wwPDB EM Validation Summary Report

Nov 4, 2024 – 04:57 AM JST

PDB ID	:	7EW6
EMDB ID	:	EMD-31348
Title	:	Barley photosystem I-LHCI-Lhca5 supercomplex
Authors	:	Wang, W.D.; Shen, L.; Tang, K.; Han, G.Y.; Zhang, X.; Shen, J.R.
Deposited on	:	2021-05-24
Resolution	:	3.40 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:

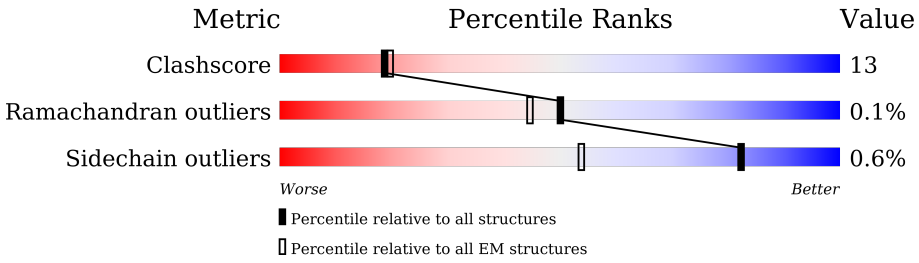
EMDB validation analysis	:	0.0.1.dev113
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.39

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 3.40 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	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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	750	77% 21%
2	B	734	84% 15%
3	C	81	73% 27%
4	D	205	8% 53% 16% 31%
5	E	147	38% 8% 54%
6	F	235	49% 17% 33%
7	H	143	20% 37% 6% 57%
8	I	36	69% 14% 17%

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Mol	Chain	Length	Quality of chain
9	J	42	19% 69% 31%
10	K	131	34% 48% 16% 36%
11	L	209	13% 54% 15% 30%
12	1	247	36% 53% 25% 23%
13	2	255	20% 58% 21% 20%
14	3	269	33% 61% 22% 17%
15	5	257	22% 54% 26% 20%

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
16	CL0	A	801	X	-	-	-
17	CLA	1	504	X	-	-	-
17	CLA	1	505	X	-	-	-
17	CLA	1	506	X	-	-	-
17	CLA	1	507	X	-	-	-
17	CLA	1	508	X	-	-	-
17	CLA	1	510	X	-	-	-
17	CLA	1	511	X	-	-	-
17	CLA	1	515	X	-	-	-
17	CLA	2	504	X	-	-	-
17	CLA	2	506	X	-	-	-
17	CLA	2	507	X	-	-	-
17	CLA	2	508	X	-	-	-
17	CLA	2	509	X	-	-	-
17	CLA	2	510	X	-	-	-
17	CLA	2	511	X	-	-	-
17	CLA	2	514	X	-	-	-
17	CLA	3	301	X	-	-	-
17	CLA	3	306	X	-	-	-
17	CLA	3	307	X	-	-	-
17	CLA	3	308	X	-	-	-
17	CLA	3	310	X	-	-	-
17	CLA	3	311	X	-	-	-
17	CLA	3	312	X	-	-	-
17	CLA	3	313	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
17	CLA	3	314	X	-	-	-
17	CLA	3	316	X	-	-	-
17	CLA	3	317	X	-	-	-
17	CLA	3	318	X	-	-	-
17	CLA	5	305	X	-	-	-
17	CLA	5	306	X	-	-	-
17	CLA	5	307	X	-	-	-
17	CLA	5	308	X	-	-	-
17	CLA	5	309	X	-	-	-
17	CLA	5	310	X	-	-	-
17	CLA	5	311	X	-	-	-
17	CLA	5	312	X	-	-	-
17	CLA	5	313	X	-	-	-
17	CLA	5	316	X	-	-	-
17	CLA	A	802	X	-	-	-
17	CLA	A	803	X	-	-	-
17	CLA	A	804	X	-	-	-
17	CLA	A	805	X	-	-	-
17	CLA	A	806	X	-	-	-
17	CLA	A	807	X	-	-	-
17	CLA	A	808	X	-	-	-
17	CLA	A	809	X	-	-	-
17	CLA	A	810	X	-	-	-
17	CLA	A	811	X	-	-	-
17	CLA	A	812	X	-	-	-
17	CLA	A	813	X	-	-	-
17	CLA	A	814	X	-	-	-
17	CLA	A	815	X	-	-	-
17	CLA	A	816	X	-	-	-
17	CLA	A	817	X	-	-	-
17	CLA	A	818	X	-	-	-
17	CLA	A	819	X	-	-	-
17	CLA	A	820	X	-	-	-
17	CLA	A	821	X	-	-	-
17	CLA	A	822	X	-	-	-
17	CLA	A	823	X	-	-	-
17	CLA	A	824	X	-	-	-
17	CLA	A	825	X	-	-	-
17	CLA	A	826	X	-	-	-
17	CLA	A	827	X	-	-	-
17	CLA	A	828	X	-	-	-
17	CLA	A	829	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
17	CLA	A	830	X	-	-	-
17	CLA	A	831	X	-	-	-
17	CLA	A	832	X	-	-	-
17	CLA	A	833	X	-	-	-
17	CLA	A	834	X	-	-	-
17	CLA	A	835	X	-	-	-
17	CLA	A	836	X	-	-	-
17	CLA	A	837	X	-	-	-
17	CLA	A	838	X	-	-	-
17	CLA	A	839	X	-	-	-
17	CLA	A	840	X	-	-	-
17	CLA	A	842	X	-	-	-
17	CLA	A	852	X	-	-	-
17	CLA	B	801	X	-	-	-
17	CLA	B	802	X	-	-	-
17	CLA	B	803	X	-	-	-
17	CLA	B	804	X	-	-	-
17	CLA	B	805	X	-	-	-
17	CLA	B	806	X	-	-	-
17	CLA	B	807	X	-	-	-
17	CLA	B	808	X	-	-	-
17	CLA	B	809	X	-	-	-
17	CLA	B	810	X	-	-	-
17	CLA	B	811	X	-	-	-
17	CLA	B	812	X	-	-	-
17	CLA	B	813	X	-	-	-
17	CLA	B	814	X	-	-	-
17	CLA	B	815	X	-	-	-
17	CLA	B	816	X	-	-	-
17	CLA	B	817	X	-	-	-
17	CLA	B	818	X	-	-	-
17	CLA	B	819	X	-	-	-
17	CLA	B	820	X	-	-	-
17	CLA	B	821	X	-	-	-
17	CLA	B	822	X	-	-	-
17	CLA	B	823	X	-	-	-
17	CLA	B	824	X	-	-	-
17	CLA	B	825	X	-	-	-
17	CLA	B	826	X	-	-	-
17	CLA	B	827	X	-	-	-
17	CLA	B	828	X	-	-	-
17	CLA	B	829	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
17	CLA	B	830	X	-	-	-
17	CLA	B	831	X	-	-	-
17	CLA	B	832	X	-	-	-
17	CLA	B	833	X	-	-	-
17	CLA	B	834	X	-	-	-
17	CLA	B	835	X	-	-	-
17	CLA	B	837	X	-	-	-
17	CLA	B	838	X	-	-	-
17	CLA	B	839	X	-	-	-
17	CLA	B	840	X	-	-	-
17	CLA	B	841	X	-	-	-
17	CLA	B	842	X	-	-	-
17	CLA	F	802	X	-	-	-
17	CLA	F	803	X	-	-	-
17	CLA	J	101	X	-	-	-
17	CLA	K	201	X	-	-	-
17	CLA	K	202	X	-	-	-
17	CLA	K	203	X	-	-	-
17	CLA	K	205	X	-	-	-
17	CLA	L	301	X	-	-	-
17	CLA	L	302	X	-	-	-
17	CLA	L	303	X	-	-	-
17	CLA	L	304	X	-	-	-
25	CHL	1	512	X	-	-	-
25	CHL	1	514	X	-	-	-
25	CHL	1	517	X	-	-	-
25	CHL	2	512	X	-	-	-
25	CHL	2	513	X	-	-	-
25	CHL	2	515	X	-	-	-
25	CHL	2	516	X	-	-	-
25	CHL	3	302	X	-	-	-
25	CHL	3	315	X	-	-	-
25	CHL	5	314	X	-	-	-
25	CHL	5	315	X	-	-	-
25	CHL	5	317	X	-	-	-

2 Entry composition (i)

There are 26 unique types of molecules in this entry. The entry contains 32973 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	5813	3812	983	1000	18	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	3834	995	1006	14	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	81	610	376	105	117	12	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	D	142	1113	716	193	201	3	0	0

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

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
5	E	68	538	341	98	99	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	F	158	1203	774	208	218	3	0	0

- Molecule 7 is a protein called Photosystem I reaction center subunit VI, chloroplastic.

Mol	Chain	Residues	Atoms				AltConf	Trace
7	H	61	Total	C	N	O	0	0
			454	303	76	75		

- Molecule 8 is a protein called Photosystem I reaction center subunit VIII.

Mol	Chain	Residues	Atoms				AltConf	Trace
8	I	30	Total	C	N	O	0	0
			232	161	35	36		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
9	J	42	Total	C	N	O	S	0	0
			333	228	51	53	1		

- Molecule 10 is a protein called Photosystem I reaction center subunit psaK, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	K	84	Total	C	N	O	S	0	0
			565	359	94	108	4		

- Molecule 11 is a protein called Photosystem I reaction center subunit XI, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	L	146	Total	C	N	O	S	0	0
			1088	716	174	197	1		

- Molecule 12 is a protein called Chlorophyll a-b binding protein Lhca1.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	1	191	Total	C	N	O	S	0	0
			1422	921	239	258	4		

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
1	73	PHE	UNK	conflict	UNP A0A287WC32
1	74	GLU	UNK	conflict	UNP A0A287WC32
1	75	ARG	UNK	conflict	UNP A0A287WC32

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

Mol	Chain	Residues	Atoms					AltConf	Trace
13	2	203	Total	C	N	O	S	0	0
			1561	1018	257	283	3		

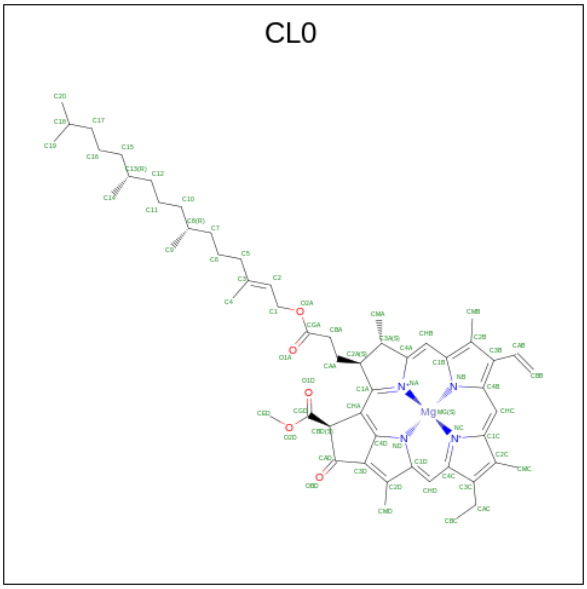
- Molecule 14 is a protein called Chlorophyll a-b binding protein, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	3	222	Total	C	N	O	S	0	0
			1629	1063	271	292	3		

- Molecule 15 is a protein called Chlorophyll a-b binding protein Lhca5.

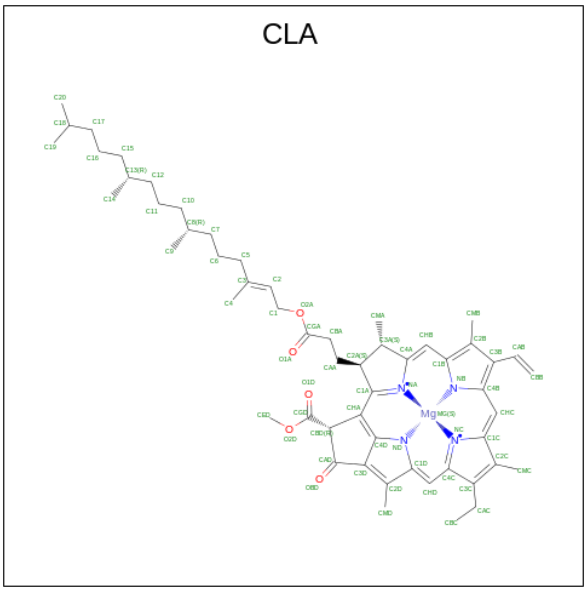
Mol	Chain	Residues	Atoms					AltConf	Trace
15	5	205	Total	C	N	O	S	0	0
			1486	962	247	270	7		

- Molecule 16 is CHLOROPHYLL A ISOMER (three-letter code: CL0) (formula: $C_{55}H_{72}MgN_4O_5$).



Mol	Chain	Residues	Atoms					AltConf
16	A	1	Total	C	Mg	N	O	0
			61	52	1	4	4	

- Molecule 17 is CHLOROPHYLL A (three-letter code: CLA) (formula: $C_{55}H_{72}MgN_4O_5$).



Mol	Chain	Residues	Atoms					AltConf
17	A	1	Total 58	C 48	Mg 1	N 4	O 5	0
17	A	1	Total 41	C 33	Mg 1	N 4	O 3	0
17	A	1	Total 52	C 42	Mg 1	N 4	O 5	0
17	A	1	Total 64	C 54	Mg 1	N 4	O 5	0
17	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
17	A	1	Total 39	C 32	Mg 1	N 4	O 2	0
17	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
17	A	1	Total 39	C 32	Mg 1	N 4	O 2	0
17	A	1	Total 54	C 44	Mg 1	N 4	O 5	0
17	A	1	Total 40	C 32	Mg 1	N 4	O 3	0
17	A	1	Total 42	C 34	Mg 1	N 4	O 3	0
17	A	1	Total 45	C 35	Mg 1	N 4	O 5	0
17	A	1	Total 42	C 34	Mg 1	N 4	O 3	0
17	A	1	Total 45	C 35	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
17	A	1	Total	C	Mg	N	O	0
			59	49	1	4	5	
17	A	1	Total	C	Mg	N	O	0
			39	32	1	4	2	
17	A	1	Total	C	Mg	N	O	0
			40	32	1	4	3	
17	A	1	Total	C	Mg	N	O	0
			40	32	1	4	3	
17	A	1	Total	C	Mg	N	O	0
			57	47	1	4	5	
17	A	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
17	A	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
17	A	1	Total	C	Mg	N	O	0
			54	44	1	4	5	
17	A	1	Total	C	Mg	N	O	0
			40	32	1	4	3	
17	A	1	Total	C	Mg	N	O	0
			59	49	1	4	5	
17	A	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
17	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
17	A	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
17	A	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
17	A	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
17	A	1	Total	C	Mg	N	O	0
			63	53	1	4	5	
17	A	1	Total	C	Mg	N	O	0
			45	37	1	4	3	
17	A	1	Total	C	Mg	N	O	0
			40	32	1	4	3	
17	A	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
17	A	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
17	A	1	Total	C	Mg	N	O	0
			55	45	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
17	A	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
17	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
17	A	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
17	A	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
17	A	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
17	A	1	Total	C	Mg	N	O	0
			57	47	1	4	5	
17	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
17	B	1	Total	C	Mg	N	O	0
			64	54	1	4	5	
17	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
17	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
17	B	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
17	B	1	Total	C	Mg	N	O	0
			39	31	1	4	3	
17	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
17	B	1	Total	C	Mg	N	O	0
			52	42	1	4	5	
17	B	1	Total	C	Mg	N	O	0
			40	32	1	4	3	
17	B	1	Total	C	Mg	N	O	0
			40	32	1	4	3	
17	B	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
17	B	1	Total	C	Mg	N	O	0
			54	44	1	4	5	
17	B	1	Total	C	Mg	N	O	0
			43	35	1	4	3	
17	B	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
17	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
17	B	1	Total	C	Mg	N	O	0
			43	35	1	4	3	
17	B	1	Total	C	Mg	N	O	0
			49	39	1	4	5	
17	B	1	Total	C	Mg	N	O	0
			59	49	1	4	5	
17	B	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
17	B	1	Total	C	Mg	N	O	0
			53	43	1	4	5	
17	B	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
17	B	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
17	B	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
17	B	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
17	B	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
17	B	1	Total	C	Mg	N	O	0
			62	52	1	4	5	
17	B	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
17	B	1	Total	C	Mg	N	O	0
			42	33	1	4	4	
17	B	1	Total	C	Mg	N	O	0
			40	32	1	4	3	
17	B	1	Total	C	Mg	N	O	0
			56	46	1	4	5	
17	B	1	Total	C	Mg	N	O	0
			43	35	1	4	3	
17	B	1	Total	C	Mg	N	O	0
			43	35	1	4	3	
17	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
17	B	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
17	B	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
17	B	1	Total	C	Mg	N	O	0
			42	34	1	4	3	

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Mol	Chain	Residues	Atoms					AltConf
17	B	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
17	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
17	B	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
17	B	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
17	B	1	Total	C	Mg	N	O	0
			54	44	1	4	5	
17	B	1	Total	C	Mg	N	O	0
			57	47	1	4	5	
17	F	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
17	F	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
17	J	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
17	K	1	Total	C	Mg	N	O	0
			37	31	1	4	1	
17	K	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
17	K	1	Total	C	Mg	N	O	0
			40	32	1	4	3	
17	K	1	Total	C	Mg	N	O	0
			39	31	1	4	3	
17	L	1	Total	C	Mg	N	O	0
			56	46	1	4	5	
17	L	1	Total	C	Mg	N	O	0
			40	32	1	4	3	
17	L	1	Total	C	Mg	N	O	0
			52	42	1	4	5	
17	L	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
17	1	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
17	1	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
17	1	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
17	1	1	Total	C	Mg	N	O	0
			42	34	1	4	3	

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Mol	Chain	Residues	Atoms					AltConf
17	1	1	Total	C	Mg	N	O	0
			40	32	1	4	3	
17	1	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
17	1	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
17	1	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
17	1	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
17	1	1	Total	C	Mg	N	O	0
			44	35	1	4	4	
17	2	1	Total	C	Mg	N	O	0
			36	30	1	4	1	
17	2	1	Total	C	Mg	N	O	0
			52	42	1	4	5	
17	2	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
17	2	1	Total	C	Mg	N	O	0
			49	41	1	4	3	
17	2	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
17	2	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
17	2	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
17	2	1	Total	C	Mg	N	O	0
			40	32	1	4	3	
17	2	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
17	3	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
17	3	1	Total	C	Mg	N	O	0
			52	42	1	4	5	
17	3	1	Total	C	Mg	N	O	0
			40	32	1	4	3	
17	3	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
17	3	1	Total	C	Mg	N	O	0
			40	32	1	4	3	
17	3	1	Total	C	Mg	N	O	0
			45	35	1	4	5	

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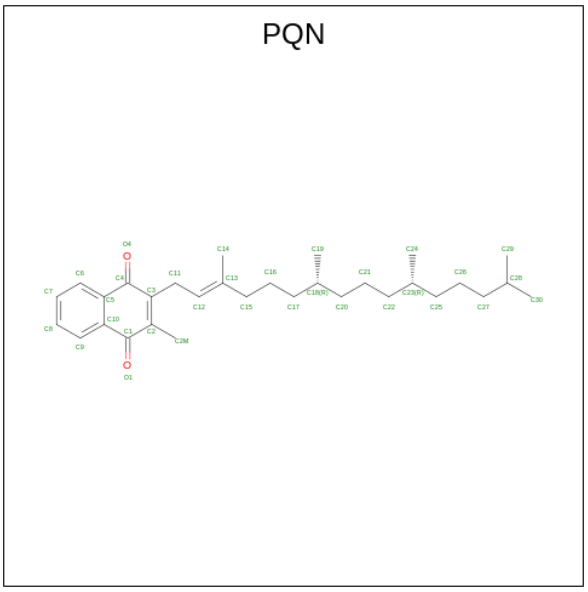
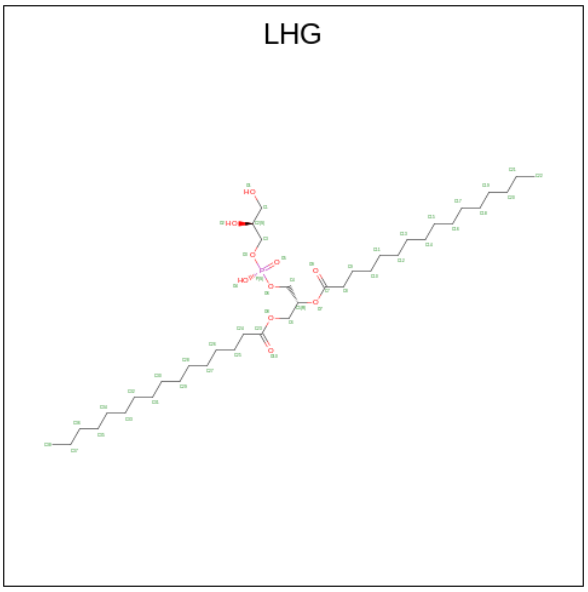
Mol	Chain	Residues	Atoms					AltConf
17	3	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
17	3	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
17	3	1	Total	C	Mg	N	O	0
			48	38	1	4	5	
17	3	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
17	3	1	Total	C	Mg	N	O	0
			37	31	1	4	1	
17	3	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
17	3	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
17	5	1	Total	C	Mg	N	O	0
			38	30	1	4	3	
17	5	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
17	5	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
17	5	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
17	5	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
17	5	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
17	5	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
17	5	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
17	5	1	Total	C	Mg	N	O	0
			40	32	1	4	3	
17	5	1	Total	C	Mg	N	O	0
			41	33	1	4	3	

- Molecule 18 is PHYLLOQUINONE (three-letter code: PQN) (formula: $C_{31}H_{46}O_2$).



Mol	Chain	Residues	Atoms			AltConf
18	A	1	Total	C	O	0
			33	31	2	
18	B	1	Total	C	O	0
			30	28	2	

- Molecule 19 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (three-letter code: LHG) (formula: $C_{38}H_{75}O_{10}P$).



Mol	Chain	Residues	Atoms				AltConf
19	A	1	Total	C	O	P	0
			49	38	10	1	

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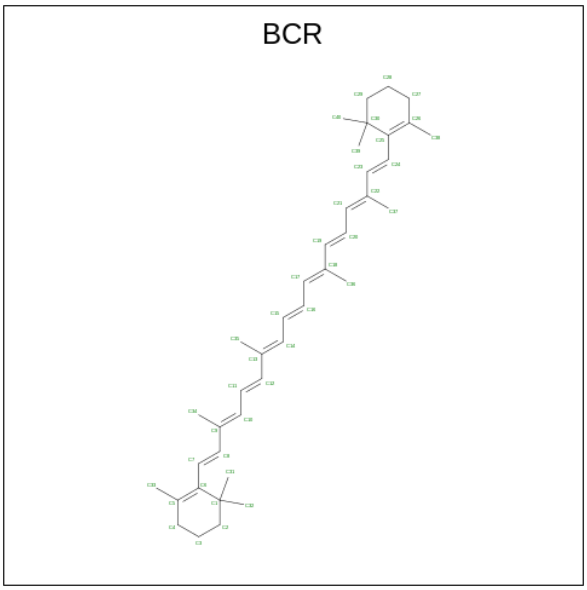
Mol	Chain	Residues	Atoms				AltConf
19	A	1	Total	C	O	P	0
			30	19	10	1	
19	B	1	Total	C	O	P	0
			38	27	10	1	
19	1	1	Total	C	O	P	0
			49	38	10	1	
19	2	1	Total	C	O	P	0
			35	24	10	1	

- Molecule 20 is BETA-CAROTENE (three-letter code: BCR) (formula: $C_{40}H_{56}$).



Mol	Chain	Residues	Atoms		AltConf
20	A	1	Total	C	0
			40	40	
20	A	1	Total	C	0
			40	40	
20	A	1	Total	C	0
			40	40	
20	A	1	Total	C	0
			40	40	
20	A	1	Total	C	0
			39	39	
20	A	1	Total	C	0
			40	40	
20	A	1	Total	C	0
			40	40	

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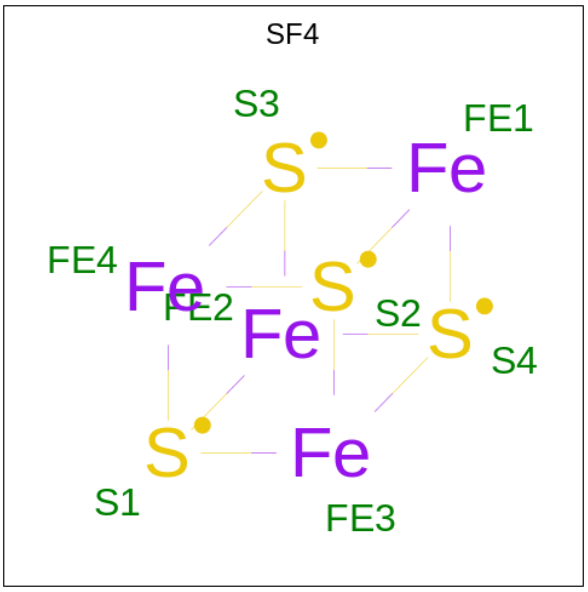
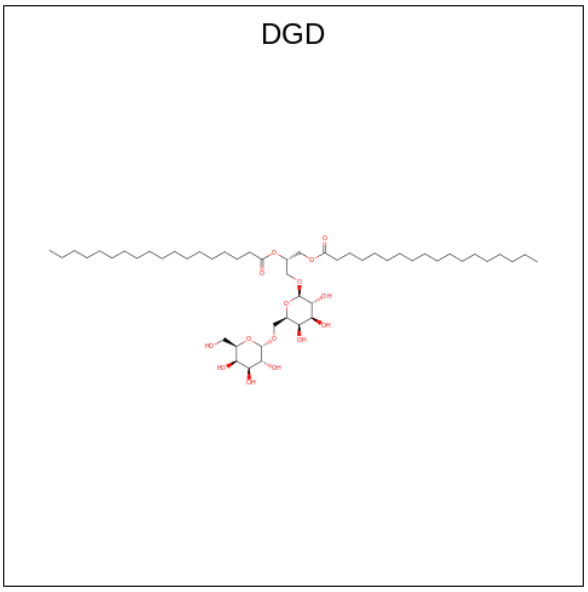
Mol	Chain	Residues	Atoms	AltConf
20	B	1	Total C 40 40	0
20	B	1	Total C 40 40	0
20	B	1	Total C 40 40	0
20	B	1	Total C 40 40	0
20	B	1	Total C 40 40	0
20	B	1	Total C 40 40	0
20	B	1	Total C 40 40	0
20	F	1	Total C 40 40	0
20	F	1	Total C 40 40	0
20	I	1	Total C 40 40	0
20	J	1	Total C 40 40	0
20	K	1	Total C 40 40	0
20	L	1	Total C 40 40	0
20	L	1	Total C 40 40	0
20	1	1	Total C 19 19	0
20	2	1	Total C 40 40	0
20	3	1	Total C 40 40	0
20	5	1	Total C 40 40	0

- Molecule 21 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe_4S_4).



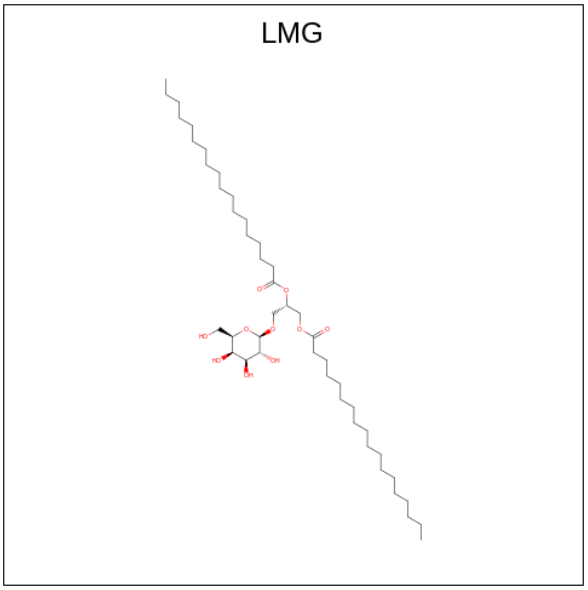
Mol	Chain	Residues	Atoms	AltConf
21	A	1	Total Fe S 8 4 4	0
21	C	1	Total Fe S 8 4 4	0
21	C	1	Total Fe S 8 4 4	0

- Molecule 22 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (three-letter code: DGD) (formula: $C_{51}H_{96}O_{15}$).



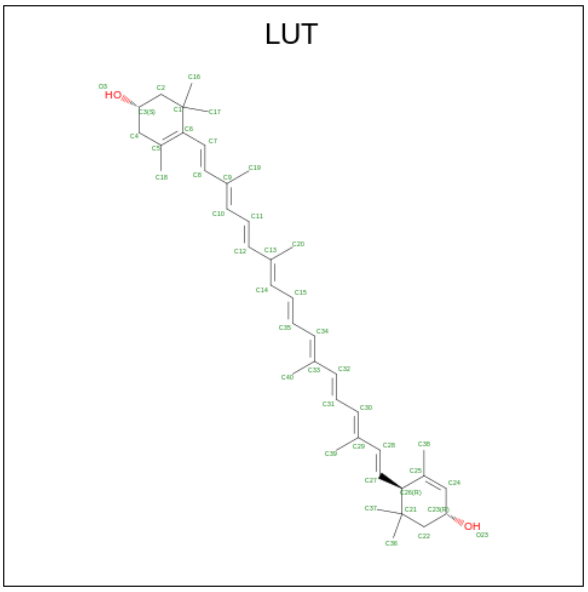
Mol	Chain	Residues	Atoms			AltConf
22	B	1	Total 59	C 44	O 15	0
22	J	1	Total 66	C 51	O 15	0

- Molecule 23 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (three-letter code: LMG) (formula: $C_{45}H_{86}O_{10}$).



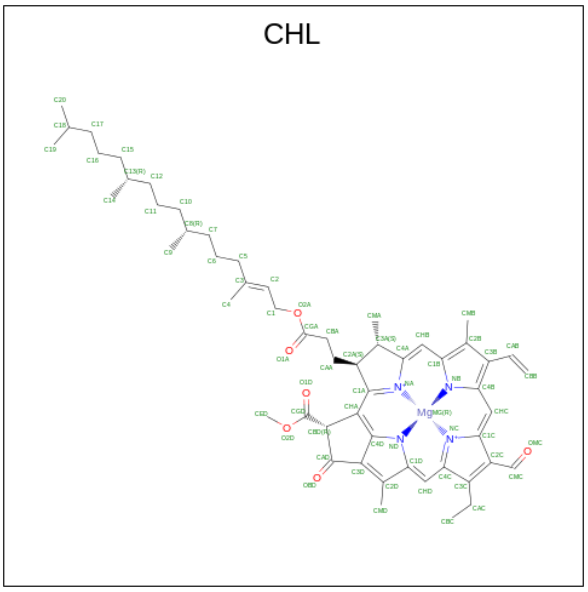
Mol	Chain	Residues	Atoms			AltConf
23	F	1	Total 30	C 20	O 10	0
23	F	1	Total 45	C 35	O 10	0
23	2	1	Total 16	C 9	O 7	0
23	2	1	Total 36	C 26	O 10	0
23	5	1	Total 32	C 22	O 10	0

- Molecule 24 is (3R,3'R,6S)-4,5-DIDEHYDRO-5,6-DIHYDRO-BETA,BETA-CAROTENE-3 ,3'-DIOL (three-letter code: LUT) (formula: $C_{40}H_{56}O_2$).



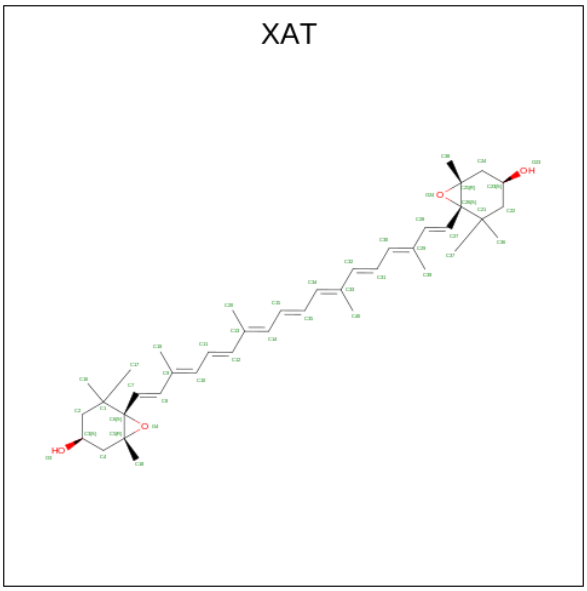
Mol	Chain	Residues	Atoms			AltConf
24	1	1	Total	C	O	0
			42	40	2	
24	1	1	Total	C	O	0
			42	40	2	
24	2	1	Total	C	O	0
			42	40	2	
24	3	1	Total	C	O	0
			42	40	2	
24	3	1	Total	C	O	0
			42	40	2	
24	5	1	Total	C	O	0
			42	40	2	

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



Mol	Chain	Residues	Atoms					AltConf
25	1	1	Total 47	C 36	Mg 1	N 4	O 6	0
25	1	1	Total 41	C 32	Mg 1	N 4	O 4	0
25	1	1	Total 41	C 32	Mg 1	N 4	O 4	0
25	2	1	Total 46	C 35	Mg 1	N 4	O 6	0
25	2	1	Total 40	C 32	Mg 1	N 4	O 3	0
25	2	1	Total 45	C 34	Mg 1	N 4	O 6	0
25	2	1	Total 43	C 34	Mg 1	N 4	O 4	0
25	3	1	Total 47	C 36	Mg 1	N 4	O 6	0
25	3	1	Total 43	C 34	Mg 1	N 4	O 4	0
25	5	1	Total 47	C 36	Mg 1	N 4	O 6	0
25	5	1	Total 46	C 35	Mg 1	N 4	O 6	0
25	5	1	Total 40	C 31	Mg 1	N 4	O 4	0

- Molecule 26 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: $C_{40}H_{56}O_4$).

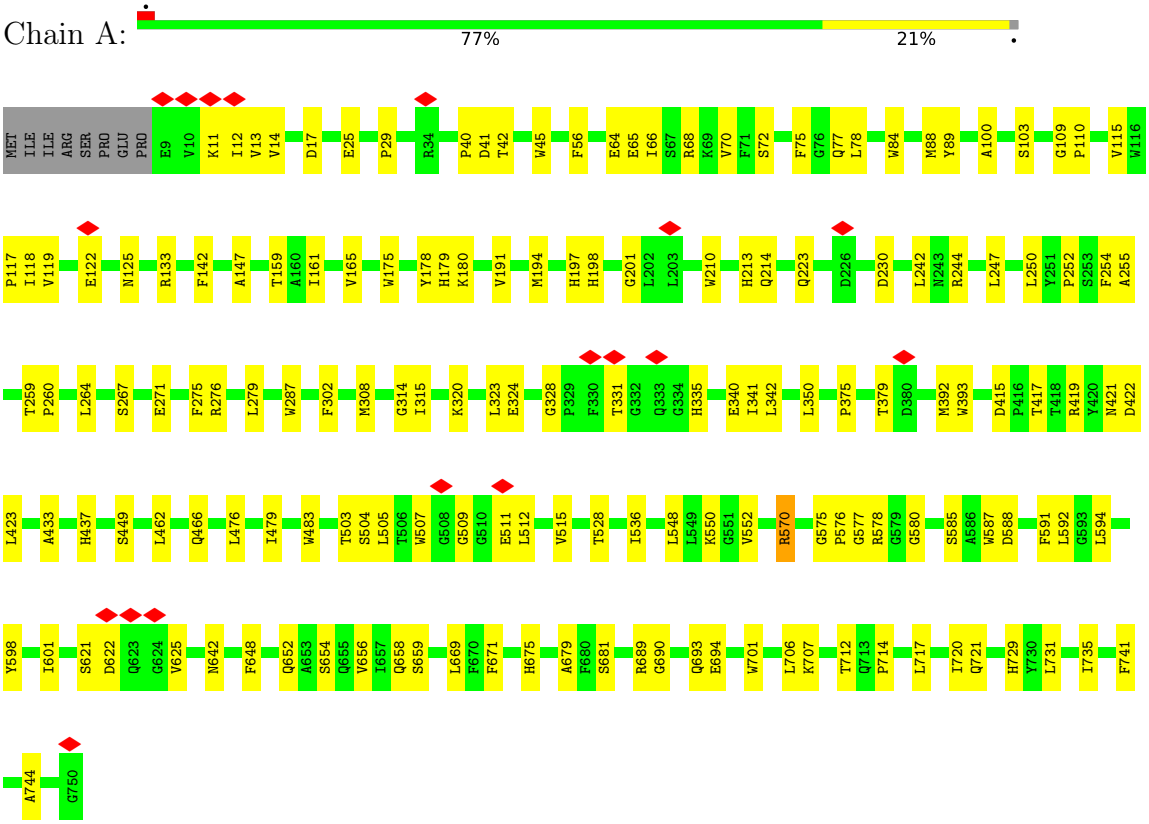


Mol	Chain	Residues	Atoms			AltConf
26	2	1	Total	C	O	0
			44	40	4	
26	5	1	Total	C	O	0
			44	40	4	

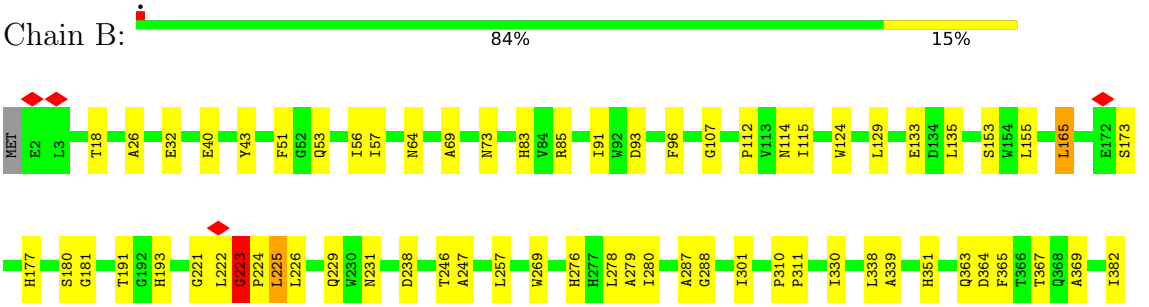
3 Residue-property plots (i)

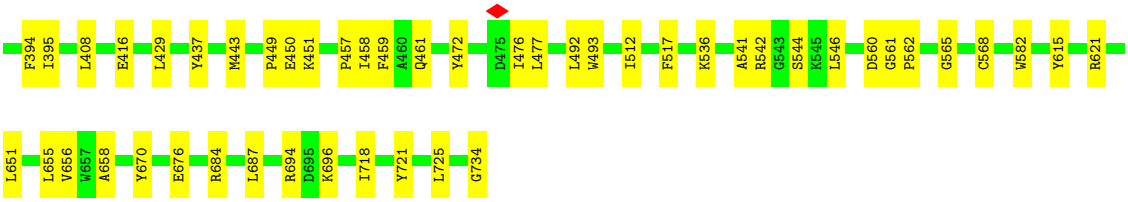
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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

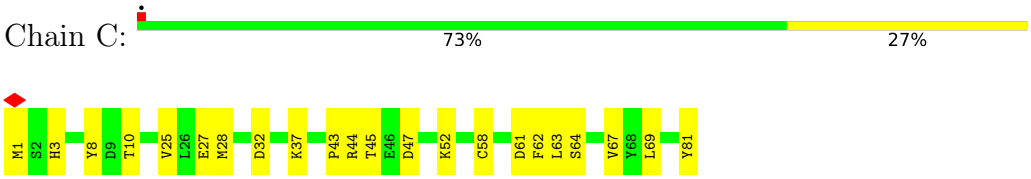


• Molecule 2: Photosystem I P700 chlorophyll a apoprotein A2

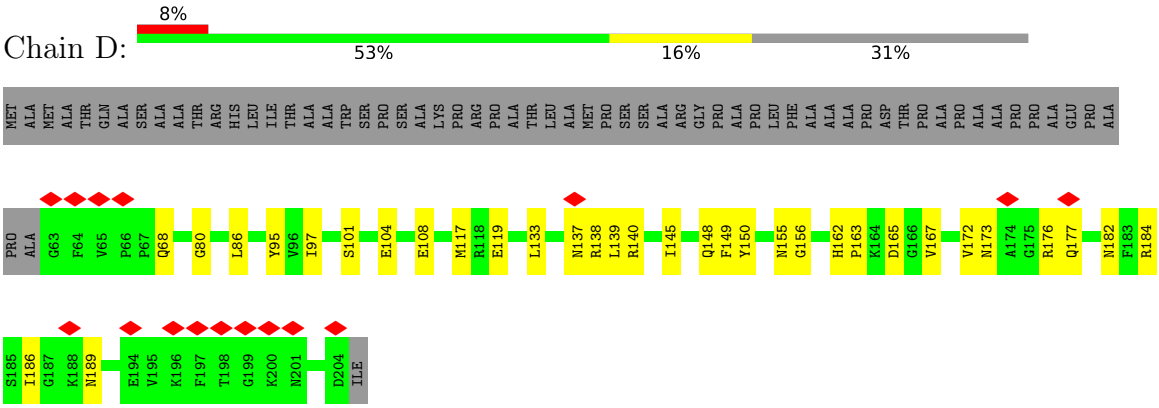




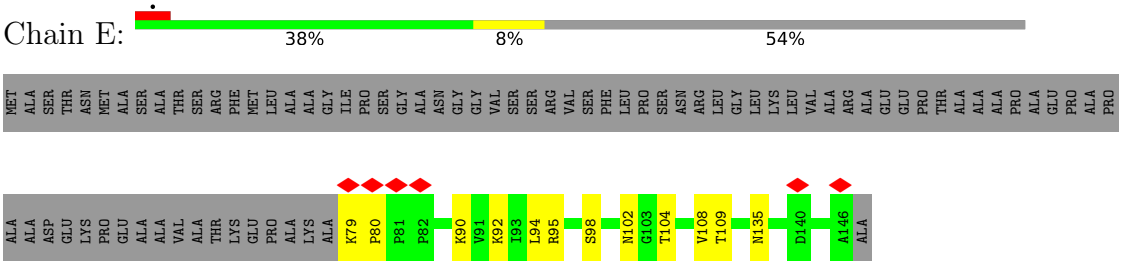
• Molecule 3: Photosystem I iron-sulfur center



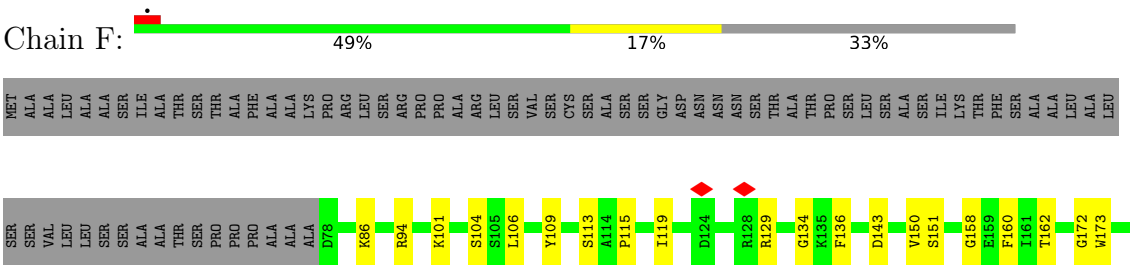
• Molecule 4: Photosystem I reaction center subunit II, chloroplastic

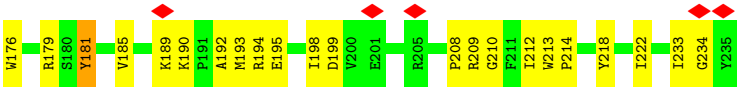


• Molecule 5: Photosystem I reaction center subunit IV, chloroplastic

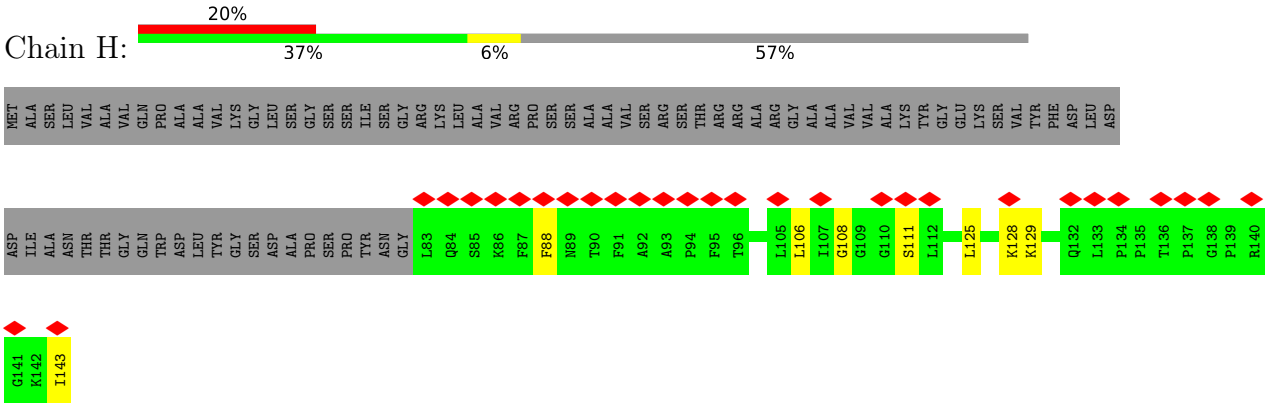


• Molecule 6: Photosystem I reaction center subunit III, chloroplastic

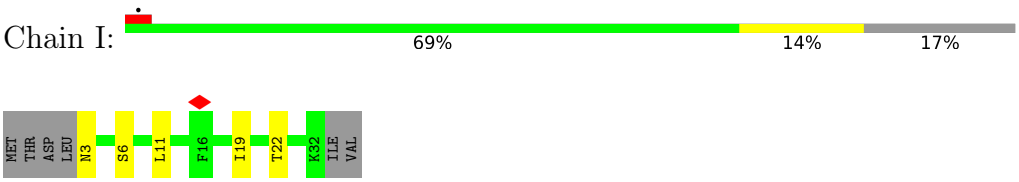




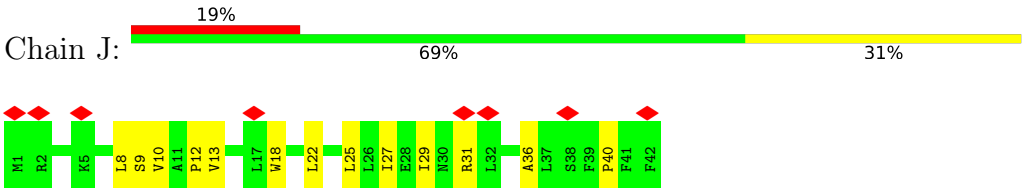
• Molecule 7: Photosystem I reaction center subunit VI, chloroplastic



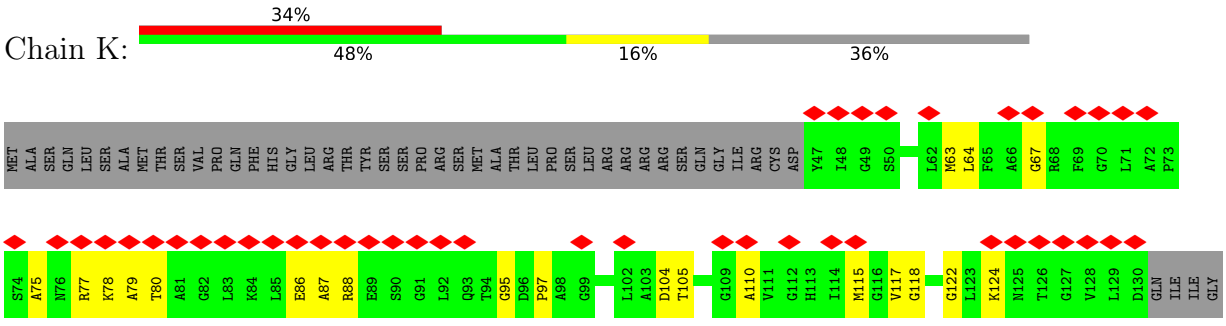
• Molecule 8: Photosystem I reaction center subunit VIII



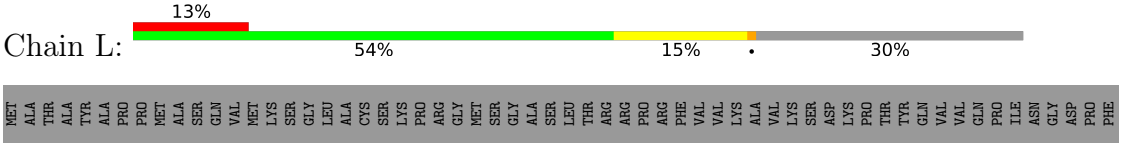
• Molecule 9: Photosystem I reaction center subunit IX

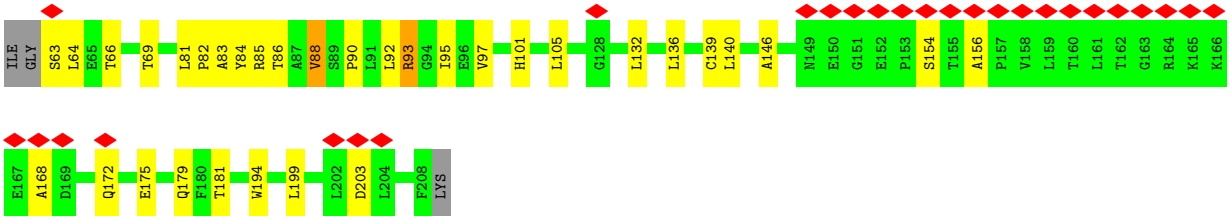


• Molecule 10: Photosystem I reaction center subunit psaK, chloroplastic

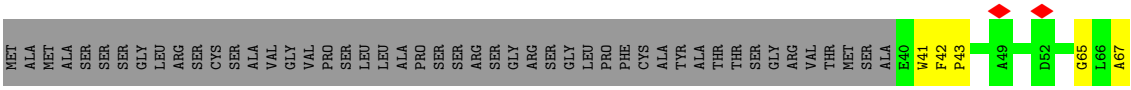


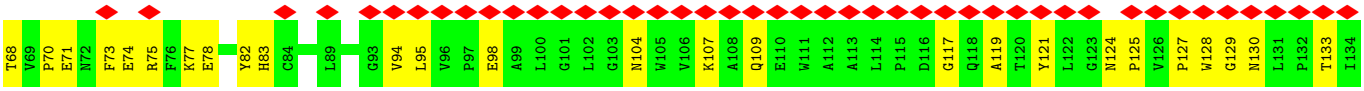
• Molecule 11: Photosystem I reaction center subunit XI, chloroplastic

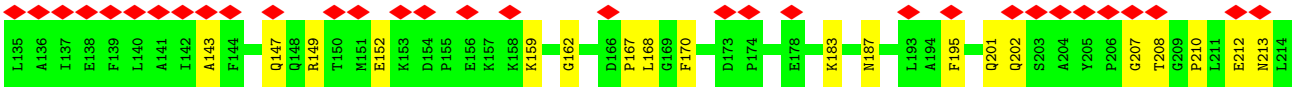


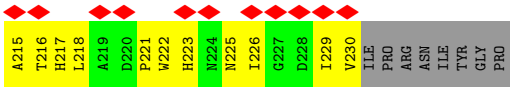


• Molecule 12: Chlorophyll a-b binding protein Lhca1

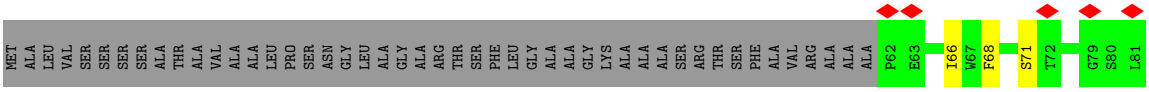


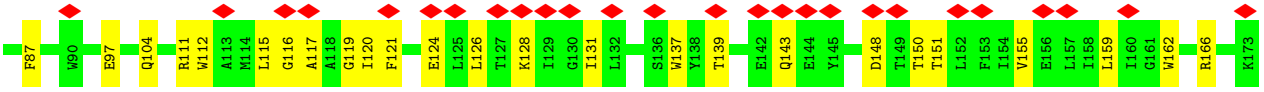


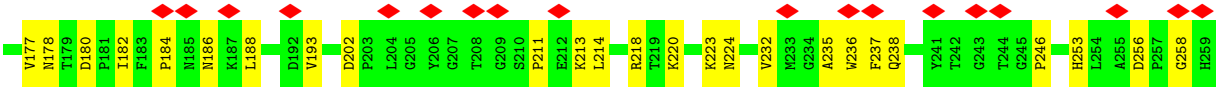


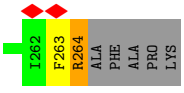


• Molecule 13: Chlorophyll a-b binding protein, chloroplastic

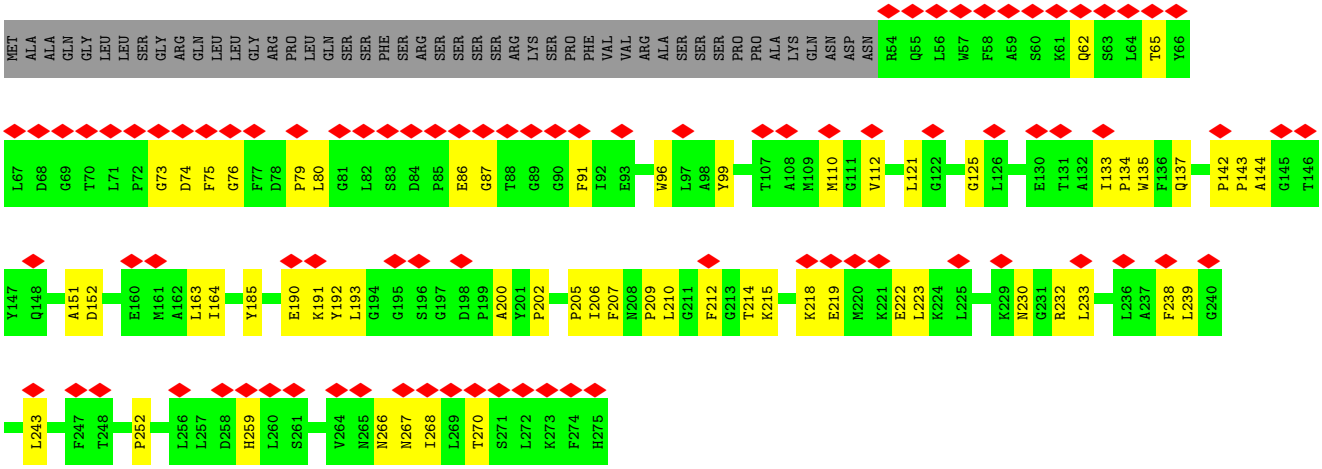






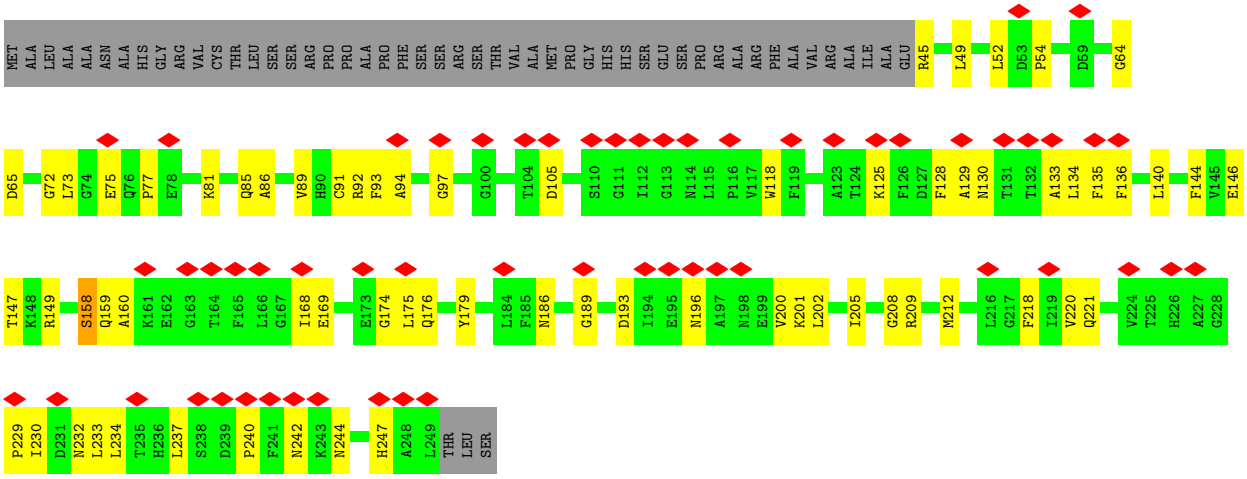


• Molecule 14: Chlorophyll a-b binding protein, chloroplastic



• Molecule 15: Chlorophyll a-b binding protein Lhca5

Chain 5:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	103844	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	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	5.056	Depositor
Minimum map value	-2.079	Depositor
Average map value	-0.001	Depositor
Map value standard deviation	0.082	Depositor
Recommended contour level	0.72	Depositor
Map size (Å)	575.08, 575.08, 575.08	wwPDB
Map dimensions	440, 440, 440	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.307, 1.307, 1.307	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: LUT, LMG, CLA, SF4, DGD, BCR, XAT, CL0, PQN, LHG, CHL

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	0.66	0/6010	0.49	0/8202
2	B	0.69	0/6058	0.51	1/8273 (0.0%)
3	C	0.73	0/621	0.53	0/840
4	D	0.61	0/1142	0.53	0/1542
5	E	0.65	0/551	0.49	0/751
6	F	0.63	2/1229 (0.2%)	0.48	0/1664
7	H	0.37	0/467	0.46	0/631
8	I	0.55	0/238	0.48	0/324
9	J	0.54	0/343	0.58	0/467
10	K	0.38	0/571	0.55	0/775
11	L	0.57	0/1120	0.52	0/1534
12	1	0.36	0/1467	0.43	0/2008
13	2	0.42	0/1616	0.46	0/2215
14	3	0.41	0/1682	0.50	0/2295
15	5	0.45	0/1527	0.50	0/2085
All	All	0.59	2/24642 (0.0%)	0.50	1/33606 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
2	B	0	1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	F	181	TYR	CE1-CZ	-8.91	1.26	1.38
6	F	181	TYR	CG-CD1	-5.10	1.32	1.39

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	223	GLY	N-CA-C	-5.13	100.26	113.10

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	222	LEU	Mainchain

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5813	0	5633	132	0
2	B	5849	0	5600	95	0
3	C	610	0	597	22	0
4	D	1113	0	1113	27	0
5	E	538	0	537	8	0
6	F	1203	0	1199	42	0
7	H	454	0	487	6	0
8	I	232	0	254	4	0
9	J	333	0	347	12	0
10	K	565	0	557	18	0
11	L	1088	0	1079	30	0
12	1	1422	0	1324	50	0
13	2	1561	0	1485	57	0
14	3	1629	0	1496	47	0
15	5	1486	0	1389	58	0
16	A	61	0	62	4	0
17	1	471	0	375	27	0
17	2	454	0	383	23	0
17	3	590	0	442	33	0
17	5	468	0	375	21	0
17	A	2024	0	1724	73	0
17	B	2118	0	1848	86	0
17	F	83	0	60	5	0
17	J	42	0	31	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
17	K	157	0	107	7	0
17	L	193	0	152	8	0
18	A	33	0	46	2	0
18	B	30	0	37	1	0
19	1	49	0	74	5	0
19	2	35	0	40	2	0
19	A	79	0	104	8	0
19	B	38	0	46	0	0
20	1	19	0	26	3	0
20	2	40	0	56	4	0
20	3	40	0	56	4	0
20	5	40	0	56	6	0
20	A	279	0	389	18	0
20	B	280	0	392	20	0
20	F	80	0	112	5	0
20	I	40	0	56	4	0
20	J	40	0	56	1	0
20	K	40	0	56	2	0
20	L	80	0	112	10	0
21	A	8	0	0	0	0
21	C	16	0	0	1	0
22	B	59	0	79	4	0
22	J	66	0	96	3	0
23	2	52	0	55	3	0
23	5	32	0	34	1	0
23	F	75	0	90	3	0
24	1	84	0	112	11	0
24	2	42	0	56	9	0
24	3	84	0	112	14	0
24	5	42	0	56	8	0
25	1	129	0	83	7	0
25	2	174	0	110	13	0
25	3	90	0	60	2	0
25	5	133	0	80	8	0
26	2	44	0	56	7	0
26	5	44	0	56	5	0
All	All	32973	0	31505	816	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 13.

The worst 5 of 816 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)
6:F:181:TYR:CE1	6:F:185:VAL:CG1	2.51	0.92
6:F:181:TYR:HE1	6:F:185:VAL:CG1	1.82	0.92
6:F:181:TYR:CE1	6:F:185:VAL:HG11	2.07	0.88
16:A:801:CL0:H13	17:B:802:CLA:OBD	1.77	0.84
6:F:181:TYR:CE1	6:F:185:VAL:HG13	2.18	0.78

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	740/750 (99%)	690 (93%)	50 (7%)	0	100 100
2	B	731/734 (100%)	688 (94%)	42 (6%)	1 (0%)	48 78
3	C	79/81 (98%)	70 (89%)	9 (11%)	0	100 100
4	D	140/205 (68%)	118 (84%)	22 (16%)	0	100 100
5	E	66/147 (45%)	61 (92%)	5 (8%)	0	100 100
6	F	156/235 (66%)	150 (96%)	6 (4%)	0	100 100
7	H	59/143 (41%)	58 (98%)	1 (2%)	0	100 100
8	I	28/36 (78%)	28 (100%)	0	0	100 100
9	J	40/42 (95%)	37 (92%)	2 (5%)	1 (2%)	4 22
10	K	82/131 (63%)	73 (89%)	9 (11%)	0	100 100
11	L	144/209 (69%)	135 (94%)	9 (6%)	0	100 100
12	1	189/247 (76%)	179 (95%)	10 (5%)	0	100 100
13	2	201/255 (79%)	185 (92%)	16 (8%)	0	100 100
14	3	220/269 (82%)	195 (89%)	25 (11%)	0	100 100
15	5	203/257 (79%)	173 (85%)	30 (15%)	0	100 100
All	All	3078/3741 (82%)	2840 (92%)	236 (8%)	2 (0%)	50 78

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	223	GLY
9	J	36	ALA

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	592/608 (97%)	589 (100%)	3 (0%)	86	91
2	B	594/601 (99%)	590 (99%)	4 (1%)	81	88
3	C	70/71 (99%)	69 (99%)	1 (1%)	62	77
4	D	119/160 (74%)	119 (100%)	0	100	100
5	E	58/112 (52%)	58 (100%)	0	100	100
6	F	120/183 (66%)	120 (100%)	0	100	100
7	H	48/110 (44%)	48 (100%)	0	100	100
8	I	26/33 (79%)	26 (100%)	0	100	100
9	J	35/36 (97%)	35 (100%)	0	100	100
10	K	52/102 (51%)	51 (98%)	1 (2%)	52	71
11	L	112/166 (68%)	110 (98%)	2 (2%)	54	73
12	1	134/196 (68%)	133 (99%)	1 (1%)	81	88
13	2	156/194 (80%)	155 (99%)	1 (1%)	84	90
14	3	147/216 (68%)	147 (100%)	0	100	100
15	5	139/202 (69%)	138 (99%)	1 (1%)	81	88
All	All	2402/2990 (80%)	2388 (99%)	14 (1%)	82	90

5 of 14 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	C	47	ASP
10	K	104	ASP
15	5	158	SER

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Mol	Chain	Res	Type
12	1	170	PHE
13	2	264	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
4	D	68	GLN

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 oligosaccharides in this entry.

5.6 Ligand geometry (i)

199 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
17	CLA	B	804	-	65,73,73	1.42	11 (16%)	76,113,113	1.42	6 (7%)
20	BCR	B	852	-	41,41,41	1.22	3 (7%)	56,56,56	2.06	18 (32%)
17	CLA	2	509	-	50,58,73	1.60	7 (14%)	58,95,113	1.63	8 (13%)
19	LHG	B	851	-	37,37,48	1.08	2 (5%)	40,43,54	1.17	4 (10%)
17	CLA	A	814	-	42,50,73	1.82	10 (23%)	48,85,113	1.73	9 (18%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
24	LUT	3	304	-	42,43,43	0.91	2 (4%)	51,60,60	1.56	10 (19%)
24	LUT	5	303	-	42,43,43	0.95	2 (4%)	51,60,60	1.83	13 (25%)
17	CLA	B	812	-	54,62,73	1.59	8 (14%)	67,100,113	1.57	13 (19%)
17	CLA	B	816	-	43,51,73	1.67	9 (20%)	49,86,113	1.66	6 (12%)
17	CLA	1	515	-	45,52,73	1.81	9 (20%)	47,87,113	1.61	6 (12%)
20	BCR	2	503	-	41,41,41	0.89	1 (2%)	56,56,56	3.62	27 (48%)
17	CLA	K	203	-	39,48,73	1.71	10 (25%)	45,82,113	1.68	8 (17%)
17	CLA	A	835	-	51,59,73	1.62	10 (19%)	59,96,113	1.75	9 (15%)
24	LUT	1	501	-	42,43,43	0.89	1 (2%)	51,60,60	1.65	11 (21%)
16	CL0	A	801	-	61,69,73	1.64	10 (16%)	70,107,113	2.21	16 (22%)
17	CLA	B	826	-	62,70,73	1.40	10 (16%)	72,109,113	1.52	10 (13%)
17	CLA	3	309	-	41,48,73	2.19	11 (26%)	50,82,113	1.57	6 (12%)
23	LMG	5	301	-	32,32,55	1.18	2 (6%)	40,40,63	1.15	3 (7%)
25	CHL	3	302	13	47,55,74	2.24	15 (31%)	50,91,114	2.81	18 (36%)
22	DGD	B	850	-	60,60,67	0.88	2 (3%)	74,74,81	1.39	11 (14%)
17	CLA	2	505	-	52,60,73	1.58	7 (13%)	60,97,113	1.53	6 (10%)
17	CLA	3	318	-	45,53,73	1.67	7 (15%)	56,89,113	1.59	8 (14%)
17	CLA	A	852	-	57,65,73	1.61	9 (15%)	66,103,113	1.43	9 (13%)
17	CLA	5	310	-	50,58,73	1.65	8 (16%)	58,95,113	1.59	8 (13%)
17	CLA	1	509	-	50,58,73	1.63	7 (14%)	58,95,113	1.60	7 (12%)
26	XAT	2	502	-	39,47,47	1.13	4 (10%)	54,74,74	2.84	20 (37%)
17	CLA	L	304	-	45,53,73	1.65	10 (22%)	52,89,113	1.88	11 (21%)
17	CLA	K	205	10	37,47,73	1.93	7 (18%)	42,81,113	1.73	8 (19%)
17	CLA	A	802	-	58,66,73	1.54	9 (15%)	67,104,113	1.51	7 (10%)
17	CLA	A	804	17	52,60,73	1.56	9 (17%)	60,97,113	1.60	7 (11%)
17	CLA	5	316	-	41,49,73	1.73	9 (21%)	47,84,113	1.80	9 (19%)
17	CLA	1	505	-	42,50,73	1.86	7 (16%)	48,85,113	1.58	8 (16%)
17	CLA	A	831	-	63,71,73	1.50	10 (15%)	77,110,113	1.53	12 (15%)
17	CLA	B	821	-	50,58,73	1.71	9 (18%)	58,95,113	1.62	8 (13%)
20	BCR	L	306	-	41,41,41	0.85	1 (2%)	56,56,56	1.96	19 (33%)
24	LUT	1	502	-	42,43,43	0.90	2 (4%)	51,60,60	1.68	11 (21%)
24	LUT	3	303	-	42,43,43	0.89	2 (4%)	51,60,60	1.51	10 (19%)
17	CLA	A	811	-	39,48,73	1.73	9 (23%)	45,82,113	1.74	10 (22%)
17	CLA	2	506	-	65,73,73	1.44	9 (13%)	76,113,113	1.51	7 (9%)
23	LMG	F	806	-	45,45,55	0.95	2 (4%)	53,53,63	1.07	4 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
20	BCR	F	801	-	41,41,41	0.99	2 (4%)	56,56,56	2.09	17 (30%)
20	BCR	J	102	-	41,41,41	1.01	2 (4%)	56,56,56	2.18	24 (42%)
20	BCR	3	305	-	41,41,41	0.90	2 (4%)	56,56,56	1.98	13 (23%)
17	CLA	B	808	-	52,60,73	1.68	9 (17%)	60,97,113	1.57	9 (15%)
25	CHL	2	512	-	46,54,74	2.17	14 (30%)	53,90,114	2.91	20 (37%)
17	CLA	B	822	-	47,55,73	1.72	10 (21%)	54,91,113	1.75	7 (12%)
17	CLA	5	311	-	42,50,73	1.72	7 (16%)	48,85,113	1.74	8 (16%)
17	CLA	B	828	-	41,49,73	1.74	10 (24%)	47,84,113	1.81	12 (25%)
17	CLA	A	813	-	45,53,73	1.69	9 (20%)	52,89,113	1.63	7 (13%)
20	BCR	B	848	-	41,41,41	1.05	2 (4%)	56,56,56	1.98	18 (32%)
25	CHL	5	317	-	41,48,74	2.34	15 (36%)	42,82,114	3.07	22 (52%)
25	CHL	2	513	-	40,48,74	2.49	16 (40%)	37,81,114	3.16	19 (51%)
17	CLA	3	314	14	55,63,73	1.58	6 (10%)	64,101,113	1.55	10 (15%)
17	CLA	A	824	-	39,48,73	1.77	8 (20%)	45,82,113	1.68	8 (17%)
17	CLA	3	313	-	48,56,73	1.71	6 (12%)	55,92,113	1.66	9 (16%)
17	CLA	2	508	-	47,55,73	1.72	7 (14%)	54,91,113	1.49	6 (11%)
17	CLA	3	316	-	38,45,73	1.80	5 (13%)	43,78,113	1.82	8 (18%)
17	CLA	5	306	-	39,48,73	1.78	6 (15%)	44,83,113	1.70	7 (15%)
17	CLA	A	808	1	65,73,73	1.42	10 (15%)	76,113,113	1.44	7 (9%)
17	CLA	3	317	-	41,49,73	1.79	8 (19%)	47,84,113	1.74	10 (21%)
20	BCR	L	305	-	41,41,41	1.00	1 (2%)	56,56,56	2.16	18 (32%)
17	CLA	A	810	17	54,62,73	1.59	10 (18%)	62,99,113	1.66	7 (11%)
17	CLA	B	833	-	65,73,73	1.39	8 (12%)	76,113,113	1.57	10 (13%)
17	CLA	B	836	-	42,50,73	1.84	9 (21%)	48,85,113	1.56	7 (14%)
17	CLA	L	301	-	56,64,73	1.59	11 (19%)	65,102,113	1.50	8 (12%)
17	CLA	1	511	-	46,54,73	1.71	9 (19%)	53,90,113	1.61	7 (13%)
23	LMG	2	519	-	36,36,55	1.09	2 (5%)	44,44,63	1.37	8 (18%)
25	CHL	1	512	-	47,55,74	2.31	16 (34%)	50,91,114	2.77	20 (40%)
17	CLA	A	838	-	65,73,73	1.46	10 (15%)	76,113,113	1.45	10 (13%)
26	XAT	5	304	-	39,47,47	1.24	5 (12%)	54,74,74	2.53	18 (33%)
17	CLA	3	307	-	39,48,73	2.01	9 (23%)	45,82,113	1.58	7 (15%)
17	CLA	A	832	-	44,53,73	1.68	10 (22%)	52,88,113	1.78	8 (15%)
17	CLA	B	806	-	38,47,73	1.98	12 (31%)	46,80,113	1.77	10 (21%)
17	CLA	B	825	-	42,50,73	1.70	10 (23%)	48,85,113	1.69	7 (14%)
17	CLA	A	826	-	60,68,73	1.48	8 (13%)	70,107,113	1.54	9 (12%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
25	CHL	1	517	12	40,49,74	2.29	14 (35%)	42,83,114	3.16	20 (47%)
17	CLA	B	830	-	56,64,73	1.72	11 (19%)	65,102,113	1.45	7 (10%)
20	BCR	A	847	-	41,41,41	0.97	2 (4%)	56,56,56	2.00	20 (35%)
22	DGD	J	103	-	67,67,67	0.83	2 (2%)	81,81,81	1.11	4 (4%)
24	LUT	2	501	-	42,43,43	0.94	1 (2%)	51,60,60	1.94	15 (29%)
25	CHL	1	514	-	40,49,74	2.55	15 (37%)	42,83,114	3.00	19 (45%)
17	CLA	B	838	-	65,73,73	1.47	10 (15%)	76,113,113	1.49	8 (10%)
17	CLA	5	305	-	38,46,73	2.22	10 (26%)	47,79,113	1.71	10 (21%)
17	CLA	B	835	-	60,68,73	1.49	9 (15%)	70,107,113	1.50	11 (15%)
17	CLA	B	823	-	42,50,73	1.76	9 (21%)	48,85,113	1.68	7 (14%)
17	CLA	A	828	-	41,49,73	1.76	10 (24%)	47,84,113	1.68	7 (14%)
17	CLA	1	510	19	46,54,73	1.73	8 (17%)	53,90,113	1.56	7 (13%)
17	CLA	1	508	-	39,48,73	1.83	6 (15%)	45,82,113	1.71	7 (15%)
17	CLA	B	837	-	50,58,73	1.62	10 (20%)	58,95,113	1.62	10 (17%)
17	CLA	B	827	-	41,49,73	1.78	10 (24%)	47,84,113	1.86	10 (21%)
23	LMG	F	805	-	30,30,55	1.22	2 (6%)	38,38,63	1.21	3 (7%)
17	CLA	A	812	-	42,50,73	1.75	10 (23%)	48,85,113	1.76	10 (20%)
25	CHL	2	515	-	45,53,74	2.23	14 (31%)	52,89,114	2.82	21 (40%)
21	SF4	C	102	3	0,12,12	-	-	-		
20	BCR	B	847	-	41,41,41	1.03	2 (4%)	56,56,56	2.35	19 (33%)
17	CLA	B	817	-	49,57,73	1.68	11 (22%)	55,93,113	1.59	7 (12%)
19	LHG	A	843	-	48,48,48	0.90	3 (6%)	51,54,54	1.29	5 (9%)
17	CLA	A	842	19	50,58,73	1.66	10 (20%)	58,95,113	1.52	8 (13%)
17	CLA	B	805	-	41,49,73	1.79	9 (21%)	47,84,113	1.75	10 (21%)
17	CLA	B	811	-	55,63,73	1.58	11 (20%)	64,101,113	1.53	7 (10%)
17	CLA	J	101	9	42,50,73	1.79	6 (14%)	48,85,113	1.68	7 (14%)
17	CLA	A	834	1	41,49,73	1.82	9 (21%)	47,84,113	1.62	7 (14%)
17	CLA	A	818	-	39,48,73	1.75	10 (25%)	45,82,113	1.74	9 (20%)
17	CLA	B	801	-	65,73,73	1.47	11 (16%)	76,113,113	1.47	10 (13%)
17	CLA	K	202	-	41,49,73	1.75	8 (19%)	47,84,113	1.70	8 (17%)
25	CHL	5	315	-	46,54,74	2.23	15 (32%)	49,90,114	2.89	21 (42%)
20	BCR	B	845	-	41,41,41	1.04	1 (2%)	56,56,56	2.07	17 (30%)
20	BCR	A	853	-	41,41,41	0.97	2 (4%)	56,56,56	2.24	18 (32%)
19	LHG	2	517	17	34,34,48	1.07	2 (5%)	37,40,54	1.21	4 (10%)
17	CLA	K	201	-	38,45,73	1.92	9 (23%)	43,78,113	1.66	6 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
17	CLA	5	312	-	46,54,73	1.73	8 (17%)	53,90,113	1.50	7 (13%)
17	CLA	B	832	-	43,51,73	1.67	9 (20%)	49,86,113	1.62	5 (10%)
17	CLA	A	830	-	50,58,73	1.59	9 (18%)	58,95,113	1.64	6 (10%)
20	BCR	B	849	-	41,41,41	1.07	2 (4%)	56,56,56	2.01	17 (30%)
17	CLA	B	820	-	53,61,73	1.68	10 (18%)	61,98,113	1.48	8 (13%)
20	BCR	5	302	-	41,41,41	0.83	0	56,56,56	1.97	13 (23%)
17	CLA	A	809	1	38,47,73	1.83	9 (23%)	39,80,113	1.63	5 (12%)
17	CLA	A	815	-	45,53,73	1.71	9 (20%)	52,89,113	1.61	8 (15%)
17	CLA	A	822	-	41,49,73	1.80	9 (21%)	47,84,113	1.79	9 (19%)
17	CLA	B	831	-	43,51,73	1.80	9 (20%)	49,86,113	1.62	7 (14%)
19	LHG	1	516	17	48,48,48	0.91	2 (4%)	51,54,54	1.16	4 (7%)
17	CLA	L	303	-	52,60,73	1.62	9 (17%)	60,97,113	1.73	10 (16%)
17	CLA	F	802	-	42,50,73	1.78	9 (21%)	48,85,113	1.68	7 (14%)
17	CLA	B	818	-	59,67,73	1.50	10 (16%)	68,105,113	1.59	9 (13%)
23	LMG	2	518	-	16,16,55	0.47	0	22,22,63	0.99	2 (9%)
17	CLA	B	819	-	41,49,73	1.77	10 (24%)	47,84,113	1.83	12 (25%)
18	PQN	B	843	-	31,31,34	1.36	2 (6%)	38,41,45	1.49	5 (13%)
20	BCR	A	846	-	41,41,41	1.05	2 (4%)	56,56,56	2.07	17 (30%)
17	CLA	A	805	-	64,72,73	1.50	12 (18%)	74,111,113	1.57	10 (13%)
17	CLA	B	810	2	39,48,73	1.75	10 (25%)	45,82,113	1.81	9 (20%)
20	BCR	I	101	-	41,41,41	1.22	3 (7%)	56,56,56	2.08	19 (33%)
17	CLA	5	308	-	60,68,73	1.52	9 (15%)	70,107,113	1.57	8 (11%)
20	BCR	F	804	-	41,41,41	1.03	1 (2%)	56,56,56	1.97	18 (32%)
17	CLA	1	513	-	65,73,73	1.53	7 (10%)	76,113,113	1.36	7 (9%)
20	BCR	B	844	-	41,41,41	0.85	1 (2%)	56,56,56	2.59	19 (33%)
17	CLA	B	802	-	64,72,73	1.46	10 (15%)	74,111,113	1.49	10 (13%)
17	CLA	B	809	-	39,48,73	1.81	10 (25%)	45,82,113	1.69	6 (13%)
17	CLA	A	829	-	55,63,73	1.60	10 (18%)	64,101,113	1.59	9 (14%)
17	CLA	3	301	-	41,49,73	1.80	9 (21%)	47,84,113	1.74	10 (21%)
21	SF4	C	101	3	0,12,12	-	-	-		
25	CHL	5	314	-	47,55,74	2.22	15 (31%)	50,91,114	2.82	21 (42%)
17	CLA	A	840	-	41,49,73	1.82	9 (21%)	47,84,113	1.64	8 (17%)
20	BCR	B	846	-	41,41,41	1.05	3 (7%)	56,56,56	2.31	18 (32%)
17	CLA	B	842	-	57,65,73	1.55	8 (14%)	66,103,113	1.46	7 (10%)
17	CLA	B	803	-	65,73,73	1.45	9 (13%)	76,113,113	1.40	10 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
17	CLA	B	815	-	65,73,73	1.50	11 (16%)	76,113,113	1.44	10 (13%)
17	CLA	A	819	-	39,48,73	1.82	9 (23%)	45,82,113	1.67	7 (15%)
17	CLA	5	313	15	39,48,73	1.80	9 (23%)	45,82,113	1.64	8 (17%)
17	CLA	A	825	-	59,67,73	1.55	10 (16%)	68,105,113	1.47	8 (11%)
17	CLA	B	824	-	45,53,73	1.74	9 (20%)	52,89,113	1.54	6 (11%)
17	CLA	A	816	-	59,67,73	1.47	8 (13%)	68,105,113	1.56	8 (11%)
25	CHL	3	315	-	43,51,74	2.17	14 (32%)	45,86,114	3.02	19 (42%)
20	BCR	A	848	-	41,41,41	1.06	2 (4%)	56,56,56	2.00	12 (21%)
17	CLA	F	803	-	41,49,73	1.77	9 (21%)	47,84,113	1.65	8 (17%)
17	CLA	3	308	-	55,63,73	1.49	9 (16%)	64,101,113	1.54	9 (14%)
17	CLA	2	504	13	34,44,73	2.06	10 (29%)	42,76,113	1.87	10 (23%)
17	CLA	3	306	-	52,60,73	1.60	7 (13%)	65,97,113	1.75	11 (16%)
17	CLA	2	511	-	39,48,73	1.82	10 (25%)	45,82,113	1.93	11 (24%)
17	CLA	2	507	13	47,56,73	1.97	9 (19%)	54,91,113	1.81	10 (18%)
20	BCR	A	849	-	40,40,41	1.04	2 (5%)	54,54,56	1.90	15 (27%)
25	CHL	2	516	13	43,51,74	2.19	13 (30%)	49,86,114	3.04	19 (38%)
19	LHG	A	844	17	29,29,48	1.20	3 (10%)	32,35,54	1.19	3 (9%)
17	CLA	5	307	15	65,73,73	1.47	8 (12%)	76,113,113	1.35	8 (10%)
17	CLA	5	309	-	45,53,73	1.72	8 (17%)	52,89,113	1.65	7 (13%)
17	CLA	A	837	-	41,49,73	1.84	11 (26%)	47,84,113	1.87	10 (21%)
17	CLA	A	820	-	57,65,73	1.53	8 (14%)	66,103,113	1.69	9 (13%)
17	CLA	A	806	1	65,73,73	1.44	9 (13%)	76,113,113	1.41	8 (10%)
17	CLA	B	829	-	39,48,73	1.77	11 (28%)	45,82,113	1.73	9 (20%)
20	BCR	K	204	-	41,41,41	0.99	2 (4%)	56,56,56	2.02	16 (28%)
17	CLA	A	807	-	37,47,73	1.78	10 (27%)	41,80,113	1.76	8 (19%)
17	CLA	B	840	-	41,49,73	1.75	9 (21%)	47,84,113	1.80	8 (17%)
17	CLA	B	841	-	54,62,73	1.56	10 (18%)	62,99,113	1.53	9 (14%)
18	PQN	A	841	-	34,34,34	1.38	2 (5%)	42,45,45	1.24	4 (9%)
17	CLA	A	817	-	39,47,73	2.03	13 (33%)	42,81,113	1.80	7 (16%)
17	CLA	B	839	-	47,55,73	1.66	9 (19%)	54,91,113	1.73	9 (16%)
17	CLA	A	821	-	42,50,73	1.78	9 (21%)	48,85,113	1.79	8 (16%)
17	CLA	A	836	-	55,63,73	1.65	10 (18%)	64,101,113	1.60	10 (15%)
17	CLA	1	507	12	42,50,73	1.71	9 (21%)	48,85,113	1.68	9 (18%)
17	CLA	B	834	-	45,53,73	1.73	9 (20%)	52,89,113	1.66	10 (19%)
17	CLA	B	814	-	41,49,73	1.78	11 (26%)	47,84,113	1.77	12 (25%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
21	SF4	A	850	1,2	0,12,12	-	-	-		
17	CLA	A	803	-	41,49,73	1.80	10 (24%)	47,84,113	1.79	10 (21%)
17	CLA	A	823	-	55,62,73	1.74	11 (20%)	60,99,113	1.54	10 (16%)
17	CLA	3	310	-	45,53,73	1.77	7 (15%)	52,89,113	1.63	9 (17%)
17	CLA	3	311	-	50,58,73	1.51	7 (14%)	58,95,113	1.74	11 (18%)
17	CLA	A	827	-	65,73,73	1.42	12 (18%)	76,113,113	1.51	9 (11%)
17	CLA	1	504	-	41,49,73	1.78	7 (17%)	47,84,113	1.60	6 (12%)
17	CLA	2	514	-	55,63,73	1.55	10 (18%)	64,101,113	1.47	8 (12%)
17	CLA	B	807	2	65,73,73	1.46	11 (16%)	76,113,113	1.42	6 (7%)
17	CLA	2	510	19	60,68,73	1.50	7 (11%)	70,107,113	1.51	9 (12%)
17	CLA	3	312	-	41,49,73	1.84	7 (17%)	47,84,113	1.63	8 (17%)
20	BCR	1	503	-	19,19,41	0.67	0	26,26,56	2.04	7 (26%)
20	BCR	A	845	-	41,41,41	1.17	4 (9%)	56,56,56	2.29	20 (35%)
17	CLA	L	302	-	41,48,73	1.92	9 (21%)	45,82,113	1.80	8 (17%)
17	CLA	B	813	-	43,51,73	1.72	9 (20%)	49,86,113	1.69	9 (18%)
17	CLA	A	833	-	39,48,73	1.74	10 (25%)	45,82,113	1.77	9 (20%)
17	CLA	1	506	-	55,63,73	1.62	8 (14%)	64,101,113	1.50	8 (12%)
20	BCR	A	851	-	41,41,41	0.91	1 (2%)	56,56,56	2.17	20 (35%)
17	CLA	A	839	-	42,50,73	1.81	10 (23%)	48,85,113	1.73	7 (14%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
17	CLA	B	804	-	1/1/15/20	14/37/115/115	-
20	BCR	B	852	-	-	6/29/63/63	0/2/2/2
17	CLA	2	509	-	1/1/12/20	10/19/97/115	-
19	LHG	B	851	-	-	18/42/42/53	-
17	CLA	A	814	-	1/1/10/20	1/10/88/115	-
24	LUT	3	304	-	-	2/29/67/67	0/2/2/2
24	LUT	5	303	-	-	2/29/67/67	0/2/2/2
17	CLA	B	812	-	1/1/13/20	6/25/101/115	-
17	CLA	B	816	-	1/1/10/20	4/11/89/115	-
17	CLA	1	515	-	1/1/10/20	6/13/87/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
20	BCR	2	503	-	-	8/29/63/63	0/2/2/2
17	CLA	K	203	-	1/1/9/20	5/8/82/115	-
17	CLA	A	835	-	1/1/12/20	12/21/99/115	-
24	LUT	1	501	-	-	2/29/67/67	0/2/2/2
16	CL0	A	801	-	3/3/18/25	5/33/125/135	-
17	CLA	B	826	-	1/1/14/20	8/34/112/115	-
17	CLA	3	309	-	-	4/10/86/115	-
23	LMG	5	301	-	-	8/27/47/70	0/1/1/1
25	CHL	3	302	13	3/3/16/26	3/17/115/137	-
22	DGD	B	850	-	-	19/48/88/95	0/2/2/2
17	CLA	3	318	-	1/1/11/20	6/15/91/115	-
17	CLA	2	505	-	-	11/22/100/115	-
17	CLA	A	852	-	1/1/13/20	9/28/106/115	-
17	CLA	5	310	-	1/1/12/20	10/19/97/115	-
17	CLA	1	509	-	-	6/19/97/115	-
26	XAT	2	502	-	-	6/31/93/93	0/4/4/4
17	CLA	L	304	-	1/1/11/20	6/13/91/115	-
17	CLA	K	205	10	1/1/9/20	0/6/80/115	-
17	CLA	A	802	-	1/1/13/20	12/29/107/115	-
17	CLA	A	804	17	1/1/12/20	5/22/100/115	-
17	CLA	5	316	-	1/1/10/20	2/8/86/115	-
17	CLA	1	505	-	1/1/10/20	3/10/88/115	-
17	CLA	A	831	-	1/1/14/20	17/35/111/115	-
17	CLA	B	821	-	1/1/12/20	5/19/97/115	-
20	BCR	L	306	-	-	6/29/63/63	0/2/2/2
24	LUT	1	502	-	-	4/29/67/67	0/2/2/2
24	LUT	3	303	-	-	2/29/67/67	0/2/2/2
17	CLA	A	811	-	1/1/9/20	2/8/82/115	-
17	CLA	2	506	-	1/1/15/20	16/37/115/115	-
23	LMG	F	806	-	-	18/40/60/70	0/1/1/1
20	BCR	F	801	-	-	6/29/63/63	0/2/2/2
20	BCR	J	102	-	-	3/29/63/63	0/2/2/2
20	BCR	3	305	-	-	8/29/63/63	0/2/2/2
17	CLA	B	808	-	1/1/12/20	7/22/100/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
25	CHL	2	512	-	3/3/16/26	3/17/113/137	-
17	CLA	B	822	-	1/1/11/20	4/16/94/115	-
17	CLA	5	311	-	1/1/10/20	4/10/88/115	-
17	CLA	B	828	-	1/1/10/20	3/8/86/115	-
17	CLA	A	813	-	1/1/11/20	9/13/91/115	-
25	CHL	5	317	-	3/3/14/26	4/8/102/137	-
20	BCR	B	848	-	-	2/29/63/63	0/2/2/2
25	CHL	2	513	-	3/3/13/26	5/10/100/137	-
17	CLA	3	314	14	1/1/13/20	13/25/103/115	-
17	CLA	A	824	-	1/1/9/20	5/8/82/115	-
17	CLA	3	313	-	1/1/11/20	10/17/95/115	-
17	CLA	2	508	-	1/1/11/20	2/15/93/115	-
17	CLA	3	316	-	1/1/8/20	0/2/76/115	-
17	CLA	5	306	-	1/1/10/20	2/6/84/115	-
17	CLA	A	808	1	1/1/15/20	8/37/115/115	-
17	CLA	3	317	-	1/1/10/20	4/8/86/115	-
20	BCR	L	305	-	-	9/29/63/63	0/2/2/2
17	CLA	A	810	17	1/1/12/20	5/24/102/115	-
17	CLA	B	833	-	1/1/15/20	4/37/115/115	-
17	CLA	B	836	-	-	4/10/88/115	-
17	CLA	L	301	-	1/1/13/20	5/27/105/115	-
17	CLA	1	511	-	1/1/11/20	5/15/93/115	-
25	CHL	1	512	-	3/3/16/26	8/17/115/137	-
23	LMG	2	519	-	-	14/31/51/70	0/1/1/1
17	CLA	A	838	-	1/1/15/20	15/37/115/115	-
26	XAT	5	304	-	-	2/31/93/93	0/4/4/4
17	CLA	3	307	-	1/1/9/20	3/8/82/115	-
17	CLA	A	832	-	1/1/10/20	5/11/89/115	-
17	CLA	B	806	-	1/1/8/20	4/8/79/115	-
17	CLA	B	825	-	1/1/10/20	3/10/88/115	-
17	CLA	A	826	-	1/1/14/20	13/31/109/115	-
25	CHL	1	517	12	3/3/14/26	5/10/104/137	-
17	CLA	B	830	-	1/1/13/20	11/27/105/115	-
20	BCR	A	847	-	-	2/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	DGD	J	103	-	-	26/55/95/95	0/2/2/2
24	LUT	2	501	-	-	0/29/67/67	0/2/2/2
25	CHL	1	514	-	3/3/14/26	4/10/104/137	-
17	CLA	B	838	-	1/1/15/20	4/37/115/115	-
17	CLA	5	305	-	1/1/9/20	1/8/80/115	-
17	CLA	B	835	-	1/1/14/20	6/31/109/115	-
17	CLA	B	823	-	1/1/10/20	4/10/88/115	-
17	CLA	A	828	-	1/1/10/20	2/8/86/115	-
17	CLA	1	510	19	1/1/11/20	7/15/93/115	-
17	CLA	1	508	-	1/1/9/20	3/8/82/115	-
17	CLA	B	837	-	1/1/12/20	5/19/97/115	-
17	CLA	B	827	-	1/1/10/20	3/8/86/115	-
23	LMG	F	805	-	-	4/25/45/70	0/1/1/1
17	CLA	A	812	-	1/1/10/20	3/10/88/115	-
25	CHL	2	515	-	3/3/16/26	6/15/111/137	-
21	SF4	C	102	3	-	-	0/6/5/5
20	BCR	B	847	-	-	5/29/63/63	0/2/2/2
17	CLA	B	817	-	1/1/11/20	7/18/96/115	-
19	LHG	A	843	-	-	13/53/53/53	-
17	CLA	A	842	19	1/1/12/20	9/19/97/115	-
17	CLA	B	805	-	1/1/10/20	2/8/86/115	-
17	CLA	B	811	-	1/1/13/20	12/25/103/115	-
17	CLA	J	101	9	1/1/10/20	7/10/88/115	-
17	CLA	A	834	1	1/1/10/20	4/8/86/115	-
17	CLA	A	818	-	1/1/9/20	4/8/82/115	-
17	CLA	B	801	-	1/1/15/20	9/37/115/115	-
17	CLA	K	202	-	1/1/10/20	2/8/86/115	-
25	CHL	5	315	-	3/3/16/26	4/15/113/137	-
20	BCR	B	845	-	-	6/29/63/63	0/2/2/2
20	BCR	A	853	-	-	2/29/63/63	0/2/2/2
19	LHG	2	517	17	-	5/39/39/53	-
17	CLA	K	201	-	1/1/8/20	0/2/76/115	-
17	CLA	5	312	-	1/1/11/20	7/15/93/115	-
17	CLA	B	832	-	1/1/10/20	3/11/89/115	-
17	CLA	A	830	-	1/1/12/20	3/19/97/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
20	BCR	B	849	-	-	3/29/63/63	0/2/2/2
17	CLA	B	820	-	1/1/12/20	5/23/101/115	-
20	BCR	5	302	-	-	9/29/63/63	0/2/2/2
17	CLA	A	809	1	1/1/9/20	1/4/84/115	-
17	CLA	A	815	-	1/1/11/20	4/13/91/115	-
17	CLA	A	822	-	1/1/10/20	2/8/86/115	-
17	CLA	B	831	-	1/1/10/20	1/11/89/115	-
19	LHG	1	516	17	-	23/53/53/53	-
17	CLA	L	303	-	1/1/12/20	12/22/100/115	-
17	CLA	F	802	-	1/1/10/20	2/10/88/115	-
17	CLA	B	818	-	1/1/13/20	16/30/108/115	-
23	LMG	2	518	-	-	3/7/27/70	0/1/1/1
17	CLA	B	819	-	1/1/10/20	0/8/86/115	-
18	PQN	B	843	-	-	7/20/40/43	0/2/2/2
20	BCR	A	846	-	-	7/29/63/63	0/2/2/2
17	CLA	A	805	-	1/1/14/20	18/36/114/115	-
17	CLA	B	810	2	1/1/9/20	2/8/82/115	-
20	BCR	I	101	-	-	4/29/63/63	0/2/2/2
17	CLA	5	308	-	1/1/14/20	14/31/109/115	-
20	BCR	F	804	-	-	2/29/63/63	0/2/2/2
17	CLA	1	513	-	-	19/37/115/115	-
20	BCR	B	844	-	-	4/29/63/63	0/2/2/2
17	CLA	B	802	-	1/1/14/20	6/35/113/115	-
17	CLA	B	809	-	1/1/9/20	2/8/82/115	-
17	CLA	A	829	-	1/1/13/20	6/25/103/115	-
17	CLA	3	301	-	1/1/10/20	2/8/86/115	-
25	CHL	5	314	-	3/3/16/26	7/17/115/137	-
21	SF4	C	101	3	-	-	0/6/5/5
17	CLA	A	840	-	1/1/10/20	2/8/86/115	-
20	BCR	B	846	-	-	6/29/63/63	0/2/2/2
17	CLA	B	842	-	1/1/13/20	15/28/106/115	-
17	CLA	B	803	-	1/1/15/20	16/37/115/115	-
17	CLA	B	815	-	1/1/15/20	7/37/115/115	-
17	CLA	A	819	-	1/1/9/20	3/8/82/115	-
17	CLA	5	313	15	1/1/9/20	2/8/82/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
17	CLA	A	825	-	1/1/13/20	8/30/108/115	-
17	CLA	B	824	-	1/1/11/20	6/13/91/115	-
17	CLA	A	816	-	1/1/13/20	12/29/107/115	-
25	CHL	3	315	-	3/3/15/26	3/12/110/137	-
20	BCR	A	848	-	-	6/29/63/63	0/2/2/2
17	CLA	F	803	-	1/1/10/20	3/8/86/115	-
17	CLA	3	308	-	1/1/13/20	14/25/103/115	-
17	CLA	2	504	13	1/1/7/20	0/2/73/115	-
17	CLA	3	306	-	1/1/13/20	14/23/99/115	-
17	CLA	2	511	-	1/1/9/20	1/8/82/115	-
17	CLA	2	507	13	2/2/11/20	5/14/88/115	-
20	BCR	A	849	-	-	2/27/61/63	0/2/2/2
25	CHL	2	516	13	3/3/15/26	8/13/109/137	-
19	LHG	A	844	17	-	11/34/34/53	-
17	CLA	5	307	15	1/1/15/20	17/37/115/115	-
17	CLA	5	309	-	1/1/11/20	5/13/91/115	-
17	CLA	A	837	-	1/1/10/20	4/8/86/115	-
17	CLA	A	820	-	1/1/13/20	10/28/106/115	-
17	CLA	A	806	1	1/1/15/20	20/37/115/115	-
17	CLA	B	829	-	1/1/9/20	2/8/82/115	-
20	BCR	K	204	-	-	8/29/63/63	0/2/2/2
17	CLA	A	807	-	1/1/8/20	1/5/79/115	-
17	CLA	B	840	-	1/1/10/20	1/8/86/115	-
17	CLA	B	841	-	1/1/12/20	8/24/102/115	-
18	PQN	A	841	-	-	13/23/43/43	0/2/2/2
17	CLA	A	817	-	1/1/9/20	0/2/82/115	-
17	CLA	B	839	-	1/1/11/20	5/16/94/115	-
17	CLA	A	821	-	1/1/10/20	2/10/88/115	-
17	CLA	A	836	-	1/1/13/20	11/25/103/115	-
17	CLA	1	507	12	1/1/10/20	4/10/88/115	-
17	CLA	B	834	-	1/1/11/20	6/13/91/115	-
17	CLA	B	814	-	1/1/10/20	5/8/86/115	-
21	SF4	A	850	1,2	-	-	0/6/5/5
17	CLA	A	803	-	1/1/10/20	0/8/86/115	-
17	CLA	A	823	-	1/1/12/20	13/25/99/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
17	CLA	3	310	-	1/1/11/20	4/13/91/115	-
17	CLA	3	311	-	1/1/12/20	8/19/97/115	-
17	CLA	A	827	-	1/1/15/20	17/37/115/115	-
17	CLA	1	504	-	1/1/10/20	5/8/86/115	-
17	CLA	2	514	-	1/1/13/20	8/25/103/115	-
17	CLA	B	807	2	1/1/15/20	11/37/115/115	-
17	CLA	2	510	19	1/1/14/20	16/31/109/115	-
17	CLA	3	312	-	1/1/10/20	5/8/86/115	-
20	BCR	1	503	-	-	4/11/28/63	0/1/1/2
20	BCR	A	845	-	-	6/29/63/63	0/2/2/2
17	CLA	L	302	-	1/1/9/20	1/8/82/115	-
17	CLA	B	813	-	1/1/10/20	3/11/89/115	-
17	CLA	A	833	-	1/1/9/20	1/8/82/115	-
17	CLA	1	506	-	1/1/13/20	9/25/103/115	-
20	BCR	A	851	-	-	6/29/63/63	0/2/2/2
17	CLA	A	839	-	1/1/10/20	3/10/88/115	-

The worst 5 of 1514 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	3	307	CLA	C4B-NB	8.26	1.42	1.35
17	3	309	CLA	C3B-C4B	7.94	1.48	1.39
17	1	513	CLA	C4B-NB	7.88	1.42	1.35
17	3	313	CLA	C4B-NB	7.60	1.42	1.35
17	1	505	CLA	C4B-NB	7.57	1.42	1.35

The worst 5 of 2004 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
20	2	503	BCR	C40-C30-C25	-12.70	89.71	110.30
16	A	801	CL0	C4A-NA-C1A	10.86	111.59	106.71
25	5	315	CHL	CMD-C2D-C1D	9.11	140.76	124.71
20	2	503	BCR	C20-C21-C22	-8.87	114.64	127.31
25	2	516	CHL	CMD-C2D-C1D	8.70	140.05	124.71

5 of 171 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
16	A	801	CL0	ND

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

5 of 1257 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
16	A	801	CL0	C1A-C2A-CAA-CBA
16	A	801	CL0	CHA-CBD-CGD-O2D
17	A	802	CLA	CHA-CBD-CGD-O1D
17	A	802	CLA	CHA-CBD-CGD-O2D
17	A	802	CLA	C6-C7-C8-C9

There are no ring outliers.

