wwPDB EM Validation Summary Report (i)

Aug 26, 2026 – 04:05 am BST

PDB ID	:	9SK3 / pdb_00009sk3
EMDB ID	:	EMD-54956
Title	:	Trimeric photosystem I of Acaryochloris marina NIES-2412
Authors	:	Leong, H.F.; Consoli, G.
Deposited on	:	2025-09-01
Resolution	:	2.63 Å(reported)

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

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

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

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

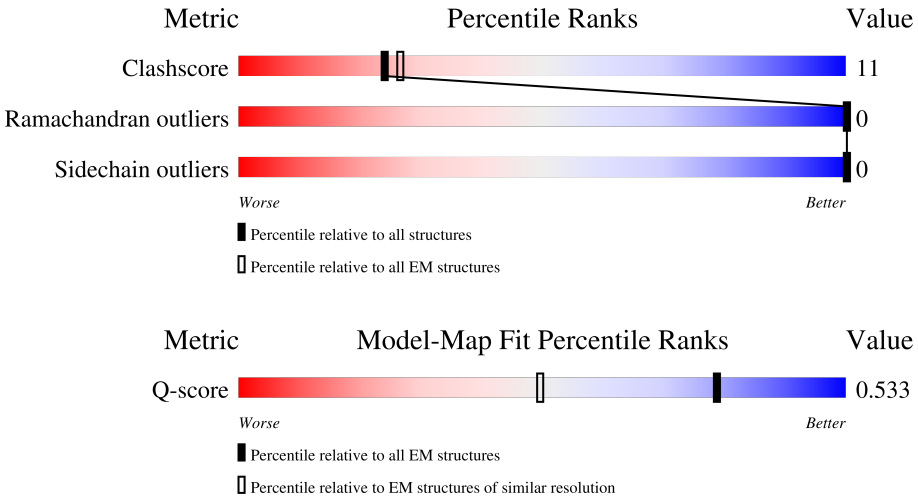
EMDB validation analysis	:	0.0.1.dev133
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4-5-2 with Phenix2.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.50

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 2.63 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	8888 (2.13 - 3.13)

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	aA	753	76% 22% .
1	bA	753	76% 22% .
1	cA	753	75% 23% .
2	aB	733	76% 24%

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Mol	Chain	Length	Quality of chain
2	bB	733	77% 23%
2	cB	733	77% 23%
3	aC	81	77% 22%
3	bC	81	77% 22%
3	cC	81	84% 15%
4	aD	139	71% 27%
4	bD	139	79% 19%
4	cD	139	77% 21%
5	aE	86	70% 8% 22%
5	bE	86	65% 13% 22%
5	cE	86	71% 7% 22%
6	aF	167	74% 11% 14%
6	bF	167	70% 16% 14%
6	cF	167	71% 14% 14%
7	aI	34	79% 18%
7	bI	34	76% 21%
7	cI	34	82% 15%
8	aJ	47	60% 15% 26%
8	bJ	47	68% 6% 26%
8	cJ	47	62% 13% 26%
9	aK	86	42% 21% 37%
9	bK	86	44% 19% 37%
9	cK	86	37% 26% 37%
10	aL	153	81% 16%
10	bL	153	80% 16%

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Mol	Chain	Length	Quality of chain
10	cL	153	82% 14%
11	aM	31	71% 29%
11	bM	31	81% 19%
11	cM	31	84% 16%
12	aX	27	63% 26% 11%
12	bX	27	81% 7% 11%
12	cX	27	70% 19% 11%

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
13	G9R	aA	1011	X	-	-	-
13	G9R	bA	1011	X	-	-	-
13	G9R	cA	1011	X	-	-	-
15	CL7	aA	1022	X	-	-	-
15	CL7	aA	1101	X	-	-	-
15	CL7	aA	1102	X	-	-	-
15	CL7	aA	1103	X	-	-	-
15	CL7	aA	1104	X	-	-	-
15	CL7	aA	1105	X	-	-	-
15	CL7	aA	1106	X	-	-	-
15	CL7	aA	1107	X	-	-	-
15	CL7	aA	1108	X	-	-	-
15	CL7	aA	1109	X	-	-	-
15	CL7	aA	1110	X	-	-	-
15	CL7	aA	1111	X	-	-	-
15	CL7	aA	1112	X	-	-	-
15	CL7	aA	1113	X	-	-	-
15	CL7	aA	1114	X	-	-	-
15	CL7	aA	1115	X	-	-	-
15	CL7	aA	1116	X	-	-	-
15	CL7	aA	1117	X	-	-	-
15	CL7	aA	1118	X	-	-	-
15	CL7	aA	1119	X	-	-	-
15	CL7	aA	1120	X	-	-	-
15	CL7	aA	1121	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
15	CL7	aA	1122	X	-	-	-
15	CL7	aA	1123	X	-	-	-
15	CL7	aA	1124	X	-	-	-
15	CL7	aA	1125	X	-	-	-
15	CL7	aA	1126	X	-	-	-
15	CL7	aA	1127	X	-	-	-
15	CL7	aA	1128	X	-	-	-
15	CL7	aA	1129	X	-	-	-
15	CL7	aA	1130	X	-	-	-
15	CL7	aA	1131	X	-	-	-
15	CL7	aA	1132	X	-	-	-
15	CL7	aA	1133	X	-	-	-
15	CL7	aA	1134	X	-	-	-
15	CL7	aA	1135	X	-	-	-
15	CL7	aA	1136	X	-	-	-
15	CL7	aA	1137	X	-	-	-
15	CL7	aA	1138	X	-	-	-
15	CL7	aA	1139	X	-	-	-
15	CL7	aA	1140	X	-	-	-
15	CL7	aA	1801	X	-	-	-
15	CL7	aB	1012	X	-	-	-
15	CL7	aB	1021	X	-	-	-
15	CL7	aB	1201	X	-	-	-
15	CL7	aB	1202	X	-	-	-
15	CL7	aB	1203	X	-	-	-
15	CL7	aB	1204	X	-	-	-
15	CL7	aB	1205	X	-	-	-
15	CL7	aB	1206	X	-	-	-
15	CL7	aB	1207	X	-	-	-
15	CL7	aB	1208	X	-	-	-
15	CL7	aB	1209	X	-	-	-
15	CL7	aB	1210	X	-	-	-
15	CL7	aB	1211	X	-	-	-
15	CL7	aB	1212	X	-	-	-
15	CL7	aB	1213	X	-	-	-
15	CL7	aB	1214	X	-	-	-
15	CL7	aB	1215	X	-	-	-
15	CL7	aB	1216	X	-	-	-
15	CL7	aB	1217	X	-	-	-
15	CL7	aB	1218	X	-	-	-
15	CL7	aB	1219	X	-	-	-
15	CL7	aB	1220	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
15	CL7	aB	1221	X	-	-	-
15	CL7	aB	1222	X	-	-	-
15	CL7	aB	1223	X	-	-	-
15	CL7	aB	1224	X	-	-	-
15	CL7	aB	1225	X	-	-	-
15	CL7	aB	1226	X	-	-	-
15	CL7	aB	1227	X	-	-	-
15	CL7	aB	1228	X	-	-	-
15	CL7	aB	1229	X	-	-	-
15	CL7	aB	1230	X	-	-	-
15	CL7	aB	1231	X	-	-	-
15	CL7	aB	1232	X	-	-	-
15	CL7	aB	1233	X	-	-	-
15	CL7	aB	1234	X	-	-	-
15	CL7	aB	1235	X	-	-	-
15	CL7	aB	1236	X	-	-	-
15	CL7	aB	1237	X	-	-	-
15	CL7	aB	1238	X	-	-	-
15	CL7	aB	1239	X	-	-	-
15	CL7	aB	1241	X	-	-	-
15	CL7	aF	1701	X	-	-	-
15	CL7	aI	1601	X	-	-	-
15	CL7	aJ	1301	X	-	-	-
15	CL7	aJ	1302	X	-	-	-
15	CL7	aK	1401	X	-	-	-
15	CL7	aK	1402	X	-	-	-
15	CL7	aL	1501	X	-	-	-
15	CL7	aL	1502	X	-	-	-
15	CL7	aL	1503	X	-	-	-
15	CL7	bA	1022	X	-	-	-
15	CL7	bA	1101	X	-	-	-
15	CL7	bA	1102	X	-	-	-
15	CL7	bA	1103	X	-	-	-
15	CL7	bA	1104	X	-	-	-
15	CL7	bA	1105	X	-	-	-
15	CL7	bA	1106	X	-	-	-
15	CL7	bA	1107	X	-	-	-
15	CL7	bA	1108	X	-	-	-
15	CL7	bA	1109	X	-	-	-
15	CL7	bA	1110	X	-	-	-
15	CL7	bA	1111	X	-	-	-
15	CL7	bA	1112	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
15	CL7	bA	1113	X	-	-	-
15	CL7	bA	1114	X	-	-	-
15	CL7	bA	1115	X	-	-	-
15	CL7	bA	1116	X	-	-	-
15	CL7	bA	1117	X	-	-	-
15	CL7	bA	1118	X	-	-	-
15	CL7	bA	1119	X	-	-	-
15	CL7	bA	1120	X	-	-	-
15	CL7	bA	1121	X	-	-	-
15	CL7	bA	1122	X	-	-	-
15	CL7	bA	1123	X	-	-	-
15	CL7	bA	1124	X	-	-	-
15	CL7	bA	1125	X	-	-	-
15	CL7	bA	1126	X	-	-	-
15	CL7	bA	1127	X	-	-	-
15	CL7	bA	1128	X	-	-	-
15	CL7	bA	1129	X	-	-	-
15	CL7	bA	1130	X	-	-	-
15	CL7	bA	1131	X	-	-	-
15	CL7	bA	1132	X	-	-	-
15	CL7	bA	1133	X	-	-	-
15	CL7	bA	1134	X	-	-	-
15	CL7	bA	1135	X	-	-	-
15	CL7	bA	1136	X	-	-	-
15	CL7	bA	1137	X	-	-	-
15	CL7	bA	1138	X	-	-	-
15	CL7	bA	1139	X	-	-	-
15	CL7	bA	1140	X	-	-	-
15	CL7	bA	1801	X	-	-	-
15	CL7	bB	1012	X	-	-	-
15	CL7	bB	1021	X	-	-	-
15	CL7	bB	1201	X	-	-	-
15	CL7	bB	1202	X	-	-	-
15	CL7	bB	1203	X	-	-	-
15	CL7	bB	1204	X	-	-	-
15	CL7	bB	1205	X	-	-	-
15	CL7	bB	1206	X	-	-	-
15	CL7	bB	1207	X	-	-	-
15	CL7	bB	1208	X	-	-	-
15	CL7	bB	1209	X	-	-	-
15	CL7	bB	1210	X	-	-	-
15	CL7	bB	1211	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
15	CL7	bB	1212	X	-	-	-
15	CL7	bB	1213	X	-	-	-
15	CL7	bB	1214	X	-	-	-
15	CL7	bB	1215	X	-	-	-
15	CL7	bB	1216	X	-	-	-
15	CL7	bB	1217	X	-	-	-
15	CL7	bB	1218	X	-	-	-
15	CL7	bB	1219	X	-	-	-
15	CL7	bB	1220	X	-	-	-
15	CL7	bB	1221	X	-	-	-
15	CL7	bB	1222	X	-	-	-
15	CL7	bB	1223	X	-	-	-
15	CL7	bB	1224	X	-	-	-
15	CL7	bB	1225	X	-	-	-
15	CL7	bB	1226	X	-	-	-
15	CL7	bB	1227	X	-	-	-
15	CL7	bB	1228	X	-	-	-
15	CL7	bB	1229	X	-	-	-
15	CL7	bB	1230	X	-	-	-
15	CL7	bB	1231	X	-	-	-
15	CL7	bB	1232	X	-	-	-
15	CL7	bB	1233	X	-	-	-
15	CL7	bB	1234	X	-	-	-
15	CL7	bB	1235	X	-	-	-
15	CL7	bB	1236	X	-	-	-
15	CL7	bB	1237	X	-	-	-
15	CL7	bB	1238	X	-	-	-
15	CL7	bB	1239	X	-	-	-
15	CL7	bB	1241	X	-	-	-
15	CL7	bF	1701	X	-	-	-
15	CL7	bI	1601	X	-	-	-
15	CL7	bJ	1301	X	-	-	-
15	CL7	bJ	1302	X	-	-	-
15	CL7	bK	1401	X	-	-	-
15	CL7	bK	1402	X	-	-	-
15	CL7	bL	1501	X	-	-	-
15	CL7	bL	1502	X	-	-	-
15	CL7	bL	1503	X	-	-	-
15	CL7	cA	1022	X	-	-	-
15	CL7	cA	1101	X	-	-	-
15	CL7	cA	1102	X	-	-	-
15	CL7	cA	1103	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
15	CL7	cA	1104	X	-	-	-
15	CL7	cA	1105	X	-	-	-
15	CL7	cA	1106	X	-	-	-
15	CL7	cA	1107	X	-	-	-
15	CL7	cA	1108	X	-	-	-
15	CL7	cA	1109	X	-	-	-
15	CL7	cA	1110	X	-	-	-
15	CL7	cA	1111	X	-	-	-
15	CL7	cA	1112	X	-	-	-
15	CL7	cA	1113	X	-	-	-
15	CL7	cA	1114	X	-	-	-
15	CL7	cA	1115	X	-	-	-
15	CL7	cA	1116	X	-	-	-
15	CL7	cA	1117	X	-	-	-
15	CL7	cA	1118	X	-	-	-
15	CL7	cA	1119	X	-	-	-
15	CL7	cA	1120	X	-	-	-
15	CL7	cA	1121	X	-	-	-
15	CL7	cA	1122	X	-	-	-
15	CL7	cA	1123	X	-	-	-
15	CL7	cA	1124	X	-	-	-
15	CL7	cA	1125	X	-	-	-
15	CL7	cA	1126	X	-	-	-
15	CL7	cA	1127	X	-	-	-
15	CL7	cA	1128	X	-	-	-
15	CL7	cA	1129	X	-	-	-
15	CL7	cA	1130	X	-	-	-
15	CL7	cA	1131	X	-	-	-
15	CL7	cA	1132	X	-	-	-
15	CL7	cA	1133	X	-	-	-
15	CL7	cA	1134	X	-	-	-
15	CL7	cA	1135	X	-	-	-
15	CL7	cA	1136	X	-	-	-
15	CL7	cA	1137	X	-	-	-
15	CL7	cA	1138	X	-	-	-
15	CL7	cA	1139	X	-	-	-
15	CL7	cA	1140	X	-	-	-
15	CL7	cA	1801	X	-	-	-
15	CL7	cB	1012	X	-	-	-
15	CL7	cB	1021	X	-	-	-
15	CL7	cB	1201	X	-	-	-
15	CL7	cB	1202	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
15	CL7	cB	1203	X	-	-	-
15	CL7	cB	1204	X	-	-	-
15	CL7	cB	1205	X	-	-	-
15	CL7	cB	1206	X	-	-	-
15	CL7	cB	1207	X	-	-	-
15	CL7	cB	1208	X	-	-	-
15	CL7	cB	1209	X	-	-	-
15	CL7	cB	1210	X	-	-	-
15	CL7	cB	1211	X	-	-	-
15	CL7	cB	1212	X	-	-	-
15	CL7	cB	1213	X	-	-	-
15	CL7	cB	1214	X	-	-	-
15	CL7	cB	1215	X	-	-	-
15	CL7	cB	1216	X	-	-	-
15	CL7	cB	1217	X	-	-	-
15	CL7	cB	1218	X	-	-	-
15	CL7	cB	1219	X	-	-	-
15	CL7	cB	1220	X	-	-	-
15	CL7	cB	1221	X	-	-	-
15	CL7	cB	1222	X	-	-	-
15	CL7	cB	1223	X	-	-	-
15	CL7	cB	1224	X	-	-	-
15	CL7	cB	1225	X	-	-	-
15	CL7	cB	1226	X	-	-	-
15	CL7	cB	1227	X	-	-	-
15	CL7	cB	1228	X	-	-	-
15	CL7	cB	1229	X	-	-	-
15	CL7	cB	1230	X	-	-	-
15	CL7	cB	1231	X	-	-	-
15	CL7	cB	1232	X	-	-	-
15	CL7	cB	1233	X	-	-	-
15	CL7	cB	1234	X	-	-	-
15	CL7	cB	1235	X	-	-	-
15	CL7	cB	1236	X	-	-	-
15	CL7	cB	1237	X	-	-	-
15	CL7	cB	1238	X	-	-	-
15	CL7	cB	1239	X	-	-	-
15	CL7	cB	1241	X	-	-	-
15	CL7	cF	1701	X	-	-	-
15	CL7	cI	1601	X	-	-	-
15	CL7	cJ	1301	X	-	-	-
15	CL7	cJ	1302	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
15	CL7	cK	1401	X	-	-	-
15	CL7	cK	1402	X	-	-	-
15	CL7	cL	1501	X	-	-	-
15	CL7	cL	1502	X	-	-	-
15	CL7	cL	1503	X	-	-	-

2 Entry composition (i)

There are 21 unique types of molecules in this entry. The entry contains 70575 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 protein PsaA.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	aA	737	Total	C	N	O	S	0	0
			5797	3785	989	991	32		
1	bA	737	Total	C	N	O	S	0	0
			5797	3785	989	991	32		
1	cA	737	Total	C	N	O	S	0	0
			5797	3785	989	991	32		

- Molecule 2 is a protein called Photosystem I protein PsaB.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	aB	731	Total	C	N	O	S	0	0
			5814	3821	966	1006	21		
2	bB	731	Total	C	N	O	S	0	0
			5814	3821	966	1006	21		
2	cB	731	Total	C	N	O	S	0	0
			5814	3821	966	1006	21		

- Molecule 3 is a protein called Photosystem I protein PsaC.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	aC	80	Total	C	N	O	S	0	0
			599	367	103	118	11		
3	bC	80	Total	C	N	O	S	0	0
			599	367	103	118	11		
3	cC	80	Total	C	N	O	S	0	0
			599	367	103	118	11		

- Molecule 4 is a protein called Photosystem I protein PsaD.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	aD	136	Total	C	N	O	S	0	0
			1039	653	180	202	4		

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Mol	Chain	Residues	Atoms					AltConf	Trace
4	bD	136	Total	C	N	O	S	0	0
			1039	653	180	202	4		
4	cD	136	Total	C	N	O	S	0	0
			1039	653	180	202	4		

- Molecule 5 is a protein called Photosystem I protein PsaE.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	aE	67	Total	C	N	O	S	0	0
			526	332	94	99	1		
5	bE	67	Total	C	N	O	S	0	0
			526	332	94	99	1		
5	cE	67	Total	C	N	O	S	0	0
			526	332	94	99	1		

- Molecule 6 is a protein called Photosystem I protein PsaF.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	aF	143	Total	C	N	O	S	0	0
			1056	666	185	201	4		
6	bF	143	Total	C	N	O	S	0	0
			1056	666	185	201	4		
6	cF	143	Total	C	N	O	S	0	0
			1056	666	185	201	4		

- Molecule 7 is a protein called Photosystem I protein PsaI.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	aI	33	Total	C	N	O	S	0	0
			250	167	36	44	3		
7	bI	33	Total	C	N	O	S	0	0
			250	167	36	44	3		
7	cI	33	Total	C	N	O	S	0	0
			250	167	36	44	3		

- Molecule 8 is a protein called Photosystem I protein PsaJ.

Mol	Chain	Residues	Atoms				AltConf	Trace
8	aJ	35	Total	C	N	O	0	0
			291	207	40	44		
8	bJ	35	Total	C	N	O	0	0
			291	207	40	44		

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Mol	Chain	Residues	Atoms				AltConf	Trace
8	cJ	35	Total 291	C 207	N 40	O 44	0	0

- Molecule 9 is a protein called Photosystem I protein PsaK.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	aK	54	Total 397	C 264	N 63	O 68	S 2	0	0
9	bK	54	Total 397	C 264	N 63	O 68	S 2	0	0
9	cK	54	Total 397	C 264	N 63	O 68	S 2	0	0

- Molecule 10 is a protein called Photosystem I protein PsaL.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	aL	148	Total 1059	C 680	N 176	O 196	S 7	0	0
10	bL	148	Total 1059	C 680	N 176	O 196	S 7	0	0
10	cL	148	Total 1059	C 680	N 176	O 196	S 7	0	0

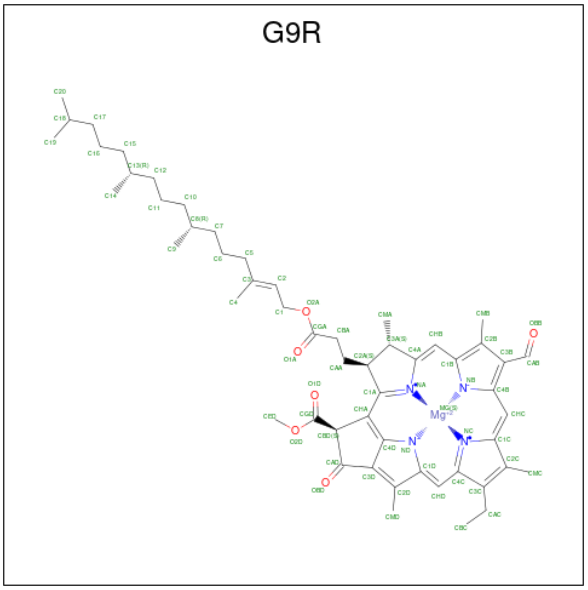
- Molecule 11 is a protein called Photosystem I protein PsaM.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	aM	31	Total 223	C 148	N 34	O 40	S 1	0	0
11	bM	31	Total 223	C 148	N 34	O 40	S 1	0	0
11	cM	31	Total 223	C 148	N 34	O 40	S 1	0	0

- Molecule 12 is a protein called Photosystem I protein PsaX2.

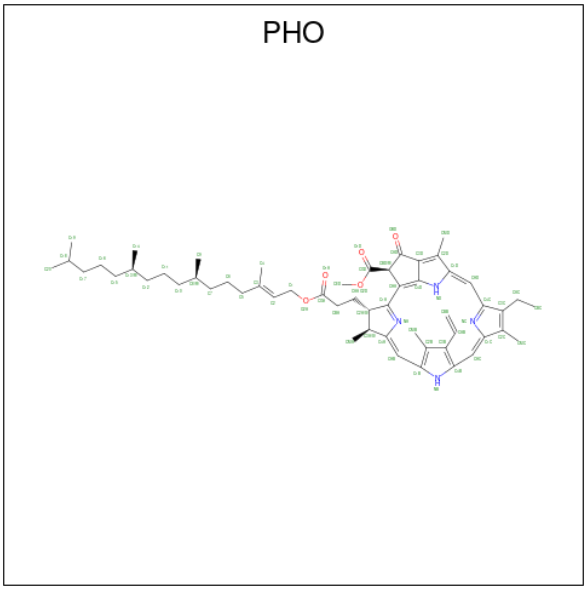
Mol	Chain	Residues	Atoms				AltConf	Trace
12	aX	24	Total 187	C 131	N 28	O 28	0	0
12	bX	24	Total 187	C 131	N 28	O 28	0	0
12	cX	24	Total 187	C 131	N 28	O 28	0	0

- Molecule 13 is CHLOROPHYLL D ISOMER (CCD ID: G9R) (formula: $C_{54}H_{70}MgN_4O_6$).



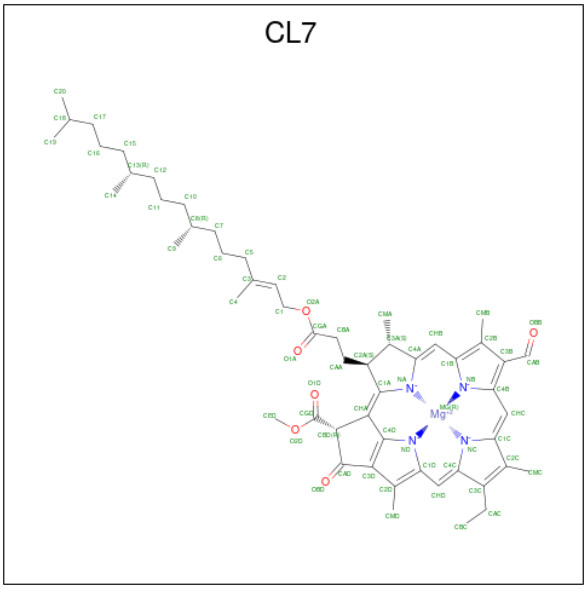
Mol	Chain	Residues	Atoms					AltConf
13	aA	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
13	bA	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
13	cA	1	Total	C	Mg	N	O	0
			65	54	1	4	6	

- Molecule 14 is PHEOPHYTIN A (CCD ID: PHO) (formula: $C_{55}H_{74}N_4O_5$).



Mol	Chain	Residues	Atoms				AltConf
14	aA	1	Total	C	N	O	0
			64	55	4	5	
14	aB	1	Total	C	N	O	0
			64	55	4	5	
14	bA	1	Total	C	N	O	0
			64	55	4	5	
14	bB	1	Total	C	N	O	0
			64	55	4	5	
14	cA	1	Total	C	N	O	0
			64	55	4	5	
14	cB	1	Total	C	N	O	0
			64	55	4	5	

- Molecule 15 is CHLOROPHYLL D (CCD ID: CL7) (formula: $C_{54}H_{70}MgN_4O_6$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
15	aA	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
15	aA	1	Total	C	Mg	N	O	0
			41	32	1	4	4	
15	aA	1	Total	C	Mg	N	O	0
			52	41	1	4	6	
15	aA	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
15	aA	1	Total	C	Mg	N	O	0
			65	54	1	4	6	

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Mol	Chain	Residues	Atoms					AltConf
15	aA	1	Total	C	Mg	N	O	0
			45	34	1	4	6	
15	aA	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
15	aA	1	Total	C	Mg	N	O	0
			45	34	1	4	6	
15	aA	1	Total	C	Mg	N	O	0
			51	40	1	4	6	
15	aA	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
15	aA	1	Total	C	Mg	N	O	0
			45	34	1	4	6	
15	aA	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
15	aA	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
15	aA	1	Total	C	Mg	N	O	0
			45	34	1	4	6	
15	aA	1	Total	C	Mg	N	O	0
			45	34	1	4	6	
15	aA	1	Total	C	Mg	N	O	0
			41	32	1	4	4	
15	aA	1	Total	C	Mg	N	O	0
			60	49	1	4	6	
15	aA	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
15	aA	1	Total	C	Mg	N	O	0
			55	44	1	4	6	
15	aA	1	Total	C	Mg	N	O	0
			55	44	1	4	6	
15	aA	1	Total	C	Mg	N	O	0
			45	34	1	4	6	
15	aA	1	Total	C	Mg	N	O	0
			55	44	1	4	6	
15	aA	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
15	aA	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
15	aA	1	Total	C	Mg	N	O	0
			50	39	1	4	6	
15	aA	1	Total	C	Mg	N	O	0
			50	39	1	4	6	

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Mol	Chain	Residues	Atoms					AltConf
15	aA	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
15	aA	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
15	aA	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
15	aA	1	Total	C	Mg	N	O	0
			50	39	1	4	6	
15	aA	1	Total	C	Mg	N	O	0
			51	40	1	4	6	
15	aA	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
15	aA	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
15	aA	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
15	aA	1	Total	C	Mg	N	O	0
			44	33	1	4	6	
15	aA	1	Total	C	Mg	N	O	0
			50	39	1	4	6	
15	aA	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
15	aA	1	Total	C	Mg	N	O	0
			55	44	1	4	6	
15	aA	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
15	aA	1	Total	C	Mg	N	O	0
			60	49	1	4	6	
15	aA	1	Total	C	Mg	N	O	0
			41	32	1	4	4	
15	aA	1	Total	C	Mg	N	O	0
			45	34	1	4	6	
15	aB	1	Total	C	Mg	N	O	0
			41	32	1	4	4	
15	aB	1	Total	C	Mg	N	O	0
			41	32	1	4	4	
15	aB	1	Total	C	Mg	N	O	0
			50	39	1	4	6	
15	aB	1	Total	C	Mg	N	O	0
			60	49	1	4	6	
15	aB	1	Total	C	Mg	N	O	0
			45	34	1	4	6	

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Mol	Chain	Residues	Atoms					AltConf
15	aB	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
15	aB	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
15	aB	1	Total	C	Mg	N	O	0
			45	34	1	4	6	
15	aB	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
15	aB	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
15	aB	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
15	aB	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
15	aB	1	Total	C	Mg	N	O	0
			54	43	1	4	6	
15	aB	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
15	aB	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
15	aB	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
15	aB	1	Total	C	Mg	N	O	0
			50	39	1	4	6	
15	aB	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
15	aB	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
15	aB	1	Total	C	Mg	N	O	0
			45	34	1	4	6	
15	aB	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
15	aB	1	Total	C	Mg	N	O	0
			55	44	1	4	6	
15	aB	1	Total	C	Mg	N	O	0
			45	34	1	4	6	
15	aB	1	Total	C	Mg	N	O	0
			45	34	1	4	6	
15	aB	1	Total	C	Mg	N	O	0
			50	39	1	4	6	
15	aB	1	Total	C	Mg	N	O	0
			55	44	1	4	6	

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Mol	Chain	Residues	Atoms					AltConf
15	aB	1	Total	C	Mg	N	O	0
			45	34	1	4	6	
15	aB	1	Total	C	Mg	N	O	0
			41	32	1	4	4	
15	aB	1	Total	C	Mg	N	O	0
			41	32	1	4	4	
15	aB	1	Total	C	Mg	N	O	0
			41	32	1	4	4	
15	aB	1	Total	C	Mg	N	O	0
			45	34	1	4	6	
15	aB	1	Total	C	Mg	N	O	0
			60	49	1	4	6	
15	aB	1	Total	C	Mg	N	O	0
			45	34	1	4	6	
15	aB	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
15	aB	1	Total	C	Mg	N	O	0
			56	45	1	4	6	
15	aB	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
15	aB	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
15	aB	1	Total	C	Mg	N	O	0
			45	34	1	4	6	
15	aB	1	Total	C	Mg	N	O	0
			45	34	1	4	6	
15	aB	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
15	aB	1	Total	C	Mg	N	O	0
			41	32	1	4	4	
15	aB	1	Total	C	Mg	N	O	0
			45	34	1	4	6	
15	aF	1	Total	C	Mg	N	O	0
			41	32	1	4	4	
15	aI	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
15	aJ	1	Total	C	Mg	N	O	0
			41	32	1	4	4	
15	aJ	1	Total	C	Mg	N	O	0
			42	33	1	4	4	
15	aK	1	Total	C	Mg	N	O	0
			45	34	1	4	6	

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Mol	Chain	Residues	Atoms					AltConf
15	aK	1	Total	C	Mg	N	O	0
			37	30	1	4	2	
15	aL	1	Total	C	Mg	N	O	0
			60	49	1	4	6	
15	aL	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
15	aL	1	Total	C	Mg	N	O	0
			60	49	1	4	6	
15	bA	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
15	bA	1	Total	C	Mg	N	O	0
			41	32	1	4	4	
15	bA	1	Total	C	Mg	N	O	0
			52	41	1	4	6	
15	bA	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
15	bA	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
15	bA	1	Total	C	Mg	N	O	0
			45	34	1	4	6	
15	bA	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
15	bA	1	Total	C	Mg	N	O	0
			45	34	1	4	6	
15	bA	1	Total	C	Mg	N	O	0
			51	40	1	4	6	
15	bA	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
15	bA	1	Total	C	Mg	N	O	0
			45	34	1	4	6	
15	bA	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
15	bA	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
15	bA	1	Total	C	Mg	N	O	0
			45	34	1	4	6	
15	bA	1	Total	C	Mg	N	O	0
			45	34	1	4	6	
15	bA	1	Total	C	Mg	N	O	0
			41	32	1	4	4	
15	bA	1	Total	C	Mg	N	O	0
			60	49	1	4	6	

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Mol	Chain	Residues	Atoms					AltConf
15	bA	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
15	bA	1	Total	C	Mg	N	O	0
			55	44	1	4	6	
15	bA	1	Total	C	Mg	N	O	0
			55	44	1	4	6	
15	bA	1	Total	C	Mg	N	O	0
			45	34	1	4	6	
15	bA	1	Total	C	Mg	N	O	0
			55	44	1	4	6	
15	bA	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
15	bA	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
15	bA	1	Total	C	Mg	N	O	0
			50	39	1	4	6	
15	bA	1	Total	C	Mg	N	O	0
			50	39	1	4	6	
15	bA	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
15	bA	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
15	bA	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
15	bA	1	Total	C	Mg	N	O	0
			50	39	1	4	6	
15	bA	1	Total	C	Mg	N	O	0
			51	40	1	4	6	
15	bA	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
15	bA	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
15	bA	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
15	bA	1	Total	C	Mg	N	O	0
			44	33	1	4	6	
15	bA	1	Total	C	Mg	N	O	0
			50	39	1	4	6	
15	bA	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
15	bA	1	Total	C	Mg	N	O	0
			55	44	1	4	6	

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

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

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Mol	Chain	Residues	Atoms					AltConf
15	bB	1	Total	C	Mg	N	O	0
			45	34	1	4	6	
15	bB	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
15	bB	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
15	bB	1	Total	C	Mg	N	O	0
			45	34	1	4	6	
15	bF	1	Total	C	Mg	N	O	0
			41	32	1	4	4	
15	bI	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
15	bJ	1	Total	C	Mg	N	O	0
			41	32	1	4	4	
15	bJ	1	Total	C	Mg	N	O	0
			42	33	1	4	4	
15	bK	1	Total	C	Mg	N	O	0
			45	34	1	4	6	
15	bK	1	Total	C	Mg	N	O	0
			37	30	1	4	2	
15	bL	1	Total	C	Mg	N	O	0
			60	49	1	4	6	
15	bL	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
15	bL	1	Total	C	Mg	N	O	0
			60	49	1	4	6	
15	cA	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
15	cA	1	Total	C	Mg	N	O	0
			41	32	1	4	4	
15	cA	1	Total	C	Mg	N	O	0
			52	41	1	4	6	
15	cA	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
15	cA	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
15	cA	1	Total	C	Mg	N	O	0
			45	34	1	4	6	
15	cA	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
15	cA	1	Total	C	Mg	N	O	0
			45	34	1	4	6	

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Mol	Chain	Residues	Atoms					AltConf
15	cA	1	Total	C	Mg	N	O	0
			51	40	1	4	6	
15	cA	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
15	cA	1	Total	C	Mg	N	O	0
			45	34	1	4	6	
15	cA	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
15	cA	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
15	cA	1	Total	C	Mg	N	O	0
			45	34	1	4	6	
15	cA	1	Total	C	Mg	N	O	0
			45	34	1	4	6	
15	cA	1	Total	C	Mg	N	O	0
			41	32	1	4	4	
15	cA	1	Total	C	Mg	N	O	0
			60	49	1	4	6	
15	cA	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
15	cA	1	Total	C	Mg	N	O	0
			55	44	1	4	6	
15	cA	1	Total	C	Mg	N	O	0
			55	44	1	4	6	
15	cA	1	Total	C	Mg	N	O	0
			45	34	1	4	6	
15	cA	1	Total	C	Mg	N	O	0
			55	44	1	4	6	
15	cA	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
15	cA	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
15	cA	1	Total	C	Mg	N	O	0
			50	39	1	4	6	
15	cA	1	Total	C	Mg	N	O	0
			50	39	1	4	6	
15	cA	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
15	cA	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
15	cA	1	Total	C	Mg	N	O	0
			65	54	1	4	6	

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Mol	Chain	Residues	Atoms					AltConf
15	cA	1	Total	C	Mg	N	O	0
			50	39	1	4	6	
15	cA	1	Total	C	Mg	N	O	0
			51	40	1	4	6	
15	cA	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
15	cA	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
15	cA	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
15	cA	1	Total	C	Mg	N	O	0
			44	33	1	4	6	
15	cA	1	Total	C	Mg	N	O	0
			50	39	1	4	6	
15	cA	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
15	cA	1	Total	C	Mg	N	O	0
			55	44	1	4	6	
15	cA	1	Total	C	Mg	N	O	0
			60	49	1	4	6	
15	cA	1	Total	C	Mg	N	O	0
			41	32	1	4	4	
15	cA	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
15	cA	1	Total	C	Mg	N	O	0
			45	34	1	4	6	
15	cB	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
15	cB	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
15	cB	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
15	cB	1	Total	C	Mg	N	O	0
			54	43	1	4	6	
15	cB	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
15	cB	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
15	cB	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
15	cB	1	Total	C	Mg	N	O	0
			65	54	1	4	6	

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

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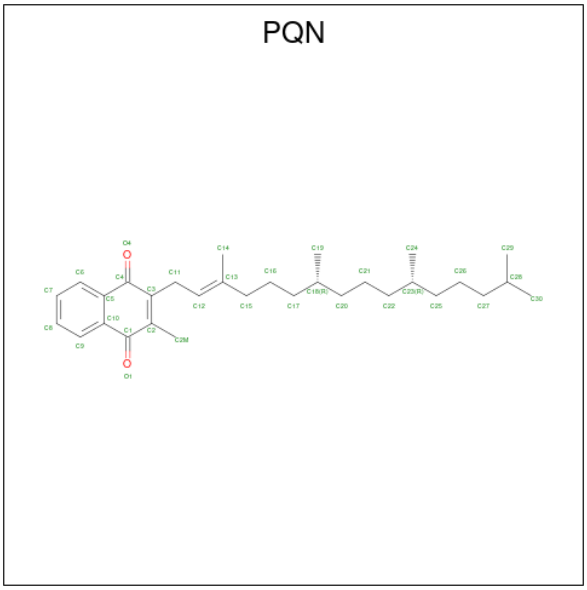
Mol	Chain	Residues	Atoms					AltConf
15	cB	1	Total	C	Mg	N	O	0
			45	34	1	4	6	
15	cB	1	Total	C	Mg	N	O	0
			45	34	1	4	6	
15	cB	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
15	cB	1	Total	C	Mg	N	O	0
			41	32	1	4	4	
15	cB	1	Total	C	Mg	N	O	0
			45	34	1	4	6	
15	cB	1	Total	C	Mg	N	O	0
			41	32	1	4	4	
15	cB	1	Total	C	Mg	N	O	0
			41	32	1	4	4	
15	cB	1	Total	C	Mg	N	O	0
			50	39	1	4	6	
15	cB	1	Total	C	Mg	N	O	0
			60	49	1	4	6	
15	cB	1	Total	C	Mg	N	O	0
			45	34	1	4	6	
15	cB	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
15	cB	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
15	cB	1	Total	C	Mg	N	O	0
			45	34	1	4	6	
15	cF	1	Total	C	Mg	N	O	0
			41	32	1	4	4	
15	cI	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
15	cJ	1	Total	C	Mg	N	O	0
			41	32	1	4	4	
15	cJ	1	Total	C	Mg	N	O	0
			42	33	1	4	4	
15	cK	1	Total	C	Mg	N	O	0
			45	34	1	4	6	
15	cK	1	Total	C	Mg	N	O	0
			37	30	1	4	2	
15	cL	1	Total	C	Mg	N	O	0
			60	49	1	4	6	
15	cL	1	Total	C	Mg	N	O	0
			65	54	1	4	6	

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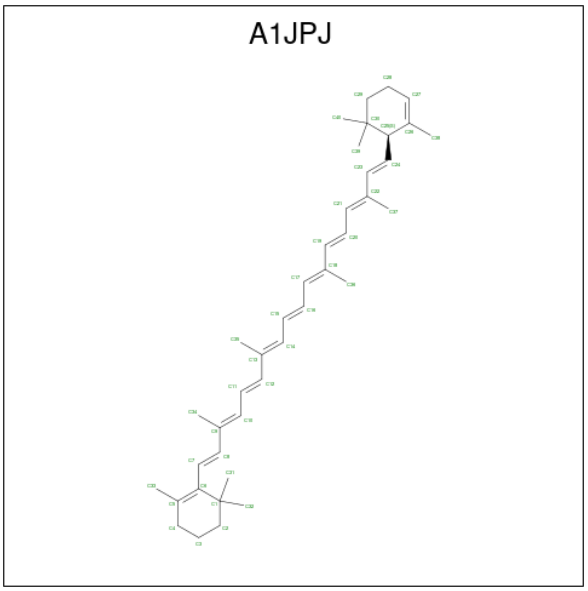
Mol	Chain	Residues	Atoms					AltConf
15	cL	1	Total	C	Mg	N	O	0
			60	49	1	4	6	

- Molecule 16 is PHYLLOQUINONE (CCD ID: PQN) (formula: $C_{31}H_{46}O_2$).



Mol	Chain	Residues	Atoms			AltConf
16	aA	1	Total	C	O	0
			33	31	2	
16	aB	1	Total	C	O	0
			33	31	2	
16	bA	1	Total	C	O	0
			33	31	2	
16	bB	1	Total	C	O	0
			33	31	2	
16	cA	1	Total	C	O	0
			33	31	2	
16	cB	1	Total	C	O	0
			33	31	2	

- Molecule 17 is (6'S)-beta,epsilon-carotene (CCD ID: A1JPJ) (formula: $C_{40}H_{56}$).



Mol	Chain	Residues	Atoms	AltConf
17	aA	1	Total C 40 40	0
17	aA	1	Total C 40 40	0
17	aA	1	Total C 40 40	0
17	aA	1	Total C 40 40	0
17	aA	1	Total C 40 40	0
17	aA	1	Total C 40 40	0
17	aB	1	Total C 40 40	0
17	aB	1	Total C 40 40	0
17	aB	1	Total C 40 40	0
17	aB	1	Total C 40 40	0
17	aB	1	Total C 40 40	0
17	aB	1	Total C 40 40	0
17	aB	1	Total C 40 40	0
17	aF	1	Total C 40 40	0

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Mol	Chain	Residues	Atoms	AltConf
17	aI	1	Total C 40 40	0
17	aI	1	Total C 40 40	0
17	aJ	1	Total C 40 40	0
17	aL	1	Total C 40 40	0
17	aL	1	Total C 40 40	0
17	bA	1	Total C 40 40	0
17	bA	1	Total C 40 40	0
17	bA	1	Total C 40 40	0
17	bA	1	Total C 40 40	0
17	bA	1	Total C 40 40	0
17	bA	1	Total C 40 40	0
17	bB	1	Total C 40 40	0
17	bB	1	Total C 40 40	0
17	bB	1	Total C 40 40	0
17	bB	1	Total C 40 40	0
17	bB	1	Total C 40 40	0
17	bB	1	Total C 40 40	0
17	bB	1	Total C 40 40	0
17	bF	1	Total C 40 40	0
17	bI	1	Total C 40 40	0
17	bI	1	Total C 40 40	0

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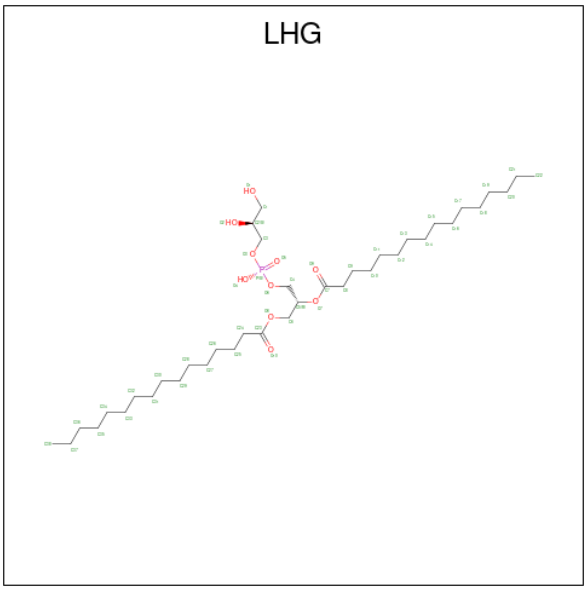
Mol	Chain	Residues	Atoms	AltConf
17	bJ	1	Total C 40 40	0
17	bL	1	Total C 40 40	0
17	bL	1	Total C 40 40	0
17	cA	1	Total C 40 40	0
17	cA	1	Total C 40 40	0
17	cA	1	Total C 40 40	0
17	cA	1	Total C 40 40	0
17	cA	1	Total C 40 40	0
17	cA	1	Total C 40 40	0
17	cB	1	Total C 40 40	0
17	cB	1	Total C 40 40	0
17	cB	1	Total C 40 40	0
17	cB	1	Total C 40 40	0
17	cB	1	Total C 40 40	0
17	cB	1	Total C 40 40	0
17	cB	1	Total C 40 40	0
17	cF	1	Total C 40 40	0
17	cI	1	Total C 40 40	0
17	cI	1	Total C 40 40	0
17	cJ	1	Total C 40 40	0
17	cL	1	Total C 40 40	0

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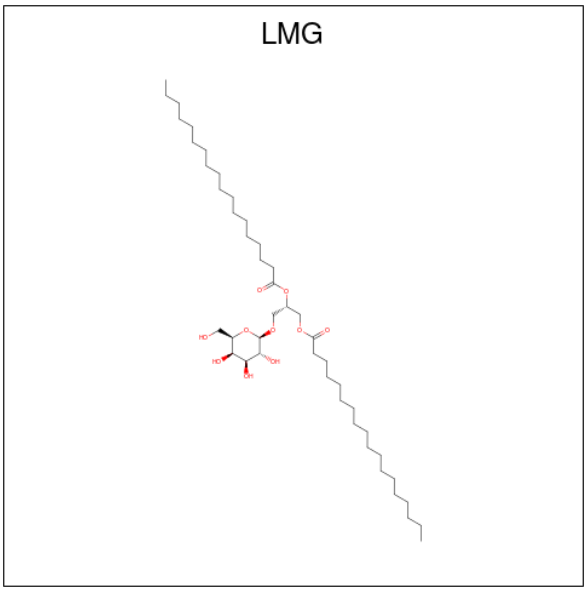
Mol	Chain	Residues	Atoms	AltConf
17	cL	1	Total C 40 40	0

- Molecule 18 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (CCD ID: LHG) (formula: $C_{38}H_{75}O_{10}P$).



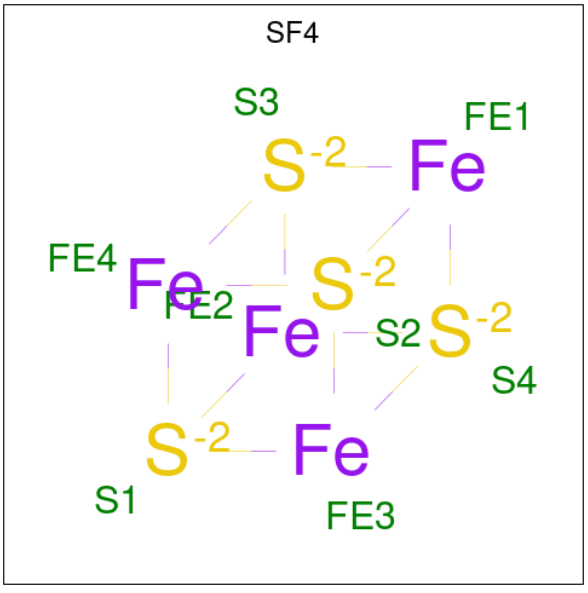
Mol	Chain	Residues	Atoms	AltConf
18	aA	1	Total C O P 49 38 10 1	0
18	aA	1	Total C O P 38 27 10 1	0
18	bA	1	Total C O P 49 38 10 1	0
18	bA	1	Total C O P 38 27 10 1	0
18	cA	1	Total C O P 49 38 10 1	0
18	cA	1	Total C O P 38 27 10 1	0

- Molecule 19 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (CCD ID: LMG) (formula: $C_{45}H_{86}O_{10}$).



Mol	Chain	Residues	Atoms			AltConf
19	aB	1	Total	C	O	0
			53	43	10	
19	bB	1	Total	C	O	0
			53	43	10	
19	cB	1	Total	C	O	0
			53	43	10	

- Molecule 20 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe_4S_4).



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

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Mol	Chain	Residues	Atoms	AltConf
20	aC	1	Total Fe S 8 4 4	0
20	aC	1	Total Fe S 8 4 4	0
20	bB	1	Total Fe S 8 4 4	0
20	bC	1	Total Fe S 8 4 4	0
20	bC	1	Total Fe S 8 4 4	0
20	cB	1	Total Fe S 8 4 4	0
20	cC	1	Total Fe S 8 4 4	0
20	cC	1	Total Fe S 8 4 4	0

- Molecule 21 is water.

Mol	Chain	Residues	Atoms	AltConf
21	aA	21	Total O 21 21	0
21	aB	6	Total O 6 6	0
21	aI	1	Total O 1 1	0
21	aJ	1	Total O 1 1	0
21	aL	2	Total O 2 2	0
21	bA	21	Total O 21 21	0
21	bB	6	Total O 6 6	0
21	bI	1	Total O 1 1	0
21	bJ	1	Total O 1 1	0
21	bL	2	Total O 2 2	0
21	cA	21	Total O 21 21	0

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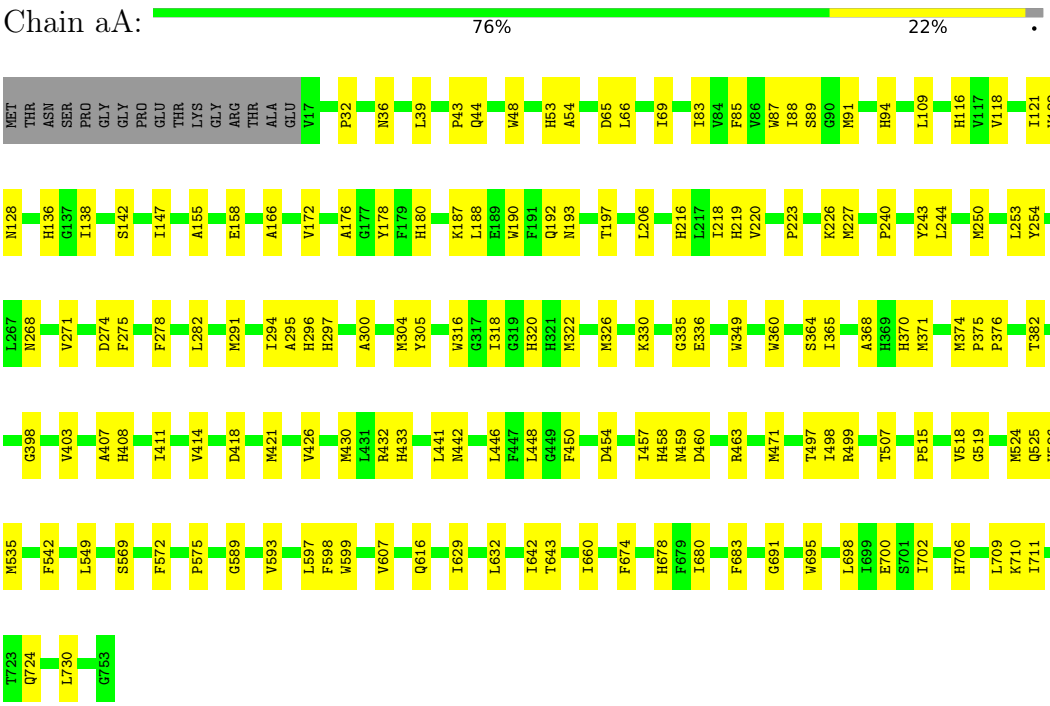
Mol	Chain	Residues	Atoms	AltConf
21	cB	6	Total O 6 6	0
21	cI	1	Total O 1 1	0
21	cJ	1	Total O 1 1	0
21	cL	2	Total O 2 2	0

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.

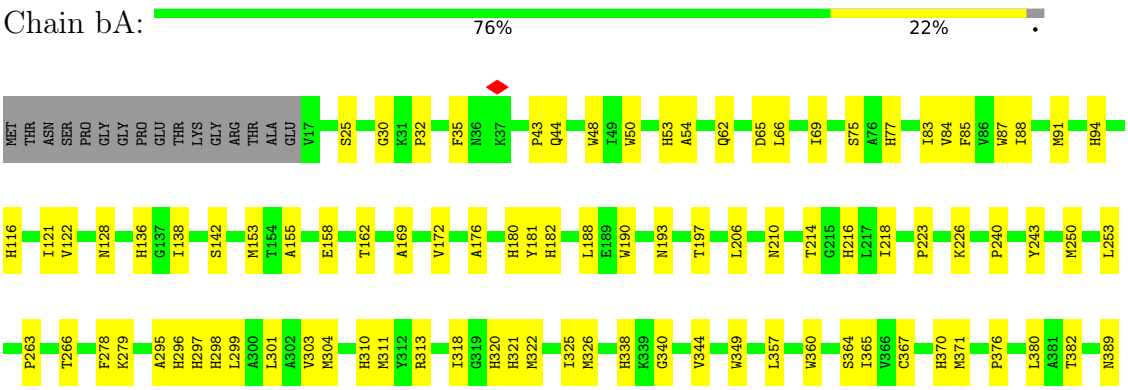
• Molecule 1: Photosystem I protein PsaA

Chain aA:



• Molecule 1: Photosystem I protein PsaA

Chain bA:

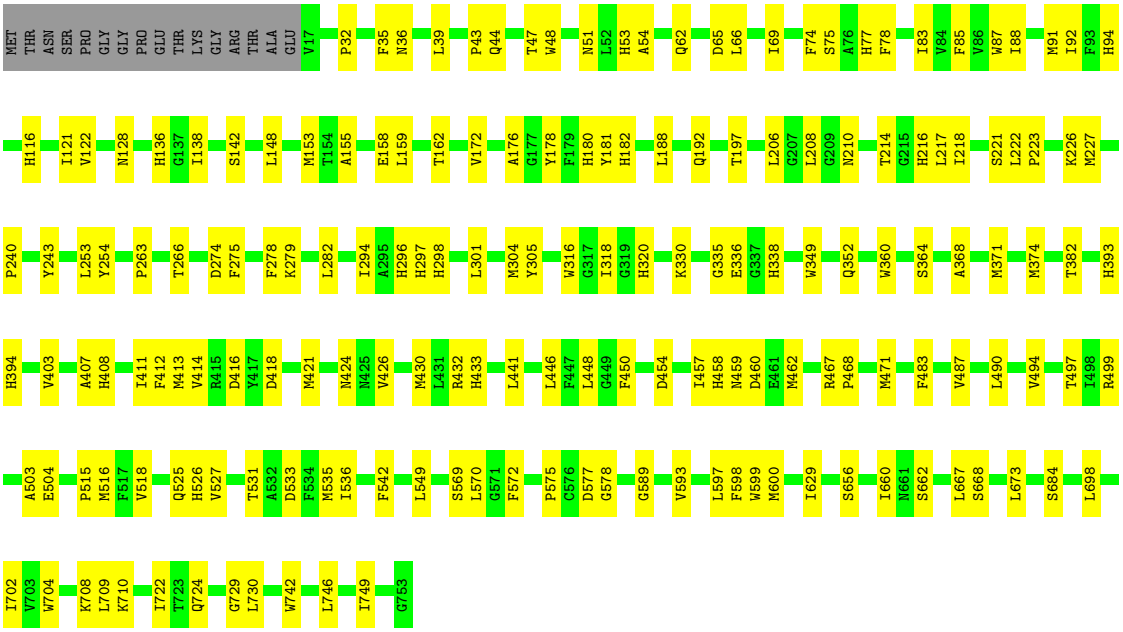




• Molecule 1: Photosystem I protein PsaA

Chain cA:

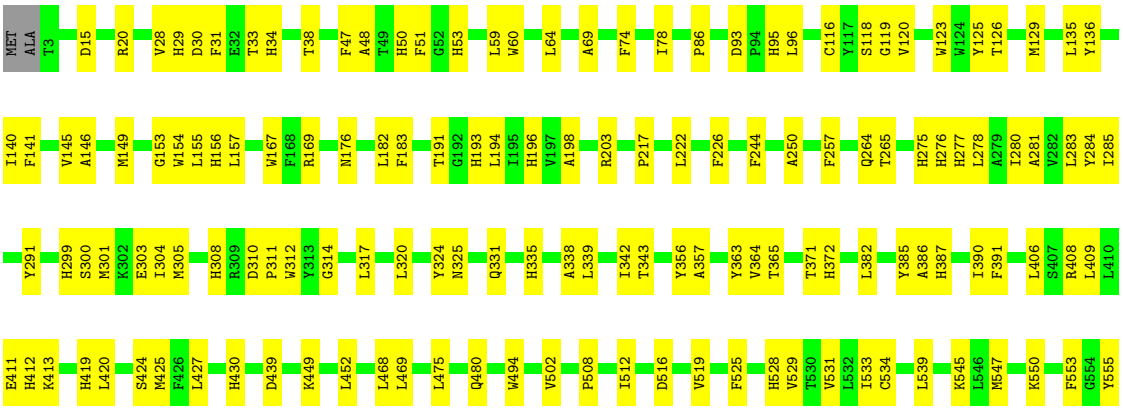




• Molecule 2: Photosystem I protein PsaB

Chain aB:



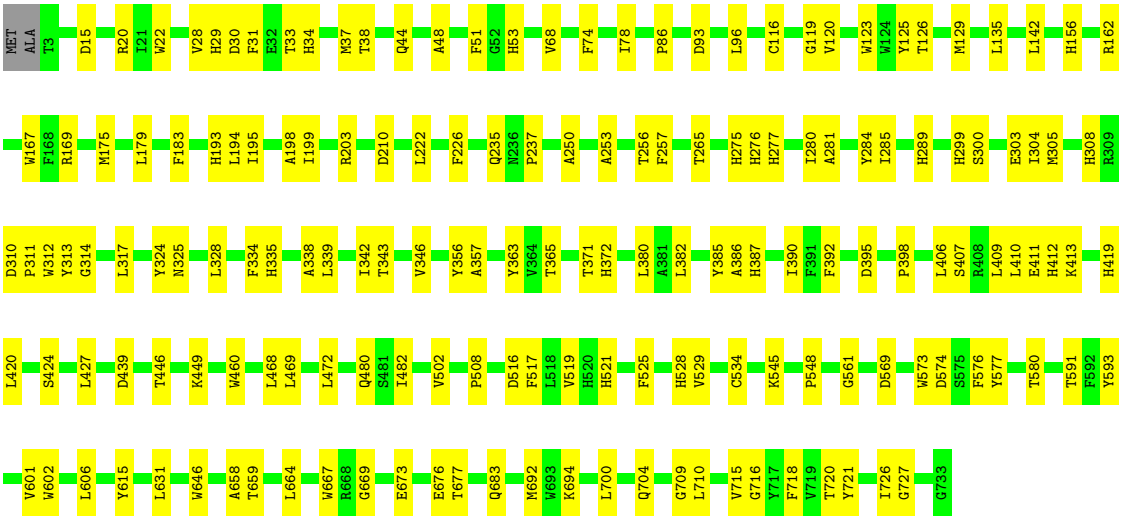




• Molecule 2: Photosystem I protein PsaB

Chain bB:

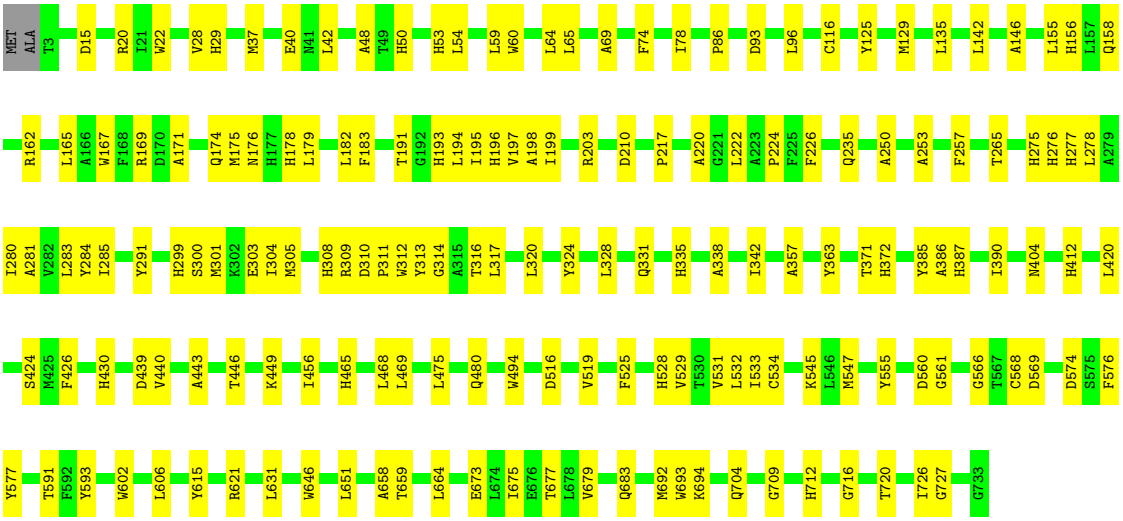




• Molecule 2: Photosystem I protein PsaB

Chain cB:

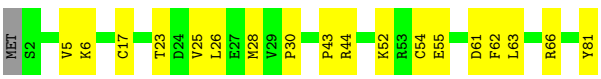




• Molecule 3: Photosystem I protein PsaC

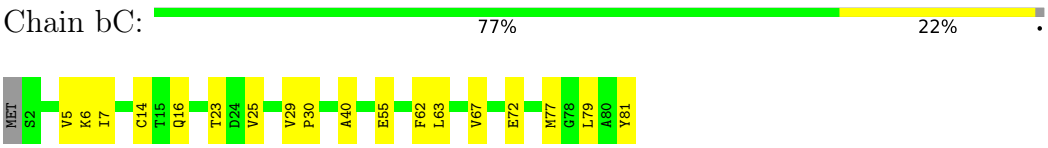
Chain aC:





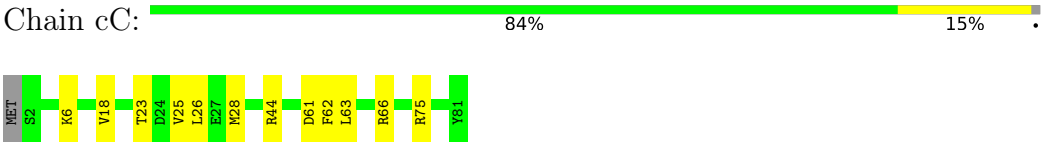
• Molecule 3: Photosystem I protein PsaC

Chain bC:



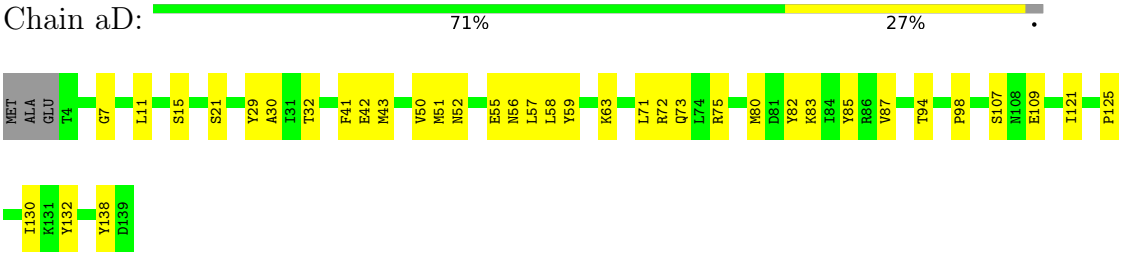
• Molecule 3: Photosystem I protein PsaC

Chain cC:



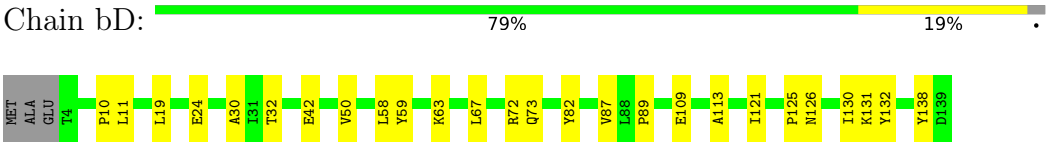
• Molecule 4: Photosystem I protein PsaD

Chain aD:



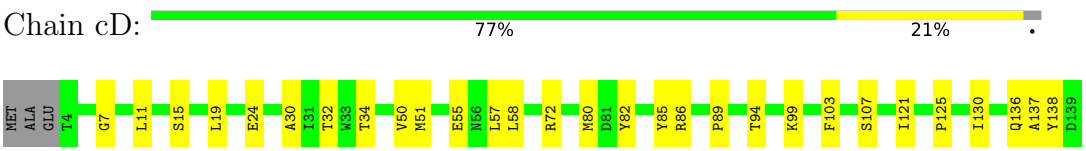
• Molecule 4: Photosystem I protein PsaD

Chain bD:



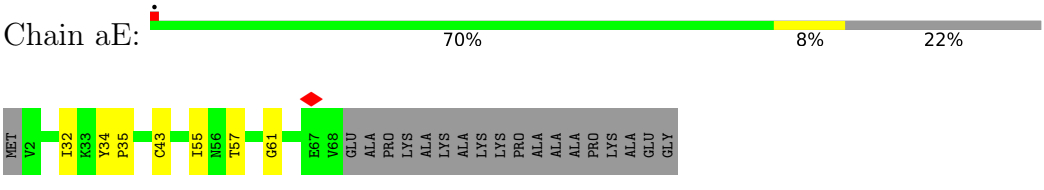
• Molecule 4: Photosystem I protein PsaD

Chain cD:



• Molecule 5: Photosystem I protein PsaE

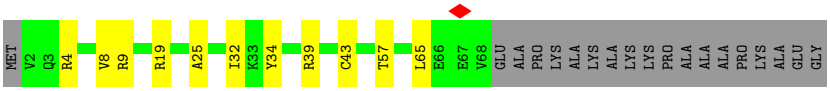
Chain aE:



• Molecule 5: Photosystem I protein PsaE

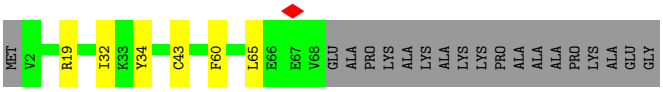
Chain bE:





• Molecule 5: Photosystem I protein PsaE





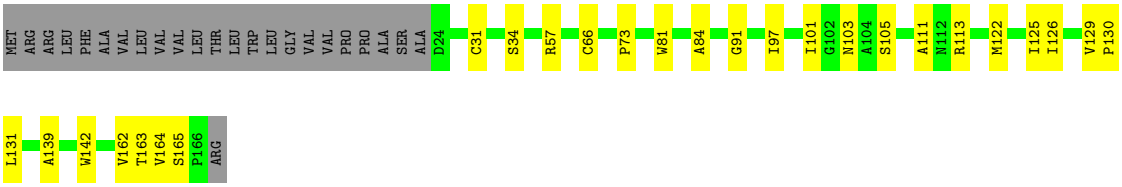
• Molecule 6: Photosystem I protein PsaF





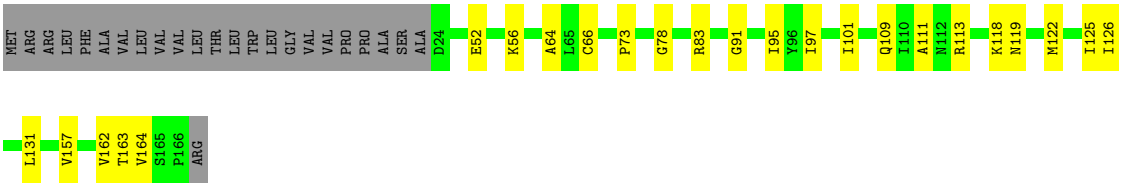
• Molecule 6: Photosystem I protein PsaF



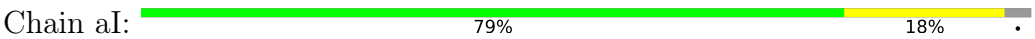


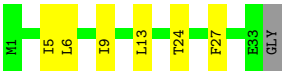
• Molecule 6: Photosystem I protein PsaF





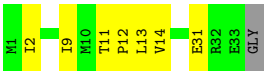
• Molecule 7: Photosystem I protein PsaI





• Molecule 7: Photosystem I protein PsaI

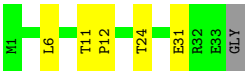




• Molecule 7: Photosystem I protein PsaI

Chain cI:





• Molecule 8: Photosystem I protein PsaJ

Chain aJ:

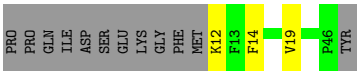




• Molecule 8: Photosystem I protein PsaJ

Chain bJ:

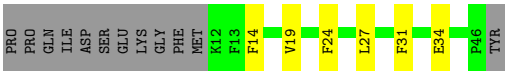




• Molecule 8: Photosystem I protein PsaJ

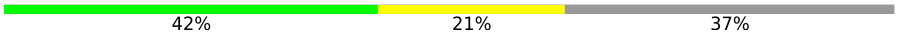
Chain cJ:

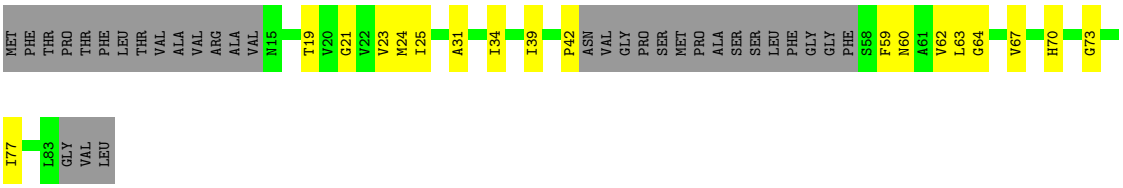




• Molecule 9: Photosystem I protein PsaK

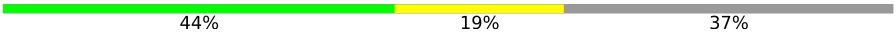
Chain aK:





• Molecule 9: Photosystem I protein PsaK

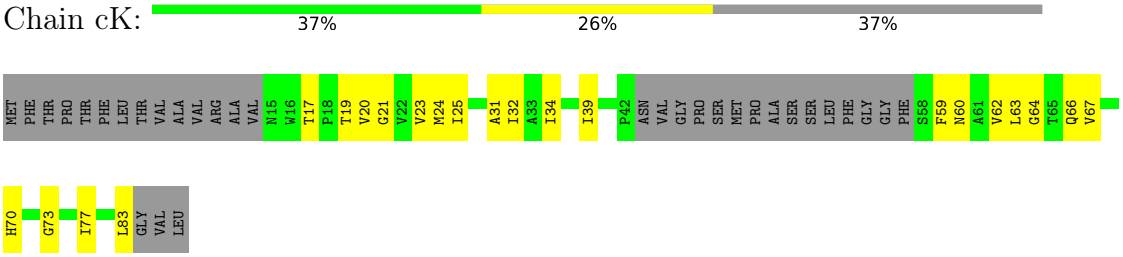
Chain bK:





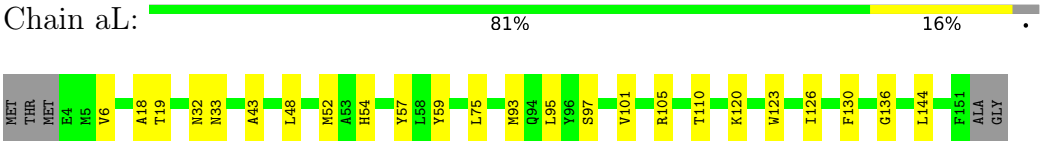
• Molecule 9: Photosystem I protein PsaK

Chain cK:



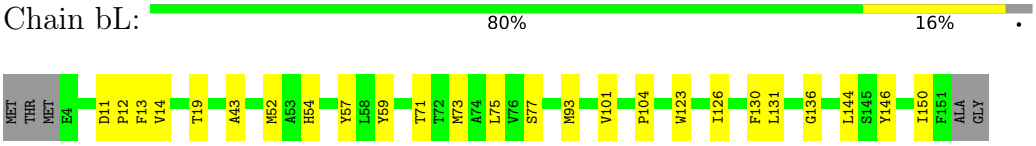
• Molecule 10: Photosystem I protein PsaL

Chain aL:



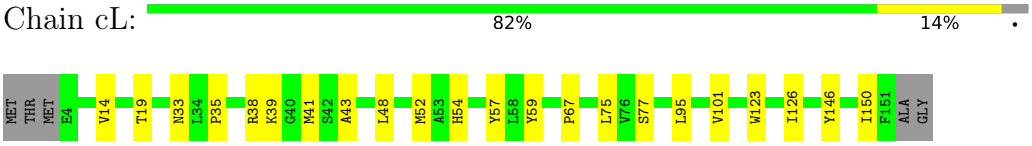
• Molecule 10: Photosystem I protein PsaL

Chain bL:



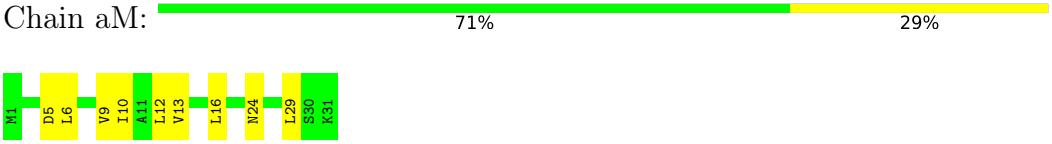
• Molecule 10: Photosystem I protein PsaL

Chain cL:



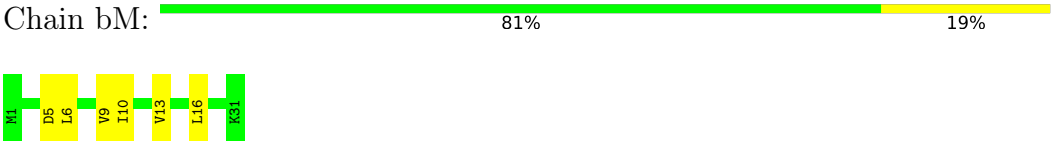
• Molecule 11: Photosystem I protein PsaM

Chain aM:



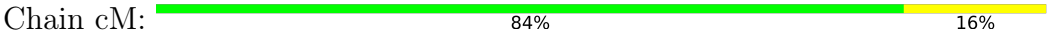
• Molecule 11: Photosystem I protein PsaM

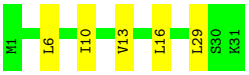
Chain bM:



• Molecule 11: Photosystem I protein PsaM

Chain cM:

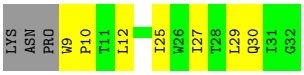




• Molecule 12: Photosystem I protein PsaX2

Chain aX:

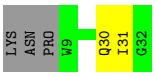




• Molecule 12: Photosystem I protein PsaX2

Chain bX:

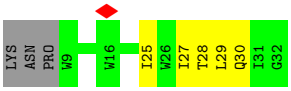




• Molecule 12: Photosystem I protein PsaX2

Chain cX:





4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	151833	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	40	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	1.435	Depositor
Minimum map value	-0.455	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.020	Depositor
Recommended contour level	0.1	Depositor
Map size (Å)	634.8, 634.8, 634.8	wwPDB
Map dimensions	600, 600, 600	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.058, 1.058, 1.058	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: LHG, LMG, PQN, CL7, SF4, A1JPJ, PHO, G9R

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|>5$	RMSZ	#$\|Z\|>5$
1	aA	0.18	0/5993	0.36	0/8165
1	bA	0.18	0/5993	0.36	0/8165
1	cA	0.18	0/5993	0.36	0/8165
2	aB	0.17	0/6030	0.35	0/8249
2	bB	0.17	0/6030	0.36	0/8249
2	cB	0.18	0/6030	0.36	0/8249
3	aC	0.16	0/609	0.36	0/825
3	bC	0.15	0/609	0.35	0/825
3	cC	0.14	0/609	0.33	0/825
4	aD	0.15	0/1058	0.39	0/1428
4	bD	0.15	0/1058	0.36	0/1428
4	cD	0.15	0/1058	0.38	0/1428
5	aE	0.11	0/536	0.31	0/725
5	bE	0.12	0/536	0.31	0/725
5	cE	0.12	0/536	0.31	0/725
6	aF	0.13	0/1078	0.33	0/1464
6	bF	0.14	0/1078	0.36	0/1464
6	cF	0.14	0/1078	0.36	0/1464
7	aI	0.18	0/255	0.34	0/346
7	bI	0.19	0/255	0.37	0/346
7	cI	0.17	0/255	0.38	0/346
8	aJ	0.13	0/303	0.36	0/412
8	bJ	0.12	0/303	0.31	0/412
8	cJ	0.13	0/303	0.32	0/412
9	aK	0.16	0/405	0.38	0/553
9	bK	0.13	0/405	0.30	0/553
9	cK	0.15	0/405	0.40	0/553
10	aL	0.20	0/1084	0.35	0/1475
10	bL	0.20	0/1084	0.41	2/1475 (0.1%)
10	cL	0.18	0/1084	0.32	0/1475
11	aM	0.20	0/223	0.42	0/304
11	bM	0.21	0/223	0.45	0/304

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| > 5$	RMSZ	$\#\|Z\| > 5$
11	cM	0.16	0/223	0.31	0/304
12	aX	0.13	0/194	0.33	0/269
12	bX	0.14	0/194	0.32	0/269
12	cX	0.14	0/194	0.33	0/269
All	All	0.17	0/53304	0.36	2/72645 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
10	bL	104	PRO	CA-C-N	-5.35	112.96	123.56
10	bL	104	PRO	C-N-CA	-5.35	112.96	123.56

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	aA	5797	0	5622	155	0
1	bA	5797	0	5623	148	0
1	cA	5797	0	5623	155	0
2	aB	5814	0	5544	153	0
2	bB	5814	0	5545	149	0
2	cB	5814	0	5545	154	0
3	aC	599	0	577	12	0
3	bC	599	0	577	16	0
3	cC	599	0	577	9	0
4	aD	1039	0	1043	26	0
4	bD	1039	0	1043	25	0
4	cD	1039	0	1043	21	0
5	aE	526	0	518	4	0
5	bE	526	0	518	7	0
5	cE	526	0	518	4	0
6	aF	1056	0	1063	14	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	bF	1056	0	1063	23	0
6	cF	1056	0	1063	16	0
7	aI	250	0	260	7	0
7	bI	250	0	260	5	0
7	cI	250	0	260	4	0
8	aJ	291	0	289	5	0
8	bJ	291	0	289	2	0
8	cJ	291	0	289	6	0
9	aK	397	0	410	14	0
9	bK	397	0	410	11	0
9	cK	397	0	410	17	0
10	aL	1059	0	1067	20	0
10	bL	1059	0	1067	18	0
10	cL	1059	0	1067	16	0
11	aM	223	0	259	8	0
11	bM	223	0	259	4	0
11	cM	223	0	259	3	0
12	aX	187	0	199	5	0
12	bX	187	0	199	2	0
12	cX	187	0	199	4	0
13	aA	65	0	0	0	0
13	bA	65	0	0	0	0
13	cA	65	0	0	0	0
14	aA	64	0	74	3	0
14	aB	64	0	74	7	0
14	bA	64	0	74	1	0
14	bB	64	0	74	6	0
14	cA	64	0	74	1	0
14	cB	64	0	74	7	0
15	aA	2346	0	2154	119	0
15	aB	2271	0	2037	100	0
15	aF	41	0	27	0	0
15	aI	65	0	70	6	0
15	aJ	83	0	55	2	0
15	aK	82	0	54	2	0
15	aL	185	0	184	7	0
15	bA	2346	0	2154	121	0
15	bB	2271	0	2037	102	0
15	bF	41	0	27	0	0
15	bI	65	0	70	2	0
15	bJ	83	0	55	1	0
15	bK	82	0	54	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
15	bL	185	0	184	6	0
15	cA	2346	0	2154	101	0
15	cB	2271	0	2037	119	0
15	cF	41	0	27	0	0
15	cI	65	0	70	4	0
15	cJ	83	0	55	4	0
15	cK	82	0	54	0	0
15	cL	185	0	184	7	0
16	aA	33	0	46	1	0
16	aB	33	0	46	0	0
16	bA	33	0	46	2	0
16	bB	33	0	46	0	0
16	cA	33	0	46	0	0
16	cB	33	0	46	0	0
17	aA	240	0	0	0	0
17	aB	280	0	0	1	0
17	aF	40	0	0	0	0
17	aI	80	0	0	0	0
17	aJ	40	0	0	0	0
17	aL	80	0	0	1	0
17	bA	240	0	0	1	0
17	bB	280	0	0	0	0
17	bF	40	0	0	0	0
17	bI	80	0	0	0	0
17	bJ	40	0	0	0	0
17	bL	80	0	0	1	0
17	cA	240	0	0	0	0
17	cB	280	0	0	1	0
17	cF	40	0	0	0	0
17	cI	80	0	0	0	0
17	cJ	40	0	0	0	0
17	cL	80	0	0	0	0
18	aA	87	0	123	5	0
18	bA	87	0	123	4	0
18	cA	87	0	123	8	0
19	aB	53	0	79	3	0
19	bB	53	0	79	3	0
19	cB	53	0	79	1	0
20	aB	8	0	0	0	0
20	aC	16	0	0	0	0
20	bB	8	0	0	0	0
20	bC	16	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
20	cB	8	0	0	0	0
20	cC	16	0	0	0	0
21	aA	21	0	0	0	0
21	aB	6	0	0	0	0
21	aI	1	0	0	0	0
21	aJ	1	0	0	0	0
21	aL	2	0	0	0	0
21	bA	21	0	0	0	0
21	bB	6	0	0	0	0
21	bI	1	0	0	0	0
21	bJ	1	0	0	0	0
21	bL	2	0	0	0	0
21	cA	21	0	0	1	0
21	cB	6	0	0	0	0
21	cI	1	0	0	0	0
21	cJ	1	0	0	0	0
21	cL	2	0	0	0	0
All	All	70575	0	65626	1464	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 11.

The worst 5 of 1464 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:aA:296:HIS:HE1	15:aA:1115:CL7:NB	1.62	0.95
2:cB:193:HIS:CE1	15:cB:1211:CL7:NA	2.42	0.87
2:aB:244:PHE:H	2:aB:264:GLN:HE22	1.29	0.80
1:bA:720:MET:HE3	1:bA:724:GLN:HG2	1.64	0.79
2:aB:335:HIS:CD2	15:aB:1221:CL7:HAA2	2.18	0.79

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	aA	735/753 (98%)	717 (98%)	18 (2%)	0	100	100
1	bA	735/753 (98%)	715 (97%)	20 (3%)	0	100	100
1	cA	735/753 (98%)	716 (97%)	19 (3%)	0	100	100
2	aB	729/733 (100%)	708 (97%)	21 (3%)	0	100	100
2	bB	729/733 (100%)	701 (96%)	28 (4%)	0	100	100
2	cB	729/733 (100%)	702 (96%)	27 (4%)	0	100	100
3	aC	78/81 (96%)	74 (95%)	4 (5%)	0	100	100
3	bC	78/81 (96%)	76 (97%)	2 (3%)	0	100	100
3	cC	78/81 (96%)	75 (96%)	3 (4%)	0	100	100
4	aD	134/139 (96%)	125 (93%)	9 (7%)	0	100	100
4	bD	134/139 (96%)	127 (95%)	7 (5%)	0	100	100
4	cD	134/139 (96%)	130 (97%)	4 (3%)	0	100	100
5	aE	65/86 (76%)	63 (97%)	2 (3%)	0	100	100
5	bE	65/86 (76%)	61 (94%)	4 (6%)	0	100	100
5	cE	65/86 (76%)	62 (95%)	3 (5%)	0	100	100
6	aF	141/167 (84%)	137 (97%)	4 (3%)	0	100	100
6	bF	141/167 (84%)	136 (96%)	5 (4%)	0	100	100
6	cF	141/167 (84%)	136 (96%)	5 (4%)	0	100	100
7	aI	31/34 (91%)	29 (94%)	2 (6%)	0	100	100
7	bI	31/34 (91%)	30 (97%)	1 (3%)	0	100	100
7	cI	31/34 (91%)	30 (97%)	1 (3%)	0	100	100
8	aJ	33/47 (70%)	33 (100%)	0	0	100	100
8	bJ	33/47 (70%)	33 (100%)	0	0	100	100
8	cJ	33/47 (70%)	33 (100%)	0	0	100	100
9	aK	50/86 (58%)	50 (100%)	0	0	100	100
9	bK	50/86 (58%)	50 (100%)	0	0	100	100
9	cK	50/86 (58%)	50 (100%)	0	0	100	100
10	aL	146/153 (95%)	142 (97%)	4 (3%)	0	100	100
10	bL	146/153 (95%)	140 (96%)	6 (4%)	0	100	100
10	cL	146/153 (95%)	141 (97%)	5 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
11	aM	29/31 (94%)	29 (100%)	0	0	100	100
11	bM	29/31 (94%)	29 (100%)	0	0	100	100
11	cM	29/31 (94%)	29 (100%)	0	0	100	100
12	aX	22/27 (82%)	21 (96%)	1 (4%)	0	100	100
12	bX	22/27 (82%)	21 (96%)	1 (4%)	0	100	100
12	cX	22/27 (82%)	21 (96%)	1 (4%)	0	100	100
All	All	6579/7011 (94%)	6372 (97%)	207 (3%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	aA	590/602 (98%)	590 (100%)	0	100	100
1	bA	590/602 (98%)	590 (100%)	0	100	100
1	cA	590/602 (98%)	590 (100%)	0	100	100
2	aB	592/593 (100%)	592 (100%)	0	100	100
2	bB	592/593 (100%)	592 (100%)	0	100	100
2	cB	592/593 (100%)	592 (100%)	0	100	100
3	aC	68/69 (99%)	68 (100%)	0	100	100
3	bC	68/69 (99%)	68 (100%)	0	100	100
3	cC	68/69 (99%)	68 (100%)	0	100	100
4	aD	110/112 (98%)	110 (100%)	0	100	100
4	bD	110/112 (98%)	110 (100%)	0	100	100
4	cD	110/112 (98%)	110 (100%)	0	100	100
5	aE	57/68 (84%)	57 (100%)	0	100	100
5	bE	57/68 (84%)	57 (100%)	0	100	100
5	cE	57/68 (84%)	57 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
6	aF	111/131 (85%)	111 (100%)	0	100	100
6	bF	111/131 (85%)	111 (100%)	0	100	100
6	cF	111/131 (85%)	111 (100%)	0	100	100
7	aI	26/26 (100%)	26 (100%)	0	100	100
7	bI	26/26 (100%)	26 (100%)	0	100	100
7	cI	26/26 (100%)	26 (100%)	0	100	100
8	aJ	31/42 (74%)	31 (100%)	0	100	100
8	bJ	31/42 (74%)	31 (100%)	0	100	100
8	cJ	31/42 (74%)	31 (100%)	0	100	100
9	aK	40/65 (62%)	40 (100%)	0	100	100
9	bK	40/65 (62%)	40 (100%)	0	100	100
9	cK	40/65 (62%)	40 (100%)	0	100	100
10	aL	110/113 (97%)	110 (100%)	0	100	100
10	bL	110/113 (97%)	110 (100%)	0	100	100
10	cL	110/113 (97%)	110 (100%)	0	100	100
11	aM	25/25 (100%)	25 (100%)	0	100	100
11	bM	25/25 (100%)	25 (100%)	0	100	100
11	cM	25/25 (100%)	25 (100%)	0	100	100
12	aX	19/22 (86%)	19 (100%)	0	100	100
12	bX	19/22 (86%)	19 (100%)	0	100	100
12	cX	19/22 (86%)	19 (100%)	0	100	100
All	All	5337/5604 (95%)	5337 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 72 such sidechains are listed below:

Mol	Chain	Res	Type
1	cA	543	GLN
12	cX	30	GLN
2	cB	29	HIS
2	cB	704	GLN
1	bA	36	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains

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

5.5 Carbohydrates

There are no oligosaccharides in this entry.

5.6 Ligand geometry

369 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
15	CL7	aB	1213	2	51,53,73	1.59	11 (21%)	56,89,113	1.41	6 (10%)
15	CL7	aB	1219	2	47,49,73	1.60	8 (17%)	51,84,113	1.46	6 (11%)
15	CL7	bB	1202	2	71,73,73	1.33	12 (16%)	80,113,113	1.22	6 (7%)
17	A1JPJ	aI	4018	-	40,41,41	1.63	8 (20%)	50,56,56	1.65	12 (24%)
15	CL7	cB	1228	2	51,53,73	1.58	11 (21%)	56,89,113	1.38	5 (8%)
17	A1JPJ	cF	4016	-	40,41,41	1.67	8 (20%)	50,56,56	1.70	10 (20%)
15	CL7	cB	1207	2	71,73,73	1.32	11 (15%)	80,113,113	1.26	7 (8%)
15	CL7	bB	1213	2	51,53,73	1.58	11 (21%)	56,89,113	1.42	6 (10%)
15	CL7	bB	1237	21	71,73,73	1.32	12 (16%)	80,113,113	1.23	5 (6%)
17	A1JPJ	cI	4019	-	40,41,41	1.66	8 (20%)	50,56,56	1.55	9 (18%)
15	CL7	bA	1126	1	71,73,73	1.41	11 (15%)	80,113,113	1.23	6 (7%)
17	A1JPJ	aA	4002	-	40,41,41	1.70	8 (20%)	50,56,56	1.64	10 (20%)
17	A1JPJ	aB	4021	-	40,41,41	1.65	8 (20%)	50,56,56	1.55	10 (20%)
15	CL7	cA	1138	-	71,73,73	1.31	11 (15%)	80,113,113	1.29	10 (12%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
15	CL7	bB	1203	2	71,73,73	1.32	11 (15%)	80,113,113	1.24	6 (7%)
15	CL7	bA	1131	1	71,73,73	1.32	12 (16%)	80,113,113	1.21	5 (6%)
15	CL7	aA	1125	1	56,58,73	1.51	11 (19%)	62,95,113	1.40	8 (12%)
15	CL7	cA	1132	1	71,73,73	1.39	14 (19%)	80,113,113	1.26	11 (13%)
15	CL7	aB	1230	2	47,49,73	1.57	11 (23%)	51,84,113	1.62	10 (19%)
15	CL7	bA	1130	1	57,59,73	1.47	11 (19%)	63,96,113	1.39	7 (11%)
15	CL7	aB	1210	2	71,73,73	1.34	11 (15%)	80,113,113	1.25	7 (8%)
15	CL7	bA	1118	1	61,63,73	1.44	10 (16%)	68,101,113	1.31	8 (11%)
15	CL7	bA	1113	1	51,53,73	1.57	10 (19%)	56,89,113	1.39	5 (8%)
15	CL7	cB	1212	2	51,53,73	1.56	10 (19%)	56,89,113	1.43	7 (12%)
15	CL7	bA	1135	1	56,58,73	1.49	11 (19%)	62,95,113	1.40	8 (12%)
15	CL7	aB	1238	21	71,73,73	1.32	11 (15%)	80,113,113	1.27	7 (8%)
15	CL7	bI	1601	21	71,73,73	1.32	12 (16%)	80,113,113	1.22	4 (5%)
15	CL7	bA	1107	1	51,53,73	1.56	11 (21%)	56,89,113	1.40	6 (10%)
15	CL7	cA	1108	1	57,59,73	1.49	10 (17%)	63,96,113	1.32	4 (6%)
15	CL7	bB	1210	2	71,73,73	1.34	10 (14%)	80,113,113	1.26	7 (8%)
15	CL7	cB	1241	2	51,53,73	1.56	10 (19%)	56,89,113	1.35	6 (10%)
15	CL7	bA	1124	21	56,58,73	1.47	11 (19%)	62,95,113	1.42	7 (11%)
15	CL7	aL	1502	10	71,73,73	1.30	11 (15%)	80,113,113	1.32	9 (11%)
15	CL7	bA	1106	1	71,73,73	1.32	12 (16%)	80,113,113	1.27	7 (8%)
20	SF4	aB	3001	1,2	0,12,12	-	-	-		
15	CL7	bB	1217	2	47,49,73	1.60	8 (17%)	51,84,113	1.46	6 (11%)
15	CL7	aJ	1302	8	47,50,73	1.63	8 (17%)	51,85,113	1.38	4 (7%)
20	SF4	bB	3001	1,2	0,12,12	-	-	-		
17	A1JPJ	cL	4023	-	40,41,41	1.66	8 (20%)	50,56,56	1.59	11 (22%)
16	PQN	aA	2001	-	34,34,34	0.36	0	42,45,45	0.65	2 (4%)
15	CL7	aF	1701	6	47,49,73	1.59	10 (21%)	51,84,113	1.46	8 (15%)
17	A1JPJ	cB	4015	-	40,41,41	1.68	8 (20%)	50,56,56	1.92	15 (30%)
15	CL7	cA	1126	1	71,73,73	1.32	11 (15%)	80,113,113	1.20	4 (5%)
15	CL7	aA	1117	1	71,73,73	1.33	10 (14%)	80,113,113	1.31	8 (10%)
15	CL7	bA	1134	1	49,52,73	1.56	10 (20%)	56,87,113	1.43	5 (8%)
16	PQN	cA	2001	-	34,34,34	0.35	0	42,45,45	0.61	1 (2%)
15	CL7	cB	1216	21	51,53,73	1.58	11 (21%)	56,89,113	1.42	6 (10%)
17	A1JPJ	bB	4004	-	40,41,41	1.73	7 (17%)	50,56,56	1.79	10 (20%)
15	CL7	cA	1117	1	71,73,73	1.33	11 (15%)	80,113,113	1.28	9 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
15	CL7	bA	1129	1	56,58,73	1.49	10 (17%)	62,95,113	1.34	8 (12%)
15	CL7	bB	1221	2	66,68,73	1.41	10 (15%)	74,107,113	1.28	8 (10%)
15	CL7	cB	1021	2	71,73,73	1.31	11 (15%)	80,113,113	1.16	5 (6%)
17	A1JPJ	bB	4006	-	40,41,41	1.78	8 (20%)	50,56,56	2.10	12 (24%)
15	CL7	cB	1211	2	61,63,73	1.43	10 (16%)	68,101,113	1.30	5 (7%)
15	CL7	aA	1135	1	56,58,73	1.50	11 (19%)	62,95,113	1.39	8 (12%)
15	CL7	bA	1116	1	66,68,73	1.38	11 (16%)	74,107,113	1.29	7 (9%)
17	A1JPJ	bB	4010	-	40,41,41	1.69	8 (20%)	50,56,56	1.76	12 (24%)
15	CL7	cA	1129	1	56,58,73	1.49	11 (19%)	62,95,113	1.37	7 (11%)
15	CL7	cJ	1301	21	47,49,73	1.63	10 (21%)	51,84,113	1.46	7 (13%)
14	PHO	aA	1013	-	58,69,69	1.99	12 (20%)	56,99,99	1.72	8 (14%)
15	CL7	cA	1128	1	71,73,73	1.33	11 (15%)	80,113,113	1.23	6 (7%)
15	CL7	bA	1133	1	71,73,73	1.33	10 (14%)	80,113,113	1.26	7 (8%)
15	CL7	cL	1501	10	66,68,73	1.38	11 (16%)	74,107,113	1.31	7 (9%)
15	CL7	aB	1235	2	66,68,73	1.37	11 (16%)	74,107,113	1.31	6 (8%)
17	A1JPJ	aA	4014	-	40,41,41	1.85	8 (20%)	50,56,56	2.10	12 (24%)
17	A1JPJ	cL	4020	-	40,41,41	1.65	8 (20%)	50,56,56	1.64	10 (20%)
15	CL7	cB	1232	21	47,49,73	1.61	9 (19%)	51,84,113	1.44	6 (11%)
15	CL7	bA	1102	15	58,60,73	1.47	9 (15%)	64,97,113	1.39	8 (12%)
15	CL7	cA	1120	1	51,53,73	1.59	11 (21%)	56,89,113	1.40	6 (10%)
15	CL7	bJ	1302	8	47,50,73	1.63	9 (19%)	51,85,113	1.35	4 (7%)
15	CL7	aA	1134	1	49,52,73	1.56	10 (20%)	56,87,113	1.44	7 (12%)
17	A1JPJ	aF	4016	-	40,41,41	1.77	8 (20%)	50,56,56	1.90	15 (30%)
15	CL7	bB	1021	2	71,73,73	1.30	11 (15%)	80,113,113	1.17	6 (7%)
20	SF4	aC	3003	3	0,12,12	-	-	-		
15	CL7	bA	1104	1	71,73,73	1.34	10 (14%)	80,113,113	1.23	6 (7%)
15	CL7	aB	1231	2	51,53,73	1.57	11 (21%)	56,89,113	1.36	4 (7%)
15	CL7	bB	1236	2	51,53,73	1.56	11 (21%)	56,89,113	1.39	5 (8%)
15	CL7	bA	1139	21	51,53,73	1.57	10 (19%)	56,89,113	1.40	5 (8%)
15	CL7	bB	1228	2	51,53,73	1.57	10 (19%)	56,89,113	1.35	3 (5%)
15	CL7	bB	1231	2	51,53,73	1.57	11 (21%)	56,89,113	1.36	4 (7%)
15	CL7	bA	1112	1	71,73,73	1.34	11 (15%)	80,113,113	1.30	8 (10%)
15	CL7	bB	1226	2	71,73,73	1.33	11 (15%)	80,113,113	1.27	9 (11%)
15	CL7	cK	1401	-	51,53,73	1.59	9 (17%)	56,89,113	1.43	5 (8%)
15	CL7	cB	1201	2	60,62,73	1.44	12 (20%)	66,99,113	1.33	6 (9%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
17	A1JPJ	bB	4021	-	40,41,41	1.66	8 (20%)	50,56,56	1.54	10 (20%)
15	CL7	cB	1238	21	71,73,73	1.32	11 (15%)	80,113,113	1.27	7 (8%)
15	CL7	bB	1230	2	47,49,73	1.57	11 (23%)	51,84,113	1.62	10 (19%)
15	CL7	bB	1224	2	62,64,73	1.42	11 (17%)	69,102,113	1.25	5 (7%)
15	CL7	cA	1109	15,1	71,73,73	1.33	9 (12%)	80,113,113	1.25	5 (6%)
20	SF4	aC	3002	3	0,12,12	-	-	-		
15	CL7	aB	1225	2	71,73,73	1.31	11 (15%)	80,113,113	1.17	7 (8%)
15	CL7	aB	1232	21	47,49,73	1.60	10 (21%)	51,84,113	1.42	6 (11%)
17	A1JPJ	bB	4017	-	40,41,41	1.67	8 (20%)	50,56,56	1.76	10 (20%)
15	CL7	aA	1120	1	51,53,73	1.59	11 (21%)	56,89,113	1.41	6 (10%)
15	CL7	cB	1219	2	47,49,73	1.61	8 (17%)	51,84,113	1.49	6 (11%)
15	CL7	cB	1222	21	51,53,73	1.55	11 (21%)	56,89,113	1.40	6 (10%)
15	CL7	cB	1203	2	71,73,73	1.32	11 (15%)	80,113,113	1.23	6 (7%)
15	CL7	aA	1123	21	71,73,73	1.35	12 (16%)	80,113,113	1.27	7 (8%)
15	CL7	aA	1115	1	47,49,73	1.60	11 (23%)	51,84,113	1.49	5 (9%)
15	CL7	cA	1022	21	71,73,73	1.33	11 (15%)	80,113,113	1.20	6 (7%)
15	CL7	aA	1114	21	51,53,73	1.58	10 (19%)	56,89,113	1.38	5 (8%)
20	SF4	bC	3002	3	0,12,12	-	-	-		
15	CL7	bA	1132	1	71,73,73	1.31	12 (16%)	80,113,113	1.31	9 (11%)
15	CL7	aA	1111	1	71,73,73	1.33	10 (14%)	80,113,113	1.25	7 (8%)
17	A1JPJ	aA	4008	-	40,41,41	1.63	8 (20%)	50,56,56	1.61	12 (24%)
15	CL7	cB	1210	2	71,73,73	1.33	10 (14%)	80,113,113	1.26	7 (8%)
15	CL7	aB	1227	2	51,53,73	1.58	11 (21%)	56,89,113	1.36	5 (8%)
15	CL7	bA	1127	1	71,73,73	1.30	12 (16%)	80,113,113	1.17	5 (6%)
15	CL7	bB	1238	21	71,73,73	1.32	11 (15%)	80,113,113	1.27	7 (8%)
17	A1JPJ	cA	4014	-	40,41,41	1.82	8 (20%)	50,56,56	2.07	12 (24%)
15	CL7	bA	1801	18	47,49,73	1.58	11 (23%)	51,84,113	1.46	6 (11%)
15	CL7	bA	1137	1	61,63,73	1.43	11 (18%)	68,101,113	1.30	7 (10%)
17	A1JPJ	cB	4006	-	40,41,41	1.79	8 (20%)	50,56,56	2.15	13 (26%)
15	CL7	aA	1105	1	51,53,73	1.55	11 (21%)	56,89,113	1.41	5 (8%)
14	PHO	cA	1013	-	58,69,69	1.98	11 (18%)	56,99,99	1.76	9 (16%)
15	CL7	aA	1140	1	66,68,73	1.37	11 (16%)	74,107,113	1.23	6 (8%)
15	CL7	cA	1113	1	51,53,73	1.56	9 (17%)	56,89,113	1.42	6 (10%)
15	CL7	bB	1012	21	71,73,73	1.32	12 (16%)	80,113,113	1.20	8 (10%)
15	CL7	aA	1022	21	71,73,73	1.32	12 (16%)	80,113,113	1.21	5 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
15	CL7	aB	1212	2	51,53,73	1.57	11 (21%)	56,89,113	1.44	7 (12%)
15	CL7	bB	1204	2	71,73,73	1.33	10 (14%)	80,113,113	1.28	7 (8%)
18	LHG	bA	5003	15	37,37,48	0.57	0	40,43,54	0.56	0
15	CL7	cB	1233	-	47,49,73	1.60	8 (17%)	51,84,113	1.45	6 (11%)
15	CL7	cI	1601	21	71,73,73	1.33	10 (14%)	80,113,113	1.24	5 (6%)
15	CL7	aB	1221	2	66,68,73	1.41	12 (18%)	74,107,113	1.29	7 (9%)
16	PQN	cB	2002	-	34,34,34	0.36	0	42,45,45	0.55	1 (2%)
15	CL7	cB	1223	2	71,73,73	1.34	11 (15%)	80,113,113	1.24	6 (7%)
17	A1JPJ	aL	4020	-	40,41,41	1.64	8 (20%)	50,56,56	1.65	10 (20%)
15	CL7	aB	1204	2	71,73,73	1.33	11 (15%)	80,113,113	1.29	7 (8%)
15	CL7	bB	1241	2	51,53,73	1.57	10 (19%)	56,89,113	1.35	5 (8%)
15	CL7	aA	1109	15,1	71,73,73	1.34	10 (14%)	80,113,113	1.26	7 (8%)
15	CL7	aA	1108	1	57,59,73	1.50	10 (17%)	63,96,113	1.31	4 (6%)
15	CL7	bA	1114	21	51,53,73	1.58	10 (19%)	56,89,113	1.38	5 (8%)
14	PHO	bA	1013	-	58,69,69	1.97	12 (20%)	56,99,99	1.73	8 (14%)
15	CL7	bB	1227	2	51,53,73	1.59	10 (19%)	56,89,113	1.41	7 (12%)
15	CL7	cB	1209	2	51,53,73	1.58	8 (15%)	56,89,113	1.40	6 (10%)
15	CL7	aB	1237	21	71,73,73	1.32	12 (16%)	80,113,113	1.23	6 (7%)
15	CL7	aB	1209	2	51,53,73	1.58	9 (17%)	56,89,113	1.42	5 (8%)
15	CL7	bA	1119	21	61,63,73	1.44	11 (18%)	68,101,113	1.33	8 (11%)
15	CL7	aB	1208	2	71,73,73	1.33	10 (14%)	80,113,113	1.20	4 (5%)
15	CL7	aB	1012	21	71,73,73	1.32	12 (16%)	80,113,113	1.20	7 (8%)
20	SF4	bC	3003	3	0,12,12	-	-	-		
15	CL7	cA	1139	21	51,53,73	1.57	11 (21%)	56,89,113	1.39	5 (8%)
17	A1JPJ	cA	4008	-	40,41,41	1.62	8 (20%)	50,56,56	1.63	11 (22%)
14	PHO	aB	1023	-	58,69,69	1.95	12 (20%)	56,99,99	1.66	8 (14%)
15	CL7	bB	1208	2	71,73,73	1.32	10 (14%)	80,113,113	1.21	6 (7%)
15	CL7	bB	1207	2	71,73,73	1.32	11 (15%)	80,113,113	1.27	8 (10%)
15	CL7	cA	1110	21	51,53,73	1.56	11 (21%)	56,89,113	1.44	6 (10%)
17	A1JPJ	cA	4002	-	40,41,41	1.68	8 (20%)	50,56,56	1.62	9 (18%)
15	CL7	aA	1137	1	61,63,73	1.43	11 (18%)	68,101,113	1.30	7 (10%)
15	CL7	aB	1021	2	71,73,73	1.30	10 (14%)	80,113,113	1.16	5 (6%)
15	CL7	cB	1236	2	51,53,73	1.55	11 (21%)	56,89,113	1.41	6 (10%)
15	CL7	bA	1115	1	47,49,73	1.61	11 (23%)	51,84,113	1.48	8 (15%)
15	CL7	aA	1119	21	61,63,73	1.44	12 (19%)	68,101,113	1.33	7 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
15	CL7	aA	1121	1	61,63,73	1.42	11 (18%)	68,101,113	1.26	5 (7%)
15	CL7	bA	1022	21	71,73,73	1.32	12 (16%)	80,113,113	1.19	5 (6%)
15	CL7	cA	1116	1	66,68,73	1.39	12 (18%)	74,107,113	1.30	7 (9%)
20	SF4	cC	3003	3	0,12,12	-	-	-		
15	CL7	cA	1106	1	71,73,73	1.31	12 (16%)	80,113,113	1.29	9 (11%)
17	A1JPJ	bI	4018	-	40,41,41	1.64	8 (20%)	50,56,56	1.66	12 (24%)
15	CL7	cB	1235	2	66,68,73	1.37	11 (16%)	74,107,113	1.32	6 (8%)
17	A1JPJ	bL	4020	-	40,41,41	1.64	8 (20%)	50,56,56	1.62	10 (20%)
17	A1JPJ	cB	4004	-	40,41,41	1.73	7 (17%)	50,56,56	1.80	10 (20%)
17	A1JPJ	aB	4004	-	40,41,41	1.72	7 (17%)	50,56,56	1.79	10 (20%)
15	CL7	aA	1106	1	71,73,73	1.31	12 (16%)	80,113,113	1.29	8 (10%)
19	LMG	cB	5002	-	53,53,55	0.51	0	61,61,63	0.65	1 (1%)
15	CL7	cB	1206	2	56,58,73	1.48	11 (19%)	62,95,113	1.38	7 (11%)
15	CL7	cB	1234	2	56,58,73	1.50	11 (19%)	62,95,113	1.39	8 (12%)
15	CL7	aB	1233	-	47,49,73	1.61	9 (19%)	51,84,113	1.47	7 (13%)
20	SF4	cB	3001	1,2	0,12,12	-	-	-		
15	CL7	bB	1220	-	51,53,73	1.57	10 (19%)	56,89,113	1.40	5 (8%)
15	CL7	bA	1120	1	51,53,73	1.59	11 (21%)	56,89,113	1.41	6 (10%)
15	CL7	bA	1128	1	71,73,73	1.32	11 (15%)	80,113,113	1.23	5 (6%)
17	A1JPJ	cB	4021	-	40,41,41	1.66	8 (20%)	50,56,56	1.55	10 (20%)
15	CL7	aB	1241	2	51,53,73	1.56	9 (17%)	56,89,113	1.38	6 (10%)
15	CL7	bB	1239	2	71,73,73	1.32	11 (15%)	80,113,113	1.26	7 (8%)
15	CL7	bA	1109	15,1	71,73,73	1.34	10 (14%)	80,113,113	1.25	6 (7%)
15	CL7	cB	1230	2	47,49,73	1.57	11 (23%)	51,84,113	1.62	8 (15%)
15	CL7	aB	1239	2	71,73,73	1.32	11 (15%)	80,113,113	1.26	7 (8%)
15	CL7	bL	1503	21	66,68,73	1.37	11 (16%)	74,107,113	1.26	6 (8%)
17	A1JPJ	cB	4017	-	40,41,41	1.67	8 (20%)	50,56,56	1.74	10 (20%)
15	CL7	bB	1225	2	71,73,73	1.32	12 (16%)	80,113,113	1.19	7 (8%)
15	CL7	cA	1134	1	49,52,73	1.56	11 (22%)	56,87,113	1.42	5 (8%)
15	CL7	aB	1201	2	60,62,73	1.44	12 (20%)	66,99,113	1.34	6 (9%)
15	CL7	aA	1128	1	71,73,73	1.33	11 (15%)	80,113,113	1.23	5 (6%)
17	A1JPJ	aB	4005	-	40,41,41	1.69	8 (20%)	50,56,56	1.77	11 (22%)
17	A1JPJ	aB	4015	-	40,41,41	1.67	8 (20%)	50,56,56	1.98	15 (30%)
15	CL7	cB	1220	-	51,53,73	1.58	11 (21%)	56,89,113	1.43	6 (10%)
15	CL7	aL	1503	21	66,68,73	1.38	11 (16%)	74,107,113	1.27	6 (8%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
19	LMG	bB	5002	-	53,53,55	0.51	0	61,61,63	0.65	1 (1%)
17	A1JPJ	cA	4011	-	40,41,41	1.64	8 (20%)	50,56,56	1.66	9 (18%)
15	CL7	aB	1220	-	51,53,73	1.57	12 (23%)	56,89,113	1.40	5 (8%)
17	A1JPJ	bB	4005	-	40,41,41	1.69	8 (20%)	50,56,56	1.77	12 (24%)
15	CL7	cA	1102	15,1	58,60,73	1.48	9 (15%)	64,97,113	1.39	7 (10%)
16	PQN	bB	2002	-	34,34,34	0.36	0	42,45,45	0.54	1 (2%)
17	A1JPJ	aI	4019	-	40,41,41	1.66	8 (20%)	50,56,56	1.56	9 (18%)
14	PHO	cB	1023	-	58,69,69	1.95	12 (20%)	56,99,99	1.63	8 (14%)
15	CL7	bA	1105	1	51,53,73	1.55	11 (21%)	56,89,113	1.41	5 (8%)
15	CL7	bA	1103	1	71,73,73	1.33	11 (15%)	80,113,113	1.24	7 (8%)
15	CL7	cA	1137	1	61,63,73	1.43	11 (18%)	68,101,113	1.32	7 (10%)
15	CL7	cA	1104	1	71,73,73	1.33	11 (15%)	80,113,113	1.25	6 (7%)
15	CL7	bA	1101	1	47,49,73	1.59	12 (25%)	51,84,113	1.50	8 (15%)
15	CL7	aB	1211	2	61,63,73	1.42	10 (16%)	68,101,113	1.32	6 (8%)
15	CL7	bL	1501	10	66,68,73	1.37	10 (15%)	74,107,113	1.31	6 (8%)
15	CL7	bA	1111	1	71,73,73	1.34	11 (15%)	80,113,113	1.25	8 (10%)
15	CL7	cB	1224	2	62,64,73	1.42	11 (17%)	69,102,113	1.23	4 (5%)
15	CL7	cB	1202	2	71,73,73	1.33	12 (16%)	80,113,113	1.22	5 (6%)
15	CL7	bA	1108	1	57,59,73	1.48	10 (17%)	63,96,113	1.31	5 (7%)
17	A1JPJ	bF	4016	-	40,41,41	1.68	8 (20%)	50,56,56	1.85	14 (28%)
15	CL7	cK	1402	9	45,45,73	1.64	10 (22%)	49,78,113	1.45	6 (12%)
15	CL7	bB	1215	2	61,63,73	1.42	12 (19%)	68,101,113	1.30	6 (8%)
15	CL7	cA	1114	21	51,53,73	1.58	10 (19%)	56,89,113	1.38	5 (8%)
15	CL7	cA	1135	1	56,58,73	1.48	11 (19%)	62,95,113	1.44	9 (14%)
15	CL7	cB	1213	2	51,53,73	1.58	11 (21%)	56,89,113	1.42	6 (10%)
15	CL7	cA	1103	1	71,73,73	1.33	11 (15%)	80,113,113	1.25	7 (8%)
15	CL7	aB	1214	2	56,58,73	1.51	11 (19%)	62,95,113	1.38	8 (12%)
15	CL7	cA	1119	21	61,63,73	1.44	11 (18%)	68,101,113	1.32	7 (10%)
15	CL7	cA	1118	1	61,63,73	1.43	10 (16%)	68,101,113	1.32	7 (10%)
15	CL7	cA	1123	21	71,73,73	1.35	12 (16%)	80,113,113	1.29	6 (7%)
17	A1JPJ	bJ	4012	-	40,41,41	1.68	8 (20%)	50,56,56	1.89	13 (26%)
14	PHO	bB	1023	-	58,69,69	1.96	12 (20%)	56,99,99	1.71	9 (16%)
15	CL7	bA	1125	1	56,58,73	1.49	12 (21%)	62,95,113	1.40	8 (12%)
17	A1JPJ	bL	4023	-	40,41,41	1.66	8 (20%)	50,56,56	1.59	11 (22%)
15	CL7	cA	1133	1	71,73,73	1.33	10 (14%)	80,113,113	1.26	7 (8%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
15	CL7	cA	1140	1	66,68,73	1.38	11 (16%)	74,107,113	1.24	6 (8%)
15	CL7	aA	1126	1	71,73,73	1.32	11 (15%)	80,113,113	1.21	5 (6%)
18	LHG	bA	5001	-	48,48,48	0.51	0	51,54,54	0.51	0
15	CL7	bA	1121	1	61,63,73	1.43	10 (16%)	68,101,113	1.27	5 (7%)
15	CL7	aA	1110	21	51,53,73	1.57	9 (17%)	56,89,113	1.44	6 (10%)
17	A1JPJ	bA	4002	-	40,41,41	1.70	8 (20%)	50,56,56	1.63	10 (20%)
15	CL7	bB	1219	2	47,49,73	1.60	8 (17%)	51,84,113	1.46	6 (11%)
15	CL7	cA	1121	1	61,63,73	1.41	10 (16%)	68,101,113	1.26	6 (8%)
20	SF4	cC	3002	3	0,12,12	-	-	-		
15	CL7	aJ	1301	21	47,49,73	1.62	10 (21%)	51,84,113	1.46	7 (13%)
13	G9R	aA	1011	1	69,73,73	1.24	9 (13%)	83,113,113	1.26	6 (7%)
15	CL7	aA	1133	1	71,73,73	1.33	10 (14%)	80,113,113	1.26	6 (7%)
18	LHG	aA	5001	-	48,48,48	0.51	0	51,54,54	0.51	0
15	CL7	bB	1212	2	51,53,73	1.57	10 (19%)	56,89,113	1.43	7 (12%)
15	CL7	aL	1501	10	66,68,73	1.38	11 (16%)	74,107,113	1.33	7 (9%)
15	CL7	cB	1231	2	51,53,73	1.57	11 (21%)	56,89,113	1.36	5 (8%)
17	A1JPJ	cI	4018	-	40,41,41	1.63	8 (20%)	50,56,56	1.66	12 (24%)
15	CL7	cB	1226	2	71,73,73	1.34	11 (15%)	80,113,113	1.25	7 (8%)
17	A1JPJ	aB	4010	-	40,41,41	1.70	8 (20%)	50,56,56	1.75	11 (22%)
15	CL7	aA	1127	1	71,73,73	1.31	11 (15%)	80,113,113	1.18	5 (6%)
15	CL7	bJ	1301	21	47,49,73	1.61	9 (19%)	51,84,113	1.46	6 (11%)
15	CL7	aB	1203	2	71,73,73	1.32	11 (15%)	80,113,113	1.24	5 (6%)
15	CL7	cL	1503	21	66,68,73	1.38	11 (16%)	74,107,113	1.27	6 (8%)
15	CL7	bA	1122	1	71,73,73	1.33	11 (15%)	80,113,113	1.23	5 (6%)
17	A1JPJ	cA	4003	-	40,41,41	1.64	8 (20%)	50,56,56	1.59	10 (20%)
15	CL7	cA	1105	1	51,53,73	1.56	11 (21%)	56,89,113	1.40	5 (8%)
15	CL7	aA	1801	18	47,49,73	1.58	10 (21%)	51,84,113	1.45	6 (11%)
15	CL7	bB	1233	-	47,49,73	1.61	8 (17%)	51,84,113	1.43	5 (9%)
15	CL7	cA	1131	1	71,73,73	1.33	12 (16%)	80,113,113	1.22	5 (6%)
17	A1JPJ	bA	4011	-	40,41,41	1.63	8 (20%)	50,56,56	1.64	8 (16%)
17	A1JPJ	aJ	4012	-	40,41,41	1.66	8 (20%)	50,56,56	1.88	13 (26%)
17	A1JPJ	bA	4008	-	40,41,41	1.62	8 (20%)	50,56,56	1.63	10 (20%)
15	CL7	cB	1221	2	66,68,73	1.42	11 (16%)	74,107,113	1.29	8 (10%)
15	CL7	aA	1112	1	71,73,73	1.33	11 (15%)	80,113,113	1.32	7 (8%)
17	A1JPJ	bI	4019	-	40,41,41	1.66	8 (20%)	50,56,56	1.56	9 (18%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
15	CL7	aA	1122	1	71,73,73	1.34	12 (16%)	80,113,113	1.23	5 (6%)
15	CL7	aB	1222	21	51,53,73	1.55	11 (21%)	56,89,113	1.39	6 (10%)
15	CL7	bB	1211	2	61,63,73	1.43	10 (16%)	68,101,113	1.32	7 (10%)
15	CL7	aB	1218	2	47,49,73	1.60	9 (19%)	51,84,113	1.48	6 (11%)
15	CL7	aB	1228	2	51,53,73	1.57	11 (21%)	56,89,113	1.37	5 (8%)
17	A1JPJ	aA	4007	-	40,41,41	1.68	8 (20%)	50,56,56	1.60	11 (22%)
15	CL7	cA	1124	21	56,58,73	1.48	11 (19%)	62,95,113	1.41	7 (11%)
16	PQN	bA	2001	-	34,34,34	0.35	0	42,45,45	0.66	1 (2%)
15	CL7	aB	1207	2	71,73,73	1.32	11 (15%)	80,113,113	1.28	7 (8%)
15	CL7	cB	1227	2	51,53,73	1.57	11 (21%)	56,89,113	1.39	6 (10%)
15	CL7	bB	1229	2	71,73,73	1.33	10 (14%)	80,113,113	1.23	6 (7%)
15	CL7	cA	1115	1	47,49,73	1.60	11 (23%)	51,84,113	1.52	6 (11%)
15	CL7	bB	1214	2	56,58,73	1.51	11 (19%)	62,95,113	1.40	8 (12%)
15	CL7	bB	1201	2	60,62,73	1.44	11 (18%)	66,99,113	1.35	6 (9%)
15	CL7	bA	1123	21	71,73,73	1.34	11 (15%)	80,113,113	1.27	7 (8%)
17	A1JPJ	bA	4014	-	40,41,41	1.85	8 (20%)	50,56,56	2.11	12 (24%)
15	CL7	cL	1502	10	71,73,73	1.31	11 (15%)	80,113,113	1.32	8 (10%)
15	CL7	aA	1124	21	56,58,73	1.48	11 (19%)	62,95,113	1.40	7 (11%)
17	A1JPJ	bB	4015	-	40,41,41	1.68	8 (20%)	50,56,56	1.91	16 (32%)
15	CL7	aI	1601	21	71,73,73	1.33	12 (16%)	80,113,113	1.24	6 (7%)
15	CL7	aB	1215	2	61,63,73	1.43	12 (19%)	68,101,113	1.31	6 (8%)
15	CL7	cB	1012	21	71,73,73	1.32	12 (16%)	80,113,113	1.19	8 (10%)
15	CL7	cF	1701	6	47,49,73	1.58	10 (21%)	51,84,113	1.47	9 (17%)
15	CL7	cB	1218	2	47,49,73	1.60	9 (19%)	51,84,113	1.48	6 (11%)
15	CL7	cA	1111	1	71,73,73	1.33	11 (15%)	80,113,113	1.24	8 (10%)
15	CL7	cB	1204	2	71,73,73	1.34	13 (18%)	80,113,113	1.30	7 (8%)
15	CL7	aA	1104	1	71,73,73	1.33	11 (15%)	80,113,113	1.25	6 (7%)
15	CL7	cB	1205	2	71,73,73	1.30	12 (16%)	80,113,113	1.28	8 (10%)
15	CL7	aB	1202	2	71,73,73	1.32	11 (15%)	80,113,113	1.21	5 (6%)
15	CL7	bB	1222	21	51,53,73	1.55	11 (21%)	56,89,113	1.39	6 (10%)
15	CL7	cA	1130	1	57,59,73	1.46	11 (19%)	63,96,113	1.37	7 (11%)
17	A1JPJ	aB	4006	-	40,41,41	1.78	8 (20%)	50,56,56	2.12	14 (28%)
18	LHG	aA	5003	15	37,37,48	0.57	0	40,43,54	0.57	0
15	CL7	cB	1229	2	71,73,73	1.34	11 (15%)	80,113,113	1.25	7 (8%)
15	CL7	bB	1235	2	66,68,73	1.37	11 (16%)	74,107,113	1.31	6 (8%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
15	CL7	bK	1401	-	51,53,73	1.59	9 (17%)	56,89,113	1.43	6 (10%)
15	CL7	cB	1215	2	61,63,73	1.41	9 (14%)	68,101,113	1.27	10 (14%)
15	CL7	bA	1140	1	66,68,73	1.38	11 (16%)	74,107,113	1.24	6 (8%)
15	CL7	bB	1205	2	71,73,73	1.30	12 (16%)	80,113,113	1.28	8 (10%)
15	CL7	bK	1402	9	45,45,73	1.64	9 (20%)	49,78,113	1.42	5 (10%)
15	CL7	cB	1208	2	71,73,73	1.32	10 (14%)	80,113,113	1.20	4 (5%)
15	CL7	aA	1130	1	57,59,73	1.47	11 (19%)	63,96,113	1.37	6 (9%)
15	CL7	cA	1122	1	71,73,73	1.33	11 (15%)	80,113,113	1.23	5 (6%)
15	CL7	aA	1118	1	61,63,73	1.44	11 (18%)	68,101,113	1.31	7 (10%)
15	CL7	aK	1401	-	51,53,73	1.59	11 (21%)	56,89,113	1.44	6 (10%)
15	CL7	aA	1113	1	51,53,73	1.56	10 (19%)	56,89,113	1.42	6 (10%)
15	CL7	aB	1236	2	51,53,73	1.56	11 (21%)	56,89,113	1.40	5 (8%)
15	CL7	cA	1127	1	71,73,73	1.31	11 (15%)	80,113,113	1.19	5 (6%)
15	CL7	aB	1234	2	56,58,73	1.50	11 (19%)	62,95,113	1.39	8 (12%)
15	CL7	aA	1107	1	51,53,73	1.57	11 (21%)	56,89,113	1.40	6 (10%)
15	CL7	bB	1234	2	56,58,73	1.50	12 (21%)	62,95,113	1.39	8 (12%)
15	CL7	cB	1214	2	56,58,73	1.51	11 (19%)	62,95,113	1.40	8 (12%)
15	CL7	bA	1117	1	71,73,73	1.33	11 (15%)	80,113,113	1.28	9 (11%)
17	A1JPJ	bA	4003	-	40,41,41	1.65	8 (20%)	50,56,56	1.60	10 (20%)
15	CL7	aA	1129	1	56,58,73	1.49	10 (17%)	62,95,113	1.37	9 (14%)
15	CL7	aB	1216	21	51,53,73	1.59	10 (19%)	56,89,113	1.39	5 (8%)
15	CL7	bA	1138	1	71,73,73	1.31	11 (15%)	80,113,113	1.29	6 (7%)
17	A1JPJ	aL	4023	-	40,41,41	1.69	8 (20%)	50,56,56	1.77	12 (24%)
15	CL7	bA	1110	21	51,53,73	1.57	10 (19%)	56,89,113	1.45	6 (10%)
15	CL7	bB	1218	2	47,49,73	1.61	11 (23%)	51,84,113	1.48	6 (11%)
15	CL7	cA	1107	1	51,53,73	1.56	11 (21%)	56,89,113	1.41	6 (10%)
15	CL7	bB	1216	21	51,53,73	1.59	11 (21%)	56,89,113	1.39	5 (8%)
15	CL7	aB	1217	2	47,49,73	1.60	8 (17%)	51,84,113	1.46	6 (11%)
15	CL7	cA	1801	18	47,49,73	1.58	11 (23%)	51,84,113	1.48	7 (13%)
13	G9R	bA	1011	1	69,73,73	1.24	9 (13%)	83,113,113	1.26	5 (6%)
15	CL7	cB	1239	2	71,73,73	1.32	12 (16%)	80,113,113	1.27	7 (8%)
15	CL7	aB	1205	2	71,73,73	1.30	12 (16%)	80,113,113	1.29	9 (11%)
17	A1JPJ	cJ	4012	-	40,41,41	1.66	8 (20%)	50,56,56	1.88	12 (24%)
17	A1JPJ	aA	4003	-	40,41,41	1.65	8 (20%)	50,56,56	1.59	10 (20%)
15	CL7	bB	1223	2	71,73,73	1.34	12 (16%)	80,113,113	1.24	6 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
19	LMG	aB	5002	-	53,53,55	0.51	0	61,61,63	0.71	1 (1%)
15	CL7	aB	1206	2	56,58,73	1.48	12 (21%)	62,95,113	1.39	7 (11%)
15	CL7	bL	1502	10	71,73,73	1.30	11 (15%)	80,113,113	1.32	8 (10%)
15	CL7	aA	1136	1	71,73,73	1.32	11 (15%)	80,113,113	1.24	6 (7%)
15	CL7	aB	1229	2	71,73,73	1.34	11 (15%)	80,113,113	1.23	7 (8%)
16	PQN	aB	2002	-	34,34,34	0.36	0	42,45,45	0.55	1 (2%)
15	CL7	aA	1101	1	47,49,73	1.59	9 (19%)	51,84,113	1.49	8 (15%)
17	A1JPJ	cA	4007	-	40,41,41	1.69	8 (20%)	50,56,56	1.62	11 (22%)
15	CL7	aB	1226	2	71,73,73	1.33	11 (15%)	80,113,113	1.28	9 (11%)
18	LHG	cA	5001	-	48,48,48	0.51	0	51,54,54	0.52	0
15	CL7	bB	1206	2	56,58,73	1.48	10 (17%)	62,95,113	1.38	8 (12%)
15	CL7	bB	1209	2	51,53,73	1.58	9 (17%)	56,89,113	1.41	5 (8%)
15	CL7	cJ	1302	8	47,50,73	1.64	8 (17%)	51,85,113	1.36	4 (7%)
15	CL7	aA	1103	1	71,73,73	1.32	11 (15%)	80,113,113	1.25	6 (7%)
17	A1JPJ	aB	4017	-	40,41,41	1.68	8 (20%)	50,56,56	1.77	10 (20%)
15	CL7	aA	1102	15,1	58,60,73	1.47	10 (17%)	64,97,113	1.37	8 (12%)
15	CL7	aA	1116	1	66,68,73	1.39	11 (16%)	74,107,113	1.29	6 (8%)
15	CL7	bB	1232	21	47,49,73	1.62	11 (23%)	51,84,113	1.43	7 (13%)
17	A1JPJ	cB	4010	-	40,41,41	1.70	8 (20%)	50,56,56	1.77	11 (22%)
15	CL7	aA	1139	21	51,53,73	1.57	10 (19%)	56,89,113	1.40	5 (8%)
15	CL7	aA	1138	1	71,73,73	1.31	11 (15%)	80,113,113	1.28	7 (8%)
15	CL7	aB	1223	2	71,73,73	1.33	12 (16%)	80,113,113	1.25	7 (8%)
15	CL7	bF	1701	6	47,49,73	1.58	11 (23%)	51,84,113	1.46	7 (13%)
13	G9R	cA	1011	1	69,73,73	1.23	9 (13%)	83,113,113	1.28	5 (6%)
15	CL7	bA	1136	1	71,73,73	1.32	11 (15%)	80,113,113	1.23	6 (7%)
18	LHG	cA	5003	15	37,37,48	0.56	0	40,43,54	0.55	0
15	CL7	aA	1132	1	71,73,73	1.39	13 (18%)	80,113,113	1.25	11 (13%)
15	CL7	cB	1237	21	71,73,73	1.32	12 (16%)	80,113,113	1.23	6 (7%)
15	CL7	cA	1125	1	56,58,73	1.50	11 (19%)	62,95,113	1.38	8 (12%)
15	CL7	cA	1112	1	71,73,73	1.33	11 (15%)	80,113,113	1.34	10 (12%)
15	CL7	aA	1131	1	71,73,73	1.33	11 (15%)	80,113,113	1.21	6 (7%)
17	A1JPJ	bA	4007	-	40,41,41	1.68	8 (20%)	50,56,56	1.61	11 (22%)
15	CL7	cA	1101	1	47,49,73	1.60	10 (21%)	51,84,113	1.50	8 (15%)
15	CL7	cB	1225	2	71,73,73	1.32	11 (15%)	80,113,113	1.18	5 (6%)
15	CL7	cA	1136	1	71,73,73	1.32	11 (15%)	80,113,113	1.23	6 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
17	A1JPJ	aA	4011	-	40,41,41	1.64	8 (20%)	50,56,56	1.63	9 (18%)
15	CL7	aK	1402	9	45,45,73	1.61	11 (24%)	49,78,113	1.41	7 (14%)
15	CL7	aB	1224	2	62,64,73	1.41	11 (17%)	69,102,113	1.29	6 (8%)
17	A1JPJ	cB	4005	-	40,41,41	1.70	8 (20%)	50,56,56	1.77	12 (24%)
15	CL7	cB	1217	2	47,49,73	1.60	8 (17%)	51,84,113	1.48	6 (11%)

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
15	CL7	aB	1213	2	2/2/11/20	11/15/91/115	-
15	CL7	aB	1219	2	2/2/10/20	4/10/86/115	-
15	CL7	bB	1202	2	2/2/15/20	22/39/115/115	-
17	A1JPJ	aI	4018	-	-	2/29/63/63	0/2/2/2
15	CL7	cB	1228	2	2/2/11/20	8/15/91/115	-
17	A1JPJ	cF	4016	-	-	6/29/63/63	0/2/2/2
15	CL7	cB	1207	2	2/2/15/20	11/39/115/115	-
15	CL7	bB	1213	2	2/2/11/20	9/15/91/115	-
15	CL7	bB	1237	21	2/2/15/20	19/39/115/115	-
17	A1JPJ	cI	4019	-	-	2/29/63/63	0/2/2/2
15	CL7	bA	1126	1	2/2/15/20	9/39/115/115	-
17	A1JPJ	aA	4002	-	-	2/29/63/63	0/2/2/2
17	A1JPJ	aB	4021	-	-	2/29/63/63	0/2/2/2
15	CL7	cA	1138	-	2/2/15/20	10/39/115/115	-
15	CL7	bB	1203	2	2/2/15/20	12/39/115/115	-
15	CL7	bA	1131	1	2/2/15/20	7/39/115/115	-
15	CL7	aA	1125	1	2/2/12/20	1/21/97/115	-
15	CL7	cA	1132	1	2/2/15/20	12/39/115/115	-
15	CL7	aB	1230	2	2/2/10/20	6/10/86/115	-
15	CL7	bA	1130	1	2/2/12/20	7/23/99/115	-
15	CL7	aB	1210	2	2/2/15/20	19/39/115/115	-
15	CL7	bA	1118	1	2/2/13/20	9/27/103/115	-
15	CL7	bA	1113	1	2/2/11/20	10/15/91/115	-
15	CL7	cB	1212	2	2/2/11/20	11/15/91/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
15	CL7	bA	1135	1	2/2/12/20	13/21/97/115	-
15	CL7	aB	1238	21	2/2/15/20	10/39/115/115	-
15	CL7	bI	1601	21	2/2/15/20	12/39/115/115	-
15	CL7	bA	1107	1	2/2/11/20	4/15/91/115	-
15	CL7	cA	1108	1	2/2/12/20	9/23/99/115	-
15	CL7	bB	1210	2	2/2/15/20	16/39/115/115	-
15	CL7	cB	1241	2	2/2/11/20	10/15/91/115	-
15	CL7	bA	1124	21	2/2/12/20	3/21/97/115	-
15	CL7	aL	1502	10	2/2/15/20	19/39/115/115	-
15	CL7	bA	1106	1	2/2/15/20	19/39/115/115	-
20	SF4	aB	3001	1,2	-	-	0/6/5/5
15	CL7	bB	1217	2	2/2/10/20	1/10/86/115	-
15	CL7	aJ	1302	8	2/2/10/20	4/9/85/115	-
20	SF4	bB	3001	1,2	-	-	0/6/5/5
17	A1JPJ	cL	4023	-	-	1/29/63/63	0/2/2/2
16	PQN	aA	2001	-	-	4/23/43/43	0/2/2/2
15	CL7	aF	1701	6	2/2/10/20	1/10/86/115	-
17	A1JPJ	cB	4015	-	-	2/29/63/63	0/2/2/2
15	CL7	cA	1126	1	2/2/15/20	10/39/115/115	-
15	CL7	aA	1117	1	2/2/15/20	15/39/115/115	-
15	CL7	bA	1134	1	2/2/10/20	7/15/87/115	-
16	PQN	cA	2001	-	-	4/23/43/43	0/2/2/2
15	CL7	cB	1216	21	2/2/11/20	3/15/91/115	-
17	A1JPJ	bB	4004	-	-	2/29/63/63	0/2/2/2
15	CL7	cA	1117	1	2/2/15/20	16/39/115/115	-
15	CL7	bA	1129	1	2/2/12/20	4/21/97/115	-
15	CL7	bB	1221	2	2/2/14/20	14/33/109/115	-
15	CL7	cB	1021	2	2/2/15/20	8/39/115/115	-
17	A1JPJ	bB	4006	-	-	6/29/63/63	0/2/2/2
15	CL7	cB	1211	2	2/2/13/20	8/27/103/115	-
15	CL7	aA	1135	1	2/2/12/20	12/21/97/115	-
15	CL7	bA	1116	1	2/2/14/20	14/33/109/115	-
17	A1JPJ	bB	4010	-	-	7/29/63/63	0/2/2/2
15	CL7	cA	1129	1	2/2/12/20	7/21/97/115	-
15	CL7	cJ	1301	21	2/2/10/20	5/10/86/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
14	PHO	aA	1013	-	-	6/37/103/103	0/5/6/6
15	CL7	cA	1128	1	2/2/15/20	6/39/115/115	-
15	CL7	bA	1133	1	2/2/15/20	11/39/115/115	-
15	CL7	cL	1501	10	2/2/14/20	17/33/109/115	-
15	CL7	aB	1235	2	2/2/14/20	13/33/109/115	-
17	A1JPJ	aA	4014	-	-	7/29/63/63	0/2/2/2
17	A1JPJ	cL	4020	-	-	5/29/63/63	0/2/2/2
15	CL7	cB	1232	21	2/2/10/20	3/10/86/115	-
15	CL7	bA	1102	15	2/2/12/20	8/24/100/115	-
15	CL7	cA	1120	1	2/2/11/20	7/15/91/115	-
15	CL7	bJ	1302	8	2/2/10/20	4/9/85/115	-
15	CL7	aA	1134	1	2/2/10/20	7/15/87/115	-
17	A1JPJ	aF	4016	-	-	9/29/63/63	0/2/2/2
15	CL7	bB	1021	2	2/2/15/20	10/39/115/115	-
20	SF4	aC	3003	3	-	-	0/6/5/5
15	CL7	bA	1104	1	2/2/15/20	19/39/115/115	-
15	CL7	aB	1231	2	2/2/11/20	0/15/91/115	-
15	CL7	bB	1236	2	2/2/11/20	8/15/91/115	-
15	CL7	bA	1139	21	2/2/11/20	10/15/91/115	-
15	CL7	bB	1228	2	2/2/11/20	8/15/91/115	-
15	CL7	bB	1231	2	2/2/11/20	4/15/91/115	-
15	CL7	bA	1112	1	2/2/15/20	14/39/115/115	-
15	CL7	bB	1226	2	2/2/15/20	13/39/115/115	-
15	CL7	cK	1401	-	2/2/11/20	6/15/91/115	-
15	CL7	cB	1201	2	2/2/12/20	10/26/102/115	-
17	A1JPJ	bB	4021	-	-	2/29/63/63	0/2/2/2
15	CL7	cB	1238	21	2/2/15/20	9/39/115/115	-
15	CL7	bB	1230	2	2/2/10/20	5/10/86/115	-
15	CL7	bB	1224	2	2/2/13/20	11/29/105/115	-
15	CL7	cA	1109	15,1	2/2/15/20	25/39/115/115	-
20	SF4	aC	3002	3	-	-	0/6/5/5
15	CL7	aB	1225	2	2/2/15/20	14/39/115/115	-
15	CL7	aB	1232	21	2/2/10/20	4/10/86/115	-
17	A1JPJ	bB	4017	-	-	4/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
15	CL7	aA	1120	1	2/2/11/20	5/15/91/115	-
15	CL7	cB	1219	2	2/2/10/20	3/10/86/115	-
15	CL7	cB	1222	21	2/2/11/20	9/15/91/115	-
15	CL7	cB	1203	2	2/2/15/20	13/39/115/115	-
15	CL7	aA	1123	21	2/2/15/20	15/39/115/115	-
15	CL7	aA	1115	1	2/2/10/20	4/10/86/115	-
15	CL7	cA	1022	21	2/2/15/20	11/39/115/115	-
15	CL7	aA	1114	21	2/2/11/20	2/15/91/115	-
20	SF4	bC	3002	3	-	-	0/6/5/5
15	CL7	bA	1132	1	2/2/15/20	14/39/115/115	-
15	CL7	aA	1111	1	2/2/15/20	14/39/115/115	-
17	A1JPJ	aA	4008	-	-	3/29/63/63	0/2/2/2
15	CL7	cB	1210	2	2/2/15/20	14/39/115/115	-
15	CL7	aB	1227	2	2/2/11/20	5/15/91/115	-
15	CL7	bA	1127	1	2/2/15/20	20/39/115/115	-
15	CL7	bB	1238	21	2/2/15/20	7/39/115/115	-
17	A1JPJ	cA	4014	-	-	8/29/63/63	0/2/2/2
15	CL7	bA	1801	18	2/2/10/20	7/10/86/115	-
15	CL7	bA	1137	1	2/2/13/20	10/27/103/115	-
17	A1JPJ	cB	4006	-	-	6/29/63/63	0/2/2/2
15	CL7	aA	1105	1	2/2/11/20	5/15/91/115	-
15	CL7	aA	1140	1	2/2/14/20	14/33/109/115	-
14	PHO	cA	1013	-	-	10/37/103/103	0/5/6/6
15	CL7	cA	1113	1	2/2/11/20	6/15/91/115	-
15	CL7	bB	1012	21	2/2/15/20	13/39/115/115	-
15	CL7	aA	1022	21	2/2/15/20	10/39/115/115	-
15	CL7	aB	1212	2	2/2/11/20	11/15/91/115	-
15	CL7	bB	1204	2	2/2/15/20	7/39/115/115	-
18	LHG	bA	5003	15	-	10/42/42/53	-
15	CL7	cB	1233	-	2/2/10/20	2/10/86/115	-
15	CL7	cI	1601	21	2/2/15/20	13/39/115/115	-
15	CL7	aB	1221	2	2/2/14/20	14/33/109/115	-
16	PQN	cB	2002	-	-	6/23/43/43	0/2/2/2
15	CL7	cB	1223	2	2/2/15/20	17/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
17	A1JPJ	aL	4020	-	-	5/29/63/63	0/2/2/2
15	CL7	aB	1204	2	2/2/15/20	5/39/115/115	-
15	CL7	bB	1241	2	2/2/11/20	10/15/91/115	-
15	CL7	aA	1109	15,1	2/2/15/20	24/39/115/115	-
15	CL7	aA	1108	1	2/2/12/20	9/23/99/115	-
15	CL7	bA	1114	21	2/2/11/20	2/15/91/115	-
14	PHO	bA	1013	-	-	11/37/103/103	0/5/6/6
15	CL7	bB	1227	2	2/2/11/20	5/15/91/115	-
15	CL7	cB	1209	2	2/2/11/20	10/15/91/115	-
15	CL7	aB	1237	21	2/2/15/20	14/39/115/115	-
15	CL7	aB	1209	2	2/2/11/20	7/15/91/115	-
15	CL7	bA	1119	21	2/2/13/20	15/27/103/115	-
15	CL7	aB	1208	2	2/2/15/20	13/39/115/115	-
15	CL7	aB	1012	21	2/2/15/20	15/39/115/115	-
20	SF4	bC	3003	3	-	-	0/6/5/5
15	CL7	cA	1139	21	2/2/11/20	10/15/91/115	-
17	A1JPJ	cA	4008	-	-	3/29/63/63	0/2/2/2
15	CL7	bB	1208	2	2/2/15/20	10/39/115/115	-
14	PHO	aB	1023	-	-	12/37/103/103	0/5/6/6
15	CL7	bB	1207	2	2/2/15/20	12/39/115/115	-
15	CL7	cA	1110	21	2/2/11/20	11/15/91/115	-
17	A1JPJ	cA	4002	-	-	2/29/63/63	0/2/2/2
15	CL7	aA	1137	1	2/2/13/20	8/27/103/115	-
15	CL7	aB	1021	2	2/2/15/20	10/39/115/115	-
15	CL7	cB	1236	2	2/2/11/20	8/15/91/115	-
15	CL7	bA	1115	1	2/2/10/20	4/10/86/115	-
15	CL7	aA	1119	21	2/2/13/20	11/27/103/115	-
15	CL7	aA	1121	1	2/2/13/20	9/27/103/115	-
15	CL7	bA	1022	21	2/2/15/20	5/39/115/115	-
15	CL7	cA	1116	1	2/2/14/20	13/33/109/115	-
20	SF4	cC	3003	3	-	-	0/6/5/5
15	CL7	cA	1106	1	2/2/15/20	19/39/115/115	-
17	A1JPJ	bI	4018	-	-	2/29/63/63	0/2/2/2
15	CL7	cB	1235	2	2/2/14/20	12/33/109/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
17	A1JPJ	bL	4020	-	-	5/29/63/63	0/2/2/2
17	A1JPJ	cB	4004	-	-	2/29/63/63	0/2/2/2
17	A1JPJ	aB	4004	-	-	2/29/63/63	0/2/2/2
15	CL7	aA	1106	1	2/2/15/20	19/39/115/115	-
19	LMG	cB	5002	-	-	15/48/68/70	0/1/1/1
15	CL7	cB	1206	2	2/2/12/20	7/21/97/115	-
15	CL7	cB	1234	2	2/2/12/20	8/21/97/115	-
15	CL7	aB	1233	-	2/2/10/20	2/10/86/115	-
20	SF4	cB	3001	1,2	-	-	0/6/5/5
15	CL7	bB	1220	-	2/2/11/20	11/15/91/115	-
15	CL7	bA	1120	1	2/2/11/20	6/15/91/115	-
15	CL7	bA	1128	1	2/2/15/20	6/39/115/115	-
17	A1JPJ	cB	4021	-	-	2/29/63/63	0/2/2/2
15	CL7	aB	1241	2	2/2/11/20	6/15/91/115	-
15	CL7	bB	1239	2	2/2/15/20	13/39/115/115	-
15	CL7	bA	1109	15,1	2/2/15/20	24/39/115/115	-
15	CL7	cB	1230	2	2/2/10/20	6/10/86/115	-
15	CL7	aB	1239	2	2/2/15/20	6/39/115/115	-
15	CL7	bL	1503	21	2/2/14/20	12/33/109/115	-
17	A1JPJ	cB	4017	-	-	4/29/63/63	0/2/2/2
15	CL7	bB	1225	2	2/2/15/20	11/39/115/115	-
15	CL7	cA	1134	1	2/2/10/20	7/15/87/115	-
15	CL7	aB	1201	2	2/2/12/20	9/26/102/115	-
15	CL7	aA	1128	1	2/2/15/20	7/39/115/115	-
17	A1JPJ	aB	4005	-	-	6/29/63/63	0/2/2/2
17	A1JPJ	aB	4015	-	-	2/29/63/63	0/2/2/2
15	CL7	cB	1220	-	2/2/11/20	8/15/91/115	-
15	CL7	aL	1503	21	2/2/14/20	12/33/109/115	-
19	LMG	bB	5002	-	-	14/48/68/70	0/1/1/1
17	A1JPJ	cA	4011	-	-	6/29/63/63	0/2/2/2
15	CL7	aB	1220	-	2/2/11/20	11/15/91/115	-
17	A1JPJ	bB	4005	-	-	6/29/63/63	0/2/2/2
15	CL7	cA	1102	15,1	2/2/12/20	7/24/100/115	-
16	PQN	bB	2002	-	-	6/23/43/43	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
17	A1JPJ	aI	4019	-	-	2/29/63/63	0/2/2/2
14	PHO	cB	1023	-	-	13/37/103/103	0/5/6/6
15	CL7	bA	1105	1	2/2/11/20	5/15/91/115	-
15	CL7	bA	1103	1	2/2/15/20	20/39/115/115	-
15	CL7	cA	1137	1	2/2/13/20	9/27/103/115	-
15	CL7	cA	1104	1	2/2/15/20	18/39/115/115	-
15	CL7	bA	1101	1	2/2/10/20	2/10/86/115	-
15	CL7	aB	1211	2	2/2/13/20	6/27/103/115	-
15	CL7	bL	1501	10	2/2/14/20	14/33/109/115	-
15	CL7	bA	1111	1	2/2/15/20	11/39/115/115	-
15	CL7	cB	1224	2	2/2/13/20	12/29/105/115	-
15	CL7	cB	1202	2	2/2/15/20	22/39/115/115	-
15	CL7	bA	1108	1	2/2/12/20	8/23/99/115	-
17	A1JPJ	bF	4016	-	-	8/29/63/63	0/2/2/2
15	CL7	cK	1402	9	2/2/8/20	2/4/76/115	-
15	CL7	bB	1215	2	2/2/13/20	7/27/103/115	-
15	CL7	cA	1114	21	2/2/11/20	4/15/91/115	-
15	CL7	cA	1135	1	2/2/12/20	12/21/97/115	-
15	CL7	cB	1213	2	2/2/11/20	9/15/91/115	-
15	CL7	cA	1103	1	2/2/15/20	16/39/115/115	-
15	CL7	aB	1214	2	2/2/12/20	6/21/97/115	-
15	CL7	cA	1119	21	2/2/13/20	13/27/103/115	-
15	CL7	cA	1118	1	2/2/13/20	12/27/103/115	-
15	CL7	cA	1123	21	2/2/15/20	18/39/115/115	-
17	A1JPJ	bJ	4012	-	-	2/29/63/63	0/2/2/2
14	PHO	bB	1023	-	-	13/37/103/103	0/5/6/6
15	CL7	bA	1125	1	2/2/12/20	2/21/97/115	-
17	A1JPJ	bL	4023	-	-	1/29/63/63	0/2/2/2
15	CL7	cA	1133	1	2/2/15/20	9/39/115/115	-
15	CL7	cA	1140	1	2/2/14/20	14/33/109/115	-
15	CL7	aA	1126	1	2/2/15/20	10/39/115/115	-
18	LHG	bA	5001	-	-	15/53/53/53	-
15	CL7	bA	1121	1	2/2/13/20	10/27/103/115	-
15	CL7	aA	1110	21	2/2/11/20	11/15/91/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
17	A1JPJ	bA	4002	-	-	2/29/63/63	0/2/2/2
15	CL7	bB	1219	2	2/2/10/20	4/10/86/115	-
15	CL7	cA	1121	1	2/2/13/20	10/27/103/115	-
20	SF4	cC	3002	3	-	-	0/6/5/5
15	CL7	aJ	1301	21	2/2/10/20	5/10/86/115	-
13	G9R	aA	1011	1	1/1/15/20	12/39/115/115	-
15	CL7	aA	1133	1	2/2/15/20	10/39/115/115	-
18	LHG	aA	5001	-	-	14/53/53/53	-
15	CL7	bB	1212	2	2/2/11/20	10/15/91/115	-
15	CL7	aL	1501	10	2/2/14/20	15/33/109/115	-
15	CL7	cB	1231	2	2/2/11/20	2/15/91/115	-
17	A1JPJ	cI	4018	-	-	2/29/63/63	0/2/2/2
15	CL7	cB	1226	2	2/2/15/20	13/39/115/115	-
17	A1JPJ	aB	4010	-	-	7/29/63/63	0/2/2/2
15	CL7	aA	1127	1	2/2/15/20	15/39/115/115	-
15	CL7	bJ	1301	21	2/2/10/20	5/10/86/115	-
15	CL7	aB	1203	2	2/2/15/20	12/39/115/115	-
15	CL7	cL	1503	21	2/2/14/20	12/33/109/115	-
15	CL7	bA	1122	1	2/2/15/20	6/39/115/115	-
17	A1JPJ	cA	4003	-	-	2/29/63/63	0/2/2/2
15	CL7	cA	1105	1	2/2/11/20	6/15/91/115	-
15	CL7	aA	1801	18	2/2/10/20	7/10/86/115	-
15	CL7	bB	1233	-	2/2/10/20	2/10/86/115	-
15	CL7	cA	1131	1	2/2/15/20	9/39/115/115	-
17	A1JPJ	bA	4011	-	-	6/29/63/63	0/2/2/2
17	A1JPJ	aJ	4012	-	-	2/29/63/63	0/2/2/2
17	A1JPJ	bA	4008	-	-	3/29/63/63	0/2/2/2
15	CL7	cB	1221	2	2/2/14/20	14/33/109/115	-
15	CL7	aA	1112	1	2/2/15/20	13/39/115/115	-
17	A1JPJ	bI	4019	-	-	2/29/63/63	0/2/2/2
15	CL7	aA	1122	1	2/2/15/20	6/39/115/115	-
15	CL7	aB	1222	21	2/2/11/20	11/15/91/115	-
15	CL7	bB	1211	2	2/2/13/20	7/27/103/115	-
15	CL7	aB	1218	2	2/2/10/20	2/10/86/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
15	CL7	aB	1228	2	2/2/11/20	10/15/91/115	-
17	A1JPJ	aA	4007	-	-	2/29/63/63	0/2/2/2
15	CL7	cA	1124	21	2/2/12/20	4/21/97/115	-
16	PQN	bA	2001	-	-	4/23/43/43	0/2/2/2
15	CL7	aB	1207	2	2/2/15/20	15/39/115/115	-
15	CL7	cB	1227	2	2/2/11/20	5/15/91/115	-
15	CL7	bB	1229	2	2/2/15/20	10/39/115/115	-
15	CL7	cA	1115	1	2/2/10/20	4/10/86/115	-
15	CL7	bB	1214	2	2/2/12/20	6/21/97/115	-
15	CL7	bB	1201	2	2/2/12/20	13/26/102/115	-
15	CL7	bA	1123	21	2/2/15/20	13/39/115/115	-
17	A1JPJ	bA	4014	-	-	7/29/63/63	0/2/2/2
15	CL7	cL	1502	10	2/2/15/20	19/39/115/115	-
15	CL7	aA	1124	21	2/2/12/20	4/21/97/115	-
17	A1JPJ	bB	4015	-	-	2/29/63/63	0/2/2/2
15	CL7	aI	1601	21	2/2/15/20	13/39/115/115	-
15	CL7	aB	1215	2	2/2/13/20	11/27/103/115	-
15	CL7	cB	1012	21	2/2/15/20	15/39/115/115	-
15	CL7	cF	1701	6	2/2/10/20	1/10/86/115	-
15	CL7	cB	1218	2	2/2/10/20	4/10/86/115	-
15	CL7	cA	1111	1	2/2/15/20	13/39/115/115	-
15	CL7	cB	1204	2	2/2/15/20	6/39/115/115	-
15	CL7	aA	1104	1	2/2/15/20	17/39/115/115	-
15	CL7	cB	1205	2	2/2/15/20	11/39/115/115	-
15	CL7	aB	1202	2	2/2/15/20	23/39/115/115	-
15	CL7	bB	1222	21	2/2/11/20	11/15/91/115	-
15	CL7	cA	1130	1	2/2/12/20	7/23/99/115	-
17	A1JPJ	aB	4006	-	-	6/29/63/63	0/2/2/2
18	LHG	aA	5003	15	-	12/42/42/53	-
15	CL7	cB	1229	2	2/2/15/20	13/39/115/115	-
15	CL7	bB	1235	2	2/2/14/20	12/33/109/115	-
15	CL7	bK	1401	-	2/2/11/20	7/15/91/115	-
15	CL7	cB	1215	2	2/2/13/20	7/27/103/115	-
15	CL7	bA	1140	1	2/2/14/20	15/33/109/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
15	CL7	bB	1205	2	2/2/15/20	11/39/115/115	-
15	CL7	bK	1402	9	2/2/8/20	2/4/76/115	-
15	CL7	cB	1208	2	2/2/15/20	11/39/115/115	-
15	CL7	aA	1130	1	2/2/12/20	7/23/99/115	-
15	CL7	cA	1122	1	2/2/15/20	9/39/115/115	-
15	CL7	aA	1118	1	2/2/13/20	11/27/103/115	-
15	CL7	aK	1401	-	2/2/11/20	7/15/91/115	-
15	CL7	aA	1113	1	2/2/11/20	11/15/91/115	-
15	CL7	aB	1236	2	2/2/11/20	7/15/91/115	-
15	CL7	cA	1127	1	2/2/15/20	16/39/115/115	-
15	CL7	aB	1234	2	2/2/12/20	7/21/97/115	-
15	CL7	aA	1107	1	2/2/11/20	4/15/91/115	-
15	CL7	bB	1234	2	2/2/12/20	8/21/97/115	-
15	CL7	cB	1214	2	2/2/12/20	3/21/97/115	-
15	CL7	bA	1117	1	2/2/15/20	16/39/115/115	-
17	A1JPJ	bA	4003	-	-	2/29/63/63	0/2/2/2
15	CL7	aA	1129	1	2/2/12/20	7/21/97/115	-
15	CL7	aB	1216	21	2/2/11/20	5/15/91/115	-
15	CL7	bA	1138	1	2/2/15/20	10/39/115/115	-
17	A1JPJ	aL	4023	-	-	2/29/63/63	0/2/2/2
15	CL7	bA	1110	21	2/2/11/20	11/15/91/115	-
15	CL7	bB	1218	2	2/2/10/20	4/10/86/115	-
15	CL7	cA	1107	1	2/2/11/20	4/15/91/115	-
15	CL7	bB	1216	21	2/2/11/20	4/15/91/115	-
15	CL7	aB	1217	2	2/2/10/20	2/10/86/115	-
15	CL7	cA	1801	18	2/2/10/20	7/10/86/115	-
13	G9R	bA	1011	1	1/1/15/20	11/39/115/115	-
15	CL7	cB	1239	2	2/2/15/20	10/39/115/115	-
15	CL7	aB	1205	2	2/2/15/20	12/39/115/115	-
17	A1JPJ	cJ	4012	-	-	2/29/63/63	0/2/2/2
17	A1JPJ	aA	4003	-	-	2/29/63/63	0/2/2/2
15	CL7	bB	1223	2	2/2/15/20	16/39/115/115	-
19	LMG	aB	5002	-	-	15/48/68/70	0/1/1/1
15	CL7	aB	1206	2	2/2/12/20	7/21/97/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
15	CL7	bL	1502	10	2/2/15/20	18/39/115/115	-
15	CL7	aA	1136	1	2/2/15/20	19/39/115/115	-
15	CL7	aB	1229	2	2/2/15/20	11/39/115/115	-
16	PQN	aB	2002	-	-	6/23/43/43	0/2/2/2
15	CL7	aA	1101	1	2/2/10/20	2/10/86/115	-
17	A1JPJ	cA	4007	-	-	2/29/63/63	0/2/2/2
15	CL7	aB	1226	2	2/2/15/20	13/39/115/115	-
18	LHG	cA	5001	-	-	18/53/53/53	-
15	CL7	bB	1206	2	2/2/12/20	6/21/97/115	-
15	CL7	bB	1209	2	2/2/11/20	8/15/91/115	-
15	CL7	cJ	1302	8	2/2/10/20	0/9/85/115	-
15	CL7	aA	1103	1	2/2/15/20	15/39/115/115	-
17	A1JPJ	aB	4017	-	-	4/29/63/63	0/2/2/2
15	CL7	aA	1102	15,1	2/2/12/20	8/24/100/115	-
15	CL7	aA	1116	1	2/2/14/20	11/33/109/115	-
15	CL7	bB	1232	21	2/2/10/20	4/10/86/115	-
17	A1JPJ	cB	4010	-	-	7/29/63/63	0/2/2/2
15	CL7	aA	1139	21	2/2/11/20	10/15/91/115	-
15	CL7	aA	1138	1	2/2/15/20	10/39/115/115	-
15	CL7	aB	1223	2	2/2/15/20	17/39/115/115	-
15	CL7	bF	1701	6	2/2/10/20	4/10/86/115	-
13	G9R	cA	1011	1	1/1/15/20	11/39/115/115	-
15	CL7	bA	1136	1	2/2/15/20	17/39/115/115	-
18	LHG	cA	5003	15	-	11/42/42/53	-
15	CL7	aA	1132	1	2/2/15/20	12/39/115/115	-
15	CL7	cB	1237	21	2/2/15/20	15/39/115/115	-
15	CL7	cA	1125	1	2/2/12/20	2/21/97/115	-
15	CL7	cA	1112	1	2/2/15/20	15/39/115/115	-
15	CL7	aA	1131	1	2/2/15/20	5/39/115/115	-
17	A1JPJ	bA	4007	-	-	2/29/63/63	0/2/2/2
15	CL7	cA	1101	1	2/2/10/20	2/10/86/115	-
15	CL7	cB	1225	2	2/2/15/20	12/39/115/115	-
15	CL7	cA	1136	1	2/2/15/20	21/39/115/115	-
17	A1JPJ	aA	4011	-	-	6/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
15	CL7	aK	1402	9	2/2/8/20	0/4/76/115	-
15	CL7	aB	1224	2	2/2/13/20	13/29/105/115	-
17	A1JPJ	cB	4005	-	-	6/29/63/63	0/2/2/2
15	CL7	cB	1217	2	2/2/10/20	0/10/86/115	-

The worst 5 of 3538 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	aA	1013	PHO	C1B-C2B	8.92	1.49	1.39
14	cA	1013	PHO	C1B-C2B	8.87	1.49	1.39
14	bA	1013	PHO	C1B-C2B	8.75	1.49	1.39
14	bB	1023	PHO	C1B-C2B	8.59	1.49	1.39
14	cB	1023	PHO	C1B-C2B	8.53	1.49	1.39

The worst 5 of 2505 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	cA	1013	PHO	C4D-CHA-CBD	-8.75	104.56	108.52
14	bB	1023	PHO	C4D-CHA-CBD	-8.57	104.64	108.52
17	bA	4014	A1JPJ	C15-C16-C17	8.48	140.85	123.47
14	bA	1013	PHO	C4D-CHA-CBD	-8.45	104.70	108.52
17	aA	4014	A1JPJ	C15-C16-C17	8.41	140.70	123.47

5 of 561 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
13	aA	1011	G9R	ND
13	bA	1011	G9R	ND
13	cA	1011	G9R	ND
15	aA	1022	CL7	NC
15	aA	1022	CL7	NA

5 of 3154 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
14	aA	1013	PHO	C1A-C2A-CAA-CBA
14	aA	1013	PHO	C3A-C2A-CAA-CBA
14	aB	1023	PHO	CBD-CGD-O2D-CED
14	bA	1013	PHO	C1A-C2A-CAA-CBA
14	bA	1013	PHO	C3A-C2A-CAA-CBA

There are no ring outliers.

