wwPDB EM Validation Summary Report (i)

Nov 9, 2026 – 08:27 PM EST

PDB ID	:	35ZQ / pdb_000035zq
EMDB ID	:	EMD-77301
Title	:	Structure of Photosystem I from Acaryochloris marina strain MU03
Authors	:	Mehra, H.M.; Gisriel, C.J.
Deposited on	:	2026-05-26
Resolution	:	1.81 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 (i) 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 (i)) were used in the production of this report:

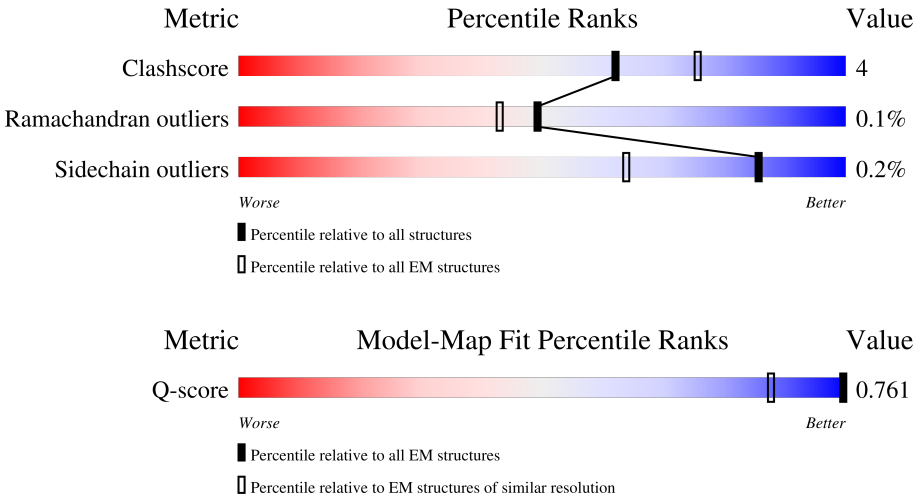
EMDB validation analysis	:	0.0.1.dev133
Mogul	:	2022.3.0, CSD as543be (2022)
MolProbity	:	4-5-2 with Phenix2.2
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.51

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 1.81 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.



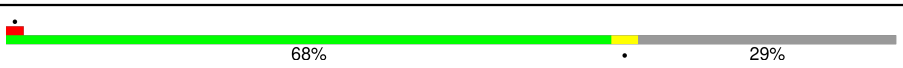
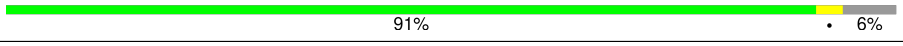
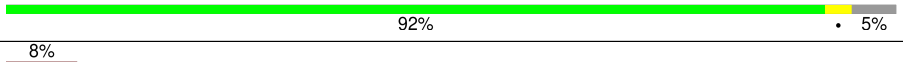
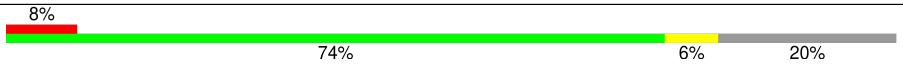
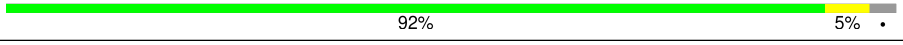
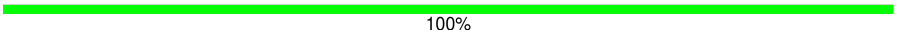
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	869 (1.31 - 2.31)

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	753	91% 8%
2	B	736	89% 7%
3	C	81	86% 12%
4	D	139	91% 7%

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Mol	Chain	Length	Quality of chain
5	E	97	
6	F	167	
7	I	34	
8	J	37	
9	K	86	
10	L	153	
11	M	31	

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
12	G9R	A	801	X	-	-	-
13	CL7	A	802	X	-	-	-
13	CL7	A	803	X	-	-	-
13	CL7	A	804	X	-	-	-
13	CL7	A	805	X	-	-	-
13	CL7	A	806	X	-	-	-
13	CL7	A	807	X	-	-	-
13	CL7	A	808	X	-	-	-
13	CL7	A	809	X	-	-	-
13	CL7	A	810	X	-	-	-
13	CL7	A	811	X	-	-	-
13	CL7	A	812	X	-	-	-
13	CL7	A	813	X	-	-	-
13	CL7	A	814	X	-	-	-
13	CL7	A	815	X	-	-	-
13	CL7	A	816	X	-	-	-
13	CL7	A	817	X	-	-	-
13	CL7	A	818	X	-	-	-
13	CL7	A	819	X	-	-	-
13	CL7	A	822	X	-	-	-
13	CL7	A	823	X	-	-	-
13	CL7	A	824	X	-	-	-
13	CL7	A	825	X	-	-	-
13	CL7	A	827	X	-	-	-
13	CL7	A	828	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
13	CL7	A	829	X	-	-	-
13	CL7	A	830	X	-	-	-
13	CL7	A	831	X	-	-	-
13	CL7	A	832	X	-	-	-
13	CL7	A	835	X	-	-	-
13	CL7	A	836	X	-	-	-
13	CL7	A	837	X	-	-	-
13	CL7	A	838	X	-	-	-
13	CL7	A	839	X	-	-	-
13	CL7	A	840	X	-	-	-
13	CL7	A	841	X	-	-	-
13	CL7	A	842	X	-	-	-
13	CL7	A	843	X	-	-	-
13	CL7	A	845	X	-	-	-
13	CL7	A	846	X	-	-	-
13	CL7	A	848	X	-	-	-
13	CL7	A	855	X	-	-	-
13	CL7	B	802	X	-	-	-
13	CL7	B	803	X	-	-	-
13	CL7	B	804	X	-	-	-
13	CL7	B	805	X	-	-	-
13	CL7	B	806	X	-	-	-
13	CL7	B	807	X	-	-	-
13	CL7	B	808	X	-	-	-
13	CL7	B	809	X	-	-	-
13	CL7	B	810	X	-	-	-
13	CL7	B	811	X	-	-	-
13	CL7	B	812	X	-	-	-
13	CL7	B	813	X	-	-	-
13	CL7	B	814	X	-	-	-
13	CL7	B	815	X	-	-	-
13	CL7	B	816	X	-	-	-
13	CL7	B	817	X	-	-	-
13	CL7	B	818	X	-	-	-
13	CL7	B	819	X	-	-	-
13	CL7	B	821	X	-	-	-
13	CL7	B	822	X	-	-	-
13	CL7	B	823	X	-	-	-
13	CL7	B	824	X	-	-	-
13	CL7	B	825	X	-	-	-
13	CL7	B	826	X	-	-	-
13	CL7	B	828	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
13	CL7	B	829	X	-	-	-
13	CL7	B	830	X	-	-	-
13	CL7	B	831	X	-	-	-
13	CL7	B	832	X	-	-	-
13	CL7	B	833	X	-	-	-
13	CL7	B	834	X	-	-	-
13	CL7	B	837	X	-	-	-
13	CL7	B	838	X	-	-	-
13	CL7	B	840	X	-	-	-
13	CL7	B	841	X	-	-	-
13	CL7	B	842	X	-	-	-
13	CL7	B	843	X	-	-	-
13	CL7	B	846	X	-	-	-
13	CL7	F	201	X	-	-	-
13	CL7	F	202	X	-	-	-
13	CL7	F	206	X	-	-	-
13	CL7	I	102	X	-	-	-
13	CL7	J	102	X	-	-	-
13	CL7	J	103	X	-	-	-
13	CL7	K	102	X	-	-	-
13	CL7	K	103	X	-	-	-
13	CL7	L	201	X	-	-	-
13	CL7	L	204	X	-	-	-
13	CL7	L	205	X	-	-	-
13	CL7	L	207	X	-	-	-
22	K3I	B	845	X	-	-	-

2 Entry composition (i)

There are 23 unique types of molecules in this entry. The entry contains 24496 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	741	5839	3813	994	1002	30	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	710	5598	3683	939	955	21	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	C	80	599	368	103	117	11	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	D	136	1037	649	180	202	6	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	E	69	540	339	96	104	1	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	F	139	1034	650	181	198	5	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
7	I	32	Total	C	N	O	S	0	0
			242	161	35	42	4		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
8	J	35	Total	C	N	O	S	0	0
			292	207	40	44	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
9	K	69	Total	C	N	O	S	0	0
			506	334	85	84	3		

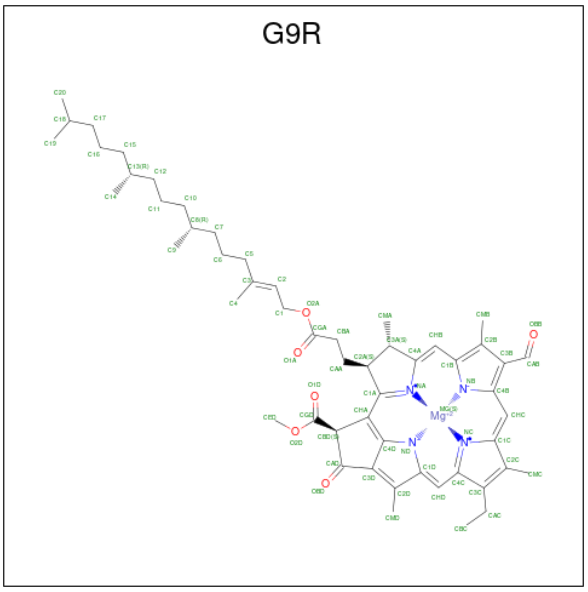
- Molecule 10 is a protein called Photosystem I reaction center subunit XI.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	L	148	Total	C	N	O	S	0	0
			1059	680	177	195	7		

- Molecule 11 is a protein called Photosystem I reaction center subunit XII.

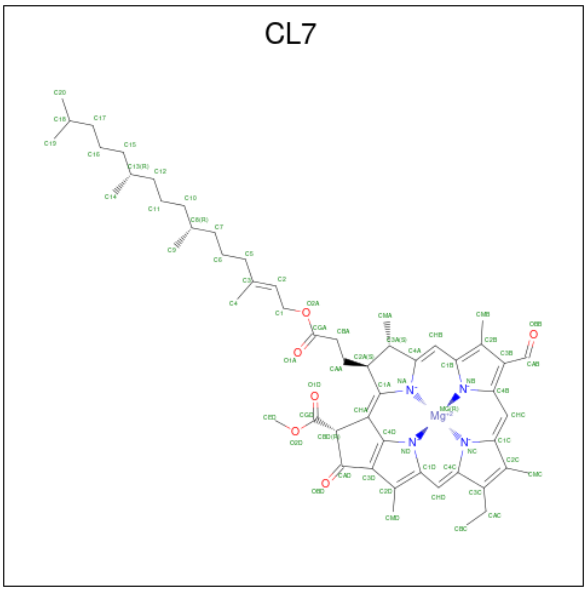
Mol	Chain	Residues	Atoms					AltConf	Trace
11	M	31	Total	C	N	O	S	0	0
			222	146	34	41	1		

- Molecule 12 is CHLOROPHYLL D ISOMER (CCD ID: G9R) (formula: $C_{54}H_{70}MgN_4O_6$).



Mol	Chain	Residues	Atoms					AltConf
12	A	1	Total	C	Mg	N	O	0
			65	54	1	4	6	

- Molecule 13 is CHLOROPHYLL D (CCD ID: CL7) (formula: $C_{54}H_{70}MgN_4O_6$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
13	A	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
13	A	1	Total	C	Mg	N	O	0
			65	54	1	4	6	

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Mol	Chain	Residues	Atoms					AltConf
13	A	1	Total	C	Mg	N	O	0
			55	44	1	4	6	
13	A	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
13	A	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
13	A	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
13	A	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
13	A	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
13	A	1	Total	C	Mg	N	O	0
			41	32	1	4	4	
13	A	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
13	A	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
13	A	1	Total	C	Mg	N	O	0
			50	39	1	4	6	
13	A	1	Total	C	Mg	N	O	0
			60	49	1	4	6	
13	A	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
13	A	1	Total	C	Mg	N	O	0
			50	39	1	4	6	
13	A	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
13	A	1	Total	C	Mg	N	O	0
			55	44	1	4	6	
13	A	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
13	A	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
13	A	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
13	A	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
13	A	1	Total	C	Mg	N	O	0
			60	49	1	4	6	

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Mol	Chain	Residues	Atoms					AltConf
13	A	1	Total	C	Mg	N	O	0
			60	49	1	4	6	
13	A	1	Total	C	Mg	N	O	0
			50	39	1	4	6	
13	A	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
13	A	1	Total	C	Mg	N	O	0
			45	34	1	4	6	
13	A	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
13	A	1	Total	C	Mg	N	O	0
			55	44	1	4	6	
13	A	1	Total	C	Mg	N	O	0
			60	49	1	4	6	
13	A	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
13	A	1	Total	C	Mg	N	O	0
			60	49	1	4	6	
13	A	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
13	A	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
13	A	1	Total	C	Mg	N	O	0
			60	49	1	4	6	
13	A	1	Total	C	Mg	N	O	0
			60	49	1	4	6	
13	A	1	Total	C	Mg	N	O	0
			50	39	1	4	6	
13	A	1	Total	C	Mg	N	O	0
			50	39	1	4	6	
13	A	1	Total	C	Mg	N	O	0
			45	34	1	4	6	
13	A	1	Total	C	Mg	N	O	0
			45	34	1	4	6	
13	A	1	Total	C	Mg	N	O	0
			41	32	1	4	4	
13	B	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
13	B	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
13	B	1	Total	C	Mg	N	O	0
			65	54	1	4	6	

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Mol	Chain	Residues	Atoms					AltConf
13	B	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
13	B	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
13	B	1	Total	C	Mg	N	O	0
			50	39	1	4	6	
13	B	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
13	B	1	Total	C	Mg	N	O	0
			41	32	1	4	4	
13	B	1	Total	C	Mg	N	O	0
			45	34	1	4	6	
13	B	1	Total	C	Mg	N	O	0
			41	32	1	4	4	
13	B	1	Total	C	Mg	N	O	0
			60	49	1	4	6	
13	B	1	Total	C	Mg	N	O	0
			41	32	1	4	4	
13	B	1	Total	C	Mg	N	O	0
			56	45	1	4	6	
13	B	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
13	B	1	Total	C	Mg	N	O	0
			50	39	1	4	6	
13	B	1	Total	C	Mg	N	O	0
			50	39	1	4	6	
13	B	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
13	B	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
13	B	1	Total	C	Mg	N	O	0
			54	43	1	4	6	
13	B	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
13	B	1	Total	C	Mg	N	O	0
			55	44	1	4	6	
13	B	1	Total	C	Mg	N	O	0
			45	34	1	4	6	
13	B	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
13	B	1	Total	C	Mg	N	O	0
			65	54	1	4	6	

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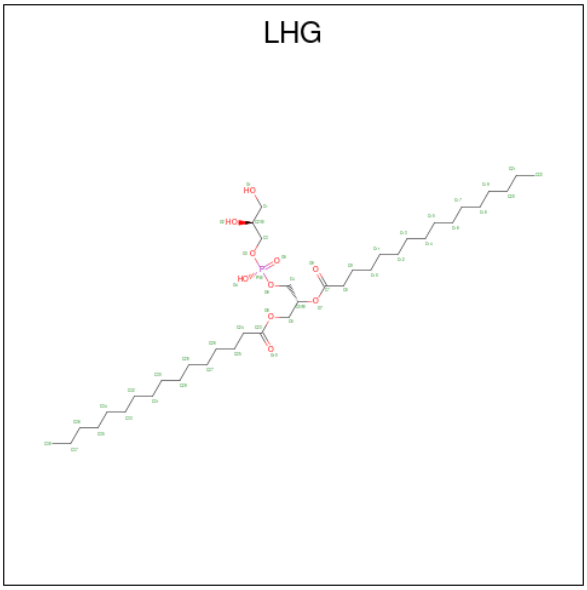
Mol	Chain	Residues	Atoms					AltConf
13	B	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
13	B	1	Total	C	Mg	N	O	0
			45	34	1	4	6	
13	B	1	Total	C	Mg	N	O	0
			45	34	1	4	6	
13	B	1	Total	C	Mg	N	O	0
			50	39	1	4	6	
13	B	1	Total	C	Mg	N	O	0
			50	39	1	4	6	
13	B	1	Total	C	Mg	N	O	0
			45	34	1	4	6	
13	B	1	Total	C	Mg	N	O	0
			45	34	1	4	6	
13	B	1	Total	C	Mg	N	O	0
			50	39	1	4	6	
13	B	1	Total	C	Mg	N	O	0
			45	34	1	4	6	
13	B	1	Total	C	Mg	N	O	0
			45	34	1	4	6	
13	B	1	Total	C	Mg	N	O	0
			45	34	1	4	6	
13	B	1	Total	C	Mg	N		0
			27	22	1	4		
13	B	1	Total	C	Mg	N	O	0
			45	34	1	4	6	
13	B	1	Total	C	Mg	N	O	0
			41	32	1	4	4	
13	F	1	Total	C	Mg	N	O	0
			60	49	1	4	6	
13	F	1	Total	C	Mg	N	O	0
			45	34	1	4	6	
13	F	1	Total	C	Mg	N	O	0
			45	34	1	4	6	
13	I	1	Total	C	Mg	N	O	0
			45	34	1	4	6	
13	J	1	Total	C	Mg	N	O	0
			60	49	1	4	6	
13	J	1	Total	C	Mg	N	O	0
			42	33	1	4	4	
13	K	1	Total	C	Mg	N	O	0
			41	32	1	4	4	

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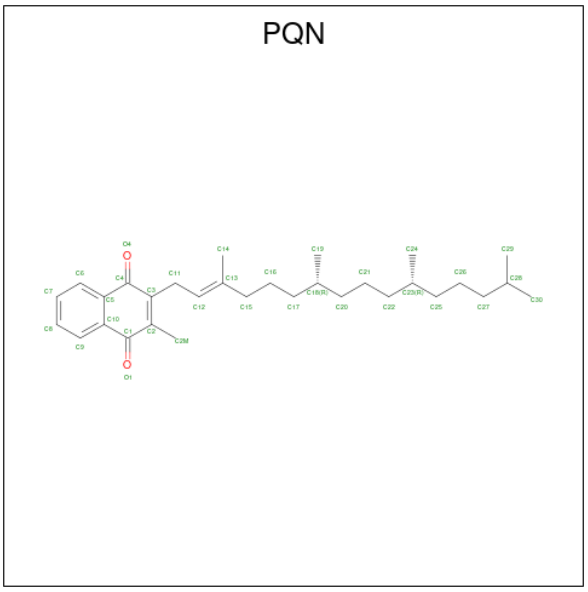
Mol	Chain	Residues	Atoms					AltConf
13	K	1	Total	C	Mg	N	O	0
			37	30	1	4	2	
13	L	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
13	L	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
13	L	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
13	L	1	Total	C	Mg	N	O	0
			65	54	1	4	6	

- Molecule 14 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (CCD ID: LHG) (formula: $C_{38}H_{75}O_{10}P$).



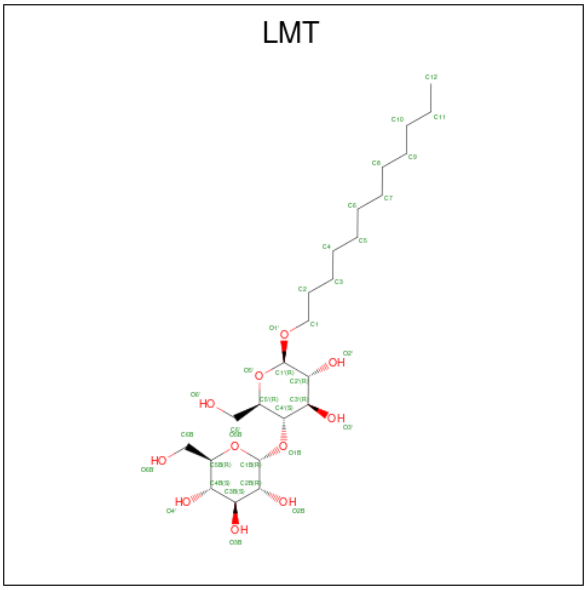
Mol	Chain	Residues	Atoms				AltConf
14	A	1	Total	C	O	P	0
			49	38	10	1	
14	A	1	Total	C	O	P	0
			46	35	10	1	
14	B	1	Total	O	P		0
			5	4	1		
14	L	1	Total	C	O	P	0
			43	32	10	1	

- Molecule 15 is PHYLLOQUINONE (CCD ID: PQN) (formula: $C_{31}H_{46}O_2$).



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

- Molecule 16 is DODECYL-BETA-D-MALTOSIDE (CCD ID: LMT) (formula: $C_{24}H_{46}O_{11}$).



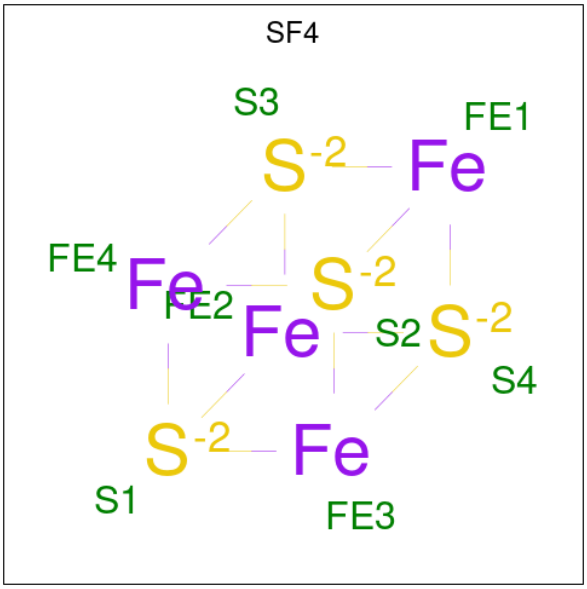
Mol	Chain	Residues	Atoms	AltConf
16	A	1	Total C O 35 24 11	0
16	A	1	Total C O 35 24 11	0

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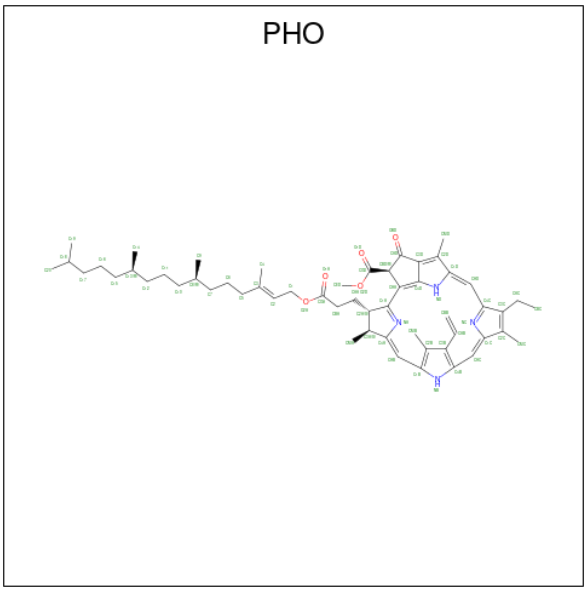
Mol	Chain	Residues	Atoms	AltConf
16	A	1	Total C O 24 18 6	0
16	B	1	Total C O 24 18 6	0
16	B	1	Total C O 22 16 6	0
16	F	1	Total C O 30 19 11	0
16	K	1	Total C O 18 12 6	0
16	L	1	Total C O 35 24 11	0

- Molecule 17 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe_4S_4).



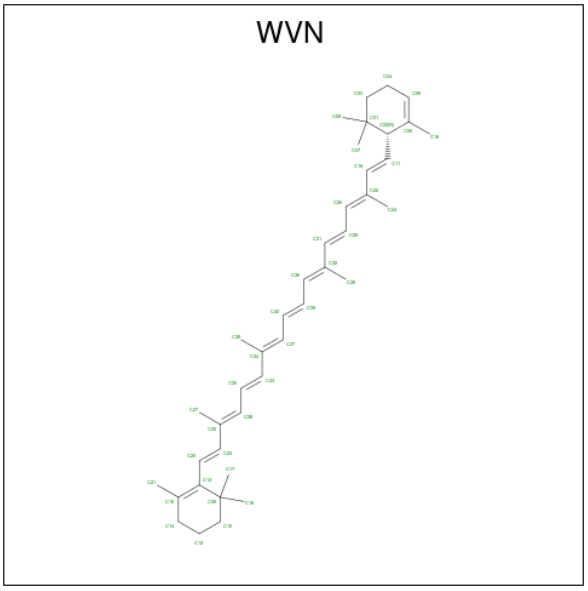
Mol	Chain	Residues	Atoms	AltConf
17	A	1	Total Fe S 8 4 4	0
17	C	1	Total Fe S 8 4 4	0
17	C	1	Total Fe S 8 4 4	0

- Molecule 18 is PHEOPHYTIN A (CCD ID: PHO) (formula: $C_{55}H_{74}N_4O_5$).



Mol	Chain	Residues	Atoms				AltConf
18	A	1	Total	C	N	O	0
			64	55	4	5	
18	B	1	Total	C	N	O	0
			64	55	4	5	

- Molecule 19 is 1,3,3-trimethyl-2-[(1E,3E,5E,7E,9E,11E,13E,15E,17E)-3,7,12,16-tetramethyl-18-[(1R)-2,6,6-trimethylcyclohex-2-en-1-yl]octadeca-1,3,5,7,9,11,13,15,17-nonaenyl]cyclohexene (CCD ID: WVN) (formula: $C_{40}H_{56}$).



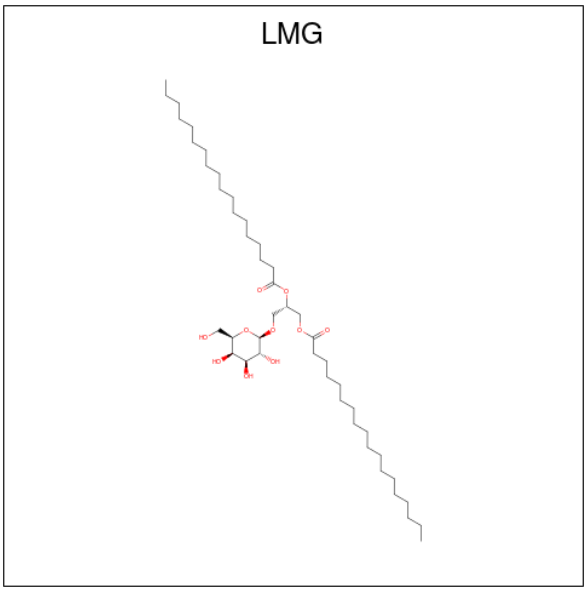
Mol	Chain	Residues	Atoms		AltConf
19	A	1	Total	C	0
			40	40	

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Mol	Chain	Residues	Atoms	AltConf
19	A	1	Total C 40 40	0
19	A	1	Total C 40 40	0
19	A	1	Total C 40 40	0
19	A	1	Total C 40 40	0
19	B	1	Total C 40 40	0
19	B	1	Total C 40 40	0
19	F	1	Total C 40 40	0
19	F	1	Total C 40 40	0
19	I	1	Total C 40 40	0
19	J	1	Total C 40 40	0
19	J	1	Total C 40 40	0
19	K	1	Total C 40 40	0
19	L	1	Total C 40 40	0
19	L	1	Total C 40 40	0
19	L	1	Total C 40 40	0
19	M	1	Total C 40 40	0

- Molecule 20 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (CCD ID: LMG) (formula: $C_{45}H_{86}O_{10}$).

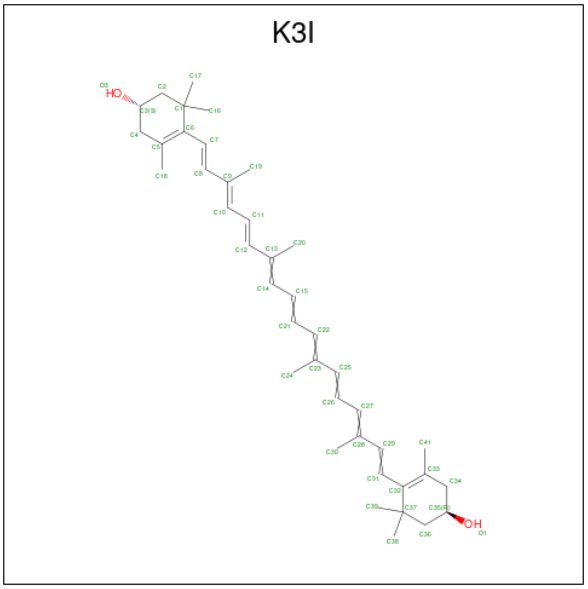


Mol	Chain	Residues	Atoms			AltConf
20	B	1	Total 55	C 45	O 10	0
20	L	1	Total 47	C 37	O 10	0

- Molecule 21 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		AltConf
21	B	1	Total 1	Ca 1	0

- Molecule 22 is Zeaxanthin (CCD ID: K3I) (formula: $C_{40}H_{56}O_2$).



Mol	Chain	Residues	Atoms			AltConf
22	B	1	Total	C	O	0
			42	40	2	

- Molecule 23 is water.

Mol	Chain	Residues	Atoms		AltConf
23	A	344	Total	O	0
			344	344	
23	B	323	Total	O	0
			323	323	
23	C	86	Total	O	0
			86	86	
23	D	78	Total	O	0
			78	78	
23	E	31	Total	O	0
			31	31	
23	F	23	Total	O	0
			23	23	
23	I	6	Total	O	0
			6	6	
23	J	9	Total	O	0
			9	9	
23	K	4	Total	O	0
			4	4	
23	L	78	Total	O	0
			78	78	
23	M	9	Total	O	0
			9	9	

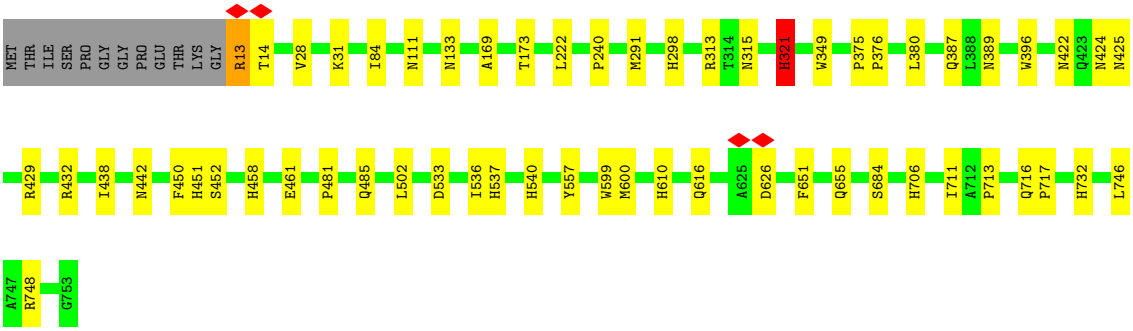
3 Residue-property plots (i)

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

• Molecule 1: Photosystem I P700 chlorophyll a apoprotein A1

Chain A:

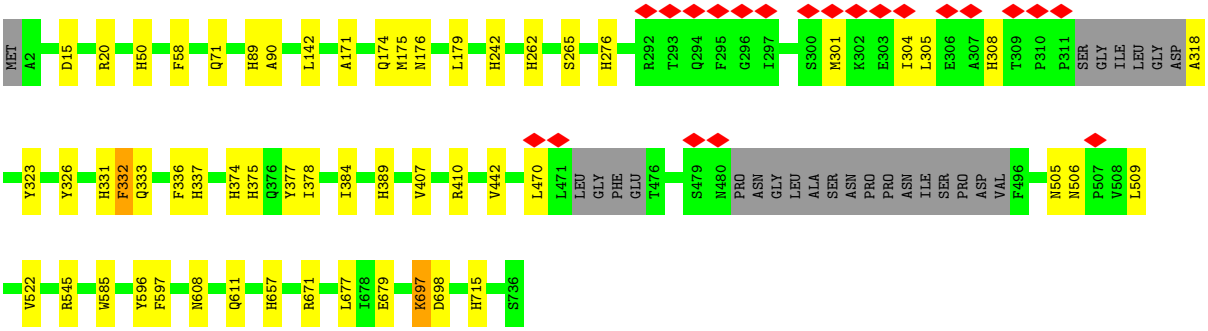




• Molecule 2: Photosystem I P700 chlorophyll a apoprotein A2

Chain B:

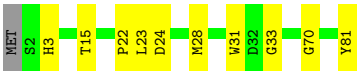




• Molecule 3: Photosystem I iron-sulfur center

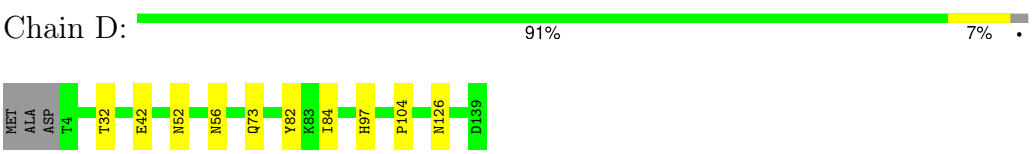
Chain C:





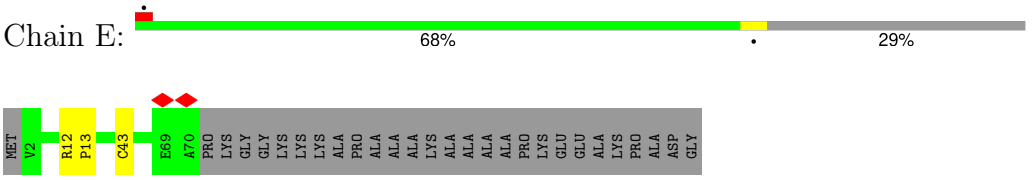
• Molecule 4: Photosystem I reaction center subunit II

Chain D:



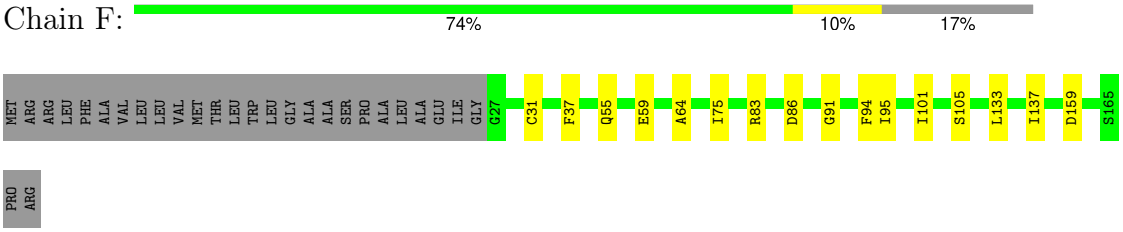
• Molecule 5: Photosystem I reaction center subunit IV

Chain E:



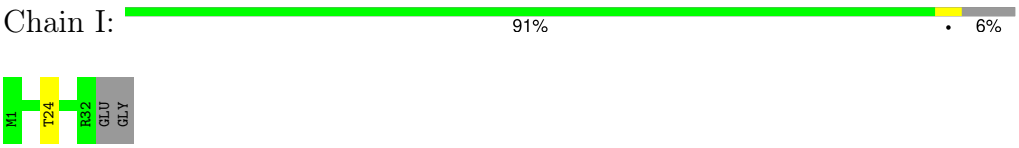
• Molecule 6: Photosystem I reaction center subunit III

Chain F:



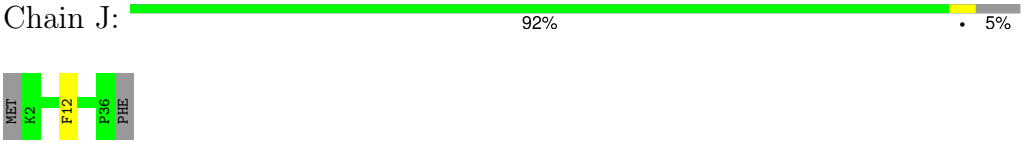
• Molecule 7: Photosystem I reaction center subunit VIII

Chain I:



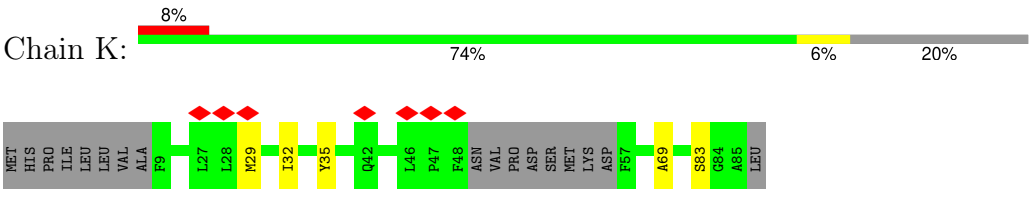
• Molecule 8: Photosystem I reaction center subunit IX

Chain J:



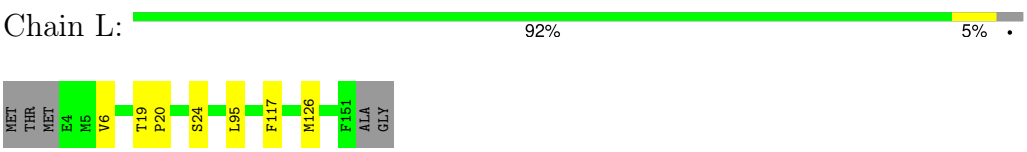
• Molecule 9: Photosystem I reaction center subunit PsaK

Chain K:



• Molecule 10: Photosystem I reaction center subunit XI

Chain L:



• Molecule 11: Photosystem I reaction center subunit XII

Chain M: 

There are no outlier residues recorded for this chain.

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	1035501	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	50	Depositor
Minimum defocus (nm)	700	Depositor
Maximum defocus (nm)	1900	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	1.767	Depositor
Minimum map value	-0.895	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.014	Depositor
Recommended contour level	0.043	Depositor
Map size (Å)	350.28, 350.28, 350.28	wwPDB
Map dimensions	500, 500, 500	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.70056, 0.70056, 0.70056	Depositor

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: PQN, LHG, LMT, K3I, CL7, PHO, LMG, WVN, SF4, CA, G9R

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	0.49	7/6036 (0.1%)	0.64	2/8224 (0.0%)
2	B	0.49	12/5804 (0.2%)	0.62	1/7930 (0.0%)
3	C	0.31	0/609	0.72	0/824
4	D	0.25	0/1057	0.59	0/1426
5	E	0.20	0/550	0.52	0/745
6	F	0.28	0/1055	0.65	0/1432
7	I	0.30	0/247	0.60	0/336
8	J	0.22	0/304	0.58	0/412
9	K	0.29	0/519	0.70	0/706
10	L	0.31	0/1084	0.57	0/1475
11	M	0.29	0/222	0.47	0/301
All	All	0.43	19/17487 (0.1%)	0.63	3/23811 (0.0%)

The worst 5 of 19 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	657	HIS	C-O	-9.42	1.13	1.24
1	A	458	HIS	C-O	-9.33	1.13	1.24
1	A	450	PHE	C-O	-8.73	1.14	1.24
1	A	537	HIS	C-O	-8.09	1.14	1.24
2	B	697	LYS	C-O	-7.84	1.14	1.24

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	458	HIS	CA-C-O	-6.39	114.06	120.90
1	A	321	HIS	N-CA-C	-5.69	99.91	109.07
2	B	671	ARG	N-CA-C	5.16	116.59	111.07

There are no chirality outliers.

There are no planarity outliers.

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	5839	0	5668	39	0
2	B	5598	0	5312	42	0
3	C	599	0	579	7	0
4	D	1037	0	1033	7	0
5	E	540	0	524	2	0
6	F	1034	0	1034	10	0
7	I	242	0	252	1	0
8	J	292	0	289	1	0
9	K	506	0	510	3	0
10	L	1059	0	1063	5	0
11	M	222	0	255	0	0
12	A	65	0	0	0	0
13	A	2417	0	2340	44	0
13	B	2011	0	1749	49	0
13	F	150	0	119	2	0
13	I	45	0	31	0	0
13	J	102	0	84	4	0
13	K	78	0	49	0	0
13	L	260	0	280	10	0
14	A	95	0	139	1	0
14	B	5	0	0	0	0
14	L	43	0	59	6	0
15	A	33	0	46	0	0
15	B	33	0	46	0	0
16	A	94	0	127	1	0
16	B	46	0	63	0	0
16	F	30	0	33	2	0
16	K	18	0	20	0	0
16	L	35	0	46	1	0
17	A	8	0	0	0	0
17	C	16	0	0	0	0
18	A	64	0	74	2	0
18	B	64	0	74	3	0
19	A	200	0	0	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
19	B	80	0	0	2	0
19	F	80	0	0	2	0
19	I	40	0	0	0	0
19	J	80	0	0	1	0
19	K	40	0	0	0	0
19	L	120	0	0	0	0
19	M	40	0	0	0	0
20	B	55	0	86	3	0
20	L	47	0	64	2	0
21	B	1	0	0	0	0
22	B	42	0	0	0	0
23	A	344	0	0	0	0
23	B	323	0	0	0	0
23	C	86	0	0	0	0
23	D	78	0	0	0	0
23	E	31	0	0	0	0
23	F	23	0	0	0	0
23	I	6	0	0	0	0
23	J	9	0	0	0	0
23	K	4	0	0	0	0
23	L	78	0	0	0	0
23	M	9	0	0	0	0
All	All	24496	0	22048	196	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 4.

The worst 5 of 196 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)
1:A:13:ARG:CZ	1:A:14:THR:HB	1.88	1.02
1:A:313:ARG:NH1	1:A:321:HIS:ND1	2.21	0.88
13:B:806:CL7:H2	13:B:806:CL7:H101	1.66	0.78
4:D:42:GLU:H	4:D:73:GLN:HE22	1.33	0.75
4:D:52:ASN:H	4:D:56:ASN:HD21	1.38	0.70

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	739/753 (98%)	720 (97%)	18 (2%)	1 (0%)	48 38
2	B	702/736 (95%)	685 (98%)	17 (2%)	0	100 100
3	C	78/81 (96%)	76 (97%)	2 (3%)	0	100 100
4	D	134/139 (96%)	129 (96%)	5 (4%)	0	100 100
5	E	67/97 (69%)	65 (97%)	2 (3%)	0	100 100
6	F	137/167 (82%)	134 (98%)	3 (2%)	0	100 100
7	I	30/34 (88%)	30 (100%)	0	0	100 100
8	J	33/37 (89%)	33 (100%)	0	0	100 100
9	K	65/86 (76%)	61 (94%)	3 (5%)	1 (2%)	8 2
10	L	146/153 (95%)	144 (99%)	2 (1%)	0	100 100
11	M	29/31 (94%)	29 (100%)	0	0	100 100
All	All	2160/2314 (93%)	2106 (98%)	52 (2%)	2 (0%)	49 38

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	626	ASP
9	K	83	SER

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	597/606 (98%)	595 (100%)	2 (0%)	86 84
2	B	558/593 (94%)	557 (100%)	1 (0%)	87 86
3	C	68/69 (99%)	68 (100%)	0	100 100
4	D	111/113 (98%)	111 (100%)	0	100 100
5	E	58/73 (80%)	58 (100%)	0	100 100
6	F	110/131 (84%)	110 (100%)	0	100 100
7	I	26/27 (96%)	26 (100%)	0	100 100
8	J	31/33 (94%)	31 (100%)	0	100 100
9	K	49/68 (72%)	49 (100%)	0	100 100
10	L	109/113 (96%)	109 (100%)	0	100 100
11	M	25/25 (100%)	25 (100%)	0	100 100
All	All	1742/1851 (94%)	1739 (100%)	3 (0%)	85 86

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	13	ARG
1	A	321	HIS
2	B	697	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 64 such sidechains are listed below:

Mol	Chain	Res	Type
4	D	136	ASN
6	F	55	GLN
1	A	540	HIS
1	A	525	GLN
6	F	107	ASN

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)

Of 132 ligands modelled in this entry, 1 is monoatomic - leaving 131 for Mogul analysis.

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	$\#\|Z\| > 2$
13	CL7	B	823	2	59,63,73	2.49	20 (33%)	68,101,113	2.51	26 (38%)
17	SF4	A	847	2,1	0,12,12	-	-	-		
19	WVN	F	205	-	40,41,41	4.09	21 (52%)	51,56,56	2.50	16 (31%)
13	CL7	A	817	1	69,73,73	2.30	20 (28%)	80,113,113	2.32	25 (31%)
13	CL7	A	809	13,1	69,73,73	2.31	22 (31%)	80,113,113	2.49	28 (35%)
13	CL7	B	829	-	49,53,73	2.65	20 (40%)	56,89,113	2.78	24 (42%)
13	CL7	K	103	9	42,45,73	2.73	21 (50%)	51,78,113	2.62	20 (39%)
13	CL7	B	824	-	49,53,73	2.66	21 (42%)	56,89,113	2.76	22 (39%)
15	PQN	B	820	-	34,34,34	1.62	2 (5%)	43,45,45	1.02	4 (9%)
13	CL7	B	833	-	49,53,73	2.67	21 (42%)	56,89,113	2.58	23 (41%)
19	WVN	J	104	-	40,41,41	4.02	21 (52%)	51,56,56	2.42	18 (35%)
13	CL7	A	819	23	69,73,73	2.29	21 (30%)	80,113,113	2.28	28 (35%)
19	WVN	A	852	-	40,41,41	3.87	20 (50%)	51,56,56	2.57	19 (37%)
13	CL7	A	829	1	54,58,73	2.62	22 (40%)	62,95,113	2.71	24 (38%)
13	CL7	A	812	1	69,73,73	2.30	22 (31%)	80,113,113	2.29	25 (31%)
13	CL7	J	102	2	64,68,73	2.32	20 (31%)	74,107,113	2.71	28 (37%)
13	CL7	L	204	10	69,73,73	2.30	21 (30%)	80,113,113	2.37	24 (30%)
13	CL7	B	806	2	69,73,73	2.25	22 (31%)	80,113,113	2.43	28 (35%)
13	CL7	B	814	2	60,64,73	2.46	20 (33%)	69,102,113	2.49	25 (36%)
16	LMT	A	844	-	24,24,36	0.50	0	29,29,47	0.81	2 (6%)
13	CL7	A	837	1	69,73,73	2.25	21 (30%)	80,113,113	2.33	23 (28%)
13	CL7	B	826	2	69,73,73	2.31	21 (30%)	80,113,113	2.34	25 (31%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
13	CL7	B	805	2	69,73,73	2.26	21 (30%)	80,113,113	2.32	25 (31%)
16	LMT	F	203	-	31,31,36	0.58	0	42,42,47	1.23	4 (9%)
13	CL7	F	201	23	64,68,73	2.42	21 (32%)	74,107,113	2.43	24 (32%)
13	CL7	A	805	1	69,73,73	2.30	22 (31%)	80,113,113	2.33	27 (33%)
13	CL7	A	814	1	64,68,73	2.40	22 (34%)	74,107,113	2.40	23 (31%)
13	CL7	B	830	2	49,53,73	2.65	21 (42%)	56,89,113	2.68	21 (37%)
13	CL7	B	817	2	54,58,73	2.60	22 (40%)	62,95,113	2.60	22 (35%)
14	LHG	B	844	13	4,4,48	1.75	2 (50%)	6,6,54	1.33	1 (16%)
19	WVN	M	101	-	40,41,41	3.92	22 (55%)	51,56,56	2.60	20 (39%)
13	CL7	A	815	1	69,73,73	2.34	22 (31%)	80,113,113	2.22	23 (28%)
13	CL7	B	837	2	54,58,73	2.62	21 (38%)	62,95,113	2.62	24 (38%)
13	CL7	A	839	23	69,73,73	2.32	22 (31%)	80,113,113	3.80	26 (32%)
13	CL7	B	810	2	49,53,73	2.62	20 (40%)	56,89,113	2.68	21 (37%)
22	K3I	B	845	-	43,43,43	3.98	22 (51%)	56,60,60	2.04	15 (26%)
13	CL7	A	807	1	69,73,73	2.28	20 (28%)	80,113,113	2.36	24 (30%)
13	CL7	B	832	2	54,58,73	2.63	23 (42%)	62,95,113	2.69	25 (40%)
13	CL7	B	838	-	49,53,73	2.67	20 (40%)	56,89,113	2.58	20 (35%)
13	CL7	B	803	2	69,73,73	2.28	21 (30%)	80,113,113	2.28	24 (30%)
13	CL7	B	825	2	69,73,73	2.31	22 (31%)	80,113,113	2.33	22 (27%)
13	CL7	A	804	13,1	59,63,73	2.51	21 (35%)	68,101,113	2.55	25 (36%)
15	PQN	A	826	-	34,34,34	1.62	2 (5%)	43,45,45	1.13	4 (9%)
13	CL7	A	824	1	69,73,73	2.31	20 (28%)	80,113,113	2.33	22 (27%)
14	LHG	A	820	-	48,48,48	0.93	2 (4%)	51,54,54	1.08	3 (5%)
19	WVN	B	848	-	40,41,41	3.84	21 (52%)	51,56,56	2.48	16 (31%)
13	CL7	L	207	23	69,73,73	2.32	20 (28%)	80,113,113	2.40	24 (30%)
13	CL7	A	825	1	69,73,73	2.31	20 (28%)	80,113,113	2.32	24 (30%)
13	CL7	A	832	1	69,73,73	2.28	23 (33%)	80,113,113	2.30	25 (31%)
19	WVN	I	101	-	40,41,41	3.95	21 (52%)	51,56,56	2.43	20 (39%)
16	LMT	A	833	-	36,36,36	0.49	0	47,47,47	1.45	8 (17%)
13	CL7	A	838	1	64,68,73	2.44	23 (35%)	74,107,113	2.48	21 (28%)
13	CL7	A	848	1	49,53,73	2.66	22 (44%)	56,89,113	4.18	21 (37%)
13	CL7	L	205	10	69,73,73	2.29	21 (30%)	80,113,113	2.40	23 (28%)
17	SF4	C	102	3	0,12,12	-	-	-		
13	CL7	A	842	23	64,68,73	2.39	21 (32%)	74,107,113	2.41	26 (35%)
18	PHO	A	849	-	58,69,69	0.92	4 (6%)	55,99,99	1.17	3 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
13	CL7	A	806	1	69,73,73	2.32	20 (28%)	80,113,113	2.37	26 (32%)
16	LMT	K	104	-	18,18,36	0.52	0	23,23,47	1.89	4 (17%)
16	LMT	L	206	-	36,36,36	0.58	0	47,47,47	0.65	0
13	CL7	A	845	1	54,58,73	2.63	21 (38%)	62,95,113	2.65	22 (35%)
13	CL7	B	846	-	45,49,73	2.77	20 (44%)	51,84,113	2.80	23 (45%)
13	CL7	B	821	2	58,62,73	2.49	21 (36%)	66,99,113	2.55	26 (39%)
19	WVN	L	202	-	40,41,41	3.90	21 (52%)	51,56,56	2.52	20 (39%)
19	WVN	B	847	-	40,41,41	3.96	20 (50%)	51,56,56	2.54	18 (35%)
13	CL7	B	816	2	54,58,73	2.63	22 (40%)	62,95,113	2.62	23 (37%)
13	CL7	B	834	-	49,53,73	2.68	21 (42%)	56,89,113	2.65	20 (35%)
13	CL7	A	816	1	54,58,73	2.64	21 (38%)	62,95,113	2.60	25 (40%)
19	WVN	L	209	-	40,41,41	3.82	21 (52%)	51,56,56	2.25	20 (39%)
19	WVN	K	101	-	40,41,41	4.00	21 (52%)	51,56,56	2.42	18 (35%)
13	CL7	L	201	1	69,73,73	2.28	21 (30%)	80,113,113	2.33	27 (33%)
13	CL7	I	102	-	49,53,73	2.63	20 (40%)	56,89,113	2.62	21 (37%)
13	CL7	A	830	1	69,73,73	2.32	20 (28%)	80,113,113	2.37	23 (28%)
13	CL7	A	818	1	59,63,73	2.48	21 (35%)	68,101,113	2.52	23 (33%)
13	CL7	B	843	14	49,53,73	2.62	21 (42%)	56,89,113	2.62	22 (39%)
13	CL7	A	841	1	64,68,73	2.38	21 (32%)	74,107,113	2.46	23 (31%)
13	CL7	B	811	2	45,49,73	2.78	22 (48%)	51,84,113	2.64	22 (43%)
19	WVN	A	851	-	40,41,41	4.01	21 (52%)	51,56,56	2.72	21 (41%)
12	G9R	A	801	1	69,73,73	2.22	22 (31%)	82,113,113	2.33	24 (29%)
20	LMG	B	827	-	55,55,55	1.51	8 (14%)	63,63,63	1.03	1 (1%)
13	CL7	F	202	6	49,53,73	2.67	22 (44%)	56,89,113	2.64	19 (33%)
13	CL7	B	822	2	69,73,73	2.27	22 (31%)	80,113,113	2.43	28 (35%)
13	CL7	B	808	2	69,73,73	2.27	22 (31%)	80,113,113	2.27	22 (27%)
13	CL7	A	835	1	59,63,73	2.49	22 (37%)	68,101,113	2.54	24 (35%)
13	CL7	A	823	1	69,73,73	2.31	21 (30%)	80,113,113	2.47	27 (33%)
13	CL7	A	808	1	69,73,73	2.32	22 (31%)	80,113,113	2.32	25 (31%)
16	LMT	B	836	-	22,22,36	0.49	0	27,27,47	0.72	0
13	CL7	B	819	2	69,73,73	2.32	21 (30%)	80,113,113	2.38	22 (27%)
13	CL7	J	103	8	44,50,73	2.69	21 (47%)	53,85,113	2.55	17 (32%)
19	WVN	A	850	-	40,41,41	3.99	20 (50%)	51,56,56	2.39	19 (37%)
14	LHG	L	208	-	42,42,48	0.99	2 (4%)	45,48,54	1.00	2 (4%)
13	CL7	A	811	1	69,73,73	2.30	22 (31%)	80,113,113	2.25	23 (28%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
17	SF4	C	101	3	0,12,12	-	-	-		
13	CL7	A	855	14	45,49,73	2.77	21 (46%)	51,84,113	2.62	20 (39%)
13	CL7	A	803	1	69,73,73	2.33	22 (31%)	80,113,113	2.36	24 (30%)
13	CL7	A	822	1	69,73,73	2.32	23 (33%)	80,113,113	2.26	24 (30%)
13	CL7	B	815	2	69,73,73	2.30	20 (28%)	80,113,113	2.31	30 (37%)
13	CL7	B	842	-	27,35,73	3.36	14 (51%)	29,60,113	2.75	14 (48%)
13	CL7	A	831	23	49,53,73	2.66	21 (42%)	56,89,113	2.57	18 (32%)
13	CL7	A	840	1	69,73,73	2.33	23 (33%)	80,113,113	2.32	25 (31%)
13	CL7	B	828	2	69,73,73	2.29	21 (30%)	80,113,113	2.36	24 (30%)
19	WVN	A	853	-	40,41,41	3.92	21 (52%)	51,56,56	2.47	20 (39%)
13	CL7	F	206	23	49,53,73	2.64	22 (44%)	56,89,113	2.65	19 (33%)
13	CL7	B	812	2	64,68,73	2.39	23 (35%)	74,107,113	2.45	22 (29%)
13	CL7	B	818	23	69,73,73	2.29	22 (31%)	80,113,113	2.32	24 (30%)
13	CL7	A	836	1	64,68,73	2.39	21 (32%)	74,107,113	2.38	27 (36%)
13	CL7	B	813	2	45,49,73	2.75	20 (44%)	51,84,113	2.65	20 (39%)
19	WVN	L	210	-	40,41,41	3.98	21 (52%)	51,56,56	2.81	22 (43%)
13	CL7	B	831	23	54,58,73	2.61	21 (38%)	62,95,113	2.73	26 (41%)
13	CL7	B	809	2	45,49,73	2.78	21 (46%)	51,84,113	2.75	20 (39%)
14	LHG	A	821	13	45,45,48	0.96	2 (4%)	48,51,54	1.05	4 (8%)
19	WVN	J	101	-	40,41,41	4.02	21 (52%)	51,56,56	2.36	22 (43%)
16	LMT	A	834	-	36,36,36	0.54	0	47,47,47	0.72	0
13	CL7	A	810	23	45,49,73	2.76	21 (46%)	51,84,113	2.85	22 (43%)
19	WVN	F	204	-	40,41,41	3.98	21 (52%)	51,56,56	2.61	20 (39%)
16	LMT	B	835	-	24,24,36	0.51	0	29,29,47	0.56	0
13	CL7	A	846	1	49,53,73	2.62	20 (40%)	56,89,113	2.66	21 (37%)
13	CL7	B	802	23	69,73,73	2.30	20 (28%)	80,113,113	2.38	28 (35%)
19	WVN	A	854	-	40,41,41	3.89	21 (52%)	51,56,56	2.31	14 (27%)
13	CL7	A	802	23	69,73,73	2.30	20 (28%)	80,113,113	2.31	23 (28%)
13	CL7	B	841	2	49,53,73	2.62	20 (40%)	56,89,113	2.94	24 (42%)
18	PHO	B	801	-	58,69,69	0.77	3 (5%)	55,99,99	1.24	3 (5%)
13	CL7	B	804	2	69,73,73	2.31	21 (30%)	80,113,113	2.30	26 (32%)
13	CL7	B	807	2	54,58,73	2.57	20 (37%)	62,95,113	2.51	22 (35%)
13	CL7	A	827	1	64,68,73	2.42	23 (35%)	74,107,113	2.44	23 (31%)
13	CL7	A	843	23	54,58,73	2.58	21 (38%)	62,95,113	2.67	28 (45%)
13	CL7	B	840	2	49,53,73	2.66	21 (42%)	56,89,113	2.63	22 (39%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
13	CL7	A	828	1	64,68,73	2.40	21 (32%)	74,107,113	2.47	25 (33%)
20	LMG	L	203	-	47,47,55	1.42	7 (14%)	55,55,63	1.37	6 (10%)
13	CL7	K	102	23	45,49,73	2.78	21 (46%)	51,84,113	2.62	18 (35%)
13	CL7	A	813	1	54,58,73	2.57	21 (38%)	62,95,113	2.67	26 (41%)