174 monomers are involved in 434 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
17	B	804	CLA	4	0
20	B	852	BCR	1	0
17	2	509	CLA	1	0
24	3	304	LUT	6	0
24	5	303	LUT	8	0
17	B	812	CLA	2	0
17	B	816	CLA	2	0
17	1	515	CLA	3	0
20	2	503	BCR	4	0
17	A	835	CLA	2	0
24	1	501	LUT	4	0
16	A	801	CL0	4	0
17	B	826	CLA	4	0
17	3	309	CLA	3	0
23	5	301	LMG	1	0
22	B	850	DGD	4	0
17	2	505	CLA	2	0
17	3	318	CLA	1	0
17	A	852	CLA	2	0
17	5	310	CLA	3	0
17	1	509	CLA	4	0
26	2	502	XAT	7	0
17	L	304	CLA	2	0
17	A	802	CLA	4	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
17	A	804	CLA	3	0
17	5	316	CLA	4	0
17	A	831	CLA	3	0
20	L	306	BCR	2	0
24	1	502	LUT	7	0
24	3	303	LUT	8	0
17	2	506	CLA	8	0
23	F	806	LMG	2	0
20	F	801	BCR	1	0
20	J	102	BCR	1	0
20	3	305	BCR	4	0
17	B	808	CLA	2	0
25	2	512	CHL	4	0
17	B	822	CLA	5	0
17	B	828	CLA	5	0
17	A	813	CLA	3	0
20	B	848	BCR	3	0
25	5	317	CHL	3	0
25	2	513	CHL	4	0
17	3	314	CLA	3	0
17	A	824	CLA	2	0
17	3	313	CLA	4	0
17	2	508	CLA	3	0
17	3	316	CLA	3	0
17	5	306	CLA	1	0
17	A	808	CLA	1	0
17	3	317	CLA	1	0
20	L	305	BCR	8	0
17	A	810	CLA	4	0
17	B	833	CLA	3	0
17	B	836	CLA	1	0
17	L	301	CLA	2	0
17	1	511	CLA	2	0
23	2	519	LMG	2	0
17	A	838	CLA	2	0
26	5	304	XAT	5	0
17	3	307	CLA	2	0
17	B	806	CLA	4	0
17	B	825	CLA	2	0
25	1	517	CHL	6	0
17	B	830	CLA	2	0
20	A	847	BCR	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
22	J	103	DGD	3	0
24	2	501	LUT	9	0
25	1	514	CHL	1	0
17	B	838	CLA	6	0
17	5	305	CLA	2	0
17	B	835	CLA	2	0
17	B	823	CLA	1	0
17	A	828	CLA	1	0
17	1	510	CLA	2	0
17	1	508	CLA	1	0
17	B	837	CLA	3	0
17	B	827	CLA	1	0
23	F	805	LMG	1	0
17	A	812	CLA	1	0
25	2	515	CHL	2	0
21	C	102	SF4	1	0
20	B	847	BCR	2	0
17	B	817	CLA	2	0
19	A	843	LHG	4	0
17	A	842	CLA	1	0
17	B	805	CLA	1	0
17	B	811	CLA	5	0
17	J	101	CLA	3	0
17	A	818	CLA	1	0
17	B	801	CLA	3	0
17	K	202	CLA	3	0
25	5	315	CHL	4	0
20	B	845	BCR	1	0
20	A	853	BCR	4	0
19	2	517	LHG	2	0
17	K	201	CLA	4	0
17	B	832	CLA	1	0
20	B	849	BCR	2	0
17	B	820	CLA	3	0
20	5	302	BCR	6	0
17	A	809	CLA	1	0
17	A	815	CLA	2	0
17	A	822	CLA	1	0
17	B	831	CLA	2	0
19	1	516	LHG	5	0
17	L	303	CLA	3	0
17	F	802	CLA	3	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
17	B	818	CLA	4	0
23	2	518	LMG	1	0
17	B	819	CLA	1	0
18	B	843	PQN	1	0
20	A	846	BCR	3	0
17	A	805	CLA	6	0
17	B	810	CLA	2	0
20	I	101	BCR	4	0
17	5	308	CLA	6	0
20	F	804	BCR	4	0
17	1	513	CLA	4	0
20	B	844	BCR	10	0
17	B	802	CLA	7	0
17	A	829	CLA	1	0
17	3	301	CLA	2	0
25	5	314	CHL	2	0
17	A	840	CLA	1	0
20	B	846	BCR	1	0
17	B	842	CLA	3	0
17	B	803	CLA	2	0
17	B	815	CLA	4	0
17	A	825	CLA	1	0
17	B	824	CLA	4	0
17	A	816	CLA	4	0
25	3	315	CHL	2	0
20	A	848	BCR	2	0
17	F	803	CLA	2	0
17	3	308	CLA	7	0
17	2	504	CLA	2	0
17	3	306	CLA	4	0
17	2	511	CLA	2	0
17	2	507	CLA	2	0
20	A	849	BCR	1	0
25	2	516	CHL	3	0
19	A	844	LHG	4	0
17	5	307	CLA	4	0
17	5	309	CLA	3	0
17	A	837	CLA	1	0
17	A	820	CLA	5	0
17	A	806	CLA	5	0
20	K	204	BCR	2	0
17	B	841	CLA	2	0

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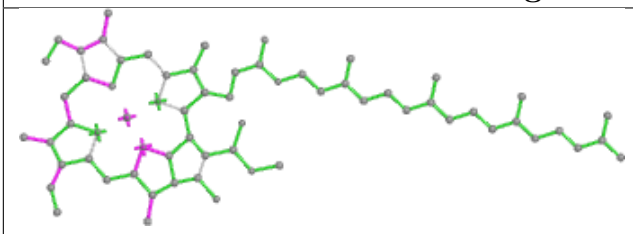
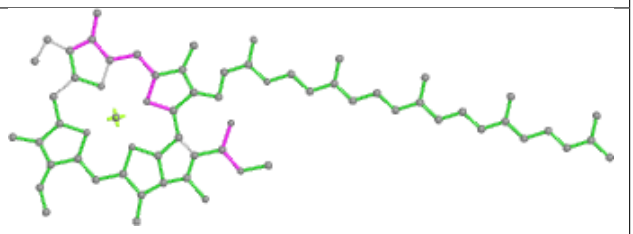
Mol	Chain	Res	Type	Clashes	Symm-Clashes
18	A	841	PQN	2	0
17	A	817	CLA	3	0
17	B	839	CLA	1	0
17	A	821	CLA	3	0
17	A	836	CLA	3	0
17	1	507	CLA	2	0
17	A	803	CLA	3	0
17	A	823	CLA	1	0
17	3	310	CLA	2	0
17	3	311	CLA	5	0
17	A	827	CLA	7	0
17	1	504	CLA	2	0
17	2	514	CLA	3	0
17	B	807	CLA	4	0
17	2	510	CLA	4	0
17	3	312	CLA	2	0
20	1	503	BCR	3	0
20	A	845	BCR	4	0
17	L	302	CLA	2	0
17	B	813	CLA	1	0
17	A	833	CLA	1	0
17	1	506	CLA	7	0
20	A	851	BCR	4	0
17	A	839	CLA	1	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.

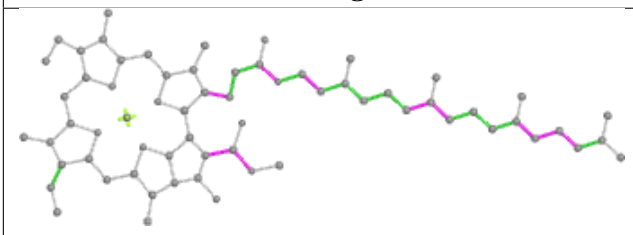
Ligand CLA B 804



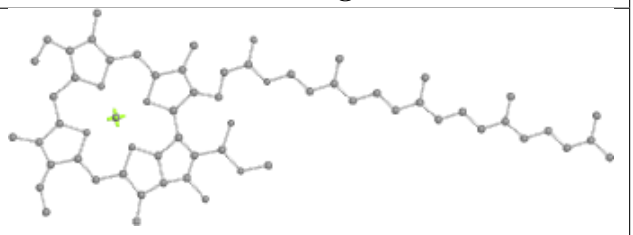
Bond lengths



Bond angles

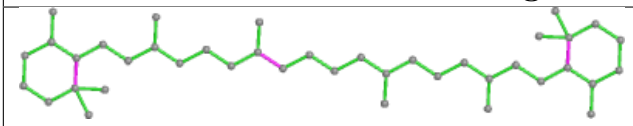


Torsions

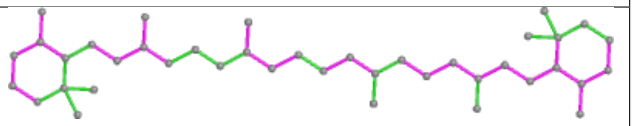


Rings

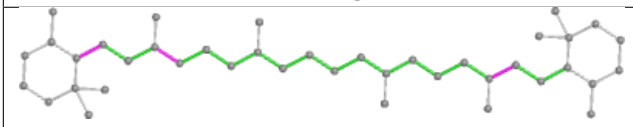
Ligand BCR B 852



Bond lengths



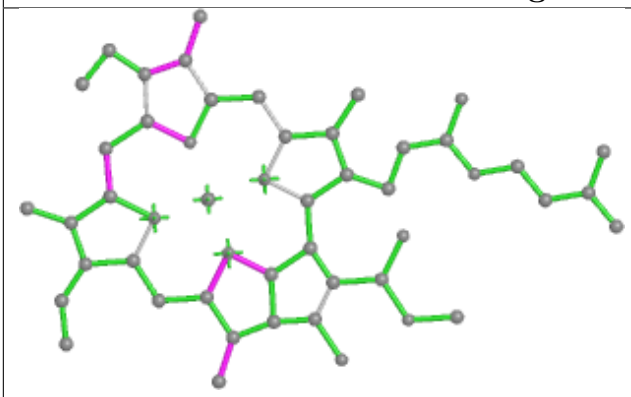
Bond angles



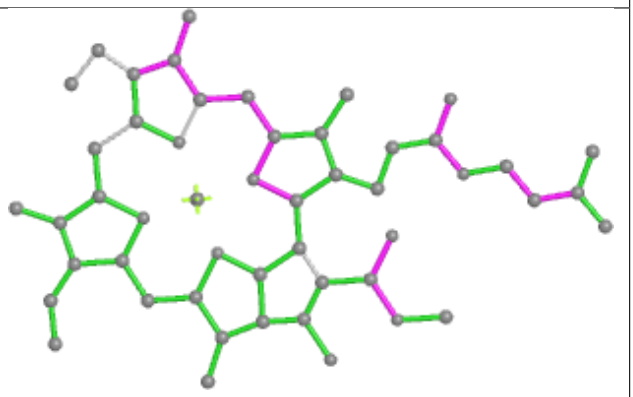
Torsions

Rings

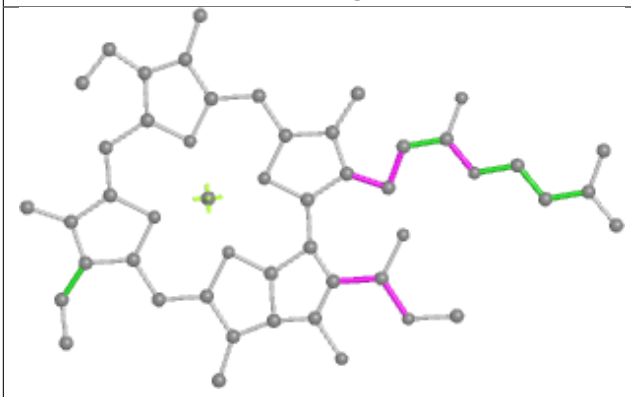
Ligand CLA 2 509



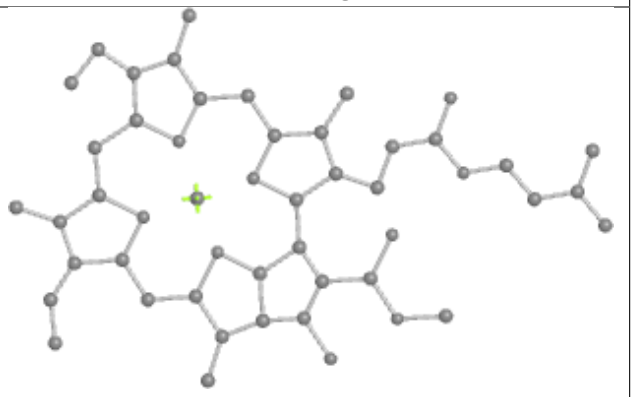
Bond lengths



Bond angles

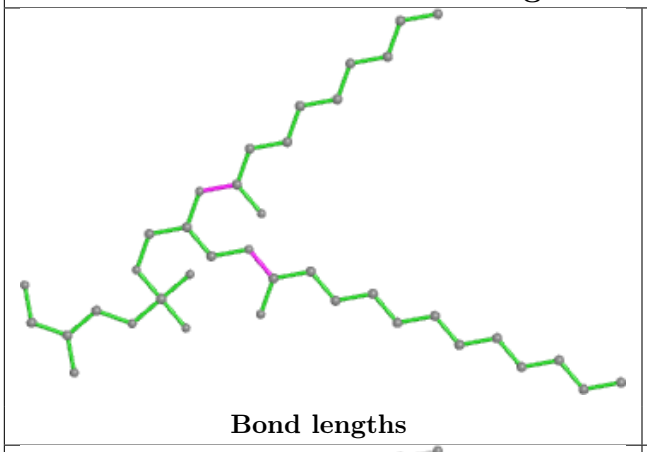


Torsions

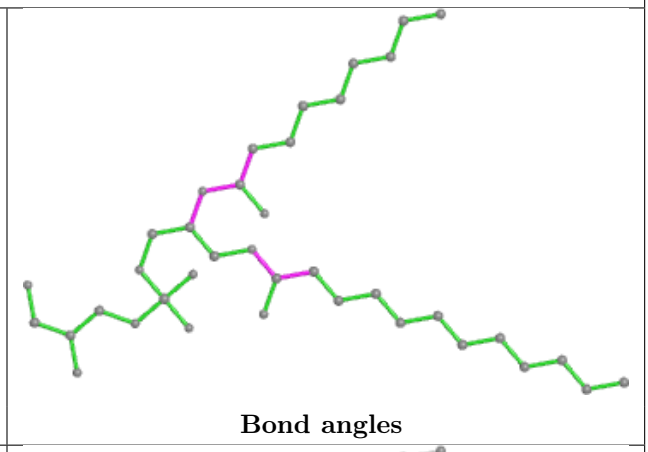


Rings

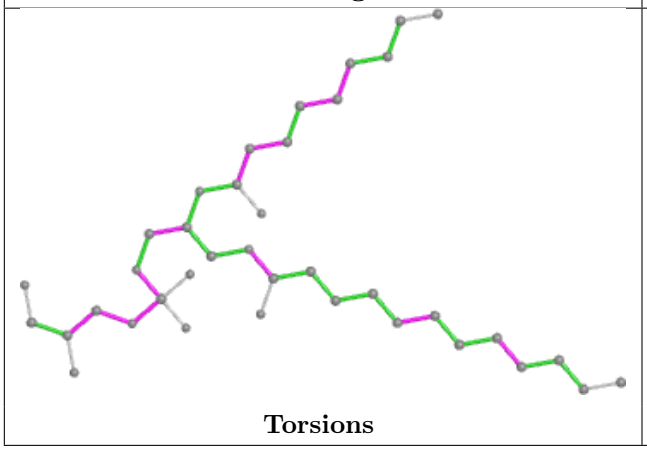
Ligand LHG B 851



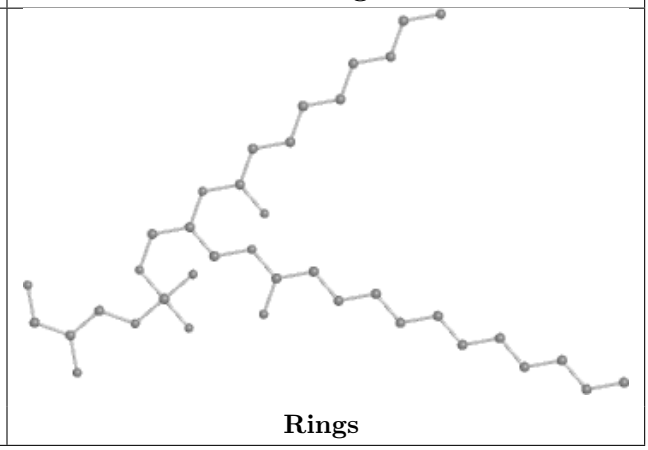
Bond lengths



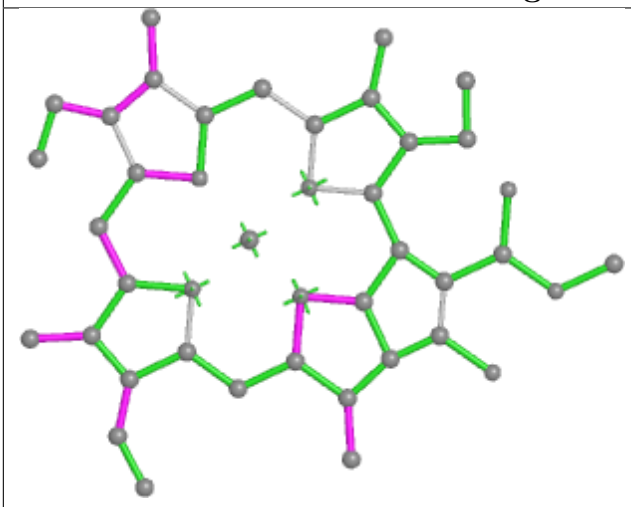
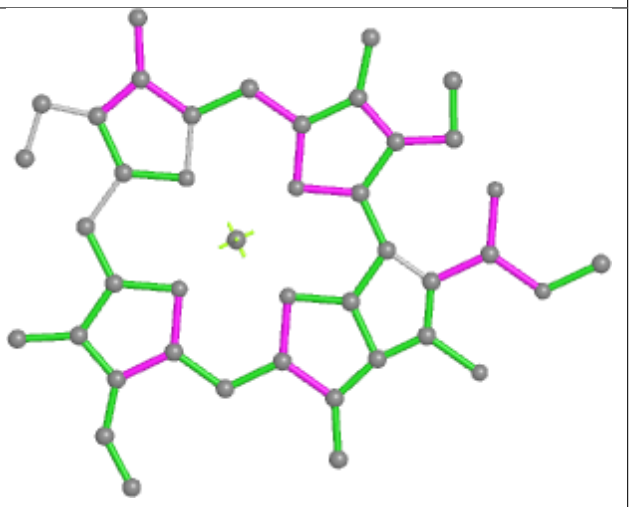
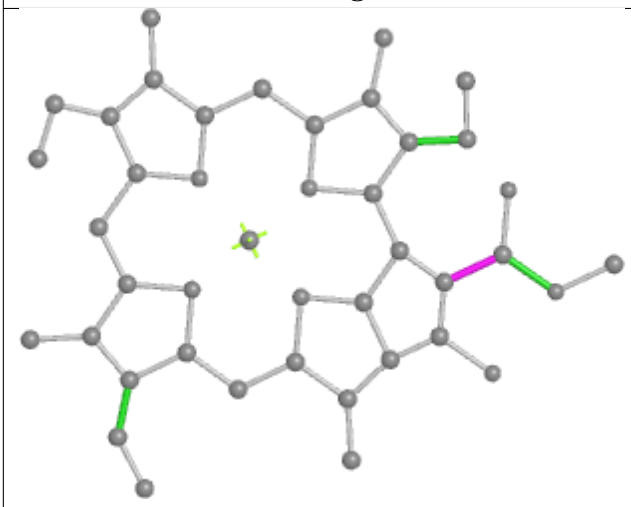
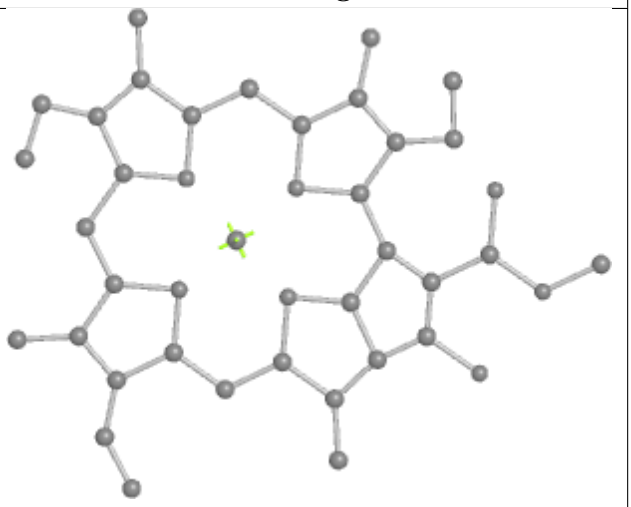
Bond angles

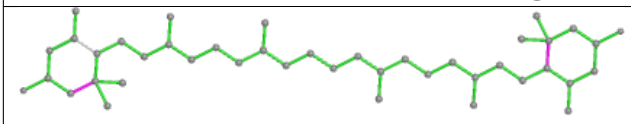
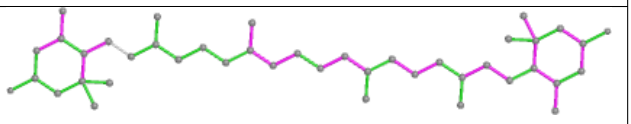
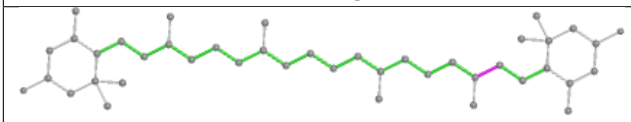
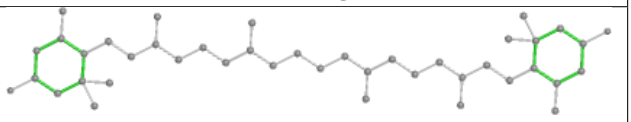


Torsions

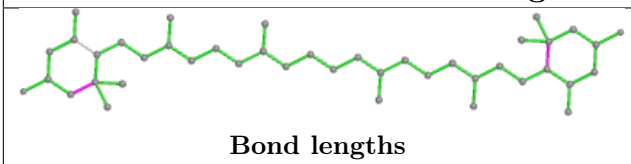


Rings

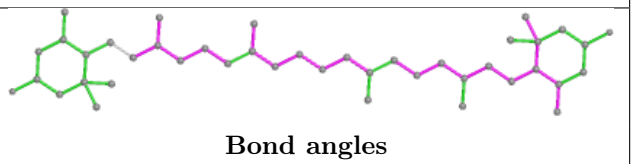
Ligand CLA A 814	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand LUT 3 304	
	
Bond lengths	Bond angles
	
Torsions	Rings

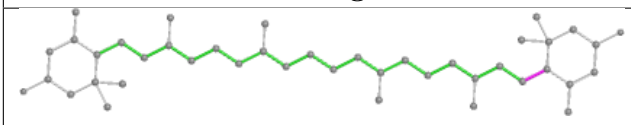
Ligand LUT 5 303



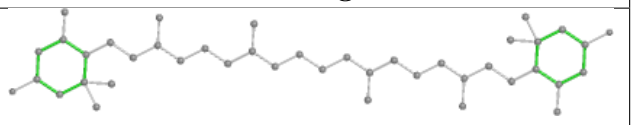
Bond lengths



Bond angles

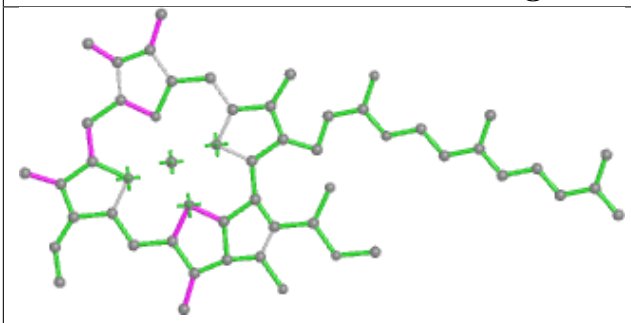


Torsions



Rings

Ligand CLA B 812



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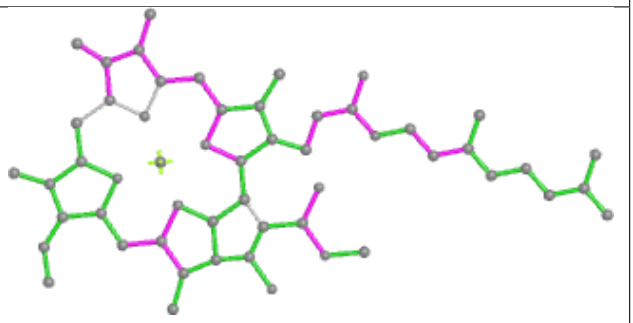
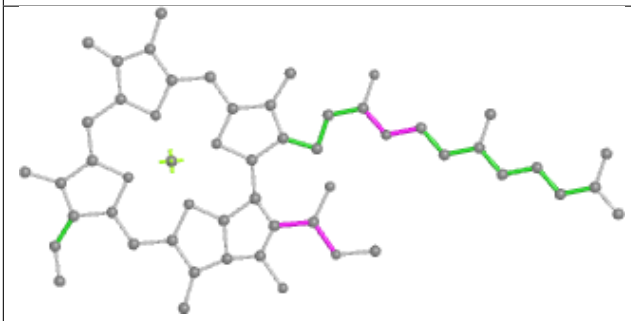


Bond angles



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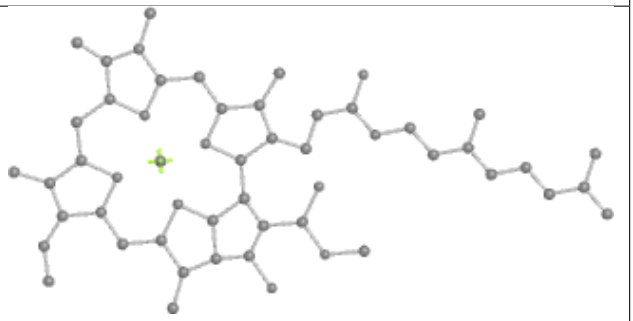
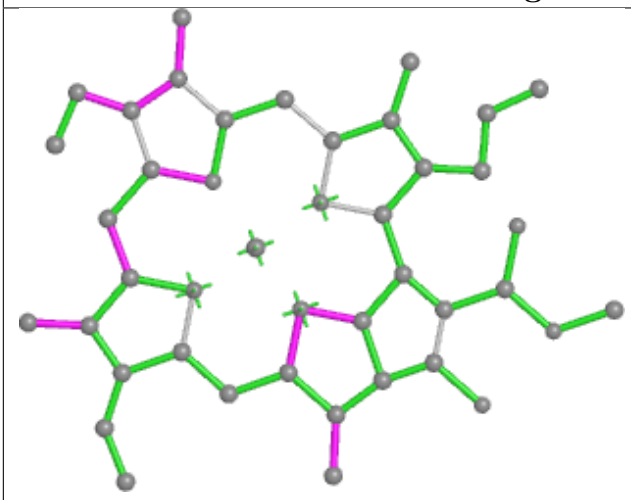


Rings

Ligand CLA B 816



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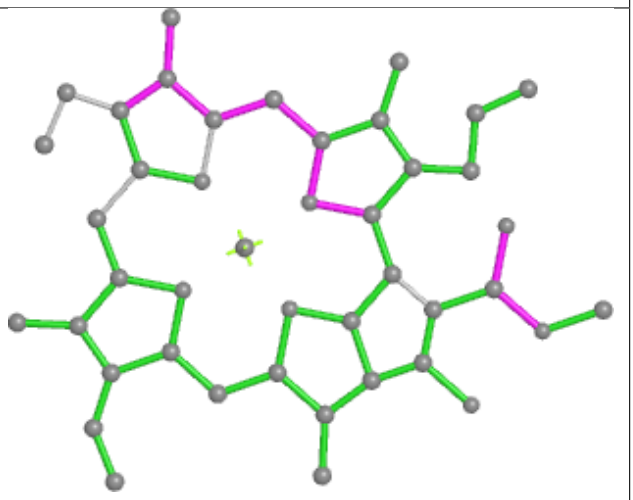
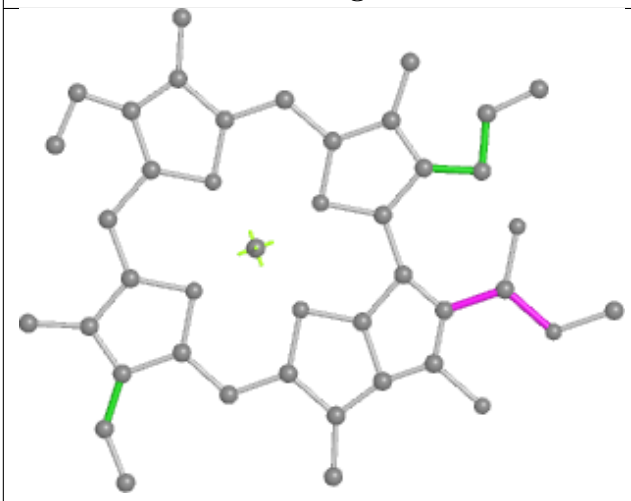


Bond angles



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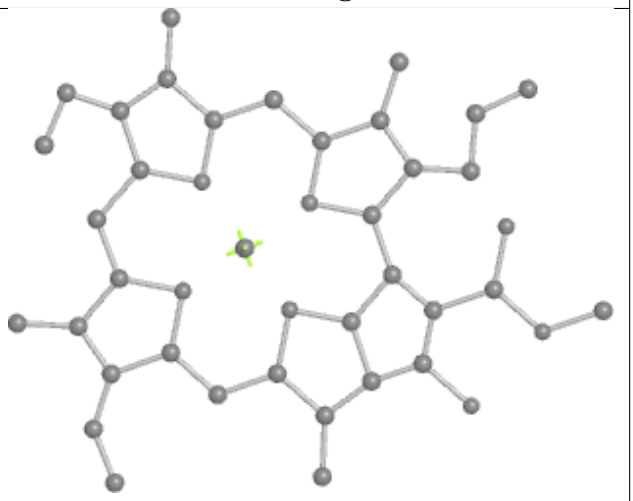
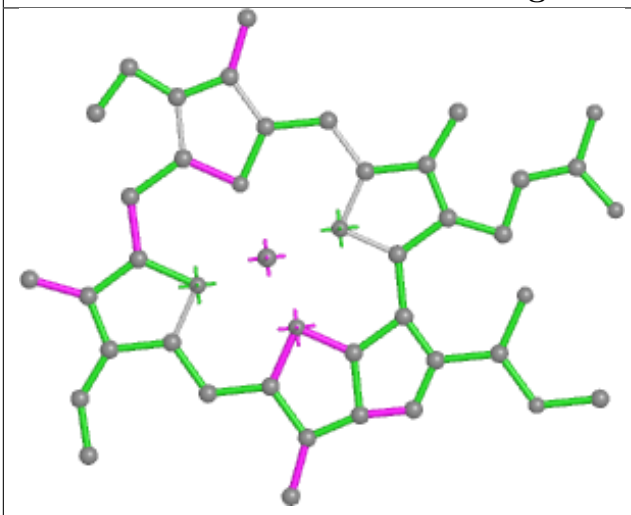
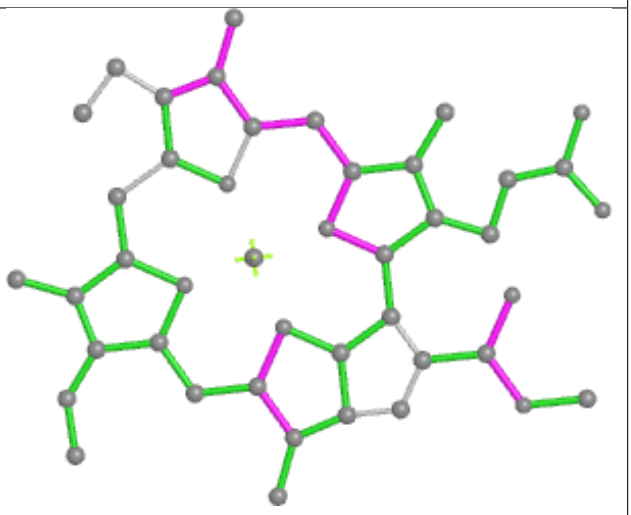


Rings

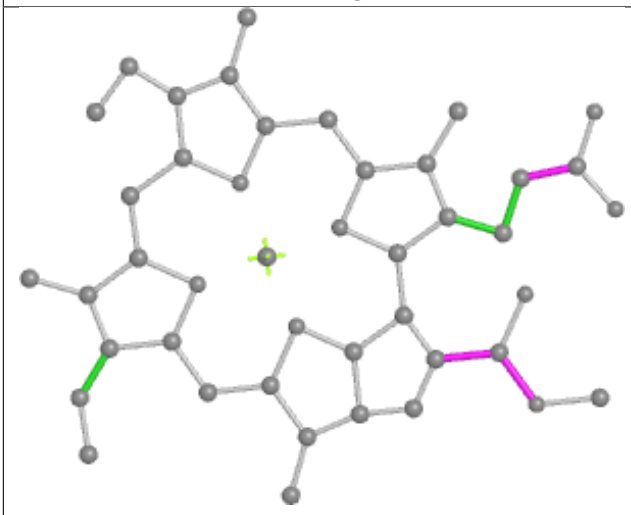
Ligand CLA 1 515



Bond lengths



Bond angles



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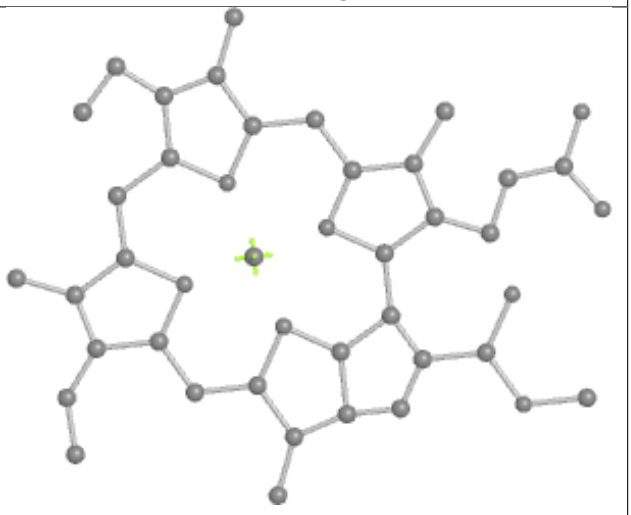
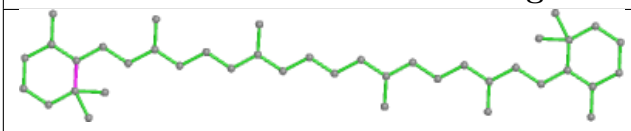


Rings

Ligand BCR 2 503



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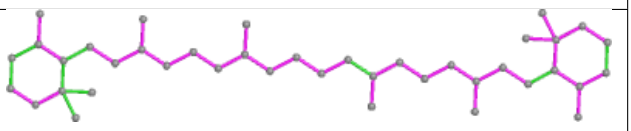
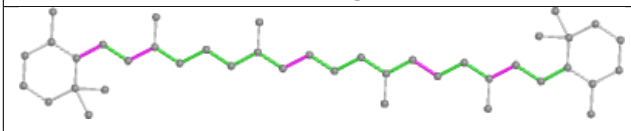


Bond angles



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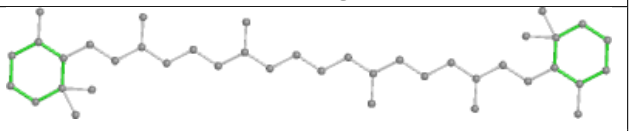
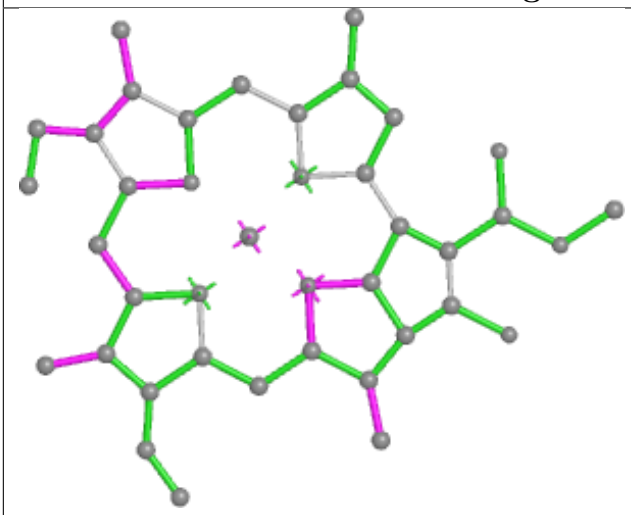


Rings

Ligand CLA K 203



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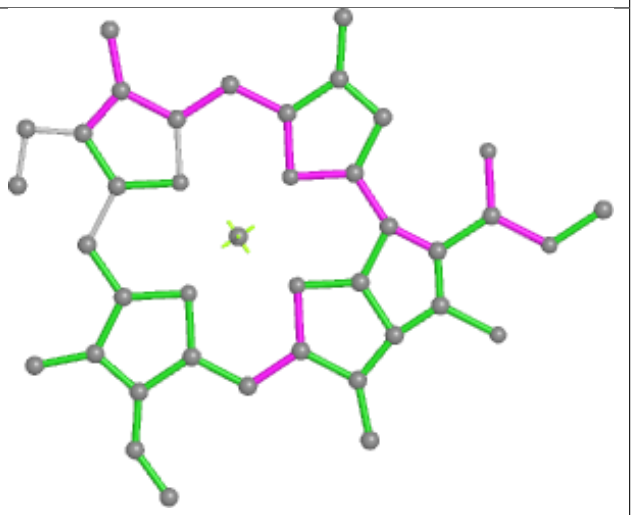
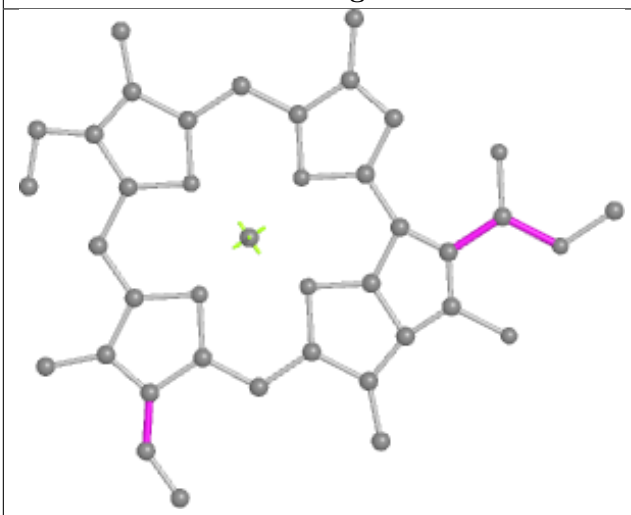
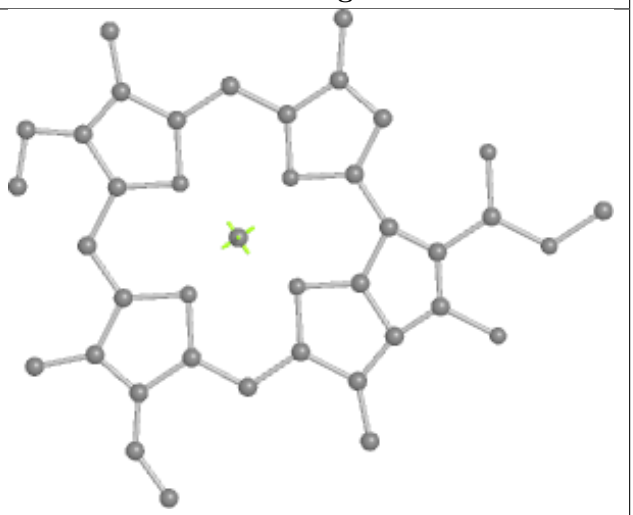


Bond angles

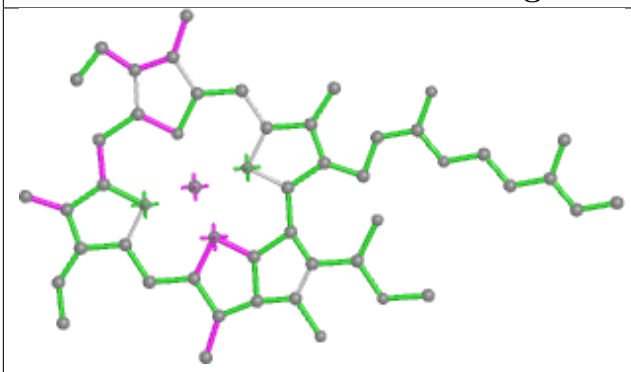


Torsions

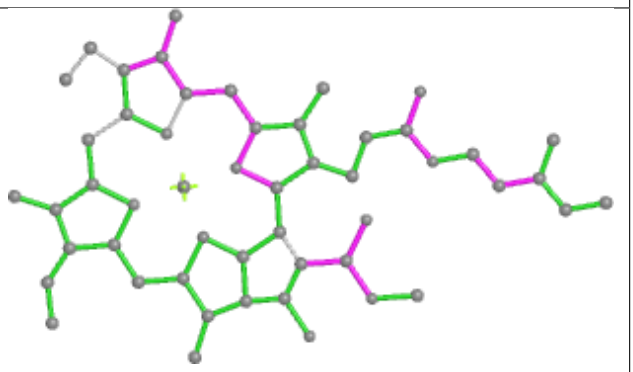


Rings

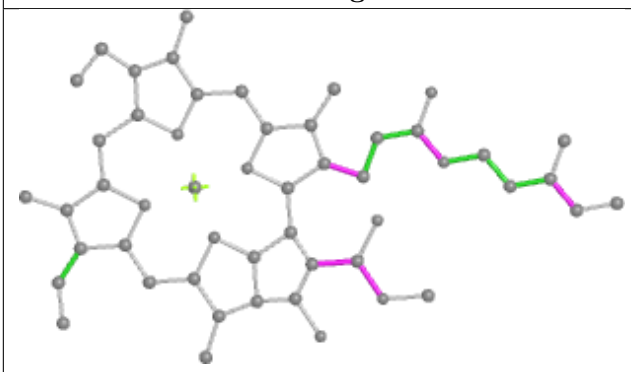
Ligand CLA A 835



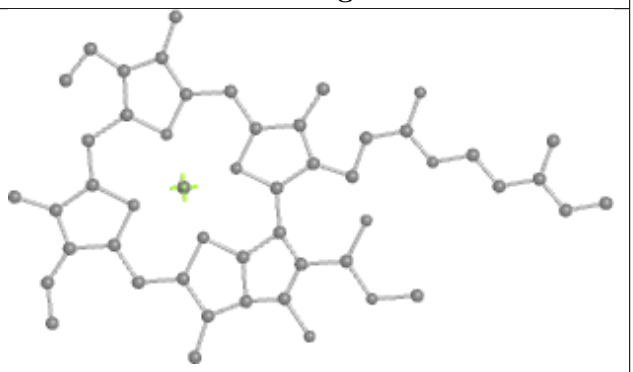
Bond lengths



Bond angles

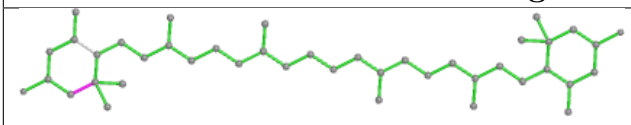


Torsions



Rings

Ligand LUT 1 501



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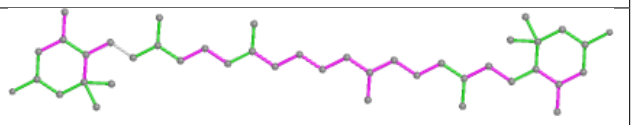
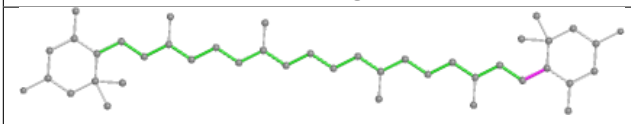
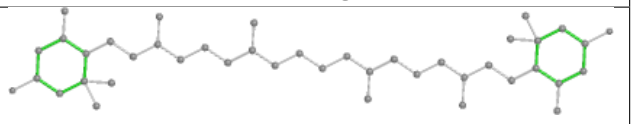


Bond angles

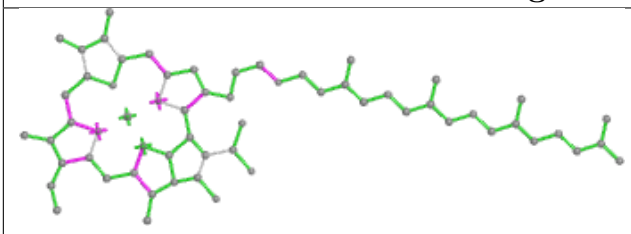


Torsions



Rings

Ligand CL0 A 801



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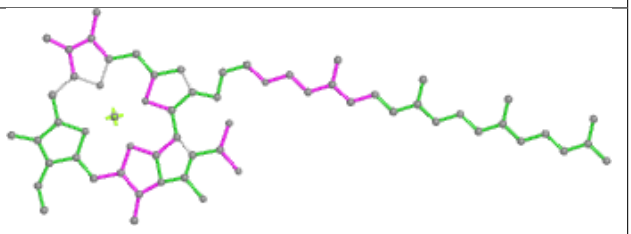
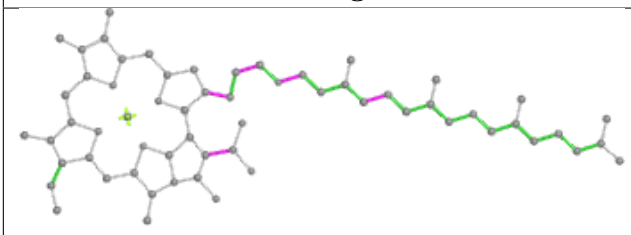
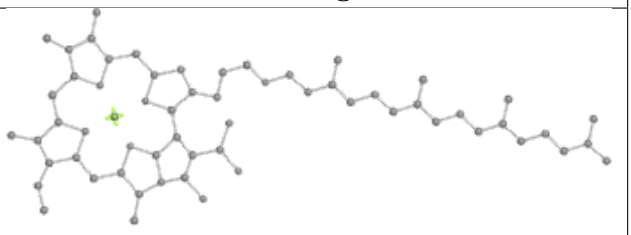


Bond angles

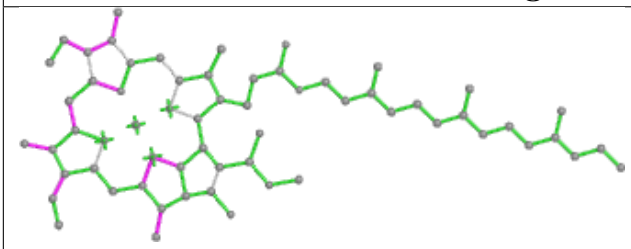


Torsions

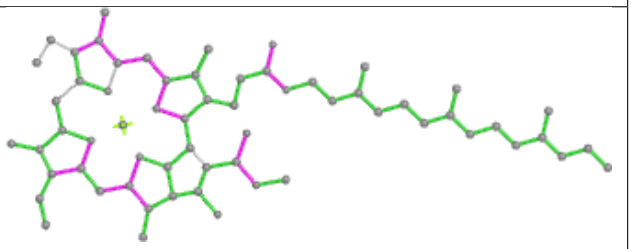


Rings

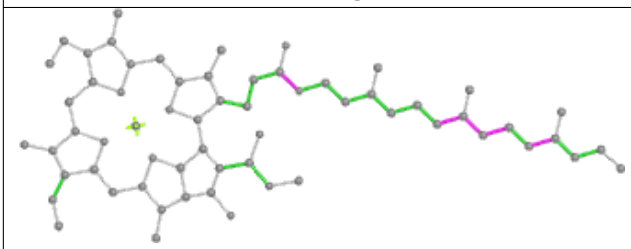
Ligand CLA B 826



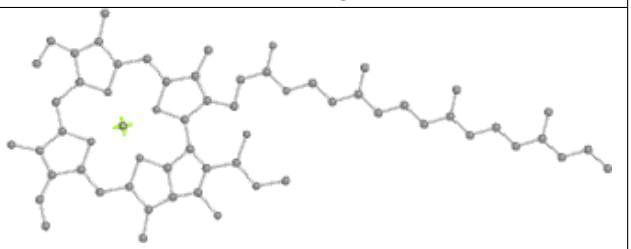
Bond lengths



Bond angles

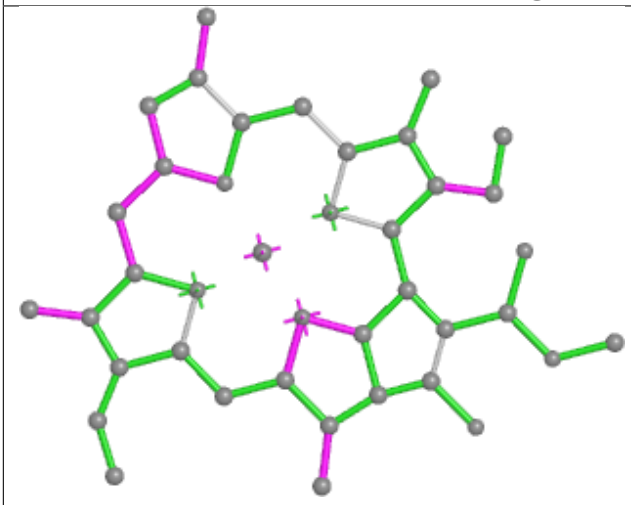


Torsions

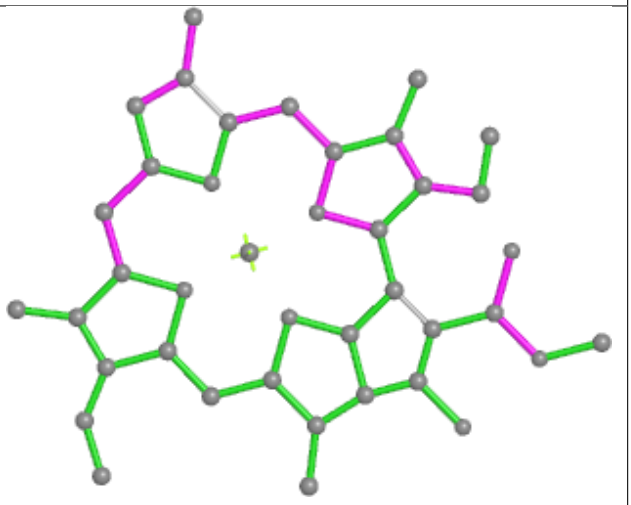


Rings

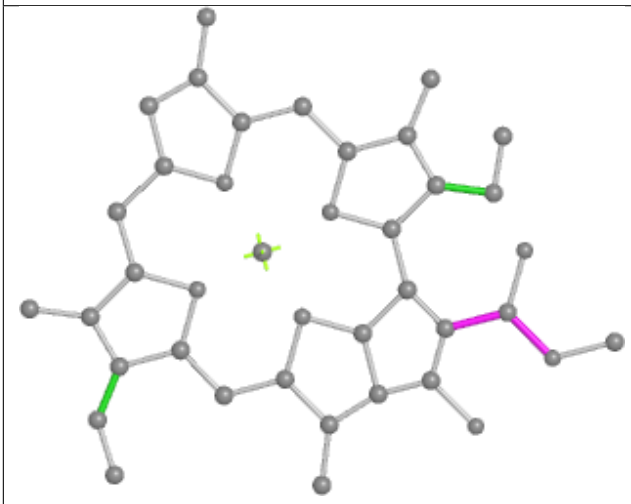
Ligand CLA 3 309



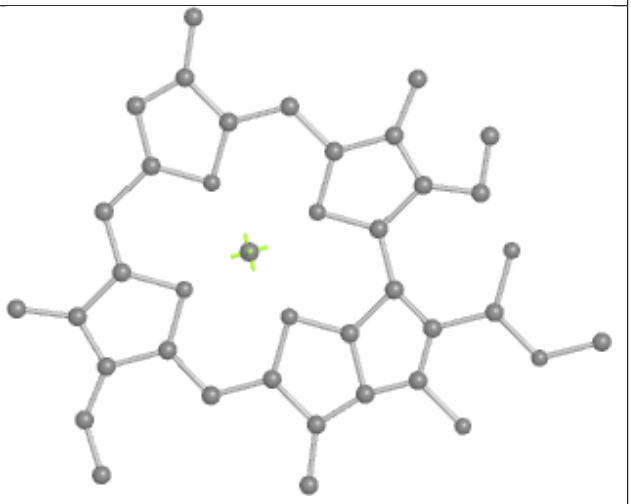
Bond lengths



Bond angles

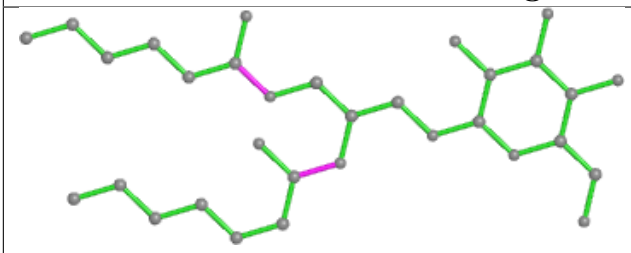


Torsions

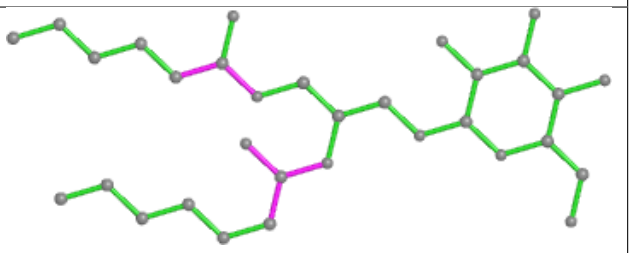


Rings

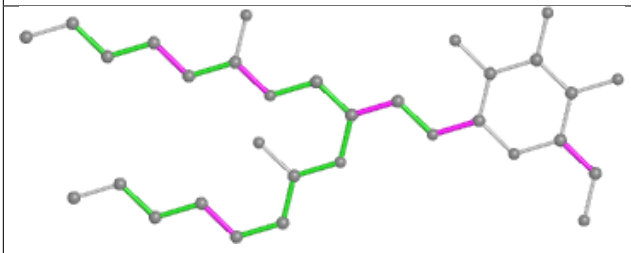
Ligand LMG 5 301



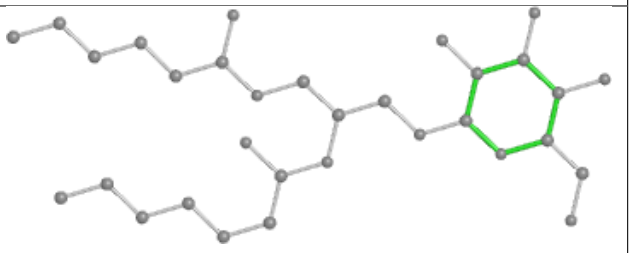
Bond lengths



Bond angles

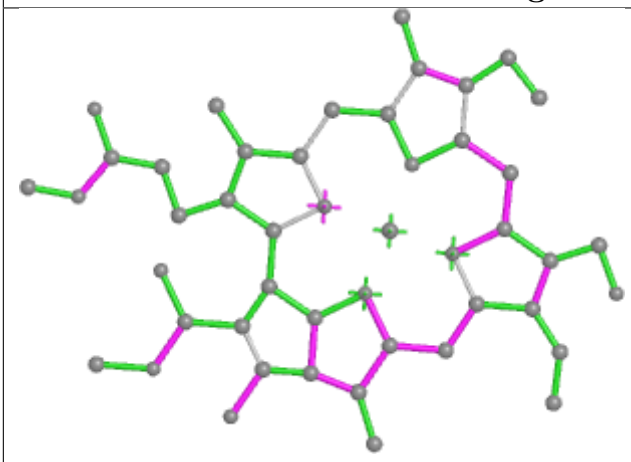


Torsions

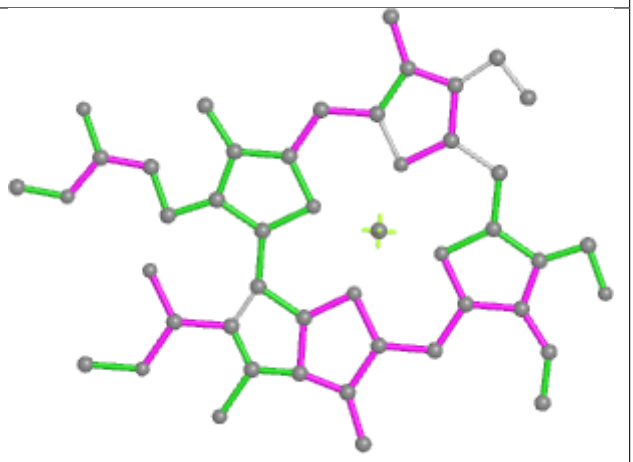


Rings

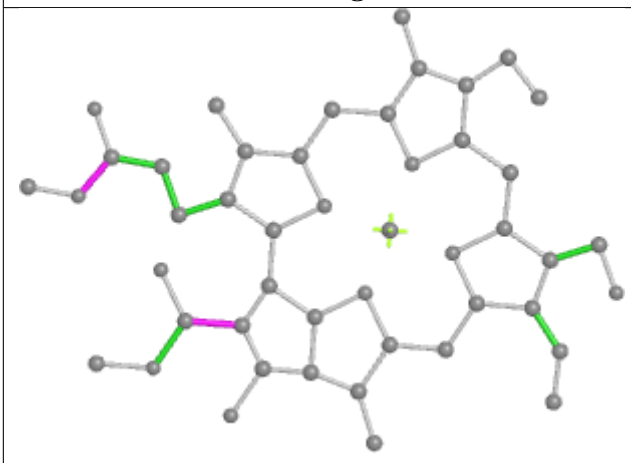
Ligand CHL 3 302



Bond lengths



Bond angles



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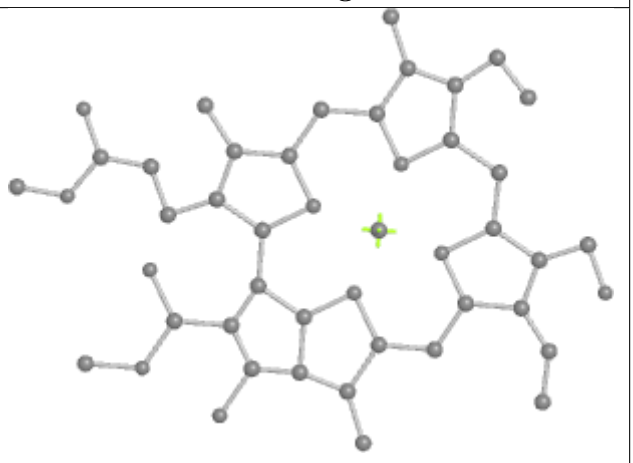
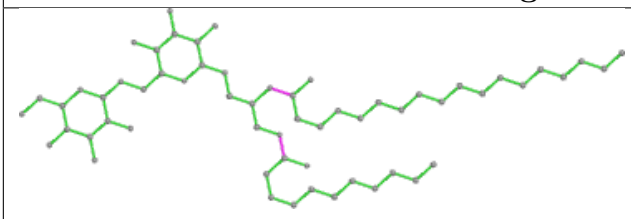
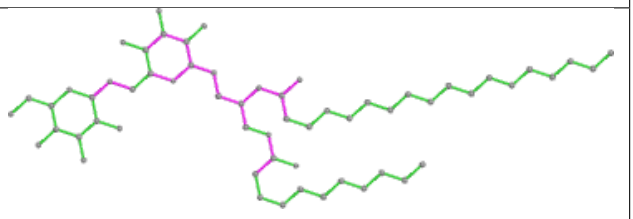


Rings

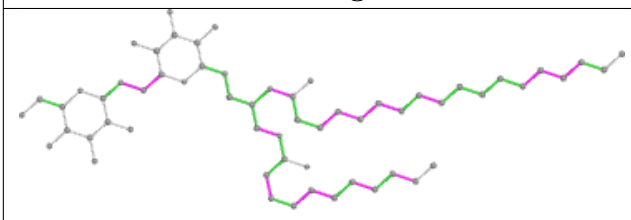
Ligand DGD B 850



Bond lengths



Bond angles



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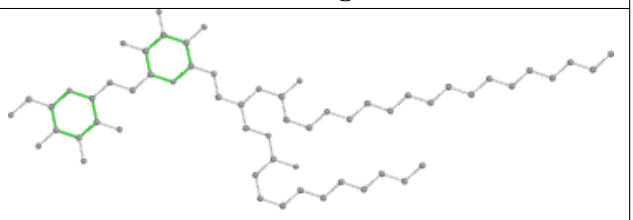
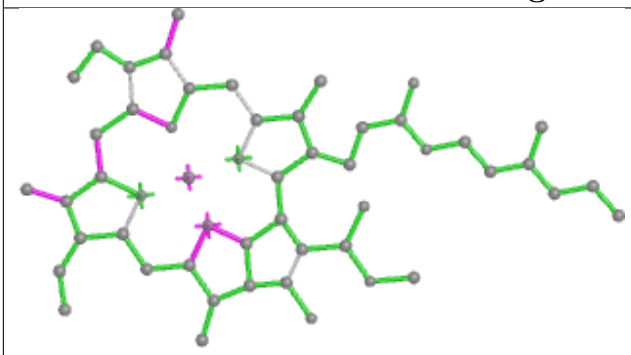
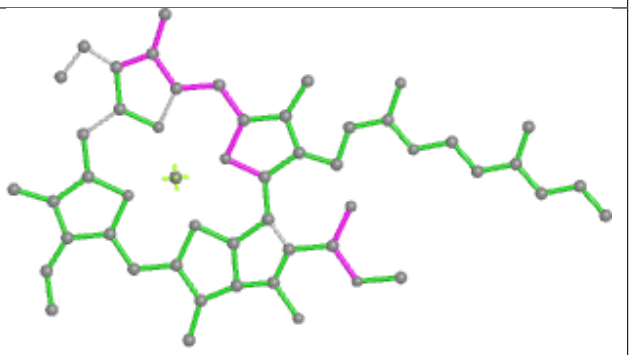
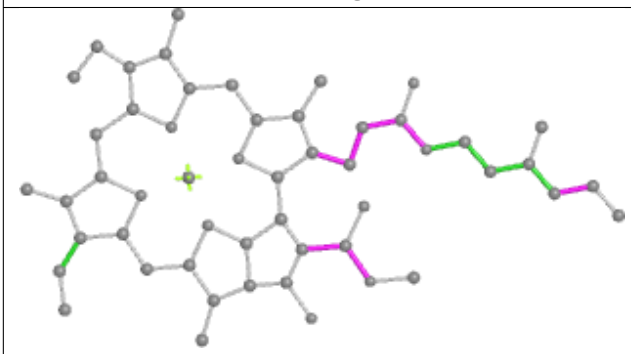
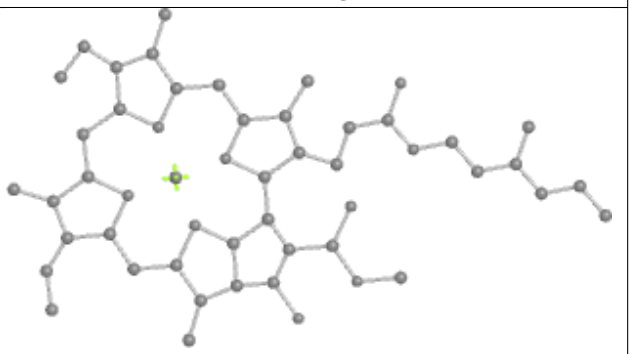
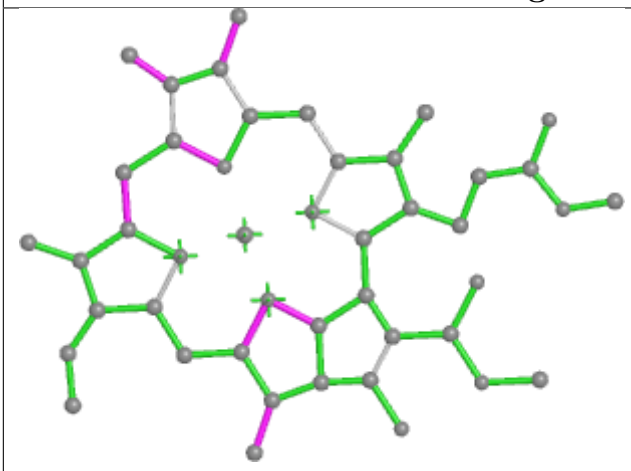


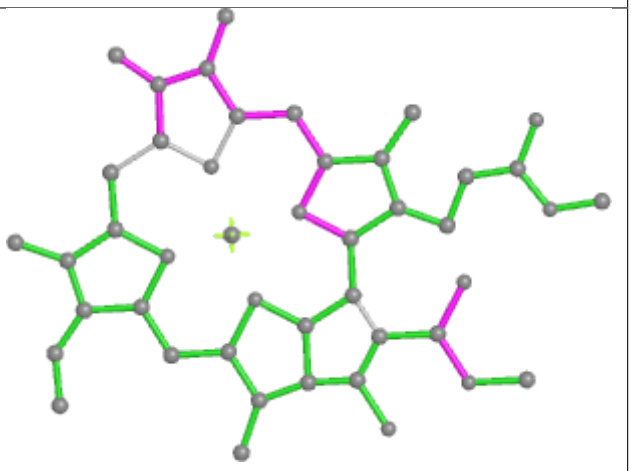
Rings

Ligand CLA 2 505	
	
Bond lengths	**Bond angles**
	
Torsions	**Rings**

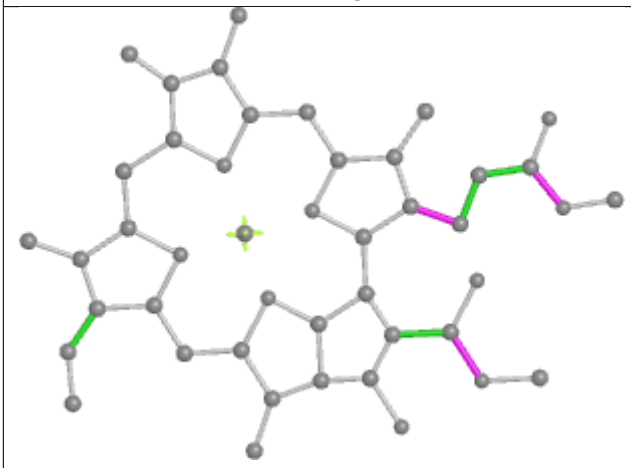
Ligand CLA 3 318



Bond lengths



Bond angles



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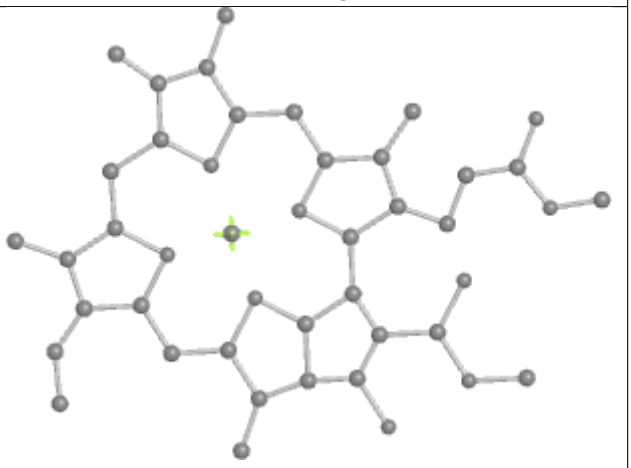
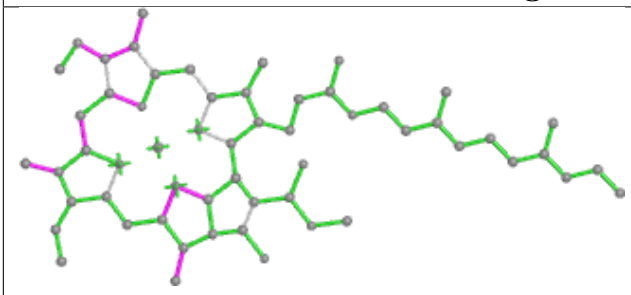


Rings

Ligand CLA A 852



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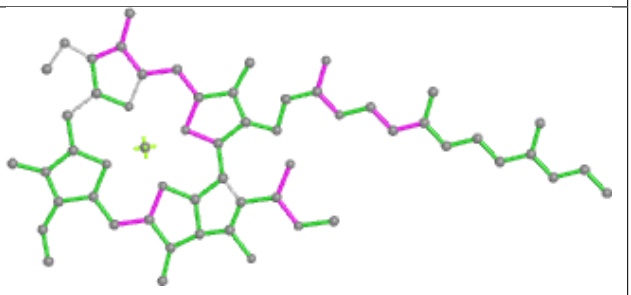
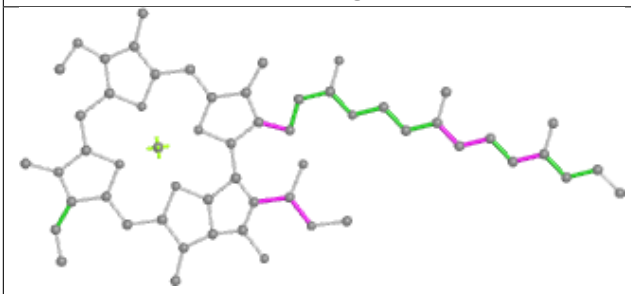


Bond angles



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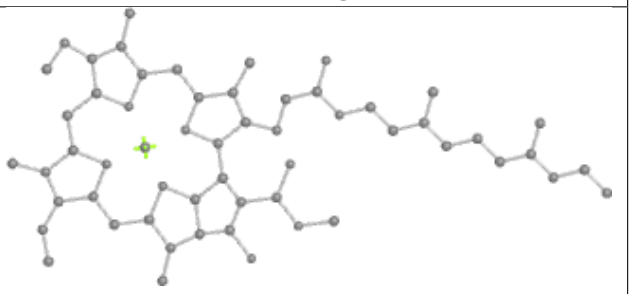
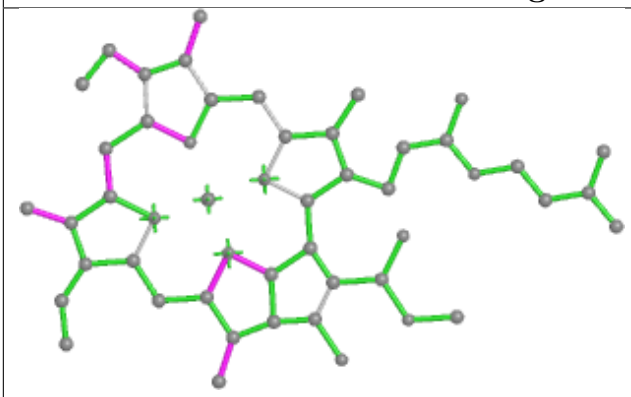


Rings

Ligand CLA 5 310



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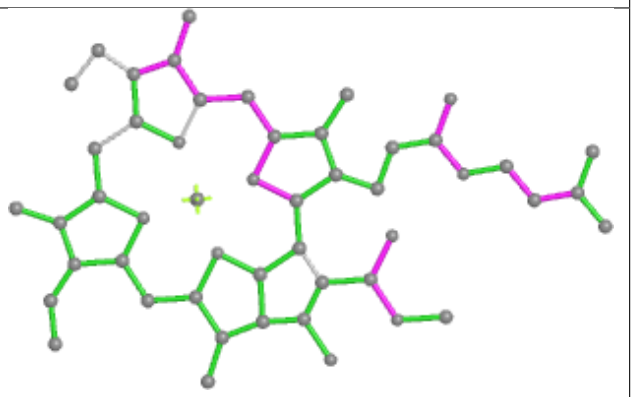
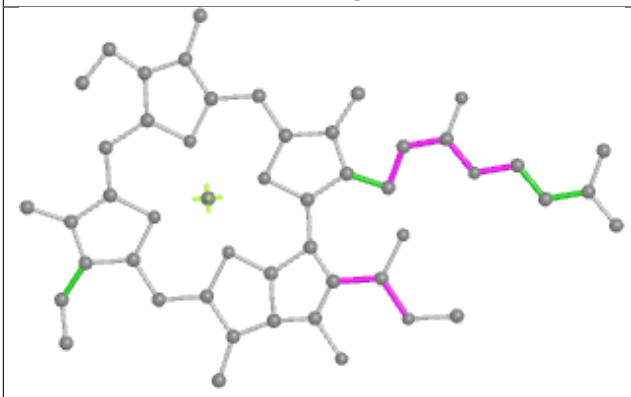


Bond angles



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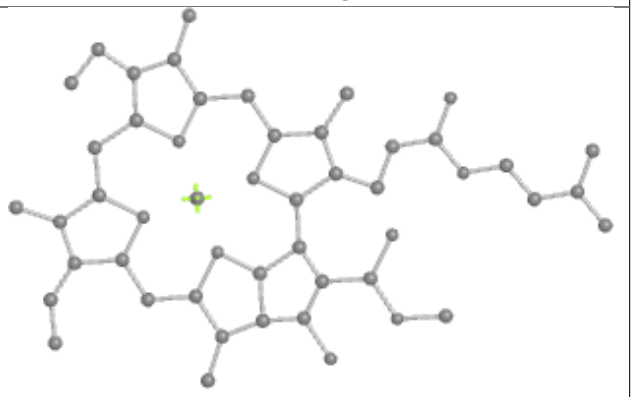
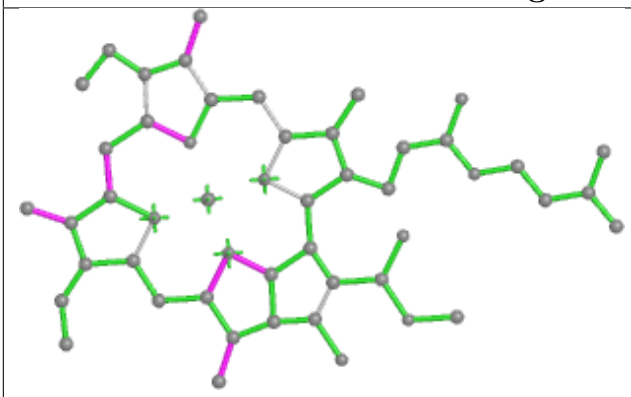


Rings

Ligand CLA 1 509



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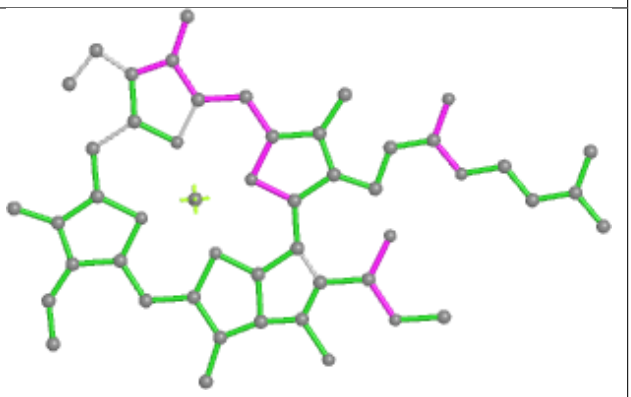
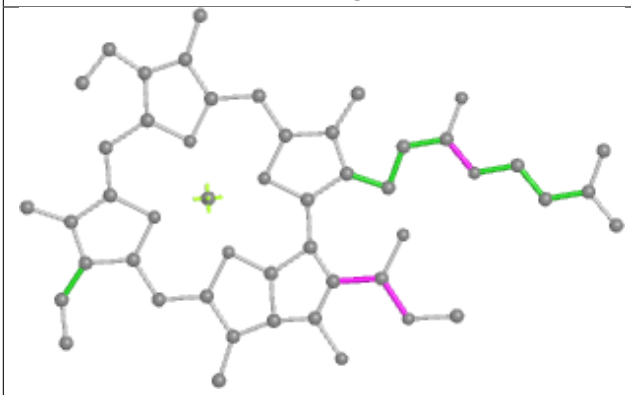


Bond angles



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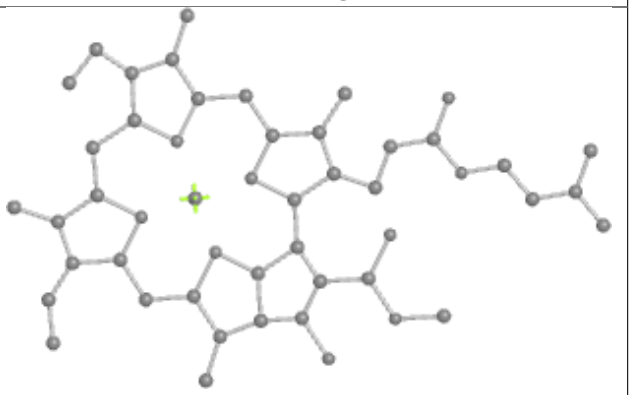
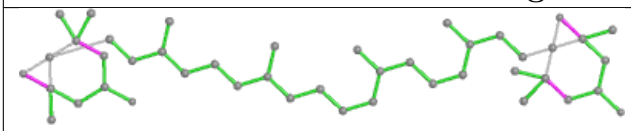
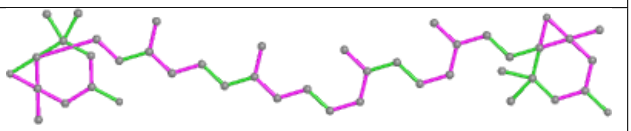


Rings

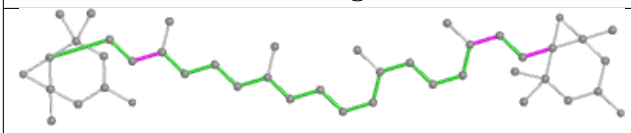
Ligand XAT 2 502



Bond lengths



Bond angles



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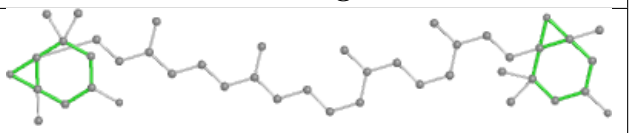
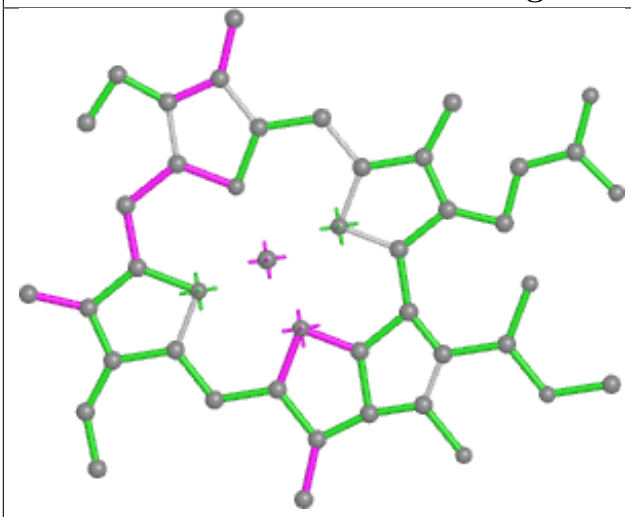


Rings

Ligand CLA L 304



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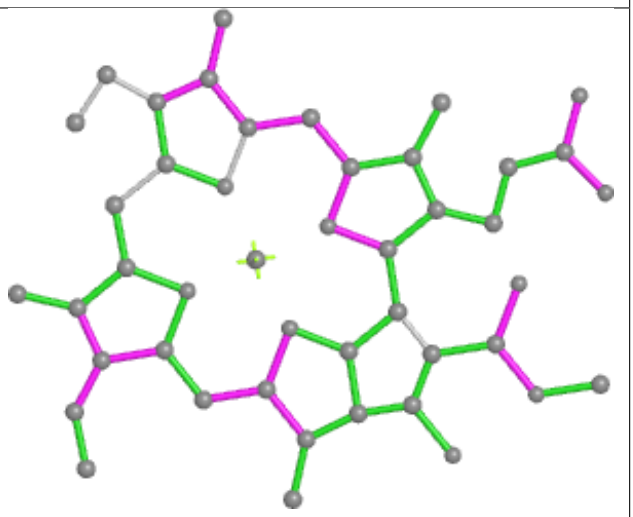
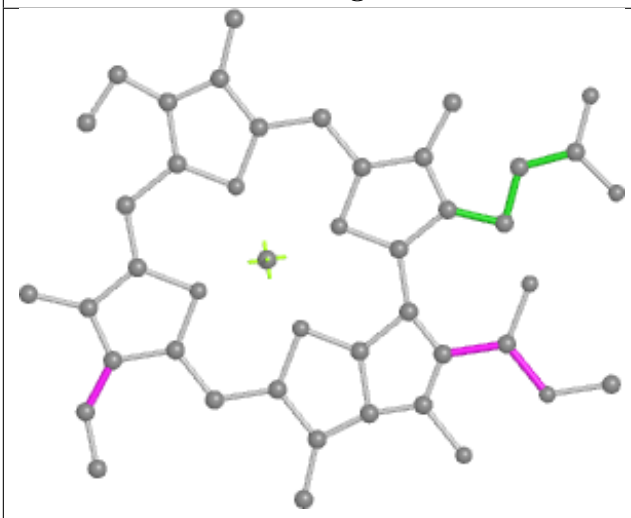


Bond angles



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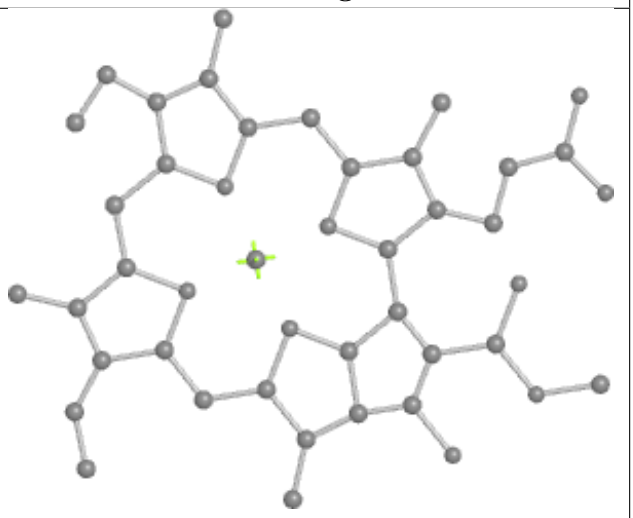
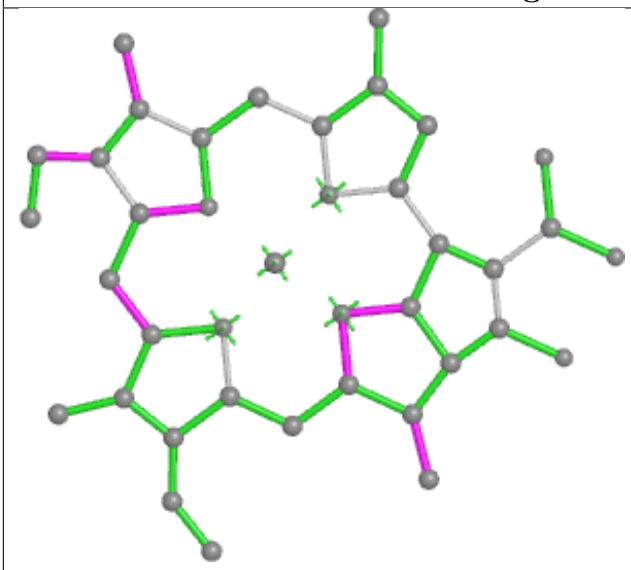


Rings

Ligand CLA K 205



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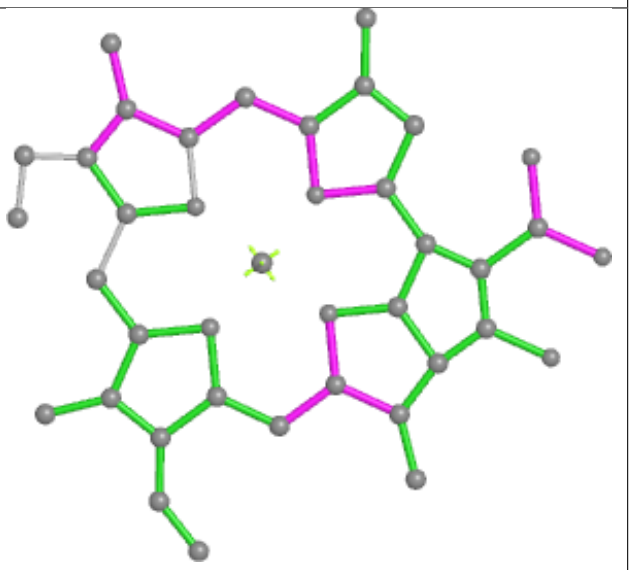
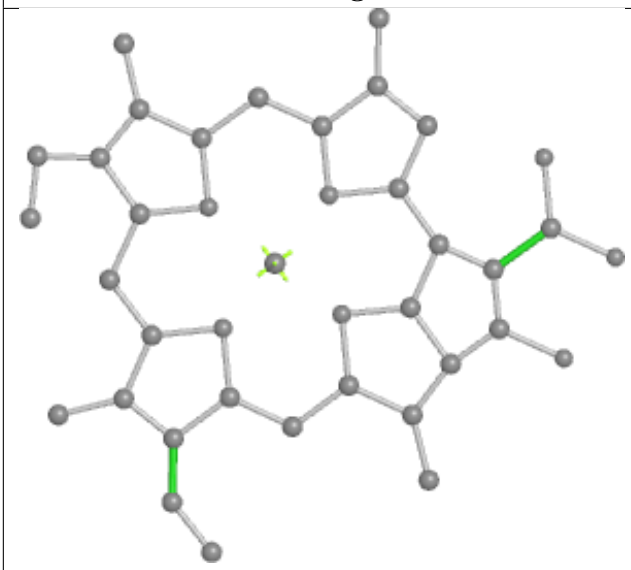