255 monomers are involved in 737 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
15	aB	1213	CL7	1	0
15	aB	1219	CL7	2	0
15	bB	1202	CL7	4	0
15	cB	1228	CL7	3	0
15	cB	1207	CL7	3	0
15	bB	1213	CL7	3	0
15	bB	1237	CL7	3	0
15	bA	1126	CL7	7	0
15	cA	1138	CL7	1	0
15	bB	1203	CL7	2	0
15	aA	1125	CL7	2	0
15	cA	1132	CL7	2	0
15	aB	1230	CL7	1	0
15	bA	1130	CL7	2	0
15	aB	1210	CL7	7	0
15	bA	1118	CL7	3	0
15	bA	1113	CL7	1	0
15	cB	1212	CL7	2	0
15	aB	1238	CL7	5	0
15	bI	1601	CL7	2	0
15	cA	1108	CL7	2	0
15	bB	1210	CL7	5	0
15	cB	1241	CL7	2	0
15	bA	1124	CL7	1	0
15	aL	1502	CL7	2	0
15	bA	1106	CL7	6	0
15	bB	1217	CL7	2	0
15	aJ	1302	CL7	2	0
16	aA	2001	PQN	1	0
15	cA	1126	CL7	7	0
15	aA	1117	CL7	2	0
15	cB	1216	CL7	2	0
15	cA	1117	CL7	2	0
15	bA	1129	CL7	3	0
15	bB	1221	CL7	4	0
15	cB	1021	CL7	2	0
15	cB	1211	CL7	7	0
15	bA	1116	CL7	8	0
15	cA	1129	CL7	3	0
15	cJ	1301	CL7	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
14	aA	1013	PHO	3	0
15	cA	1128	CL7	4	0
15	bA	1133	CL7	7	0
15	cL	1501	CL7	3	0
15	aB	1235	CL7	3	0
15	bA	1102	CL7	2	0
15	cA	1120	CL7	3	0
15	bJ	1302	CL7	1	0
15	aA	1134	CL7	1	0
15	bB	1021	CL7	2	0
15	bA	1104	CL7	5	0
15	bB	1236	CL7	2	0
15	bA	1139	CL7	1	0
15	bB	1228	CL7	5	0
15	bA	1112	CL7	2	0
15	bB	1226	CL7	8	0
15	cB	1201	CL7	4	0
15	cB	1238	CL7	5	0
15	bB	1230	CL7	2	0
15	bB	1224	CL7	2	0
15	cA	1109	CL7	5	0
15	aA	1120	CL7	4	0
15	cB	1219	CL7	3	0
15	cB	1222	CL7	5	0
15	cB	1203	CL7	5	0
15	aA	1123	CL7	2	0
15	aA	1115	CL7	3	0
15	aA	1114	CL7	1	0
15	bA	1132	CL7	3	0
15	aA	1111	CL7	4	0
15	cB	1210	CL7	8	0
15	aB	1227	CL7	1	0
15	bA	1127	CL7	9	0
15	bB	1238	CL7	5	0
15	bA	1137	CL7	1	0
15	aA	1105	CL7	1	0
14	cA	1013	PHO	1	0
15	aA	1140	CL7	2	0
15	aA	1022	CL7	1	0
15	aB	1212	CL7	3	0
15	bB	1204	CL7	3	0
18	bA	5003	LHG	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
15	cI	1601	CL7	4	0
15	aB	1221	CL7	4	0
15	cB	1223	CL7	4	0
15	aB	1204	CL7	4	0
15	bB	1241	CL7	3	0
15	aA	1109	CL7	5	0
15	aA	1108	CL7	5	0
14	bA	1013	PHO	1	0
15	bB	1227	CL7	6	0
15	cB	1209	CL7	1	0
15	aB	1237	CL7	2	0
15	aB	1209	CL7	1	0
15	bA	1119	CL7	5	0
15	aB	1208	CL7	7	0
20	bC	3003	SF4	1	0
15	cA	1139	CL7	1	0
14	aB	1023	PHO	7	0
15	bB	1208	CL7	2	0
15	bB	1207	CL7	4	0
15	cA	1110	CL7	2	0
15	aA	1137	CL7	2	0
15	aB	1021	CL7	1	0
15	cB	1236	CL7	4	0
15	bA	1115	CL7	2	0
15	aA	1119	CL7	8	0
15	aA	1121	CL7	2	0
15	cA	1116	CL7	8	0
15	cA	1106	CL7	4	0
15	cB	1235	CL7	3	0
15	aA	1106	CL7	5	0
19	cB	5002	LMG	1	0
15	cB	1206	CL7	2	0
15	cB	1234	CL7	1	0
15	bB	1220	CL7	2	0
15	bA	1120	CL7	5	0
15	bA	1128	CL7	4	0
15	aB	1241	CL7	2	0
15	bB	1239	CL7	3	0
15	bA	1109	CL7	6	0
15	cB	1230	CL7	3	0
15	aB	1239	CL7	3	0
15	bL	1503	CL7	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
15	aB	1201	CL7	3	0
15	aA	1128	CL7	5	0
17	aB	4005	A1JPJ	1	0
15	cB	1220	CL7	3	0
15	aL	1503	CL7	2	0
19	bB	5002	LMG	3	0
15	aB	1220	CL7	1	0
15	cA	1102	CL7	2	0
14	cB	1023	PHO	7	0
15	bA	1105	CL7	1	0
15	bA	1103	CL7	9	0
15	cA	1137	CL7	2	0
15	cA	1104	CL7	6	0
15	bA	1101	CL7	6	0
15	aB	1211	CL7	3	0
15	bL	1501	CL7	3	0
15	bA	1111	CL7	4	0
15	cB	1224	CL7	2	0
15	cB	1202	CL7	7	0
15	bA	1108	CL7	4	0
15	bB	1215	CL7	1	0
15	cB	1213	CL7	2	0
15	cA	1103	CL7	6	0
15	aB	1214	CL7	1	0
15	cA	1119	CL7	4	0
15	cA	1118	CL7	4	0
15	cA	1123	CL7	5	0
14	bB	1023	PHO	6	0
15	bA	1125	CL7	3	0
17	bL	4023	A1JPJ	1	0
15	cA	1133	CL7	3	0
15	cA	1140	CL7	2	0
15	aA	1126	CL7	7	0
18	bA	5001	LHG	3	0
15	bA	1121	CL7	2	0
15	aA	1110	CL7	2	0
15	bB	1219	CL7	2	0
15	cA	1121	CL7	2	0
15	aA	1133	CL7	6	0
18	aA	5001	LHG	4	0
15	bB	1212	CL7	3	0
15	aL	1501	CL7	3	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
15	cB	1231	CL7	3	0
15	cB	1226	CL7	5	0
15	aA	1127	CL7	8	0
15	aB	1203	CL7	5	0
15	cL	1503	CL7	2	0
15	bA	1122	CL7	4	0
15	cA	1105	CL7	1	0
15	cB	1221	CL7	5	0
15	aA	1112	CL7	3	0
15	aA	1122	CL7	3	0
15	aB	1222	CL7	3	0
15	bB	1211	CL7	4	0
15	aB	1218	CL7	2	0
15	aB	1228	CL7	5	0
15	cA	1124	CL7	1	0
16	bA	2001	PQN	2	0
15	aB	1207	CL7	3	0
15	cB	1227	CL7	5	0
15	bB	1229	CL7	4	0
15	cA	1115	CL7	2	0
15	bB	1214	CL7	4	0
15	bB	1201	CL7	2	0
15	bA	1123	CL7	4	0
17	bA	4014	A1JPJ	1	0
15	cL	1502	CL7	2	0
15	aA	1124	CL7	1	0
15	aI	1601	CL7	6	0
15	aB	1215	CL7	1	0
15	cB	1218	CL7	4	0
15	cA	1111	CL7	3	0
15	cB	1204	CL7	5	0
15	aA	1104	CL7	4	0
15	cB	1205	CL7	3	0
15	aB	1202	CL7	5	0
15	bB	1222	CL7	3	0
15	cA	1130	CL7	2	0
18	aA	5003	LHG	1	0
15	cB	1229	CL7	5	0
15	bB	1235	CL7	7	0
15	cB	1215	CL7	2	0
15	bA	1140	CL7	3	0
15	bB	1205	CL7	4	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
15	bK	1402	CL7	1	0
15	cB	1208	CL7	6	0
15	aA	1130	CL7	2	0
15	cA	1122	CL7	4	0
15	aA	1118	CL7	4	0
15	aA	1113	CL7	4	0
15	aB	1236	CL7	1	0
15	cA	1127	CL7	7	0
15	aB	1234	CL7	1	0
15	cB	1214	CL7	3	0
15	bA	1117	CL7	2	0
15	aA	1129	CL7	5	0
15	aB	1216	CL7	3	0
15	bA	1138	CL7	5	0
17	aL	4023	A1JPJ	1	0
15	bA	1110	CL7	2	0
15	bB	1218	CL7	3	0
15	bB	1216	CL7	1	0
15	cB	1239	CL7	4	0
15	aB	1205	CL7	4	0
15	bB	1223	CL7	3	0
19	aB	5002	LMG	3	0
15	aB	1206	CL7	1	0
15	bL	1502	CL7	2	0
15	aA	1136	CL7	1	0
15	aB	1229	CL7	6	0
15	aA	1101	CL7	4	0
15	aB	1226	CL7	7	0
18	cA	5001	LHG	6	0
15	bB	1209	CL7	1	0
15	cJ	1302	CL7	3	0
15	aA	1103	CL7	4	0
15	aA	1102	CL7	1	0
15	aA	1116	CL7	4	0
15	aA	1138	CL7	6	0
15	aB	1223	CL7	4	0
15	bA	1136	CL7	1	0
18	cA	5003	LHG	2	0
15	aA	1132	CL7	2	0
15	cB	1237	CL7	3	0
15	cA	1112	CL7	2	0
15	aA	1131	CL7	2	0

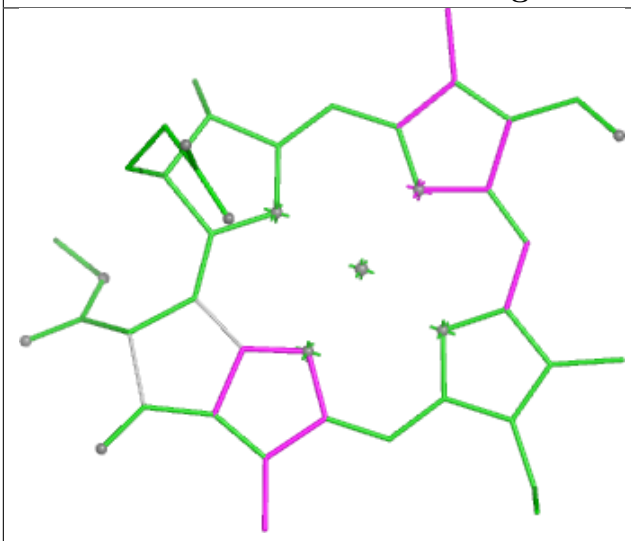
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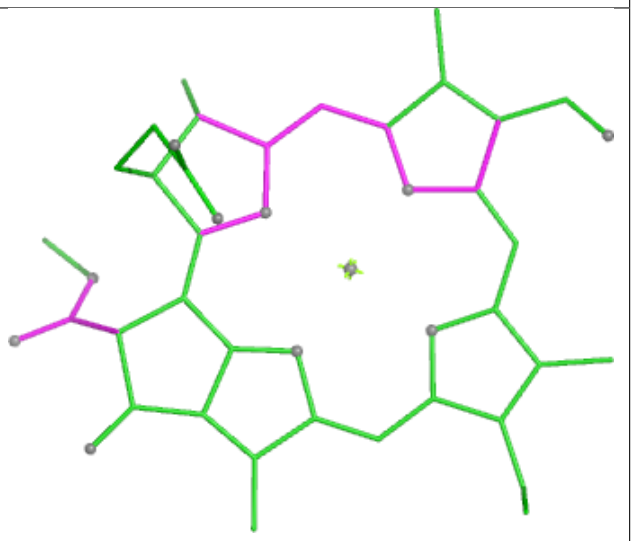
Mol	Chain	Res	Type	Clashes	Symm-Clashes
15	cA	1101	CL7	5	0
15	cA	1136	CL7	1	0
15	aK	1402	CL7	2	0
15	aB	1224	CL7	4	0
17	cB	4005	A1JPJ	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

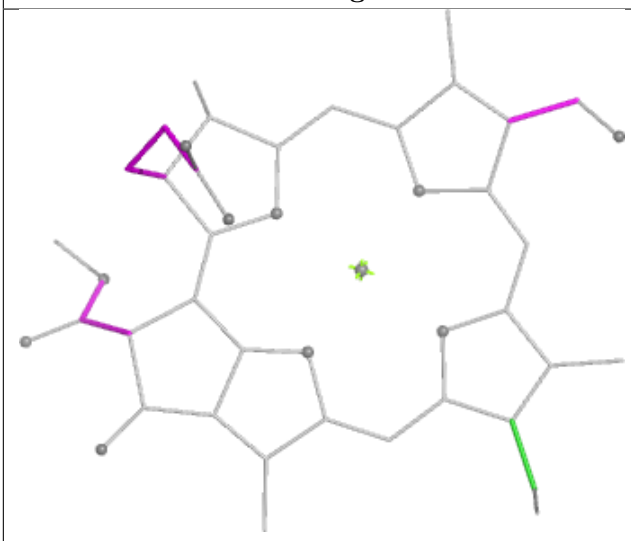
Ligand CL7 aB 1213



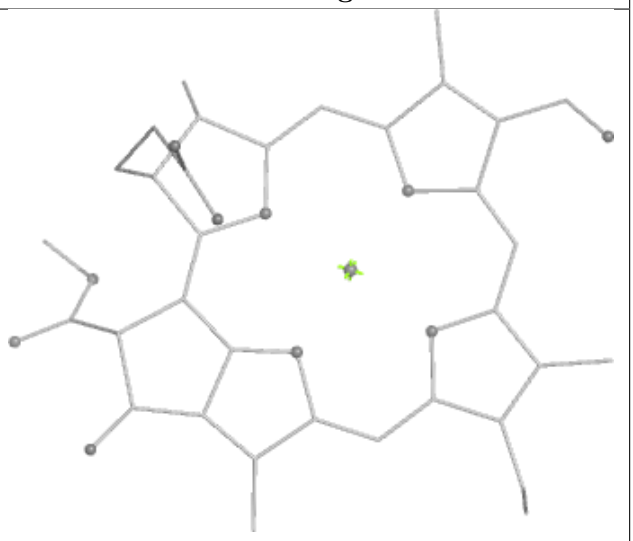
Bond lengths



Bond angles

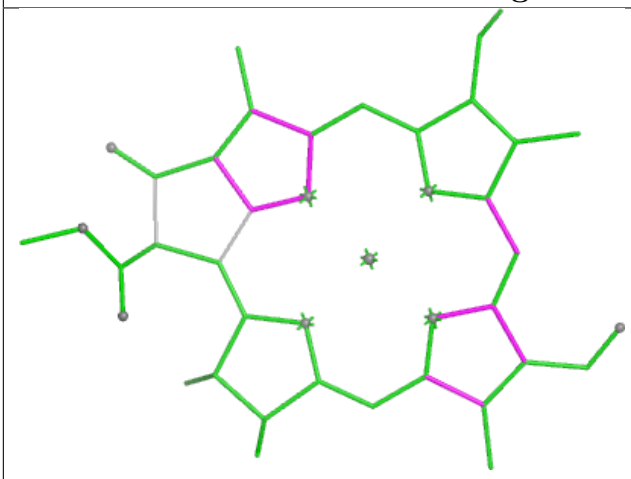


Torsions

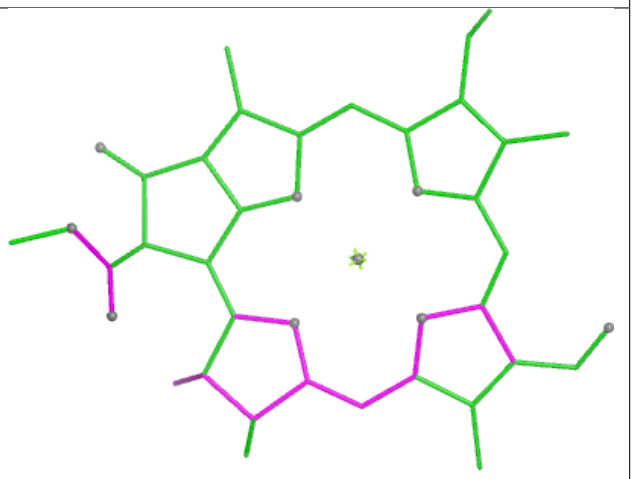


Rings

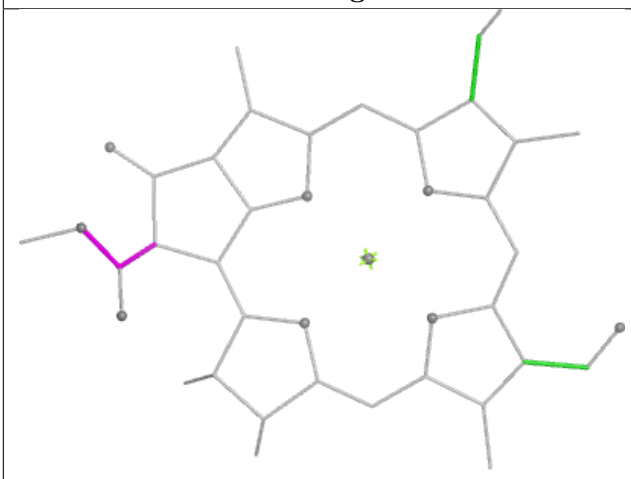
Ligand CL7 aB 1219



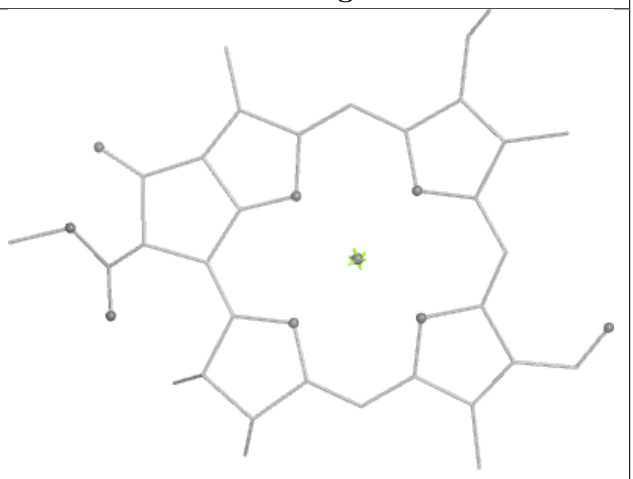
Bond lengths



Bond angles

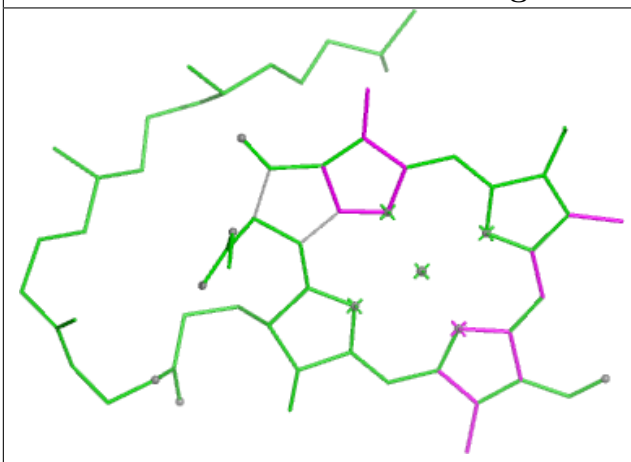


Torsions

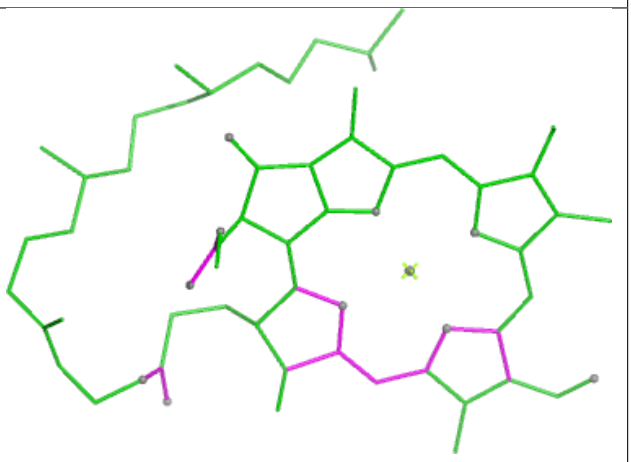


Rings

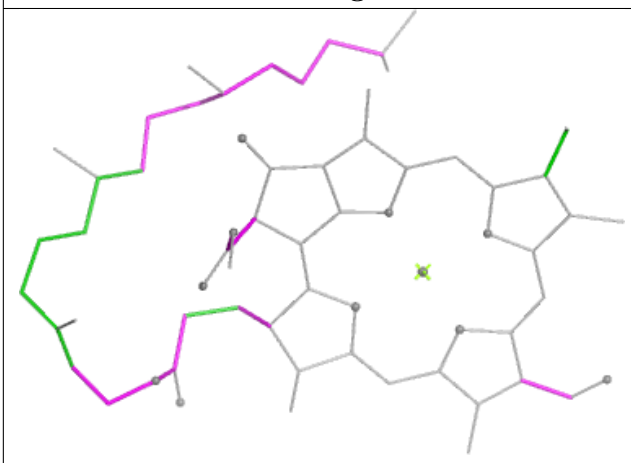
Ligand CL7 bB 1202



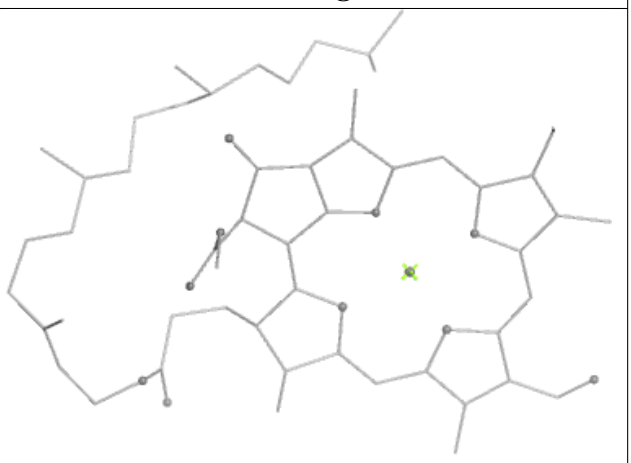
Bond lengths



Bond angles

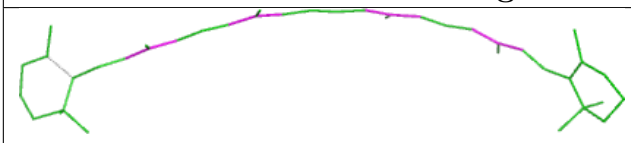


Torsions



Rings

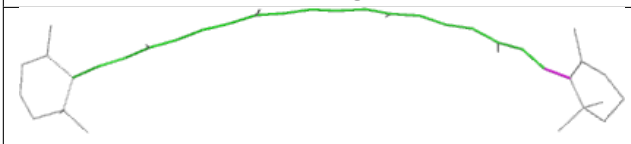
Ligand A1JPJ aI 4018



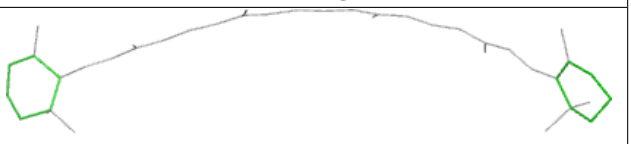
Bond lengths



Bond angles

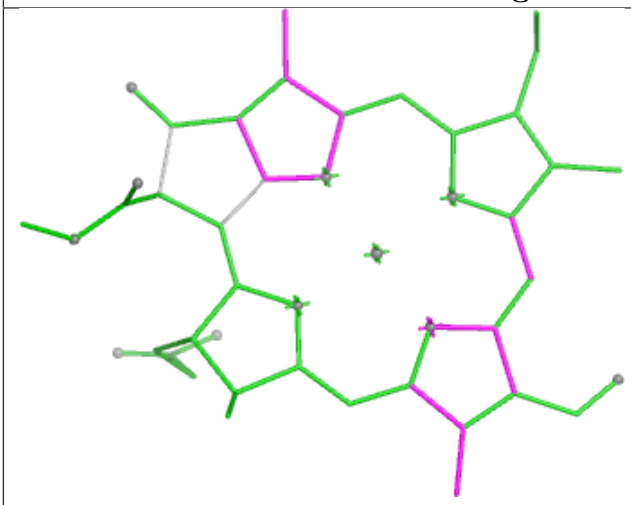


Torsions

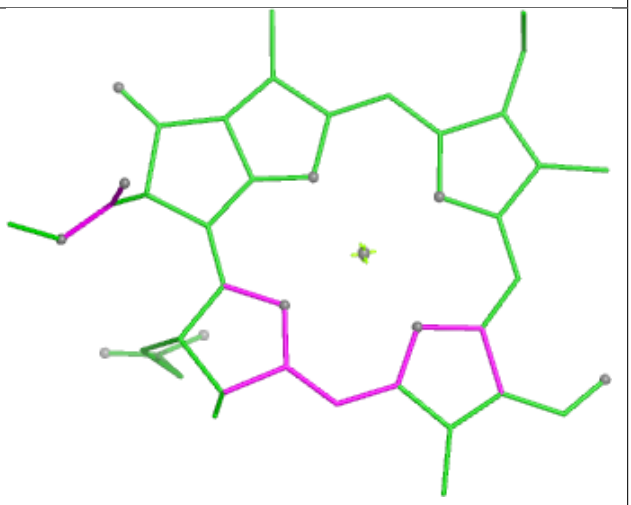


Rings

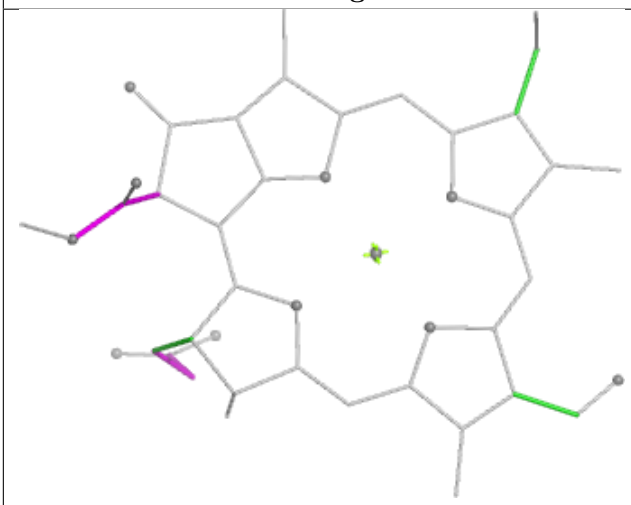
Ligand CL7 cB 1228



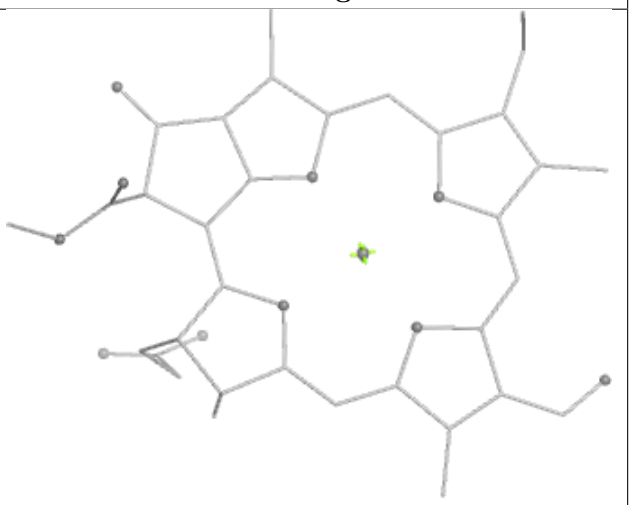
Bond lengths



Bond angles

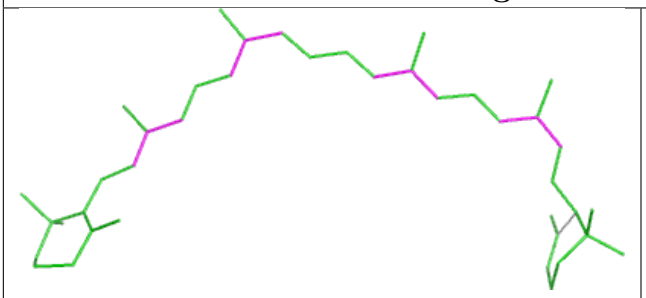


Torsions

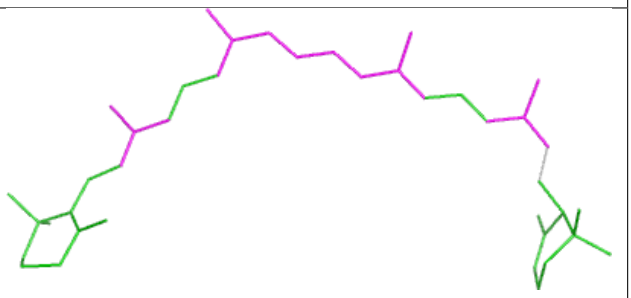


Rings

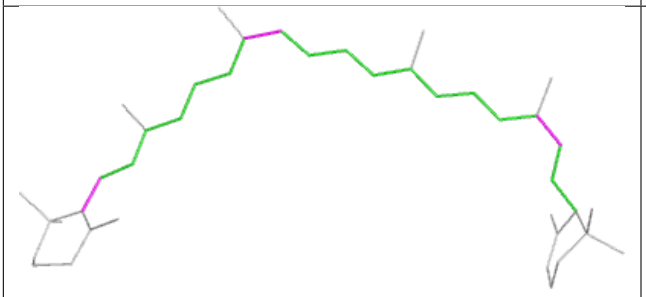
Ligand A1JPJ cF 4016



Bond lengths



Bond angles

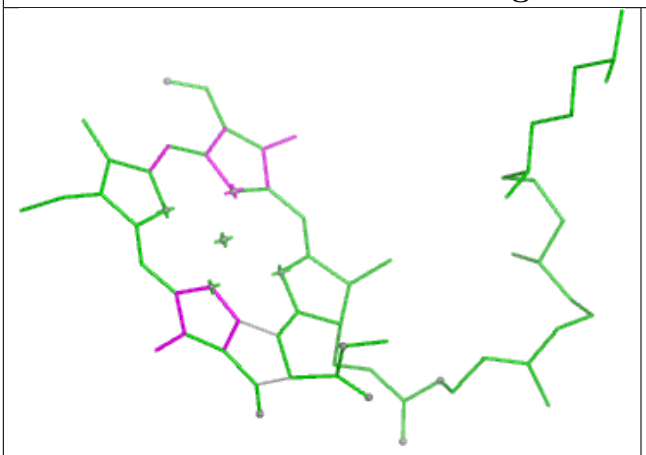


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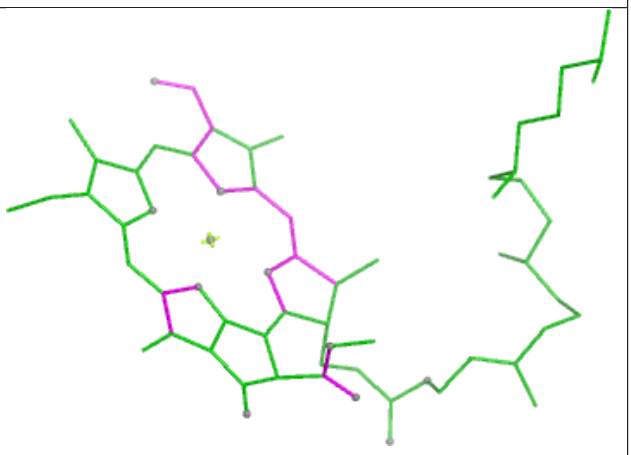


Rings

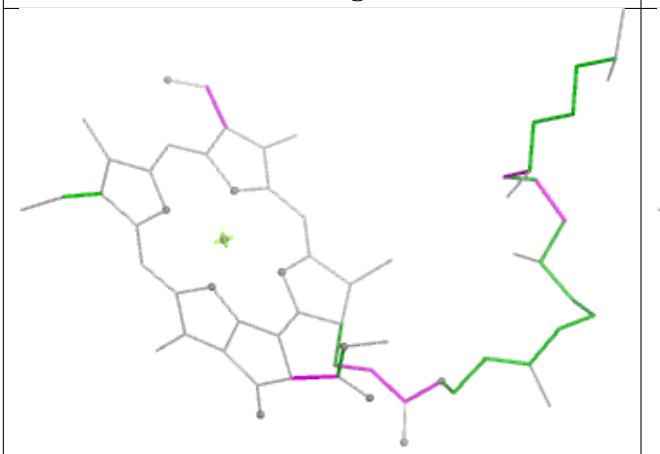
Ligand CL7 cB 1207



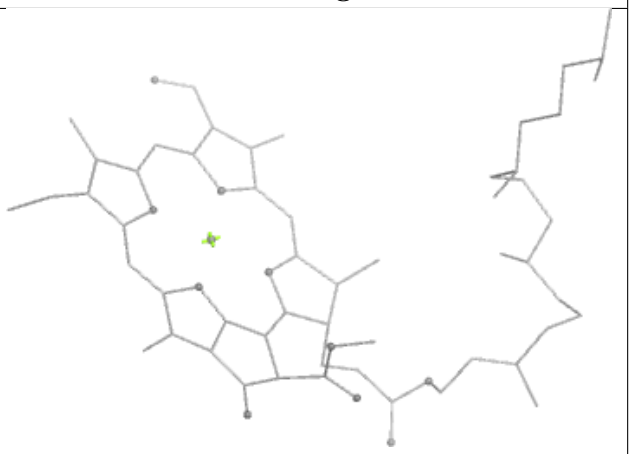
Bond lengths



Bond angles

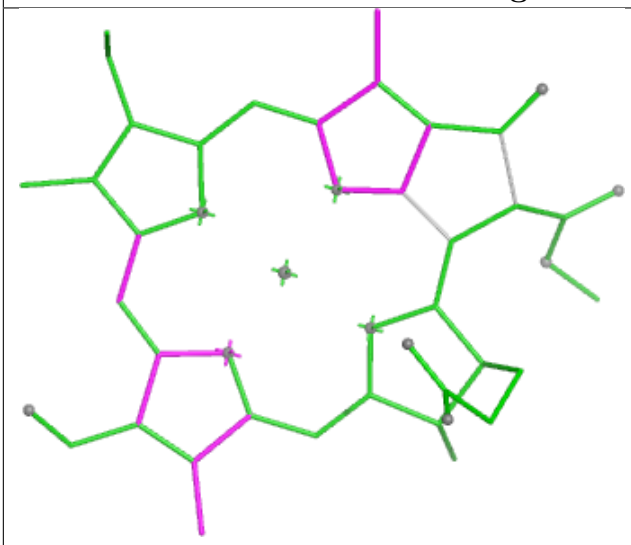


Torsions

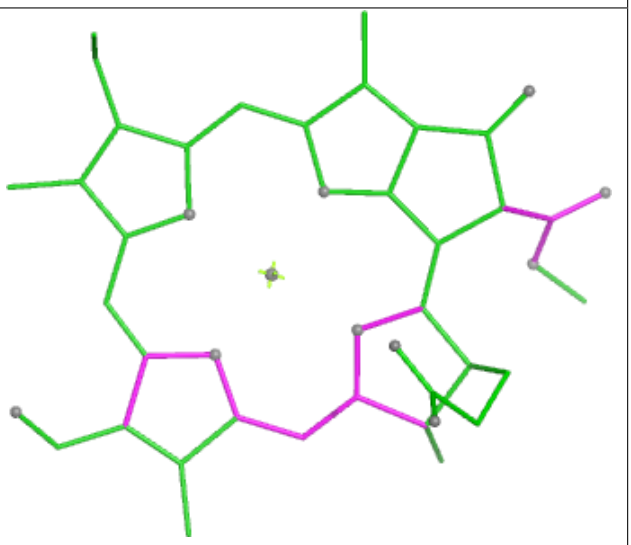


Rings

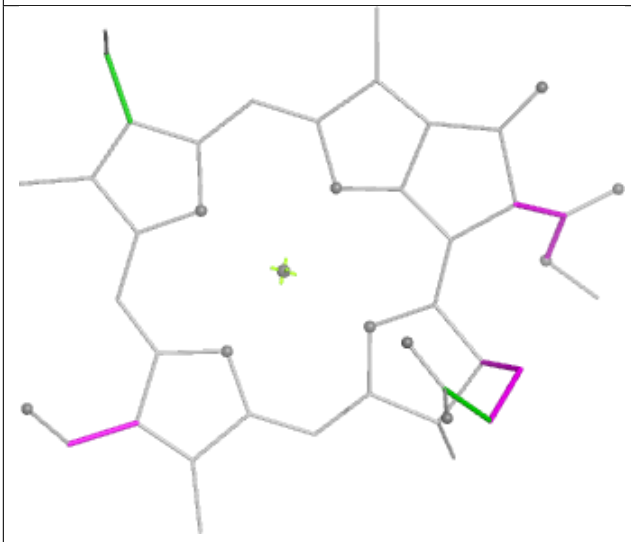
Ligand CL7 bB 1213



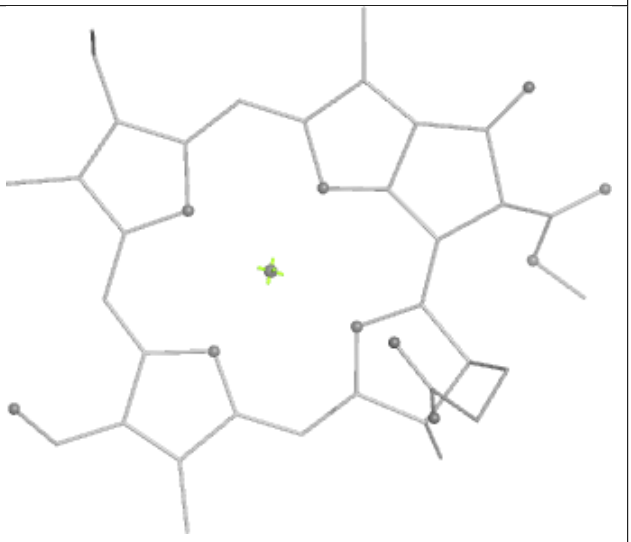
Bond lengths



Bond angles

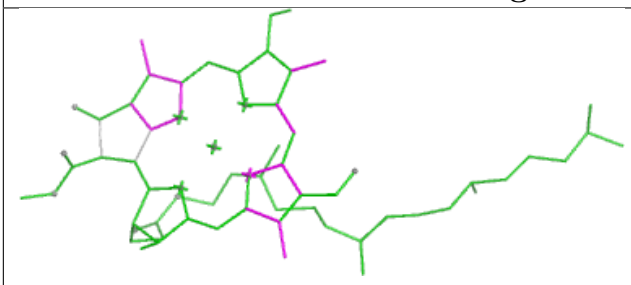


Torsions

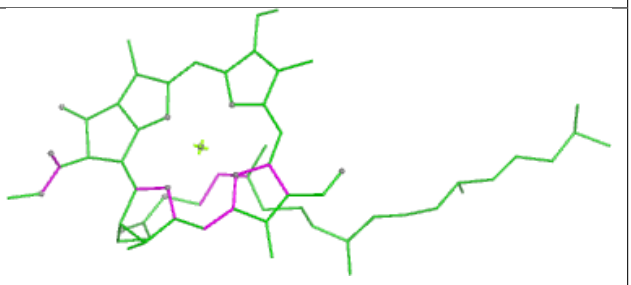


Rings

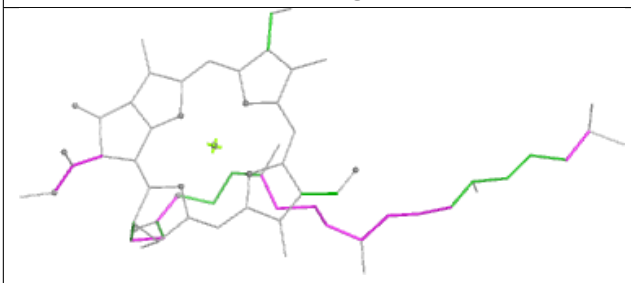
Ligand CL7 bB 1237



Bond lengths



Bond angles

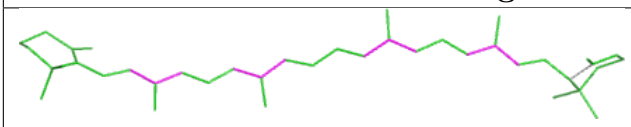


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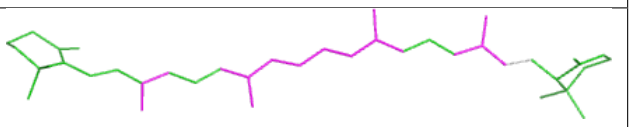


Rings

Ligand A1JPJ cI 4019



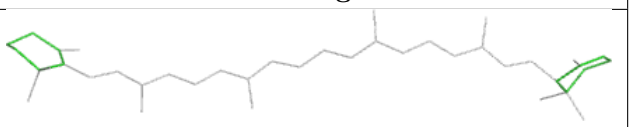
Bond lengths



Bond angles

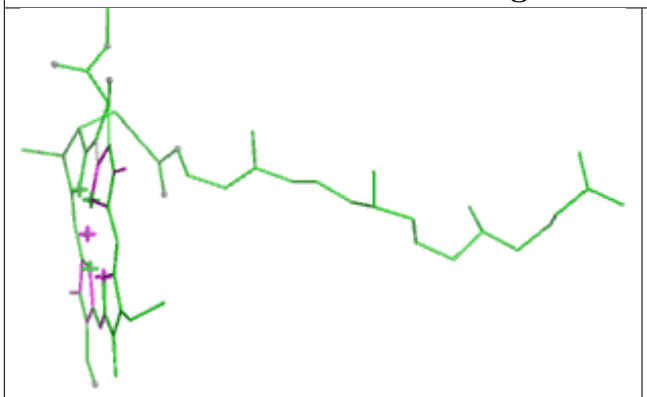


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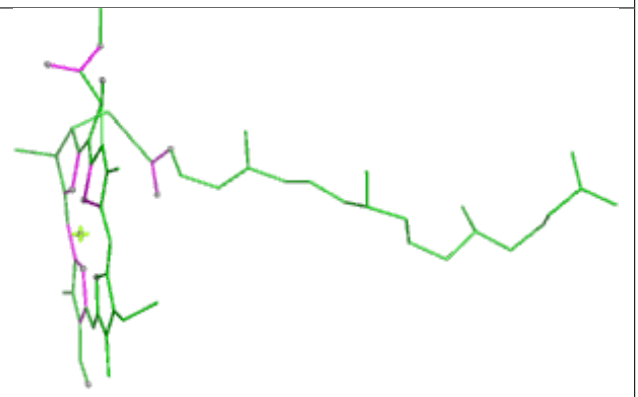


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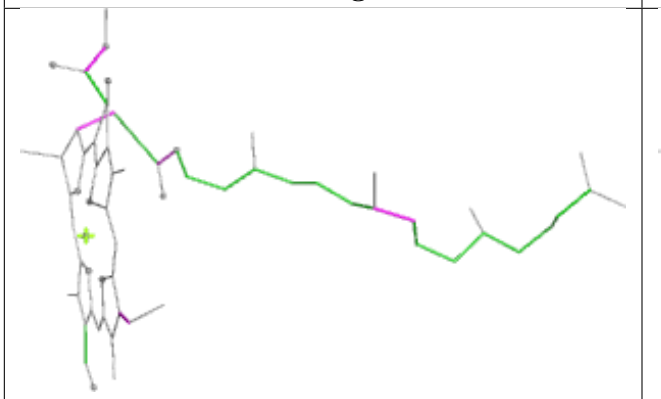
Ligand CL7 bA 1126



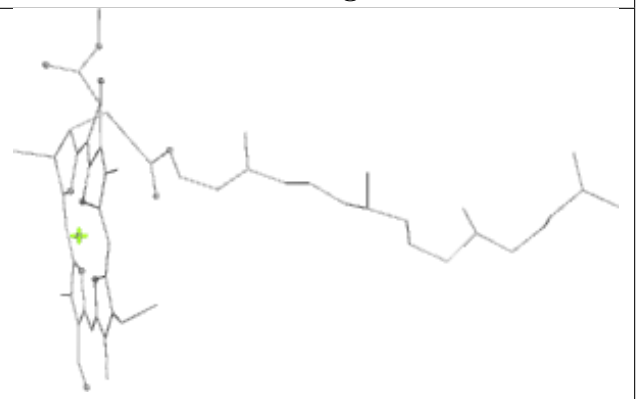
Bond lengths



Bond angles

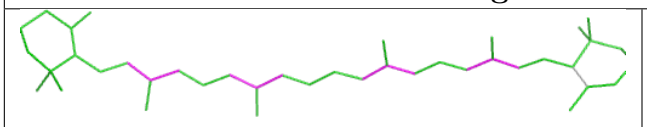


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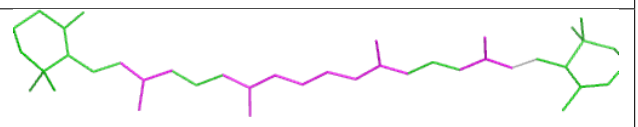


Rings

Ligand A1JPJ aA 4002



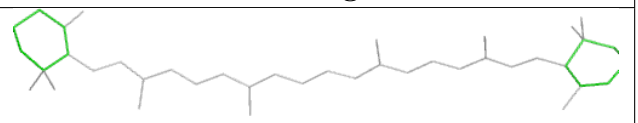
Bond lengths



Bond angles

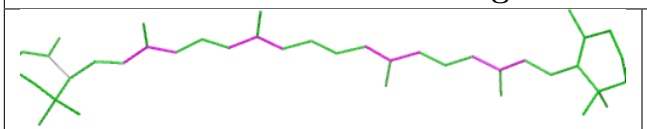


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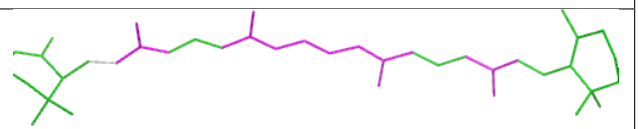


Rings

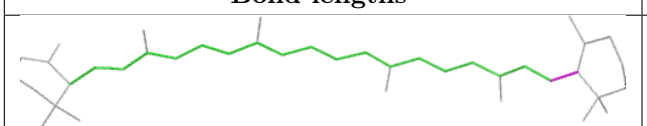
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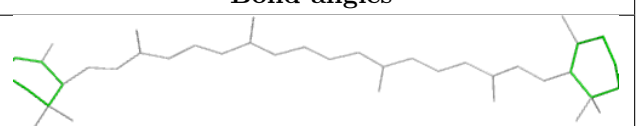
Bond lengths



Bond angles

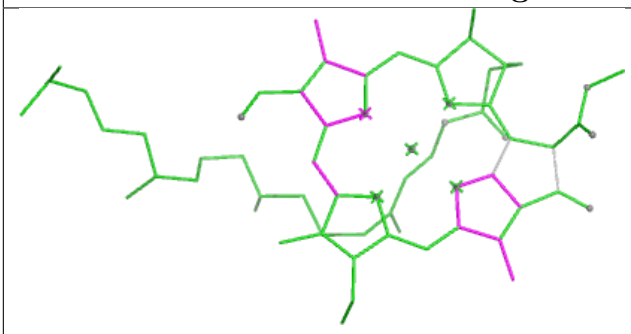


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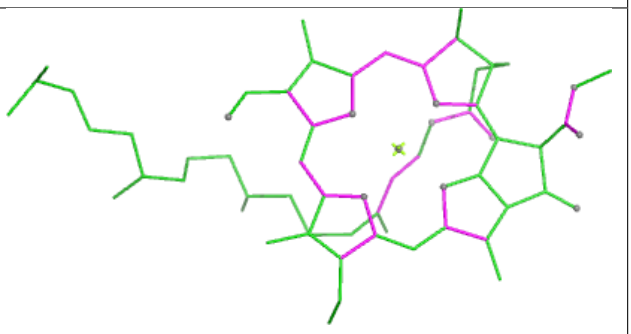


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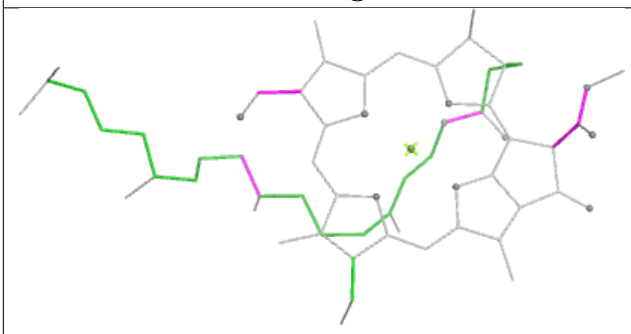
Ligand CL7 cA 1138



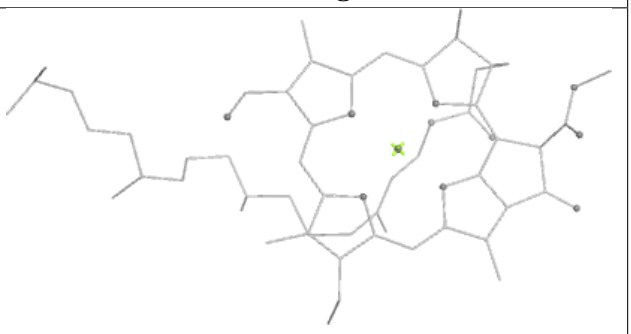
Bond lengths



Bond angles

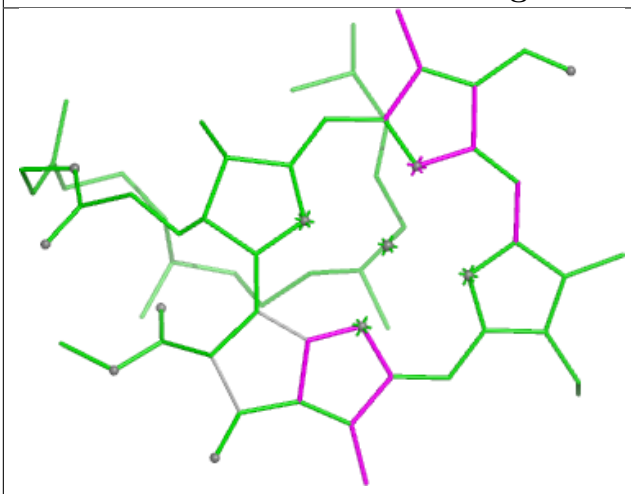


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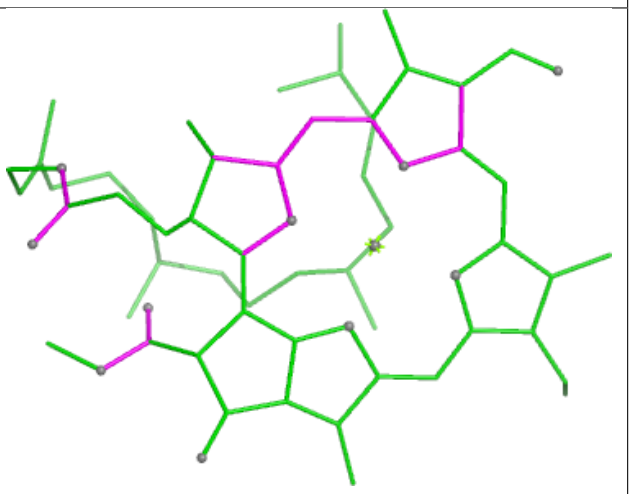


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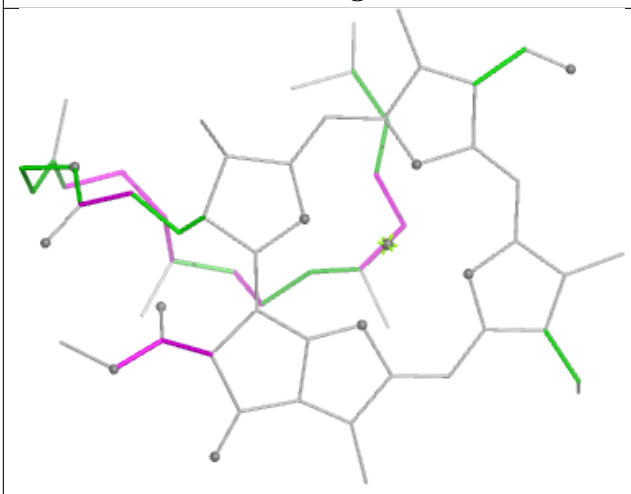
Ligand CL7 bB 1203



Bond lengths



Bond angles

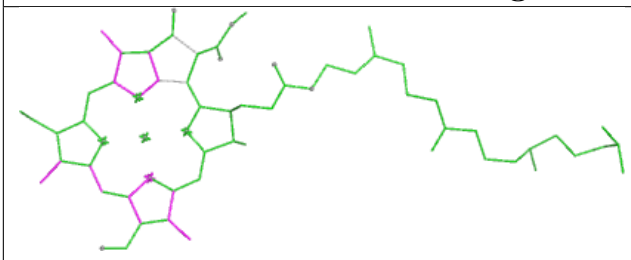


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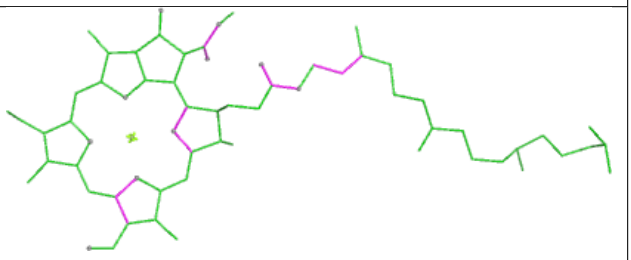


Rings

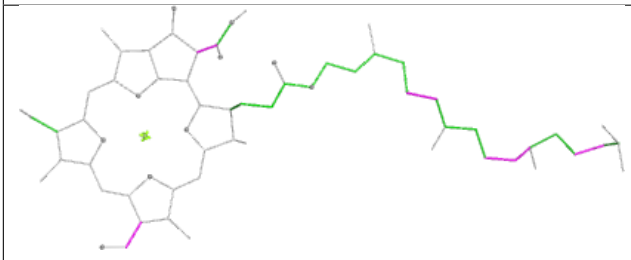
Ligand CL7 bA 1131



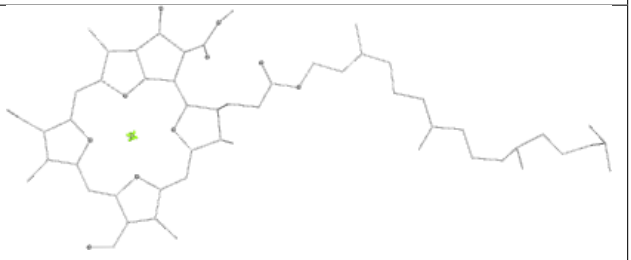
Bond lengths



Bond angles

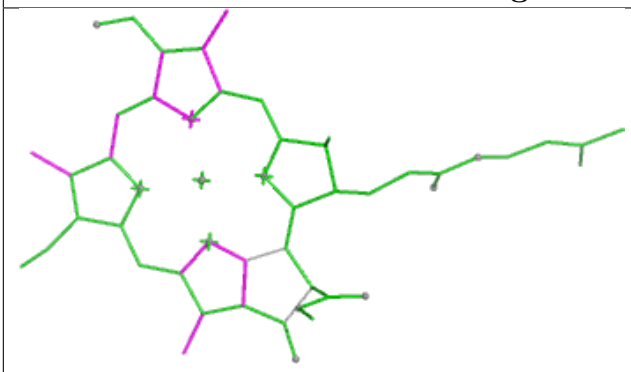


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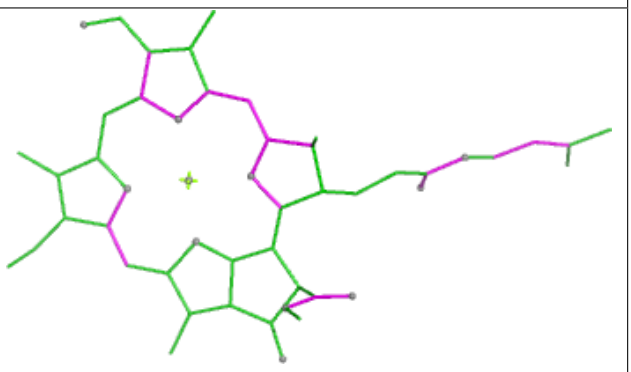


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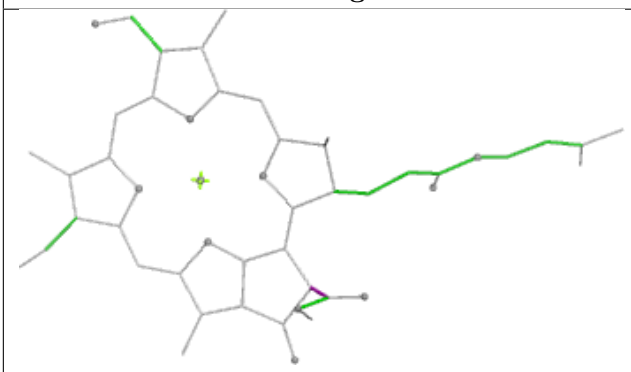
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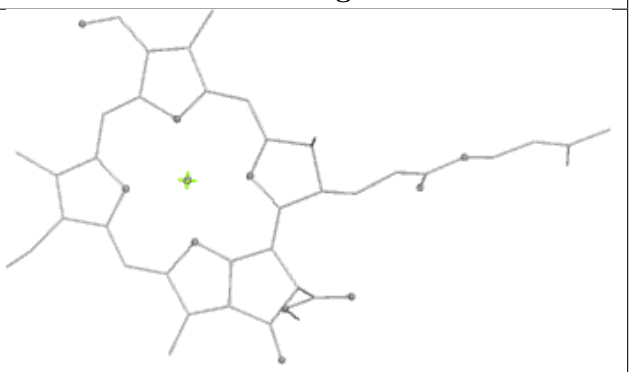
Bond lengths



Bond angles

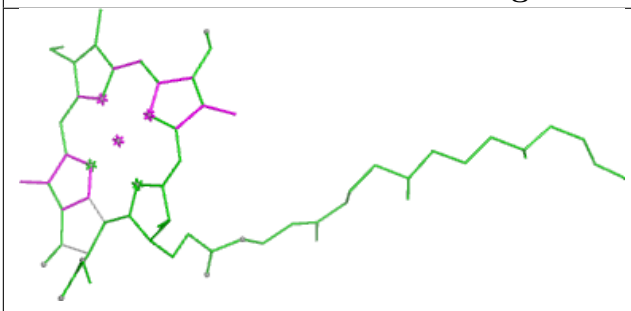


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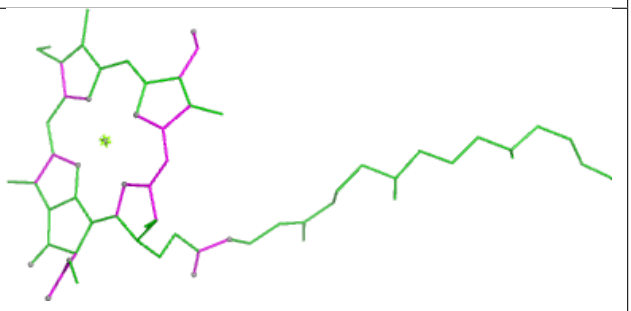


Rings

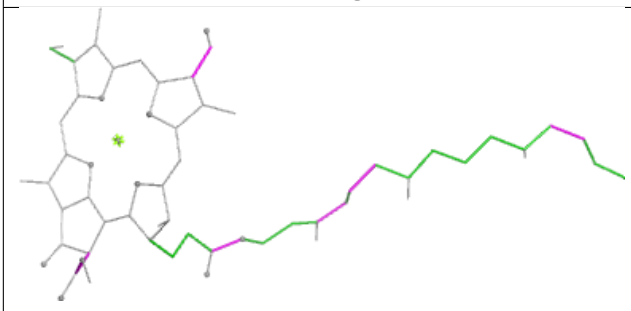
Ligand CL7 cA 1132



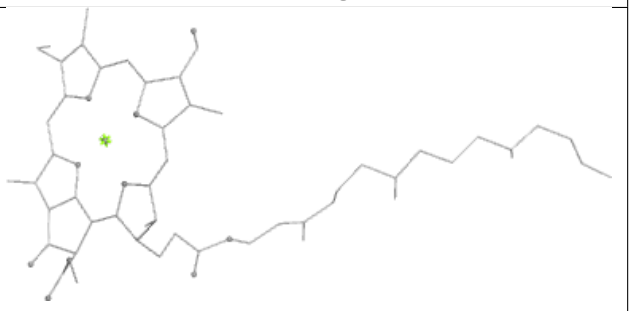
Bond lengths



Bond angles

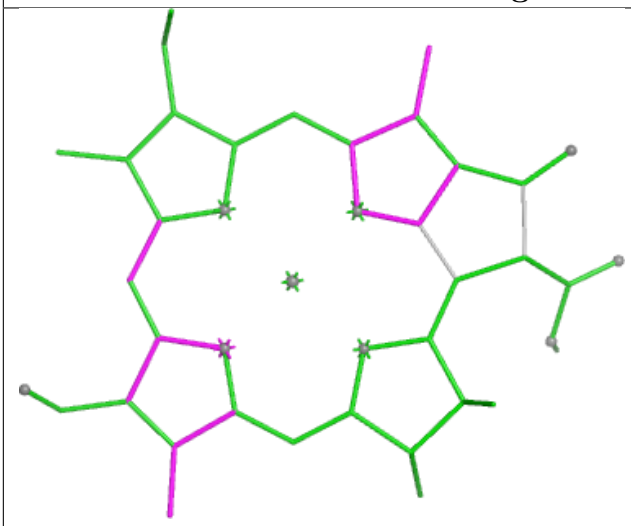


Torsions

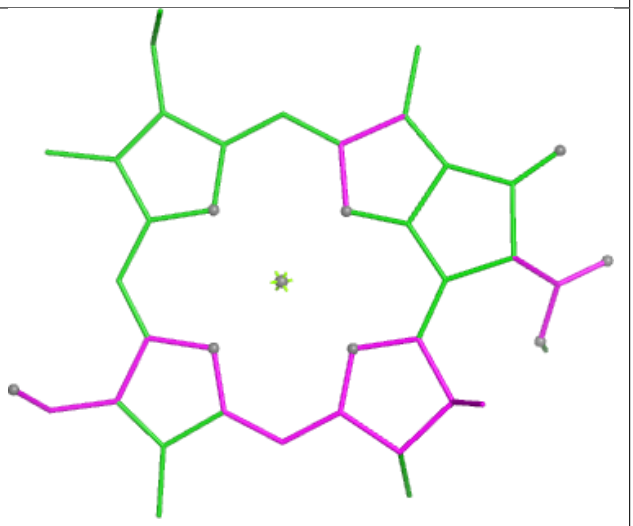


Rings

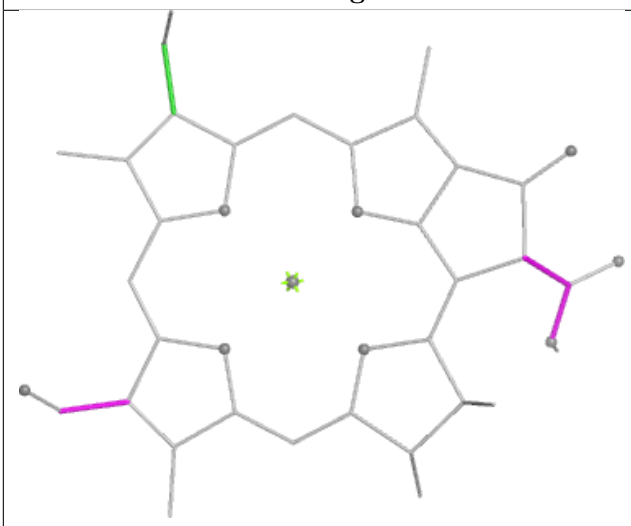
Ligand CL7 aB 1230



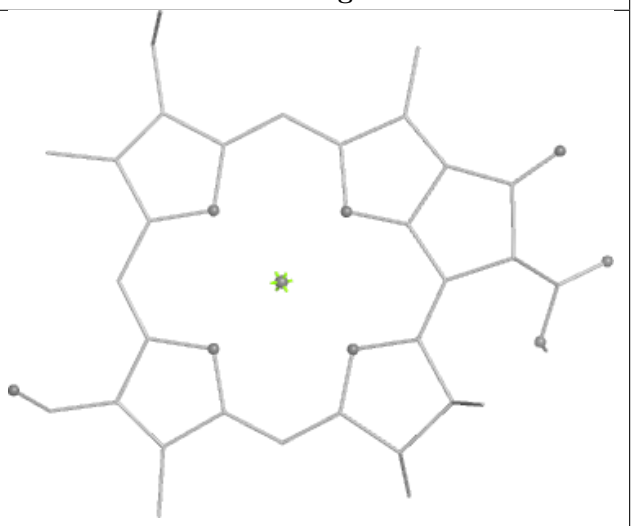
Bond lengths



Bond angles

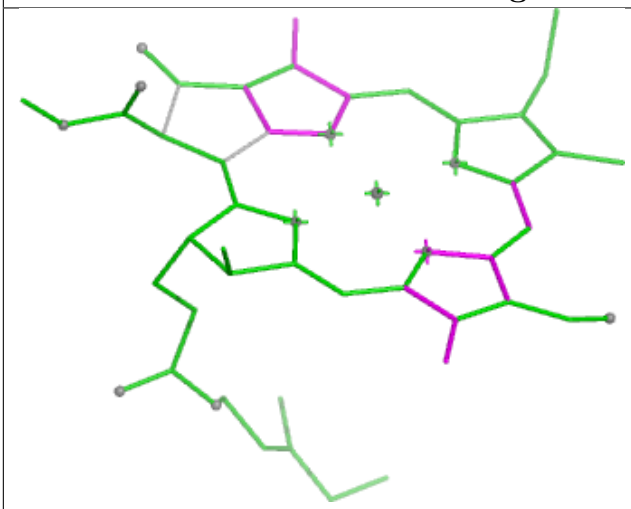


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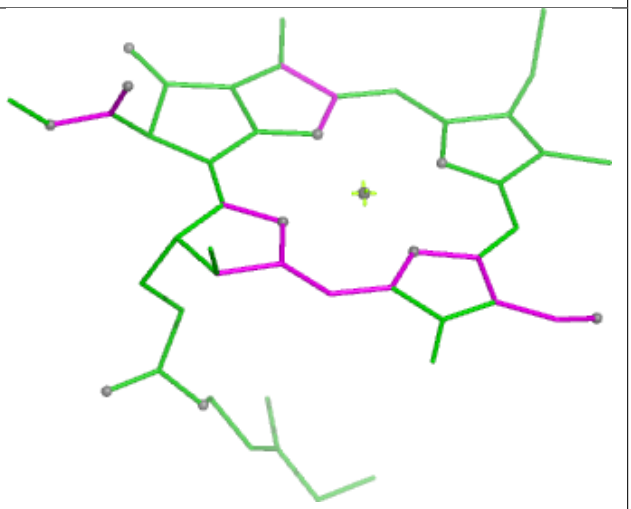


Rings

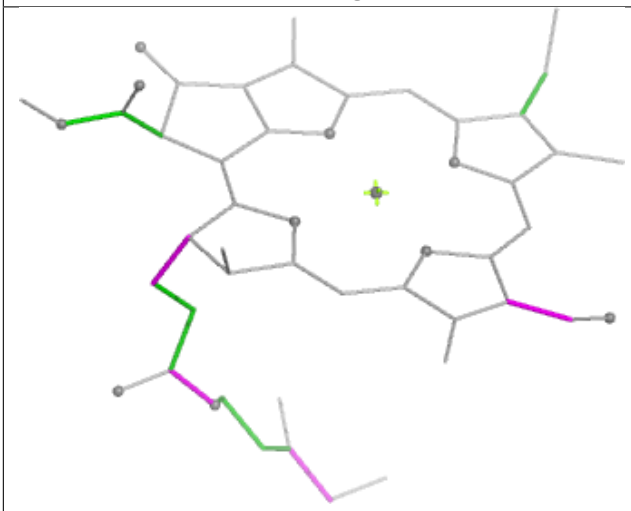
Ligand CL7 bA 1130



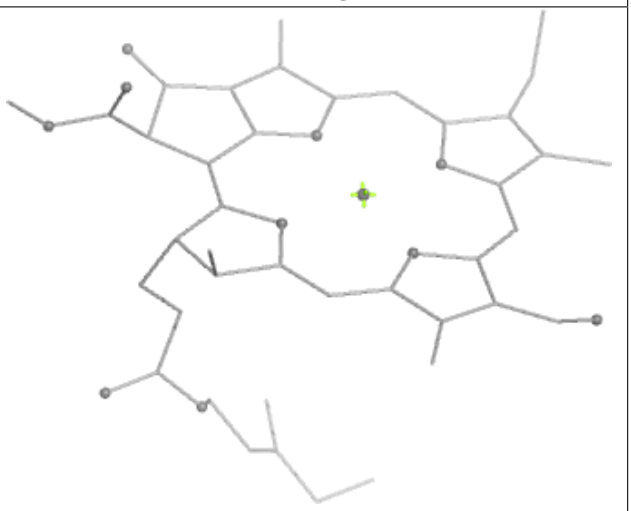
Bond lengths



Bond angles

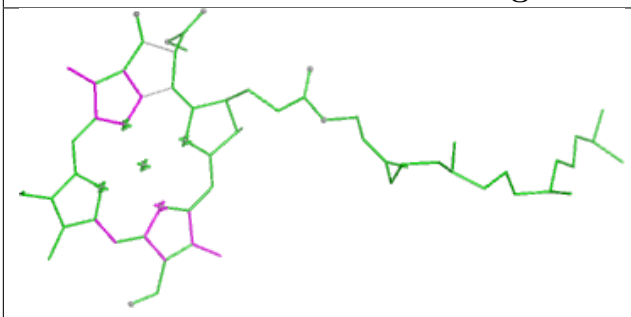


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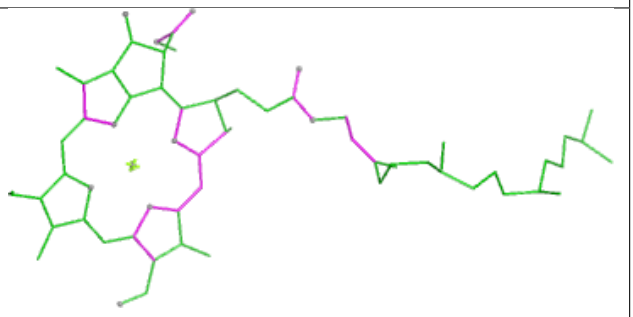


Rings

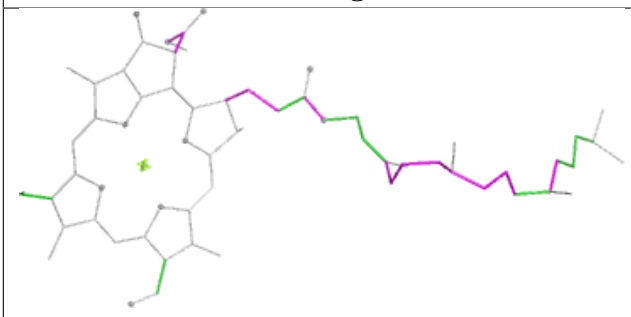
Ligand CL7 aB 1210



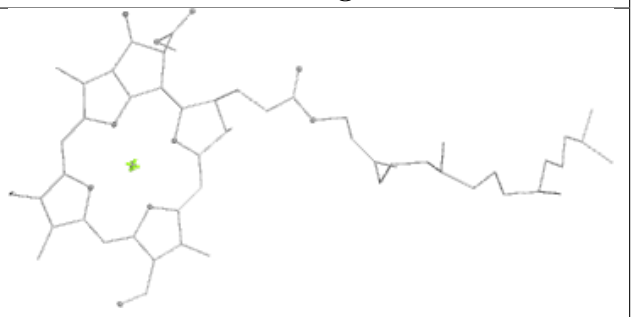
Bond lengths



Bond angles

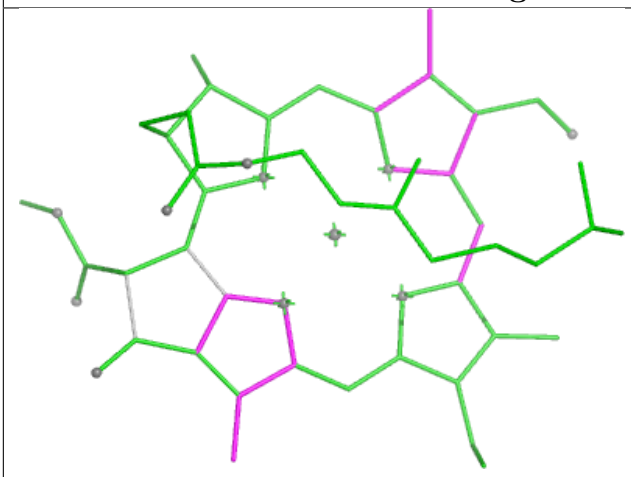


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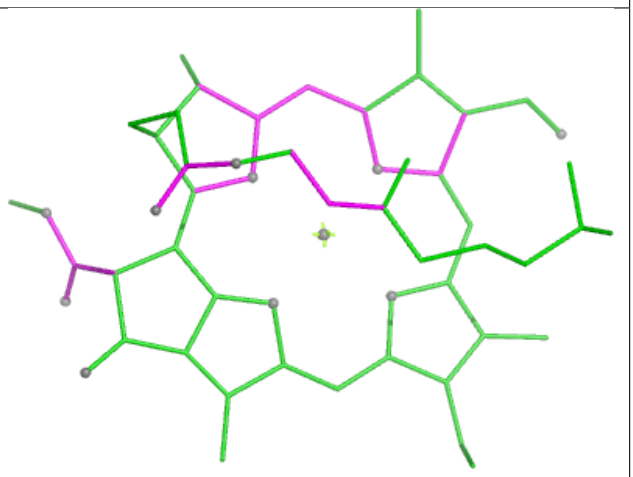


Rings

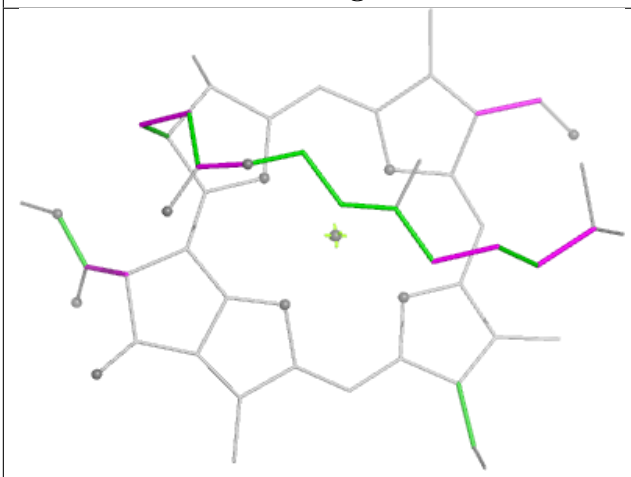
Ligand CL7 bA 1118



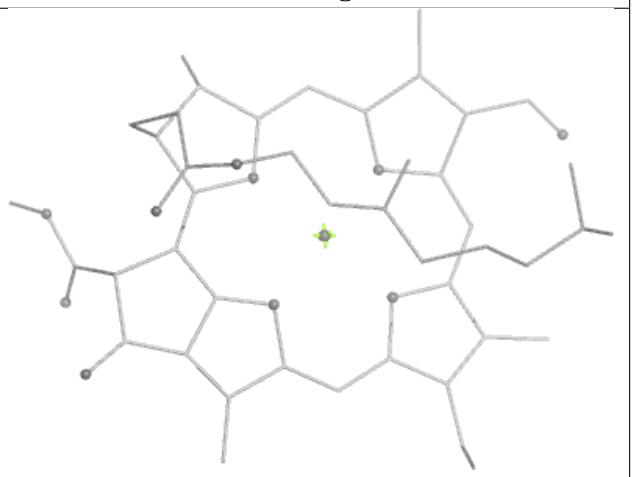
Bond lengths



Bond angles

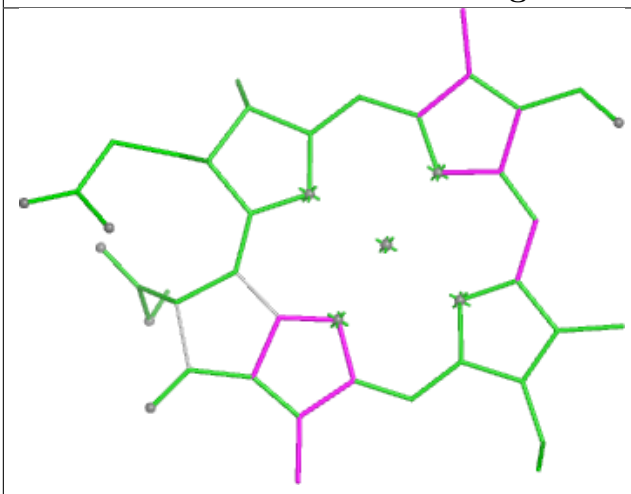


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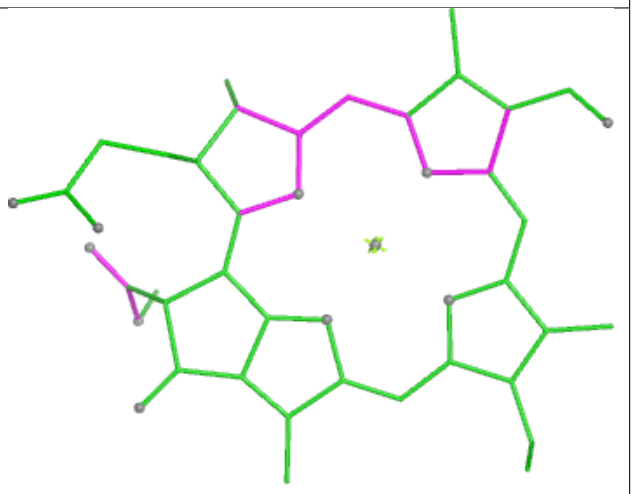


Rings

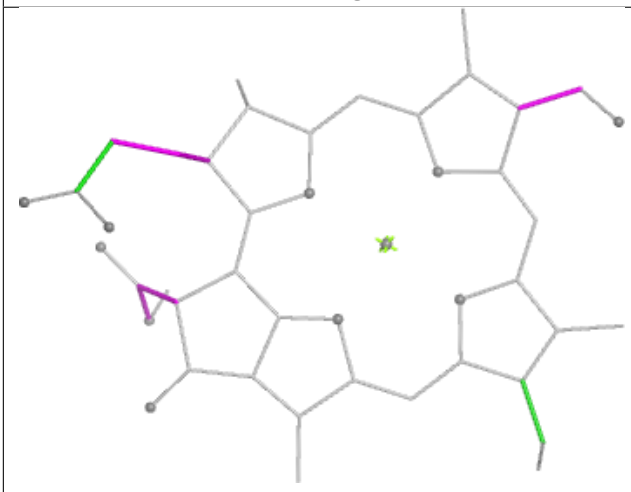
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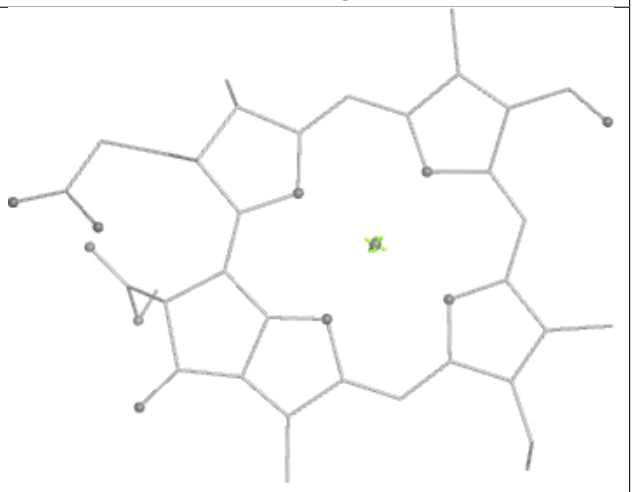
Bond lengths



Bond angles

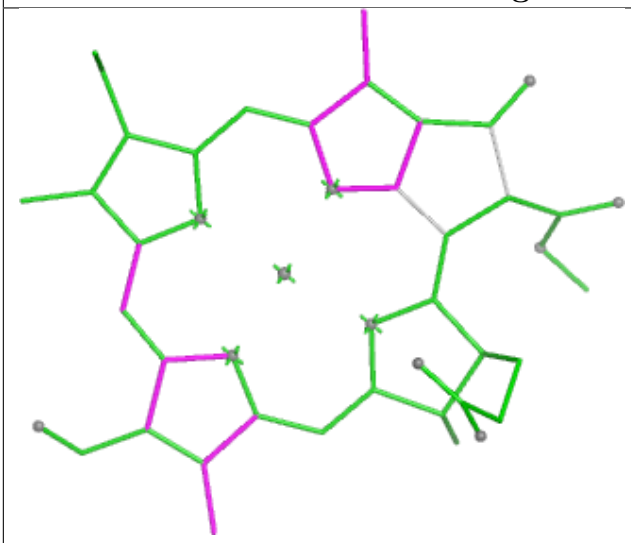


Torsions

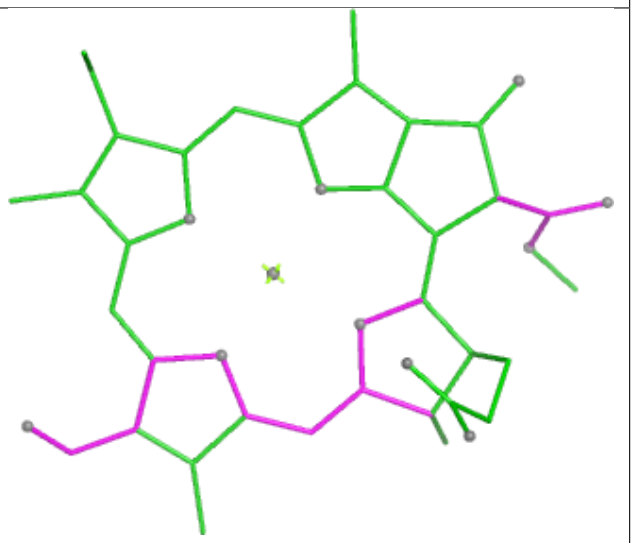


Rings

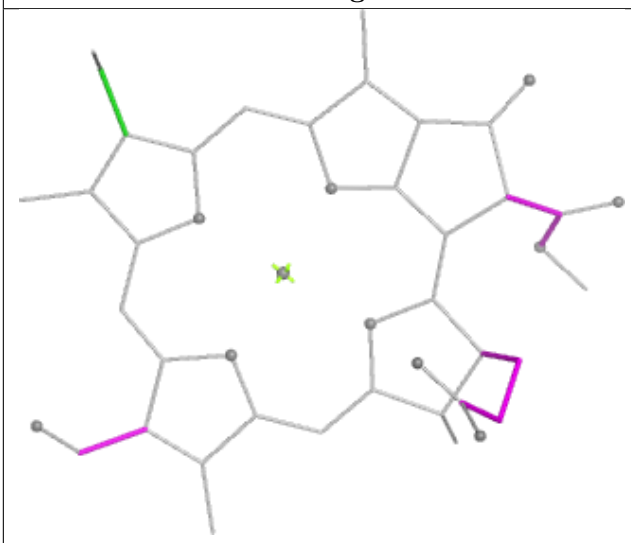
Ligand CL7 cB 1212



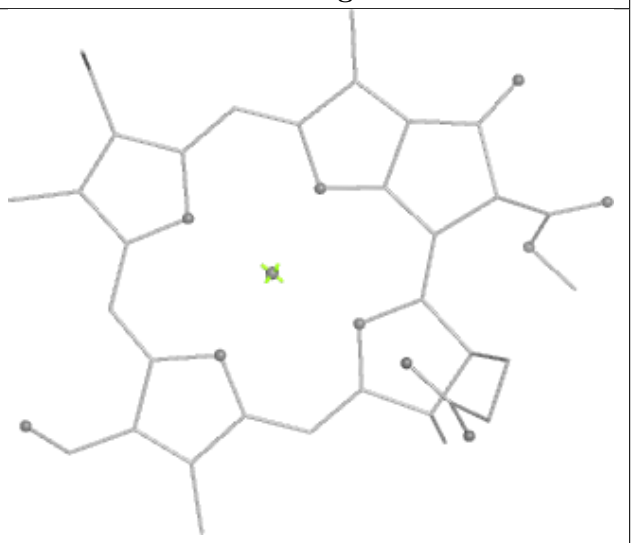
Bond lengths



Bond angles

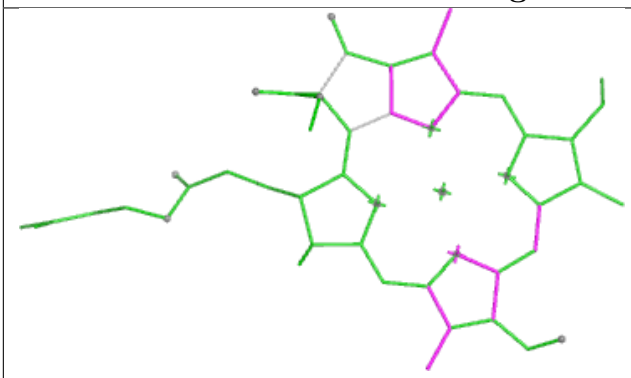


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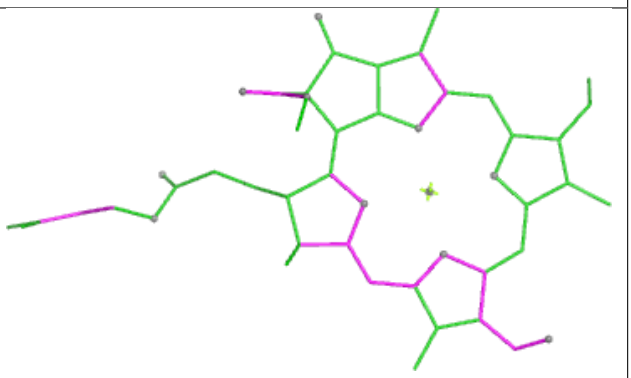


Rings

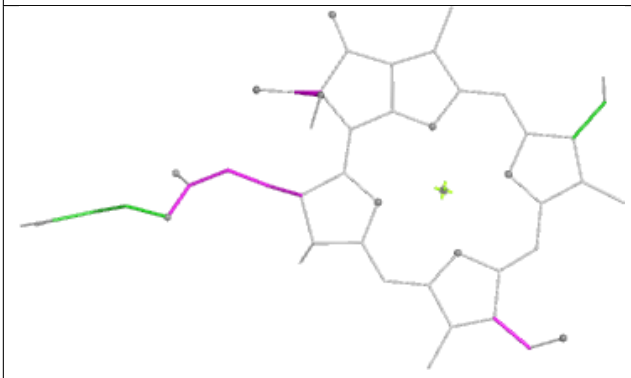
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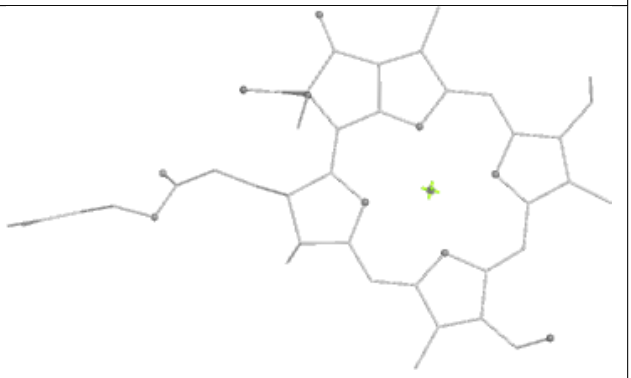
Bond lengths



Bond angles

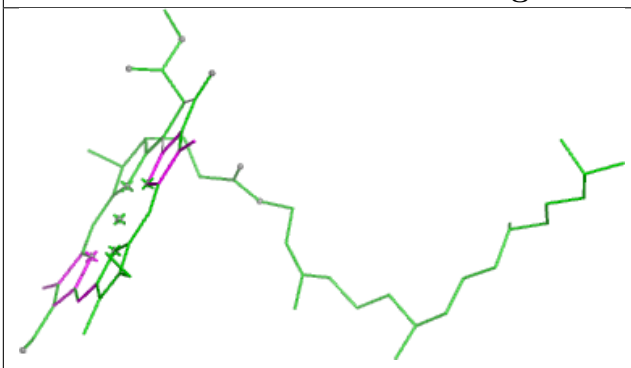


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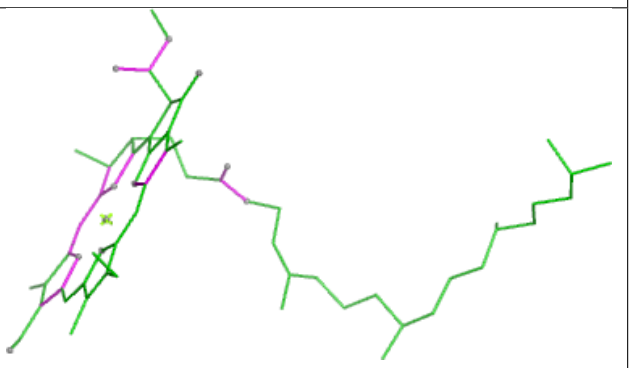


Rings

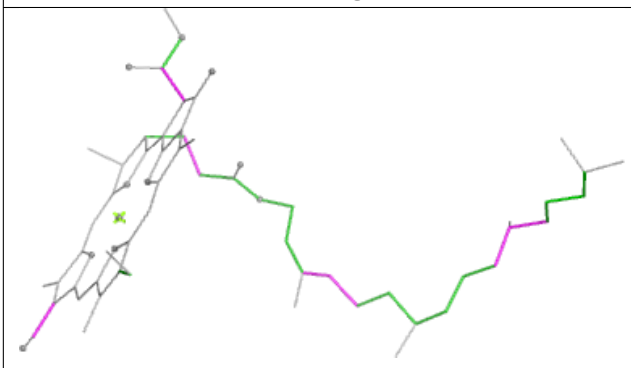
Ligand CL7 aB 1238



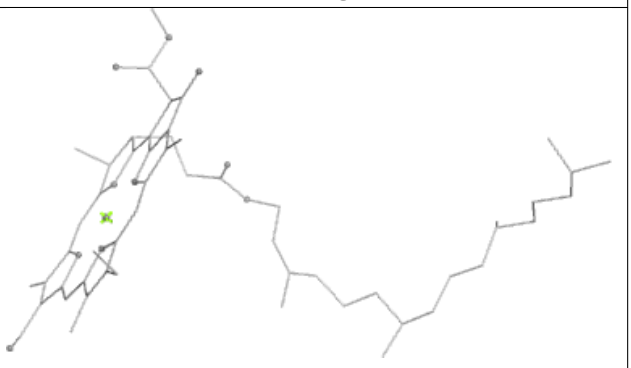
Bond lengths



Bond angles

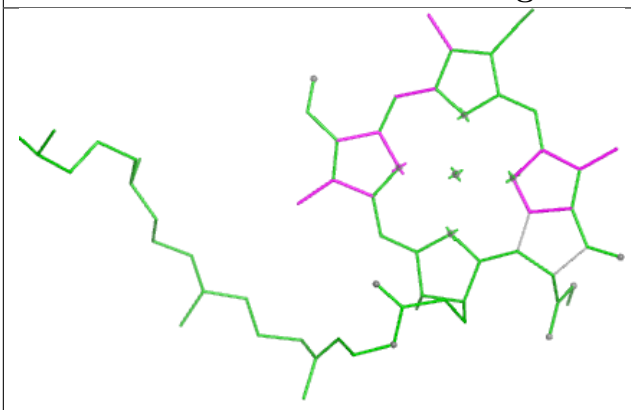


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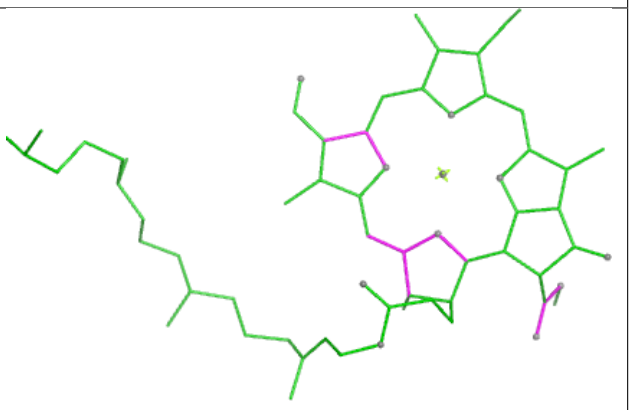


Rings

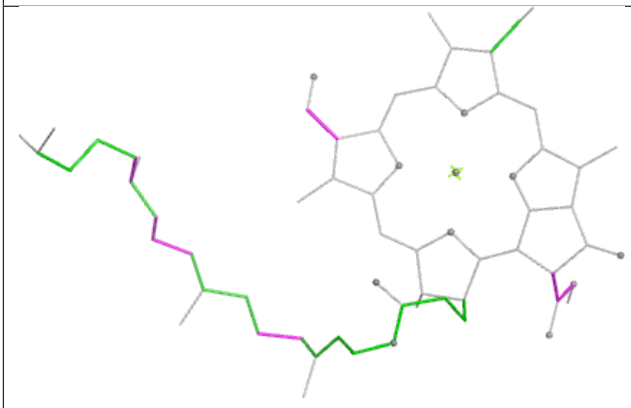
Ligand CL7 bI 1601



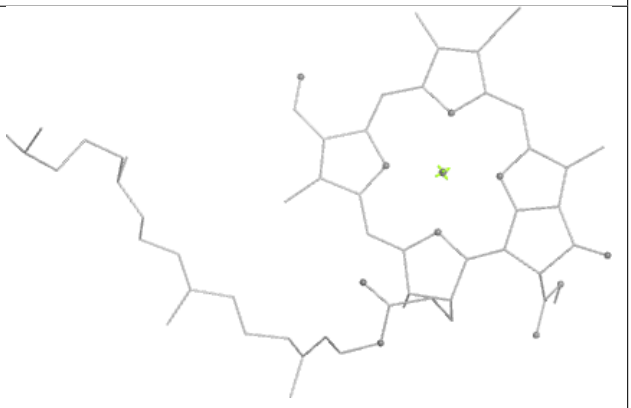
Bond lengths



Bond angles

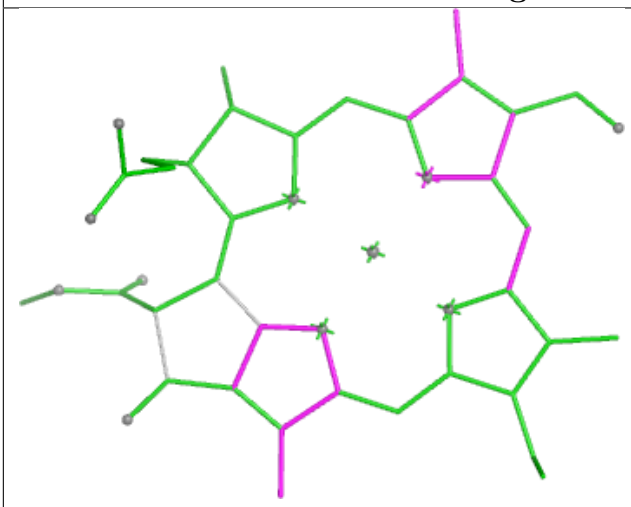


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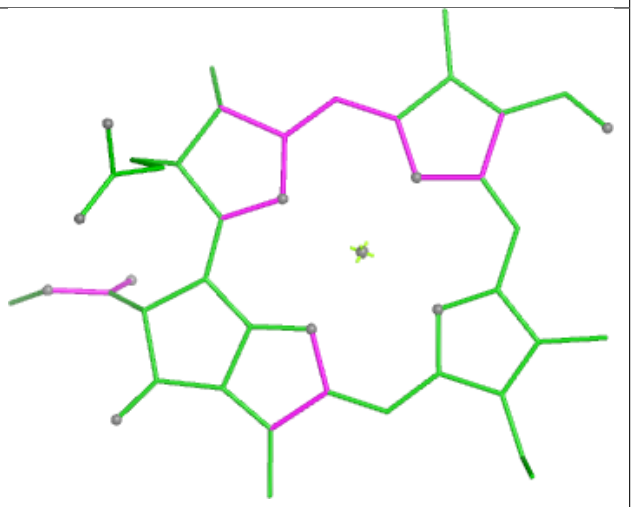


Rings

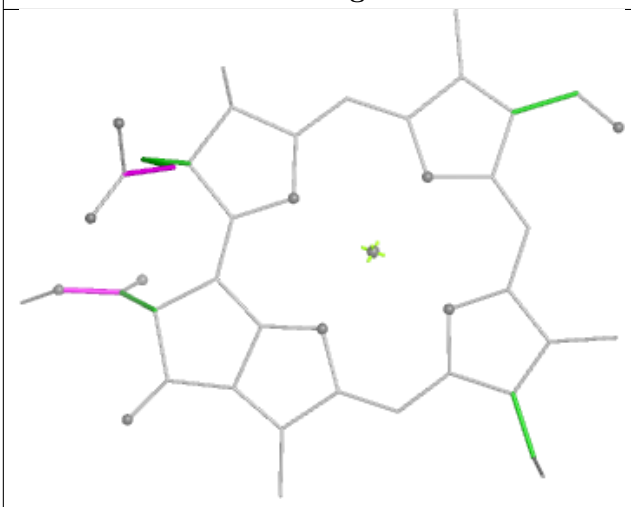
Ligand CL7 bA 1107



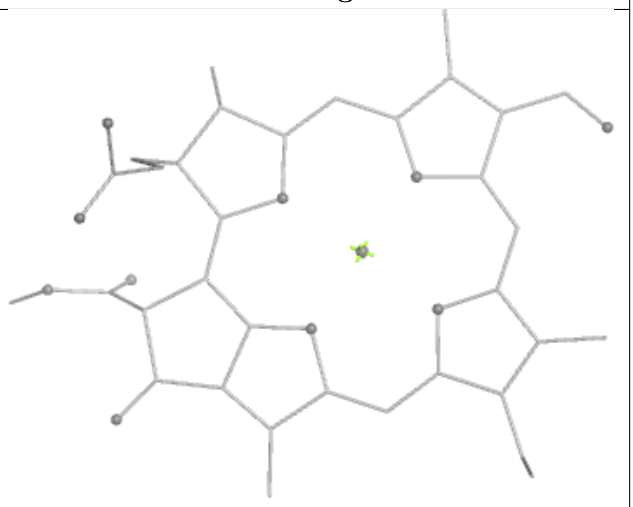
Bond lengths



Bond angles

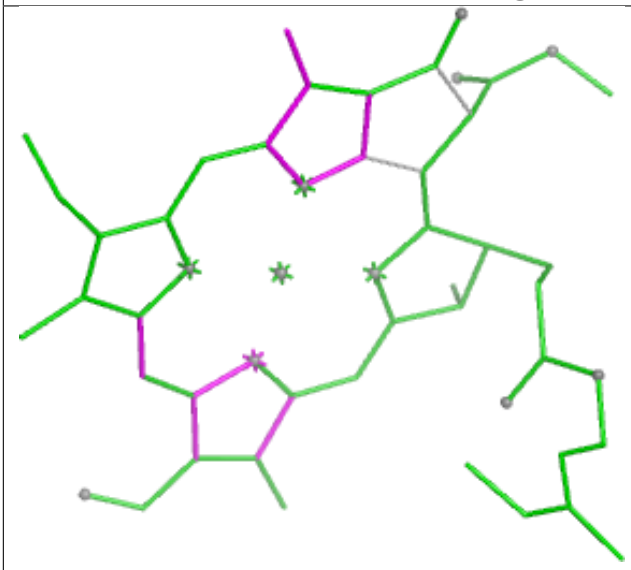


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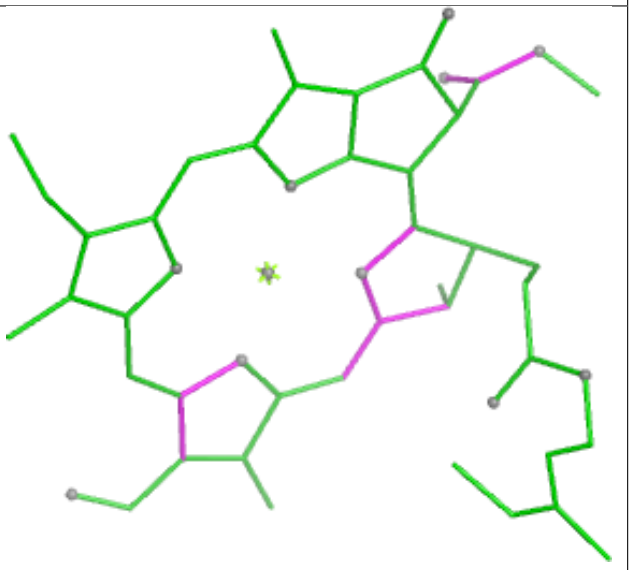


Rings

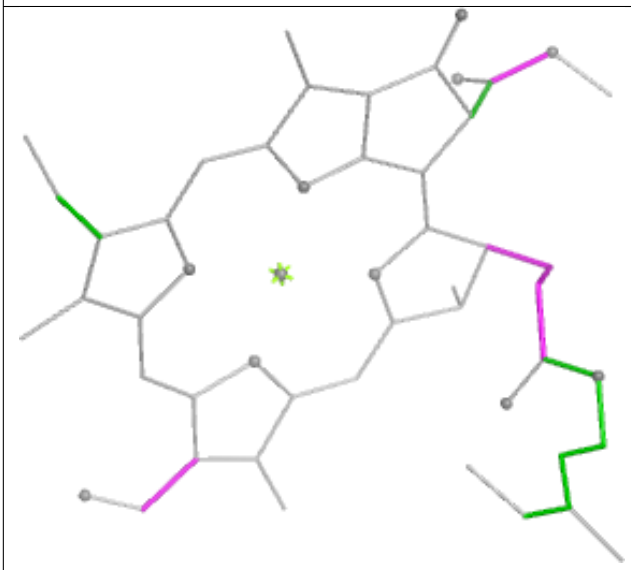
Ligand CL7 cA 1108



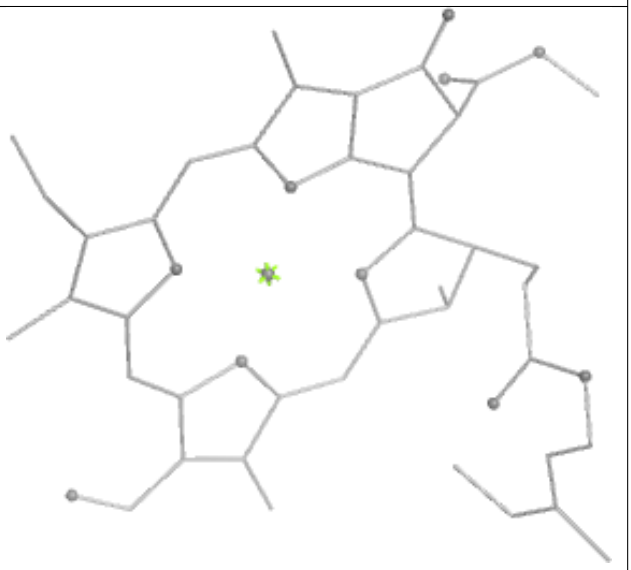
Bond lengths



Bond angles

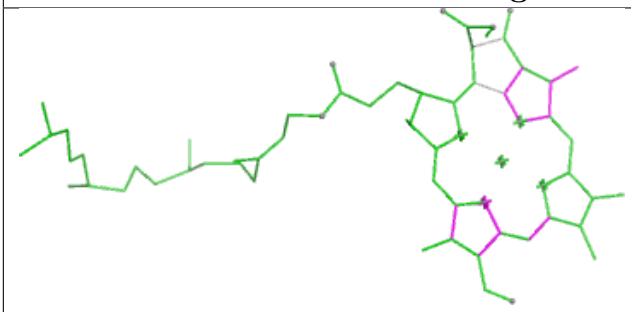


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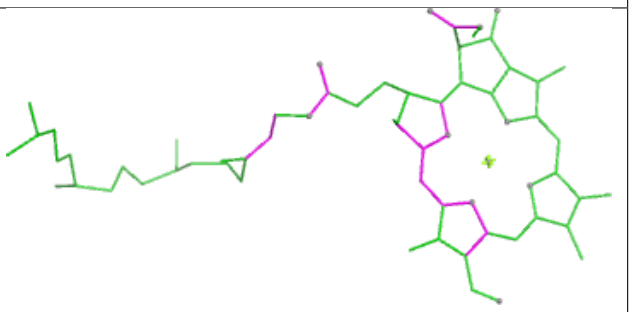


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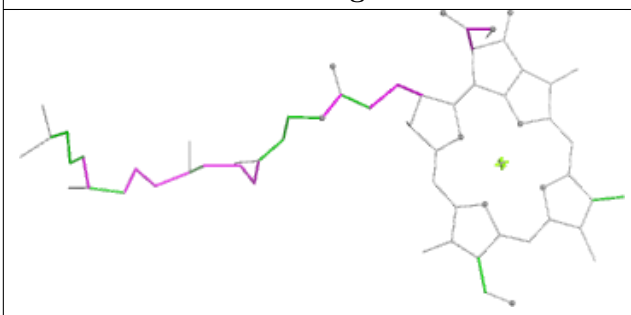
Ligand CL7 bB 1210



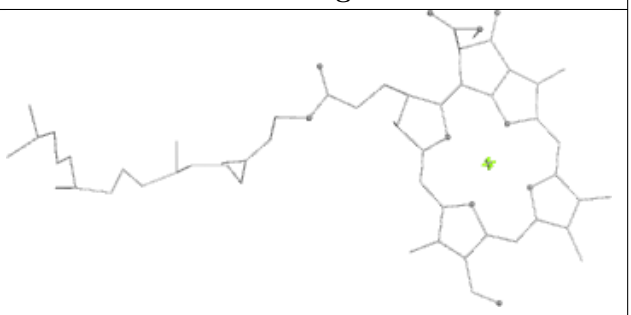
Bond lengths



Bond angles

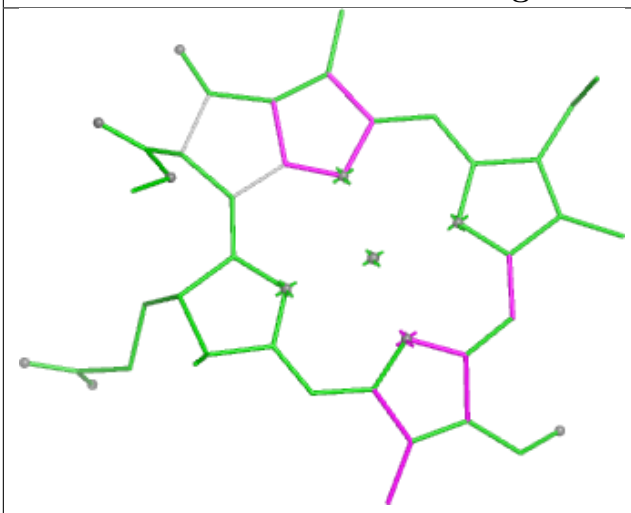


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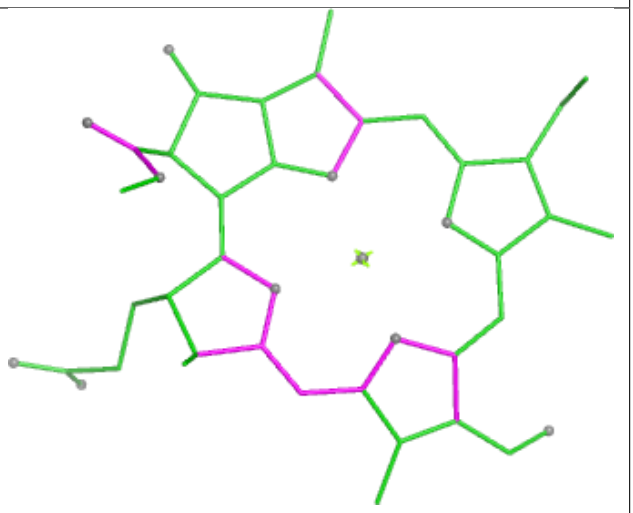


Rings

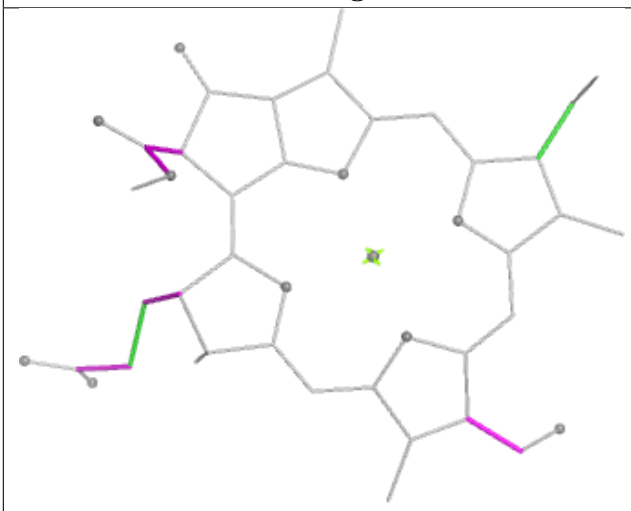
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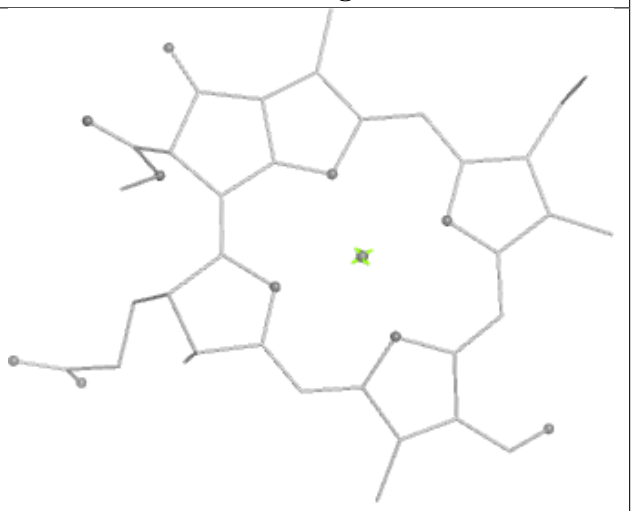
Bond lengths



Bond angles

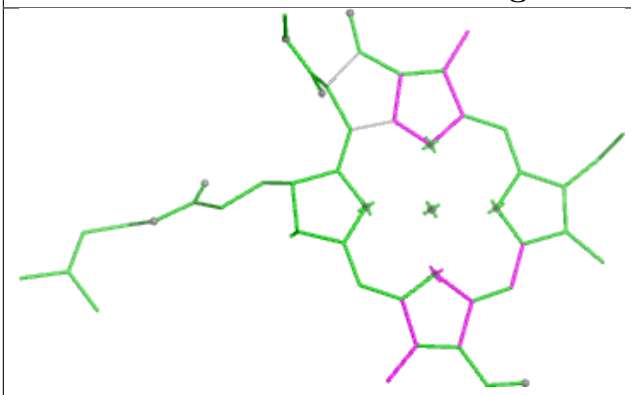


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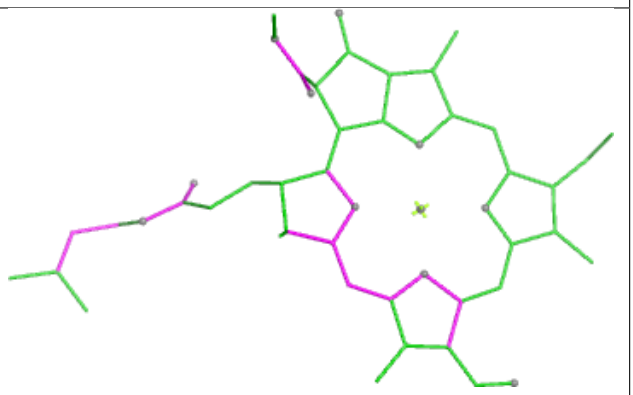


Rings

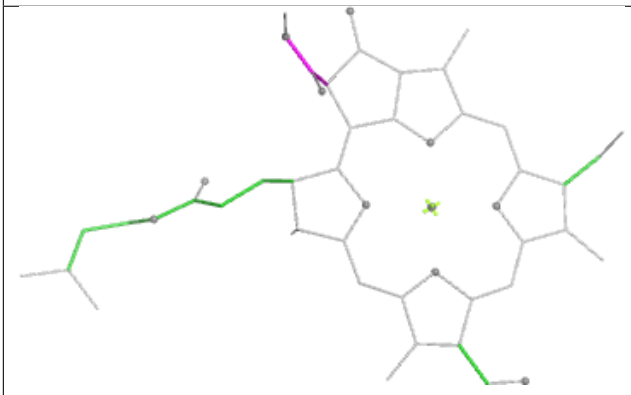
Ligand CL7 bA 1124



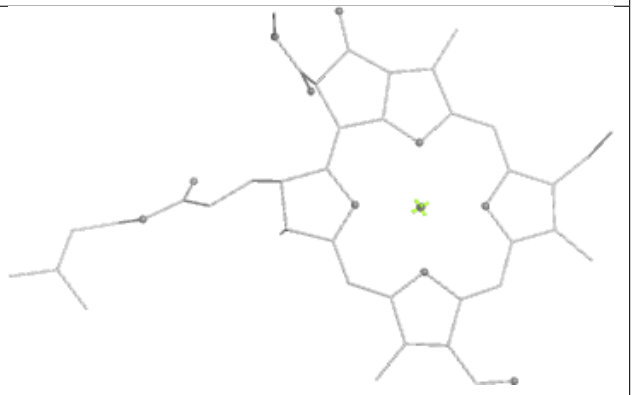
Bond lengths



Bond angles

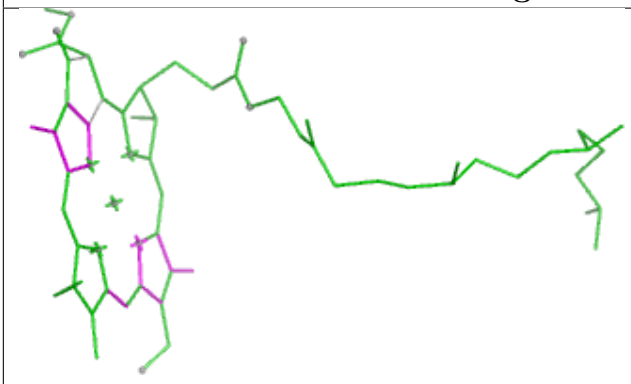


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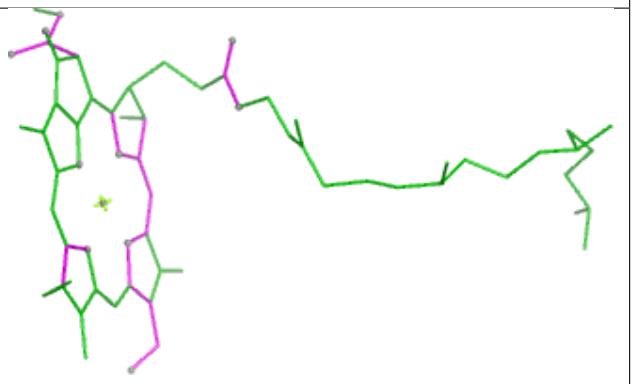


Rings

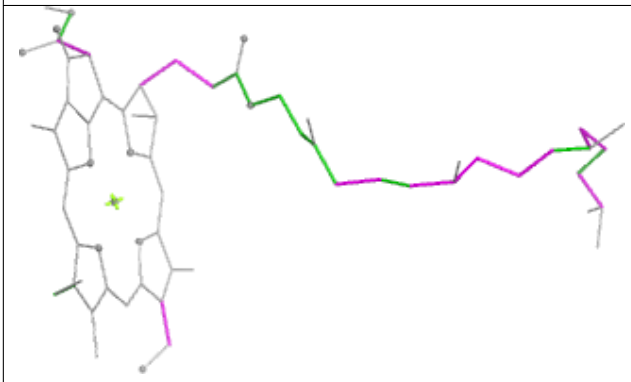
Ligand CL7 aL 1502



Bond lengths



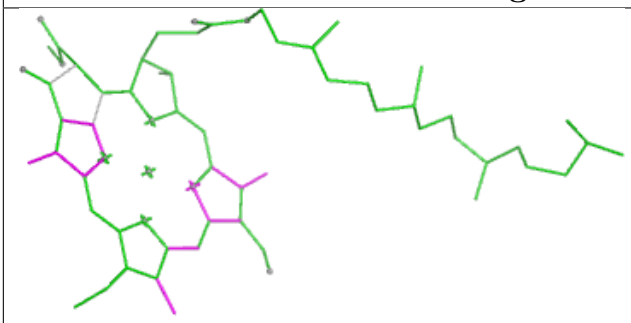
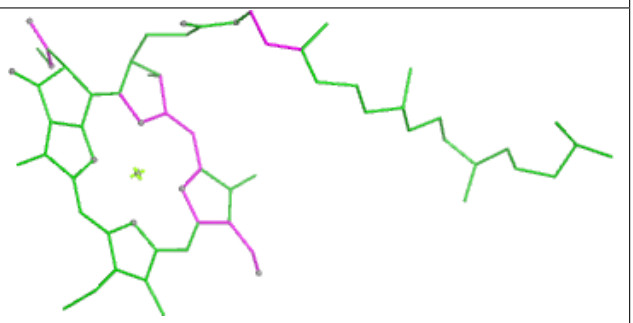
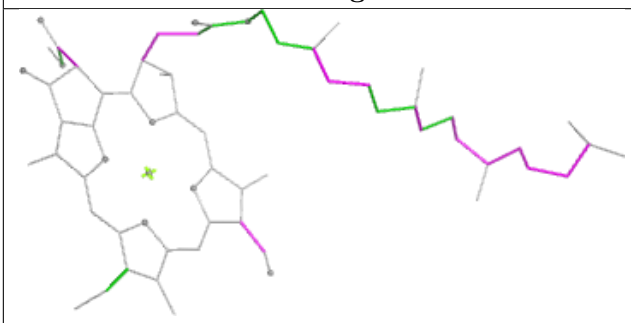
Bond angles



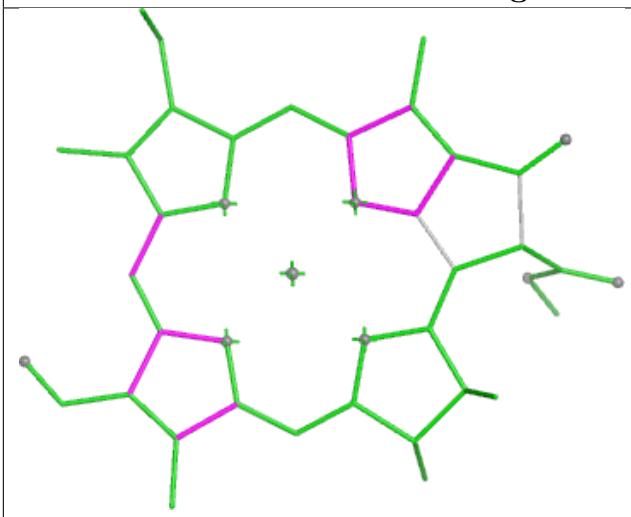
Torsions



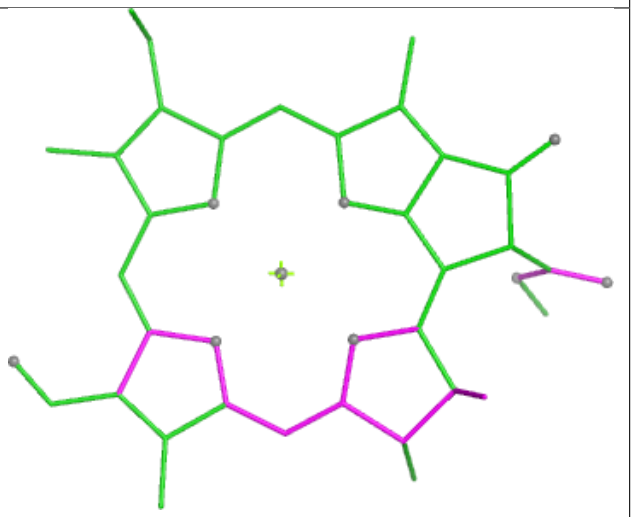
Rings

Ligand CL7 bA 1106	
	
Bond lengths	**Bond angles**
	
Torsions	**Rings**

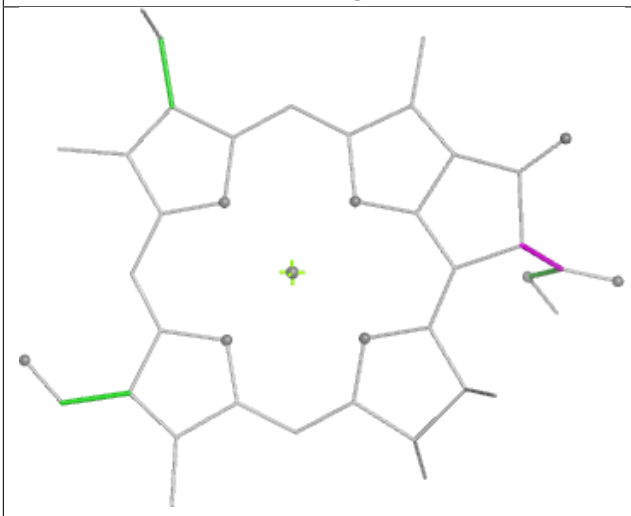
Ligand CL7 bB 1217



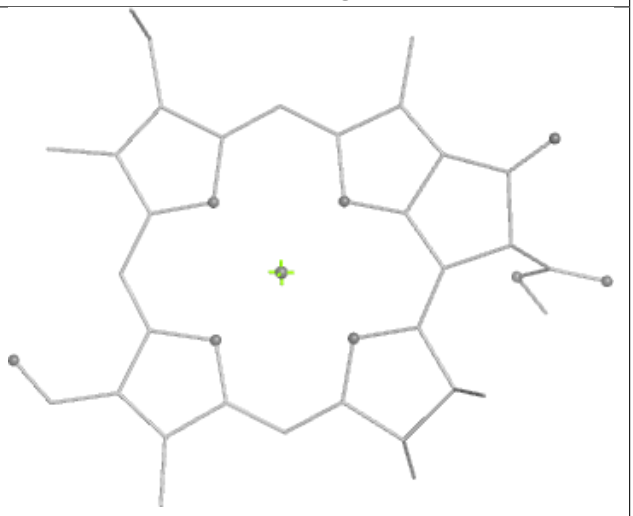
Bond lengths



Bond angles

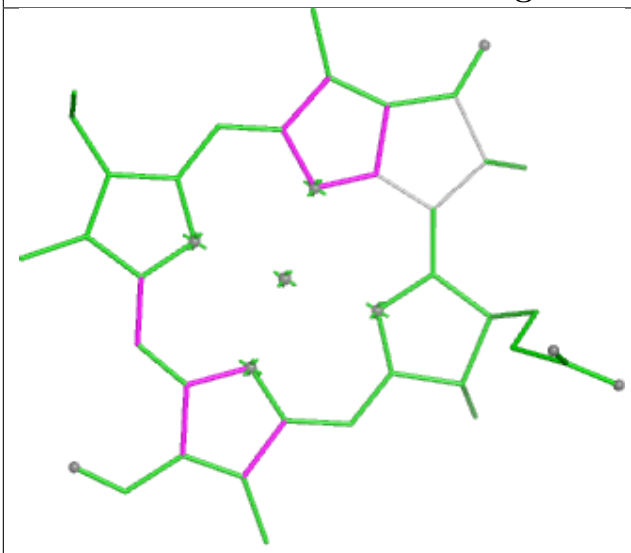


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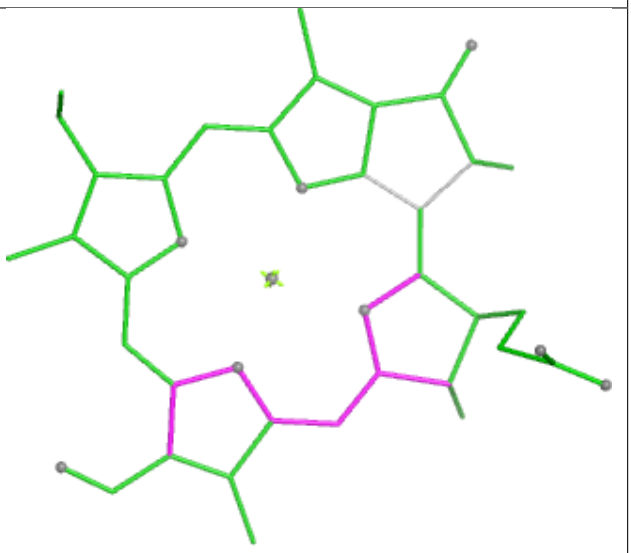


Rings

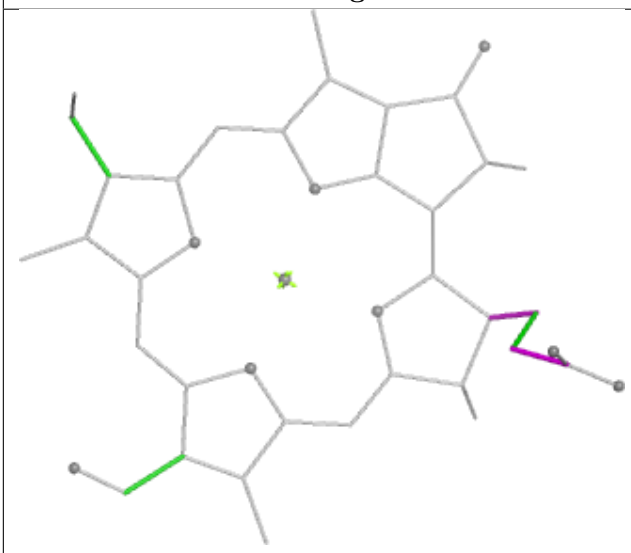
Ligand CL7 aJ 1302



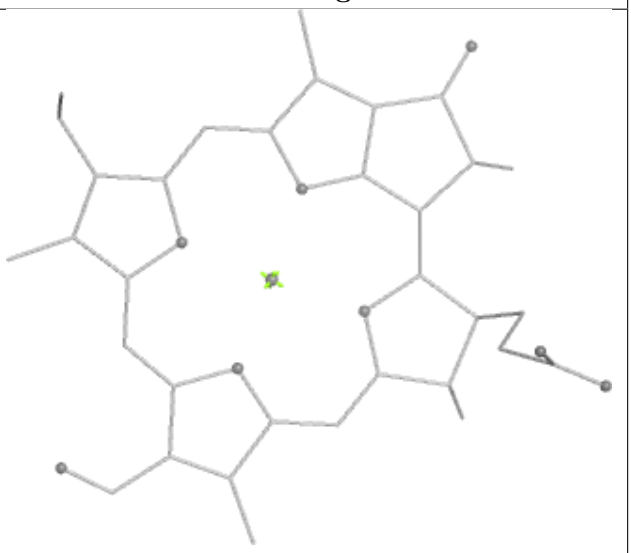
Bond lengths



Bond angles

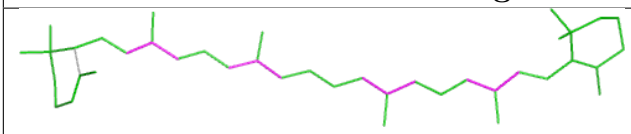


Torsions



Rings

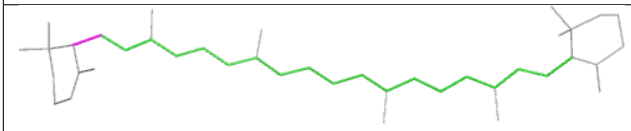
Ligand A1JPJ cL 4023



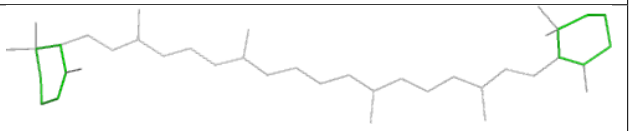
Bond lengths



Bond angles

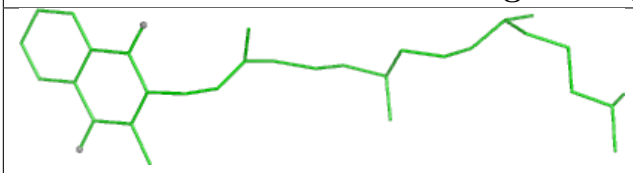


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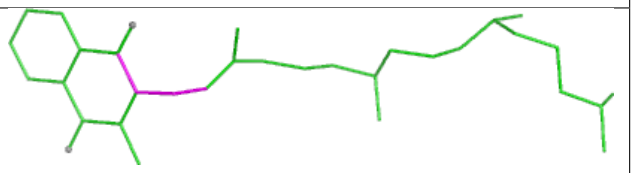


Rings

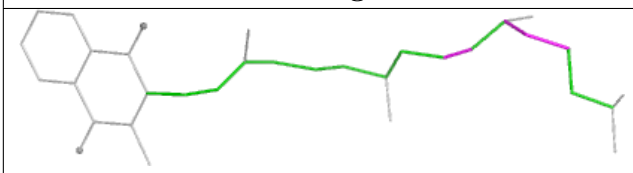
Ligand PQN aA 2001



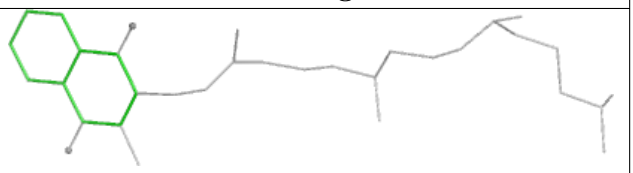
Bond lengths



Bond angles

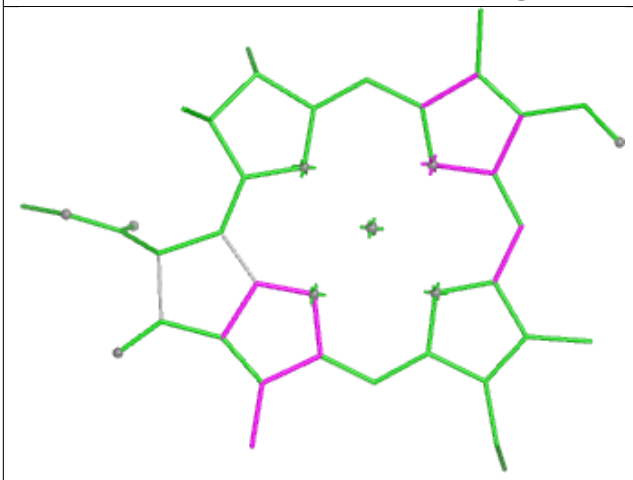


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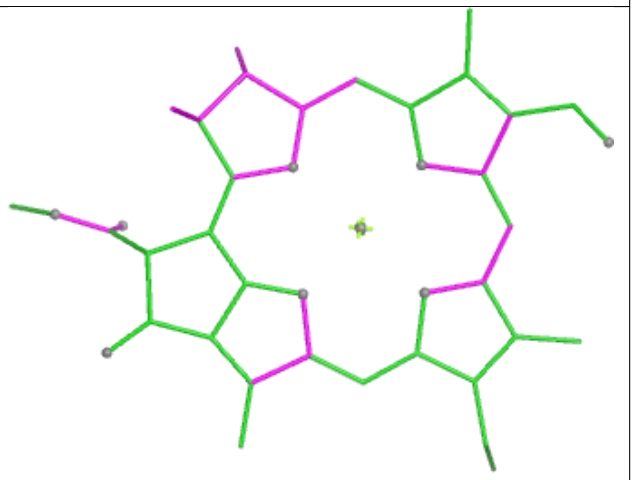