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
13	CL7	B	823	2	2/2/13/20	7/27/103/115	-
19	WVN	F	205	-	-	11/29/63/63	0/2/2/2
17	SF4	A	847	2,1	-	-	0/6/5/5
13	CL7	A	817	1	2/2/15/20	15/39/115/115	-
13	CL7	A	809	13,1	2/2/15/20	15/39/115/115	-
13	CL7	B	829	-	1/1/11/20	9/15/91/115	-
13	CL7	K	103	9	2/2/8/20	2/4/76/115	-
13	CL7	B	824	-	1/1/11/20	5/15/91/115	-
15	PQN	B	820	-	-	2/23/43/43	0/2/2/2
13	CL7	B	833	-	2/2/11/20	4/15/91/115	-
19	WVN	J	104	-	-	5/29/63/63	0/2/2/2
13	CL7	A	819	23	2/2/15/20	6/39/115/115	-
19	WVN	A	852	-	-	4/29/63/63	0/2/2/2
13	CL7	A	829	1	2/2/12/20	9/21/97/115	-
13	CL7	A	812	1	2/2/15/20	13/39/115/115	-
13	CL7	J	102	2	2/2/14/20	16/33/109/115	-
13	CL7	L	204	10	2/2/15/20	17/39/115/115	-
13	CL7	B	806	2	2/2/15/20	12/39/115/115	-
13	CL7	B	814	2	2/2/13/20	8/29/105/115	-
16	LMT	A	844	-	-	7/15/35/61	0/1/1/2
13	CL7	A	837	1	2/2/15/20	7/39/115/115	-
13	CL7	B	826	2	2/2/15/20	11/39/115/115	-
13	CL7	B	805	2	2/2/15/20	8/39/115/115	-
16	LMT	F	203	-	-	7/16/56/61	0/2/2/2
13	CL7	F	201	23	2/2/14/20	11/33/109/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
13	CL7	A	805	1	1/1/15/20	13/39/115/115	-
13	CL7	A	814	1	2/2/14/20	9/33/109/115	-
13	CL7	B	830	2	2/2/11/20	6/15/91/115	-
13	CL7	B	817	2	2/2/12/20	6/21/97/115	-
19	WVN	M	101	-	-	5/29/63/63	0/2/2/2
13	CL7	A	815	1	2/2/15/20	13/39/115/115	-
13	CL7	B	837	2	2/2/12/20	7/21/97/115	-
13	CL7	A	839	23	2/2/15/20	12/39/115/115	-
13	CL7	B	810	2	2/2/11/20	4/15/91/115	-
22	K3I	B	845	-	1/1/12/26	4/29/67/67	0/2/2/2
13	CL7	A	807	1	2/2/15/20	15/39/115/115	-
13	CL7	B	832	2	2/2/12/20	9/21/97/115	-
13	CL7	B	838	-	2/2/11/20	11/15/91/115	-
13	CL7	B	803	2	2/2/15/20	6/39/115/115	-
13	CL7	B	825	2	2/2/15/20	18/39/115/115	-
13	CL7	A	804	13,1	2/2/13/20	9/27/103/115	-
15	PQN	A	826	-	-	5/23/43/43	0/2/2/2
13	CL7	A	824	1	2/2/15/20	9/39/115/115	-
14	LHG	A	820	-	-	29/53/53/53	-
19	WVN	B	848	-	-	1/29/63/63	0/2/2/2
13	CL7	L	207	23	2/2/15/20	12/39/115/115	-
13	CL7	A	825	1	2/2/15/20	13/39/115/115	-
13	CL7	A	832	1	2/2/15/20	13/39/115/115	-
19	WVN	I	101	-	-	8/29/63/63	0/2/2/2
16	LMT	A	833	-	-	10/21/61/61	0/2/2/2
13	CL7	A	838	1	2/2/14/20	16/33/109/115	-
13	CL7	A	848	1	2/2/11/20	10/15/91/115	-
13	CL7	L	205	10	2/2/15/20	10/39/115/115	-
17	SF4	C	102	3	-	-	0/6/5/5
13	CL7	A	842	23	2/2/14/20	9/33/109/115	-
18	PHO	A	849	-	-	17/37/103/103	0/5/6/6
13	CL7	A	806	1	2/2/15/20	19/39/115/115	-
16	LMT	K	104	-	-	6/9/29/61	0/1/1/2
16	LMT	L	206	-	-	9/21/61/61	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
13	CL7	A	845	1	2/2/12/20	7/21/97/115	-
13	CL7	B	846	-	2/2/10/20	4/10/86/115	-
13	CL7	B	821	2	2/2/12/20	9/26/102/115	-
19	WVN	L	202	-	-	6/29/63/63	0/2/2/2
19	WVN	B	847	-	-	8/29/63/63	0/2/2/2
13	CL7	B	816	2	2/2/12/20	7/21/97/115	-
13	CL7	B	834	-	2/2/11/20	8/15/91/115	-
13	CL7	A	816	1	2/2/12/20	5/21/97/115	-
19	WVN	L	209	-	-	2/29/63/63	0/2/2/2
19	WVN	K	101	-	-	6/29/63/63	0/2/2/2
13	CL7	L	201	1	2/2/15/20	11/39/115/115	-
13	CL7	I	102	-	1/1/11/20	6/15/91/115	-
13	CL7	A	830	1	2/2/15/20	19/39/115/115	-
13	CL7	A	818	1	2/2/13/20	7/27/103/115	-
13	CL7	B	843	14	2/2/11/20	7/15/91/115	-
13	CL7	A	841	1	2/2/14/20	13/33/109/115	-
13	CL7	B	811	2	2/2/10/20	3/10/86/115	-
19	WVN	A	851	-	-	6/29/63/63	0/2/2/2
12	G9R	A	801	1	1/1/15/20	7/39/115/115	-
20	LMG	B	827	-	-	23/50/70/70	0/1/1/1
13	CL7	F	202	6	2/2/11/20	7/15/91/115	-
13	CL7	B	822	2	1/1/15/20	9/39/115/115	-
13	CL7	B	808	2	2/2/15/20	12/39/115/115	-
13	CL7	A	835	1	2/2/13/20	10/27/103/115	-
13	CL7	A	823	1	2/2/15/20	17/39/115/115	-
13	CL7	A	808	1	2/2/15/20	16/39/115/115	-
16	LMT	B	836	-	-	4/13/33/61	0/1/1/2
13	CL7	B	819	2	2/2/15/20	19/39/115/115	-
13	CL7	J	103	8	2/2/10/20	6/9/85/115	-
19	WVN	A	850	-	-	7/29/63/63	0/2/2/2
14	LHG	L	208	-	-	24/47/47/53	-
13	CL7	A	811	1	2/2/15/20	14/39/115/115	-
17	SF4	C	101	3	-	-	0/6/5/5
13	CL7	A	855	14	2/2/10/20	4/10/86/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
13	CL7	A	803	1	2/2/15/20	14/39/115/115	-
13	CL7	A	822	1	2/2/15/20	6/39/115/115	-
13	CL7	B	815	2	2/2/15/20	18/39/115/115	-
13	CL7	B	842	-	2/2/5/20	-	-
13	CL7	A	831	23	2/2/11/20	5/15/91/115	-
13	CL7	A	840	1	2/2/15/20	12/39/115/115	-
13	CL7	B	828	2	2/2/15/20	11/39/115/115	-
19	WVN	A	853	-	-	6/29/63/63	0/2/2/2
13	CL7	F	206	23	2/2/11/20	4/15/91/115	-
13	CL7	B	812	2	2/2/14/20	15/33/109/115	-
13	CL7	B	818	23	2/2/15/20	10/39/115/115	-
13	CL7	A	836	1	2/2/14/20	14/33/109/115	-
13	CL7	B	813	2	2/2/10/20	4/10/86/115	-
19	WVN	L	210	-	-	4/29/63/63	0/2/2/2
13	CL7	B	831	23	2/2/12/20	8/21/97/115	-
13	CL7	B	809	2	2/2/10/20	4/10/86/115	-
14	LHG	A	821	13	-	25/50/50/53	-
19	WVN	J	101	-	-	3/29/63/63	0/2/2/2
16	LMT	A	834	-	-	5/21/61/61	0/2/2/2
13	CL7	A	810	23	2/2/10/20	6/10/86/115	-
19	WVN	F	204	-	-	6/29/63/63	0/2/2/2
16	LMT	B	835	-	-	8/15/35/61	0/1/1/2
13	CL7	A	846	1	2/2/11/20	6/15/91/115	-
13	CL7	B	802	23	2/2/15/20	11/39/115/115	-
19	WVN	A	854	-	-	7/29/63/63	0/2/2/2
13	CL7	A	802	23	2/2/15/20	8/39/115/115	-
13	CL7	B	841	2	2/2/11/20	4/15/91/115	-
18	PHO	B	801	-	-	7/37/103/103	0/5/6/6
13	CL7	B	804	2	2/2/15/20	8/39/115/115	-
13	CL7	B	807	2	2/2/12/20	4/21/97/115	-
13	CL7	A	827	1	2/2/14/20	12/33/109/115	-
13	CL7	A	843	23	2/2/12/20	4/21/97/115	-
13	CL7	B	840	2	2/2/11/20	6/15/91/115	-
13	CL7	A	828	1	2/2/14/20	15/33/109/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
20	LMG	L	203	-	-	13/42/62/70	0/1/1/1
13	CL7	K	102	23	2/2/10/20	4/10/86/115	-
13	CL7	A	813	1	2/2/12/20	2/21/97/115	-

The worst 5 of 2351 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	K	101	WVN	C15-C13	14.83	1.59	1.34
19	J	101	WVN	C15-C13	14.82	1.59	1.34
19	F	205	WVN	C15-C13	14.63	1.59	1.34
19	I	101	WVN	C15-C13	14.63	1.59	1.34
19	M	101	WVN	C15-C13	14.61	1.59	1.34

The worst 5 of 2549 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
13	A	839	CL7	O2A-CGA-O1A	-21.15	70.72	123.63
13	A	848	CL7	O2A-CGA-O1A	-20.52	70.56	123.33
13	A	839	CL7	O2A-CGA-CBA	14.46	155.93	111.83
13	A	848	CL7	O1A-CGA-CBA	10.58	156.64	123.09
13	A	839	CL7	O1A-CGA-CBA	-9.84	85.28	123.78

5 of 179 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
12	A	801	G9R	ND
13	A	802	CL7	NC
13	A	802	CL7	NA
13	A	803	CL7	NC
13	A	803	CL7	NA

5 of 1166 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
13	A	802	CL7	C4B-C3B-CAB-OBB
13	A	804	CL7	C2B-C3B-CAB-OBB
13	A	804	CL7	C4B-C3B-CAB-OBB
13	A	805	CL7	C1A-C2A-CAA-CBA
13	A	805	CL7	C2B-C3B-CAB-OBB

There are no ring outliers.

77 monomers are involved in 120 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
13	B	823	CL7	1	0
13	A	817	CL7	3	0
13	A	809	CL7	2	0
13	B	829	CL7	1	0
13	B	824	CL7	1	0
13	B	833	CL7	6	0
13	A	819	CL7	3	0
13	A	812	CL7	1	0
13	J	102	CL7	4	0
13	L	204	CL7	1	0
13	B	806	CL7	3	0
13	B	814	CL7	1	0
13	A	837	CL7	1	0
13	B	826	CL7	1	0
13	B	805	CL7	1	0
16	F	203	LMT	2	0
13	F	201	CL7	1	0
13	A	805	CL7	2	0
13	A	814	CL7	3	0
13	B	817	CL7	2	0
13	A	815	CL7	2	0
13	B	810	CL7	1	0
13	B	832	CL7	2	0
13	B	838	CL7	1	0
13	B	803	CL7	1	0
13	B	825	CL7	1	0
13	A	804	CL7	1	0
13	A	824	CL7	1	0
19	B	848	WVN	1	0
13	L	207	CL7	2	0
13	A	825	CL7	1	0
13	A	832	CL7	3	0
16	A	833	LMT	1	0
13	L	205	CL7	3	0
18	A	849	PHO	2	0
13	A	806	CL7	2	0
16	L	206	LMT	1	0
13	B	846	CL7	12	0
13	B	821	CL7	2	0
19	B	847	WVN	1	0
13	B	816	CL7	1	0
13	B	834	CL7	1	0

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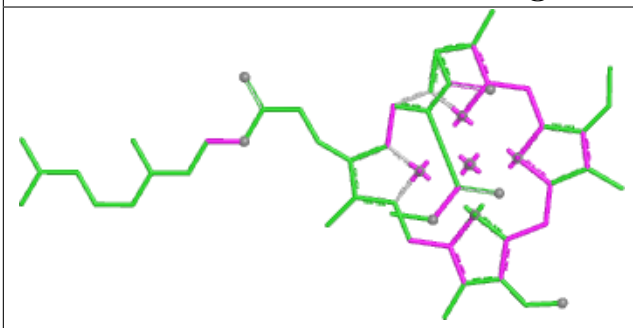
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
13	L	201	CL7	4	0
13	A	830	CL7	2	0
13	B	843	CL7	1	0
13	A	841	CL7	1	0
20	B	827	LMG	3	0
13	B	822	CL7	2	0
13	B	808	CL7	1	0
13	A	835	CL7	2	0
13	A	823	CL7	2	0
13	A	808	CL7	3	0
13	B	819	CL7	1	0
19	A	850	WVN	1	0
14	L	208	LHG	6	0
13	A	855	CL7	1	0
13	A	803	CL7	4	0
13	B	815	CL7	1	0
13	A	840	CL7	2	0
13	B	828	CL7	2	0
19	A	853	WVN	1	0
13	F	206	CL7	1	0
13	B	818	CL7	2	0
13	B	831	CL7	1	0
14	A	821	LHG	1	0
19	J	101	WVN	1	0
19	F	204	WVN	2	0
13	B	802	CL7	3	0
13	A	802	CL7	2	0
13	B	841	CL7	4	0
18	B	801	PHO	3	0
13	B	804	CL7	1	0
13	A	827	CL7	2	0
13	A	843	CL7	1	0
13	B	840	CL7	1	0
13	A	828	CL7	1	0
20	L	203	LMG	2	0

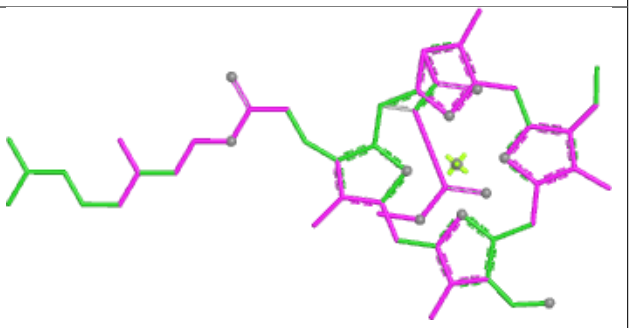
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring

in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

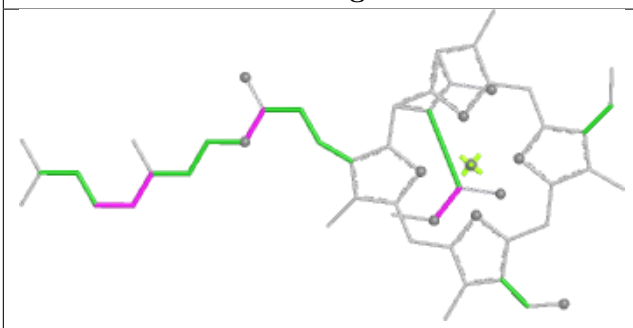
Ligand CL7 B 823



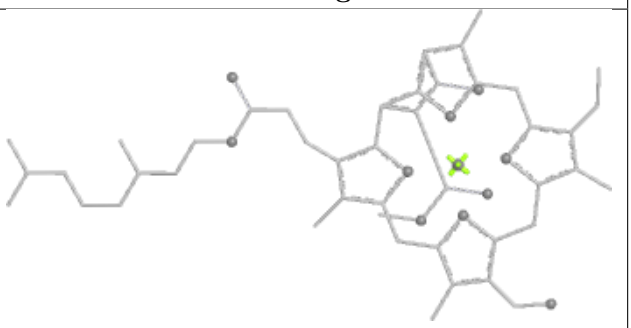
Bond lengths



Bond angles

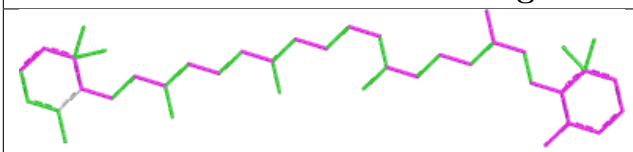


Torsions

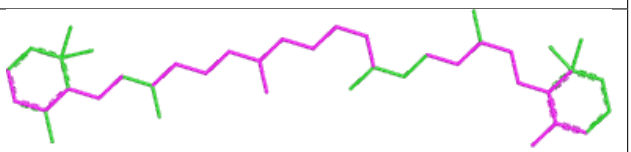


Rings

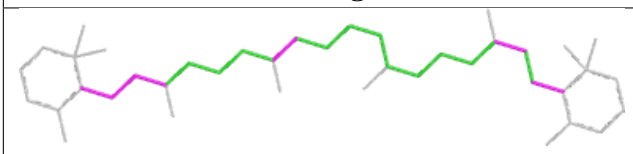
Ligand WVN F 205



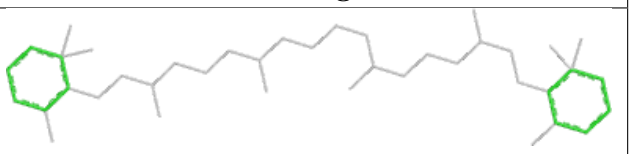
Bond lengths



Bond angles

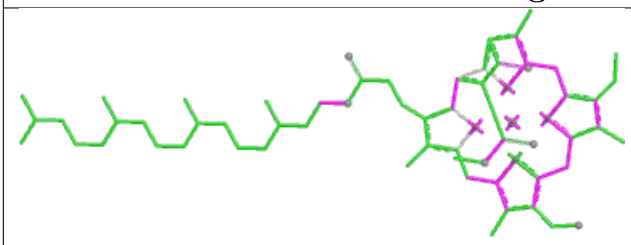


Torsions

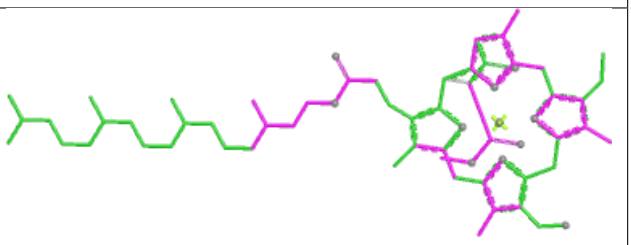


Rings

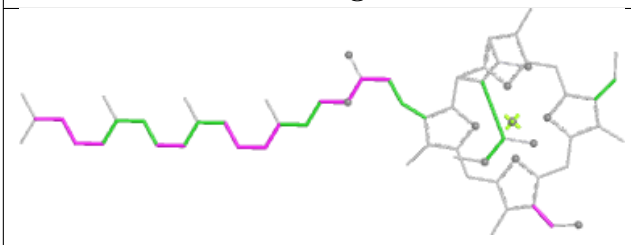
Ligand CL7 A 817



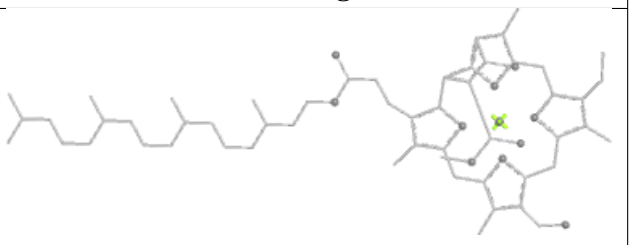
Bond lengths



Bond angles

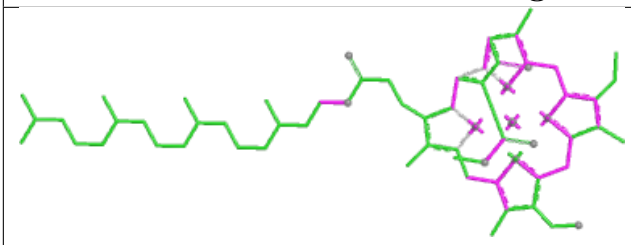


Torsions

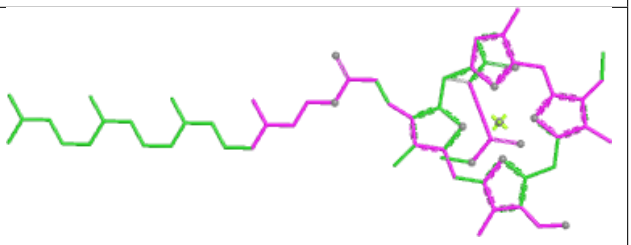


Rings

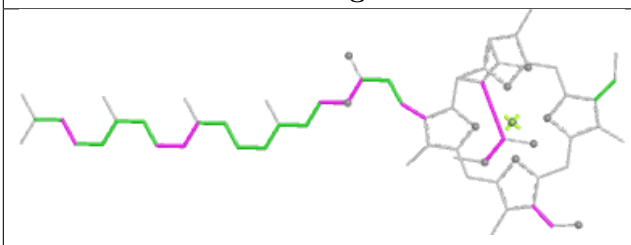
Ligand CL7 A 809



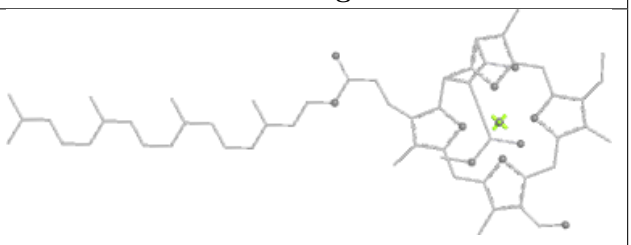
Bond lengths



Bond angles

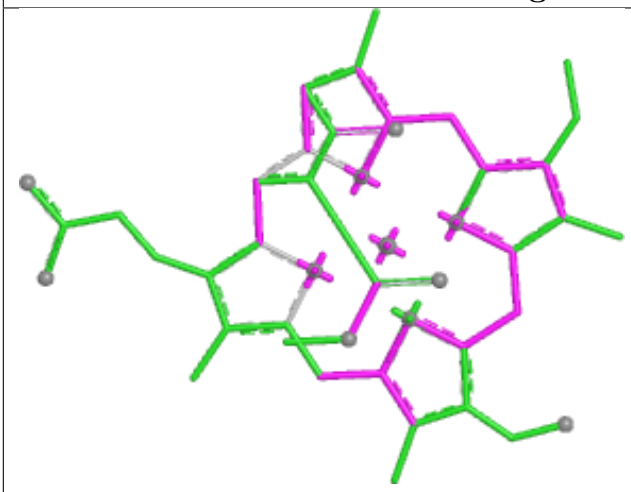


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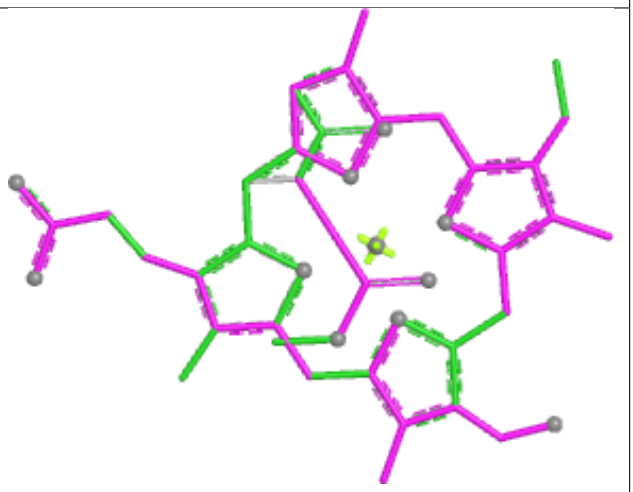


Rings

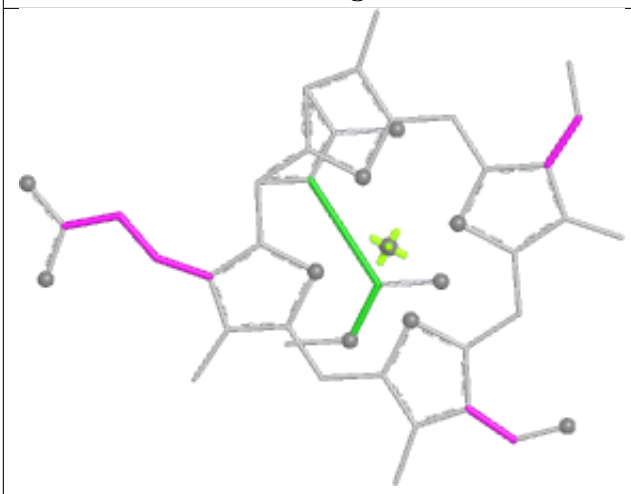
Ligand CL7 B 829



Bond lengths



Bond angles

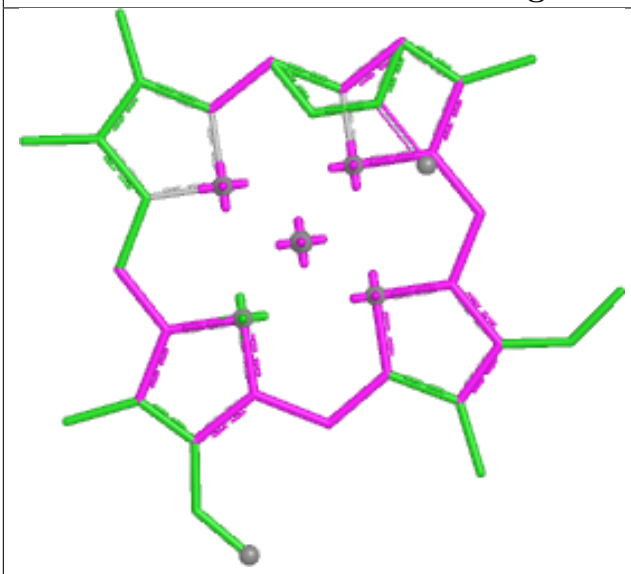


Torsions

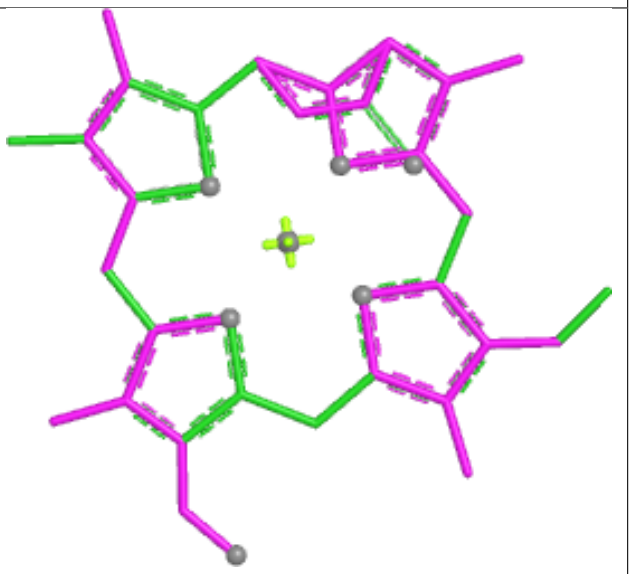


Rings

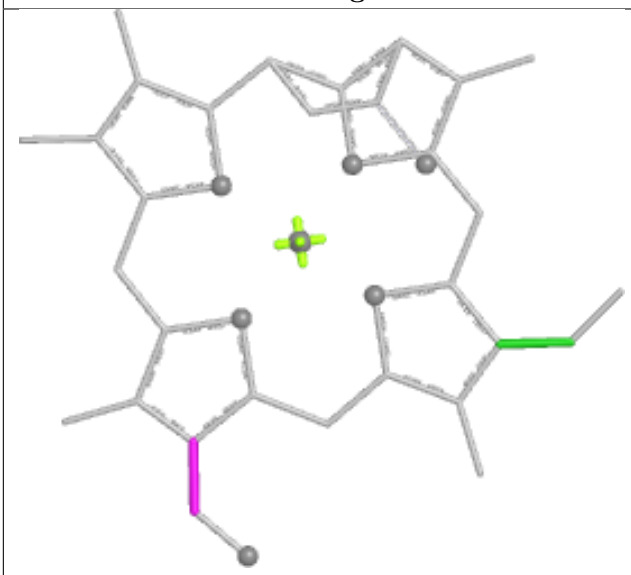
Ligand CL7 K 103



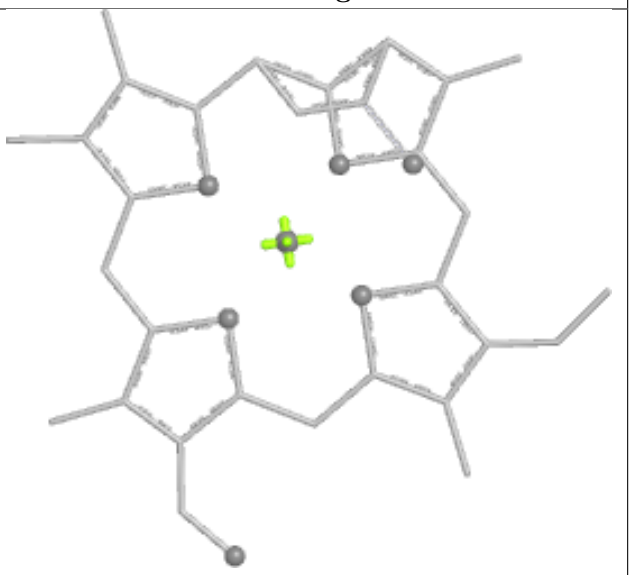
Bond lengths



Bond angles

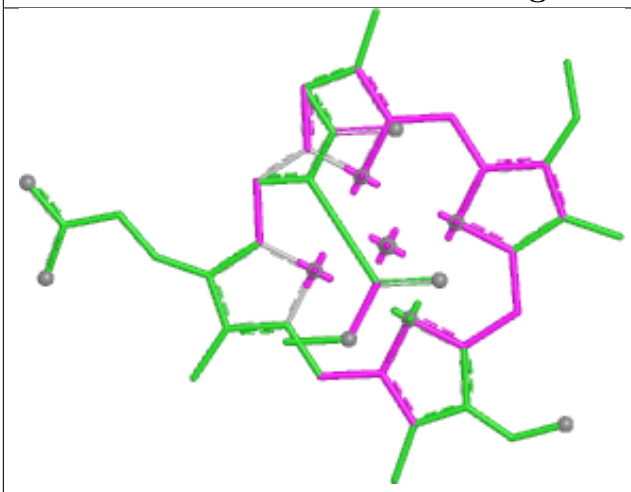


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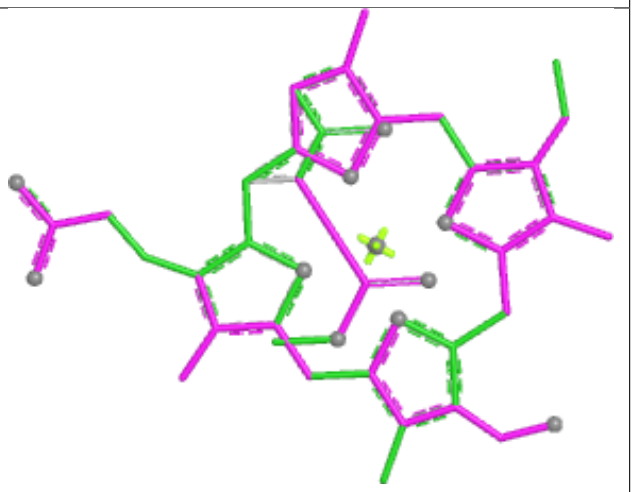


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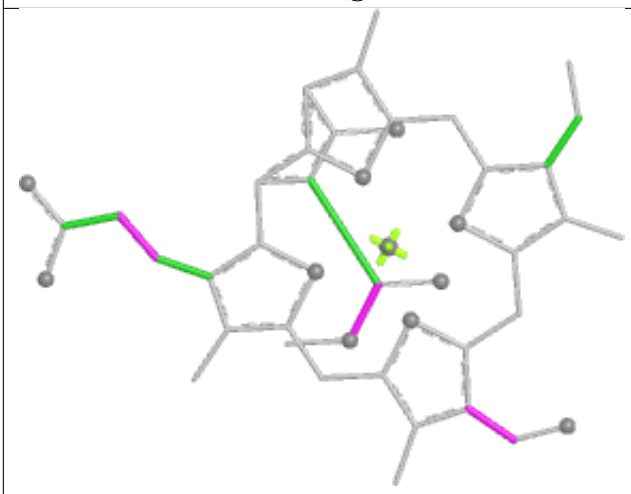
Ligand CL7 B 824



Bond lengths



Bond angles

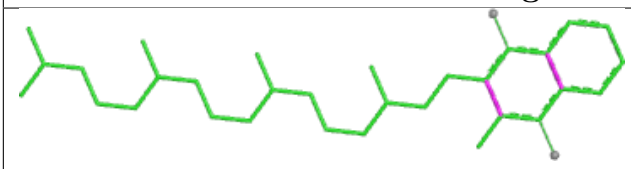


Torsions

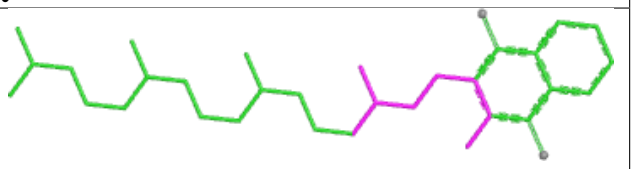


Rings

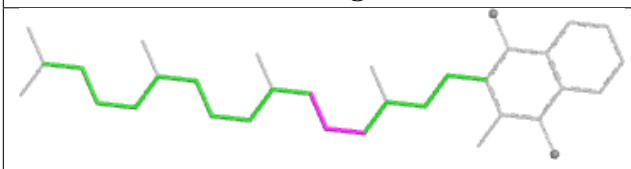
Ligand PQN B 820



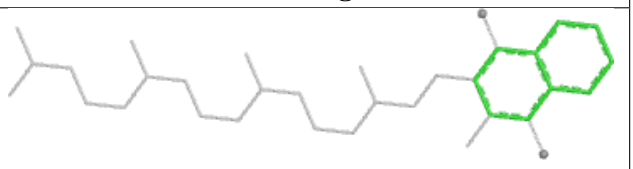
Bond lengths



Bond angles

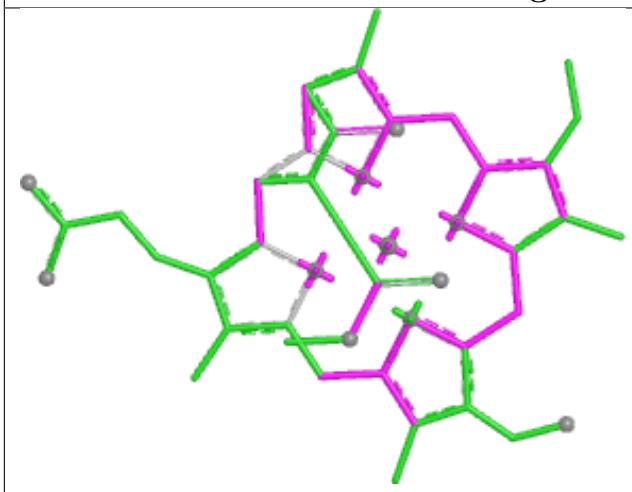


Torsions

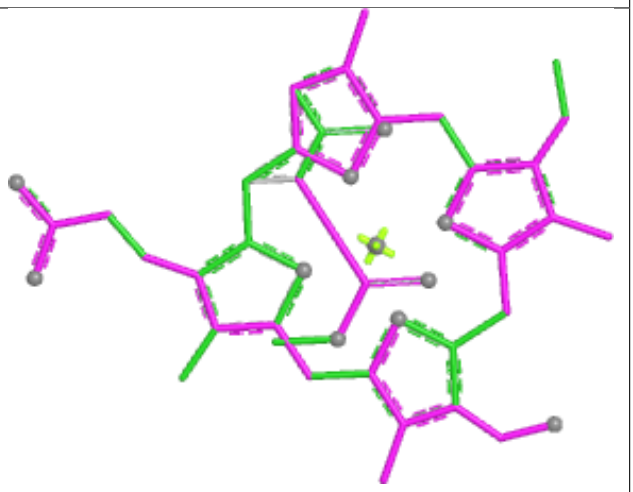


Rings

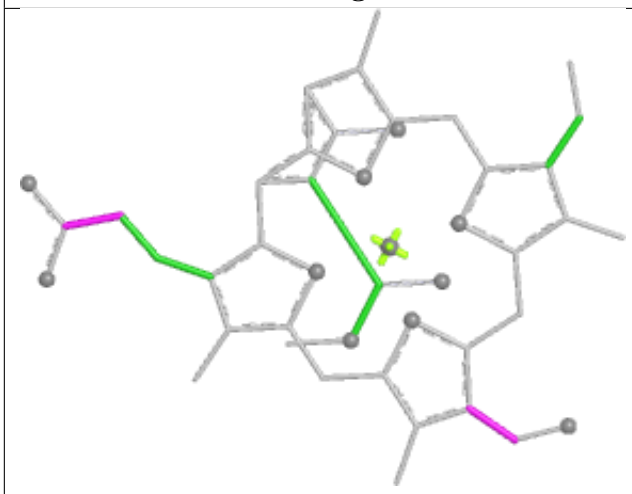
Ligand CL7 B 833



Bond lengths



Bond angles

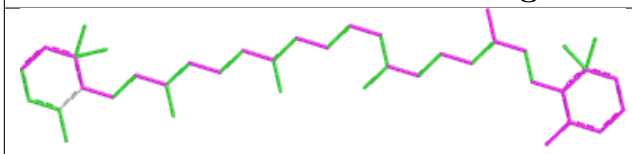


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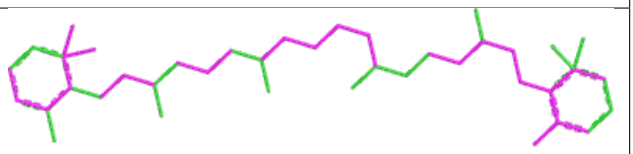


Rings

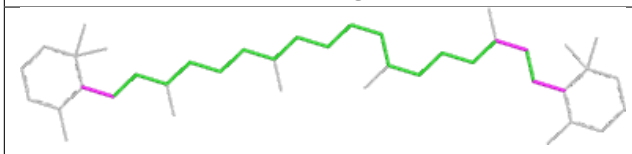
Ligand WVN J 104



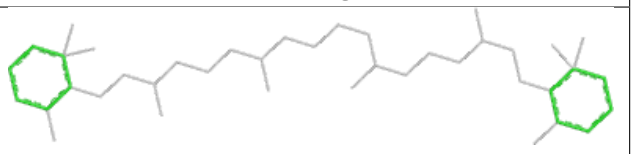
Bond lengths



Bond angles

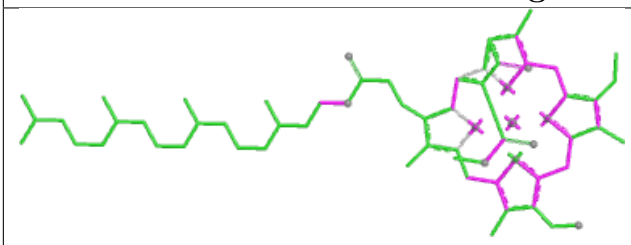


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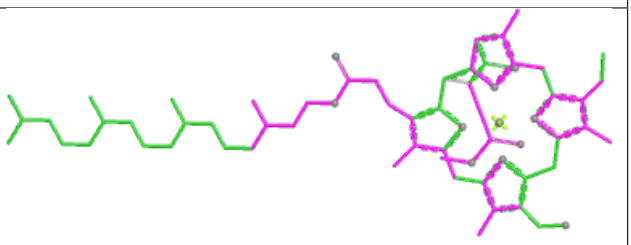


Rings

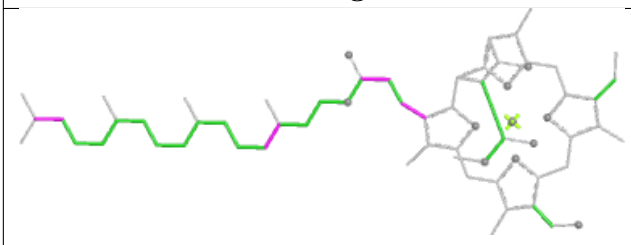
Ligand CL7 A 819



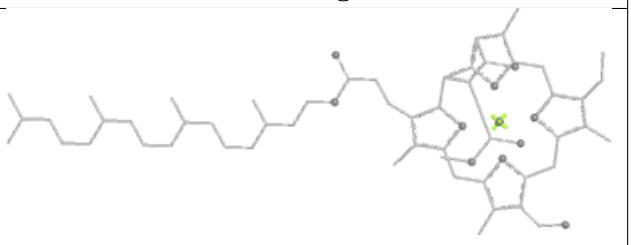
Bond lengths



Bond angles

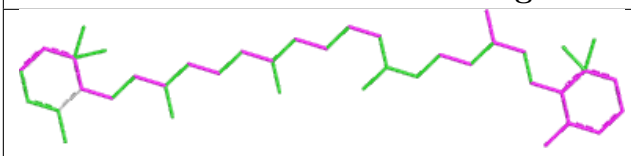


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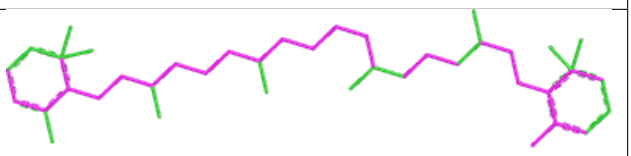


Rings

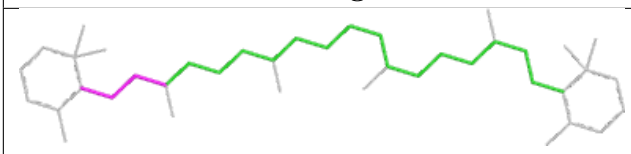
Ligand WVN A 852



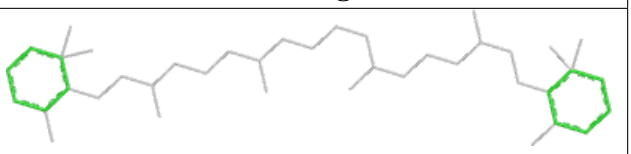
Bond lengths



Bond angles

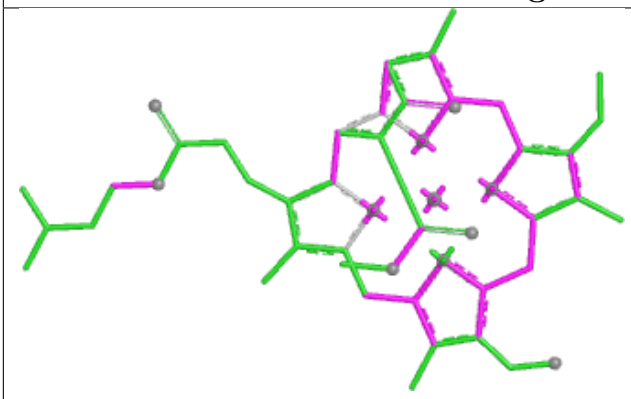


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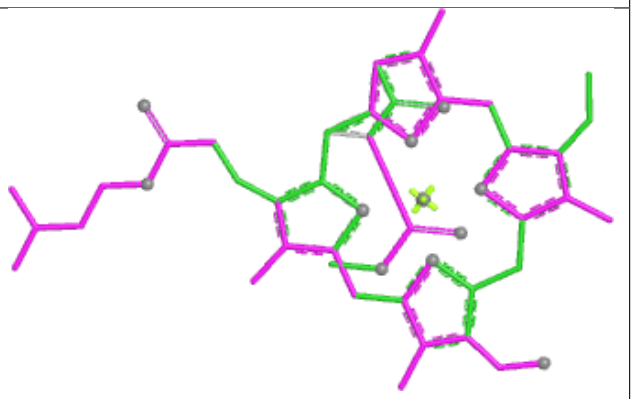


Rings

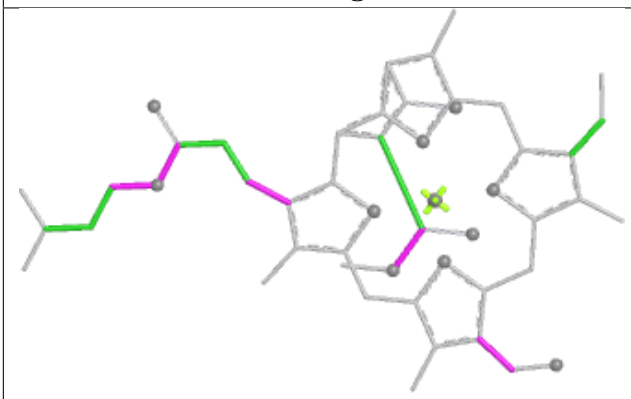
Ligand CL7 A 829



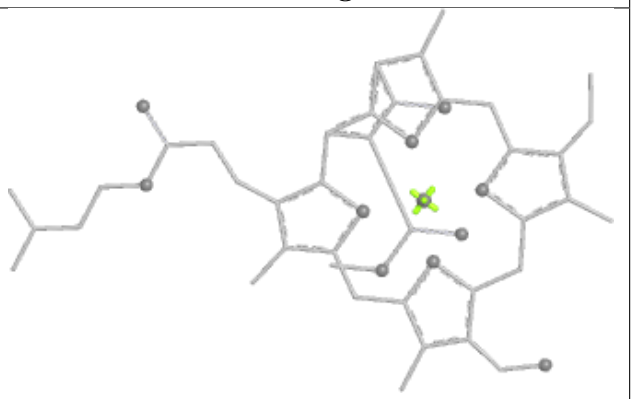
Bond lengths



Bond angles

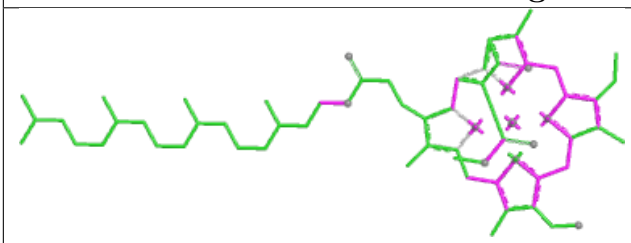


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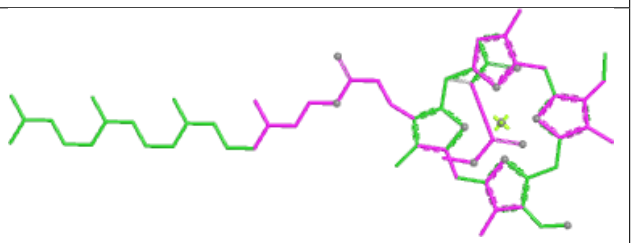


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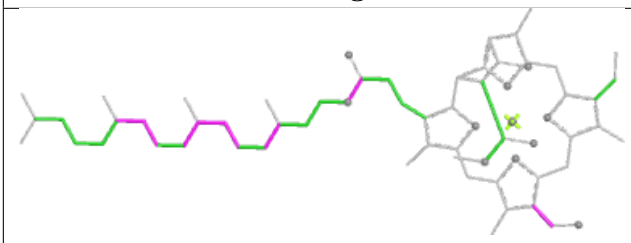
Ligand CL7 A 812



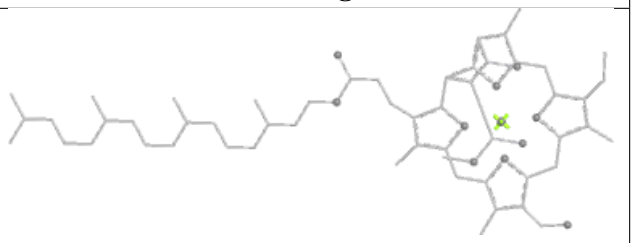
Bond lengths



Bond angles

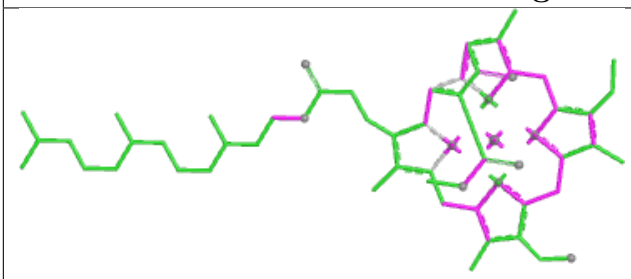


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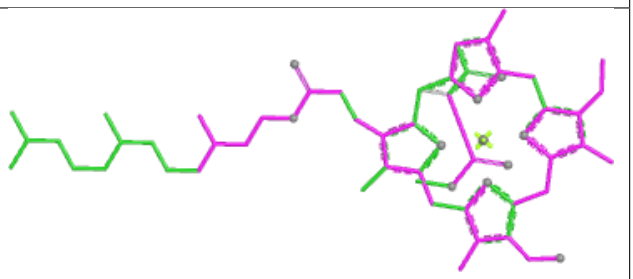


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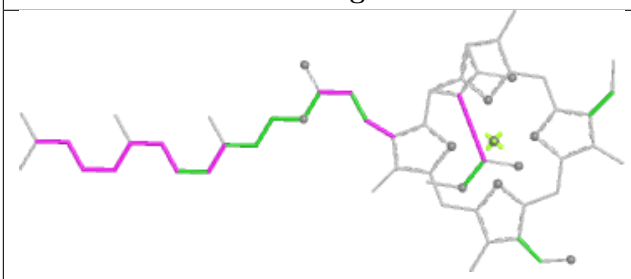
Ligand CL7 J 102



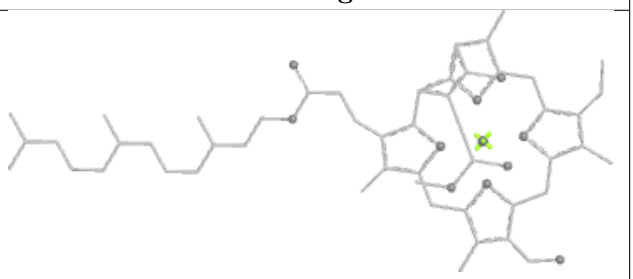
Bond lengths



Bond angles

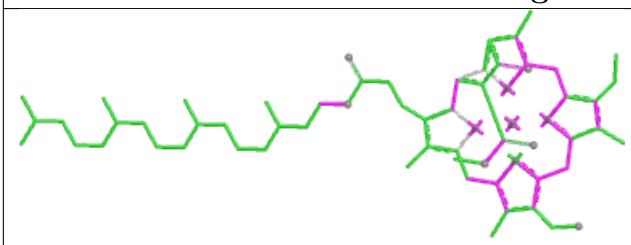


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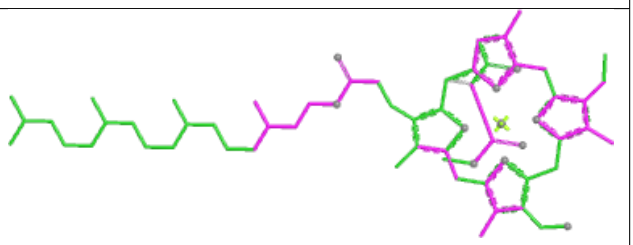


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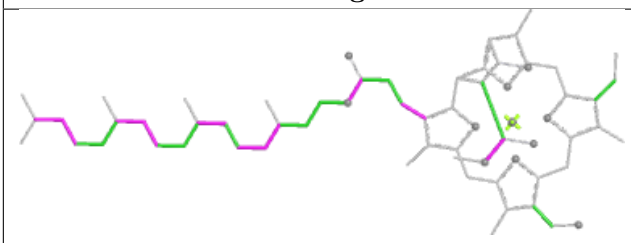
Ligand CL7 L 204



