wwPDB EM Validation Summary Report

Dec 19, 2022 – 05:44 am GMT

PDB ID	:	6YEZ
EMDB ID	:	EMD-10798
Title	:	Plant PSI-ferredoxin-plastocyanin supercomplex
Authors	:	Caspy, I.; Nelson, N.; Shkolnisky, Y.; Klaiman, D.; Sheinker, A.
Deposited on	:	2020-03-25
Resolution	:	2.70 Å(reported)
Based on initial model	:	5L8R

This is a wwPDB EM Validation Summary Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/EMValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references ⓘ) were used in the production of this report:

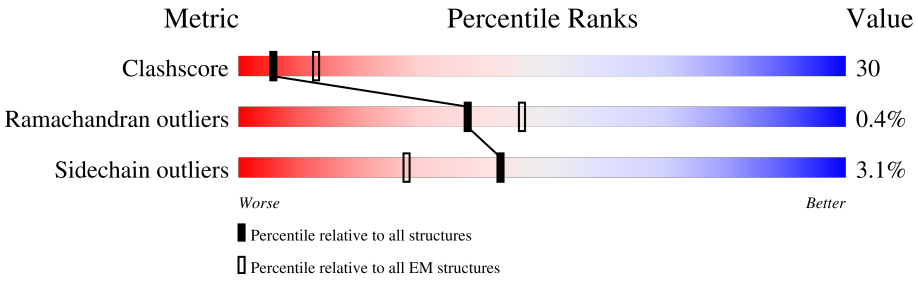
EMDB validation analysis	:	0.0.1.dev43
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.3

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 2.70 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



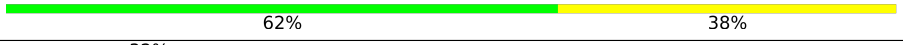
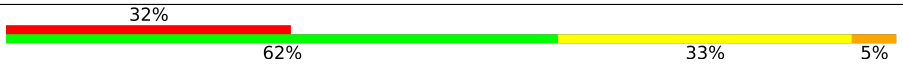
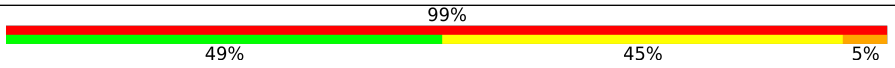
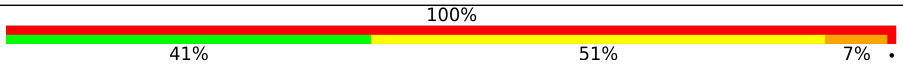
Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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

Mol	Chain	Length	Quality of chain
1	A	743	65% 33%
2	B	733	71% 27%
3	C	80	68% 31%
4	D	143	71% 27%
5	E	66	5% 86% 12%
6	F	154	73% 25%
7	G	97	74% 24%
8	H	93	65% 32%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
9	I	31	
10	J	42	
11	K	81	
12	L	159	
13	1	193	
14	2	208	
15	3	221	
16	4	198	
17	N	97	
18	P	99	

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
19	CL0	A	1011	X	-	-	-
20	CLA	1	601	X	-	-	-
20	CLA	1	602	X	-	-	-
20	CLA	1	603	X	-	-	-
20	CLA	1	604	X	-	-	-
20	CLA	1	605	X	-	-	-
20	CLA	1	606	X	-	-	-
20	CLA	1	607	X	-	-	-
20	CLA	1	608	X	-	-	-
20	CLA	1	611	X	-	-	-
20	CLA	1	613	X	-	-	-
20	CLA	1	614	X	-	-	-
20	CLA	2	601	X	-	-	-
20	CLA	2	602	X	-	-	-
20	CLA	2	603	X	-	-	-
20	CLA	2	604	X	-	X	-
20	CLA	2	605	X	-	-	-
20	CLA	2	606	X	-	X	-
20	CLA	2	607	X	-	-	-
20	CLA	2	608	X	-	-	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
20	CLA	2	612	X	-	-	-
20	CLA	3	601	X	-	-	-
20	CLA	3	602	X	-	-	-
20	CLA	3	603	X	-	-	-
20	CLA	3	605	X	-	-	-
20	CLA	3	606	X	-	-	-
20	CLA	3	608	X	-	-	-
20	CLA	3	610	X	-	-	-
20	CLA	3	612	X	-	-	-
20	CLA	3	613	X	-	-	-
20	CLA	3	614	X	-	-	-
20	CLA	3	617	X	-	-	-
20	CLA	4	601	X	-	X	-
20	CLA	4	602	X	-	-	-
20	CLA	4	603	X	-	-	-
20	CLA	4	604	X	-	X	-
20	CLA	4	606	X	-	-	-
20	CLA	4	607	X	-	-	-
20	CLA	4	608	X	-	-	-
20	CLA	4	609	X	-	-	-
20	CLA	4	612	X	-	X	-
20	CLA	4	617	X	-	-	-
20	CLA	A	1012	X	-	-	-
20	CLA	A	1013	X	-	-	-
20	CLA	A	1101	X	-	-	-
20	CLA	A	1102	X	-	-	-
20	CLA	A	1103	X	-	-	-
20	CLA	A	1104	X	-	-	-
20	CLA	A	1105	X	-	-	-
20	CLA	A	1106	X	-	-	-
20	CLA	A	1107	X	-	-	-
20	CLA	A	1108	X	-	-	-
20	CLA	A	1109	X	-	-	-
20	CLA	A	1110	X	-	-	-
20	CLA	A	1111	X	-	-	-
20	CLA	A	1112	X	-	-	-
20	CLA	A	1113	X	-	-	-
20	CLA	A	1114	X	-	-	-
20	CLA	A	1115	X	-	-	-
20	CLA	A	1116	X	-	-	-
20	CLA	A	1117	X	-	-	-
20	CLA	A	1118	X	-	-	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
20	CLA	A	1119	X	-	-	-
20	CLA	A	1120	X	-	-	-
20	CLA	A	1121	X	-	-	-
20	CLA	A	1122	X	-	-	-
20	CLA	A	1123	X	-	-	-
20	CLA	A	1124	X	-	-	-
20	CLA	A	1125	X	-	-	-
20	CLA	A	1126	X	-	X	-
20	CLA	A	1127	X	-	-	-
20	CLA	A	1128	X	-	-	-
20	CLA	A	1129	X	-	-	-
20	CLA	A	1130	X	-	-	-
20	CLA	A	1131	X	-	-	-
20	CLA	A	1132	X	-	X	-
20	CLA	A	1133	X	-	-	-
20	CLA	A	1134	X	-	-	-
20	CLA	A	1135	X	-	-	-
20	CLA	A	1136	X	-	-	-
20	CLA	A	1137	X	-	-	-
20	CLA	A	1138	X	-	-	-
20	CLA	A	1139	X	-	-	-
20	CLA	A	1140	X	-	-	-
20	CLA	A	1141	X	-	-	-
20	CLA	B	1021	X	-	-	-
20	CLA	B	1022	X	-	-	-
20	CLA	B	1023	X	-	-	-
20	CLA	B	1201	X	-	-	-
20	CLA	B	1202	X	-	-	-
20	CLA	B	1203	X	-	-	-
20	CLA	B	1204	X	-	-	-
20	CLA	B	1205	X	-	-	-
20	CLA	B	1206	X	-	-	-
20	CLA	B	1207	X	-	-	-
20	CLA	B	1208	X	-	-	-
20	CLA	B	1209	X	-	-	-
20	CLA	B	1210	X	-	-	-
20	CLA	B	1211	X	-	-	-
20	CLA	B	1212	X	-	-	-
20	CLA	B	1213	X	-	-	-
20	CLA	B	1214	X	-	-	-
20	CLA	B	1215	X	-	-	-
20	CLA	B	1216	X	-	-	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
20	CLA	B	1217	X	-	-	-
20	CLA	B	1218	X	-	-	-
20	CLA	B	1219	X	-	-	-
20	CLA	B	1220	X	-	-	-
20	CLA	B	1221	X	-	-	-
20	CLA	B	1222	X	-	-	-
20	CLA	B	1223	X	-	-	-
20	CLA	B	1224	X	-	-	-
20	CLA	B	1225	X	-	-	-
20	CLA	B	1226	X	-	-	-
20	CLA	B	1227	X	-	-	-
20	CLA	B	1228	X	-	-	-
20	CLA	B	1229	X	-	-	-
20	CLA	B	1230	X	-	-	-
20	CLA	B	1231	X	-	-	-
20	CLA	B	1232	X	-	-	-
20	CLA	B	1234	X	-	-	-
20	CLA	B	1235	X	-	-	-
20	CLA	B	1236	X	-	-	-
20	CLA	B	1237	X	-	-	-
20	CLA	B	1238	X	-	-	-
20	CLA	B	1239	X	-	-	-
20	CLA	B	1240	X	-	-	-
20	CLA	F	1301	X	-	-	-
20	CLA	F	1302	X	-	-	-
20	CLA	G	1601	X	-	-	-
20	CLA	G	1602	X	-	-	-
20	CLA	G	1603	X	-	-	-
20	CLA	H	1701	X	-	X	-
20	CLA	J	1901	X	-	-	-
20	CLA	K	1401	X	-	-	-
20	CLA	K	1402	X	-	-	-
20	CLA	K	1403	X	-	-	-
20	CLA	K	1404	X	-	-	-
20	CLA	L	1501	X	-	-	-
20	CLA	L	1502	X	-	-	-
20	CLA	L	1503	X	-	-	-
22	BCR	2	503	-	-	X	-
22	BCR	H	4021	-	-	X	-
22	BCR	L	4019	-	-	X	-
25	SF4	C	3003	-	-	X	-
29	LUT	1	502	-	-	X	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
29	LUT	2	501	X	-	-	-
29	LUT	3	502	X	-	-	-
30	CHL	1	609	X	-	-	-
30	CHL	1	610	X	-	-	-
30	CHL	1	612	X	-	-	-
30	CHL	2	609	X	-	X	-
30	CHL	2	610	X	-	-	-
30	CHL	2	611	X	-	-	-
30	CHL	2	613	X	-	-	-
30	CHL	2	615	X	-	-	-
30	CHL	3	604	X	-	-	-
30	CHL	3	607	X	-	-	-
30	CHL	3	611	X	-	-	-
30	CHL	4	610	X	-	-	-
30	CHL	4	611	X	-	-	-
30	CHL	4	613	X	-	-	-
30	CHL	4	615	X	-	-	-
31	XAT	2	502	X	-	-	-
31	XAT	4	502	X	-	-	-

2 Entry composition (i)

There are 36 unique types of molecules in this entry. The entry contains 39217 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	743	5858	3839	998	1003	18	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	B	733	5857	3848	998	997	14	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	C	80	612	379	107	115	11	0	0

- Molecule 4 is a protein called PsaD.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	D	143	1132	731	194	204	3	0	0

- Molecule 5 is a protein called PsaE.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
5	E	66	528	336	93	99	0	0

- Molecule 6 is a protein called PsaF.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	F	154	1206	782	207	215	2	0	0

- Molecule 7 is a protein called PsaG.

Mol	Chain	Residues	Atoms				AltConf	Trace
7	G	97	Total	C	N	O	0	0
			757	492	125	140		

- Molecule 8 is a protein called PsaH.

Mol	Chain	Residues	Atoms				AltConf	Trace
8	H	93	Total	C	N	O	0	0
			712	466	112	134		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
9	I	31	Total	C	N	O	S	0	0
			240	165	38	36	1		

- Molecule 10 is a protein called PsaJ.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	J	42	Total	C	N	O	S	0	0
			338	231	51	55	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
11	K	81	Total	C	N	O	S	0	0
			569	362	99	105	3		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
K	86	ALA	VAL	conflict	UNP E1C9L3

- Molecule 12 is a protein called PsaL.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	L	159	Total	C	N	O	S	0	0
			1197	788	191	217	1		

- Molecule 13 is a protein called Lhca1.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	1	193	Total	C	N	O	S	0	0
			1508	982	252	269	5		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
14	2	208	Total	C	N	O	S	0	0
			1620	1059	265	292	4		

- Molecule 15 is a protein called Chlorophyll a-b binding protein 3, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	3	221	Total	C	N	O	S	0	0
			1706	1118	278	305	5		

- Molecule 16 is a protein called Chlorophyll a-b binding protein P4, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	4	198	Total	C	N	O	S	0	0
			1559	1022	253	281	3		

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
4	89	LYS	ARG	conflict	UNP Q9SQL2
4	128	ASP	ALA	conflict	UNP Q9SQL2
4	149	PHE	SER	conflict	UNP Q9SQL2

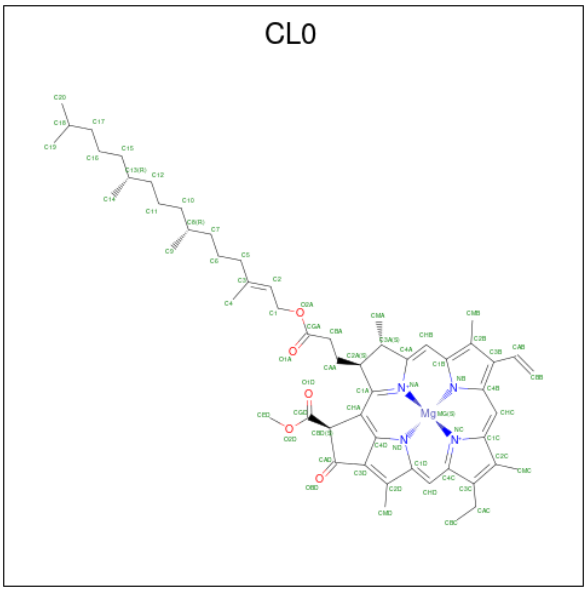
- Molecule 17 is a protein called Ferredoxin-1, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	N	97	Total	C	N	O	S	0	0
			724	448	111	160	5		

- Molecule 18 is a protein called Plastocyanin, chloroplastic.

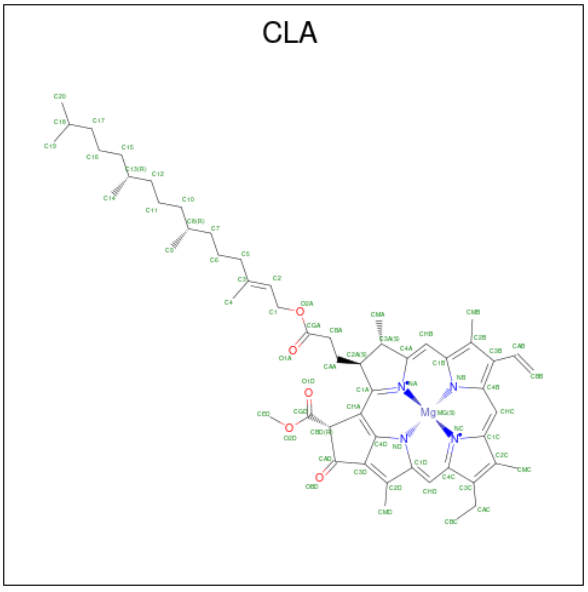
Mol	Chain	Residues	Atoms					AltConf	Trace
18	P	99	Total	C	N	O	S	0	0
			728	460	115	150	3		

- Molecule 19 is CHLOROPHYLL A ISOMER (three-letter code: CL0) (formula: $C_{55}H_{72}MgN_4O_5$).



Mol	Chain	Residues	Atoms					AltConf
19	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

- Molecule 20 is CHLOROPHYLL A (three-letter code: CLA) (formula: $C_{55}H_{72}MgN_4O_5$).



Mol	Chain	Residues	Atoms					AltConf
20	A	1	Total	C	Mg	N	O	0
			2643	2213	43	172	215	
20	A	1	Total	C	Mg	N	O	0
			2643	2213	43	172	215	
20	A	1	Total	C	Mg	N	O	0
			2643	2213	43	172	215	

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf
20	A	1	Total 2643	C 2213	Mg 43	N 172	O 215	0
20	A	1	Total 2643	C 2213	Mg 43	N 172	O 215	0
20	A	1	Total 2643	C 2213	Mg 43	N 172	O 215	0
20	A	1	Total 2643	C 2213	Mg 43	N 172	O 215	0
20	A	1	Total 2643	C 2213	Mg 43	N 172	O 215	0
20	A	1	Total 2643	C 2213	Mg 43	N 172	O 215	0
20	A	1	Total 2643	C 2213	Mg 43	N 172	O 215	0
20	A	1	Total 2643	C 2213	Mg 43	N 172	O 215	0
20	A	1	Total 2643	C 2213	Mg 43	N 172	O 215	0
20	A	1	Total 2643	C 2213	Mg 43	N 172	O 215	0
20	A	1	Total 2643	C 2213	Mg 43	N 172	O 215	0
20	A	1	Total 2643	C 2213	Mg 43	N 172	O 215	0
20	A	1	Total 2643	C 2213	Mg 43	N 172	O 215	0
20	A	1	Total 2643	C 2213	Mg 43	N 172	O 215	0
20	A	1	Total 2643	C 2213	Mg 43	N 172	O 215	0
20	A	1	Total 2643	C 2213	Mg 43	N 172	O 215	0
20	A	1	Total 2643	C 2213	Mg 43	N 172	O 215	0
20	A	1	Total 2643	C 2213	Mg 43	N 172	O 215	0
20	A	1	Total 2643	C 2213	Mg 43	N 172	O 215	0
20	A	1	Total 2643	C 2213	Mg 43	N 172	O 215	0
20	A	1	Total 2643	C 2213	Mg 43	N 172	O 215	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf
20	A	1	Total 2643	C 2213	Mg 43	N 172	O 215	0
20	A	1	Total 2643	C 2213	Mg 43	N 172	O 215	0
20	A	1	Total 2643	C 2213	Mg 43	N 172	O 215	0
20	A	1	Total 2643	C 2213	Mg 43	N 172	O 215	0
20	A	1	Total 2643	C 2213	Mg 43	N 172	O 215	0
20	A	1	Total 2643	C 2213	Mg 43	N 172	O 215	0
20	A	1	Total 2643	C 2213	Mg 43	N 172	O 215	0
20	A	1	Total 2643	C 2213	Mg 43	N 172	O 215	0
20	A	1	Total 2643	C 2213	Mg 43	N 172	O 215	0
20	A	1	Total 2643	C 2213	Mg 43	N 172	O 215	0
20	A	1	Total 2643	C 2213	Mg 43	N 172	O 215	0
20	A	1	Total 2643	C 2213	Mg 43	N 172	O 215	0
20	A	1	Total 2643	C 2213	Mg 43	N 172	O 215	0
20	A	1	Total 2643	C 2213	Mg 43	N 172	O 215	0
20	A	1	Total 2643	C 2213	Mg 43	N 172	O 215	0
20	A	1	Total 2643	C 2213	Mg 43	N 172	O 215	0
20	A	1	Total 2643	C 2213	Mg 43	N 172	O 215	0
20	A	1	Total 2643	C 2213	Mg 43	N 172	O 215	0
20	A	1	Total 2643	C 2213	Mg 43	N 172	O 215	0
20	B	1	Total 2610	C 2190	Mg 42	N 168	O 210	0
20	B	1	Total 2610	C 2190	Mg 42	N 168	O 210	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms	AltConf
20	B	1	Total C Mg N O 2610 2190 42 168 210	0
20	B	1	Total C Mg N O 2610 2190 42 168 210	0
20	B	1	Total C Mg N O 2610 2190 42 168 210	0
20	B	1	Total C Mg N O 2610 2190 42 168 210	0
20	B	1	Total C Mg N O 2610 2190 42 168 210	0
20	B	1	Total C Mg N O 2610 2190 42 168 210	0
20	B	1	Total C Mg N O 2610 2190 42 168 210	0
20	B	1	Total C Mg N O 2610 2190 42 168 210	0
20	B	1	Total C Mg N O 2610 2190 42 168 210	0
20	B	1	Total C Mg N O 2610 2190 42 168 210	0
20	B	1	Total C Mg N O 2610 2190 42 168 210	0
20	B	1	Total C Mg N O 2610 2190 42 168 210	0
20	B	1	Total C Mg N O 2610 2190 42 168 210	0
20	B	1	Total C Mg N O 2610 2190 42 168 210	0
20	B	1	Total C Mg N O 2610 2190 42 168 210	0
20	B	1	Total C Mg N O 2610 2190 42 168 210	0
20	B	1	Total C Mg N O 2610 2190 42 168 210	0
20	B	1	Total C Mg N O 2610 2190 42 168 210	0
20	B	1	Total C Mg N O 2610 2190 42 168 210	0
20	B	1	Total C Mg N O 2610 2190 42 168 210	0
20	B	1	Total C Mg N O 2610 2190 42 168 210	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms	AltConf
20	B	1	Total C Mg N O 2610 2190 42 168 210	0
20	B	1	Total C Mg N O 2610 2190 42 168 210	0
20	B	1	Total C Mg N O 2610 2190 42 168 210	0
20	B	1	Total C Mg N O 2610 2190 42 168 210	0
20	B	1	Total C Mg N O 2610 2190 42 168 210	0
20	B	1	Total C Mg N O 2610 2190 42 168 210	0
20	B	1	Total C Mg N O 2610 2190 42 168 210	0
20	B	1	Total C Mg N O 2610 2190 42 168 210	0
20	B	1	Total C Mg N O 2610 2190 42 168 210	0
20	B	1	Total C Mg N O 2610 2190 42 168 210	0
20	B	1	Total C Mg N O 2610 2190 42 168 210	0
20	B	1	Total C Mg N O 2610 2190 42 168 210	0
20	B	1	Total C Mg N O 2610 2190 42 168 210	0
20	B	1	Total C Mg N O 2610 2190 42 168 210	0
20	B	1	Total C Mg N O 2610 2190 42 168 210	0
20	B	1	Total C Mg N O 2610 2190 42 168 210	0
20	B	1	Total C Mg N O 2610 2190 42 168 210	0
20	B	1	Total C Mg N O 2610 2190 42 168 210	0
20	B	1	Total C Mg N O 2610 2190 42 168 210	0
20	F	1	Total C Mg N O 130 110 2 8 10	0
20	F	1	Total C Mg N O 130 110 2 8 10	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms	AltConf
20	G	1	Total C Mg N O 166 136 3 12 15	0
20	G	1	Total C Mg N O 166 136 3 12 15	0
20	G	1	Total C Mg N O 166 136 3 12 15	0
20	H	1	Total C Mg N O 60 50 1 4 5	0
20	J	1	Total C Mg N O 50 40 1 4 5	0
20	K	1	Total C Mg N O 199 159 4 16 20	0
20	K	1	Total C Mg N O 199 159 4 16 20	0
20	K	1	Total C Mg N O 199 159 4 16 20	0
20	K	1	Total C Mg N O 199 159 4 16 20	0
20	L	1	Total C Mg N O 160 130 3 12 15	0
20	L	1	Total C Mg N O 160 130 3 12 15	0
20	L	1	Total C Mg N O 160 130 3 12 15	0
20	1	1	Total C Mg N O 608 498 11 44 55	0
20	1	1	Total C Mg N O 608 498 11 44 55	0
20	1	1	Total C Mg N O 608 498 11 44 55	0
20	1	1	Total C Mg N O 608 498 11 44 55	0
20	1	1	Total C Mg N O 608 498 11 44 55	0
20	1	1	Total C Mg N O 608 498 11 44 55	0
20	1	1	Total C Mg N O 608 498 11 44 55	0
20	1	1	Total C Mg N O 608 498 11 44 55	0
20	1	1	Total C Mg N O 608 498 11 44 55	0

Continued on next page...

Continued from previous page...

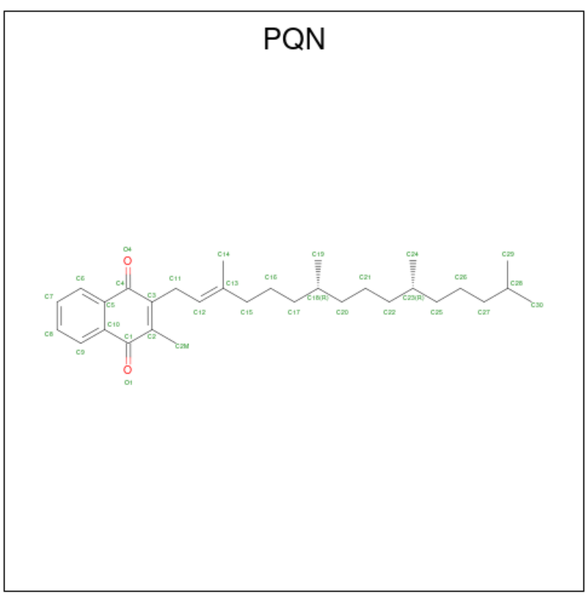
Mol	Chain	Residues	Atoms	AltConf
20	1	1	Total C Mg N O 608 498 11 44 55	0
20	1	1	Total C Mg N O 608 498 11 44 55	0
20	2	1	Total C Mg N O 522 432 9 36 45	0
20	2	1	Total C Mg N O 522 432 9 36 45	0
20	2	1	Total C Mg N O 522 432 9 36 45	0
20	2	1	Total C Mg N O 522 432 9 36 45	0
20	2	1	Total C Mg N O 522 432 9 36 45	0
20	2	1	Total C Mg N O 522 432 9 36 45	0
20	2	1	Total C Mg N O 522 432 9 36 45	0
20	2	1	Total C Mg N O 522 432 9 36 45	0
20	2	1	Total C Mg N O 522 432 9 36 45	0
20	3	1	Total C Mg N O 578 470 11 44 53	0
20	3	1	Total C Mg N O 578 470 11 44 53	0
20	3	1	Total C Mg N O 578 470 11 44 53	0
20	3	1	Total C Mg N O 578 470 11 44 53	0
20	3	1	Total C Mg N O 578 470 11 44 53	0
20	3	1	Total C Mg N O 578 470 11 44 53	0
20	3	1	Total C Mg N O 578 470 11 44 53	0
20	3	1	Total C Mg N O 578 470 11 44 53	0
20	3	1	Total C Mg N O 578 470 11 44 53	0
20	3	1	Total C Mg N O 578 470 11 44 53	0

Continued on next page...

Continued from previous page...

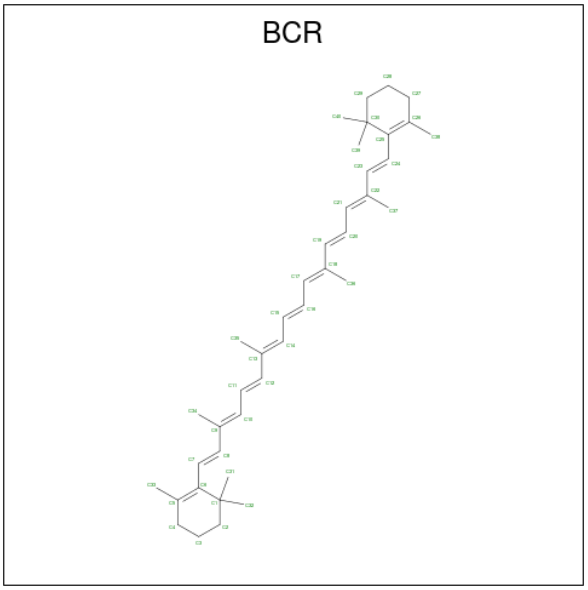
Mol	Chain	Residues	Atoms	AltConf
20	3	1	Total C Mg N O 578 470 11 44 53	0
20	4	1	Total C Mg N O 631 521 11 44 55	0
20	4	1	Total C Mg N O 631 521 11 44 55	0
20	4	1	Total C Mg N O 631 521 11 44 55	0
20	4	1	Total C Mg N O 631 521 11 44 55	0
20	4	1	Total C Mg N O 631 521 11 44 55	0
20	4	1	Total C Mg N O 631 521 11 44 55	0
20	4	1	Total C Mg N O 631 521 11 44 55	0
20	4	1	Total C Mg N O 631 521 11 44 55	0
20	4	1	Total C Mg N O 631 521 11 44 55	0
20	4	1	Total C Mg N O 631 521 11 44 55	0
20	4	1	Total C Mg N O 631 521 11 44 55	0

- Molecule 21 is PHYLLOQUINONE (three-letter code: PQN) (formula: $C_{31}H_{46}O_2$).



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

- Molecule 22 is BETA-CAROTENE (three-letter code: BCR) (formula: $C_{40}H_{56}$).



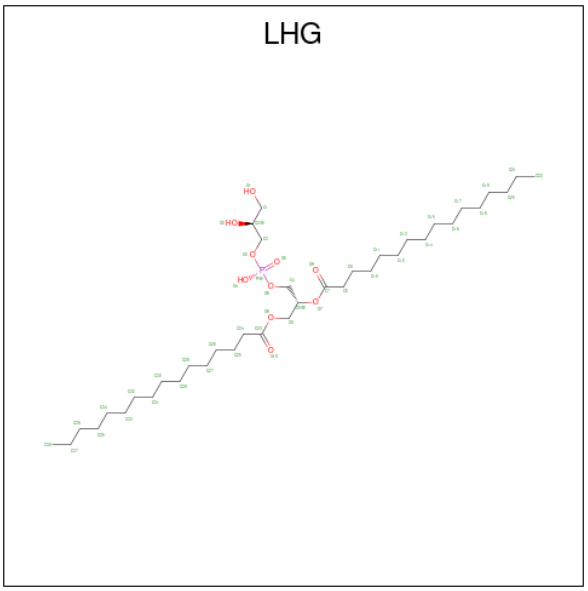
Mol	Chain	Residues	Atoms	AltConf
22	A	1	Total C 240 240	0
22	A	1	Total C 240 240	0
22	A	1	Total C 240 240	0
22	A	1	Total C 240 240	0
22	A	1	Total C 240 240	0
22	A	1	Total C 240 240	0
22	B	1	Total C 200 200	0
22	B	1	Total C 200 200	0
22	B	1	Total C 200 200	0
22	B	1	Total C 200 200	0

Continued on next page...

Continued from previous page...

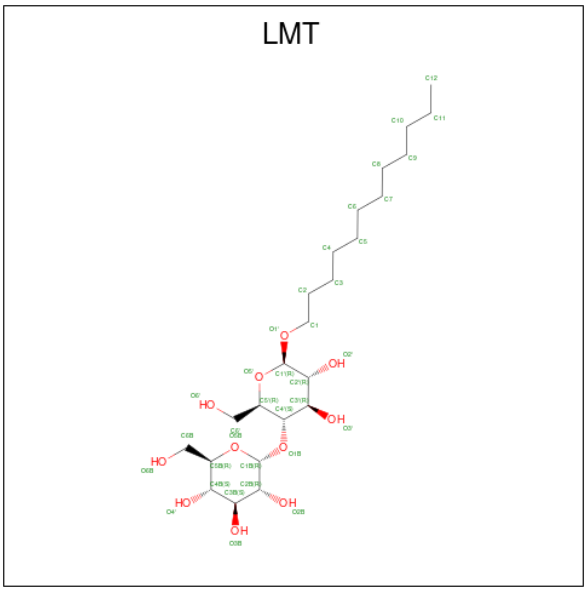
Mol	Chain	Residues	Atoms	AltConf
22	B	1	Total C 200 200	0
22	F	1	Total C 80 80	0
22	F	1	Total C 80 80	0
22	G	1	Total C 40 40	0
22	H	1	Total C 40 40	0
22	I	1	Total C 80 80	0
22	I	1	Total C 80 80	0
22	J	1	Total C 40 40	0
22	K	1	Total C 80 80	0
22	K	1	Total C 80 80	0
22	L	1	Total C 80 80	0
22	L	1	Total C 80 80	0
22	1	1	Total C 80 80	0
22	1	1	Total C 80 80	0
22	2	1	Total C 40 40	0
22	3	1	Total C 80 80	0
22	3	1	Total C 80 80	0

- Molecule 23 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (three-letter code: LHG) (formula: $C_{38}H_{75}O_{10}P$).



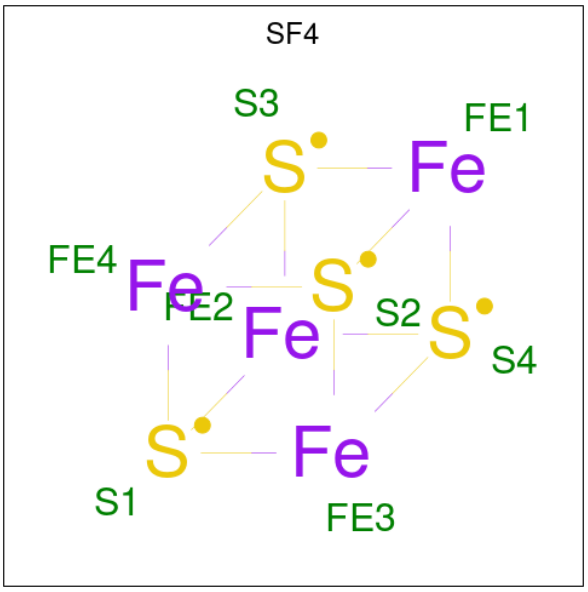
Mol	Chain	Residues	Atoms	AltConf
23	A	1	Total C O P 89 67 20 2	0
23	A	1	Total C O P 89 67 20 2	0
23	B	1	Total C O P 70 48 20 2	0
23	B	1	Total C O P 70 48 20 2	0
23	1	1	Total C O P 49 38 10 1	0
23	2	1	Total C O P 35 24 10 1	0
23	3	1	Total C O P 17 8 8 1	0
23	4	1	Total C O P 35 24 10 1	0

- Molecule 24 is DODECYL-BETA-D-MALTOSIDE (three-letter code: LMT) (formula: $C_{24}H_{46}O_{11}$).



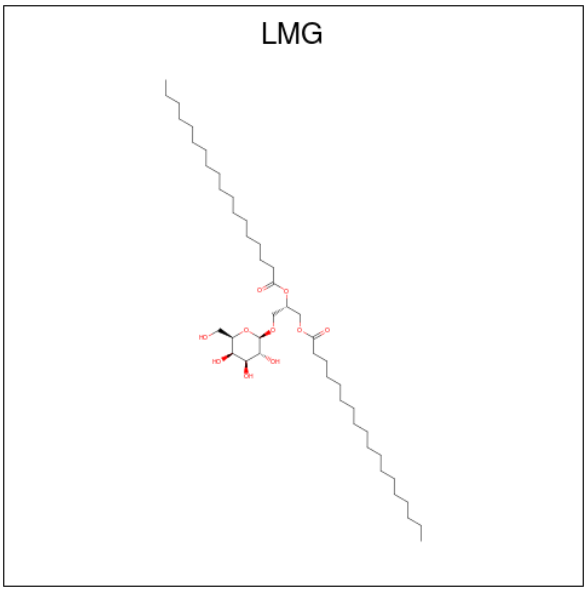
Mol	Chain	Residues	Atoms			AltConf
24	A	1	Total 35	C 24	O 11	0
24	B	1	Total 63	C 41	O 22	0
24	B	1	Total 63	C 41	O 22	0
24	G	1	Total 66	C 44	O 22	0
24	G	1	Total 66	C 44	O 22	0
24	2	1	Total 35	C 24	O 11	0

- Molecule 25 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe_4S_4).



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

- Molecule 26 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (three-letter code: LMG) (formula: $C_{45}H_{86}O_{10}$).



Mol	Chain	Residues	Atoms			AltConf
26	A	1	Total 50	C 40	O 10	0
26	B	1	Total 102	C 72	O 30	0
26	B	1	Total 102	C 72	O 30	0
26	B	1	Total 102	C 72	O 30	0
26	F	1	Total 160	C 114	O 46	0
26	F	1	Total 160	C 114	O 46	0
26	F	1	Total 160	C 114	O 46	0
26	F	1	Total 160	C 114	O 46	0
26	F	1	Total 160	C 114	O 46	0
26	G	1	Total 124	C 94	O 30	0
26	G	1	Total 124	C 94	O 30	0
26	G	1	Total 124	C 94	O 30	0
26	1	1	Total 46	C 36	O 10	0
26	2	1	Total 134	C 88	O 46	0
26	2	1	Total 134	C 88	O 46	0
26	2	1	Total 134	C 88	O 46	0
26	2	1	Total 134	C 88	O 46	0
26	2	1	Total 134	C 88	O 46	0
26	3	1	Total 30	C 20	O 10	0

- Molecule 27 is CALCIUM ION (three-letter code: CA) (formula: Ca).

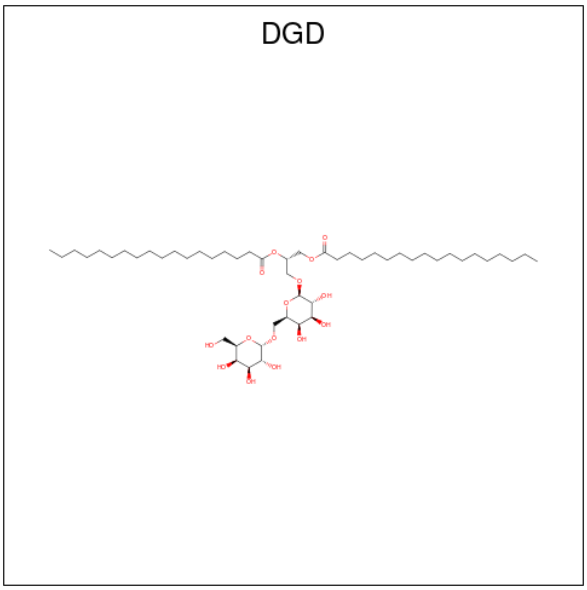
Mol	Chain	Residues	Atoms		AltConf
27	A	1	Total 1	Ca 1	0

Continued on next page...

Continued from previous page...

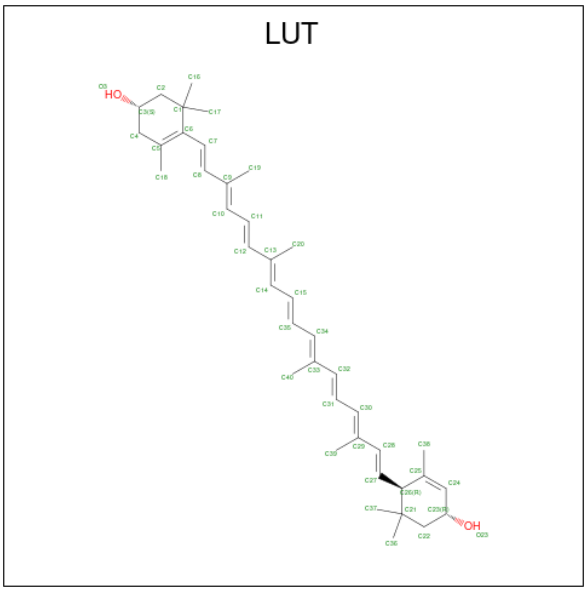
Mol	Chain	Residues	Atoms	AltConf
27	B	1	Total Ca 1 1	0

- Molecule 28 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (three-letter code: DGD) (formula: $C_{51}H_{96}O_{15}$).



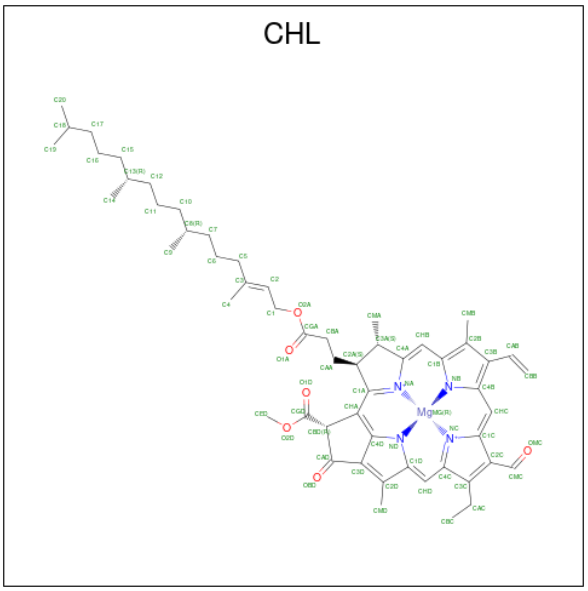
Mol	Chain	Residues	Atoms	AltConf
28	B	1	Total C O 61 46 15	0
28	F	1	Total C O 57 42 15	0
28	G	1	Total C O 47 32 15	0
28	J	1	Total C O 58 43 15	0
28	1	1	Total C O 41 26 15	0
28	3	1	Total C O 51 36 15	0
28	4	1	Total C O 51 36 15	0

- Molecule 29 is (3R,3'R,6S)-4,5-DIDEHYDRO-5,6-DIHYDRO-BETA,BETA-CAROTENE-3,3'-DIOL (three-letter code: LUT) (formula: $C_{40}H_{56}O_2$).



Mol	Chain	Residues	Atoms	AltConf
29	J	1	Total C O 42 40 2	0
29	1	1	Total C O 84 80 4	0
29	1	1	Total C O 84 80 4	0
29	2	1	Total C O 42 40 2	0
29	3	1	Total C O 84 80 4	0
29	3	1	Total C O 84 80 4	0
29	4	1	Total C O 42 40 2	0

- Molecule 30 is CHLOROPHYLL B (three-letter code: CHL) (formula: $C_{55}H_{70}MgN_4O_6$).



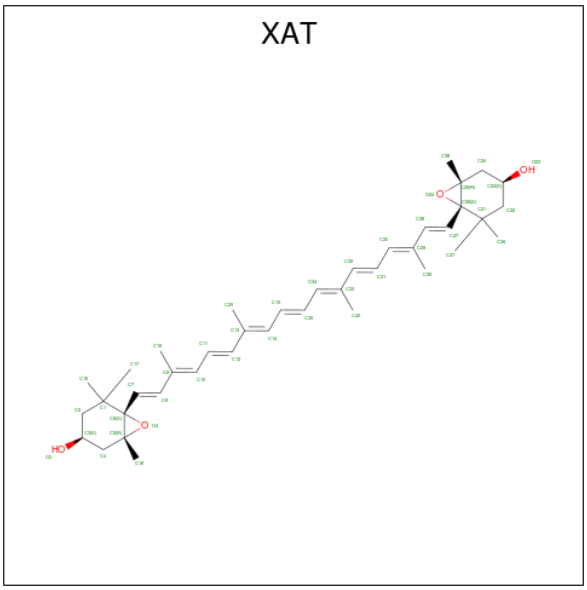
Mol	Chain	Residues	Atoms					AltConf
30	1	1	Total	C	Mg	N	O	0
			164	131	3	12	18	
30	1	1	Total	C	Mg	N	O	0
			164	131	3	12	18	
30	1	1	Total	C	Mg	N	O	0
			164	131	3	12	18	
30	2	1	Total	C	Mg	N	O	0
			272	217	5	20	30	
30	2	1	Total	C	Mg	N	O	0
			272	217	5	20	30	
30	2	1	Total	C	Mg	N	O	0
			272	217	5	20	30	
30	2	1	Total	C	Mg	N	O	0
			272	217	5	20	30	
30	2	1	Total	C	Mg	N	O	0
			272	217	5	20	30	
30	3	1	Total	C	Mg	N	O	0
			164	131	3	12	18	
30	3	1	Total	C	Mg	N	O	0
			164	131	3	12	18	
30	3	1	Total	C	Mg	N	O	0
			164	131	3	12	18	
30	4	1	Total	C	Mg	N	O	0
			202	160	4	16	22	
30	4	1	Total	C	Mg	N	O	0
			202	160	4	16	22	
30	4	1	Total	C	Mg	N	O	0
			202	160	4	16	22	

Continued on next page...

Continued from previous page...

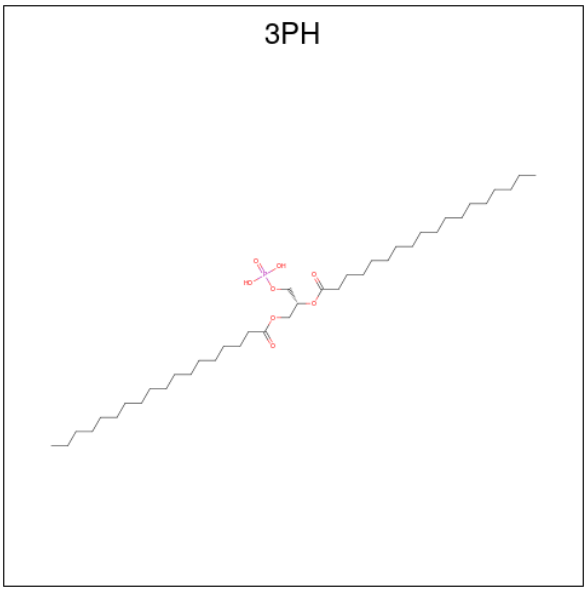
Mol	Chain	Residues	Atoms					AltConf
30	4	1	Total	C	Mg	N	O	0
			202	160	4	16	22	

- Molecule 31 is (3S,5R,6S,3'S,5'R,6'S)-5,6,5',6'-DIEPOXY-5,6,5',6'- TETRAHYDRO-BETA ,BETA-CAROTENE-3,3'-DIOL (three-letter code: XAT) (formula: $C_{40}H_{56}O_4$).



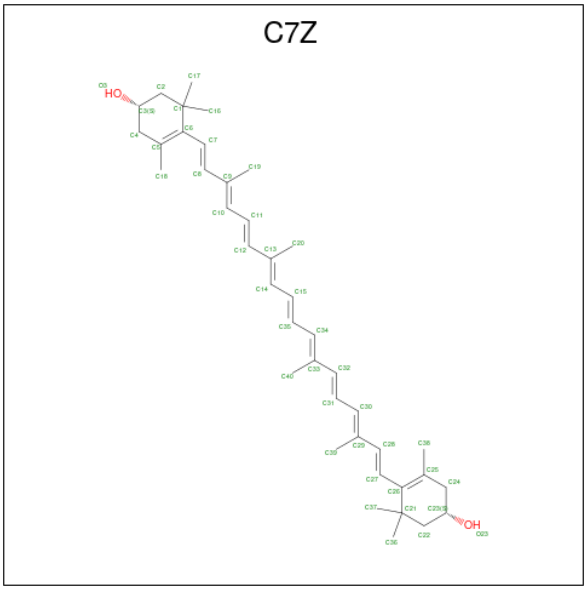
Mol	Chain	Residues	Atoms			AltConf
31	2	1	Total	C	O	0
			44	40	4	
31	4	1	Total	C	O	0
			44	40	4	

- Molecule 32 is 1,2-DIACYL-GLYCEROL-3-SN-PHOSPHATE (three-letter code: 3PH) (formula: $C_{39}H_{77}O_8P$).



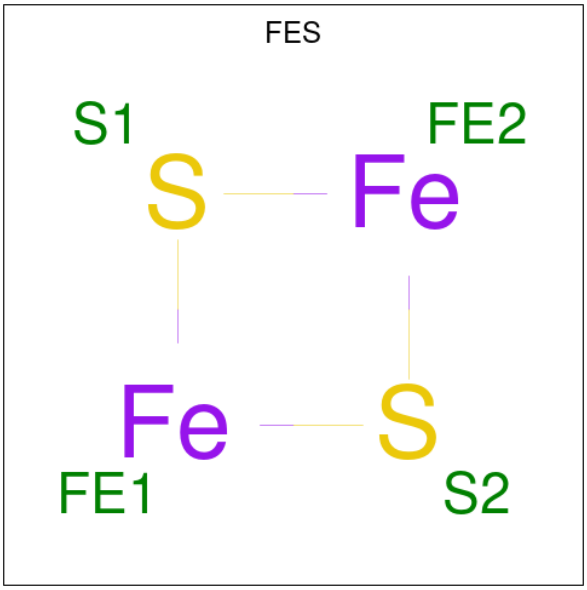
Mol	Chain	Residues	Atoms				AltConf
32	2	1	Total	C	O	P	0
			33	24	8	1	

- Molecule 33 is (1 {S})-3,5,5-trimethyl-4-[(1 {E},3 {E},5 {E},7 {E},9 {E},11 {E},13 {E},15 {E},17 {E})-3,7,12,16-tetramethyl-18-[(4 {S})-2,6,6-trimethyl-4-oxidanyl-cyclohexen-1-yl]octadeca-1,3,5,7,9,11,13,15,17-nonaenyl]cyclohex-3-en-1-ol (three-letter code: C7Z) (formula: $C_{40}H_{56}O_2$).



Mol	Chain	Residues	Atoms			AltConf
33	4	1	Total	C	O	0
			42	40	2	

- Molecule 34 is FE2/S2 (INORGANIC) CLUSTER (three-letter code: FES) (formula: Fe_2S_2).



Mol	Chain	Residues	Atoms			AltConf
			Total	Fe	S	
34	N	1	4	2	2	0

- Molecule 35 is COPPER (II) ION (three-letter code: CU) (formula: Cu).

Mol	Chain	Residues	Atoms		AltConf
			Total	Cu	
35	P	1	1	1	0

- Molecule 36 is water.

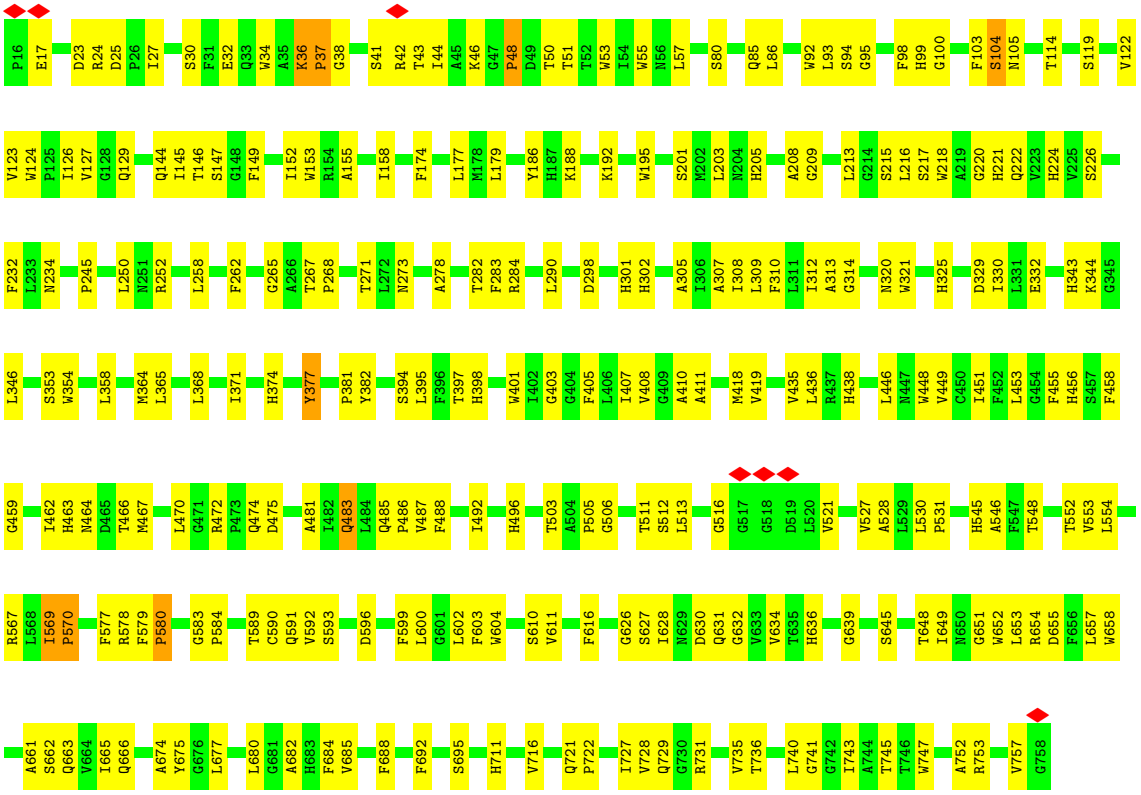
Mol	Chain	Residues	Atoms		AltConf
			Total	O	
36	B	2	2	2	0

3 Residue-property plots (i)

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

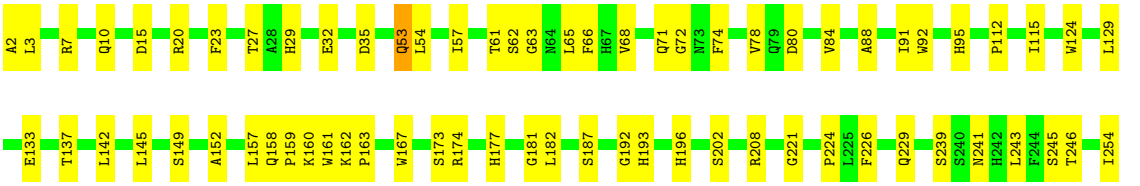
• Molecule 1: Photosystem I P700 chlorophyll a apoprotein A1

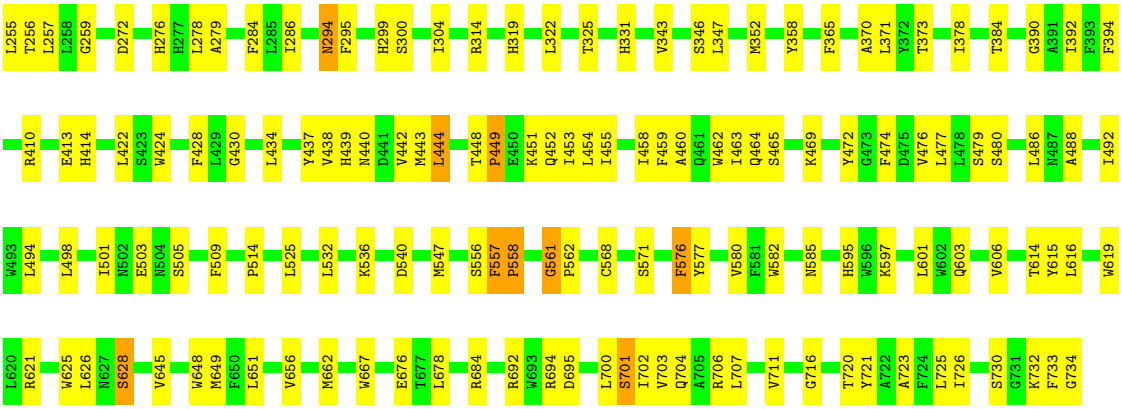
Chain A:



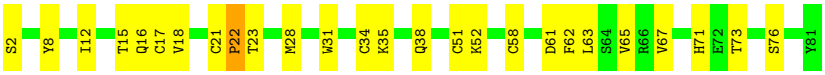
• Molecule 2: Photosystem I P700 chlorophyll a apoprotein A2

Chain B:

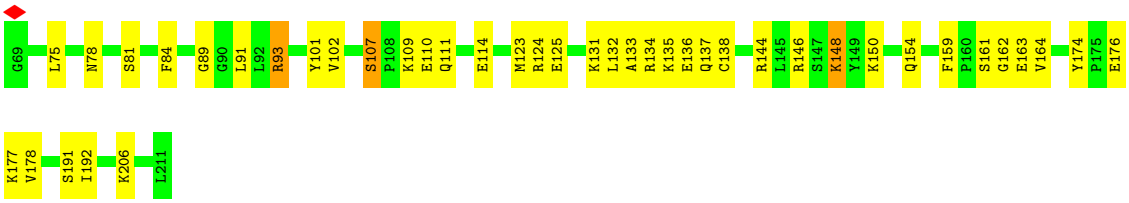




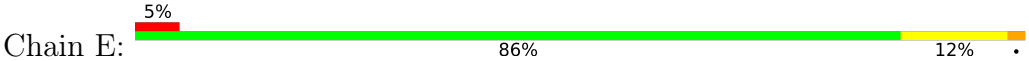
• Molecule 3: Photosystem I iron-sulfur center

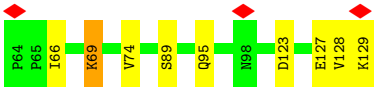


• Molecule 4: PsaD

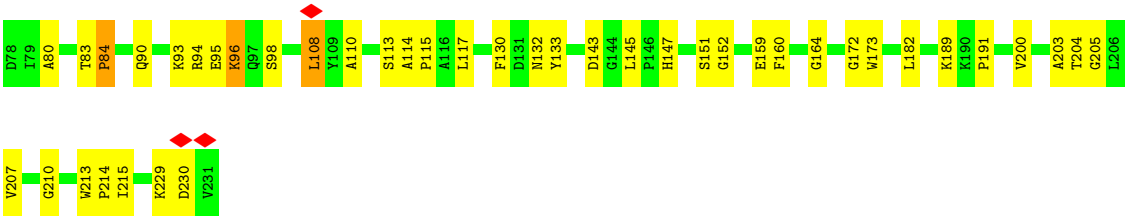


• Molecule 5: PsaE



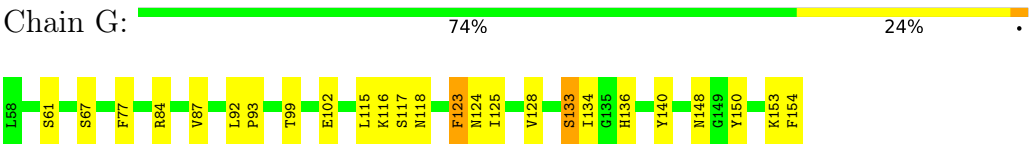


• Molecule 6: PsaF



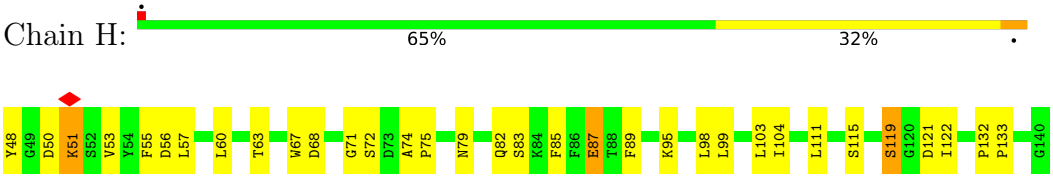
• Molecule 7: PsaG

Chain G:



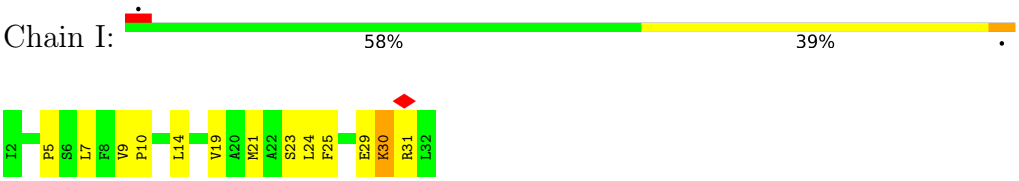
• Molecule 8: PsaH

Chain H:



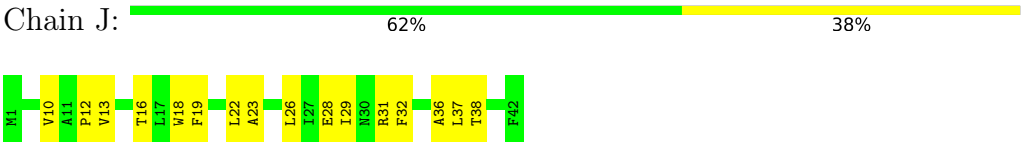
• Molecule 9: Photosystem I reaction center subunit VIII

Chain I:



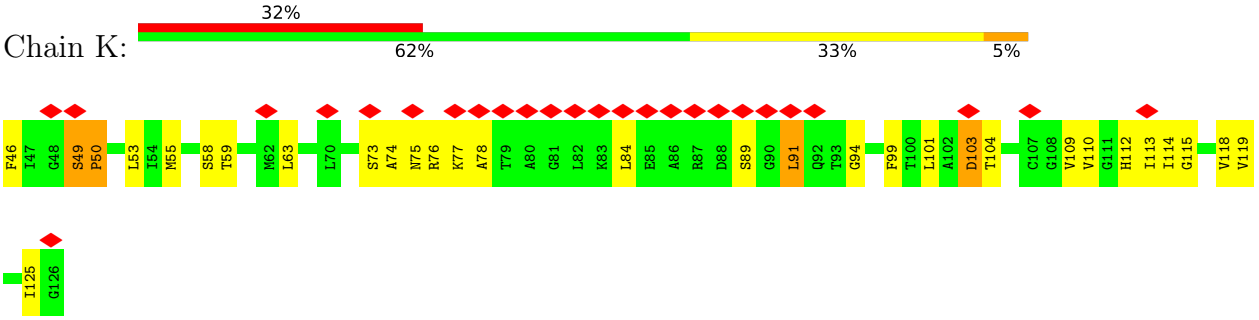
• Molecule 10: PsaJ

Chain J:



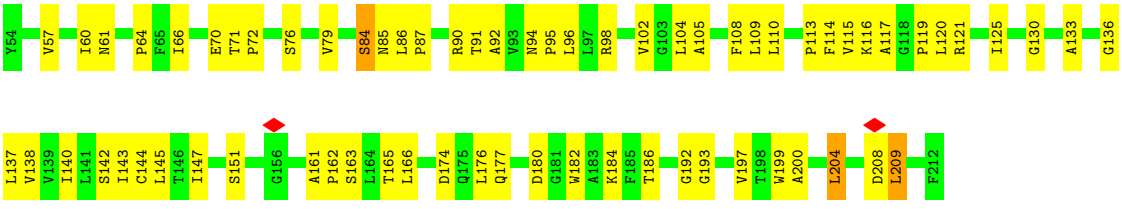
• Molecule 11: Photosystem I reaction center subunit X psaK

Chain K:



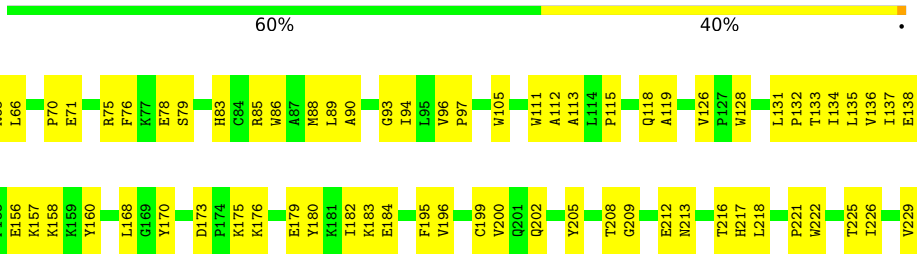
• Molecule 12: PsaL

Chain L:



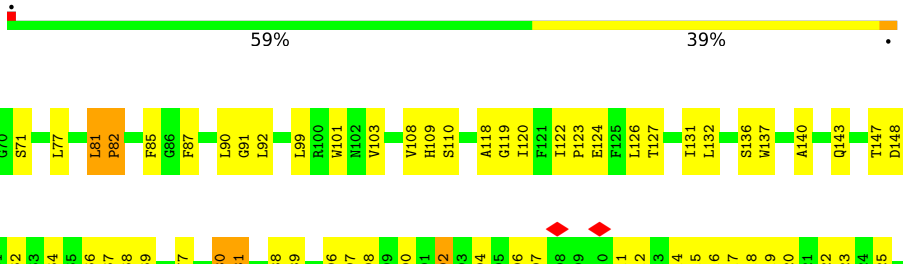
• Molecule 13: Lhca1

Chain 1:



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

Chain 2:

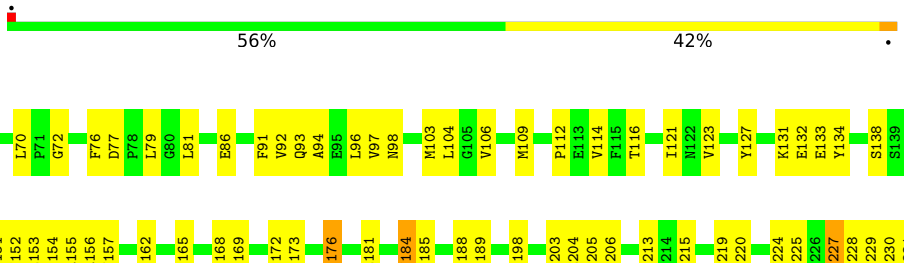


• Molecule 15: Chlorophyll a-b binding protein 3, chloroplastic

Chain 3:

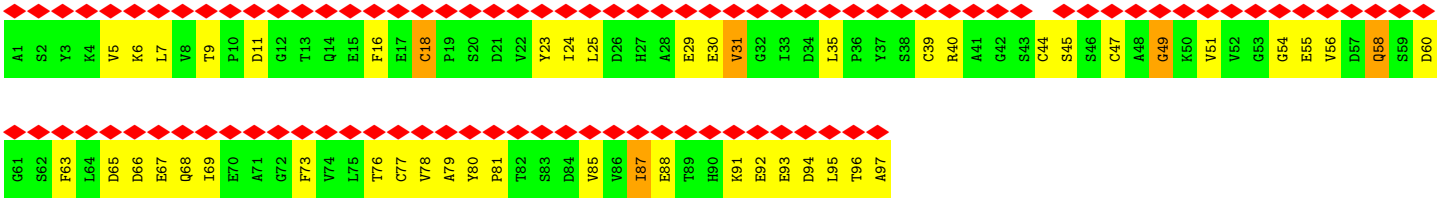
• Molecule 16: Chlorophyll a-b binding protein P4, chloroplastic

Chain 4:



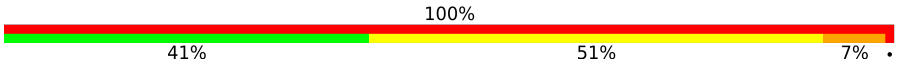
• Molecule 17: Ferredoxin-1, chloroplastic

Chain N:



• Molecule 18: Plastocyanin, chloroplastic

Chain P:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	102216	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	47.05	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	105000	Depositor
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.184	Depositor
Minimum map value	-0.047	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.006	Depositor
Recommended contour level	0.022	Depositor
Map size (Å)	246.6, 246.6, 246.6	wwPDB
Map dimensions	300, 300, 300	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.822, 0.822, 0.822	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 3PH, LUT, C7Z, CA, CL0, SF4, LMG, LHG, CLA, XAT, LMT, CU, DGD, BCR, FES, CHL, PQN

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	0.55	4/6057 (0.1%)	0.51	2/8264 (0.0%)
2	B	0.54	5/6069 (0.1%)	0.51	2/8286 (0.0%)
3	C	0.77	2/625 (0.3%)	0.65	1/846 (0.1%)
4	D	0.42	0/1163	0.52	0/1572
5	E	0.43	0/540	0.49	0/734
6	F	0.65	2/1234 (0.2%)	0.60	1/1670 (0.1%)
7	G	0.40	0/776	0.47	0/1054
8	H	0.47	0/733	0.52	0/995
9	I	0.40	0/246	0.57	0/335
10	J	0.43	0/349	0.46	0/476
11	K	0.48	0/576	0.62	0/779
12	L	0.64	2/1232 (0.2%)	0.62	1/1684 (0.1%)
13	1	0.39	0/1558	0.49	0/2125
14	2	0.68	4/1679 (0.2%)	0.60	2/2302 (0.1%)
15	3	0.49	1/1760 (0.1%)	0.60	1/2390 (0.0%)
16	4	0.50	1/1608 (0.1%)	0.53	0/2191
17	N	0.83	2/736 (0.3%)	1.04	4/1000 (0.4%)
18	P	0.94	3/743 (0.4%)	0.78	1/1009 (0.1%)
All	All	0.56	26/27684 (0.1%)	0.57	15/37712 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
18	P	0	2

The worst 5 of 26 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	37	PRO	N-CA	13.91	1.70	1.47
14	2	82	PRO	N-CA	13.88	1.70	1.47
1	A	570	PRO	N-CA	13.70	1.70	1.47
6	F	84	PRO	N-CA	13.69	1.70	1.47
2	B	449	PRO	N-CA	13.62	1.70	1.47

The worst 5 of 15 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
17	N	49	GLY	O-C-N	-12.13	103.28	122.70
17	N	40	ARG	NE-CZ-NH2	-9.45	115.58	120.30
2	B	558	PRO	CA-N-CD	-9.05	98.83	111.50
17	N	49	GLY	C-N-CA	8.93	144.01	121.70
1	A	570	PRO	CA-N-CD	-8.19	100.04	111.50

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
18	P	15	VAL	Peptide
18	P	35	PHE	Peptide

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	5858	0	5719	345	0
2	B	5857	0	5653	223	0
3	C	612	0	591	28	0
4	D	1132	0	1141	47	0
5	E	528	0	528	5	0
6	F	1206	0	1231	48	0
7	G	757	0	743	22	0
8	H	712	0	701	37	0
9	I	240	0	264	31	0
10	J	338	0	345	31	0
11	K	569	0	596	41	0
12	L	1197	0	1197	92	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
13	1	1508	0	1489	118	0
14	2	1620	0	1557	132	0
15	3	1706	0	1661	124	0
16	4	1559	0	1527	141	0
17	N	724	0	672	71	0
18	P	728	0	699	85	0
19	A	65	0	72	12	0
20	1	608	0	563	103	0
20	2	522	0	499	105	0
20	3	578	0	495	70	0
20	4	631	0	595	170	0
20	A	2643	0	2749	387	0
20	B	2610	0	2747	268	0
20	F	130	0	144	20	0
20	G	166	0	153	21	0
20	H	60	0	58	21	0
20	J	50	0	38	7	0
20	K	199	0	158	17	0
20	L	160	0	134	52	0
21	A	33	0	46	7	0
21	B	33	0	46	3	0
22	1	80	0	105	5	0
22	2	40	0	53	24	0
22	3	80	0	105	14	0
22	A	240	0	316	27	0
22	B	200	0	265	20	0
22	F	80	0	105	11	0
22	G	40	0	53	5	0
22	H	40	0	53	21	0
22	I	80	0	105	17	0
22	J	40	0	53	5	0
22	K	80	0	106	17	0
22	L	80	0	106	47	0
23	1	49	0	74	11	0
23	2	35	0	40	7	0
23	3	17	0	12	0	0
23	4	35	0	40	11	0
23	A	89	0	127	3	0
23	B	70	0	86	6	0
24	2	35	0	46	8	0
24	A	35	0	45	1	0
24	B	63	0	68	1	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
24	G	66	0	79	0	0
25	A	8	0	0	0	0
25	C	16	0	0	3	0
26	1	46	0	65	8	0
26	2	134	0	133	17	0
26	3	30	0	30	0	0
26	A	50	0	73	3	0
26	B	102	0	114	16	0
26	F	160	0	188	7	0
26	G	124	0	161	14	0
27	A	1	0	0	0	0
27	B	1	0	0	0	0
28	1	41	0	40	1	0
28	3	51	0	60	3	0
28	4	51	0	60	4	0
28	B	61	0	83	7	0
28	F	57	0	75	18	0
28	G	47	0	52	3	0
28	J	58	0	77	10	0
29	1	84	0	110	40	0
29	2	42	0	55	13	0
29	3	84	0	110	9	0
29	4	42	0	55	20	0
29	J	42	0	55	10	0
30	1	164	0	134	32	0
30	2	272	0	223	50	0
30	3	164	0	136	13	0
30	4	202	0	152	11	0
31	2	44	0	56	14	0
31	4	44	0	56	14	0
32	2	33	0	39	5	0
33	4	42	0	0	4	0
34	N	4	0	0	0	0
35	P	1	0	0	0	0
36	B	2	0	0	0	0
All	All	39217	0	39245	2384	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 30.

The worst 5 of 2384 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:558:PRO:N	2:B:558:PRO:CA	1.69	1.44
14:2:181:PRO:CA	14:2:181:PRO:N	1.70	1.43
6:F:84:PRO:N	6:F:84:PRO:CA	1.70	1.41
1:A:570:PRO:N	1:A:570:PRO:CA	1.70	1.41
3:C:22:PRO:CA	3:C:22:PRO:N	1.69	1.38

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	741/743 (100%)	713 (96%)	25 (3%)	3 (0%)	34 60
2	B	731/733 (100%)	700 (96%)	31 (4%)	0	100 100
3	C	78/80 (98%)	77 (99%)	1 (1%)	0	100 100
4	D	141/143 (99%)	136 (96%)	5 (4%)	0	100 100
5	E	64/66 (97%)	58 (91%)	6 (9%)	0	100 100
6	F	152/154 (99%)	145 (95%)	7 (5%)	0	100 100
7	G	95/97 (98%)	92 (97%)	3 (3%)	0	100 100
8	H	91/93 (98%)	83 (91%)	7 (8%)	1 (1%)	14 34
9	I	29/31 (94%)	26 (90%)	3 (10%)	0	100 100
10	J	40/42 (95%)	40 (100%)	0	0	100 100
11	K	79/81 (98%)	71 (90%)	6 (8%)	2 (2%)	5 14
12	L	157/159 (99%)	146 (93%)	10 (6%)	1 (1%)	25 50
13	1	191/193 (99%)	185 (97%)	6 (3%)	0	100 100
14	2	206/208 (99%)	190 (92%)	15 (7%)	1 (0%)	29 54
15	3	219/221 (99%)	197 (90%)	22 (10%)	0	100 100
16	4	196/198 (99%)	188 (96%)	8 (4%)	0	100 100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
17	N	95/97 (98%)	82 (86%)	11 (12%)	2 (2%)	7 18
18	P	97/99 (98%)	85 (88%)	10 (10%)	2 (2%)	7 18
All	All	3402/3438 (99%)	3214 (94%)	176 (5%)	12 (0%)	38 60

5 of 12 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	639	GLY
11	K	50	PRO
12	L	209	LEU
17	N	66	ASP
1	A	580	PRO

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	604/604 (100%)	589 (98%)	15 (2%)	47 76
2	B	598/598 (100%)	580 (97%)	18 (3%)	41 70
3	C	69/69 (100%)	68 (99%)	1 (1%)	67 86
4	D	122/122 (100%)	115 (94%)	7 (6%)	20 44
5	E	58/58 (100%)	56 (97%)	2 (3%)	37 66
6	F	125/126 (99%)	123 (98%)	2 (2%)	62 85
7	G	82/82 (100%)	78 (95%)	4 (5%)	25 52
8	H	75/75 (100%)	71 (95%)	4 (5%)	22 48
9	I	27/27 (100%)	25 (93%)	2 (7%)	13 32
10	J	35/35 (100%)	35 (100%)	0	100 100
11	K	59/59 (100%)	57 (97%)	2 (3%)	37 66
12	L	126/126 (100%)	121 (96%)	5 (4%)	31 60
13	1	158/158 (100%)	154 (98%)	4 (2%)	47 76
14	2	167/167 (100%)	165 (99%)	2 (1%)	71 88

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
15	3	171/172 (99%)	166 (97%)	5 (3%)	42 71
16	4	164/164 (100%)	156 (95%)	8 (5%)	25 52
17	N	82/82 (100%)	78 (95%)	4 (5%)	25 52
18	P	79/79 (100%)	76 (96%)	3 (4%)	33 62
All	All	2801/2803 (100%)	2713 (97%)	88 (3%)	43 69

5 of 88 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
12	L	79	VAL
15	3	236	LEU
12	L	151	SER
13	1	175	LYS
16	4	133	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 8 such sidechains are listed below:

Mol	Chain	Res	Type
18	P	95	GLN
17	N	58	GLN
12	L	61	ASN
8	H	79	ASN
14	2	238	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 244 ligands modelled in this entry, 3 are monoatomic - leaving 241 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	$\#\|Z\| > 2$
20	CLA	B	1213	-	60,68,73	1.44	7 (11%)	70,107,113	2.01	16 (22%)
20	CLA	4	603	-	65,73,73	1.33	7 (10%)	76,113,113	1.88	15 (19%)
20	CLA	3	605	-	55,63,73	1.49	7 (12%)	64,101,113	2.20	19 (29%)
20	CLA	K	1404	11	46,54,73	1.61	9 (19%)	53,90,113	2.09	12 (22%)
26	LMG	3	802	-	30,30,55	0.56	0	38,38,63	1.14	3 (7%)
20	CLA	A	1137	-	65,73,73	1.39	7 (10%)	76,113,113	1.98	16 (21%)
22	BCR	A	4017	-	41,41,41	1.84	5 (12%)	56,56,56	4.79	19 (33%)
30	CHL	3	604	-	66,74,74	0.89	2 (3%)	73,114,114	1.39	9 (12%)
23	LHG	4	801	-	34,34,48	0.42	0	37,40,54	1.14	3 (8%)
20	CLA	A	1131	-	65,73,73	1.39	8 (12%)	76,113,113	1.97	17 (22%)
22	BCR	K	4001	-	41,41,41	1.87	4 (9%)	56,56,56	4.35	15 (26%)
22	BCR	A	4007	-	41,41,41	1.87	6 (14%)	56,56,56	4.37	16 (28%)
20	CLA	L	1503	-	50,58,73	1.53	7 (14%)	58,95,113	2.19	17 (29%)
20	CLA	L	1501	12	50,58,73	1.52	8 (16%)	58,95,113	2.22	16 (27%)
20	CLA	2	606	-	50,58,73	1.53	7 (14%)	58,95,113	2.24	18 (31%)
22	BCR	2	503	-	41,41,41	1.95	5 (12%)	56,56,56	5.26	27 (48%)
30	CHL	1	609	13	56,64,74	0.93	3 (5%)	61,102,114	1.41	10 (16%)
31	XAT	4	502	-	39,47,47	0.78	1 (2%)	54,74,74	2.07	13 (24%)
20	CLA	B	1023	-	65,73,73	1.42	9 (13%)	76,113,113	1.92	16 (21%)
20	CLA	B	1240	23	65,73,73	1.39	8 (12%)	76,113,113	2.10	21 (27%)
30	CHL	2	611	-	48,56,74	1.00	3 (6%)	51,92,114	1.55	11 (21%)
25	SF4	C	3002	3	0,12,12	-	-	-		
26	LMG	2	805	-	30,30,55	0.52	0	38,38,63	1.08	2 (5%)
20	CLA	G	1601	-	55,63,73	1.51	6 (10%)	64,101,113	2.10	19 (29%)
29	LUT	3	502	-	42,43,43	2.32	1 (2%)	51,60,60	2.10	13 (25%)
30	CHL	2	610	-	56,64,74	0.89	3 (5%)	61,102,114	1.41	11 (18%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
20	CLA	A	1132	-	65,73,73	1.34	7 (10%)	76,113,113	2.00	16 (21%)
20	CLA	1	607	-	46,54,73	1.62	7 (15%)	53,90,113	2.12	13 (24%)
22	BCR	H	4021	-	41,41,41	1.87	4 (9%)	56,56,56	4.40	17 (30%)
26	LMG	F	5003	-	36,36,55	0.72	1 (2%)	44,44,63	1.08	3 (6%)
22	BCR	J	4012	-	41,41,41	1.85	4 (9%)	56,56,56	4.21	19 (33%)
20	CLA	A	1136	-	65,73,73	1.39	7 (10%)	76,113,113	1.90	16 (21%)
20	CLA	A	1134	1	55,63,73	1.50	7 (12%)	64,101,113	2.08	14 (21%)
20	CLA	B	1230	-	58,66,73	1.44	7 (12%)	67,104,113	2.15	18 (26%)
20	CLA	A	1106	1	65,73,73	1.38	8 (12%)	76,113,113	2.03	19 (25%)
20	CLA	B	1232	-	55,63,73	1.53	7 (12%)	64,101,113	2.15	19 (29%)
20	CLA	A	1122	-	65,73,73	1.39	7 (10%)	76,113,113	1.95	14 (18%)
20	CLA	A	1103	-	65,73,73	1.37	8 (12%)	76,113,113	2.11	19 (25%)
24	LMT	B	5008	-	32,32,36	1.31	6 (18%)	43,43,47	1.02	3 (6%)
20	CLA	3	613	-	46,54,73	1.59	7 (15%)	53,90,113	2.17	14 (26%)
20	CLA	4	602	-	50,58,73	1.52	8 (16%)	58,95,113	2.12	16 (27%)
20	CLA	3	602	-	52,60,73	1.53	8 (15%)	60,97,113	2.24	18 (30%)
20	CLA	B	1239	-	65,73,73	1.42	7 (10%)	76,113,113	1.98	19 (25%)
30	CHL	4	610	-	47,55,74	1.16	5 (10%)	50,91,114	1.56	12 (24%)
20	CLA	A	1124	-	55,63,73	1.50	8 (14%)	64,101,113	2.13	17 (26%)
20	CLA	3	614	-	42,50,73	1.68	7 (16%)	48,85,113	2.27	13 (27%)
22	BCR	L	4020	-	41,41,41	1.87	4 (9%)	56,56,56	4.45	18 (32%)
20	CLA	B	1214	-	65,73,73	1.41	8 (12%)	76,113,113	2.01	16 (21%)
20	CLA	B	1206	2	65,73,73	1.39	7 (10%)	76,113,113	2.00	17 (22%)
20	CLA	A	1105	-	60,68,73	1.42	8 (13%)	70,107,113	2.13	17 (24%)
26	LMG	B	5003	-	35,35,55	0.73	1 (2%)	43,43,63	1.13	3 (6%)
20	CLA	A	1126	-	65,73,73	1.42	8 (12%)	76,113,113	1.95	16 (21%)
20	CLA	A	1108	-	50,58,73	1.60	8 (16%)	58,95,113	2.21	19 (32%)
20	CLA	1	601	13	65,73,73	1.36	7 (10%)	76,113,113	2.07	20 (26%)
20	CLA	A	1114	-	46,54,73	1.64	7 (15%)	53,90,113	2.16	14 (26%)
20	CLA	B	1237	-	65,73,73	1.35	7 (10%)	76,113,113	2.05	20 (26%)
20	CLA	1	614	13	60,68,73	1.44	7 (11%)	70,107,113	2.07	17 (24%)
26	LMG	B	5007	-	34,34,55	0.50	0	42,42,63	1.07	3 (7%)
23	LHG	A	5002	-	48,48,48	0.38	0	51,54,54	1.13	5 (9%)
20	CLA	1	613	-	45,53,73	1.68	7 (15%)	52,89,113	2.02	13 (25%)
33	C7Z	4	505	-	43,43,43	5.25	17 (39%)	58,60,60	5.54	32 (55%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
23	LHG	A	5001	20	39,39,48	0.45	0	42,45,54	1.25	4 (9%)
20	CLA	3	617	-	60,68,73	1.38	7 (11%)	70,107,113	2.03	17 (24%)
20	CLA	A	1117	-	65,73,73	1.39	8 (12%)	76,113,113	1.93	16 (21%)
20	CLA	2	603	14	65,73,73	1.37	9 (13%)	76,113,113	1.99	18 (23%)
24	LMT	G	5004	-	36,36,36	1.20	6 (16%)	47,47,47	1.05	3 (6%)
29	LUT	1	501	-	42,43,43	2.38	2 (4%)	51,60,60	2.02	16 (31%)
22	BCR	3	506	-	41,41,41	1.92	4 (9%)	56,56,56	4.40	18 (32%)
20	CLA	B	1204	-	65,73,73	1.38	8 (12%)	76,113,113	2.01	17 (22%)
20	CLA	2	607	23	60,68,73	1.38	6 (10%)	70,107,113	2.13	19 (27%)
30	CHL	1	610	13	47,55,74	1.12	4 (8%)	50,91,114	1.31	8 (16%)
20	CLA	B	1201	-	65,73,73	1.36	7 (10%)	76,113,113	1.99	15 (19%)
20	CLA	4	607	-	60,68,73	1.40	8 (13%)	70,107,113	2.03	18 (25%)
20	CLA	J	1901	10	50,58,73	1.55	9 (18%)	58,95,113	2.25	17 (29%)
20	CLA	B	1203	-	65,73,73	1.37	7 (10%)	76,113,113	1.96	17 (22%)
20	CLA	1	604	-	65,73,73	1.36	7 (10%)	76,113,113	1.99	17 (22%)
20	CLA	1	605	-	65,73,73	1.34	7 (10%)	76,113,113	2.17	18 (23%)
23	LHG	3	801	30	16,16,48	0.83	1 (6%)	17,20,54	0.68	0
20	CLA	4	608	-	46,54,73	1.58	8 (17%)	53,90,113	2.18	15 (28%)
28	DGD	J	5001	-	59,59,67	1.06	6 (10%)	73,73,81	1.02	2 (2%)
22	BCR	I	4020	-	41,41,41	1.86	4 (9%)	56,56,56	4.36	16 (28%)
28	DGD	4	802	-	52,52,67	0.89	2 (3%)	66,66,81	1.03	2 (3%)
20	CLA	A	1119	-	65,73,73	1.39	8 (12%)	76,113,113	2.01	20 (26%)
24	LMT	B	5006	-	33,33,36	1.24	6 (18%)	44,44,47	1.00	3 (6%)
20	CLA	G	1603	-	65,73,73	1.37	9 (13%)	76,113,113	2.16	18 (23%)
30	CHL	4	615	-	43,51,74	1.03	2 (4%)	45,86,114	1.41	9 (20%)
20	CLA	1	603	-	55,63,73	1.49	7 (12%)	64,101,113	2.20	19 (29%)
20	CLA	A	1012	-	65,73,73	1.42	7 (10%)	76,113,113	2.01	15 (19%)
20	CLA	A	1130	-	55,63,73	1.47	7 (12%)	64,101,113	2.10	18 (28%)
20	CLA	K	1402	-	60,68,73	1.40	8 (13%)	70,107,113	2.09	19 (27%)
22	BCR	B	4004	-	41,41,41	1.93	4 (9%)	56,56,56	4.84	23 (41%)
22	BCR	G	4011	-	41,41,41	1.87	4 (9%)	56,56,56	4.56	18 (32%)
26	LMG	2	802	-	25,25,55	0.53	0	33,33,63	1.27	3 (9%)
20	CLA	A	1127	-	65,73,73	1.40	9 (13%)	76,113,113	1.96	18 (23%)
28	DGD	B	5005	-	62,62,67	1.11	6 (9%)	76,76,81	1.03	4 (5%)
20	CLA	4	601	16	60,68,73	1.39	7 (11%)	70,107,113	2.01	16 (22%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
20	CLA	A	1115	-	65,73,73	1.37	7 (10%)	76,113,113	2.02	13 (17%)
20	CLA	A	1113	-	45,53,73	1.62	7 (15%)	52,89,113	2.17	15 (28%)
20	CLA	A	1121	-	60,68,73	1.45	7 (11%)	70,107,113	2.08	16 (22%)
20	CLA	A	1138	-	65,73,73	1.38	8 (12%)	76,113,113	1.93	15 (19%)
20	CLA	B	1205	-	65,73,73	1.38	7 (10%)	76,113,113	2.03	18 (23%)
22	BCR	B	4010	-	41,41,41	1.84	5 (12%)	56,56,56	4.26	15 (26%)
26	LMG	A	5006	-	50,50,55	1.04	5 (10%)	58,58,63	1.19	3 (5%)
20	CLA	L	1502	-	60,68,73	1.38	7 (11%)	70,107,113	2.06	17 (24%)
20	CLA	B	1212	-	55,63,73	1.48	8 (14%)	64,101,113	2.17	16 (25%)
26	LMG	F	5001	-	30,30,55	0.52	0	38,38,63	1.21	2 (5%)
20	CLA	2	608	-	50,58,73	1.60	7 (14%)	58,95,113	2.33	17 (29%)
20	CLA	B	1217	-	46,54,73	1.64	7 (15%)	53,90,113	2.17	13 (24%)
26	LMG	F	5006	-	13,13,55	0.54	0	18,18,63	0.77	0
30	CHL	2	613	-	46,54,74	1.00	3 (6%)	49,90,114	1.48	9 (18%)
26	LMG	G	5006	-	25,25,55	0.56	0	33,33,63	1.34	4 (12%)
29	LUT	J	4013	-	42,43,43	2.26	2 (4%)	51,60,60	2.41	18 (35%)
30	CHL	3	607	23	51,59,74	0.99	3 (5%)	55,96,114	1.39	10 (18%)
34	FES	N	101	17	0,4,4	-	-	-		
20	CLA	4	606	-	50,58,73	1.55	6 (12%)	58,95,113	2.23	19 (32%)
21	PQN	A	2001	-	34,34,34	0.37	0	42,45,45	1.26	4 (9%)
26	LMG	2	804	-	30,30,55	0.54	0	38,38,63	1.14	3 (7%)
20	CLA	B	1238	36	65,73,73	1.33	8 (12%)	76,113,113	1.98	15 (19%)
26	LMG	F	5002	-	47,47,55	0.97	4 (8%)	55,55,63	1.20	4 (7%)
20	CLA	G	1602	-	46,54,73	1.65	7 (15%)	53,90,113	2.14	17 (32%)
26	LMG	F	5004	-	34,34,55	0.46	0	42,42,63	1.12	2 (4%)
20	CLA	A	1116	-	56,64,73	1.50	8 (14%)	65,102,113	2.11	17 (26%)
26	LMG	1	802	-	46,46,55	0.94	3 (6%)	54,54,63	1.07	2 (3%)
20	CLA	1	606	-	50,58,73	1.57	7 (14%)	58,95,113	2.25	20 (34%)
20	CLA	A	1013	-	65,73,73	1.40	7 (10%)	76,113,113	1.94	20 (26%)
20	CLA	A	1140	-	65,73,73	1.38	7 (10%)	76,113,113	1.94	17 (22%)
26	LMG	B	5004	-	33,33,55	0.54	0	41,41,63	1.32	6 (14%)
22	BCR	K	4002	-	41,41,41	1.87	4 (9%)	56,56,56	4.47	18 (32%)
20	CLA	B	1231	-	60,68,73	1.45	8 (13%)	70,107,113	2.10	15 (21%)
23	LHG	B	5001	20	20,20,48	0.59	0	23,26,54	1.48	2 (8%)
20	CLA	3	601	-	55,63,73	1.46	7 (12%)	64,101,113	2.24	21 (32%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
20	CLA	A	1125	-	65,73,73	1.38	8 (12%)	76,113,113	2.09	20 (26%)
20	CLA	B	1215	-	65,73,73	1.37	8 (12%)	76,113,113	2.12	20 (26%)
20	CLA	2	601	-	60,68,73	1.43	7 (11%)	70,107,113	1.96	16 (22%)
20	CLA	B	1208	-	60,68,73	1.44	7 (11%)	70,107,113	1.96	14 (20%)
20	CLA	A	1118	-	50,58,73	1.56	7 (14%)	58,95,113	2.33	18 (31%)
20	CLA	2	612	-	55,63,73	1.46	7 (12%)	64,101,113	2.13	16 (25%)
20	CLA	K	1403	-	48,56,73	1.58	7 (14%)	55,92,113	2.22	16 (29%)
22	BCR	3	503	-	41,41,41	1.83	4 (9%)	56,56,56	4.41	17 (30%)
20	CLA	H	1701	8	60,68,73	1.39	8 (13%)	70,107,113	2.01	16 (22%)
23	LHG	1	801	-	48,48,48	0.44	0	51,54,54	1.20	3 (5%)
20	CLA	B	1221	-	65,73,73	1.39	7 (10%)	76,113,113	2.09	22 (28%)
29	LUT	2	501	-	42,43,43	2.34	3 (7%)	51,60,60	2.42	17 (33%)
20	CLA	A	1129	-	65,73,73	1.38	7 (10%)	76,113,113	2.00	16 (21%)
20	CLA	4	605	-	60,68,73	1.46	7 (11%)	70,107,113	2.01	19 (27%)
20	CLA	A	1109	-	65,73,73	1.36	7 (10%)	76,113,113	2.01	18 (23%)
22	BCR	F	4016	-	41,41,41	1.87	5 (12%)	56,56,56	4.29	15 (26%)
20	CLA	B	1209	-	46,54,73	1.56	7 (15%)	53,90,113	2.14	13 (24%)
22	BCR	B	4005	-	41,41,41	1.86	4 (9%)	56,56,56	4.33	17 (30%)
22	BCR	1	504	-	41,41,41	1.90	4 (9%)	56,56,56	4.66	14 (25%)
20	CLA	A	1141	23	60,68,73	1.40	7 (11%)	70,107,113	2.02	18 (25%)
20	CLA	B	1222	36	65,73,73	1.37	8 (12%)	76,113,113	2.06	20 (26%)
20	CLA	2	604	14	65,73,73	1.34	8 (12%)	76,113,113	1.97	17 (22%)
20	CLA	A	1101	-	65,73,73	1.33	8 (12%)	76,113,113	2.01	17 (22%)
20	CLA	K	1401	-	45,53,73	1.60	7 (15%)	52,89,113	2.16	13 (25%)
20	CLA	A	1123	-	65,73,73	1.35	7 (10%)	76,113,113	2.00	19 (25%)
20	CLA	B	1219	-	65,73,73	1.35	8 (12%)	76,113,113	2.02	17 (22%)
20	CLA	B	1220	-	55,63,73	1.50	8 (14%)	64,101,113	2.08	13 (20%)
22	BCR	1	503	-	41,41,41	1.86	4 (9%)	56,56,56	4.19	14 (25%)
23	LHG	B	5002	-	48,48,48	0.40	0	51,54,54	1.10	3 (5%)
20	CLA	B	1202	-	65,73,73	1.37	7 (10%)	76,113,113	1.99	19 (25%)
20	CLA	4	604	-	60,68,73	1.40	8 (13%)	70,107,113	2.06	16 (22%)
22	BCR	B	4009	-	41,41,41	1.82	4 (9%)	56,56,56	4.20	14 (25%)
24	LMT	2	808	-	36,36,36	0.41	0	47,47,47	0.73	1 (2%)
23	LHG	2	801	20	34,34,48	0.44	0	37,40,54	1.13	2 (5%)
28	DGD	G	5003	-	48,48,67	0.84	1 (2%)	62,62,81	1.01	2 (3%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
20	CLA	B	1216	-	65,73,73	1.36	7 (10%)	76,113,113	1.92	16 (21%)
20	CLA	A	1120	-	60,68,73	1.44	7 (11%)	70,107,113	2.01	14 (20%)
20	CLA	B	1226	-	65,73,73	1.40	7 (10%)	76,113,113	2.11	18 (23%)
22	BCR	A	4008	-	41,41,41	1.87	6 (14%)	56,56,56	4.05	17 (30%)
30	CHL	4	613	-	61,69,74	1.08	4 (6%)	67,108,114	1.38	12 (17%)
20	CLA	B	1021	-	65,73,73	1.40	9 (13%)	76,113,113	2.03	19 (25%)
29	LUT	1	502	-	42,43,43	2.40	2 (4%)	51,60,60	2.15	11 (21%)
22	BCR	A	4003	-	41,41,41	1.86	4 (9%)	56,56,56	4.23	20 (35%)
30	CHL	1	612	-	61,69,74	1.05	4 (6%)	67,108,114	1.37	11 (16%)
20	CLA	B	1225	-	65,73,73	1.38	8 (12%)	76,113,113	2.00	18 (23%)
20	CLA	B	1211	-	65,73,73	1.37	8 (12%)	76,113,113	2.07	19 (25%)
20	CLA	A	1112	-	65,73,73	1.39	7 (10%)	76,113,113	1.96	18 (23%)
21	PQN	B	2002	-	34,34,34	0.41	0	42,45,45	1.28	4 (9%)
20	CLA	B	1224	-	65,73,73	1.39	7 (10%)	76,113,113	2.01	16 (21%)
20	CLA	B	1235	-	65,73,73	1.36	7 (10%)	76,113,113	2.02	20 (26%)
20	CLA	B	1228	-	60,68,73	1.41	7 (11%)	70,107,113	2.05	14 (20%)
20	CLA	A	1107	1	65,73,73	1.35	7 (10%)	76,113,113	2.09	19 (25%)
22	BCR	B	4006	-	41,41,41	1.87	4 (9%)	56,56,56	4.24	21 (37%)
20	CLA	3	612	-	50,58,73	1.53	8 (16%)	58,95,113	2.20	15 (25%)
28	DGD	F	5005	-	58,58,67	1.05	4 (6%)	72,72,81	1.12	5 (6%)
20	CLA	F	1302	6	65,73,73	1.37	7 (10%)	76,113,113	1.92	14 (18%)
20	CLA	3	603	15	55,63,73	1.50	7 (12%)	64,101,113	2.19	18 (28%)
22	BCR	A	4011	-	41,41,41	1.86	5 (12%)	56,56,56	4.30	19 (33%)
20	CLA	A	1111	-	65,73,73	1.38	8 (12%)	76,113,113	2.06	19 (25%)
22	BCR	L	4019	-	41,41,41	1.92	4 (9%)	56,56,56	4.38	17 (30%)
20	CLA	A	1135	-	51,59,73	1.55	7 (13%)	59,96,113	2.25	17 (28%)
32	3PH	2	807	-	32,32,47	1.01	4 (12%)	36,37,52	1.20	2 (5%)
20	CLA	2	602	-	52,60,73	1.51	8 (15%)	60,97,113	2.15	17 (28%)
24	LMT	G	5005	-	32,32,36	1.23	5 (15%)	43,43,47	1.02	2 (4%)
20	CLA	B	1022	-	65,73,73	1.44	8 (12%)	76,113,113	1.94	16 (21%)
26	LMG	G	5001	-	49,49,55	1.00	4 (8%)	57,57,63	1.17	5 (8%)
26	LMG	G	5002	-	50,50,55	1.06	4 (8%)	58,58,63	1.21	4 (6%)
20	CLA	B	1210	-	65,73,73	1.42	8 (12%)	76,113,113	2.09	21 (27%)
20	CLA	B	1218	-	65,73,73	1.37	7 (10%)	76,113,113	2.00	16 (21%)
20	CLA	A	1110	-	55,63,73	1.51	7 (12%)	64,101,113	2.17	19 (29%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
20	CLA	1	602	13	46,54,73	1.63	8 (17%)	53,90,113	2.07	14 (26%)
20	CLA	4	612	-	65,73,73	1.34	8 (12%)	76,113,113	1.98	16 (21%)
20	CLA	B	1207	-	65,73,73	1.34	7 (10%)	76,113,113	1.99	17 (22%)
20	CLA	B	1223	-	65,73,73	1.36	8 (12%)	76,113,113	2.06	19 (25%)
20	CLA	F	1301	-	65,73,73	1.36	8 (12%)	76,113,113	2.00	17 (22%)
22	BCR	A	4002	-	41,41,41	1.85	5 (12%)	56,56,56	4.24	17 (30%)
30	CHL	2	615	-	56,64,74	0.92	3 (5%)	61,102,114	1.44	13 (21%)
22	BCR	F	4014	-	41,41,41	1.84	4 (9%)	56,56,56	4.27	17 (30%)
31	XAT	2	502	-	39,47,47	0.80	1 (2%)	54,74,74	2.23	15 (27%)
30	CHL	2	609	-	66,74,74	0.85	3 (4%)	73,114,114	1.33	12 (16%)
28	DGD	3	803	-	52,52,67	0.89	2 (3%)	66,66,81	1.14	4 (6%)
20	CLA	B	1227	-	65,73,73	1.37	7 (10%)	76,113,113	1.99	18 (23%)
20	CLA	A	1139	-	65,73,73	1.38	8 (12%)	76,113,113	2.02	18 (23%)
26	LMG	2	803	-	36,36,55	0.64	1 (2%)	44,44,63	1.05	3 (6%)
20	CLA	A	1128	-	65,73,73	1.40	7 (10%)	76,113,113	2.07	18 (23%)
28	DGD	1	803	-	42,42,67	0.86	1 (2%)	56,56,81	1.05	3 (5%)
26	LMG	2	806	-	13,13,55	0.57	0	18,18,63	0.56	0
30	CHL	3	611	-	47,55,74	1.17	3 (6%)	50,91,114	1.54	11 (22%)
20	CLA	B	1229	-	65,73,73	1.37	8 (12%)	76,113,113	2.06	20 (26%)
20	CLA	B	1236	-	50,58,73	1.57	7 (14%)	58,95,113	2.26	17 (29%)
25	SF4	C	3003	3	0,12,12	-	-	-		
20	CLA	1	611	-	65,73,73	1.35	7 (10%)	76,113,113	2.02	16 (21%)
24	LMT	A	5004	-	36,36,36	1.21	7 (19%)	47,47,47	1.08	3 (6%)
30	CHL	4	611	-	51,59,74	1.05	3 (5%)	55,96,114	1.46	12 (21%)
20	CLA	4	617	-	65,73,73	1.32	8 (12%)	76,113,113	2.04	15 (19%)
22	BCR	I	4018	-	41,41,41	1.94	4 (9%)	56,56,56	3.88	19 (33%)
20	CLA	3	608	-	48,56,73	1.55	8 (16%)	55,92,113	2.19	16 (29%)
29	LUT	4	501	-	42,43,43	2.40	4 (9%)	51,60,60	2.17	15 (29%)
29	LUT	3	501	-	42,43,43	2.35	2 (4%)	51,60,60	2.20	18 (35%)
20	CLA	A	1102	-	65,73,73	1.38	7 (10%)	76,113,113	2.02	17 (22%)
20	CLA	2	605	-	65,73,73	1.34	7 (10%)	76,113,113	2.05	20 (26%)
20	CLA	3	606	-	50,58,73	1.58	9 (18%)	58,95,113	2.13	13 (22%)
19	CL0	A	1011	-	65,73,73	2.18	16 (24%)	76,113,113	2.50	25 (32%)
20	CLA	A	1133	-	65,73,73	1.39	8 (12%)	76,113,113	1.91	17 (22%)
20	CLA	B	1234	-	55,63,73	1.51	8 (14%)	64,101,113	2.11	16 (25%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
20	CLA	1	608	-	46,54,73	1.62	7 (15%)	53,90,113	2.23	14 (26%)
20	CLA	A	1104	-	65,73,73	1.39	8 (12%)	76,113,113	2.05	19 (25%)
20	CLA	3	610	15	65,73,73	1.34	7 (10%)	76,113,113	2.00	19 (25%)
25	SF4	A	3001	1,2	0,12,12	-	-	-		
20	CLA	4	609	16	50,58,73	1.53	7 (14%)	58,95,113	2.21	16 (27%)