Rings

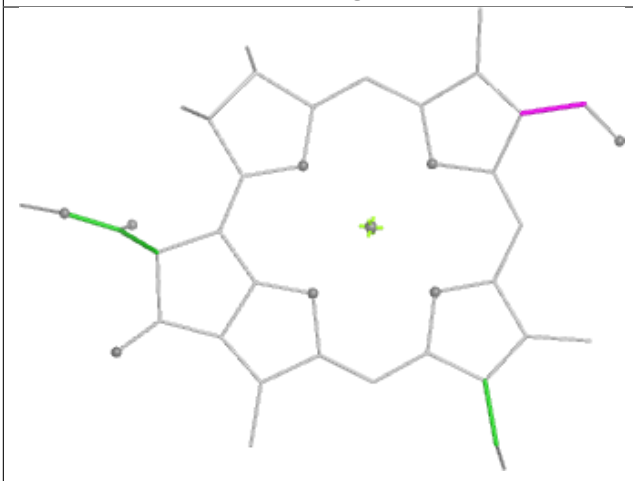
Ligand CL7 aF 1701



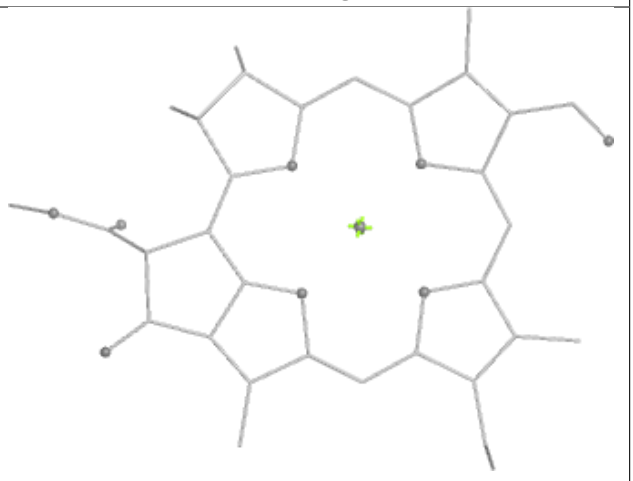
Bond lengths



Bond angles

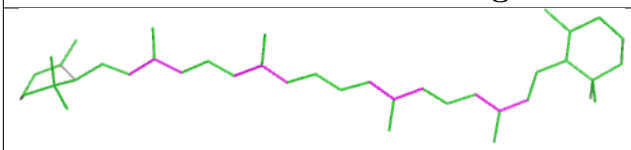


Torsions

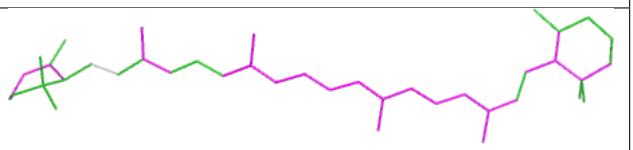


Rings

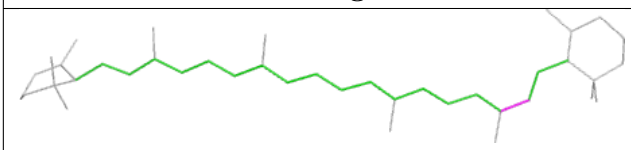
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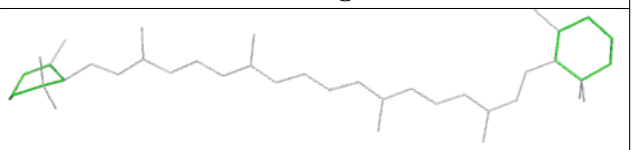
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Bond angles

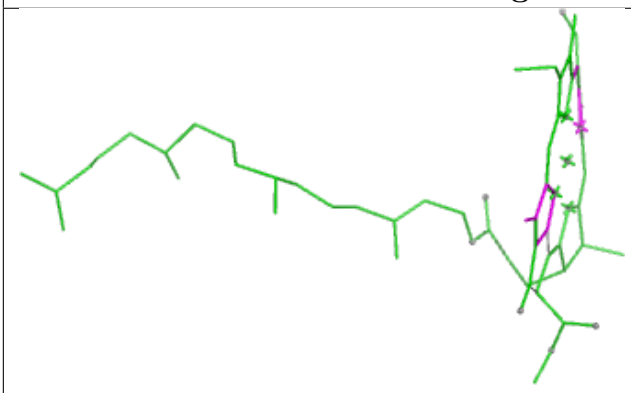


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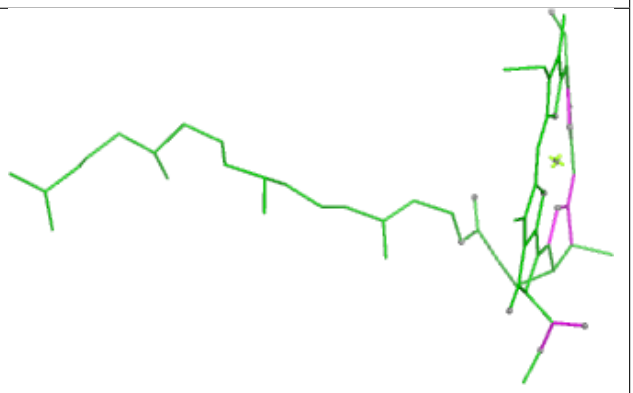


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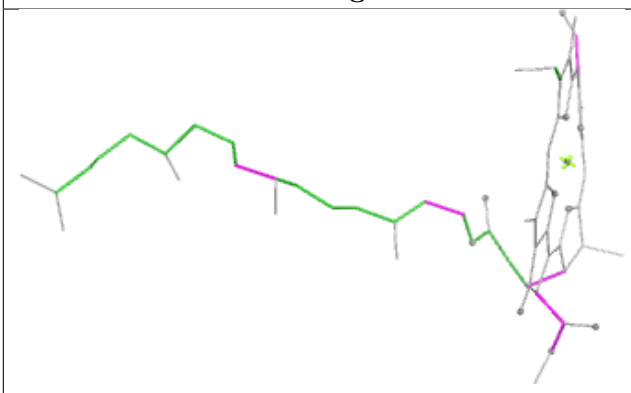
Ligand CL7 cA 1126



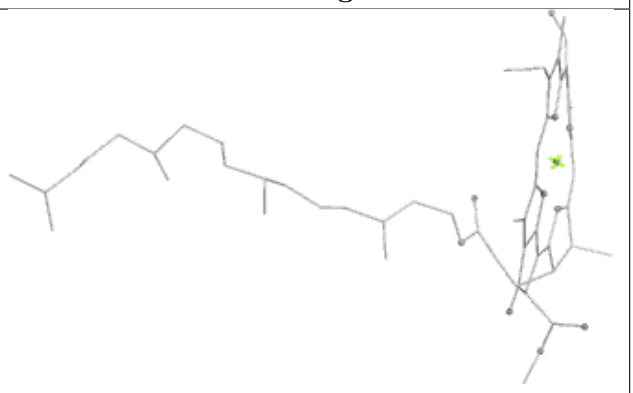
Bond lengths



Bond angles

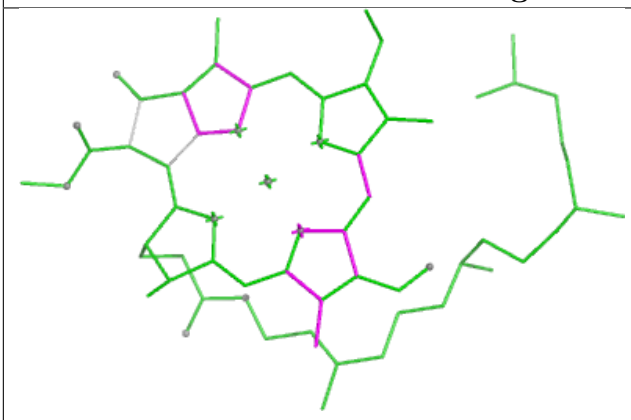


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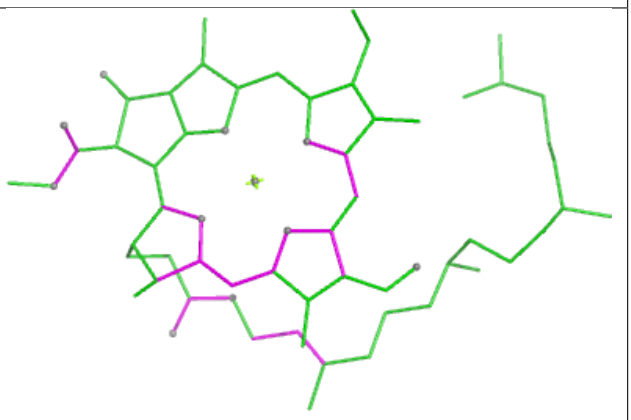


Rings

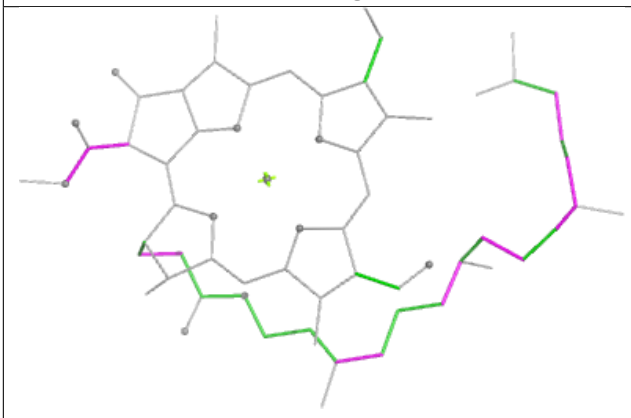
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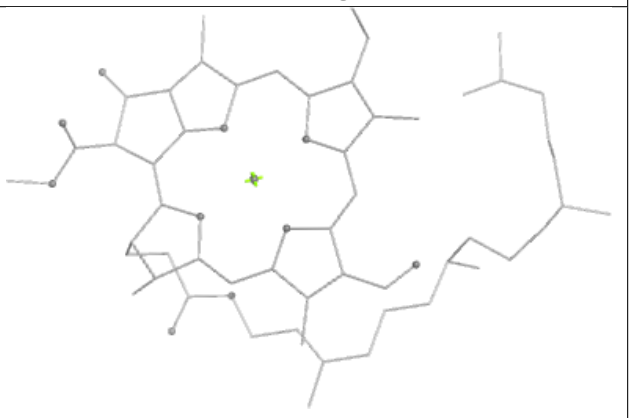
Bond lengths



Bond angles

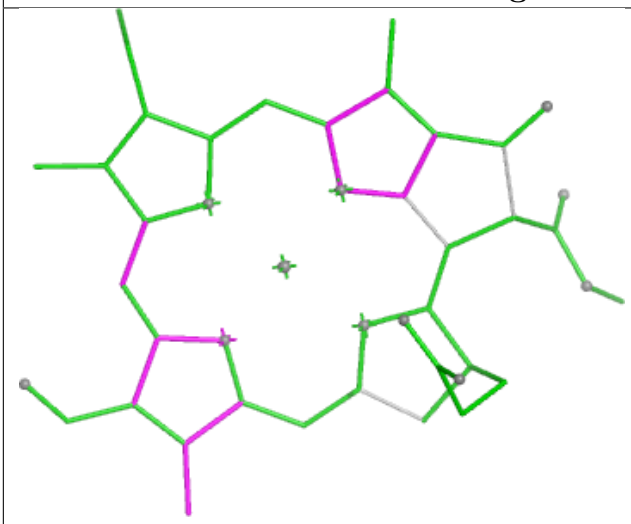


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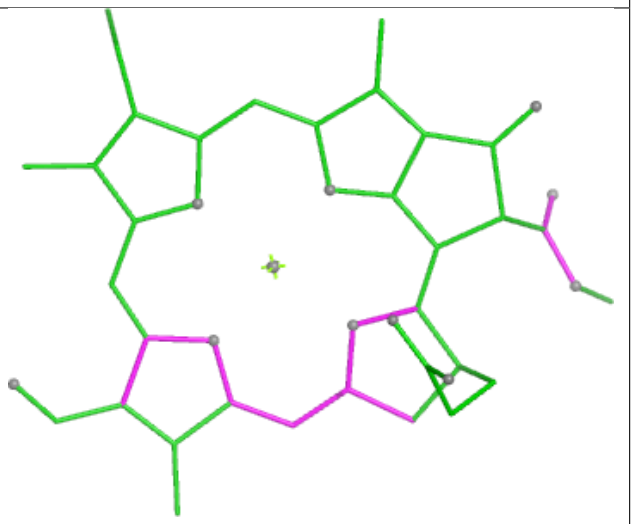


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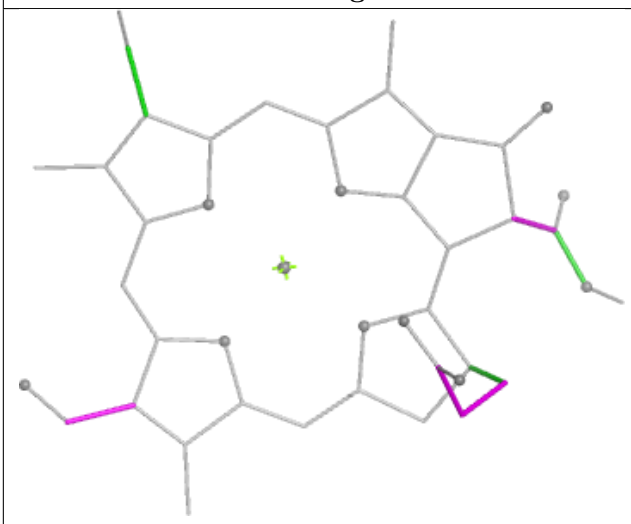
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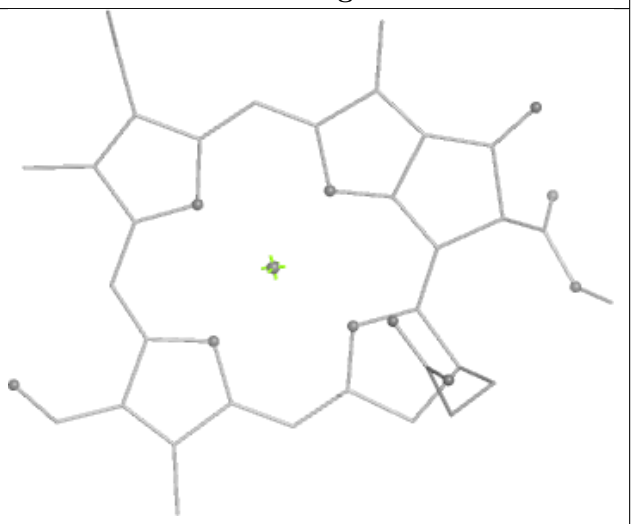
Bond lengths



Bond angles



Torsions



Rings

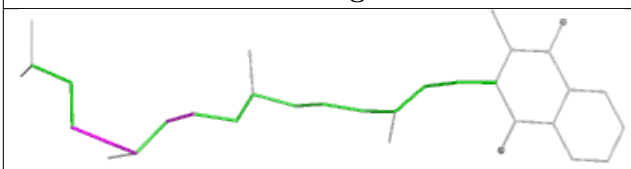
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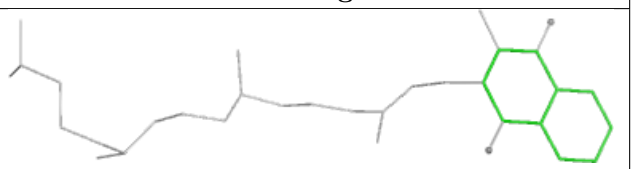
Bond lengths



Bond angles

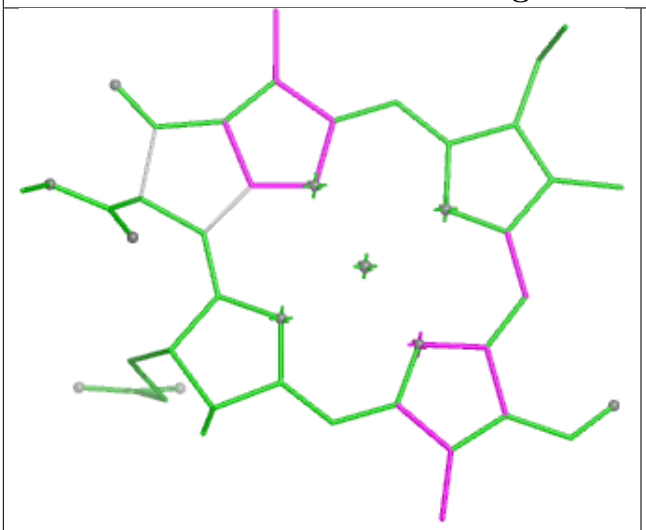


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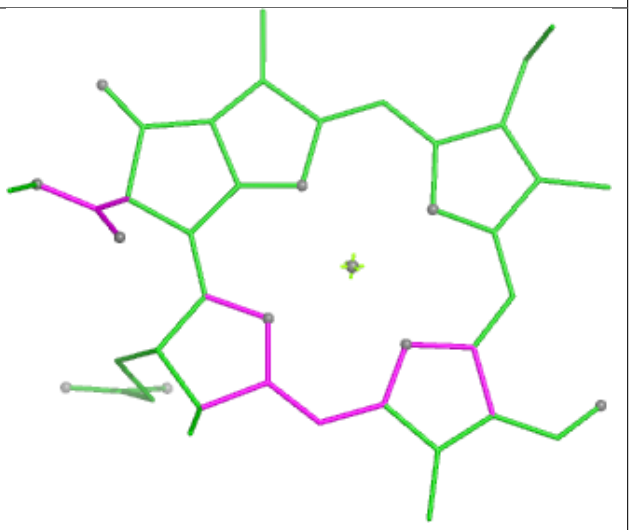


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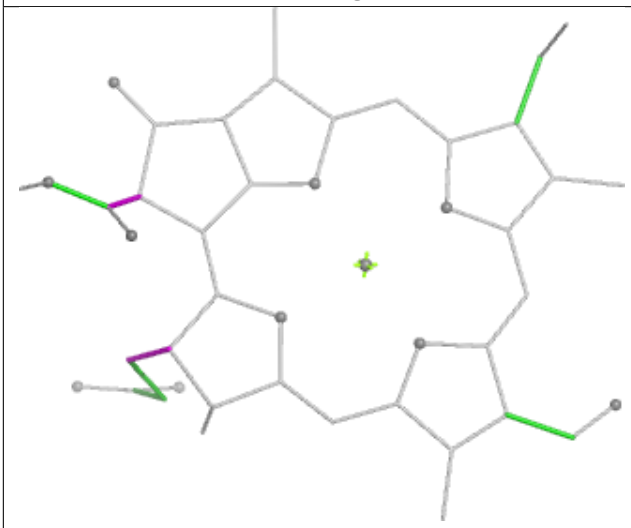
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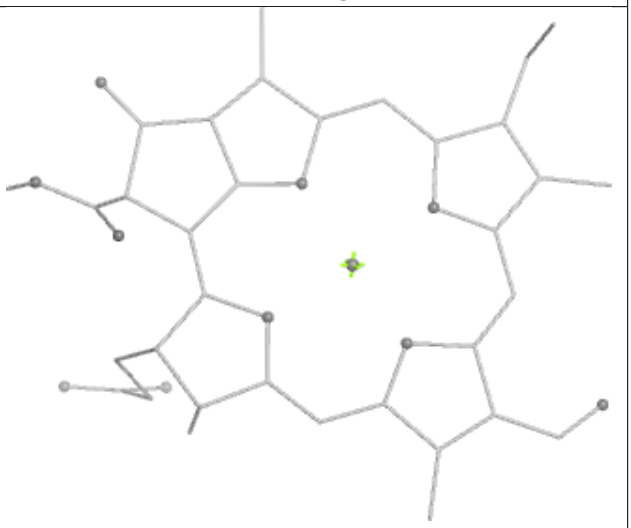
Bond lengths



Bond angles

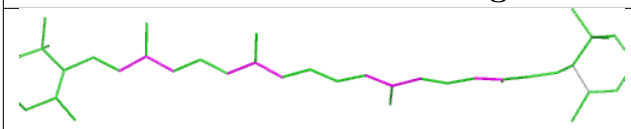


Torsions



Rings

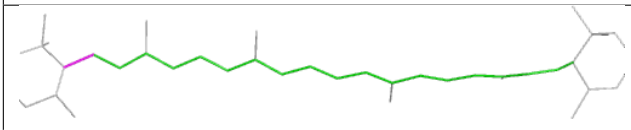
Ligand A1JPJ bB 4004



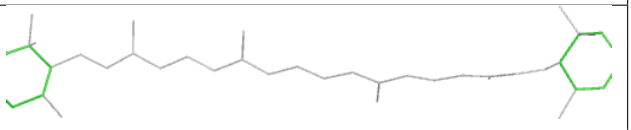
Bond lengths



Bond angles

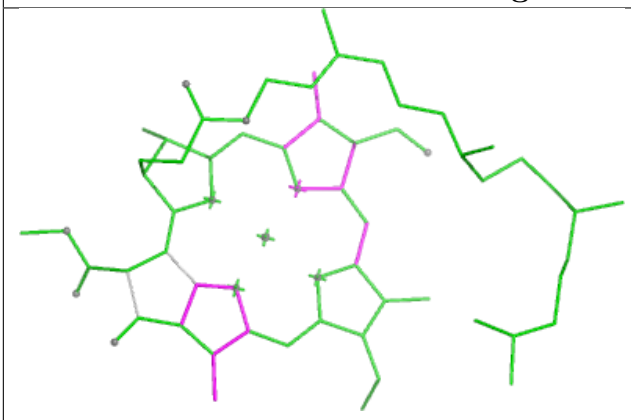


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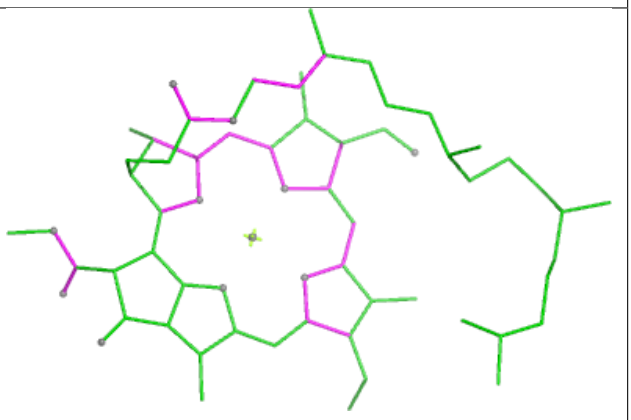


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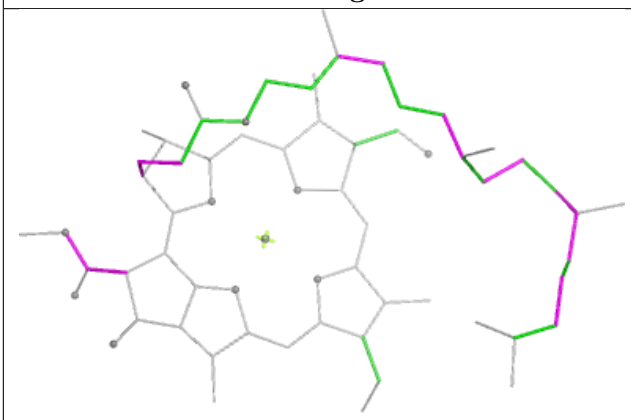
Ligand CL7 cA 1117



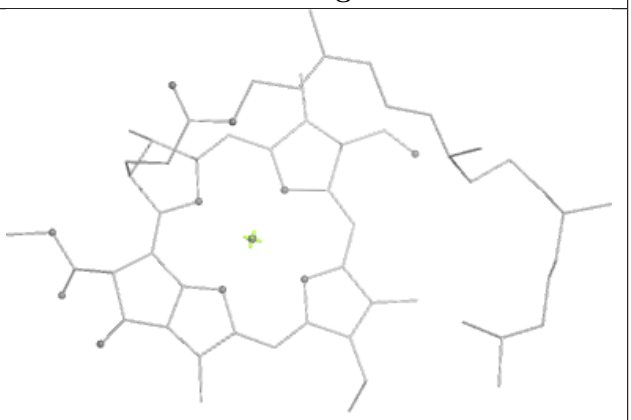
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Bond angles

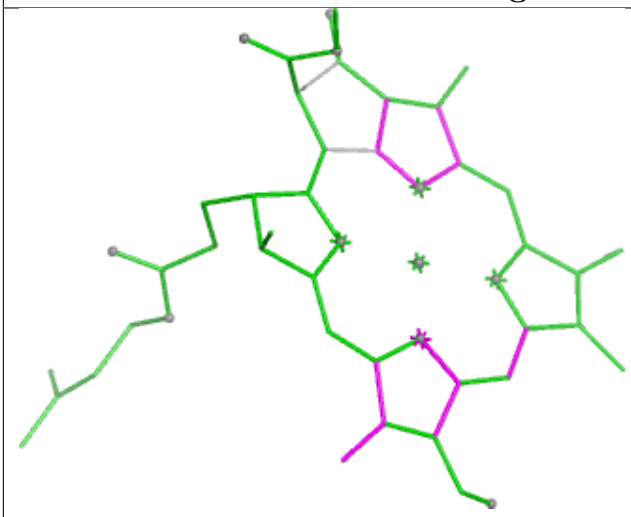


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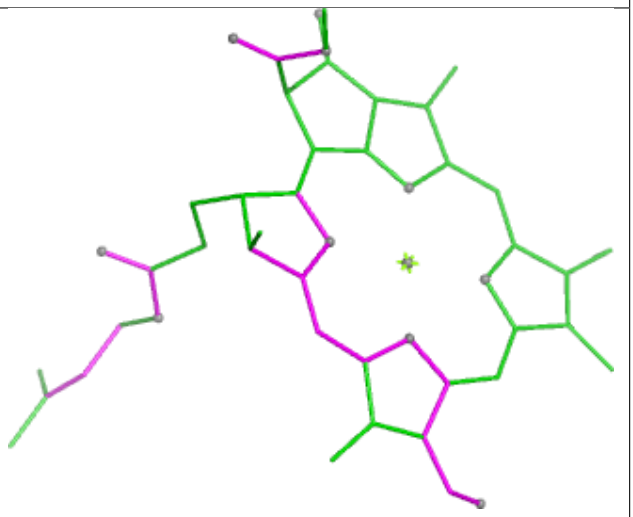


Rings

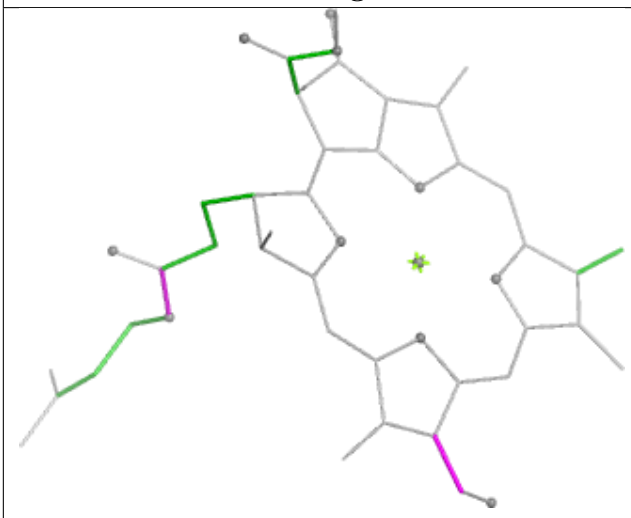
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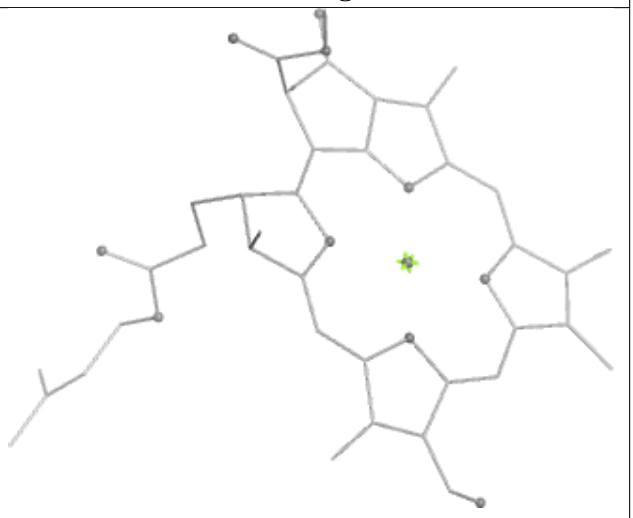
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Bond angles

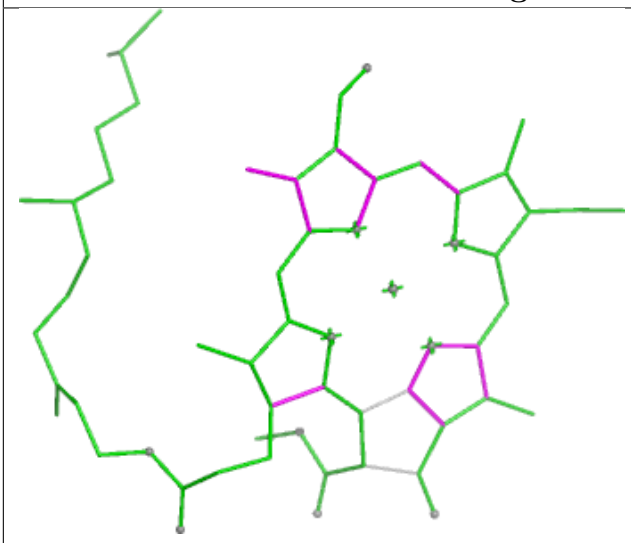


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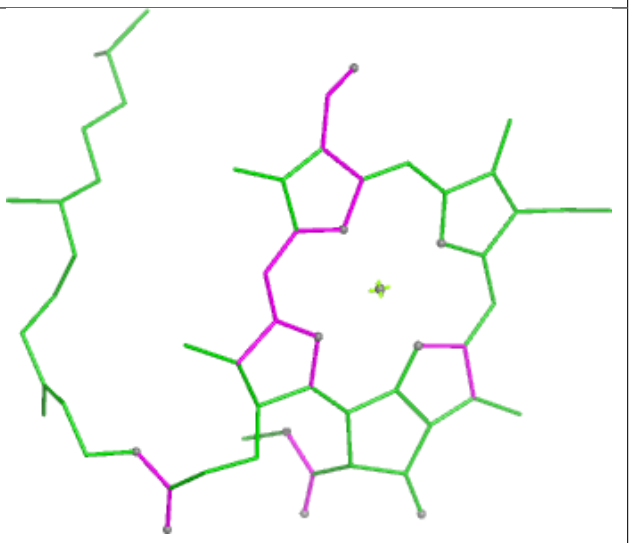


Rings

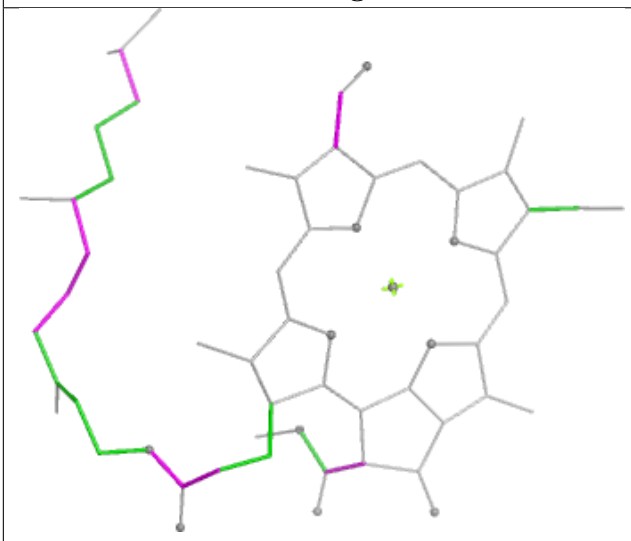
Ligand CL7 bB 1221



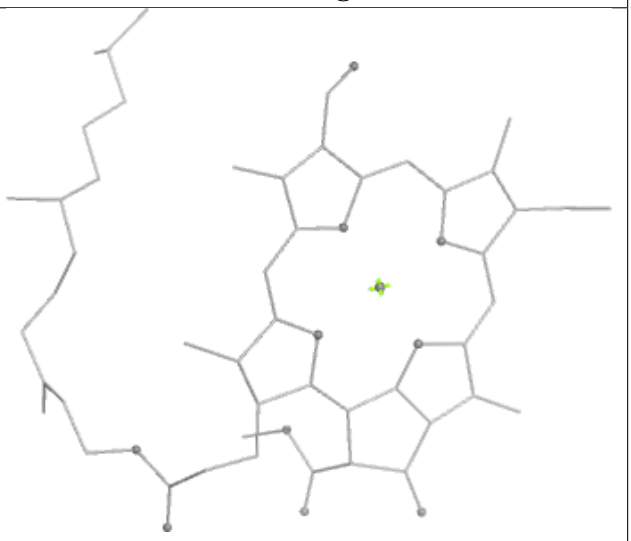
Bond lengths



Bond angles

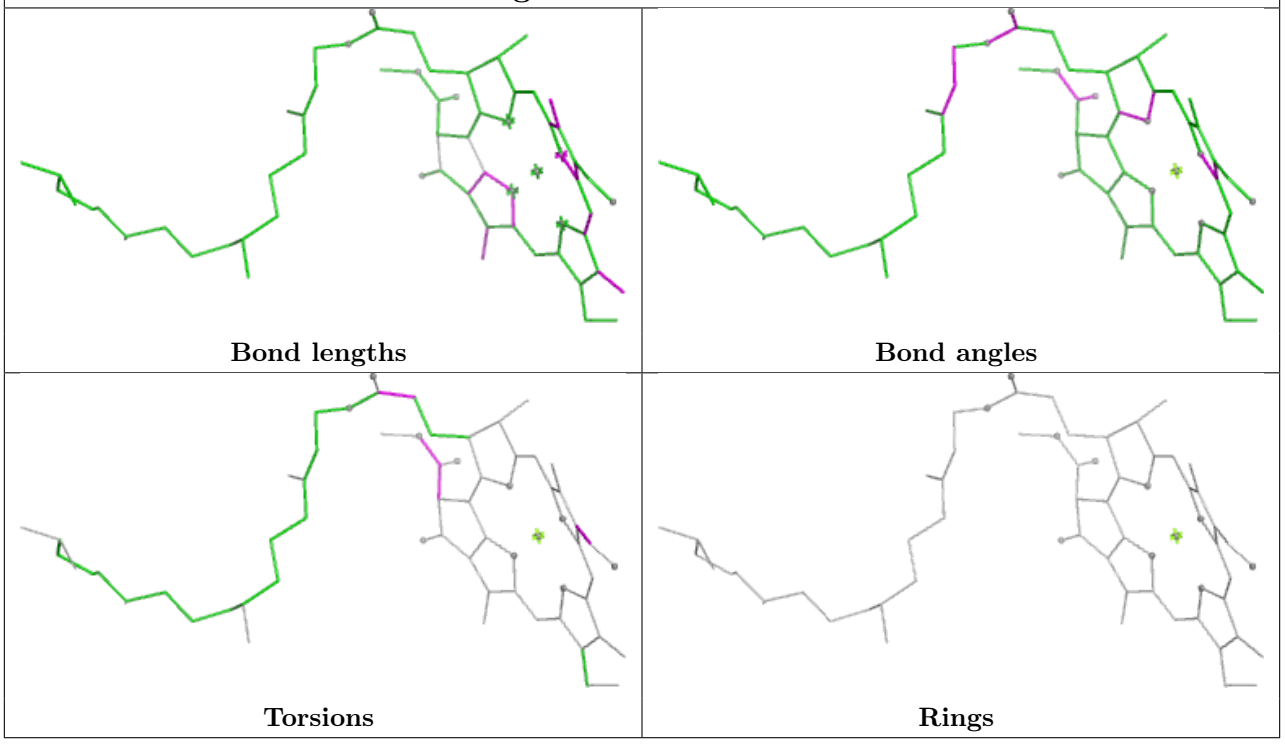


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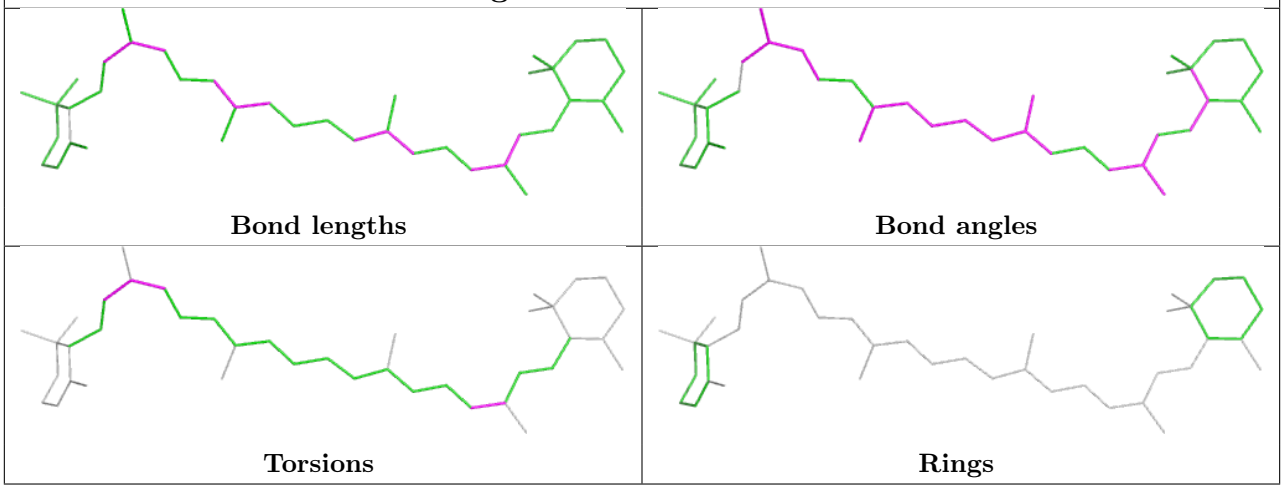


Rings

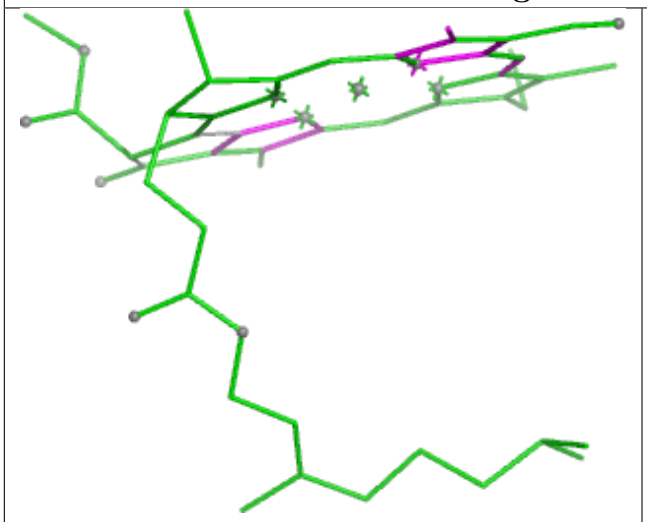
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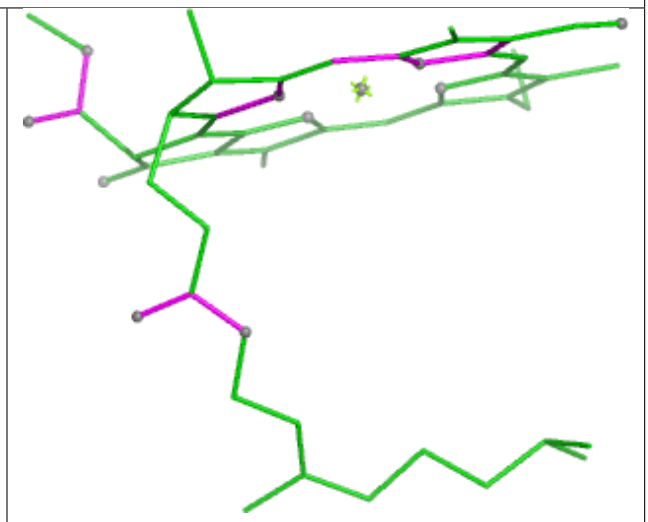
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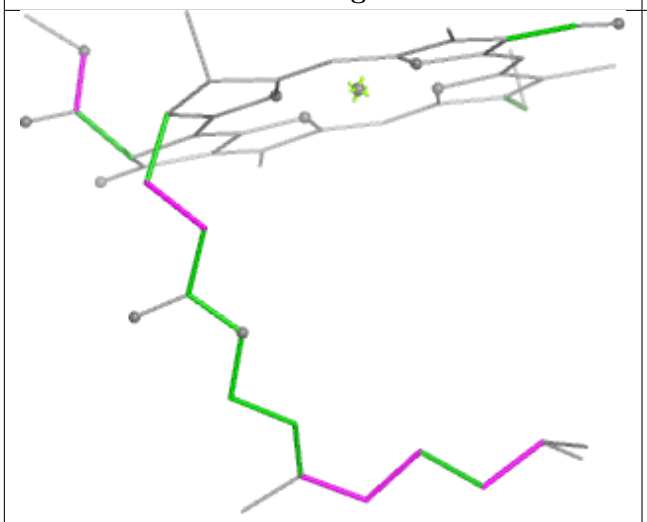
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Bond lengths



Bond angles

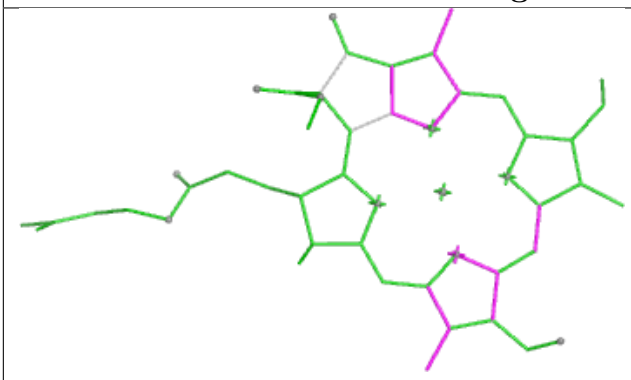


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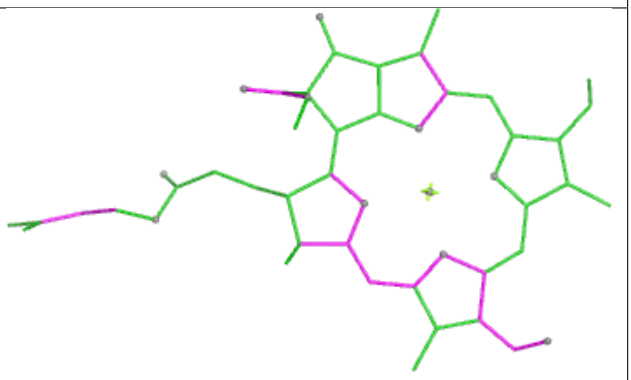


Rings

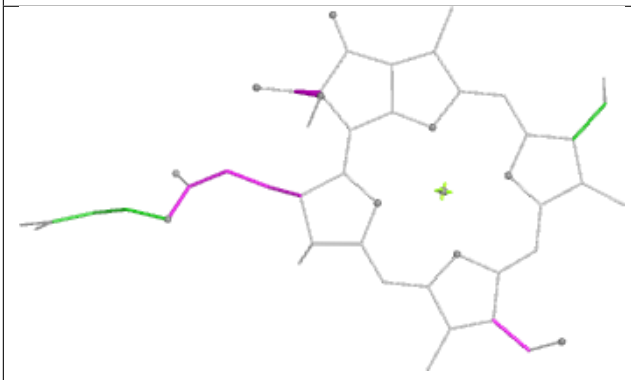
Ligand CL7 aA 1135



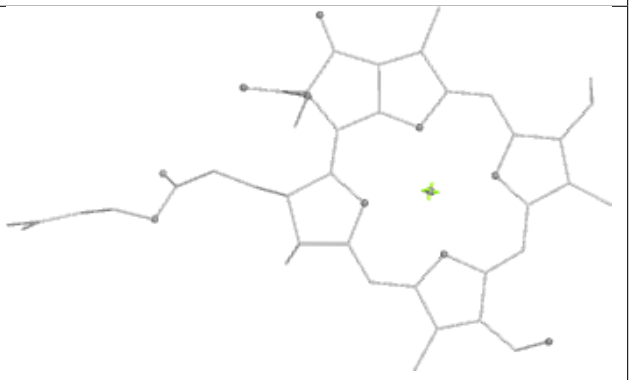
Bond lengths



Bond angles

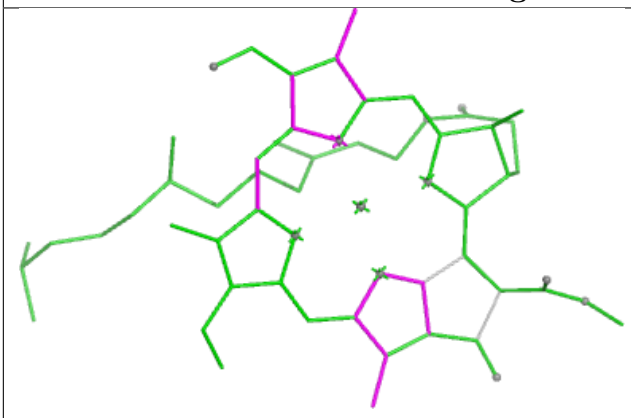


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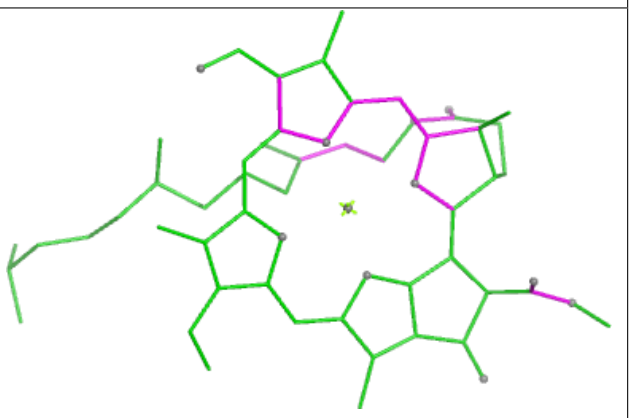


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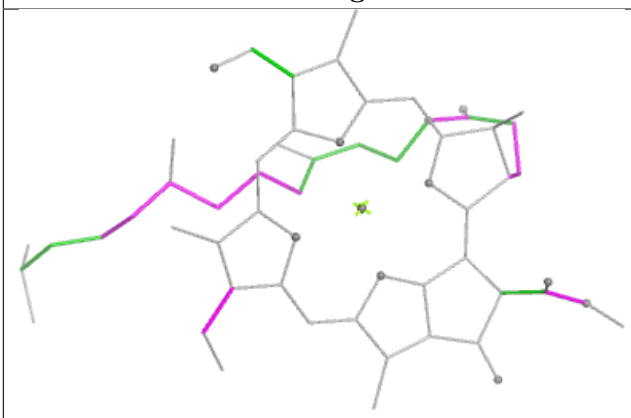
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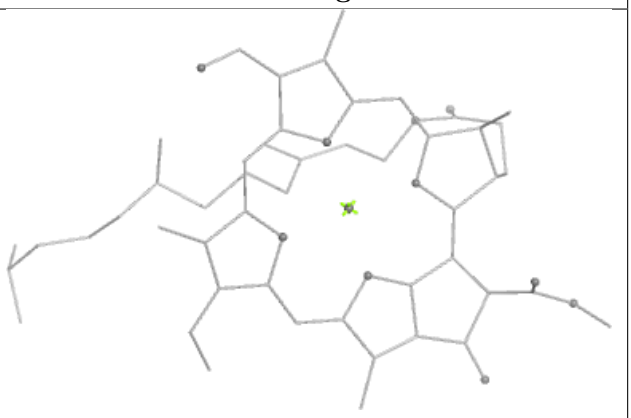
Bond lengths



Bond angles

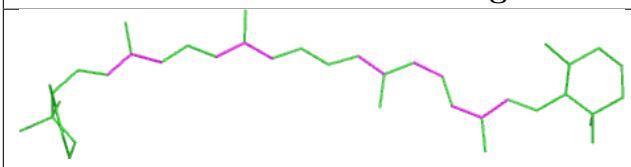


Torsions



Rings

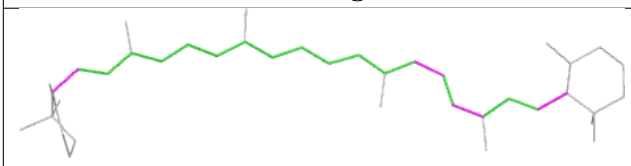
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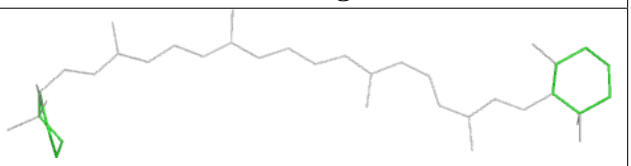
Bond lengths



Bond angles

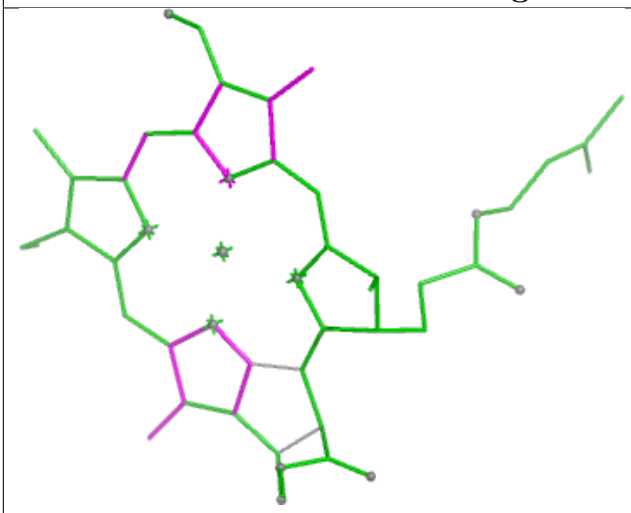


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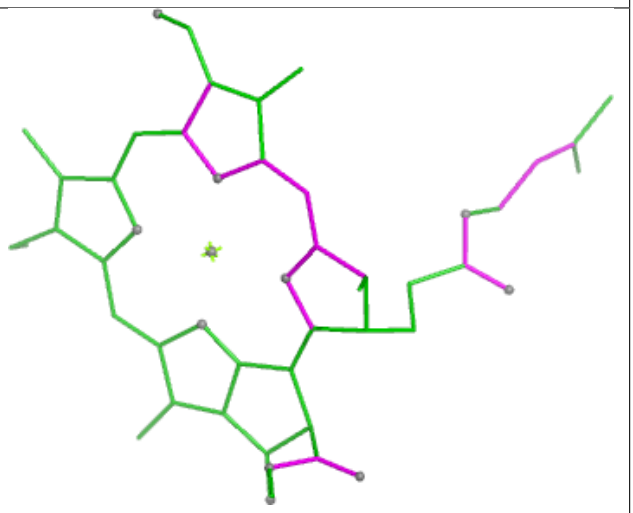


Rings

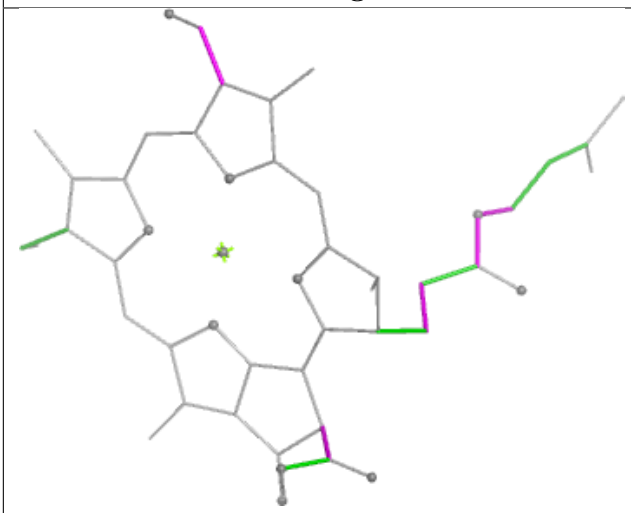
Ligand CL7 cA 1129



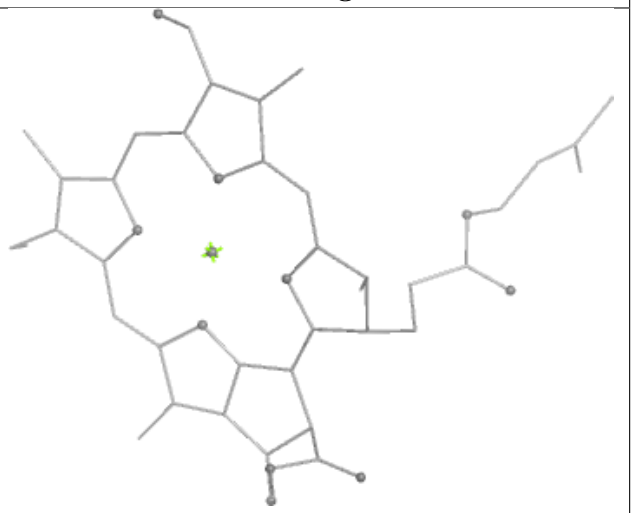
Bond lengths



Bond angles

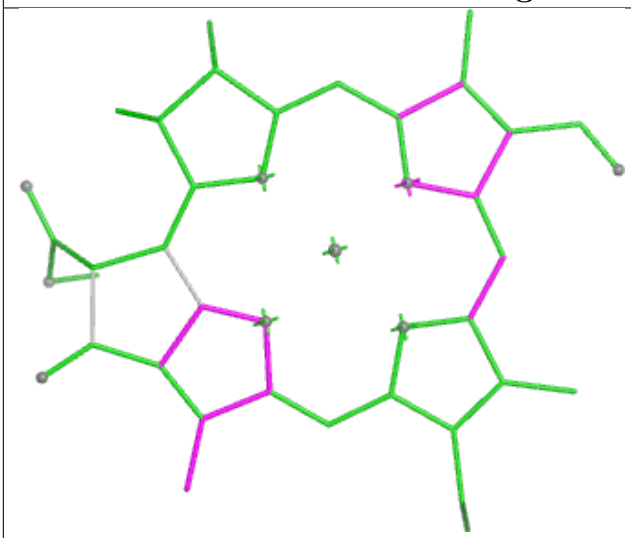


Torsions

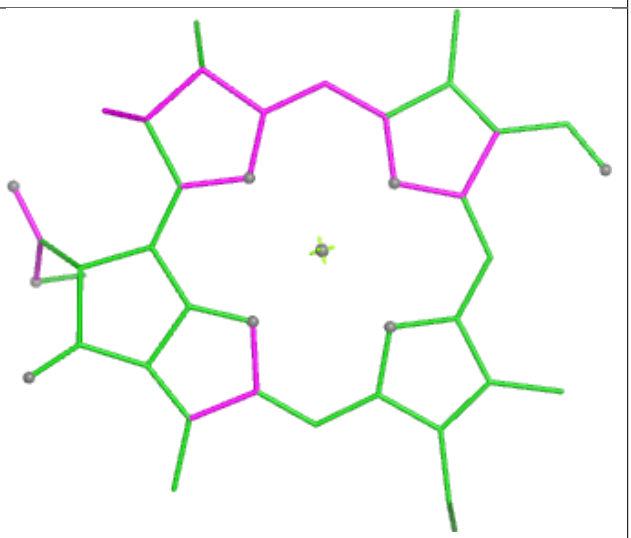


Rings

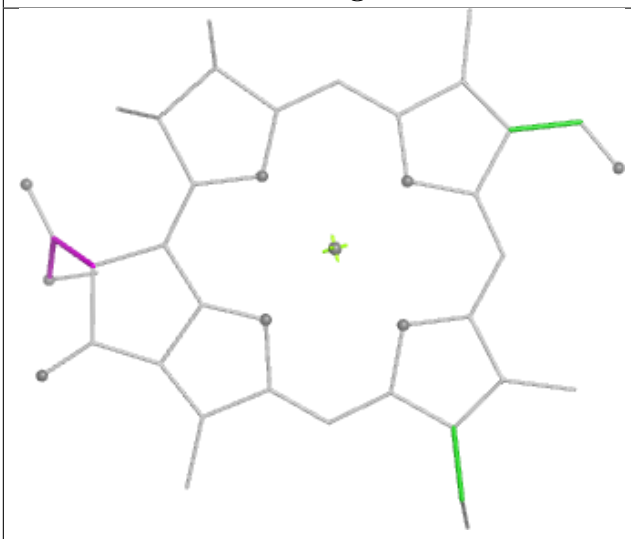
Ligand CL7 cJ 1301



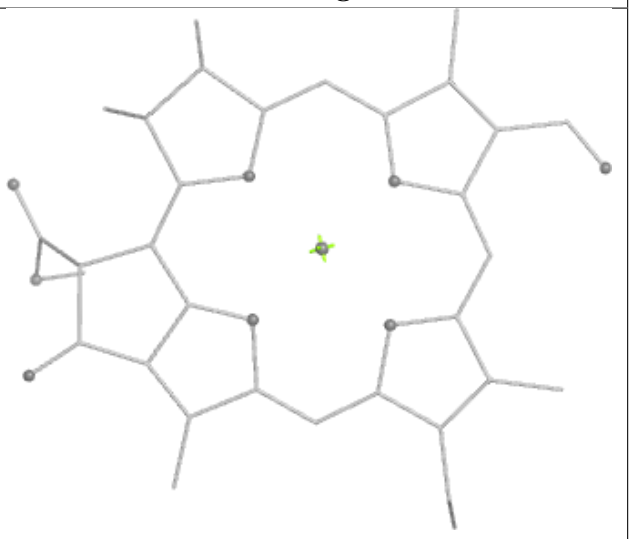
Bond lengths



Bond angles

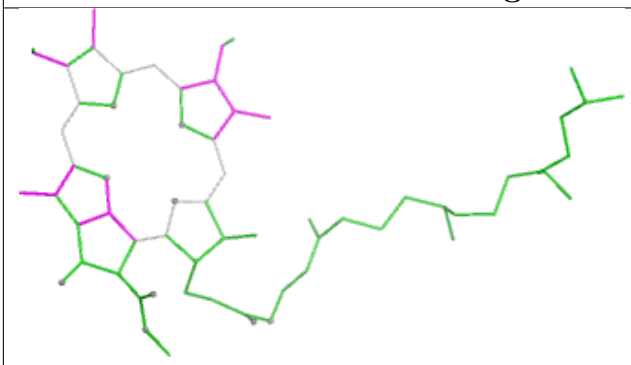


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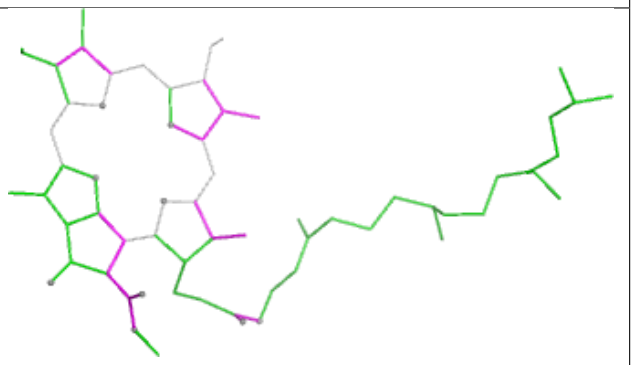


Rings

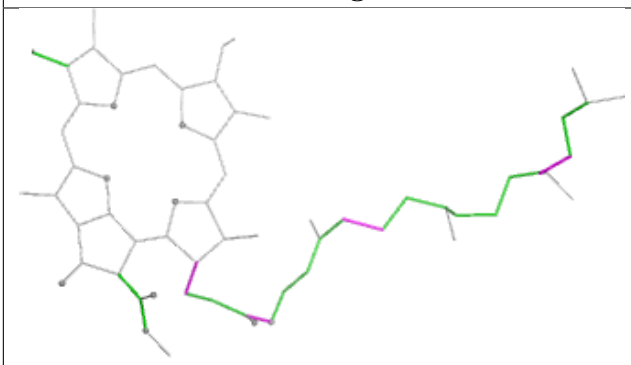
Ligand PHO aA 1013



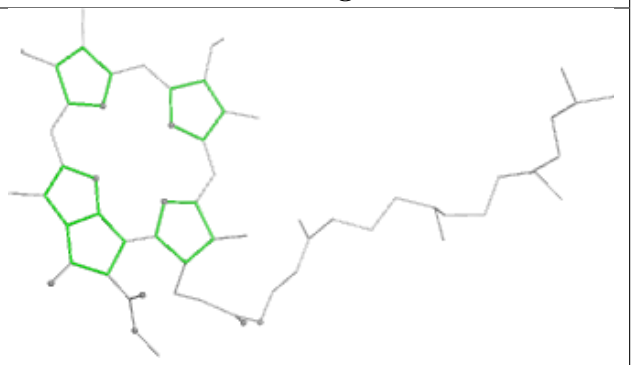
Bond lengths



Bond angles

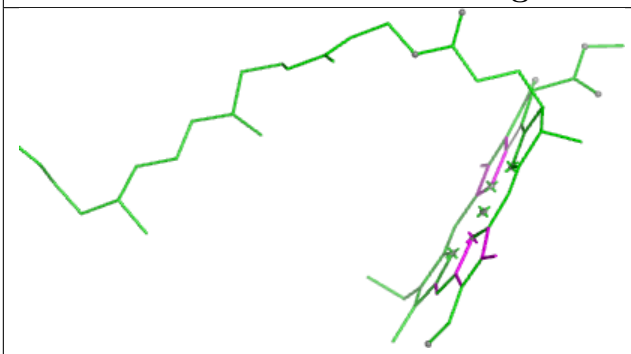


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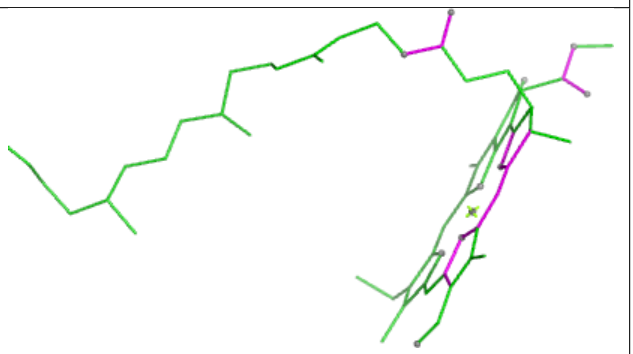


Rings

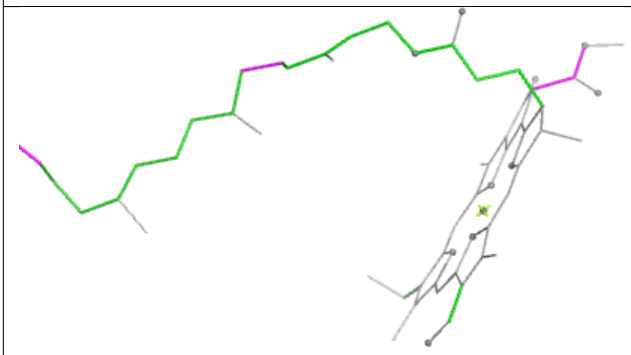
Ligand CL7 cA 1128



Bond lengths



Bond angles

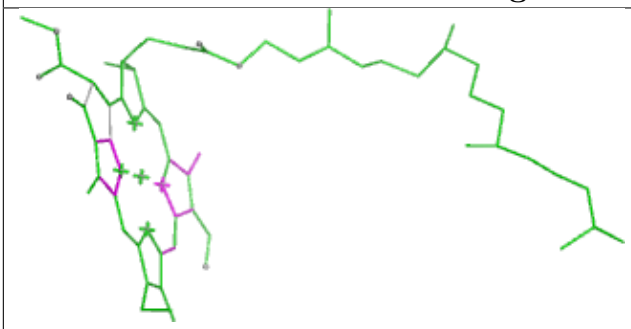


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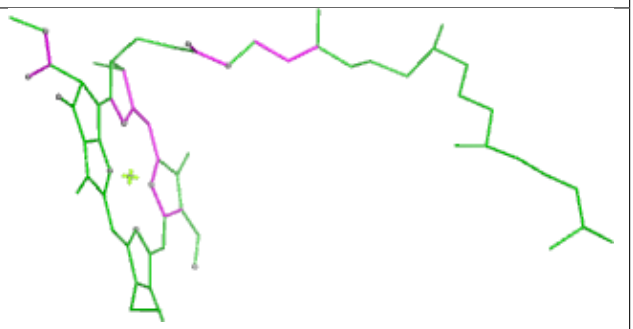


Rings

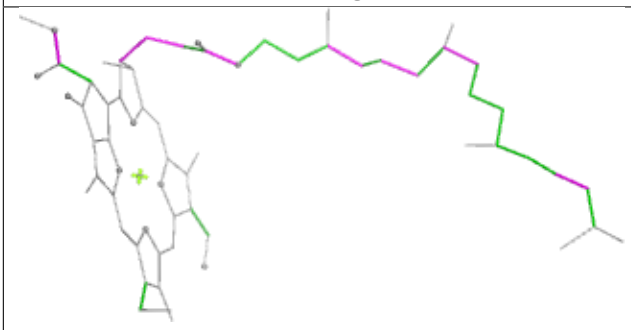
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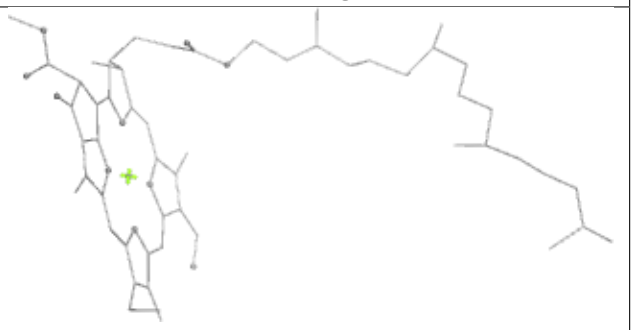
Bond lengths



Bond angles

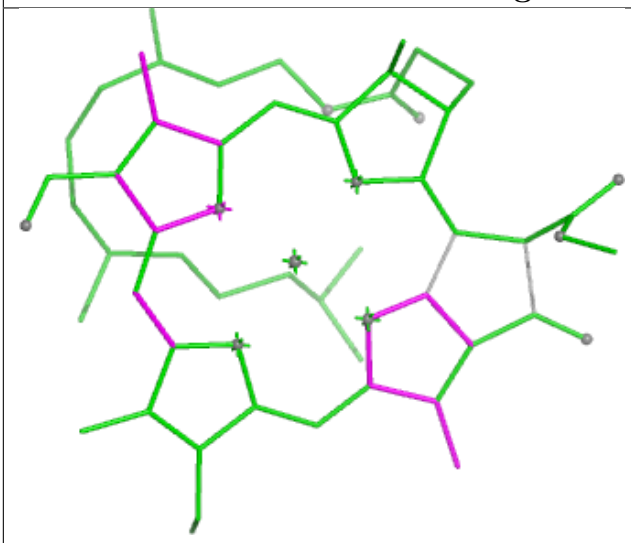


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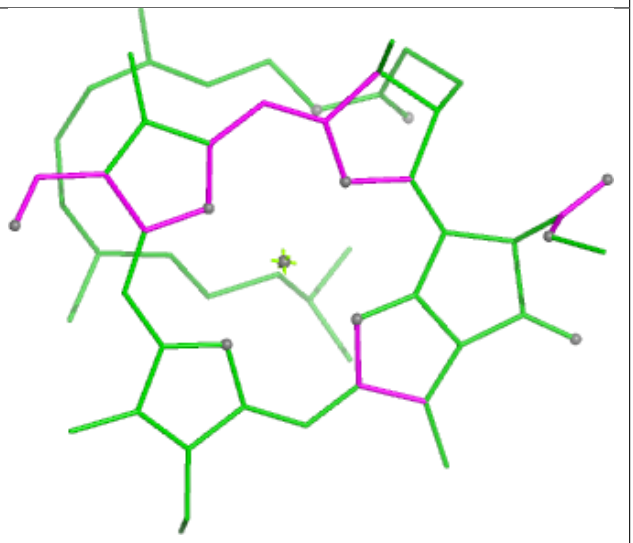


Rings

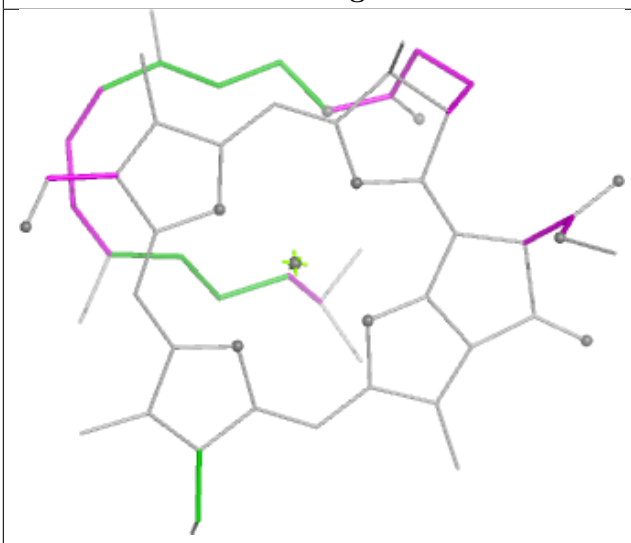
Ligand CL7 cL 1501



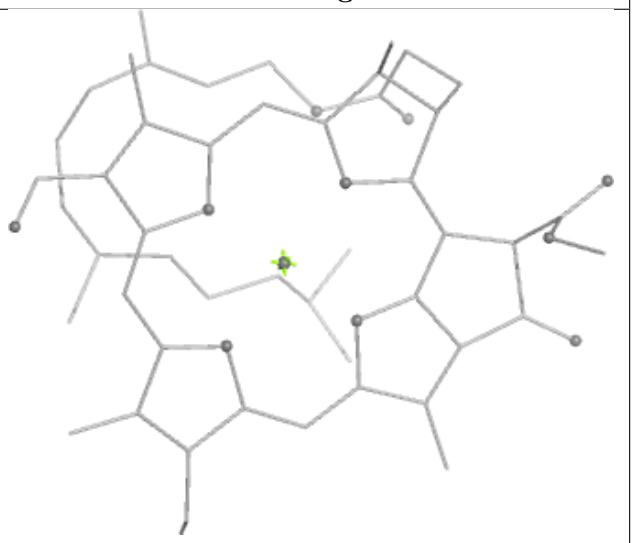
Bond lengths



Bond angles

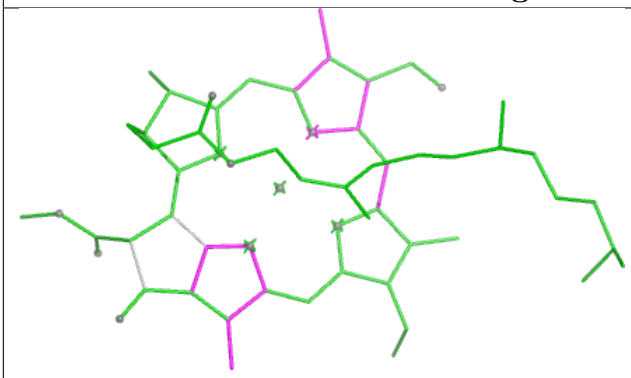


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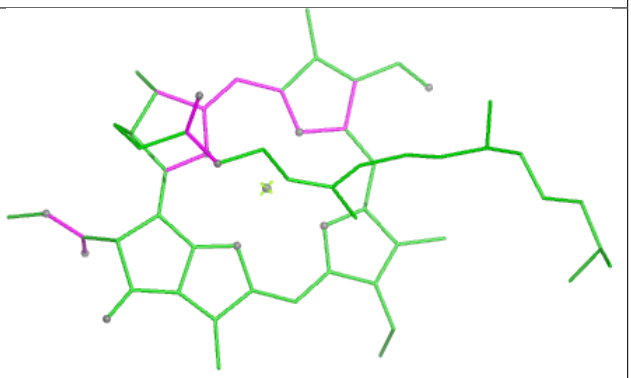


Rings

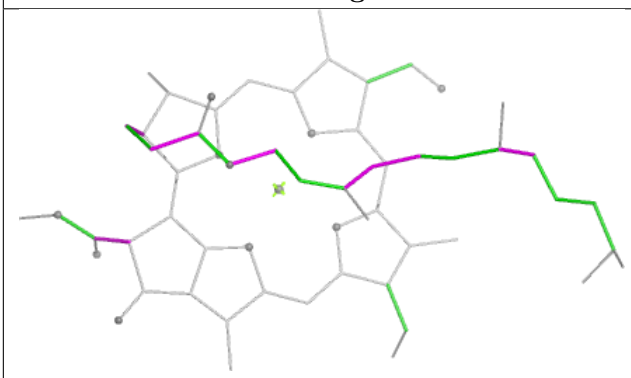
Ligand CL7 aB 1235



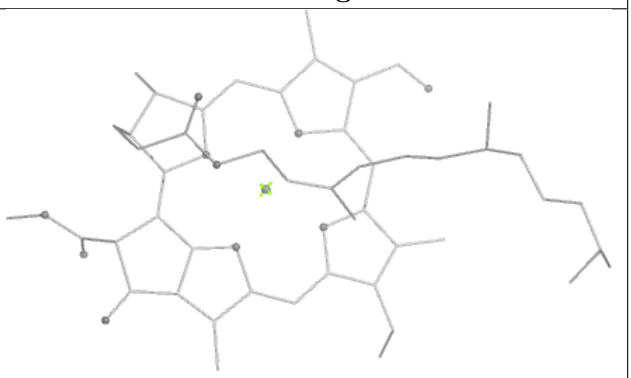
Bond lengths



Bond angles

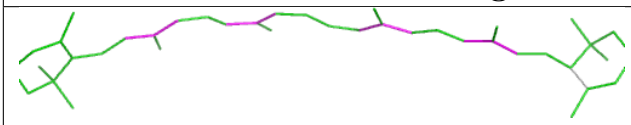


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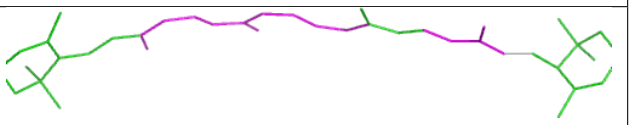


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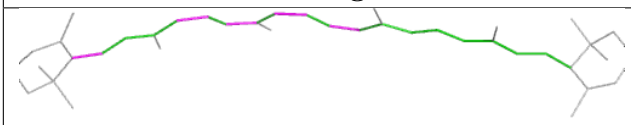
Ligand A1JPJ aA 4014



Bond lengths



Bond angles



Torsions

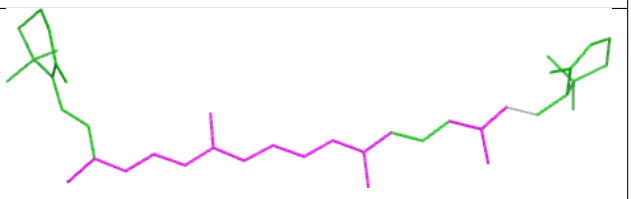


Rings

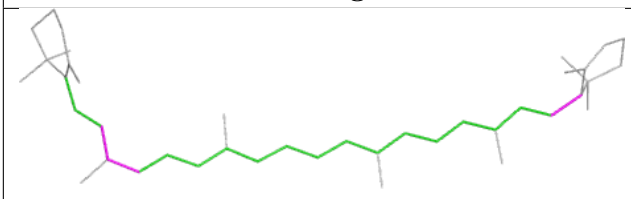
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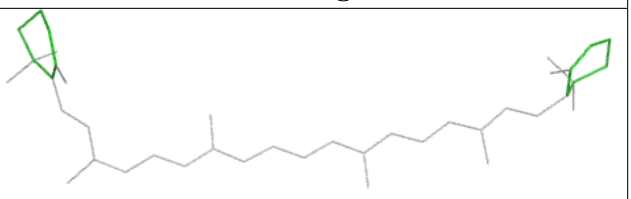
Bond lengths



Bond angles

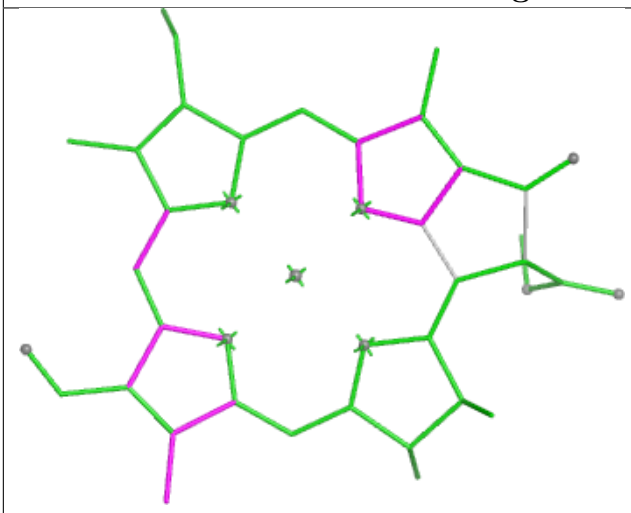


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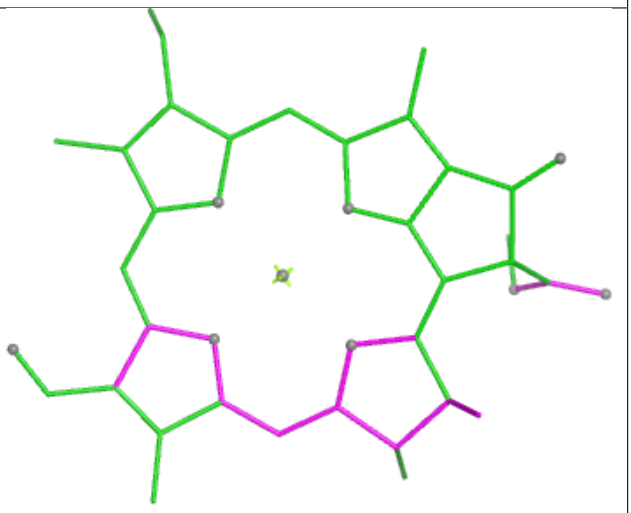


Rings

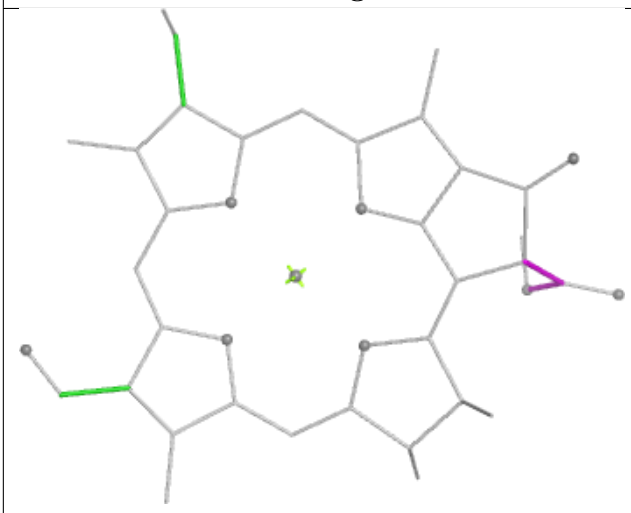
Ligand CL7 cB 1232



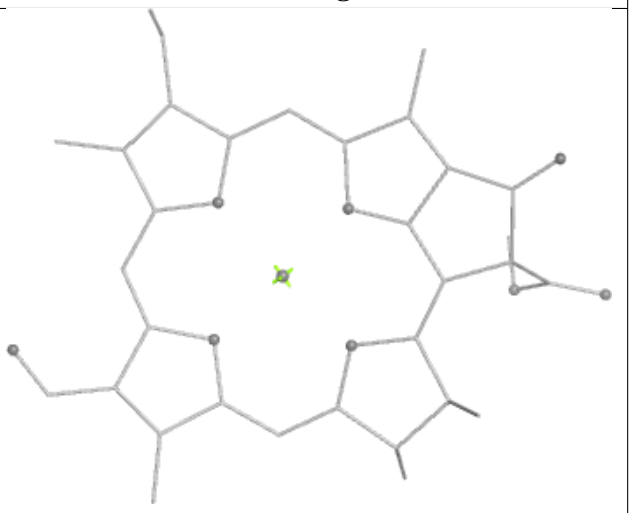
Bond lengths



Bond angles

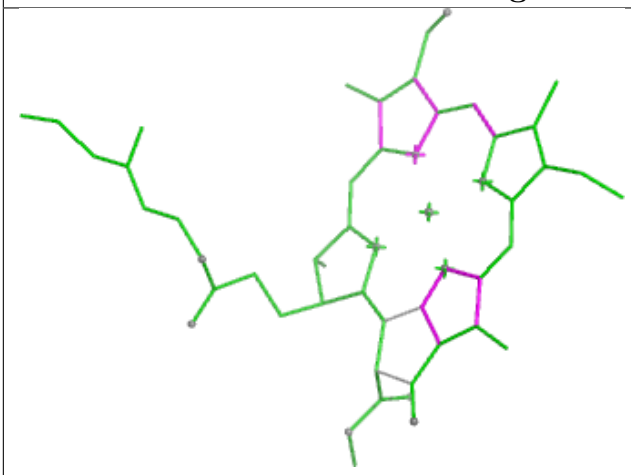


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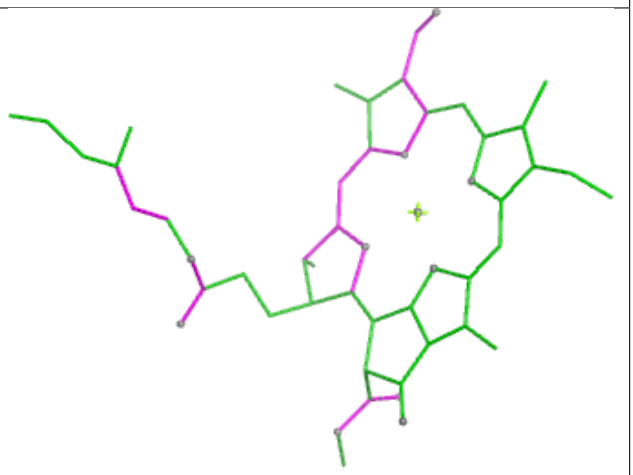


Rings

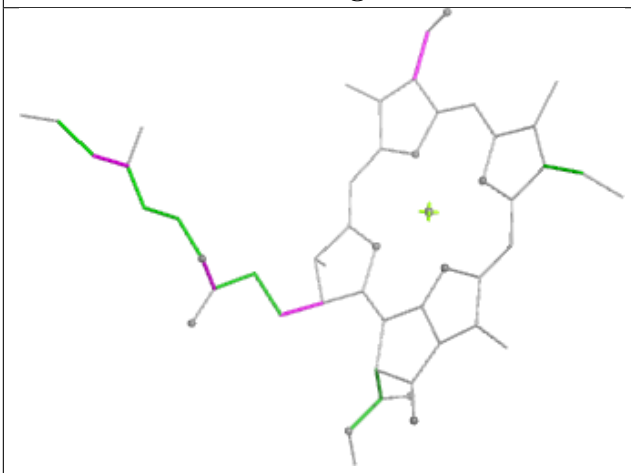
Ligand CL7 bA 1102



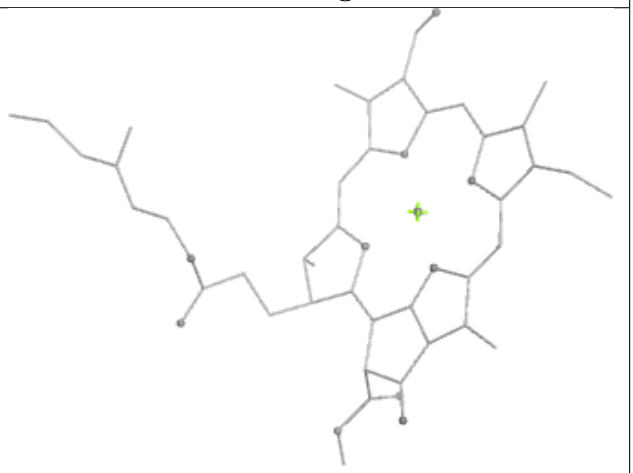
Bond lengths



Bond angles

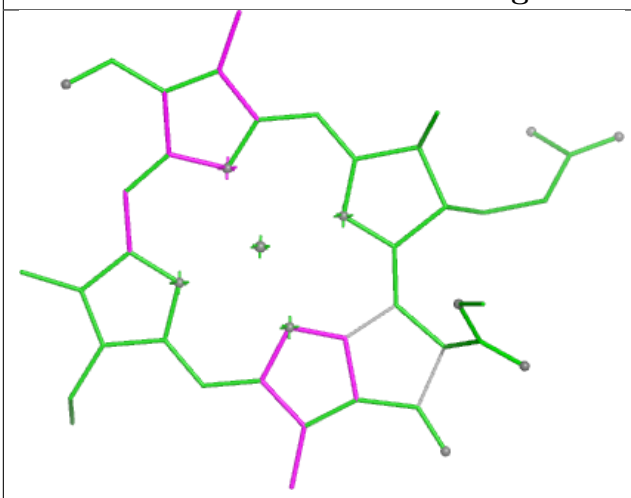


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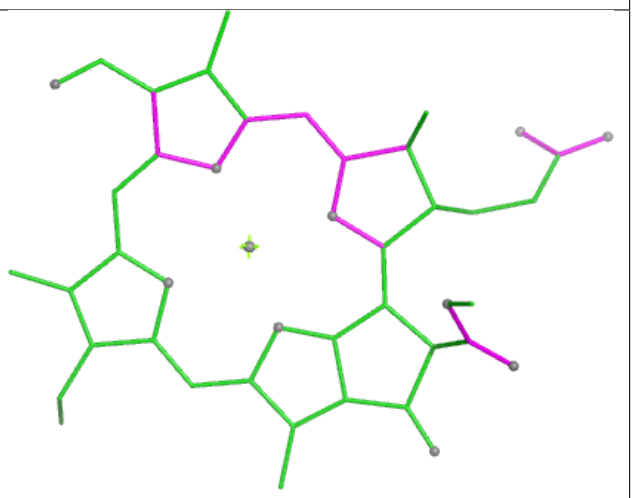


Rings

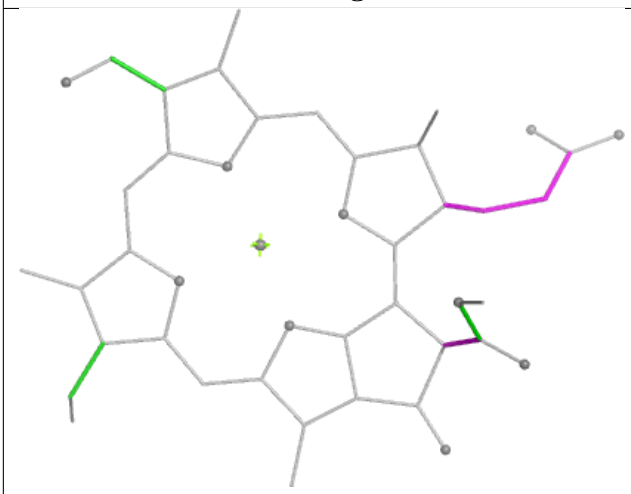
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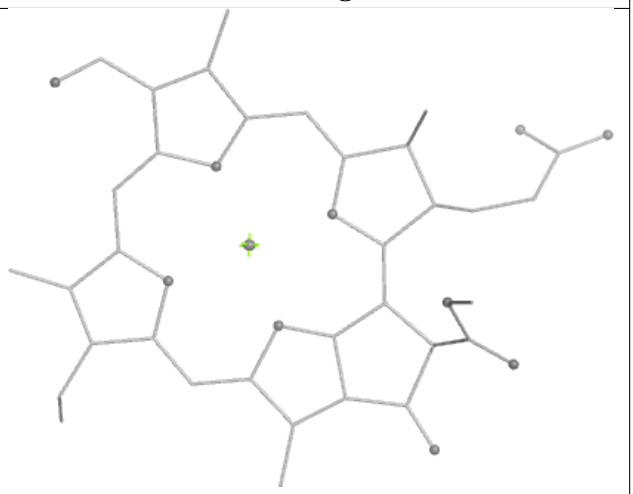
Bond lengths



Bond angles

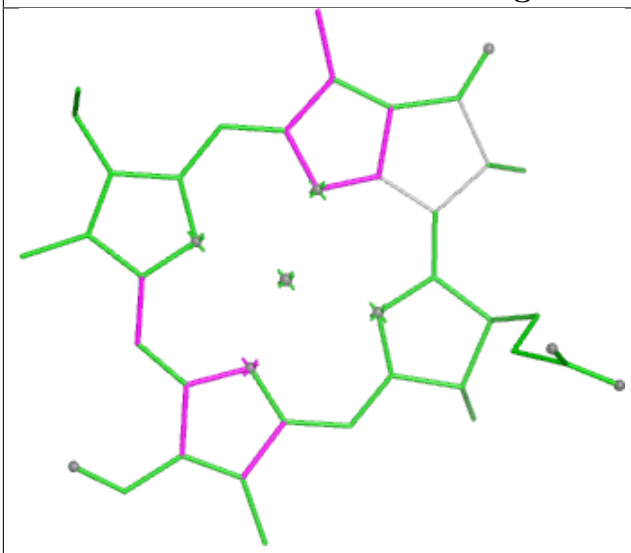


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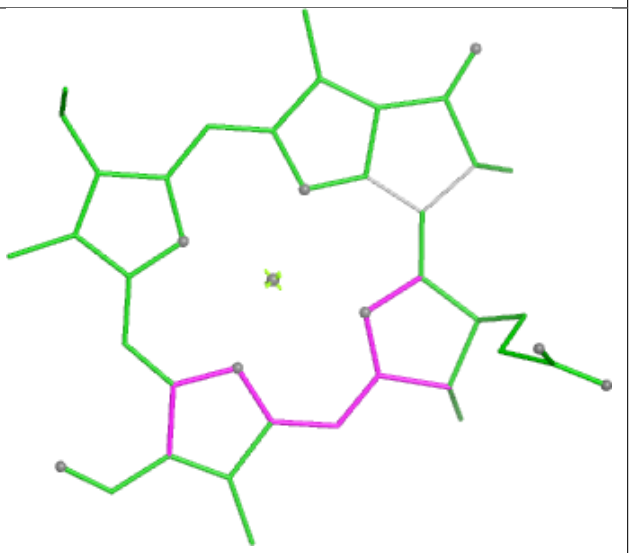


Rings

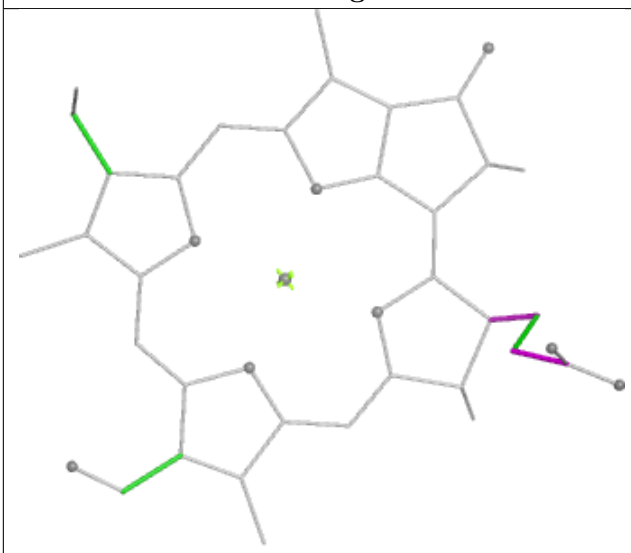
Ligand CL7 bJ 1302



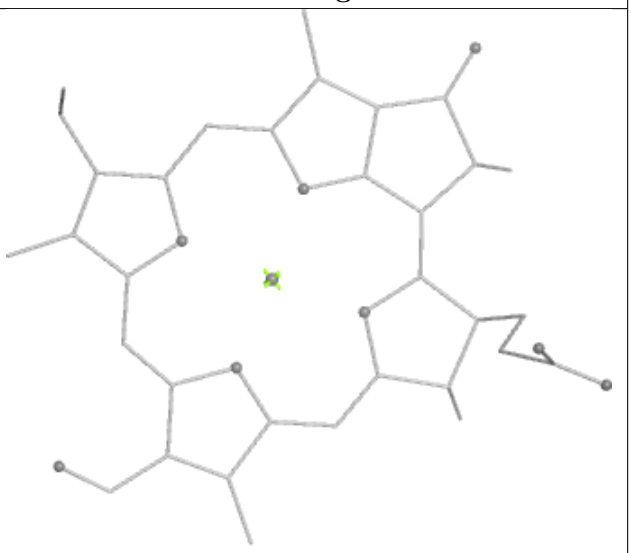
Bond lengths



Bond angles

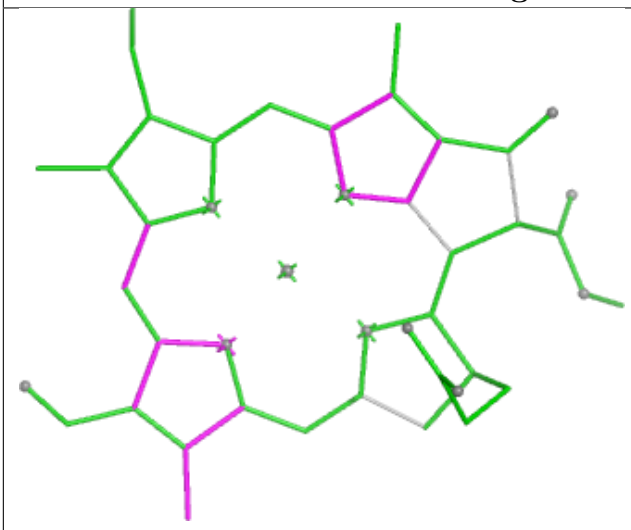


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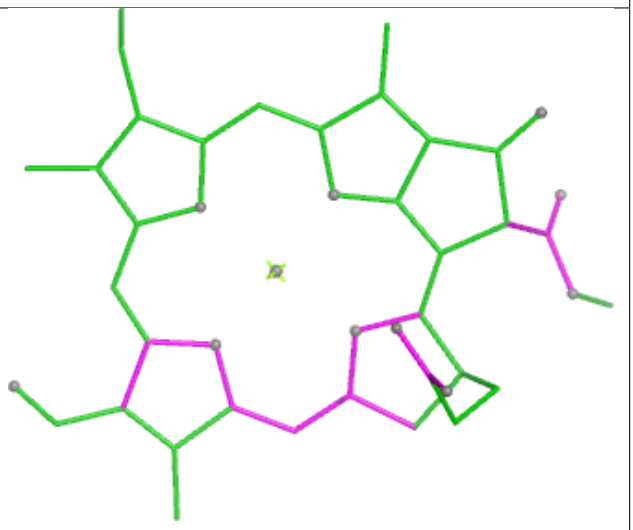


Rings

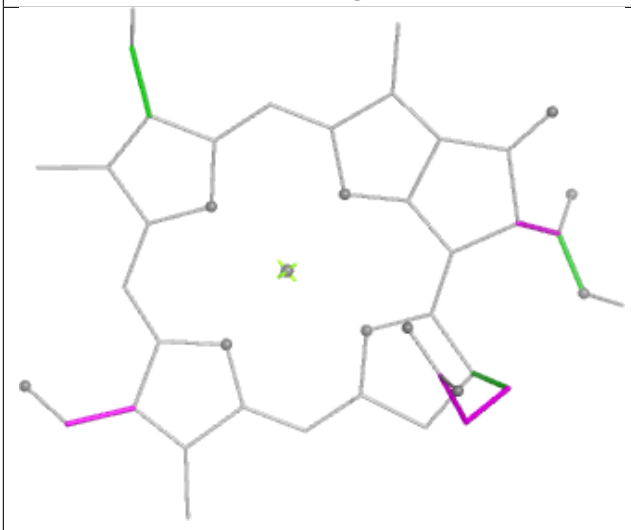
Ligand CL7 aA 1134



Bond lengths



Bond angles

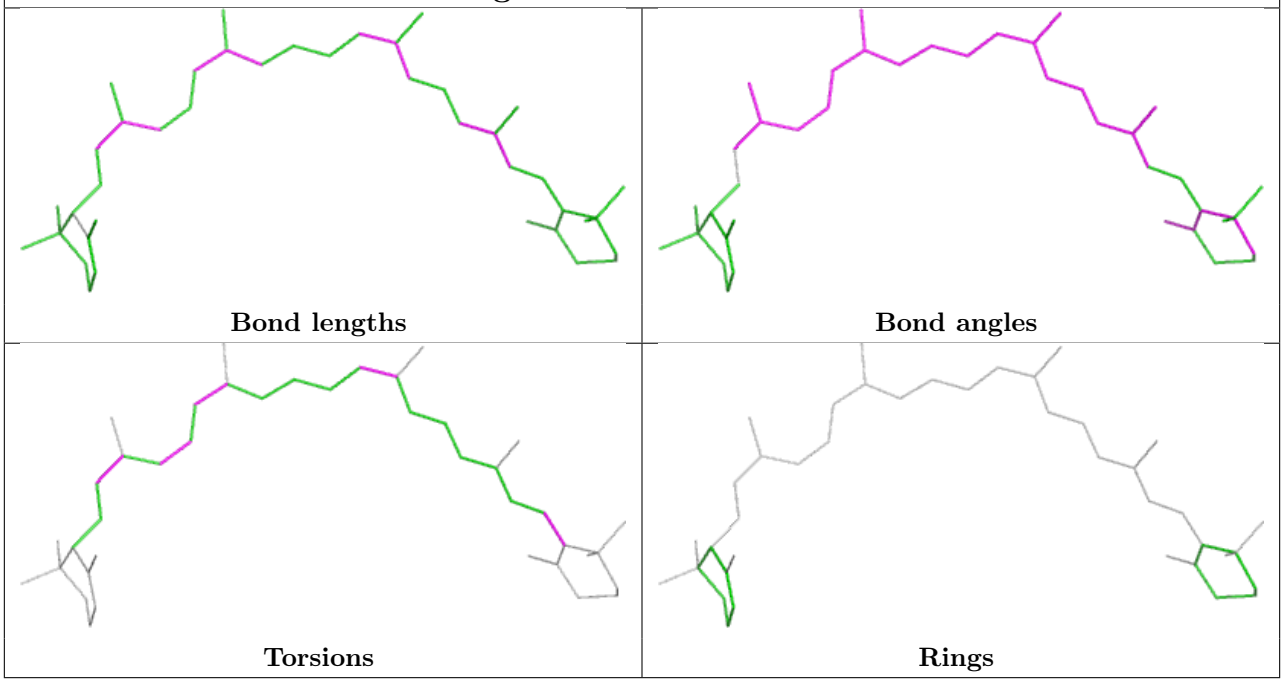


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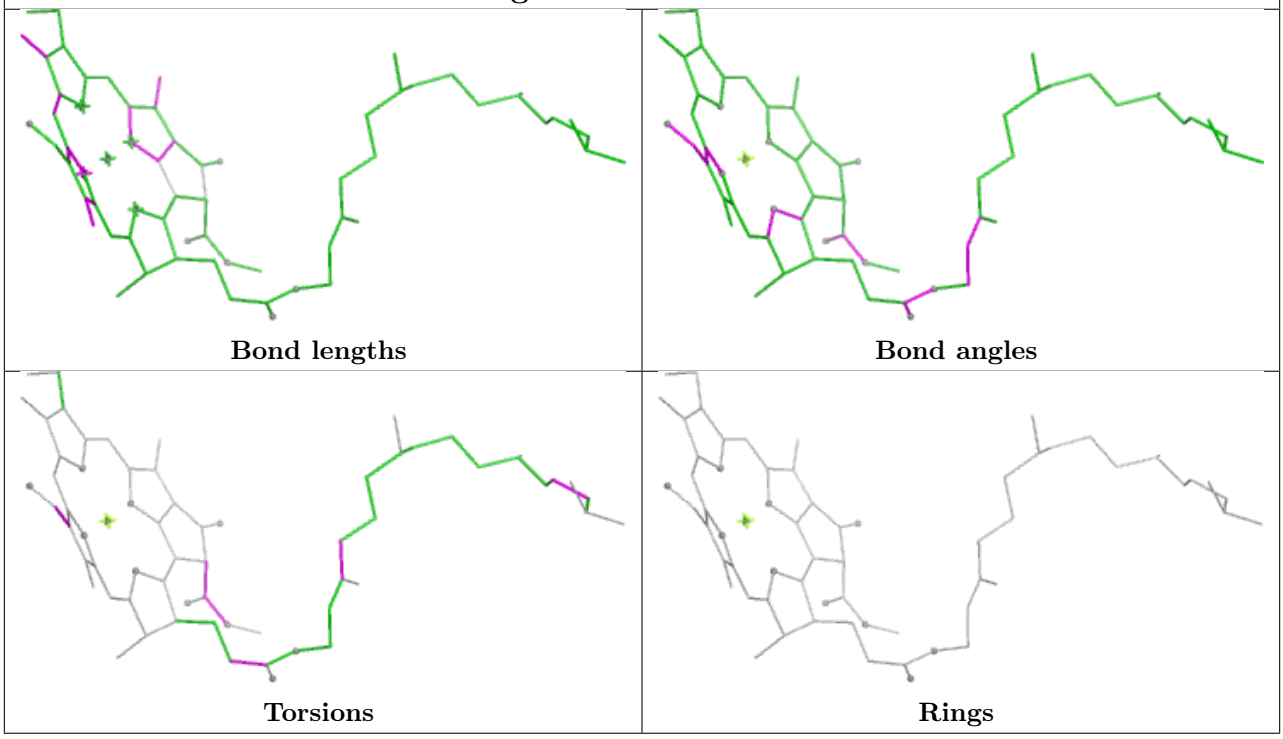


Rings

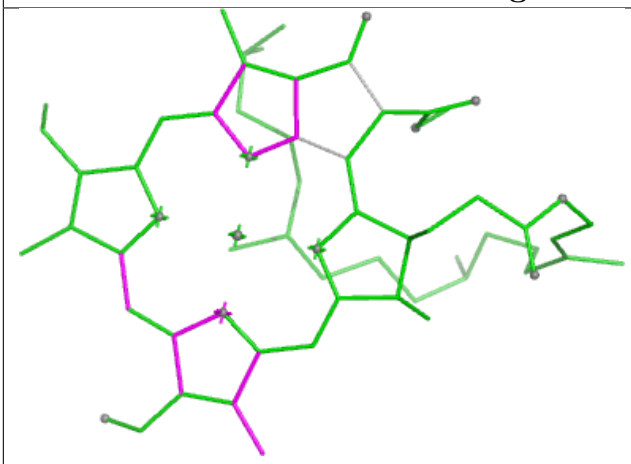
Ligand A1JPJ aF 4016



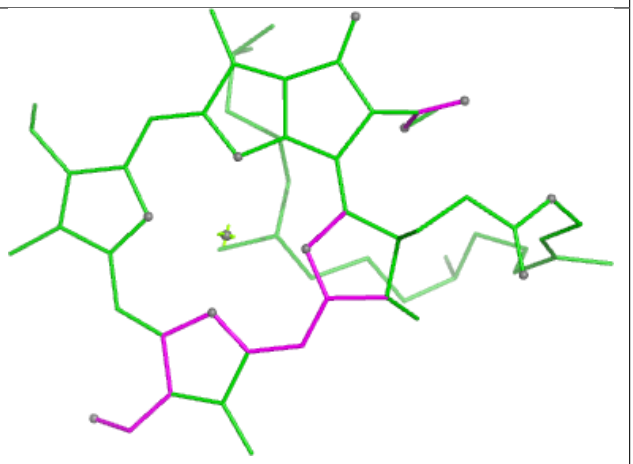
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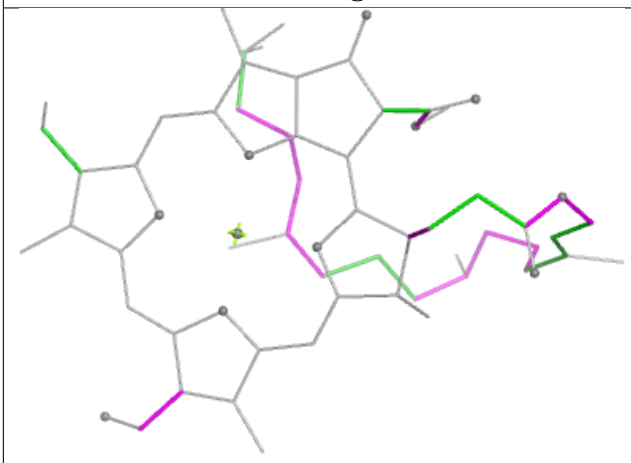
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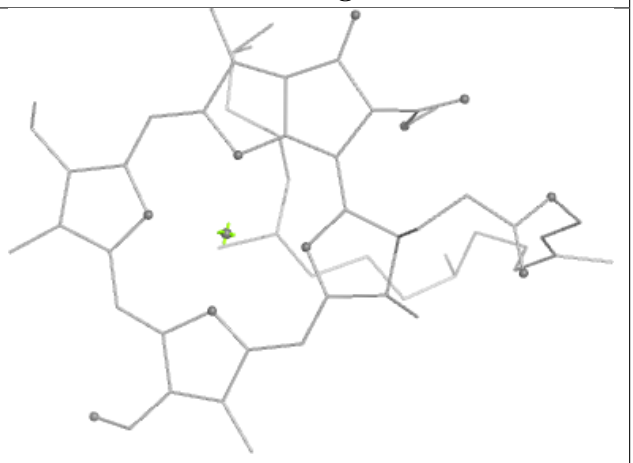
Bond lengths



Bond angles

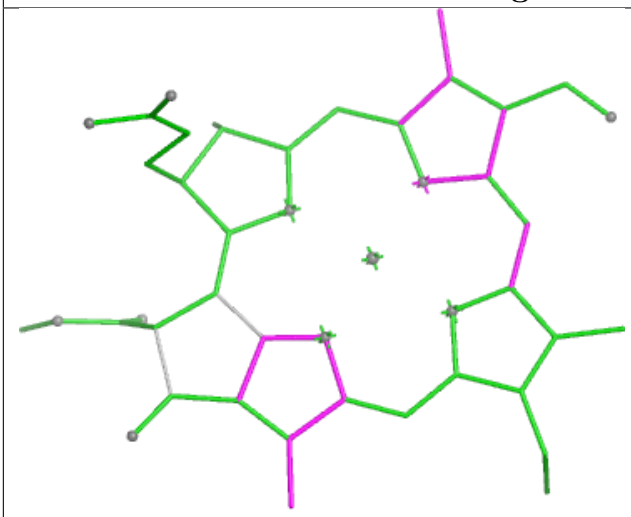


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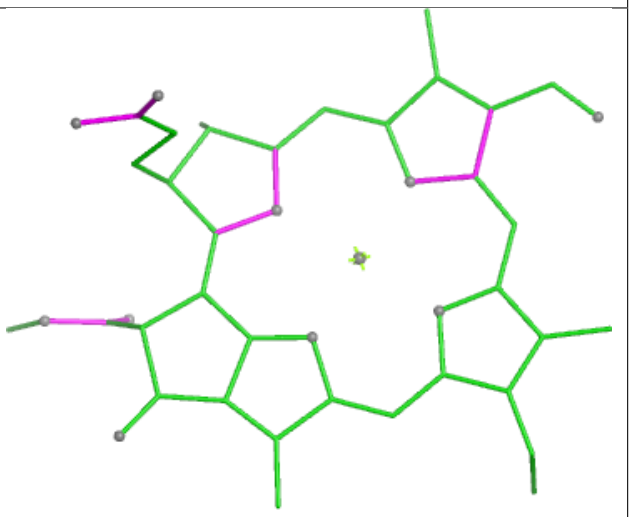


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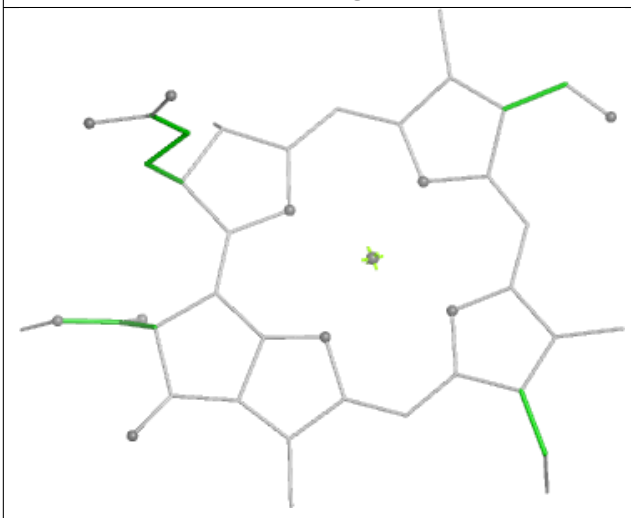
Ligand CL7 aB 1231



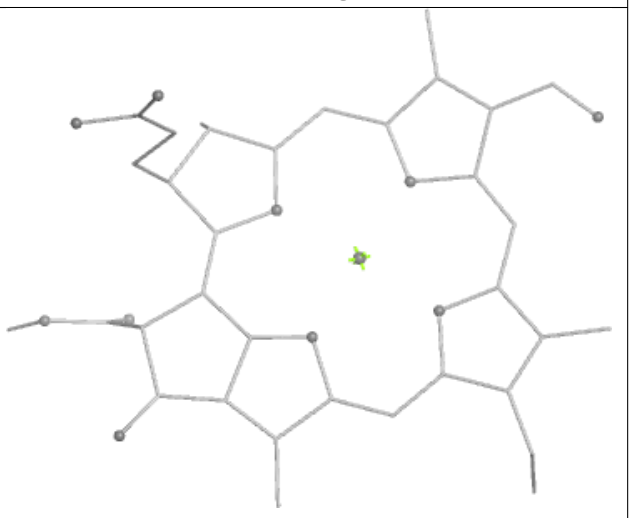
Bond lengths



Bond angles

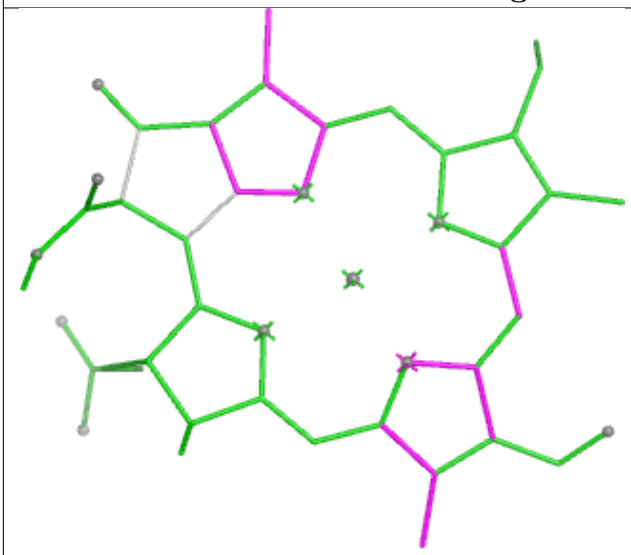


Torsions



Rings

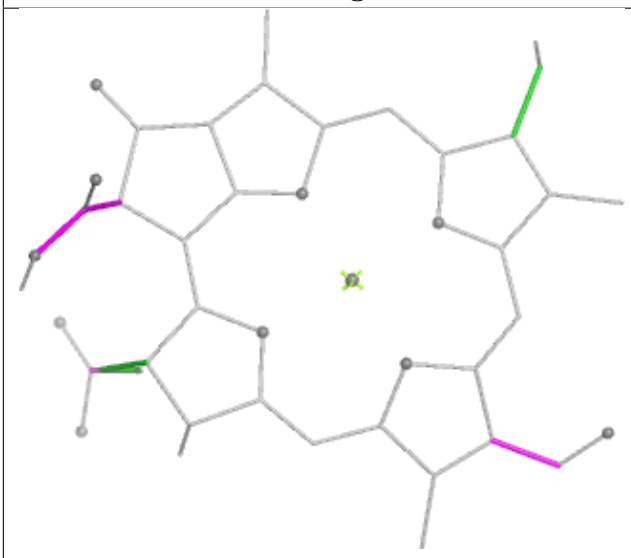
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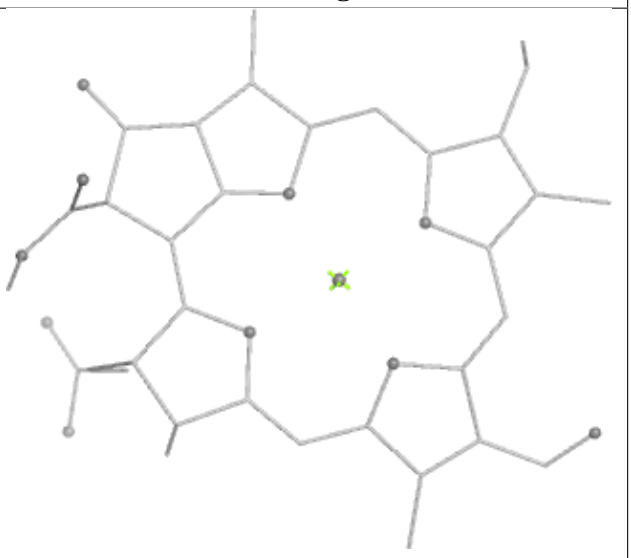
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Bond angles

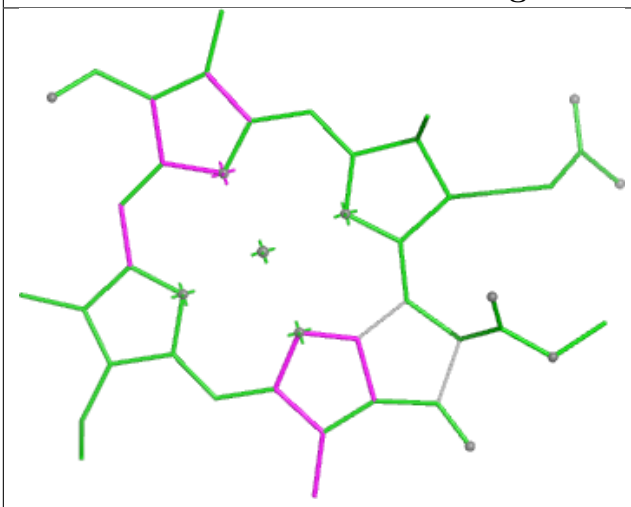


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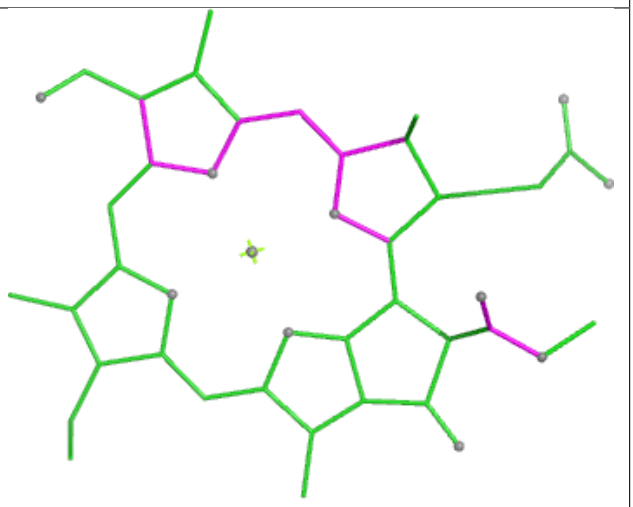


Rings

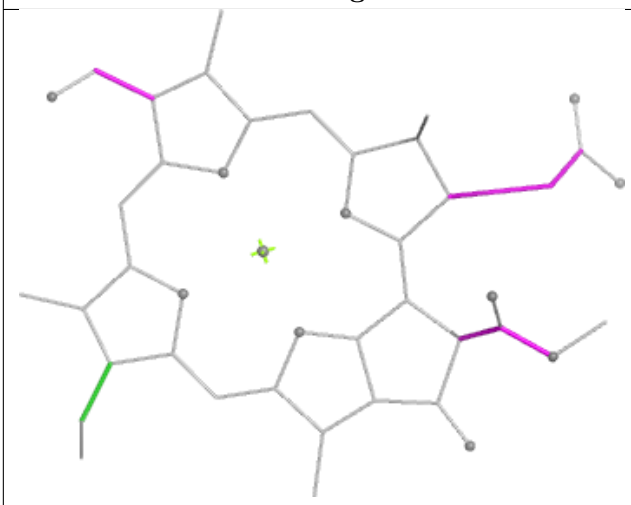
Ligand CL7 bA 1139



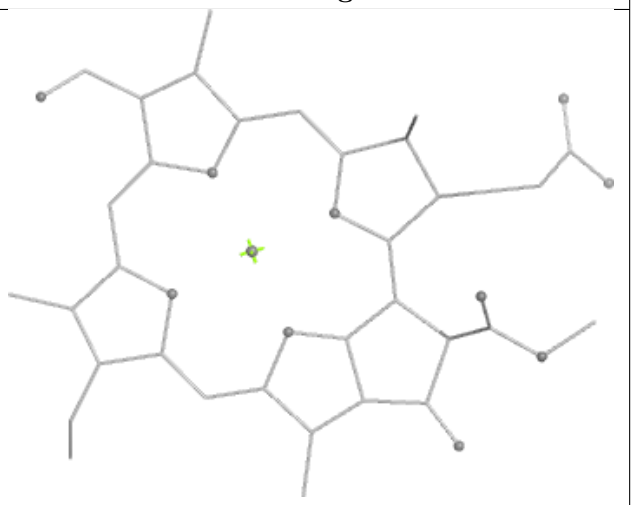
Bond lengths



Bond angles

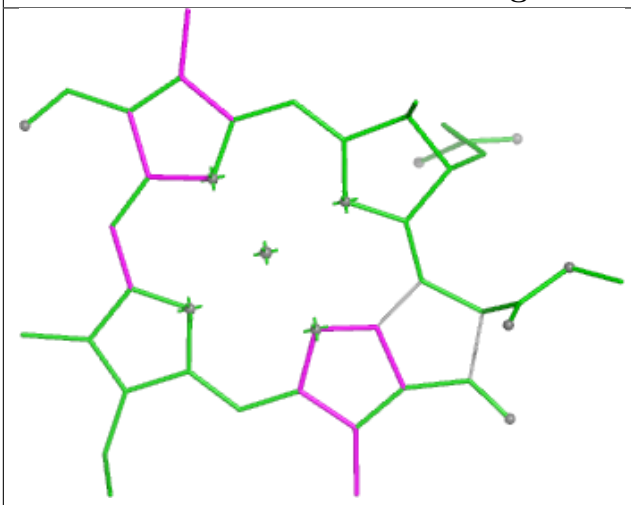


Torsions

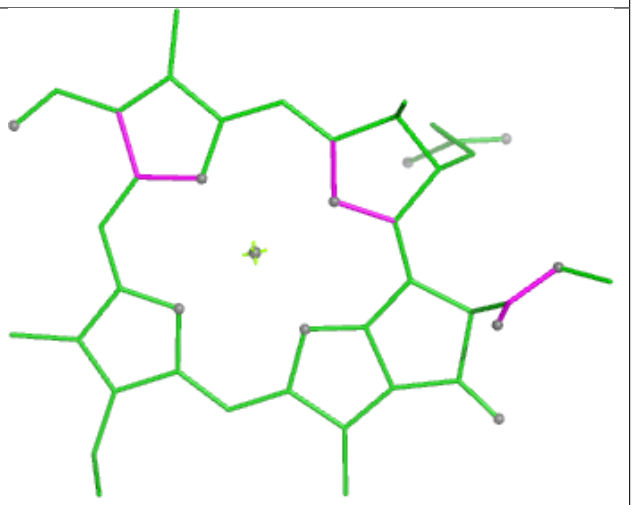


Rings

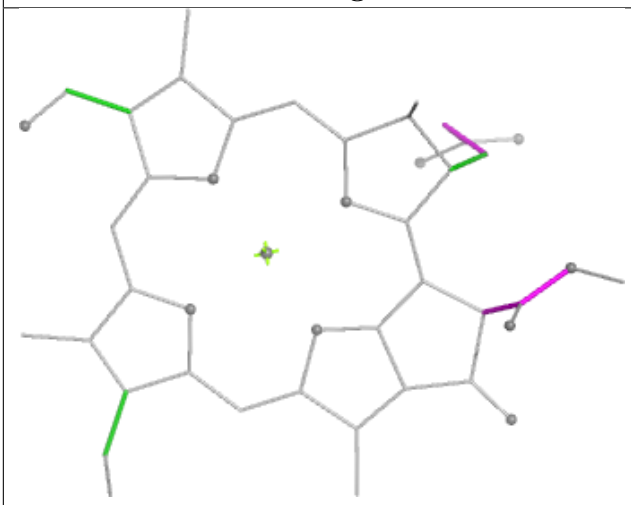
Ligand CL7 bB 1228



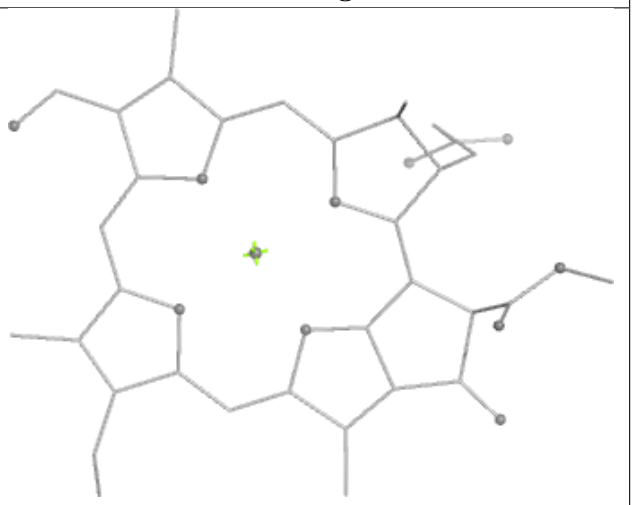
Bond lengths



Bond angles

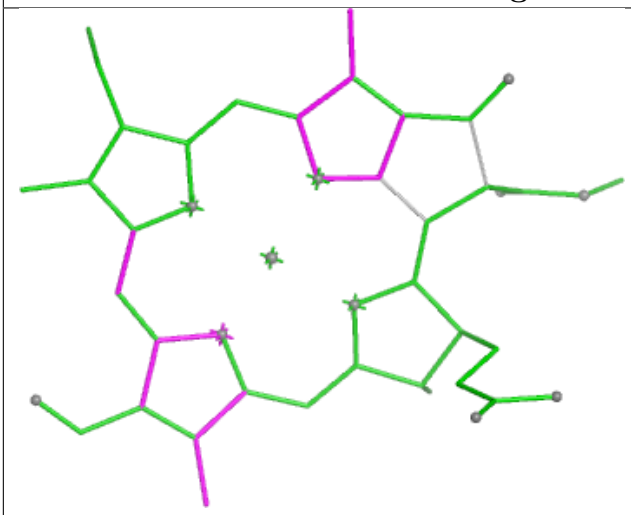


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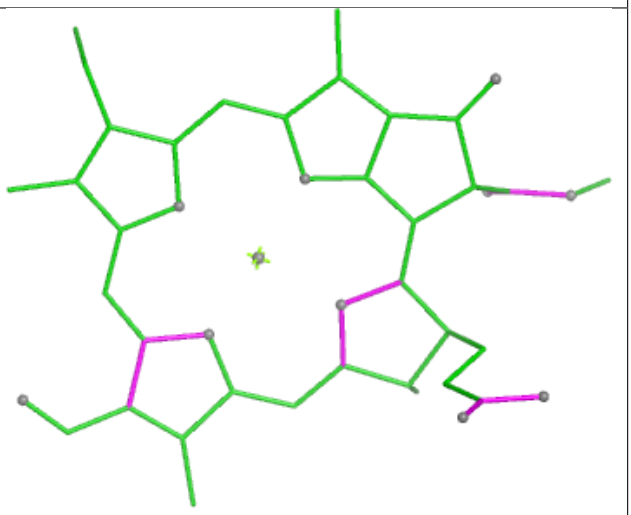


Rings

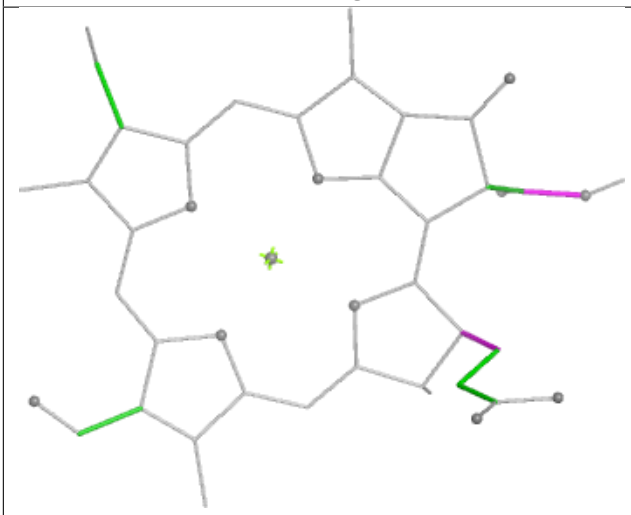
Ligand CL7 bB 1231



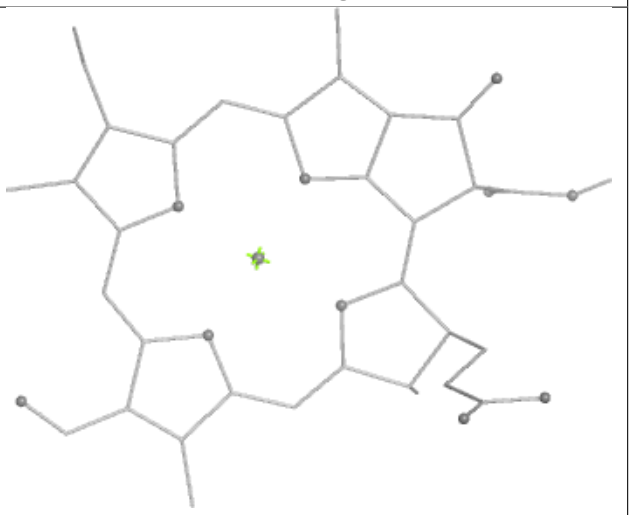
Bond lengths



Bond angles

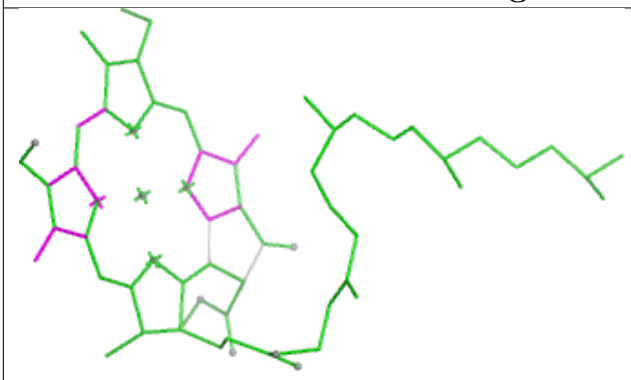


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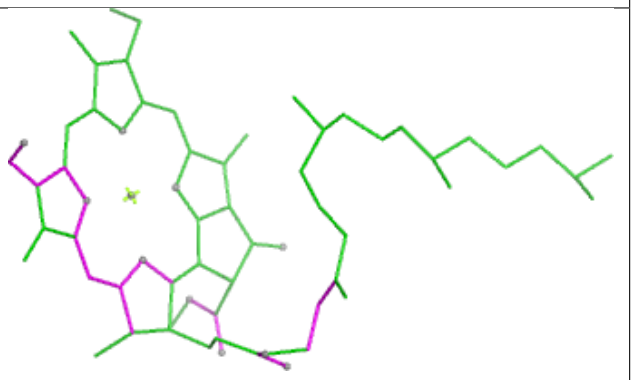


Rings

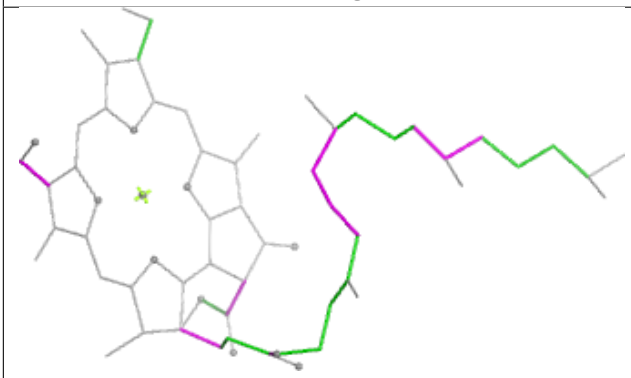
Ligand CL7 bA 1112



Bond lengths



Bond angles

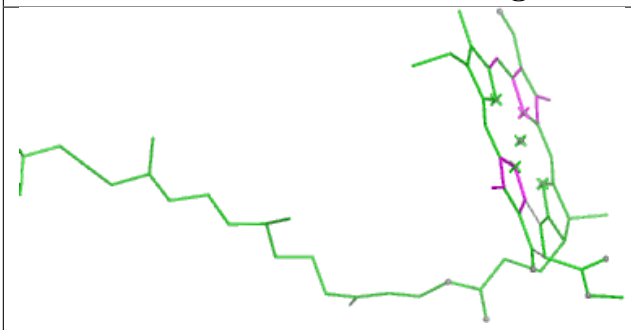


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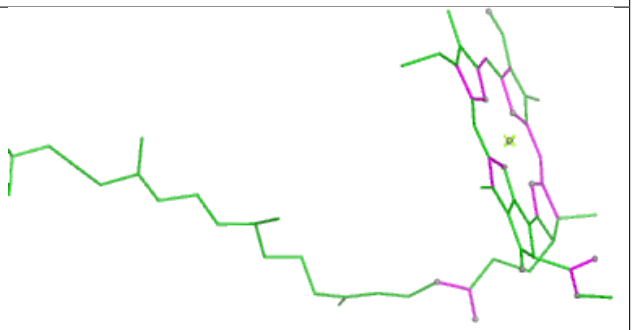


Rings

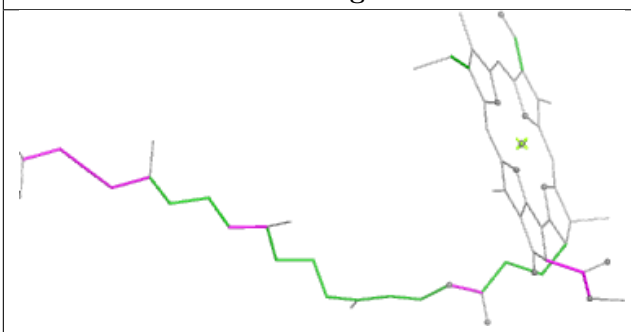
Ligand CL7 bB 1226



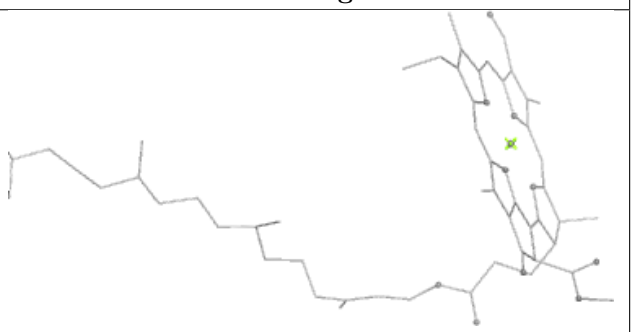
Bond lengths



Bond angles

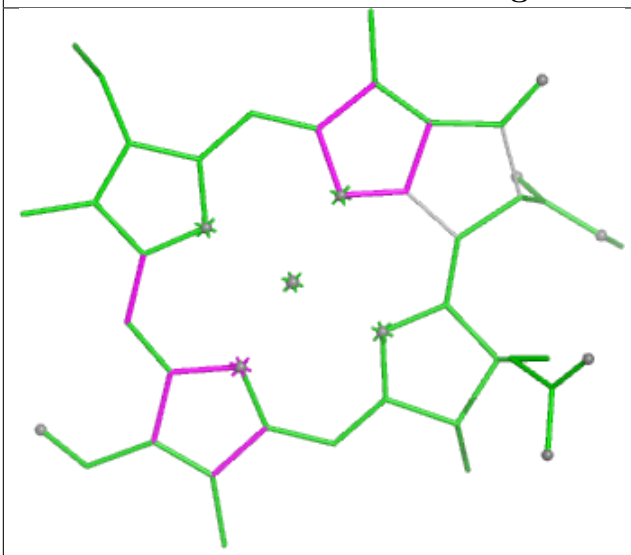


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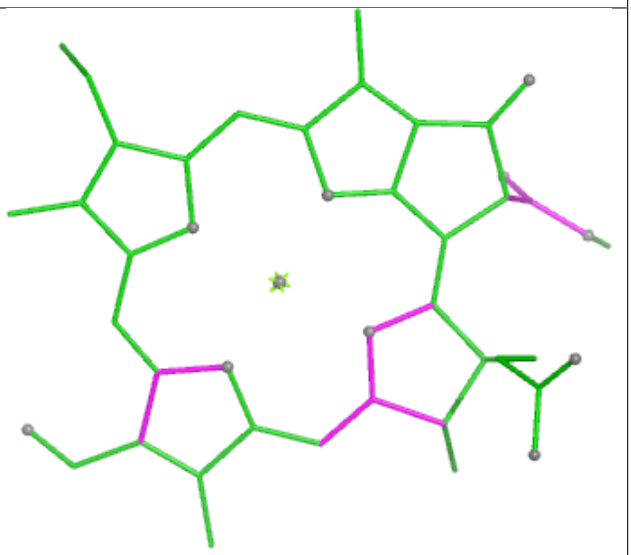


Rings

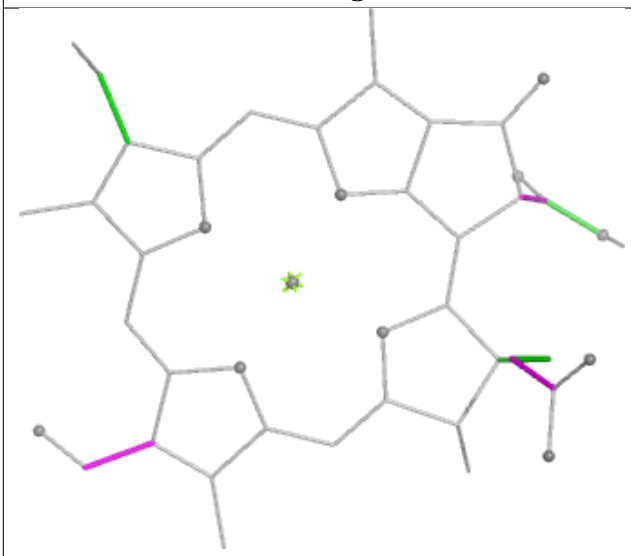
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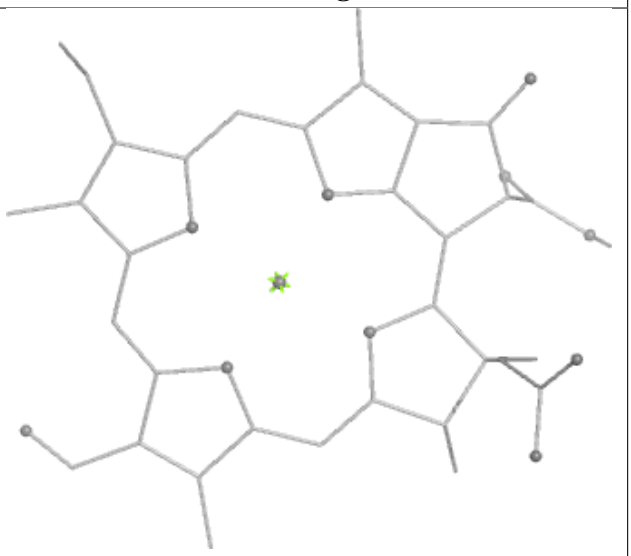
Bond lengths



Bond angles

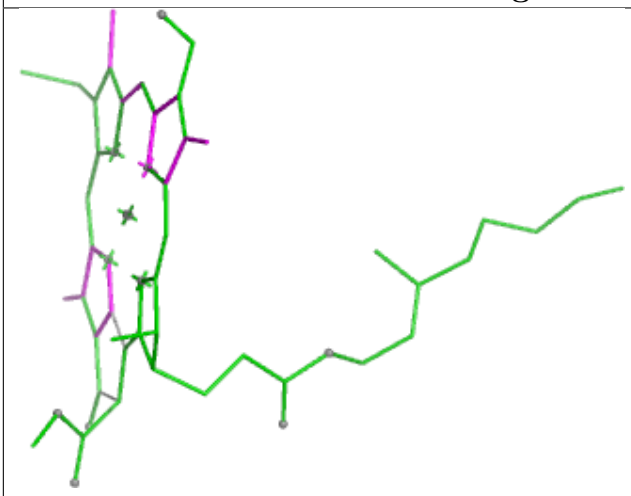


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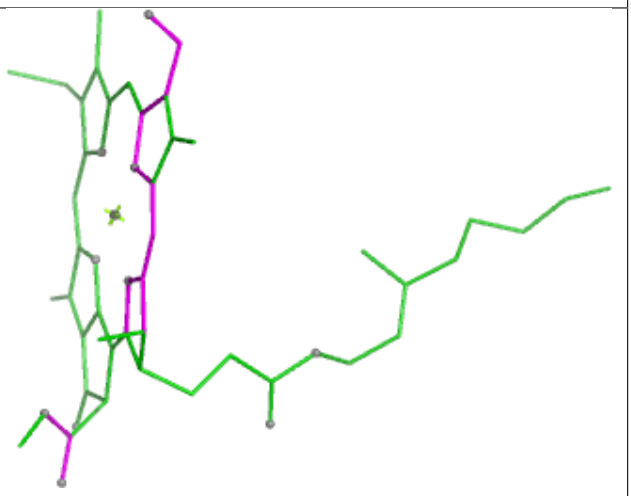


Rings

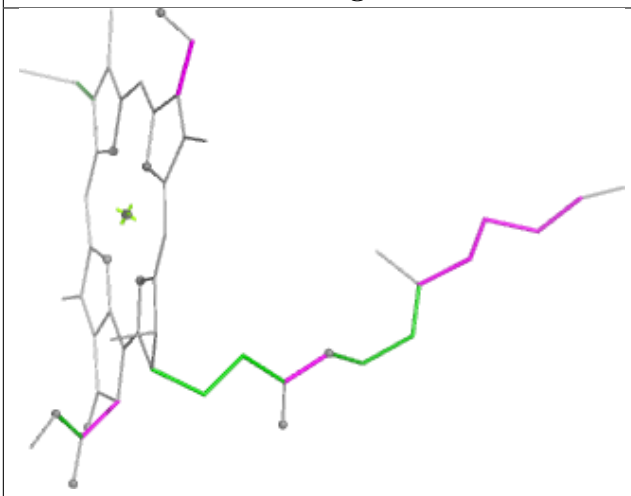
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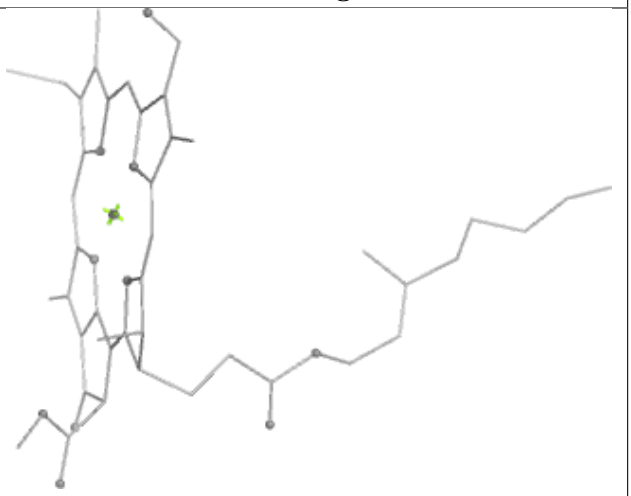
Bond lengths



Bond angles

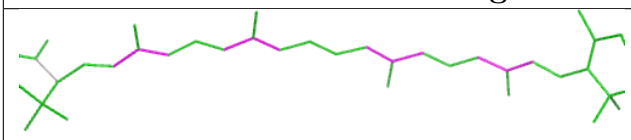


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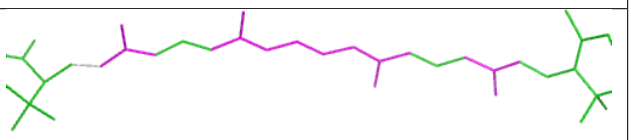


Rings

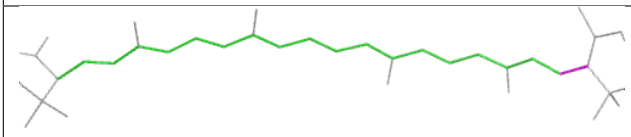
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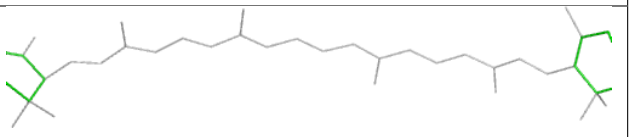
Bond lengths



Bond angles

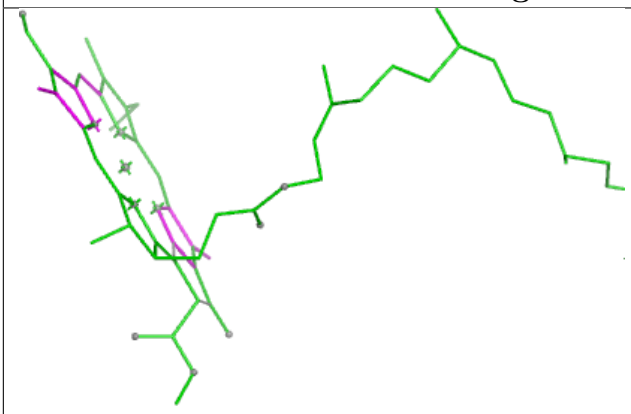


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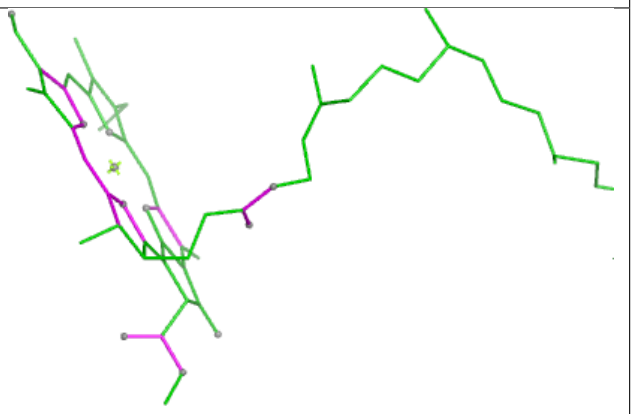


