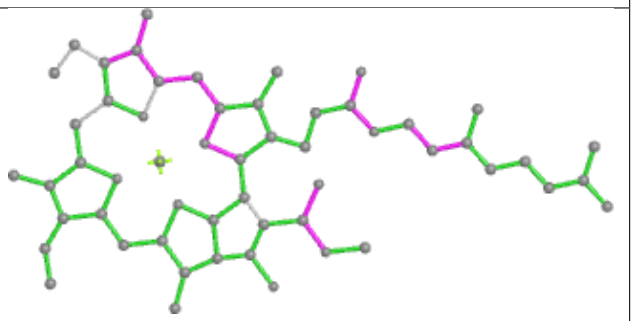


Rings

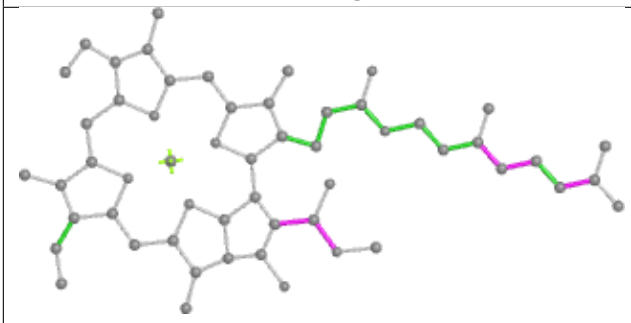
Ligand CLA B 822



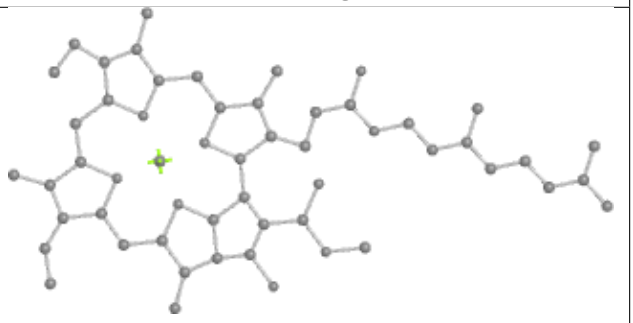
Bond lengths



Bond angles

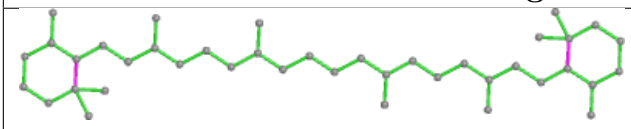


Torsions

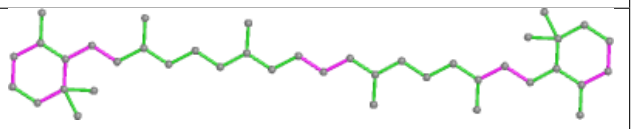


Rings

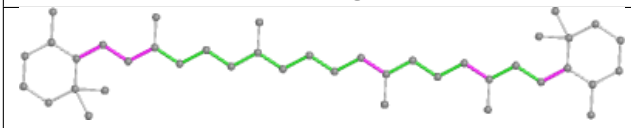
Ligand BCR 3 620



Bond lengths



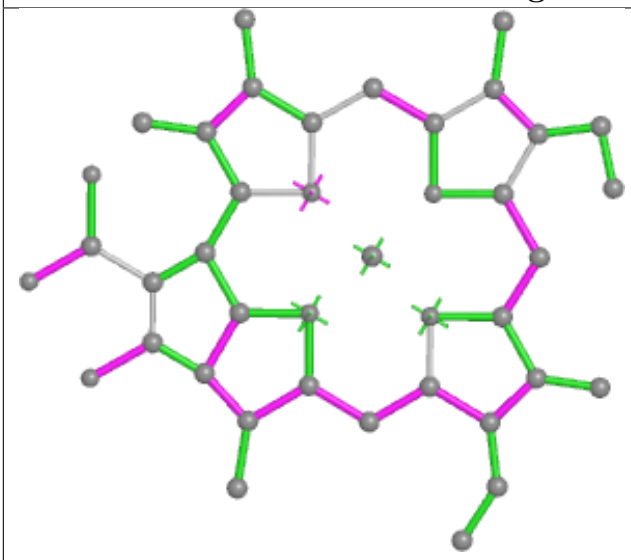
Bond angles



Torsions

Rings

Ligand CHL 3 608



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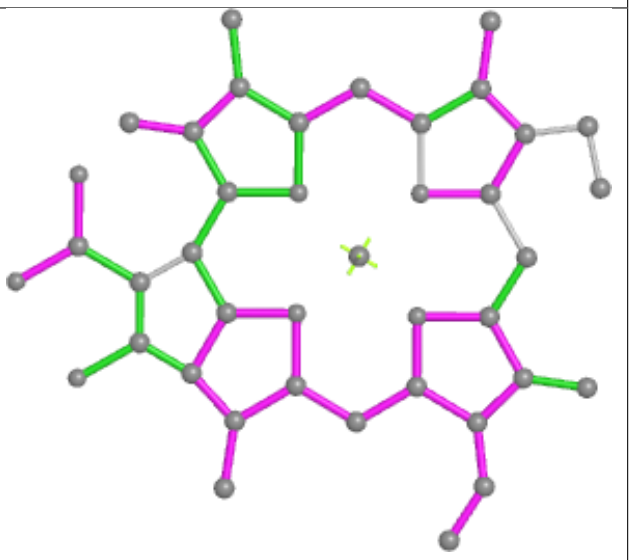
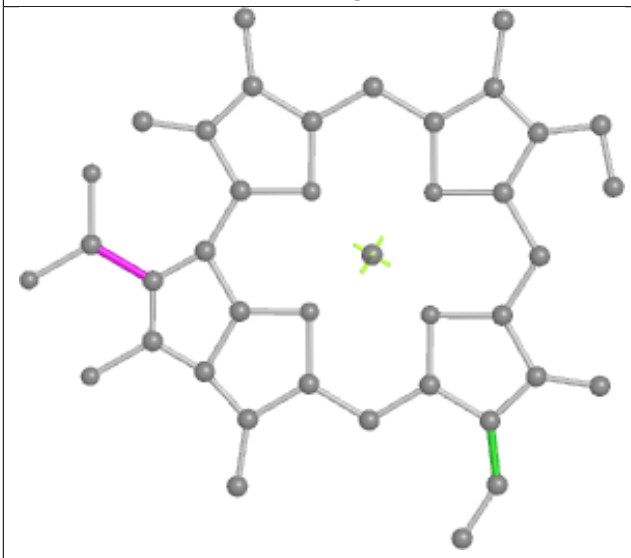
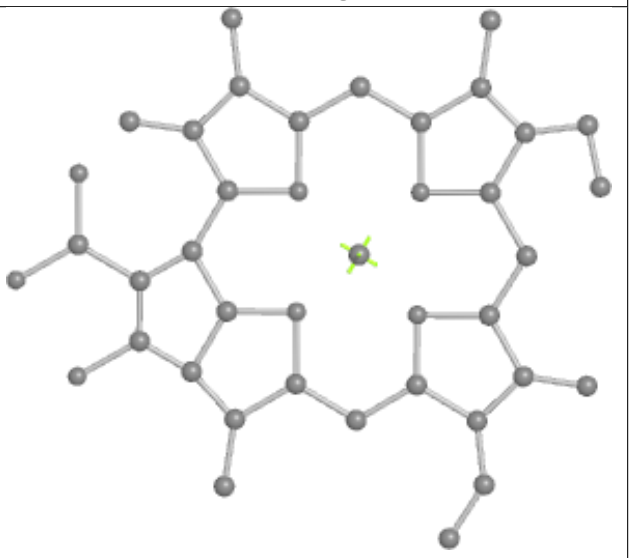


Bond angles

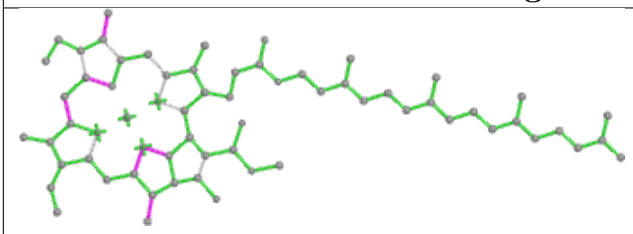


Torsions

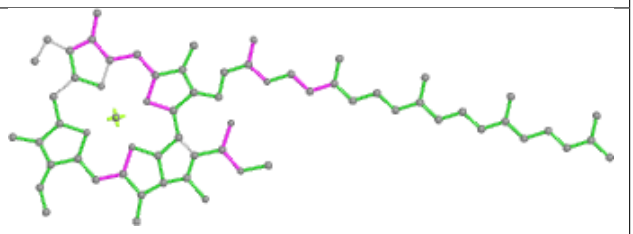


Rings

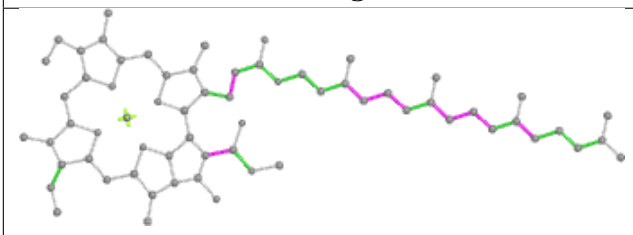
Ligand CLA B 807



Bond lengths



Bond angles



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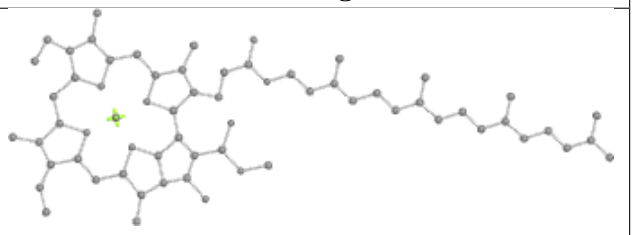
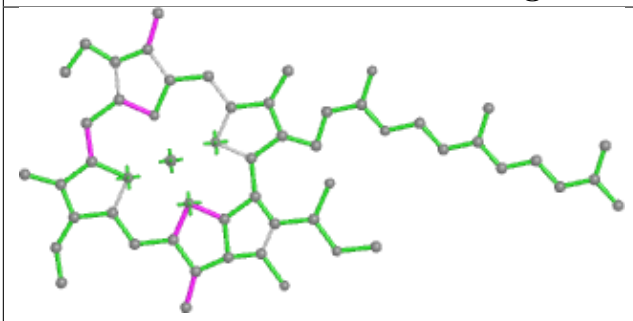
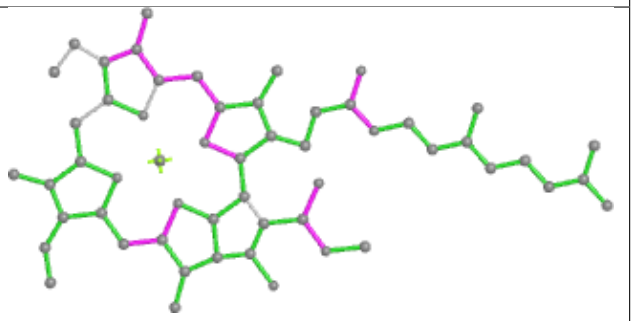


Rings

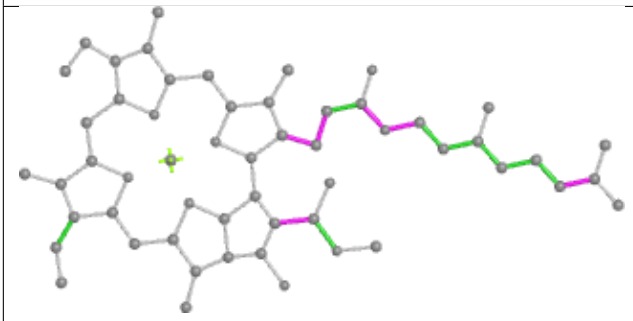
Ligand CLA A 825



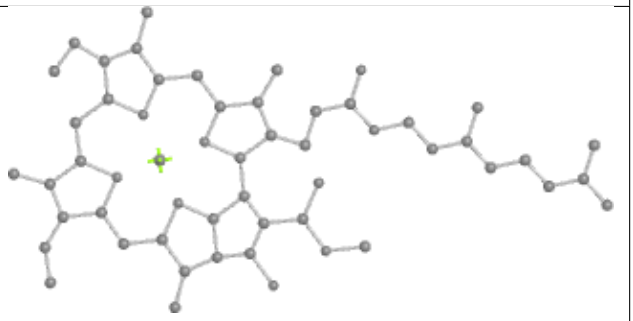
Bond lengths



Bond angles

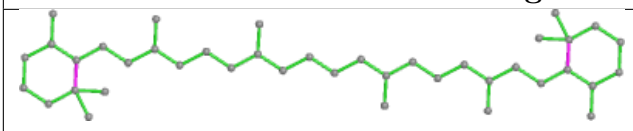


Torsions



Rings

Ligand BCR L 301



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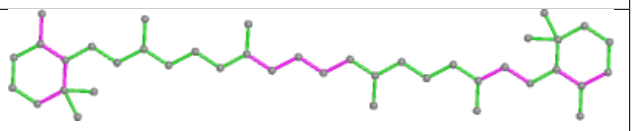
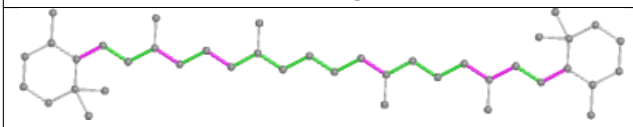


Bond angles



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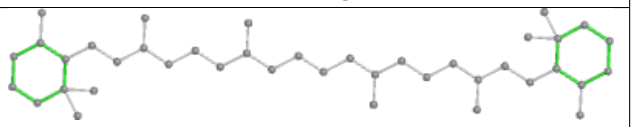
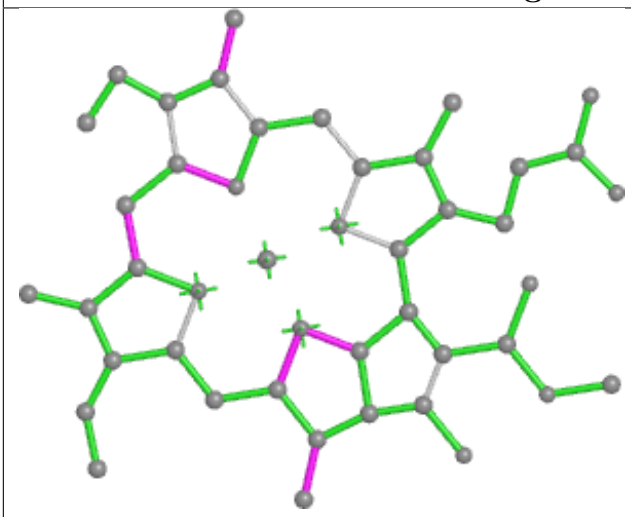
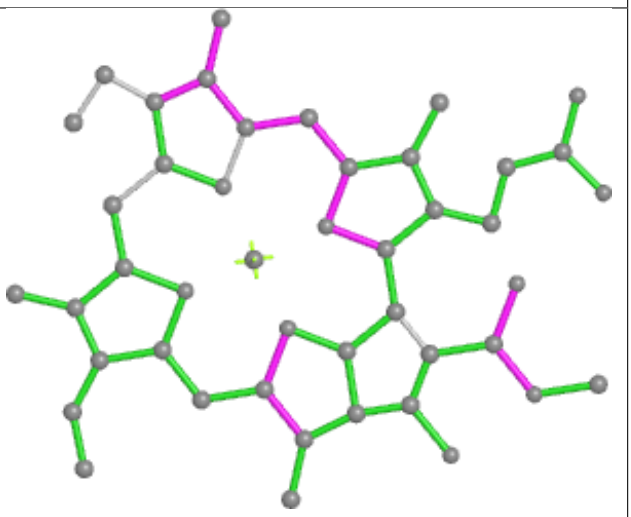


Rings

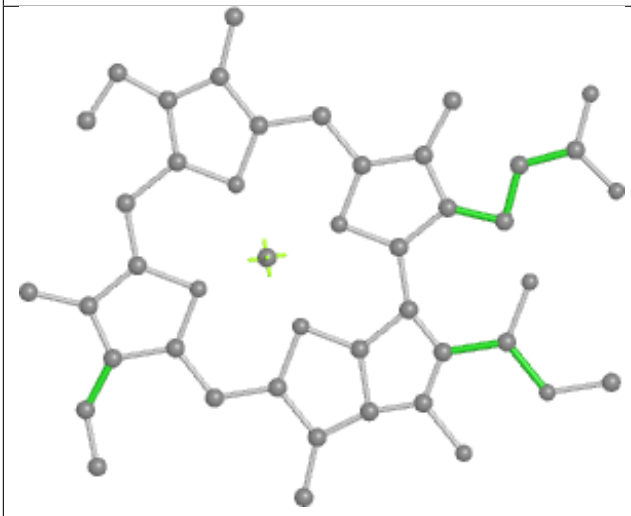
Ligand CLA B 829



Bond lengths



Bond angles



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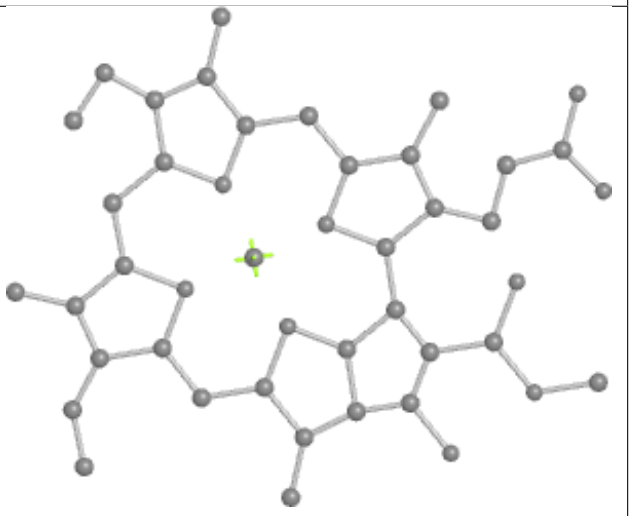
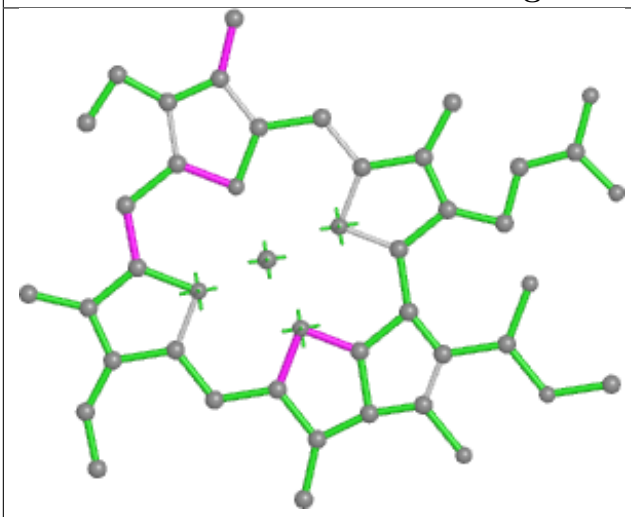


Rings

Ligand CLA A 833



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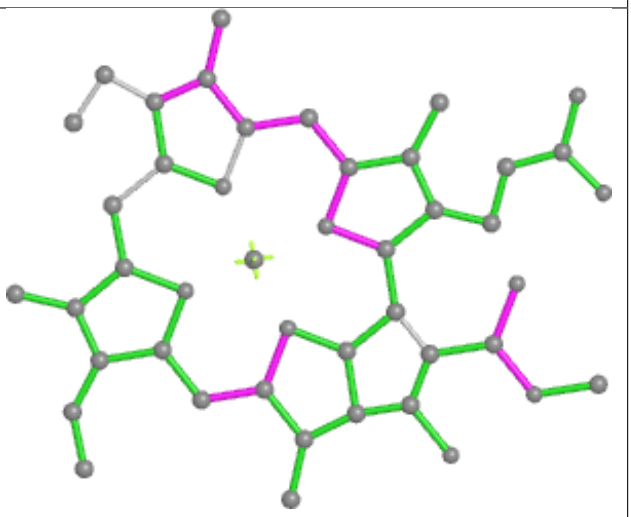
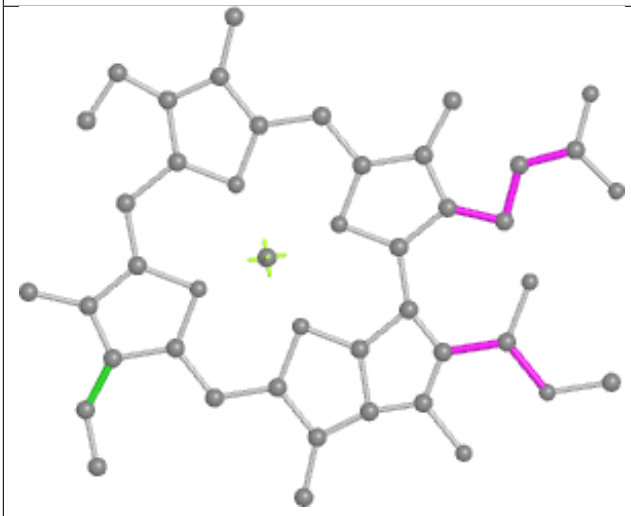


Bond angles



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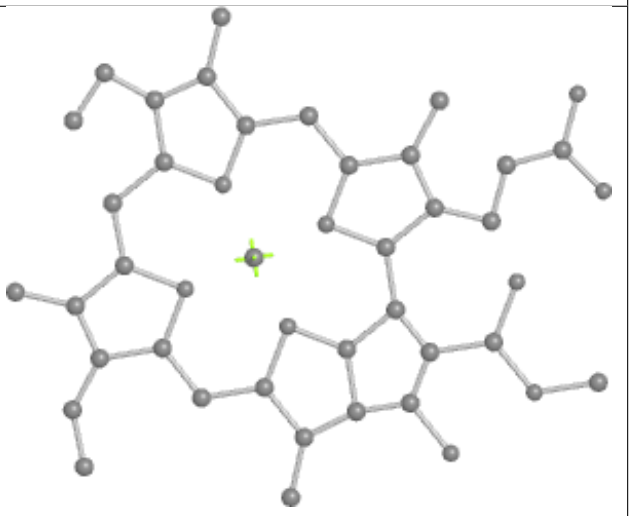
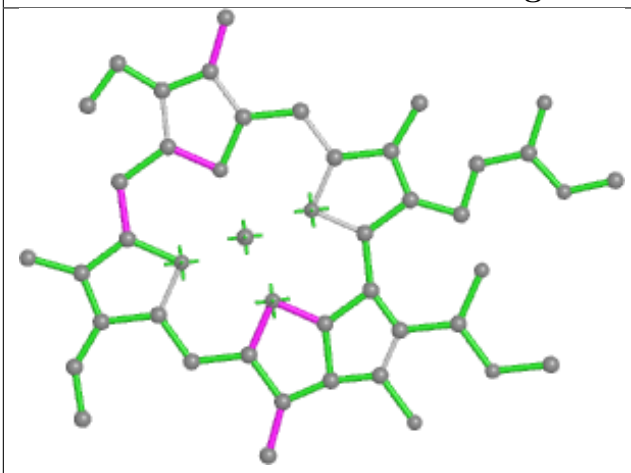
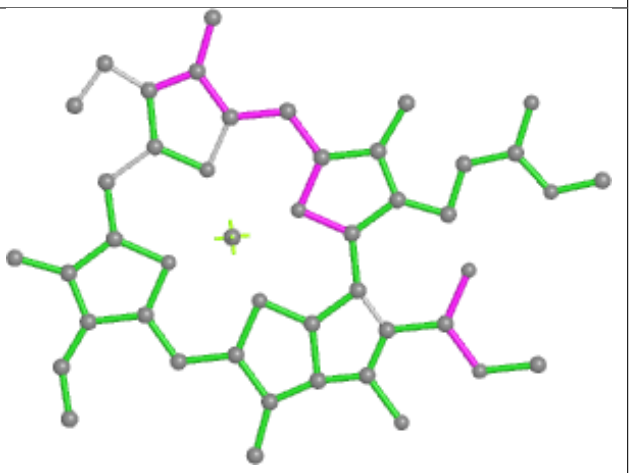


Rings

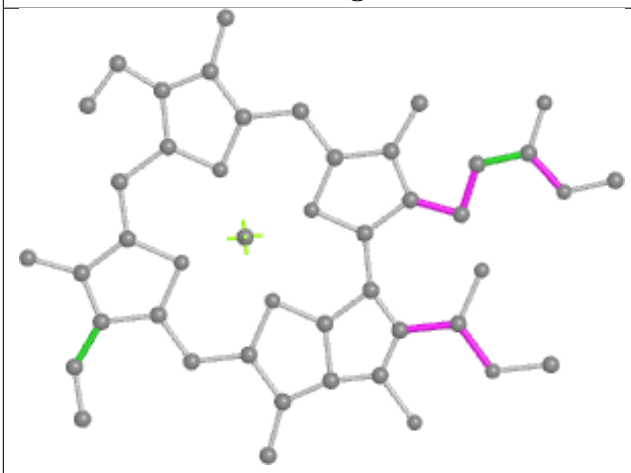
Ligand CLA B 810



Bond lengths



Bond angles



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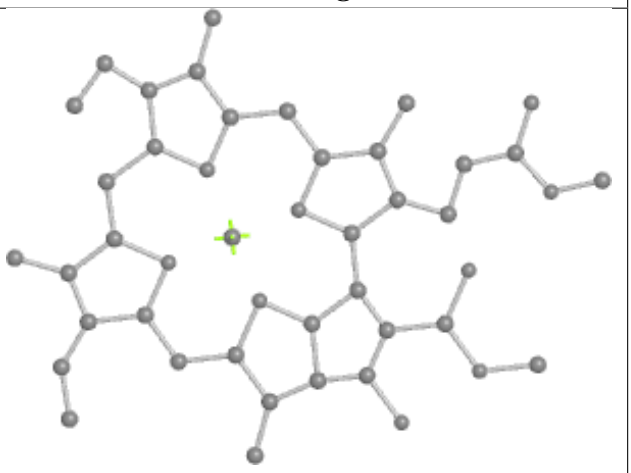
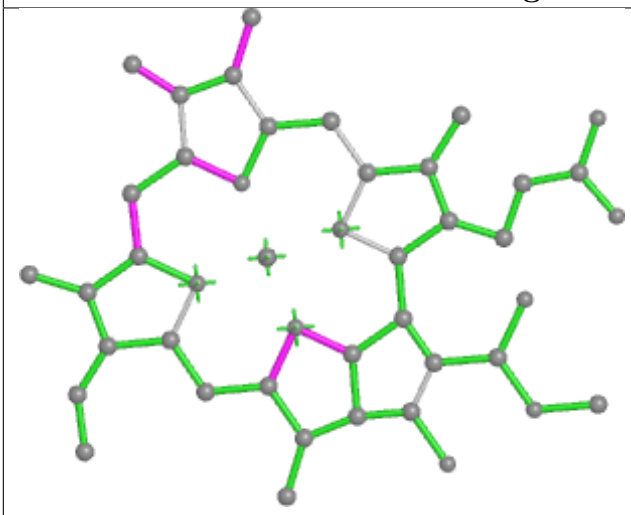
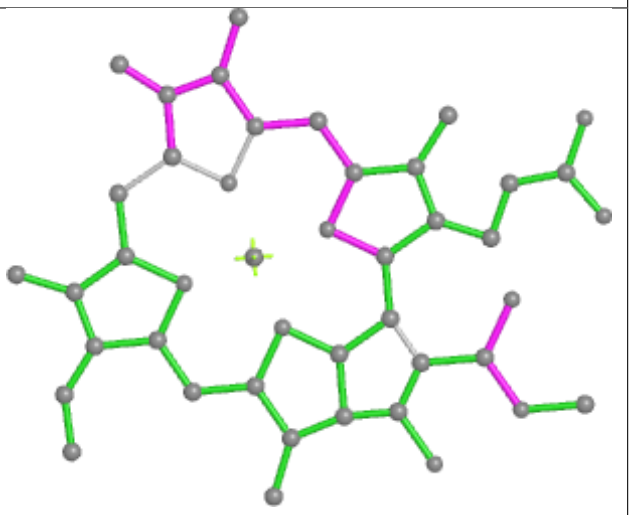


Rings

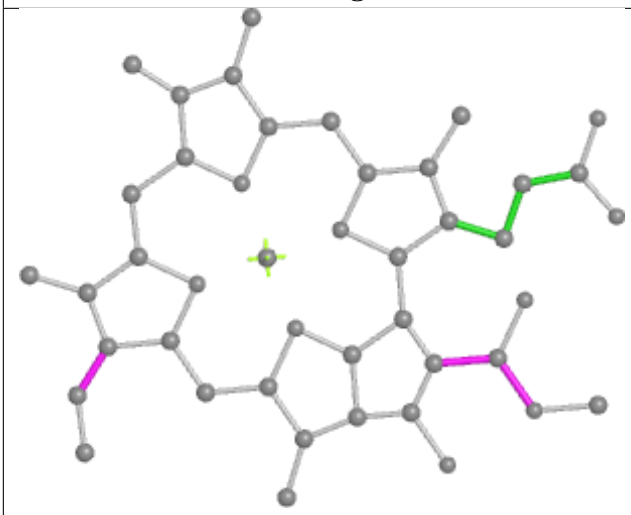
Ligand CLA K 204



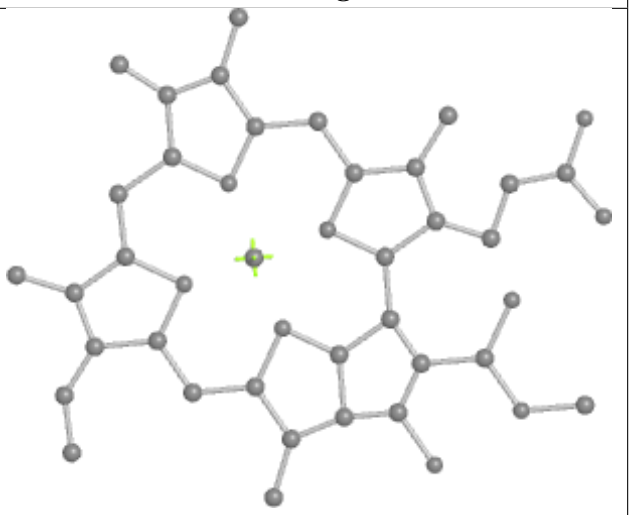
Bond lengths



Bond angles

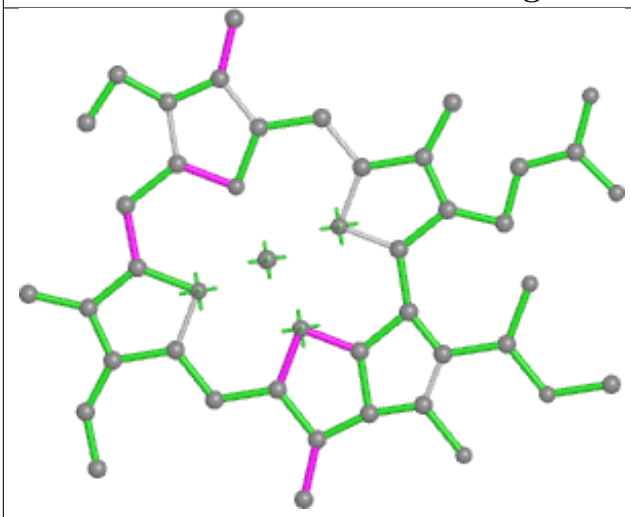


Torsions

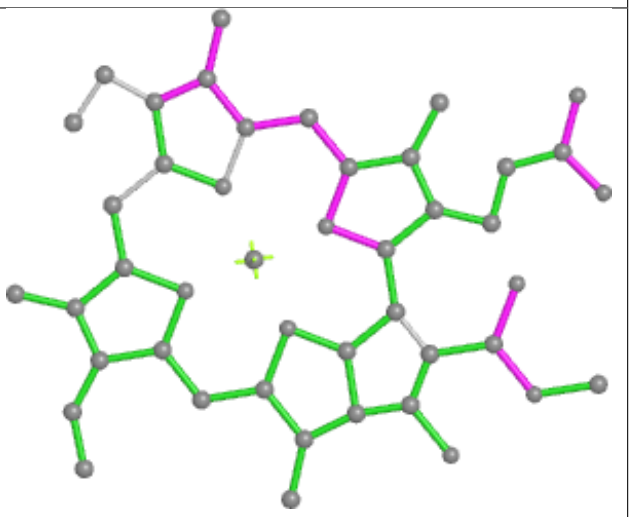


Rings

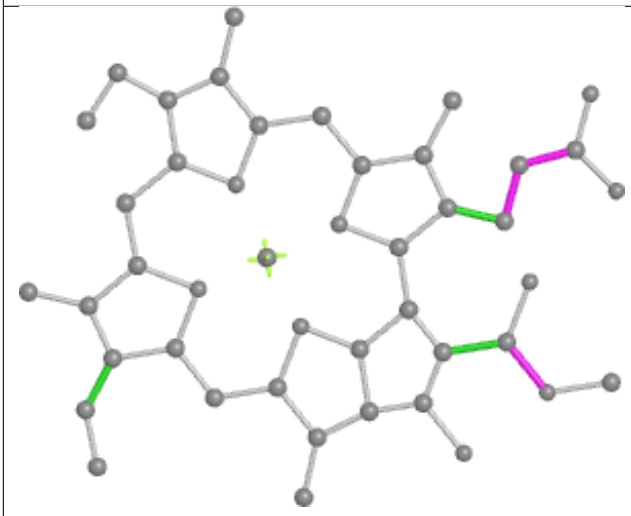
Ligand CLA K 206



Bond lengths



Bond angles



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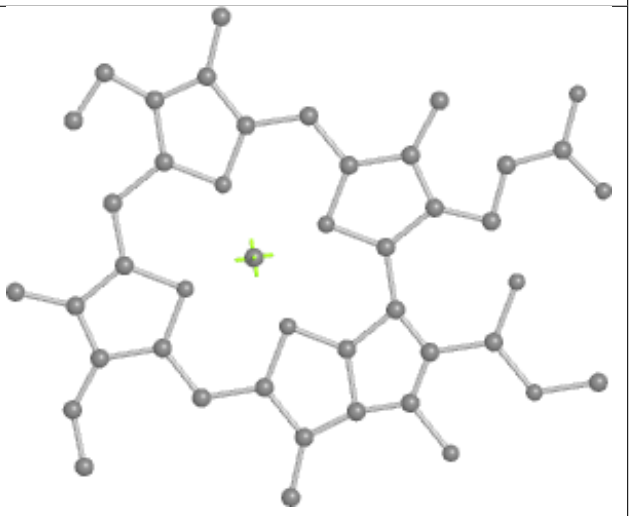
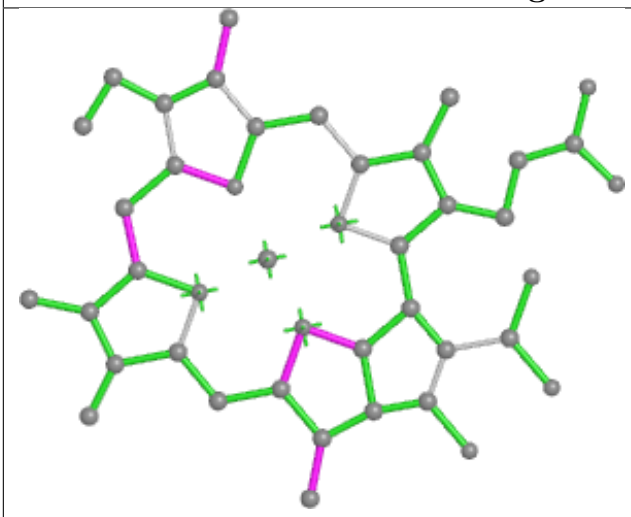
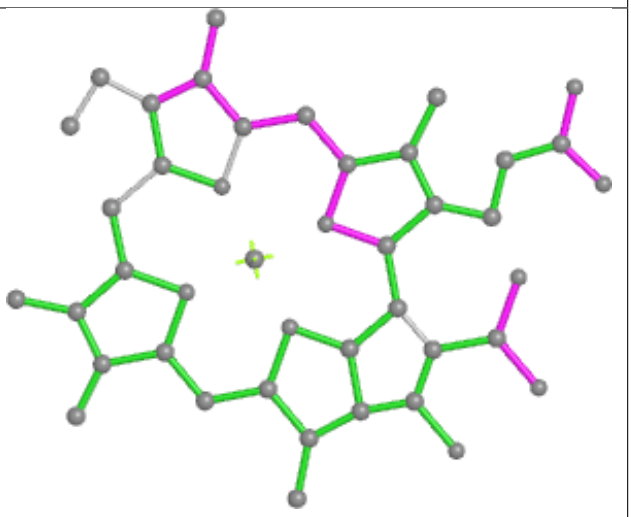


Rings

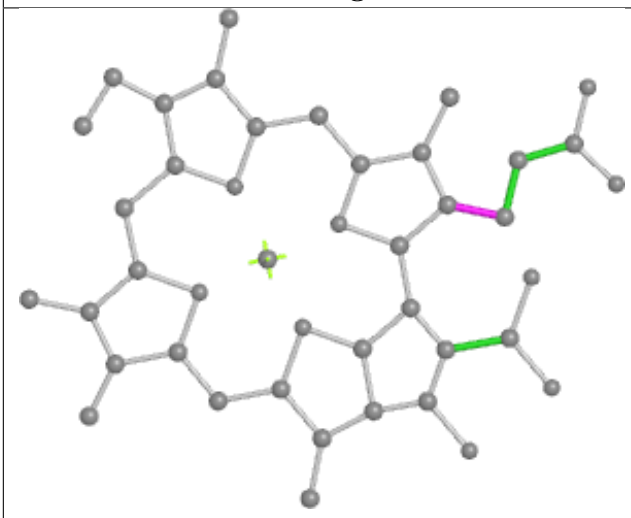
Ligand CLA 6 610



Bond lengths



Bond angles



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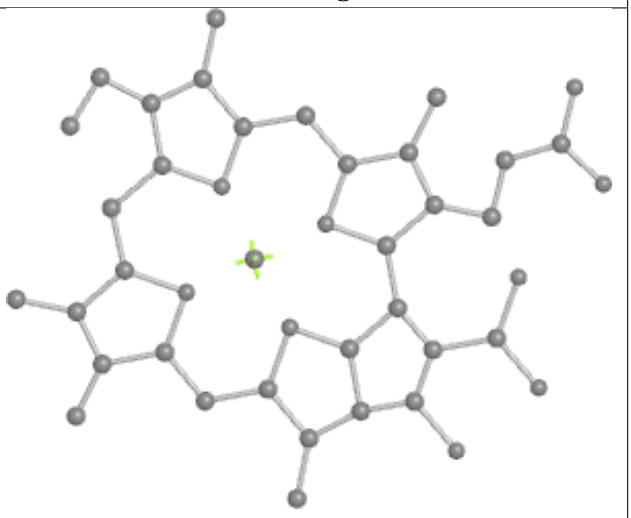
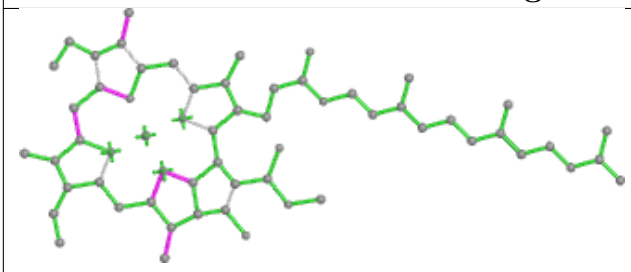


Rings

Ligand CLA B 836



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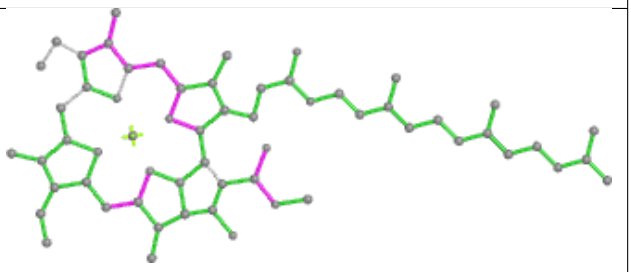
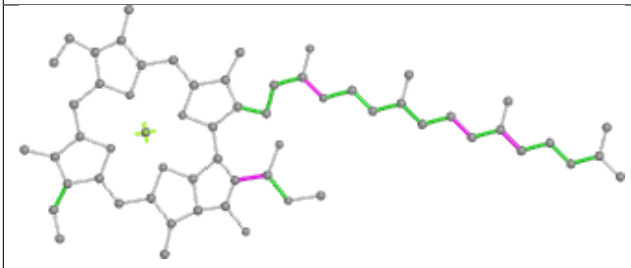


Bond angles



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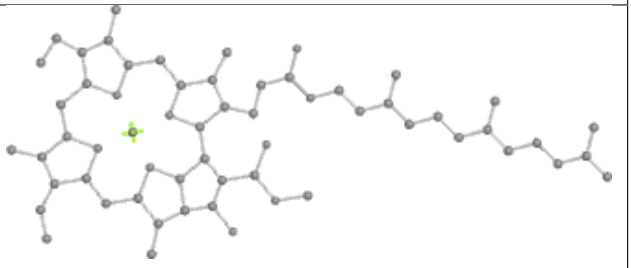
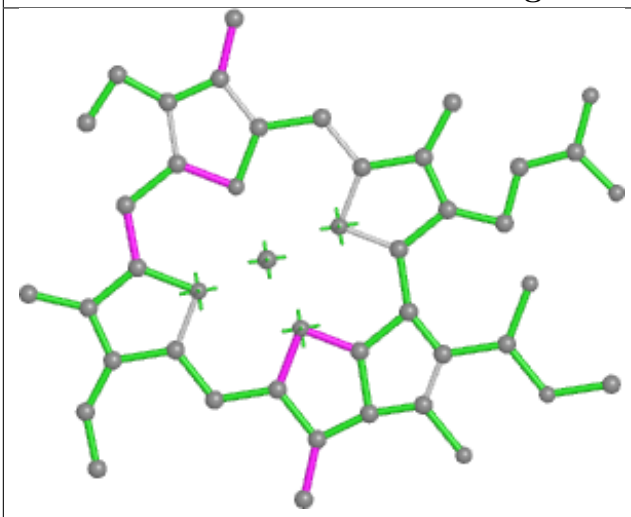
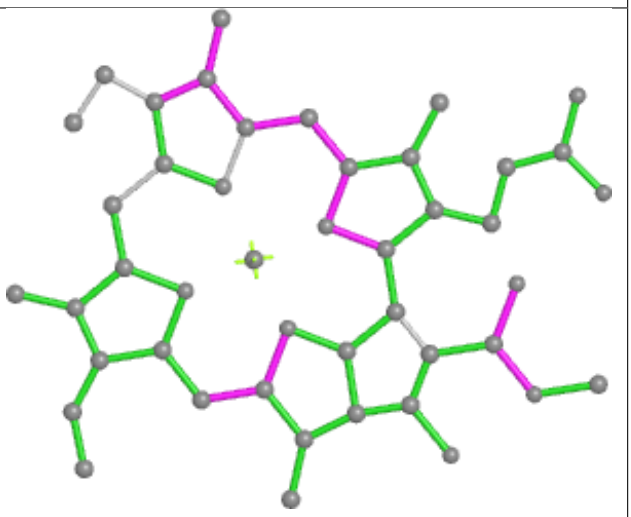


Rings

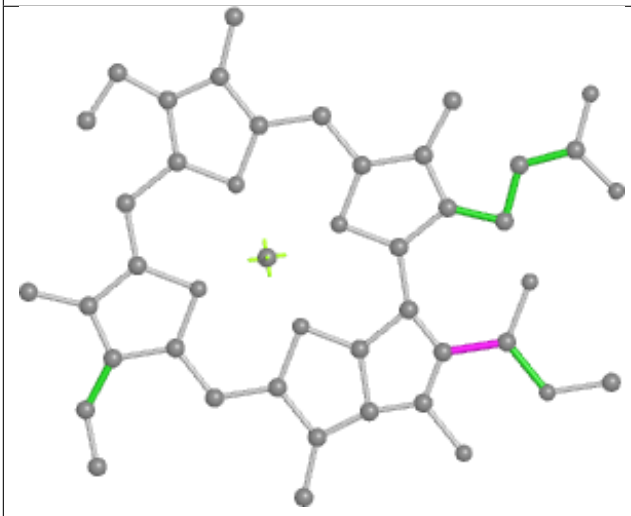
Ligand CLA B 830



Bond lengths



Bond angles



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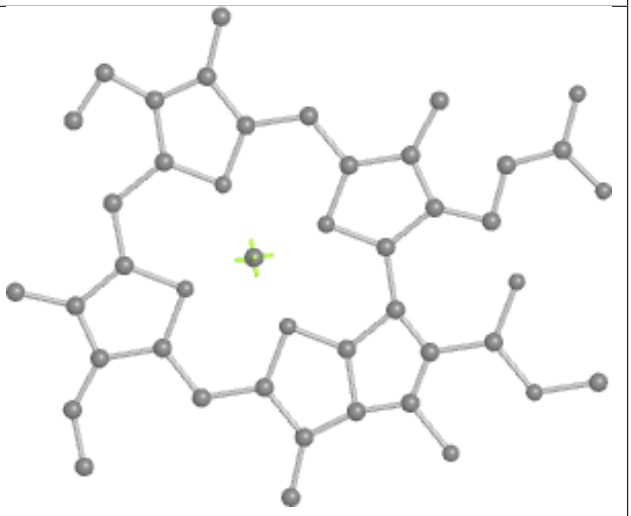
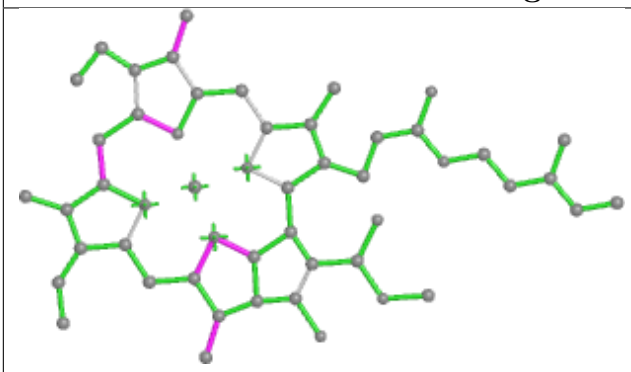
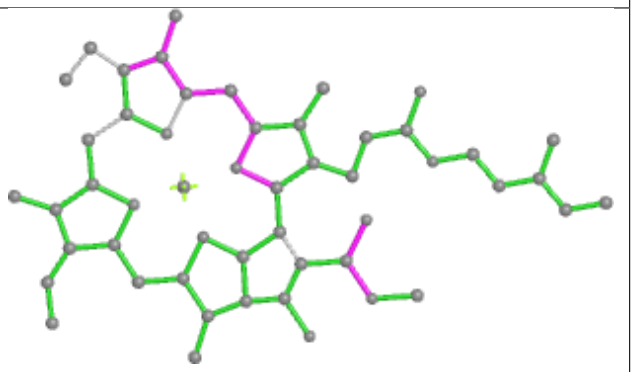
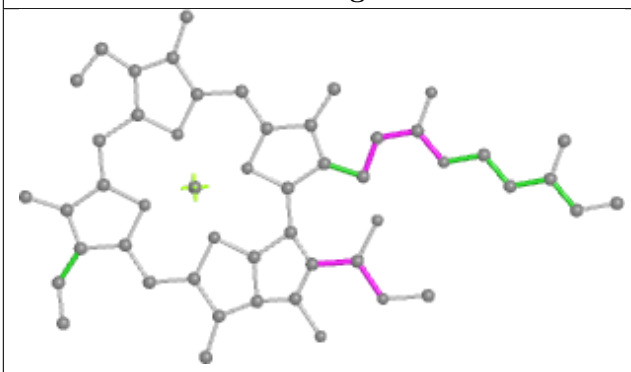
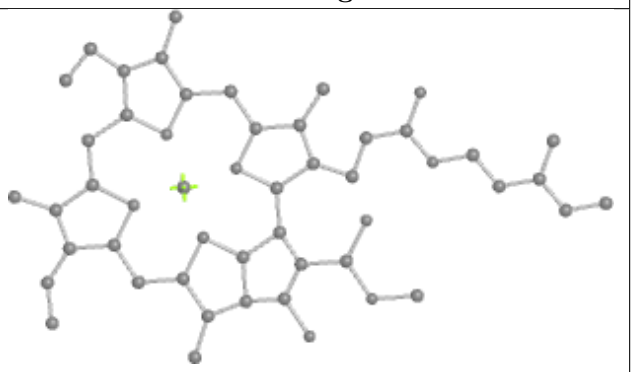
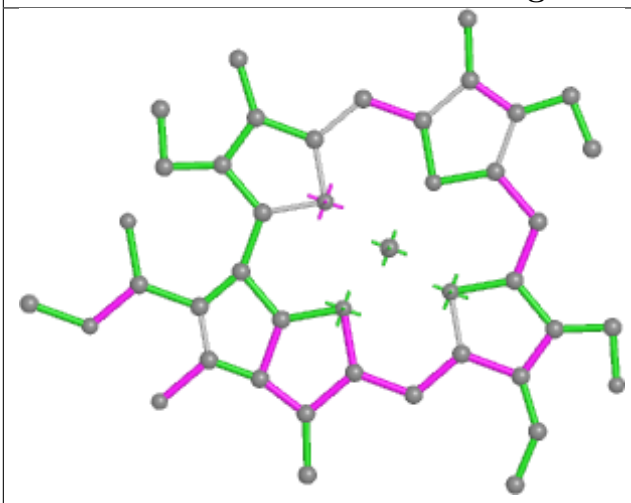


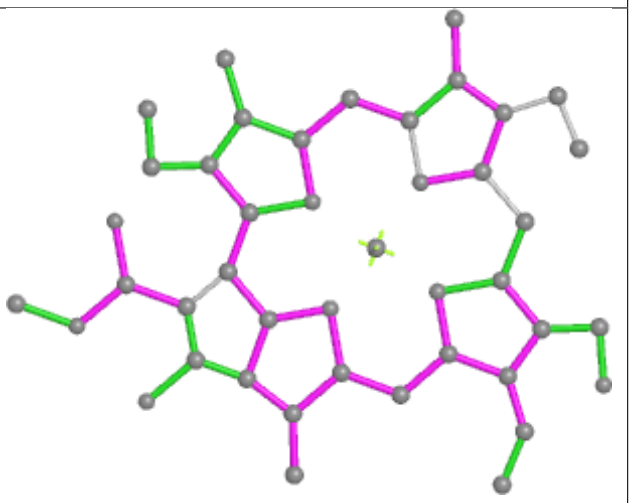
Rings

Ligand CLA A 824	
 Bond lengths	 Bond angles
 Torsions	 Rings

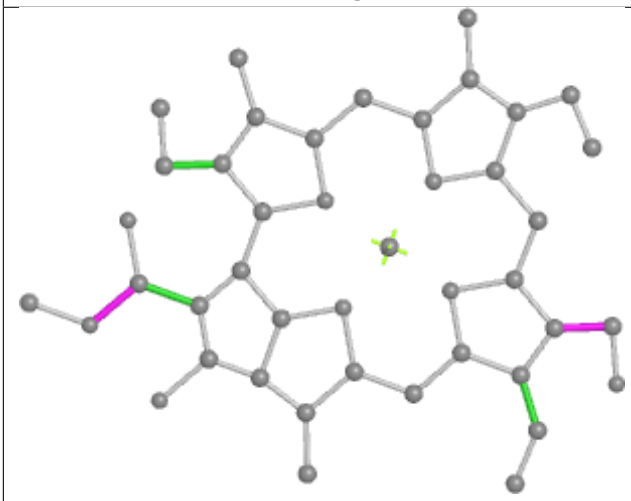
Ligand CHL 5 615



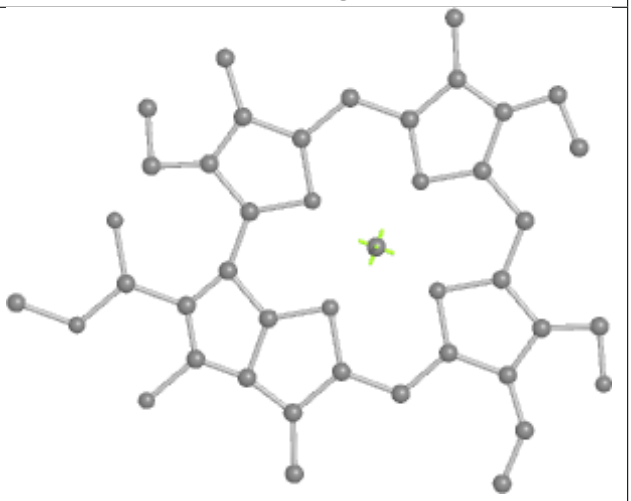
Bond lengths



Bond angles

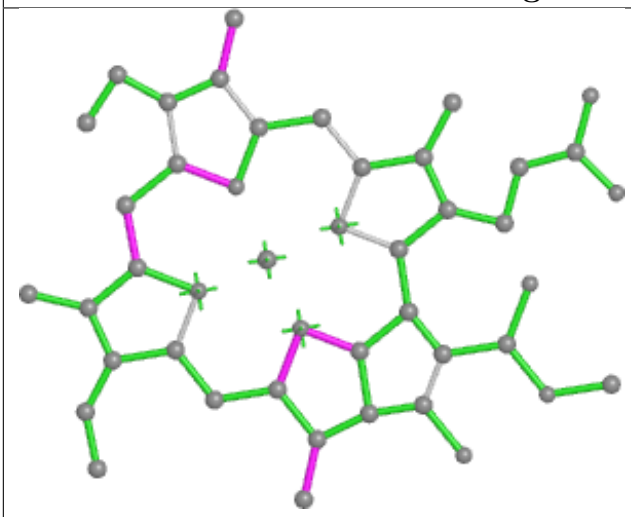


Torsions

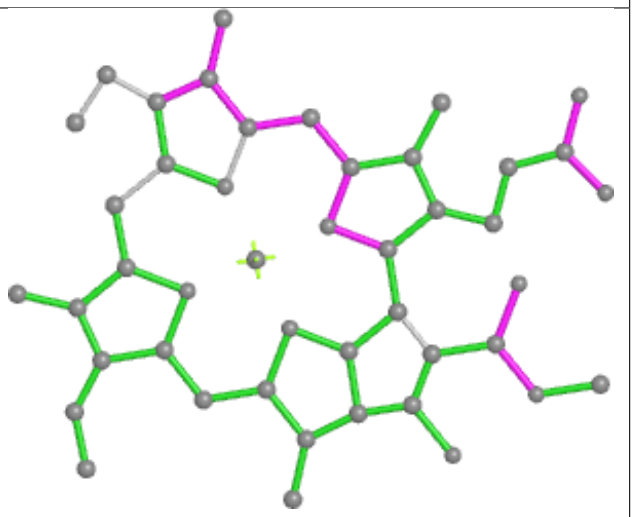


Rings

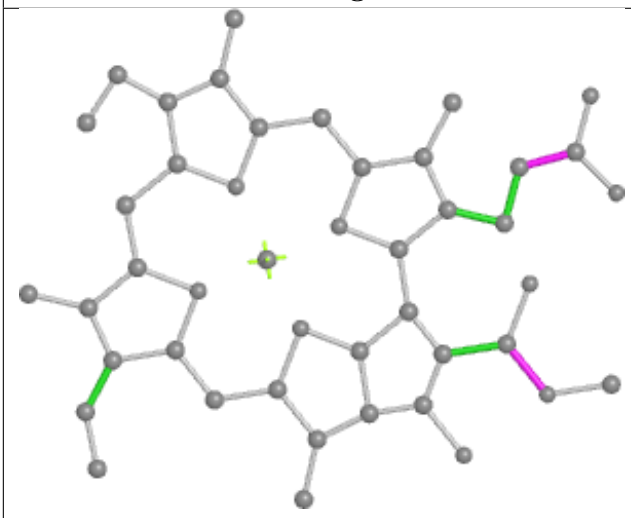
Ligand CLA K 203



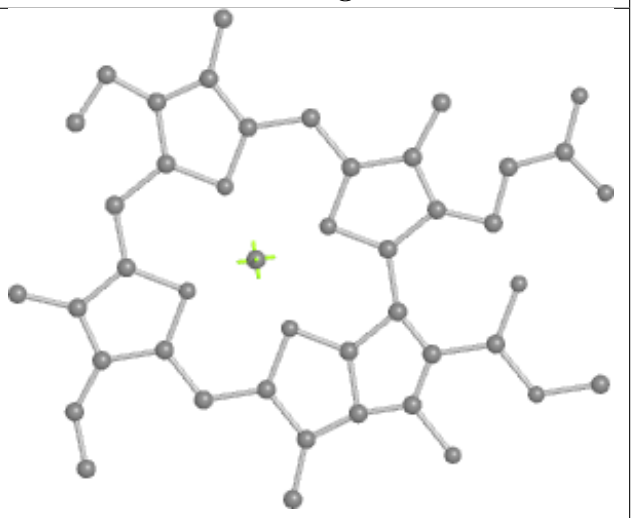
Bond lengths



Bond angles

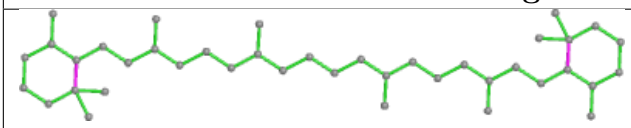


Torsions



Rings

Ligand BCR B 848



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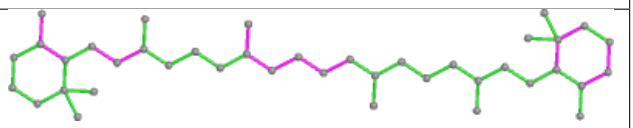
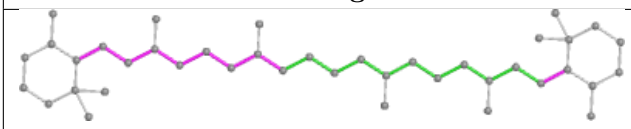
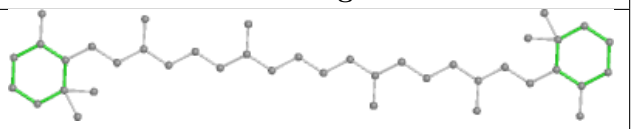


Bond angles

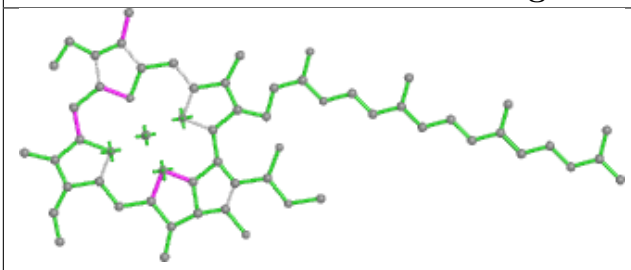


Torsions



Rings

Ligand CLA 3 602



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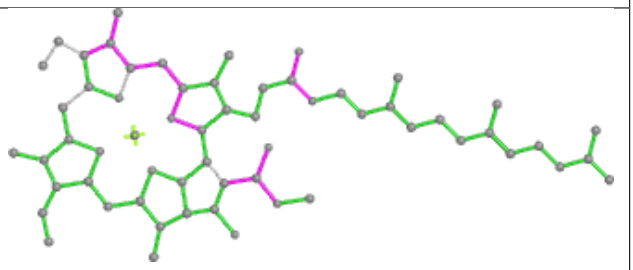
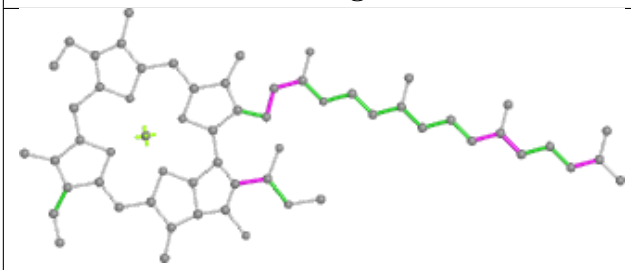
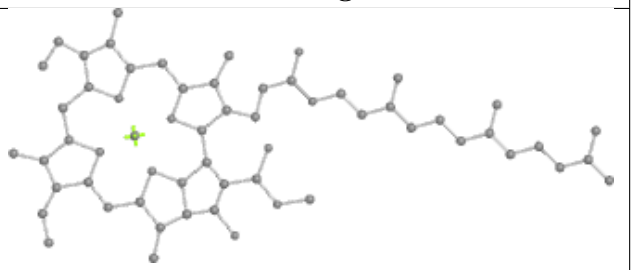


Bond angles

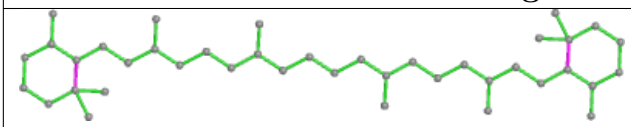


Torsions

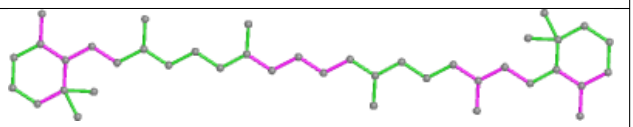


Rings

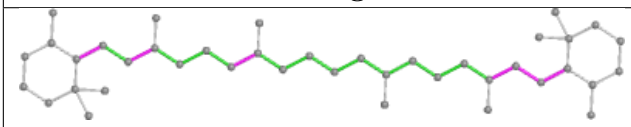
Ligand BCR A 851



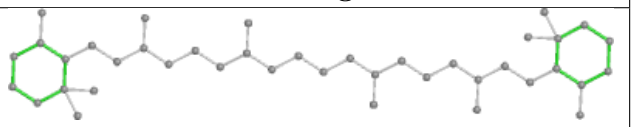
Bond lengths



Bond angles

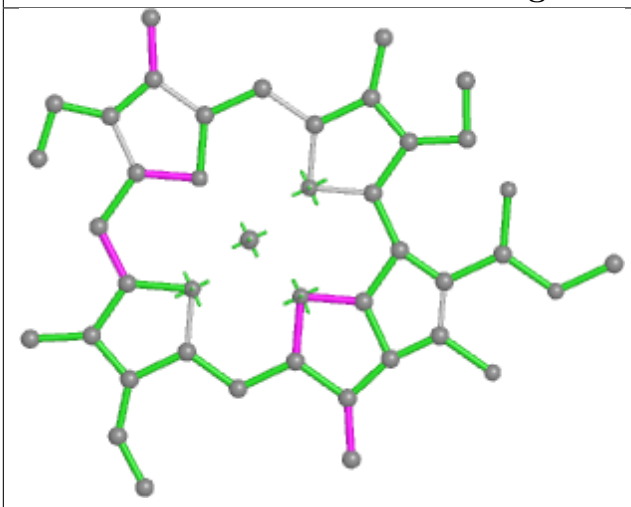


Torsions



Rings

Ligand CLA 2 614



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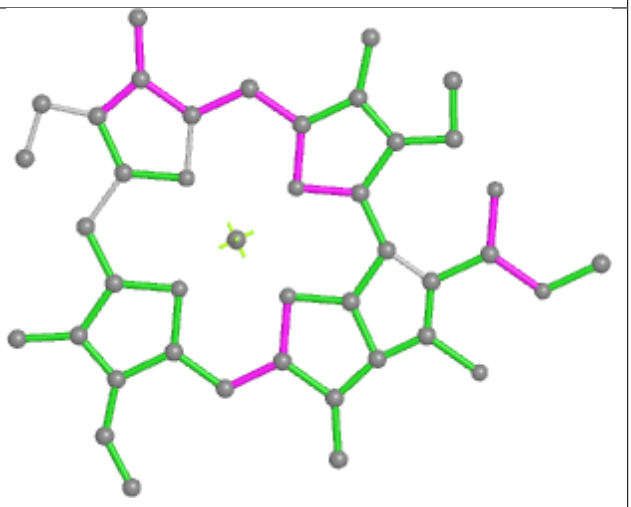
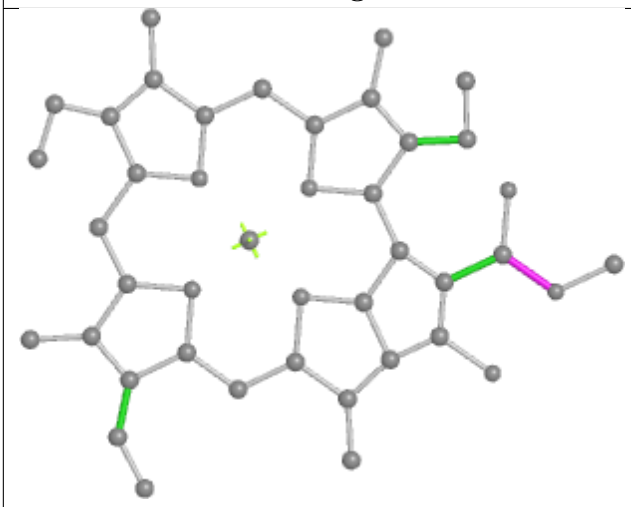
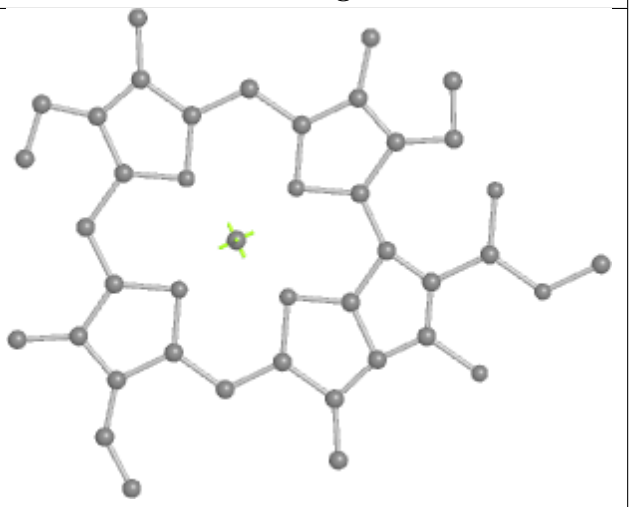


Bond angles

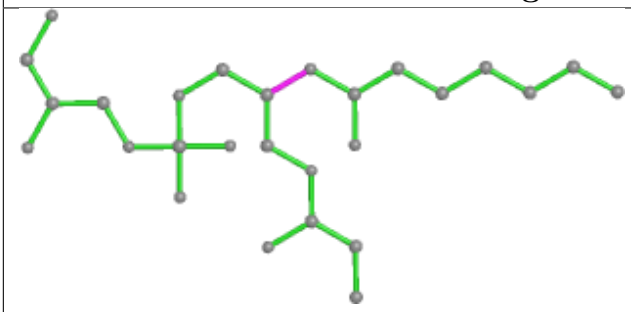


Torsions



Rings

Ligand LHG A 847



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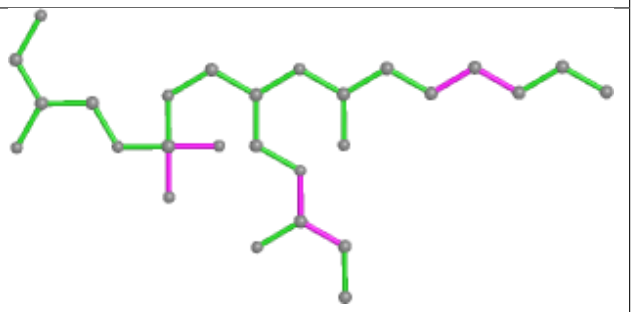
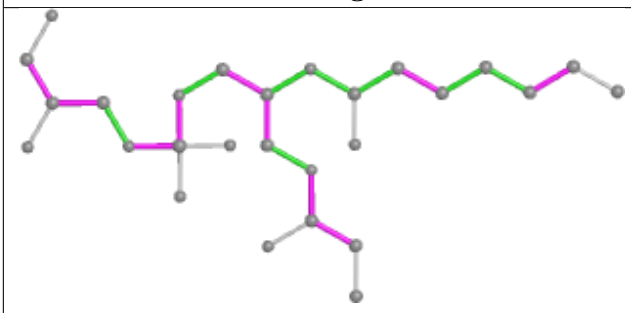
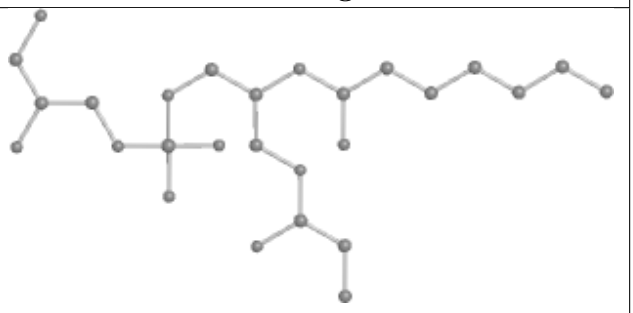