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
20	CLA	B	1213	-	1/1/14/20	8/31/109/115	-
20	CLA	4	603	-	1/1/15/20	17/37/115/115	-
20	CLA	3	605	-	1/1/13/20	8/25/103/115	-
20	CLA	K	1404	11	1/1/11/20	5/15/93/115	-
26	LMG	3	802	-	-	14/25/45/70	0/1/1/1
20	CLA	A	1137	-	1/1/15/20	18/37/115/115	-
30	CHL	3	604	-	4/4/20/26	12/39/137/137	-
22	BCR	A	4017	-	-	6/29/63/63	0/2/2/2
23	LHG	4	801	-	-	19/39/39/53	-
20	CLA	A	1131	-	1/1/15/20	11/37/115/115	-
22	BCR	K	4001	-	-	12/29/63/63	0/2/2/2
22	BCR	A	4007	-	-	9/29/63/63	0/2/2/2
20	CLA	L	1503	-	1/1/12/20	9/19/97/115	-
20	CLA	L	1501	12	1/1/12/20	12/19/97/115	-
20	CLA	2	606	-	1/1/12/20	9/19/97/115	-
30	CHL	1	609	13	4/4/18/26	0/27/125/137	-
22	BCR	2	503	-	-	14/29/63/63	0/2/2/2
20	CLA	B	1023	-	1/1/15/20	11/37/115/115	-
20	CLA	B	1240	23	1/1/15/20	20/37/115/115	-
30	CHL	2	611	-	3/3/16/26	3/18/116/137	-
25	SF4	C	3002	3	-	-	0/6/5/5
26	LMG	2	805	-	-	8/25/45/70	0/1/1/1
20	CLA	G	1601	-	1/1/13/20	9/25/103/115	-
29	LUT	3	502	-	1/1/12/27	11/29/67/67	0/2/2/2

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
30	CHL	2	610	-	4/4/18/26	4/27/125/137	-
20	CLA	A	1132	-	1/1/15/20	13/37/115/115	-
20	CLA	1	607	-	1/1/11/20	7/15/93/115	-
22	BCR	H	4021	-	-	12/29/63/63	0/2/2/2
26	LMG	F	5003	-	-	6/31/51/70	0/1/1/1
22	BCR	J	4012	-	-	12/29/63/63	0/2/2/2
20	CLA	A	1136	-	1/1/15/20	14/37/115/115	-
20	CLA	A	1134	1	1/1/13/20	14/25/103/115	-
20	CLA	B	1230	-	1/1/13/20	14/29/107/115	-
20	CLA	A	1106	1	1/1/15/20	19/37/115/115	-
20	CLA	B	1232	-	1/1/13/20	13/25/103/115	-
20	CLA	A	1122	-	1/1/15/20	16/37/115/115	-
20	CLA	A	1103	-	1/1/15/20	22/37/115/115	-
24	LMT	B	5008	-	-	8/17/57/61	0/2/2/2
20	CLA	3	613	-	1/1/11/20	7/15/93/115	-
20	CLA	4	602	-	1/1/12/20	7/19/97/115	-
20	CLA	3	602	-	1/1/12/20	9/22/100/115	-
20	CLA	B	1239	-	1/1/15/20	20/37/115/115	-
30	CHL	4	610	-	3/3/16/26	2/17/115/137	-
26	LMG	F	5001	-	-	7/25/45/70	0/1/1/1
20	CLA	A	1124	-	1/1/13/20	8/25/103/115	-
20	CLA	3	614	-	1/1/10/20	3/10/88/115	-
22	BCR	L	4020	-	-	9/29/63/63	0/2/2/2
20	CLA	B	1214	-	1/1/15/20	14/37/115/115	-
20	CLA	B	1206	2	1/1/15/20	20/37/115/115	-
20	CLA	A	1105	-	1/1/14/20	19/31/109/115	-
26	LMG	B	5003	-	-	8/30/50/70	0/1/1/1
20	CLA	A	1126	-	1/1/15/20	21/37/115/115	-
20	CLA	A	1108	-	1/1/12/20	7/19/97/115	-
20	CLA	1	601	13	1/1/15/20	20/37/115/115	-
20	CLA	A	1114	-	1/1/11/20	8/15/93/115	-
20	CLA	B	1237	-	1/1/15/20	21/37/115/115	-
20	CLA	1	614	13	1/1/14/20	15/31/109/115	-
26	LMG	B	5007	-	-	11/29/49/70	0/1/1/1

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
23	LHG	A	5002	-	-	37/53/53/53	-
20	CLA	1	613	-	1/1/11/20	6/13/91/115	-
33	C7Z	4	505	-	-	16/29/67/67	0/2/2/2
23	LHG	A	5001	20	-	22/44/44/53	-
20	CLA	3	617	-	1/1/14/20	12/31/109/115	-
20	CLA	A	1117	-	1/1/15/20	19/37/115/115	-
20	CLA	2	603	14	1/1/15/20	15/37/115/115	-
24	LMT	G	5004	-	-	10/21/61/61	0/2/2/2
29	LUT	1	501	-	-	3/29/67/67	0/2/2/2
22	BCR	3	506	-	-	14/29/63/63	0/2/2/2
20	CLA	B	1204	-	1/1/15/20	22/37/115/115	-
20	CLA	2	607	23	1/1/14/20	15/31/109/115	-
30	CHL	1	610	13	3/3/16/26	7/17/115/137	-
20	CLA	B	1201	-	1/1/15/20	19/37/115/115	-
20	CLA	4	607	-	1/1/14/20	15/31/109/115	-
20	CLA	J	1901	10	1/1/12/20	8/19/97/115	-
20	CLA	B	1203	-	1/1/15/20	15/37/115/115	-
20	CLA	1	604	-	1/1/15/20	17/37/115/115	-
20	CLA	1	605	-	1/1/15/20	18/37/115/115	-
23	LHG	3	801	30	-	13/19/19/53	-
20	CLA	4	608	-	1/1/11/20	6/15/93/115	-
28	DGD	J	5001	-	-	13/47/87/95	0/2/2/2
22	BCR	I	4020	-	-	15/29/63/63	0/2/2/2
28	DGD	4	802	-	-	17/40/80/95	0/2/2/2
20	CLA	A	1119	-	1/1/15/20	18/37/115/115	-
24	LMT	B	5006	-	-	7/18/58/61	0/2/2/2
20	CLA	G	1603	-	1/1/15/20	17/37/115/115	-
30	CHL	4	615	-	3/3/15/26	2/12/110/137	-
20	CLA	1	603	-	1/1/13/20	10/25/103/115	-
20	CLA	A	1012	-	1/1/15/20	20/37/115/115	-
20	CLA	A	1130	-	1/1/13/20	12/25/103/115	-
20	CLA	K	1402	-	1/1/14/20	20/31/109/115	-
22	BCR	B	4004	-	-	12/29/63/63	0/2/2/2
22	BCR	G	4011	-	-	9/29/63/63	0/2/2/2

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
26	LMG	2	802	-	-	8/20/40/70	0/1/1/1
20	CLA	A	1127	-	1/1/15/20	19/37/115/115	-
28	DGD	B	5005	-	-	19/50/90/95	0/2/2/2
20	CLA	4	601	16	1/1/14/20	14/31/109/115	-
20	CLA	A	1115	-	1/1/15/20	22/37/115/115	-
20	CLA	A	1113	-	1/1/11/20	9/13/91/115	-
20	CLA	A	1121	-	1/1/14/20	14/31/109/115	-
20	CLA	A	1138	-	1/1/15/20	17/37/115/115	-
20	CLA	B	1205	-	1/1/15/20	16/37/115/115	-
31	XAT	4	502	-	2/2/12/26	2/31/93/93	0/4/4/4
22	BCR	B	4010	-	-	13/29/63/63	0/2/2/2
20	CLA	L	1502	-	1/1/14/20	21/31/109/115	-
20	CLA	B	1212	-	1/1/13/20	9/25/103/115	-
26	LMG	A	5006	-	-	11/45/65/70	0/1/1/1
20	CLA	2	608	-	1/1/12/20	7/19/97/115	-
20	CLA	B	1217	-	1/1/11/20	5/15/93/115	-
26	LMG	F	5006	-	-	1/4/24/70	0/1/1/1
30	CHL	2	613	-	3/3/16/26	6/15/113/137	-
26	LMG	G	5006	-	-	11/20/40/70	0/1/1/1
29	LUT	J	4013	-	-	7/29/67/67	0/2/2/2
30	CHL	3	607	23	3/3/17/26	6/21/119/137	-
34	FES	N	101	17	-	-	0/1/1/1
20	CLA	4	606	-	1/1/12/20	7/19/97/115	-
21	PQN	A	2001	-	-	3/23/43/43	0/2/2/2
26	LMG	2	804	-	-	8/25/45/70	0/1/1/1
20	CLA	B	1238	36	1/1/15/20	17/37/115/115	-
26	LMG	F	5002	-	-	11/42/62/70	0/1/1/1
20	CLA	G	1602	-	1/1/11/20	8/15/93/115	-
26	LMG	F	5004	-	-	8/29/49/70	0/1/1/1
20	CLA	A	1116	-	1/1/13/20	11/27/105/115	-
26	LMG	1	802	-	-	8/41/61/70	0/1/1/1
20	CLA	1	606	-	1/1/12/20	7/19/97/115	-
20	CLA	A	1013	-	1/1/15/20	18/37/115/115	-
20	CLA	A	1140	-	1/1/15/20	12/37/115/115	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
26	LMG	B	5004	-	-	13/28/48/70	0/1/1/1
22	BCR	K	4002	-	-	11/29/63/63	0/2/2/2
20	CLA	B	1231	-	1/1/14/20	10/31/109/115	-
23	LHG	B	5001	20	-	14/23/23/53	-
20	CLA	3	601	-	1/1/13/20	14/25/103/115	-
20	CLA	A	1125	-	1/1/15/20	18/37/115/115	-
20	CLA	B	1215	-	1/1/15/20	16/37/115/115	-
20	CLA	2	601	-	1/1/14/20	12/31/109/115	-
20	CLA	B	1208	-	1/1/14/20	13/31/109/115	-
20	CLA	A	1118	-	1/1/12/20	7/19/97/115	-
20	CLA	2	612	-	1/1/13/20	12/25/103/115	-
20	CLA	K	1403	-	1/1/11/20	9/17/95/115	-
29	LUT	2	501	-	1/1/12/27	5/29/67/67	0/2/2/2
20	CLA	H	1701	8	1/1/14/20	17/31/109/115	-
22	BCR	3	503	-	-	15/29/63/63	0/2/2/2
20	CLA	B	1221	-	1/1/15/20	21/37/115/115	-
23	LHG	1	801	-	-	29/53/53/53	-
20	CLA	A	1129	-	1/1/15/20	15/37/115/115	-
20	CLA	4	605	-	-	13/31/109/115	-
20	CLA	A	1109	-	1/1/15/20	13/37/115/115	-
22	BCR	F	4016	-	-	15/29/63/63	0/2/2/2
20	CLA	B	1209	-	1/1/11/20	6/15/93/115	-
22	BCR	B	4005	-	-	10/29/63/63	0/2/2/2
22	BCR	1	504	-	-	14/29/63/63	0/2/2/2
20	CLA	A	1141	23	1/1/14/20	14/31/109/115	-
20	CLA	B	1222	36	1/1/15/20	22/37/115/115	-
20	CLA	2	604	14	1/1/15/20	17/37/115/115	-
20	CLA	A	1101	-	1/1/15/20	18/37/115/115	-
20	CLA	K	1401	-	1/1/11/20	8/13/91/115	-
20	CLA	A	1123	-	1/1/15/20	15/37/115/115	-
20	CLA	B	1219	-	1/1/15/20	20/37/115/115	-
20	CLA	B	1220	-	1/1/13/20	12/25/103/115	-
22	BCR	1	503	-	-	16/29/63/63	0/2/2/2
23	LHG	B	5002	-	-	30/53/53/53	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
20	CLA	B	1202	-	1/1/15/20	15/37/115/115	-
20	CLA	4	604	-	1/1/14/20	16/31/109/115	-
22	BCR	B	4009	-	-	9/29/63/63	0/2/2/2
24	LMT	2	808	-	-	2/21/61/61	0/2/2/2
23	LHG	2	801	20	-	19/39/39/53	-
28	DGD	G	5003	-	-	11/36/76/95	0/2/2/2
20	CLA	B	1216	-	1/1/15/20	12/37/115/115	-
20	CLA	A	1120	-	1/1/14/20	15/31/109/115	-
20	CLA	B	1226	-	1/1/15/20	20/37/115/115	-
30	CHL	4	613	-	4/4/19/26	8/33/131/137	-
22	BCR	A	4008	-	-	13/29/63/63	0/2/2/2
20	CLA	B	1021	-	1/1/15/20	16/37/115/115	-
29	LUT	1	502	-	-	5/29/67/67	0/2/2/2
22	BCR	A	4003	-	-	13/29/63/63	0/2/2/2
30	CHL	1	612	-	4/4/19/26	8/33/131/137	-
20	CLA	B	1225	-	1/1/15/20	16/37/115/115	-
20	CLA	B	1211	-	1/1/15/20	22/37/115/115	-
20	CLA	A	1112	-	1/1/15/20	19/37/115/115	-
21	PQN	B	2002	-	-	8/23/43/43	0/2/2/2
20	CLA	B	1224	-	1/1/15/20	18/37/115/115	-
20	CLA	B	1235	-	1/1/15/20	17/37/115/115	-
20	CLA	B	1228	-	1/1/14/20	16/31/109/115	-
20	CLA	A	1107	1	1/1/15/20	17/37/115/115	-
22	BCR	B	4006	-	-	12/29/63/63	0/2/2/2
20	CLA	3	612	-	1/1/12/20	11/19/97/115	-
28	DGD	F	5005	-	-	18/46/86/95	0/2/2/2
20	CLA	F	1302	6	1/1/15/20	17/37/115/115	-
20	CLA	3	603	15	1/1/13/20	15/25/103/115	-
22	BCR	A	4011	-	-	16/29/63/63	0/2/2/2
20	CLA	A	1111	-	1/1/15/20	20/37/115/115	-
22	BCR	L	4019	-	-	14/29/63/63	0/2/2/2
20	CLA	A	1135	-	1/1/12/20	8/21/99/115	-
32	3PH	2	807	-	-	16/34/34/49	-
20	CLA	2	602	-	1/1/12/20	8/22/100/115	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	LMT	G	5005	-	-	6/17/57/61	0/2/2/2
20	CLA	B	1022	-	1/1/15/20	4/37/115/115	-
26	LMG	G	5001	-	-	21/44/64/70	0/1/1/1
26	LMG	G	5002	-	-	18/45/65/70	0/1/1/1
20	CLA	B	1210	-	1/1/15/20	16/37/115/115	-
20	CLA	B	1218	-	1/1/15/20	10/37/115/115	-
20	CLA	A	1110	-	1/1/13/20	6/25/103/115	-
20	CLA	1	602	13	1/1/11/20	6/15/93/115	-
20	CLA	4	612	-	1/1/15/20	17/37/115/115	-
20	CLA	B	1207	-	1/1/15/20	24/37/115/115	-
20	CLA	B	1223	-	1/1/15/20	14/37/115/115	-
20	CLA	F	1301	-	1/1/15/20	17/37/115/115	-
22	BCR	A	4002	-	-	11/29/63/63	0/2/2/2
30	CHL	2	615	-	4/4/18/26	5/27/125/137	-
22	BCR	F	4014	-	-	9/29/63/63	0/2/2/2
31	XAT	2	502	-	2/2/12/26	4/31/93/93	0/4/4/4
30	CHL	2	609	-	4/4/20/26	9/39/137/137	-
28	DGD	3	803	-	-	10/40/80/95	0/2/2/2
20	CLA	B	1227	-	1/1/15/20	13/37/115/115	-
20	CLA	A	1139	-	1/1/15/20	14/37/115/115	-
26	LMG	2	803	-	-	12/31/51/70	0/1/1/1
20	CLA	A	1128	-	1/1/15/20	16/37/115/115	-
28	DGD	1	803	-	-	15/30/70/95	0/2/2/2
26	LMG	2	806	-	-	1/4/24/70	0/1/1/1
30	CHL	3	611	-	3/3/16/26	0/17/115/137	-
20	CLA	B	1229	-	1/1/15/20	12/37/115/115	-
20	CLA	B	1236	-	1/1/12/20	10/19/97/115	-
25	SF4	C	3003	3	-	-	0/6/5/5
20	CLA	1	611	-	1/1/15/20	14/37/115/115	-
24	LMT	A	5004	-	-	9/21/61/61	0/2/2/2
30	CHL	4	611	-	3/3/17/26	2/21/119/137	-
20	CLA	4	617	-	1/1/15/20	20/37/115/115	-
22	BCR	I	4018	-	-	14/29/63/63	0/2/2/2
20	CLA	3	608	-	1/1/11/20	4/17/95/115	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
29	LUT	4	501	-	-	5/29/67/67	0/2/2/2
29	LUT	3	501	-	-	5/29/67/67	0/2/2/2
20	CLA	A	1102	-	1/1/15/20	23/37/115/115	-
20	CLA	2	605	-	1/1/15/20	22/37/115/115	-
20	CLA	3	606	-	1/1/12/20	12/19/97/115	-
19	CL0	A	1011	-	3/3/20/25	7/37/135/135	-
20	CLA	A	1133	-	1/1/15/20	15/37/115/115	-
20	CLA	B	1234	-	1/1/13/20	9/25/103/115	-
20	CLA	1	608	-	1/1/11/20	5/15/93/115	-
20	CLA	A	1104	-	1/1/15/20	17/37/115/115	-
20	CLA	3	610	15	1/1/15/20	21/37/115/115	-
25	SF4	A	3001	1,2	-	-	0/6/5/5
20	CLA	4	609	16	1/1/12/20	10/19/97/115	-

The worst 5 of 1347 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	1	502	LUT	C24-C25	14.56	1.51	1.33
33	4	505	C7Z	C34-C33	14.48	1.55	1.35
33	4	505	C7Z	C30-C29	14.33	1.54	1.35
29	4	501	LUT	C24-C25	14.28	1.50	1.33
29	1	501	LUT	C24-C25	14.27	1.50	1.33

The worst 5 of 3346 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	A	4017	BCR	C16-C15-C14	18.16	160.67	123.47
22	H	4021	BCR	C10-C11-C12	18.10	179.72	123.22
22	B	4004	BCR	C11-C10-C9	17.84	152.77	127.31
22	3	506	BCR	C10-C11-C12	17.71	178.49	123.22
22	1	504	BCR	C10-C11-C12	17.60	178.15	123.22

5 of 201 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
19	A	1011	CL0	NA
19	A	1011	CL0	NC
19	A	1011	CL0	ND
20	A	1101	CLA	ND

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atom
20	A	1102	CLA	ND

5 of 2969 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
20	A	1101	CLA	C2-C1-O2A-CGA
20	A	1101	CLA	CHA-CBD-CGD-O1D
20	A	1101	CLA	CHA-CBD-CGD-O2D
20	A	1102	CLA	C3A-C2A-CAA-CBA
20	A	1103	CLA	C1A-C2A-CAA-CBA

There are no ring outliers.

229 monomers are involved in 1607 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
20	B	1213	CLA	3	0
20	4	603	CLA	16	0
20	3	605	CLA	6	0
20	K	1404	CLA	3	0
20	A	1137	CLA	4	0
22	A	4017	BCR	8	0
30	3	604	CHL	3	0
23	4	801	LHG	11	0
20	A	1131	CLA	10	0
22	K	4001	BCR	9	0
22	A	4007	BCR	5	0
20	L	1503	CLA	17	0
20	L	1501	CLA	18	0
20	2	606	CLA	21	0
22	2	503	BCR	24	0
30	1	609	CHL	16	0
31	4	502	XAT	14	0
20	B	1023	CLA	3	0
20	B	1240	CLA	9	0
30	2	611	CHL	5	0
25	C	3002	SF4	1	0
26	2	805	LMG	1	0
20	G	1601	CLA	6	0
29	3	502	LUT	4	0
30	2	610	CHL	16	0
20	A	1132	CLA	27	0
20	1	607	CLA	1	0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
22	H	4021	BCR	21	0
26	F	5003	LMG	3	0
22	J	4012	BCR	5	0
20	A	1136	CLA	12	0
20	A	1134	CLA	10	0
20	B	1230	CLA	9	0
20	A	1106	CLA	11	0
20	B	1232	CLA	10	0
20	A	1122	CLA	8	0
20	A	1103	CLA	18	0
24	B	5008	LMT	1	0
20	3	613	CLA	2	0
20	4	602	CLA	18	0
20	3	602	CLA	2	0
20	B	1239	CLA	8	0
30	4	610	CHL	3	0
20	A	1124	CLA	4	0
20	3	614	CLA	1	0
22	L	4020	BCR	19	0
20	B	1214	CLA	9	0
20	B	1206	CLA	10	0
20	A	1105	CLA	12	0
26	B	5003	LMG	13	0
20	A	1126	CLA	22	0
20	A	1108	CLA	5	0
20	1	601	CLA	13	0
20	A	1114	CLA	3	0
20	B	1237	CLA	20	0
20	1	614	CLA	5	0
26	B	5007	LMG	1	0
23	A	5002	LHG	2	0
20	1	613	CLA	9	0
33	4	505	C7Z	4	0
23	A	5001	LHG	1	0
20	3	617	CLA	18	0
20	A	1117	CLA	15	0
20	2	603	CLA	9	0
29	1	501	LUT	6	0
22	3	506	BCR	3	0
20	B	1204	CLA	9	0
20	2	607	CLA	9	0
30	1	610	CHL	10	0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
20	B	1201	CLA	5	0
20	4	607	CLA	12	0
20	J	1901	CLA	7	0
20	B	1203	CLA	4	0
20	1	604	CLA	15	0
20	1	605	CLA	9	0
20	4	608	CLA	14	0
28	J	5001	DGD	10	0
22	I	4020	BCR	10	0
28	4	802	DGD	4	0
20	A	1119	CLA	13	0
20	G	1603	CLA	13	0
30	4	615	CHL	3	0
20	1	603	CLA	20	0
20	A	1012	CLA	11	0
20	A	1130	CLA	3	0
20	K	1402	CLA	3	0
22	B	4004	BCR	5	0
22	G	4011	BCR	5	0
26	2	802	LMG	10	0
20	A	1127	CLA	12	0
28	B	5005	DGD	7	0
20	4	601	CLA	36	0
20	A	1115	CLA	10	0
20	A	1113	CLA	19	0
20	A	1121	CLA	3	0
20	A	1138	CLA	4	0
20	B	1205	CLA	9	0
22	B	4010	BCR	3	0
26	A	5006	LMG	3	0
20	L	1502	CLA	18	0
20	B	1212	CLA	5	0
26	F	5001	LMG	1	0
20	2	608	CLA	10	0
20	B	1217	CLA	1	0
30	2	613	CHL	5	0
26	G	5006	LMG	1	0
29	J	4013	LUT	10	0
30	3	607	CHL	1	0
20	4	606	CLA	4	0
21	A	2001	PQN	7	0
26	2	804	LMG	2	0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
20	B	1238	CLA	9	0
26	F	5002	LMG	3	0
20	G	1602	CLA	2	0
20	A	1116	CLA	13	0
26	1	802	LMG	8	0
20	1	606	CLA	10	0
20	A	1013	CLA	13	0
20	A	1140	CLA	7	0
26	B	5004	LMG	2	0
22	K	4002	BCR	8	0
20	B	1231	CLA	5	0
23	B	5001	LHG	2	0
20	3	601	CLA	13	0
20	A	1125	CLA	11	0
20	B	1215	CLA	4	0
20	2	601	CLA	8	0
20	B	1208	CLA	3	0
20	A	1118	CLA	3	0
20	2	612	CLA	14	0
22	3	503	BCR	11	0
20	H	1701	CLA	21	0
23	1	801	LHG	11	0
20	B	1221	CLA	4	0
29	2	501	LUT	13	0
20	A	1129	CLA	2	0
20	4	605	CLA	12	0
20	A	1109	CLA	15	0
22	F	4016	BCR	9	0
20	B	1209	CLA	4	0
22	B	4005	BCR	3	0
22	1	504	BCR	4	0
20	A	1141	CLA	3	0
20	B	1222	CLA	8	0
20	2	604	CLA	25	0
20	A	1101	CLA	16	0
20	K	1401	CLA	11	0
20	A	1123	CLA	10	0
20	B	1219	CLA	5	0
20	B	1220	CLA	3	0
22	1	503	BCR	1	0
23	B	5002	LHG	4	0
20	B	1202	CLA	7	0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
20	4	604	CLA	26	0
22	B	4009	BCR	4	0
24	2	808	LMT	8	0
23	2	801	LHG	7	0
28	G	5003	DGD	3	0
20	B	1216	CLA	7	0
20	A	1120	CLA	4	0
20	B	1226	CLA	7	0
22	A	4008	BCR	4	0
30	4	613	CHL	5	0
20	B	1021	CLA	11	0
29	1	502	LUT	34	0
30	1	612	CHL	6	0
20	B	1225	CLA	11	0
20	B	1211	CLA	11	0
20	A	1112	CLA	15	0
21	B	2002	PQN	3	0
20	B	1224	CLA	5	0
20	B	1235	CLA	5	0
20	B	1228	CLA	4	0
20	A	1107	CLA	10	0
22	B	4006	BCR	5	0
20	3	612	CLA	9	0
28	F	5005	DGD	18	0
20	F	1302	CLA	8	0
20	3	603	CLA	10	0
22	A	4011	BCR	7	0
20	A	1111	CLA	13	0
22	L	4019	BCR	28	0
20	A	1135	CLA	5	0
32	2	807	3PH	5	0
20	2	602	CLA	3	0
20	B	1022	CLA	11	0
26	G	5001	LMG	5	0
26	G	5002	LMG	8	0
20	B	1210	CLA	11	0
20	B	1218	CLA	9	0
20	A	1110	CLA	8	0
20	1	602	CLA	2	0
20	4	612	CLA	21	0
20	B	1207	CLA	12	0
20	B	1223	CLA	6	0

Continued on next page...

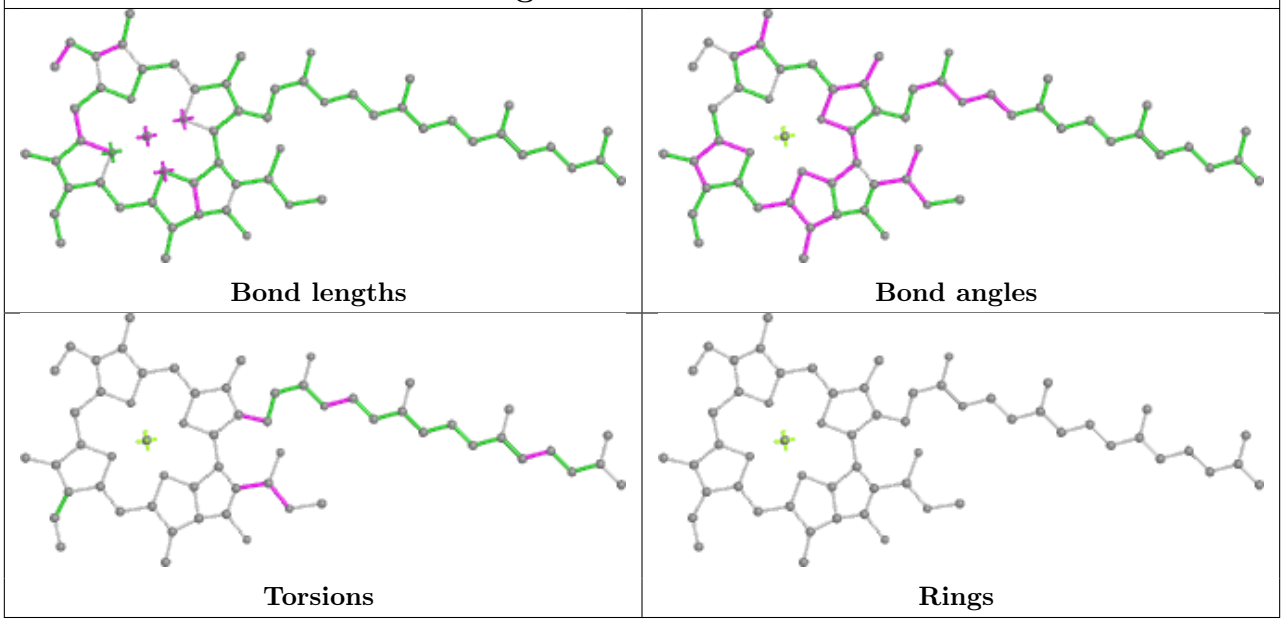
Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
20	F	1301	CLA	12	0
22	A	4002	BCR	3	0
30	2	615	CHL	4	0
22	F	4014	BCR	2	0
31	2	502	XAT	14	0
30	2	609	CHL	21	0
28	3	803	DGD	3	0
20	B	1227	CLA	7	0
20	A	1139	CLA	11	0
26	2	803	LMG	4	0
20	A	1128	CLA	5	0
28	1	803	DGD	1	0
30	3	611	CHL	9	0
20	B	1229	CLA	8	0
20	B	1236	CLA	2	0
25	C	3003	SF4	2	0
20	1	611	CLA	10	0
24	A	5004	LMT	1	0
30	4	611	CHL	1	0
20	4	617	CLA	12	0
22	I	4018	BCR	8	0
20	3	608	CLA	5	0
29	4	501	LUT	20	0
29	3	501	LUT	5	0
20	A	1102	CLA	6	0
20	2	605	CLA	11	0
20	3	606	CLA	7	0
19	A	1011	CL0	12	0
20	A	1133	CLA	12	0
20	B	1234	CLA	12	0
20	1	608	CLA	10	0
20	A	1104	CLA	7	0
20	3	610	CLA	3	0
20	4	609	CLA	16	0

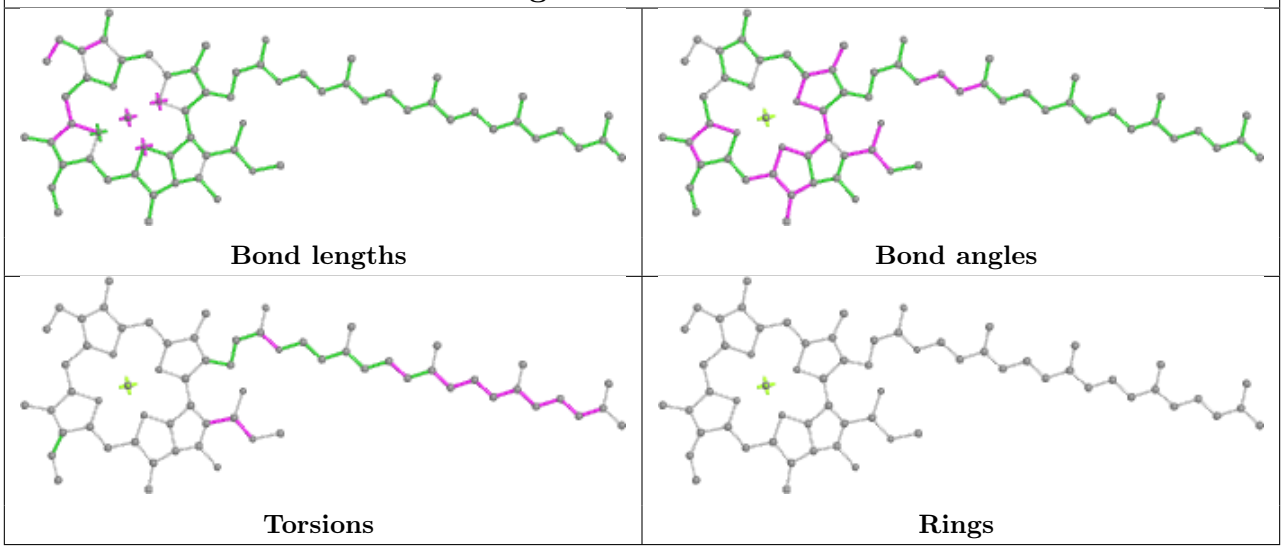
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