Rings

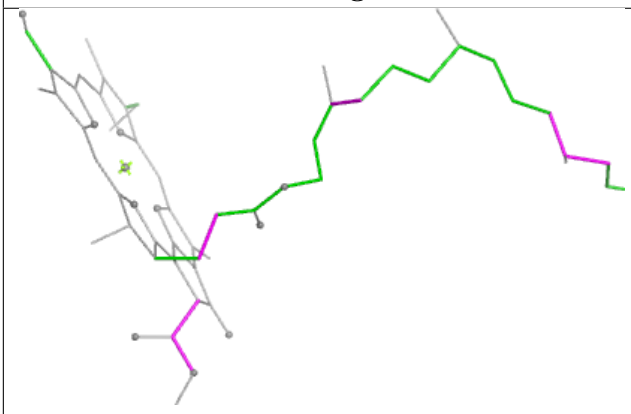
Ligand CL7 cB 1238



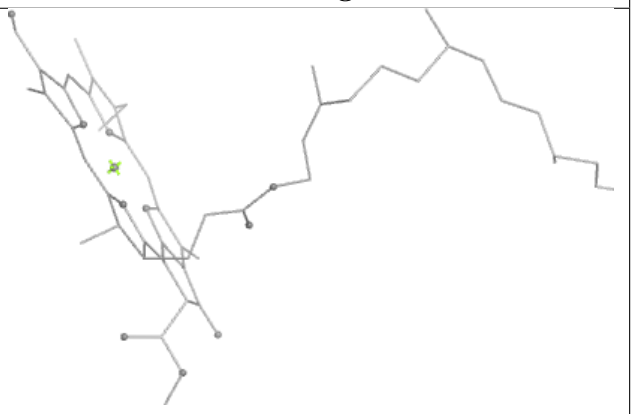
Bond lengths



Bond angles

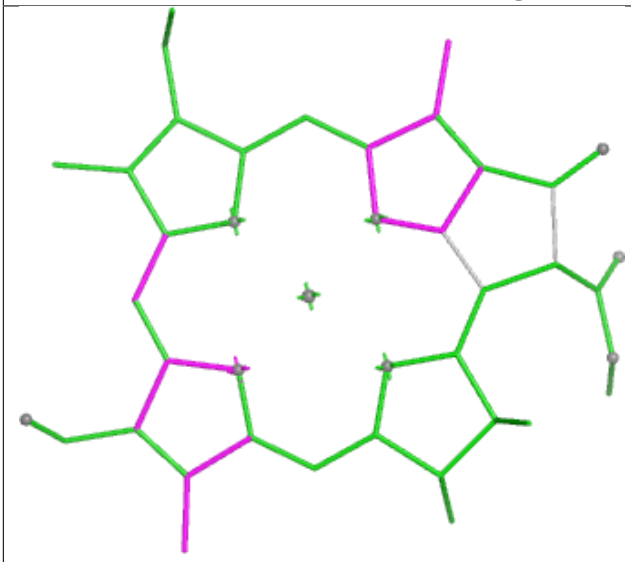


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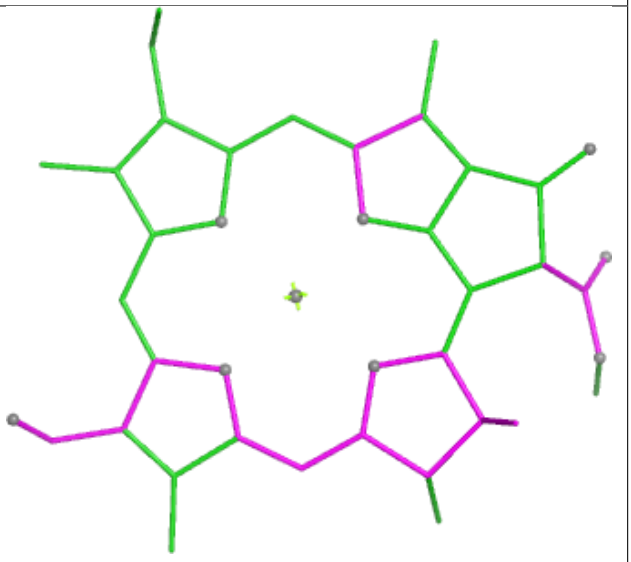


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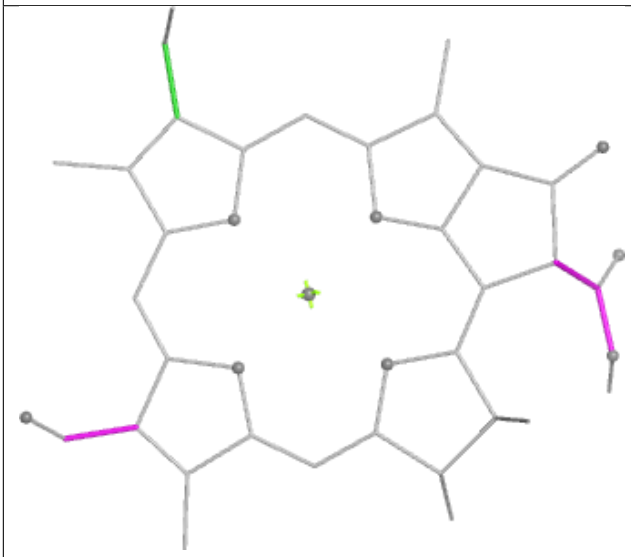
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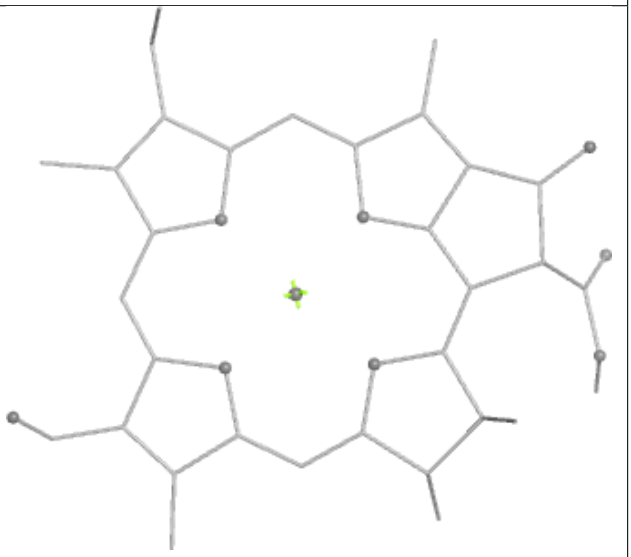
Bond lengths



Bond angles

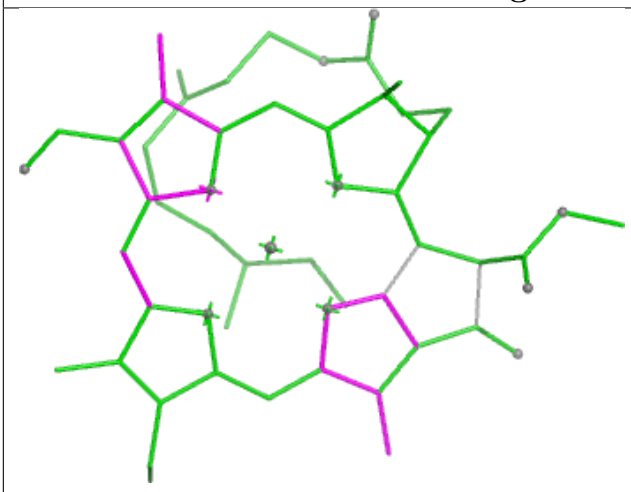


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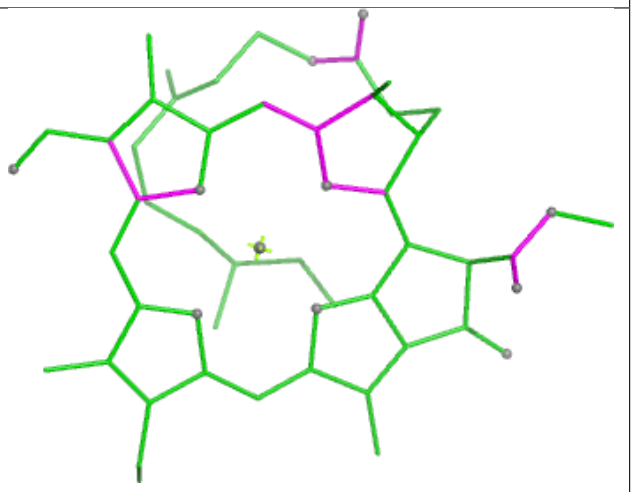


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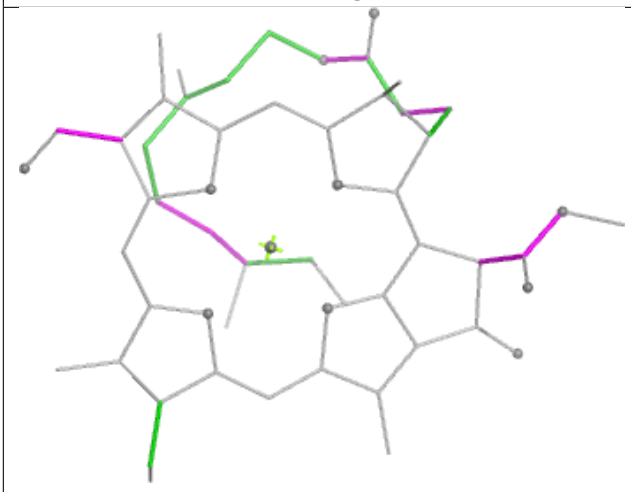
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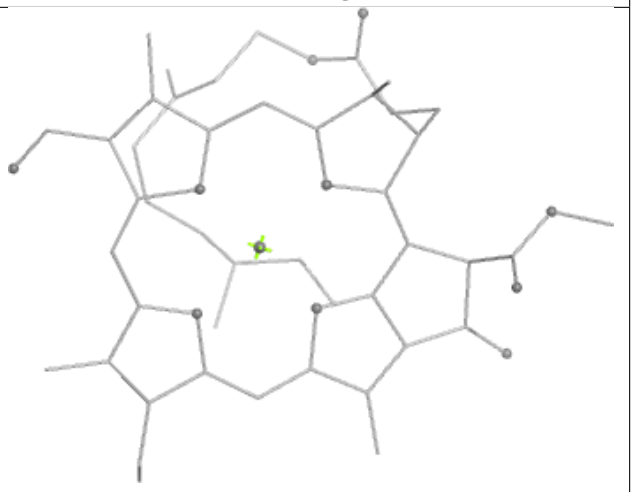
Bond lengths



Bond angles



Torsions



Rings

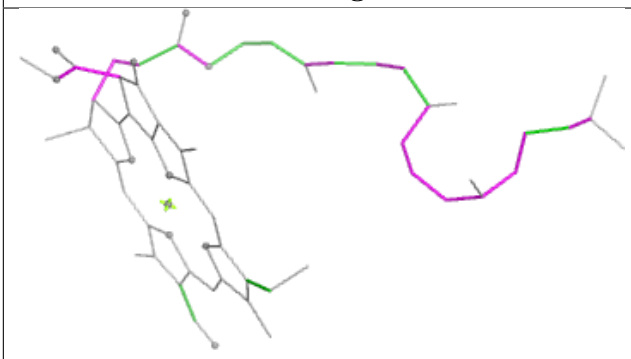
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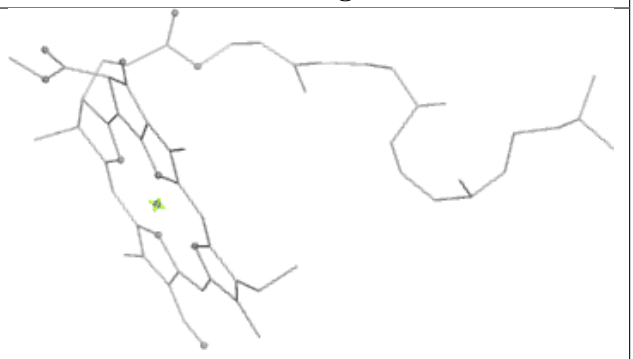
Bond lengths



Bond angles

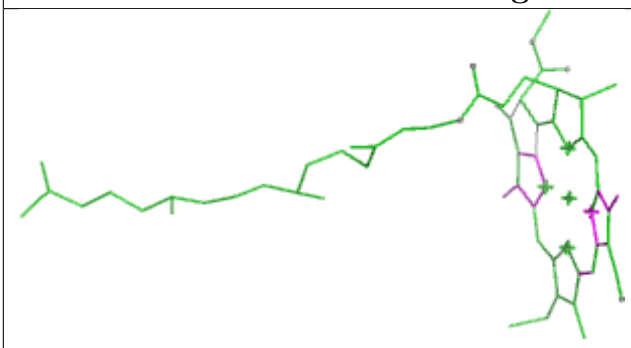


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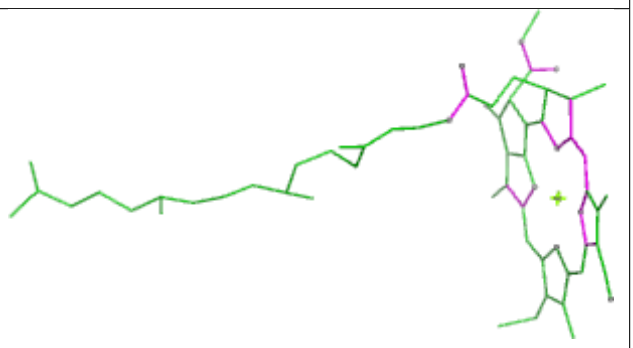


Rings

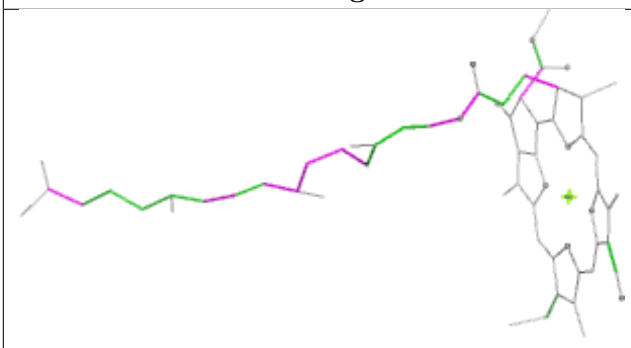
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Bond lengths



Bond angles

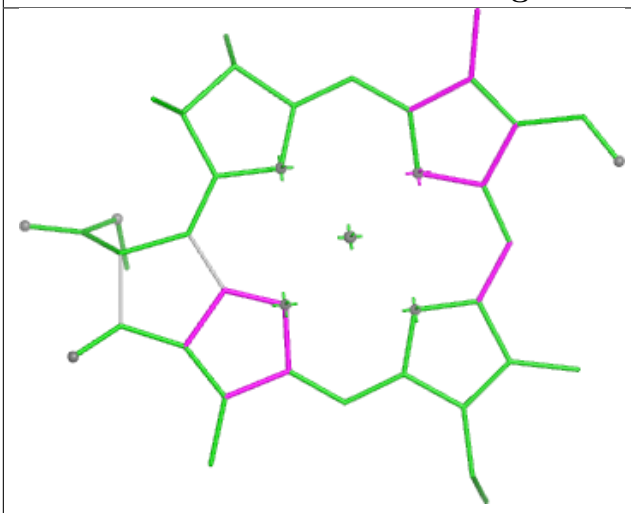


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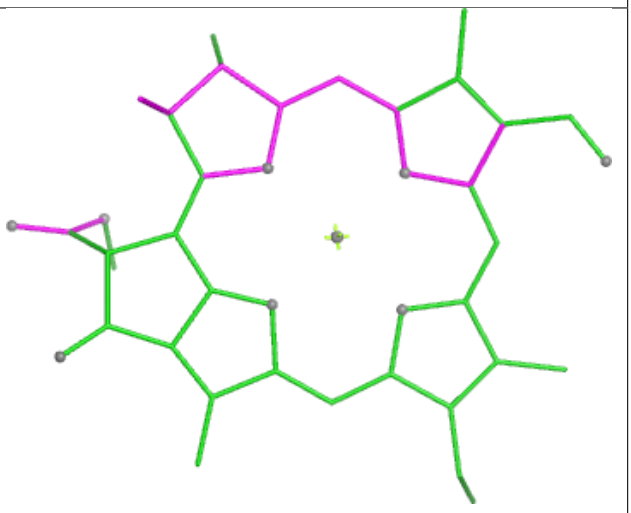


Rings

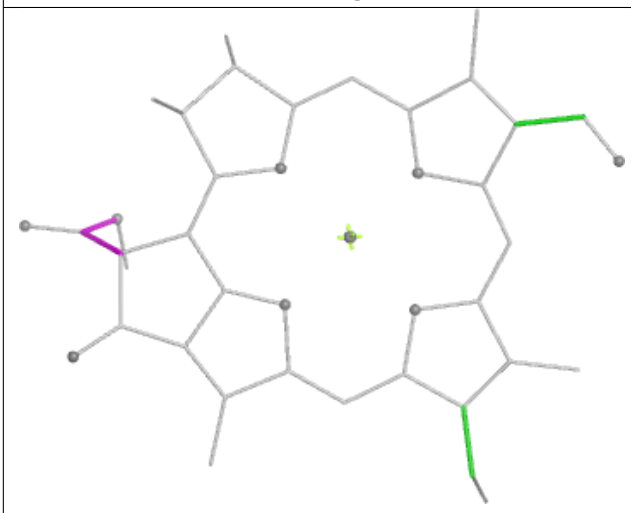
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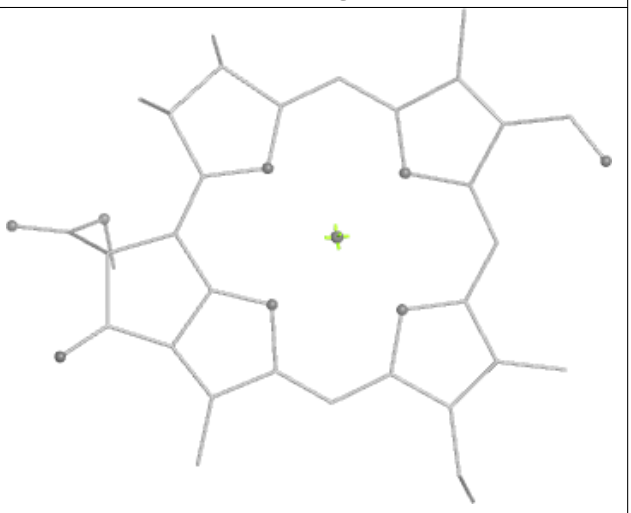
Bond lengths



Bond angles

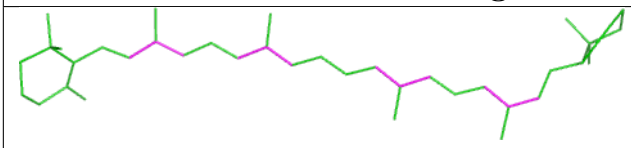


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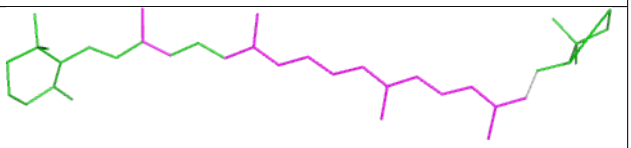


Rings

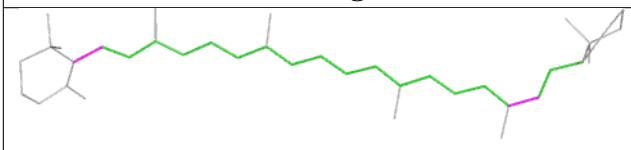
Ligand A1JPJ bB 4017



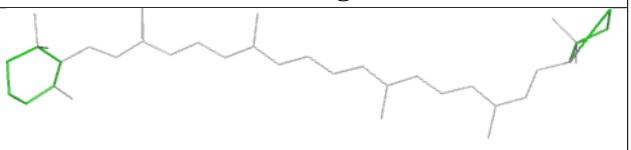
Bond lengths



Bond angles

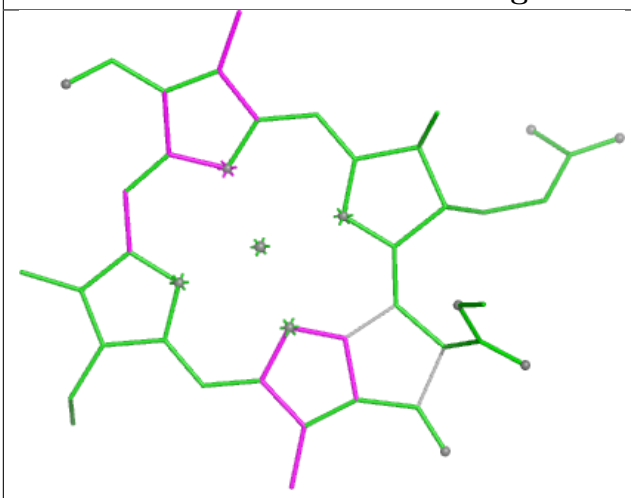


Torsions

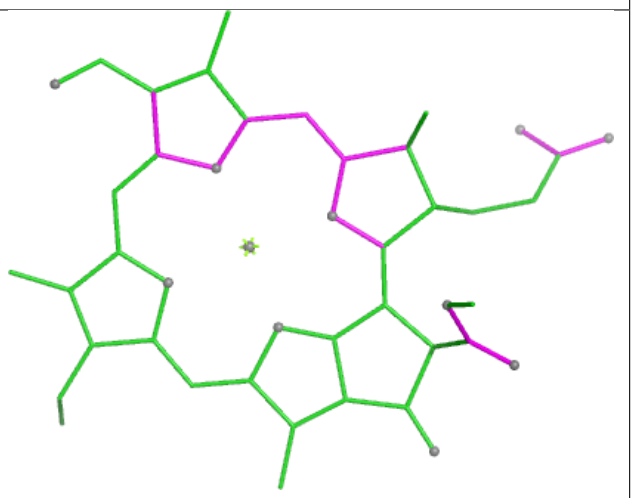


Rings

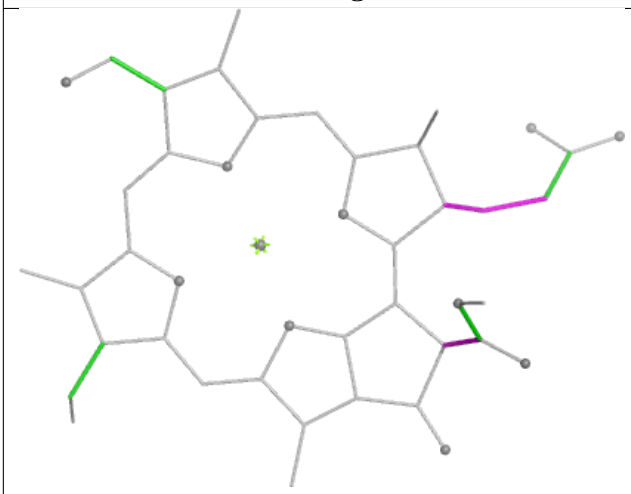
Ligand CL7 aA 1120



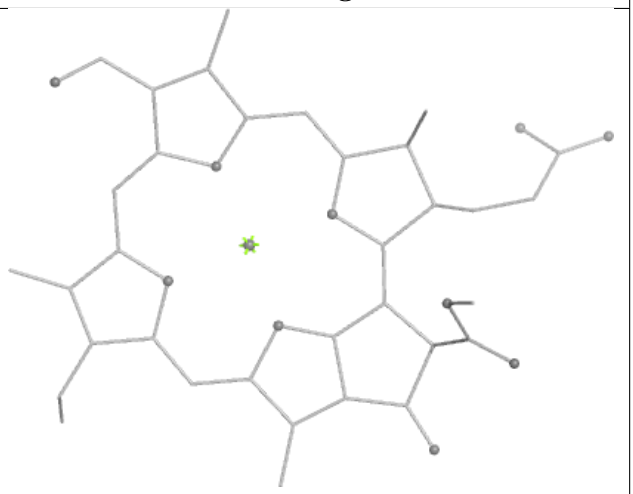
Bond lengths



Bond angles

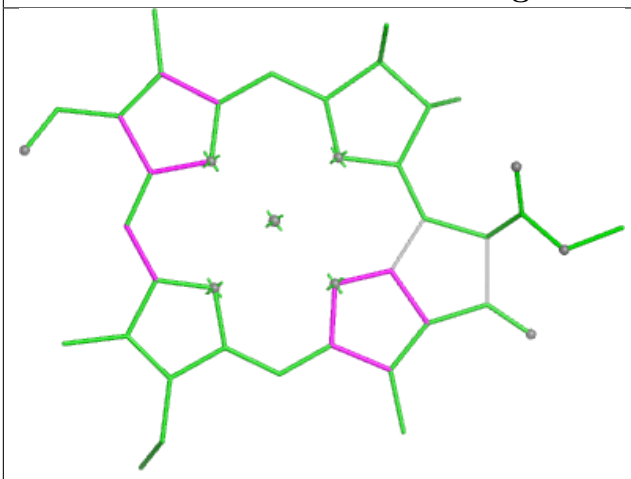


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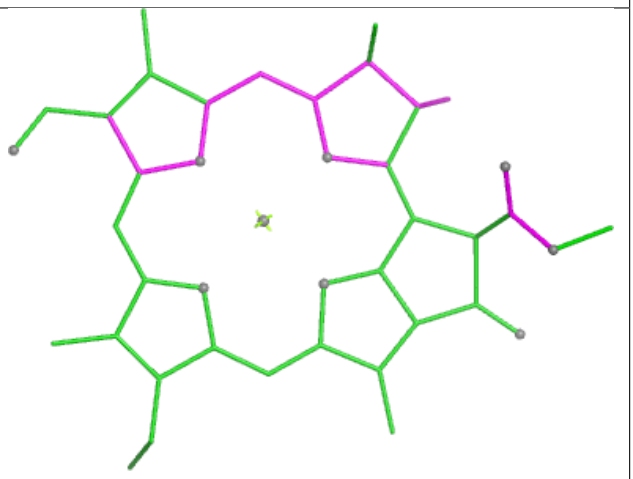


Rings

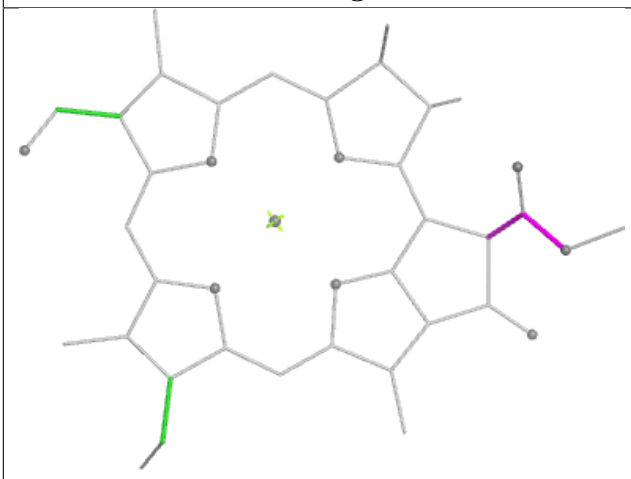
Ligand CL7 cB 1219



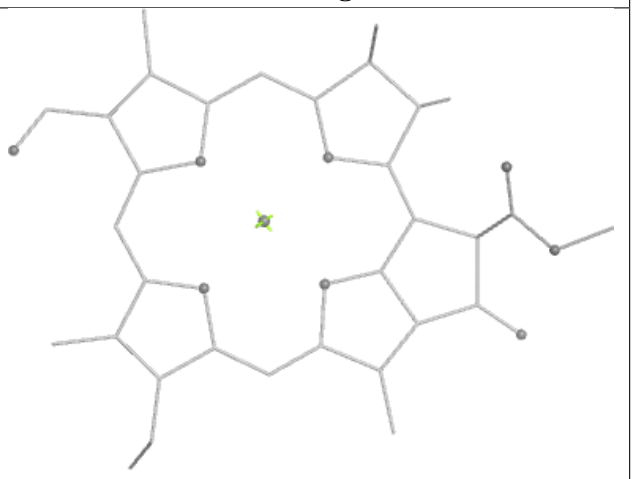
Bond lengths



Bond angles

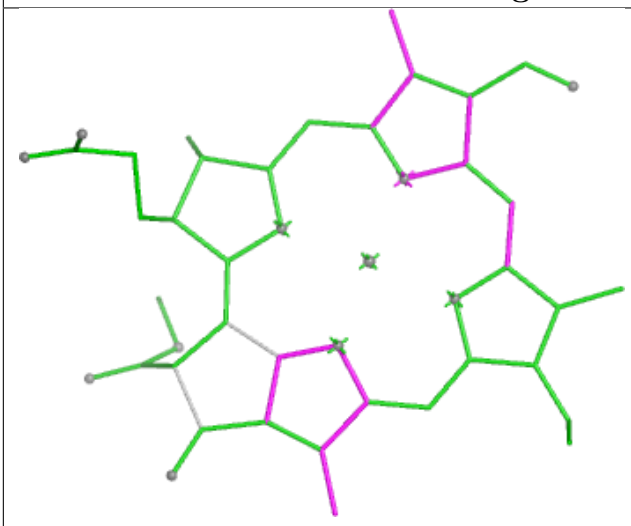


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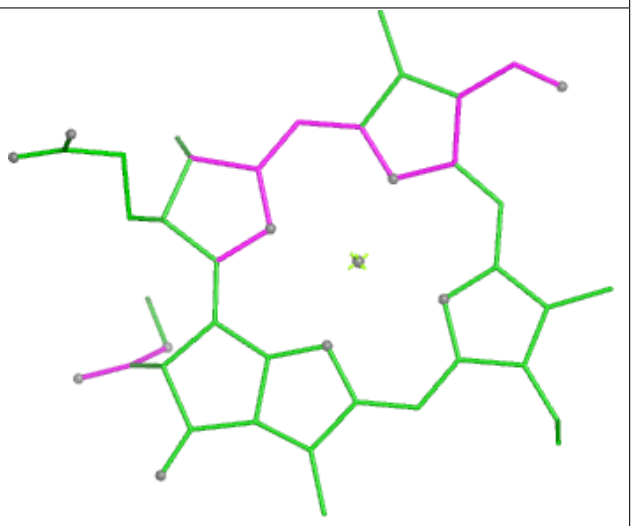


Rings

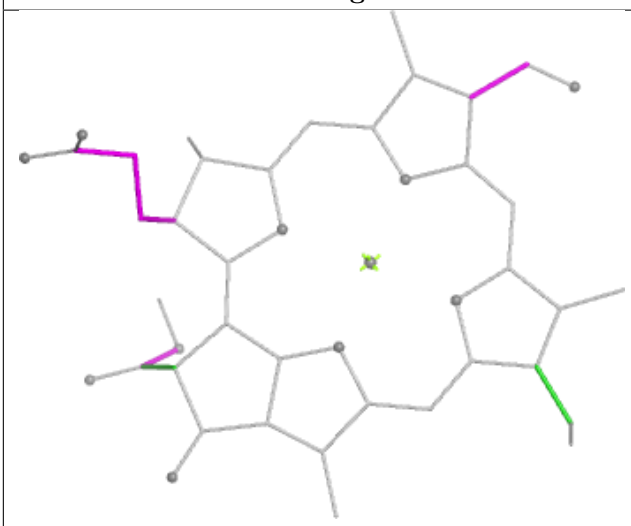
Ligand CL7 cB 1222



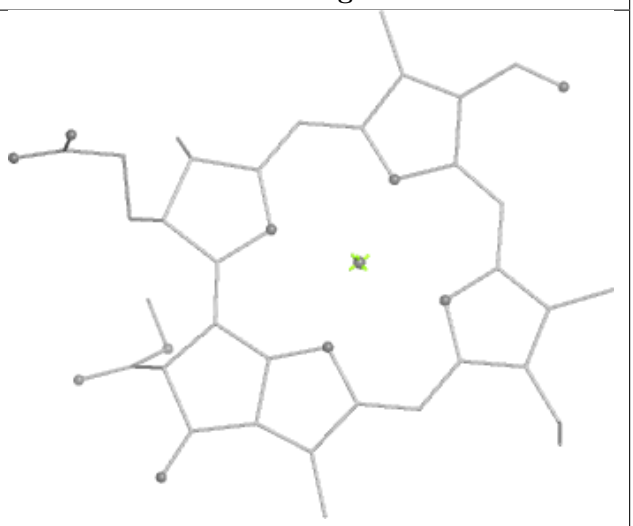
Bond lengths



Bond angles

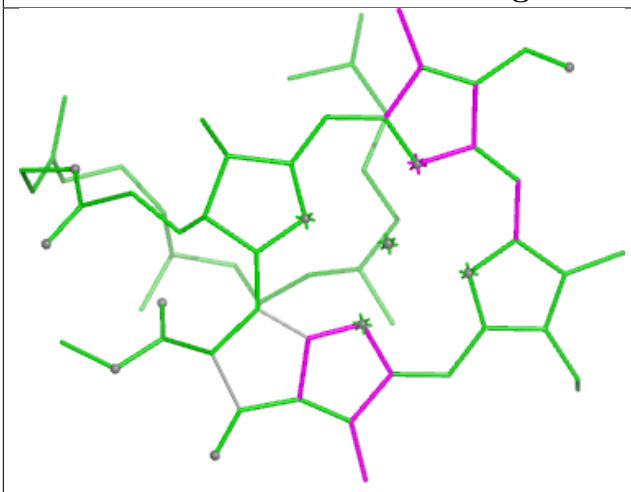


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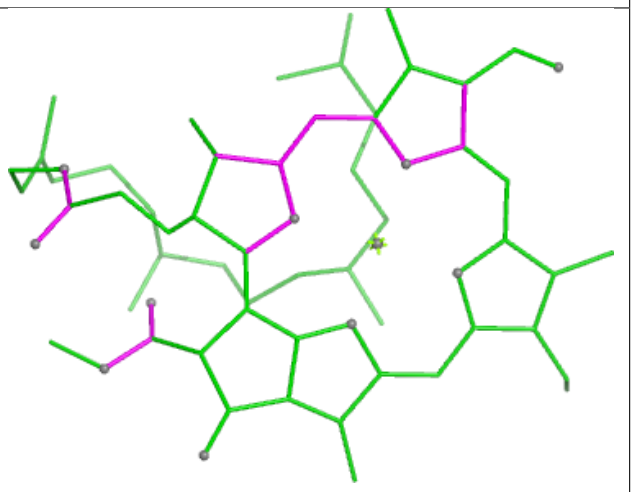


Rings

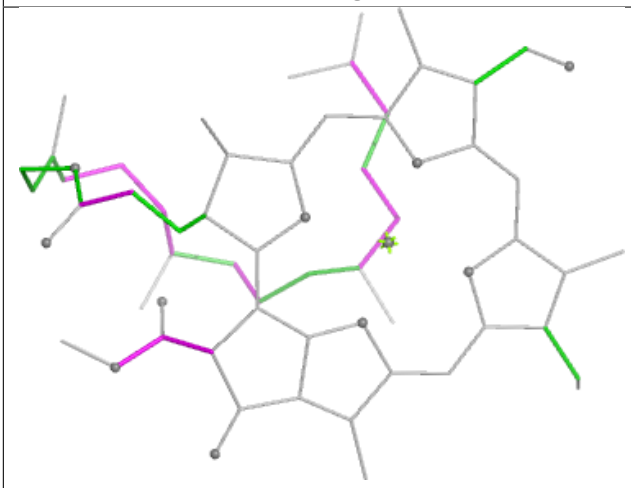
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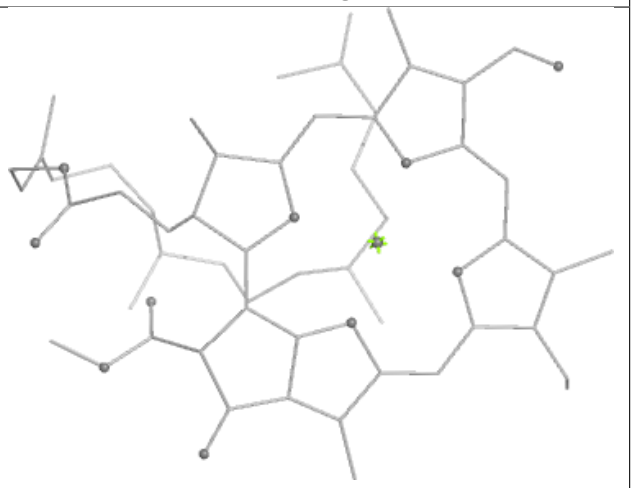
Bond lengths



Bond angles

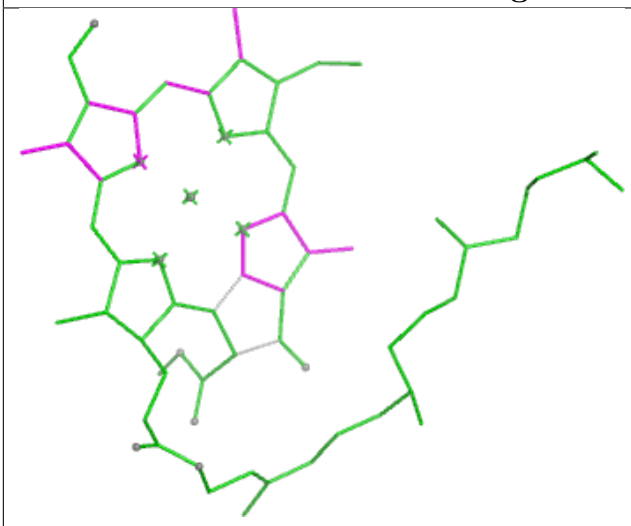


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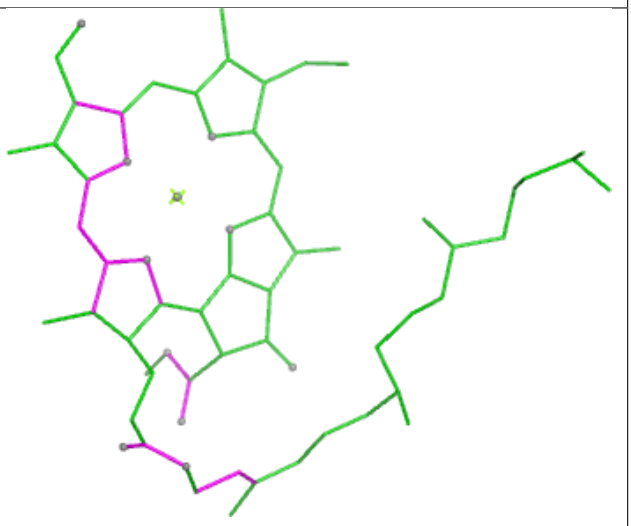


Rings

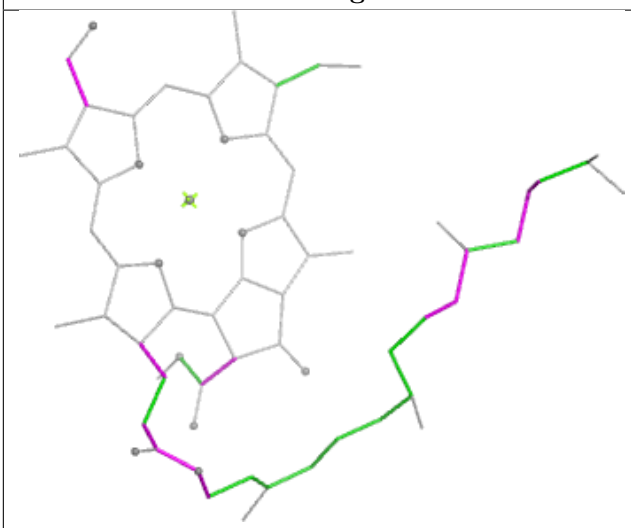
Ligand CL7 aA 1123



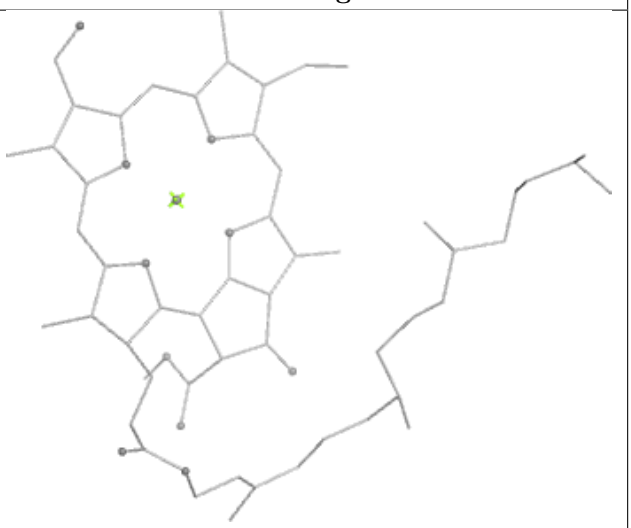
Bond lengths



Bond angles

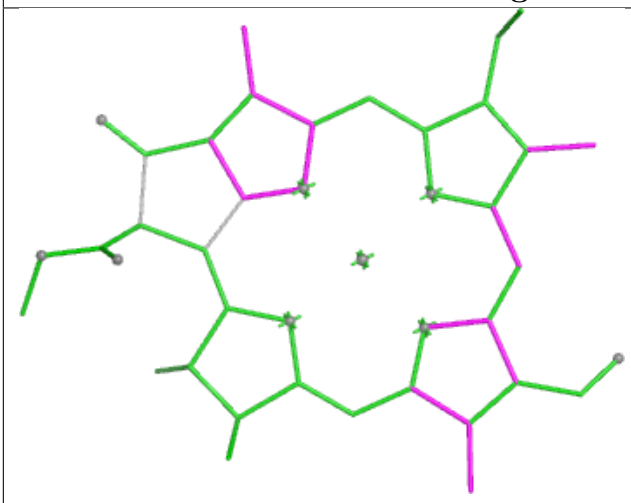


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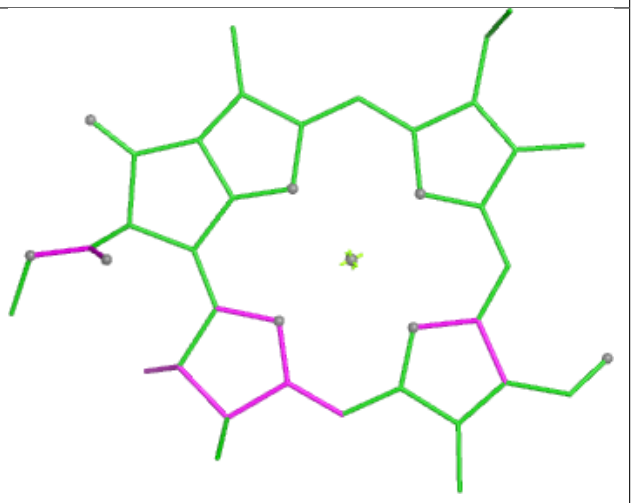


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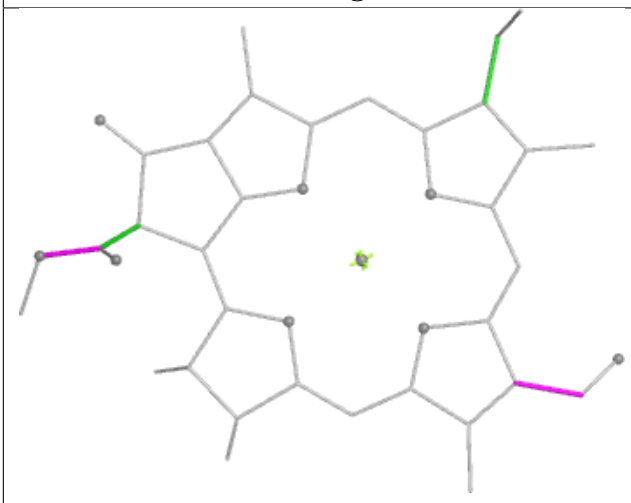
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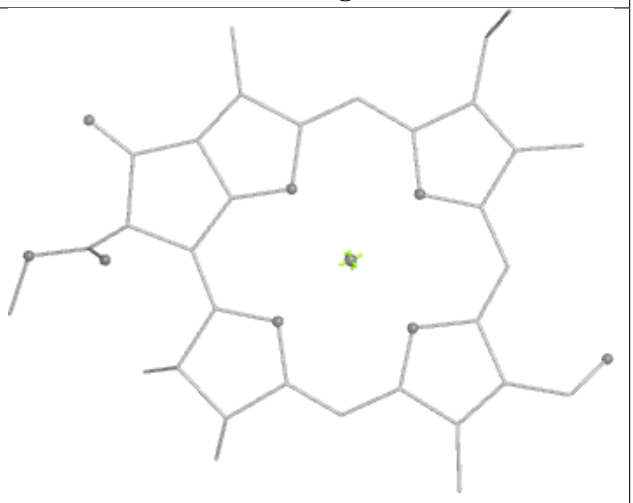
Bond lengths



Bond angles

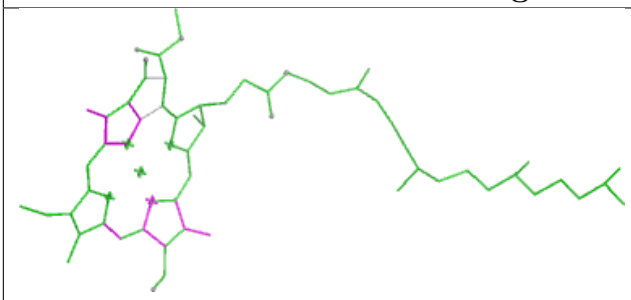


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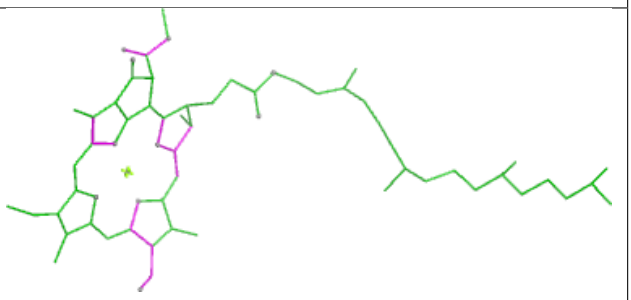


Rings

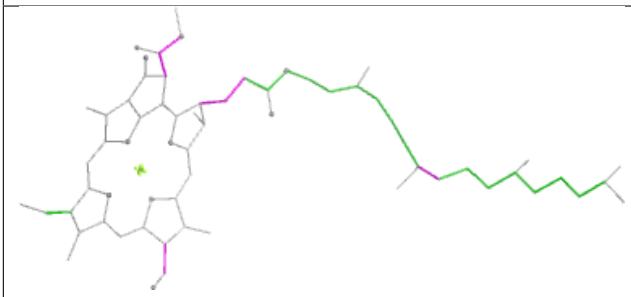
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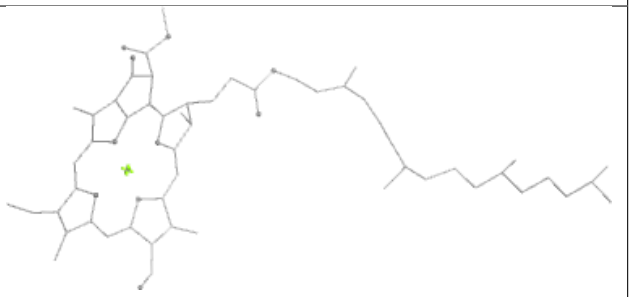
Bond lengths



Bond angles

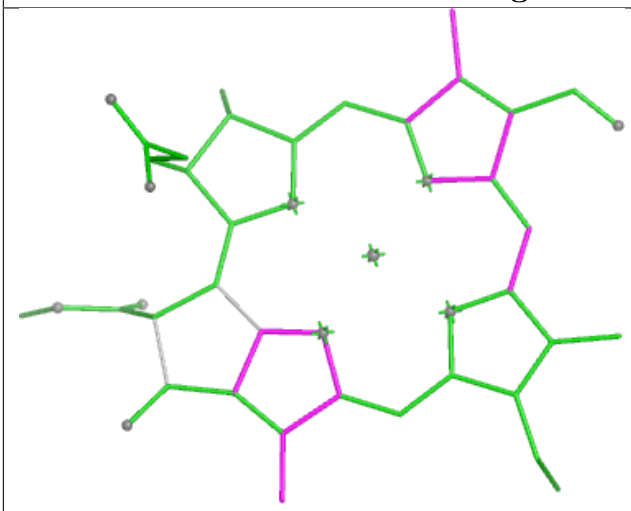


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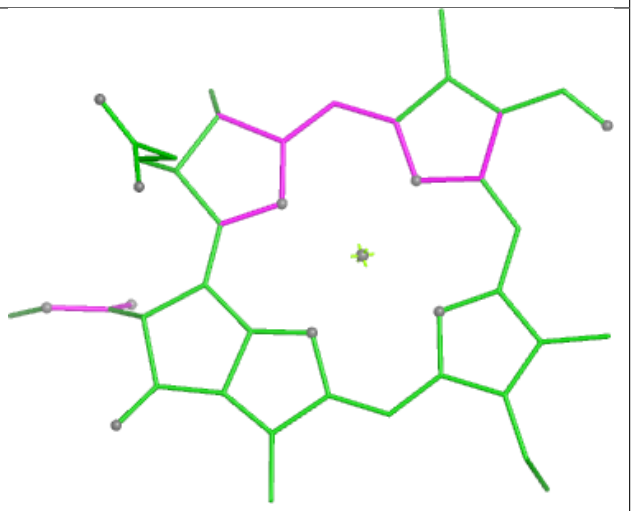


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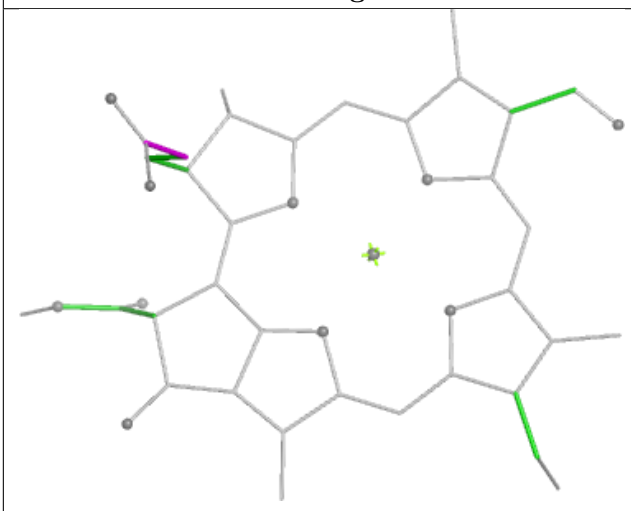
Ligand CL7 aA 1114



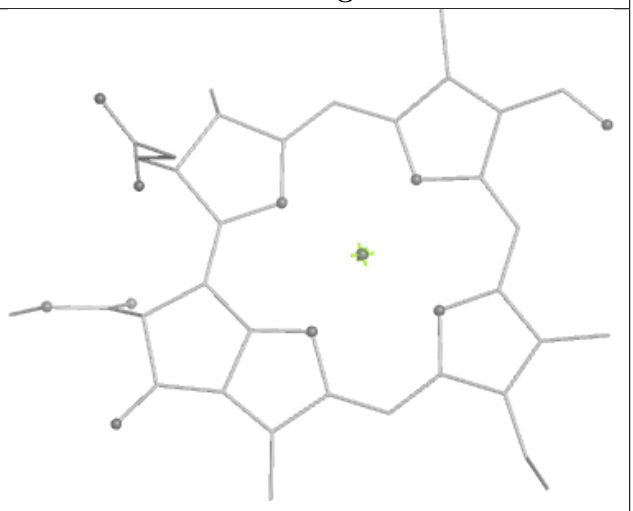
Bond lengths



Bond angles

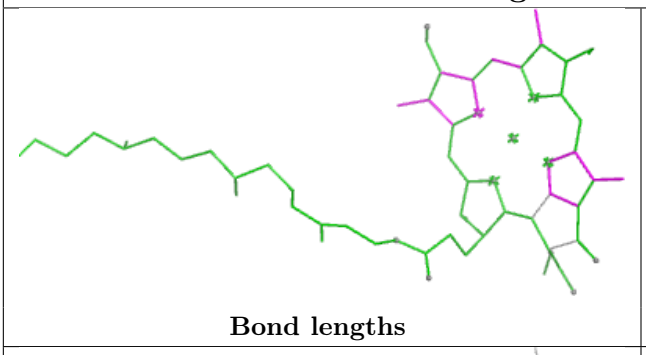


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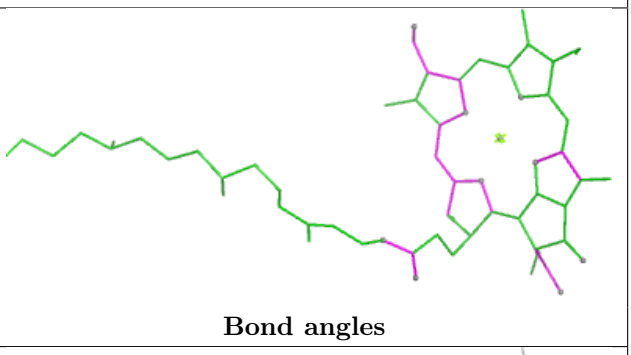


Rings

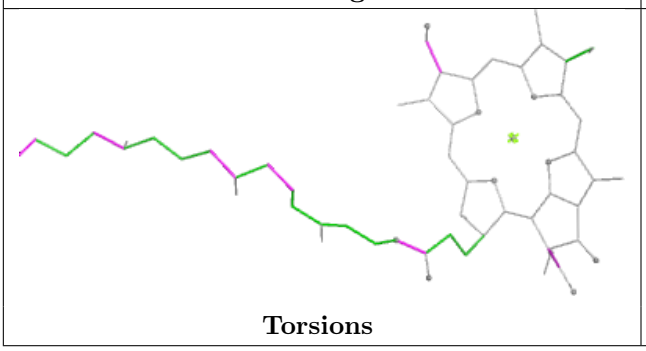
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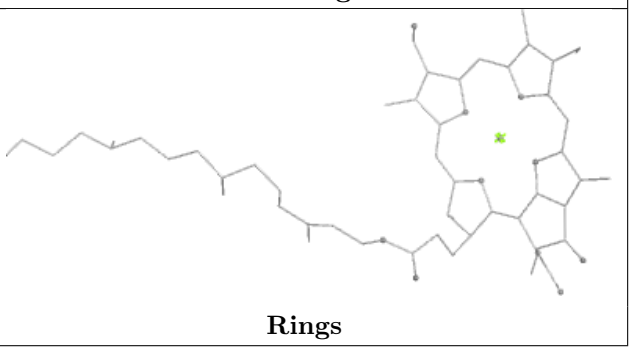
Bond lengths



Bond angles

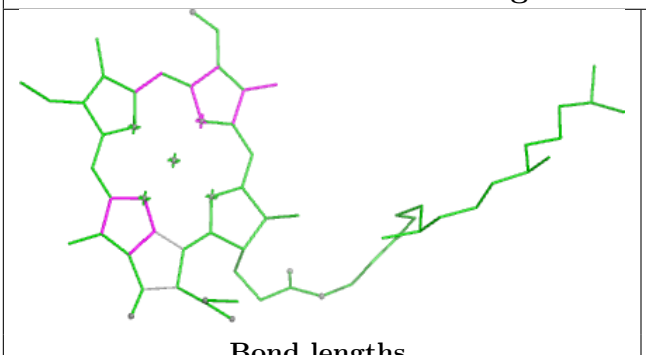


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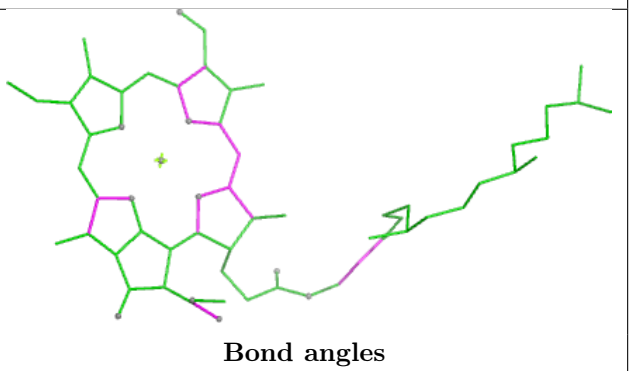


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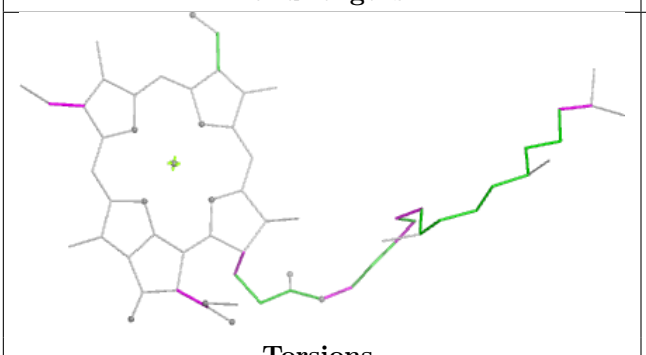
Ligand CL7 aA 1111



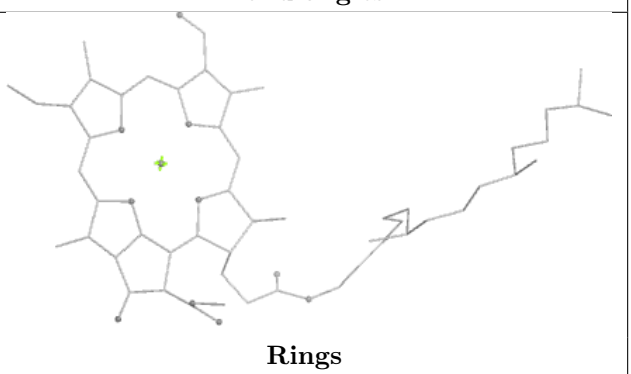
Bond lengths



Bond angles

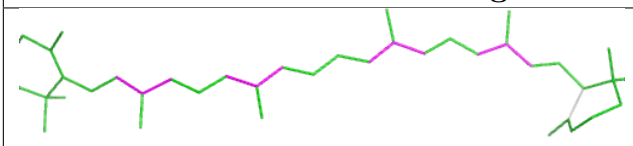


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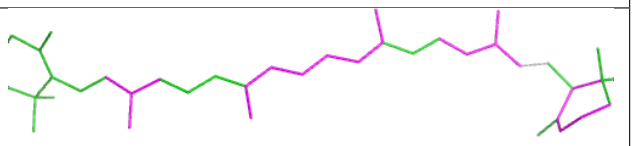


Rings

Ligand A1JPJ aA 4008



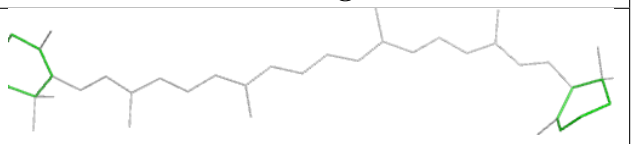
Bond lengths



Bond angles

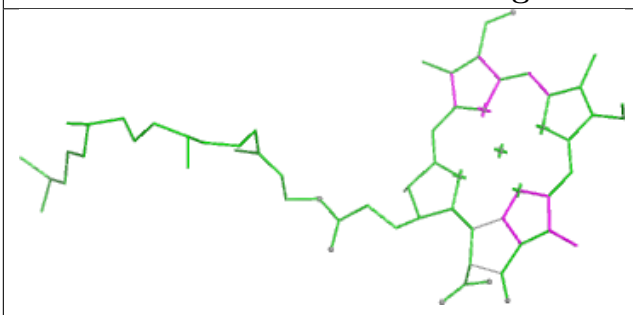


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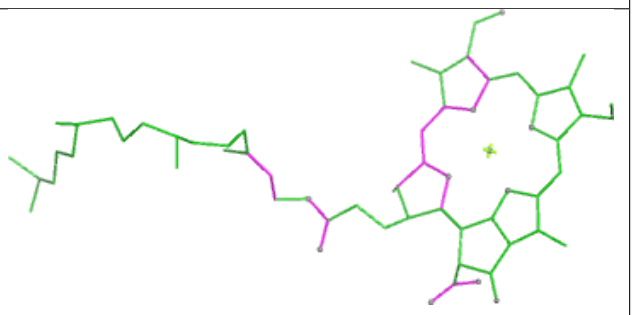


Rings

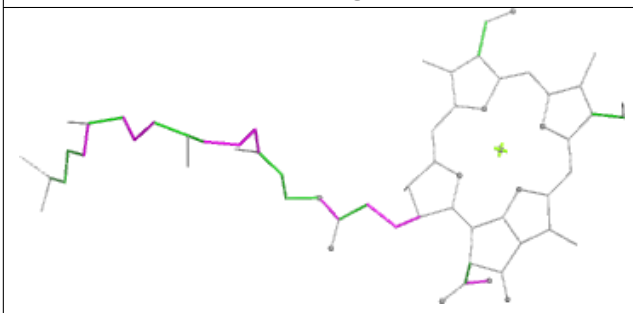
Ligand CL7 cB 1210



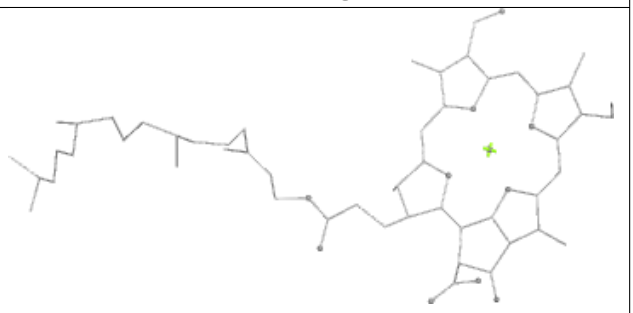
Bond lengths



Bond angles

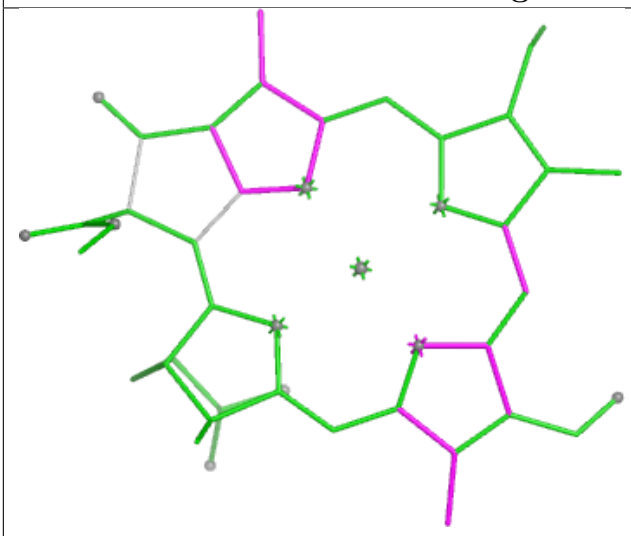


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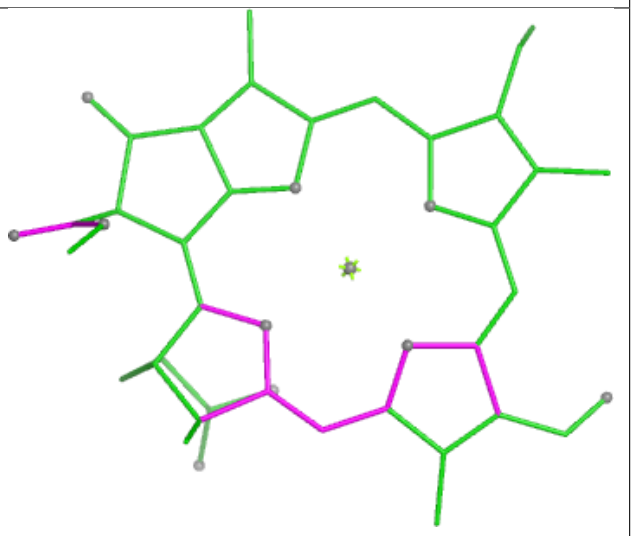


Rings

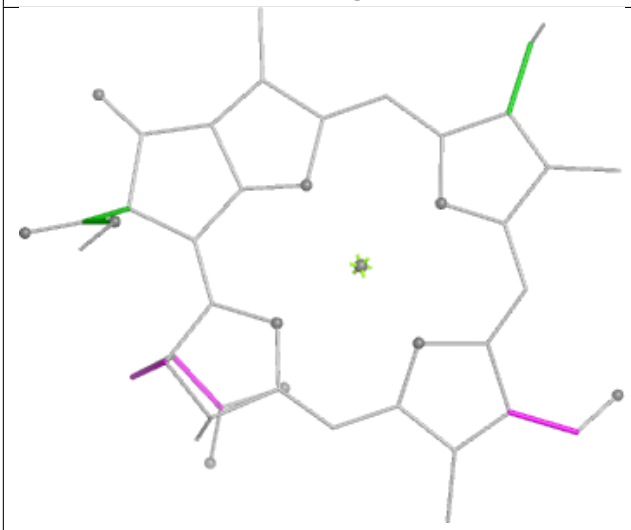
Ligand CL7 aB 1227



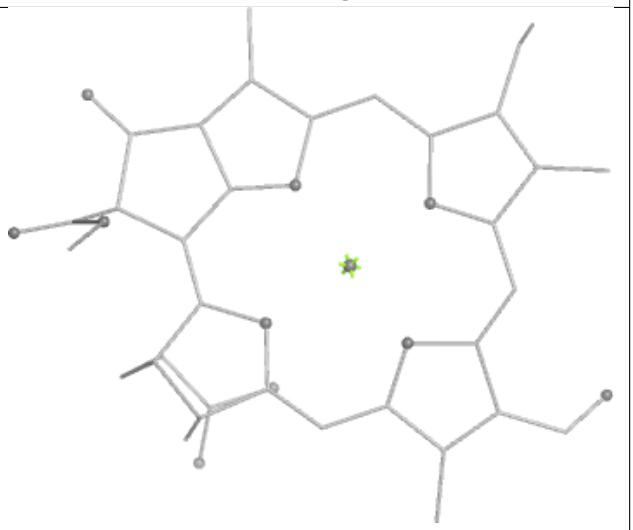
Bond lengths



Bond angles

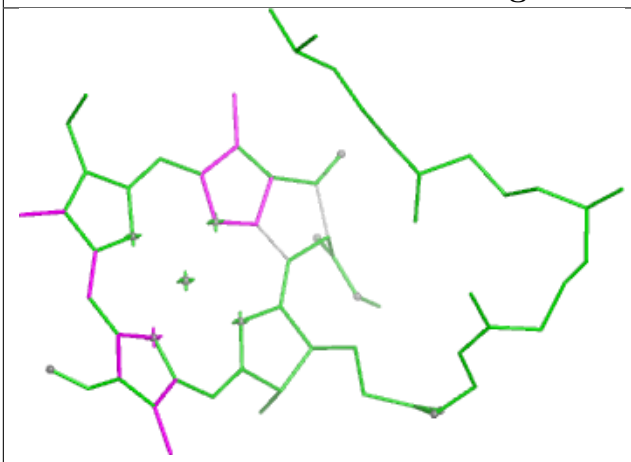


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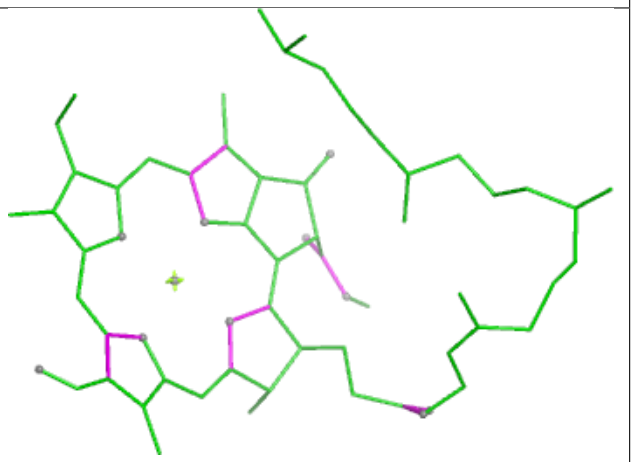


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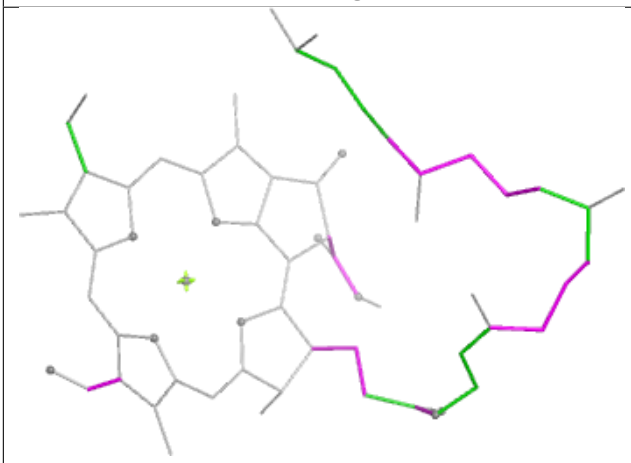
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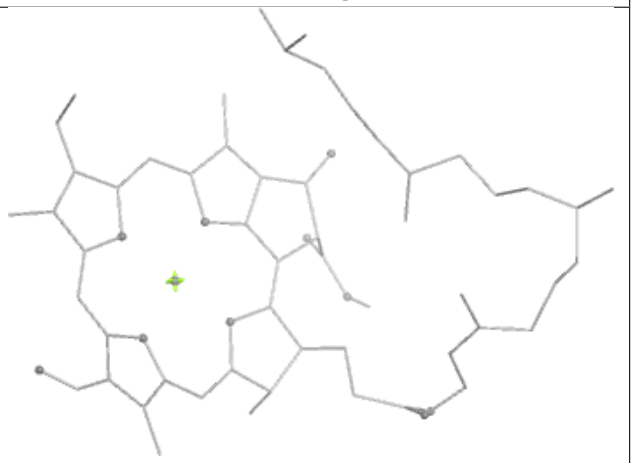
Bond lengths



Bond angles

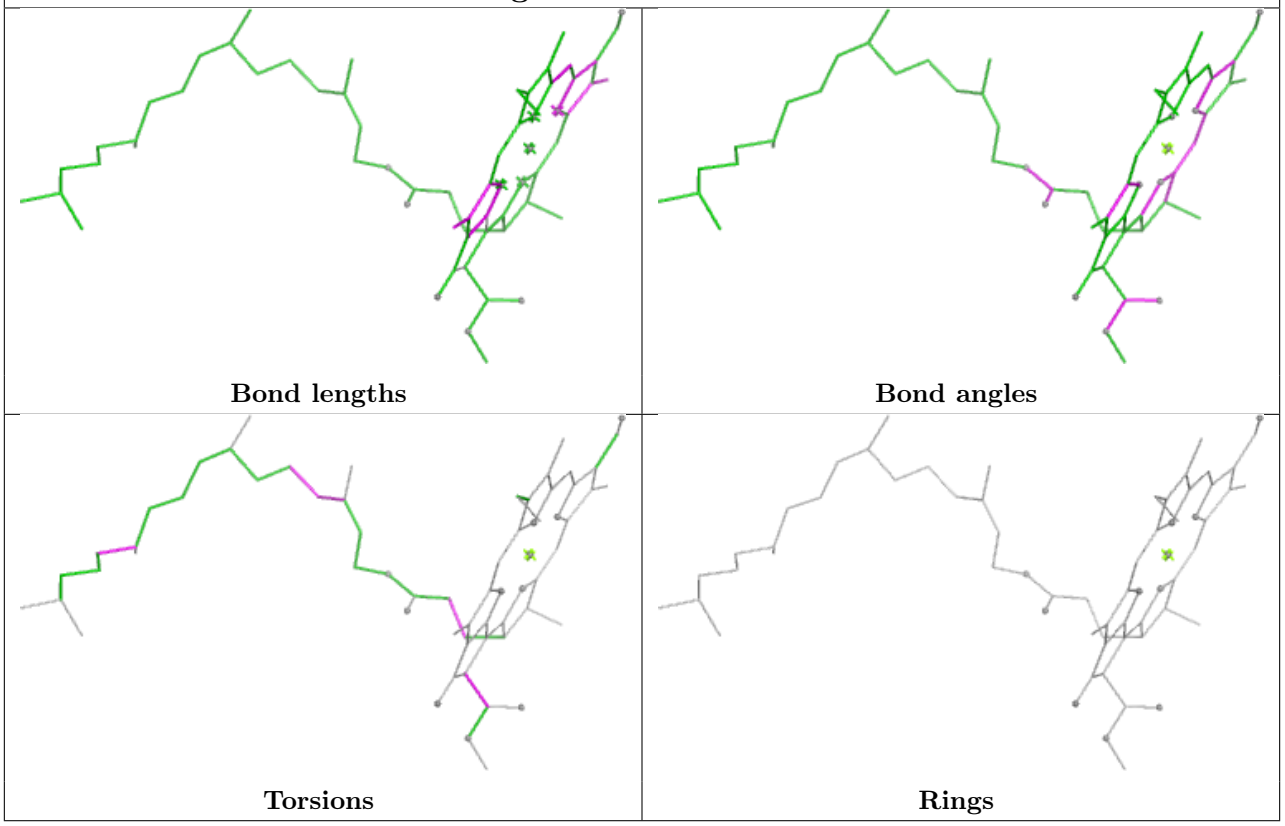


Torsions

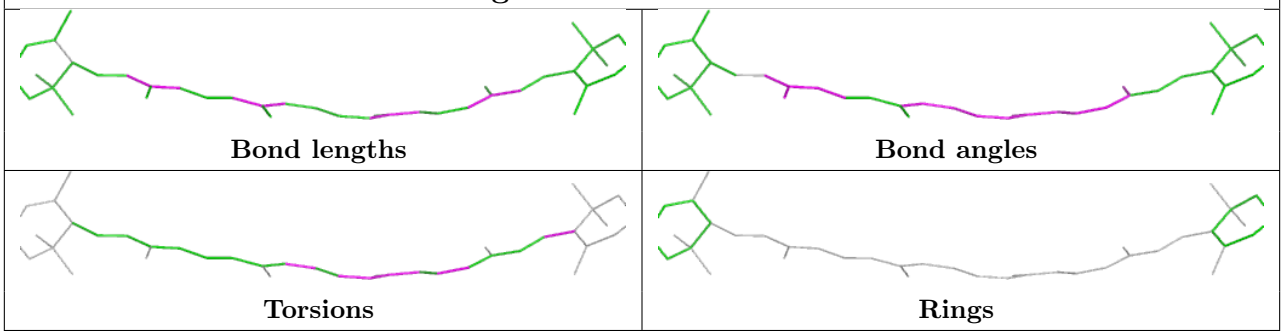


Rings

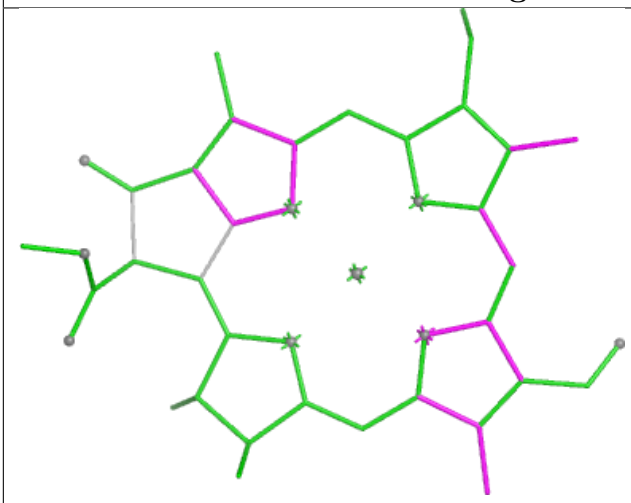
Ligand CL7 bB 1238



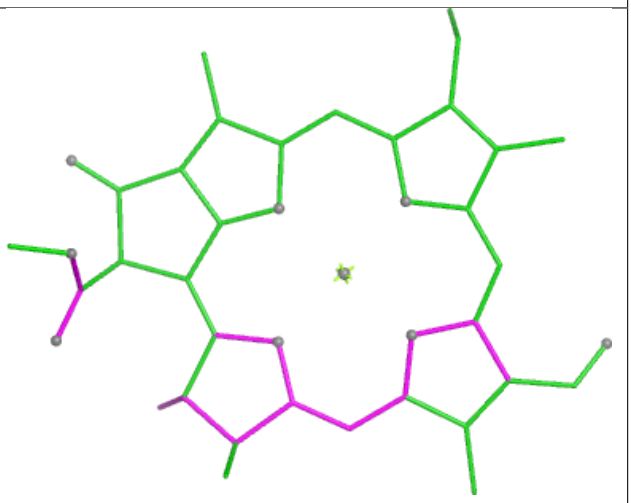
Ligand A1JPJ cA 4014



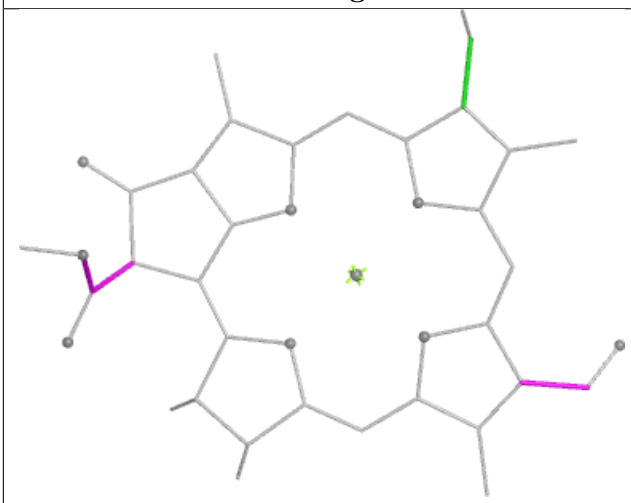
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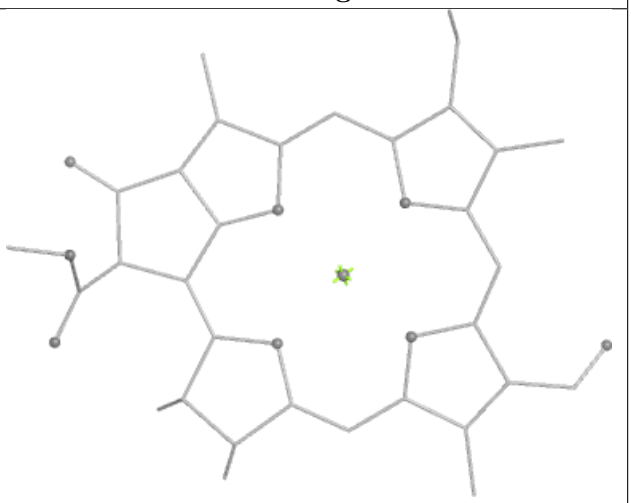
Bond lengths



Bond angles

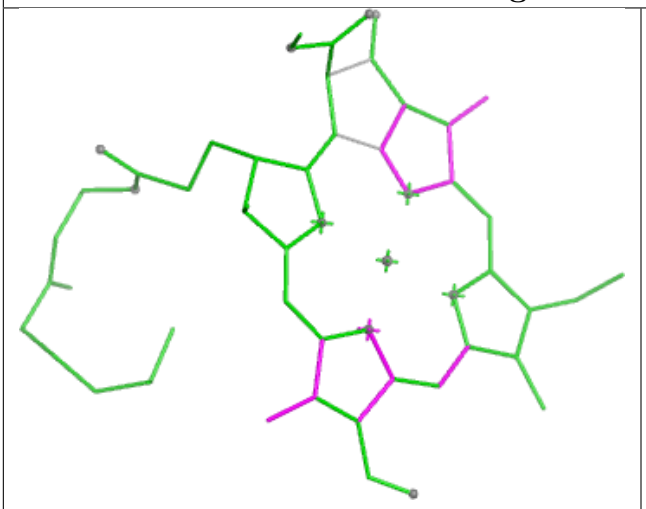


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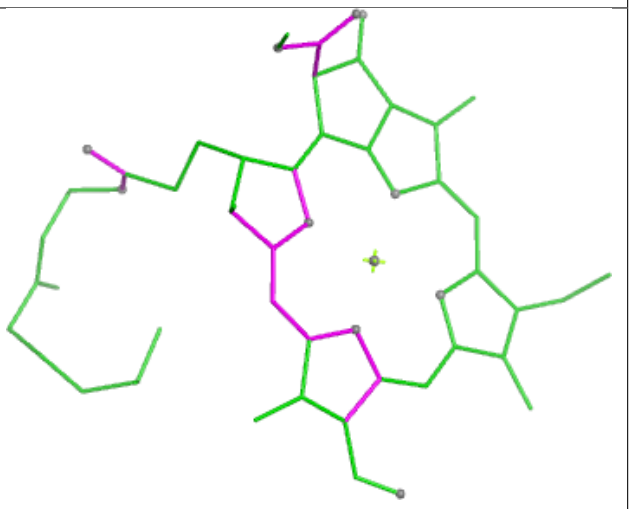


Rings

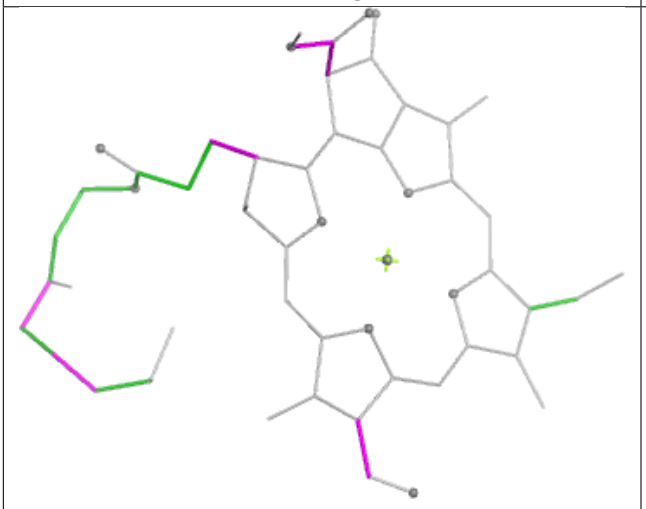
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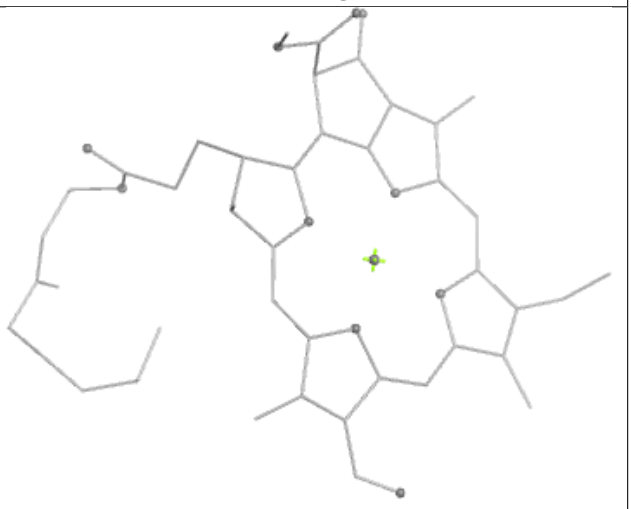
Bond lengths



Bond angles

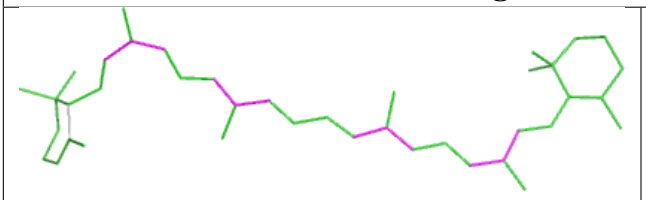


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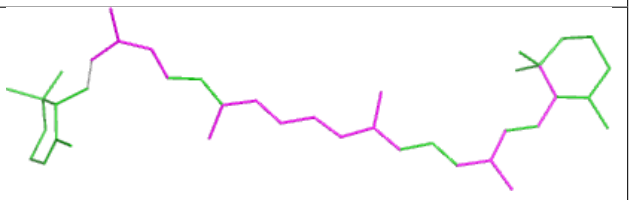


Rings

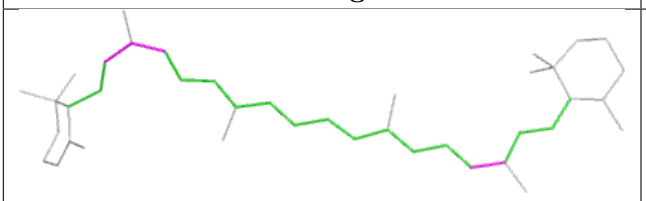
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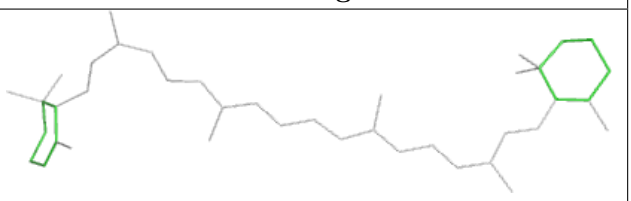
Bond lengths



Bond angles

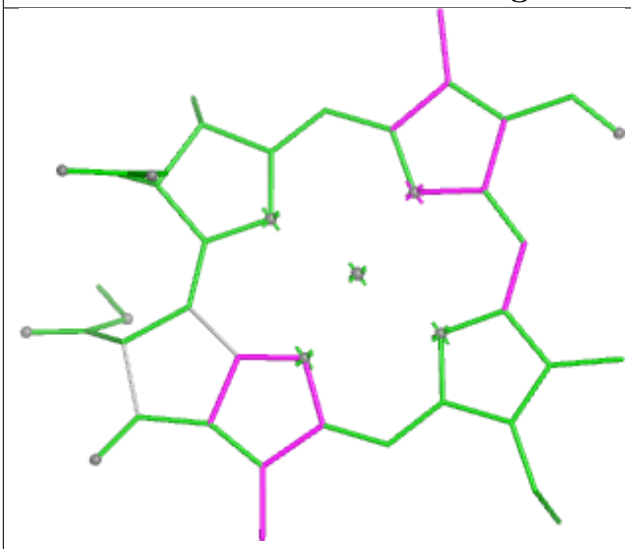


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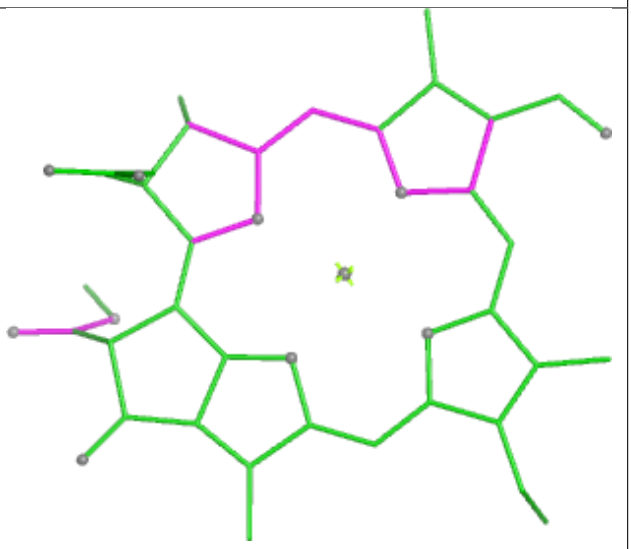


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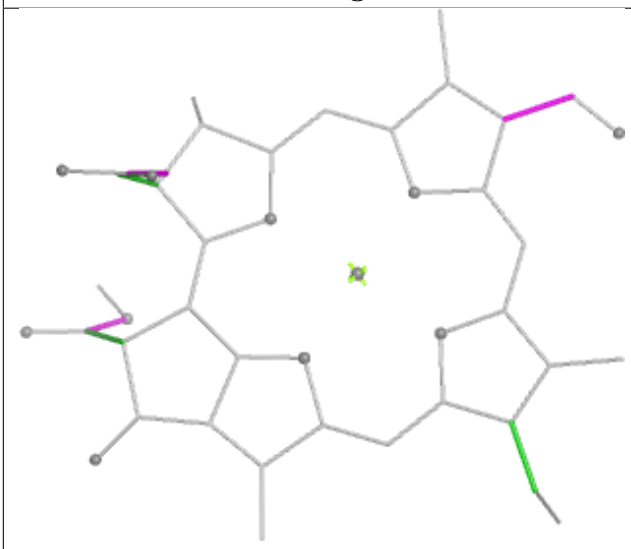
Ligand CL7 aA 1105



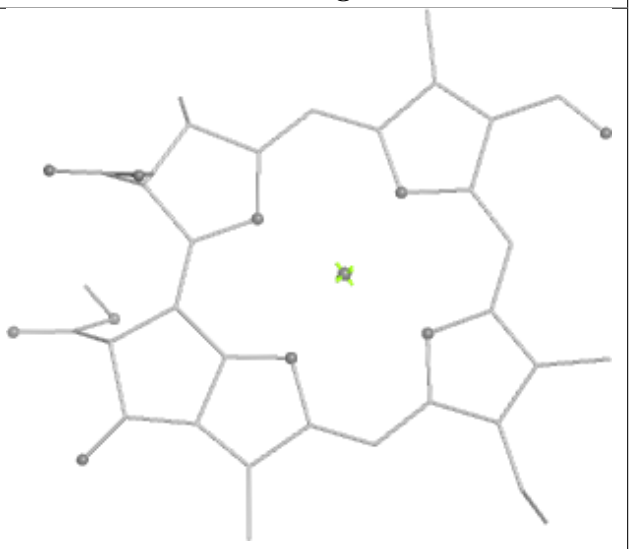
Bond lengths



Bond angles

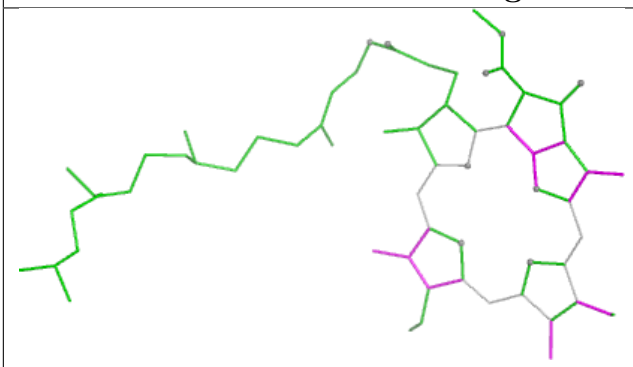


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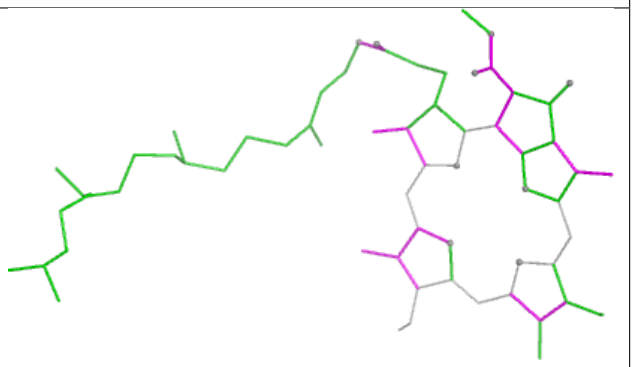


Rings

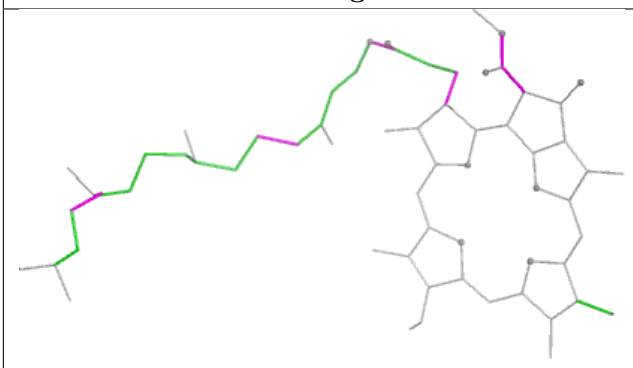
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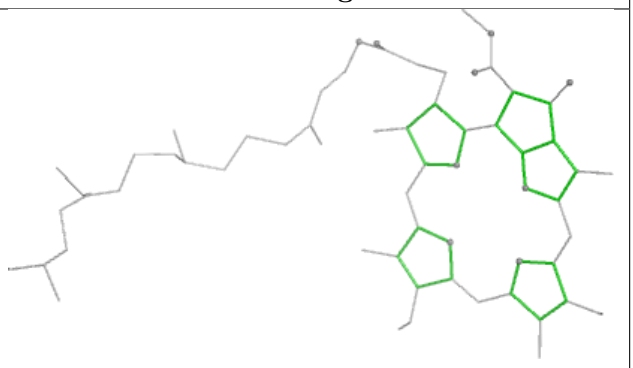
Bond lengths



Bond angles

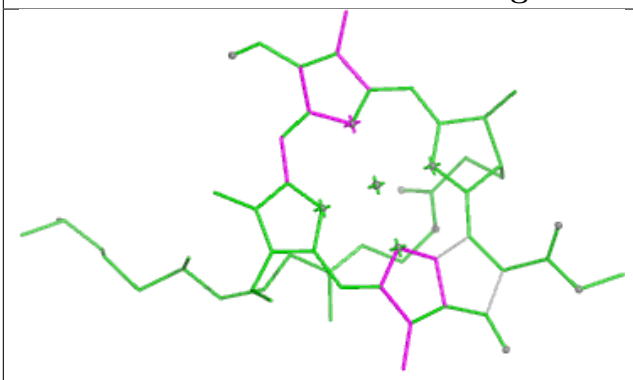


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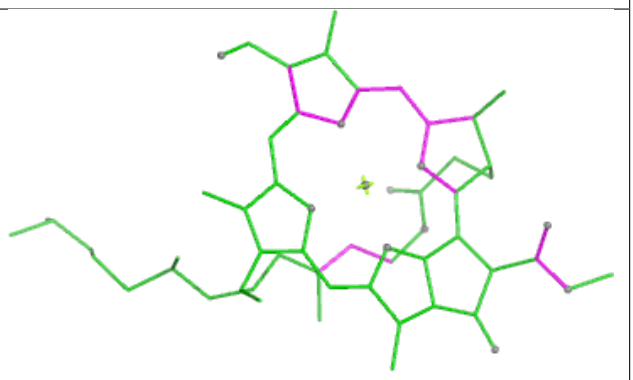


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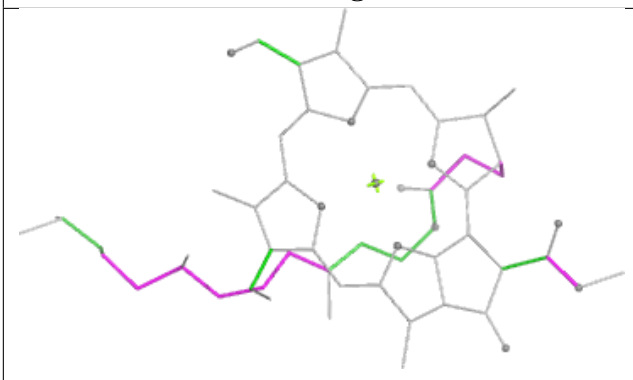
Ligand CL7 aA 1140



Bond lengths



Bond angles

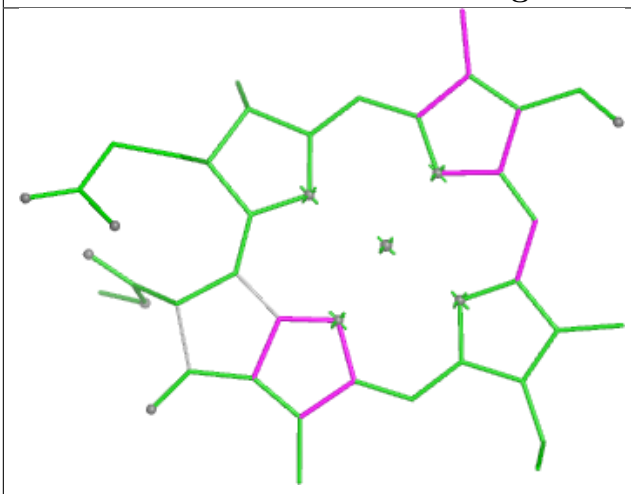


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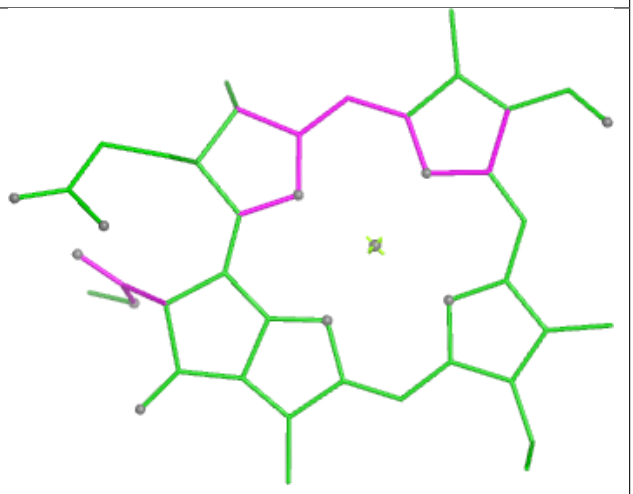


Rings

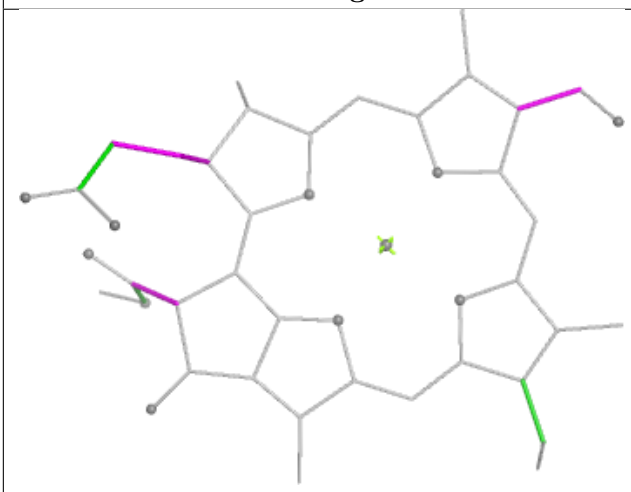
Ligand CL7 cA 1113



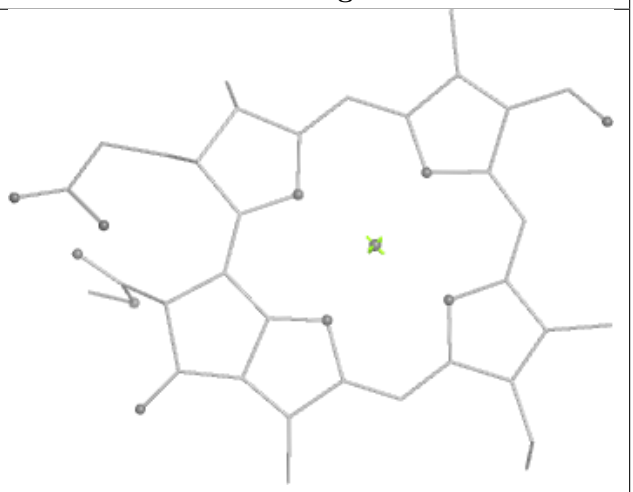
Bond lengths



Bond angles

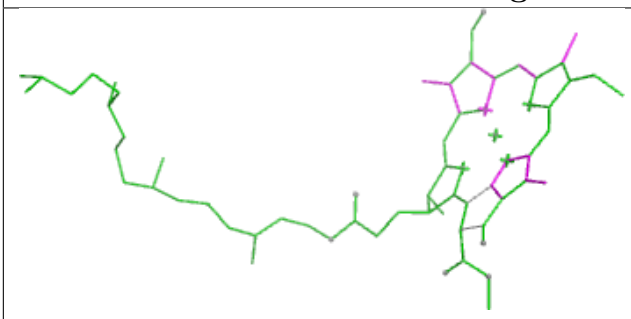


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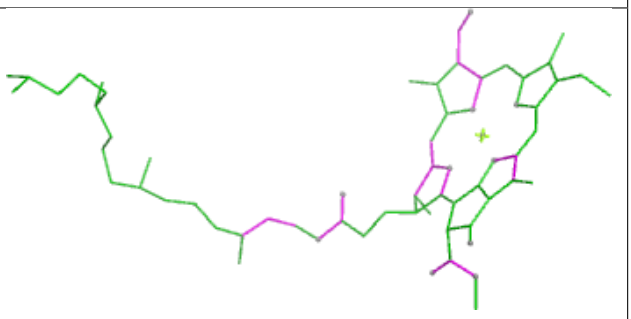


Rings

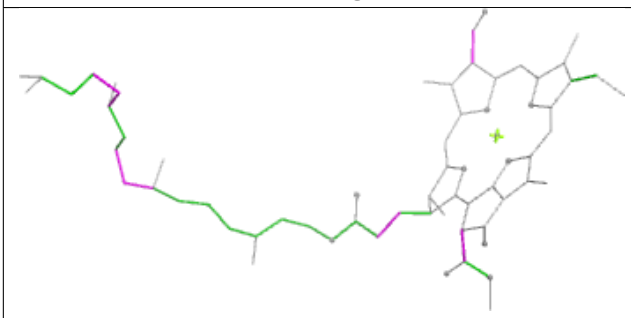
Ligand CL7 bB 1012



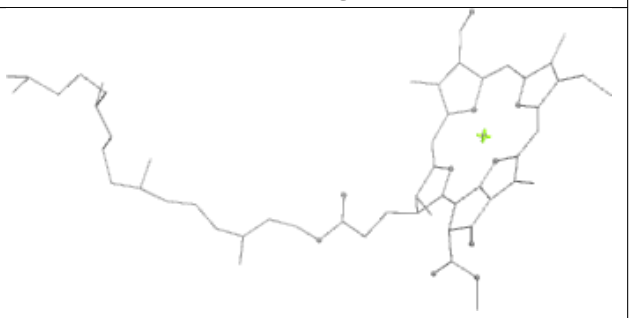
Bond lengths



Bond angles

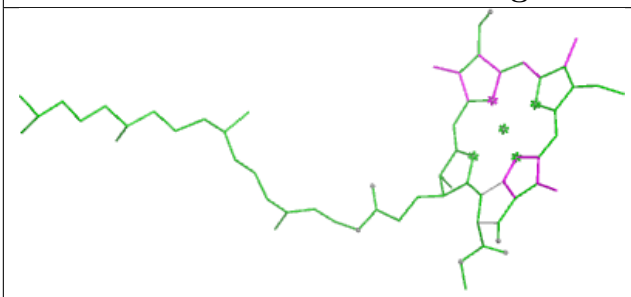


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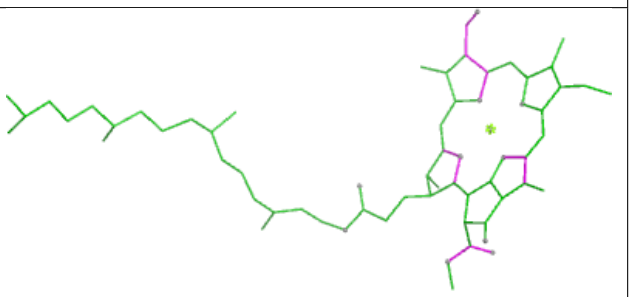


Rings

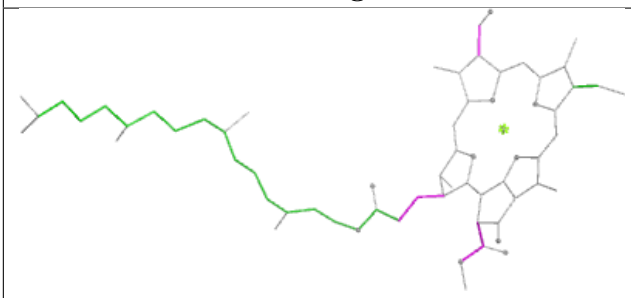
Ligand CL7 aA 1022



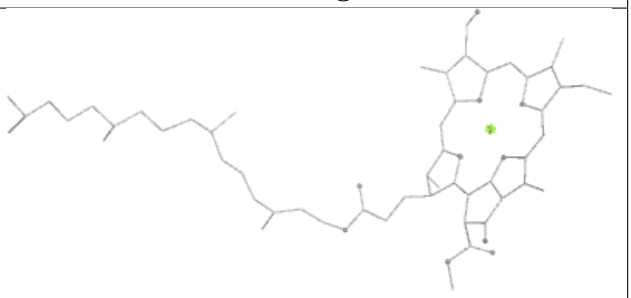
Bond lengths



Bond angles

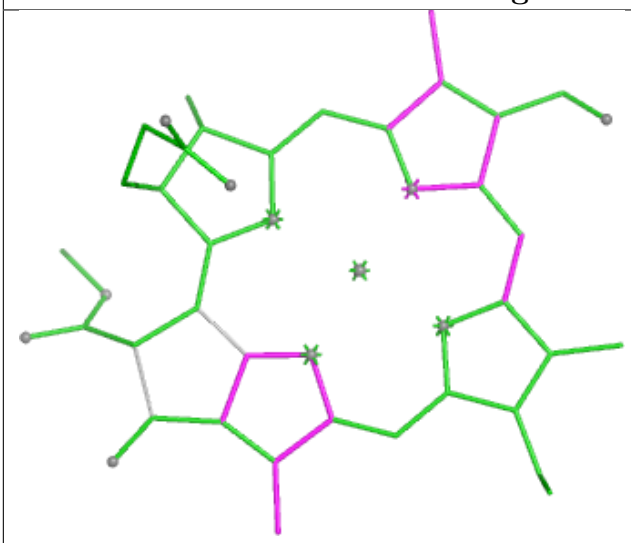


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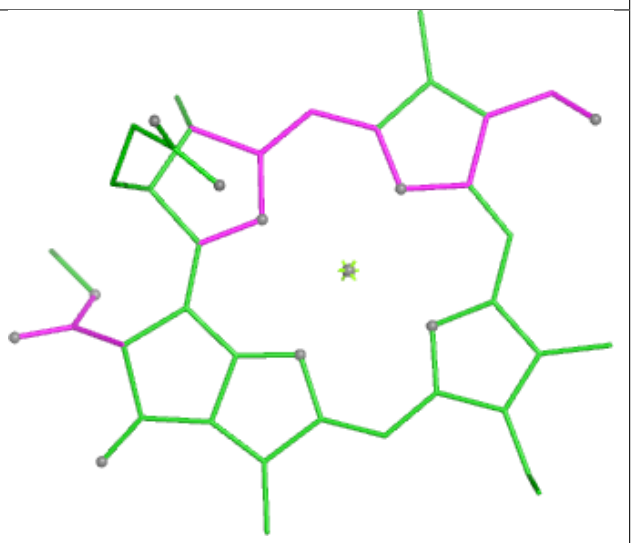


Rings

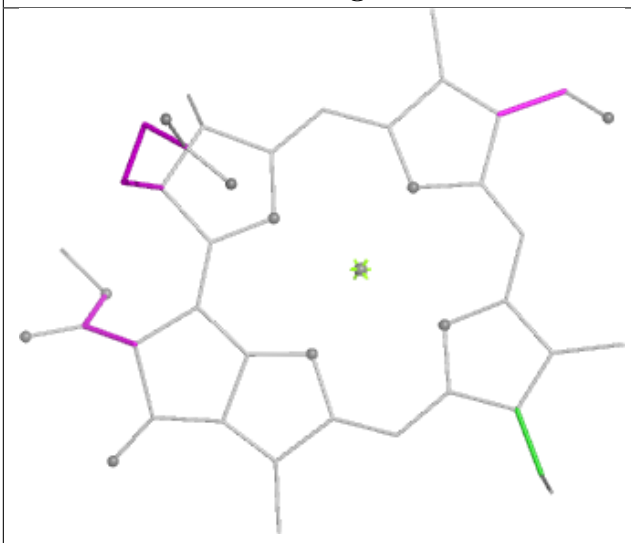
Ligand CL7 aB 1212



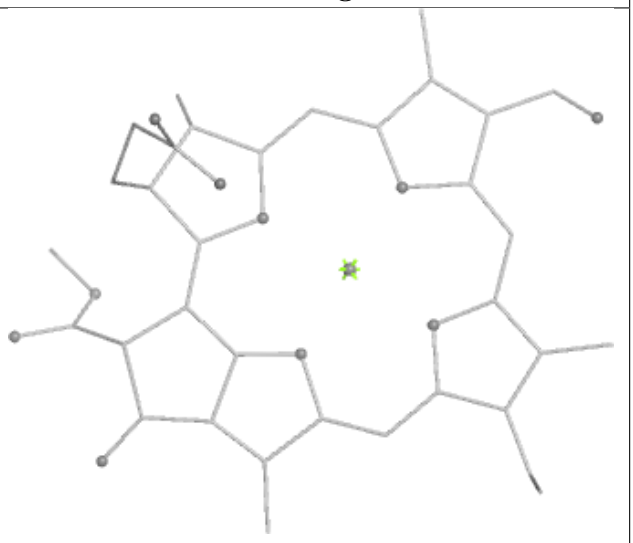
Bond lengths



Bond angles

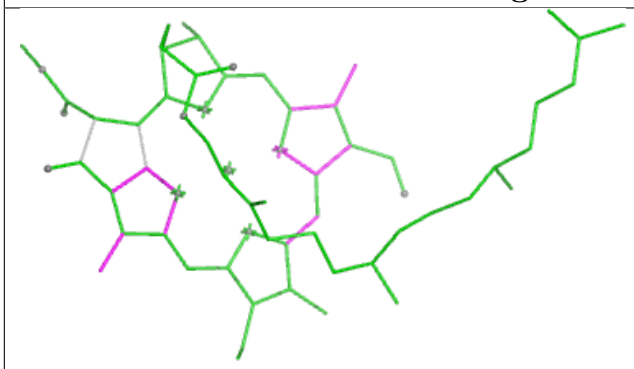


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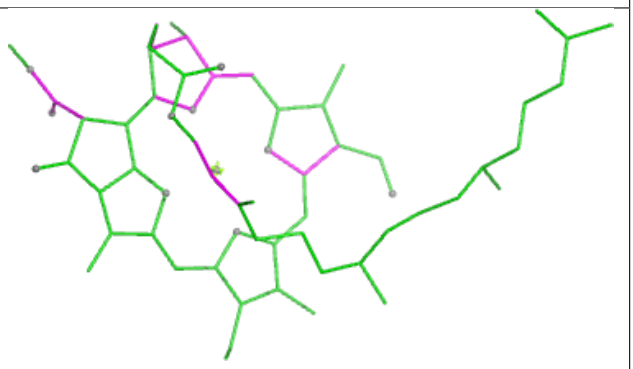


Rings

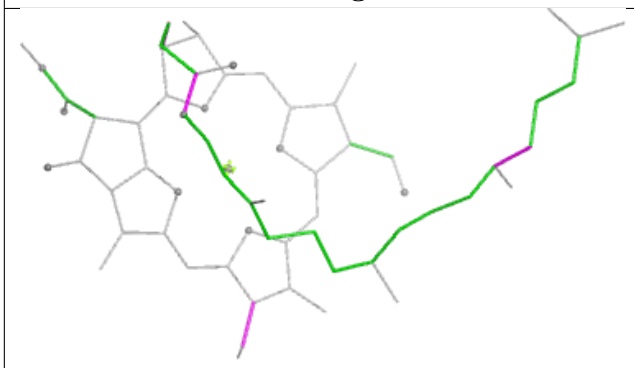
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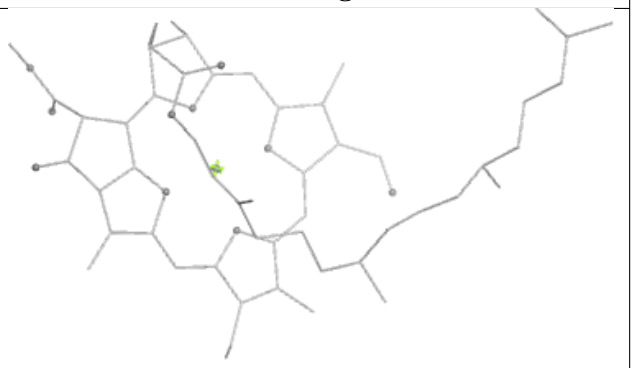
Bond lengths



Bond angles

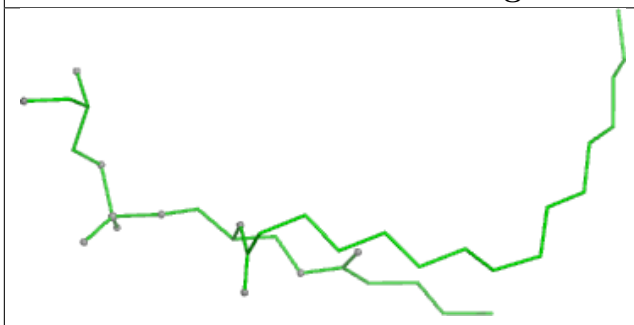


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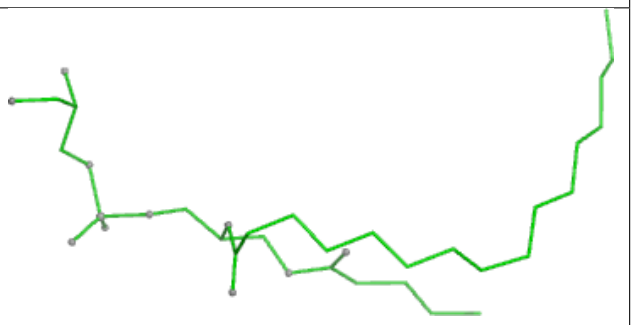


Rings

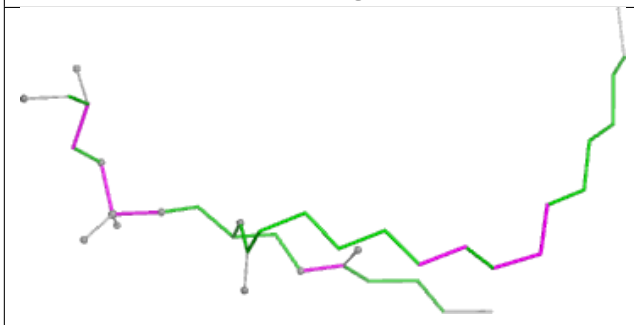
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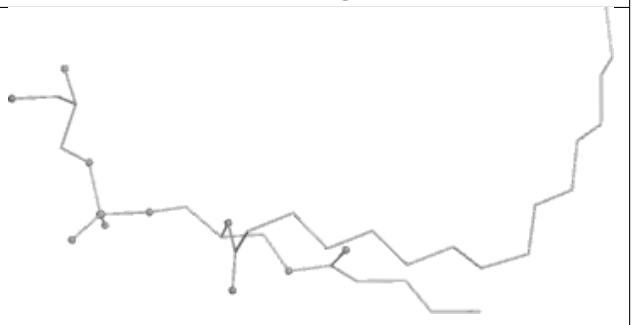
Bond lengths



Bond angles

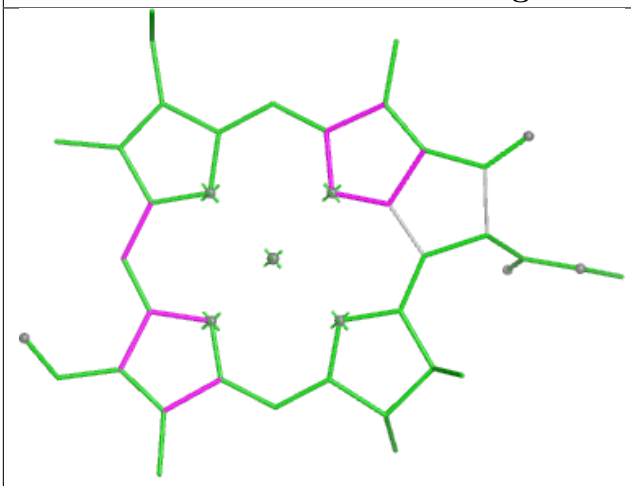


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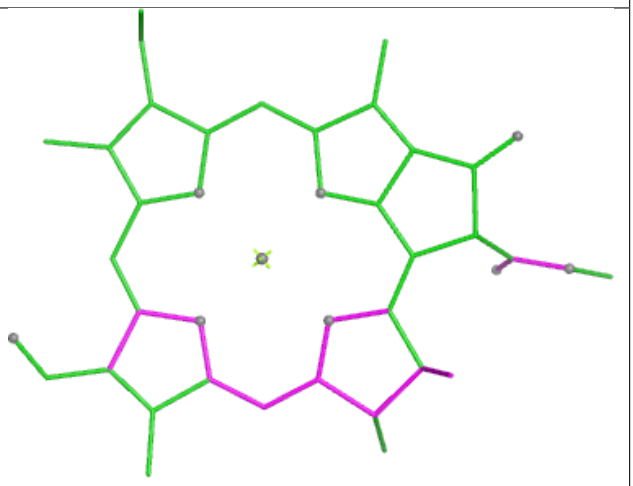


Rings

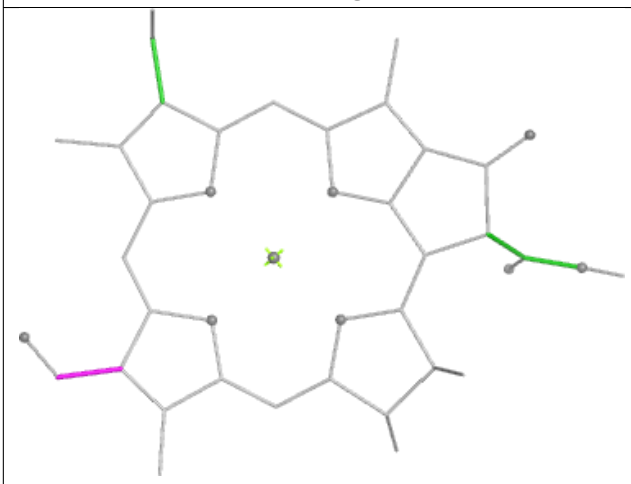
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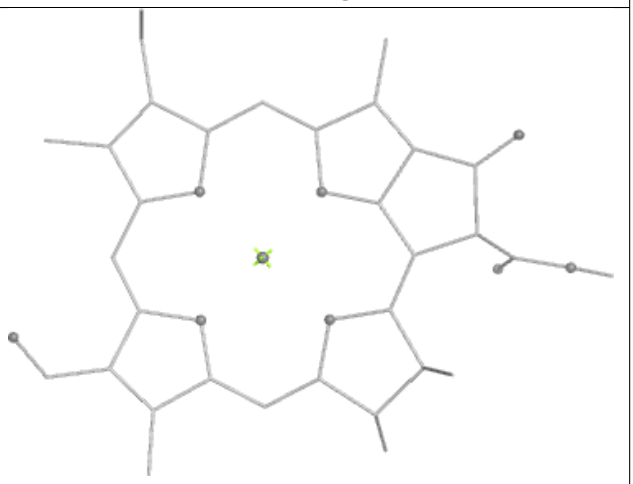
Bond lengths



Bond angles

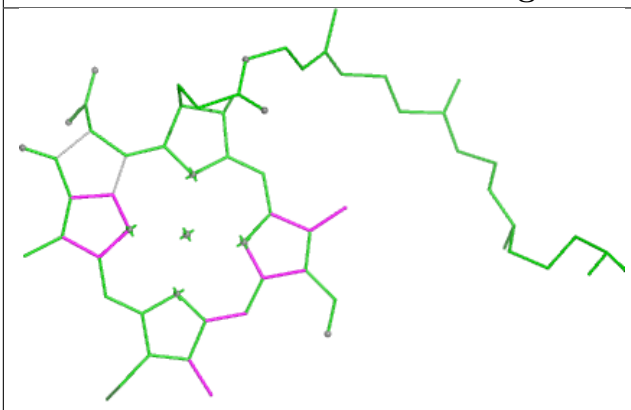


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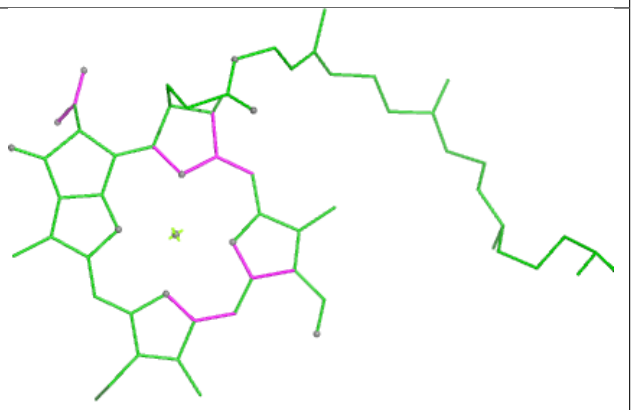


Rings

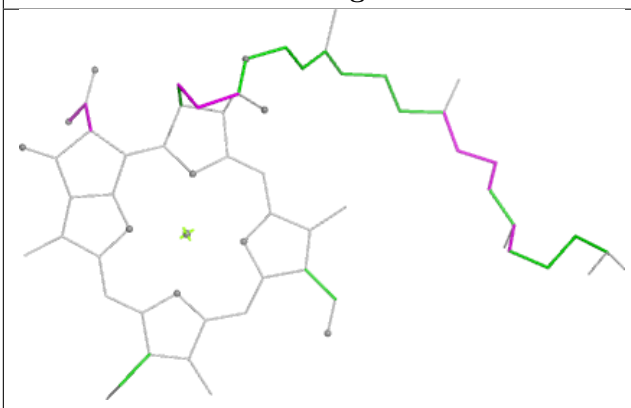
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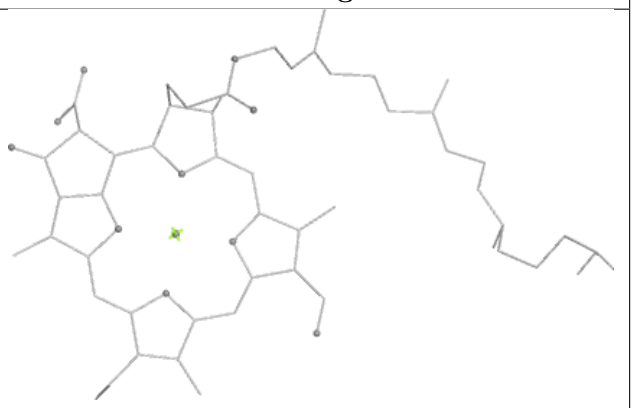
Bond lengths



Bond angles

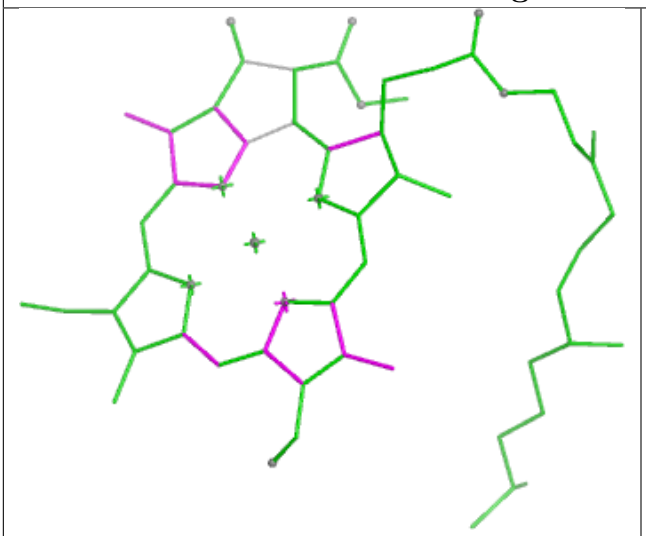


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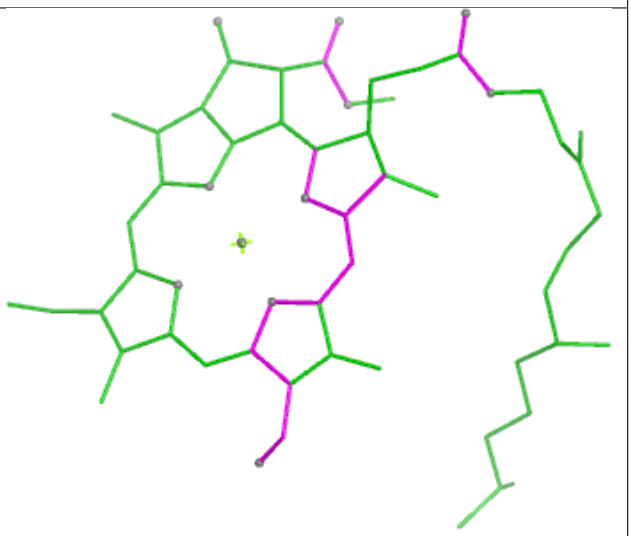


Rings

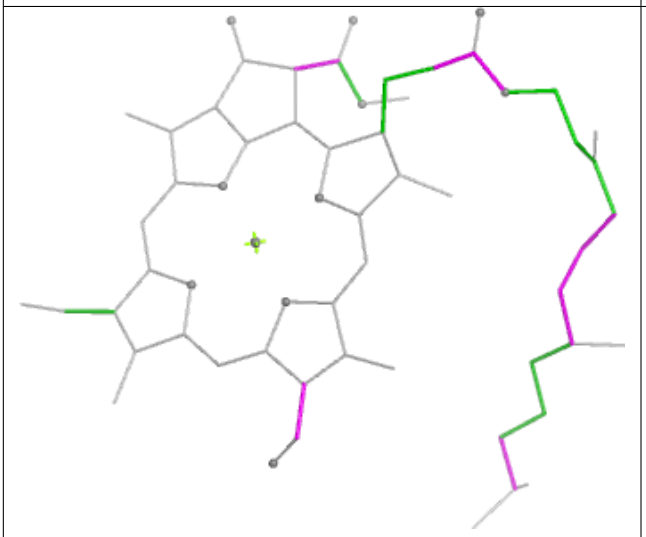
Ligand CL7 aB 1221



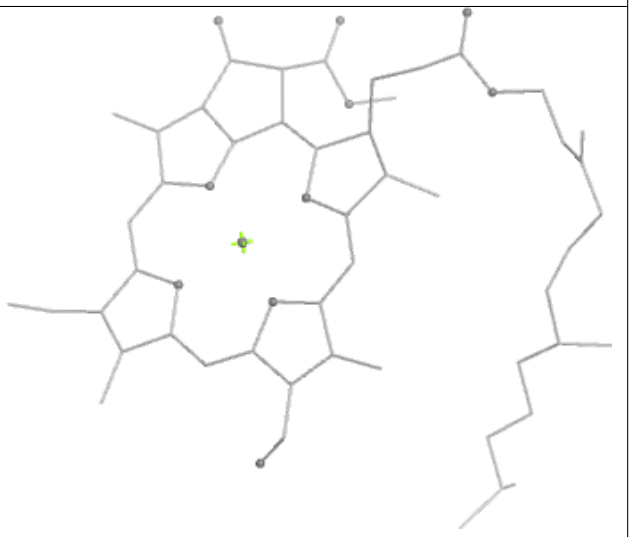
Bond lengths



Bond angles

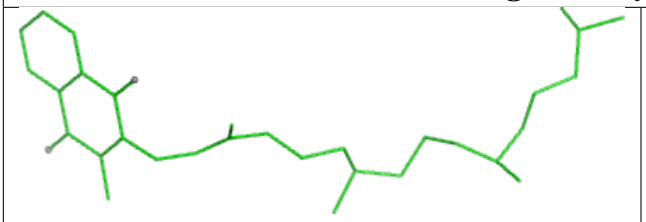


Torsions

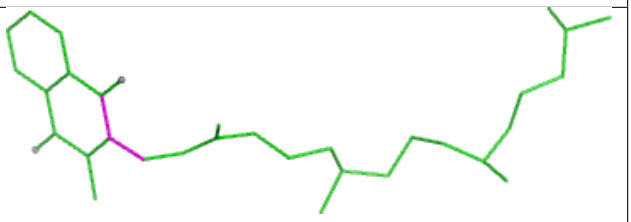


Rings

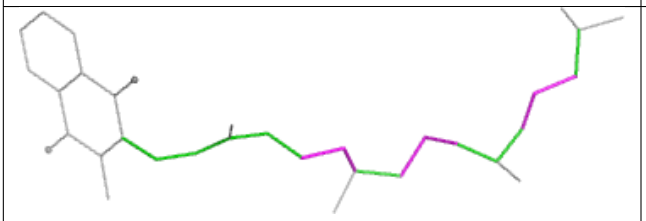
Ligand PQN cB 2002



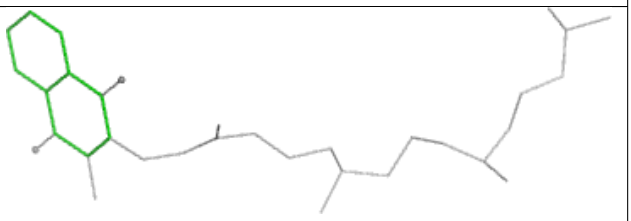
Bond lengths



Bond angles

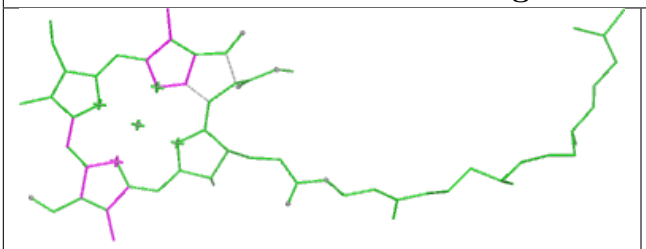


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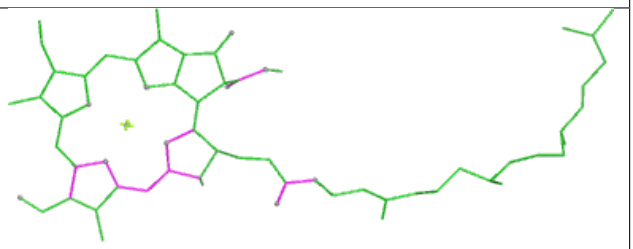


Rings

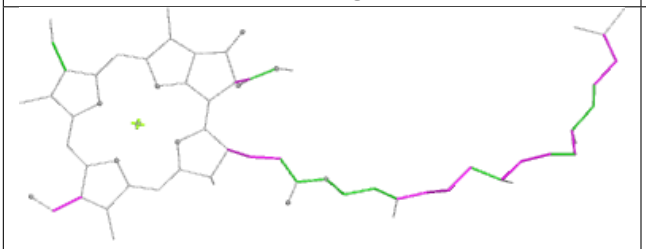
Ligand CL7 cB 1223



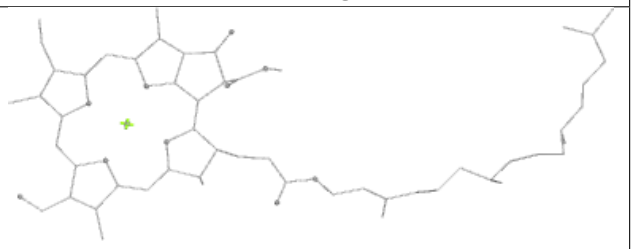
Bond lengths



Bond angles

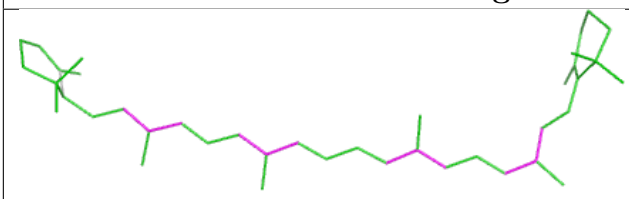


Torsions

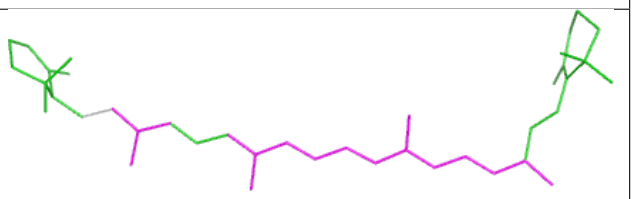


Rings

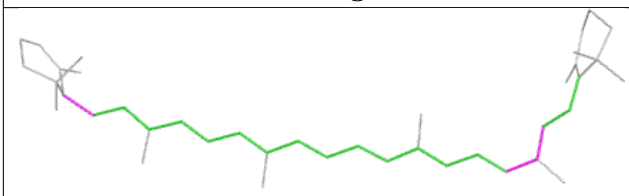
Ligand A1JPJ aL 4020



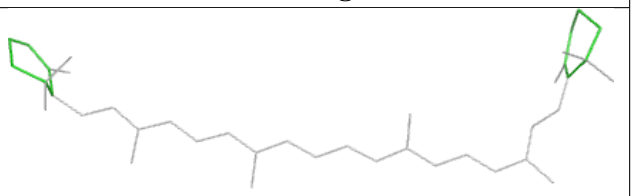
Bond lengths



Bond angles

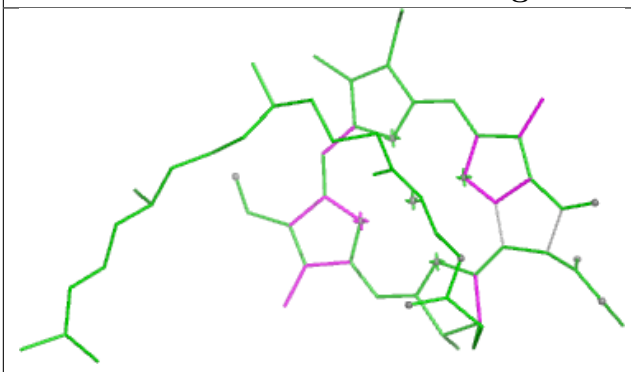


Torsions

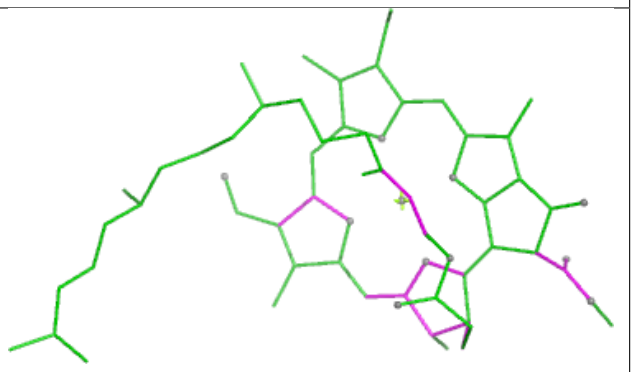


Rings

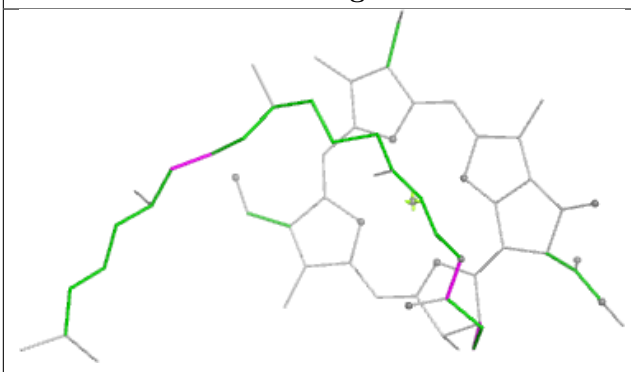
Ligand CL7 aB 1204



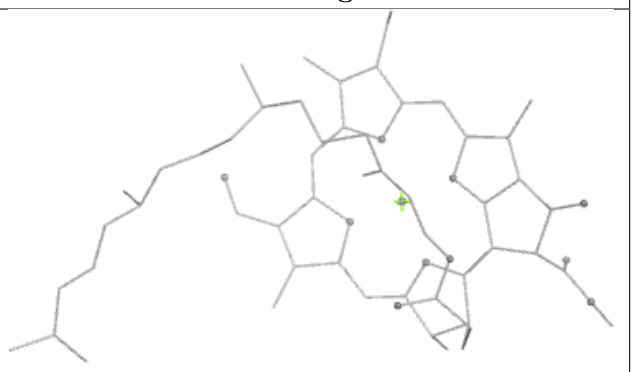
Bond lengths



Bond angles

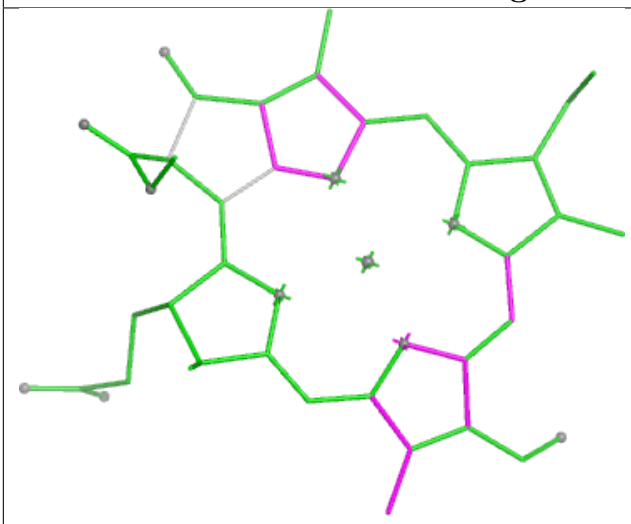


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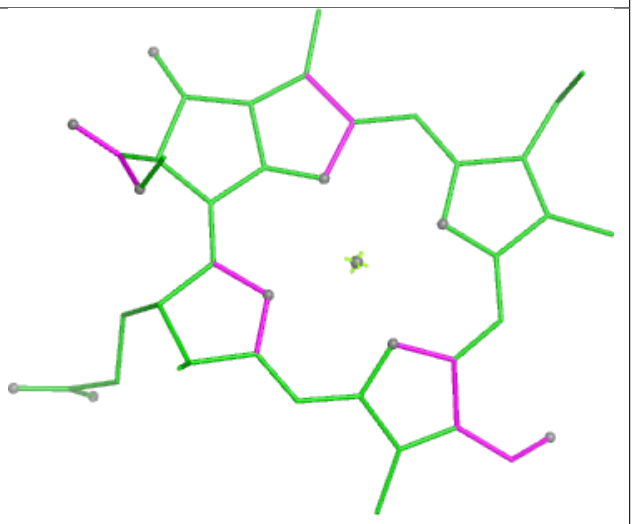


Rings

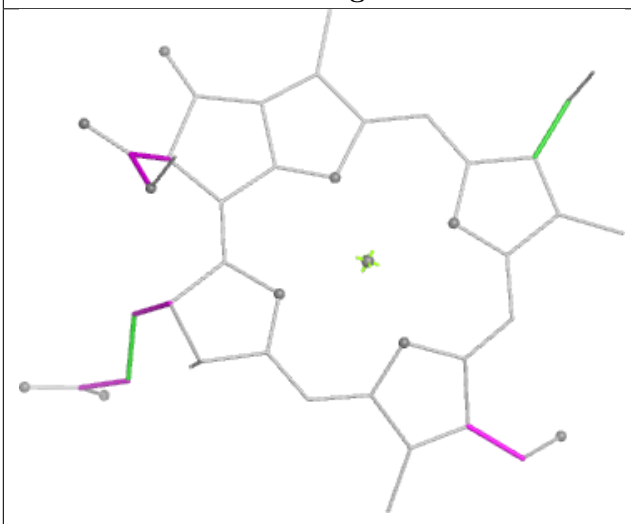
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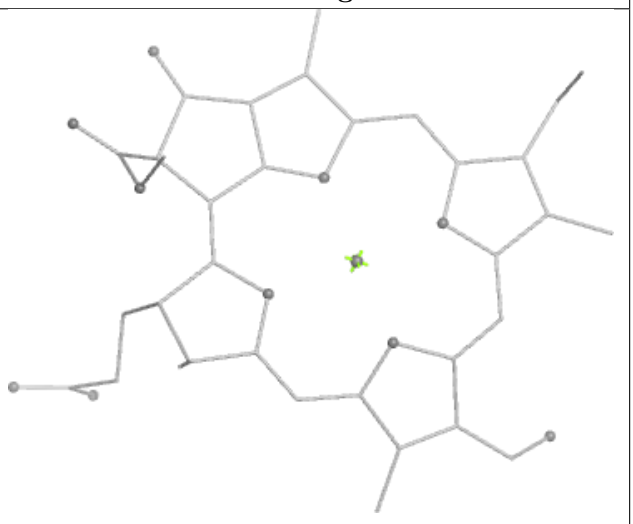
Bond lengths



Bond angles

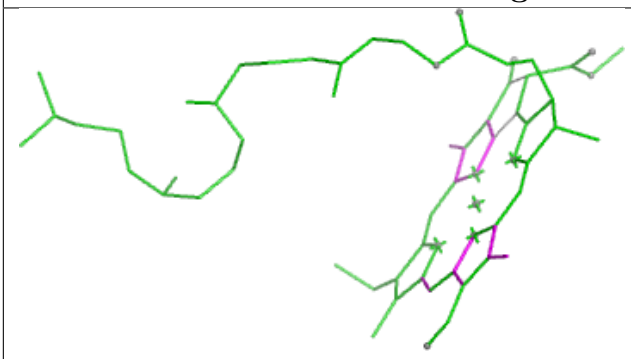


Torsions



Rings

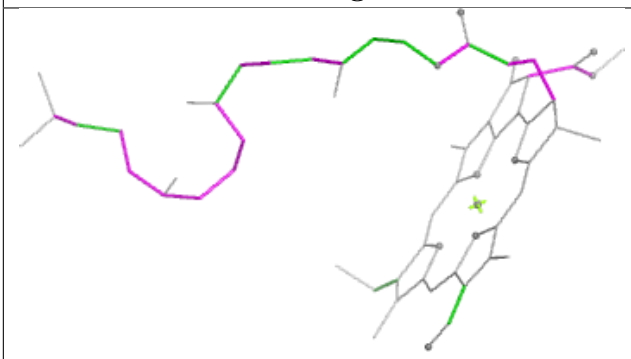
Ligand CL7 aA 1109



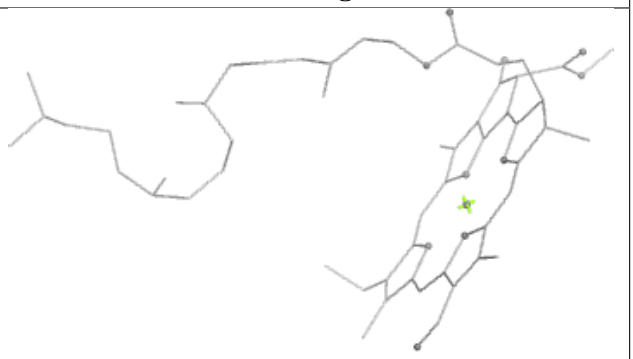
Bond lengths



Bond angles

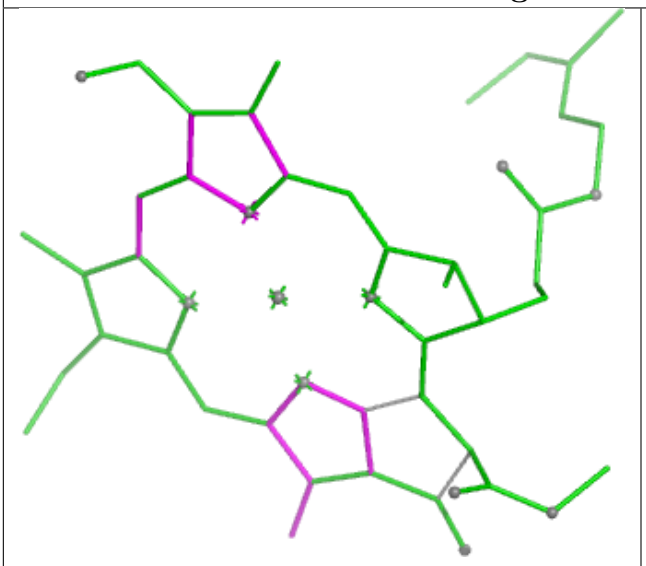


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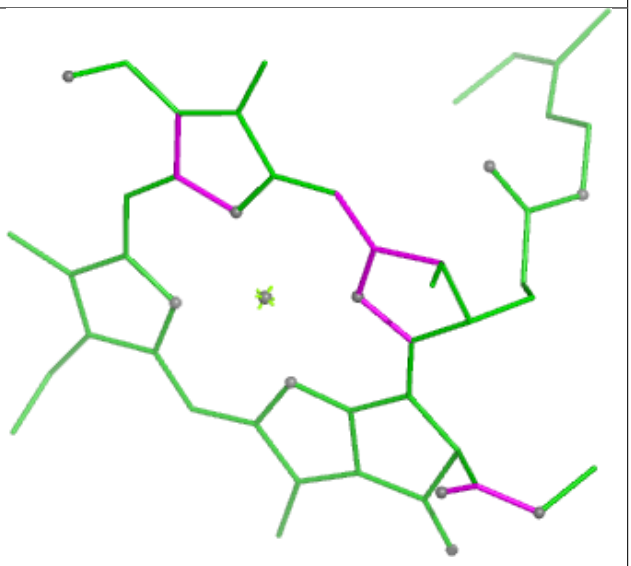


Rings

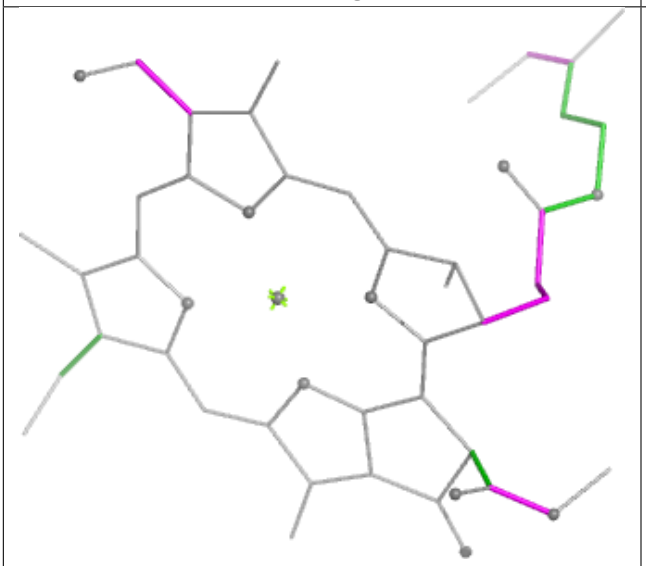
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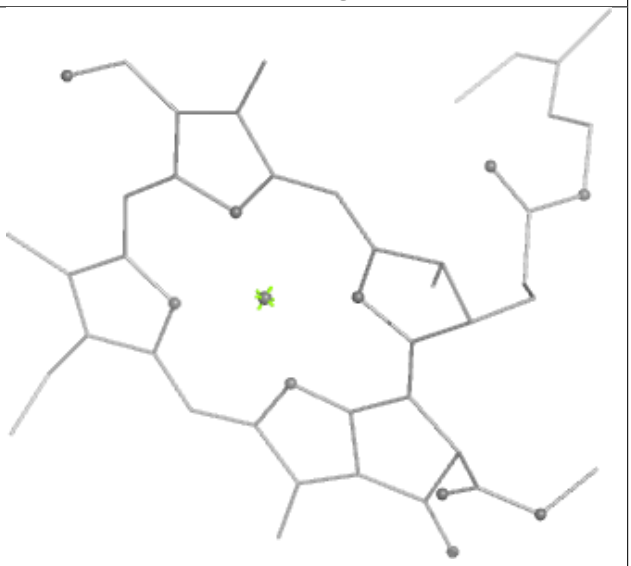
Bond lengths