Bond angles



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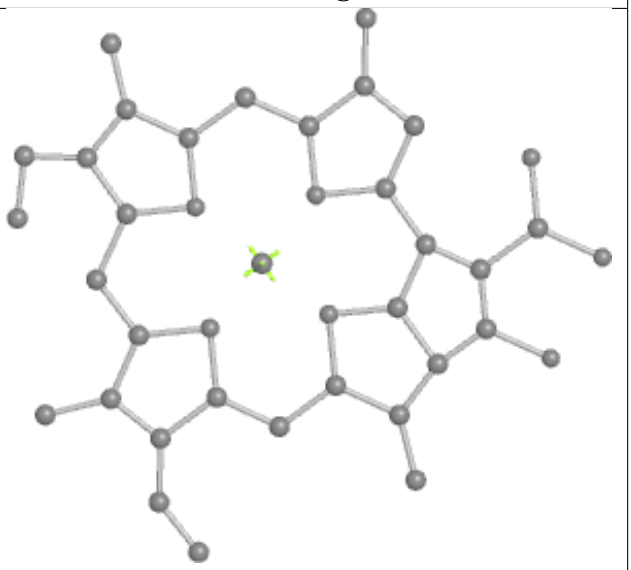
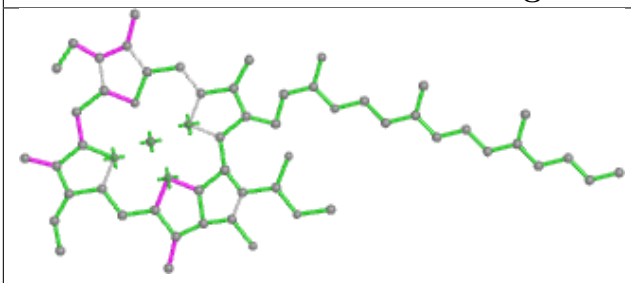


Rings

Ligand CLA A 802



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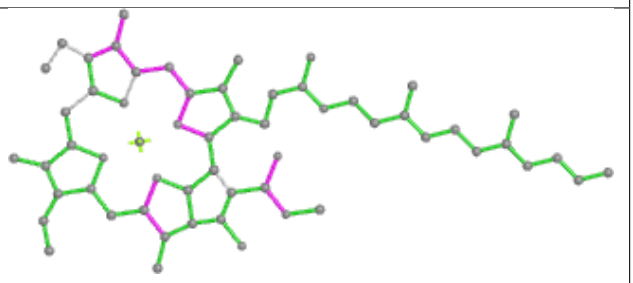
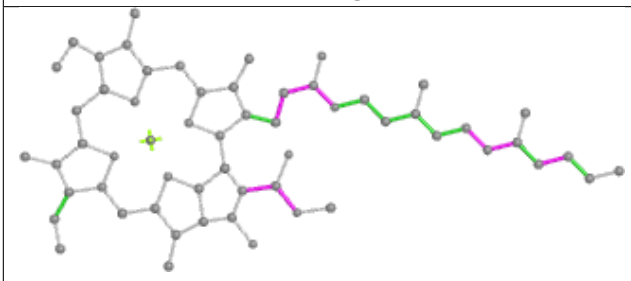


Bond angles



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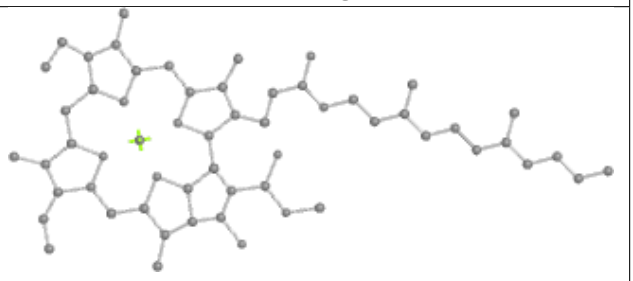
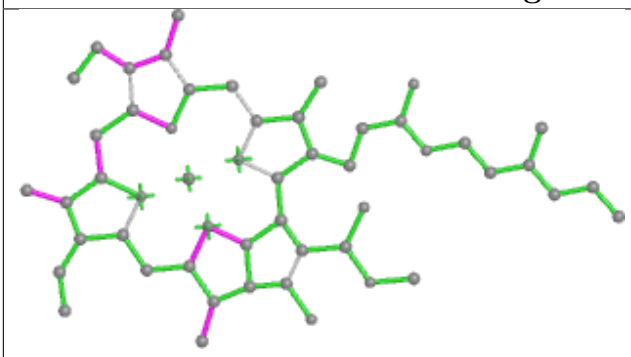


Rings

Ligand CLA A 804



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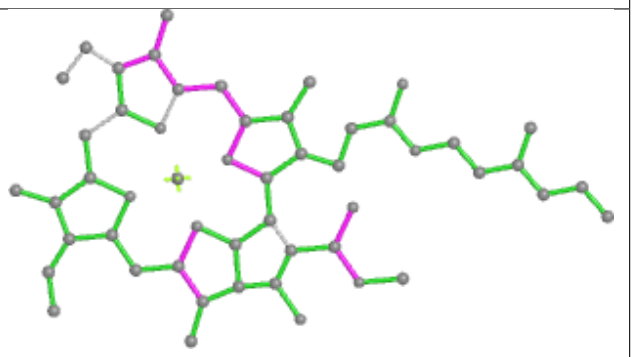
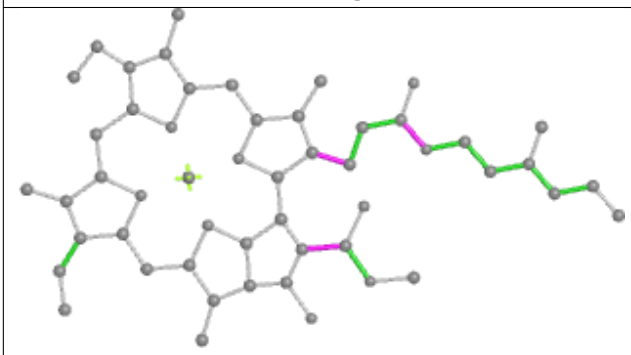


Bond angles



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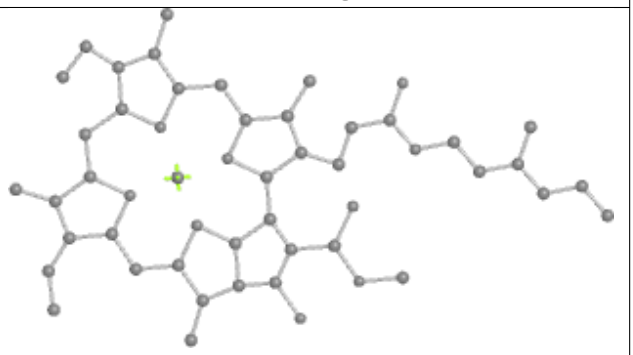
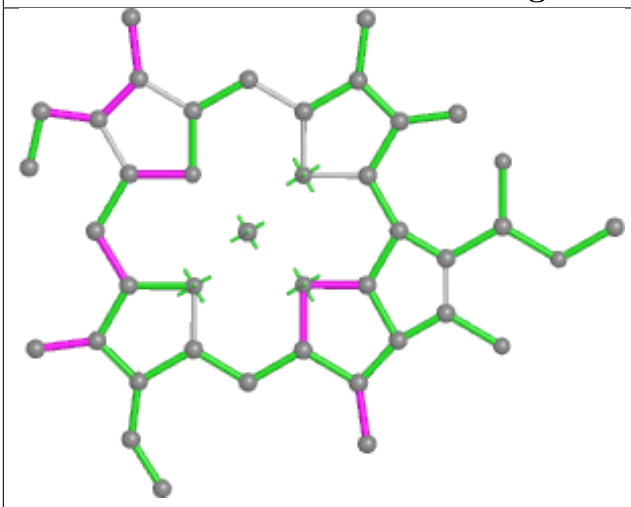
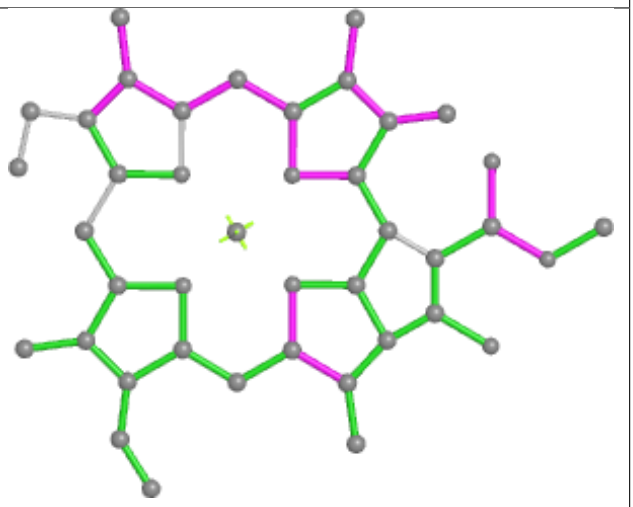


Rings

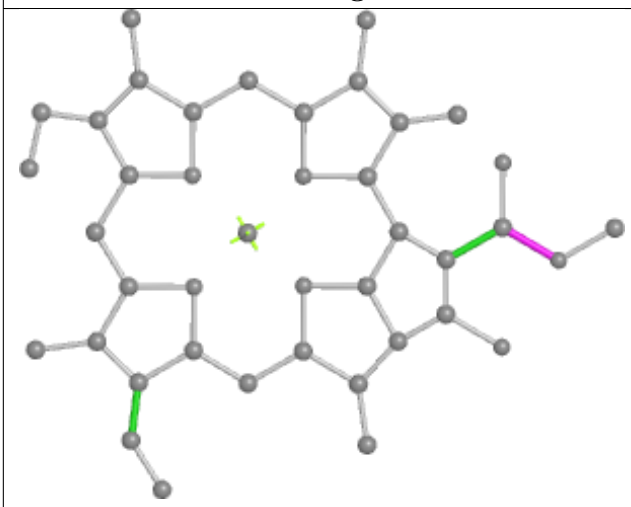
Ligand CLA 5 316



Bond lengths



Bond angles



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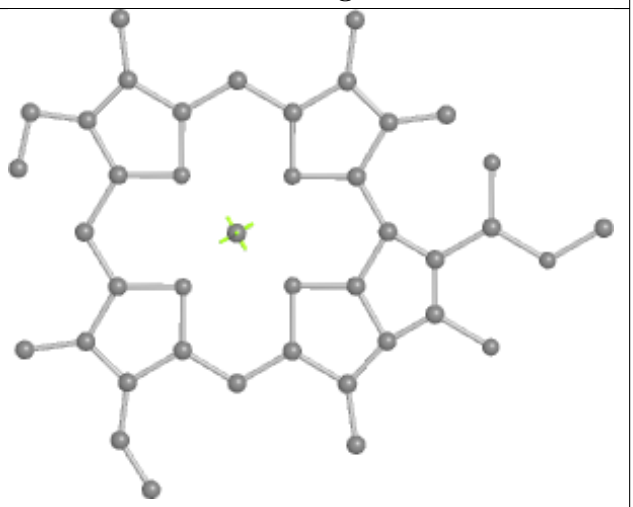
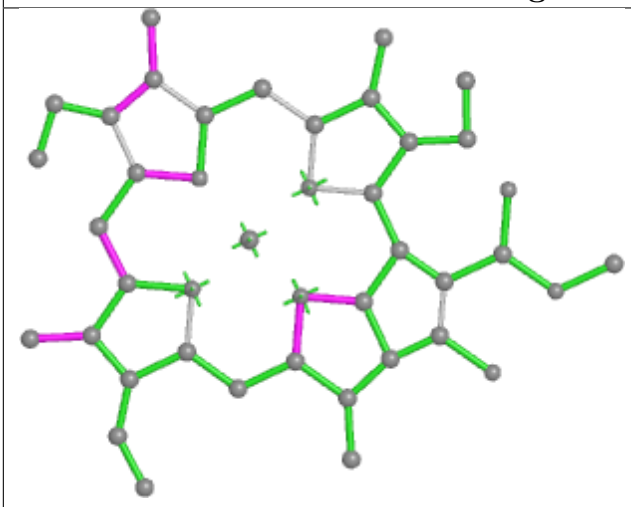
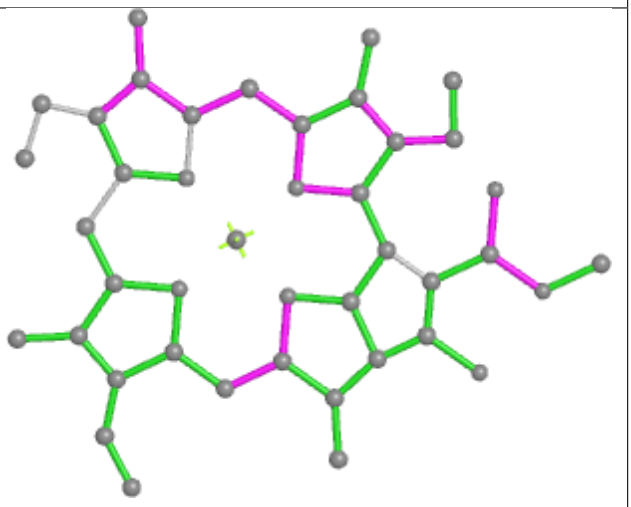


Rings

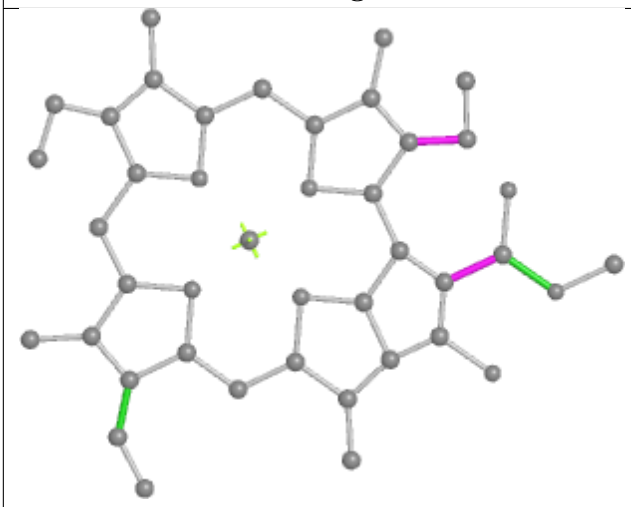
Ligand CLA 1 505



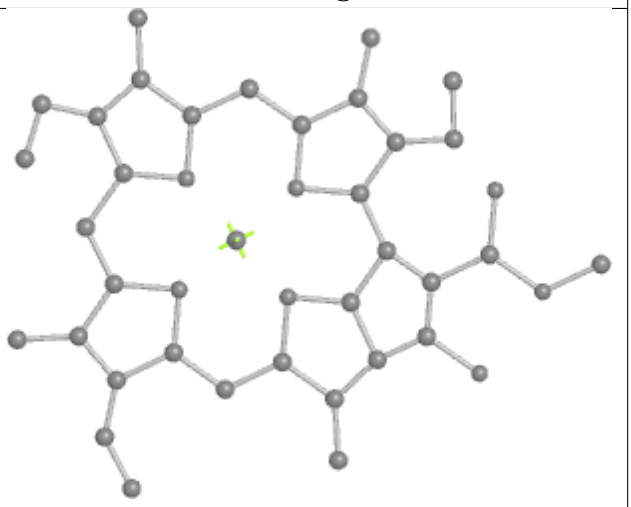
Bond lengths



Bond angles

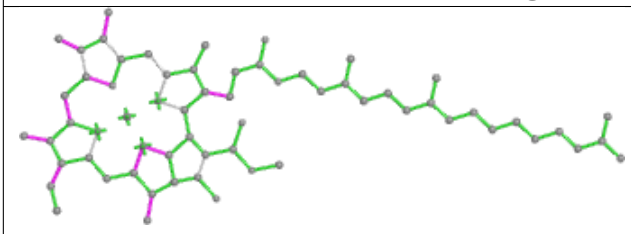


Torsions



Rings

Ligand CLA A 831



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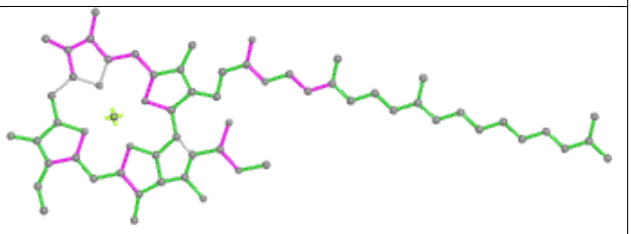
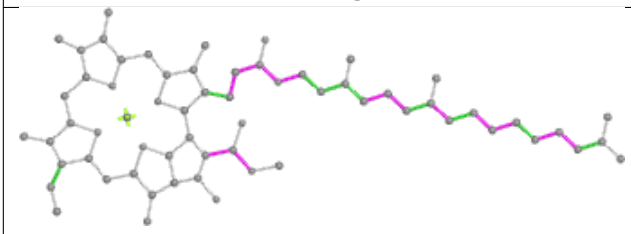
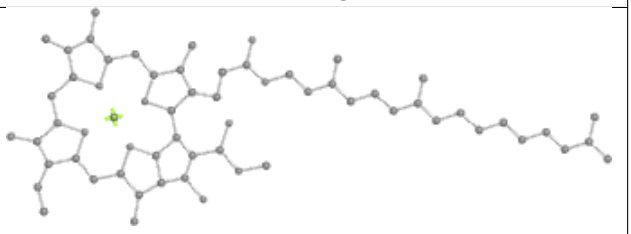


Bond angles

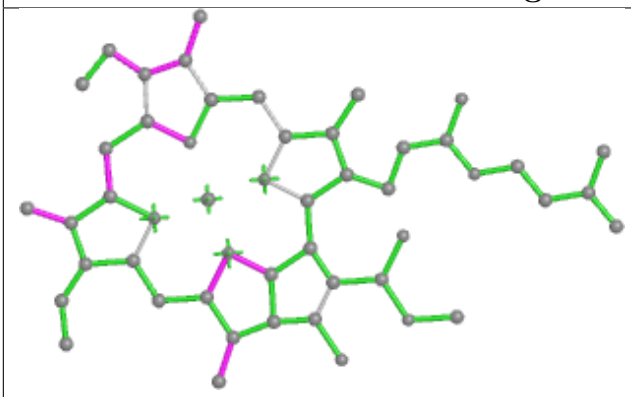


Torsions



Rings

Ligand CLA B 821



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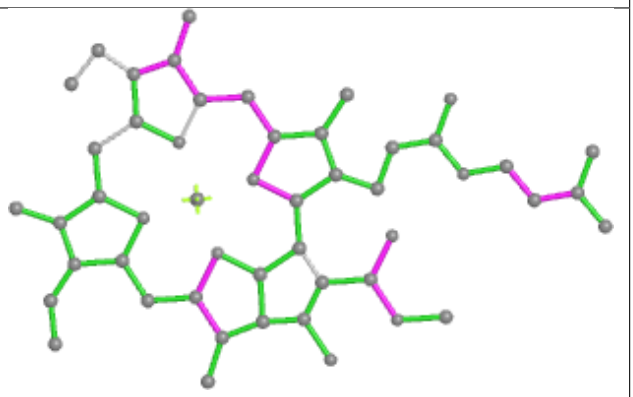
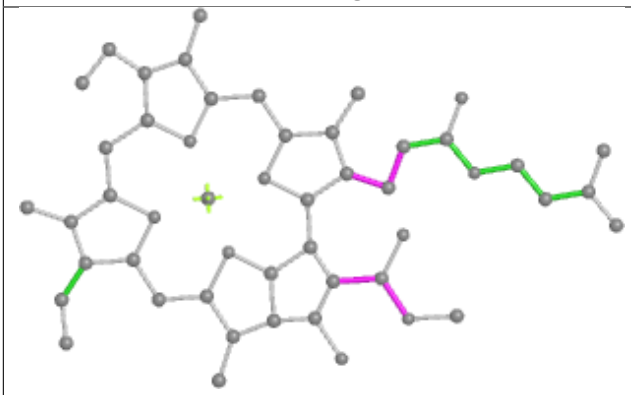
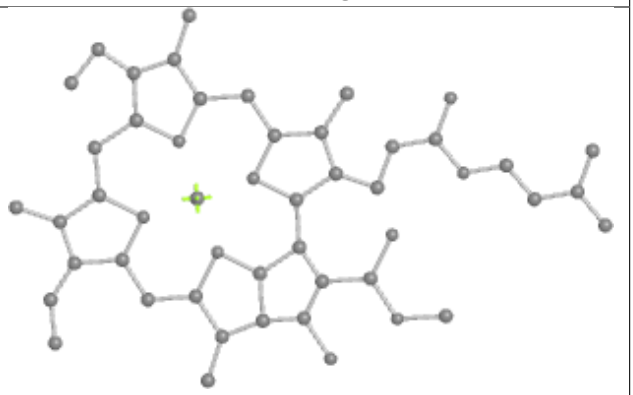


Bond angles

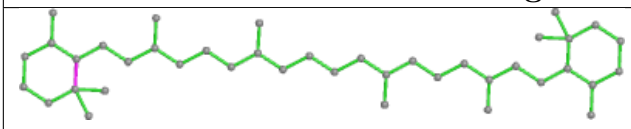


Torsions



Rings

Ligand BCR L 306



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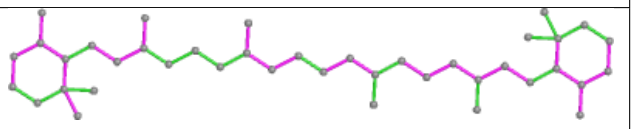
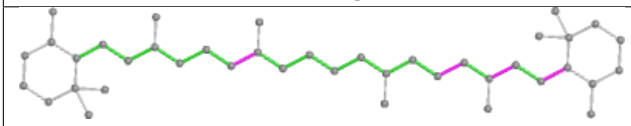


Bond angles



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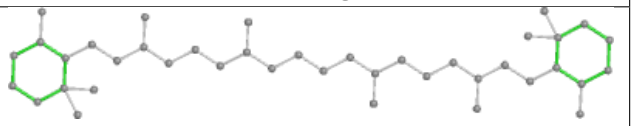
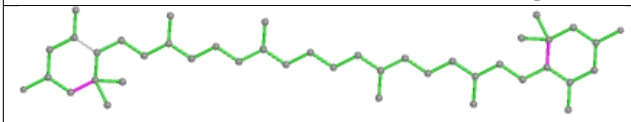


Rings

Ligand LUT 1 502



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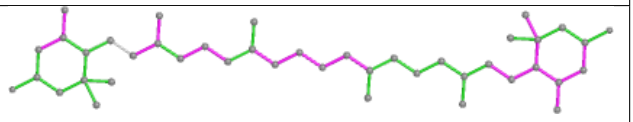
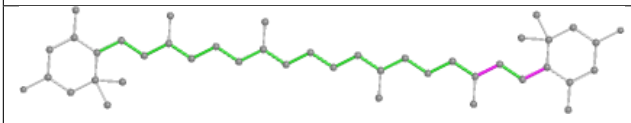
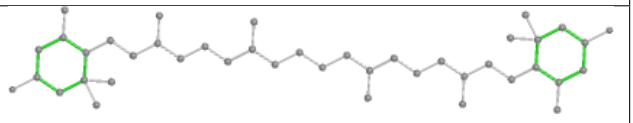


Bond angles

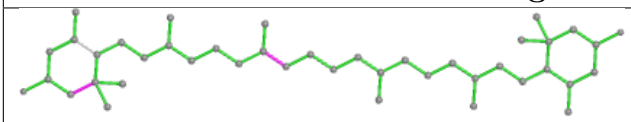


Torsions



Rings

Ligand LUT 3 303



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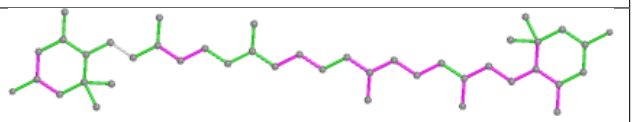
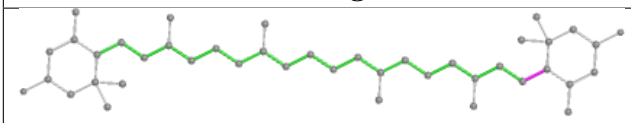


Bond angles



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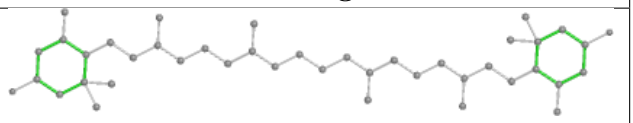
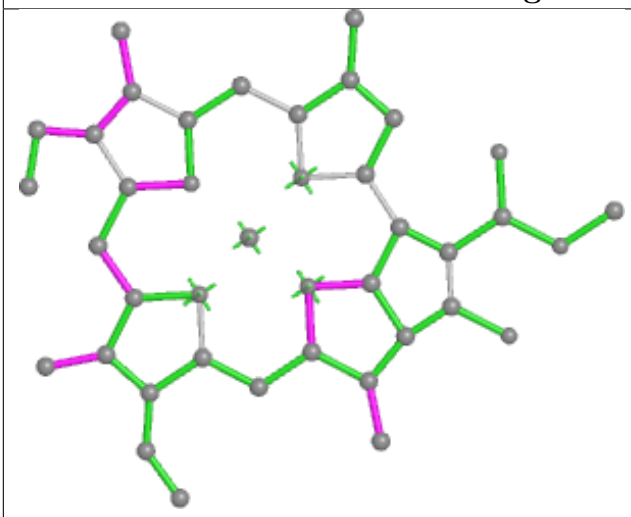


Rings

Ligand CLA A 811



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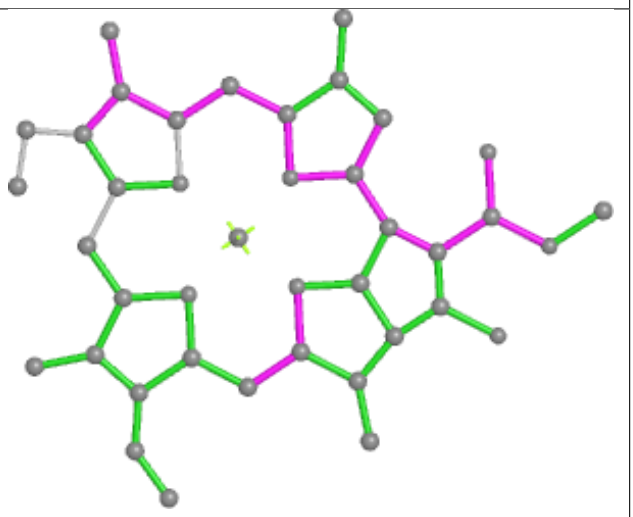
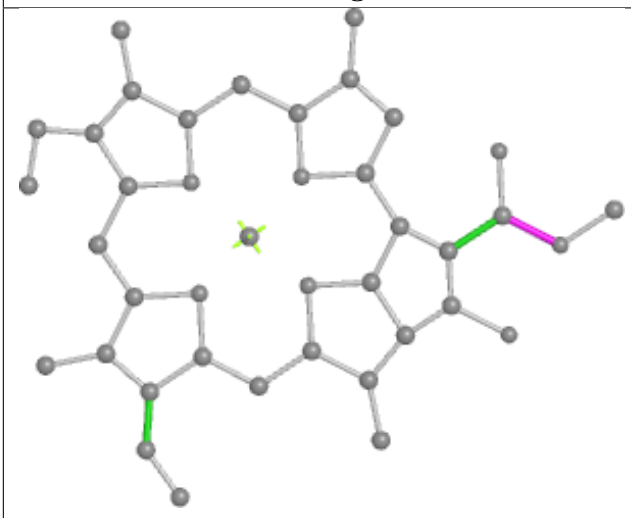


Bond angles



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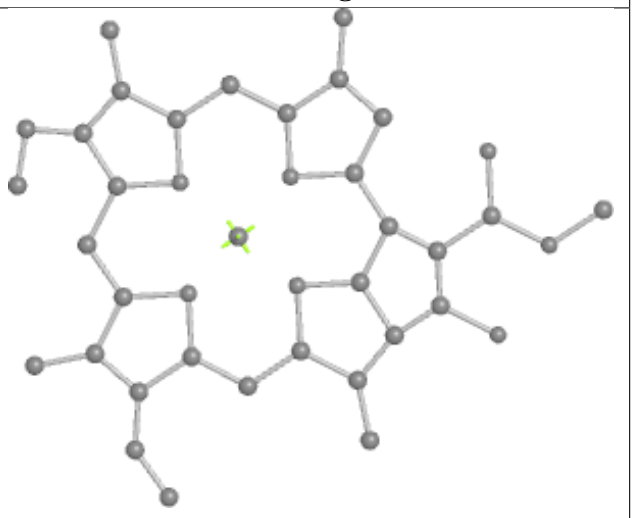
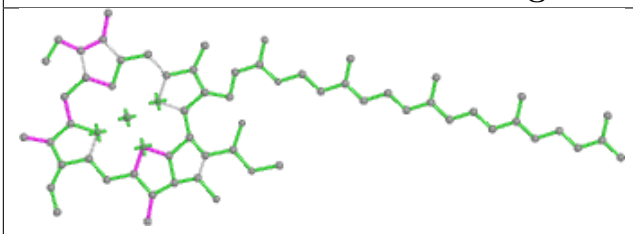


Rings

Ligand CLA 2 506



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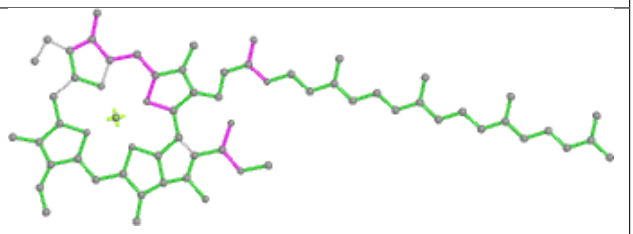

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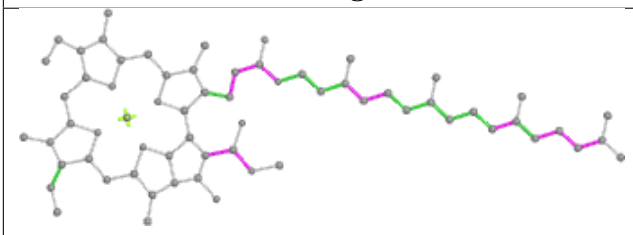

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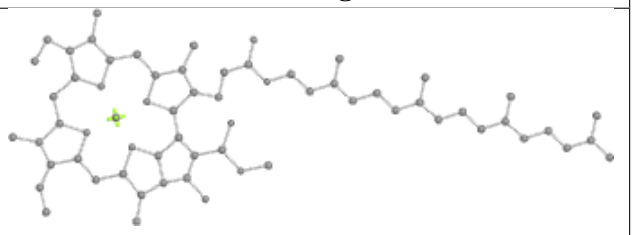
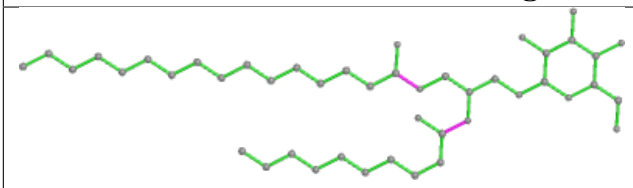


Rings

Ligand LMG F 806



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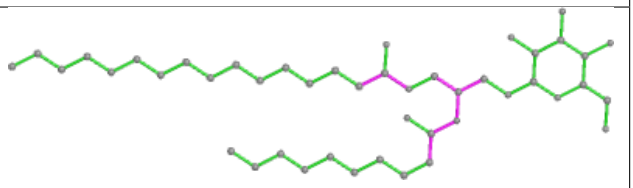
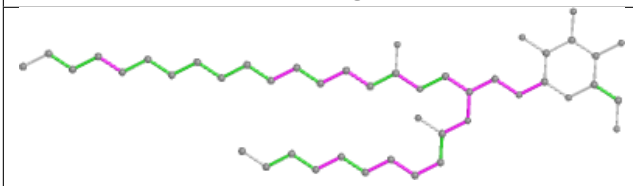


Bond angles



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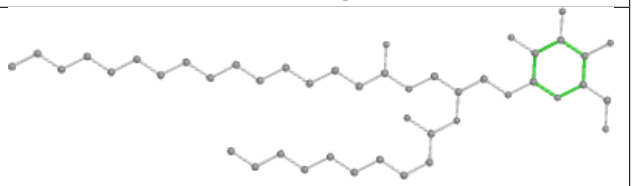
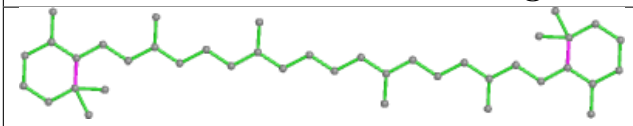


Rings

Ligand BCR F 801



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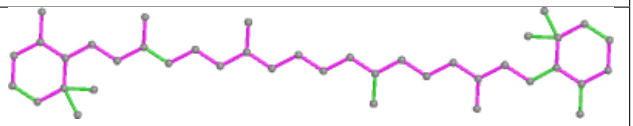
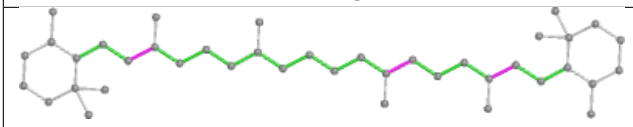


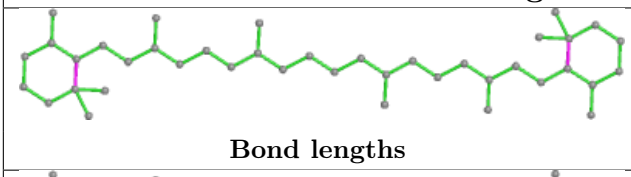
Bond angles



Torsions

Rings

Ligand BCR J 102



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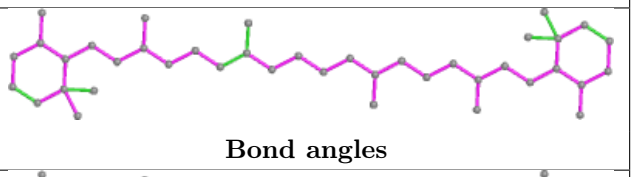

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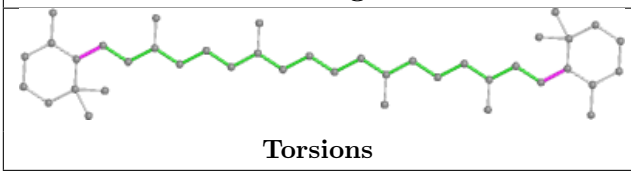

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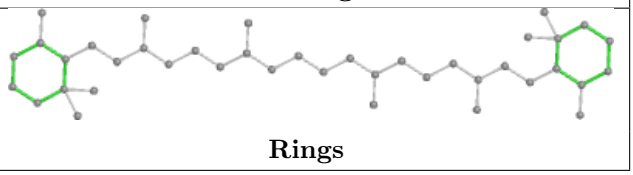
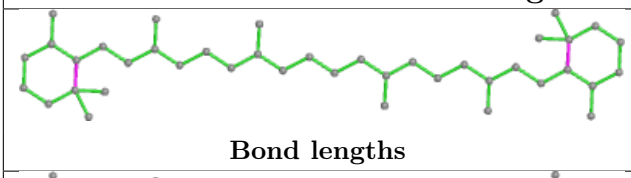


Rings

Ligand BCR 3 305



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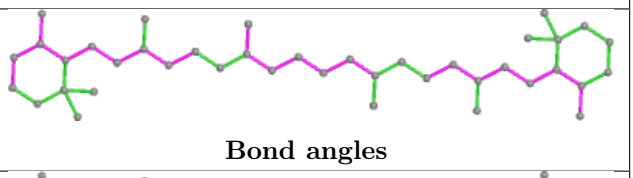
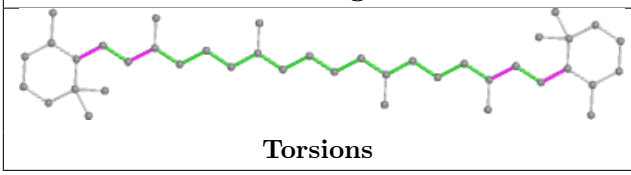


Bond angles



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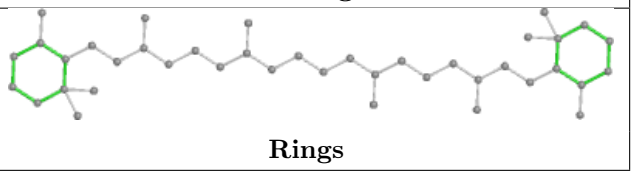
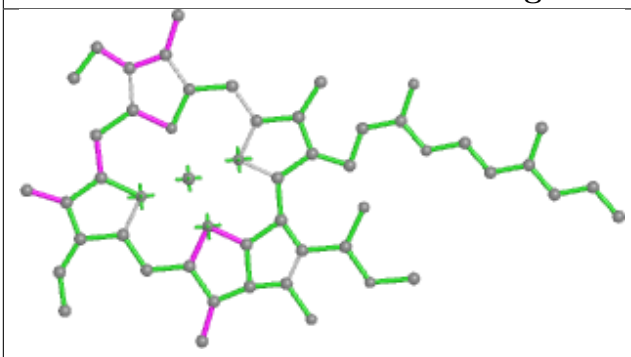


Rings

Ligand CLA B 808



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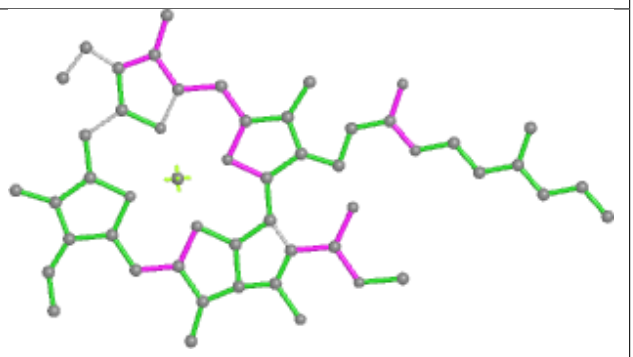
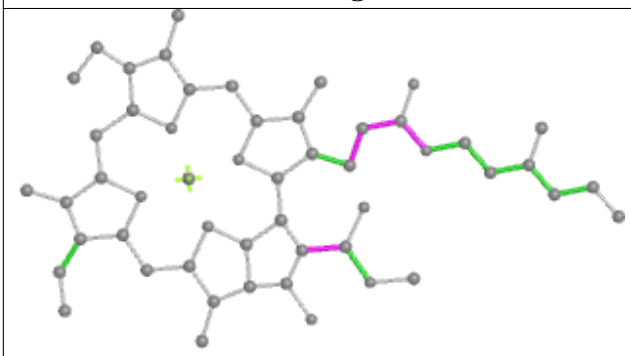


Bond angles



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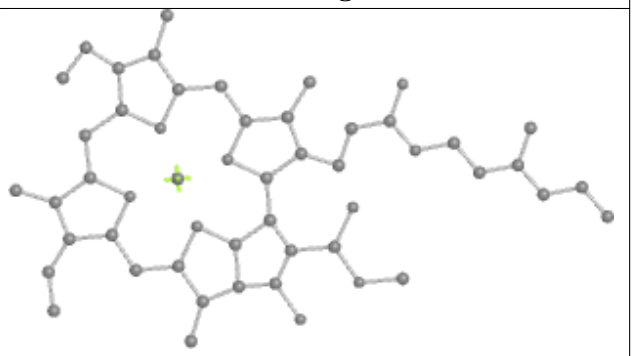
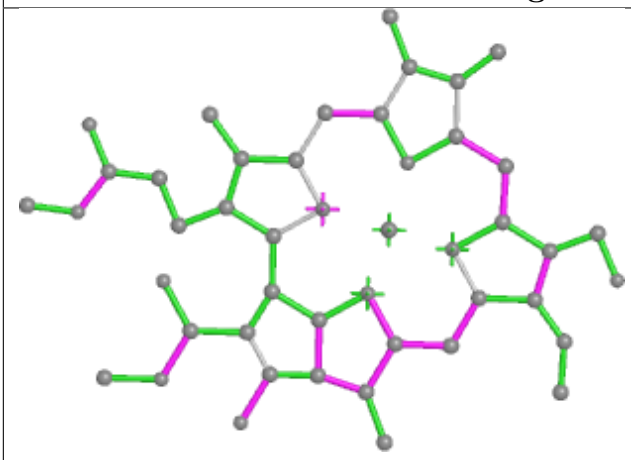
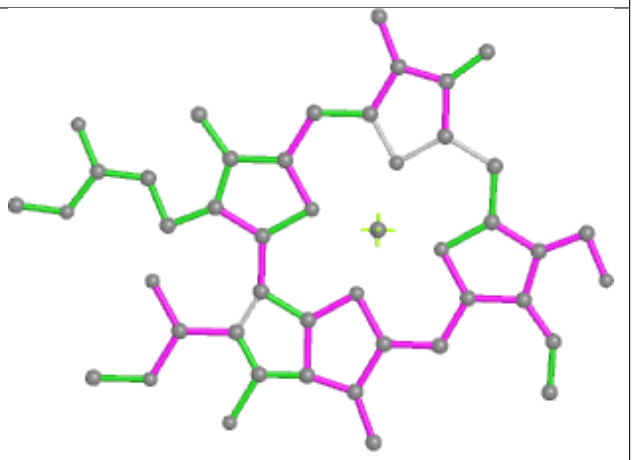


Rings

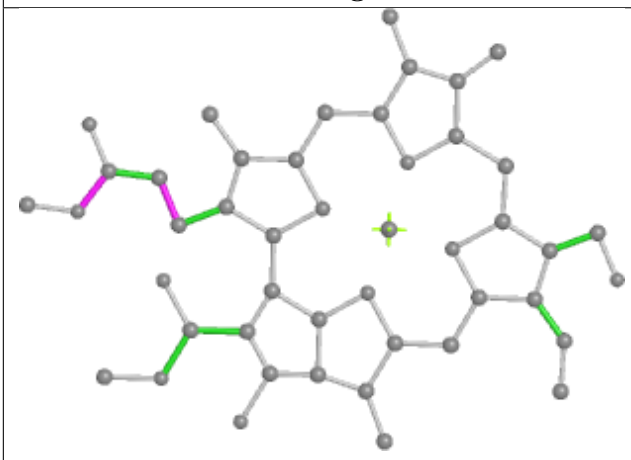
Ligand CHL 2 512



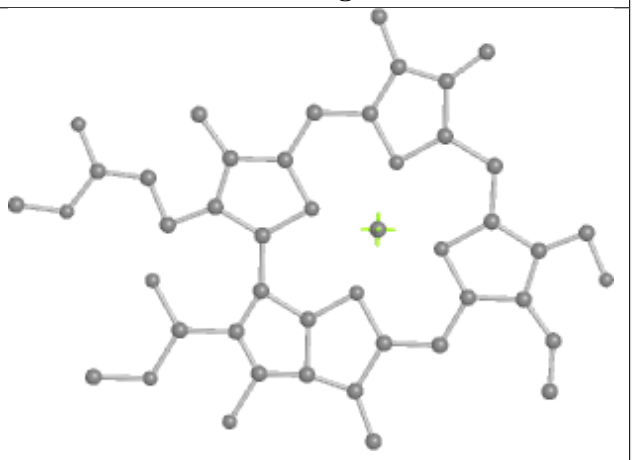
Bond lengths



Bond angles

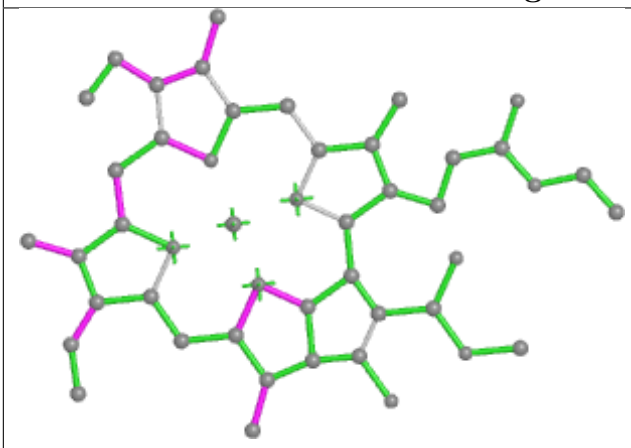


Torsions

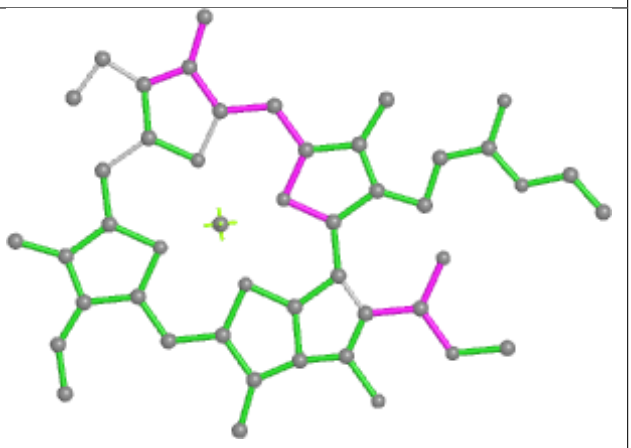


Rings

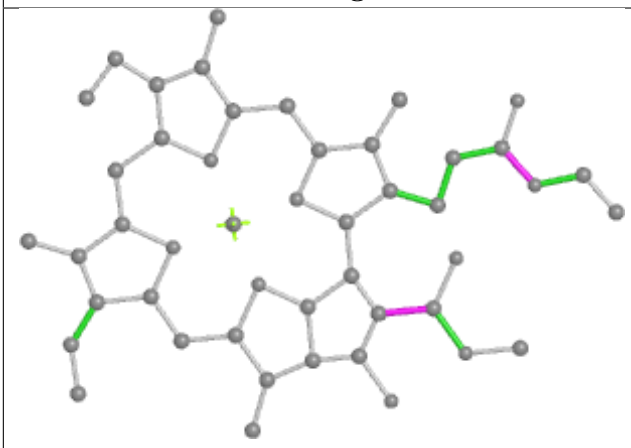
Ligand CLA B 822



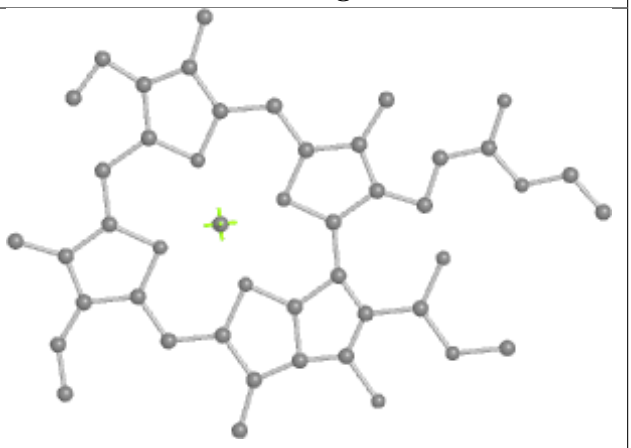
Bond lengths



Bond angles

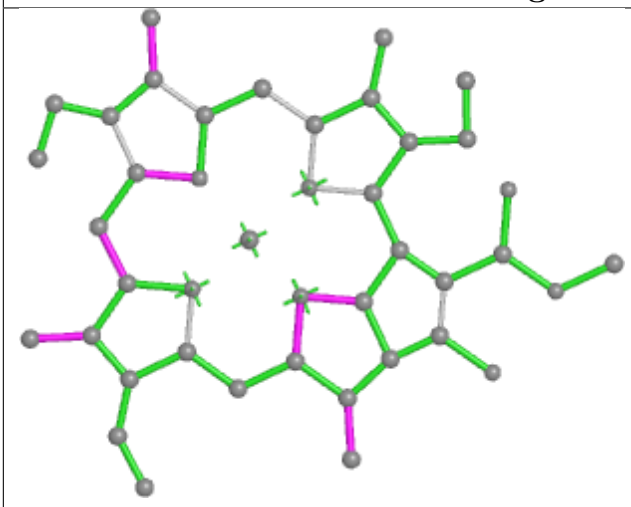


Torsions

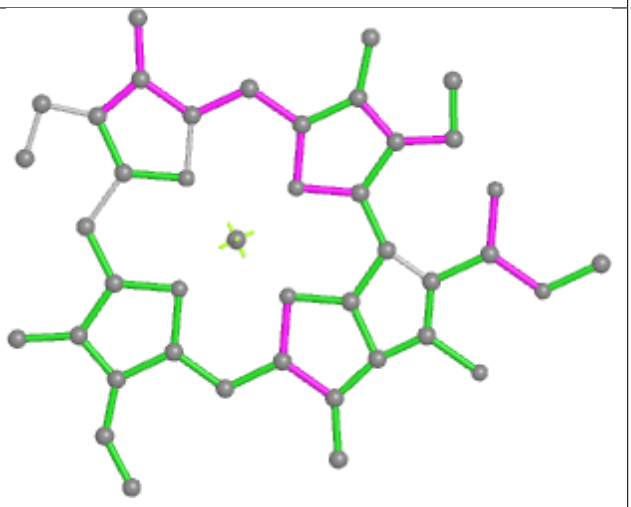


Rings

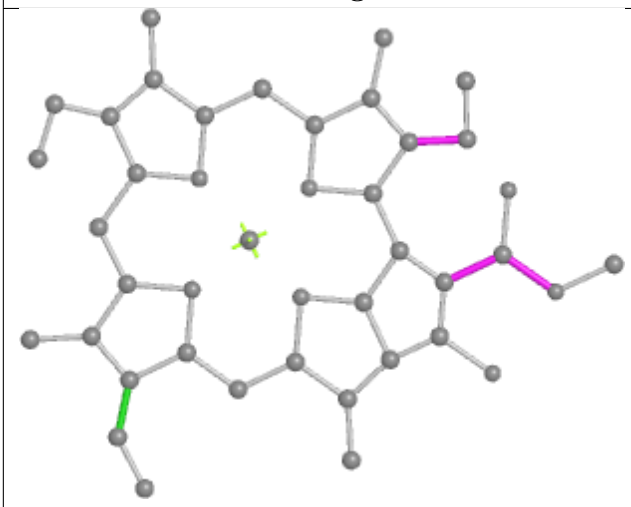
Ligand CLA 5 311



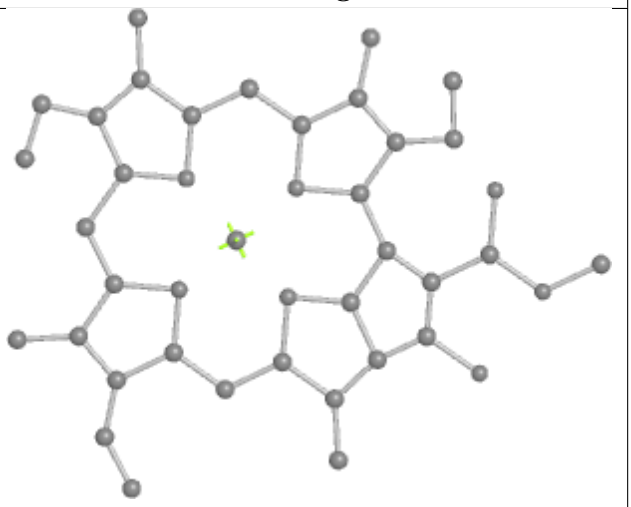
Bond lengths



Bond angles

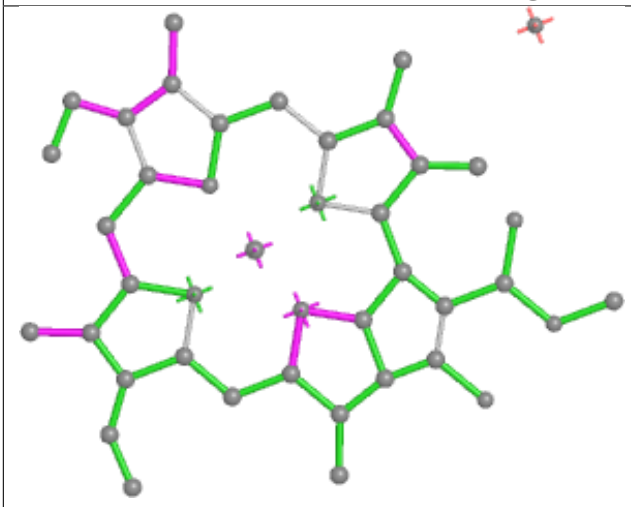


Torsions



Rings

Ligand CLA B 828



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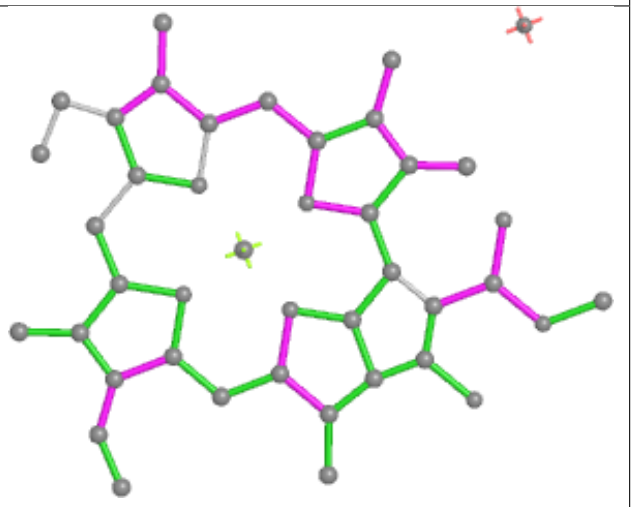
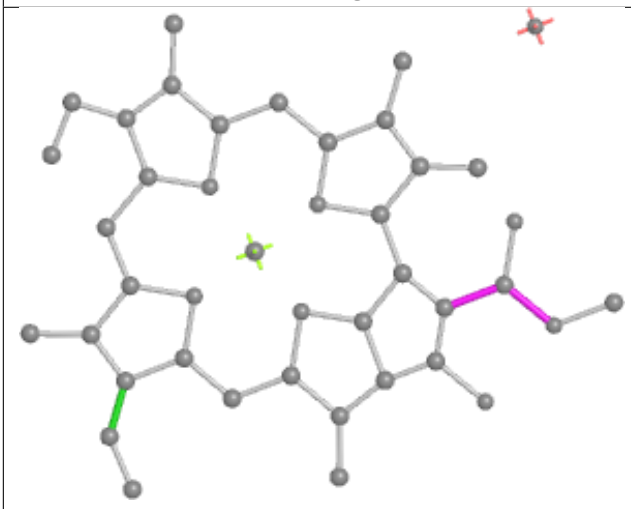
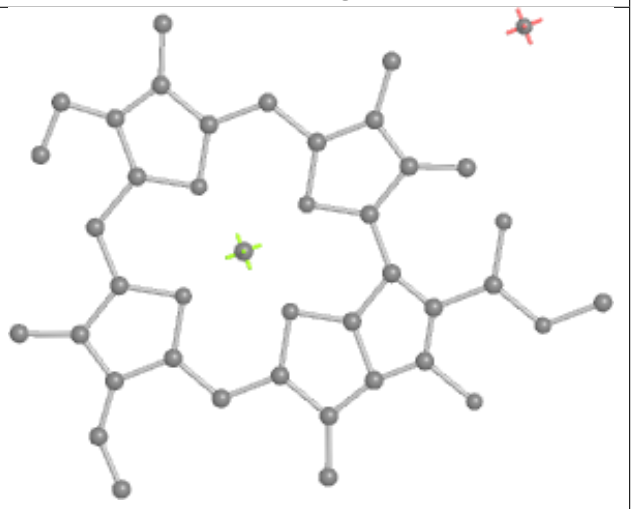


Bond angles

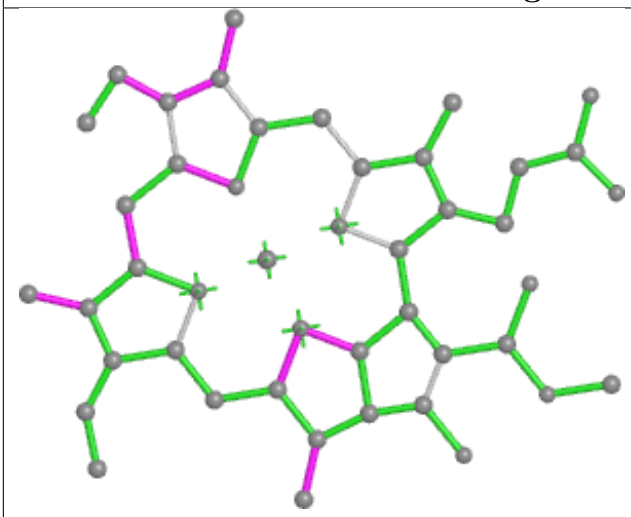


Torsions

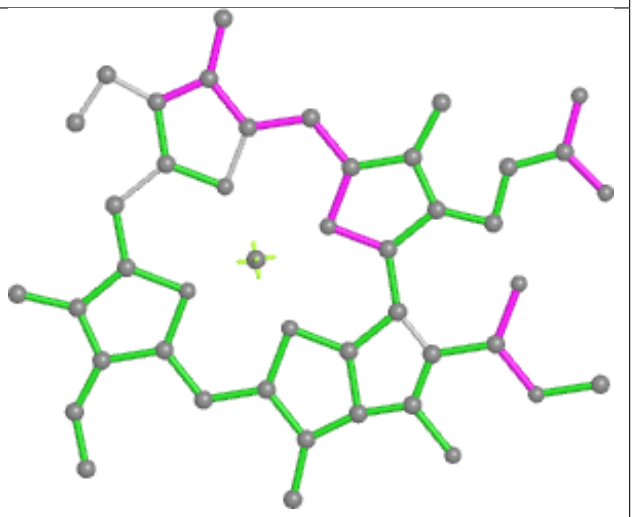


Rings

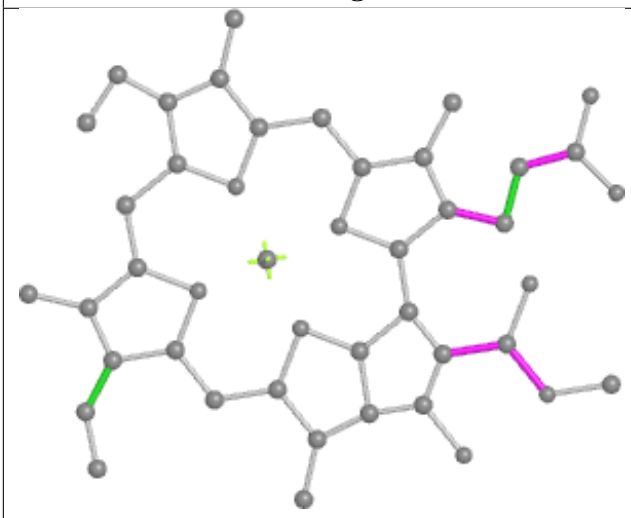
Ligand CLA A 813



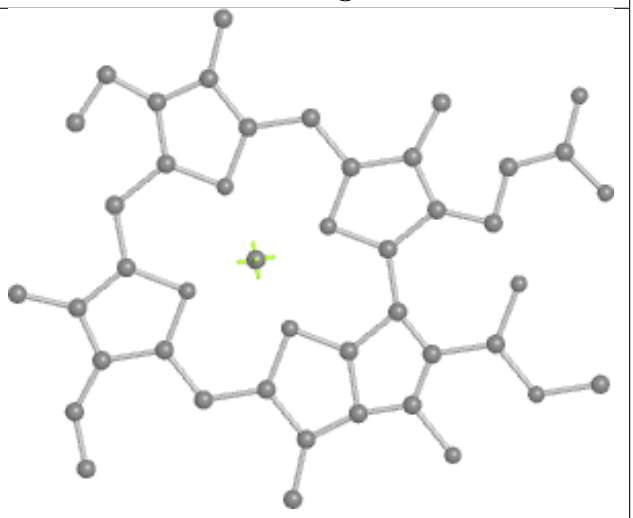
Bond lengths



Bond angles

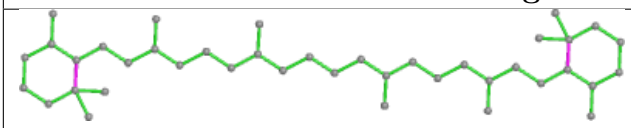


Torsions



Rings

Ligand BCR B 848



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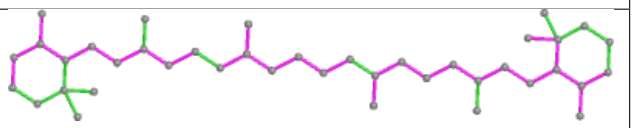
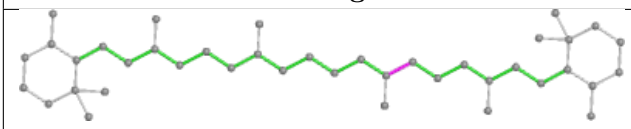


Bond angles



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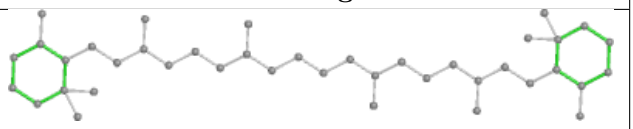
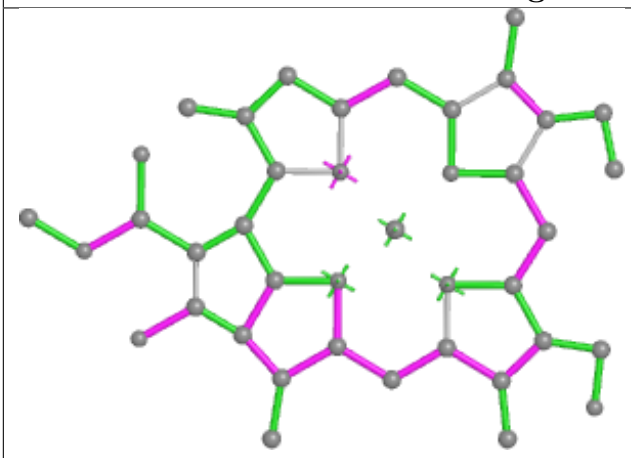


Rings

Ligand CHL 5 317



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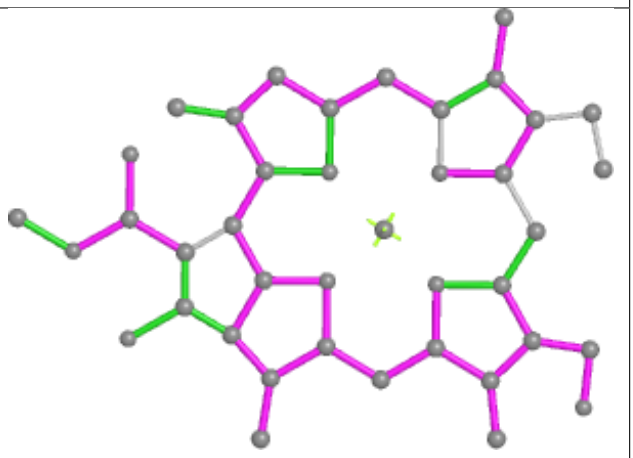
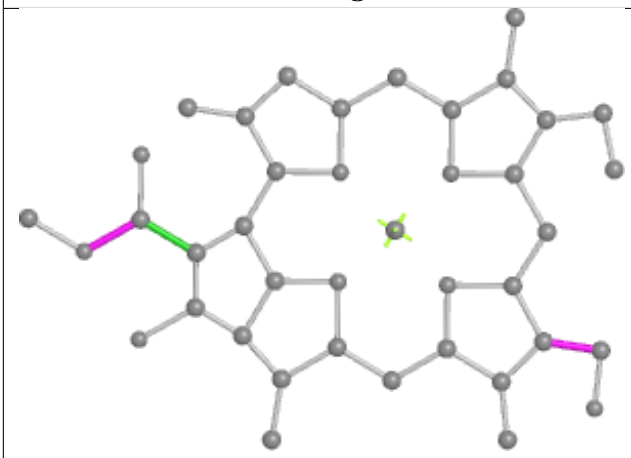


Bond angles



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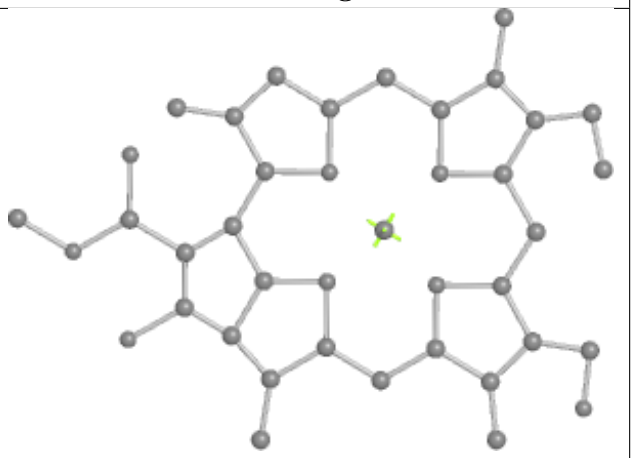
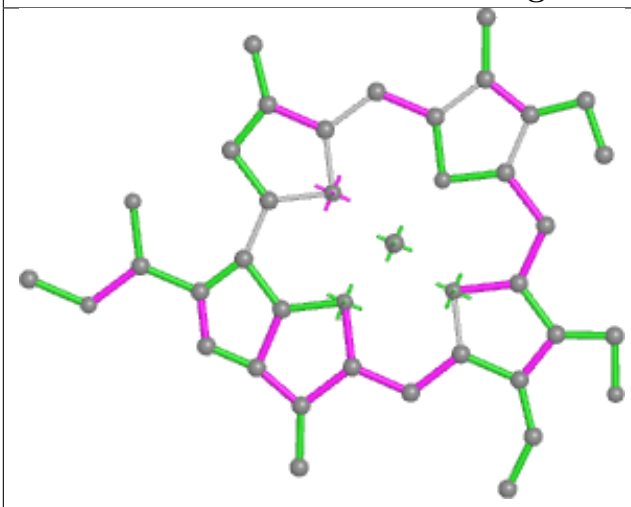


Rings

Ligand CHL 2 513



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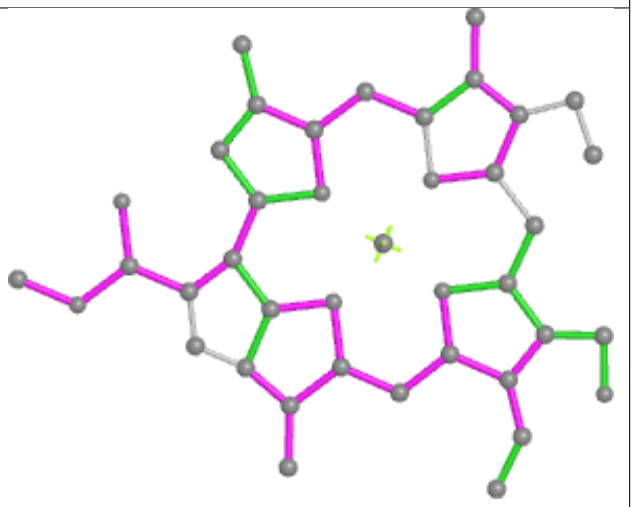
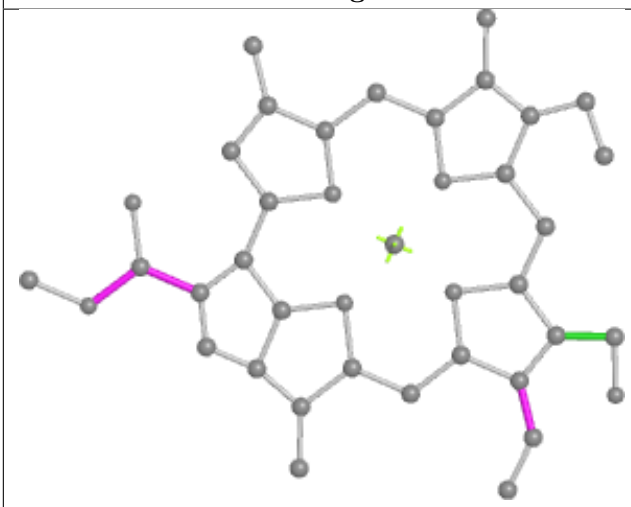


Bond angles



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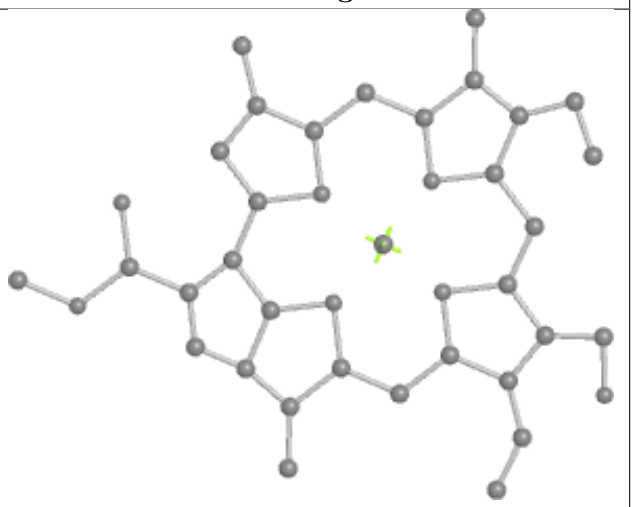
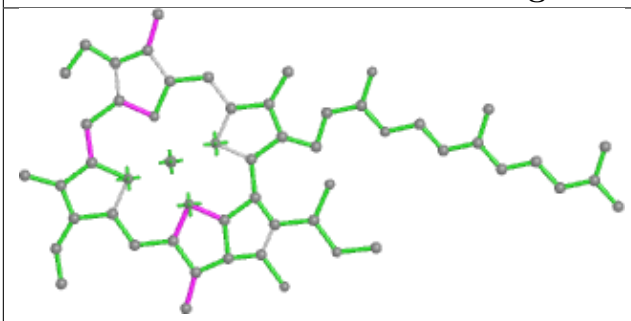


Rings

Ligand CLA 3 314



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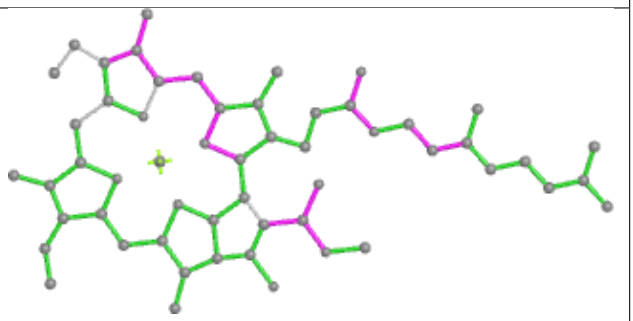
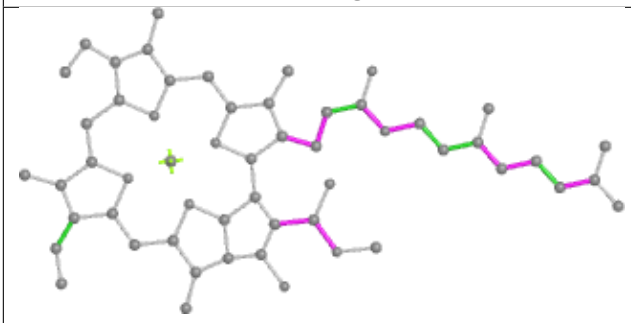


Bond angles



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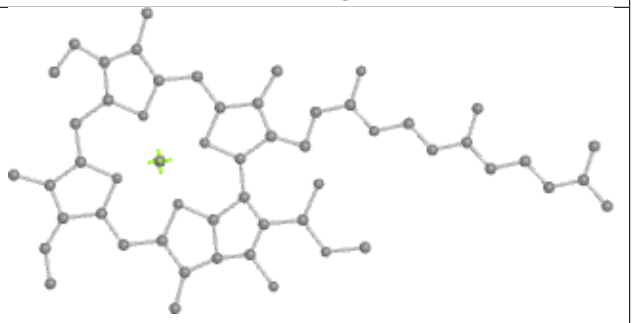
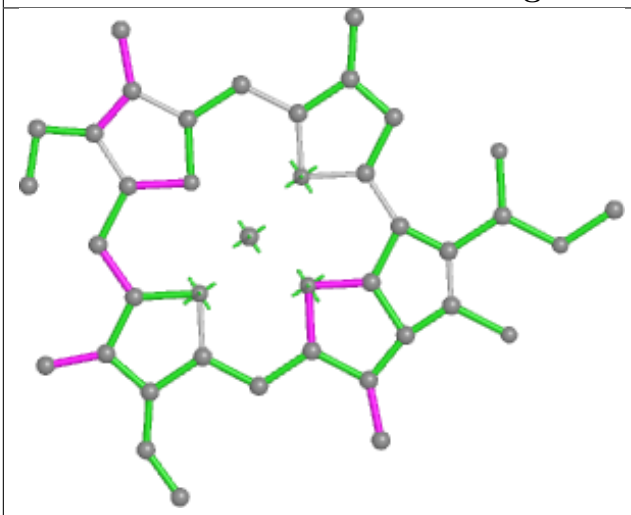


Rings

Ligand CLA A 824



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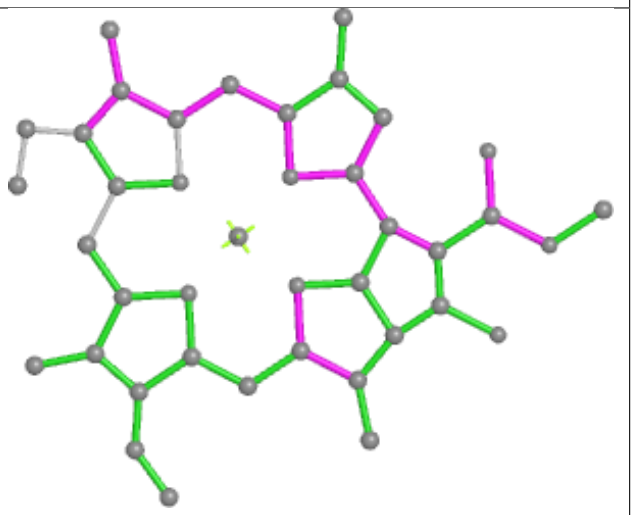
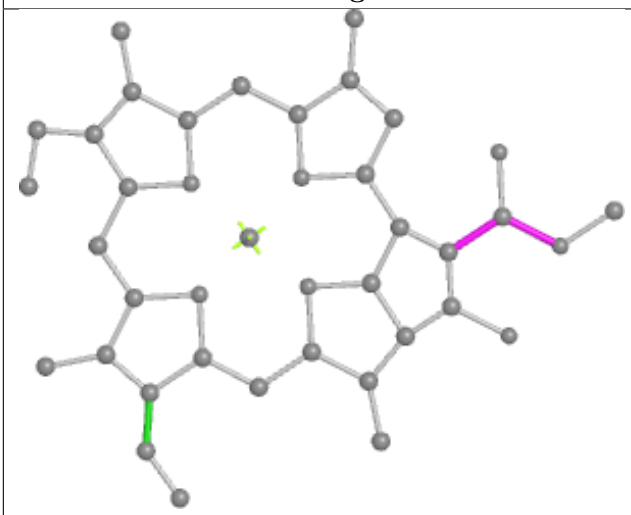


Bond angles



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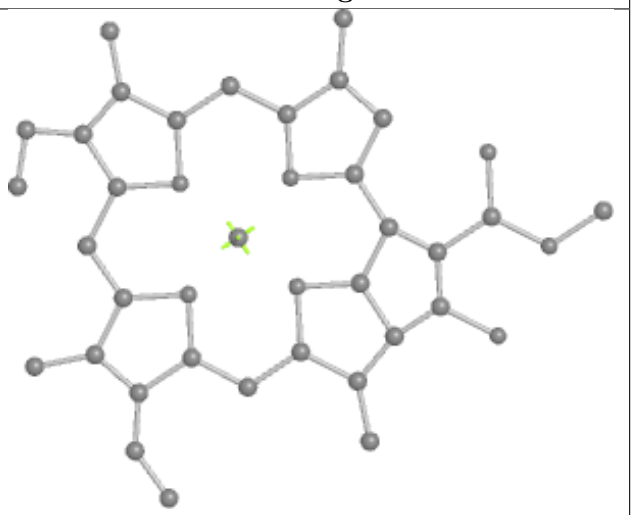
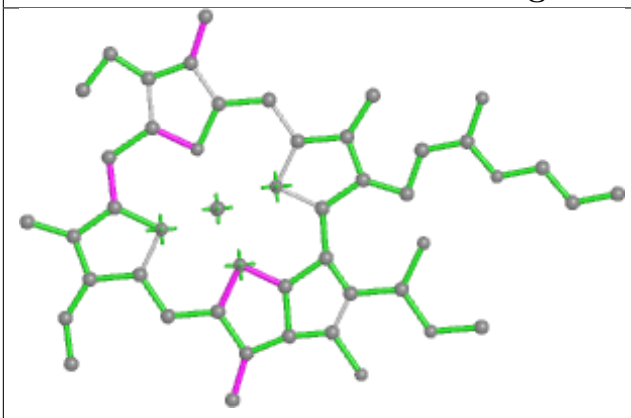


Rings

Ligand CLA 3 313



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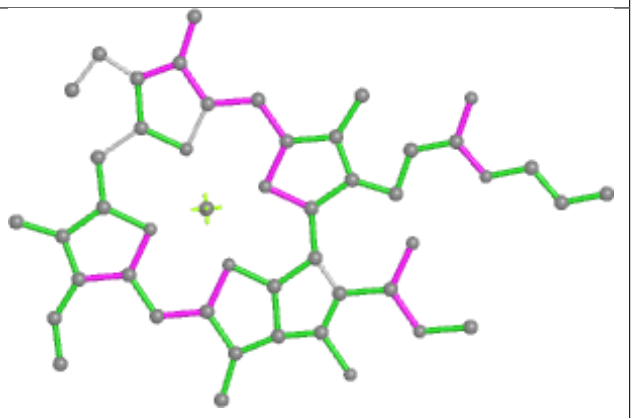
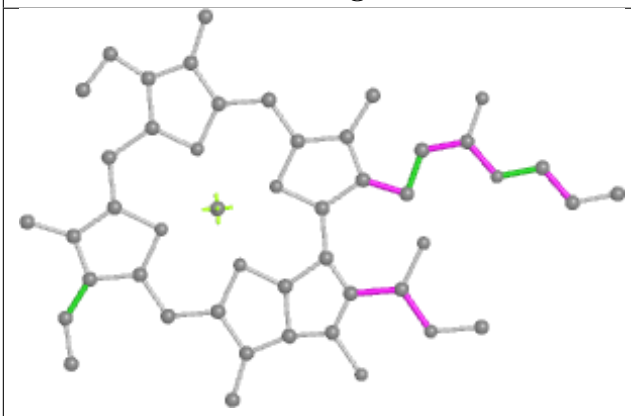


Bond angles



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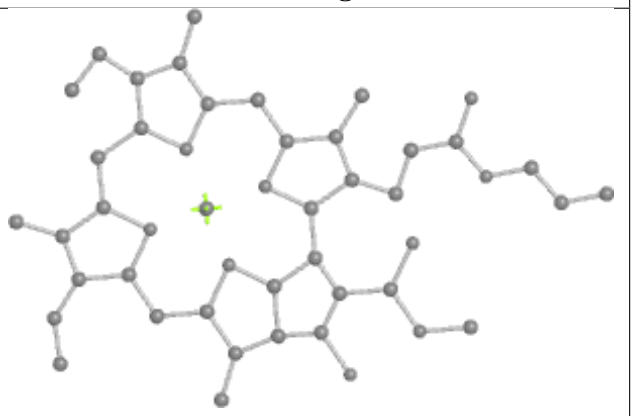
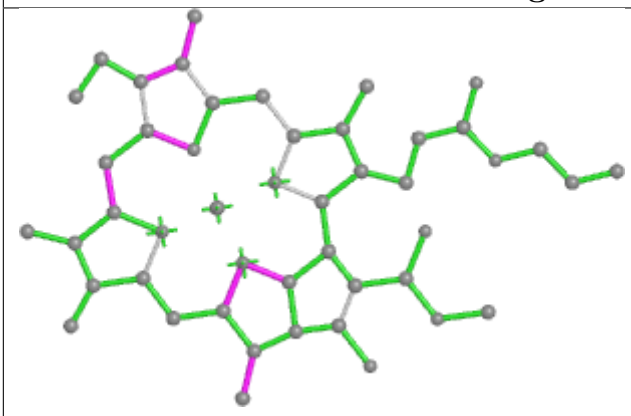


Rings

Ligand CLA 2 508



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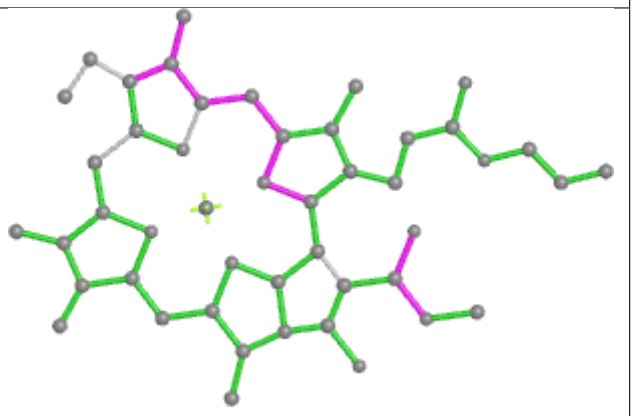
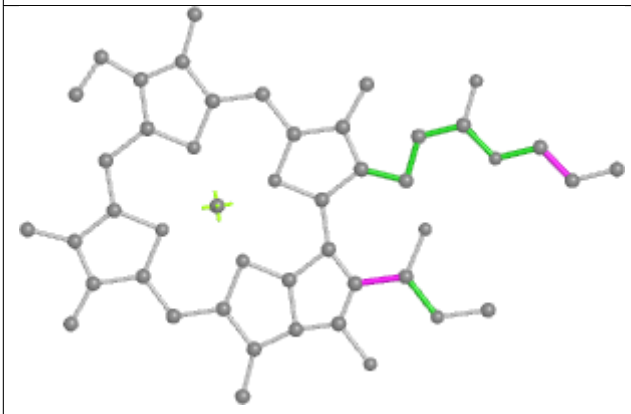
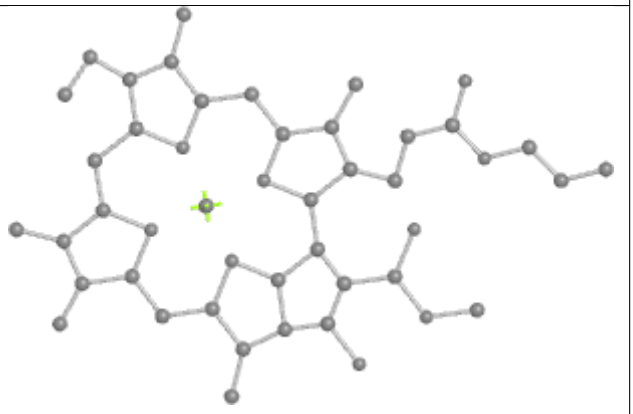


Bond angles

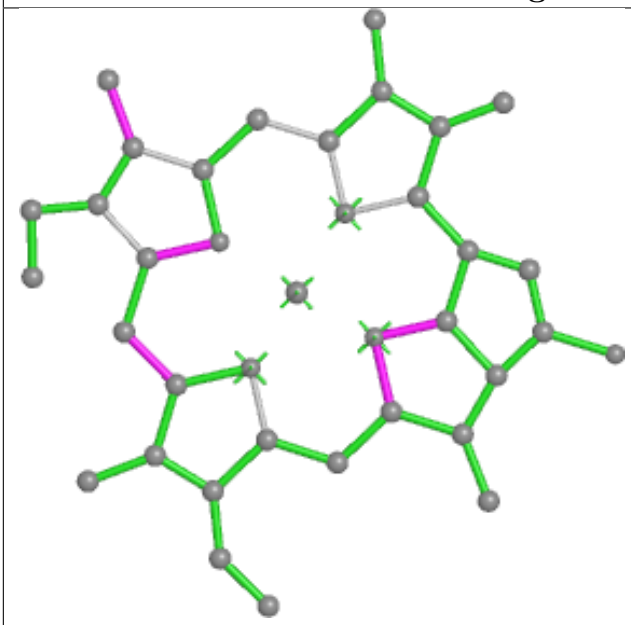


Torsions



Rings

Ligand CLA 3 316



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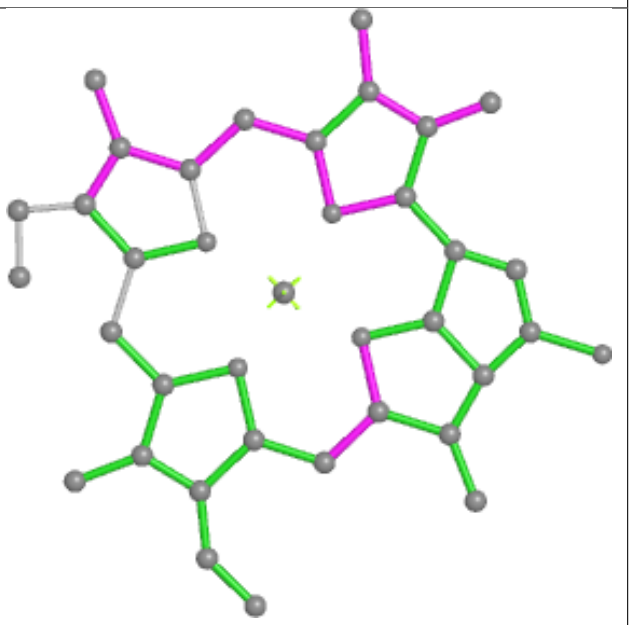
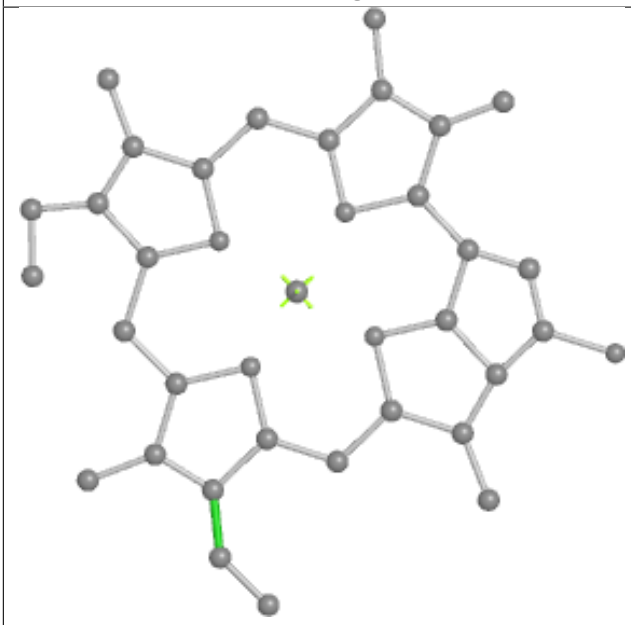


Bond angles



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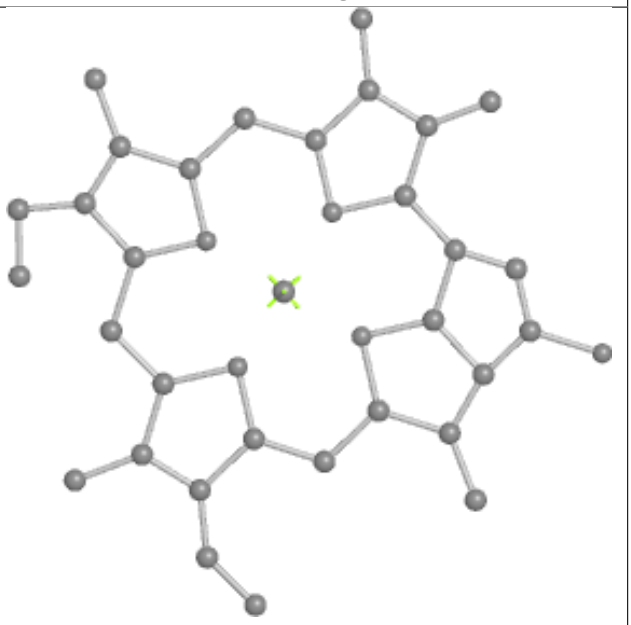
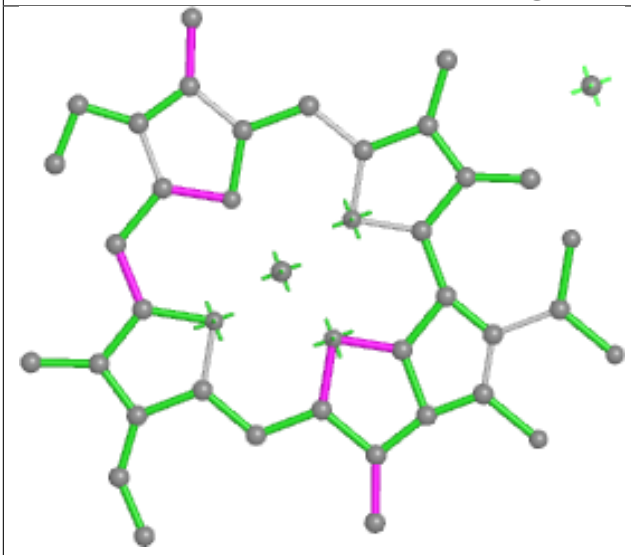


Rings

Ligand CLA 5 306



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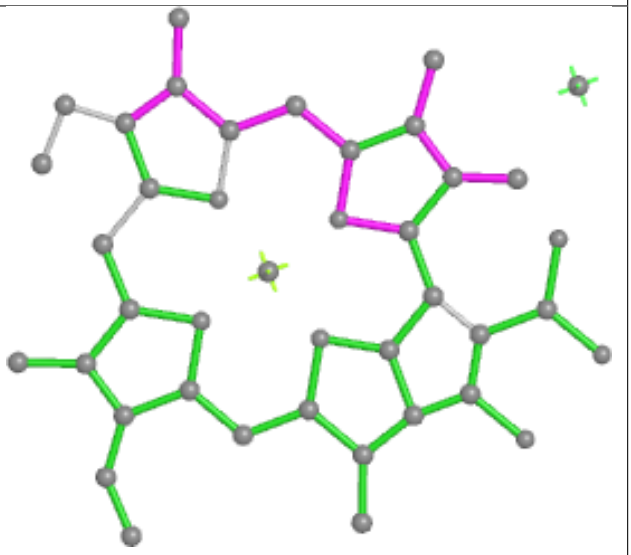
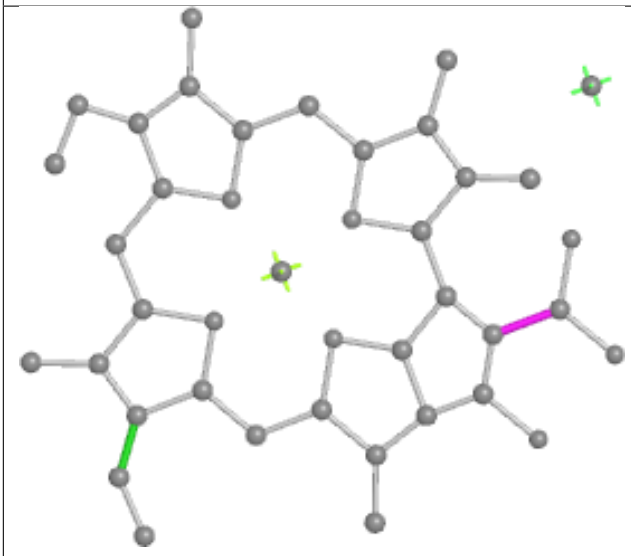


Bond angles



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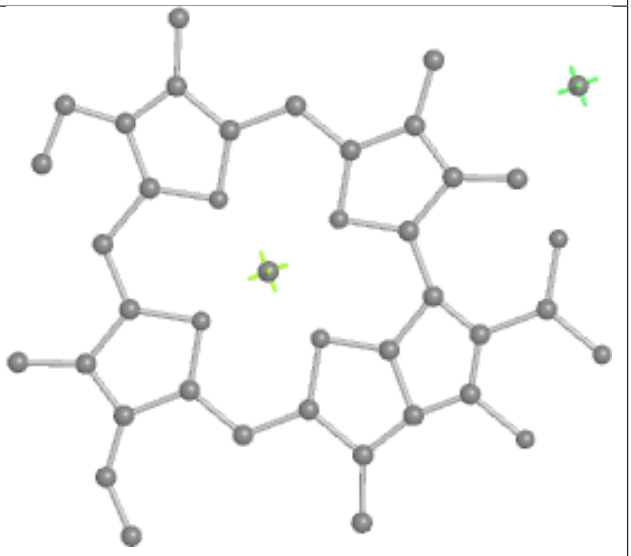
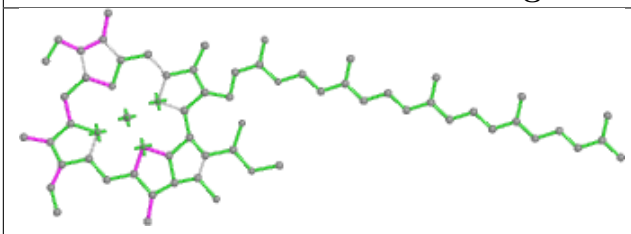