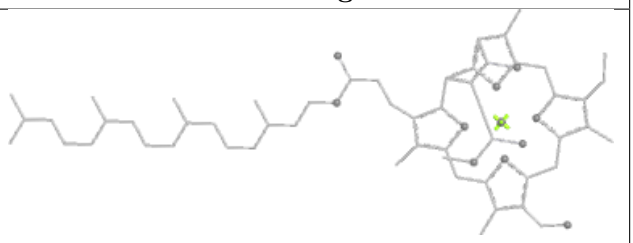
Bond lengths



Bond angles

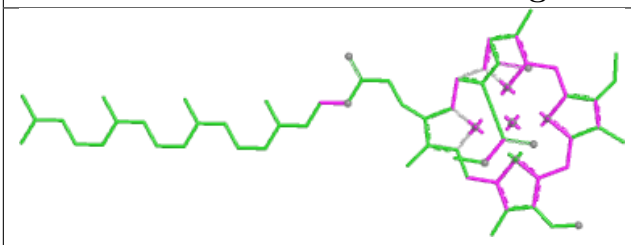


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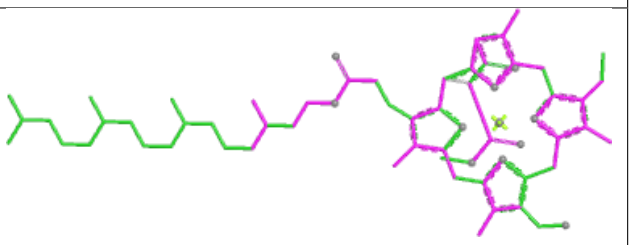


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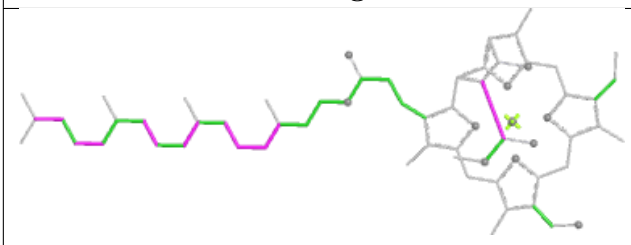
Ligand CL7 B 806



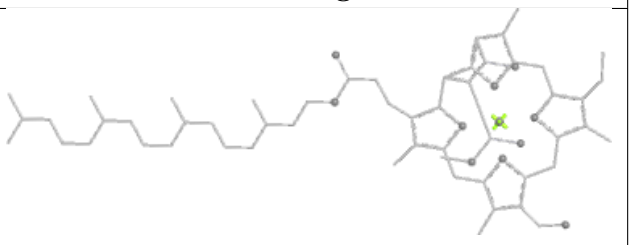
Bond lengths



Bond angles

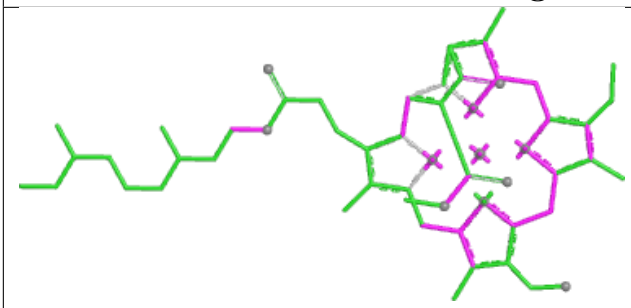


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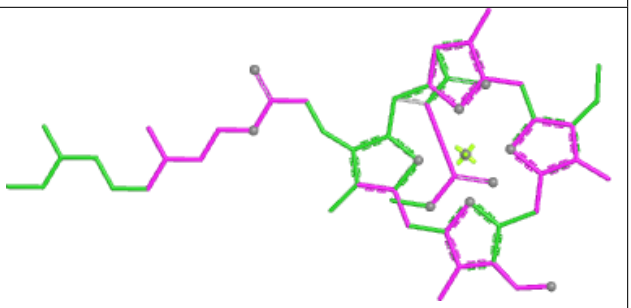


Rings

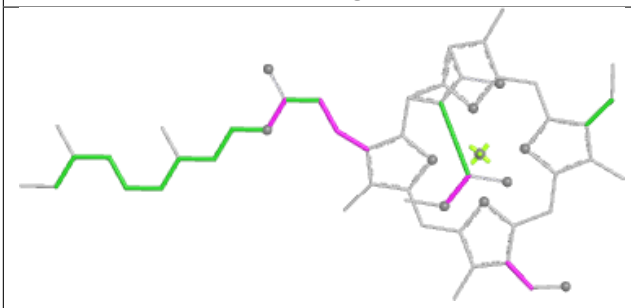
Ligand CL7 B 814



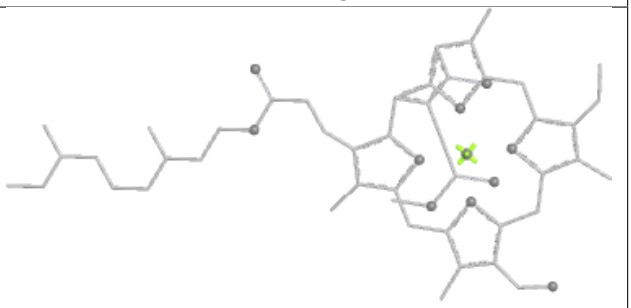
Bond lengths



Bond angles

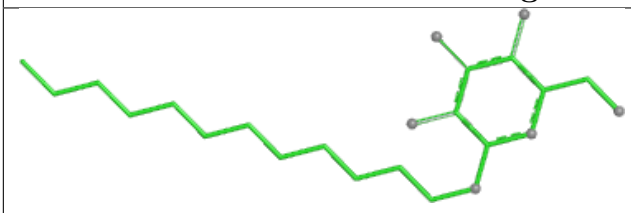


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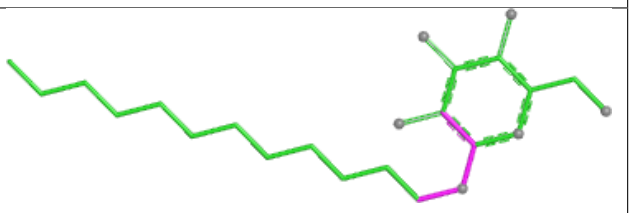


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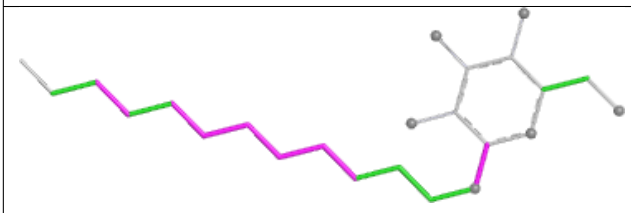
Ligand LMT A 844



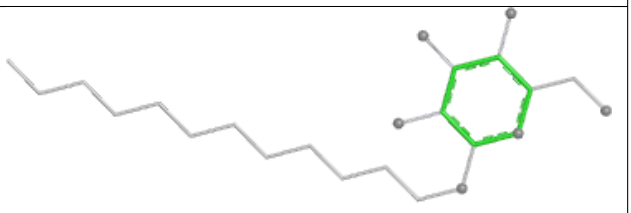
Bond lengths



Bond angles

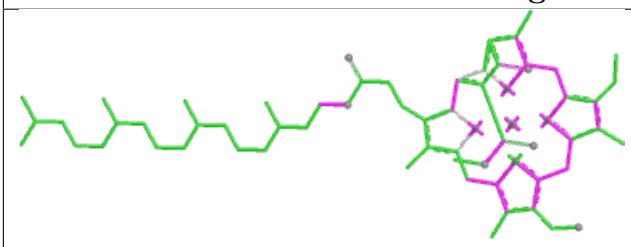


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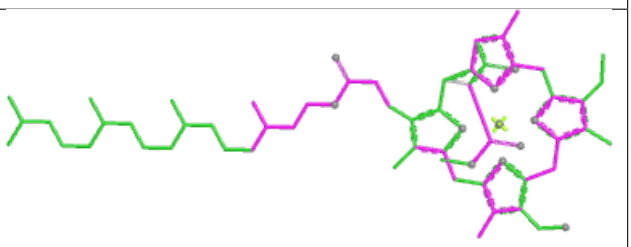


Rings

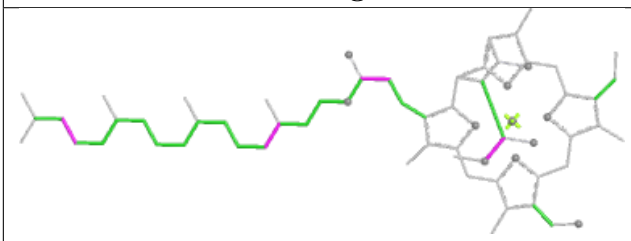
Ligand CL7 A 837



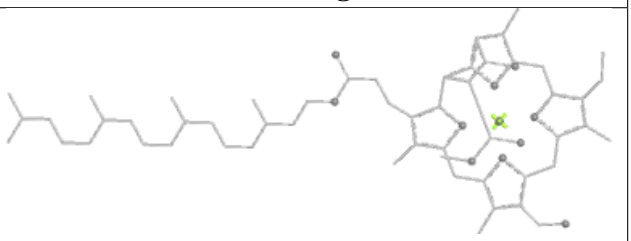
Bond lengths



Bond angles

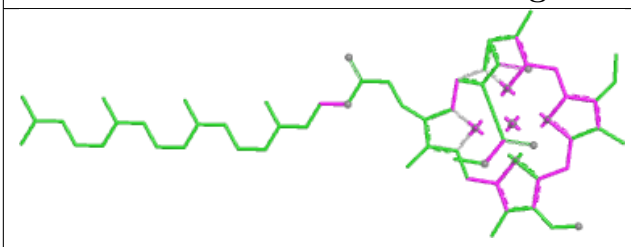


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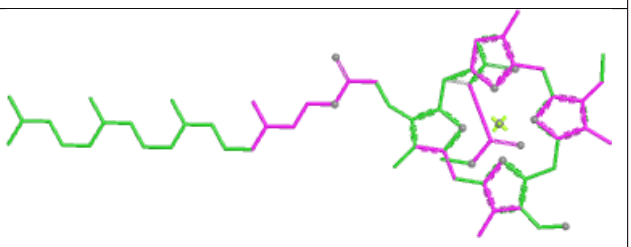


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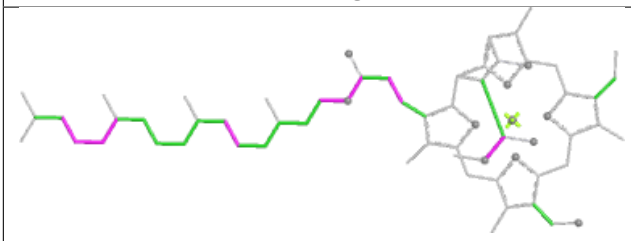
Ligand CL7 B 826



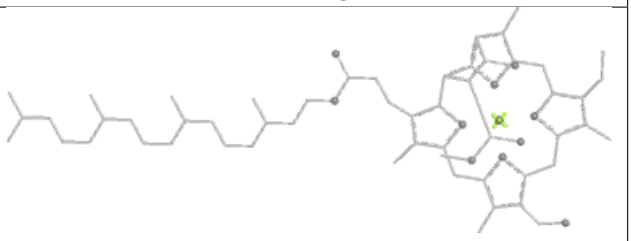
Bond lengths



Bond angles

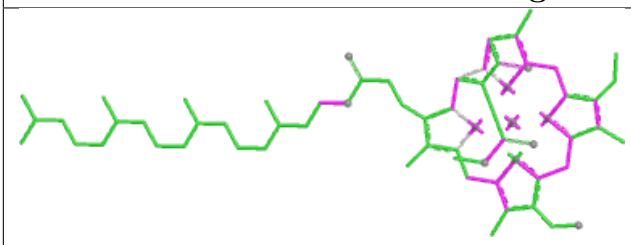


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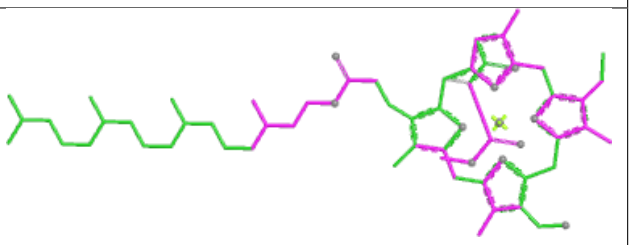


Rings

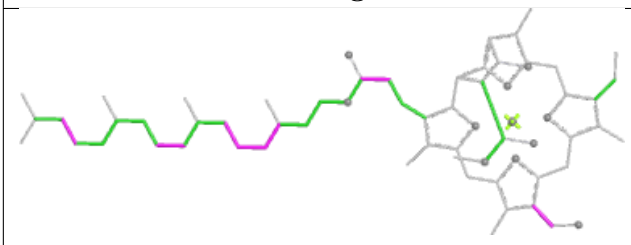
Ligand CL7 B 805



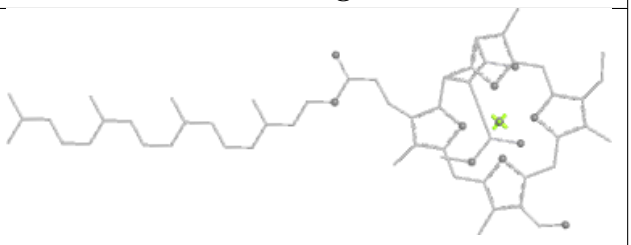
Bond lengths



Bond angles

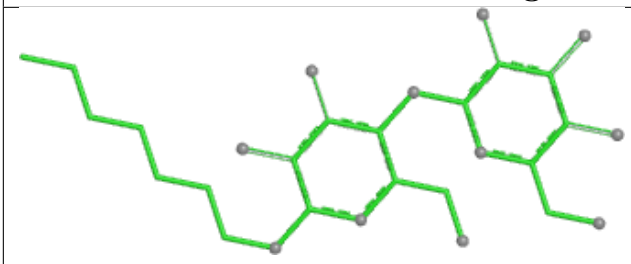


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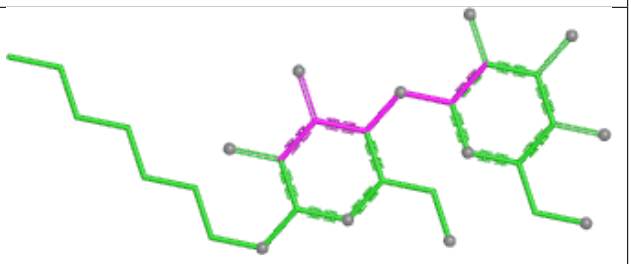


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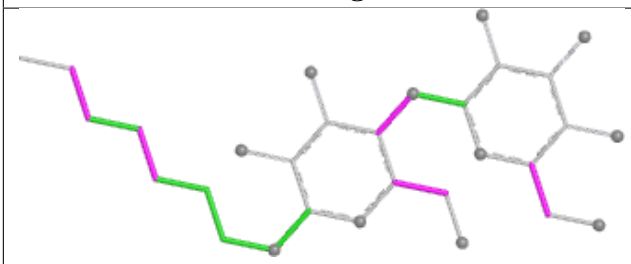
Ligand LMT F 203



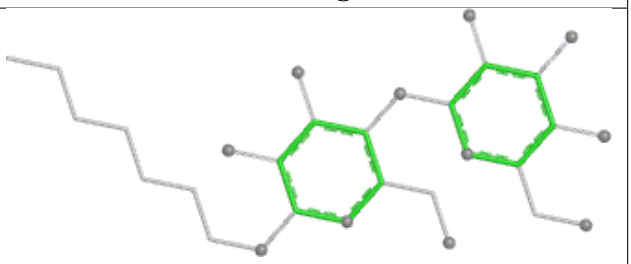
Bond lengths



Bond angles

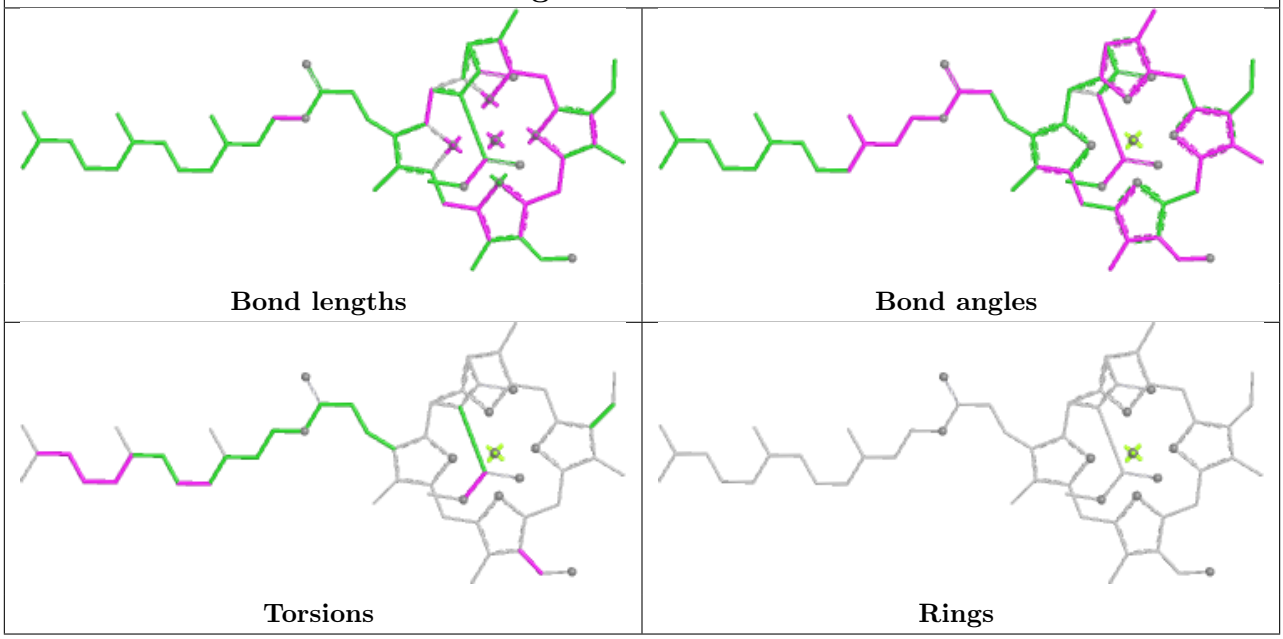


Torsions

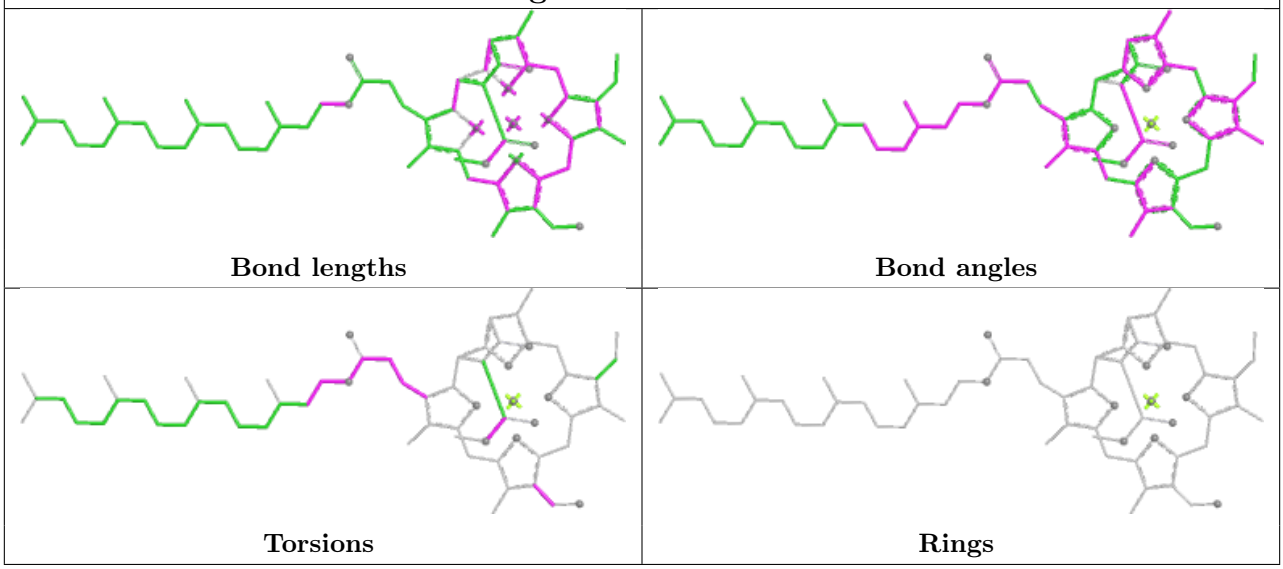


Rings

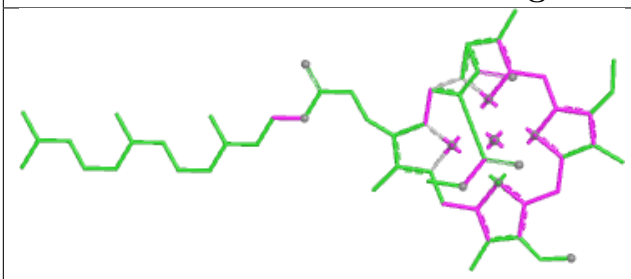
Ligand CL7 F 201



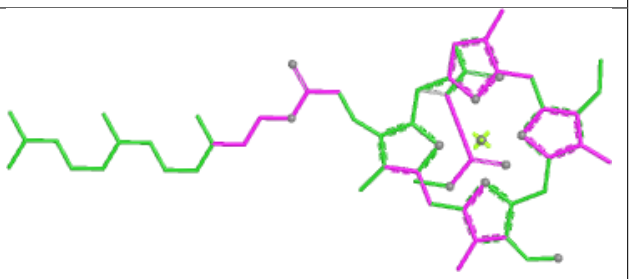
Ligand CL7 A 805



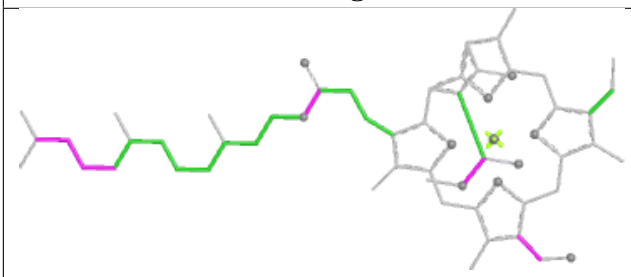
Ligand CL7 A 814



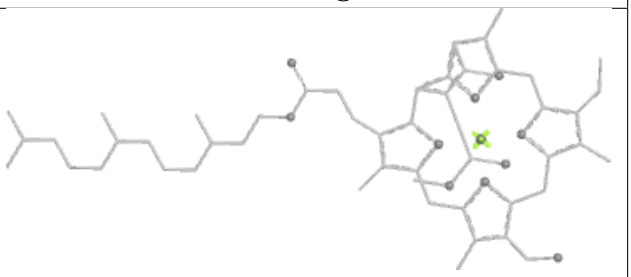
Bond lengths



Bond angles



Torsions

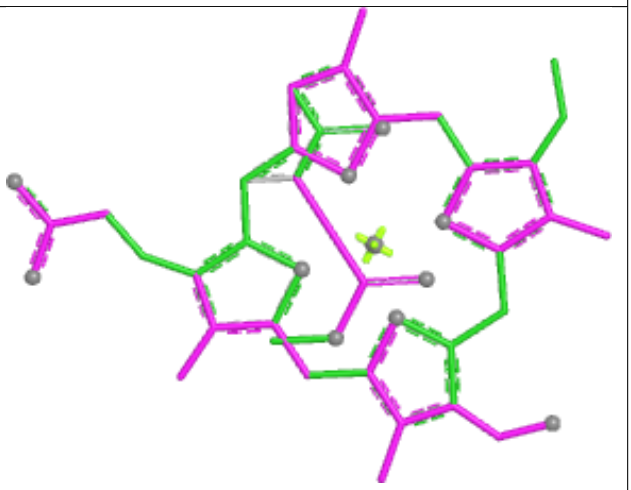


Rings

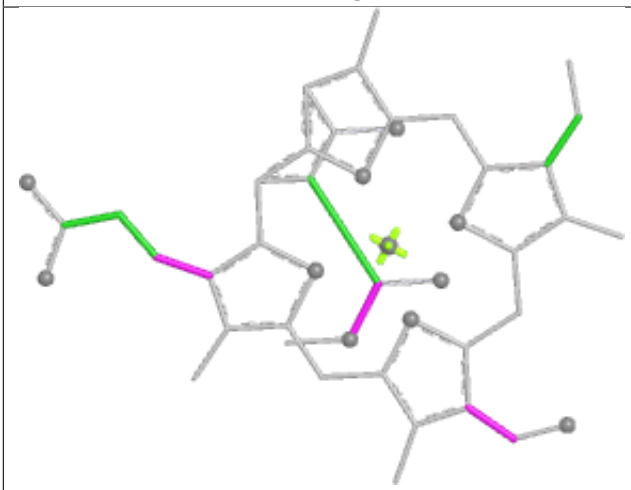
Ligand CL7 B 830



Bond lengths



Bond angles

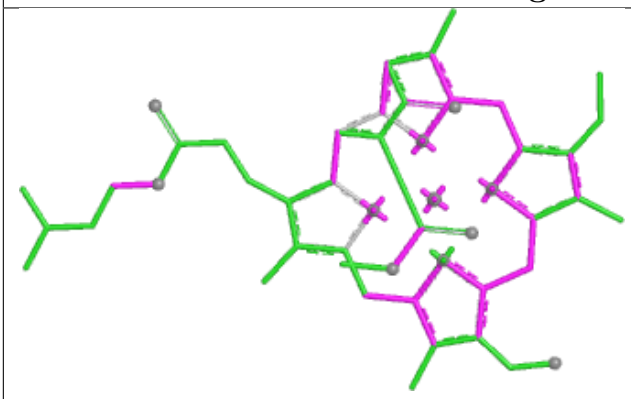


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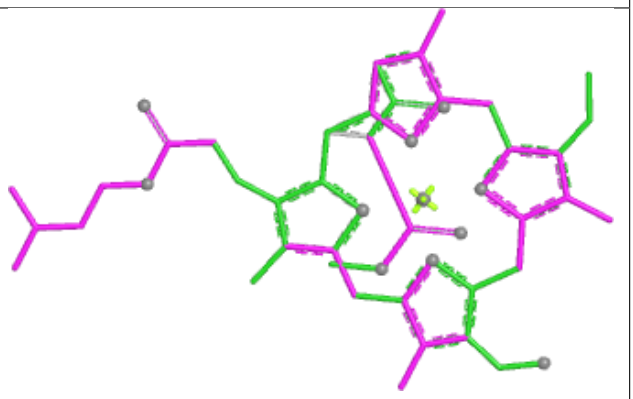


Rings

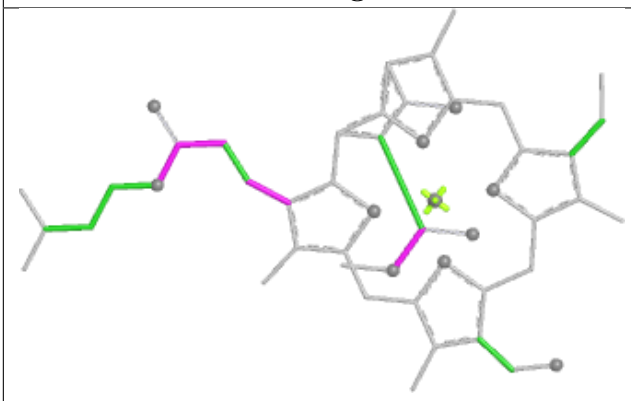
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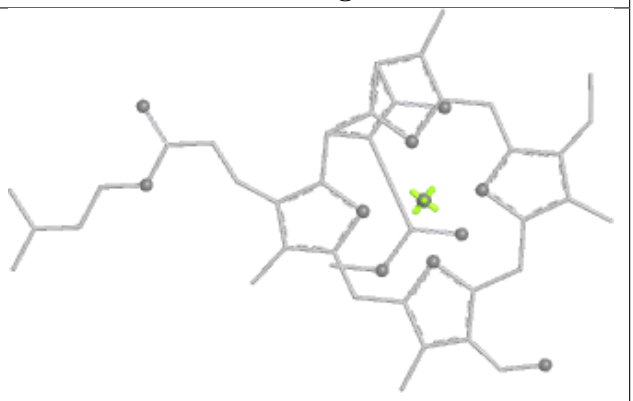
Bond lengths



Bond angles

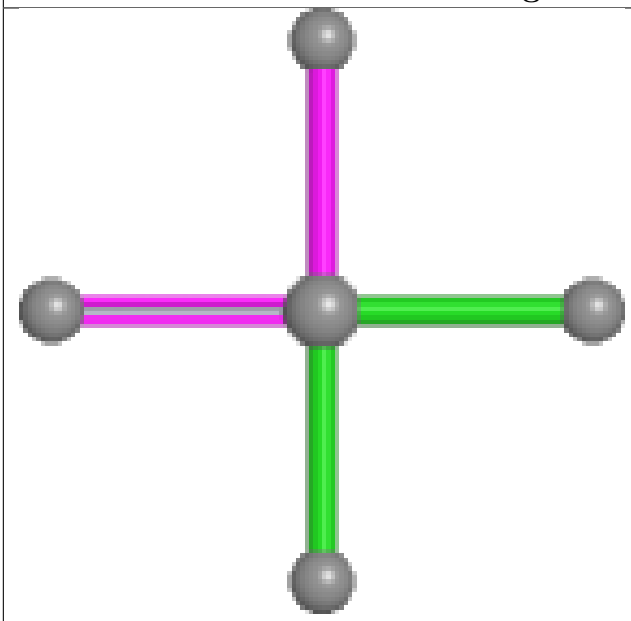


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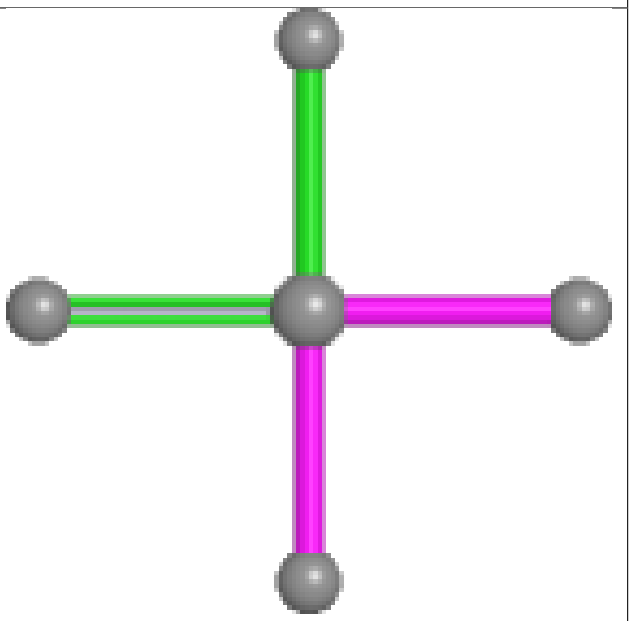


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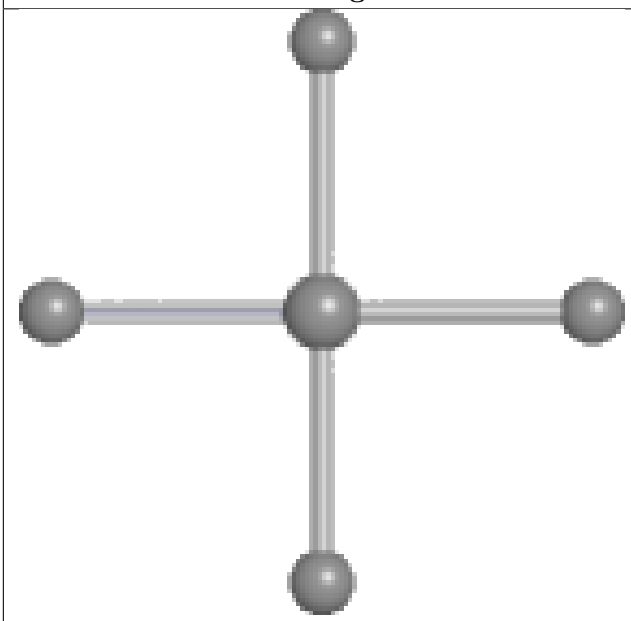
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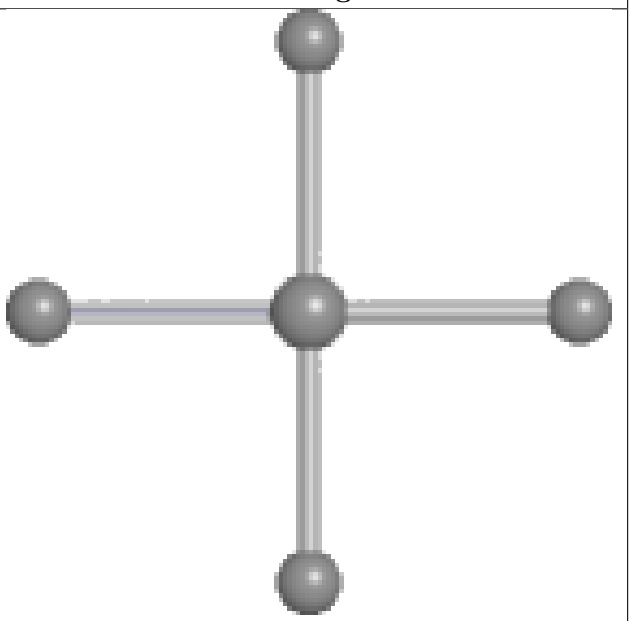
Bond lengths



Bond angles

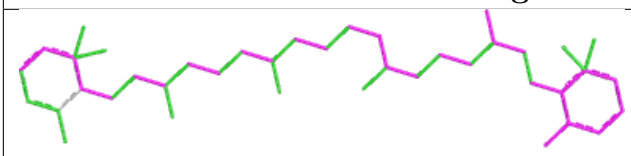


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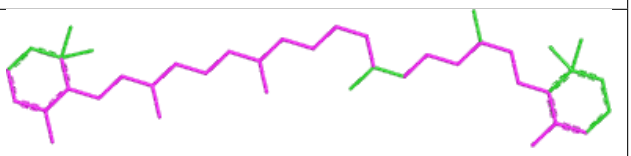


Rings

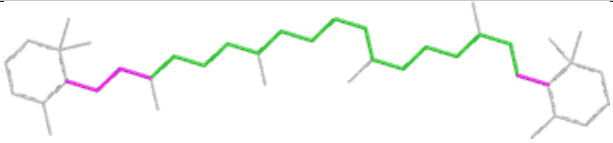
Ligand WVN M 101



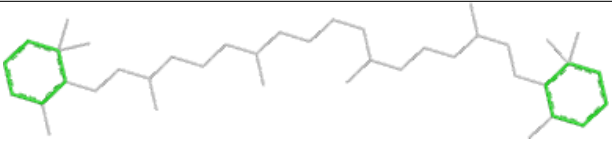
Bond lengths



Bond angles

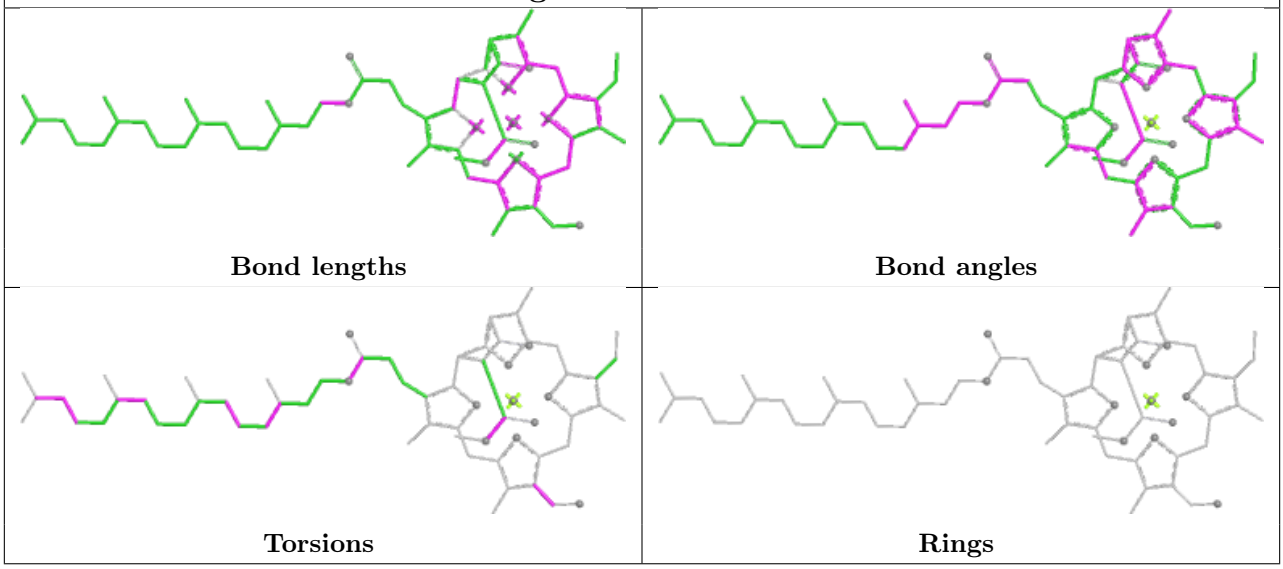


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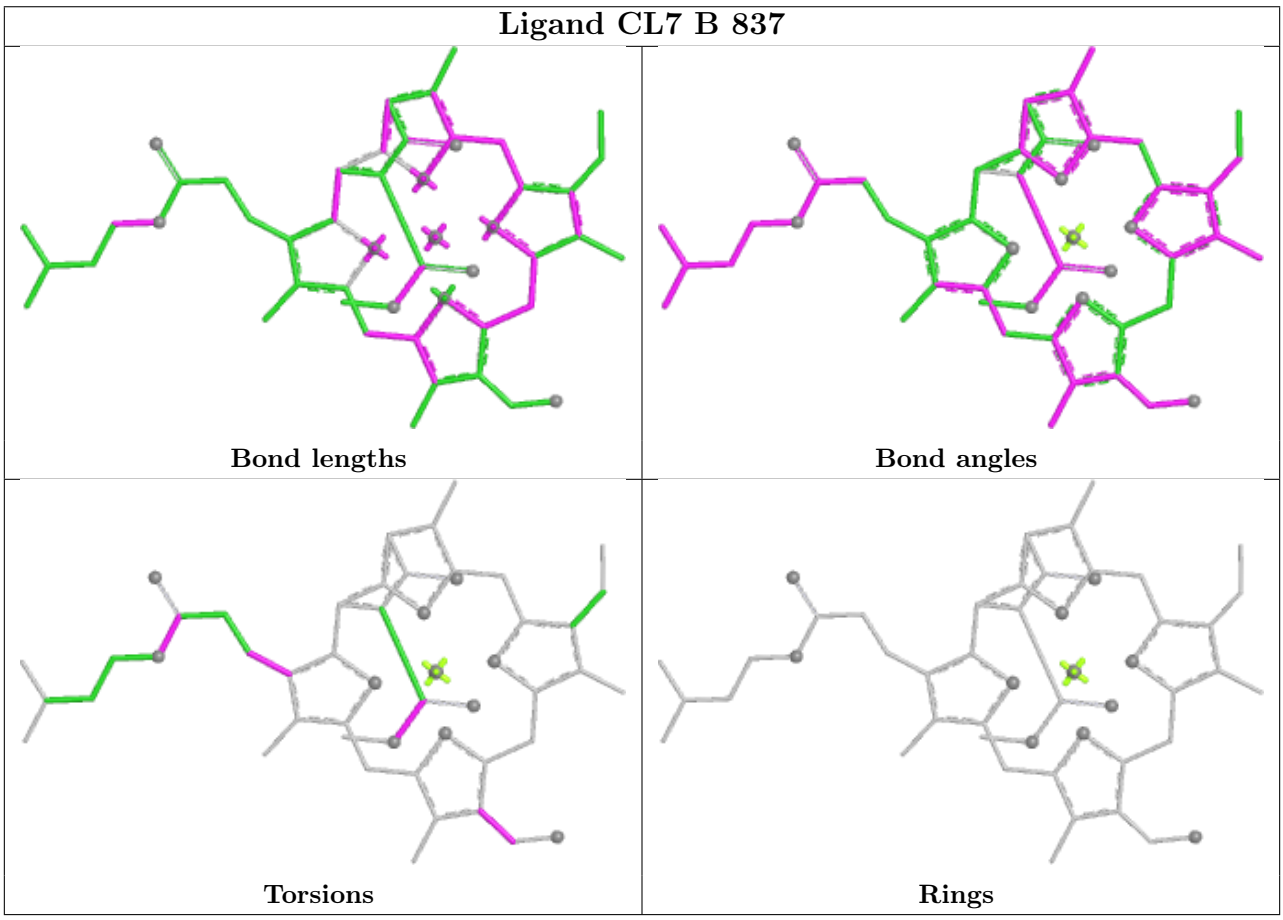


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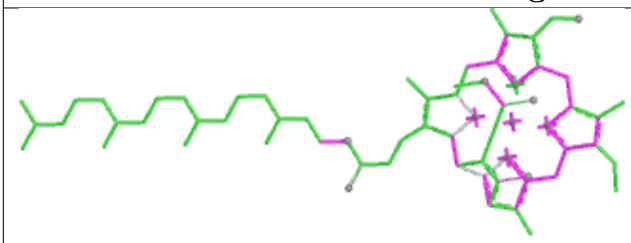
Ligand CL7 A 815



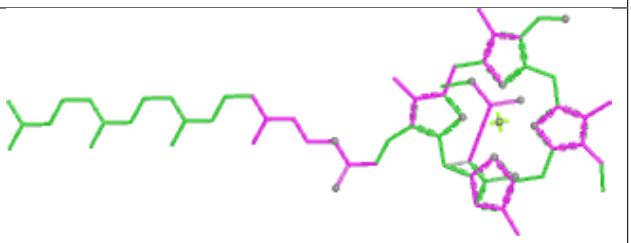
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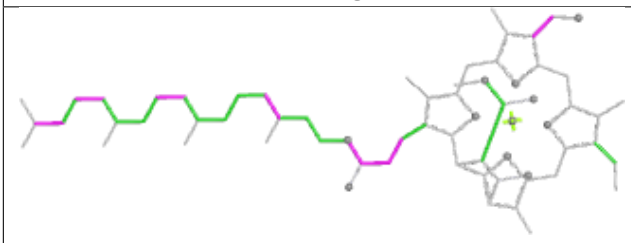
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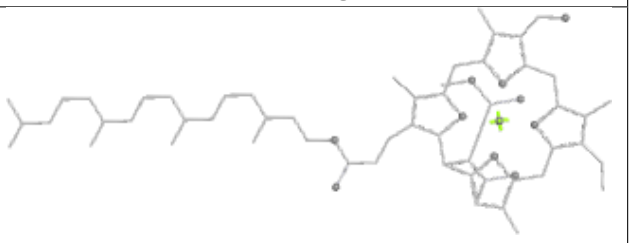
Bond lengths



Bond angles

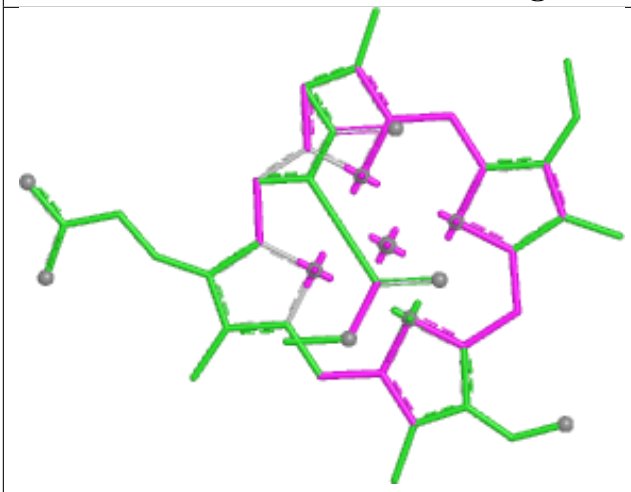


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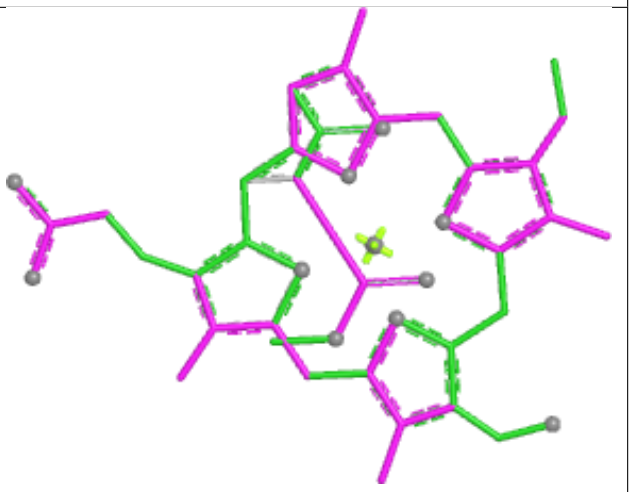


Rings

Ligand CL7 B 810



Bond lengths



Bond angles

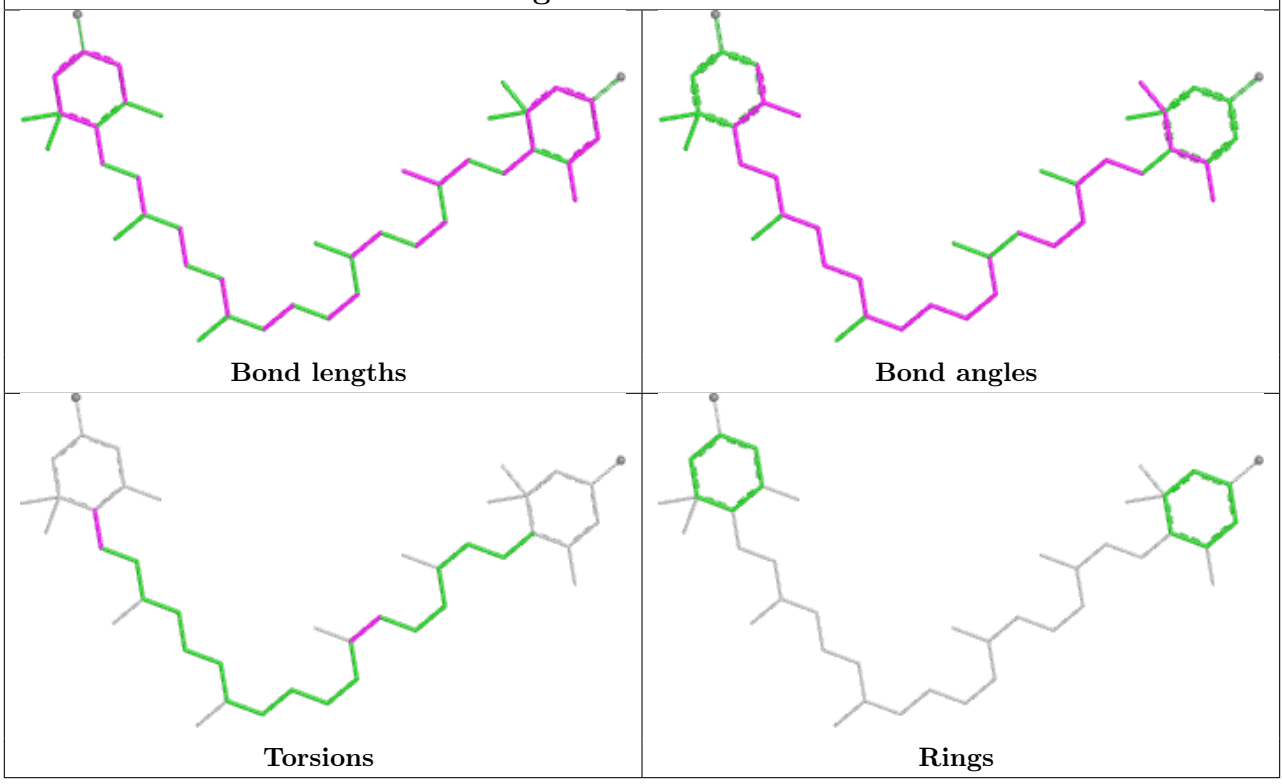


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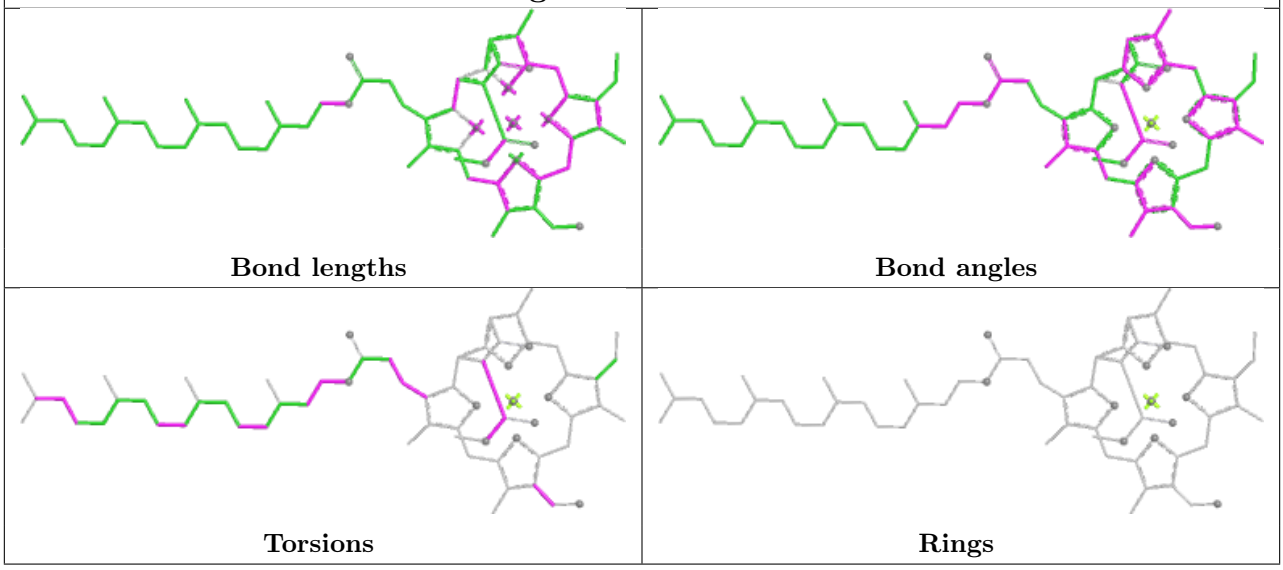


Rings

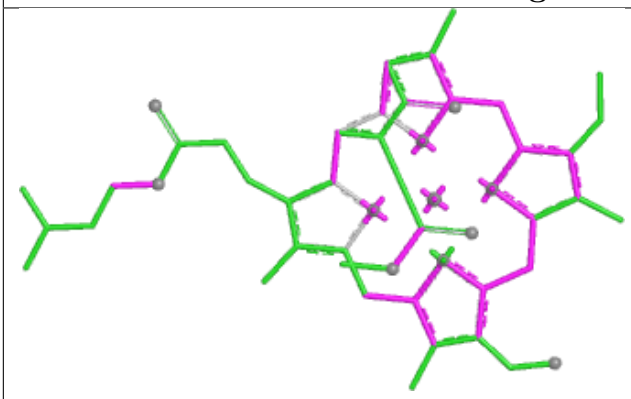
Ligand K3I B 845



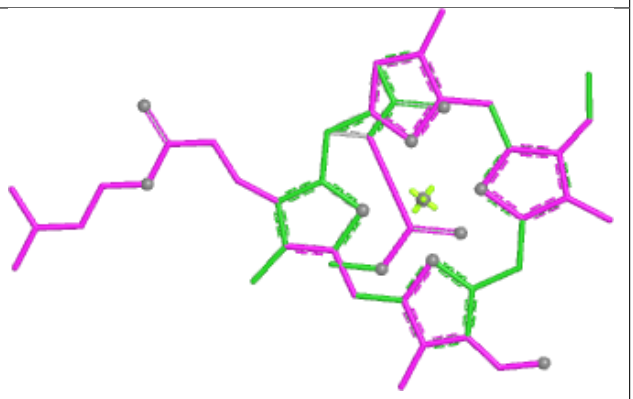
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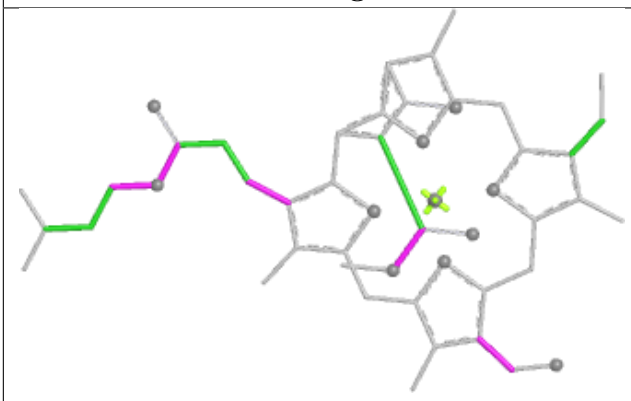
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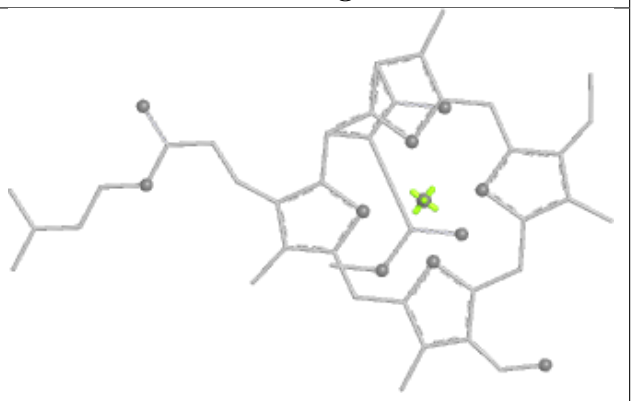
Bond lengths



Bond angles

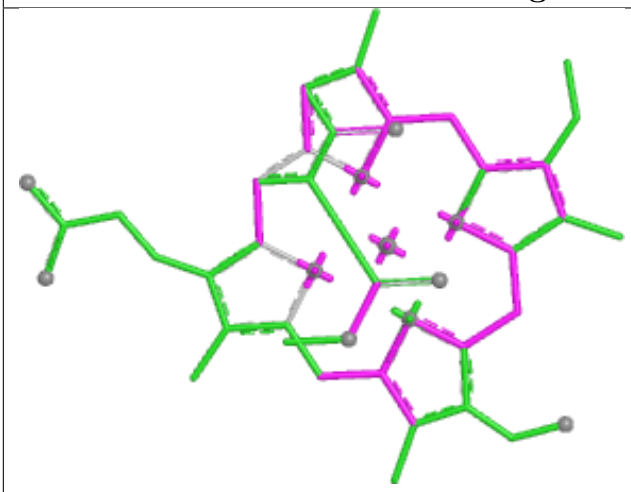


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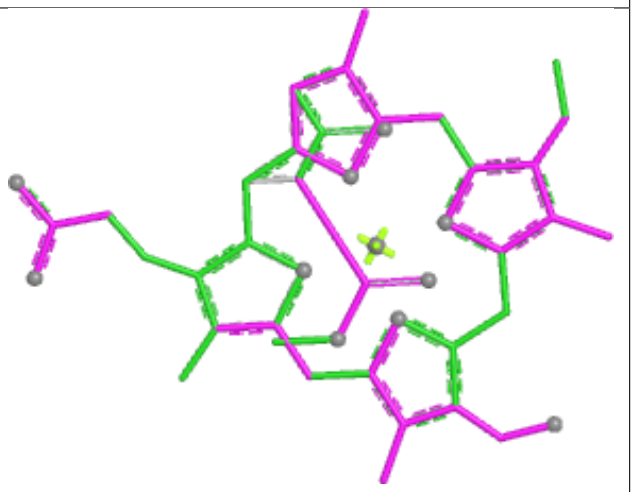