Bond angles

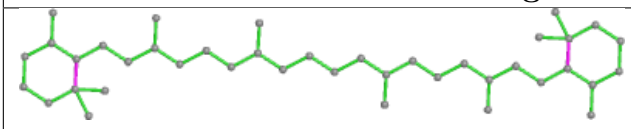


Torsions

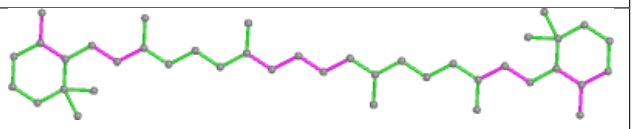


Rings

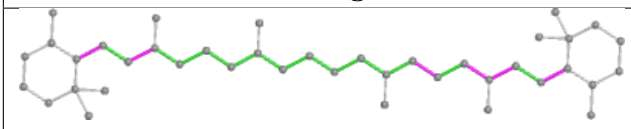
Ligand BCR B 843



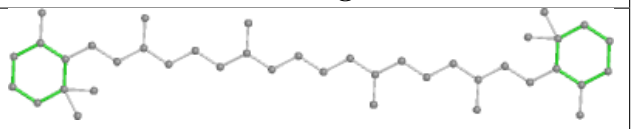
Bond lengths



Bond angles

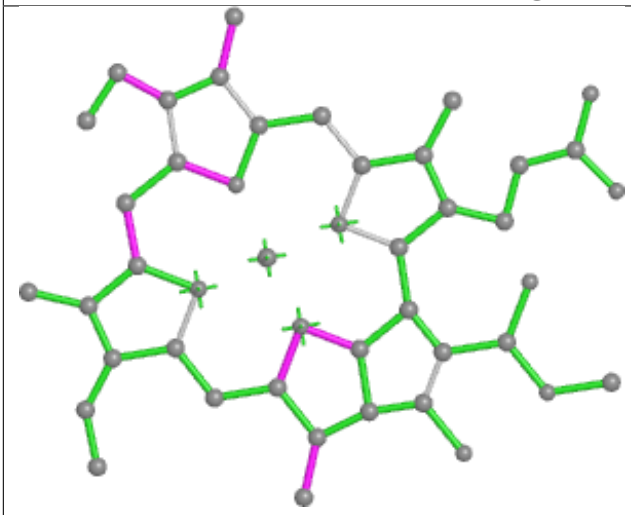


Torsions

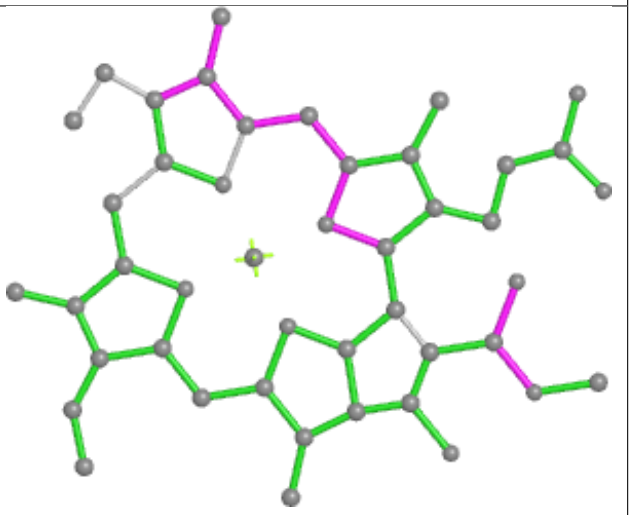


Rings

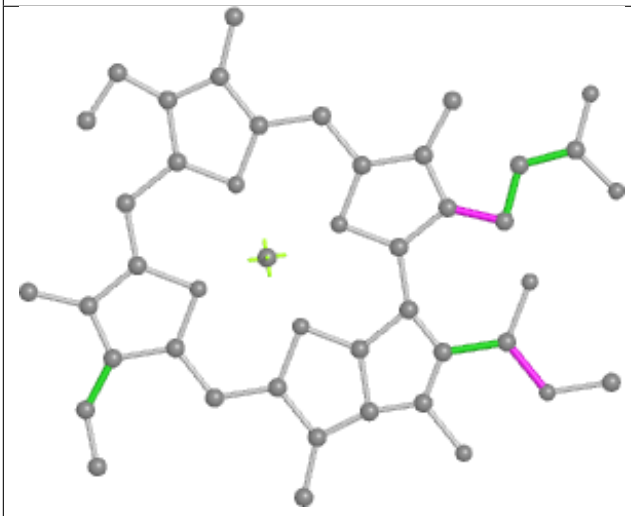
Ligand CLA 2 610



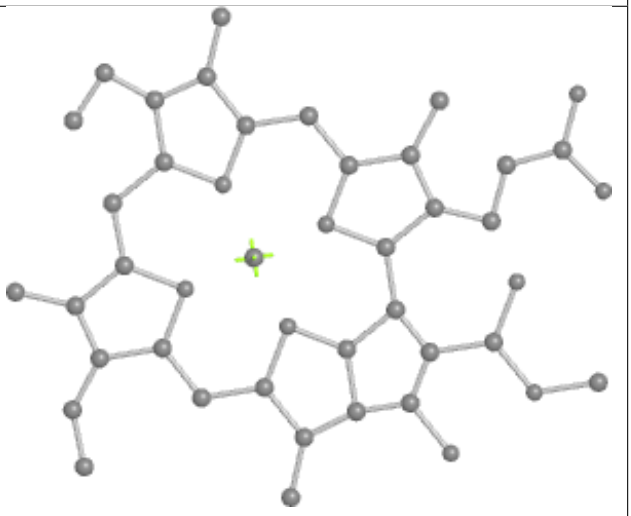
Bond lengths



Bond angles

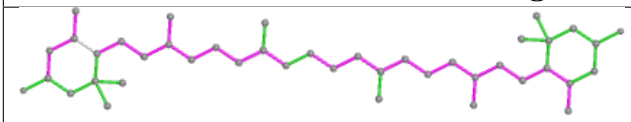


Torsions

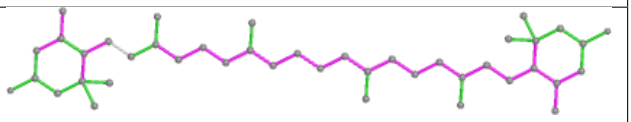


Rings

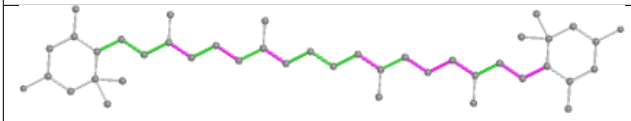
Ligand LUT 6 617



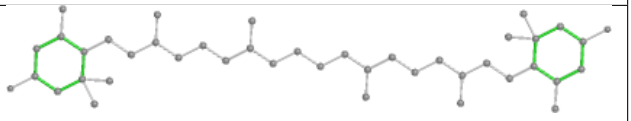
Bond lengths



Bond angles

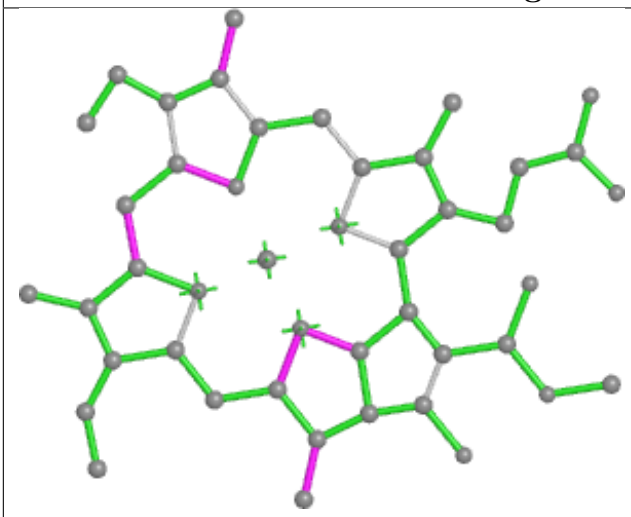


Torsions

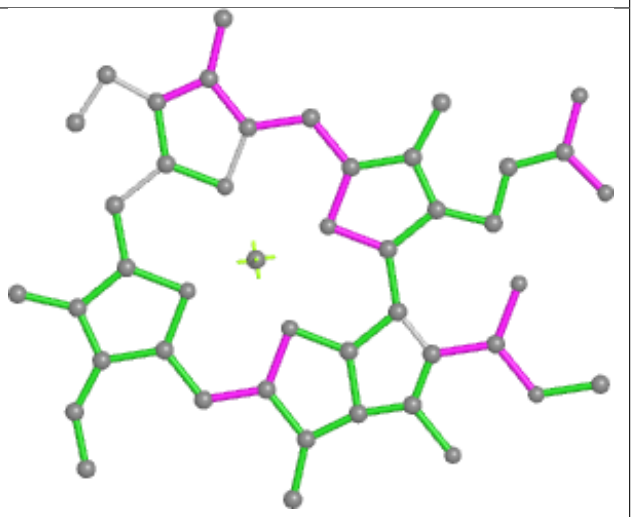


Rings

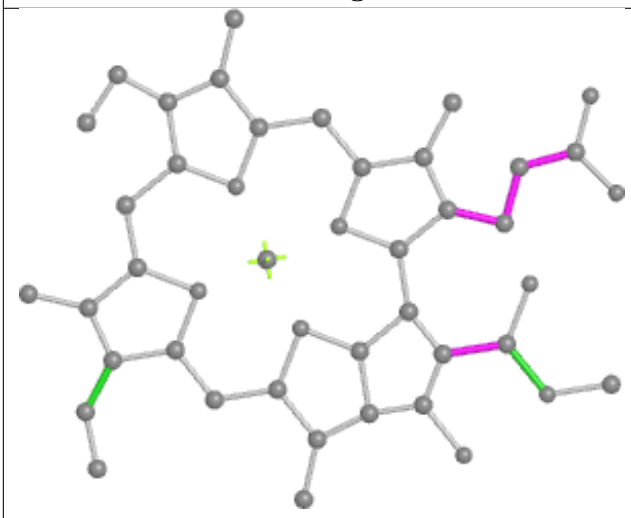
Ligand CLA B 832



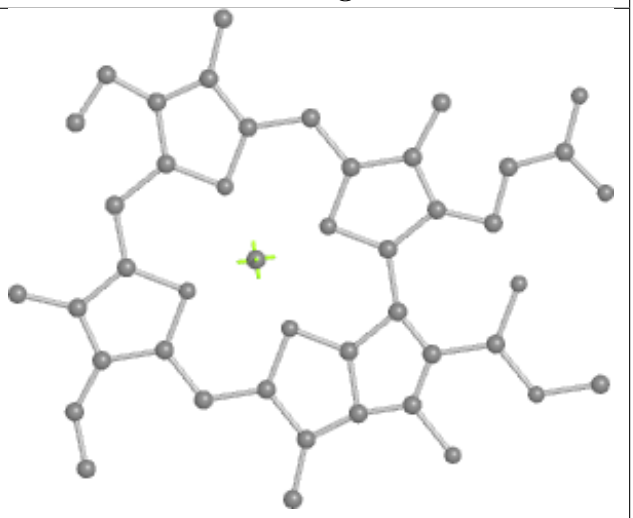
Bond lengths



Bond angles

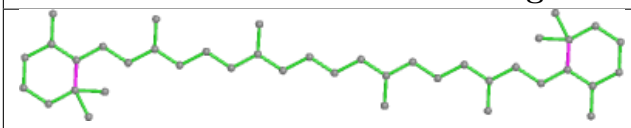


Torsions

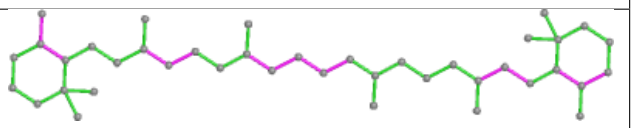


Rings

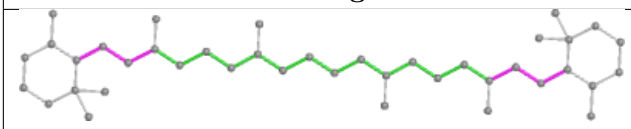
Ligand BCR 3 622



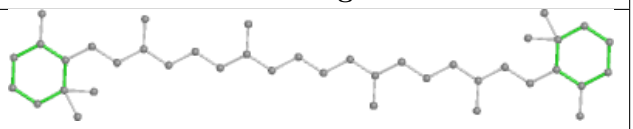
Bond lengths



Bond angles

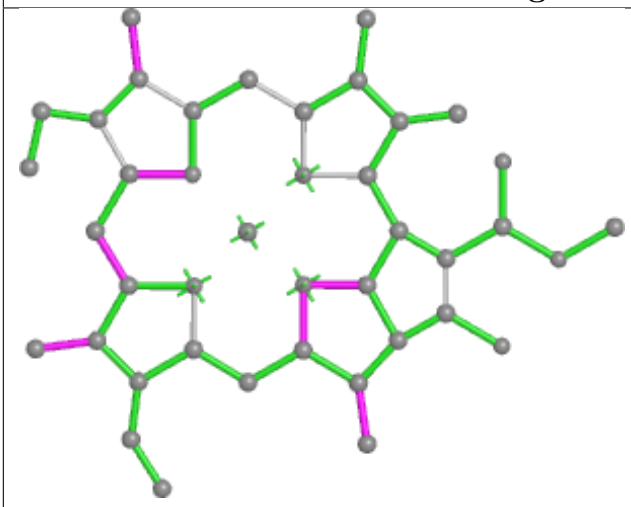


Torsions



Rings

Ligand CLA 3 610



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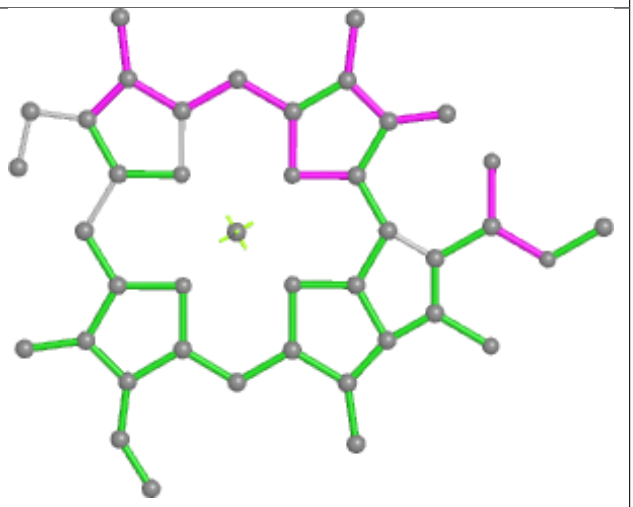
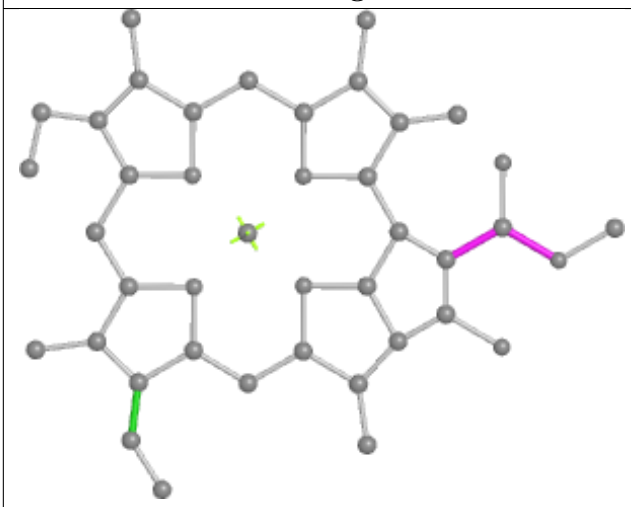
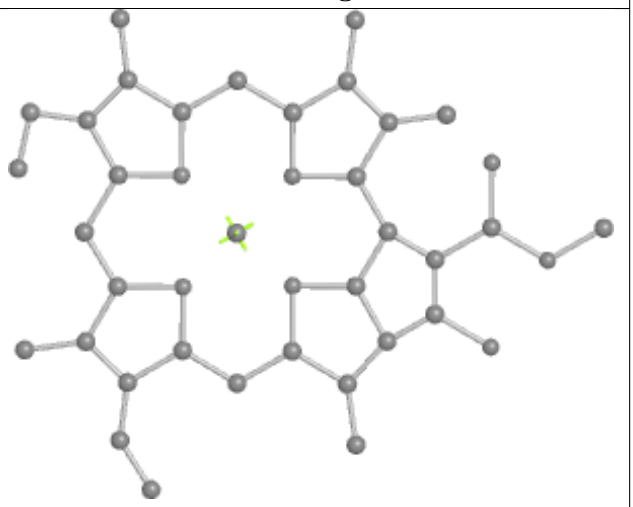


Bond angles

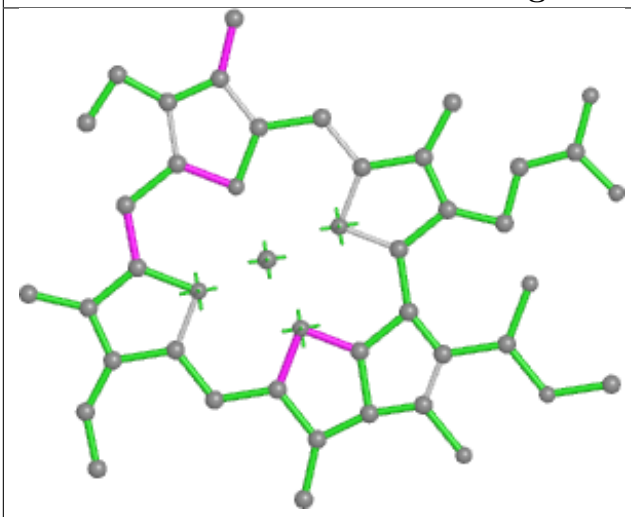


Torsions

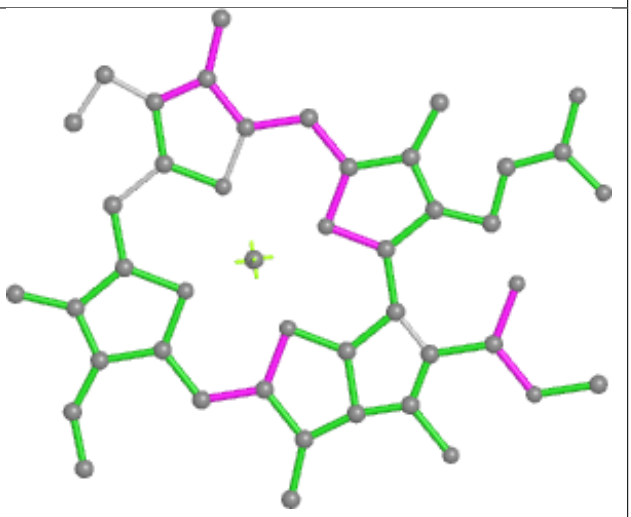


Rings

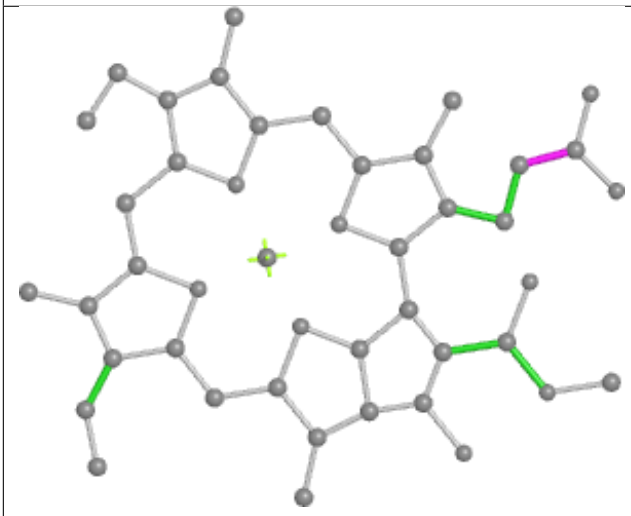
Ligand CLA 5 601



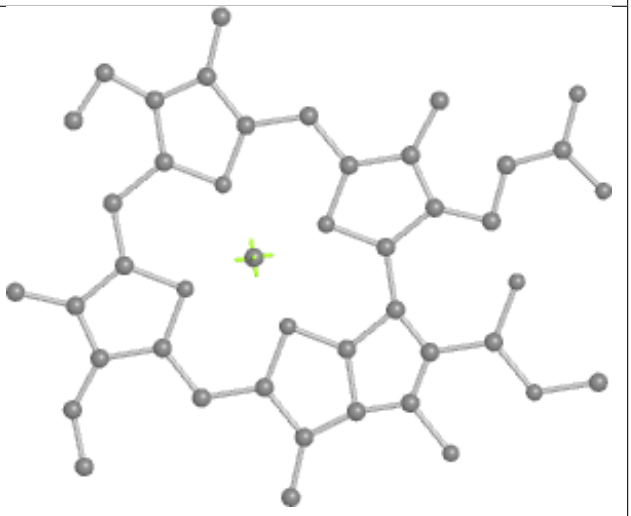
Bond lengths



Bond angles

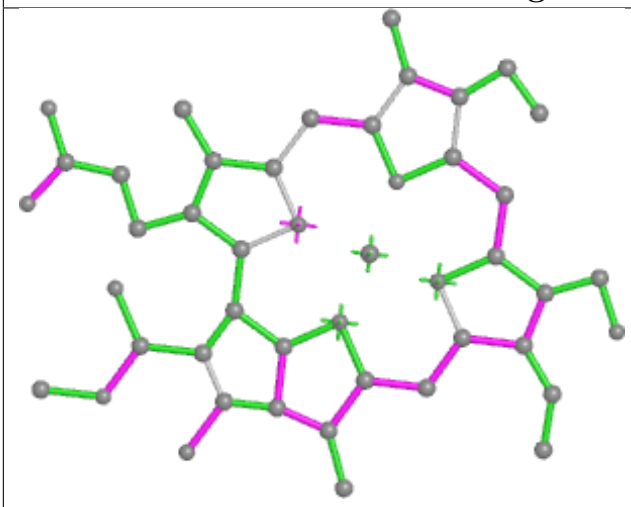


Torsions

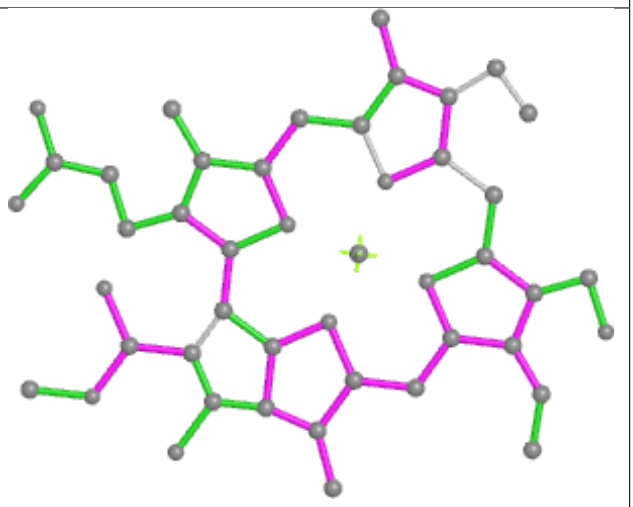


Rings

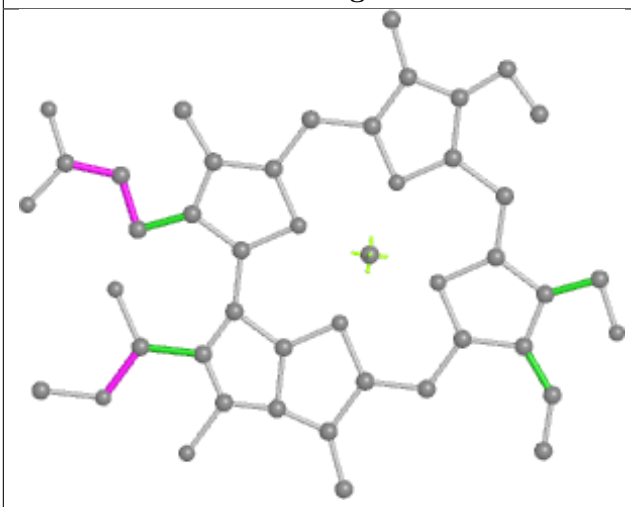
Ligand CHL 2 606



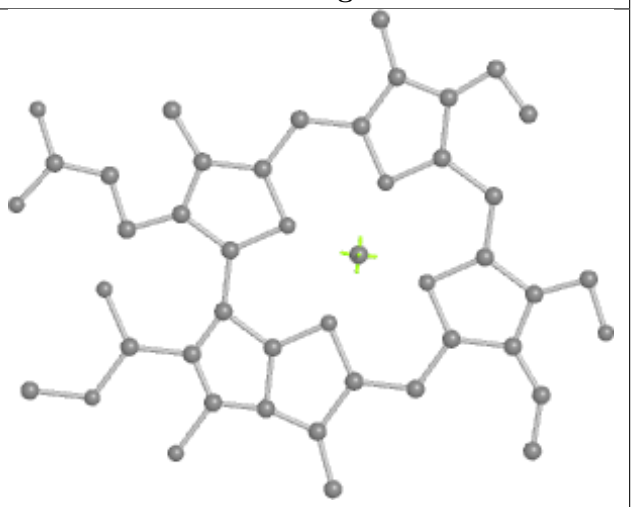
Bond lengths



Bond angles

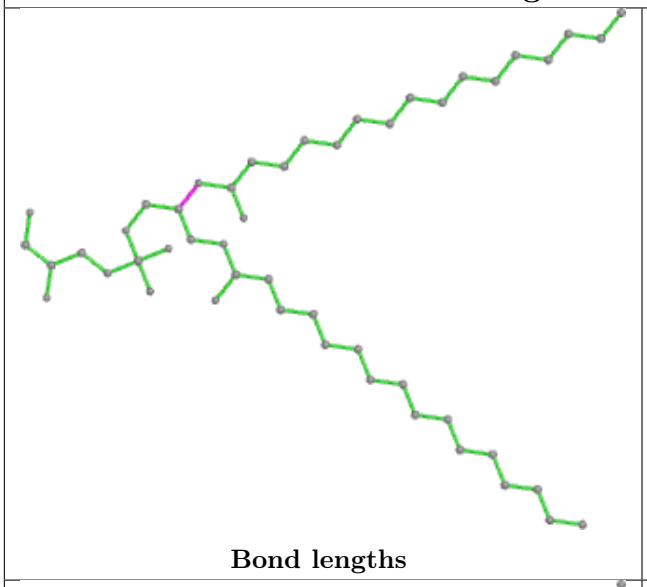


Torsions

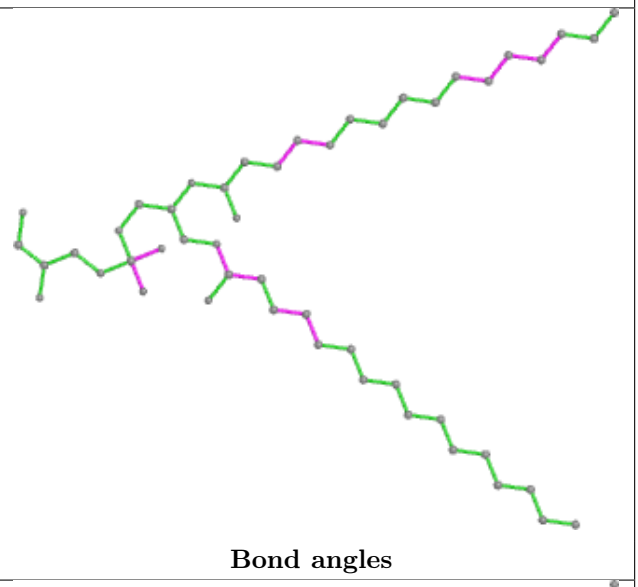


Rings

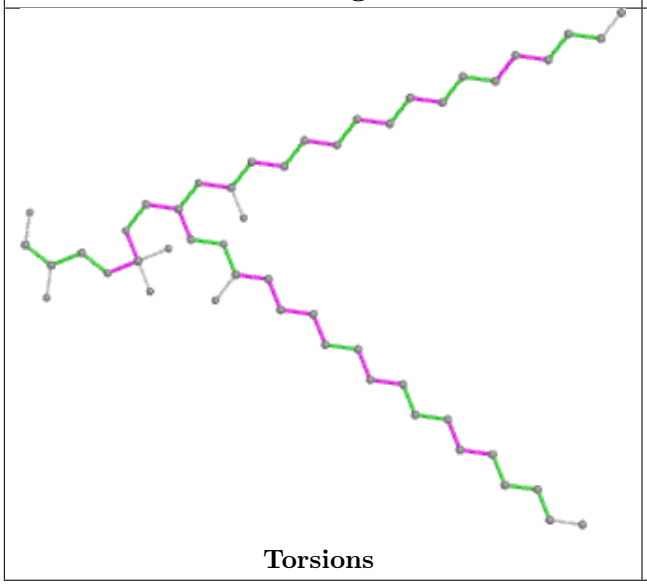
Ligand LHG A 846



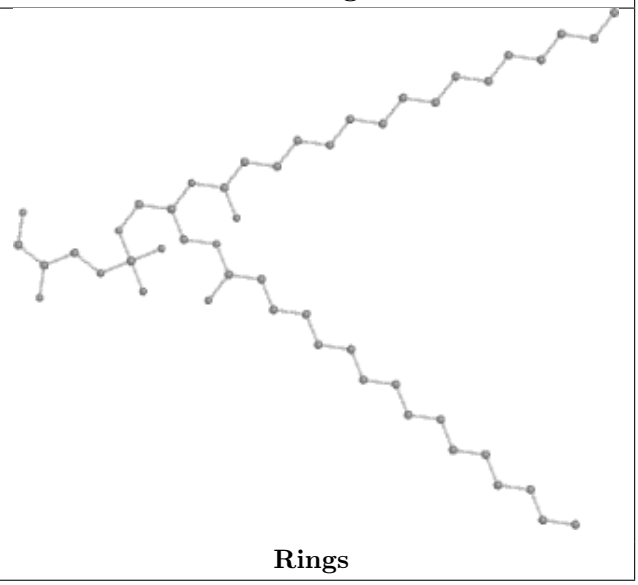
Bond lengths



Bond angles

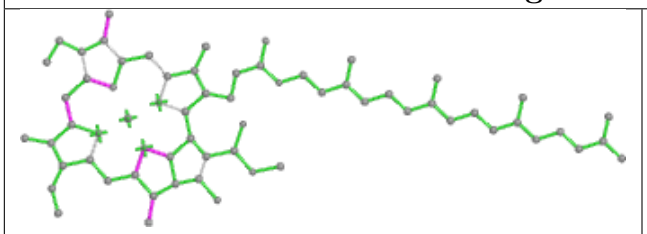


Torsions

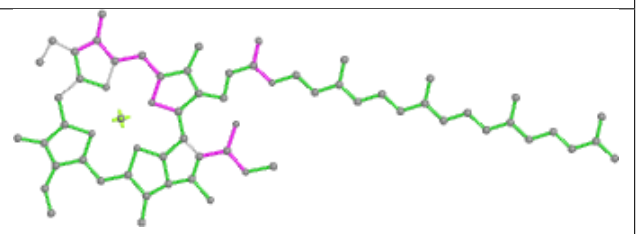


Rings

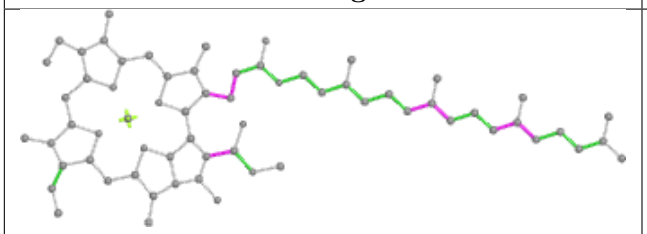
Ligand CLA B 805



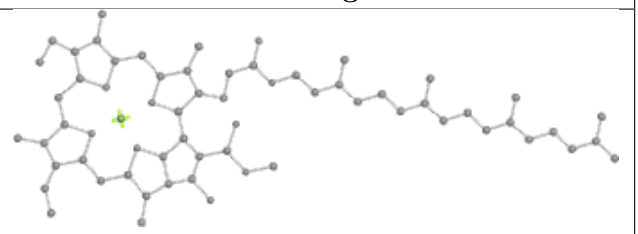
Bond lengths



Bond angles

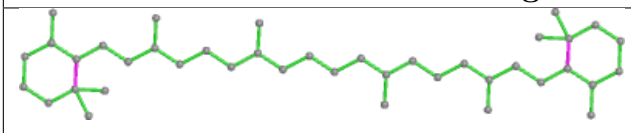


Torsions

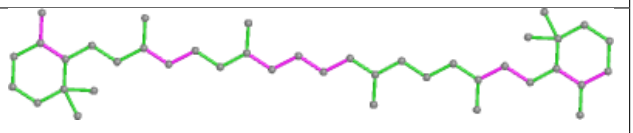


Rings

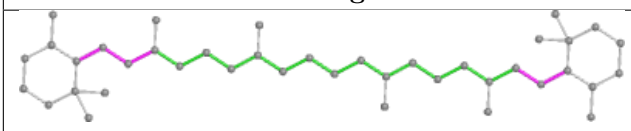
Ligand BCR A 849



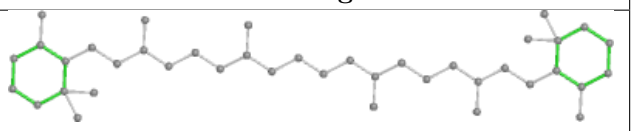
Bond lengths



Bond angles

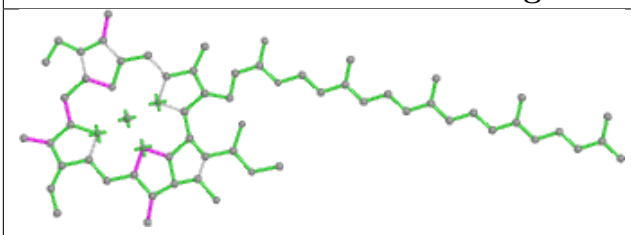


Torsions



Rings

Ligand CLA A 835



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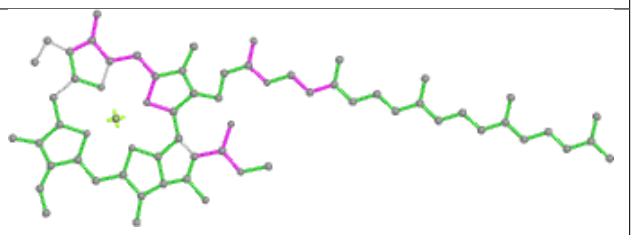
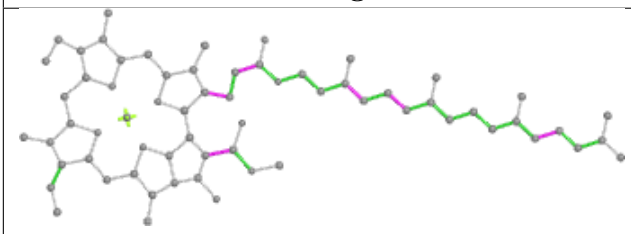
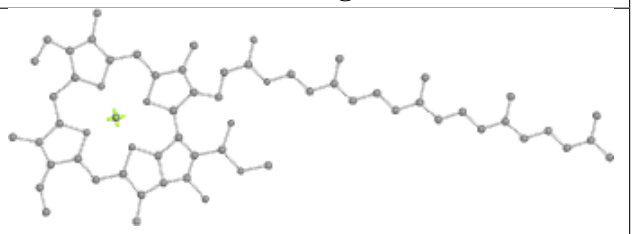


Bond angles

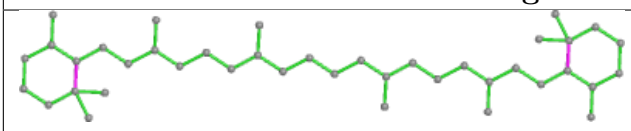


Torsions

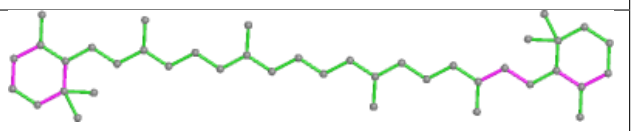


Rings

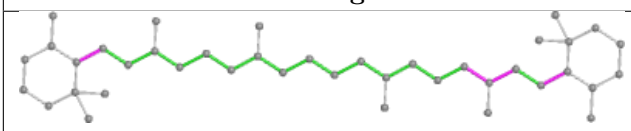
Ligand BCR A 848



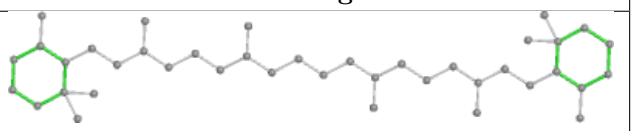
Bond lengths



Bond angles

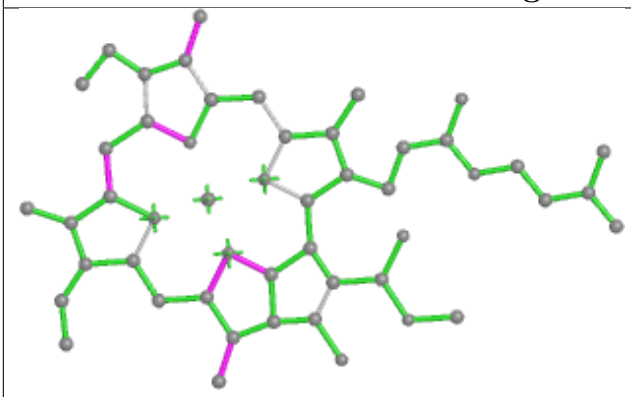


Torsions

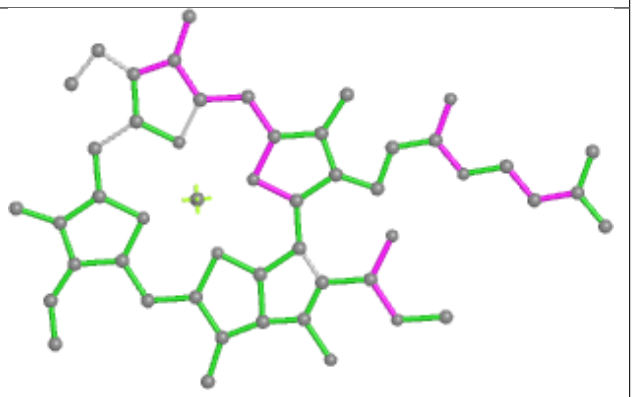


Rings

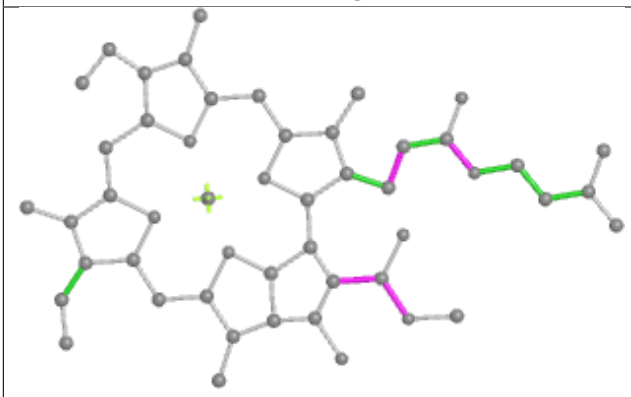
Ligand CLA G 203



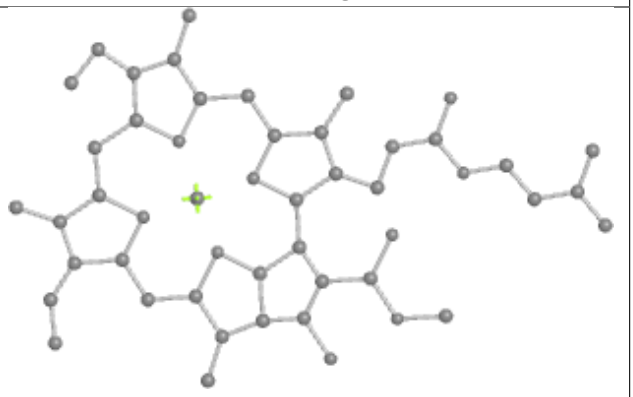
Bond lengths



Bond angles

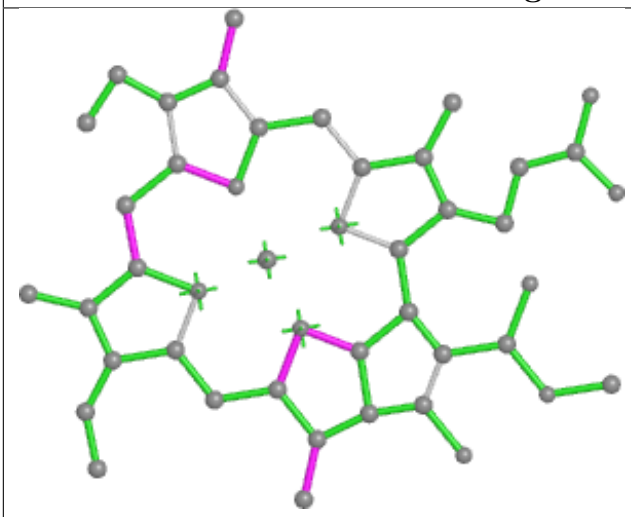


Torsions

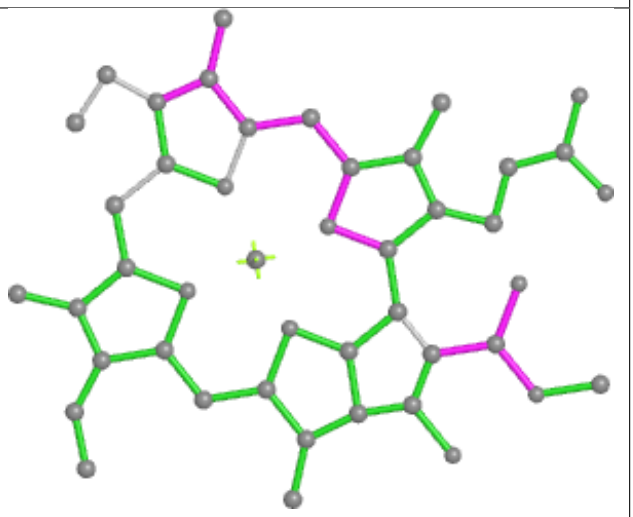


Rings

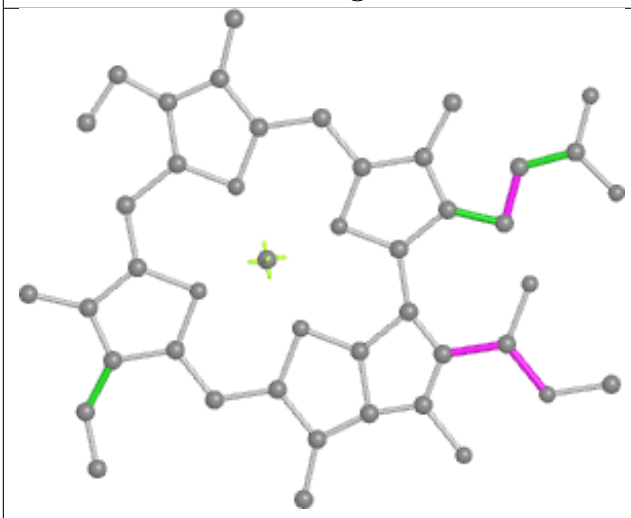
Ligand CLA B 804



Bond lengths



Bond angles



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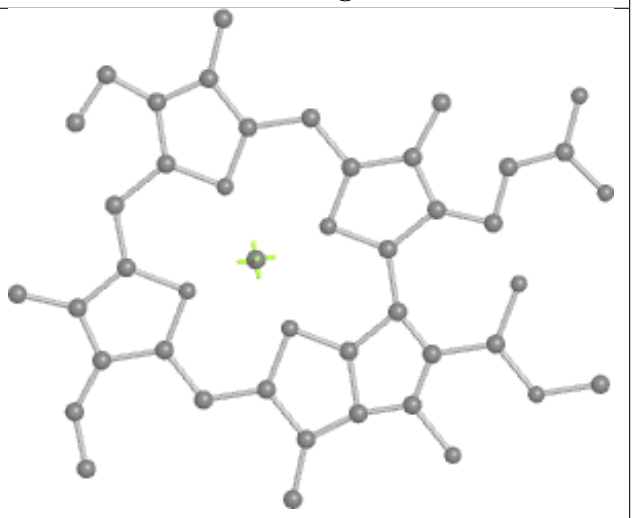
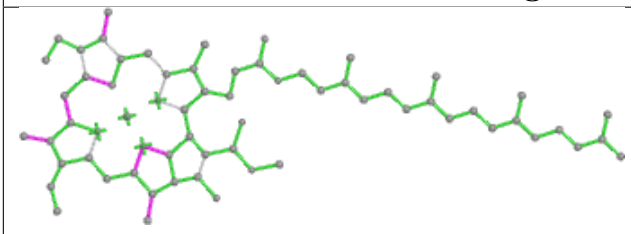


Rings

Ligand CLA A 841



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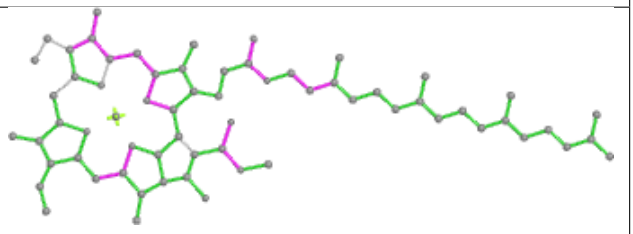
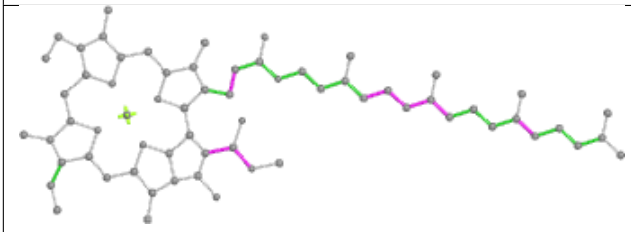
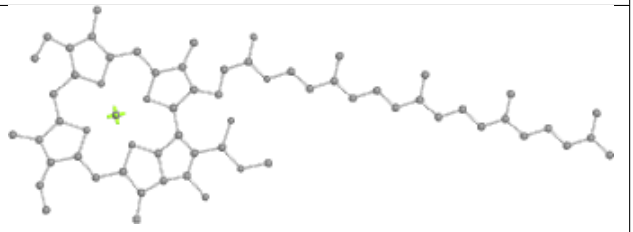


Bond angles

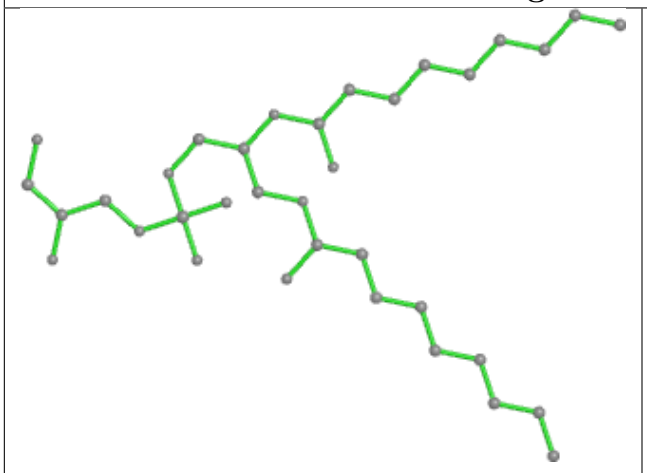


Torsions

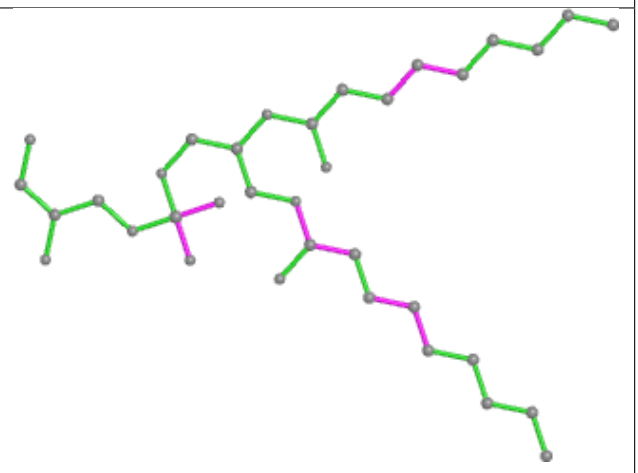


Rings

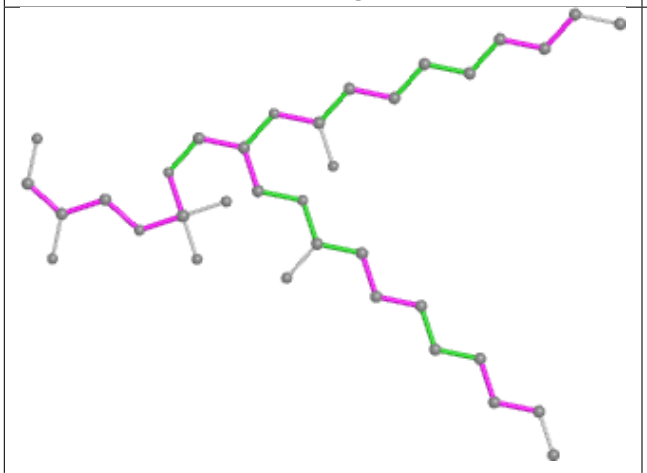
Ligand LHG 2 622



Bond lengths



Bond angles



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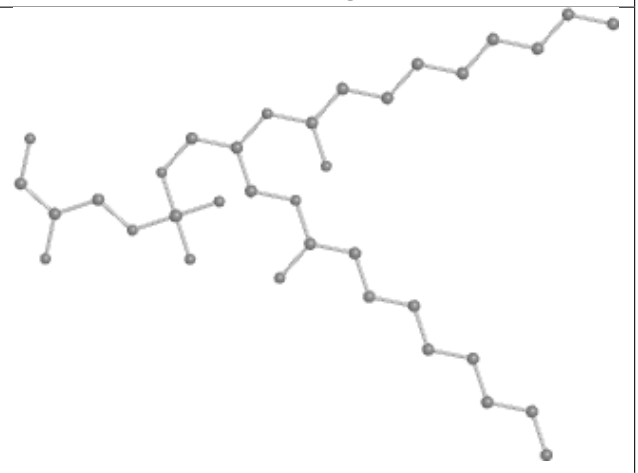
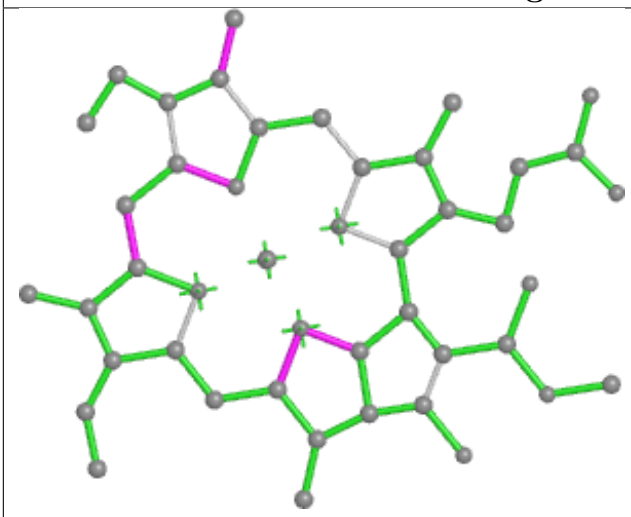
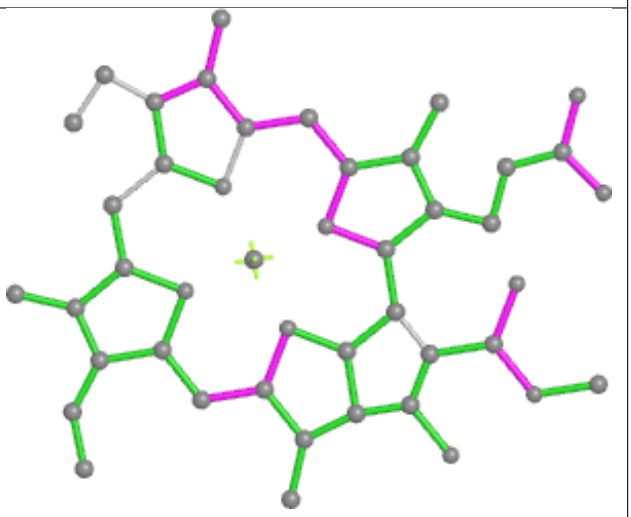