Rings

Ligand CLA A 808



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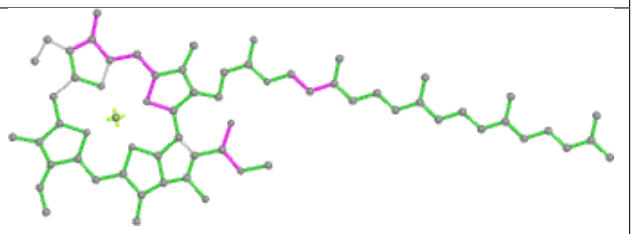
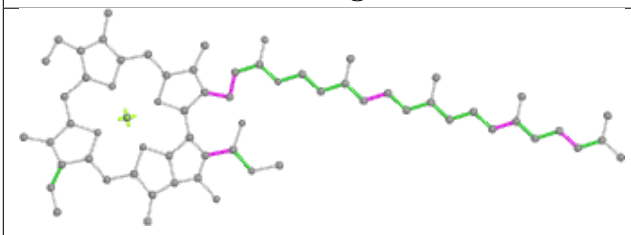
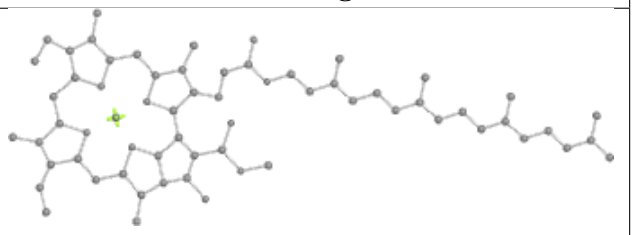


Bond angles

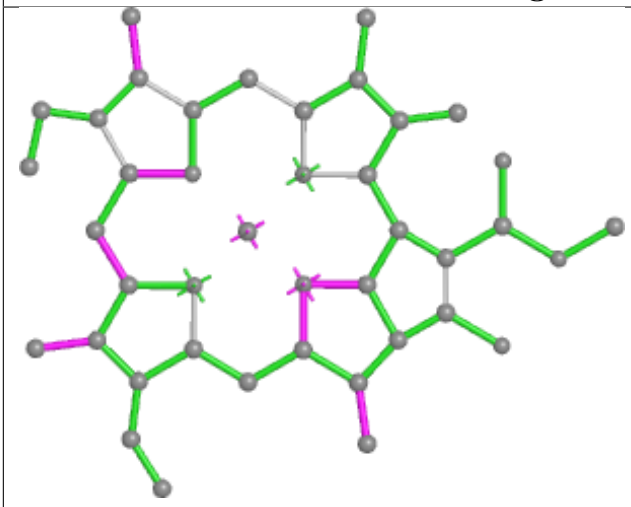


Torsions

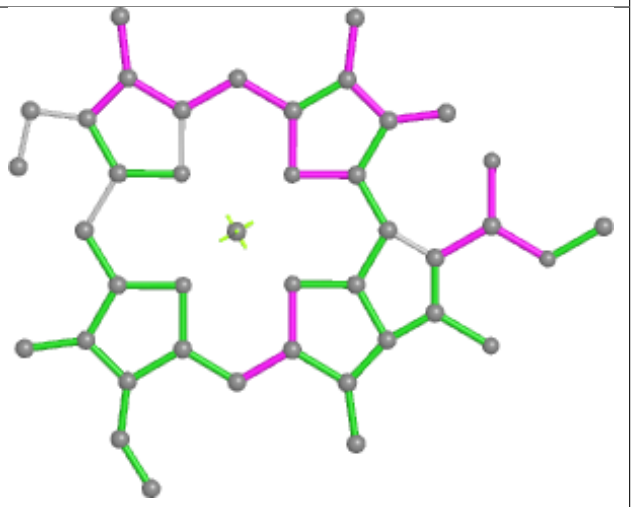


Rings

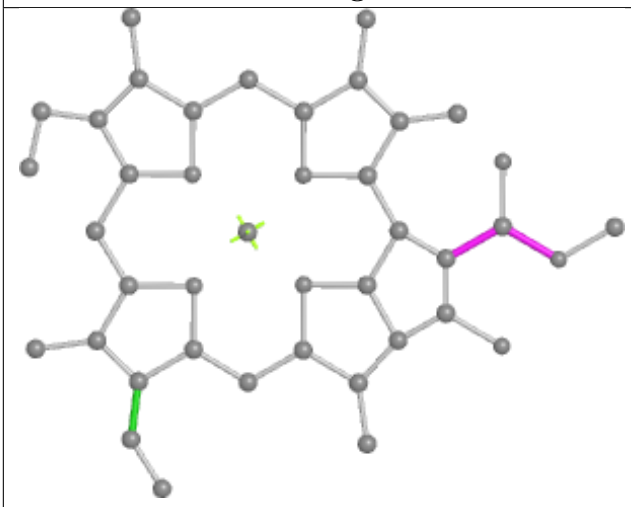
Ligand CLA 3 317



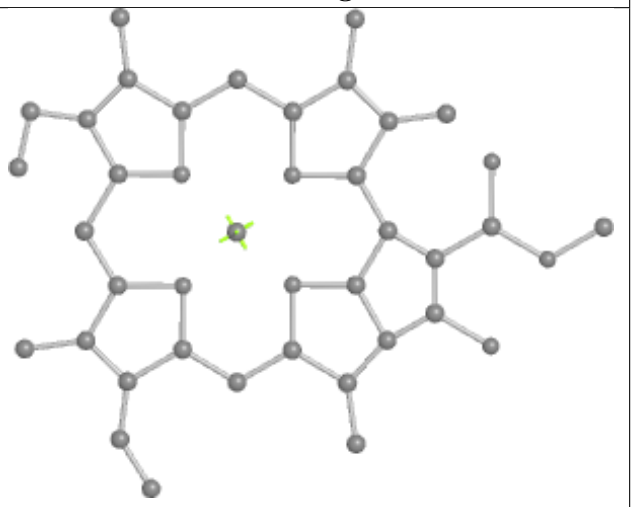
Bond lengths



Bond angles

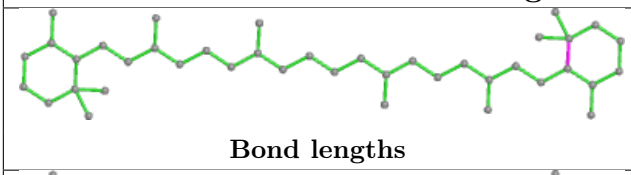


Torsions

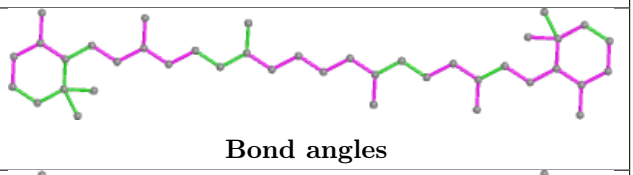


Rings

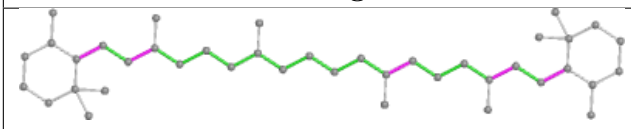
Ligand BCR L 305



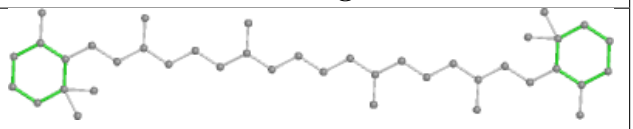
Bond lengths



Bond angles

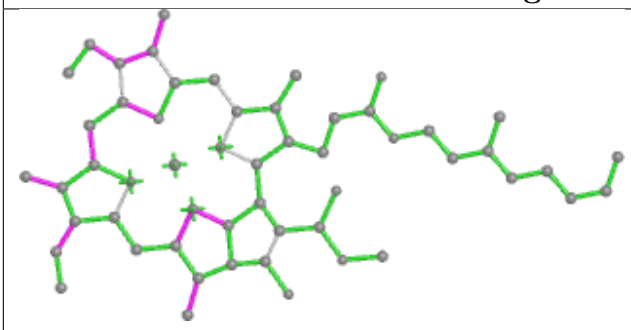


Torsions

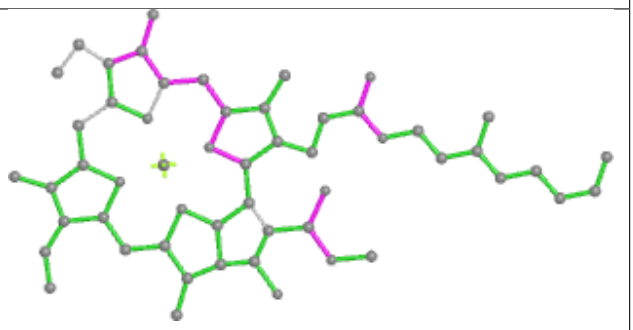


Rings

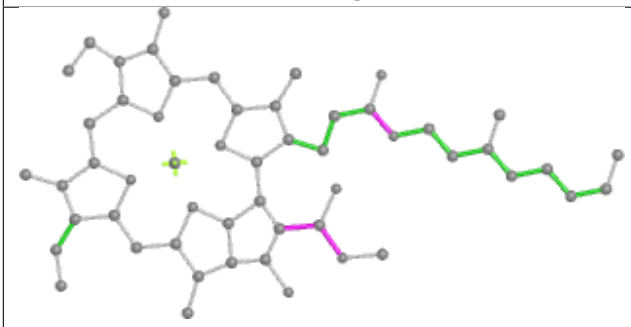
Ligand CLA A 810



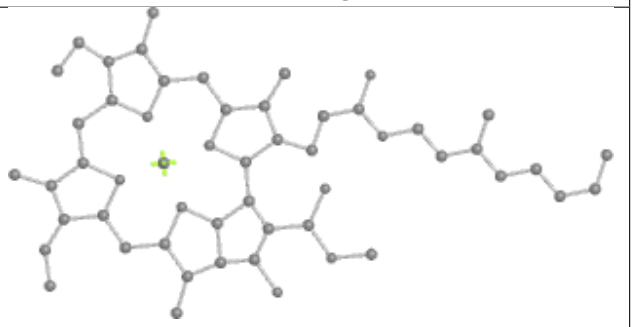
Bond lengths



Bond angles

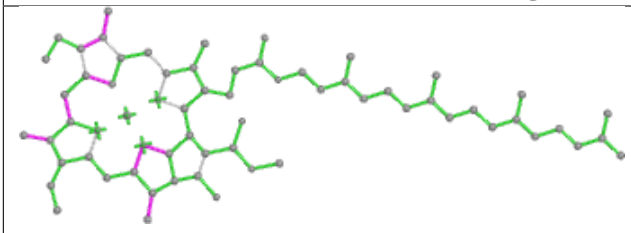


Torsions

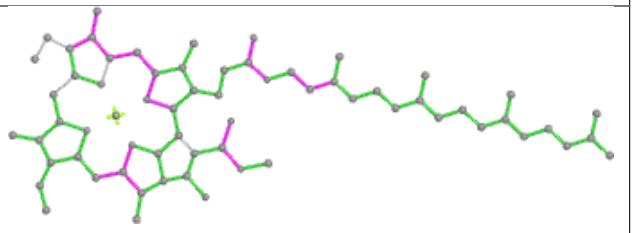


Rings

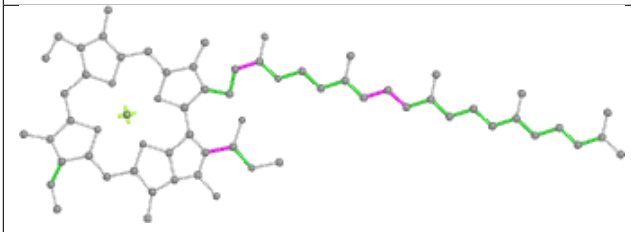
Ligand CLA B 833



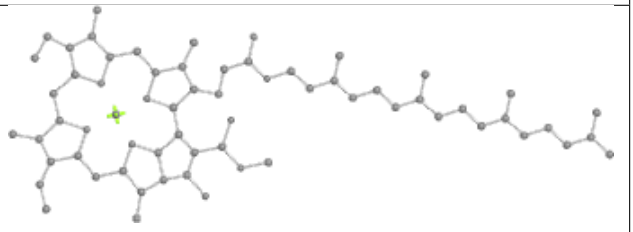
Bond lengths



Bond angles

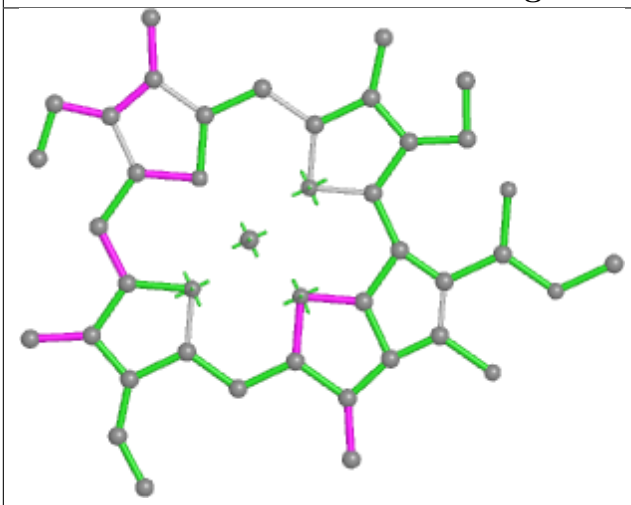


Torsions

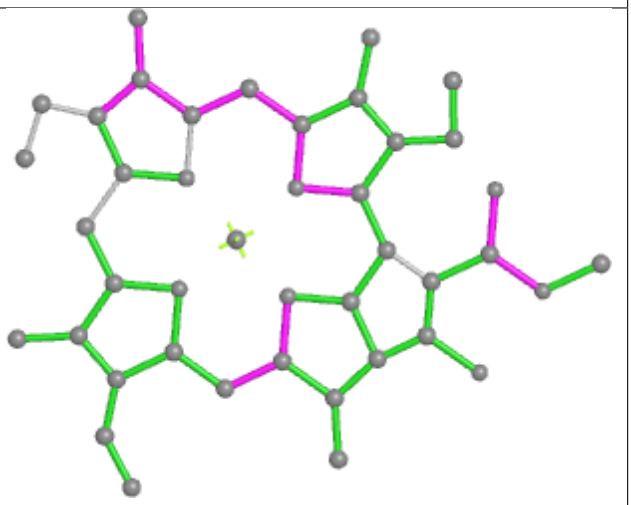


Rings

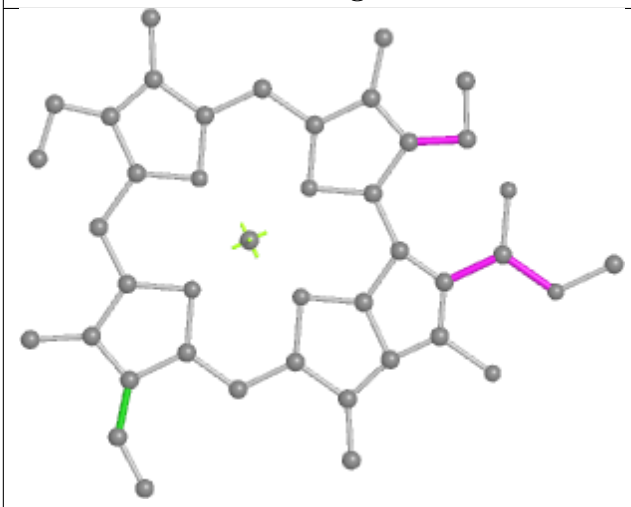
Ligand CLA B 836



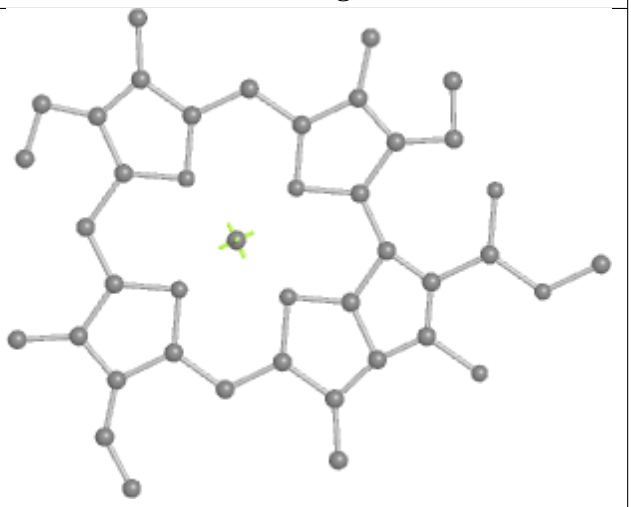
Bond lengths



Bond angles

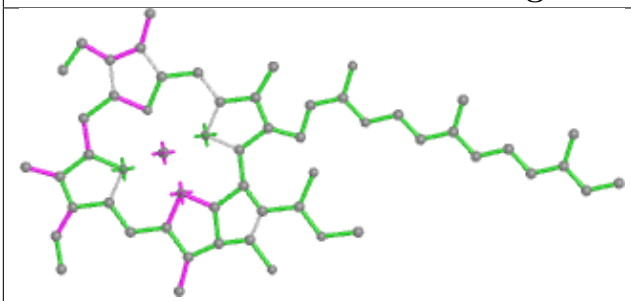


Torsions

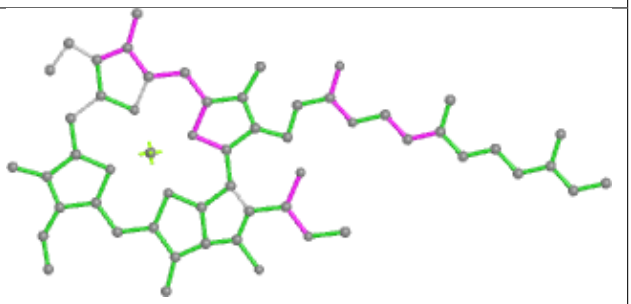


Rings

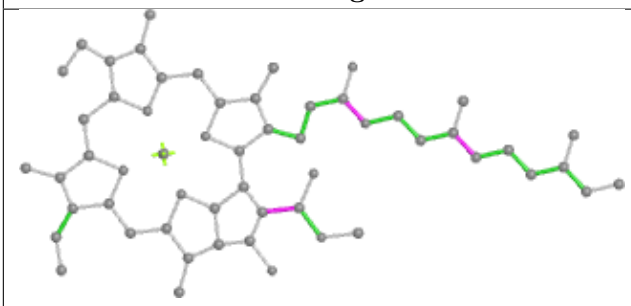
Ligand CLA L 301



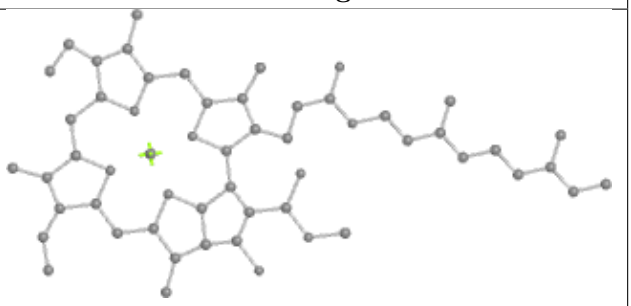
Bond lengths



Bond angles

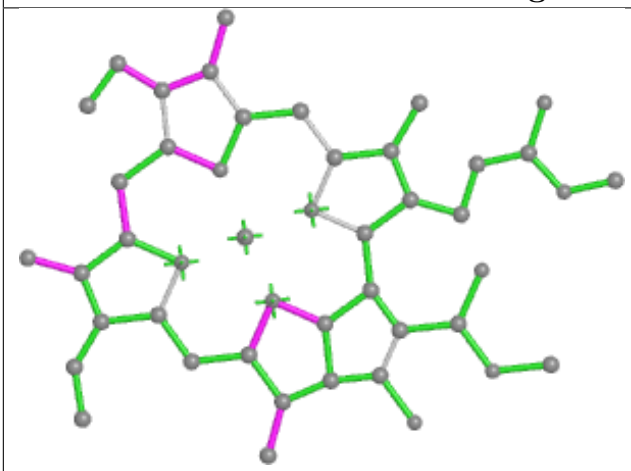


Torsions

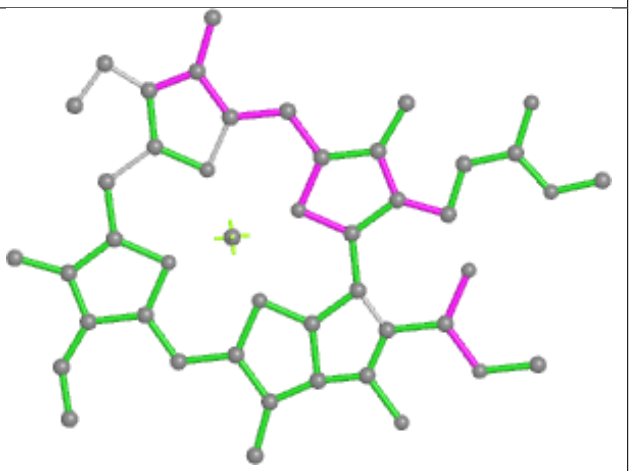


Rings

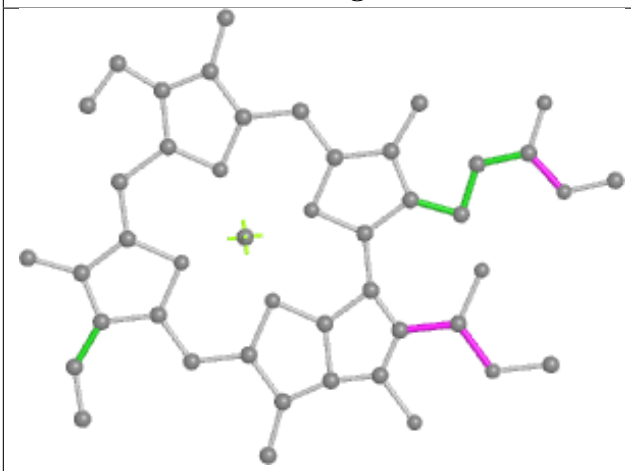
Ligand CLA 1 511



Bond lengths



Bond angles



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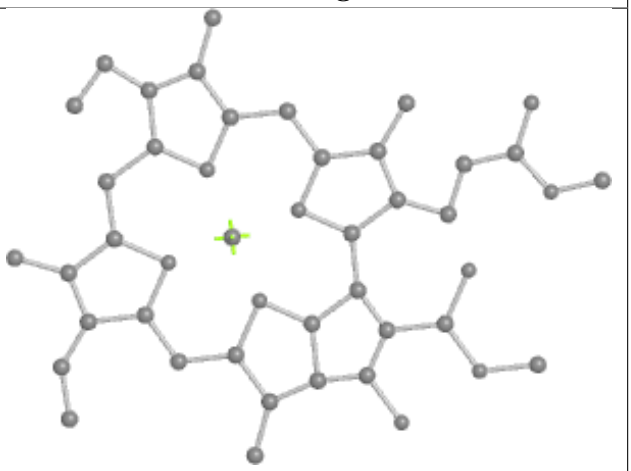
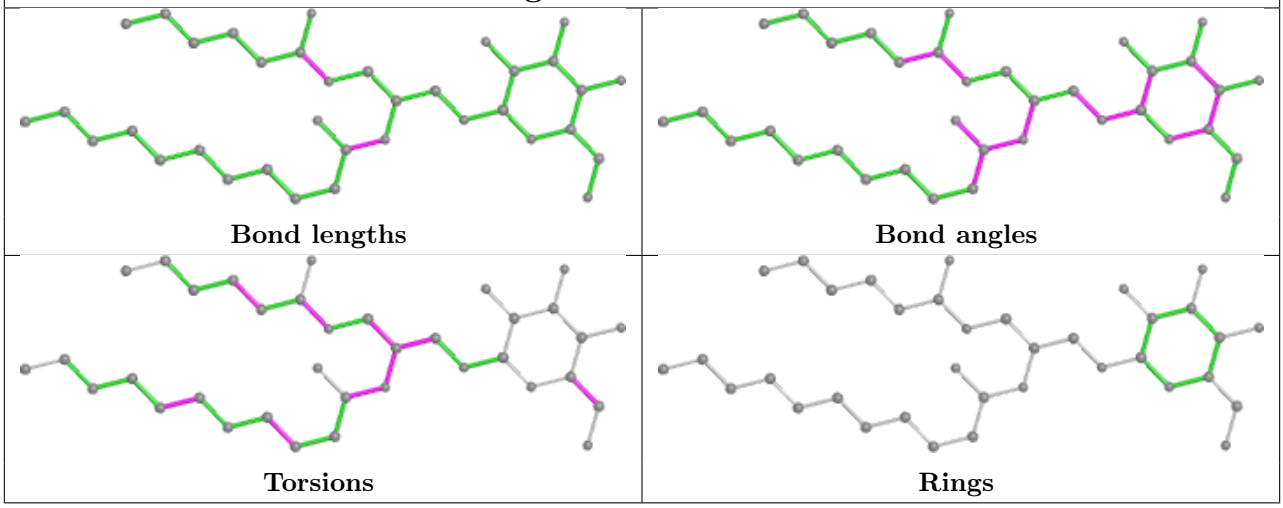
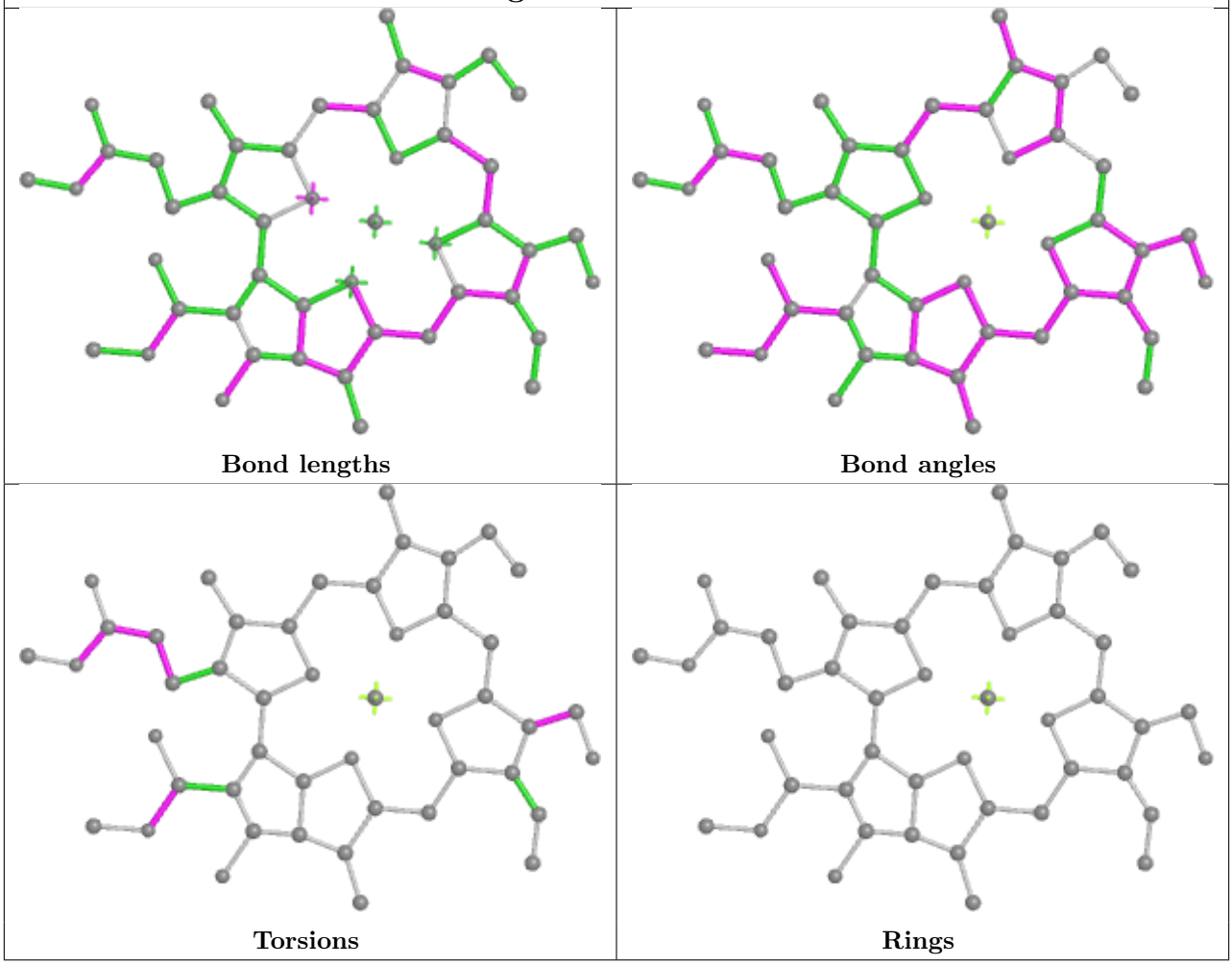


Rings

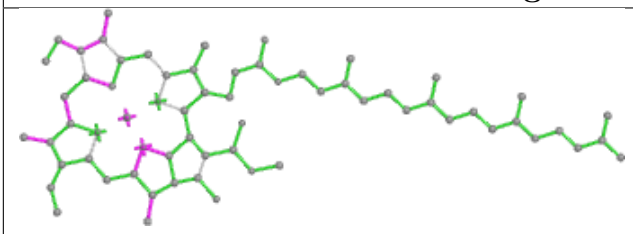
Ligand LMG 2 519



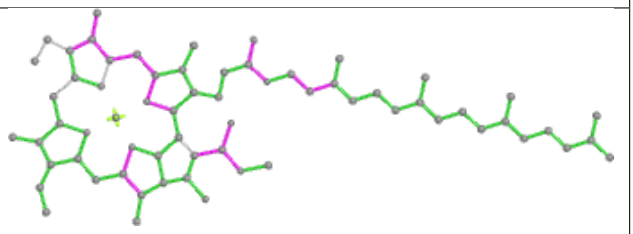
Ligand CHL 1 512



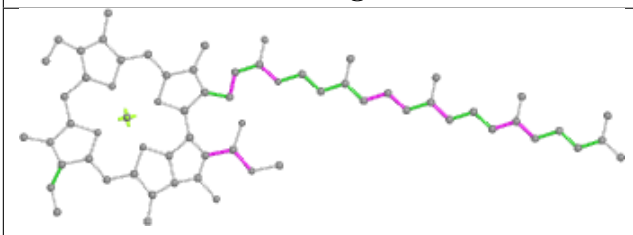
Ligand CLA A 838



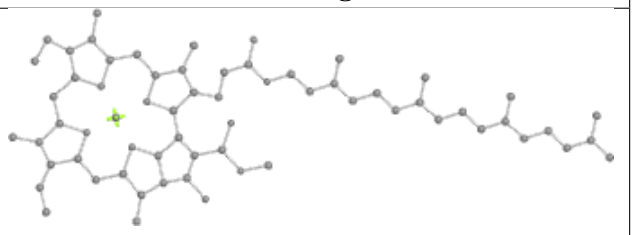
Bond lengths



Bond angles

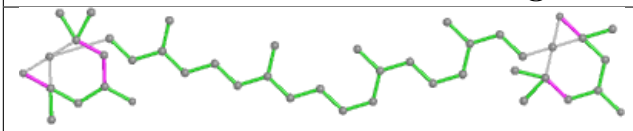


Torsions

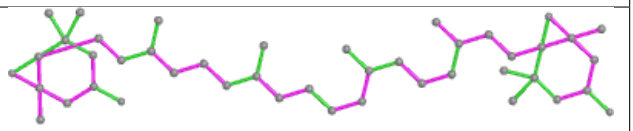


Rings

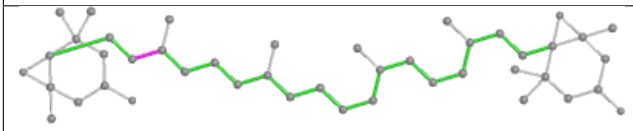
Ligand XAT 5 304



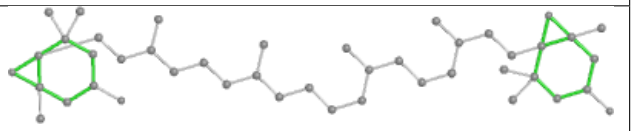
Bond lengths



Bond angles

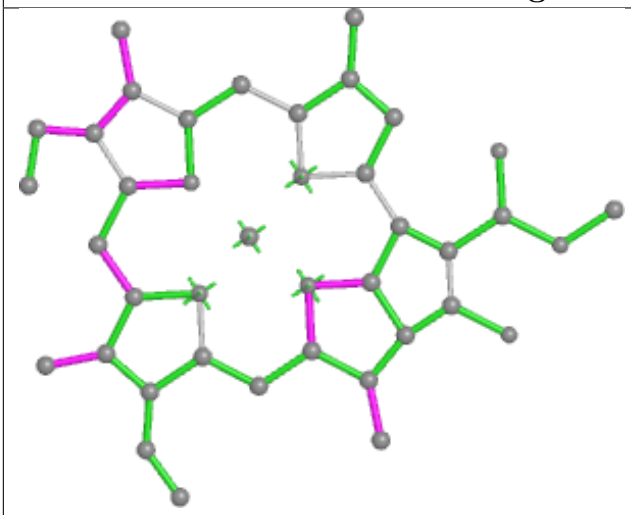


Torsions

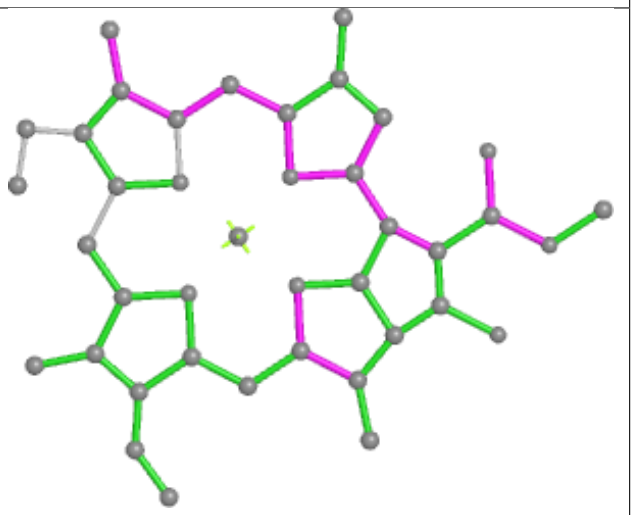


Rings

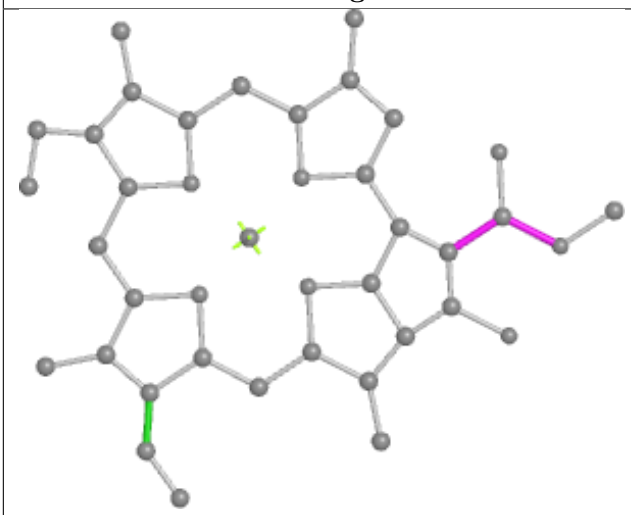
Ligand CLA 3 307



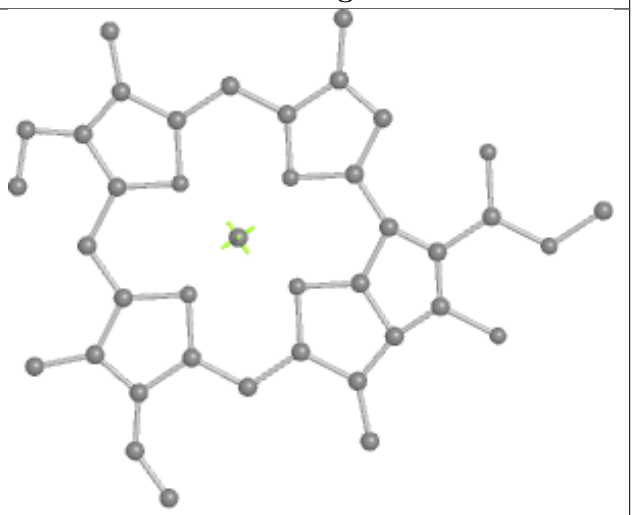
Bond lengths



Bond angles

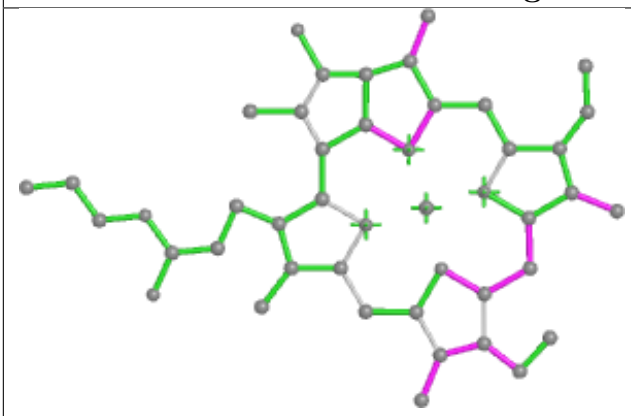


Torsions

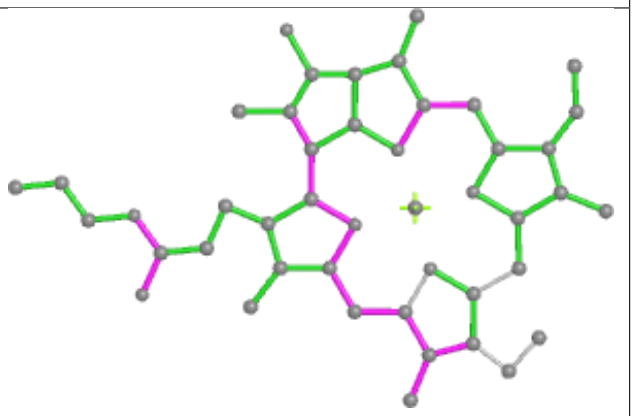


Rings

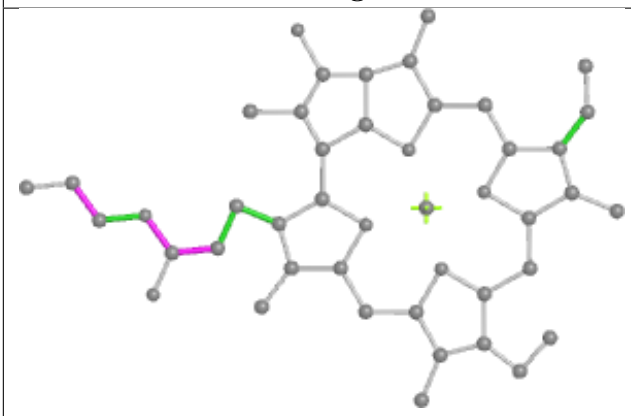
Ligand CLA A 832



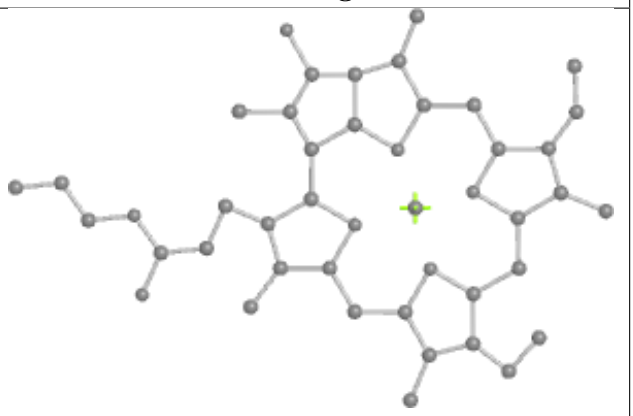
Bond lengths



Bond angles

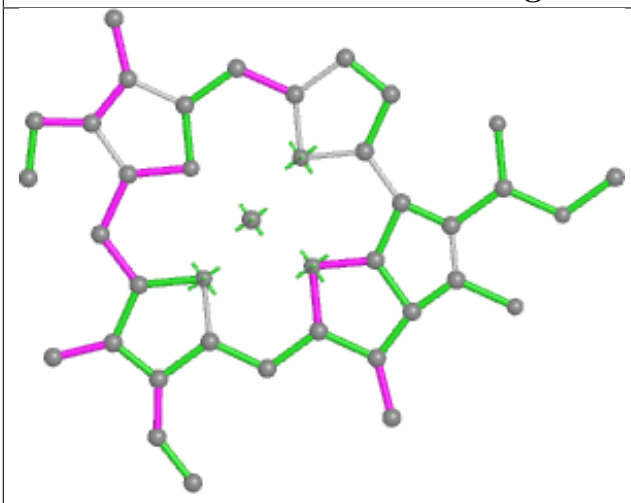


Torsions

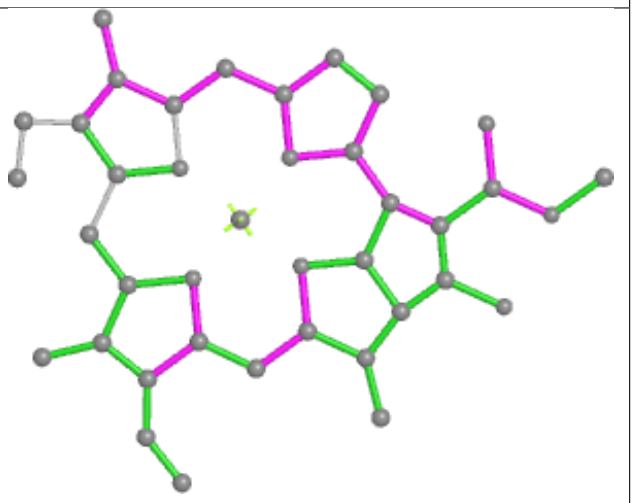


Rings

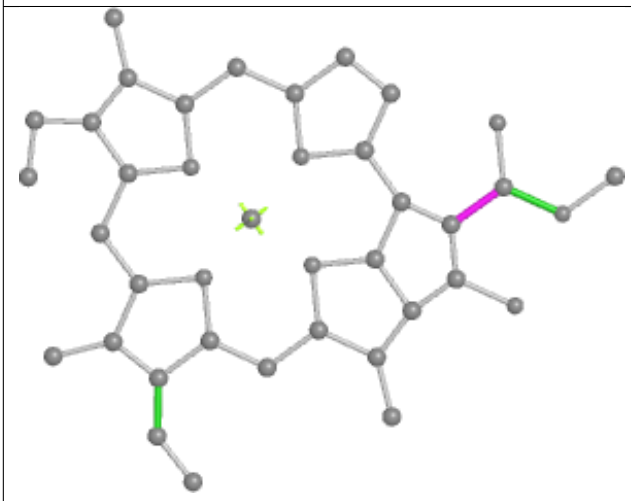
Ligand CLA B 806



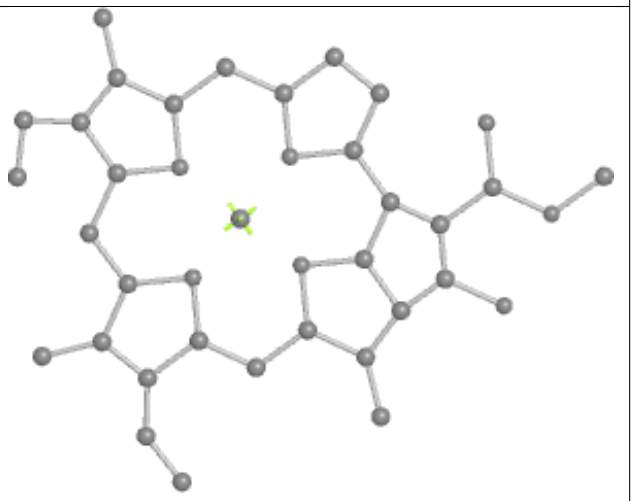
Bond lengths



Bond angles

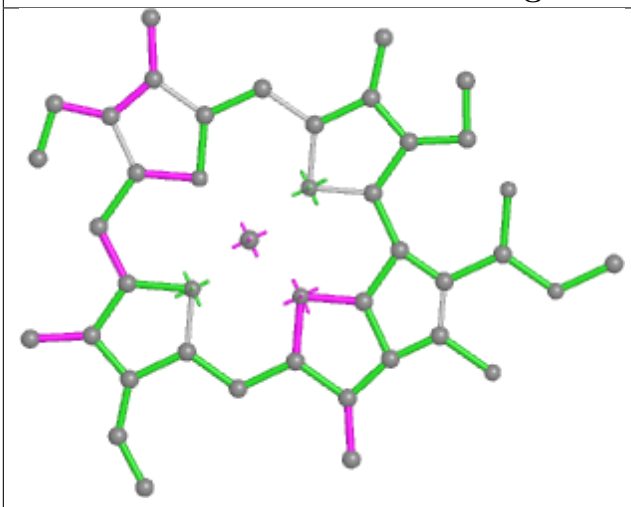


Torsions

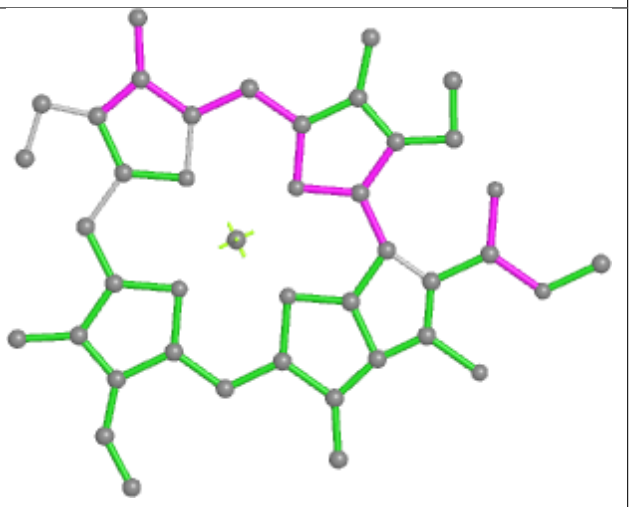


Rings

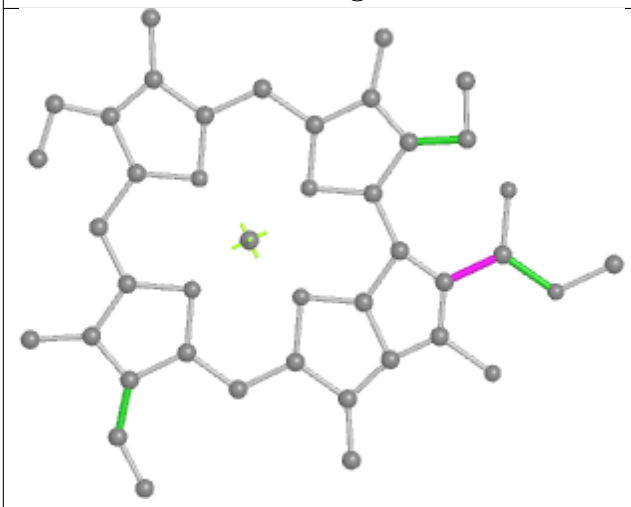
Ligand CLA B 825



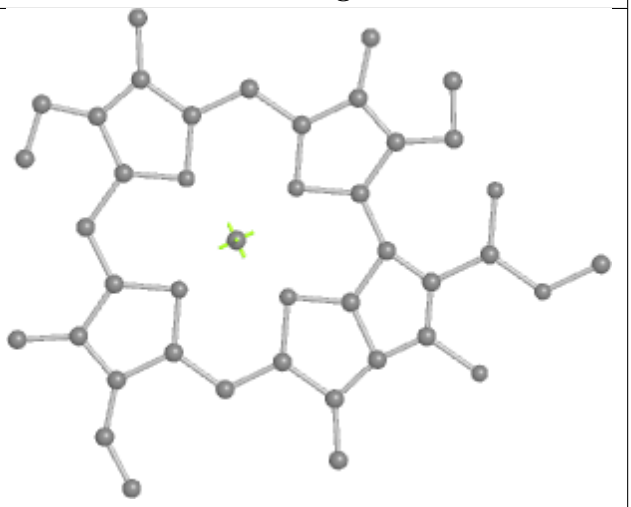
Bond lengths



Bond angles

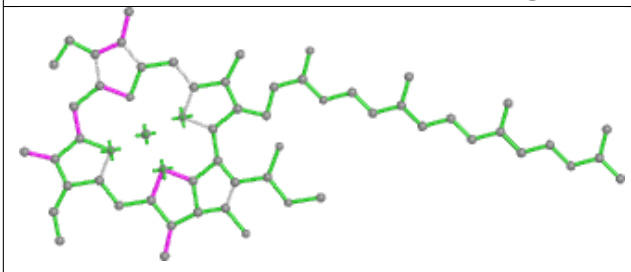


Torsions

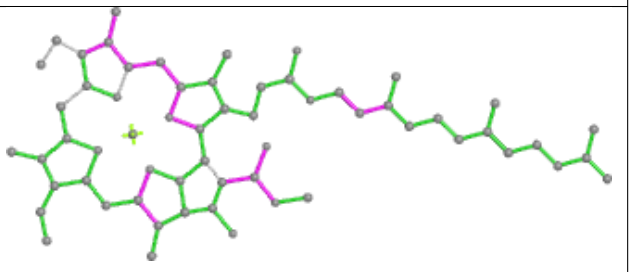


Rings

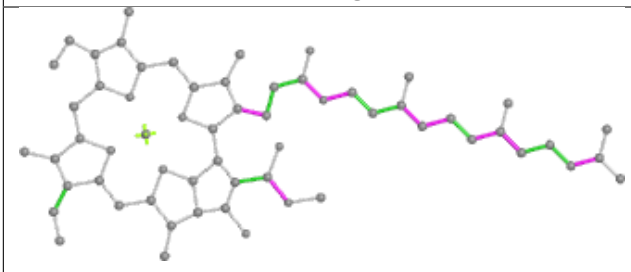
Ligand CLA A 826



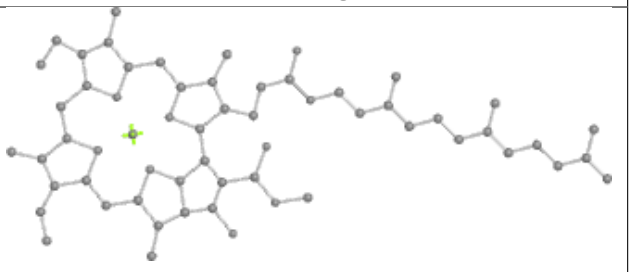
Bond lengths



Bond angles

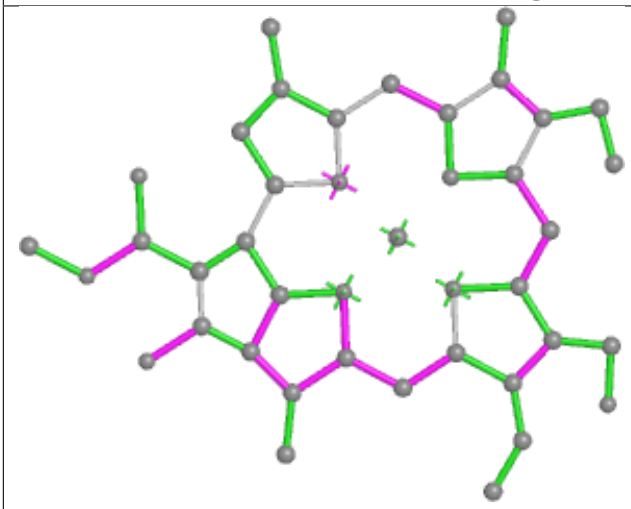


Torsions

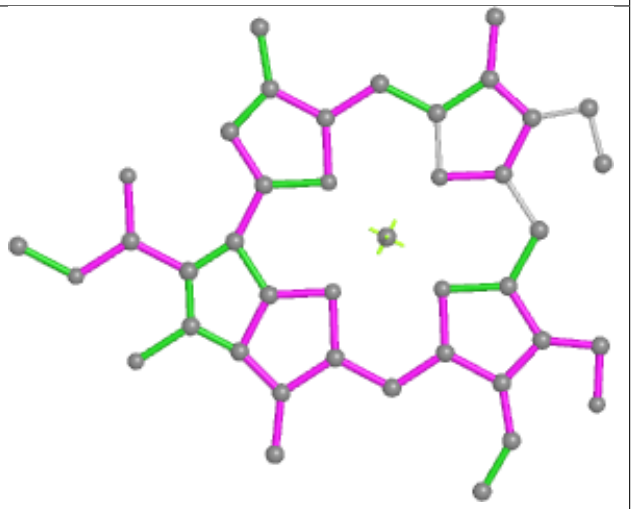


Rings

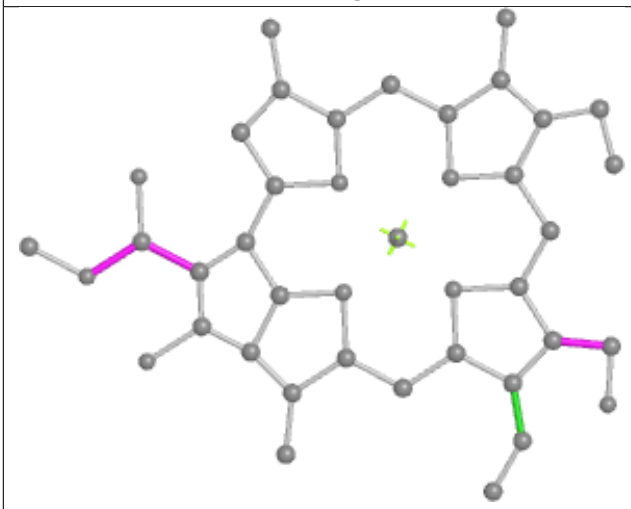
Ligand CHL 1 517



Bond lengths



Bond angles



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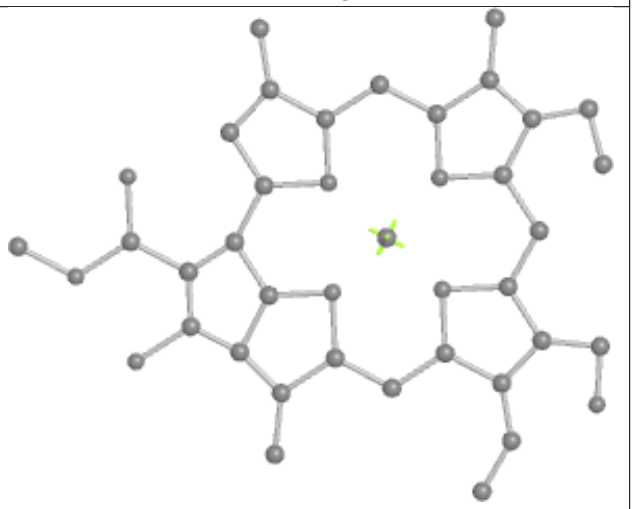
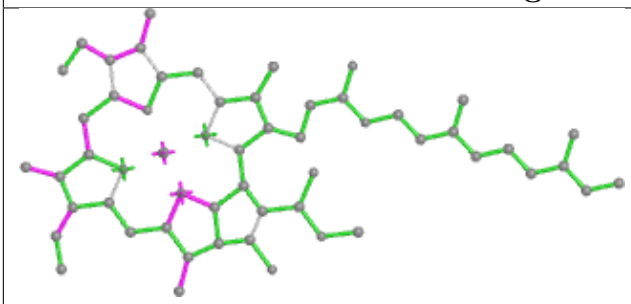
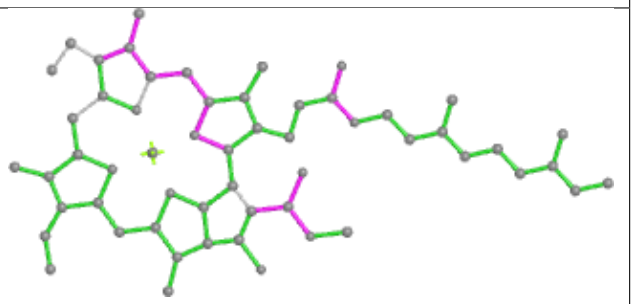


Rings

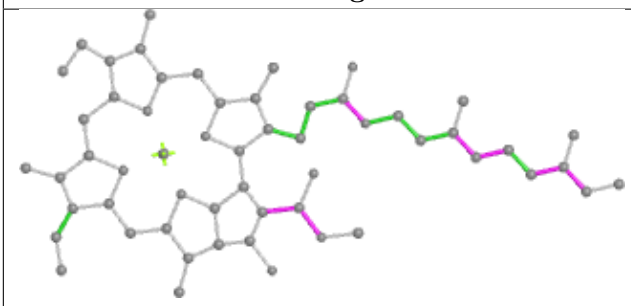
Ligand CLA B 830



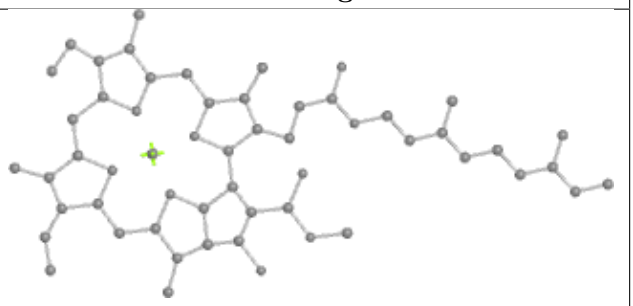
Bond lengths



Bond angles

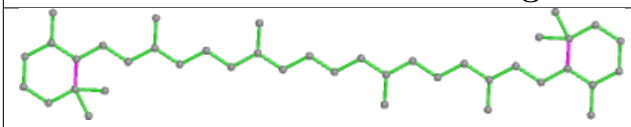


Torsions

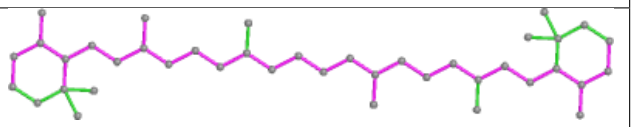


Rings

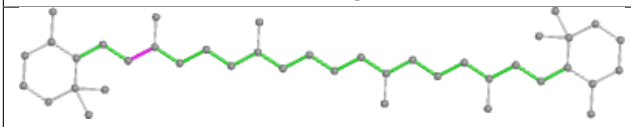
Ligand BCR A 847



Bond lengths



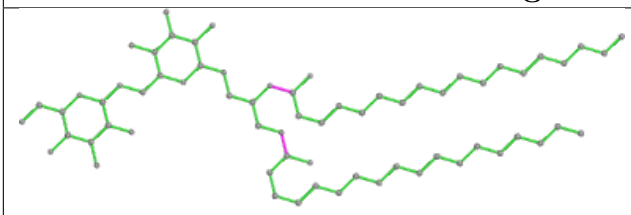
Bond angles



Torsions

Rings

Ligand DGD J 103



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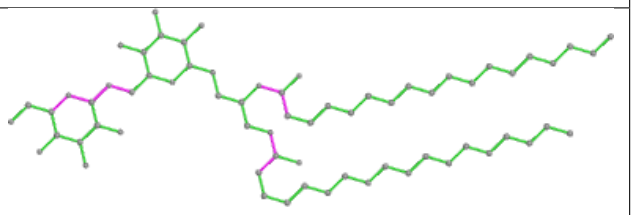
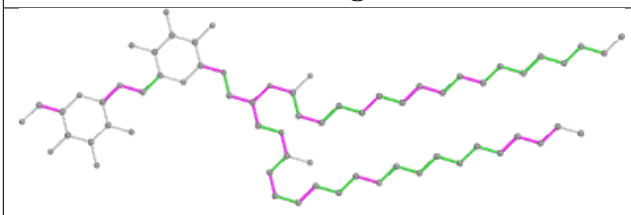


Bond angles



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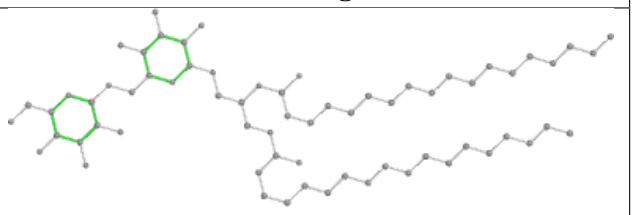
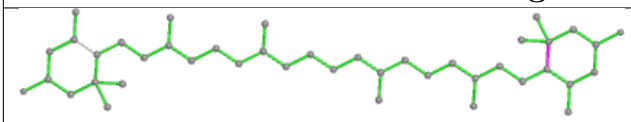


Rings

Ligand LUT 2 501



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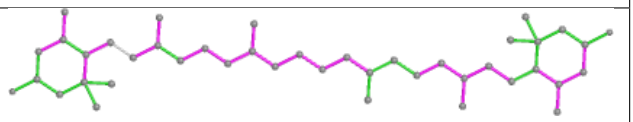
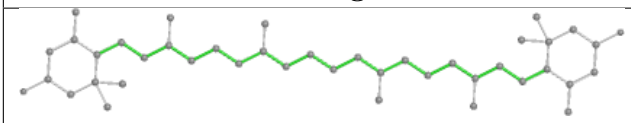


Bond angles



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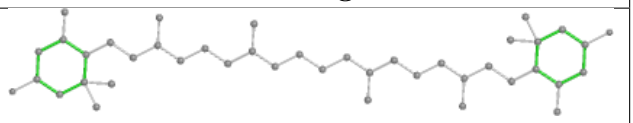
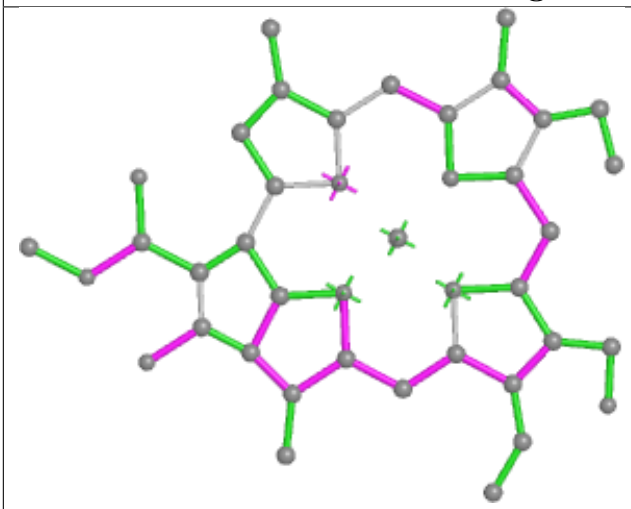


Rings

Ligand CHL 1 514



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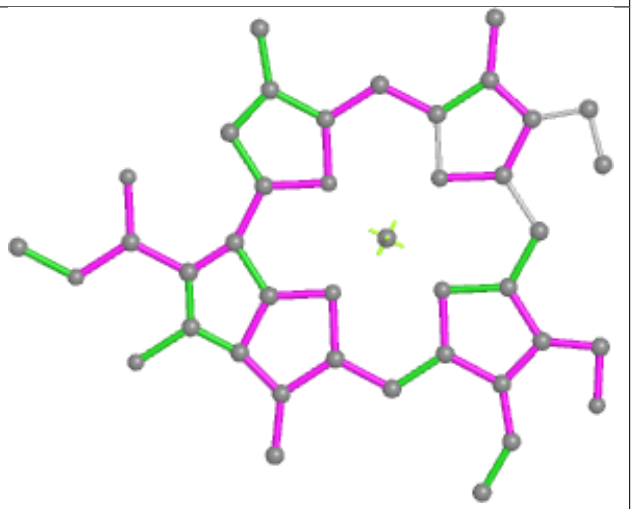
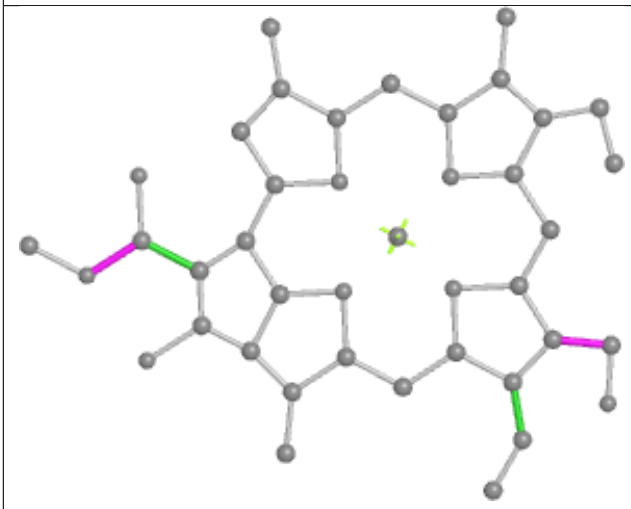
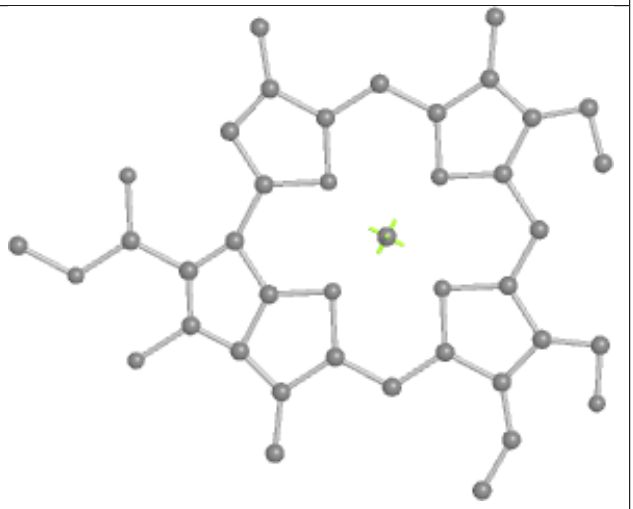


Bond angles

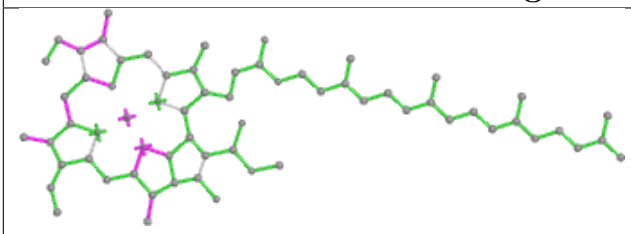


Torsions



Rings

Ligand CLA B 838



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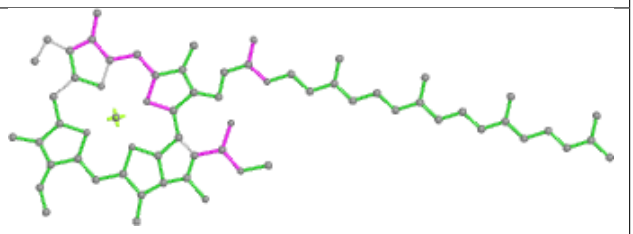
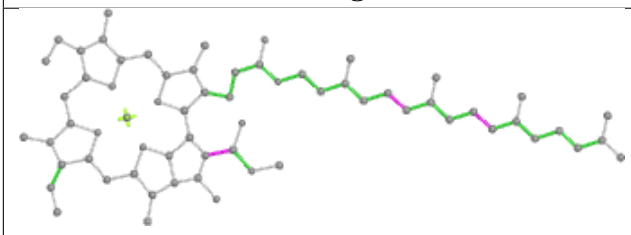


Bond angles



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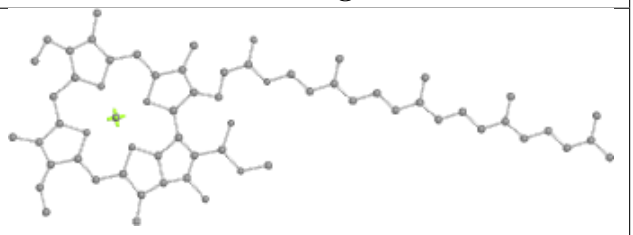
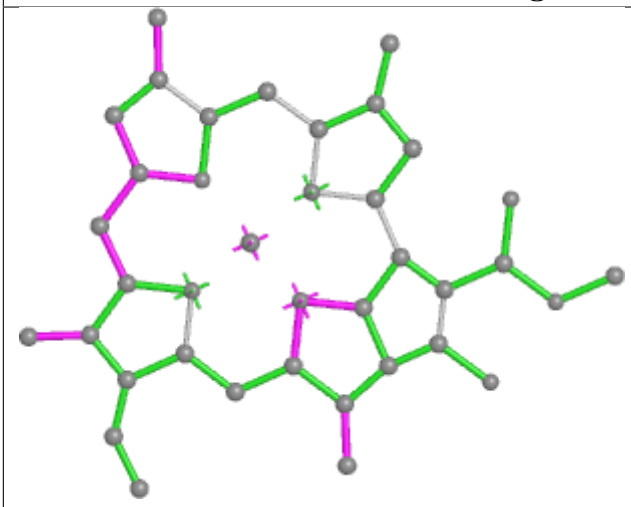


Rings

Ligand CLA 5 305



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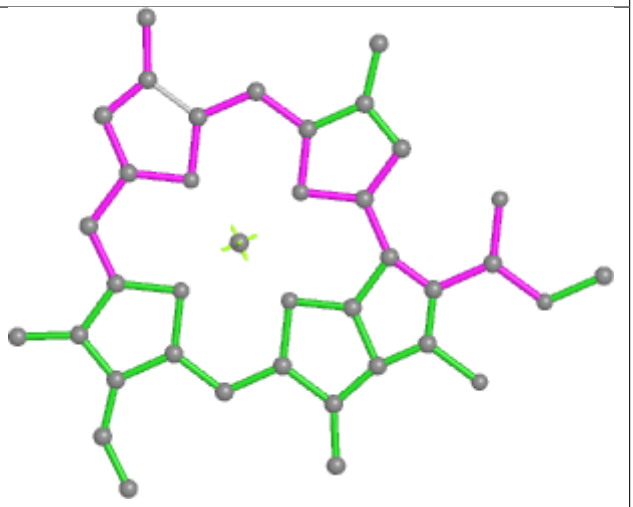
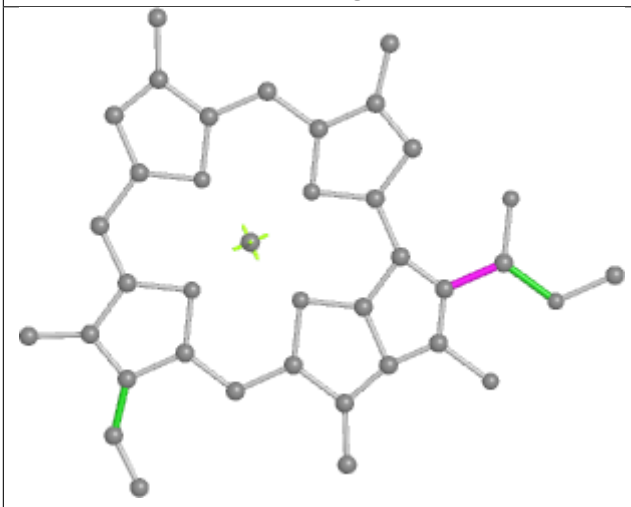
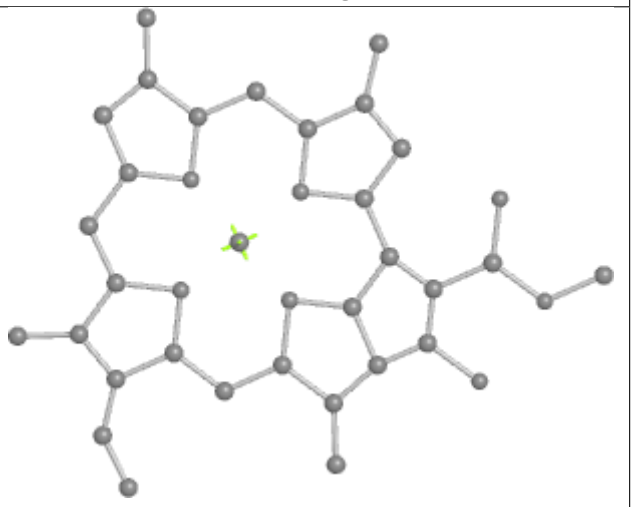


Bond angles

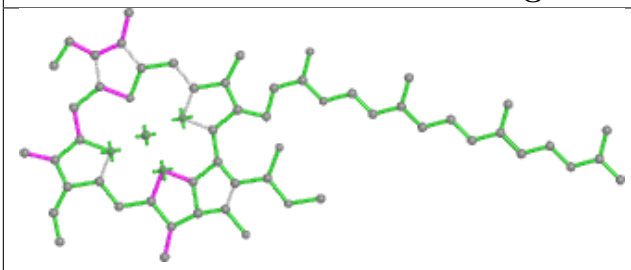


Torsions



Rings

Ligand CLA B 835



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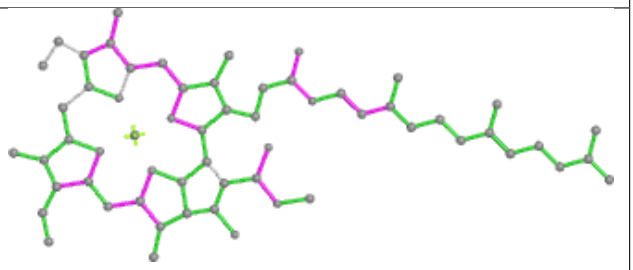
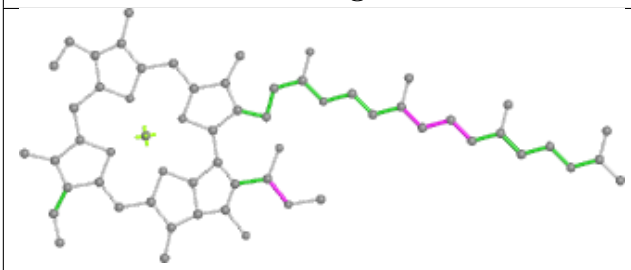


Bond angles



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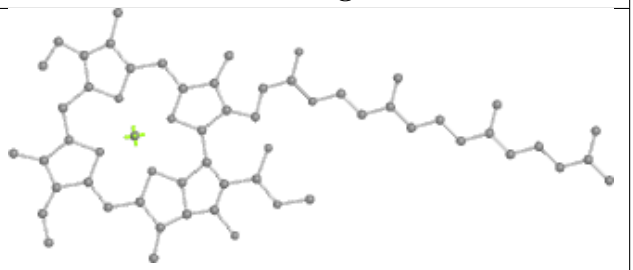
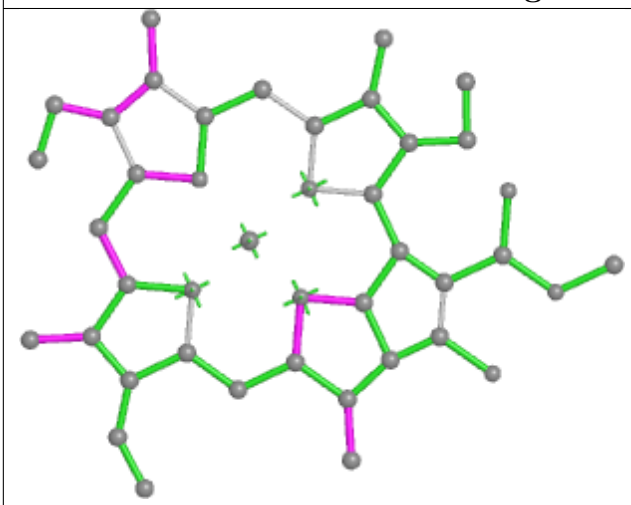


Rings

Ligand CLA B 823



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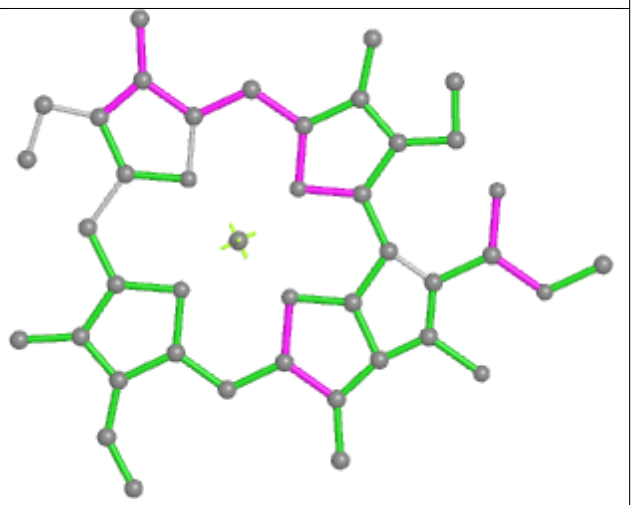
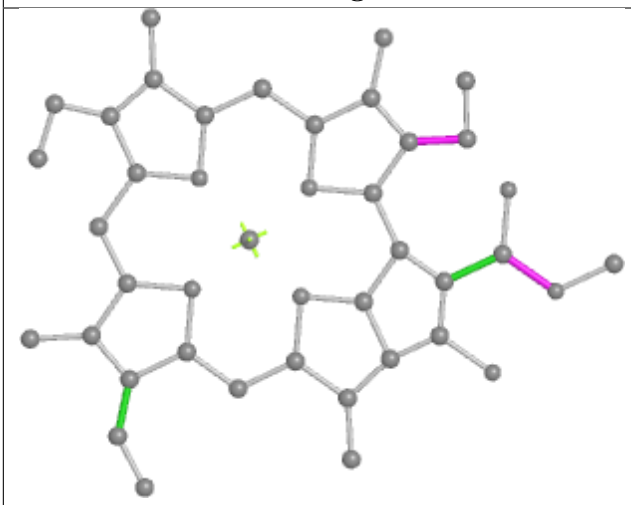
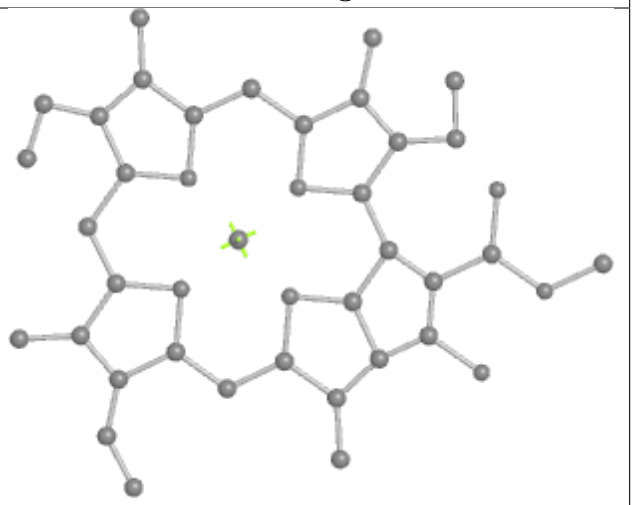


Bond angles

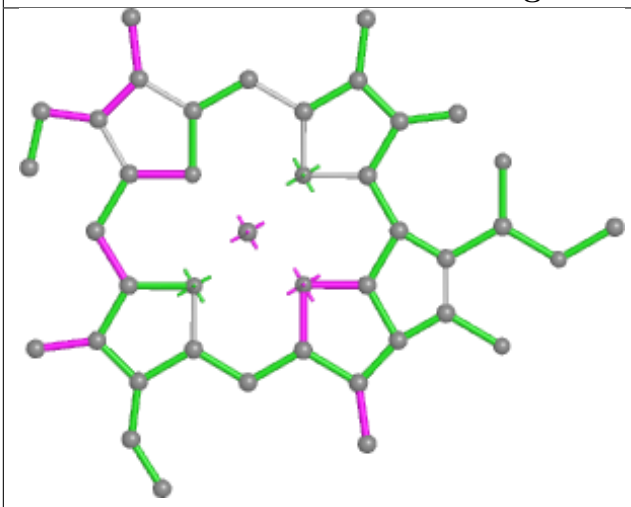


Torsions

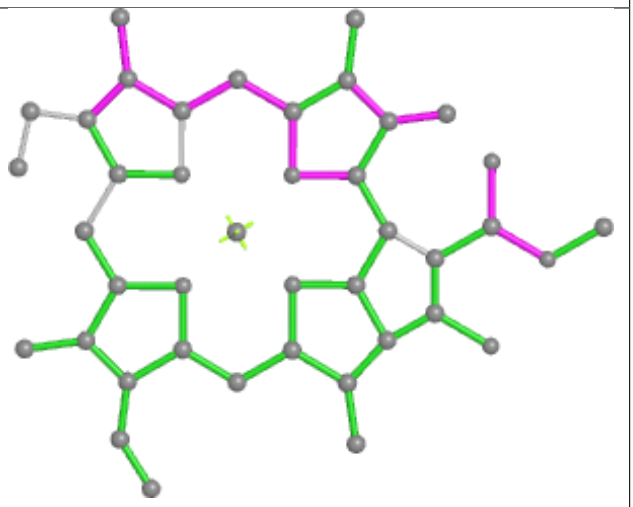


Rings

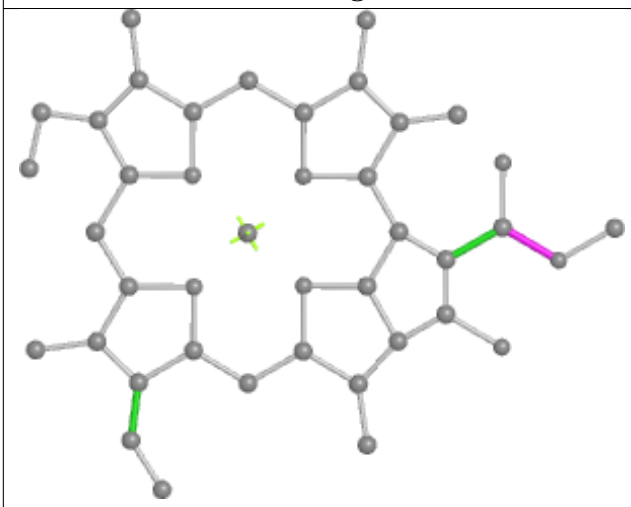
Ligand CLA A 828



Bond lengths



Bond angles



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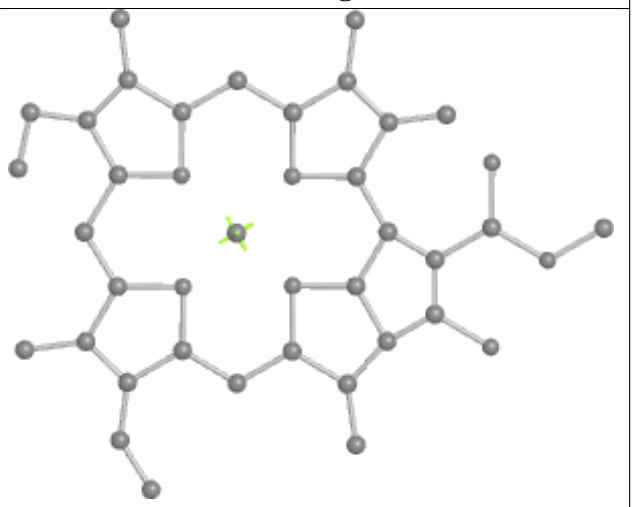
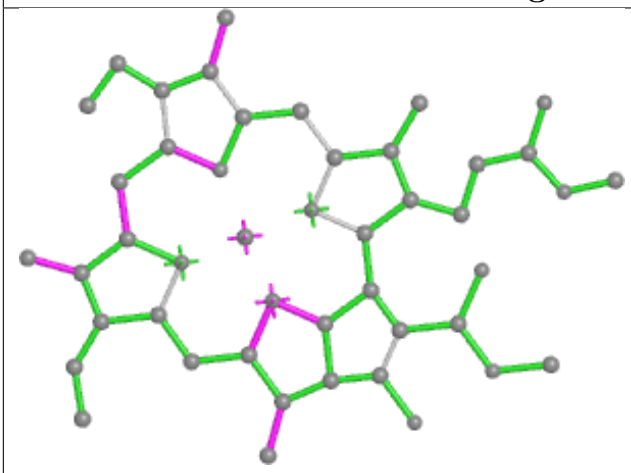


Rings

Ligand CLA 1 510



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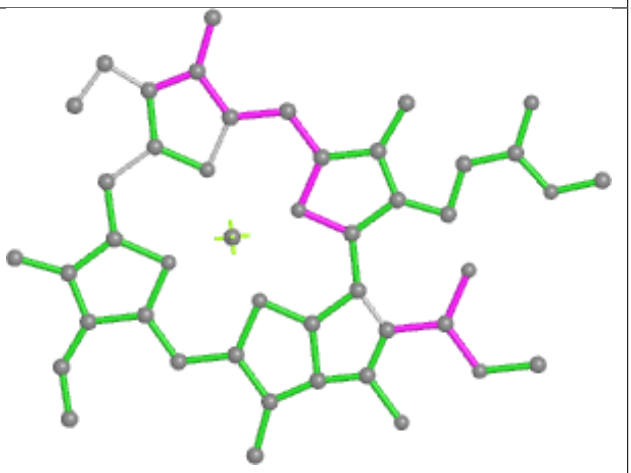
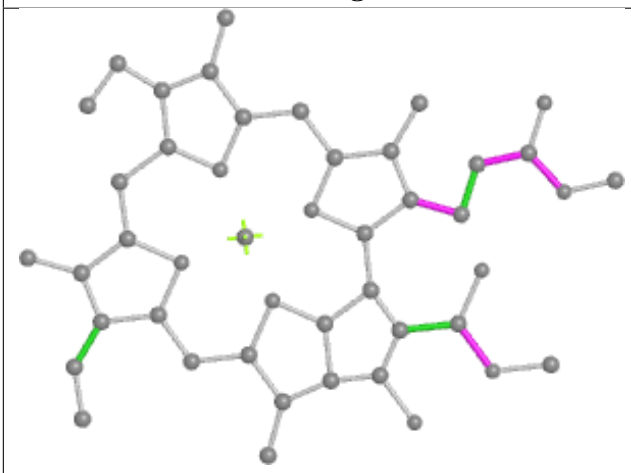


Bond angles



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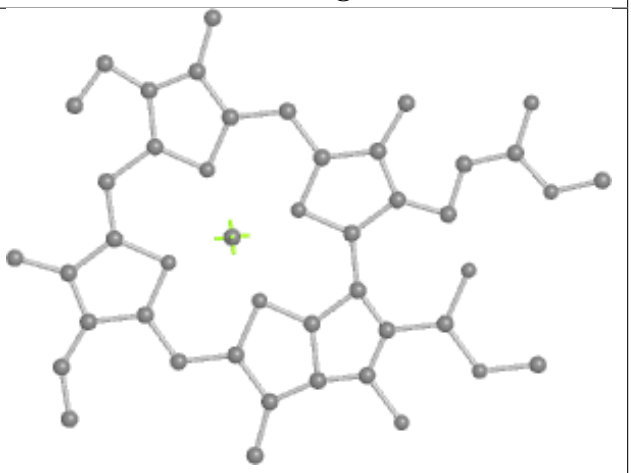
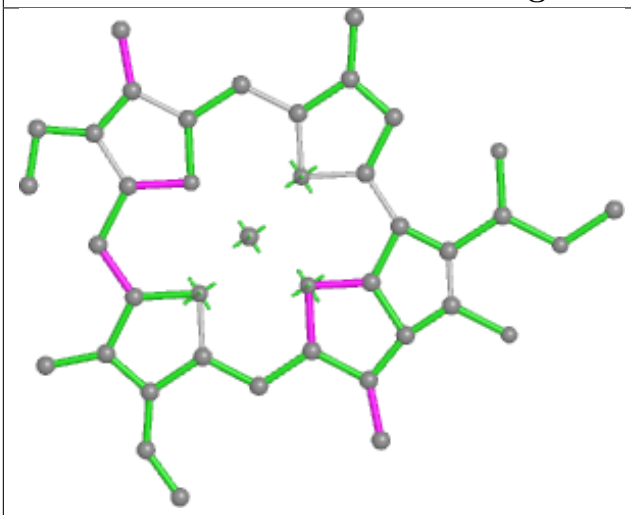


Rings

Ligand CLA 1 508



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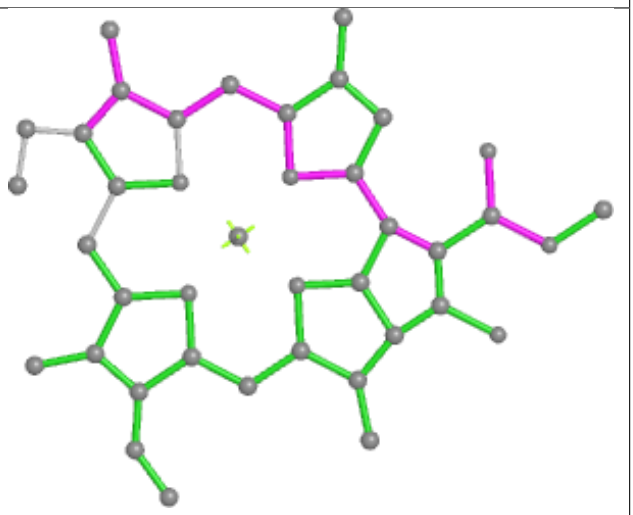
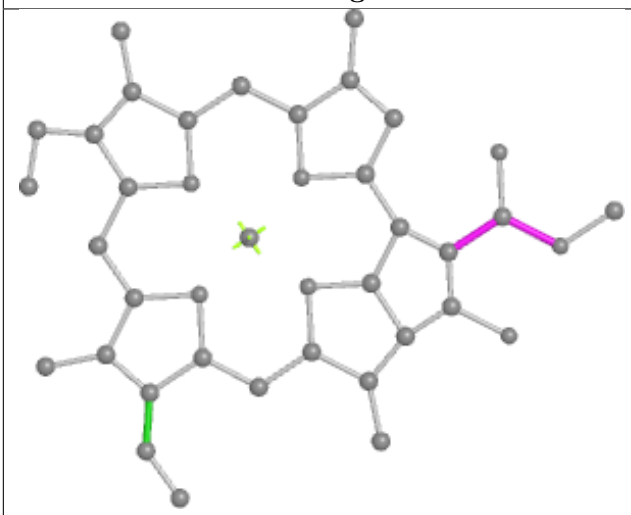


Bond angles



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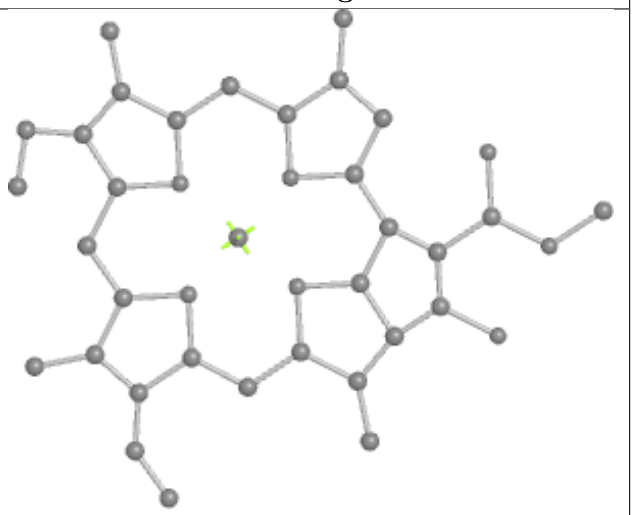
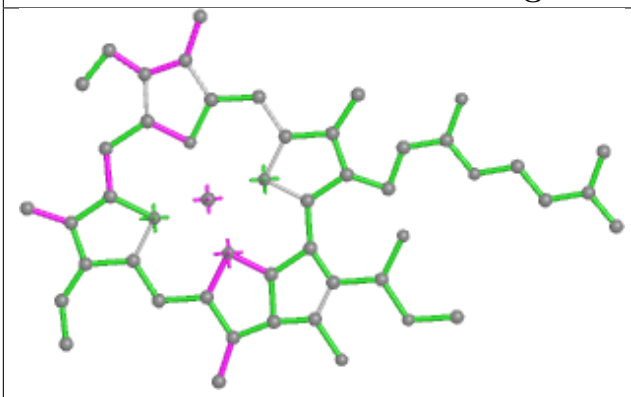


Rings

Ligand CLA B 837



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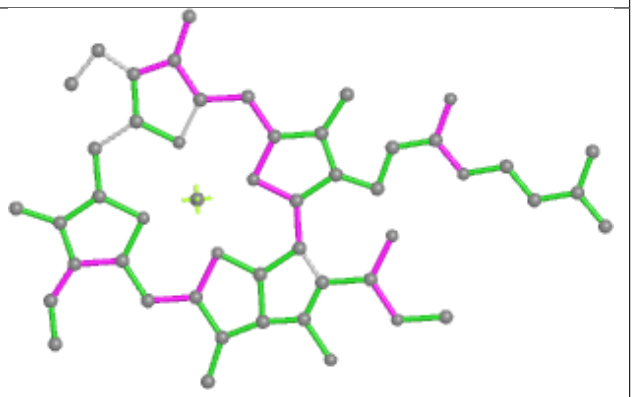
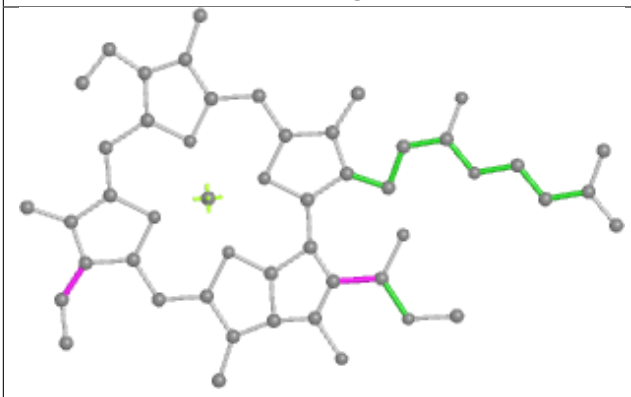