Rings

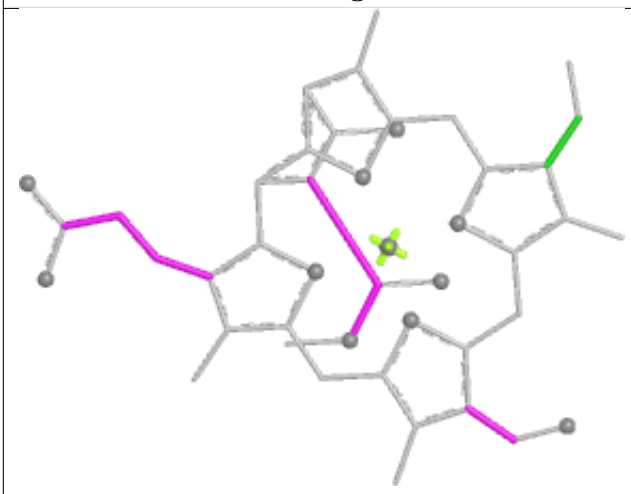
Ligand CL7 B 838



Bond lengths



Bond angles

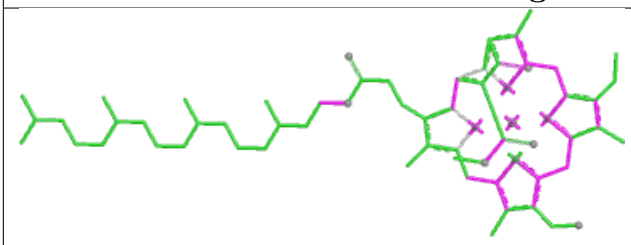


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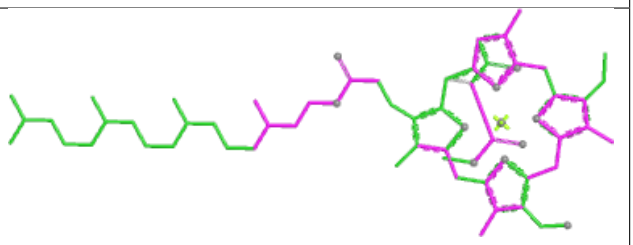


Rings

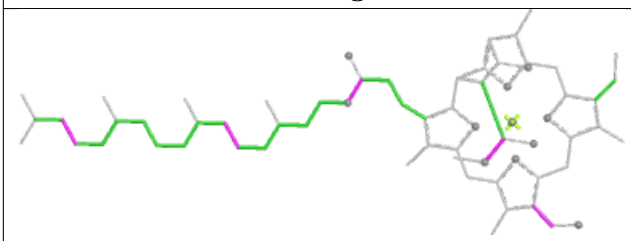
Ligand CL7 B 803



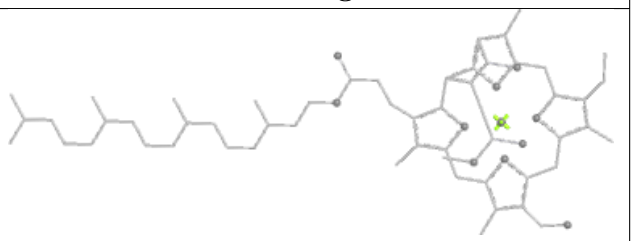
Bond lengths



Bond angles

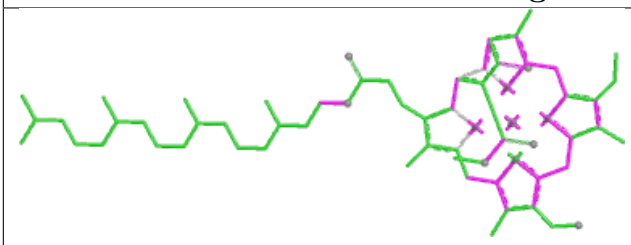


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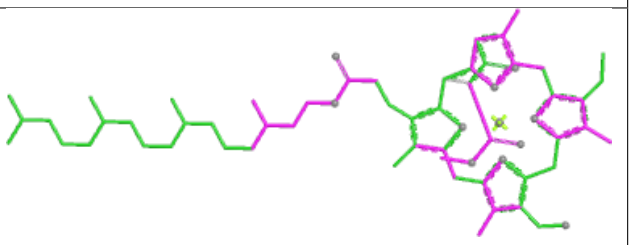


Rings

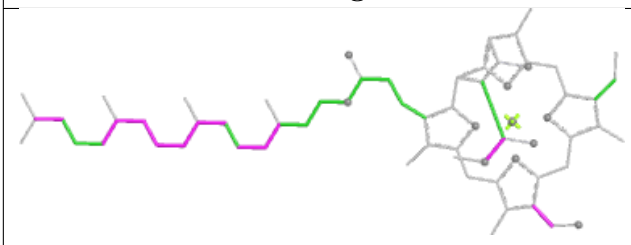
Ligand CL7 B 825



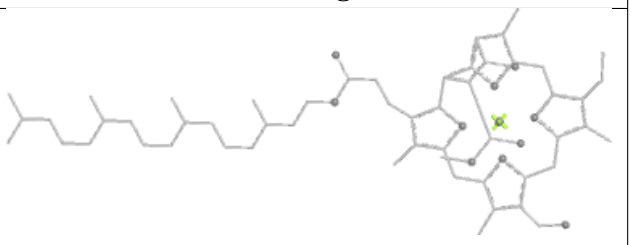
Bond lengths



Bond angles

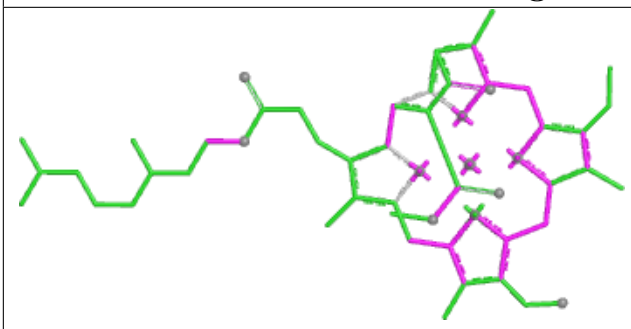


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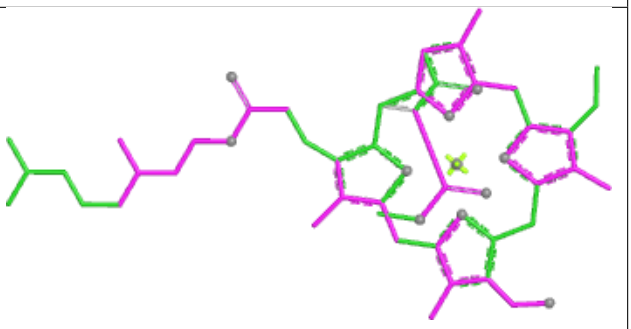


Rings

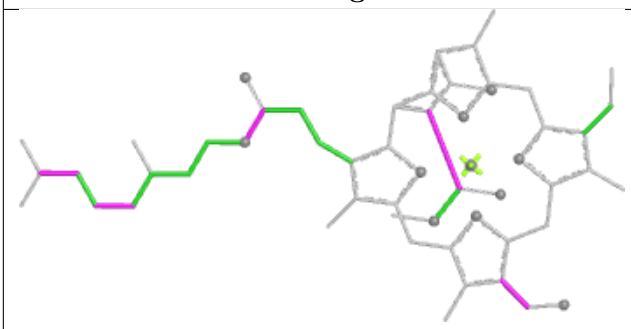
Ligand CL7 A 804



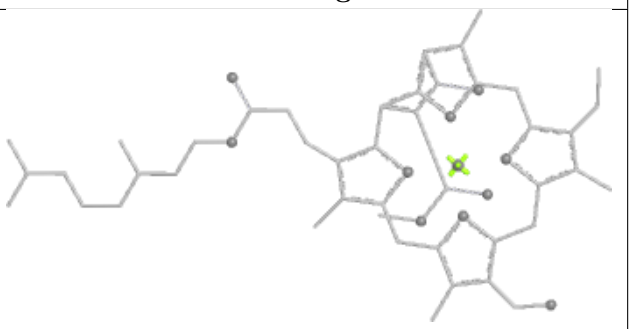
Bond lengths



Bond angles

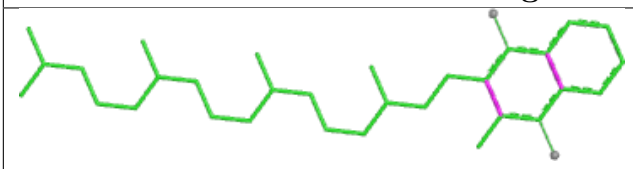


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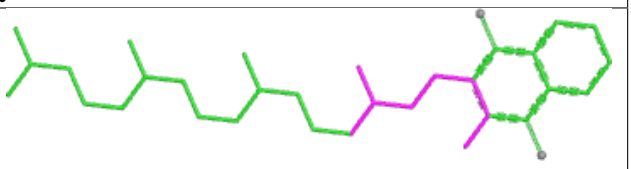


Rings

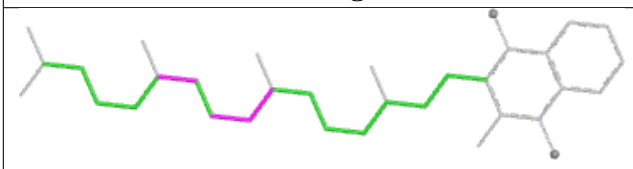
Ligand PQN A 826



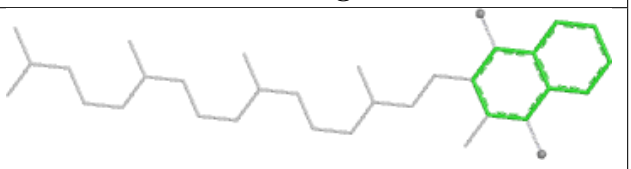
Bond lengths



Bond angles

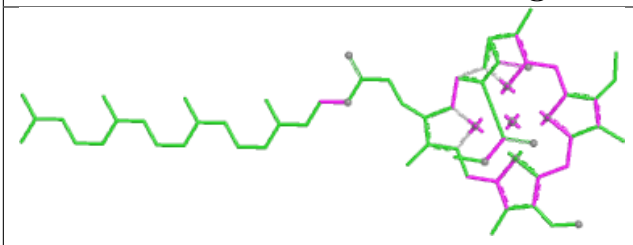


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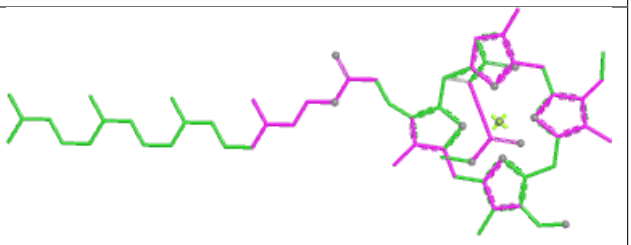


Rings

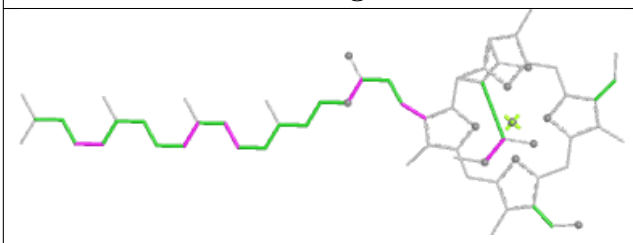
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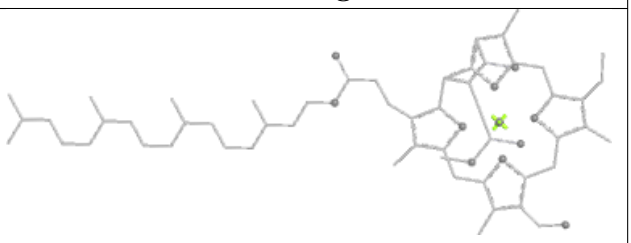
Bond lengths



Bond angles

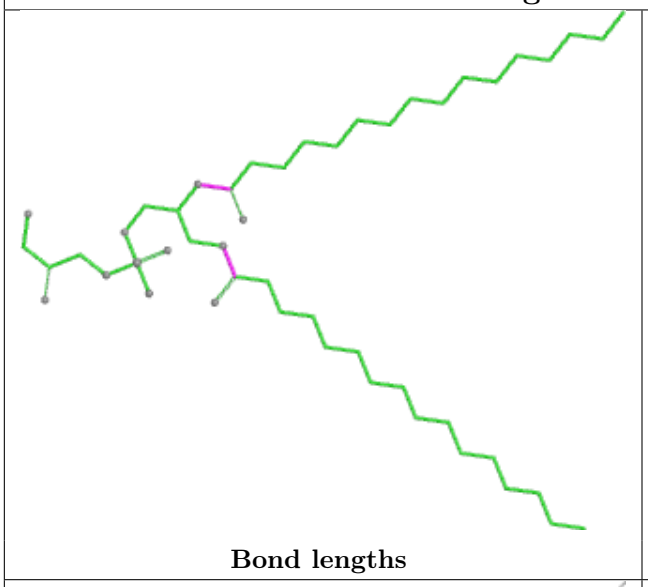


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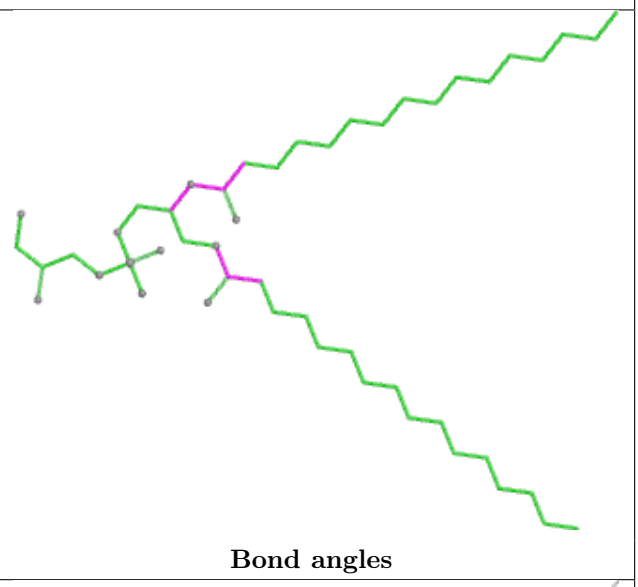


Rings

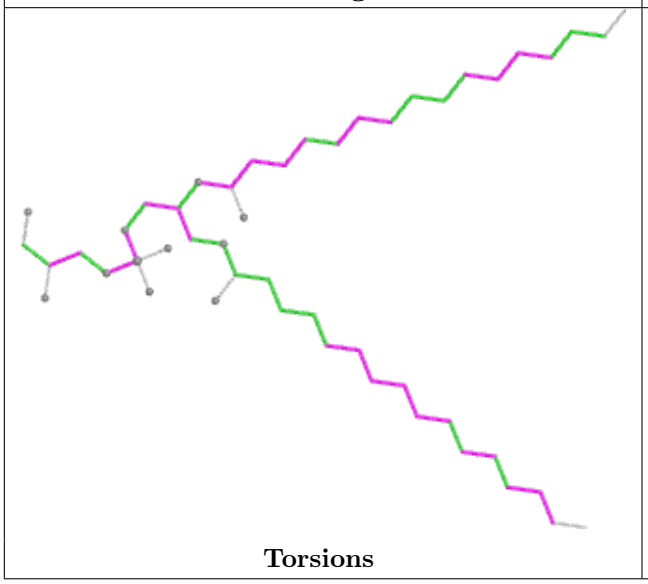
Ligand LHG A 820



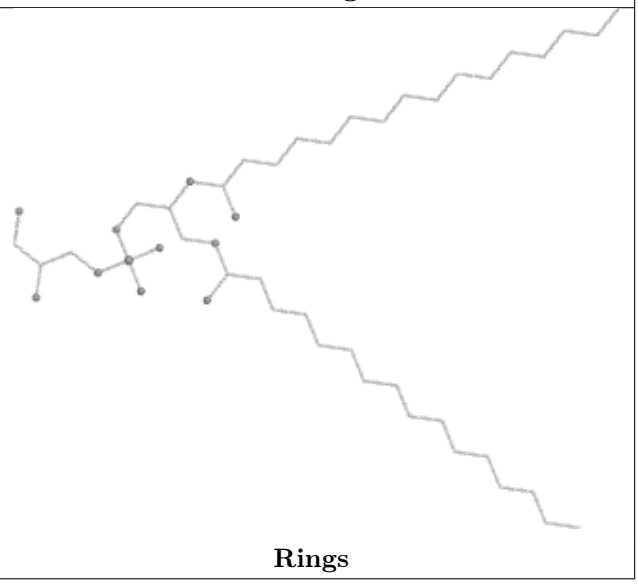
Bond lengths



Bond angles

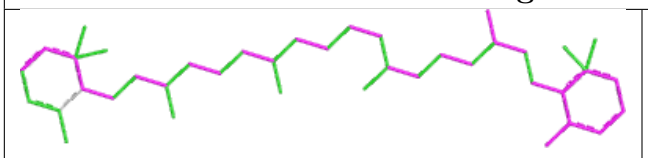


Torsions

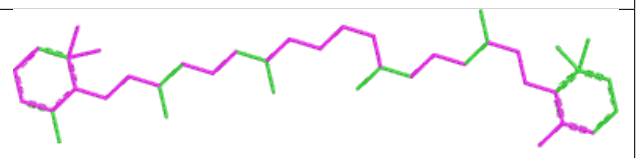


Rings

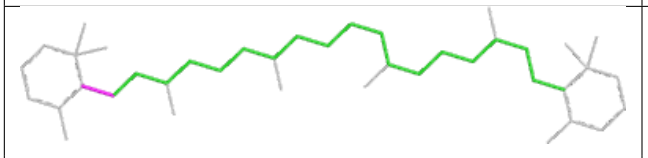
Ligand WVN B 848



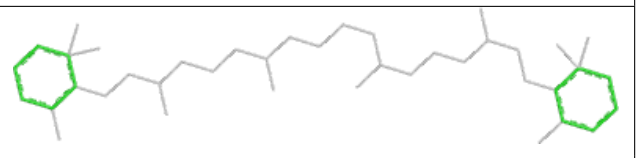
Bond lengths



Bond angles

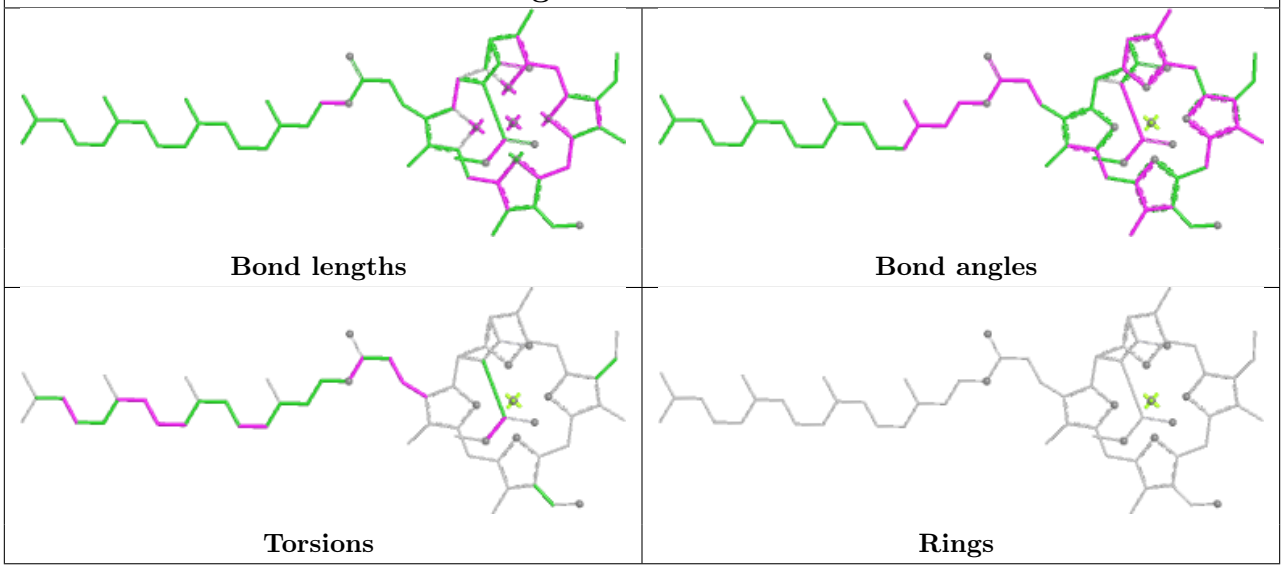


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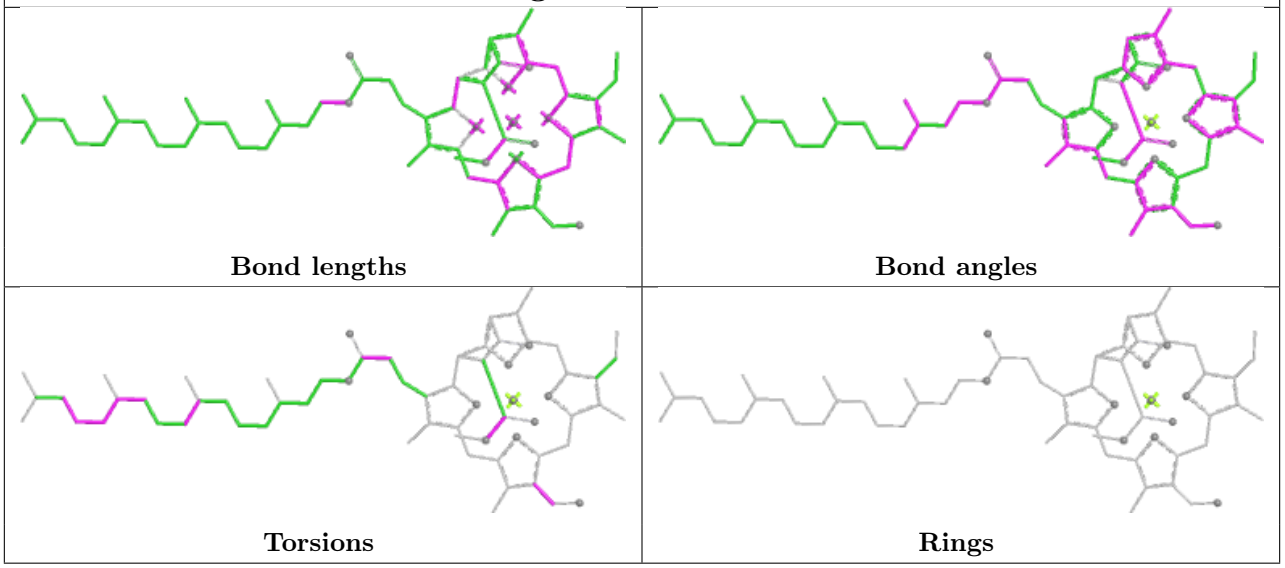


Rings

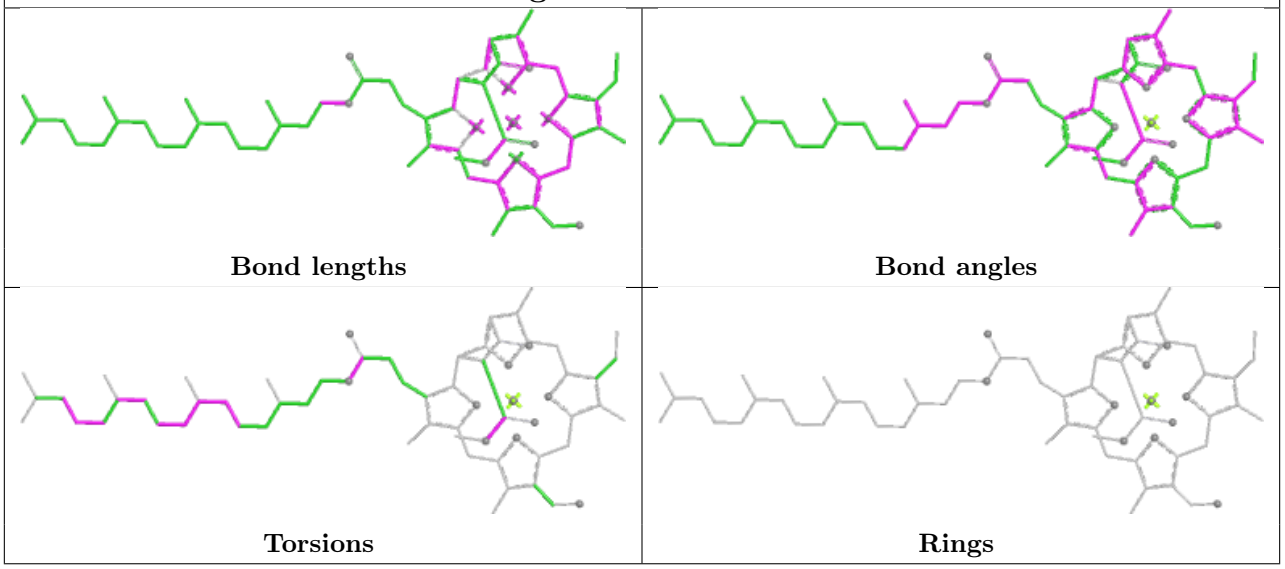
Ligand CL7 L 207



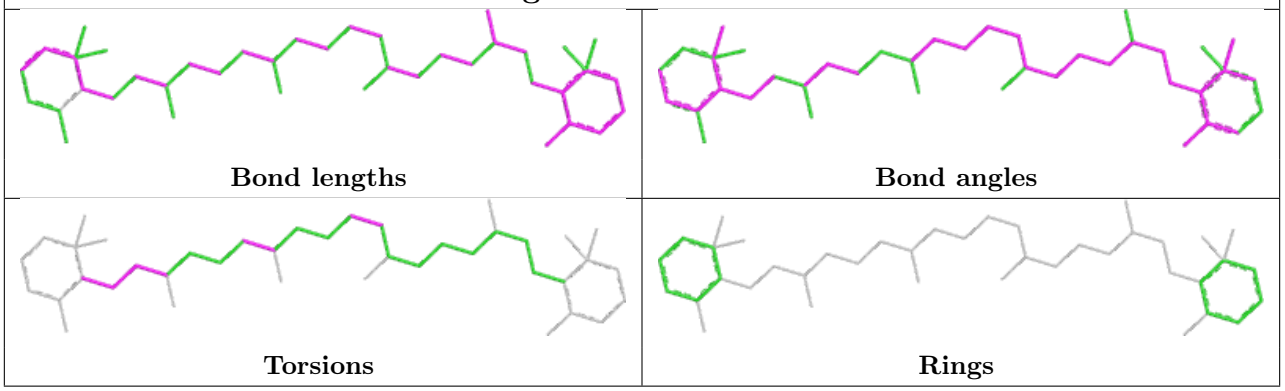
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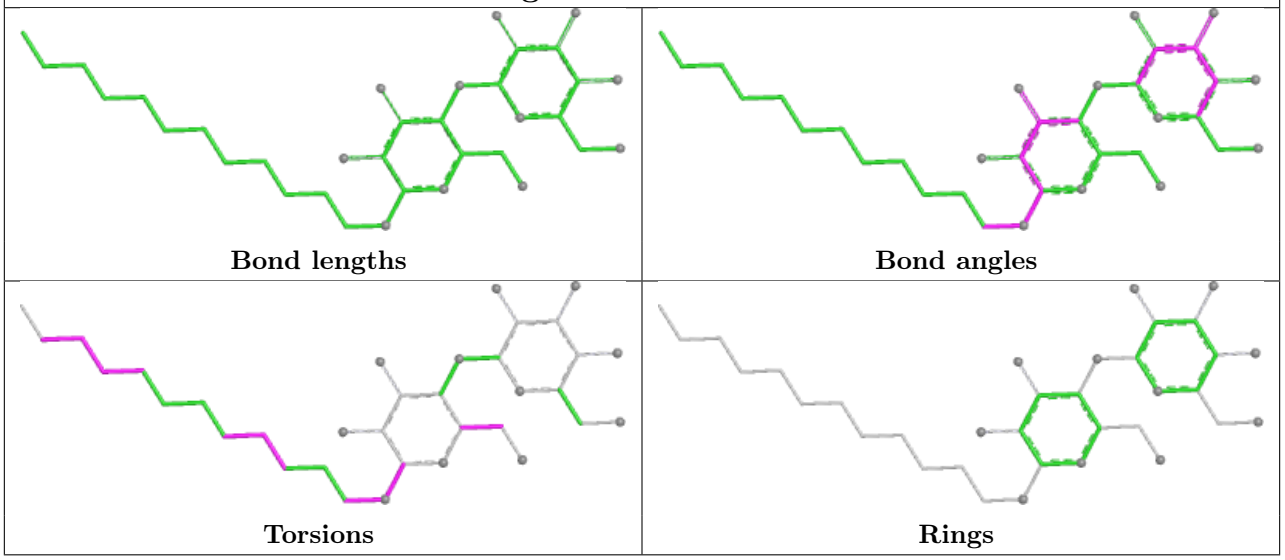
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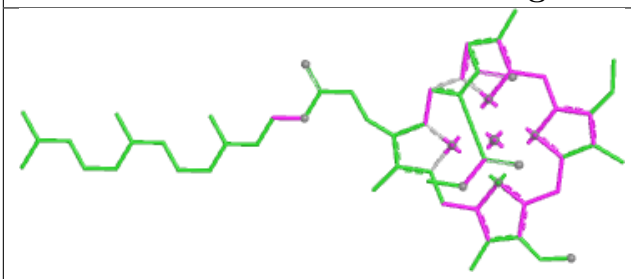
Ligand WVN I 101



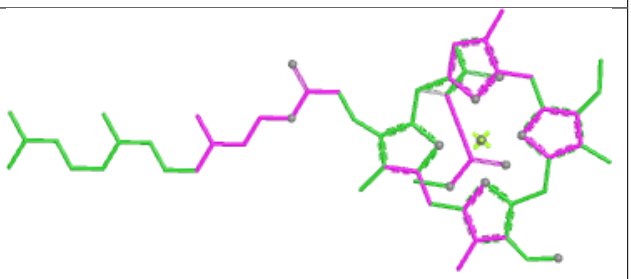
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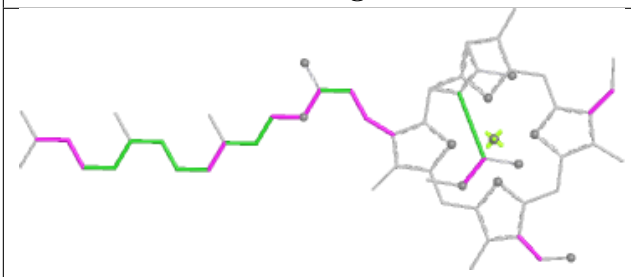
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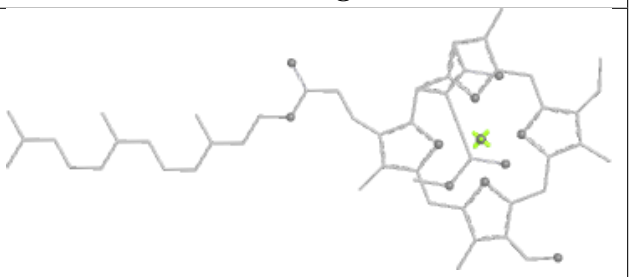
Bond lengths



Bond angles

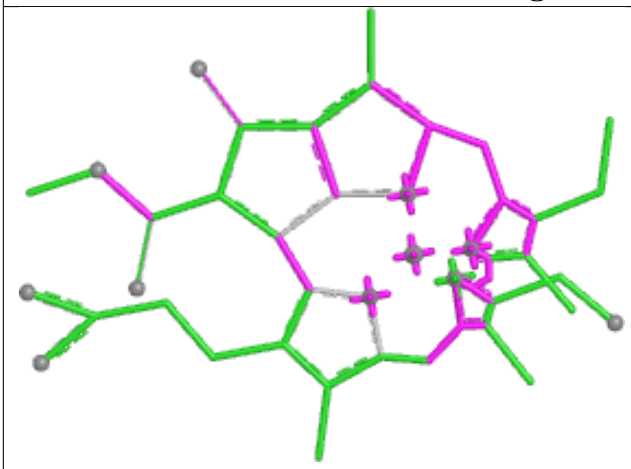


Torsions

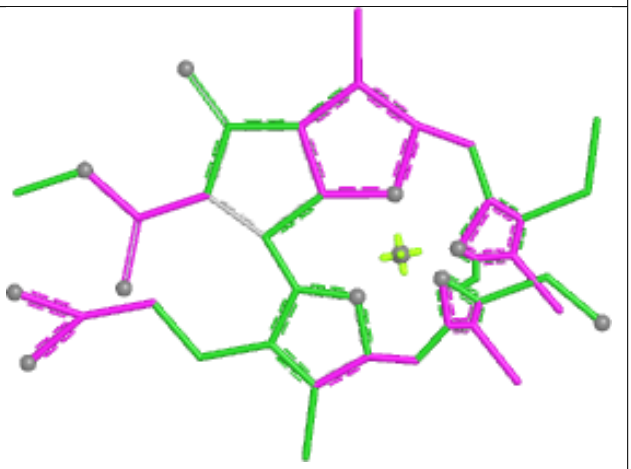


Rings

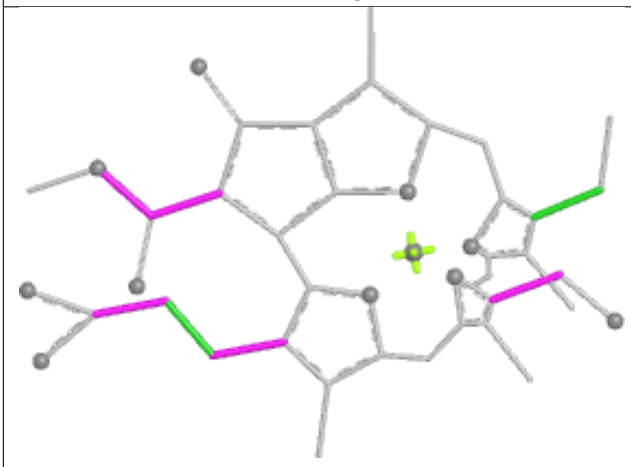
Ligand CL7 A 848



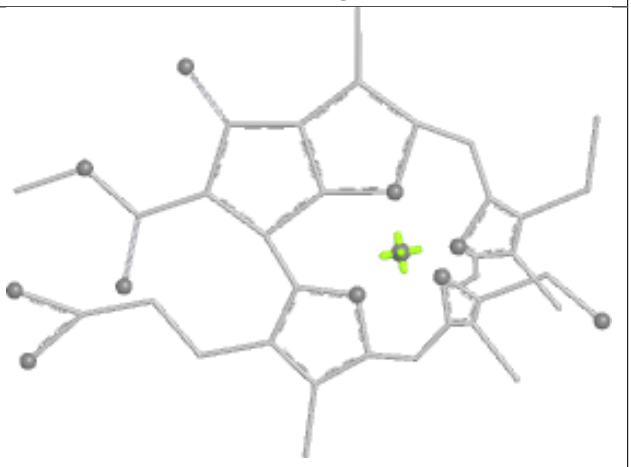
Bond lengths



Bond angles

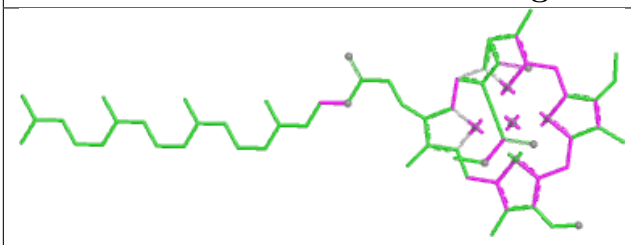


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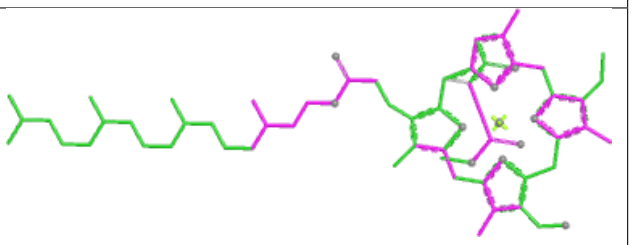


Rings

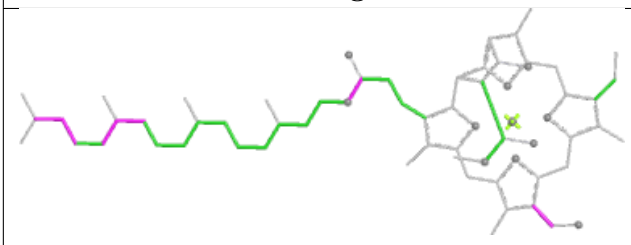
Ligand CL7 L 205



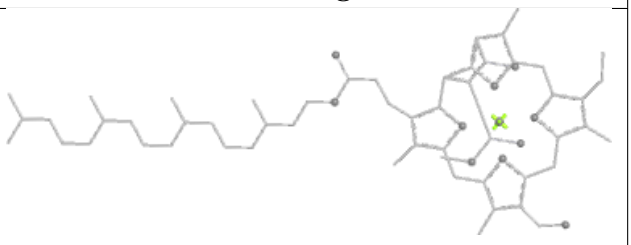
Bond lengths



Bond angles

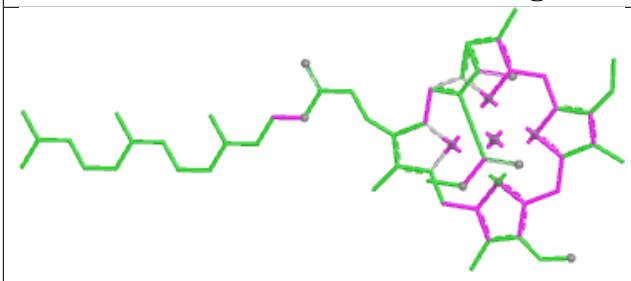


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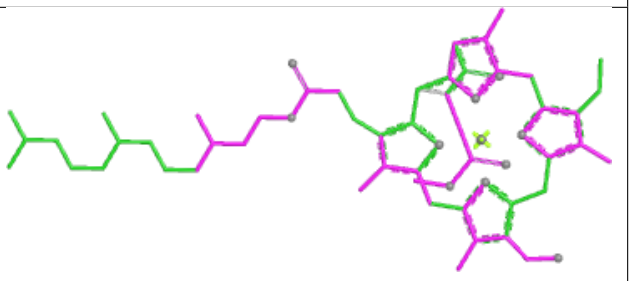


Rings

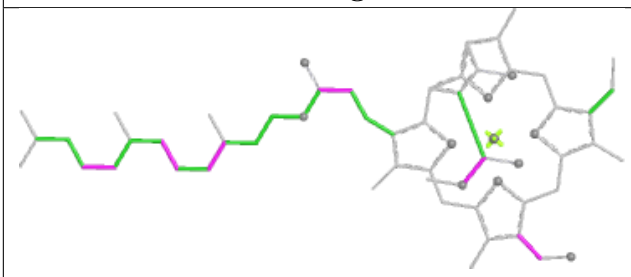
Ligand CL7 A 842



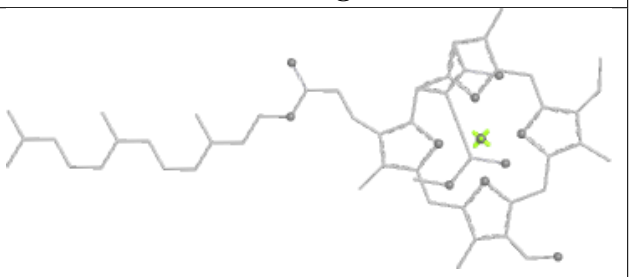
Bond lengths



Bond angles

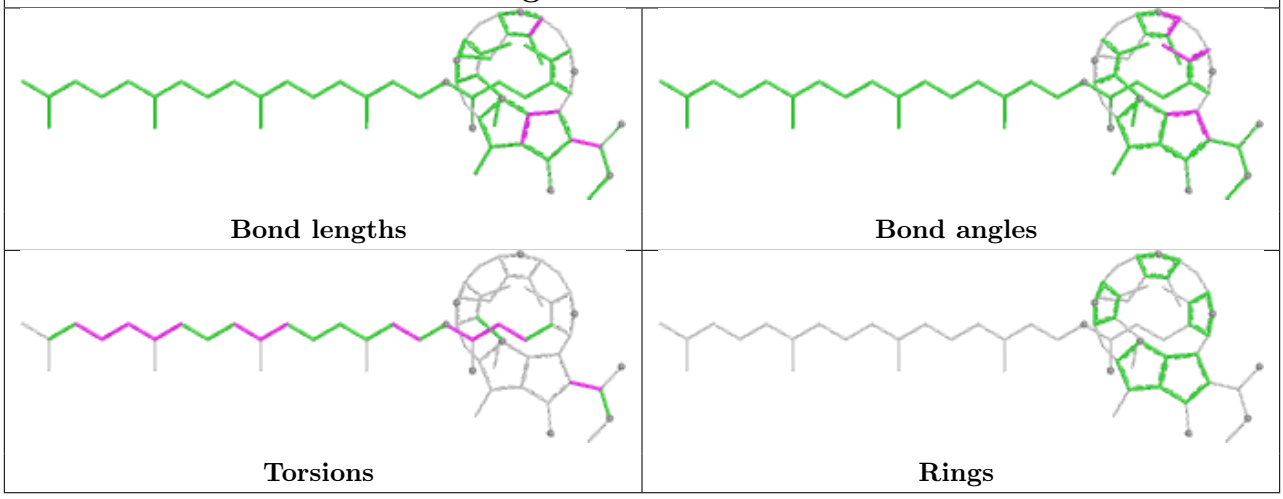


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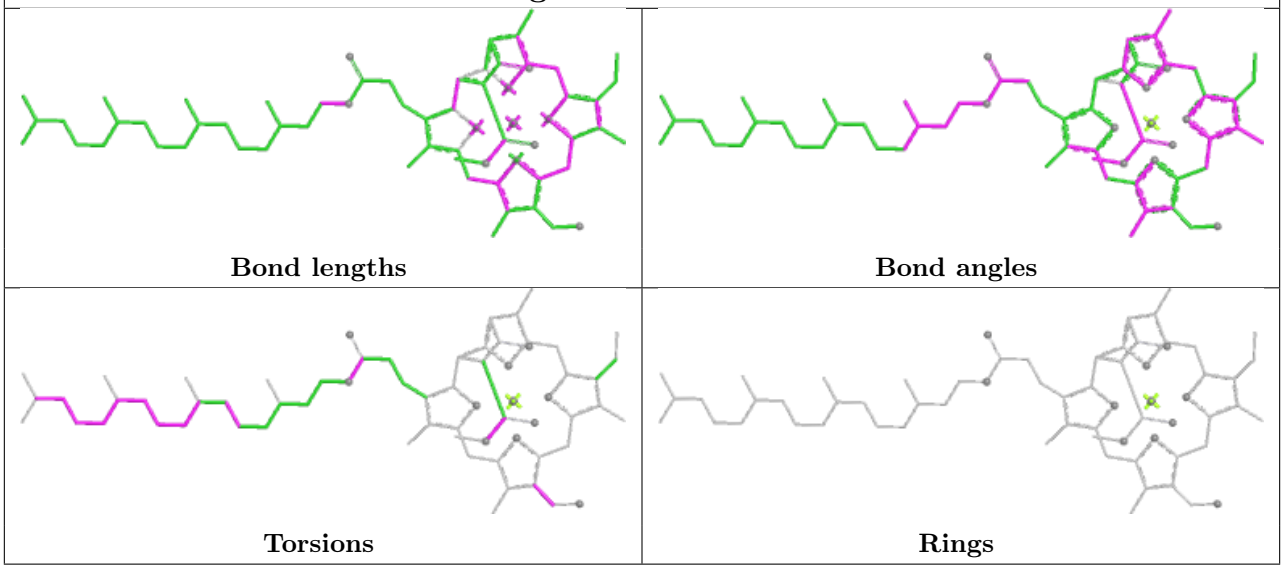


Rings

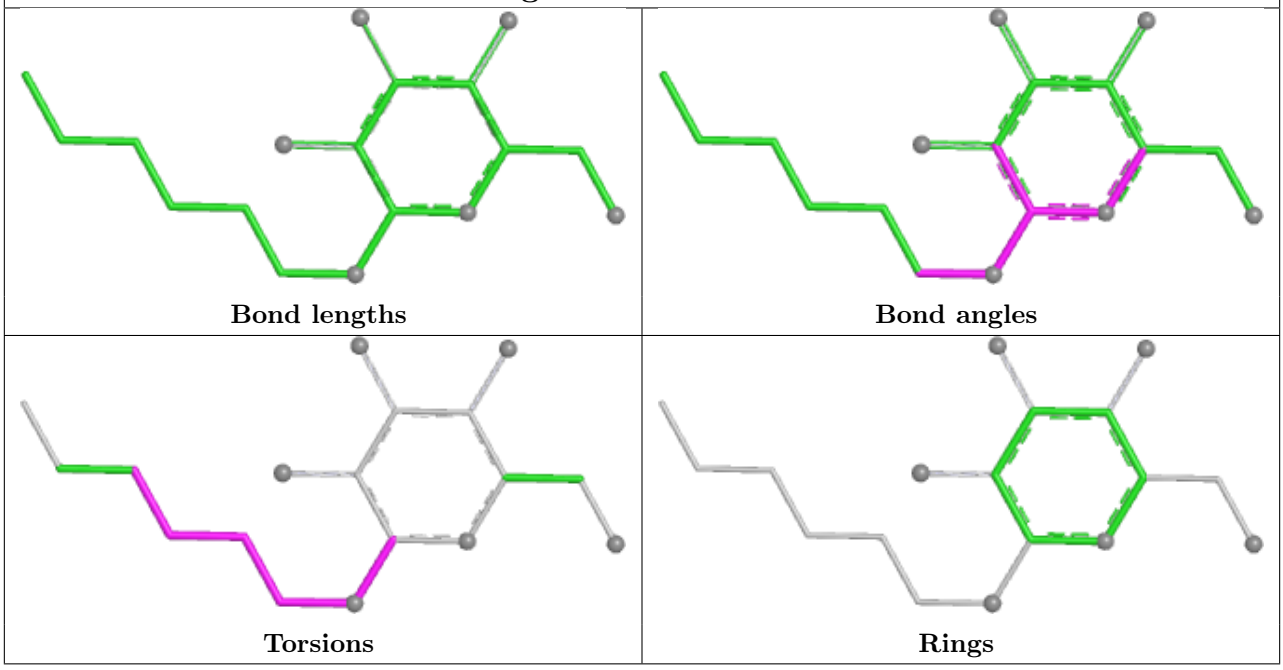
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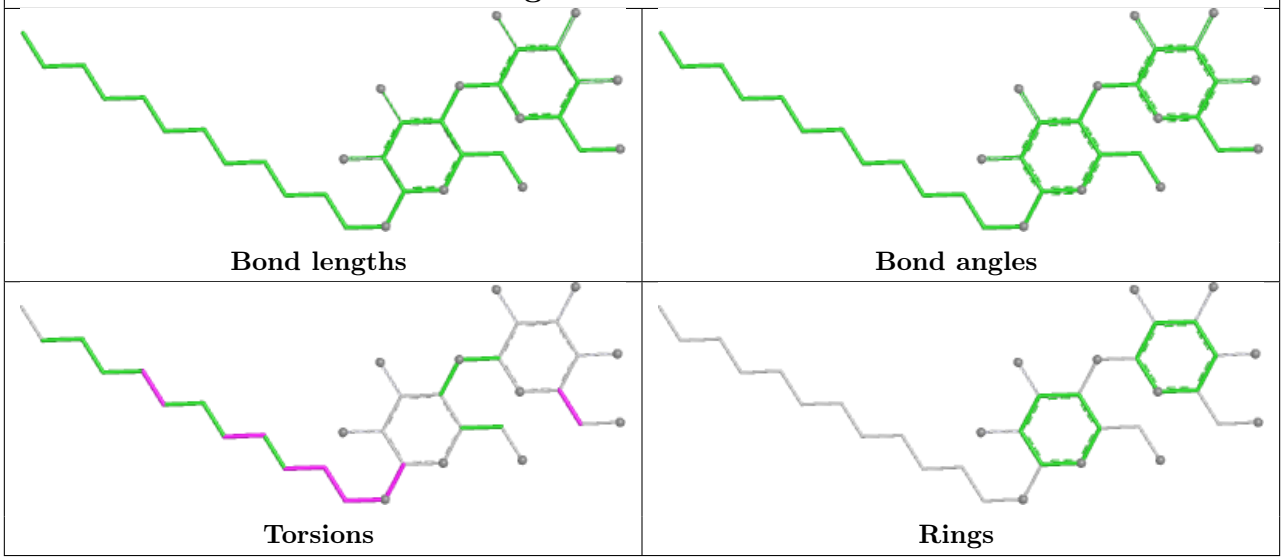
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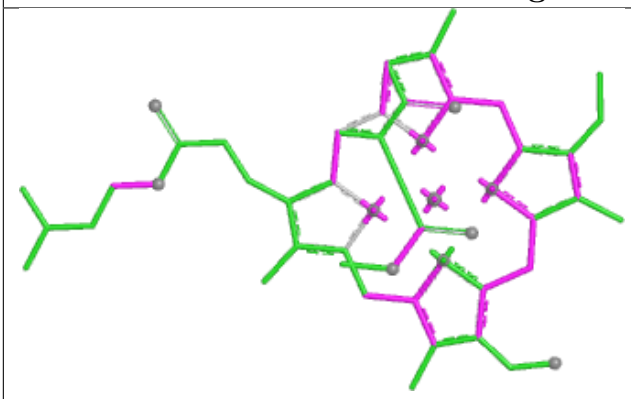
Ligand LMT K 104



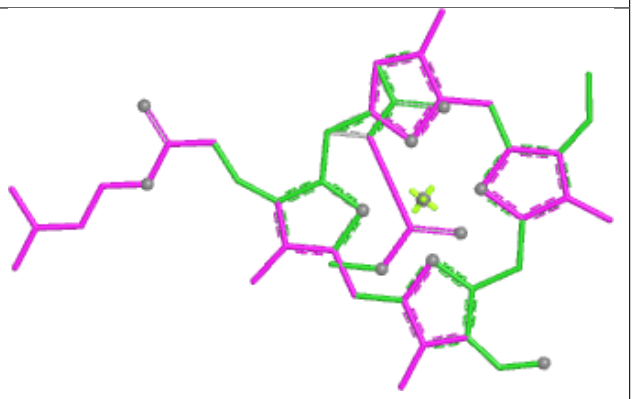
Ligand LMT L 206



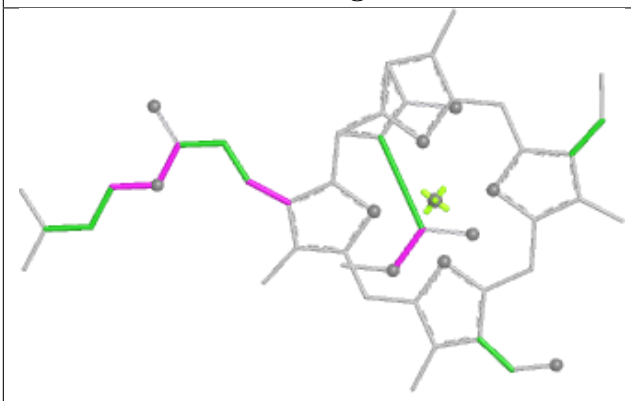
Ligand CL7 A 845



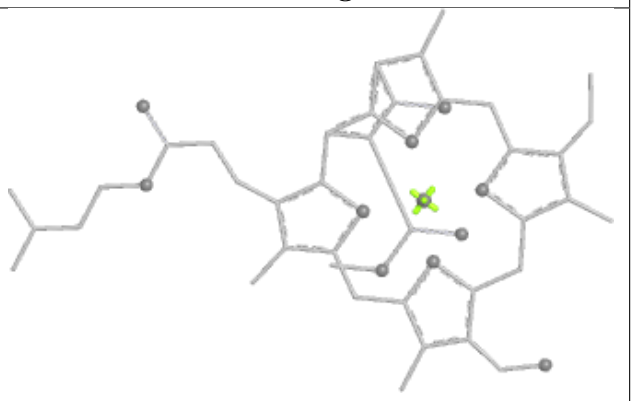
Bond lengths



Bond angles

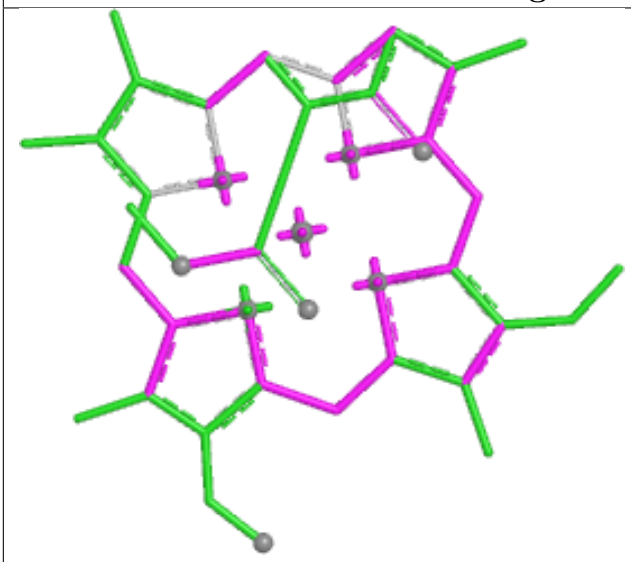


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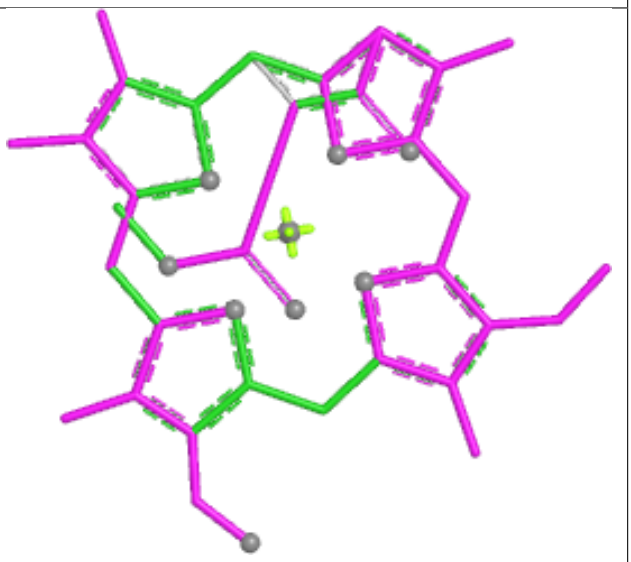