Rings

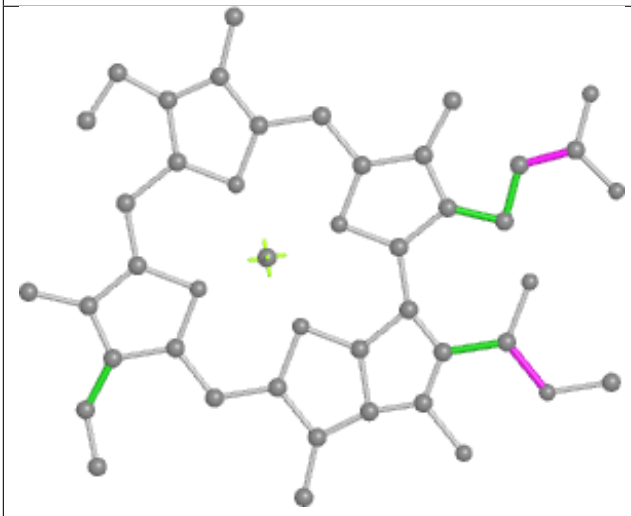
Ligand CLA F 303



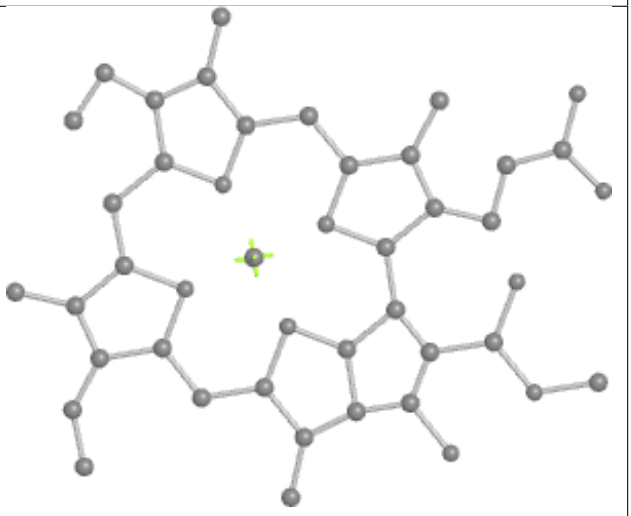
Bond lengths



Bond angles

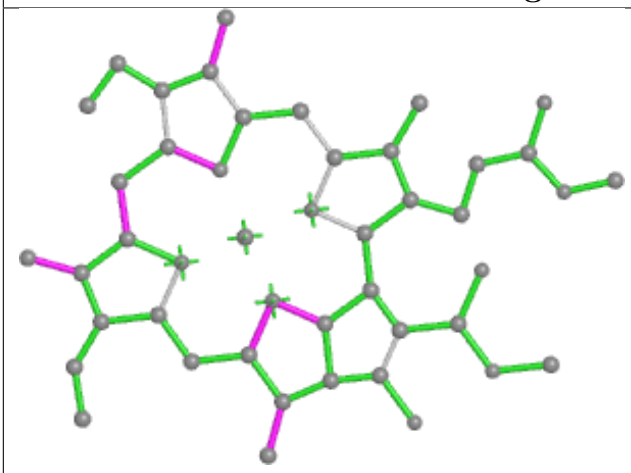


Torsions

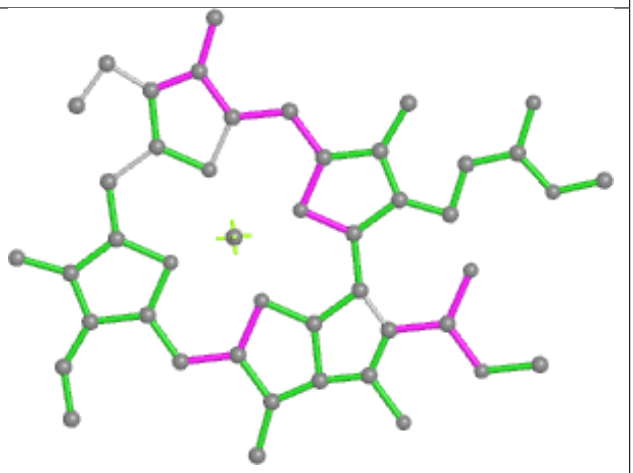


Rings

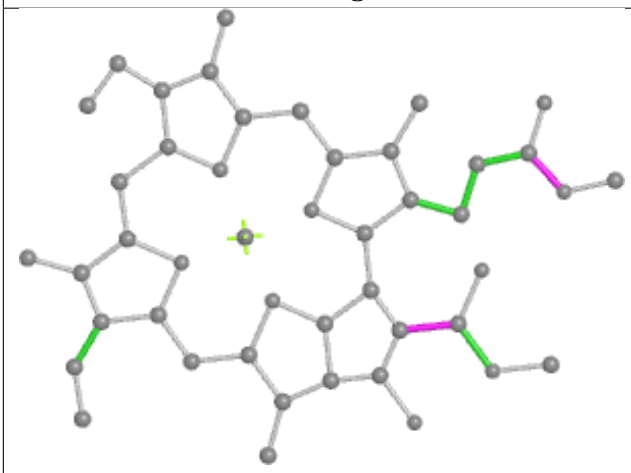
Ligand CLA B 837



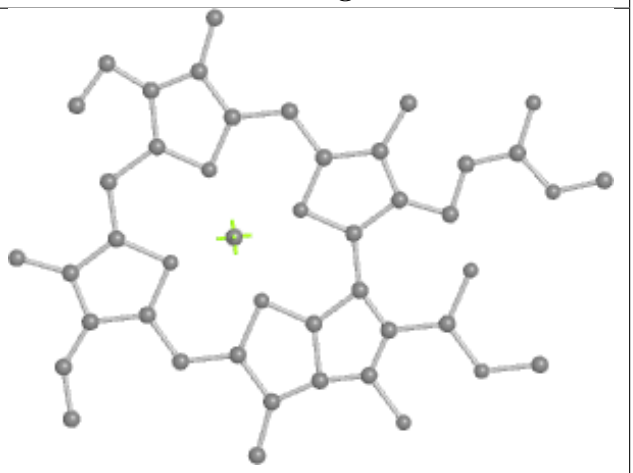
Bond lengths



Bond angles

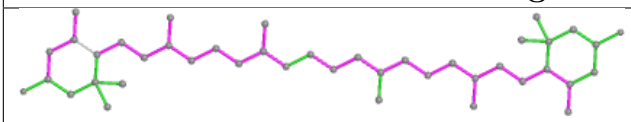


Torsions

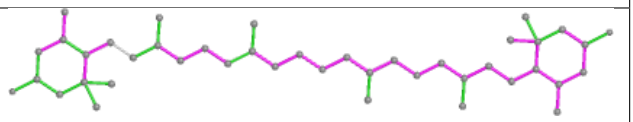


Rings

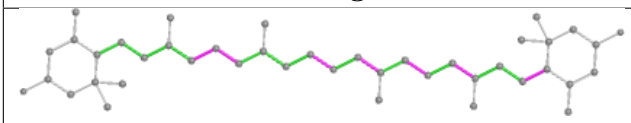
Ligand LUT 5 619



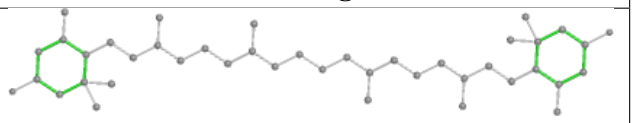
Bond lengths



Bond angles

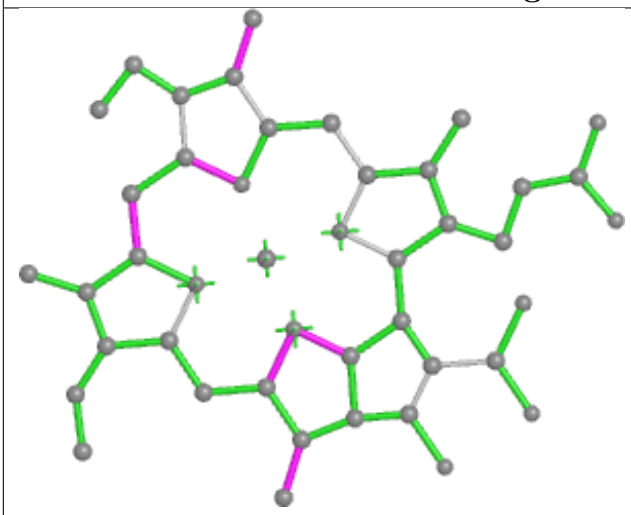


Torsions

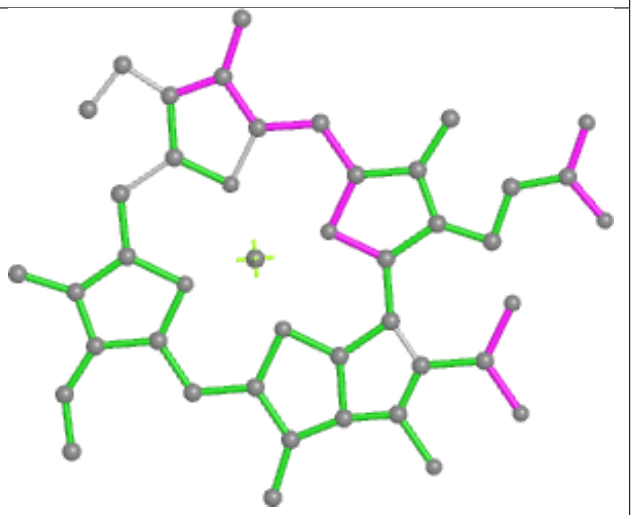


Rings

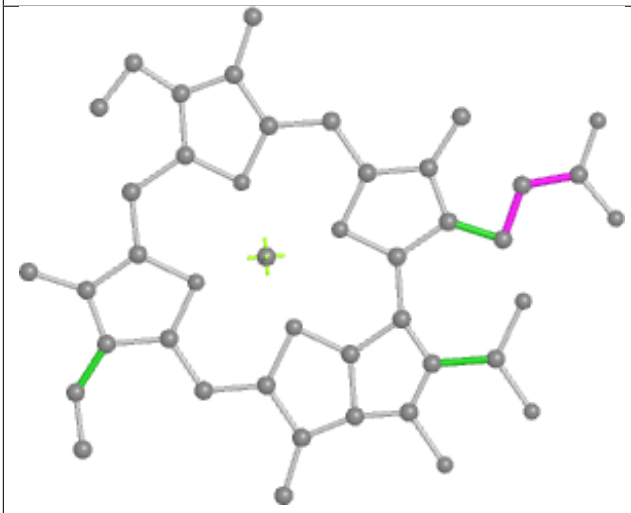
Ligand CLA A 842



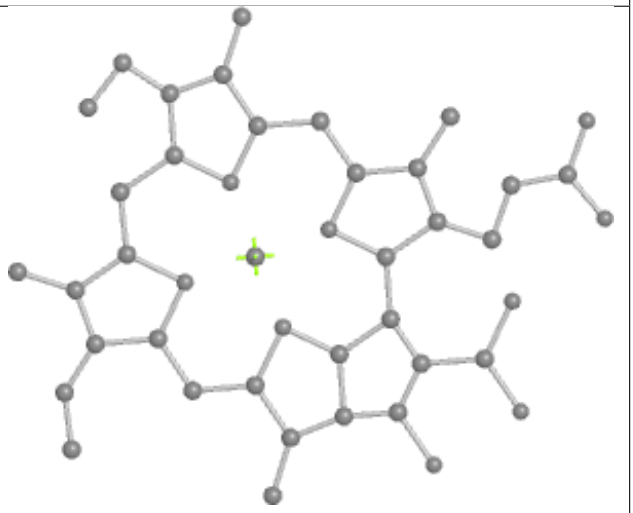
Bond lengths



Bond angles

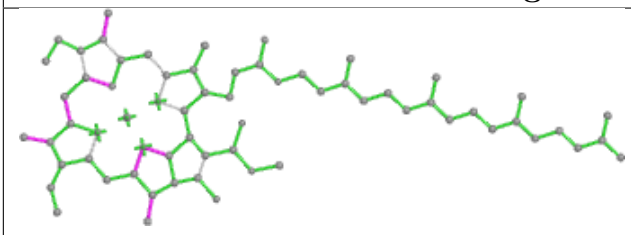


Torsions

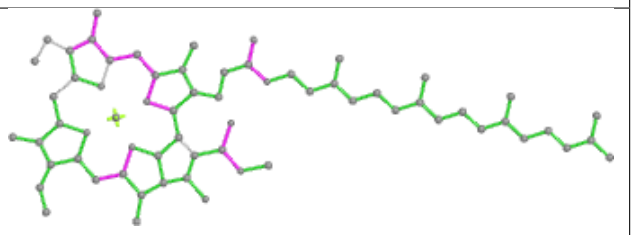


Rings

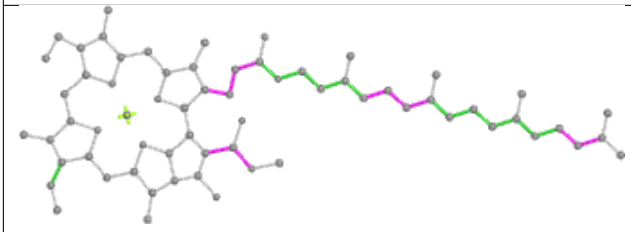
Ligand CLA A 814



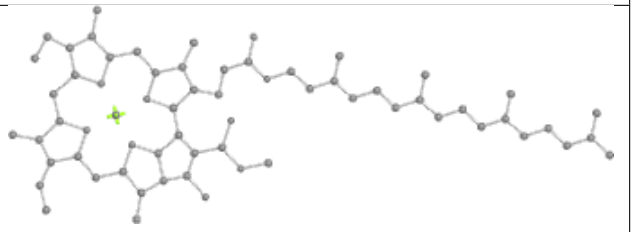
Bond lengths



Bond angles

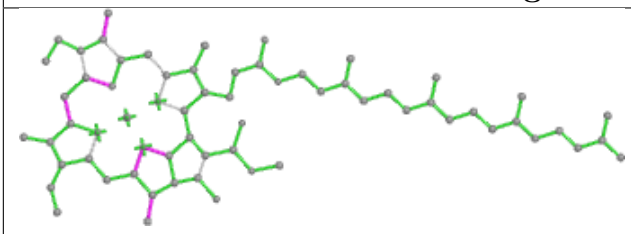


Torsions

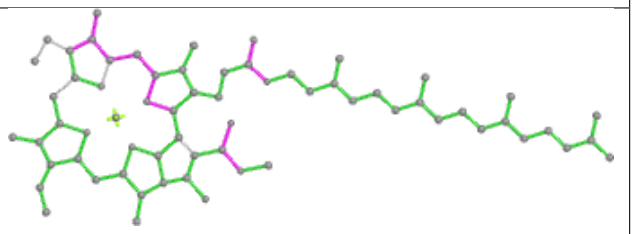


Rings

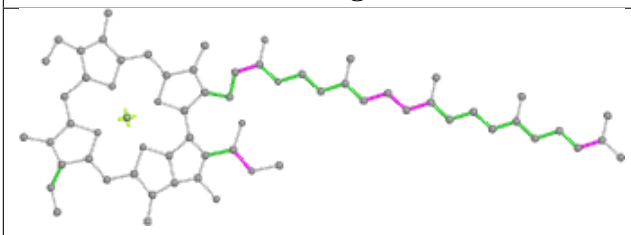
Ligand CLA A 801



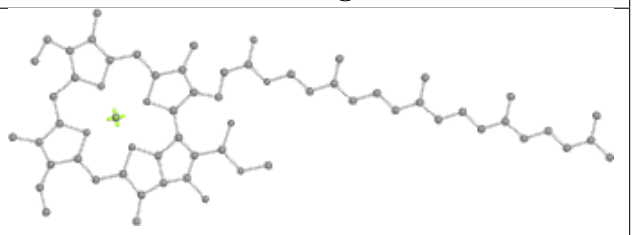
Bond lengths



Bond angles

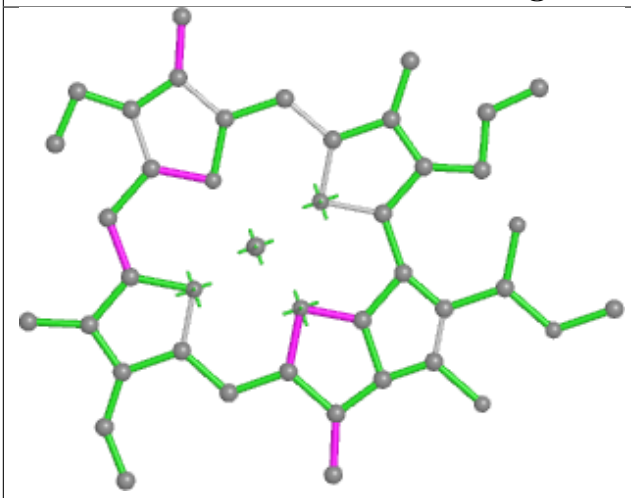


Torsions

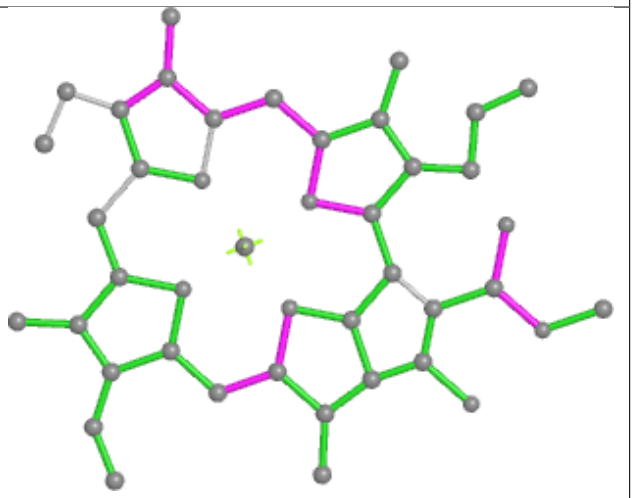


Rings

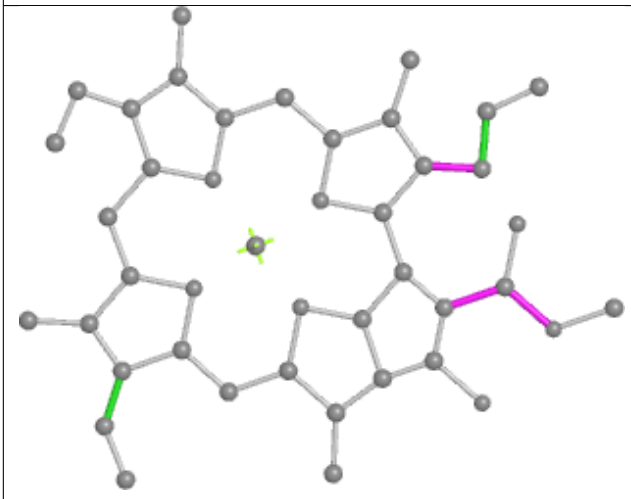
Ligand CLA 5 614



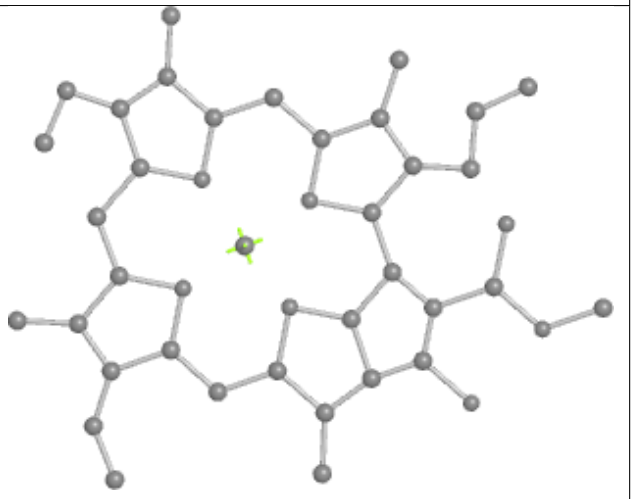
Bond lengths



Bond angles

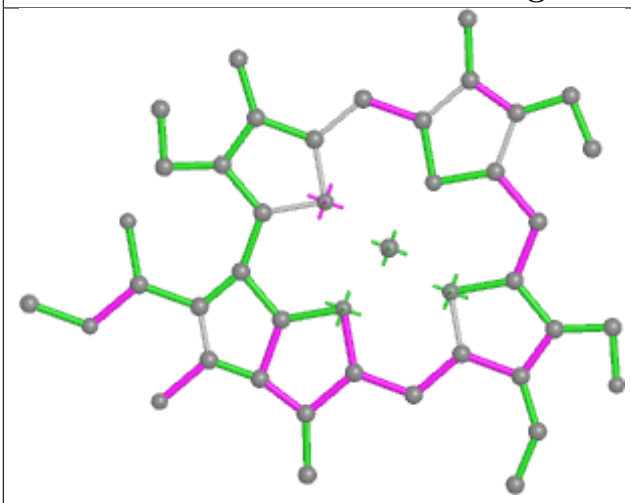


Torsions

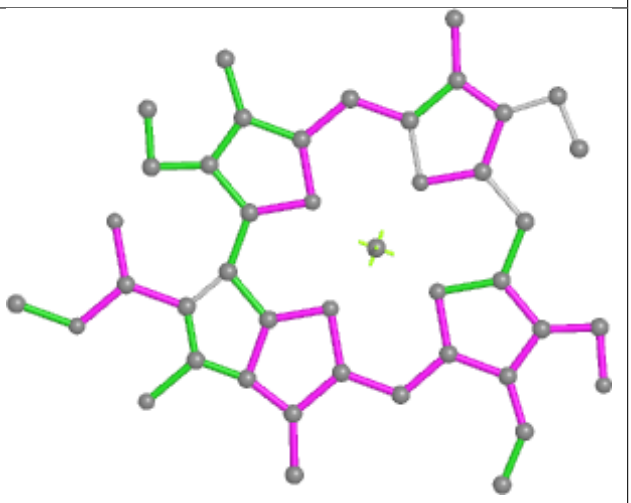


Rings

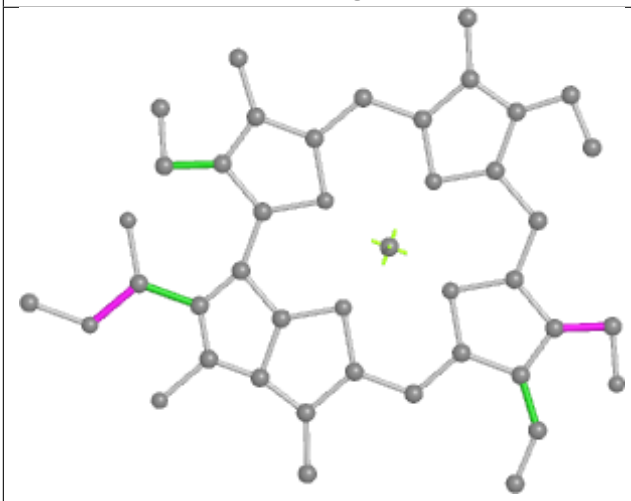
Ligand CHL 2 607



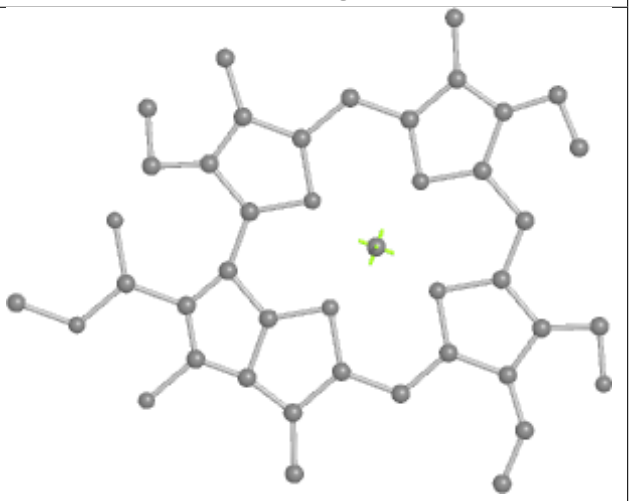
Bond lengths



Bond angles

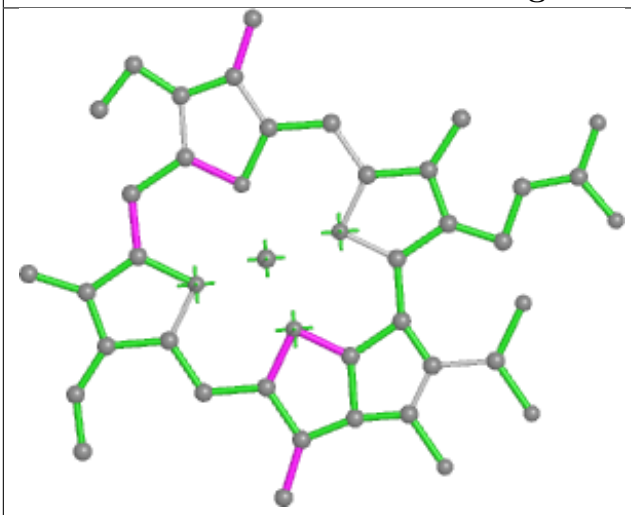


Torsions

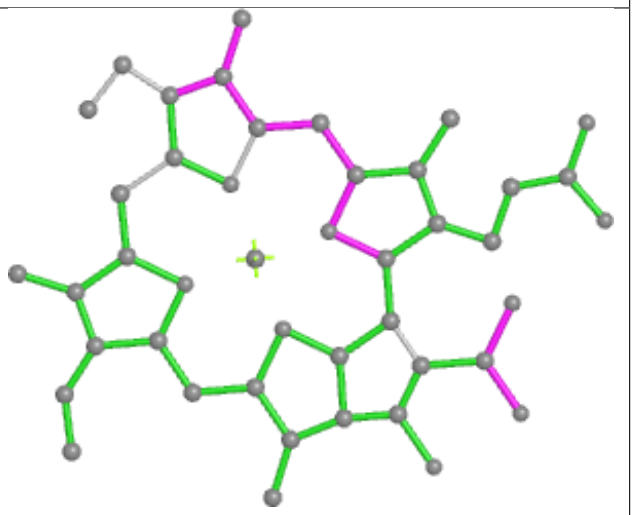


Rings

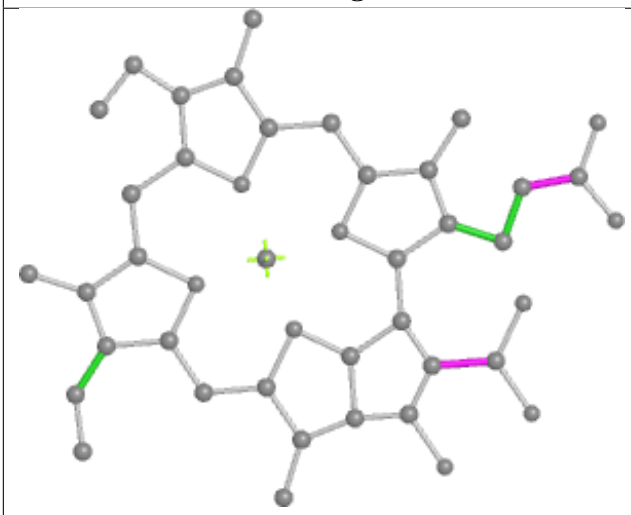
Ligand CLA 5 603



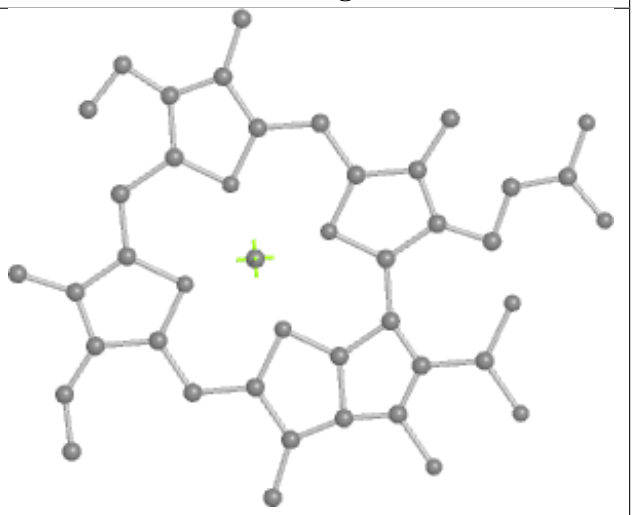
Bond lengths



Bond angles

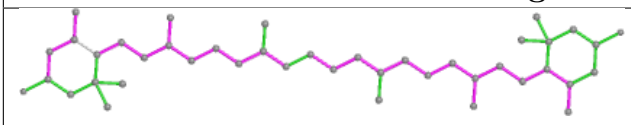


Torsions



Rings

Ligand LUT 2 619



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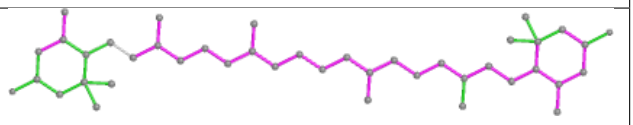
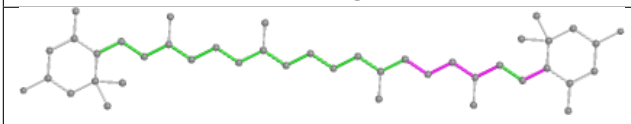
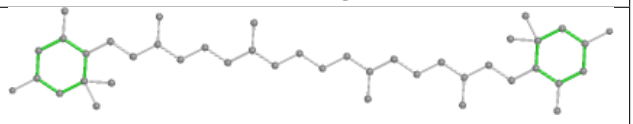


Bond angles

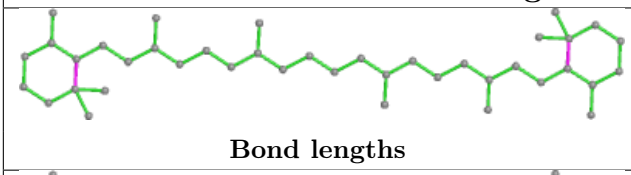


Torsions

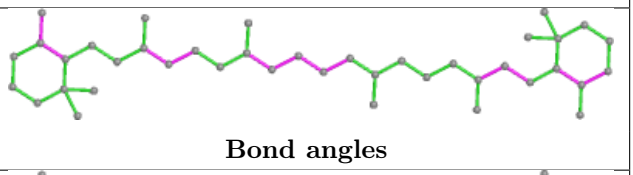


Rings

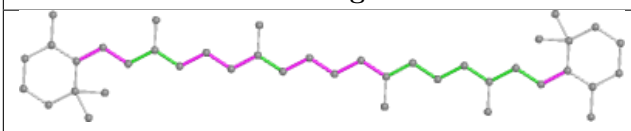
Ligand BCR F 302



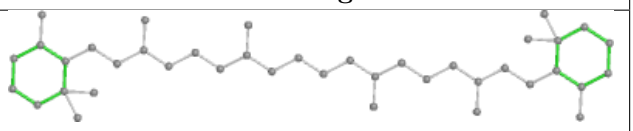
Bond lengths



Bond angles

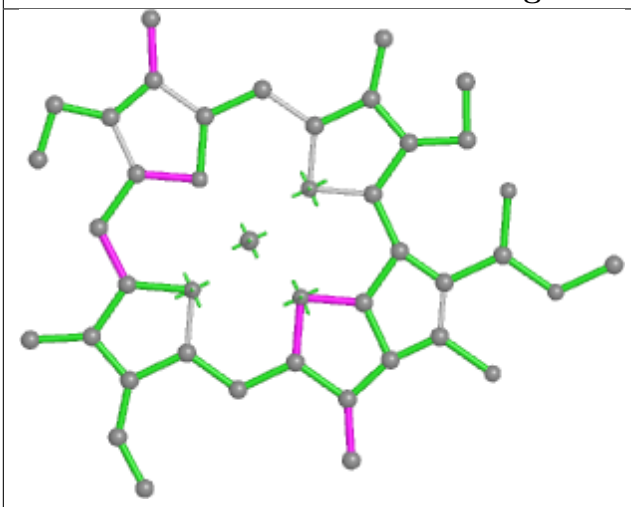


Torsions

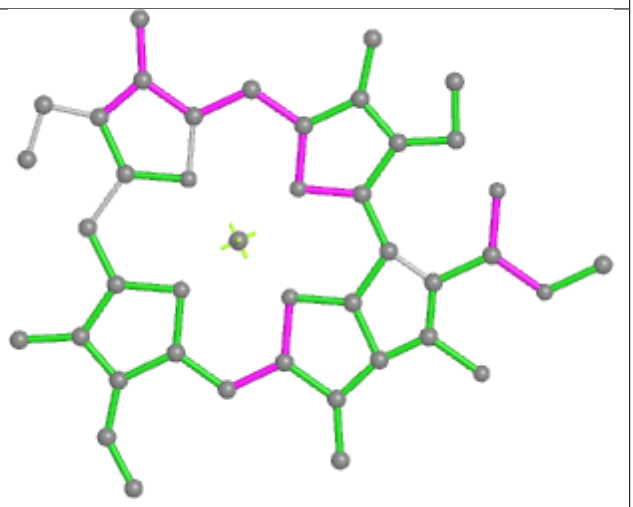


Rings

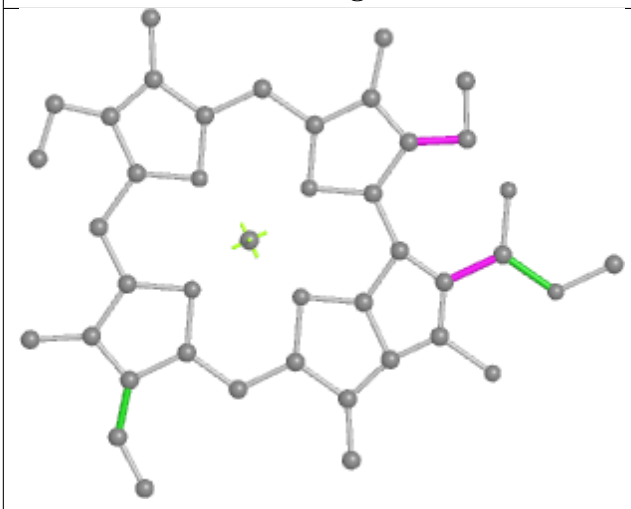
Ligand CLA A 816



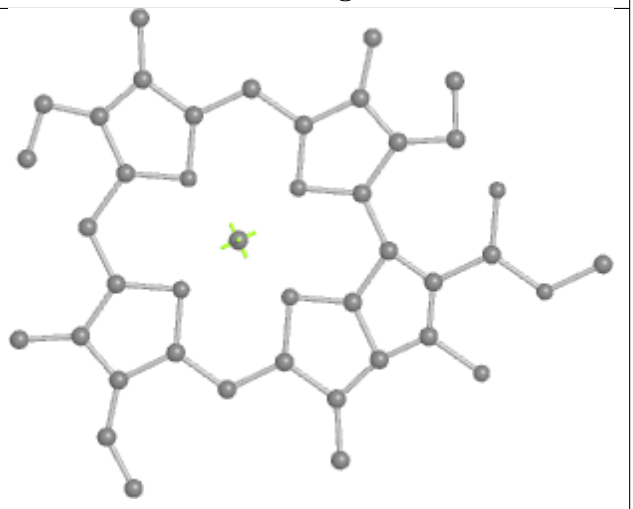
Bond lengths



Bond angles

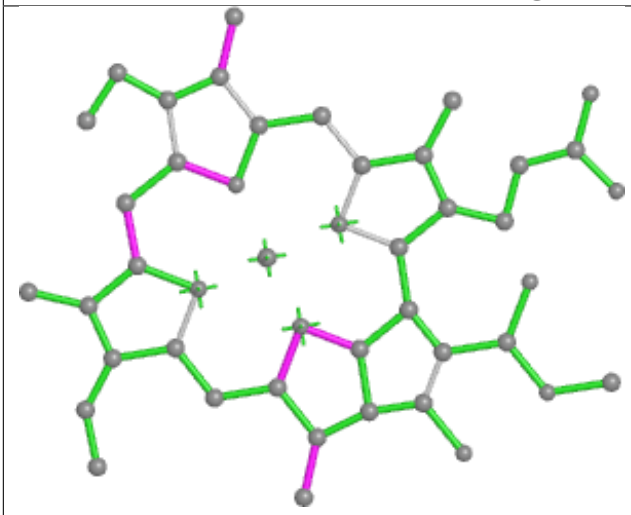


Torsions

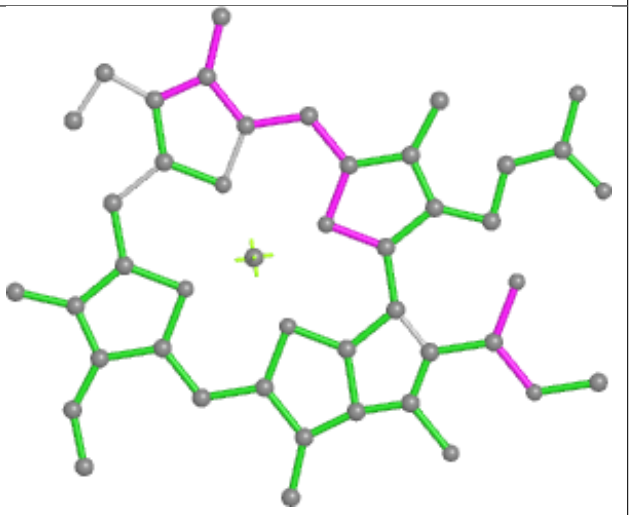


Rings

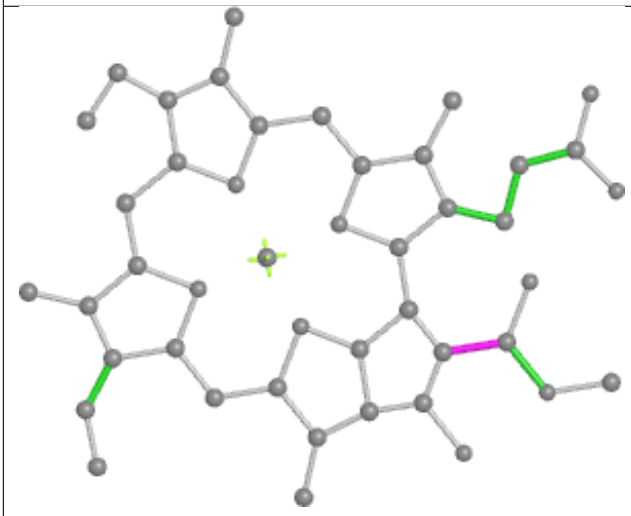
Ligand CLA 3 609



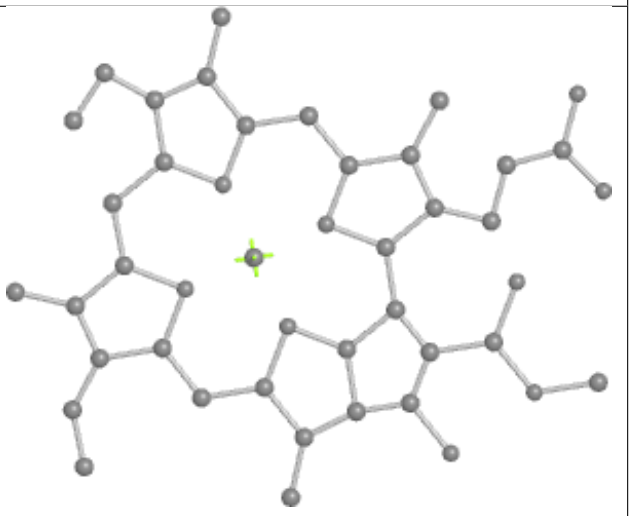
Bond lengths



Bond angles

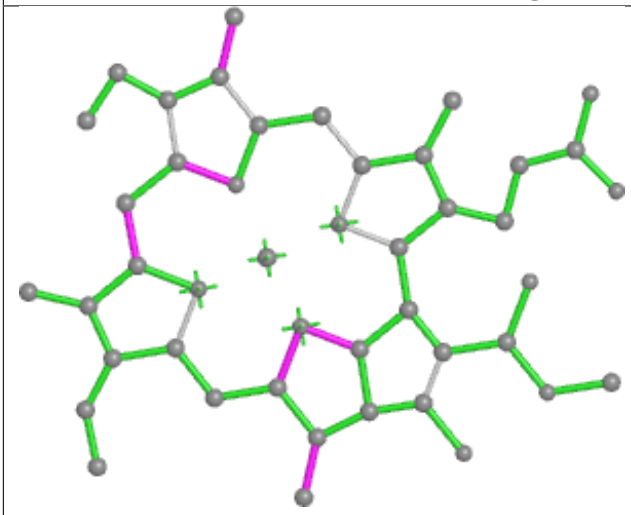


Torsions

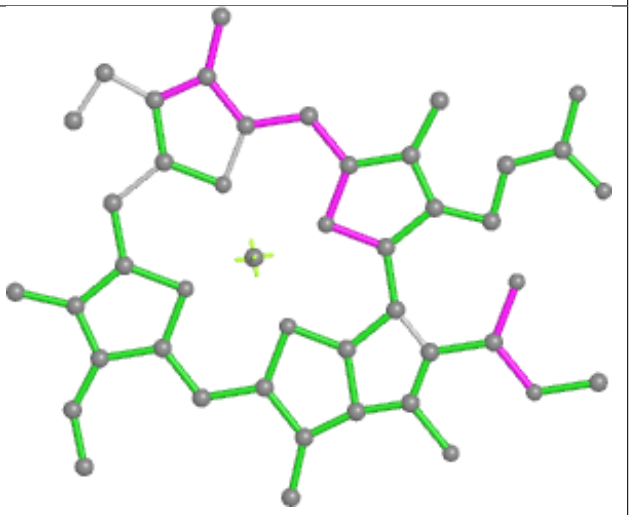


Rings

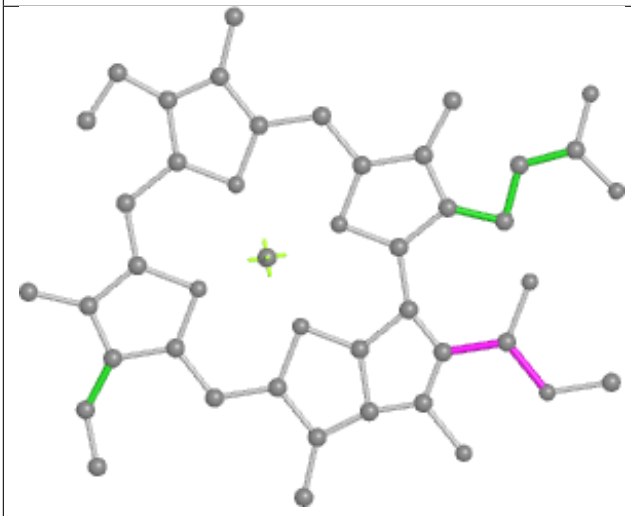
Ligand CLA F 301



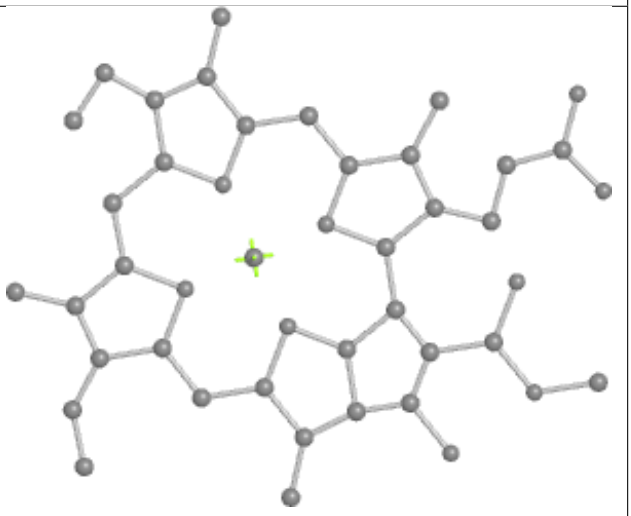
Bond lengths



Bond angles

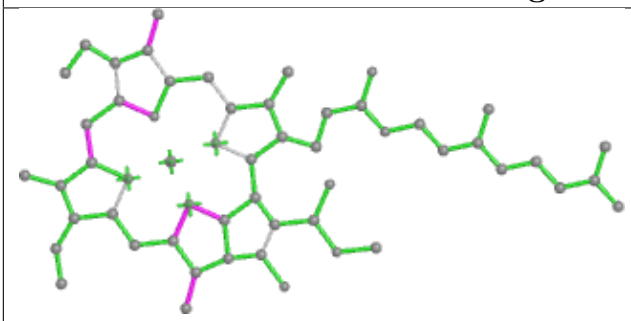


Torsions

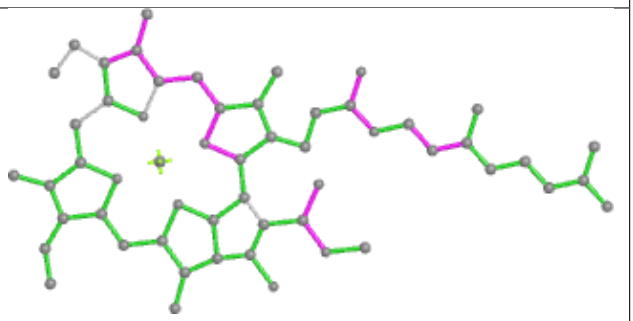


Rings

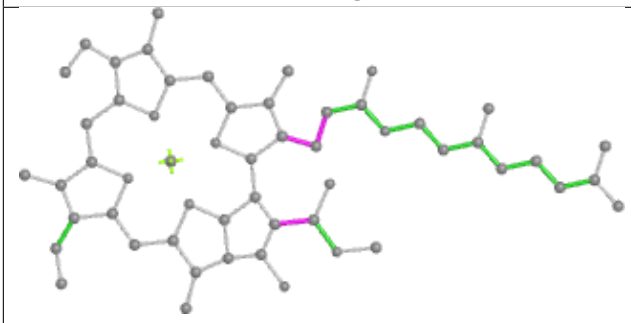
Ligand CLA 5 610



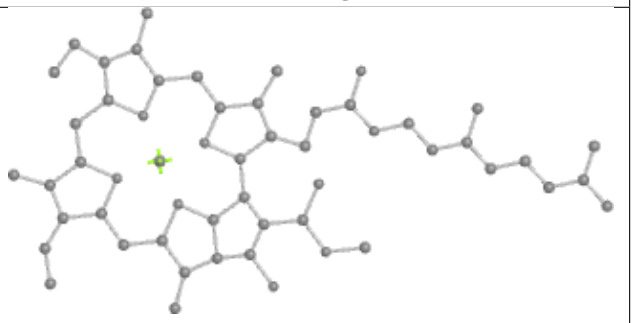
Bond lengths



Bond angles

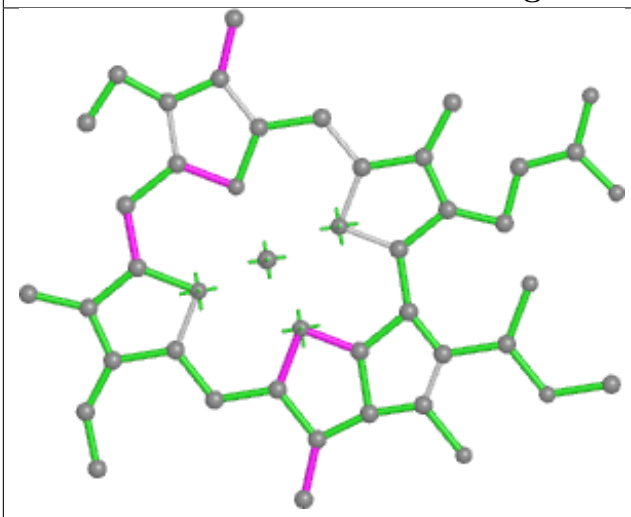


Torsions

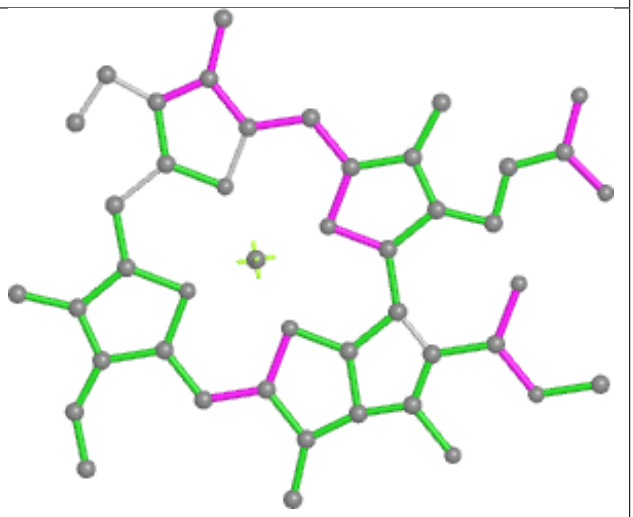


Rings

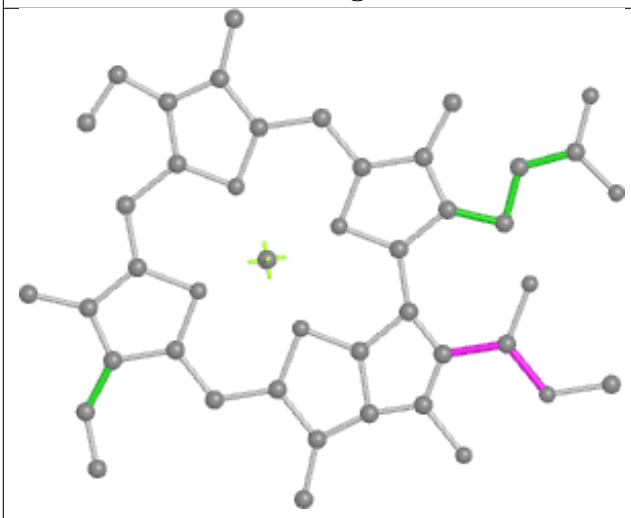
Ligand CLA A 815



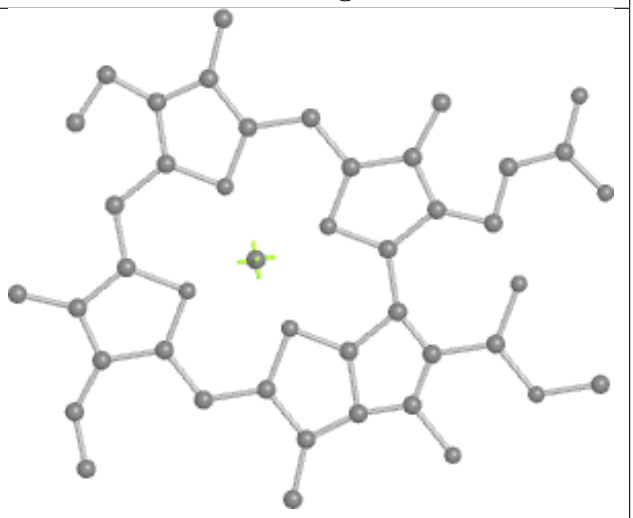
Bond lengths



Bond angles

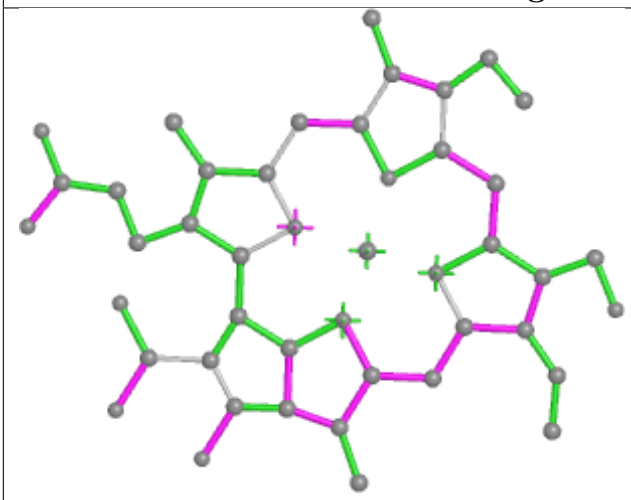


Torsions

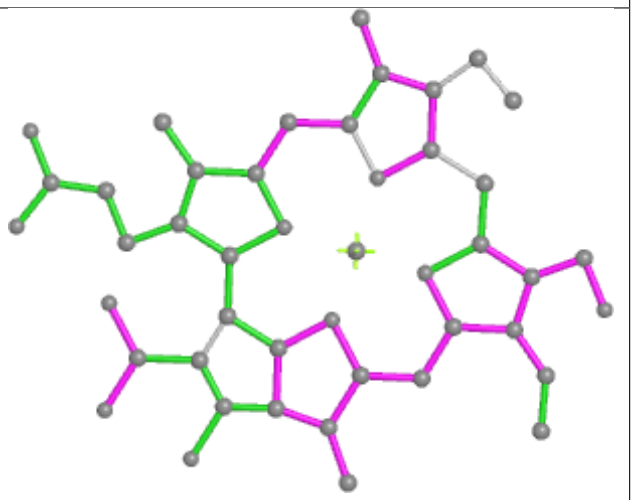


Rings

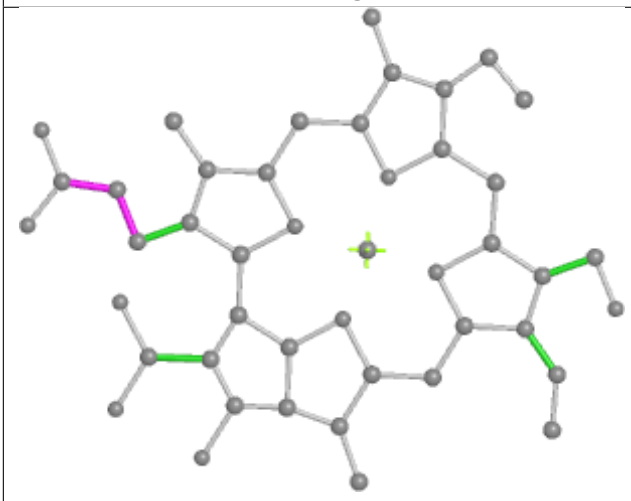
Ligand CHL 6 601



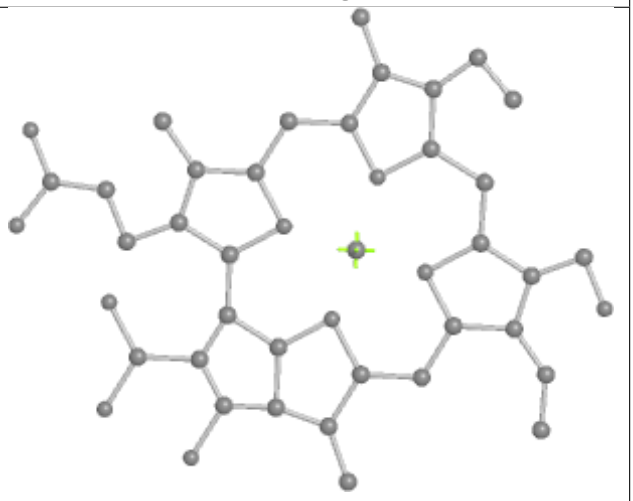
Bond lengths



Bond angles

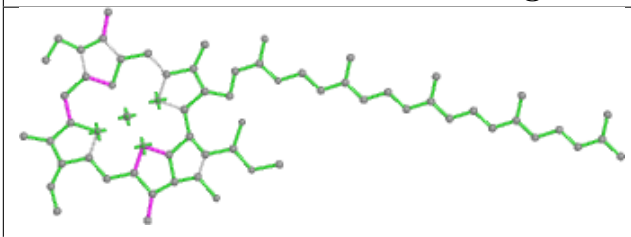


Torsions

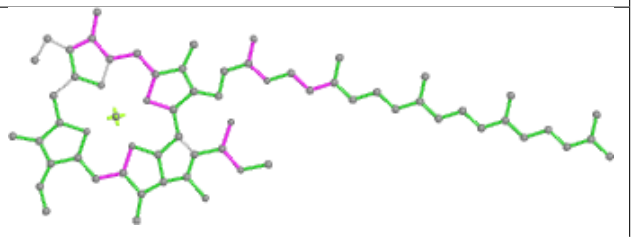


Rings

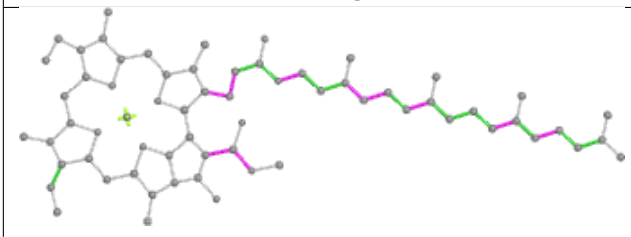
Ligand CLA A 854



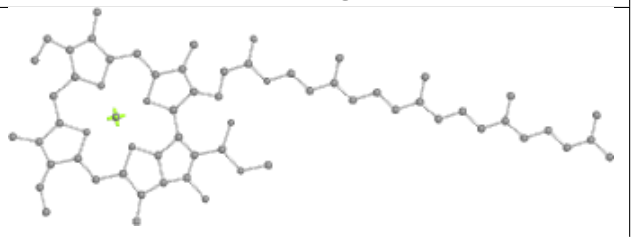
Bond lengths



Bond angles

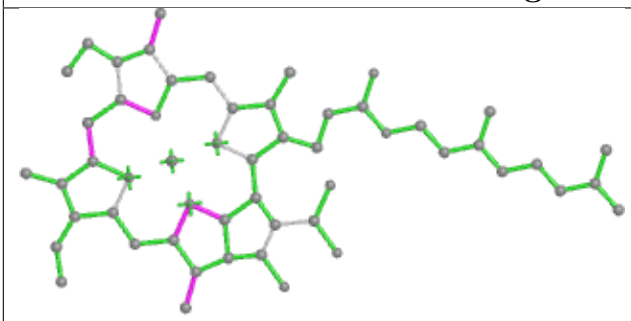


Torsions

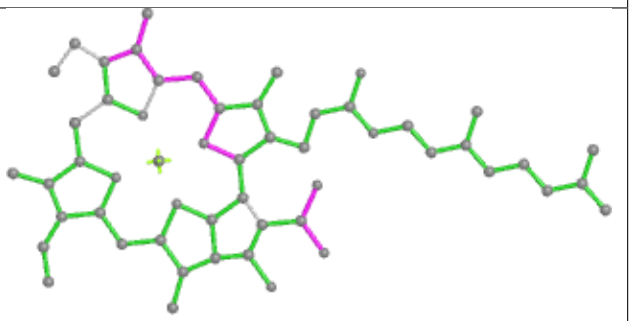


Rings

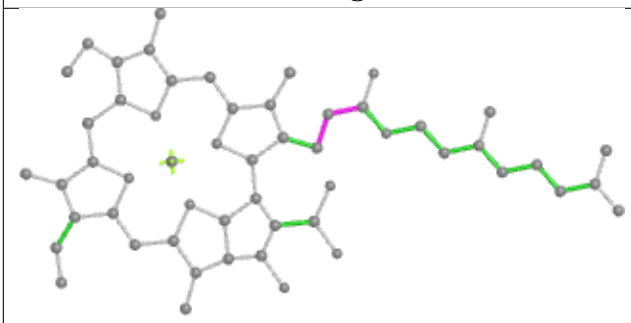
Ligand CLA B 816



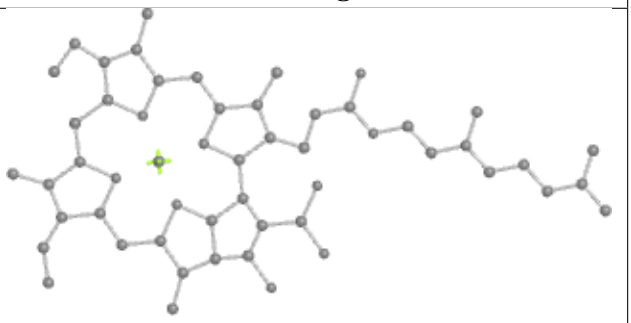
Bond lengths



Bond angles

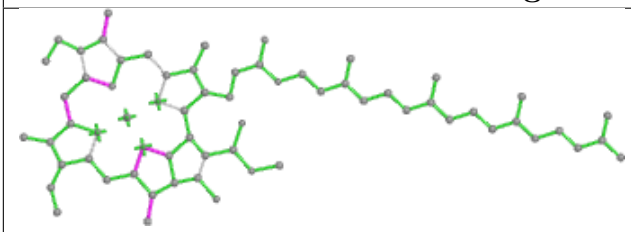


Torsions

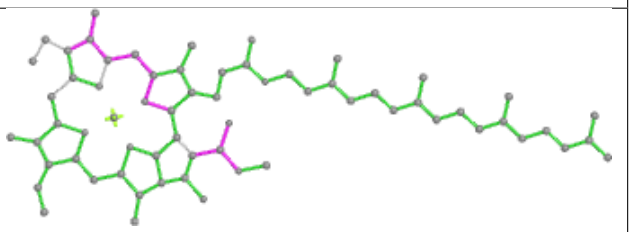


Rings

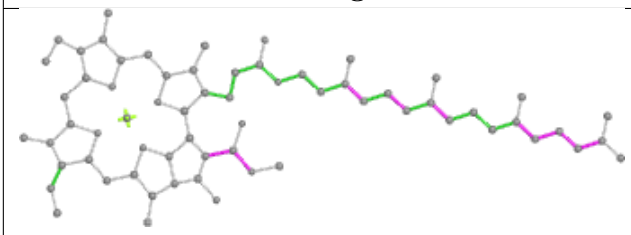
Ligand CLA A 831



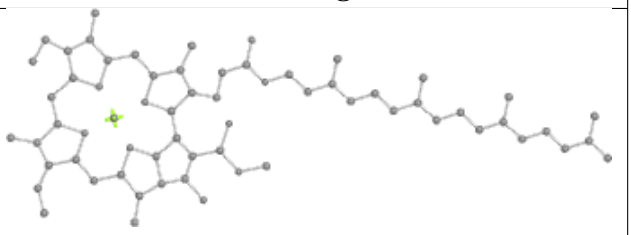
Bond lengths



Bond angles

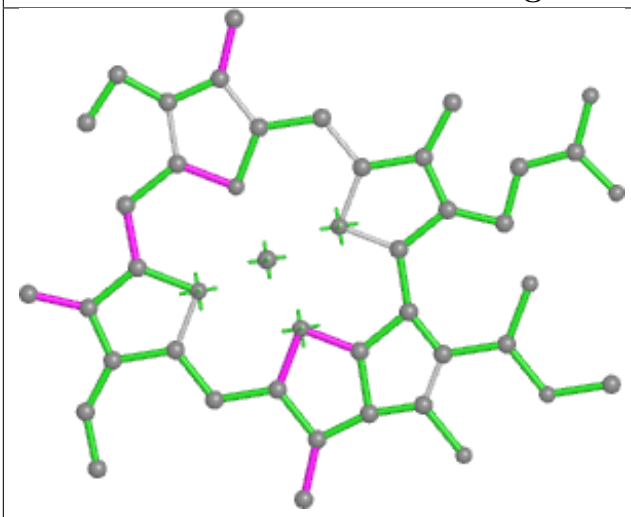


Torsions

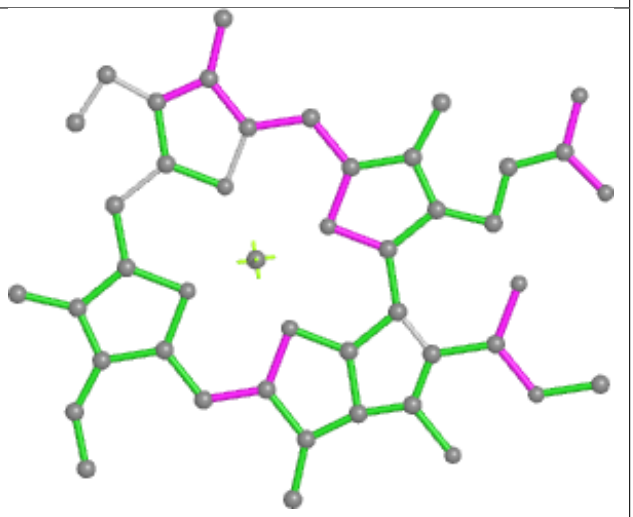


Rings

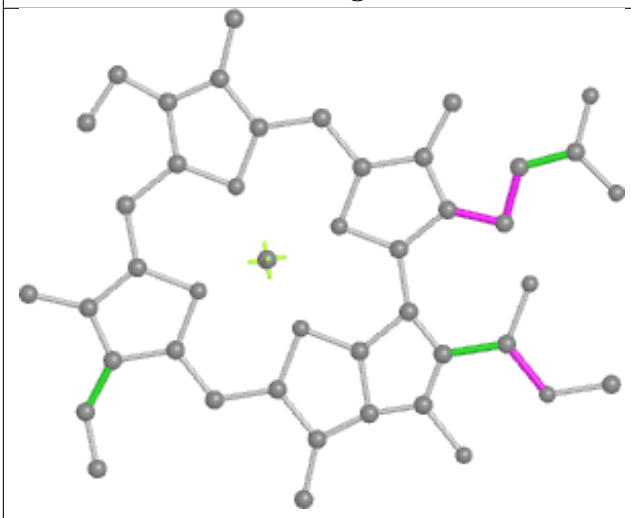
Ligand CLA B 827



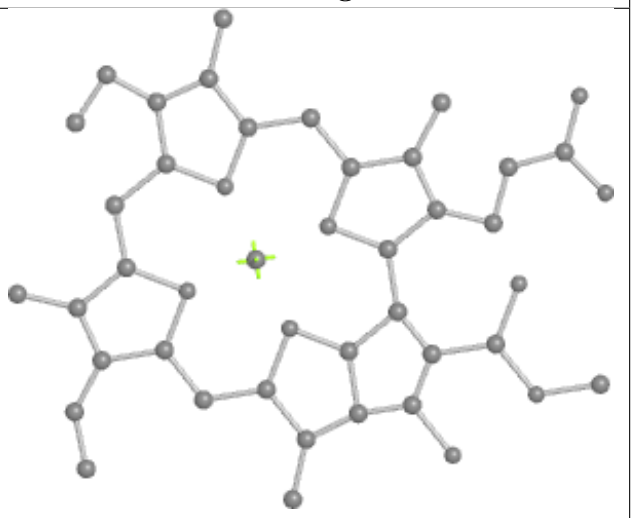
Bond lengths



Bond angles

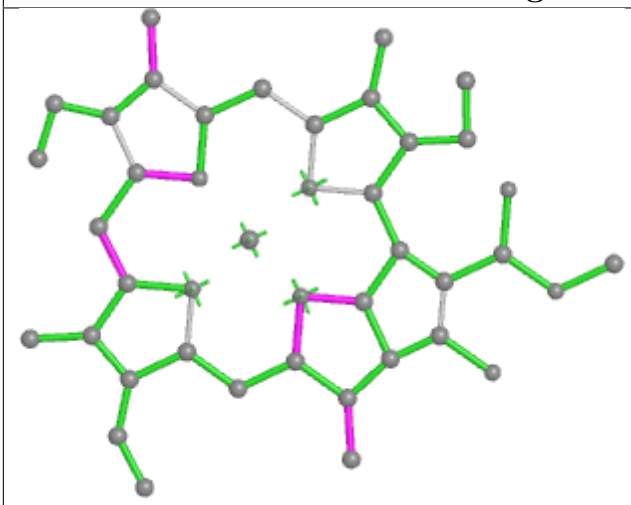


Torsions

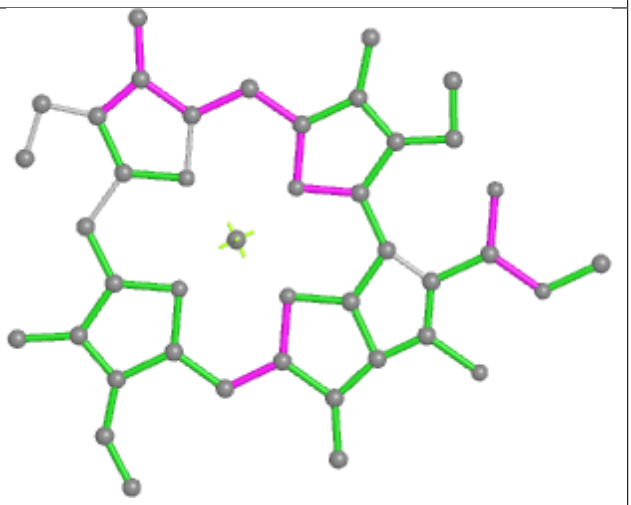


Rings

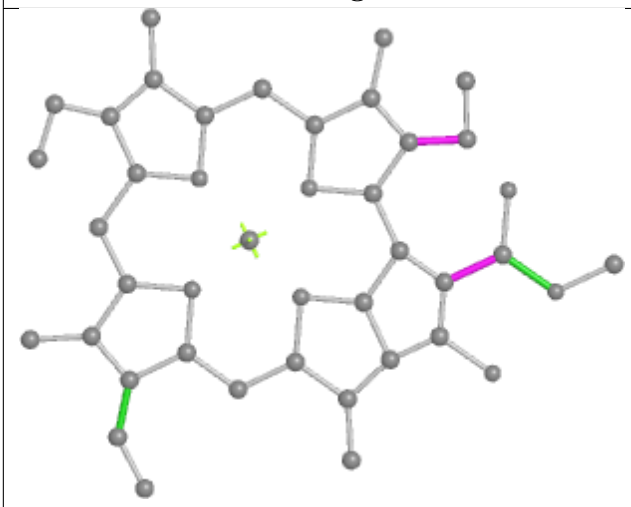
Ligand CLA L 304



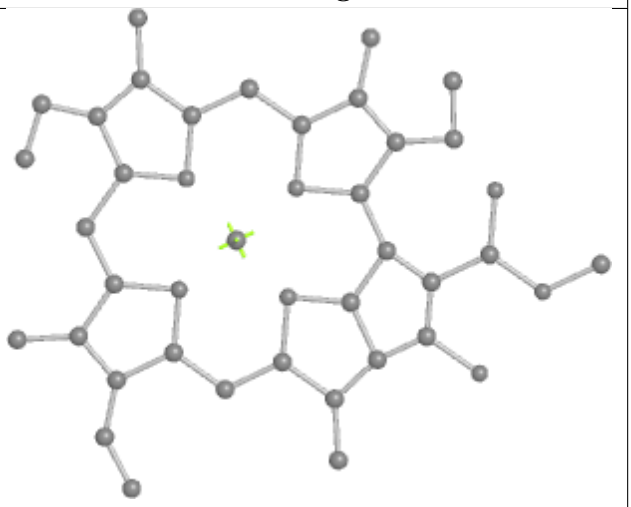
Bond lengths



Bond angles

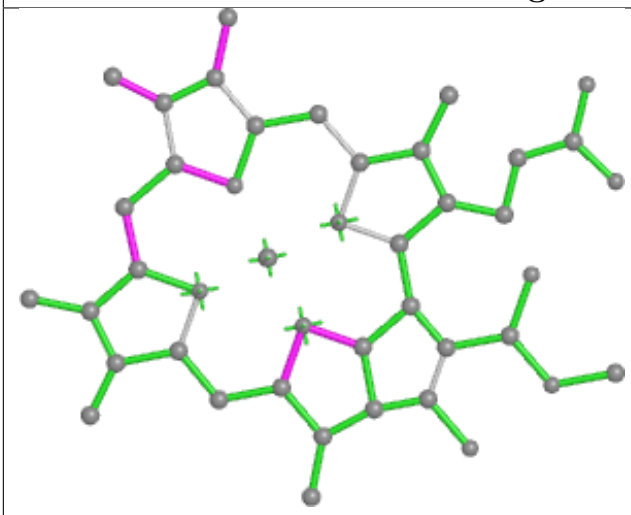


Torsions

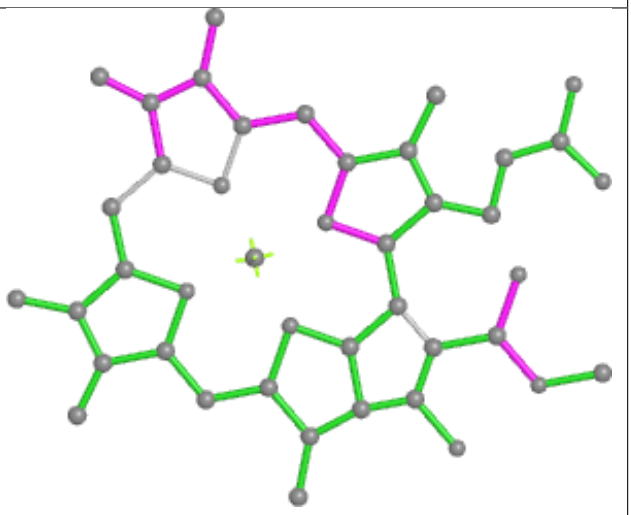


Rings

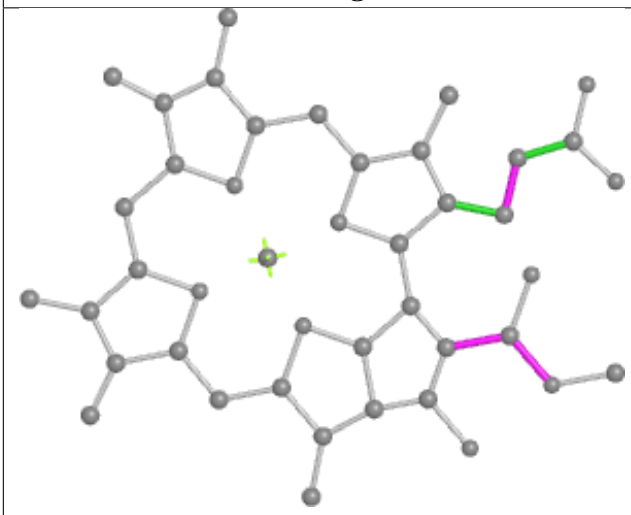
Ligand CLA 6 616



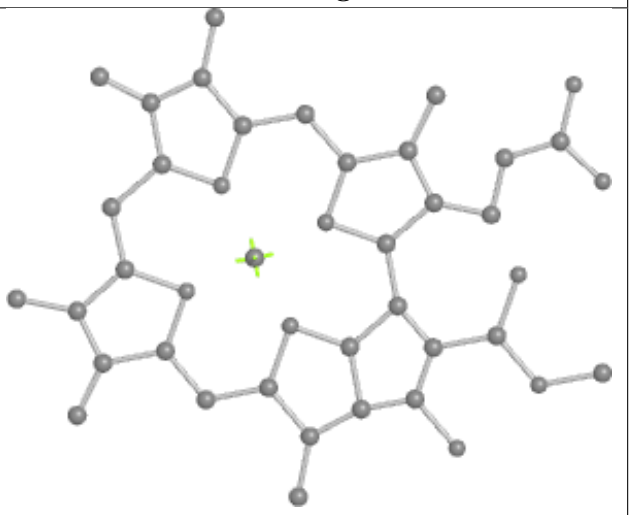
Bond lengths



Bond angles

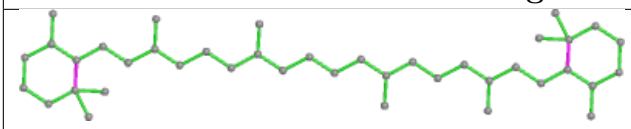


Torsions



Rings

Ligand BCR 5 621



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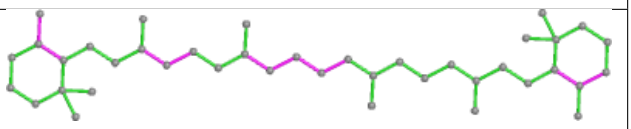

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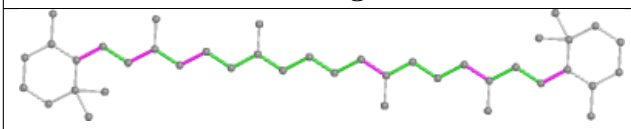

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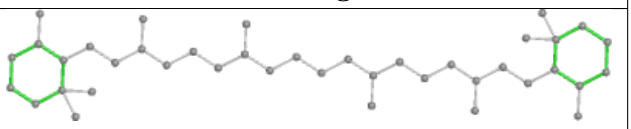
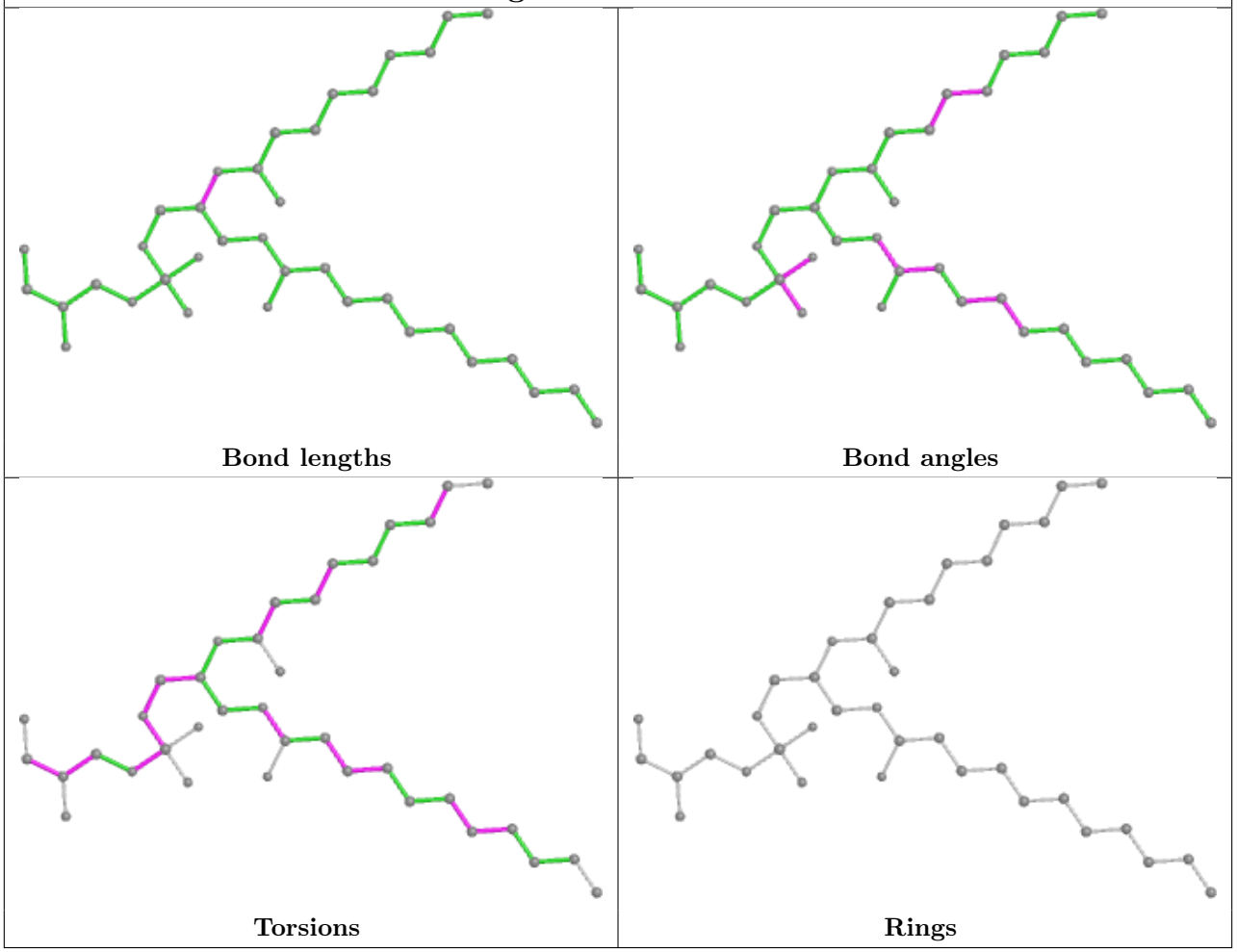
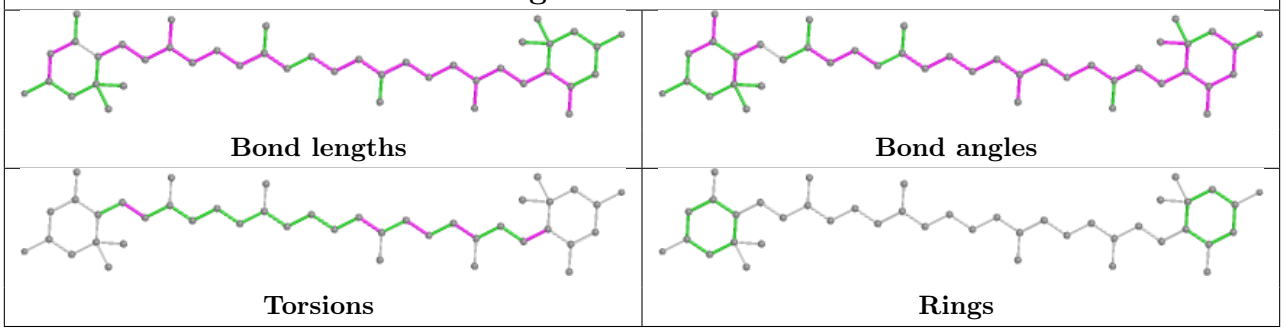


Rings

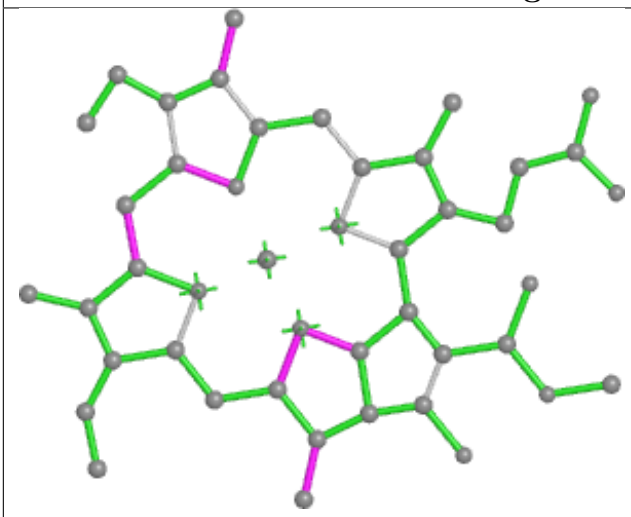
Ligand LHG 5 622



Ligand LUT 3 618



Ligand CLA A 809



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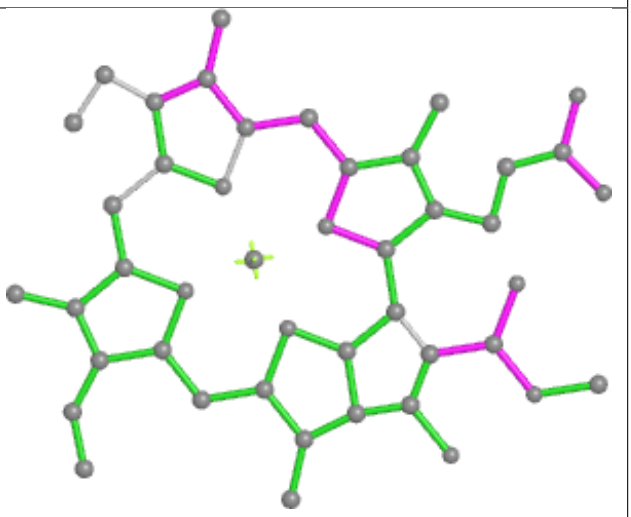
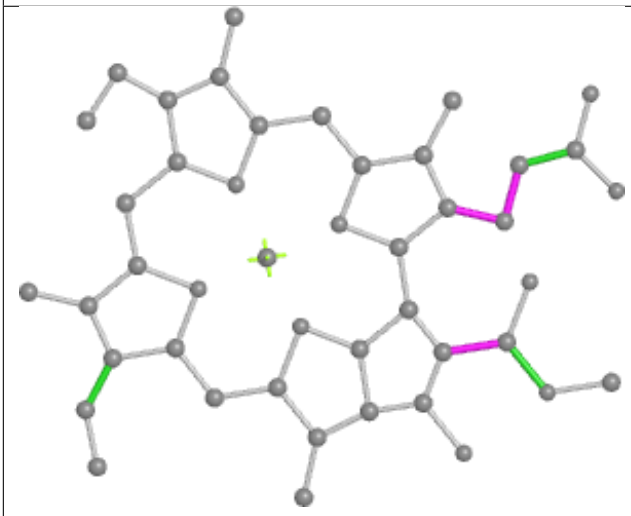


Bond angles



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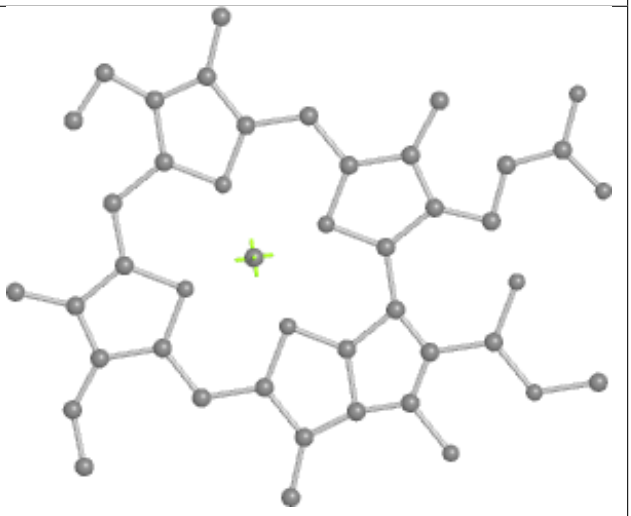
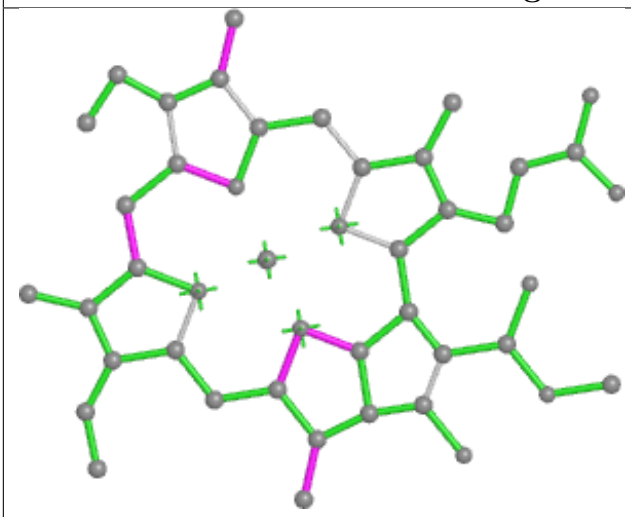