Bond angles



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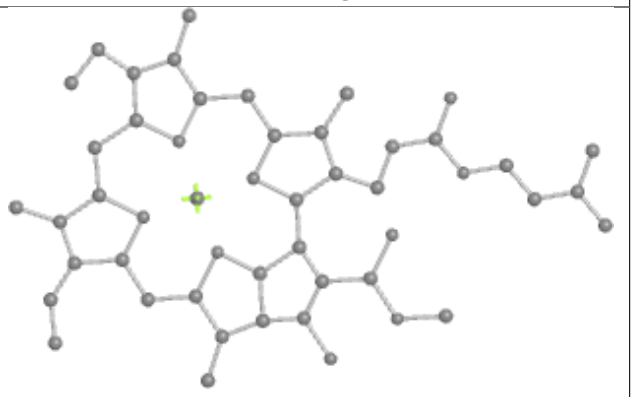
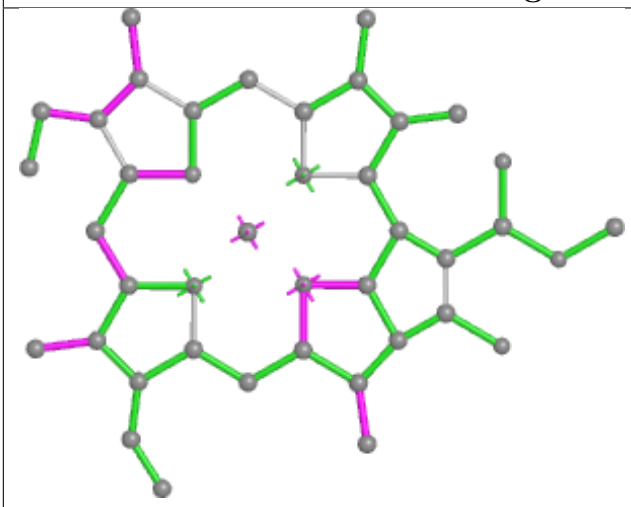
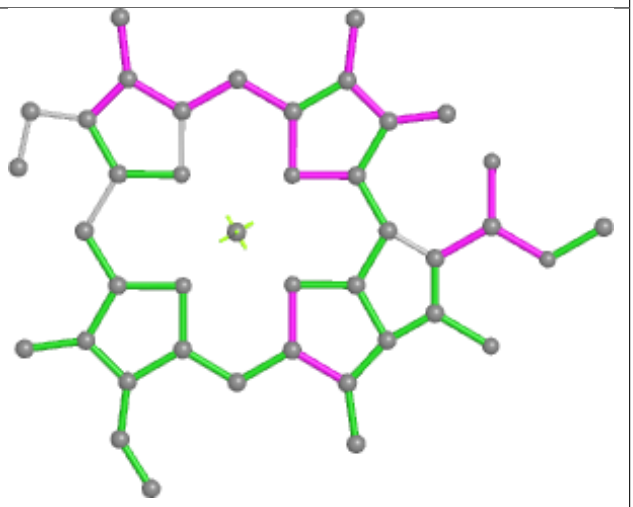


Rings

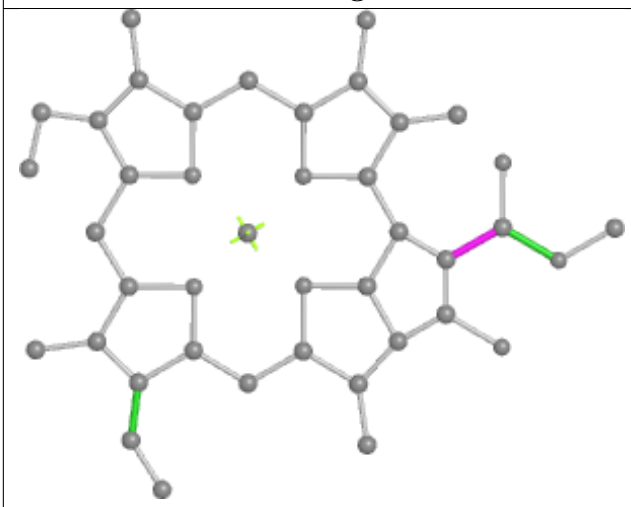
Ligand CLA B 827



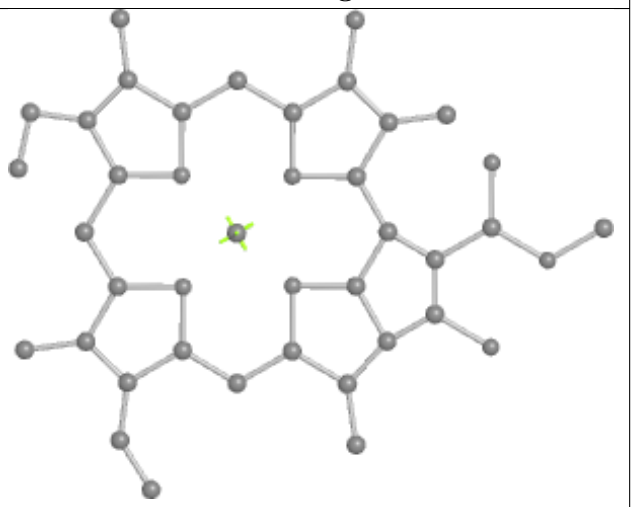
Bond lengths



Bond angles

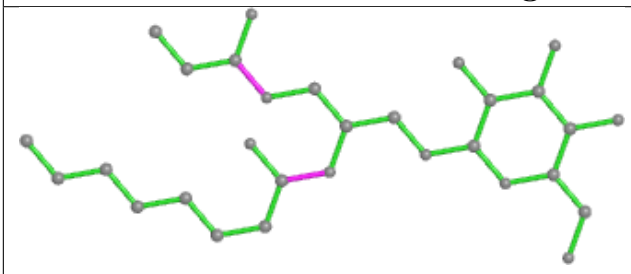


Torsions

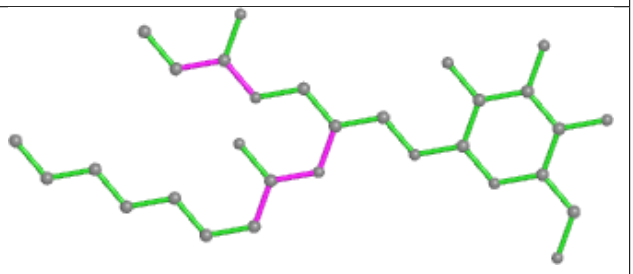


Rings

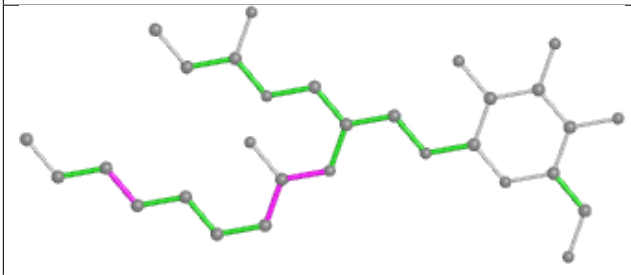
Ligand LMG F 805



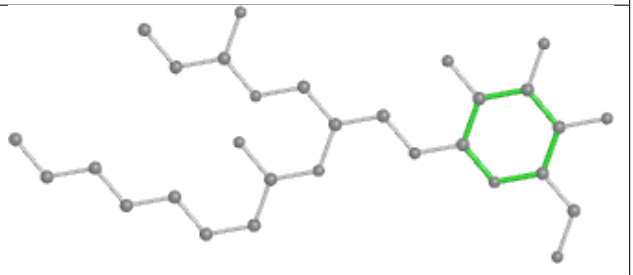
Bond lengths



Bond angles

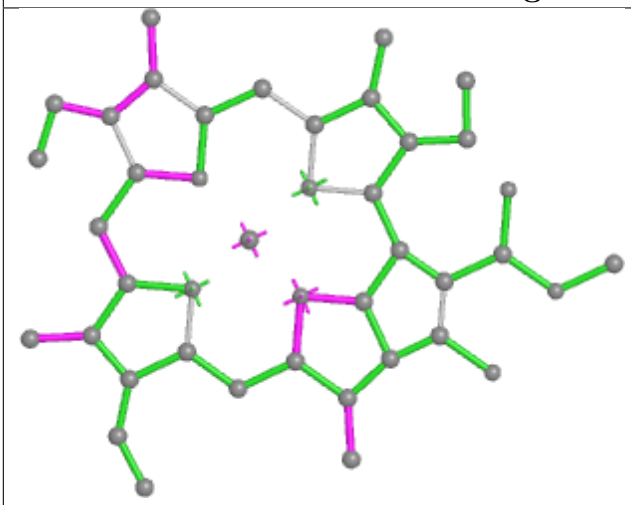


Torsions

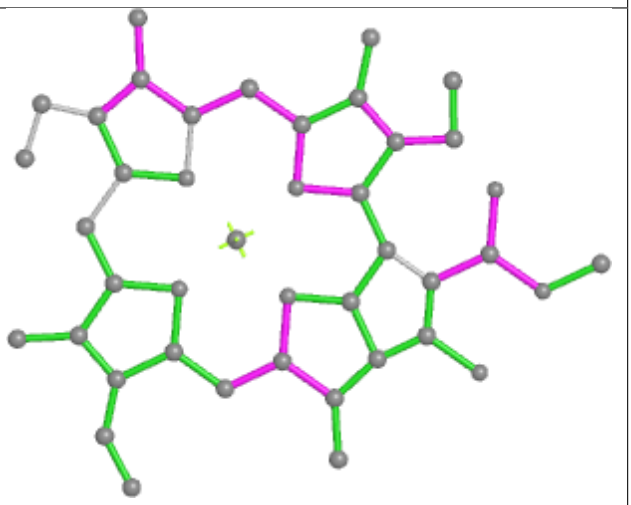


Rings

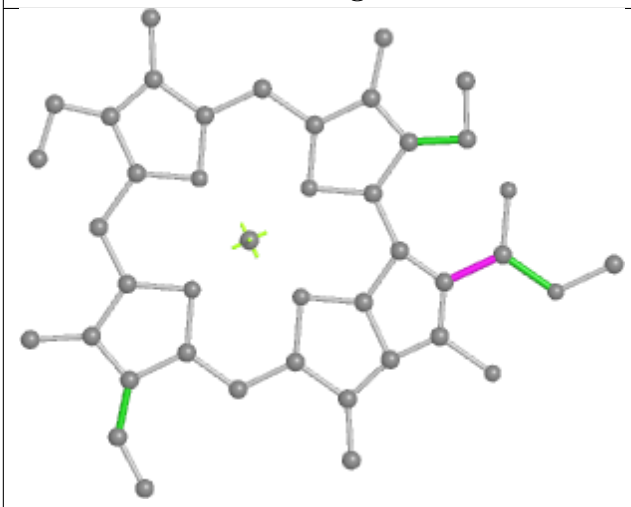
Ligand CLA A 812



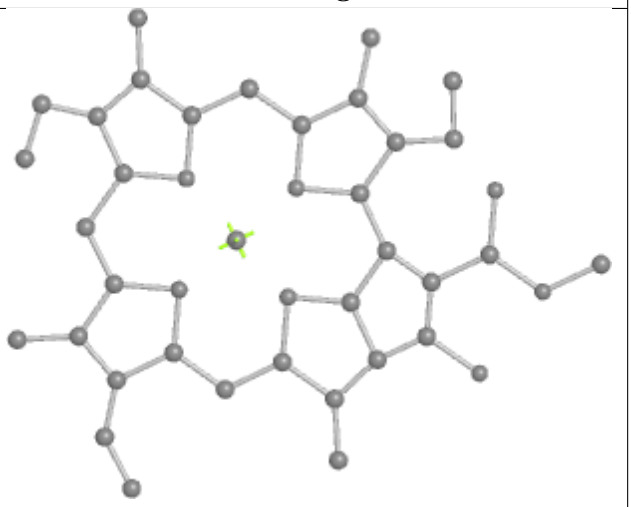
Bond lengths



Bond angles

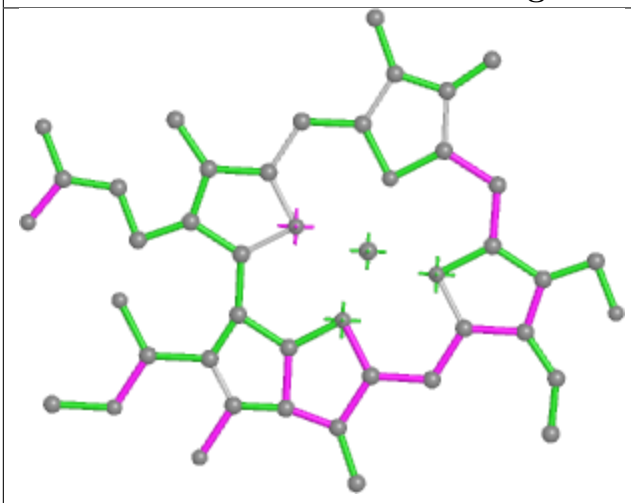


Torsions



Rings

Ligand CHL 2 515



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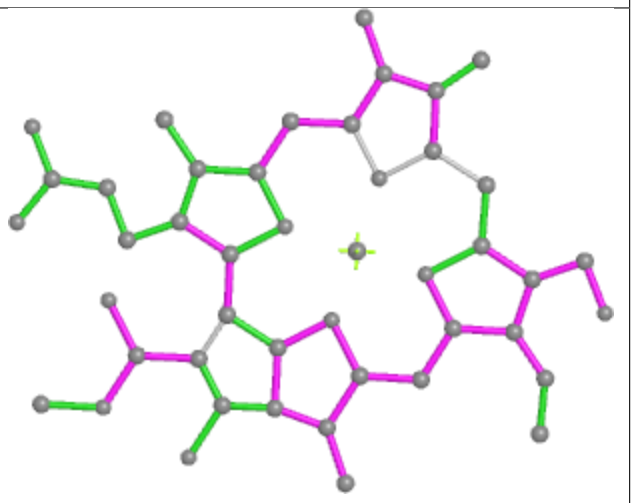
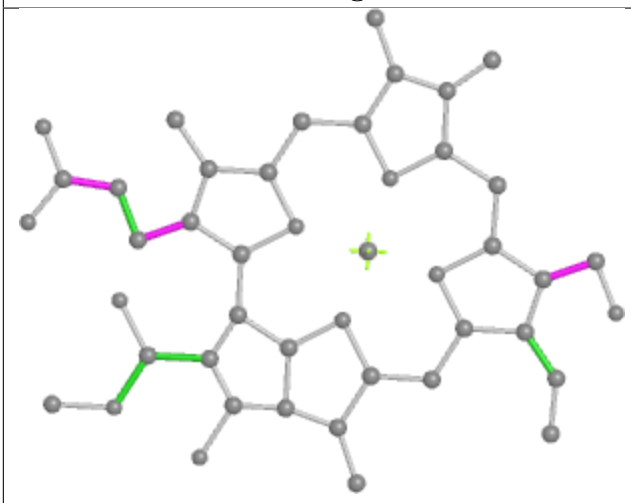
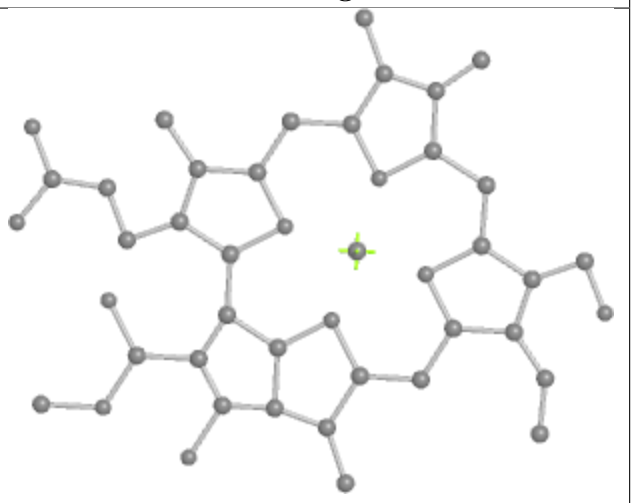


Bond angles

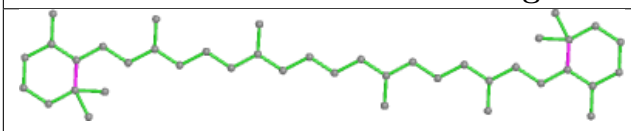


Torsions



Rings

Ligand BCR B 847



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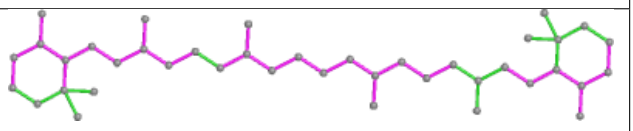
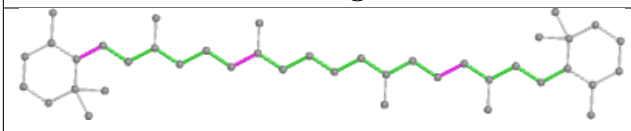
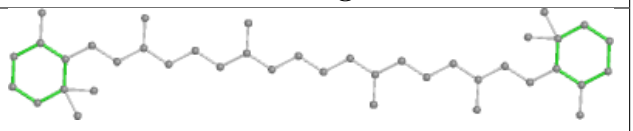


Bond angles

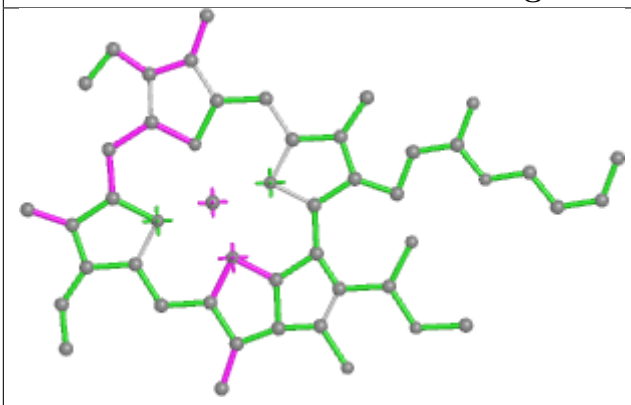


Torsions



Rings

Ligand CLA B 817



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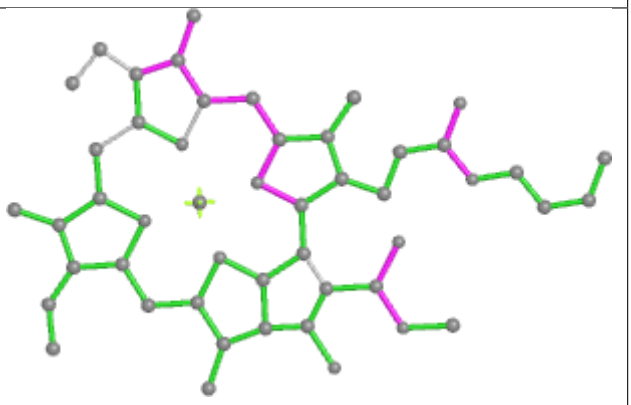
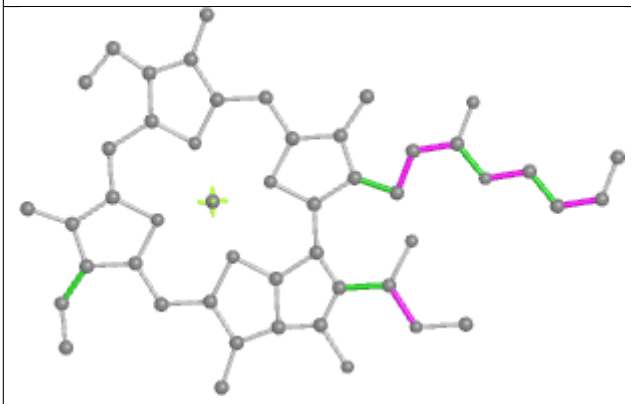
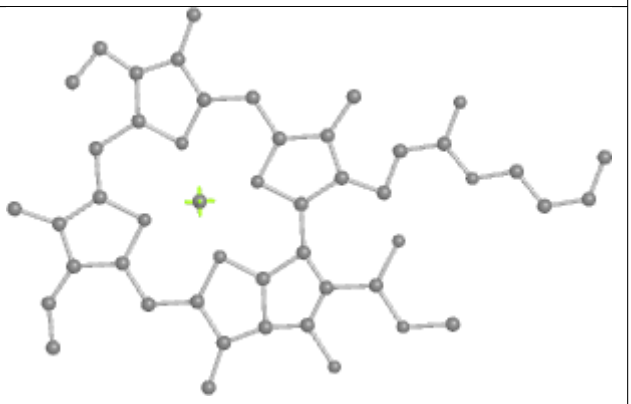


Bond angles

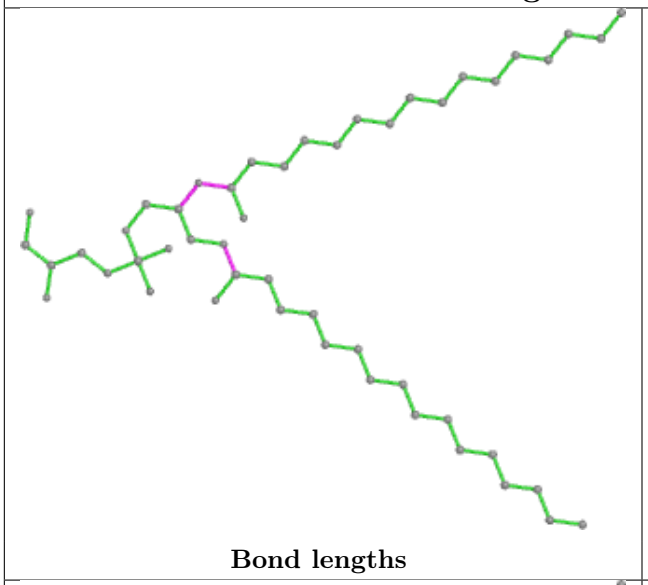


Torsions



Rings

Ligand LHG A 843



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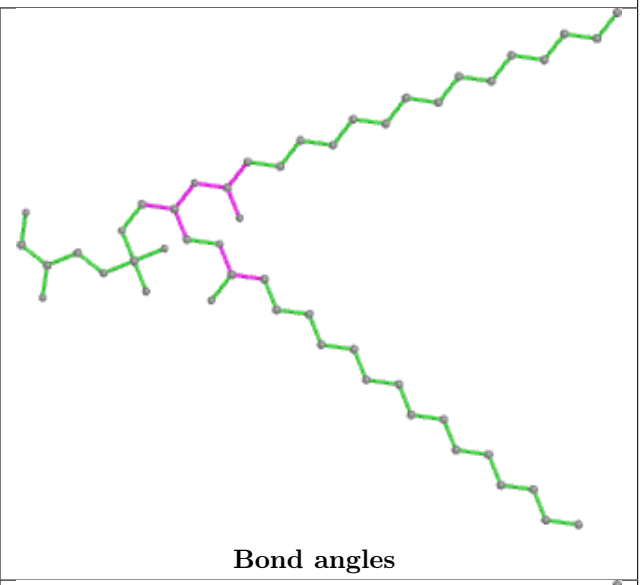
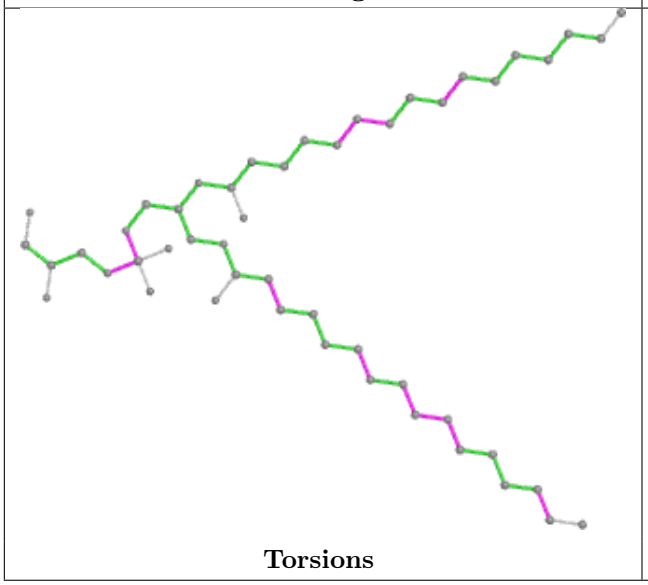


Bond angles



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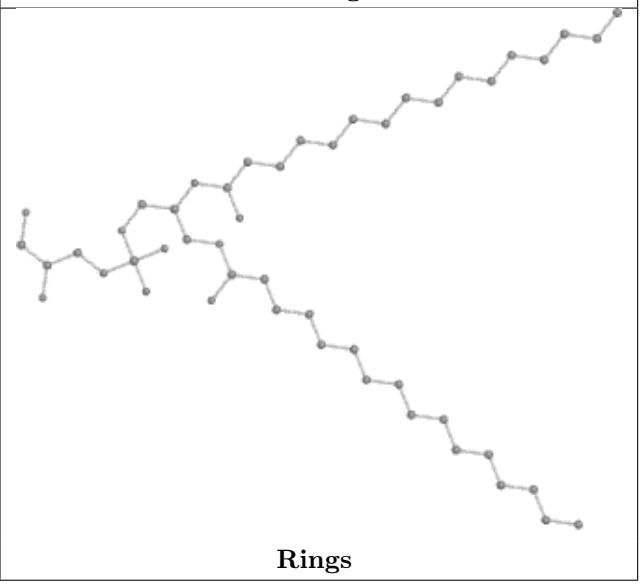
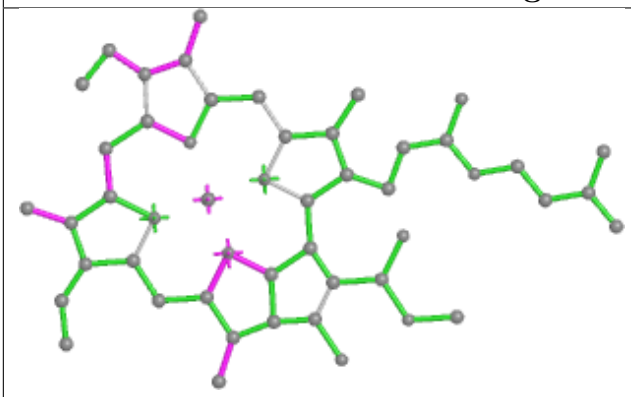
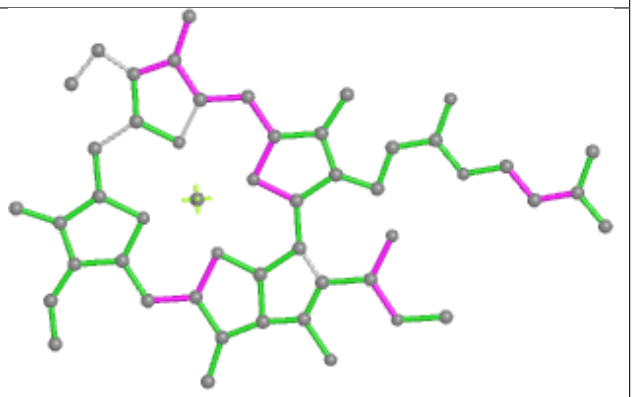


Rings

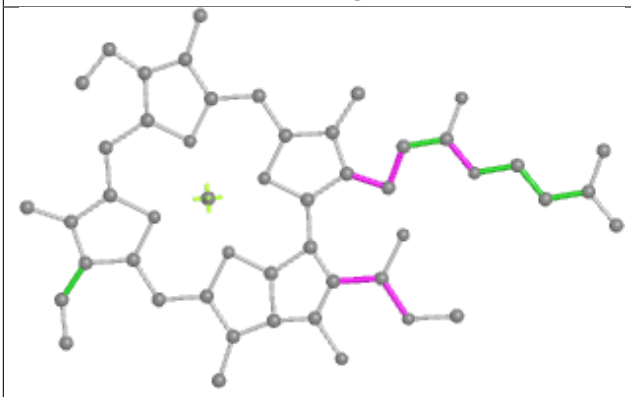
Ligand CLA A 842



Bond lengths



Bond angles



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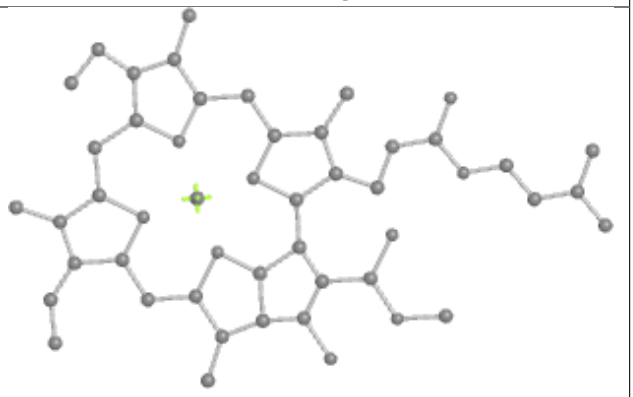
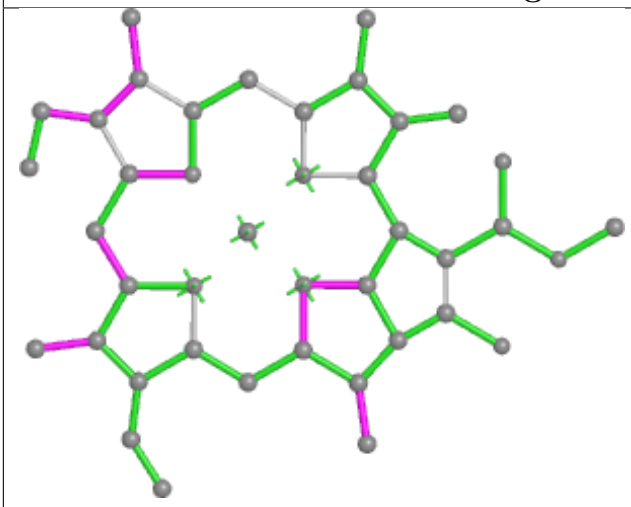
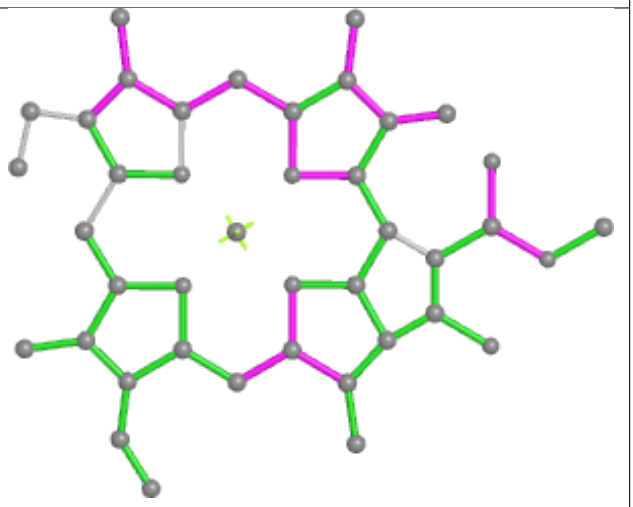


Rings

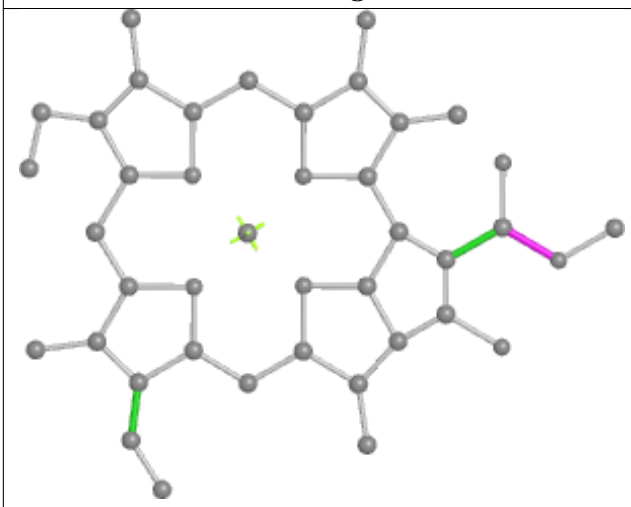
Ligand CLA B 805



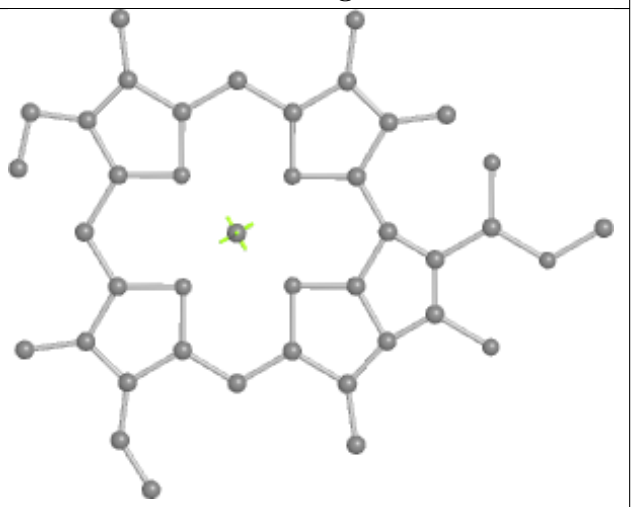
Bond lengths



Bond angles

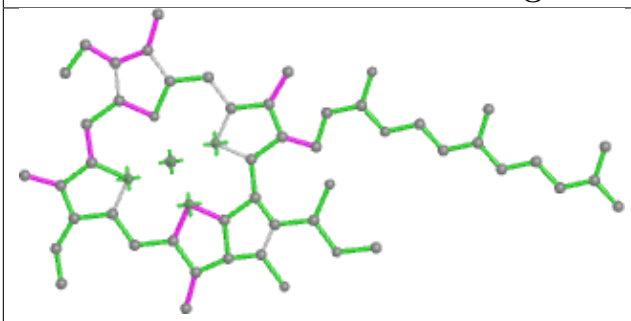


Torsions

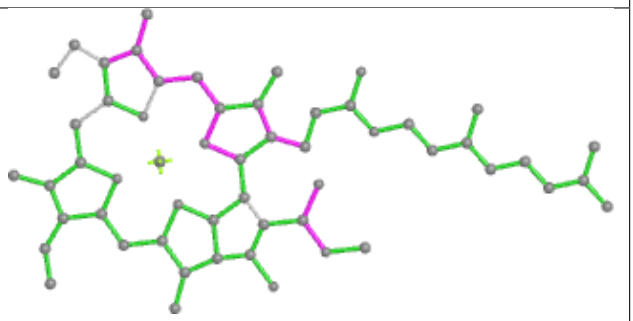


Rings

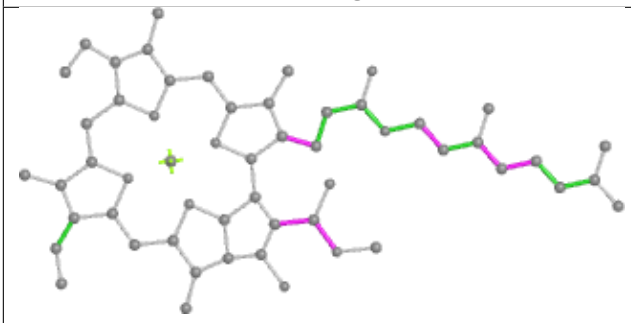
Ligand CLA B 811



Bond lengths



Bond angles



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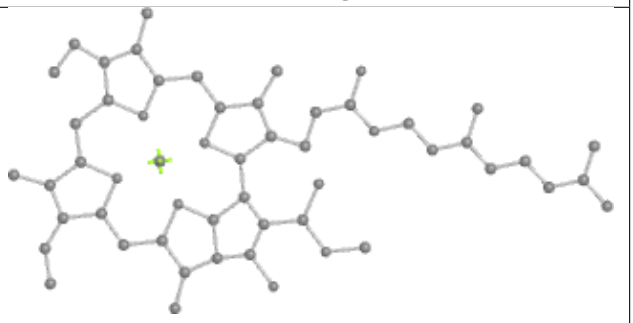
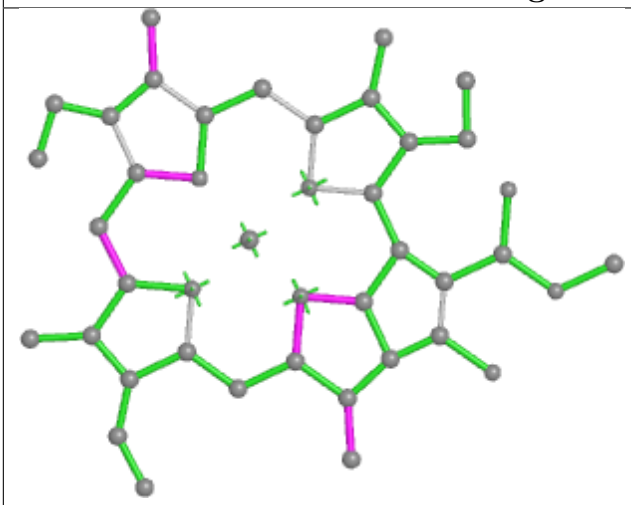
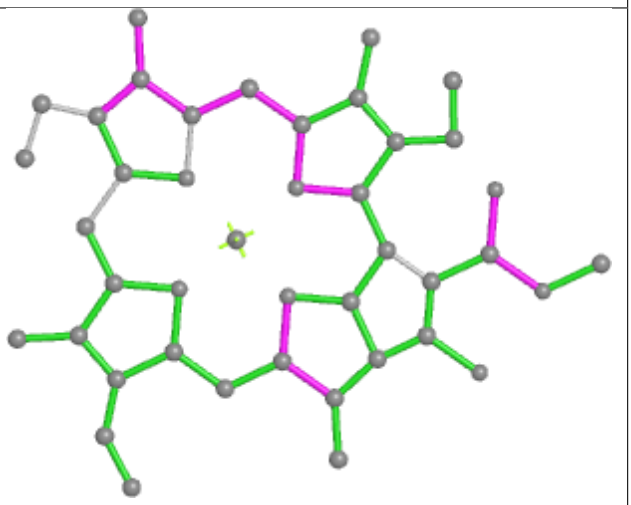


Rings

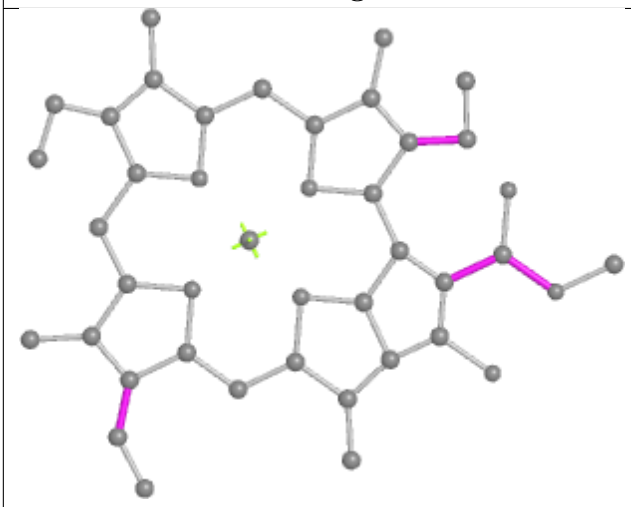
Ligand CLA J 101



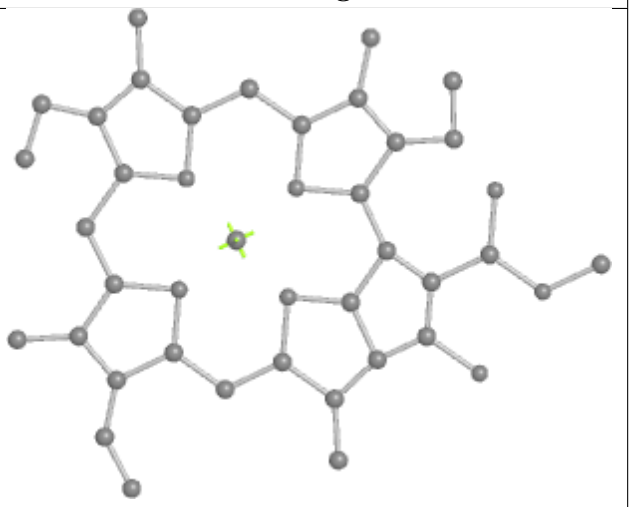
Bond lengths



Bond angles

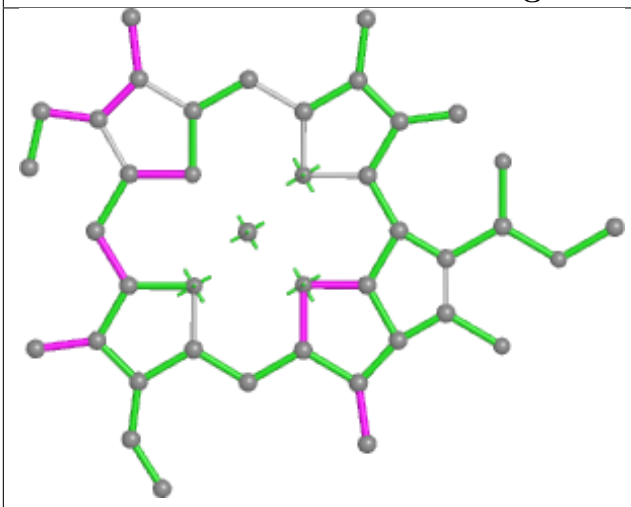


Torsions

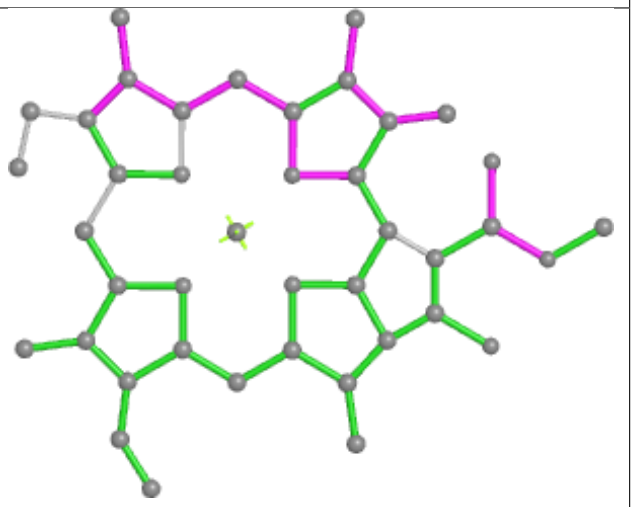


Rings

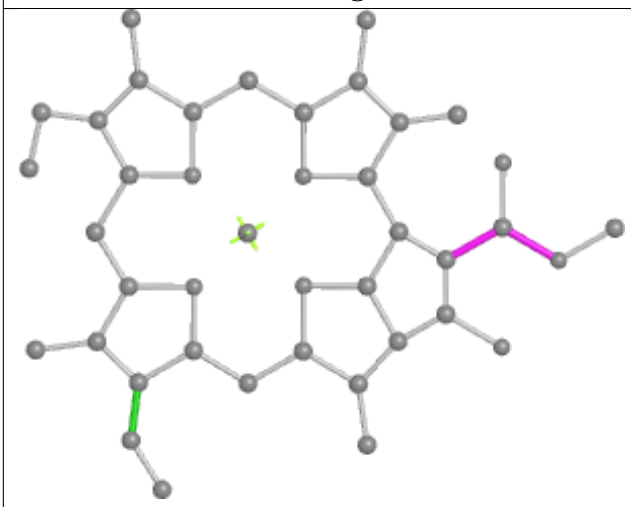
Ligand CLA A 834



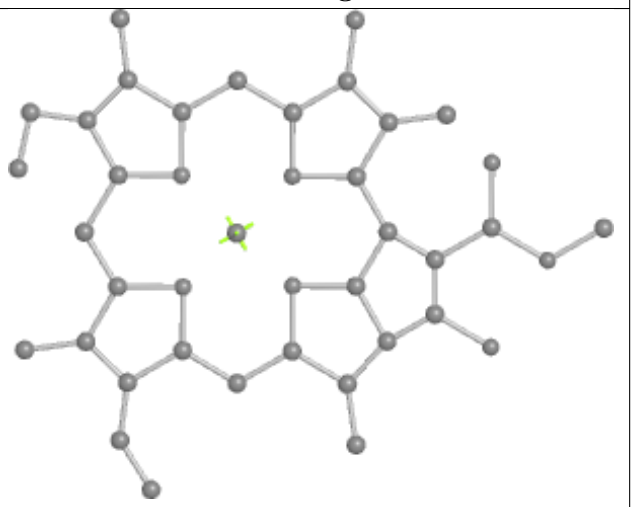
Bond lengths



Bond angles

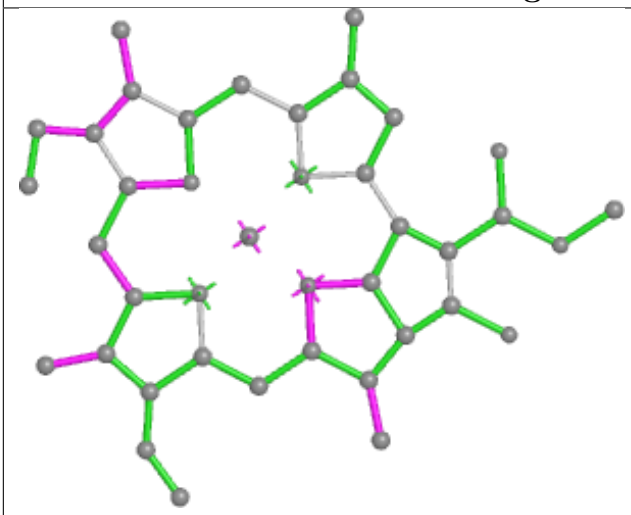


Torsions

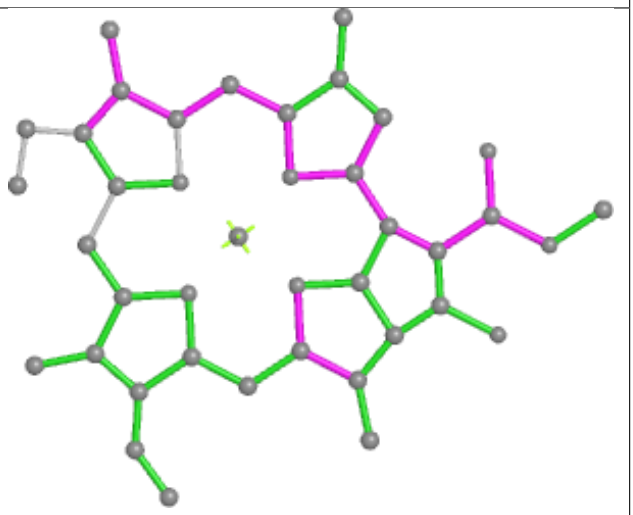


Rings

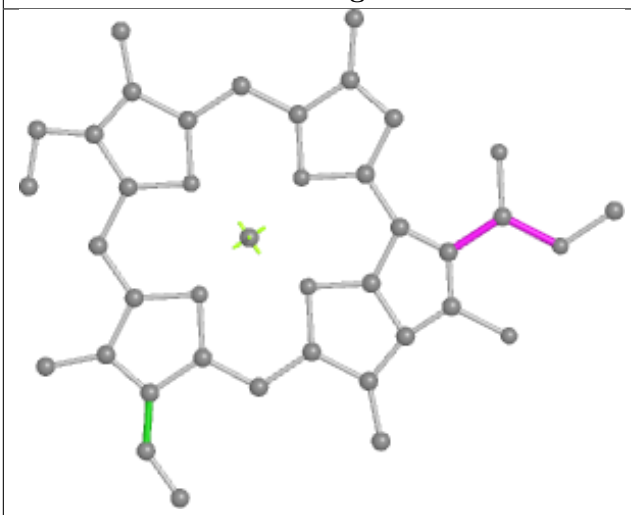
Ligand CLA A 818



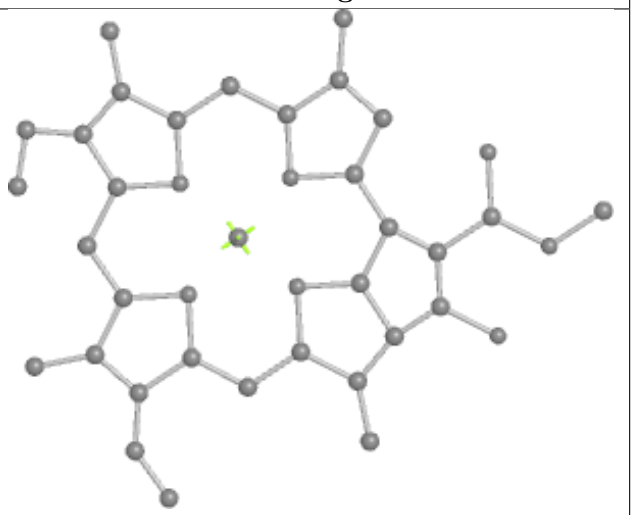
Bond lengths



Bond angles

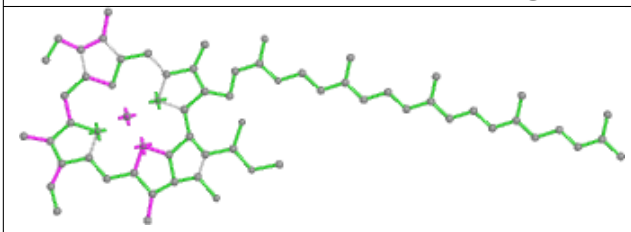


Torsions

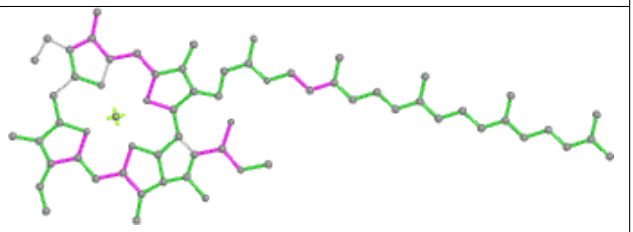


Rings

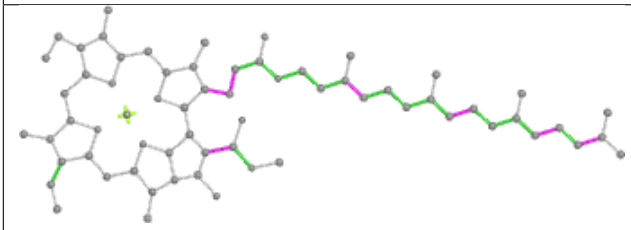
Ligand CLA B 801



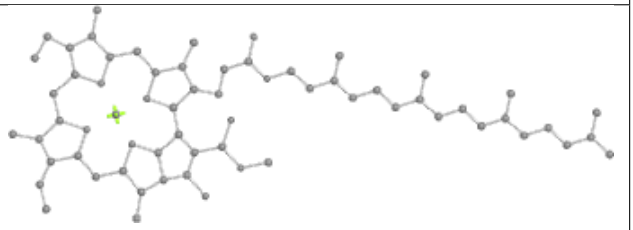
Bond lengths



Bond angles

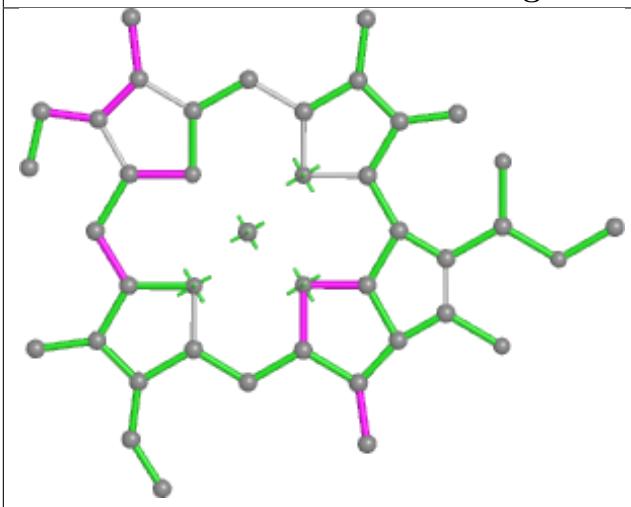


Torsions

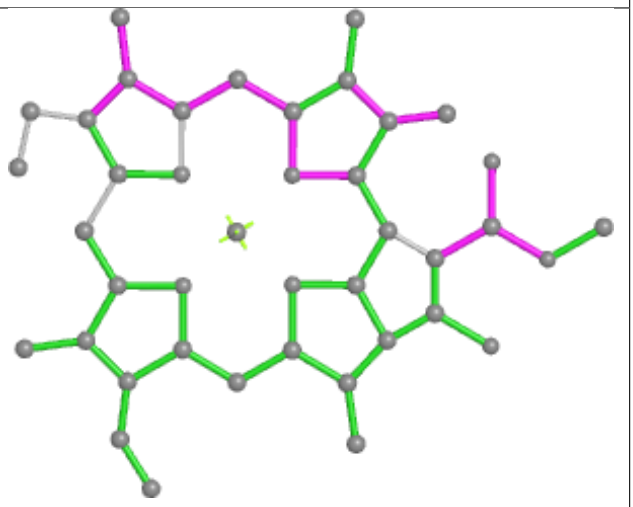


Rings

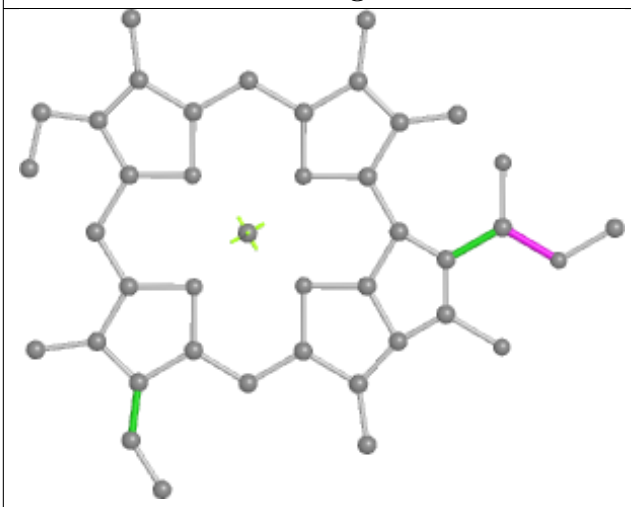
Ligand CLA K 202



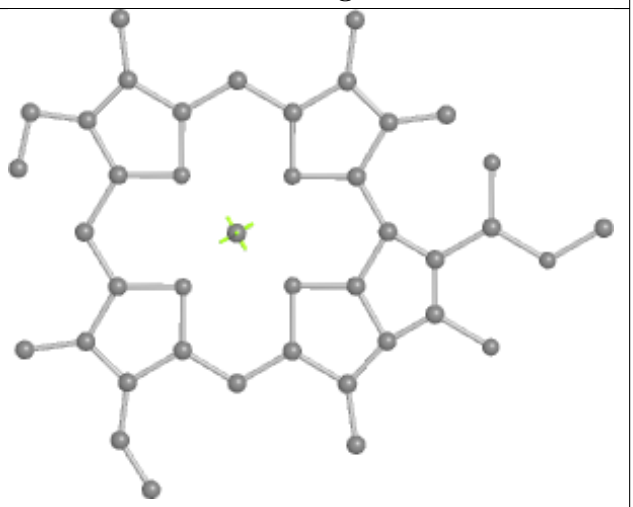
Bond lengths



Bond angles

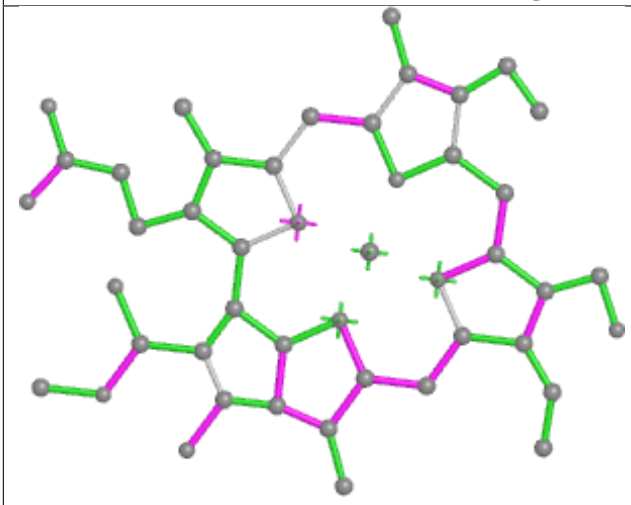


Torsions

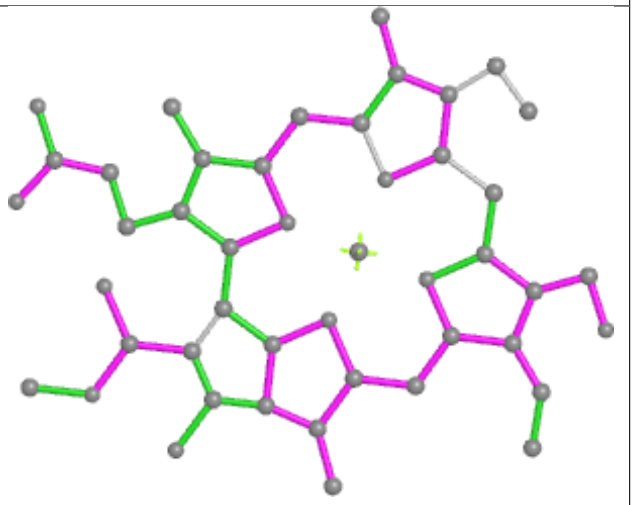


Rings

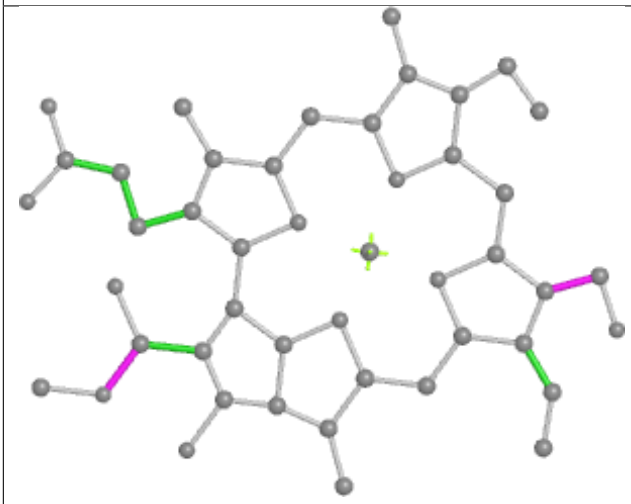
Ligand CHL 5 315



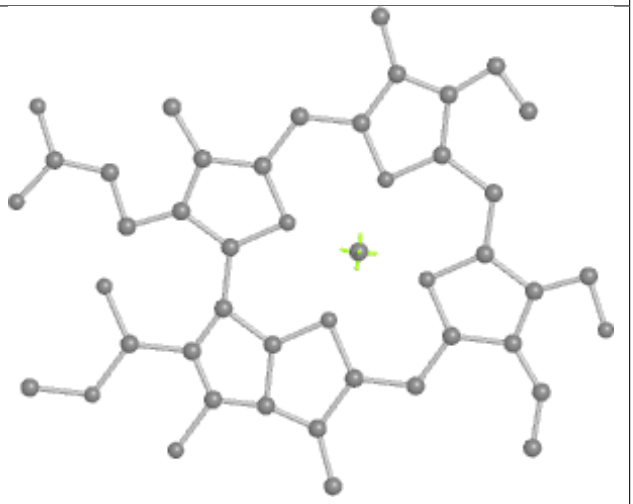
Bond lengths



Bond angles

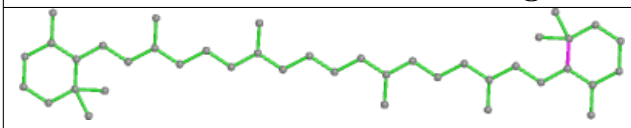


Torsions

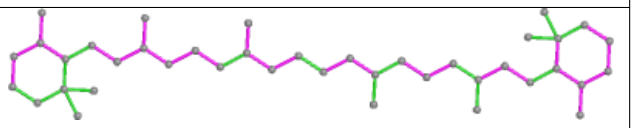


Rings

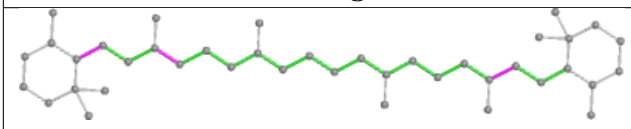
Ligand BCR B 845



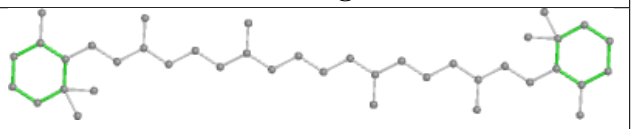
Bond lengths



Bond angles

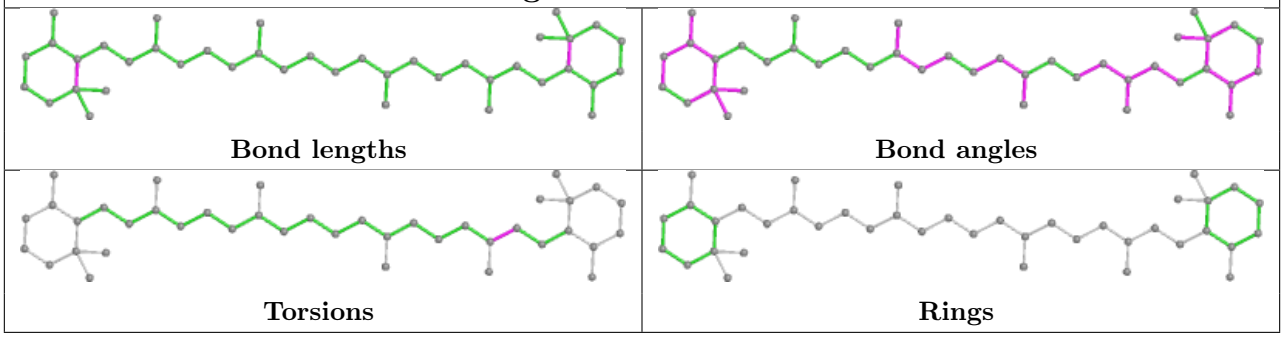


Torsions

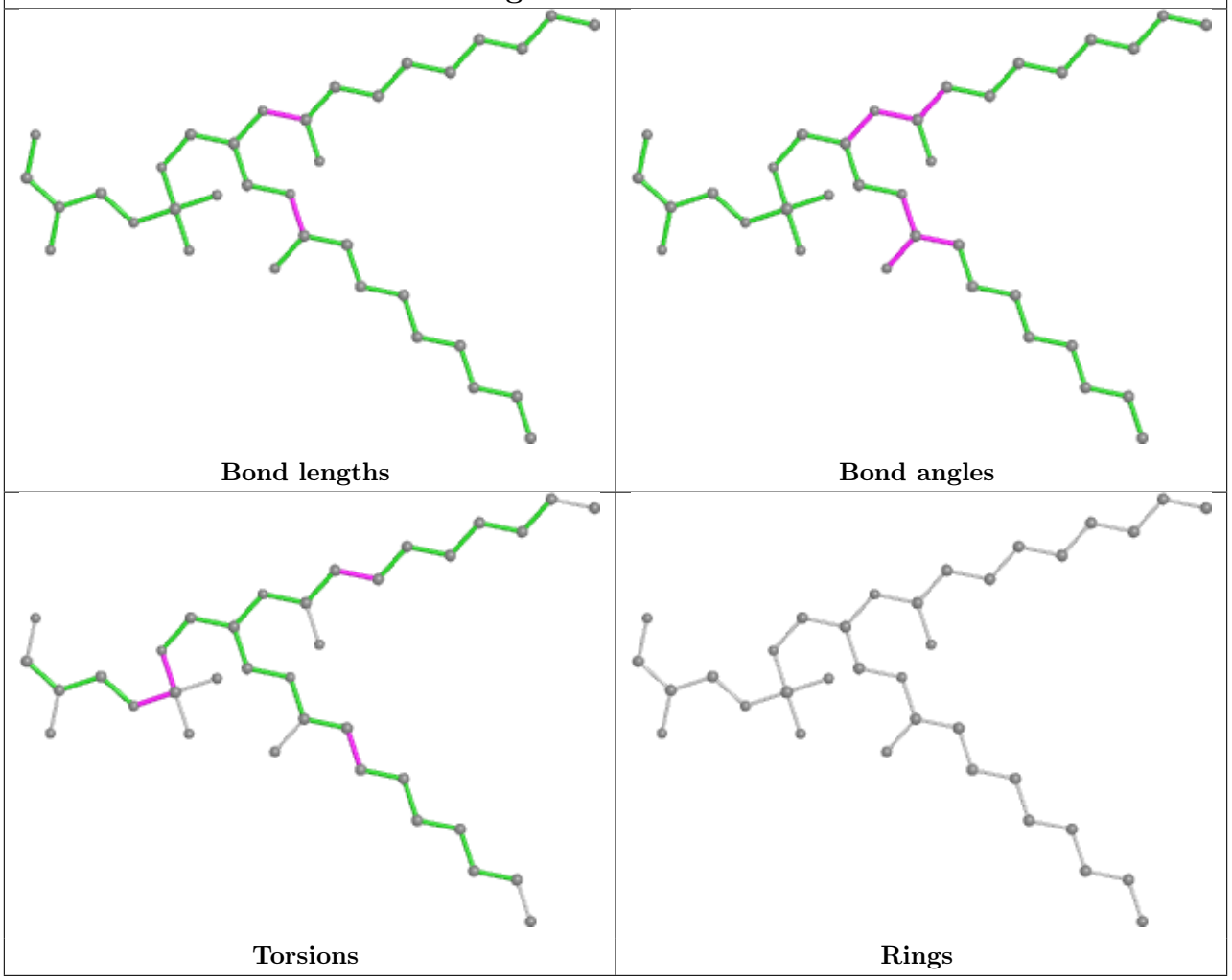


Rings

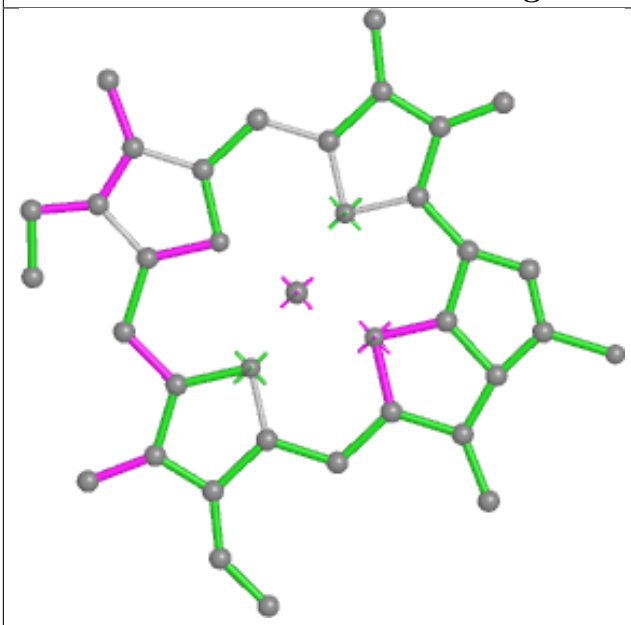
Ligand BCR A 853



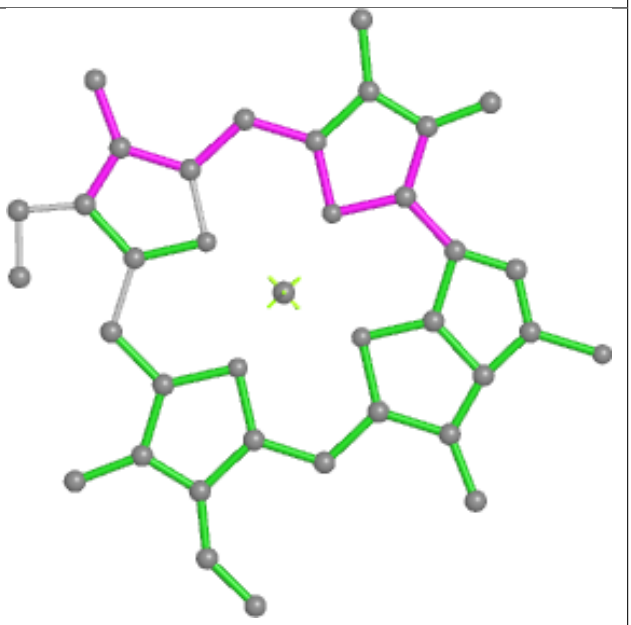
Ligand LHG 2 517



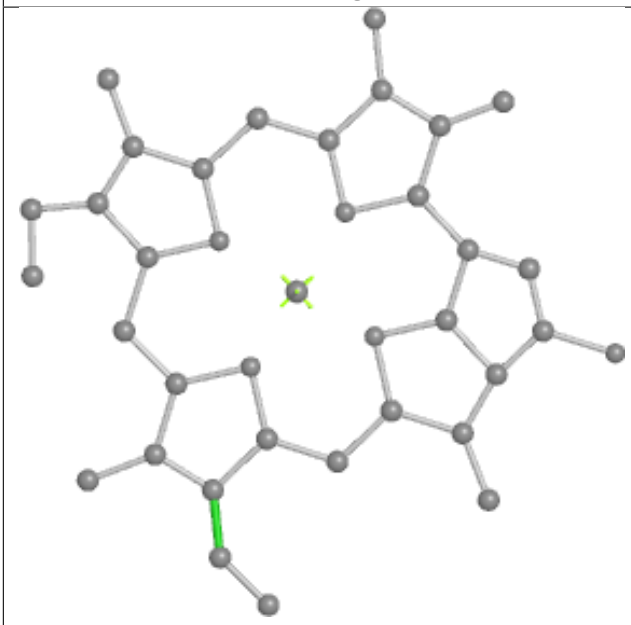
Ligand CLA K 201



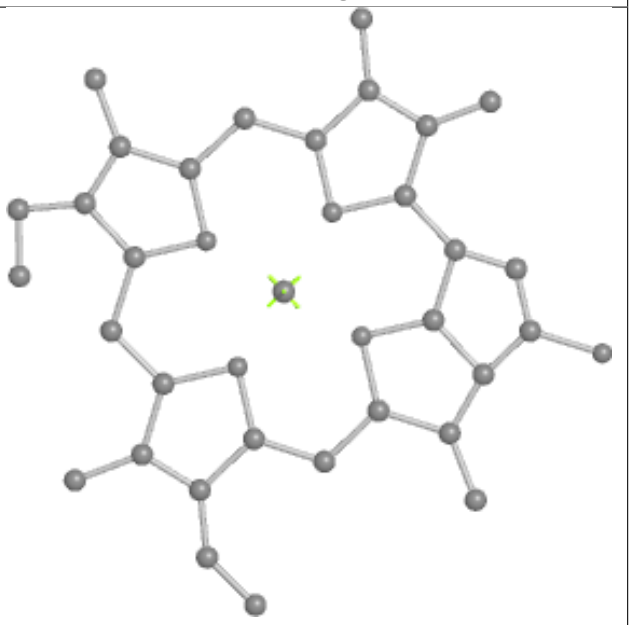
Bond lengths



Bond angles

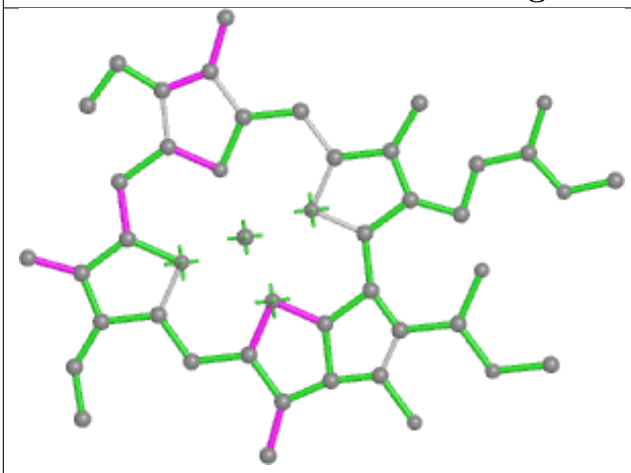


Torsions

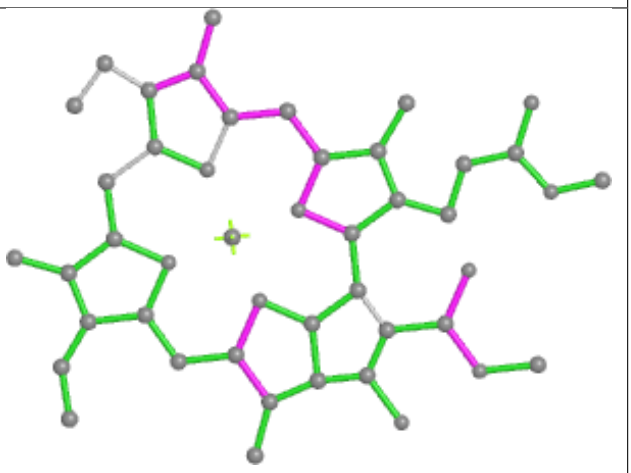


Rings

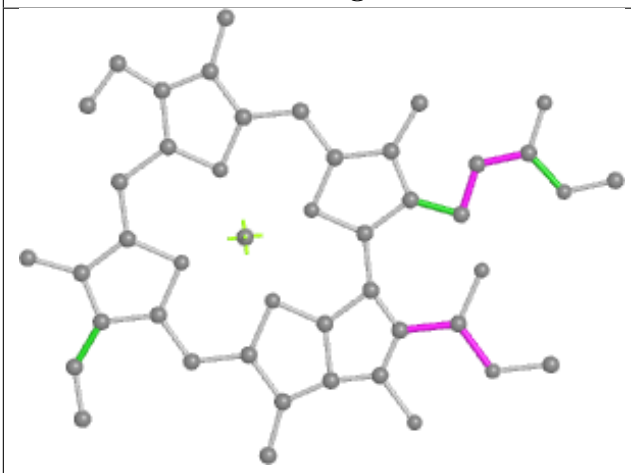
Ligand CLA 5 312



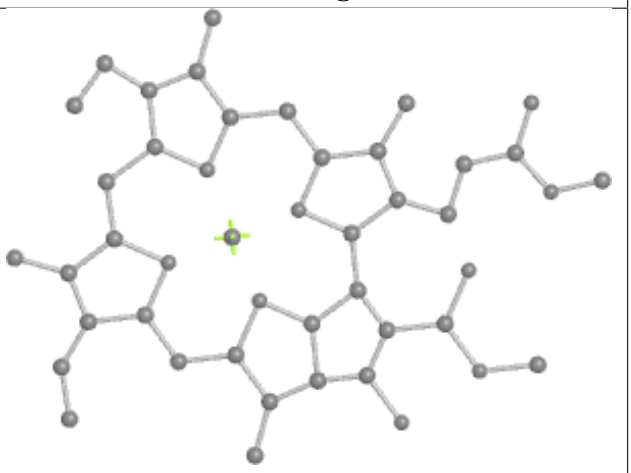
Bond lengths



Bond angles

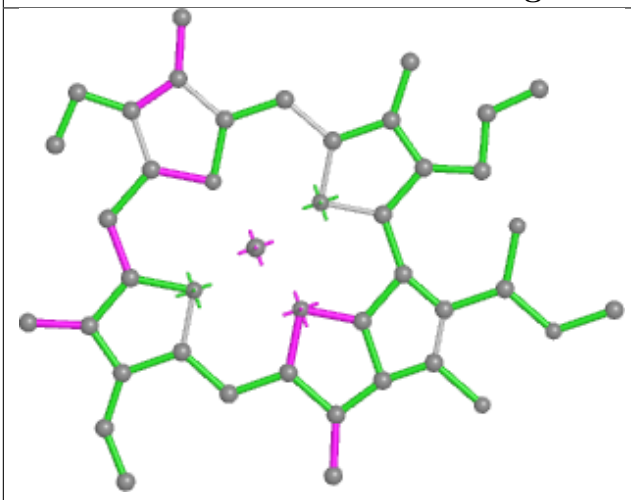


Torsions

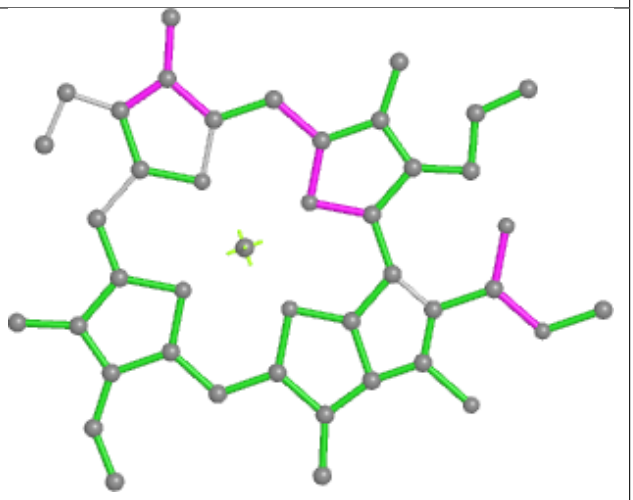


Rings

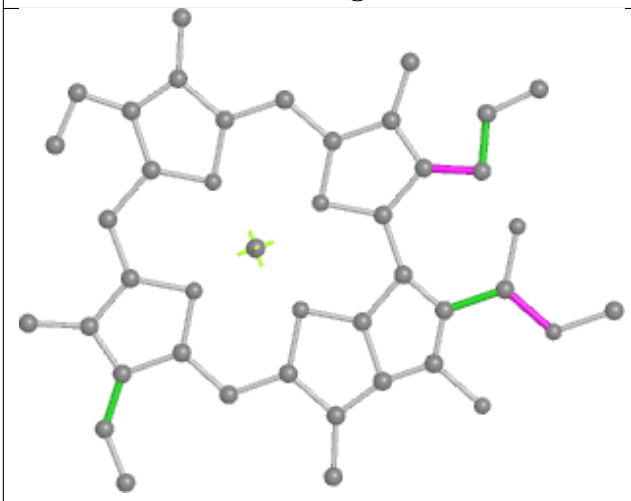
Ligand CLA B 832



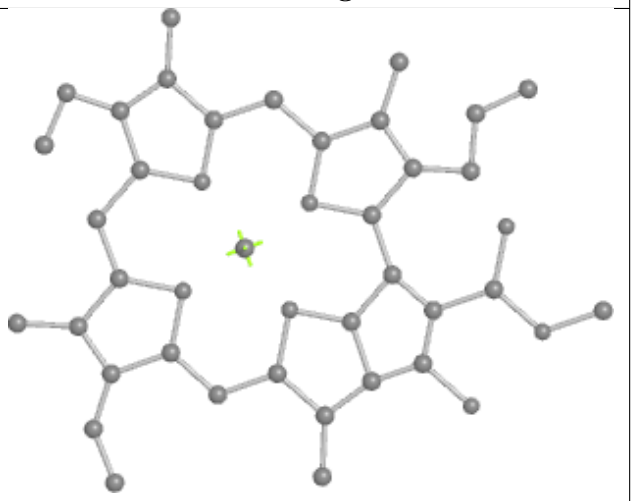
Bond lengths



Bond angles

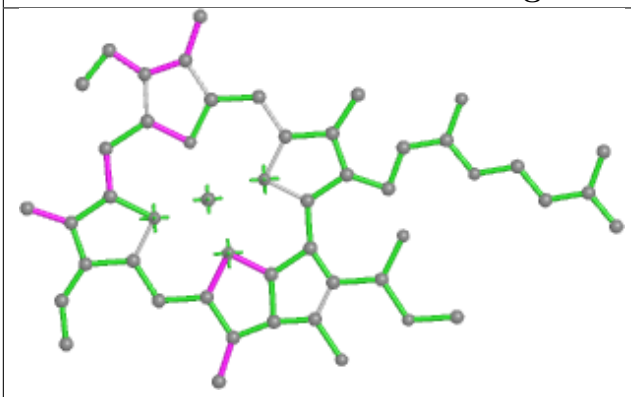


Torsions



Rings

Ligand CLA A 830



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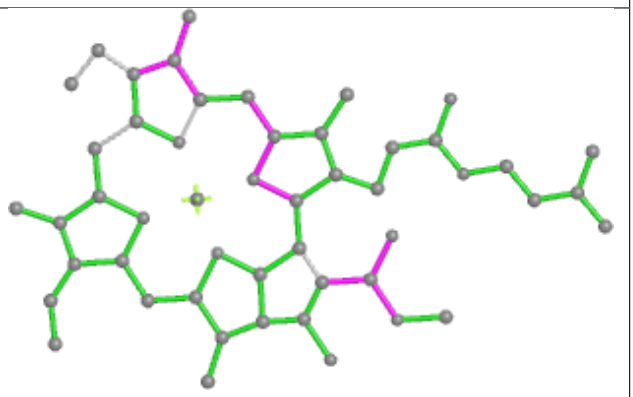
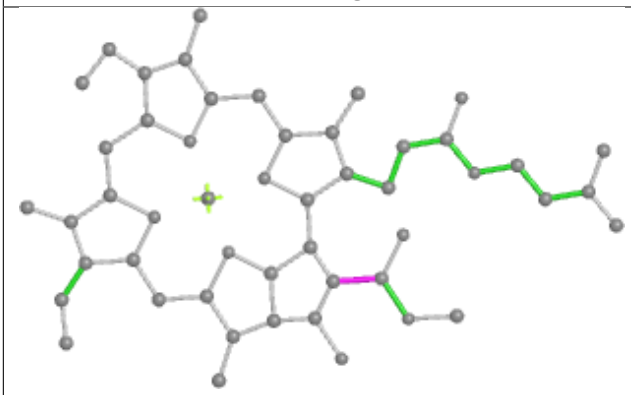


Bond angles



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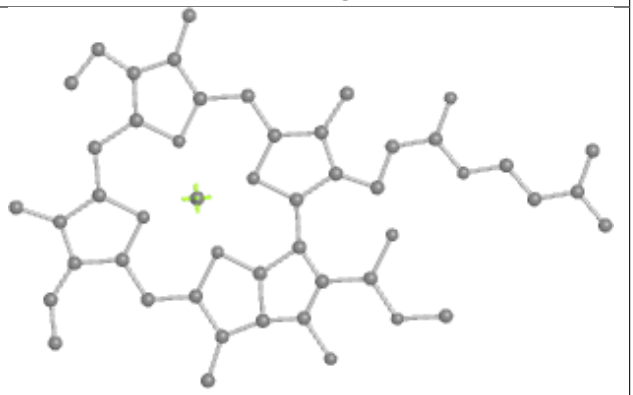
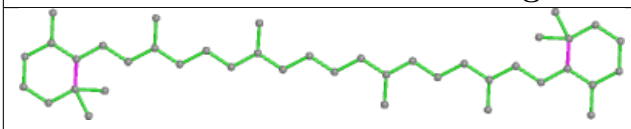
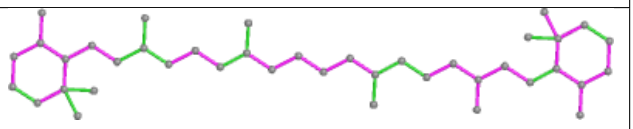


Rings

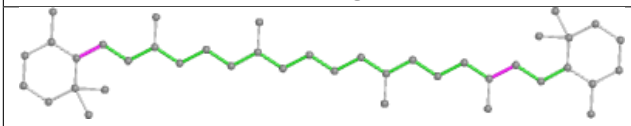
Ligand BCR B 849



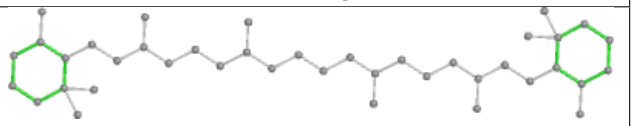
Bond lengths



Bond angles

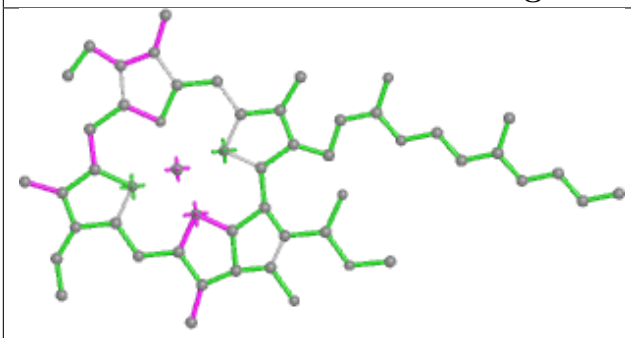


Torsions

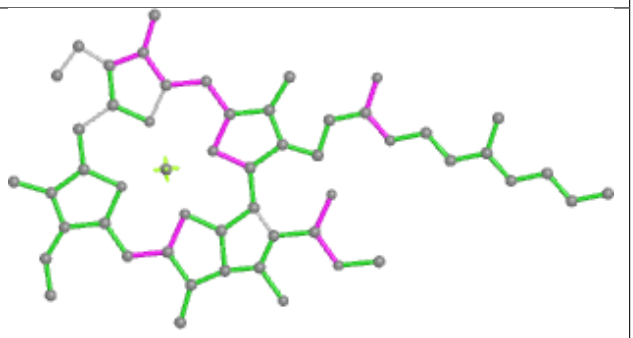


Rings

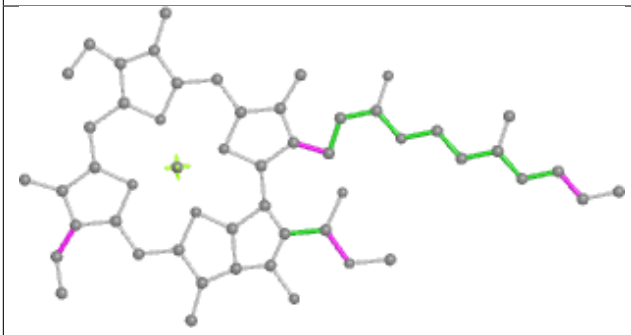
Ligand CLA B 820



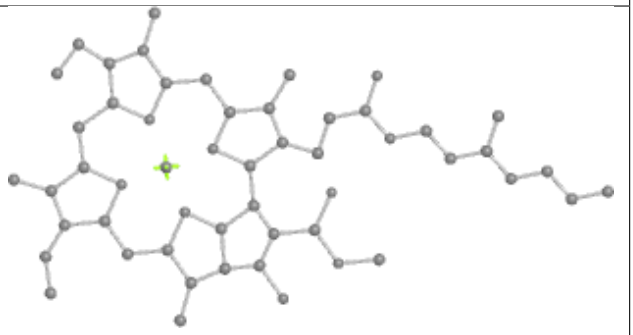
Bond lengths



Bond angles

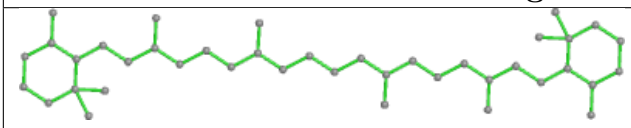


Torsions



Rings

Ligand BCR 5 302



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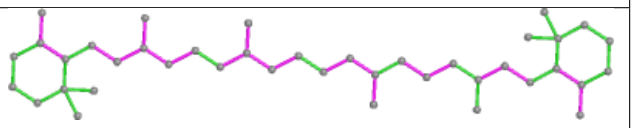
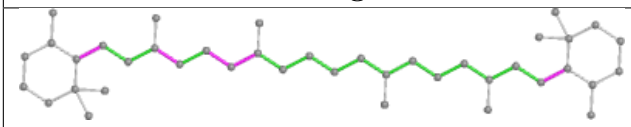


Bond angles



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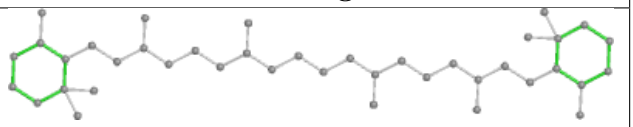
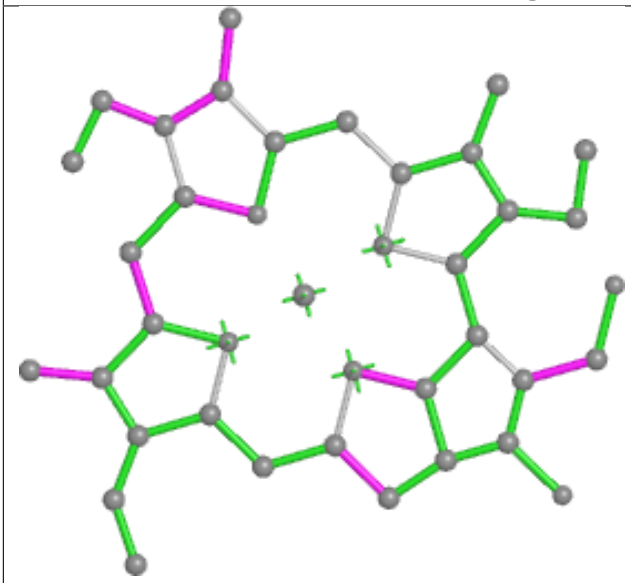
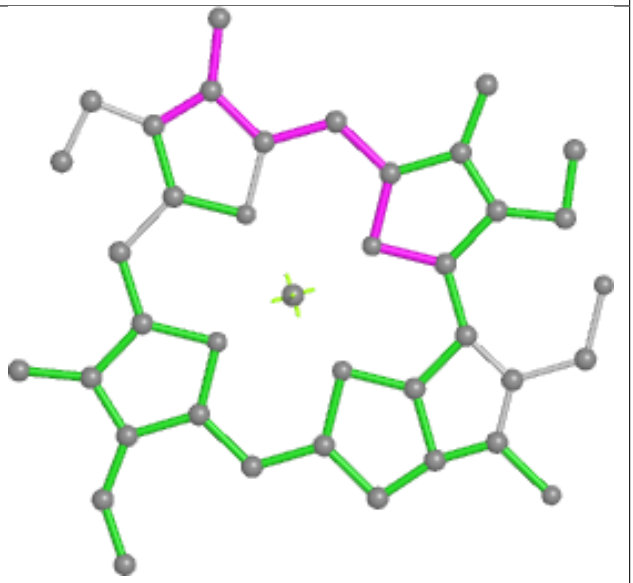


Rings

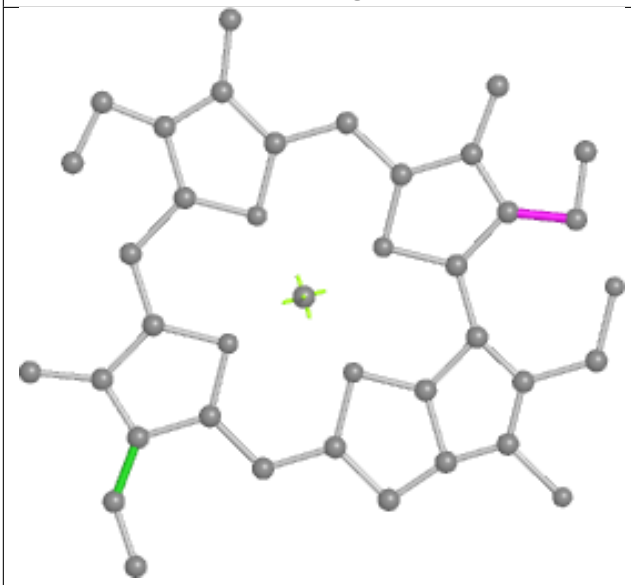
Ligand CLA A 809



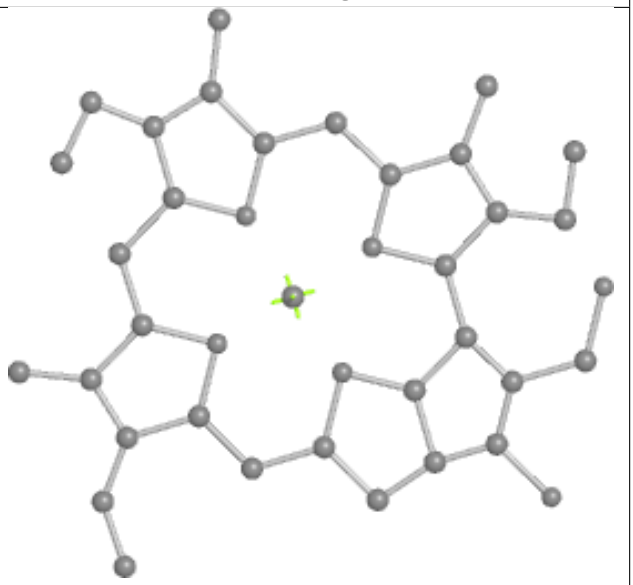
Bond lengths



Bond angles

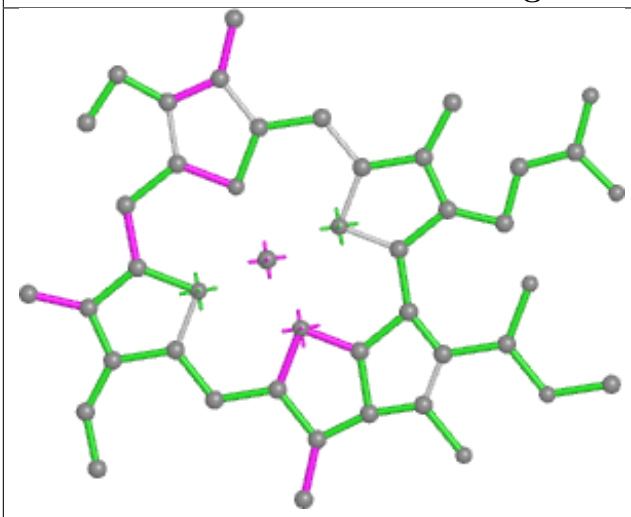


Torsions



Rings

Ligand CLA A 815



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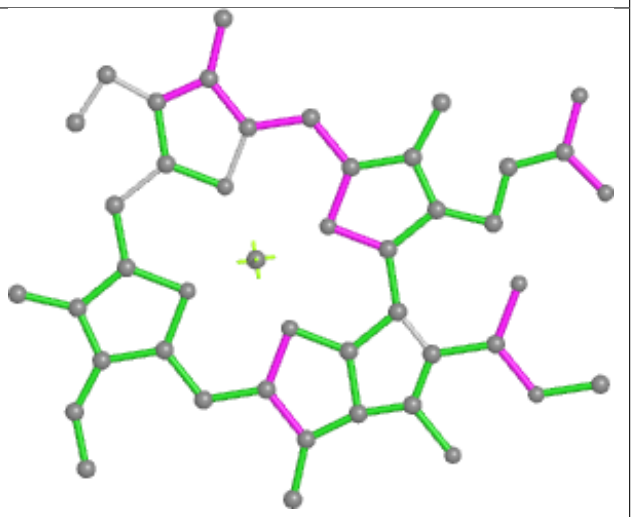
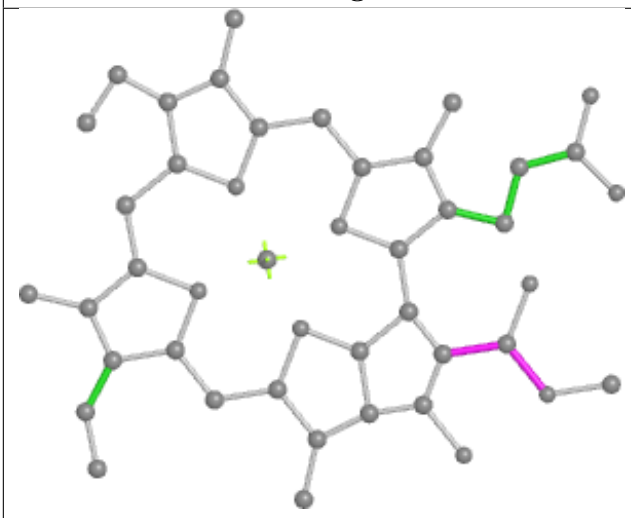