Rings

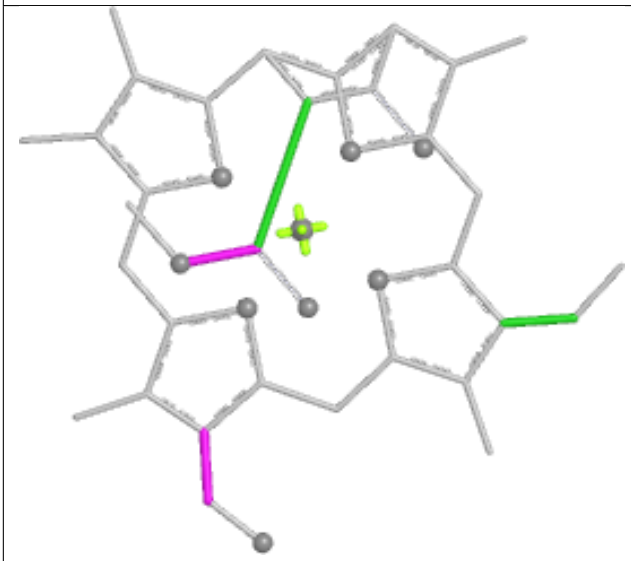
Ligand CL7 B 846



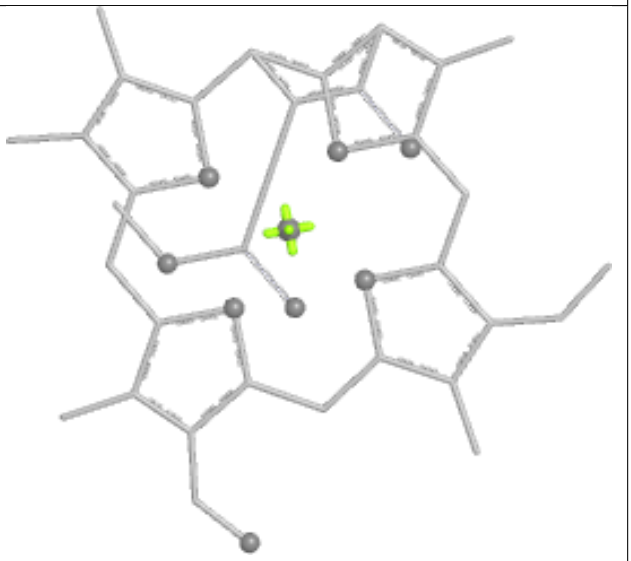
Bond lengths



Bond angles

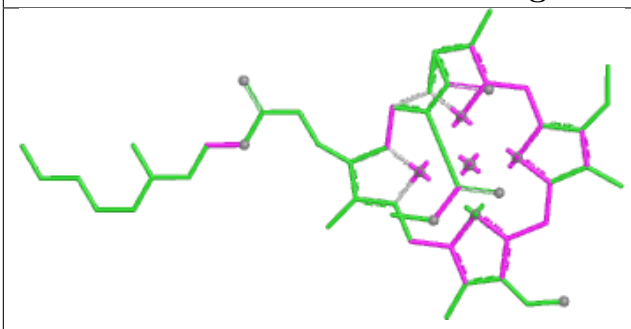


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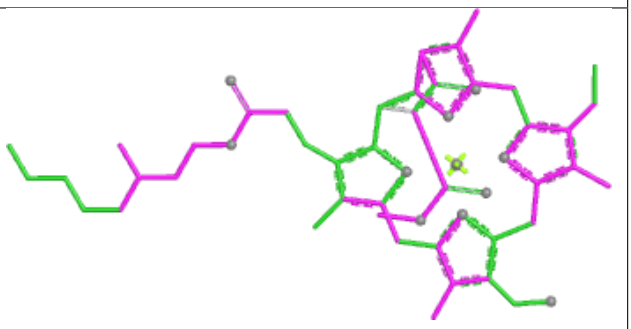


Rings

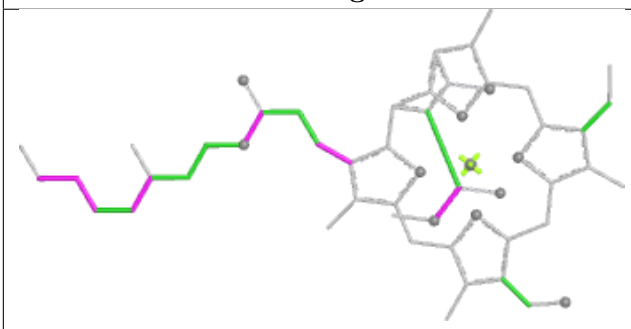
Ligand CL7 B 821



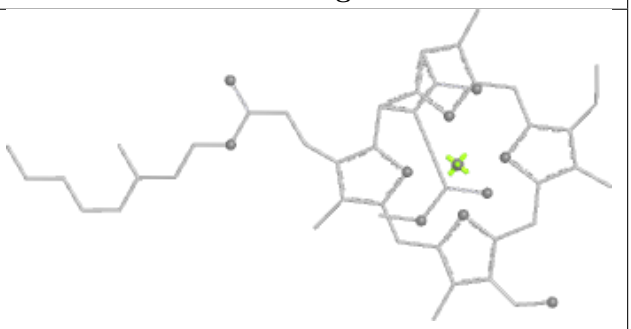
Bond lengths



Bond angles

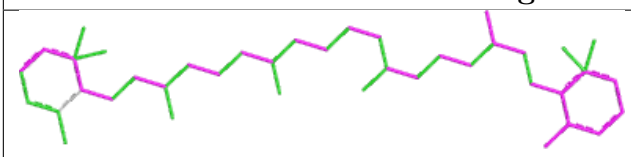


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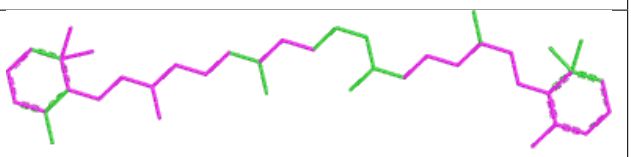


Rings

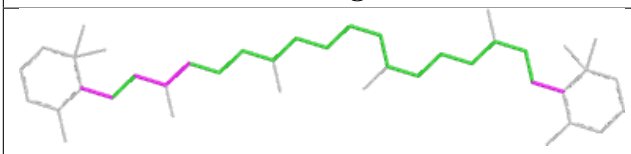
Ligand WVN L 202



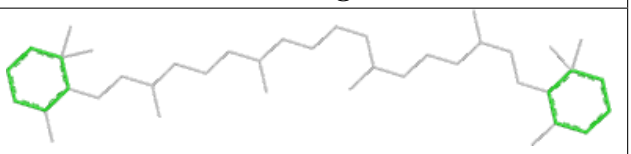
Bond lengths



Bond angles

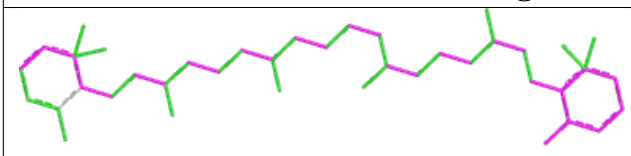


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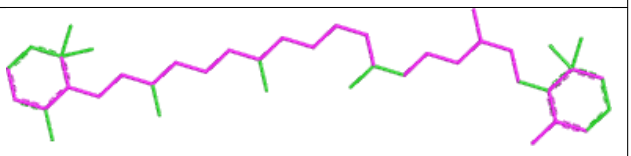


Rings

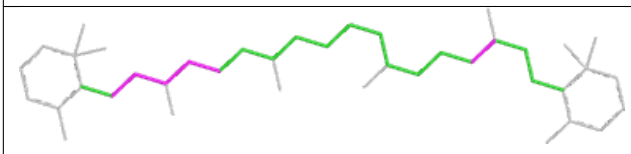
Ligand WVN B 847



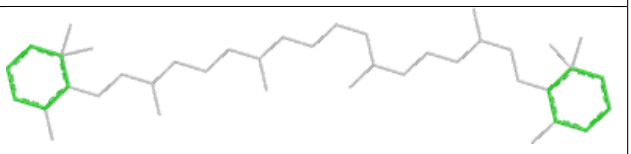
Bond lengths



Bond angles

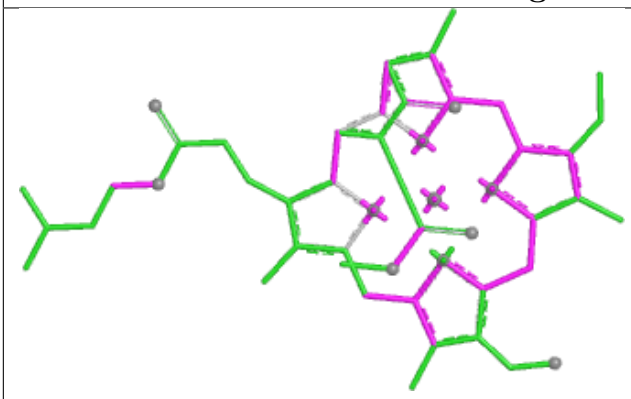


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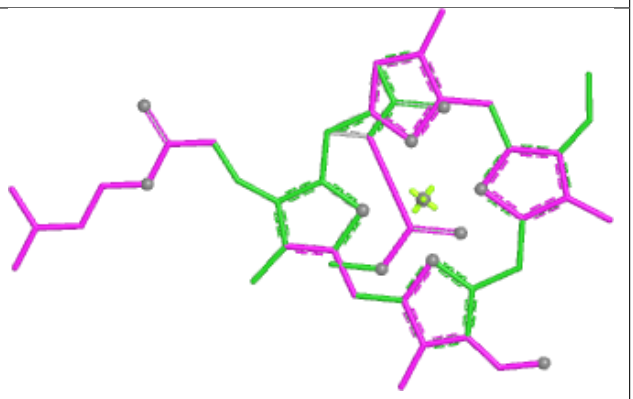


Rings

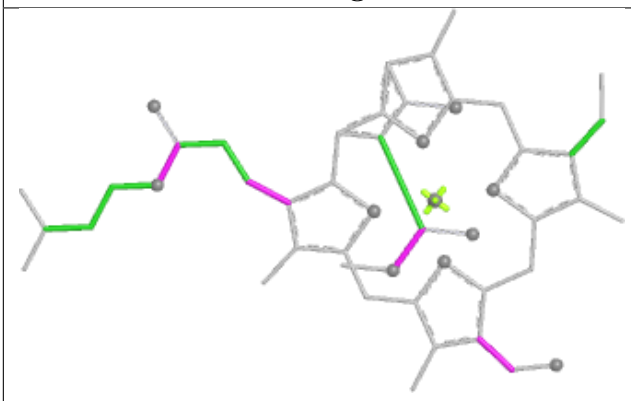
Ligand CL7 B 816



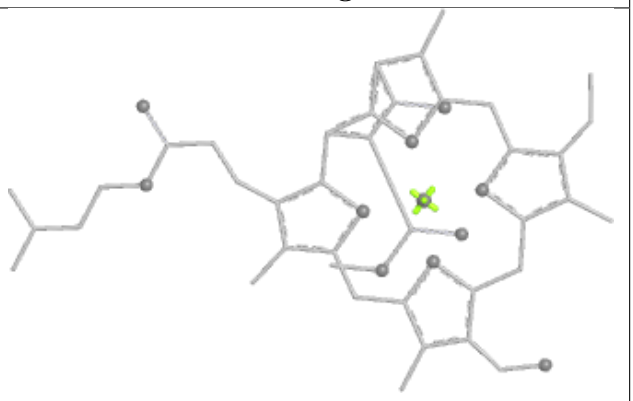
Bond lengths



Bond angles

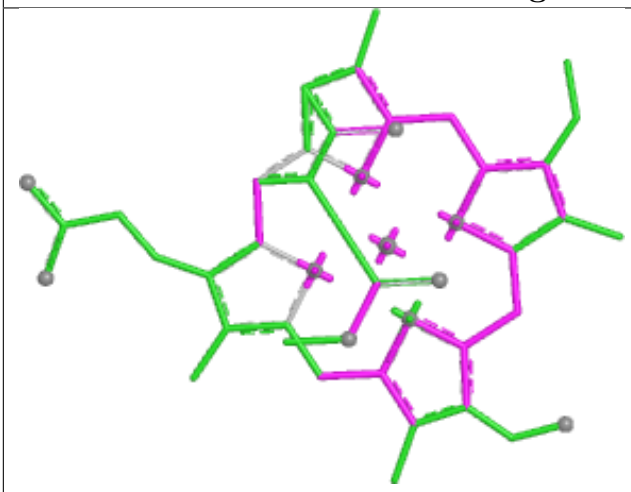


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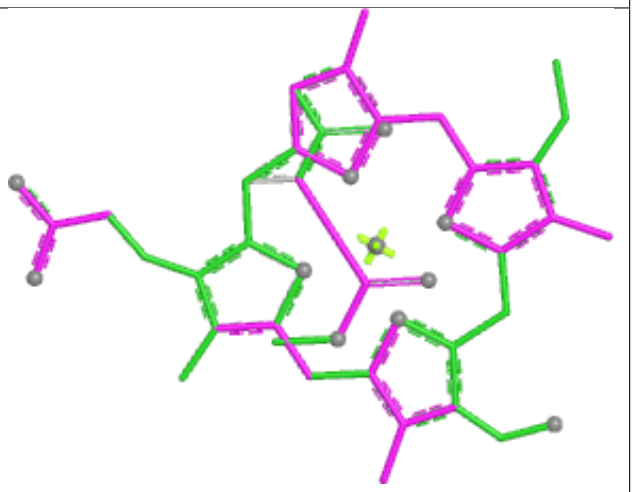


Rings

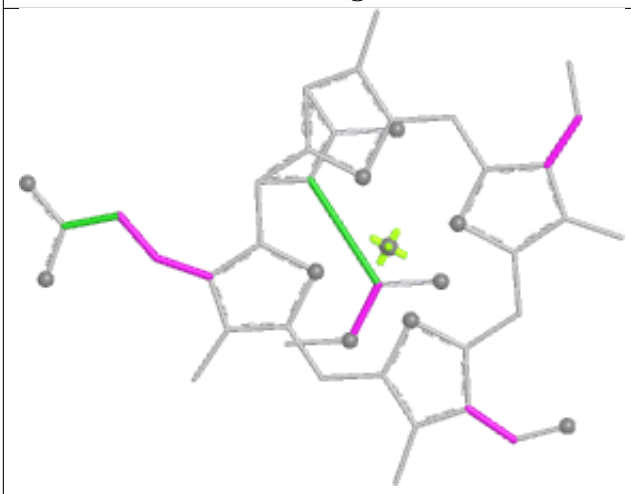
Ligand CL7 B 834



Bond lengths



Bond angles

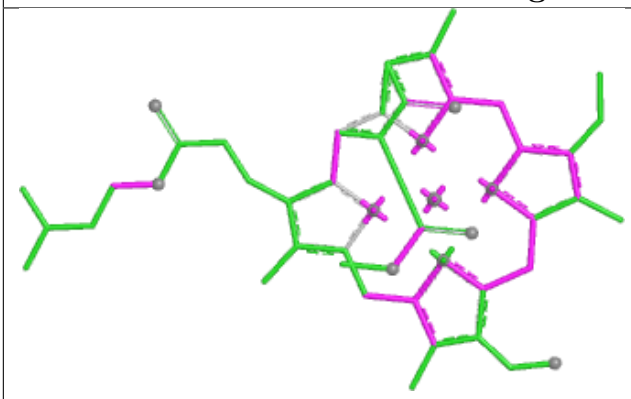


Torsions

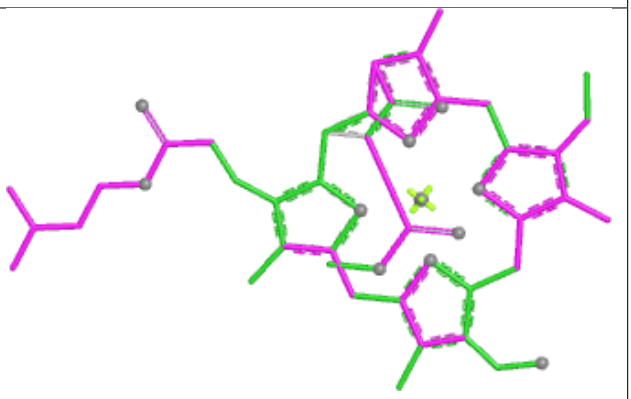


Rings

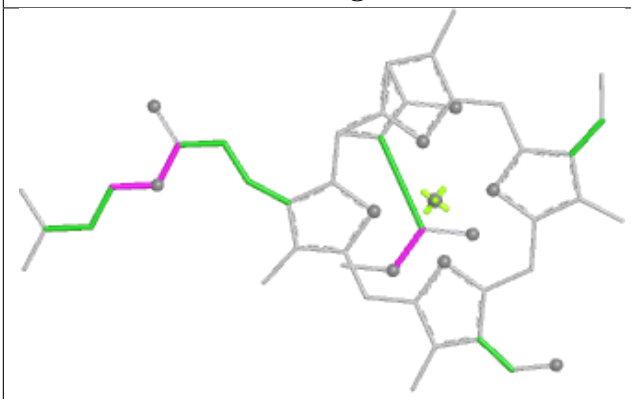
Ligand CL7 A 816



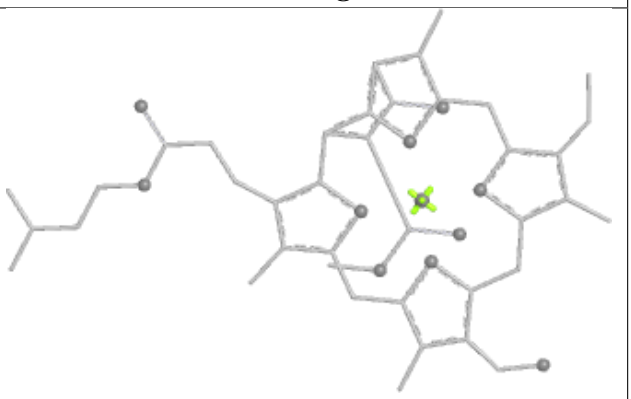
Bond lengths



Bond angles

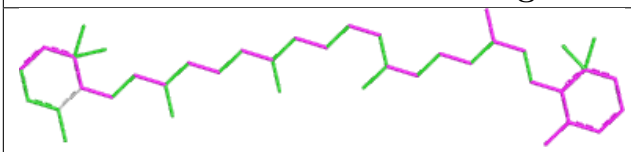


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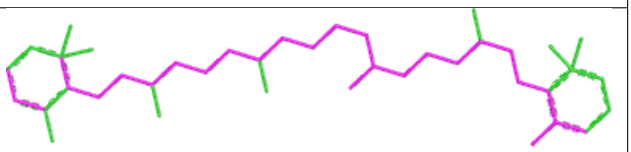


Rings

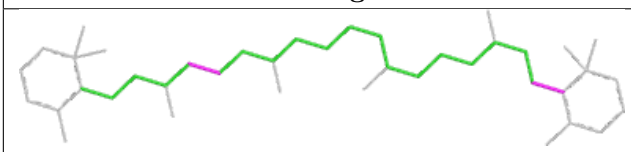
Ligand WVN L 209



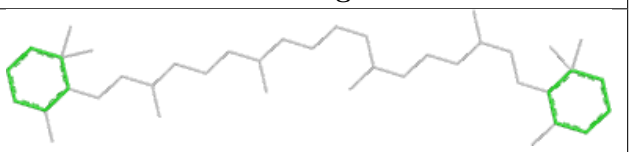
Bond lengths



Bond angles

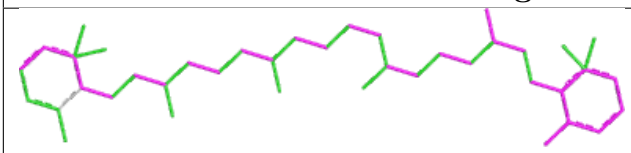


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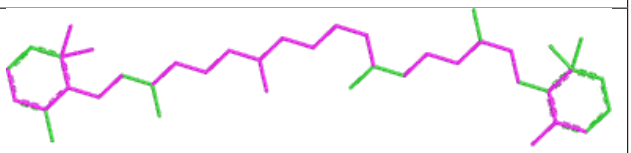


Rings

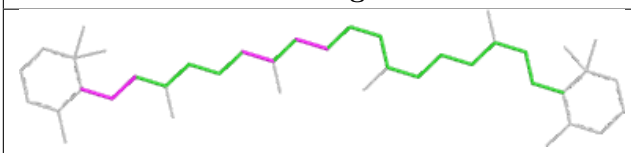
Ligand WVN K 101



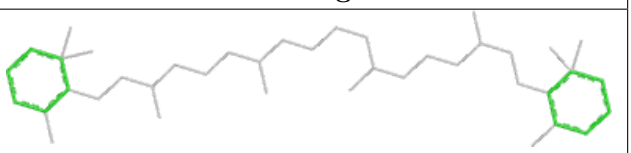
Bond lengths



Bond angles

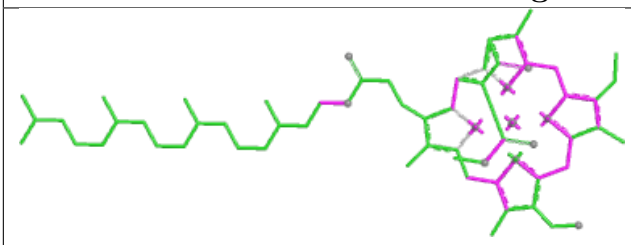


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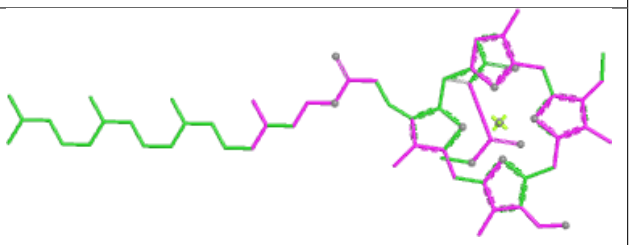


Rings

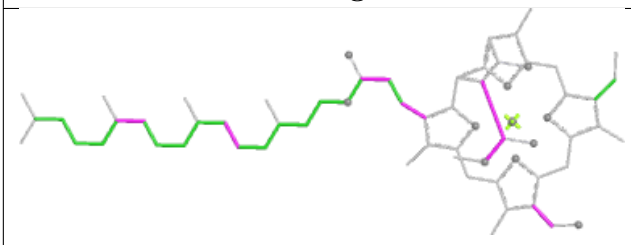
Ligand CL7 L 201



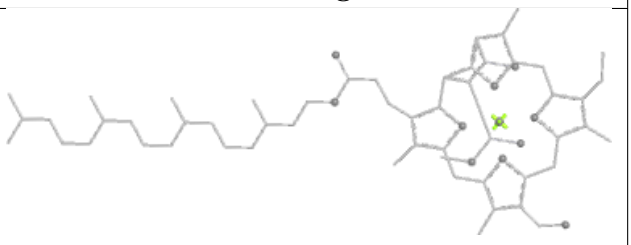
Bond lengths



Bond angles

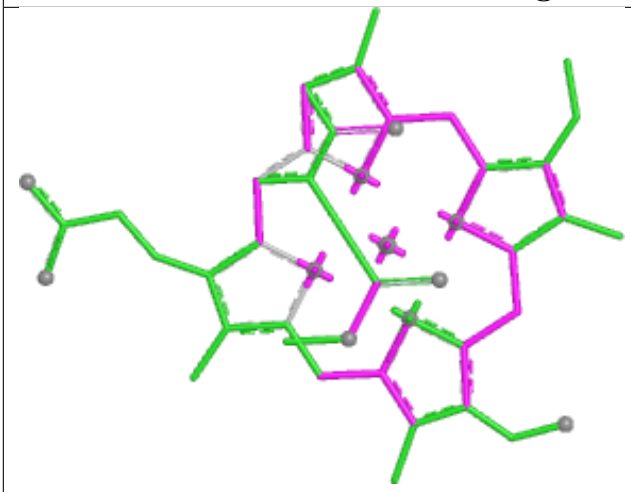


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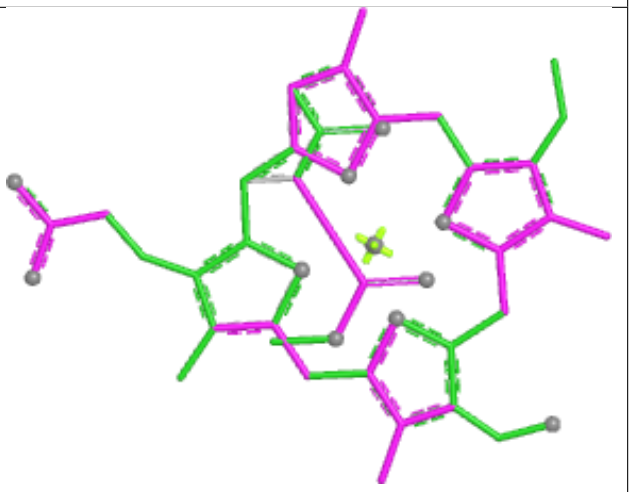


Rings

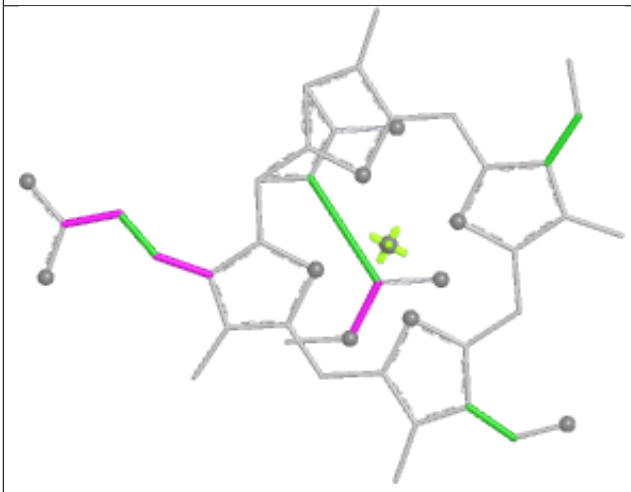
Ligand CL7 I 102



Bond lengths



Bond angles

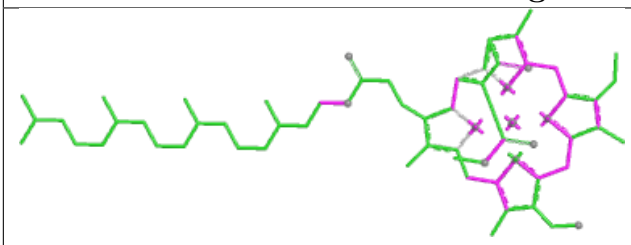


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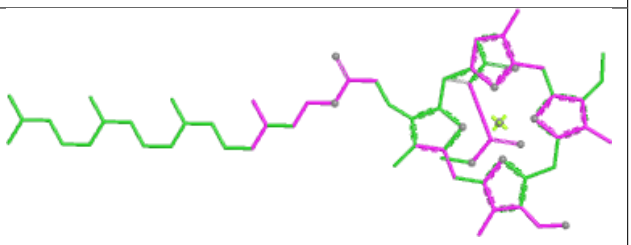


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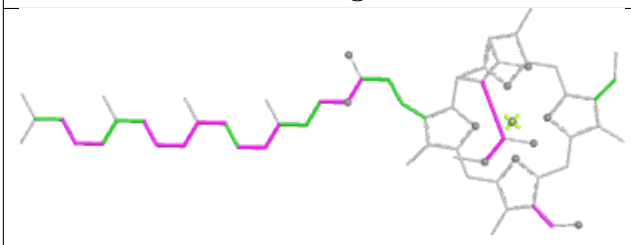
Ligand CL7 A 830



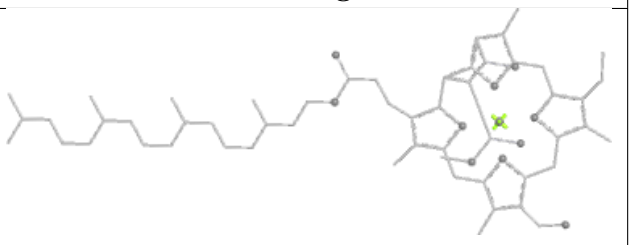
Bond lengths



Bond angles

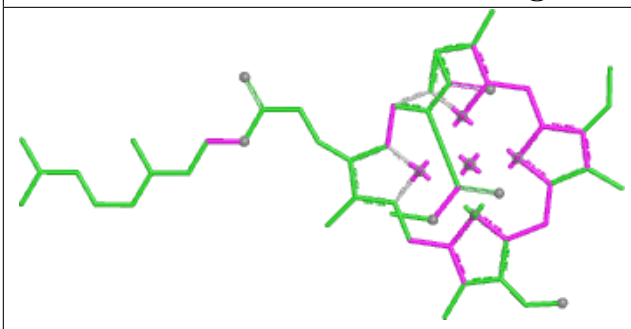


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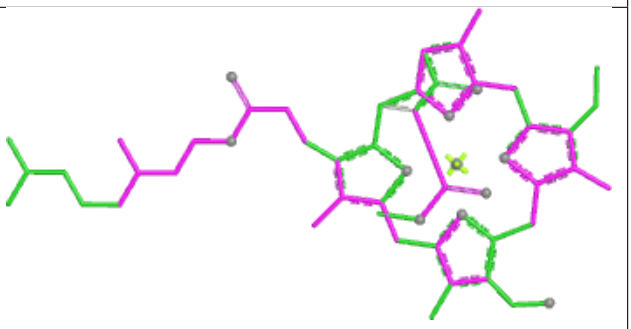


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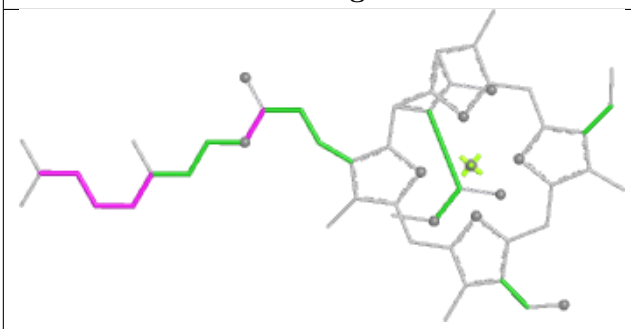
Ligand CL7 A 818



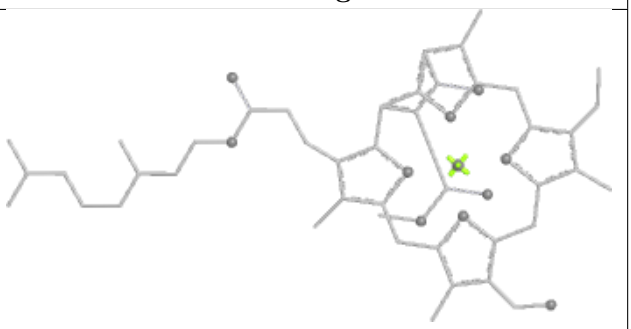
Bond lengths



Bond angles

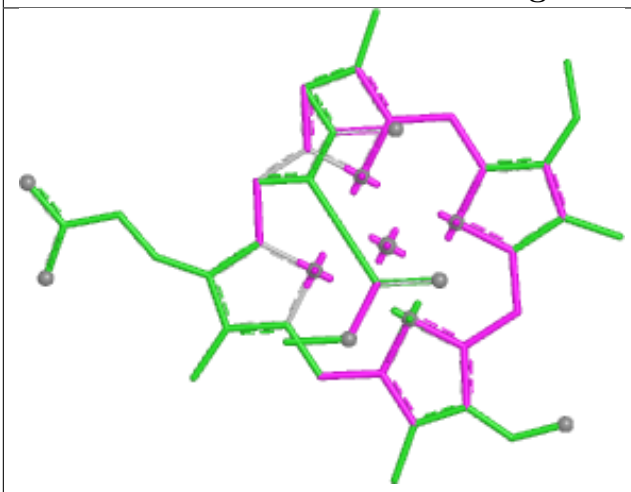


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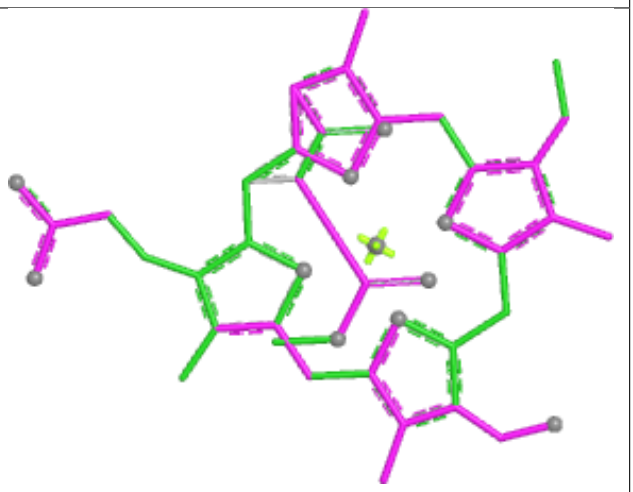


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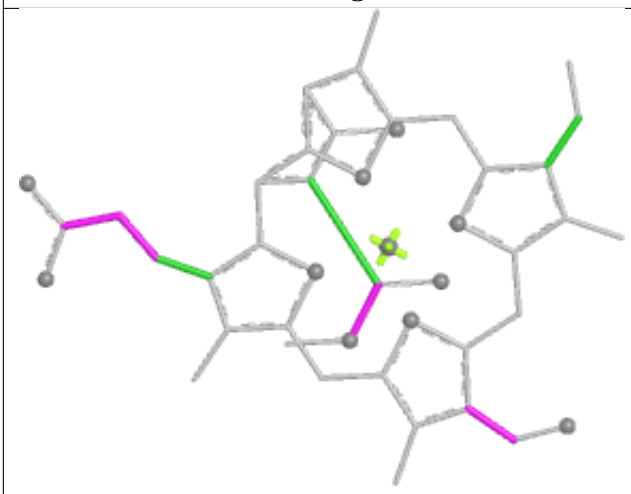
Ligand CL7 B 843



Bond lengths



Bond angles

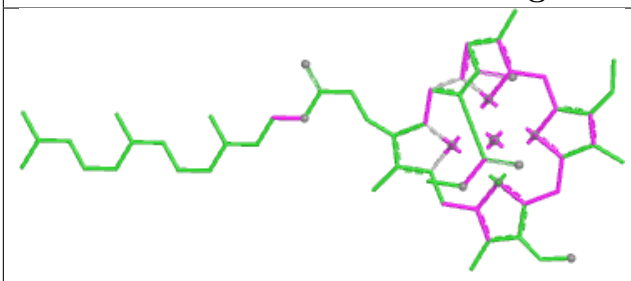


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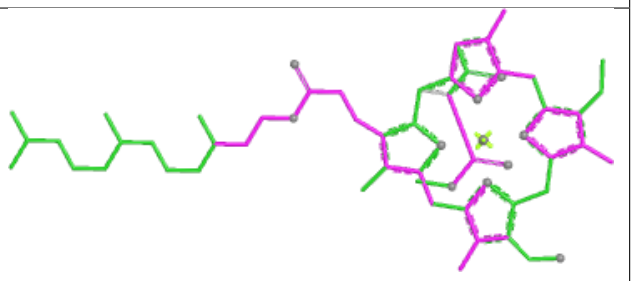


Rings

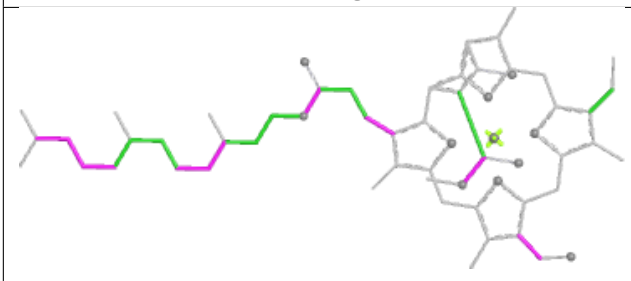
Ligand CL7 A 841



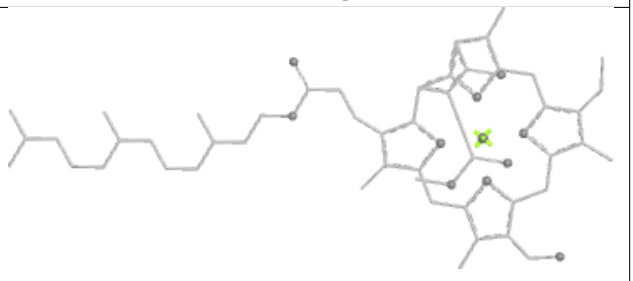
Bond lengths



Bond angles

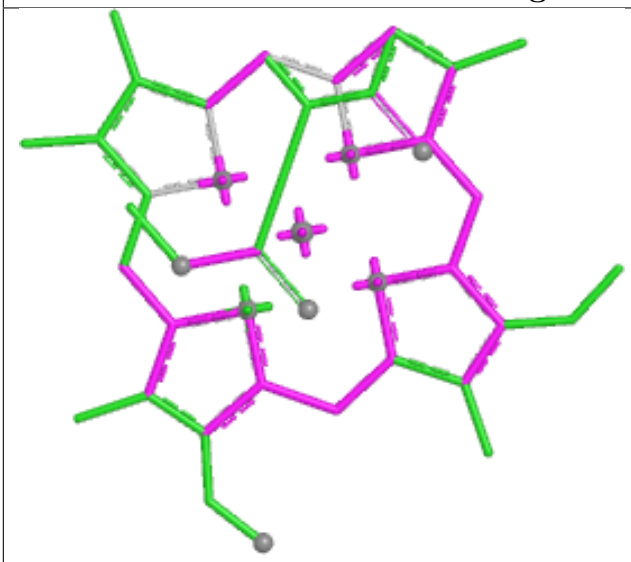


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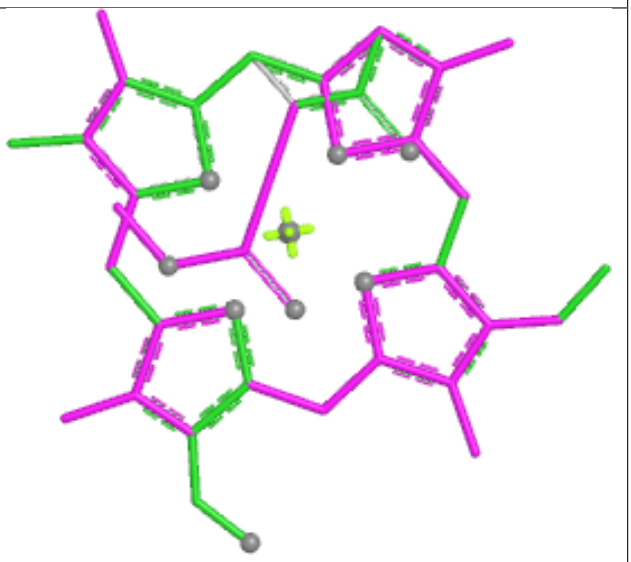


Rings

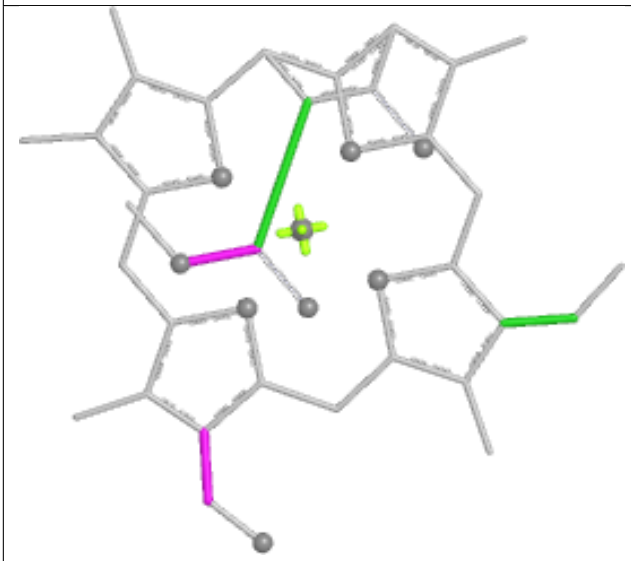
Ligand CL7 B 811



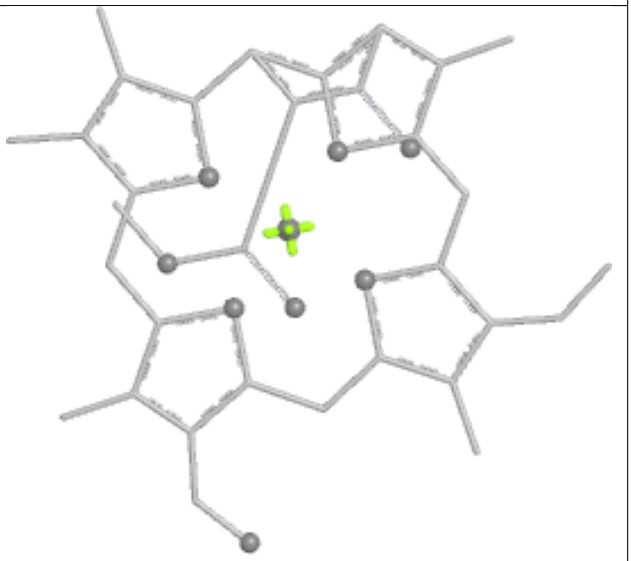
Bond lengths



Bond angles

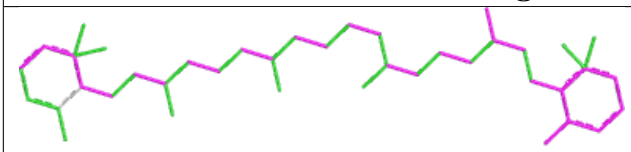


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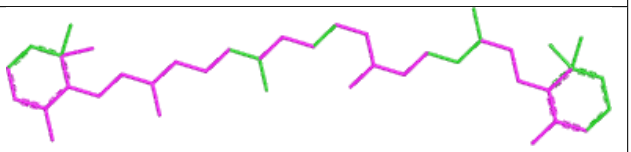


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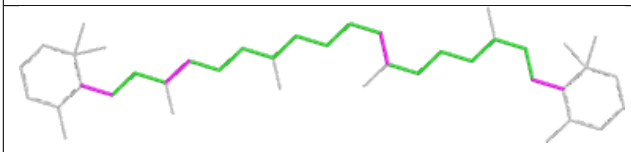
Ligand WVN A 851



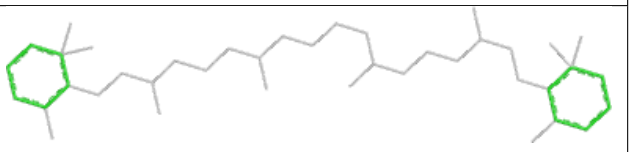
Bond lengths



Bond angles

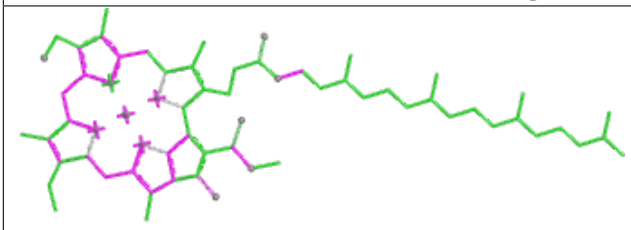


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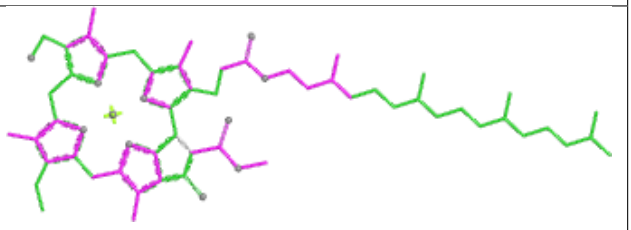


Rings

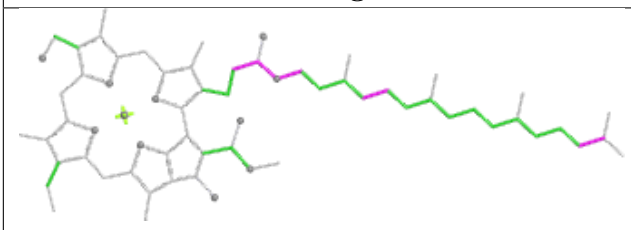
Ligand G9R A 801



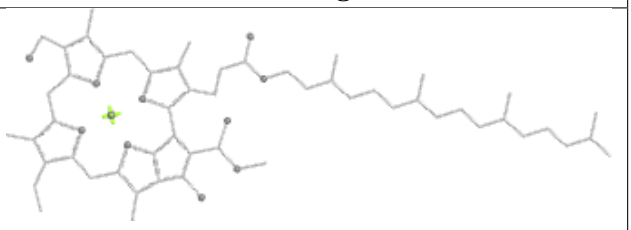
Bond lengths



Bond angles



Torsions



Rings

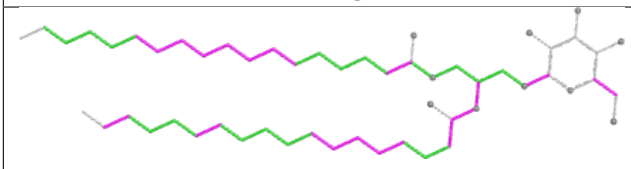
Ligand LMG B 827



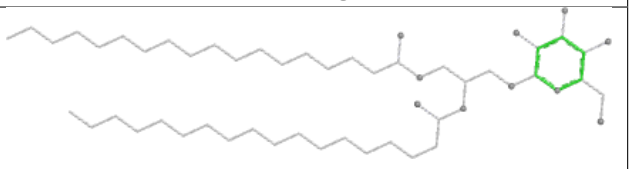
Bond lengths



Bond angles

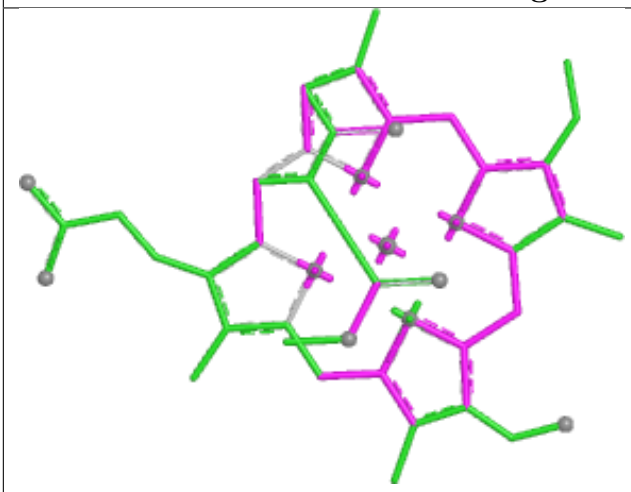


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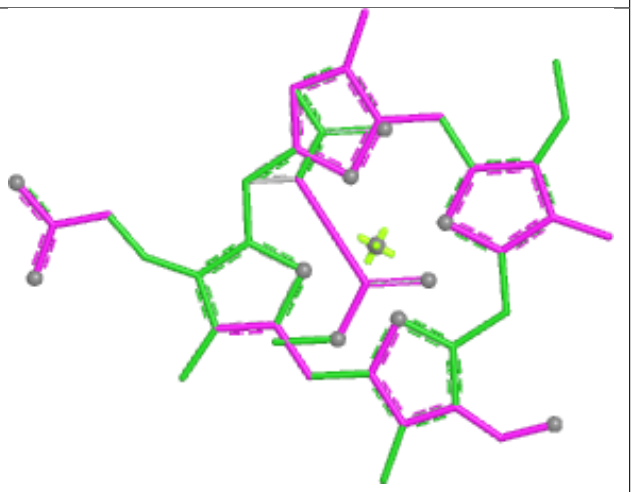


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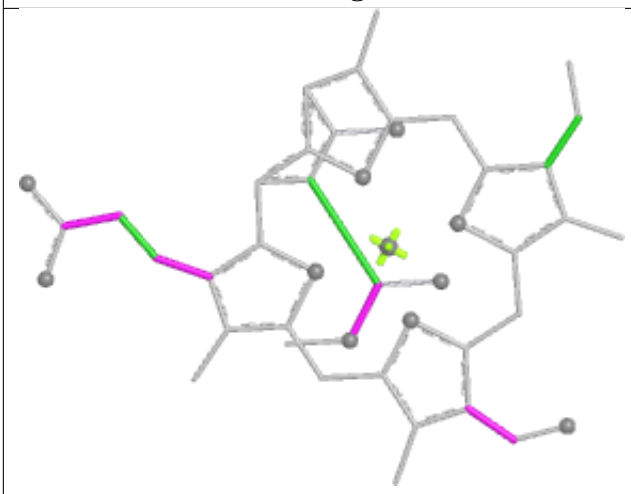
Ligand CL7 F 202



Bond lengths



Bond angles

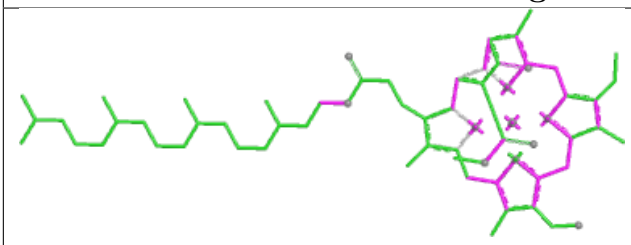


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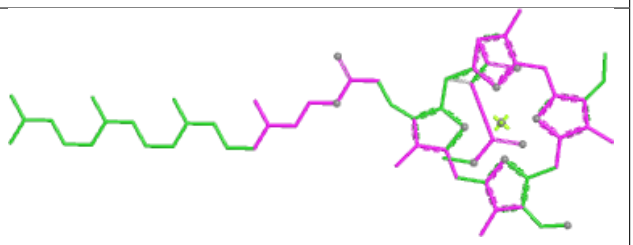


Rings

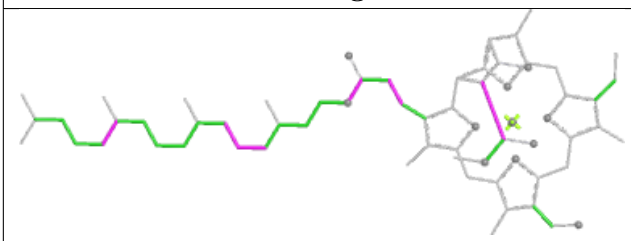
Ligand CL7 B 822



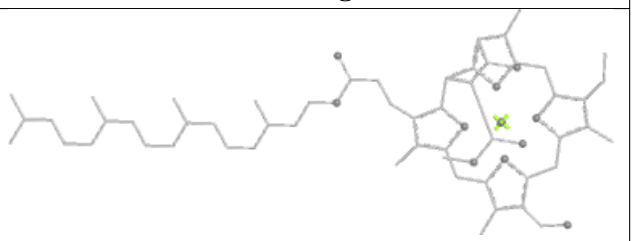
Bond lengths



Bond angles

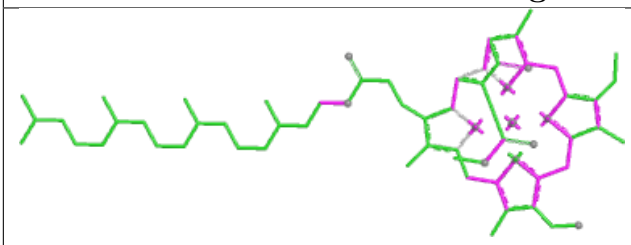


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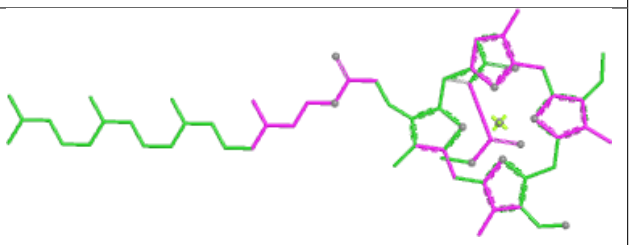


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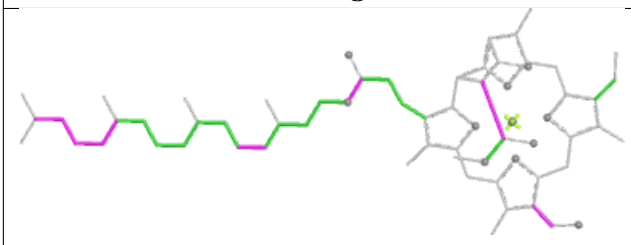
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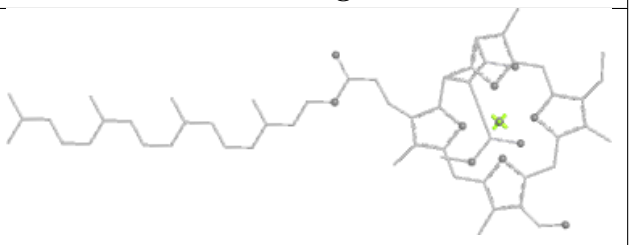
Bond lengths