Rings

Ligand CLA A 802



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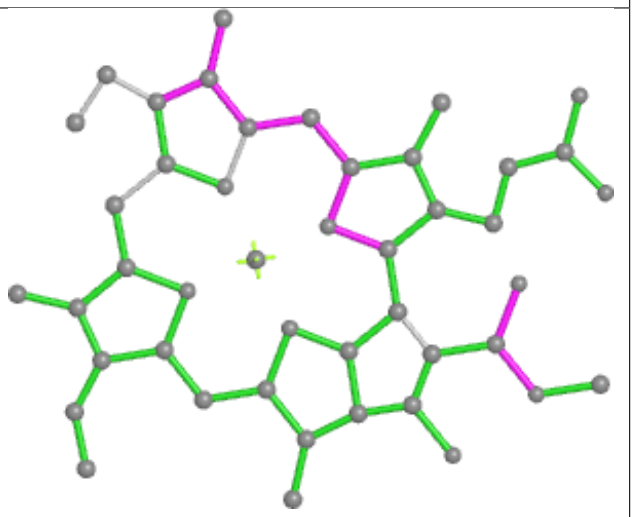
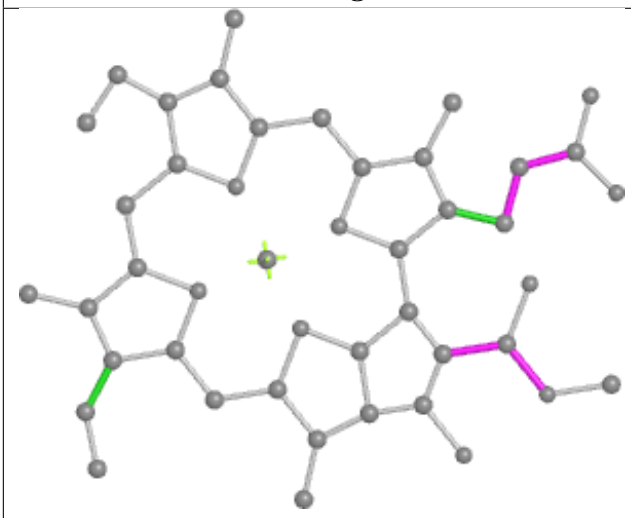


Bond angles



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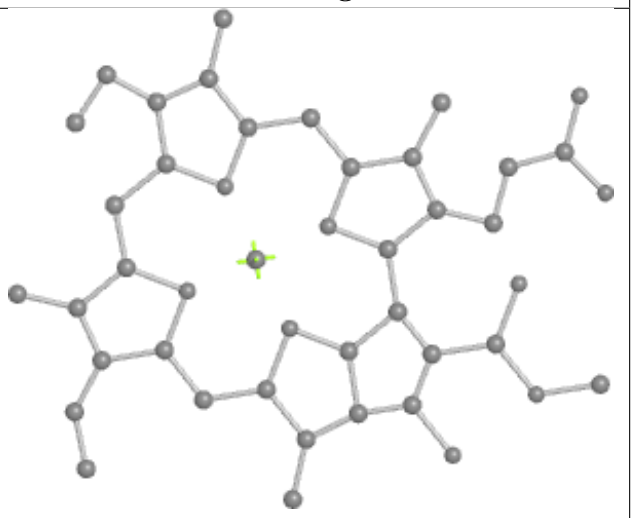
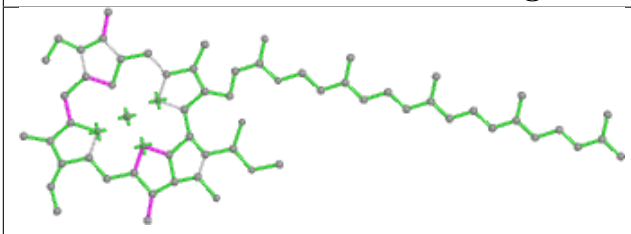


Rings

Ligand CLA A 827



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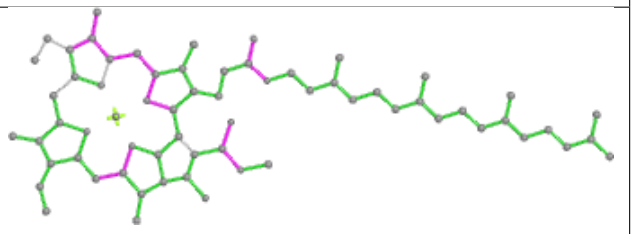
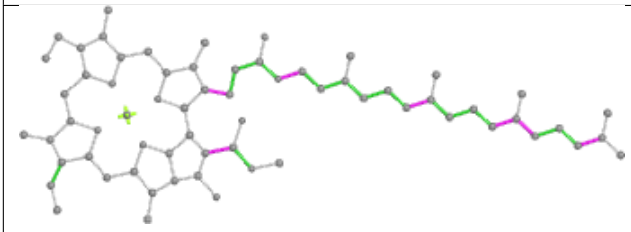


Bond angles



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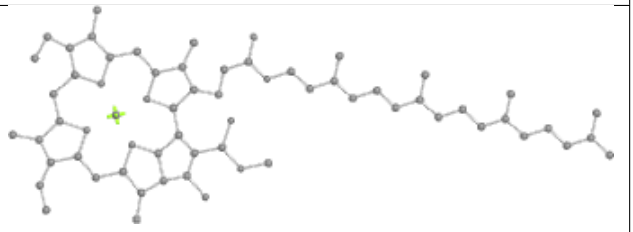
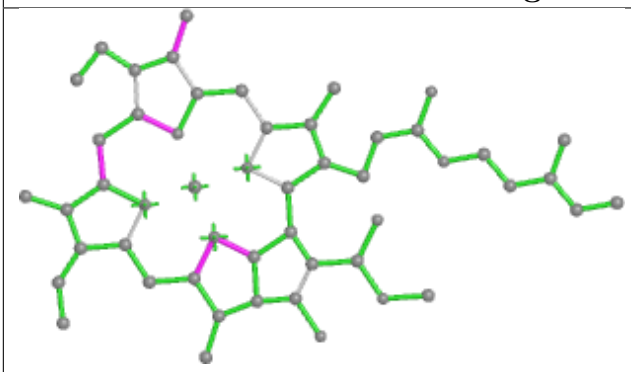
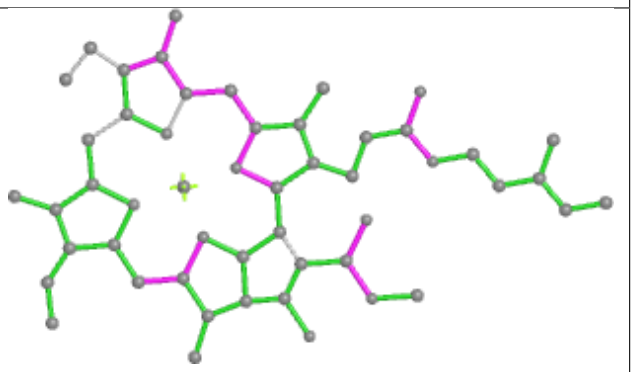
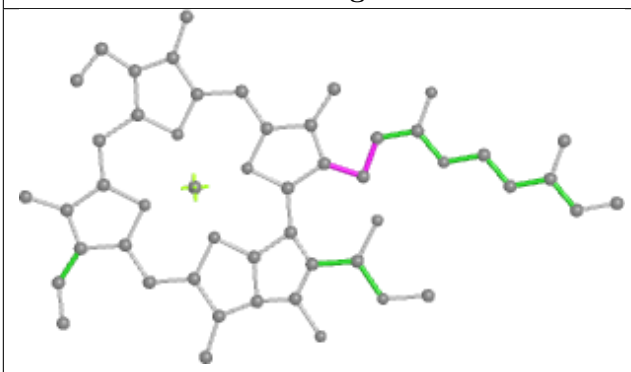
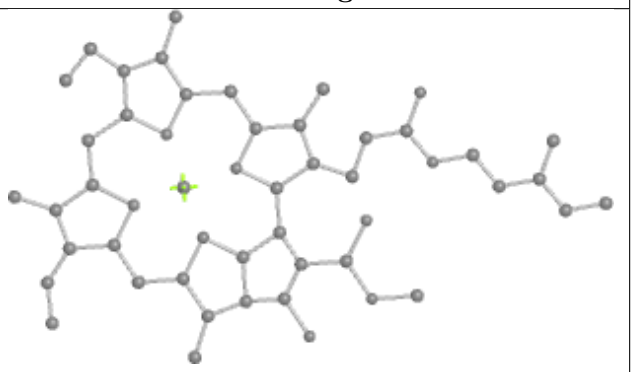
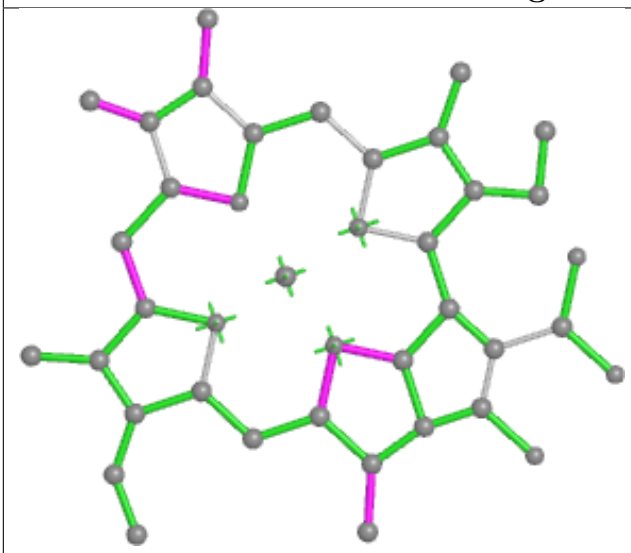


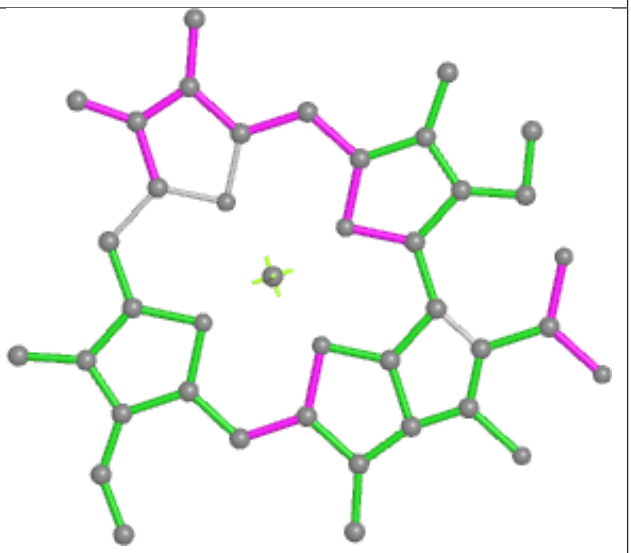
Rings

Ligand CLA A 838	
	
Bond lengths	**Bond angles**
	
Torsions	**Rings**

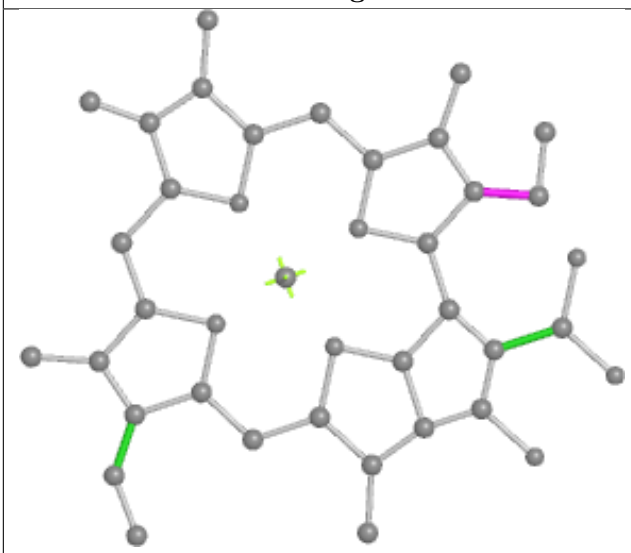
Ligand CLA 3 607



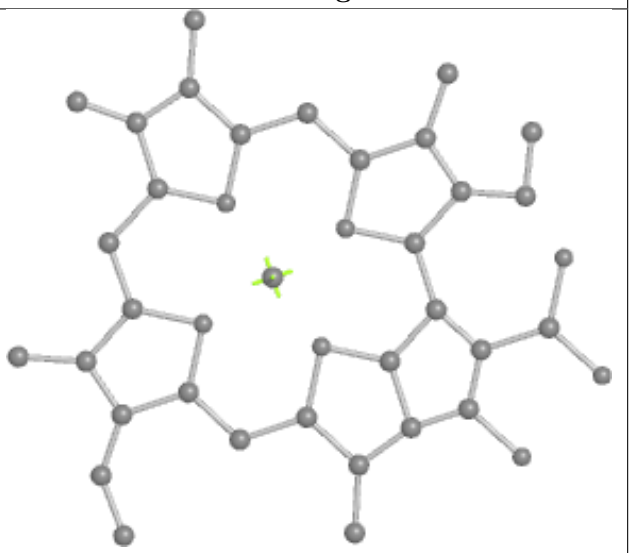
Bond lengths



Bond angles

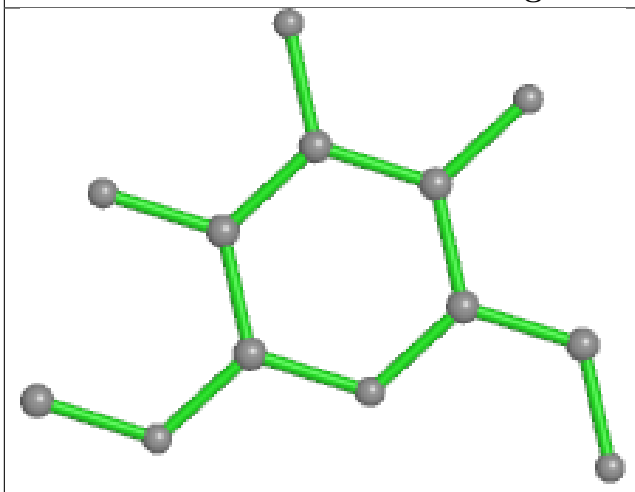


Torsions



Rings

Ligand LMG 2 617



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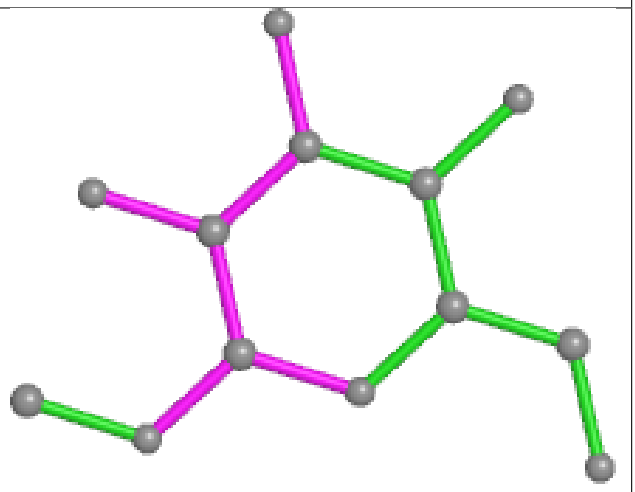
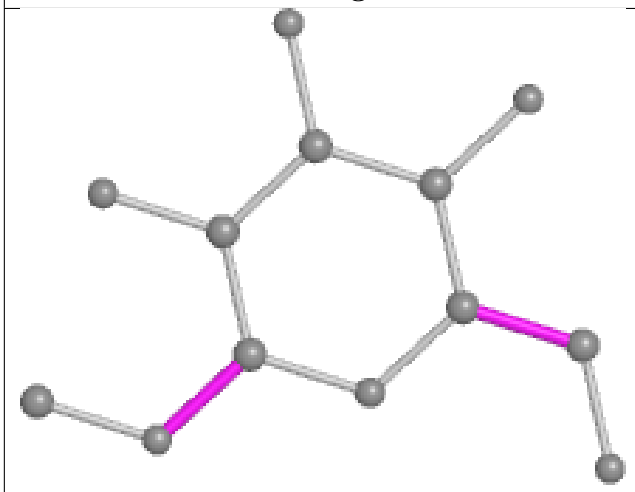


Bond angles



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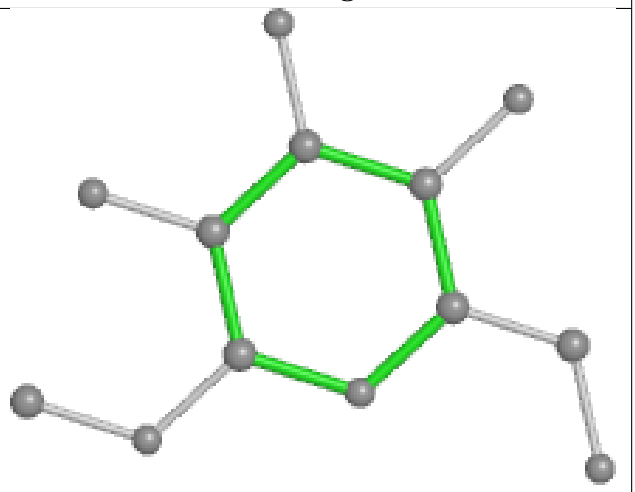
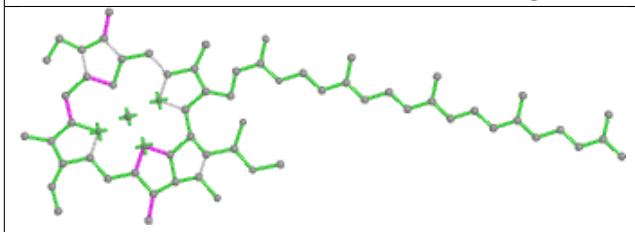
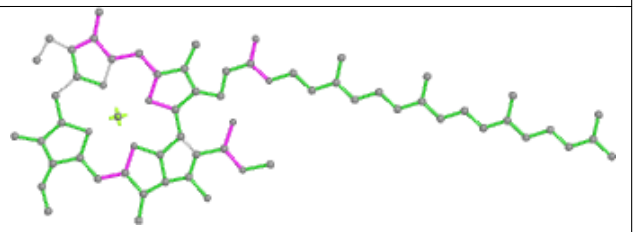


Rings

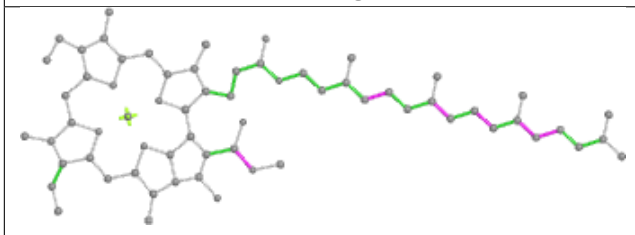
Ligand CLA B 809



Bond lengths



Bond angles



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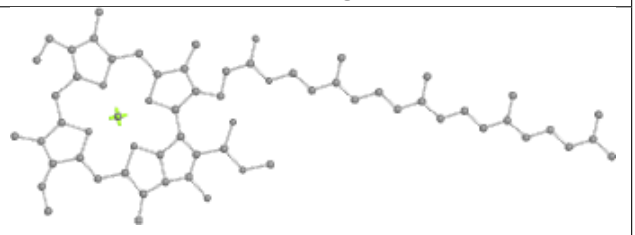
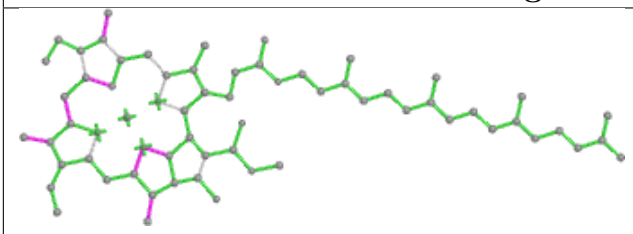
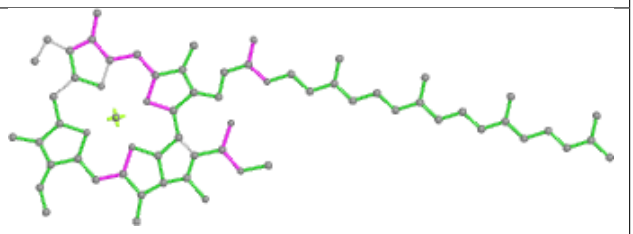


Rings

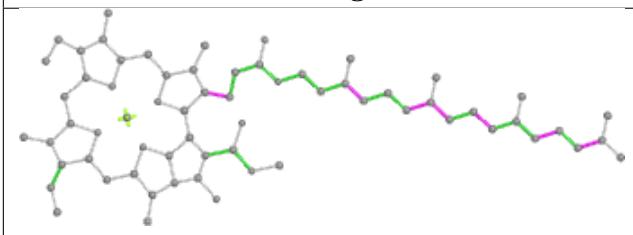
Ligand CLA B 825



Bond lengths



Bond angles



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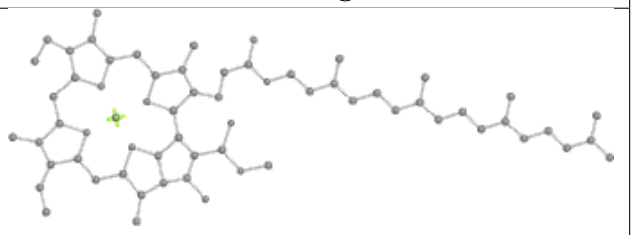
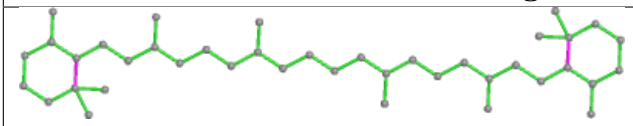
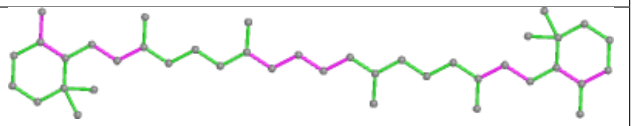


Rings

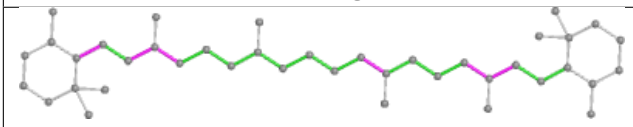
Ligand BCR A 852



Bond lengths



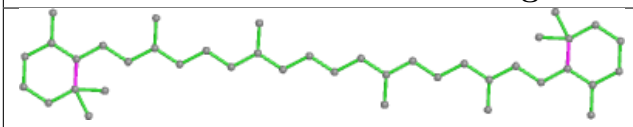
Bond angles



Torsions

Rings

Ligand BCR G 205



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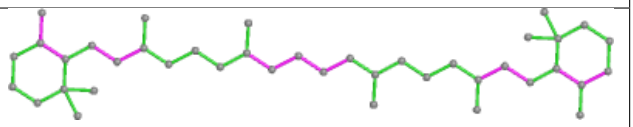
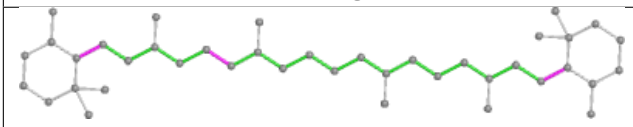
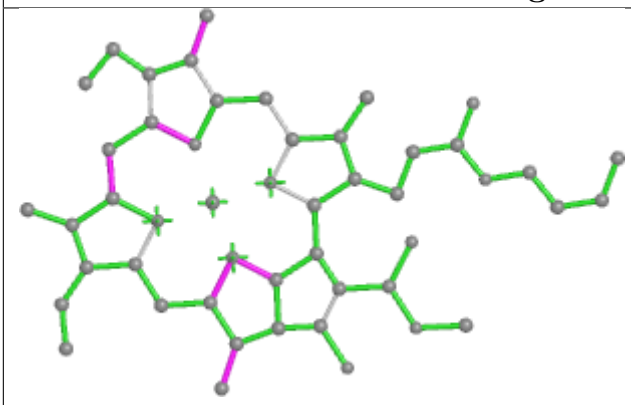
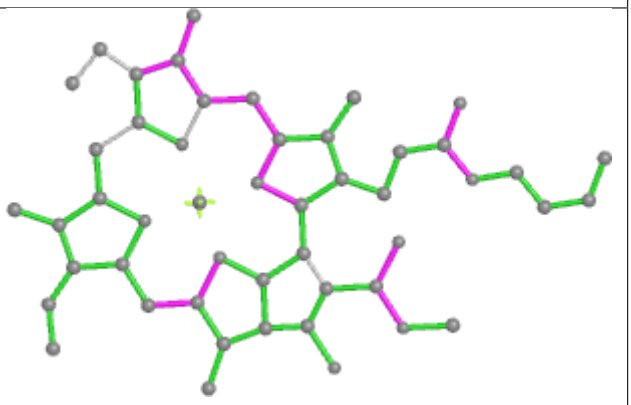
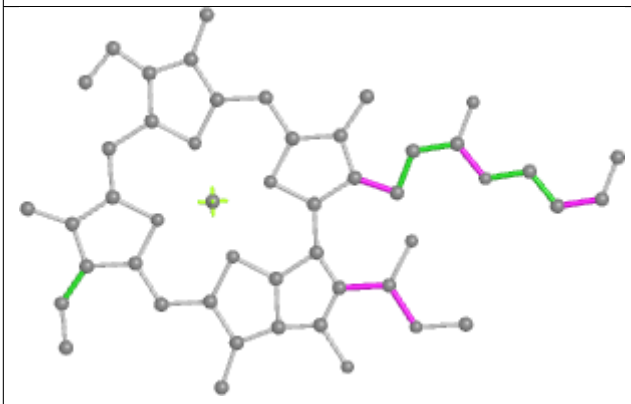
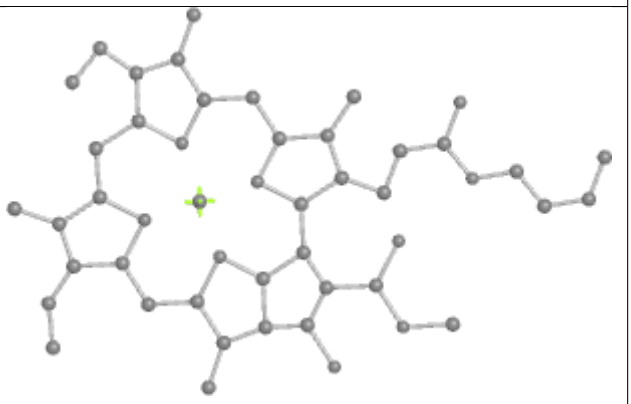


Bond angles

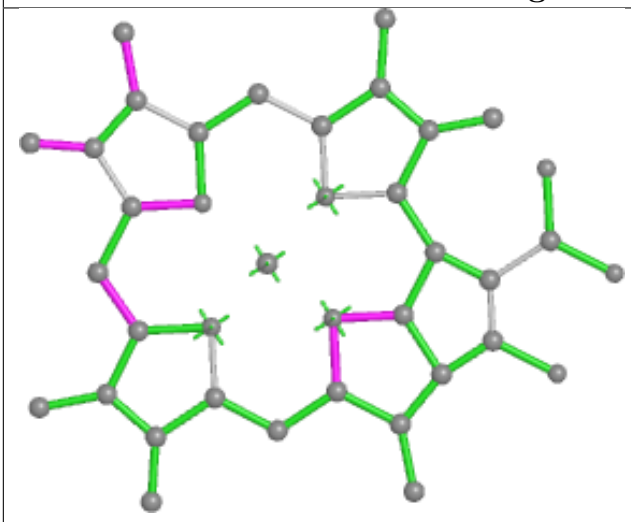


Torsions

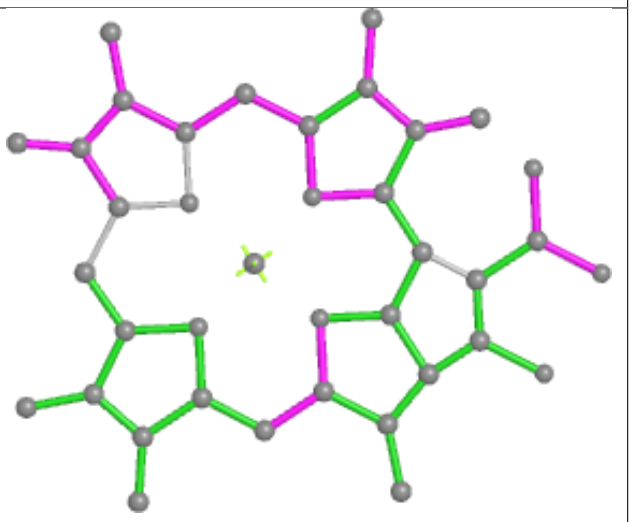
Rings

Ligand CLA 6 604	
 Bond lengths	 Bond angles
 Torsions	 Rings

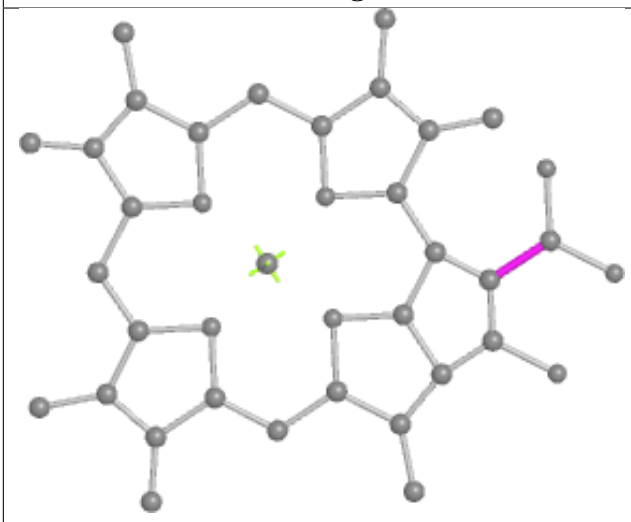
Ligand CLA 6 614



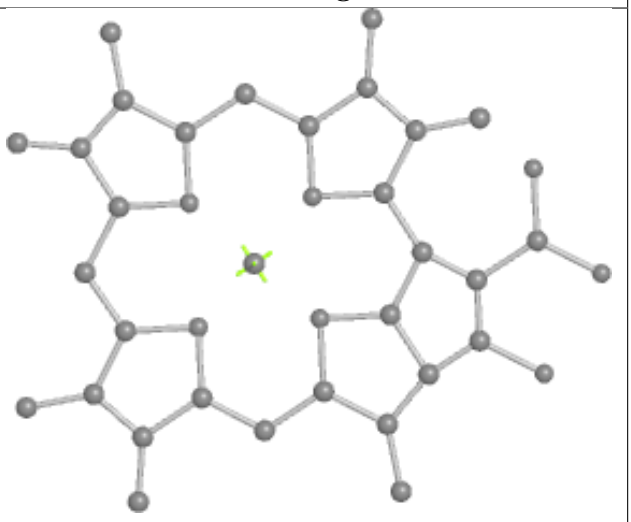
Bond lengths



Bond angles

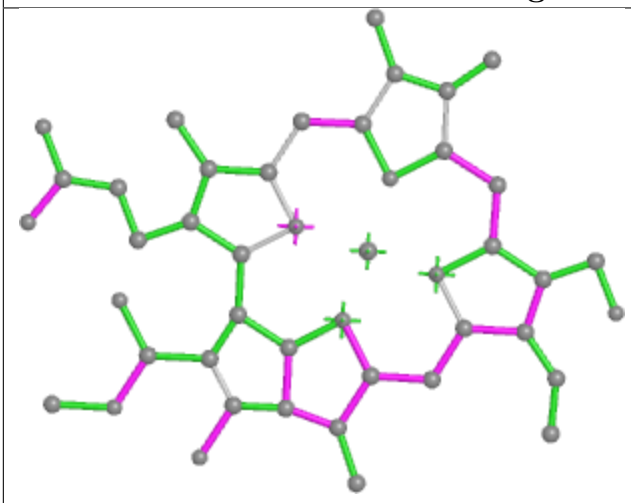


Torsions

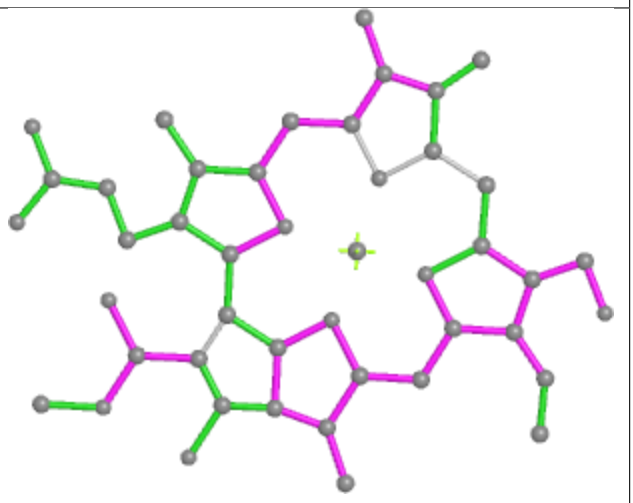


Rings

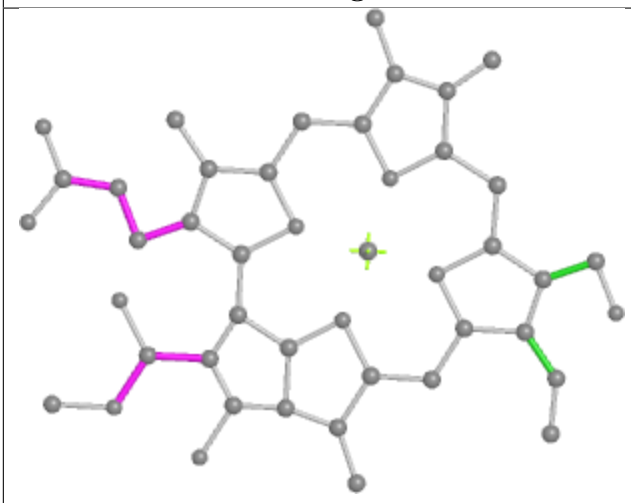
Ligand CHL 2 601



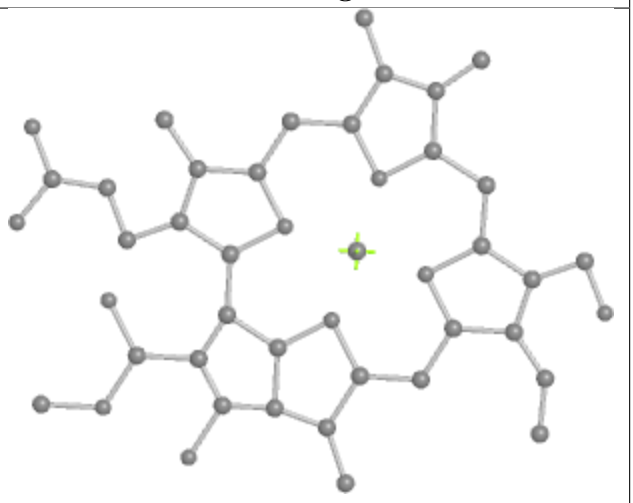
Bond lengths



Bond angles

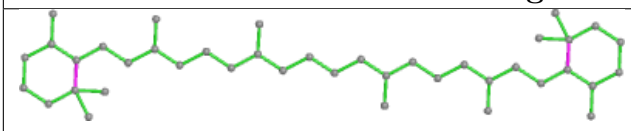


Torsions

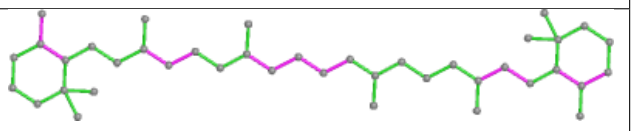


Rings

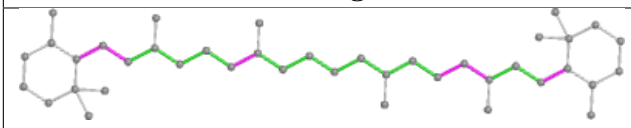
Ligand BCR 2 621



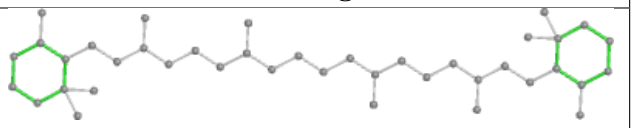
Bond lengths



Bond angles

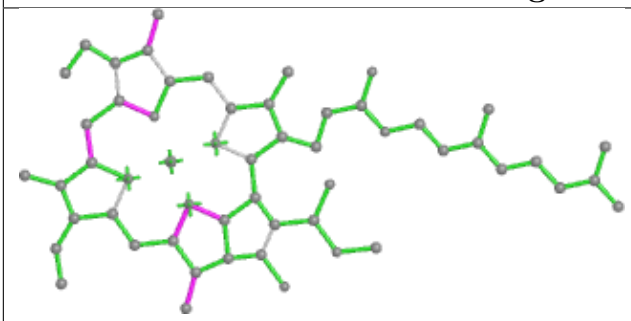


Torsions



Rings

Ligand CLA 6 603



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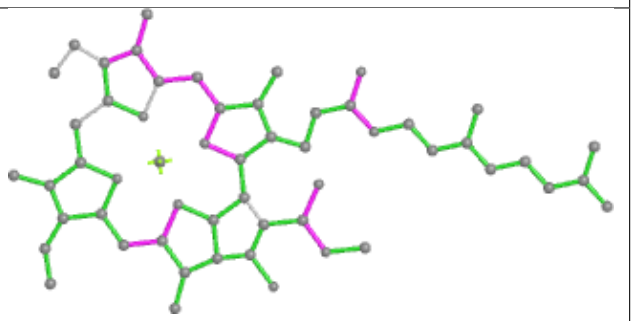
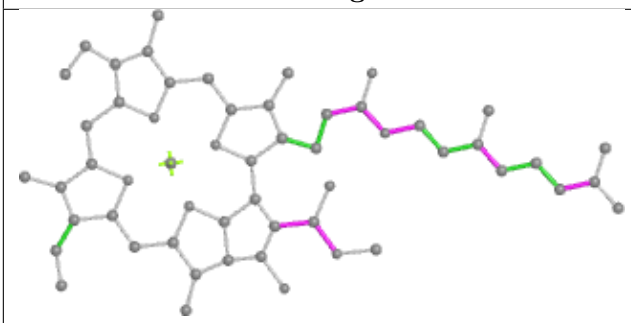


Bond angles



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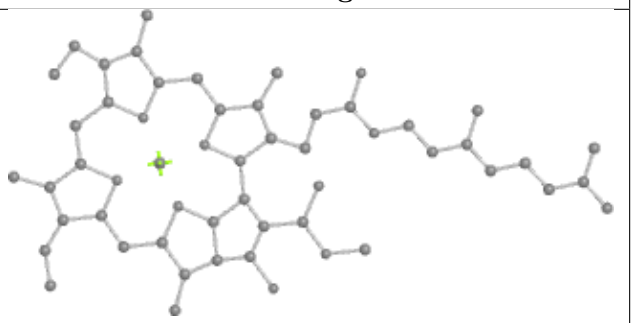
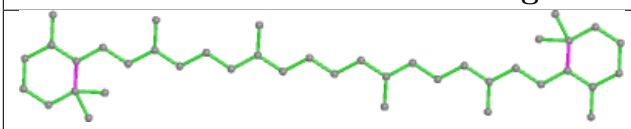


Rings

Ligand BCR K 207



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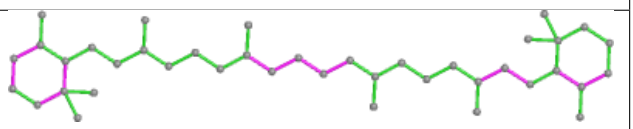
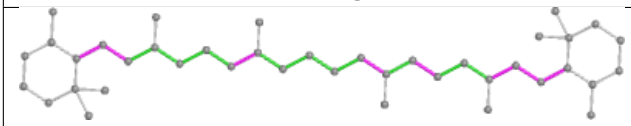


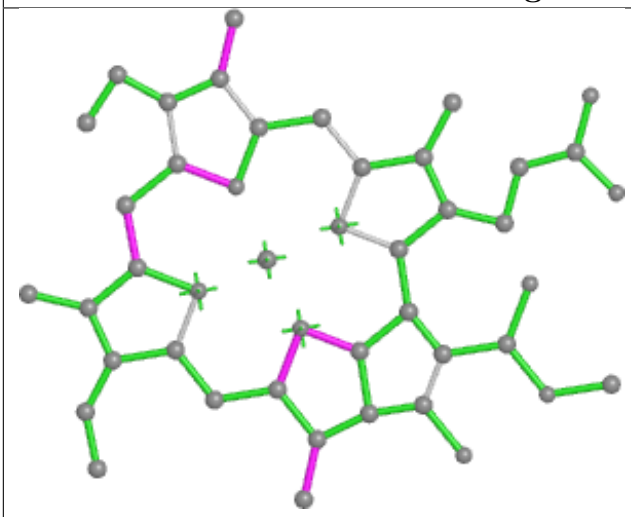
Bond angles



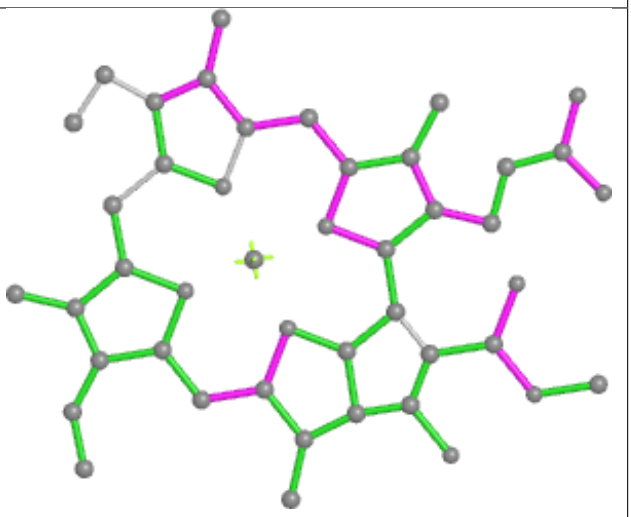
Torsions

Rings

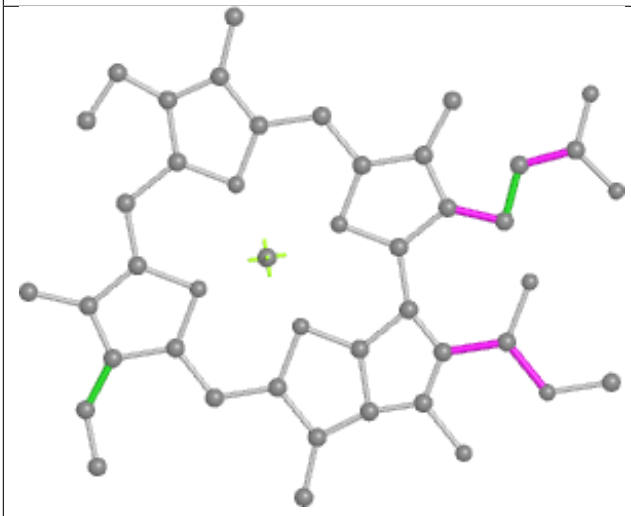
Ligand CLA B 833



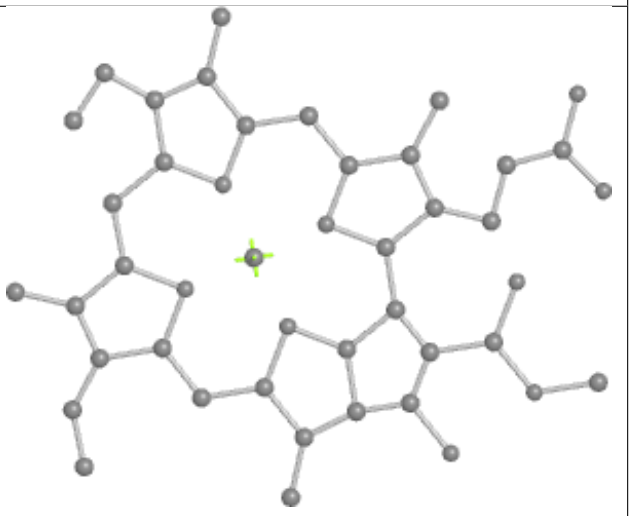
Bond lengths



Bond angles

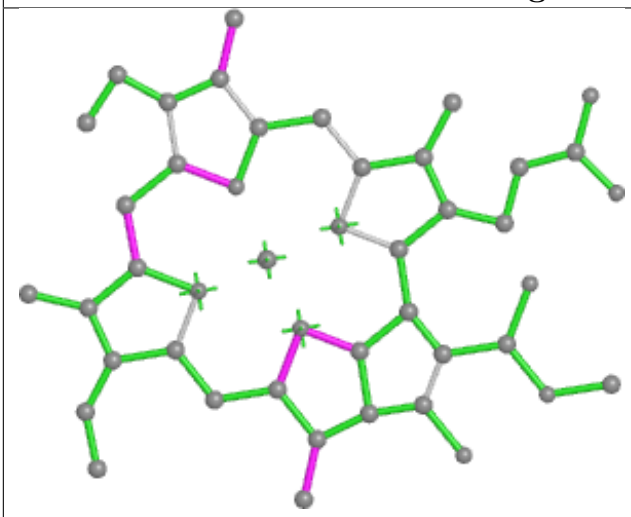


Torsions



Rings

Ligand CLA 5 613



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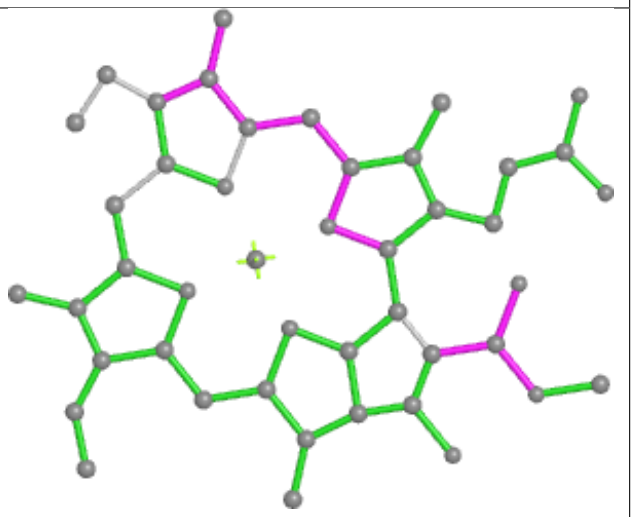
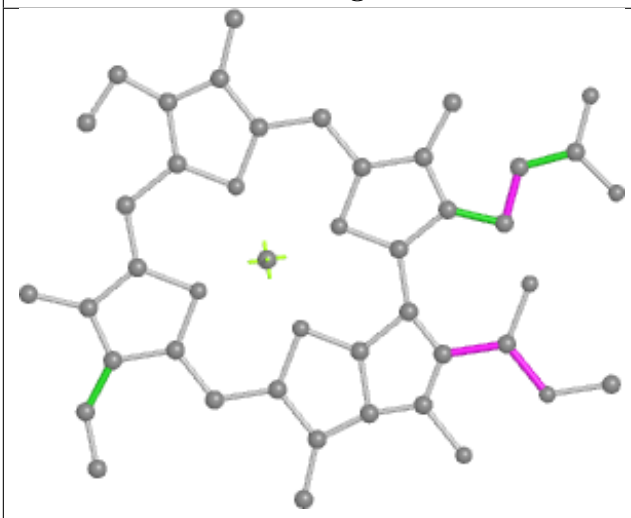
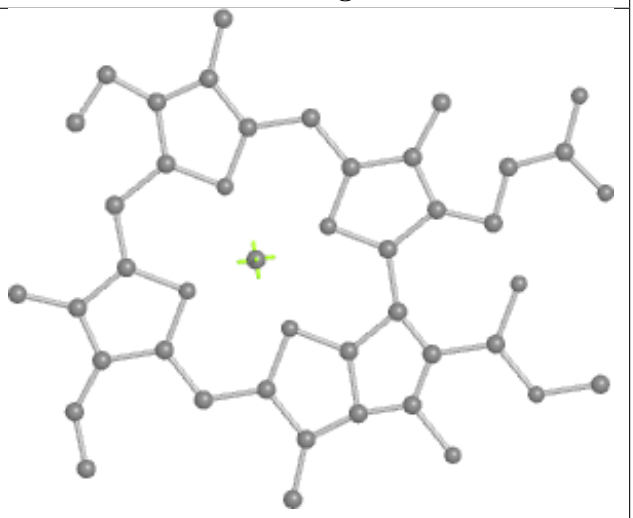


Bond angles

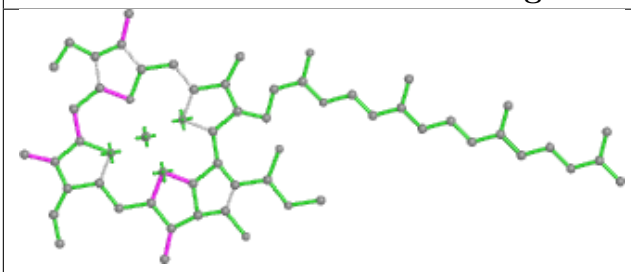


Torsions

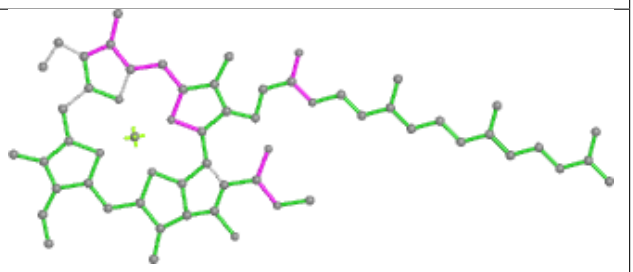


Rings

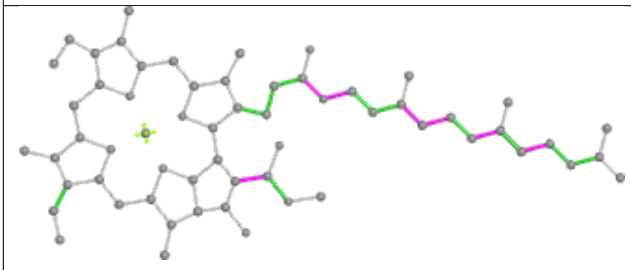
Ligand CLA B 815



Bond lengths



Bond angles



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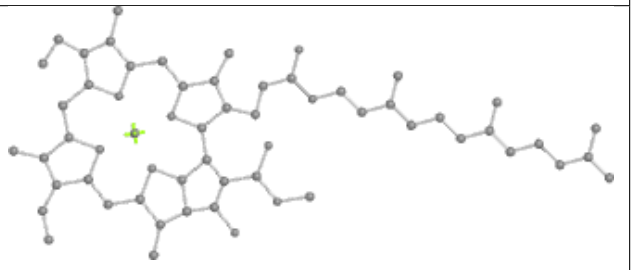
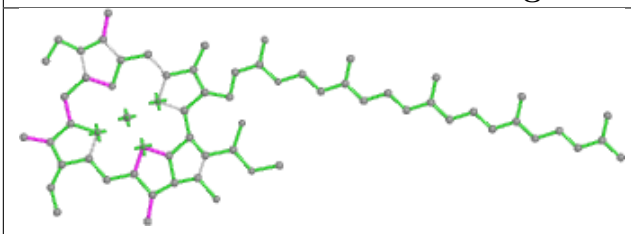


Rings

Ligand CLA A 818



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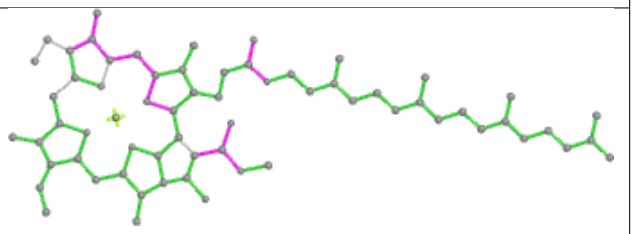
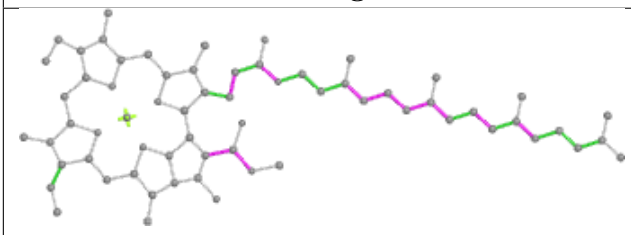
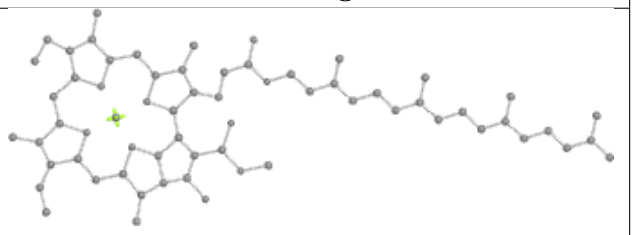


Bond angles

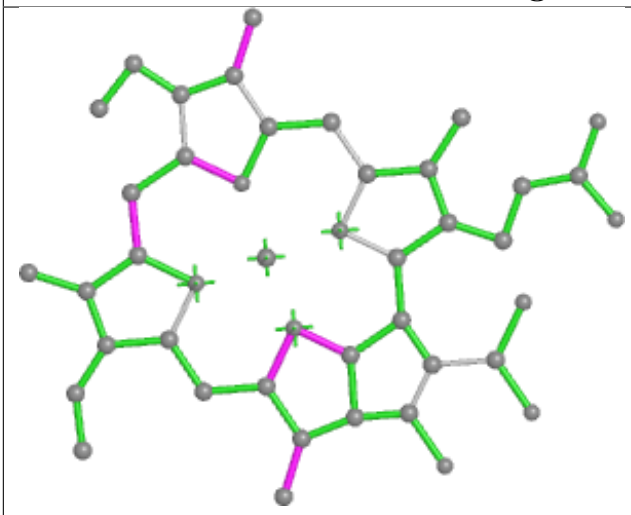


Torsions



Rings

Ligand CLA 6 608



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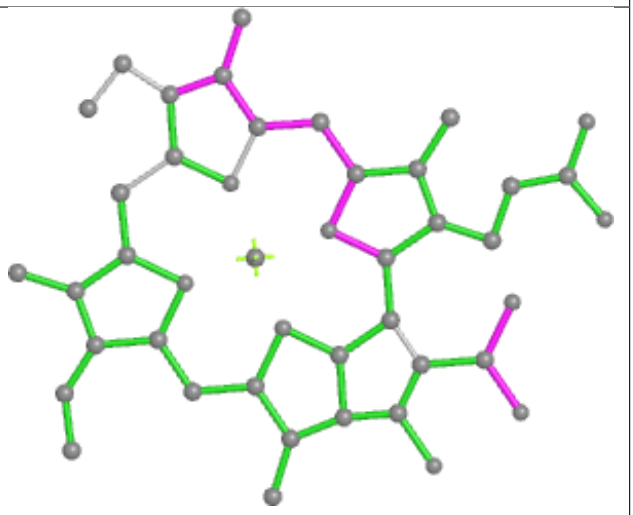
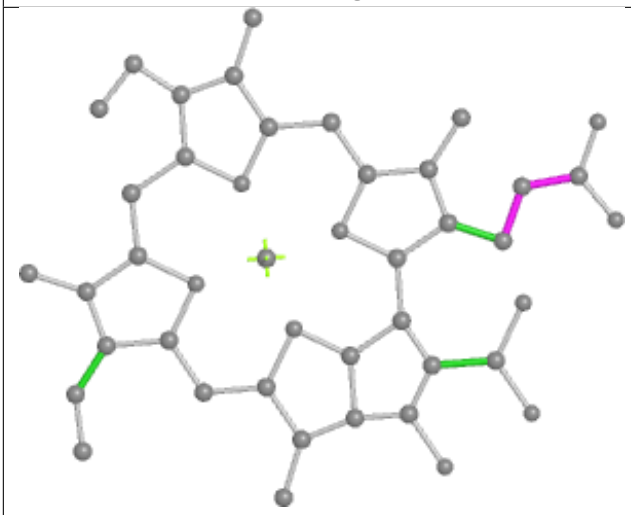


Bond angles



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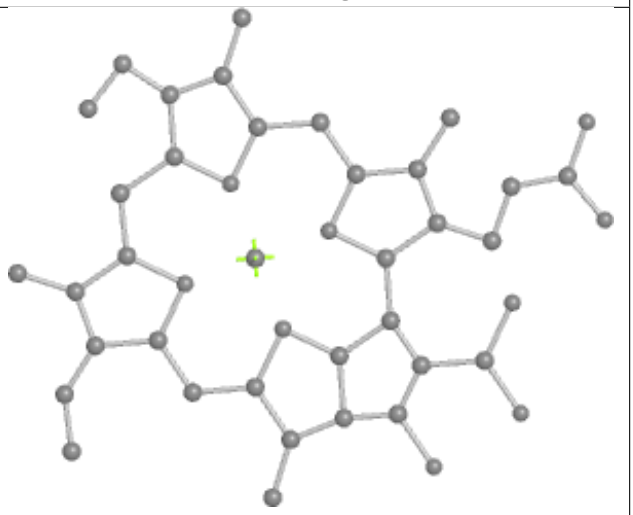
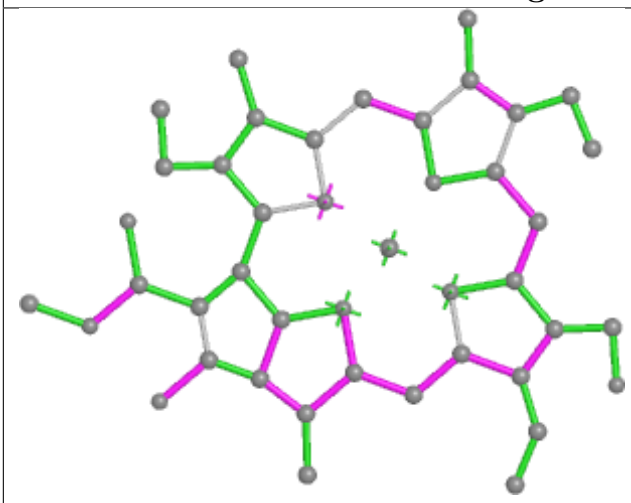
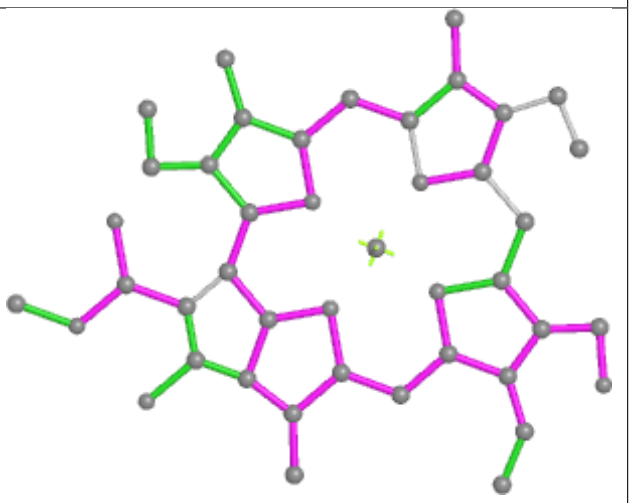