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

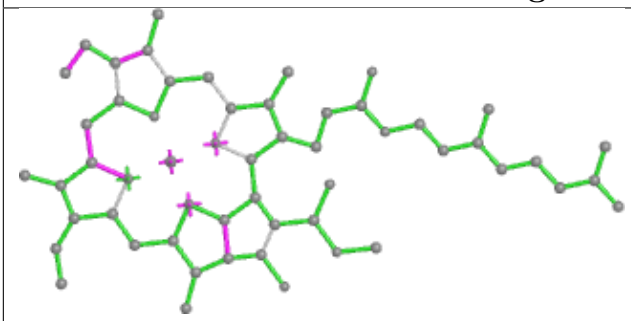
Ligand CLA B 1213



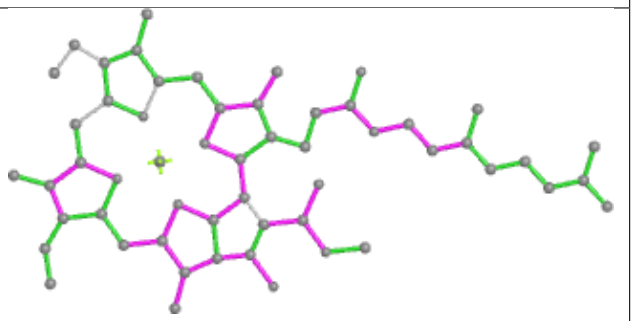
Ligand CLA 4 603



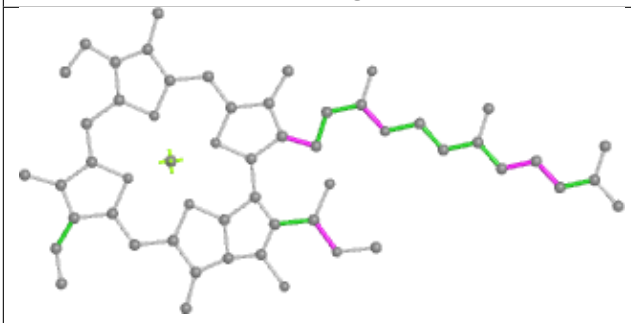
Ligand CLA 3 605



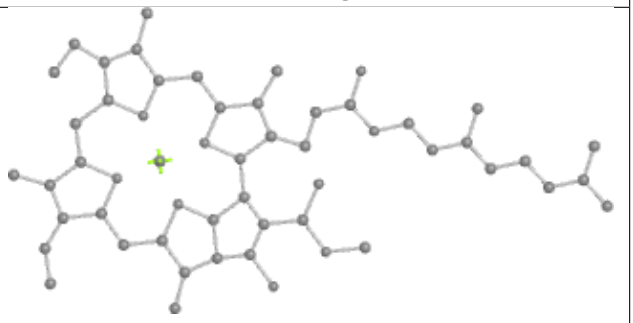
Bond lengths



Bond angles

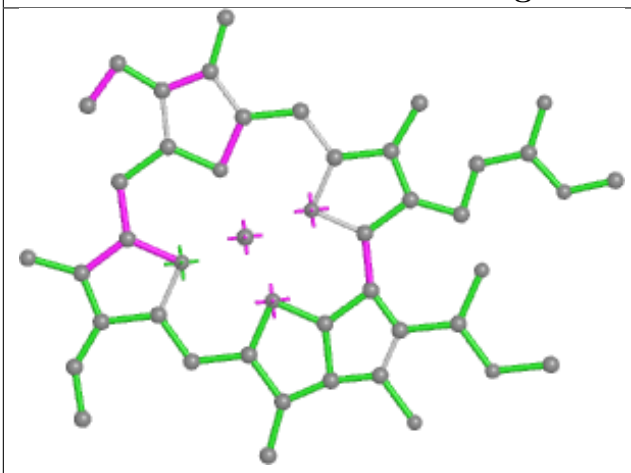


Torsions

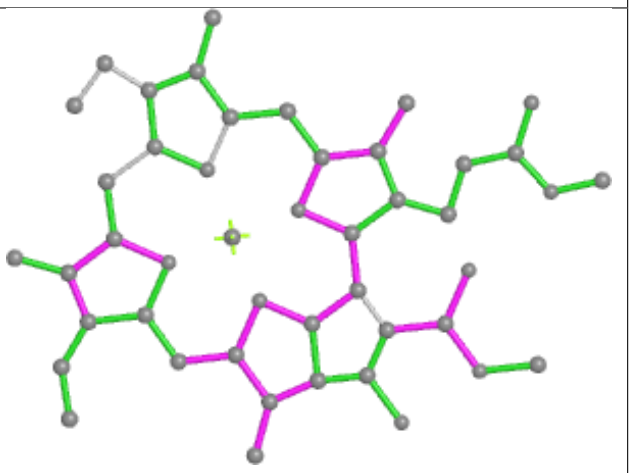


Rings

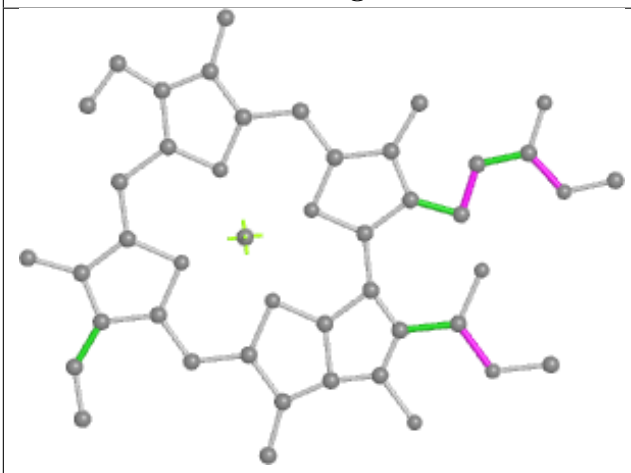
Ligand CLA K 1404



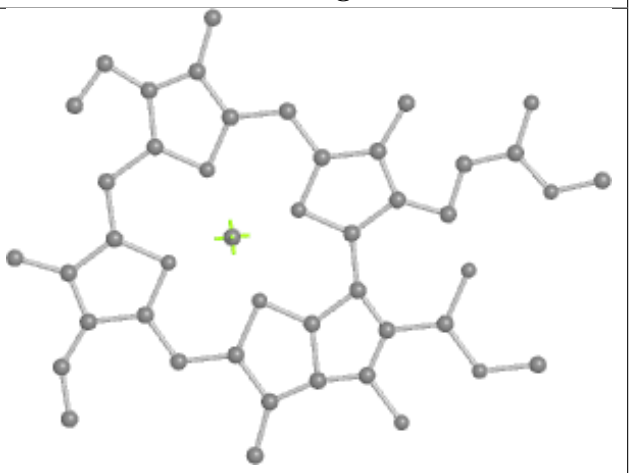
Bond lengths



Bond angles

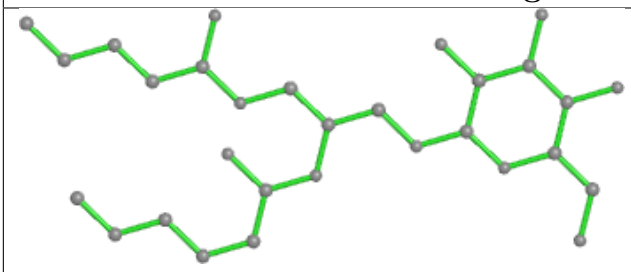


Torsions

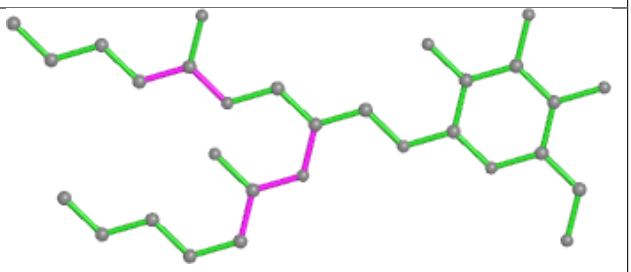


Rings

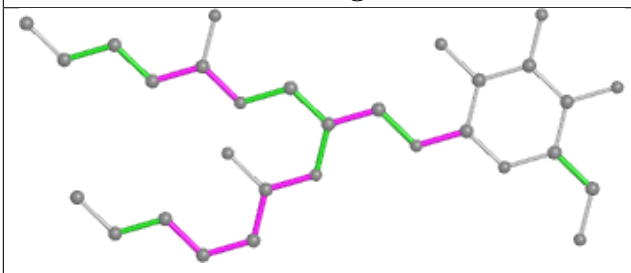
Ligand LMG 3 802



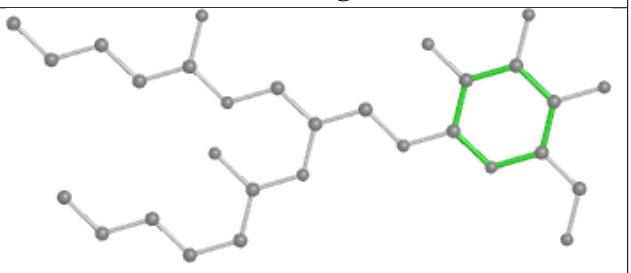
Bond lengths



Bond angles

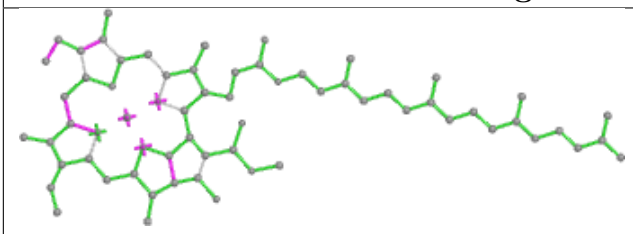


Torsions

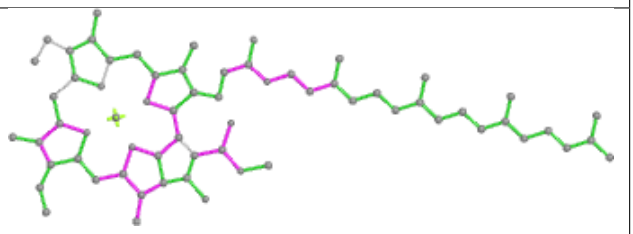


Rings

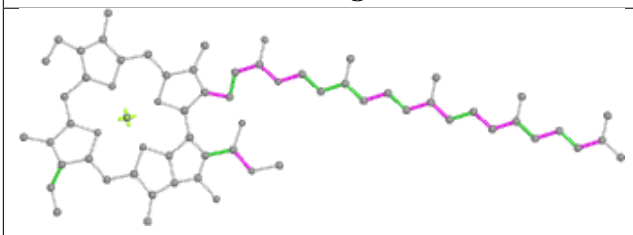
Ligand CLA A 1137



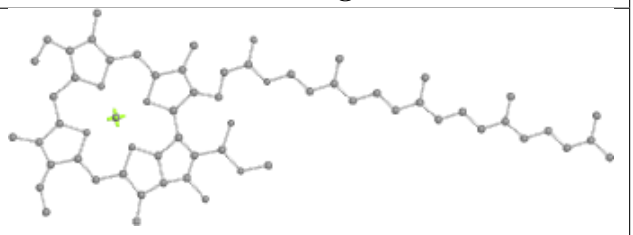
Bond lengths



Bond angles

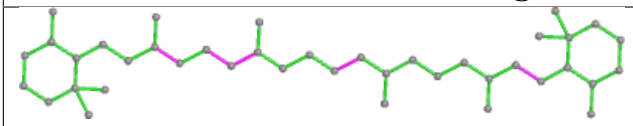


Torsions

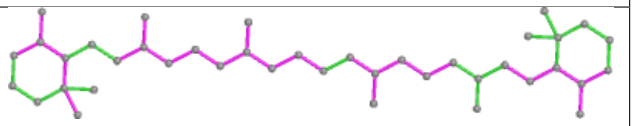


Rings

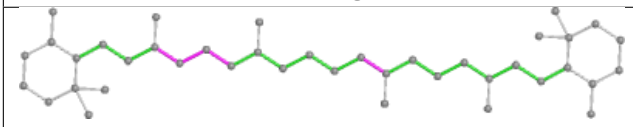
Ligand BCR A 4017



Bond lengths



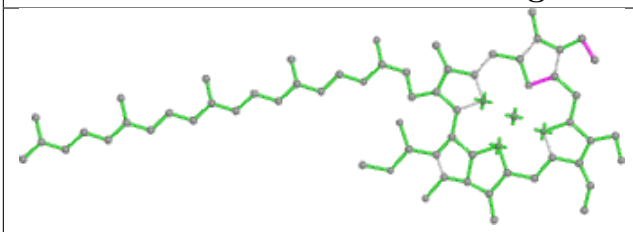
Bond angles



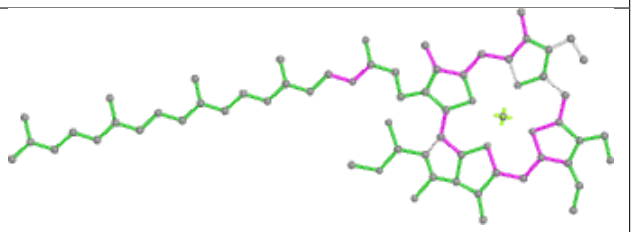
Torsions

Rings

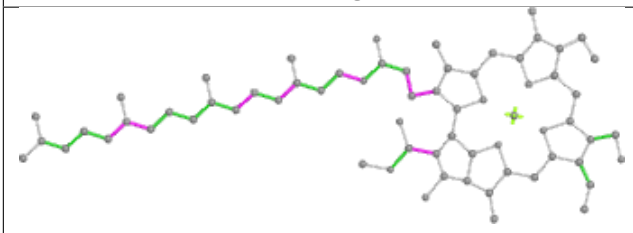
Ligand CHL 3 604



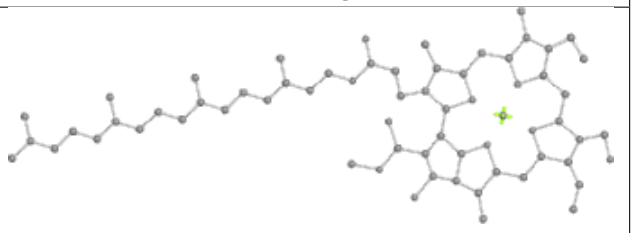
Bond lengths



Bond angles

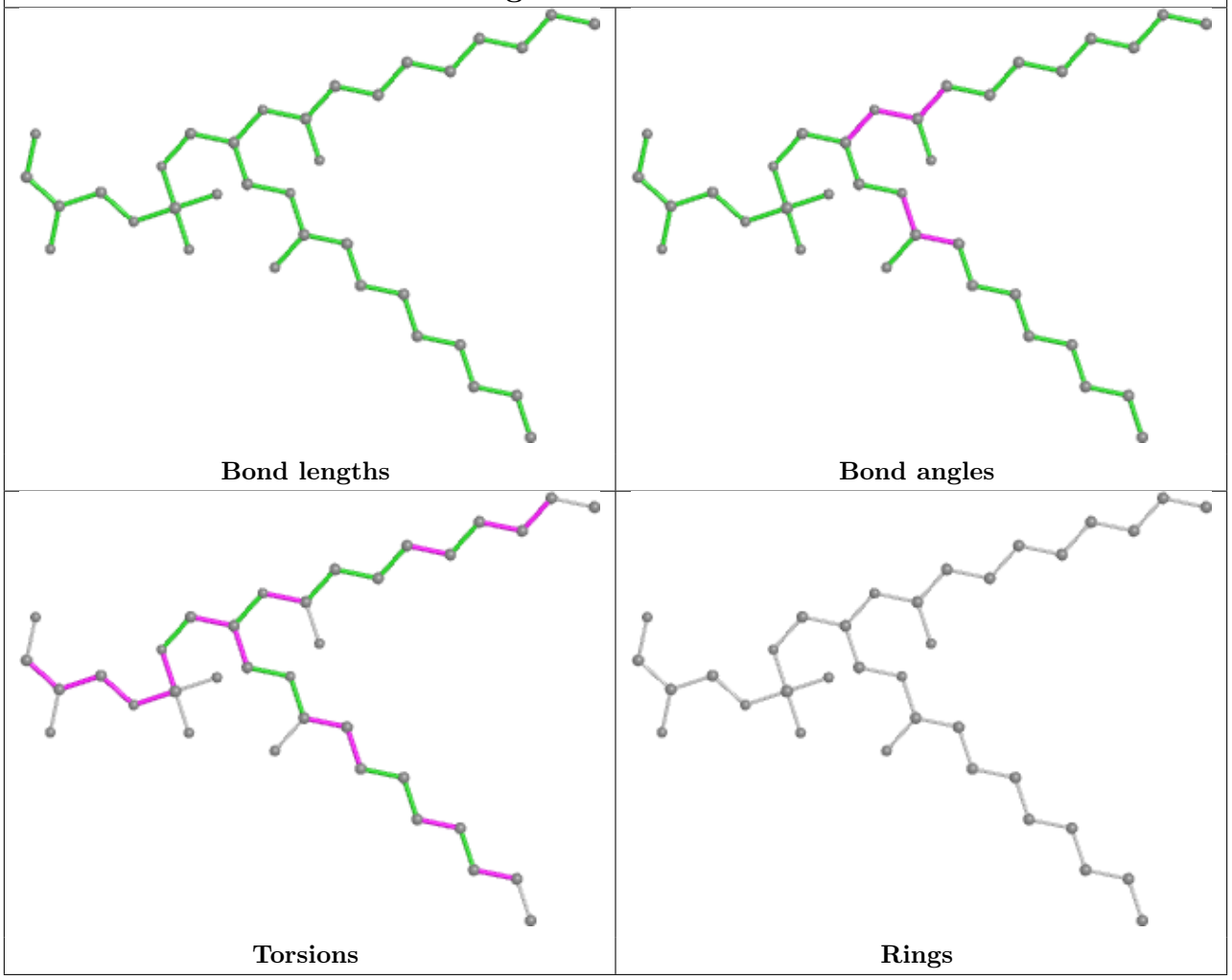


Torsions

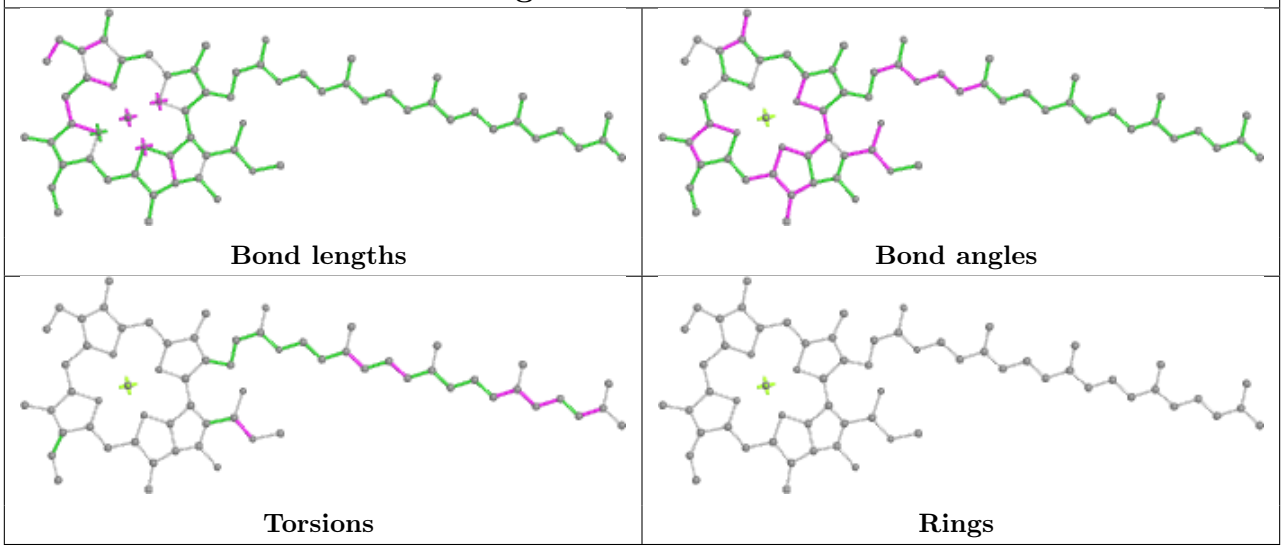


Rings

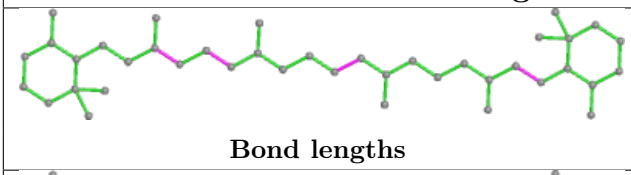
Ligand LHG 4 801



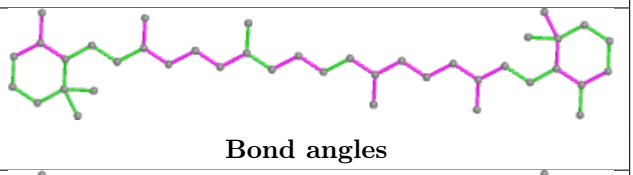
Ligand CLA A 1131



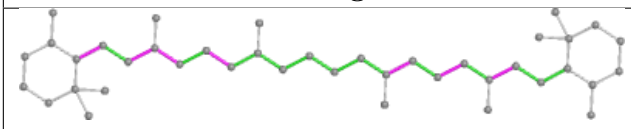
Ligand BCR K 4001



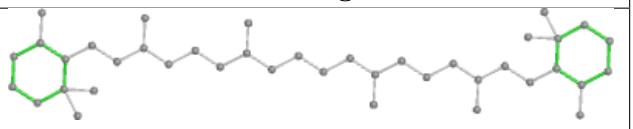
Bond lengths



Bond angles

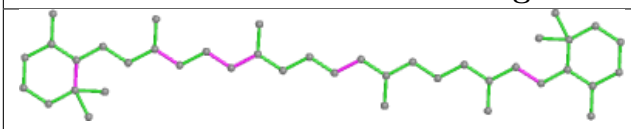


Torsions

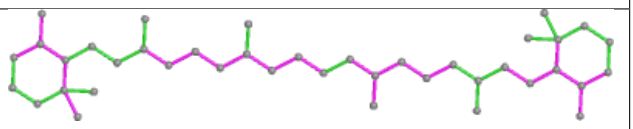


Rings

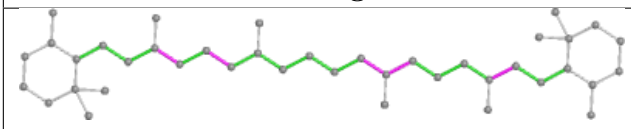
Ligand BCR A 4007



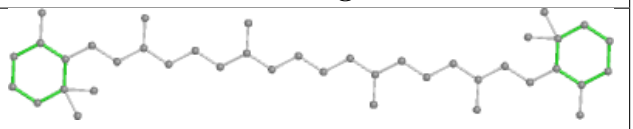
Bond lengths



Bond angles

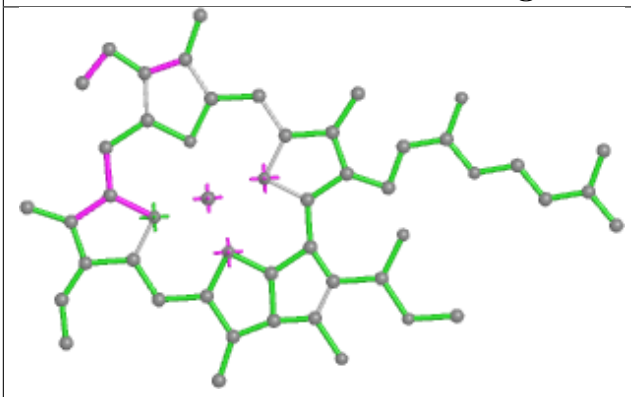


Torsions

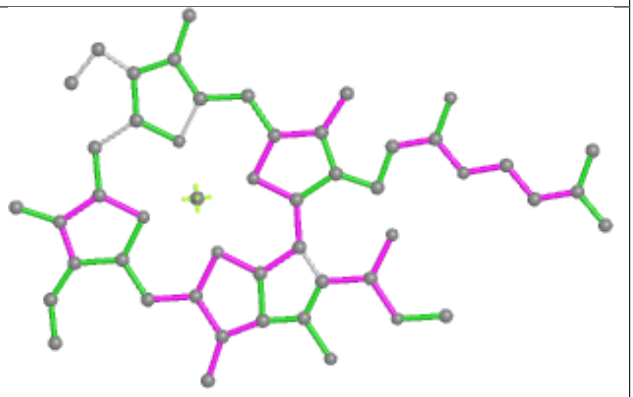


Rings

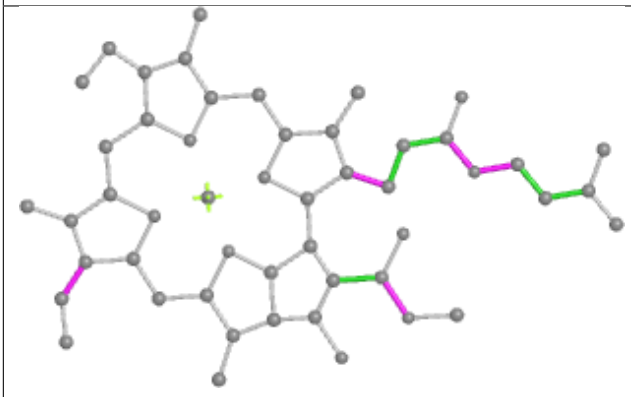
Ligand CLA L 1503



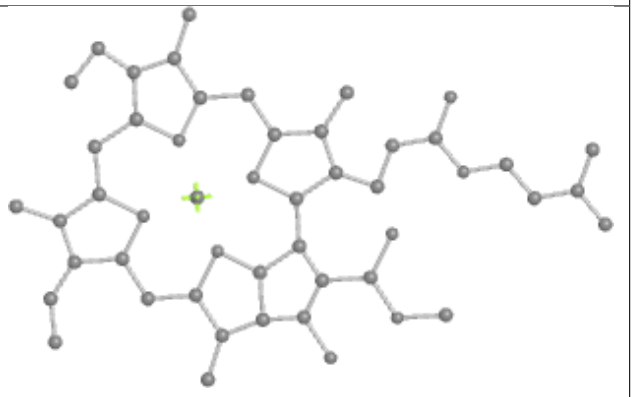
Bond lengths



Bond angles

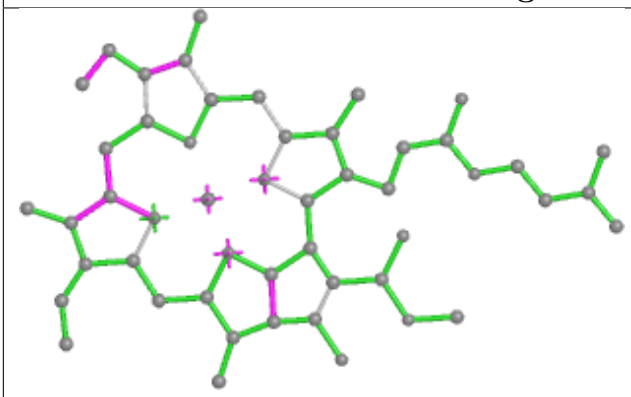


Torsions

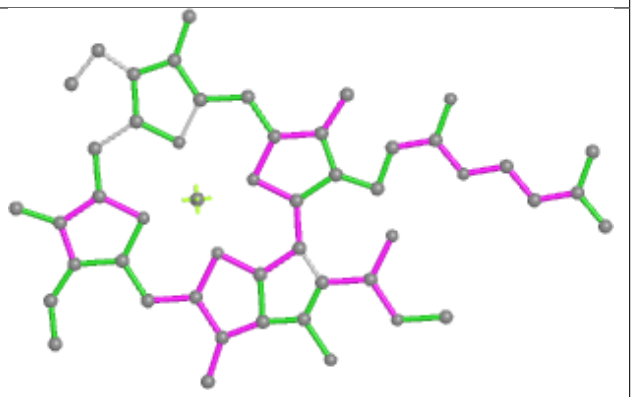


Rings

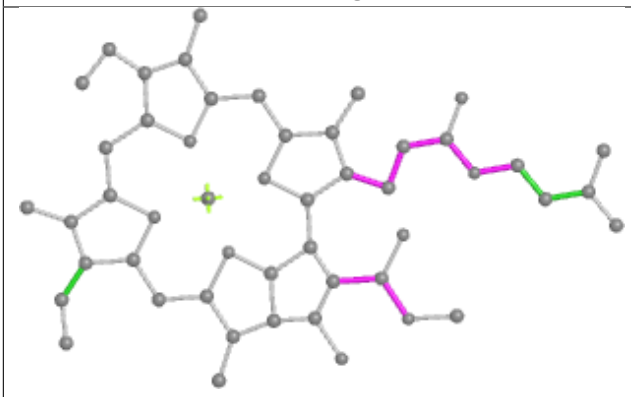
Ligand CLA L 1501



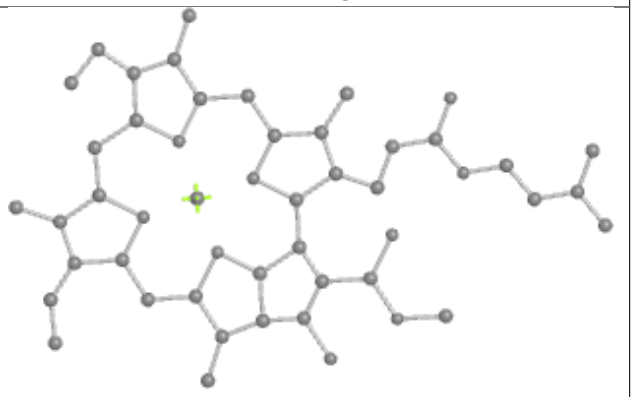
Bond lengths



Bond angles

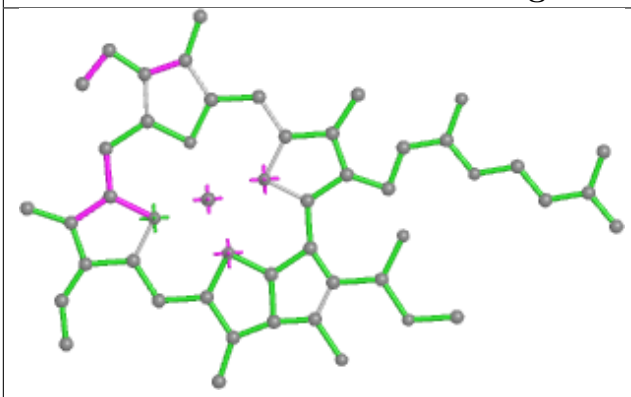


Torsions

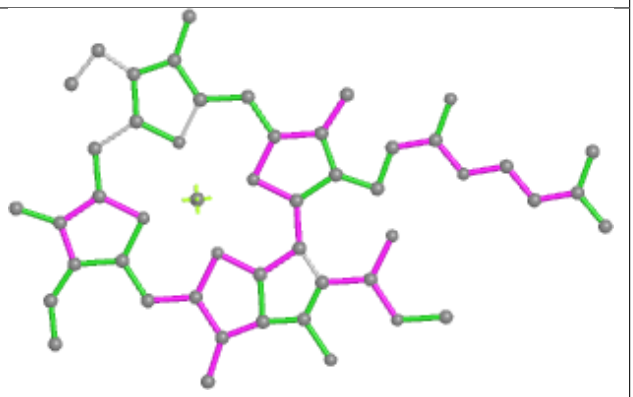


Rings

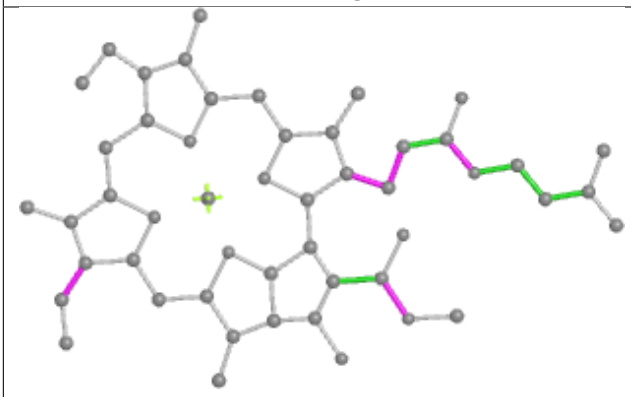
Ligand CLA 2 606



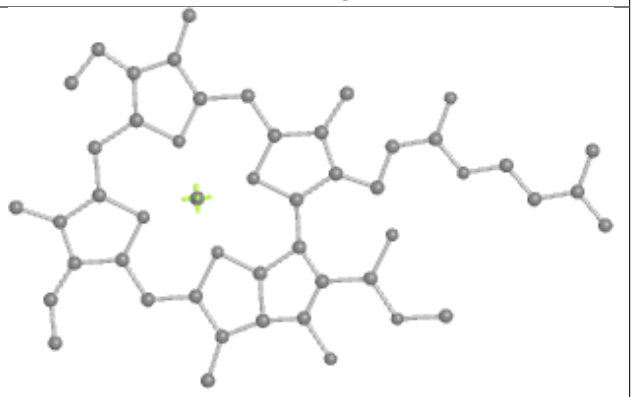
Bond lengths



Bond angles

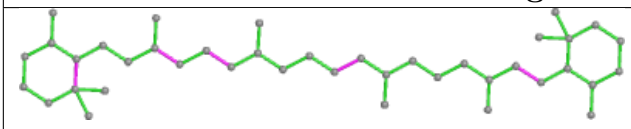


Torsions

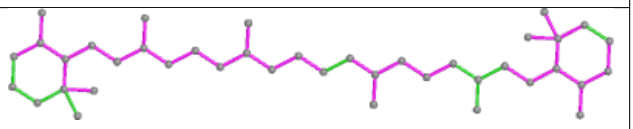


Rings

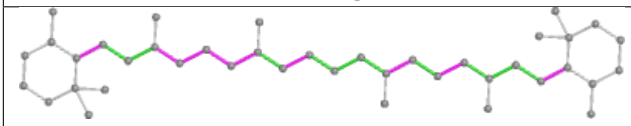
Ligand BCR 2 503



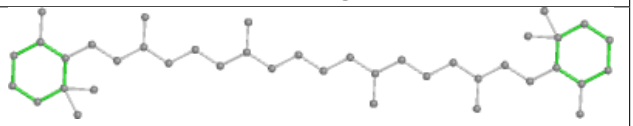
Bond lengths



Bond angles

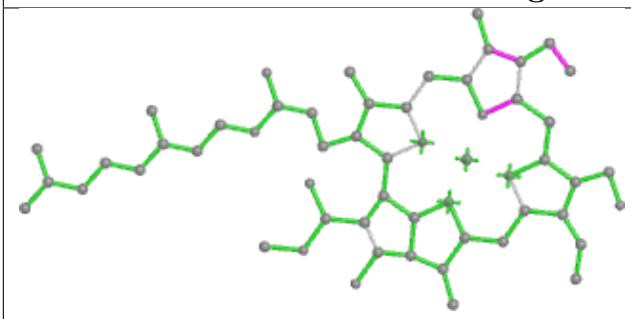


Torsions

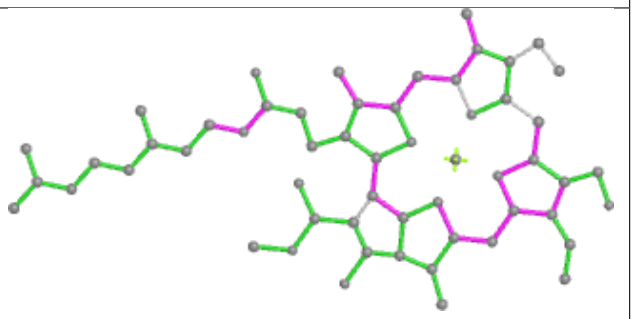


Rings

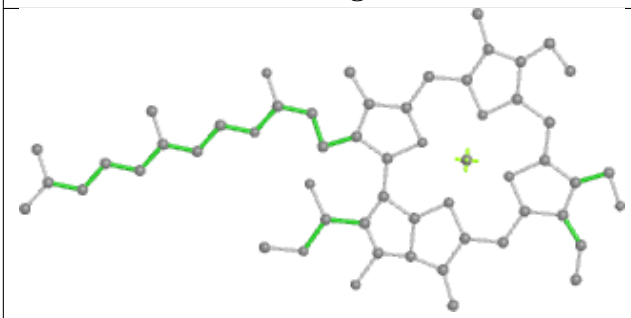
Ligand CHL 1 609



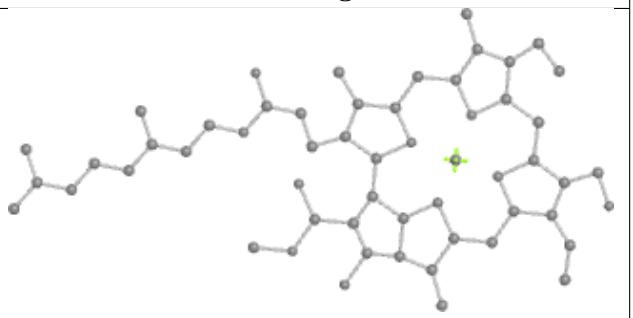
Bond lengths



Bond angles

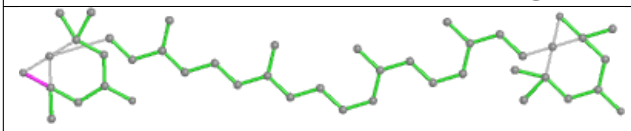


Torsions

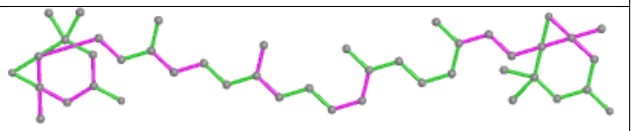


Rings

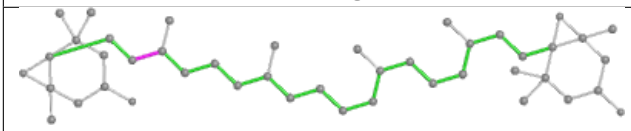
Ligand XAT 4 502



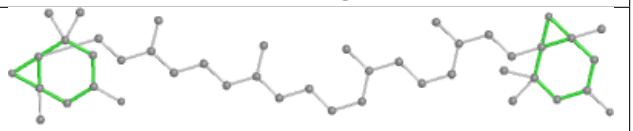
Bond lengths



Bond angles

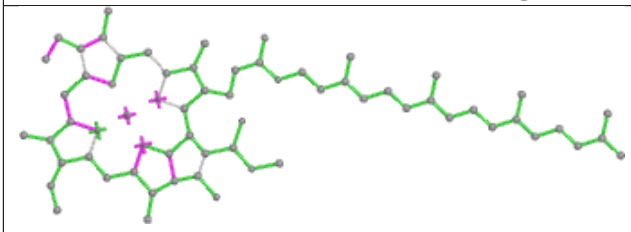


Torsions

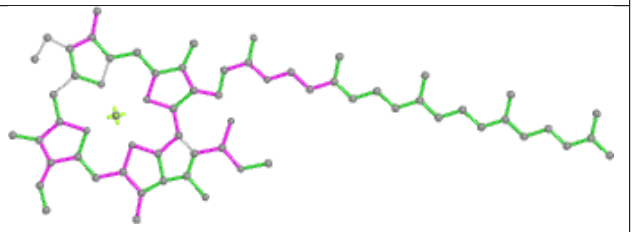


Rings

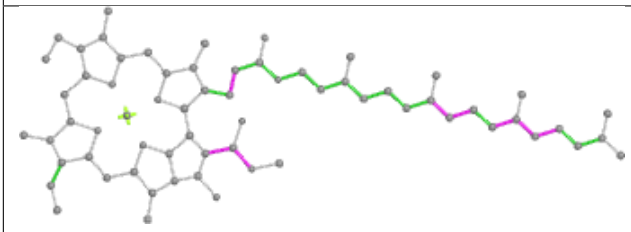
Ligand CLA B 1023



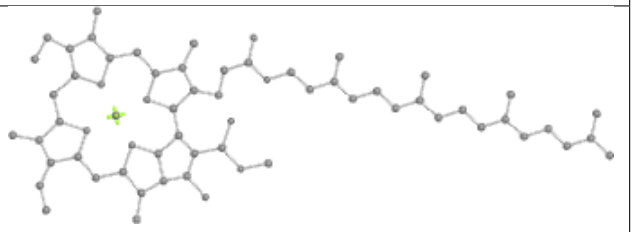
Bond lengths



Bond angles

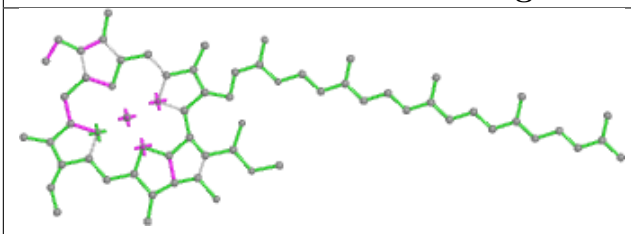


Torsions

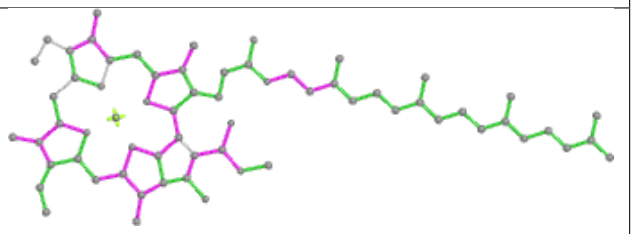


Rings

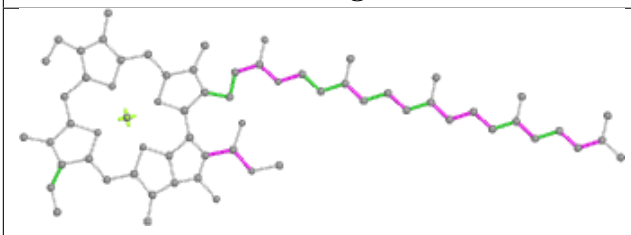
Ligand CLA B 1240



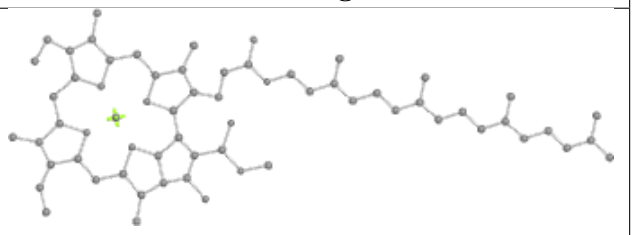
Bond lengths



Bond angles

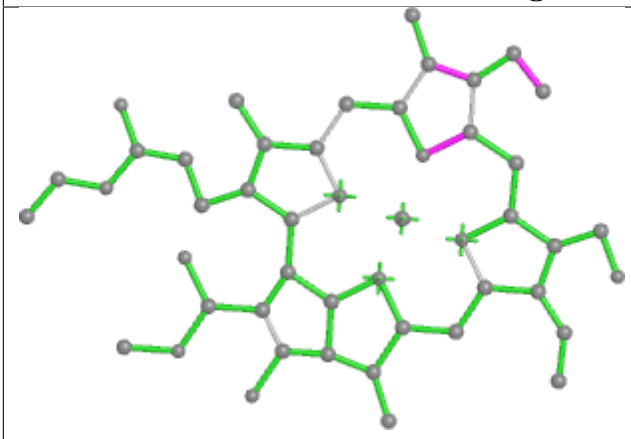


Torsions

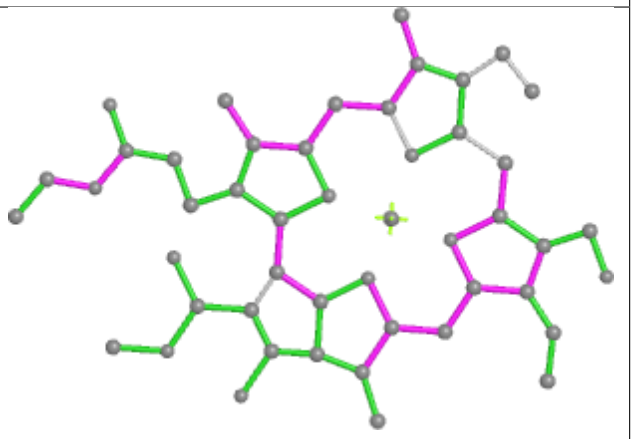


Rings

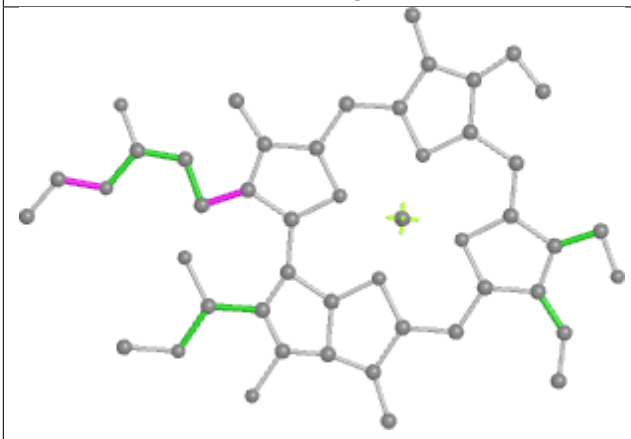
Ligand CHL 2 611



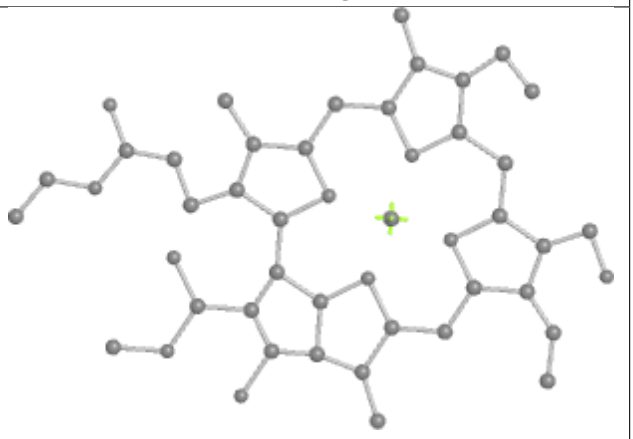
Bond lengths



Bond angles

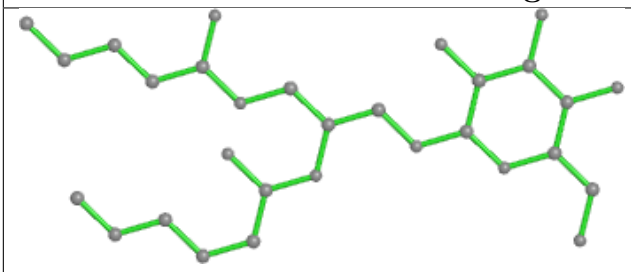


Torsions

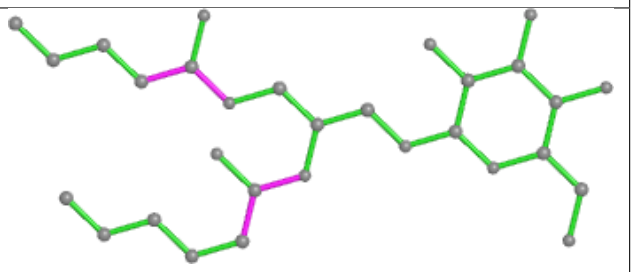


Rings

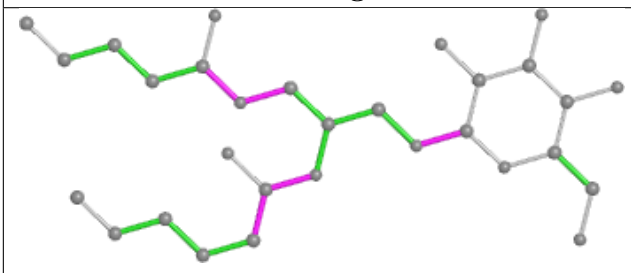
Ligand LMG 2 805



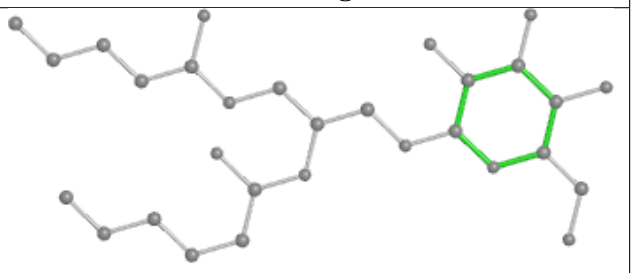
Bond lengths



Bond angles

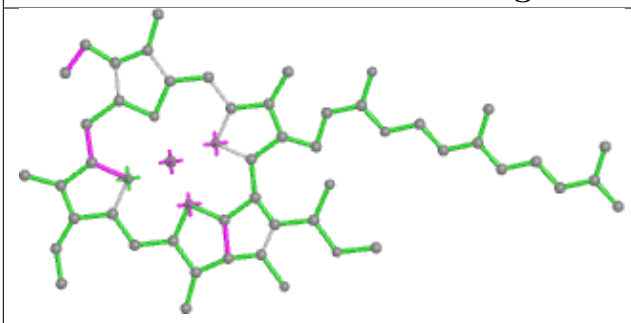


Torsions

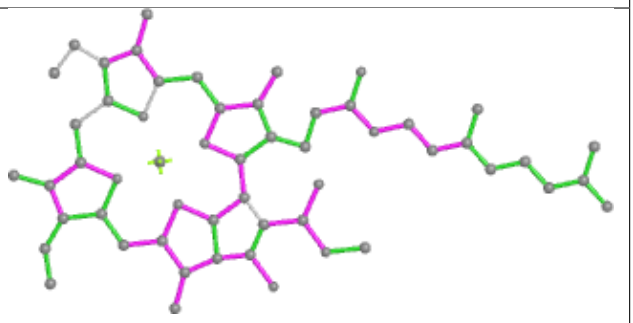


Rings

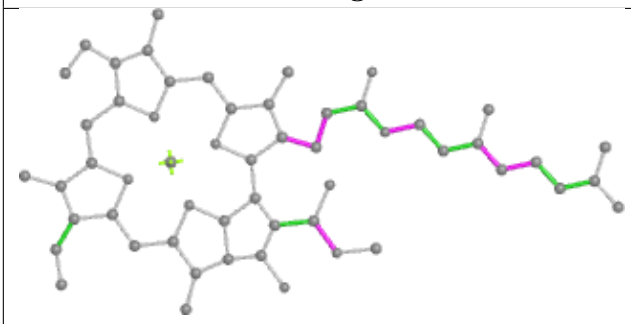
Ligand CLA G 1601



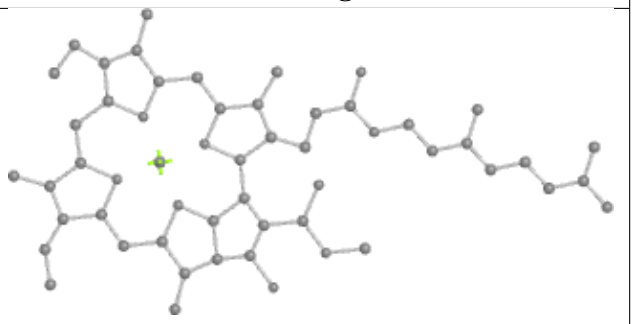
Bond lengths



Bond angles

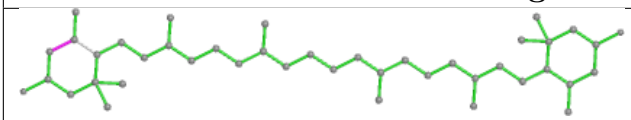


Torsions

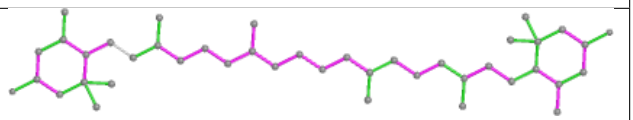


Rings

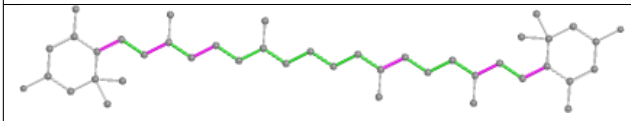
Ligand LUT 3 502



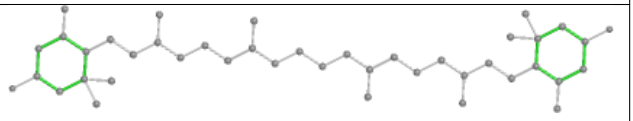
Bond lengths



Bond angles

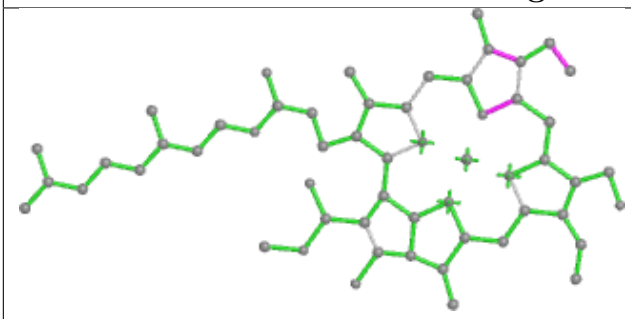


Torsions

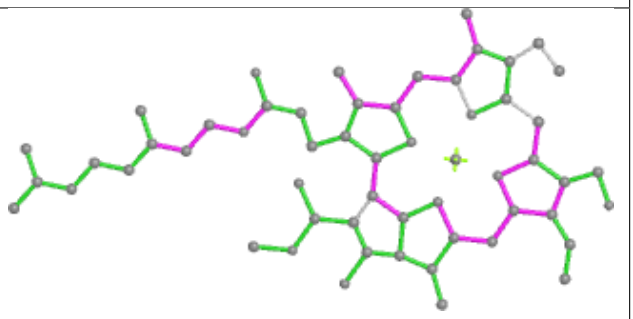


Rings

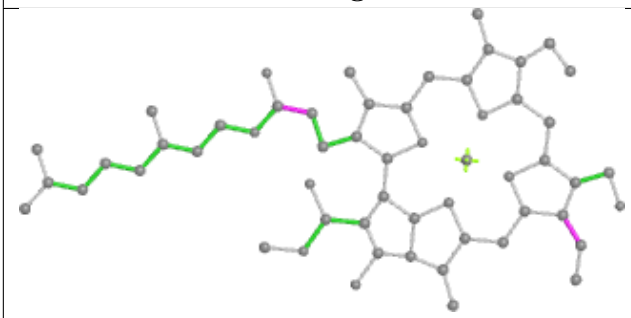
Ligand CHL 2 610



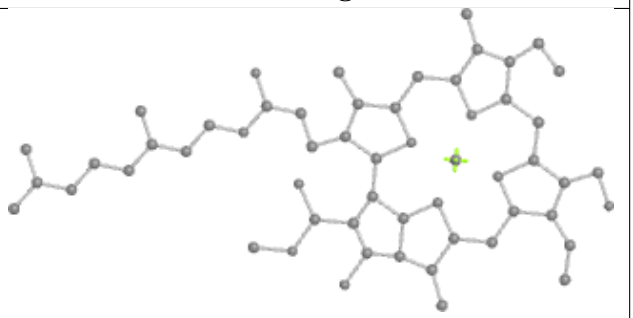
Bond lengths



Bond angles

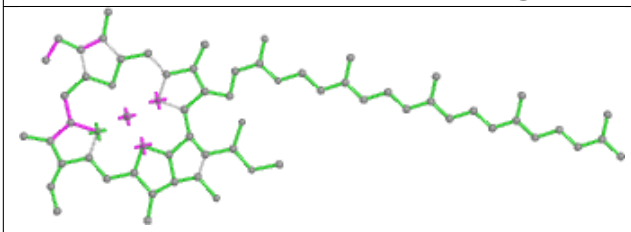


Torsions

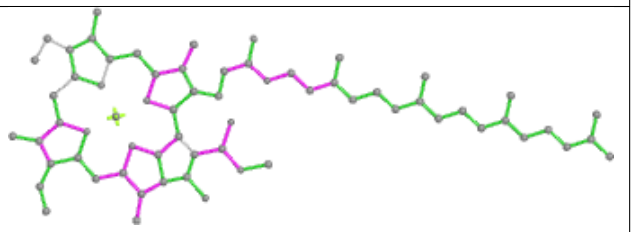


Rings

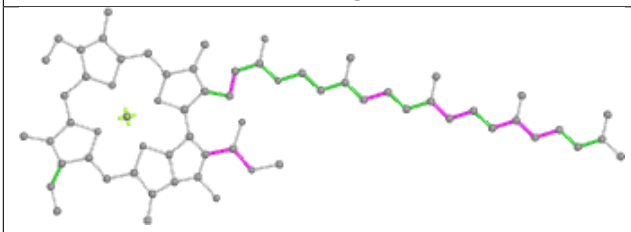
Ligand CLA A 1132



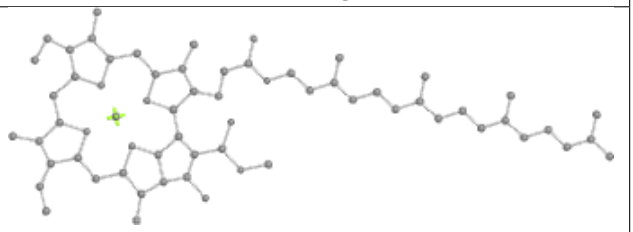
Bond lengths



Bond angles

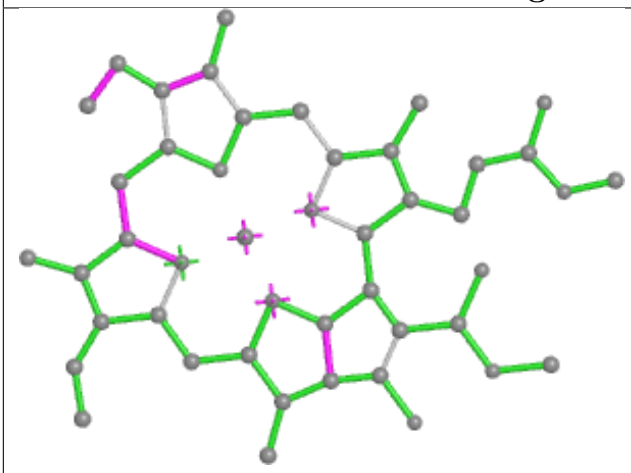


Torsions

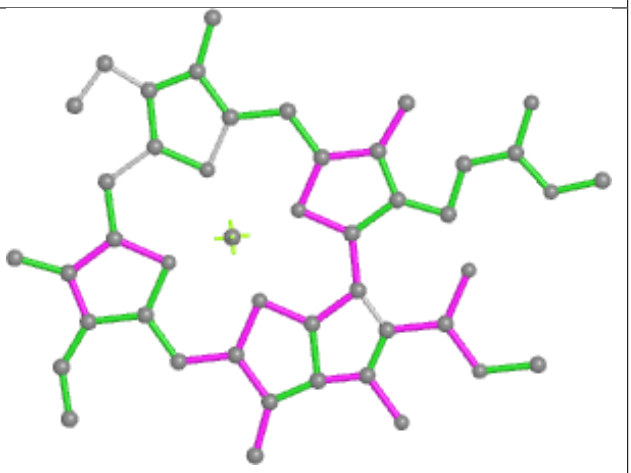


Rings

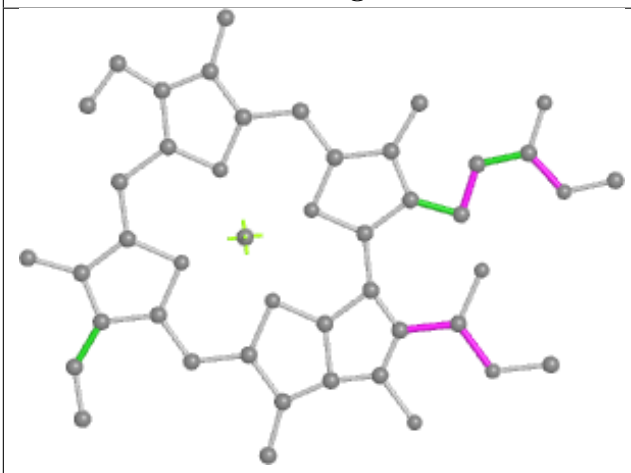
Ligand CLA 1 607



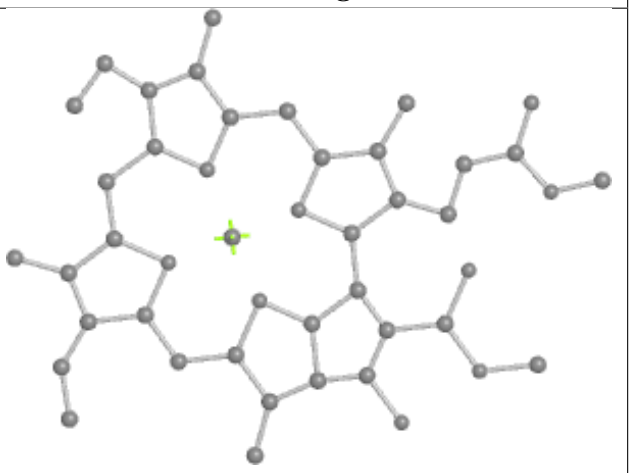
Bond lengths



Bond angles

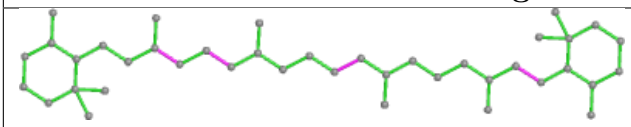


Torsions

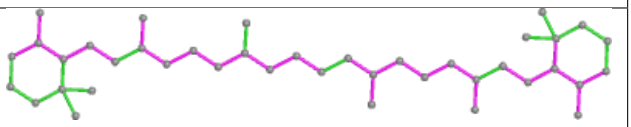


Rings

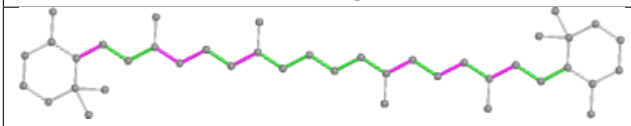
Ligand BCR H 4021



Bond lengths



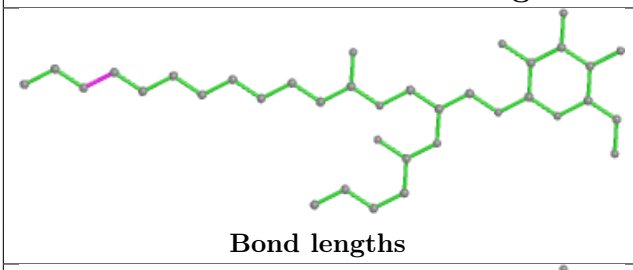
Bond angles



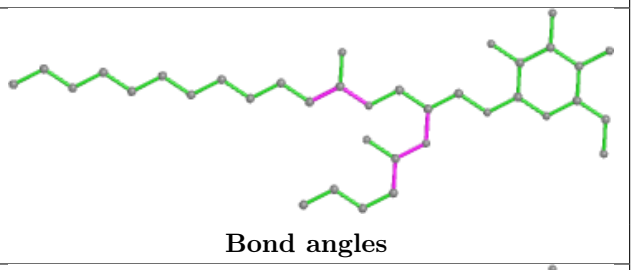
Torsions

Rings

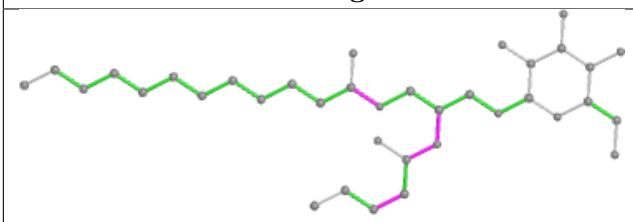
Ligand LMG F 5003



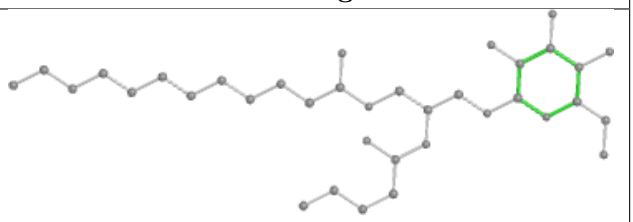
Bond lengths



Bond angles

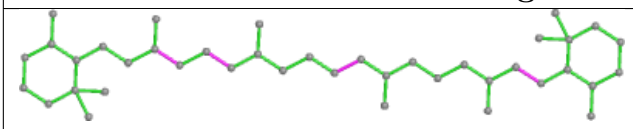


Torsions

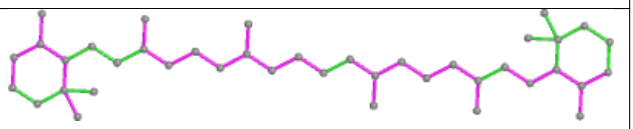


Rings

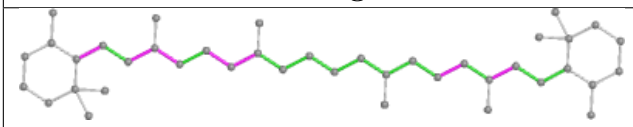
Ligand BCR J 4012



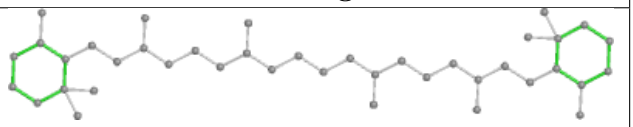
Bond lengths



Bond angles

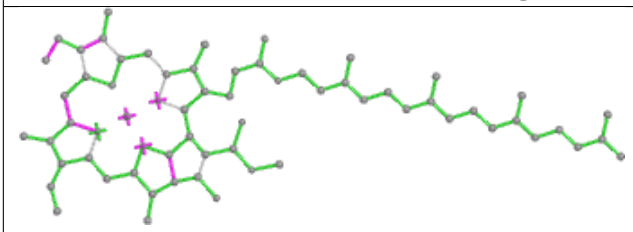


Torsions

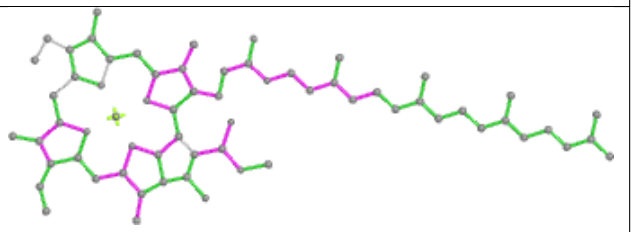


Rings

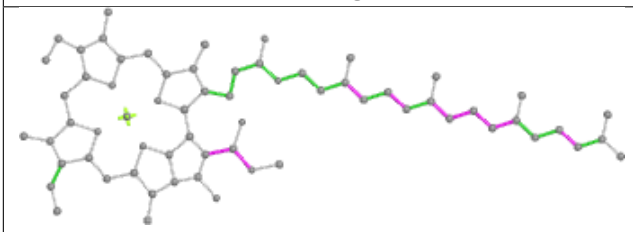
Ligand CLA A 1136



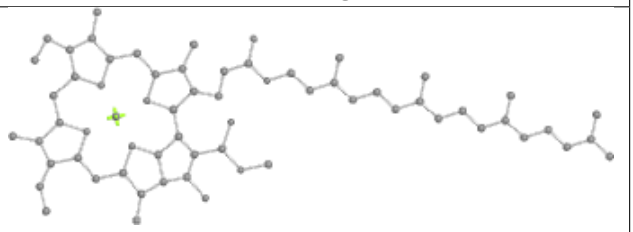
Bond lengths



Bond angles

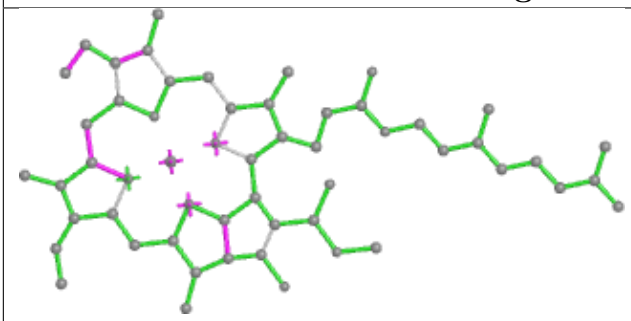


Torsions

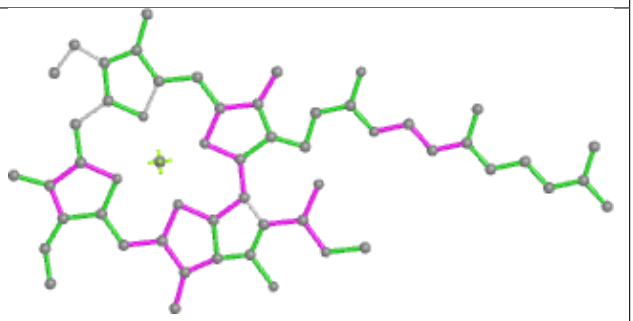


Rings

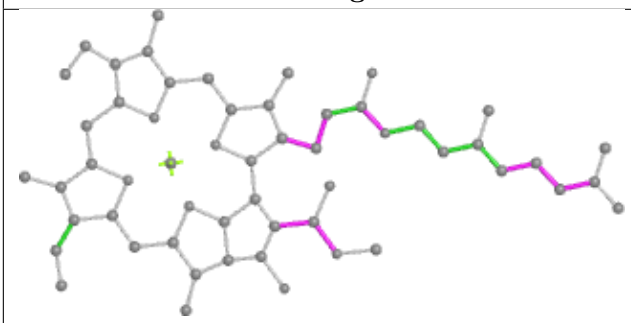
Ligand CLA A 1134



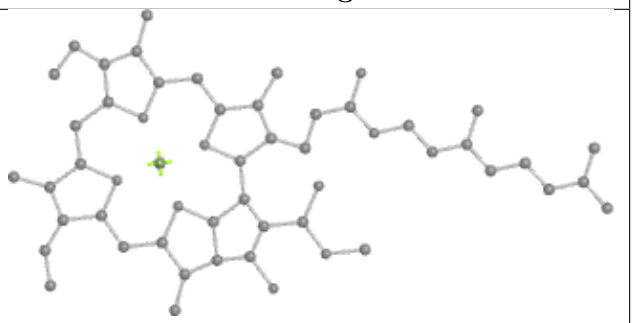
Bond lengths



Bond angles

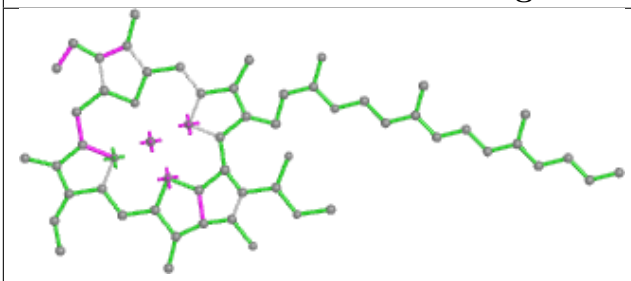


Torsions

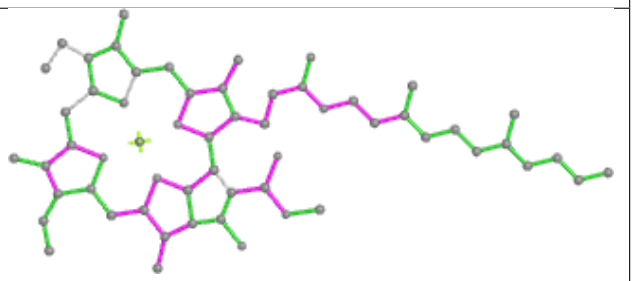


Rings

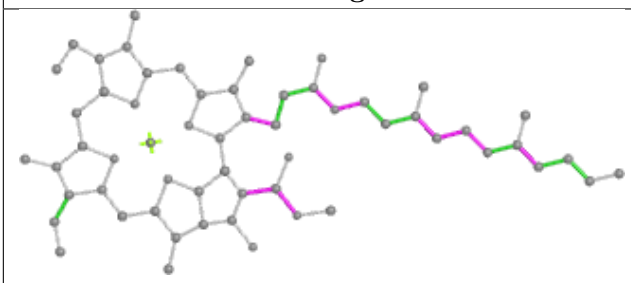
Ligand CLA B 1230



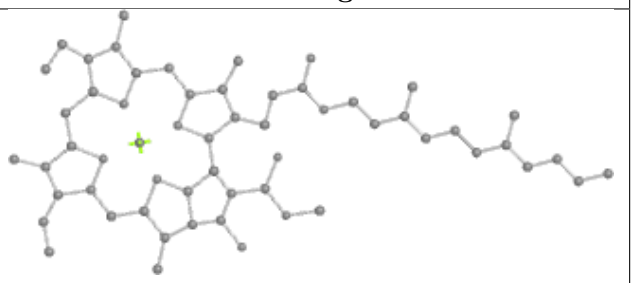
Bond lengths



Bond angles

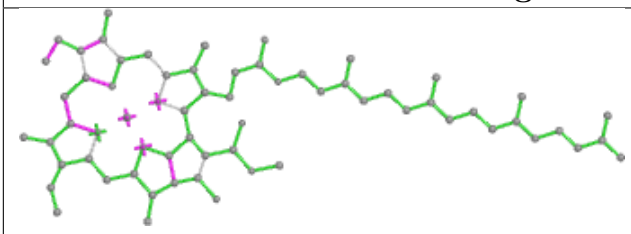


Torsions

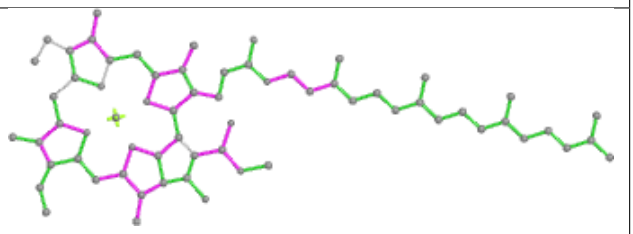


Rings

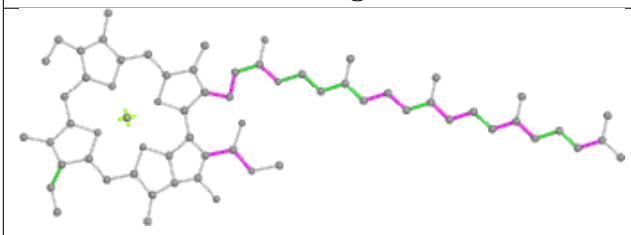
Ligand CLA A 1106



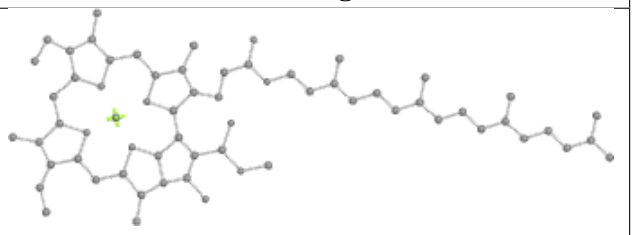
Bond lengths



Bond angles

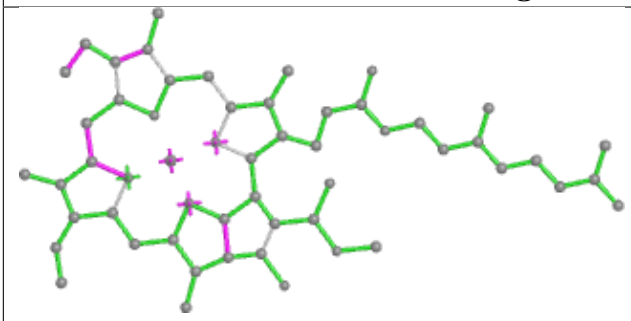


Torsions

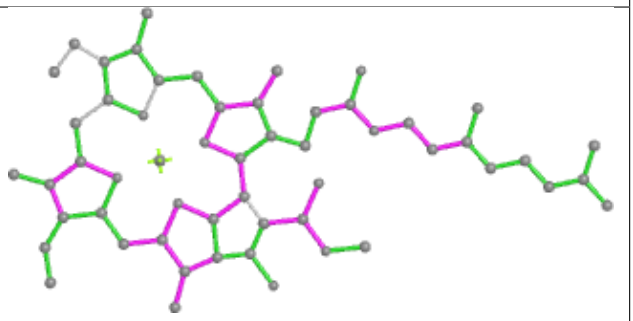


Rings

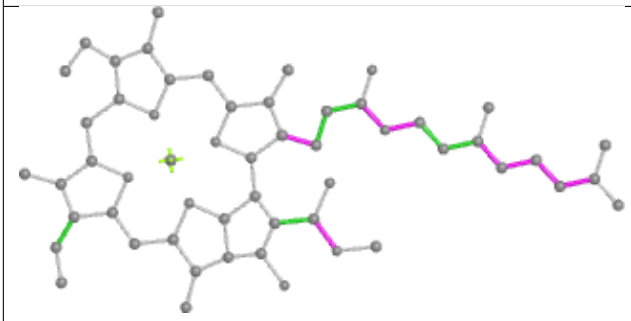
Ligand CLA B 1232



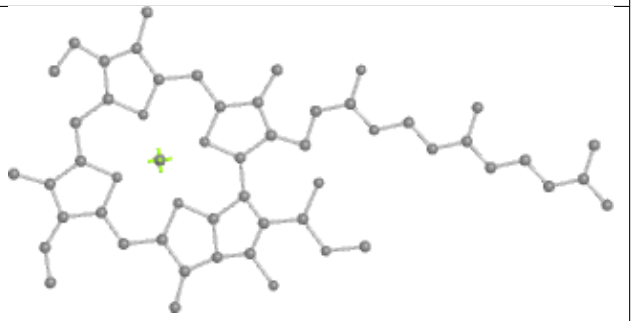
Bond lengths



Bond angles

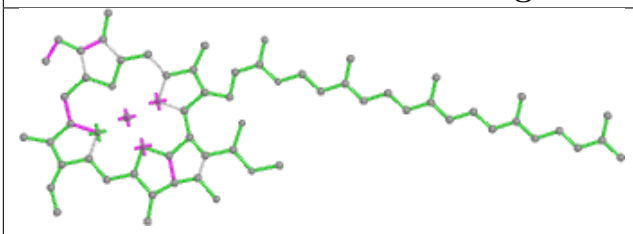


Torsions

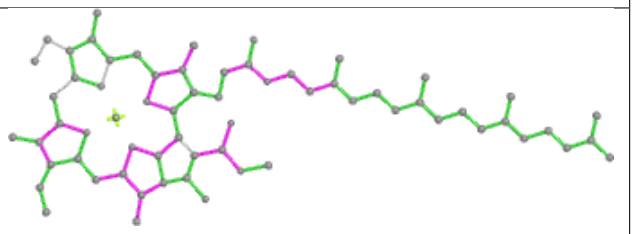


Rings

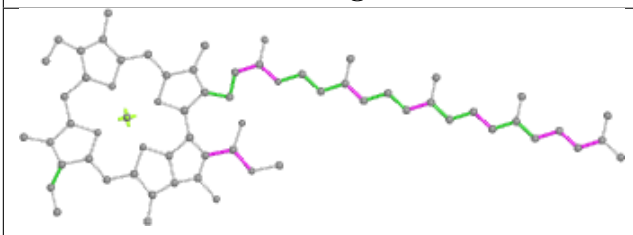
Ligand CLA A 1122



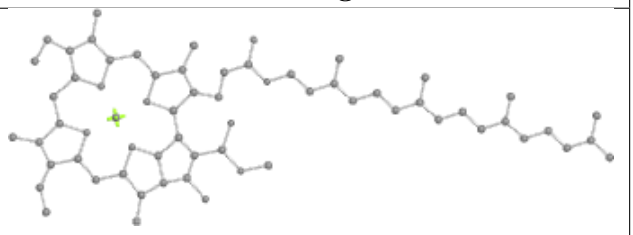
Bond lengths



Bond angles

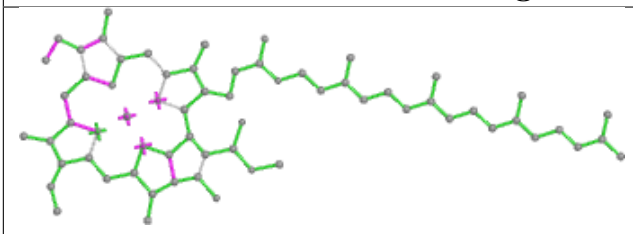


Torsions

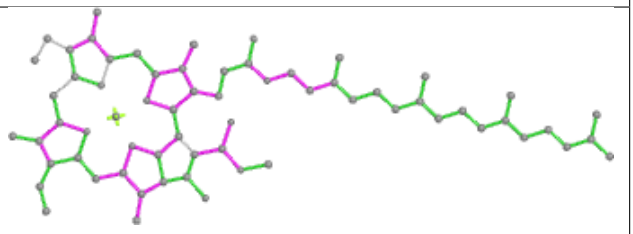


Rings

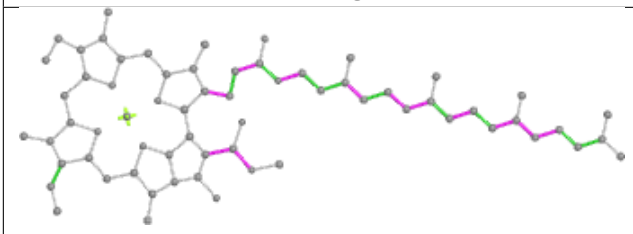
Ligand CLA A 1103



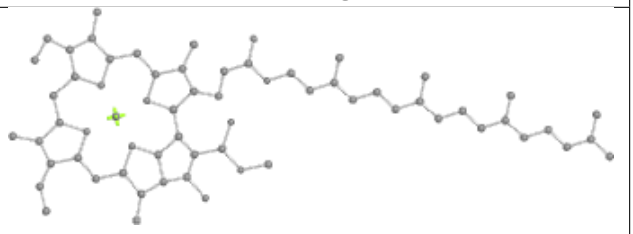
Bond lengths



Bond angles

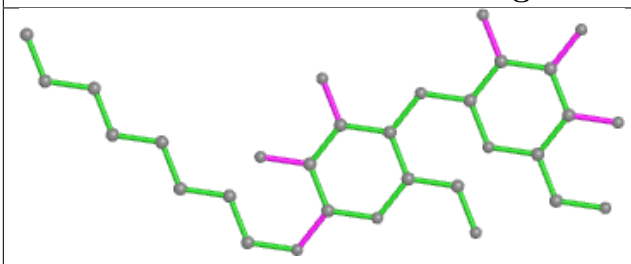


Torsions

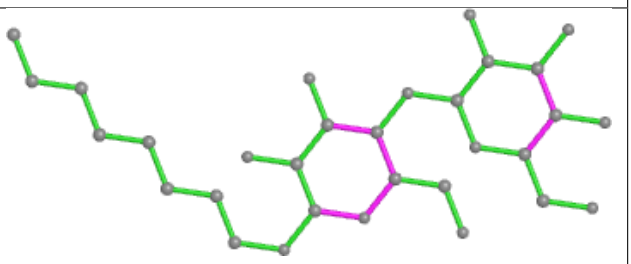


Rings

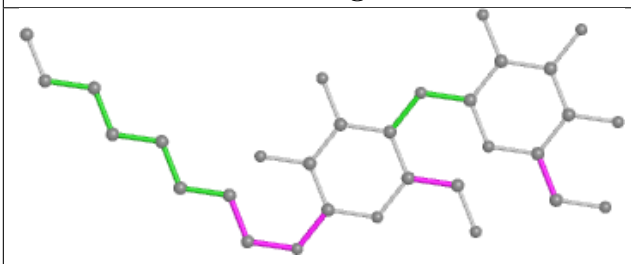
Ligand LMT B 5008



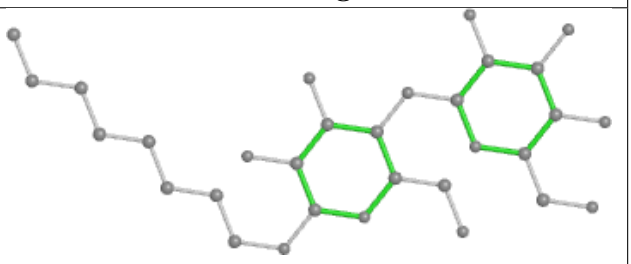
Bond lengths



Bond angles

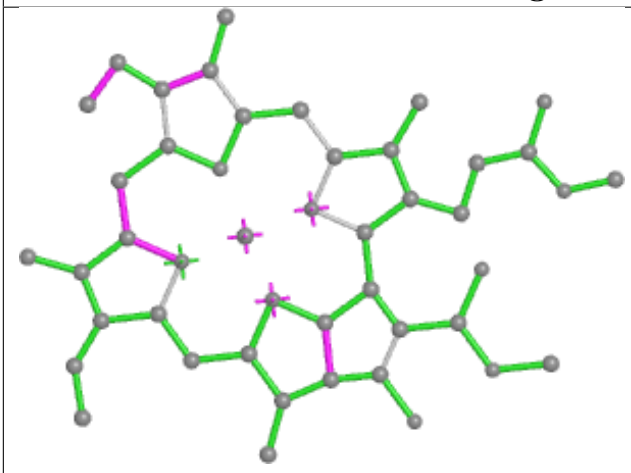


Torsions

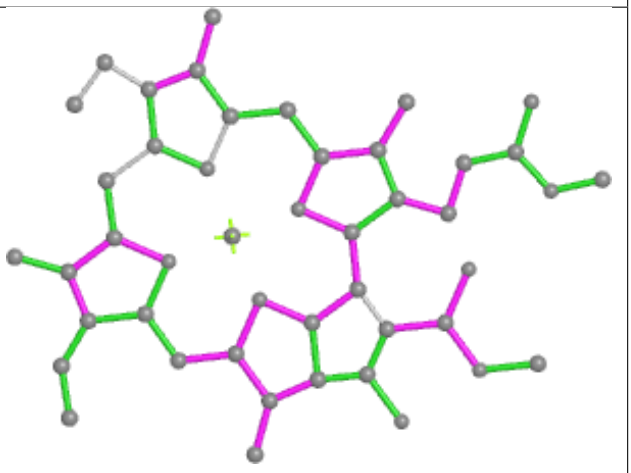


Rings

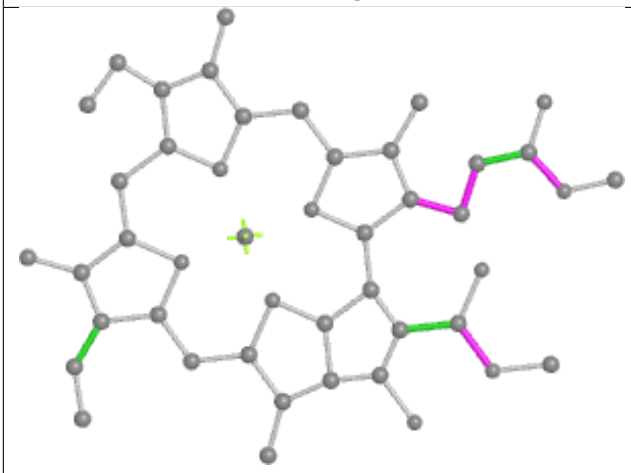
Ligand CLA 3 613



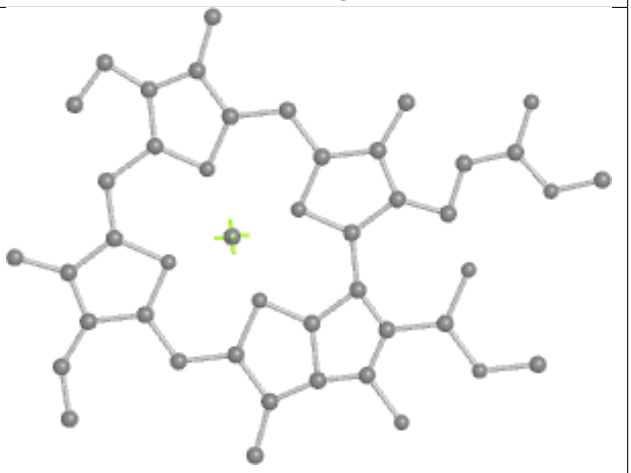
Bond lengths



Bond angles

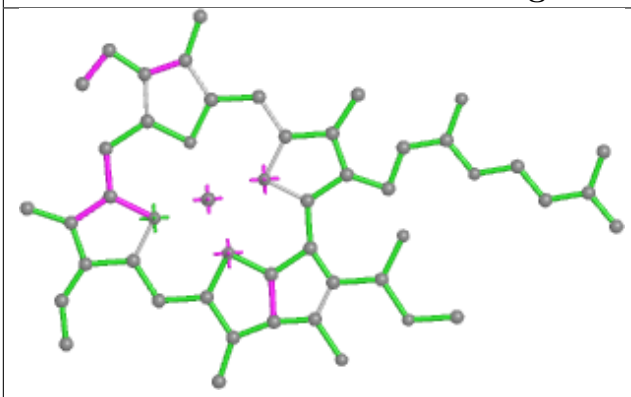


Torsions

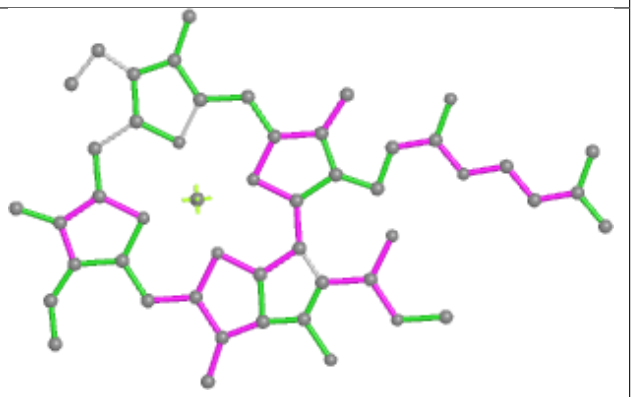


Rings

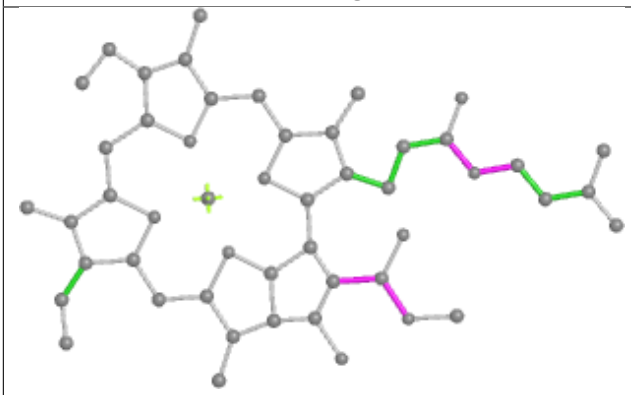
Ligand CLA 4 602



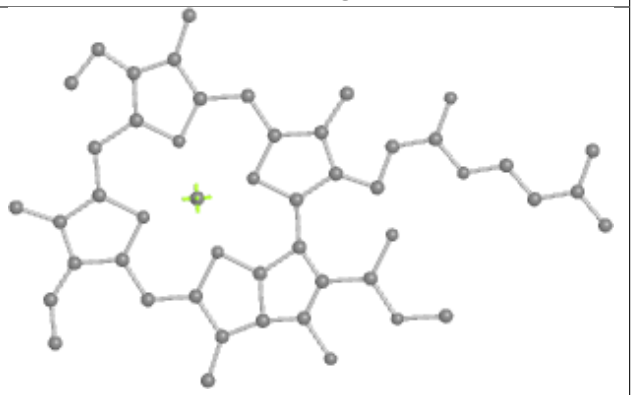
Bond lengths



Bond angles

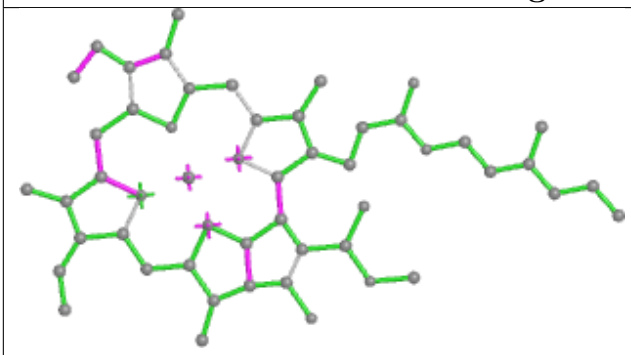


Torsions

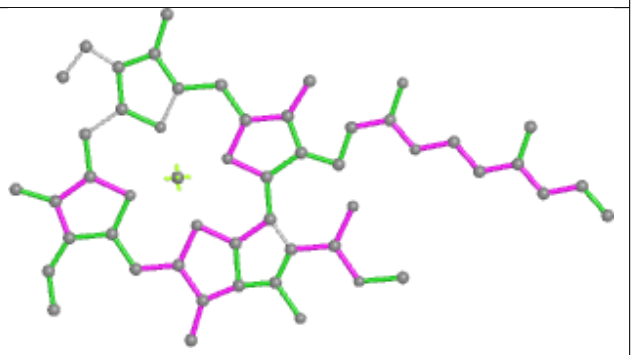


Rings

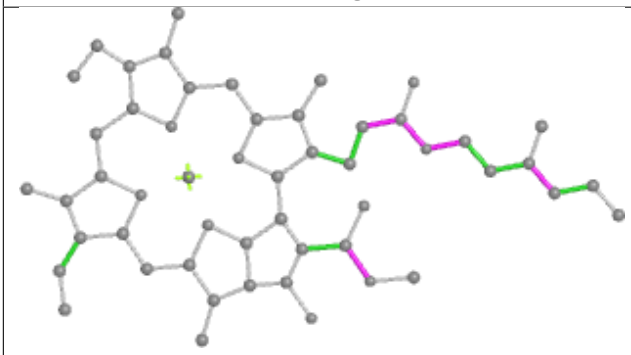
Ligand CLA 3 602



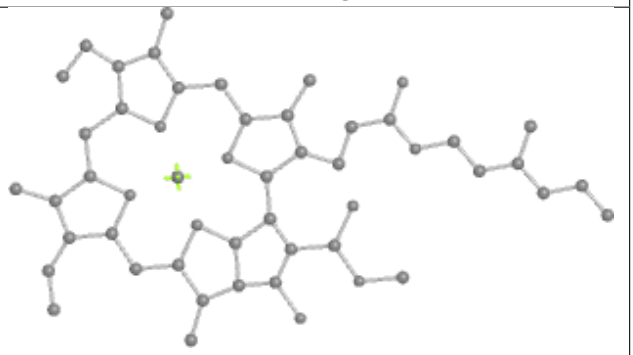
Bond lengths



Bond angles

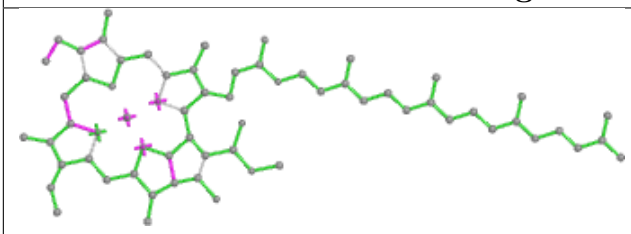


Torsions

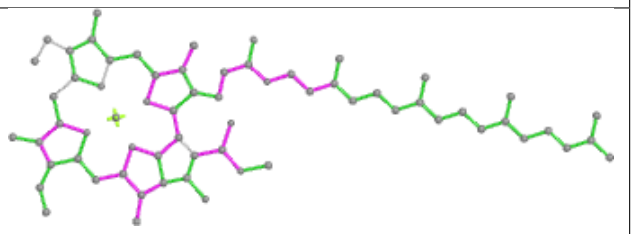


Rings

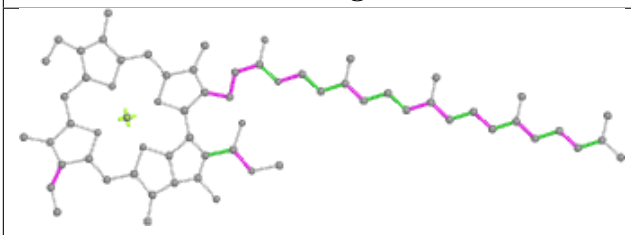
Ligand CLA B 1239



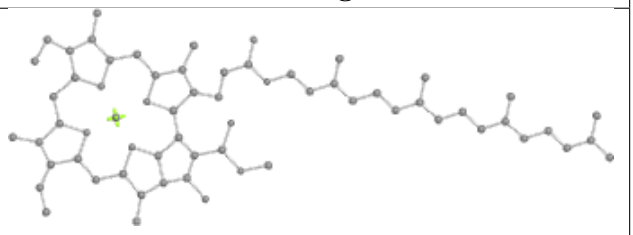
Bond lengths



Bond angles

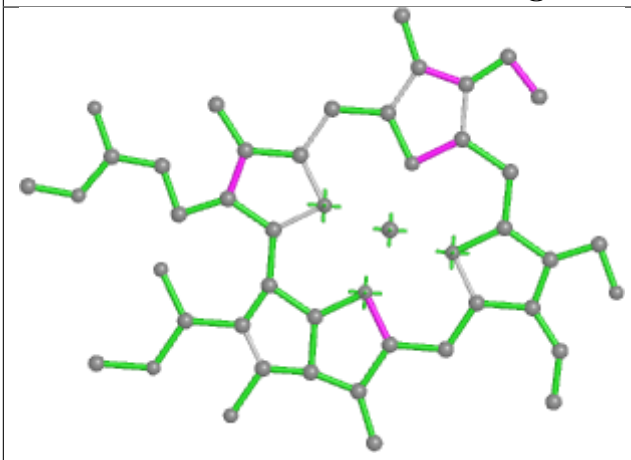


Torsions

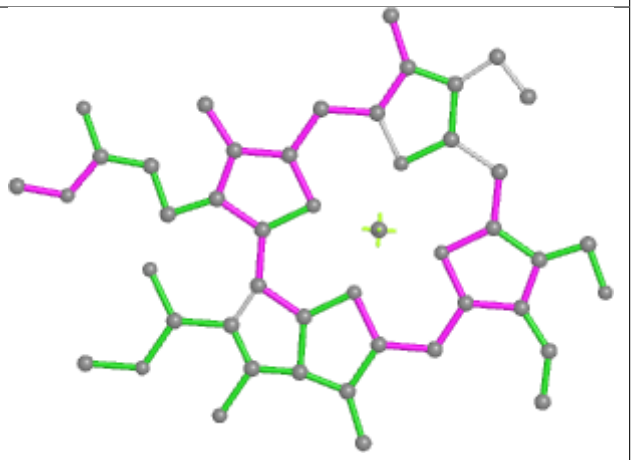


Rings

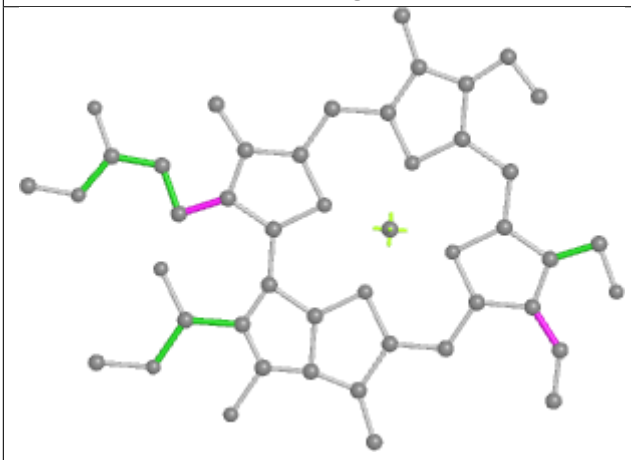
Ligand CHL 4 610



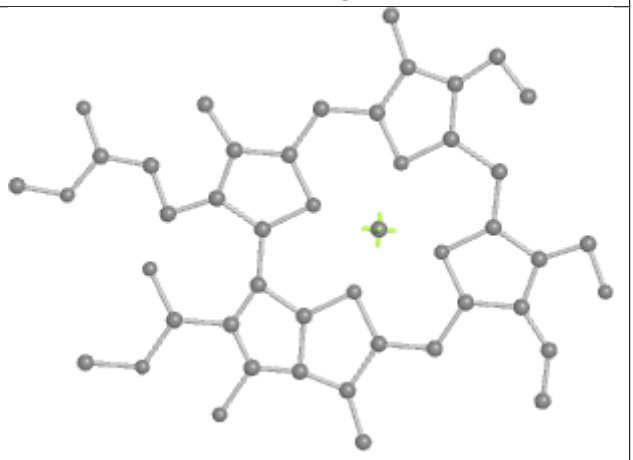
Bond lengths



Bond angles

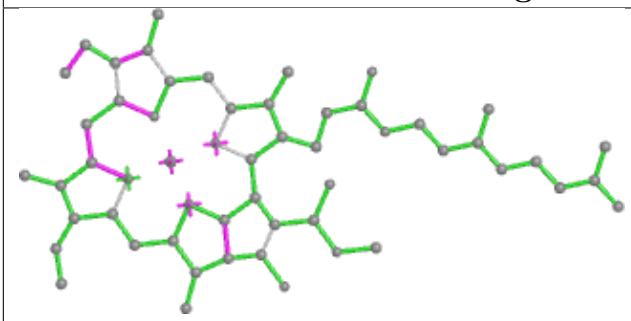


Torsions

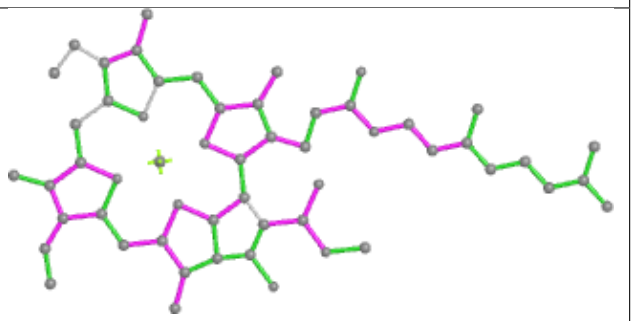


Rings

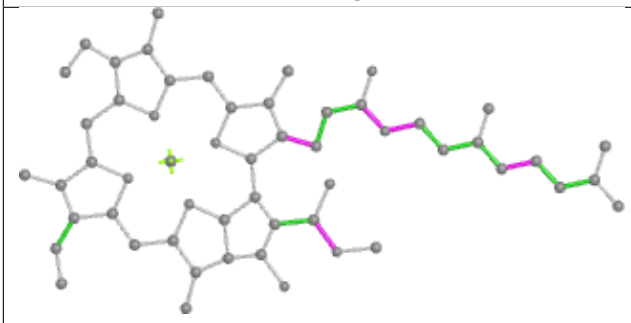
Ligand CLA A 1124



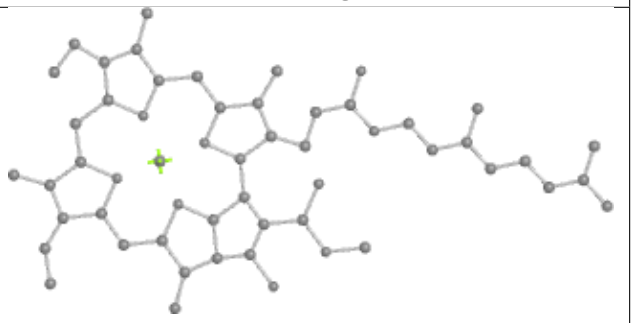
Bond lengths



Bond angles

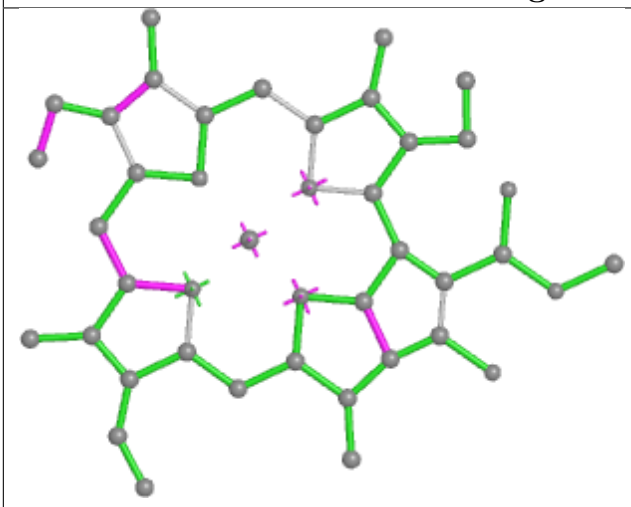


Torsions

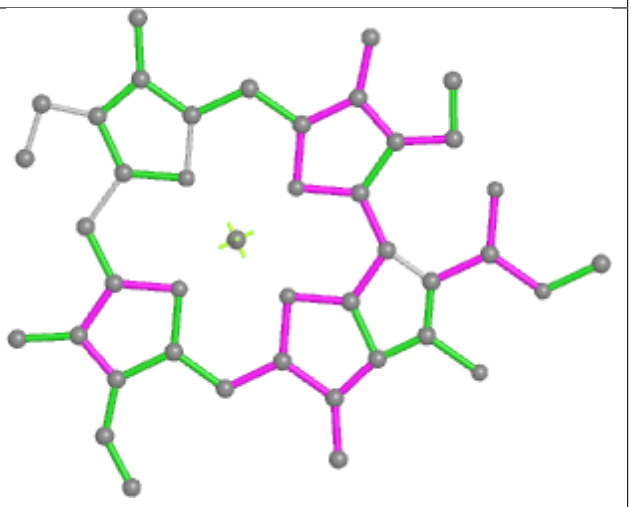


Rings

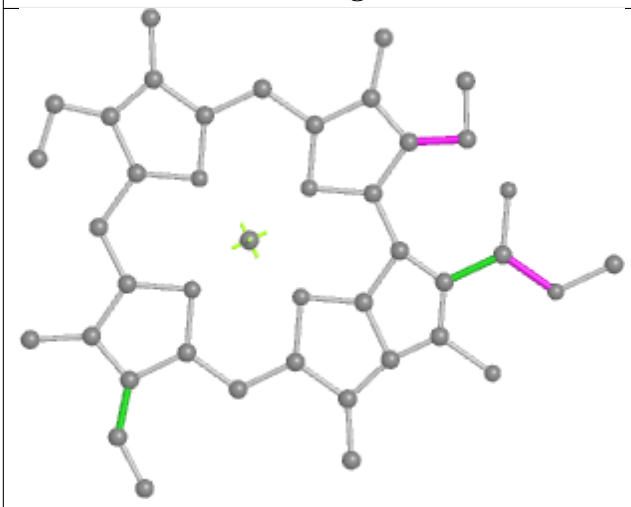
Ligand CLA 3 614



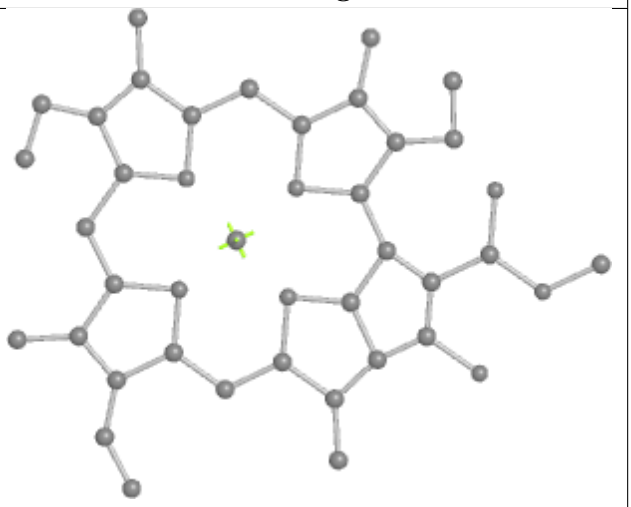
Bond lengths



Bond angles

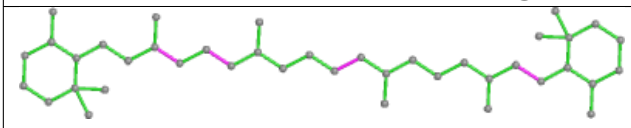


Torsions

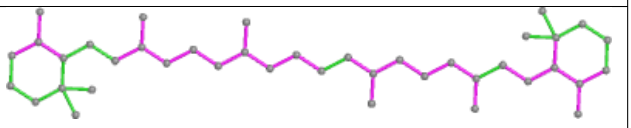


Rings

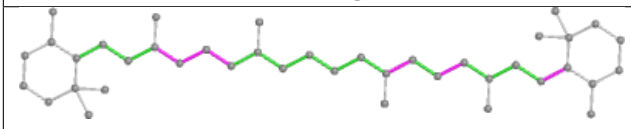
Ligand BCR L 4020



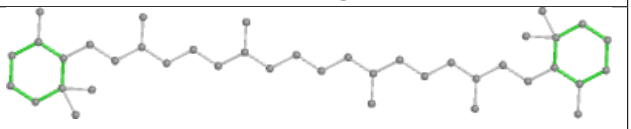
Bond lengths



Bond angles

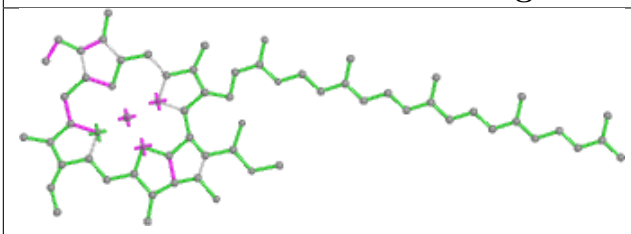


Torsions

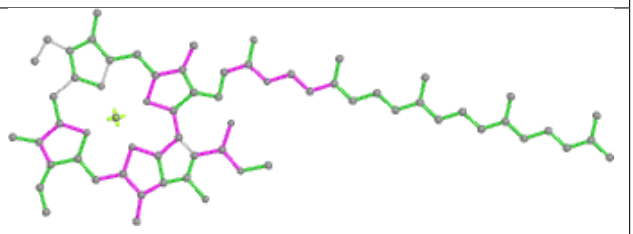


Rings

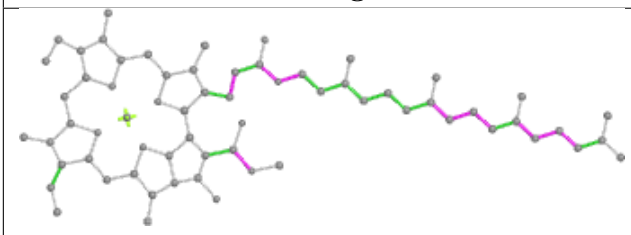
Ligand CLA B 1214



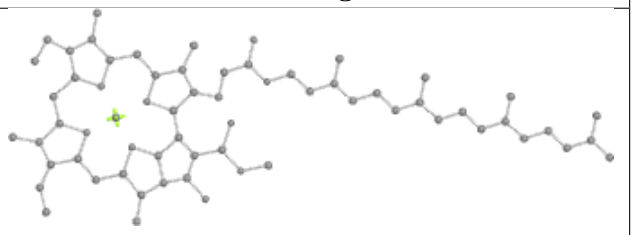
Bond lengths



Bond angles

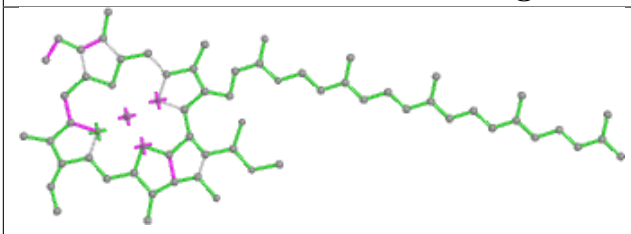


Torsions

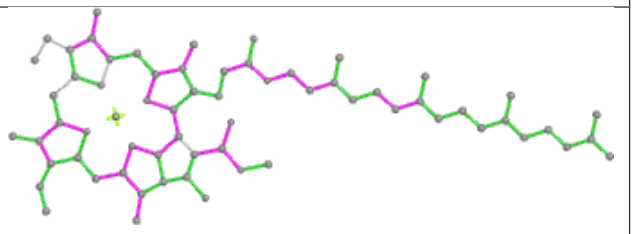


Rings

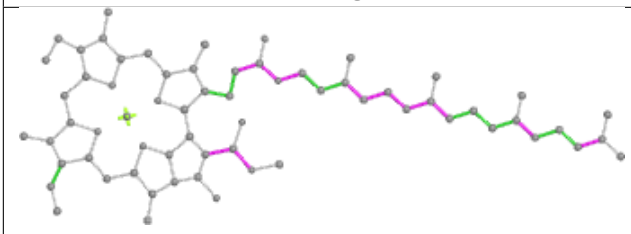
Ligand CLA B 1206



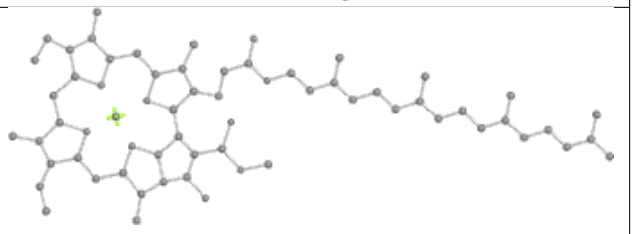
Bond lengths



Bond angles

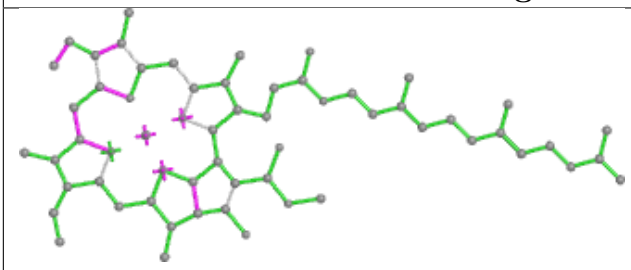


Torsions

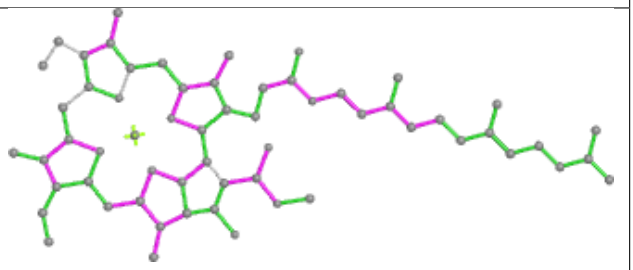


Rings

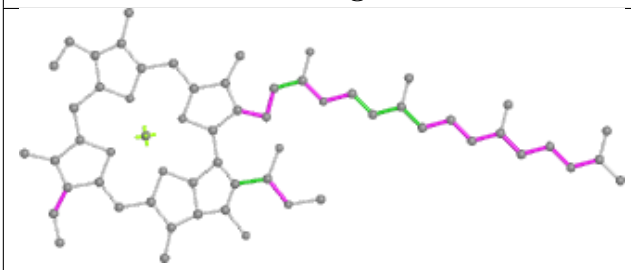
Ligand CLA A 1105



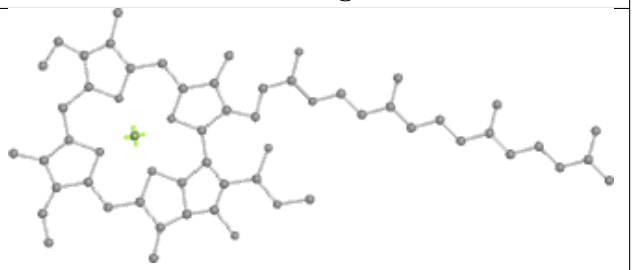
Bond lengths



Bond angles

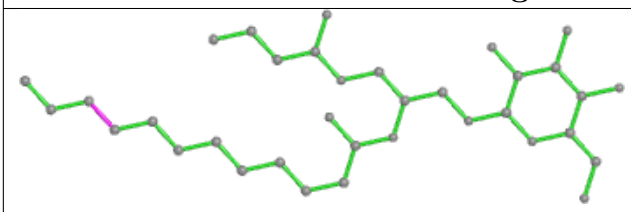


Torsions

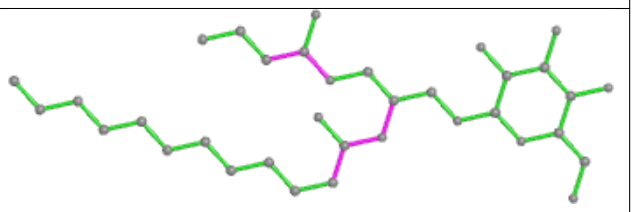


Rings

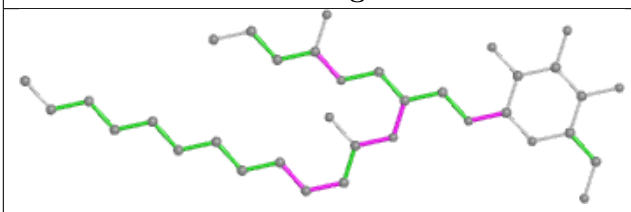
Ligand LMG B 5003



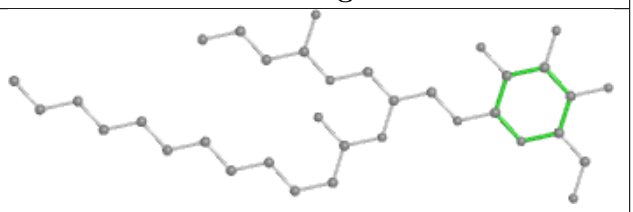
Bond lengths



Bond angles

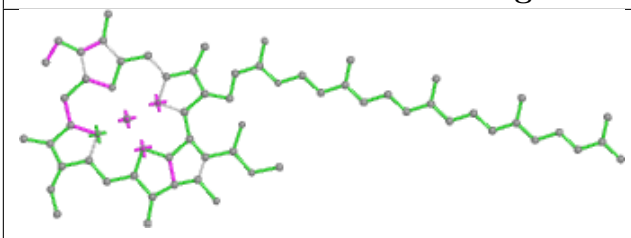


Torsions

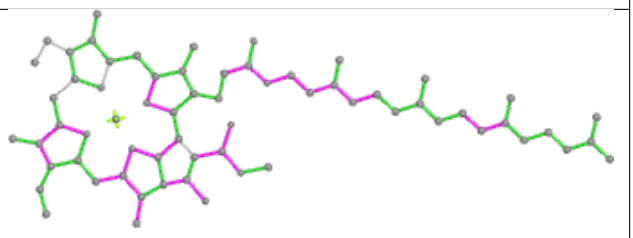


Rings

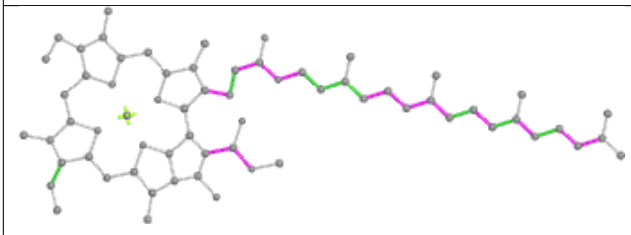
Ligand CLA A 1126



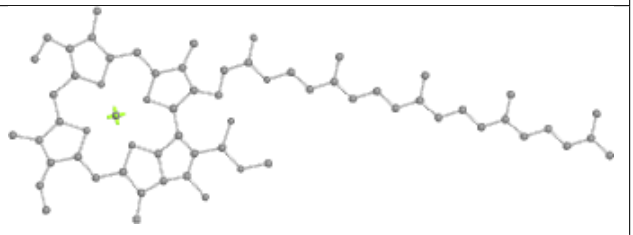
Bond lengths



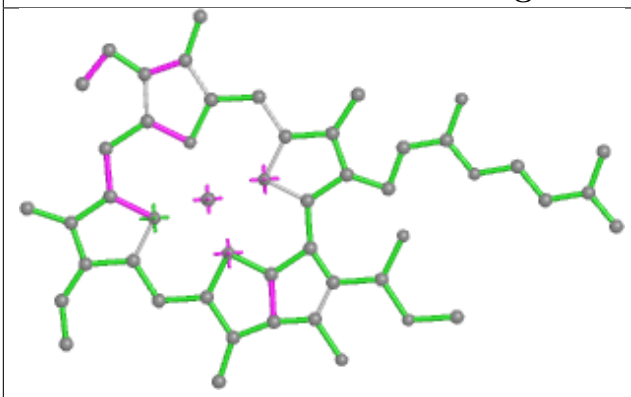
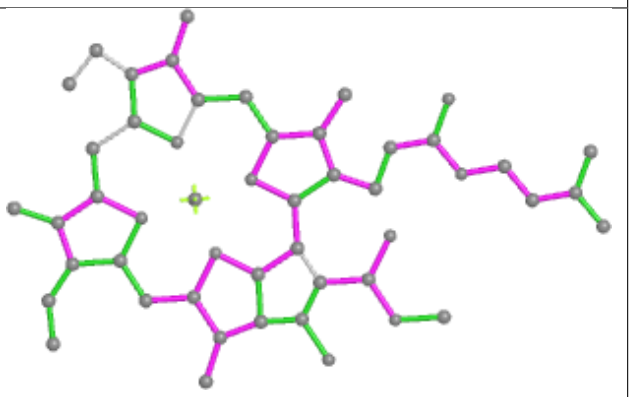
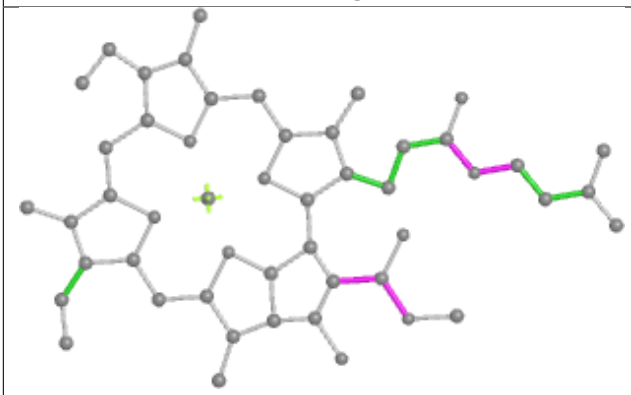
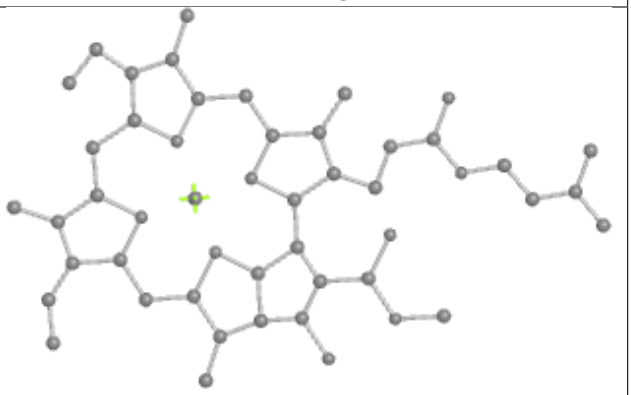
Bond angles

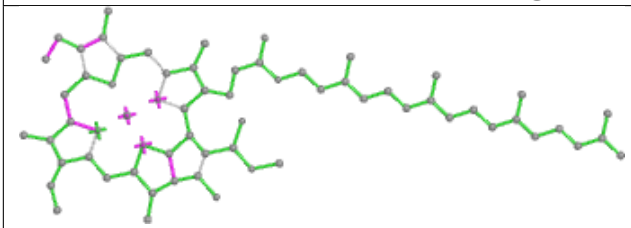
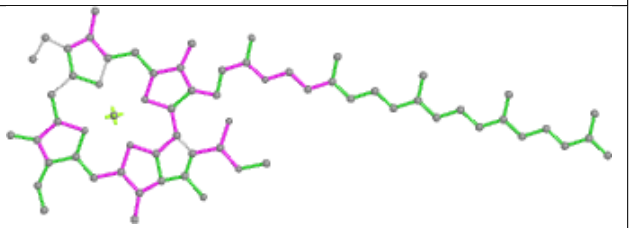
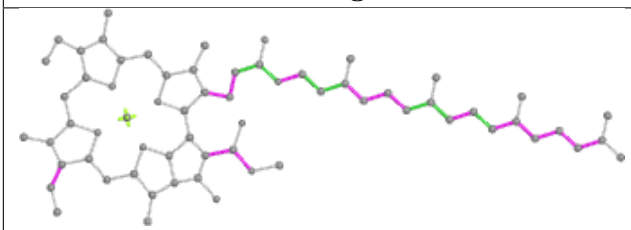
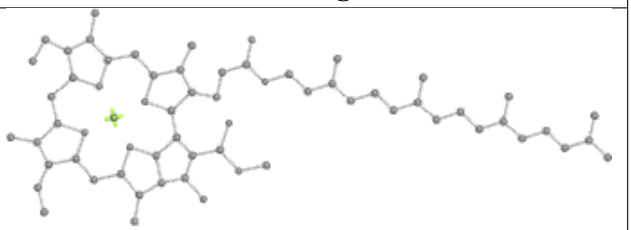


Torsions

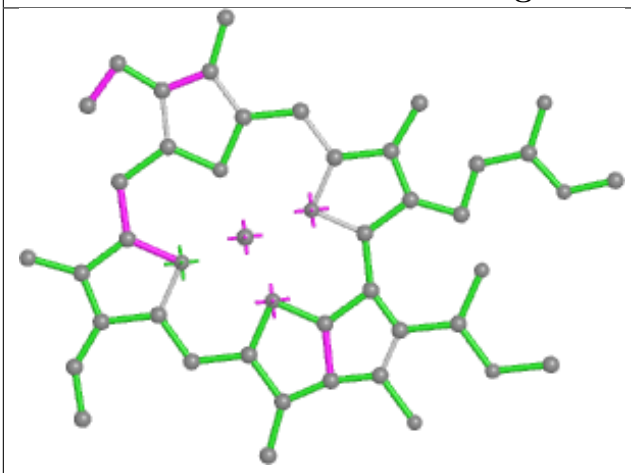


Rings

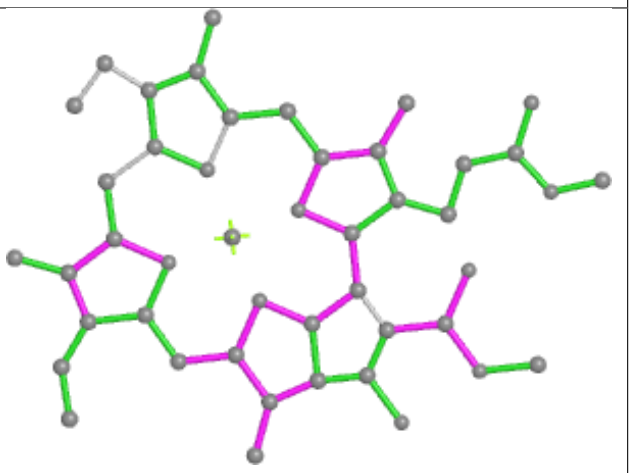
Ligand CLA A 1108	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA 1 601	
 Bond lengths	 Bond angles
 Torsions	 Rings