Bond angles

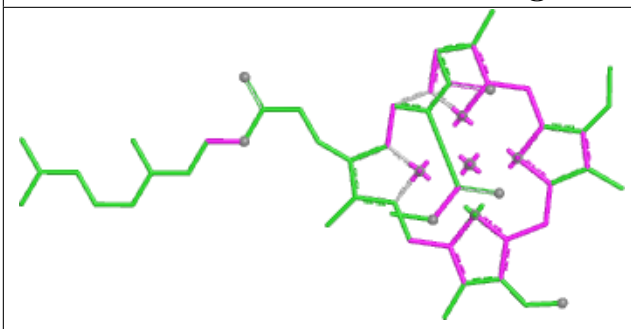


Torsions

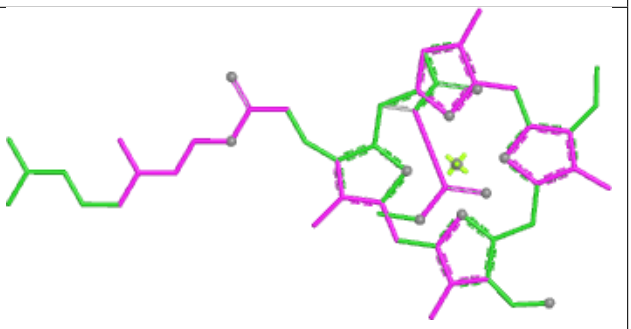


Rings

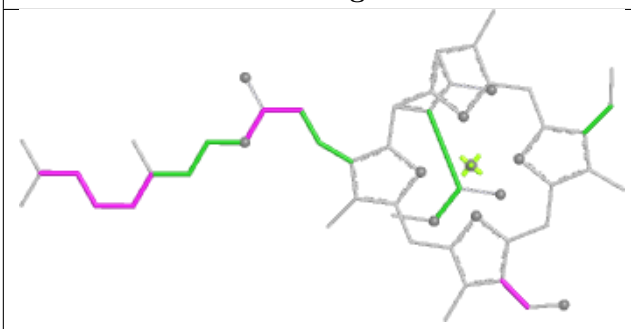
Ligand CL7 A 835



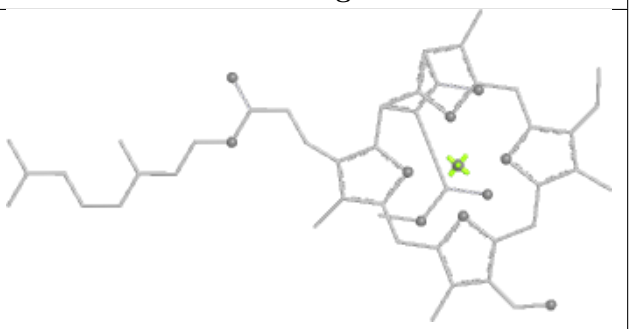
Bond lengths



Bond angles

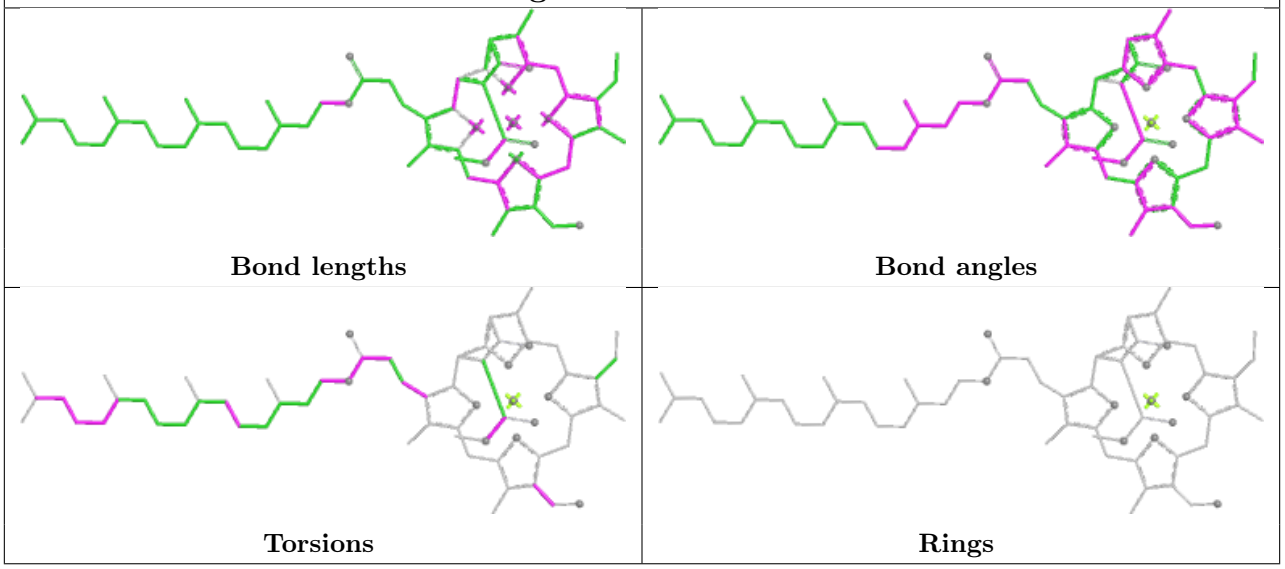


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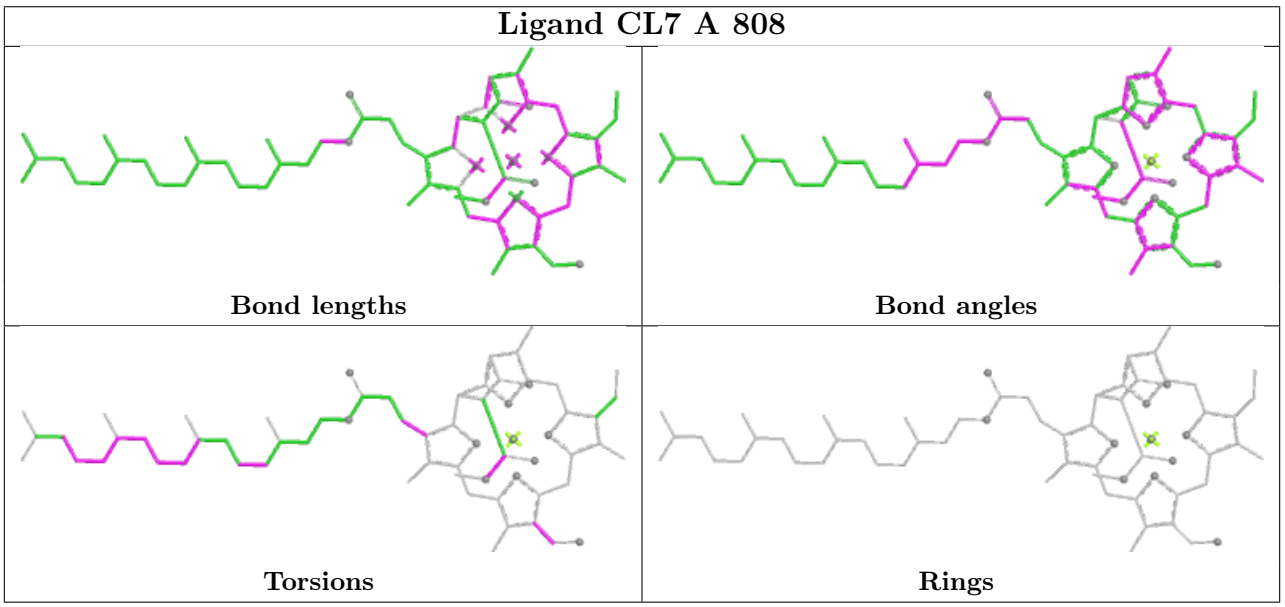


Rings

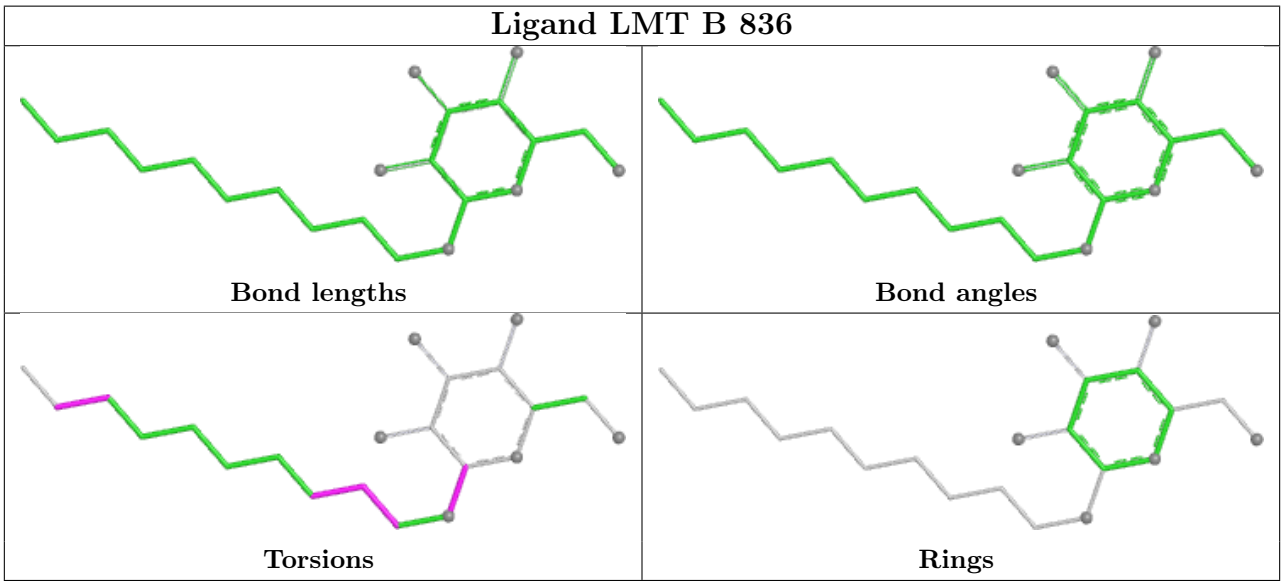
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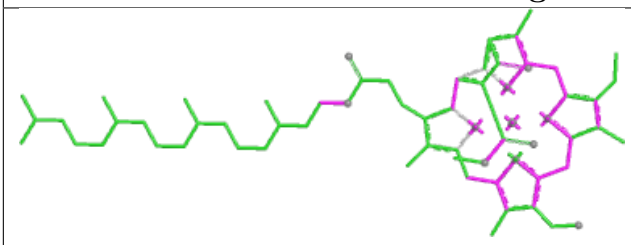
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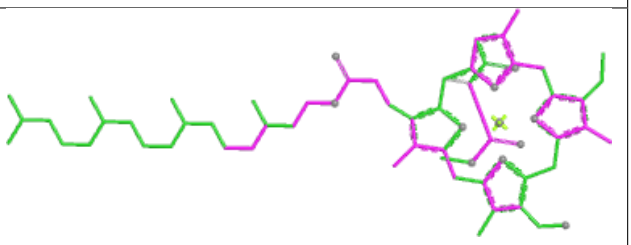
Ligand LMT B 836



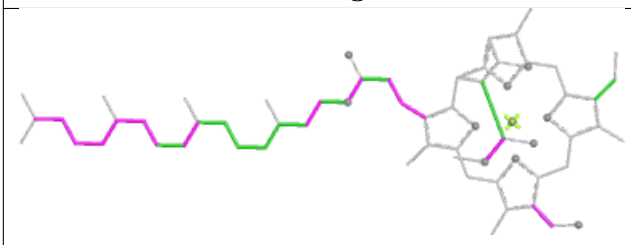
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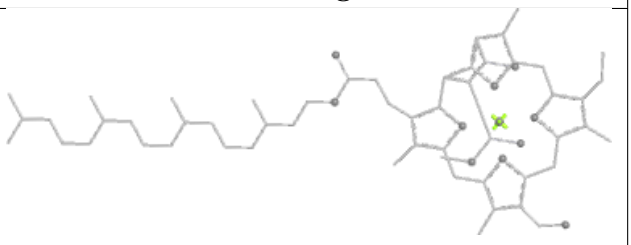
Bond lengths



Bond angles



Torsions

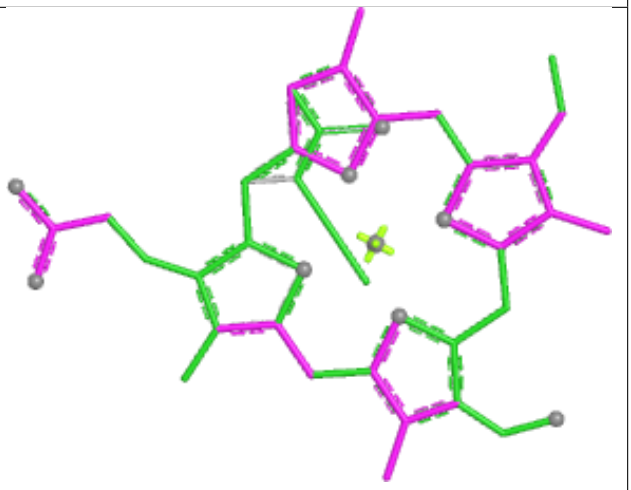


Rings

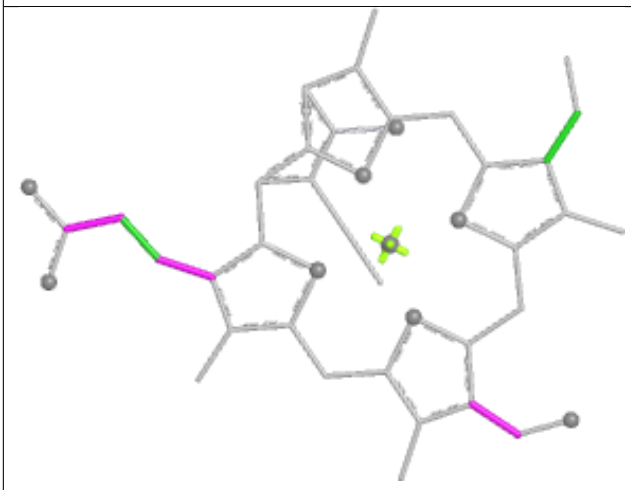
Ligand CL7 J 103



Bond lengths



Bond angles

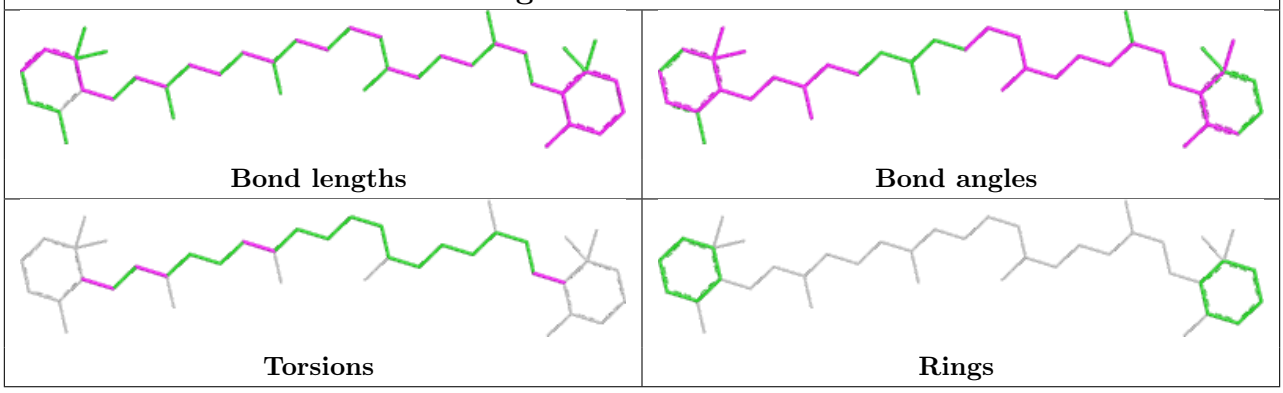


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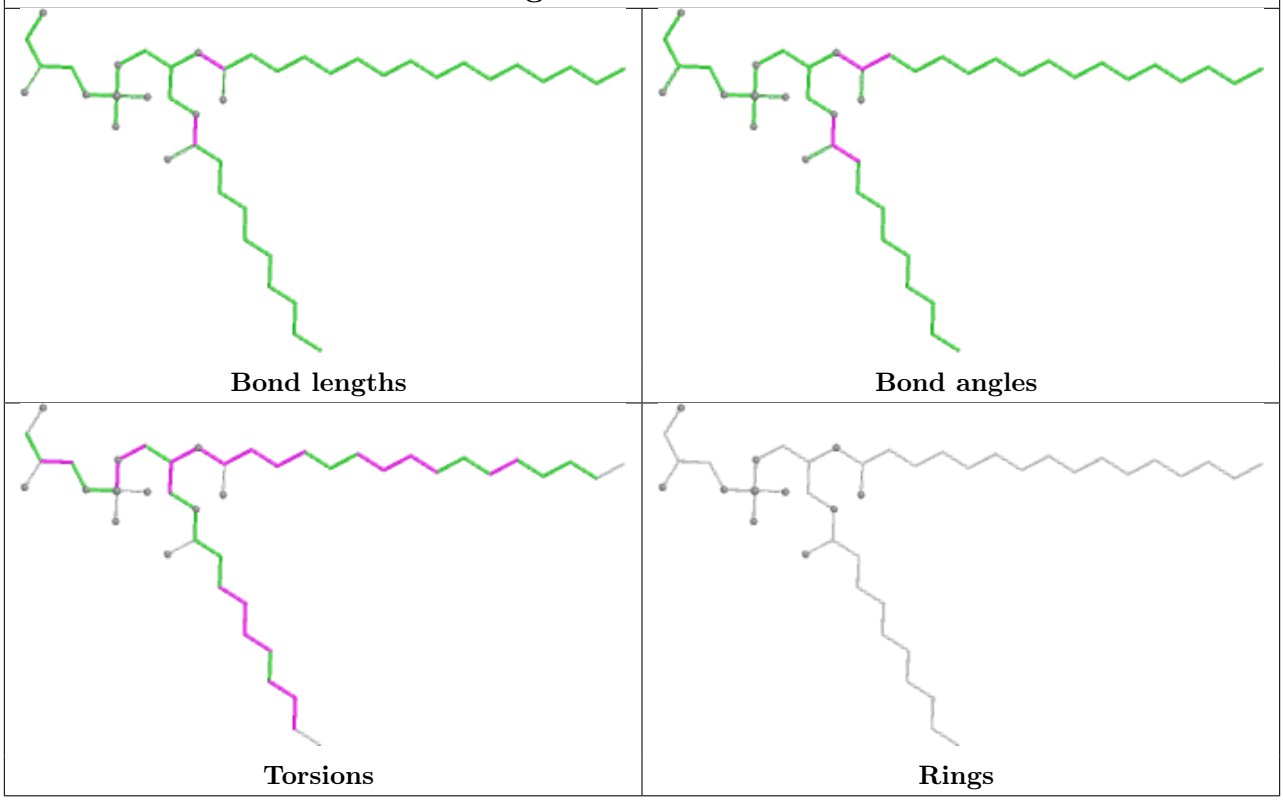


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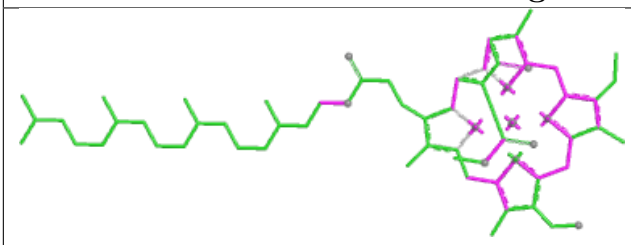
Ligand WVN A 850



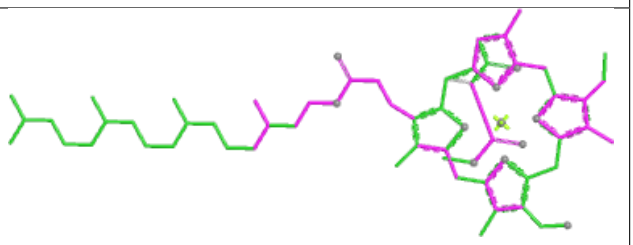
Ligand LHG L 208



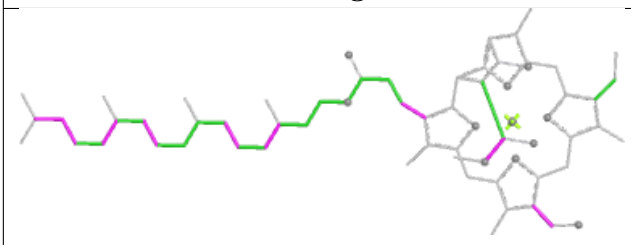
Ligand CL7 A 811



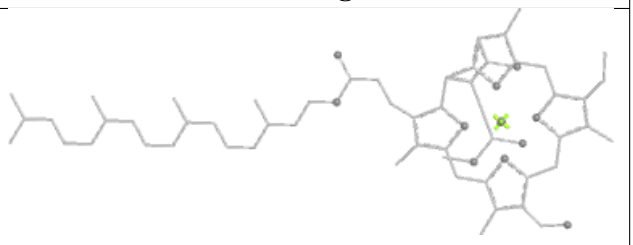
Bond lengths



Bond angles

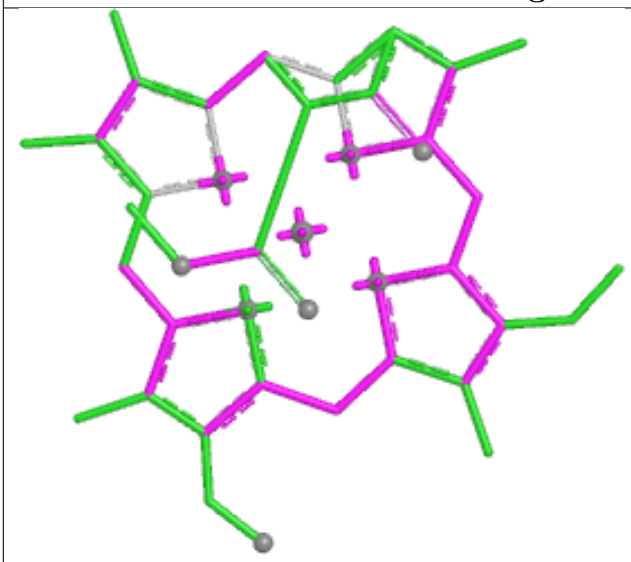


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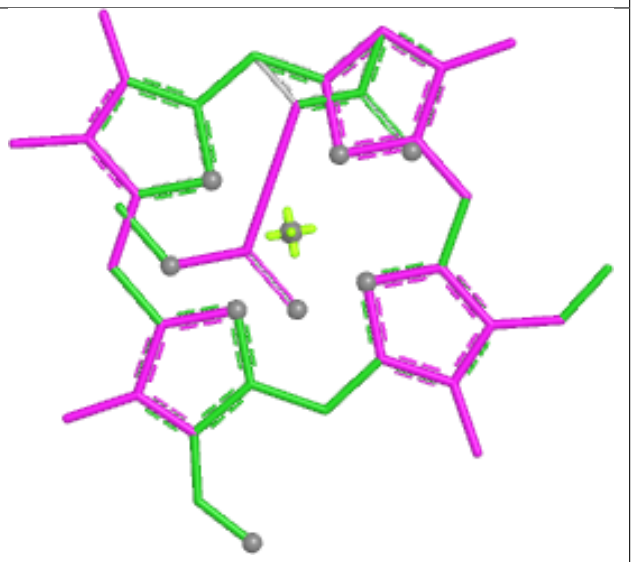


Rings

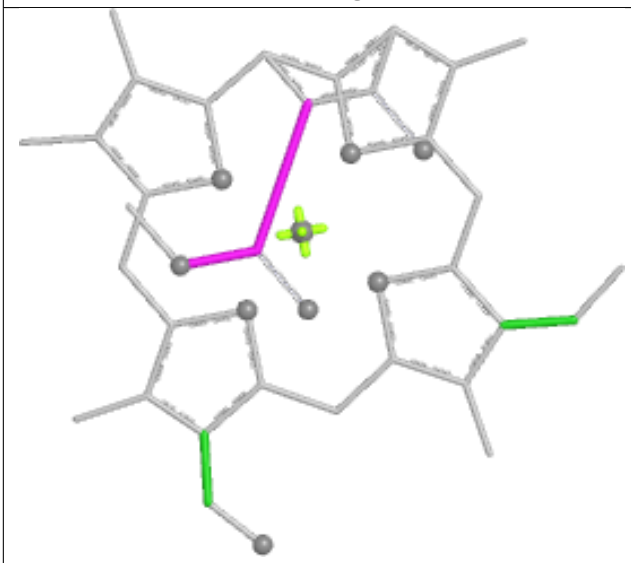
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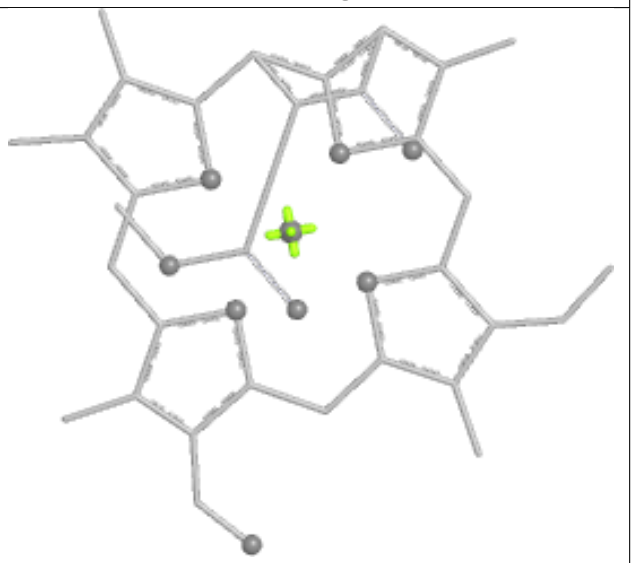
Bond lengths



Bond angles

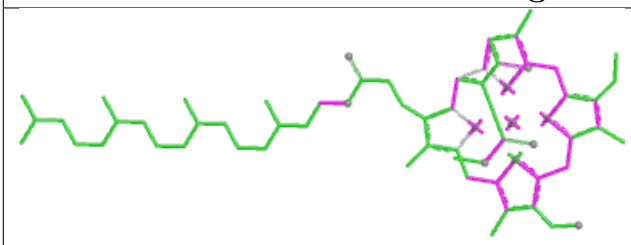


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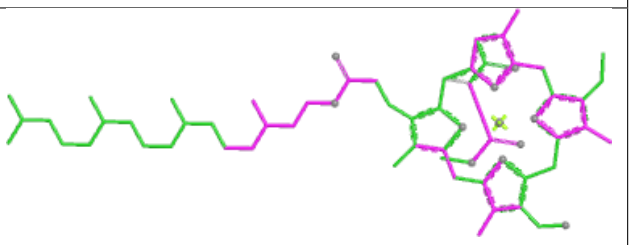


Rings

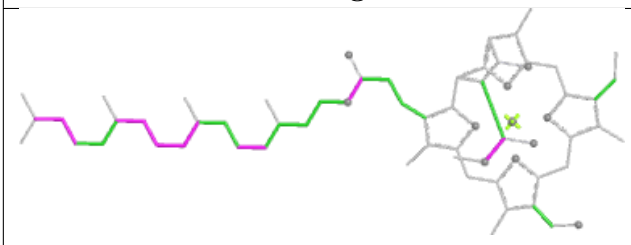
Ligand CL7 A 803



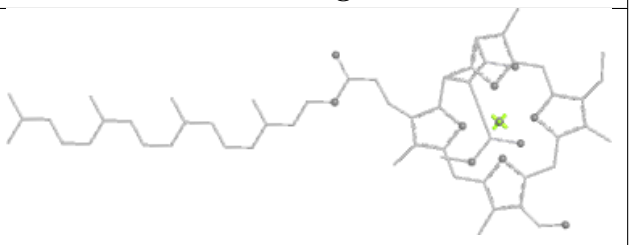
Bond lengths



Bond angles

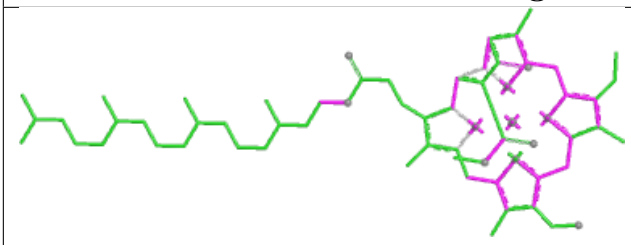


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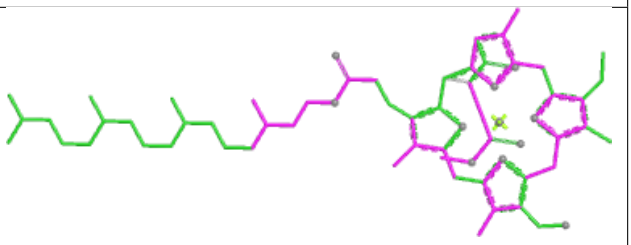


Rings

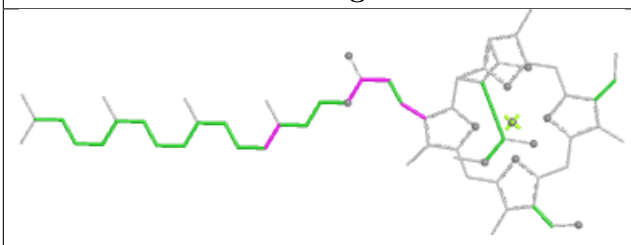
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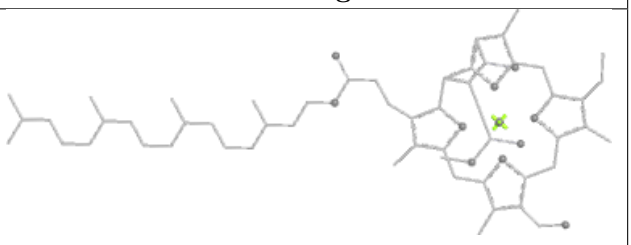
Bond lengths



Bond angles

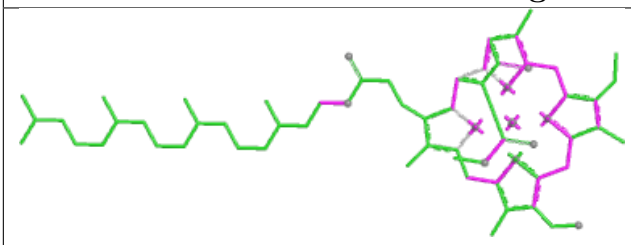


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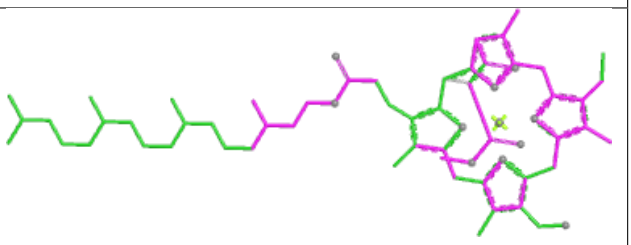


Rings

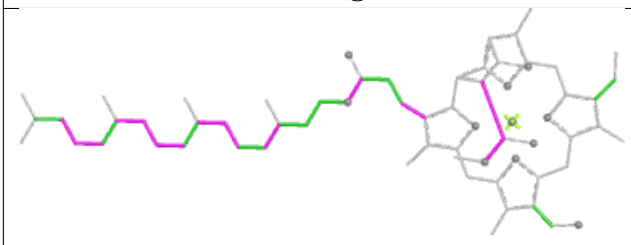
Ligand CL7 B 815



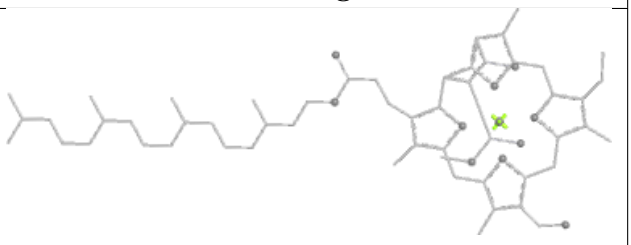
Bond lengths



Bond angles

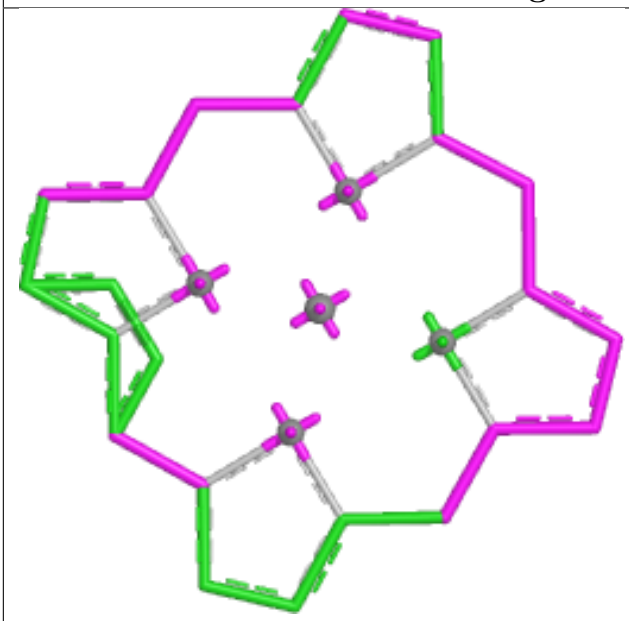


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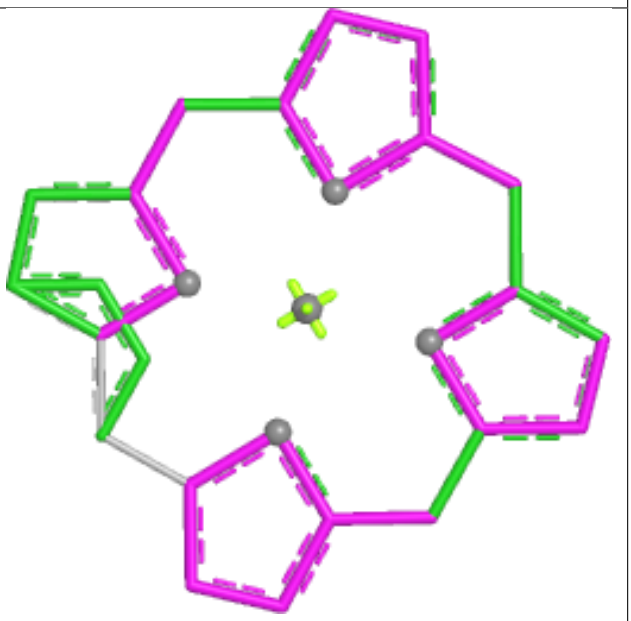


Rings

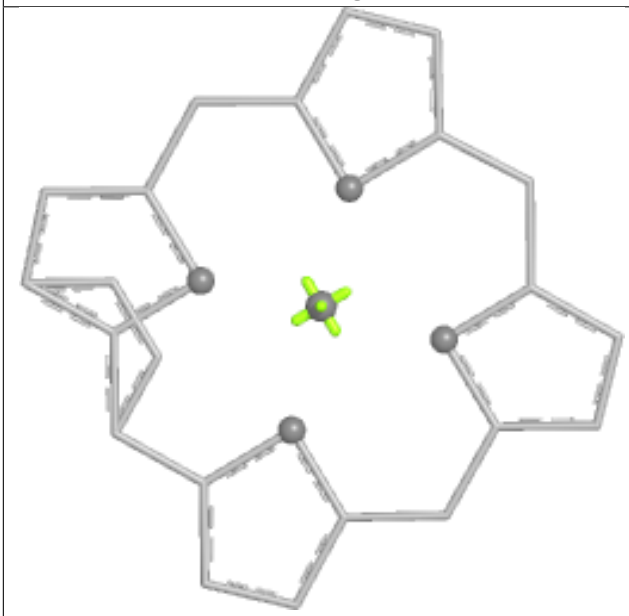
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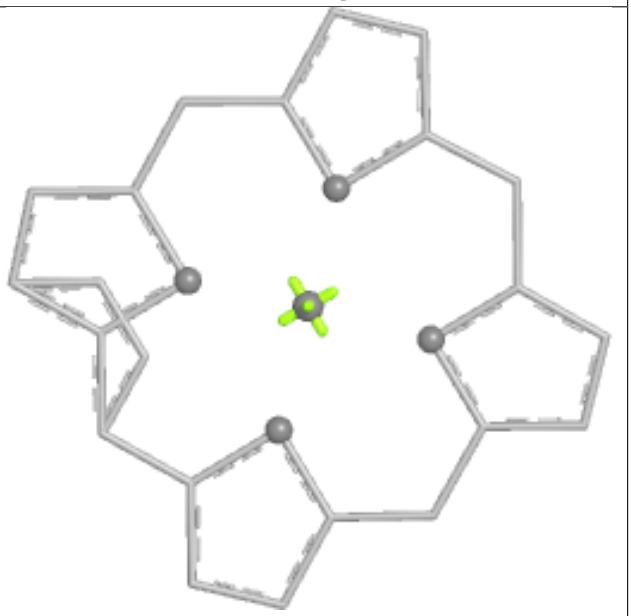
Bond lengths



Bond angles

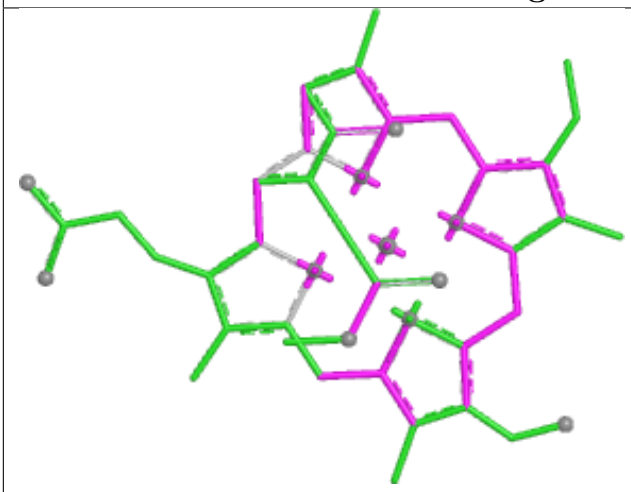


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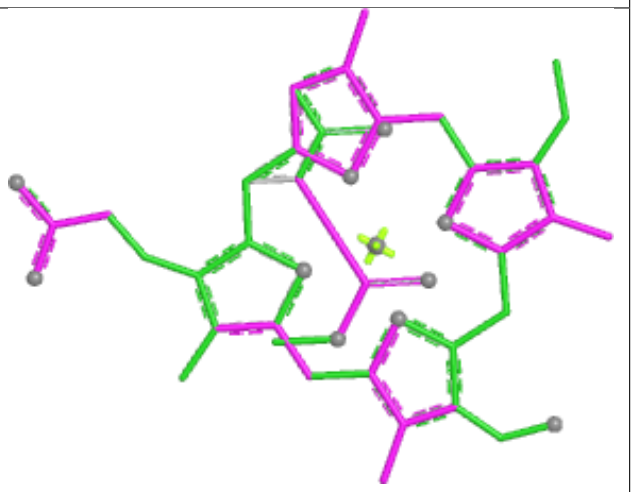


Rings

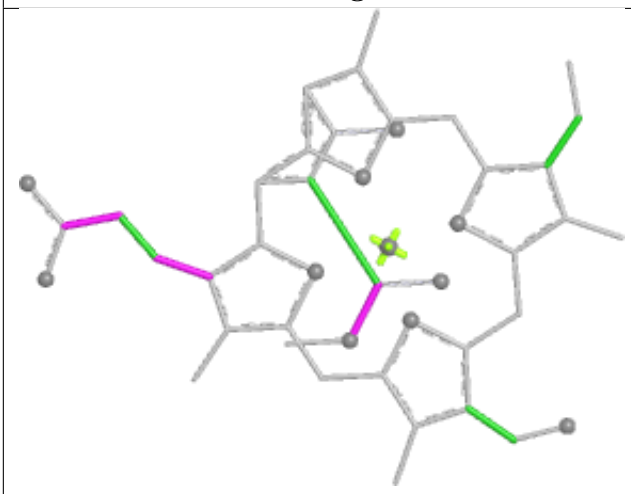
Ligand CL7 A 831



Bond lengths



Bond angles

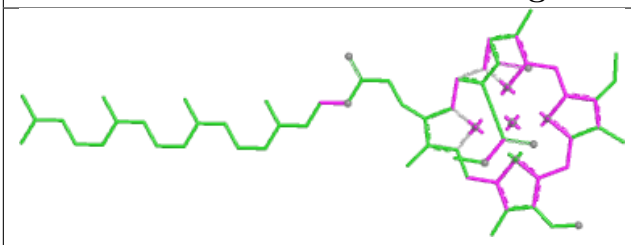


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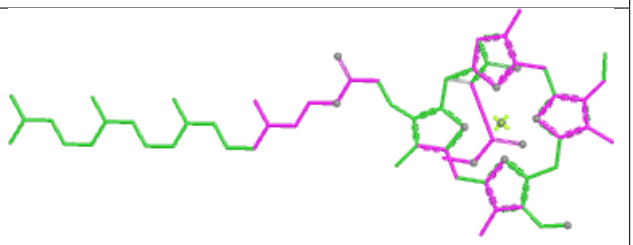


Rings

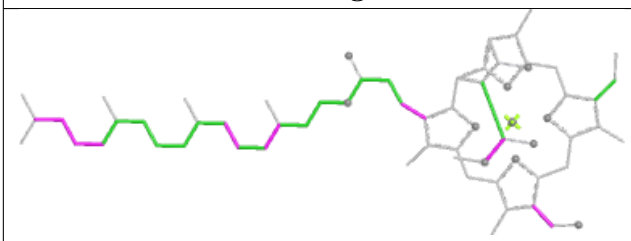
Ligand CL7 A 840



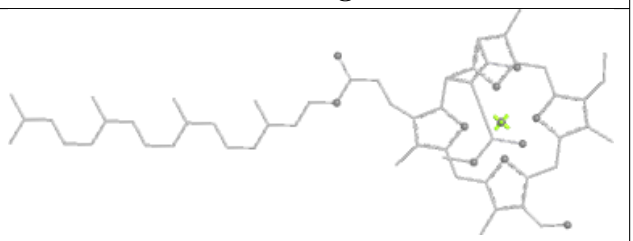
Bond lengths



Bond angles

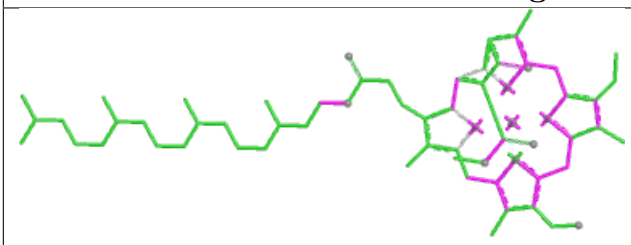


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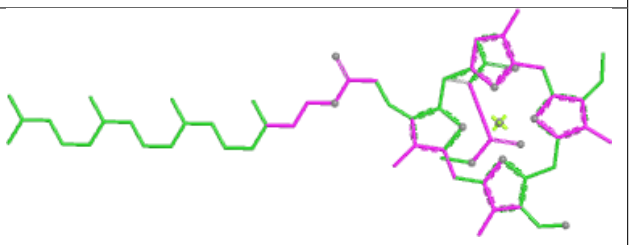


Rings

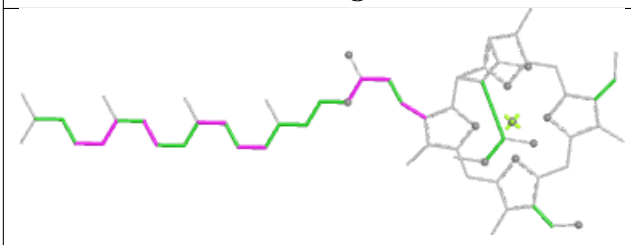
Ligand CL7 B 828



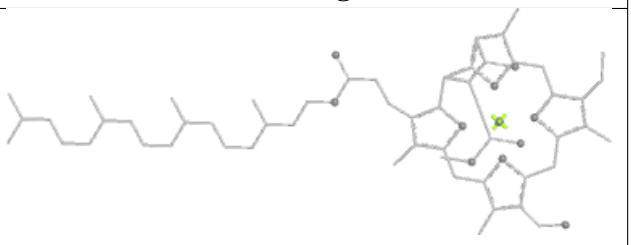
Bond lengths



Bond angles

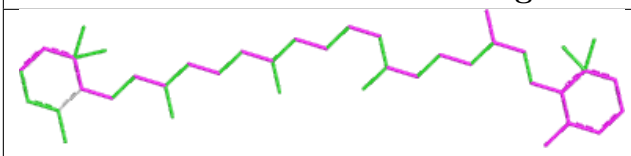


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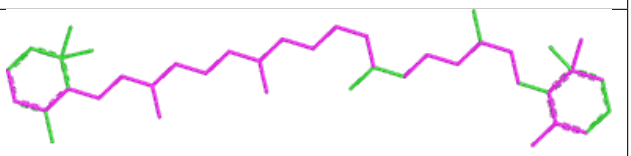


Rings

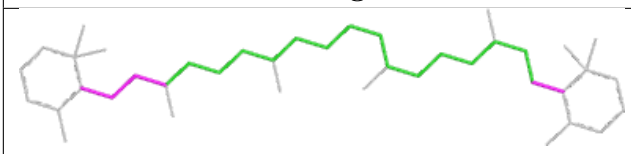
Ligand WVN A 853



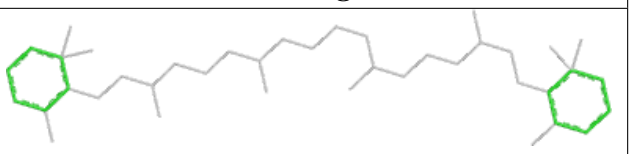
Bond lengths



Bond angles

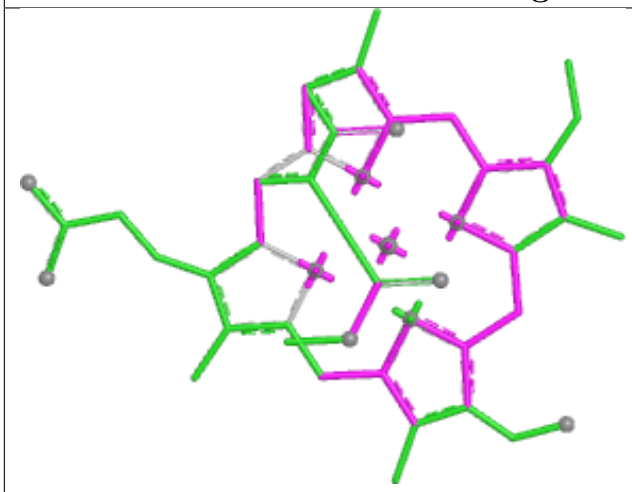


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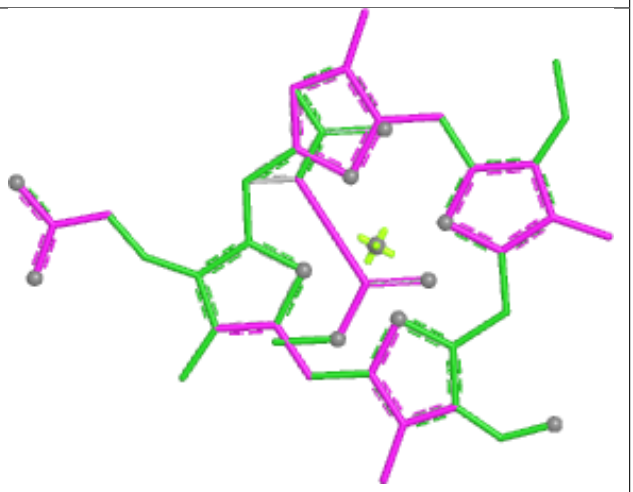


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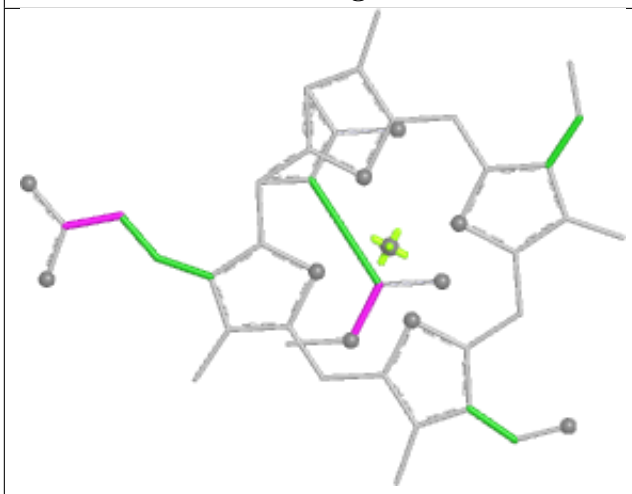
Ligand CL7 F 206



Bond lengths



Bond angles

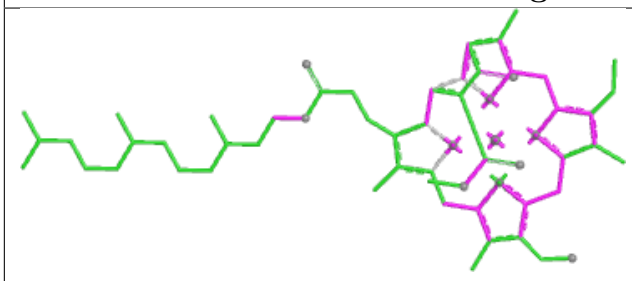


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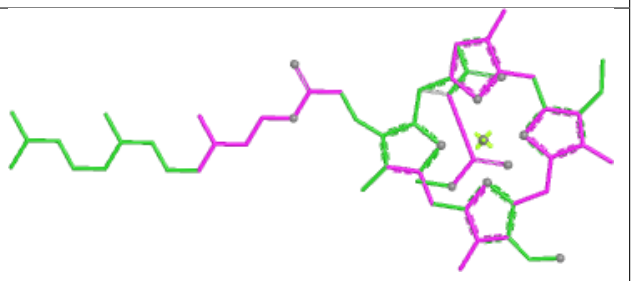


Rings

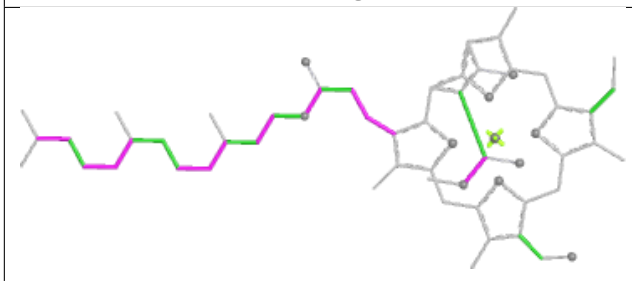
Ligand CL7 B 812



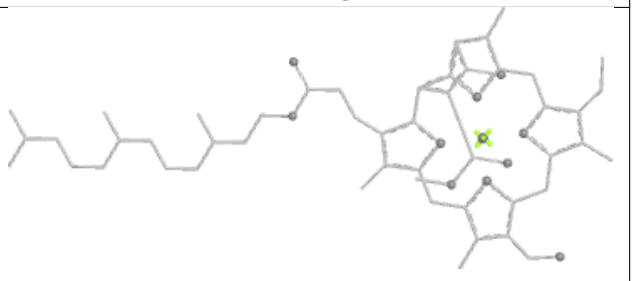
Bond lengths



Bond angles

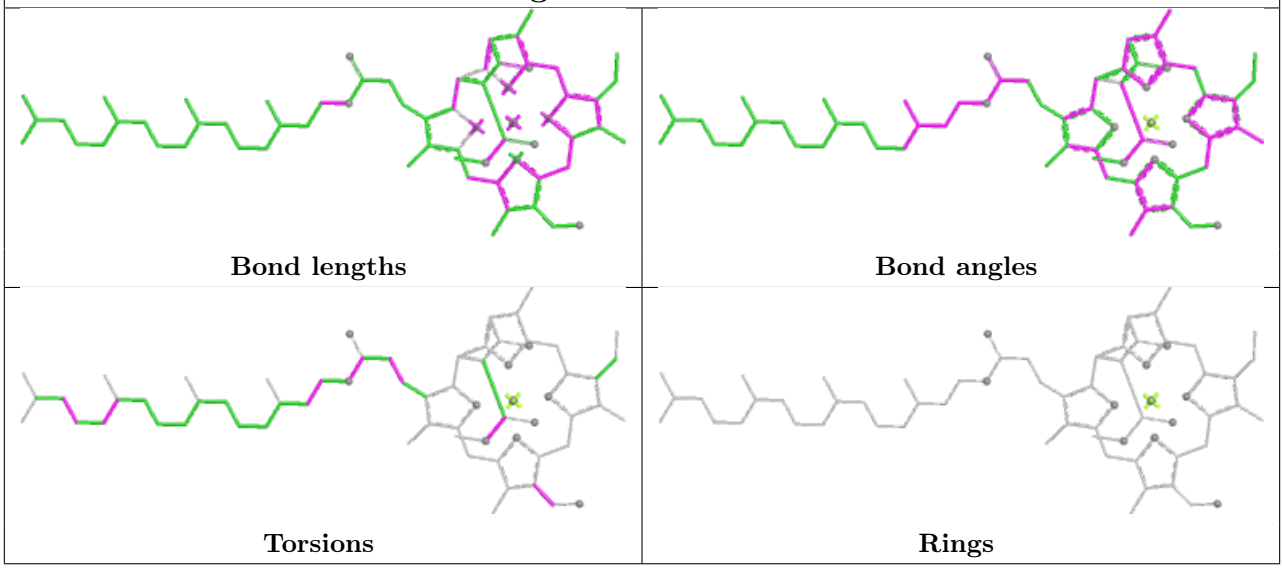


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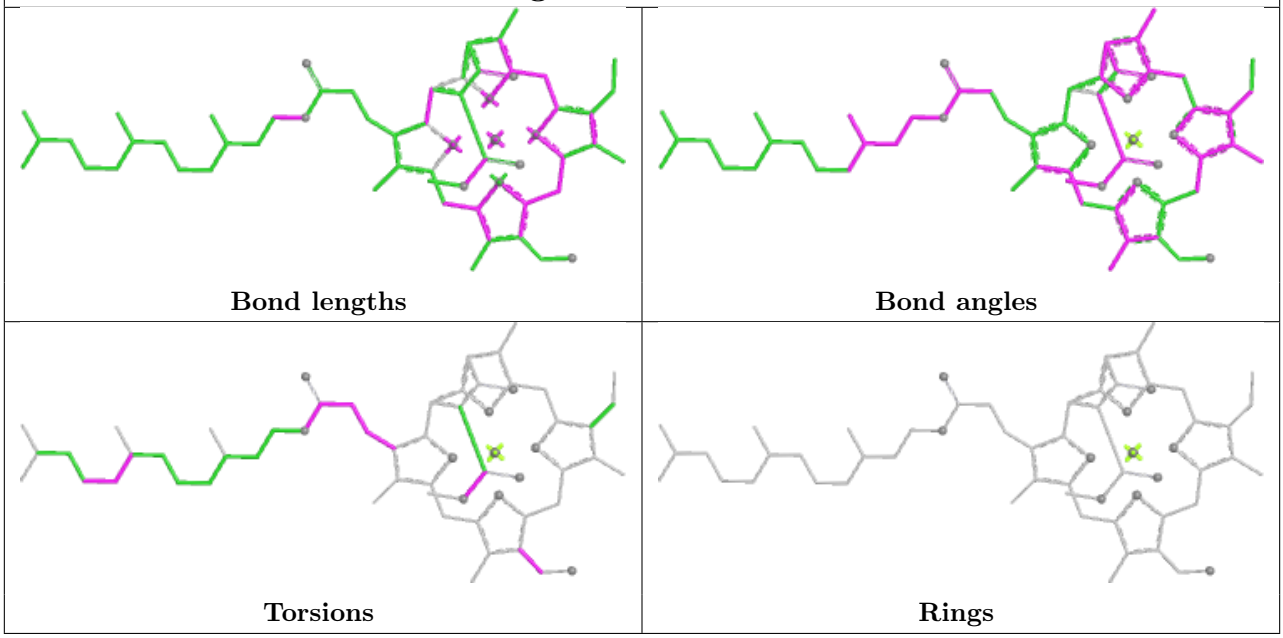