Rings

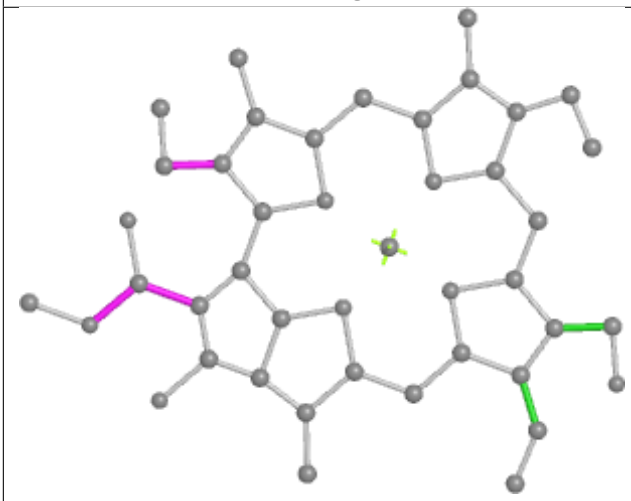
Ligand CHL 5 607



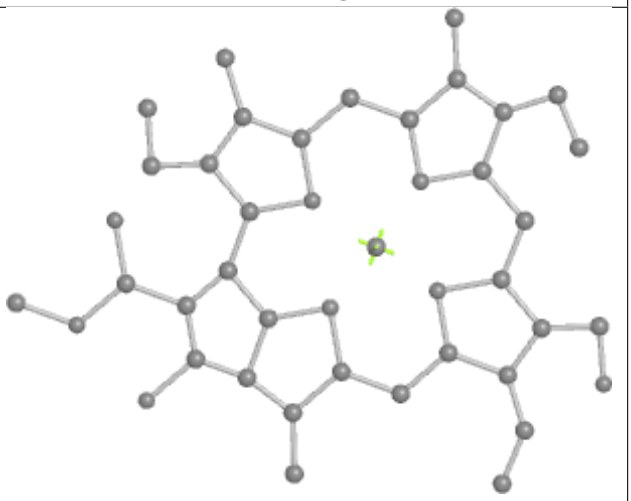
Bond lengths



Bond angles

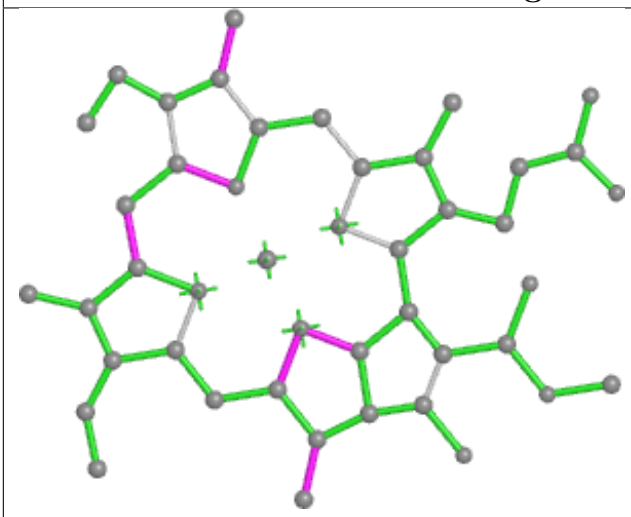


Torsions

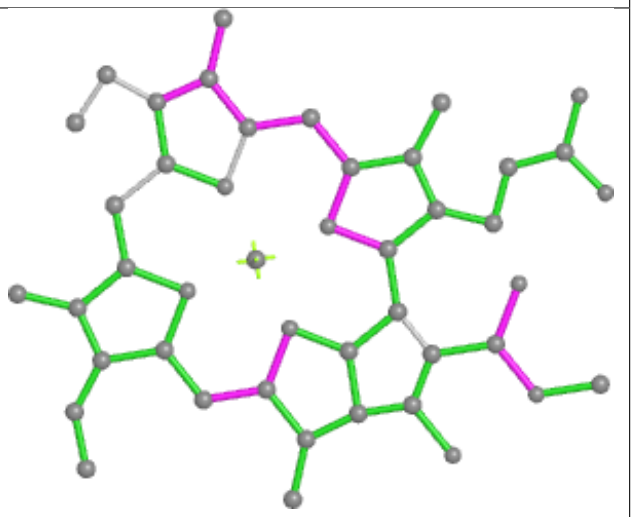


Rings

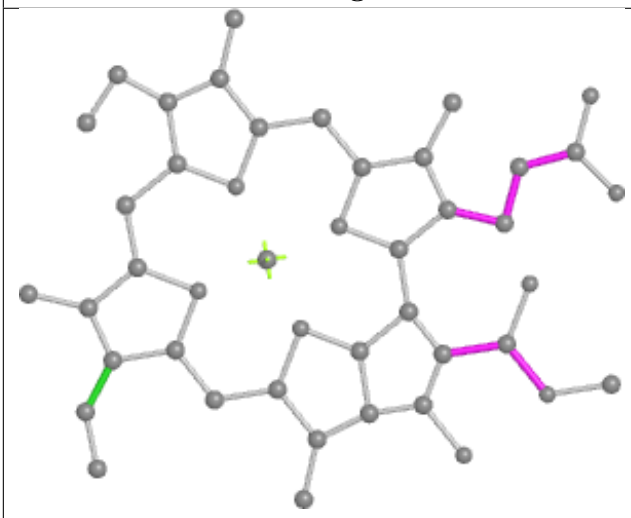
Ligand CLA B 835



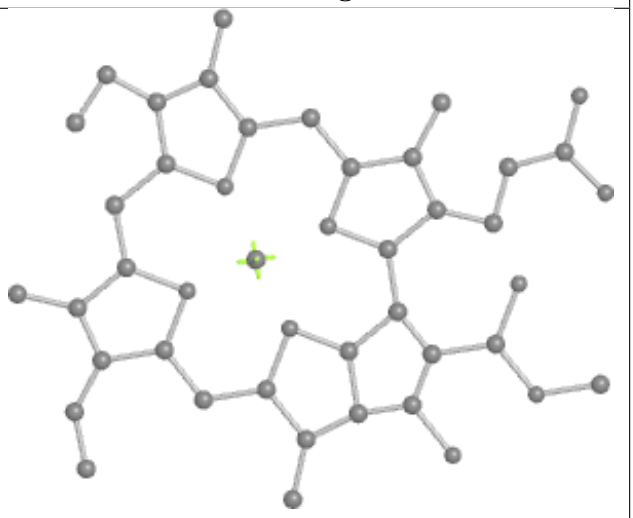
Bond lengths



Bond angles

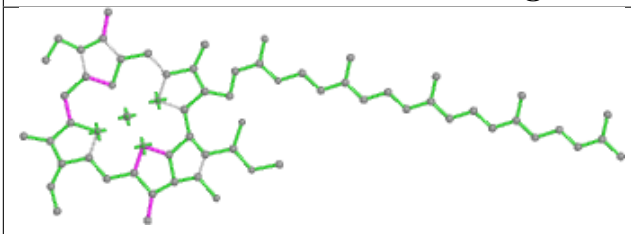


Torsions

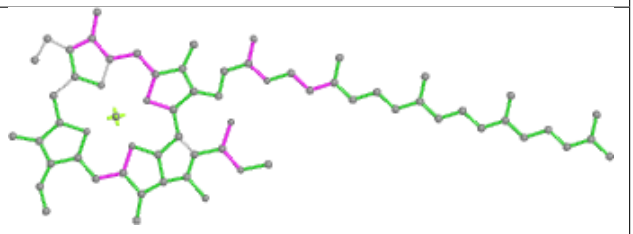


Rings

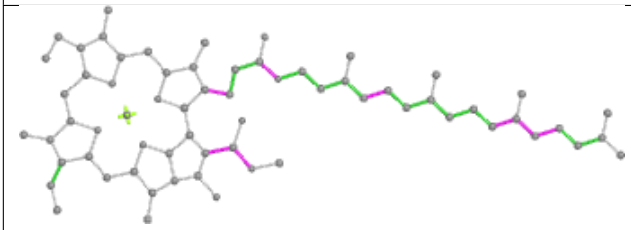
Ligand CLA B 841



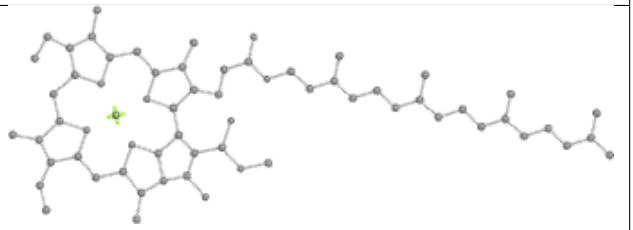
Bond lengths



Bond angles

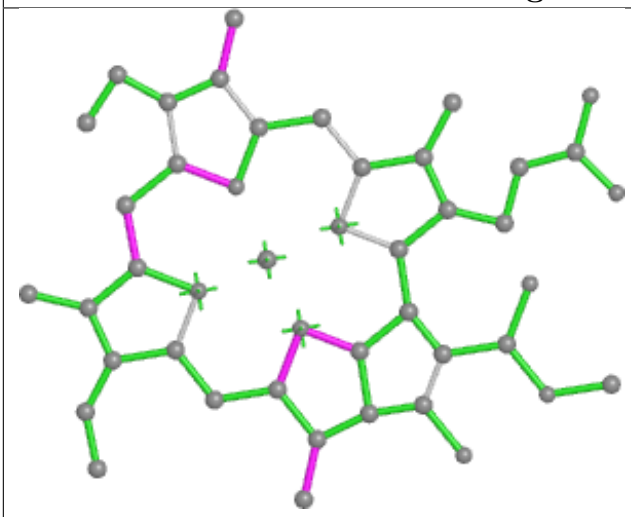


Torsions

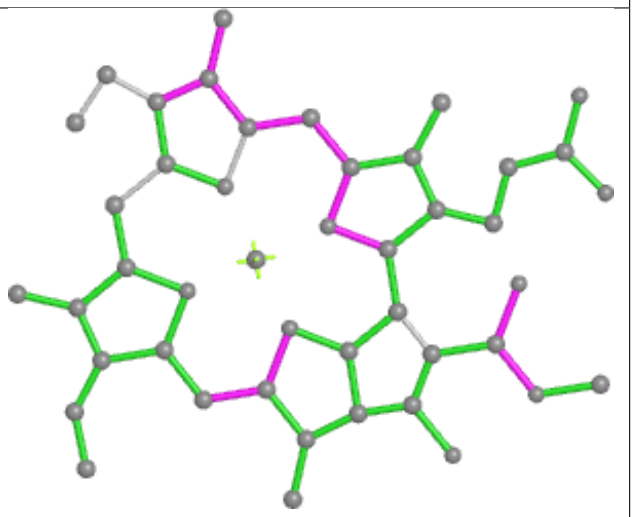


Rings

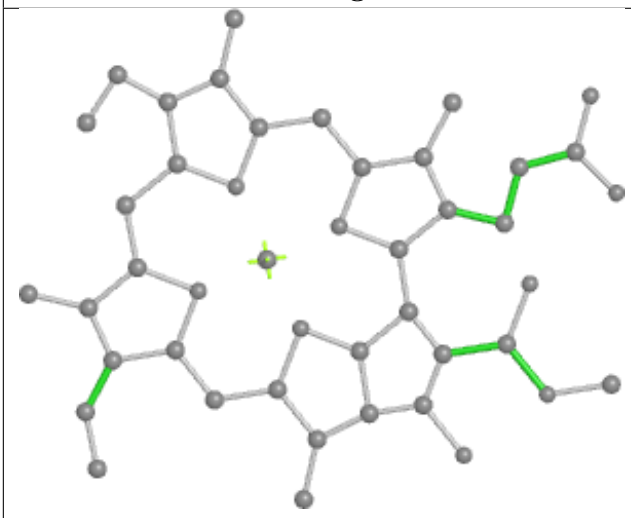
Ligand CLA L 303



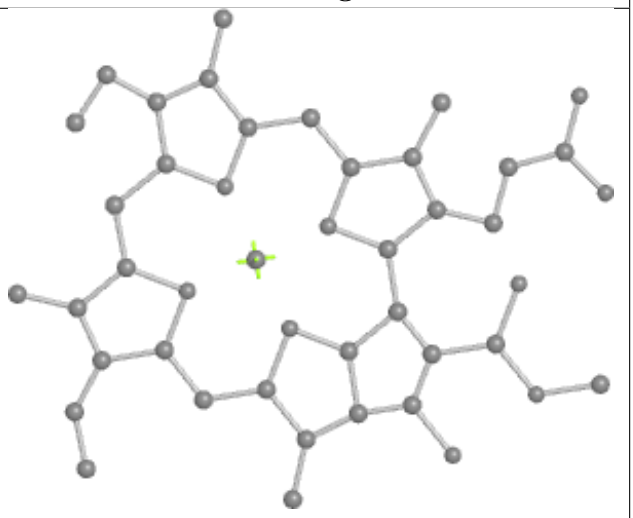
Bond lengths



Bond angles

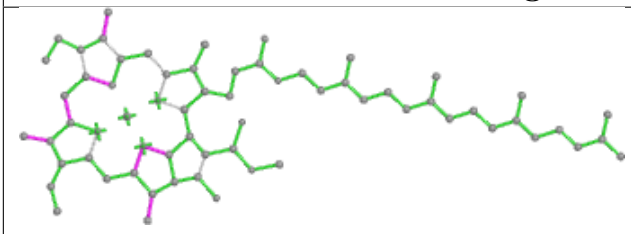


Torsions

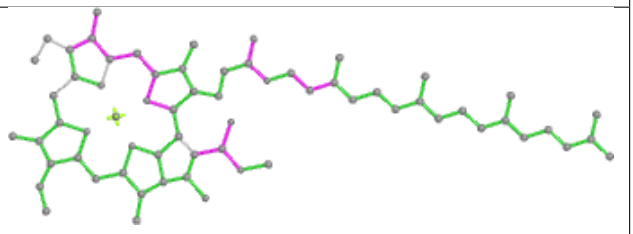


Rings

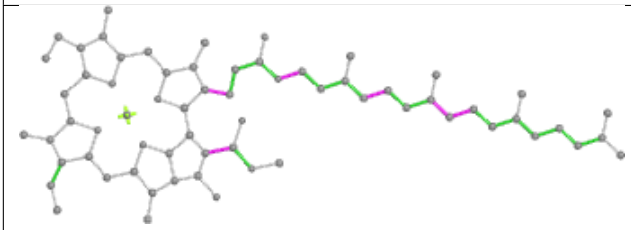
Ligand CLA A 804



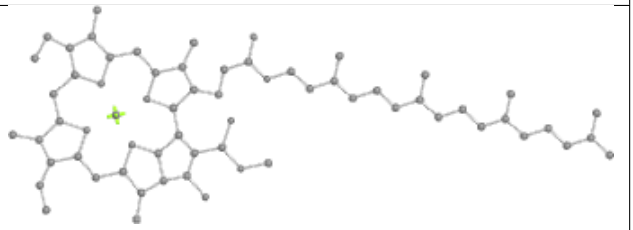
Bond lengths



Bond angles

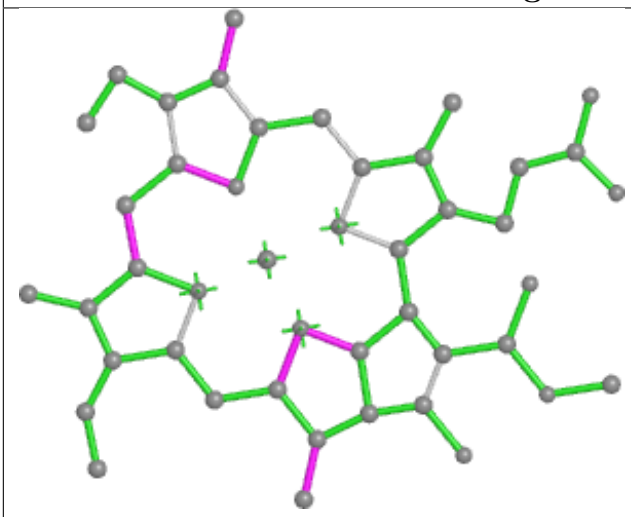


Torsions

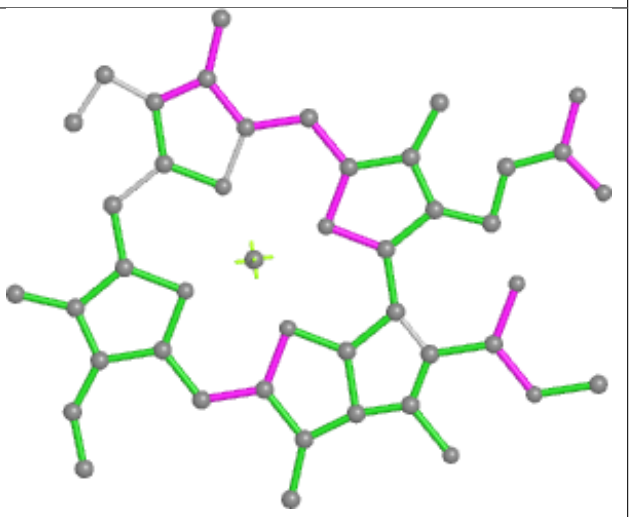


Rings

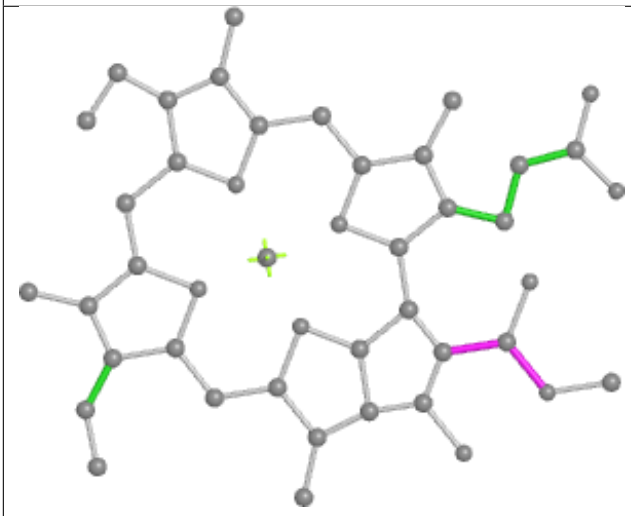
Ligand CLA A 808



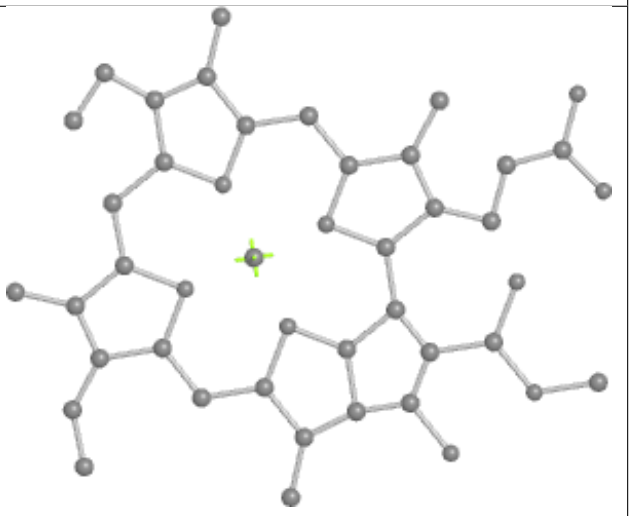
Bond lengths



Bond angles

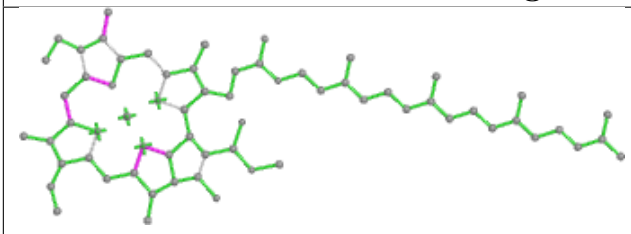


Torsions

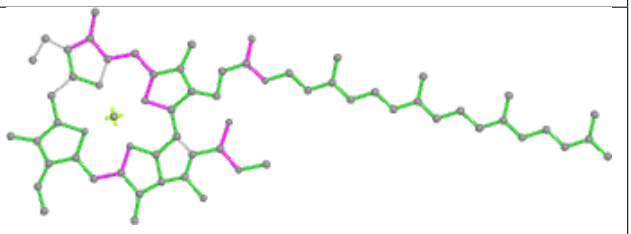


Rings

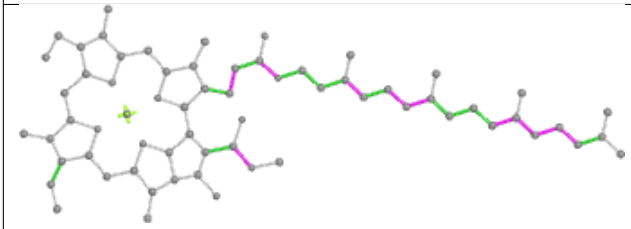
Ligand CLA A 839



Bond lengths



Bond angles



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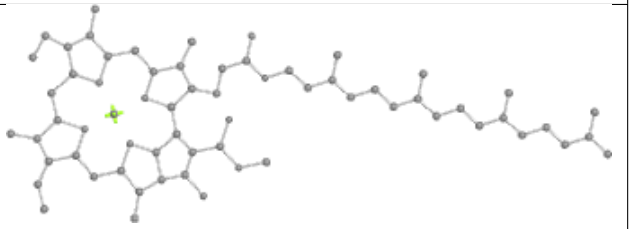
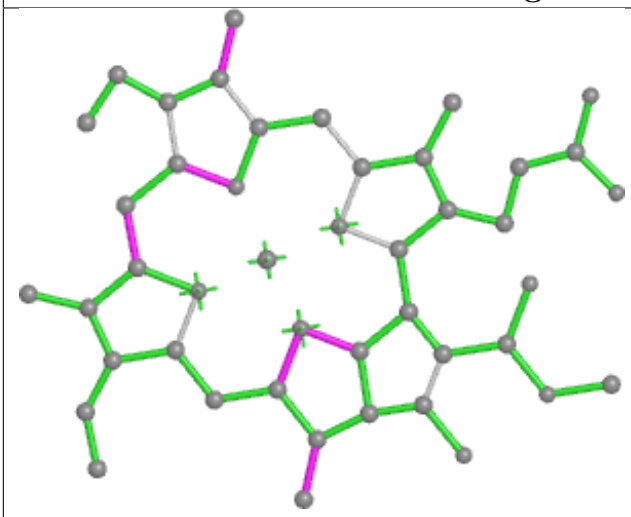
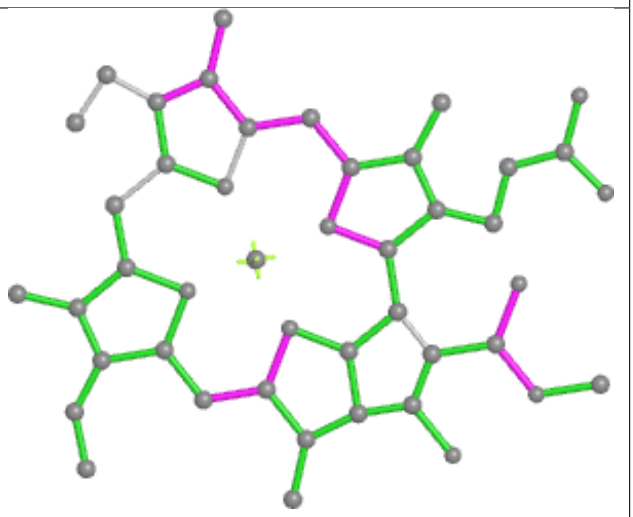


Rings

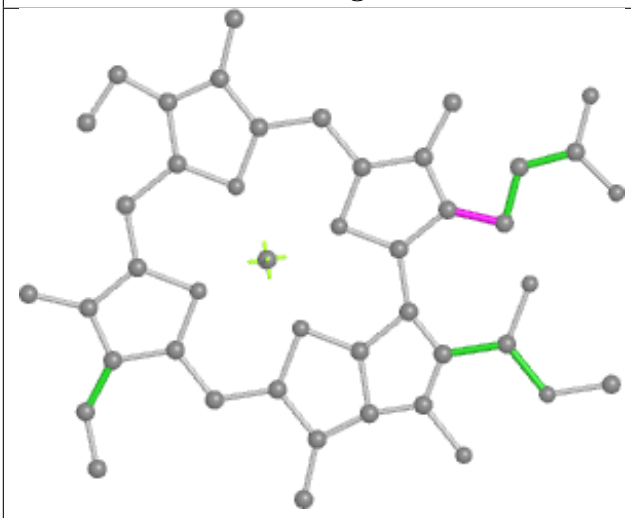
Ligand CLA B 818



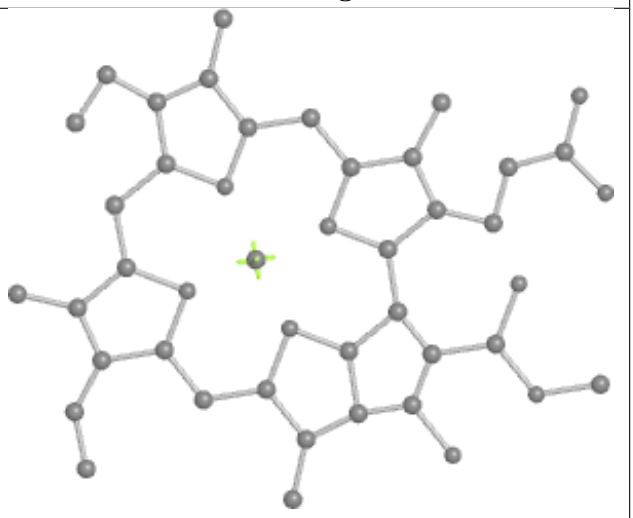
Bond lengths



Bond angles

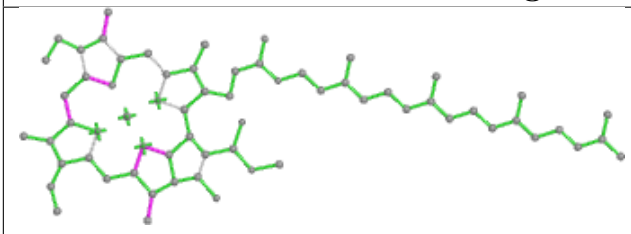


Torsions

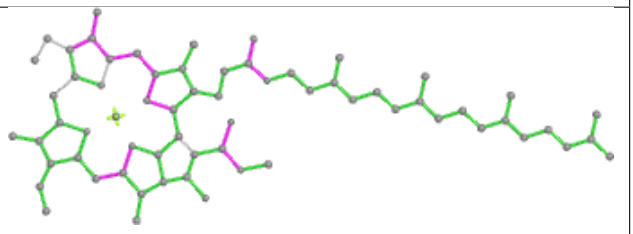


Rings

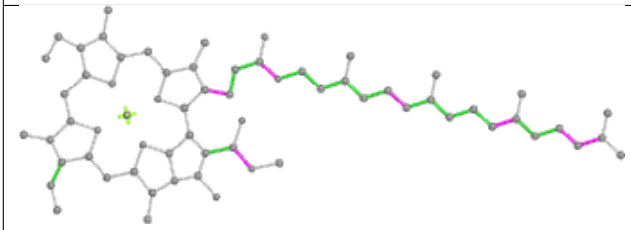
Ligand CLA A 812



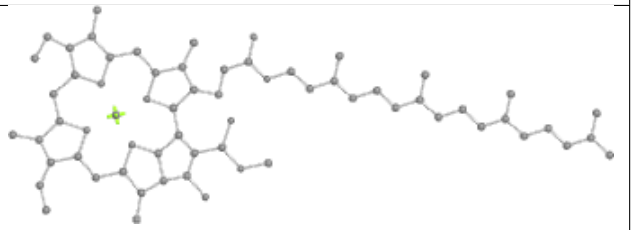
Bond lengths



Bond angles

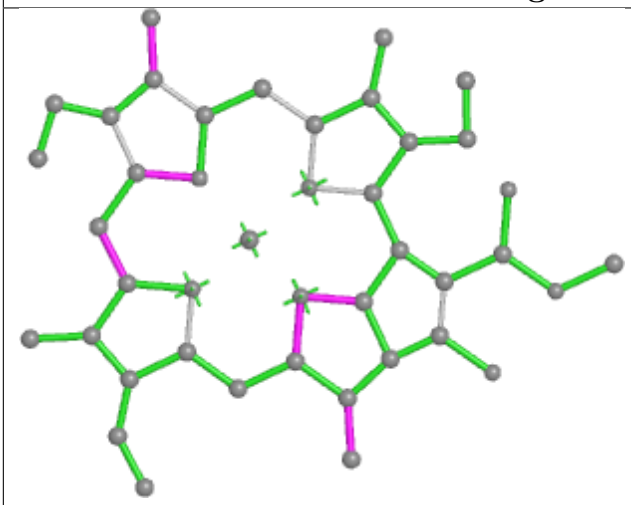


Torsions

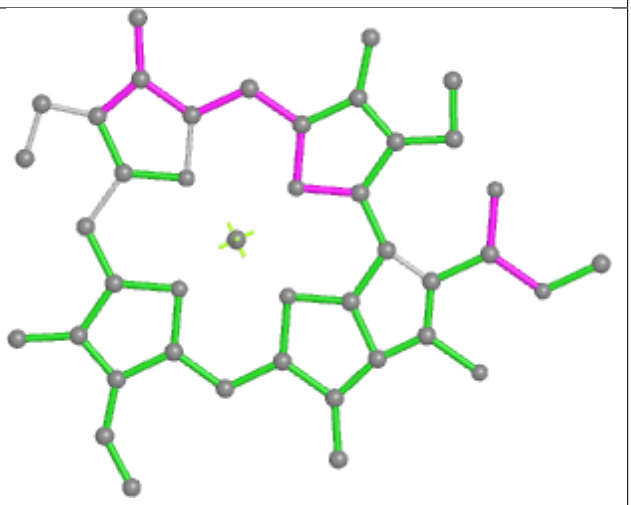


Rings

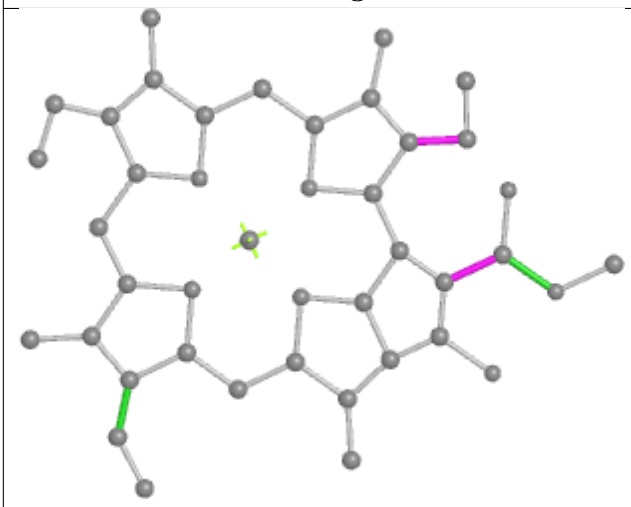
Ligand CLA J 101



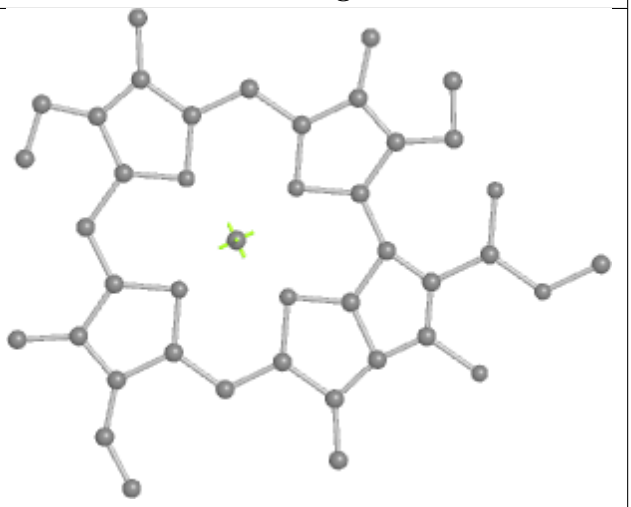
Bond lengths



Bond angles

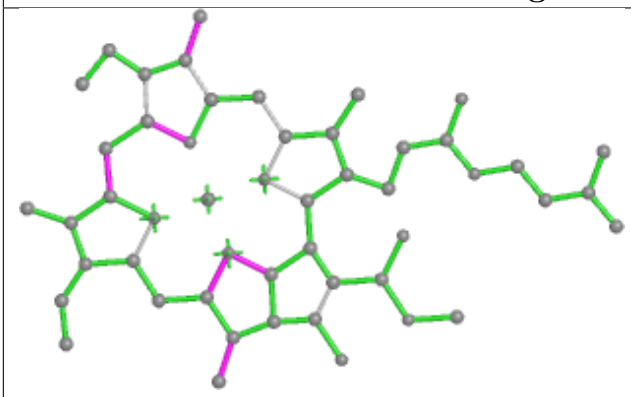


Torsions

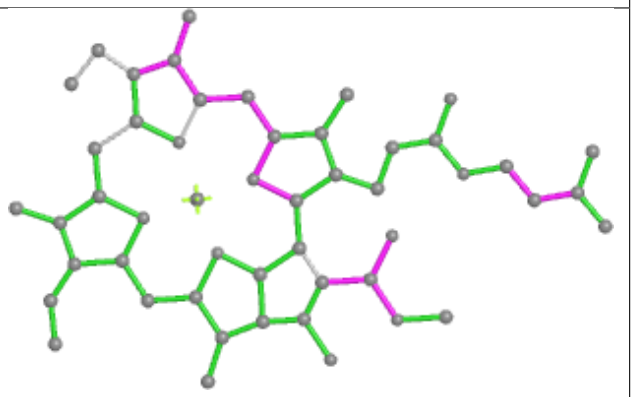


Rings

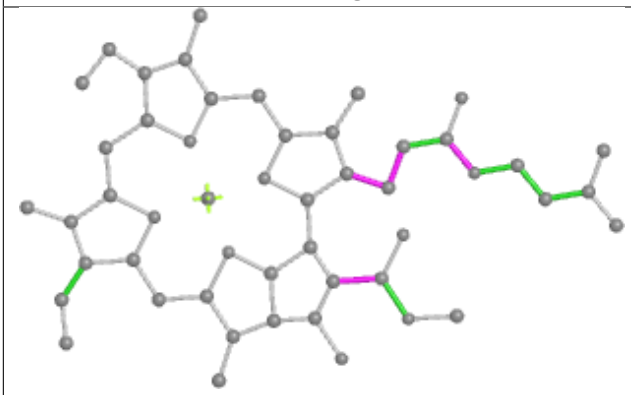
Ligand CLA 2 604



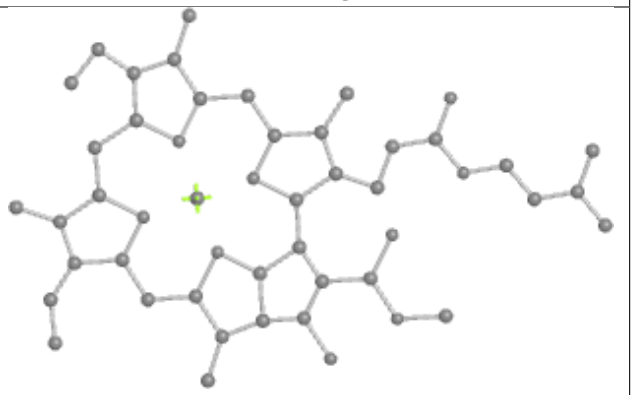
Bond lengths



Bond angles

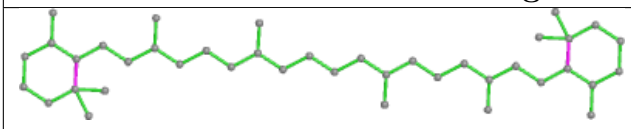


Torsions

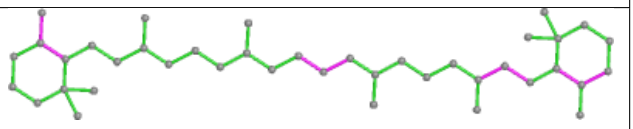


Rings

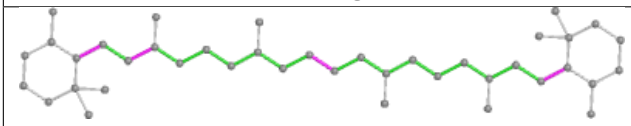
Ligand BCR B 801



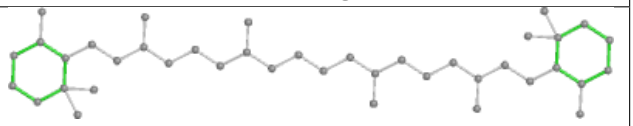
Bond lengths



Bond angles

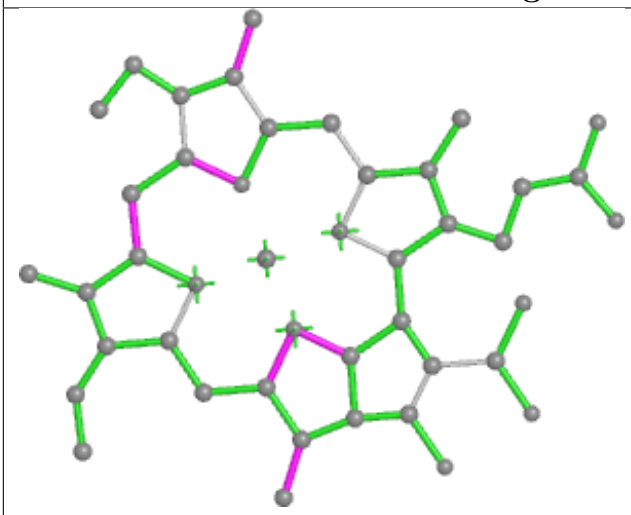


Torsions

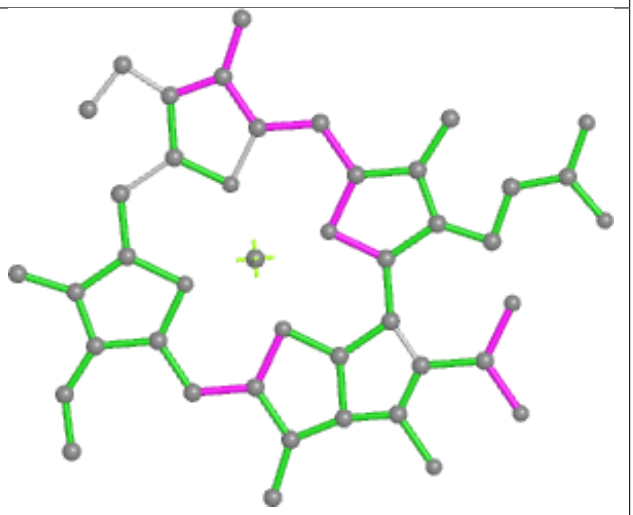


Rings

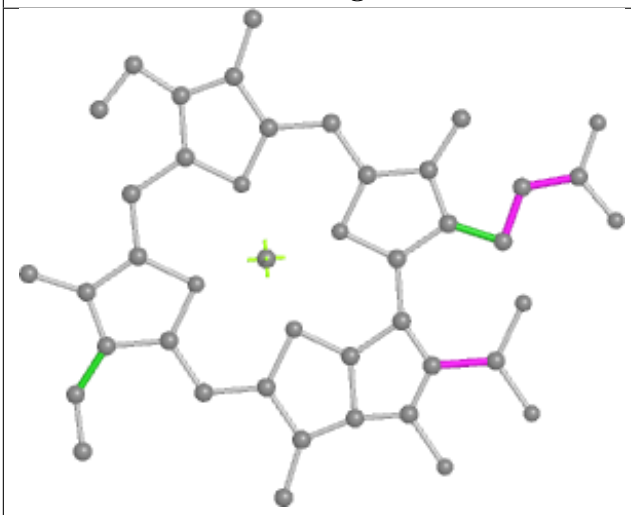
Ligand CLA G 204



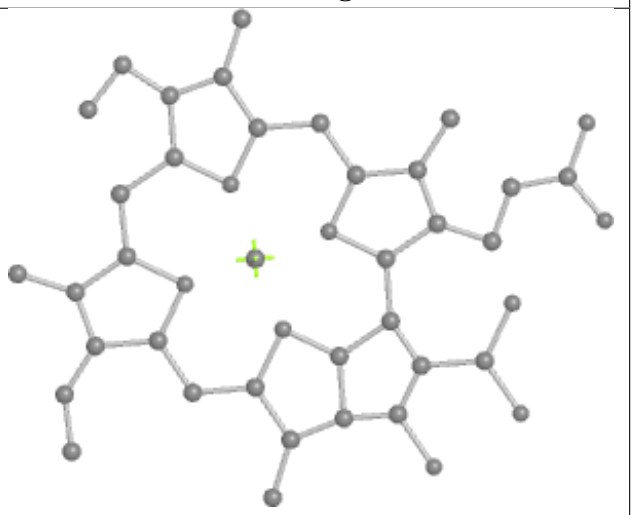
Bond lengths



Bond angles

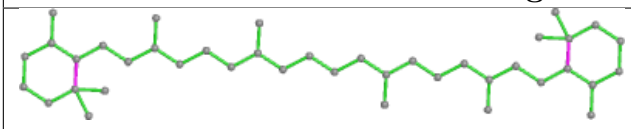


Torsions



Rings

Ligand BCR J 102



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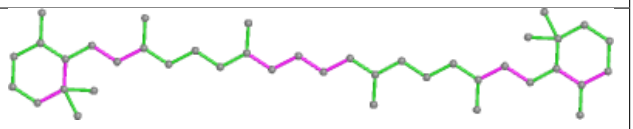
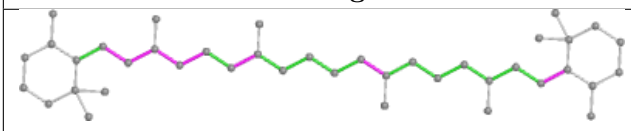


Bond angles



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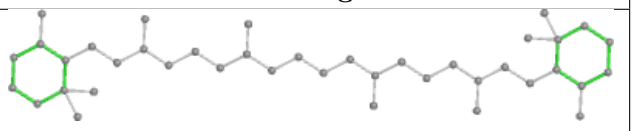
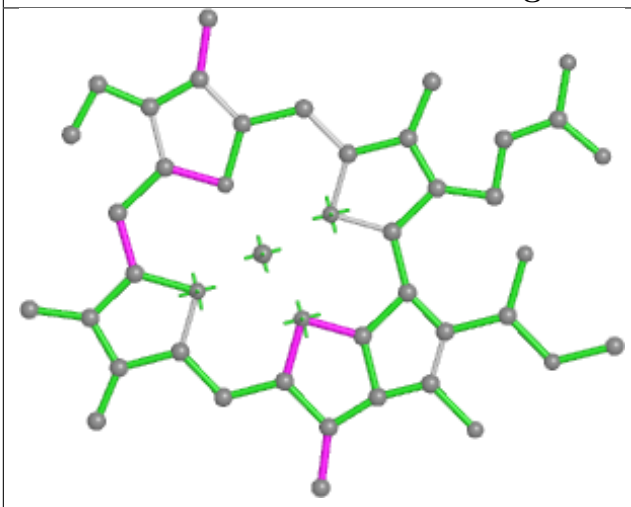
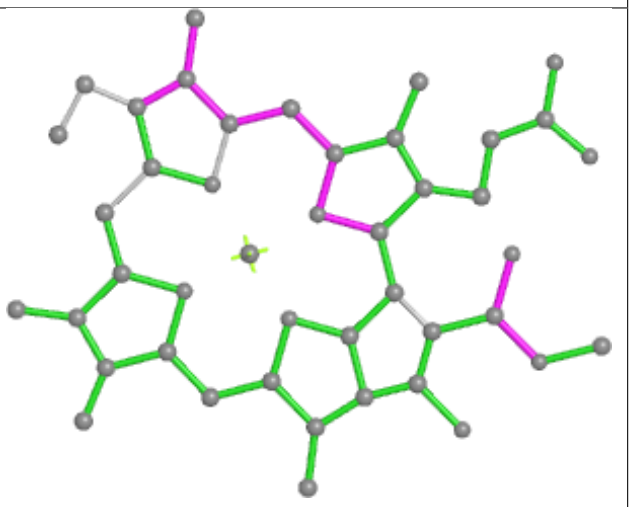


Rings

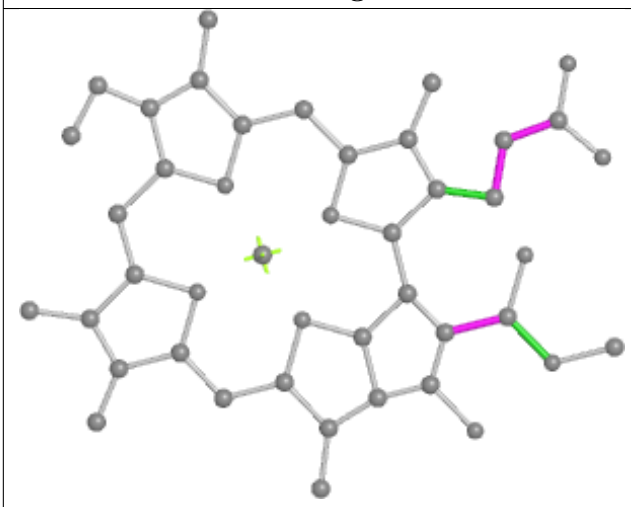
Ligand CLA A 823



Bond lengths



Bond angles



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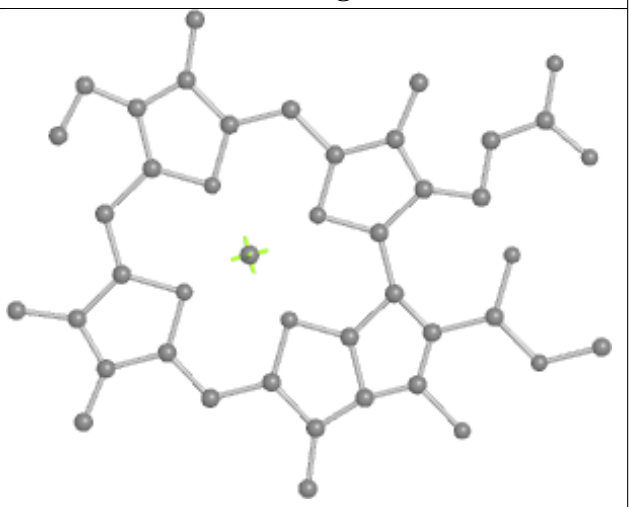
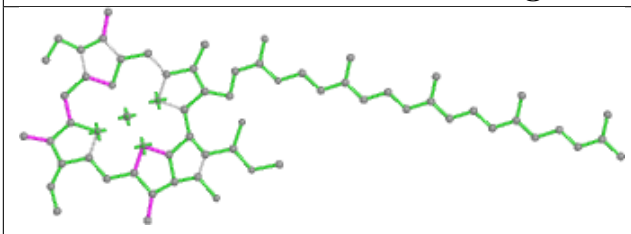
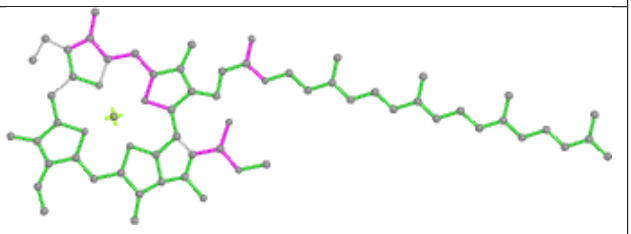


Rings

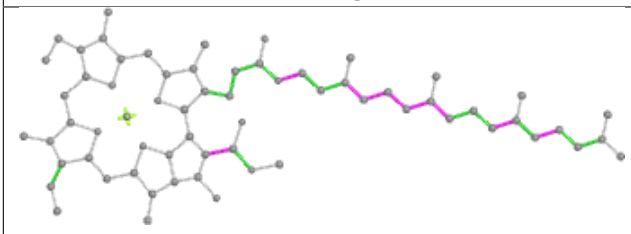
Ligand CLA B 826



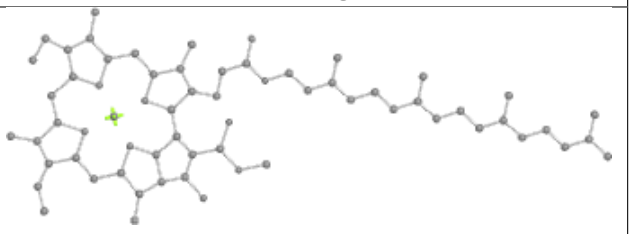
Bond lengths



Bond angles

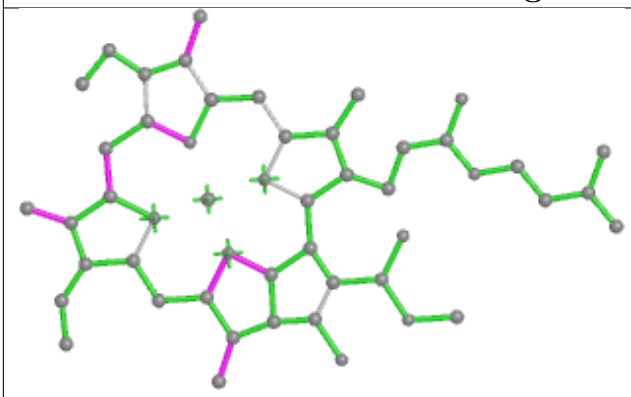


Torsions

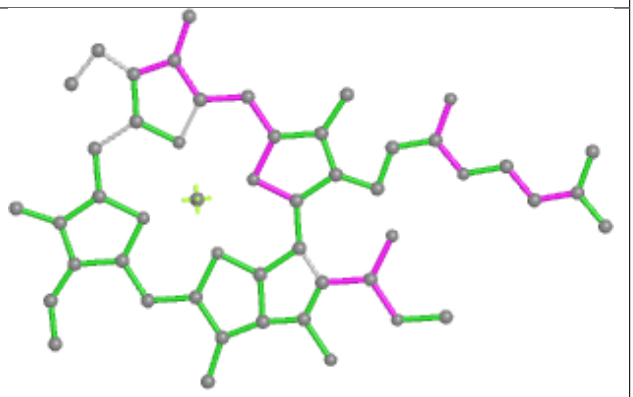


Rings

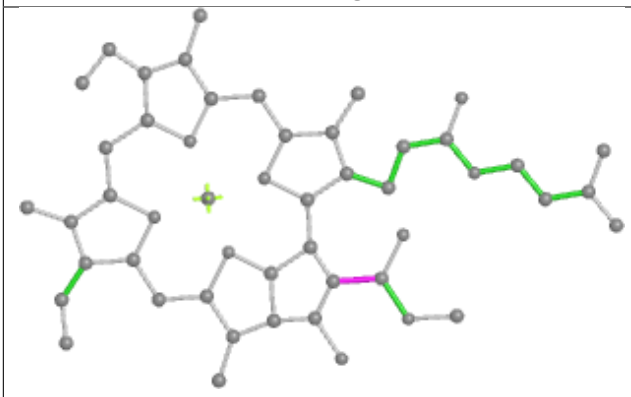
Ligand CLA B 808



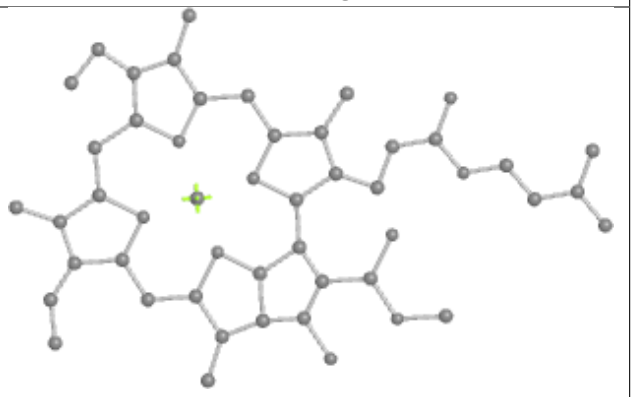
Bond lengths



Bond angles

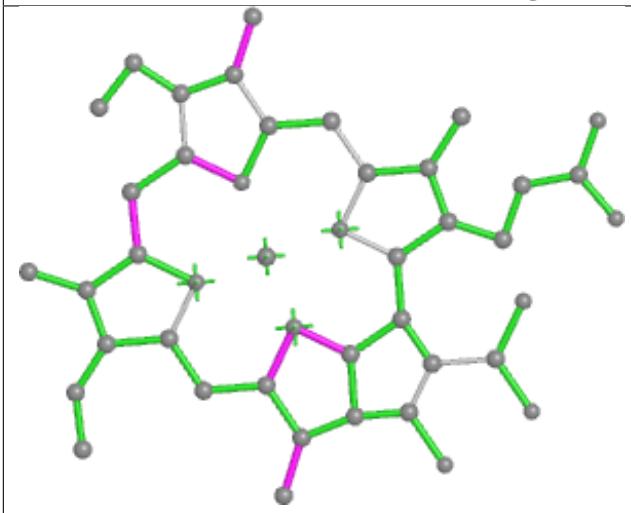


Torsions

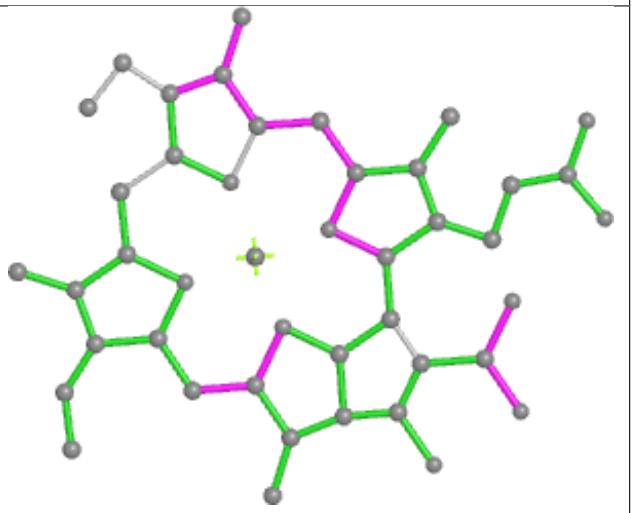


Rings

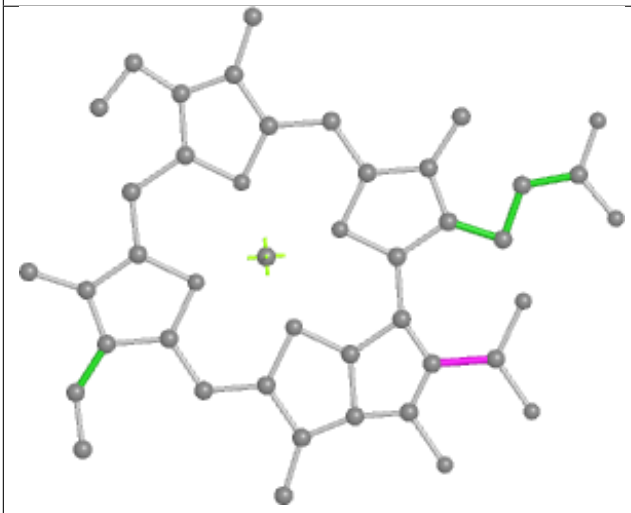
Ligand CLA B 814



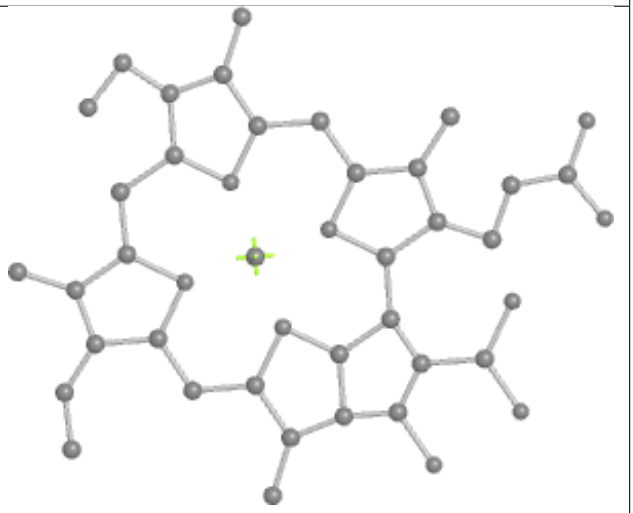
Bond lengths



Bond angles

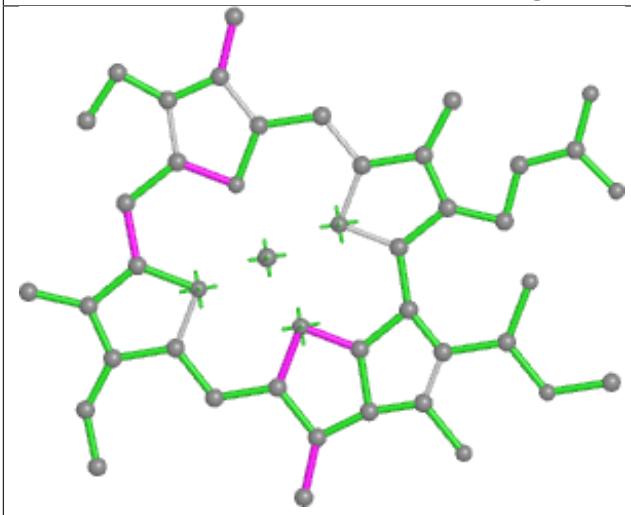


Torsions

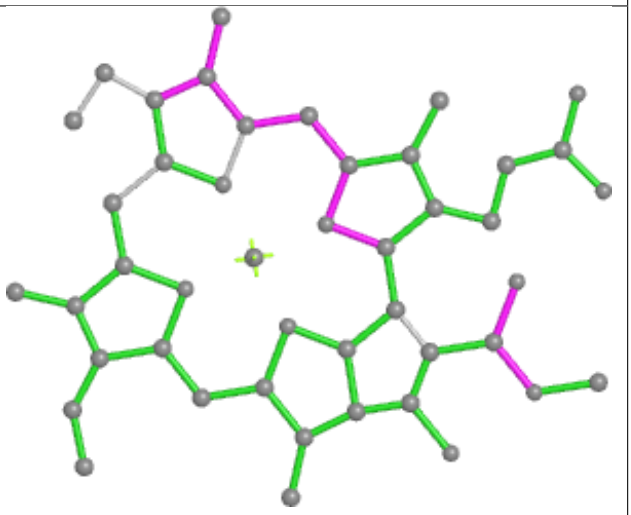


Rings

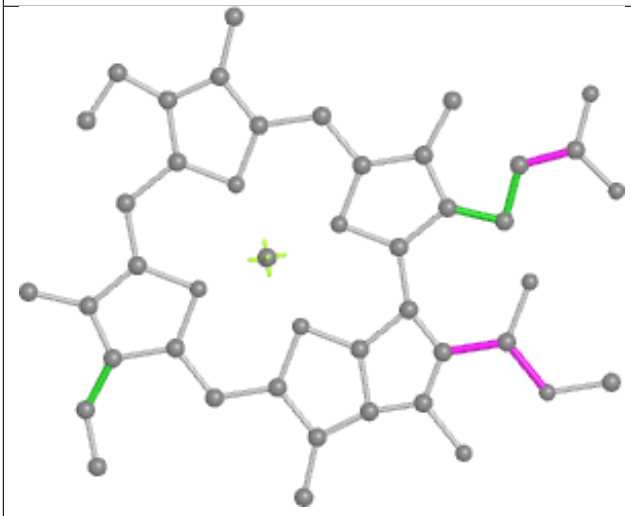
Ligand CLA 2 603



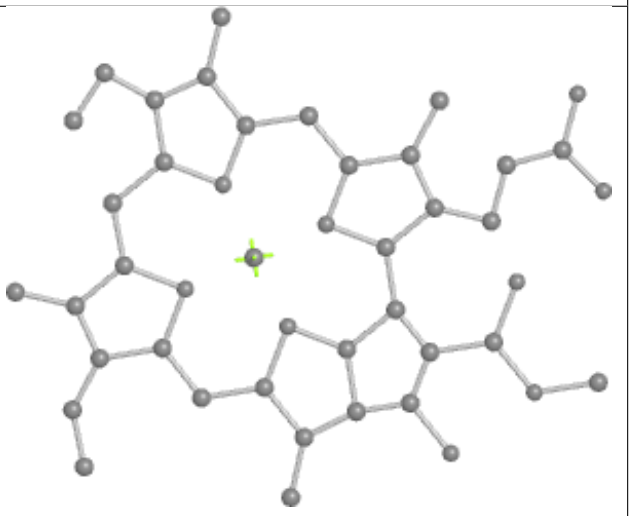
Bond lengths



Bond angles

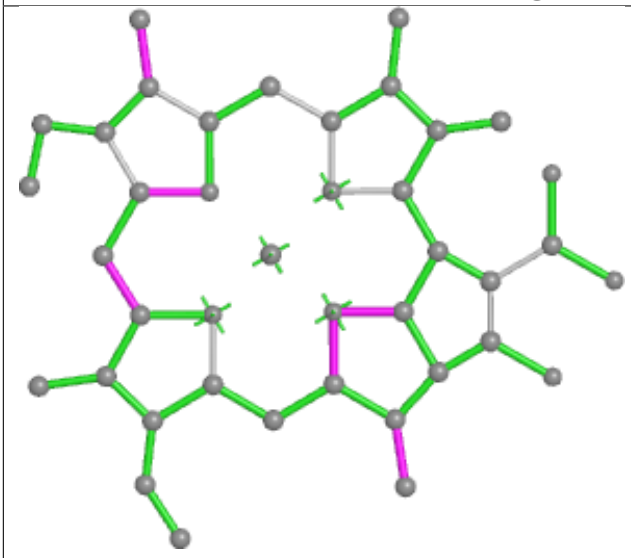


Torsions

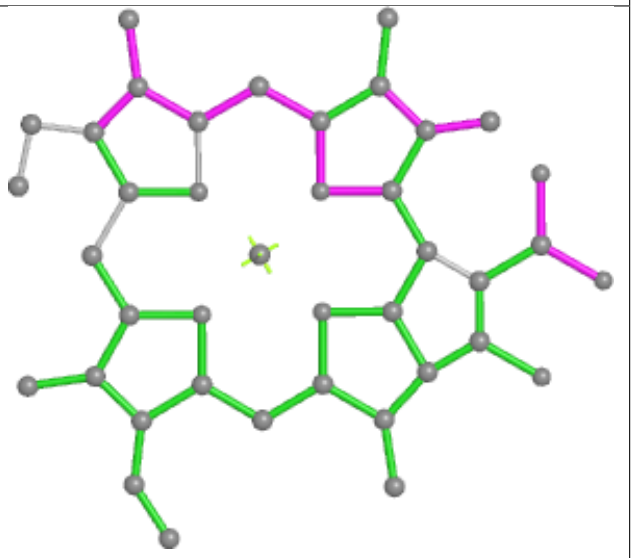


Rings

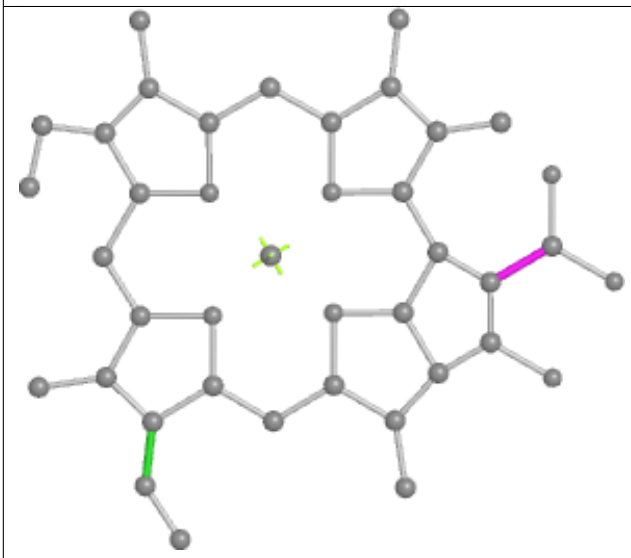
Ligand CLA 3 614



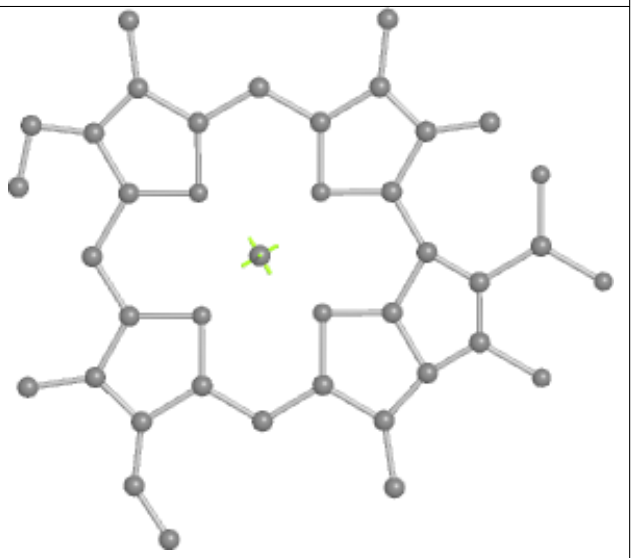
Bond lengths



Bond angles

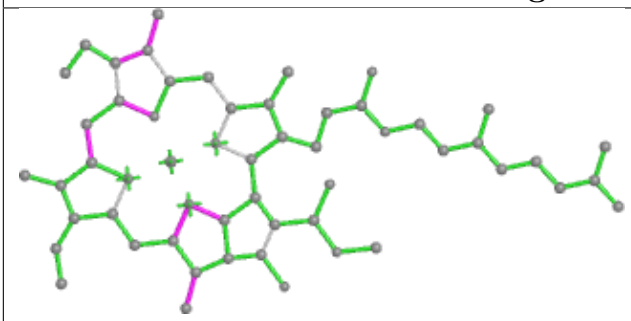


Torsions

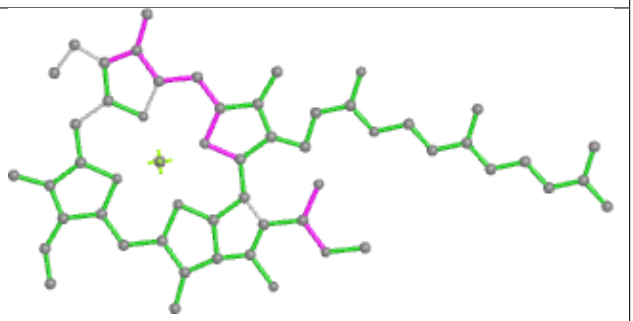


Rings

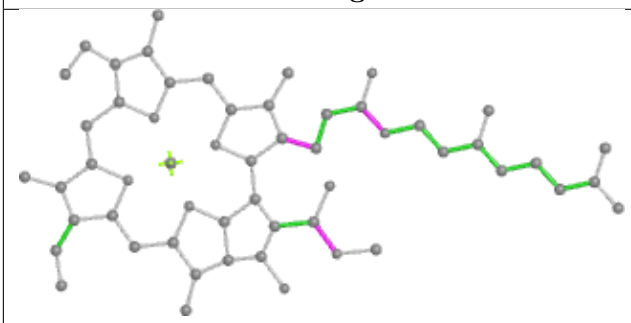
Ligand CLA 3 603



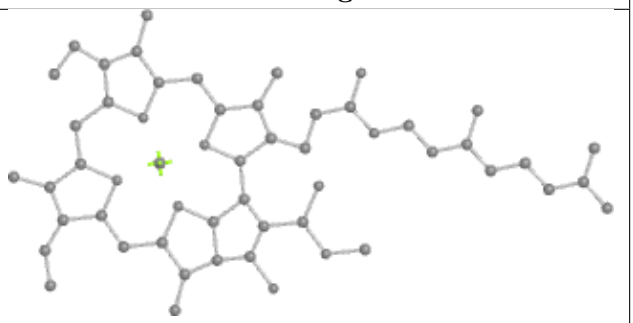
Bond lengths



Bond angles

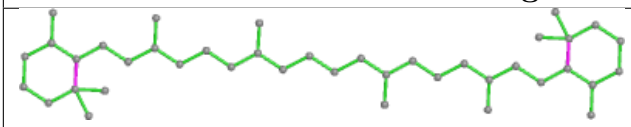


Torsions

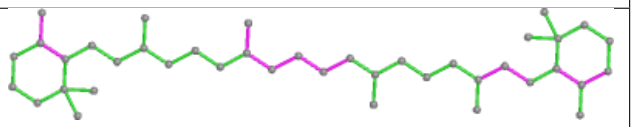


Rings

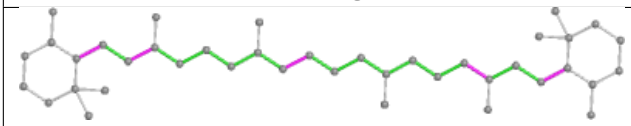
Ligand BCR K 202



Bond lengths



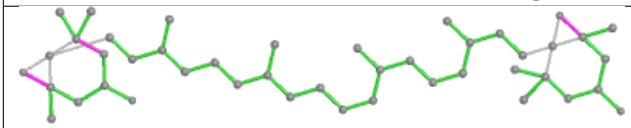
Bond angles



Torsions

Rings

Ligand XAT 5 620



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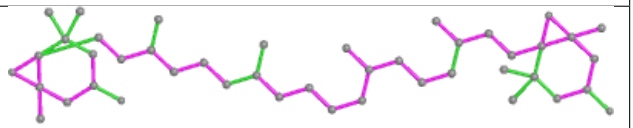
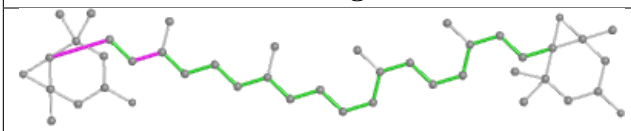
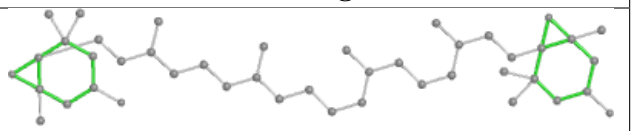


Bond angles

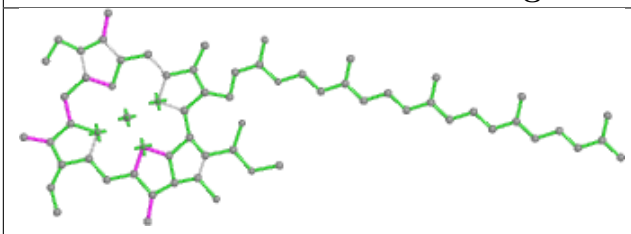


Torsions

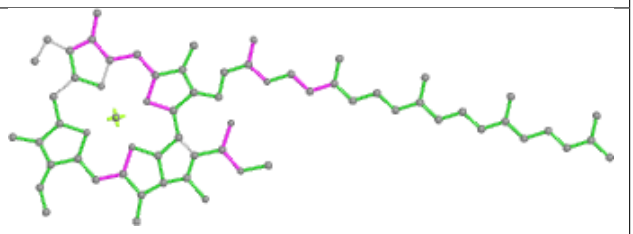


Rings

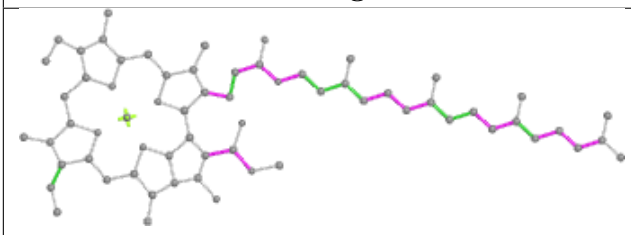
Ligand CLA A 829



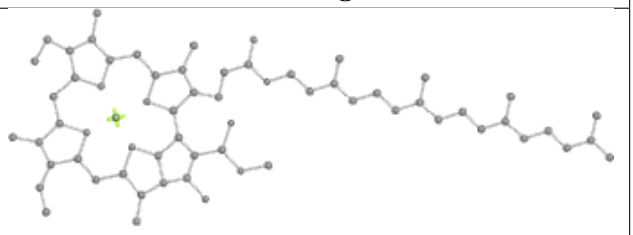
Bond lengths



Bond angles

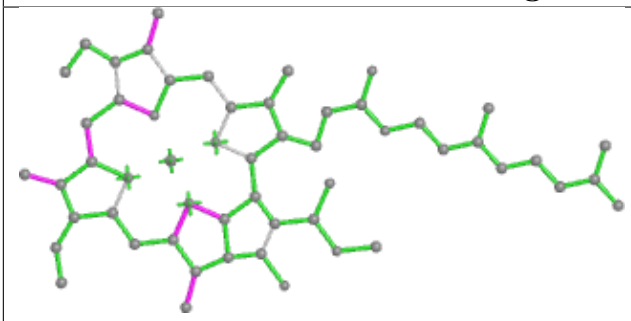


Torsions

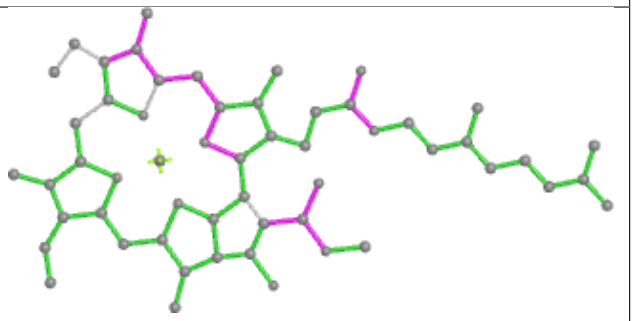


Rings

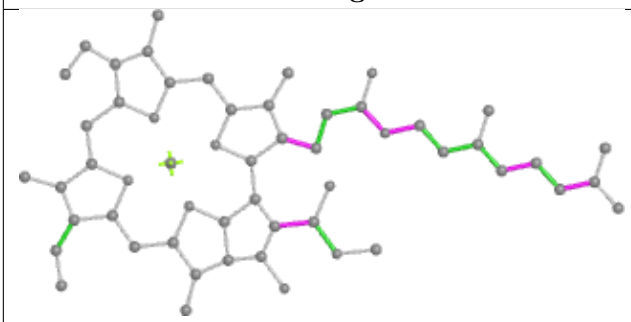
Ligand CLA A 805



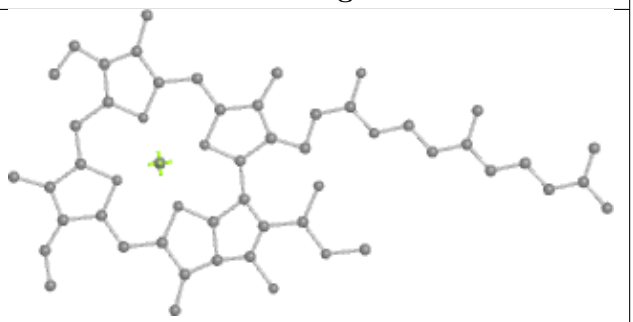
Bond lengths



Bond angles

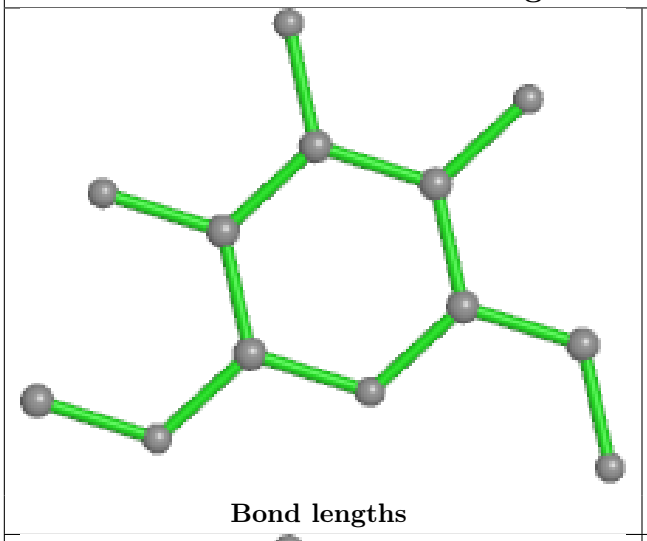


Torsions

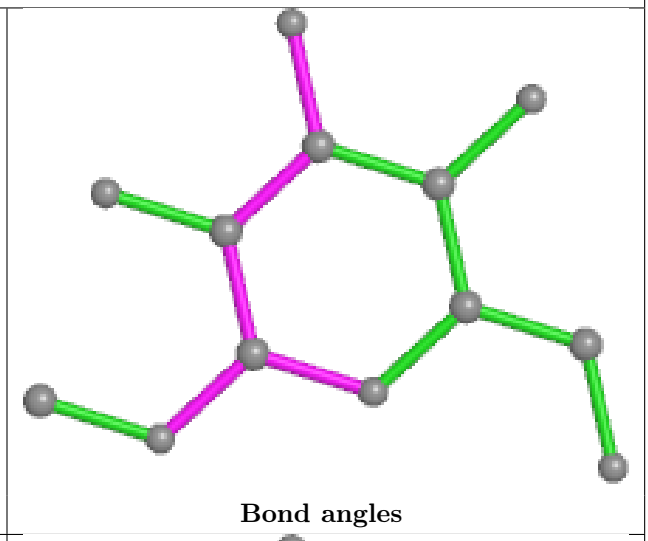


Rings

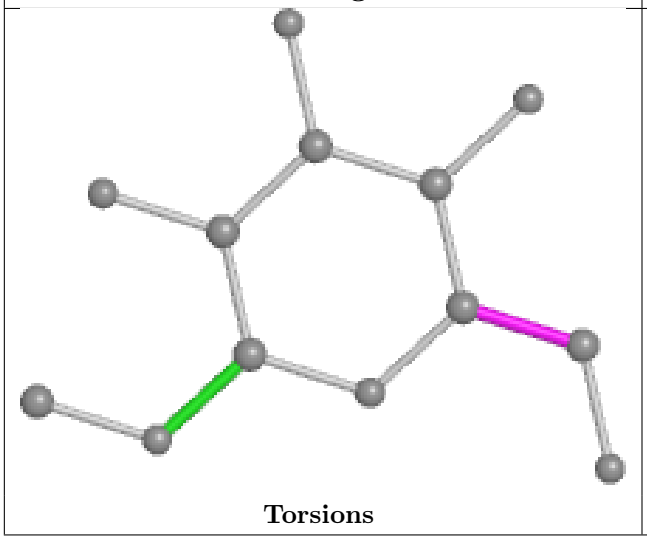
Ligand LMG 2 618



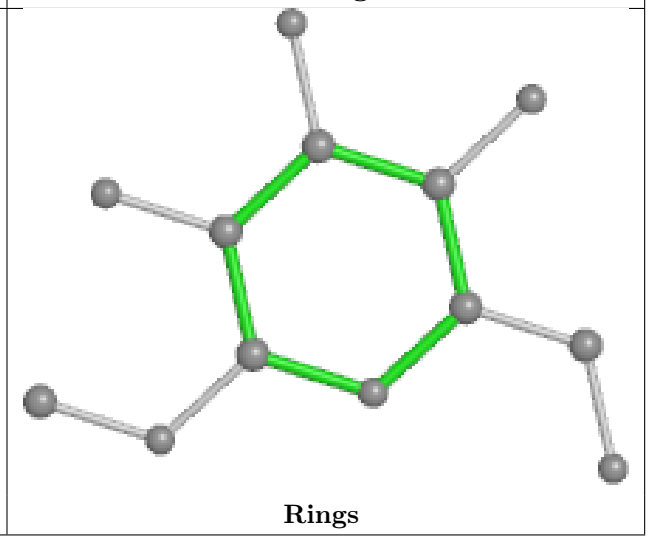
Bond lengths



Bond angles

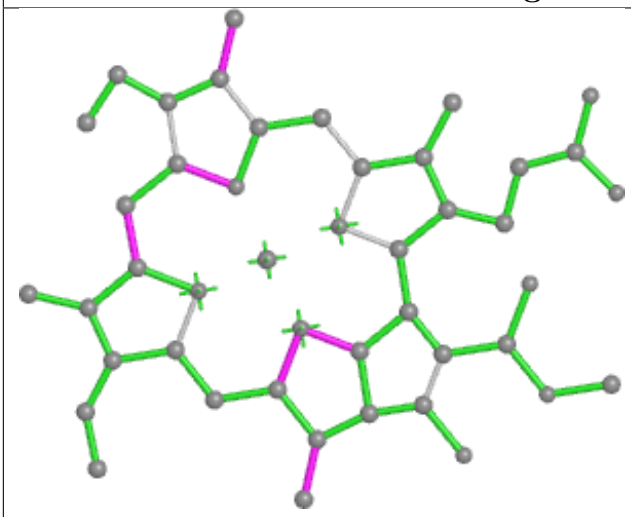


Torsions

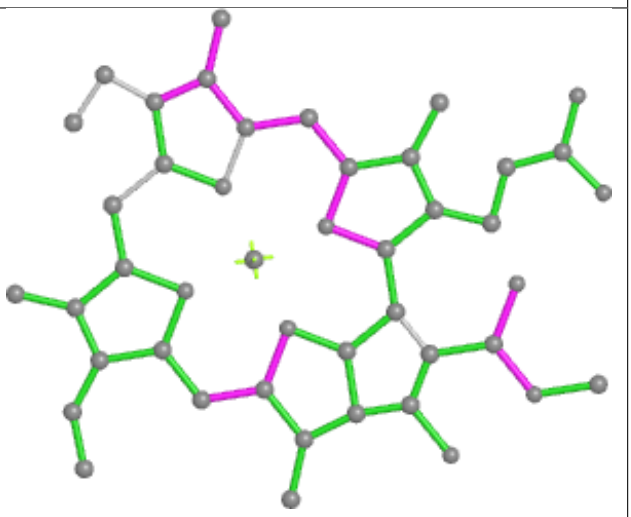


Rings

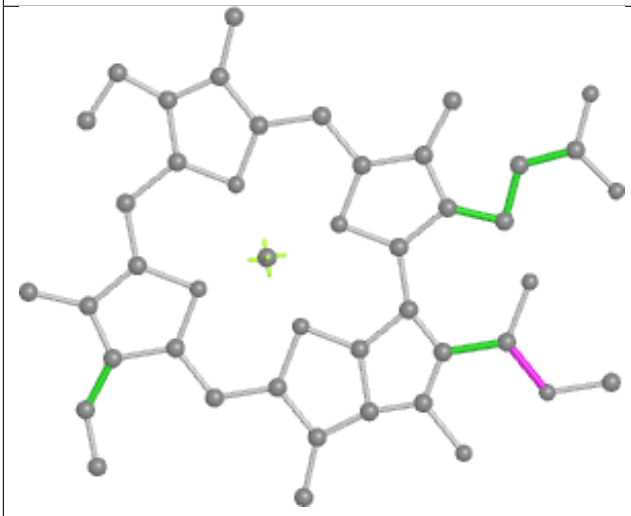
Ligand CLA A 811



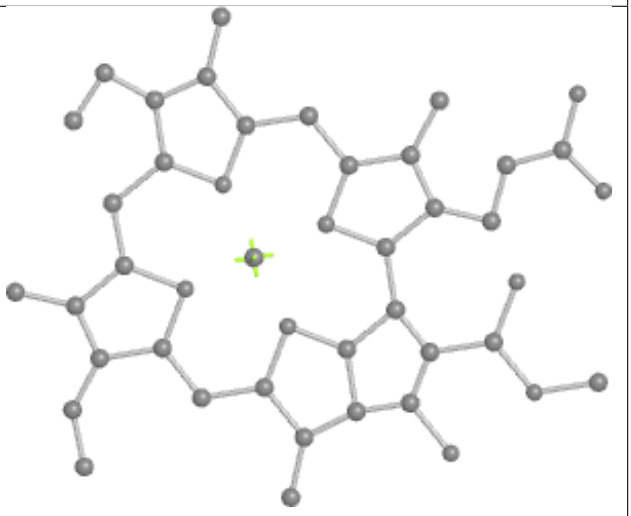
Bond lengths



Bond angles

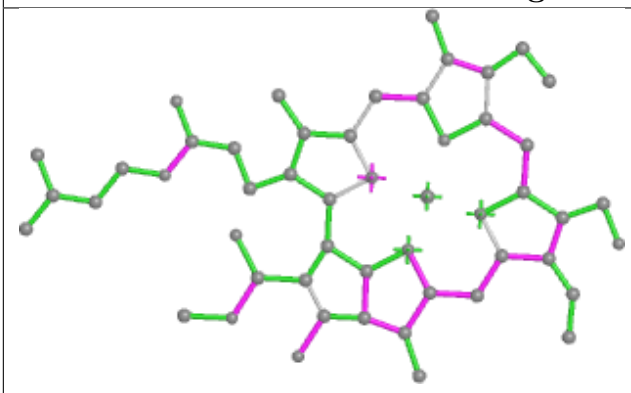


Torsions

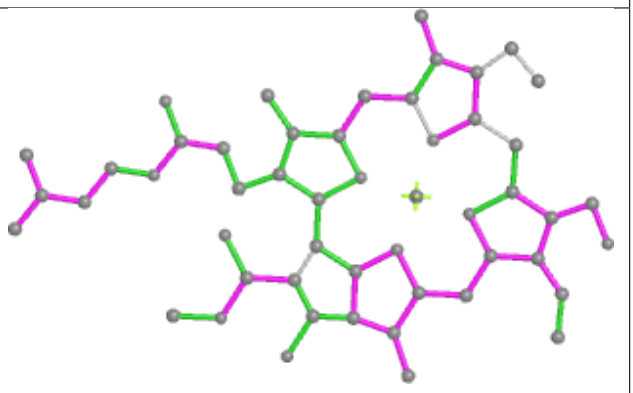


Rings

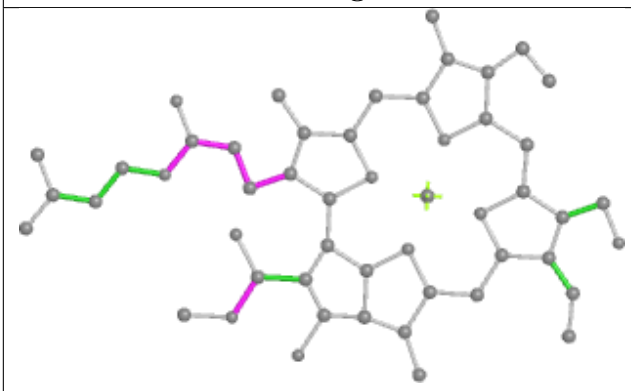
Ligand CHL 5 608



Bond lengths



Bond angles



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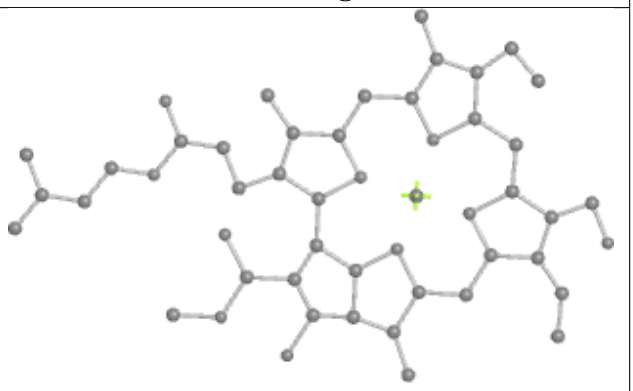
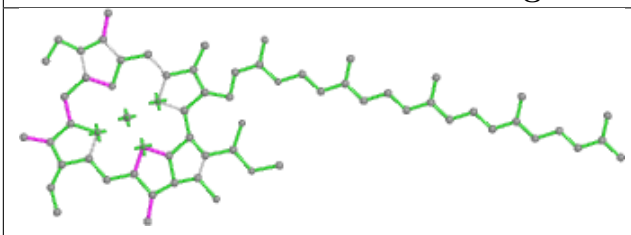
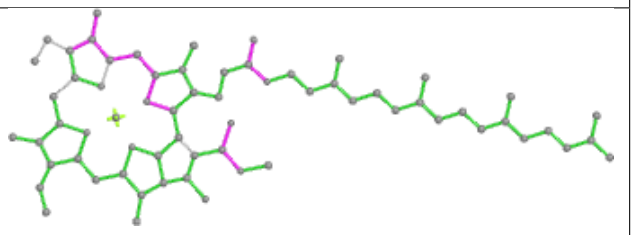