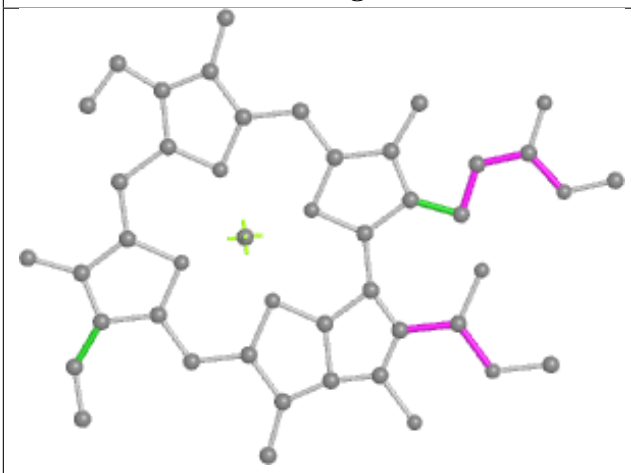
Ligand CLA A 1114



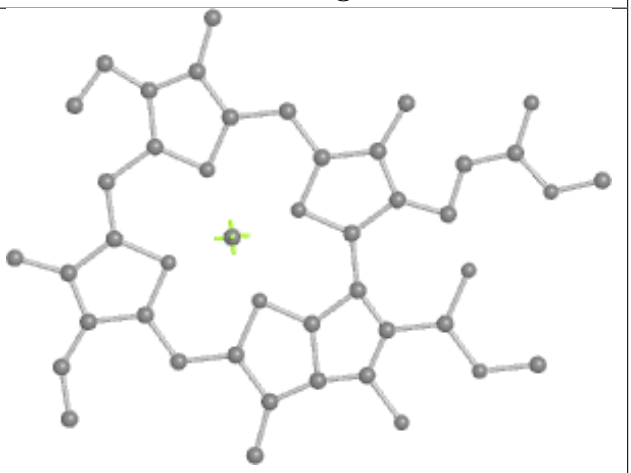
Bond lengths



Bond angles

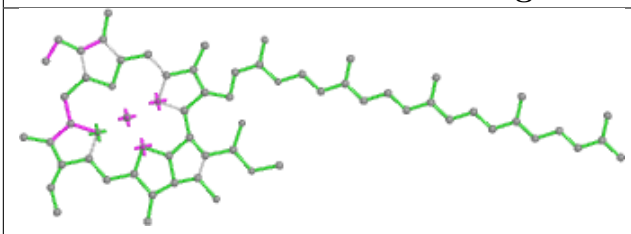


Torsions

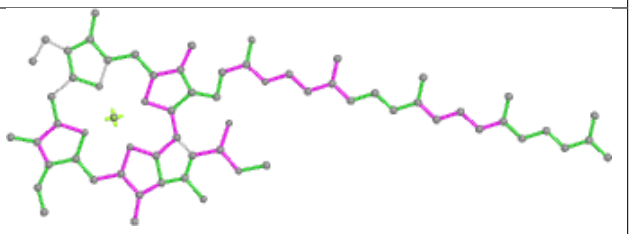


Rings

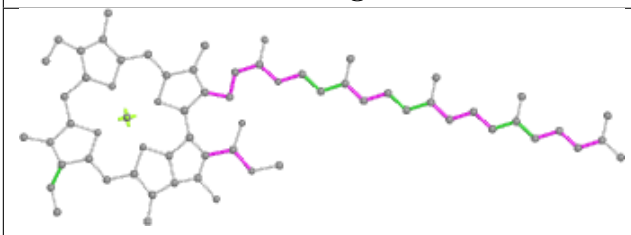
Ligand CLA B 1237



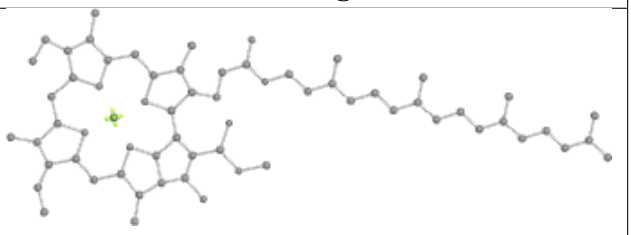
Bond lengths



Bond angles

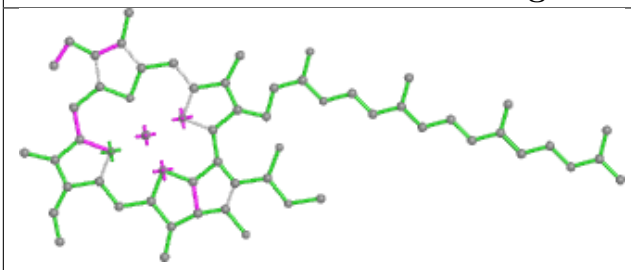


Torsions

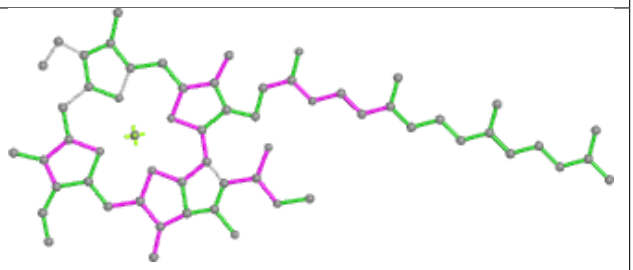


Rings

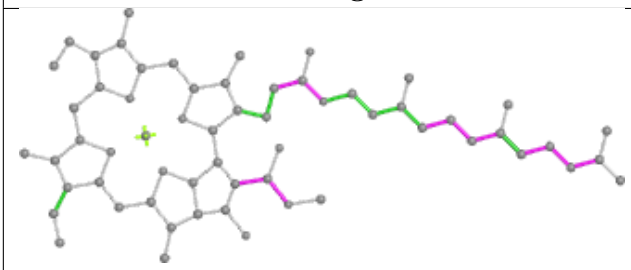
Ligand CLA 1 614



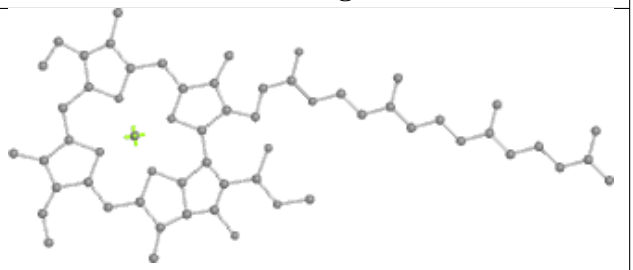
Bond lengths



Bond angles

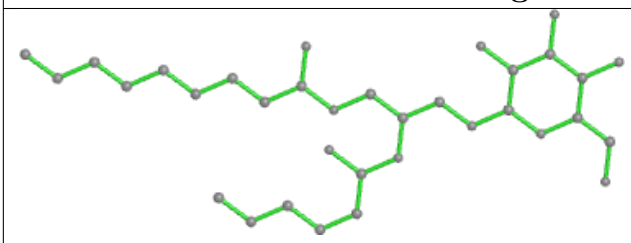


Torsions

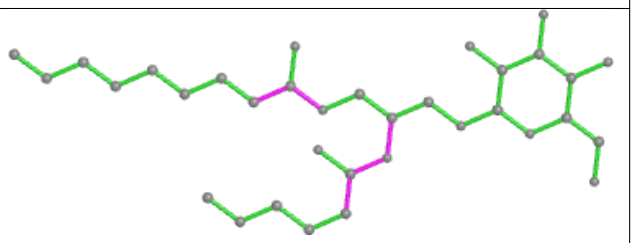


Rings

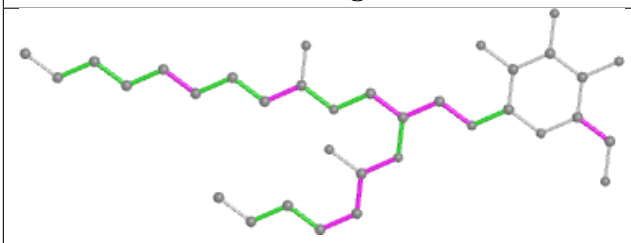
Ligand LMG B 5007



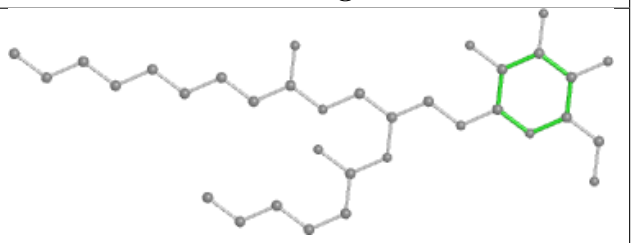
Bond lengths



Bond angles

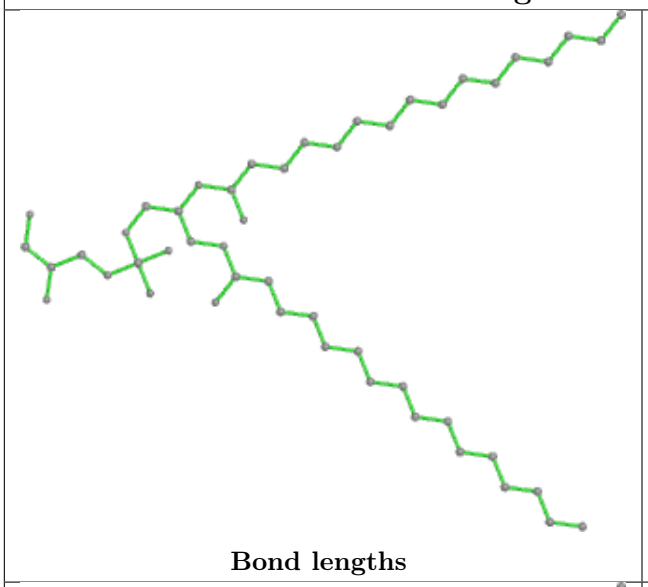


Torsions

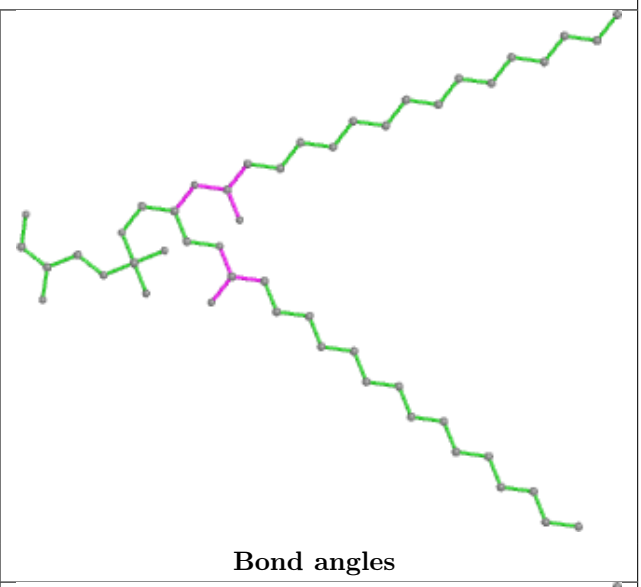


Rings

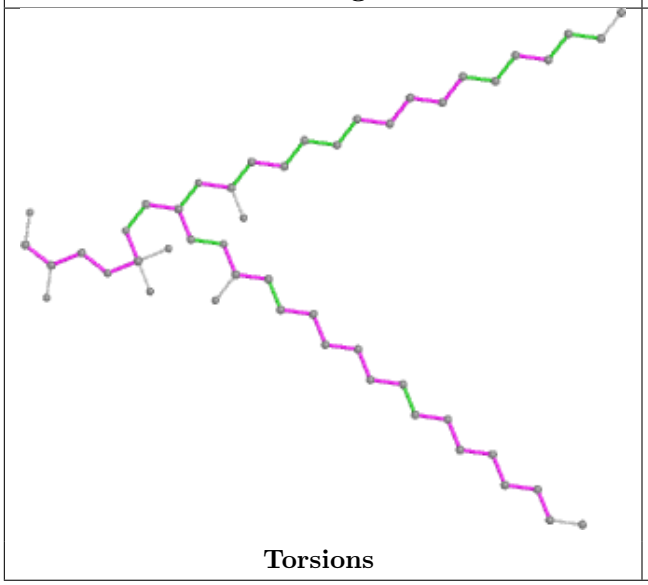
Ligand LHG A 5002



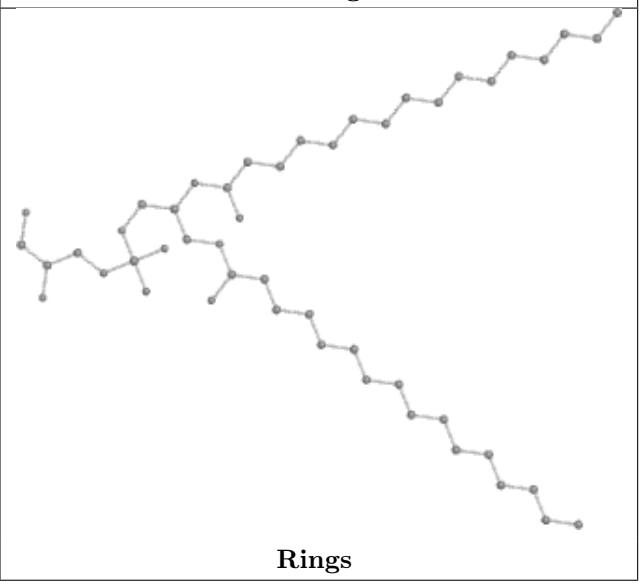
Bond lengths



Bond angles

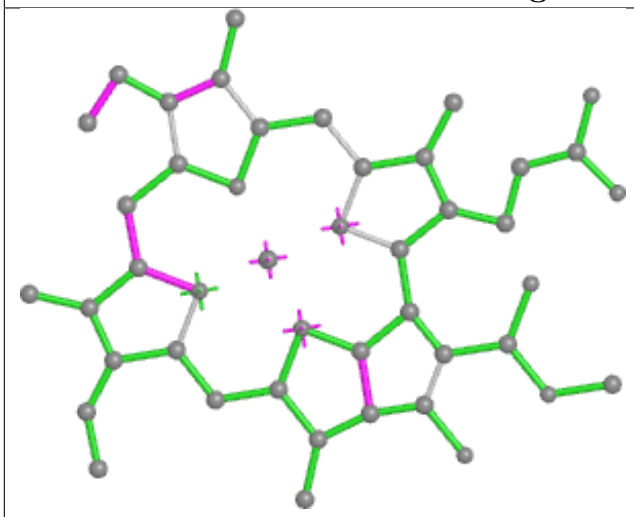


Torsions

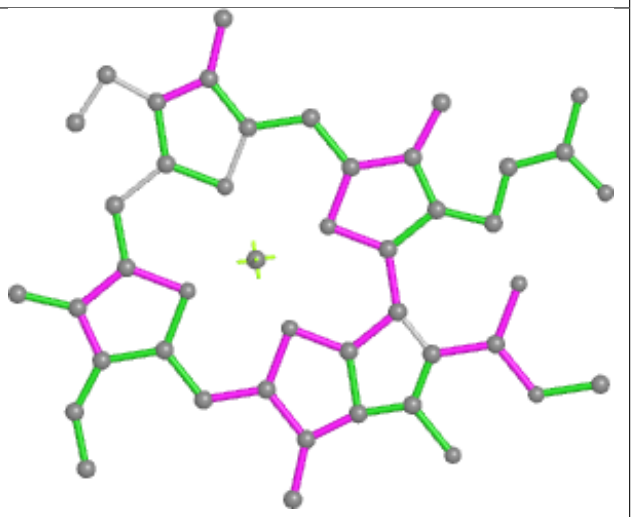


Rings

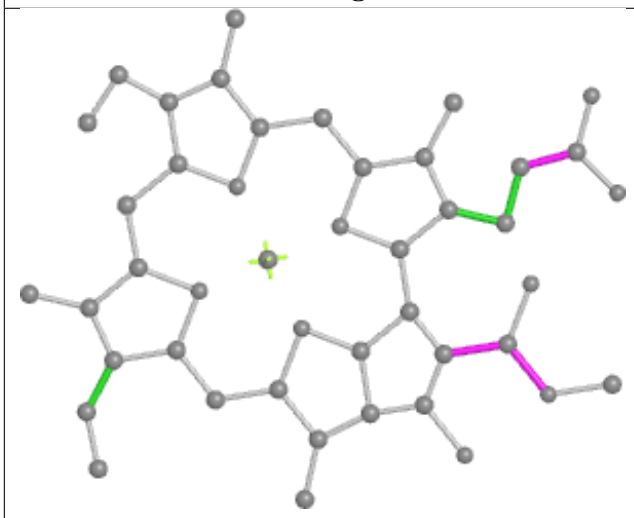
Ligand CLA 1 613



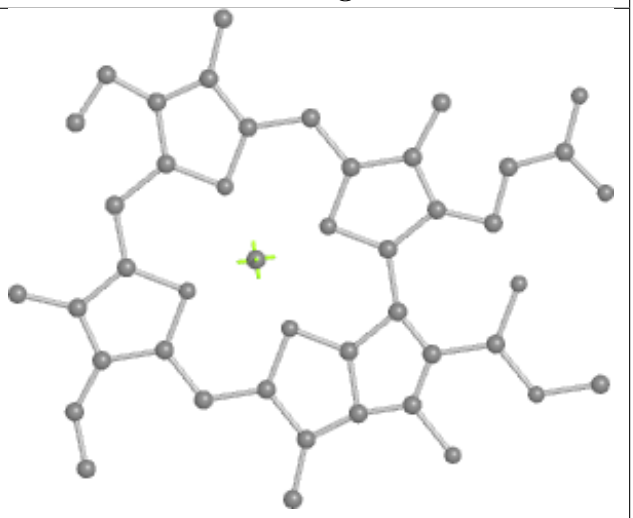
Bond lengths



Bond angles

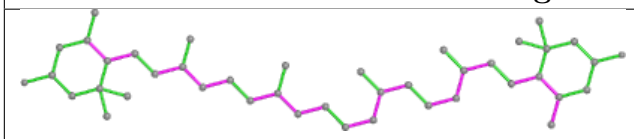


Torsions

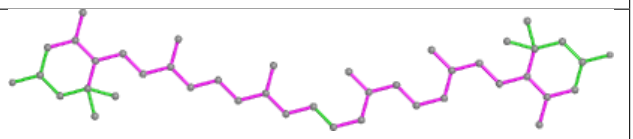


Rings

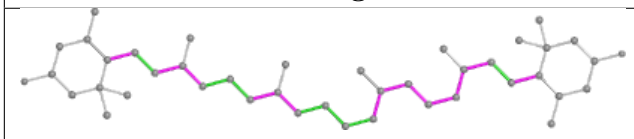
Ligand C7Z 4 505



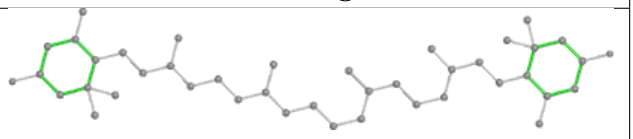
Bond lengths



Bond angles

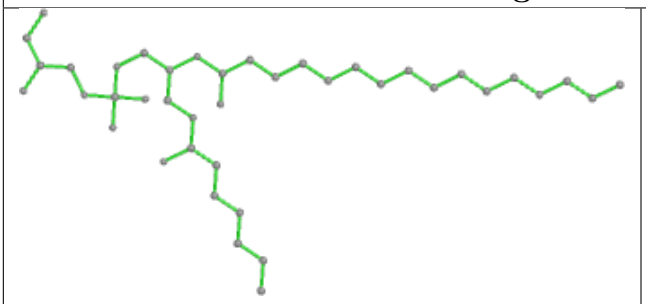


Torsions

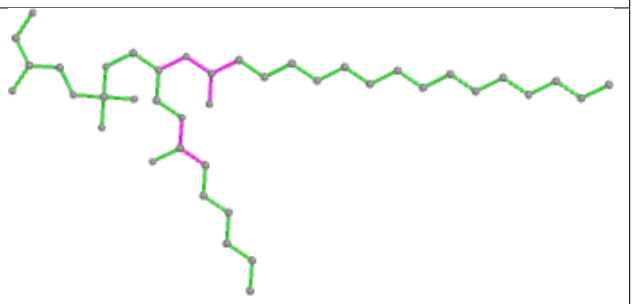


Rings

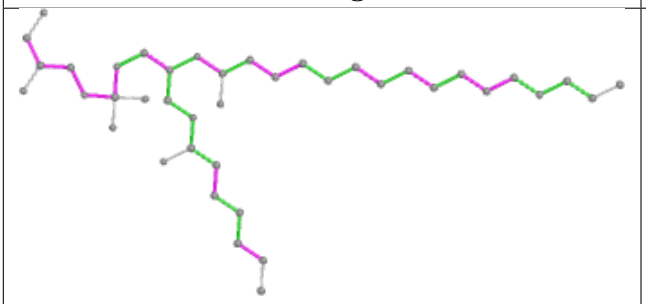
Ligand LHG A 5001



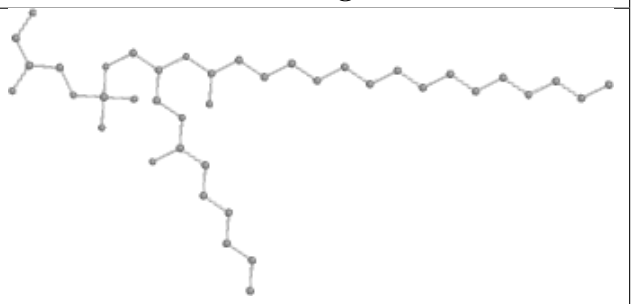
Bond lengths



Bond angles

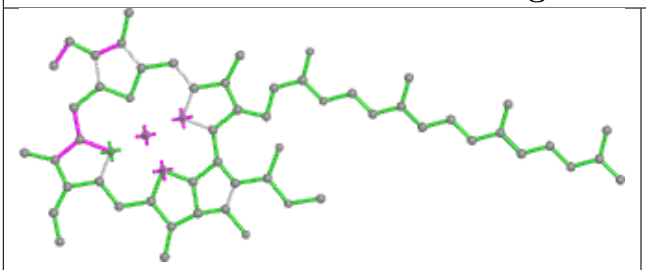


Torsions

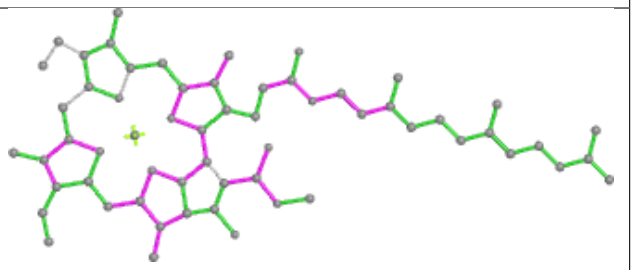


Rings

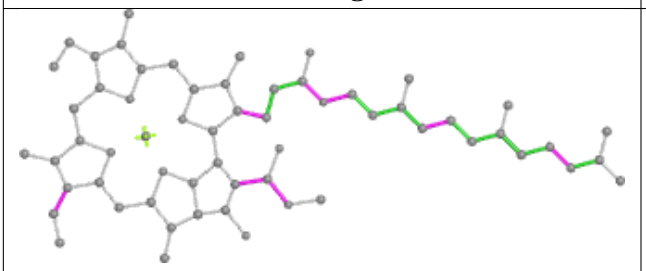
Ligand CLA 3 617



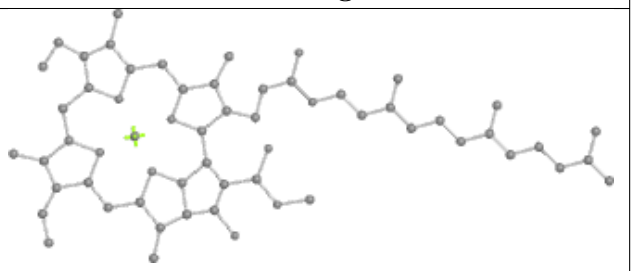
Bond lengths



Bond angles

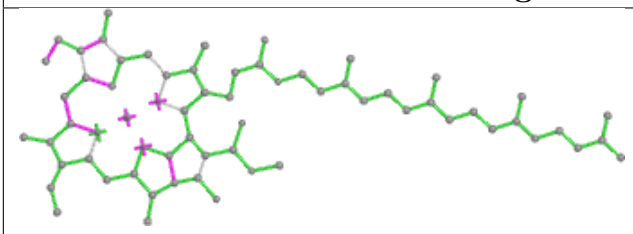


Torsions

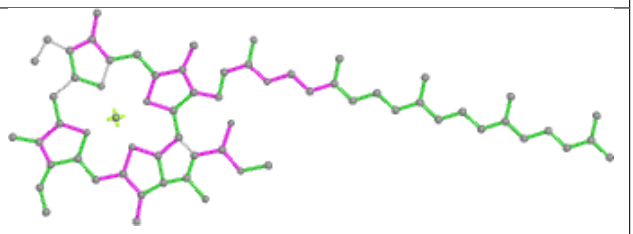


Rings

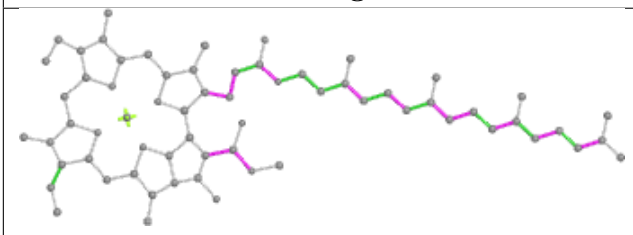
Ligand CLA A 1117



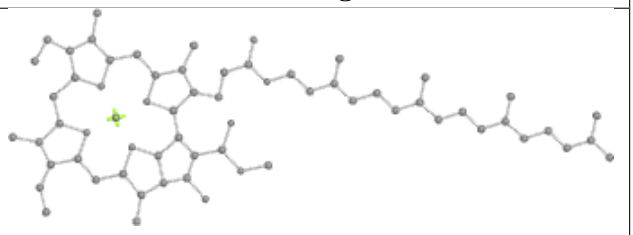
Bond lengths



Bond angles

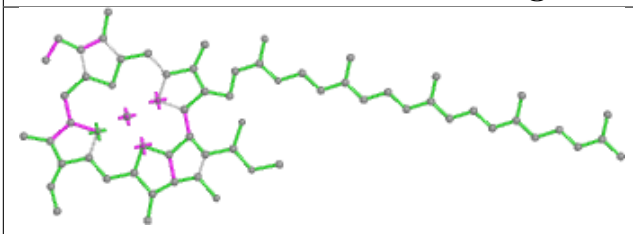


Torsions

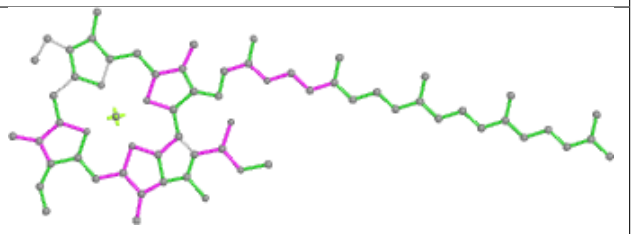


Rings

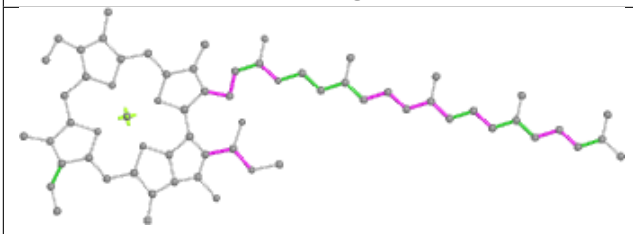
Ligand CLA 2 603



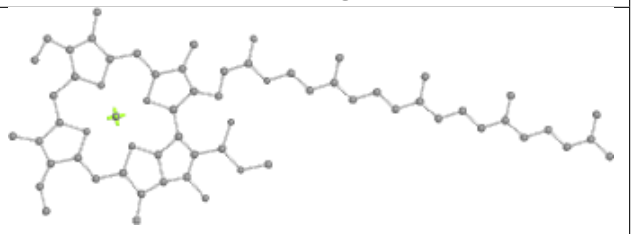
Bond lengths



Bond angles

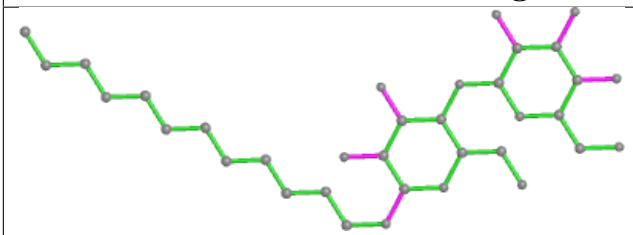


Torsions

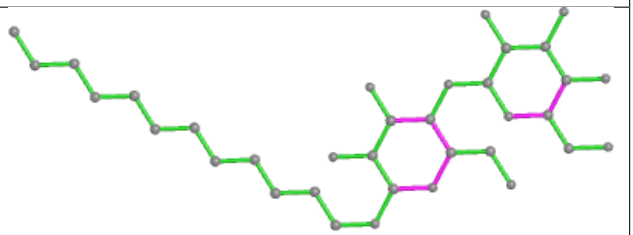


Rings

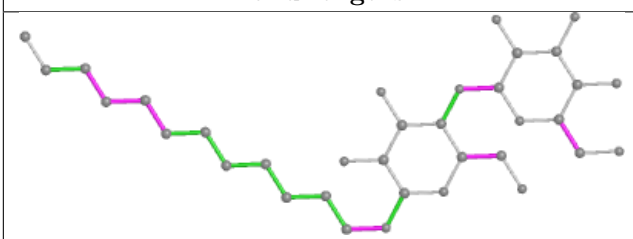
Ligand LMT G 5004



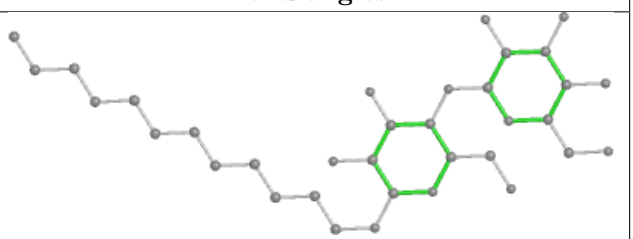
Bond lengths



Bond angles

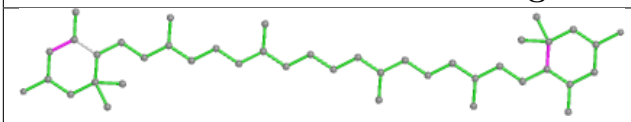


Torsions

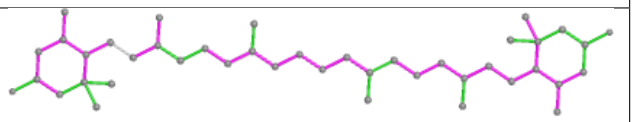


Rings

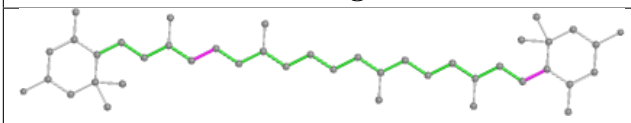
Ligand LUT 1 501



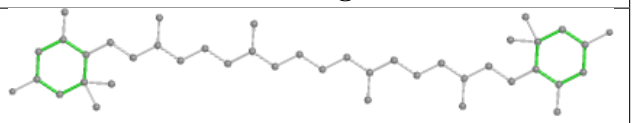
Bond lengths



Bond angles

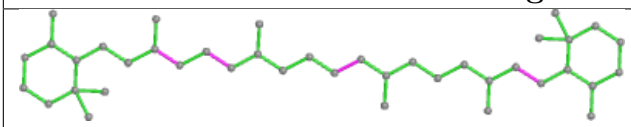


Torsions

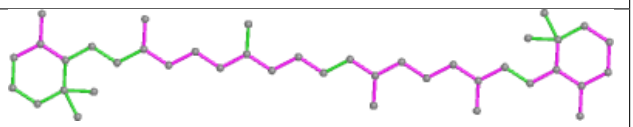


Rings

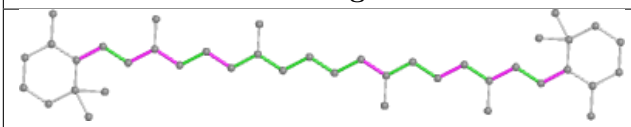
Ligand BCR 3 506



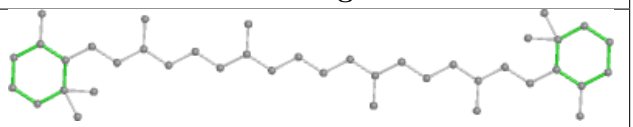
Bond lengths



Bond angles

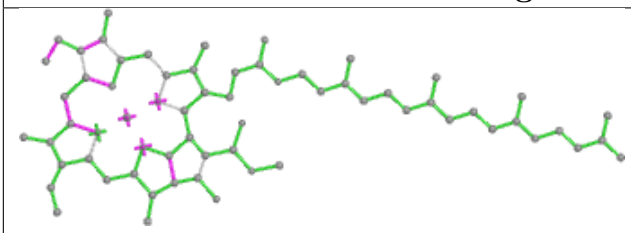


Torsions

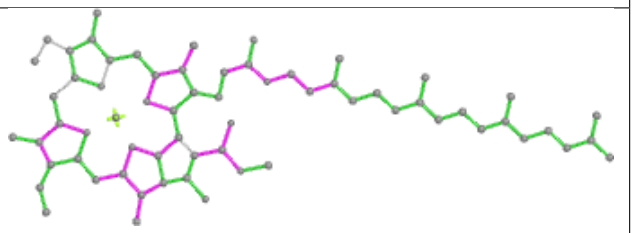


Rings

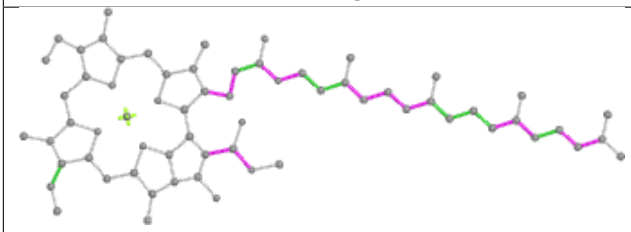
Ligand CLA B 1204



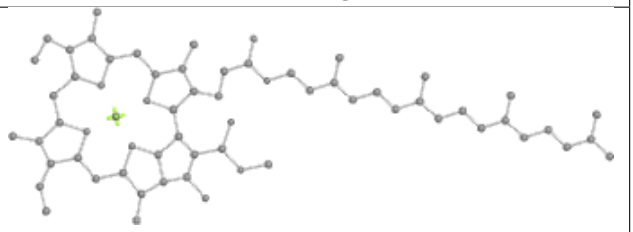
Bond lengths



Bond angles

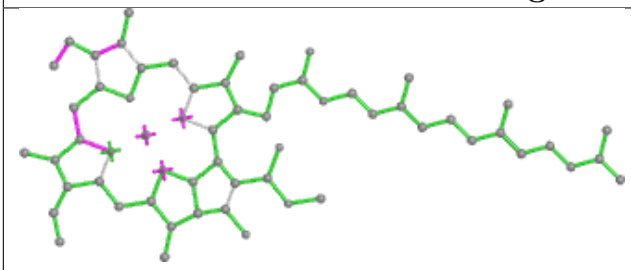


Torsions

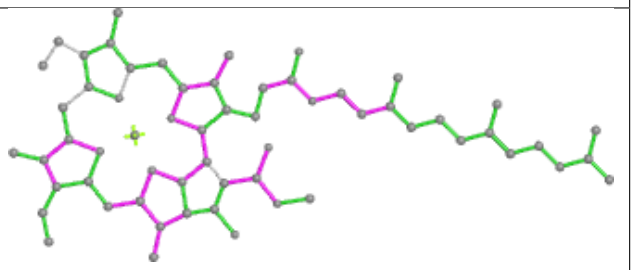


Rings

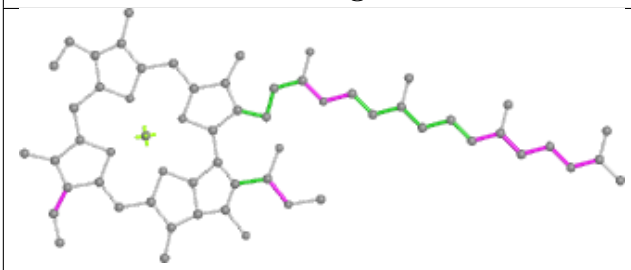
Ligand CLA 2 607



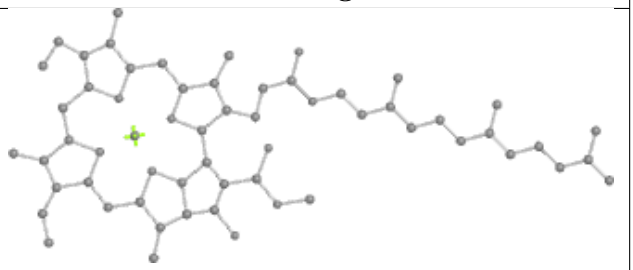
Bond lengths



Bond angles

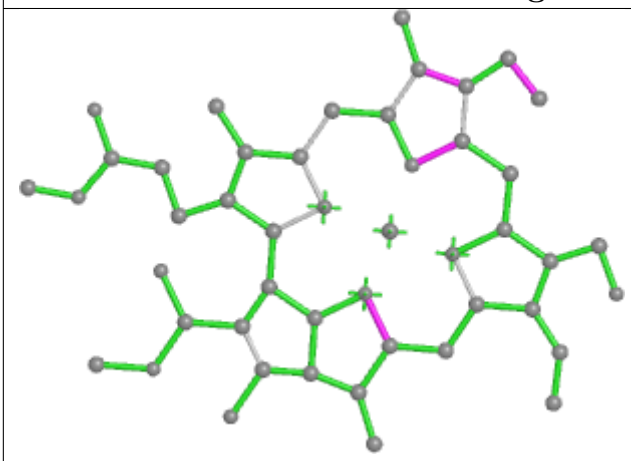


Torsions

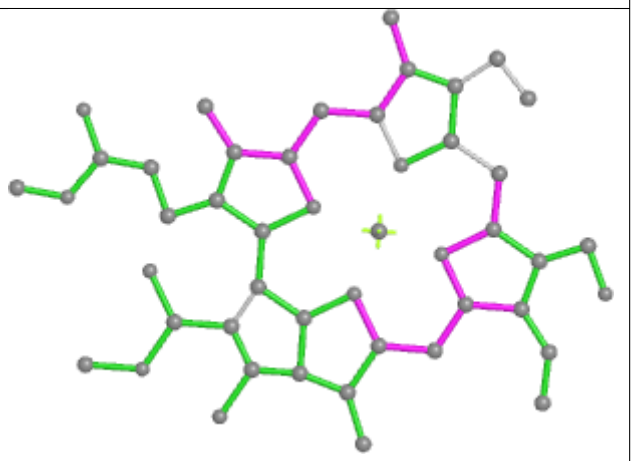


Rings

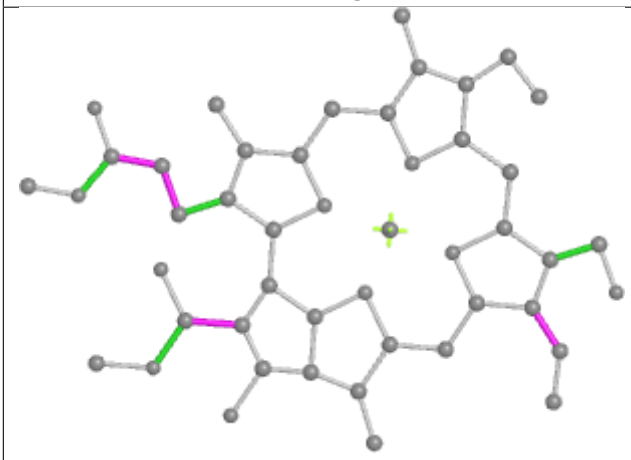
Ligand CHL 1 610



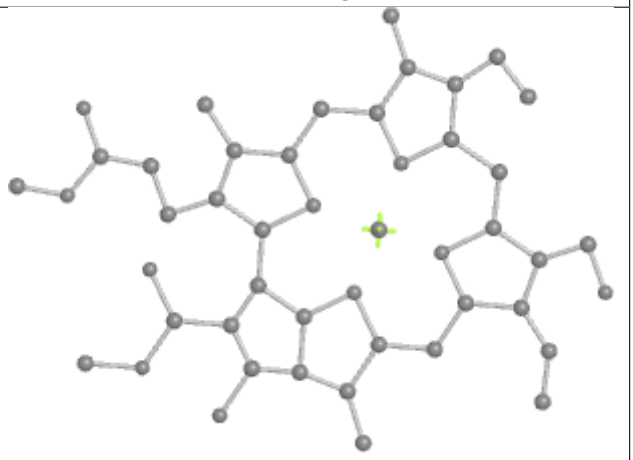
Bond lengths



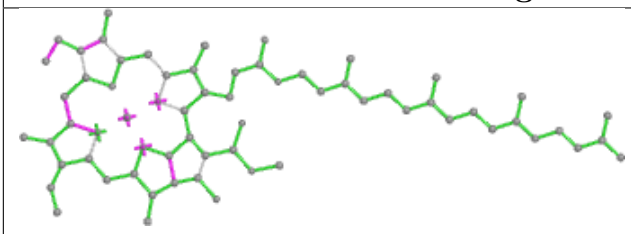
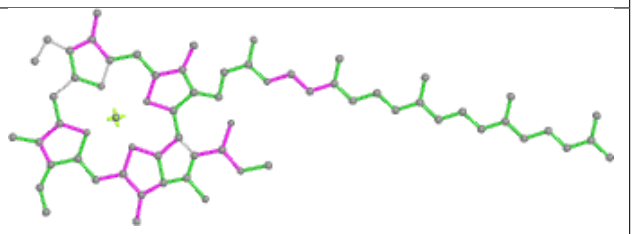
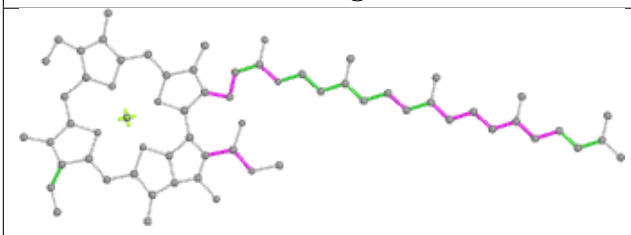
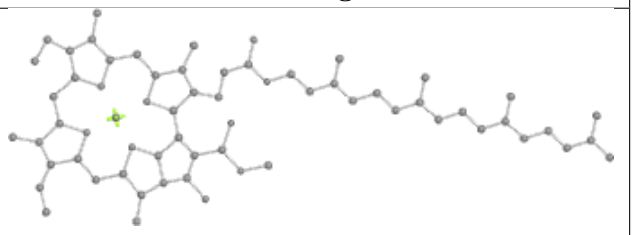
Bond angles

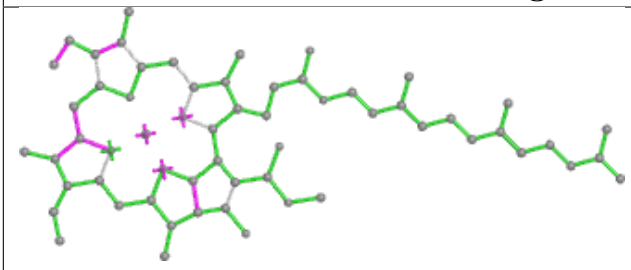
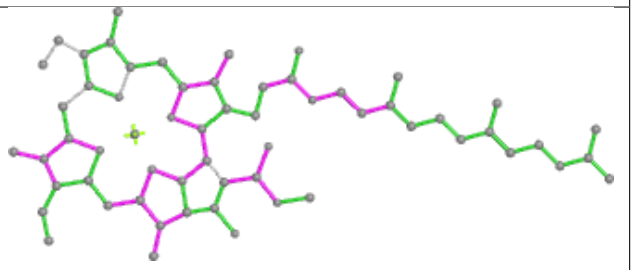
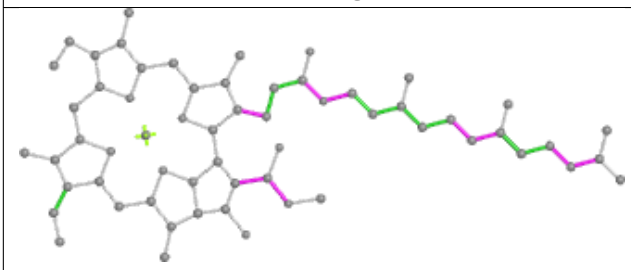
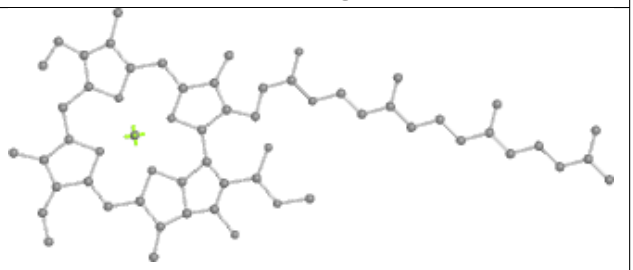


Torsions

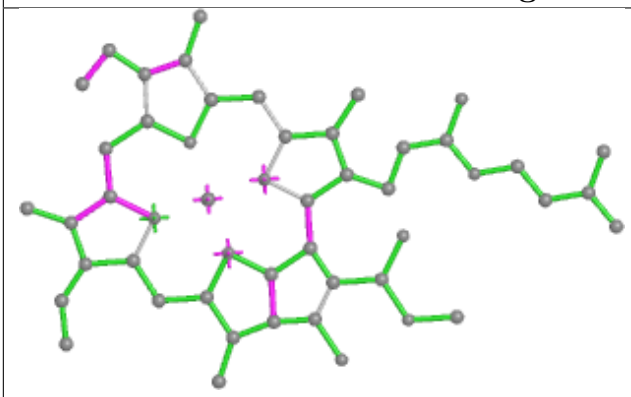


Rings

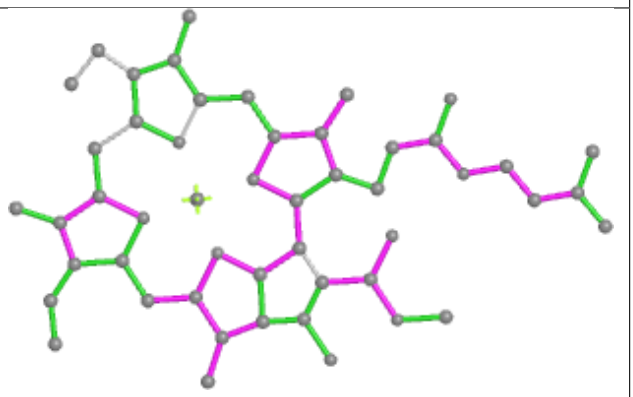
Ligand CLA B 1201	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA 4 607	
 Bond lengths	 Bond angles
 Torsions	 Rings