Bond angles



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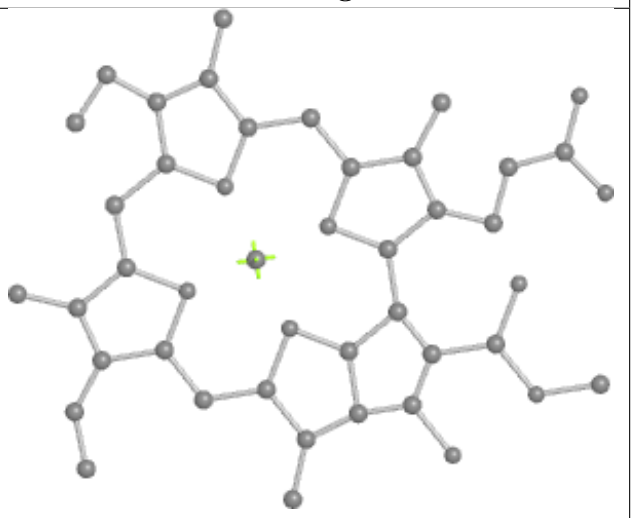
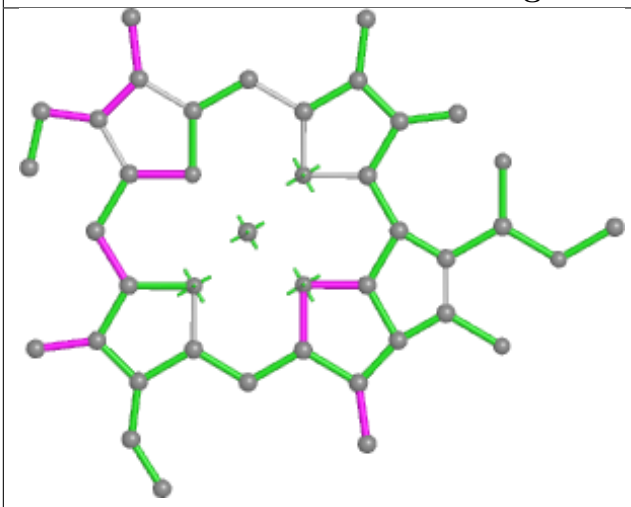


Rings

Ligand CLA A 822



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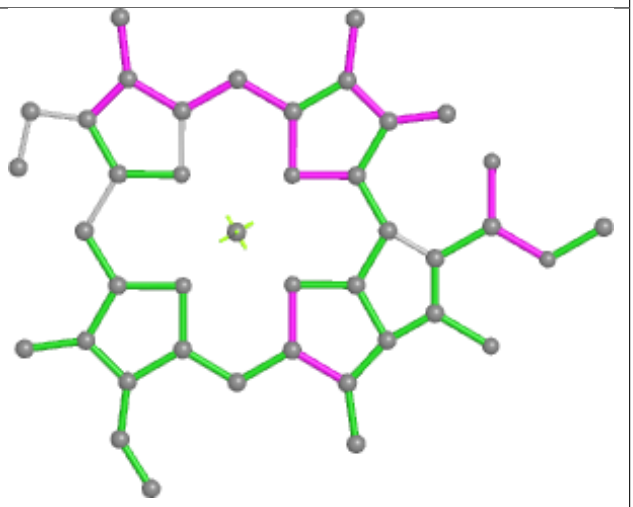
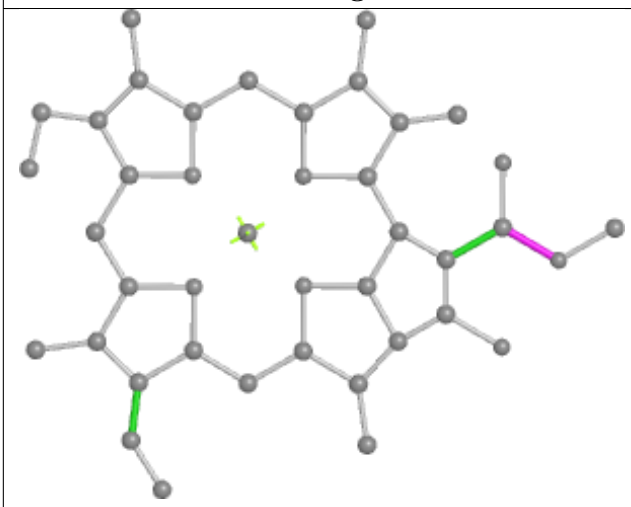


Bond angles



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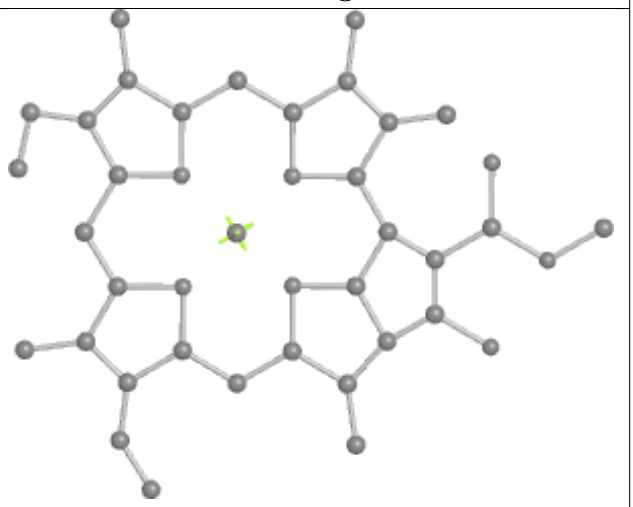
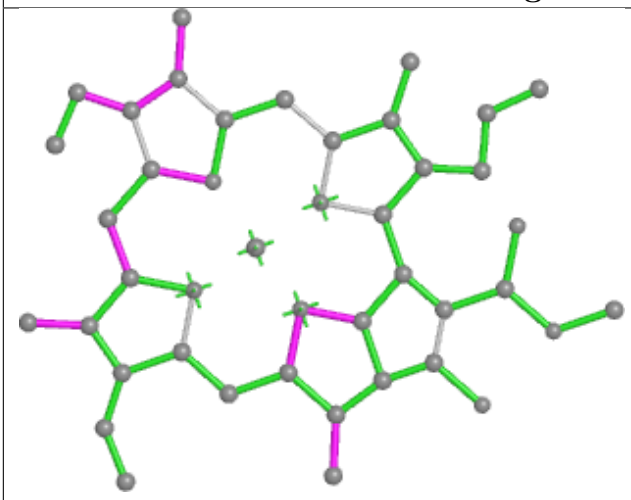
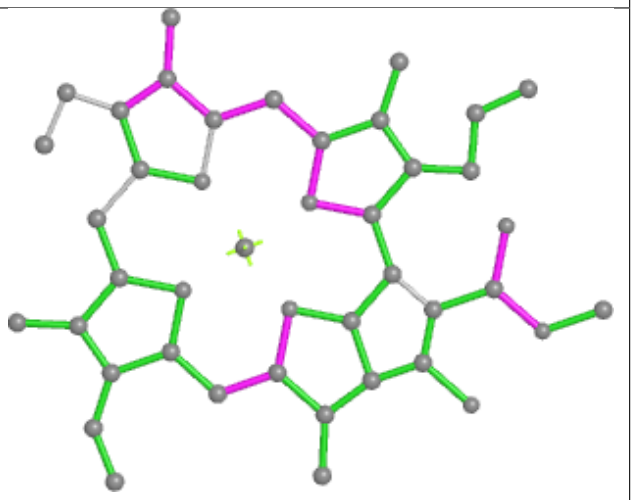


Rings

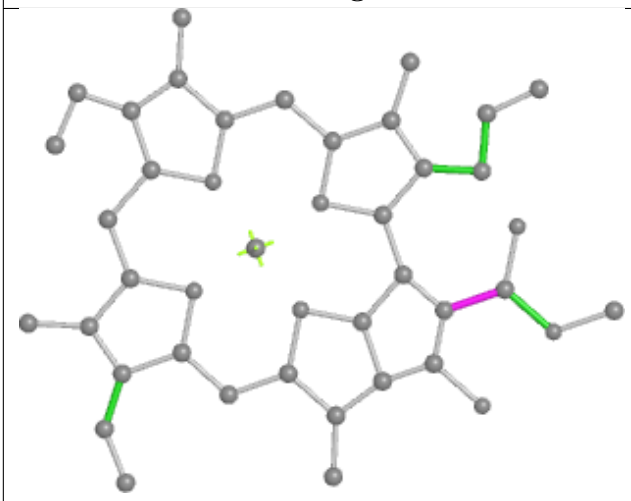
Ligand CLA B 831



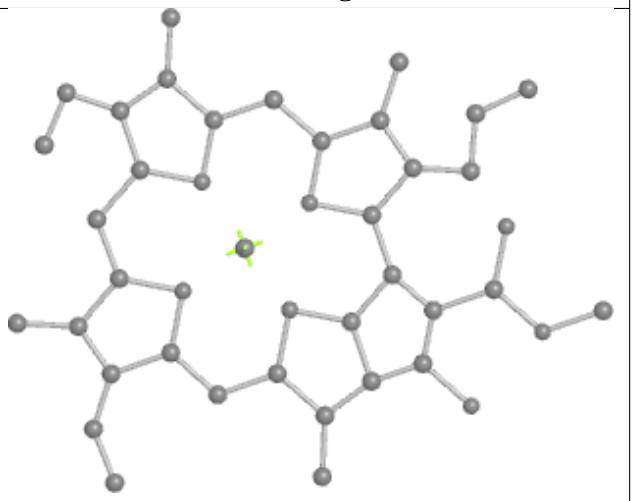
Bond lengths



Bond angles

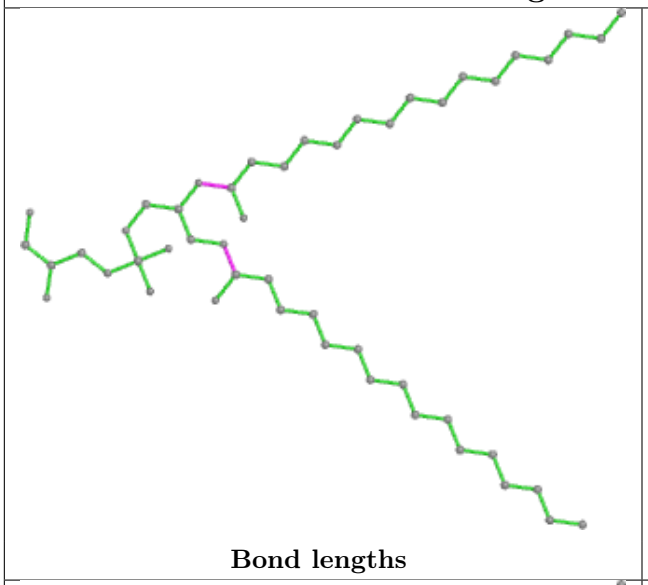


Torsions

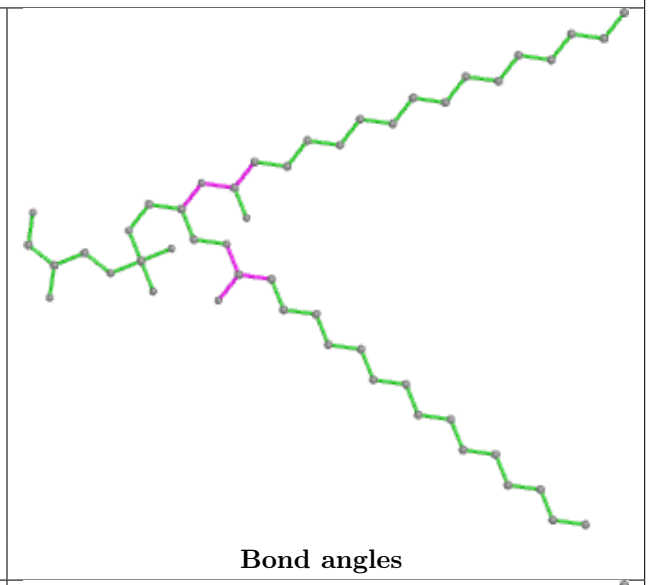


Rings

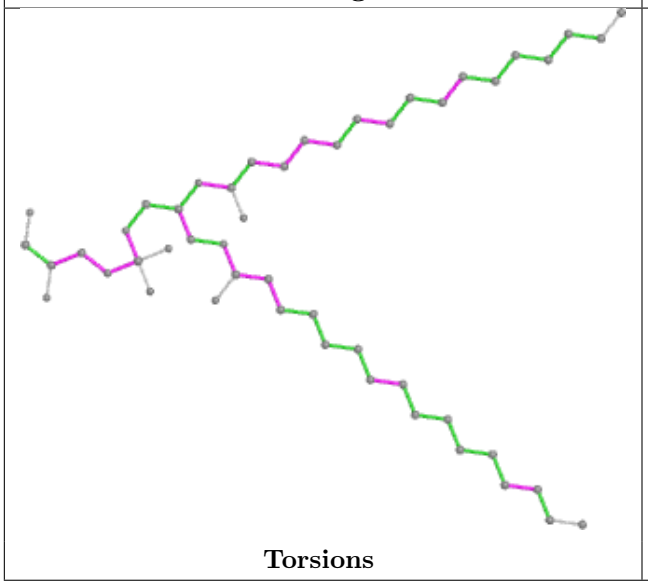
Ligand LHG 1 516



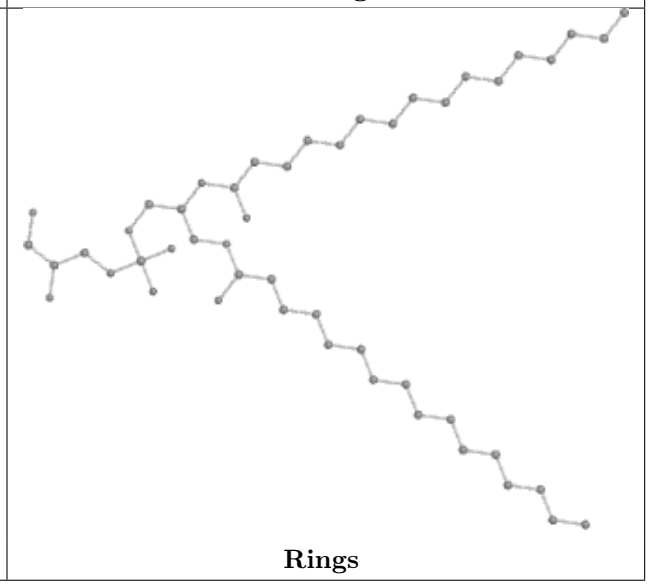
Bond lengths



Bond angles

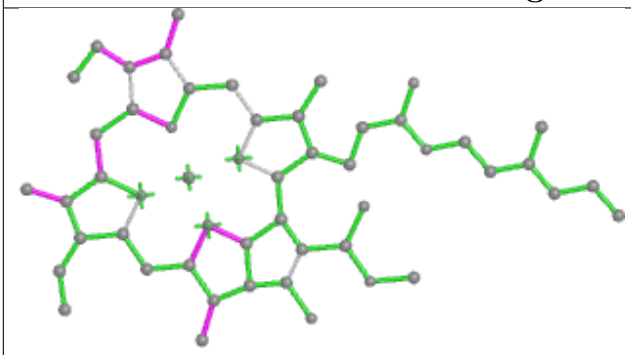


Torsions

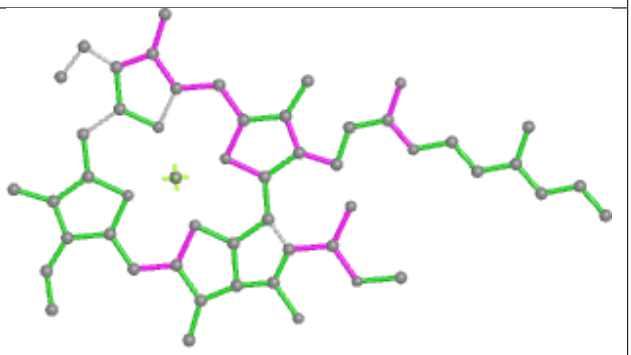


Rings

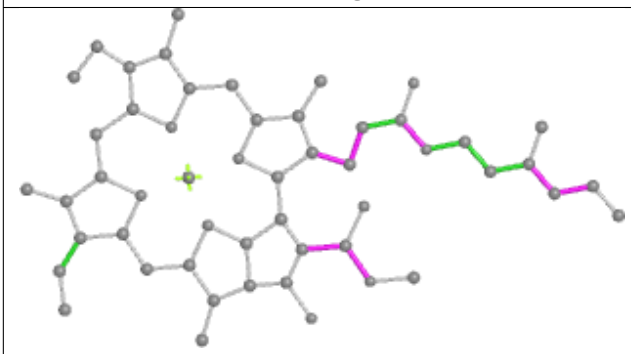
Ligand CLA L 303



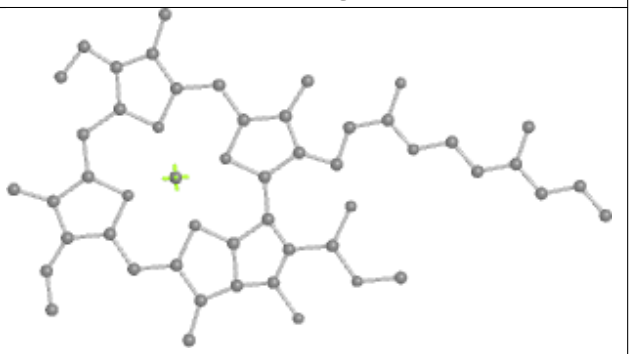
Bond lengths



Bond angles

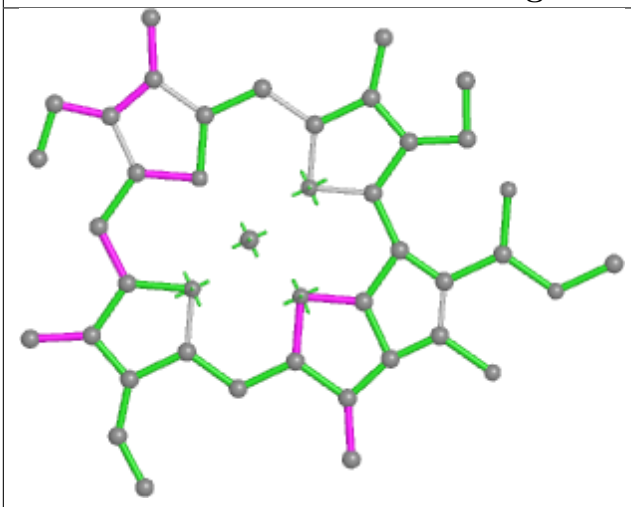


Torsions

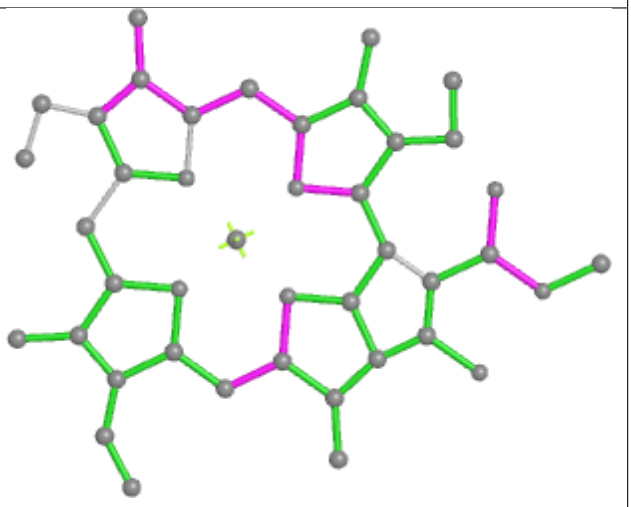


Rings

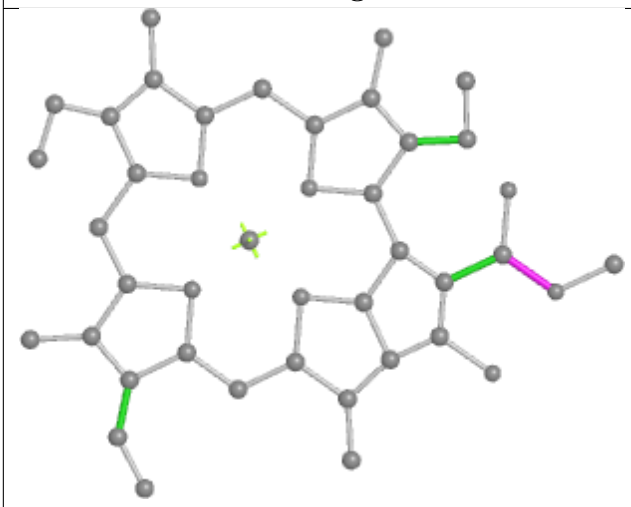
Ligand CLA F 802



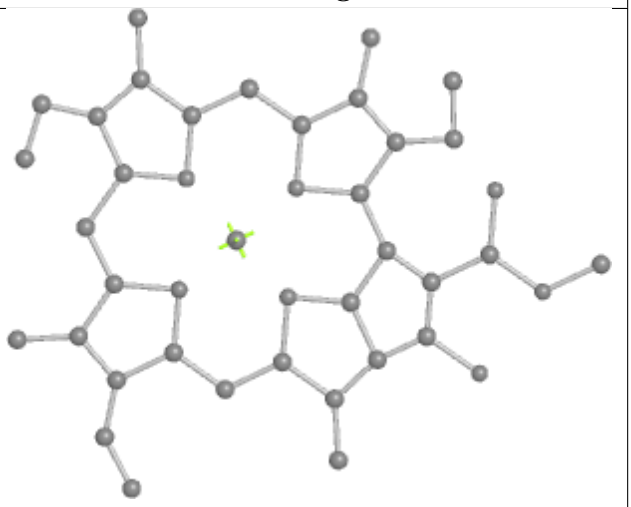
Bond lengths



Bond angles

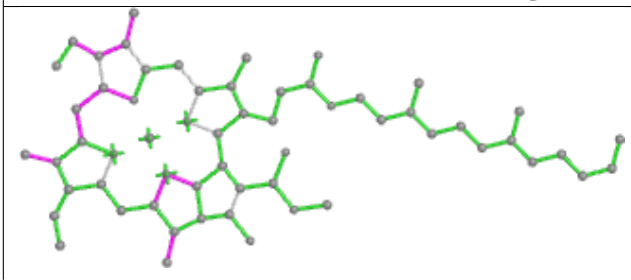


Torsions

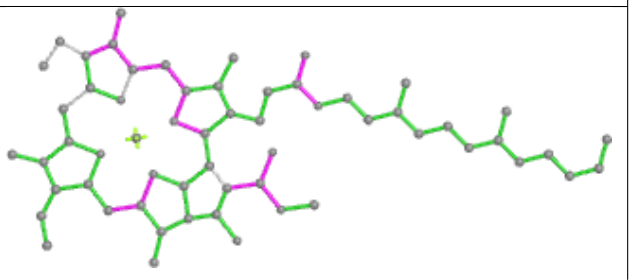


Rings

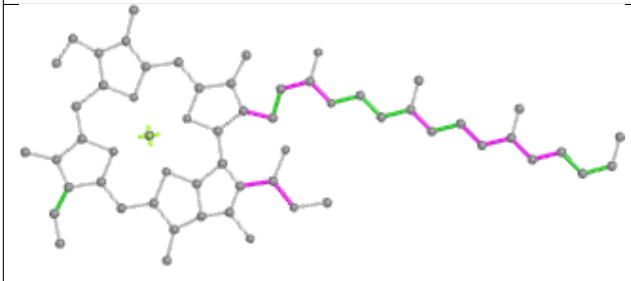
Ligand CLA B 818



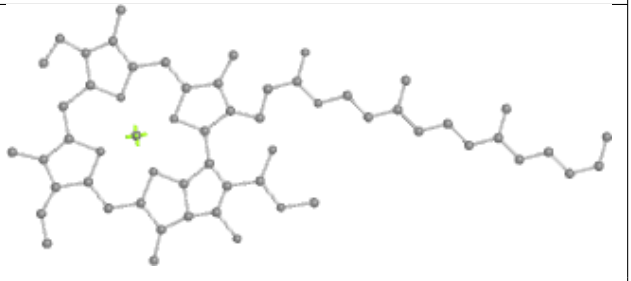
Bond lengths



Bond angles

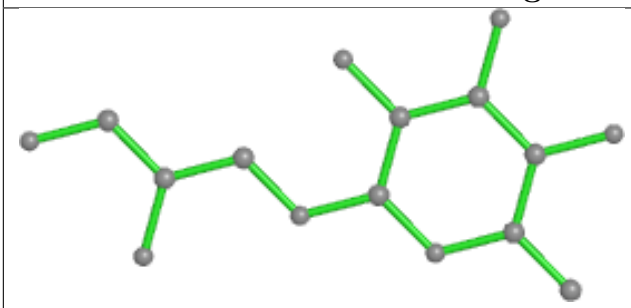


Torsions

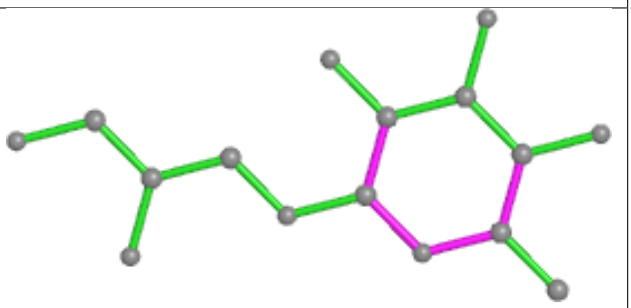


Rings

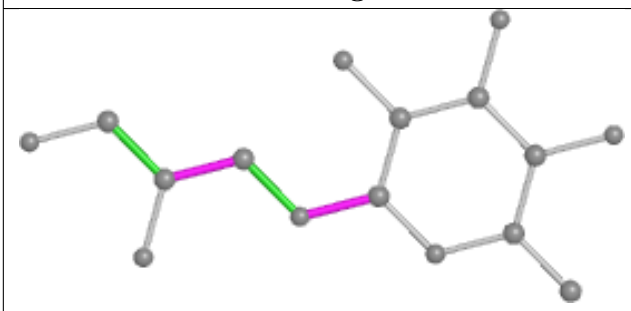
Ligand LMG 2 518



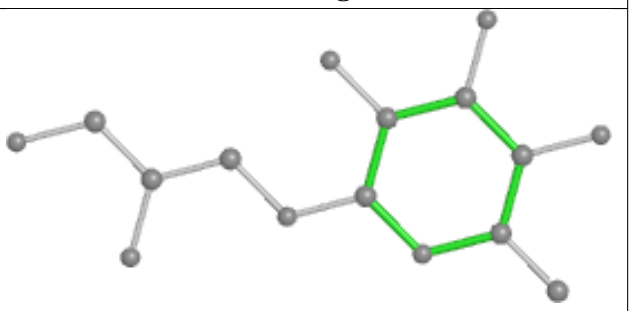
Bond lengths



Bond angles

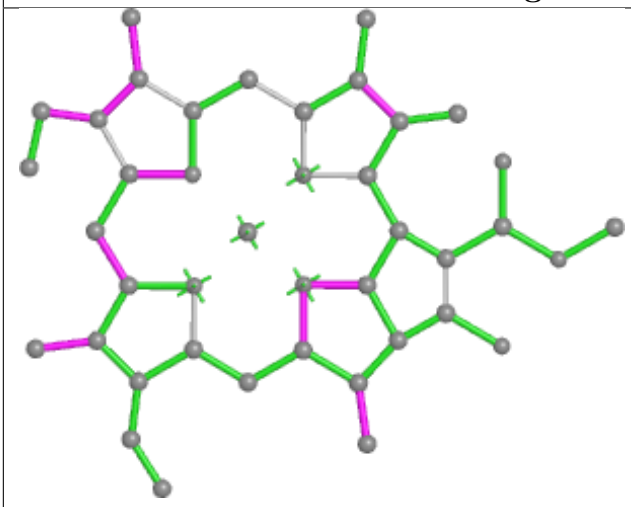


Torsions



Rings

Ligand CLA B 819



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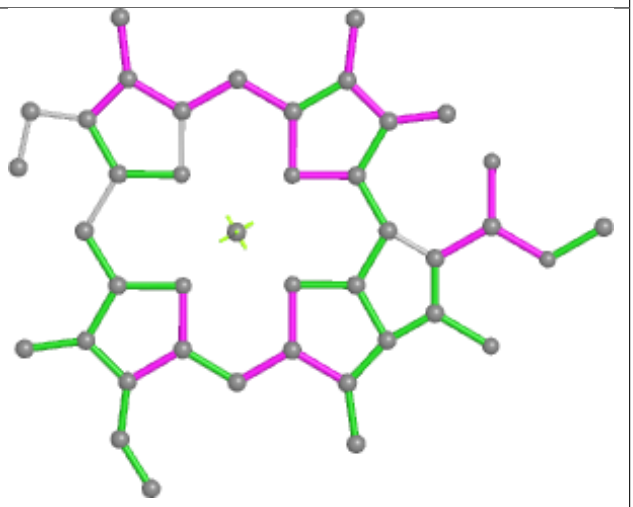
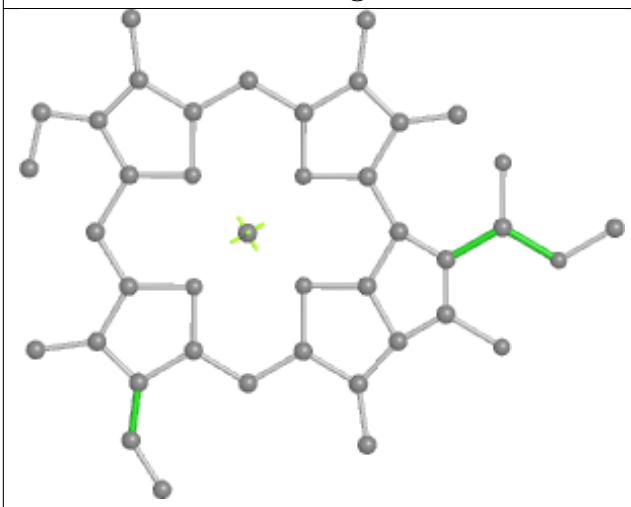
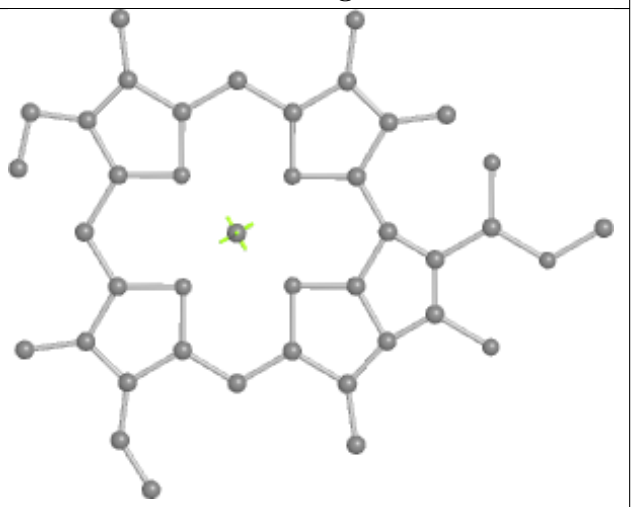


Bond angles

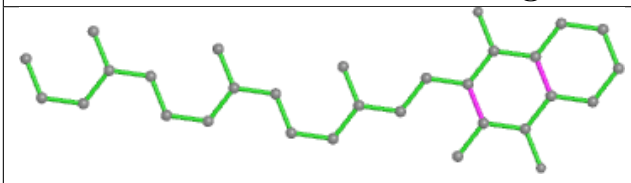


Torsions



Rings

Ligand PQN B 843



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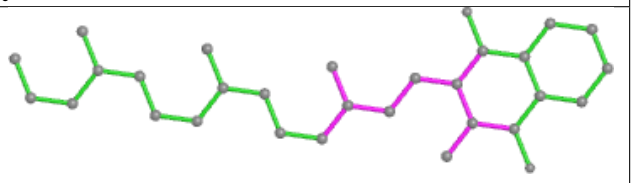
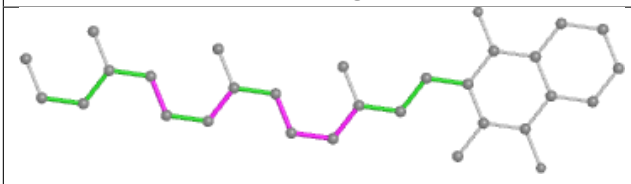
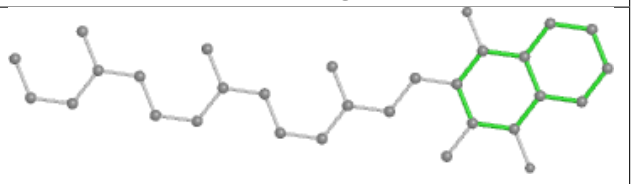


Bond angles

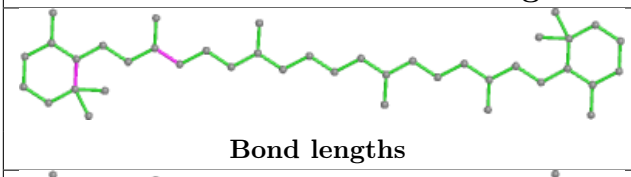


Torsions



Rings

Ligand BCR A 846



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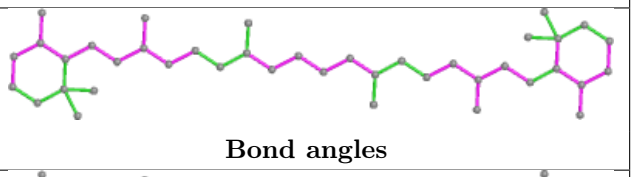
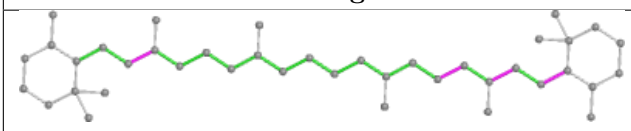


Bond angles



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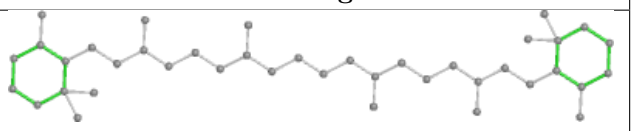
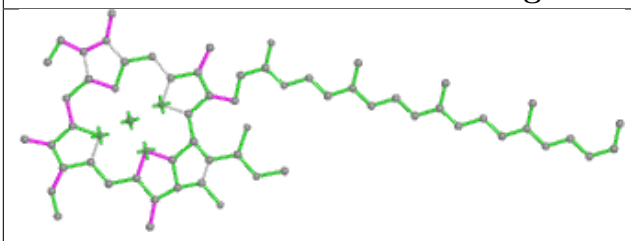


Rings

Ligand CLA A 805



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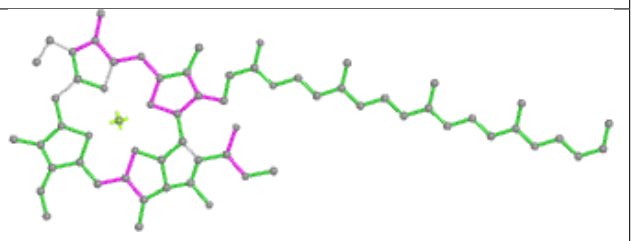
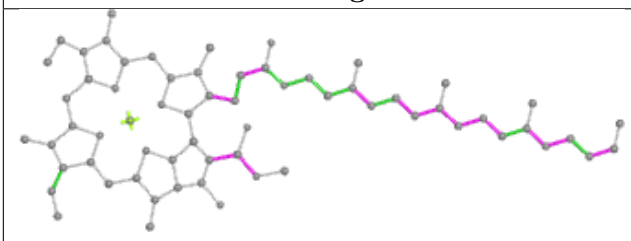


Bond angles



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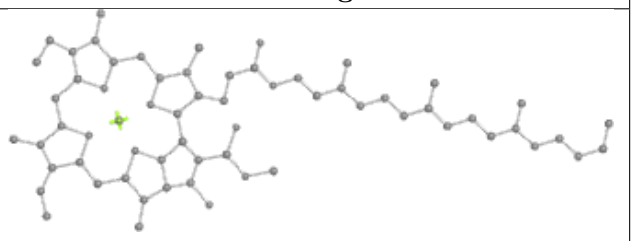
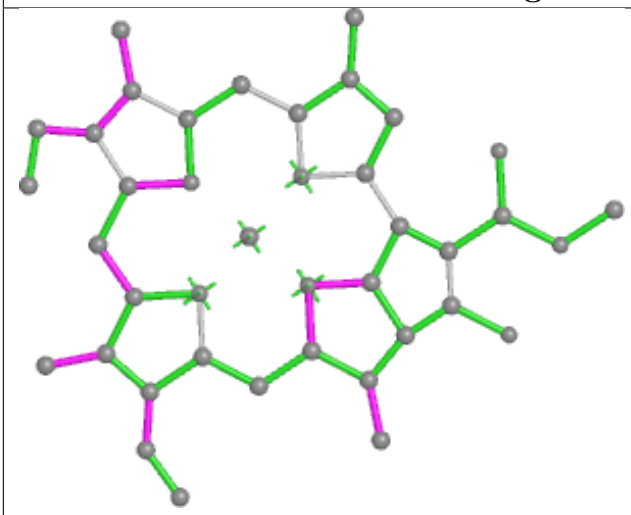


Rings

Ligand CLA B 810



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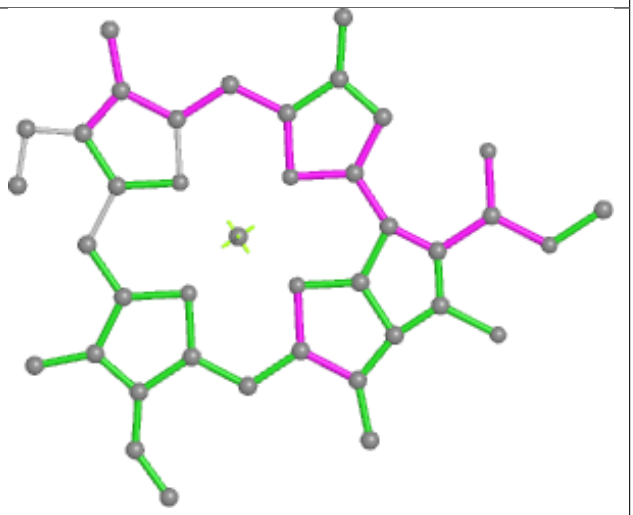
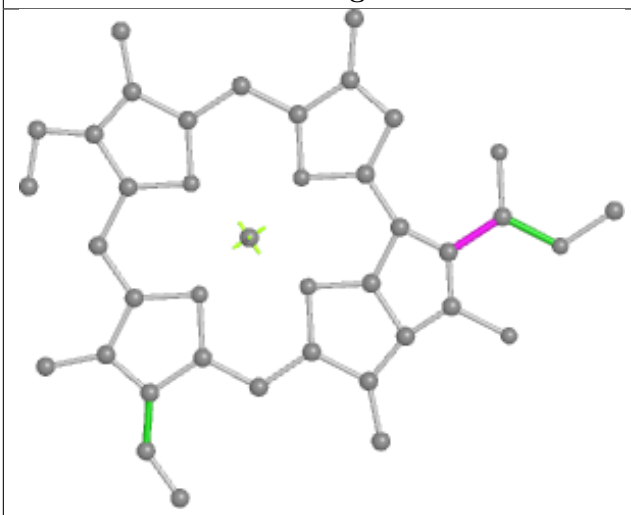
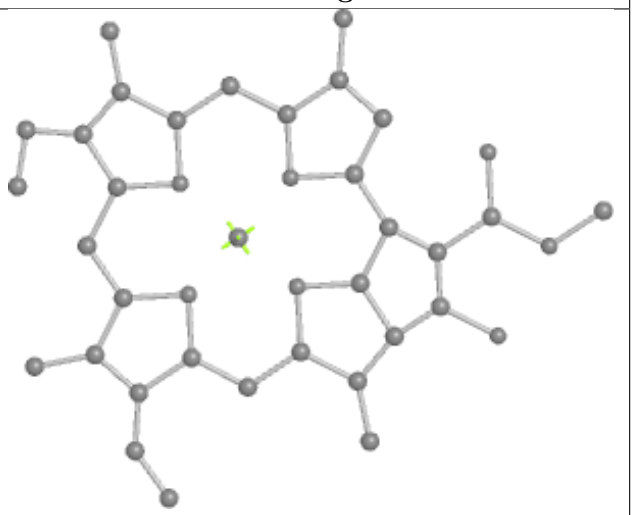


Bond angles

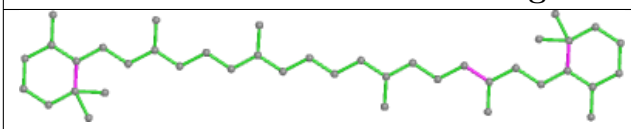


Torsions



Rings

Ligand BCR I 101



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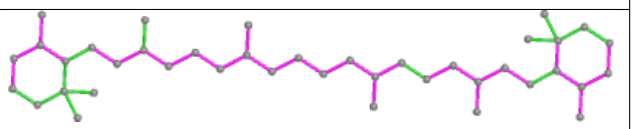
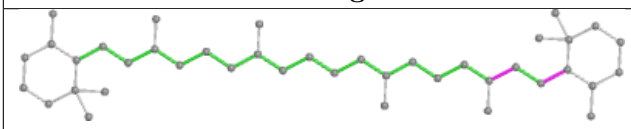
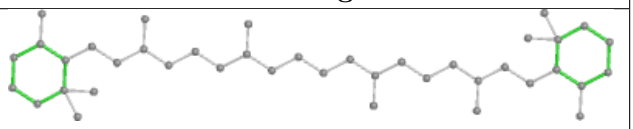


Bond angles

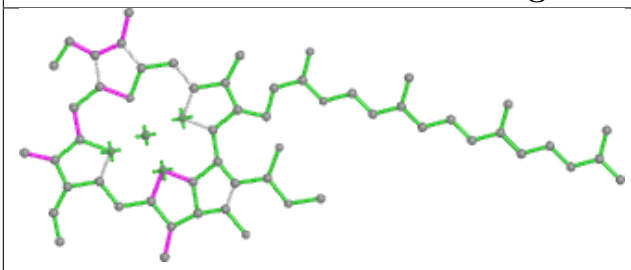


Torsions



Rings

Ligand CLA 5 308



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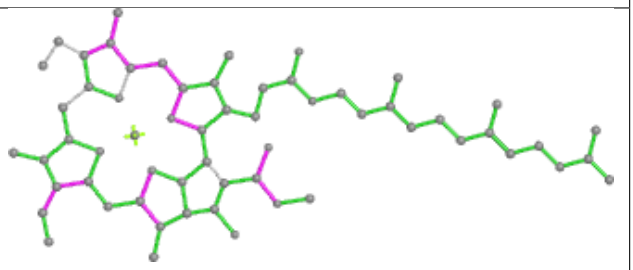
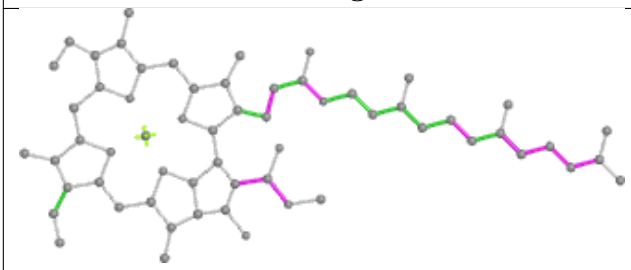


Bond angles



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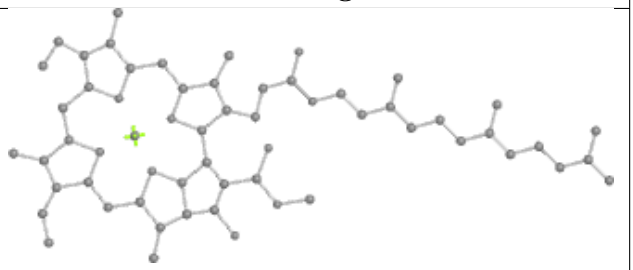
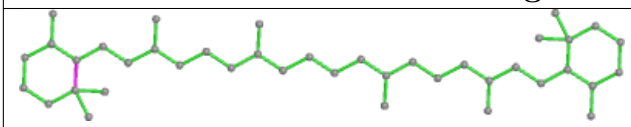


Rings

Ligand BCR F 804



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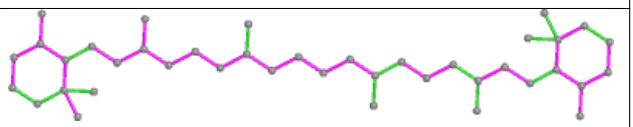
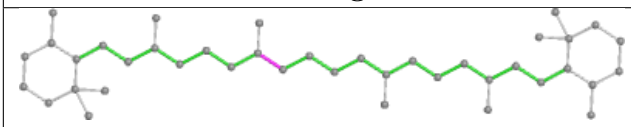


Bond angles



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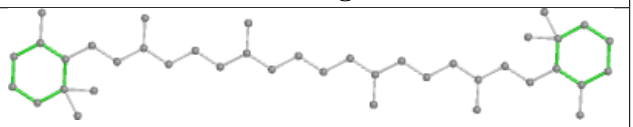
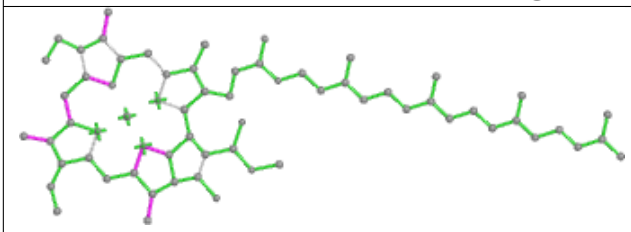


Rings

Ligand CLA 1 513



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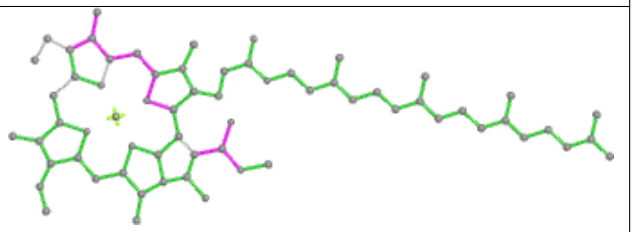
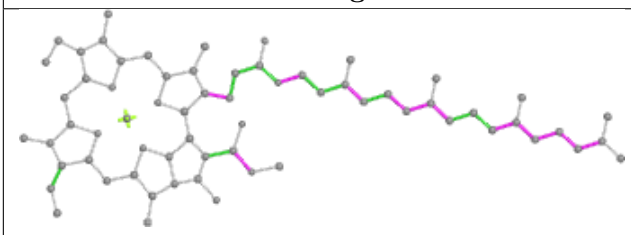


Bond angles



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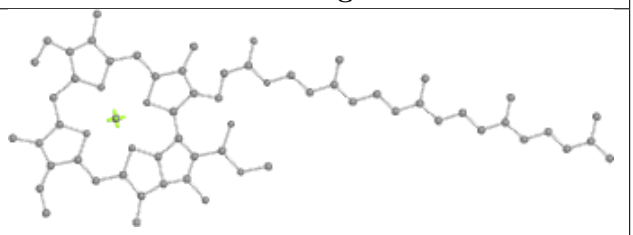
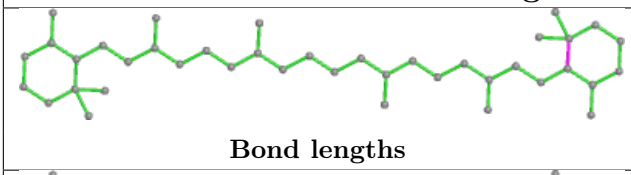


Rings

Ligand BCR B 844



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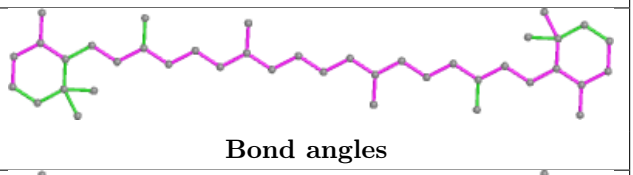
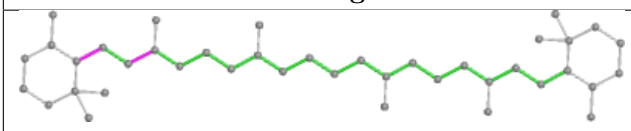


Bond angles



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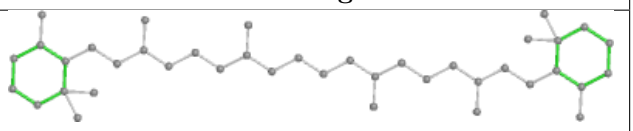
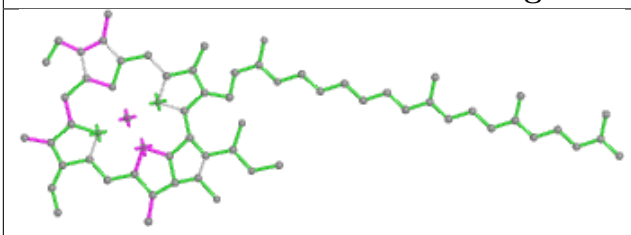
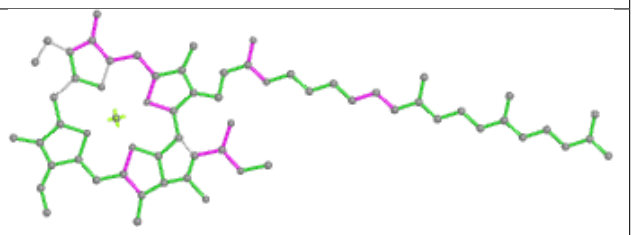


Rings

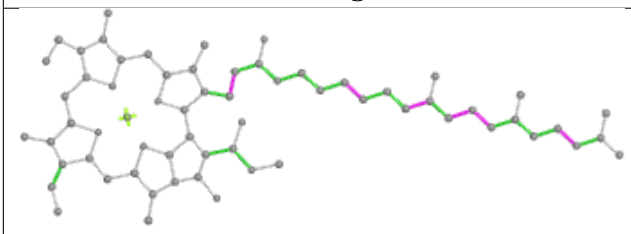
Ligand CLA B 802



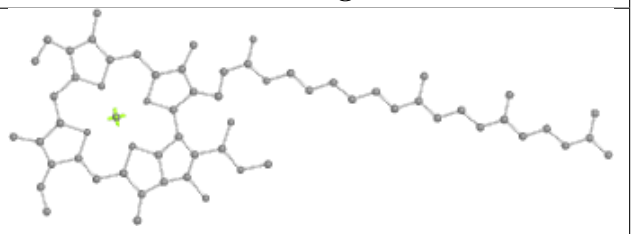
Bond lengths



Bond angles

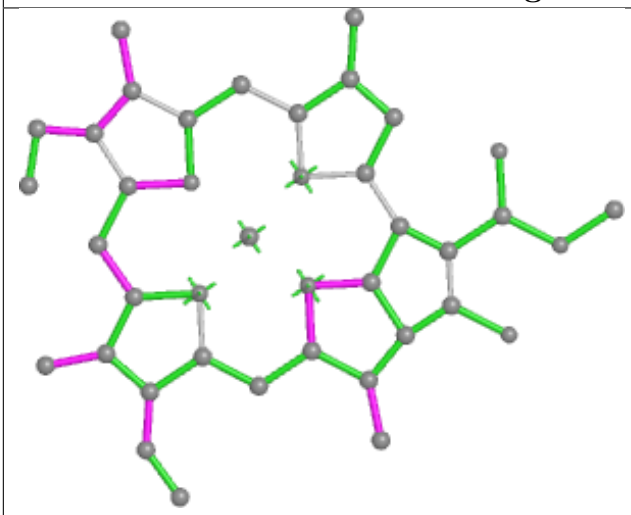


Torsions

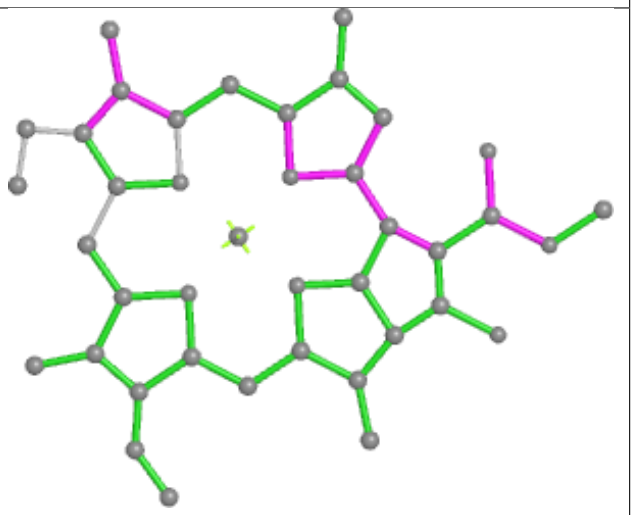


Rings

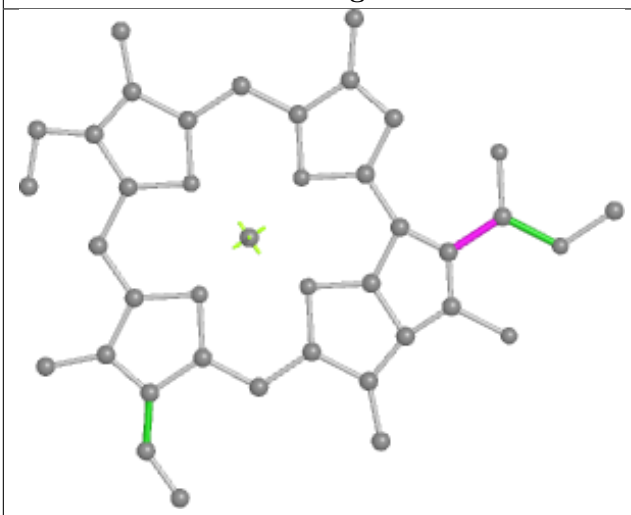
Ligand CLA B 809



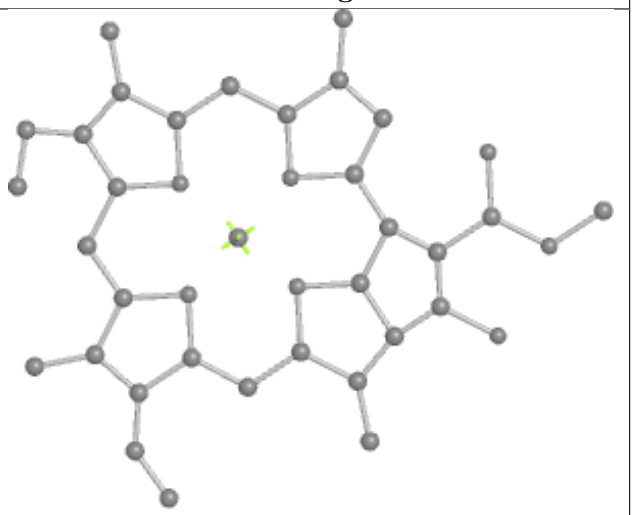
Bond lengths



Bond angles

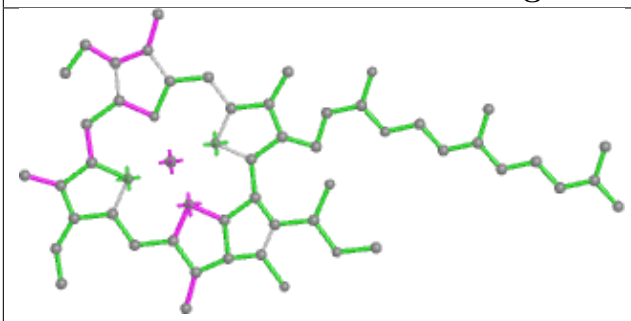


Torsions

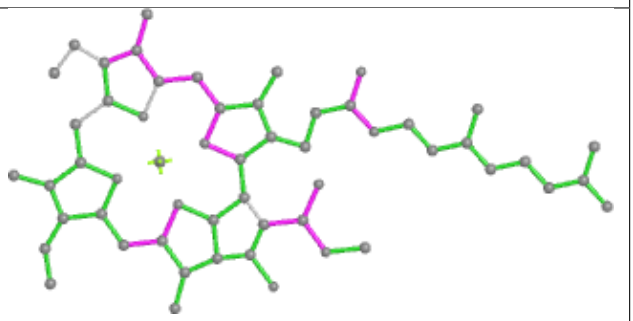


Rings

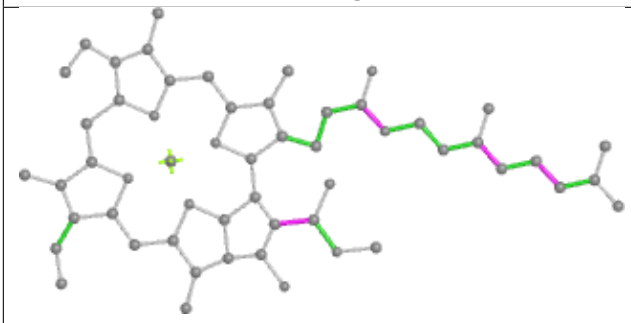
Ligand CLA A 829



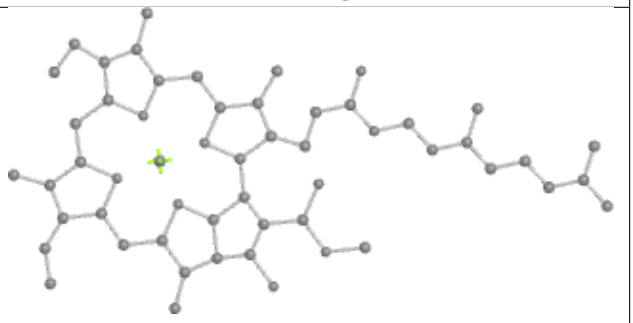
Bond lengths



Bond angles

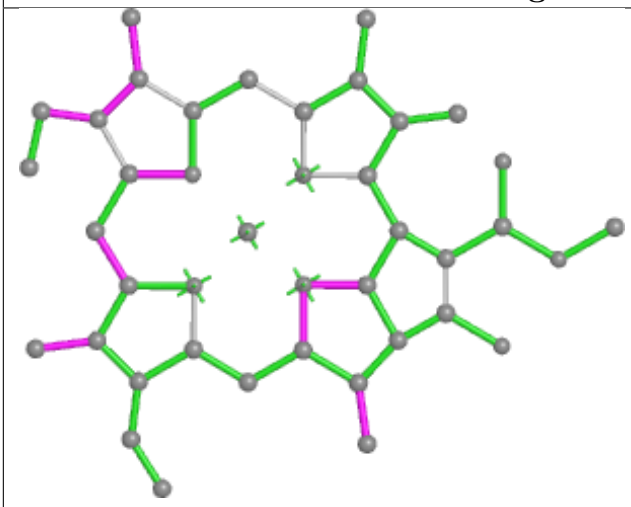


Torsions



Rings

Ligand CLA 3 301



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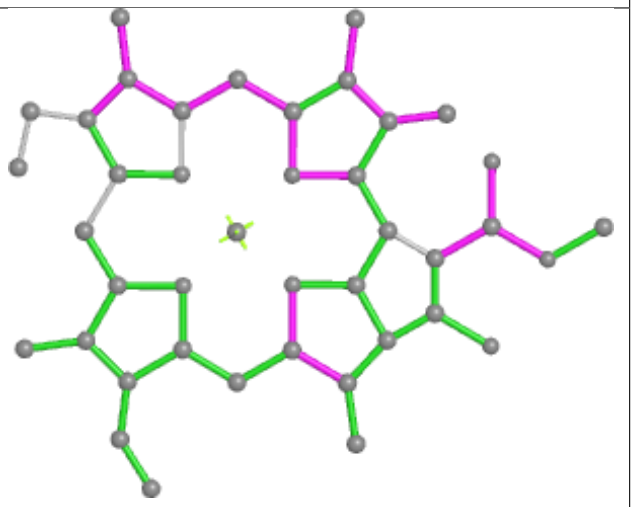

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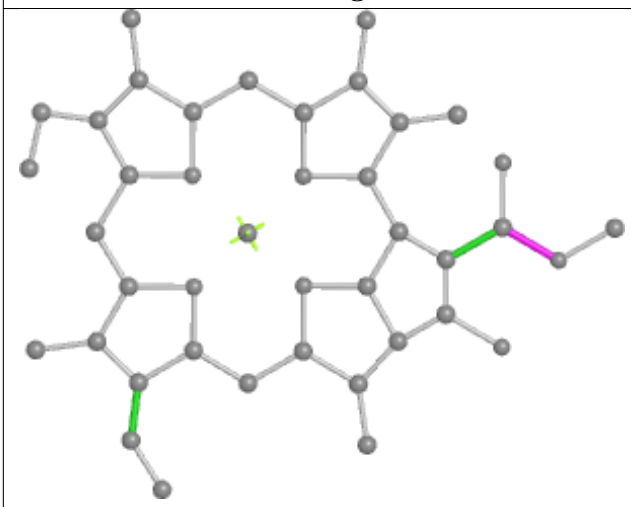
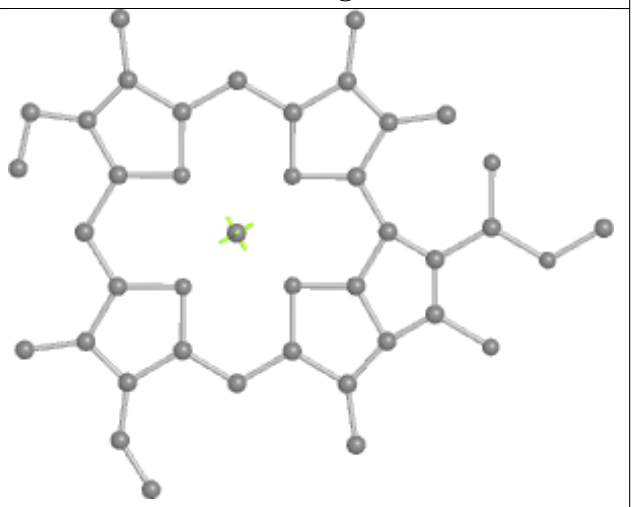
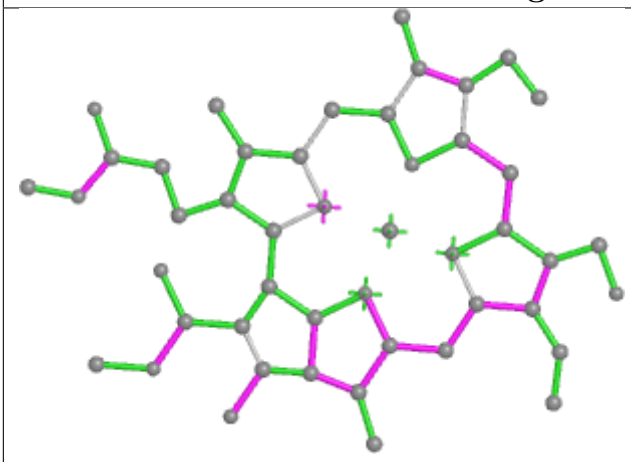


Torsions



Rings

Ligand CHL 5 314



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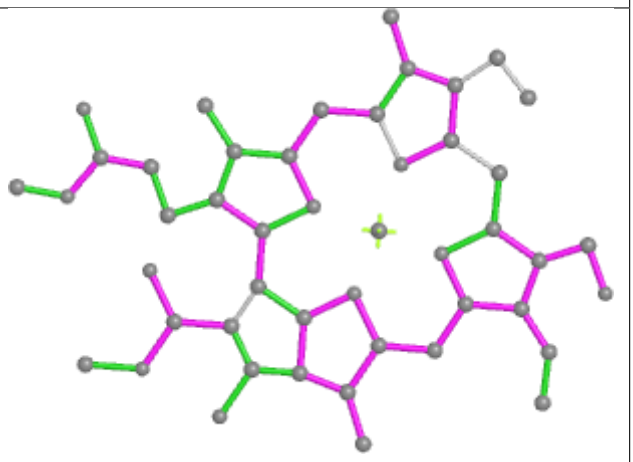
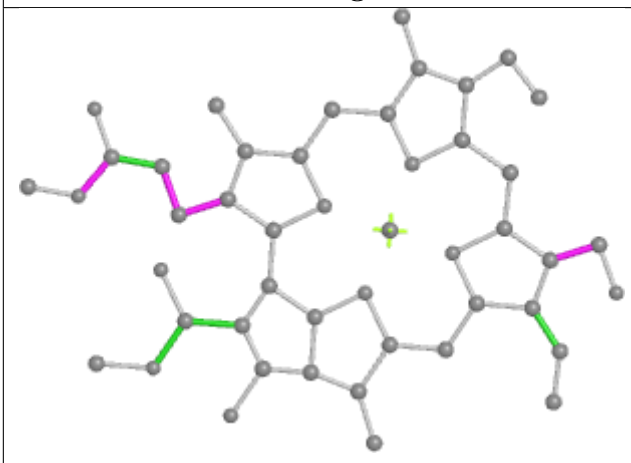


Bond angles



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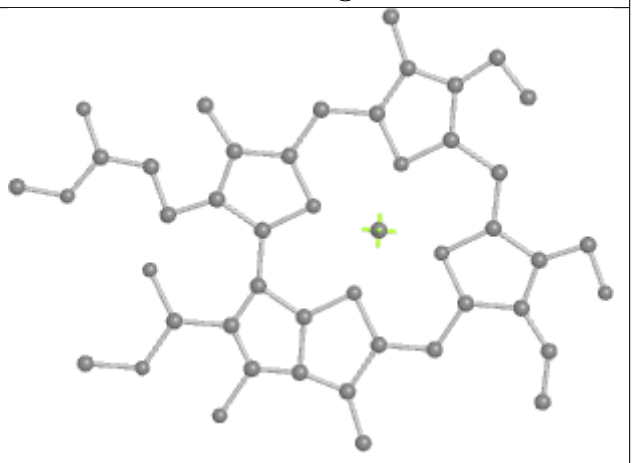
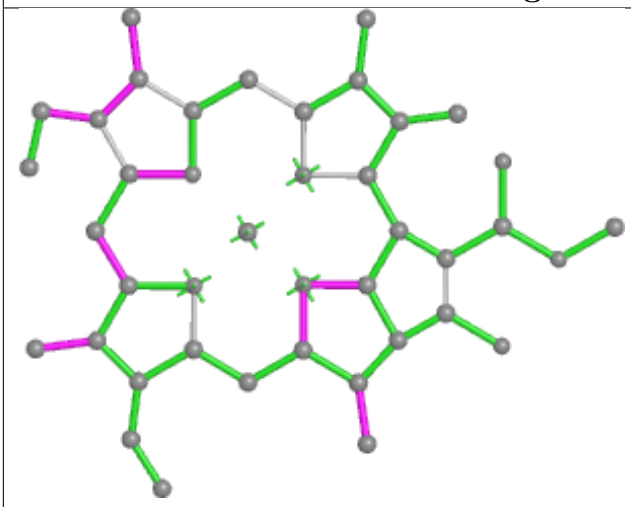


Rings

Ligand CLA A 840



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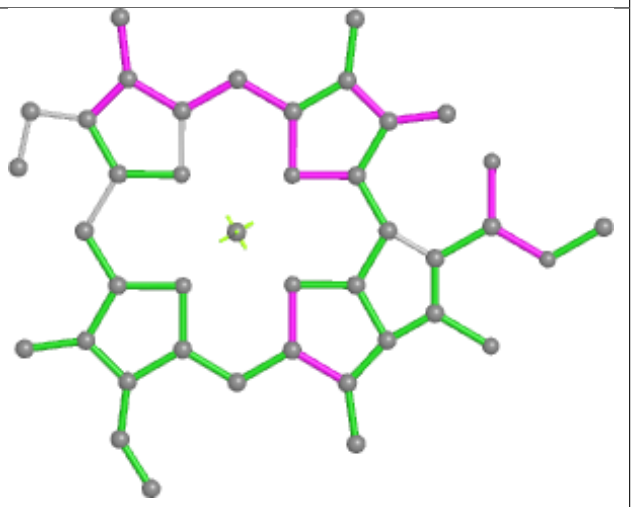
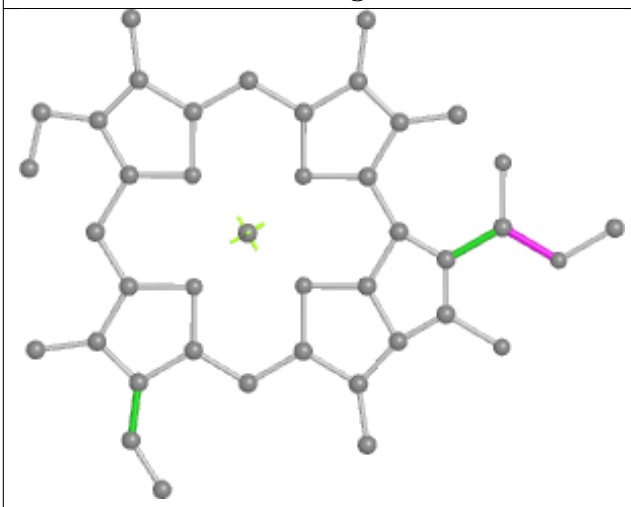


Bond angles



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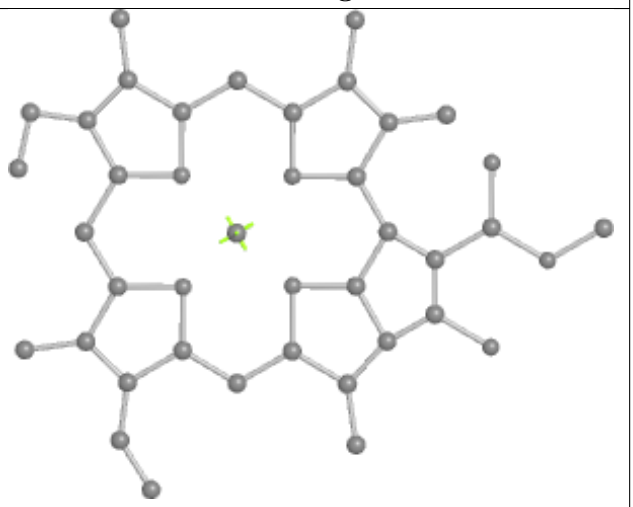
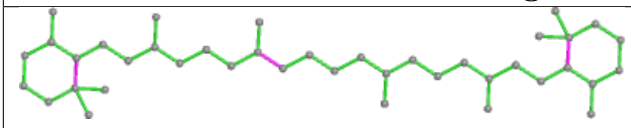


Rings

Ligand BCR B 846



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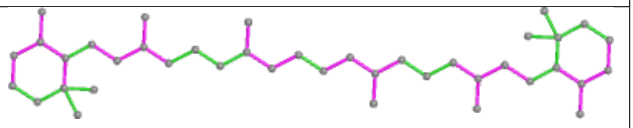
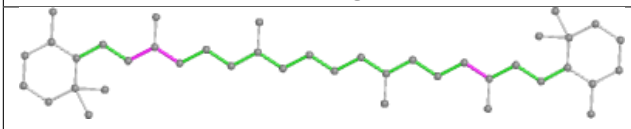


Bond angles



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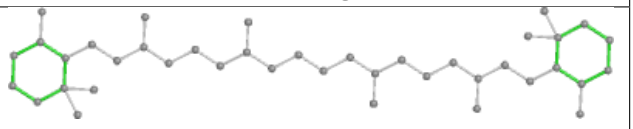
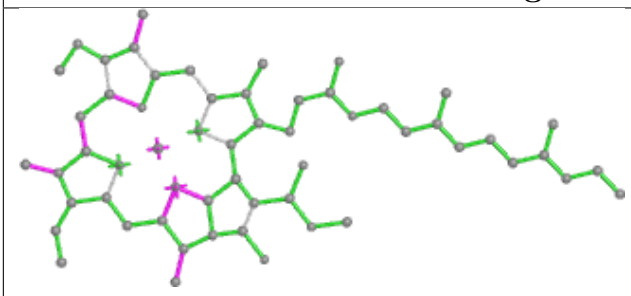
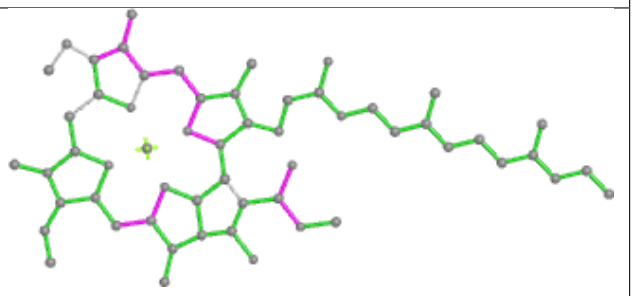


Rings

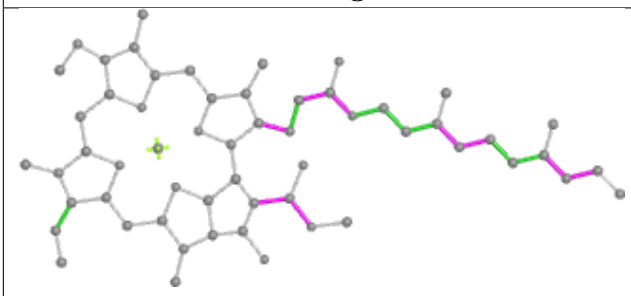
Ligand CLA B 842



Bond lengths



Bond angles



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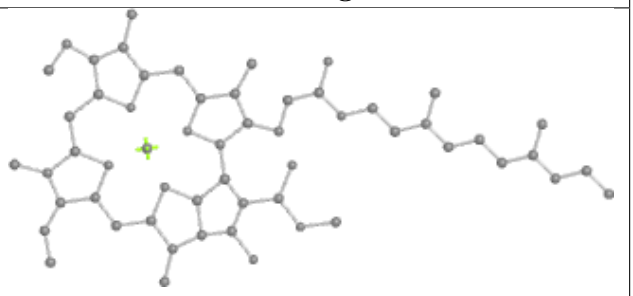
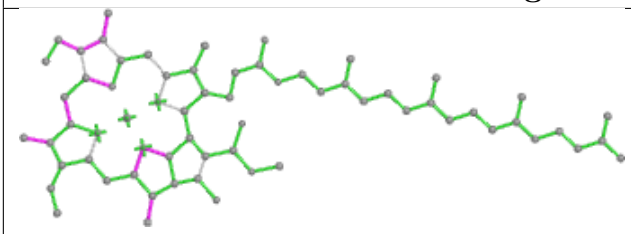


Rings

Ligand CLA B 803



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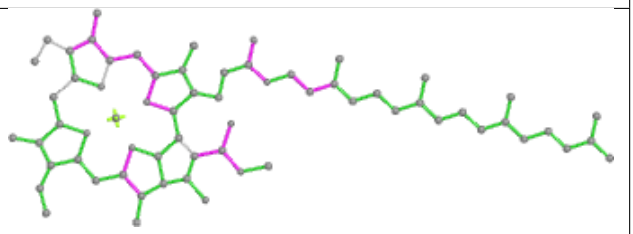
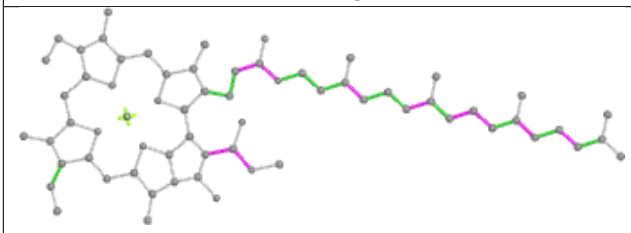


Bond angles



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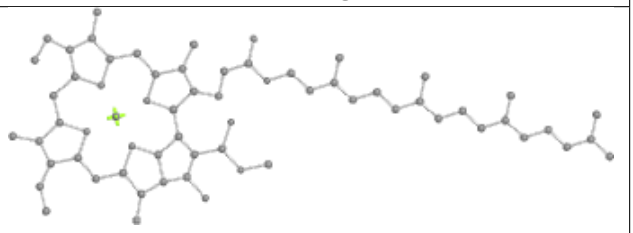
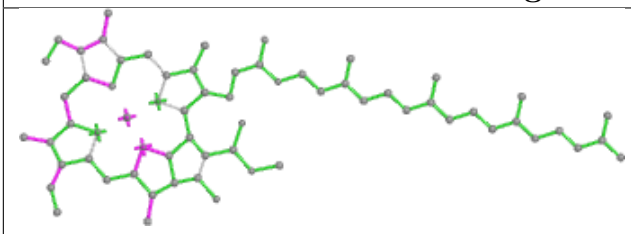


Rings

Ligand CLA B 815



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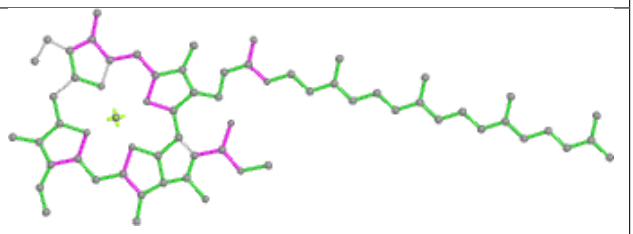
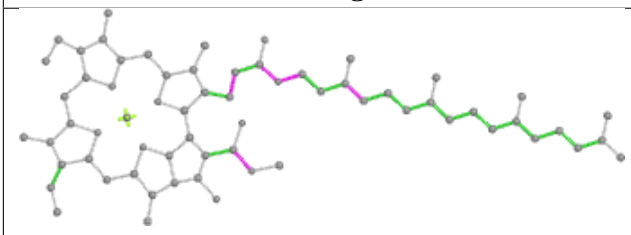


Bond angles



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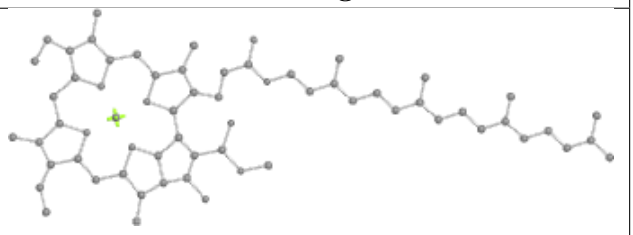
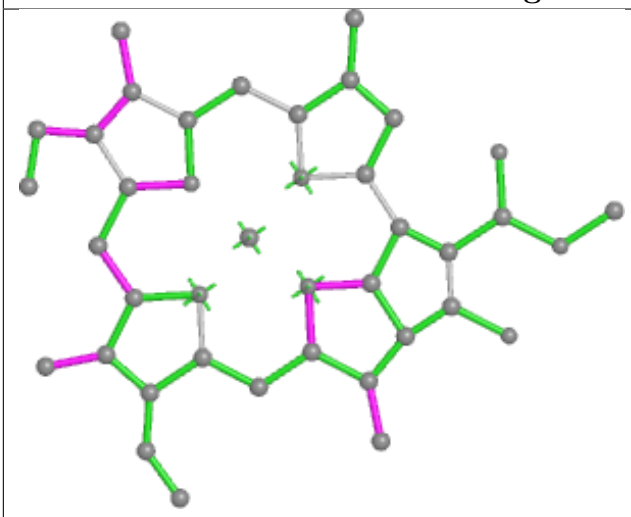


Rings

Ligand CLA A 819



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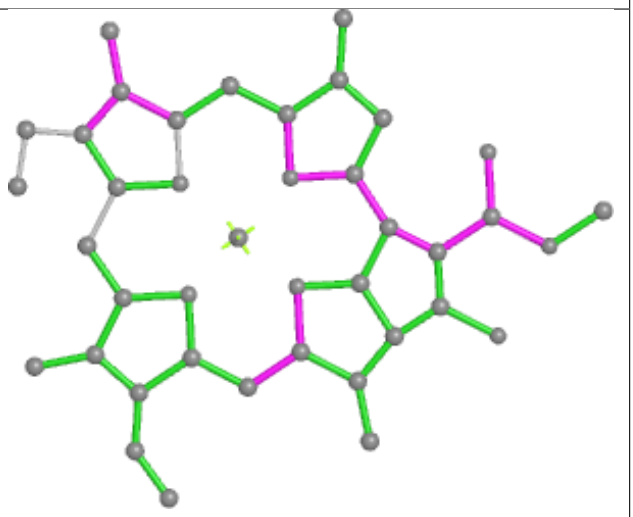
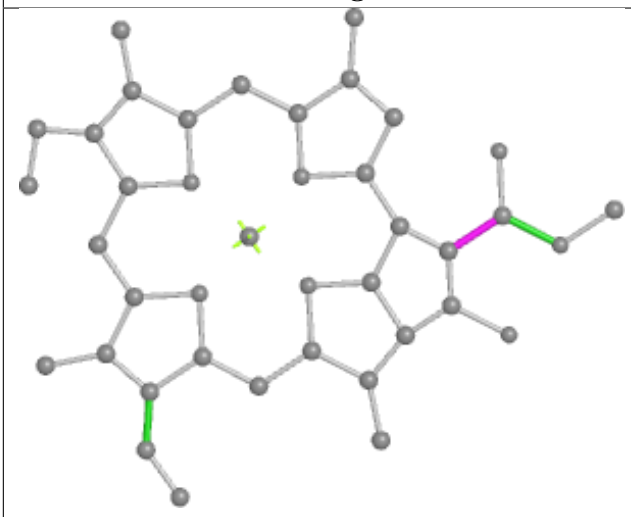


Bond angles



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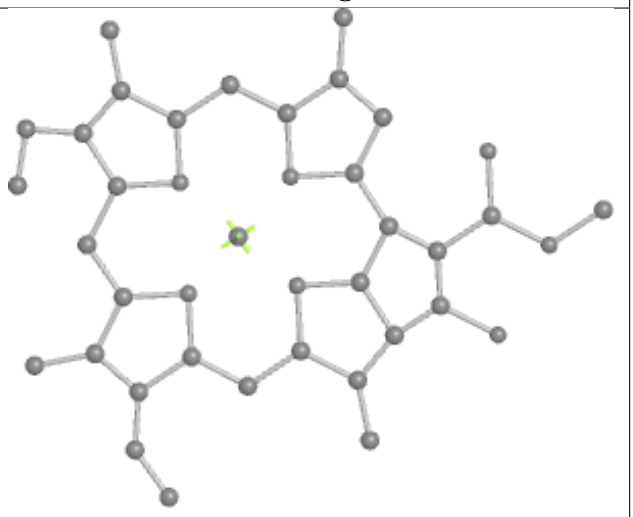
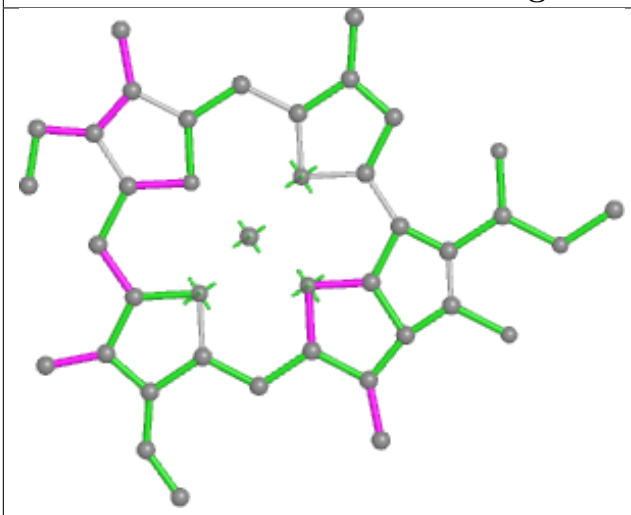


Rings

Ligand CLA 5 313



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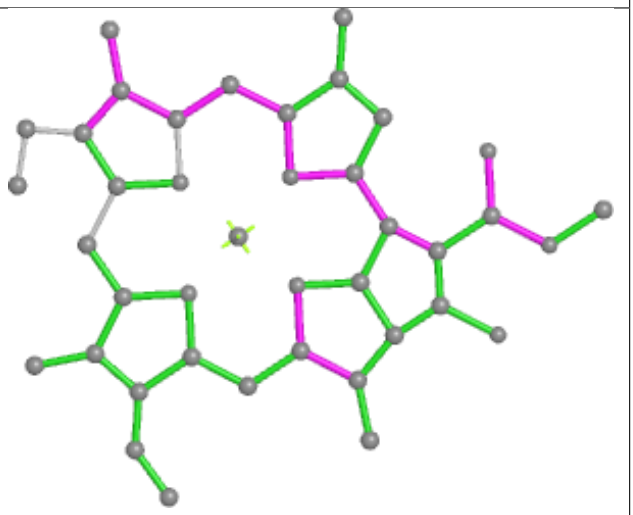
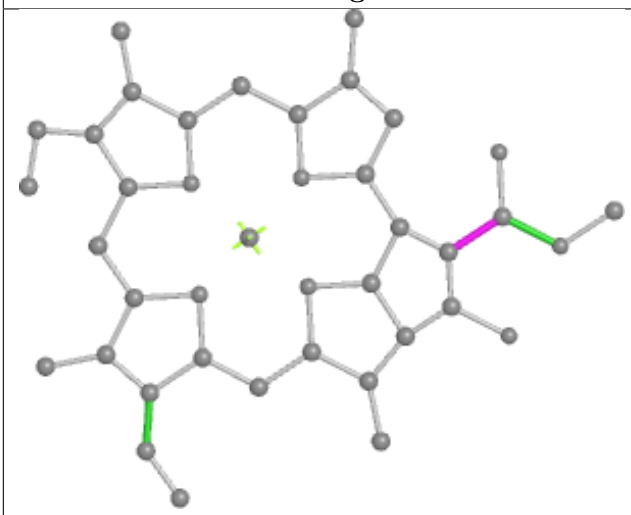


Bond angles



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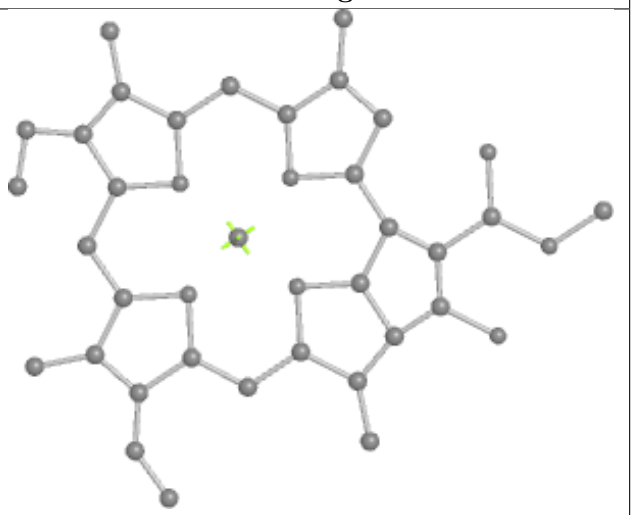
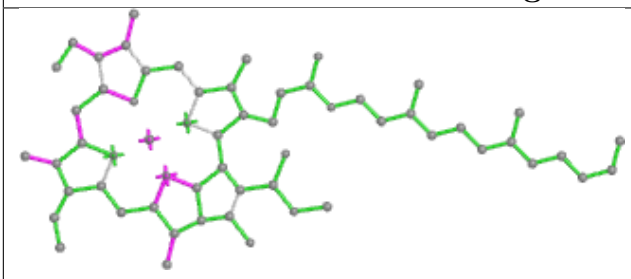
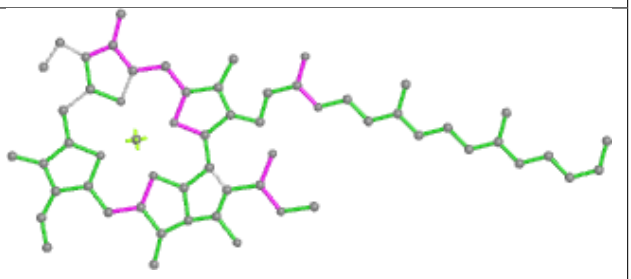


Rings

Ligand CLA A 825	
	
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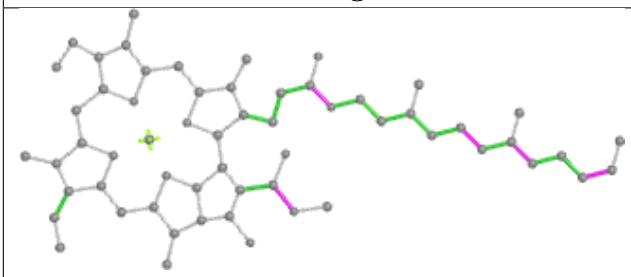
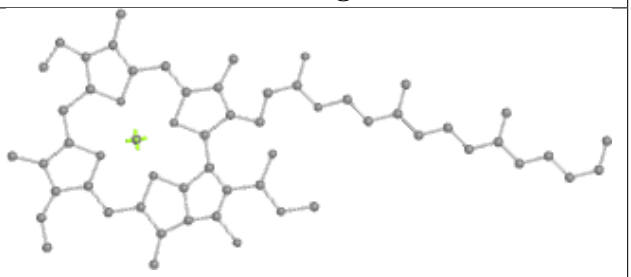
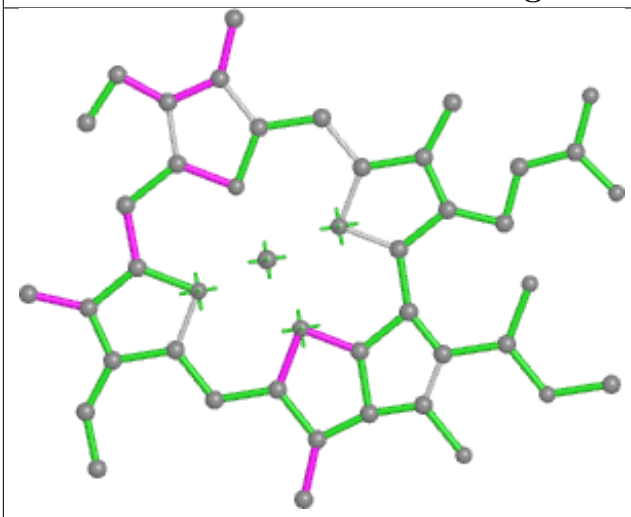
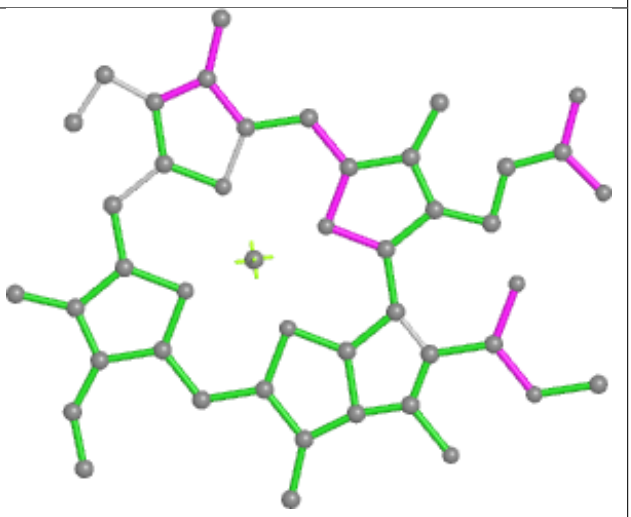
	