Rings

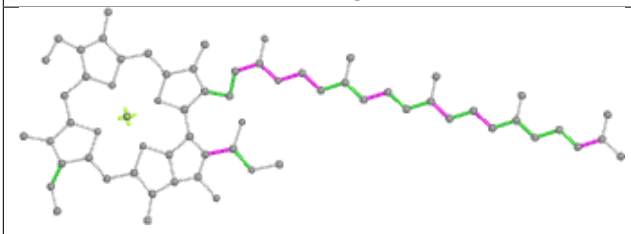
Ligand CLA A 806



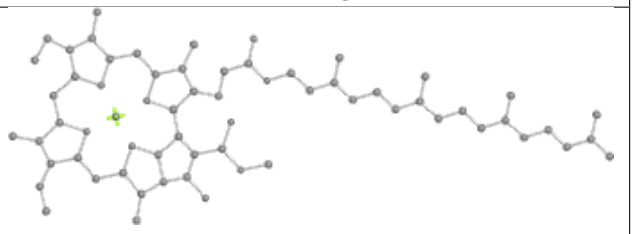
Bond lengths



Bond angles

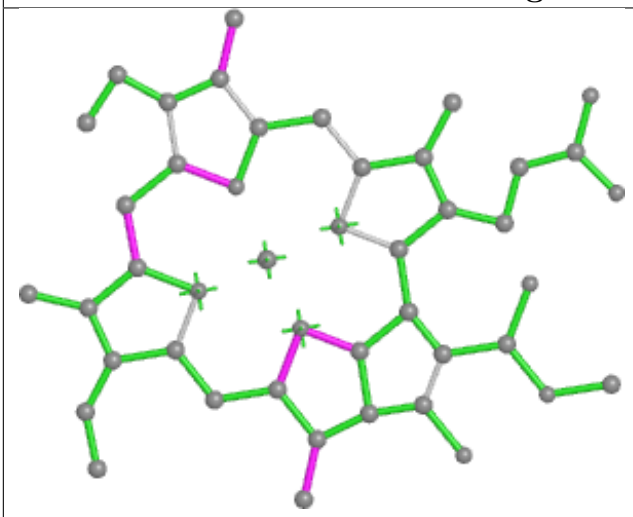


Torsions

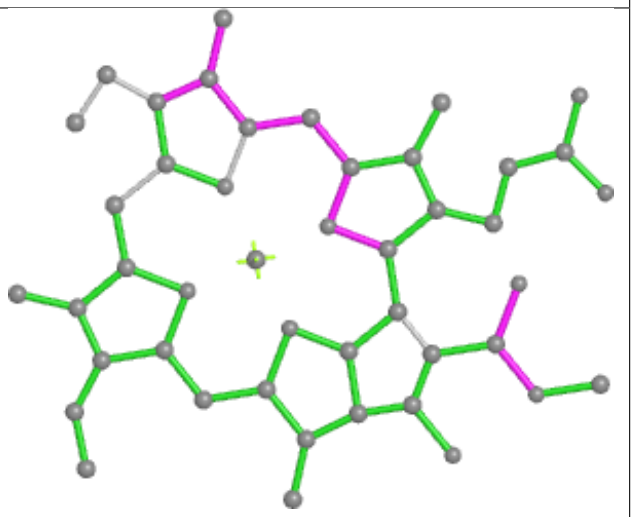


Rings

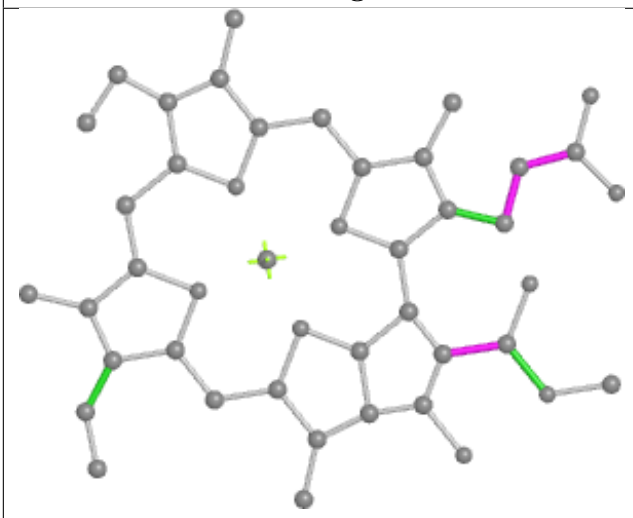
Ligand CLA F 305



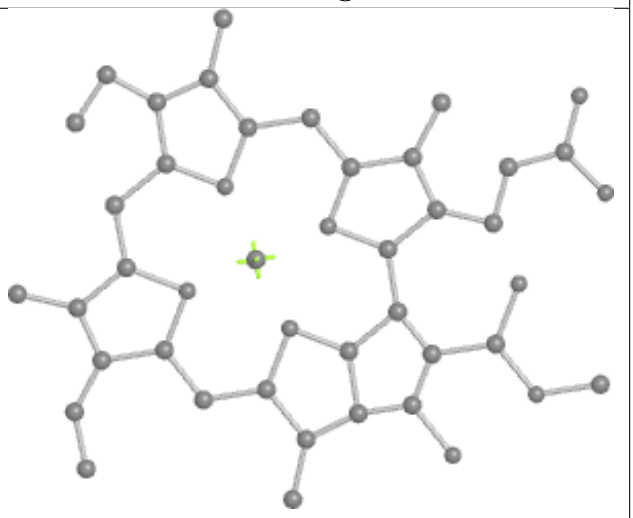
Bond lengths



Bond angles

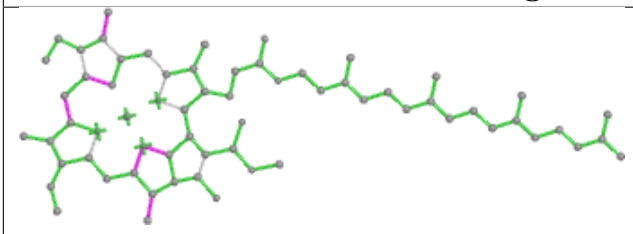


Torsions

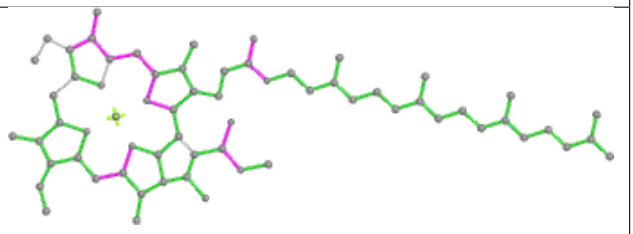


Rings

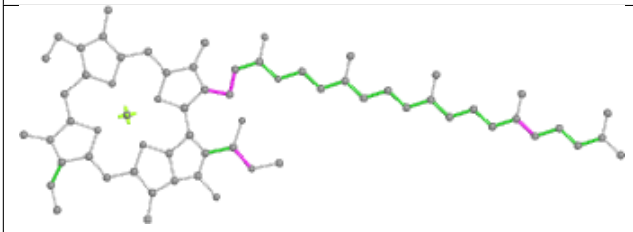
Ligand CLA A 803



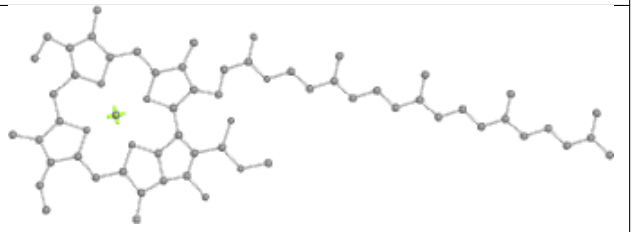
Bond lengths



Bond angles

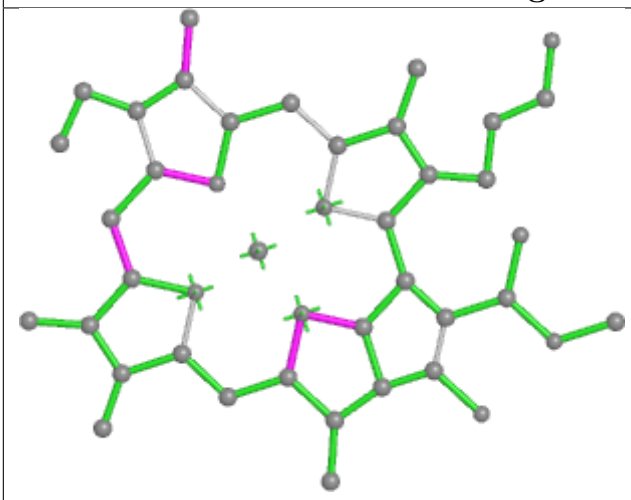


Torsions

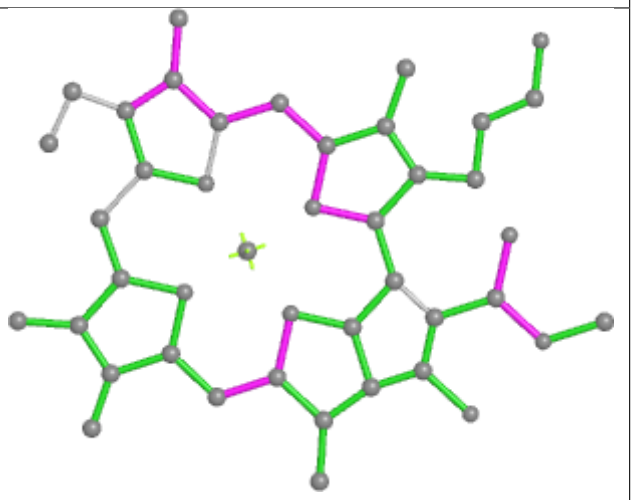


Rings

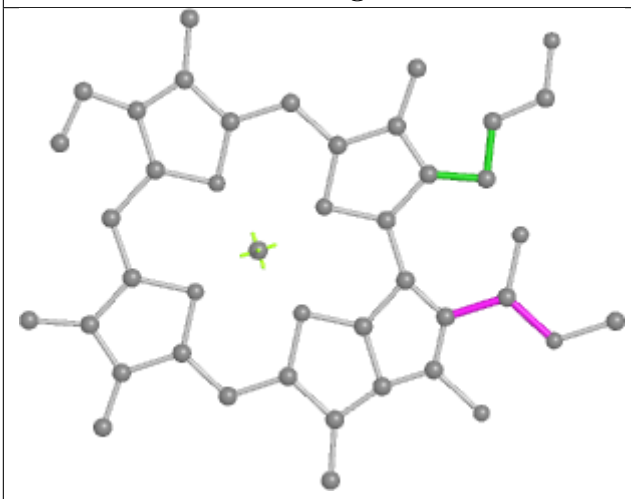
Ligand CLA 5 604



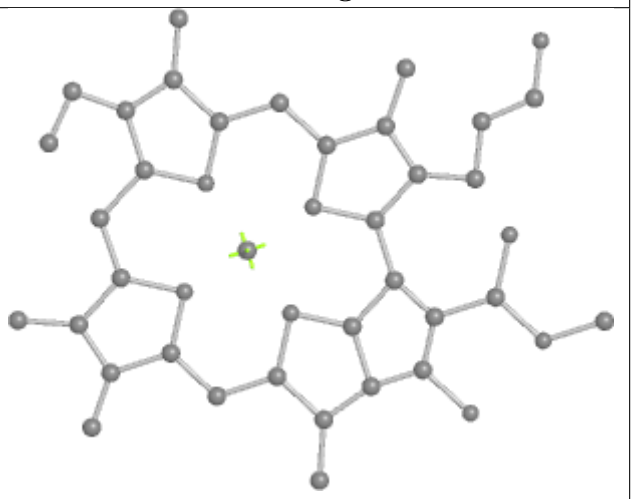
Bond lengths



Bond angles

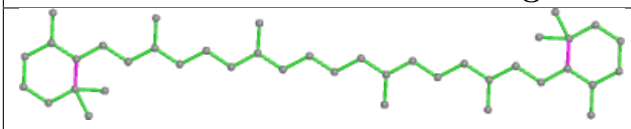


Torsions

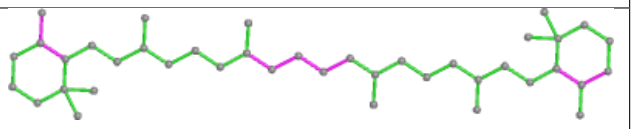


Rings

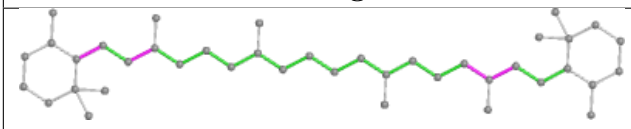
Ligand BCR B 844



Bond lengths



Bond angles



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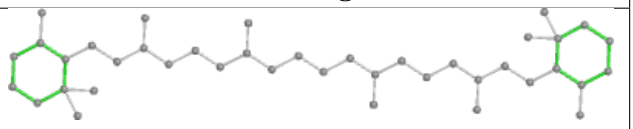
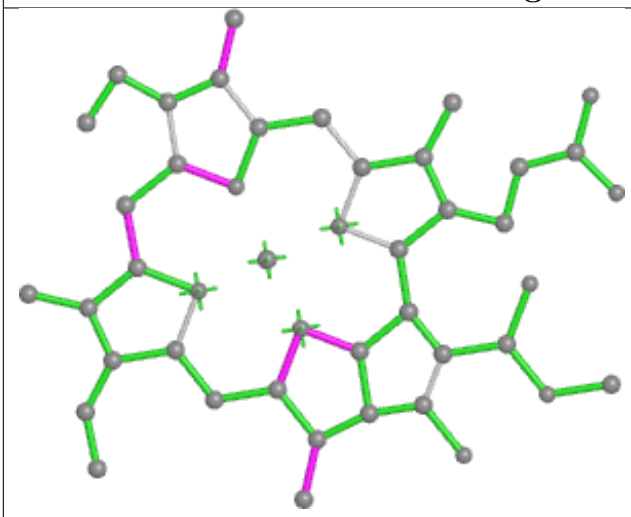


Rings

Ligand CLA B 834



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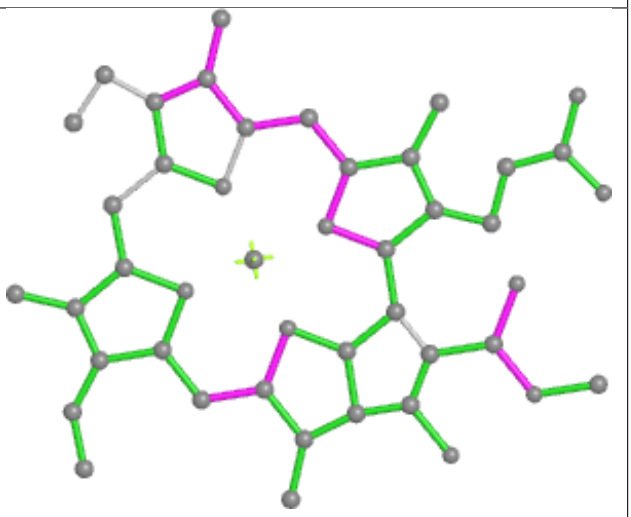
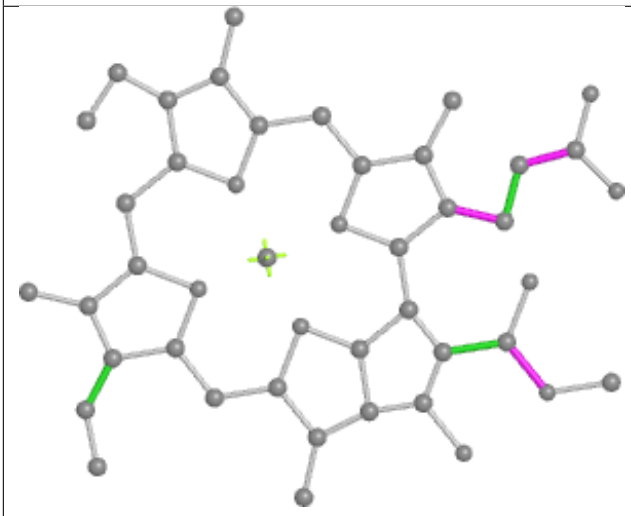


Bond angles



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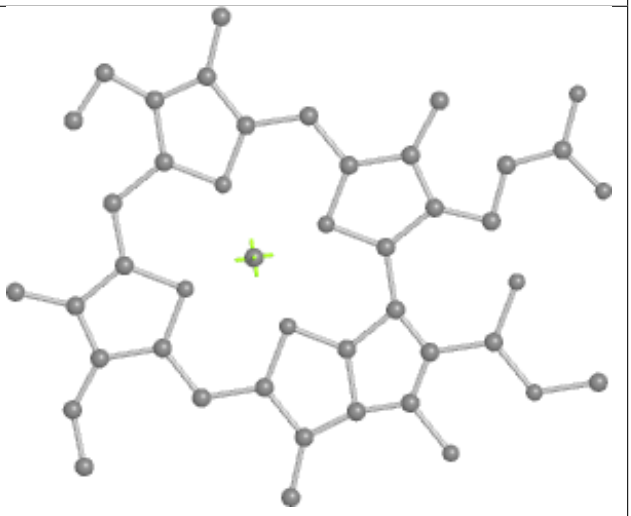
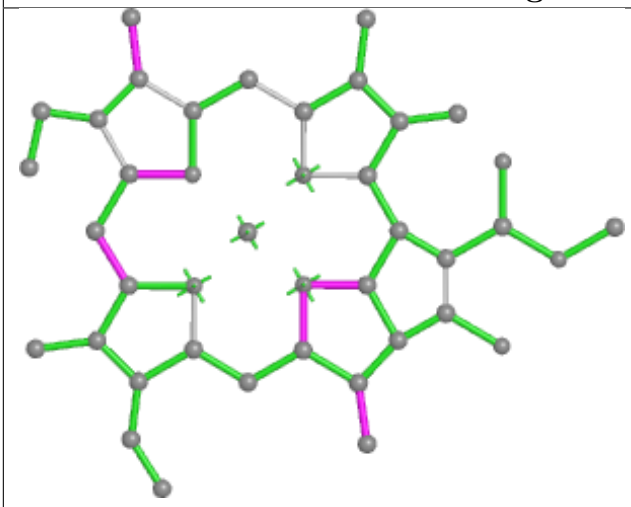
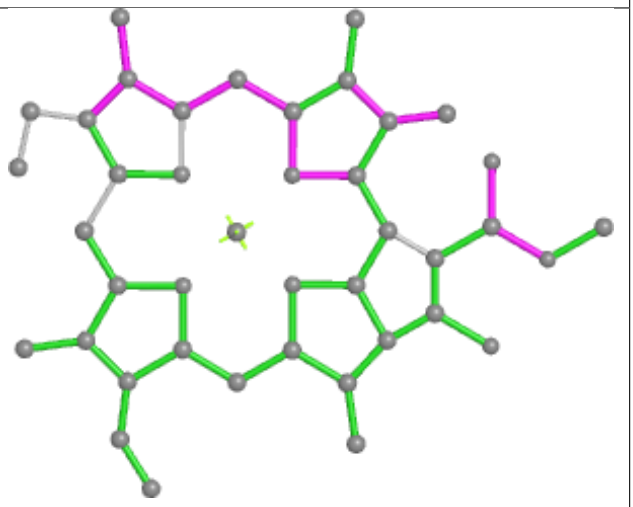


Rings

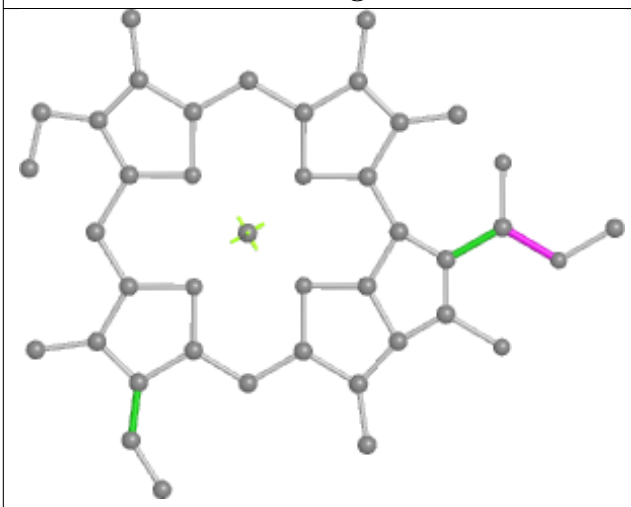
Ligand CLA F 304



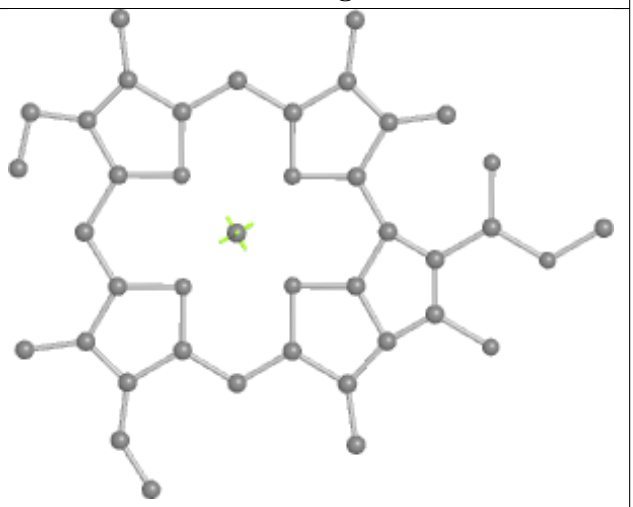
Bond lengths



Bond angles

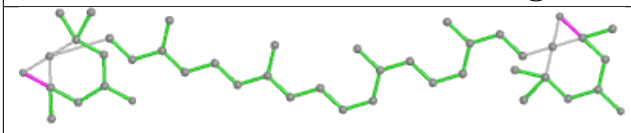


Torsions

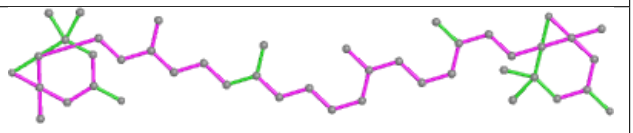


Rings

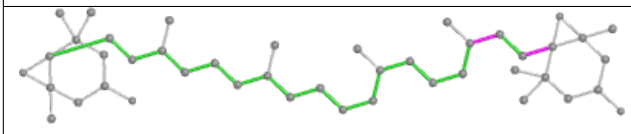
Ligand XAT 2 620



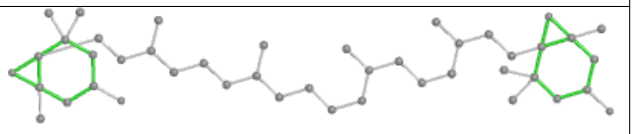
Bond lengths



Bond angles

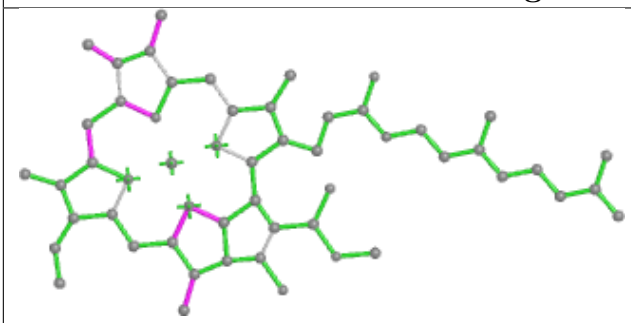


Torsions

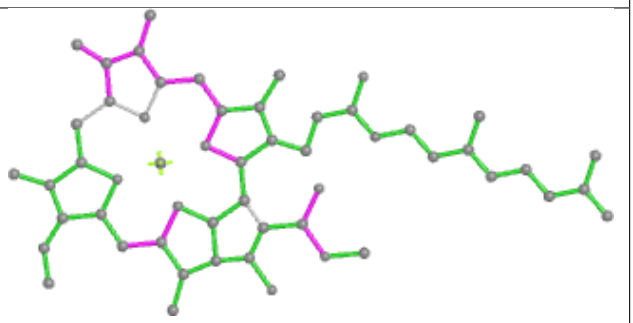


Rings

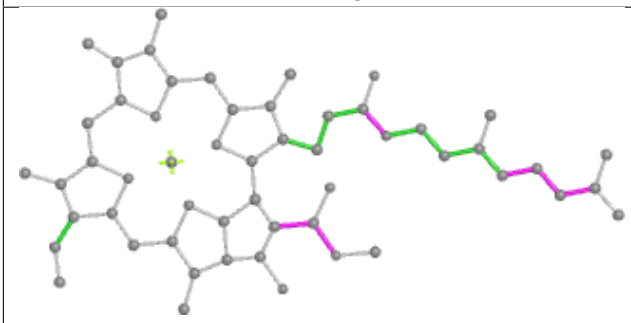
Ligand CLA B 811



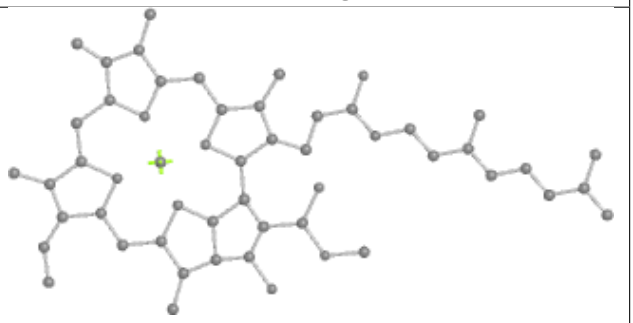
Bond lengths



Bond angles

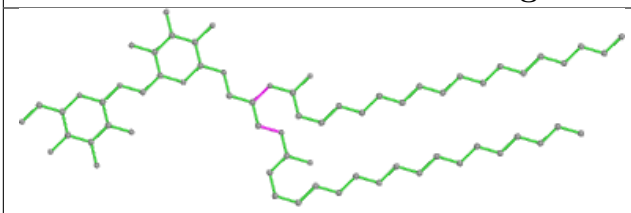


Torsions

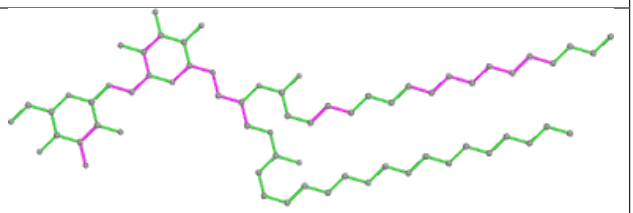


Rings

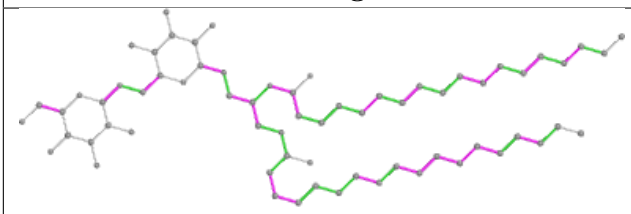
Ligand DGD B 850



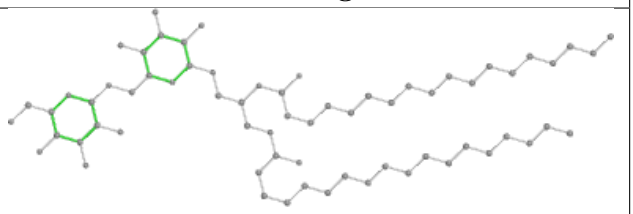
Bond lengths



Bond angles

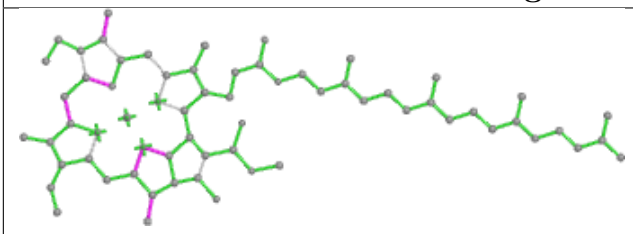


Torsions

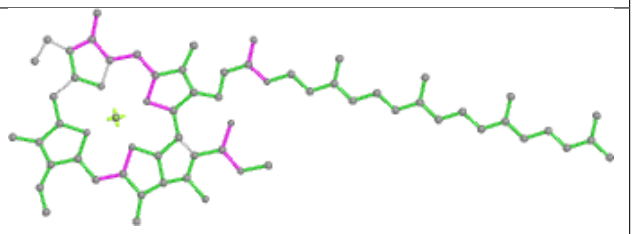


Rings

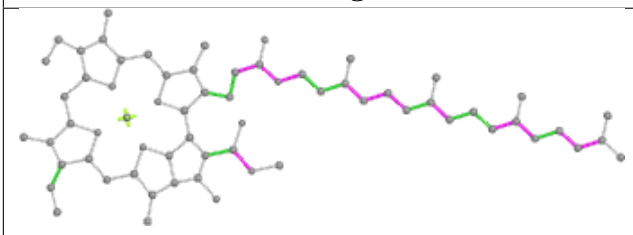
Ligand CLA B 806



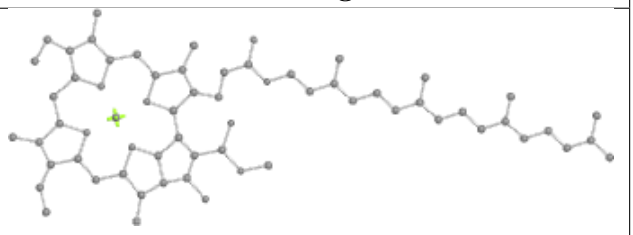
Bond lengths



Bond angles

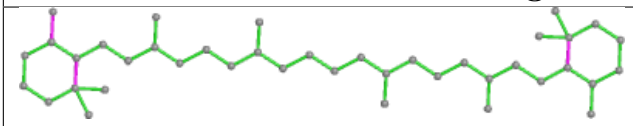


Torsions

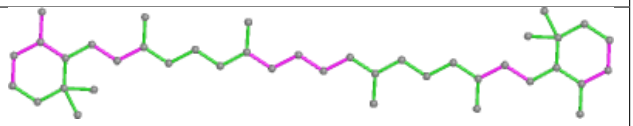


Rings

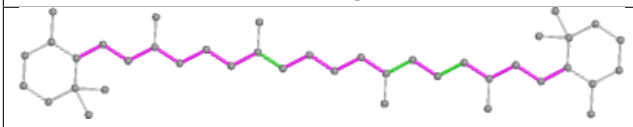
Ligand BCR J 103



Bond lengths



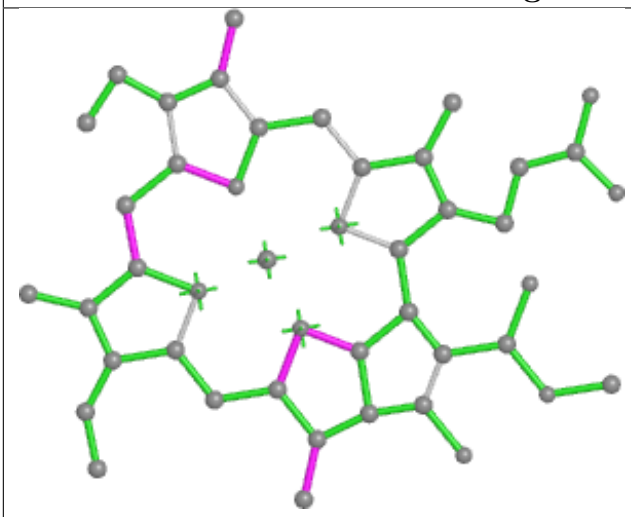
Bond angles



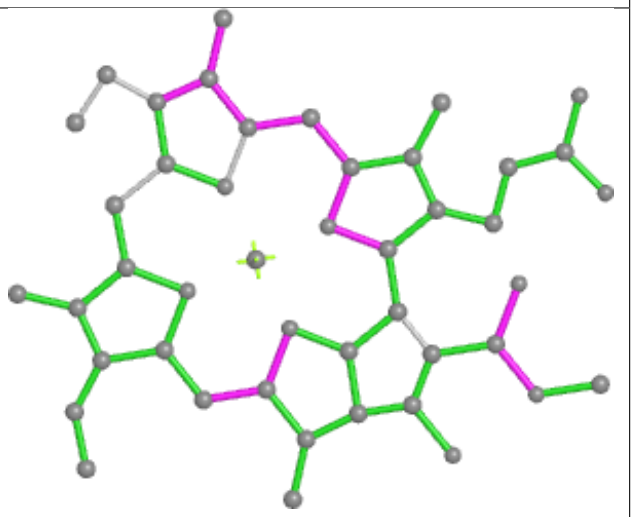
Torsions

Rings

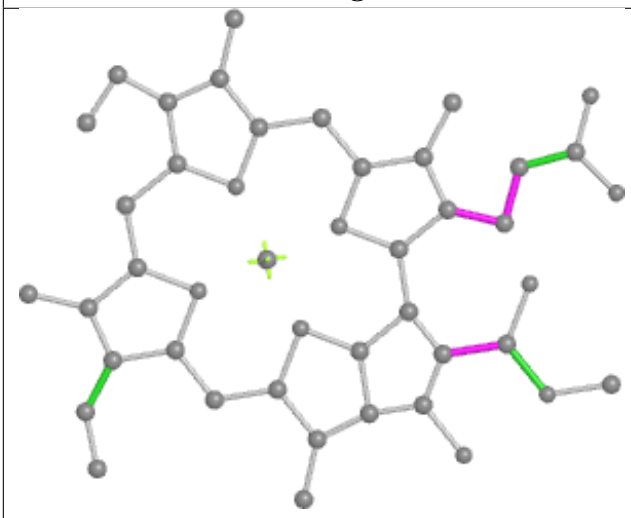
Ligand CLA A 820



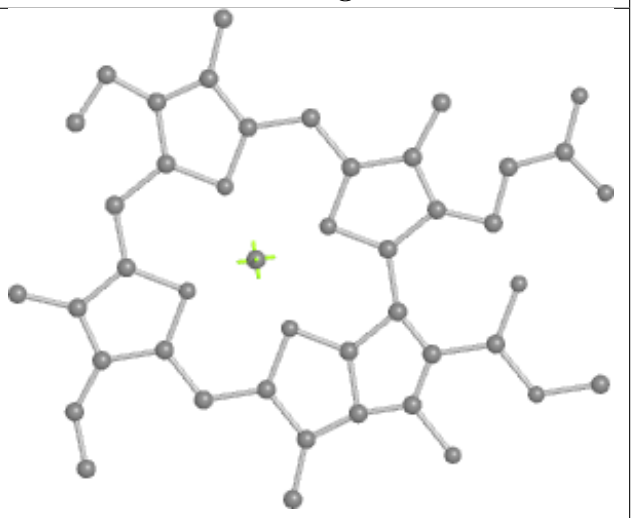
Bond lengths



Bond angles

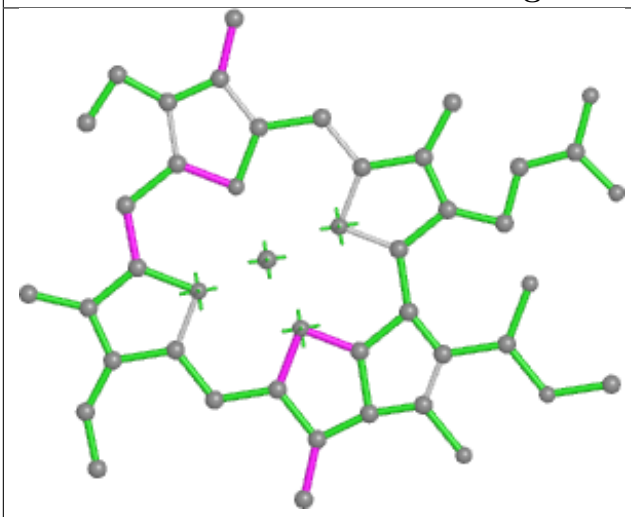


Torsions

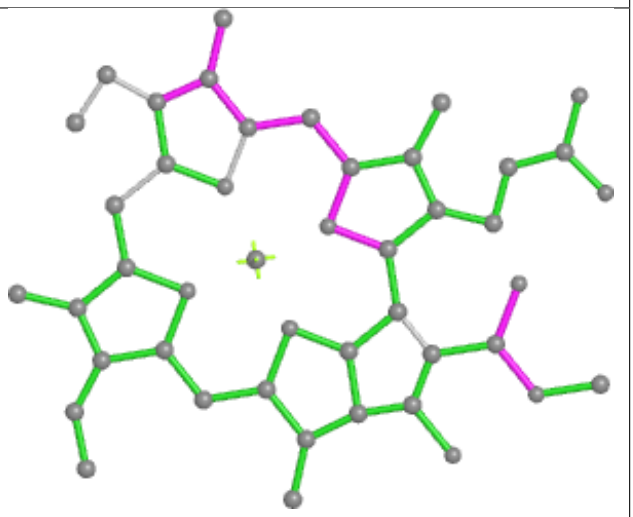


Rings

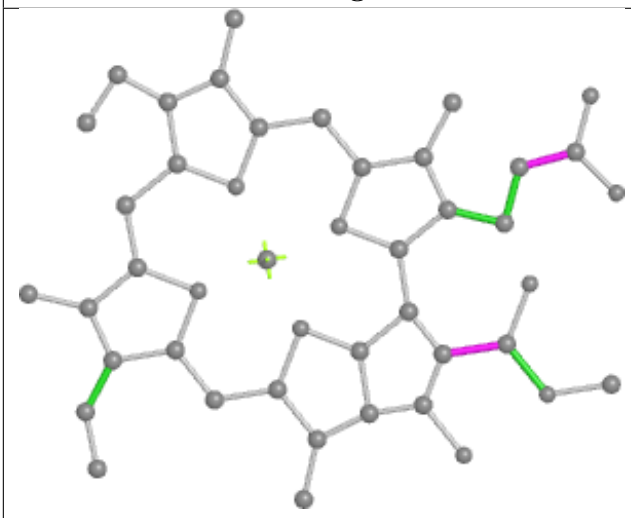
Ligand CLA A 840



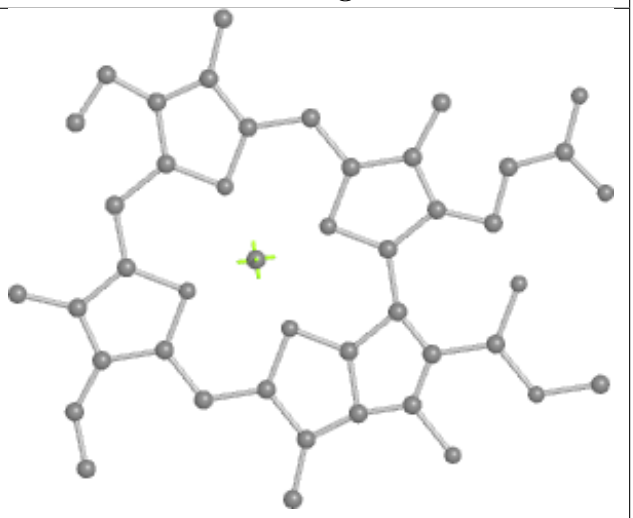
Bond lengths



Bond angles

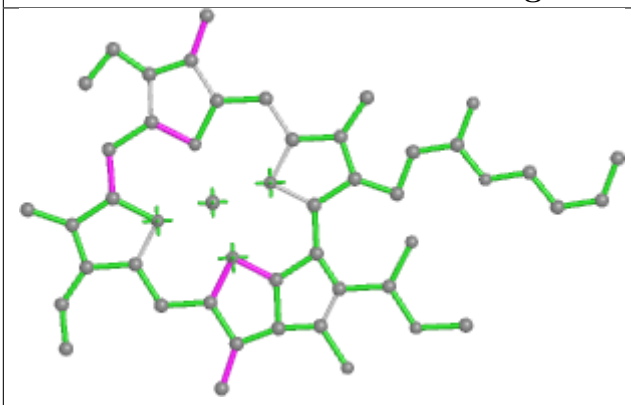


Torsions

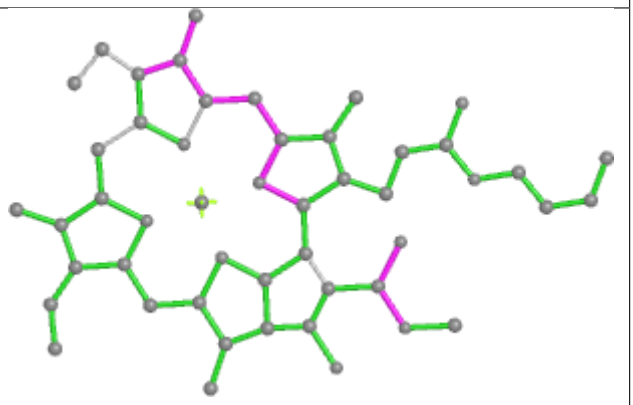


Rings

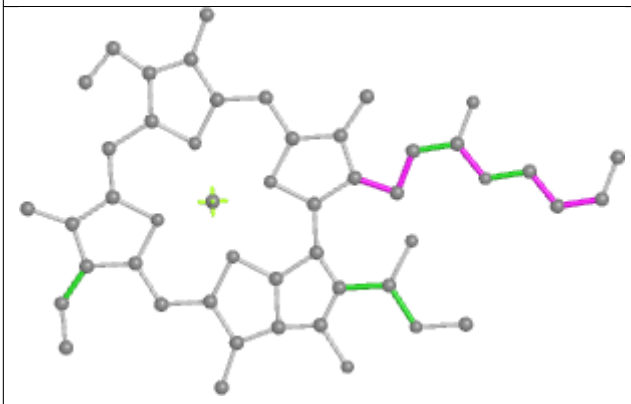
Ligand CLA B 831



Bond lengths



Bond angles



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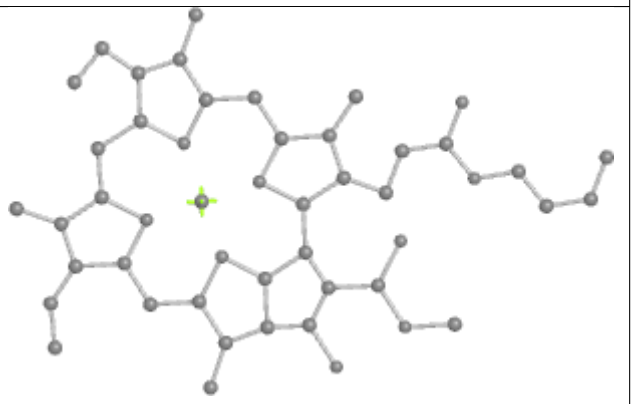
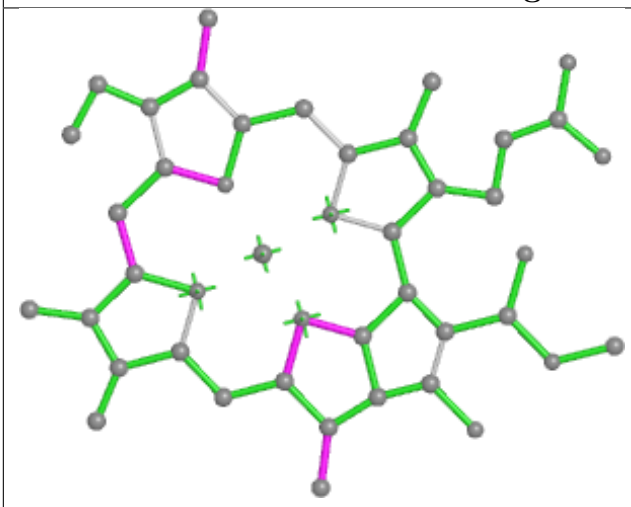
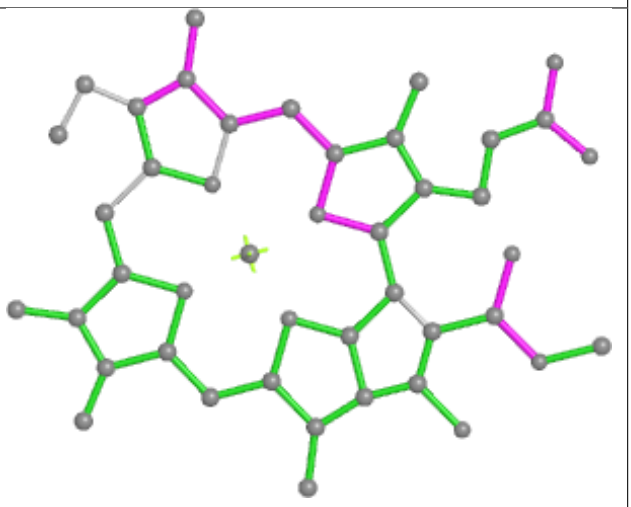


Rings

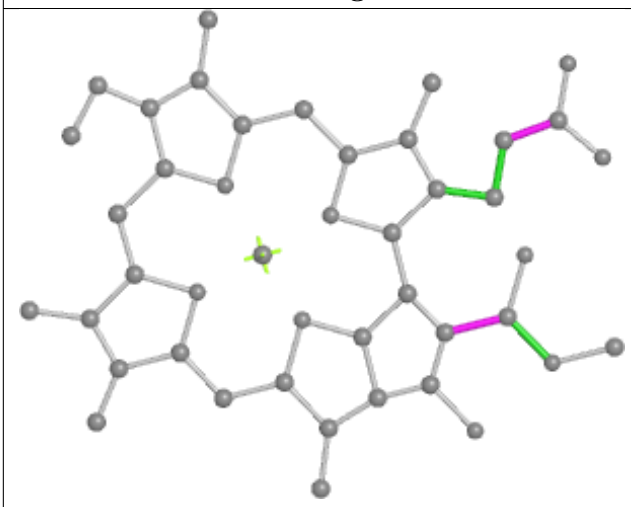
Ligand CLA A 821



Bond lengths



Bond angles



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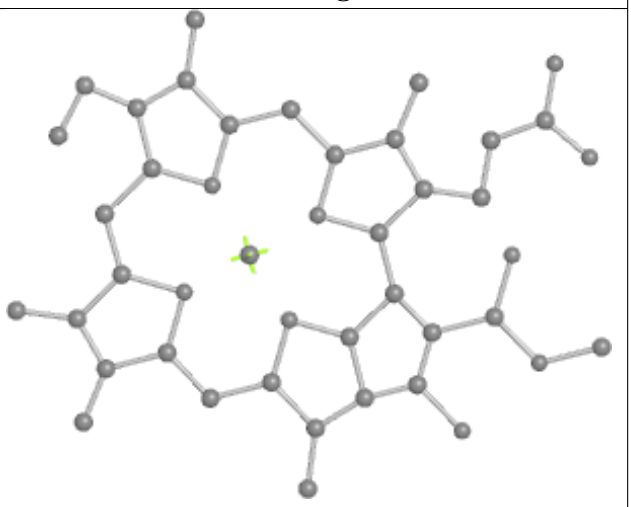
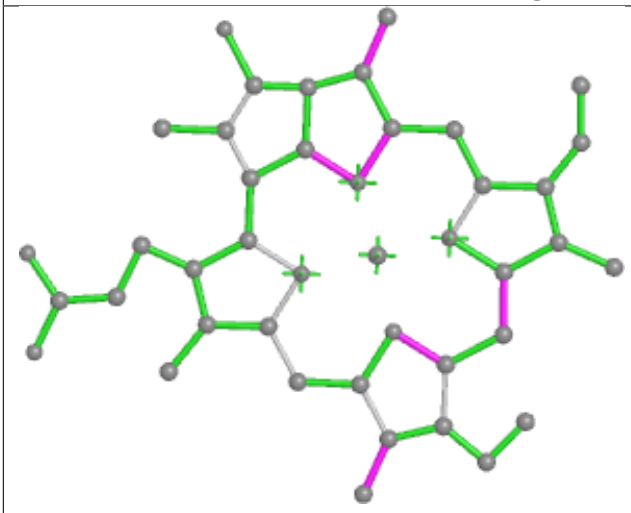


Rings

Ligand CLA 2 611



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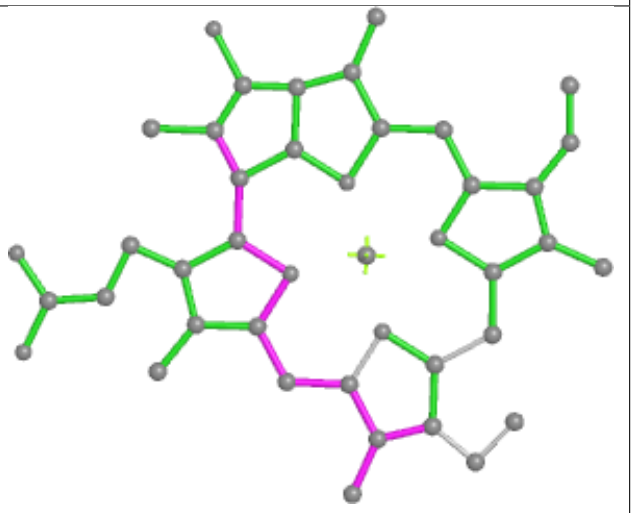
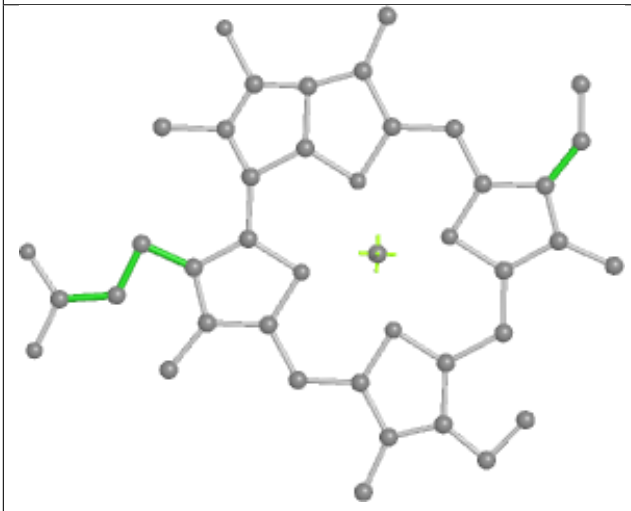
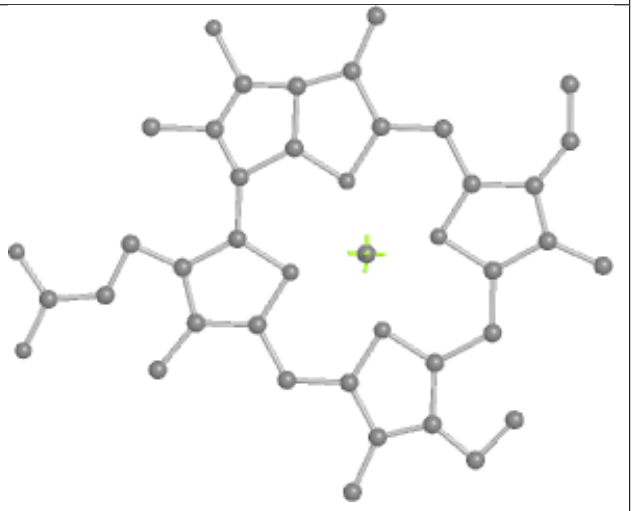


Bond angles

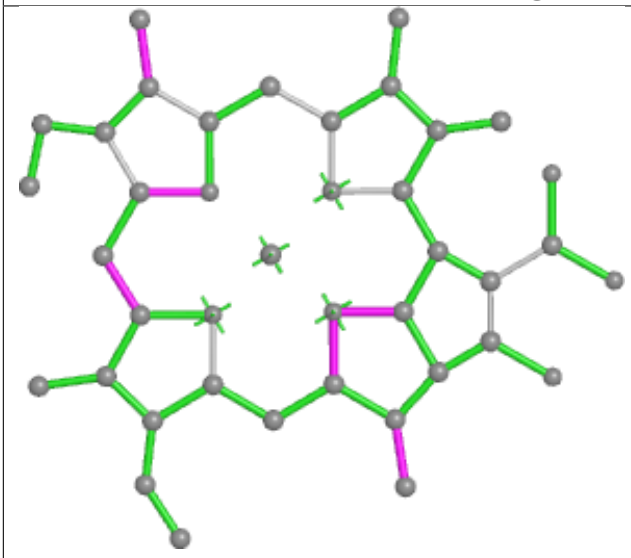


Torsions

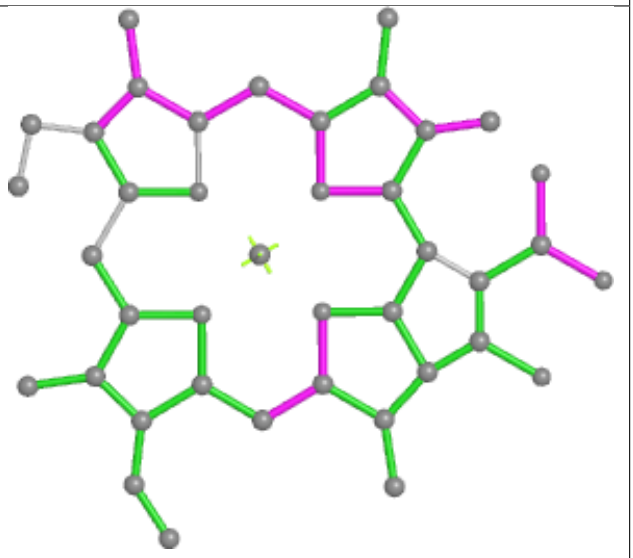


Rings

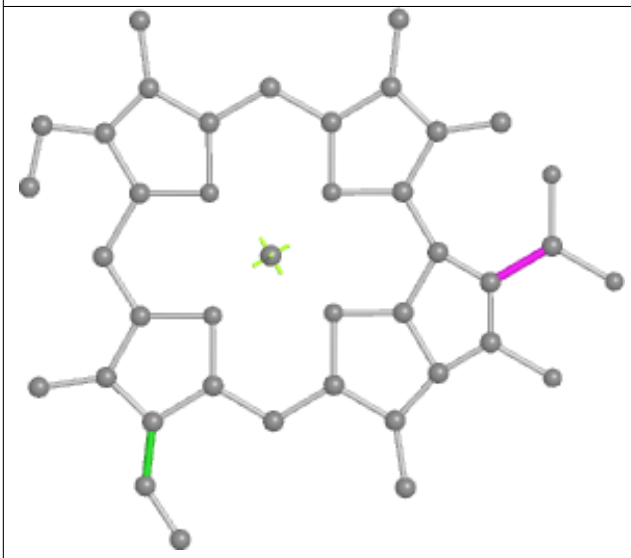
Ligand CLA 3 617



Bond lengths



Bond angles



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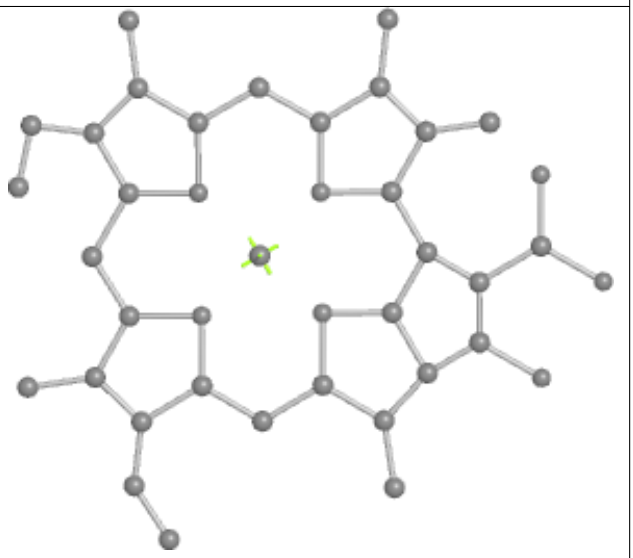
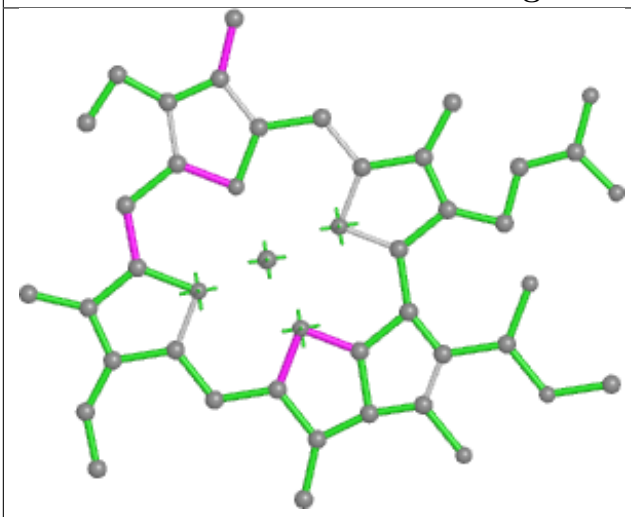
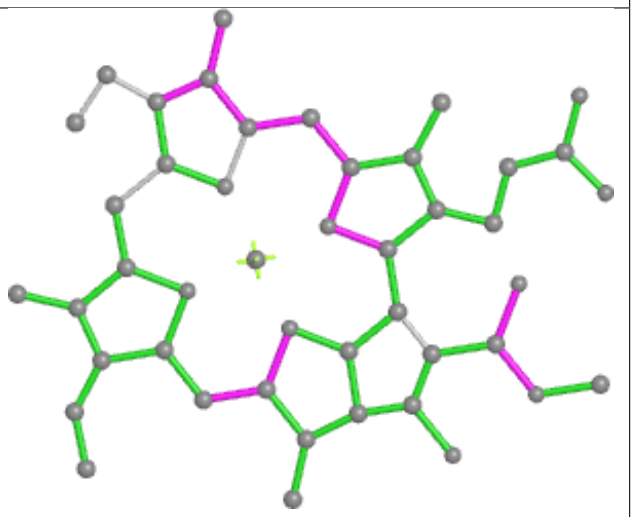