Bond angles

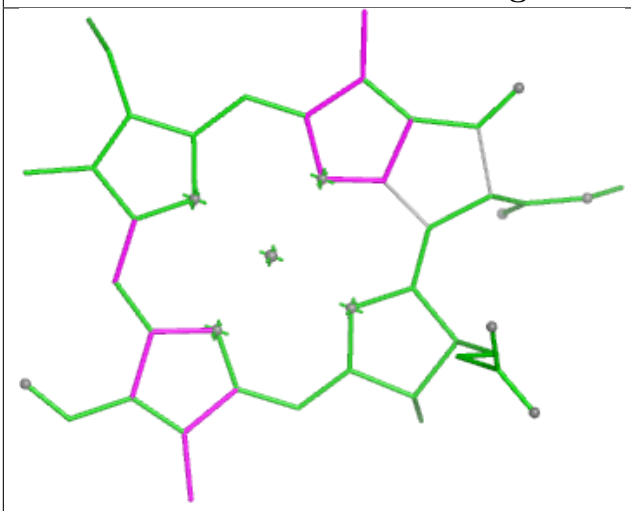


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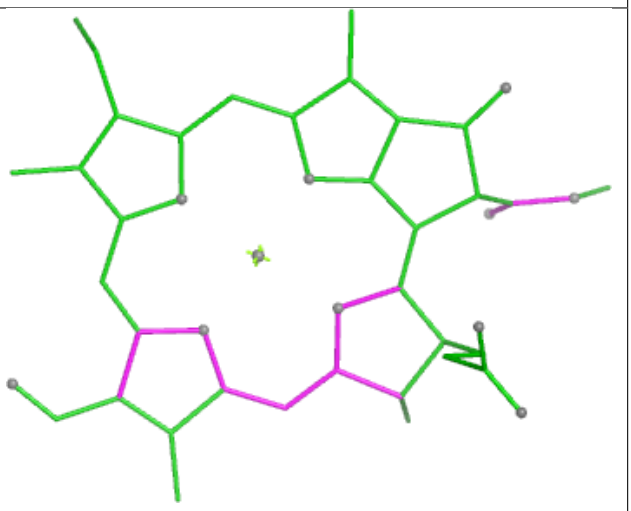


Rings

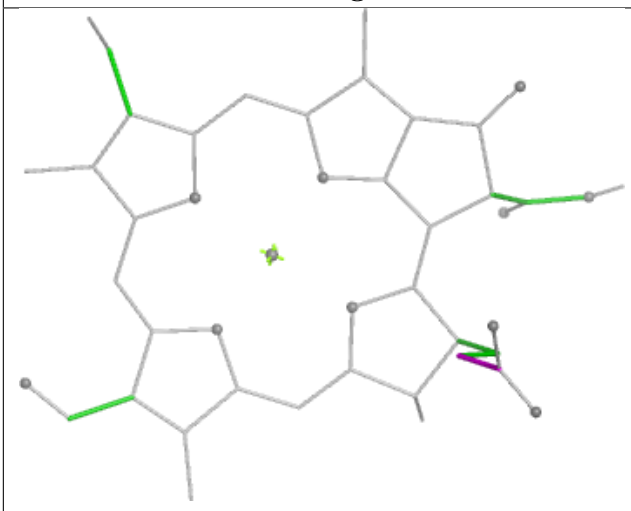
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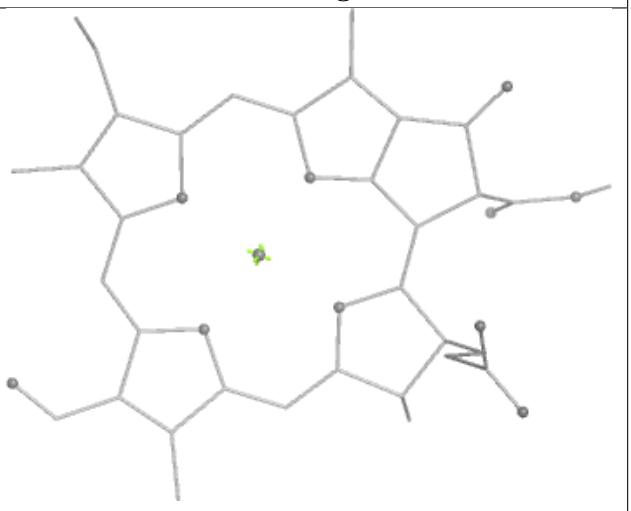
Bond lengths



Bond angles

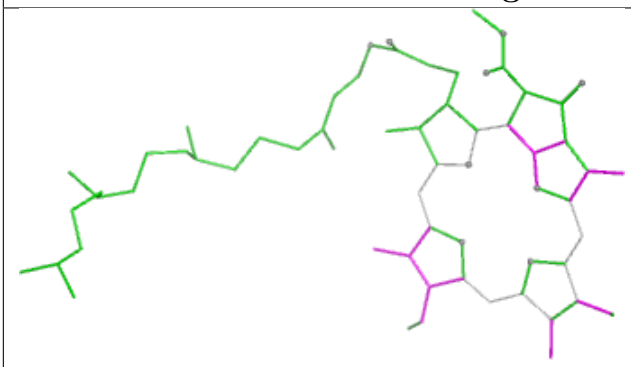


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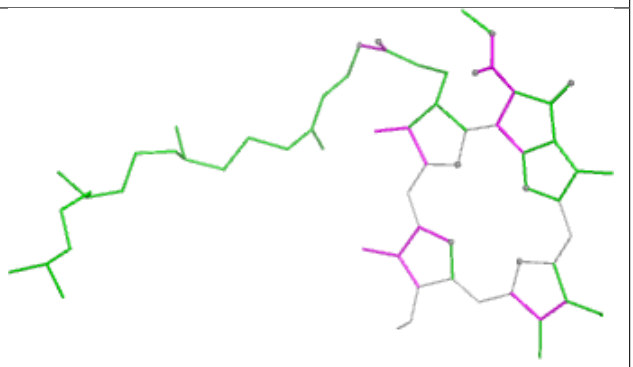


Rings

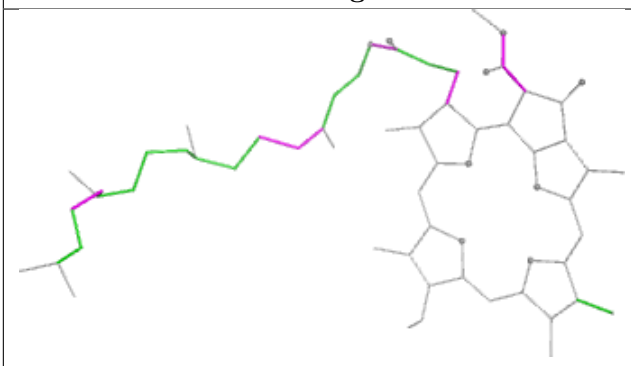
Ligand PHO bA 1013



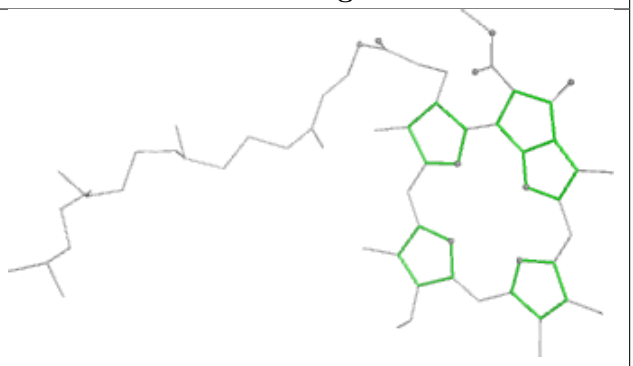
Bond lengths



Bond angles

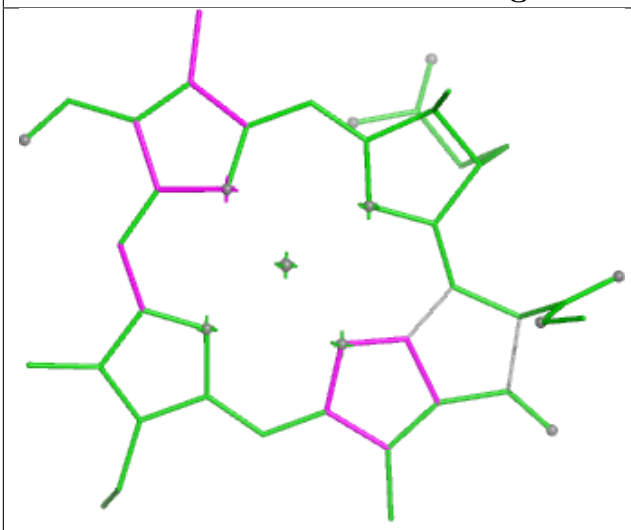


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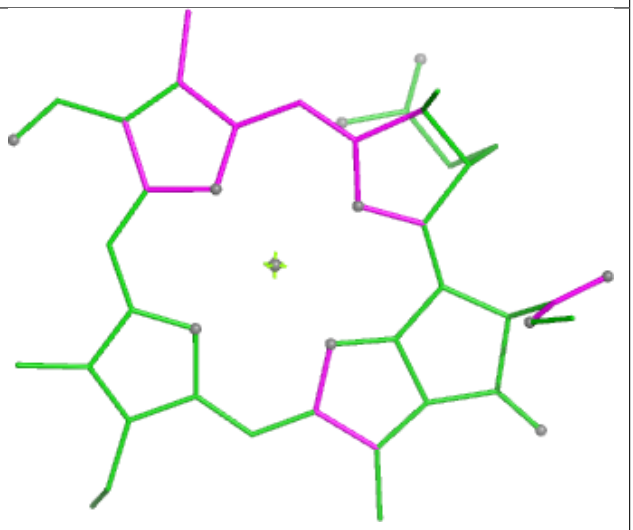


Rings

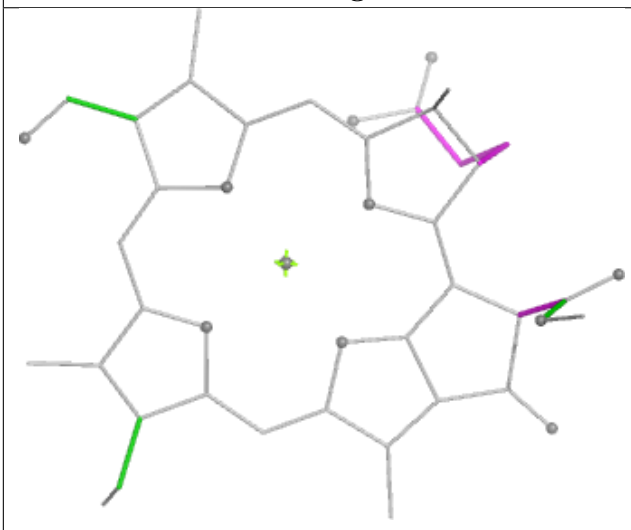
Ligand CL7 bB 1227



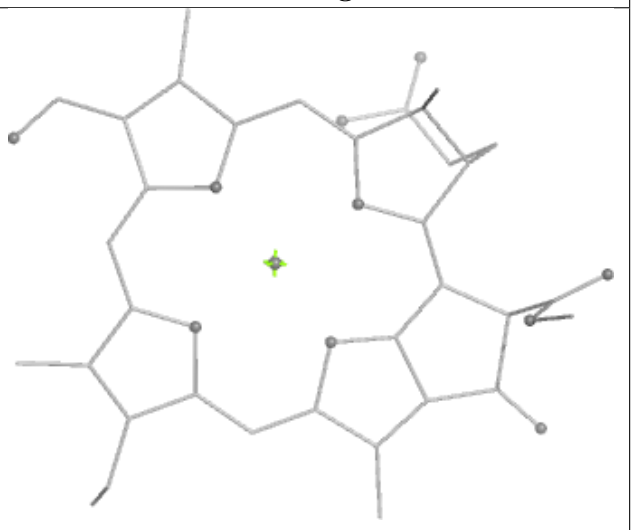
Bond lengths



Bond angles

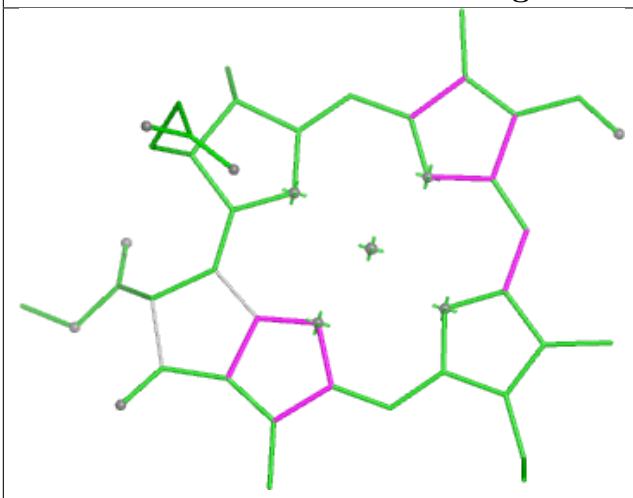


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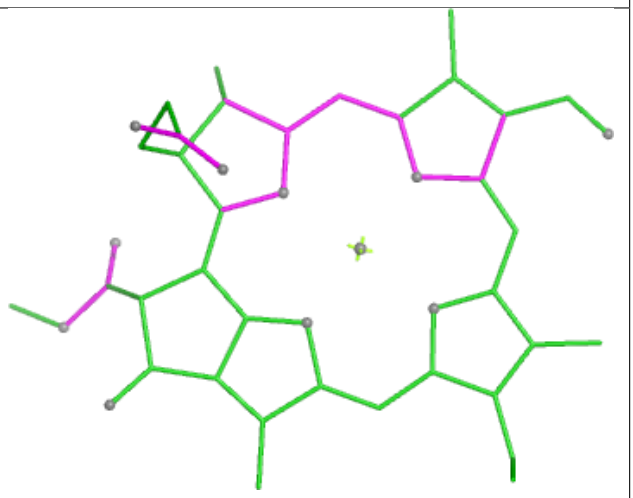


Rings

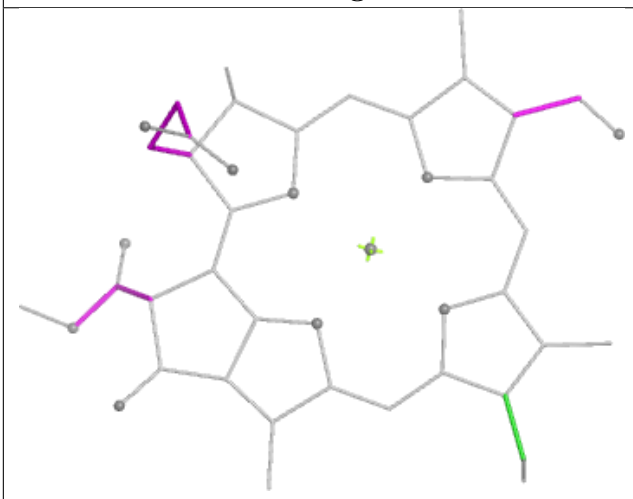
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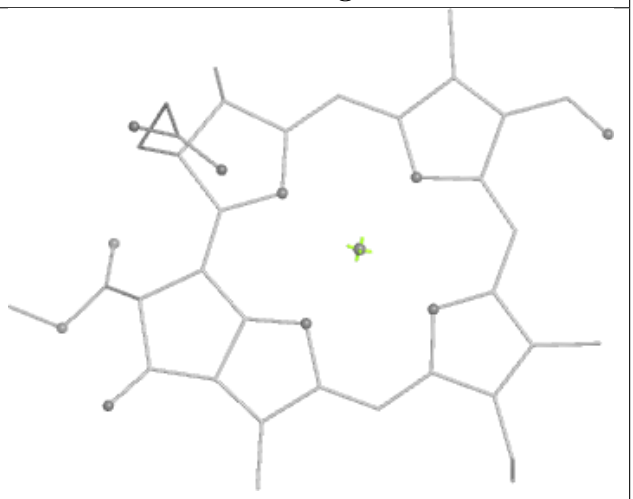
Bond lengths



Bond angles

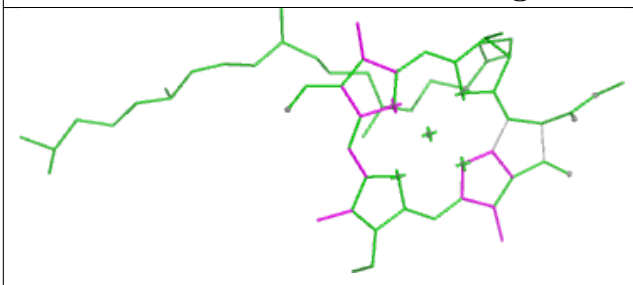


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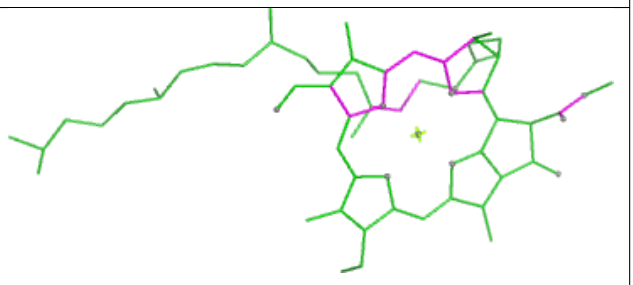


Rings

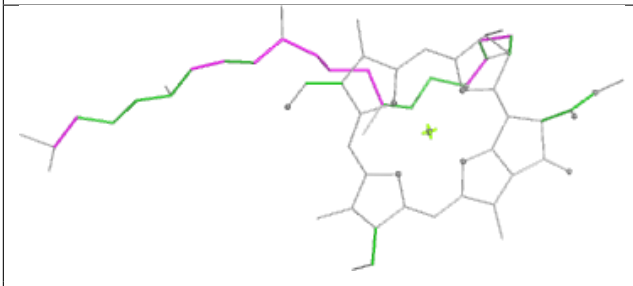
Ligand CL7 aB 1237



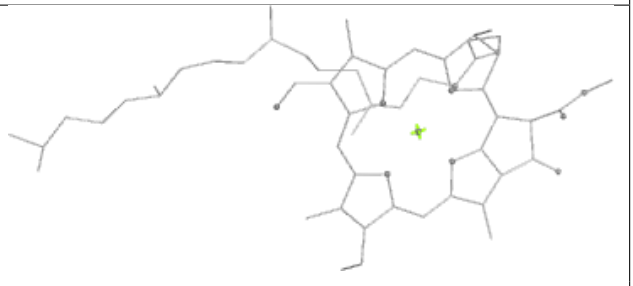
Bond lengths



Bond angles

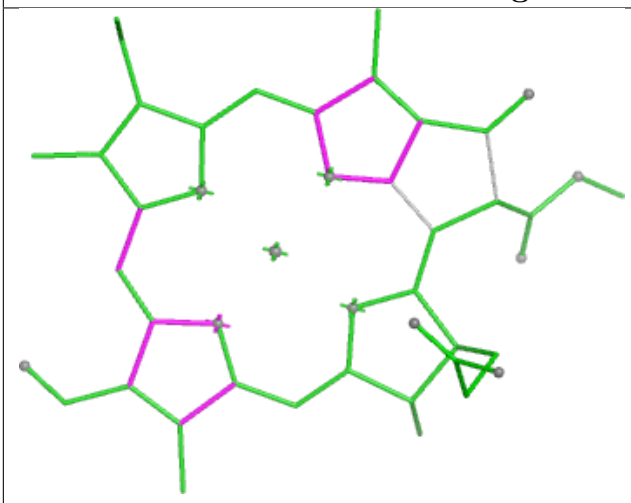


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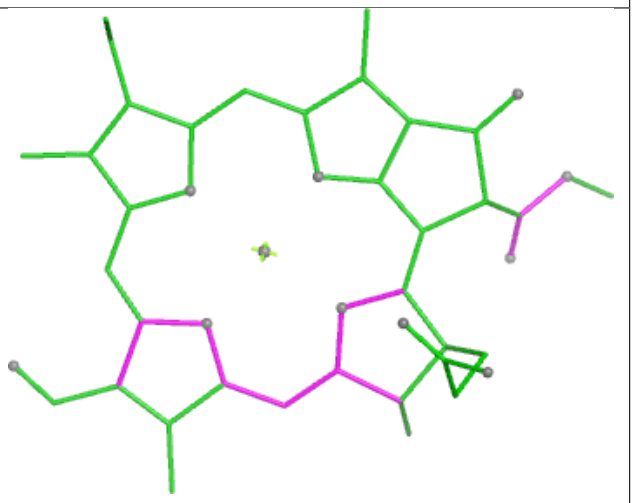


Rings

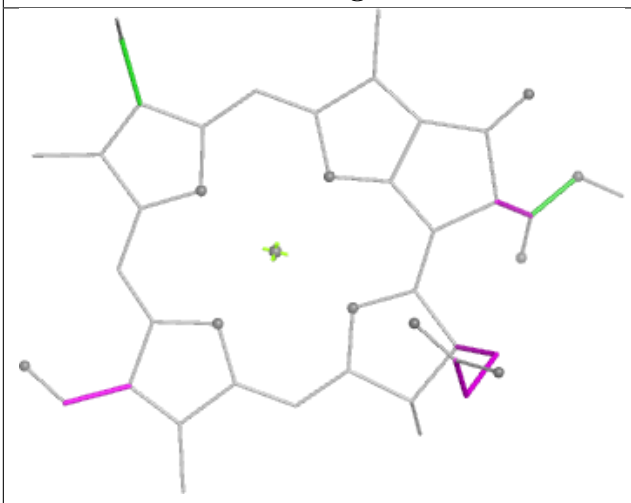
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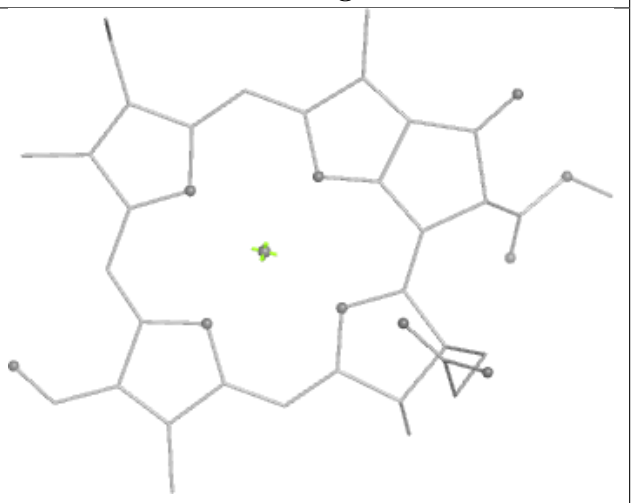
Bond lengths



Bond angles

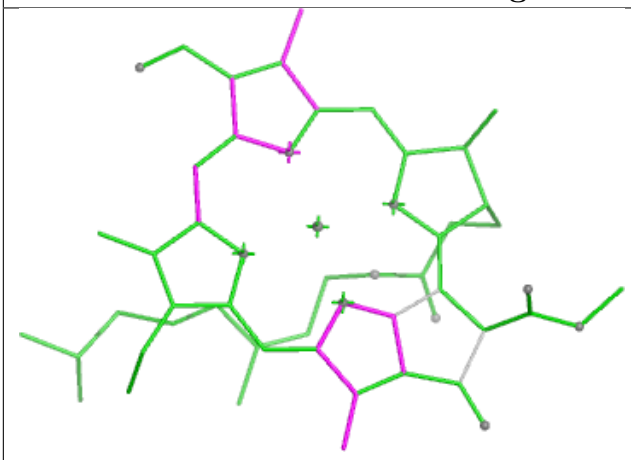


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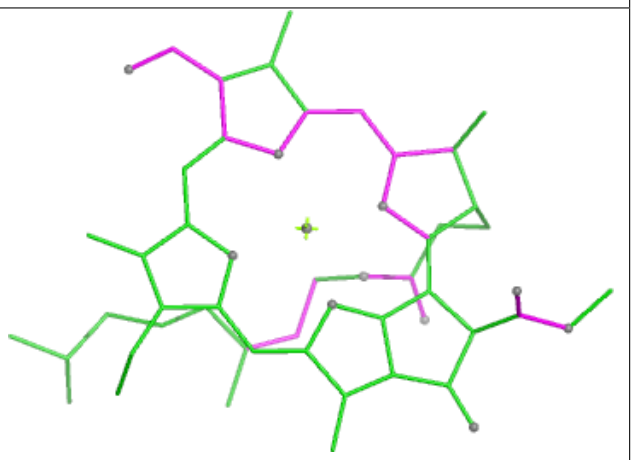


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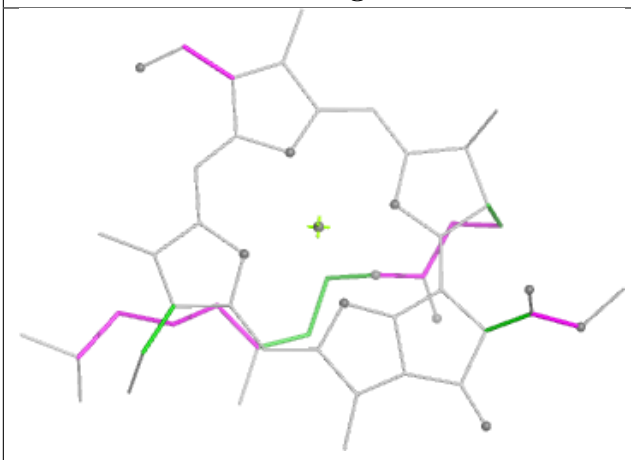
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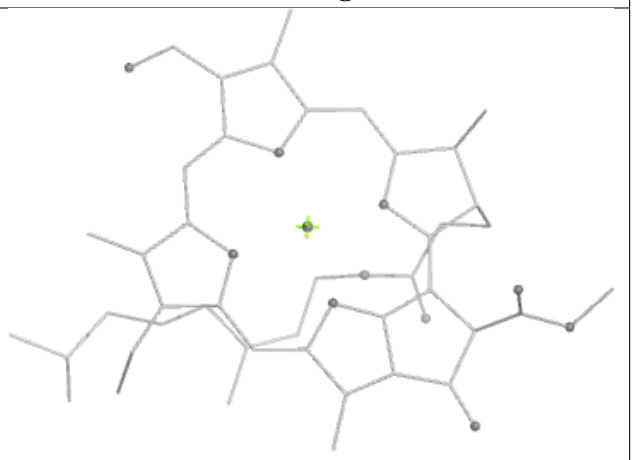
Bond lengths



Bond angles

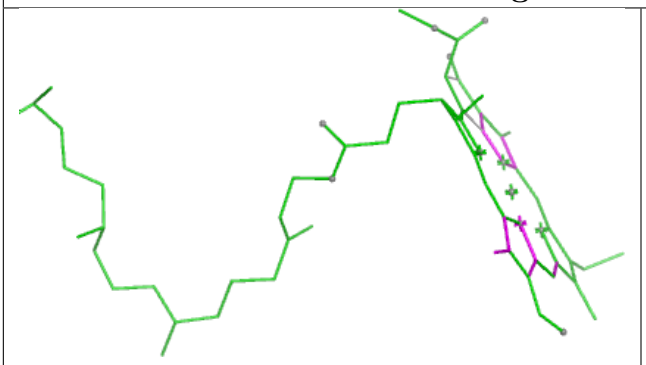


Torsions

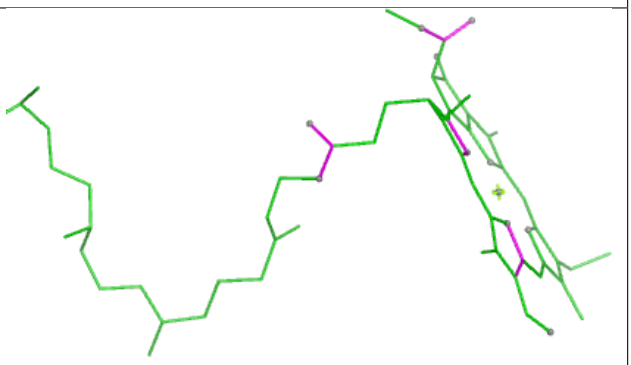


Rings

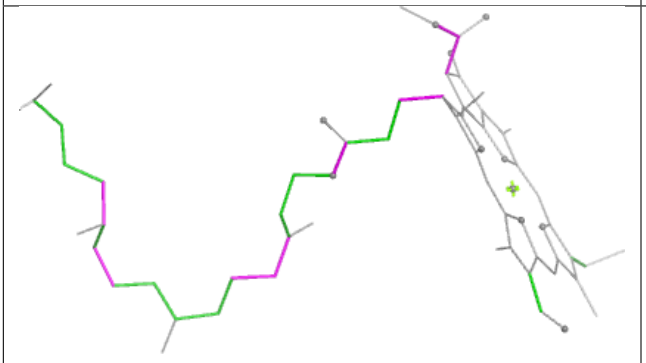
Ligand CL7 aB 1208



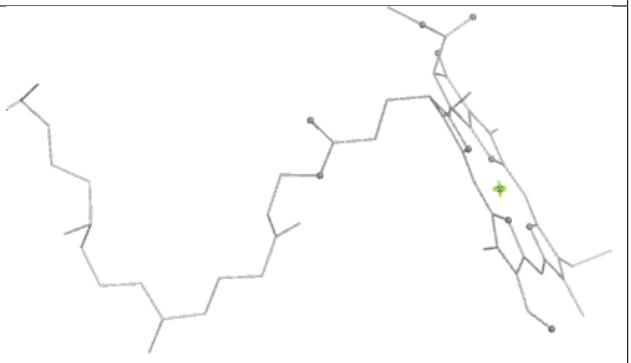
Bond lengths



Bond angles

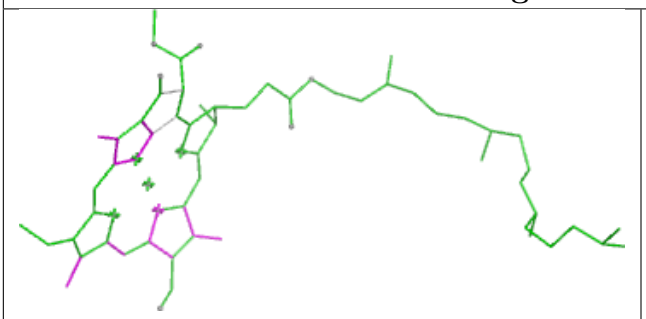


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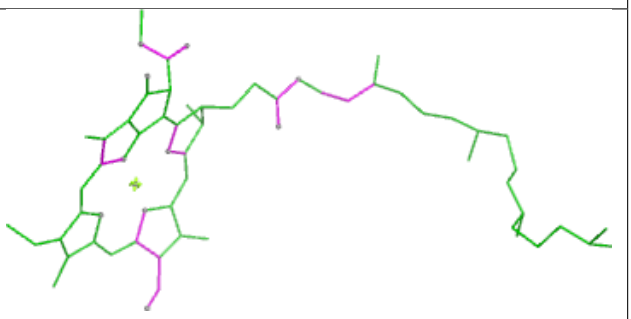


Rings

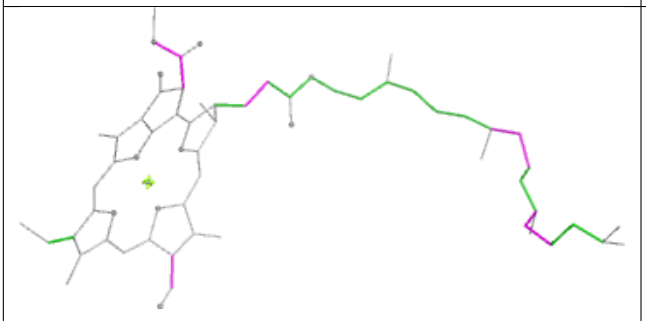
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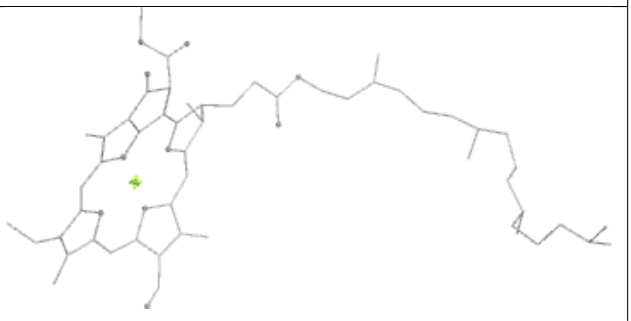
Bond lengths



Bond angles

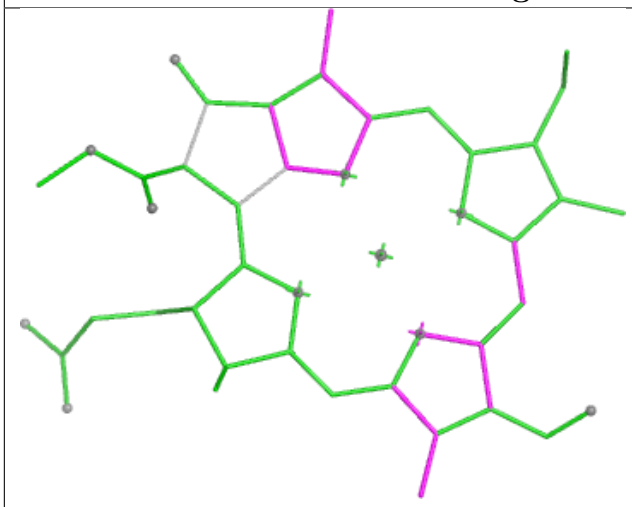


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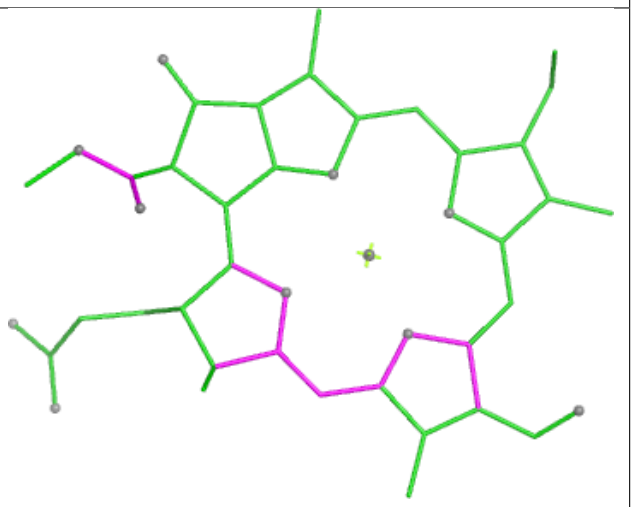


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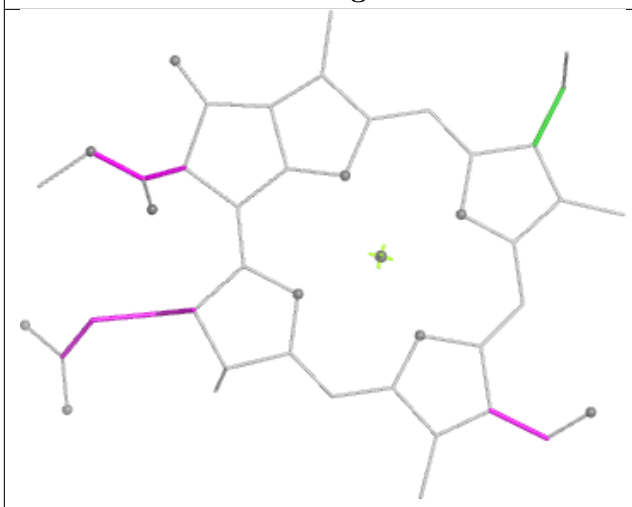
Ligand CL7 cA 1139



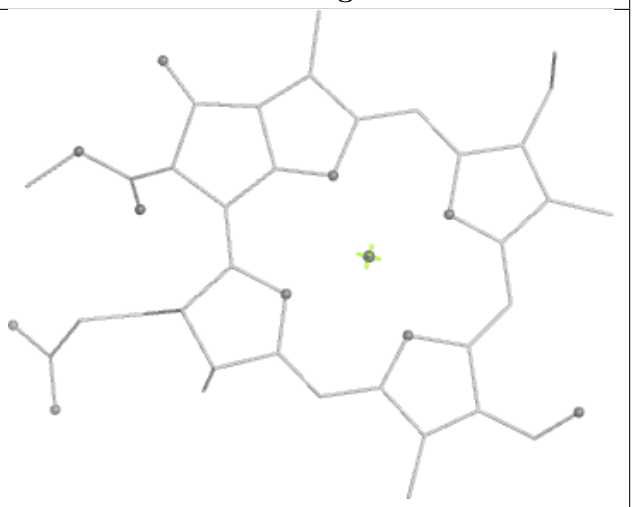
Bond lengths



Bond angles

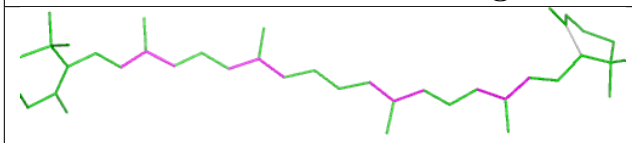


Torsions



Rings

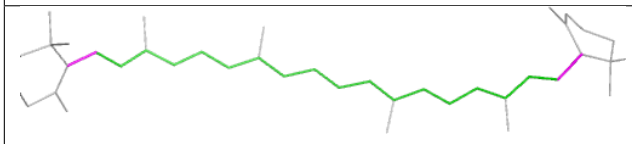
Ligand A1JPJ cA 4008



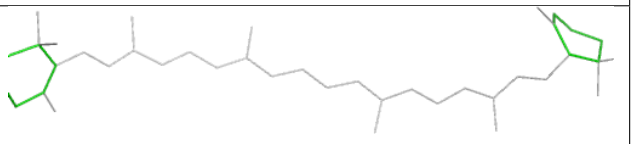
Bond lengths



Bond angles

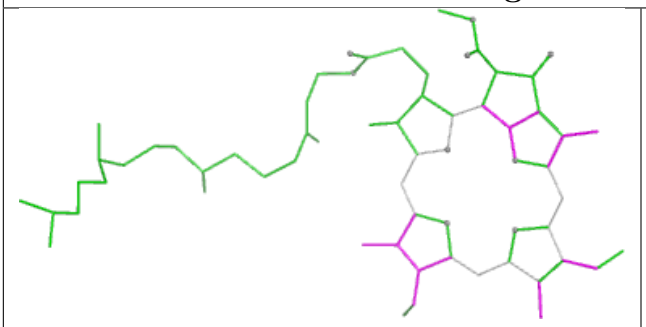


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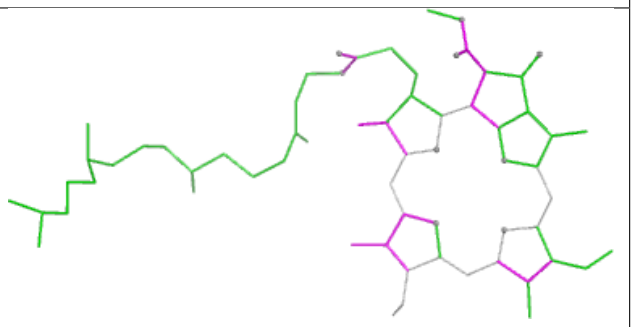


Rings

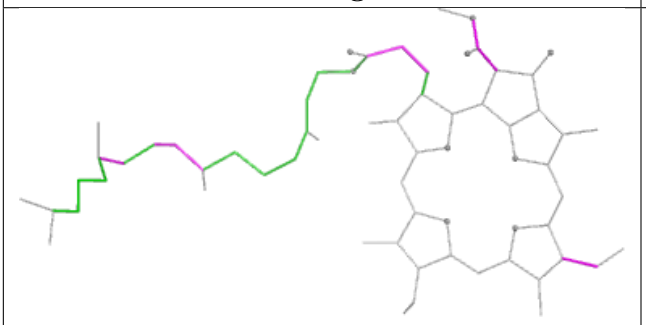
Ligand PHO aB 1023



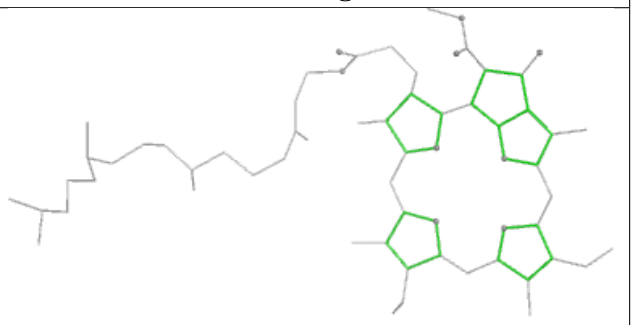
Bond lengths



Bond angles

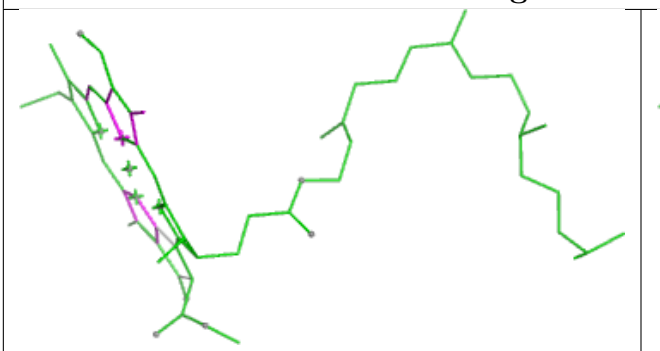


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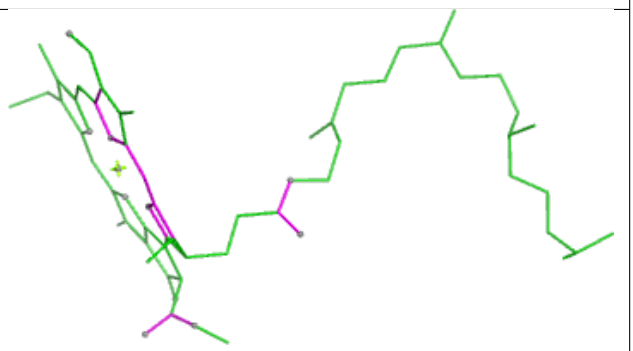


Rings

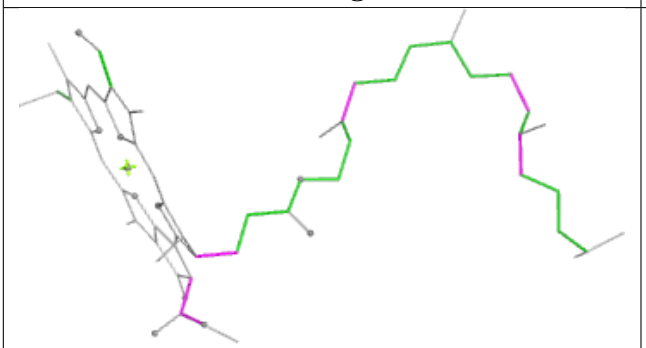
Ligand CL7 bB 1208



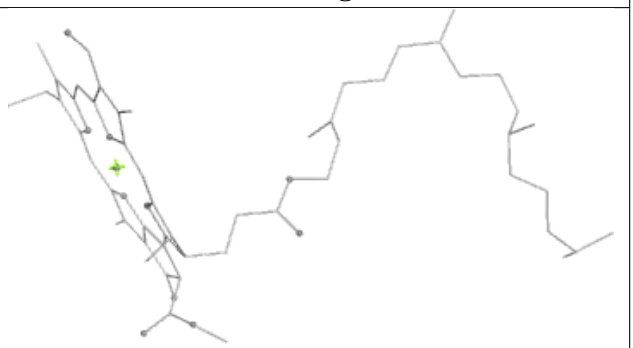
Bond lengths



Bond angles

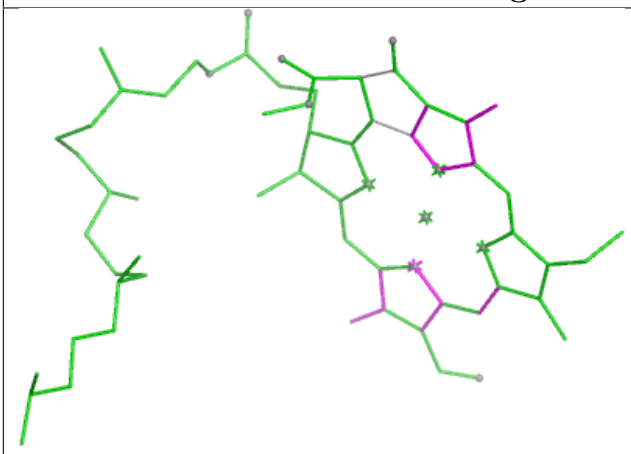


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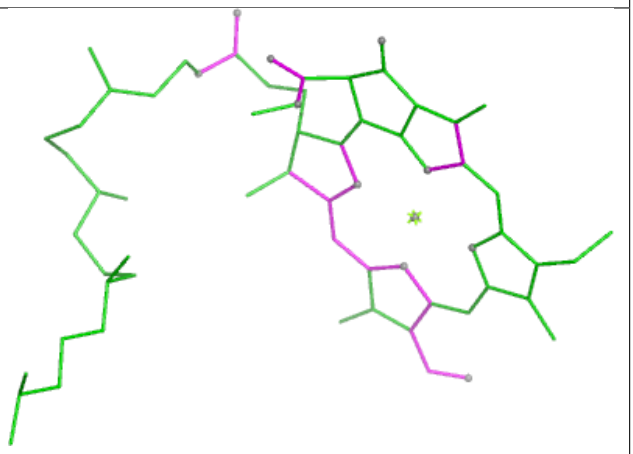


Rings

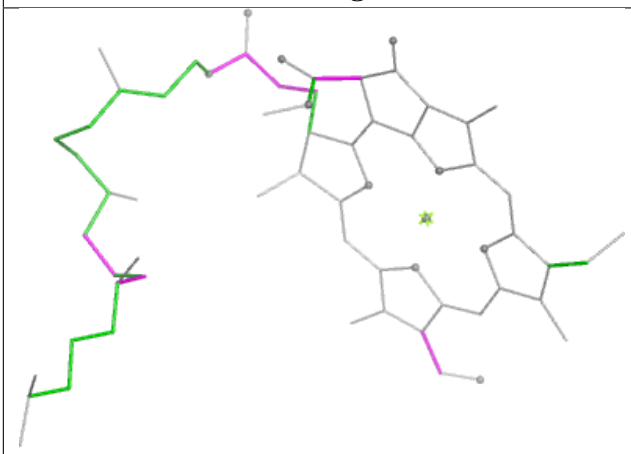
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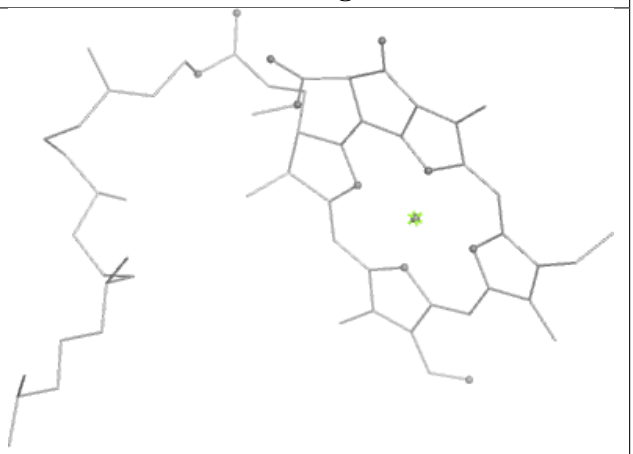
Bond lengths



Bond angles

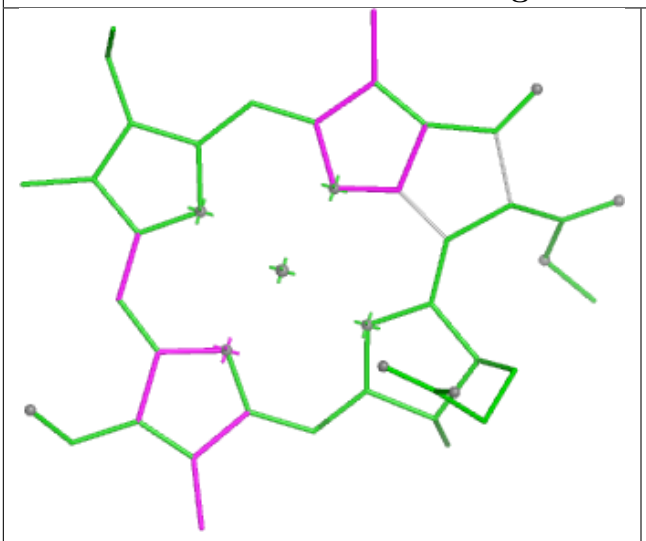


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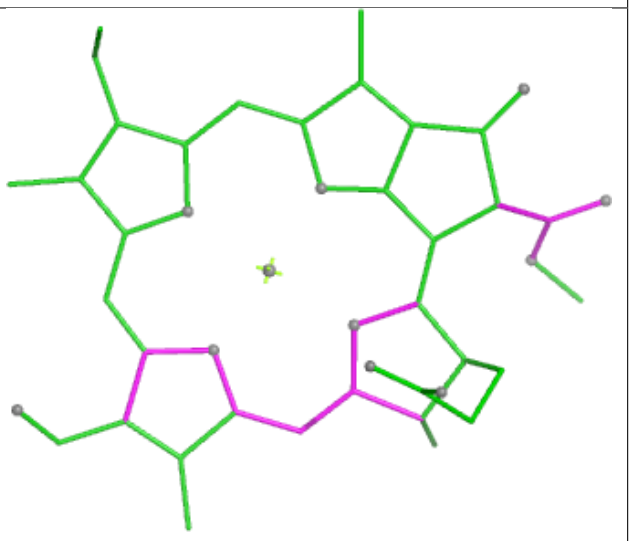


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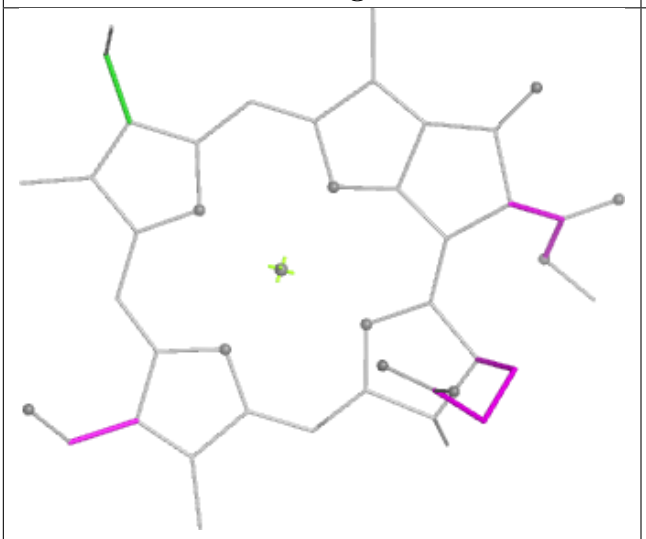
Ligand CL7 cA 1110



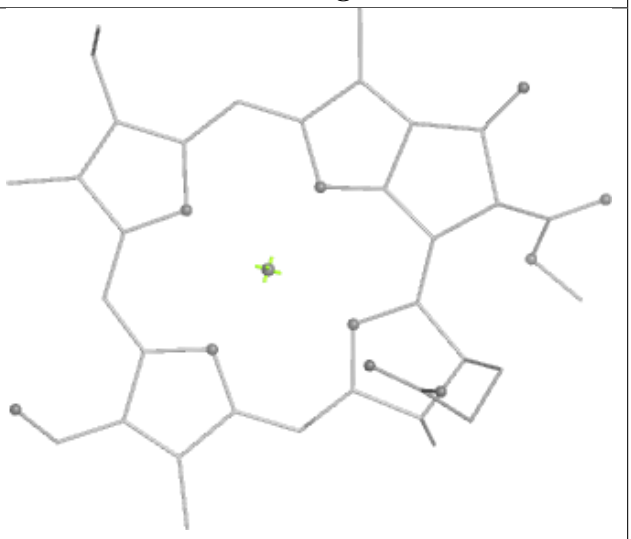
Bond lengths



Bond angles

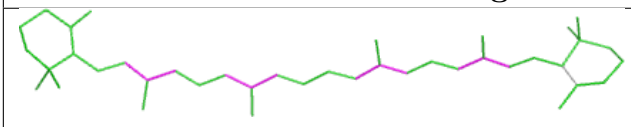


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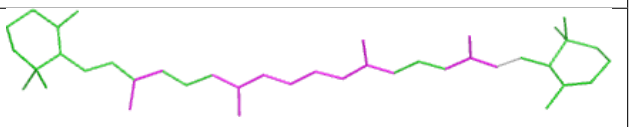


Rings

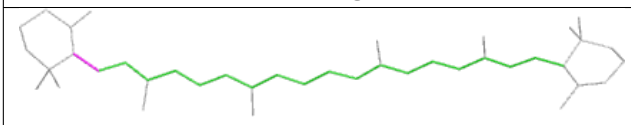
Ligand A1JPJ cA 4002



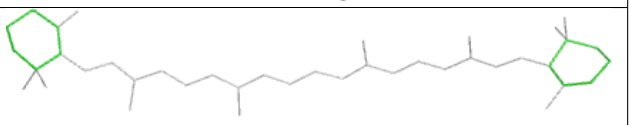
Bond lengths



Bond angles

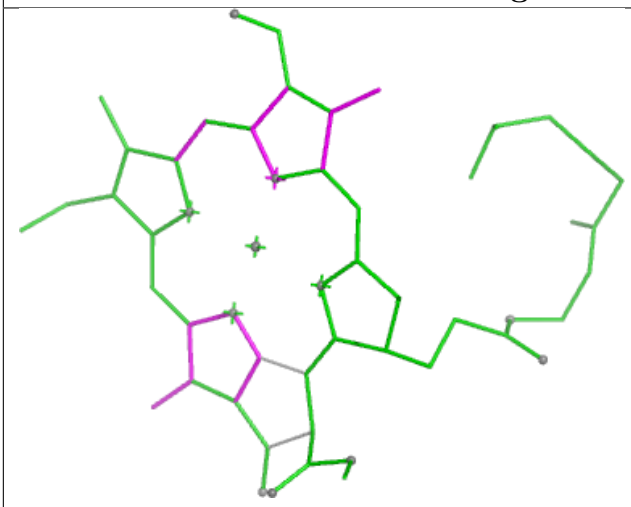


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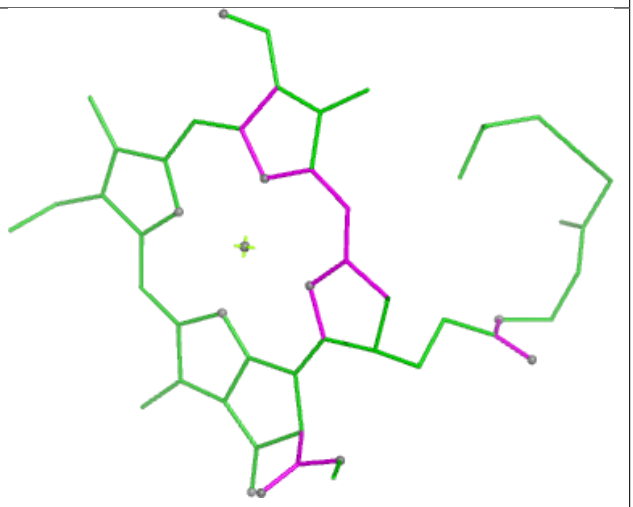


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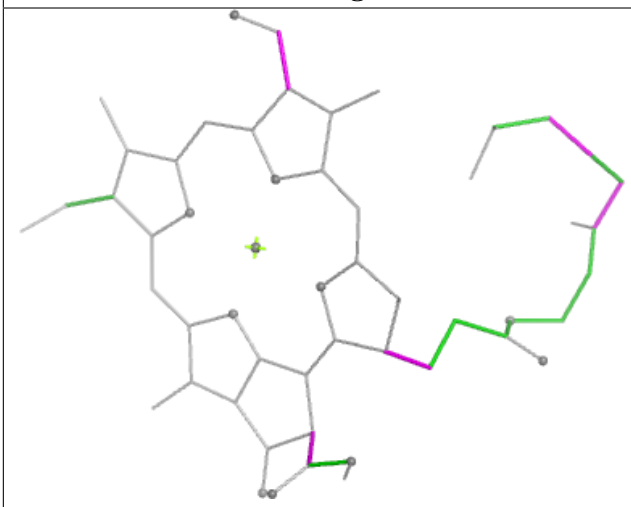
Ligand CL7 aA 1137



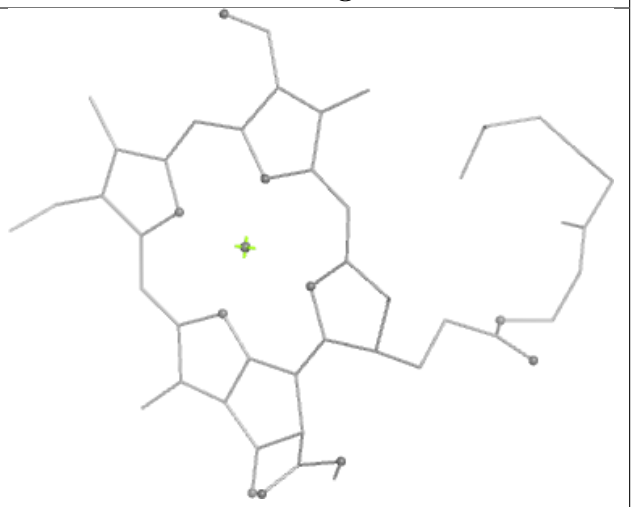
Bond lengths



Bond angles

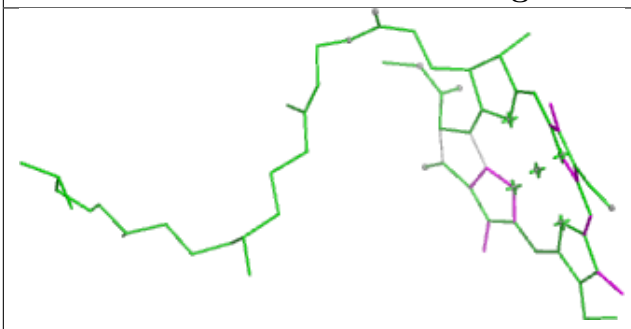


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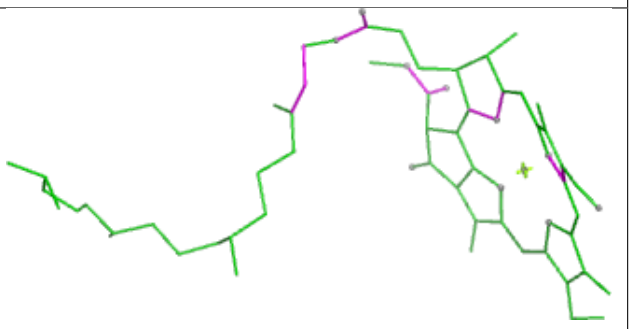


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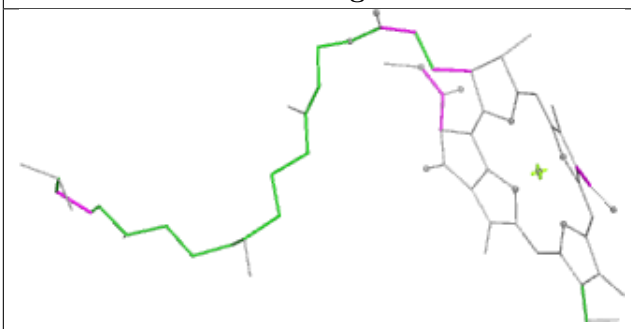
Ligand CL7 aB 1021



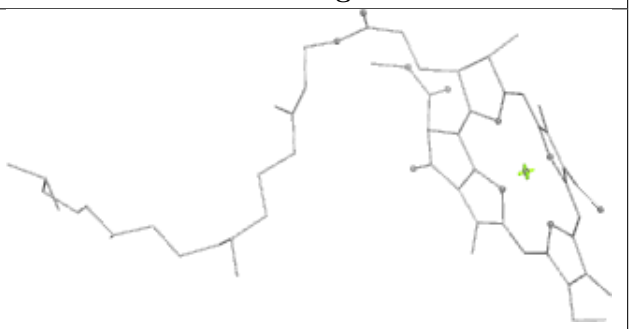
Bond lengths



Bond angles

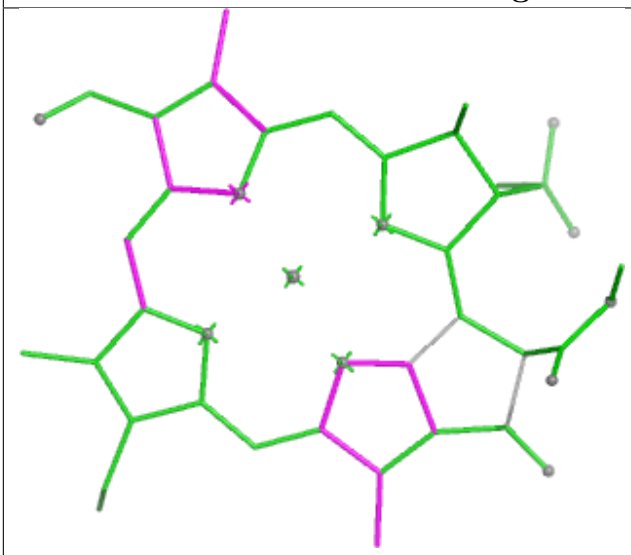


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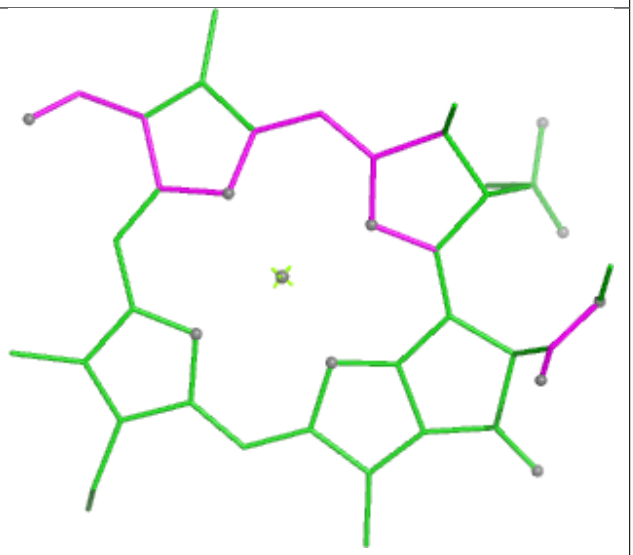


Rings

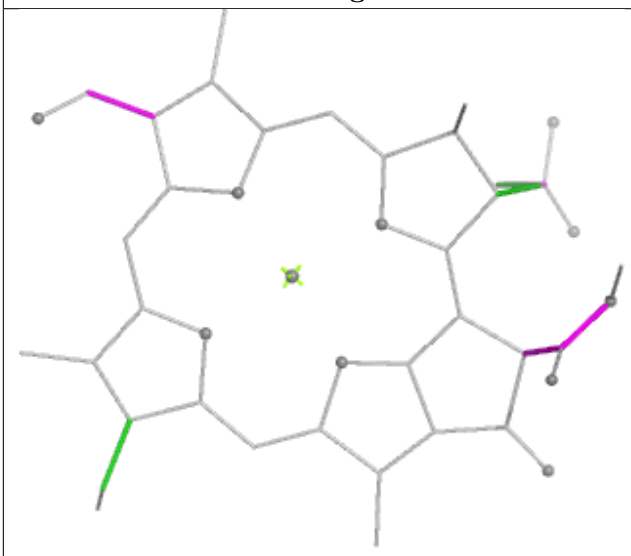
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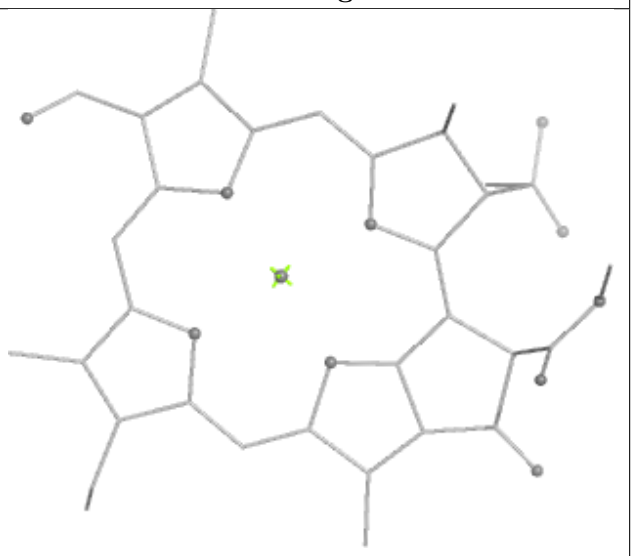
Bond lengths



Bond angles

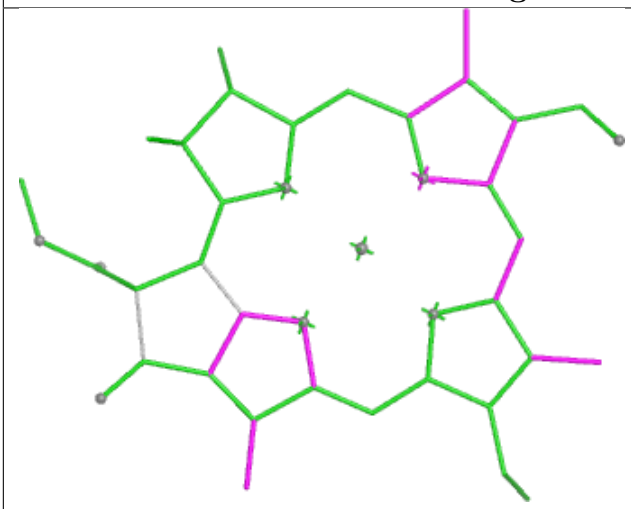


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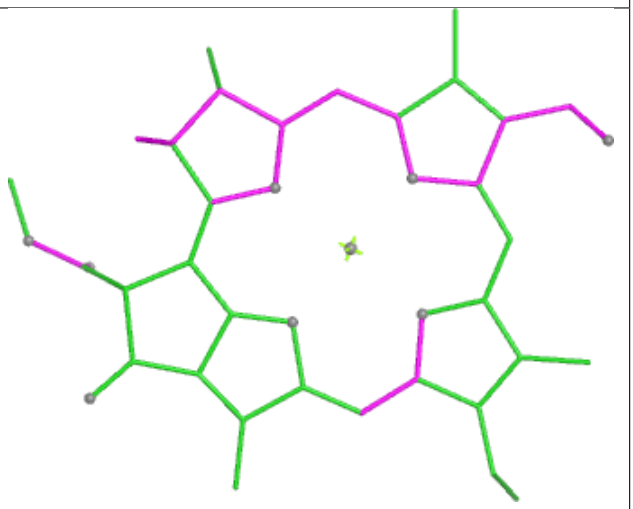


Rings

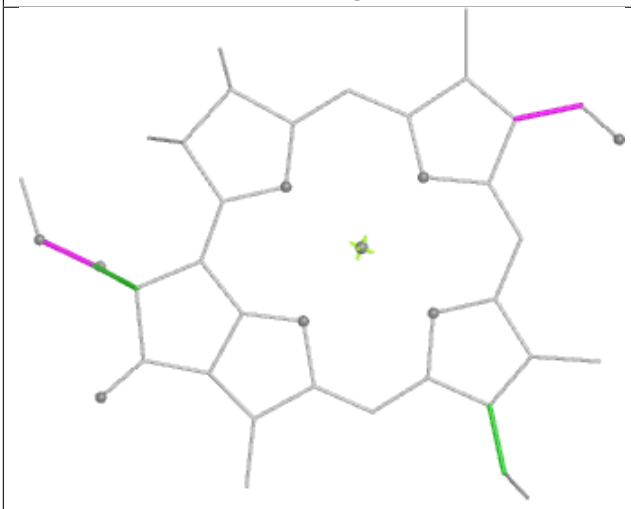
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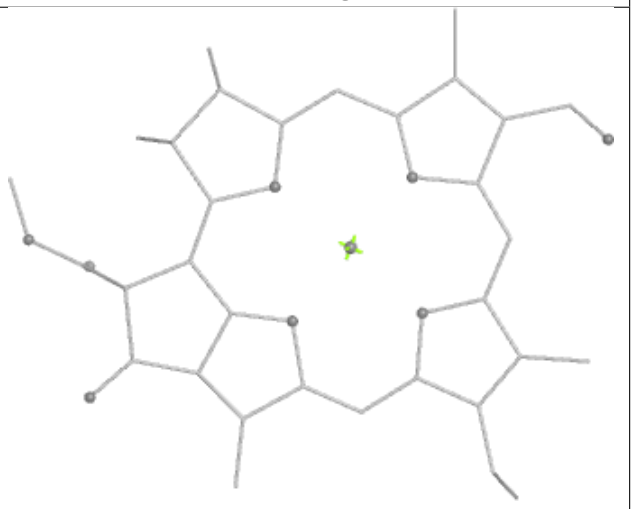
Bond lengths



Bond angles

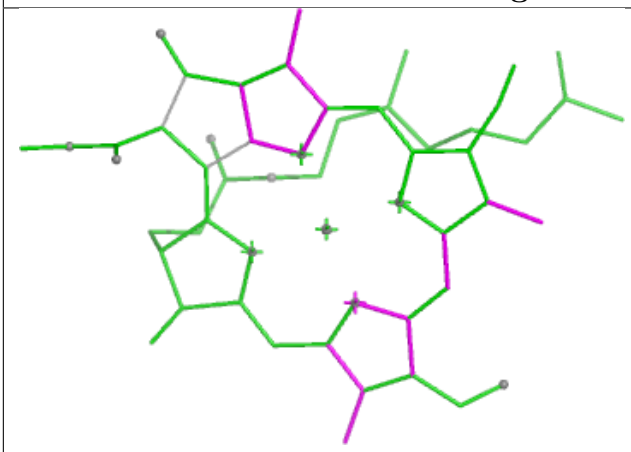


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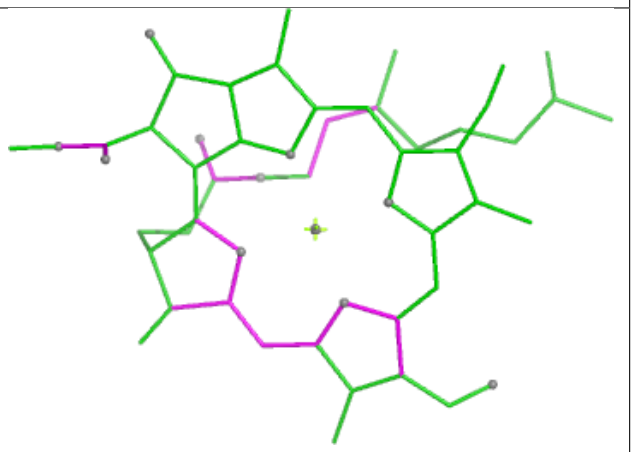


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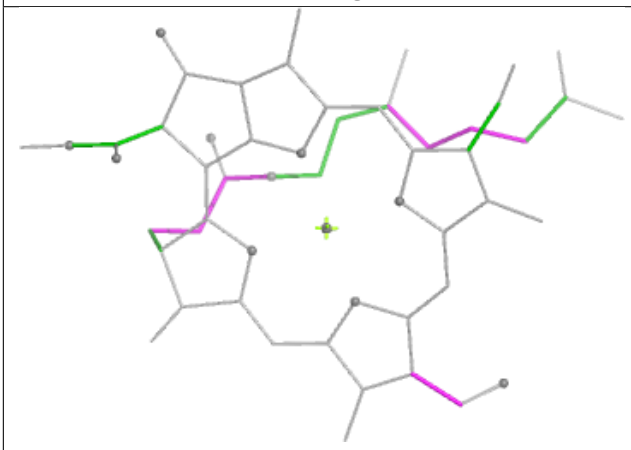
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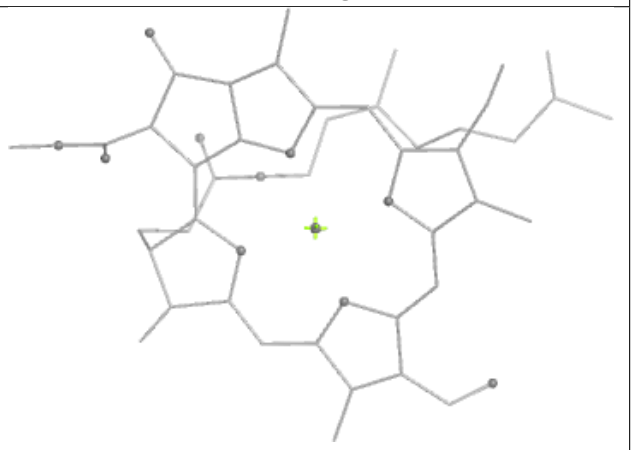
Bond lengths



Bond angles

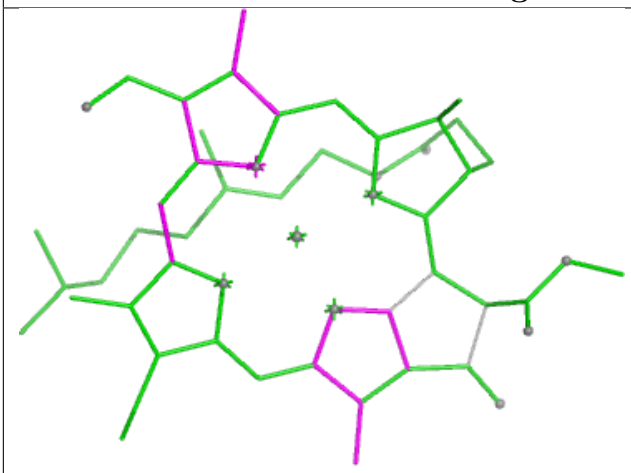


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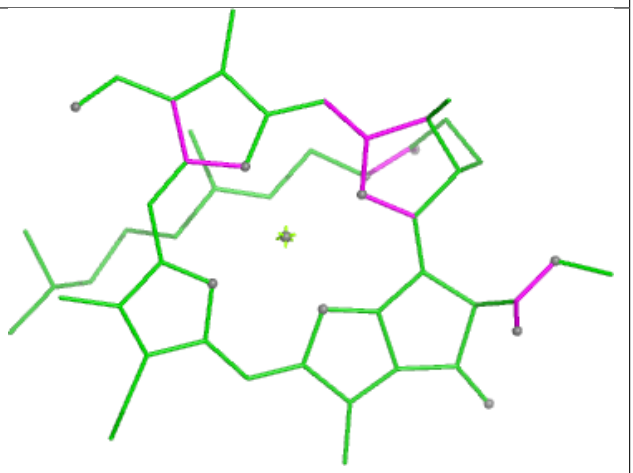


Rings

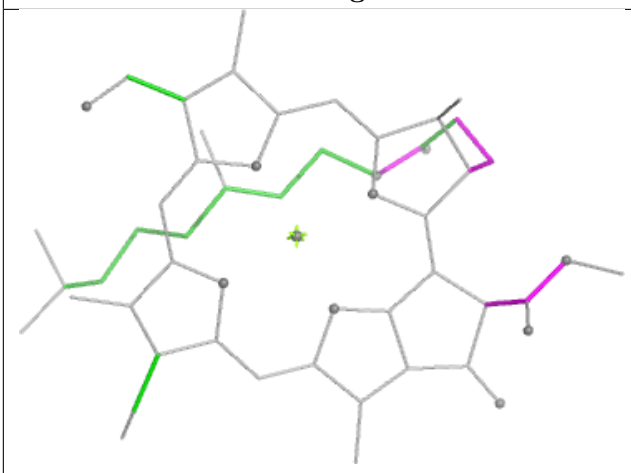
Ligand CL7 aA 1121



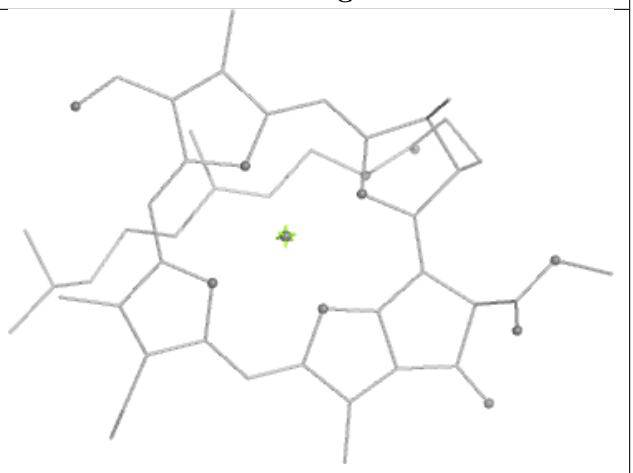
Bond lengths



Bond angles

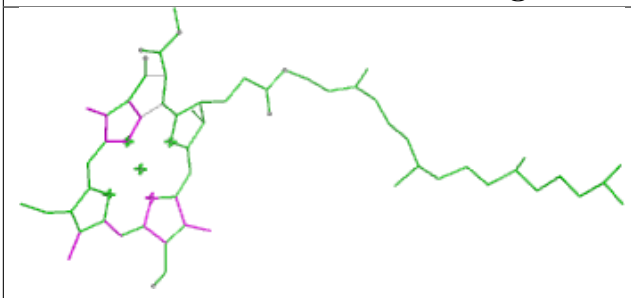


Torsions

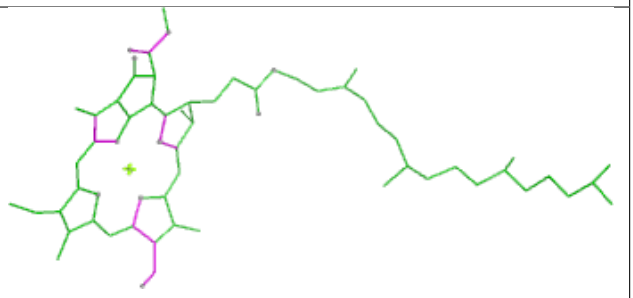


Rings

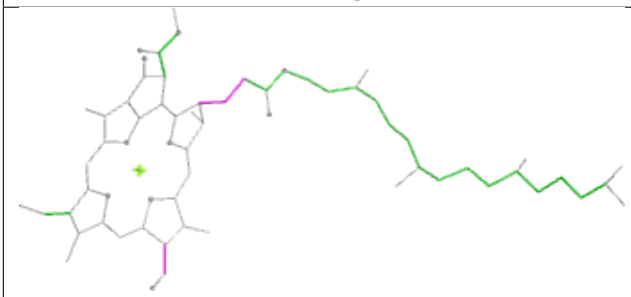
Ligand CL7 bA 1022



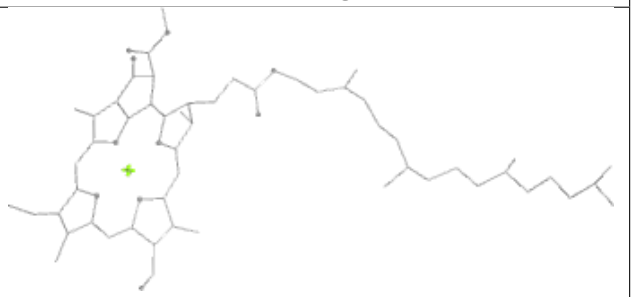
Bond lengths



Bond angles

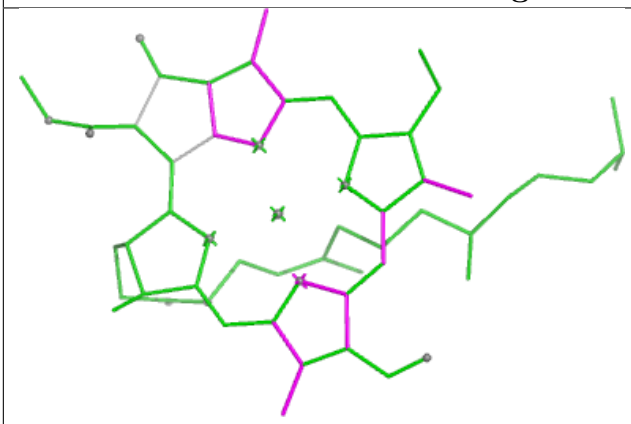


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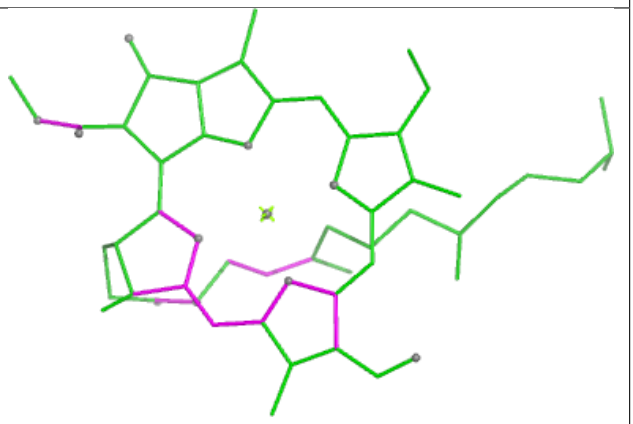


Rings

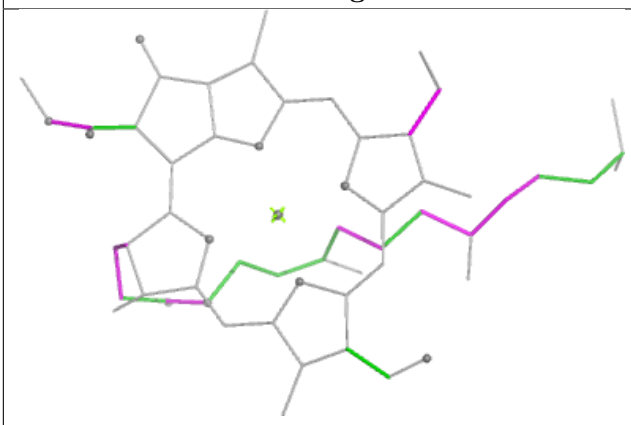
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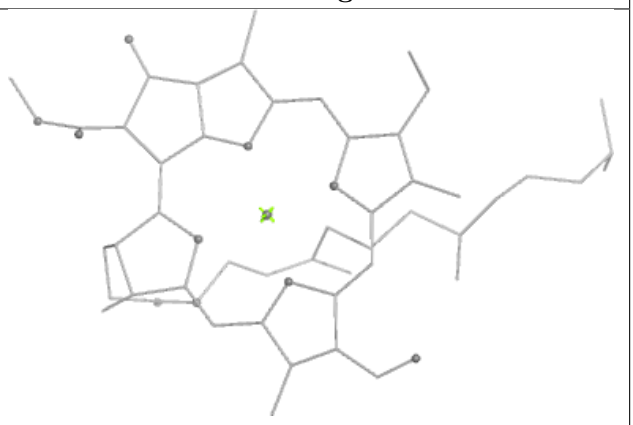
Bond lengths



Bond angles

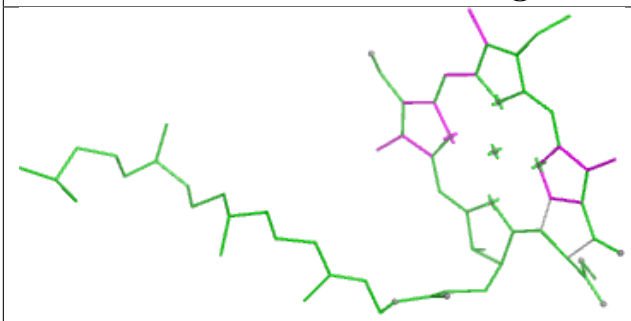


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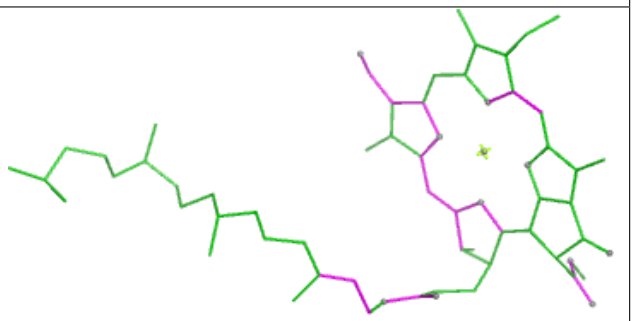


Rings

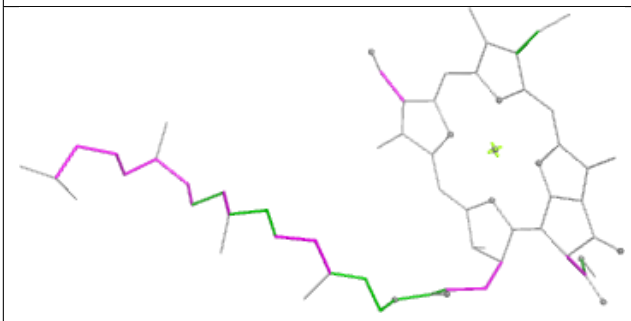
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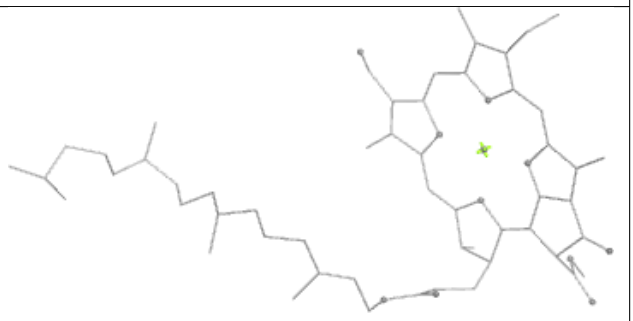
Bond lengths



Bond angles

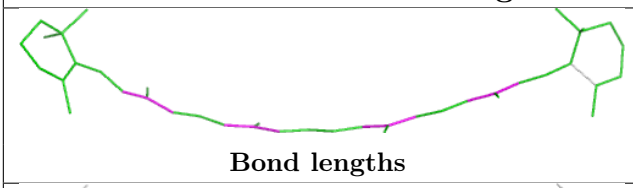


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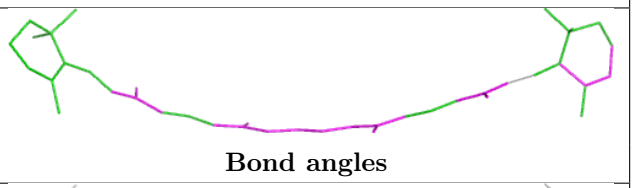


Rings

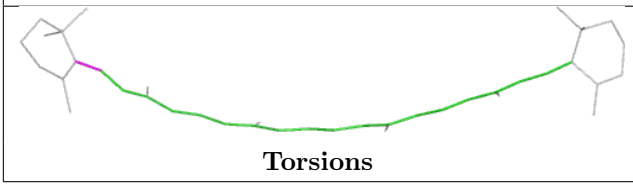
Ligand A1JPJ bI 4018



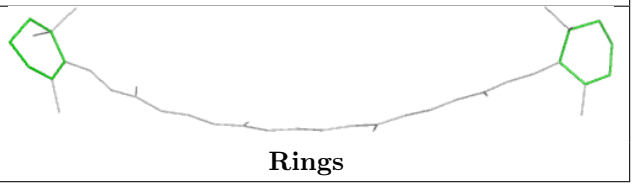
Bond lengths



Bond angles

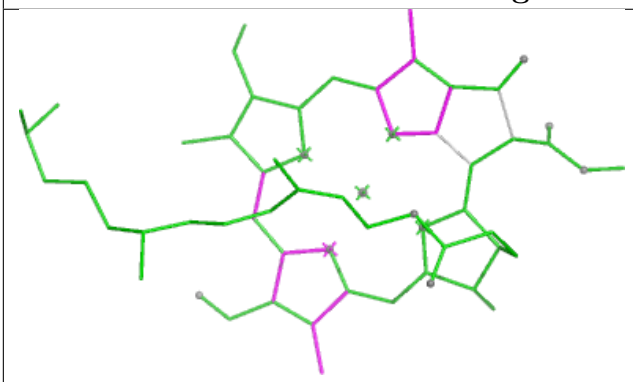


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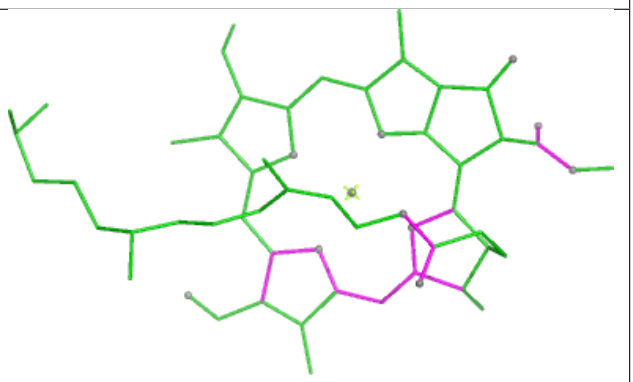


Rings

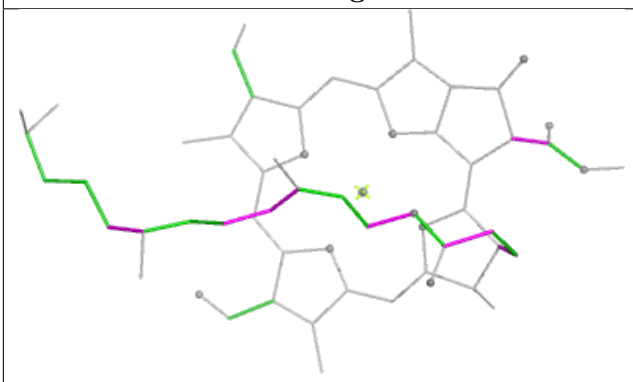
Ligand CL7 cB 1235



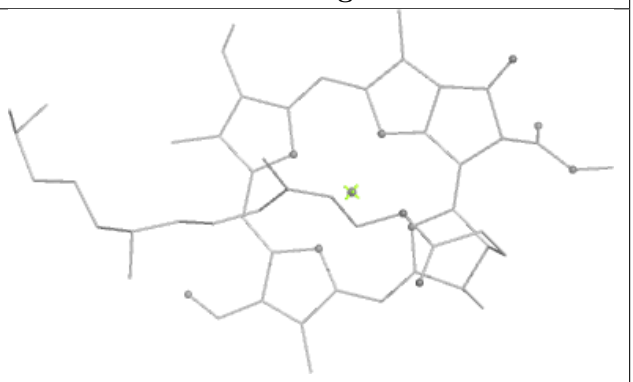
Bond lengths



Bond angles

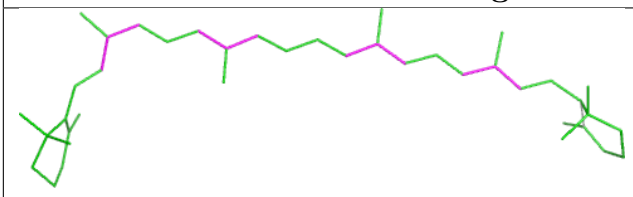


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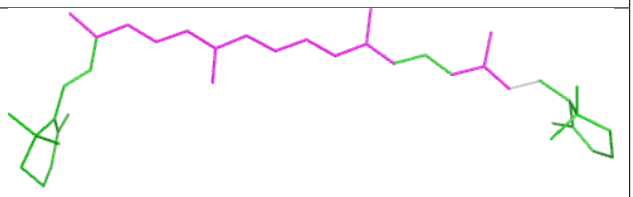


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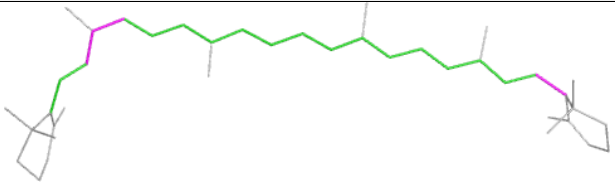
Ligand A1JPJ bL 4020



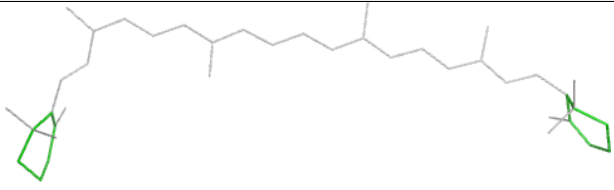
Bond lengths



Bond angles

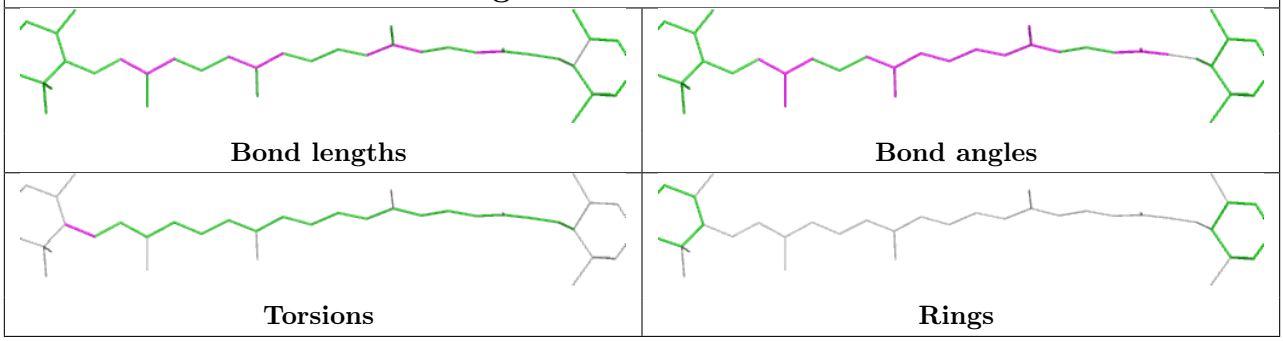


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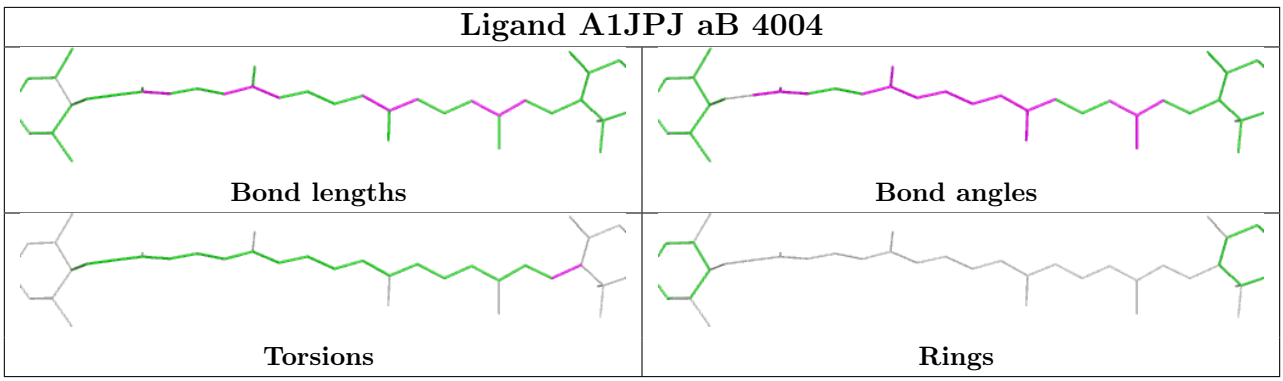


Rings

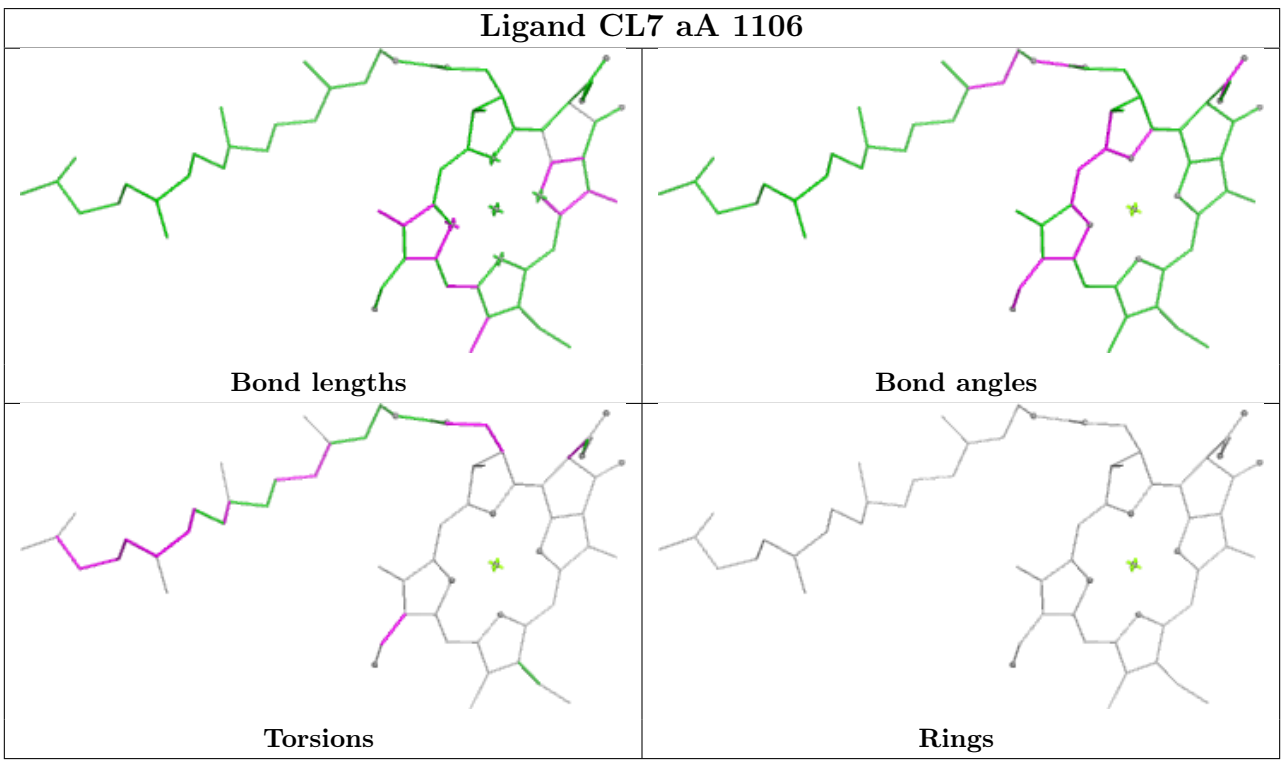
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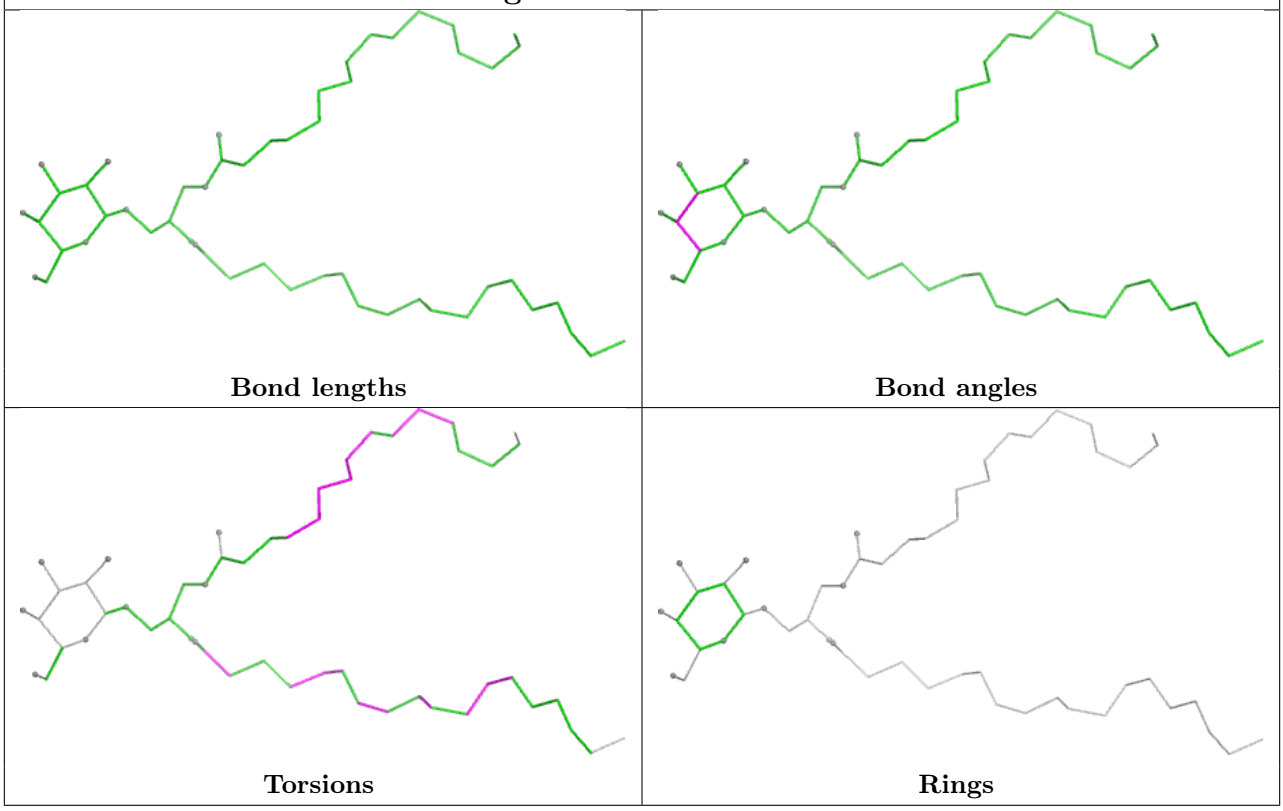
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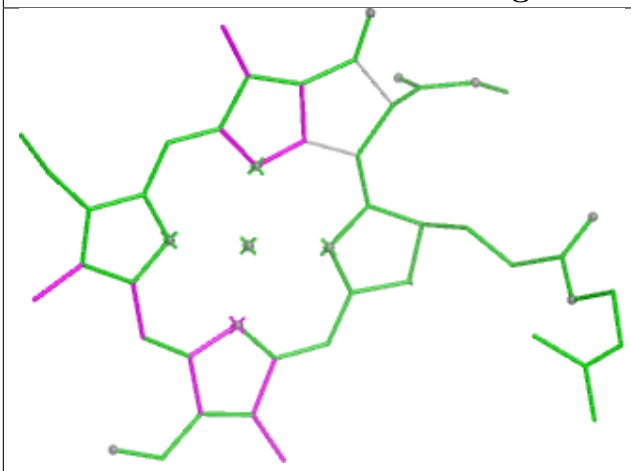
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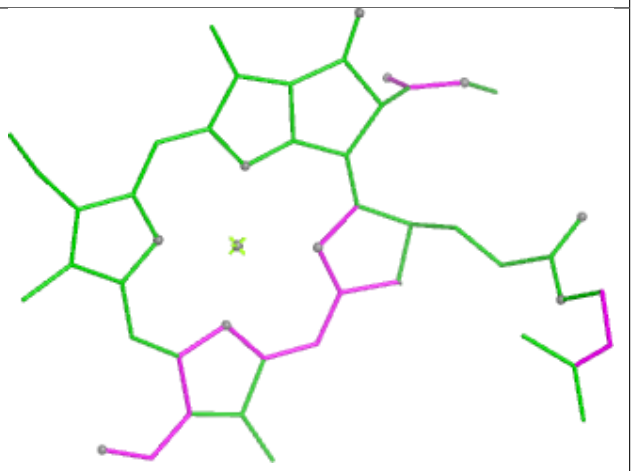
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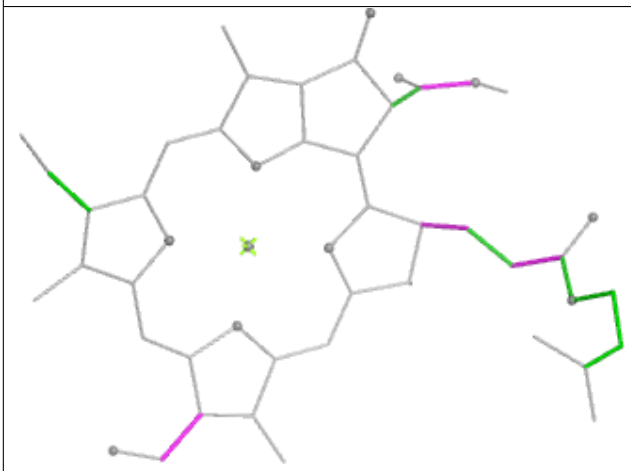
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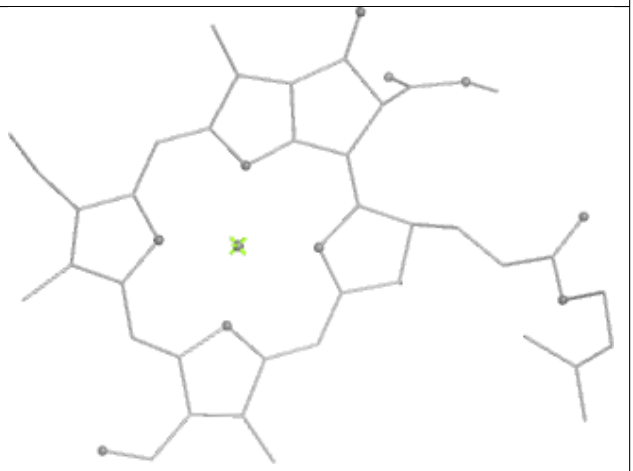
Bond lengths



Bond angles

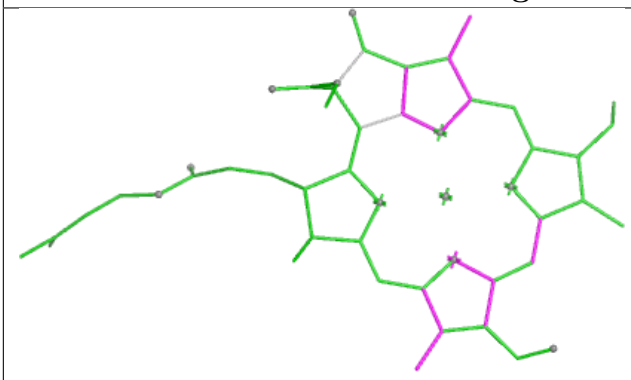


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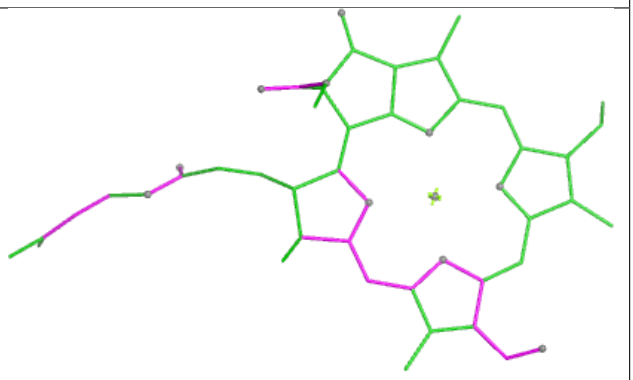


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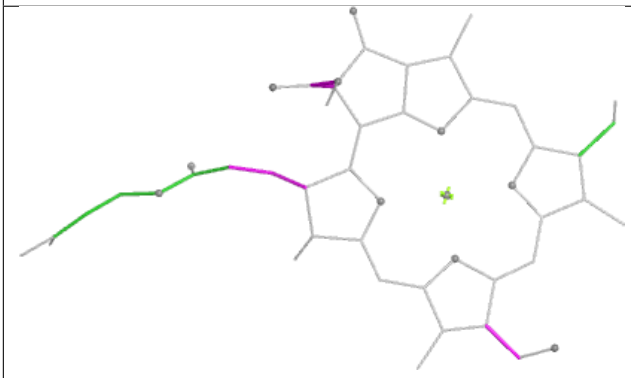
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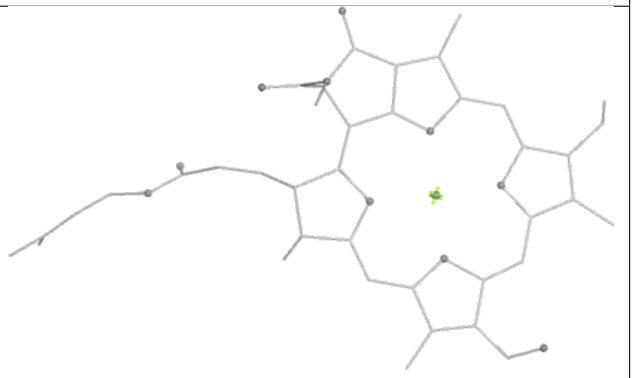
Bond lengths



Bond angles

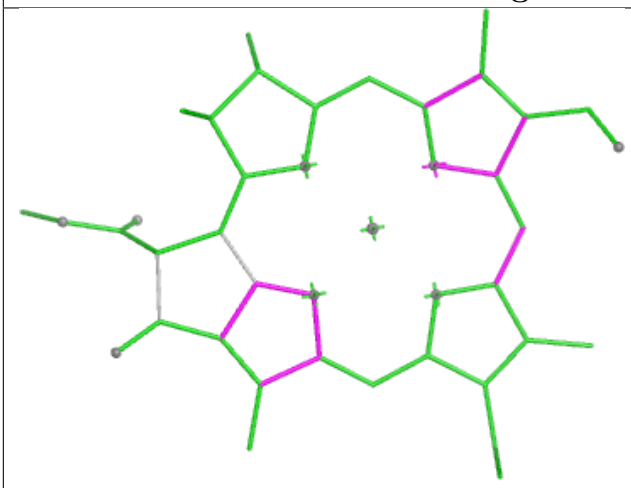


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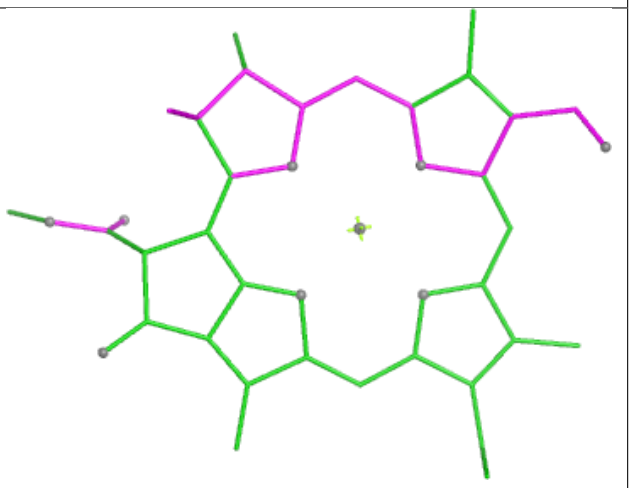


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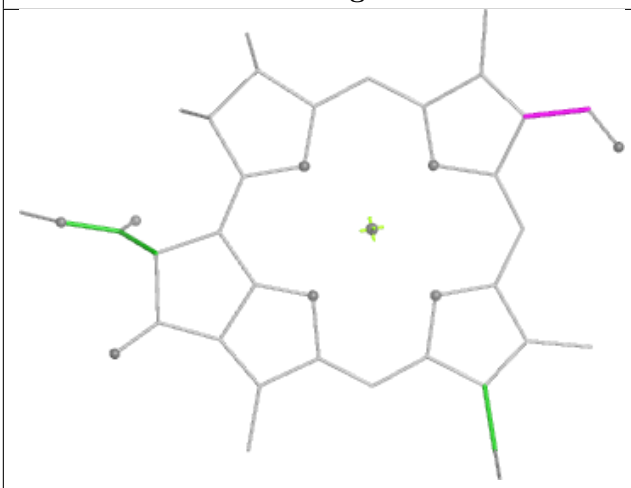
Ligand CL7 aB 1233



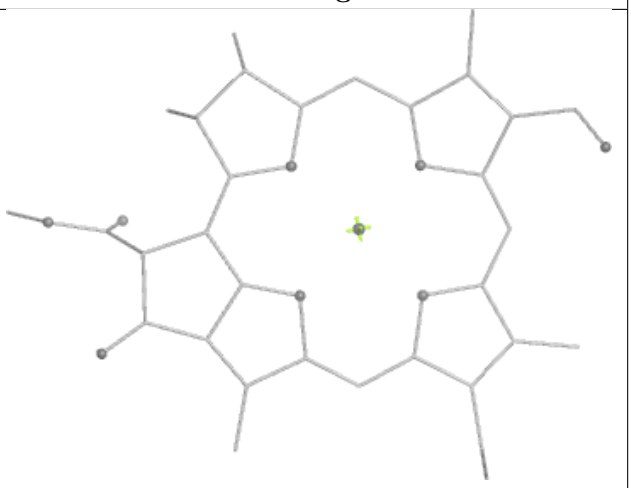
Bond lengths



Bond angles

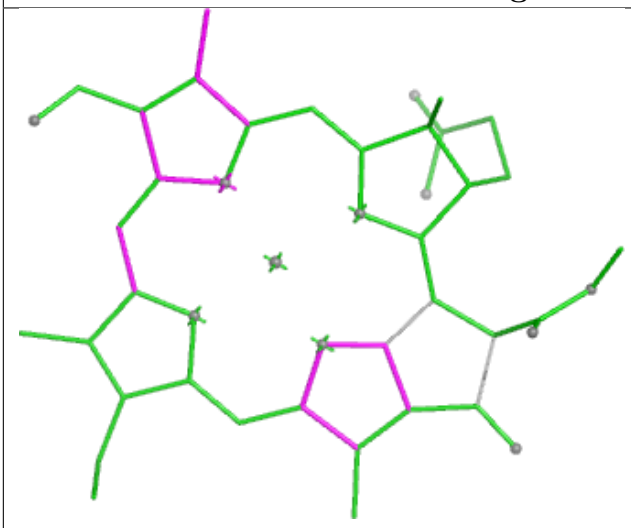


Torsions



Rings

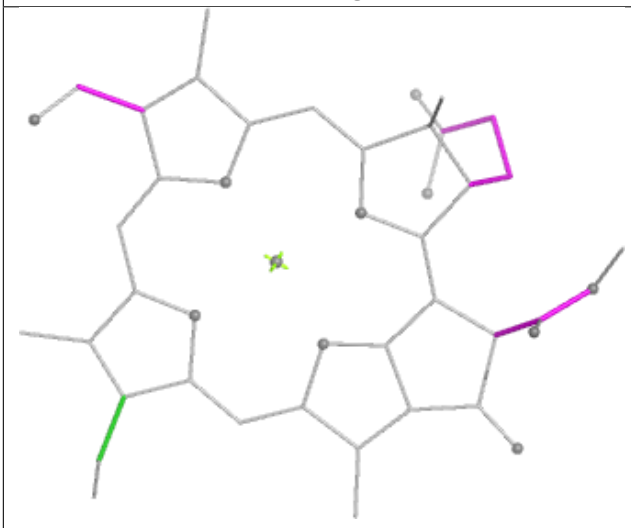
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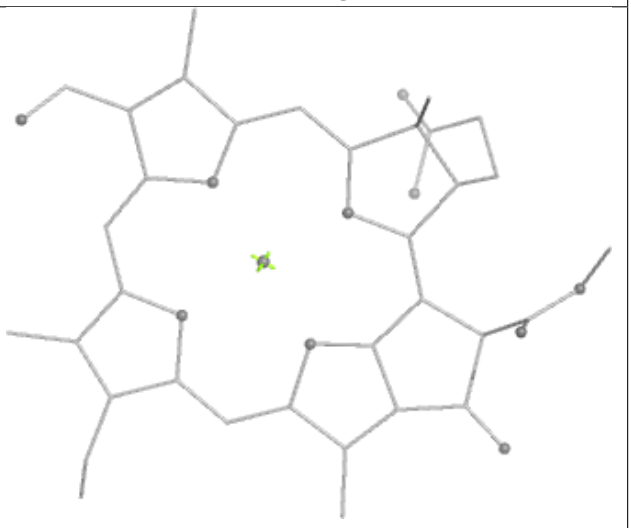
Bond lengths



Bond angles

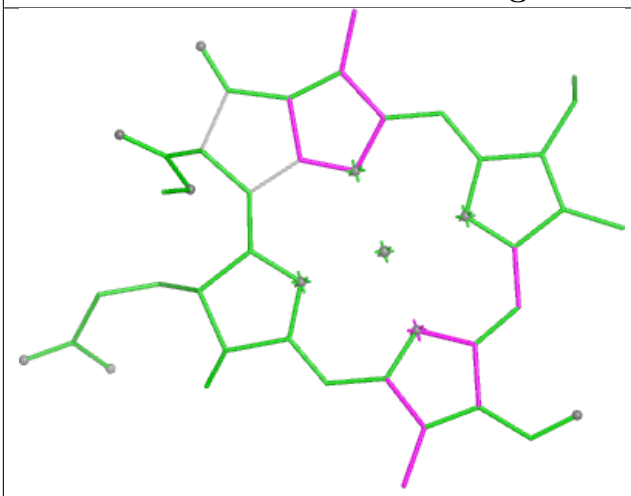


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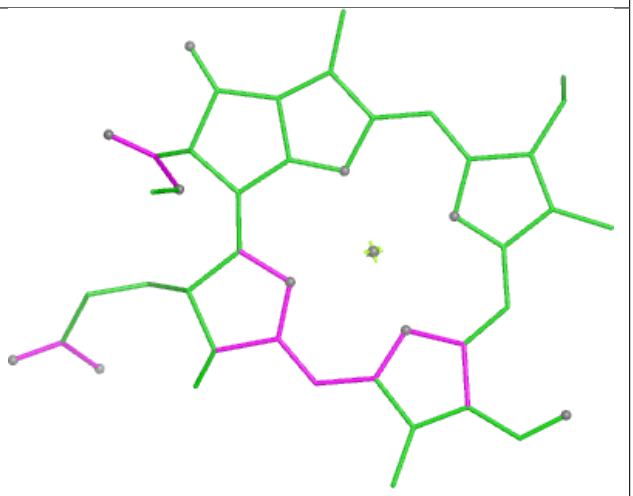


Rings

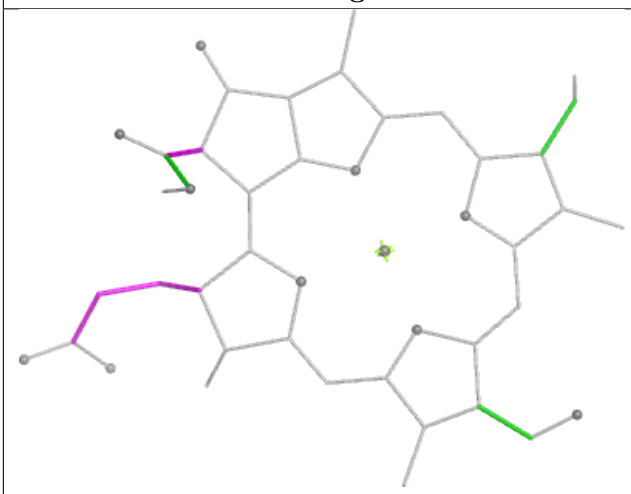
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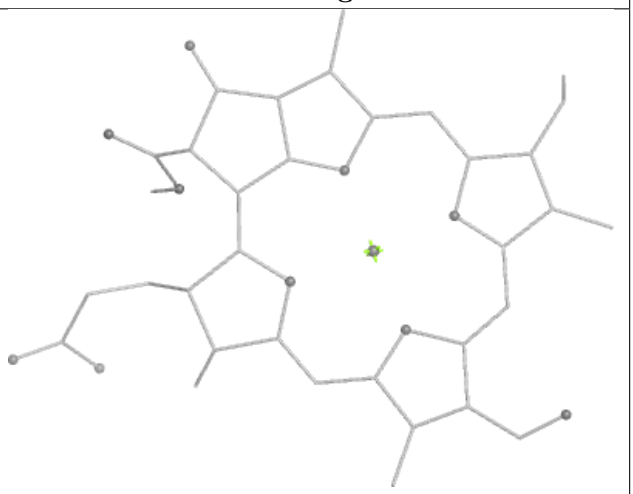
Bond lengths



Bond angles

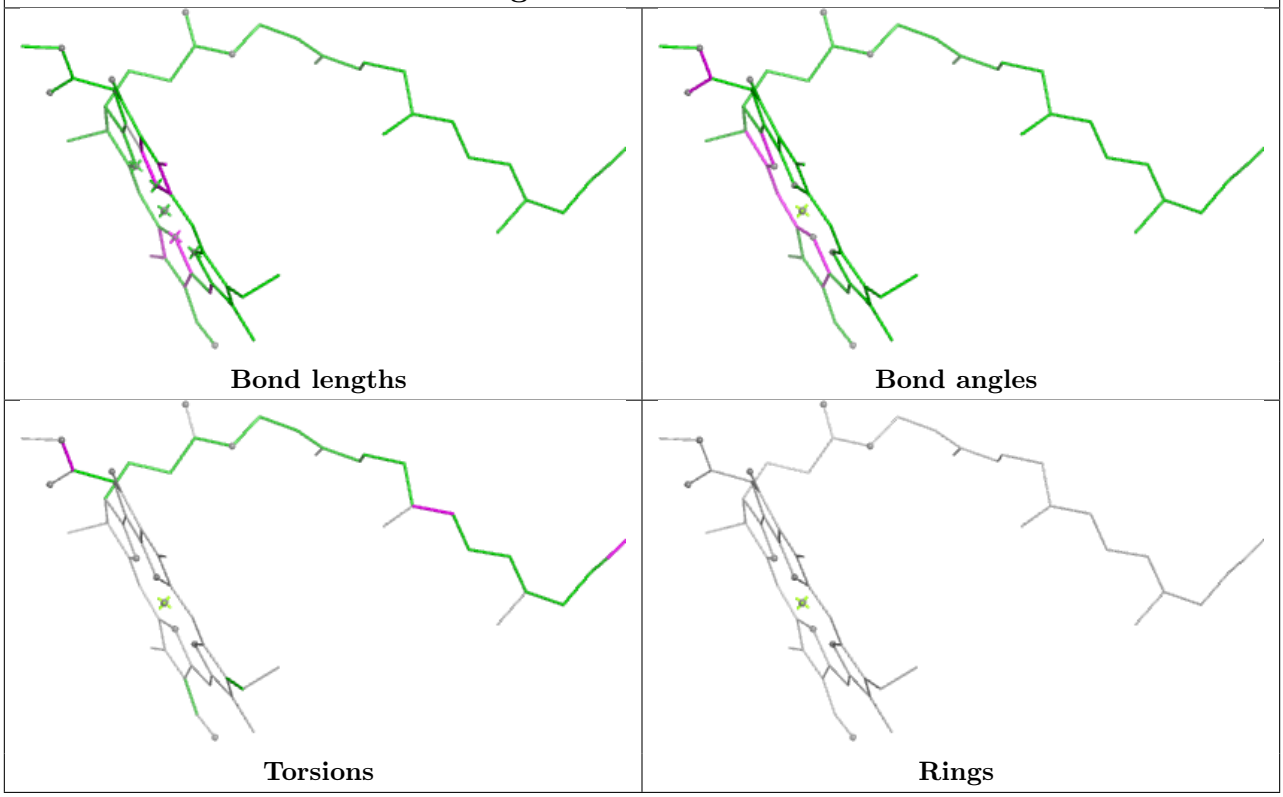


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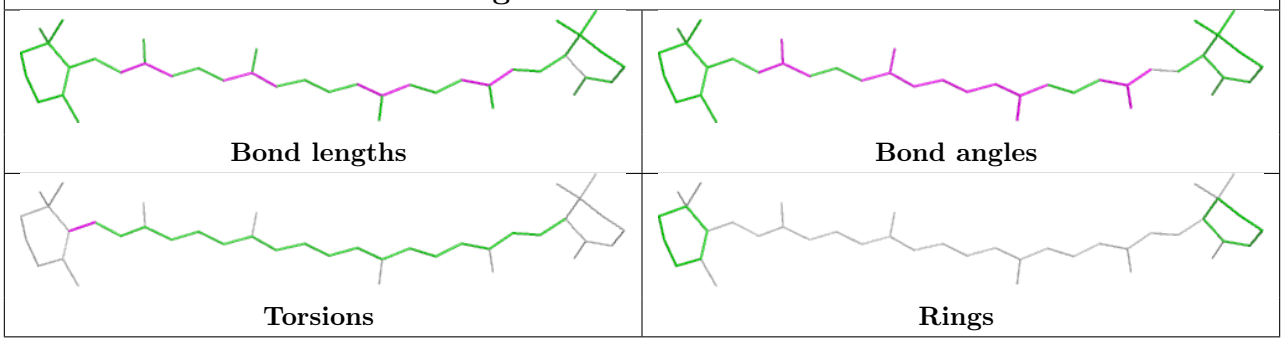


Rings

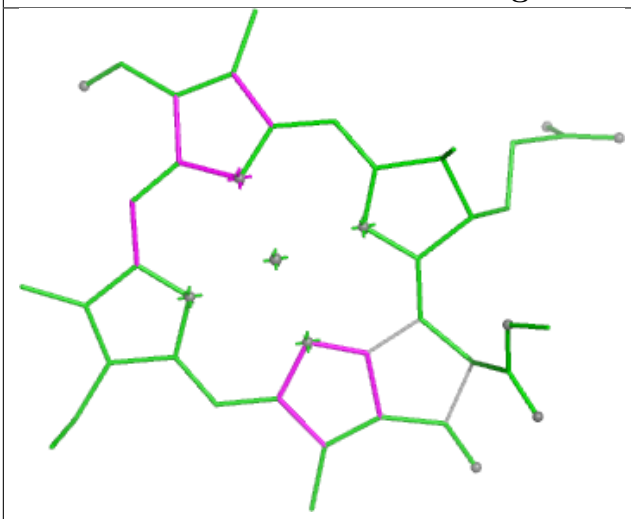
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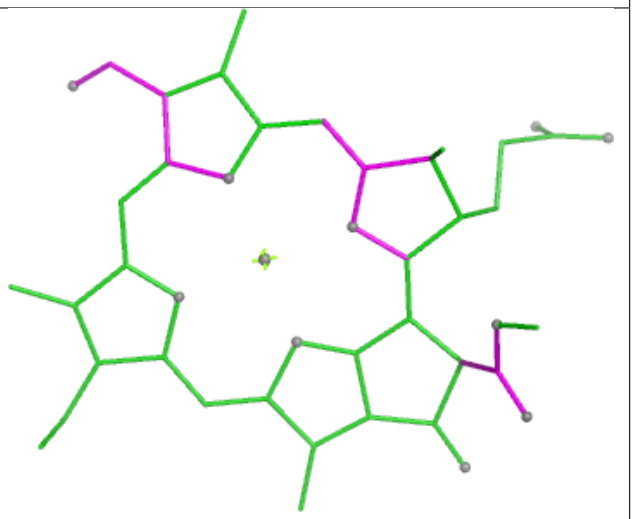
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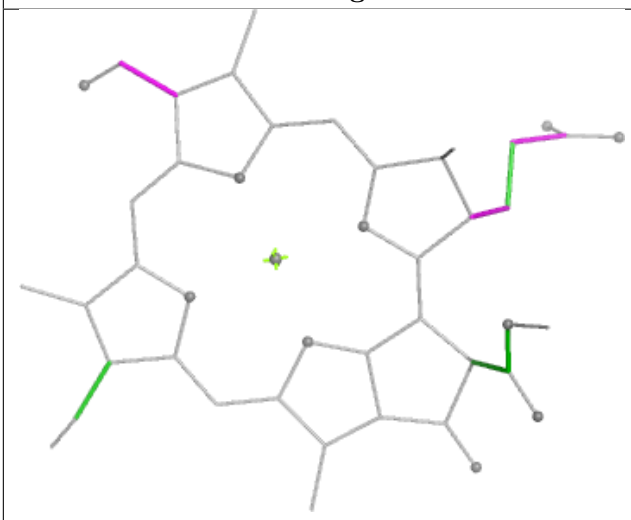
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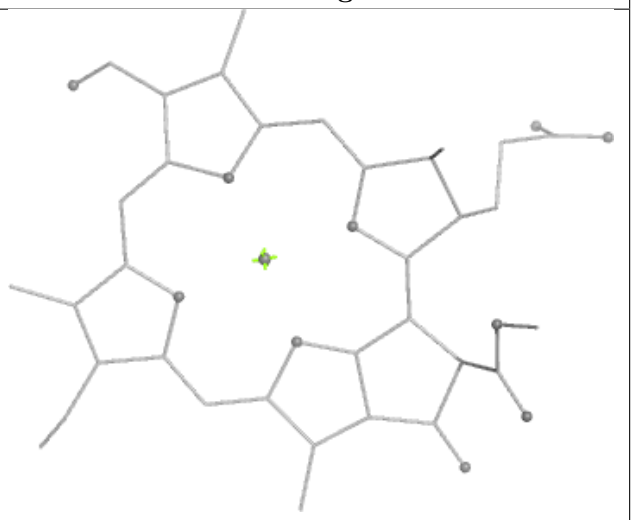
Bond lengths



Bond angles

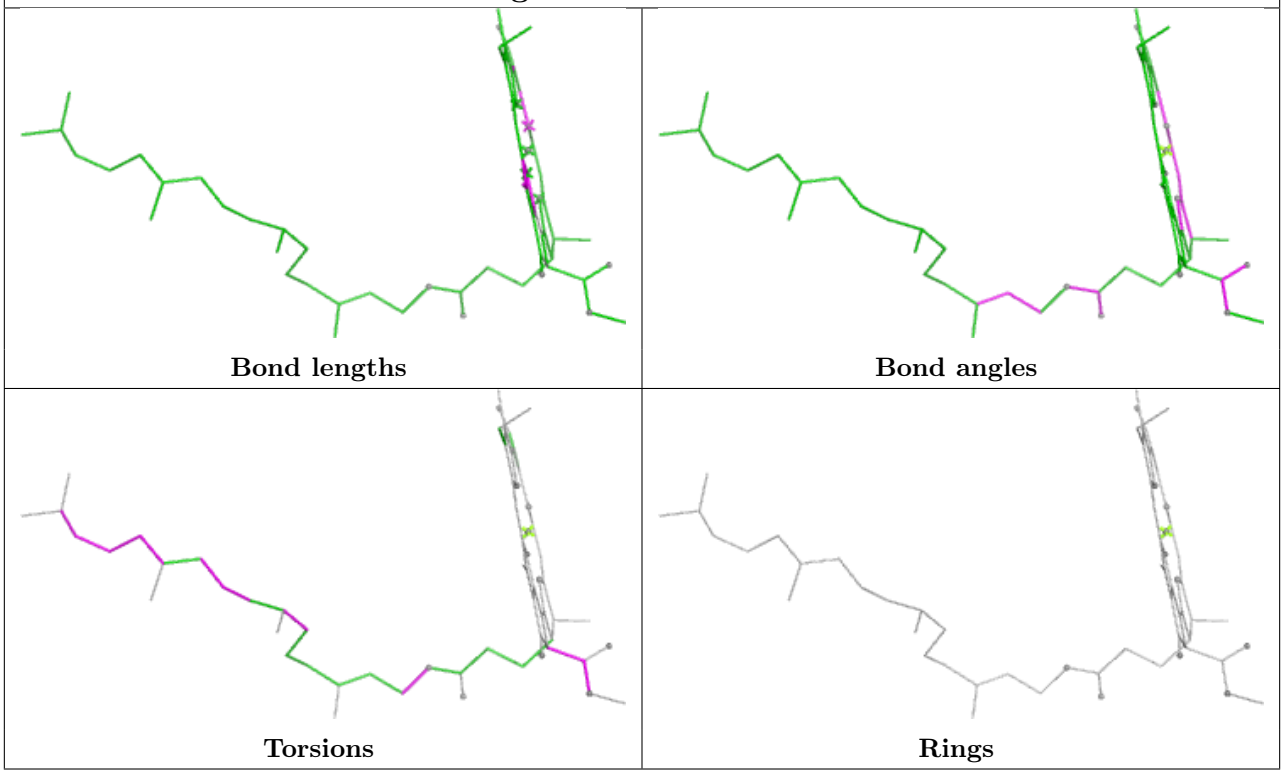


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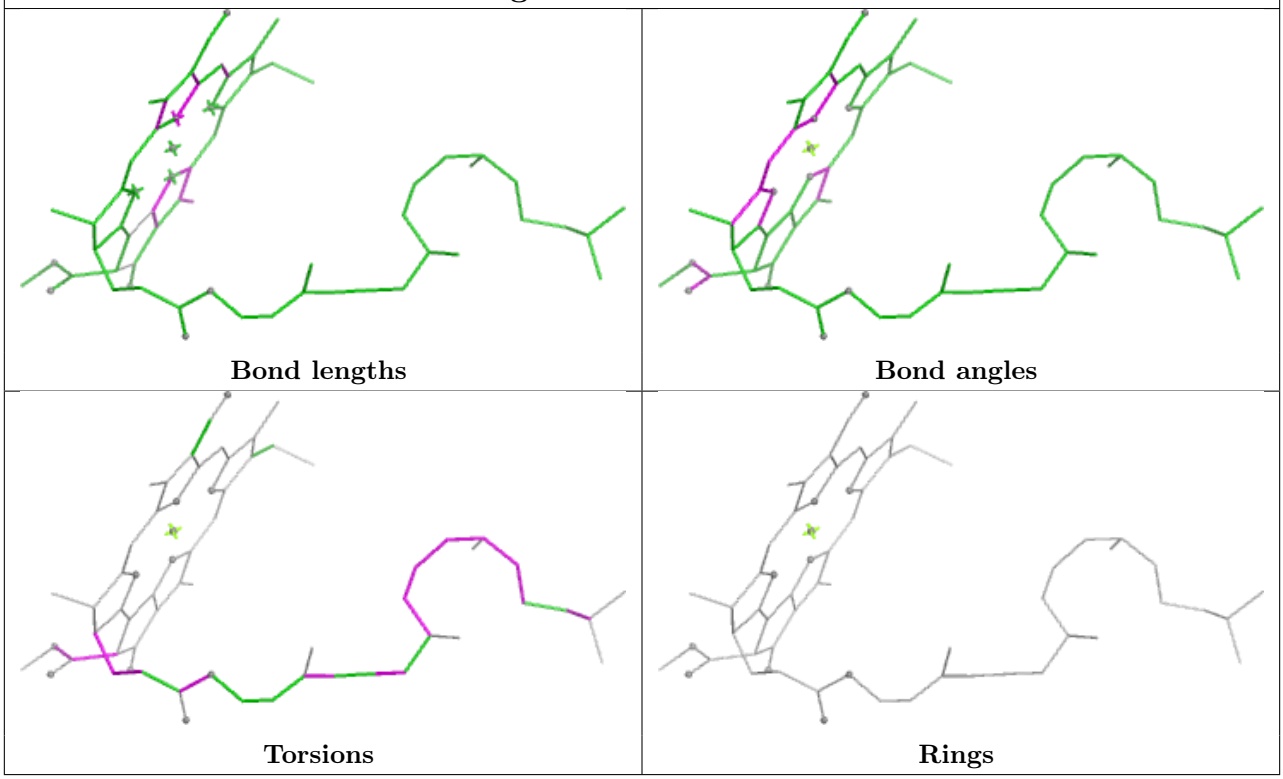


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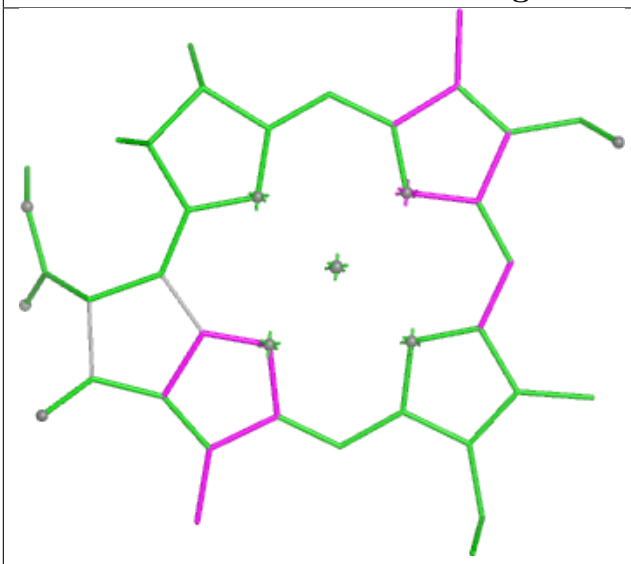
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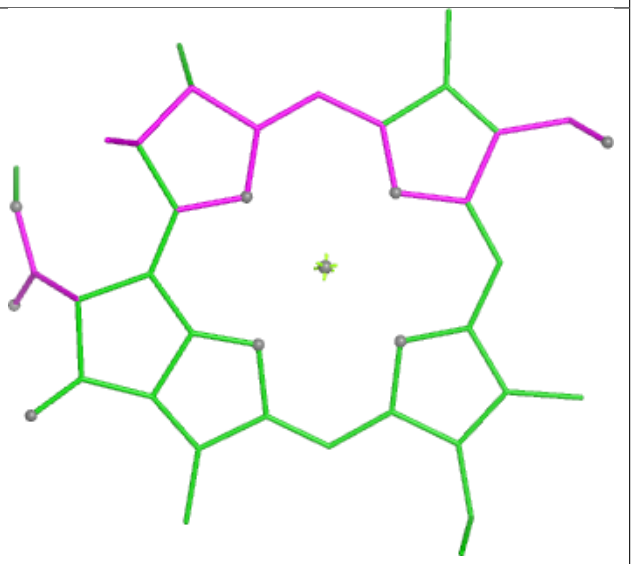
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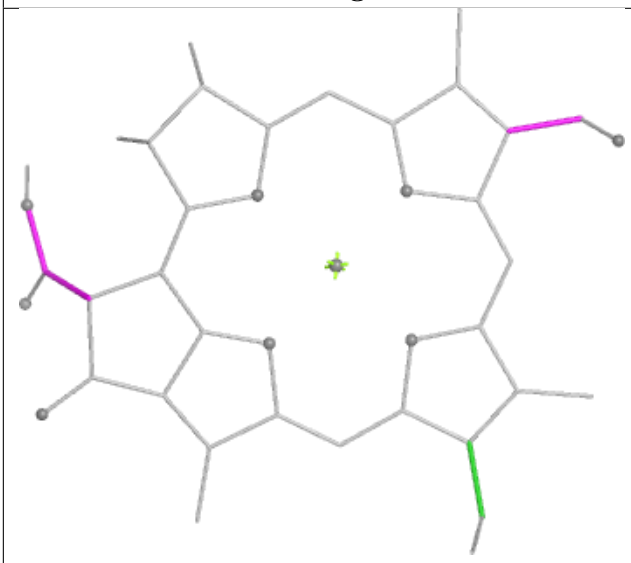
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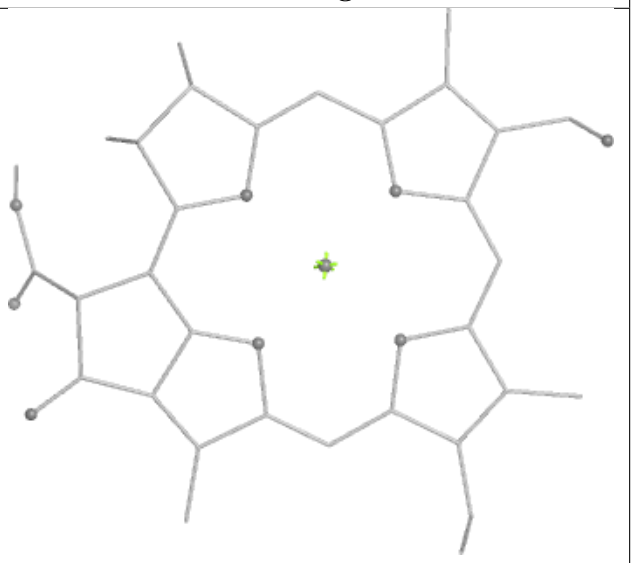
Bond lengths



Bond angles

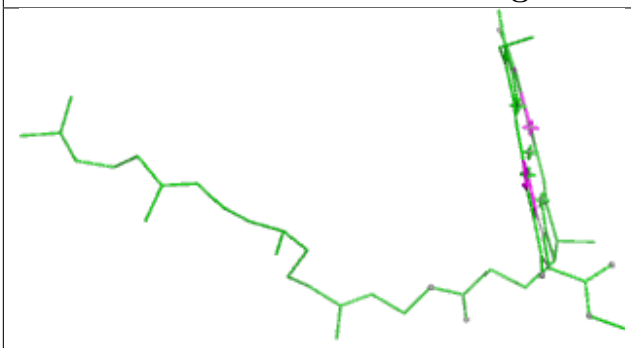


Torsions

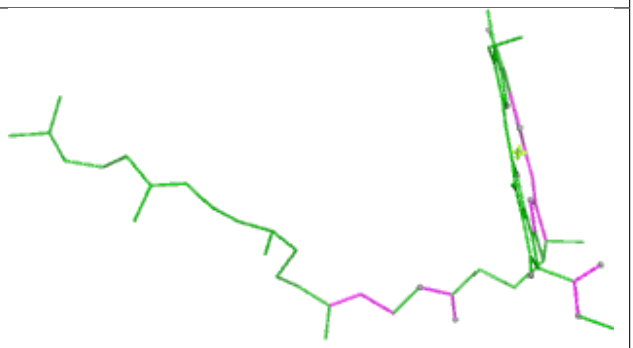


Rings

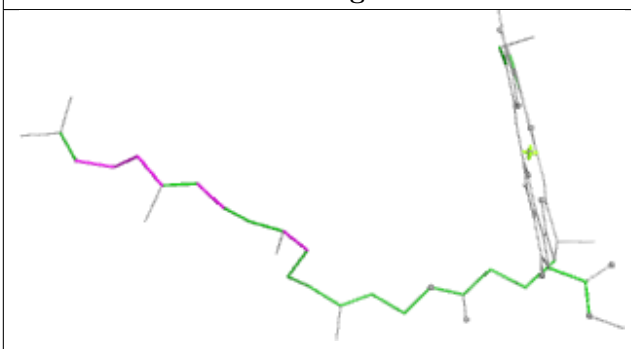
Ligand CL7 aB 1239



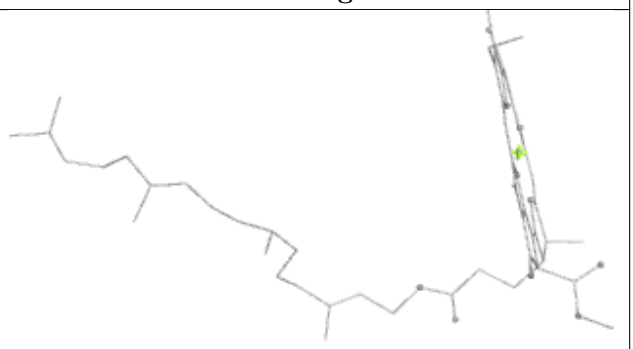
Bond lengths



Bond angles

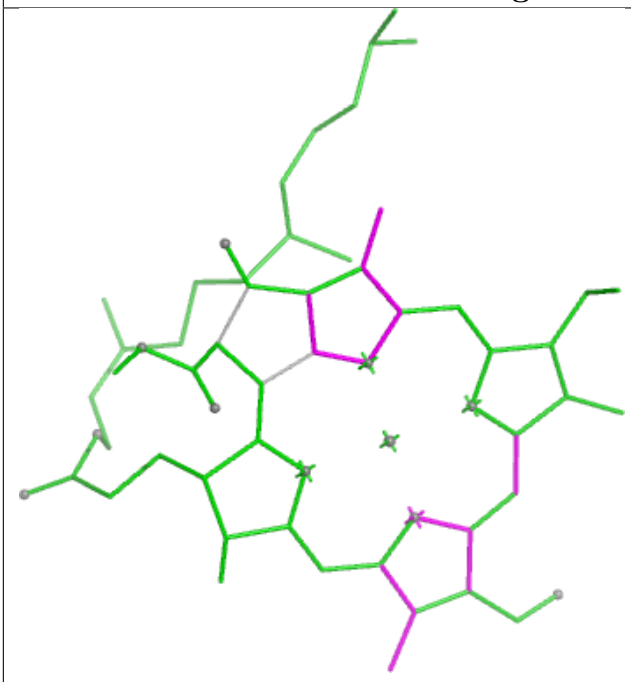


Torsions

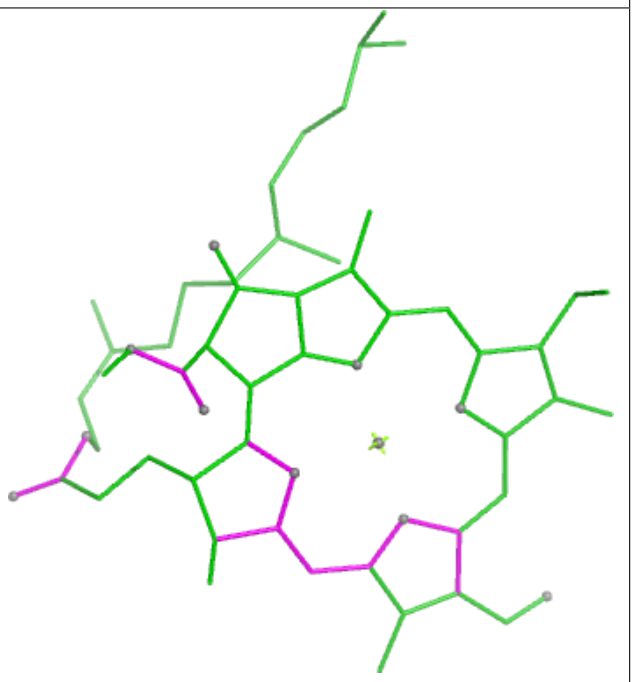


Rings

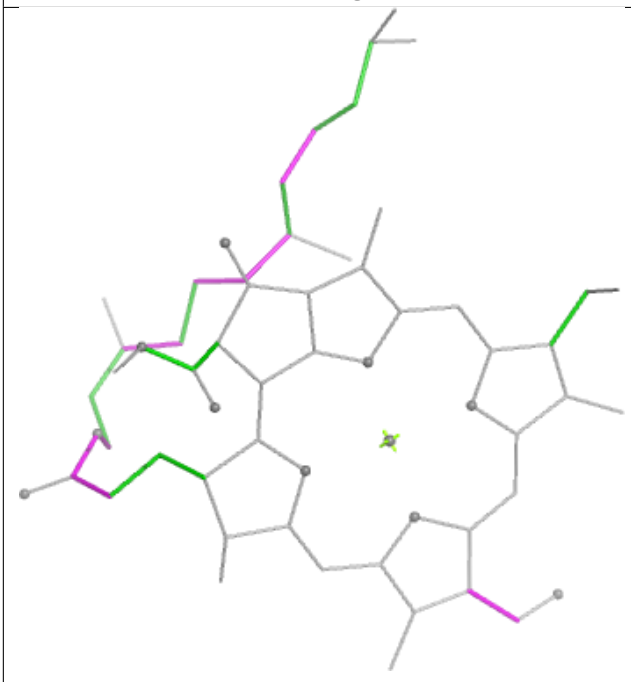
Ligand CL7 bL 1503



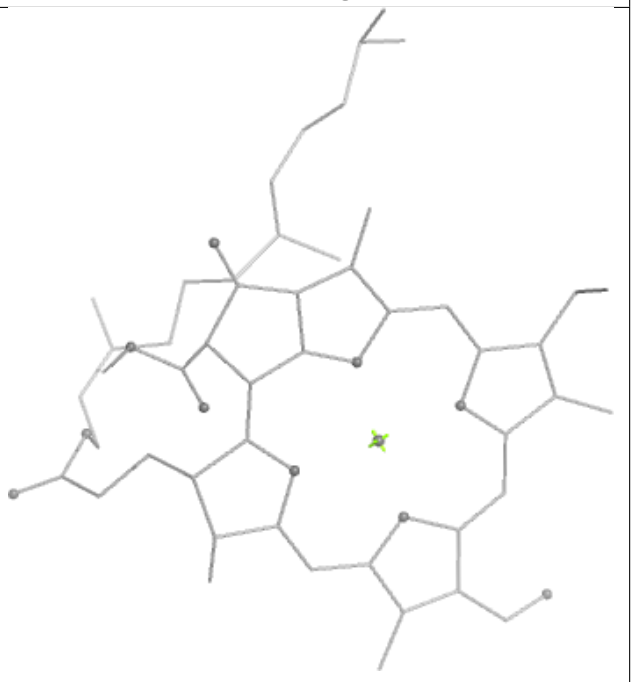
Bond lengths



Bond angles

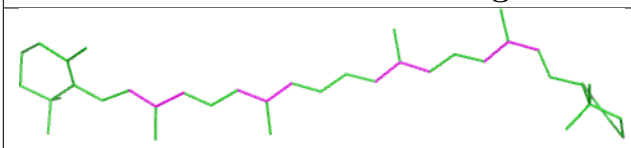


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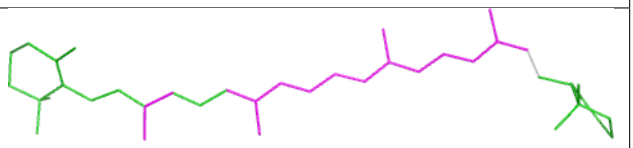