Torsions	**Rings**

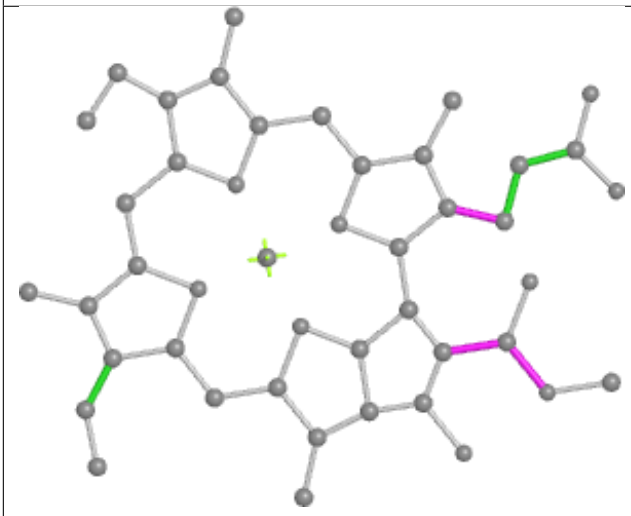
Ligand CLA B 824



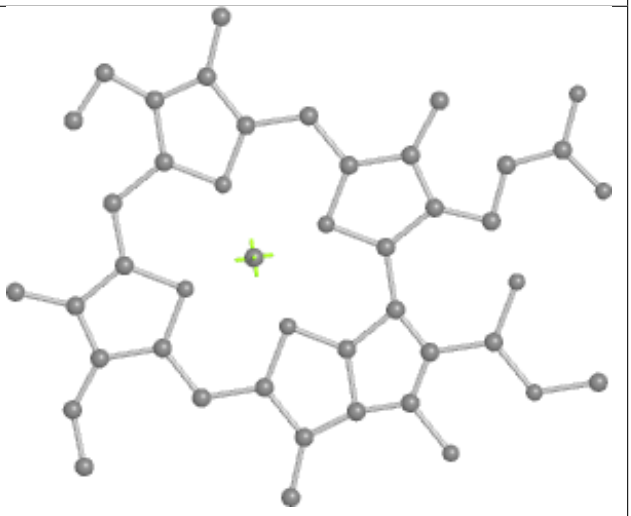
Bond lengths



Bond angles

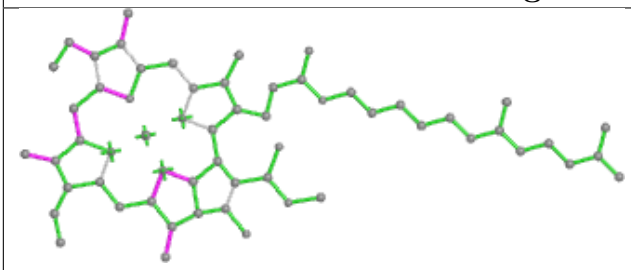


Torsions



Rings

Ligand CLA A 816



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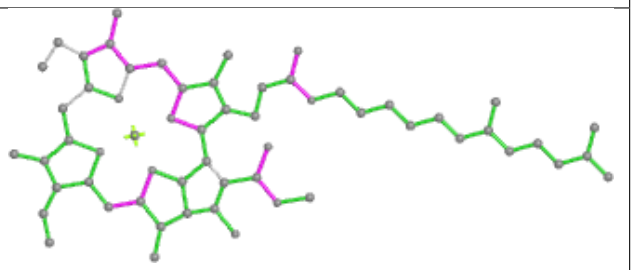
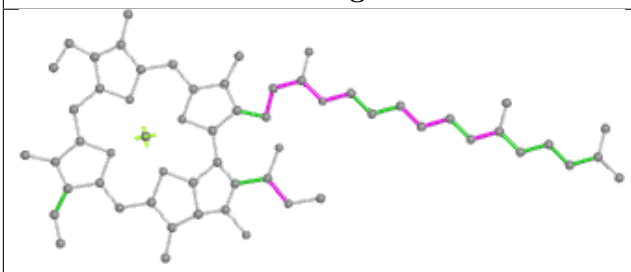


Bond angles



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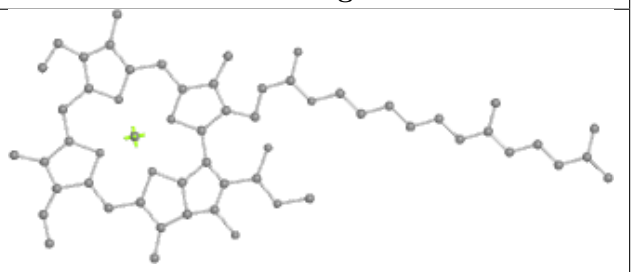
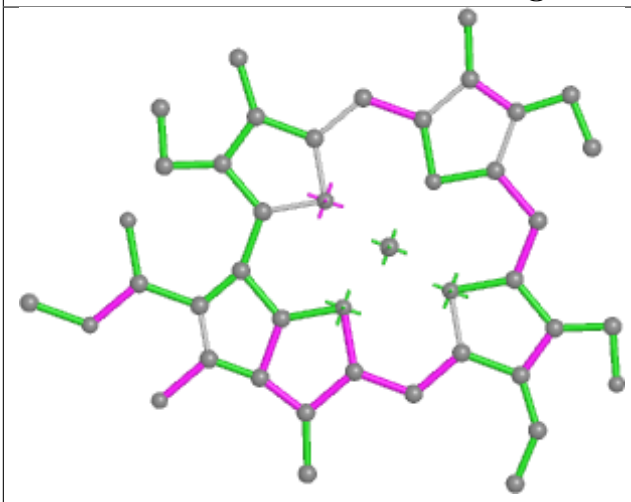
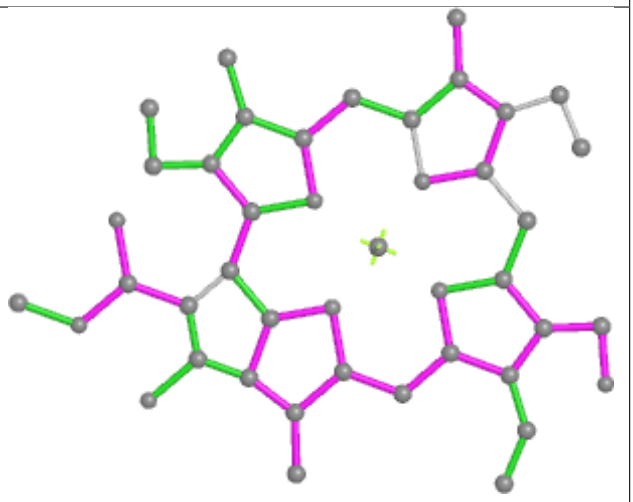


Rings

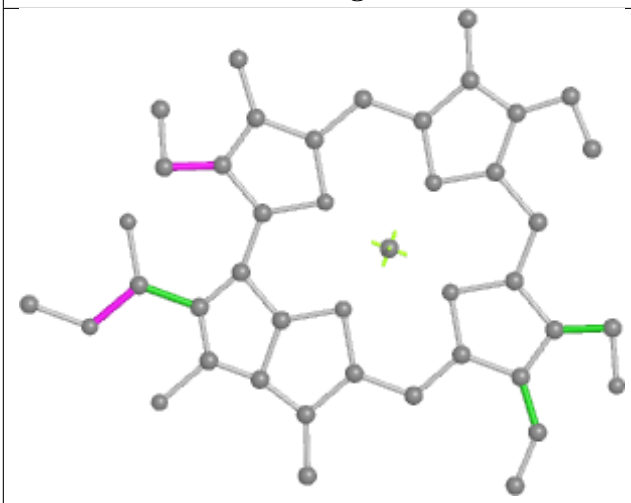
Ligand CHL 3 315



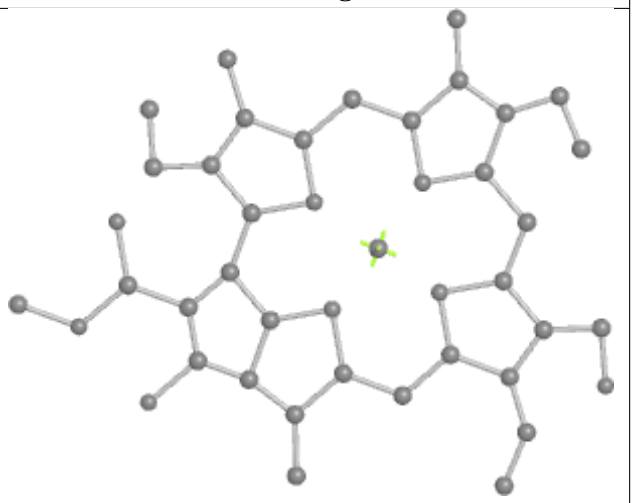
Bond lengths



Bond angles

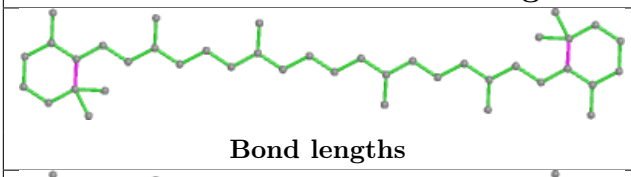


Torsions

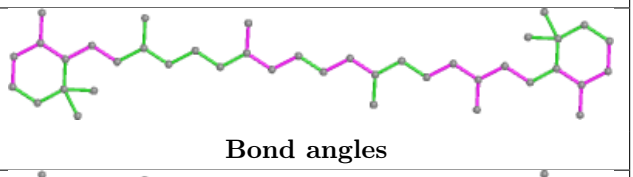


Rings

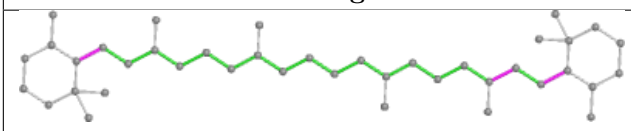
Ligand BCR A 848



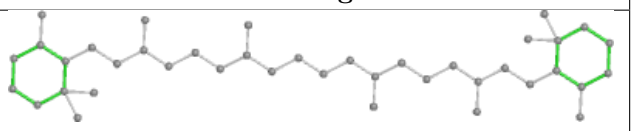
Bond lengths



Bond angles

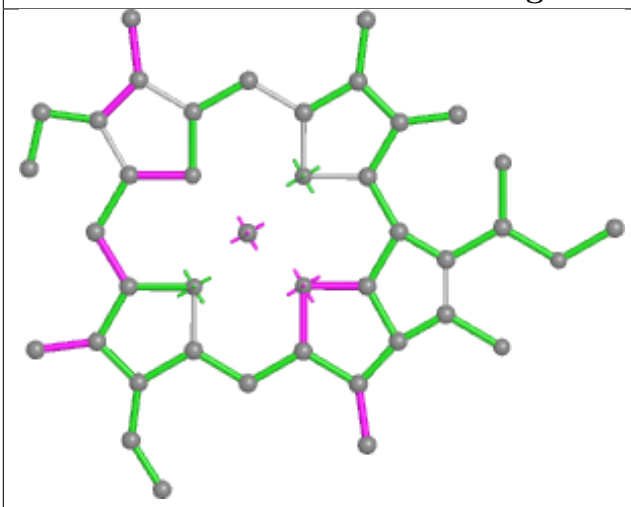


Torsions



Rings

Ligand CLA F 803



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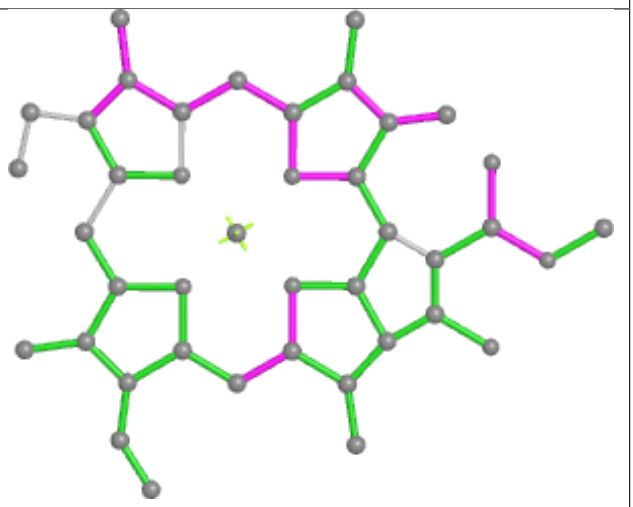
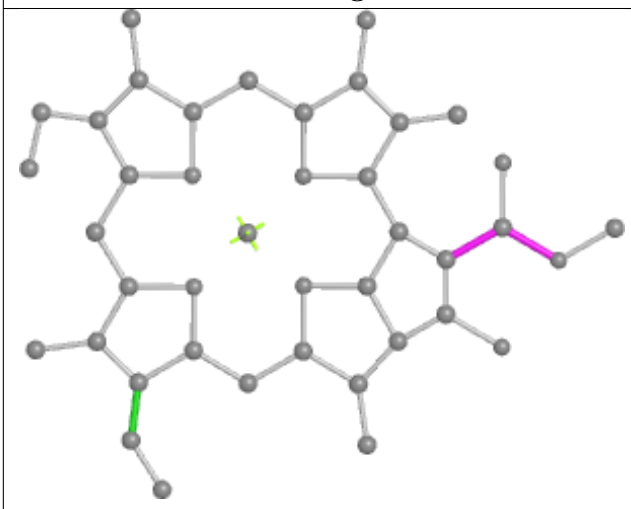


Bond angles



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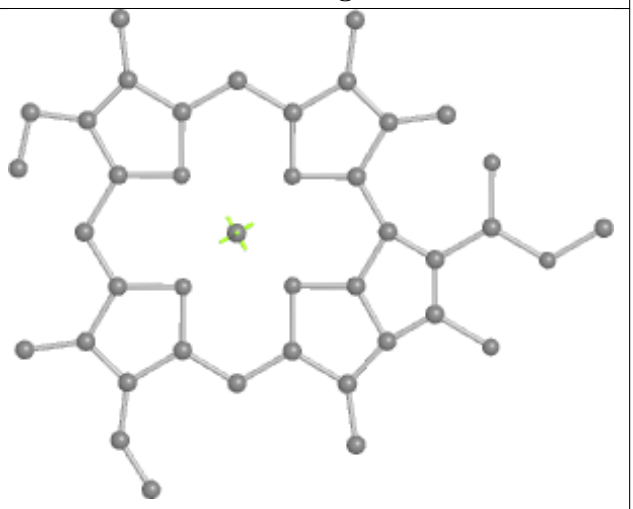
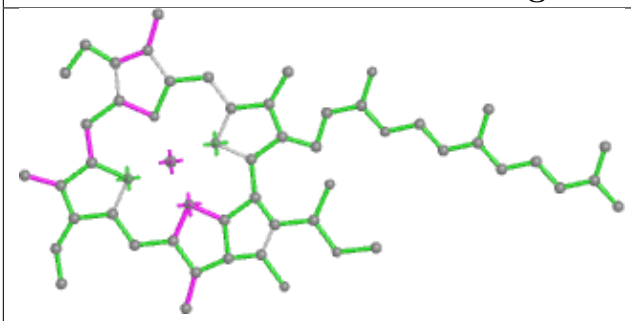


Rings

Ligand CLA 3 308



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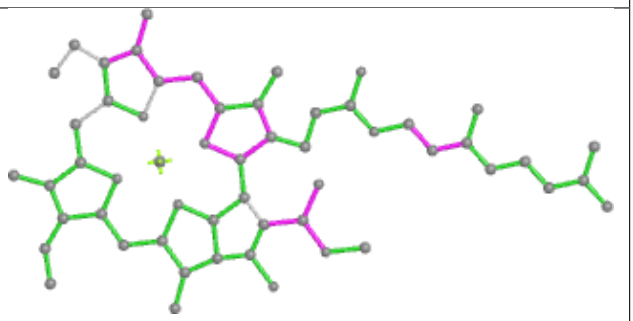
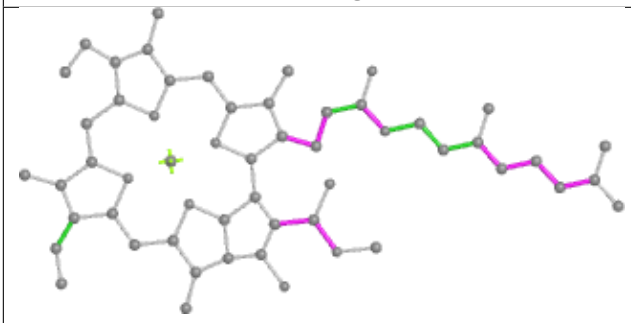


Bond angles



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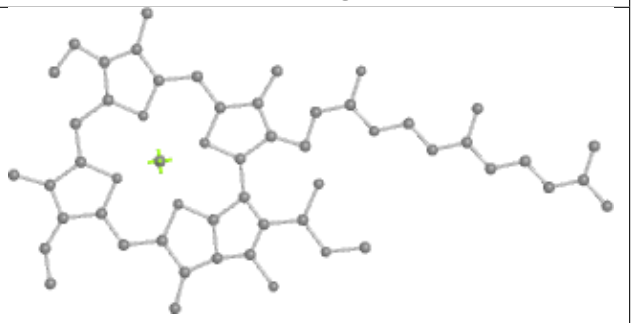
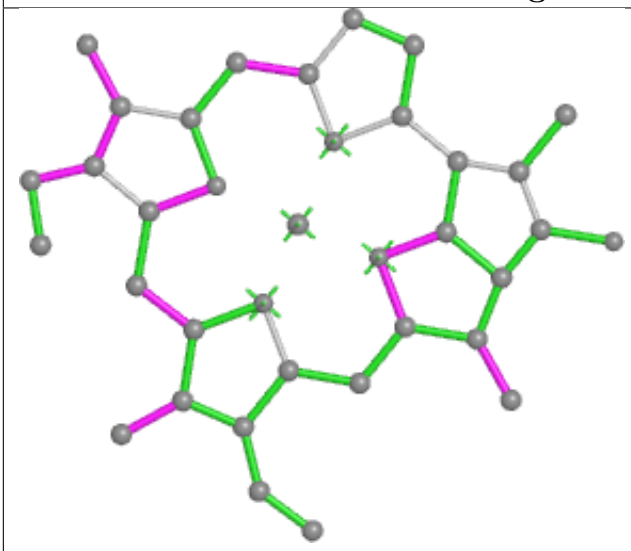


Rings

Ligand CLA 2 504



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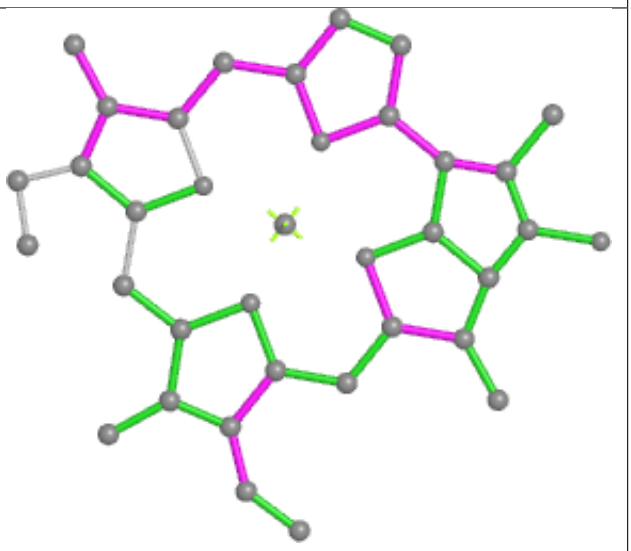
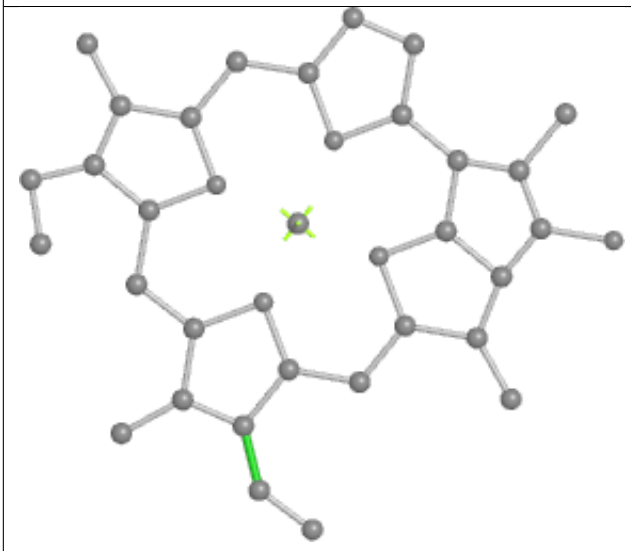


Bond angles



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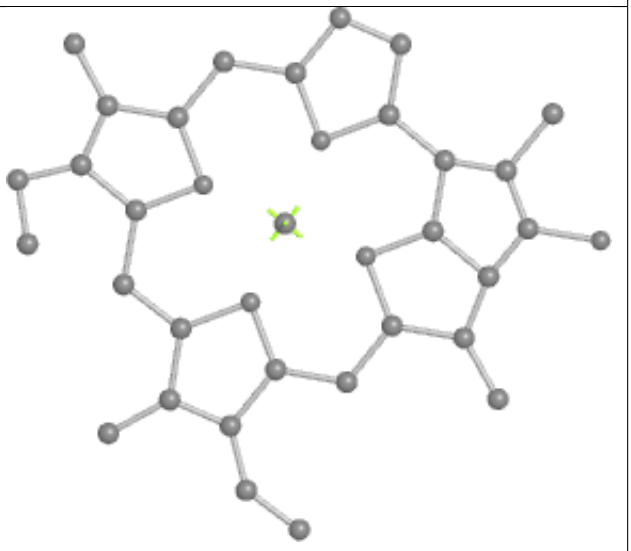
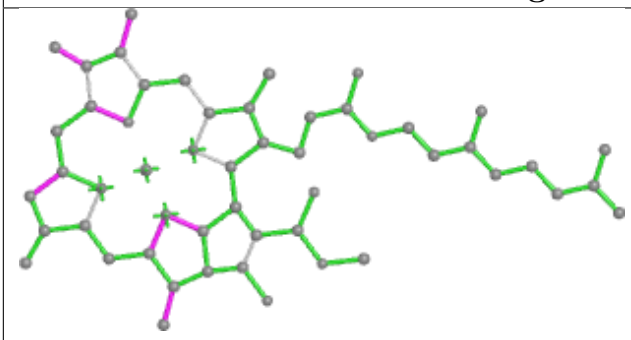


Rings

Ligand CLA 3 306



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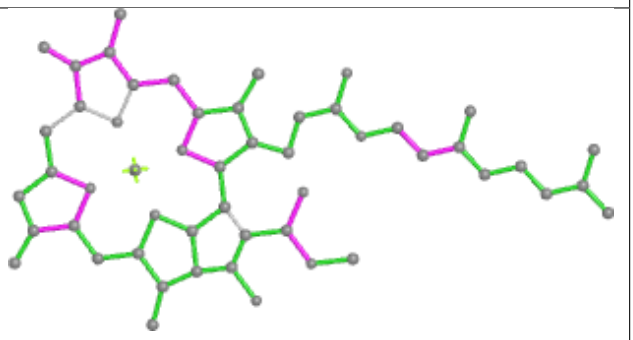
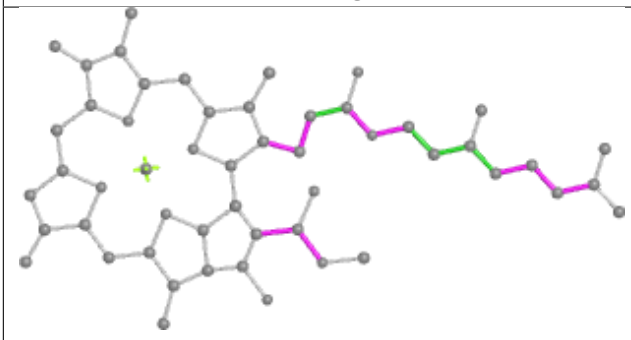


Bond angles



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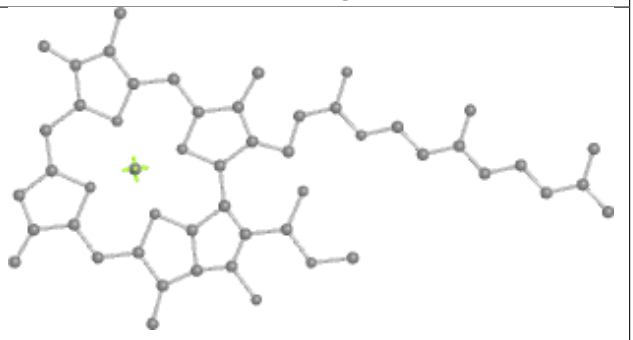
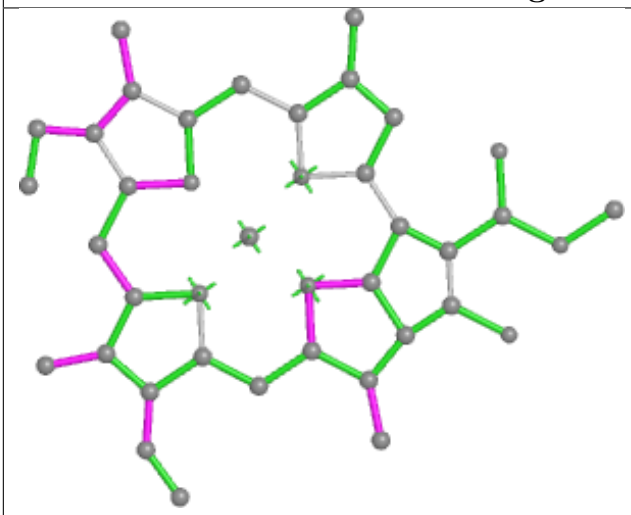


Rings

Ligand CLA 2 511



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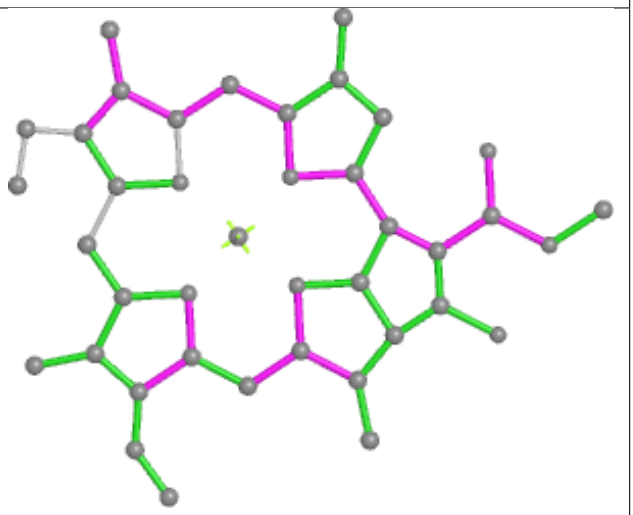
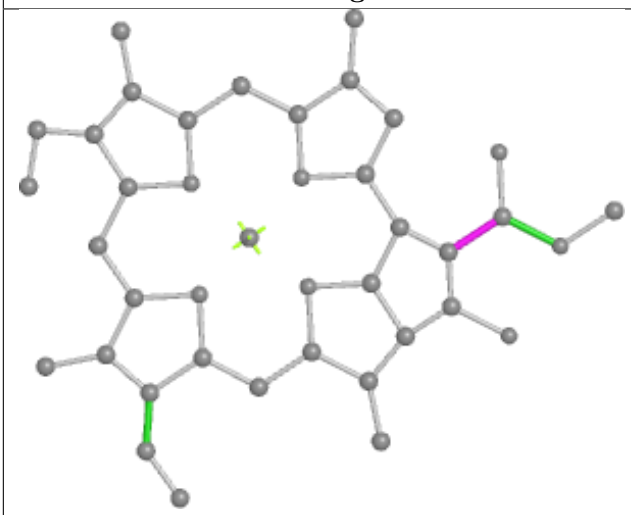
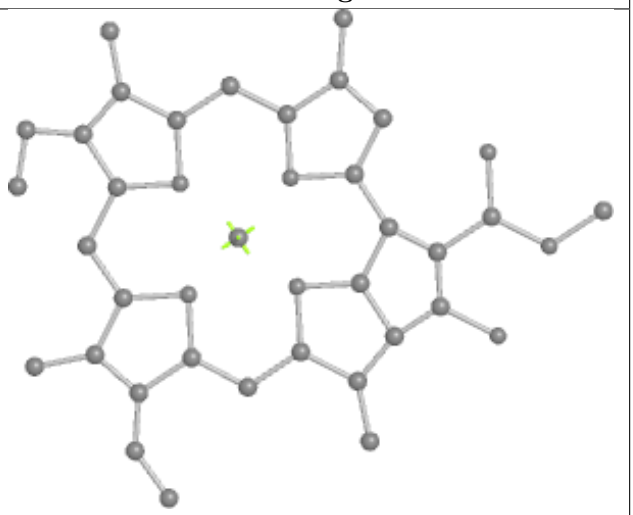


Bond angles

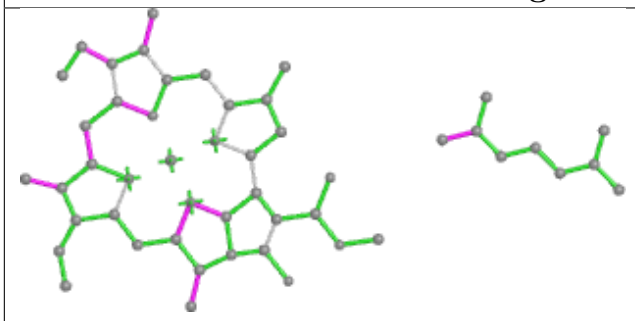


Torsions



Rings

Ligand CLA 2 507



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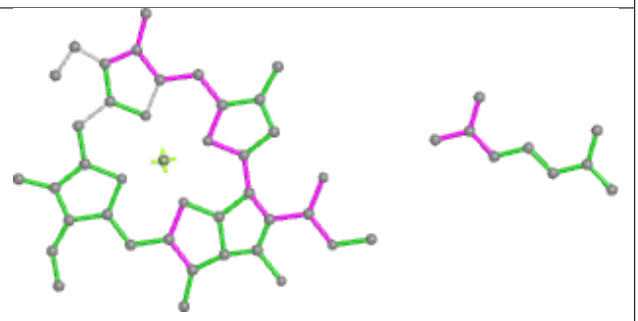
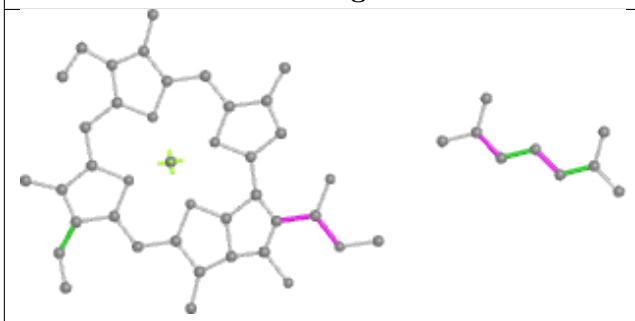


Bond angles



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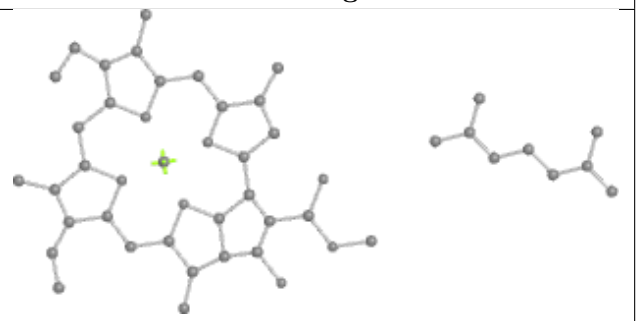
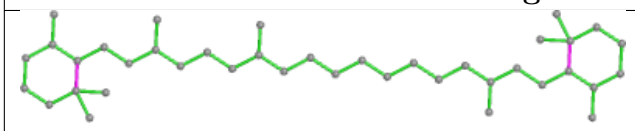


Rings

Ligand BCR A 849



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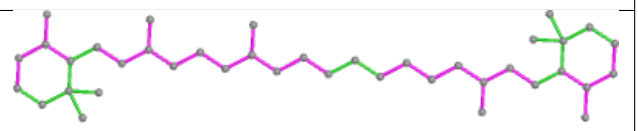
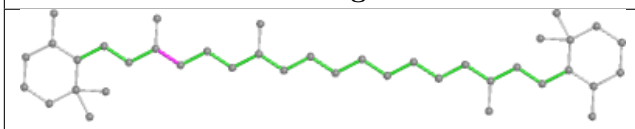


Bond angles



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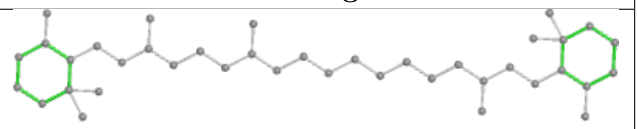
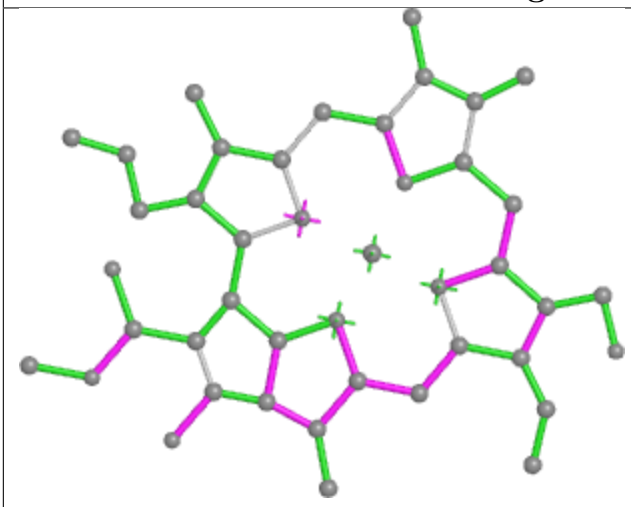


Rings

Ligand CHL 2 516



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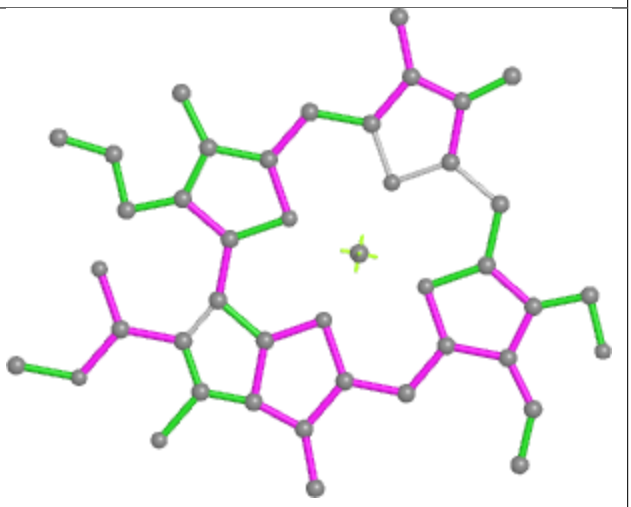
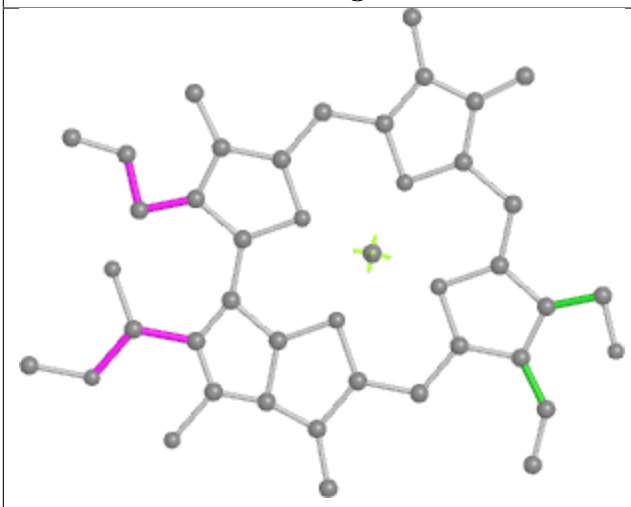


Bond angles



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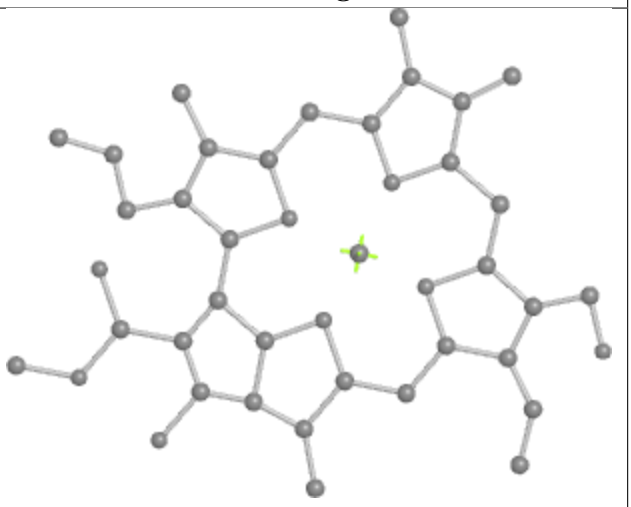
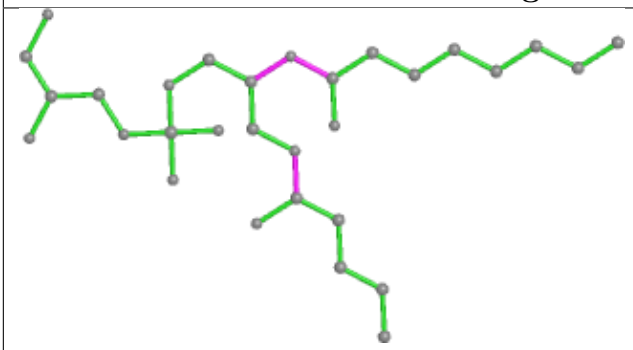


Rings

Ligand LHG A 844



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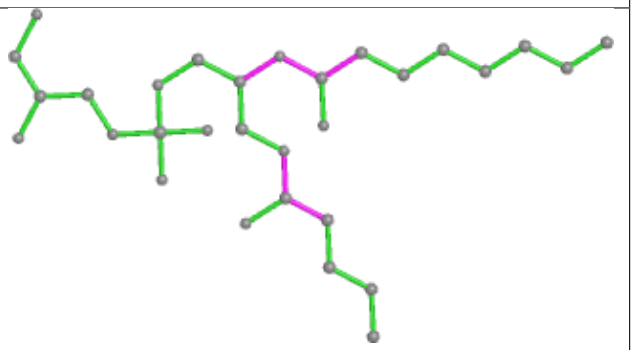
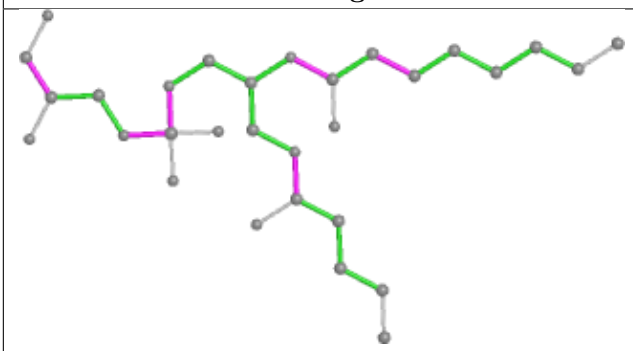


Bond angles



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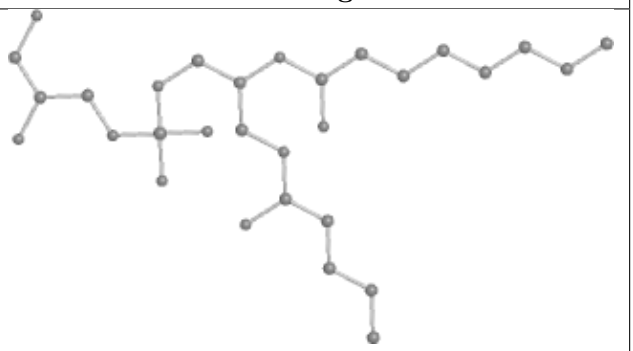
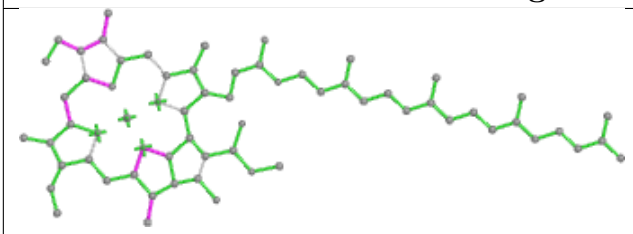


Rings

Ligand CLA 5 307



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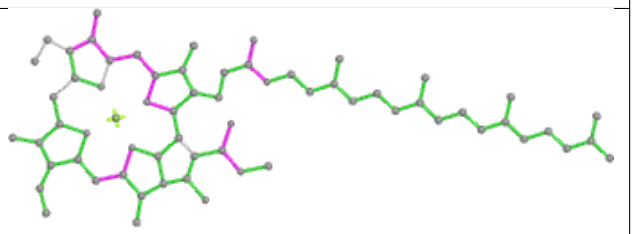
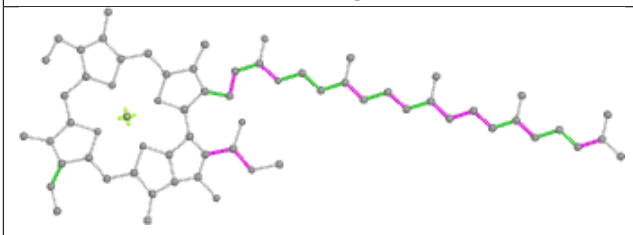


Bond angles



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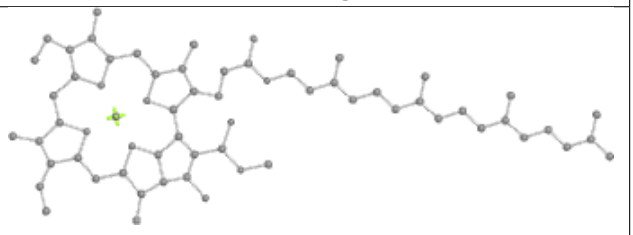
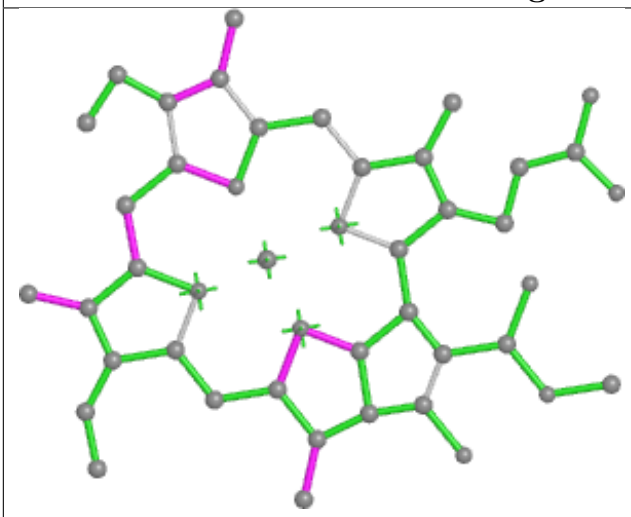


Rings

Ligand CLA 5 309



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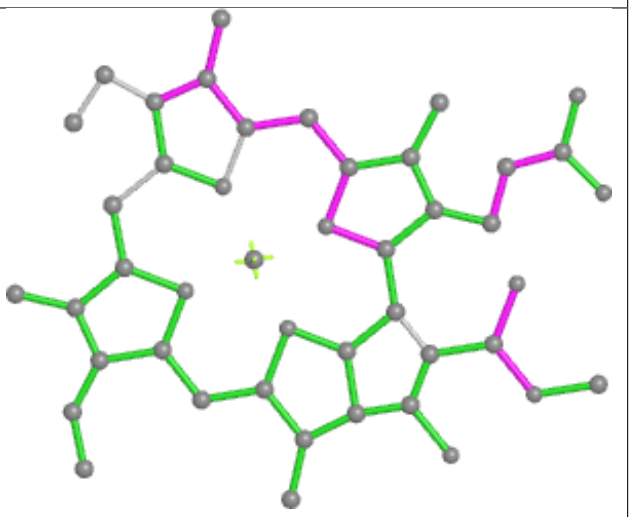
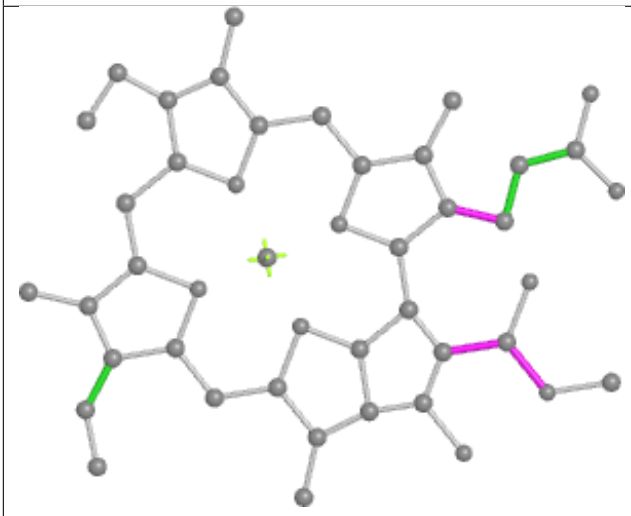


Bond angles



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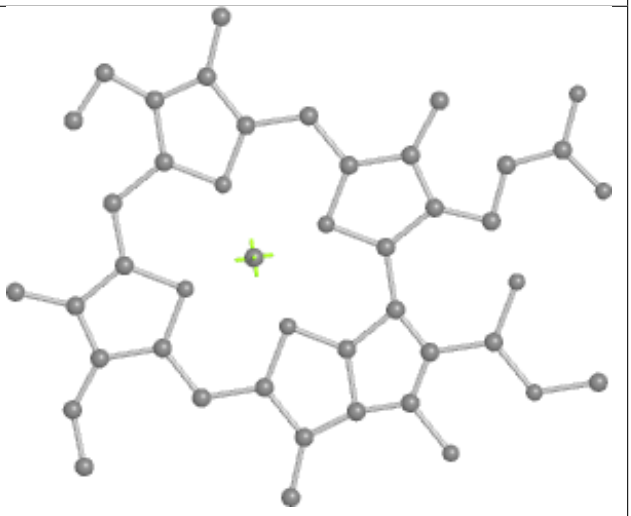
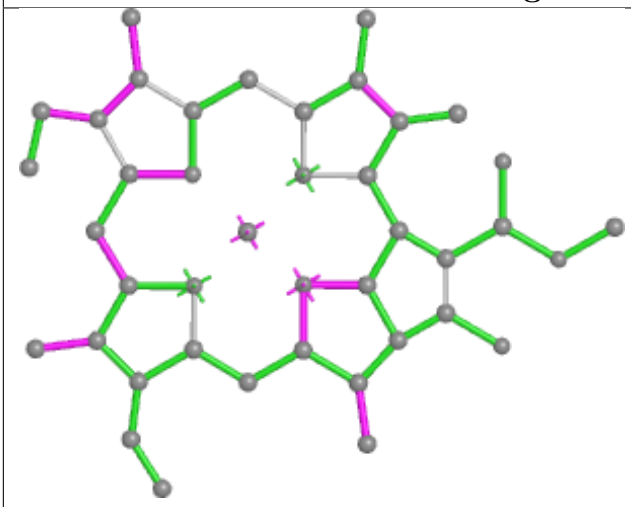


Rings

Ligand CLA A 837



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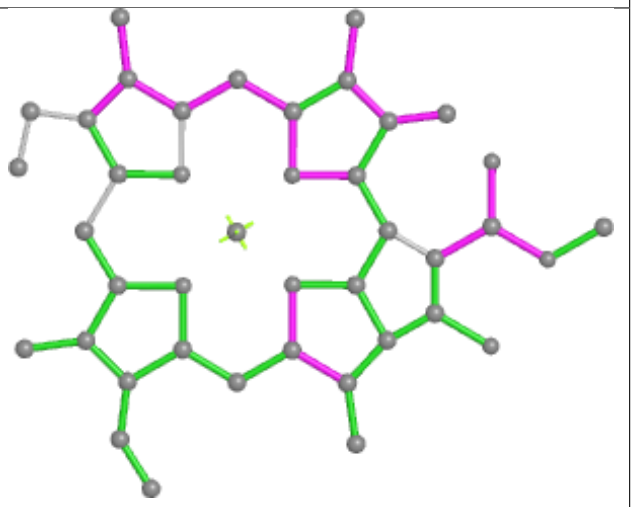
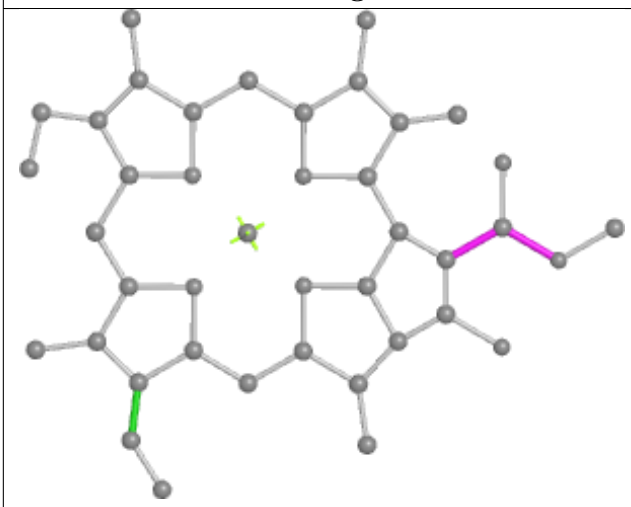


Bond angles



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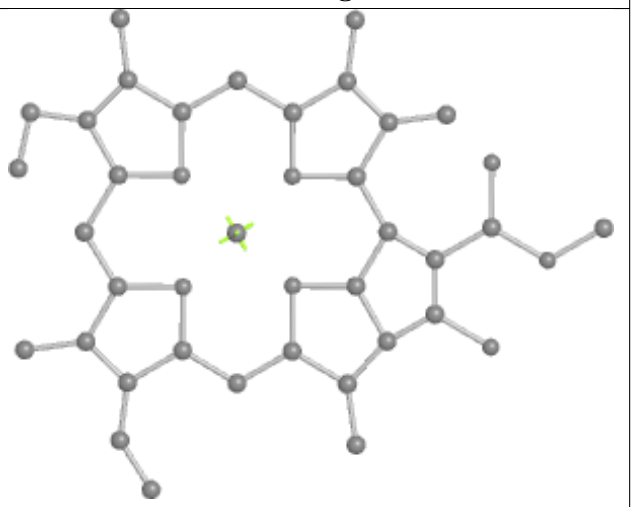
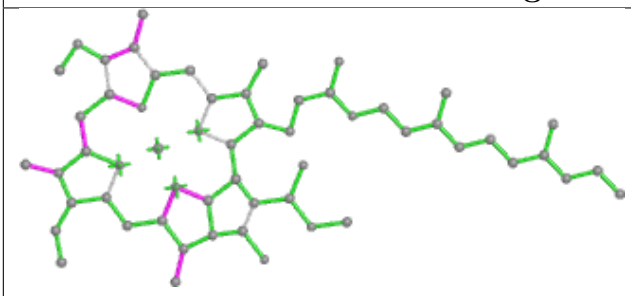
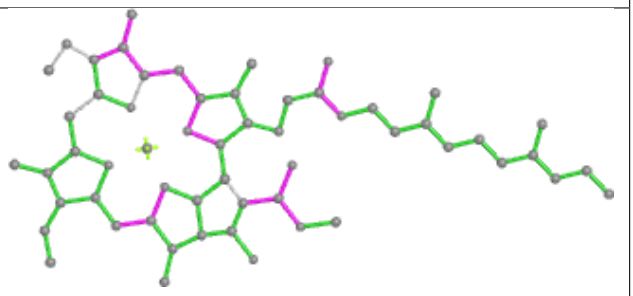


Rings

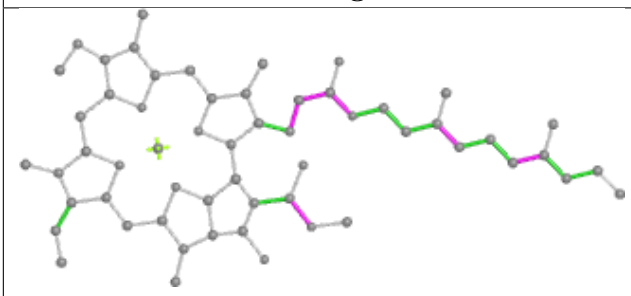
Ligand CLA A 820



Bond lengths



Bond angles



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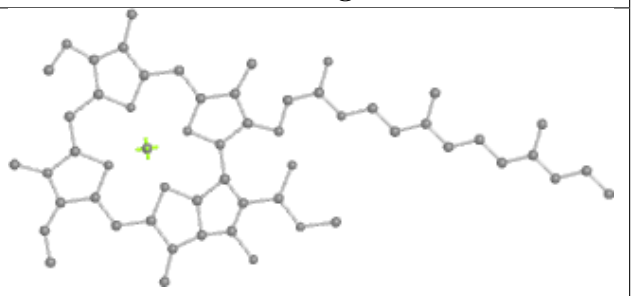
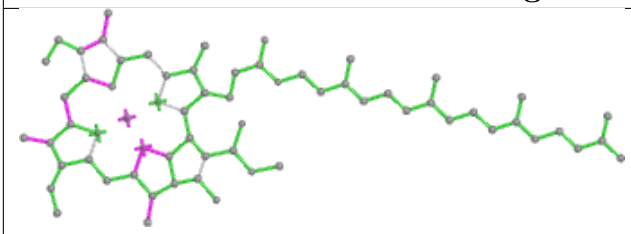
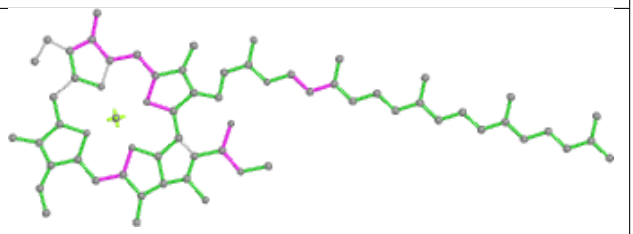


Rings

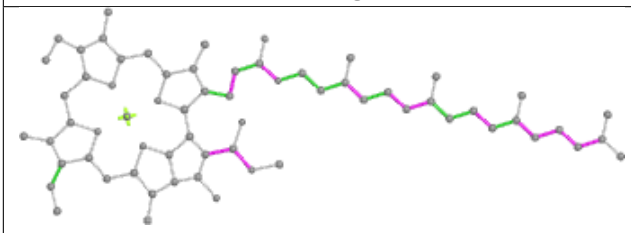
Ligand CLA A 806



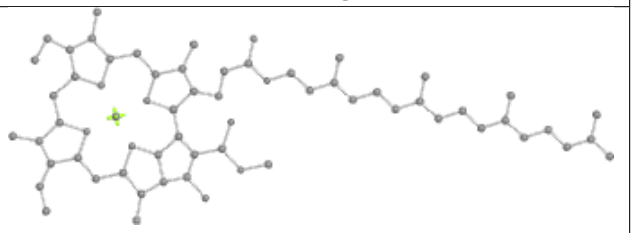
Bond lengths



Bond angles

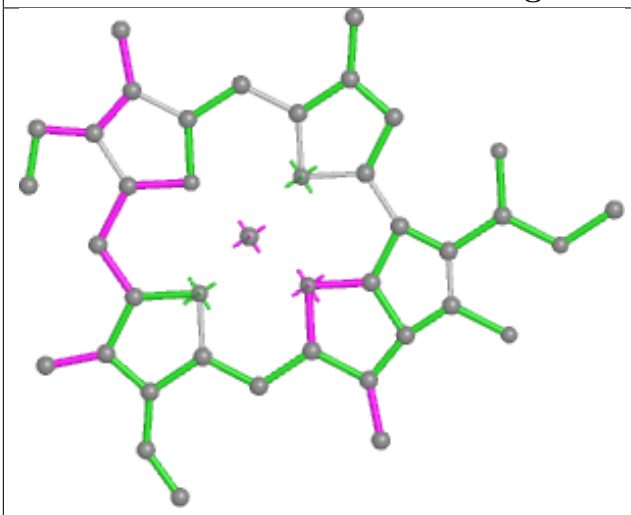


Torsions

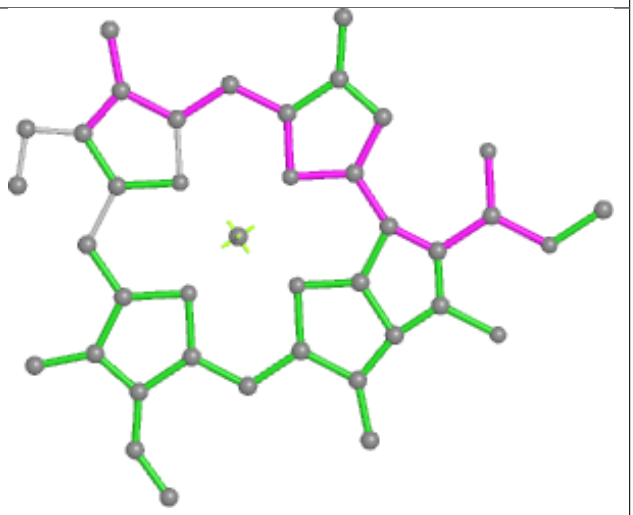


Rings

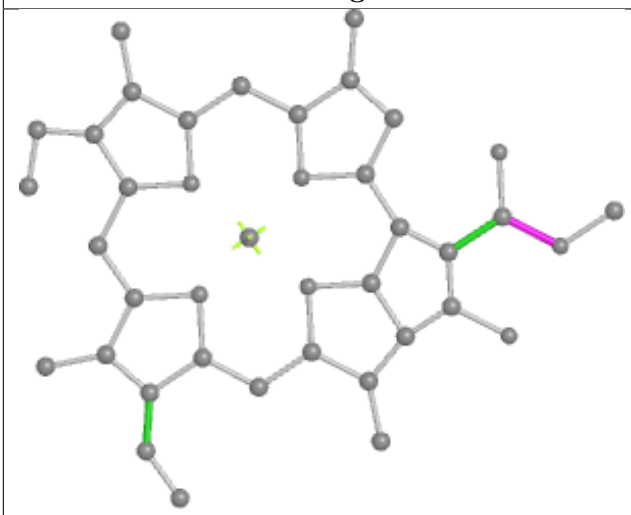
Ligand CLA B 829



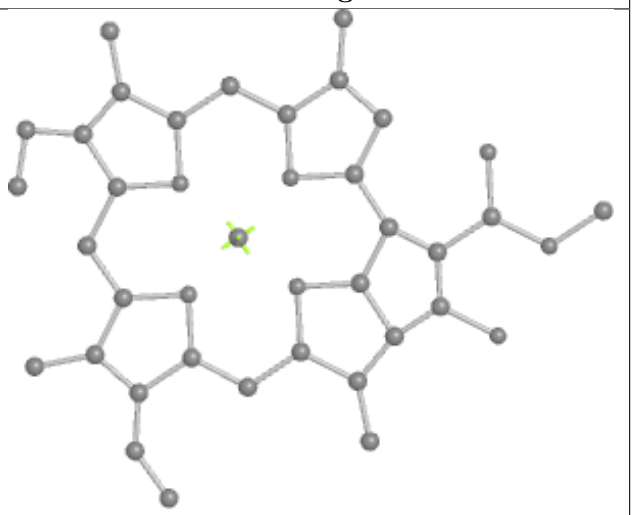
Bond lengths



Bond angles

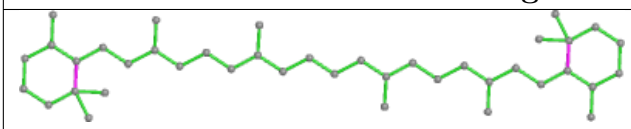


Torsions

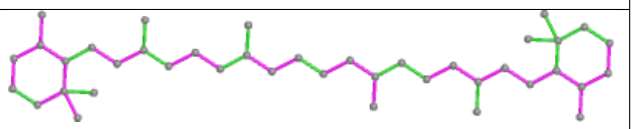


Rings

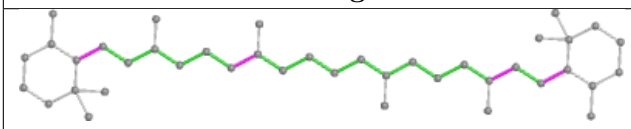
Ligand BCR K 204



Bond lengths



Bond angles



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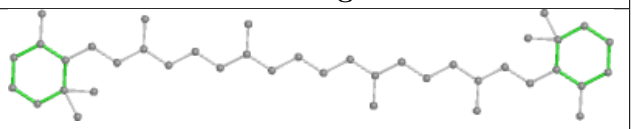
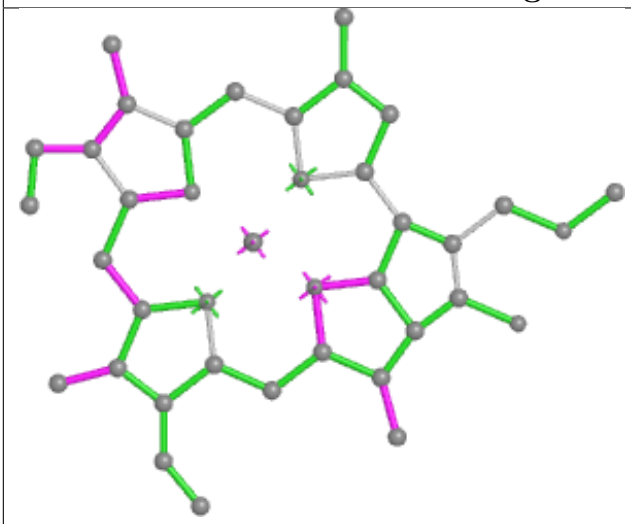
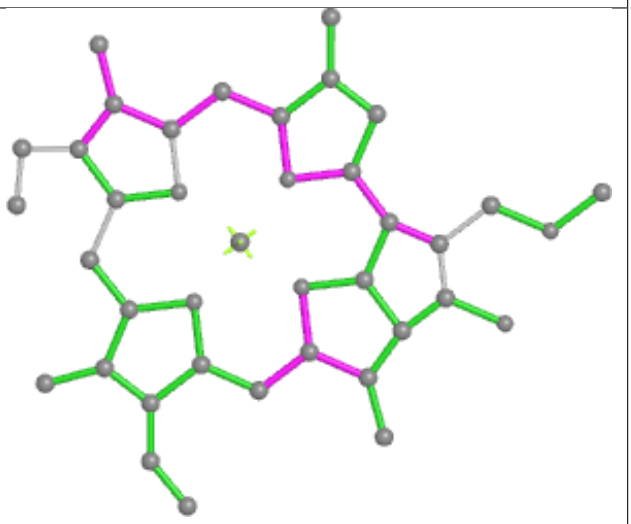


Rings

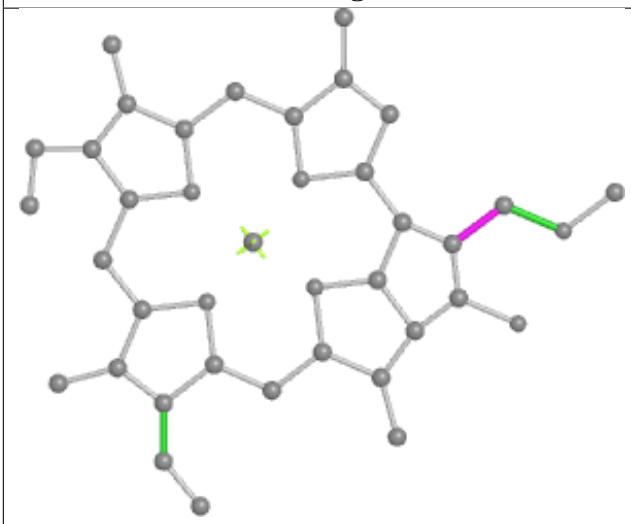
Ligand CLA A 807



Bond lengths



Bond angles



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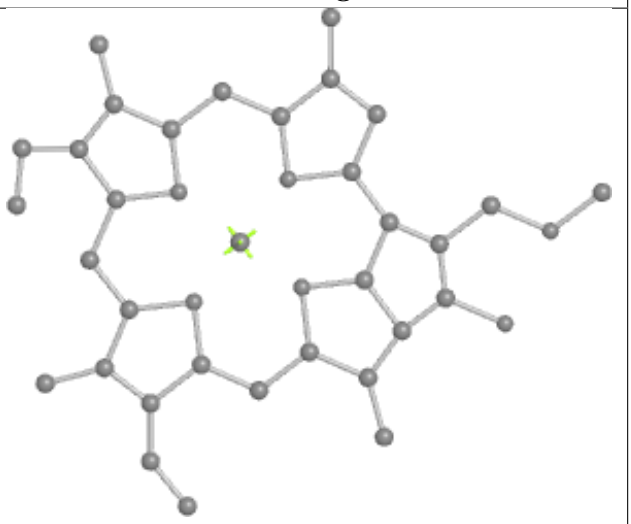
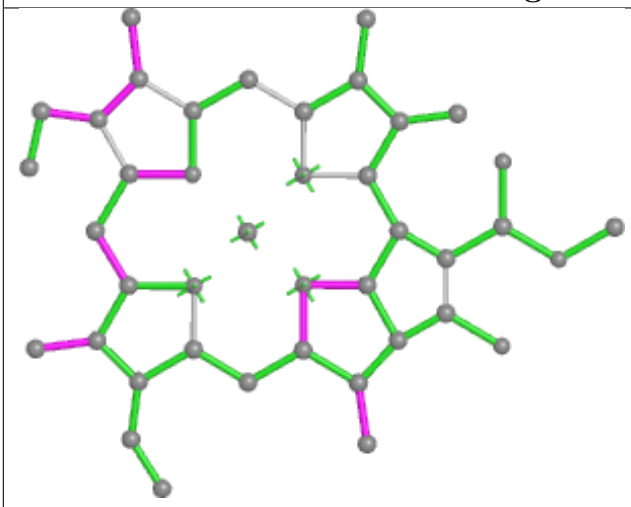
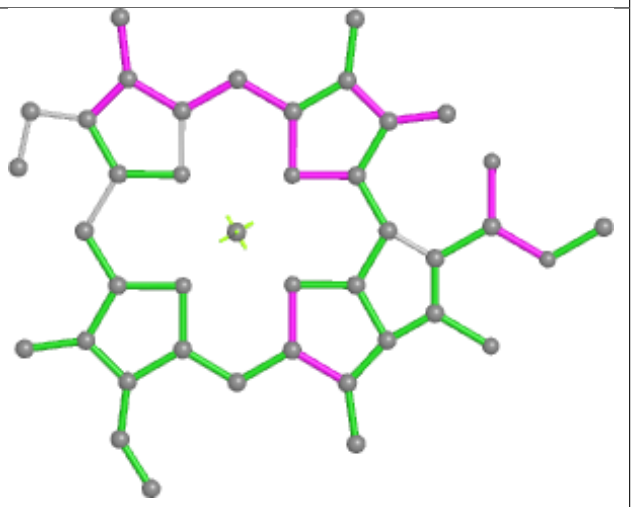


Rings

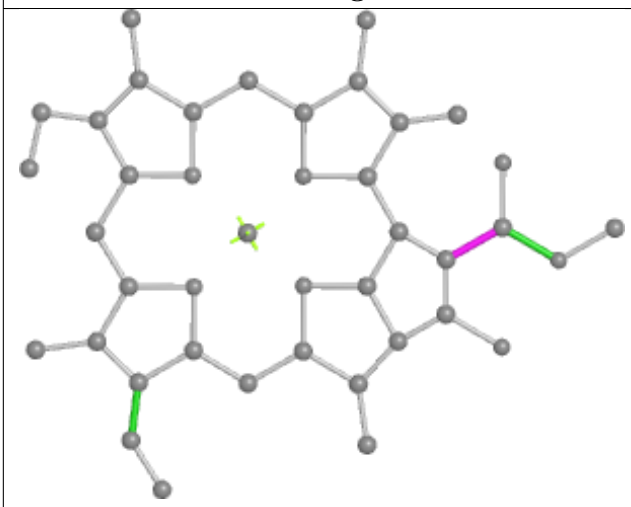
Ligand CLA B 840



Bond lengths



Bond angles



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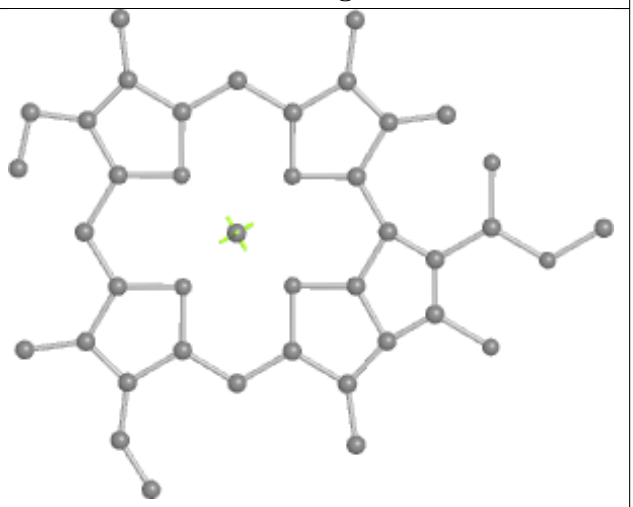
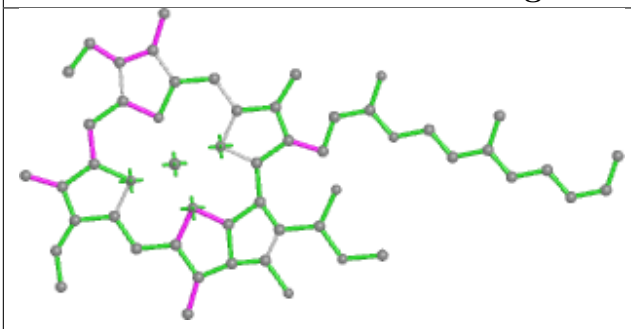


Rings

Ligand CLA B 841



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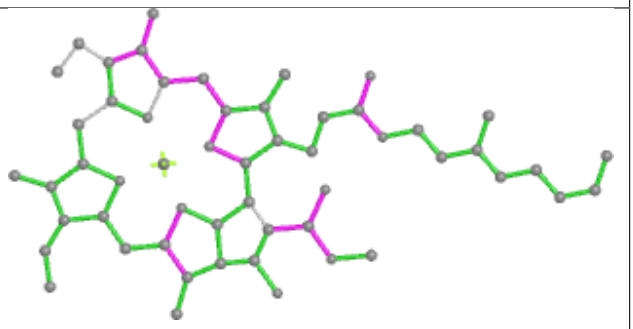
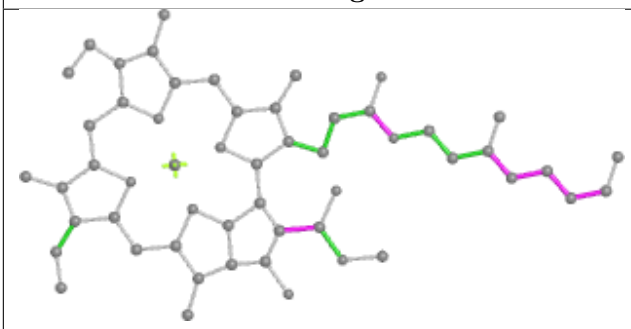


Bond angles



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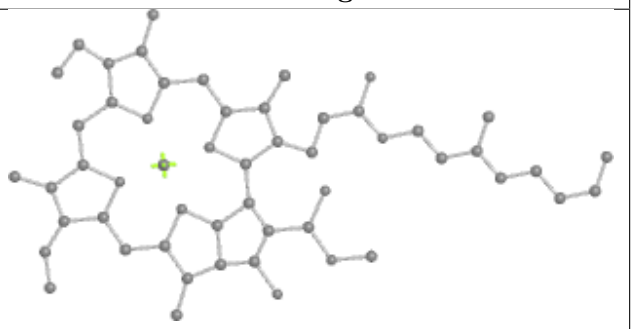
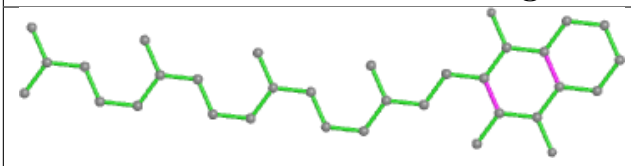


Rings

Ligand PQN A 841



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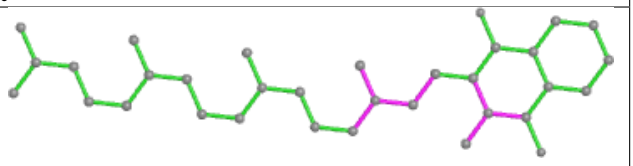
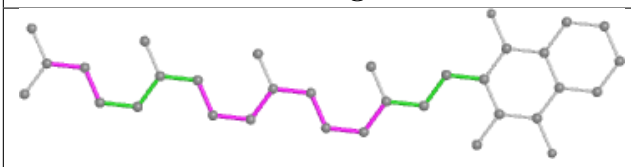


Bond angles



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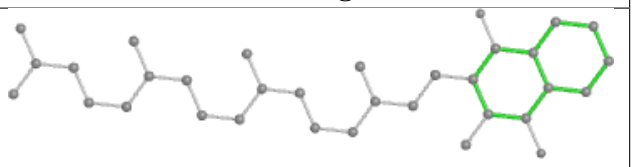
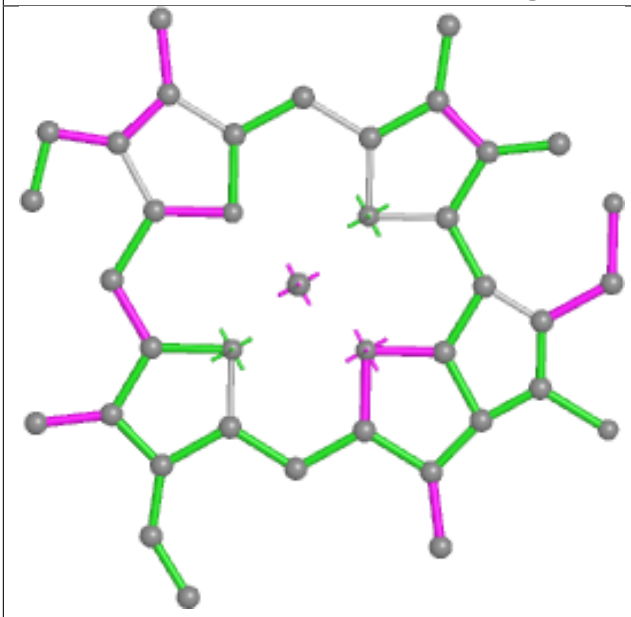


Rings

Ligand CLA A 817



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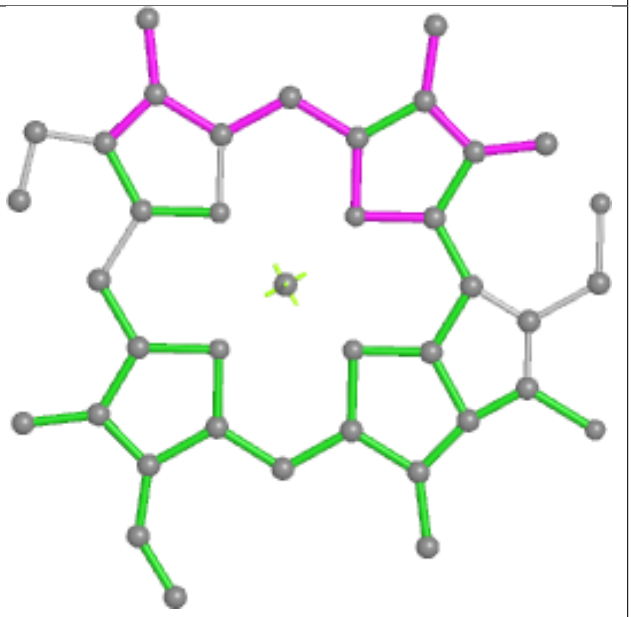
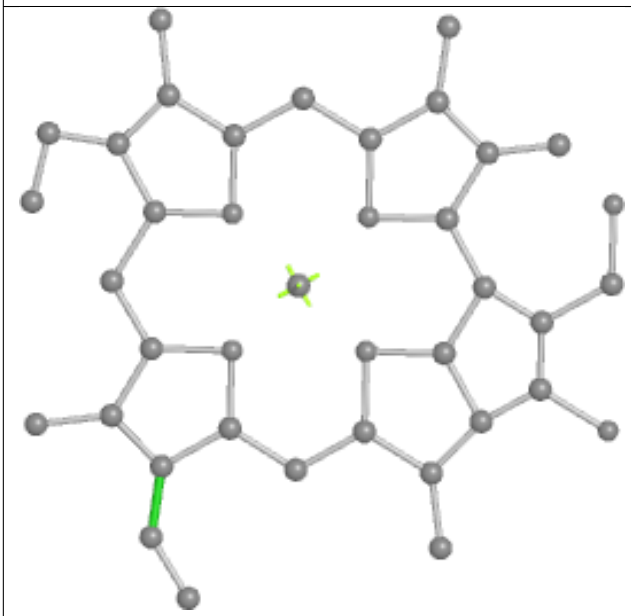


Bond angles



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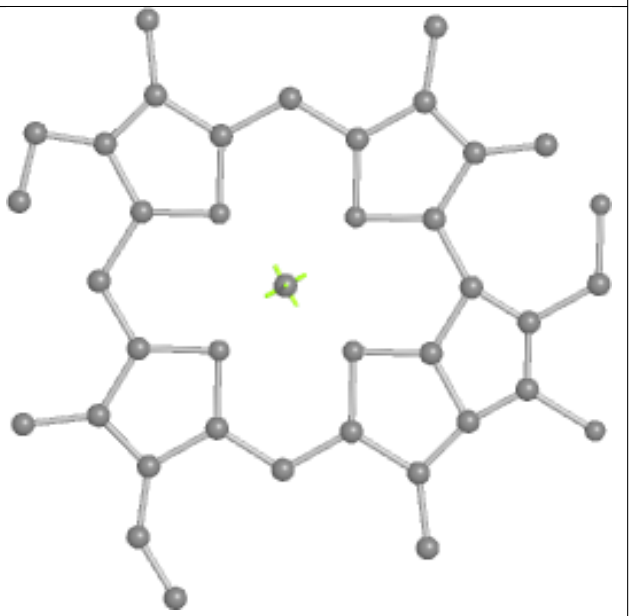
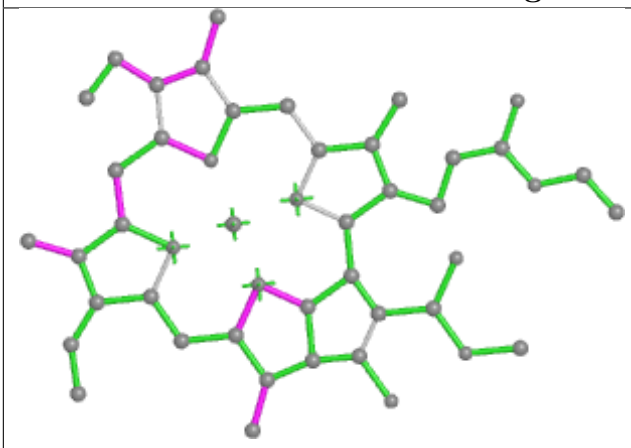


Rings

Ligand CLA B 839



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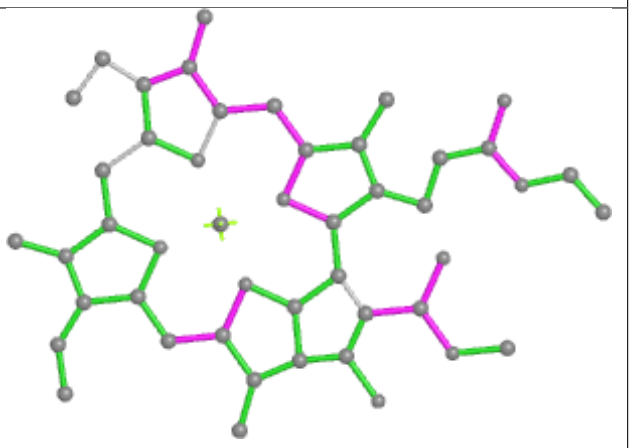
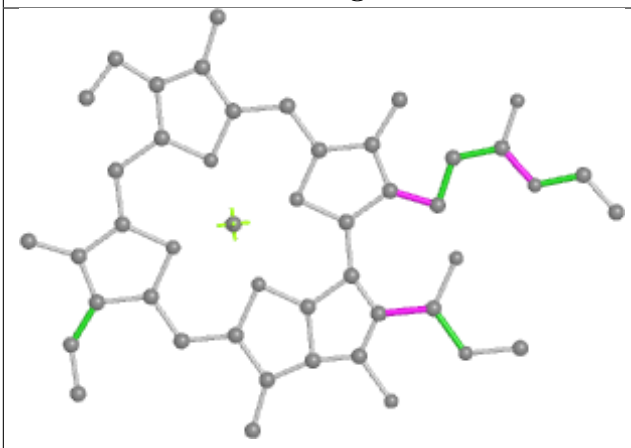


Bond angles



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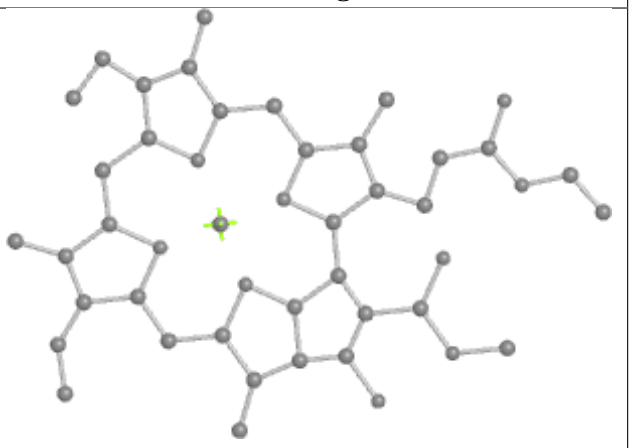
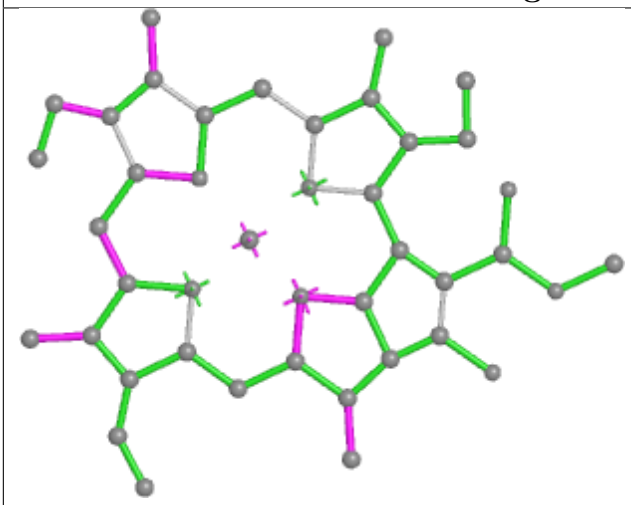
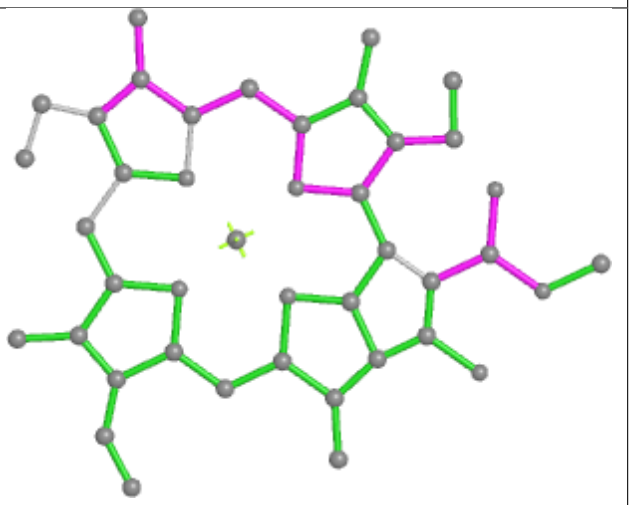


Rings

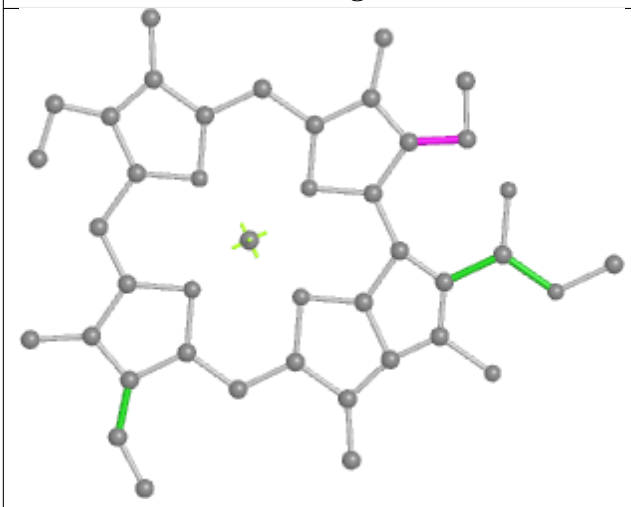
Ligand CLA A 821



Bond lengths



Bond angles



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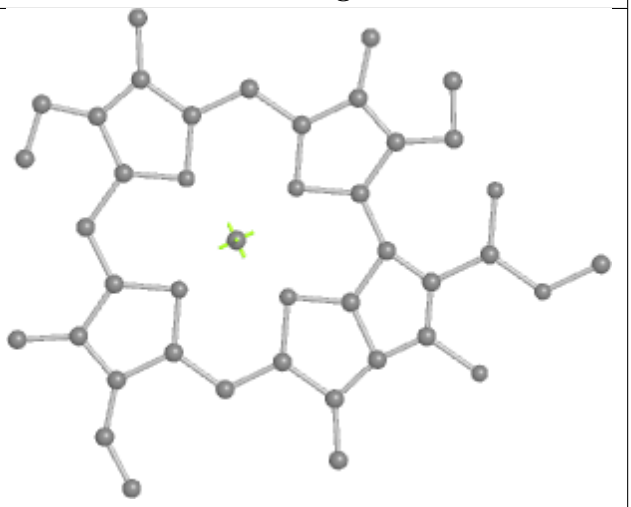
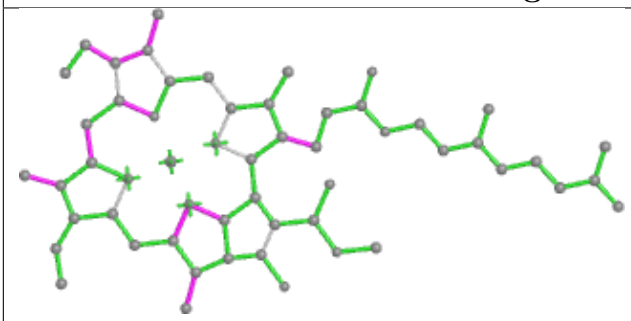


Rings

Ligand CLA A 836



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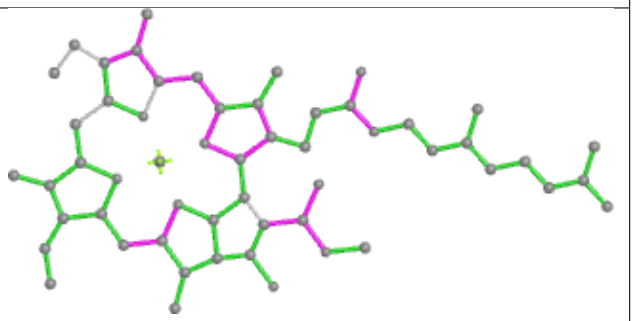
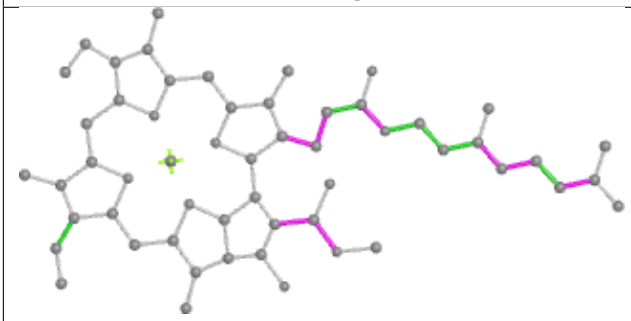


Bond angles



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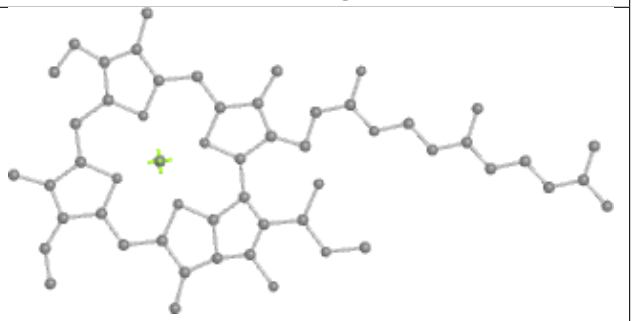
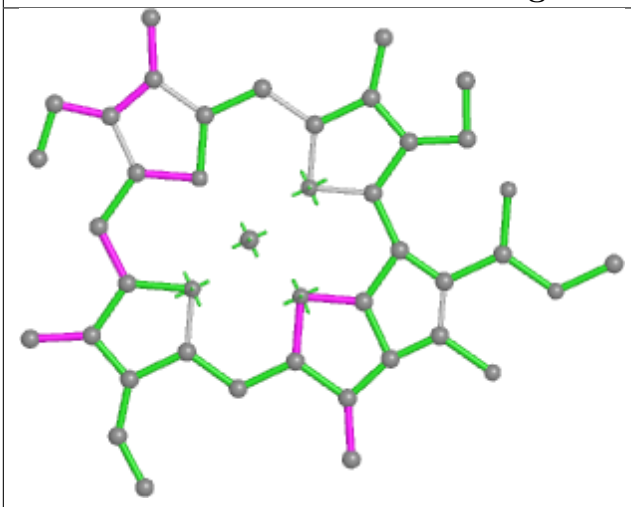


Rings

Ligand CLA 1 507



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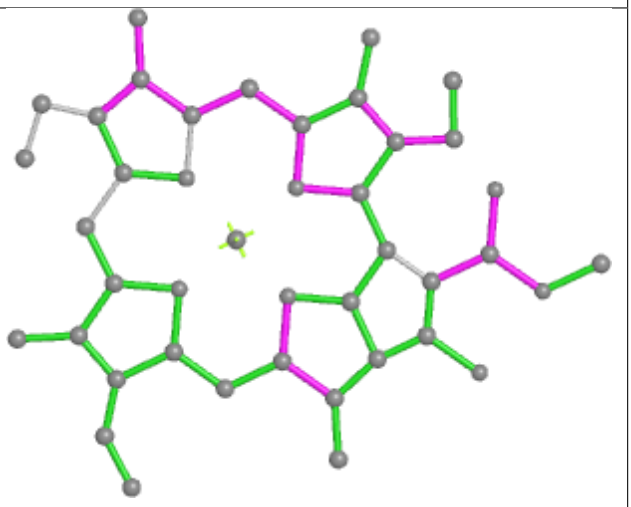
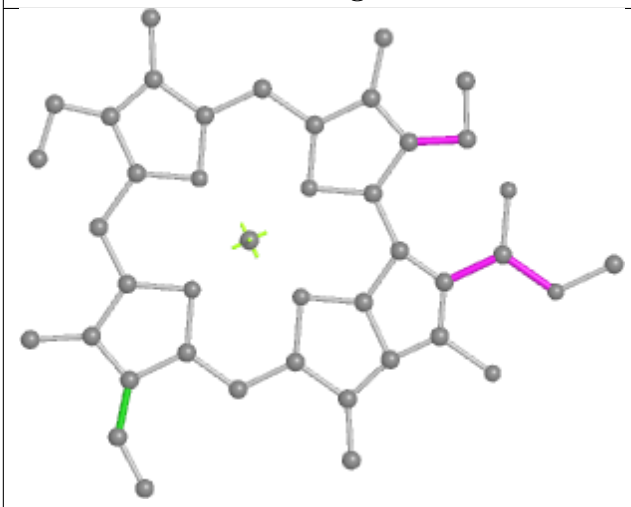