Rings

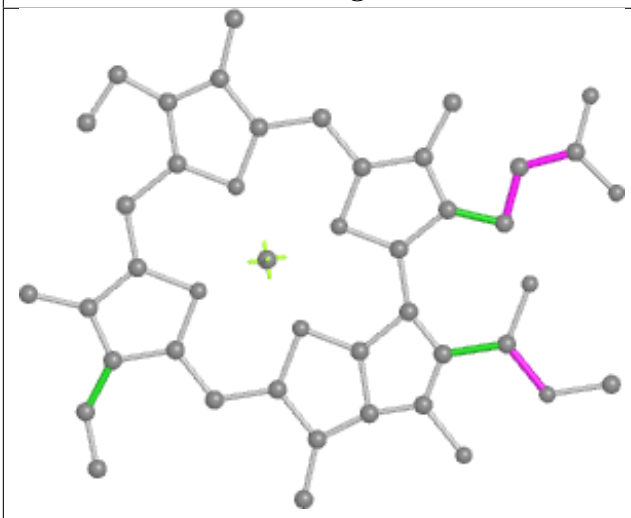
Ligand CLA G 201



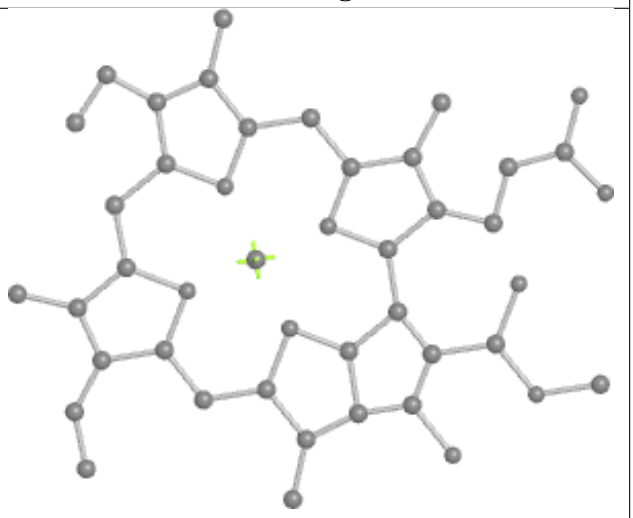
Bond lengths



Bond angles

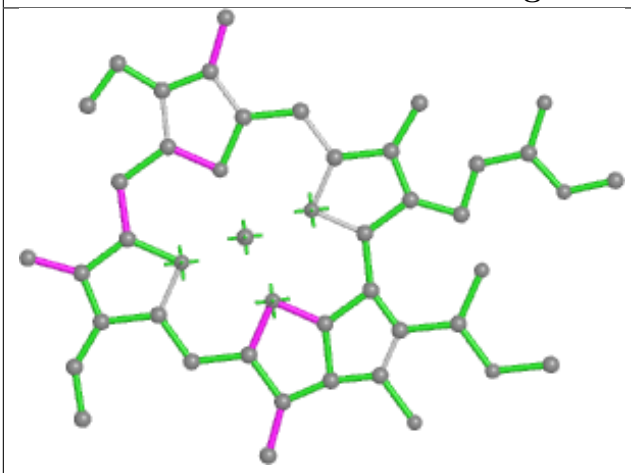


Torsions

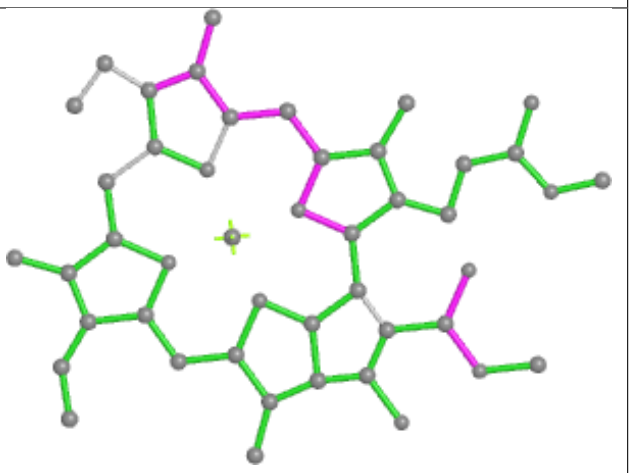


Rings

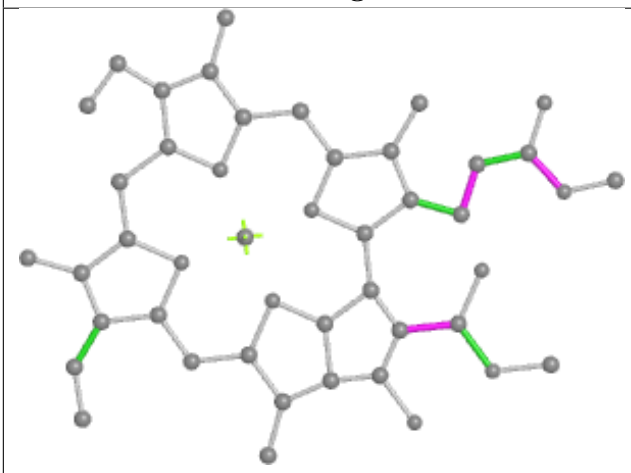
Ligand CLA A 828



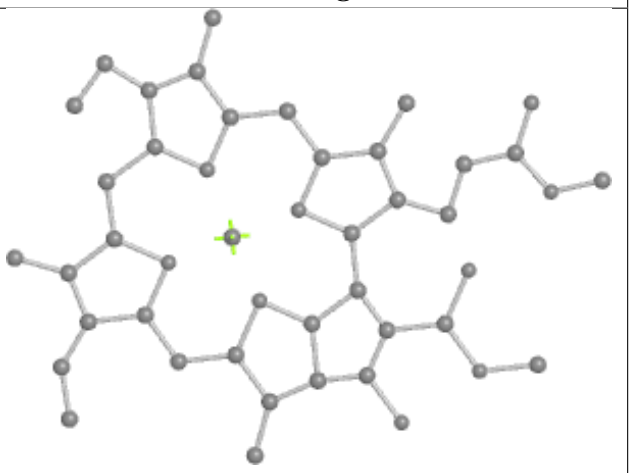
Bond lengths



Bond angles

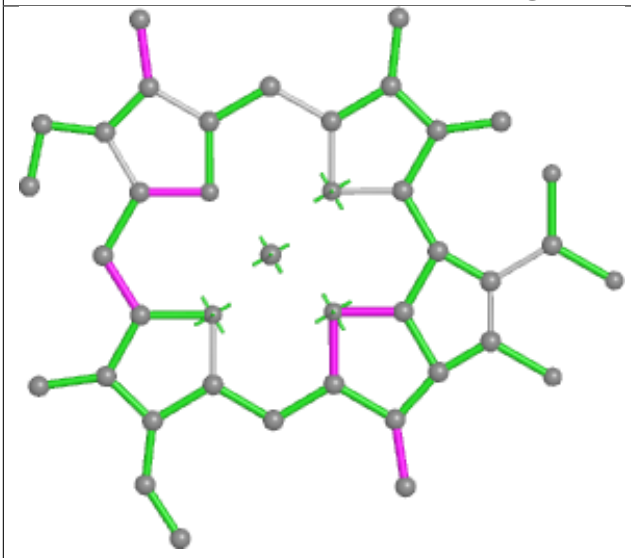


Torsions

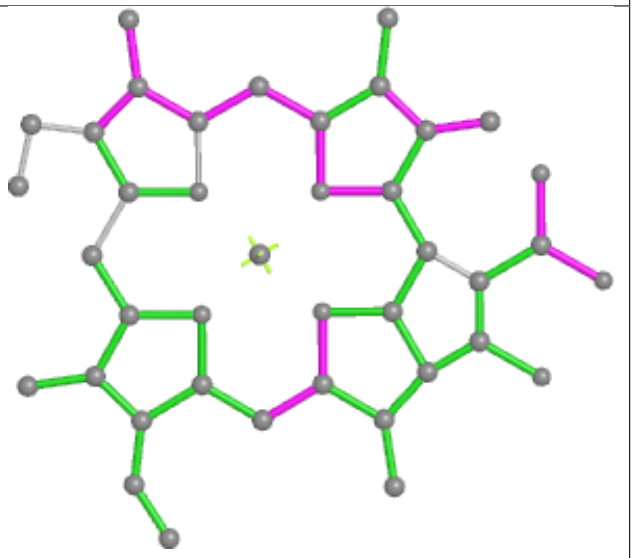


Rings

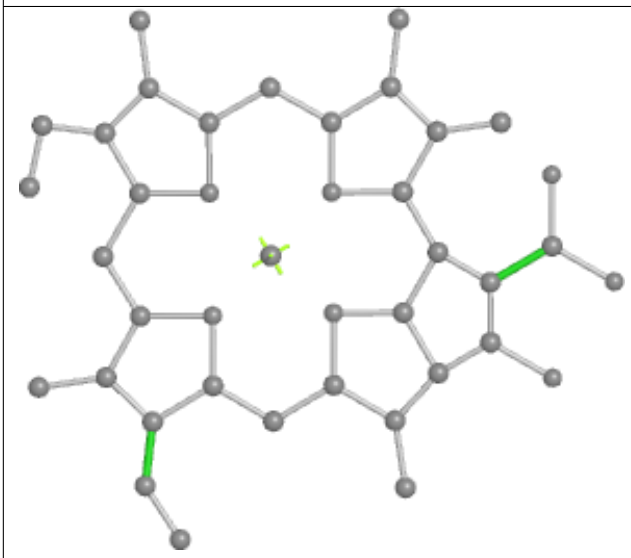
Ligand CLA A 817



Bond lengths



Bond angles



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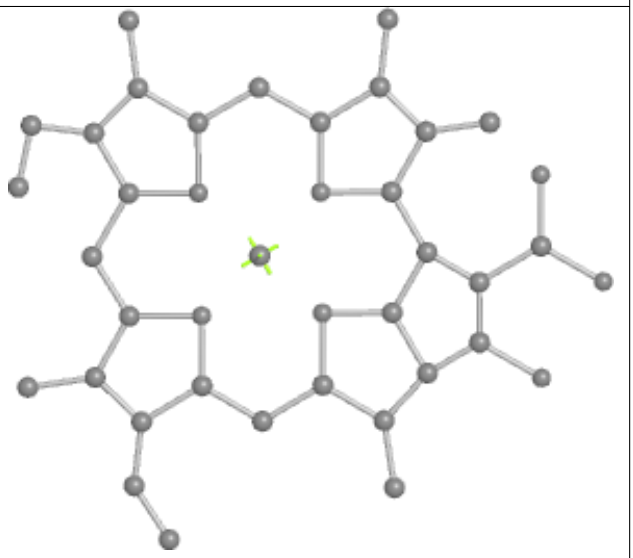
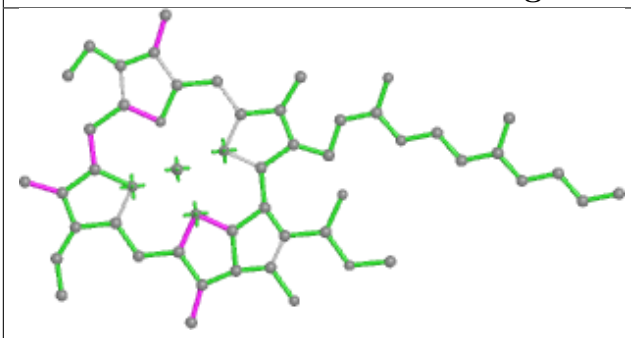
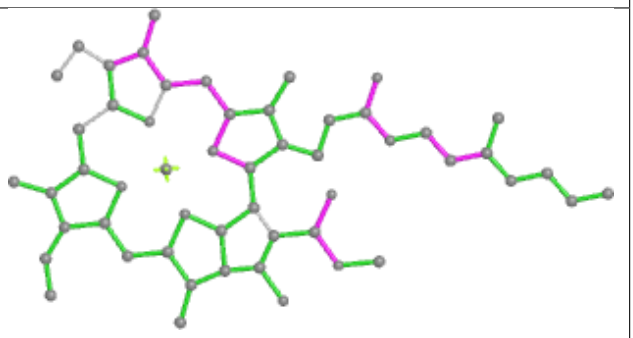


Rings

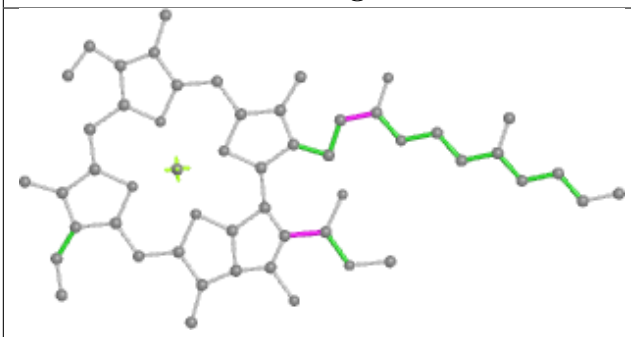
Ligand CLA B 802



Bond lengths



Bond angles



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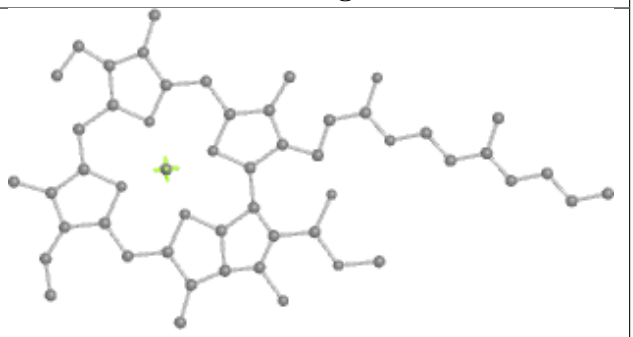
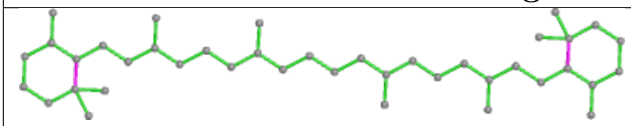
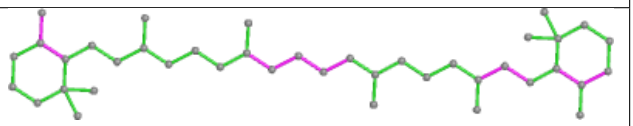