Rings

Ligand A1JPJ cB 4017



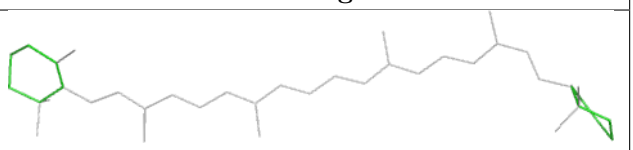
Bond lengths



Bond angles

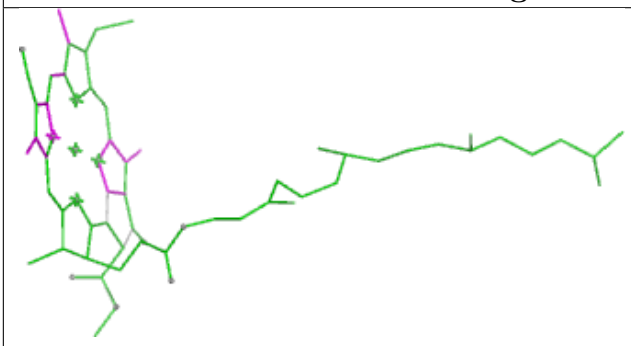


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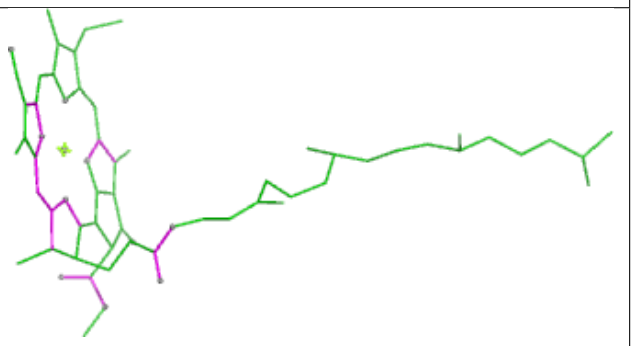


Rings

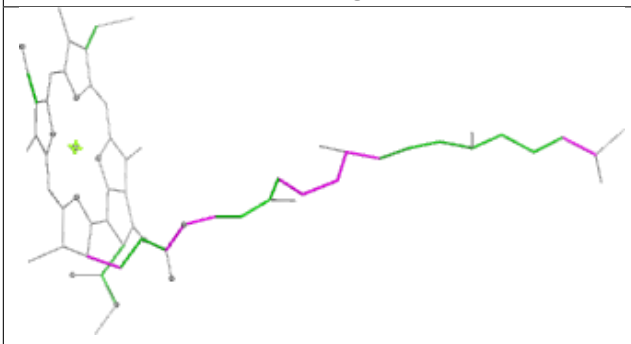
Ligand CL7 bB 1225



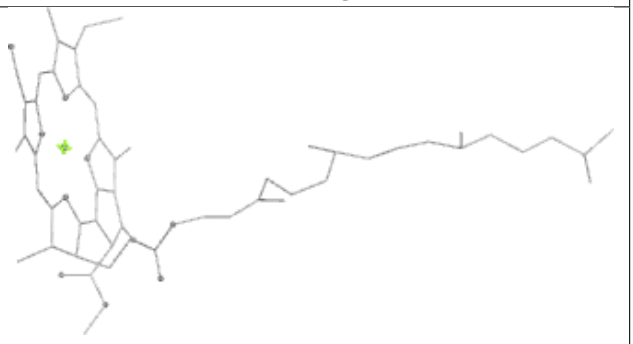
Bond lengths



Bond angles

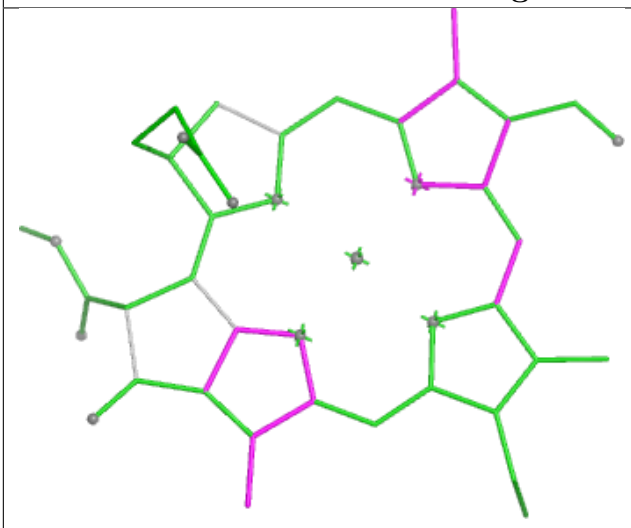


Torsions

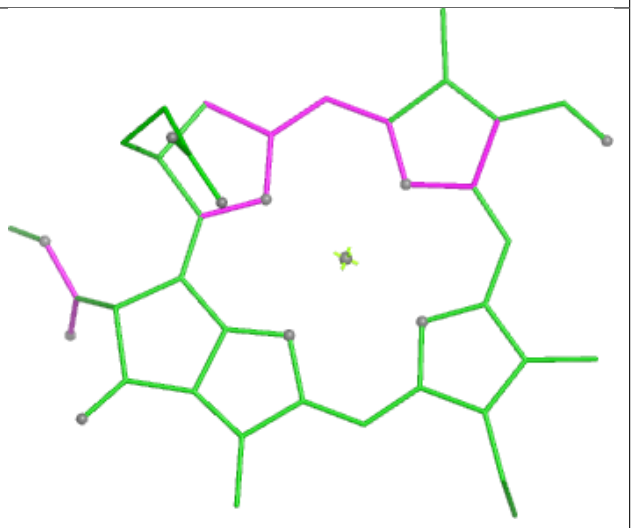


Rings

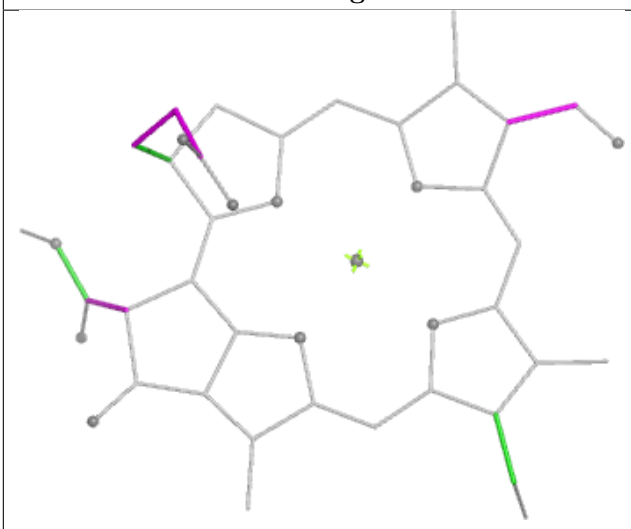
Ligand CL7 cA 1134



Bond lengths



Bond angles

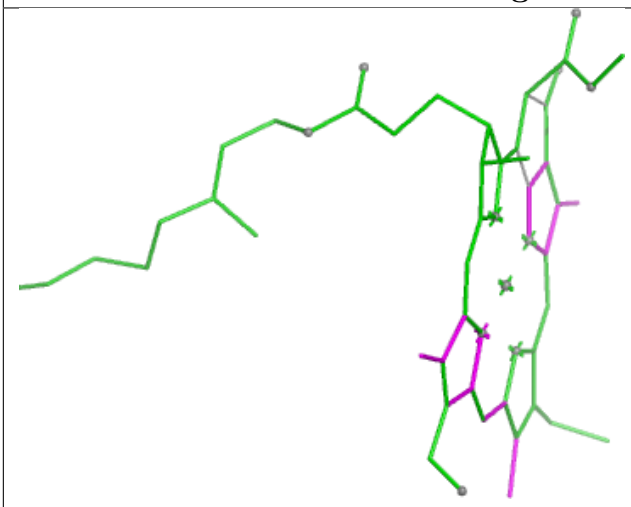


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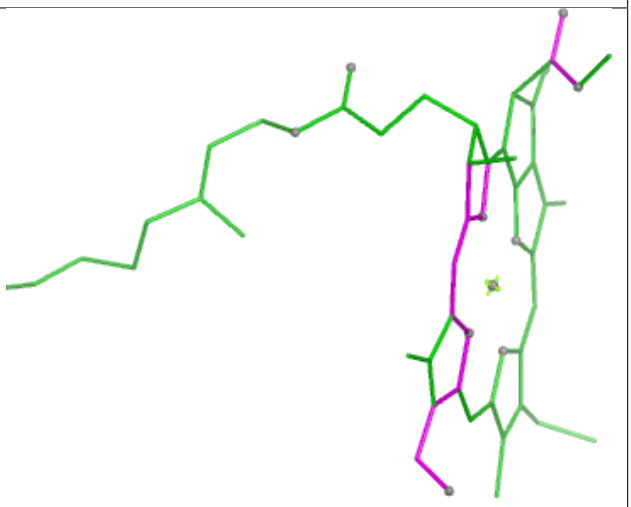


Rings

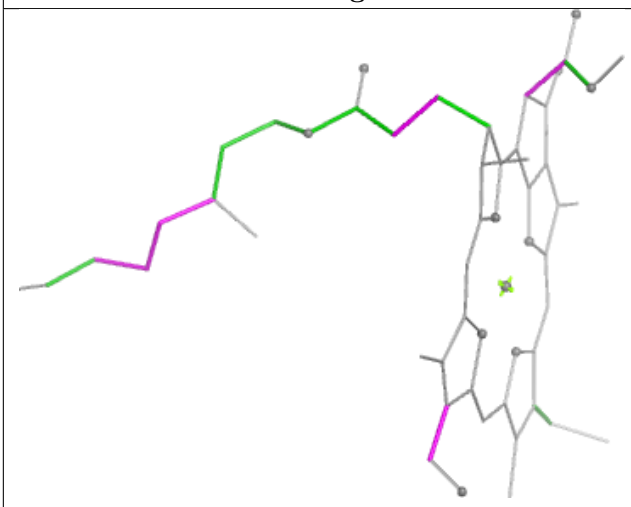
Ligand CL7 aB 1201



Bond lengths



Bond angles

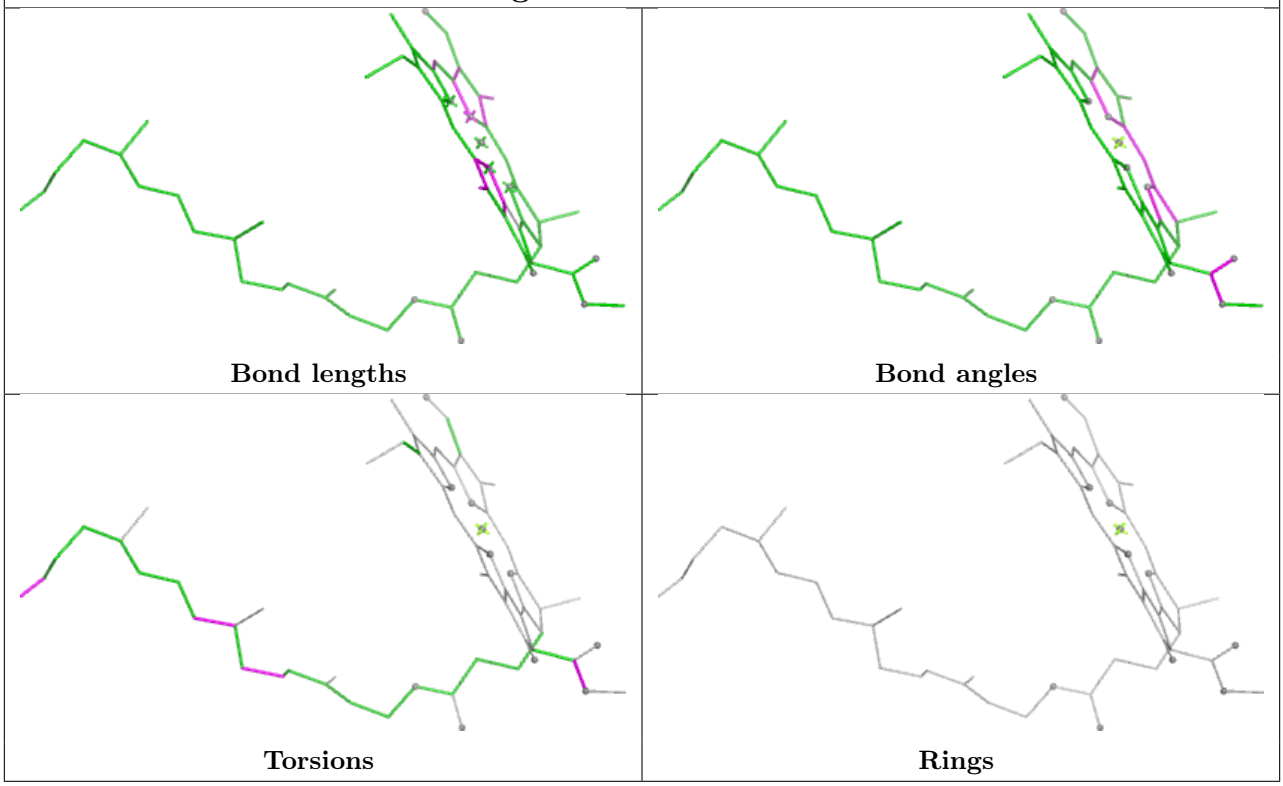


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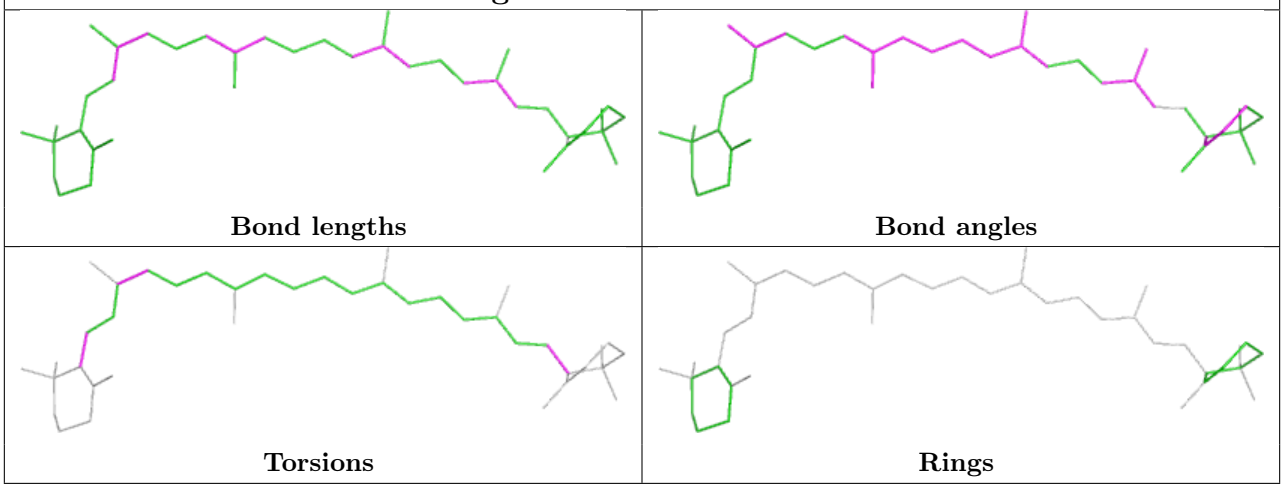


Rings

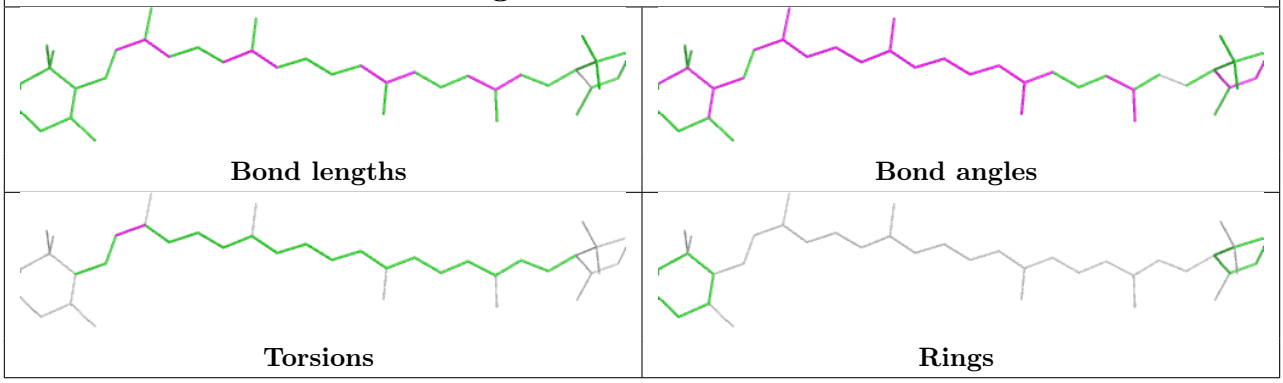
Ligand CL7 aA 1128



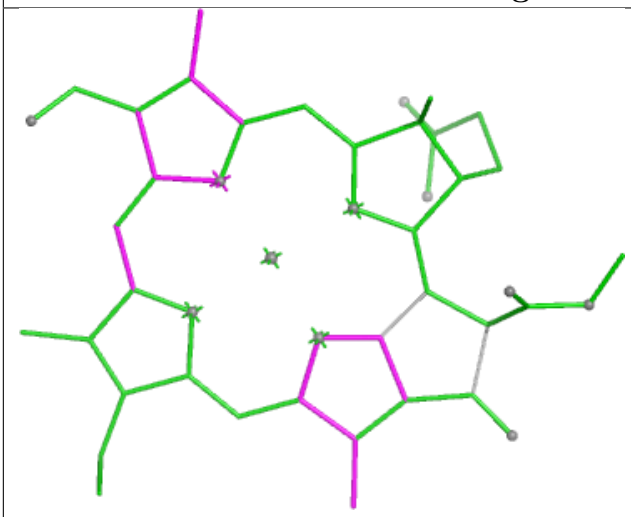
Ligand A1JPJ aB 4005



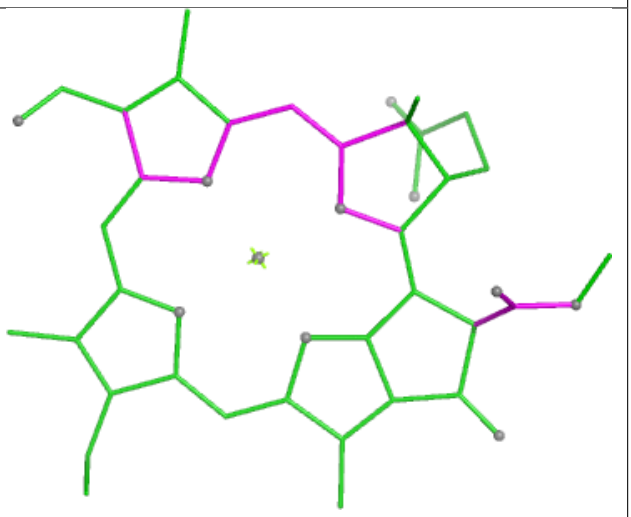
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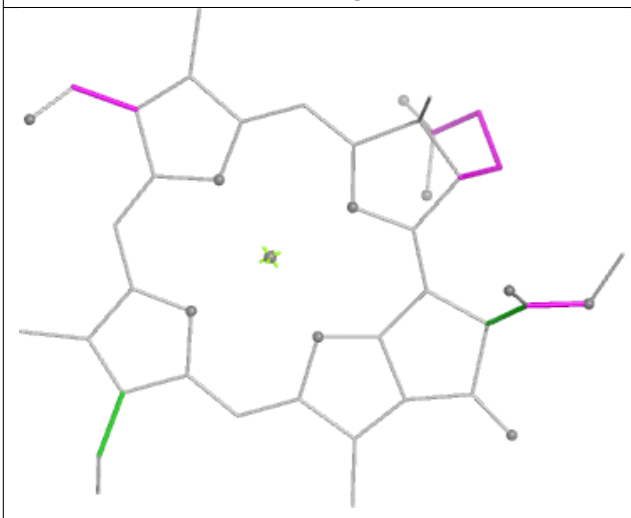
Ligand CL7 cB 1220



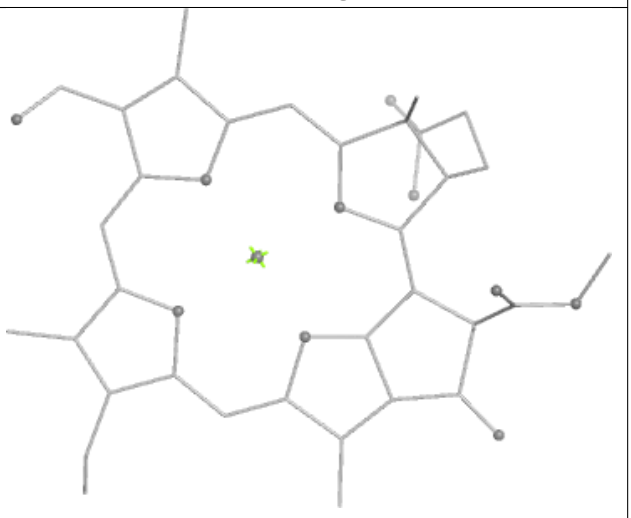
Bond lengths



Bond angles

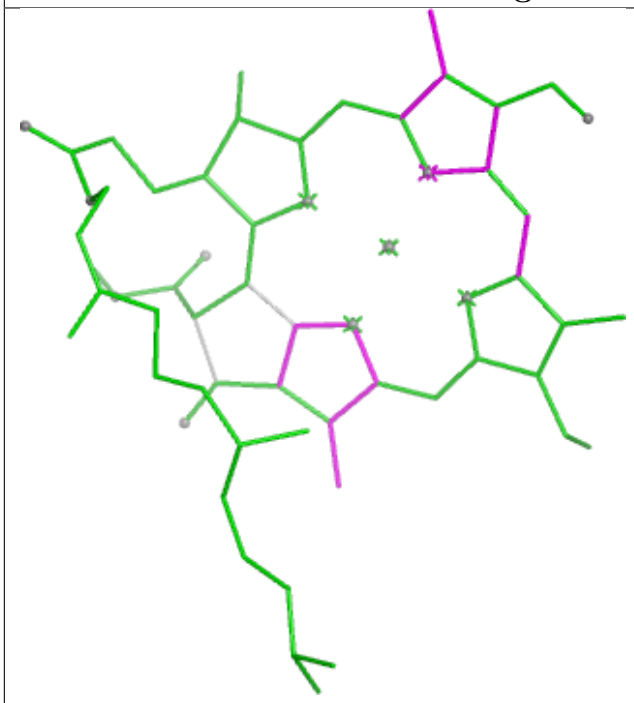


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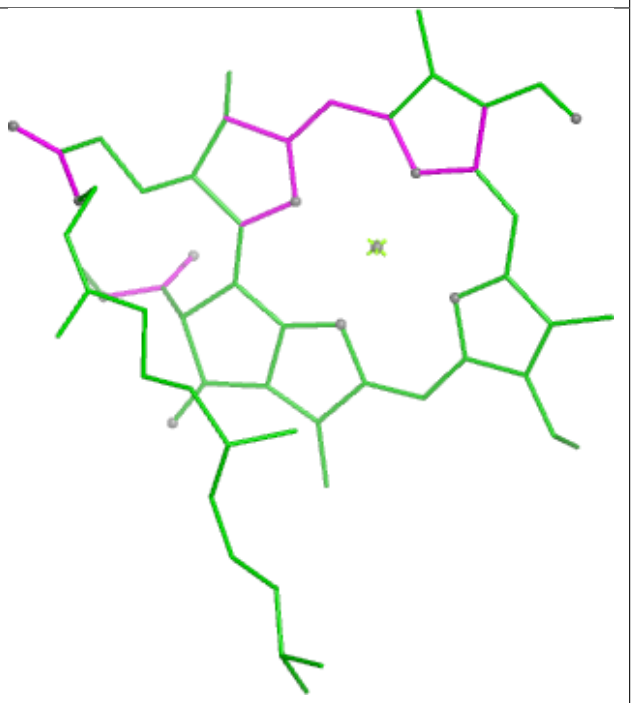


Rings

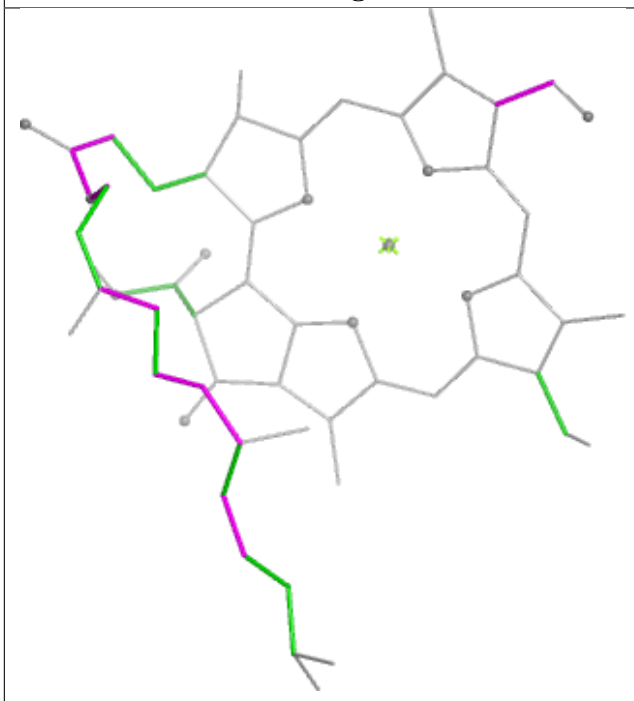
Ligand CL7 aL 1503



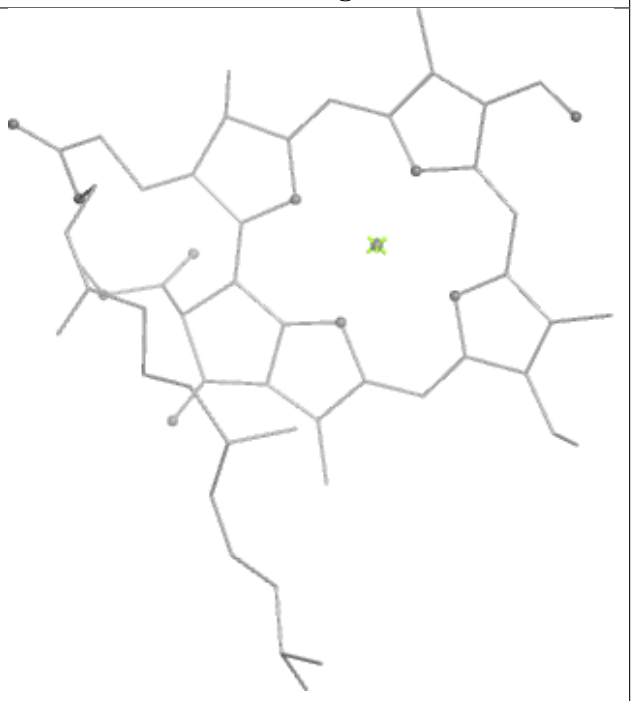
Bond lengths



Bond angles

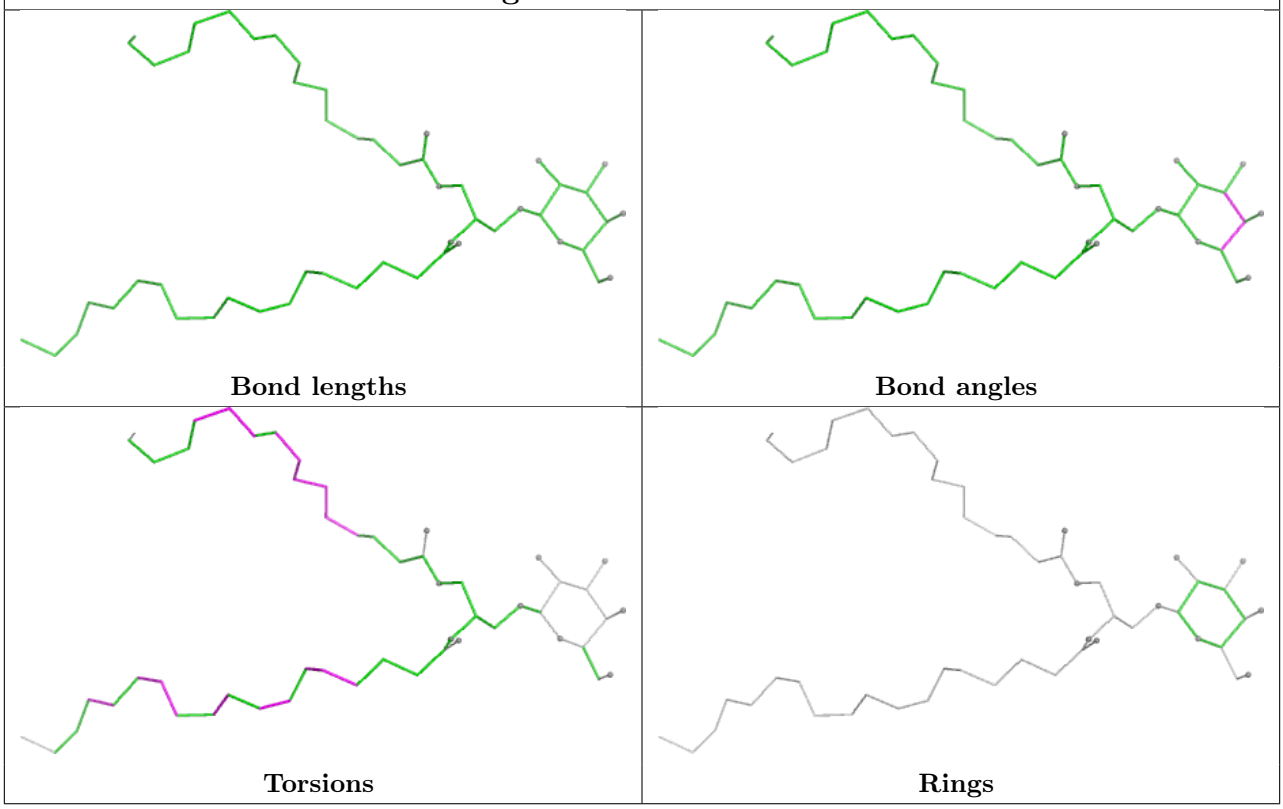


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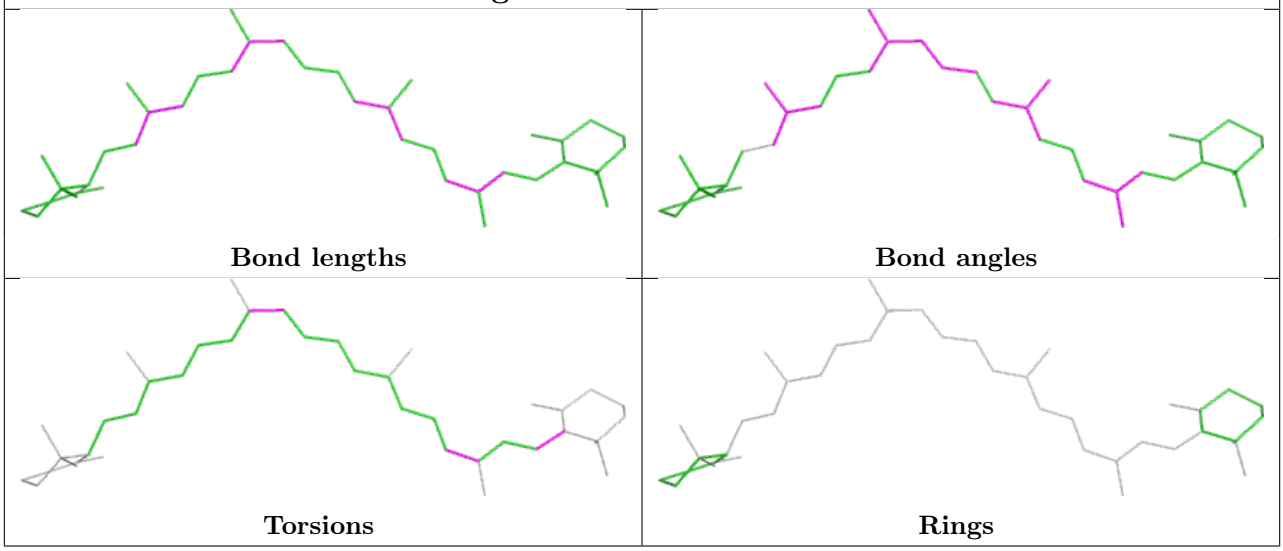


Rings

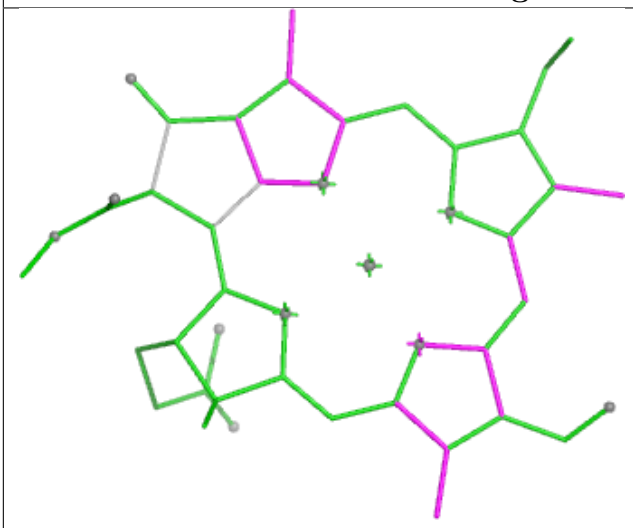
Ligand LMG bB 5002



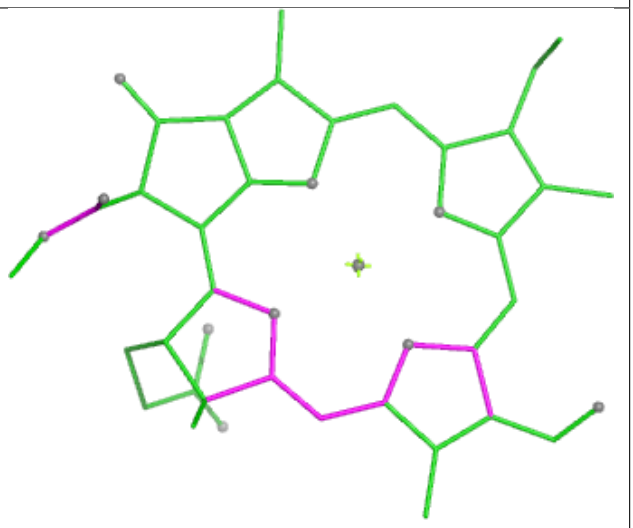
Ligand A1JPJ cA 4011



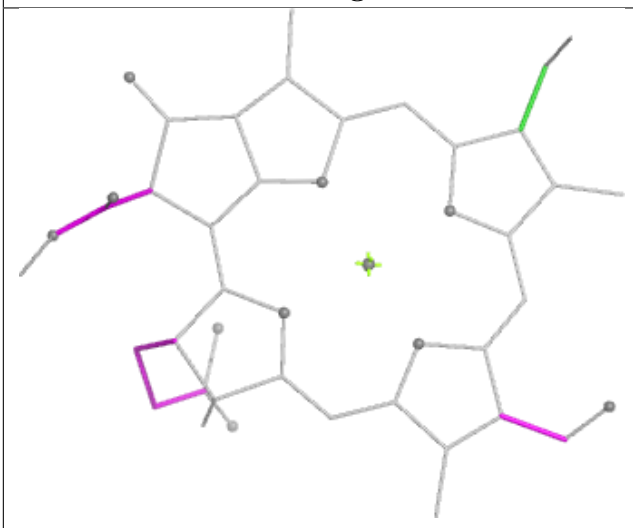
Ligand CL7 aB 1220



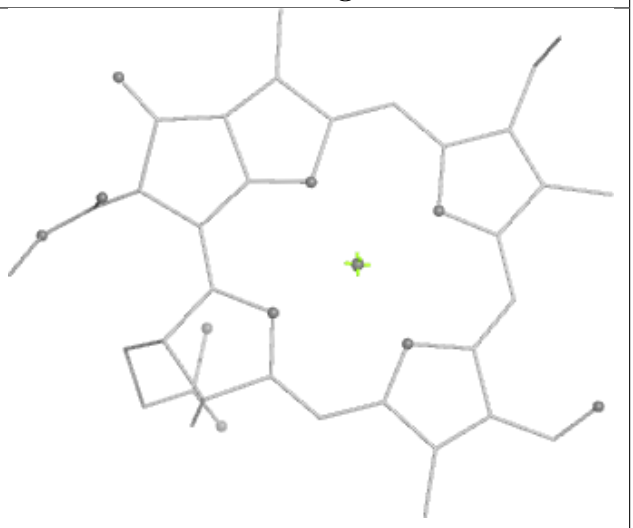
Bond lengths



Bond angles

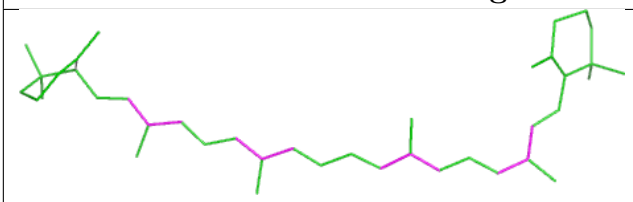


Torsions

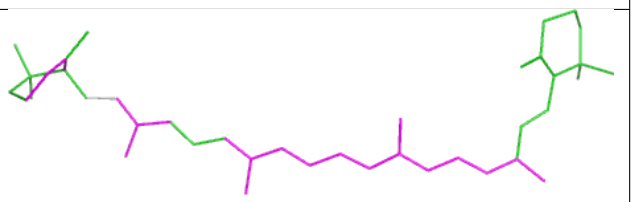


Rings

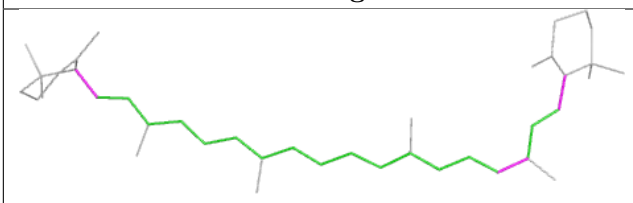
Ligand A1JPJ bB 4005



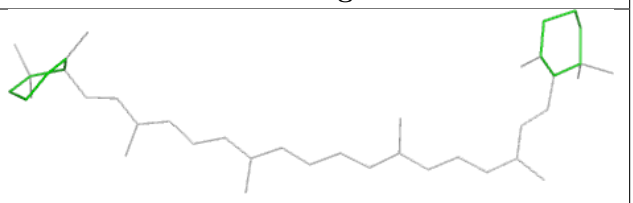
Bond lengths



Bond angles

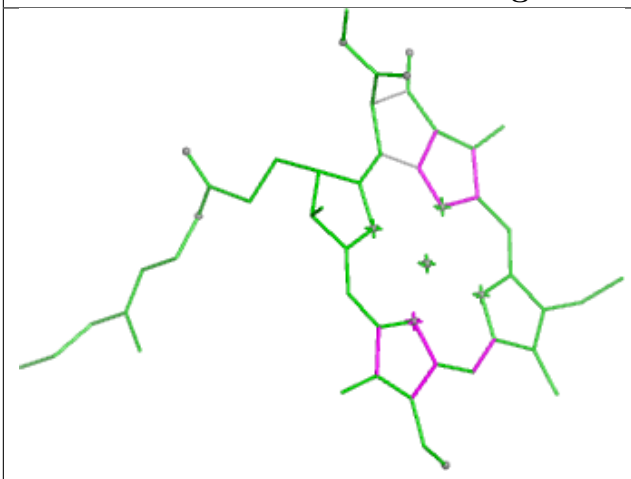


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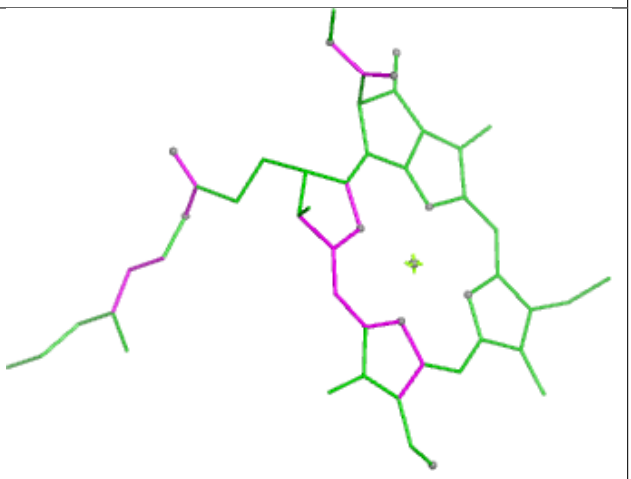


Rings

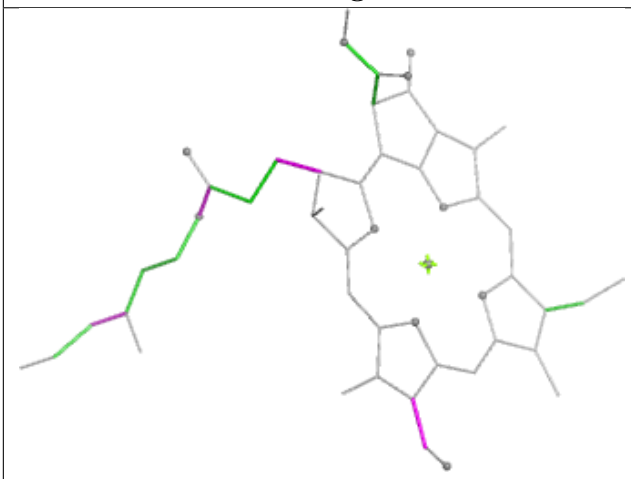
Ligand CL7 cA 1102



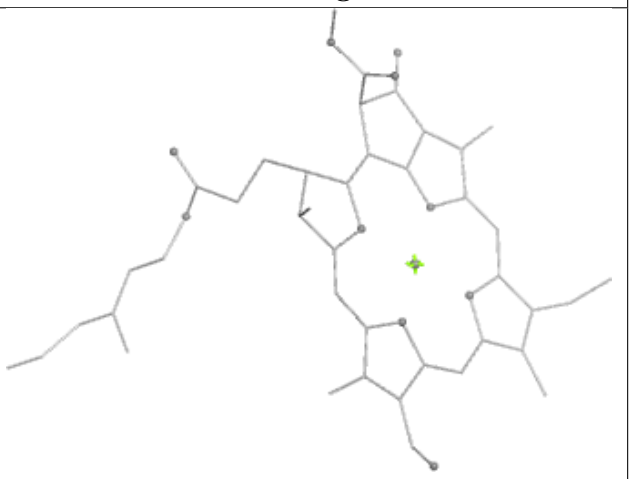
Bond lengths



Bond angles

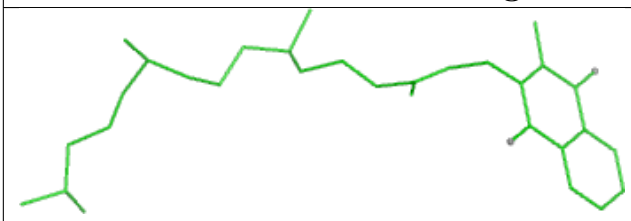


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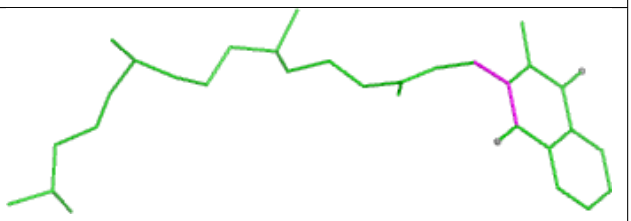


Rings

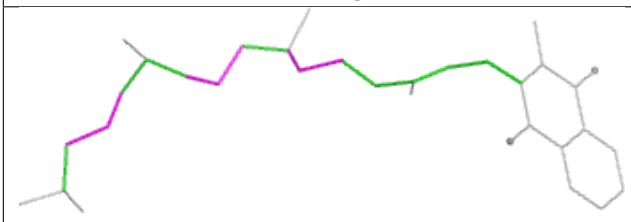
Ligand PQN bB 2002



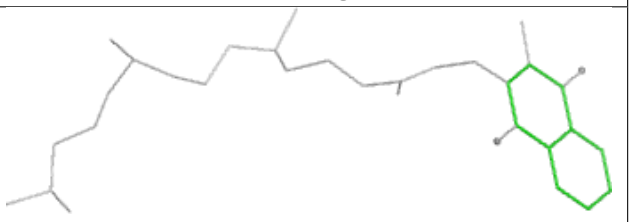
Bond lengths



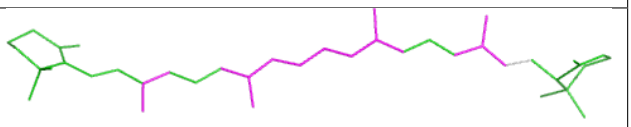
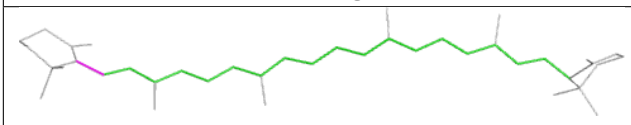
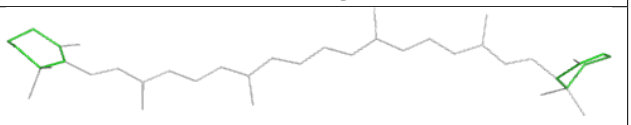
Bond angles

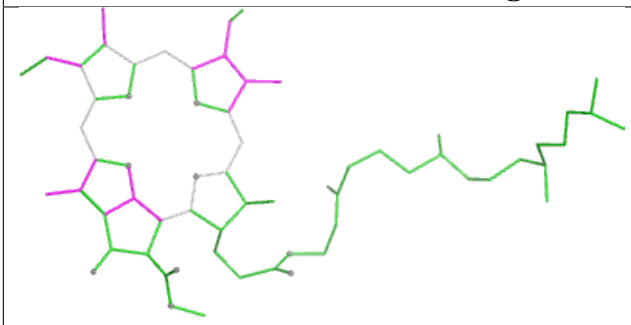
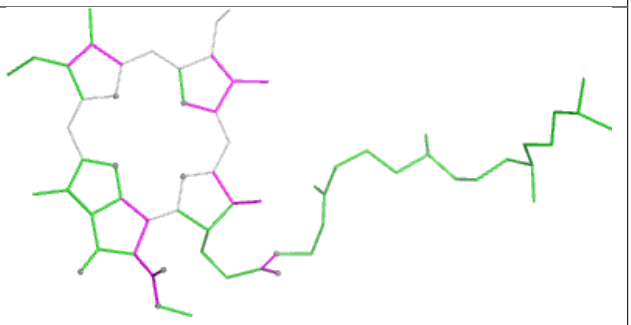
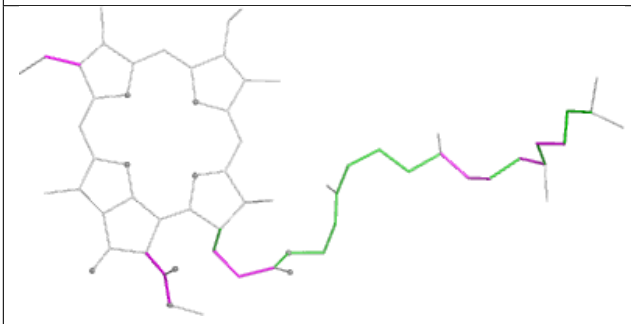
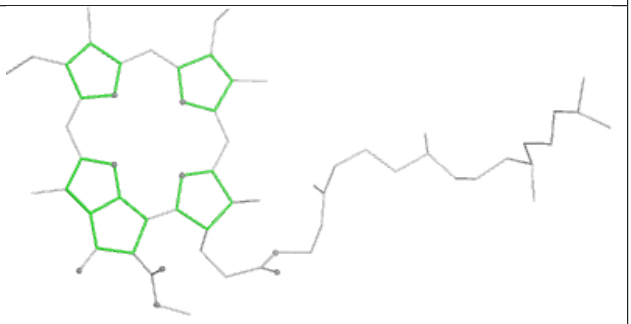


Torsions

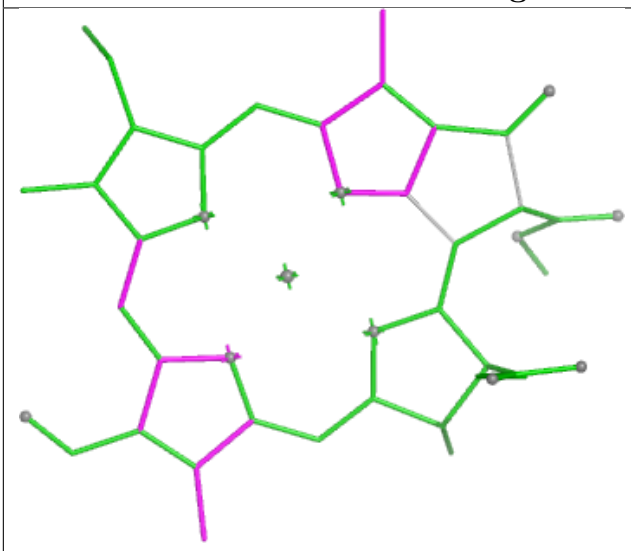


Rings

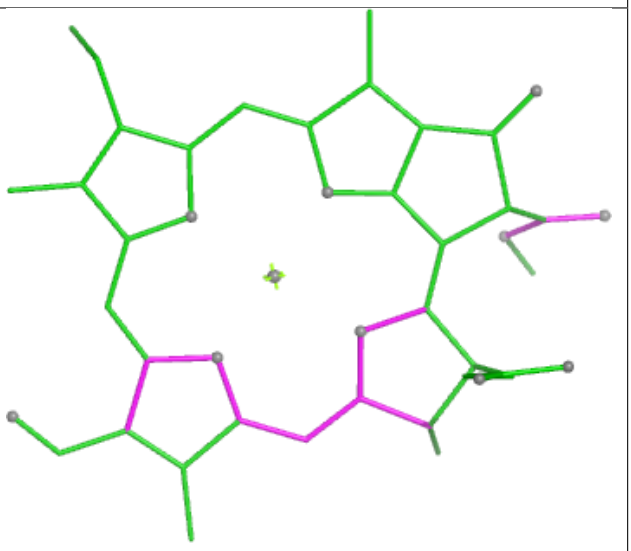
Ligand A1JPJ aI 4019	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand PHO cB 1023	
 Bond lengths	 Bond angles
 Torsions	 Rings

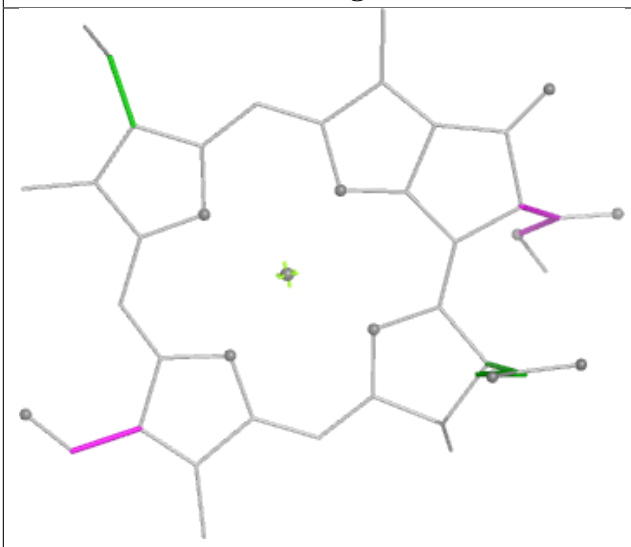
Ligand CL7 bA 1105



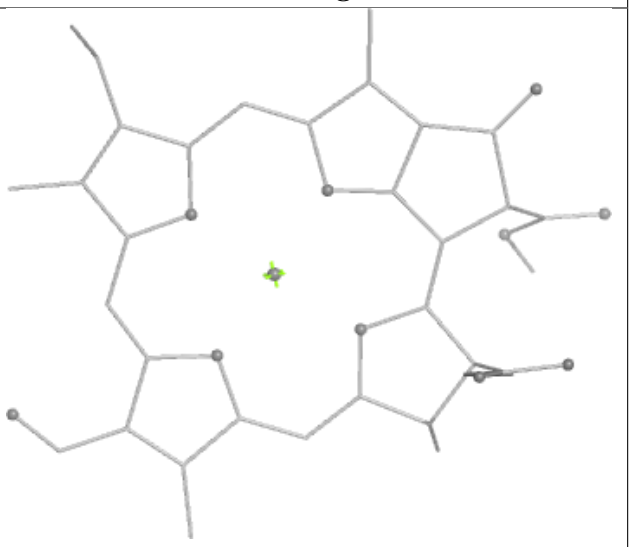
Bond lengths



Bond angles

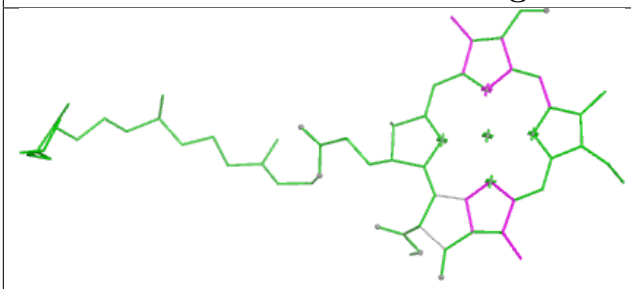


Torsions

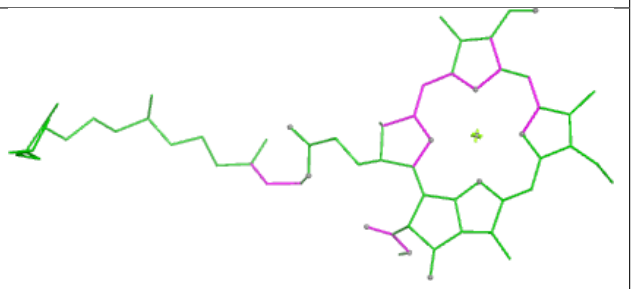


Rings

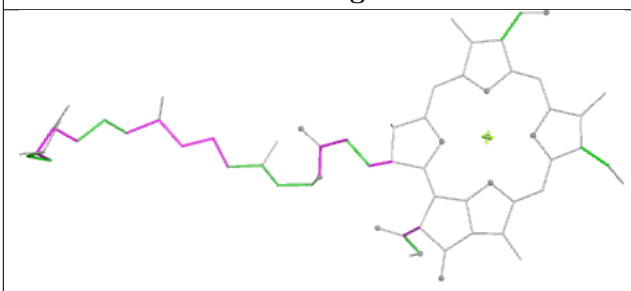
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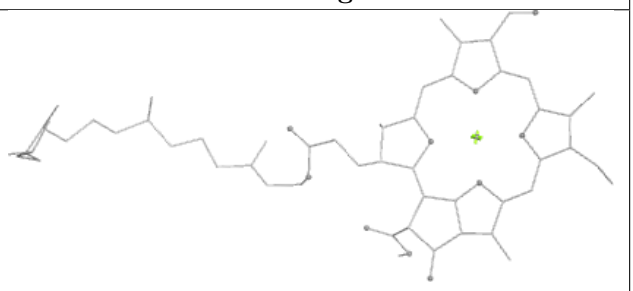
Bond lengths



Bond angles

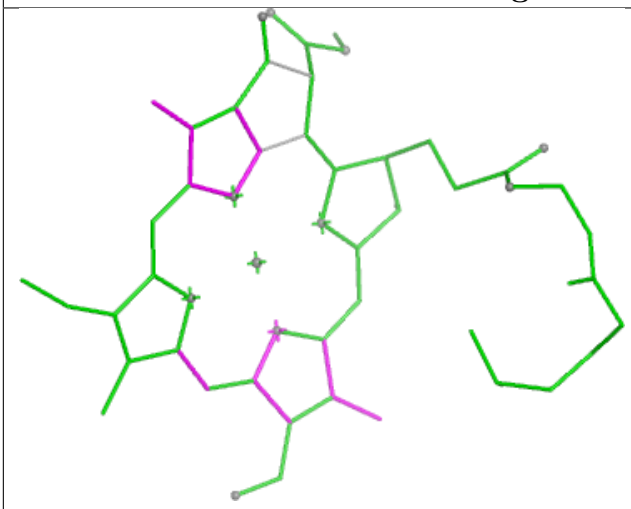


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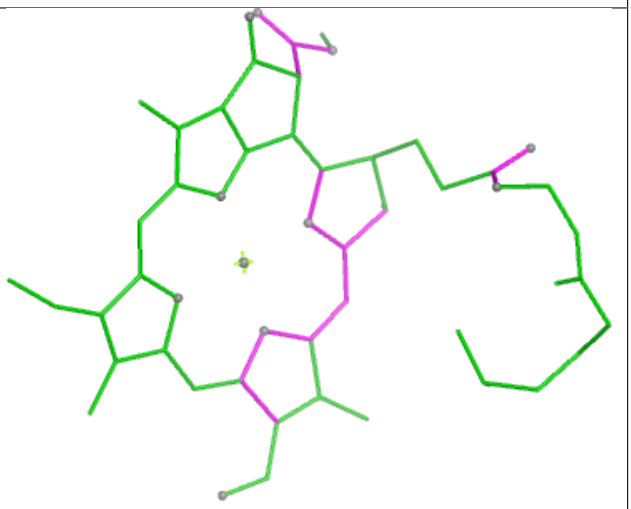


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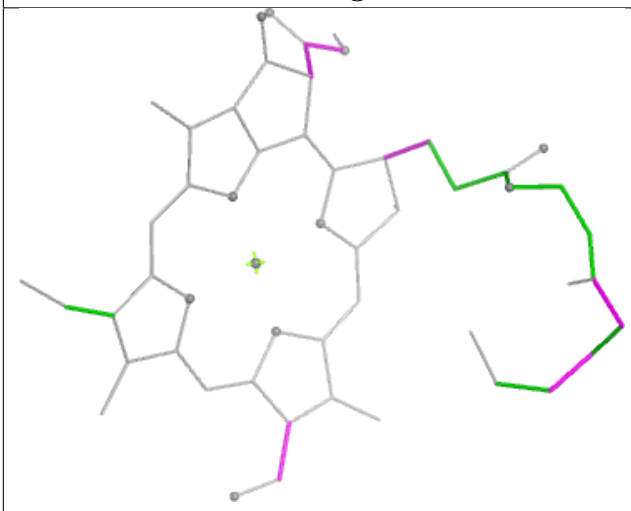
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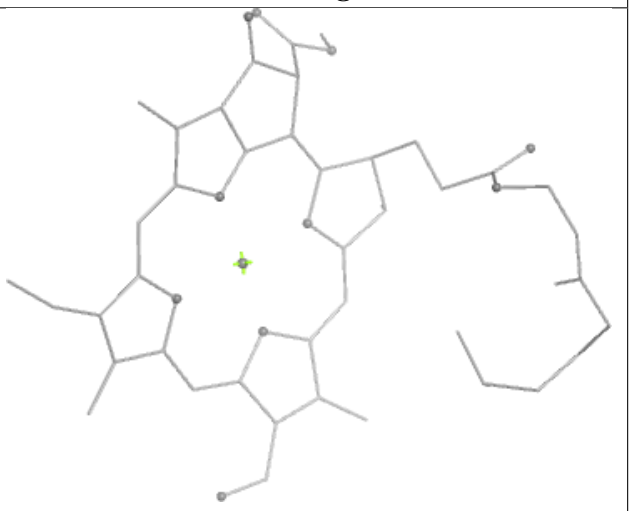
Bond lengths



Bond angles

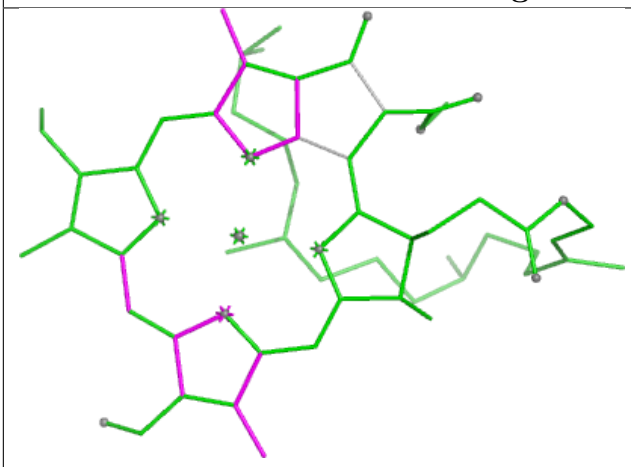


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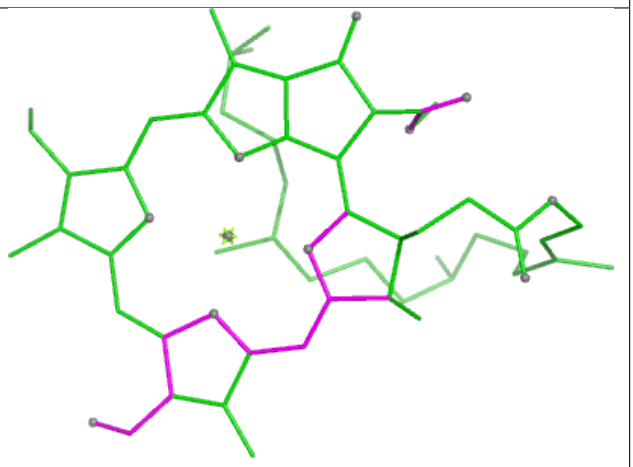


Rings

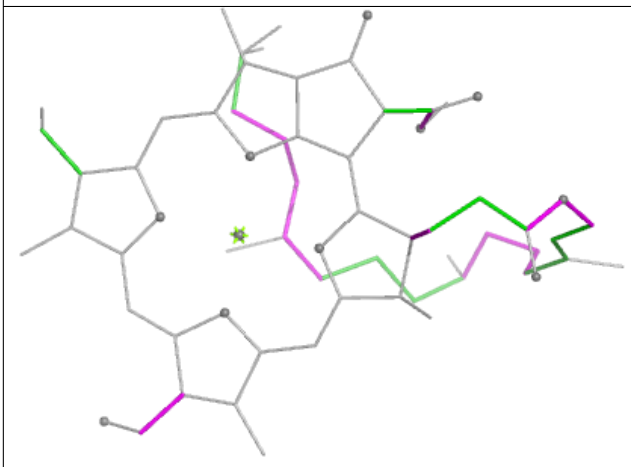
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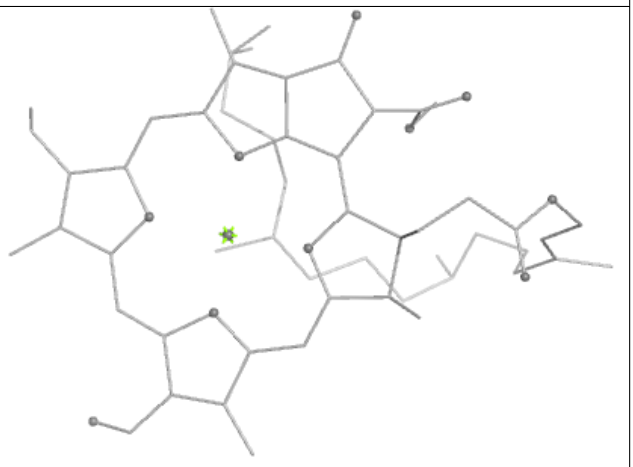
Bond lengths



Bond angles

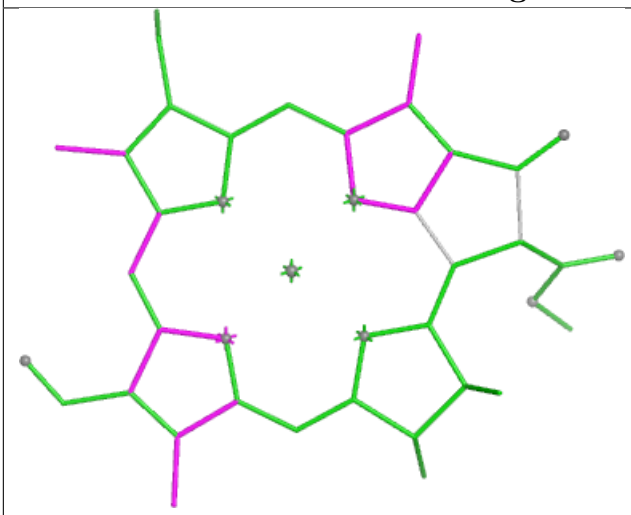


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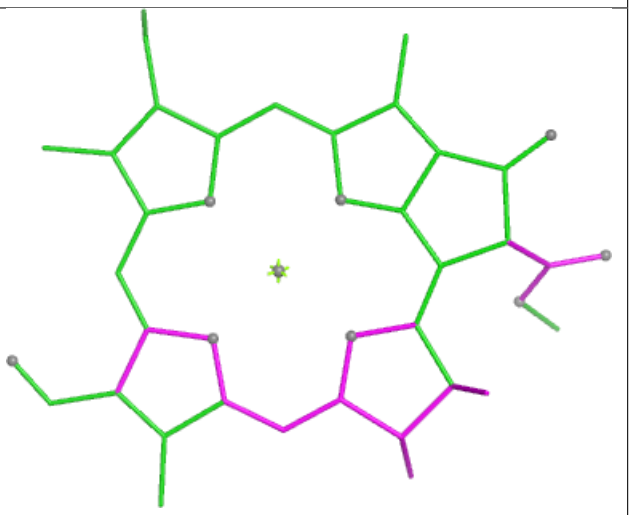


Rings

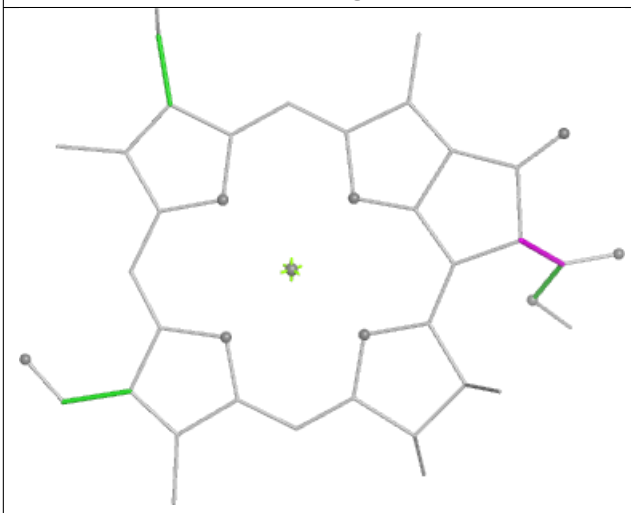
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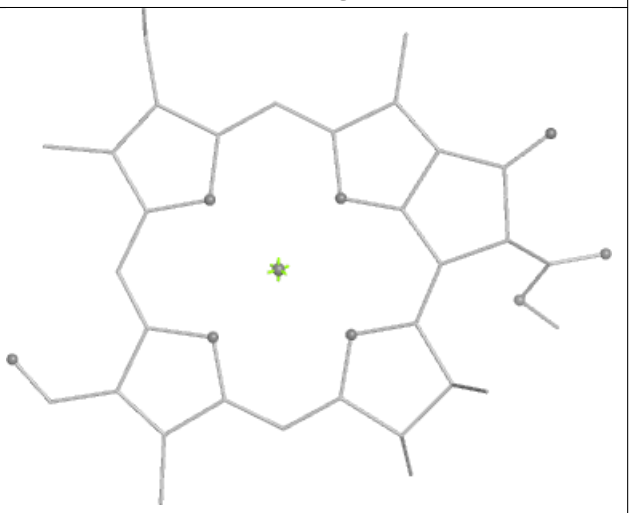
Bond lengths



Bond angles

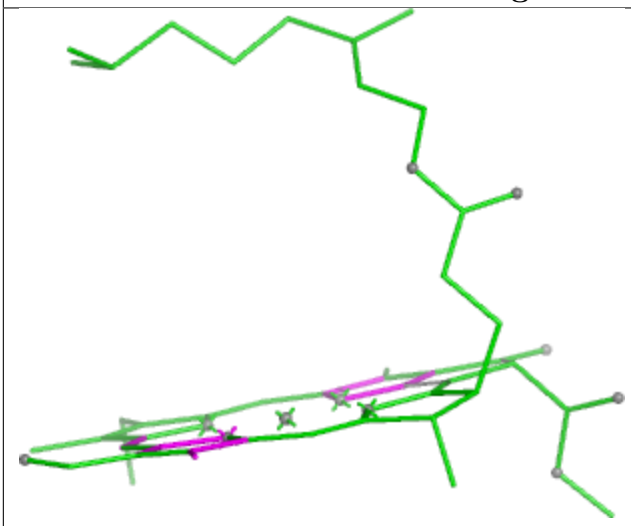


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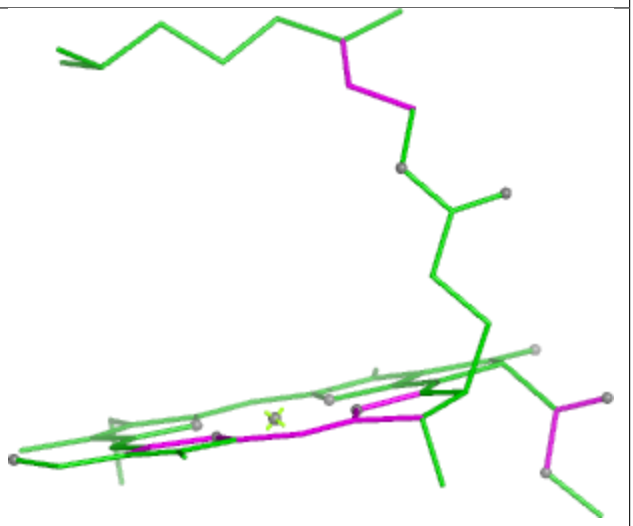


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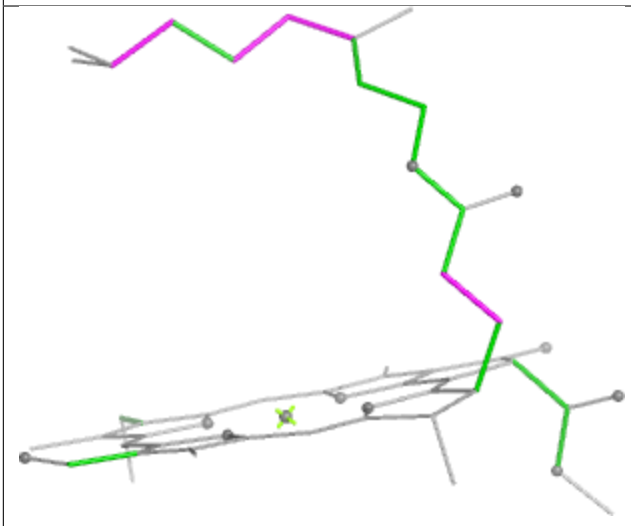
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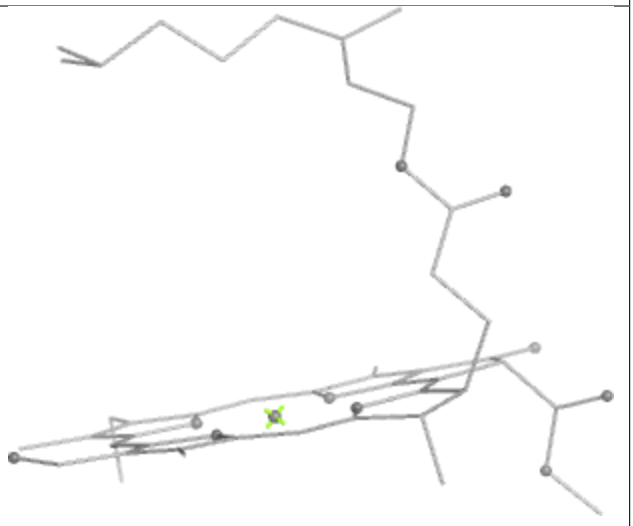
Bond lengths



Bond angles

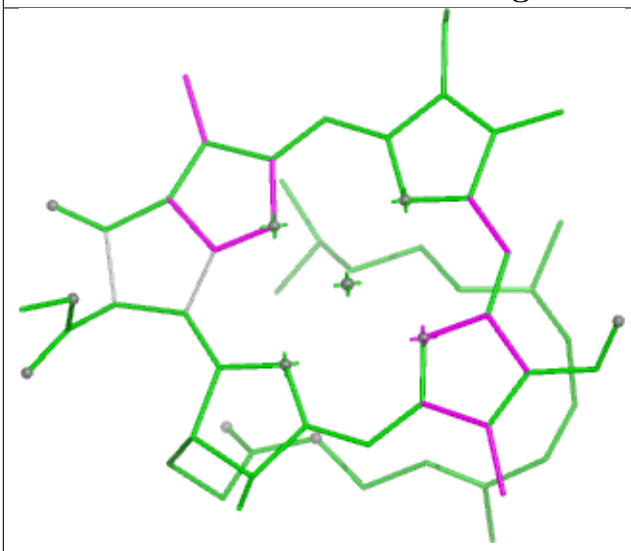


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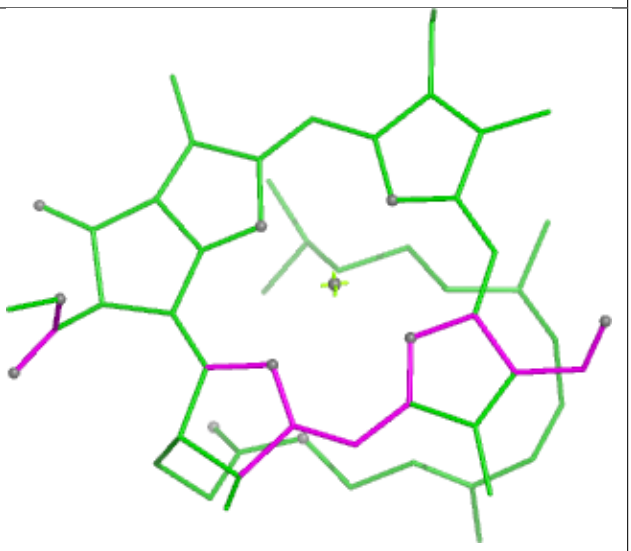


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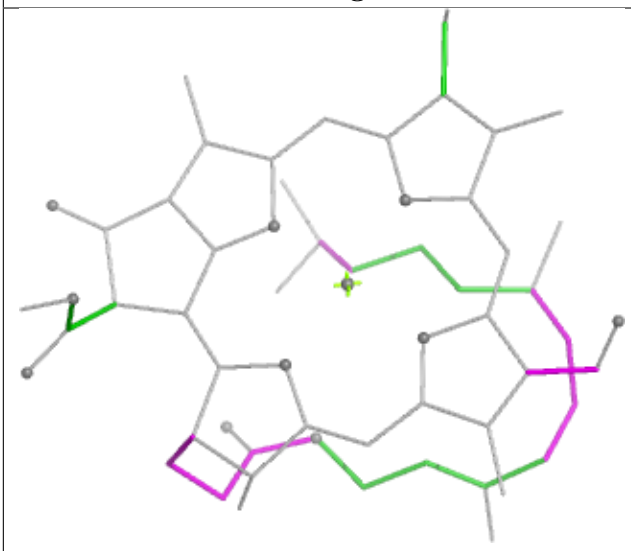
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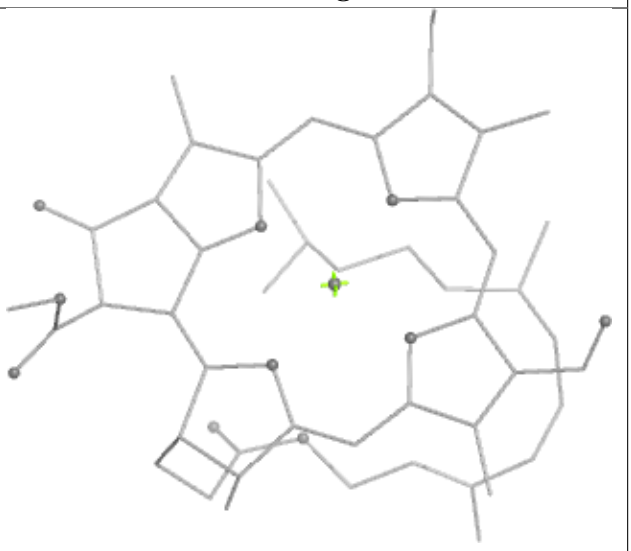
Bond lengths



Bond angles

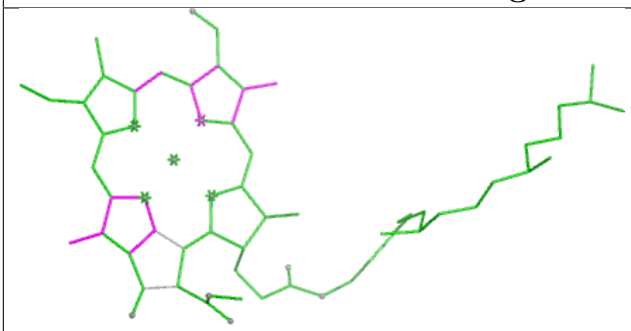


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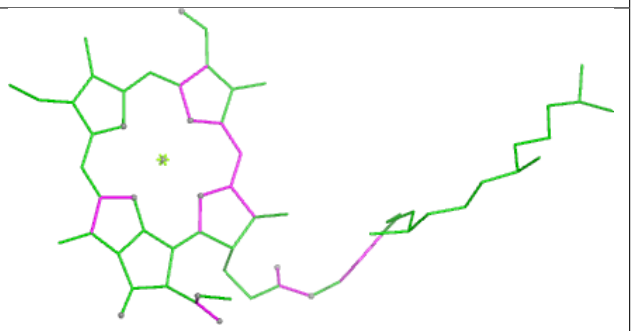


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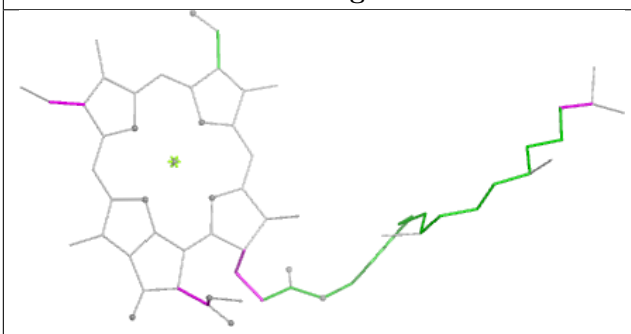
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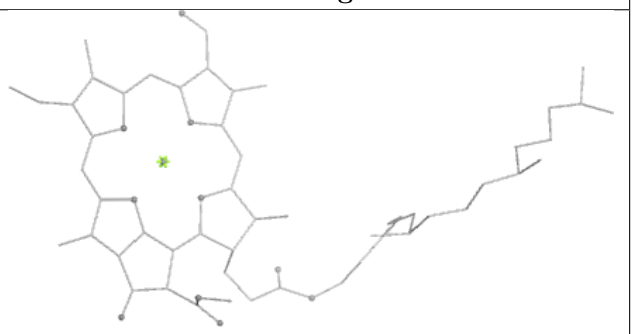
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Bond angles

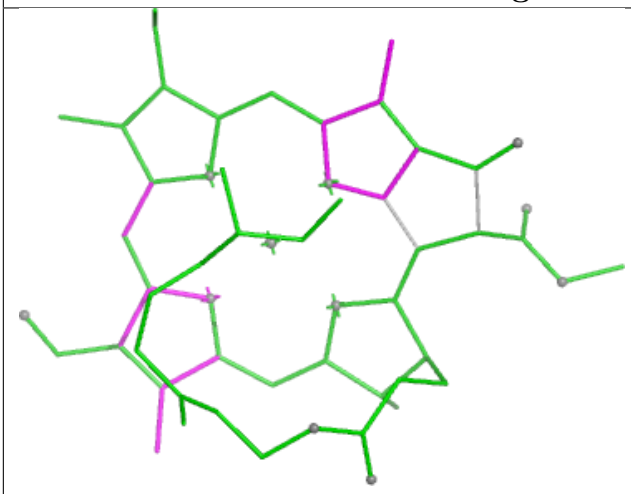


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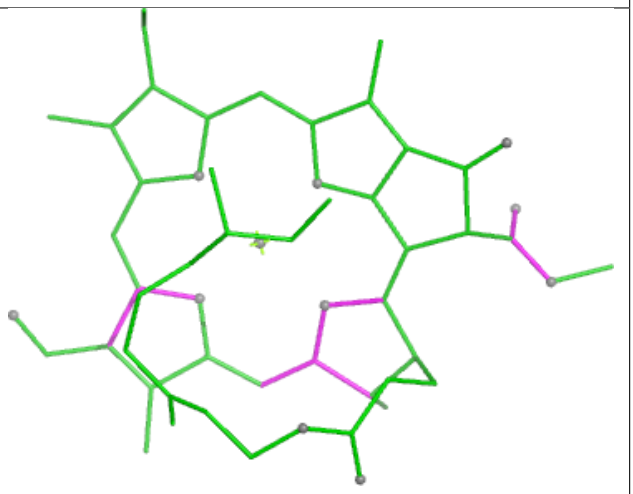


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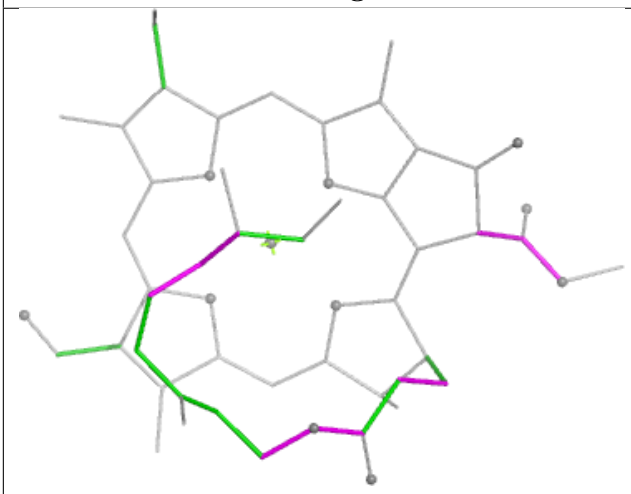
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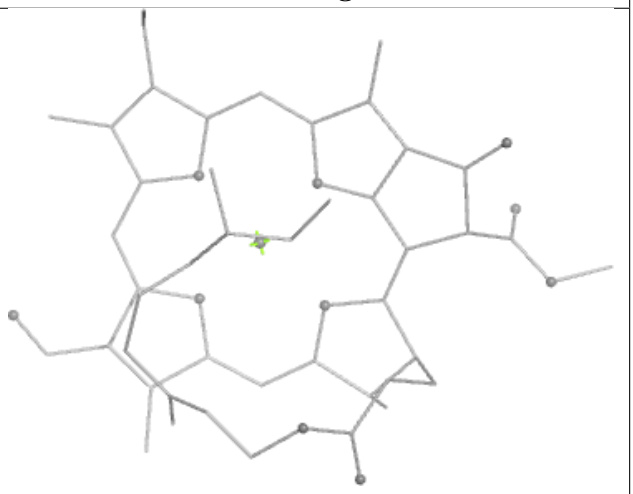
Bond lengths



Bond angles

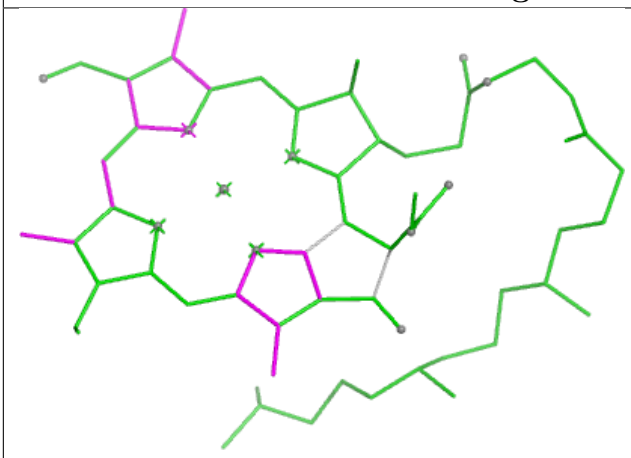


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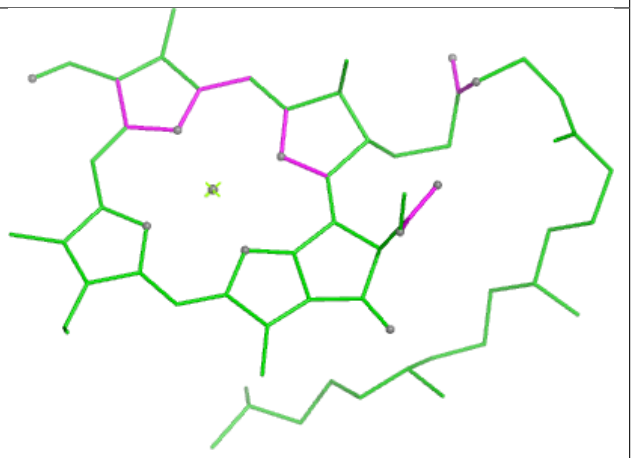


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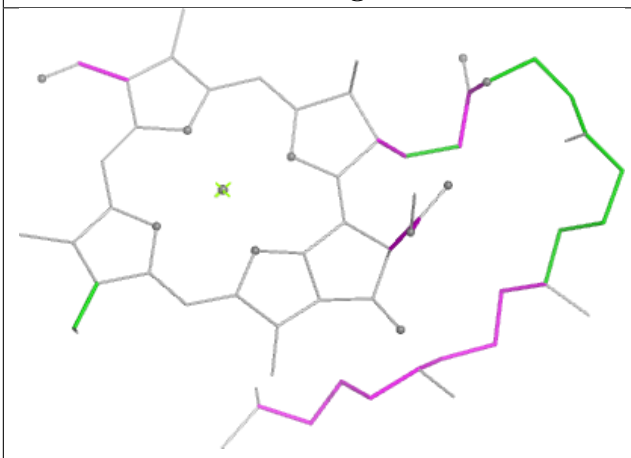
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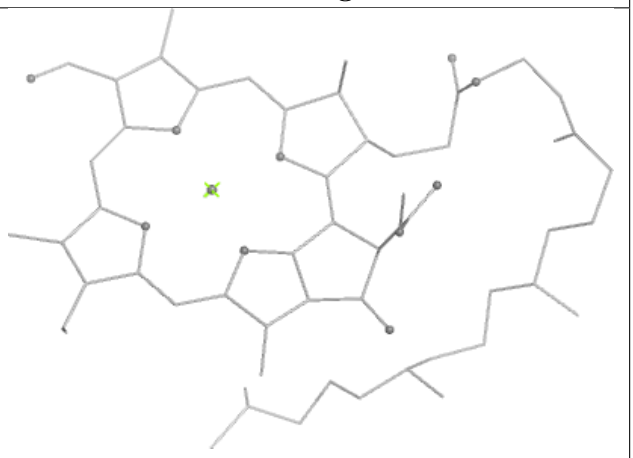
Bond lengths



Bond angles

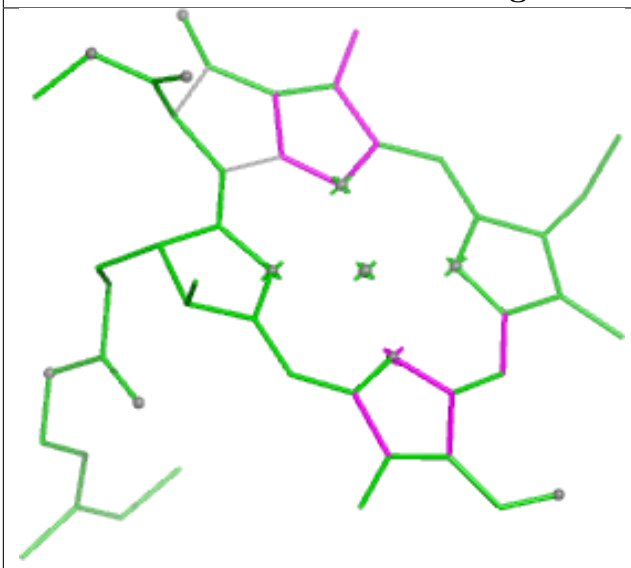


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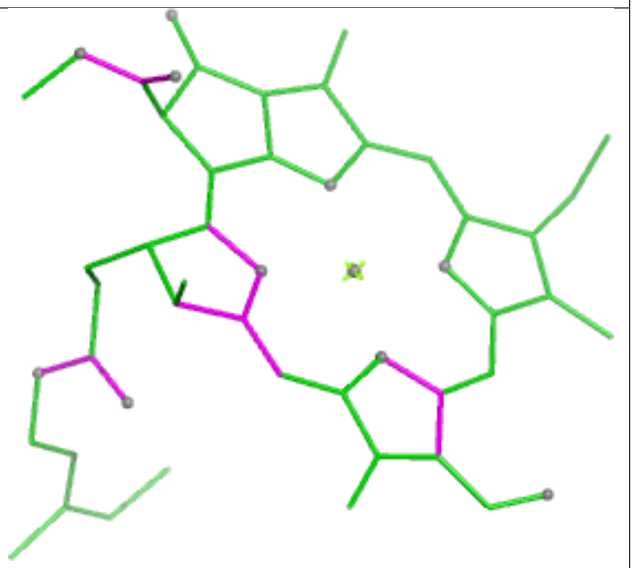


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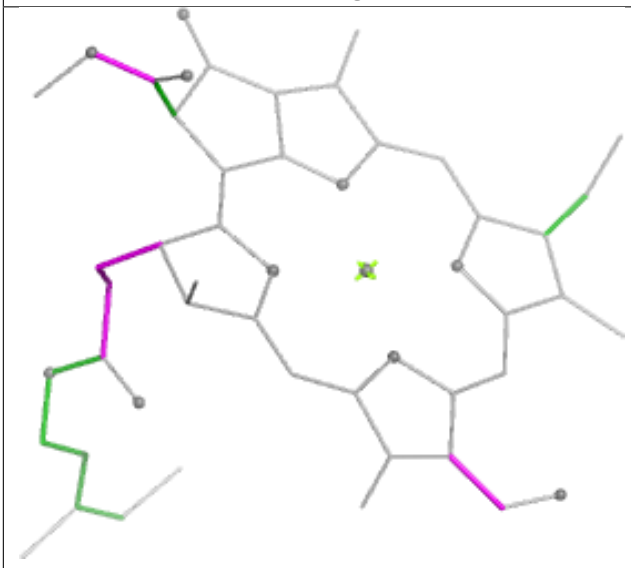
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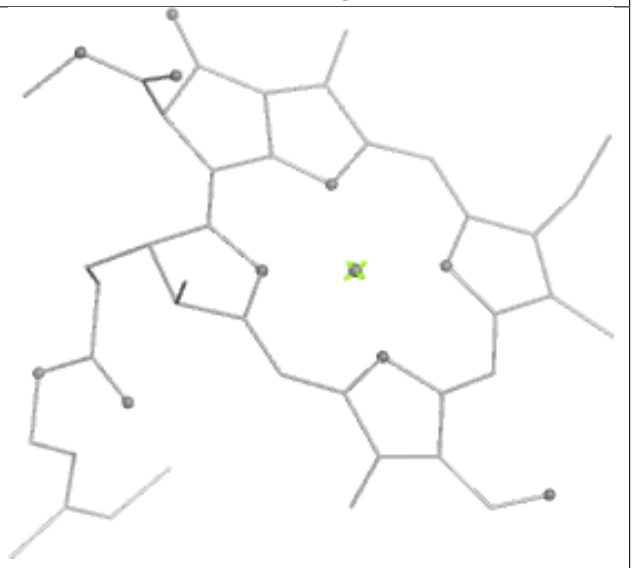
Bond lengths



Bond angles

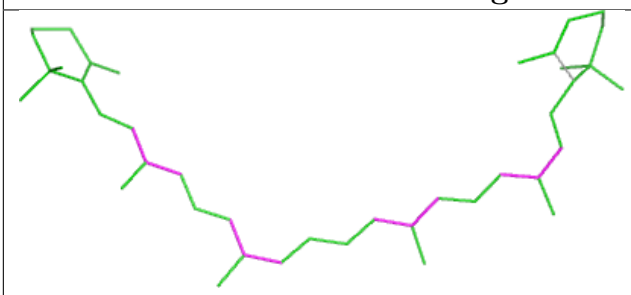


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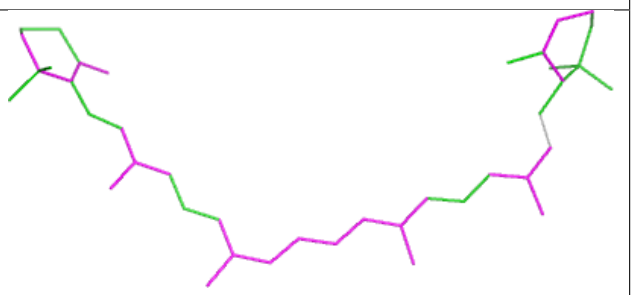


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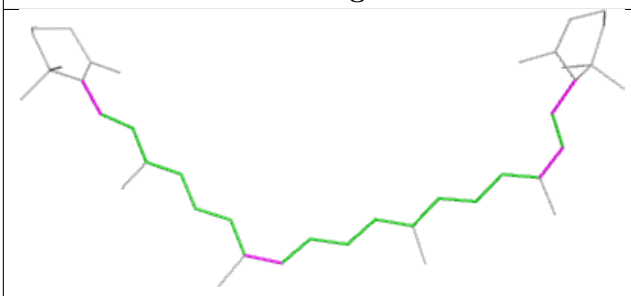
Ligand A1JPJ bF 4016



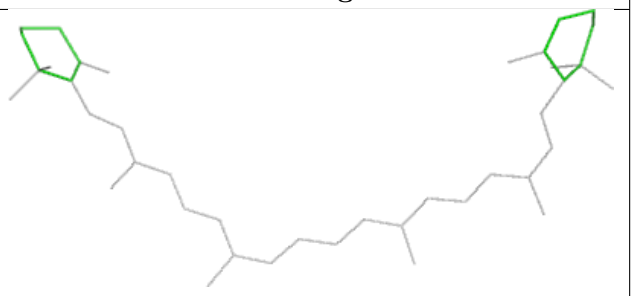
Bond lengths



Bond angles

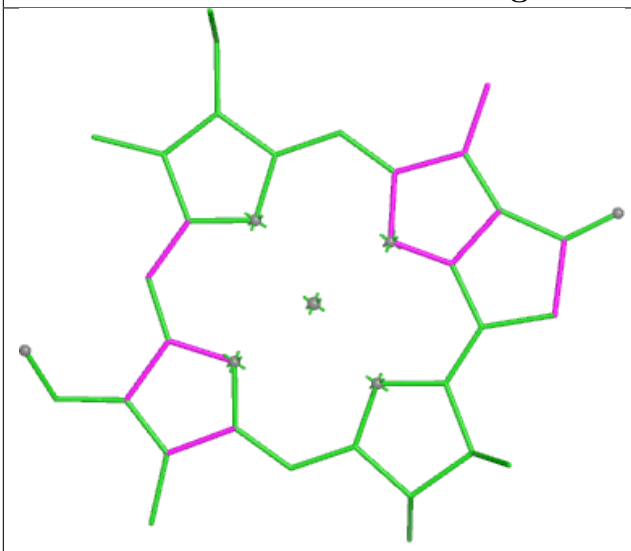


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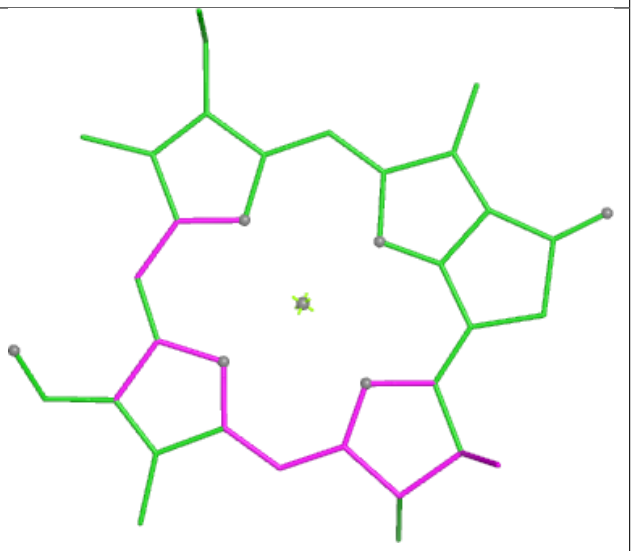


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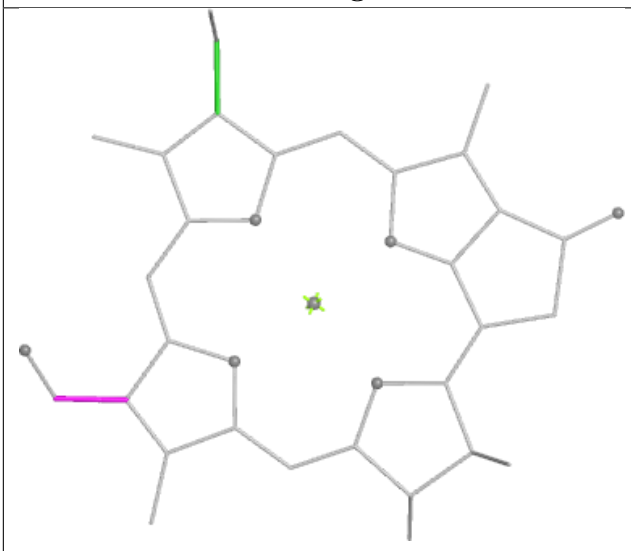
Ligand CL7 cK 1402



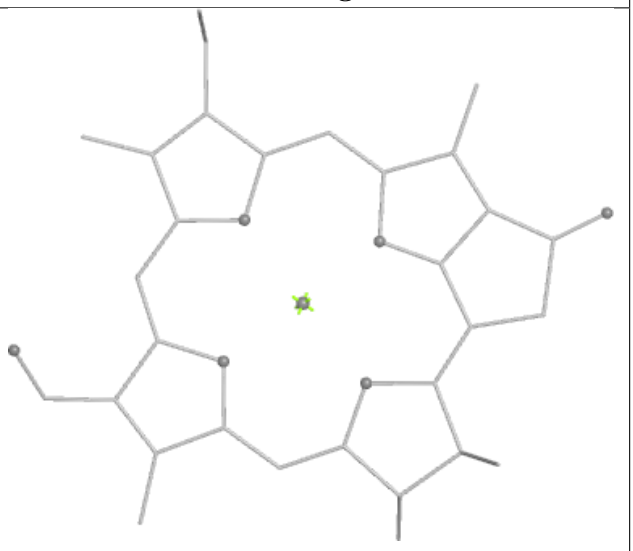
Bond lengths



Bond angles

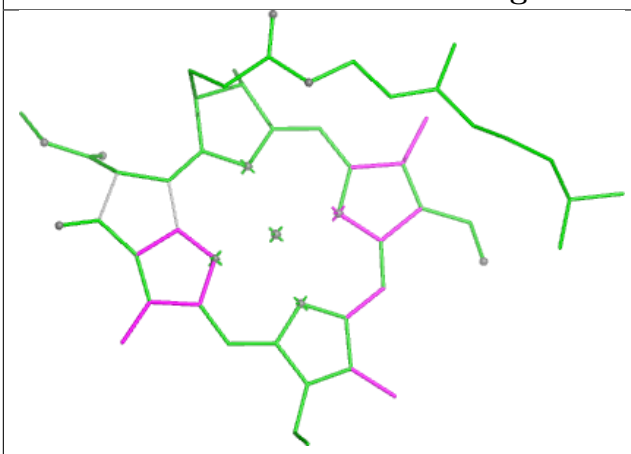


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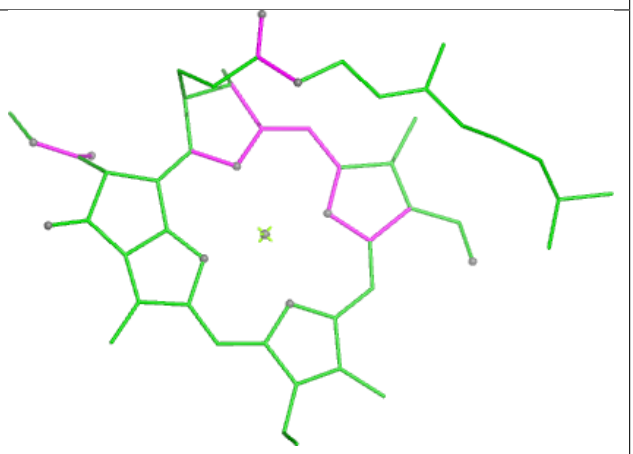


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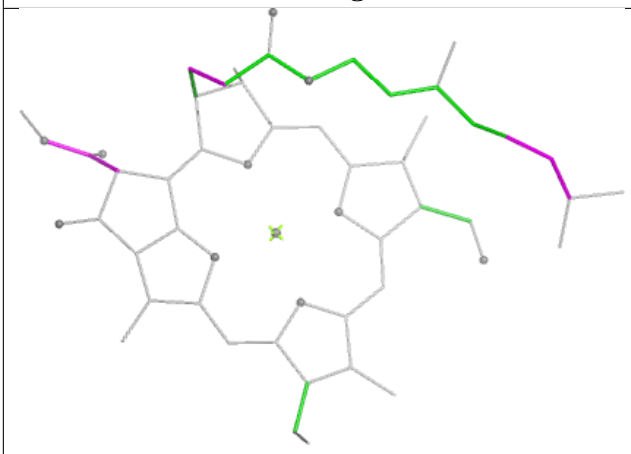
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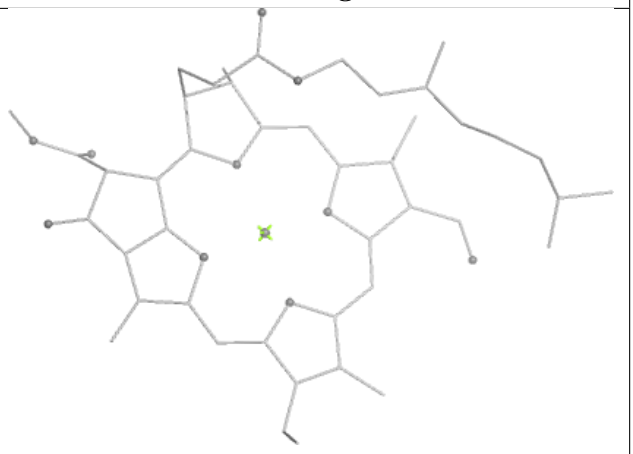
Bond lengths



Bond angles

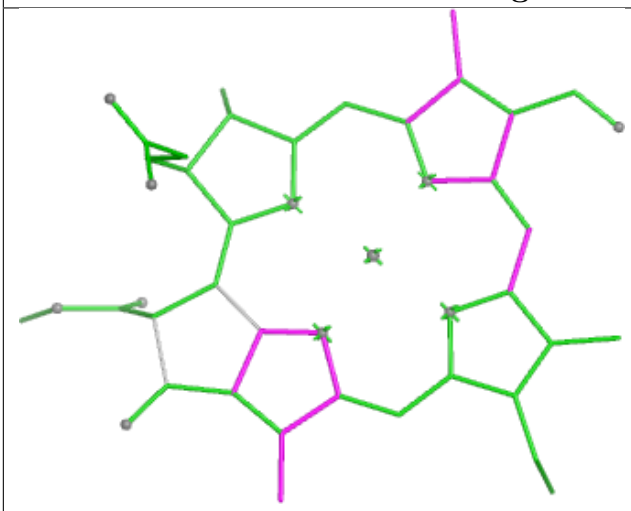


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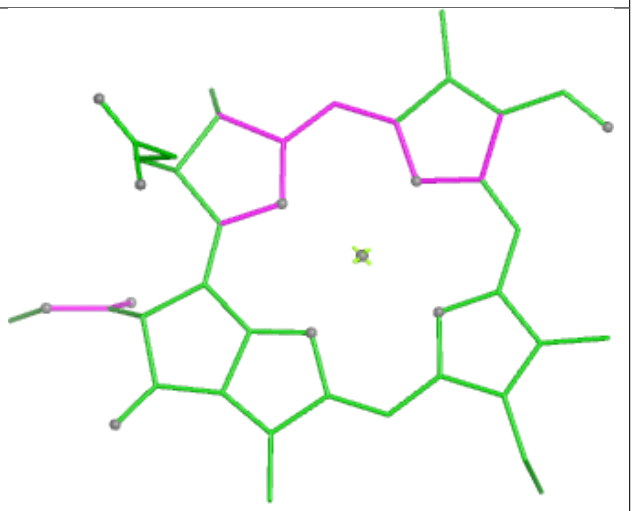


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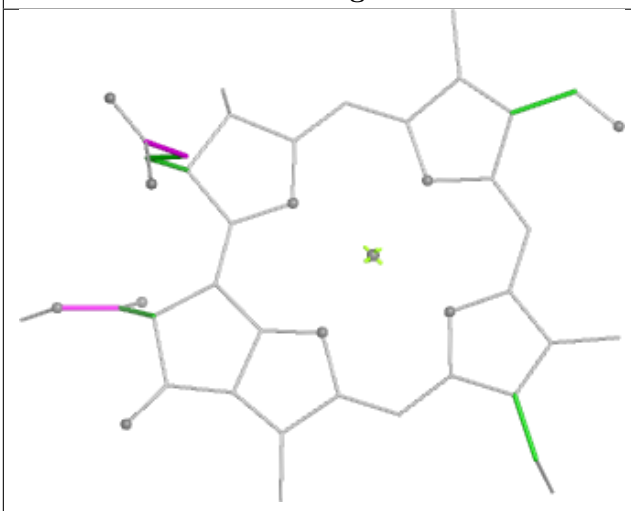
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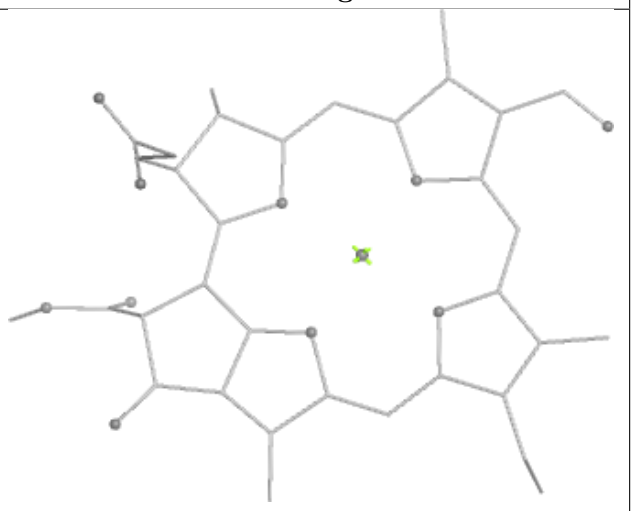
Bond lengths



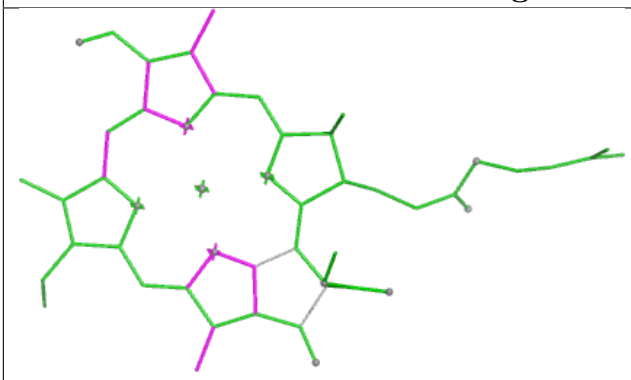
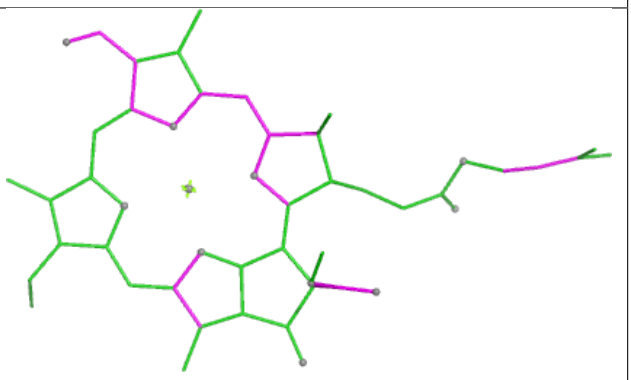
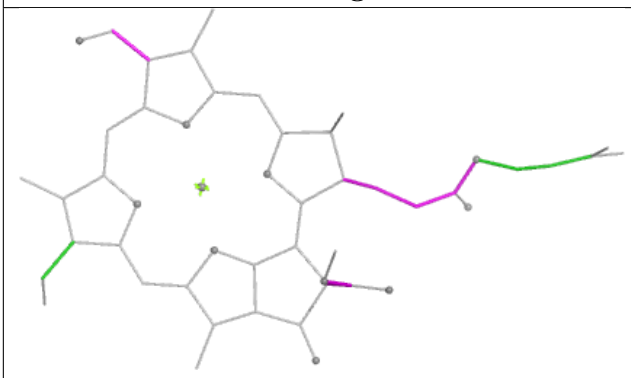
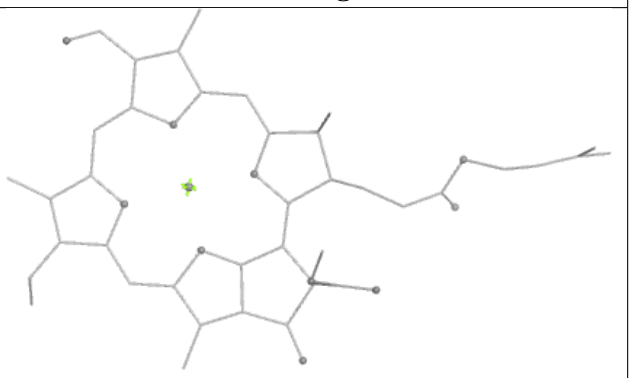
Bond angles



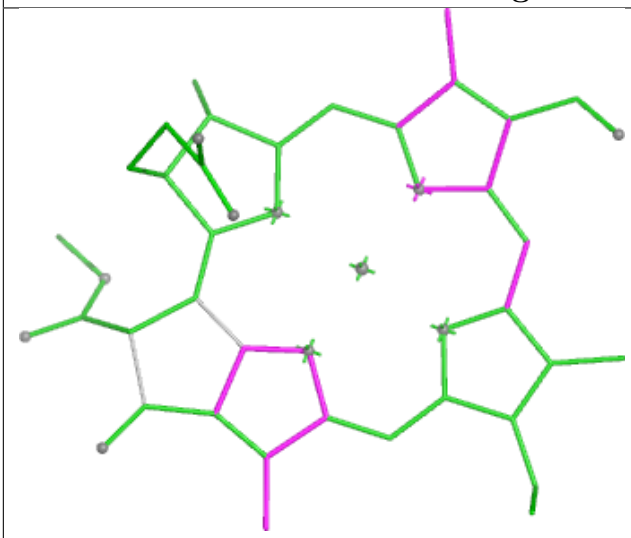
Torsions



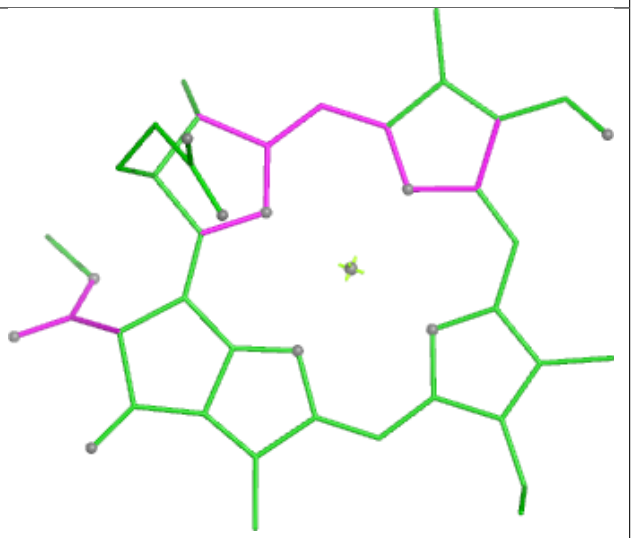
Rings

Ligand CL7 cA 1135	
	
Bond lengths	**Bond angles**
	
Torsions	**Rings**

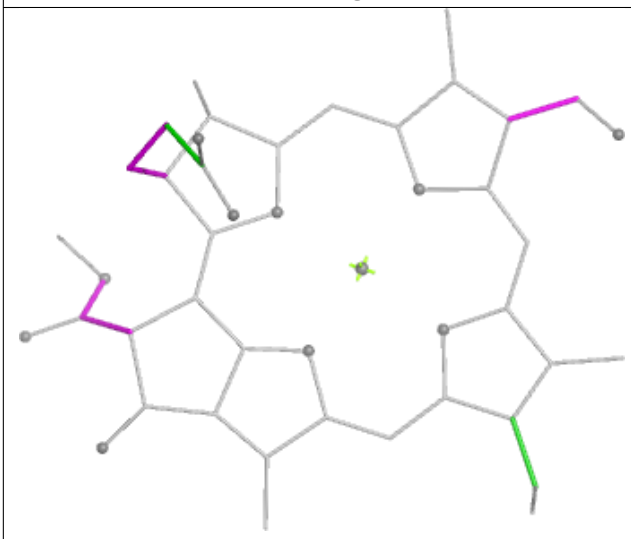
Ligand CL7 cB 1213



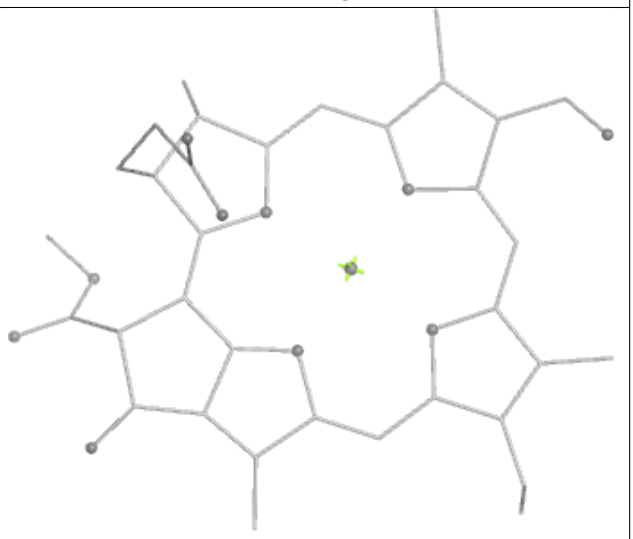
Bond lengths



Bond angles

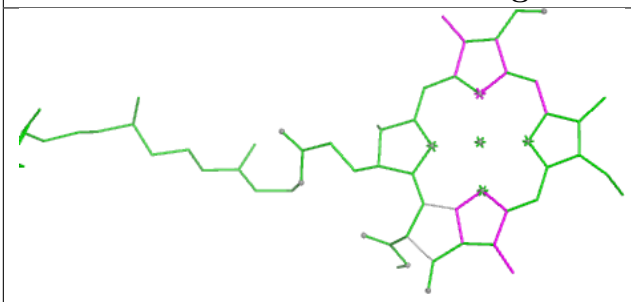


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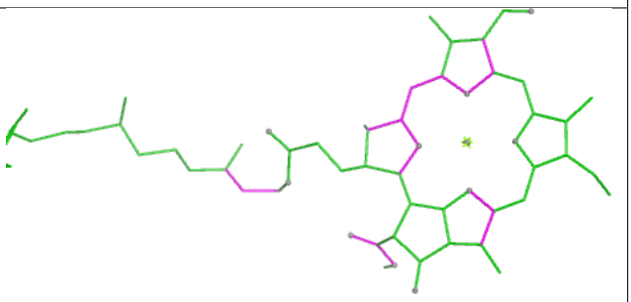


Rings

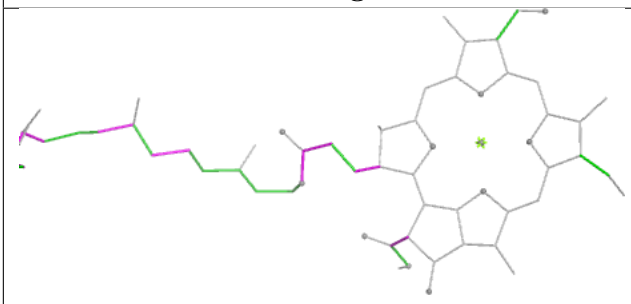
Ligand CL7 cA 1103



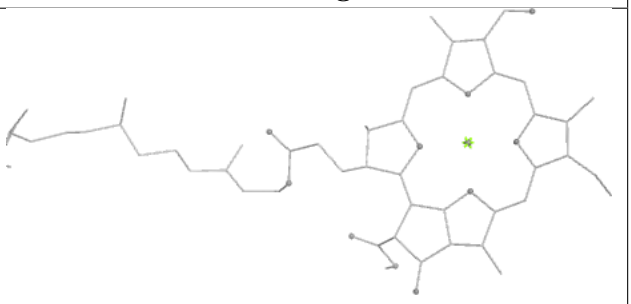
Bond lengths



Bond angles

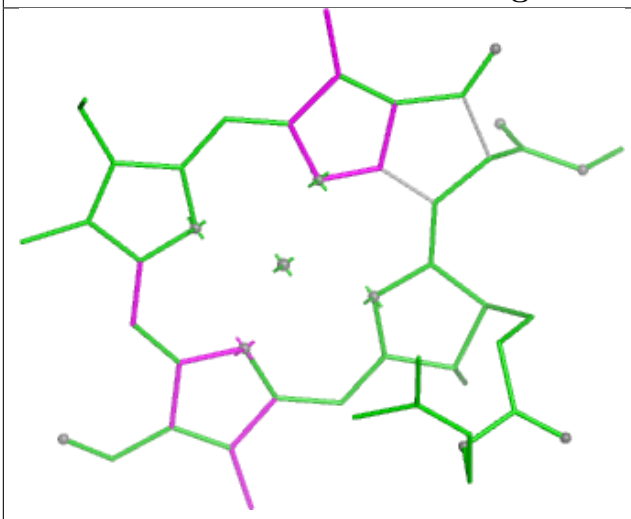


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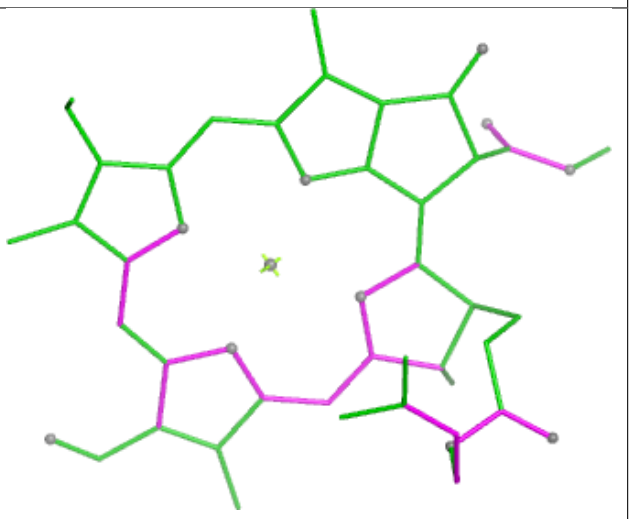


Rings

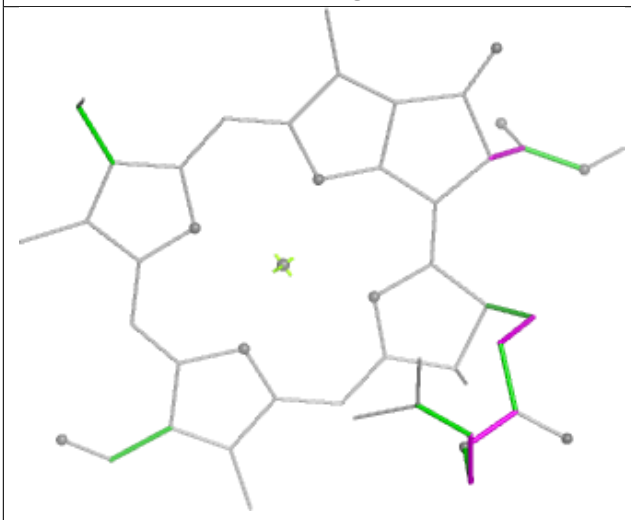
Ligand CL7 aB 1214



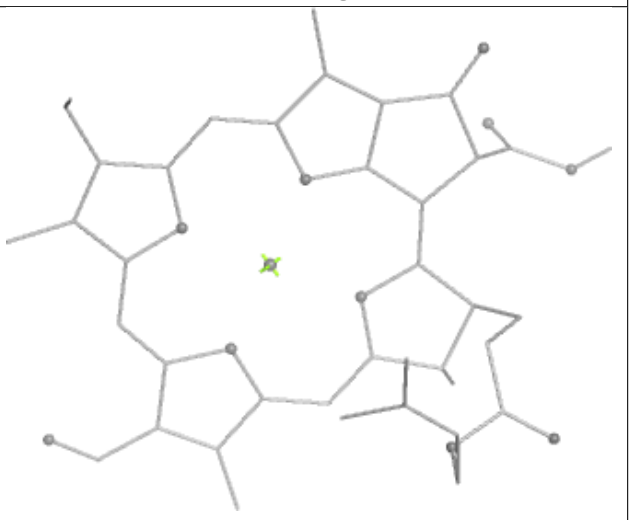
Bond lengths



Bond angles

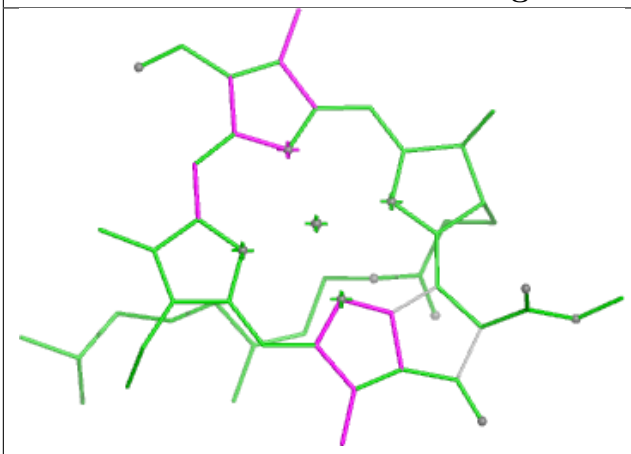


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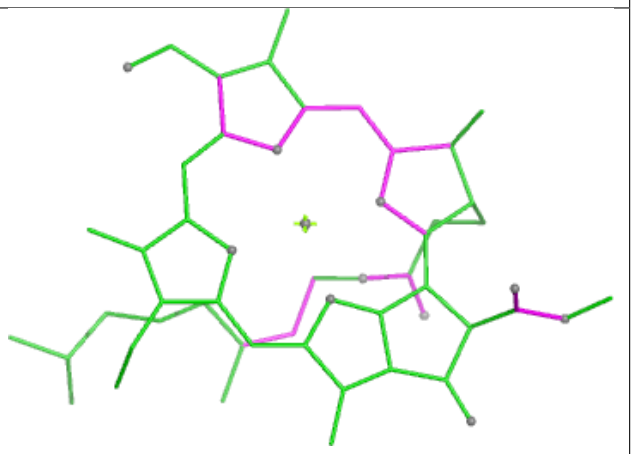


Rings

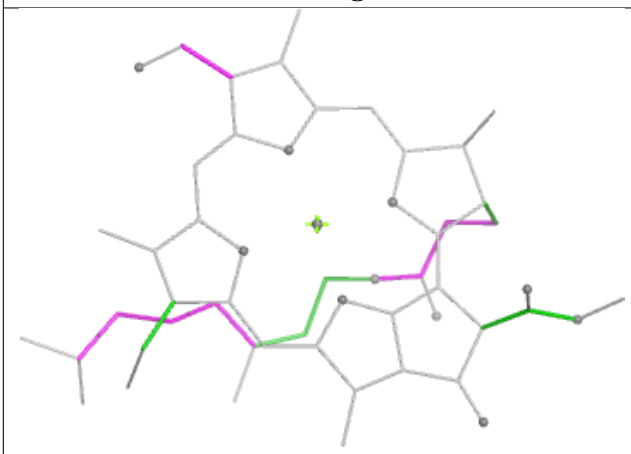
Ligand CL7 cA 1119



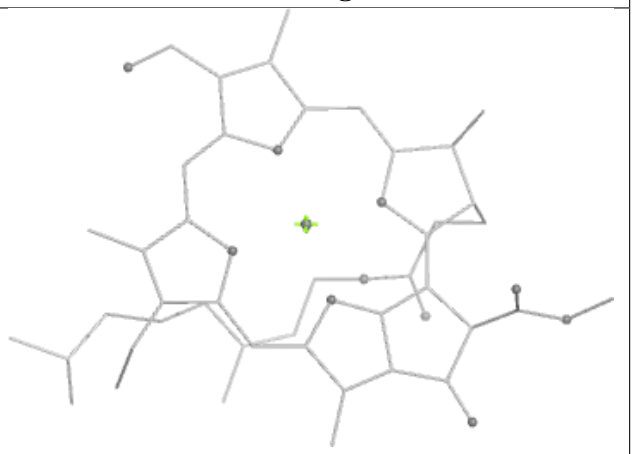
Bond lengths



Bond angles

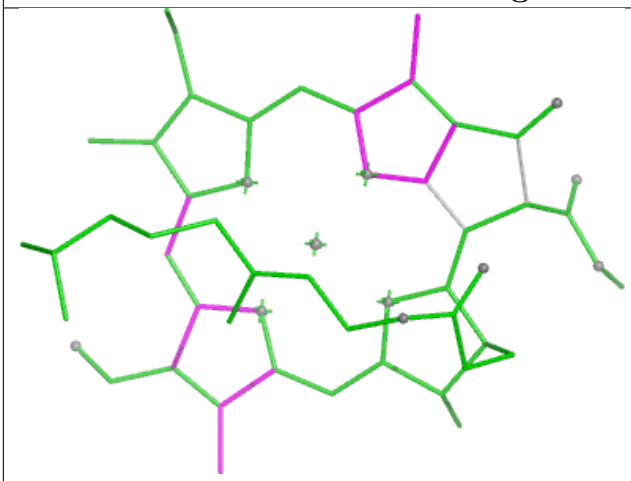


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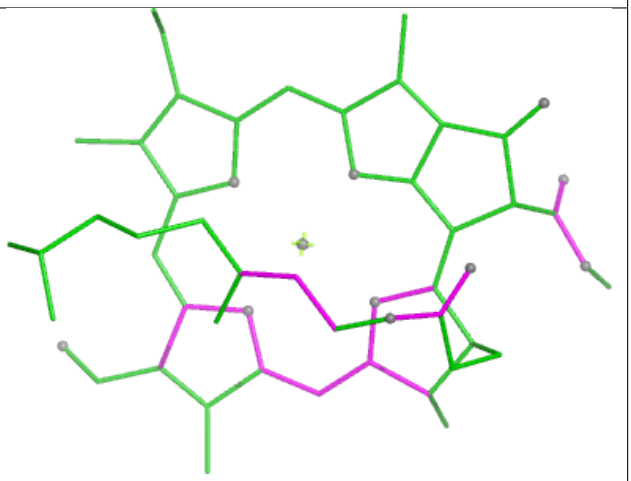


Rings

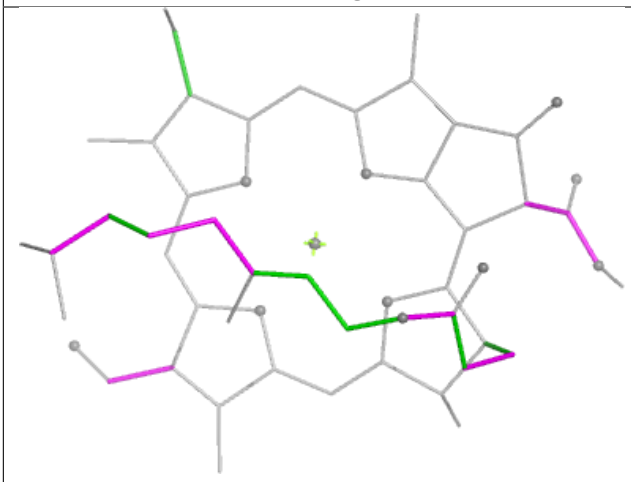
Ligand CL7 cA 1118



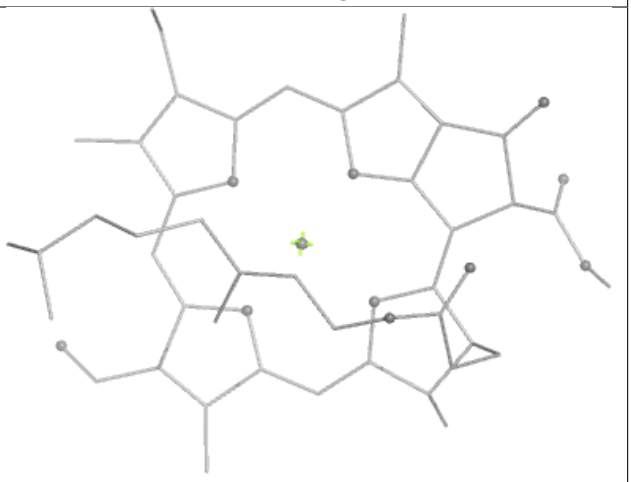
Bond lengths



Bond angles

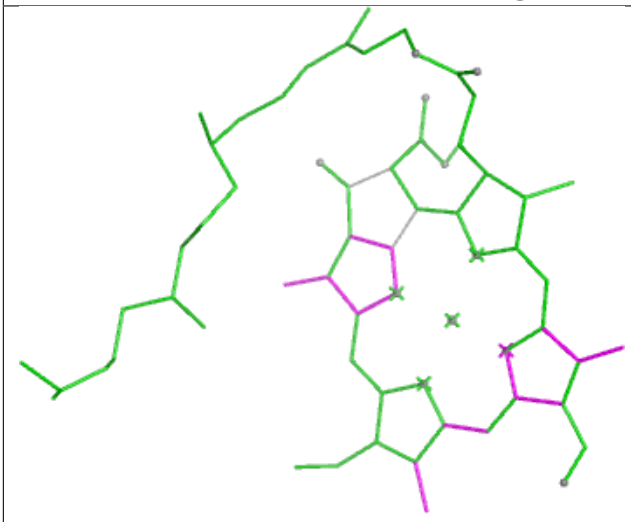


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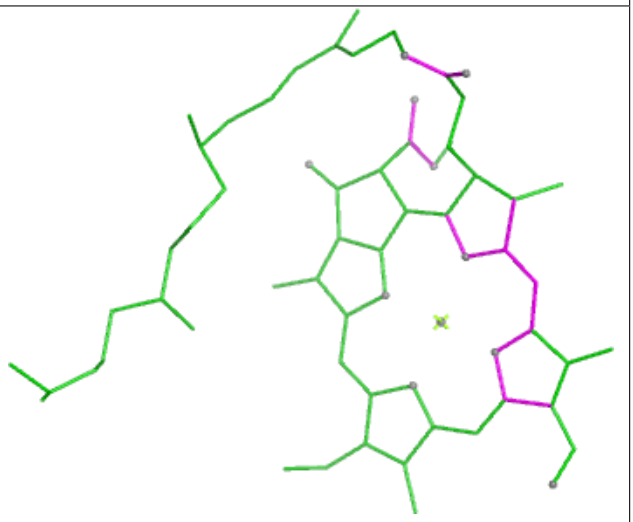


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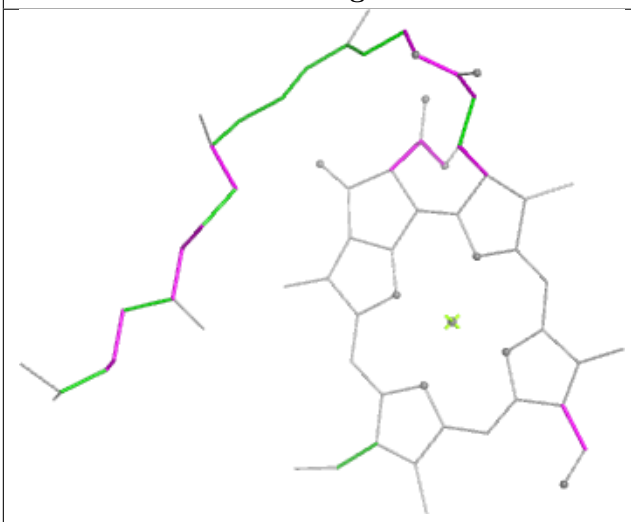
Ligand CL7 cA 1123



Bond lengths



Bond angles

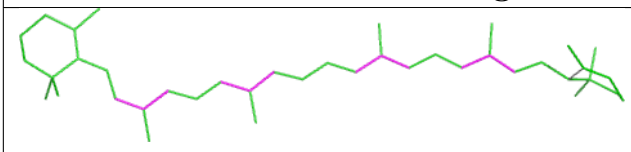


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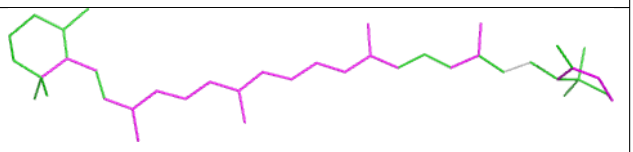


Rings

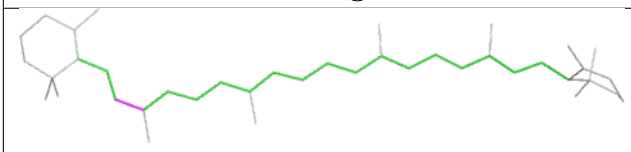
Ligand A1JPJ bJ 4012



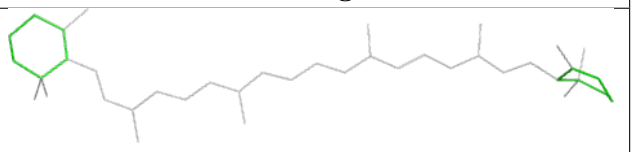
Bond lengths



Bond angles

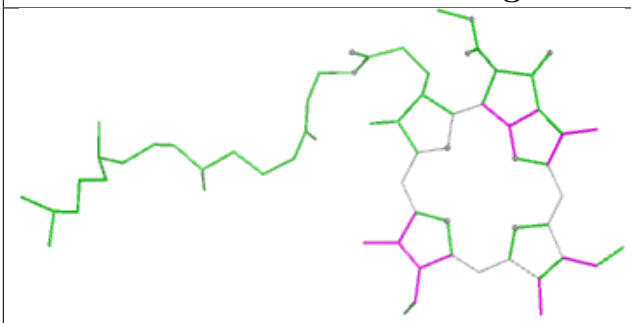


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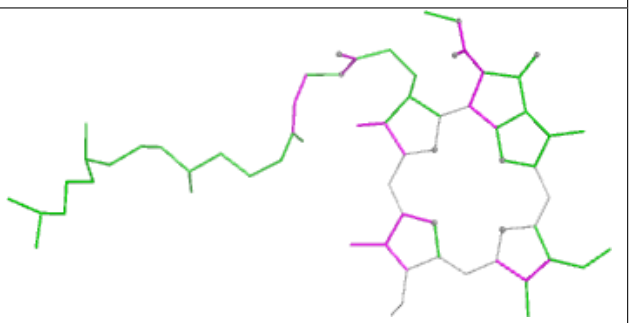


Rings

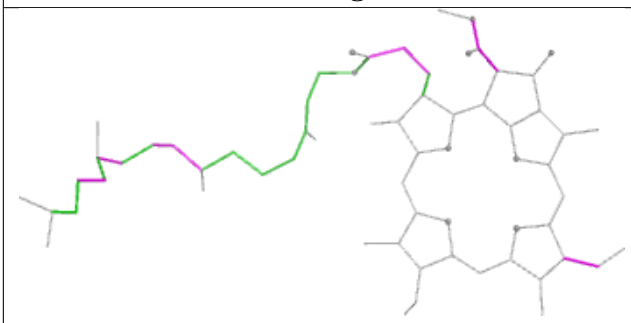
Ligand PHO bB 1023



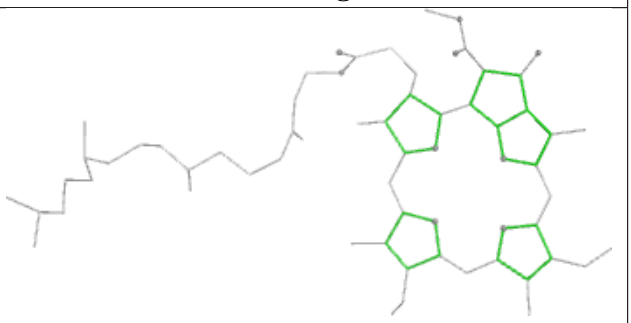
Bond lengths



Bond angles

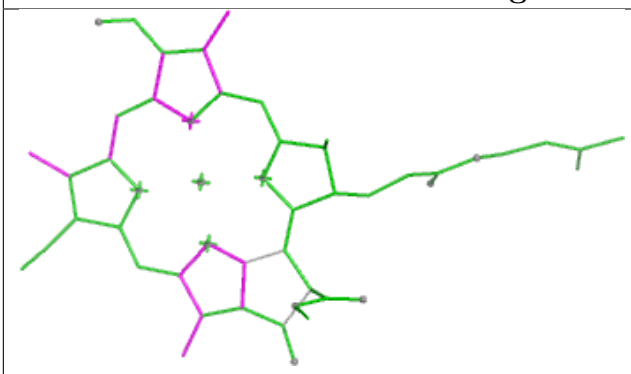


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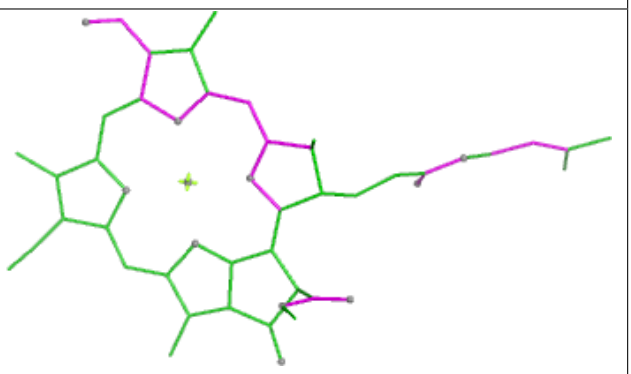