Bond angles



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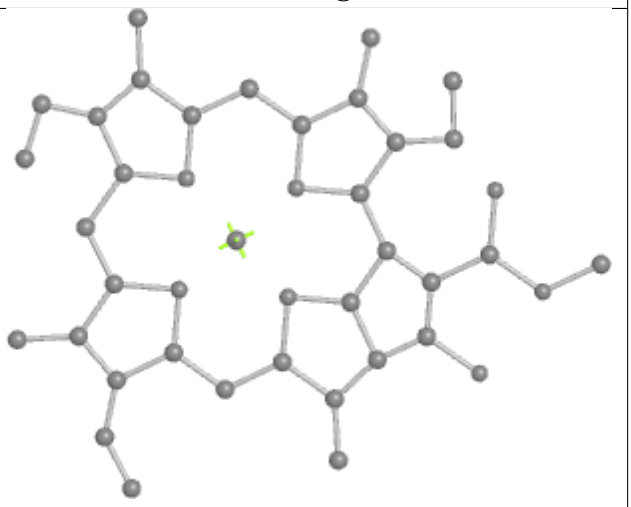
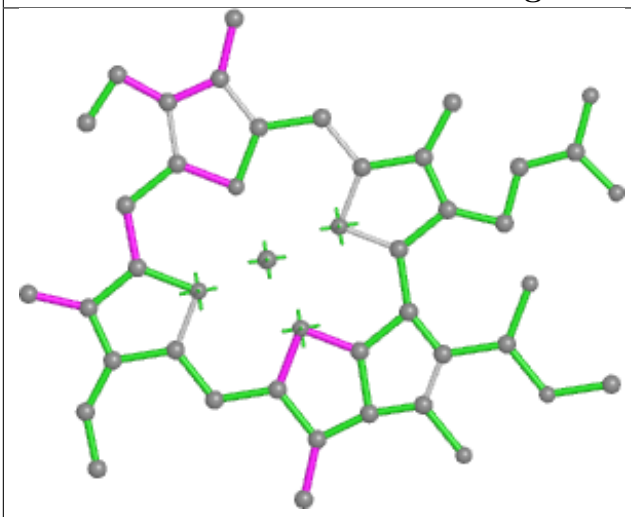


Rings

Ligand CLA B 834



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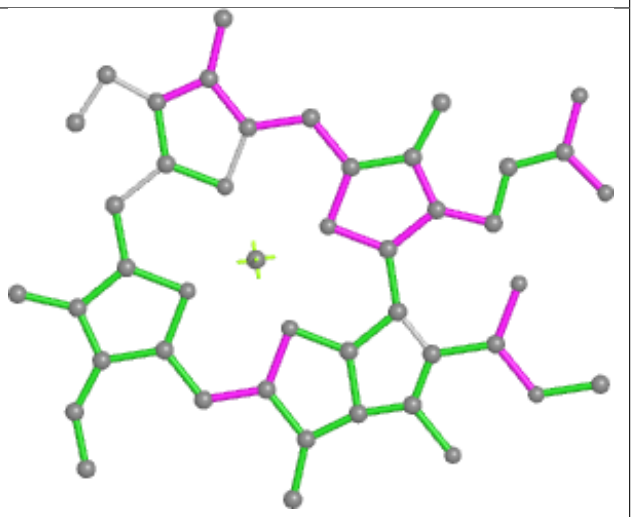
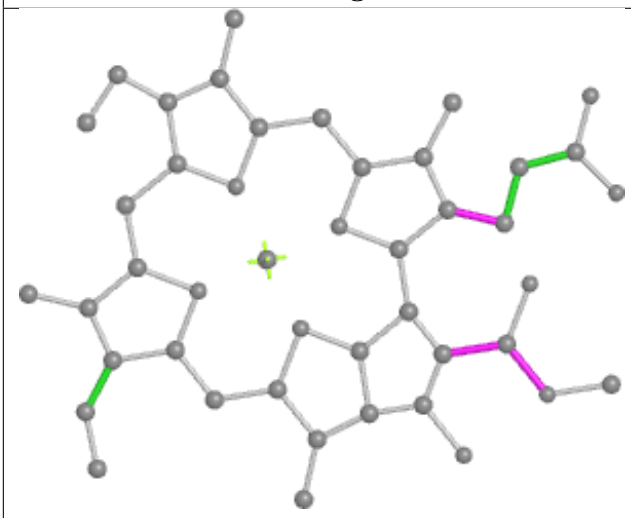


Bond angles



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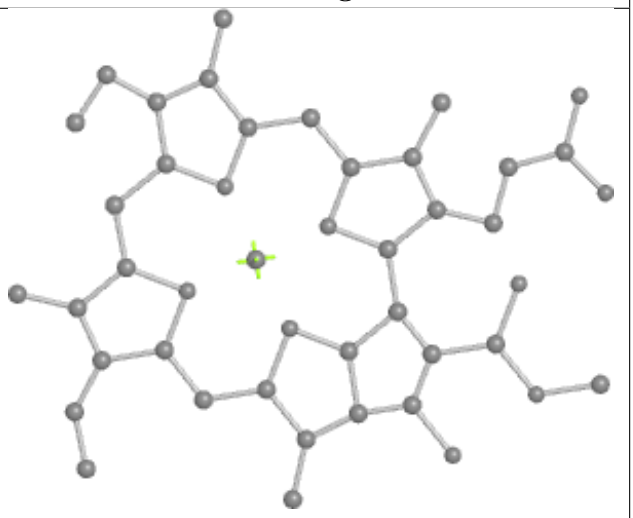
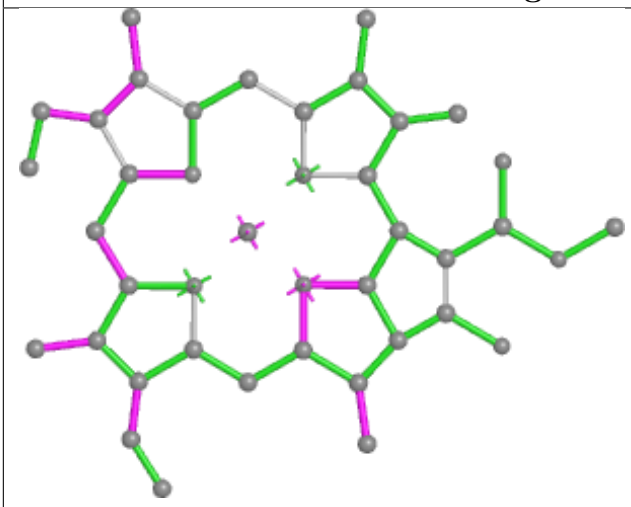
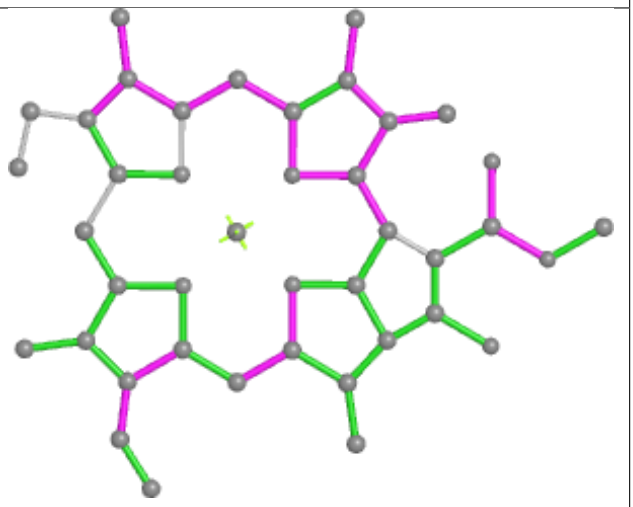


Rings

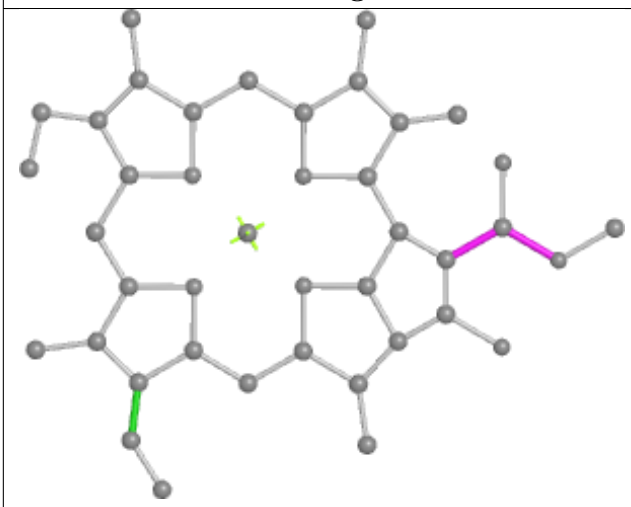
Ligand CLA B 814



Bond lengths



Bond angles



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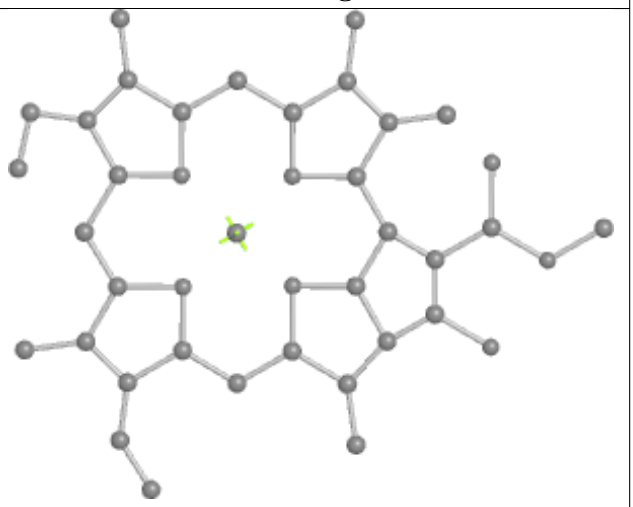
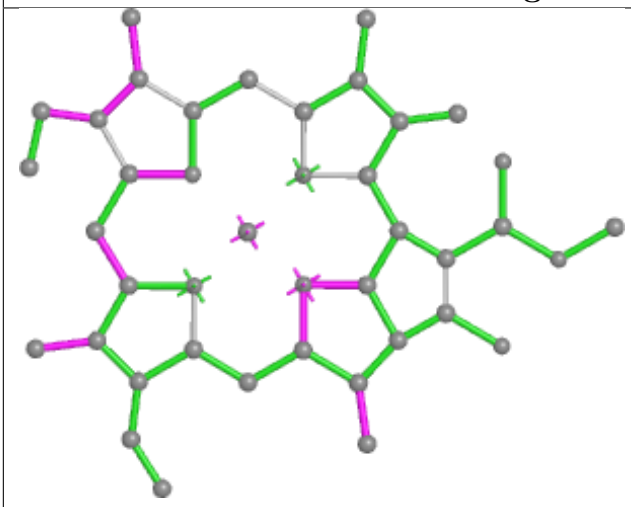
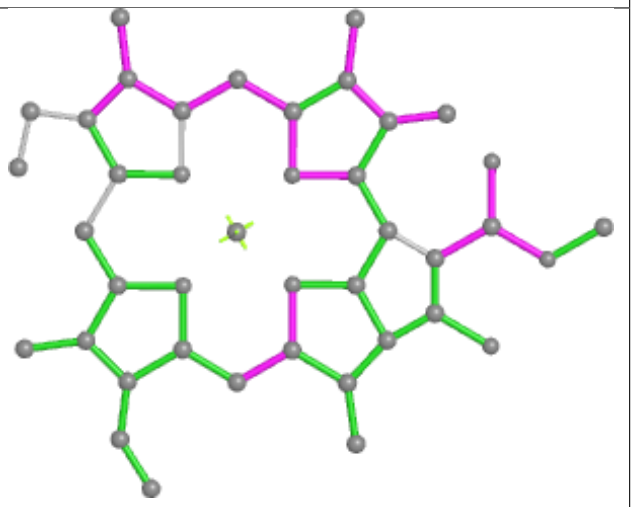
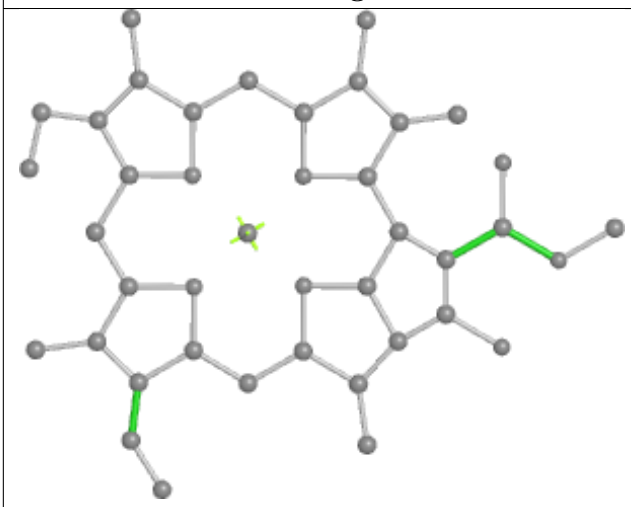
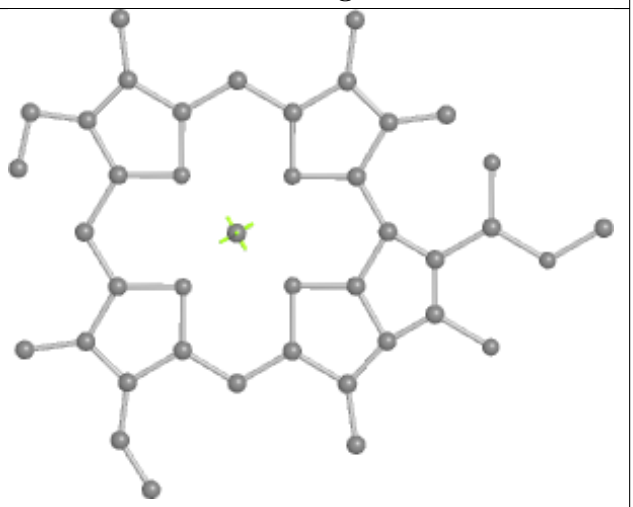
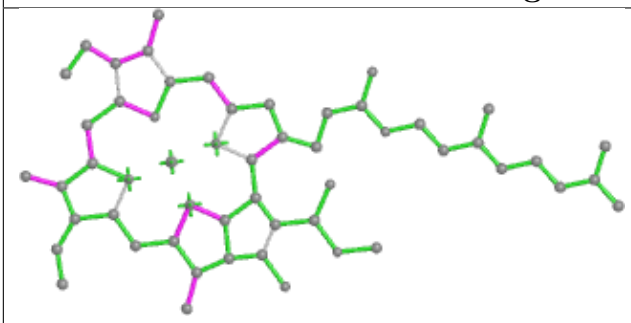


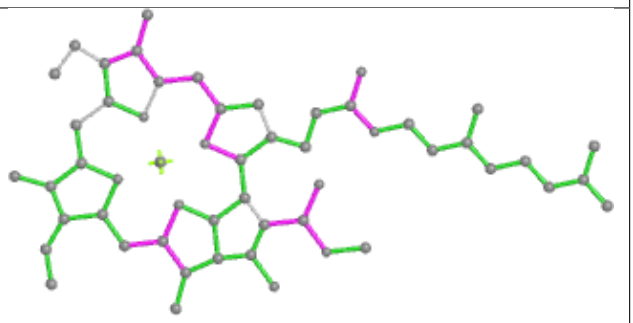
Rings

Ligand CLA A 803	
	
Bond lengths	**Bond angles**
	
Torsions	**Rings**

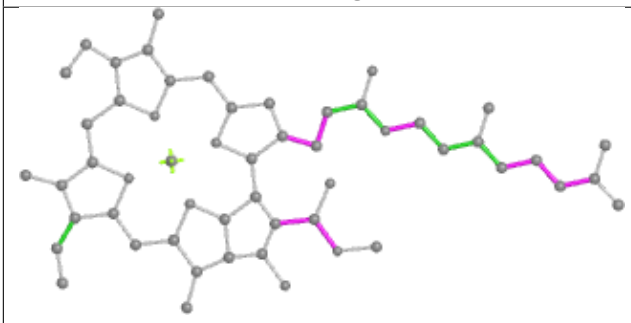
Ligand CLA A 823



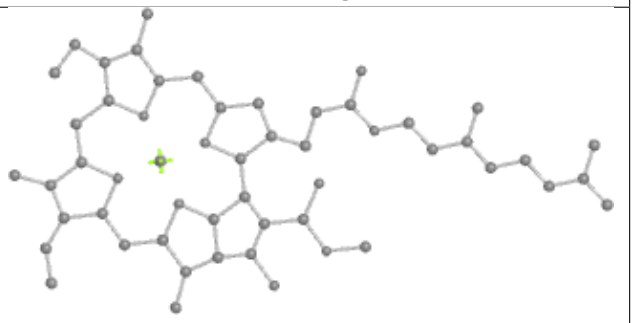
Bond lengths



Bond angles

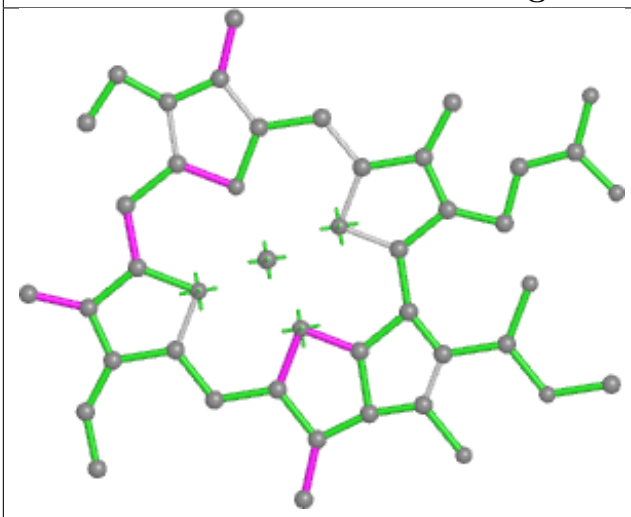


Torsions

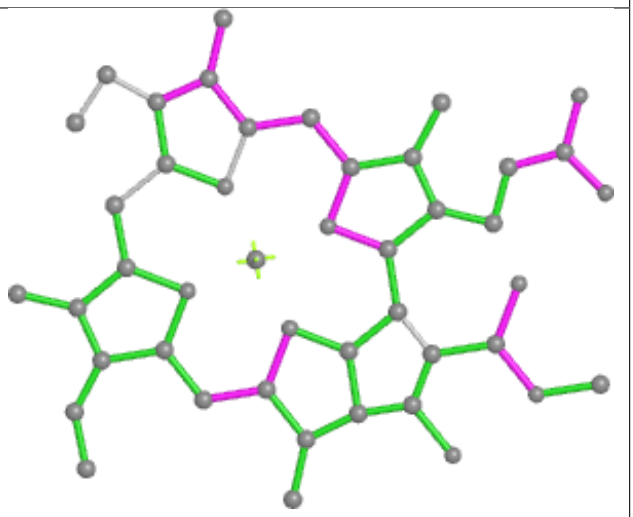


Rings

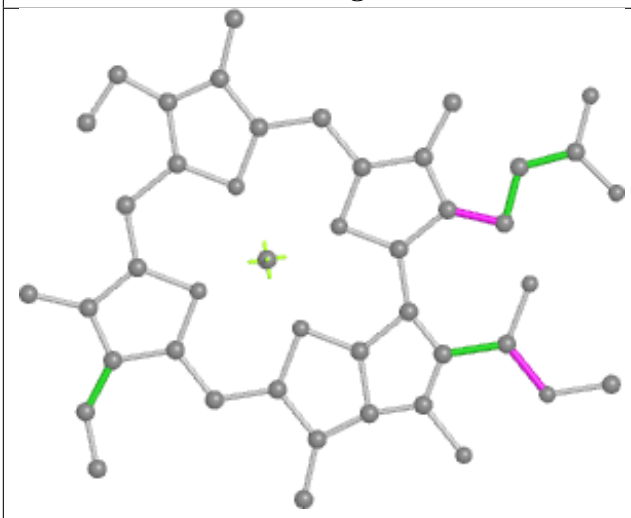
Ligand CLA 3 310



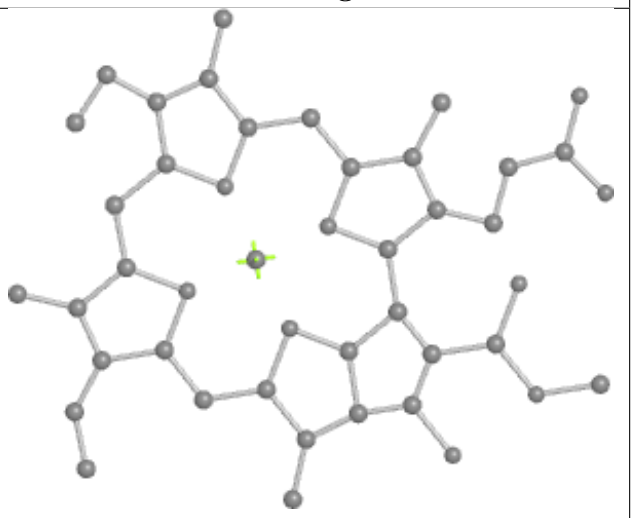
Bond lengths



Bond angles

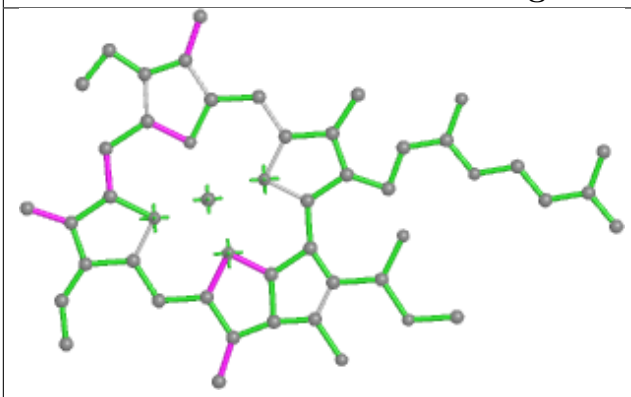


Torsions



Rings

Ligand CLA 3 311



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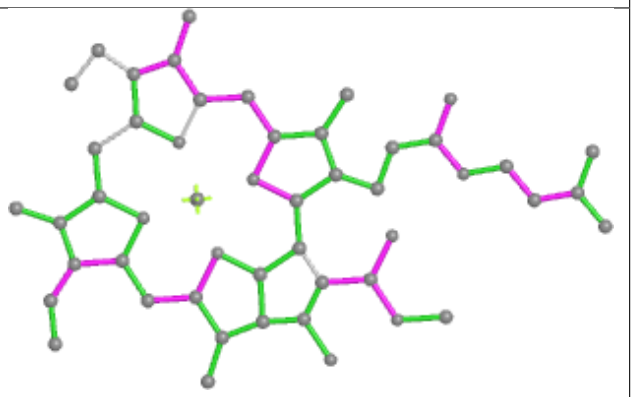

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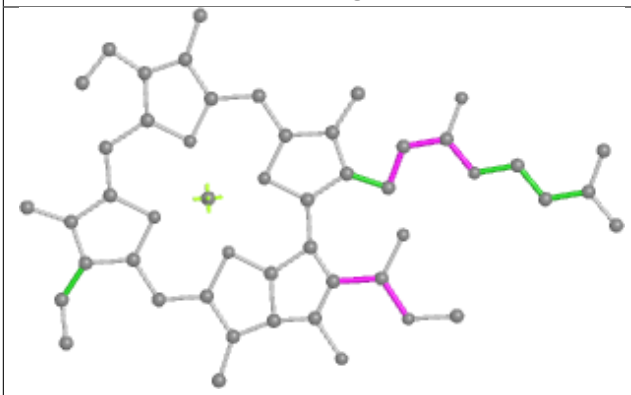
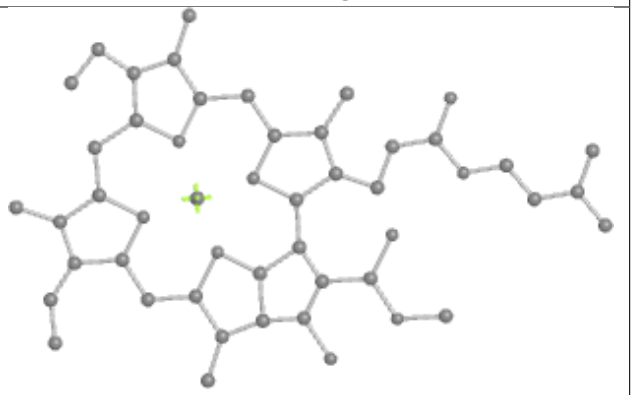
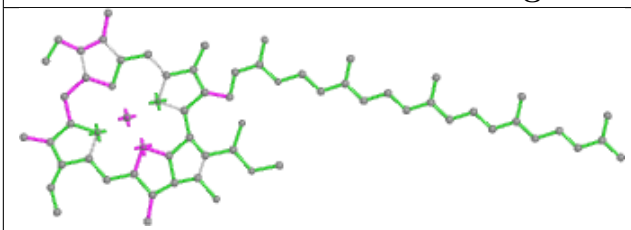


Torsions



Rings

Ligand CLA A 827



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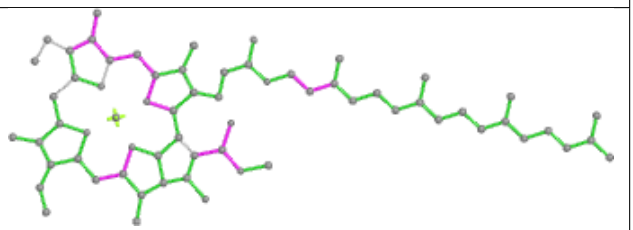
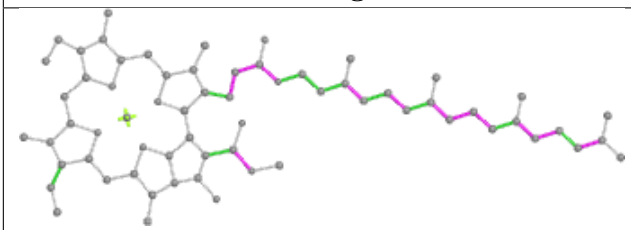
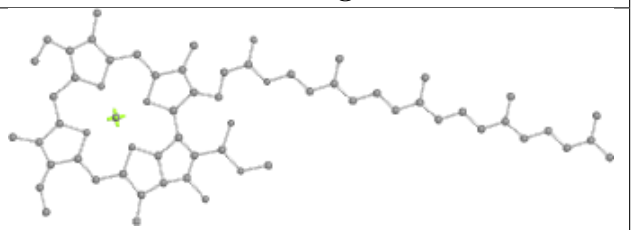


Bond angles

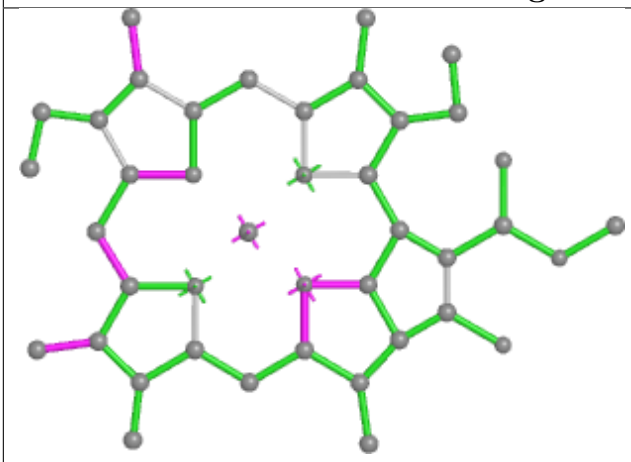


Torsions



Rings

Ligand CLA 1 504



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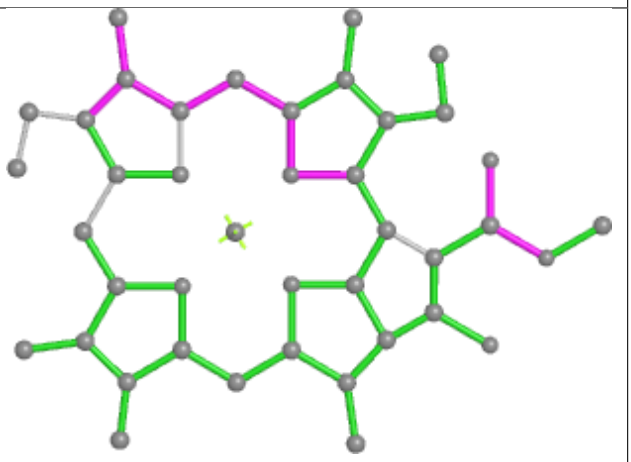
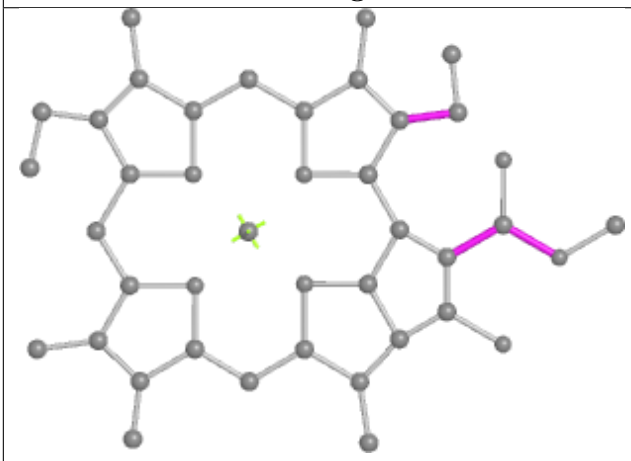


Bond angles



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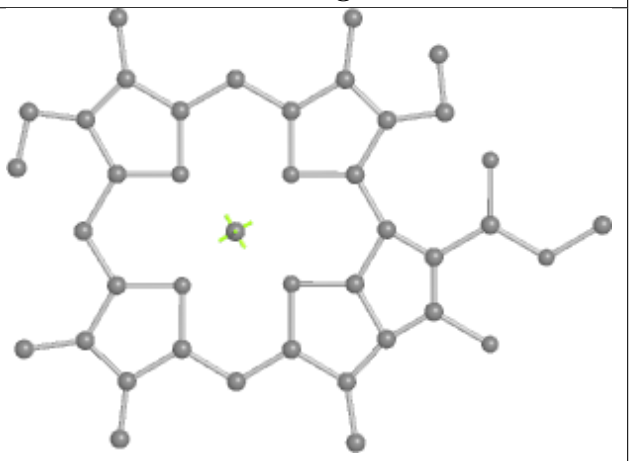
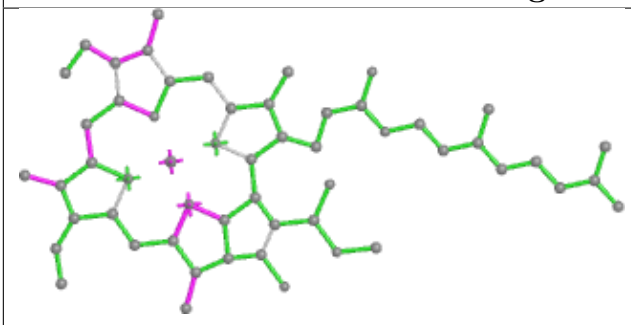


Rings

Ligand CLA 2 514



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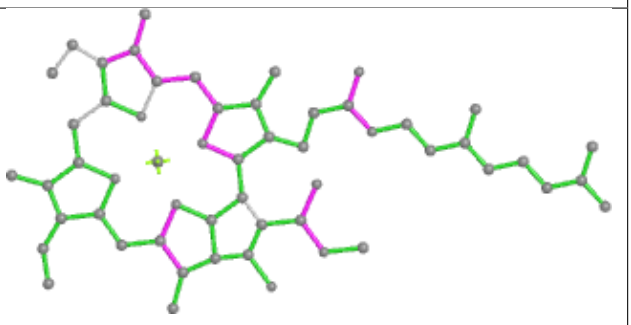
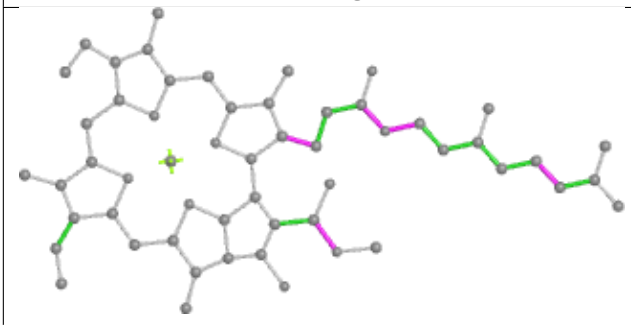


Bond angles



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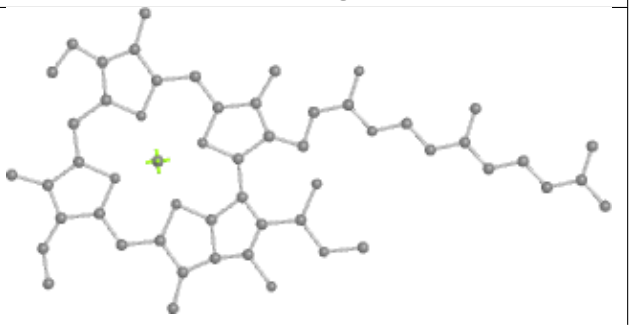
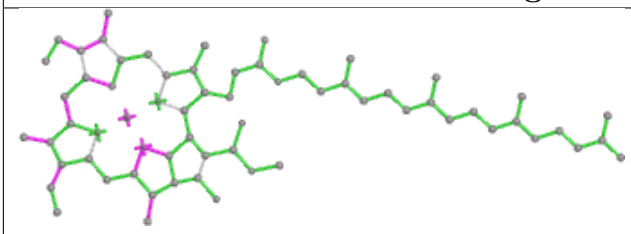


Rings

Ligand CLA B 807



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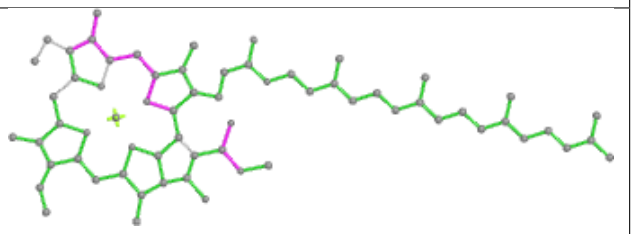
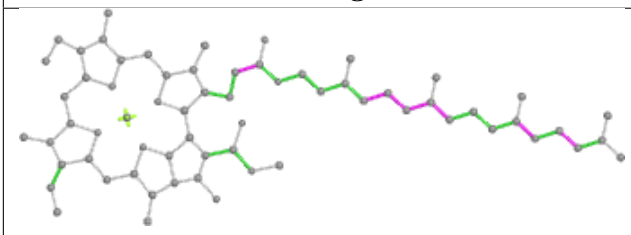


Bond angles



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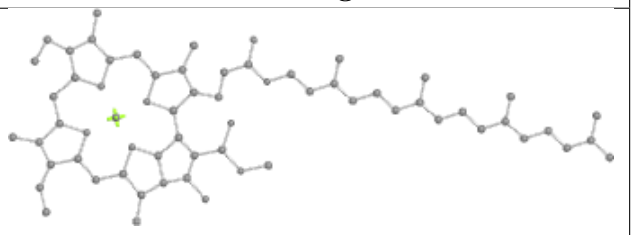
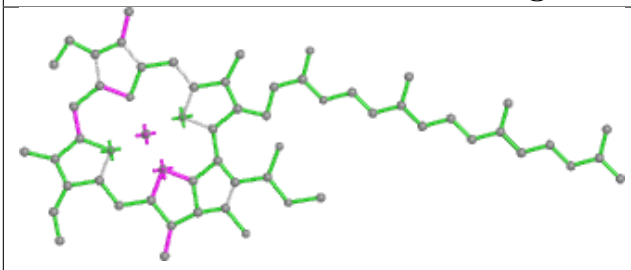


Rings

Ligand CLA 2 510



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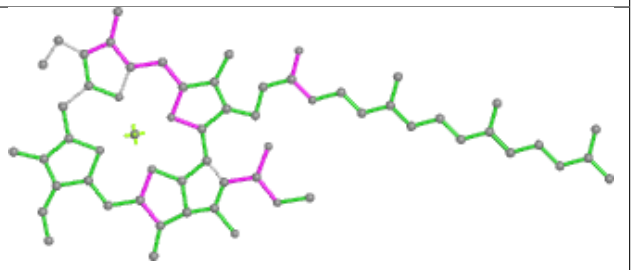
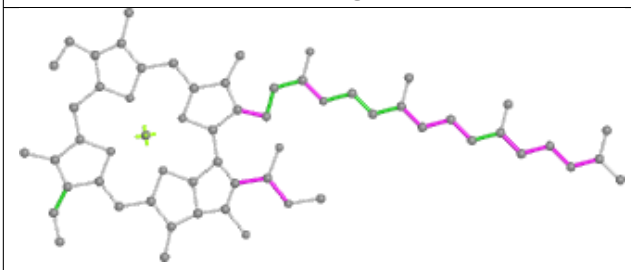


Bond angles



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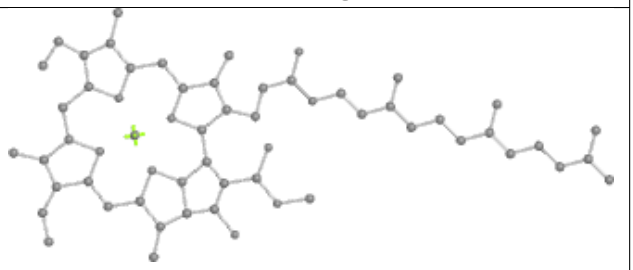
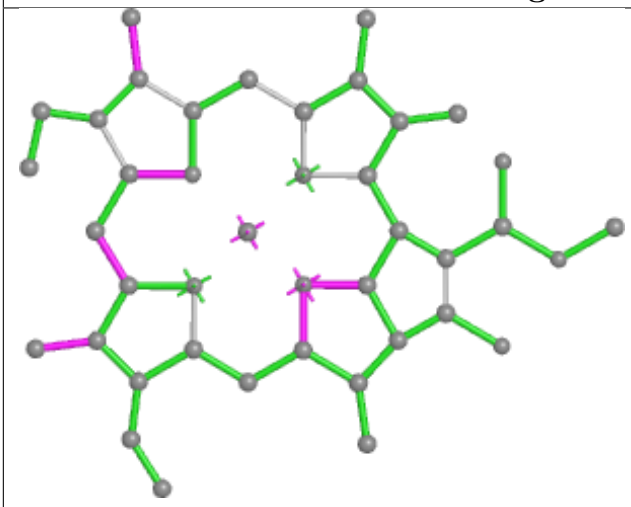


Rings

Ligand CLA 3 312



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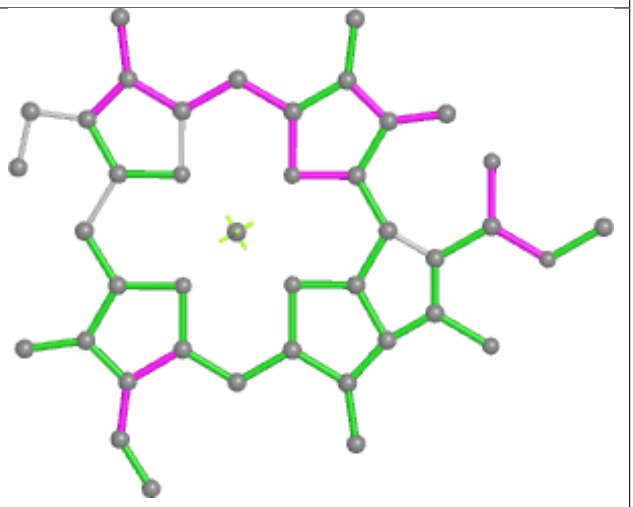
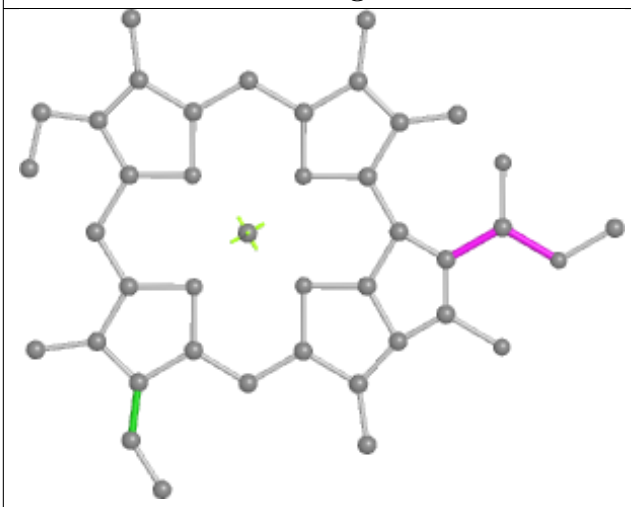


Bond angles



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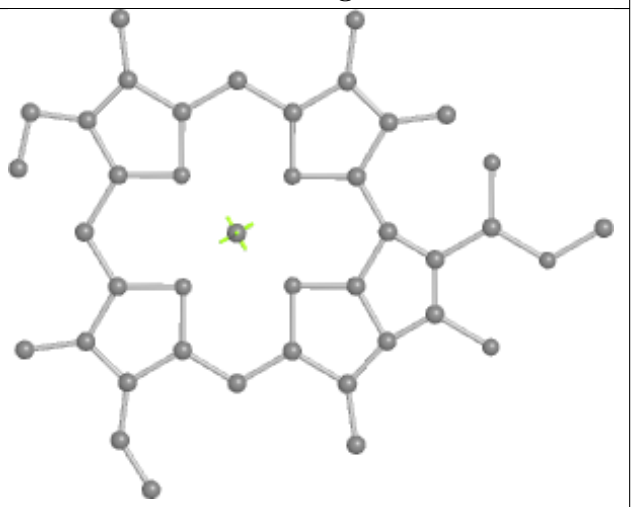
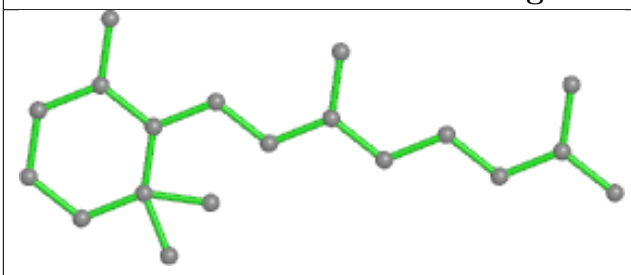


Rings

Ligand BCR 1 503



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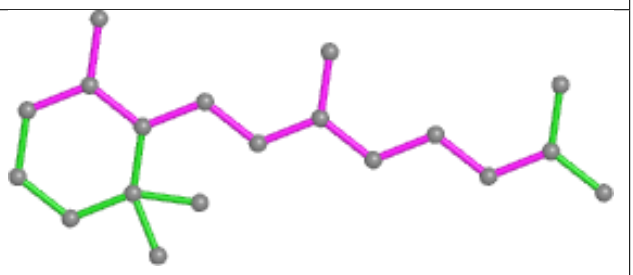
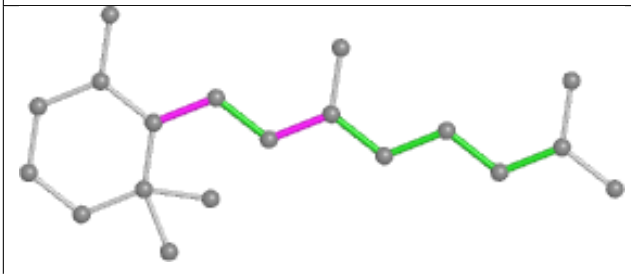


Bond angles



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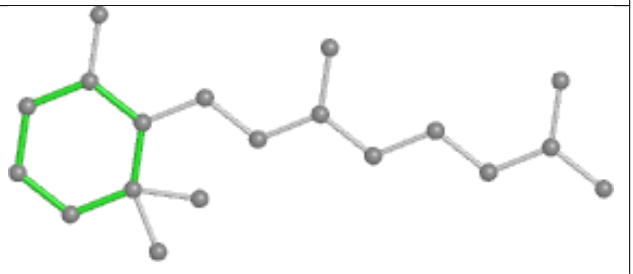
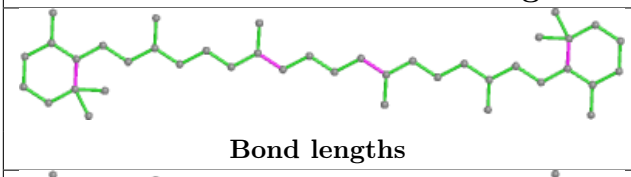


Rings

Ligand BCR A 845



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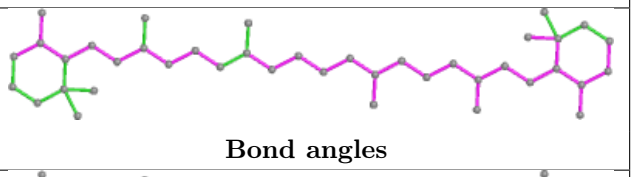
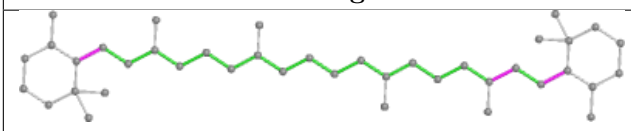
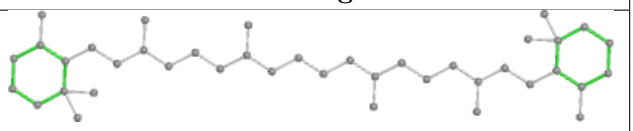


Bond angles

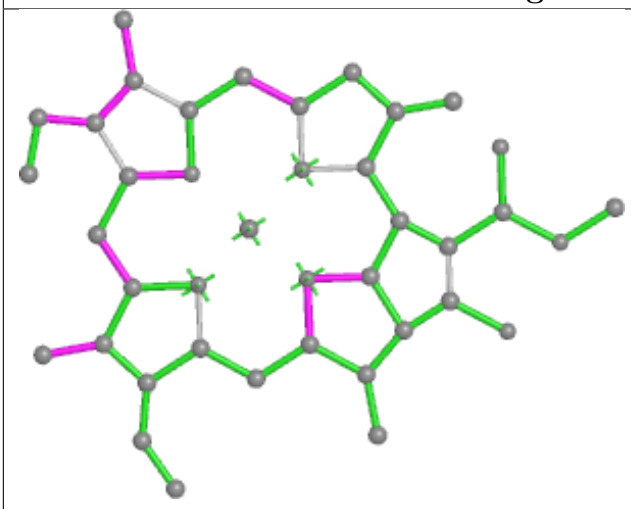


Torsions



Rings

Ligand CLA L 302



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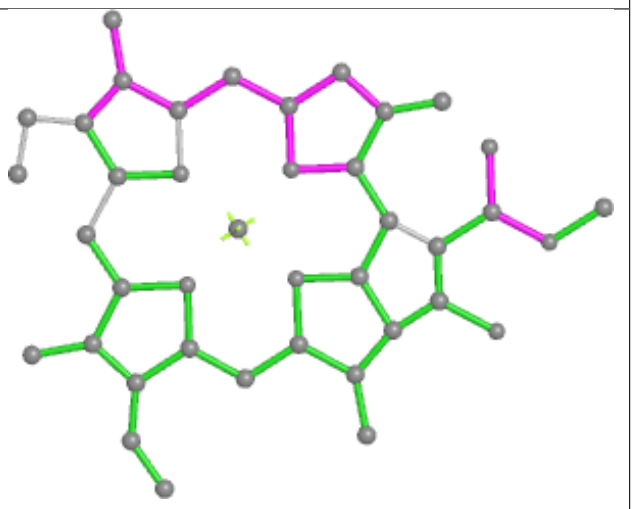
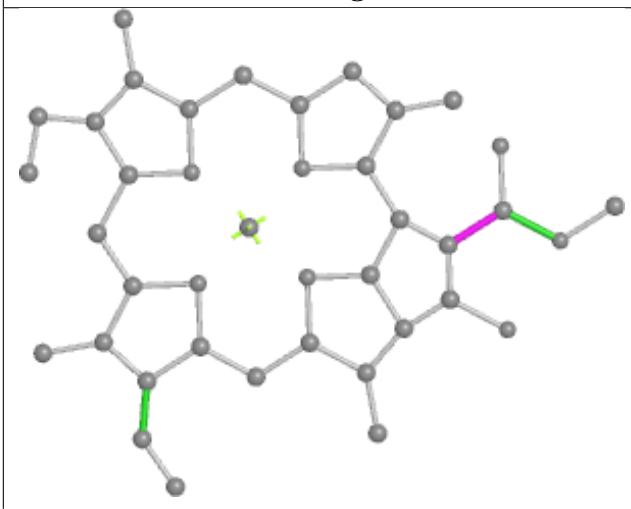


Bond angles



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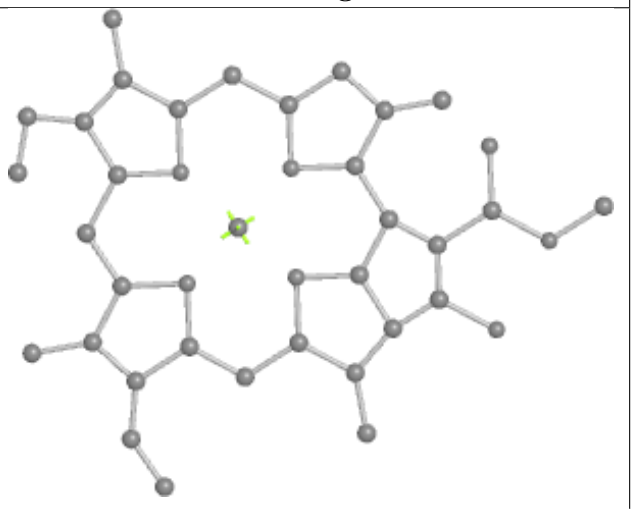
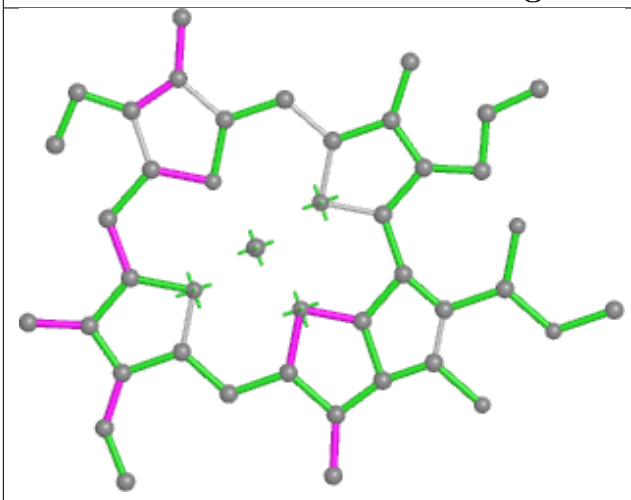
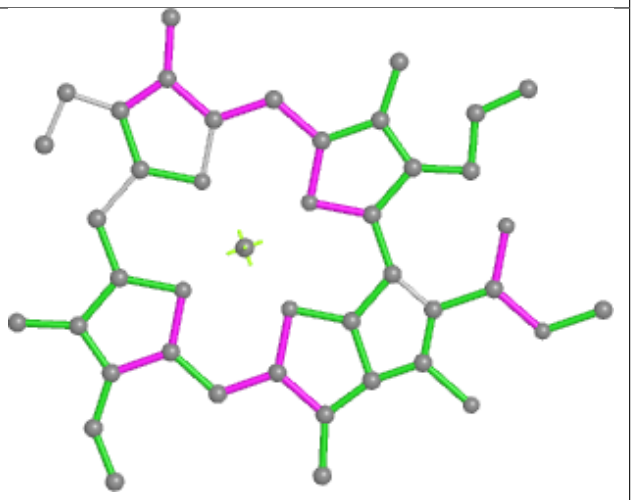


Rings

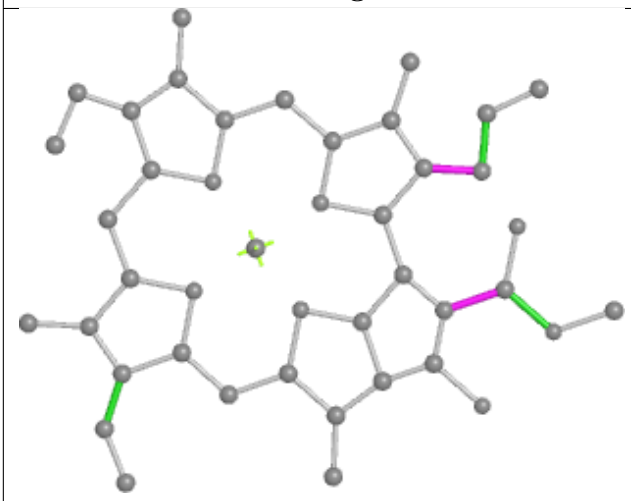
Ligand CLA B 813



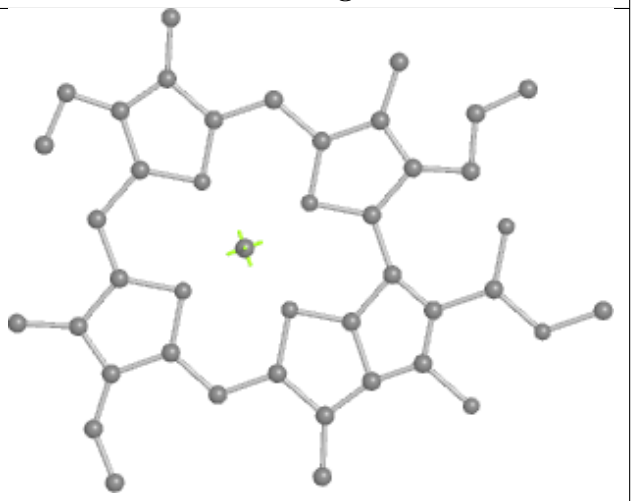
Bond lengths



Bond angles

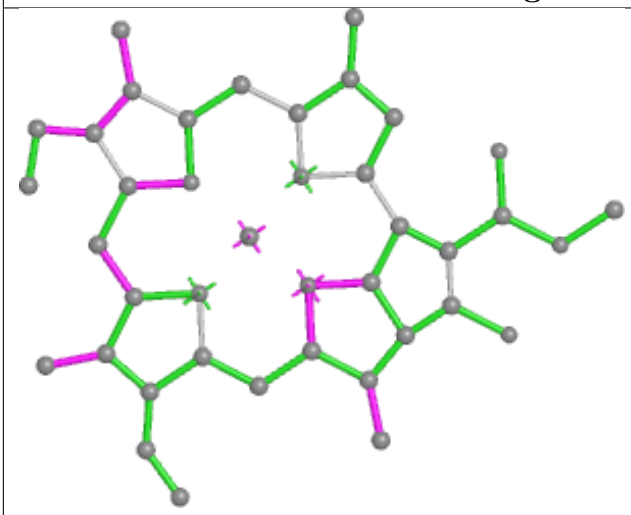


Torsions

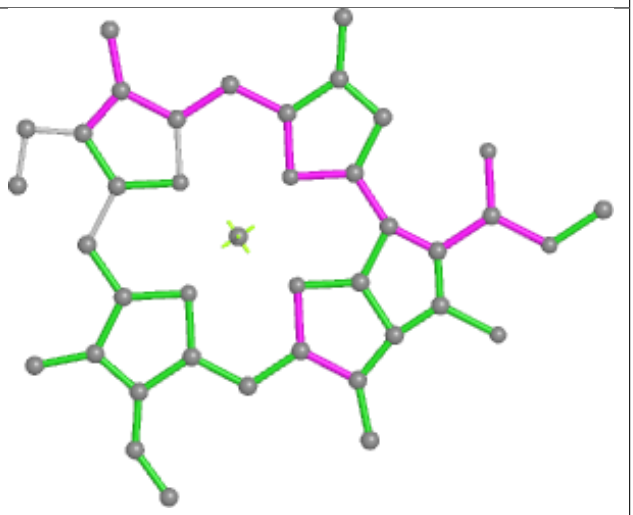


Rings

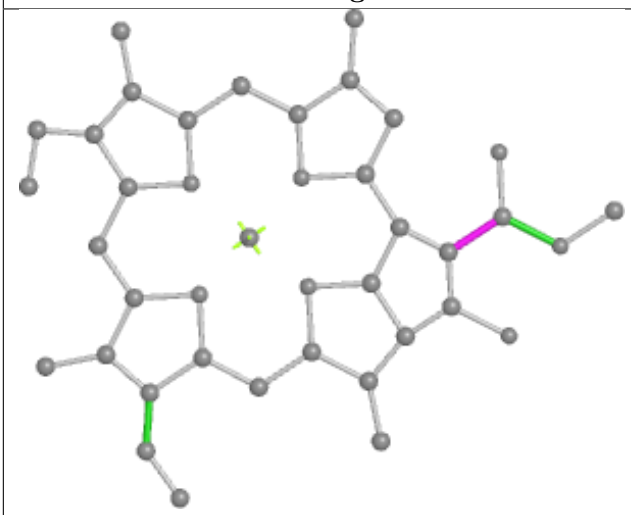
Ligand CLA A 833



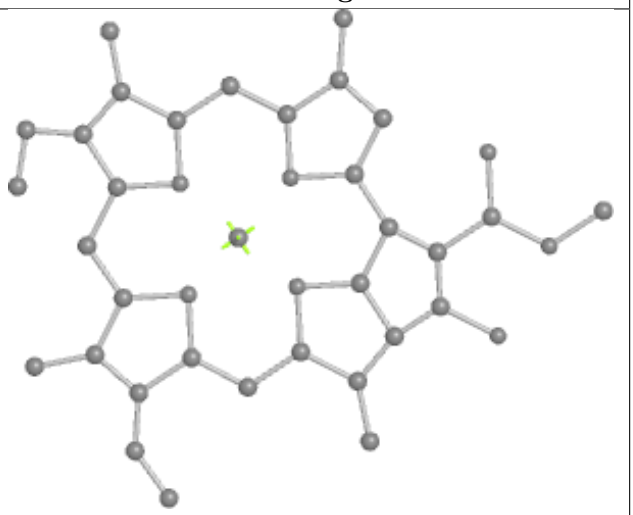
Bond lengths



Bond angles

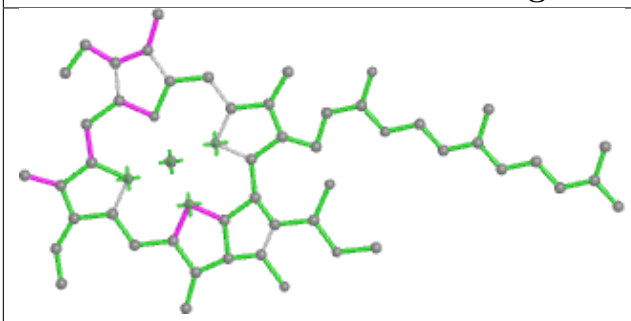


Torsions

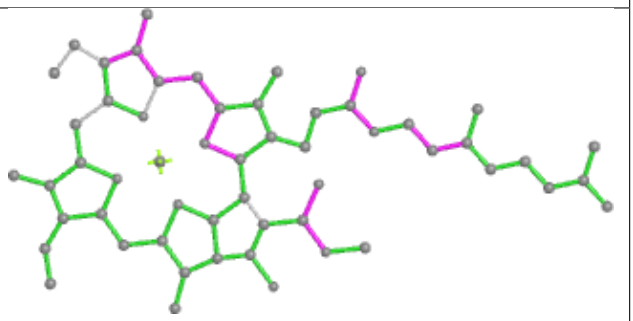


Rings

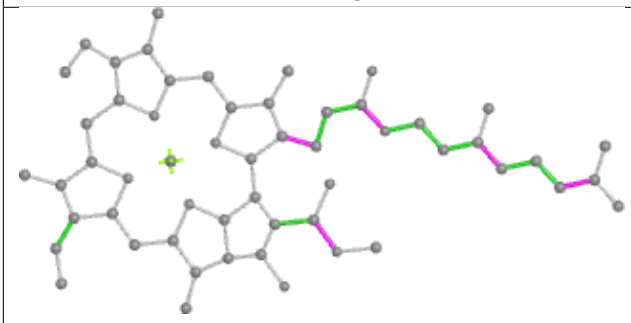
Ligand CLA 1 506



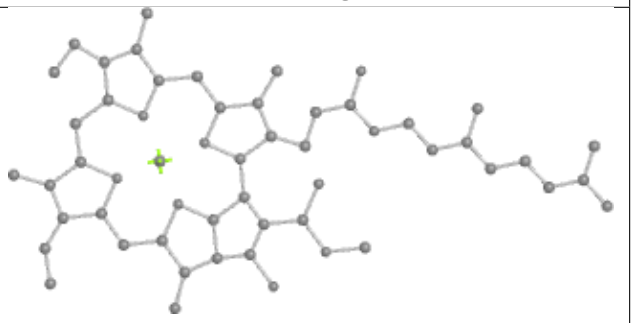
Bond lengths



Bond angles

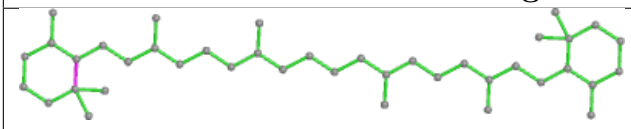


Torsions

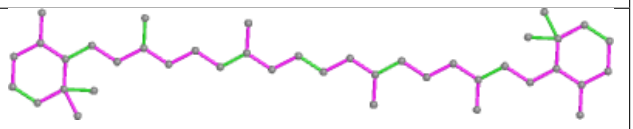


Rings

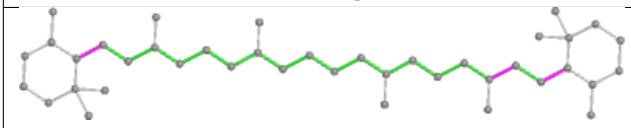
Ligand BCR A 851



Bond lengths



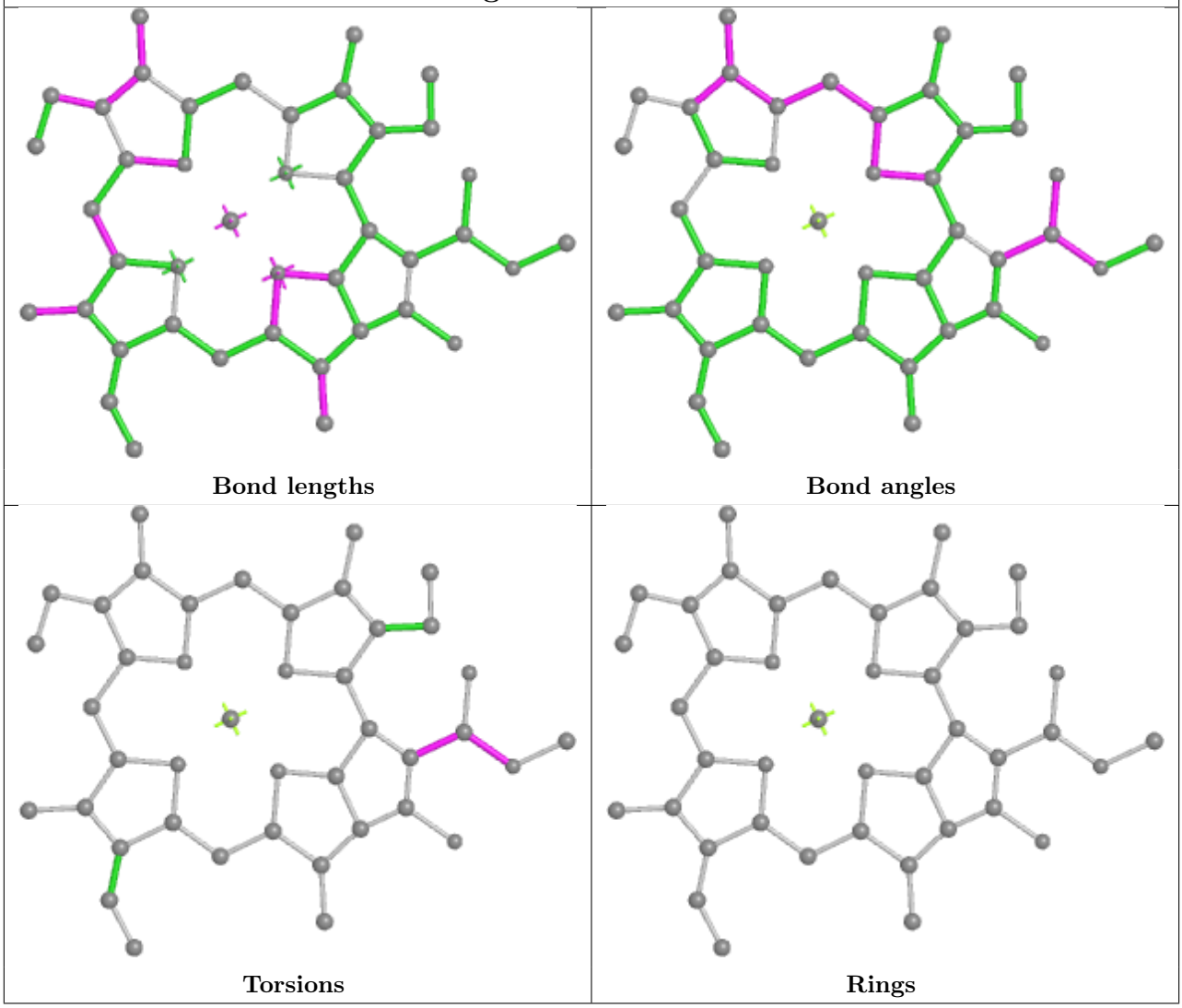
Bond angles



Torsions

Rings

Ligand CLA A 839



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.

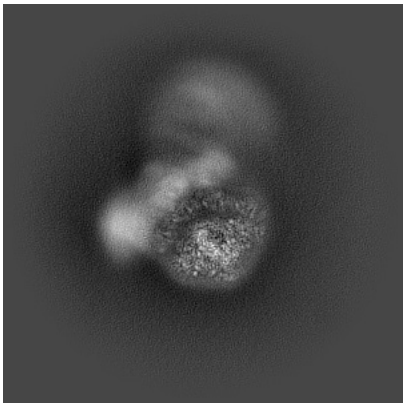
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-31348. These allow visual inspection of the internal detail of the map and identification of artifacts.

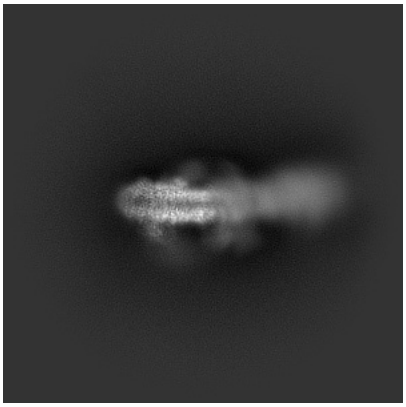
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

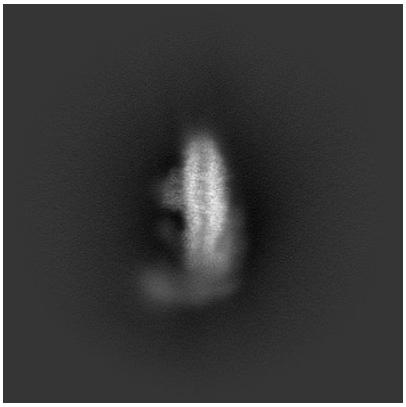
6.1.1 Primary map



X



Y

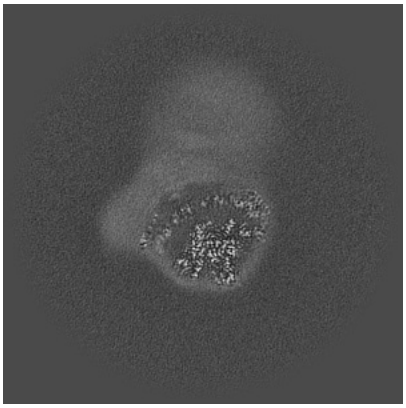


Z

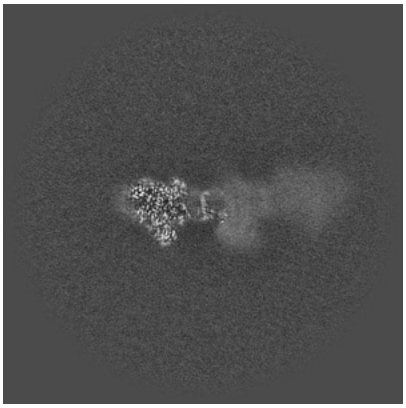
The images above show the map projected in three orthogonal directions.

6.2 Central slices

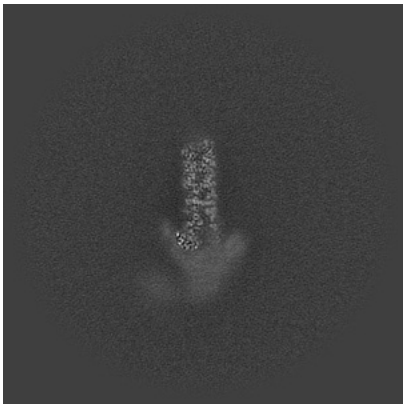
6.2.1 Primary map



X Index: 220



Y Index: 220

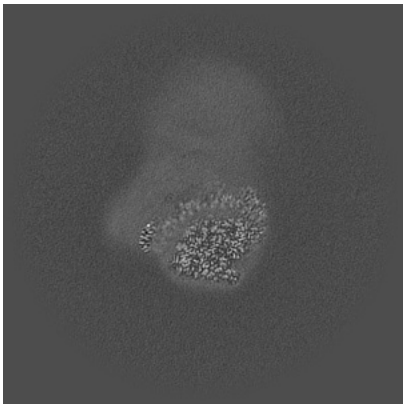


Z Index: 220

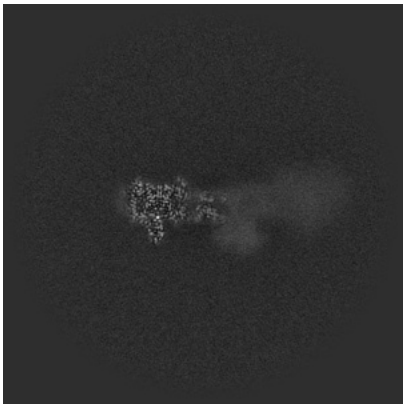
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

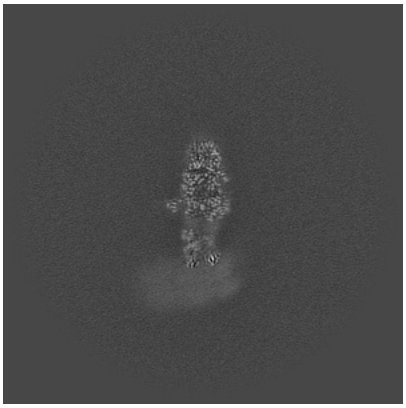
6.3.1 Primary map



X Index: 229



Y Index: 231

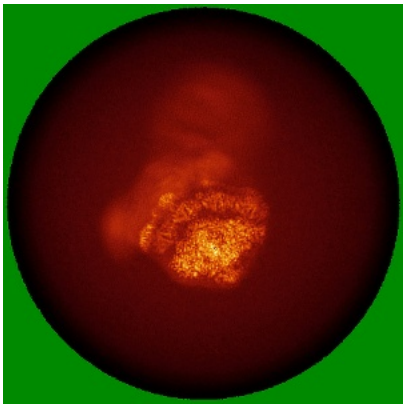


Z Index: 188

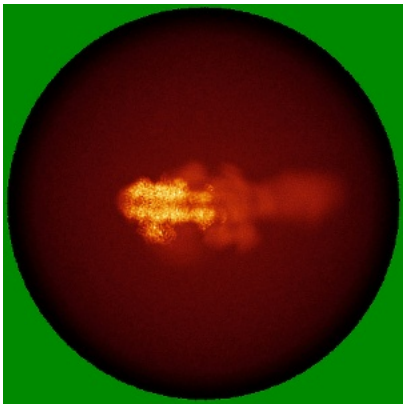
The images above show the largest variance slices of the map in three orthogonal directions.

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

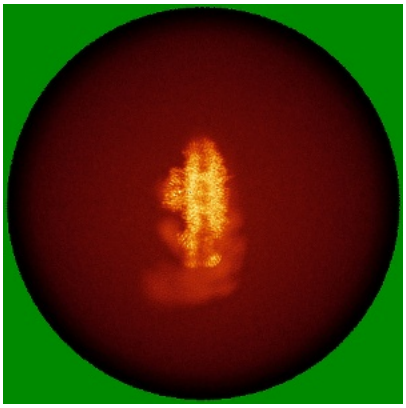
6.4.1 Primary map



X



Y

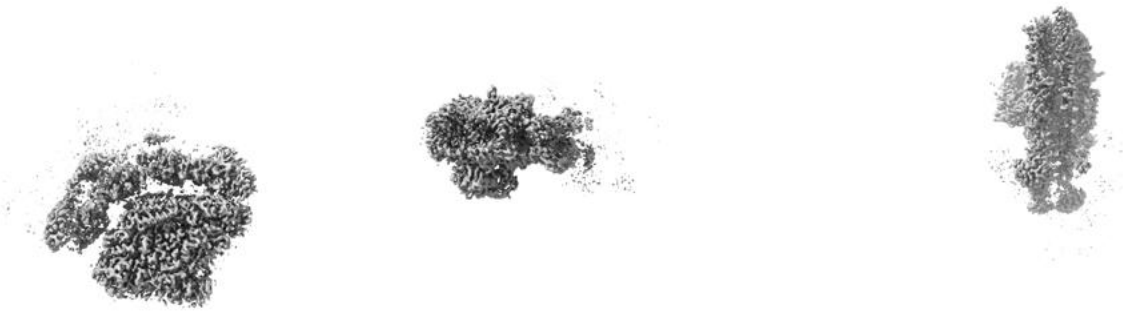


Z

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

6.5 Orthogonal surface views (i)

6.5.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.72. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

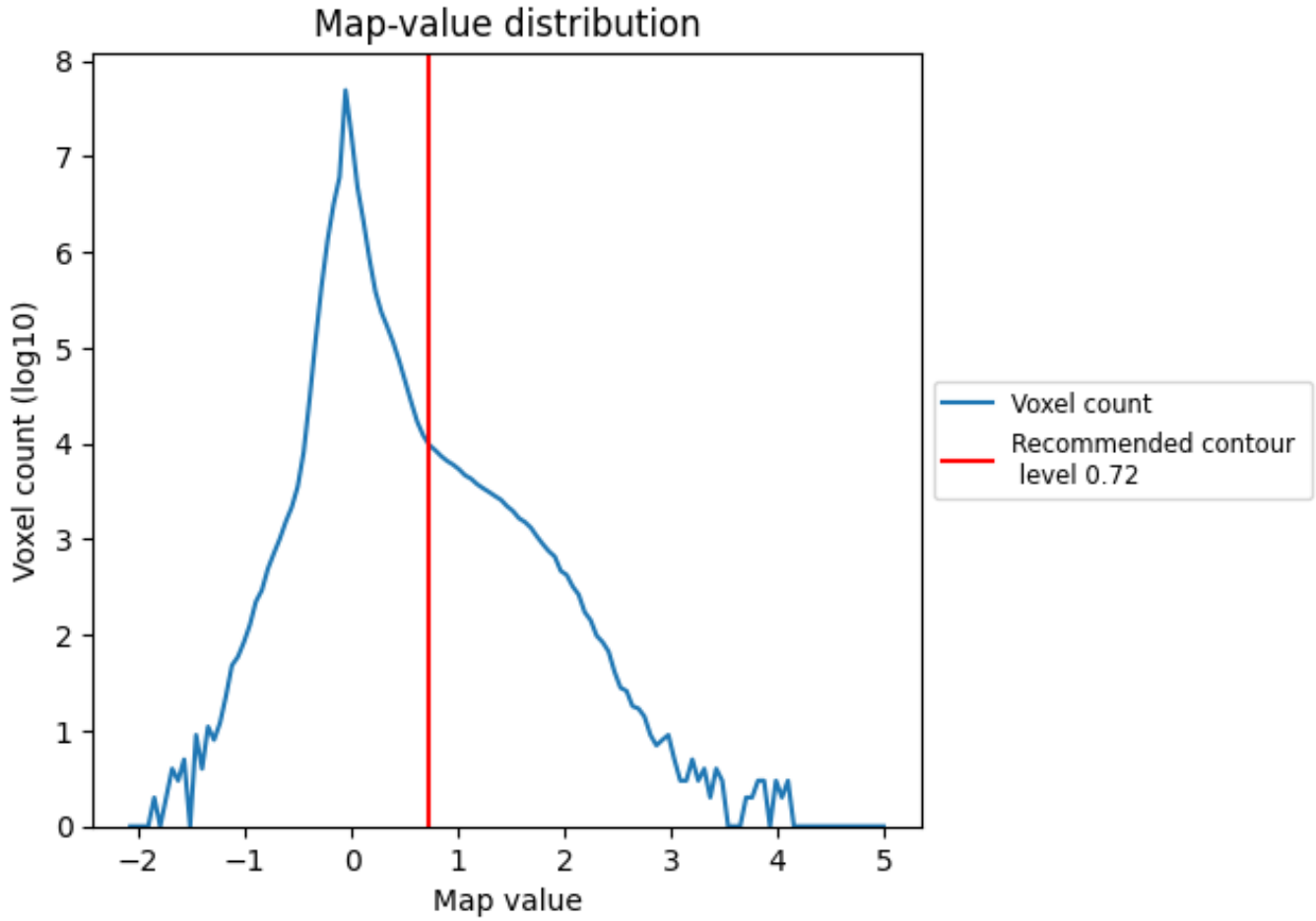
6.6 Mask visualisation (i)

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

7 Map analysis

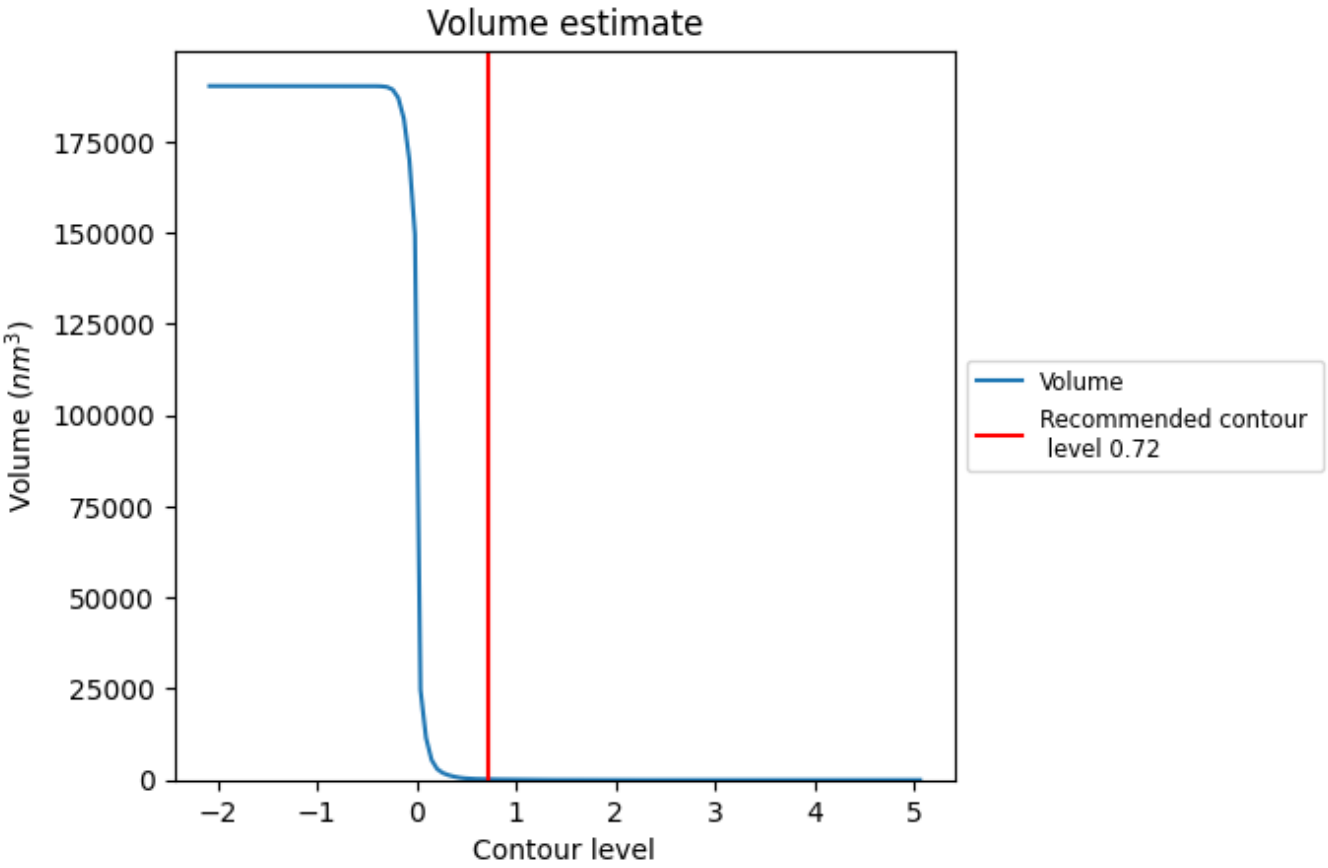
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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

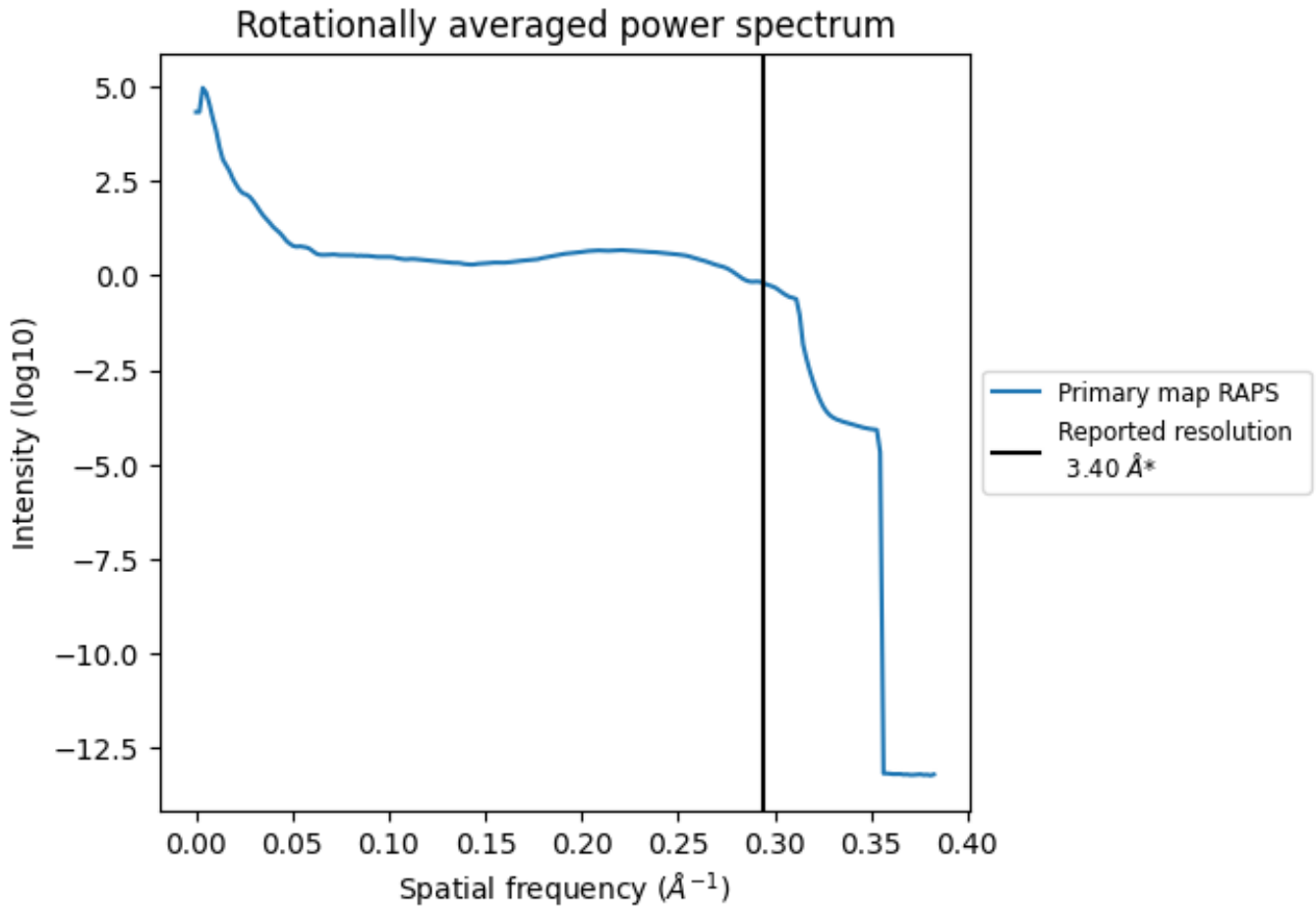
7.2 Volume estimate (i)



The volume at the recommended contour level is 189 nm^3; this corresponds to an approximate mass of 170 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 0.294 $Å^{-1}$

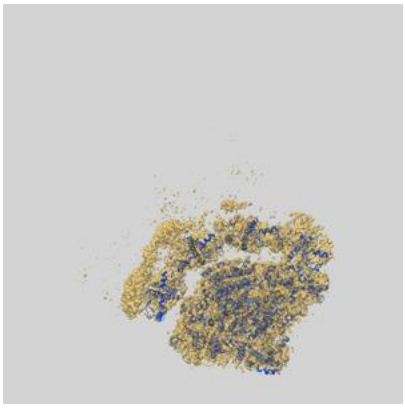
8 Fourier-Shell correlation

This section was not generated. No FSC curve or half-maps provided.

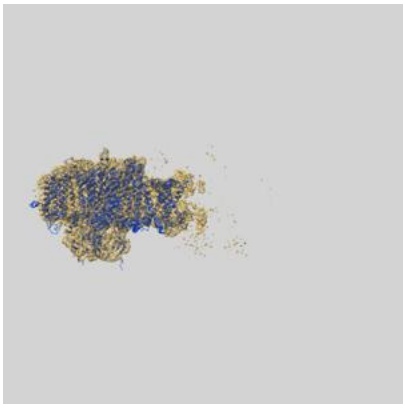
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-31348 and PDB model 7EW6. Per-residue inclusion information can be found in section 3 on page 25.

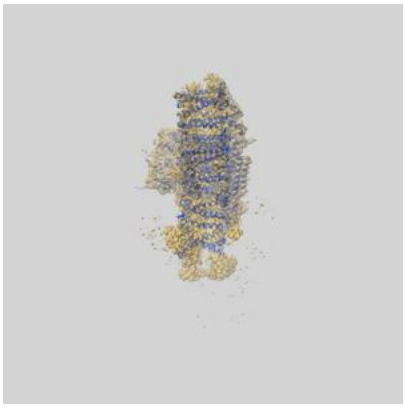
9.1 Map-model overlay



X



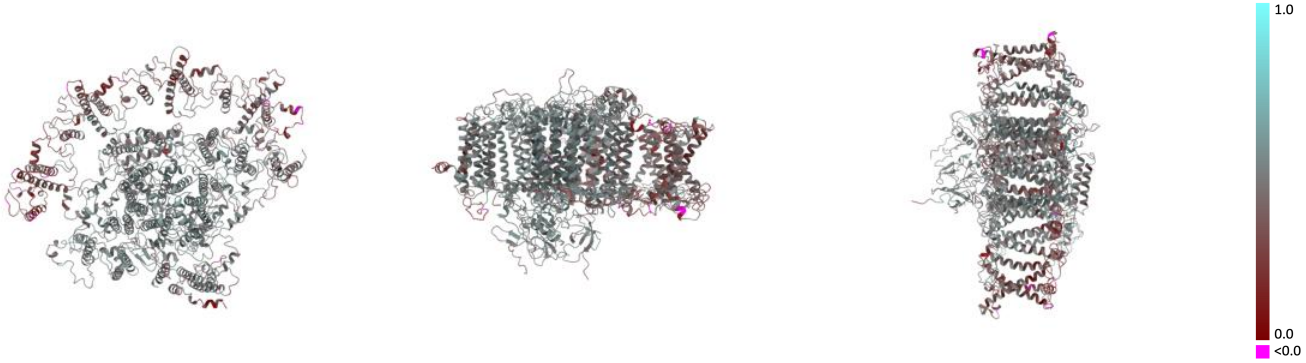
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.72 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.

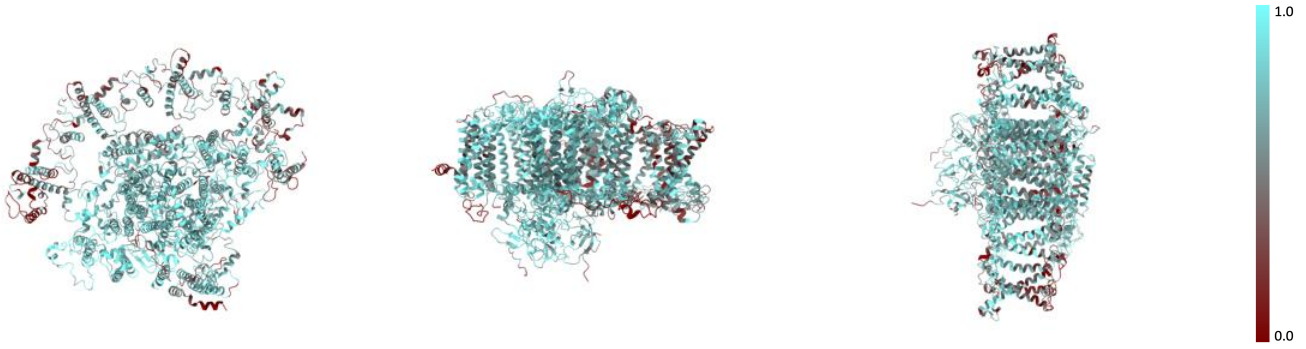
9.2 Q-score mapped to coordinate model (i)



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.

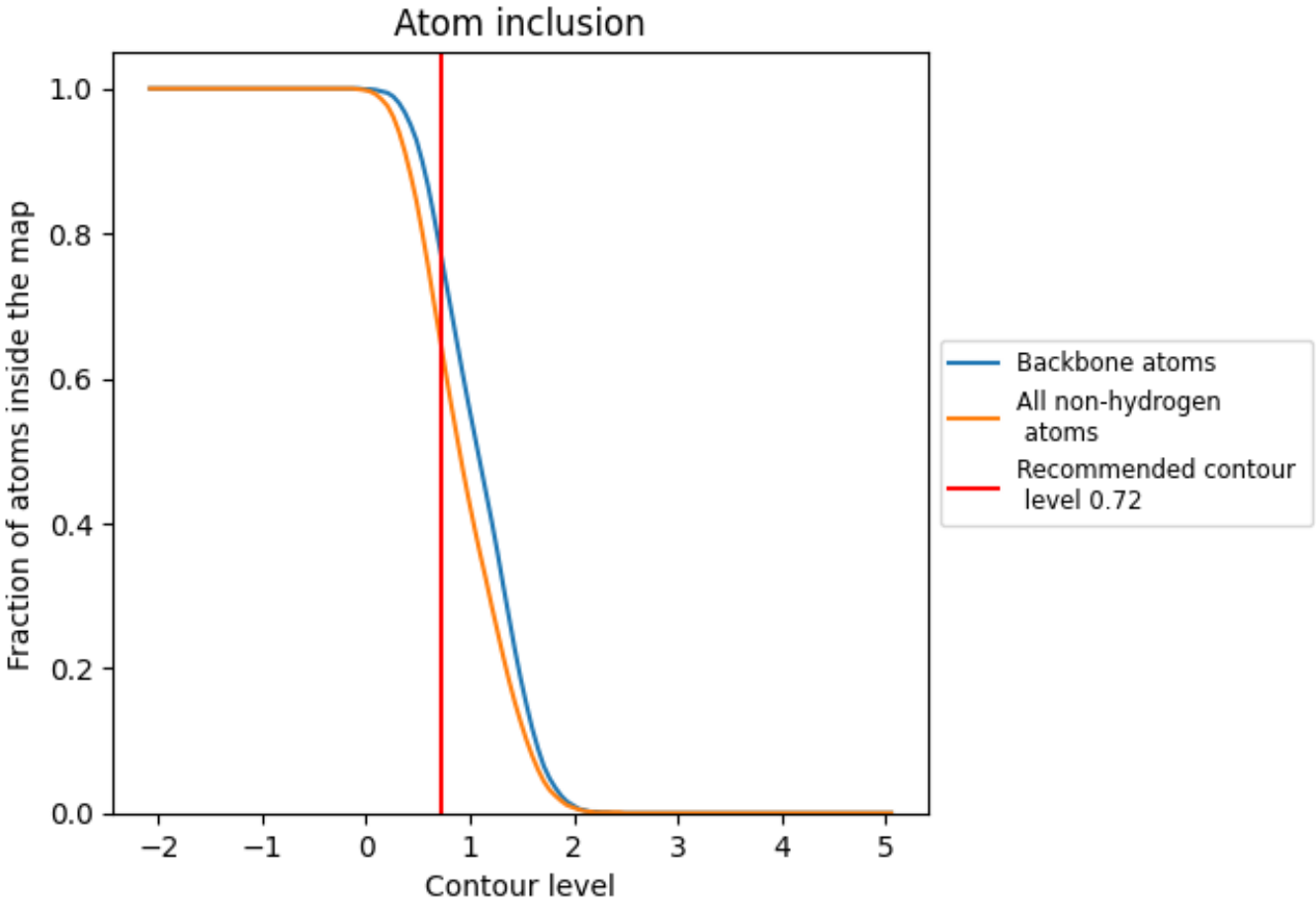
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.72).

9.4 Atom inclusion (i)



At the recommended contour level, 77% of all backbone atoms, 65% 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 (0.72) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6480	0.4660
1	0.3980	0.3020
2	0.5250	0.3870
3	0.4570	0.3520
5	0.5640	0.3970
A	0.7350	0.5220
B	0.7690	0.5240
C	0.8610	0.5200
D	0.6940	0.4910
E	0.6980	0.4810
F	0.6450	0.4880
H	0.3740	0.3900
I	0.6750	0.5100
J	0.4840	0.4810
K	0.3900	0.3820
L	0.6170	0.4580