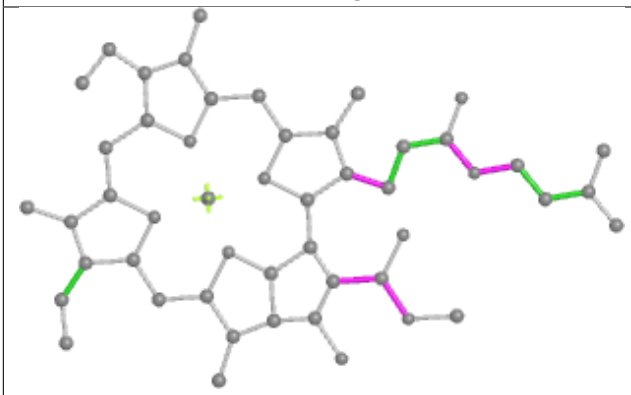
Ligand CLA J 1901



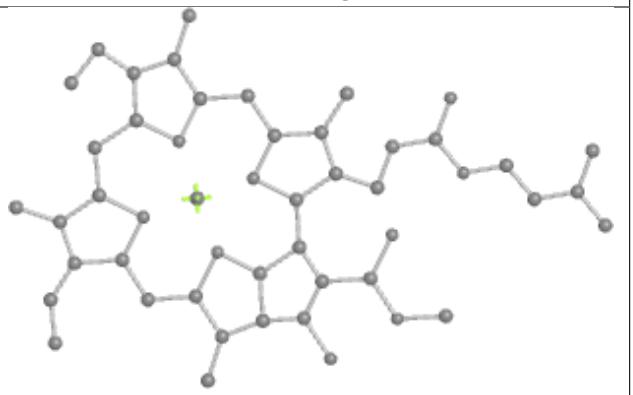
Bond lengths



Bond angles

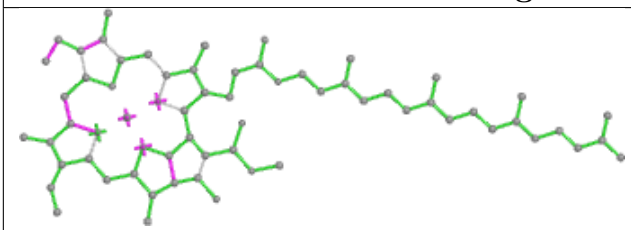


Torsions

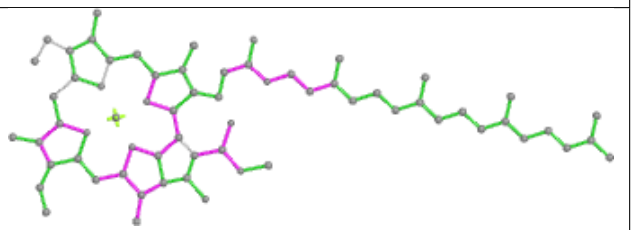


Rings

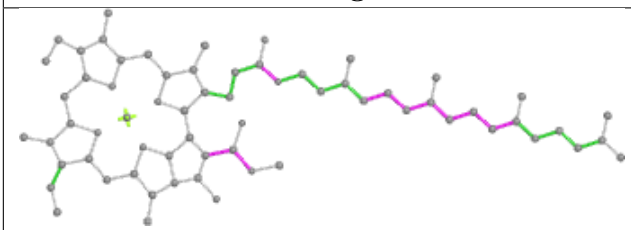
Ligand CLA B 1203



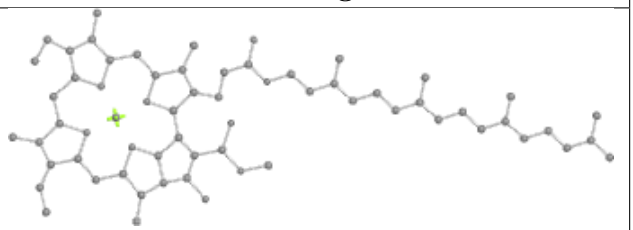
Bond lengths



Bond angles

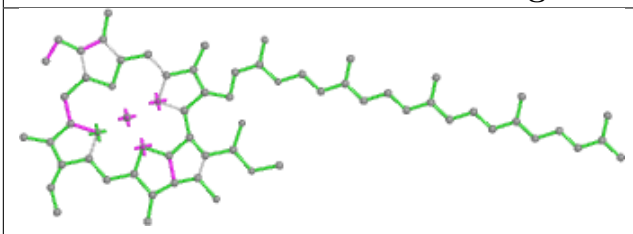


Torsions

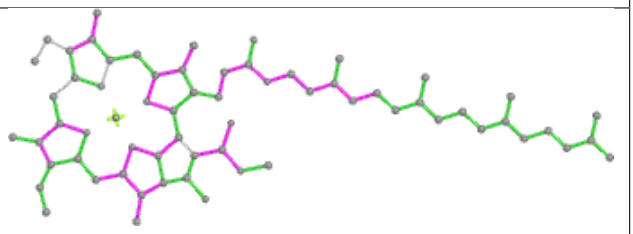


Rings

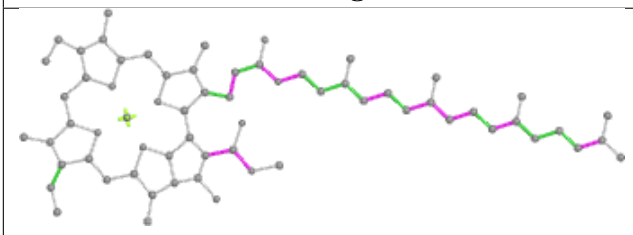
Ligand CLA 1 604



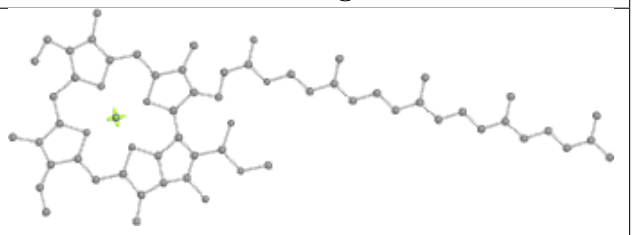
Bond lengths



Bond angles

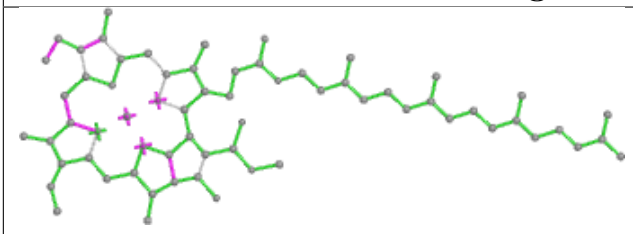


Torsions

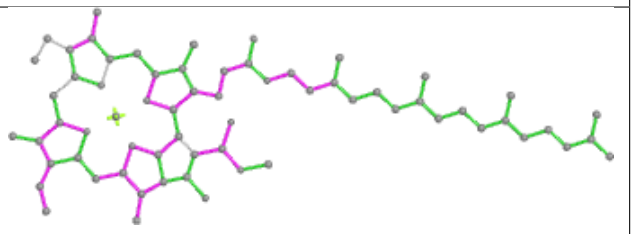


Rings

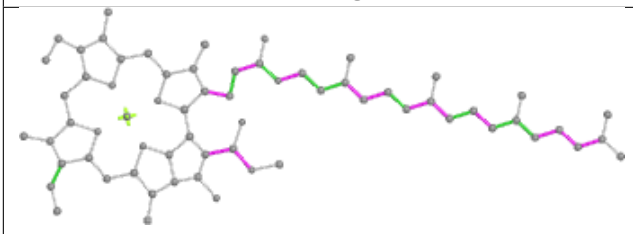
Ligand CLA 1 605



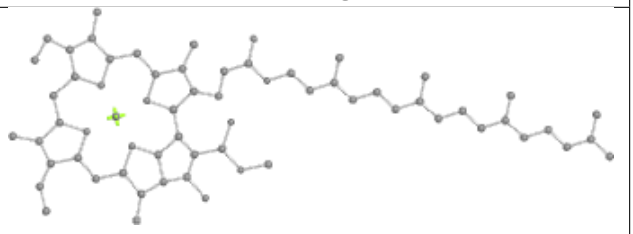
Bond lengths



Bond angles

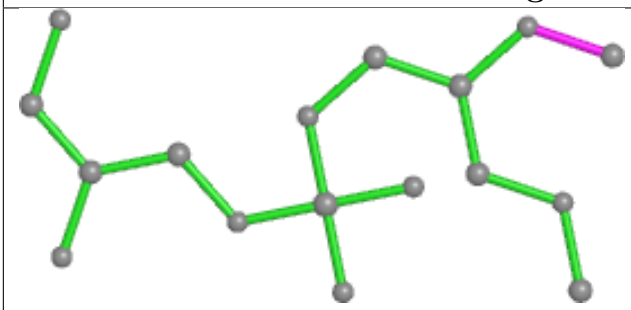


Torsions

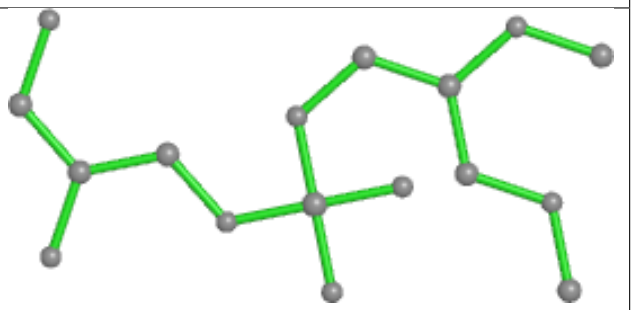


Rings

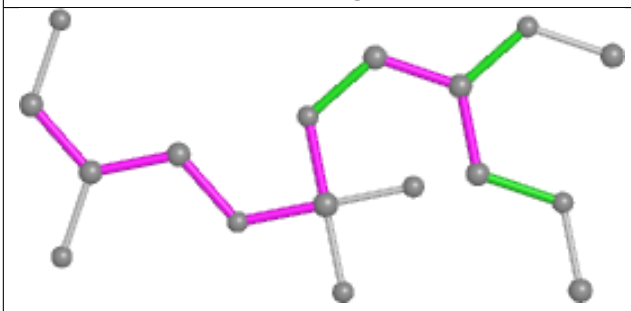
Ligand LHG 3 801



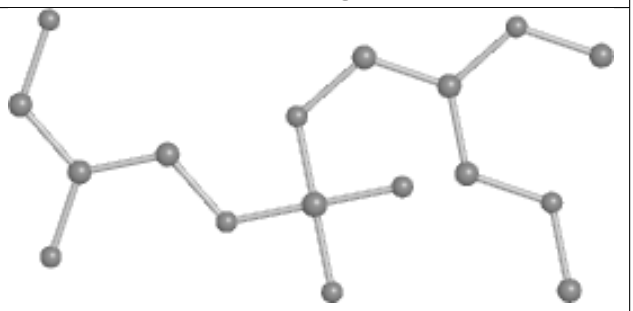
Bond lengths



Bond angles

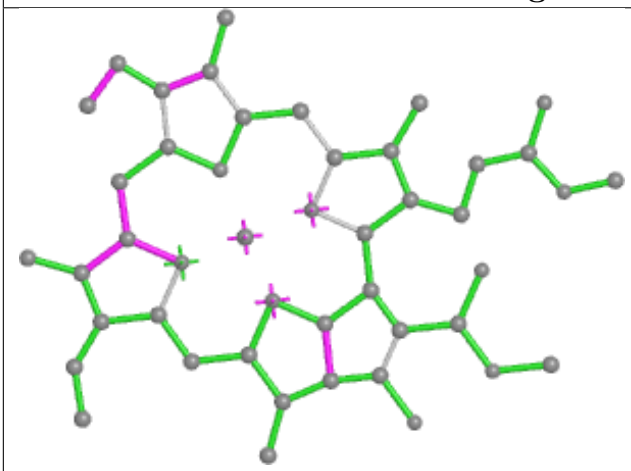


Torsions

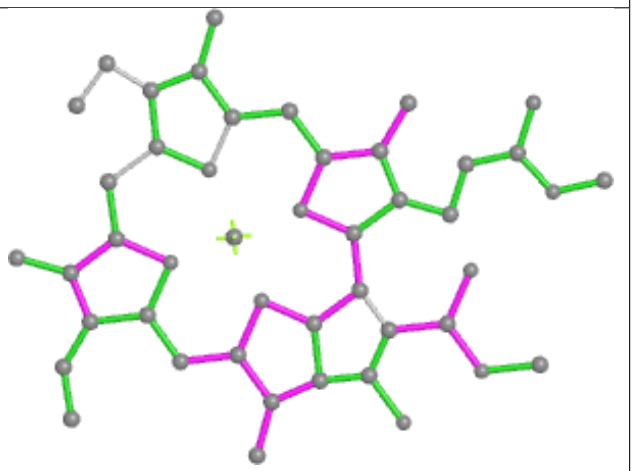


Rings

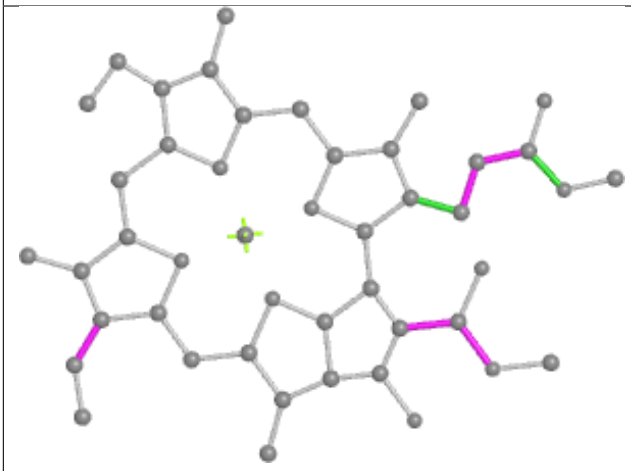
Ligand CLA 4 608



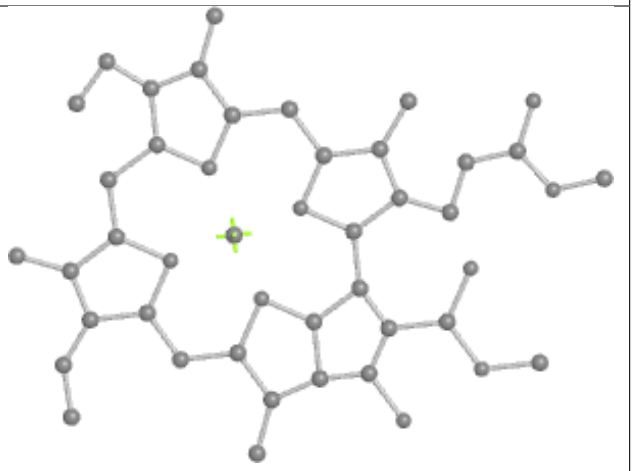
Bond lengths



Bond angles

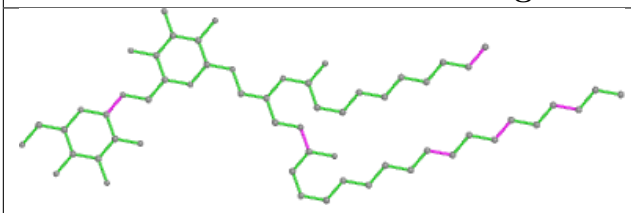


Torsions

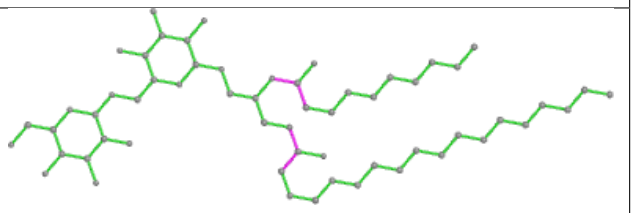


Rings

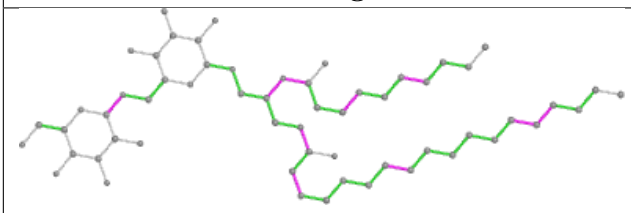
Ligand DGD J 5001



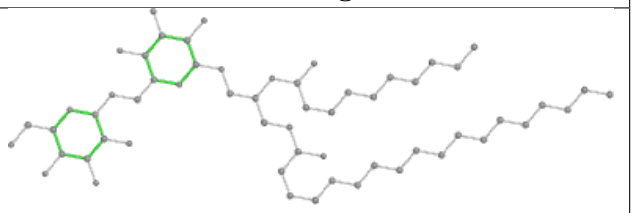
Bond lengths



Bond angles

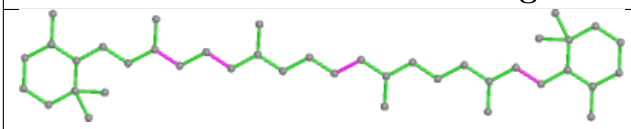


Torsions

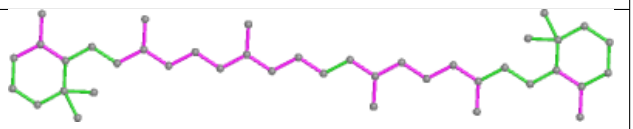


Rings

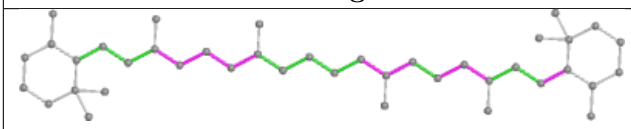
Ligand BCR I 4020



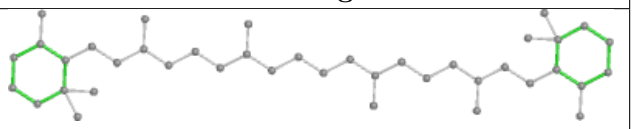
Bond lengths



Bond angles

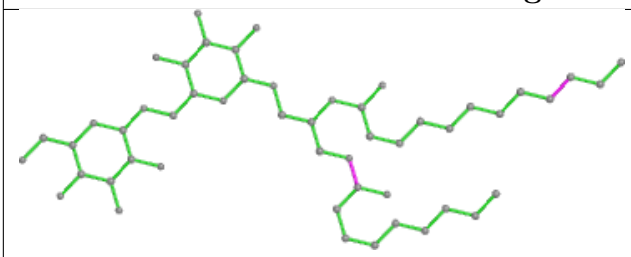


Torsions

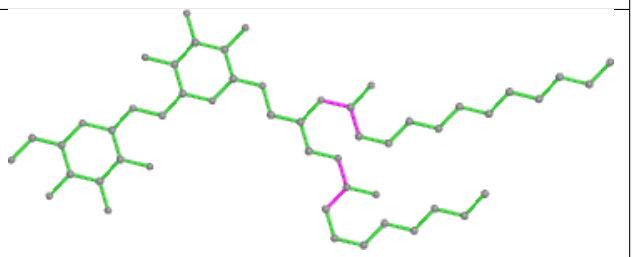


Rings

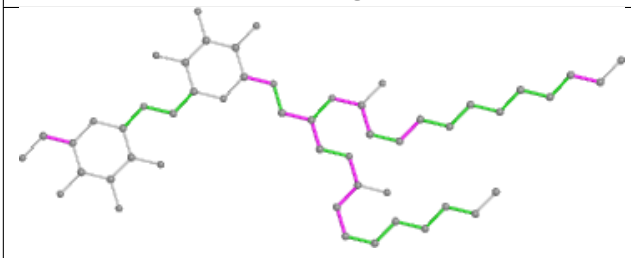
Ligand DGD 4 802



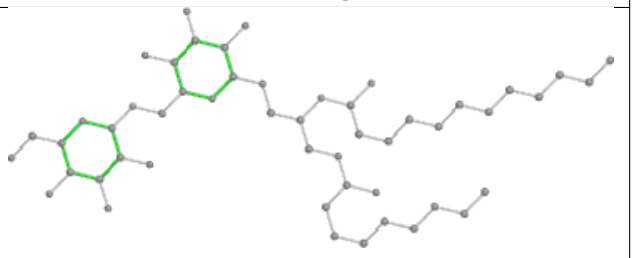
Bond lengths



Bond angles

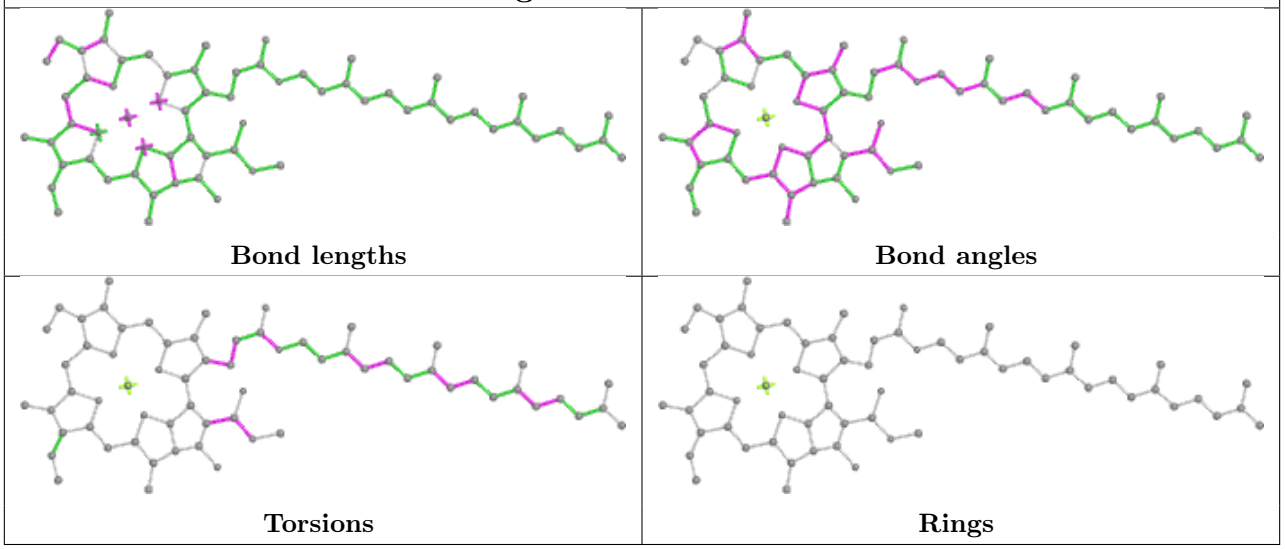


Torsions

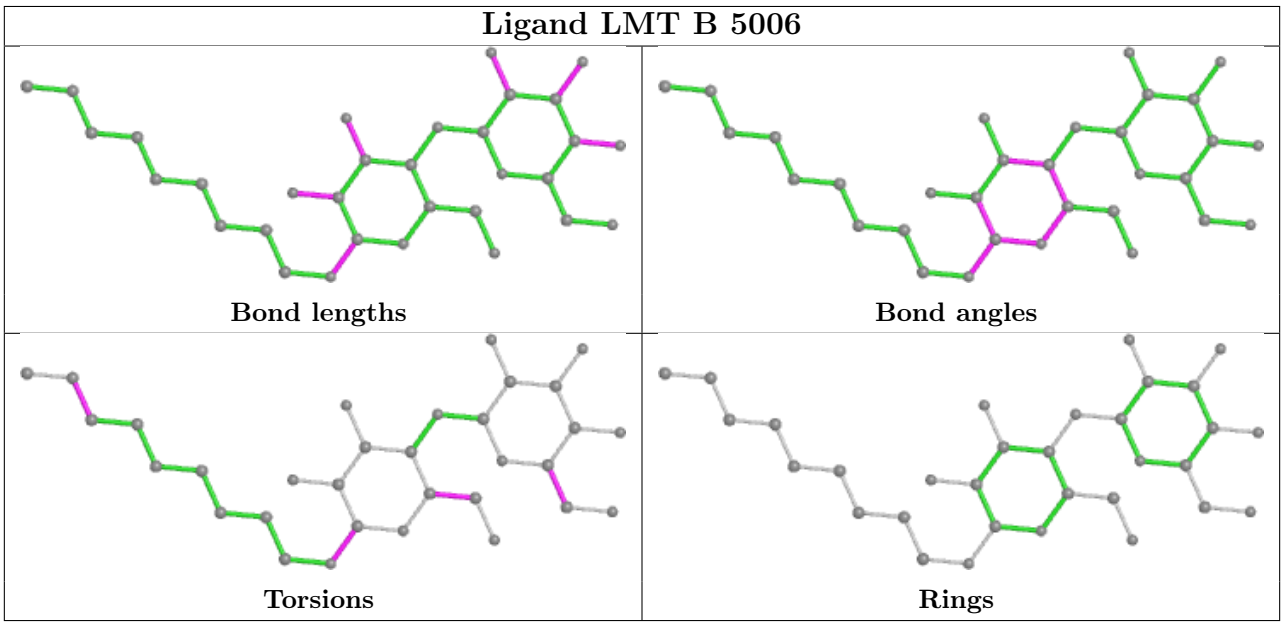


Rings

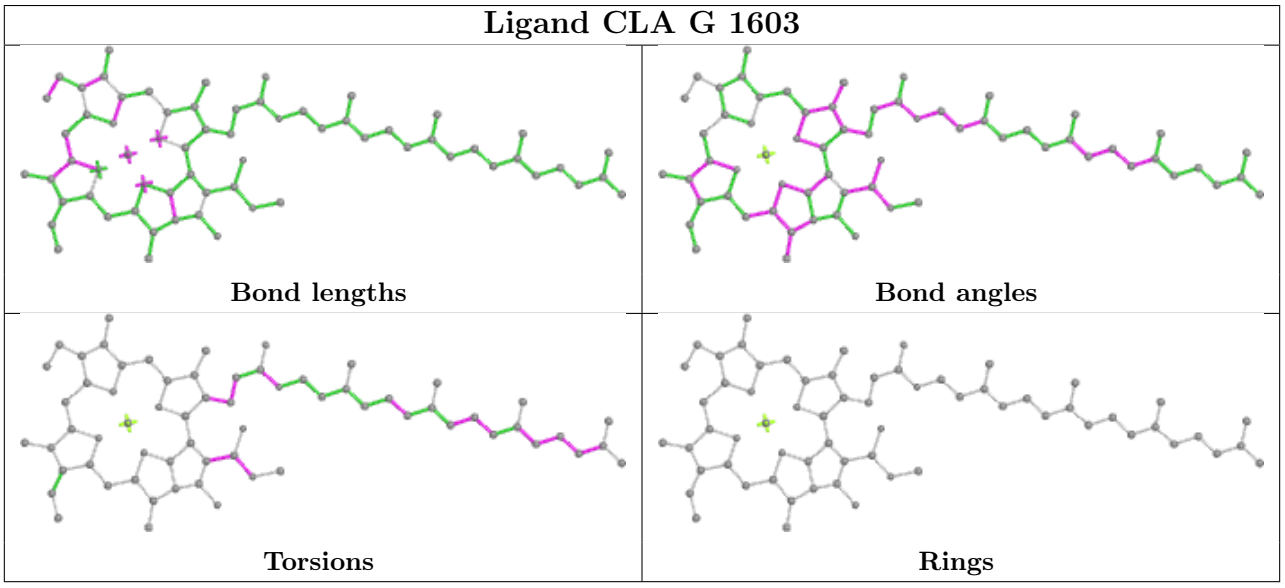
Ligand CLA A 1119



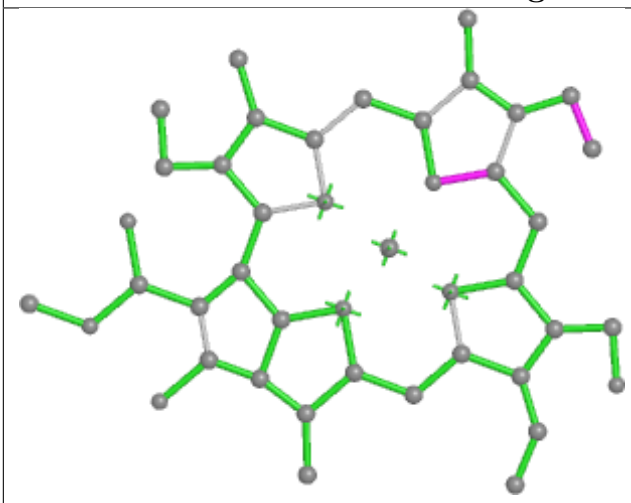
Ligand LMT B 5006



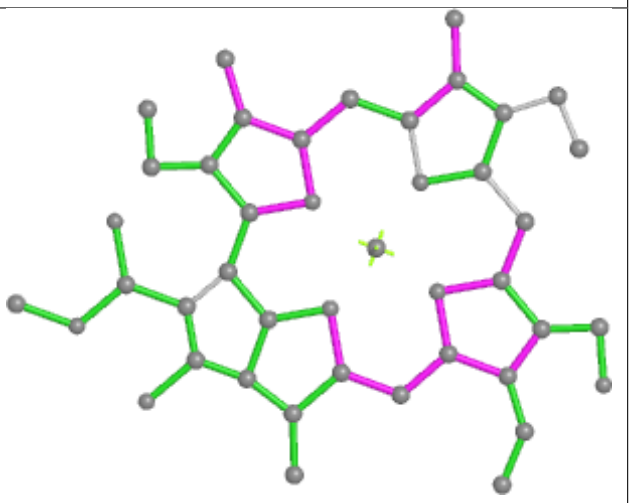
Ligand CLA G 1603



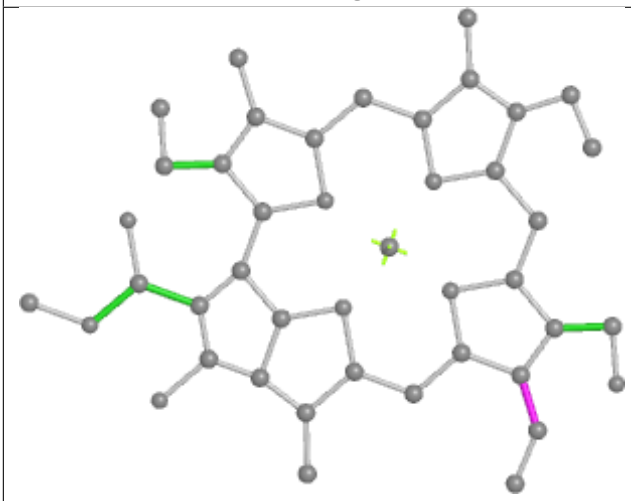
Ligand CHL 4 615



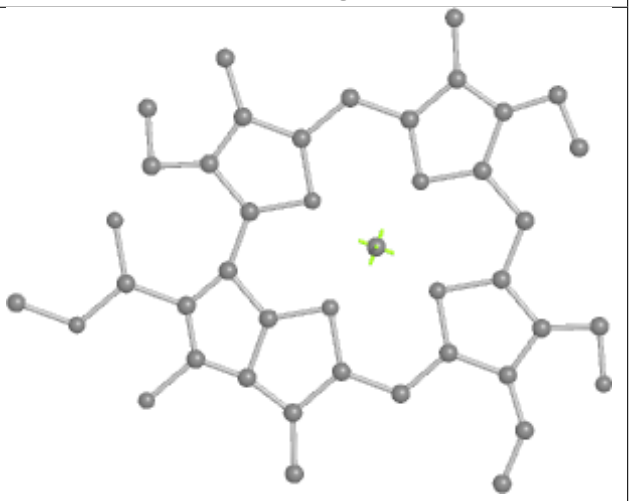
Bond lengths



Bond angles

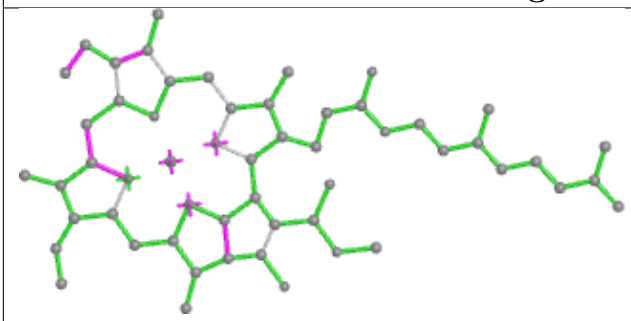


Torsions

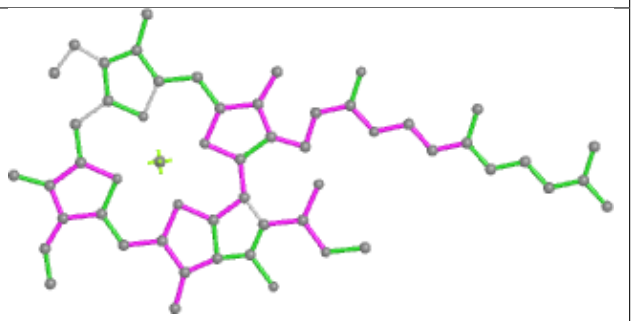


Rings

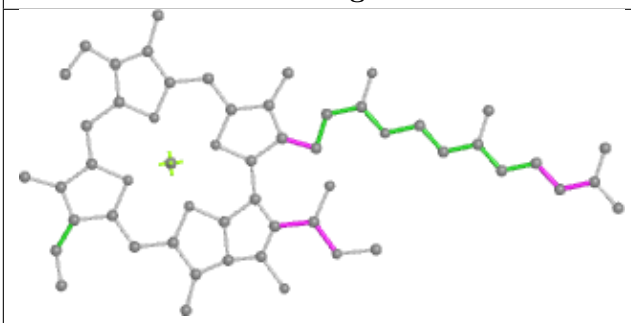
Ligand CLA 1 603



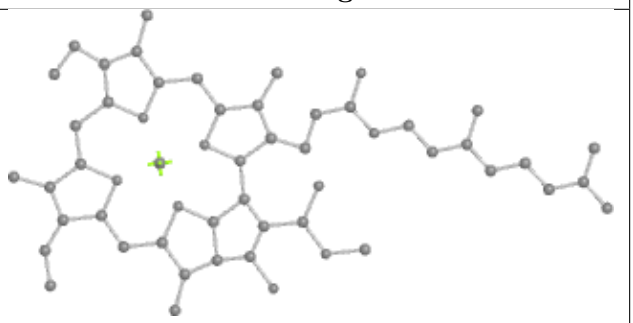
Bond lengths



Bond angles

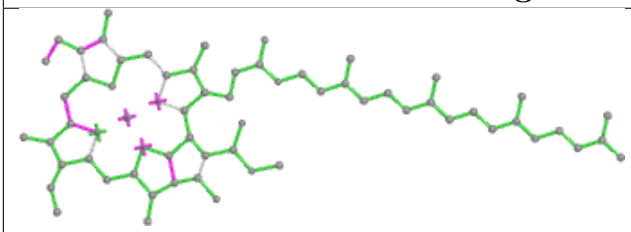


Torsions

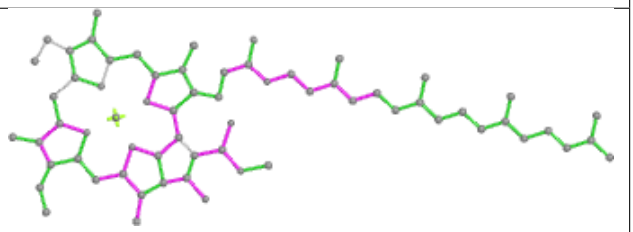


Rings

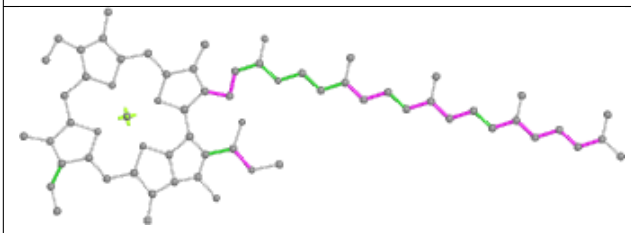
Ligand CLA A 1012



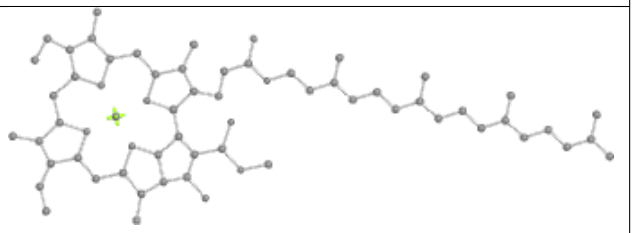
Bond lengths



Bond angles

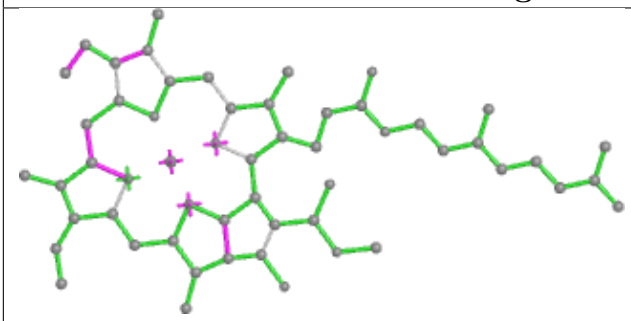


Torsions

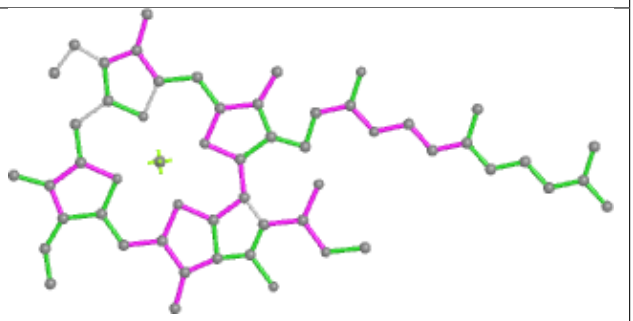


Rings

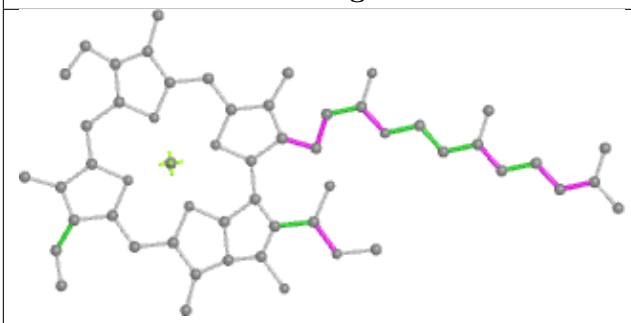
Ligand CLA A 1130



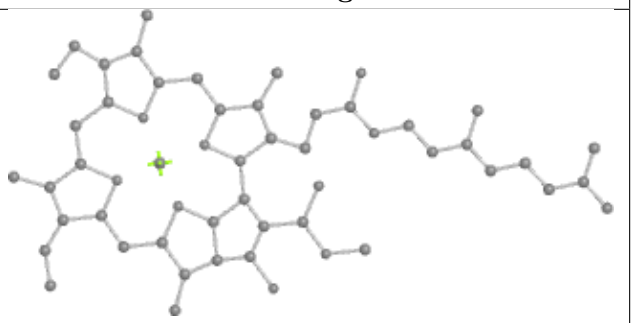
Bond lengths



Bond angles

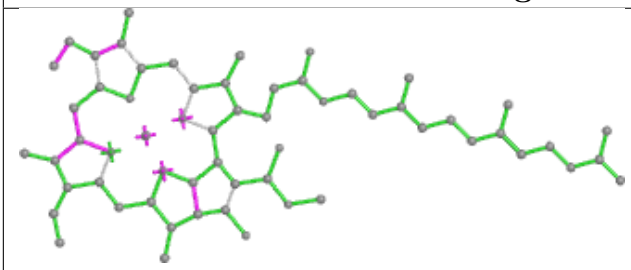


Torsions

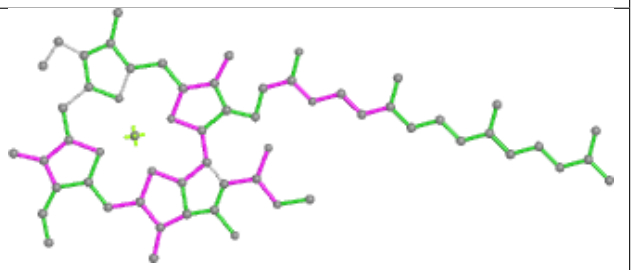


Rings

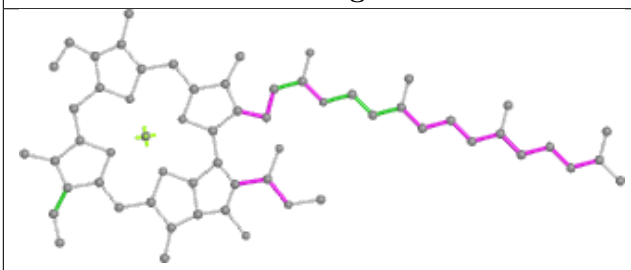
Ligand CLA K 1402



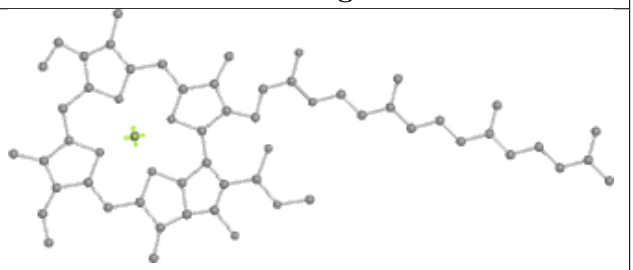
Bond lengths



Bond angles

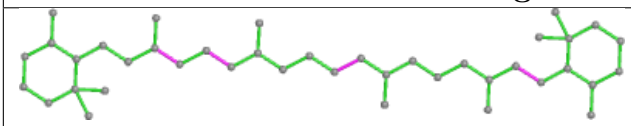


Torsions

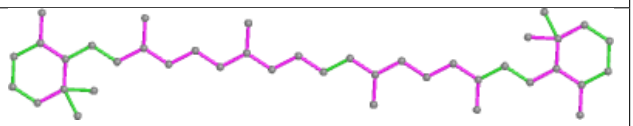


Rings

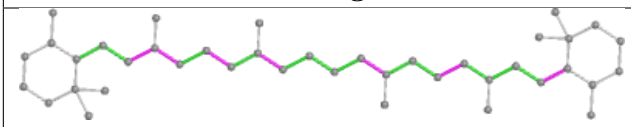
Ligand BCR B 4004



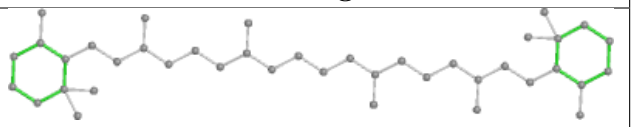
Bond lengths



Bond angles

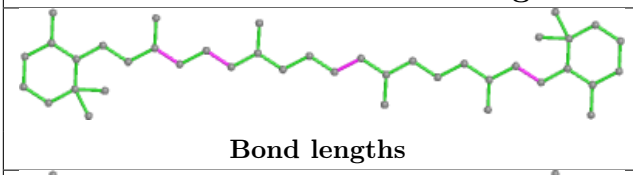


Torsions

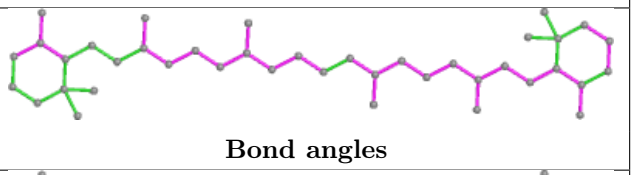


Rings

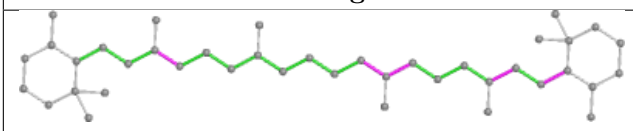
Ligand BCR G 4011



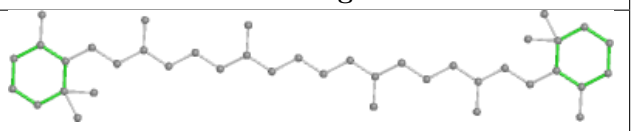
Bond lengths



Bond angles

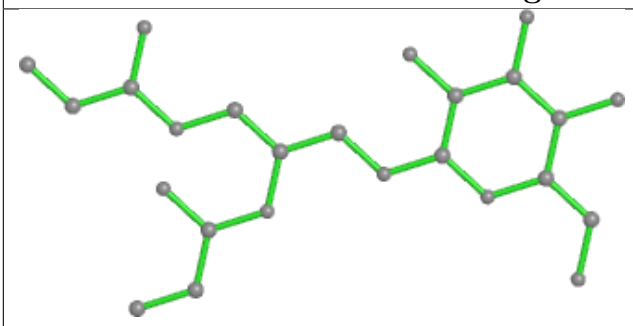


Torsions

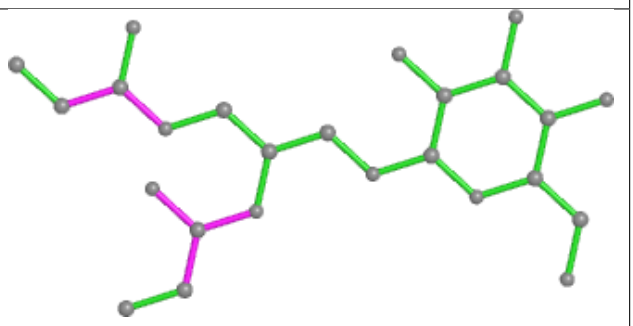


Rings

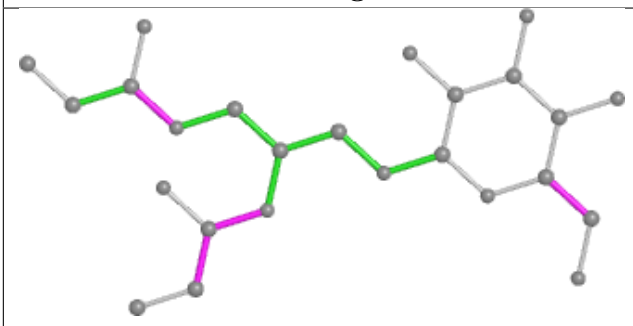
Ligand LMG 2 802



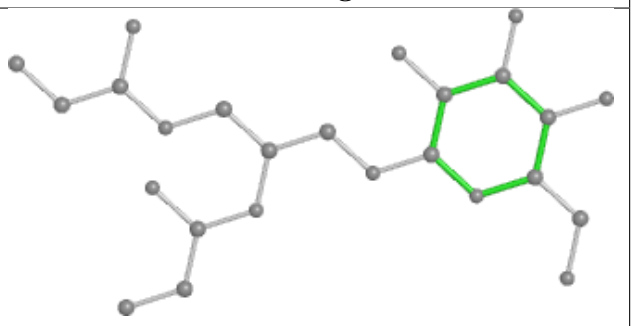
Bond lengths



Bond angles

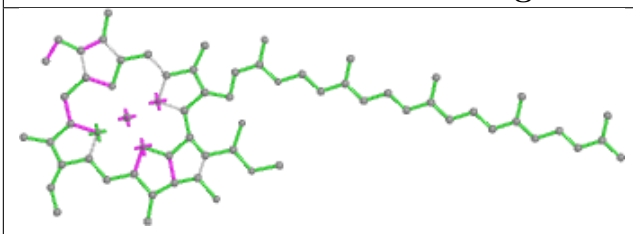


Torsions

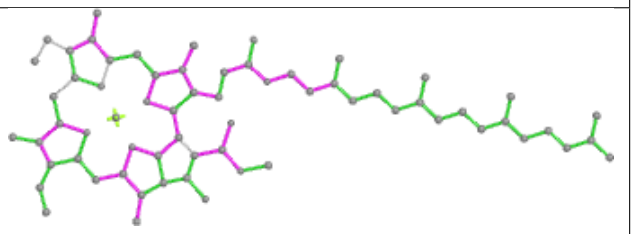


Rings

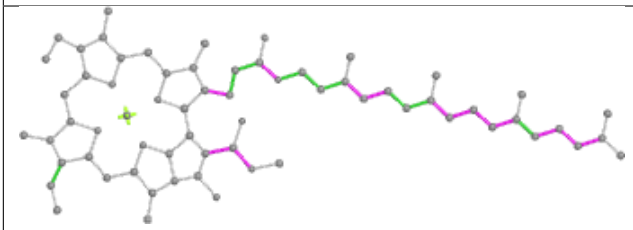
Ligand CLA A 1127



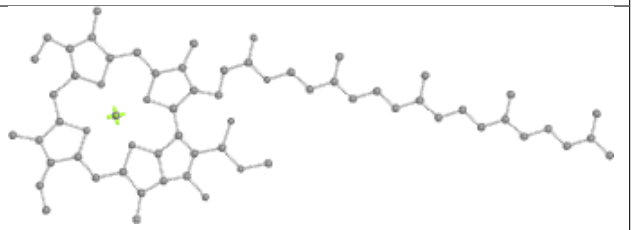
Bond lengths



Bond angles

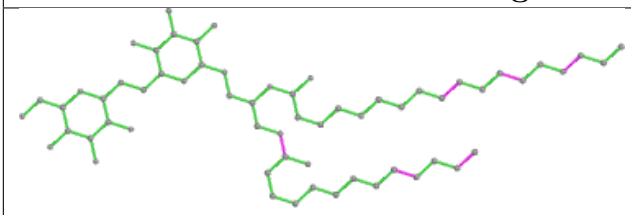


Torsions

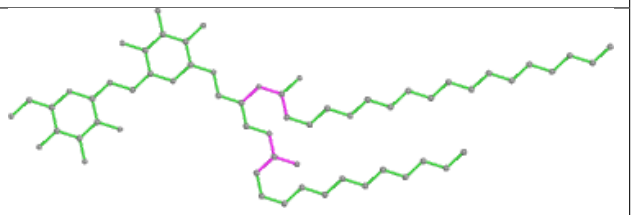


Rings

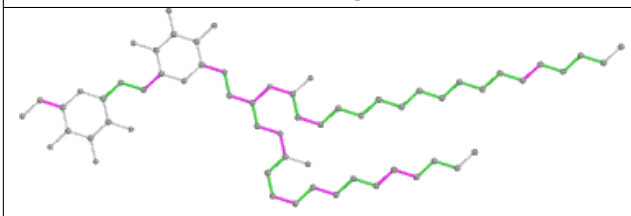
Ligand DGD B 5005



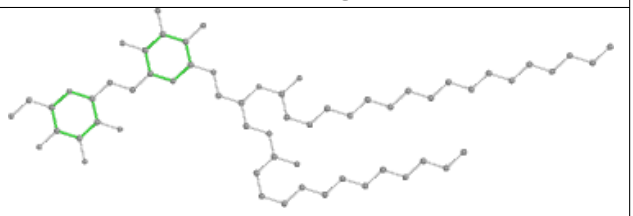
Bond lengths



Bond angles

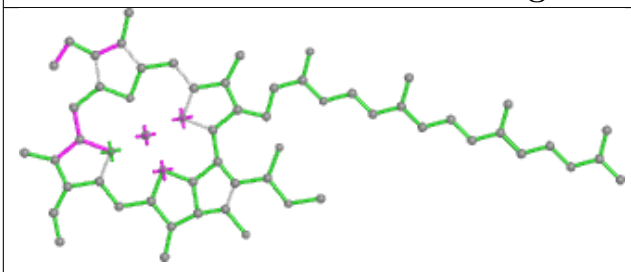


Torsions

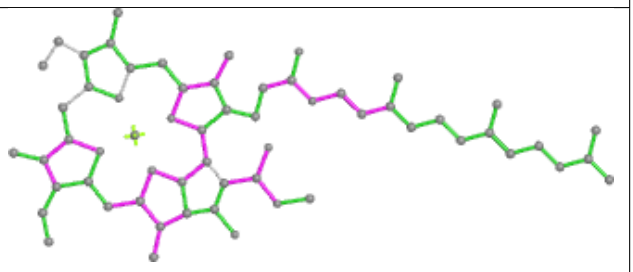


Rings

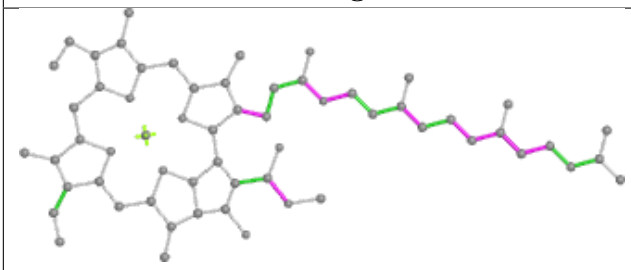
Ligand CLA 4 601



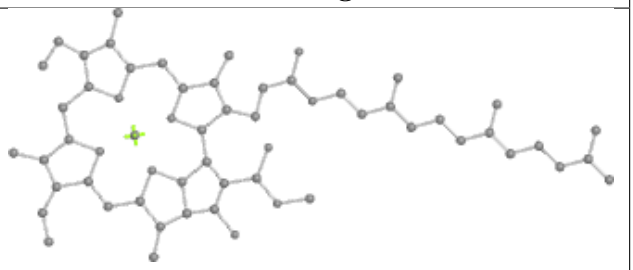
Bond lengths



Bond angles

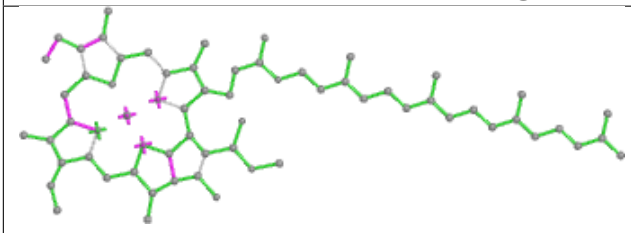


Torsions

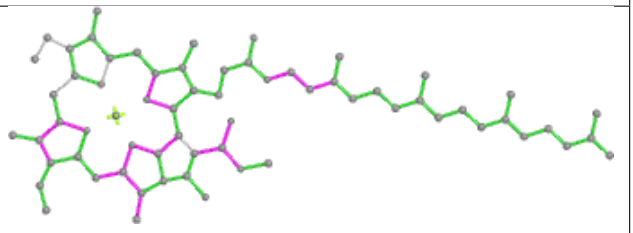


Rings

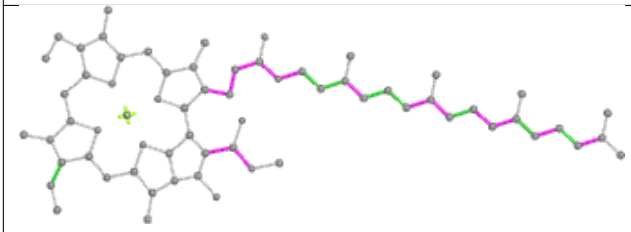
Ligand CLA A 1115



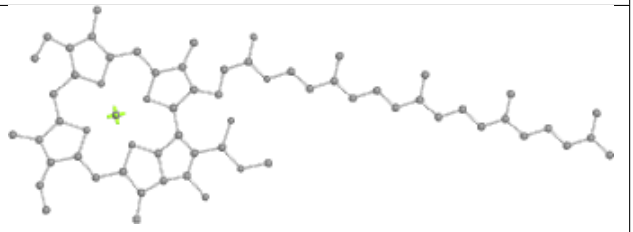
Bond lengths



Bond angles

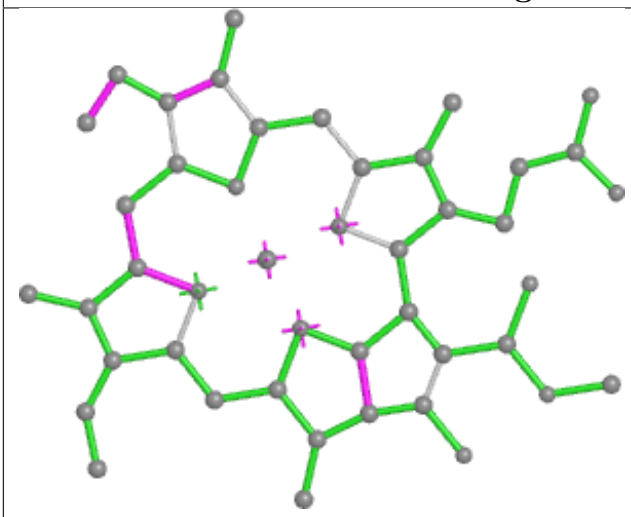


Torsions

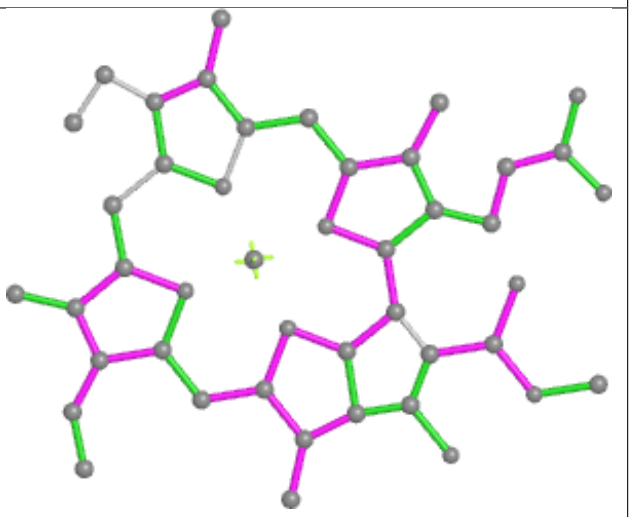


Rings

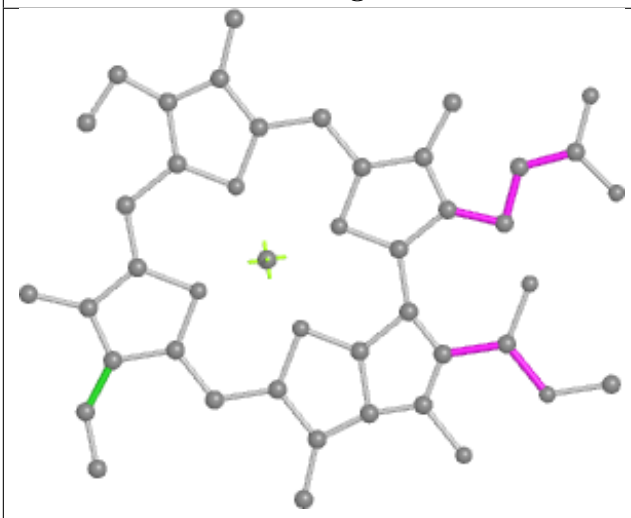
Ligand CLA A 1113



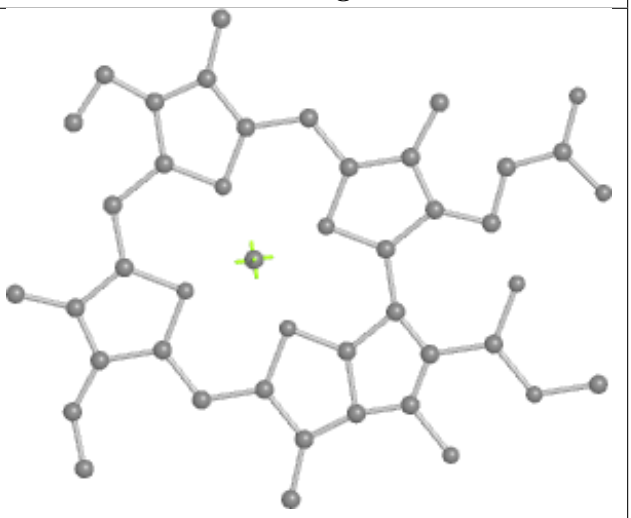
Bond lengths



Bond angles

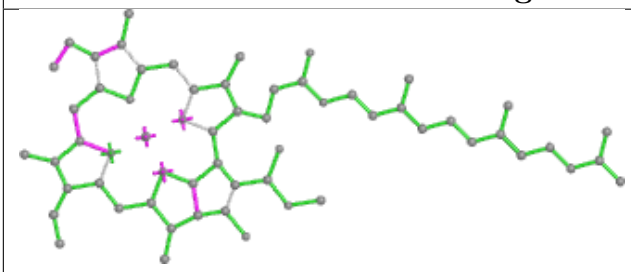


Torsions

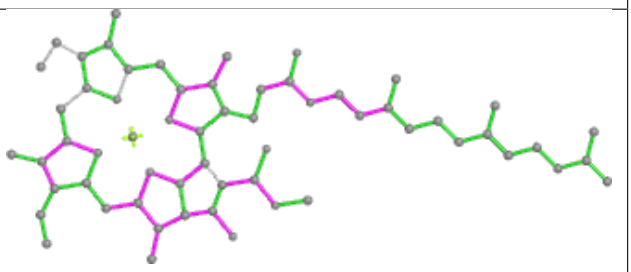


Rings

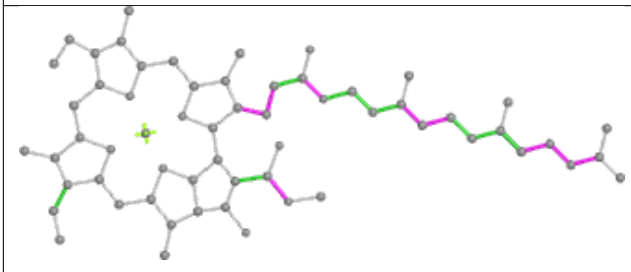
Ligand CLA A 1121



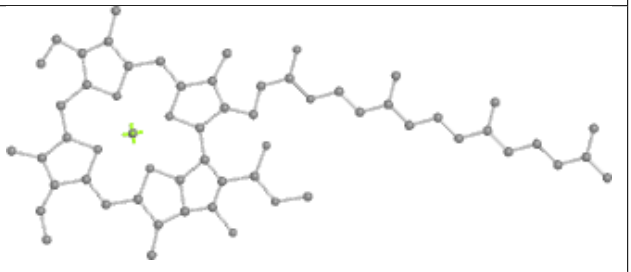
Bond lengths



Bond angles

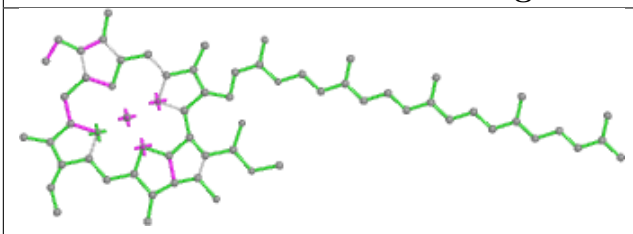


Torsions

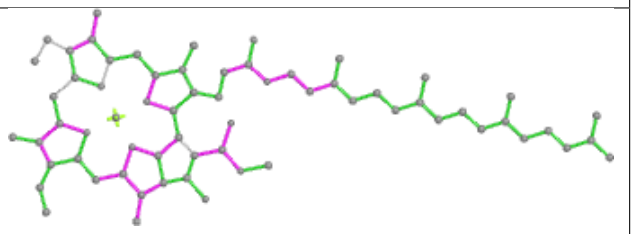


Rings

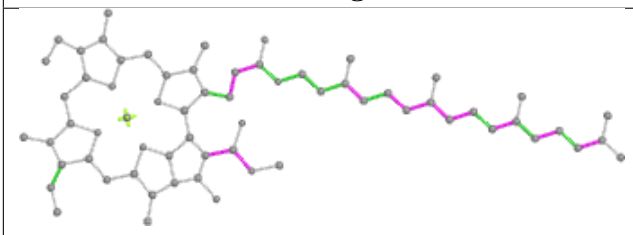
Ligand CLA A 1138



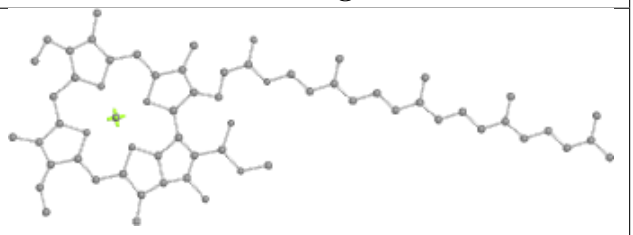
Bond lengths



Bond angles

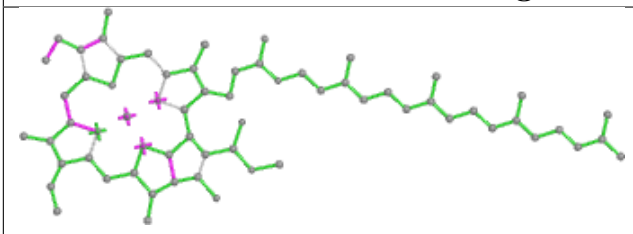


Torsions

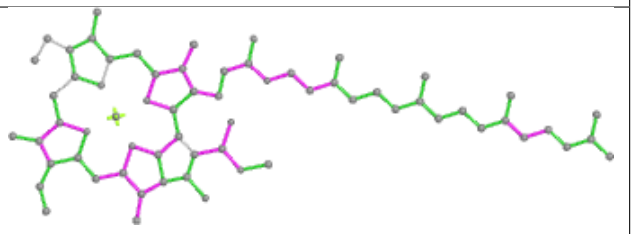


Rings

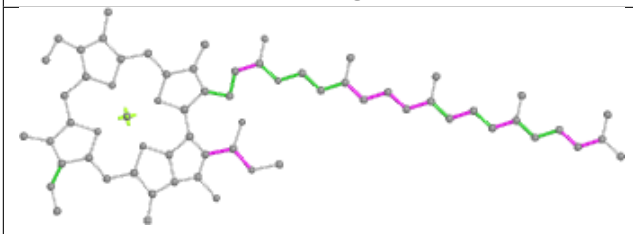
Ligand CLA B 1205



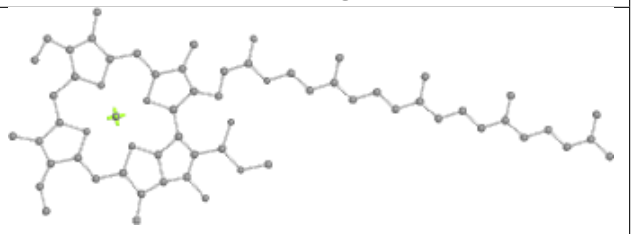
Bond lengths



Bond angles

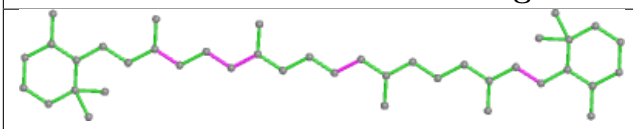


Torsions

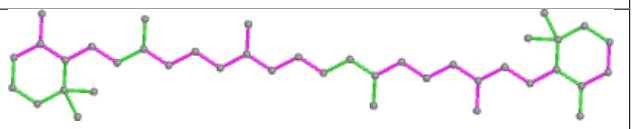


Rings

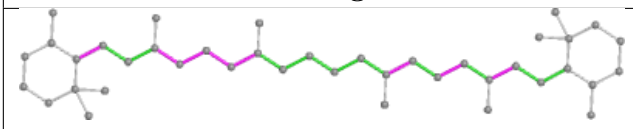
Ligand BCR B 4010



Bond lengths



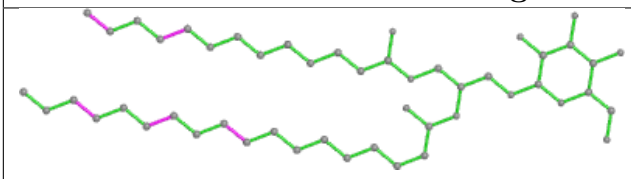
Bond angles



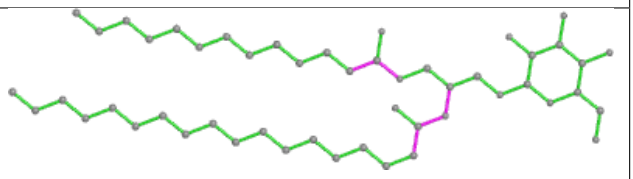
Torsions

Rings

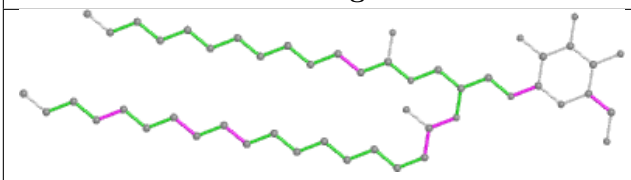
Ligand LMG A 5006



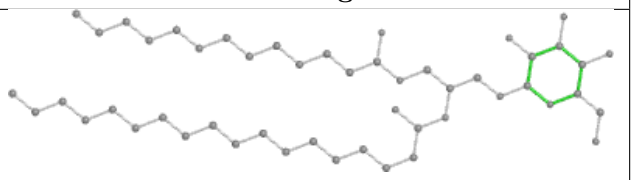
Bond lengths



Bond angles

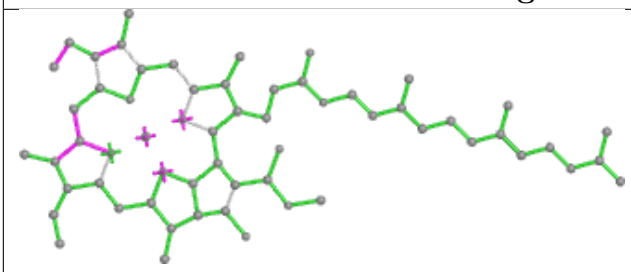


Torsions

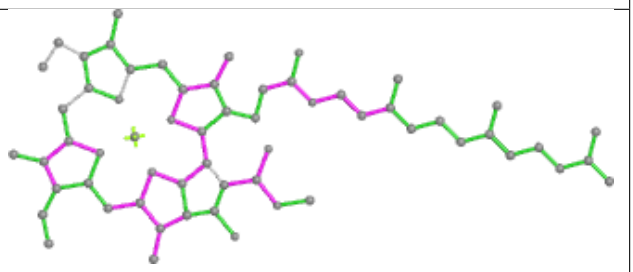


Rings

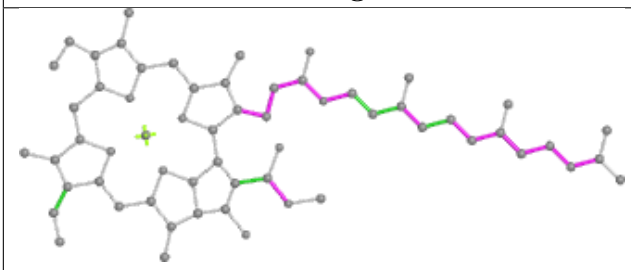
Ligand CLA L 1502



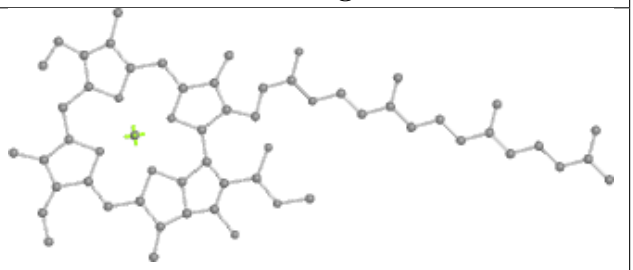
Bond lengths



Bond angles

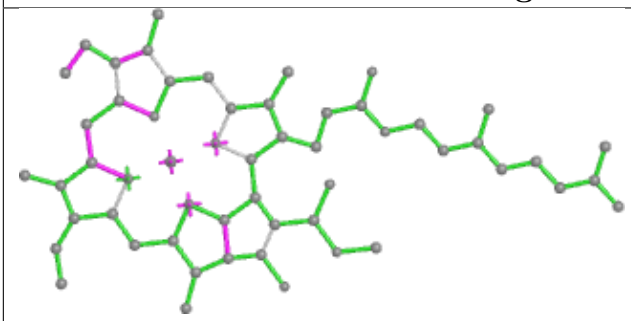


Torsions

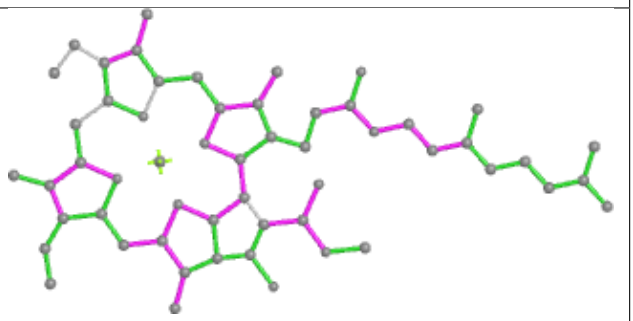


Rings