Rings

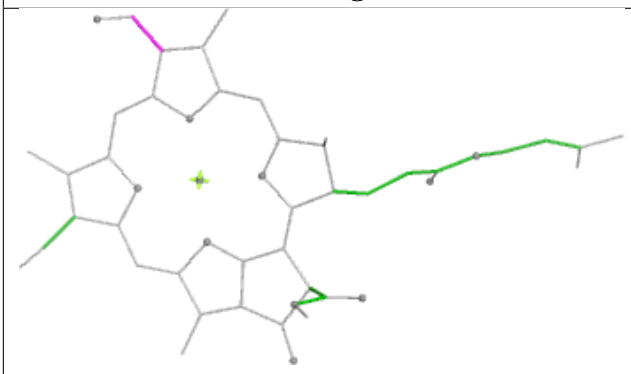
Ligand CL7 bA 1125



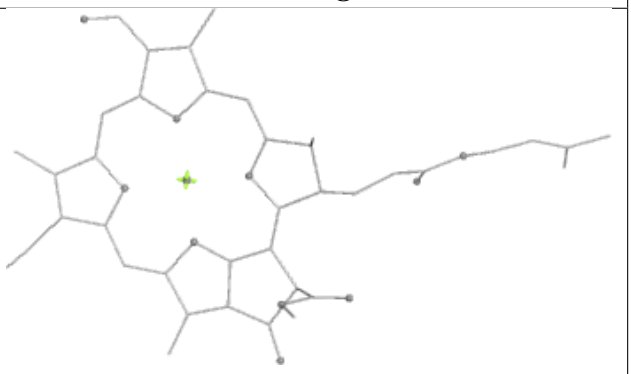
Bond lengths



Bond angles

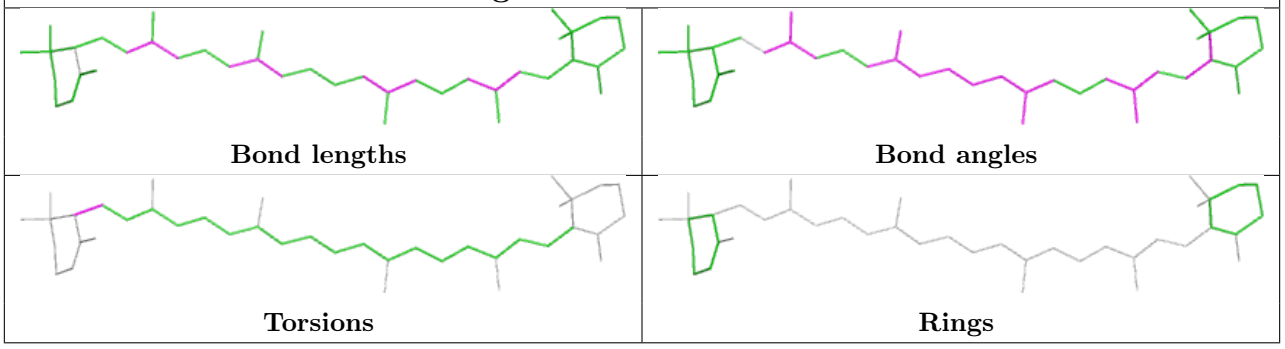


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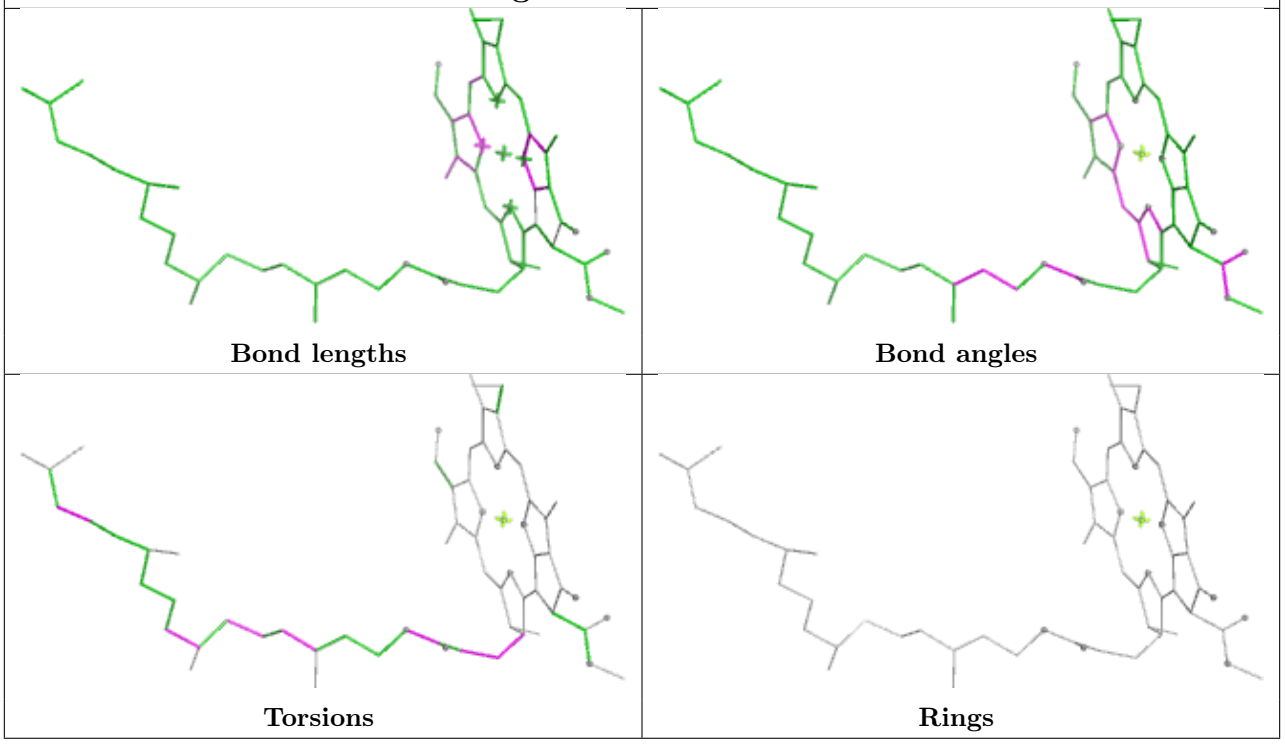


Rings

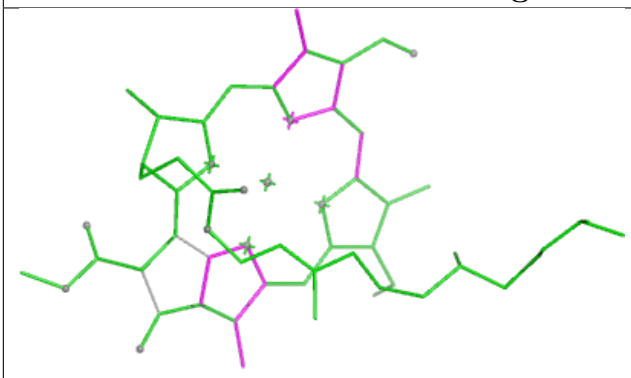
Ligand A1JPJ bL 4023



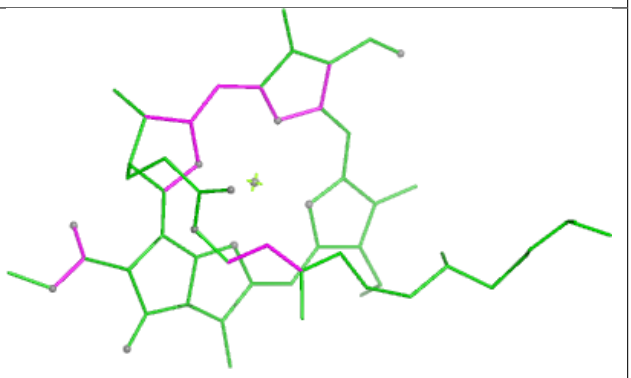
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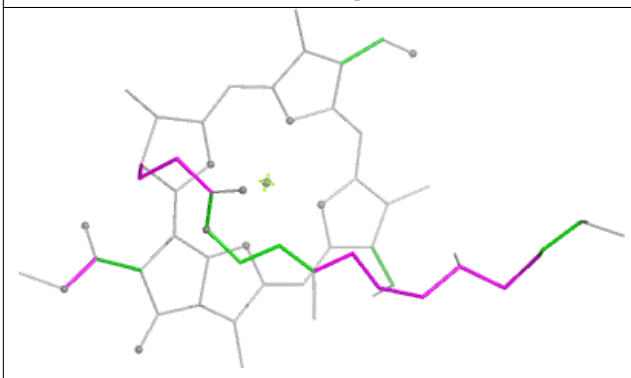
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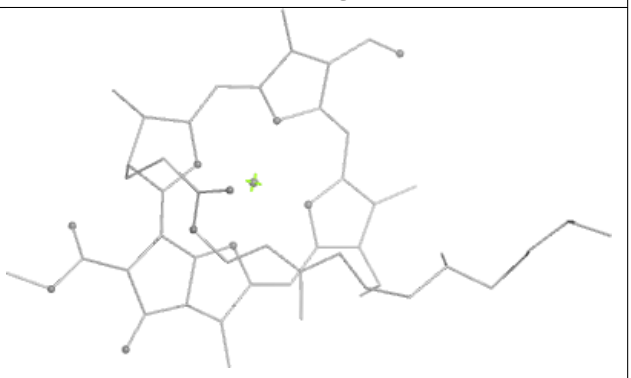
Bond lengths



Bond angles

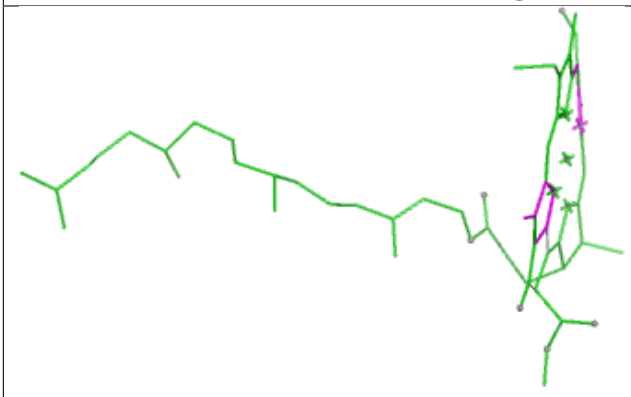


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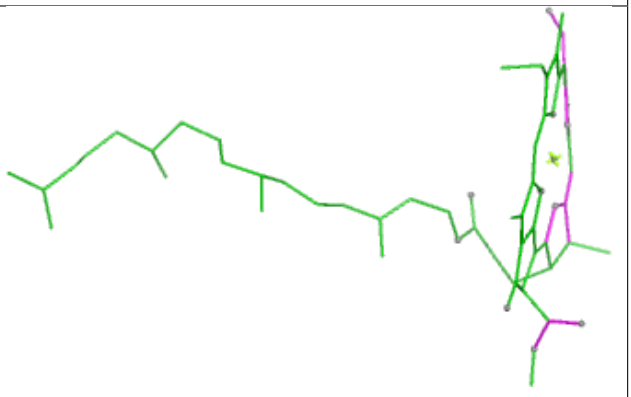


Rings

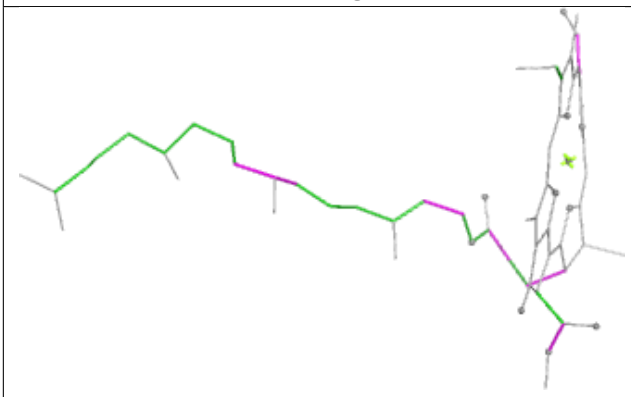
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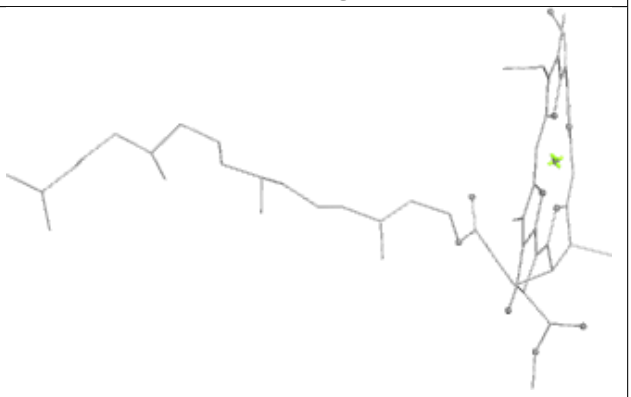
Bond lengths



Bond angles

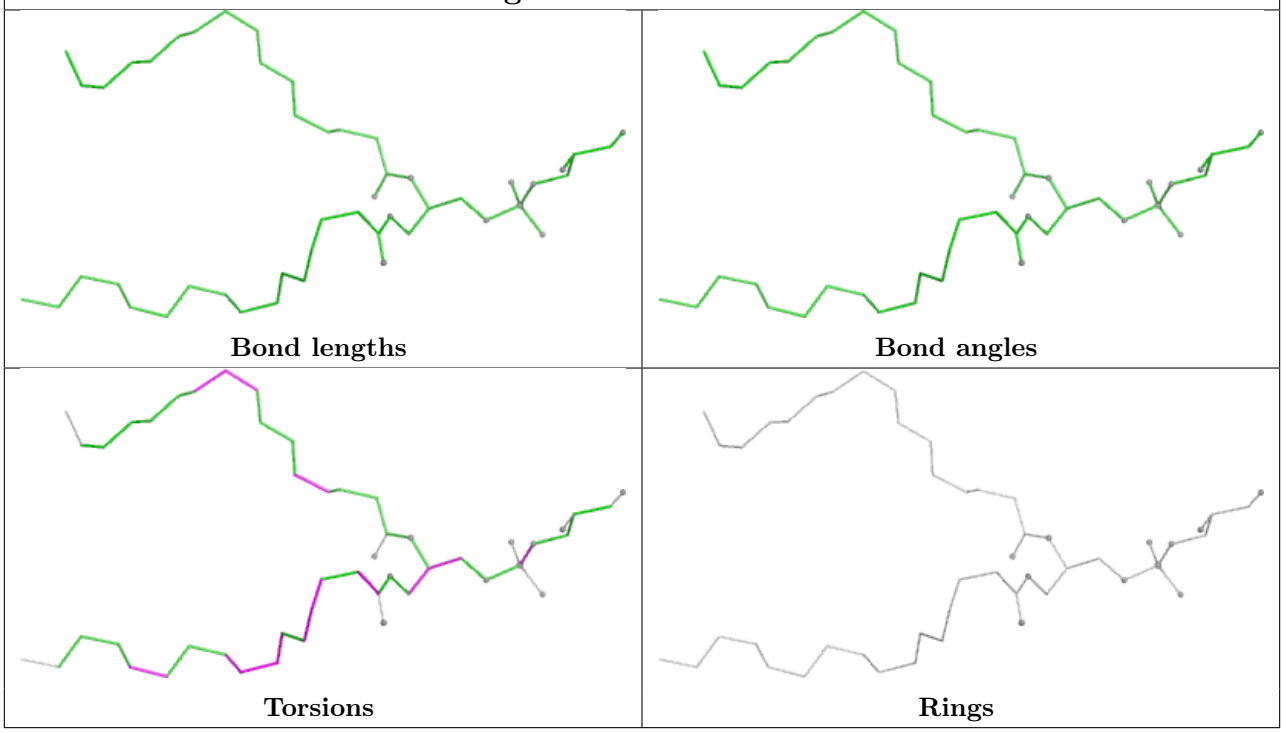


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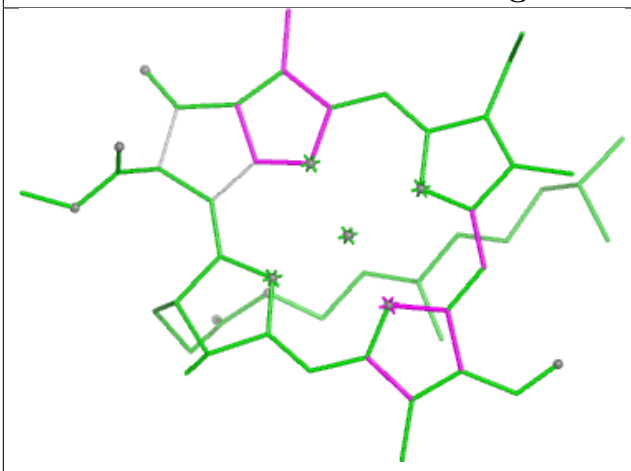


Rings

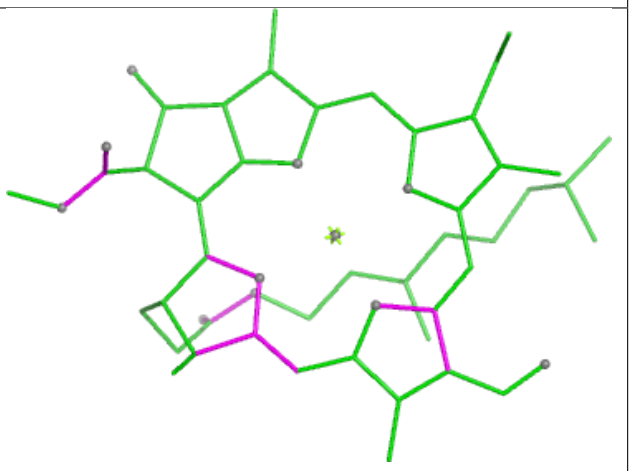
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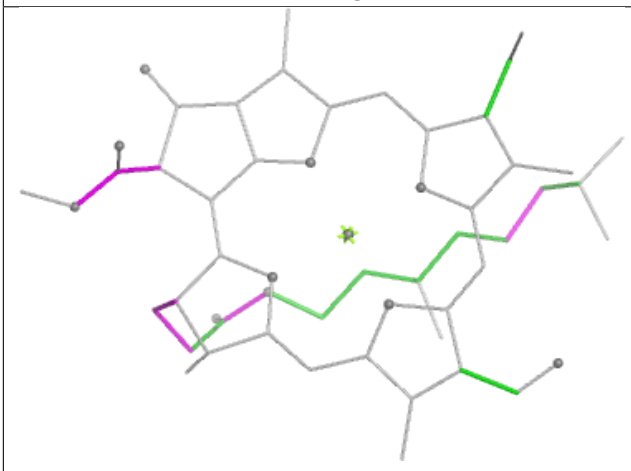
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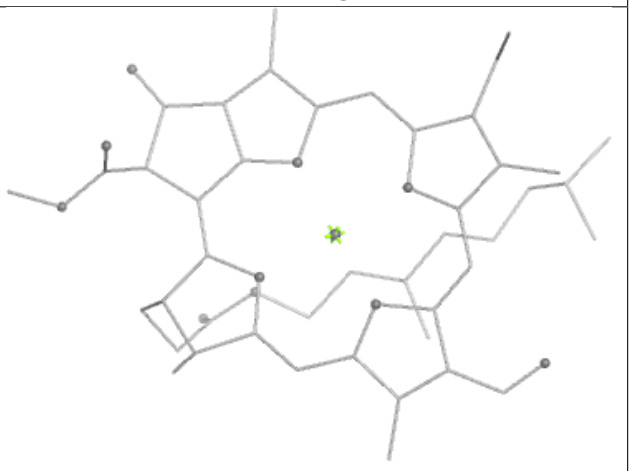
Bond lengths



Bond angles

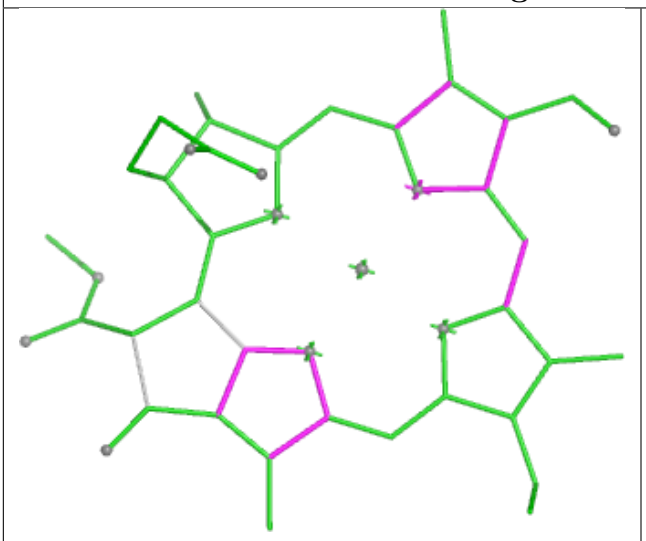


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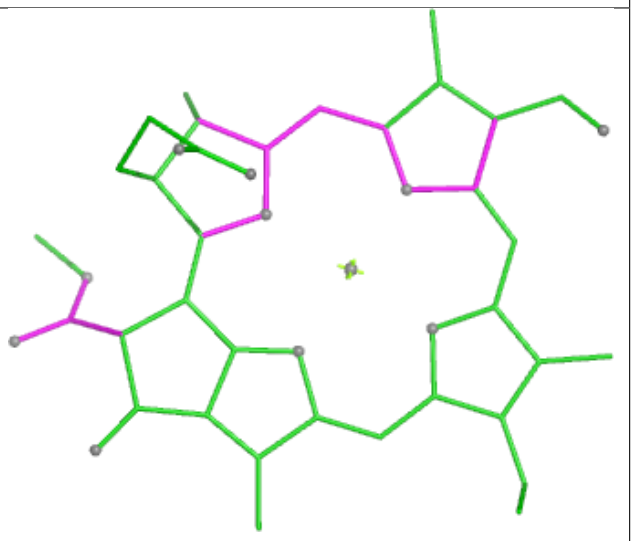


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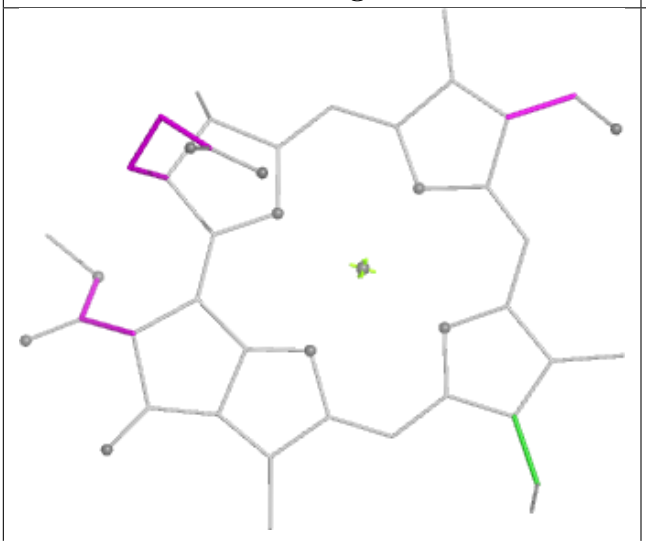
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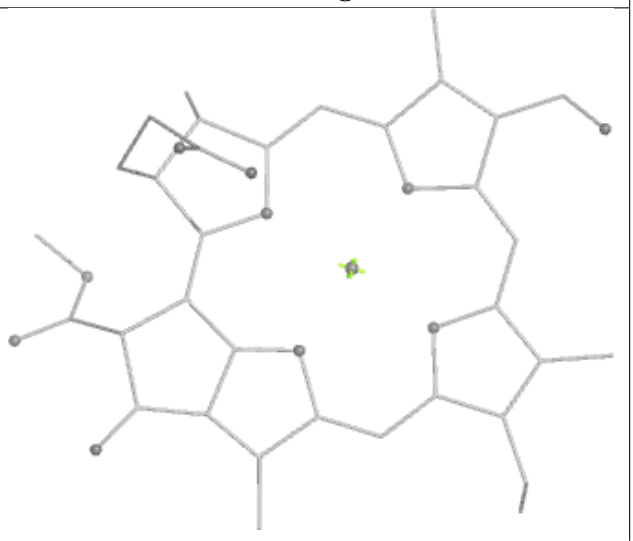
Bond lengths



Bond angles



Torsions



Rings

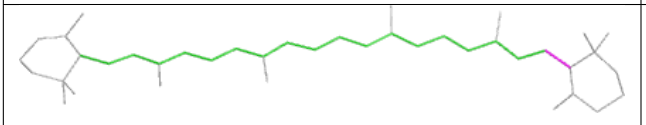
Ligand A1JPJ bA 4002



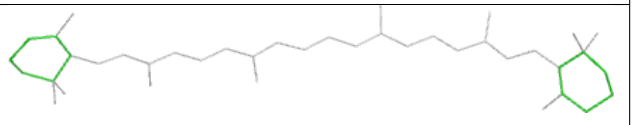
Bond lengths



Bond angles

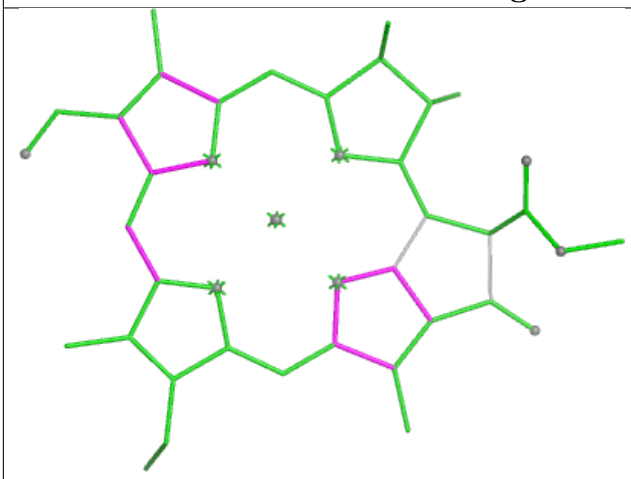


Torsions

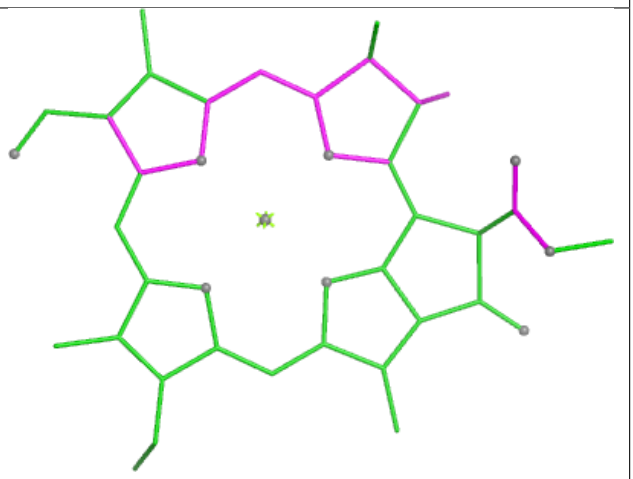


Rings

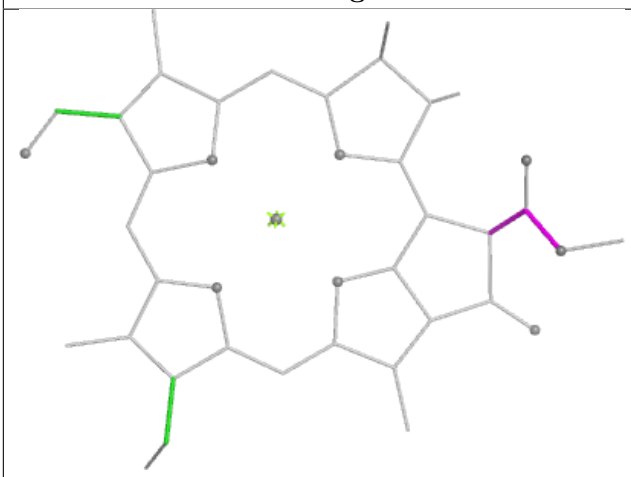
Ligand CL7 bB 1219



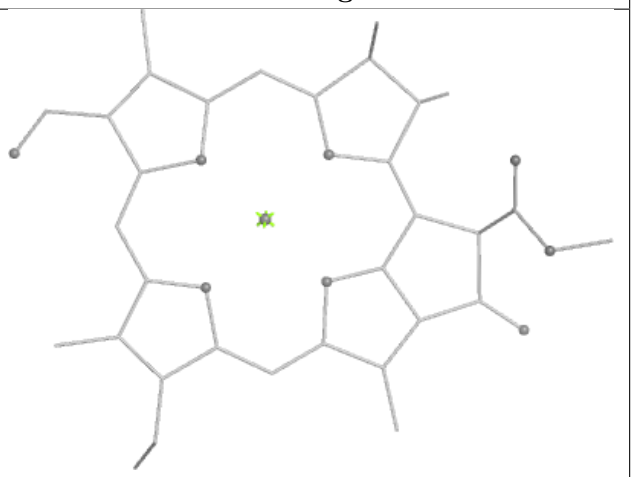
Bond lengths



Bond angles

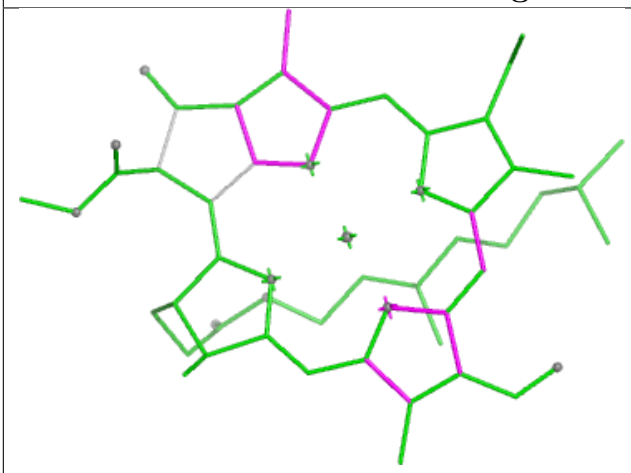


Torsions

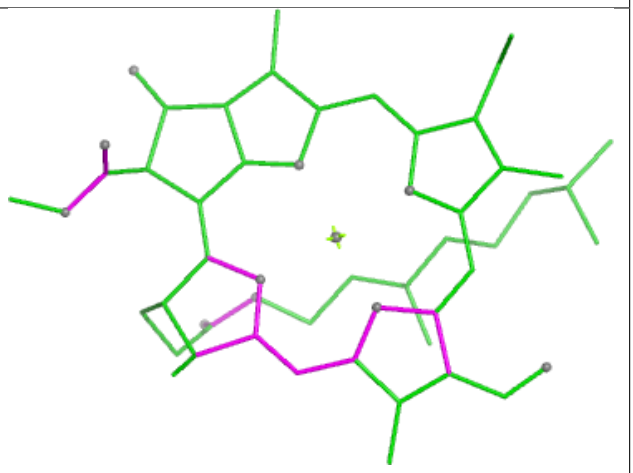


Rings

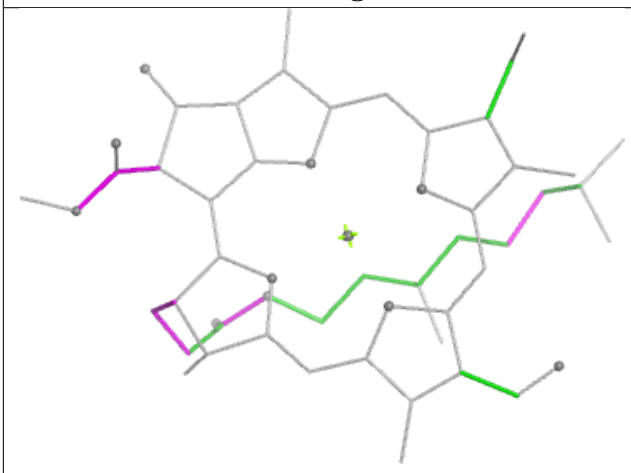
Ligand CL7 cA 1121



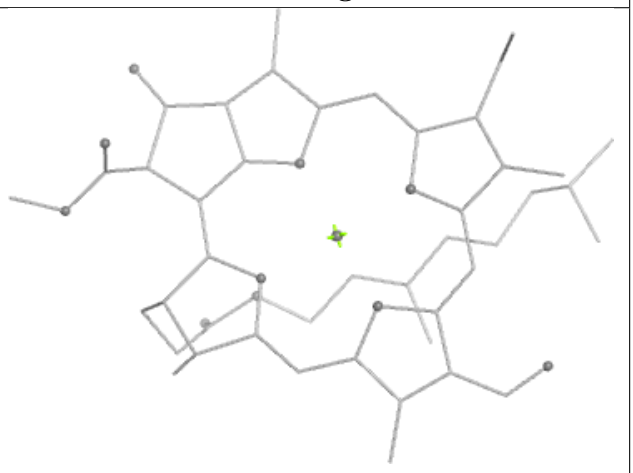
Bond lengths



Bond angles

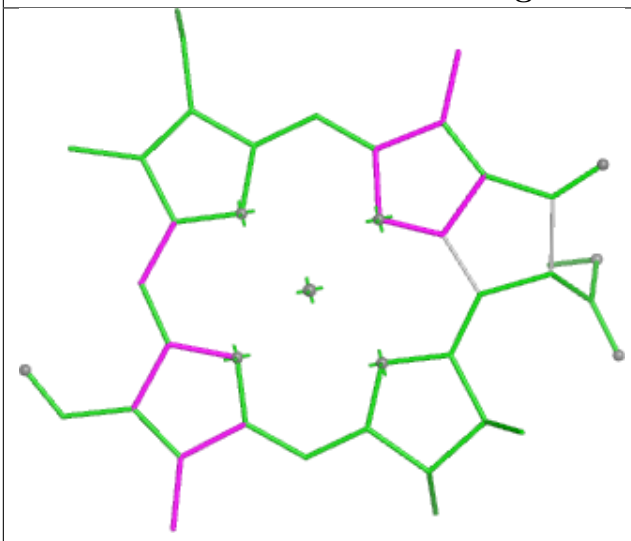


Torsions

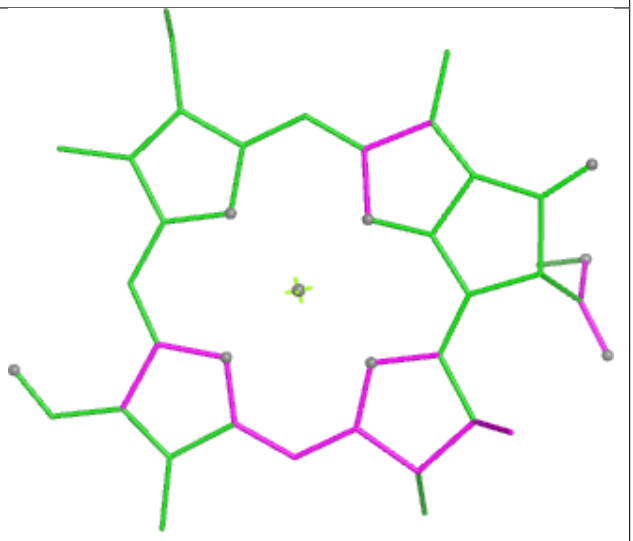


Rings

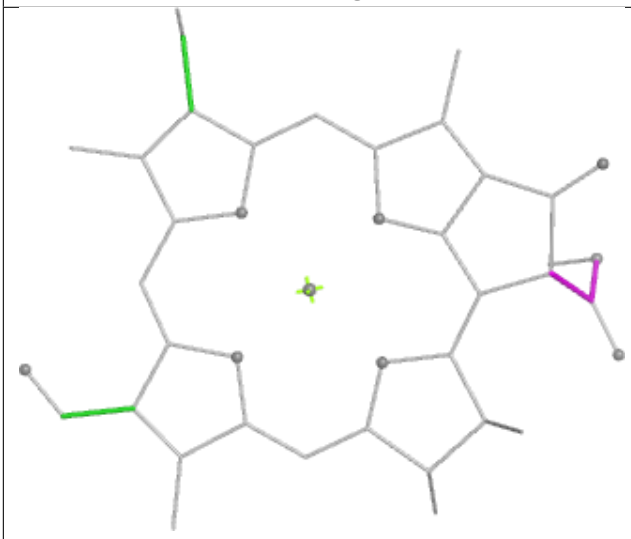
Ligand CL7 aJ 1301



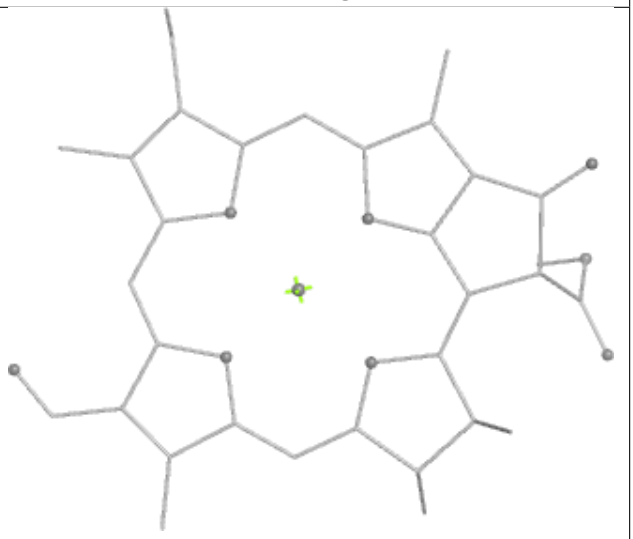
Bond lengths



Bond angles

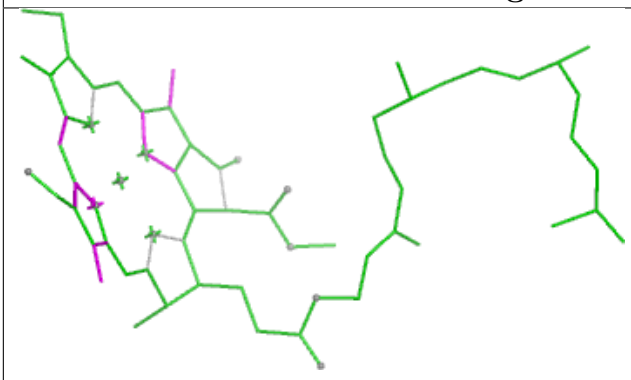


Torsions

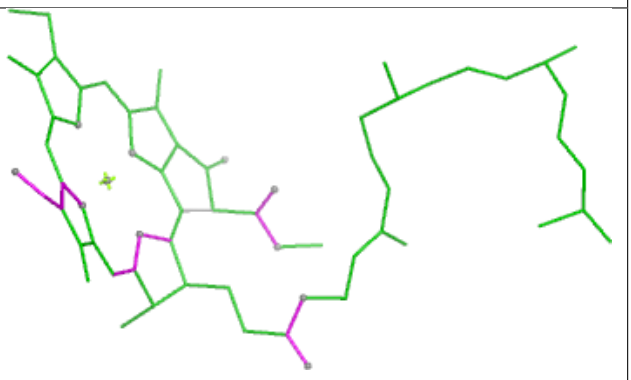


Rings

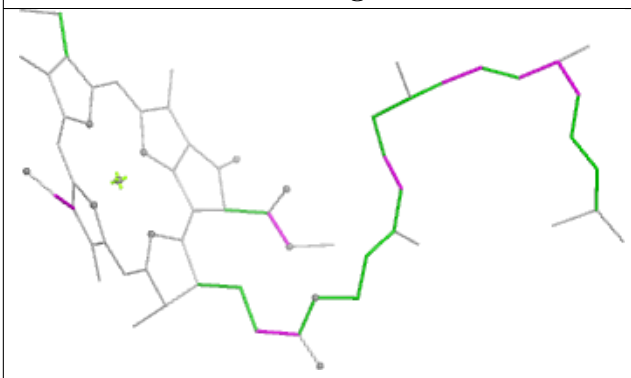
Ligand G9R aA 1011



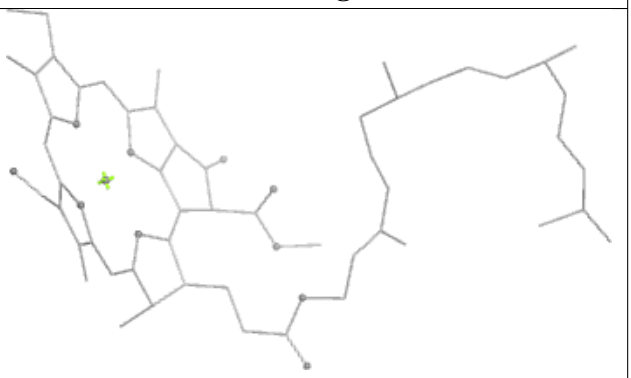
Bond lengths



Bond angles

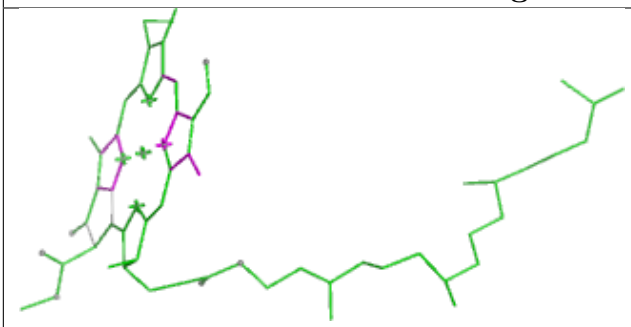


Torsions

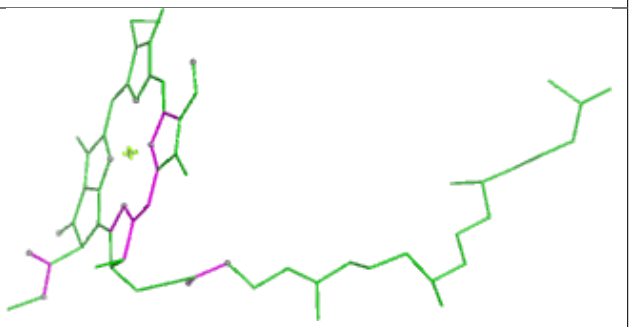


Rings

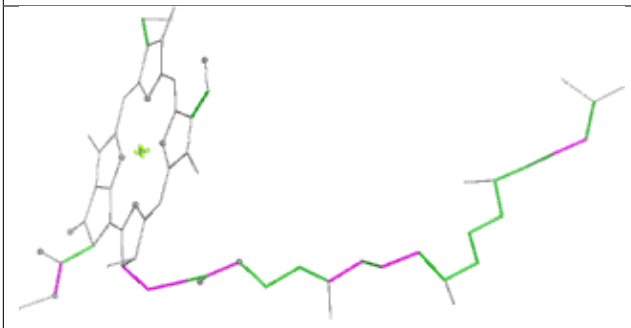
Ligand CL7 aA 1133



Bond lengths



Bond angles

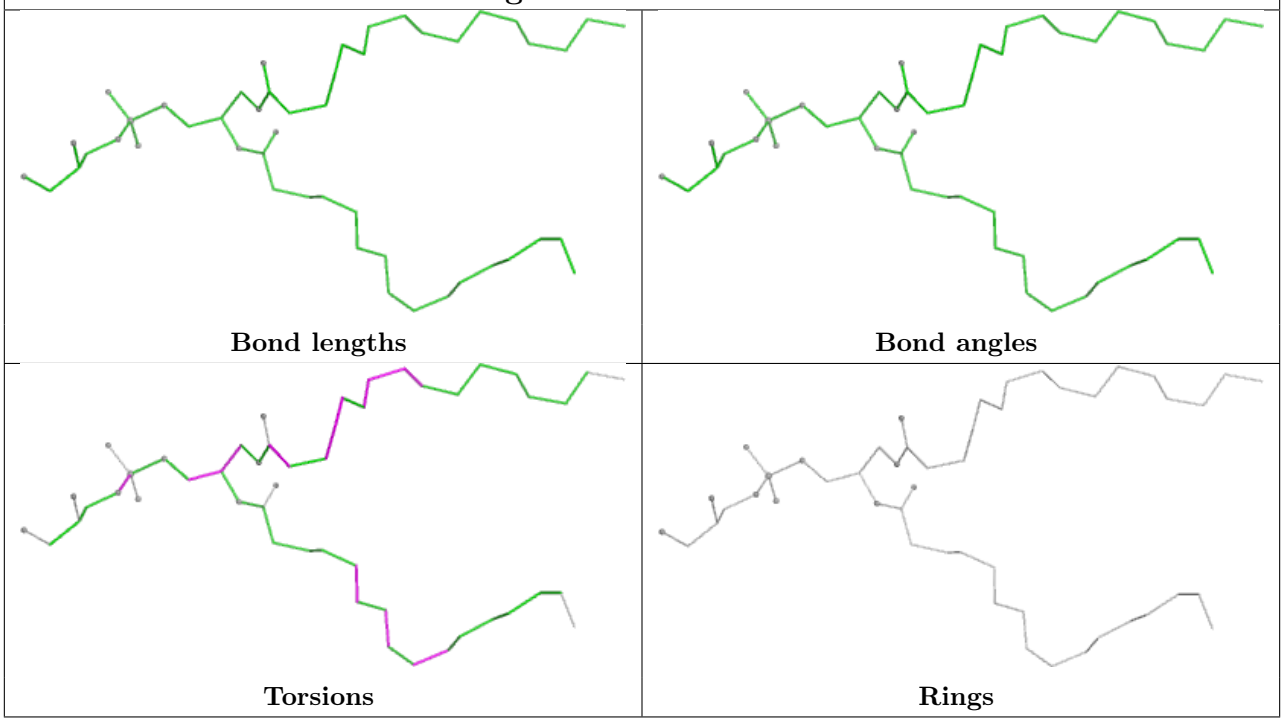


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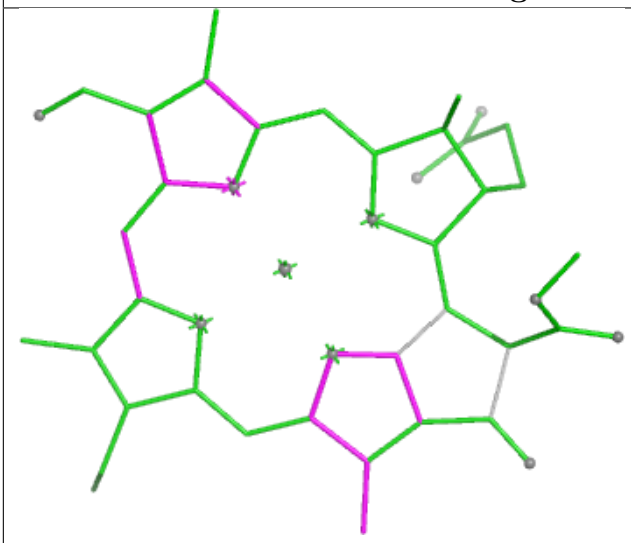


Rings

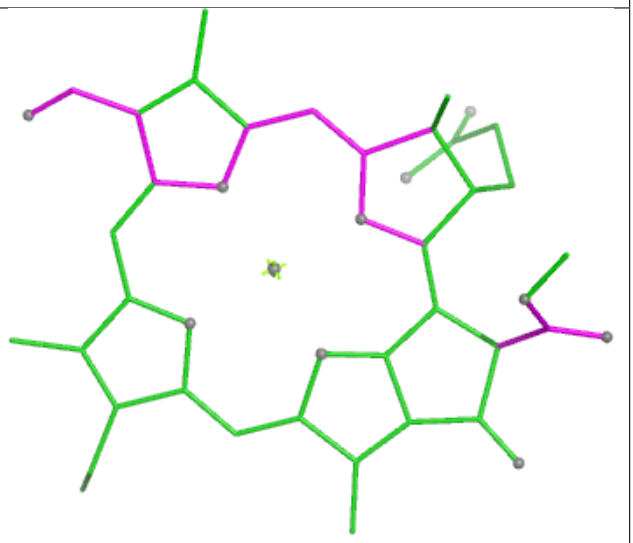
Ligand LHG aA 5001



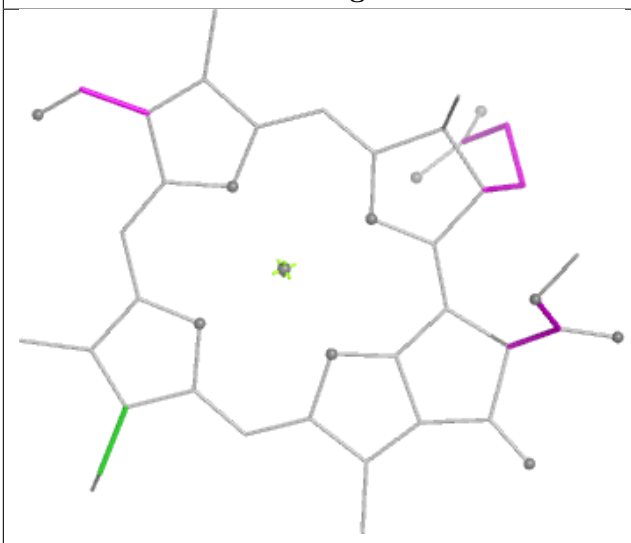
Ligand CL7 bB 1212



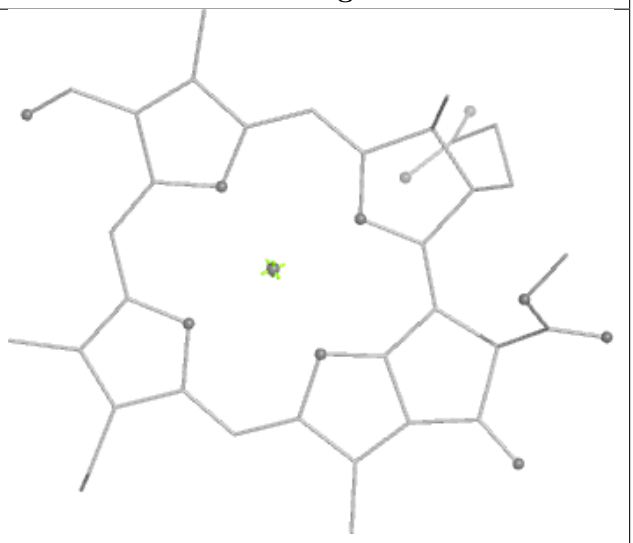
Bond lengths



Bond angles

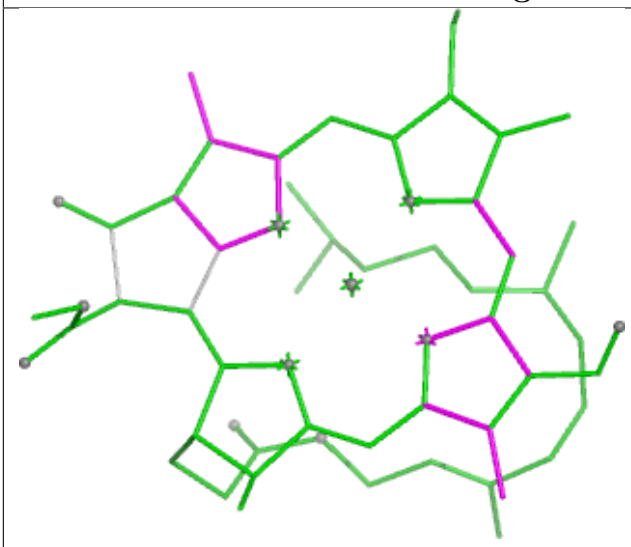


Torsions

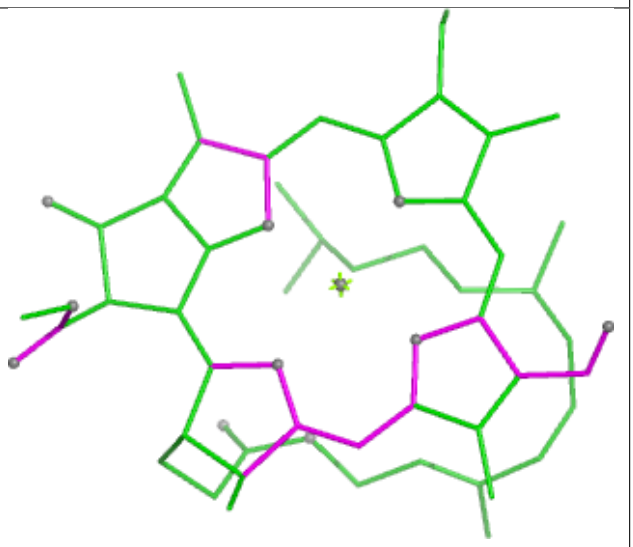


Rings

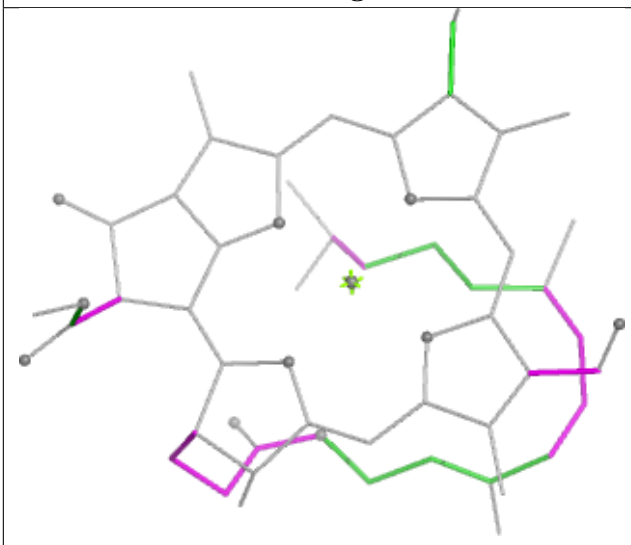
Ligand CL7 aL 1501



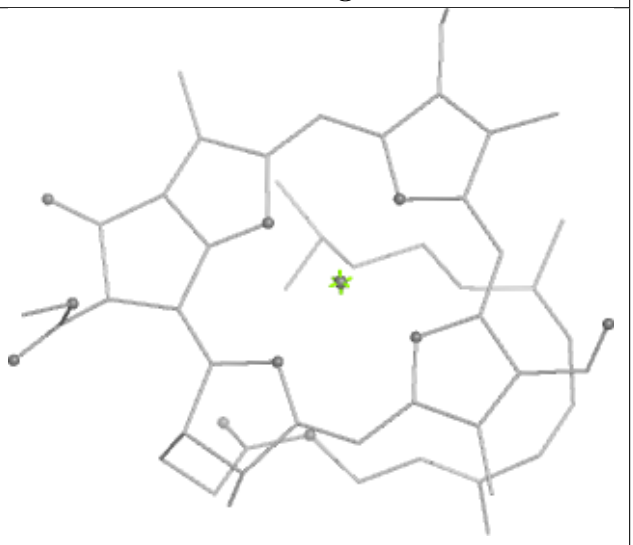
Bond lengths



Bond angles

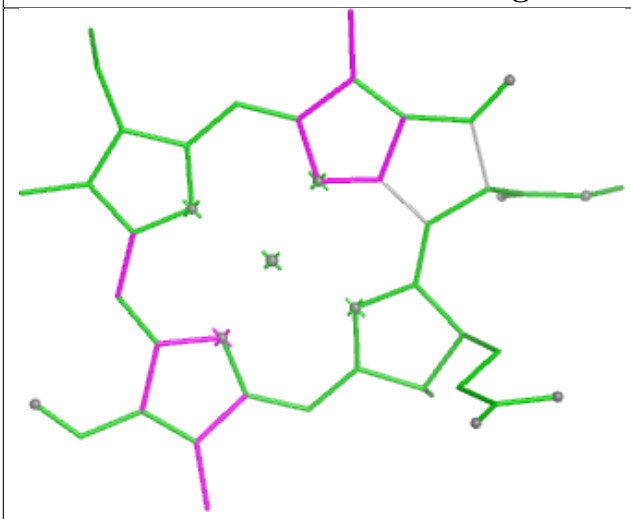


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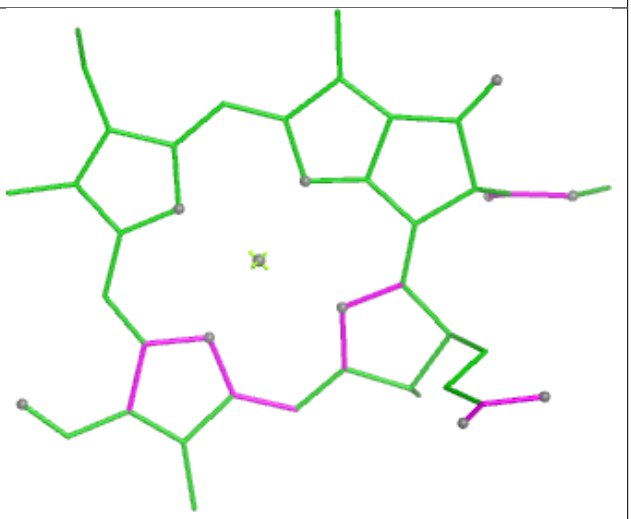


Rings

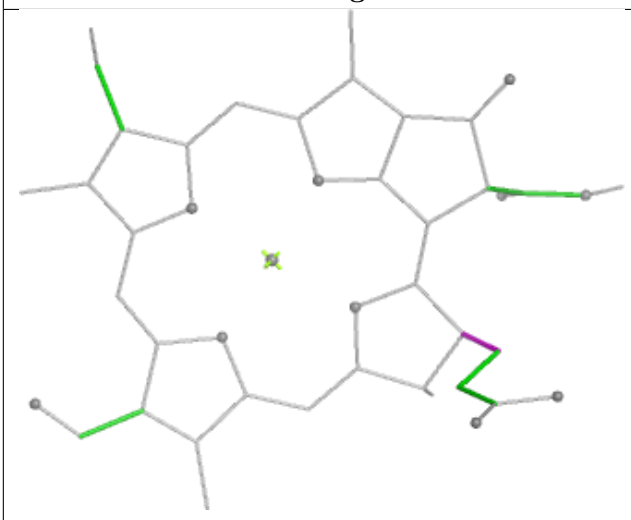
Ligand CL7 cB 1231



Bond lengths



Bond angles

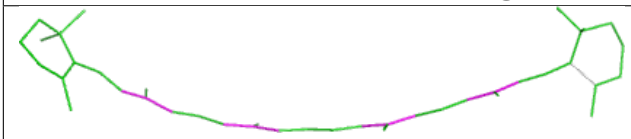


Torsions

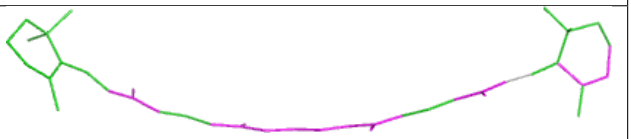


Rings

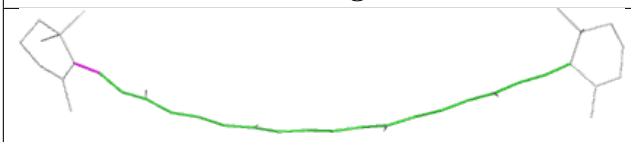
Ligand A1JPJ cI 4018



Bond lengths



Bond angles

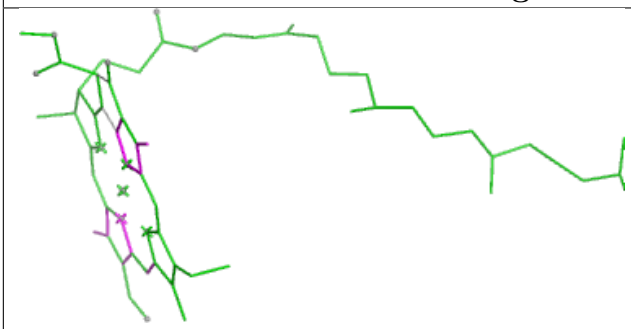


Torsions

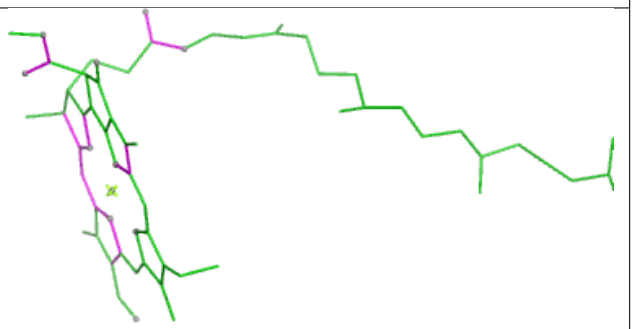


Rings

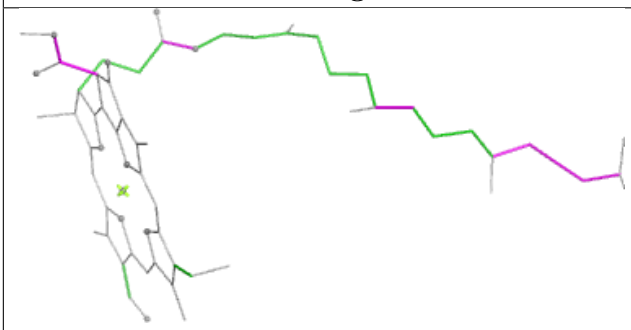
Ligand CL7 cB 1226



Bond lengths



Bond angles

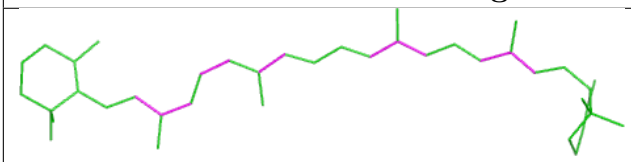


Torsions

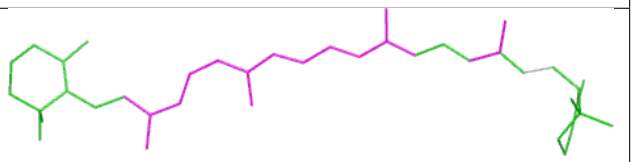


Rings

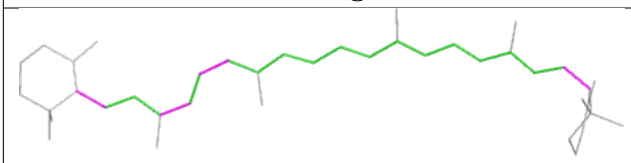
Ligand A1JPJ aB 4010



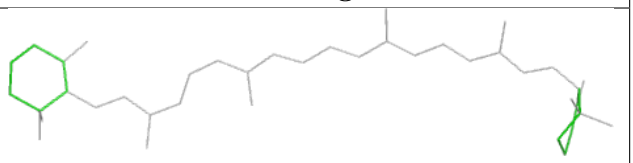
Bond lengths



Bond angles

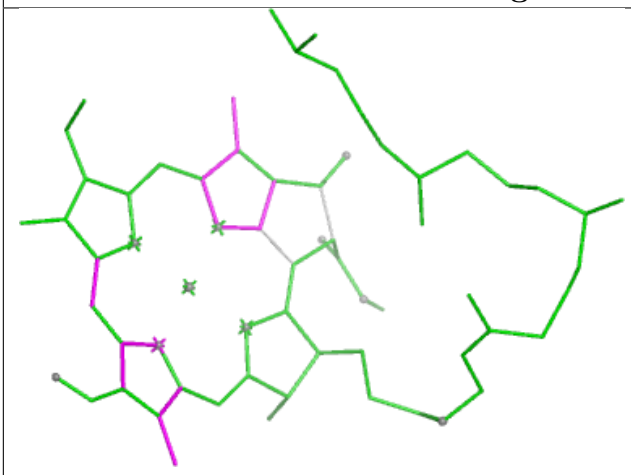


Torsions

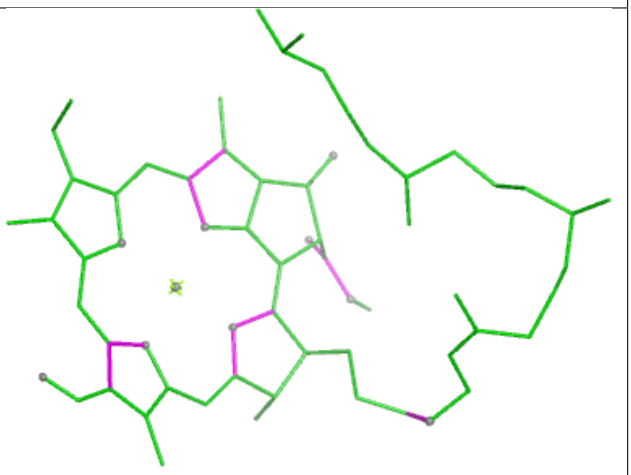


Rings

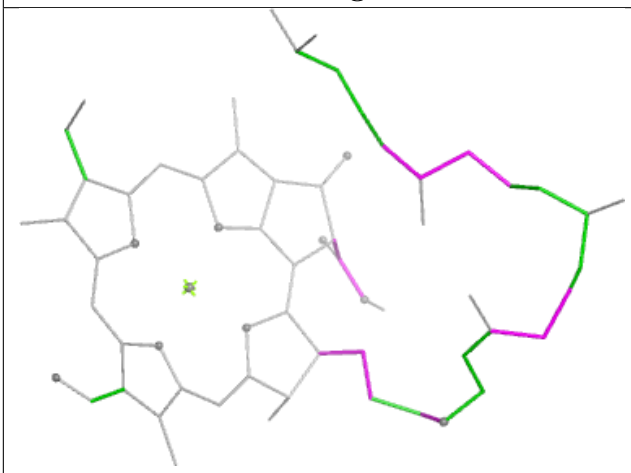
Ligand CL7 aA 1127



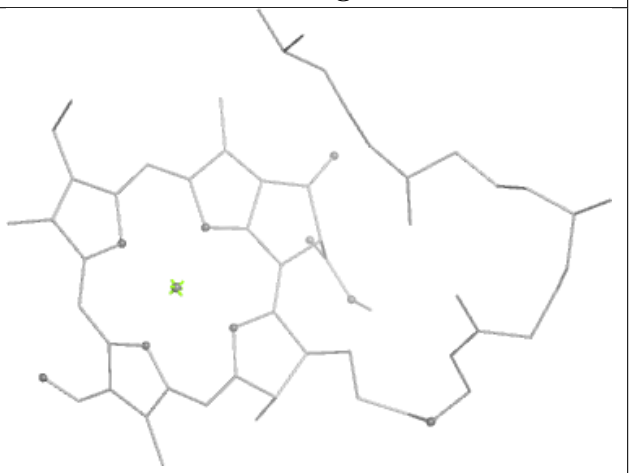
Bond lengths



Bond angles

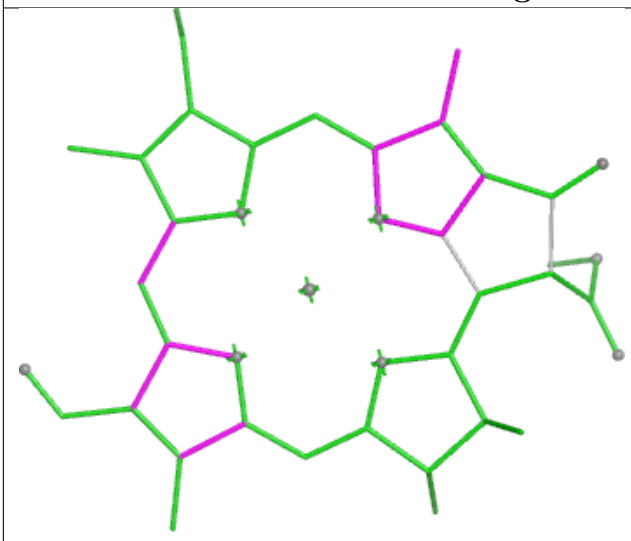


Torsions

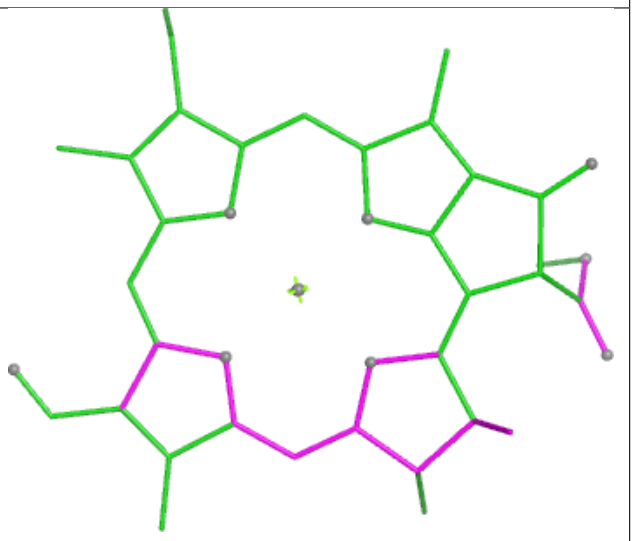


Rings

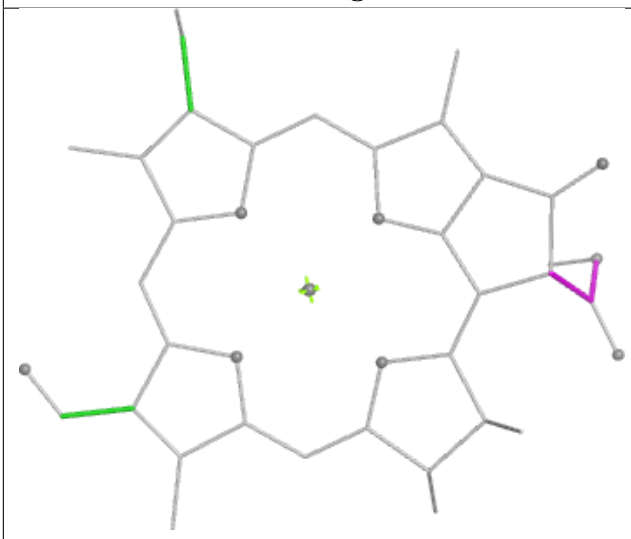
Ligand CL7 bJ 1301



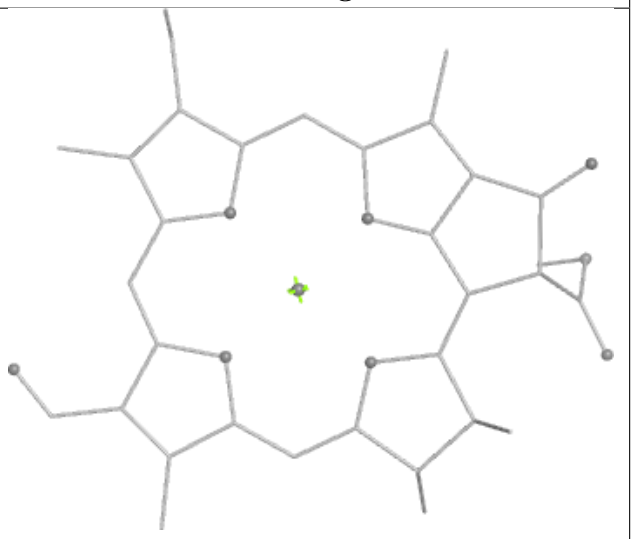
Bond lengths



Bond angles

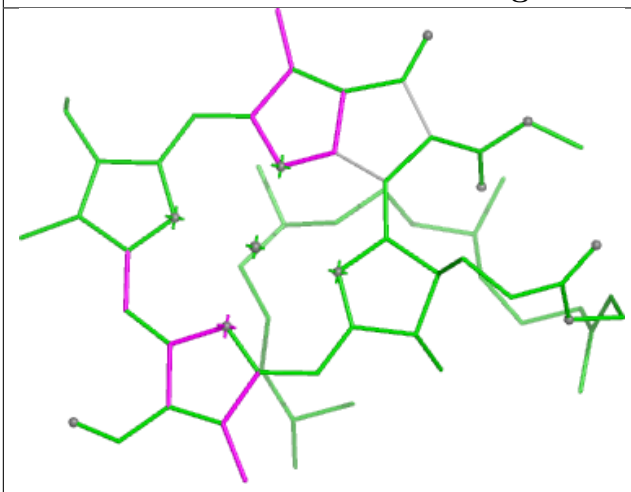


Torsions

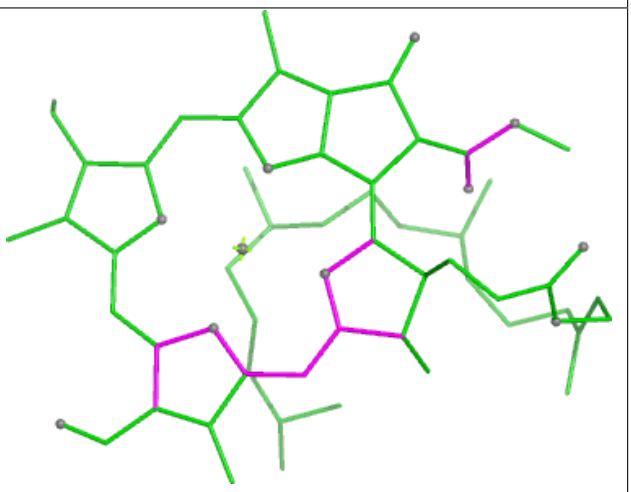


Rings

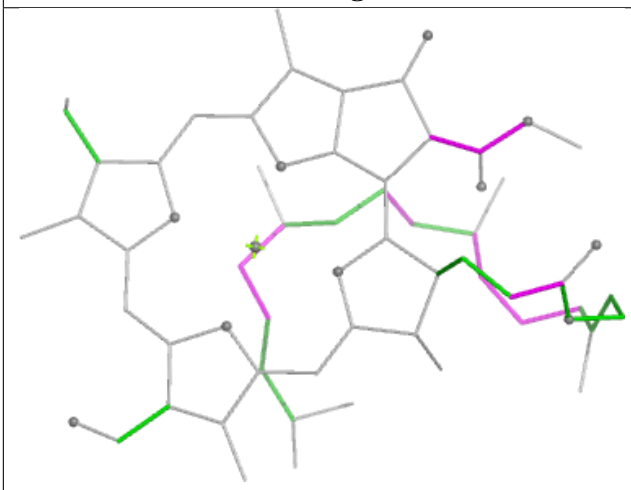
Ligand CL7 aB 1203



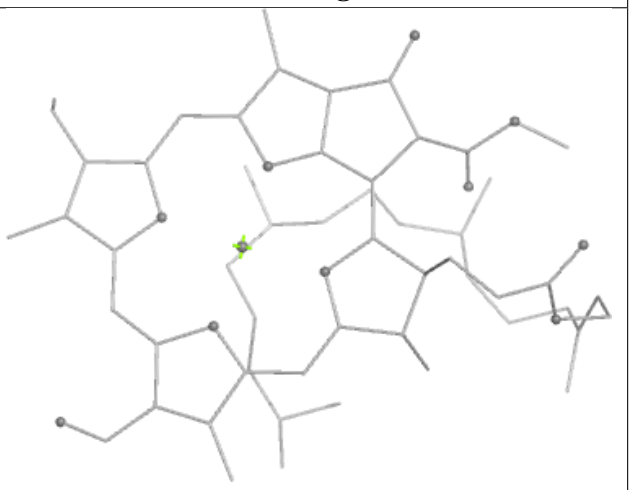
Bond lengths



Bond angles

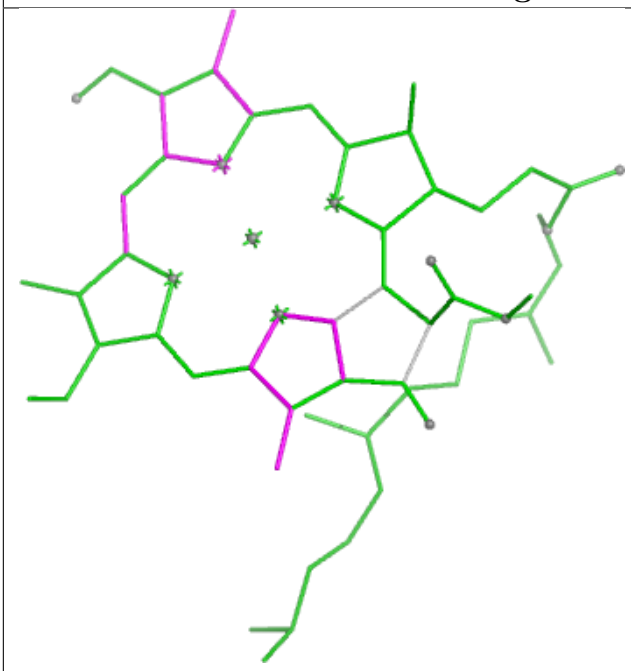


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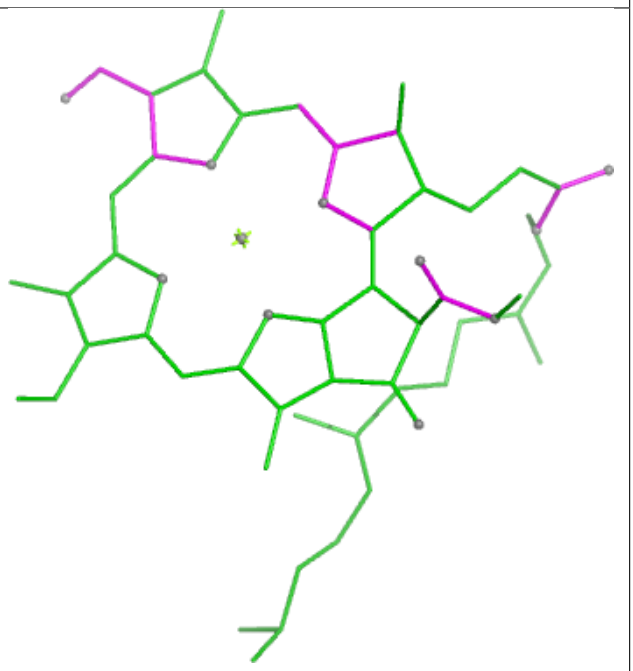


Rings

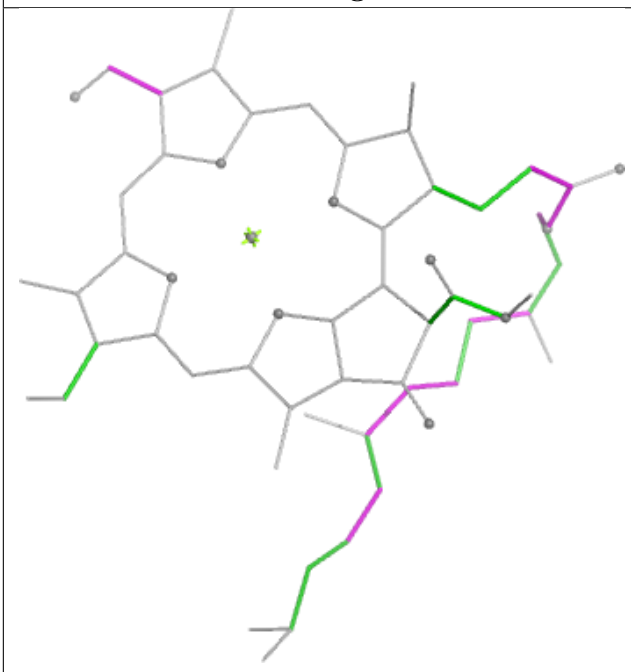
Ligand CL7 cL 1503



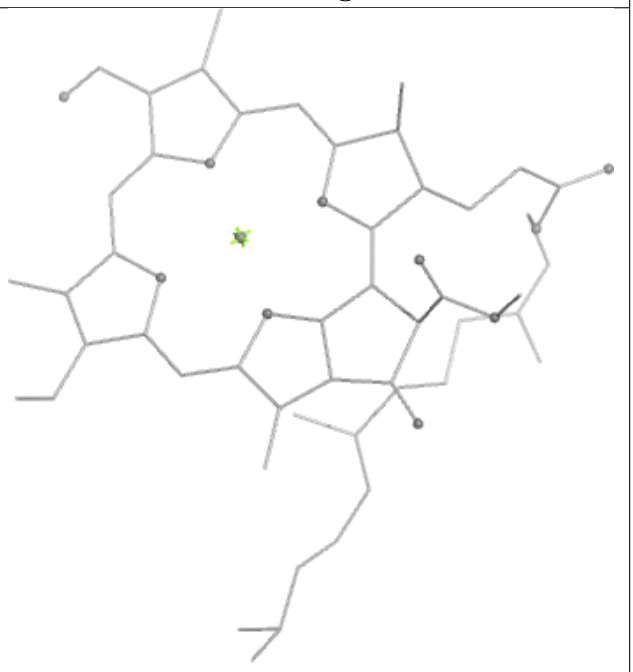
Bond lengths



Bond angles

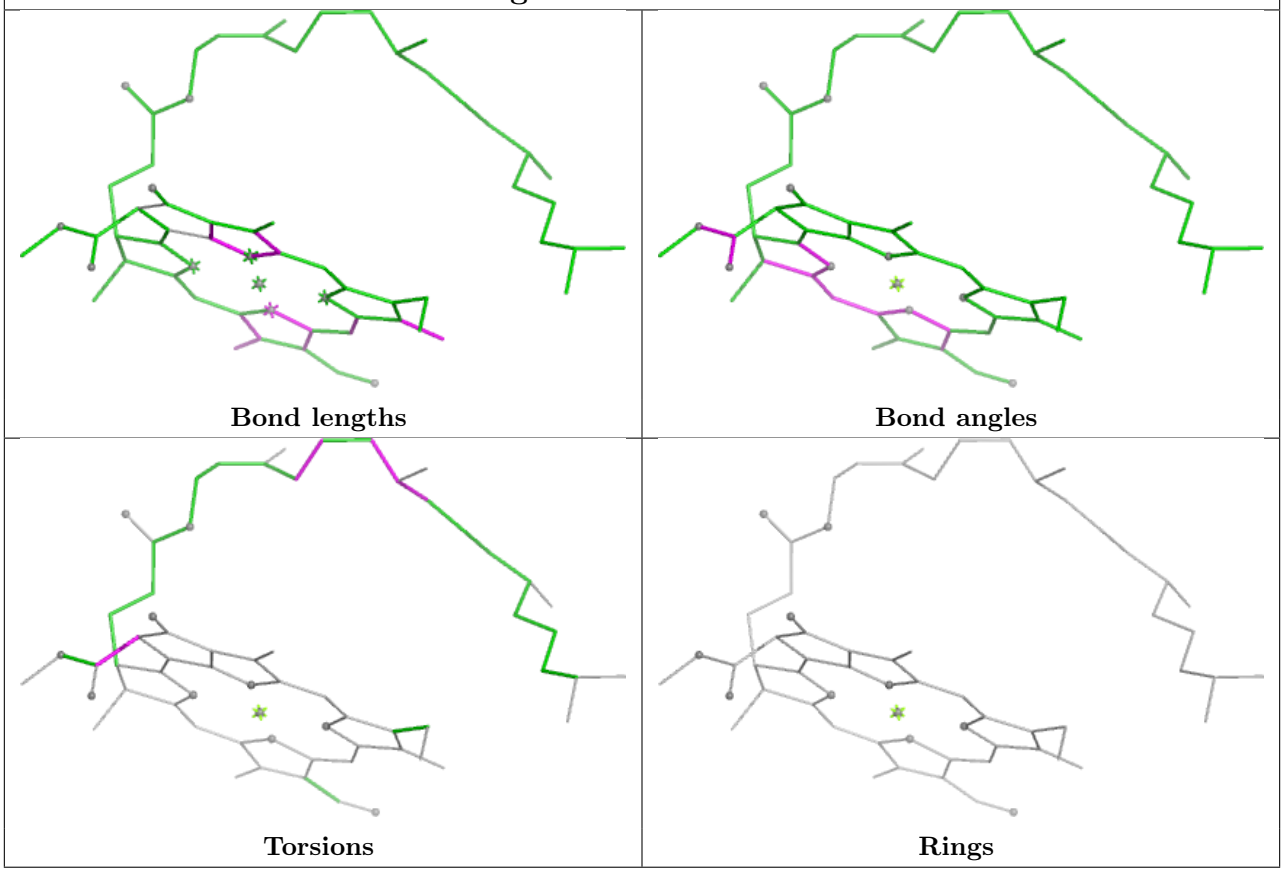


Torsions

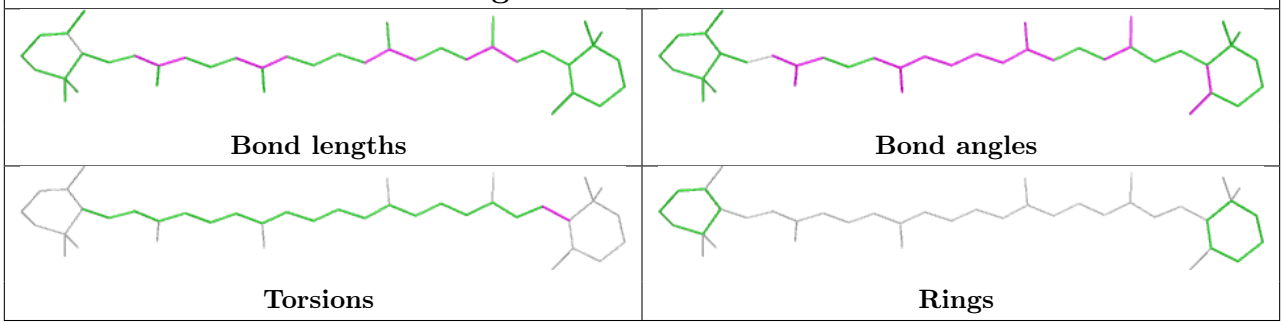


Rings

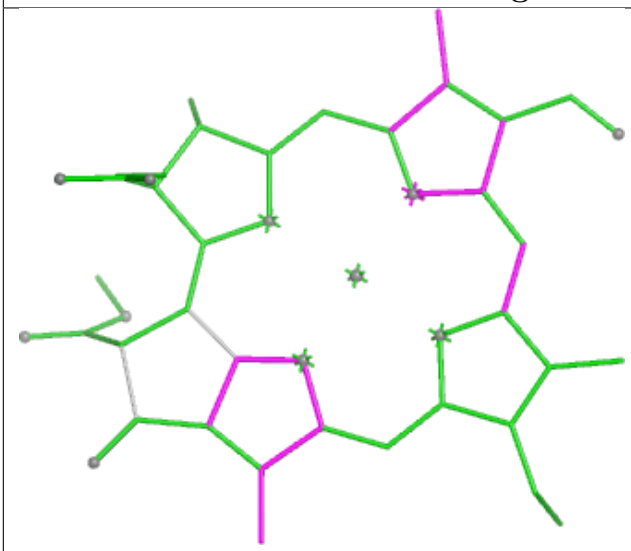
Ligand CL7 bA 1122



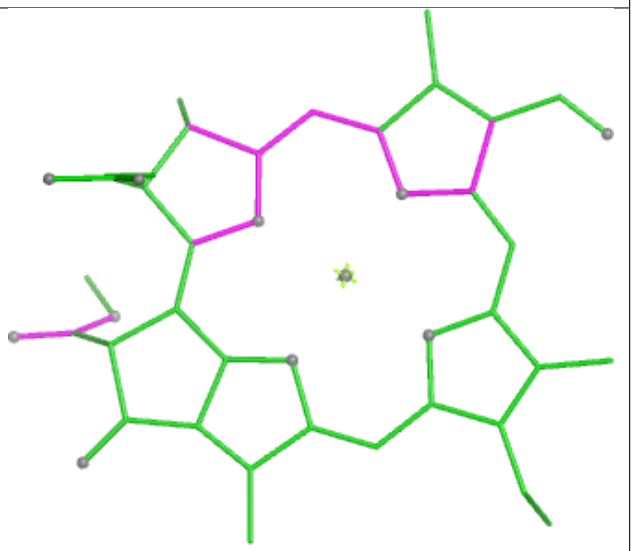
Ligand A1JPJ cA 4003



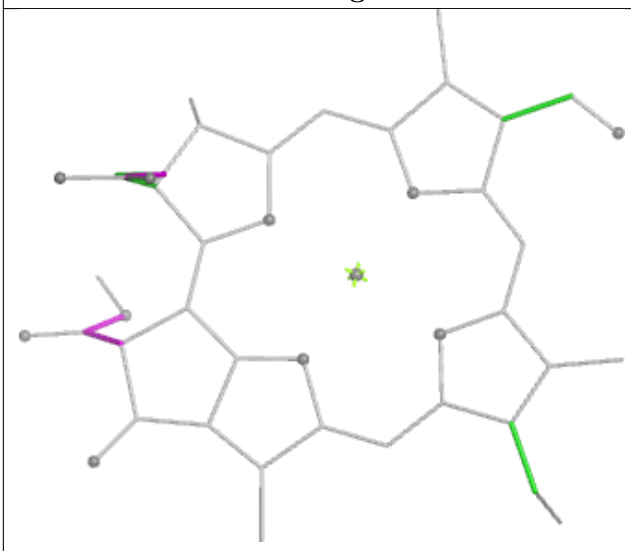
Ligand CL7 cA 1105



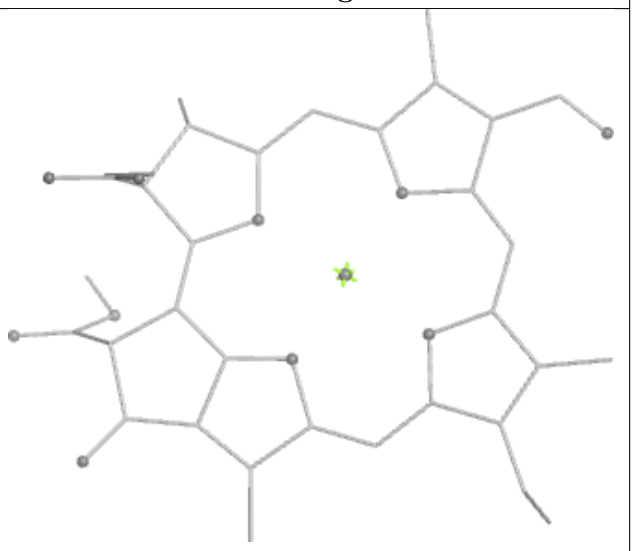
Bond lengths



Bond angles

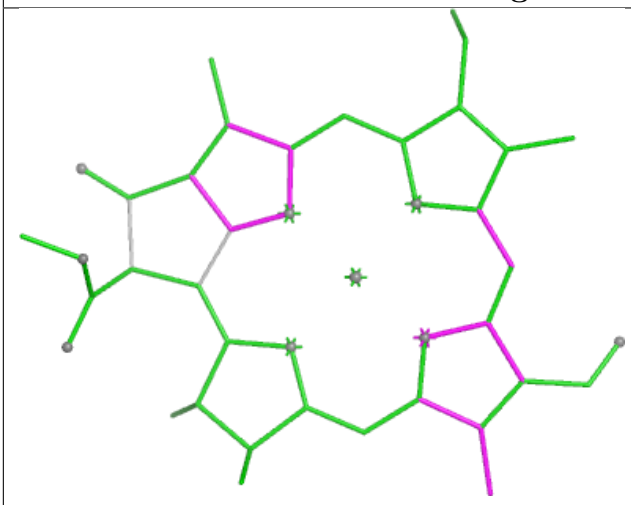


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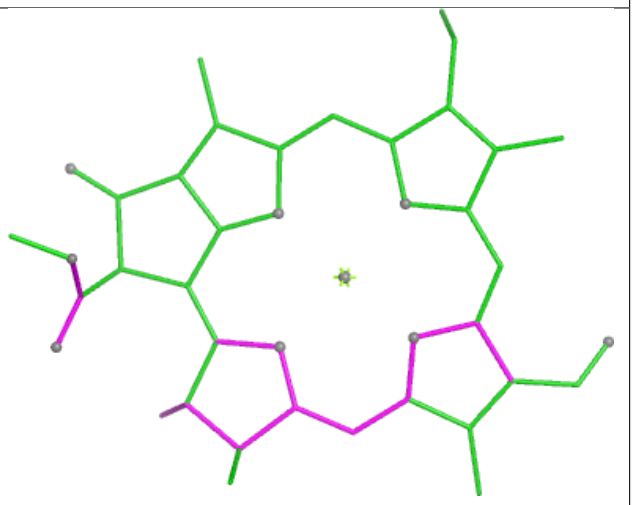


Rings

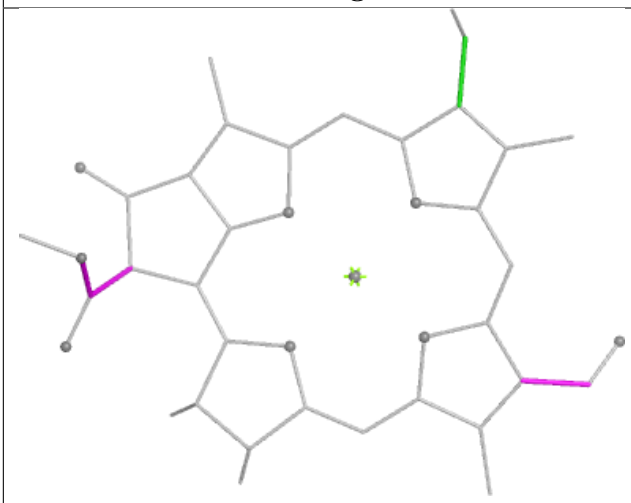
Ligand CL7 aA 1801



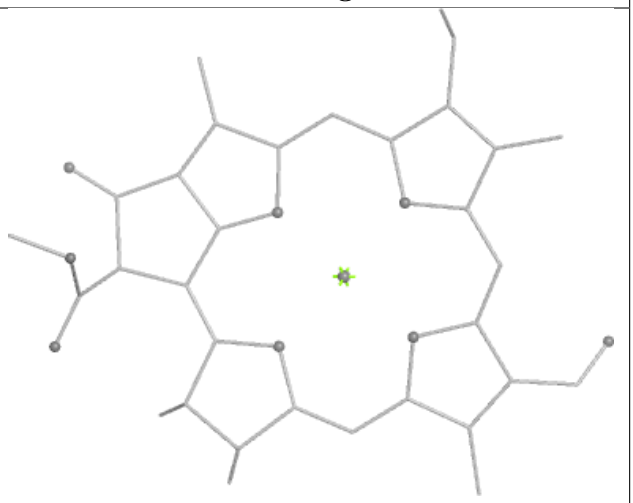
Bond lengths



Bond angles

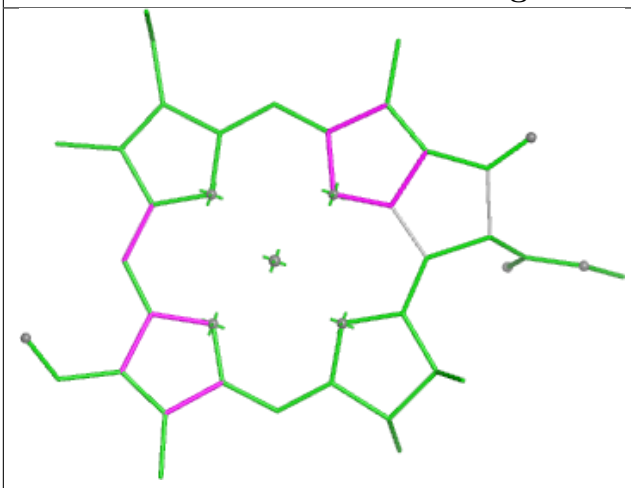


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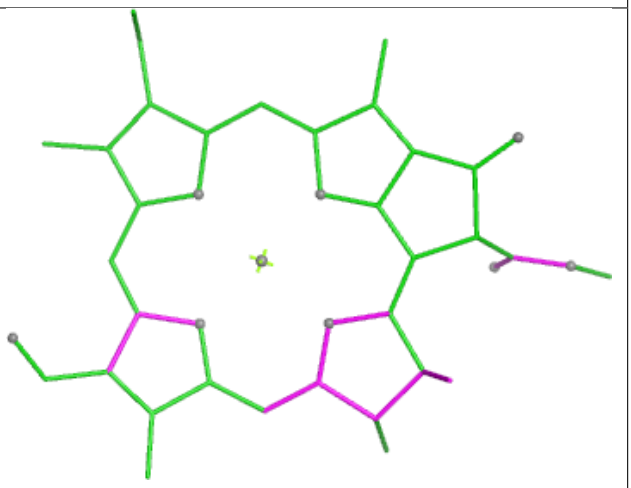


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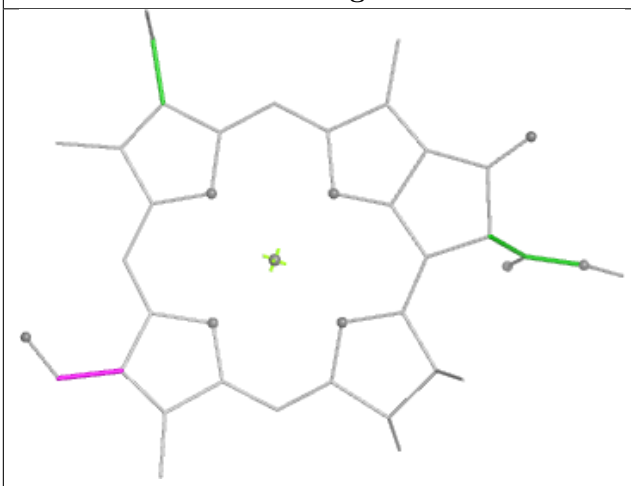
Ligand CL7 bB 1233



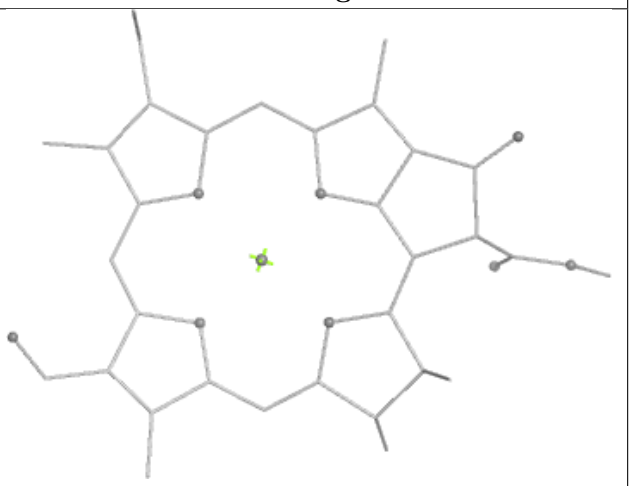
Bond lengths



Bond angles

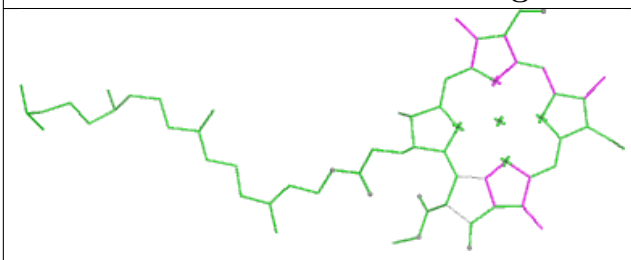


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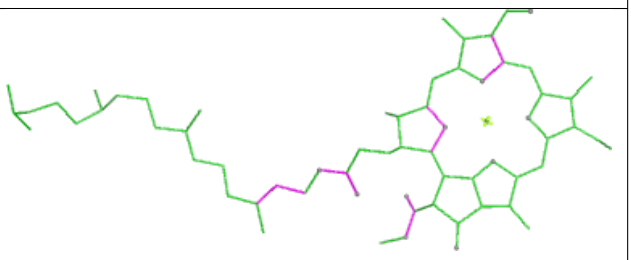


Rings

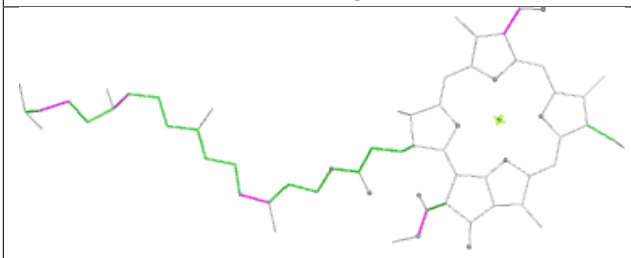
Ligand CL7 cA 1131



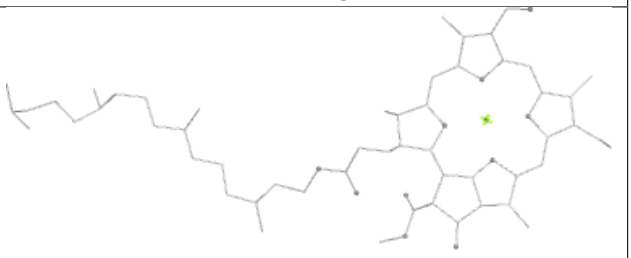
Bond lengths



Bond angles

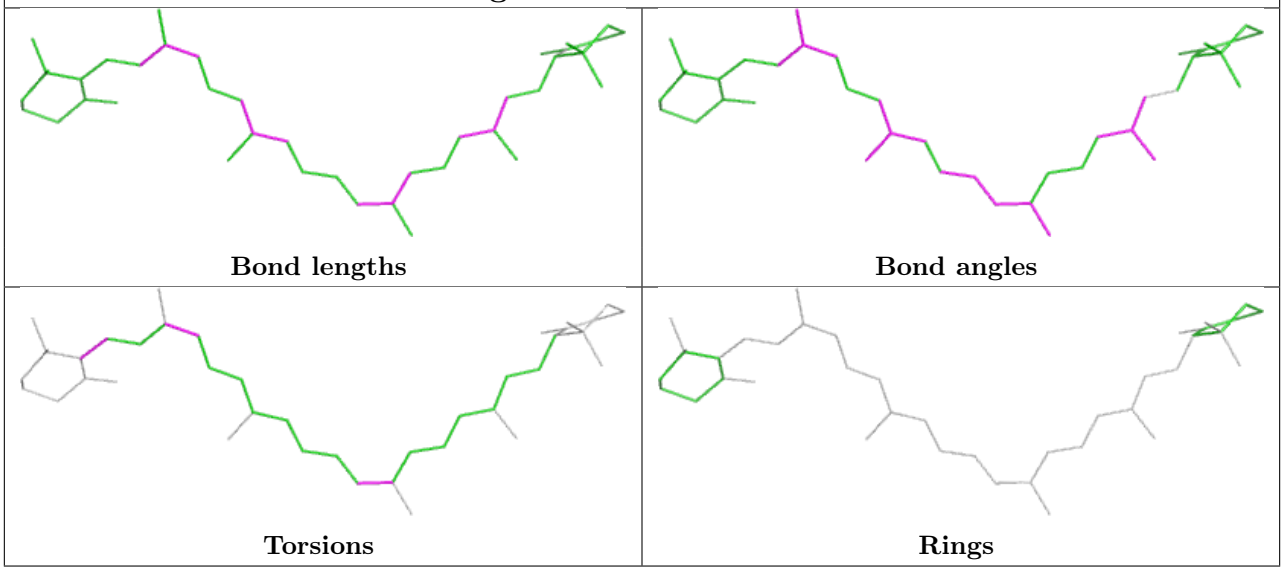


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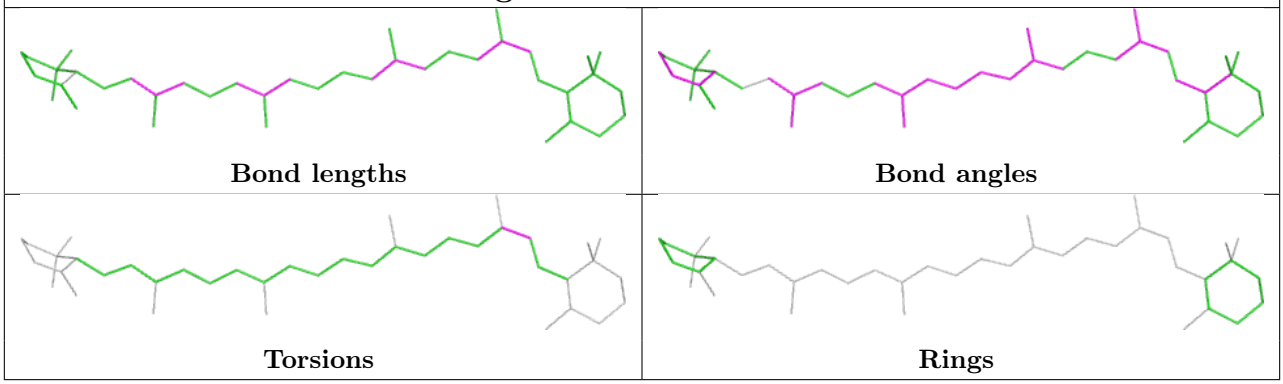


Rings

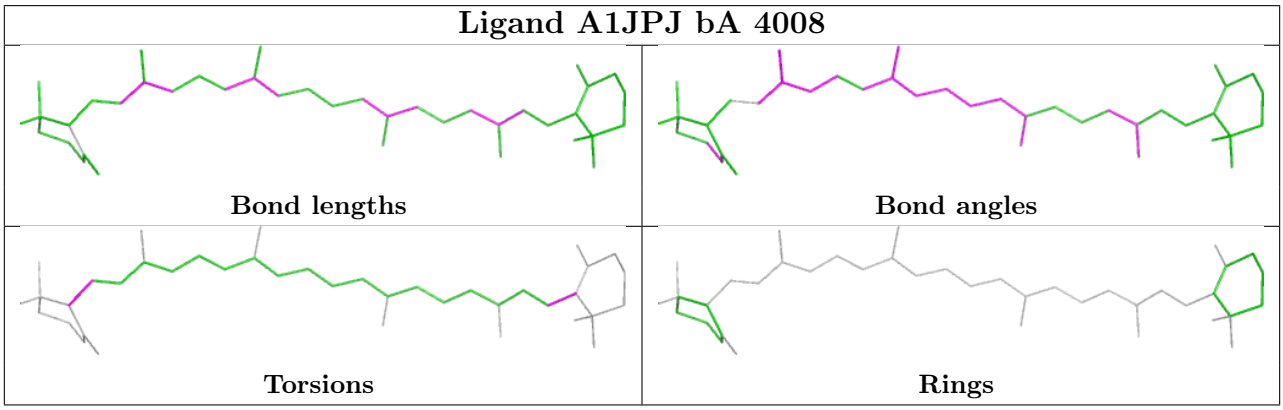
Ligand A1JPJ bA 4011



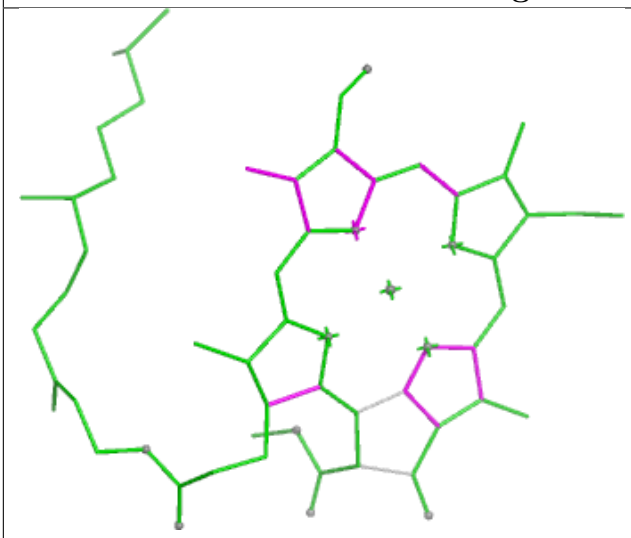
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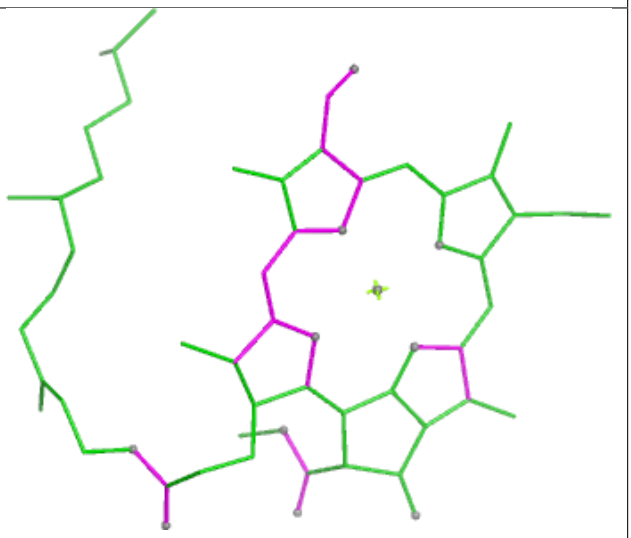
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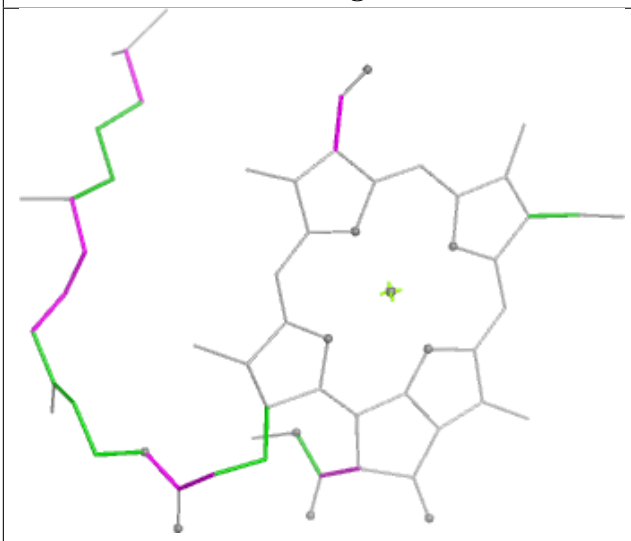
Ligand CL7 cB 1221



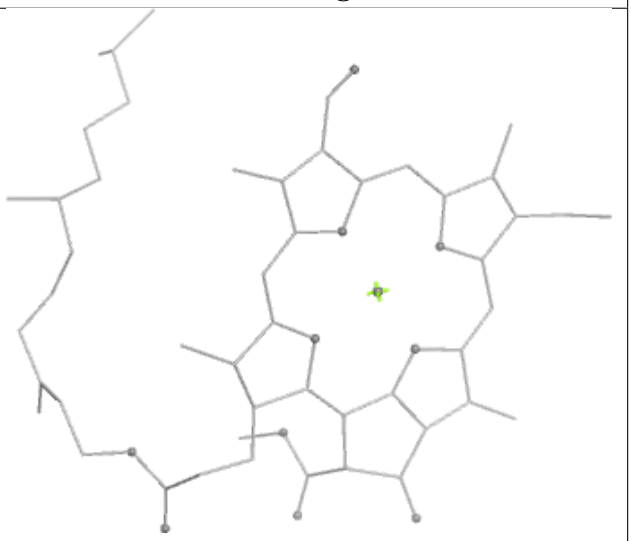
Bond lengths



Bond angles

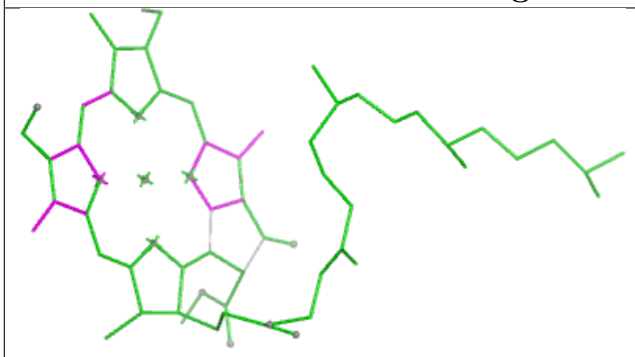


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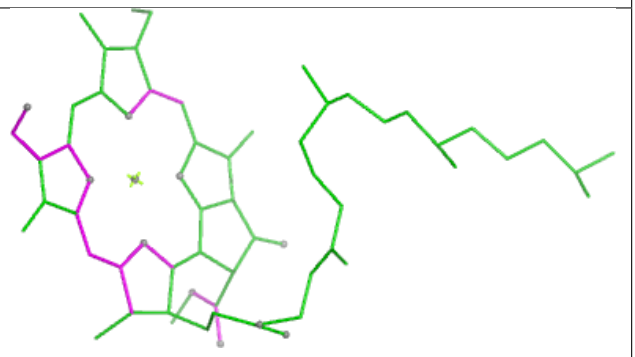


Rings

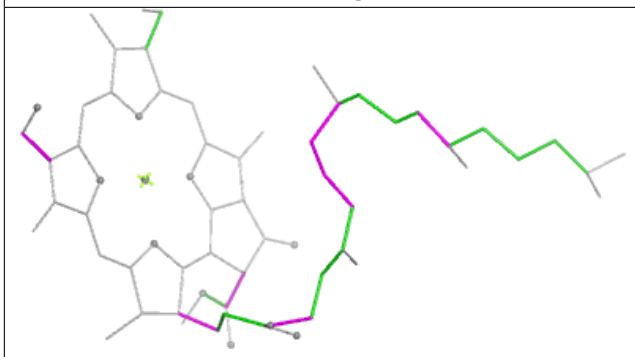
Ligand CL7 aA 1112



Bond lengths



Bond angles

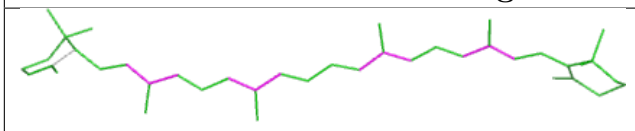


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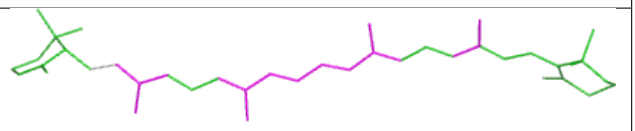


Rings

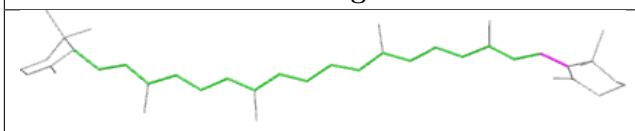
Ligand A1JPJ bI 4019



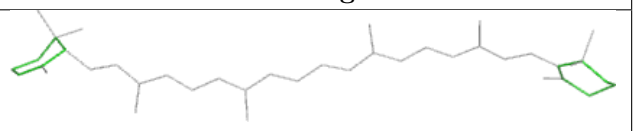
Bond lengths



Bond angles

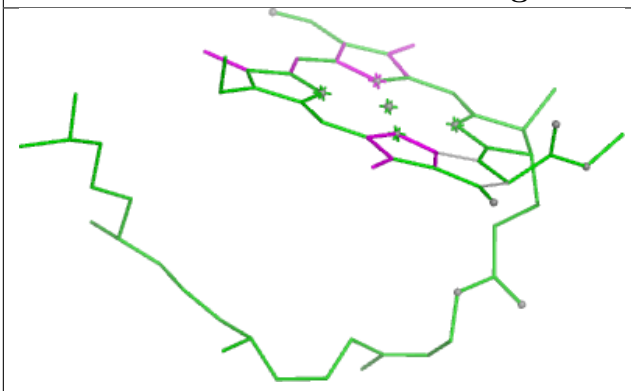


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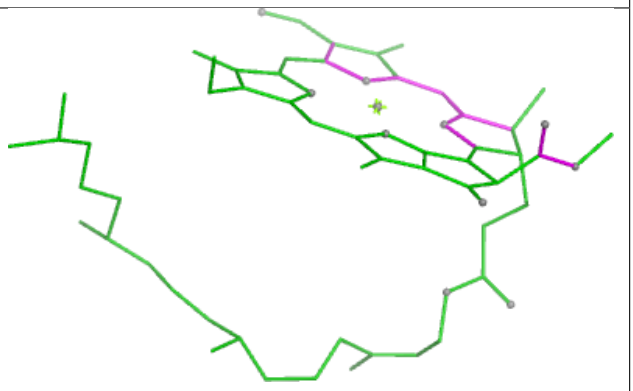


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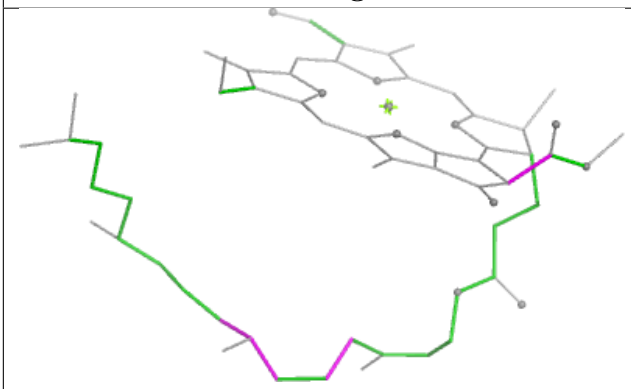
Ligand CL7 aA 1122



Bond lengths



Bond angles

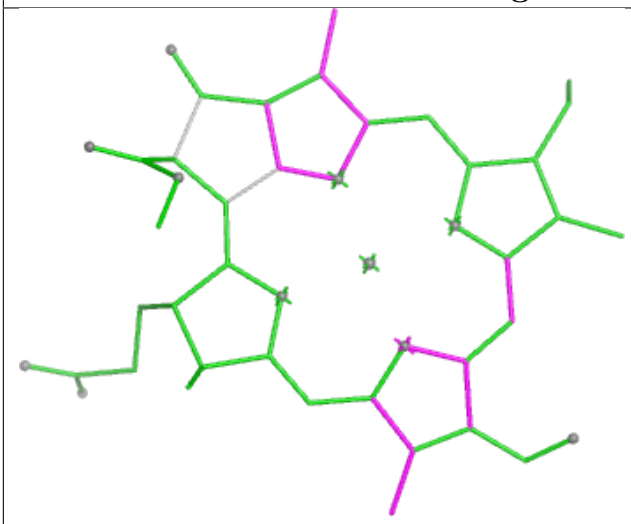


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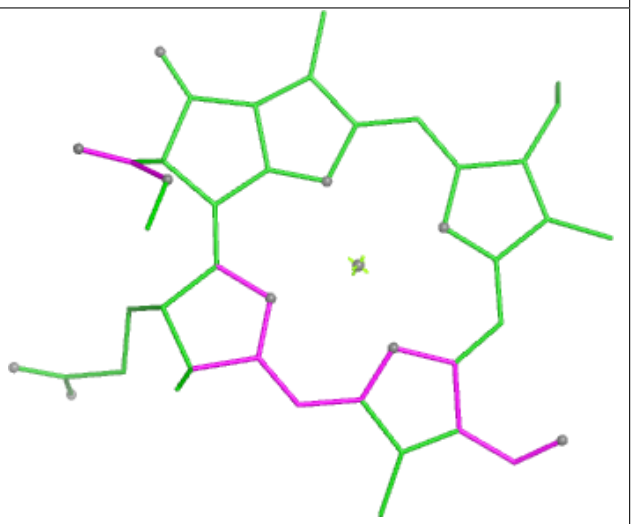


Rings

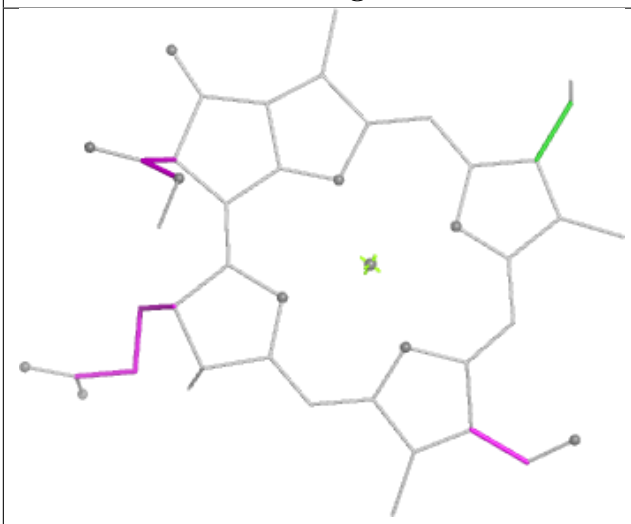
Ligand CL7 aB 1222



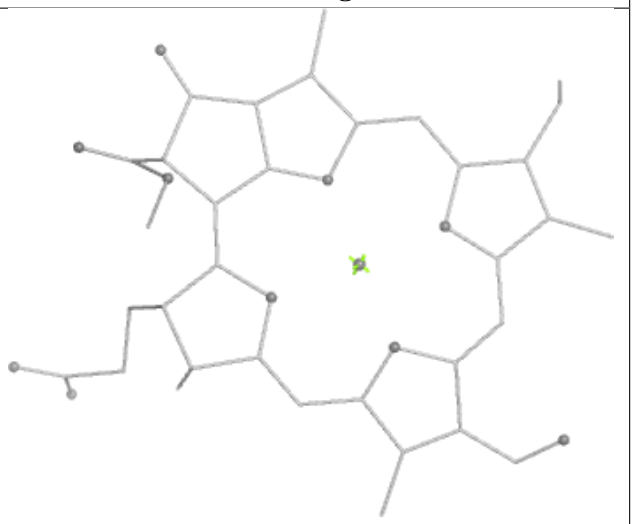
Bond lengths



Bond angles

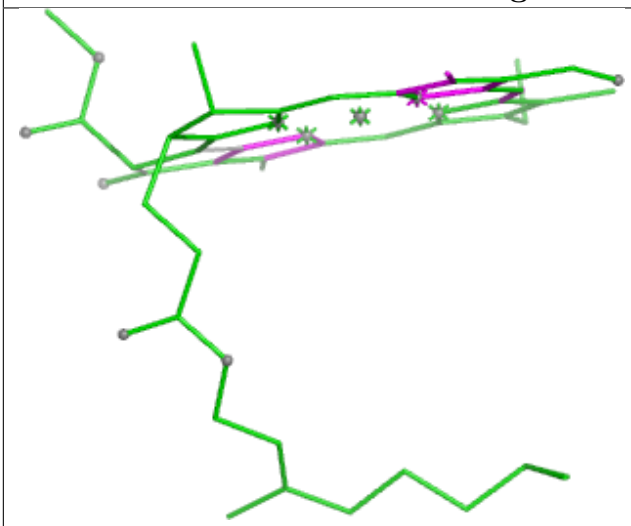


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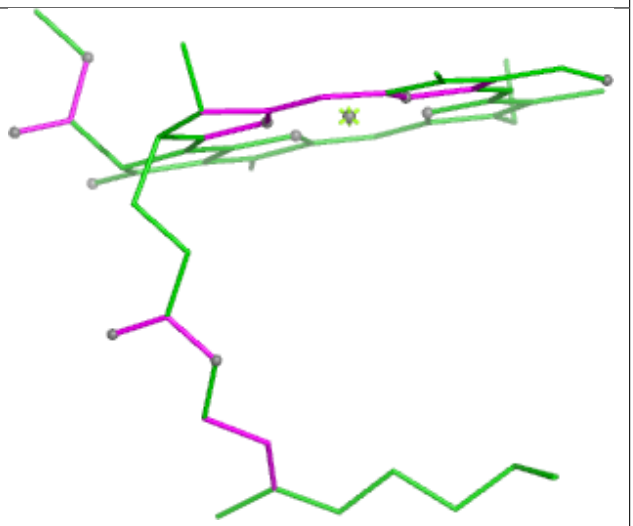


Rings

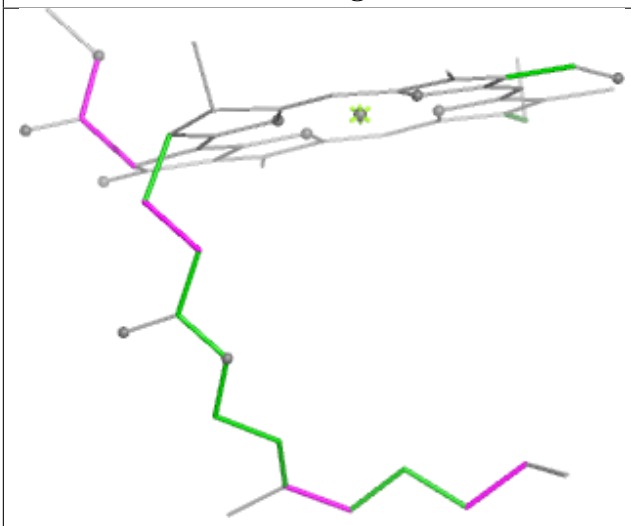
Ligand CL7 bB 1211



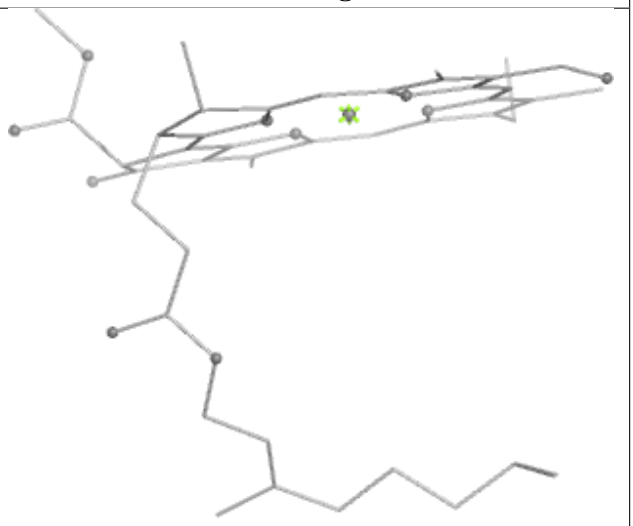
Bond lengths



Bond angles

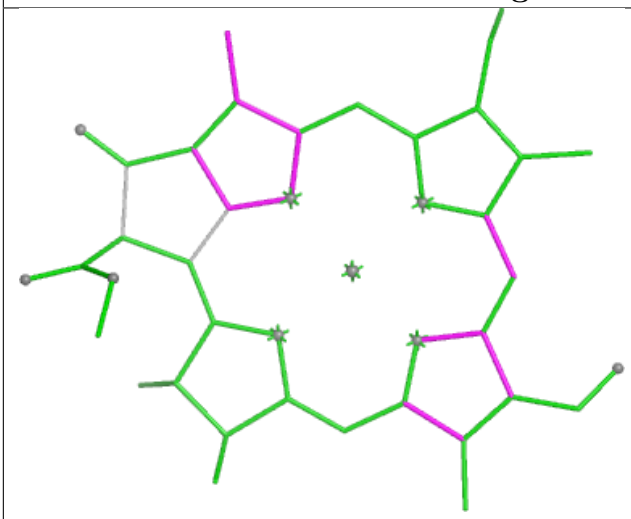


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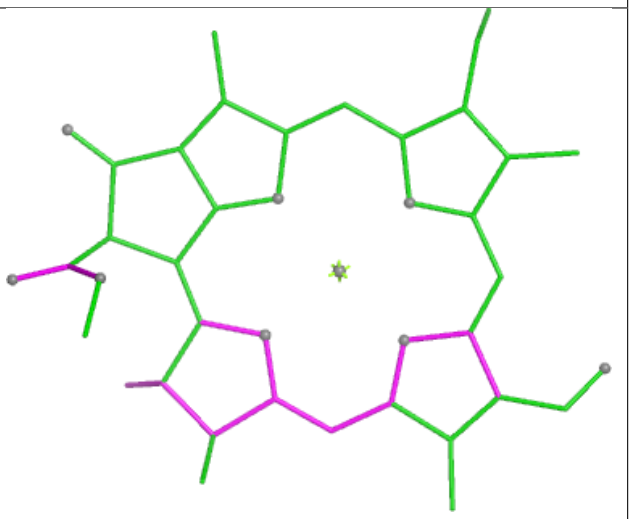


Rings

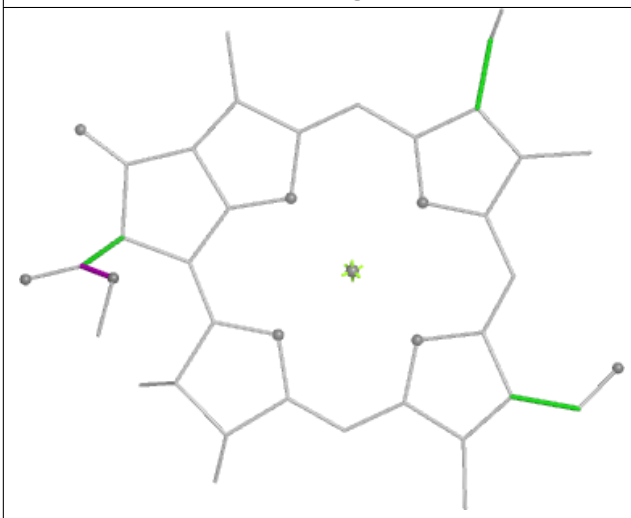
Ligand CL7 aB 1218



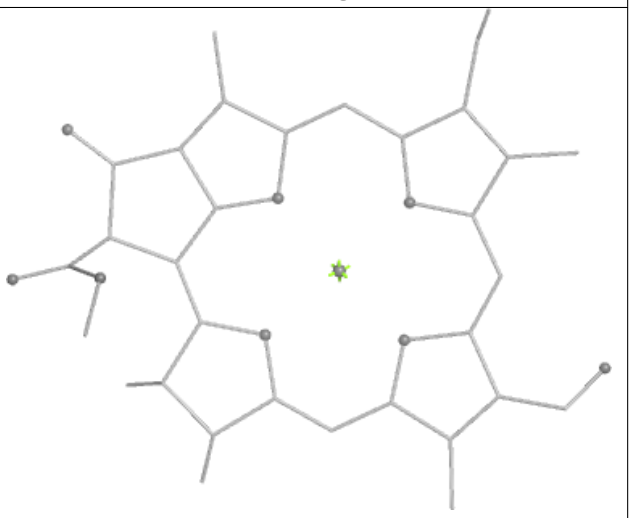
Bond lengths



Bond angles

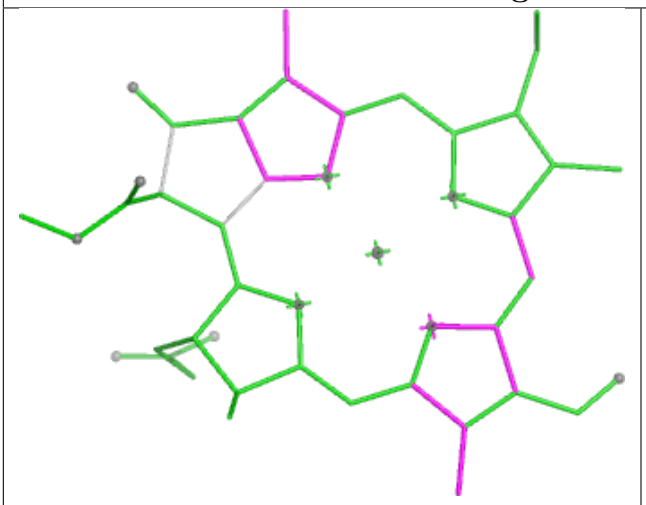


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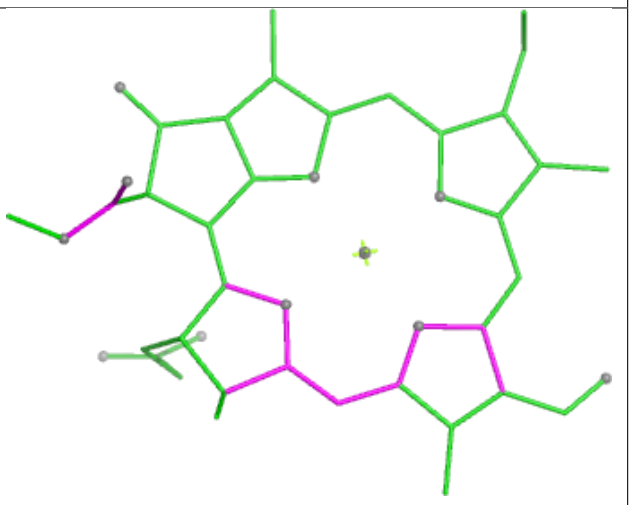


Rings

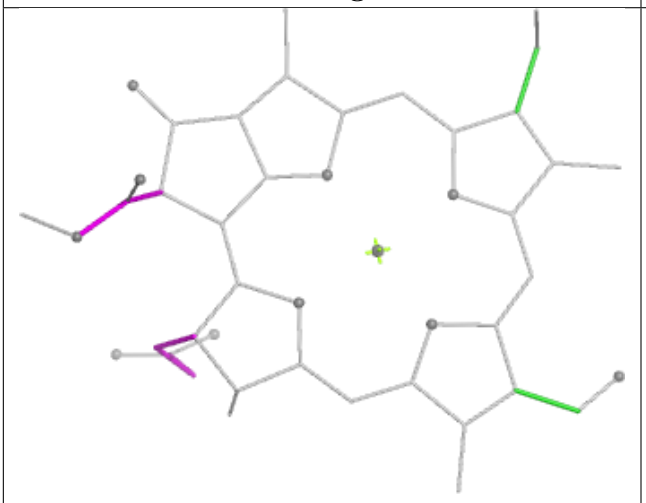
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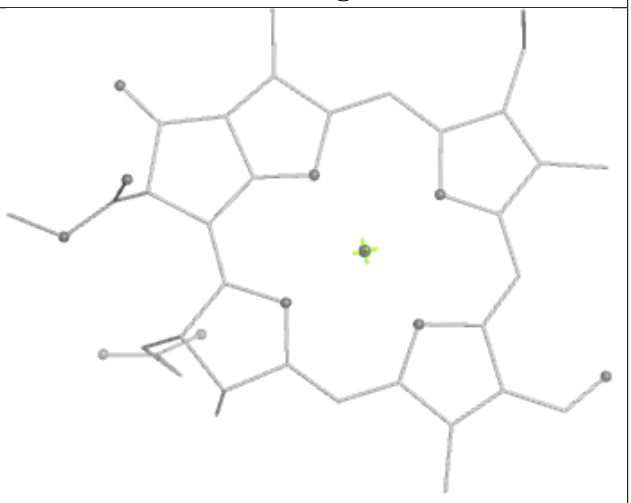
Bond lengths



Bond angles



Torsions

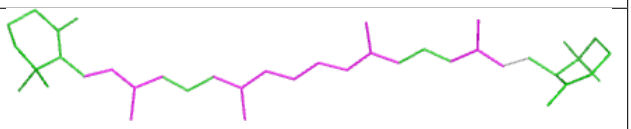


Rings

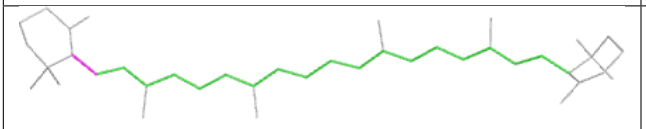
Ligand A1JPJ aA 4007



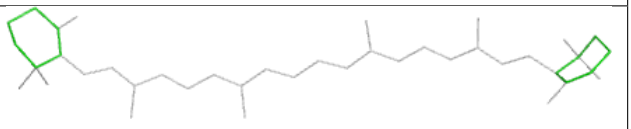
Bond lengths



Bond angles

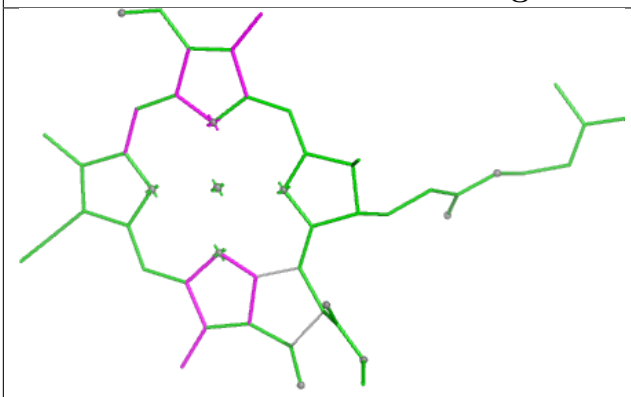


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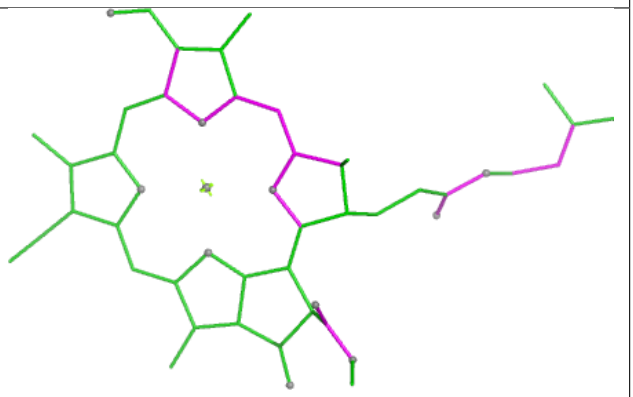


Rings

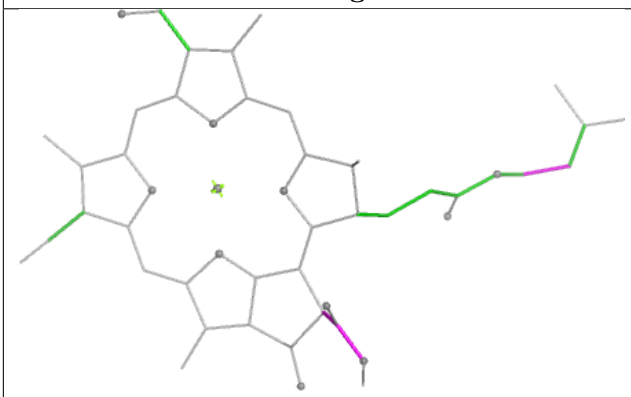
Ligand CL7 cA 1124



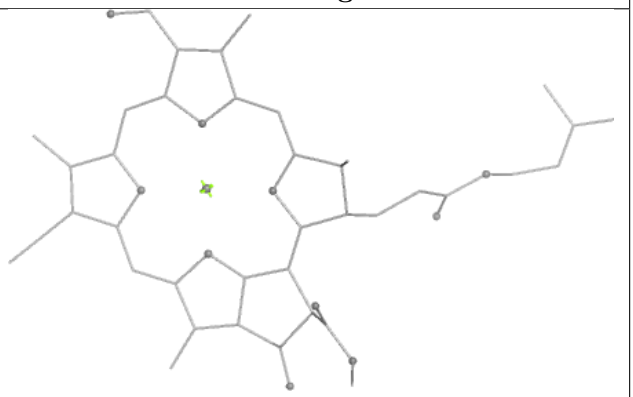
Bond lengths



Bond angles

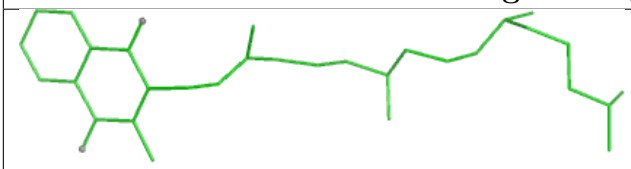


Torsions



Rings

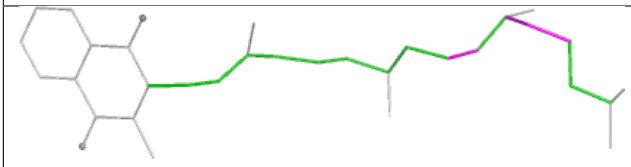
Ligand PQN bA 2001



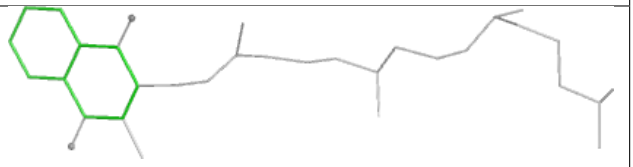
Bond lengths



Bond angles

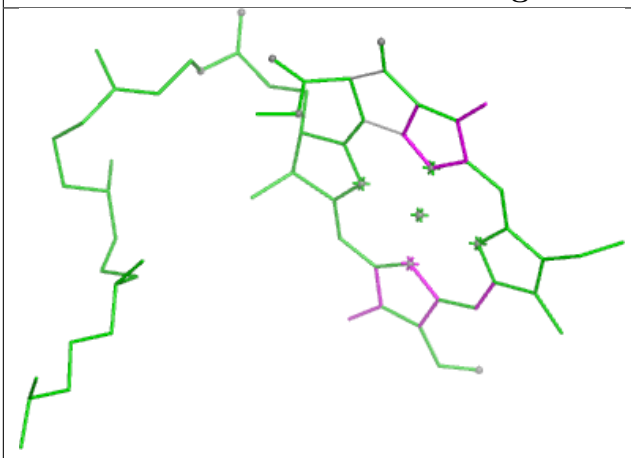


Torsions

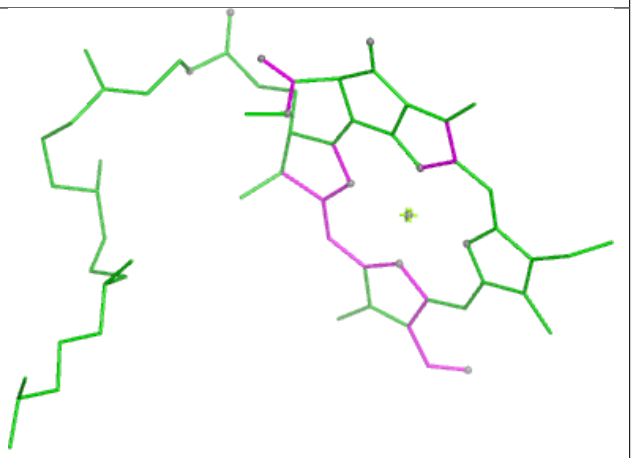


Rings

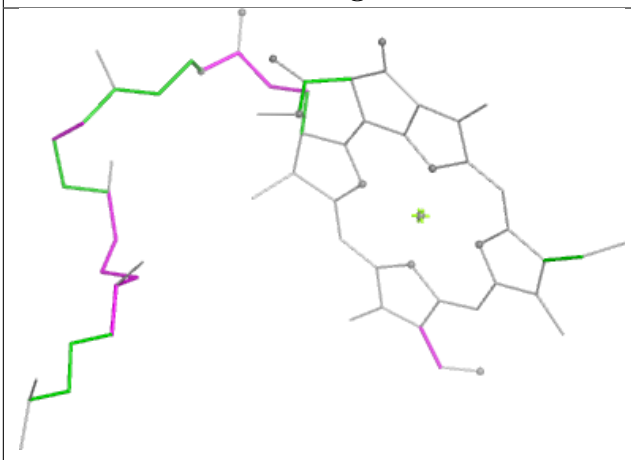
Ligand CL7 aB 1207



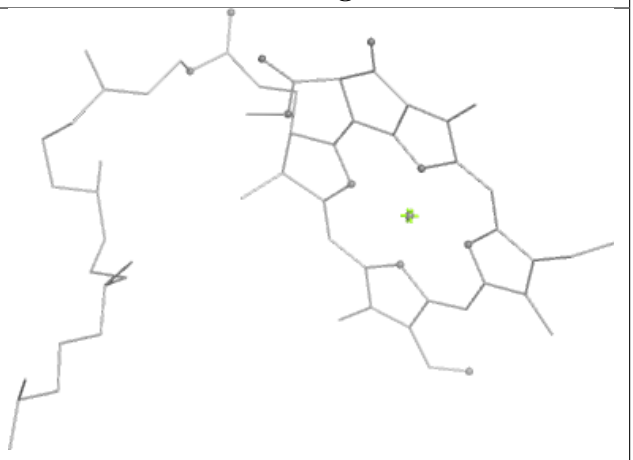
Bond lengths



Bond angles

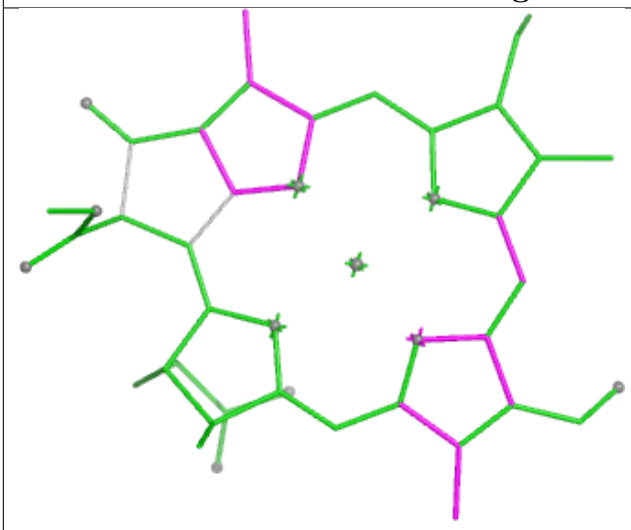


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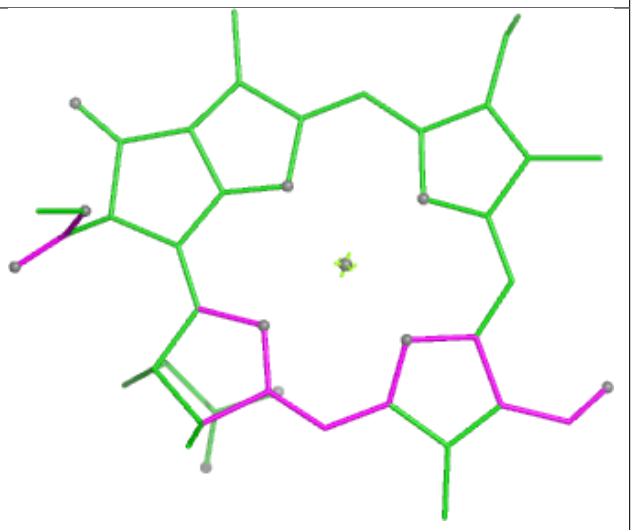


Rings

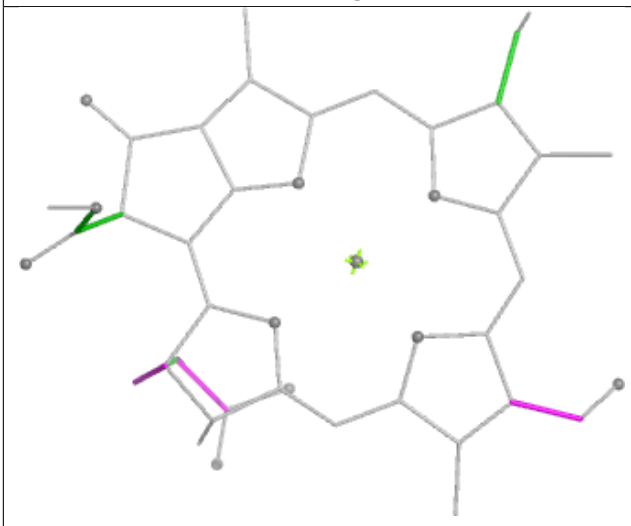
Ligand CL7 cB 1227



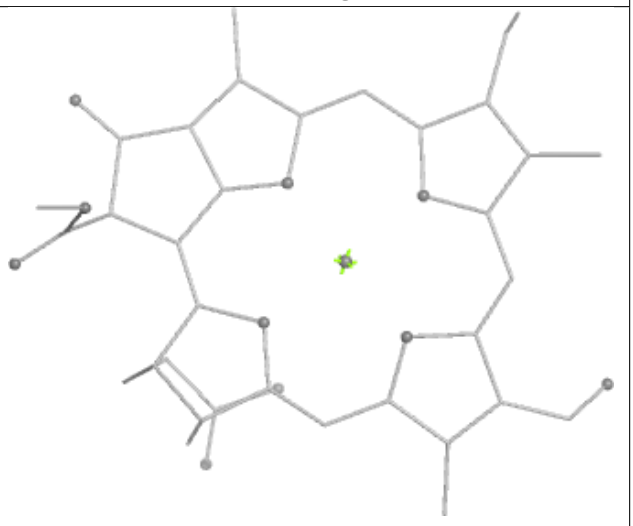
Bond lengths



Bond angles

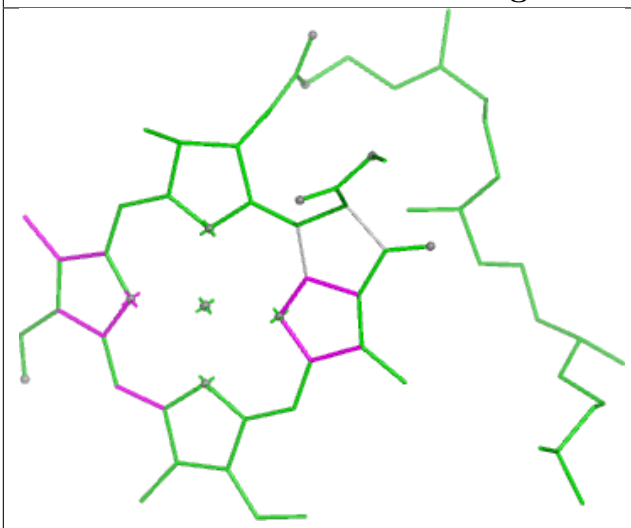


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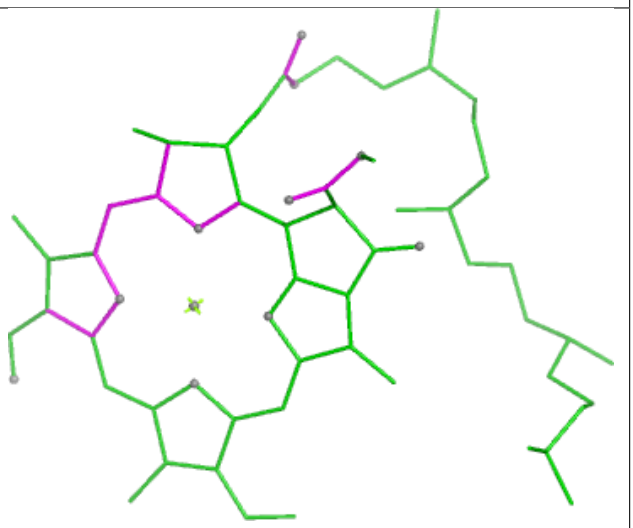