Rings

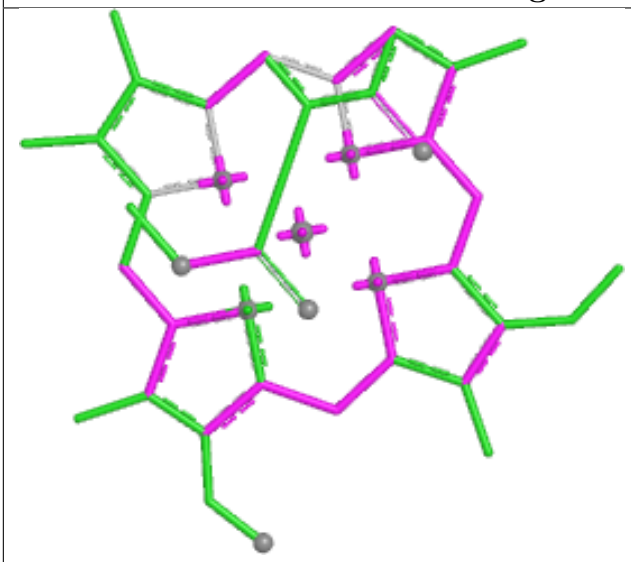
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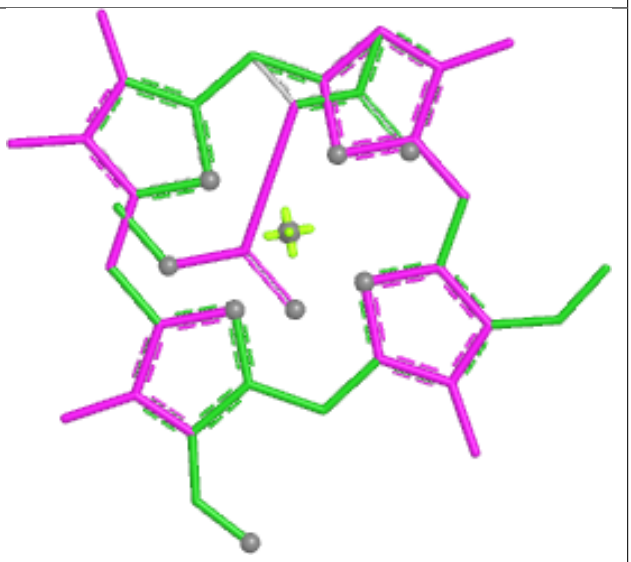
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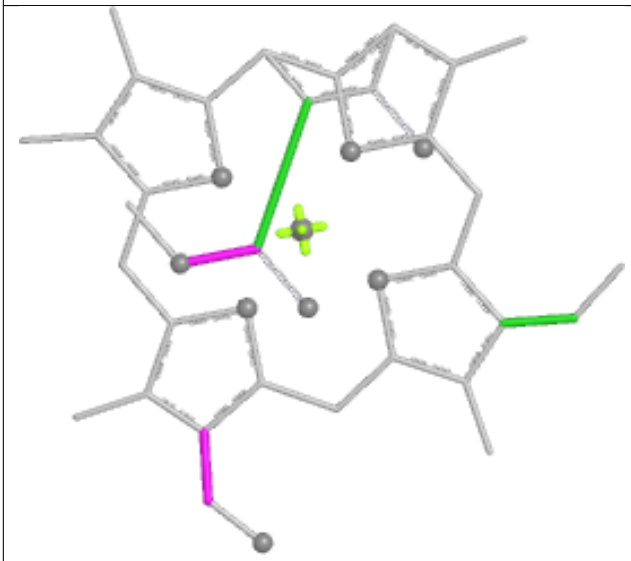
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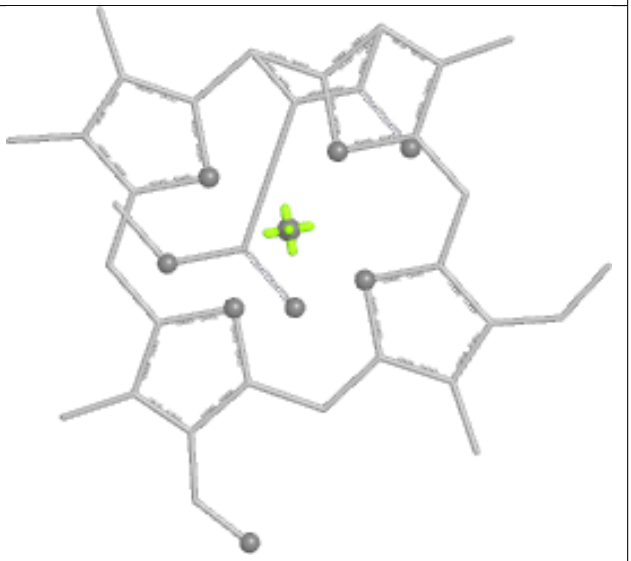
Bond lengths



Bond angles

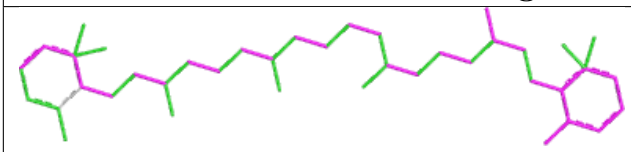


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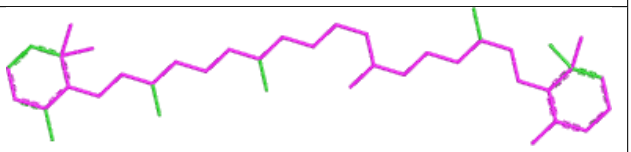


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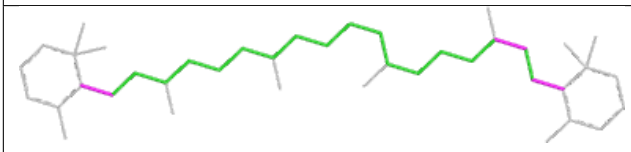
Ligand WVN L 210



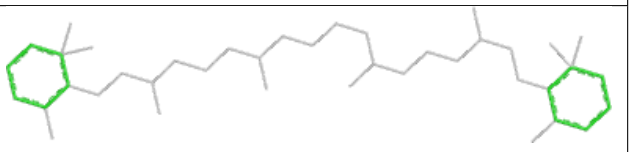
Bond lengths



Bond angles

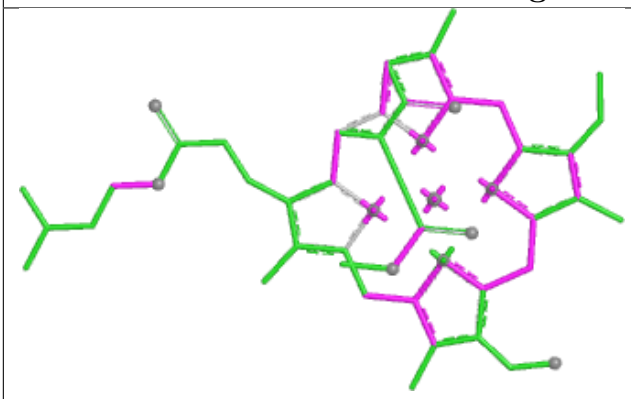


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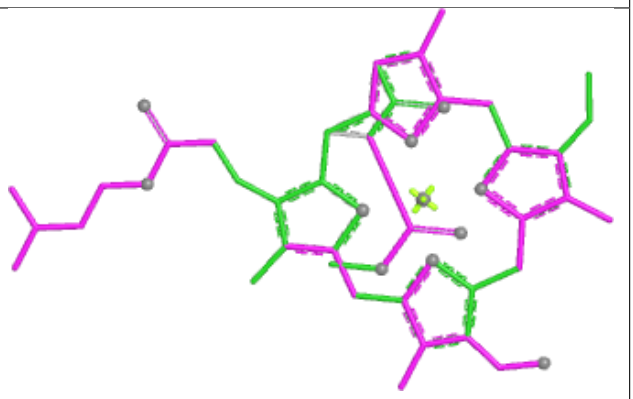


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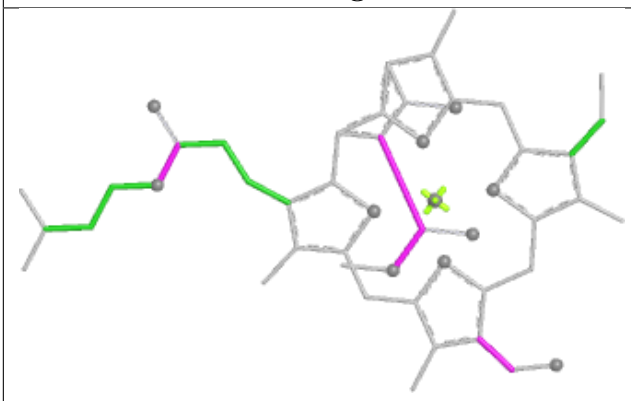
Ligand CL7 B 831



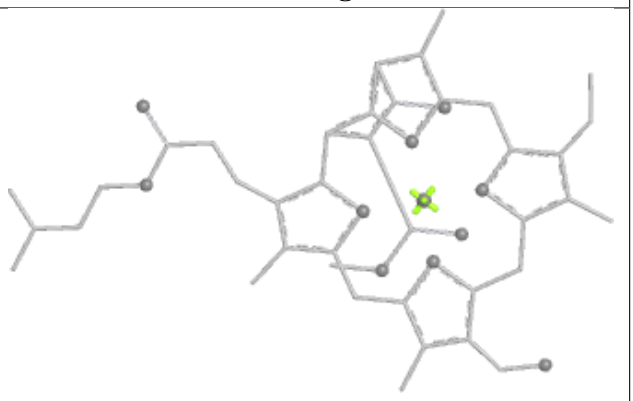
Bond lengths



Bond angles

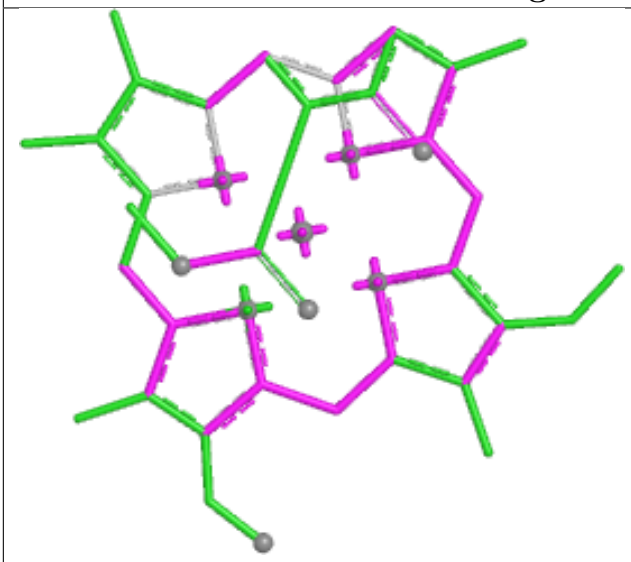


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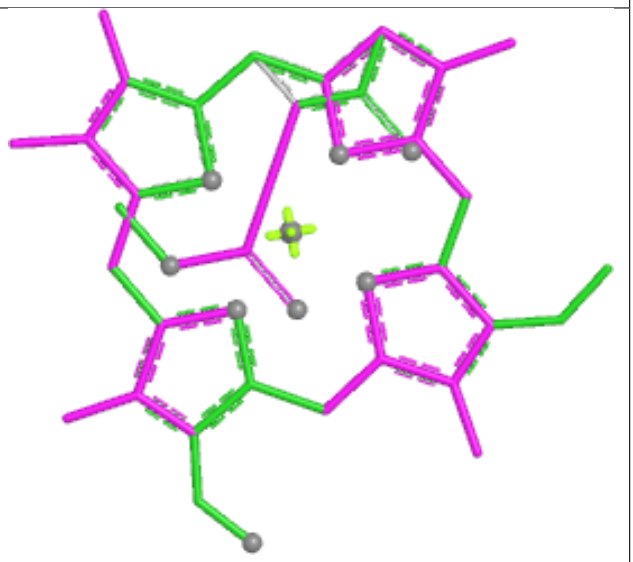


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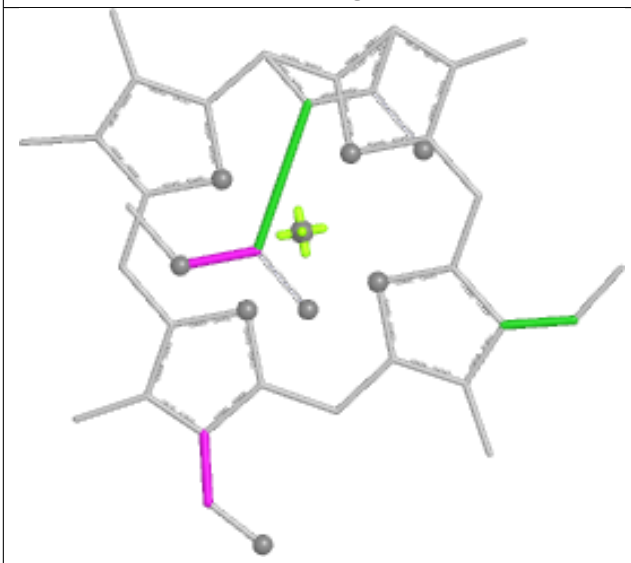
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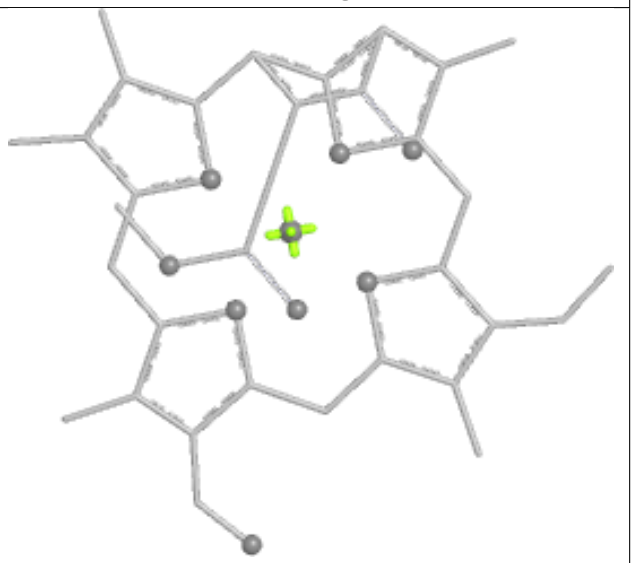
Bond lengths



Bond angles

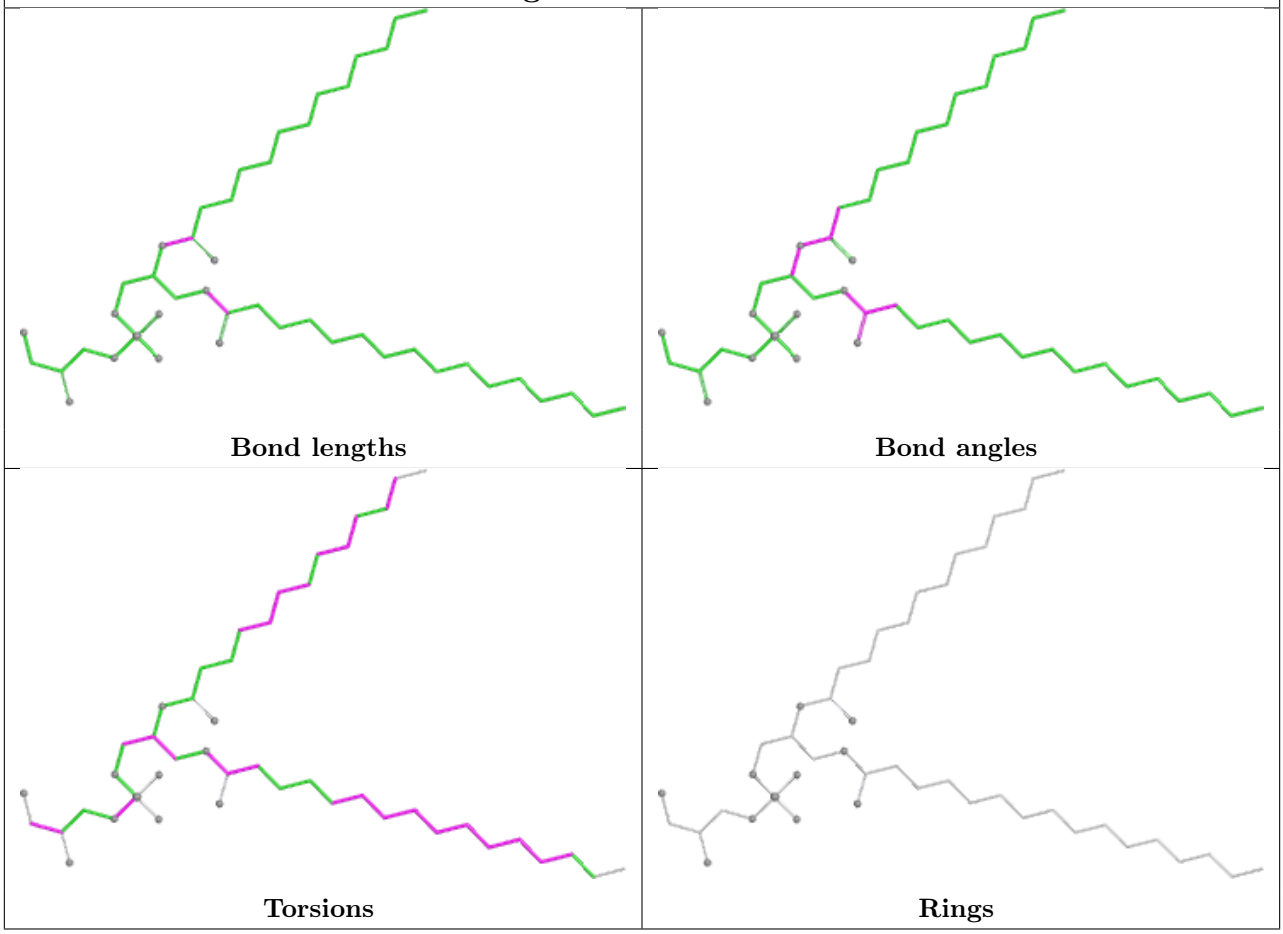


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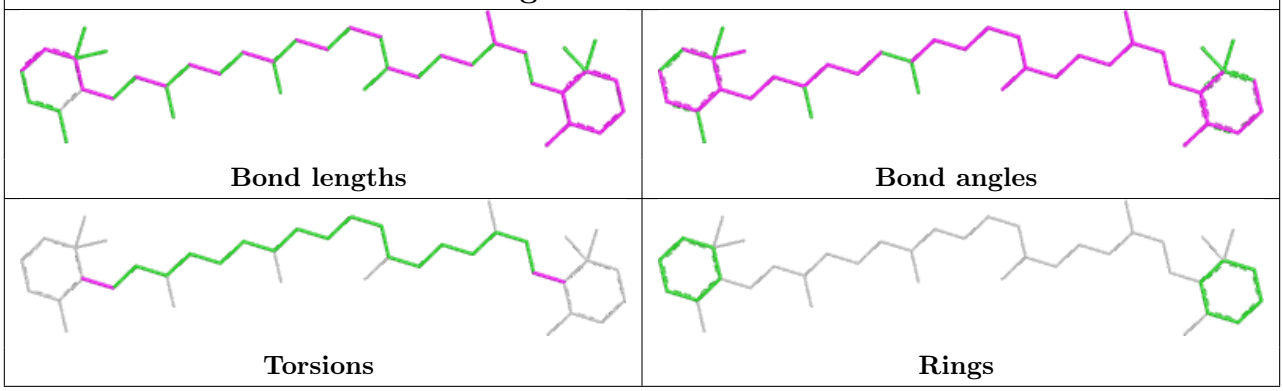


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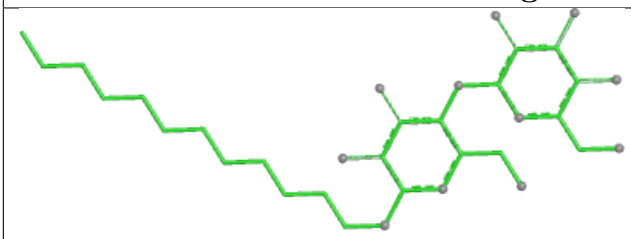
Ligand LHG A 821



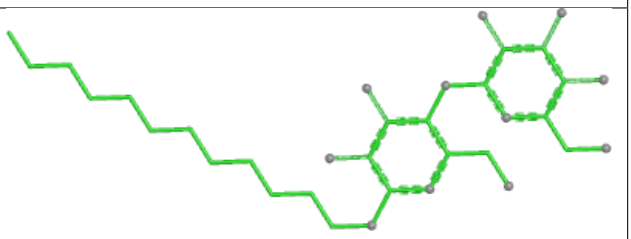
Ligand WVN J 101



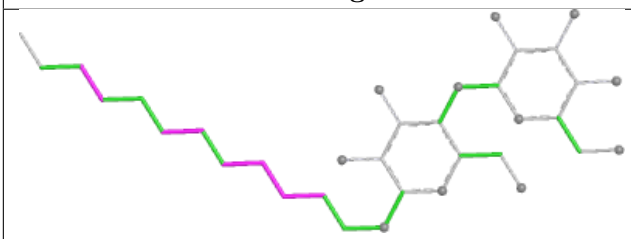
Ligand LMT A 834



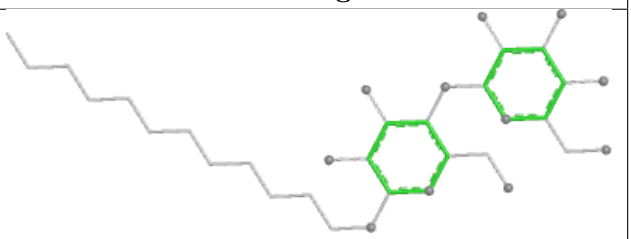
Bond lengths



Bond angles

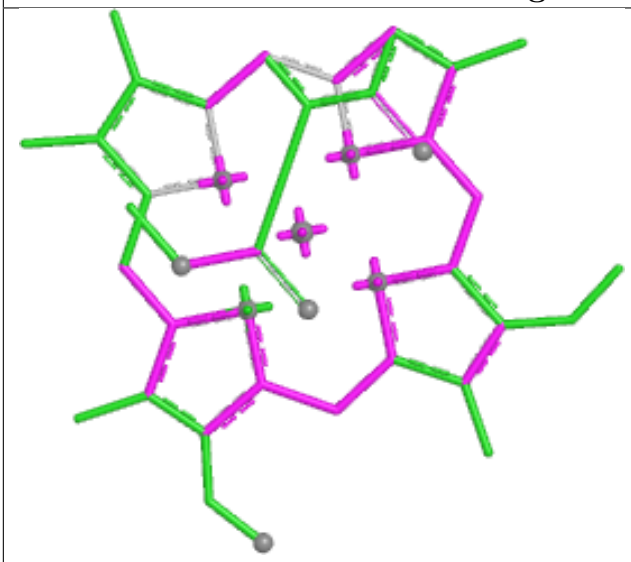


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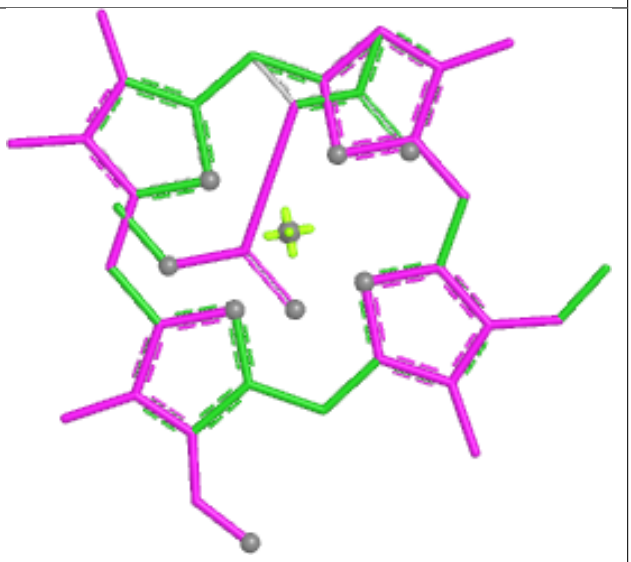


Rings

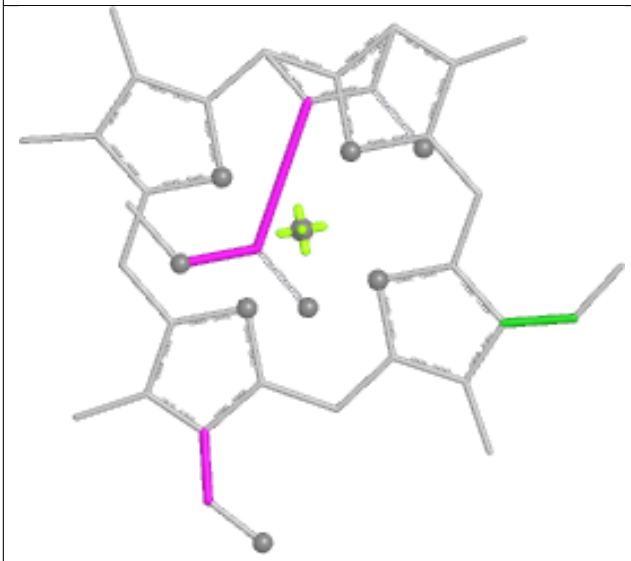
Ligand CL7 A 810



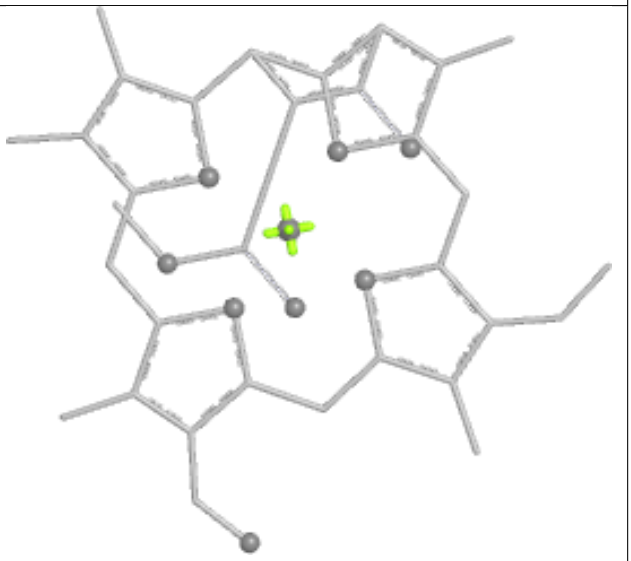
Bond lengths



Bond angles

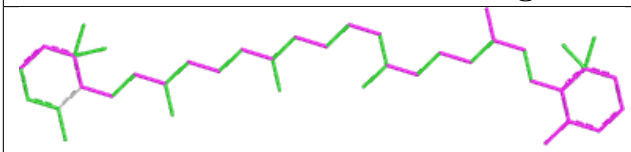


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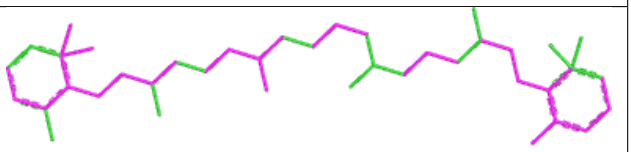


Rings

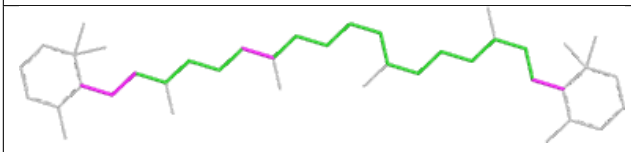
Ligand WVN F 204



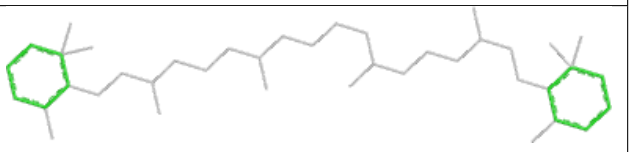
Bond lengths



Bond angles

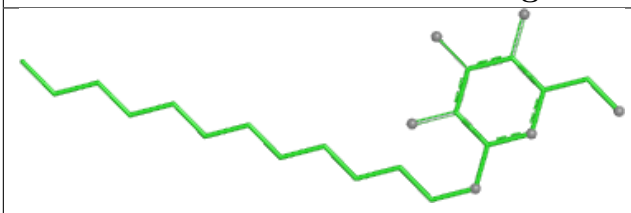


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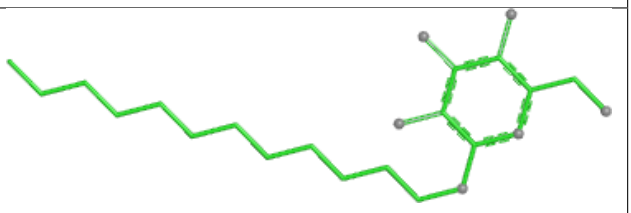


Rings

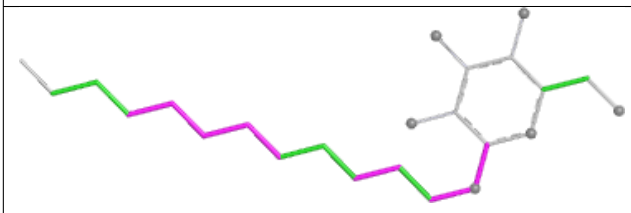
Ligand LMT B 835



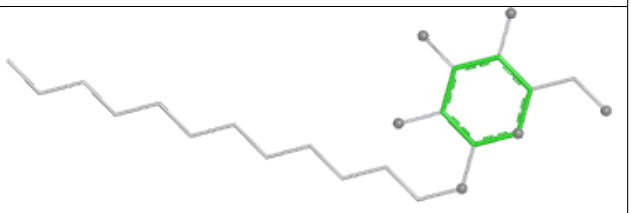
Bond lengths



Bond angles

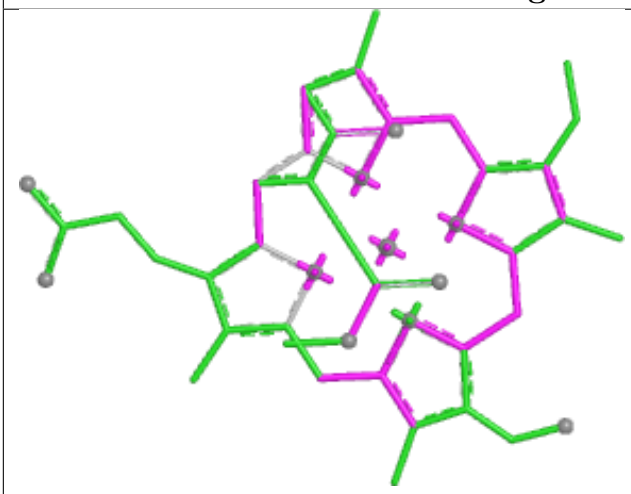


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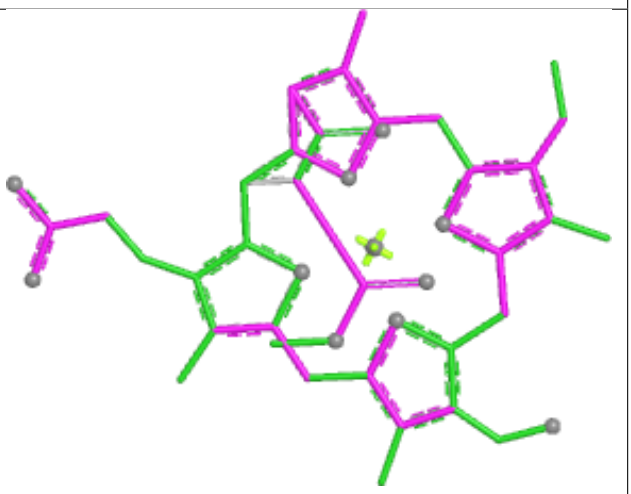


Rings

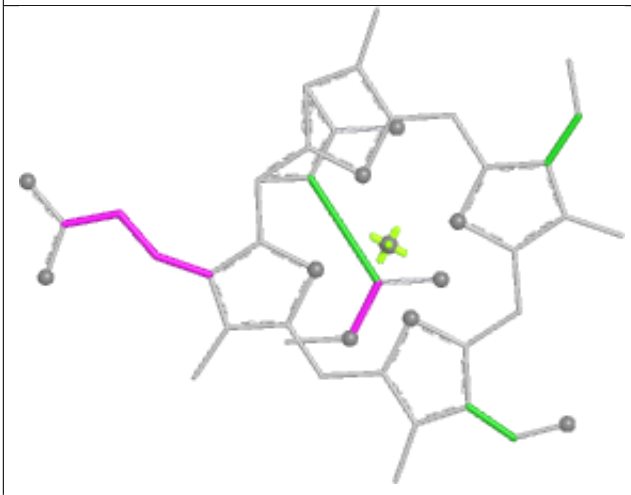
Ligand CL7 A 846



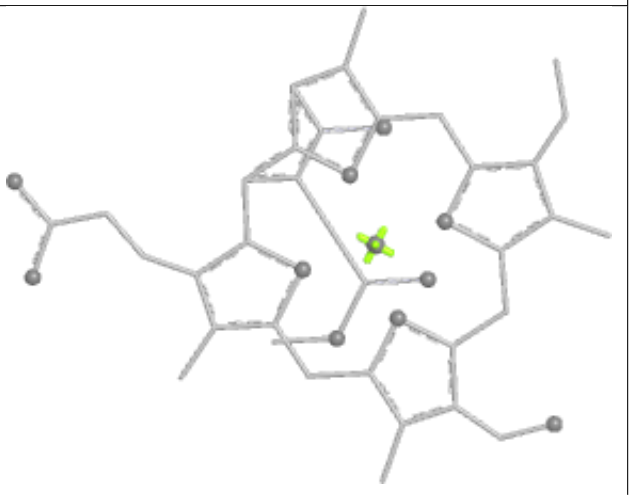
Bond lengths



Bond angles

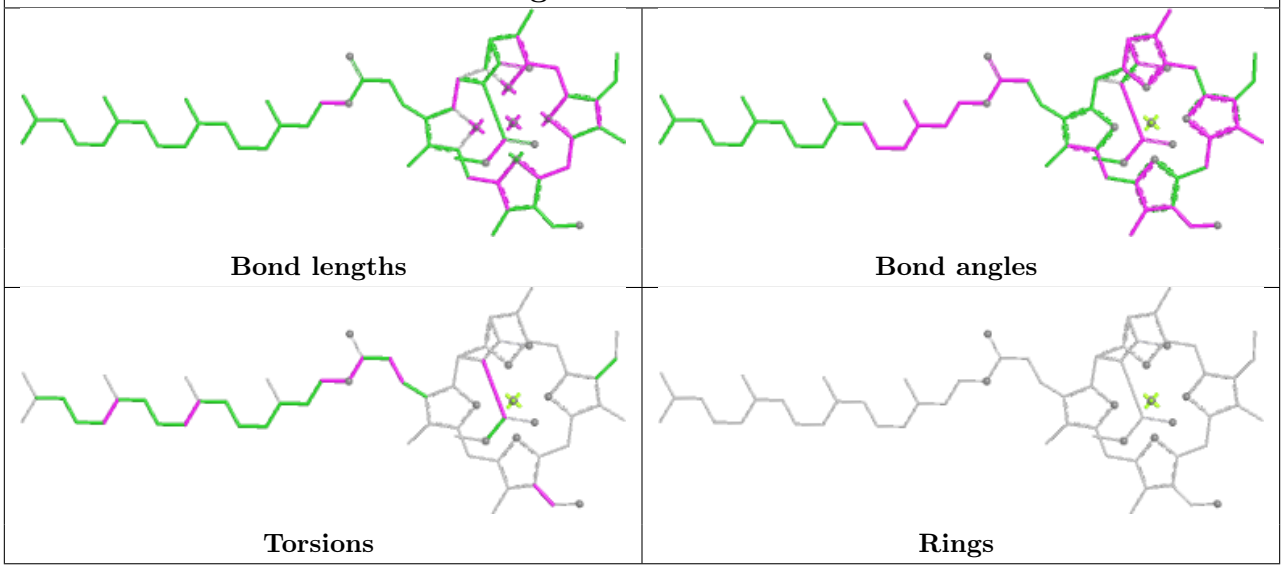


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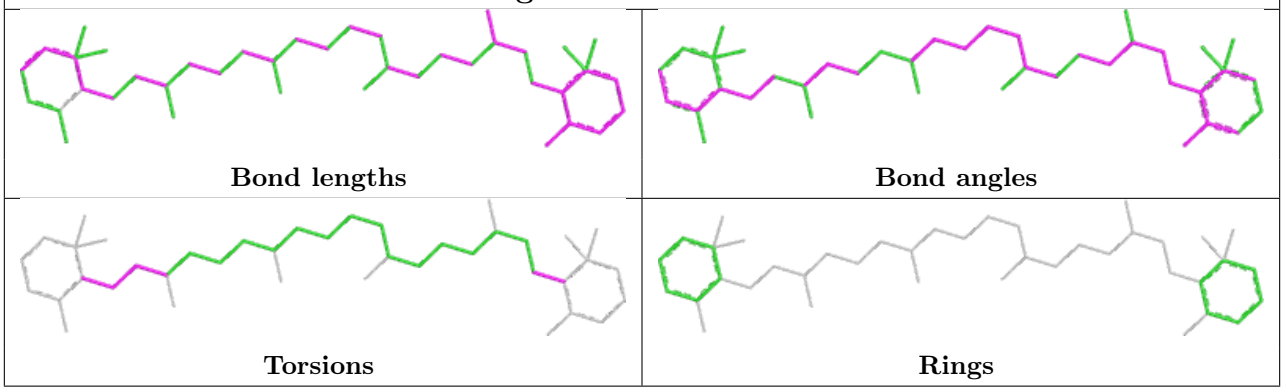


Rings

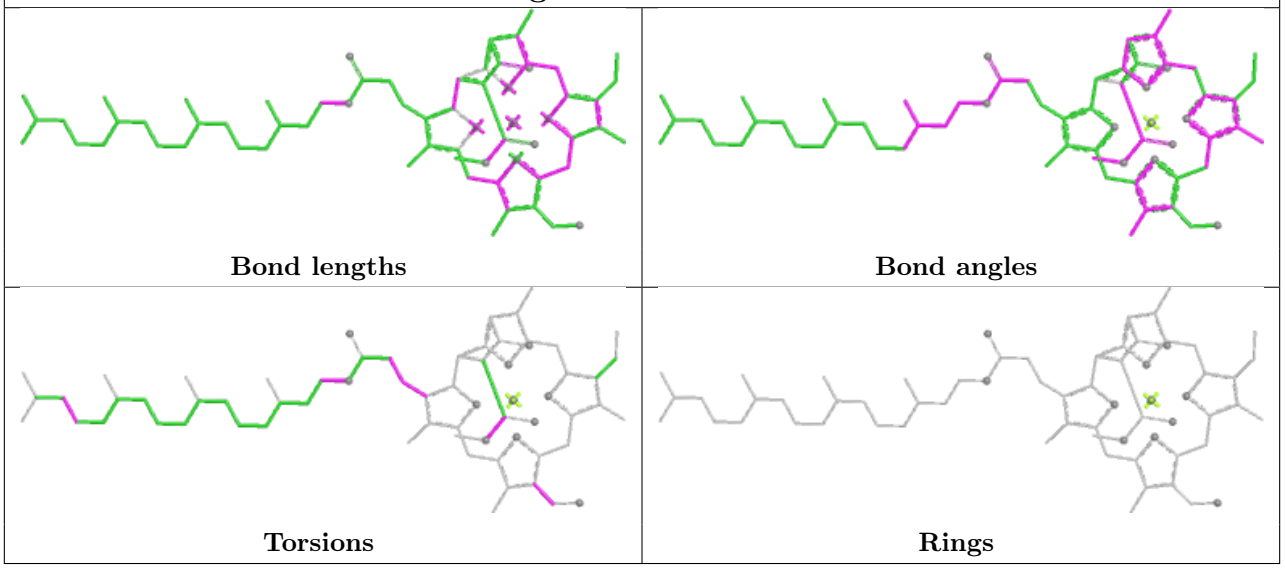
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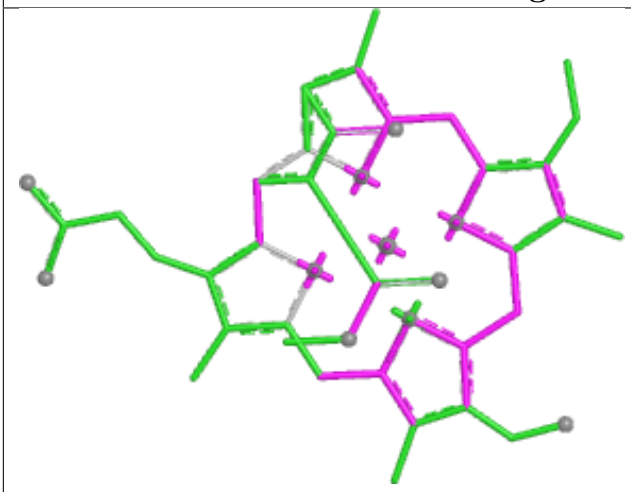
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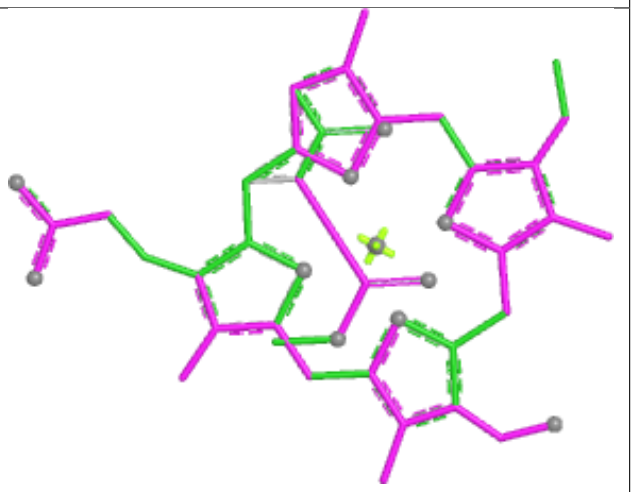
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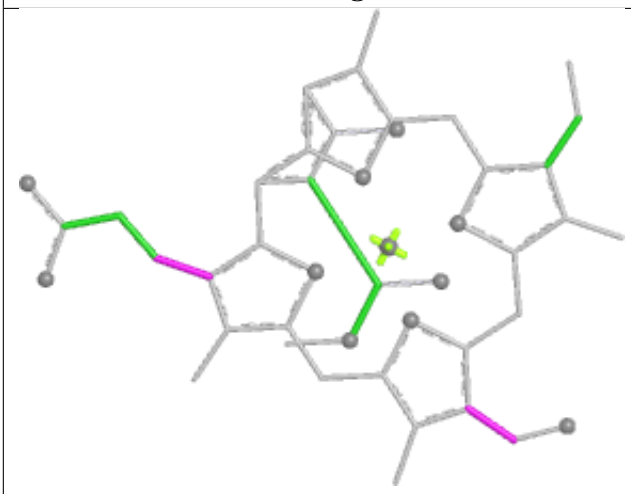
Ligand CL7 B 841



Bond lengths



Bond angles

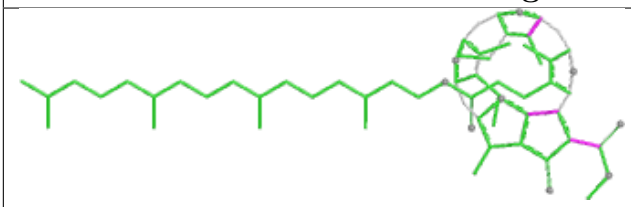


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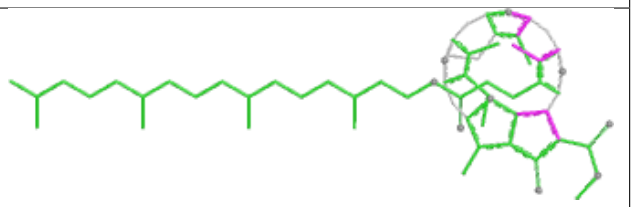


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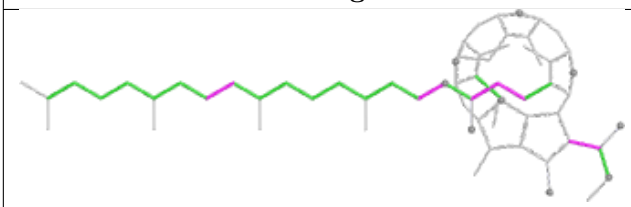
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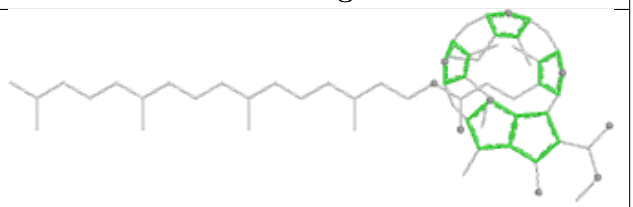
Bond lengths



Bond angles

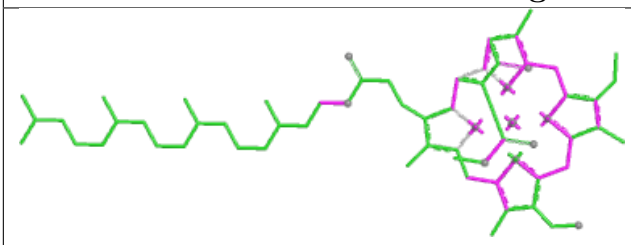


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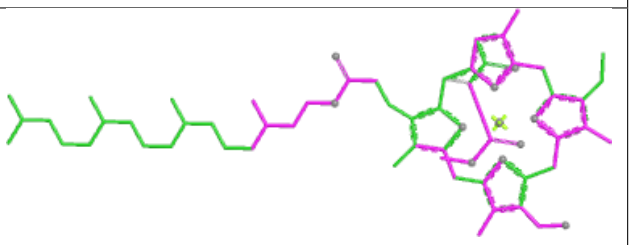


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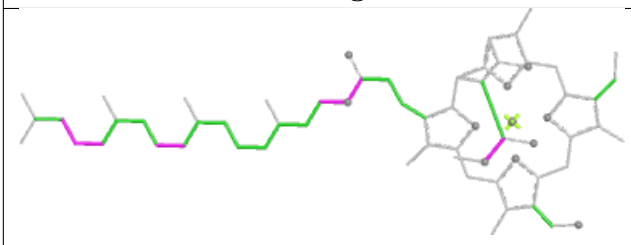
Ligand CL7 B 804



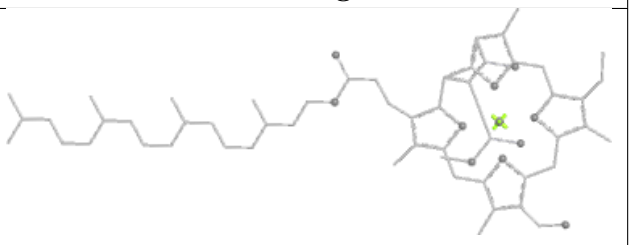
Bond lengths



Bond angles

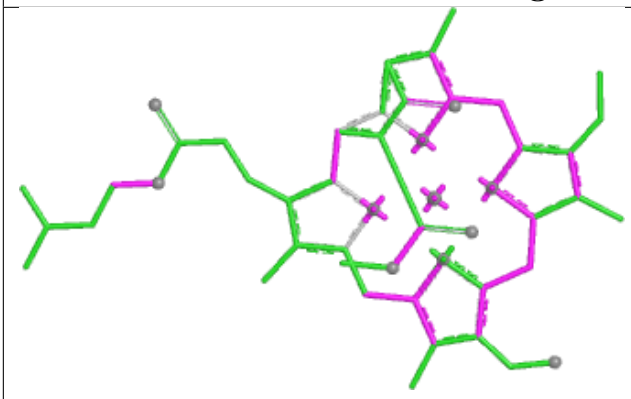


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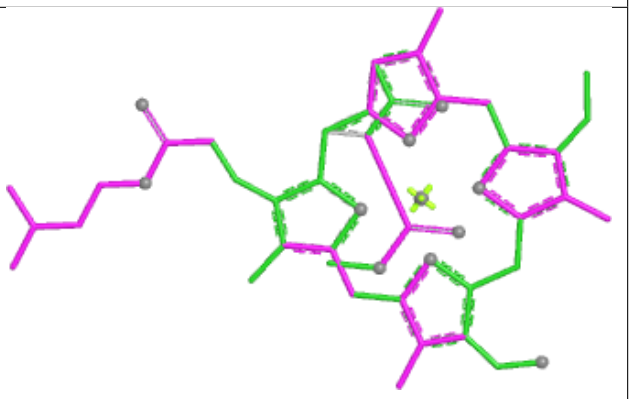