Rings

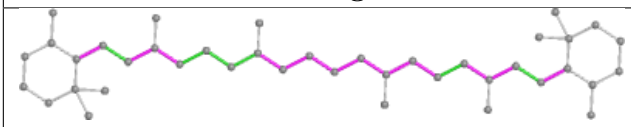
Ligand BCR B 845



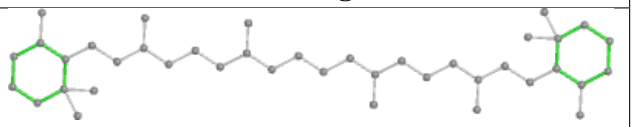
Bond lengths



Bond angles

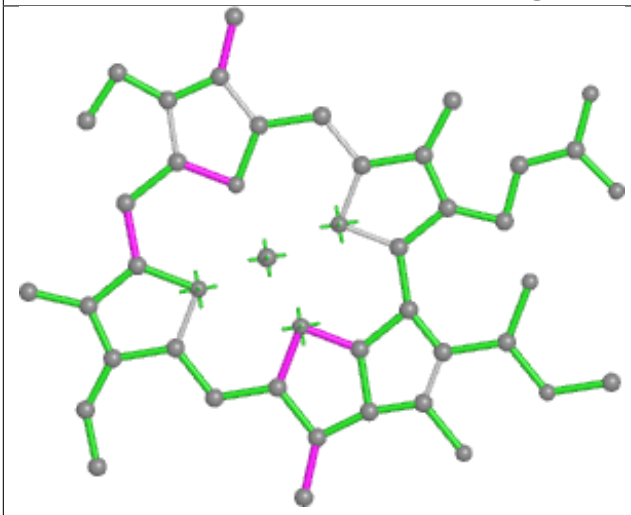


Torsions

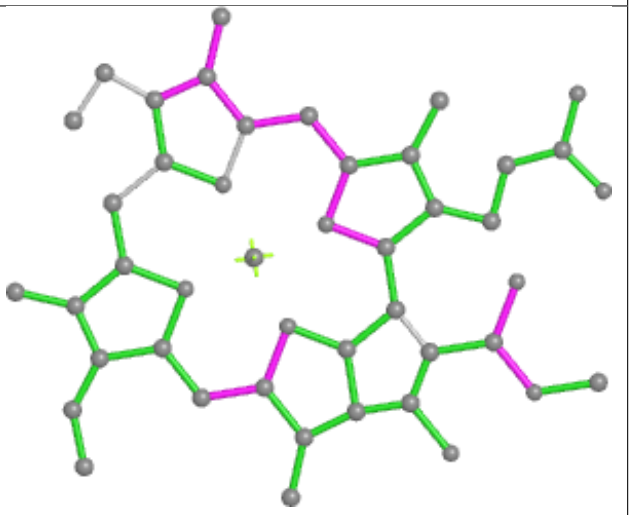


Rings

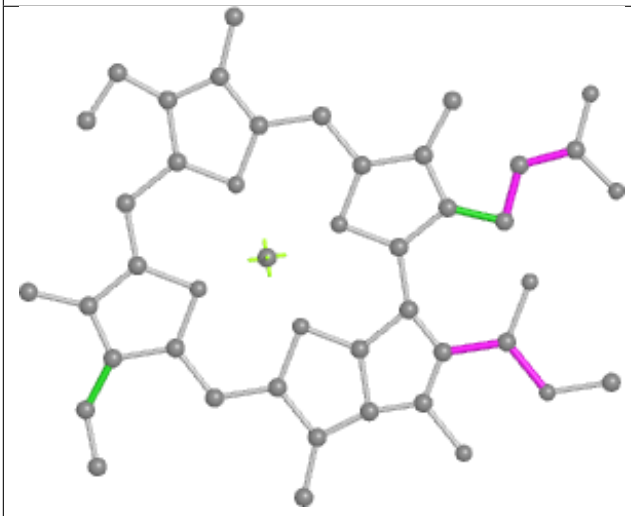
Ligand CLA 6 602



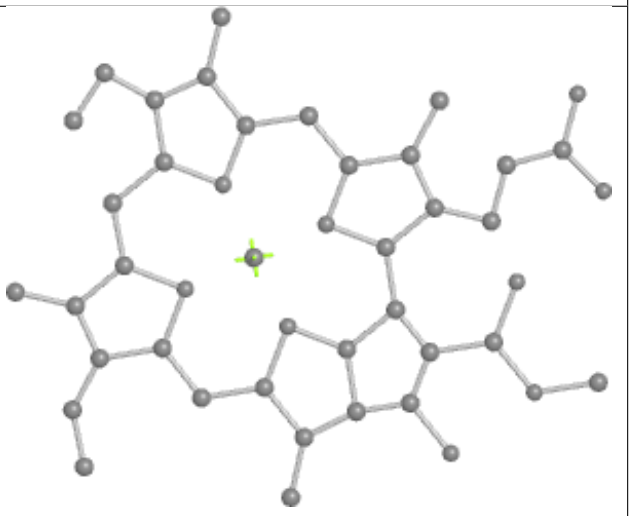
Bond lengths



Bond angles

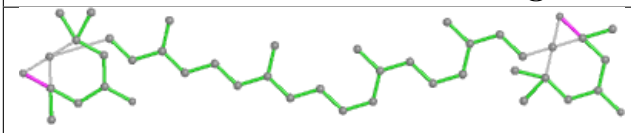


Torsions

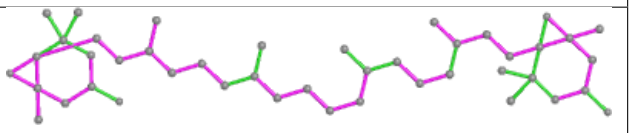


Rings

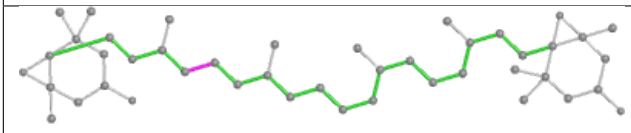
Ligand XAT 6 619



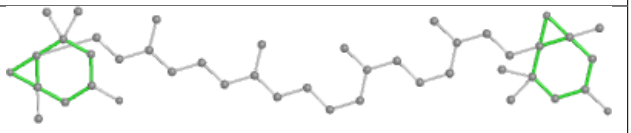
Bond lengths



Bond angles

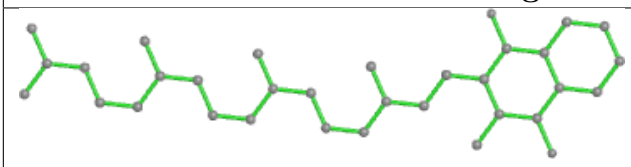


Torsions

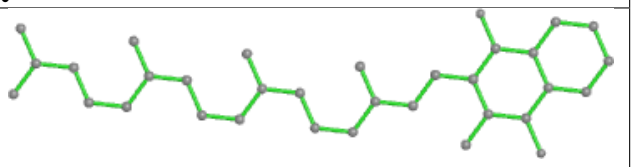


Rings

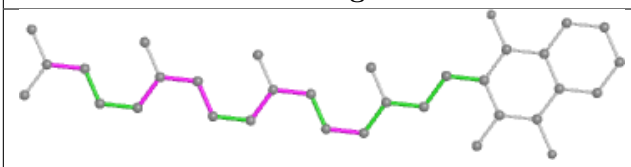
Ligand PQN B 842



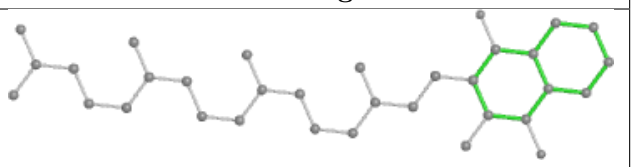
Bond lengths



Bond angles

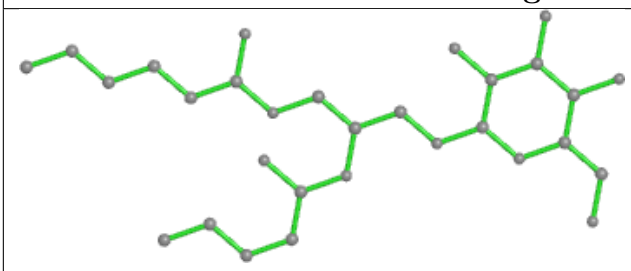


Torsions

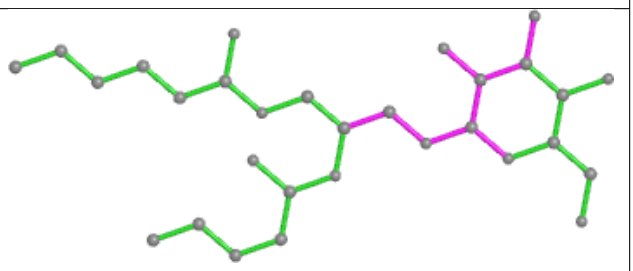


Rings

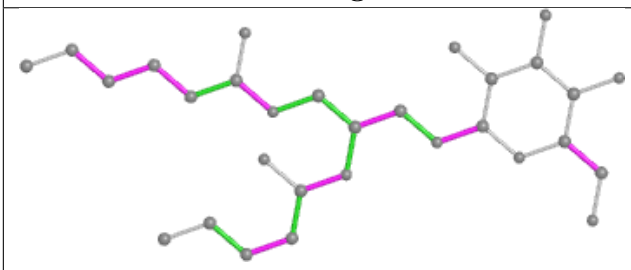
Ligand LMG J 104



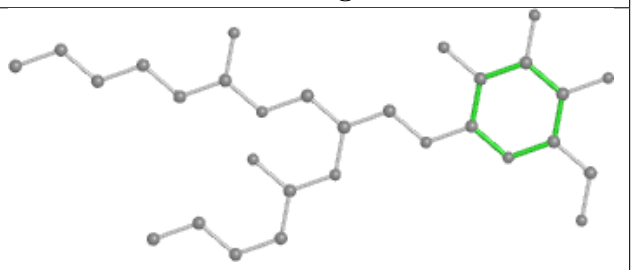
Bond lengths



Bond angles

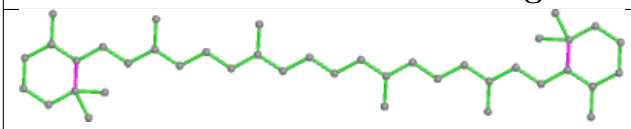


Torsions

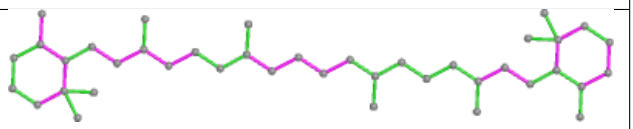


Rings

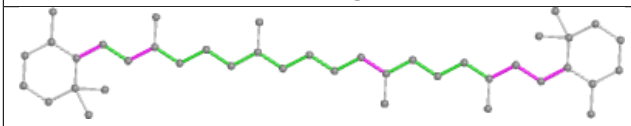
Ligand BCR L 305



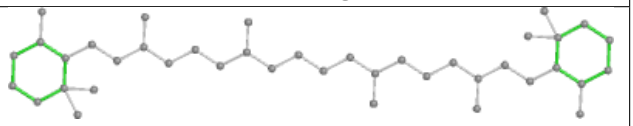
Bond lengths



Bond angles

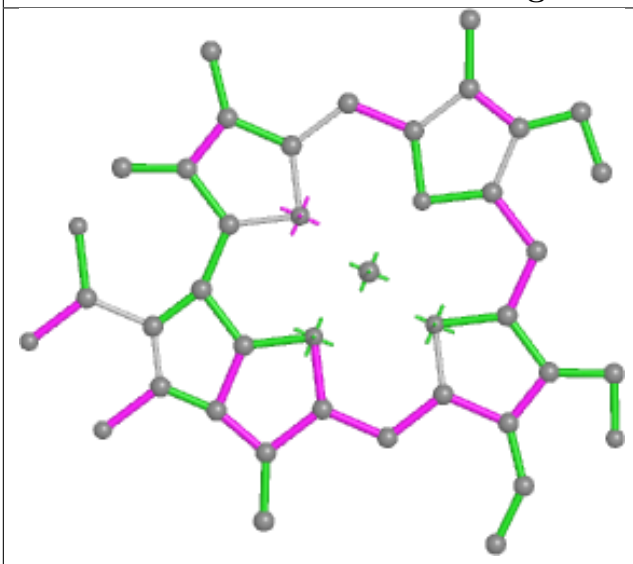


Torsions

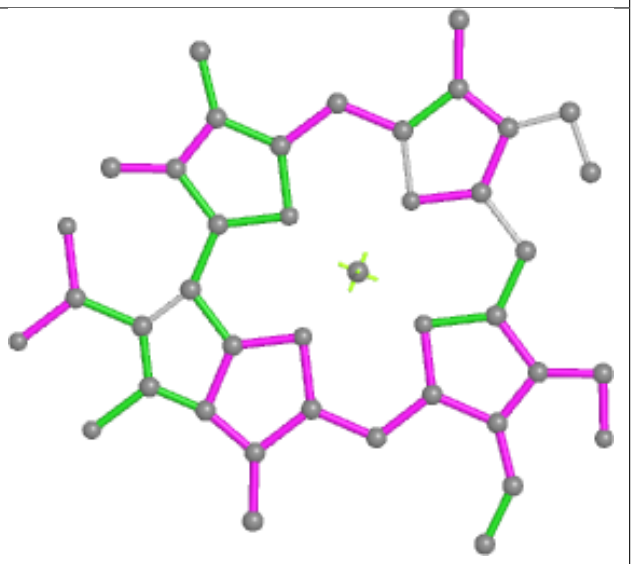


Rings

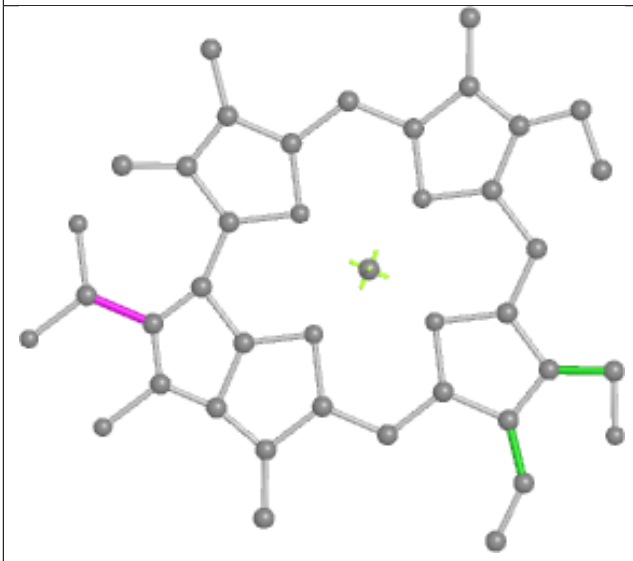
Ligand CHL 2 608



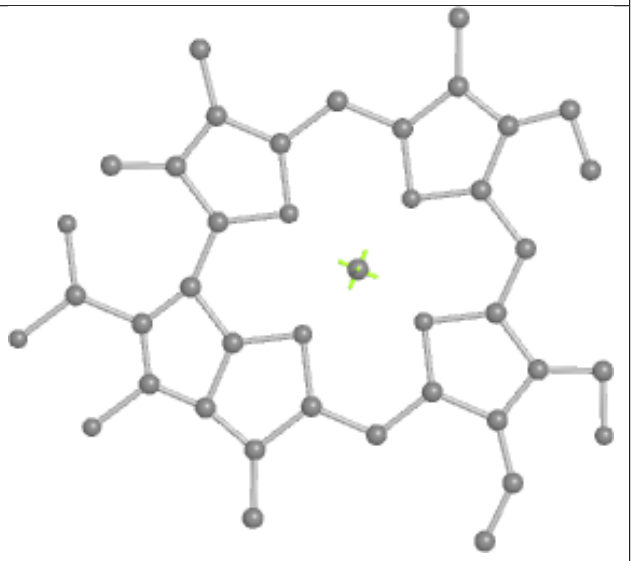
Bond lengths



Bond angles

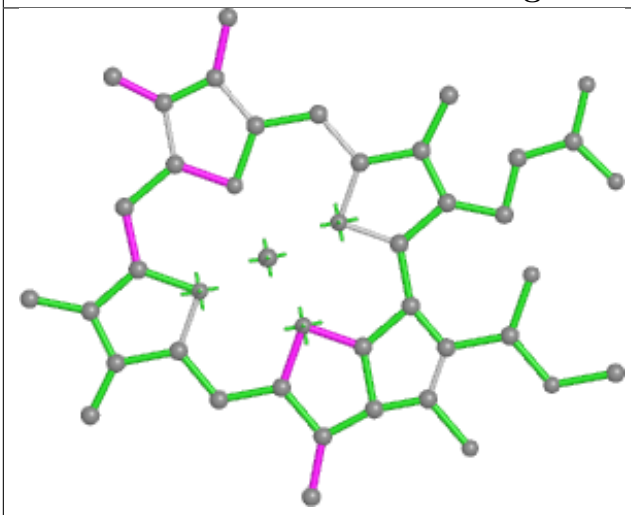


Torsions

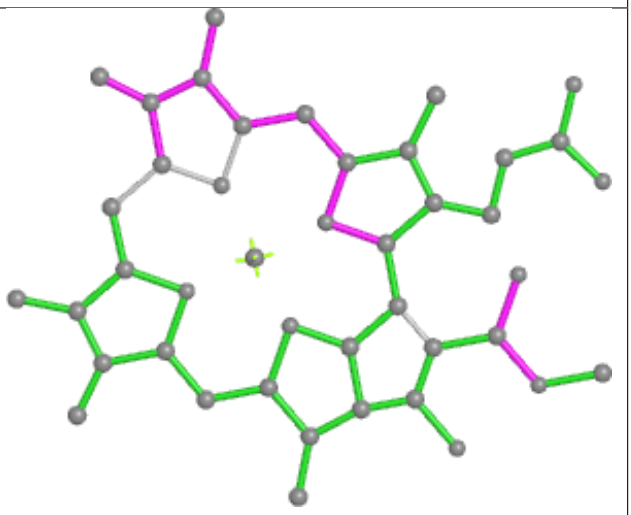


Rings

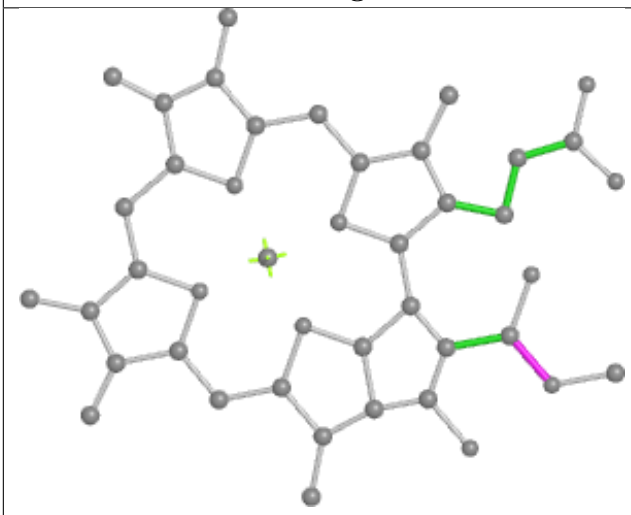
Ligand CLA A 822



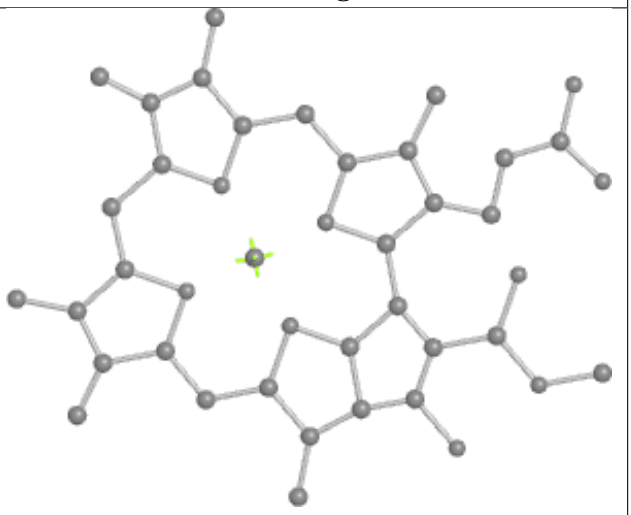
Bond lengths



Bond angles

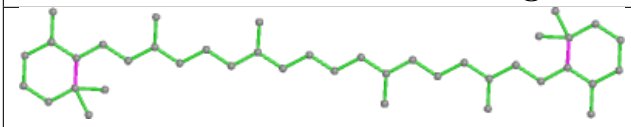


Torsions

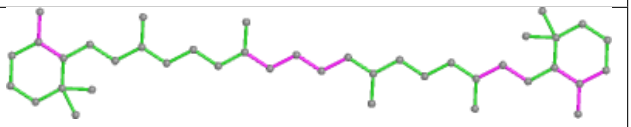


Rings

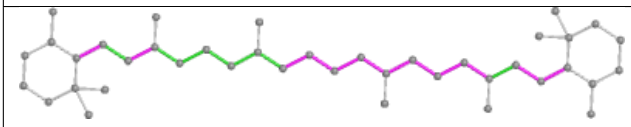
Ligand BCR B 846



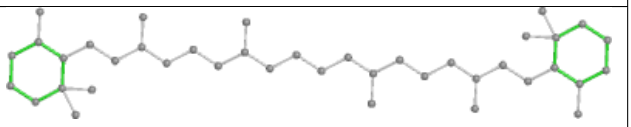
Bond lengths



Bond angles

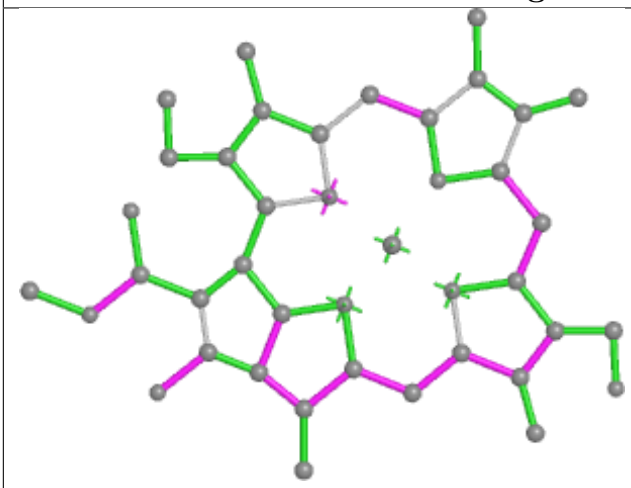


Torsions

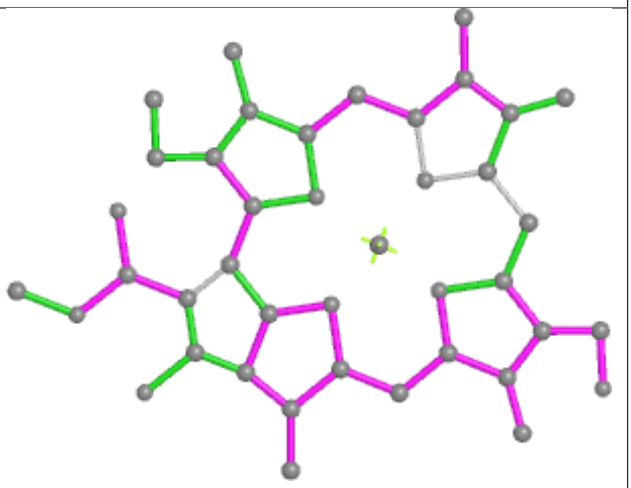


Rings

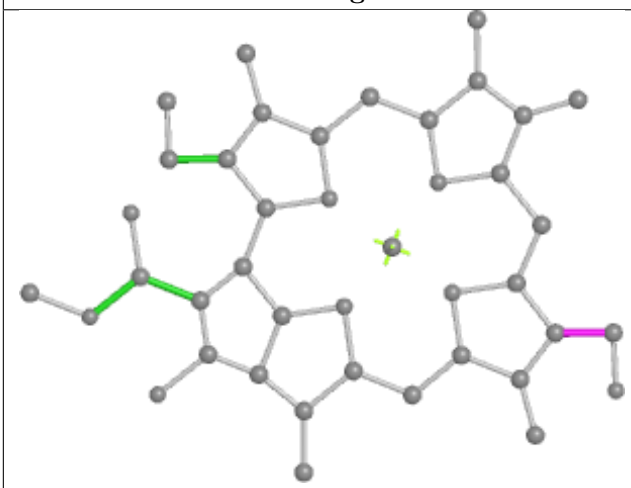
Ligand CHL 5 606



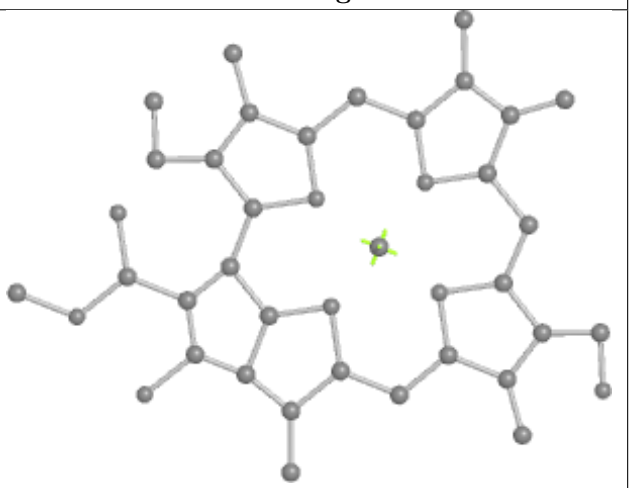
Bond lengths



Bond angles

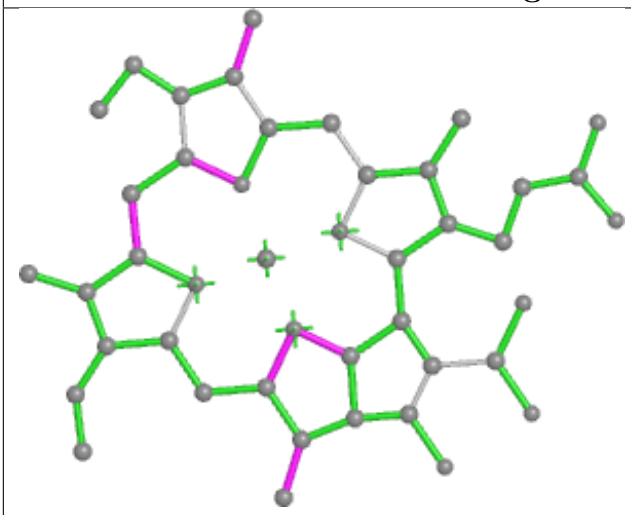


Torsions

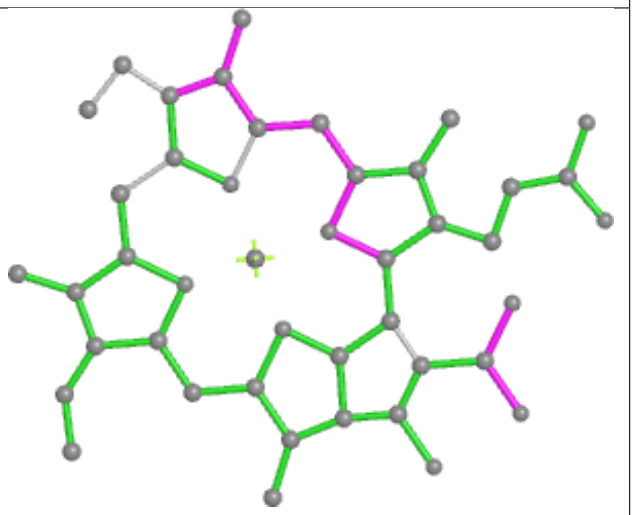


Rings

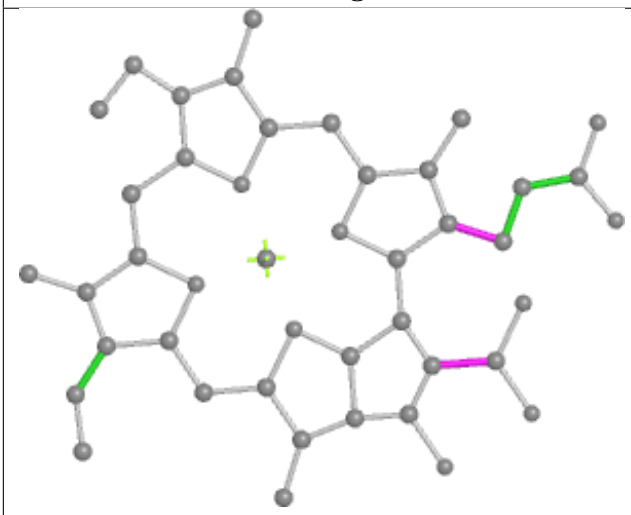
Ligand CLA A 807



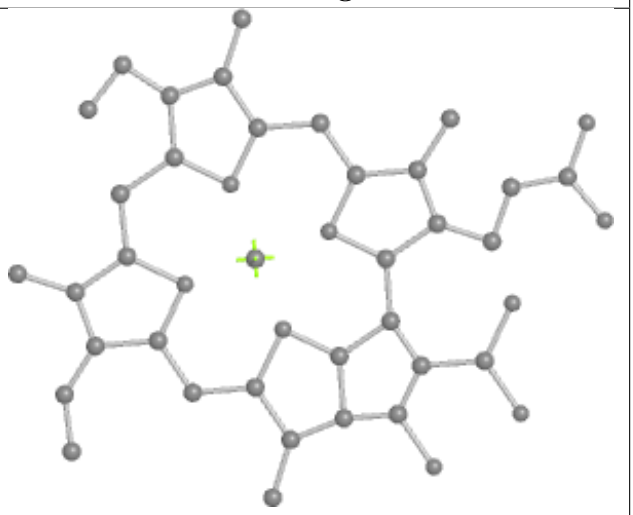
Bond lengths



Bond angles

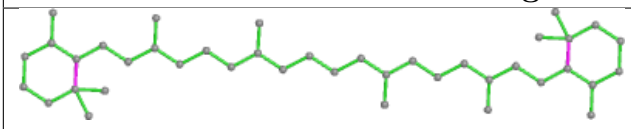


Torsions

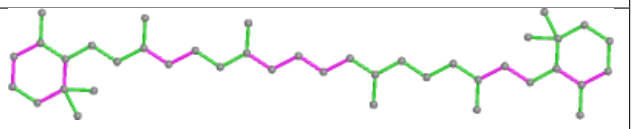


Rings

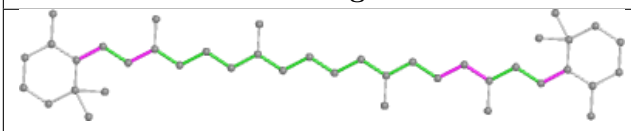
Ligand BCR A 856



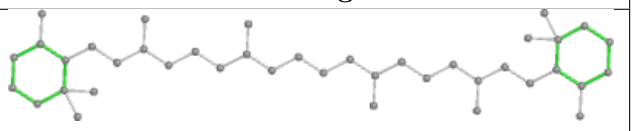
Bond lengths



Bond angles

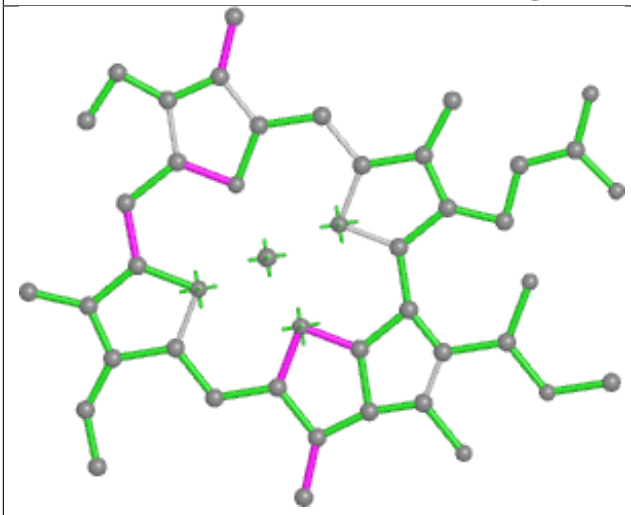


Torsions

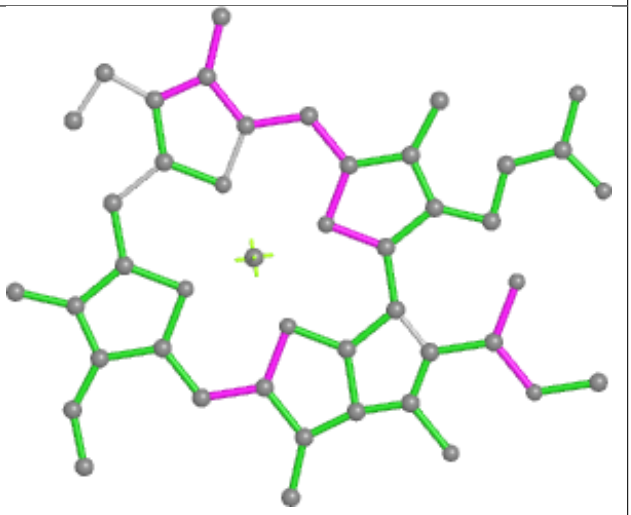


Rings

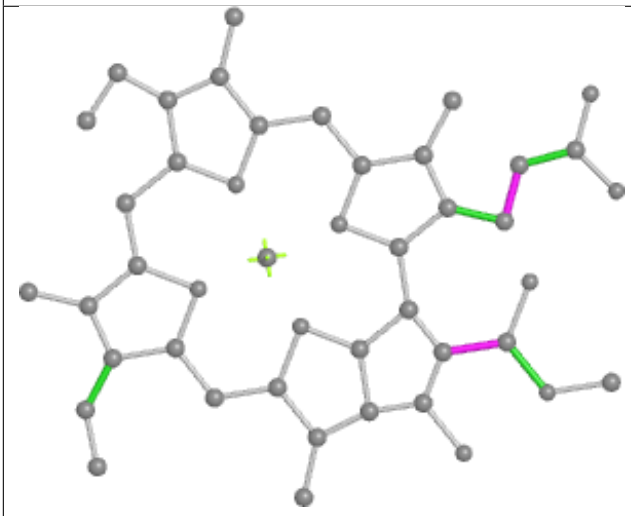
Ligand CLA L 302



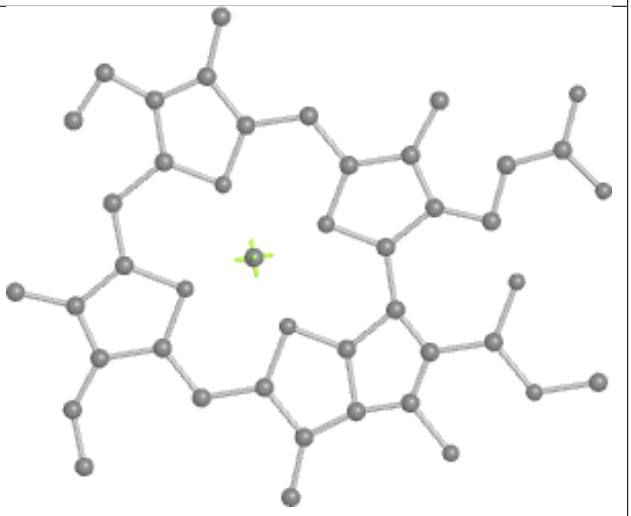
Bond lengths



Bond angles

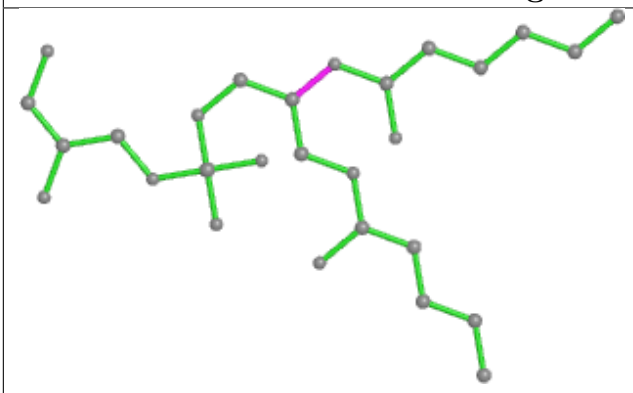


Torsions

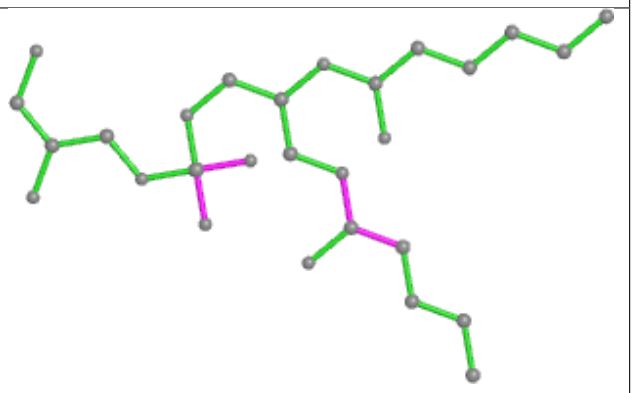


Rings

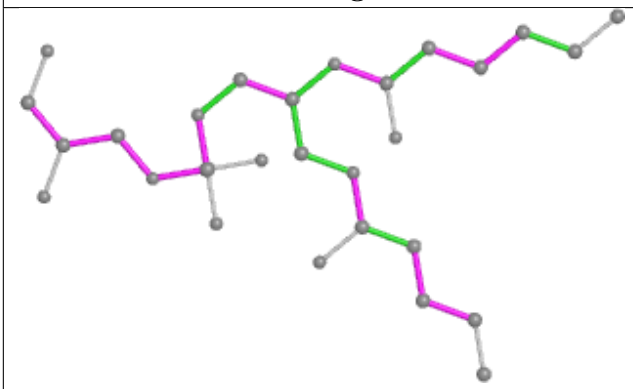
Ligand LHG 6 620



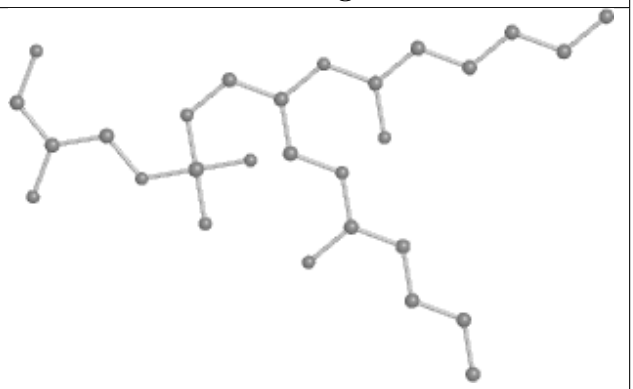
Bond lengths



Bond angles

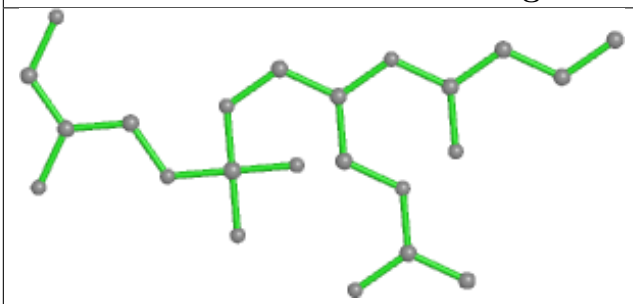


Torsions

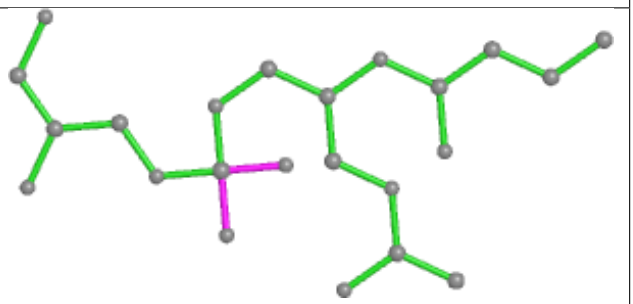


Rings

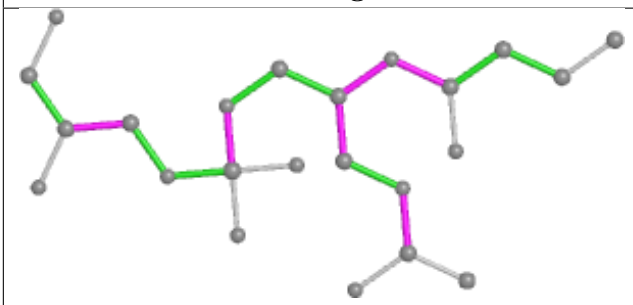
Ligand LHG B 851



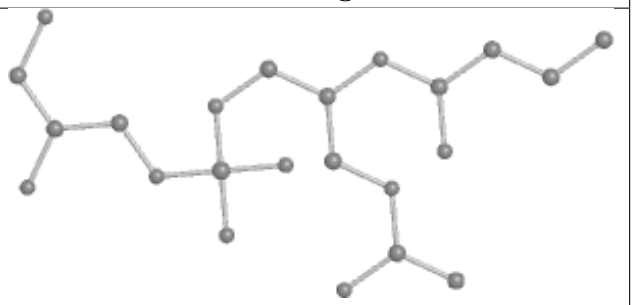
Bond lengths



Bond angles

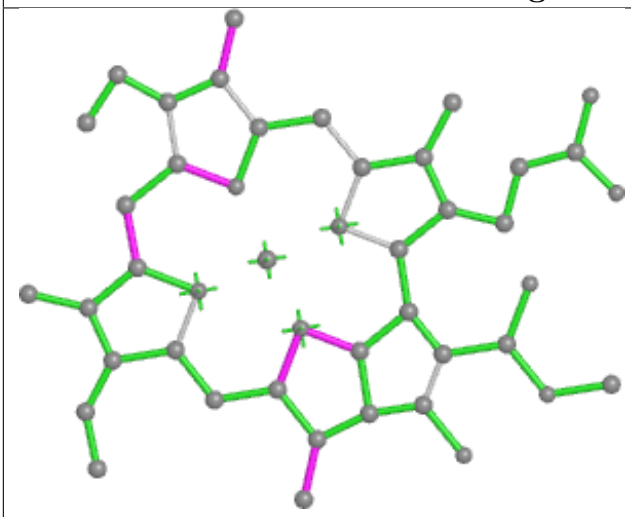


Torsions

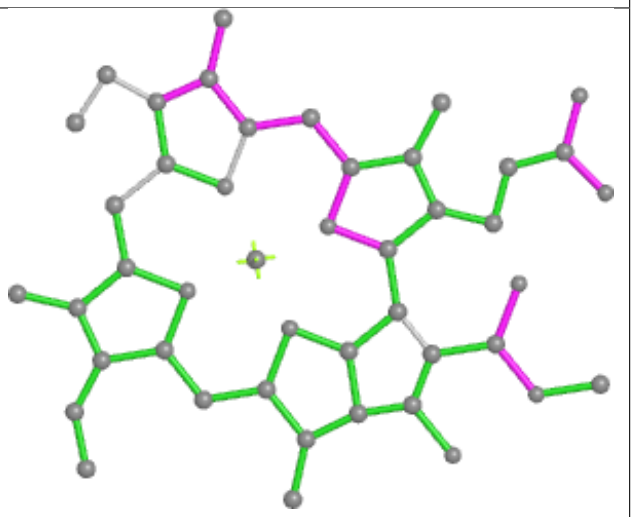


Rings

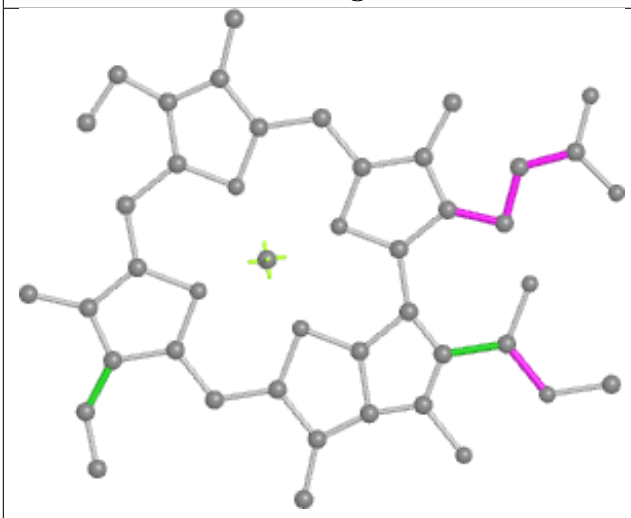
Ligand CLA 6 613



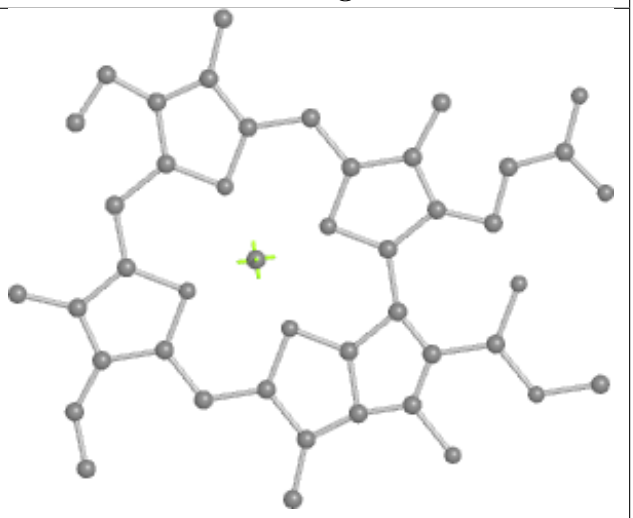
Bond lengths



Bond angles

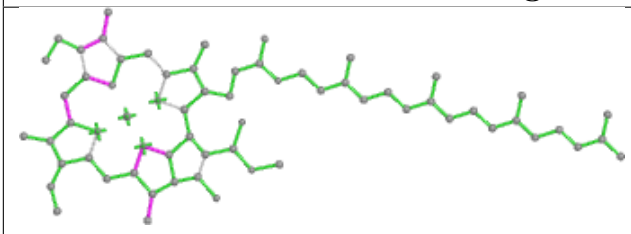


Torsions

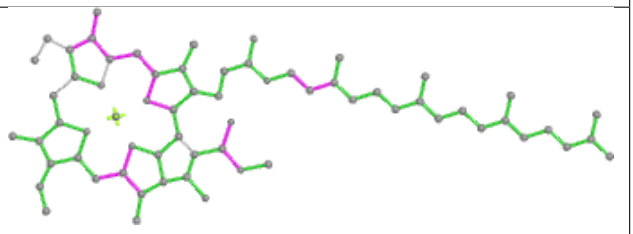


Rings

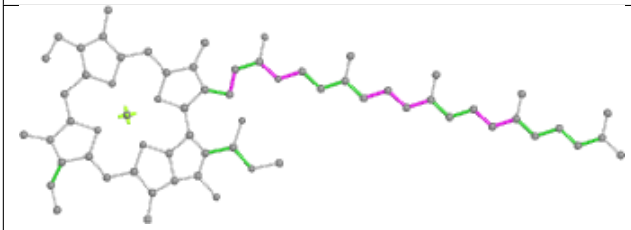
Ligand CLA A 843



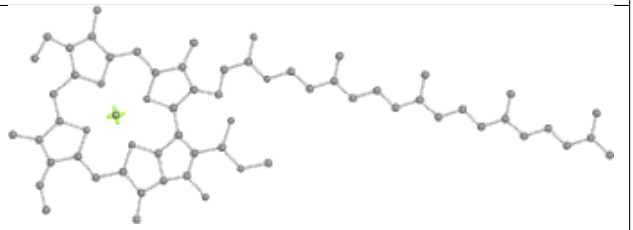
Bond lengths



Bond angles

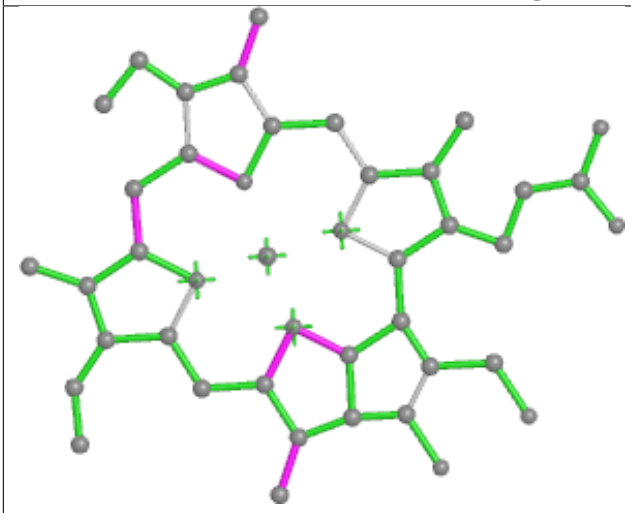


Torsions

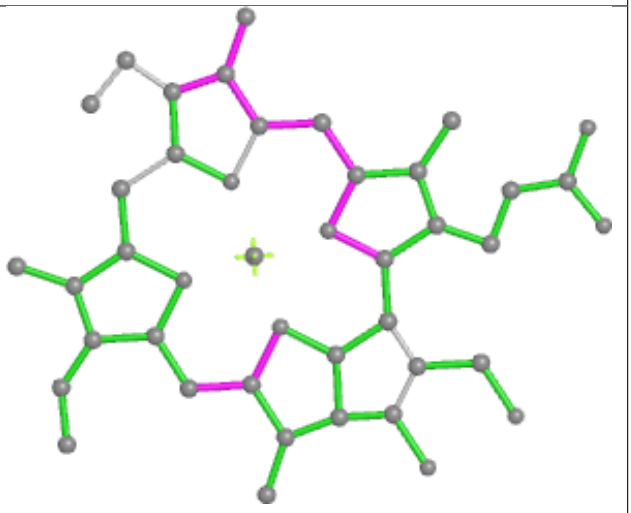


Rings

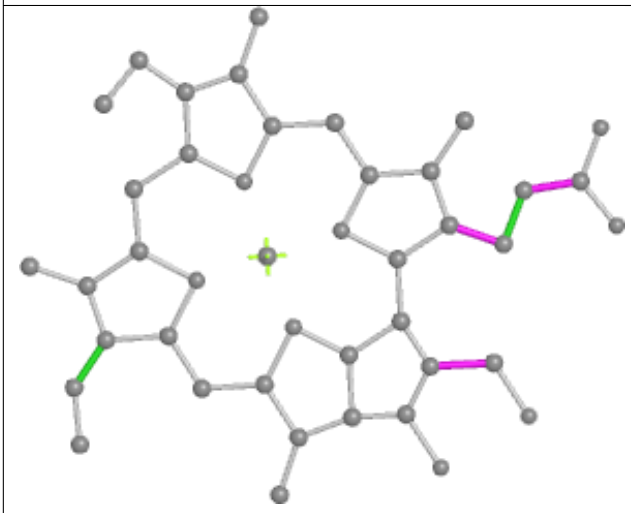
Ligand CLA 5 609



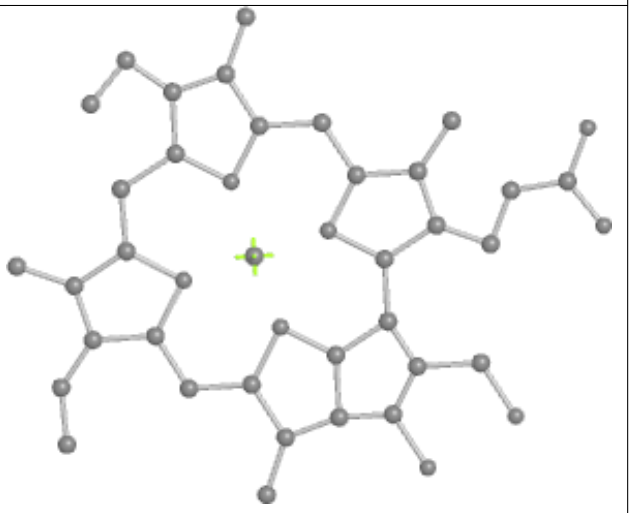
Bond lengths



Bond angles

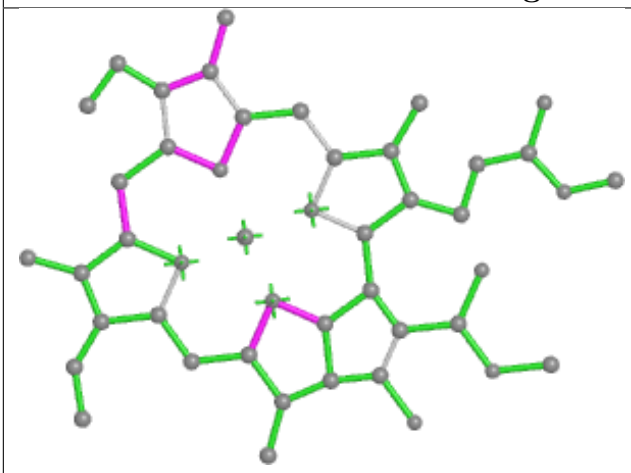


Torsions

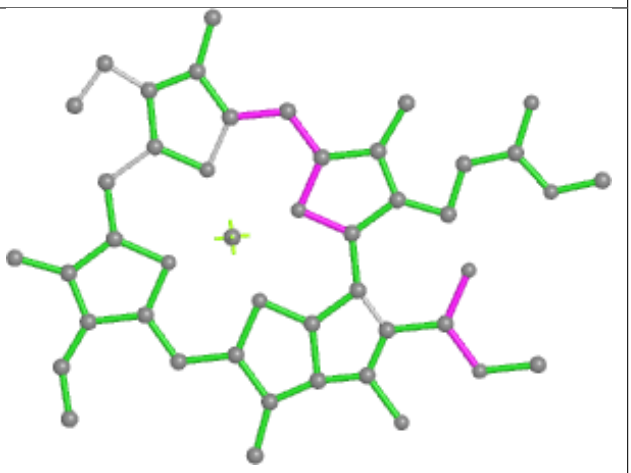


Rings

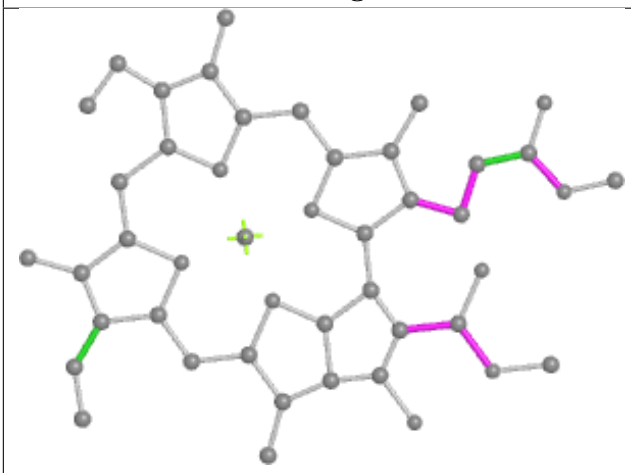
Ligand CLA K 201



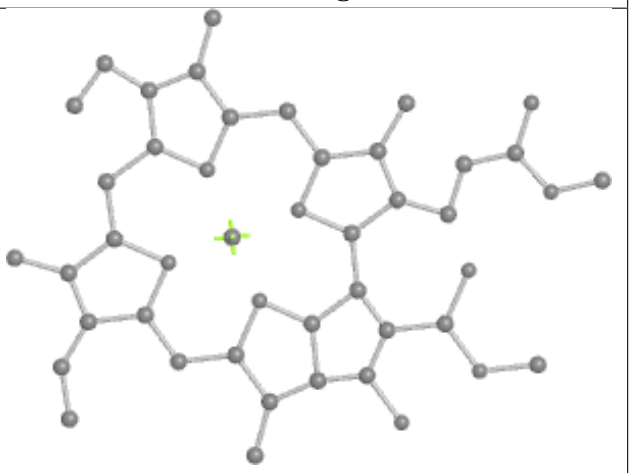
Bond lengths



Bond angles

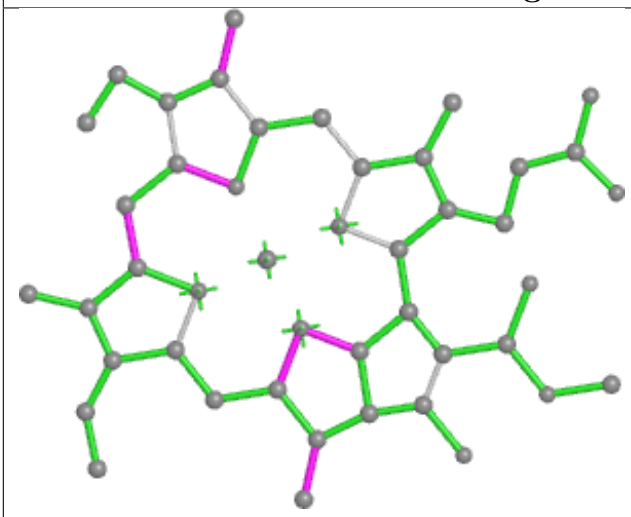


Torsions

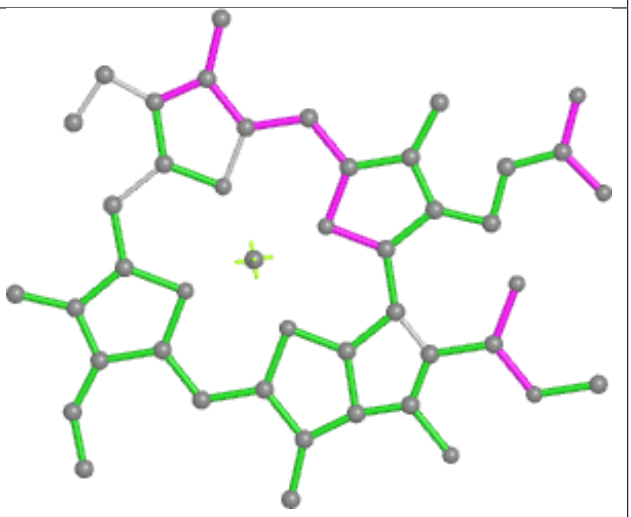


Rings

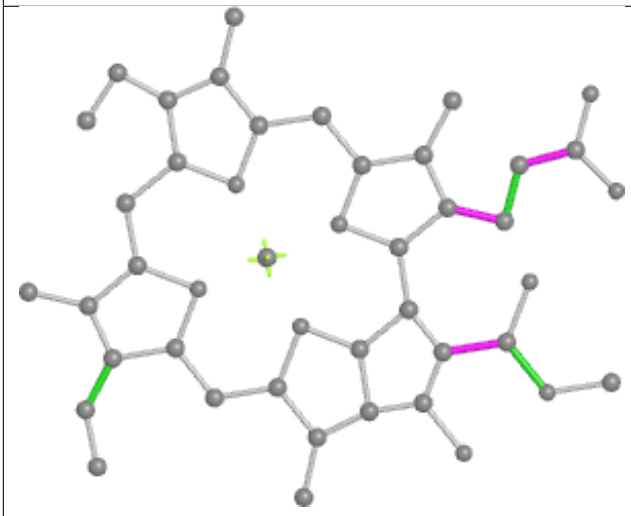
Ligand CLA A 810



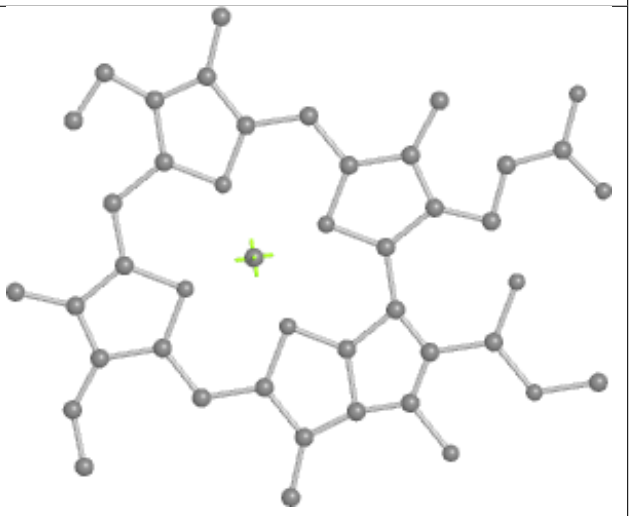
Bond lengths



Bond angles

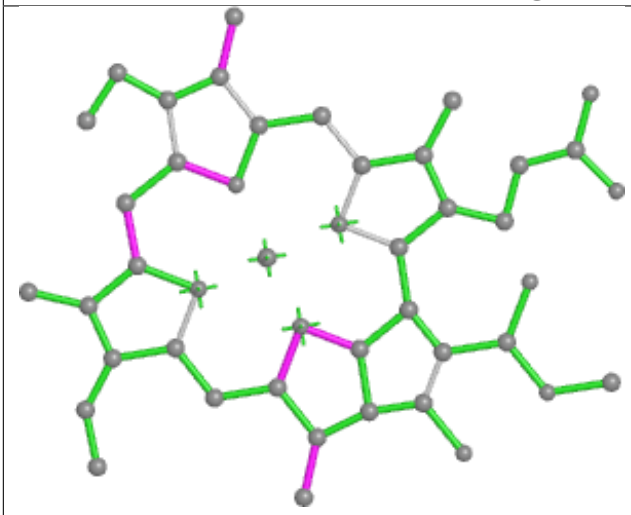


Torsions

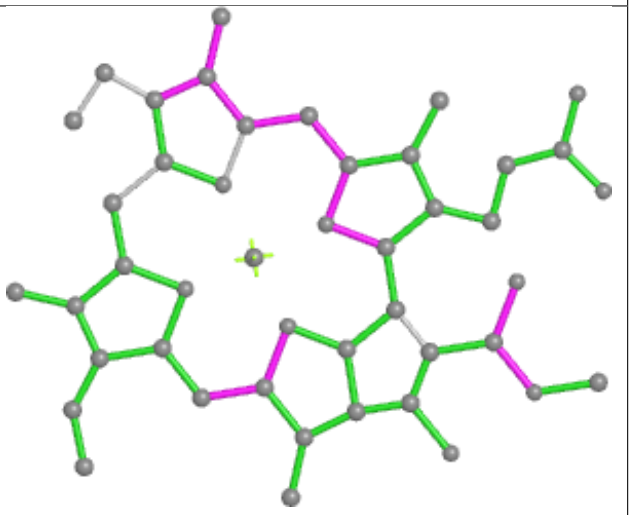


Rings

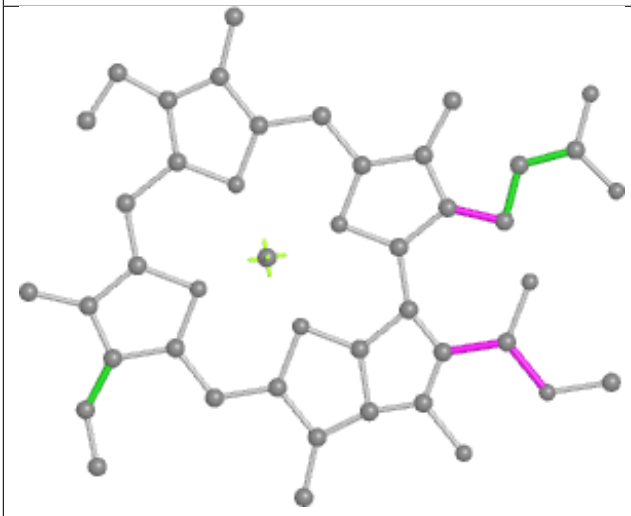
Ligand CLA 2 602



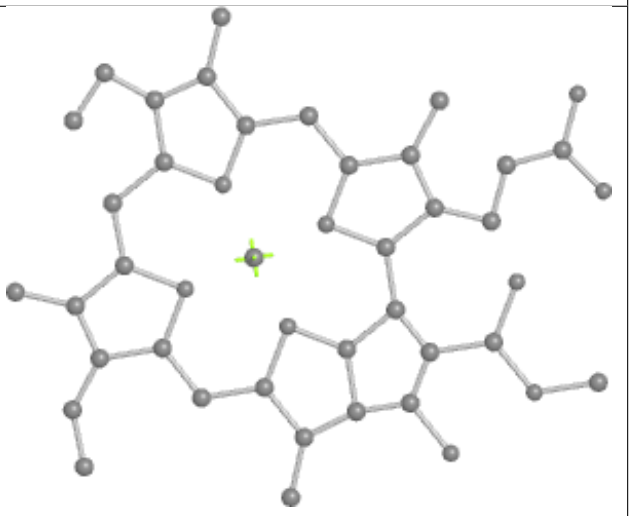
Bond lengths



Bond angles

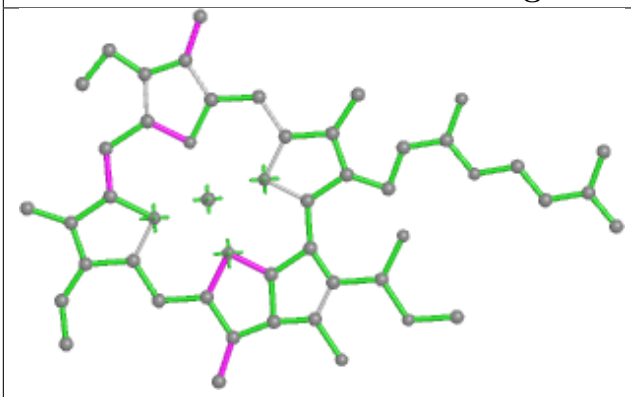


Torsions

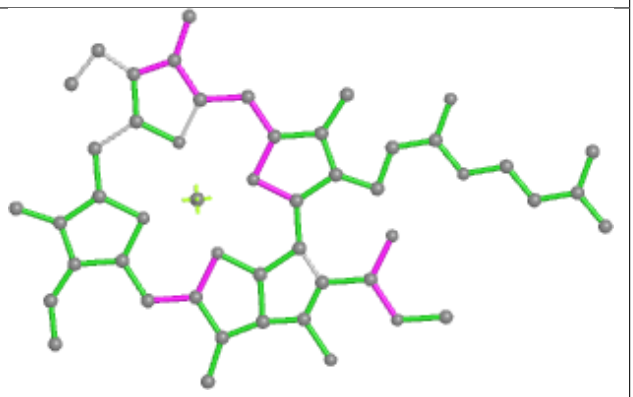


Rings

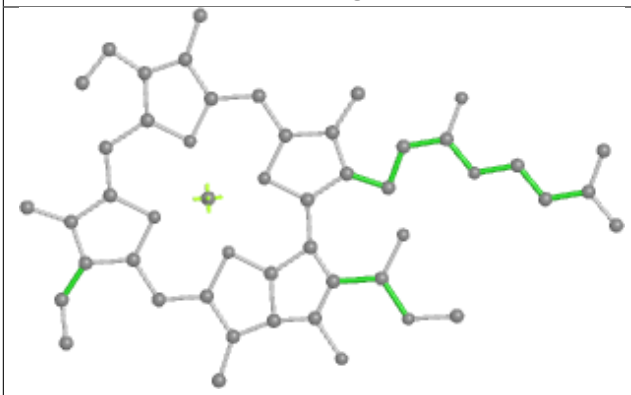
Ligand CLA A 836



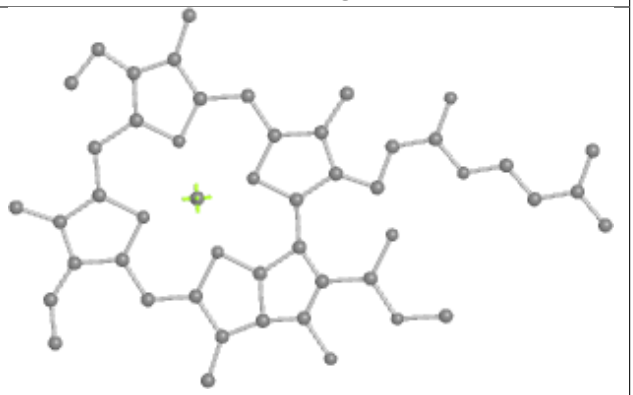
Bond lengths



Bond angles

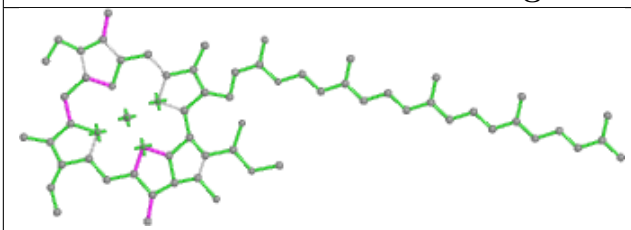


Torsions

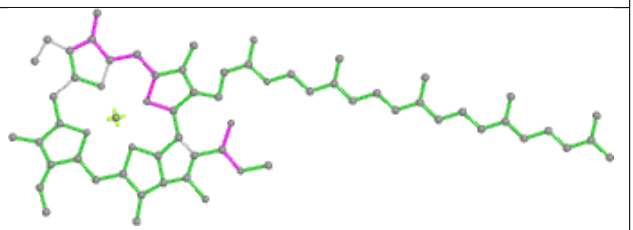


Rings

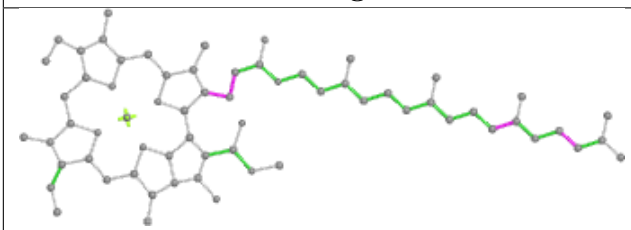
Ligand CLA A 830



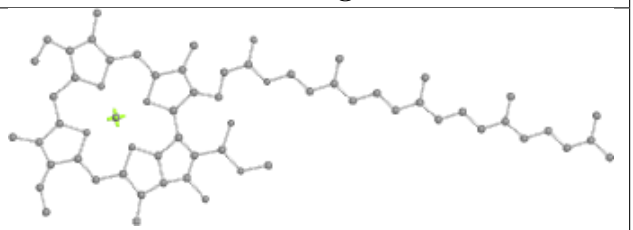
Bond lengths



Bond angles

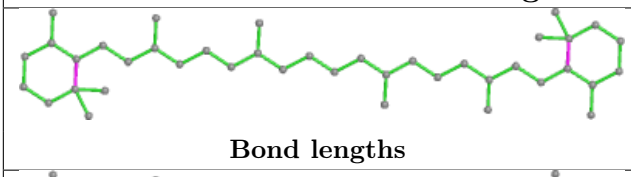


Torsions

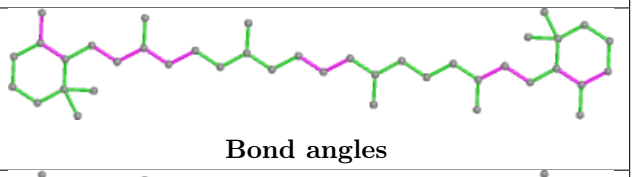


Rings

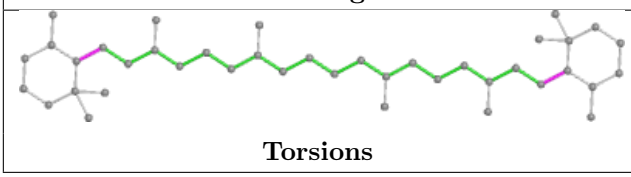
Ligand BCR A 850



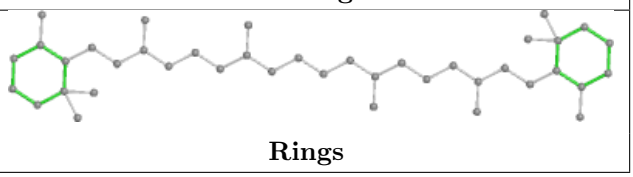
Bond lengths



Bond angles

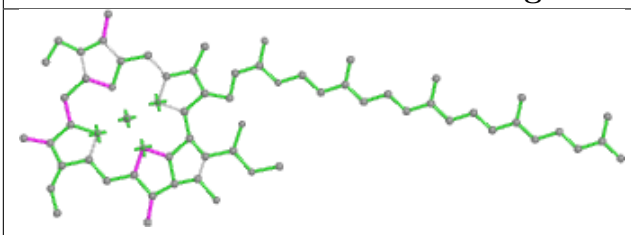


Torsions

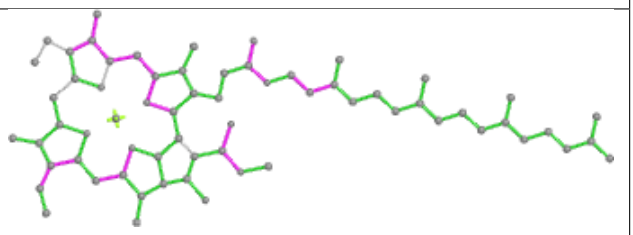


Rings

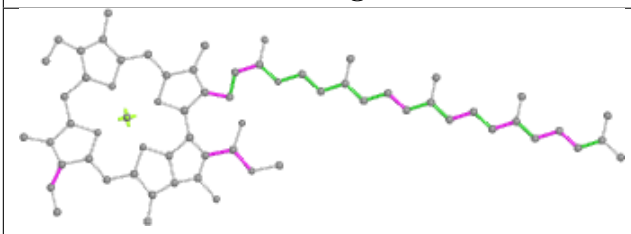
Ligand CLA B 813



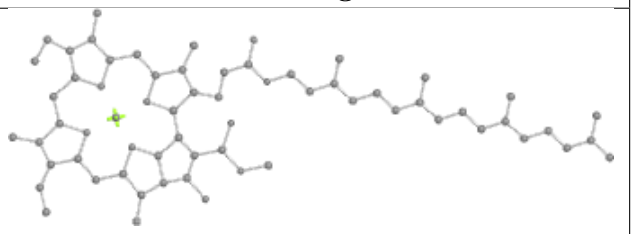
Bond lengths



Bond angles

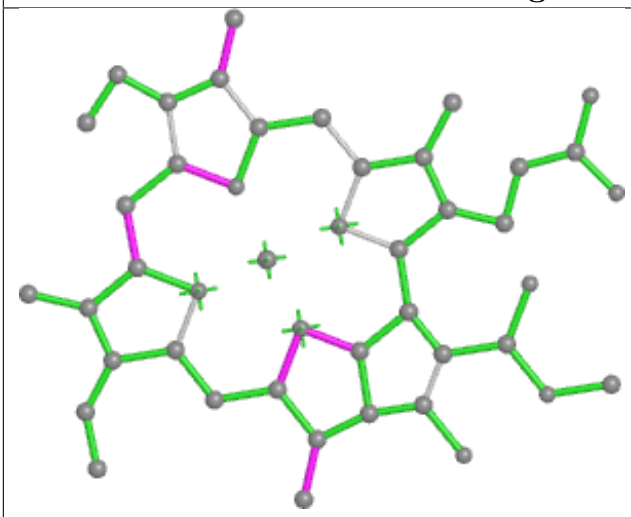


Torsions

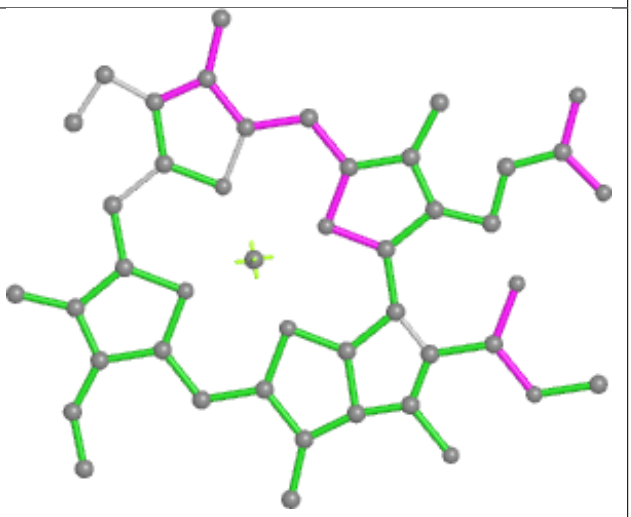


Rings

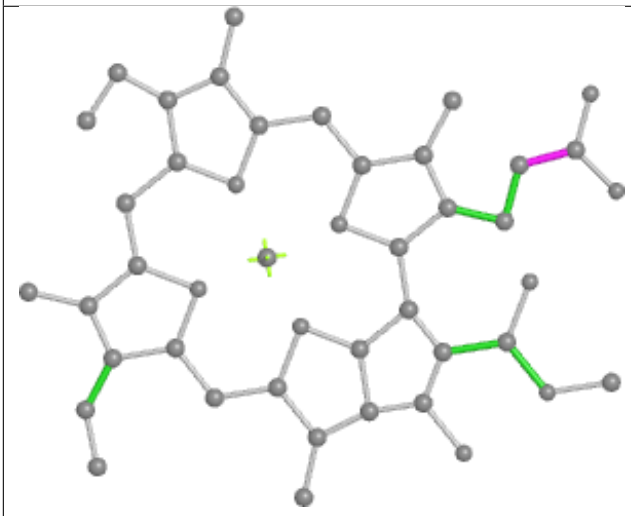
Ligand CLA 6 612



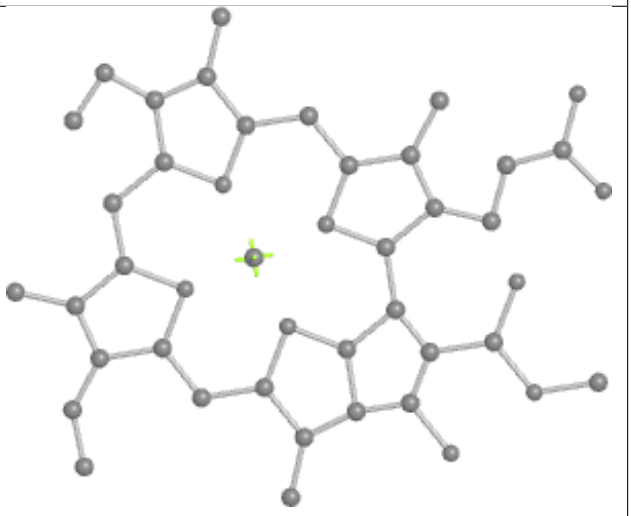
Bond lengths



Bond angles

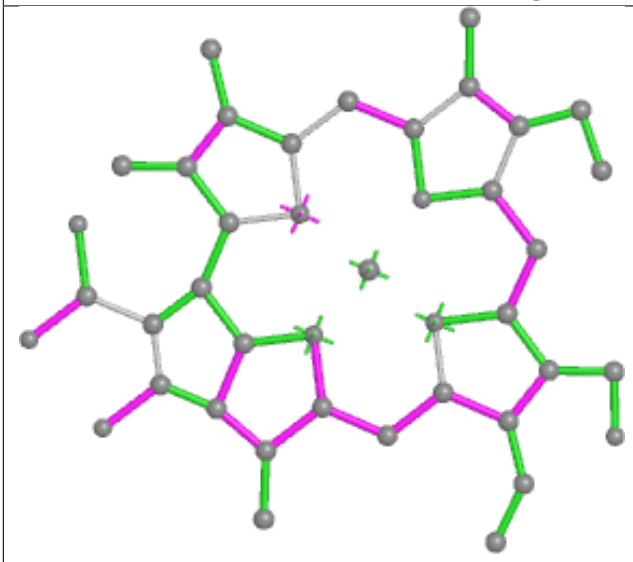


Torsions

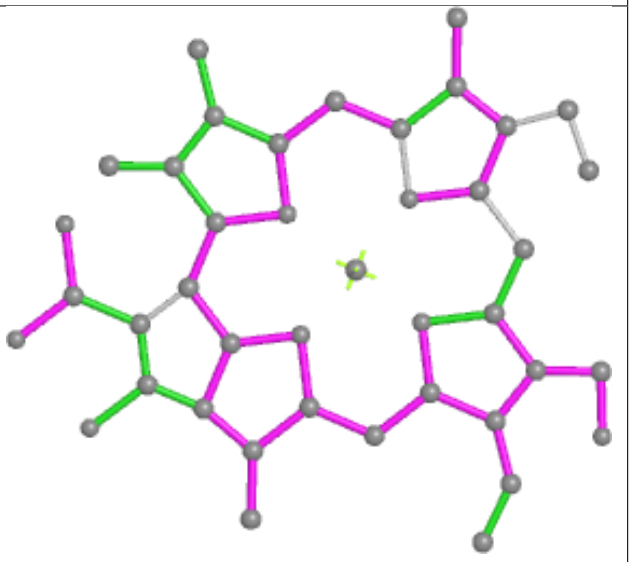


Rings

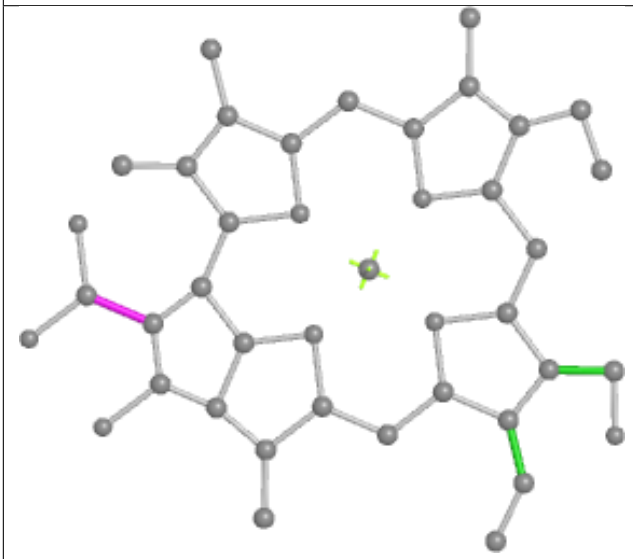
Ligand CHL 6 607



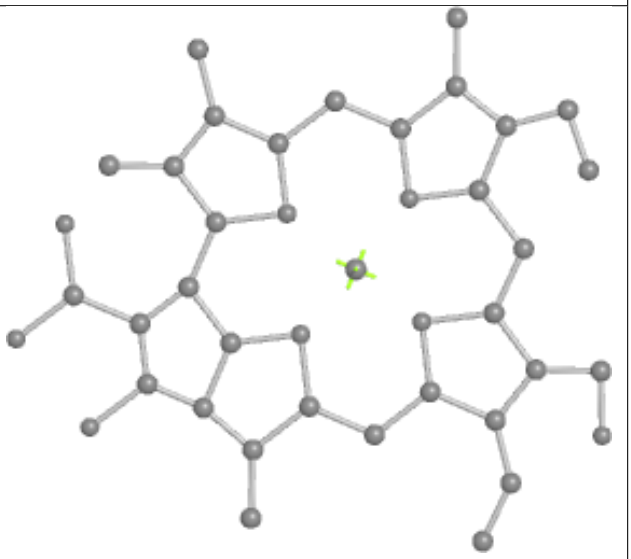
Bond lengths



Bond angles

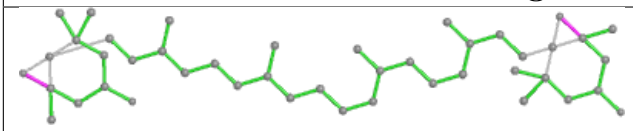


Torsions

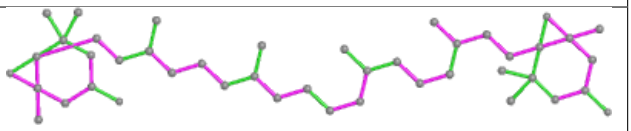


Rings

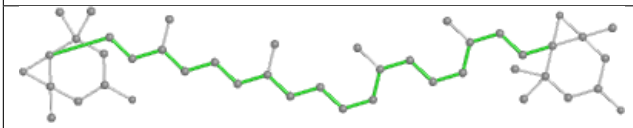
Ligand XAT 3 619



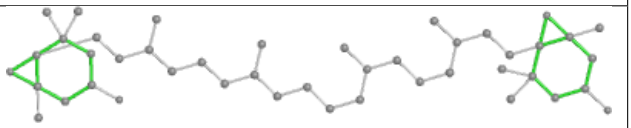
Bond lengths



Bond angles

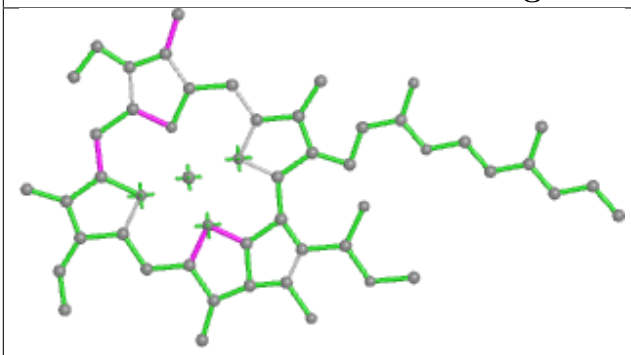


Torsions

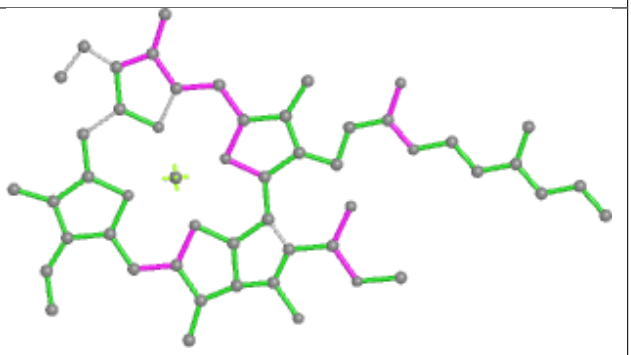


Rings

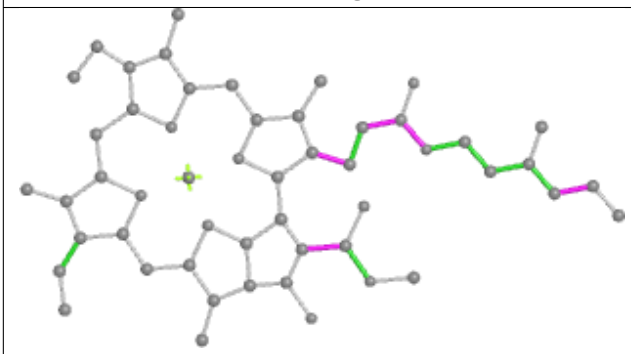
Ligand CLA A 845



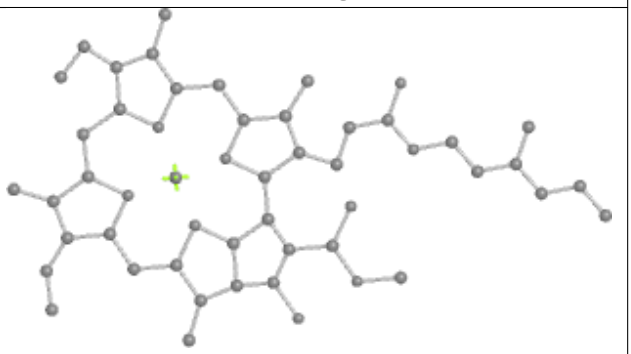
Bond lengths



Bond angles

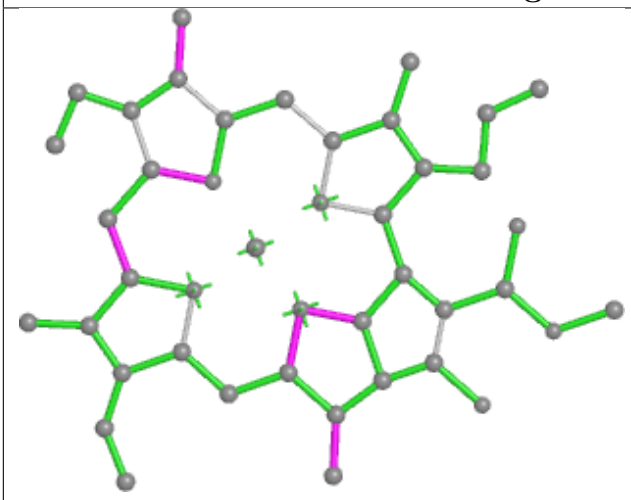


Torsions

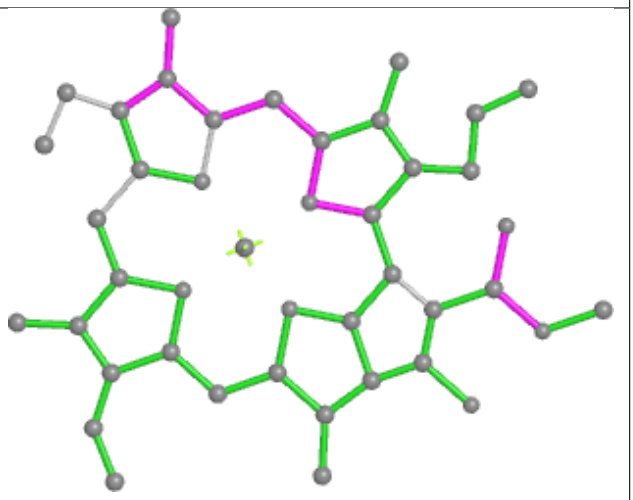


Rings

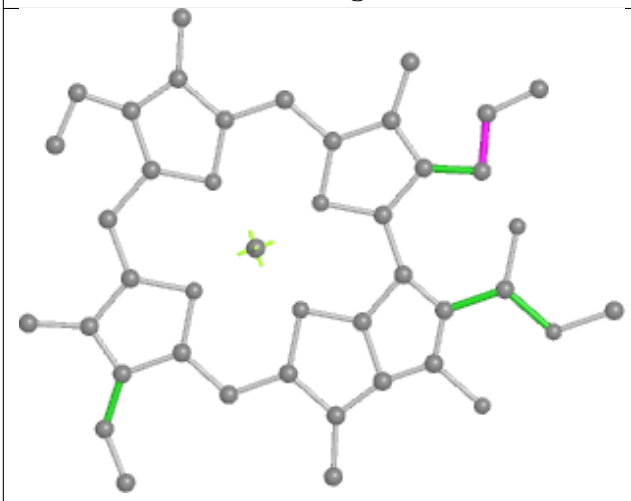
Ligand CLA B 820



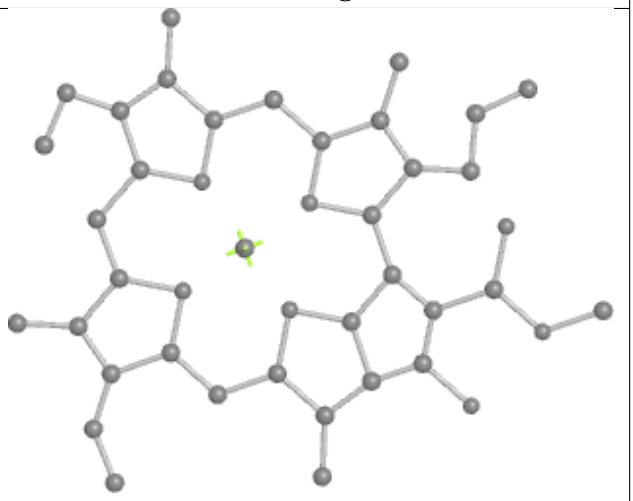
Bond lengths



Bond angles

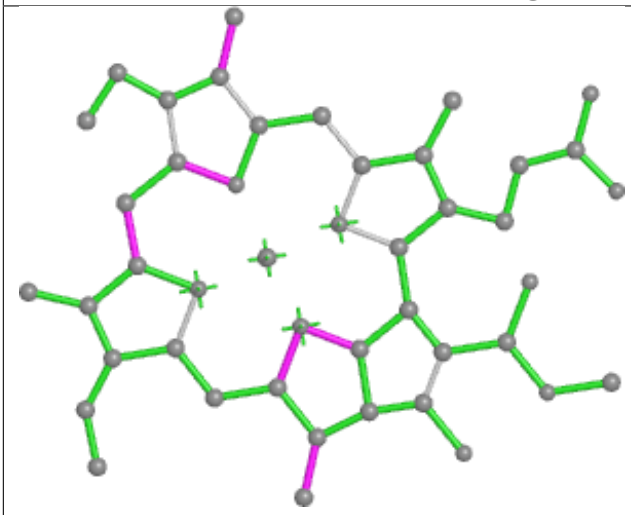


Torsions

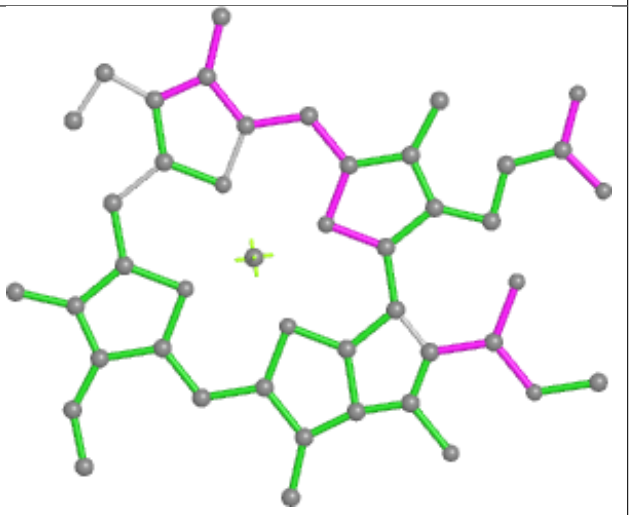


Rings

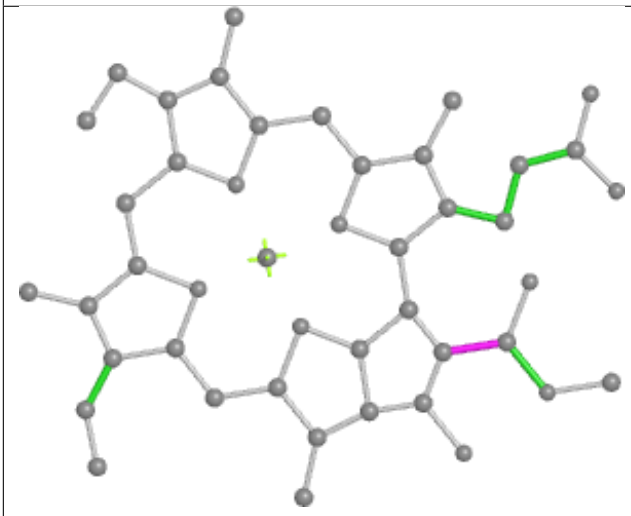
Ligand CLA B 824



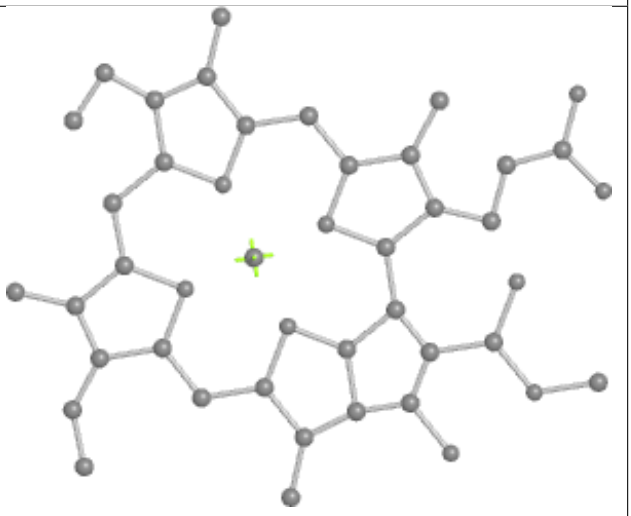
Bond lengths



Bond angles

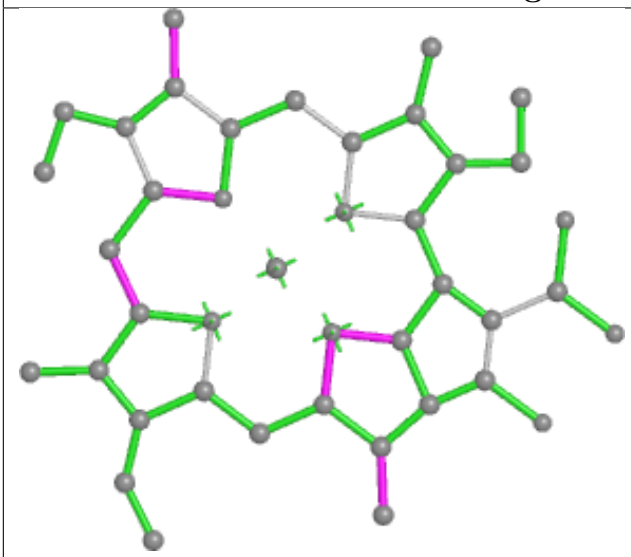


Torsions

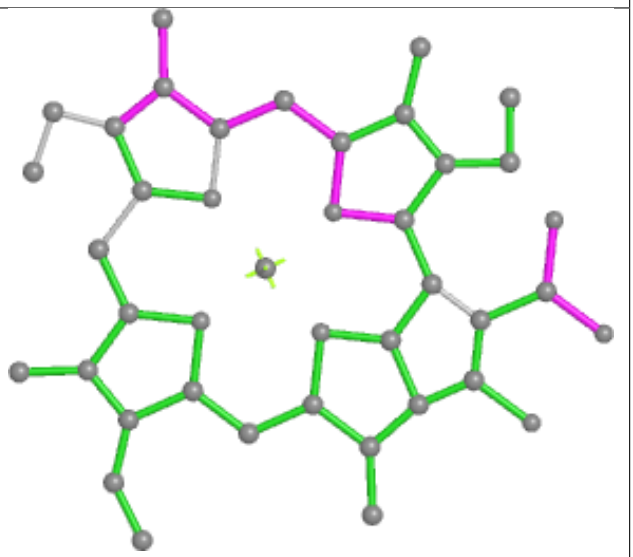


Rings

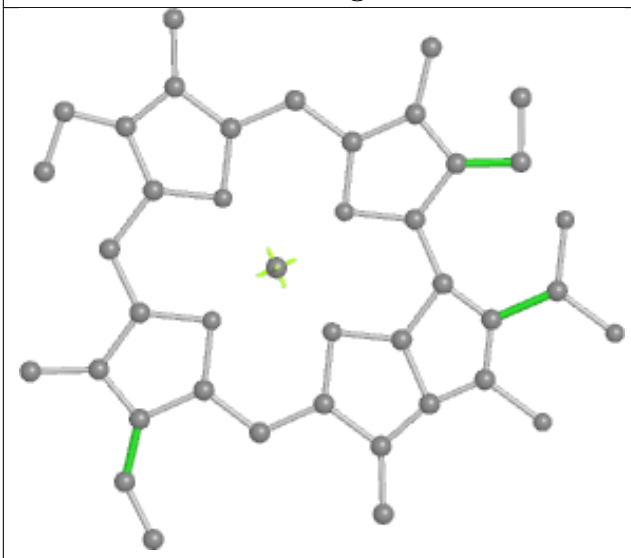
Ligand CLA B 839



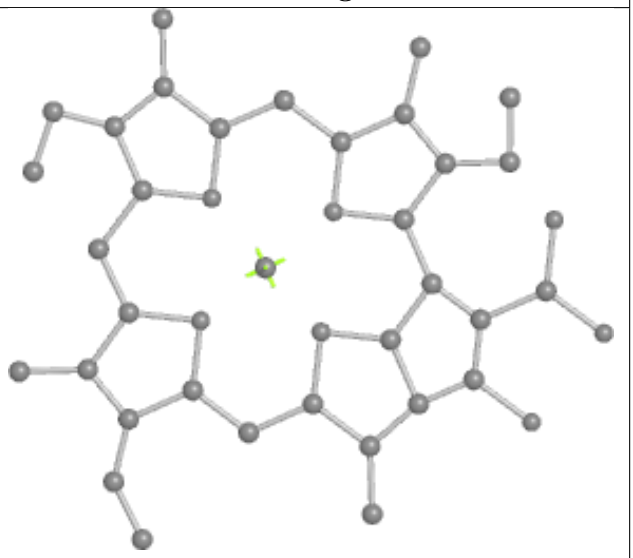
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

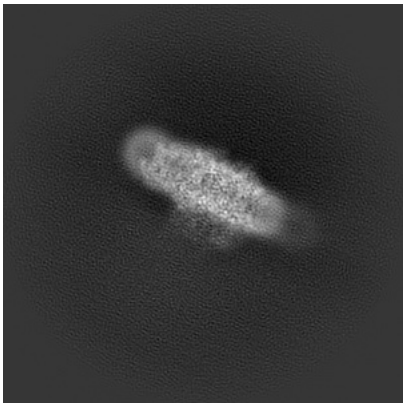
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-0821. These allow visual inspection of the internal detail of the map and identification of artifacts.

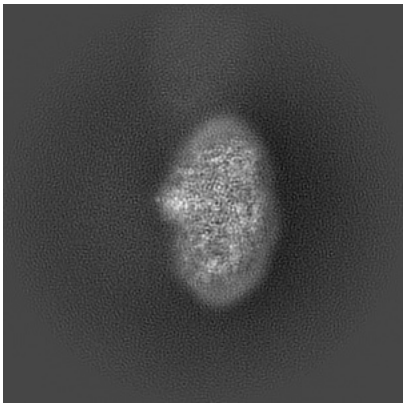
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

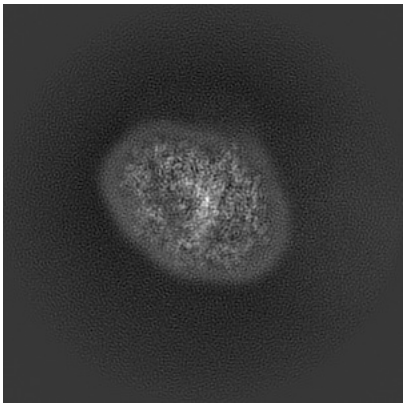
6.1.1 Primary map



X



Y

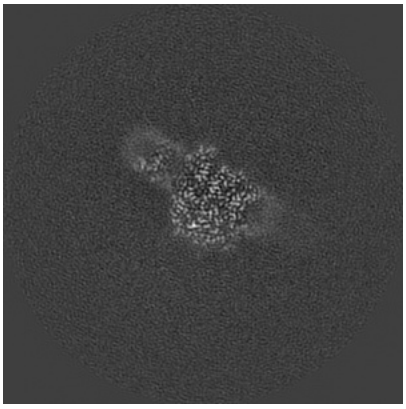


Z

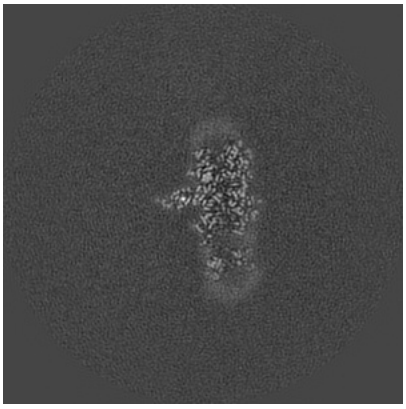
The images above show the map projected in three orthogonal directions.

6.2 Central slices

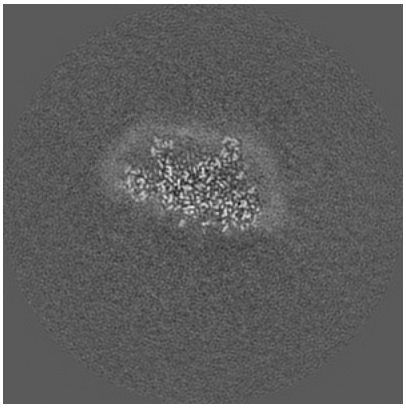
6.2.1 Primary map



X Index: 192



Y Index: 192

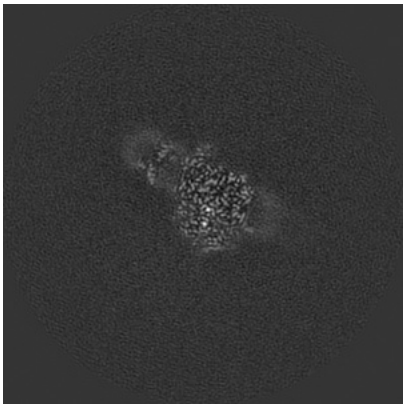


Z Index: 192

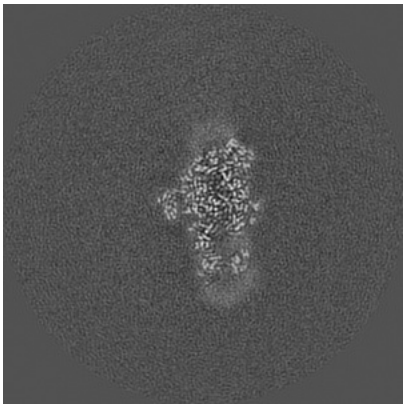
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

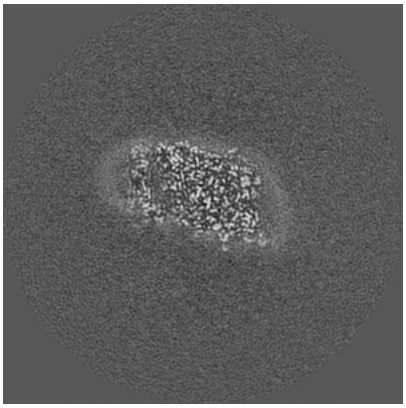
6.3.1 Primary map



X Index: 196



Y Index: 200



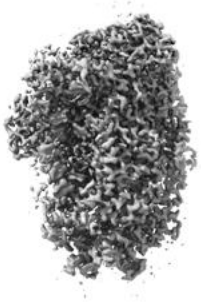
Z Index: 204

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

6.4 Orthogonal surface views (i)

6.4.1 Primary map

X



Y

Z

The images above show the 3D surface view of the map at the recommended contour level 0.03. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

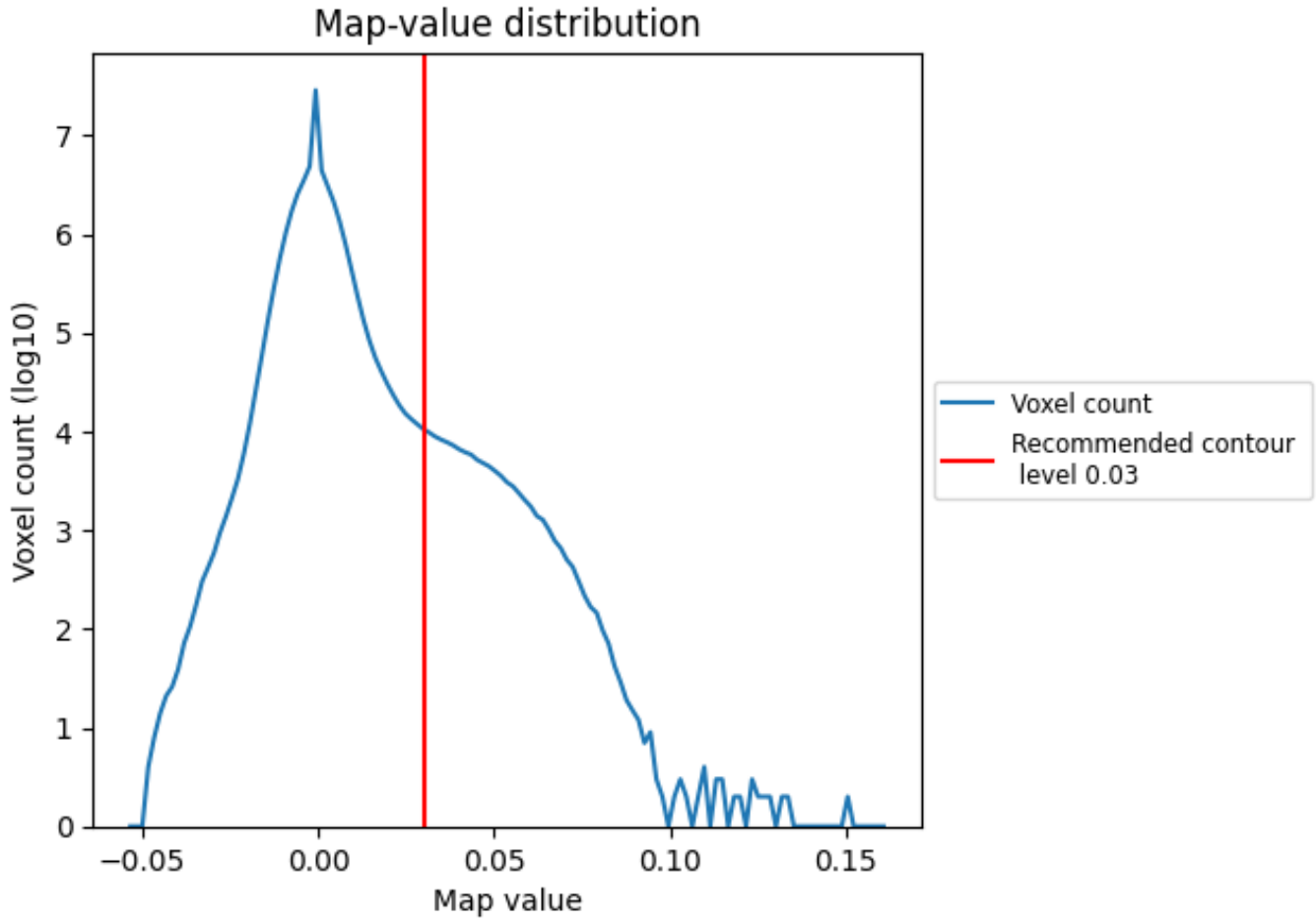
6.5 Mask visualisation (i)

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

7 Map analysis

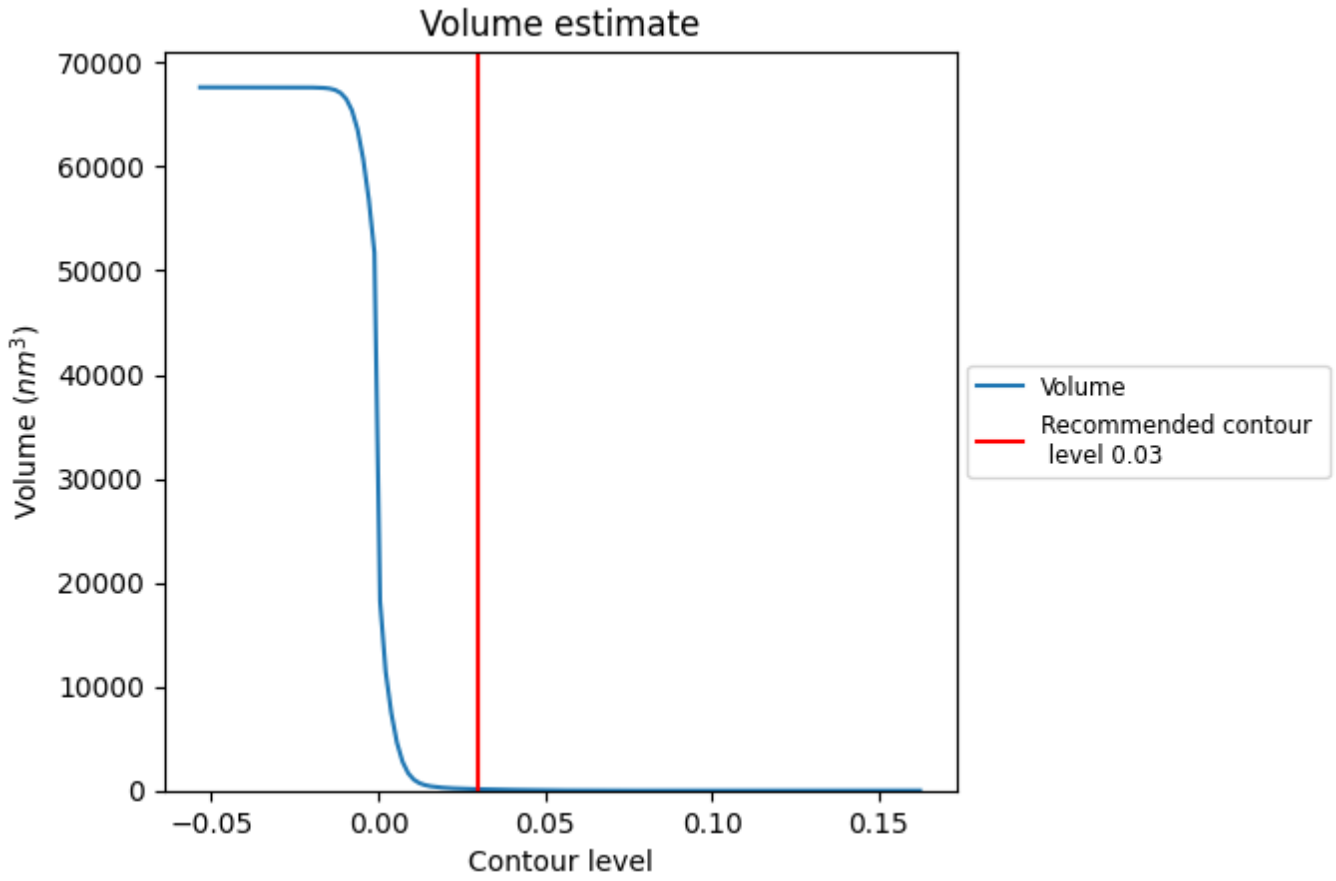
This section contains the results of statistical analysis of the map.

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.

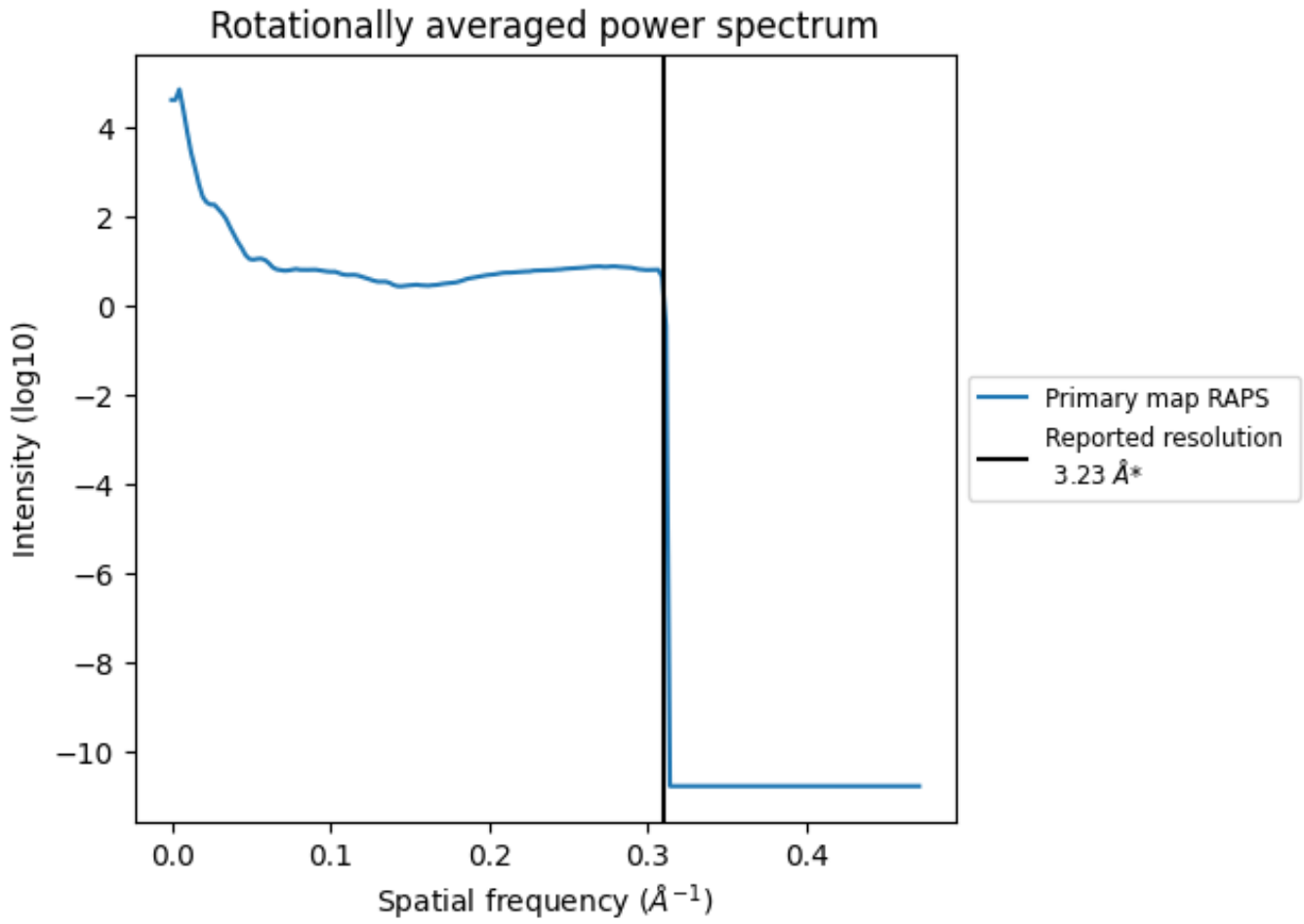
7.2 Volume estimate (i)



The volume at the recommended contour level is 134 nm^3; this corresponds to an approximate mass of 121 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)

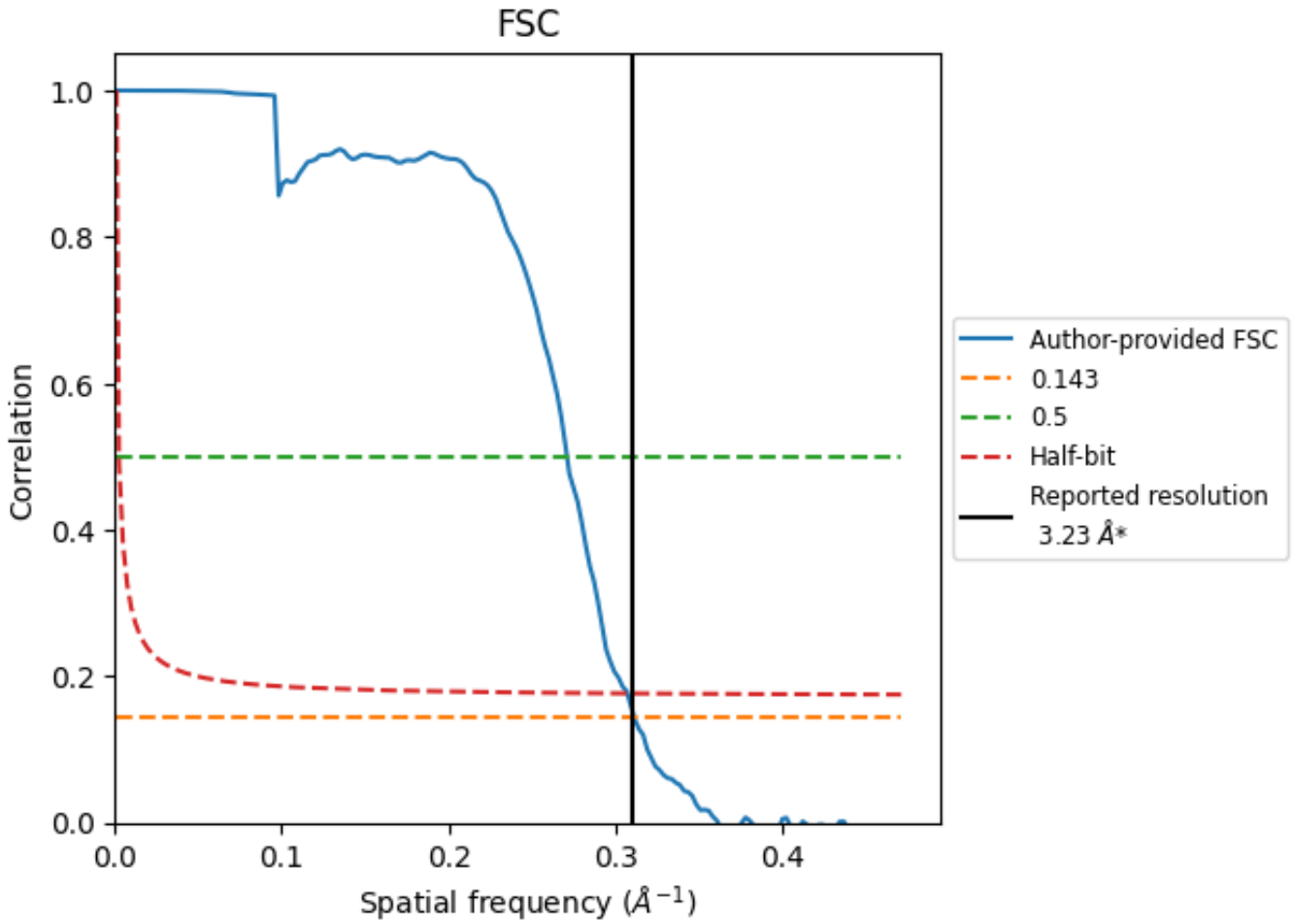


*Reported resolution corresponds to spatial frequency of 0.310 Å^{-1}

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 0.310 Å^{-1}

8.2 Resolution estimates (i)

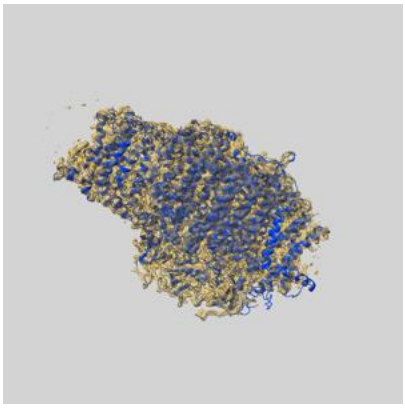
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.23	-	-
Author-provided FSC curve	3.21	3.69	3.26
Unmasked-calculated*	-	-	-

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

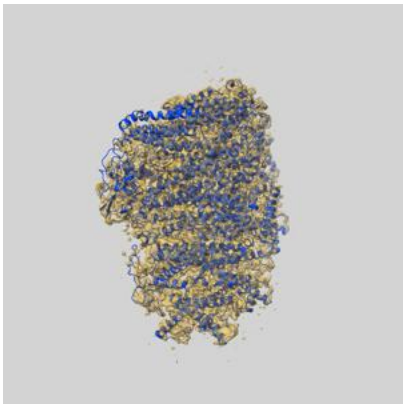
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-0821 and PDB model 6L35. Per-residue inclusion information can be found in section 3 on page 26.

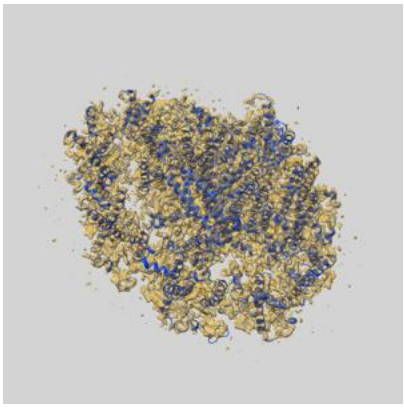
9.1 Map-model overlay



X



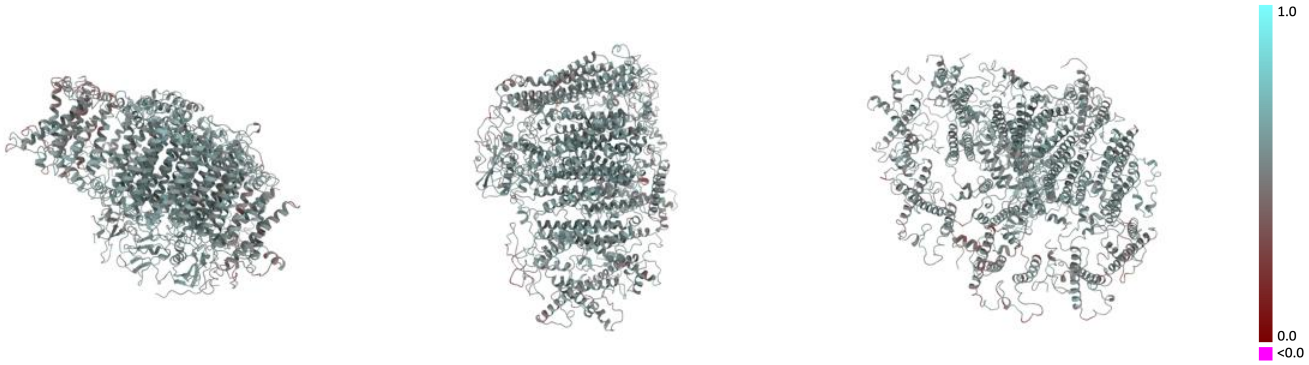
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.03 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.

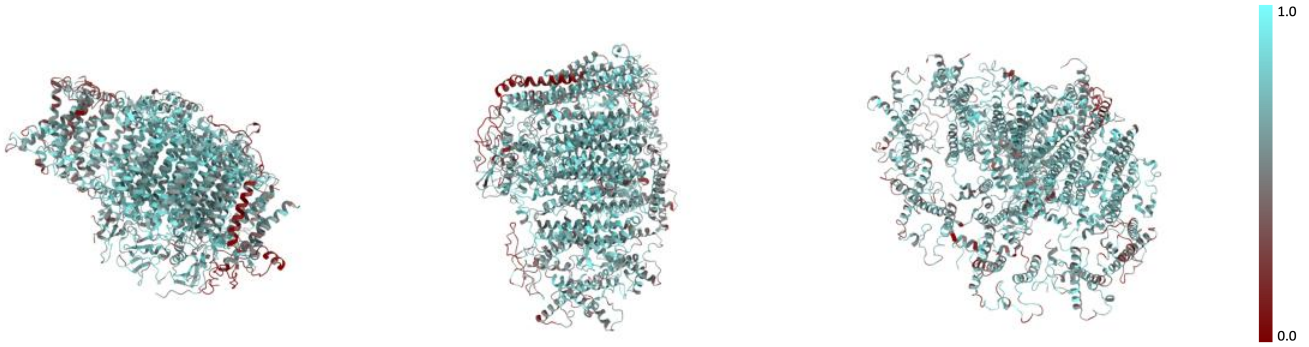
9.2 Q-score mapped to coordinate model (i)



X Y Z

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.

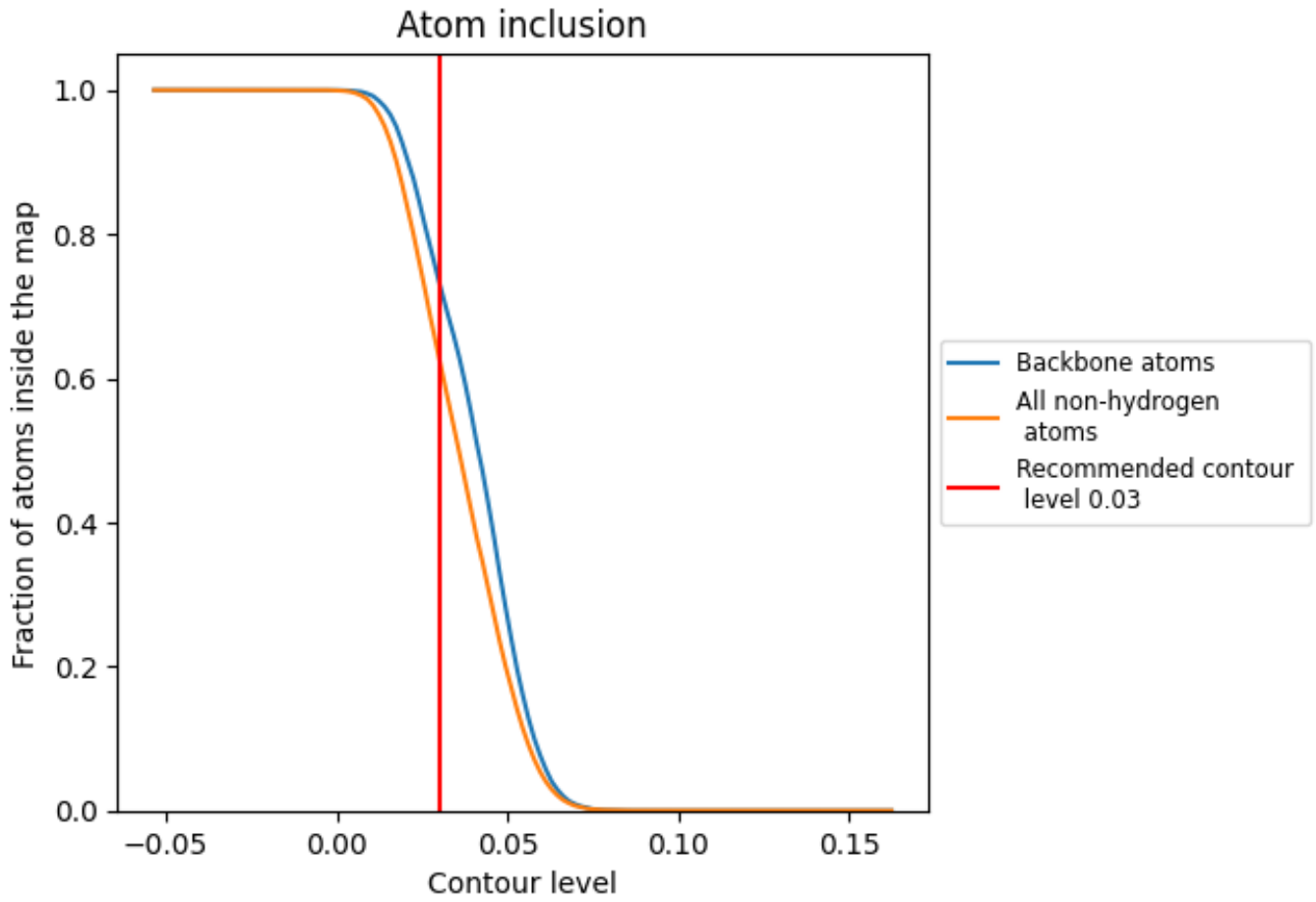
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

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 (0.03).

9.4 Atom inclusion (i)



At the recommended contour level, 73% of all backbone atoms, 63% 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 (0.03) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6283	0.5450
2	0.5838	0.5210
3	0.5714	0.5210
5	0.5621	0.4890
6	0.5767	0.5130
A	0.7031	0.5700
B	0.7097	0.5730
C	0.7404	0.5450
D	0.6355	0.5470
E	0.6674	0.5550
F	0.6184	0.5420
G	0.5077	0.5190
H	0.1309	0.4850
I	0.5559	0.5500
J	0.5629	0.5490
K	0.4193	0.5040
L	0.4854	0.5170
M	0.6066	0.5250