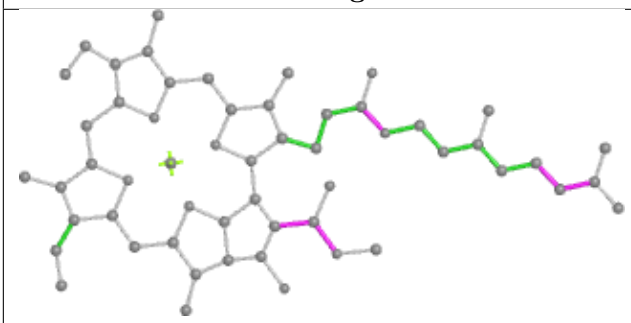
Ligand CLA B 1212



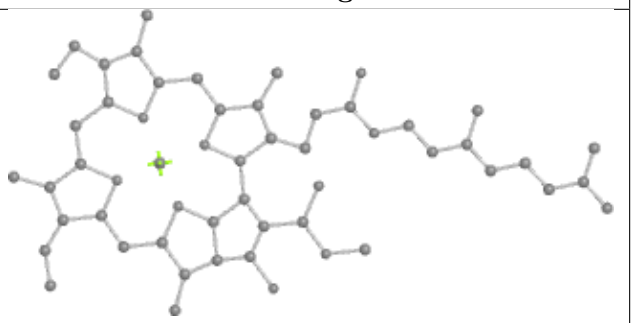
Bond lengths



Bond angles

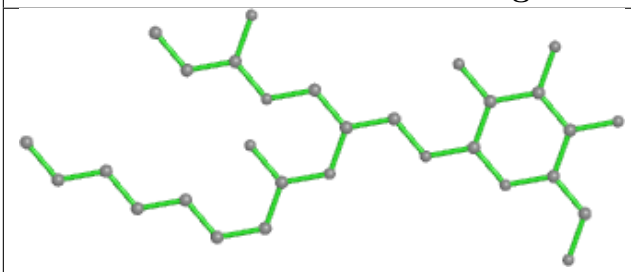


Torsions

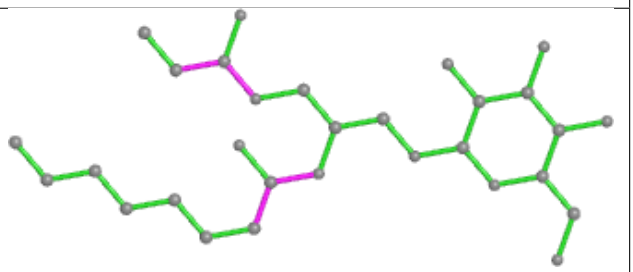


Rings

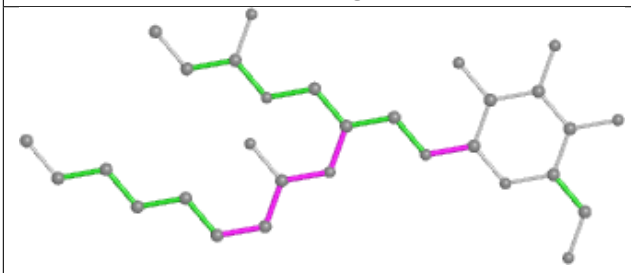
Ligand LMG F 5001



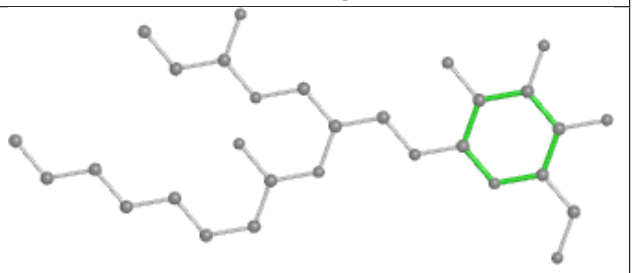
Bond lengths



Bond angles

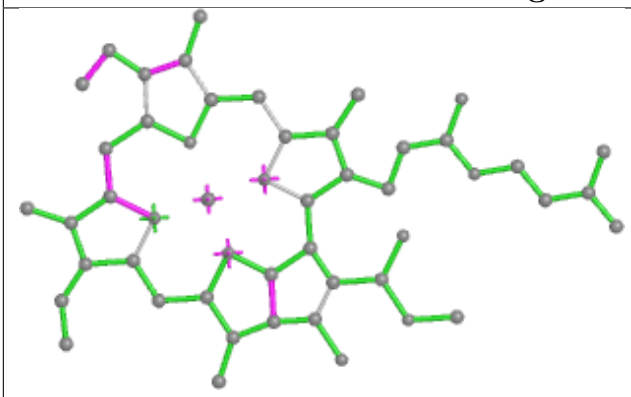


Torsions

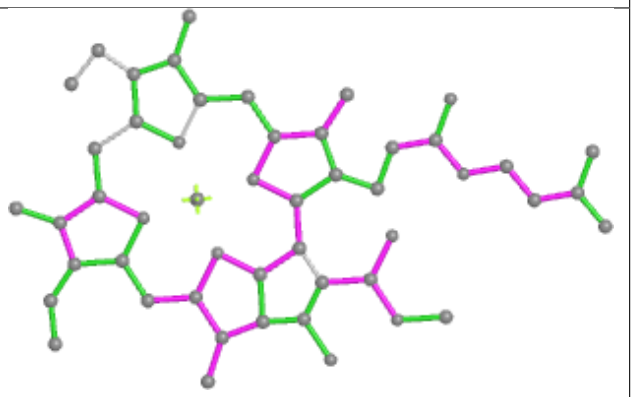


Rings

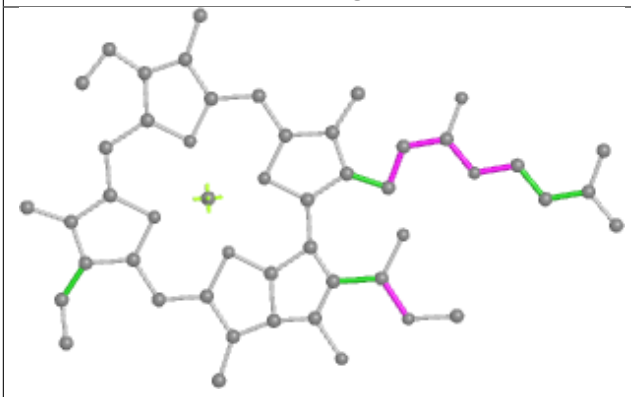
Ligand CLA 2 608



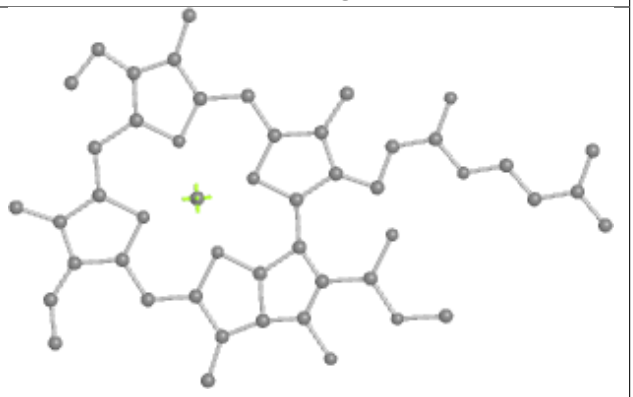
Bond lengths



Bond angles

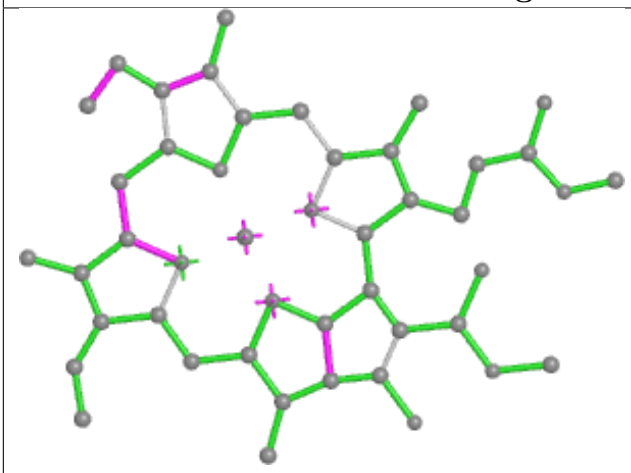


Torsions

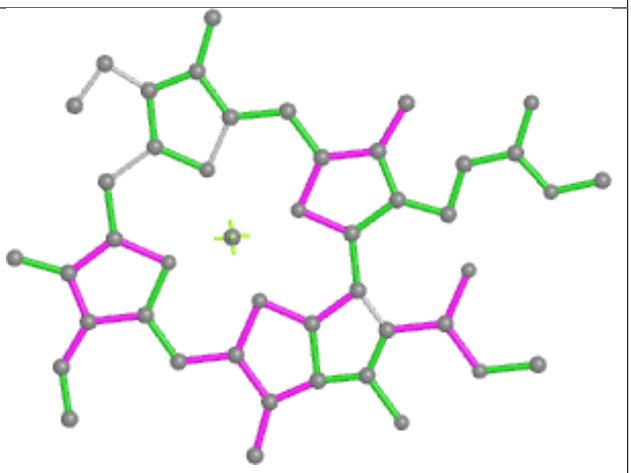


Rings

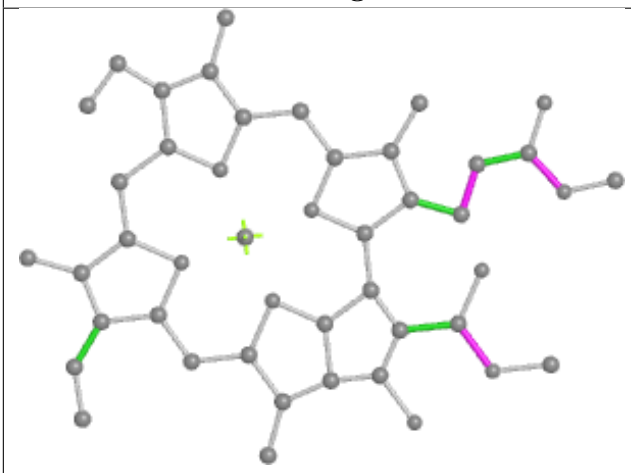
Ligand CLA B 1217



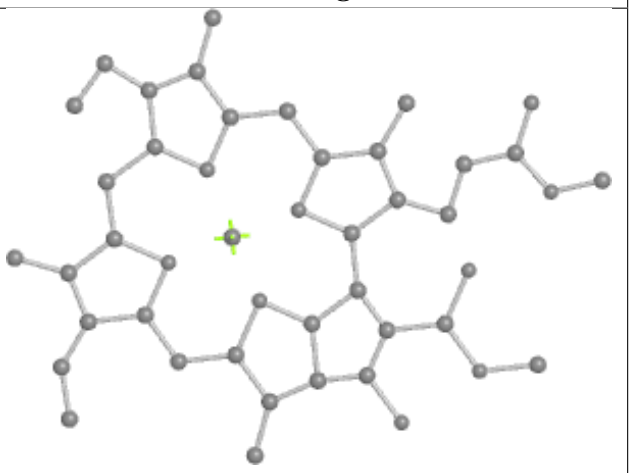
Bond lengths



Bond angles

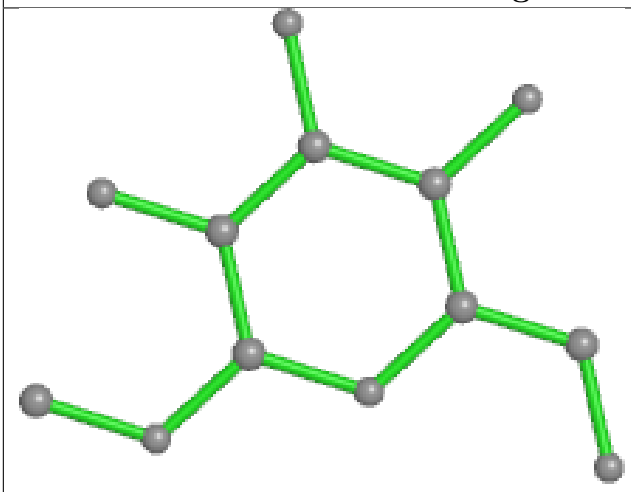


Torsions

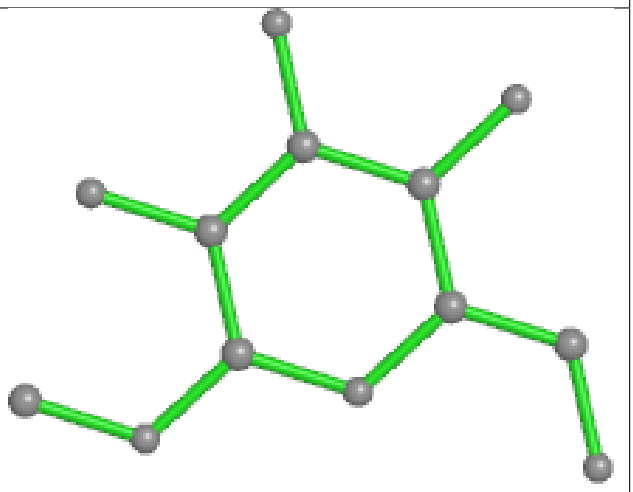


Rings

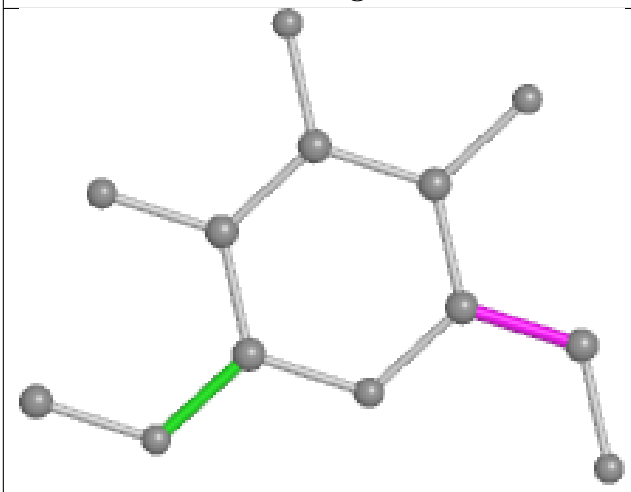
Ligand LMG F 5006



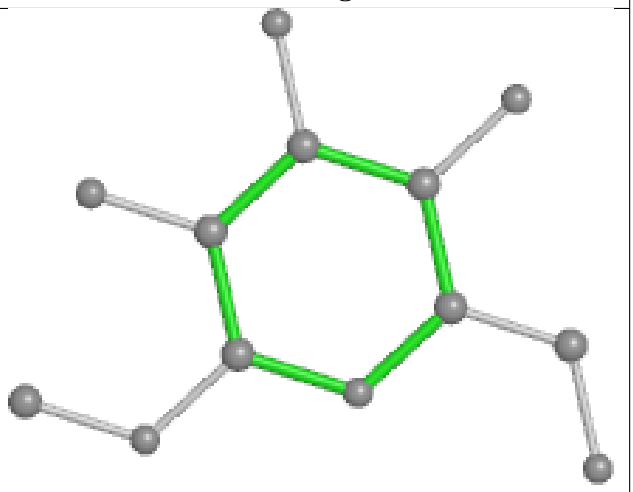
Bond lengths



Bond angles

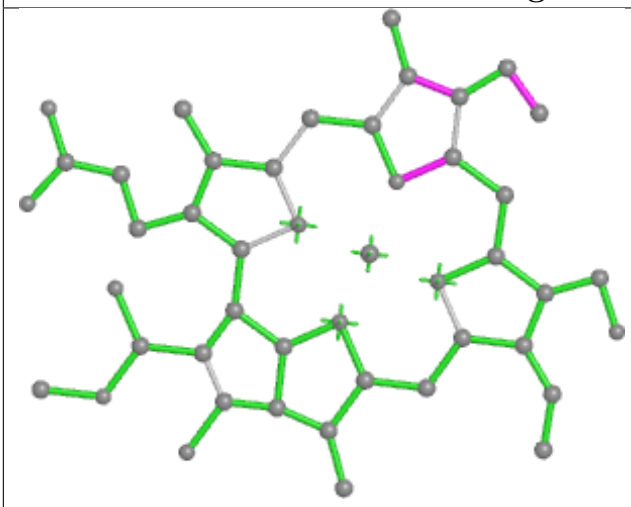


Torsions

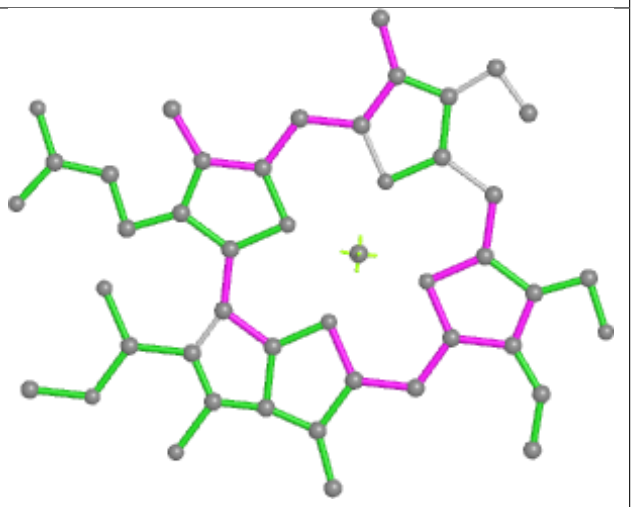


Rings

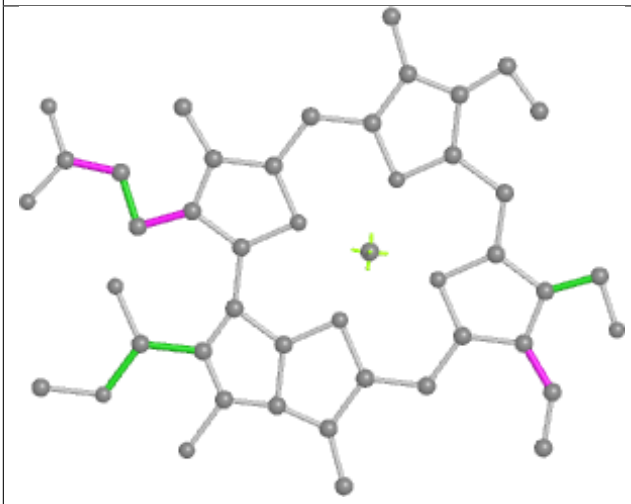
Ligand CHL 2 613



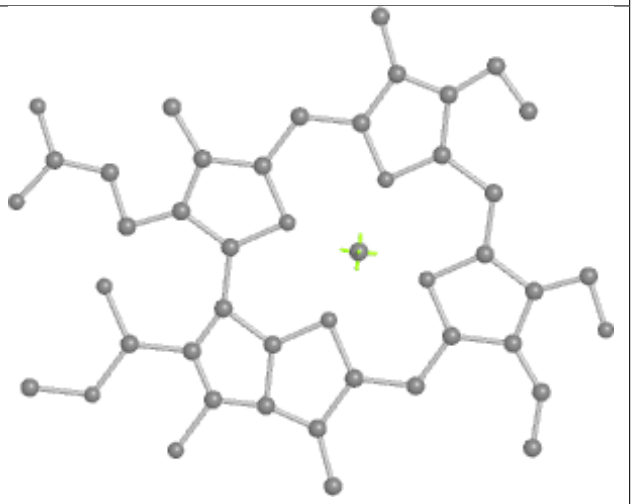
Bond lengths



Bond angles

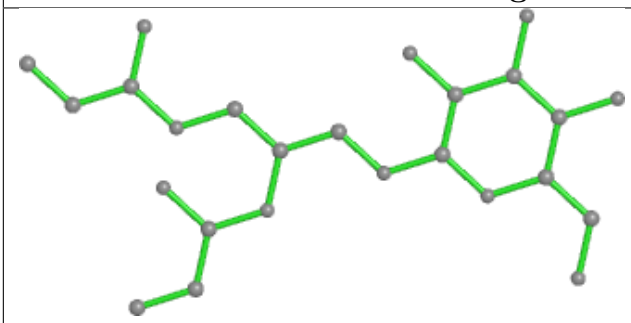


Torsions

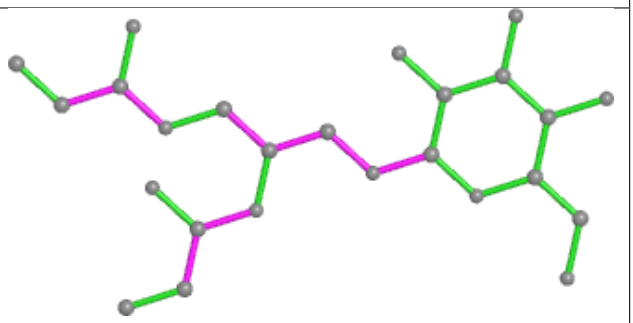


Rings

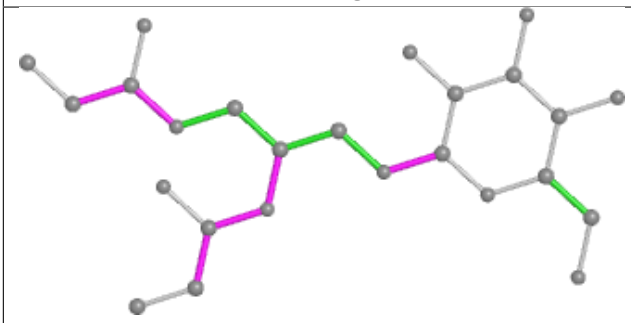
Ligand LMG G 5006



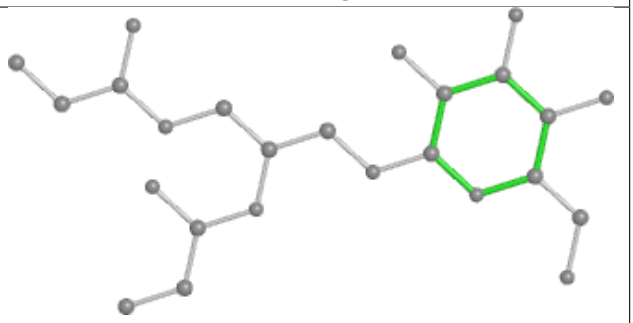
Bond lengths



Bond angles

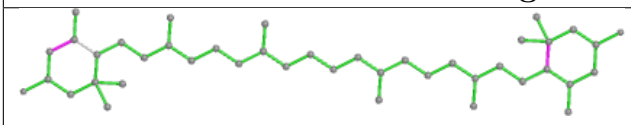


Torsions

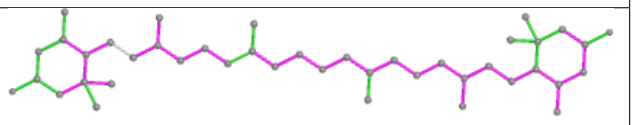


Rings

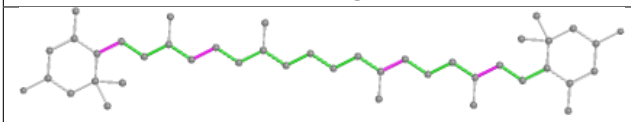
Ligand LUT J 4013



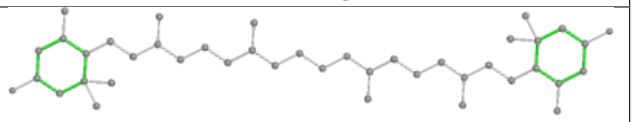
Bond lengths



Bond angles

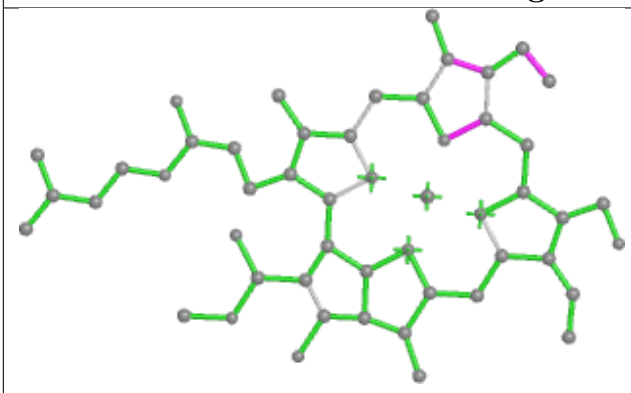


Torsions

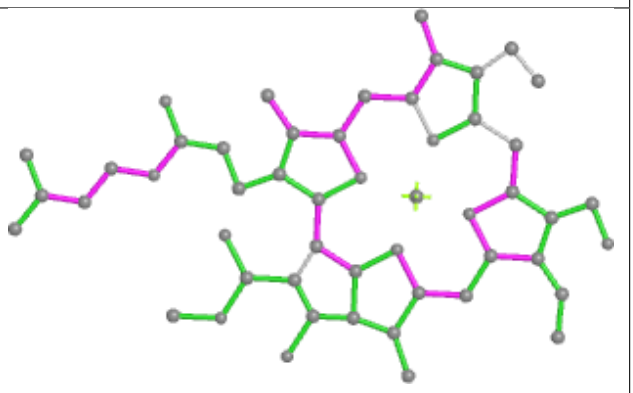


Rings

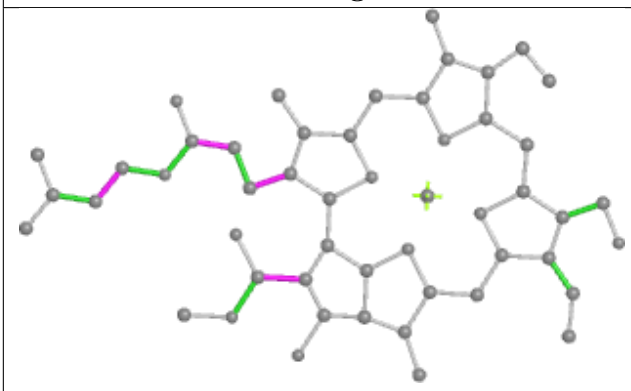
Ligand CHL 3 607



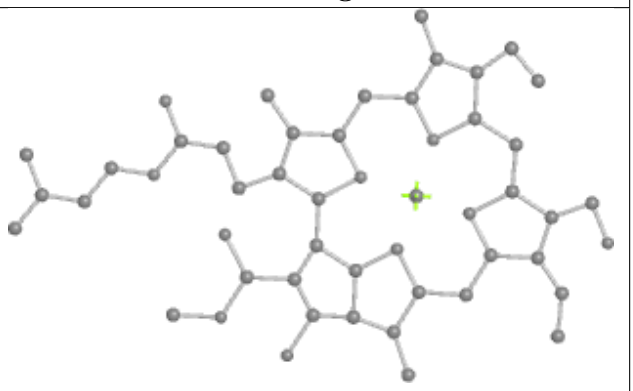
Bond lengths



Bond angles

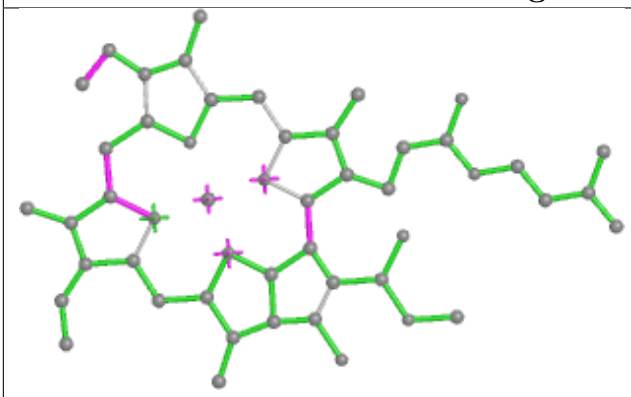


Torsions

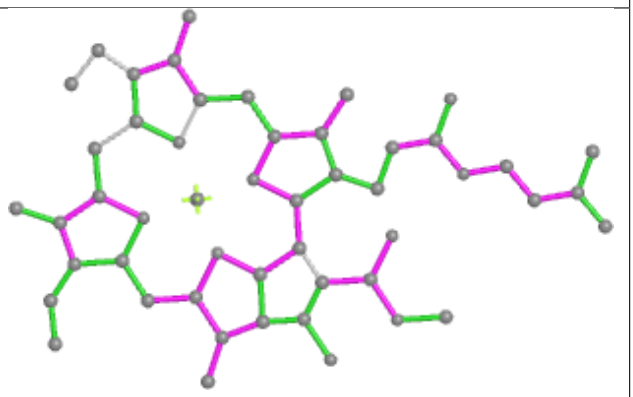


Rings

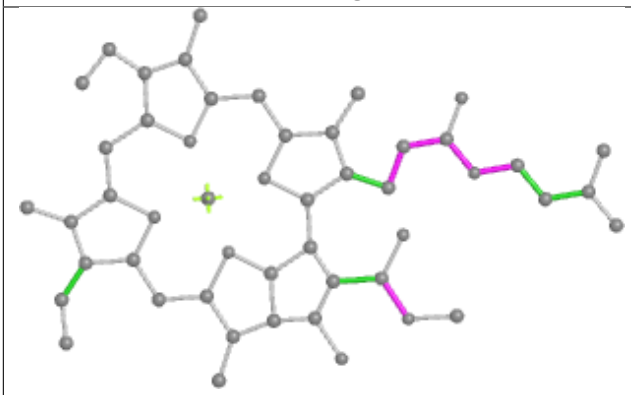
Ligand CLA 4 606



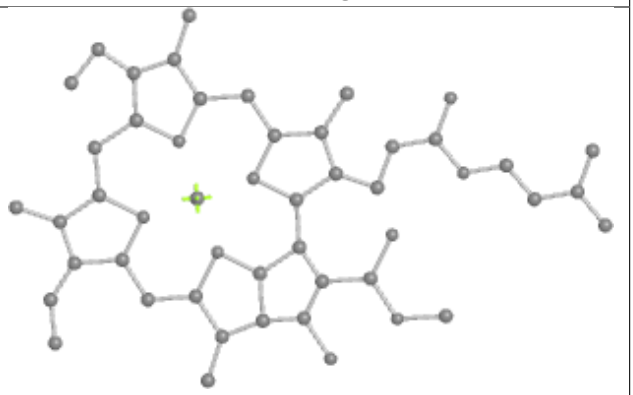
Bond lengths



Bond angles

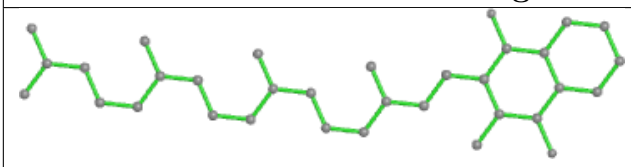


Torsions

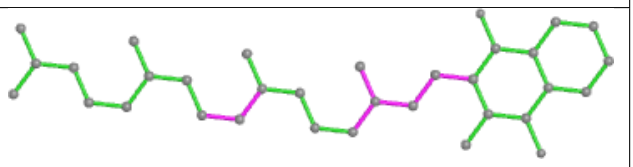


Rings

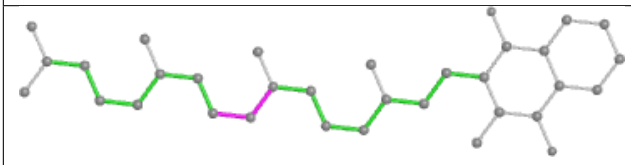
Ligand PQN A 2001



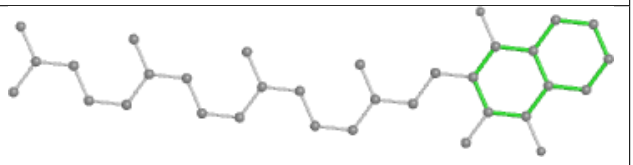
Bond lengths



Bond angles

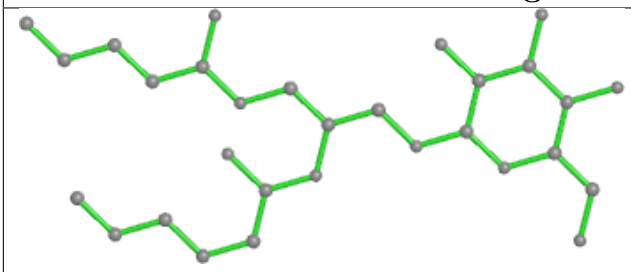


Torsions

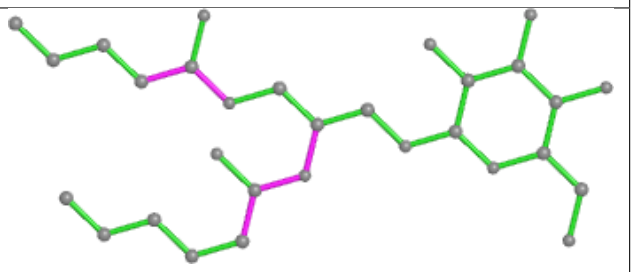


Rings

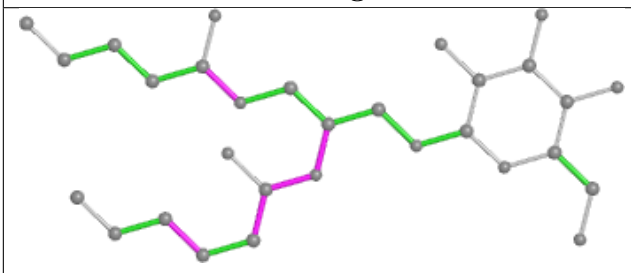
Ligand LMG 2 804



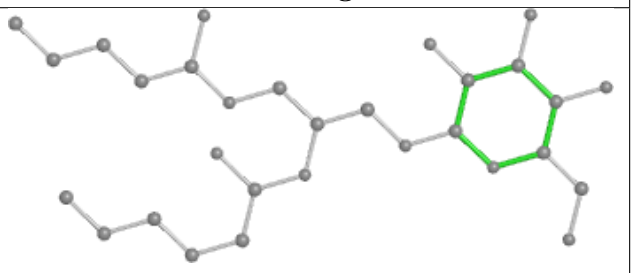
Bond lengths



Bond angles

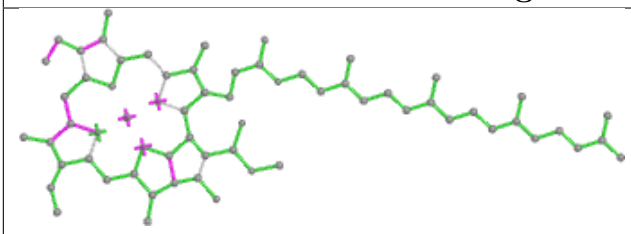


Torsions

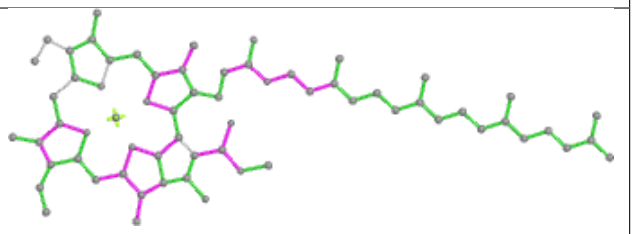


Rings

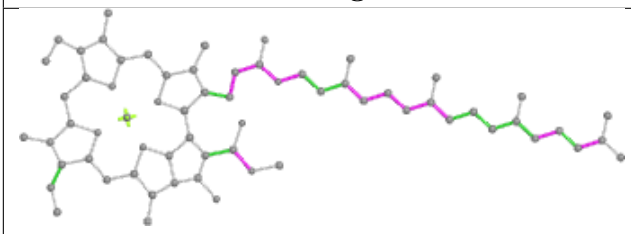
Ligand CLA B 1238



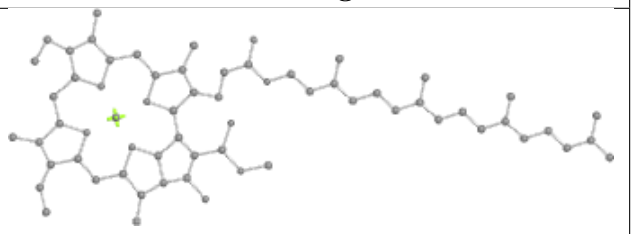
Bond lengths



Bond angles

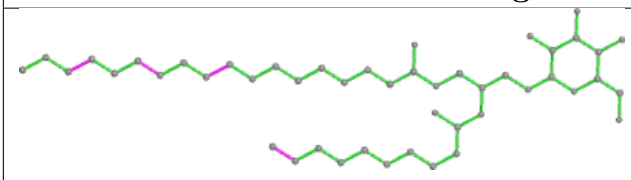


Torsions

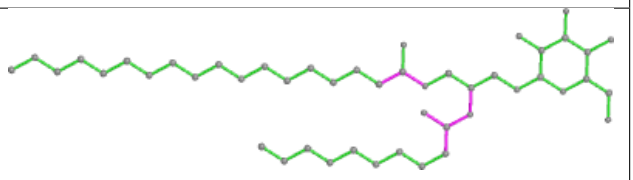


Rings

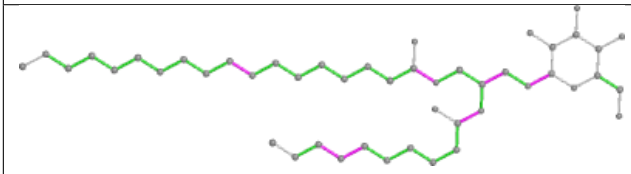
Ligand LMG F 5002



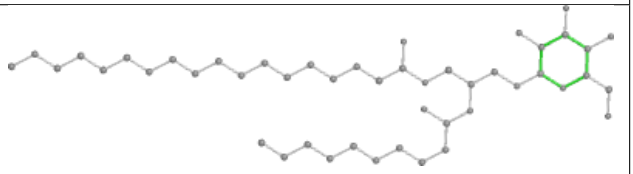
Bond lengths



Bond angles

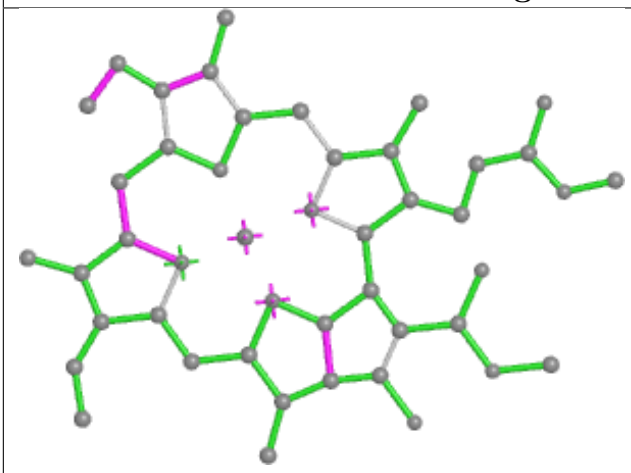


Torsions

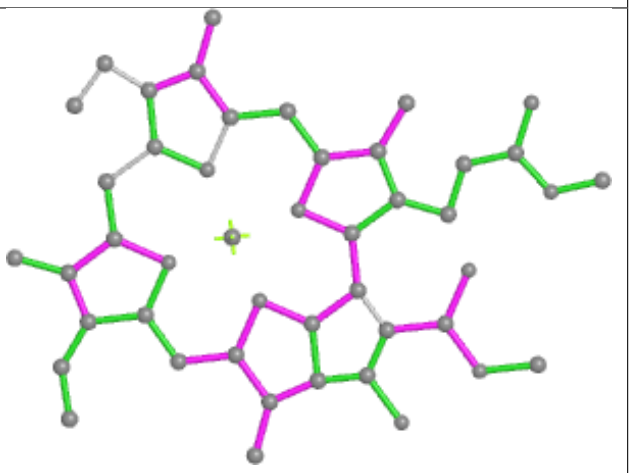


Rings

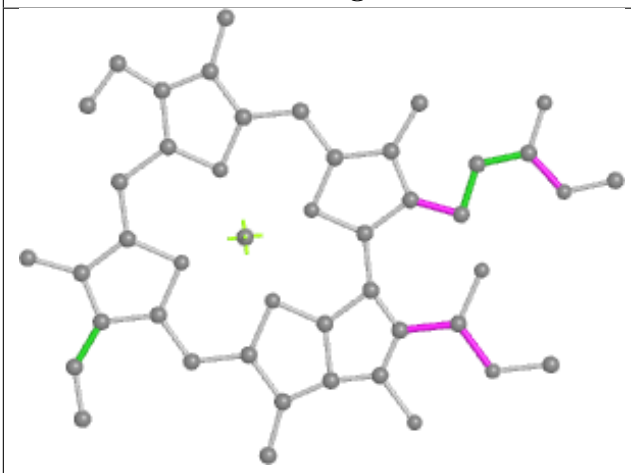
Ligand CLA G 1602



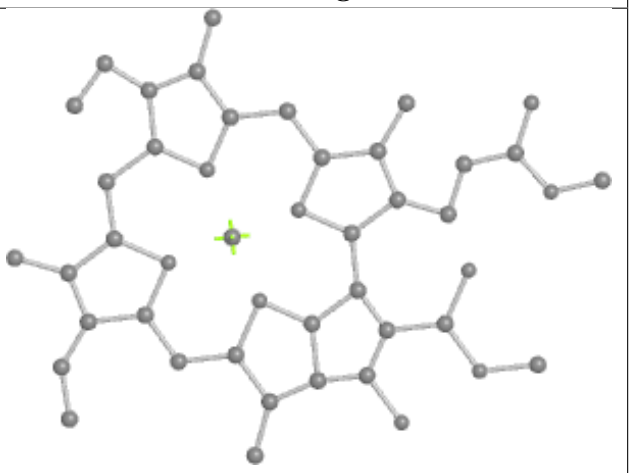
Bond lengths



Bond angles

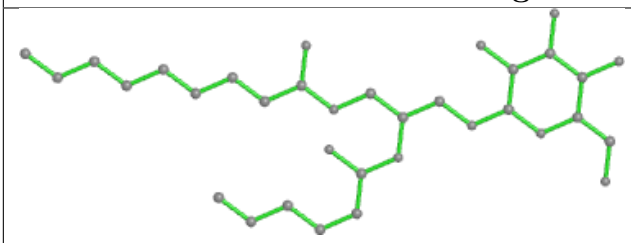


Torsions

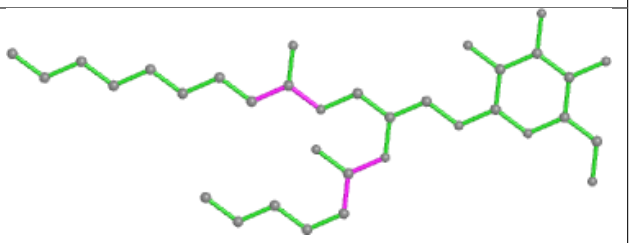


Rings

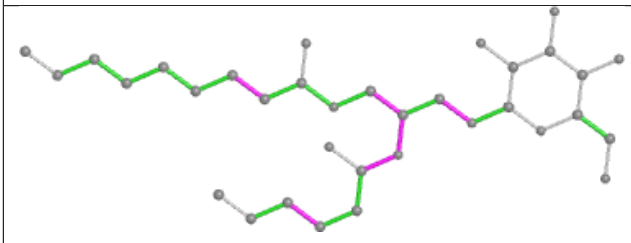
Ligand LMG F 5004



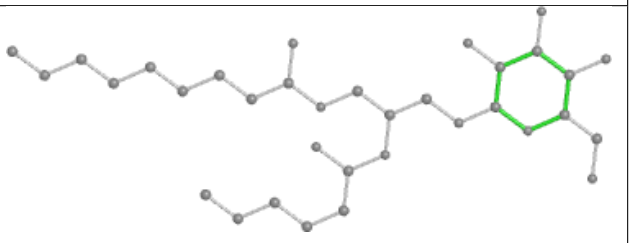
Bond lengths



Bond angles

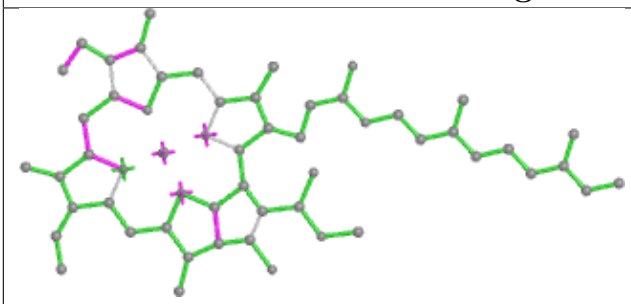


Torsions

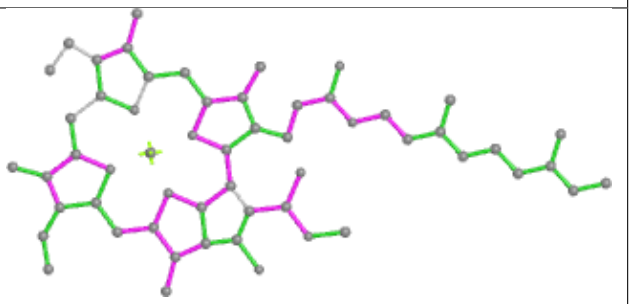


Rings

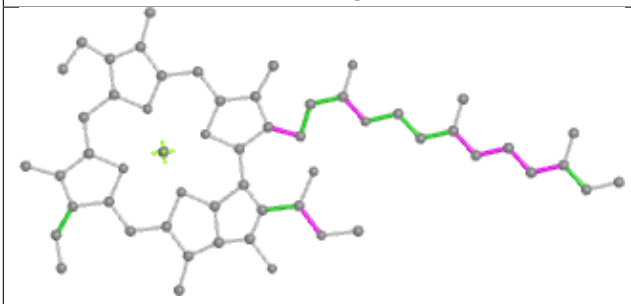
Ligand CLA A 1116



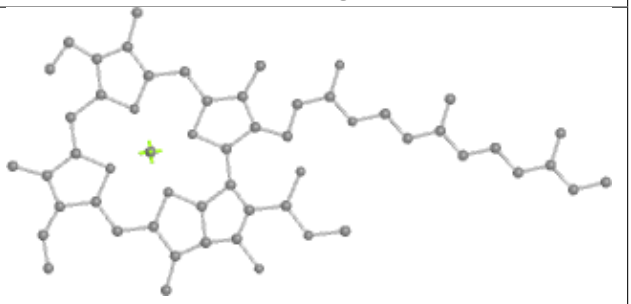
Bond lengths



Bond angles

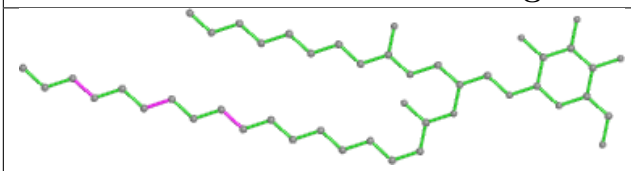


Torsions

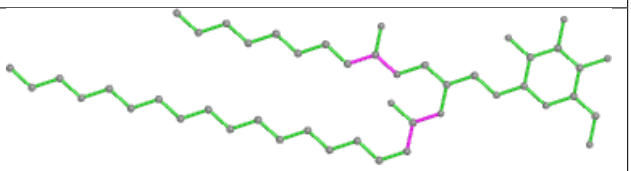


Rings

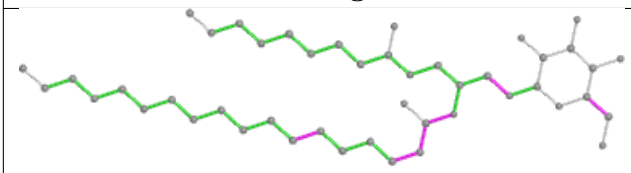
Ligand LMG 1 802



Bond lengths



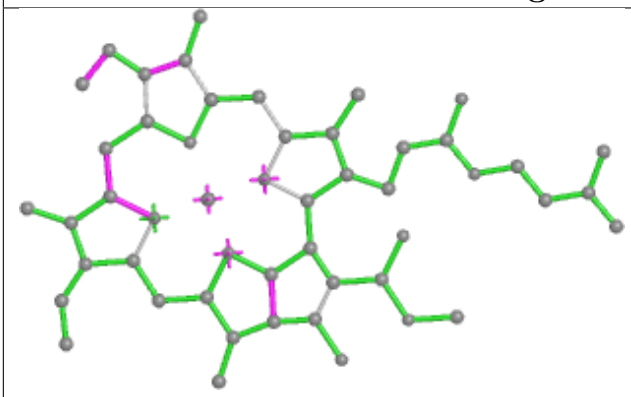
Bond angles



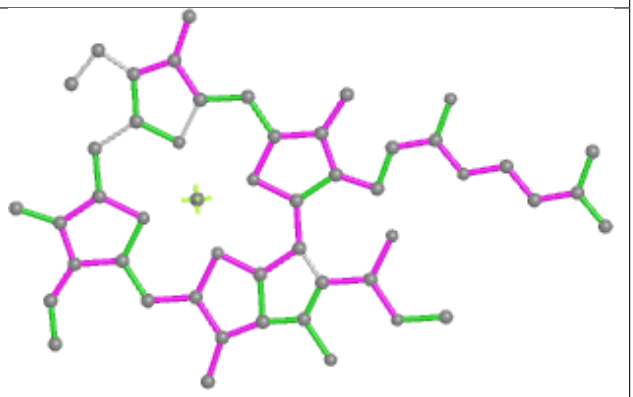
Torsions

Rings

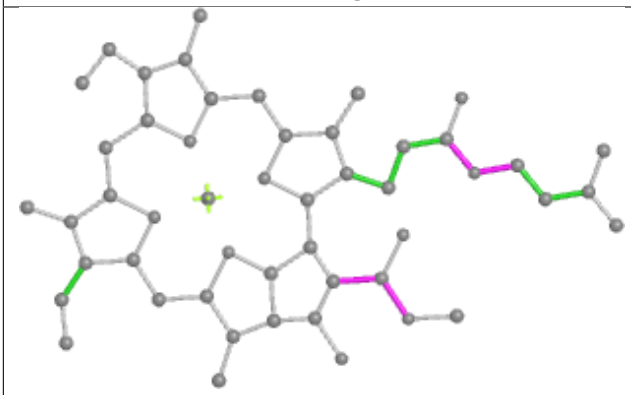
Ligand CLA 1 606



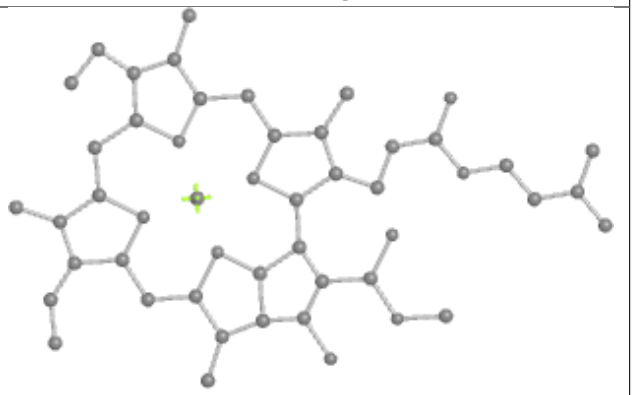
Bond lengths



Bond angles

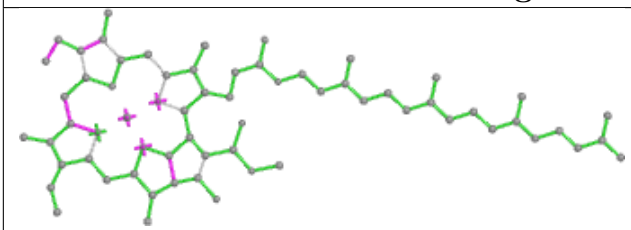


Torsions

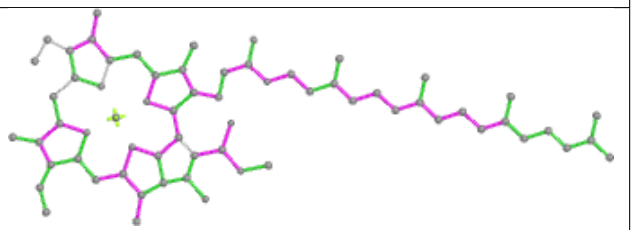


Rings

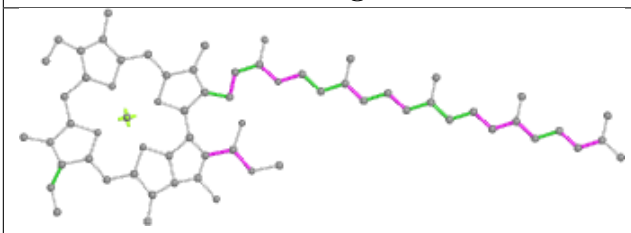
Ligand CLA A 1013



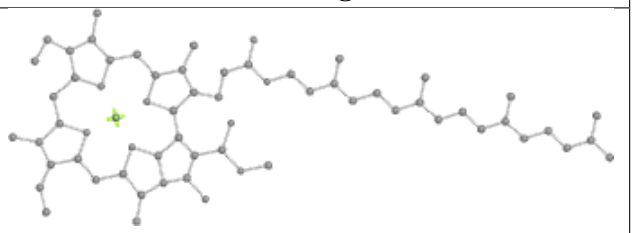
Bond lengths



Bond angles

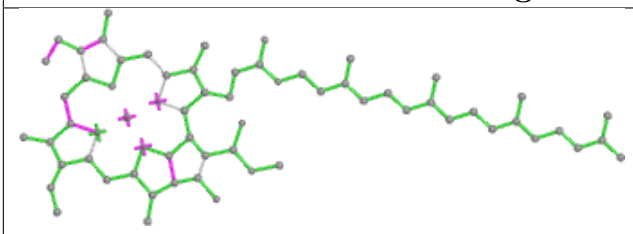


Torsions

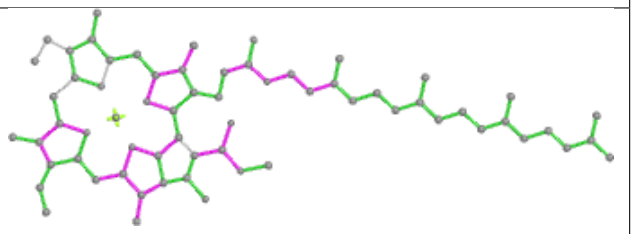


Rings

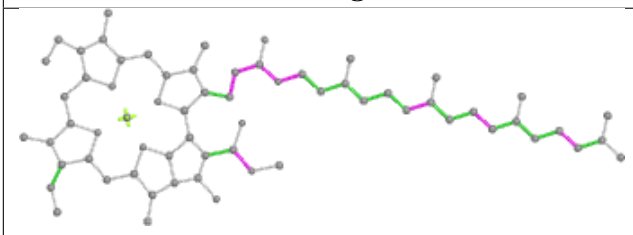
Ligand CLA A 1140



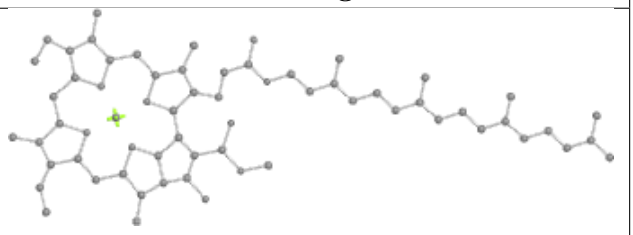
Bond lengths



Bond angles

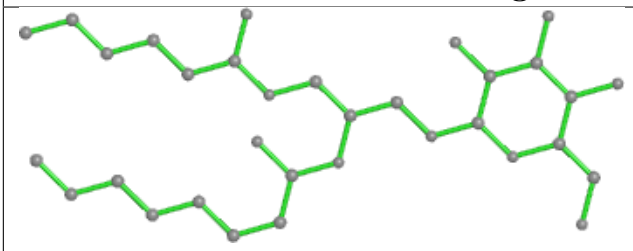


Torsions

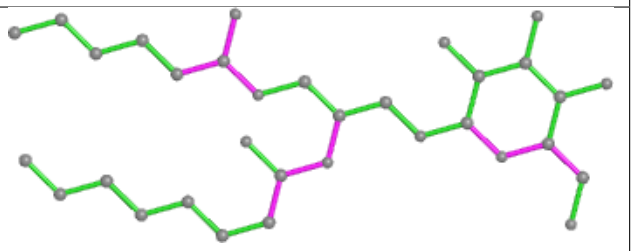


Rings

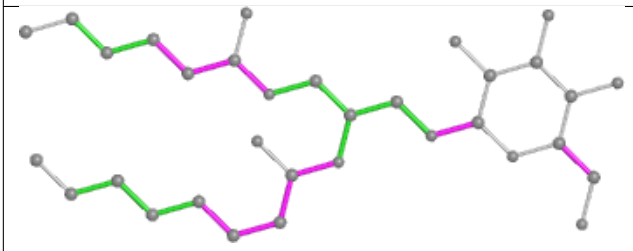
Ligand LMG B 5004



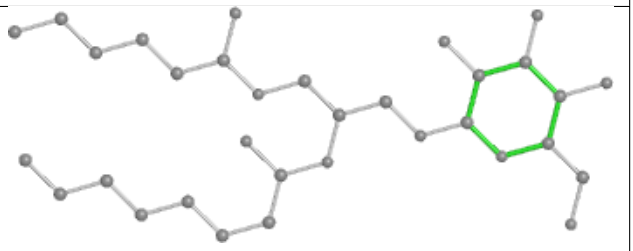
Bond lengths



Bond angles

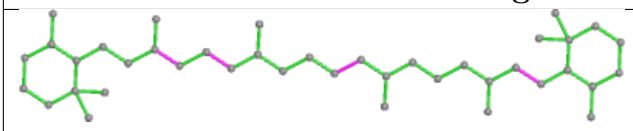


Torsions

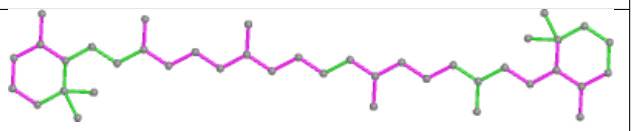


Rings

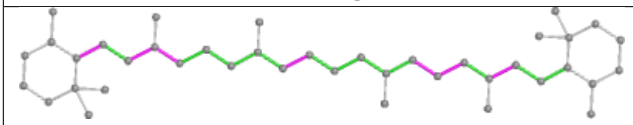
Ligand BCR K 4002



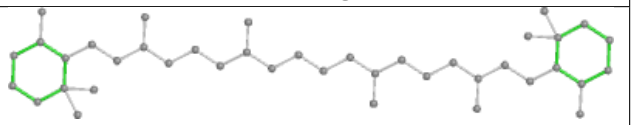
Bond lengths



Bond angles

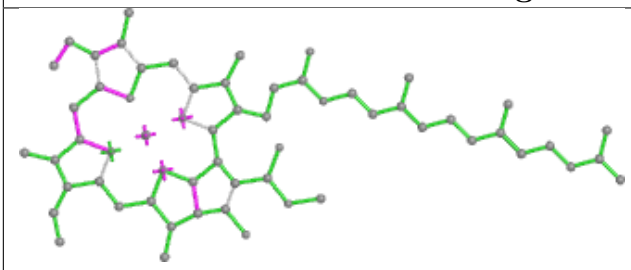


Torsions

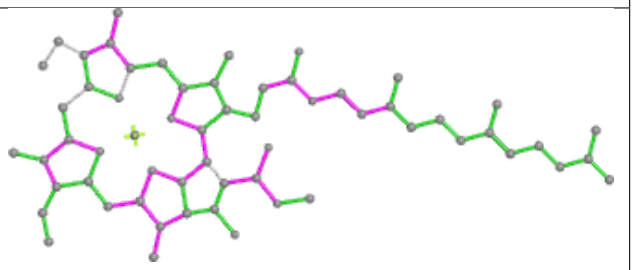


Rings

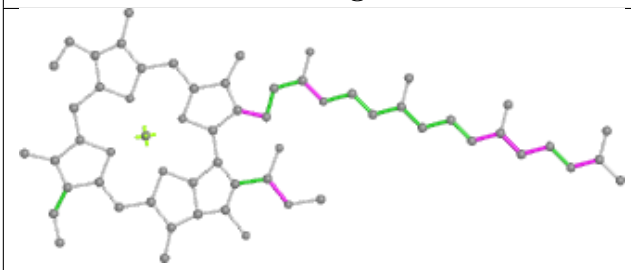
Ligand CLA B 1231



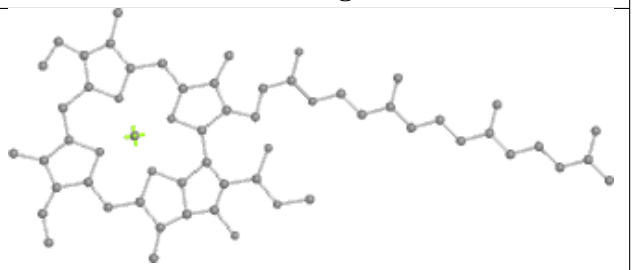
Bond lengths



Bond angles

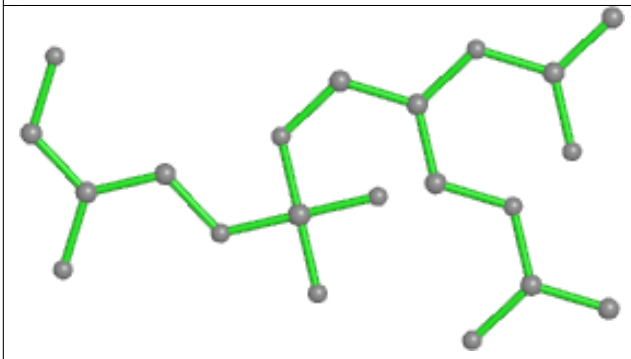


Torsions

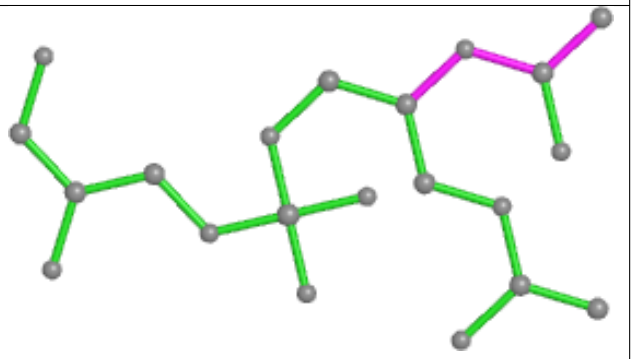


Rings

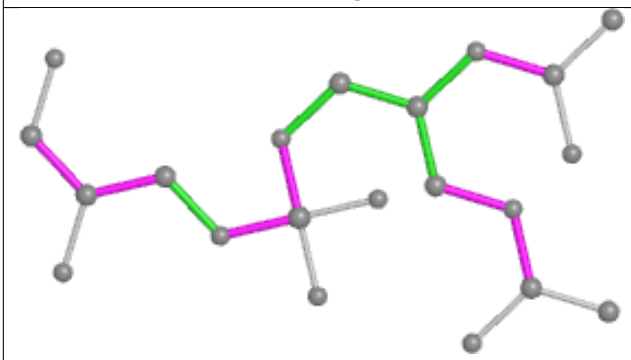
Ligand LHG B 5001



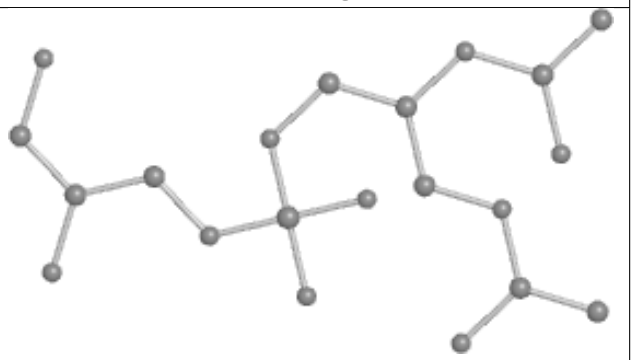
Bond lengths



Bond angles

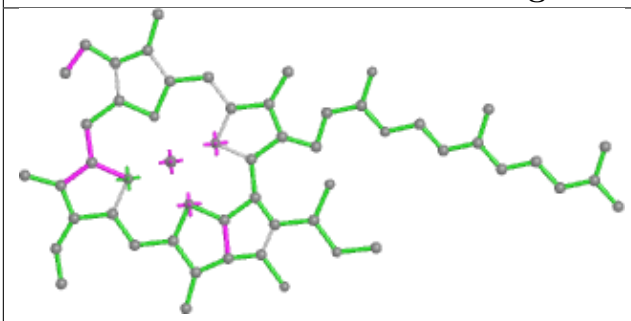


Torsions

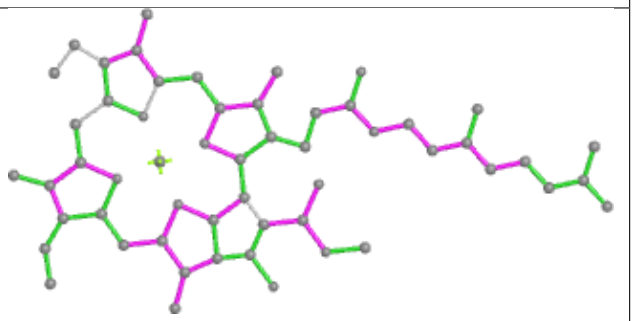


Rings

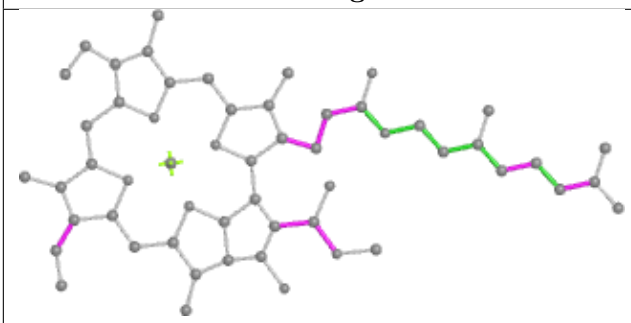
Ligand CLA 3 601



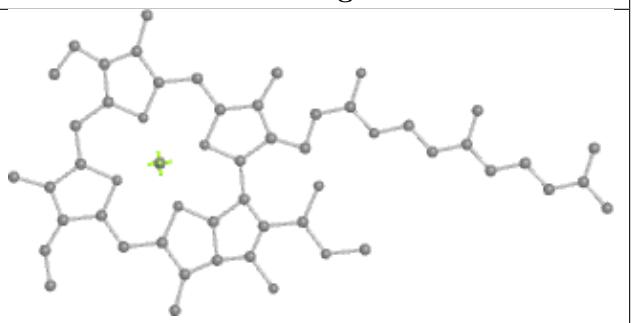
Bond lengths



Bond angles

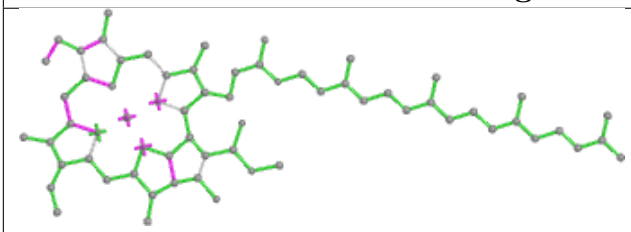


Torsions

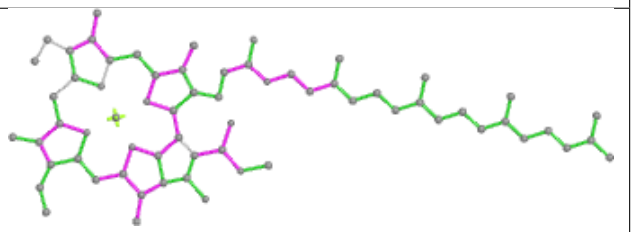


Rings

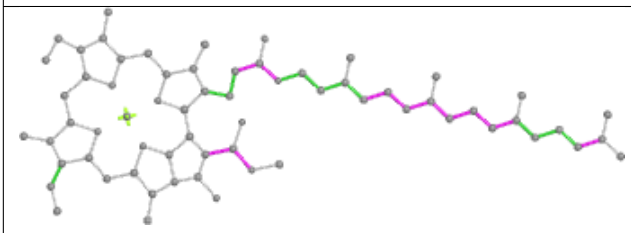
Ligand CLA A 1125



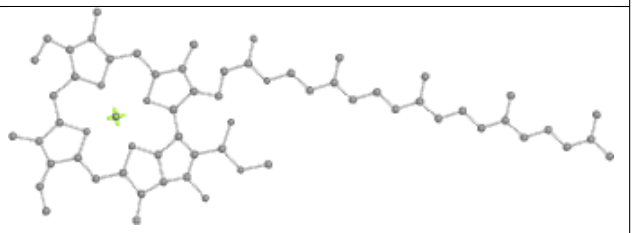
Bond lengths



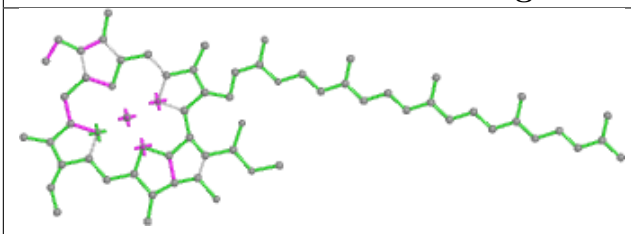
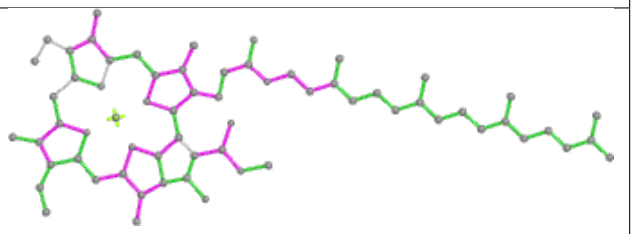
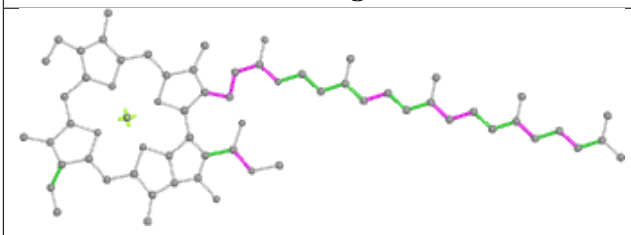
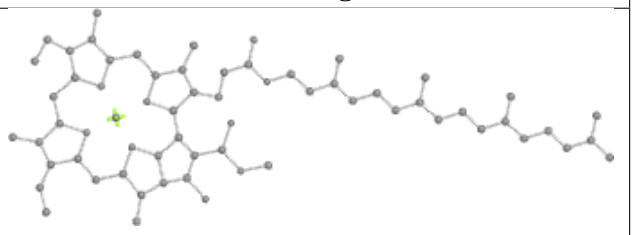
Bond angles

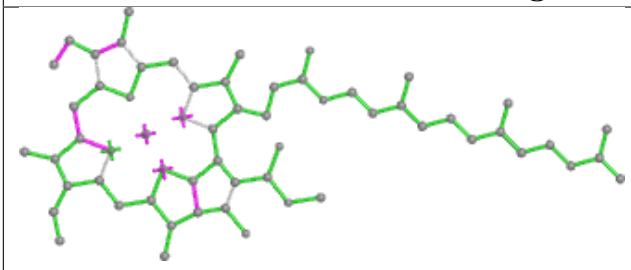
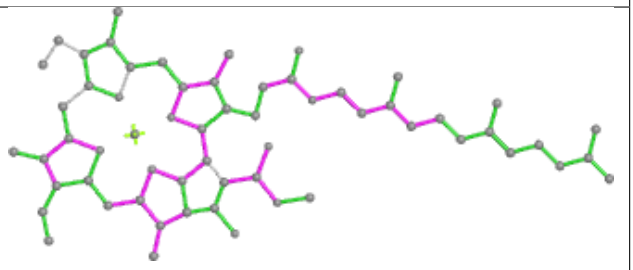
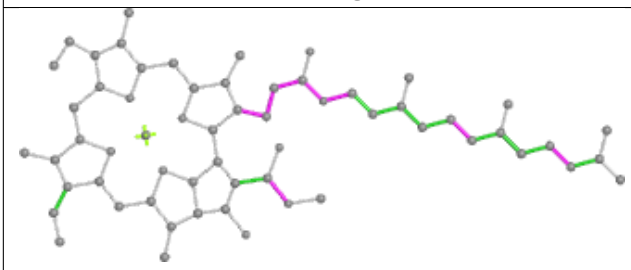
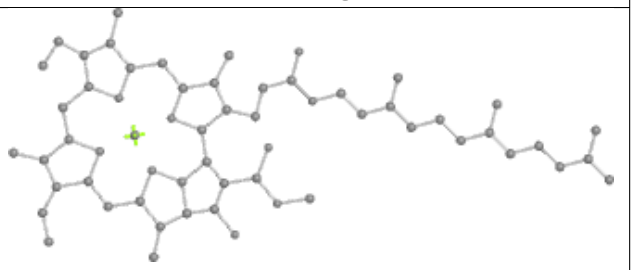


Torsions

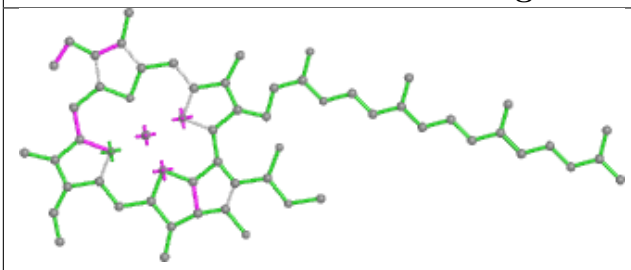


Rings

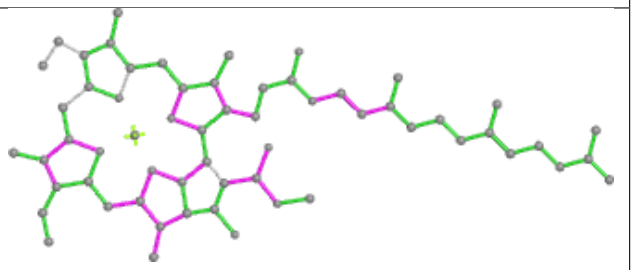
Ligand CLA B 1215	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA 2 601	
 Bond lengths	 Bond angles
 Torsions	 Rings