Rings

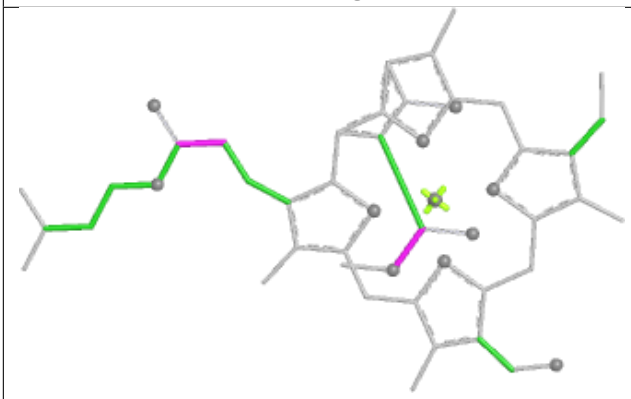
Ligand CL7 B 807



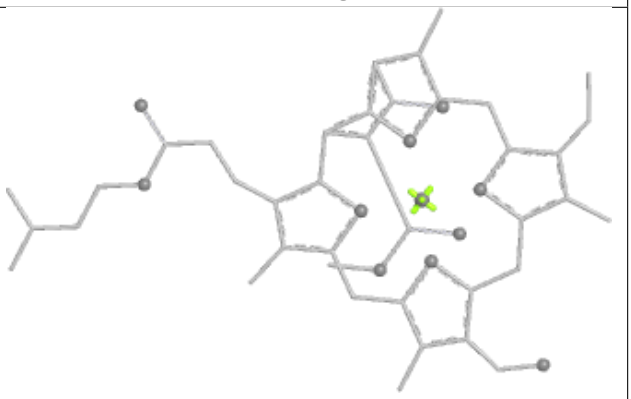
Bond lengths



Bond angles

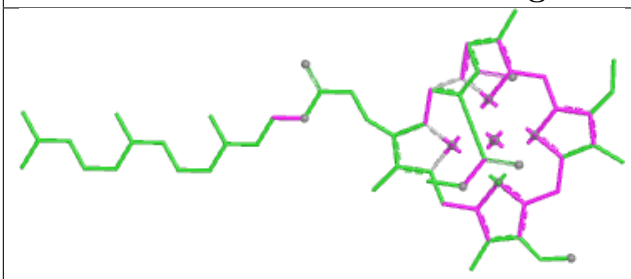


Torsions

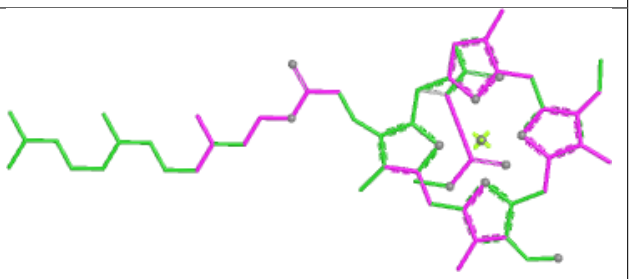


Rings

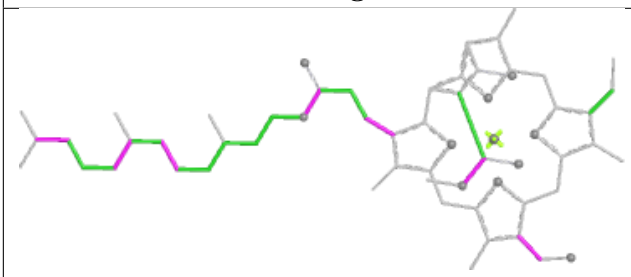
Ligand CL7 A 827



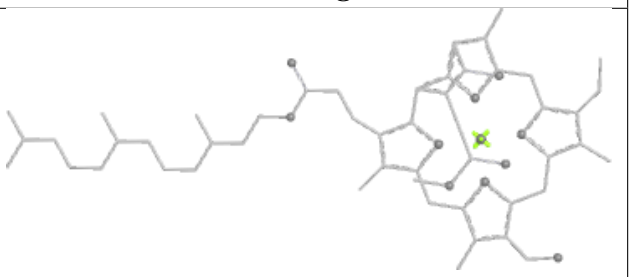
Bond lengths



Bond angles

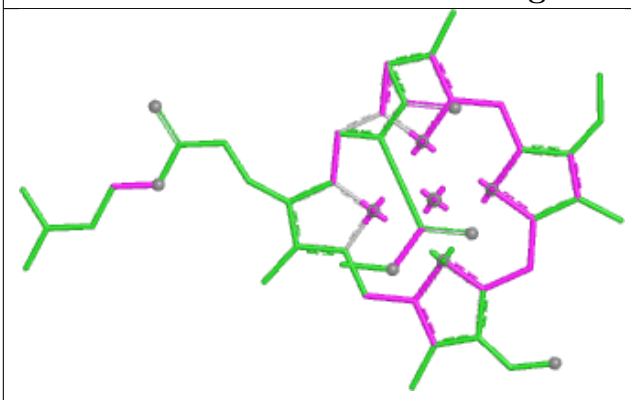


Torsions

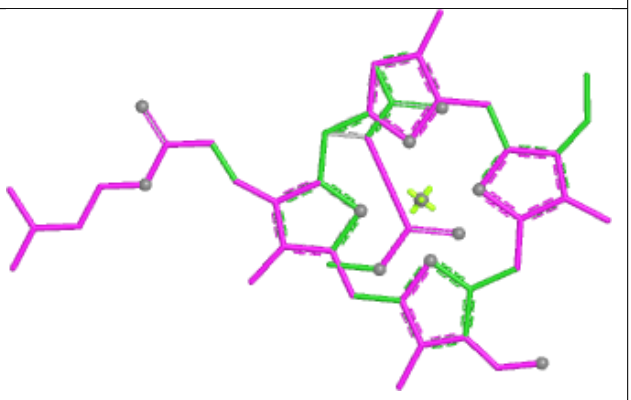


Rings

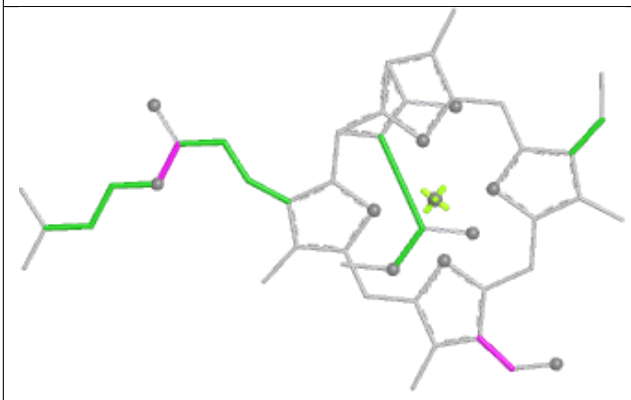
Ligand CL7 A 843



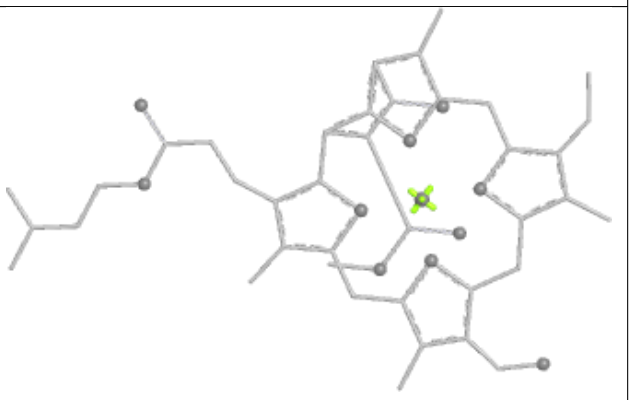
Bond lengths



Bond angles

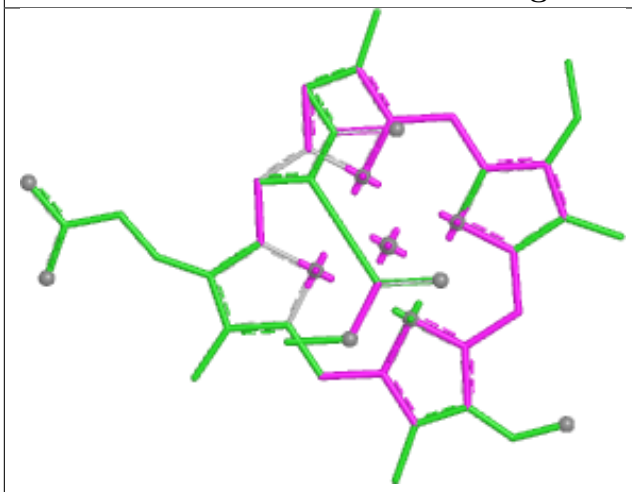


Torsions

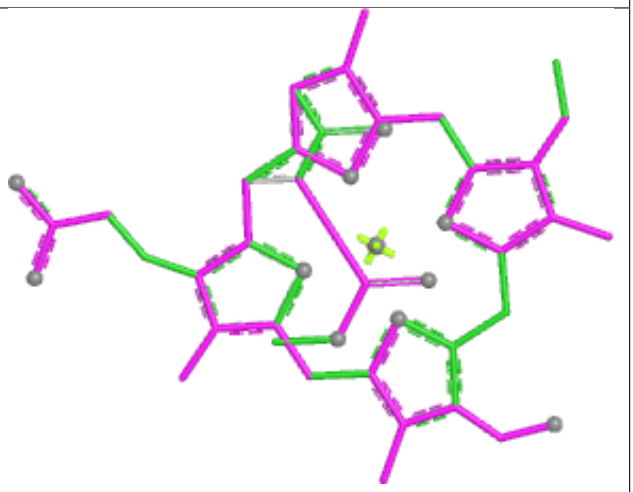


Rings

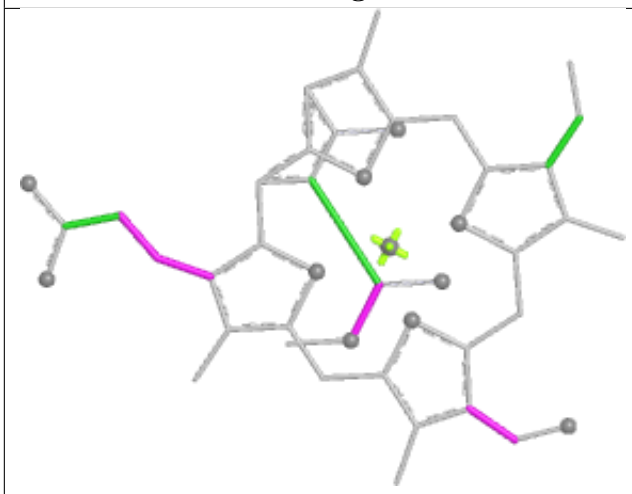
Ligand CL7 B 840



Bond lengths



Bond angles

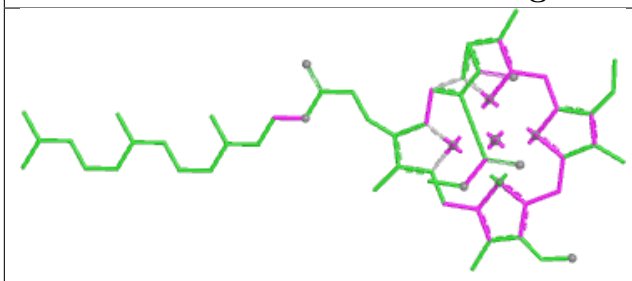


Torsions

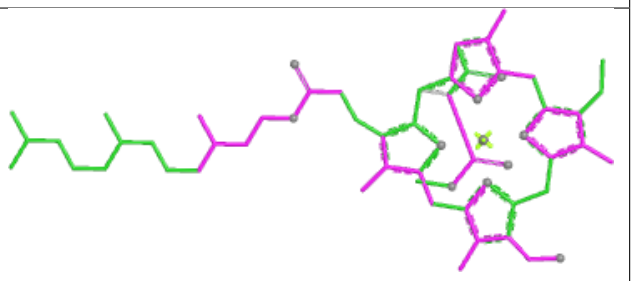


Rings

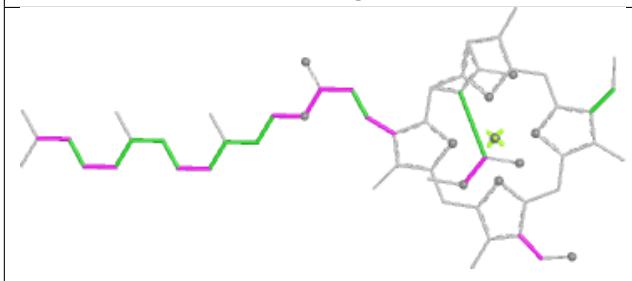
Ligand CL7 A 828



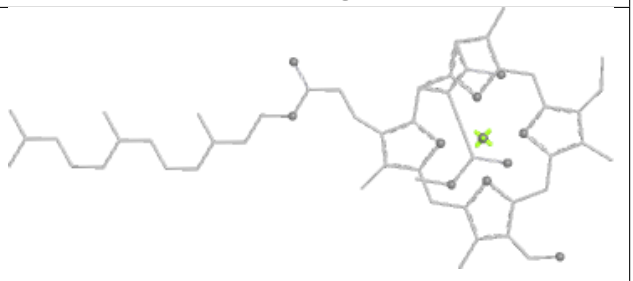
Bond lengths



Bond angles

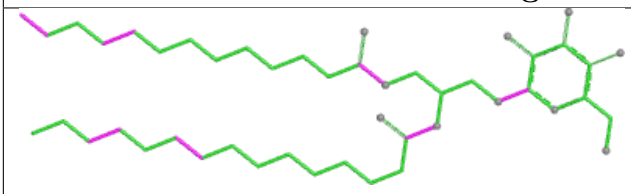


Torsions

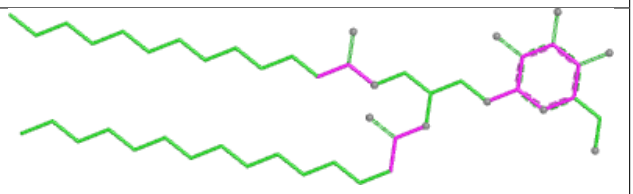


Rings

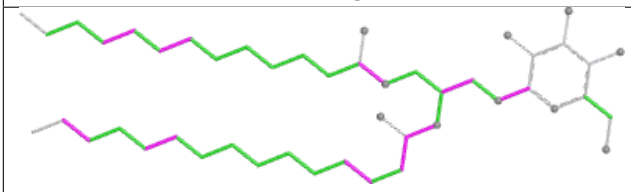
Ligand LMG L 203



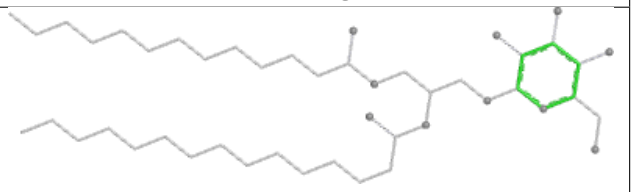
Bond lengths



Bond angles

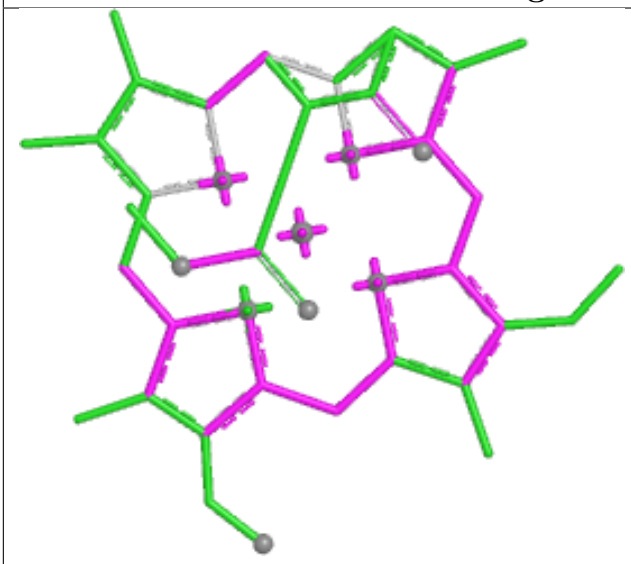


Torsions

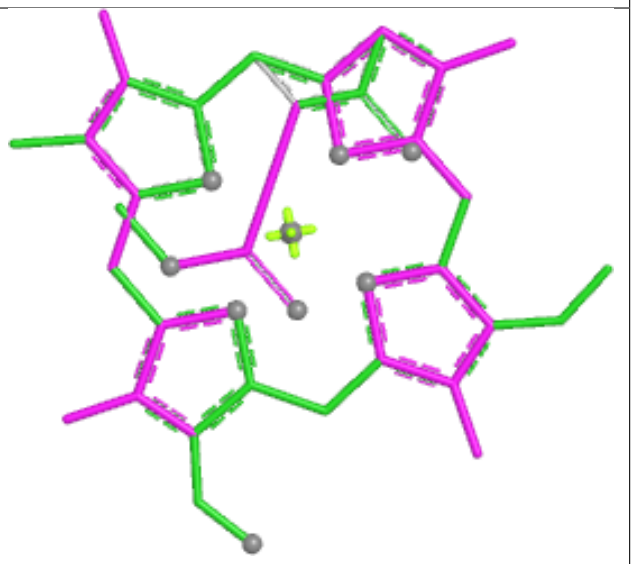


Rings

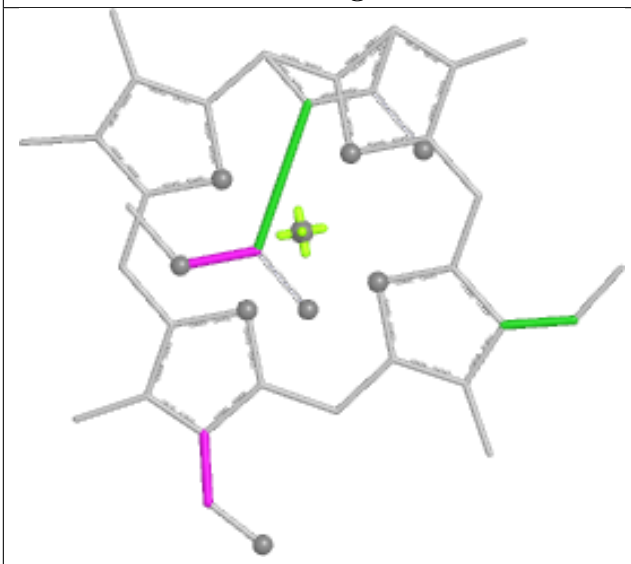
Ligand CL7 K 102



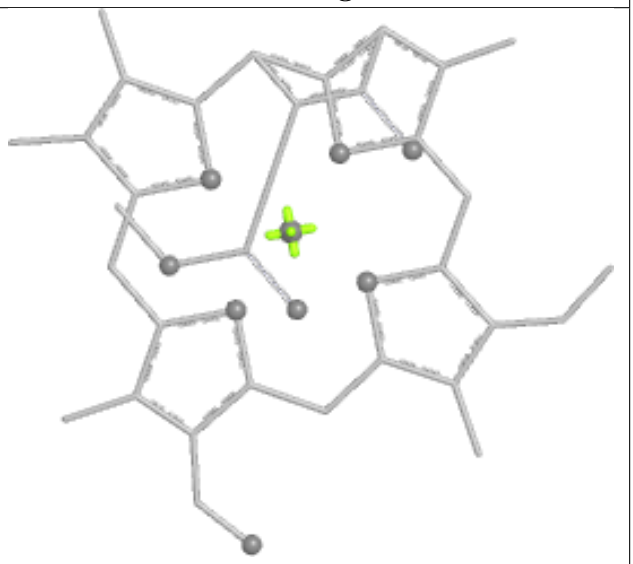
Bond lengths



Bond angles

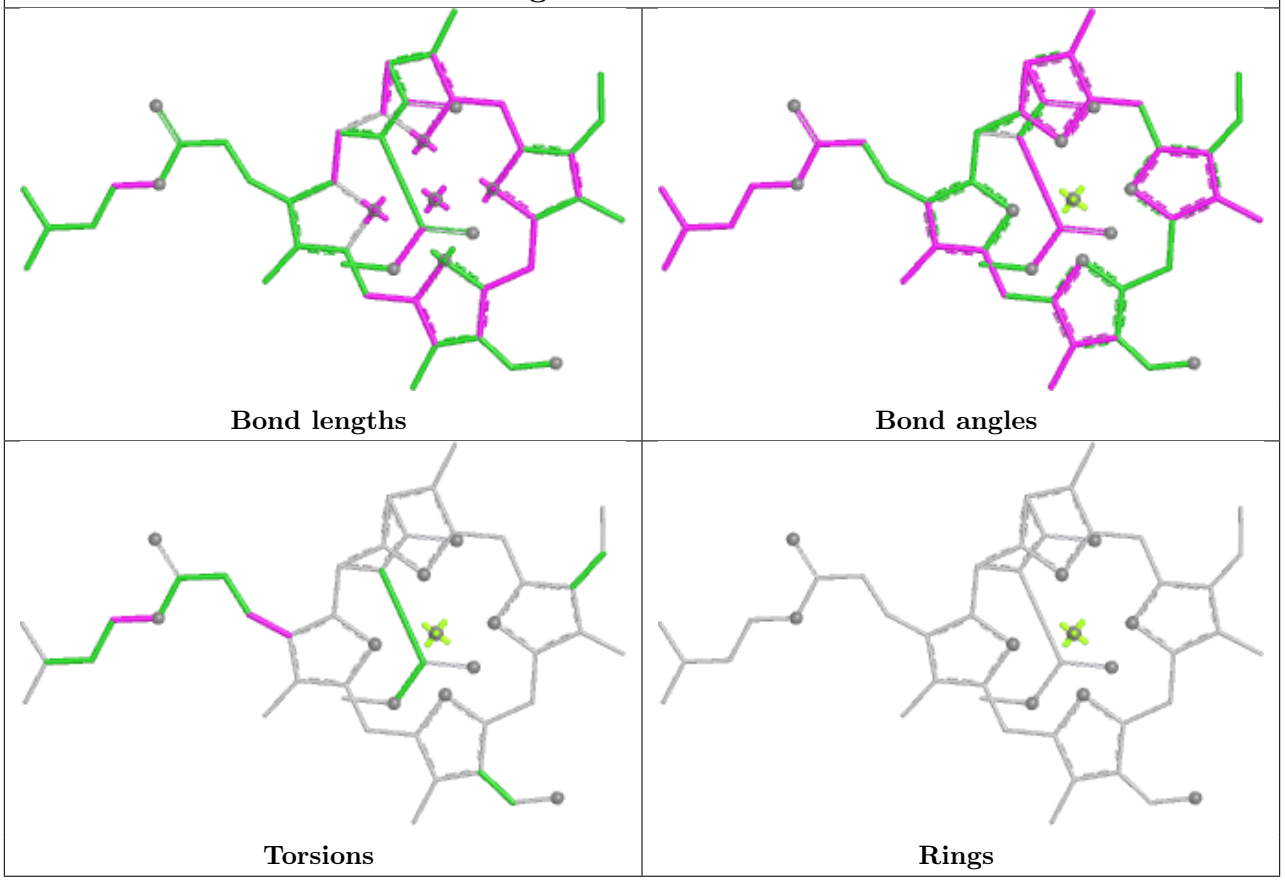


Torsions



Rings

Ligand CL7 A 813



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.

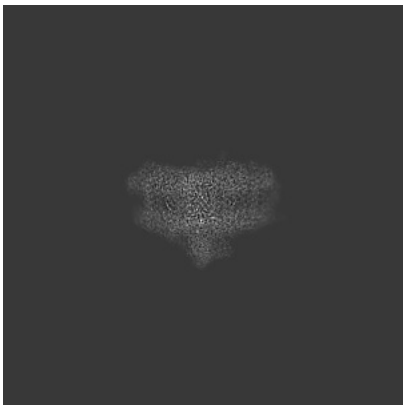
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-77301. These allow visual inspection of the internal detail of the map and identification of artifacts.

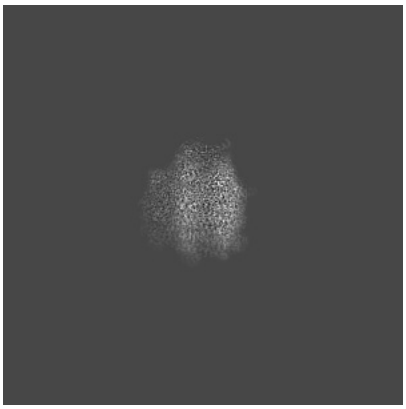
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

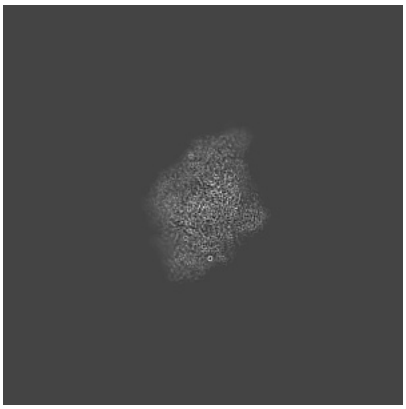
6.1.1 Primary map



X

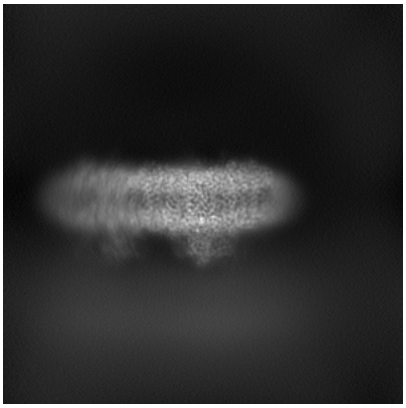


Y

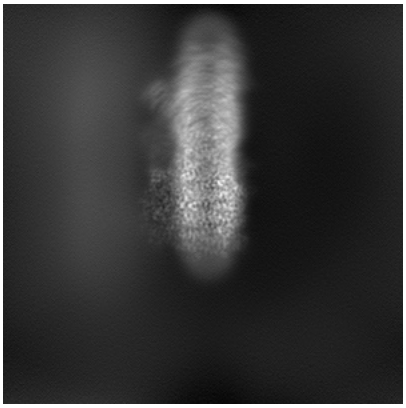


Z

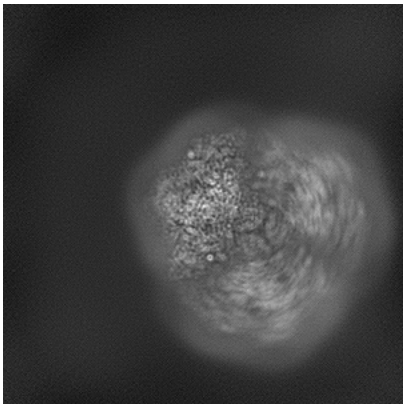
6.1.2 Raw map



X



Y



Z

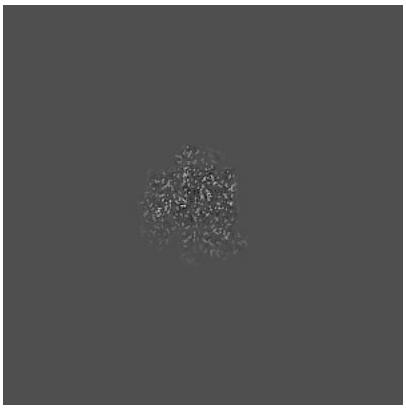
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

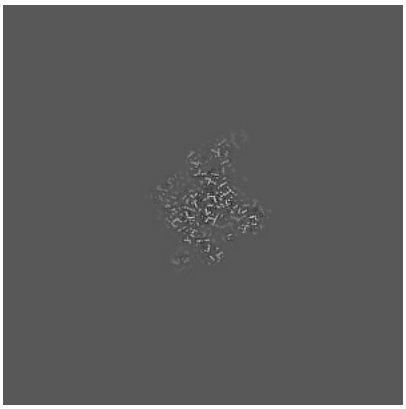
6.2.1 Primary map



X Index: 250

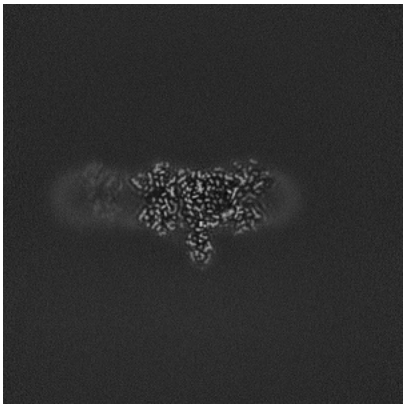


Y Index: 250

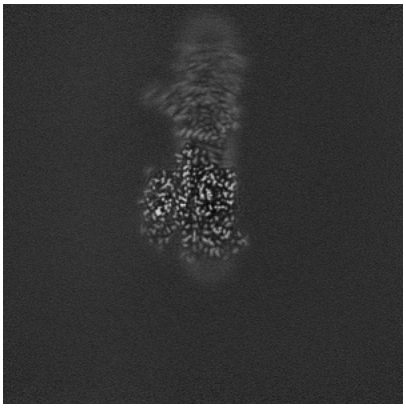


Z Index: 250

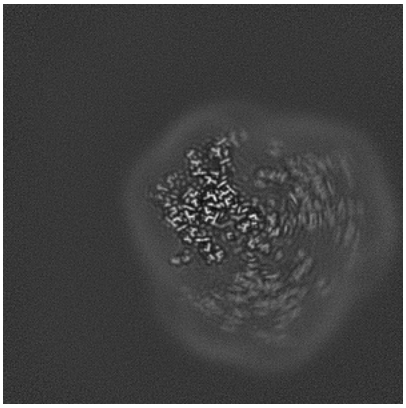
6.2.2 Raw map



X Index: 250



Y Index: 250



Z Index: 250

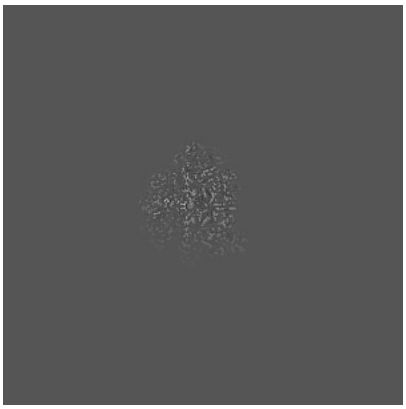
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

6.3.1 Primary map



X Index: 257

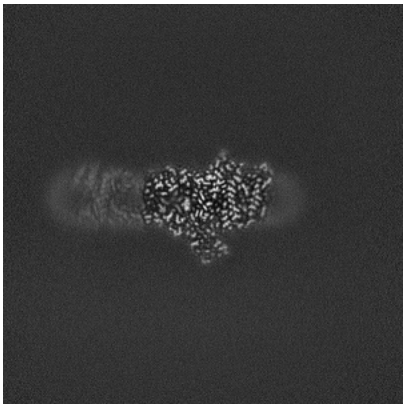


Y Index: 247

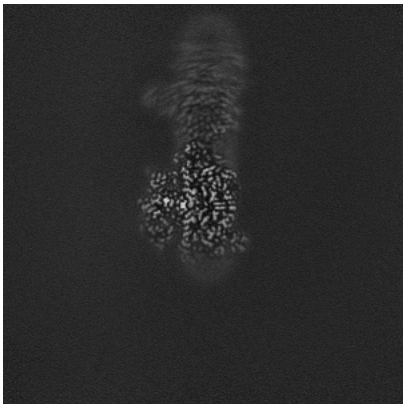


Z Index: 271

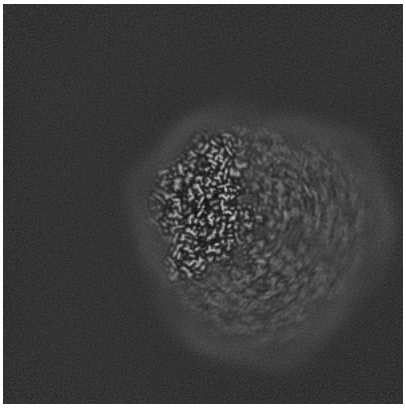
6.3.2 Raw map



X Index: 264



Y Index: 247

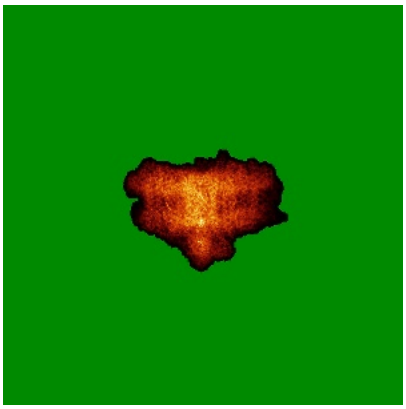


Z Index: 271

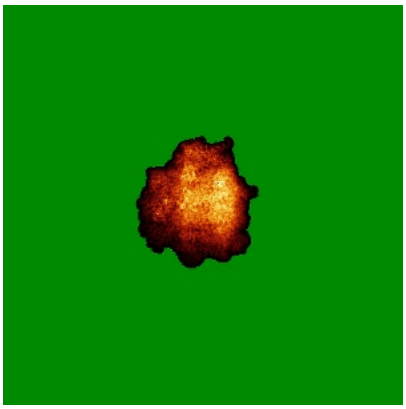
The images above show the largest variance slices of the map in three orthogonal directions.

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

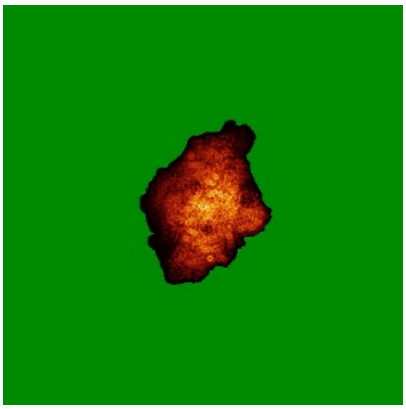
6.4.1 Primary map



X

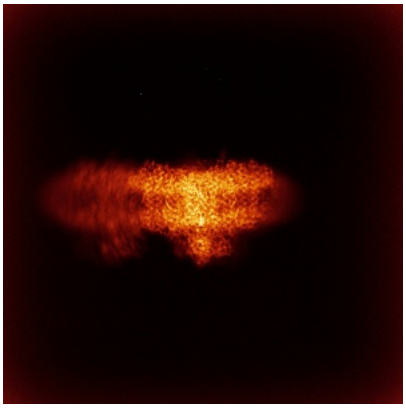


Y

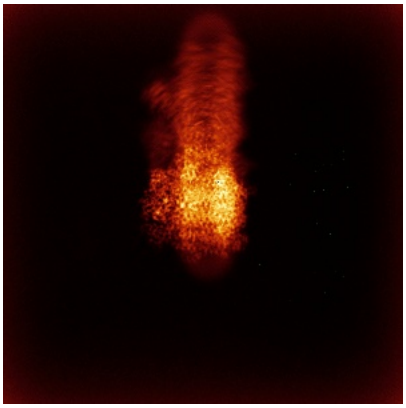


Z

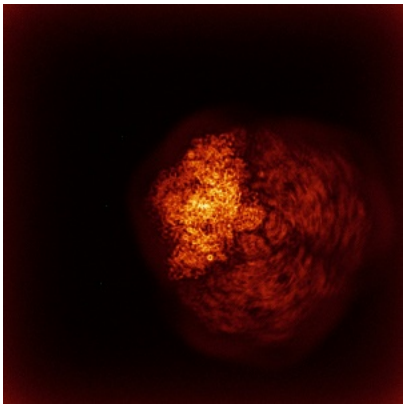
6.4.2 Raw map



X



Y

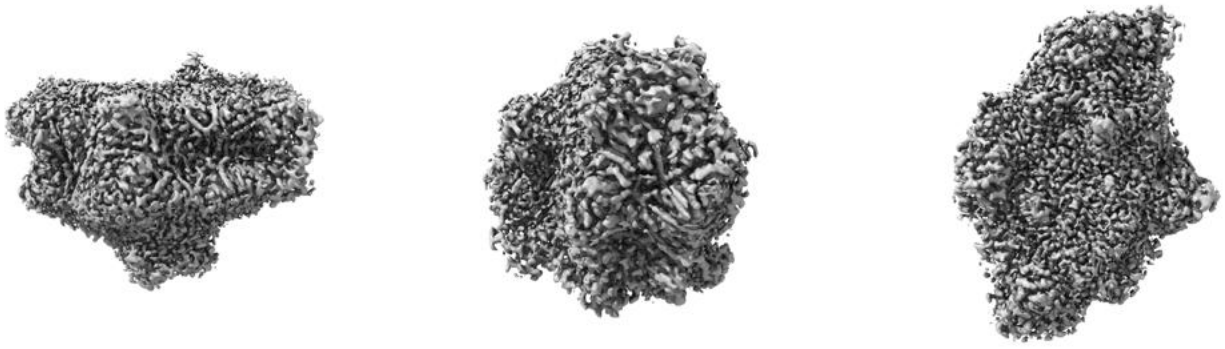


Z

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

6.5.2 Raw map



X Y Z

These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

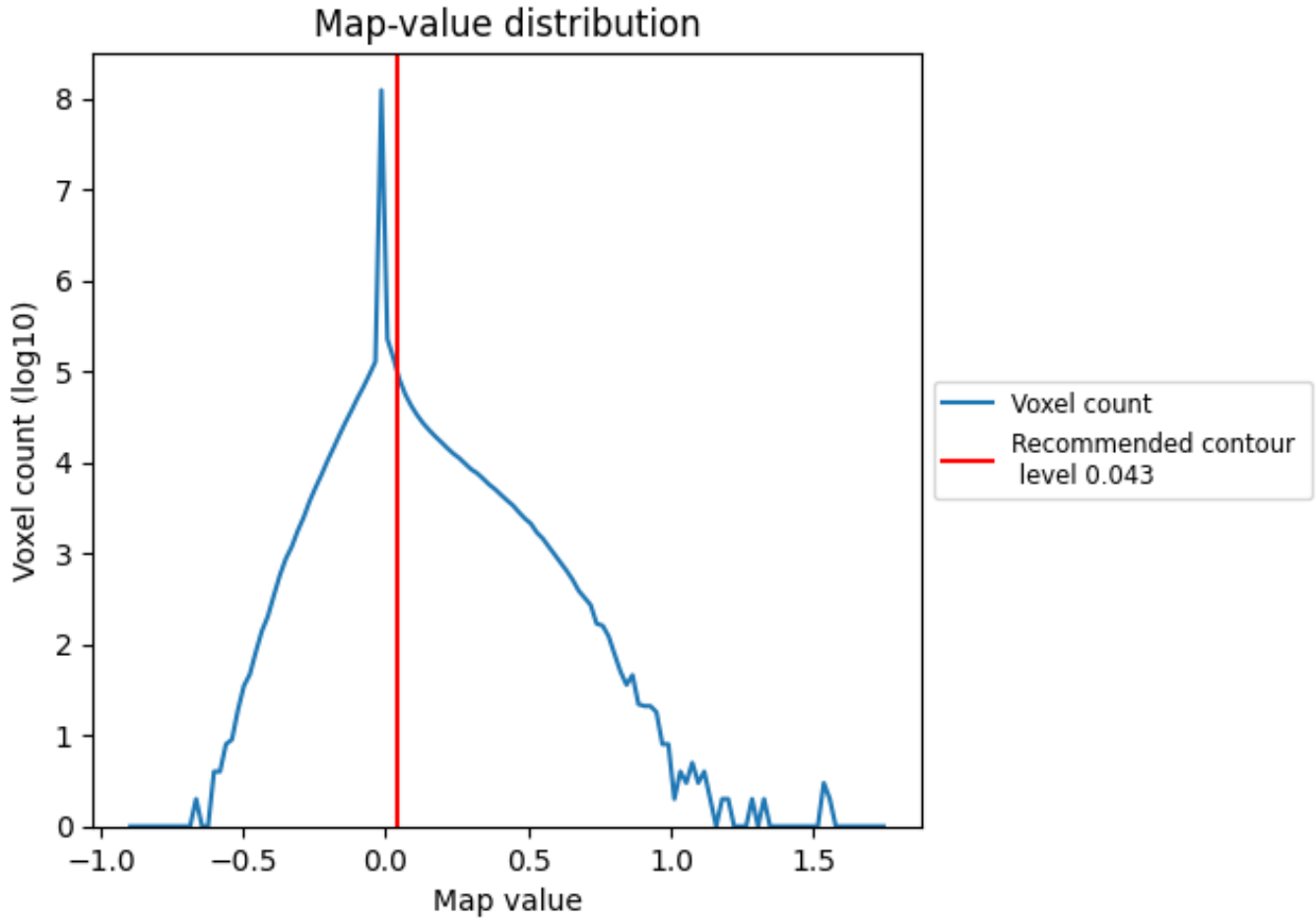
6.6 Mask visualisation (i)

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

7 Map analysis

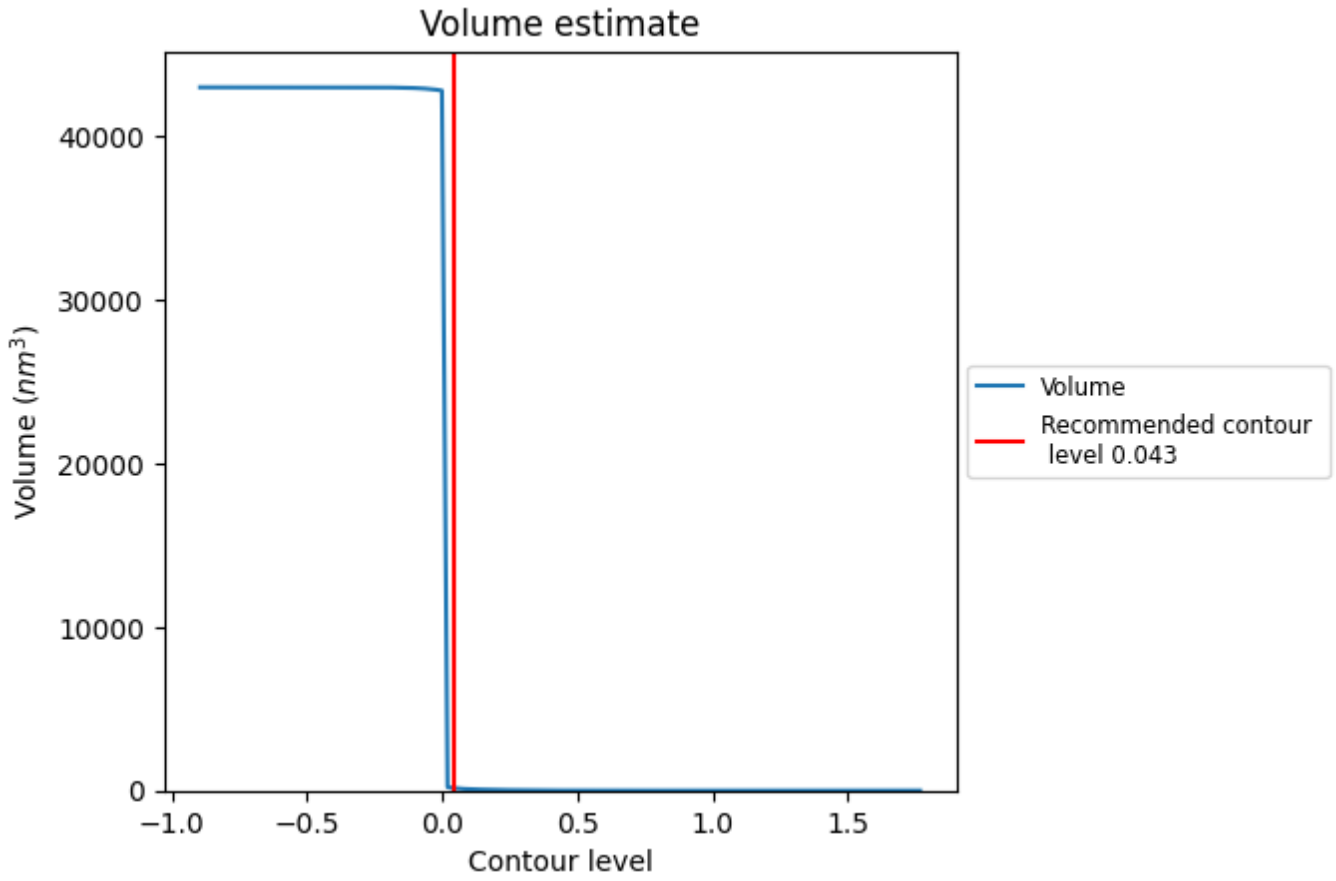
This section contains the results of statistical analysis of the map.

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.

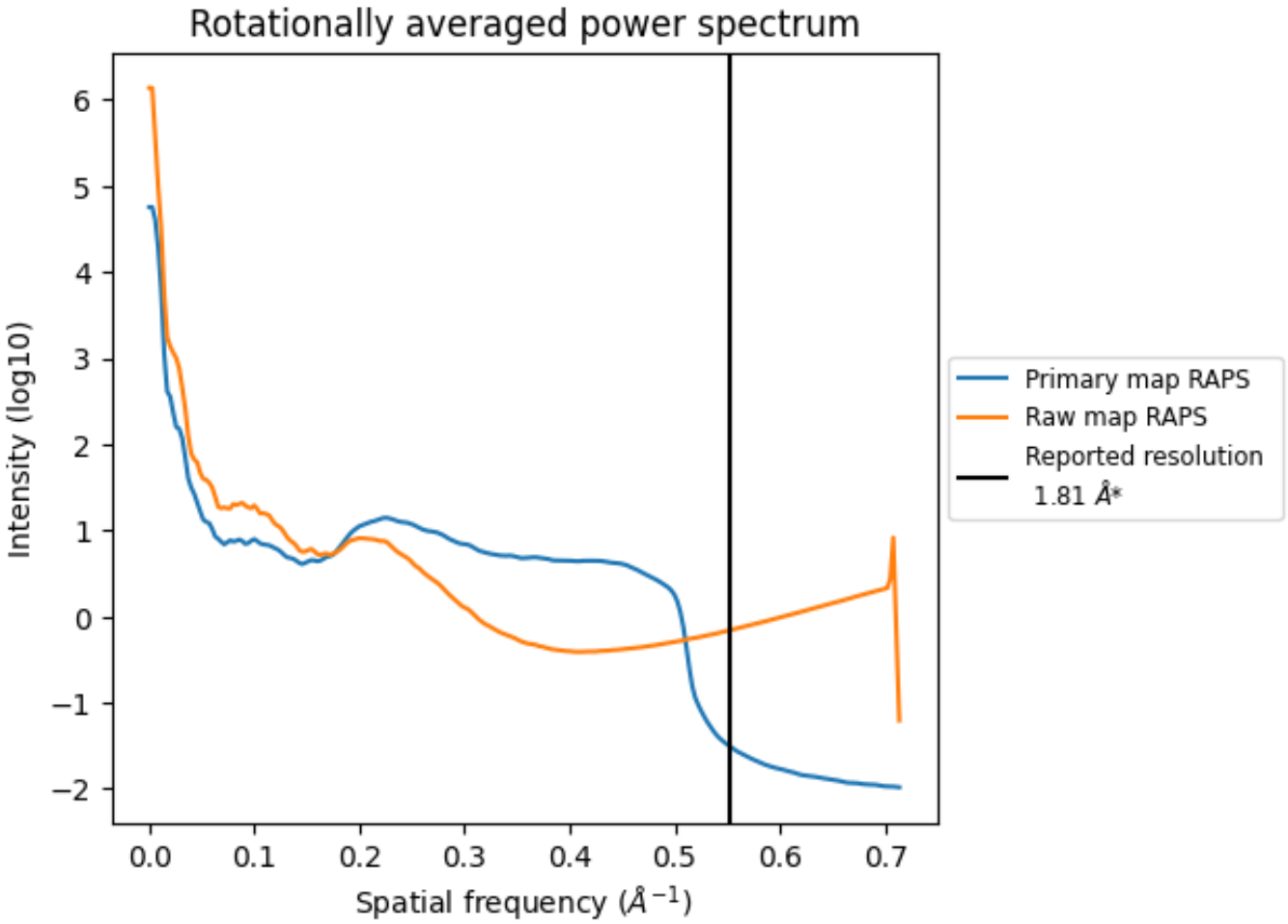
7.2 Volume estimate



The volume at the recommended contour level is 150 nm^3; this corresponds to an approximate mass of 136 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)

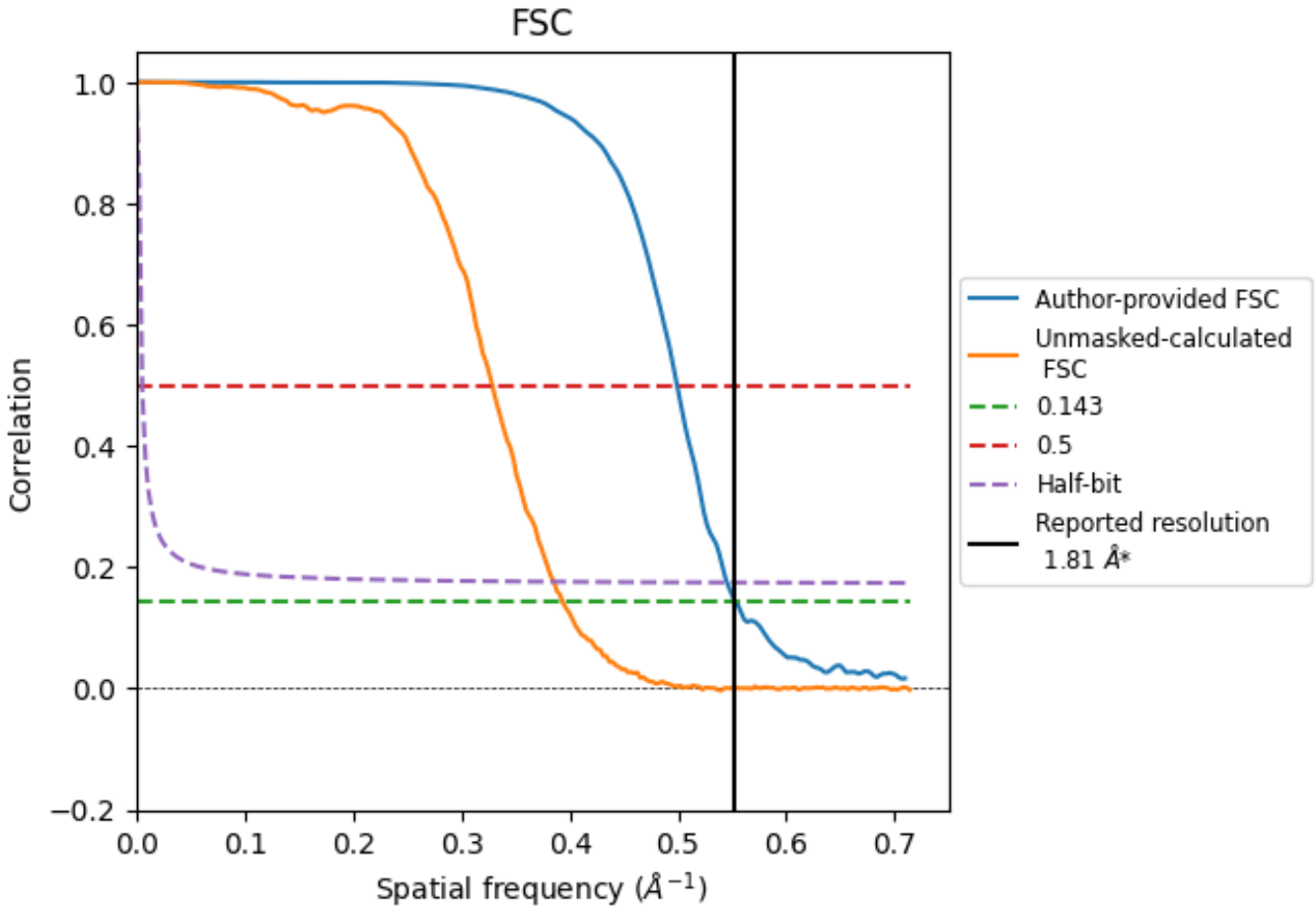


*Reported resolution corresponds to spatial frequency of 0.552 Å^{-1}

8 Fourier-Shell correlation

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

8.1 FSC



*Reported resolution corresponds to spatial frequency of 0.552 Å^{-1}

8.2 Resolution estimates (i)

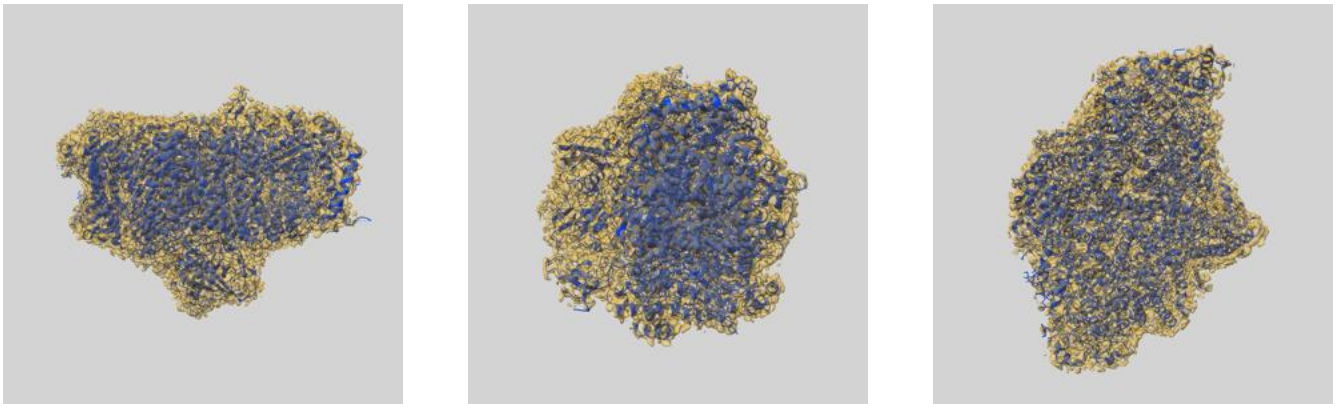
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	1.81	-	-
Author-provided FSC curve	1.81	2.00	1.83
Unmasked-calculated*	2.54	3.04	2.59

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 2.54 differs from the reported value 1.81 by more than 10 %

9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-77301 and PDB model 35ZQ. Per-residue inclusion information can be found in section 3 on page 20.

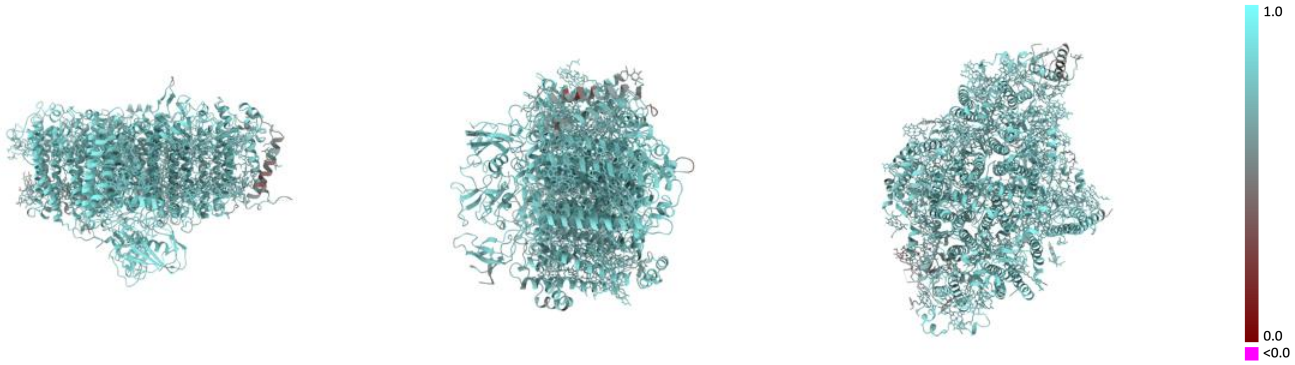
9.1 Map-model overlay



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.043 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.

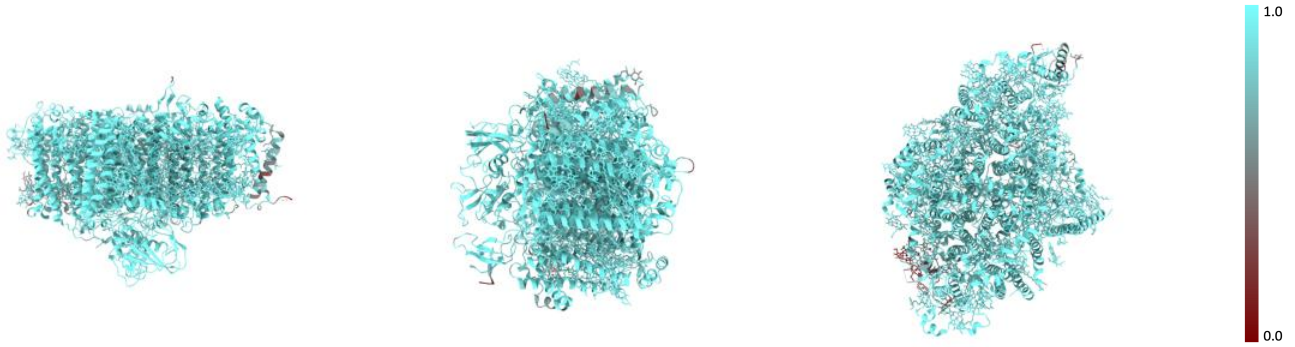
9.2 Q-score mapped to coordinate model (i)



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.

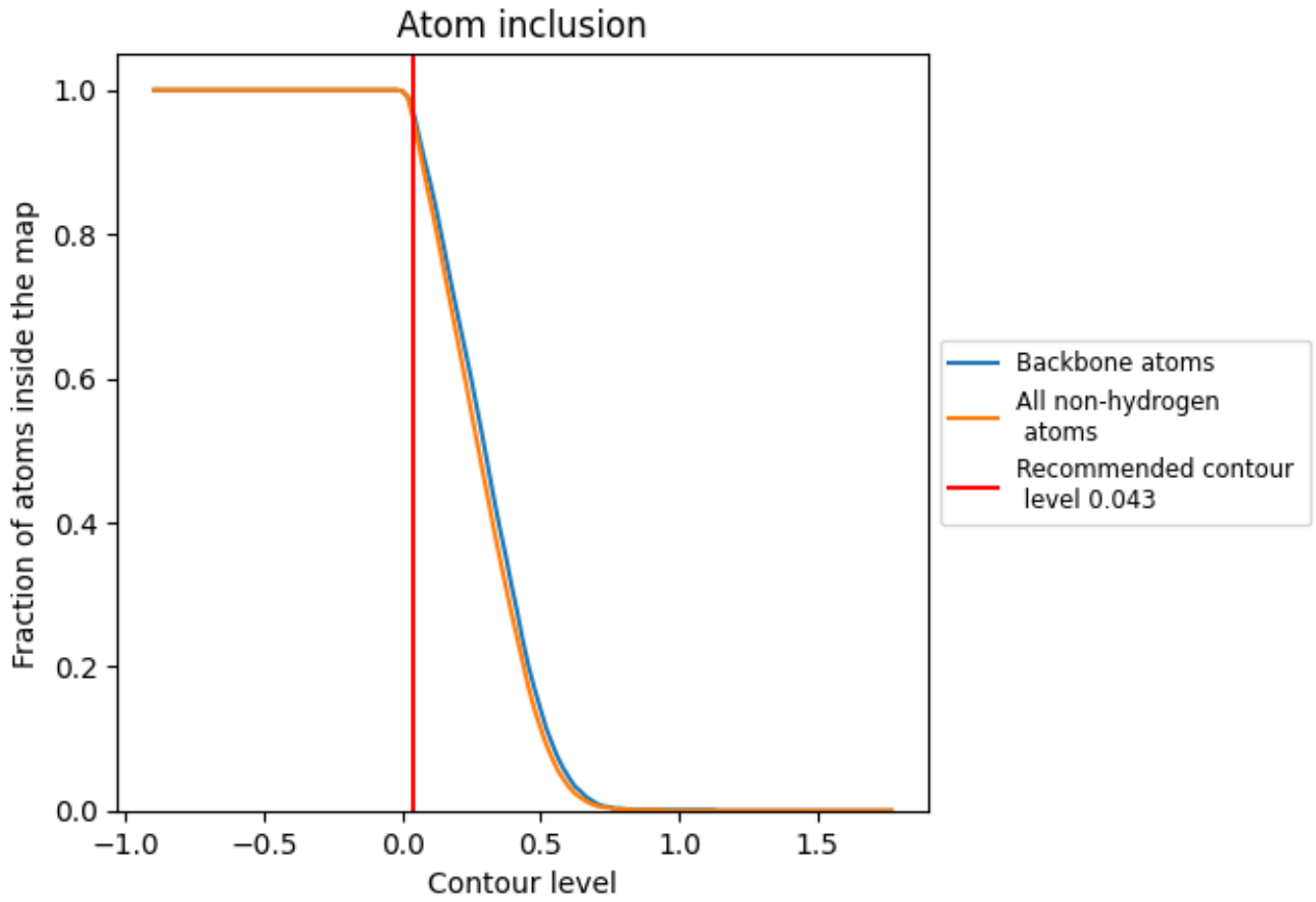
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.043).

9.4 Atom inclusion (i)



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

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.043) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.9550	0.7610
A	0.9810	0.7830
B	0.9350	0.7560
C	0.9920	0.7990
D	0.9780	0.7700
E	0.9180	0.7240
F	0.9290	0.7100
I	0.9880	0.7800
J	0.9810	0.7590
K	0.7650	0.5780
L	0.9690	0.7680
M	0.9730	0.7690