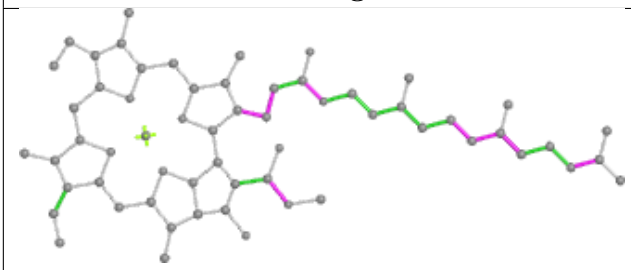
Ligand CLA B 1208



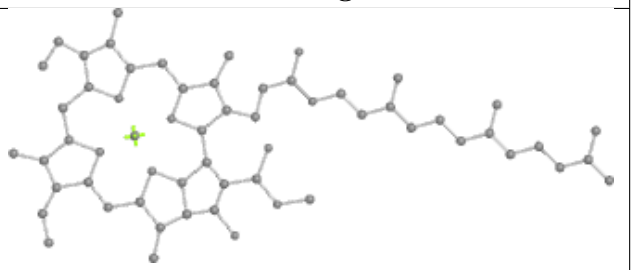
Bond lengths



Bond angles

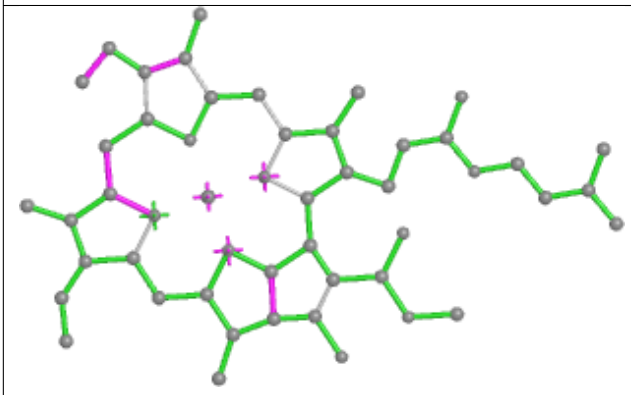


Torsions

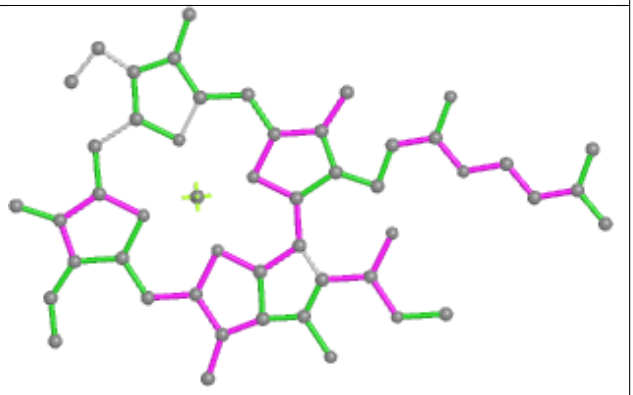


Rings

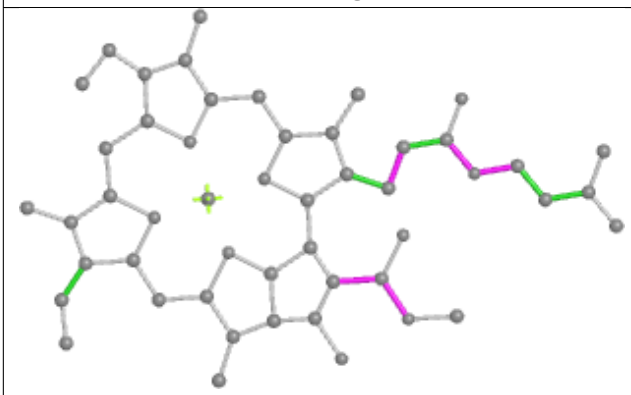
Ligand CLA A 1118



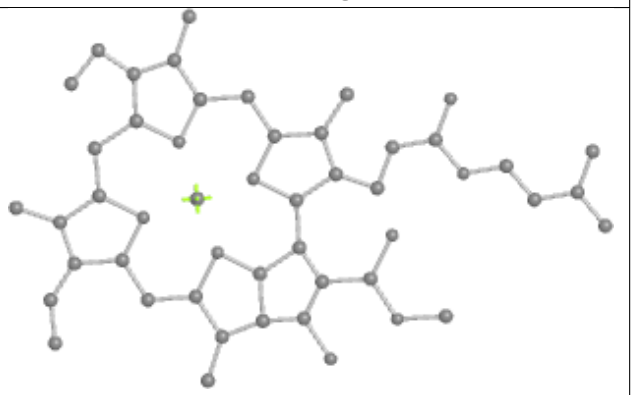
Bond lengths



Bond angles

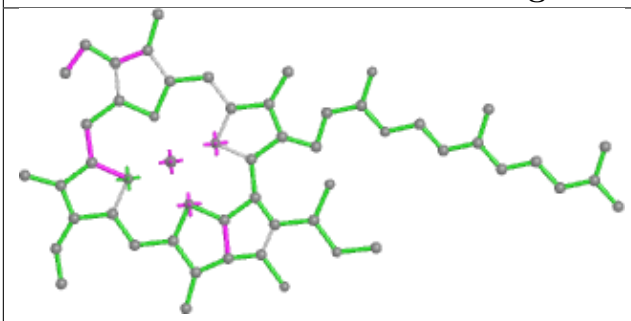


Torsions

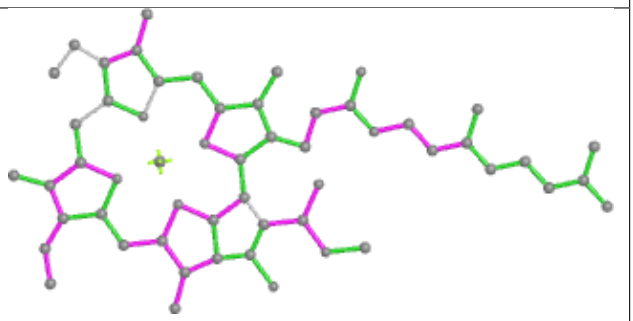


Rings

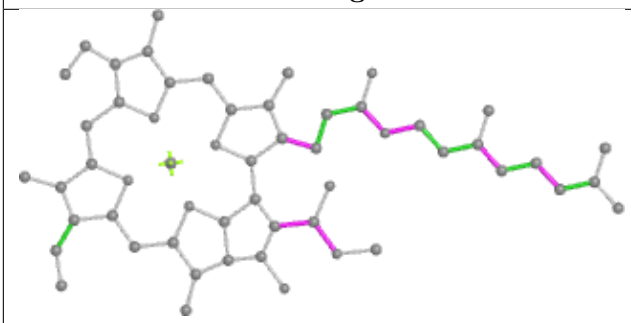
Ligand CLA 2 612



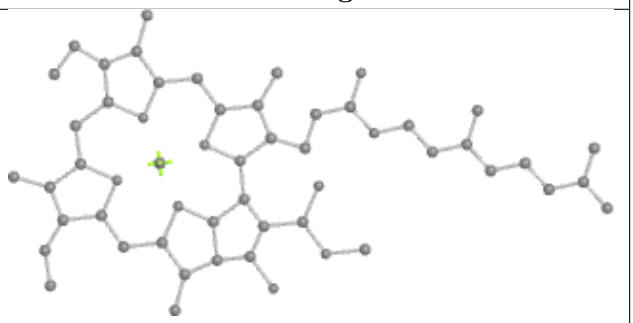
Bond lengths



Bond angles

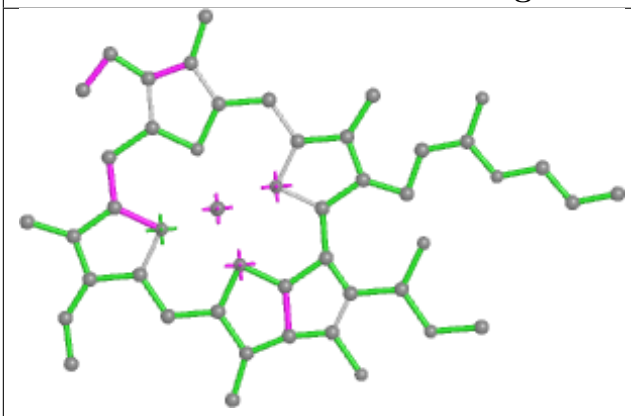


Torsions

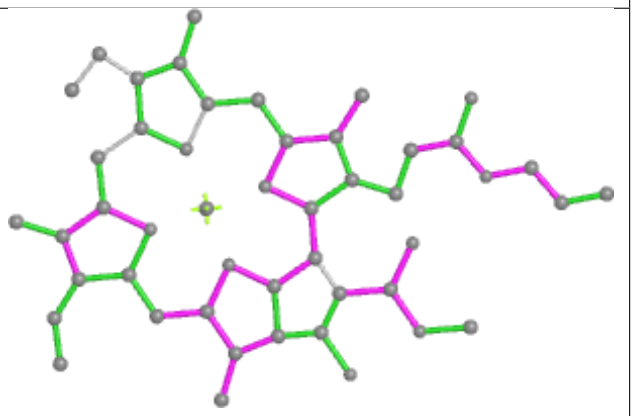


Rings

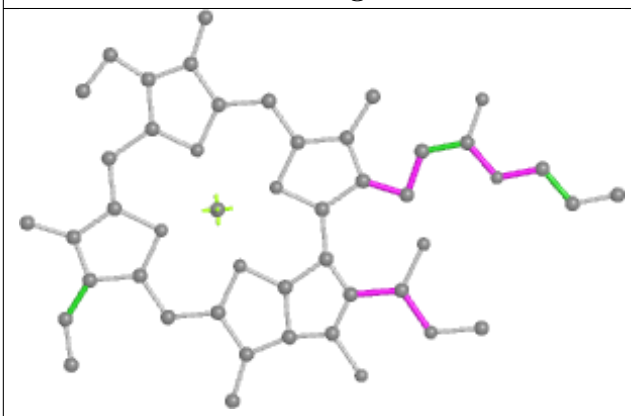
Ligand CLA K 1403



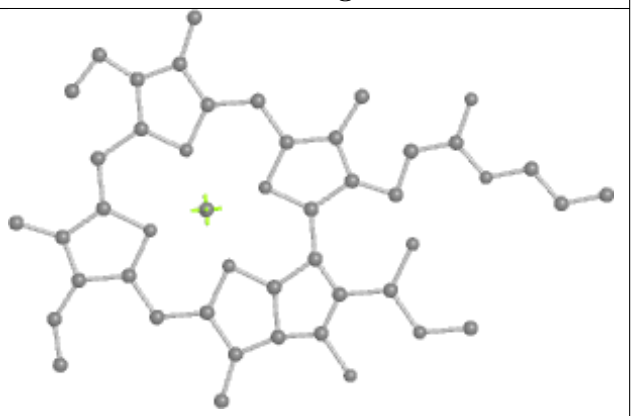
Bond lengths



Bond angles

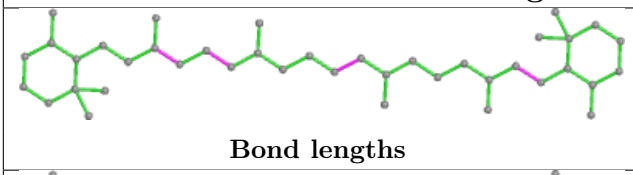


Torsions

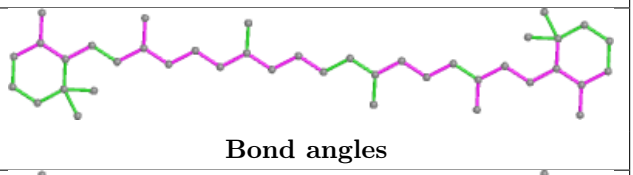


Rings

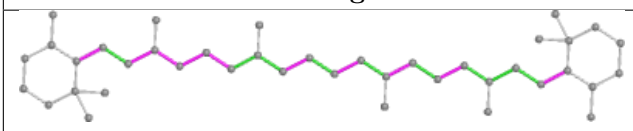
Ligand BCR 3 503



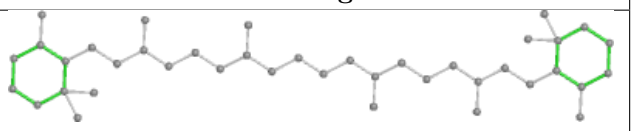
Bond lengths



Bond angles

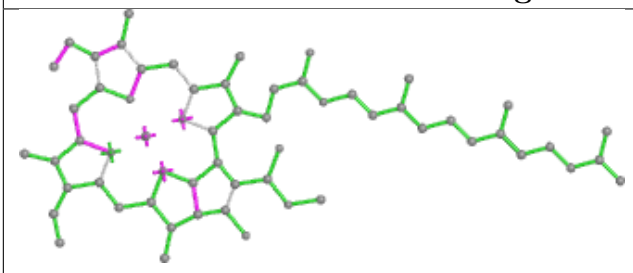


Torsions

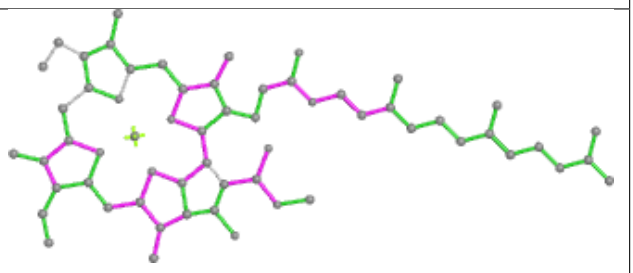


Rings

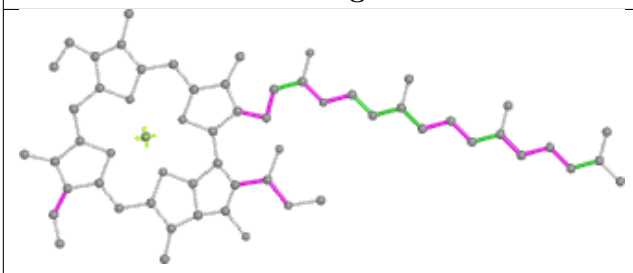
Ligand CLA H 1701



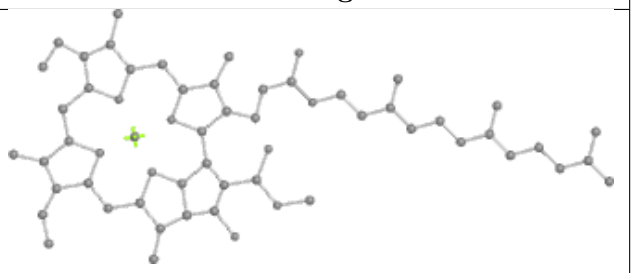
Bond lengths



Bond angles

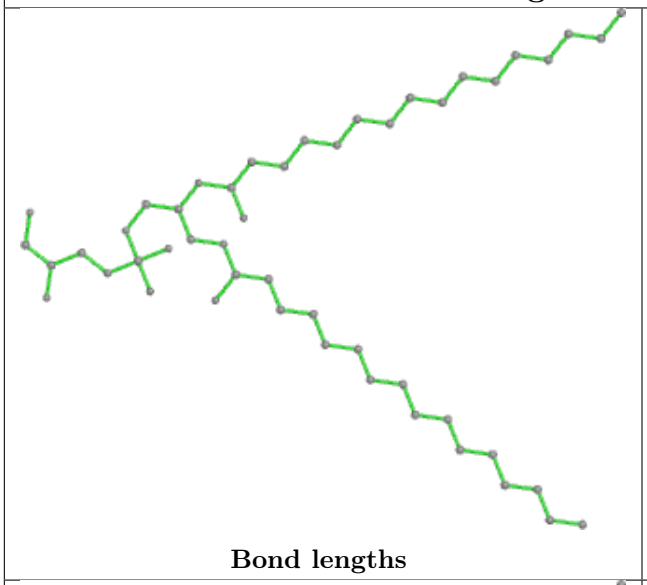


Torsions

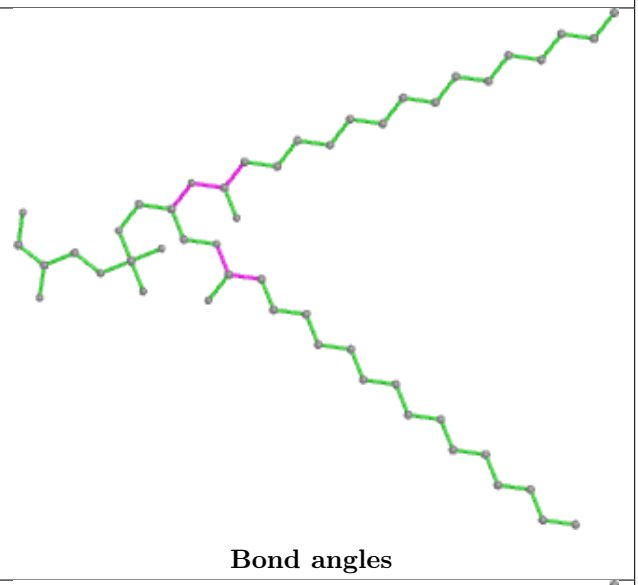


Rings

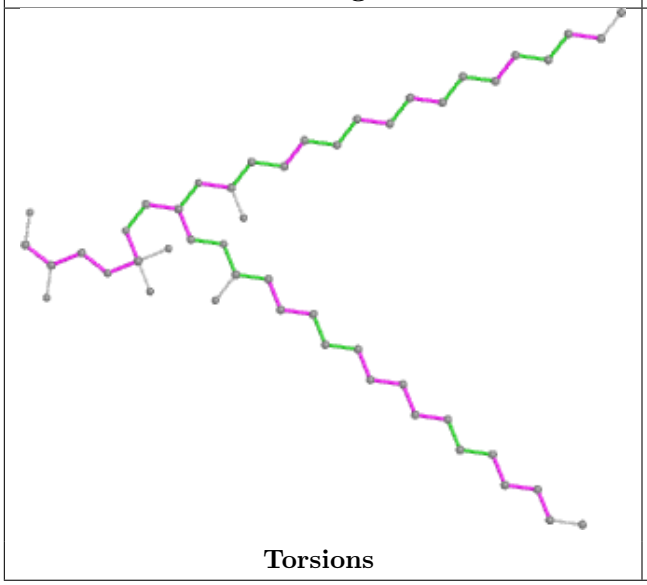
Ligand LHG 1 801



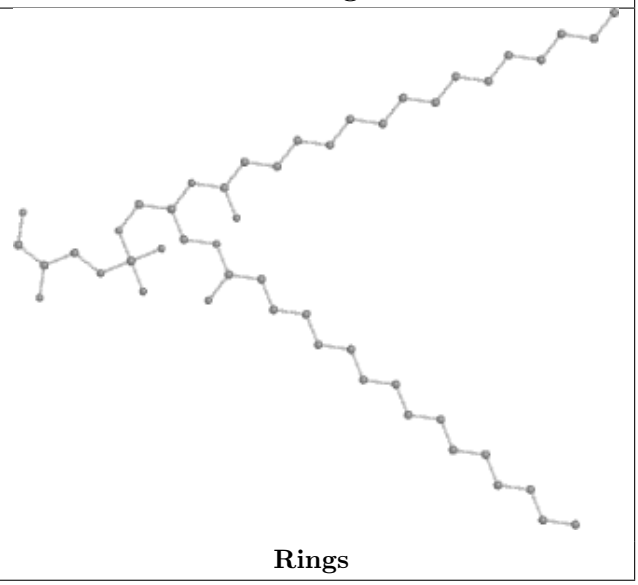
Bond lengths



Bond angles

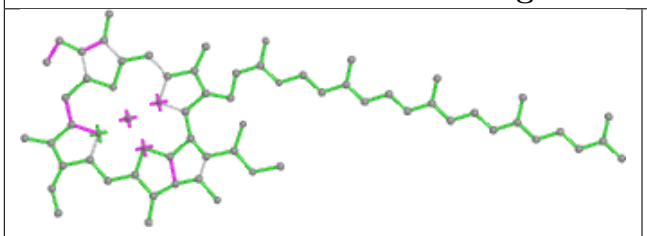


Torsions

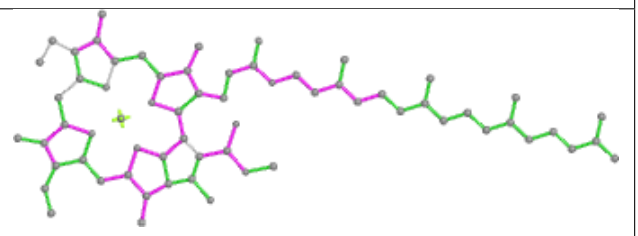


Rings

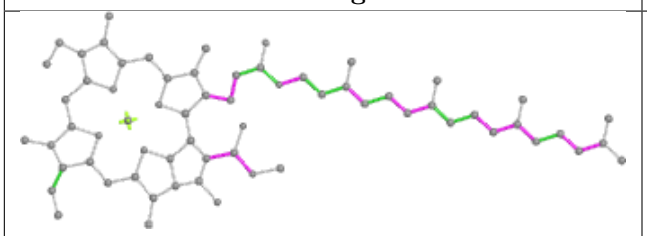
Ligand CLA B 1221



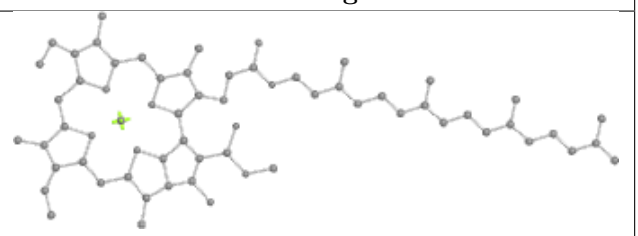
Bond lengths



Bond angles

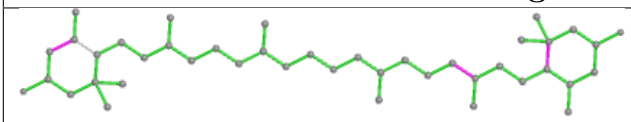


Torsions

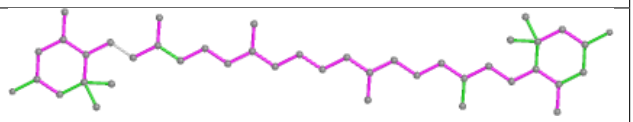


Rings

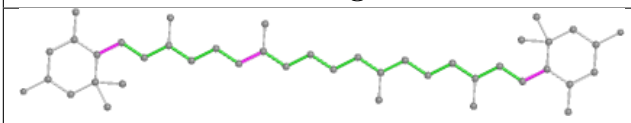
Ligand LUT 2 501



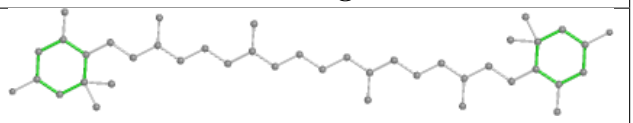
Bond lengths



Bond angles

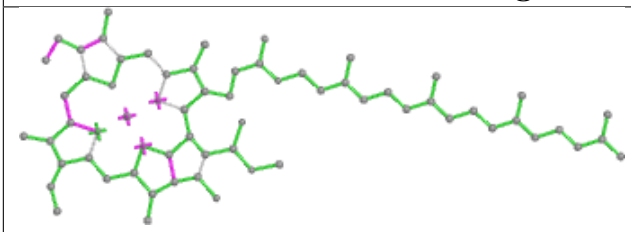


Torsions

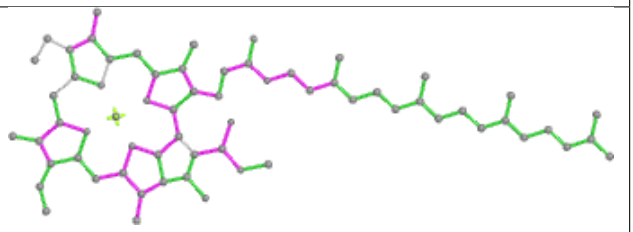


Rings

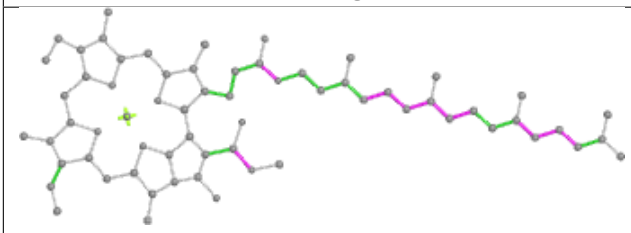
Ligand CLA A 1129



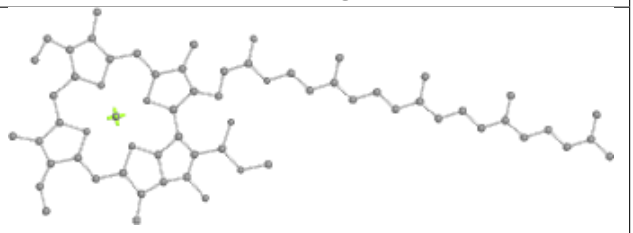
Bond lengths



Bond angles

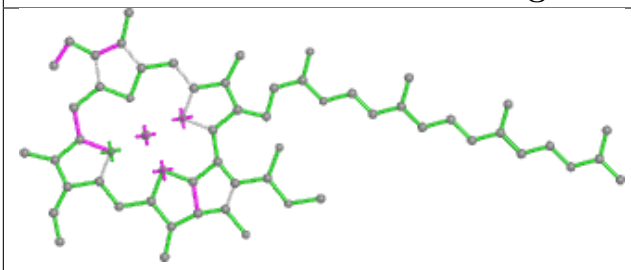


Torsions

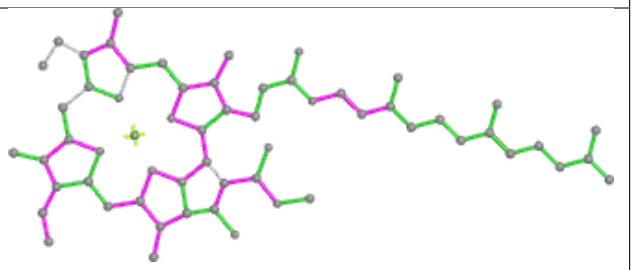


Rings

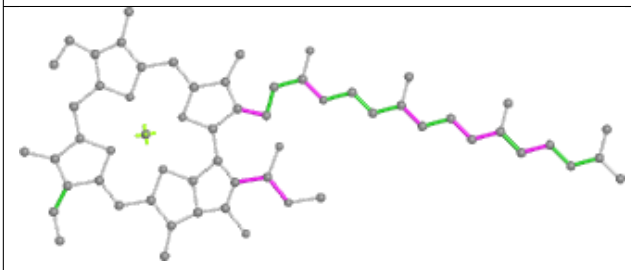
Ligand CLA 4 605



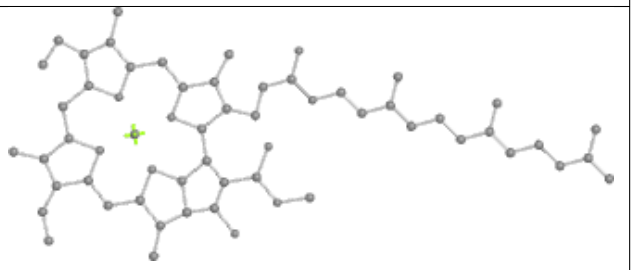
Bond lengths



Bond angles

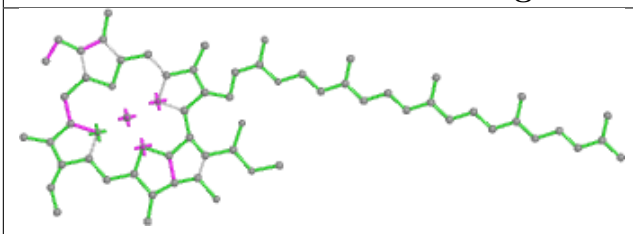


Torsions

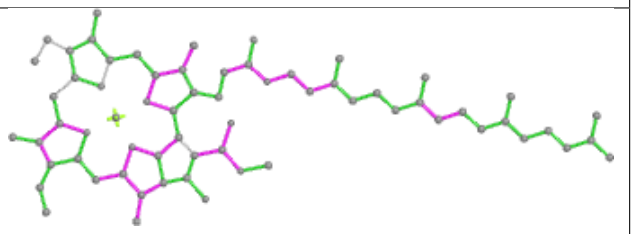


Rings

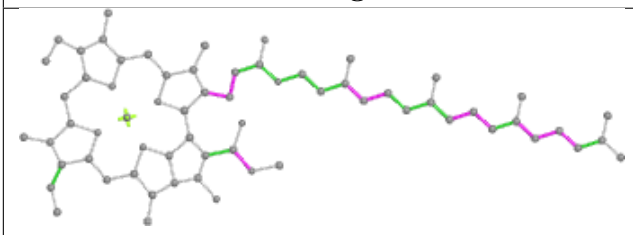
Ligand CLA A 1109



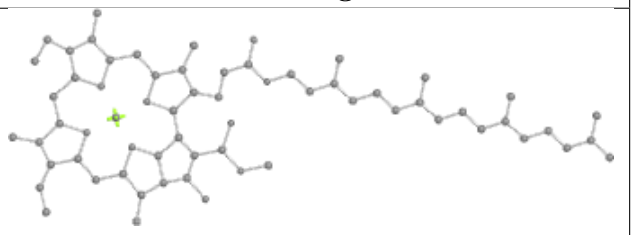
Bond lengths



Bond angles

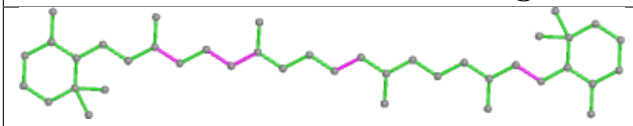


Torsions

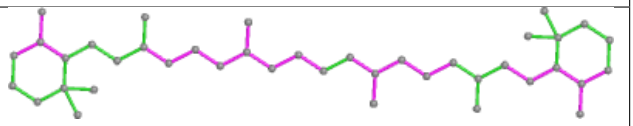


Rings

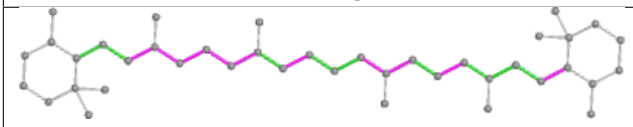
Ligand BCR F 4016



Bond lengths



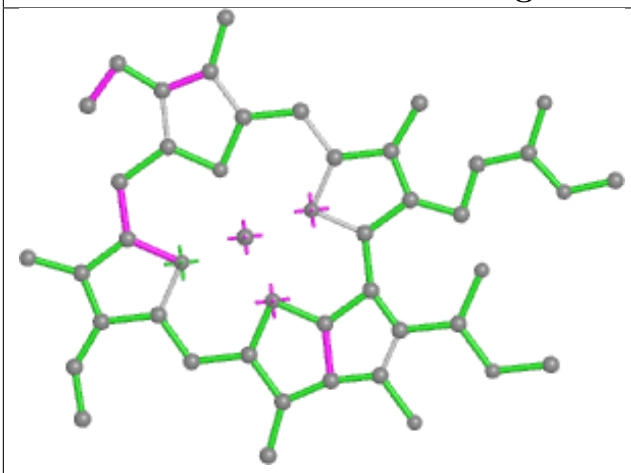
Bond angles



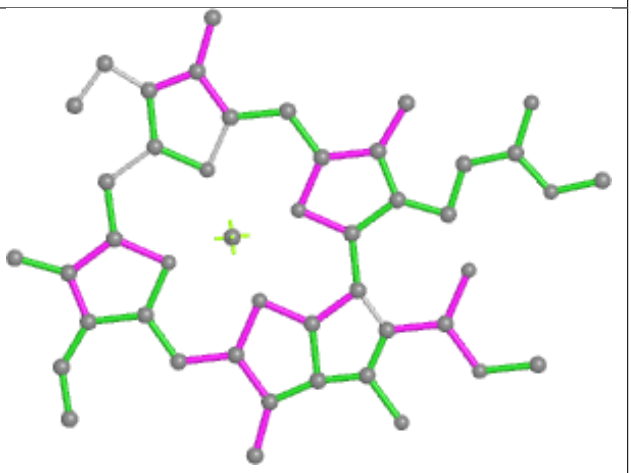
Torsions

Rings

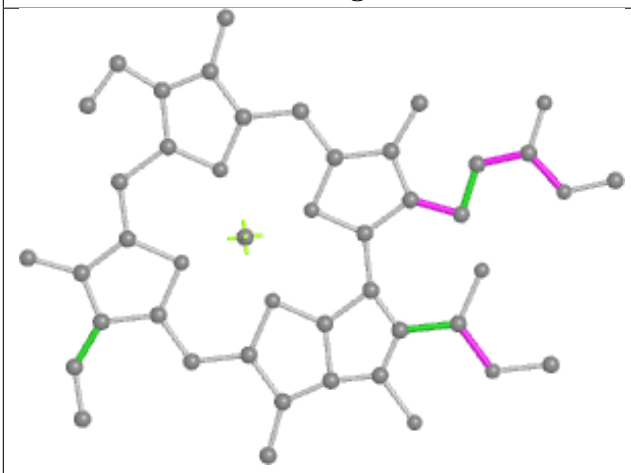
Ligand CLA B 1209



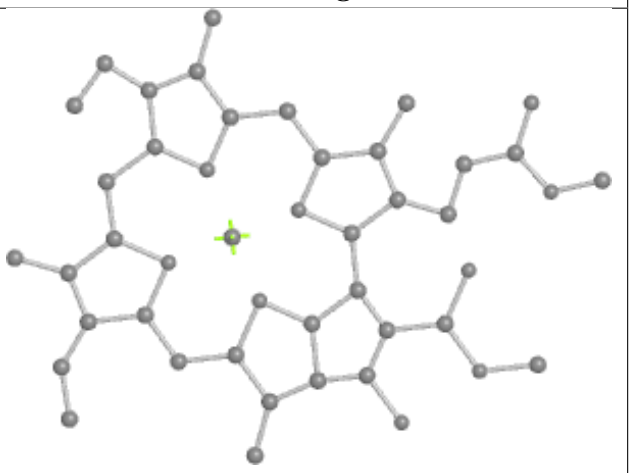
Bond lengths



Bond angles

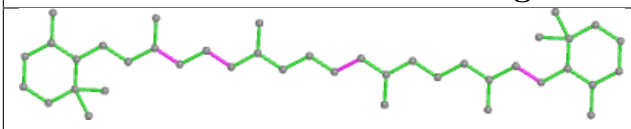


Torsions

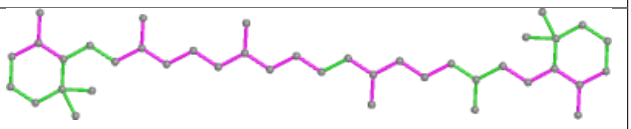


Rings

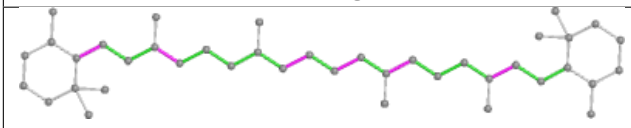
Ligand BCR B 4005



Bond lengths



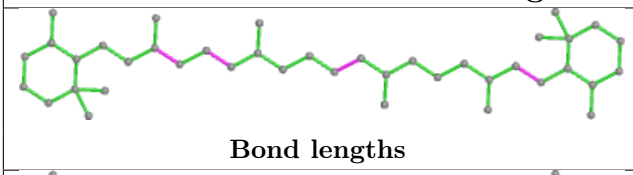
Bond angles



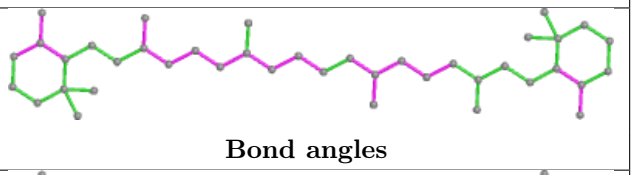
Torsions

Rings

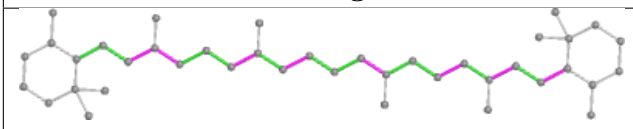
Ligand BCR 1 504



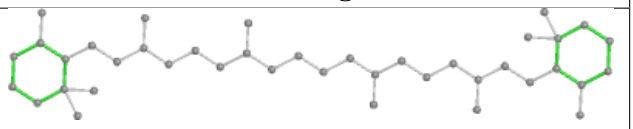
Bond lengths



Bond angles

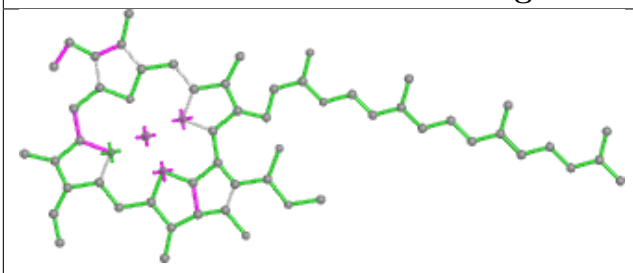


Torsions

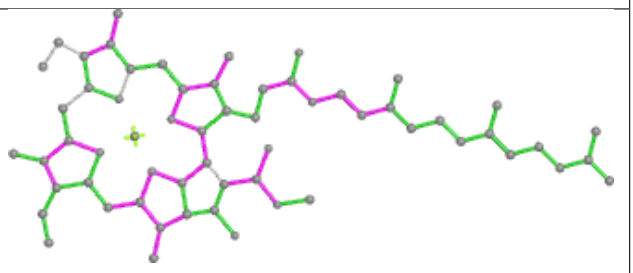


Rings

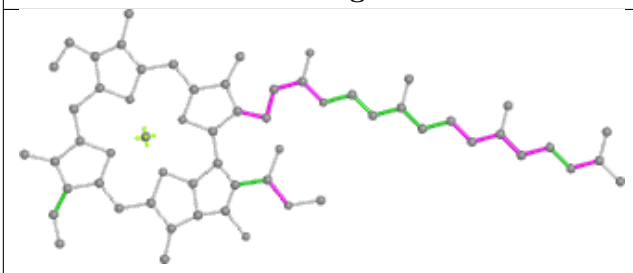
Ligand CLA A 1141



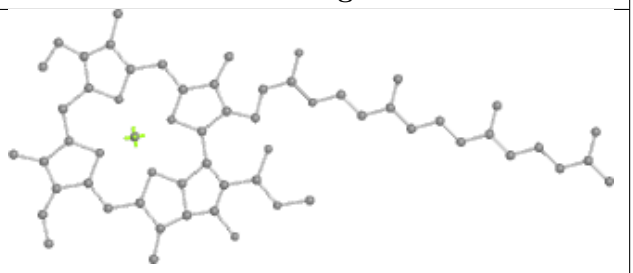
Bond lengths



Bond angles

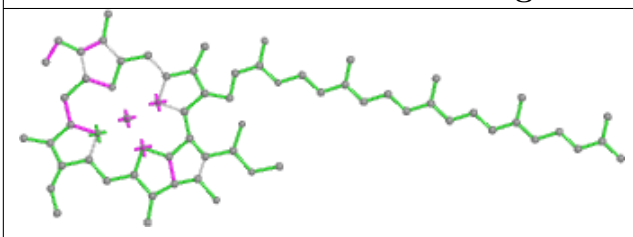


Torsions

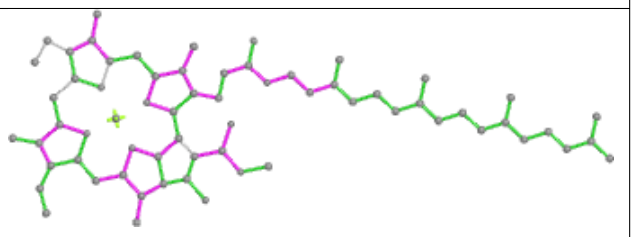


Rings

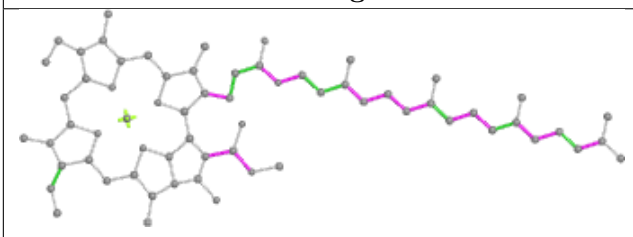
Ligand CLA B 1222



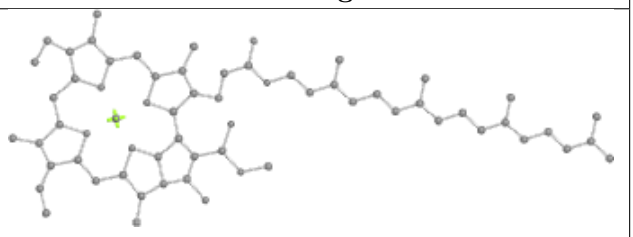
Bond lengths



Bond angles

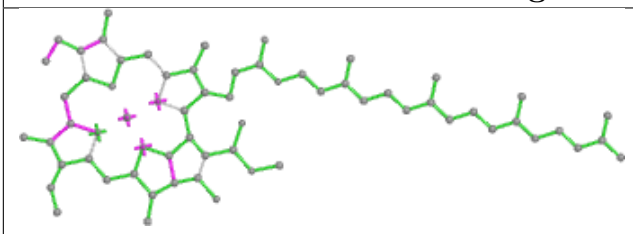


Torsions

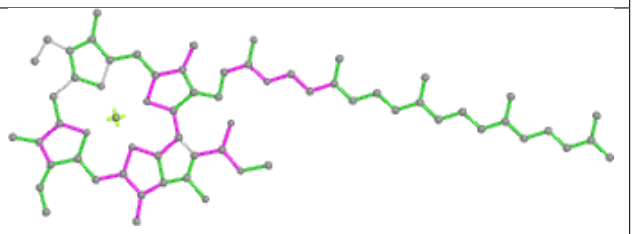


Rings

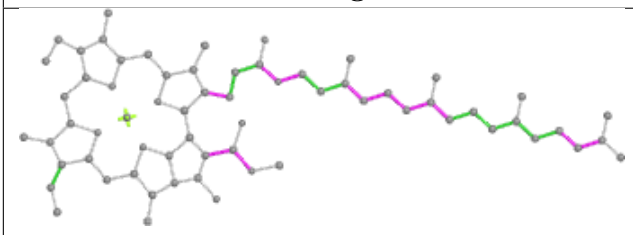
Ligand CLA 2 604



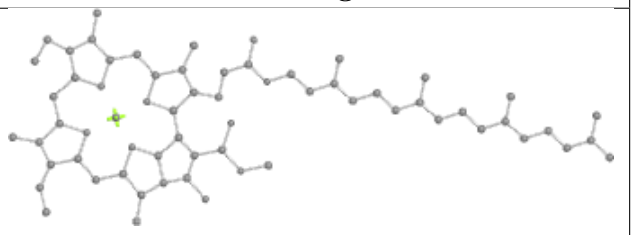
Bond lengths



Bond angles

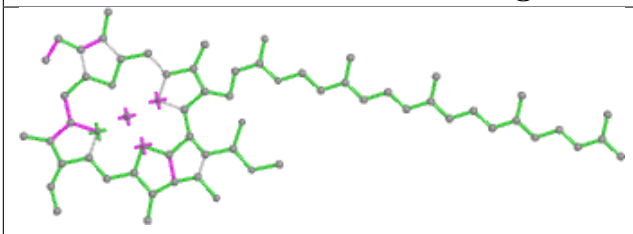


Torsions

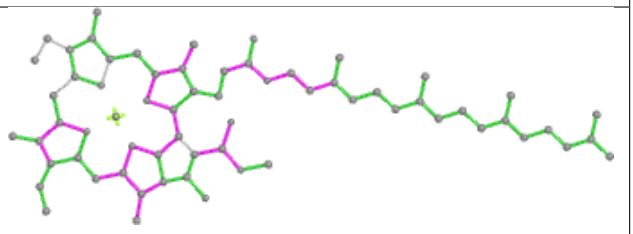


Rings

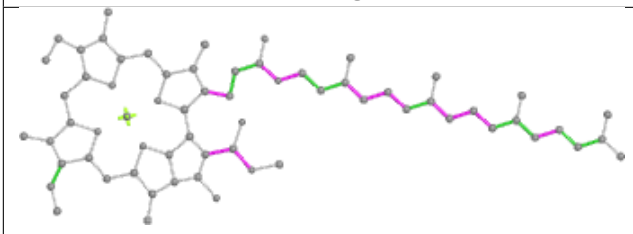
Ligand CLA A 1101



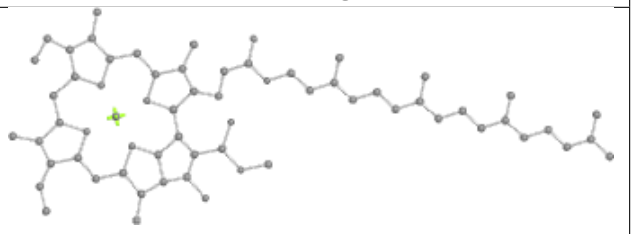
Bond lengths



Bond angles

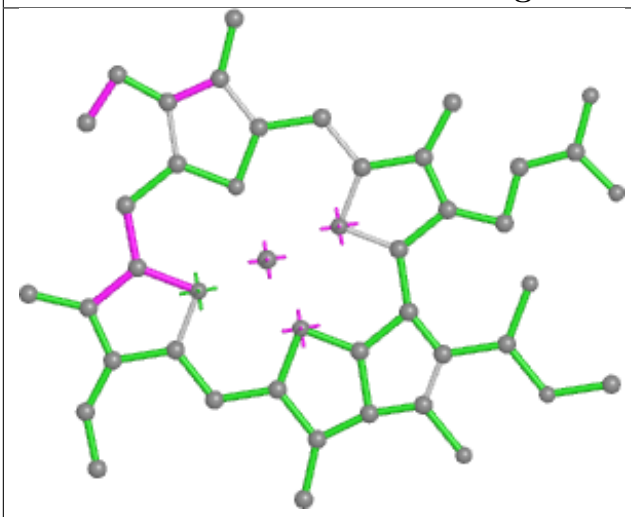


Torsions

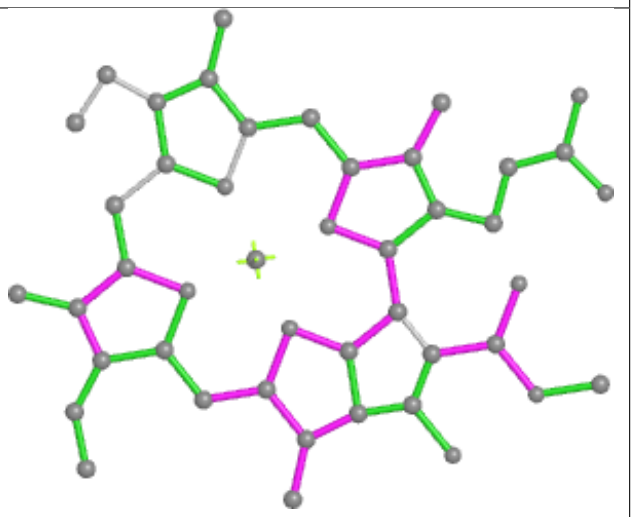


Rings

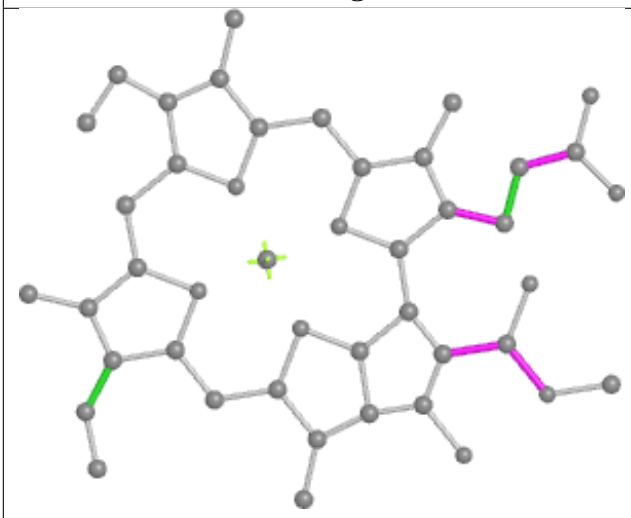
Ligand CLA K 1401



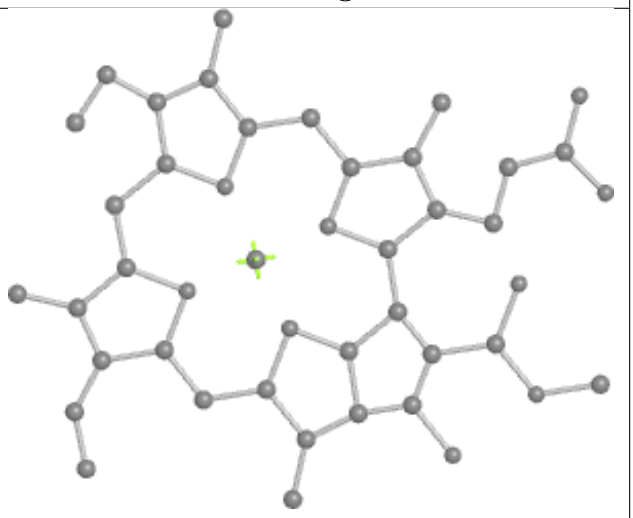
Bond lengths



Bond angles

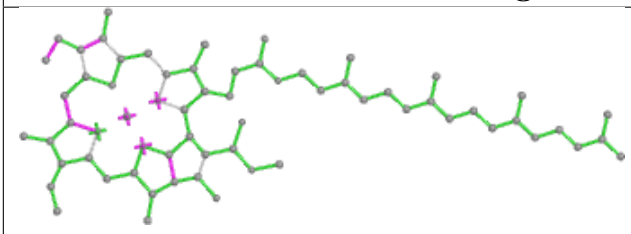


Torsions

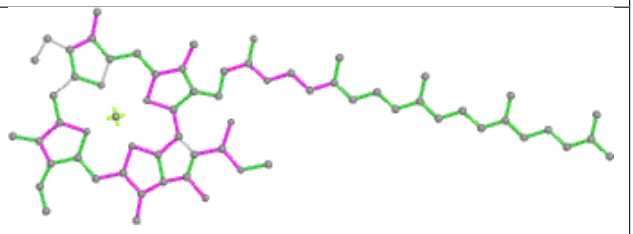


Rings

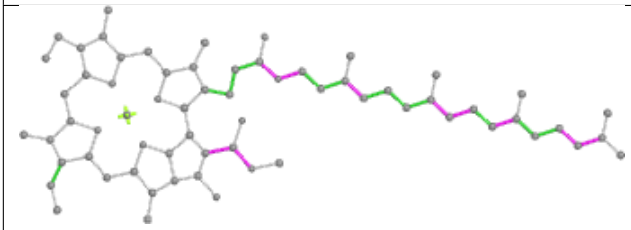
Ligand CLA A 1123



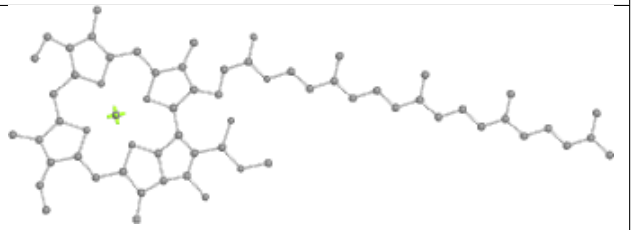
Bond lengths



Bond angles

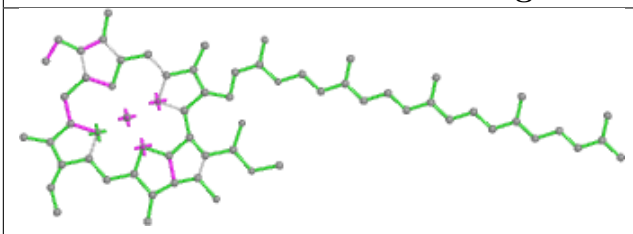


Torsions

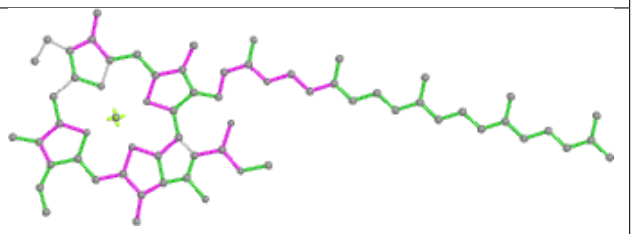


Rings

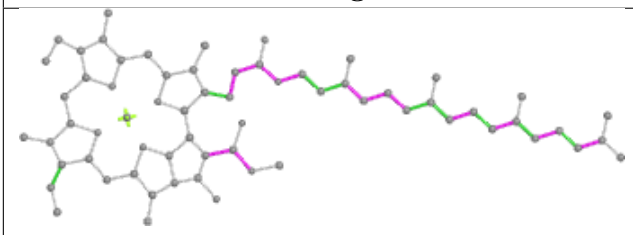
Ligand CLA B 1219



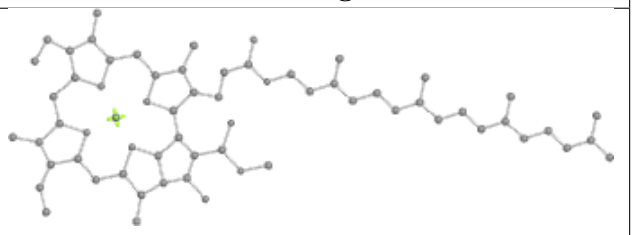
Bond lengths



Bond angles

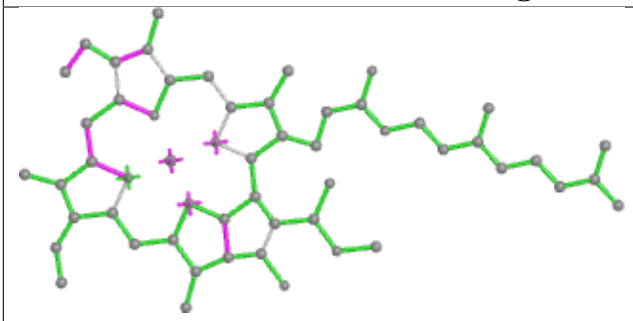


Torsions

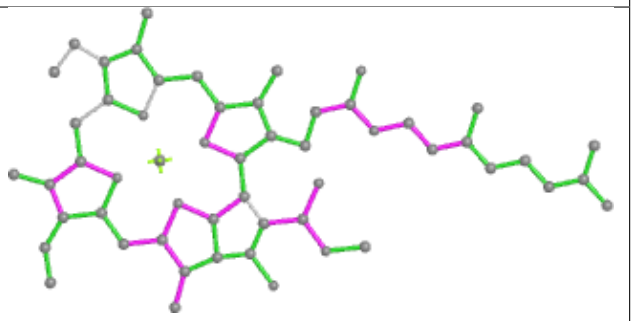


Rings

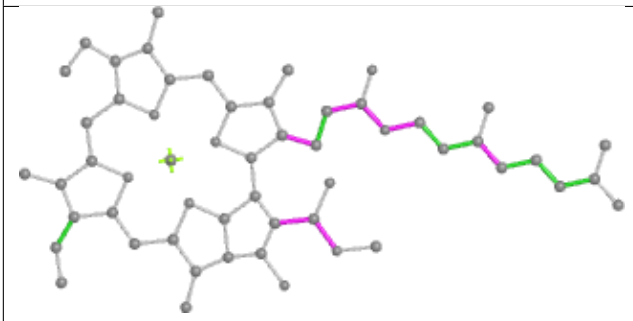
Ligand CLA B 1220



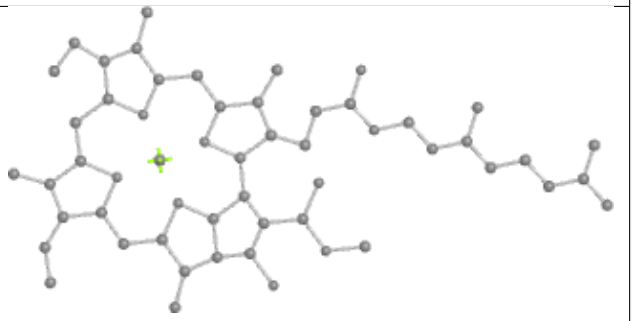
Bond lengths



Bond angles

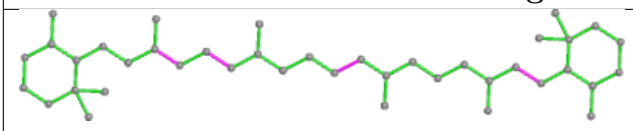


Torsions

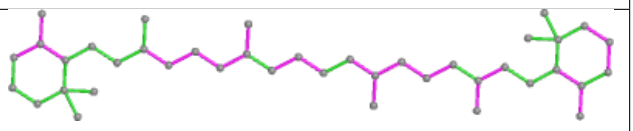


Rings

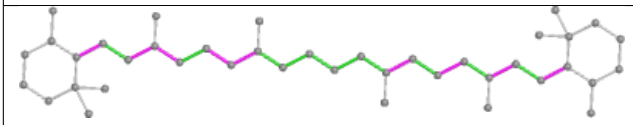
Ligand BCR 1 503



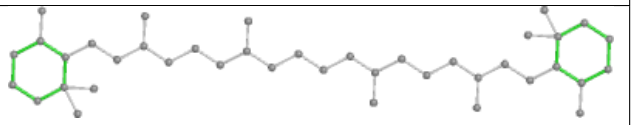
Bond lengths



Bond angles

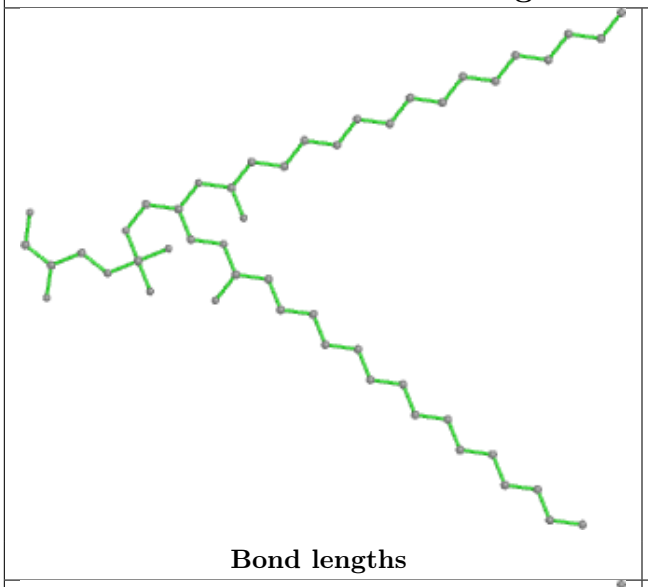


Torsions

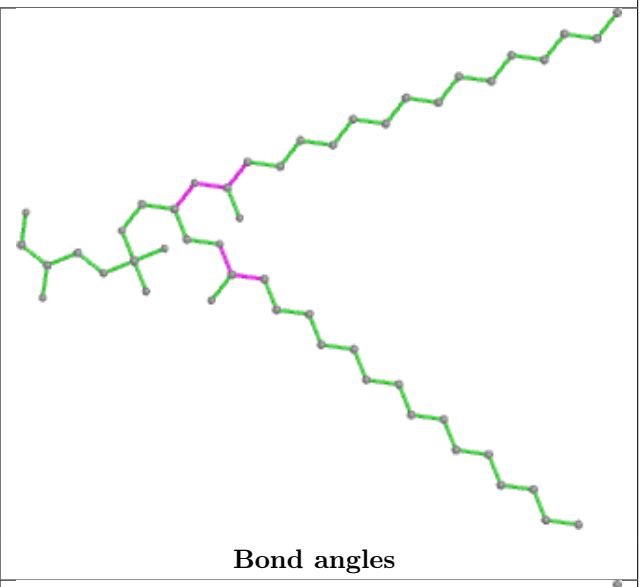


Rings

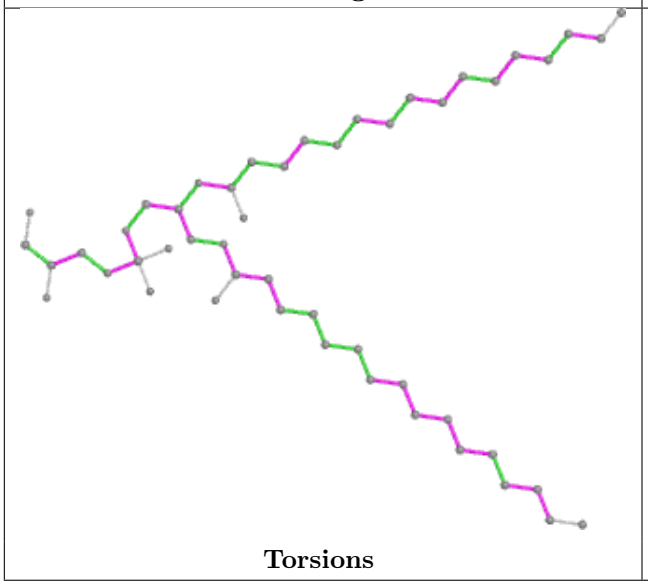
Ligand LHG B 5002



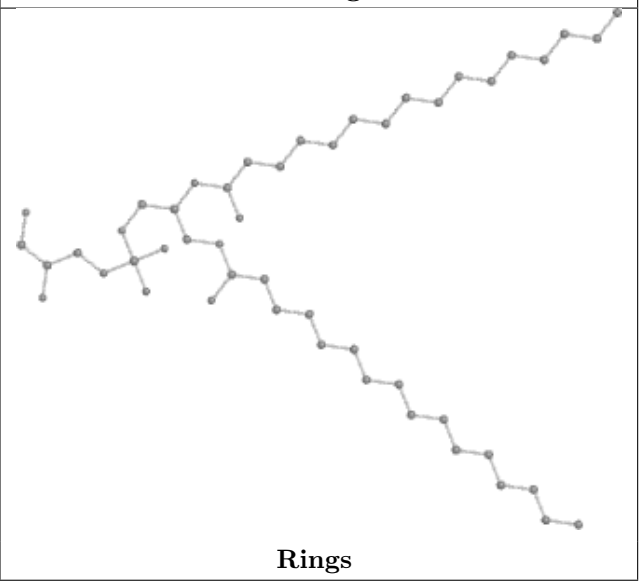
Bond lengths



Bond angles

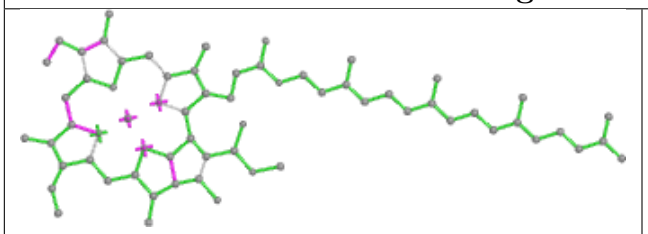


Torsions

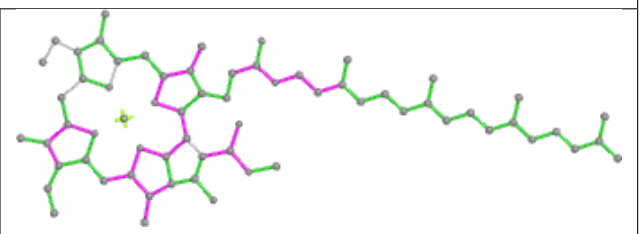


Rings

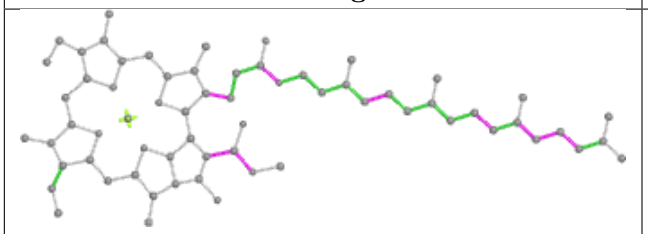
Ligand CLA B 1202



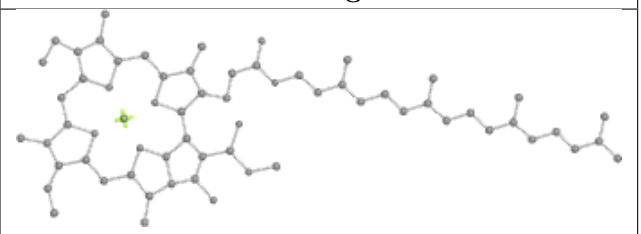
Bond lengths



Bond angles

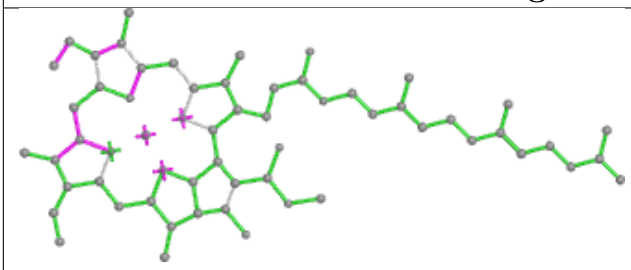


Torsions

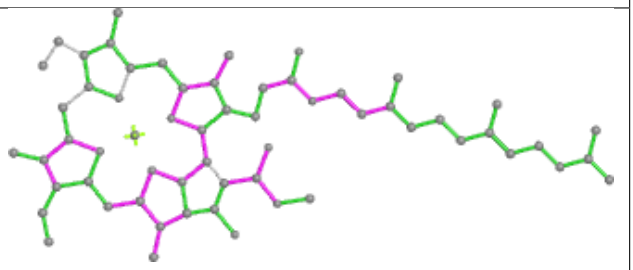


Rings

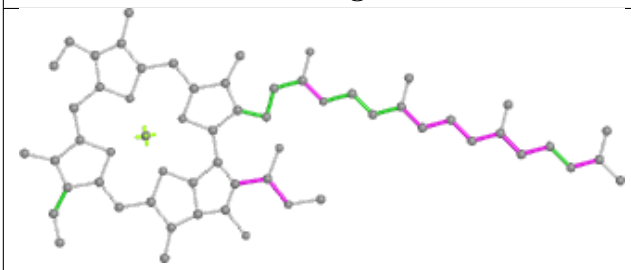
Ligand CLA 4 604



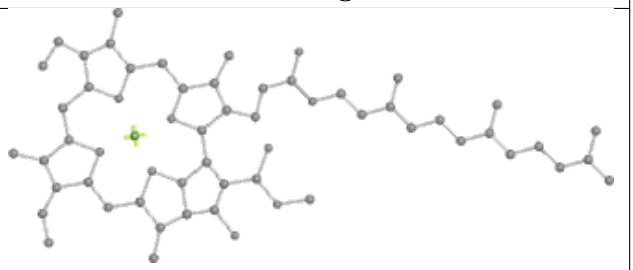
Bond lengths



Bond angles

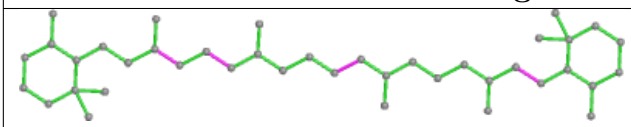


Torsions

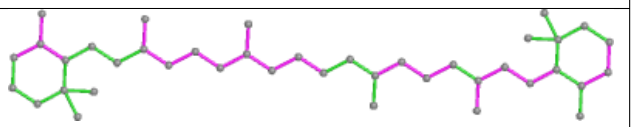


Rings

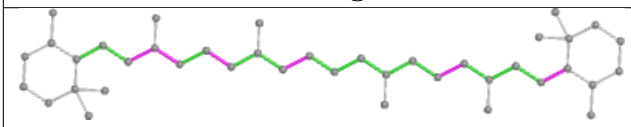
Ligand BCR B 4009



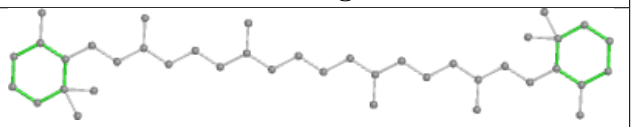
Bond lengths



Bond angles

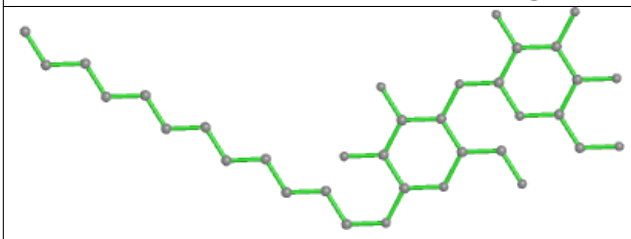


Torsions

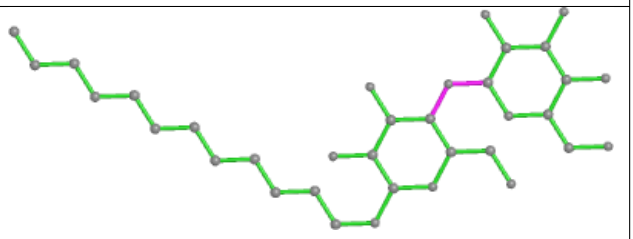


Rings

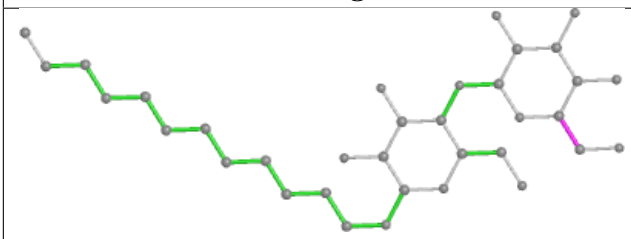
Ligand LMT 2 808



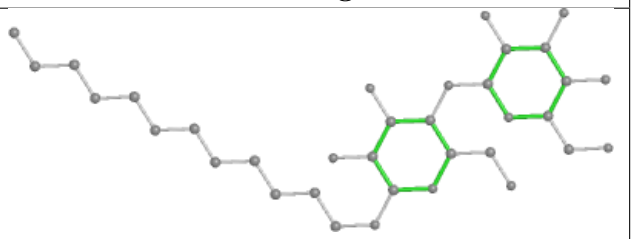
Bond lengths



Bond angles

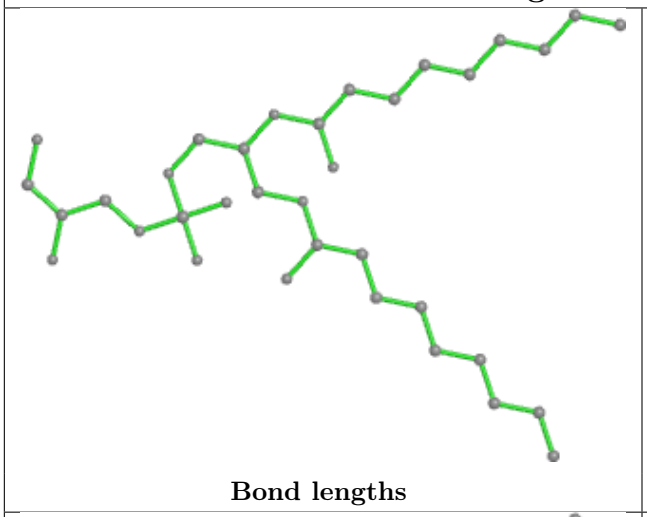


Torsions

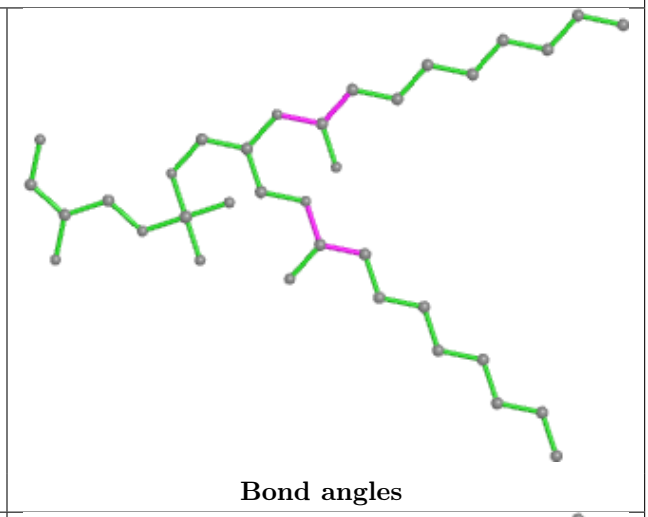


Rings

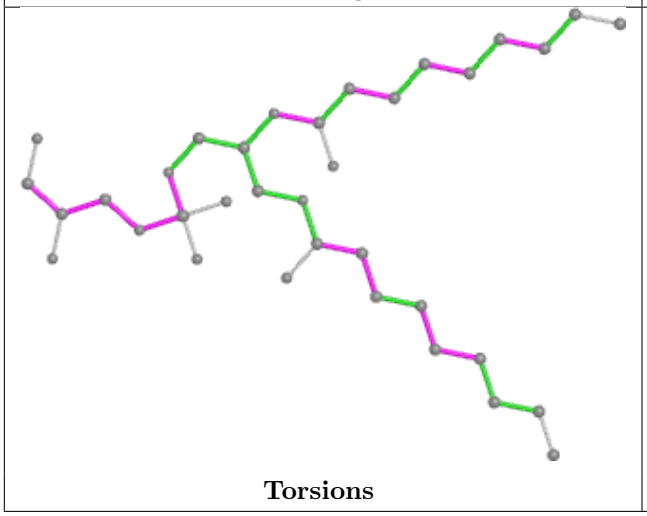
Ligand LHG 2 801



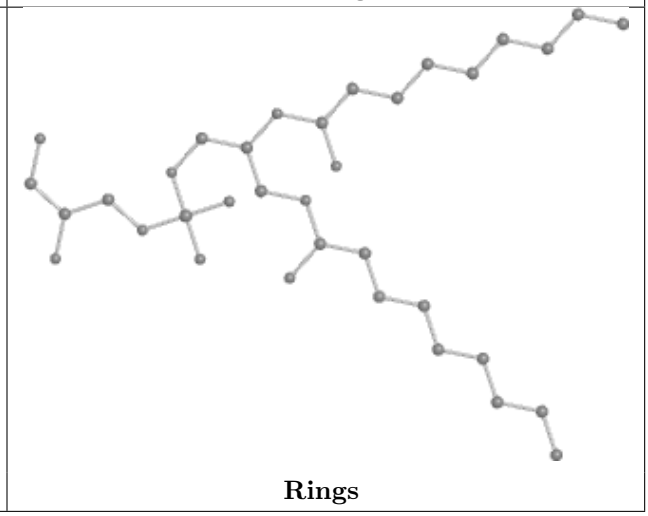
Bond lengths



Bond angles

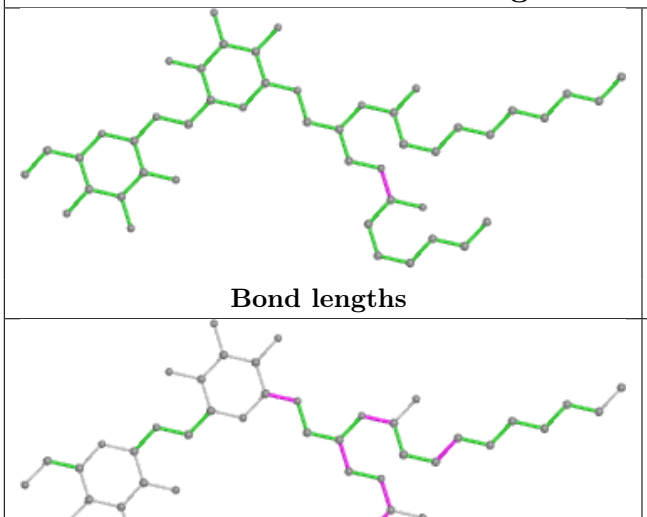


Torsions

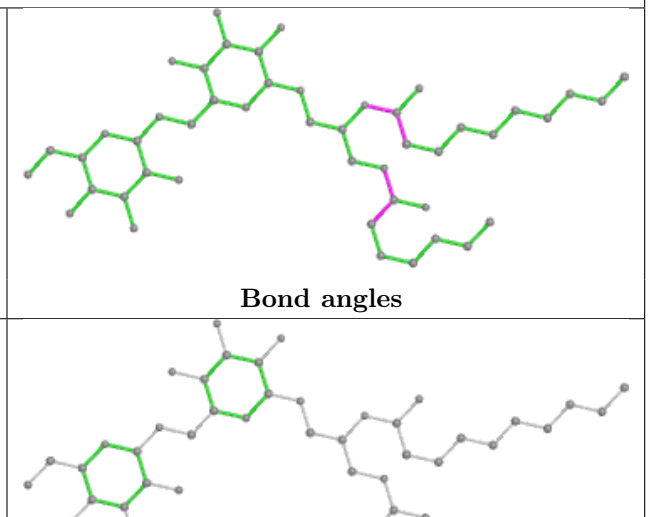


Rings

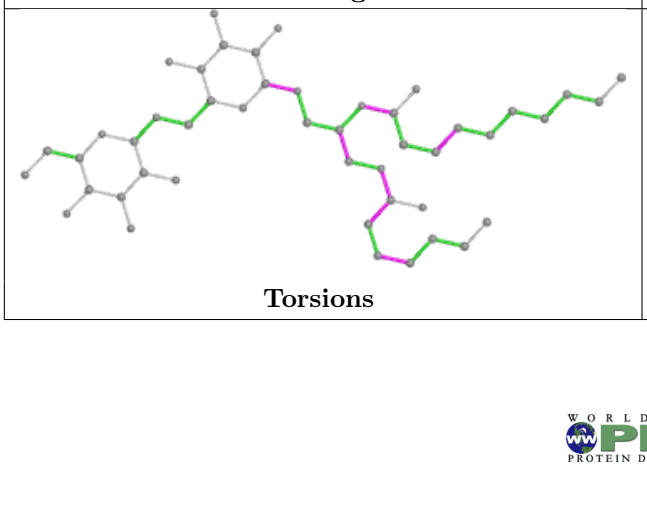
Ligand DGD G 5003



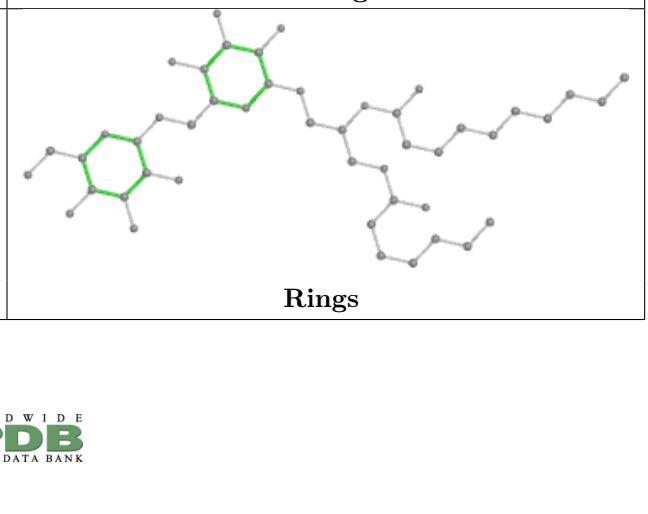
Bond lengths



Bond angles

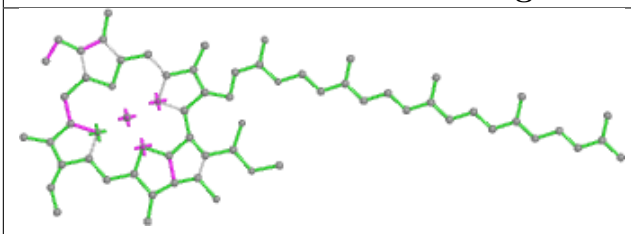


Torsions

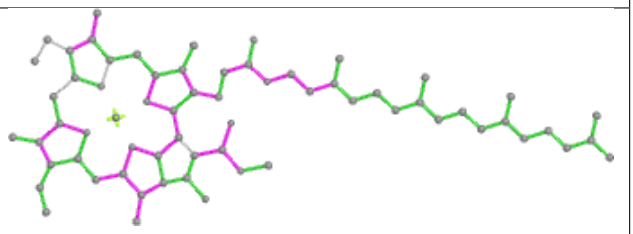


Rings

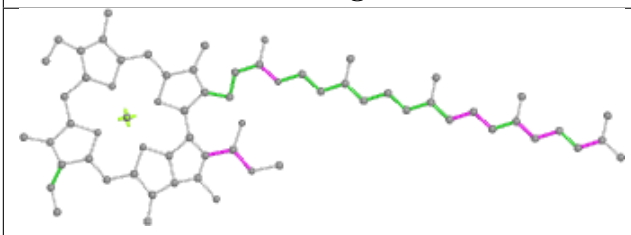
Ligand CLA B 1216



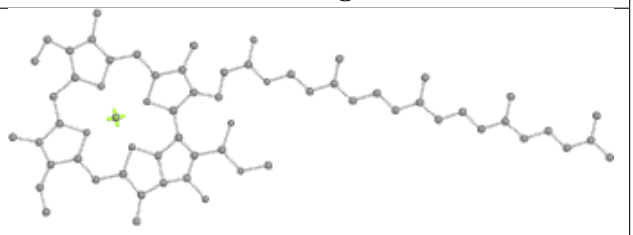
Bond lengths



Bond angles

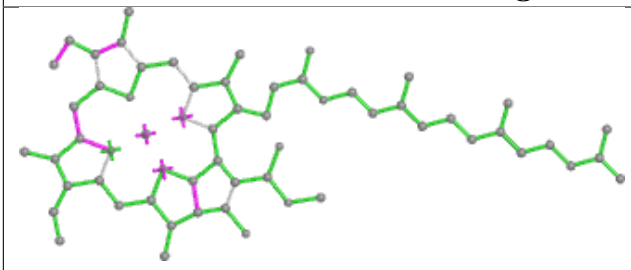


Torsions

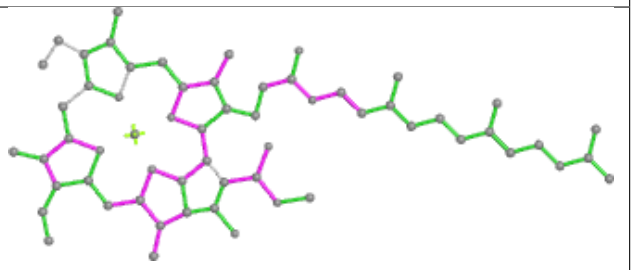


Rings

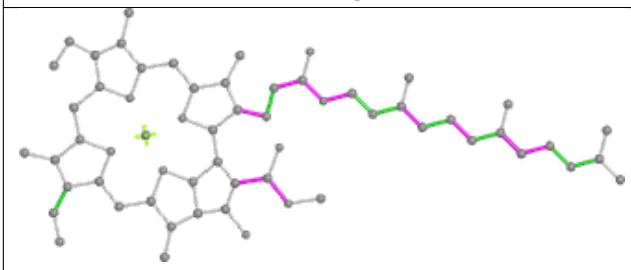
Ligand CLA A 1120



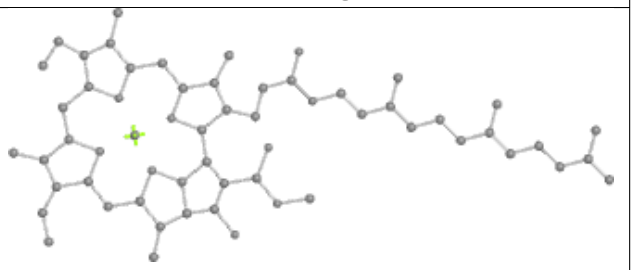
Bond lengths



Bond angles

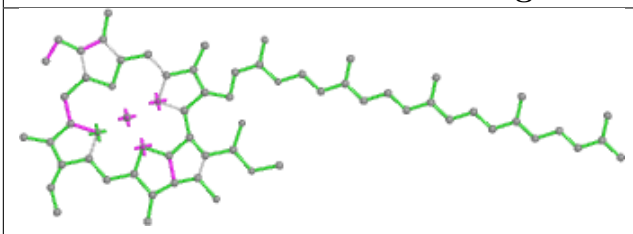


Torsions

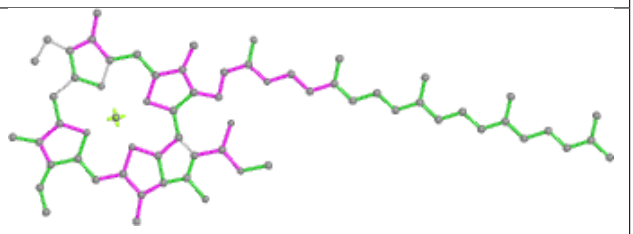


Rings

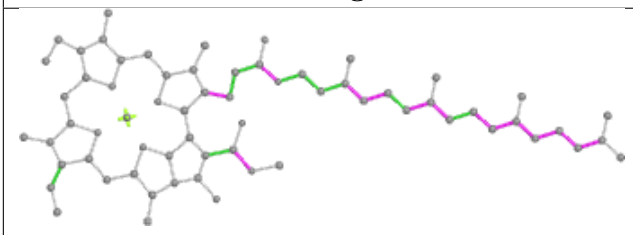
Ligand CLA B 1226



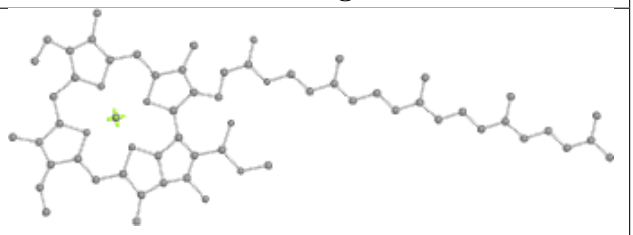
Bond lengths



Bond angles

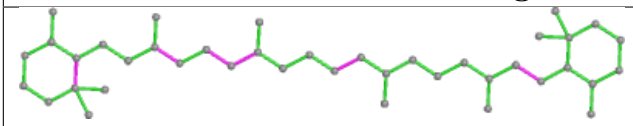


Torsions

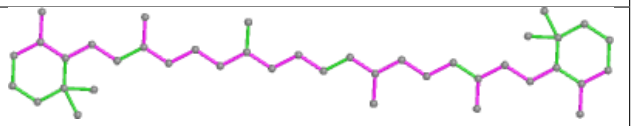


Rings

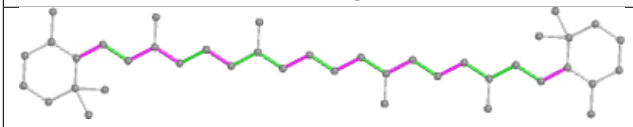
Ligand BCR A 4008



Bond lengths



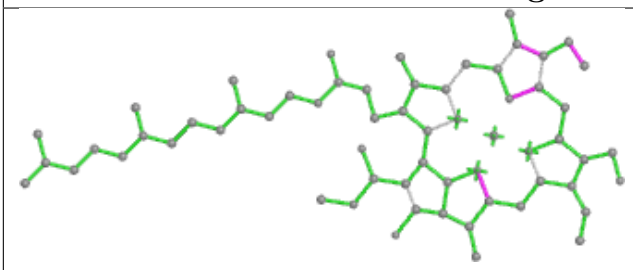
Bond angles



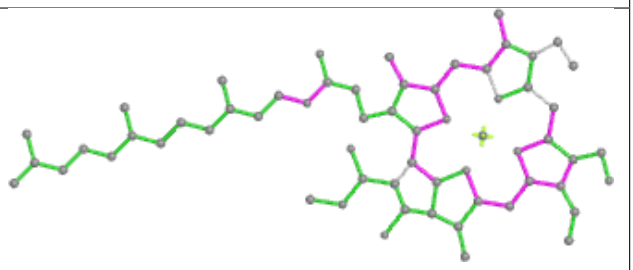
Torsions

Rings

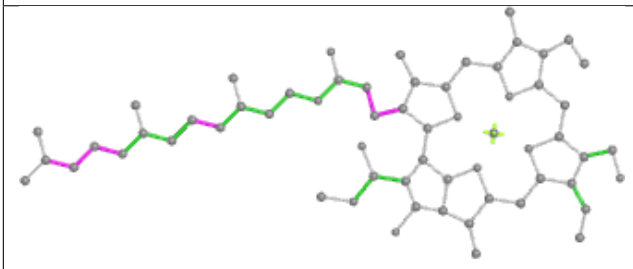
Ligand CHL 4 613



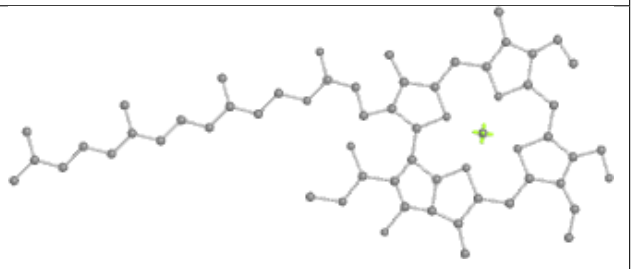
Bond lengths



Bond angles

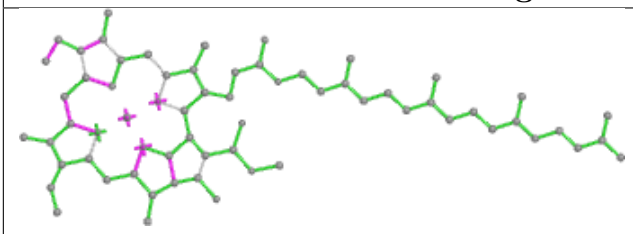


Torsions

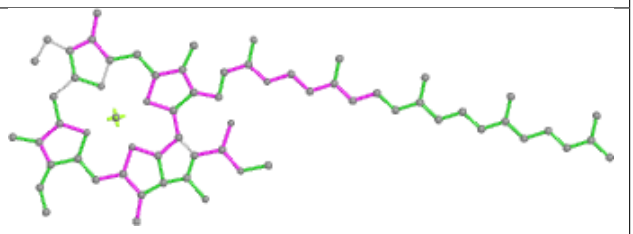


Rings

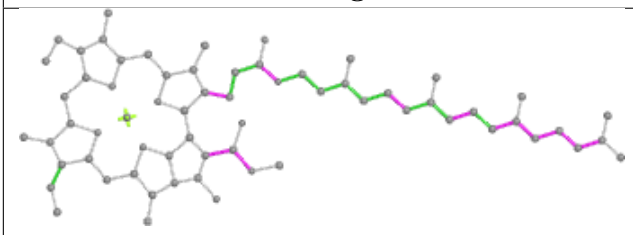
Ligand CLA B 1021



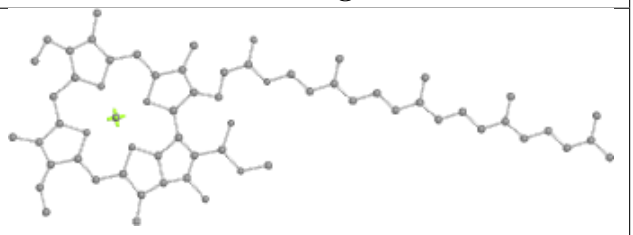
Bond lengths



Bond angles

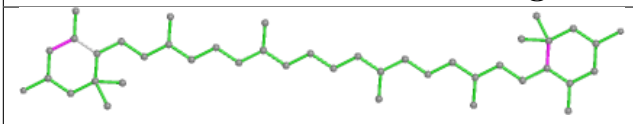


Torsions

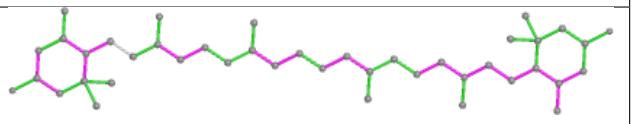


Rings

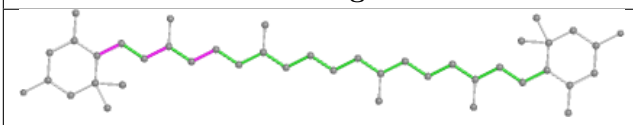
Ligand LUT 1 502



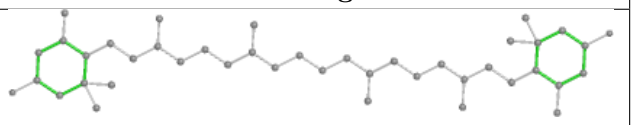
Bond lengths



Bond angles

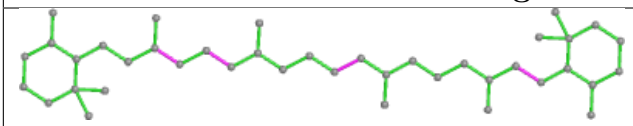


Torsions

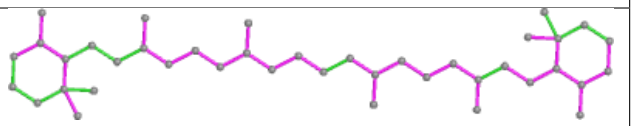


Rings

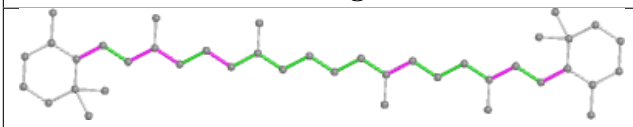
Ligand BCR A 4003



Bond lengths



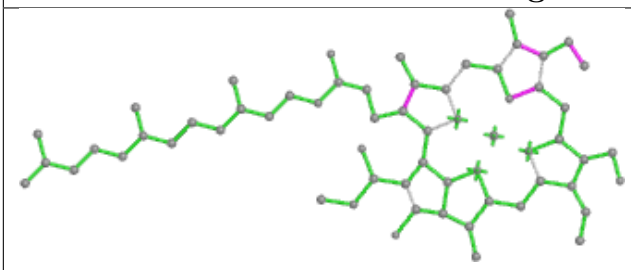
Bond angles



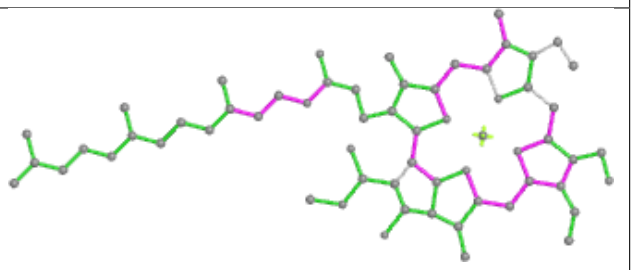
Torsions

Rings

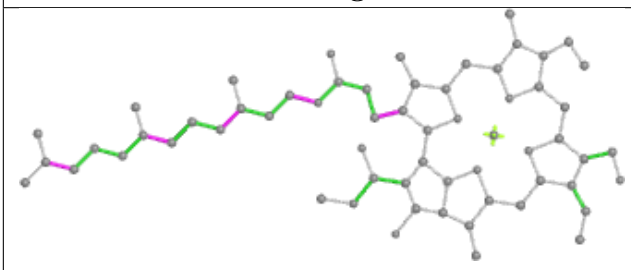
Ligand CHL 1 612



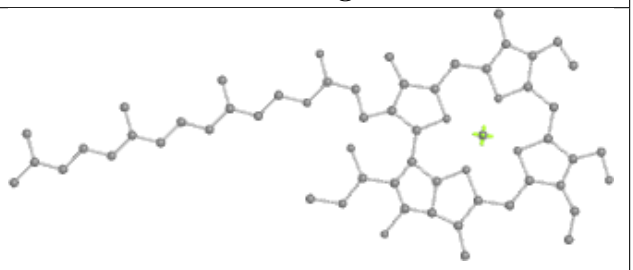
Bond lengths



Bond angles

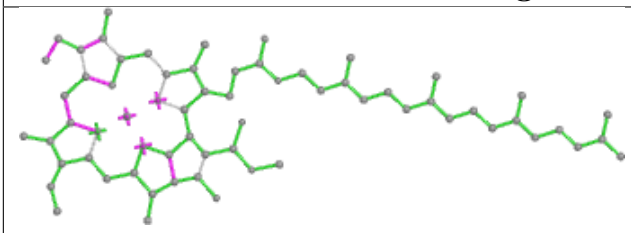


Torsions

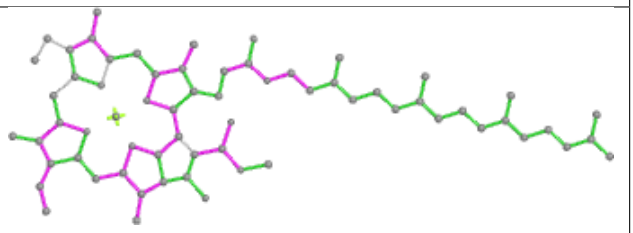


Rings

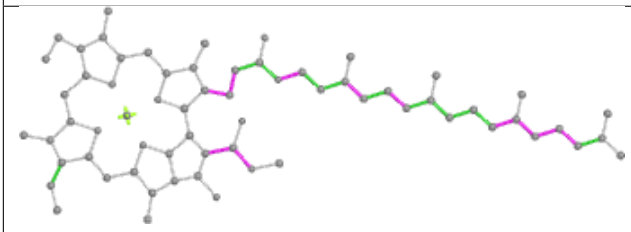
Ligand CLA B 1225



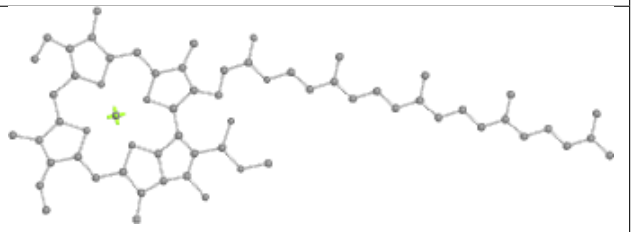
Bond lengths



Bond angles

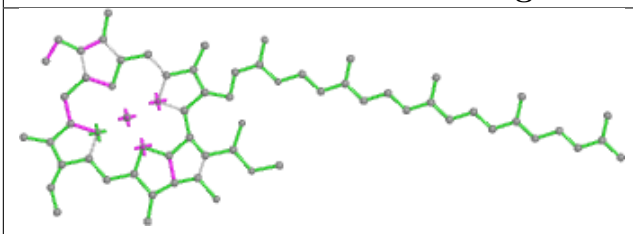


Torsions

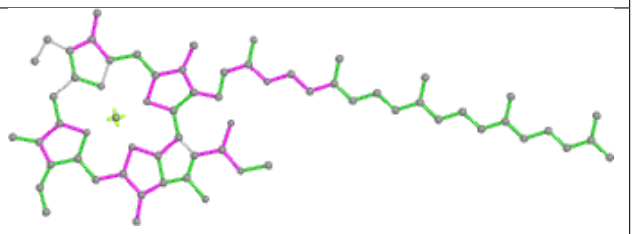


Rings

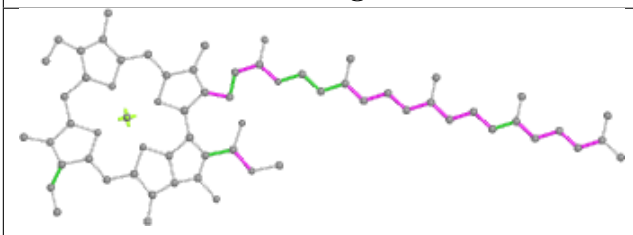
Ligand CLA B 1211



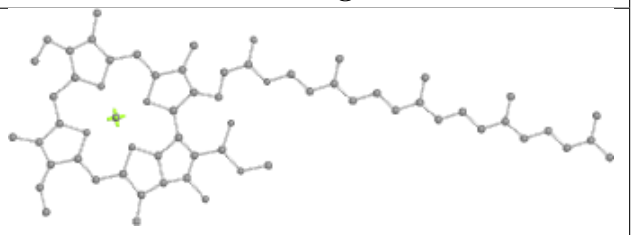
Bond lengths



Bond angles

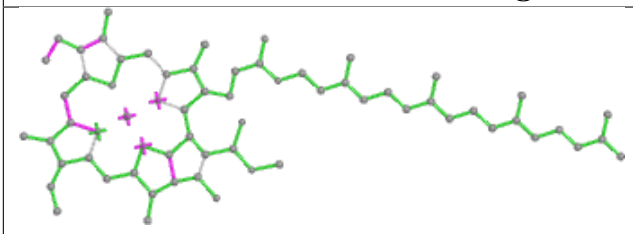


Torsions

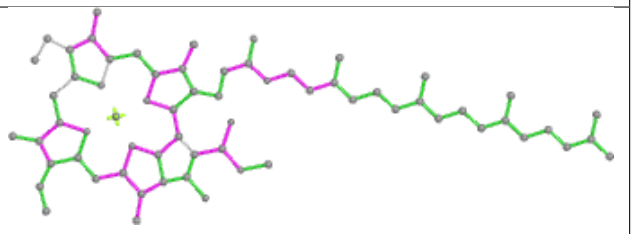


Rings

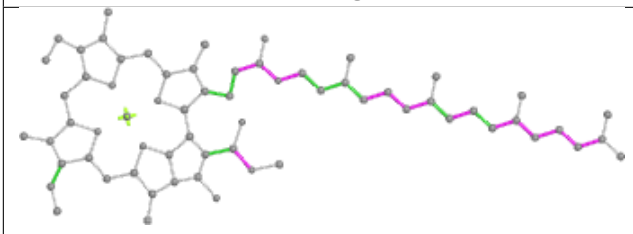
Ligand CLA A 1112



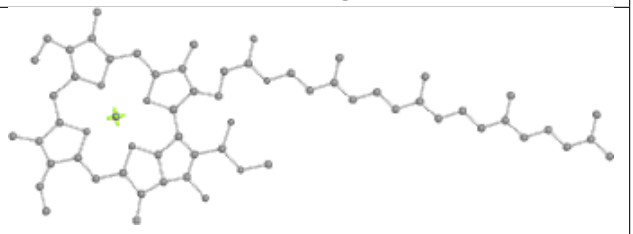
Bond lengths



Bond angles

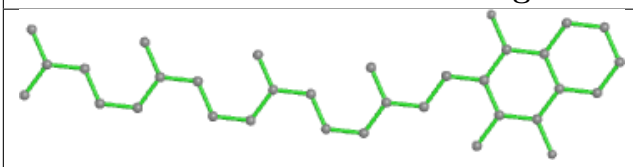


Torsions

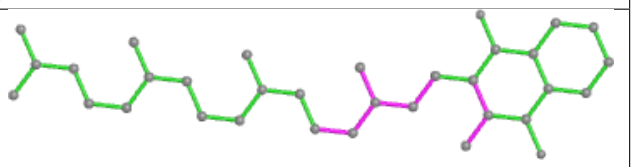


Rings

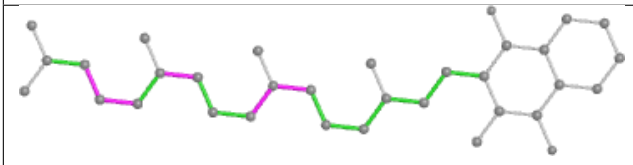
Ligand PQN B 2002



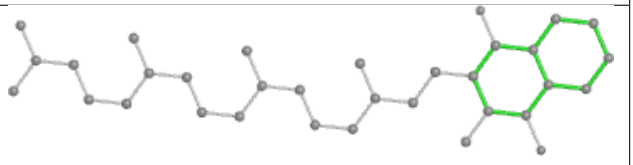
Bond lengths



Bond angles

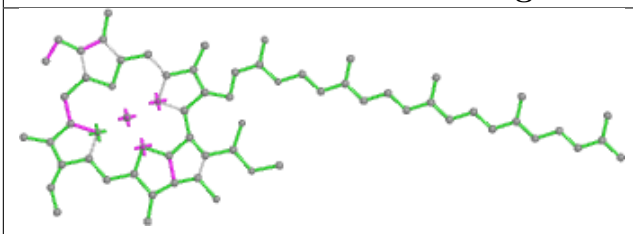


Torsions

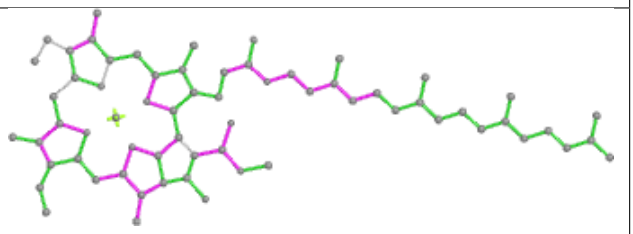


Rings

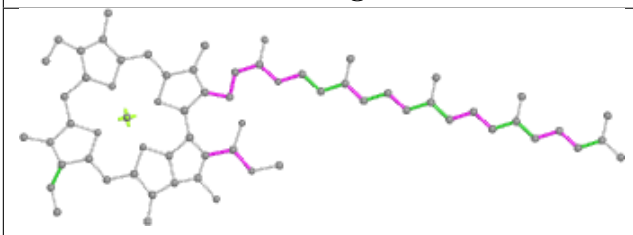
Ligand CLA B 1224



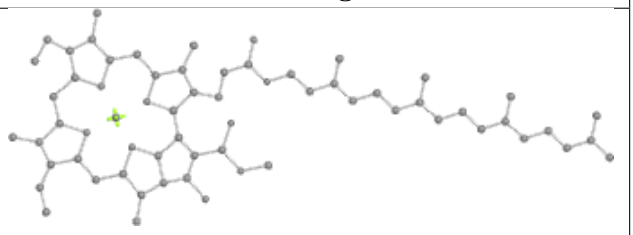
Bond lengths



Bond angles

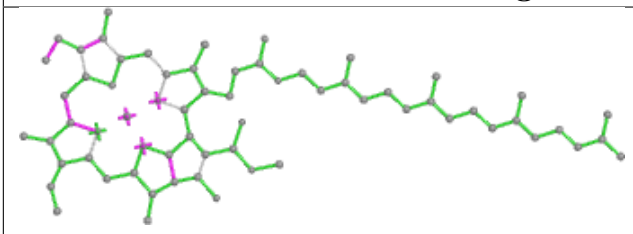


Torsions

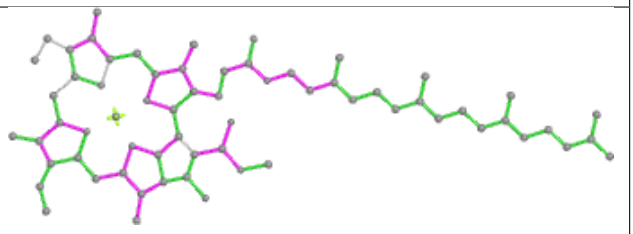


Rings

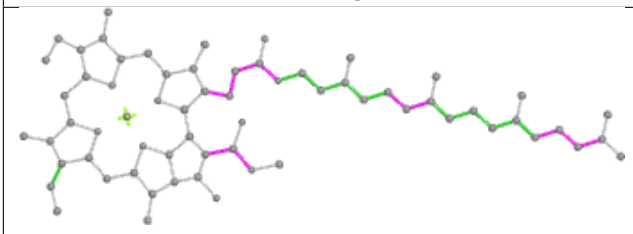
Ligand CLA B 1235



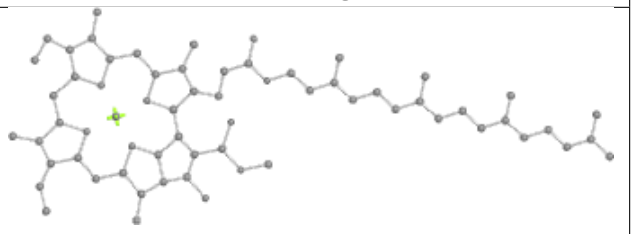
Bond lengths



Bond angles

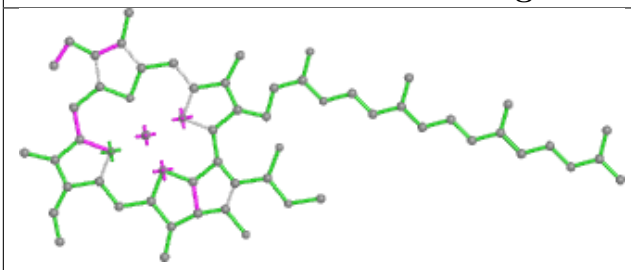


Torsions

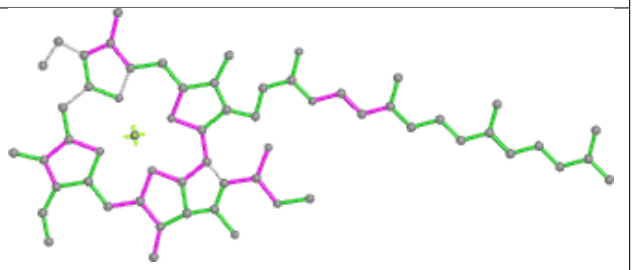


Rings

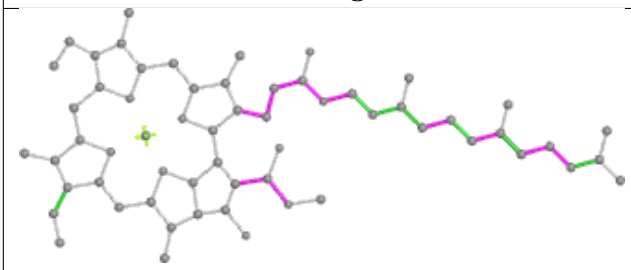
Ligand CLA B 1228



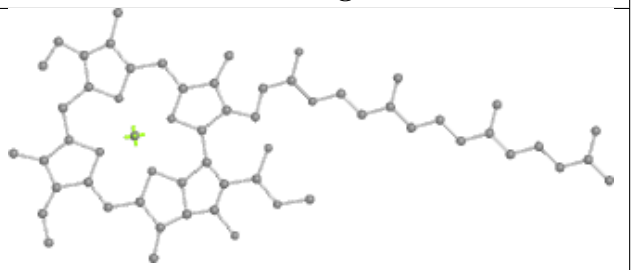
Bond lengths



Bond angles

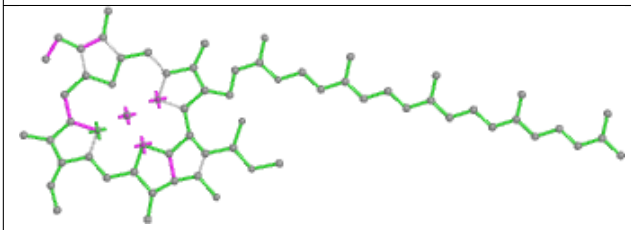


Torsions

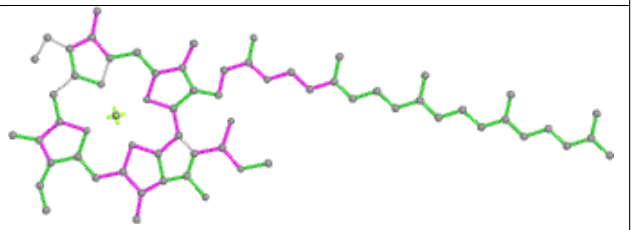


Rings

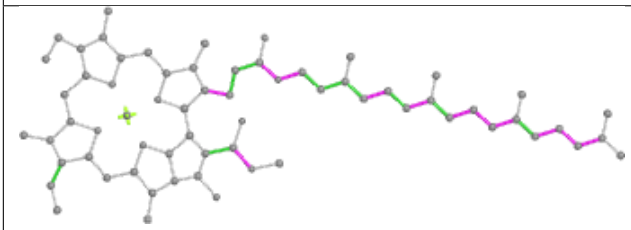
Ligand CLA A 1107



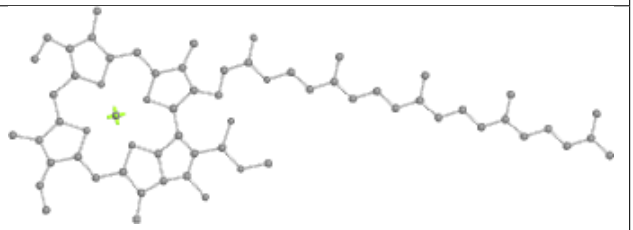
Bond lengths



Bond angles

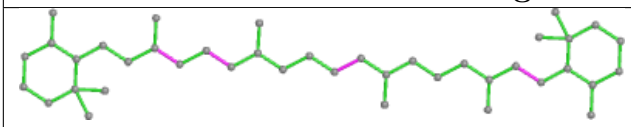


Torsions

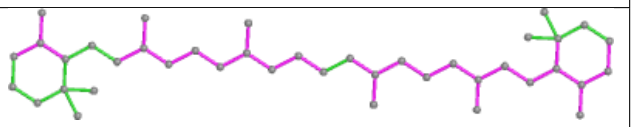


Rings

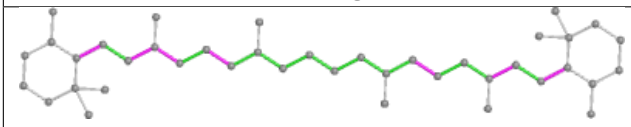
Ligand BCR B 4006



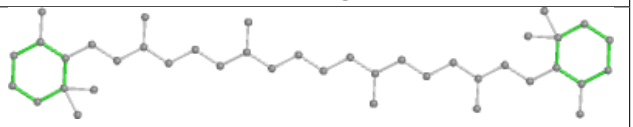
Bond lengths



Bond angles

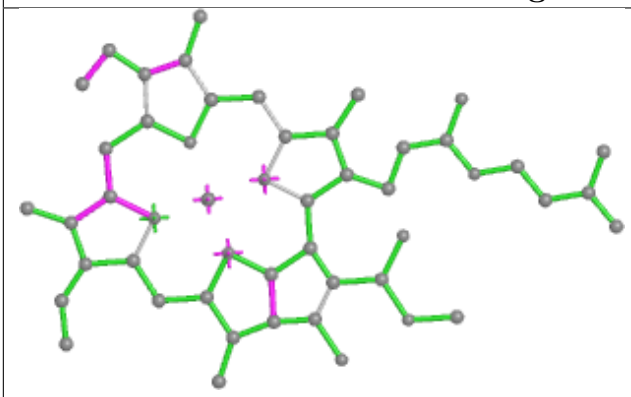


Torsions

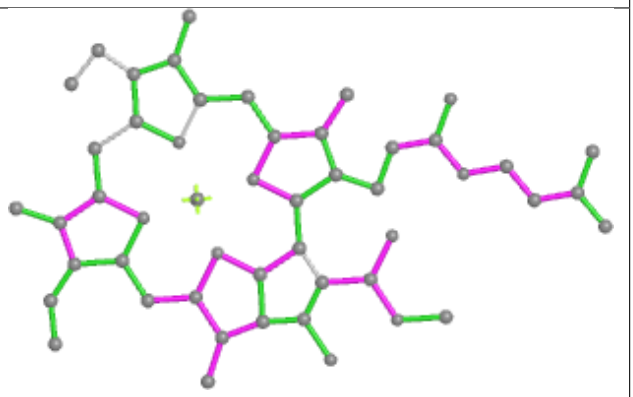


Rings

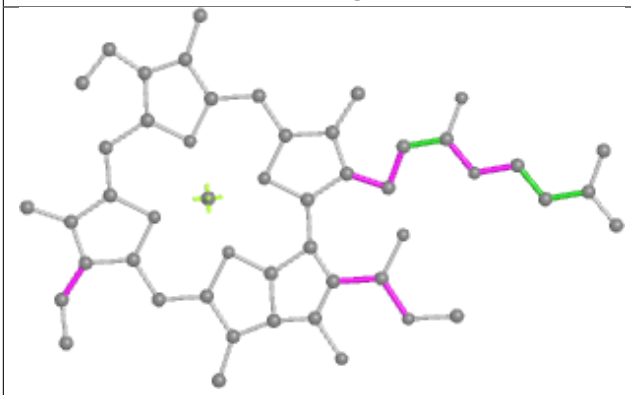
Ligand CLA 3 612



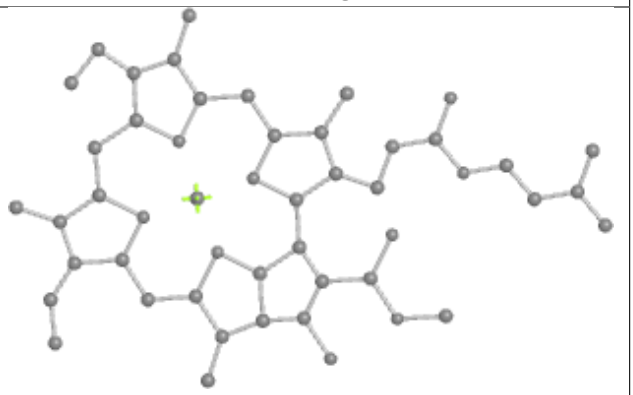
Bond lengths



Bond angles

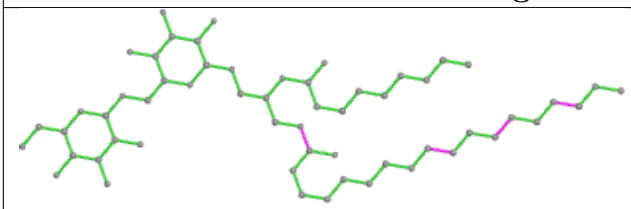


Torsions

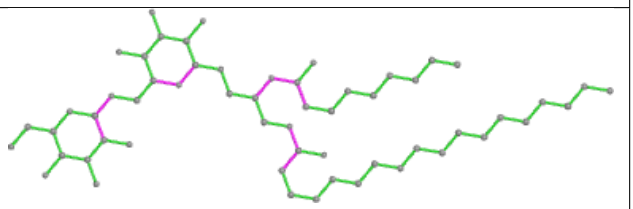


Rings

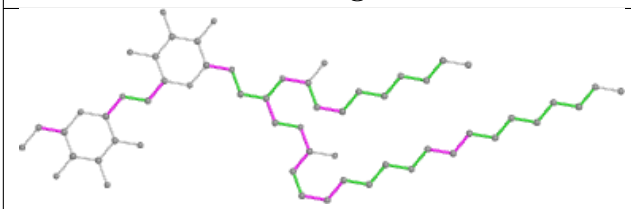
Ligand DGD F 5005



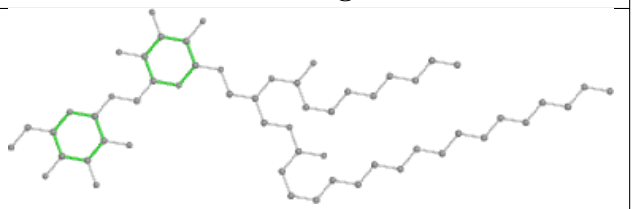
Bond lengths



Bond angles

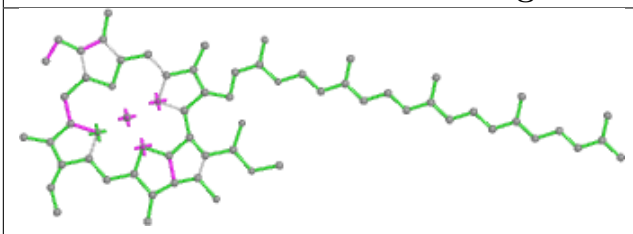


Torsions

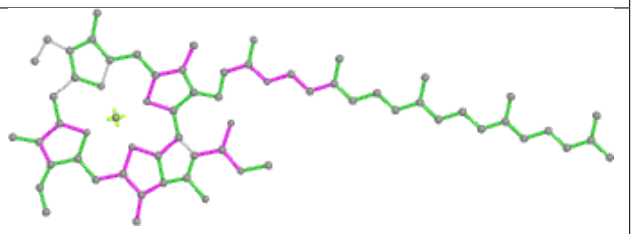


Rings

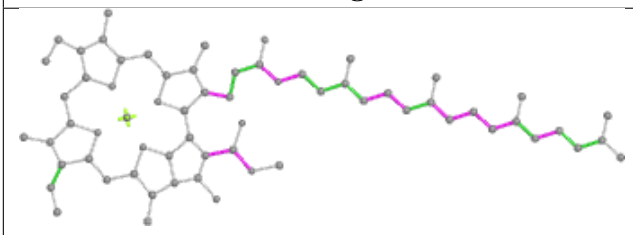
Ligand CLA F 1302



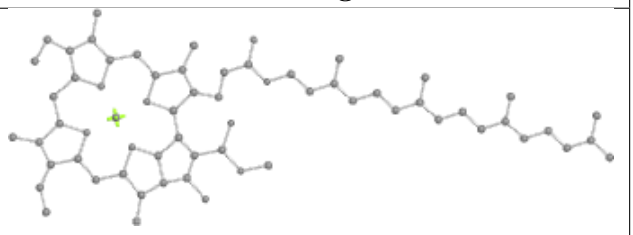
Bond lengths



Bond angles

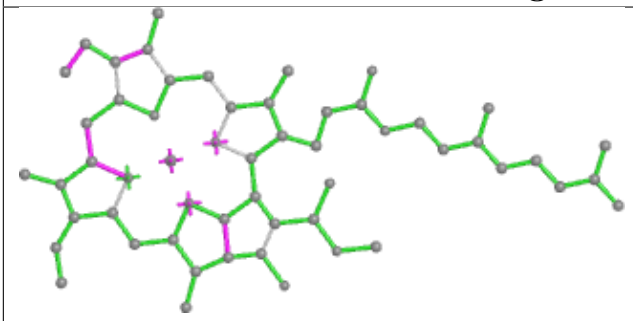


Torsions

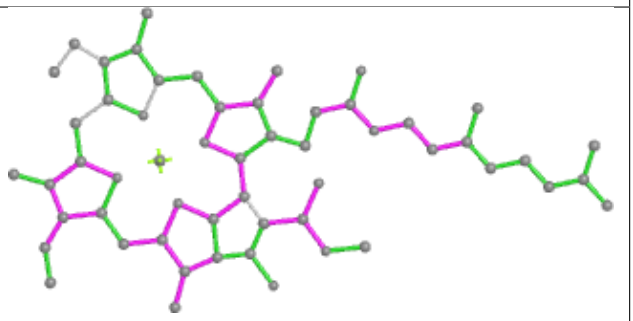


Rings

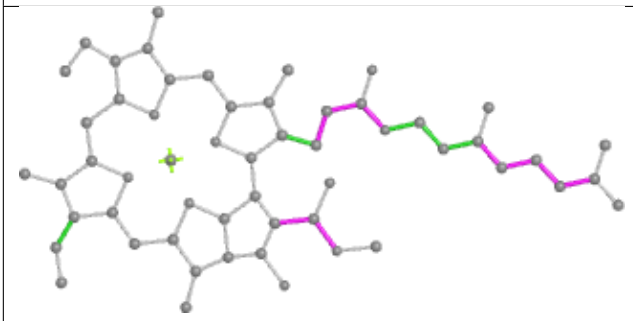
Ligand CLA 3 603



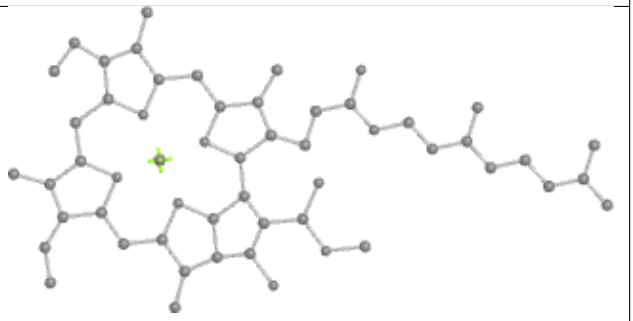
Bond lengths



Bond angles

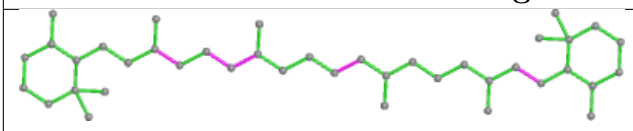


Torsions

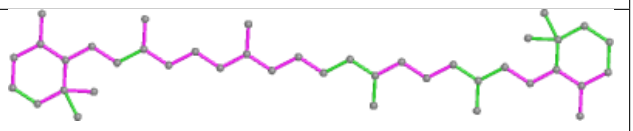


Rings

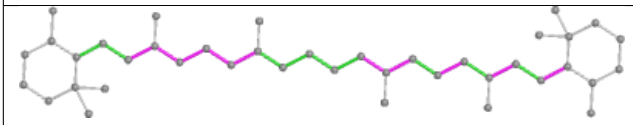
Ligand BCR A 4011



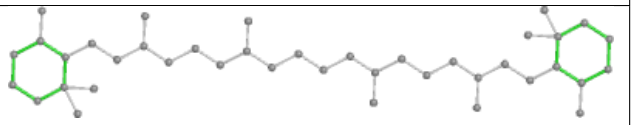
Bond lengths



Bond angles

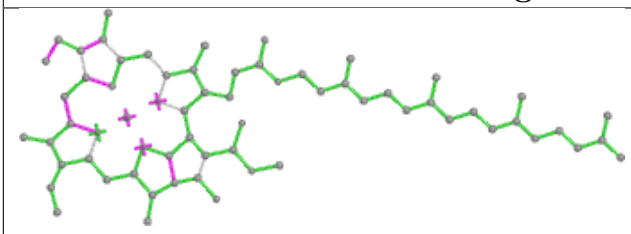


Torsions

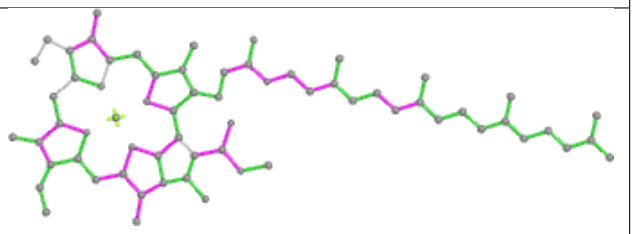


Rings

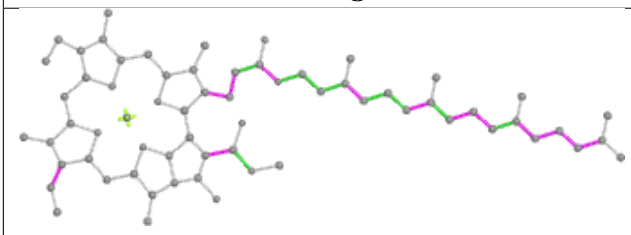
Ligand CLA A 1111



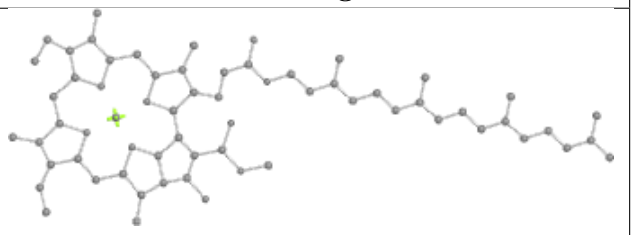
Bond lengths



Bond angles

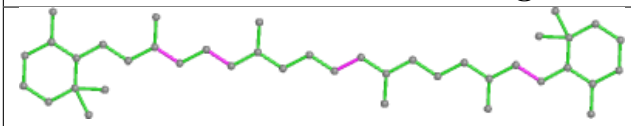


Torsions

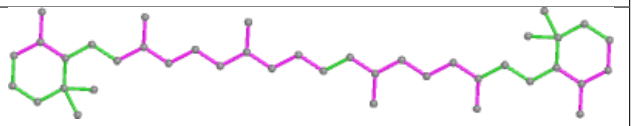


Rings

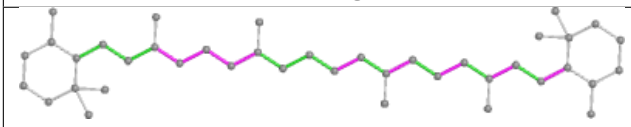
Ligand BCR L 4019



Bond lengths



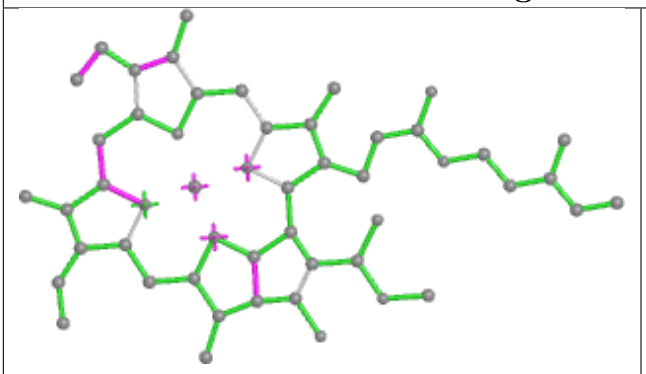
Bond angles



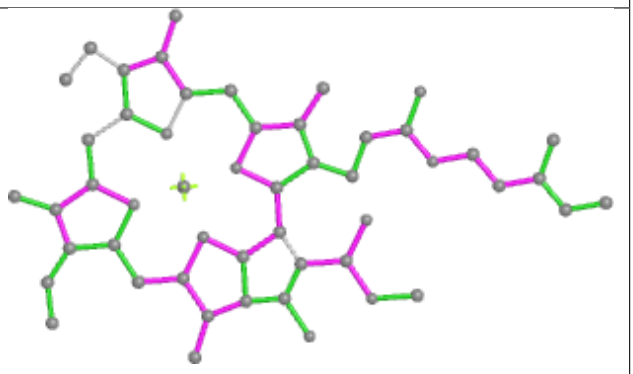
Torsions

Rings

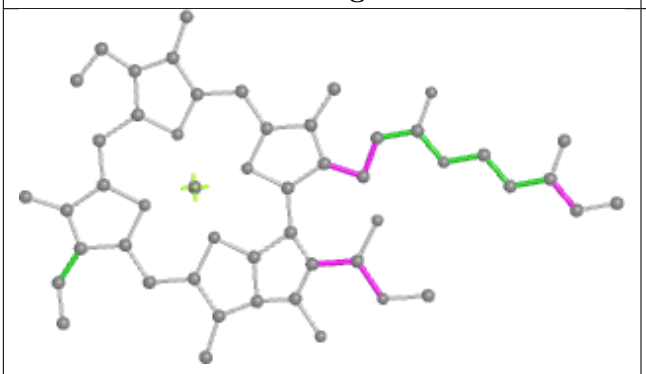
Ligand CLA A 1135



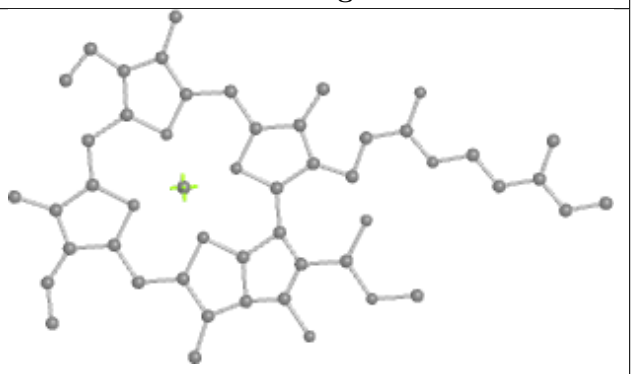
Bond lengths



Bond angles

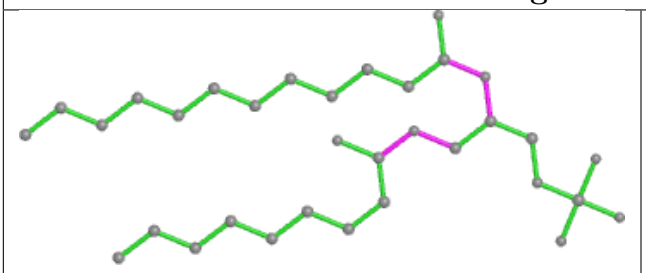


Torsions

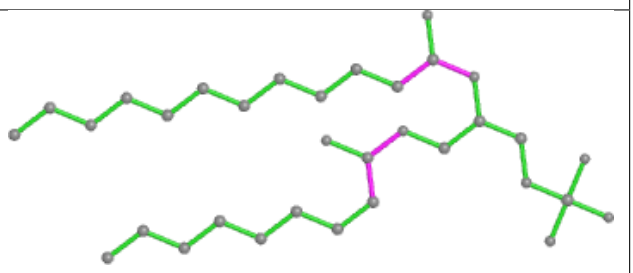


Rings

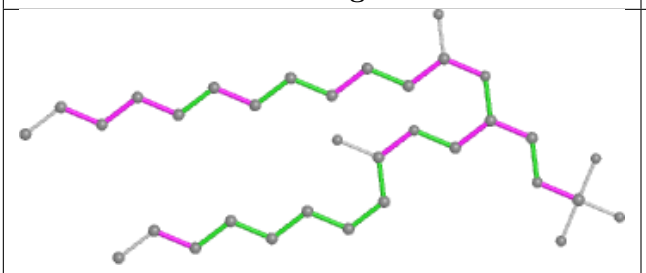
Ligand 3PH 2 807



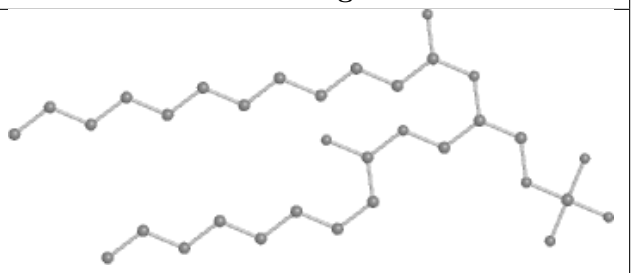
Bond lengths



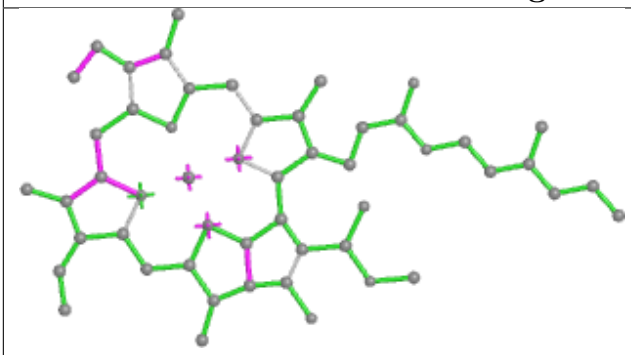
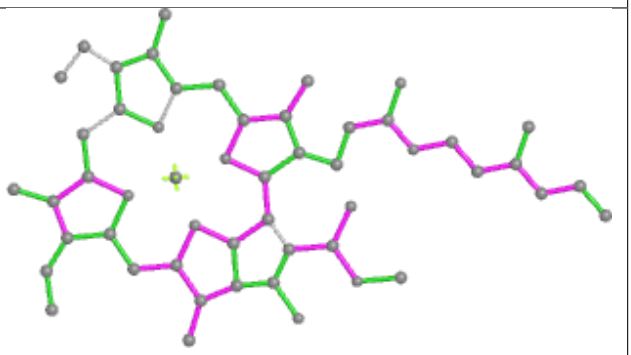
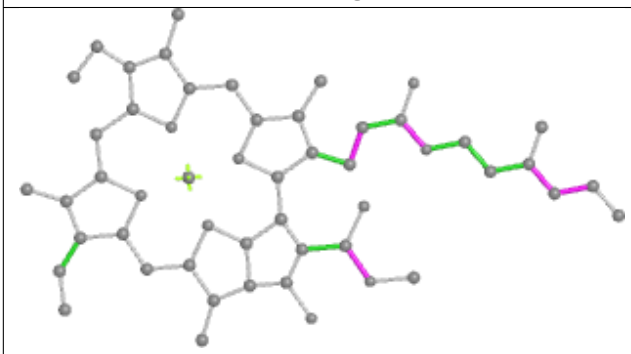
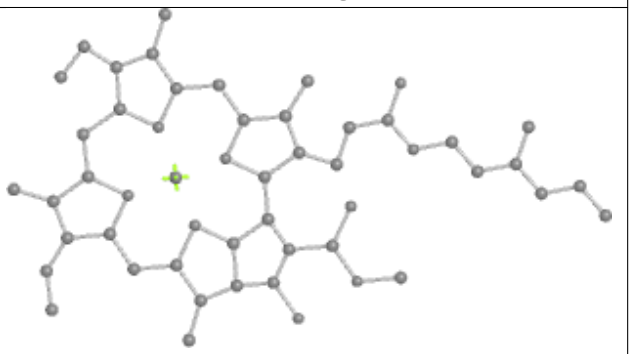
Bond angles

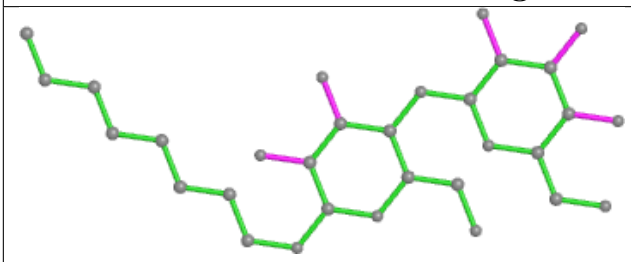
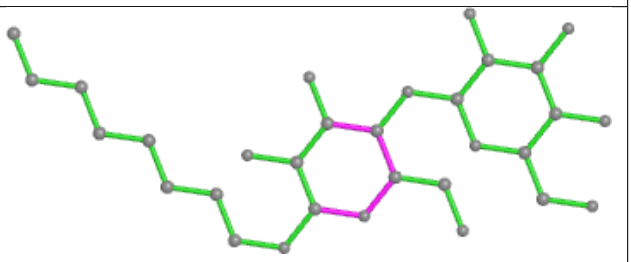
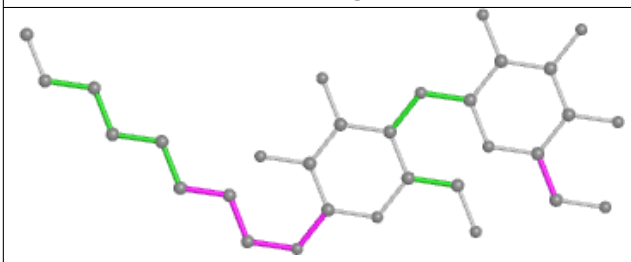
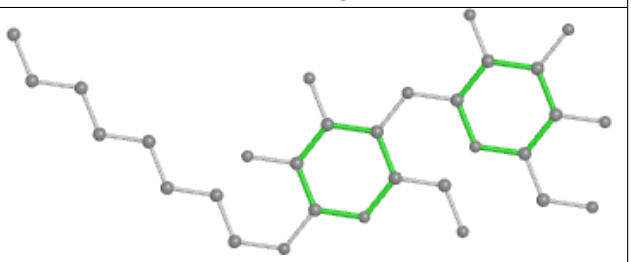


Torsions

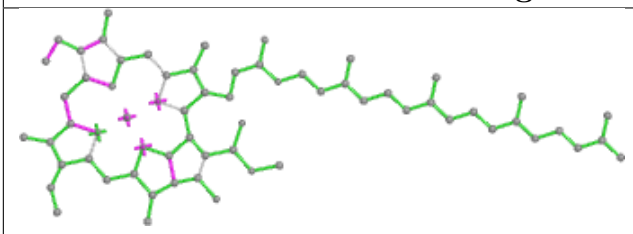


Rings

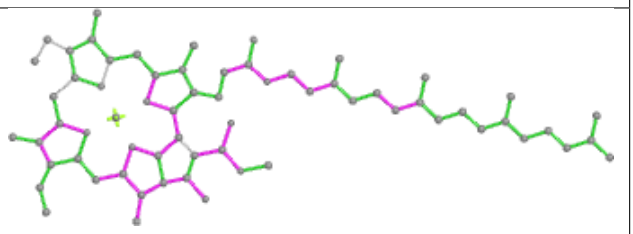
Ligand CLA 2 602	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand LMT G 5005	
 Bond lengths	 Bond angles
 Torsions	 Rings

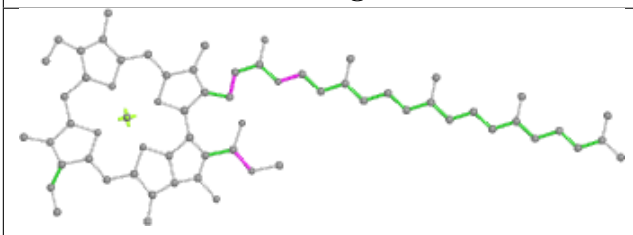
Ligand CLA B 1022



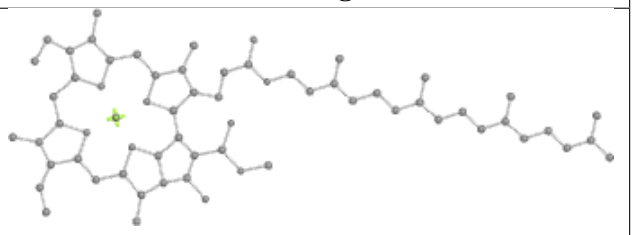
Bond lengths



Bond angles

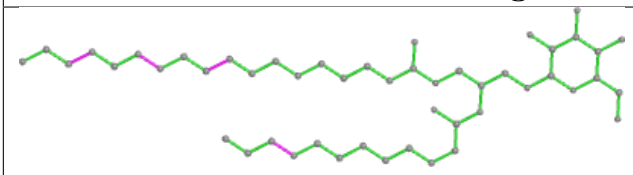


Torsions

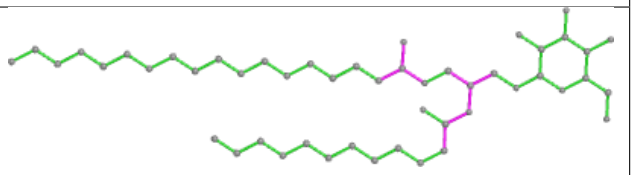


Rings

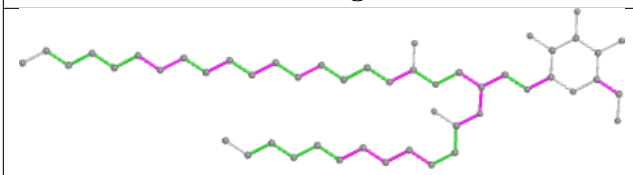
Ligand LMG G 5001



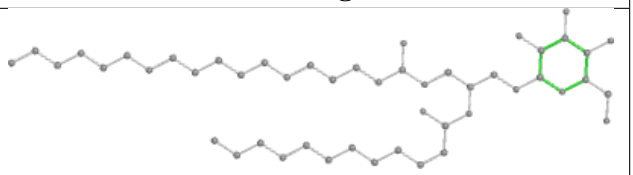
Bond lengths



Bond angles

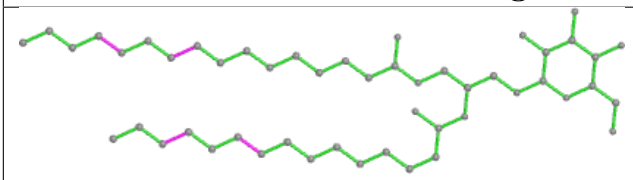


Torsions

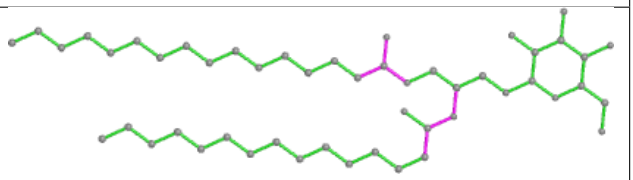


Rings

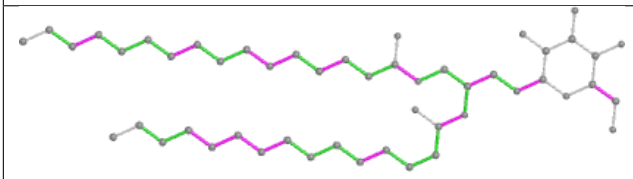
Ligand LMG G 5002



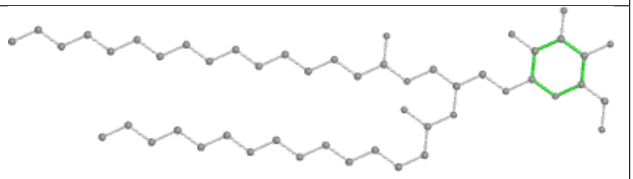
Bond lengths



Bond angles

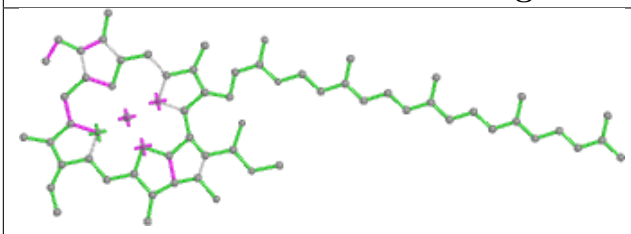


Torsions

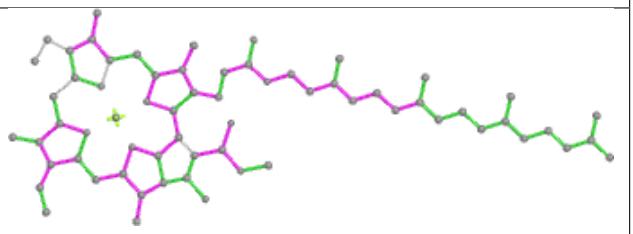


Rings

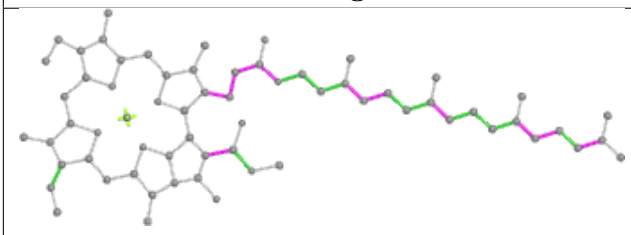
Ligand CLA B 1210



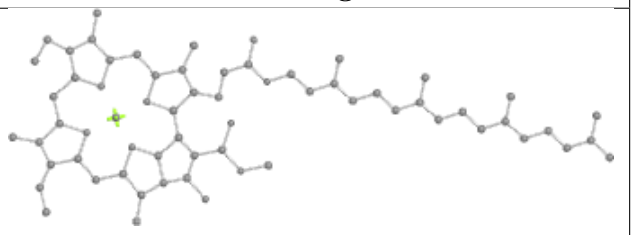
Bond lengths



Bond angles

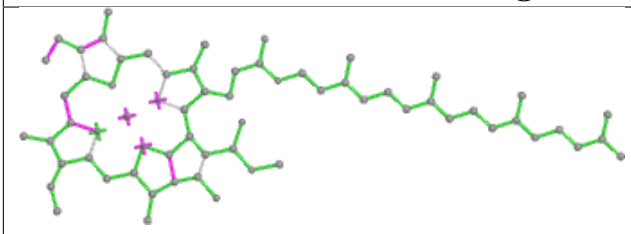


Torsions

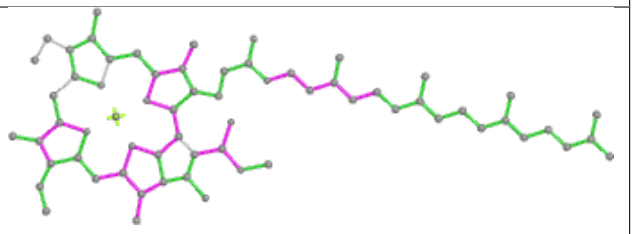


Rings

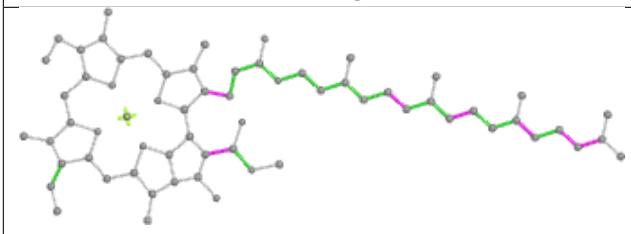
Ligand CLA B 1218



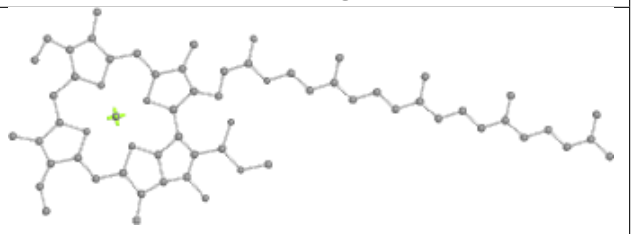
Bond lengths



Bond angles

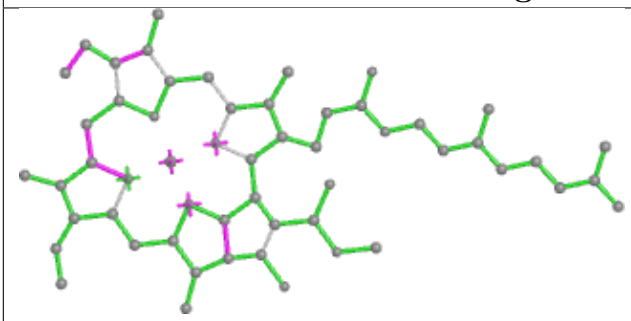


Torsions

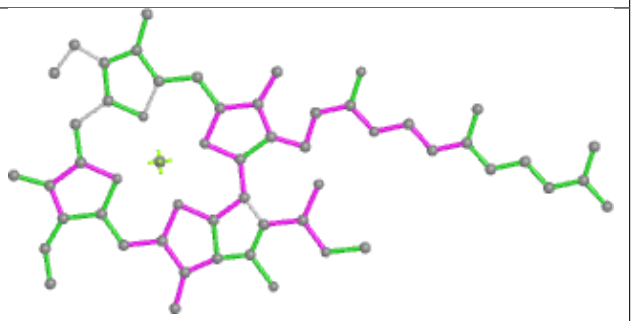


Rings

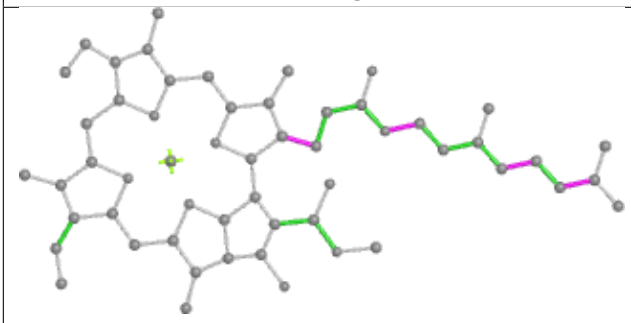
Ligand CLA A 1110



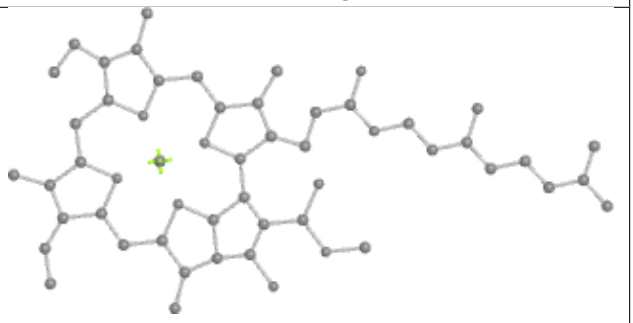
Bond lengths



Bond angles

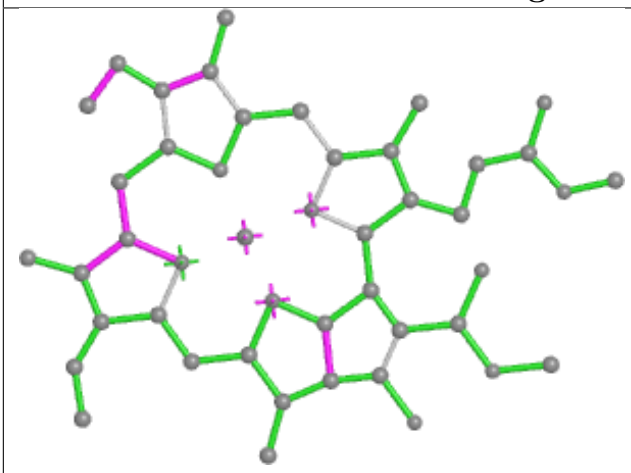


Torsions

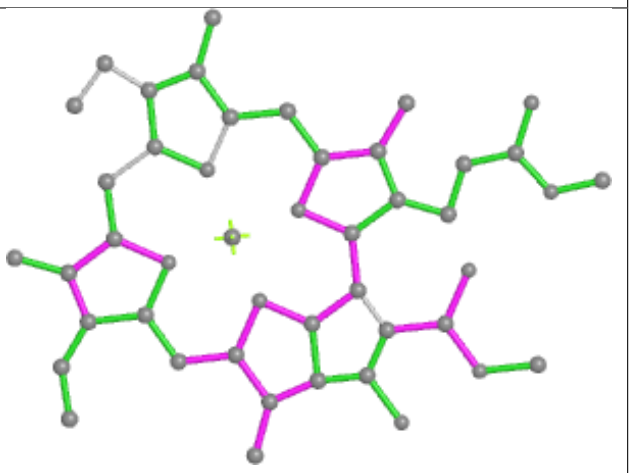


Rings

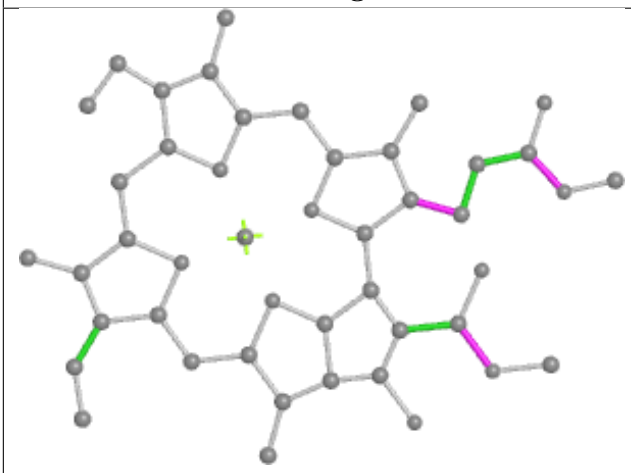
Ligand CLA 1 602



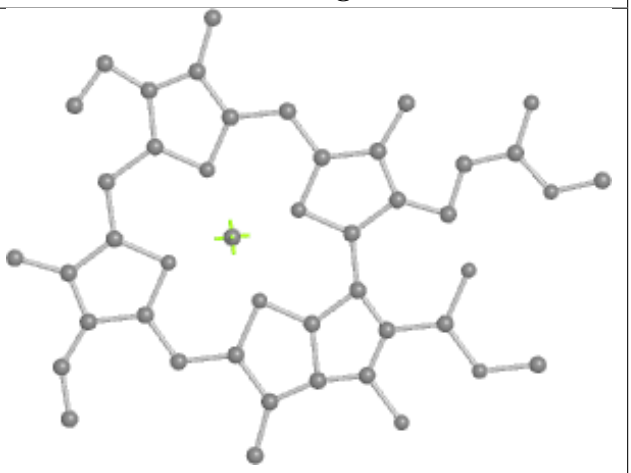
Bond lengths



Bond angles

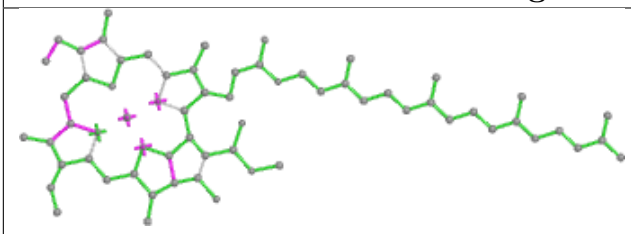


Torsions

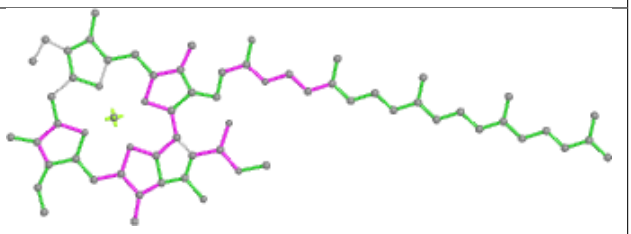


Rings

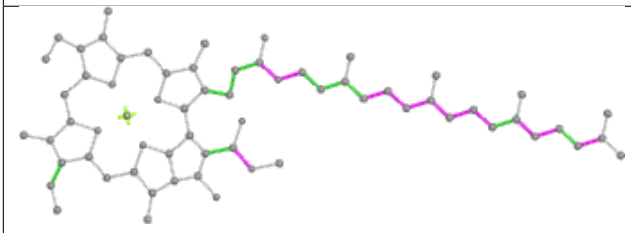
Ligand CLA 4 612



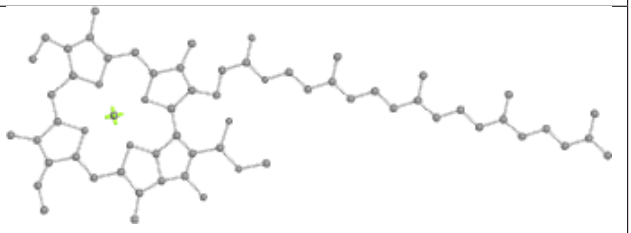
Bond lengths



Bond angles

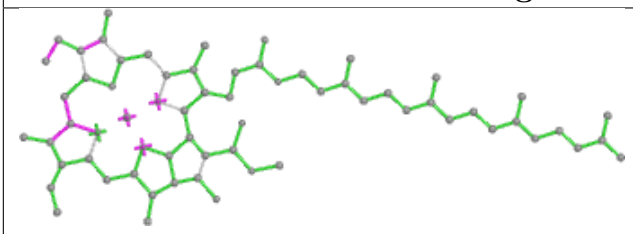


Torsions

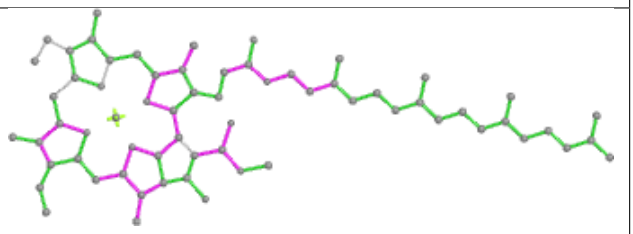


Rings

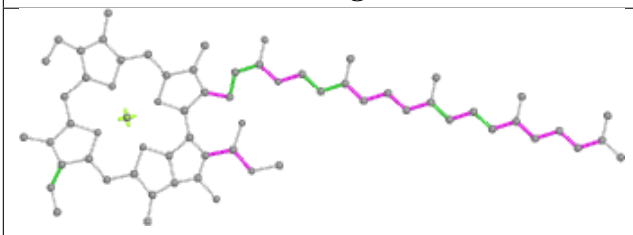
Ligand CLA B 1207



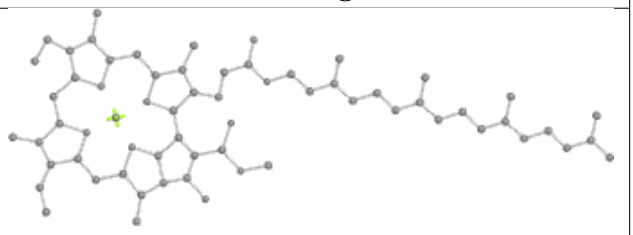
Bond lengths



Bond angles

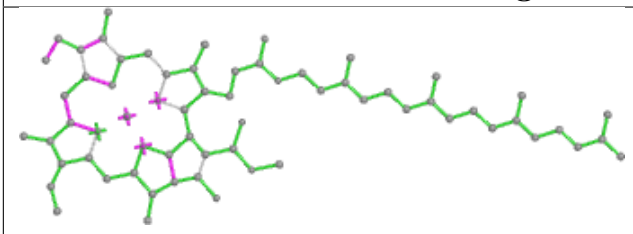


Torsions

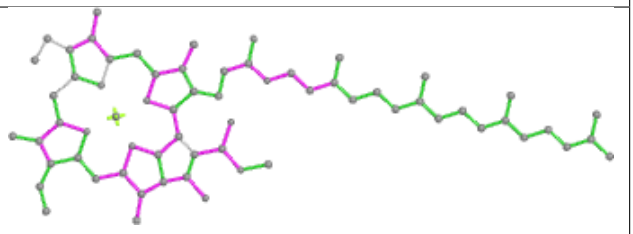


Rings

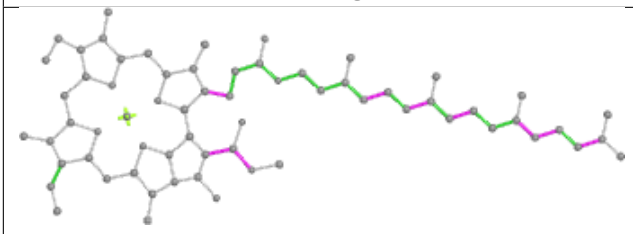
Ligand CLA B 1223



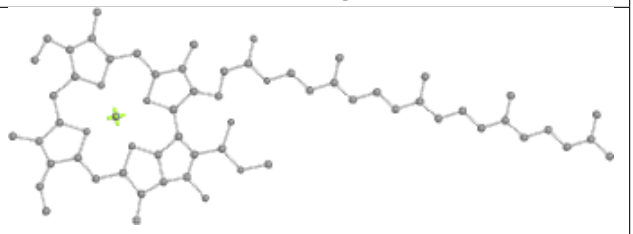
Bond lengths



Bond angles

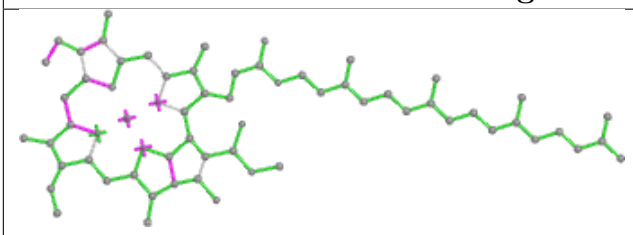


Torsions

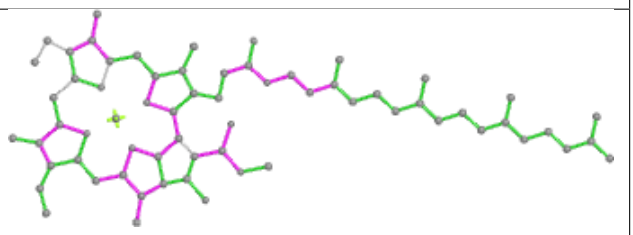


Rings

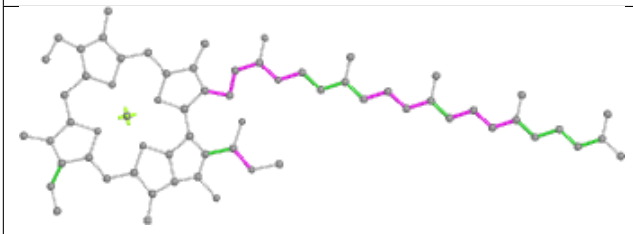
Ligand CLA F 1301



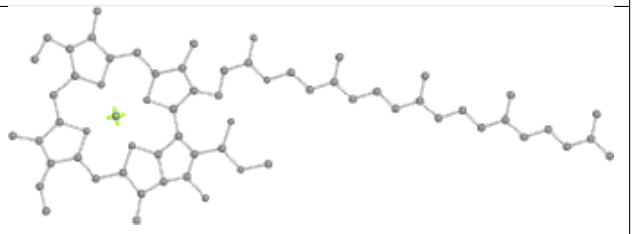
Bond lengths



Bond angles

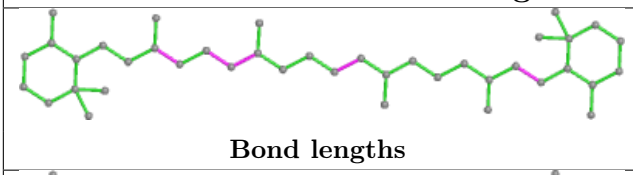


Torsions

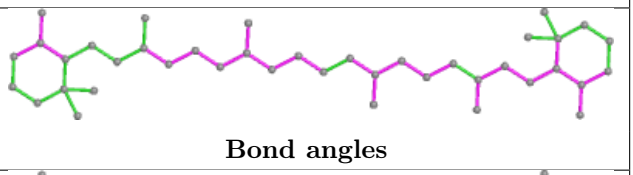


Rings

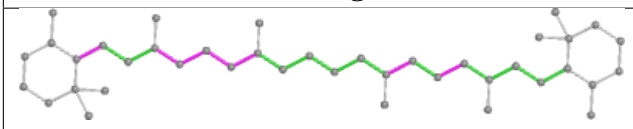
Ligand BCR A 4002



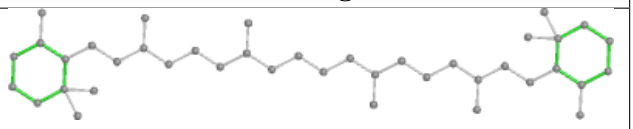
Bond lengths



Bond angles

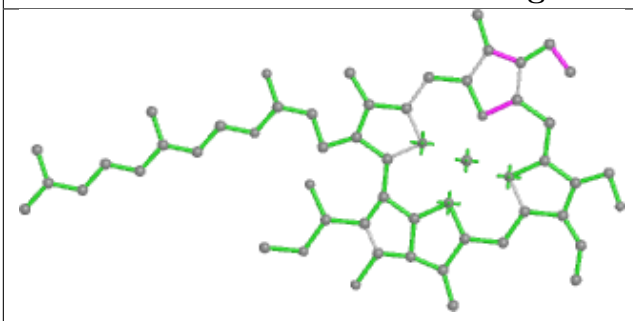


Torsions

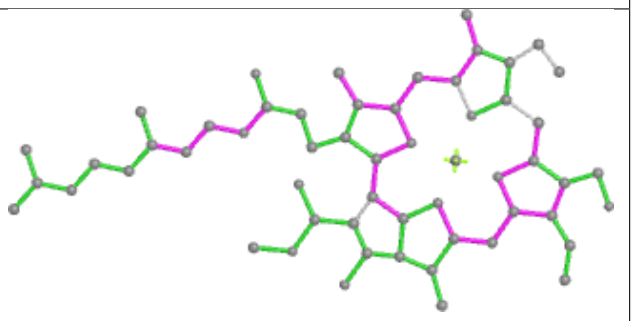


Rings

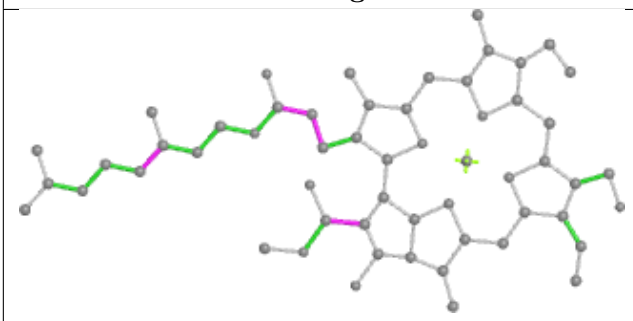
Ligand CHL 2 615



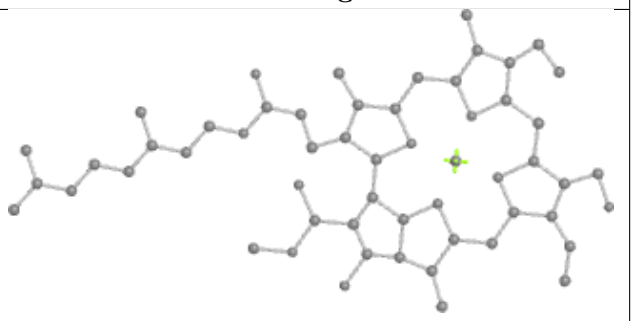
Bond lengths



Bond angles

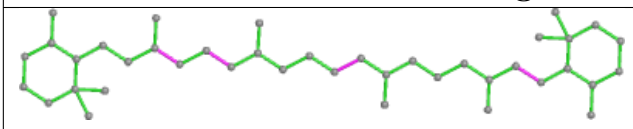


Torsions

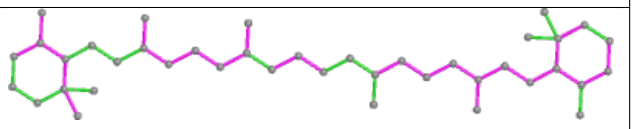


Rings

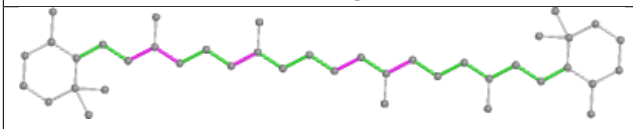
Ligand BCR F 4014



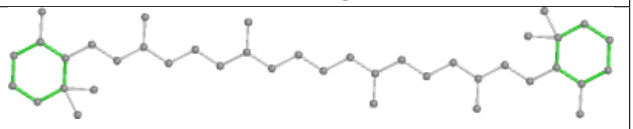
Bond lengths



Bond angles

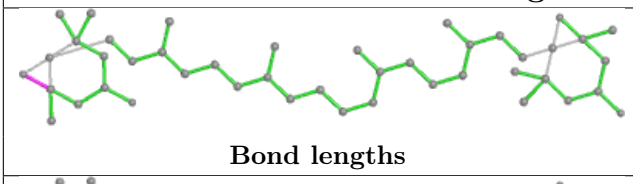


Torsions

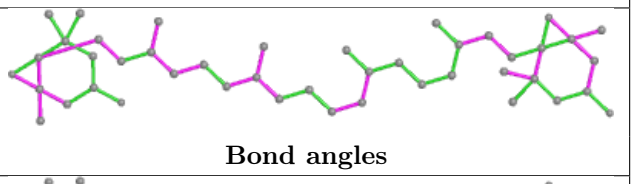


Rings

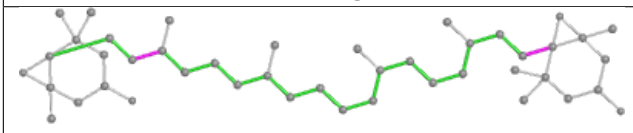
Ligand XAT 2 502



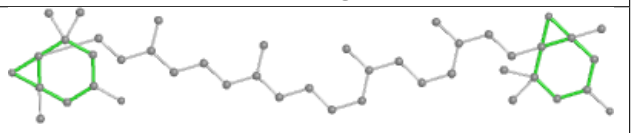
Bond lengths



Bond angles

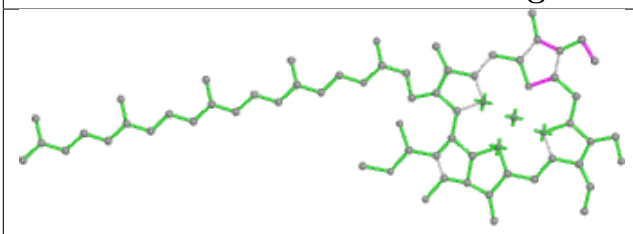


Torsions

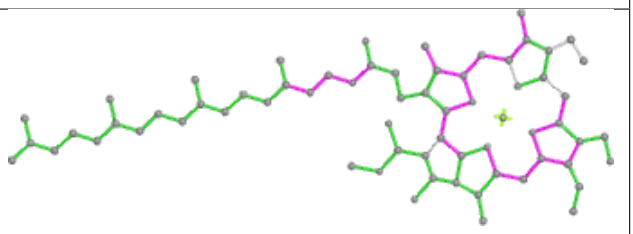


Rings

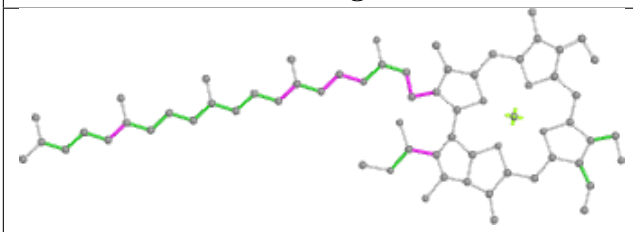
Ligand CHL 2 609



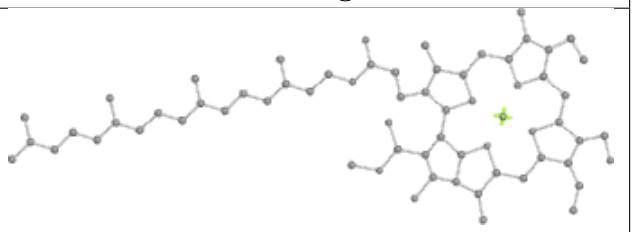
Bond lengths



Bond angles

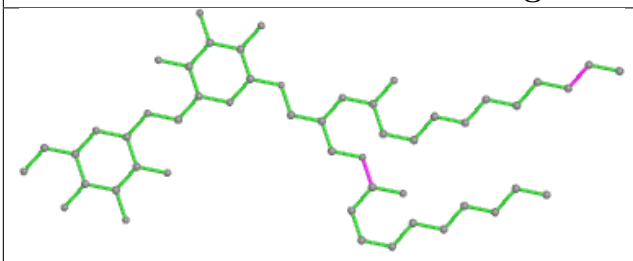


Torsions

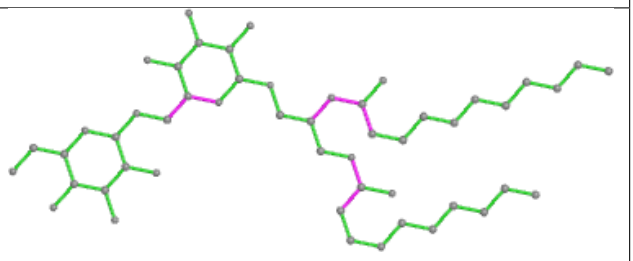


Rings

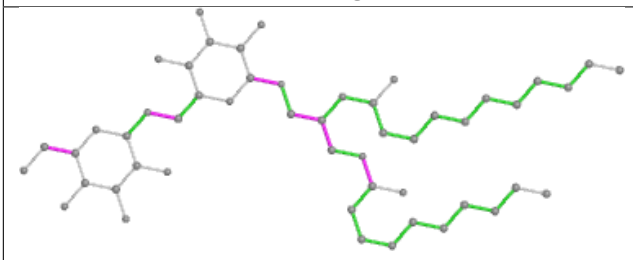
Ligand DGD 3 803



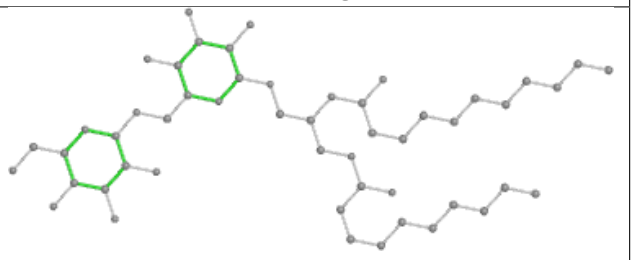
Bond lengths



Bond angles

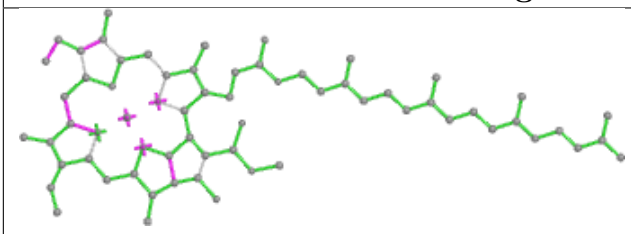


Torsions

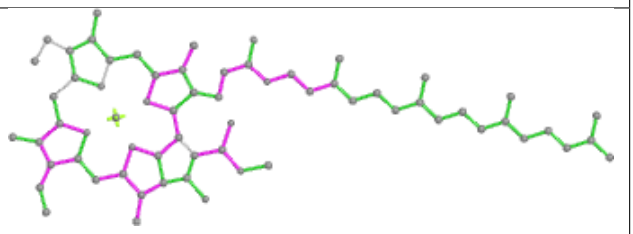


Rings

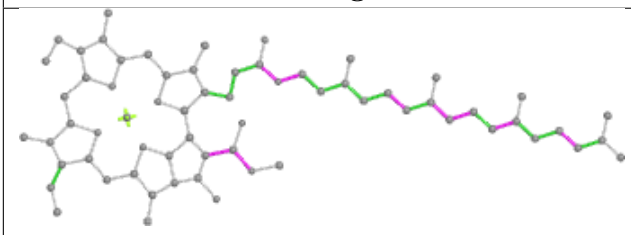
Ligand CLA B 1227



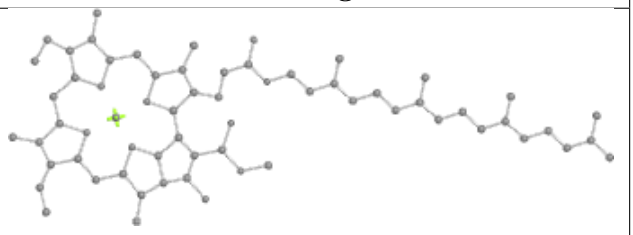
Bond lengths



Bond angles

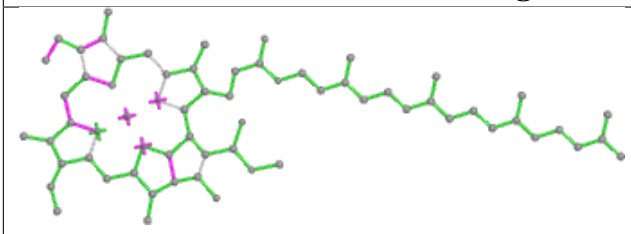


Torsions

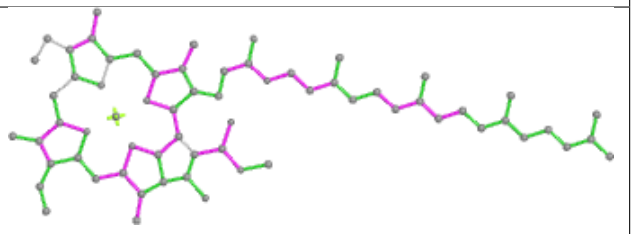


Rings

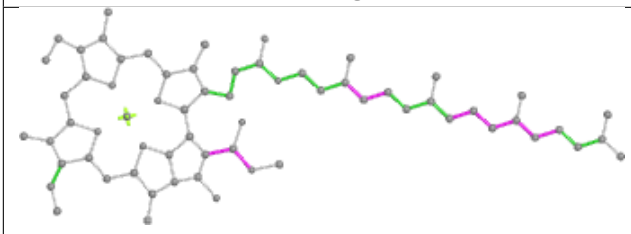
Ligand CLA A 1139



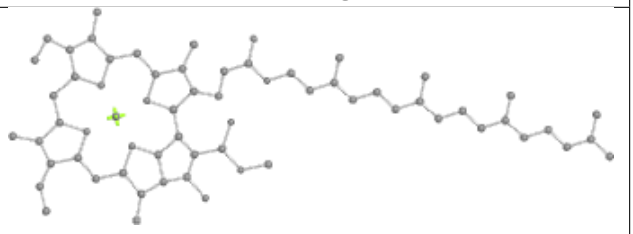
Bond lengths



Bond angles

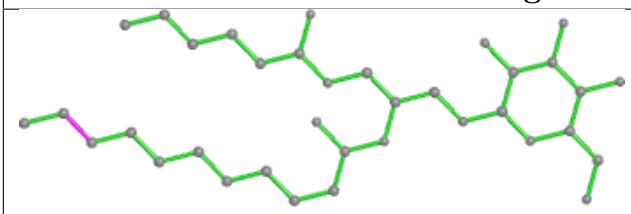


Torsions

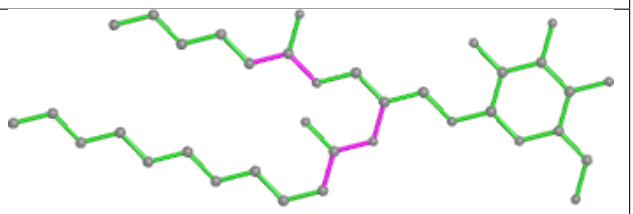


Rings

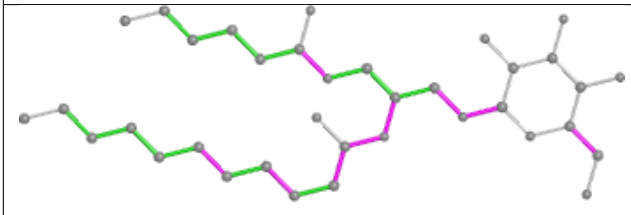
Ligand LMG 2 803



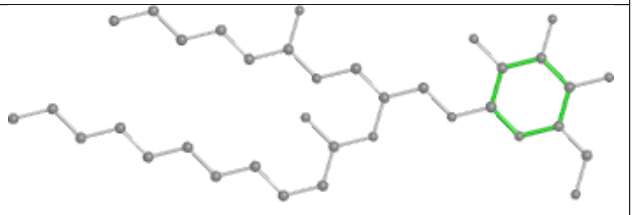
Bond lengths



Bond angles

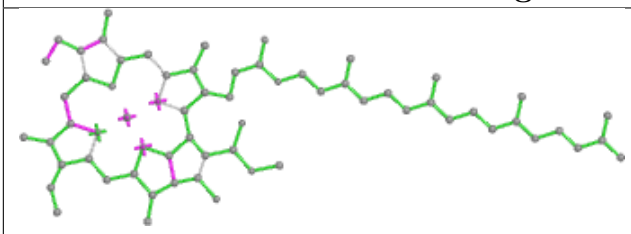


Torsions

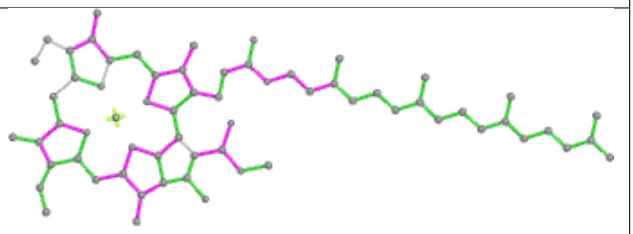


Rings

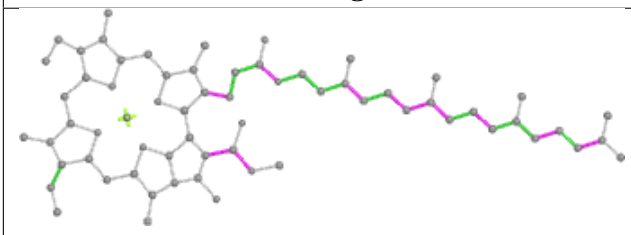
Ligand CLA A 1128



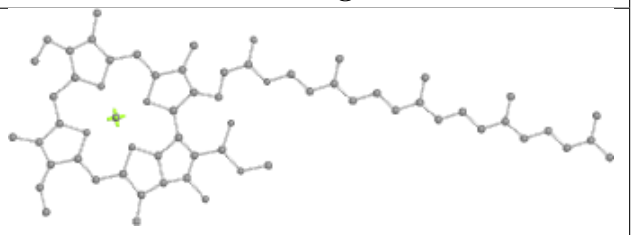
Bond lengths



Bond angles

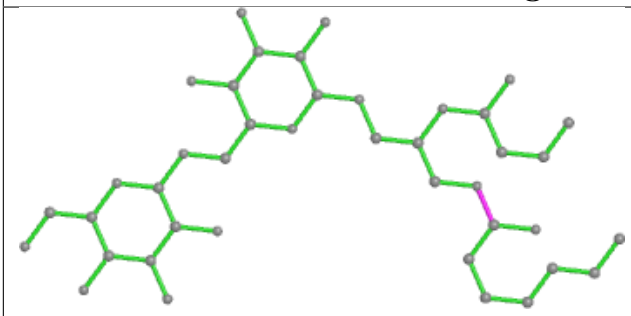


Torsions

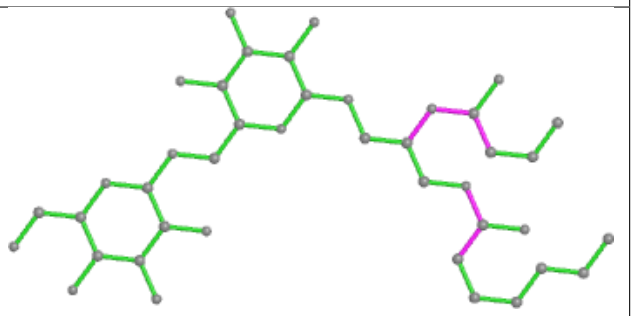


Rings

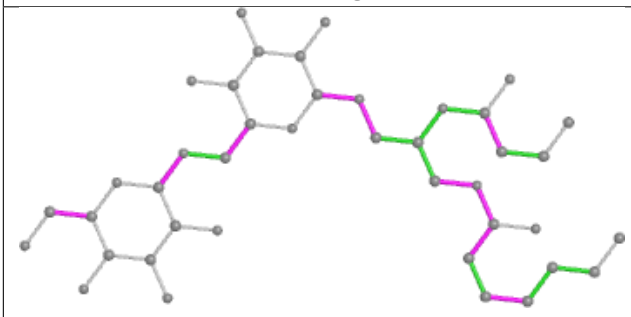
Ligand DGD 1 803



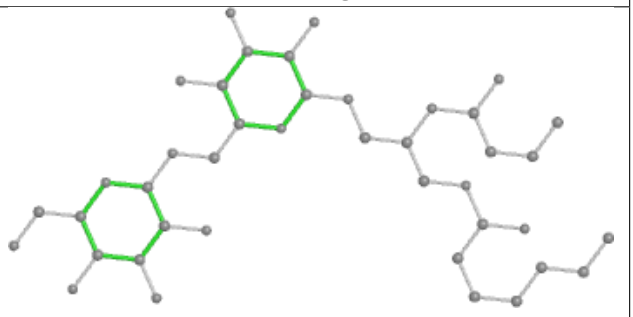
Bond lengths



Bond angles

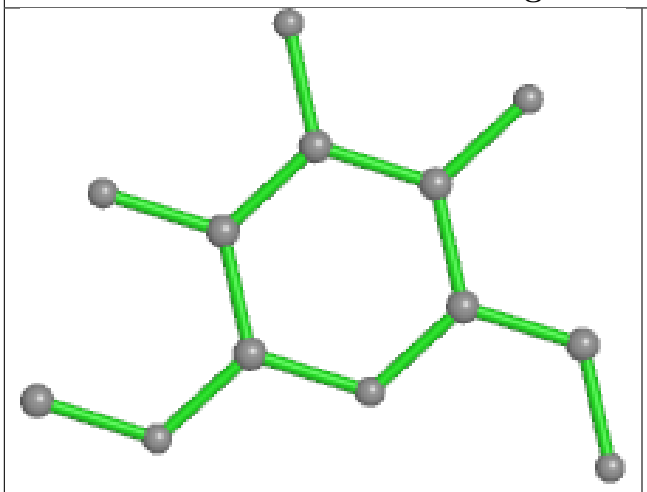


Torsions

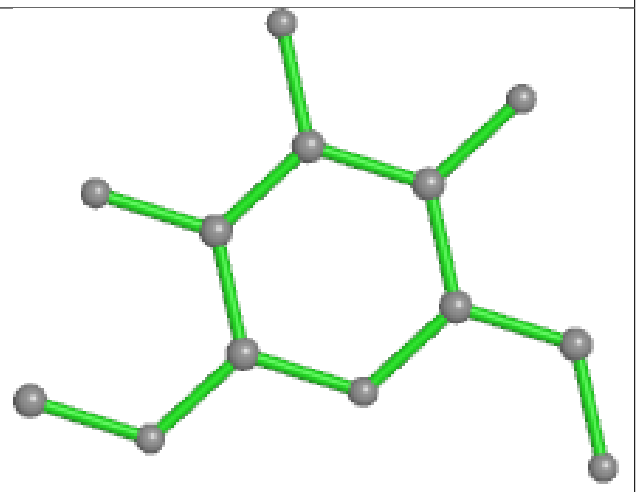


Rings

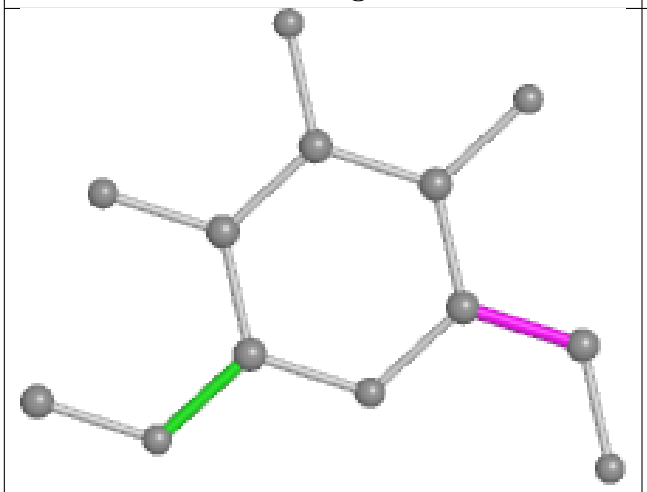
Ligand LMG 2 806



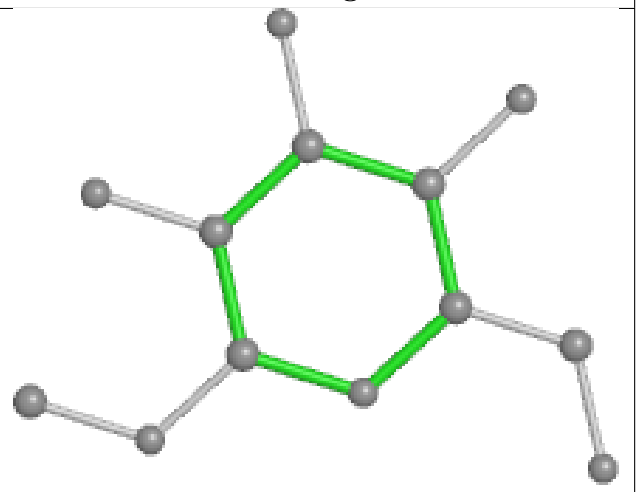
Bond lengths



Bond angles

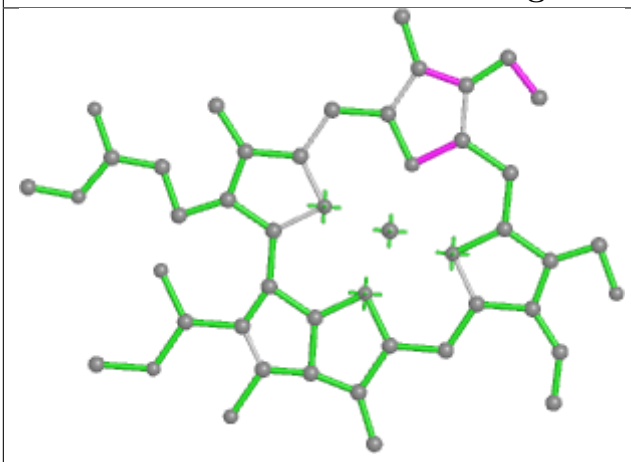


Torsions

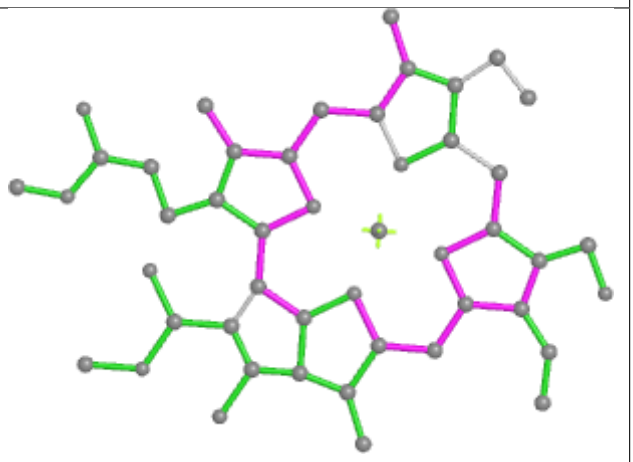


Rings

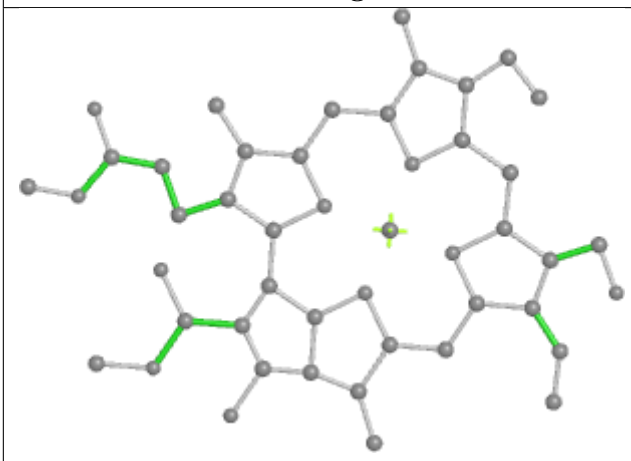
Ligand CHL 3 611



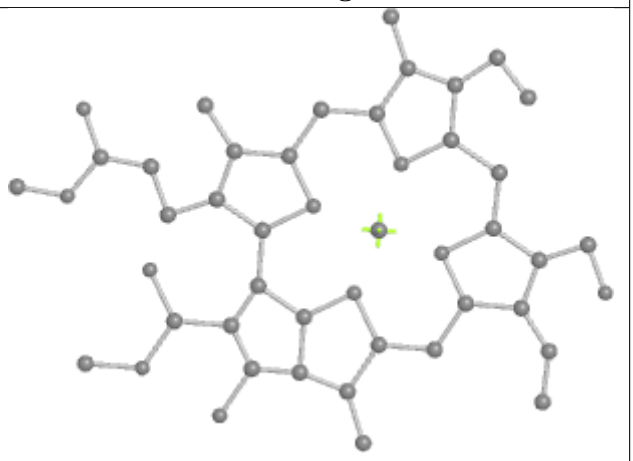
Bond lengths



Bond angles

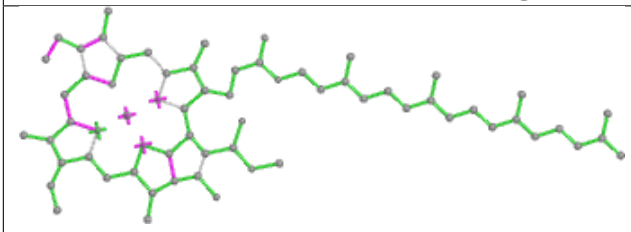


Torsions

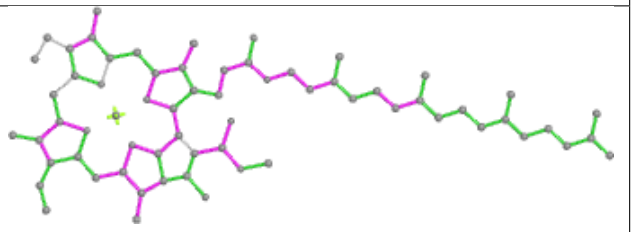


Rings

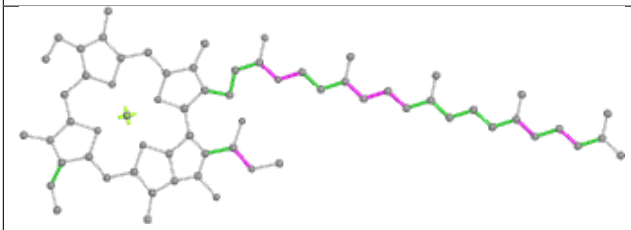
Ligand CLA B 1229



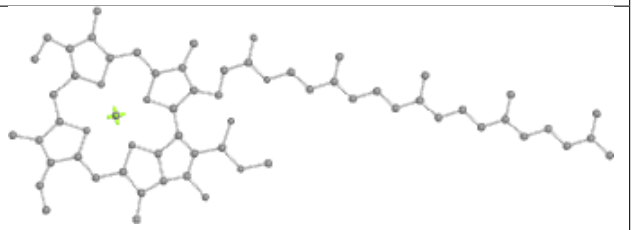
Bond lengths



Bond angles

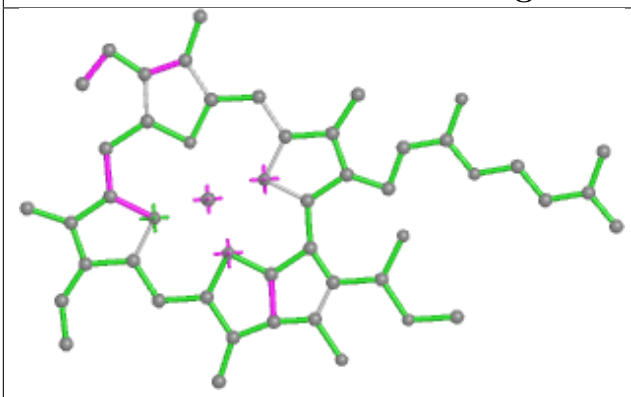


Torsions

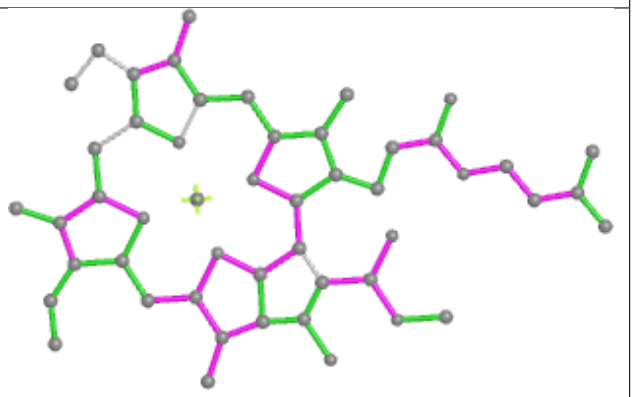


Rings

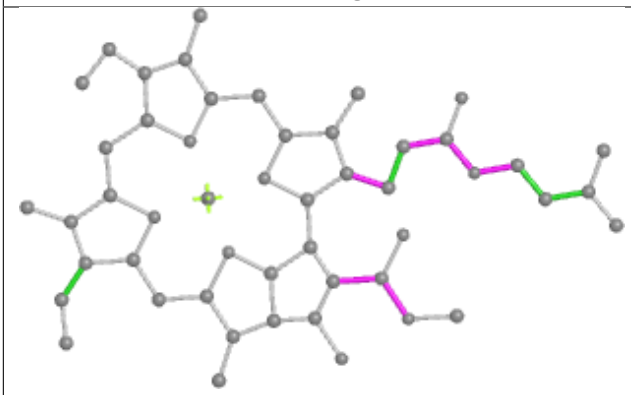
Ligand CLA B 1236



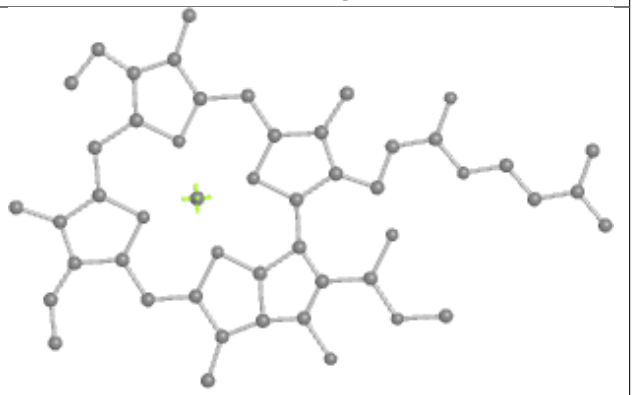
Bond lengths



Bond angles

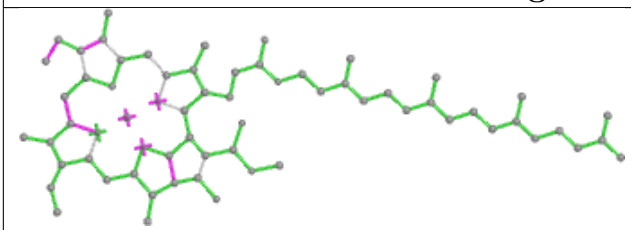


Torsions

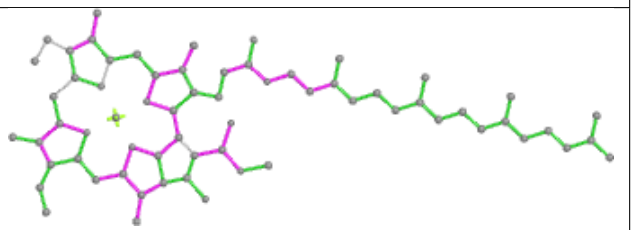


Rings

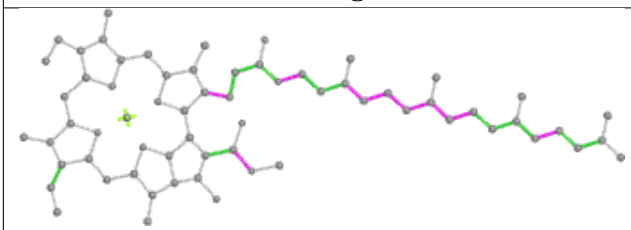
Ligand CLA 1 611



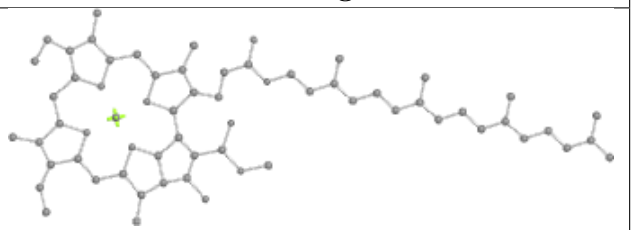
Bond lengths



Bond angles

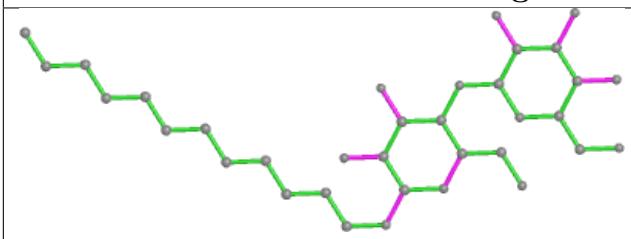


Torsions

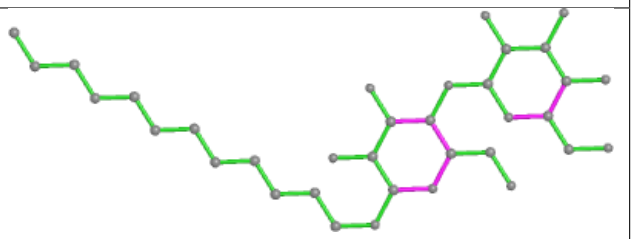


Rings

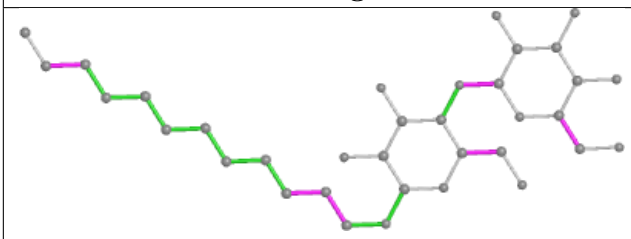
Ligand LMT A 5004



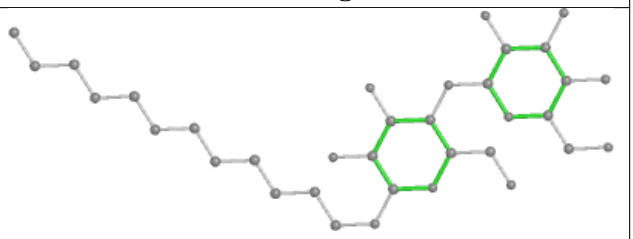
Bond lengths



Bond angles

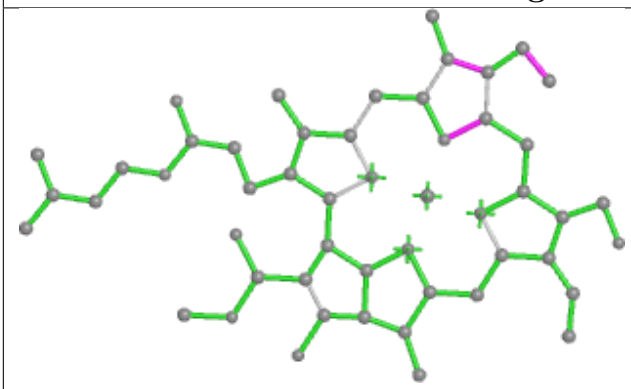


Torsions

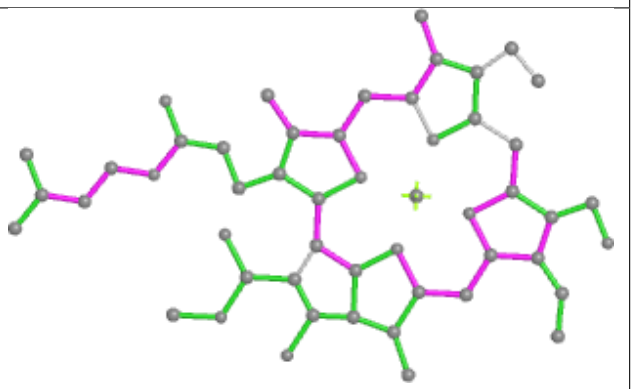


Rings

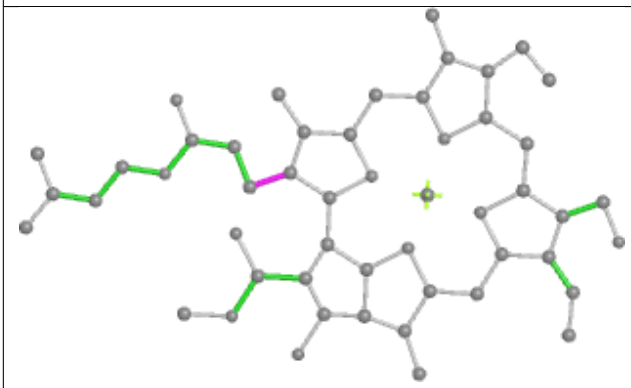
Ligand CHL 4 611



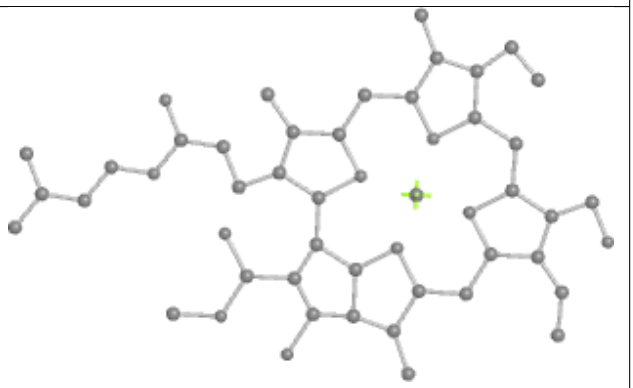
Bond lengths



Bond angles

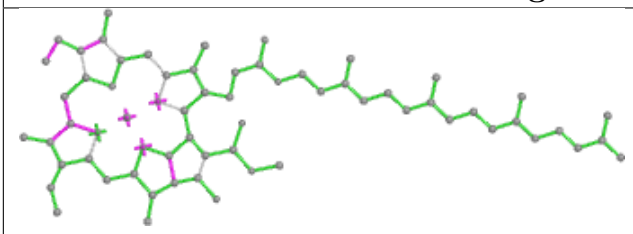


Torsions

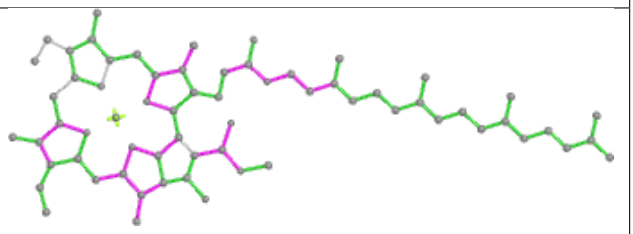


Rings

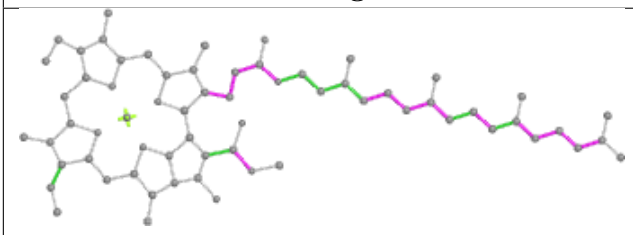
Ligand CLA 4 617



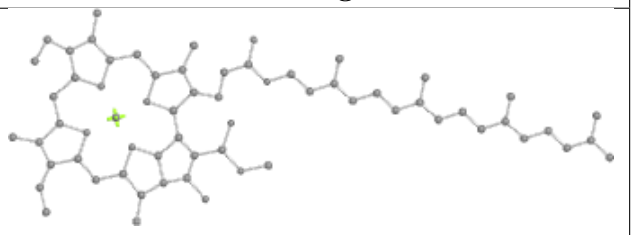
Bond lengths



Bond angles

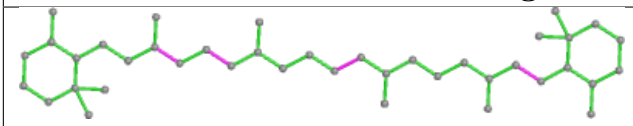


Torsions

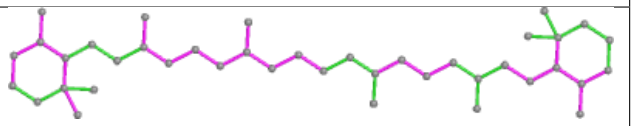


Rings

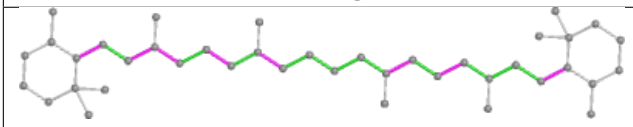
Ligand BCR I 4018



Bond lengths



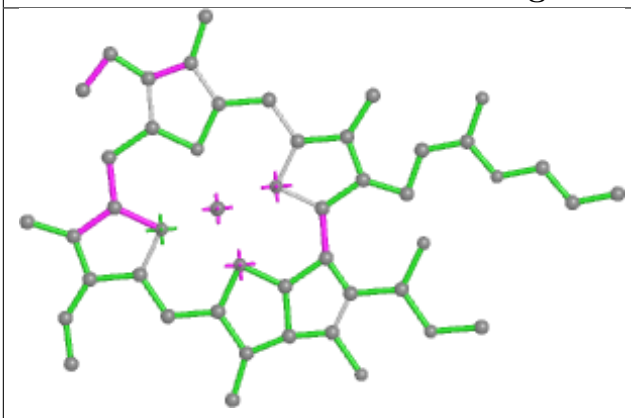
Bond angles



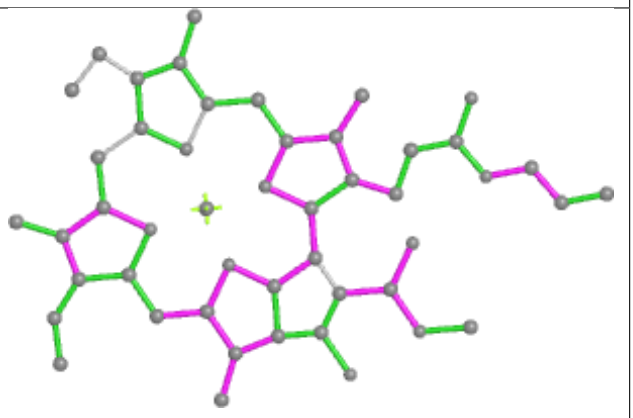
Torsions

Rings

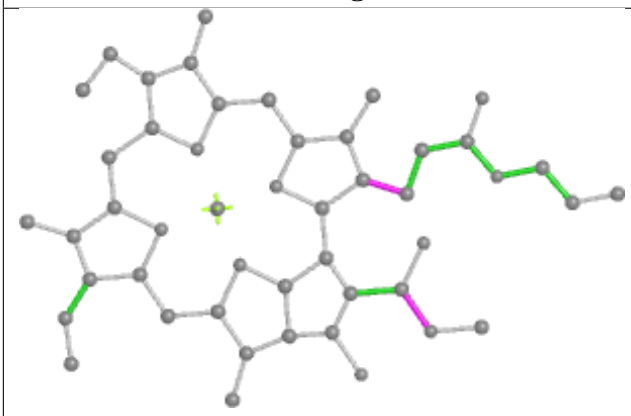
Ligand CLA 3 608



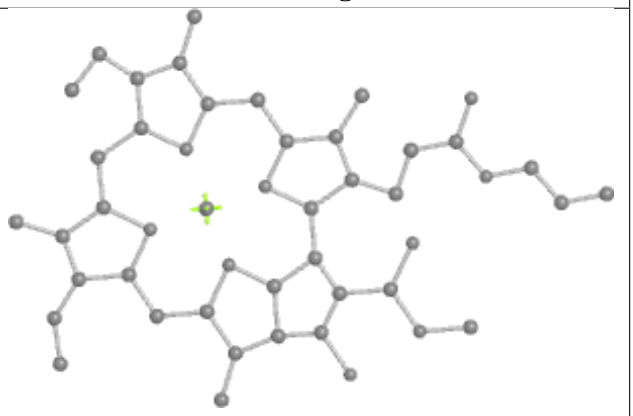
Bond lengths



Bond angles

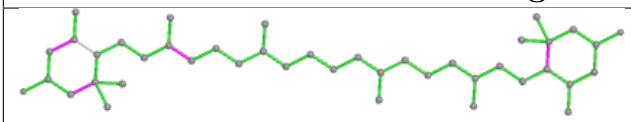


Torsions

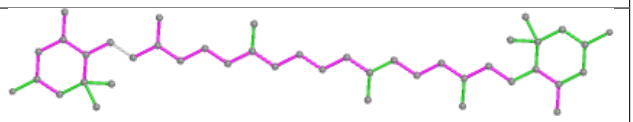


Rings

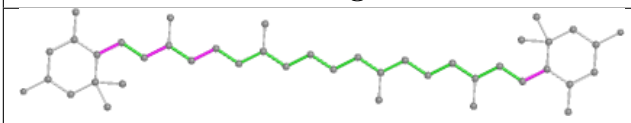
Ligand LUT 4 501



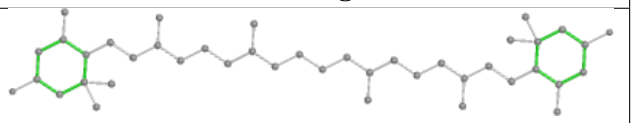
Bond lengths



Bond angles

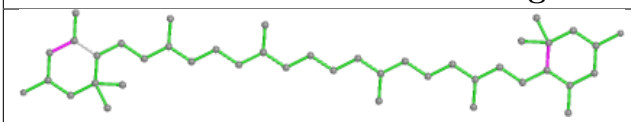


Torsions

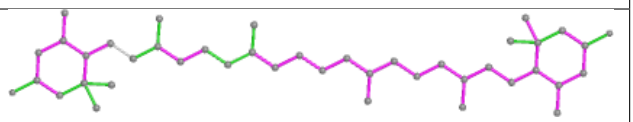


Rings

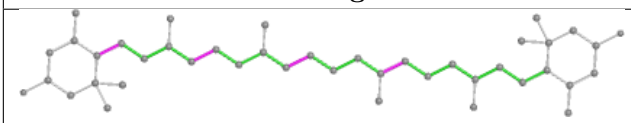
Ligand LUT 3 501



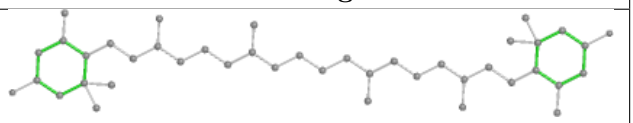
Bond lengths



Bond angles

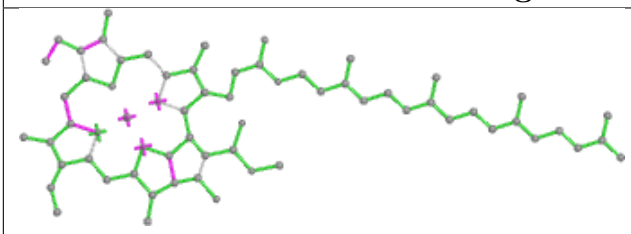


Torsions

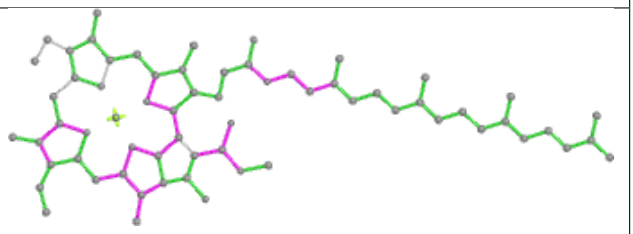


Rings

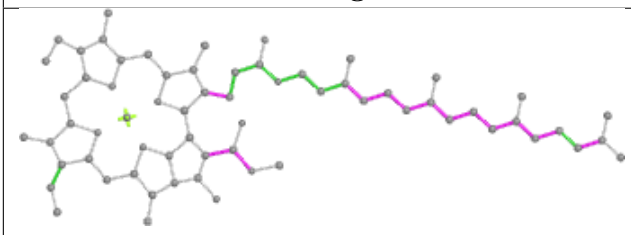
Ligand CLA A 1102



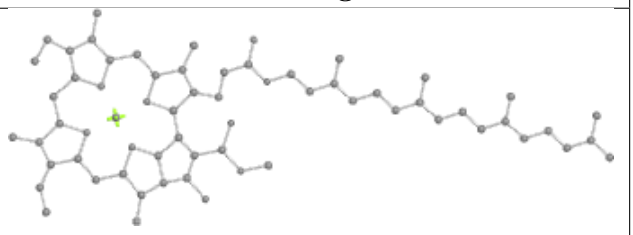
Bond lengths



Bond angles

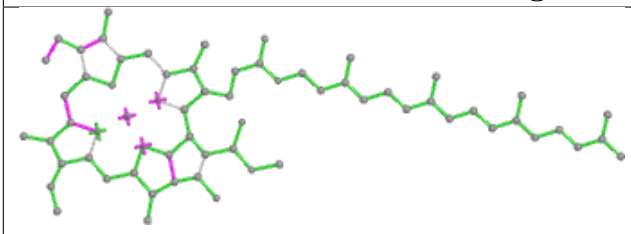


Torsions

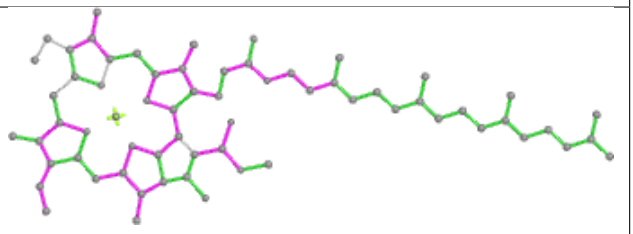


Rings

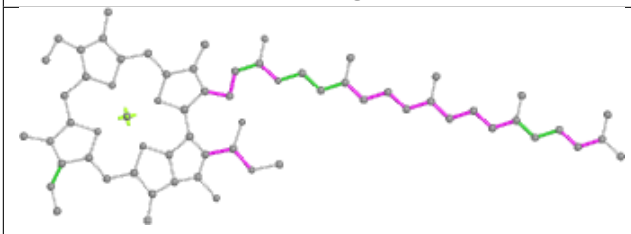
Ligand CLA 2 605



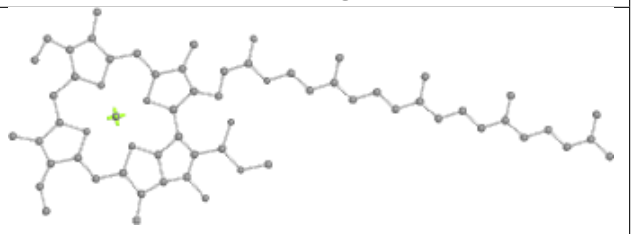
Bond lengths



Bond angles

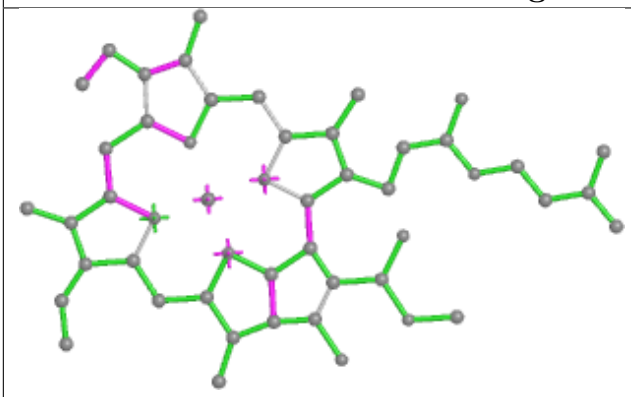


Torsions

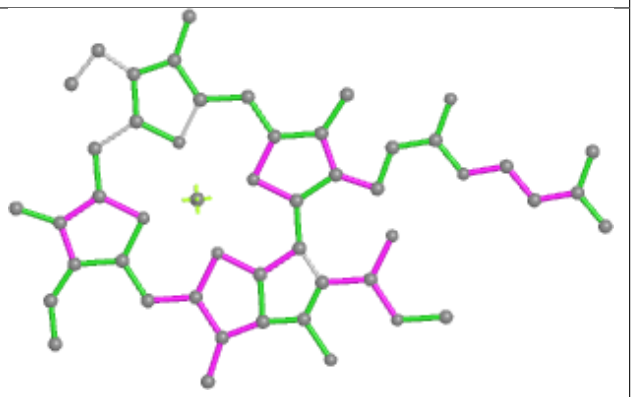


Rings

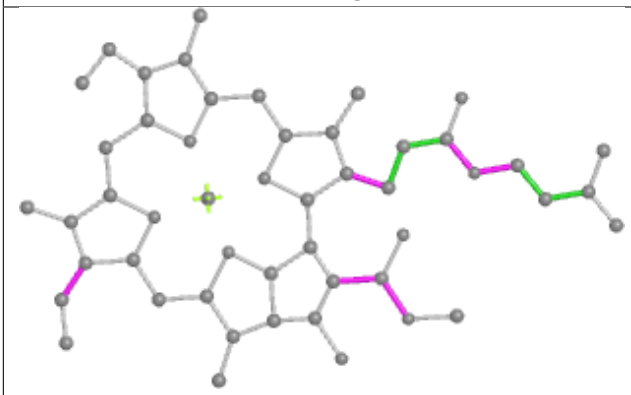
Ligand CLA 3 606



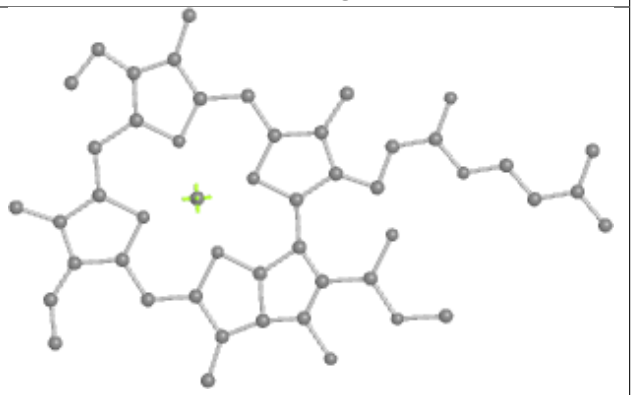
Bond lengths



Bond angles

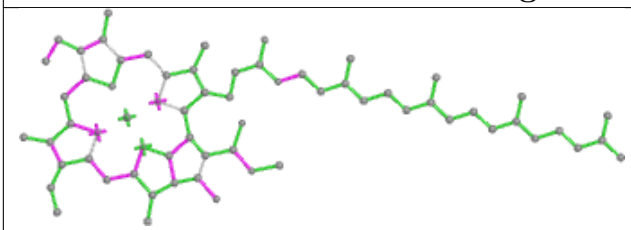


Torsions

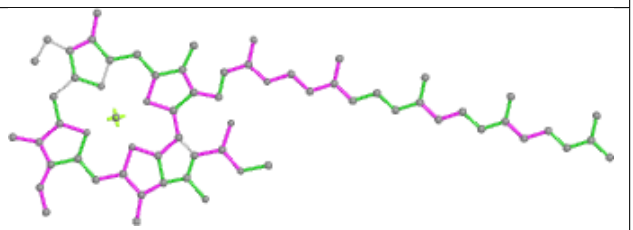


Rings

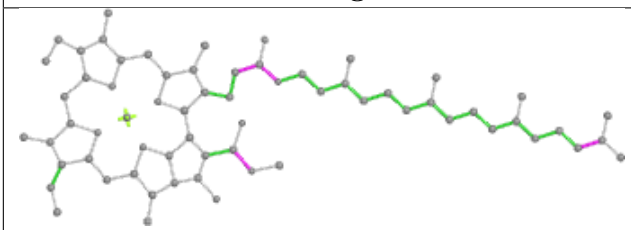
Ligand CL0 A 1011



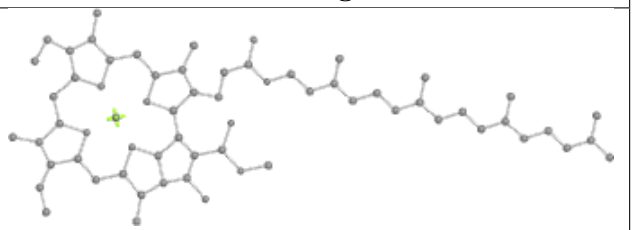
Bond lengths



Bond angles

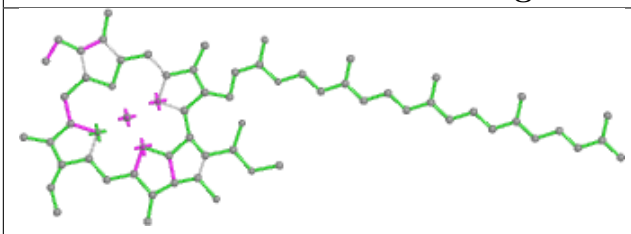


Torsions

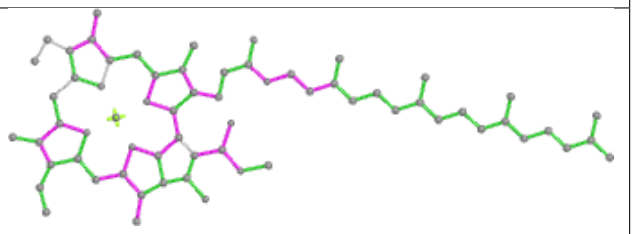


Rings

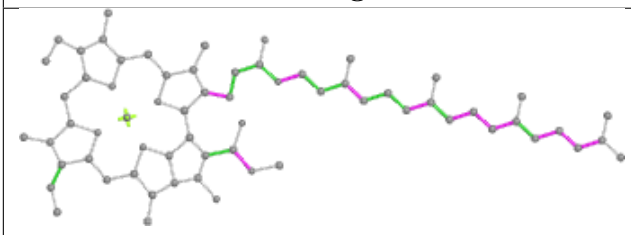
Ligand CLA A 1133



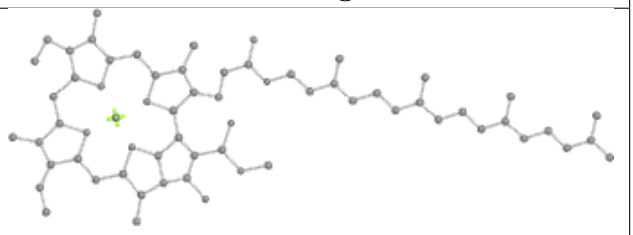
Bond lengths



Bond angles

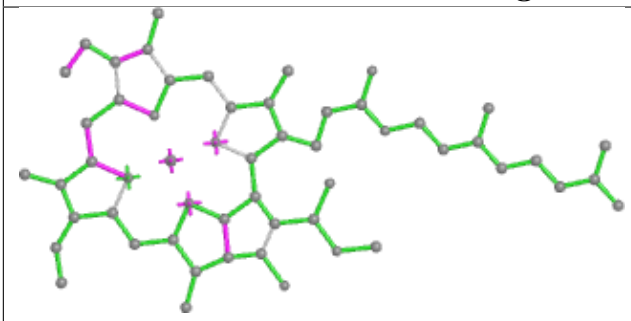


Torsions

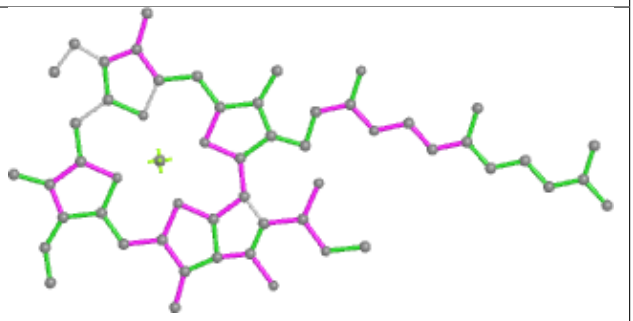


Rings

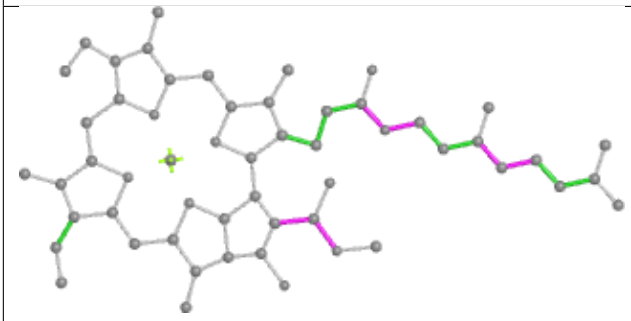
Ligand CLA B 1234



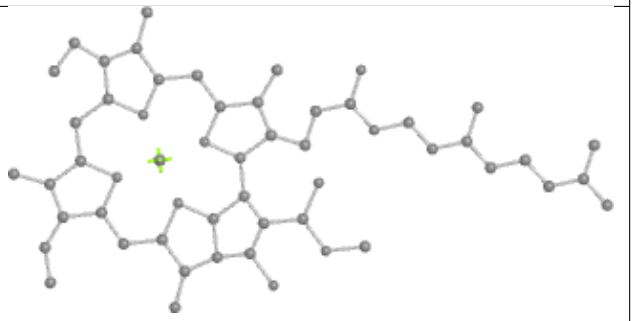
Bond lengths



Bond angles

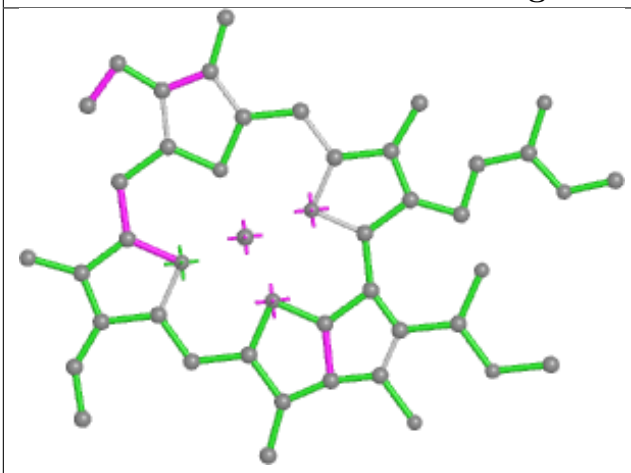


Torsions

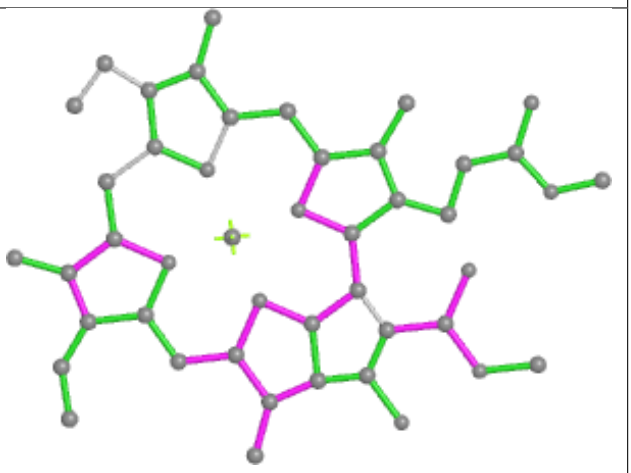


Rings

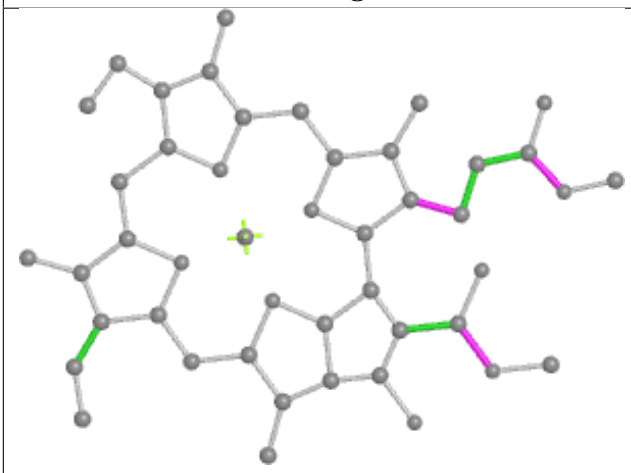
Ligand CLA 1 608



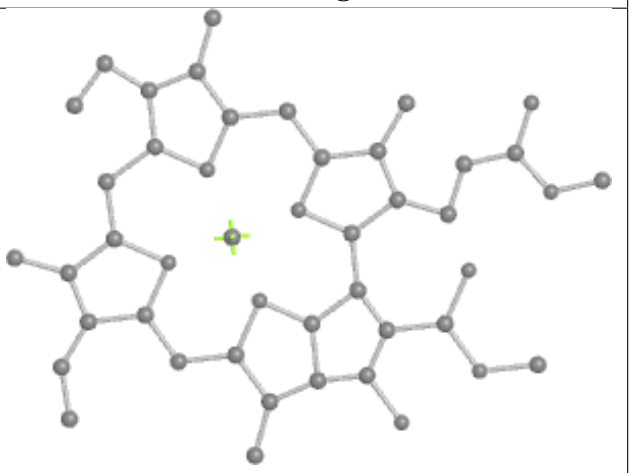
Bond lengths



Bond angles

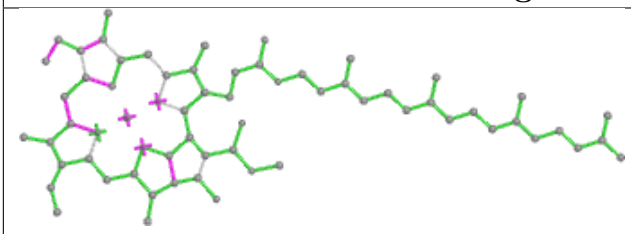


Torsions

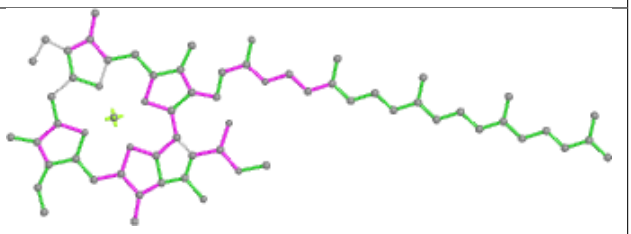


Rings

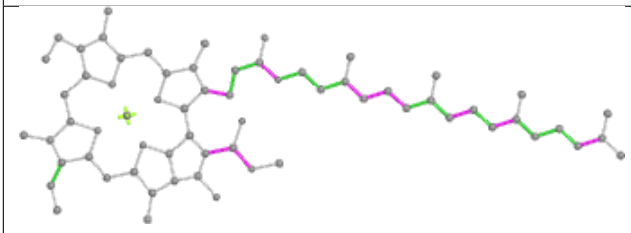
Ligand CLA A 1104



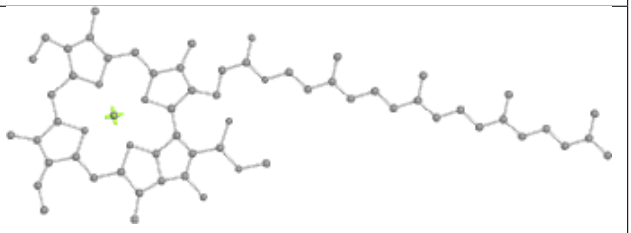
Bond lengths



Bond angles

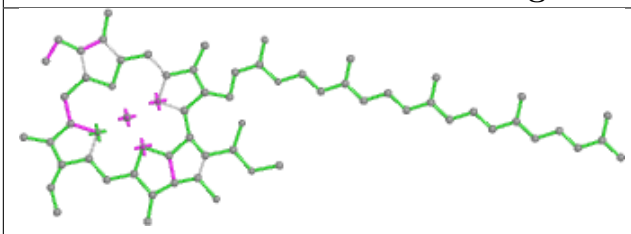


Torsions

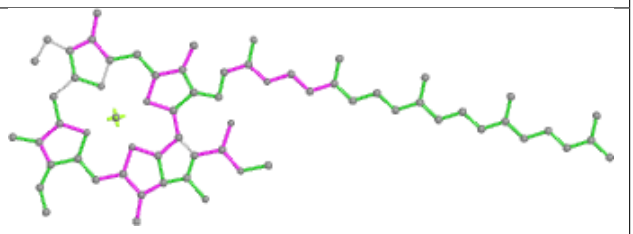


Rings

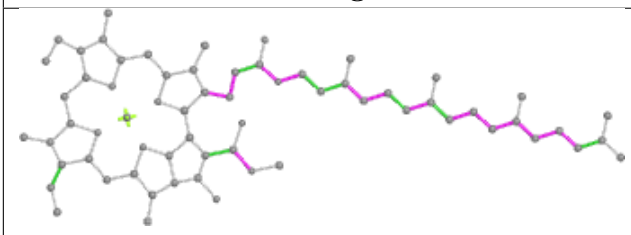
Ligand CLA 3 610



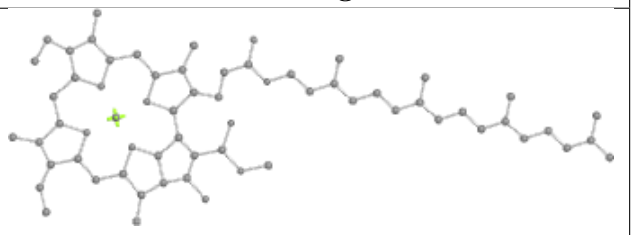
Bond lengths



Bond angles

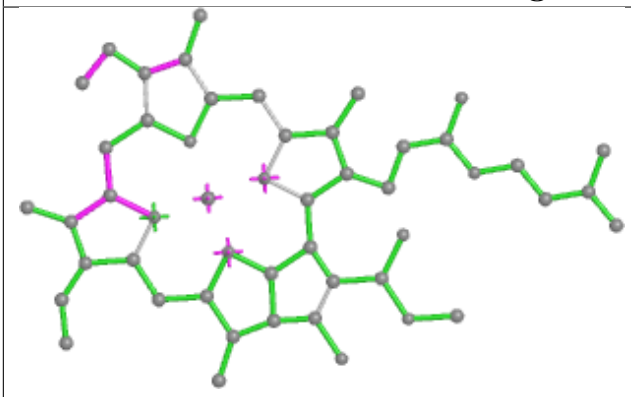


Torsions

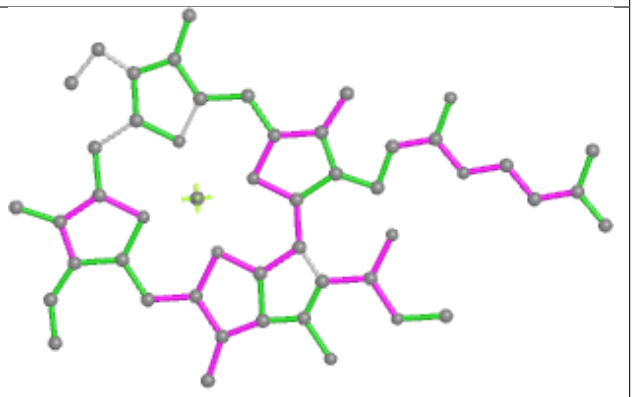


Rings

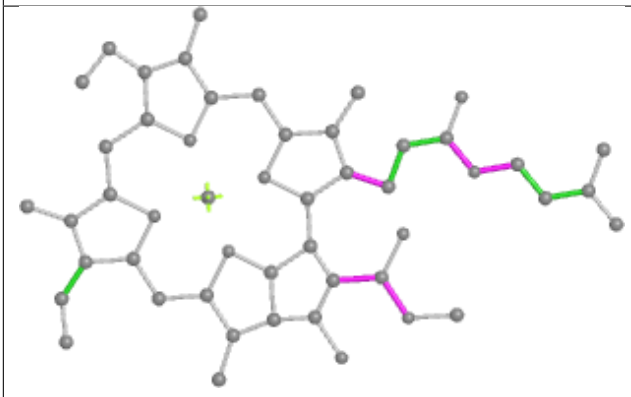
Ligand CLA 4 609



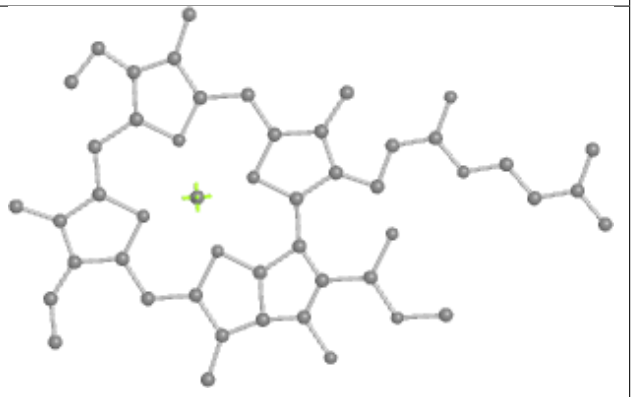
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
17	N	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	N	35:LEU	C	36:PRO	N	1.19

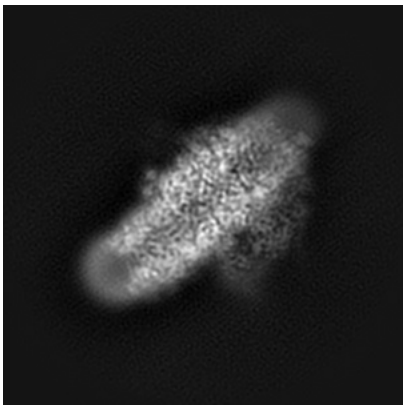
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-10798. These allow visual inspection of the internal detail of the map and identification of artifacts.

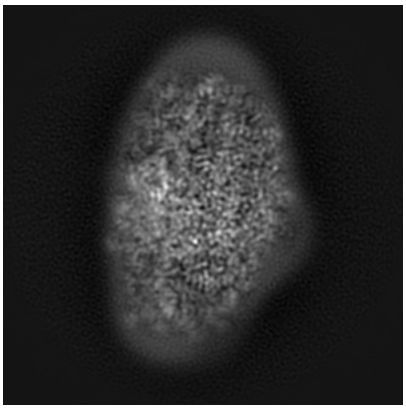
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

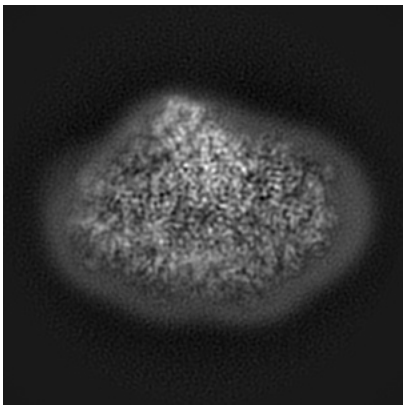
6.1.1 Primary map



X

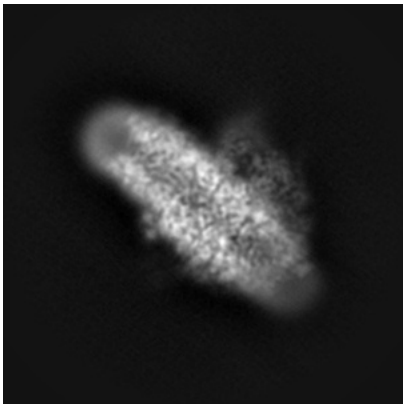


Y

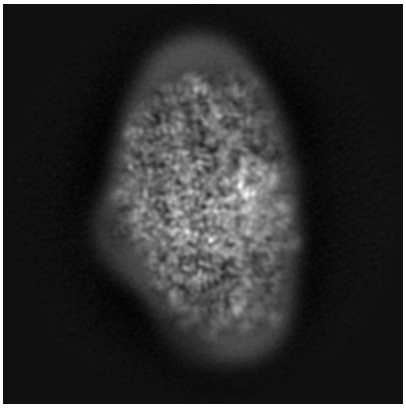


Z

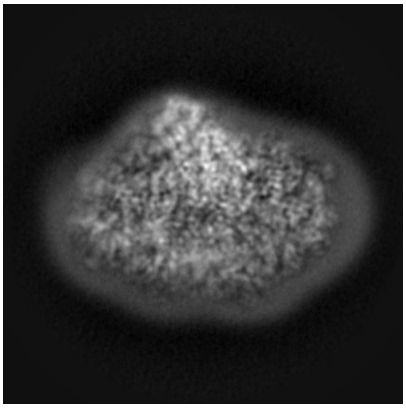
6.1.2 Raw map



X



Y

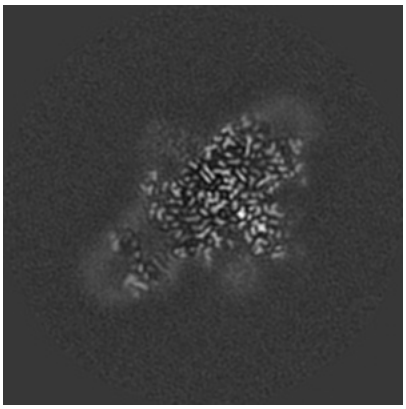


Z

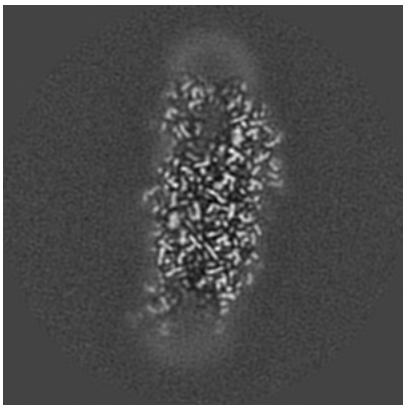
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

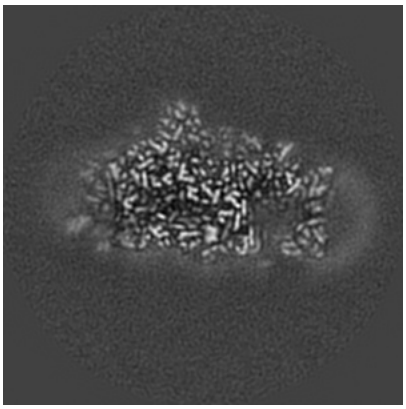
6.2.1 Primary map



X Index: 150

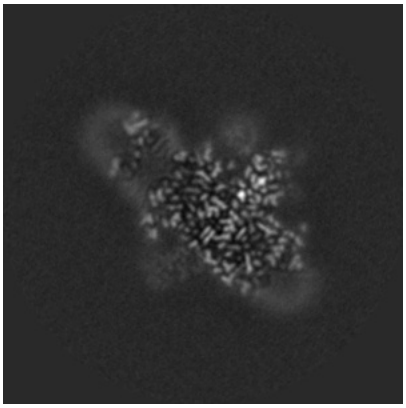


Y Index: 150

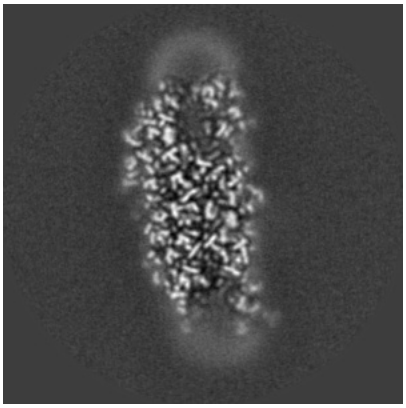


Z Index: 150

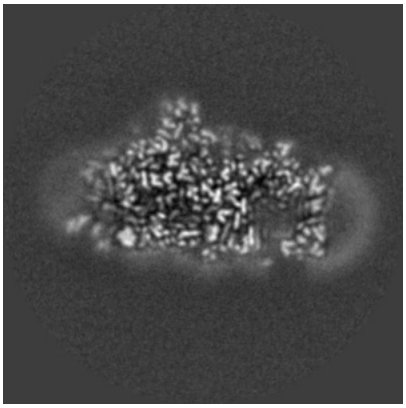
6.2.2 Raw map



X Index: 150



Y Index: 150

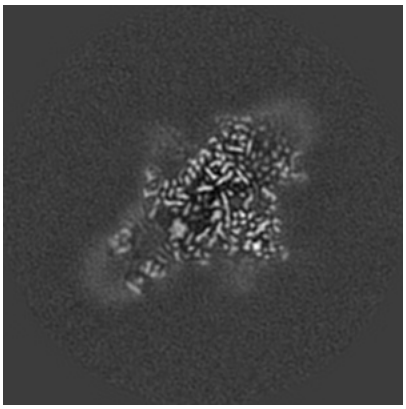


Z Index: 150

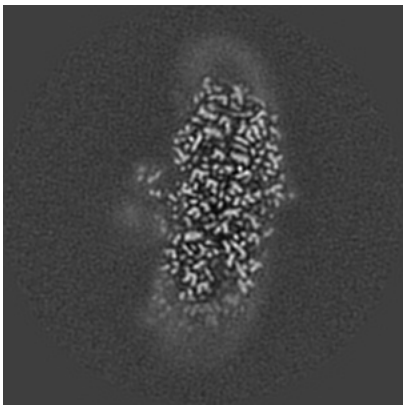
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

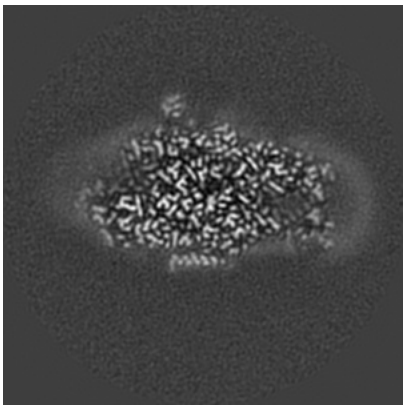
6.3.1 Primary map



X Index: 154

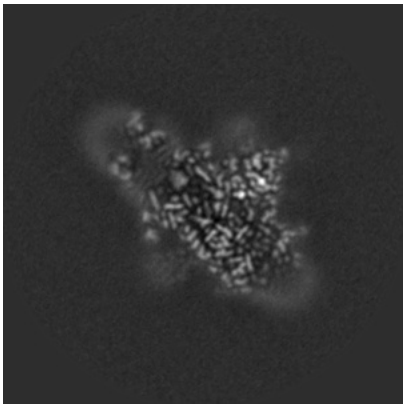


Y Index: 164

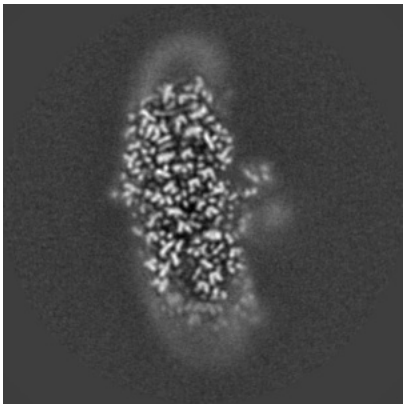


Z Index: 161

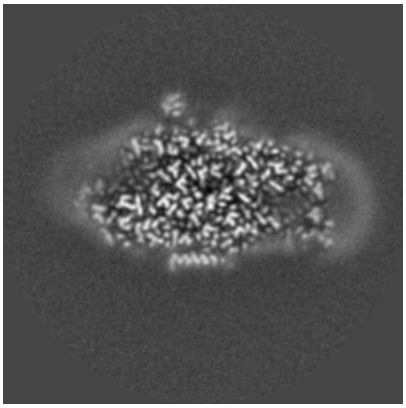
6.3.2 Raw map



X Index: 153



Y Index: 164



Z Index: 138

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

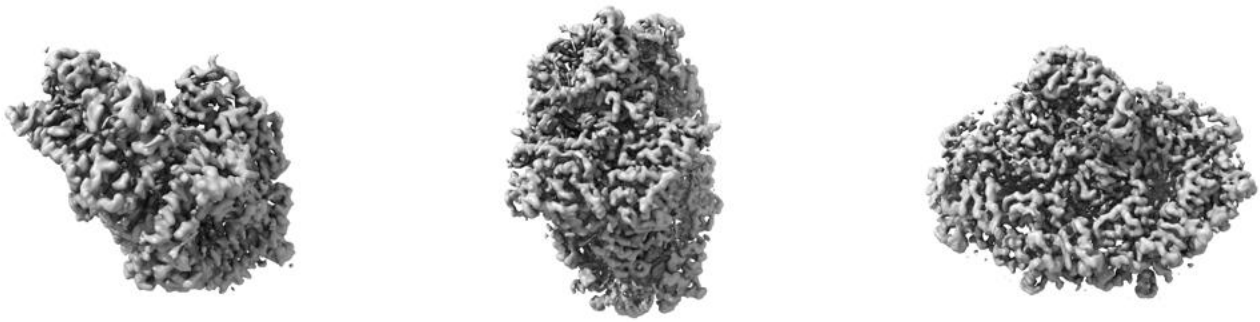
6.4 Orthogonal surface views (i)

6.4.1 Primary map

X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.022. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.4.2 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.

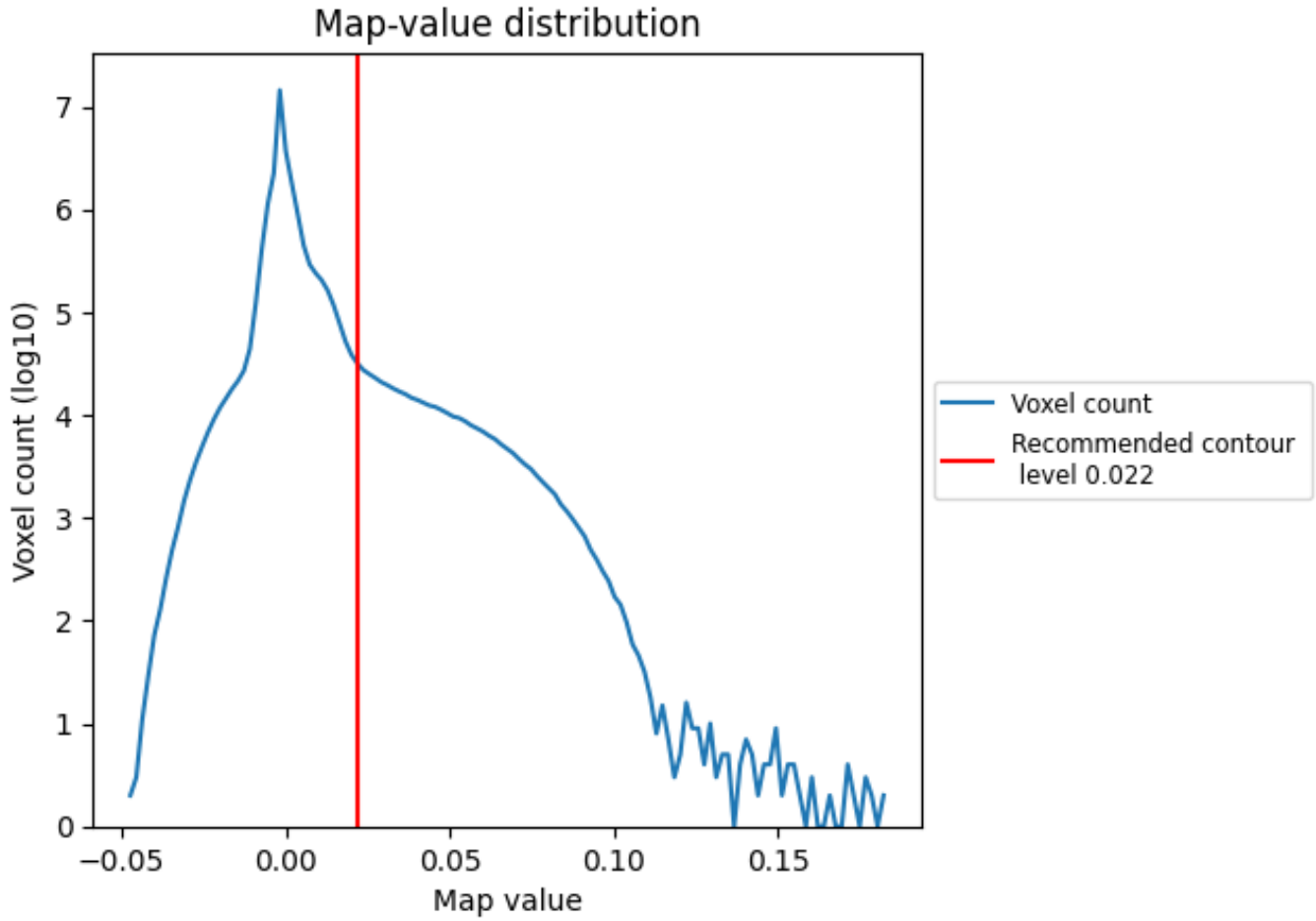
6.5 Mask visualisation (i)

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

7 Map analysis

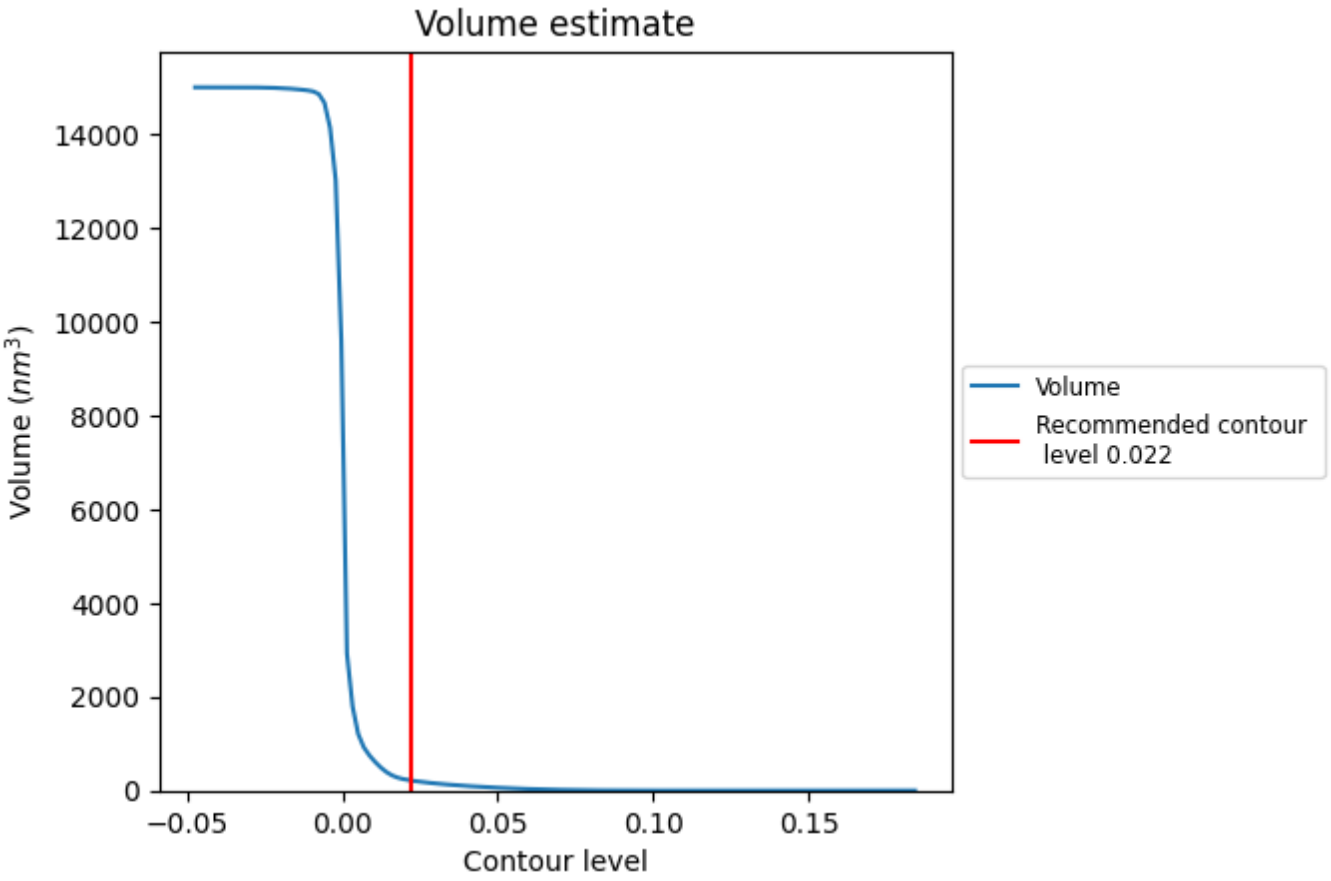
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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

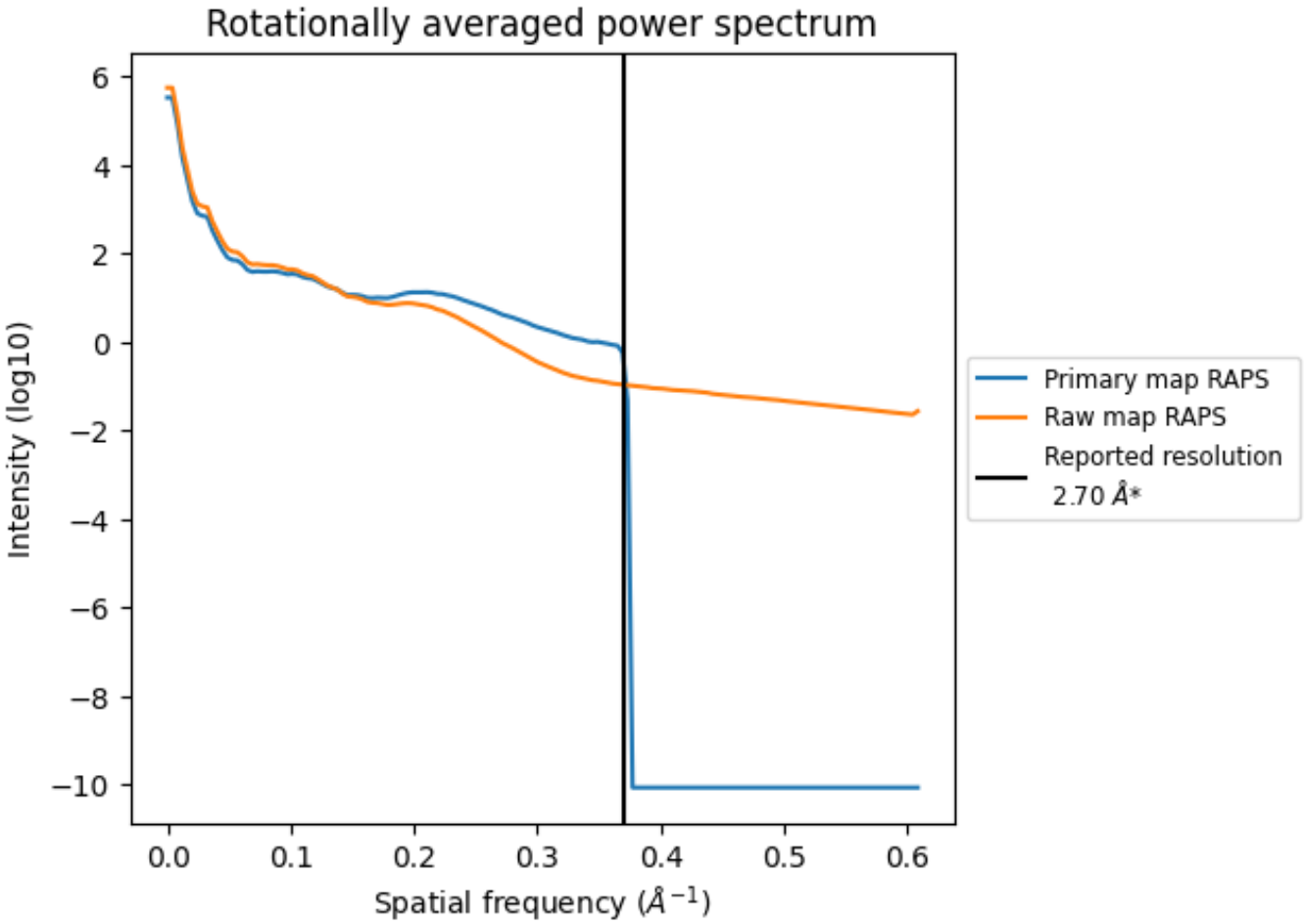
7.2 Volume estimate (i)



The volume at the recommended contour level is 215 nm^3; this corresponds to an approximate mass of 195 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)

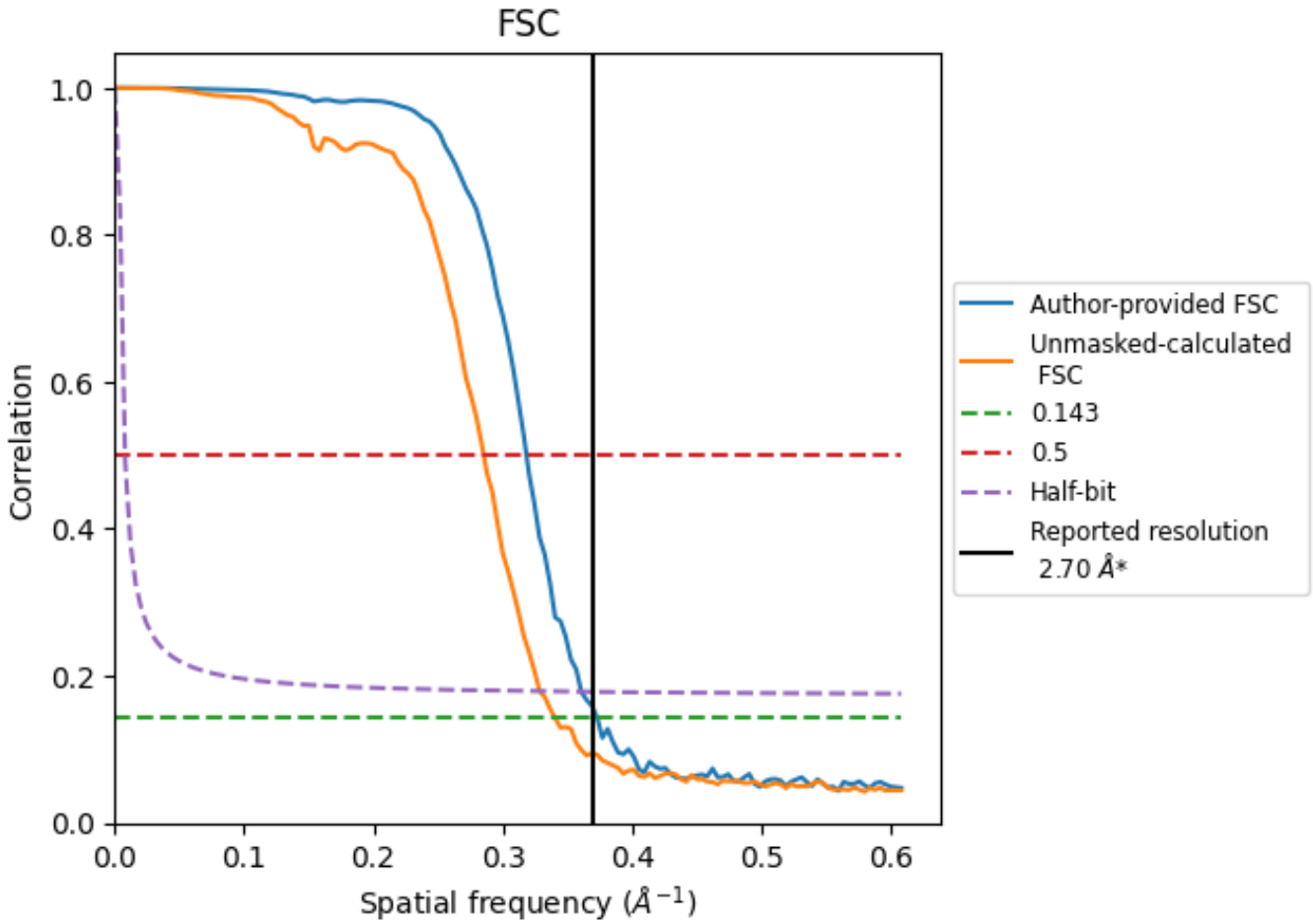


*Reported resolution corresponds to spatial frequency of 0.370 $Å^{-1}$

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 0.370 Å^{-1}

8.2 Resolution estimates (i)

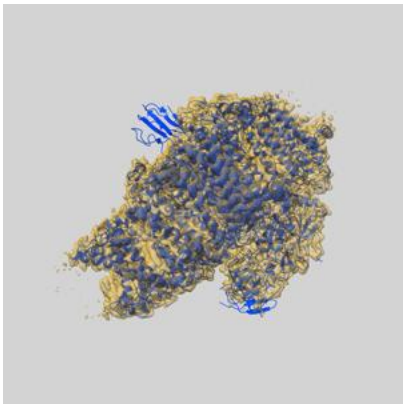
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.70	-	-
Author-provided FSC curve	2.68	3.14	2.77
Unmasked-calculated*	2.94	3.50	3.04

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

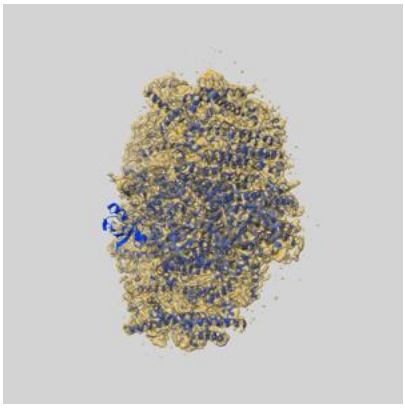
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-10798 and PDB model 6YEZ. Per-residue inclusion information can be found in section 3 on page 31.

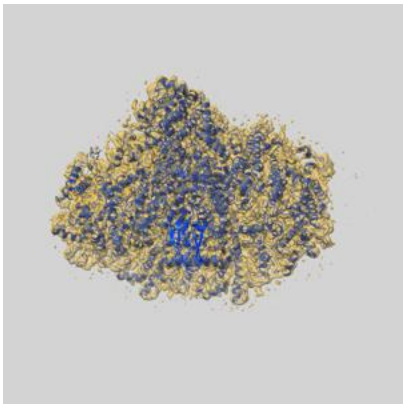
9.1 Map-model overlay



X



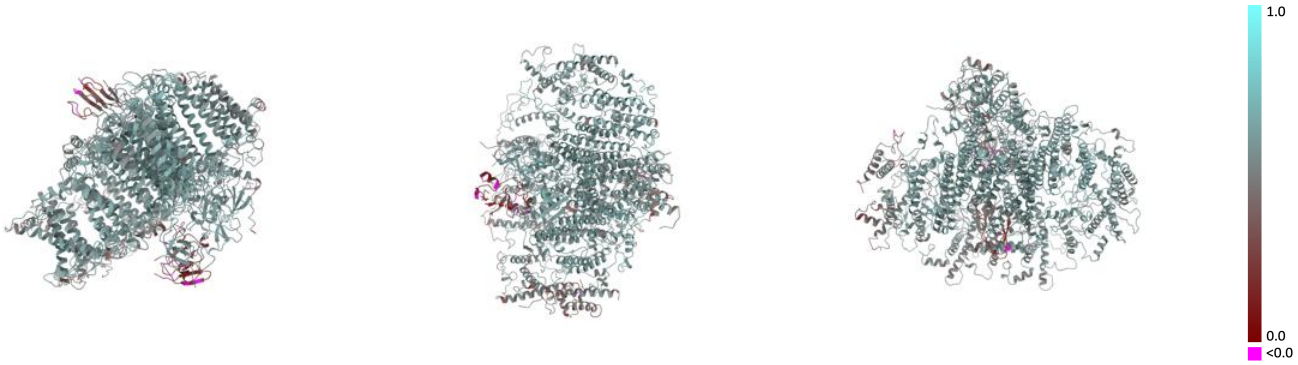
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.022 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.

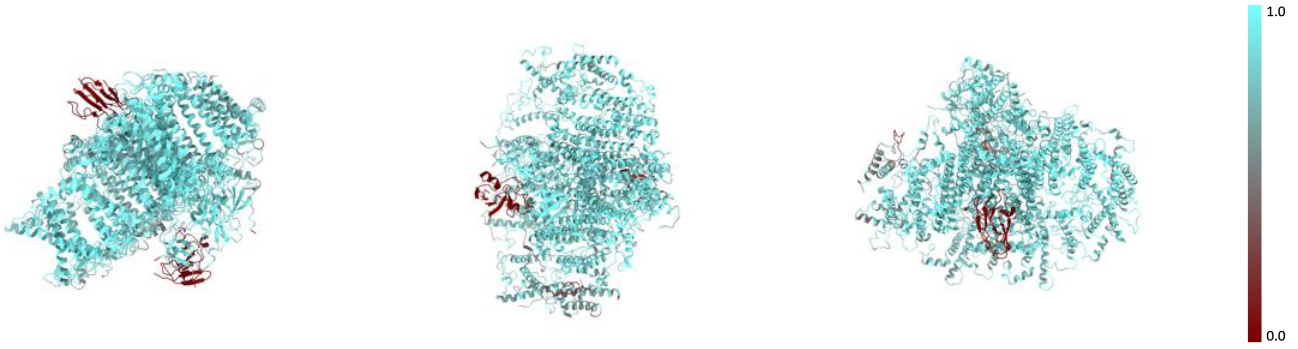
9.2 Q-score mapped to coordinate model (i)



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.

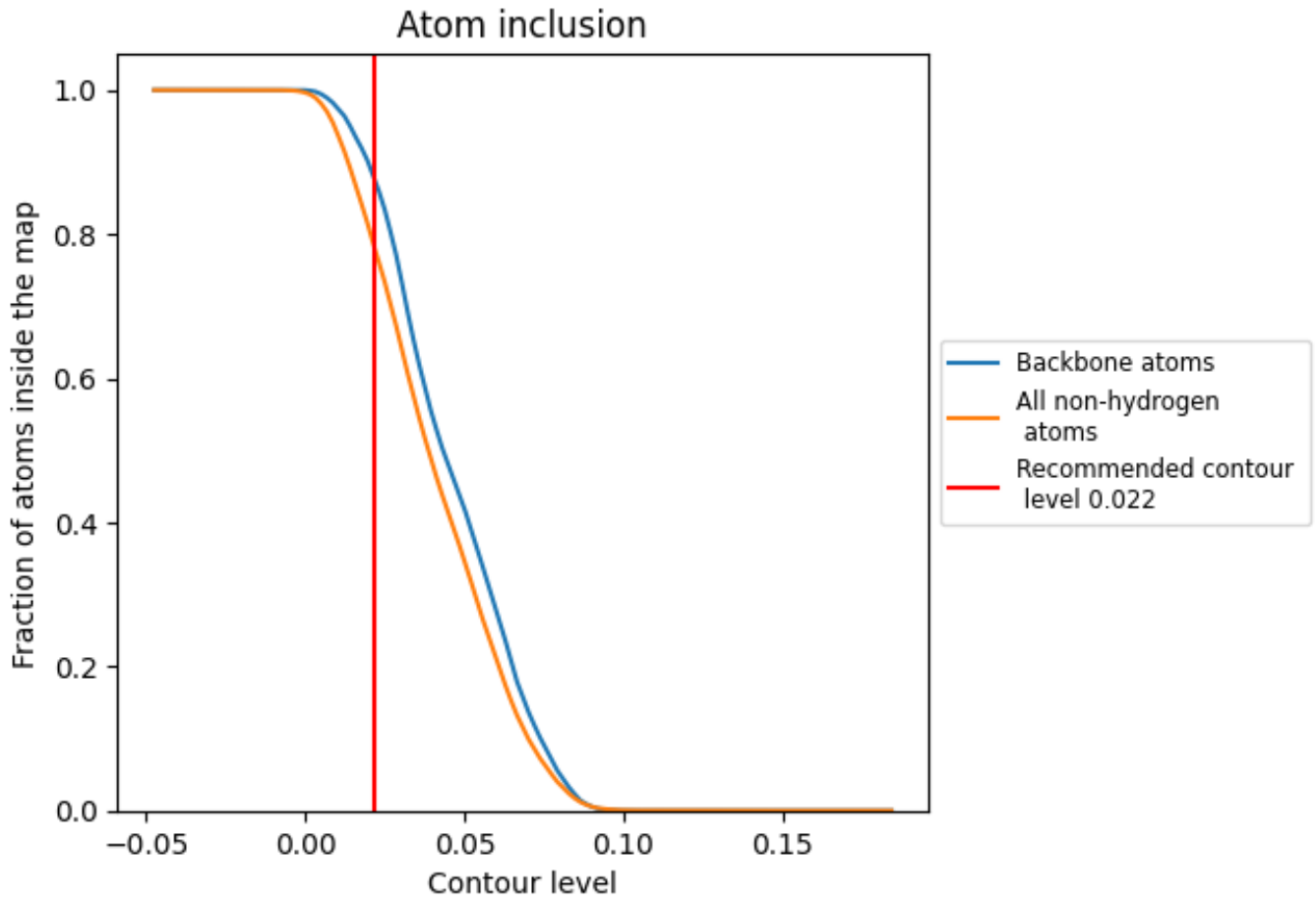
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.022).

9.4 Atom inclusion (i)



At the recommended contour level, 87% of all backbone atoms, 78% 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 (0.022) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7780	0.5360
1	0.7916	0.5340
2	0.7137	0.4750
3	0.7212	0.4840
4	0.7870	0.5180
A	0.8473	0.5710
B	0.8781	0.5920
C	0.9266	0.5930
D	0.8899	0.5660
E	0.8307	0.5480
F	0.7674	0.5400
G	0.7332	0.5090
H	0.7481	0.4990
I	0.7893	0.5460
J	0.7544	0.5320
K	0.4649	0.4130
L	0.8331	0.5480
N	0.0568	0.2140
P	0.0041	0.3360