Rings

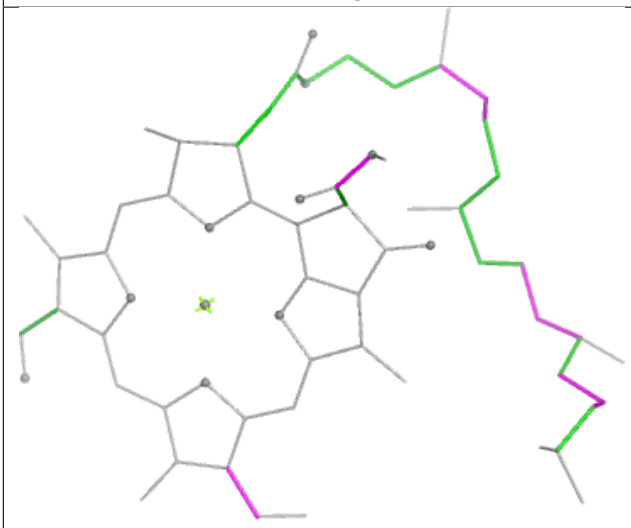
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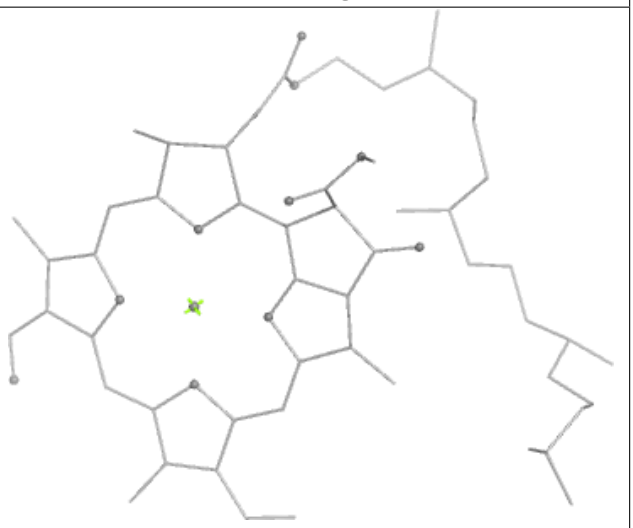
Bond lengths



Bond angles

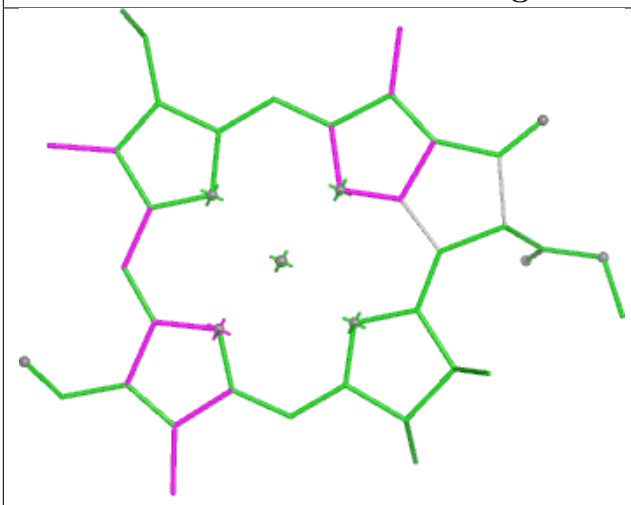


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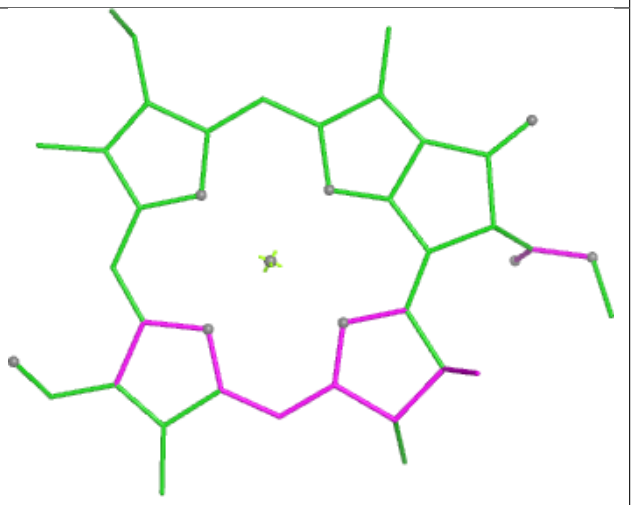


Rings

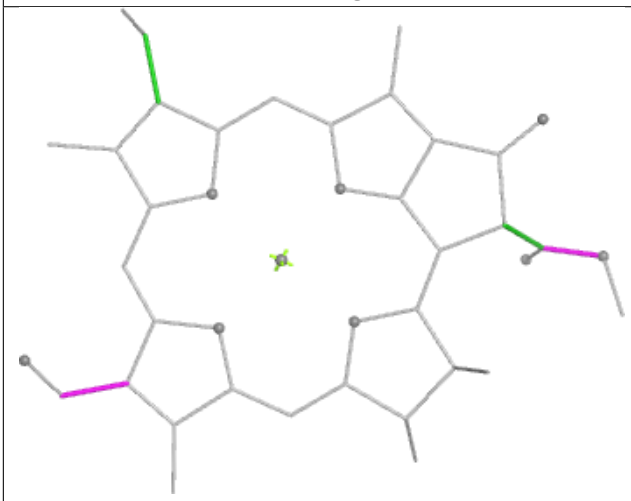
Ligand CL7 cA 1115



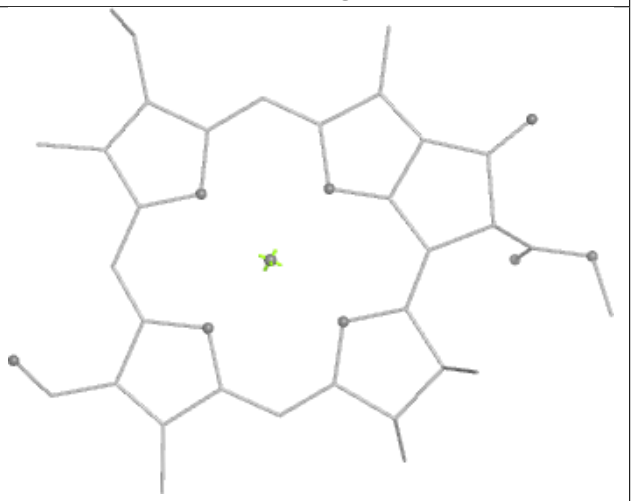
Bond lengths



Bond angles

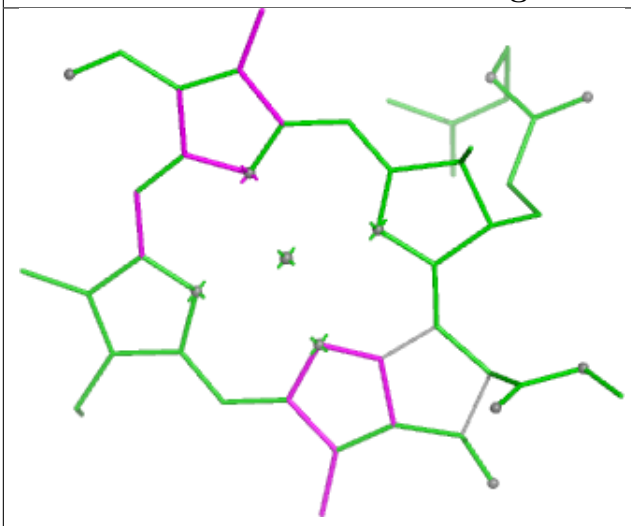


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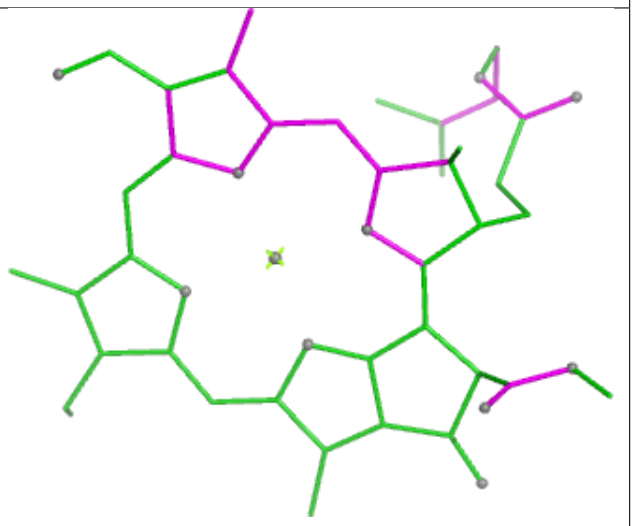


Rings

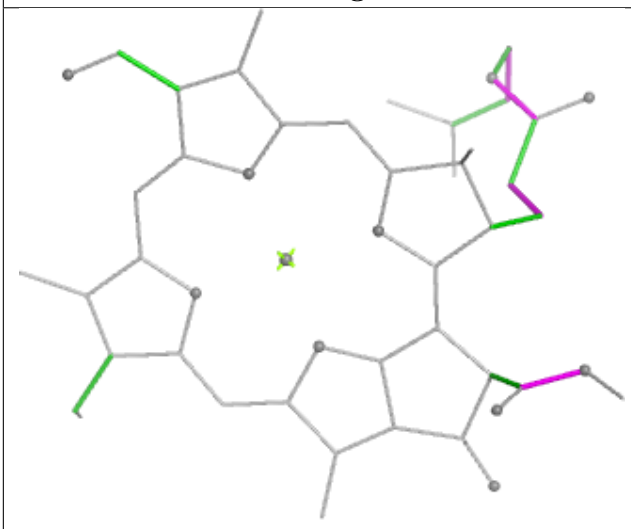
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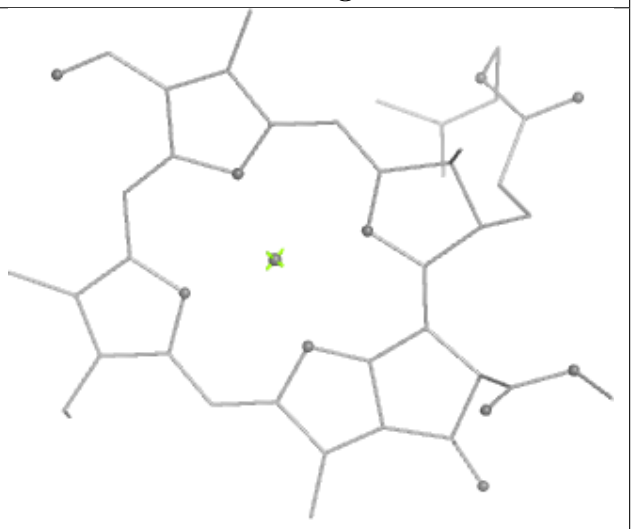
Bond lengths



Bond angles

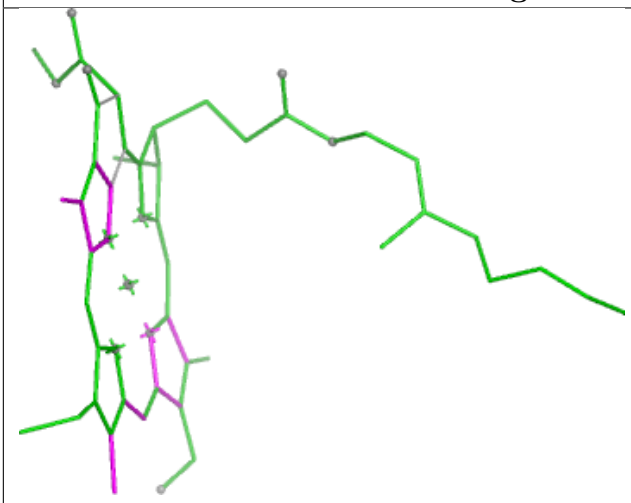


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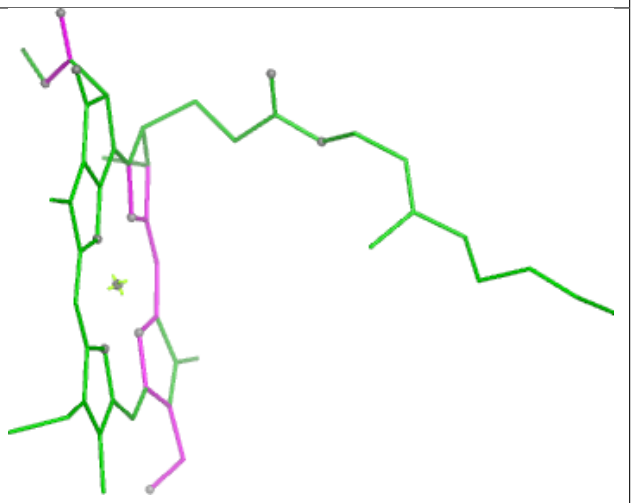


Rings

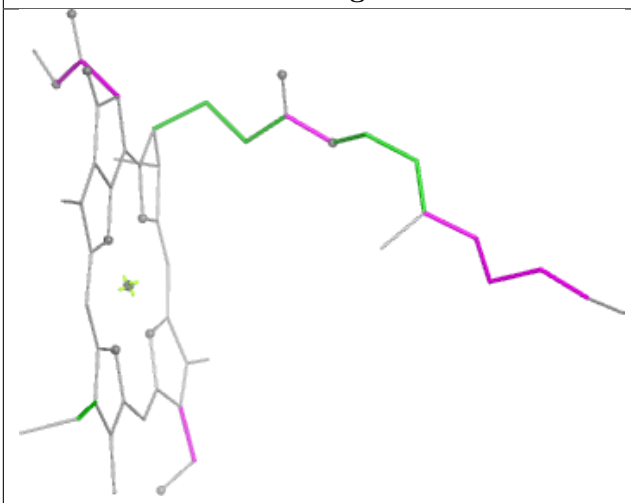
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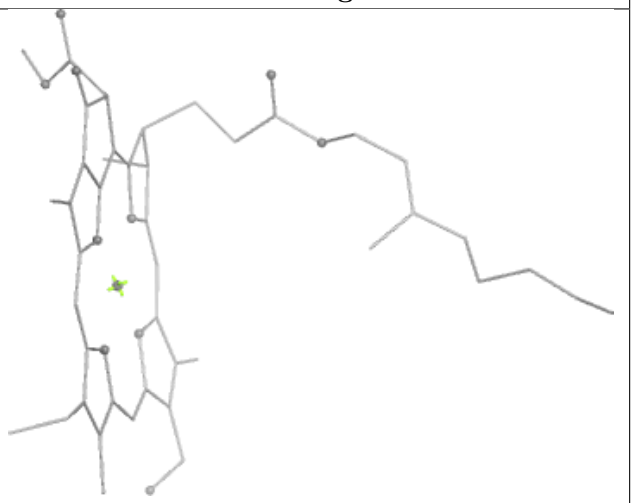
Bond lengths



Bond angles

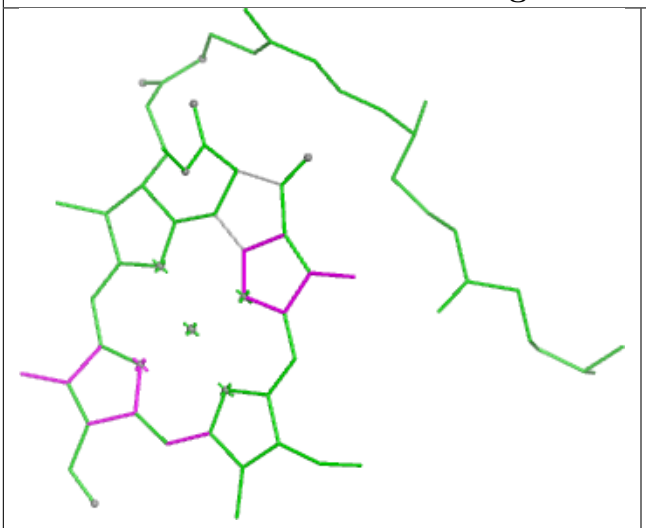


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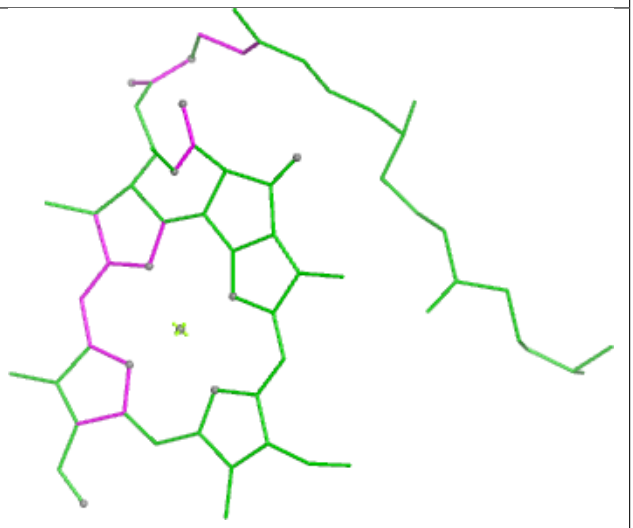


Rings

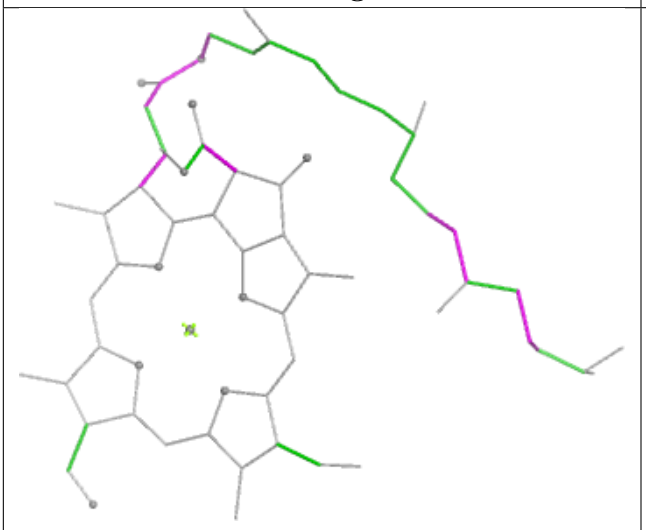
Ligand CL7 bA 1123



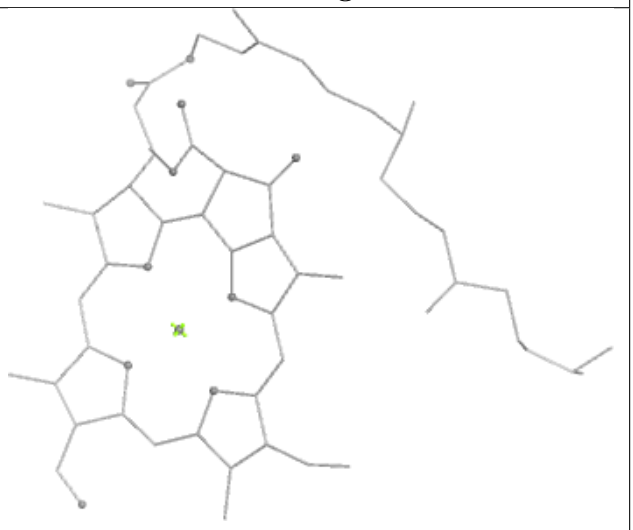
Bond lengths



Bond angles

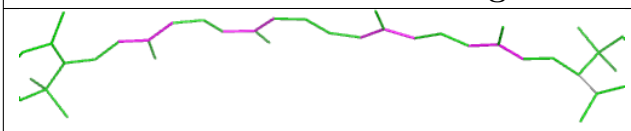


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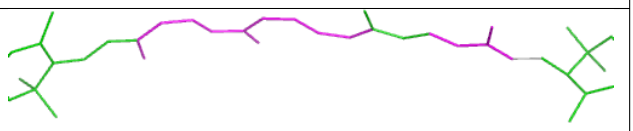


Rings

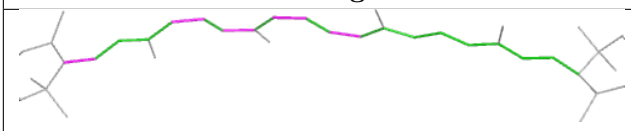
Ligand A1JPJ bA 4014



Bond lengths



Bond angles

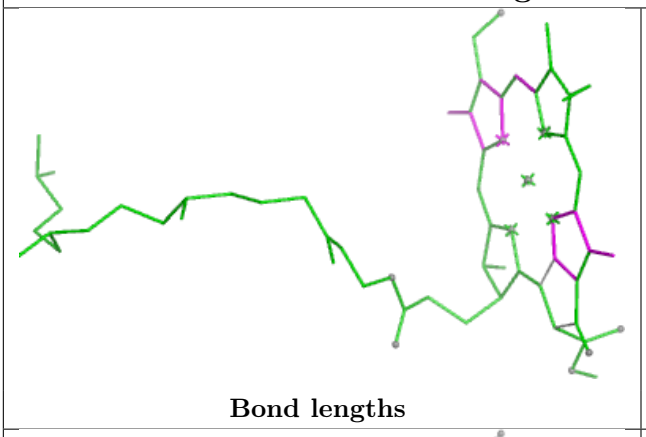


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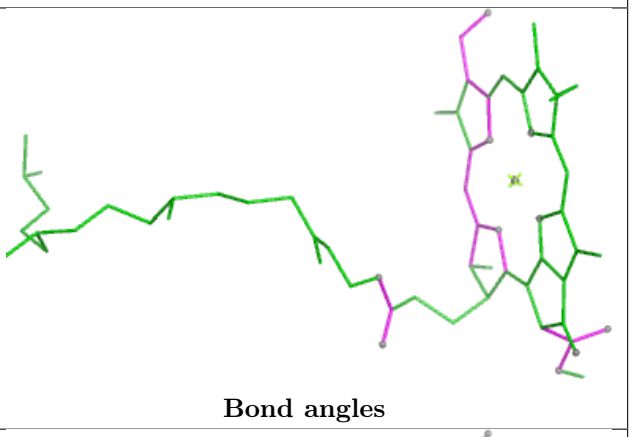


Rings

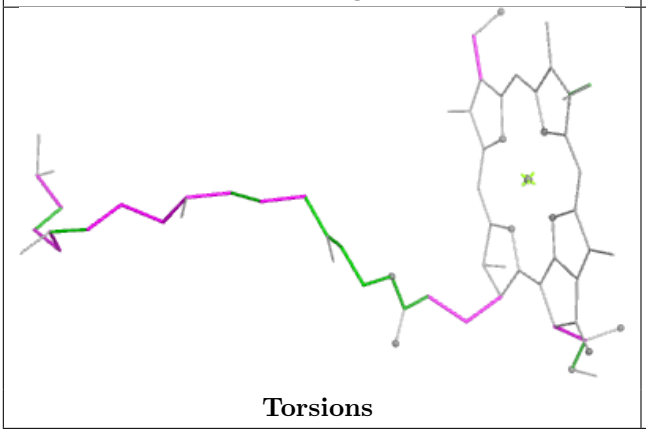
Ligand CL7 cL 1502



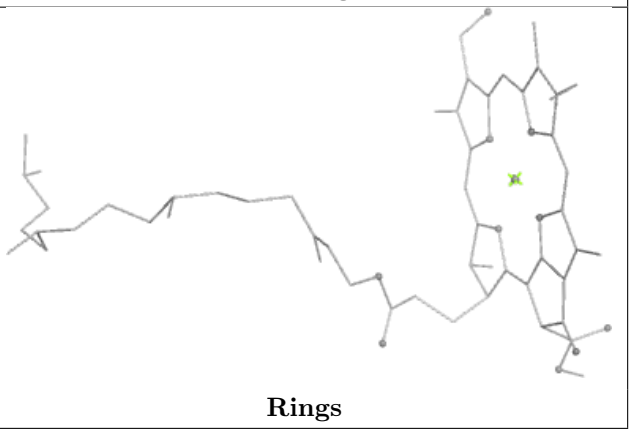
Bond lengths



Bond angles

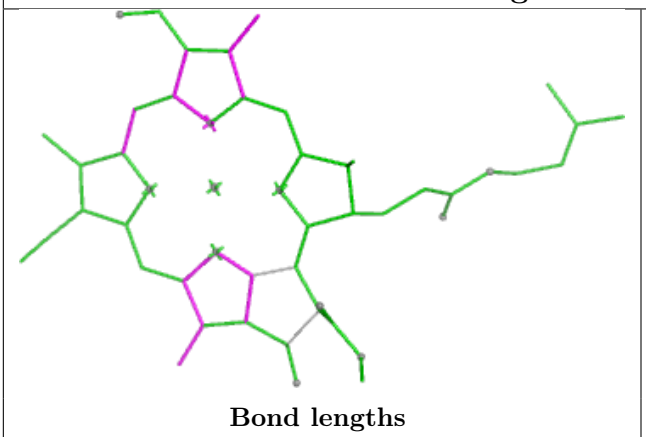


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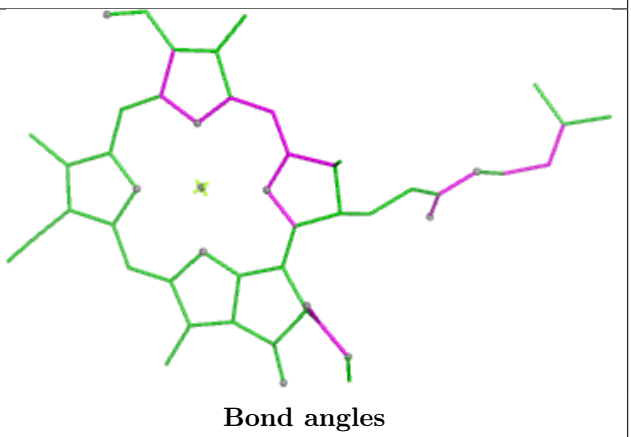


Rings

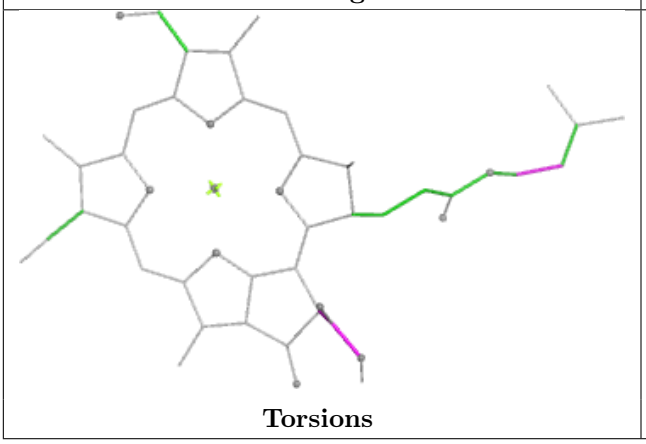
Ligand CL7 aA 1124



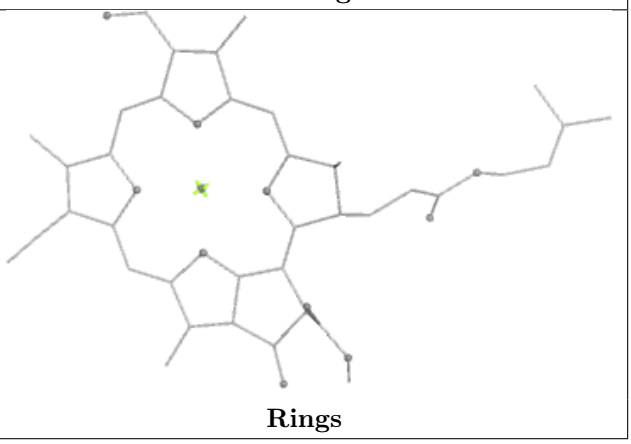
Bond lengths



Bond angles

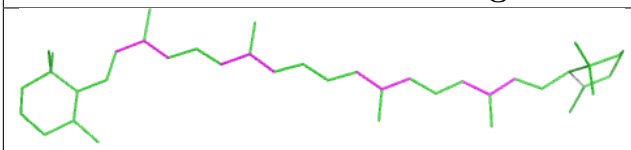


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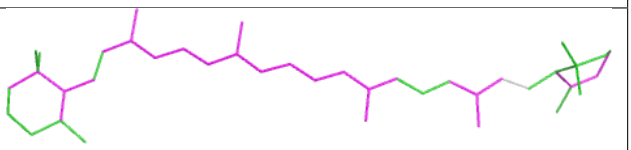


Rings

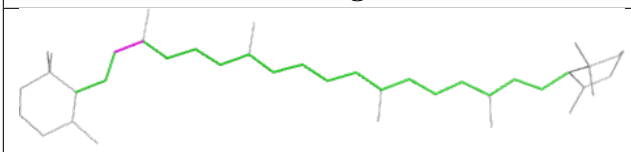
Ligand A1JPJ bB 4015



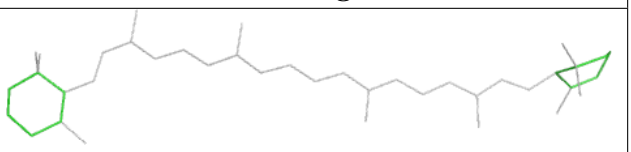
Bond lengths



Bond angles

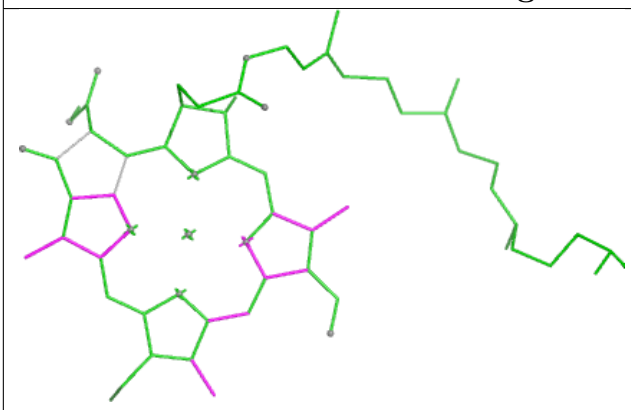


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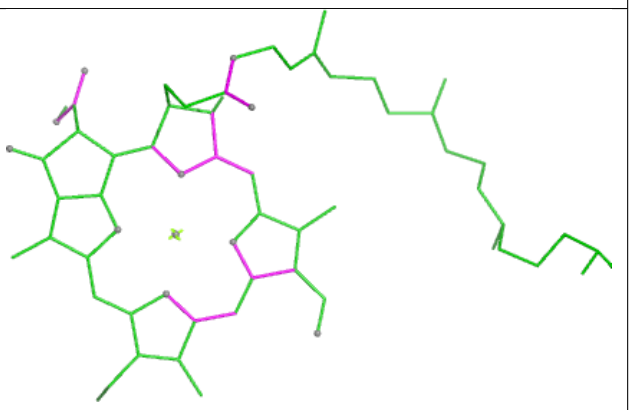


Rings

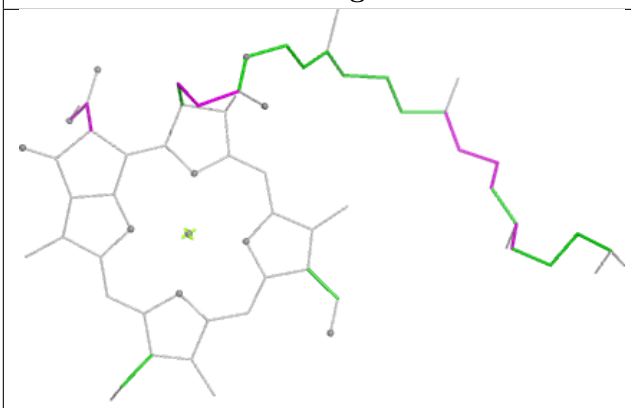
Ligand CL7 aI 1601



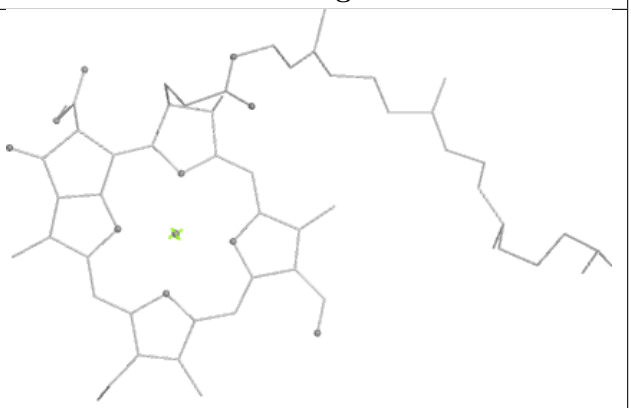
Bond lengths



Bond angles

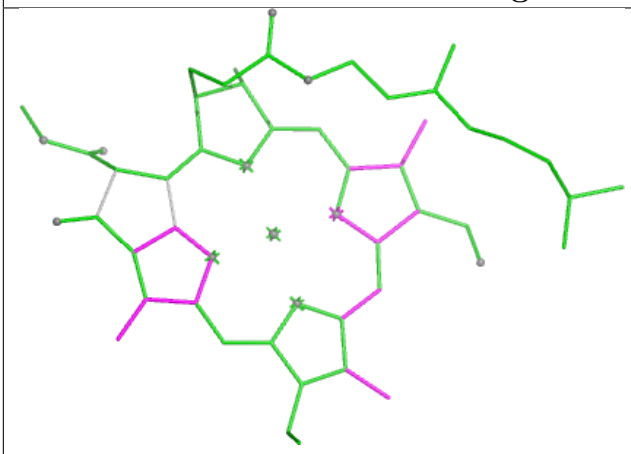


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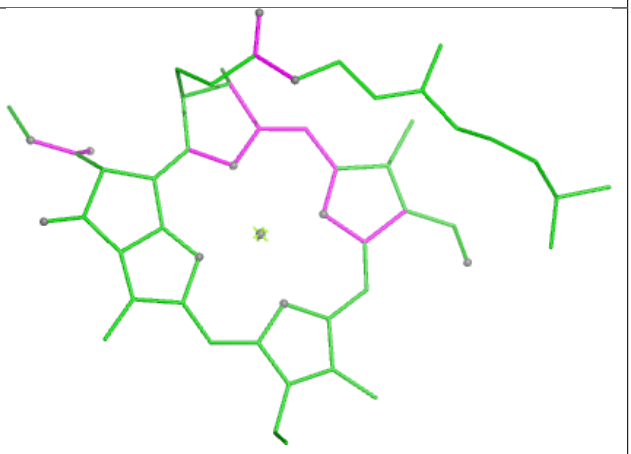


Rings

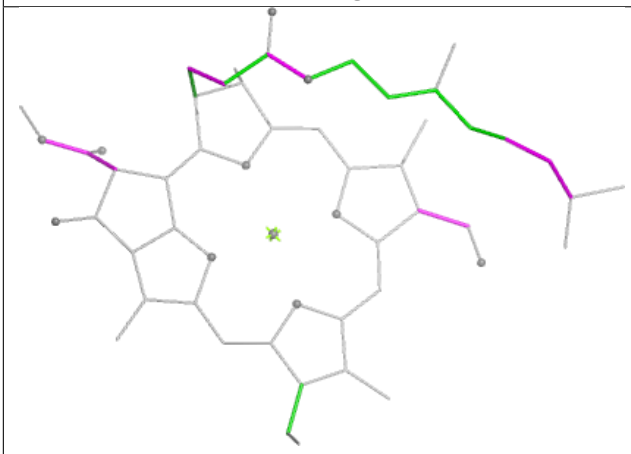
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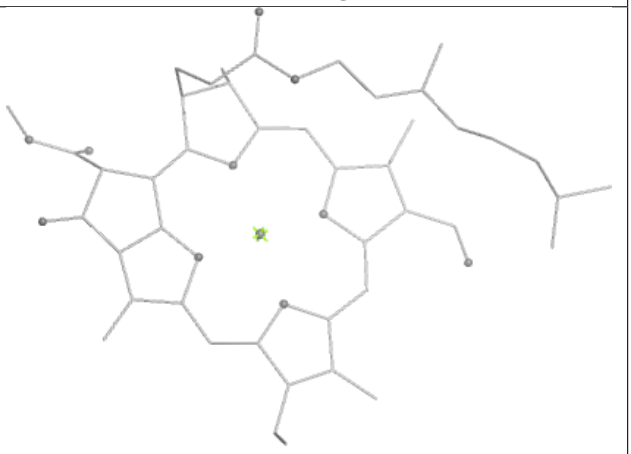
Bond lengths



Bond angles

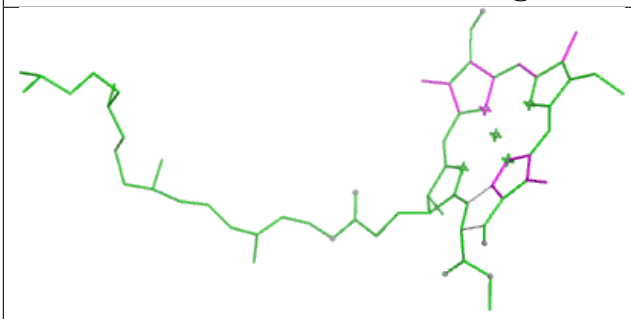


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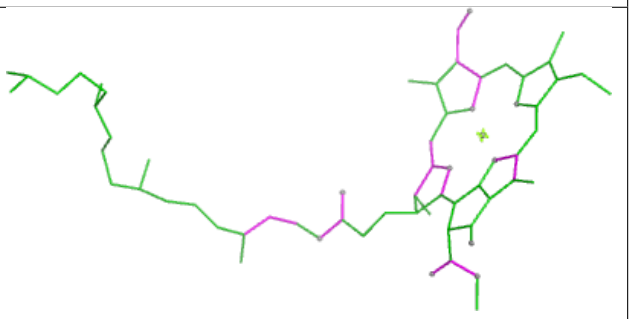


Rings

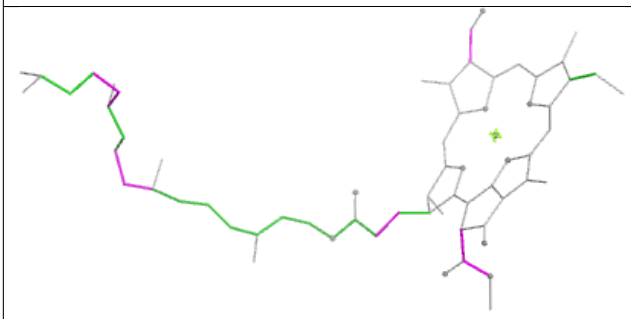
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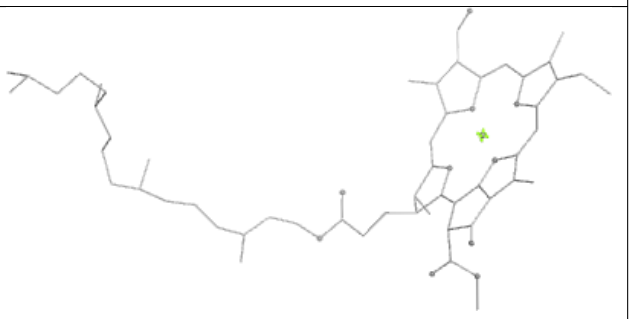
Bond lengths



Bond angles

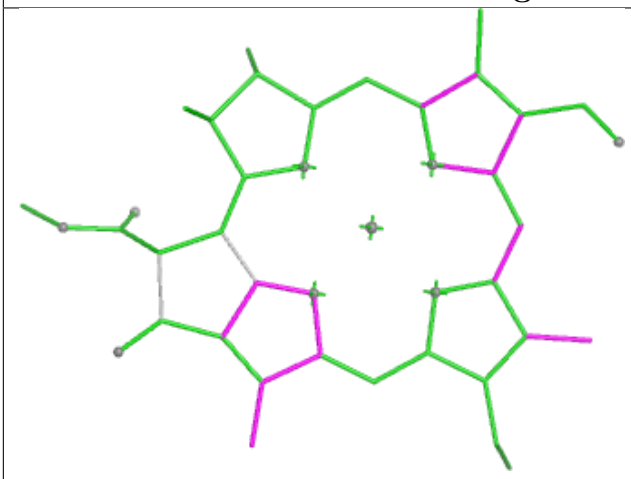


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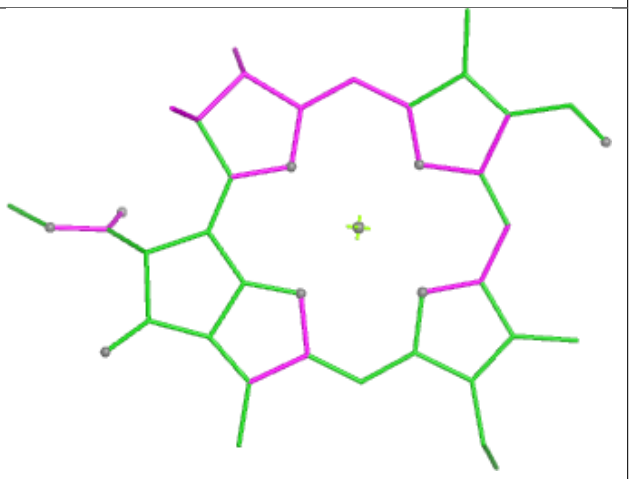


Rings

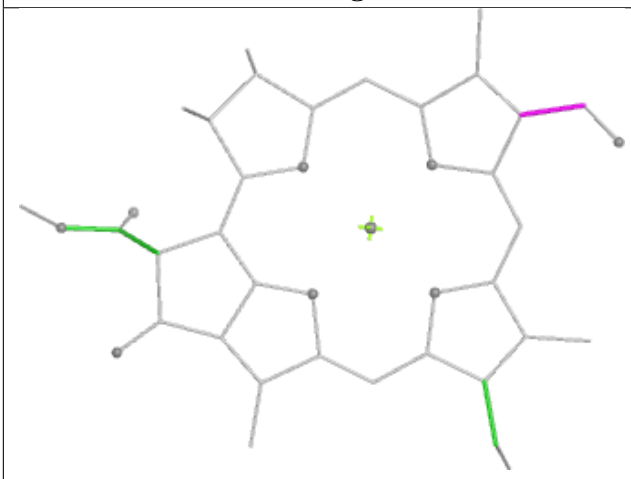
Ligand CL7 cF 1701



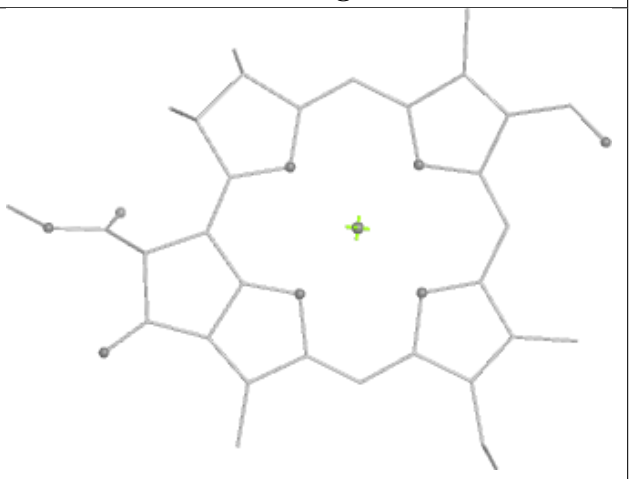
Bond lengths



Bond angles

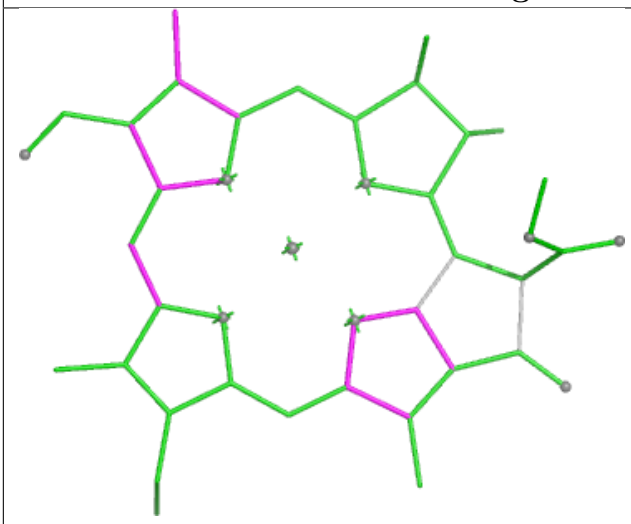


Torsions

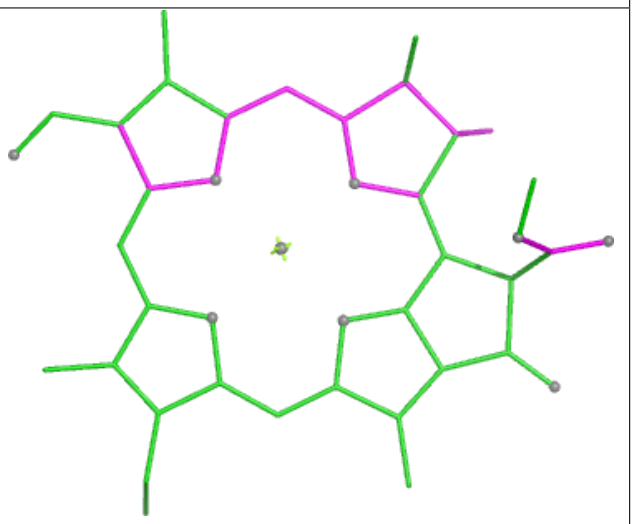


Rings

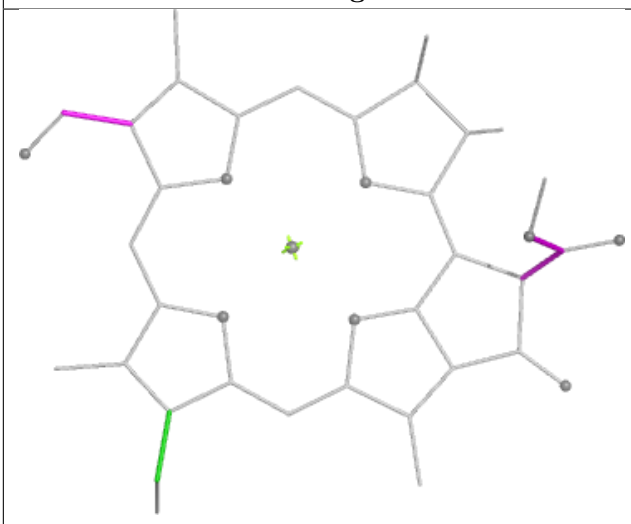
Ligand CL7 cB 1218



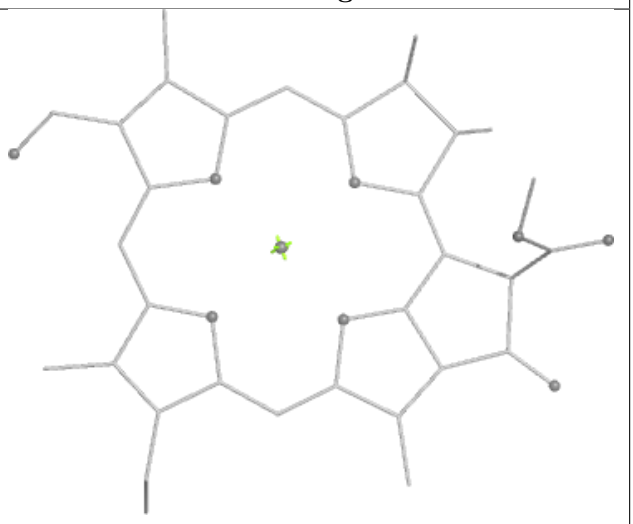
Bond lengths



Bond angles

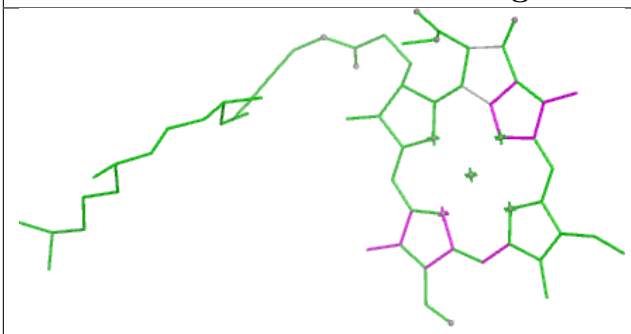


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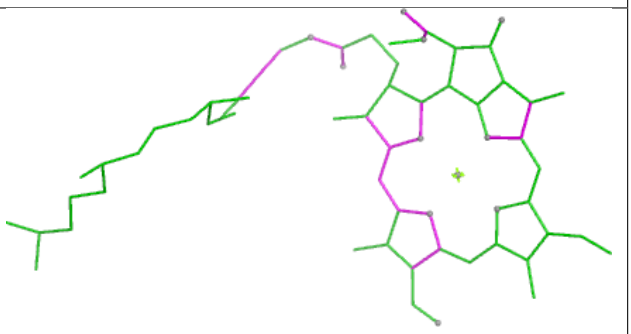


Rings

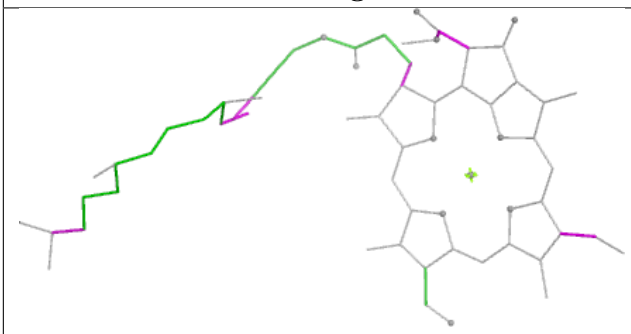
Ligand CL7 cA 1111



Bond lengths



Bond angles

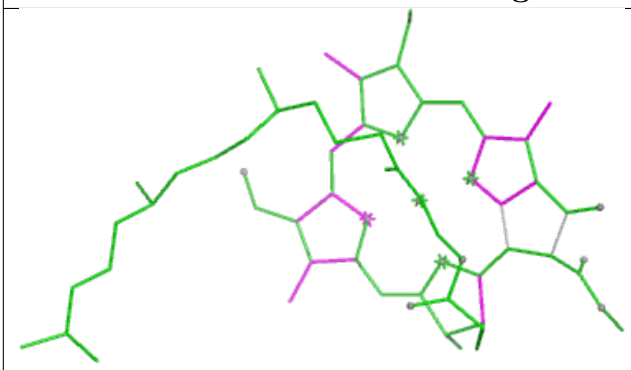


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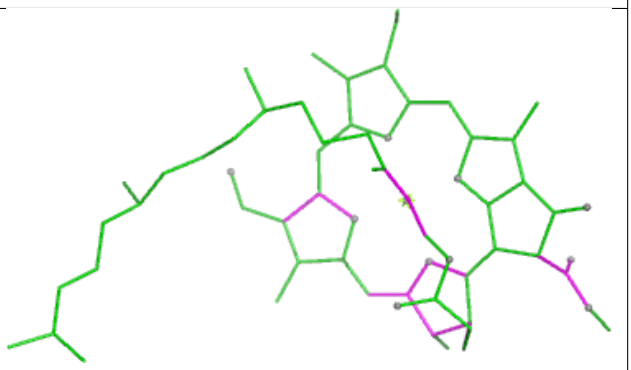


Rings

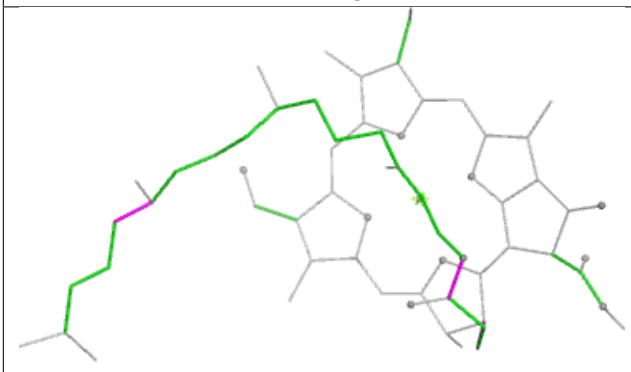
Ligand CL7 cB 1204



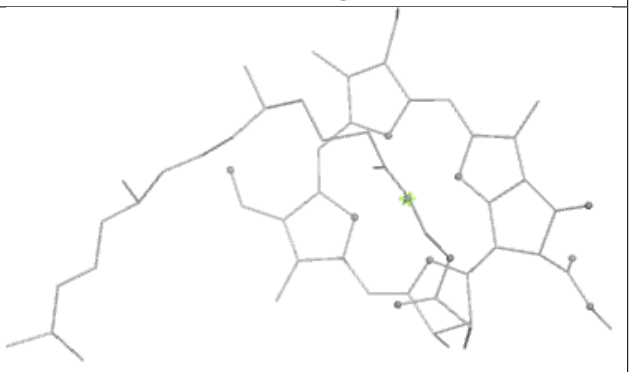
Bond lengths



Bond angles

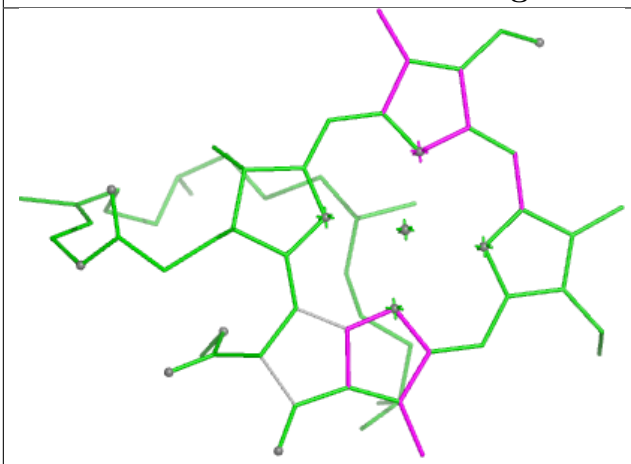


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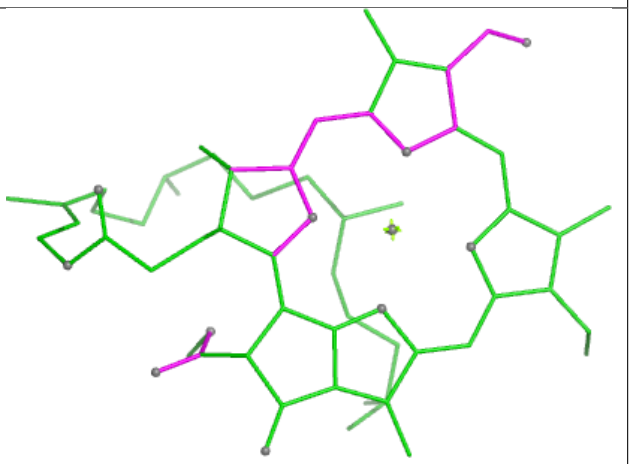


Rings

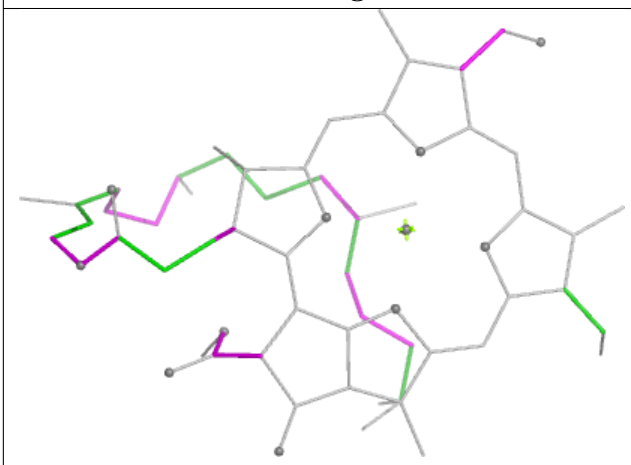
Ligand CL7 aA 1104



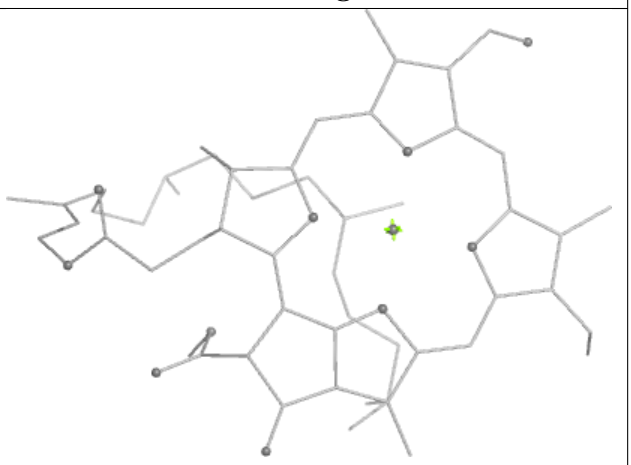
Bond lengths



Bond angles

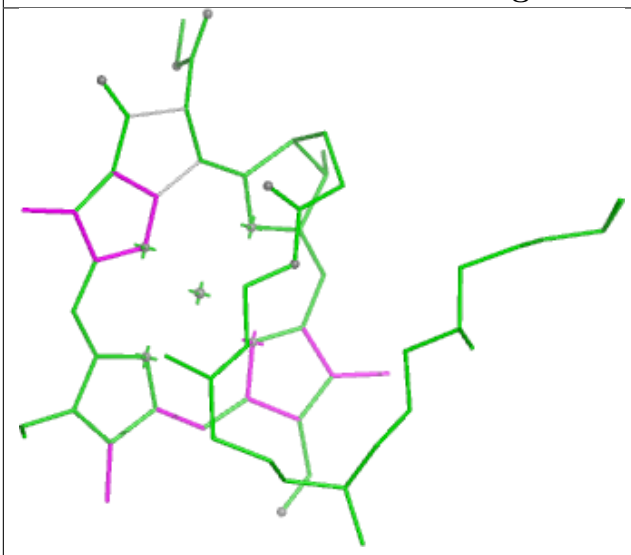


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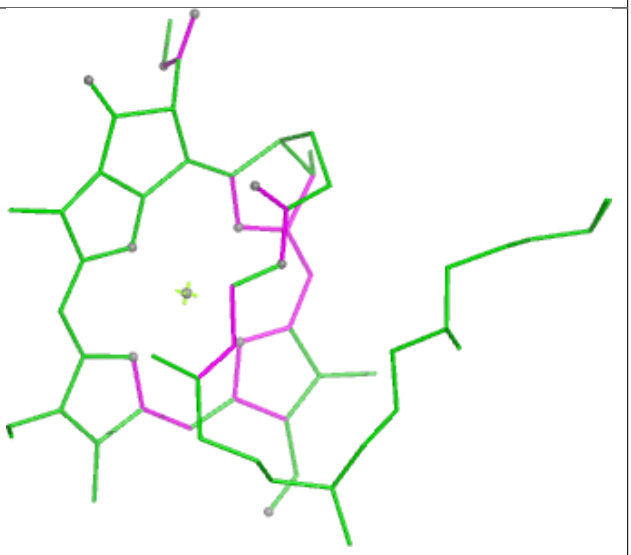


Rings

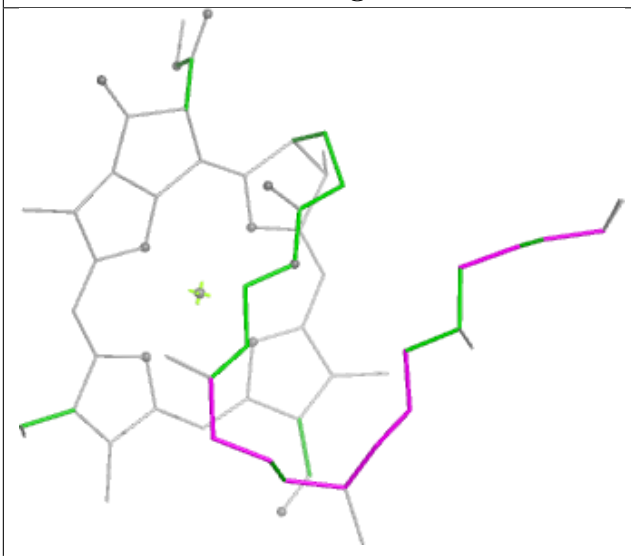
Ligand CL7 cB 1205



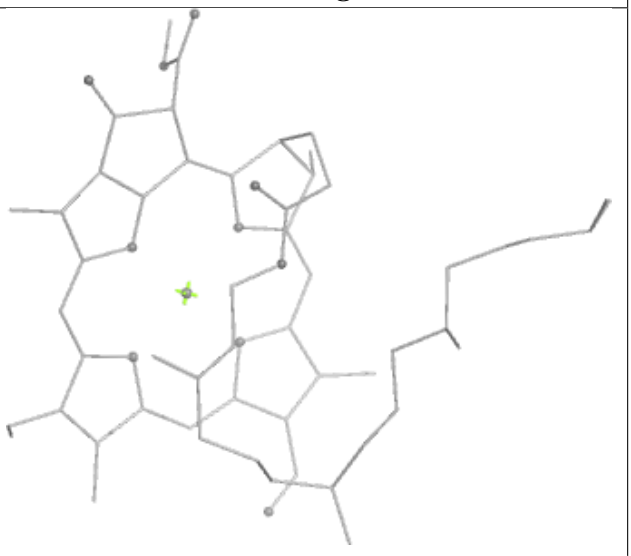
Bond lengths



Bond angles

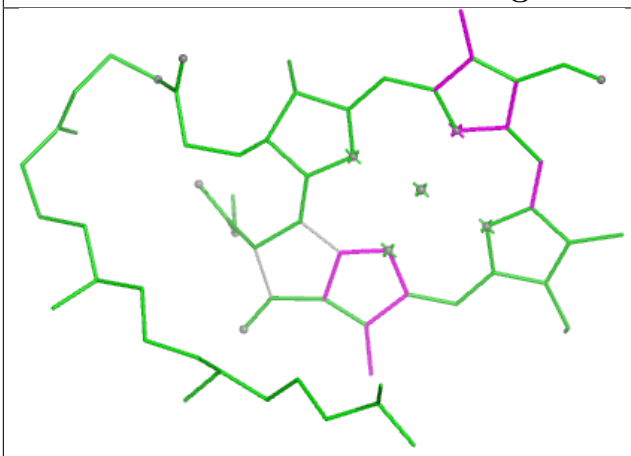


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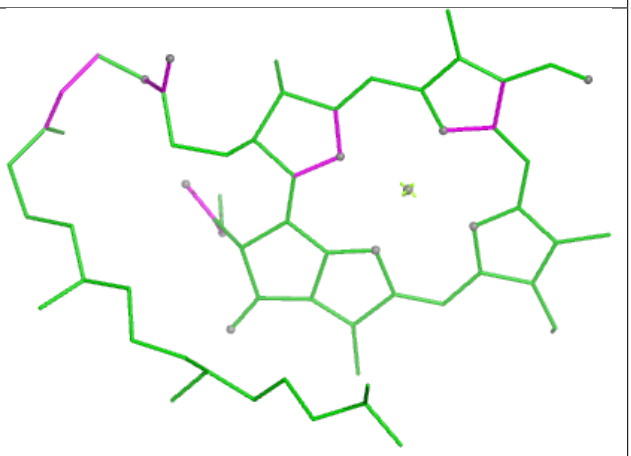


Rings

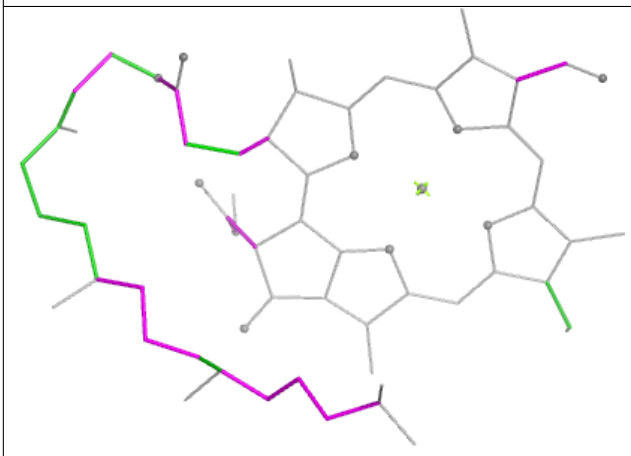
Ligand CL7 aB 1202



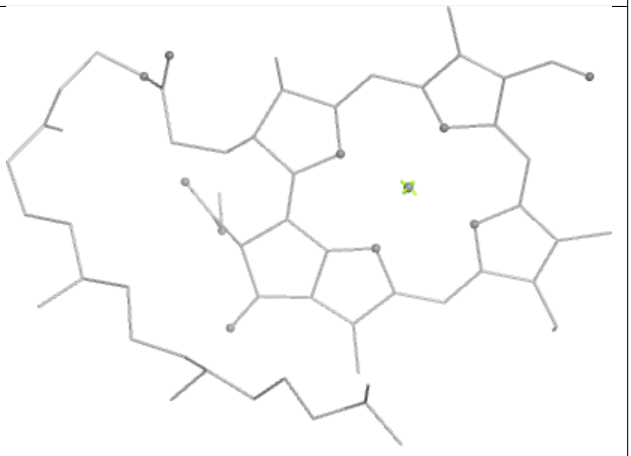
Bond lengths



Bond angles

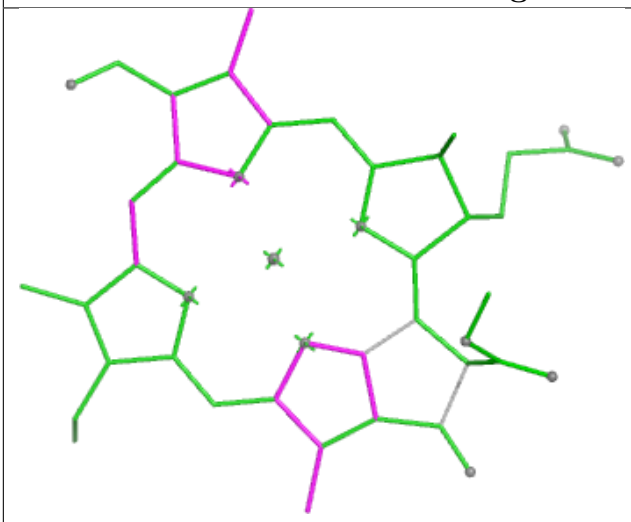


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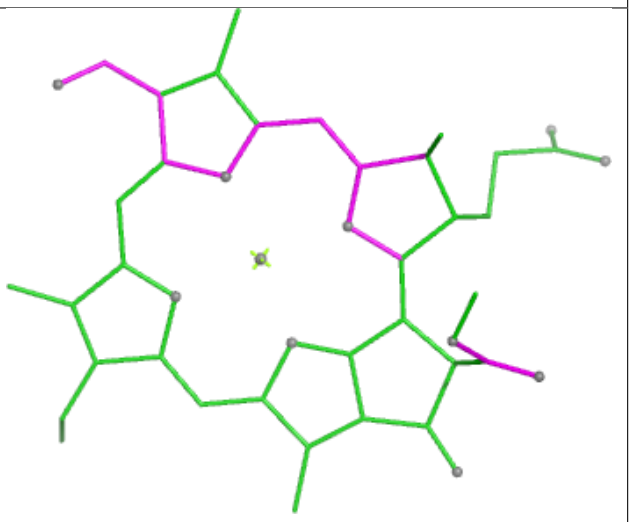


Rings

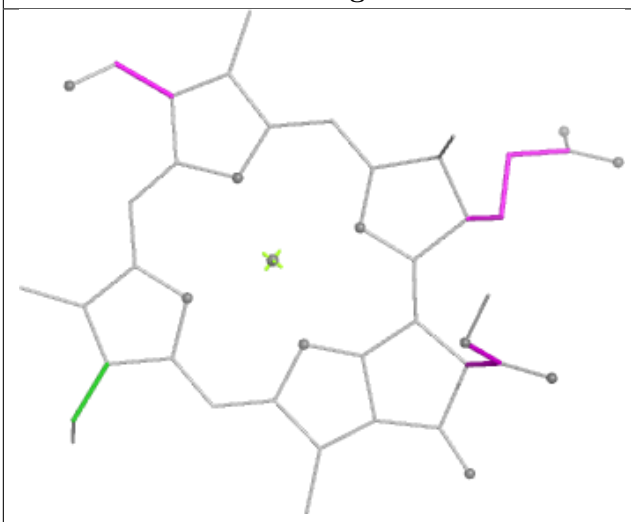
Ligand CL7 bB 1222



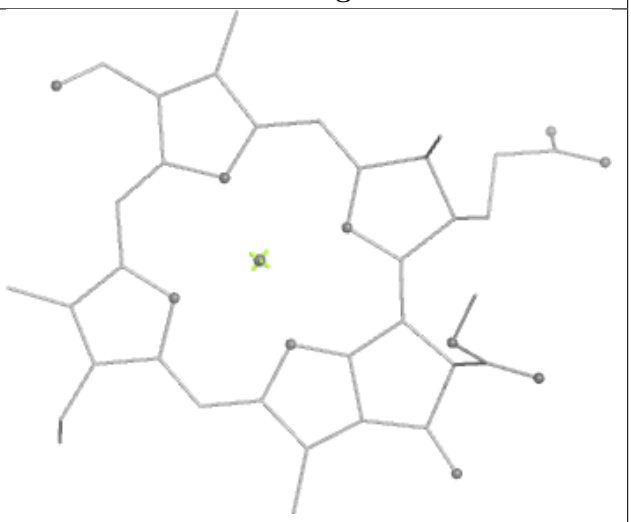
Bond lengths



Bond angles

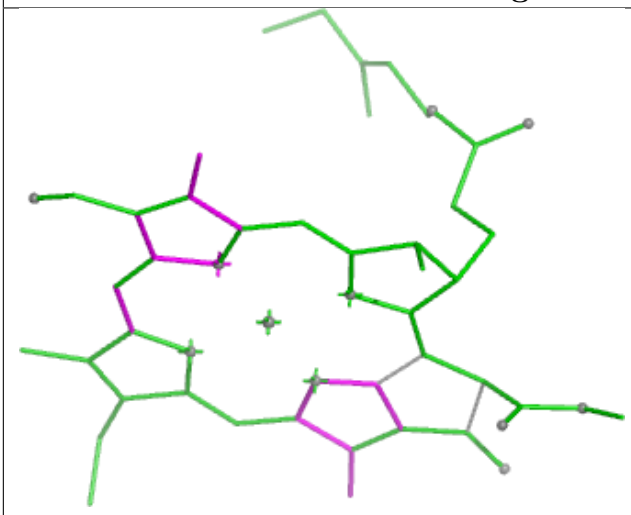


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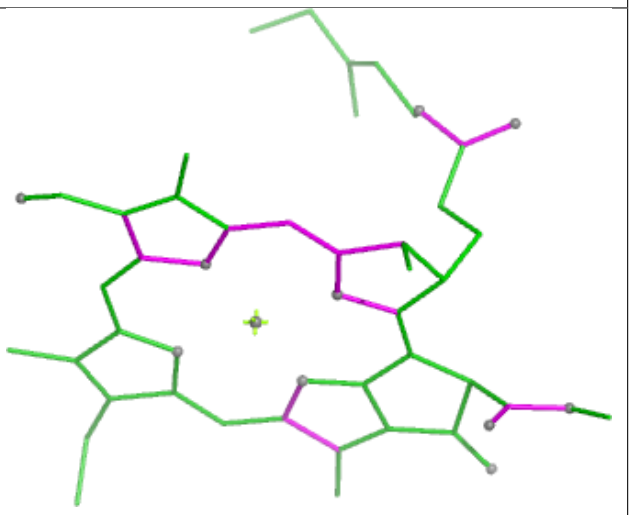


Rings

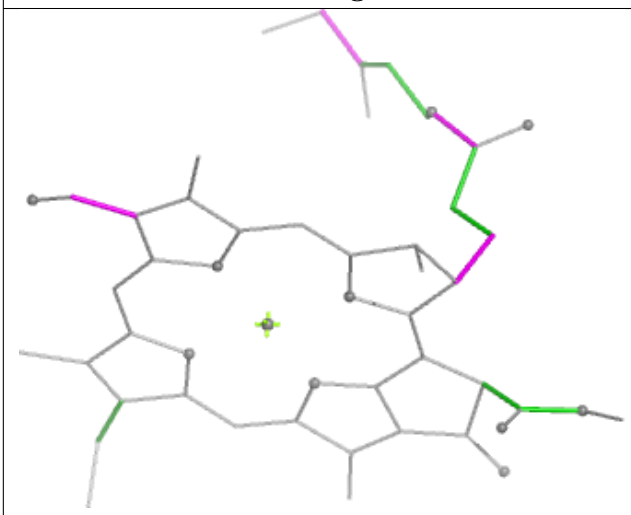
Ligand CL7 cA 1130



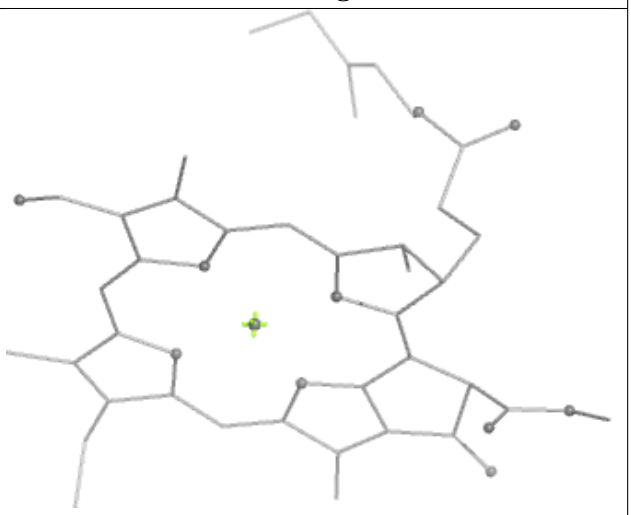
Bond lengths



Bond angles

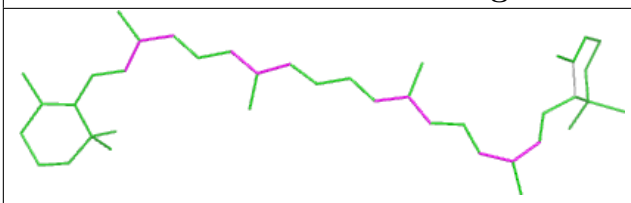


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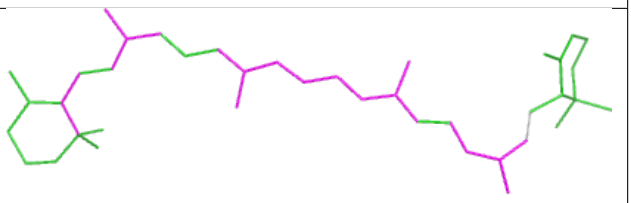


Rings

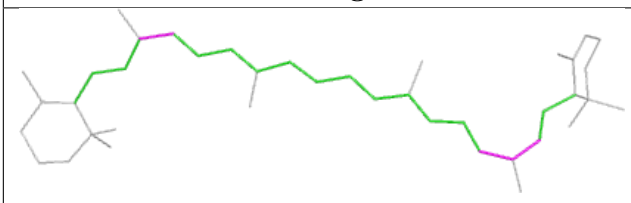
Ligand A1JPJ aB 4006



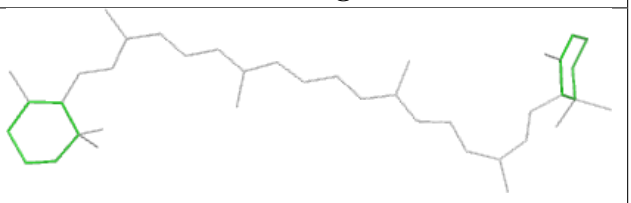
Bond lengths



Bond angles

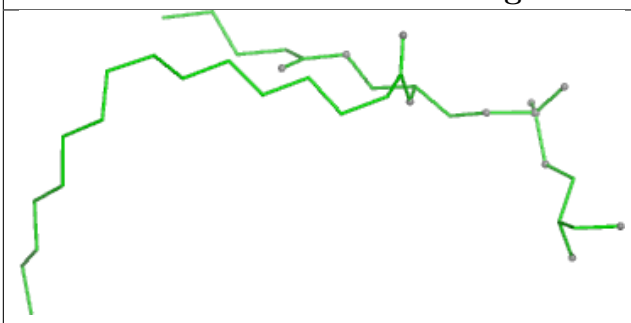


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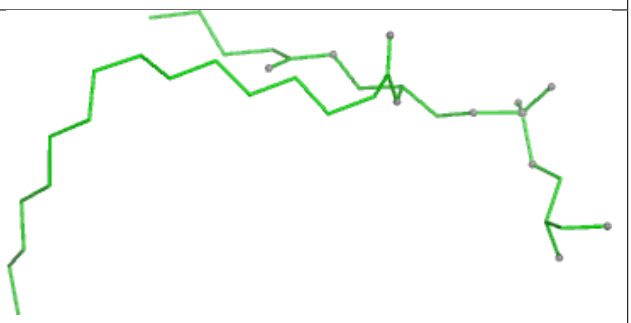


Rings

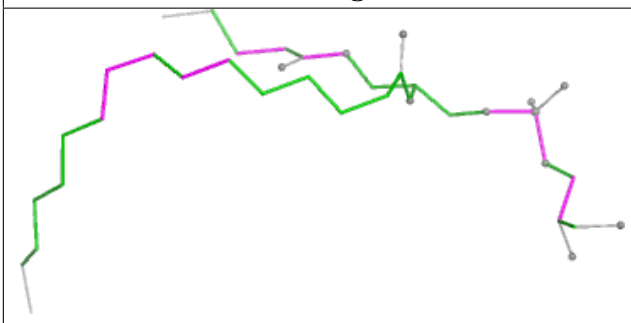
Ligand LHG aA 5003



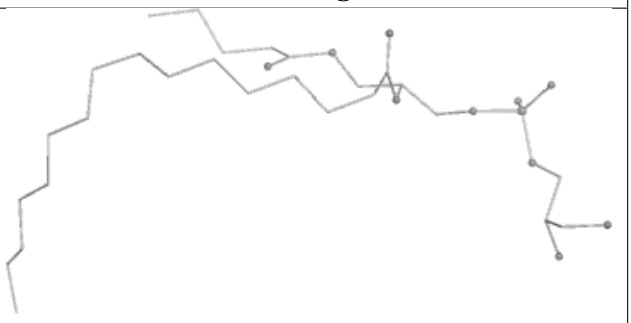
Bond lengths



Bond angles

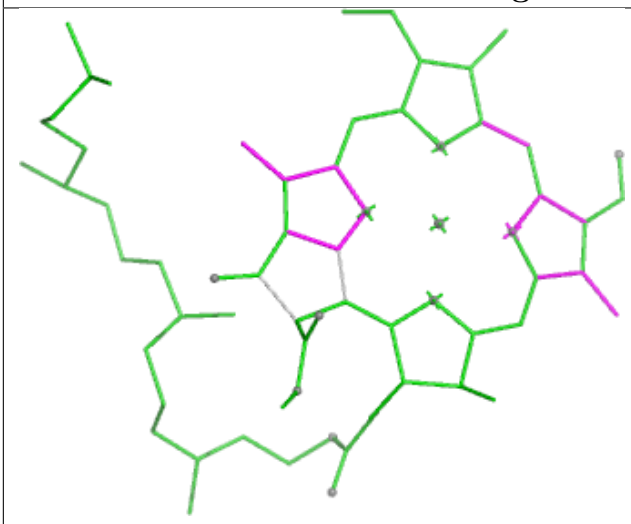


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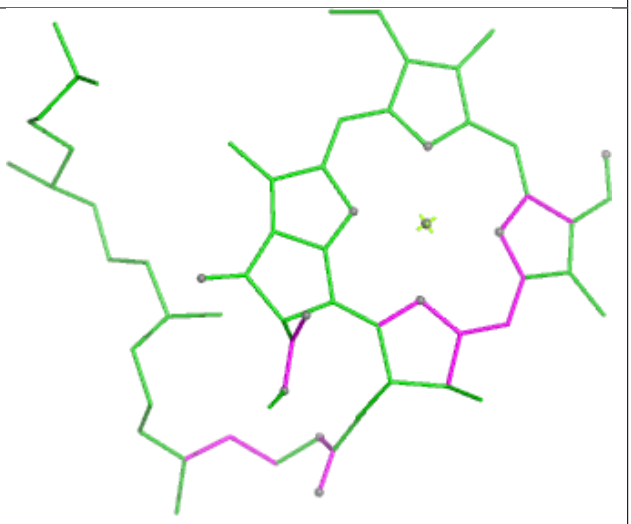


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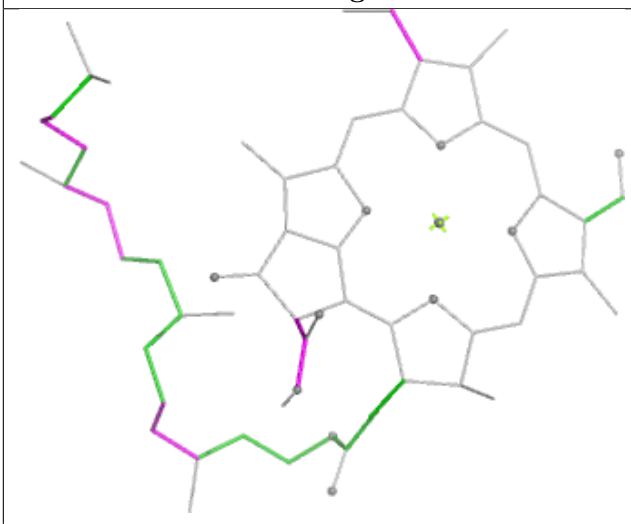
Ligand CL7 cB 1229



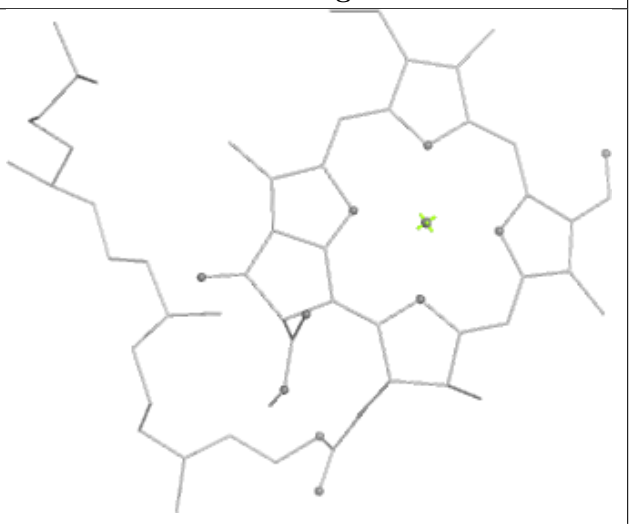
Bond lengths



Bond angles

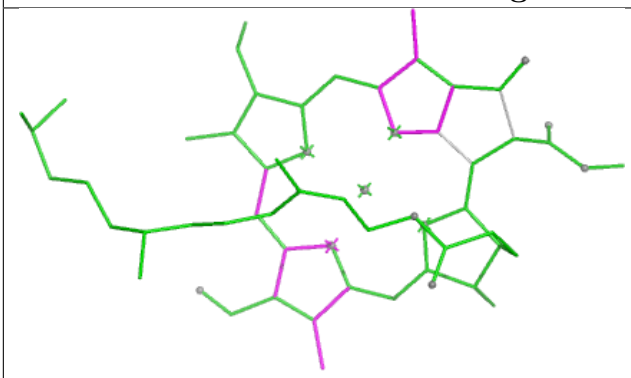


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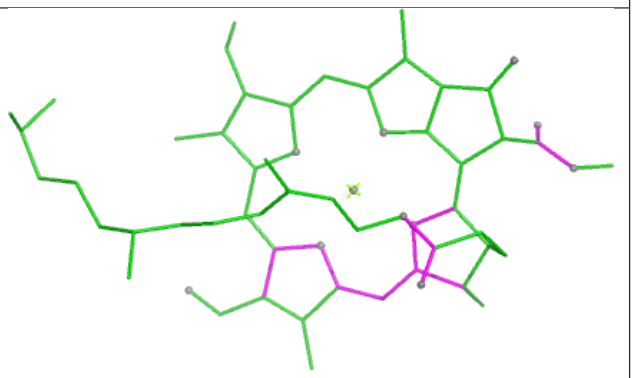


Rings

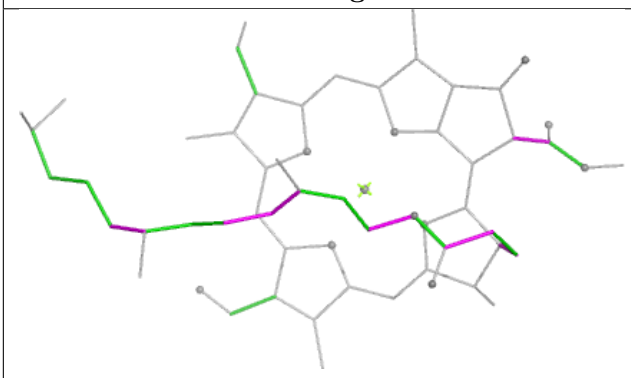
Ligand CL7 bB 1235



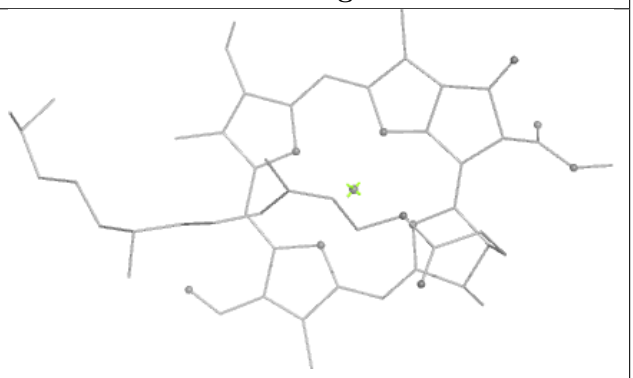
Bond lengths



Bond angles

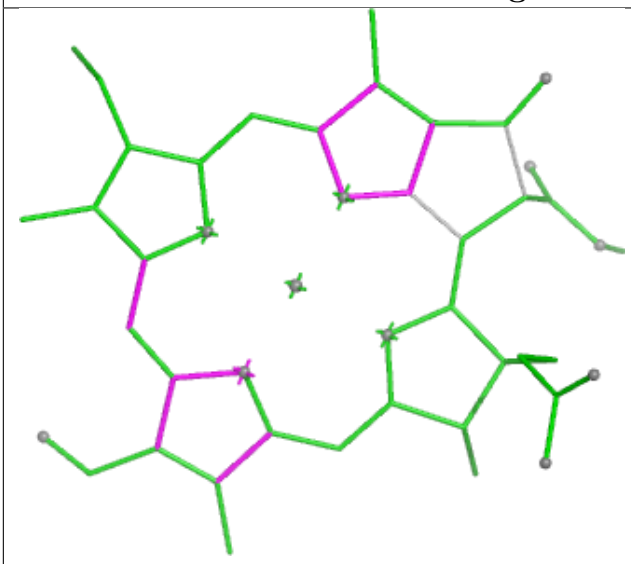


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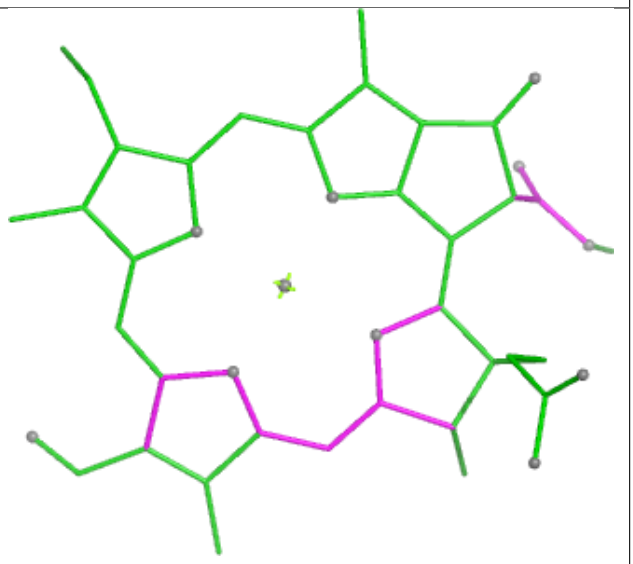


Rings

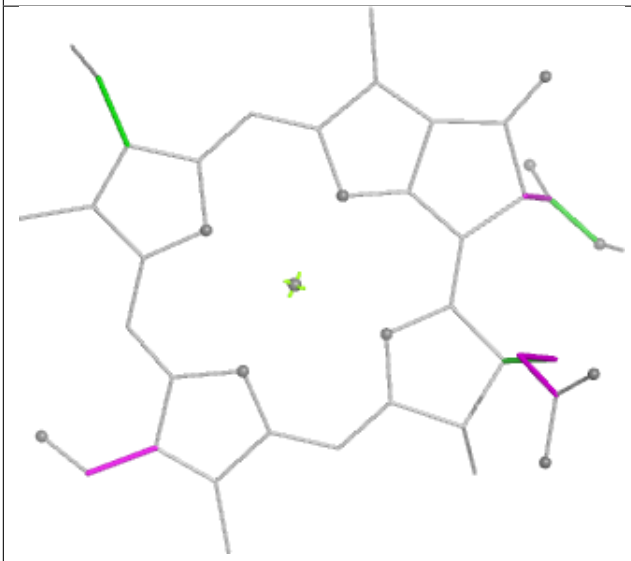
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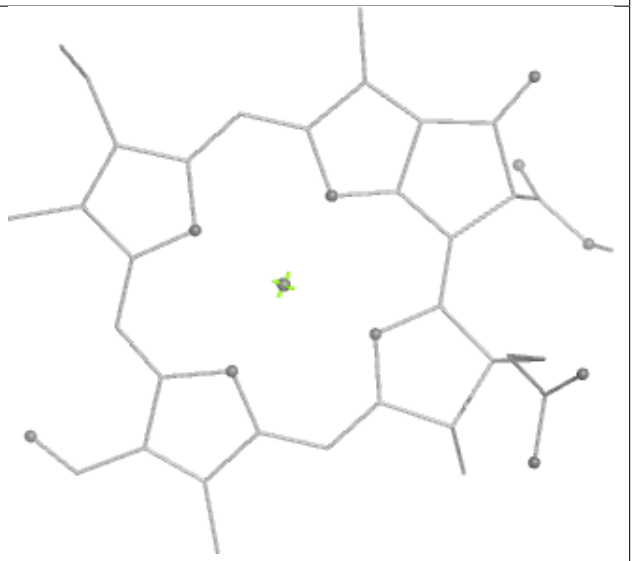
Bond lengths



Bond angles

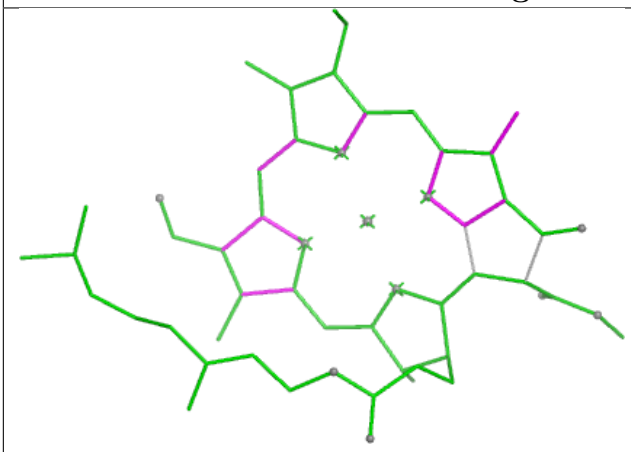


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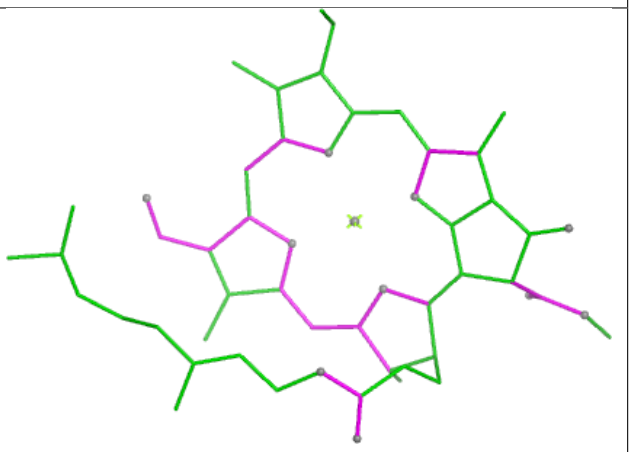


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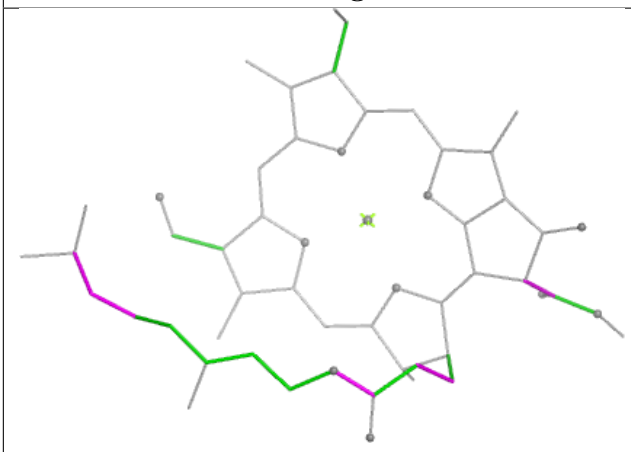
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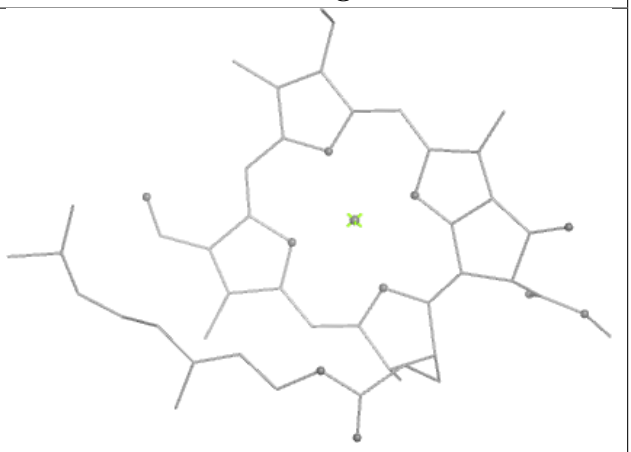
Bond lengths



Bond angles

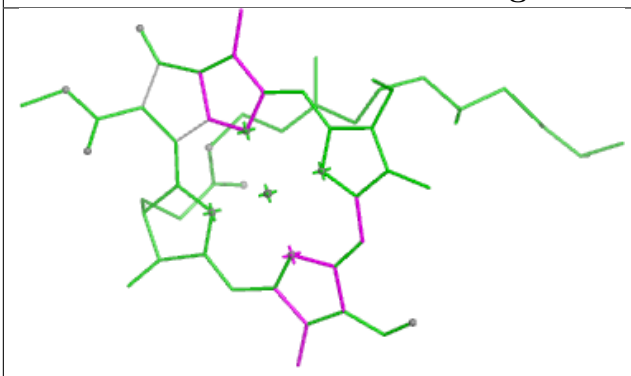


Torsions

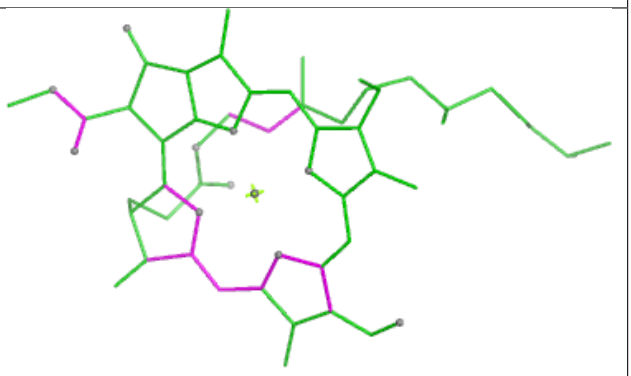


Rings

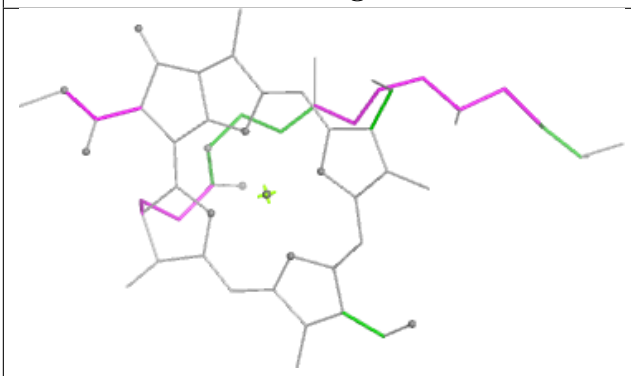
Ligand CL7 bA 1140



Bond lengths



Bond angles

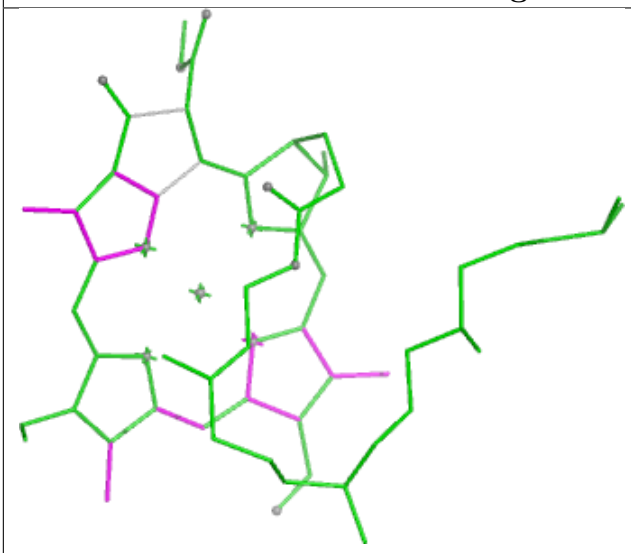


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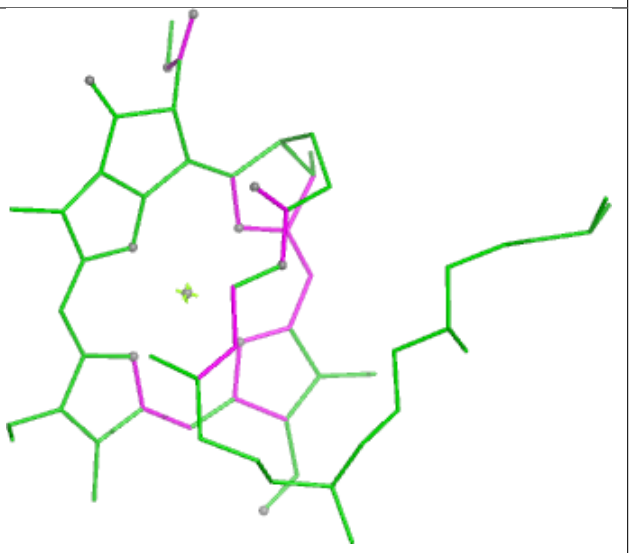


Rings

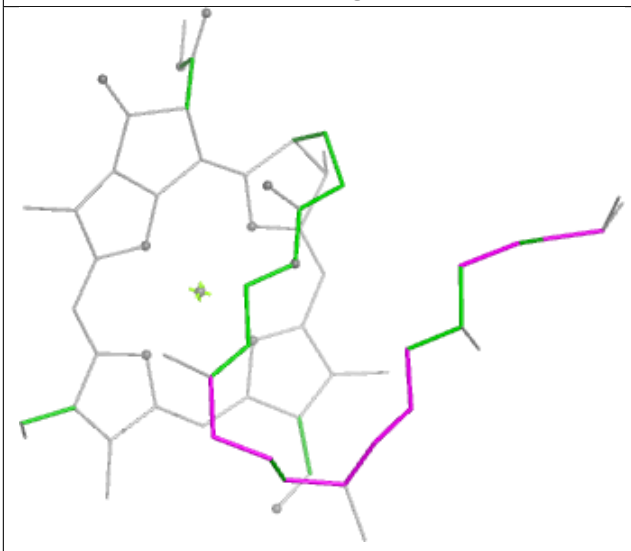
Ligand CL7 bB 1205



Bond lengths



Bond angles

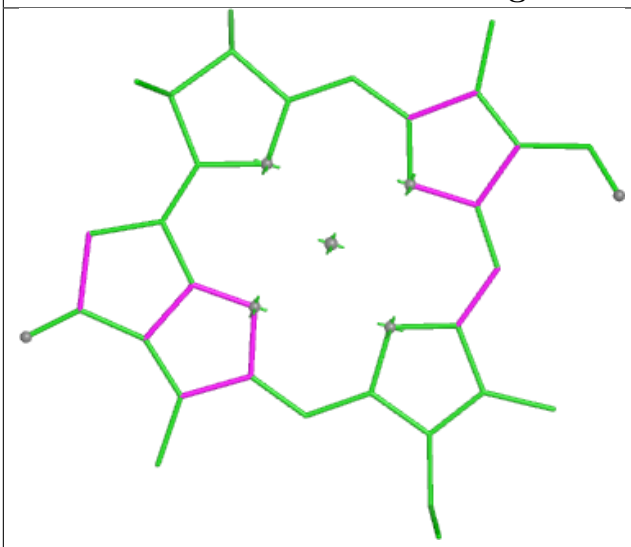


Torsions



Rings

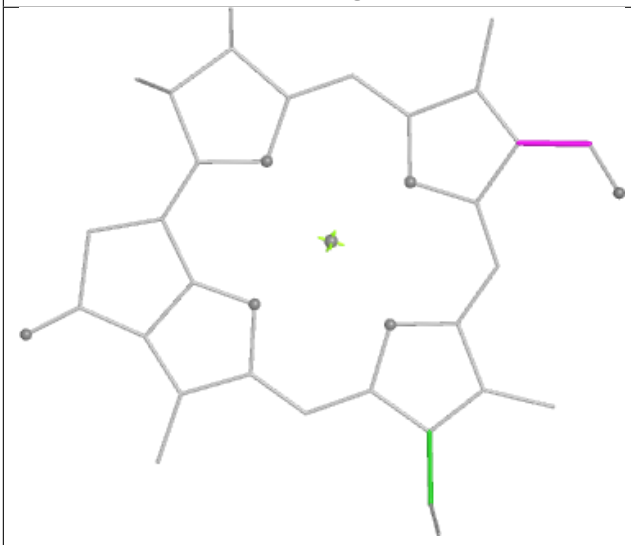
Ligand CL7 bK 1402



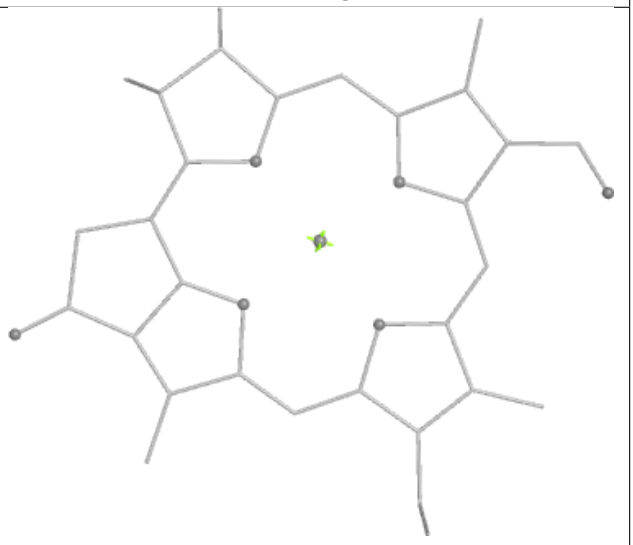
Bond lengths



Bond angles

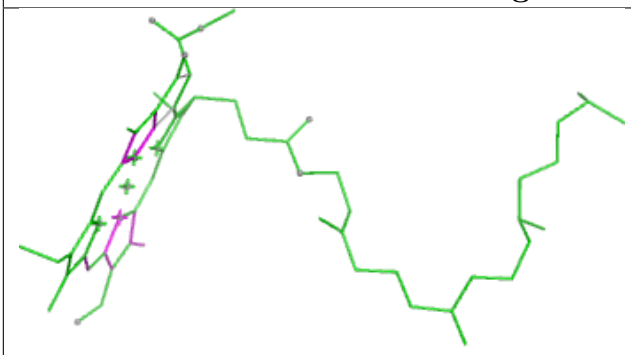


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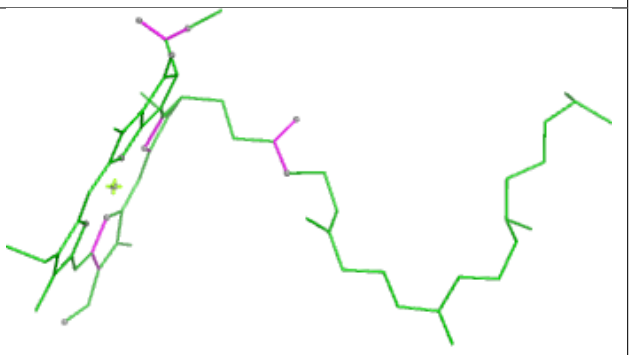


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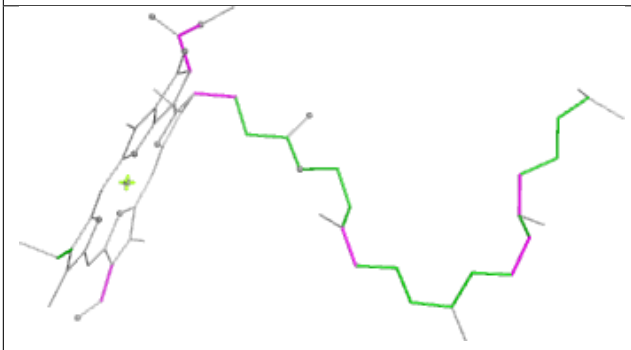
Ligand CL7 cB 1208



Bond lengths



Bond angles

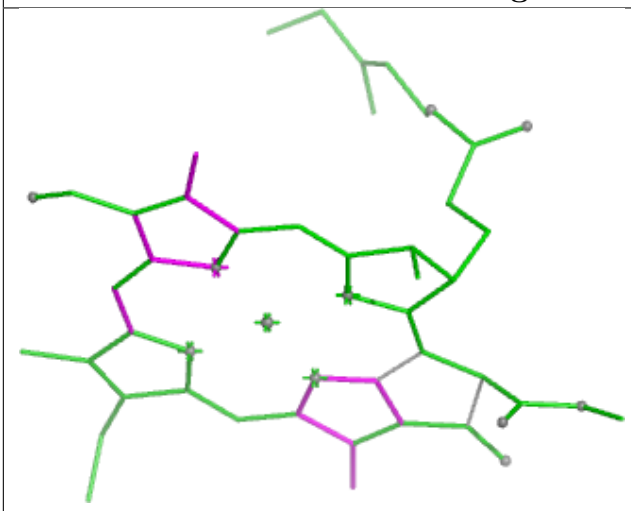


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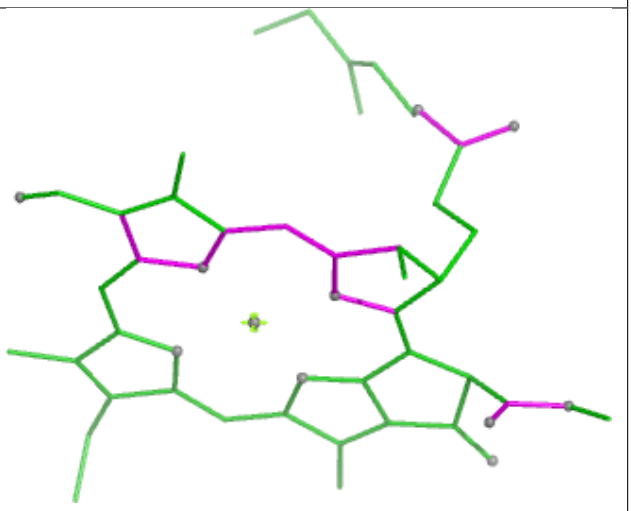


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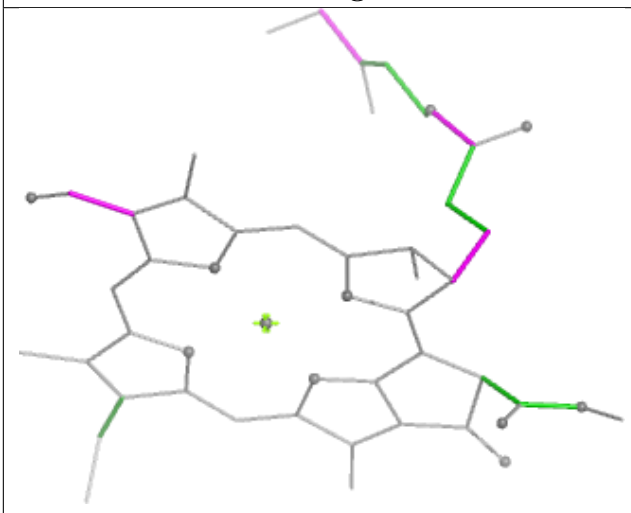
Ligand CL7 aA 1130



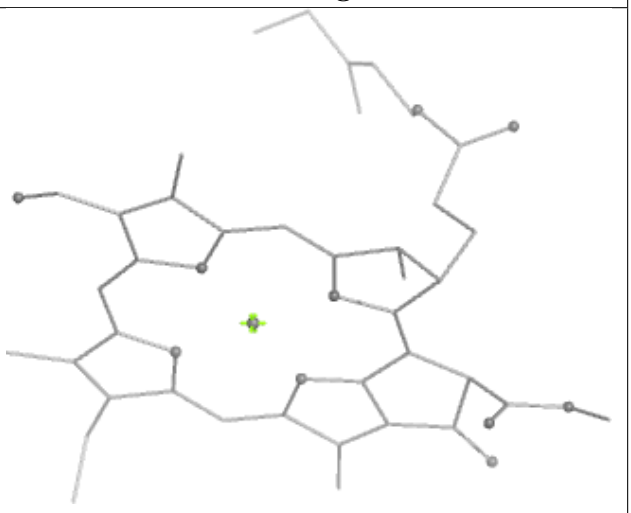
Bond lengths



Bond angles

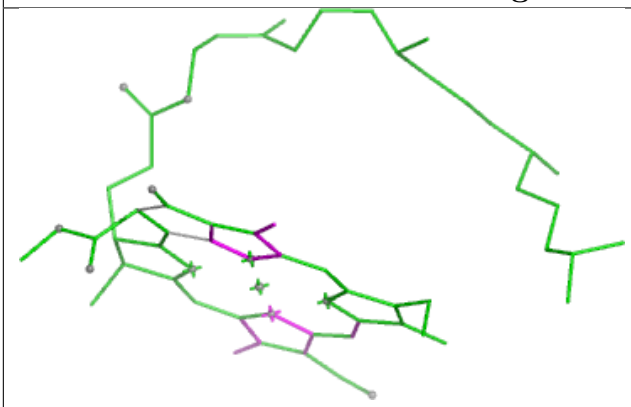


Torsions



Rings

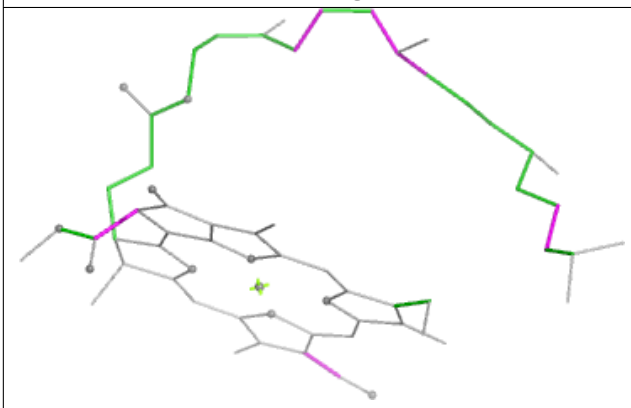
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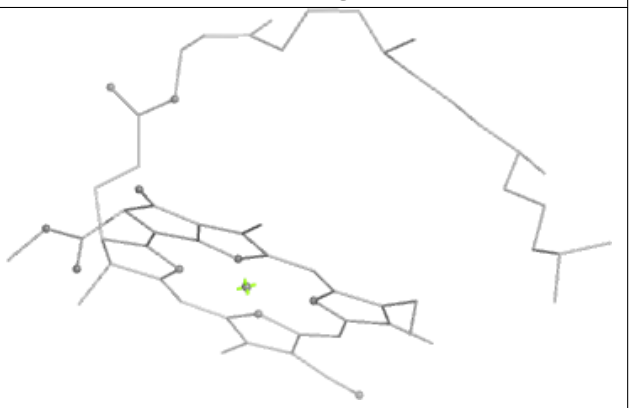
Bond lengths



Bond angles

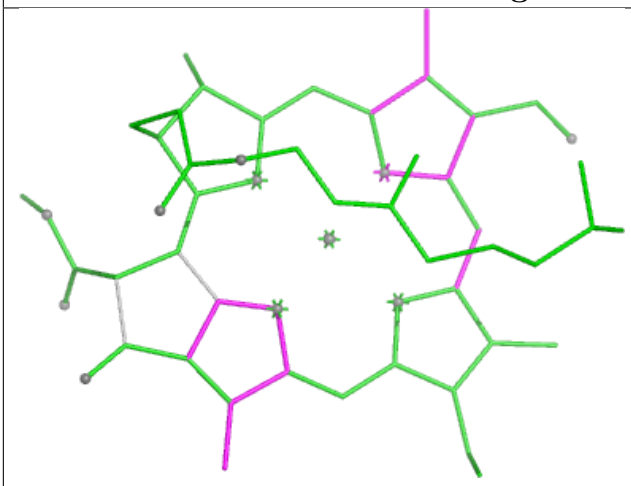


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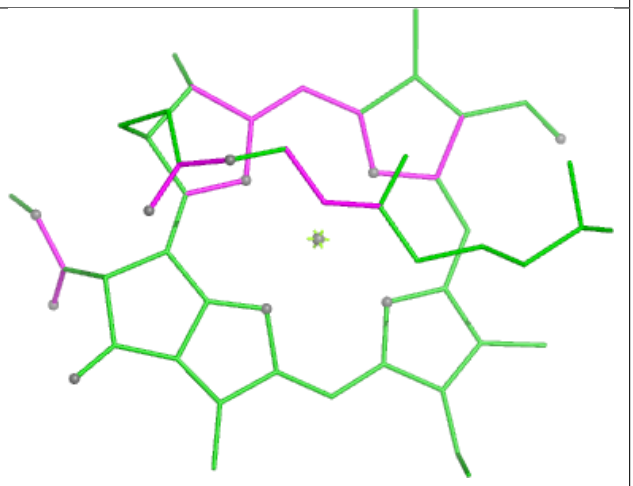


Rings

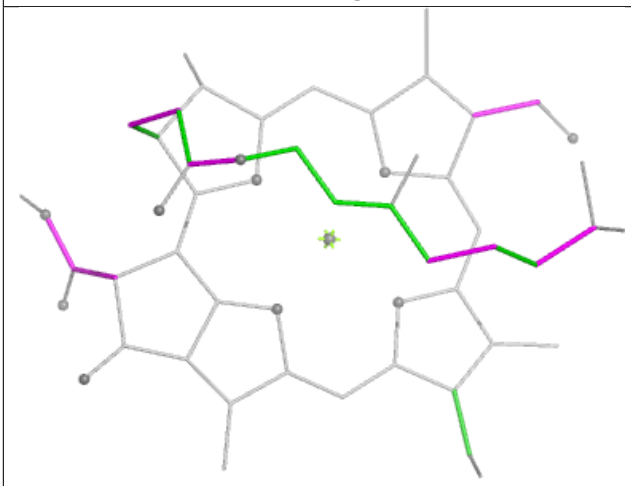
Ligand CL7 aA 1118



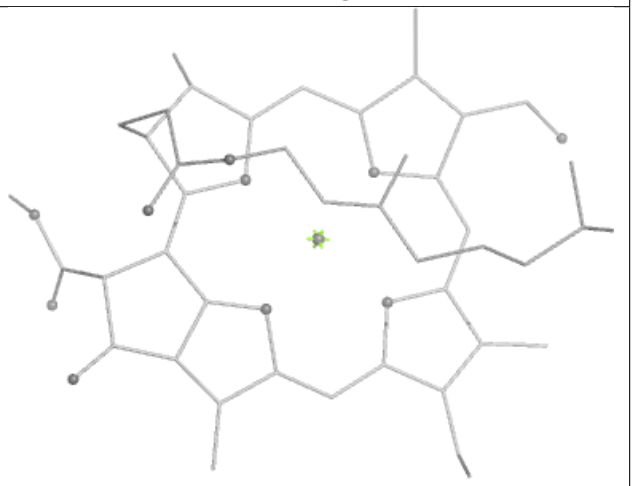
Bond lengths



Bond angles

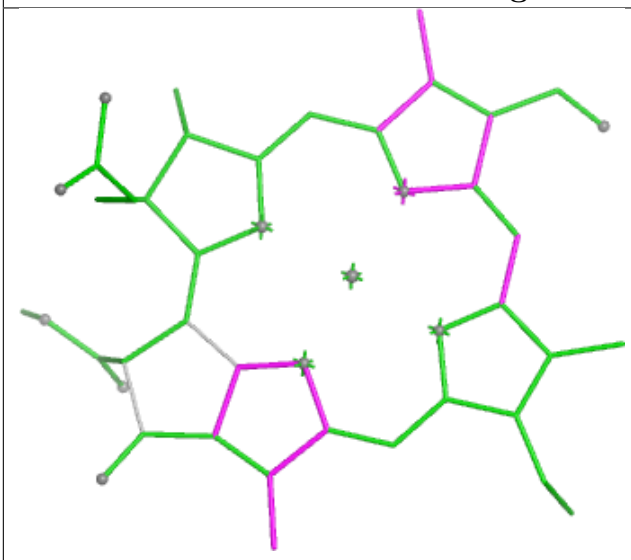


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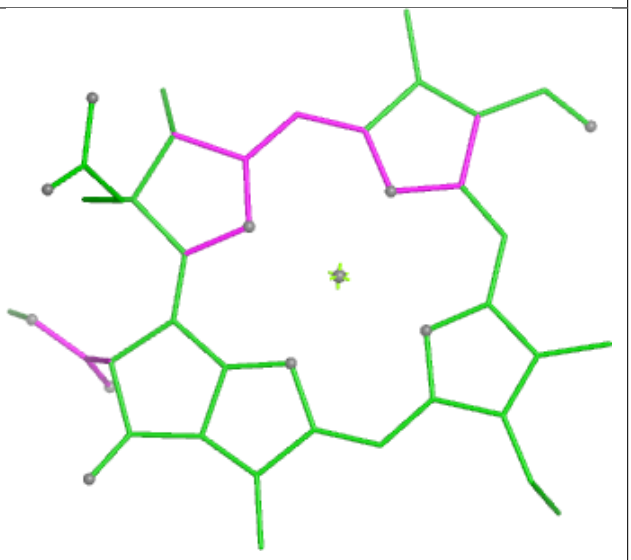


Rings

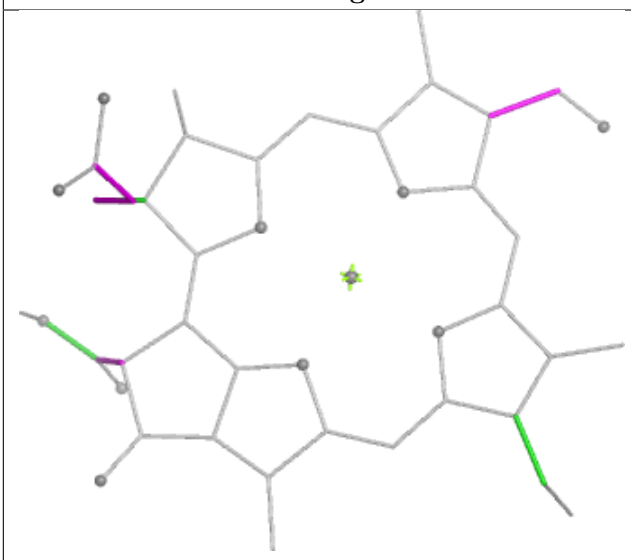
Ligand CL7 aK 1401



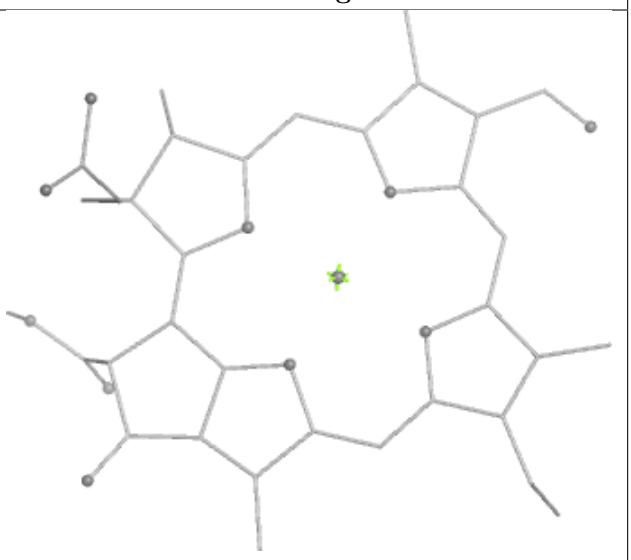
Bond lengths



Bond angles

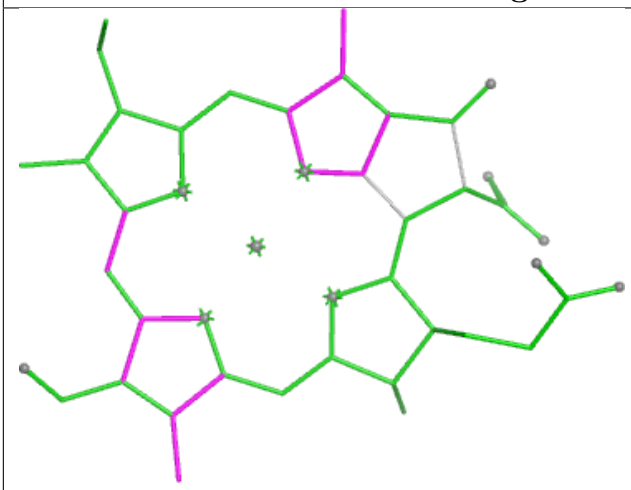


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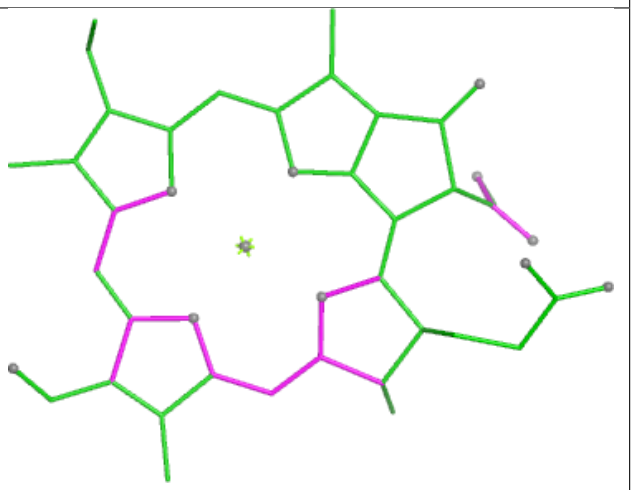


Rings

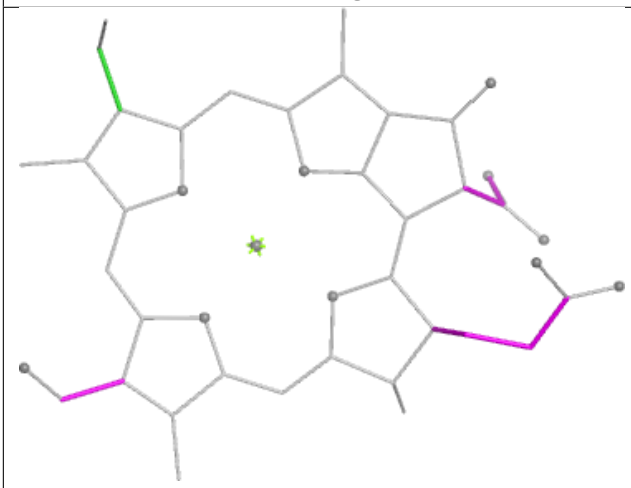
Ligand CL7 aA 1113



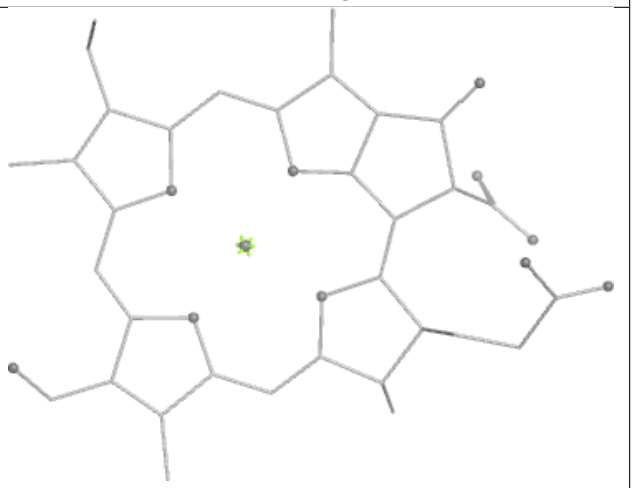
Bond lengths



Bond angles

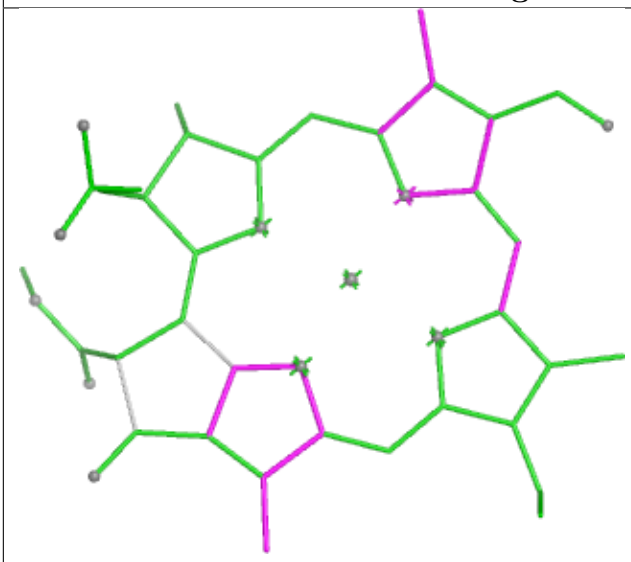


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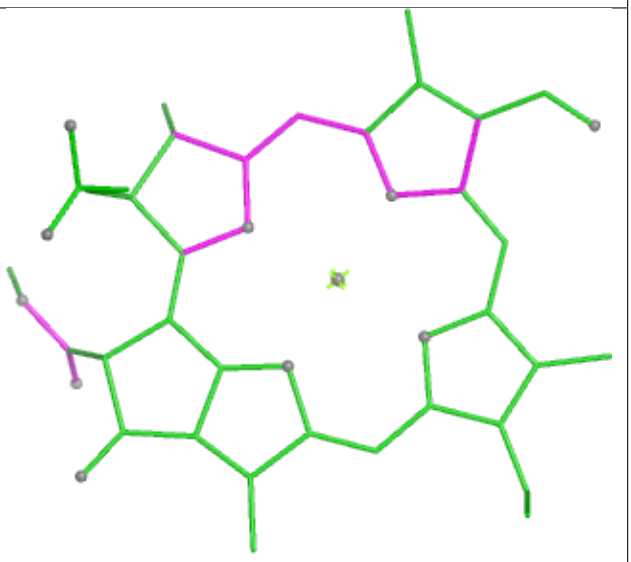


Rings

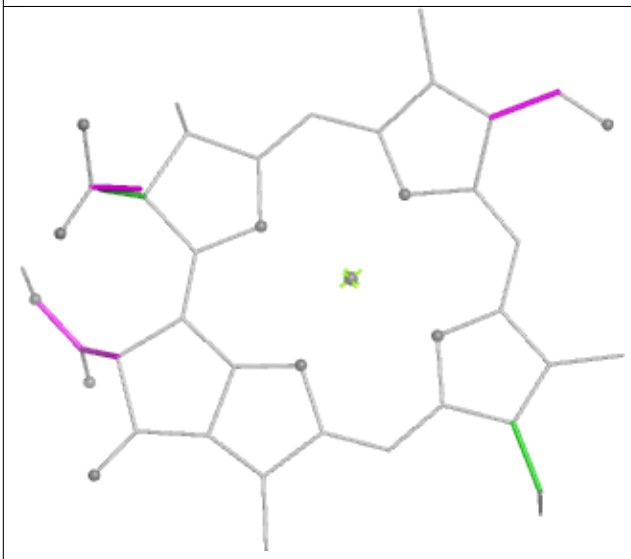
Ligand CL7 aB 1236



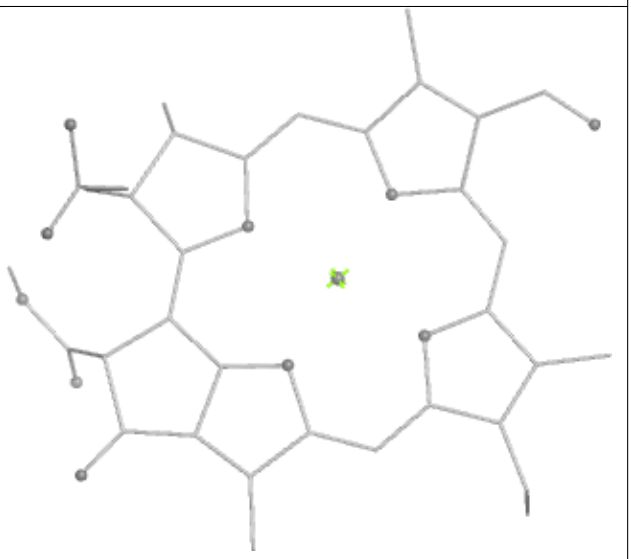
Bond lengths



Bond angles

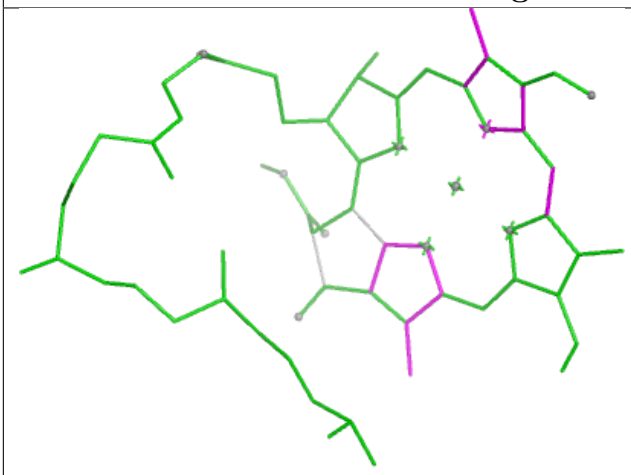


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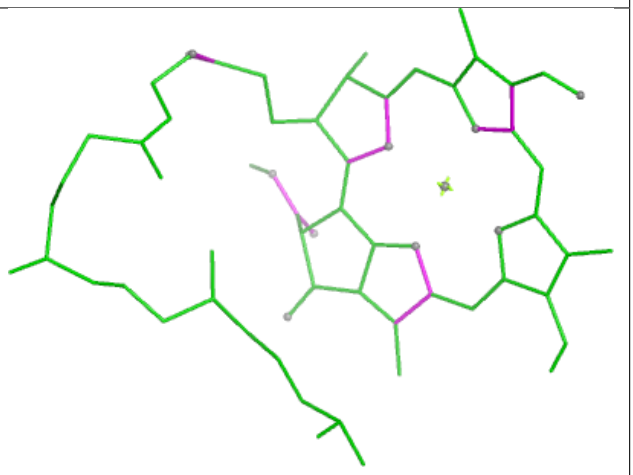


Rings

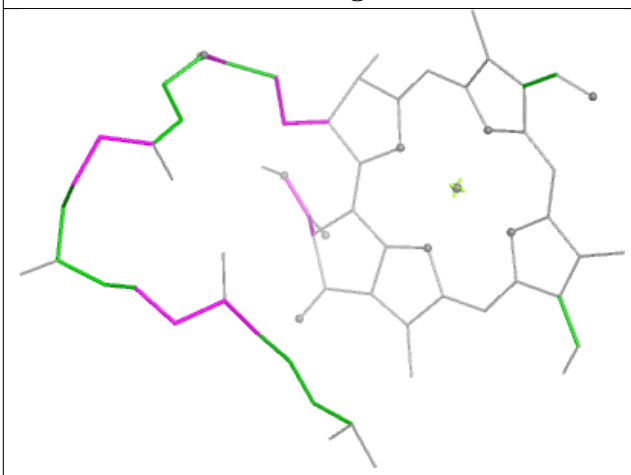
Ligand CL7 cA 1127



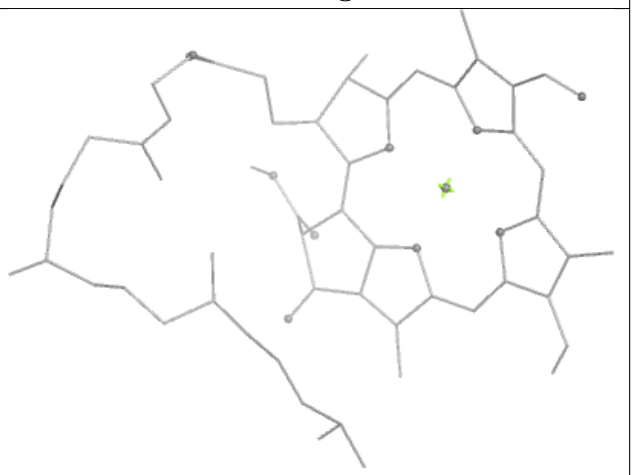
Bond lengths



Bond angles

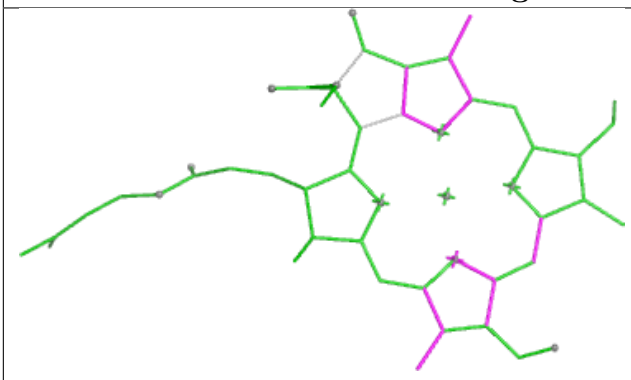


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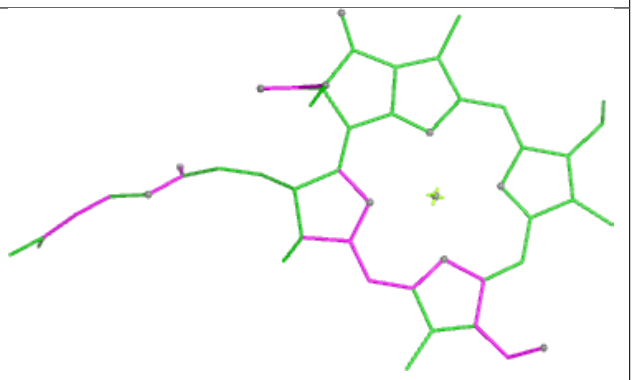


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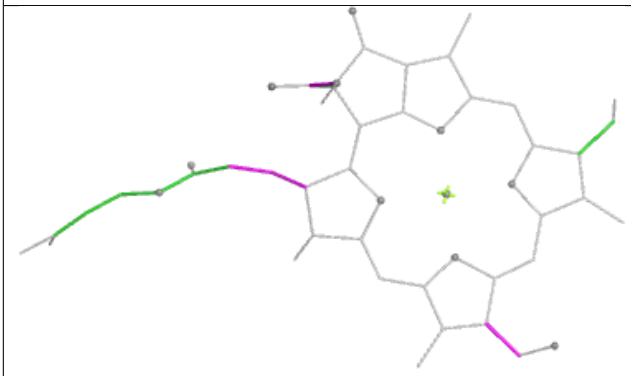
Ligand CL7 aB 1234



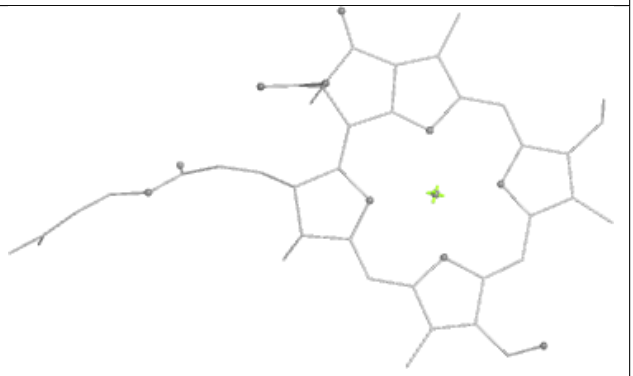
Bond lengths



Bond angles

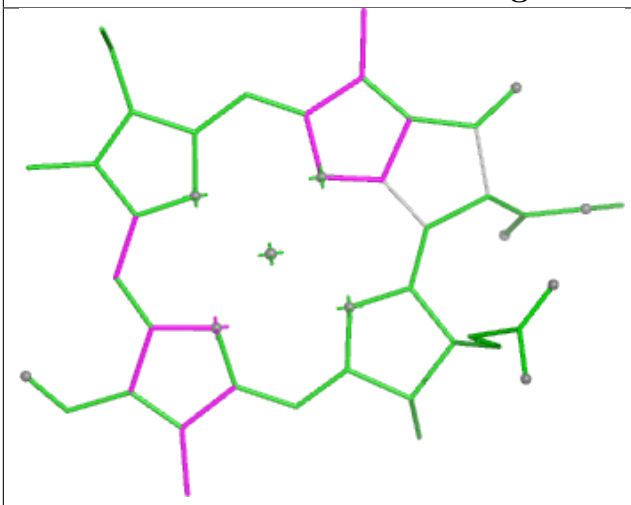


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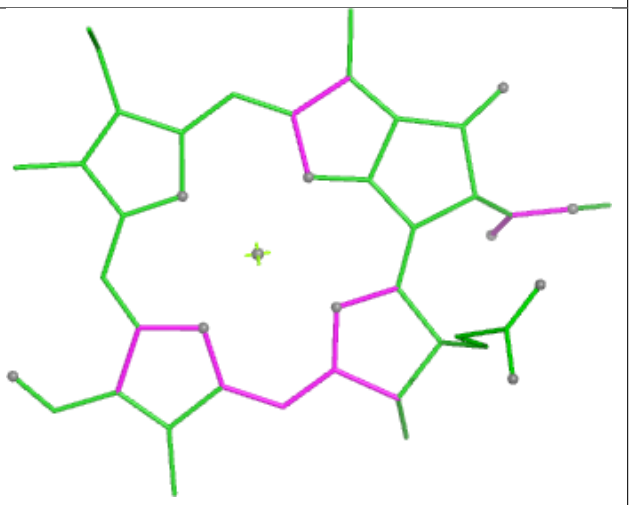


Rings

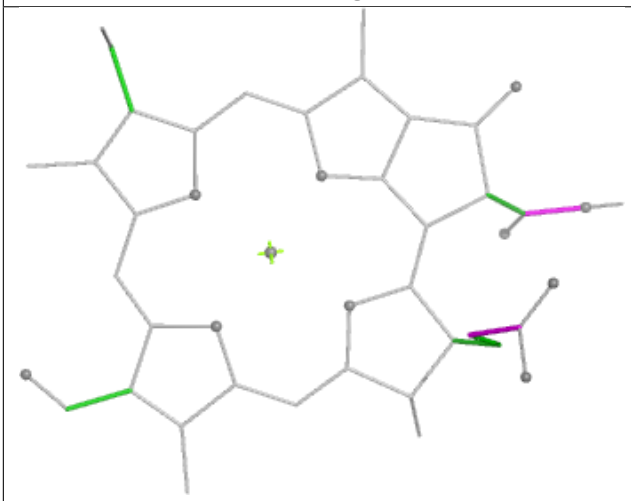
Ligand CL7 aA 1107



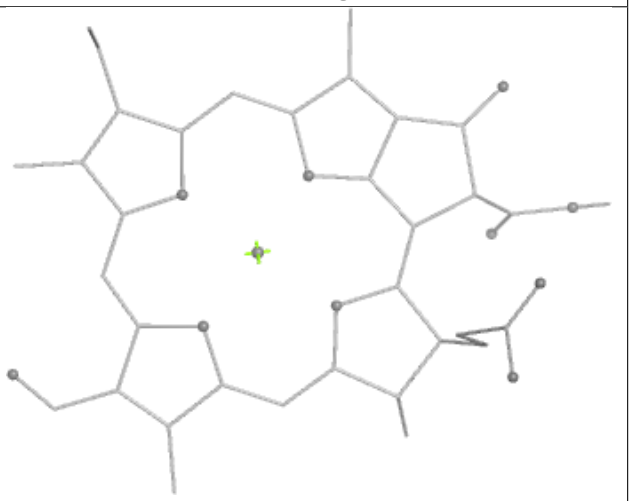
Bond lengths



Bond angles

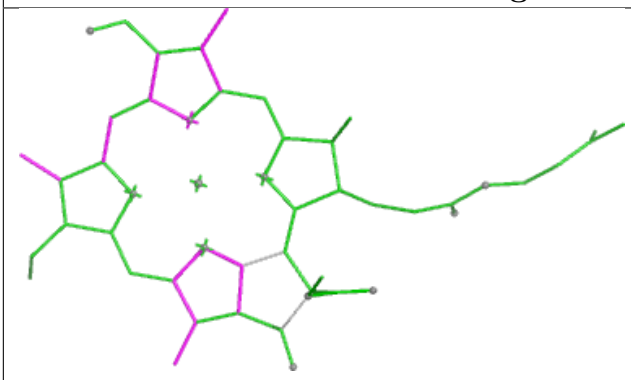


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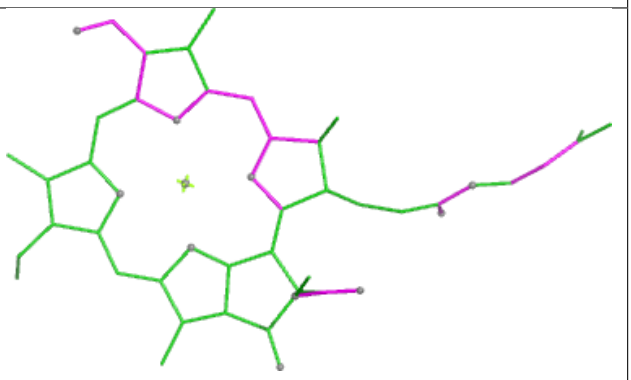


Rings

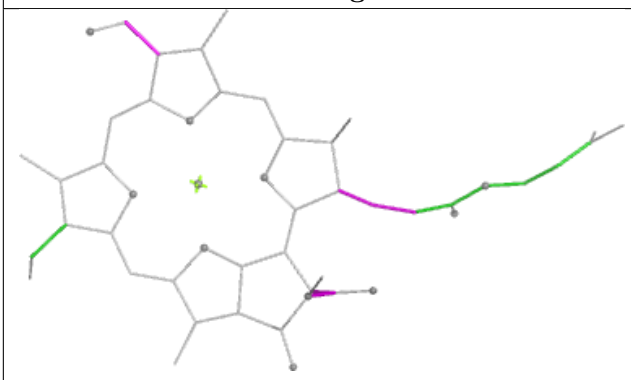
Ligand CL7 bB 1234



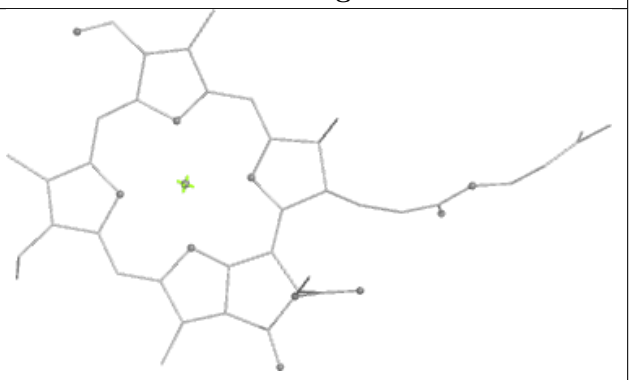
Bond lengths



Bond angles

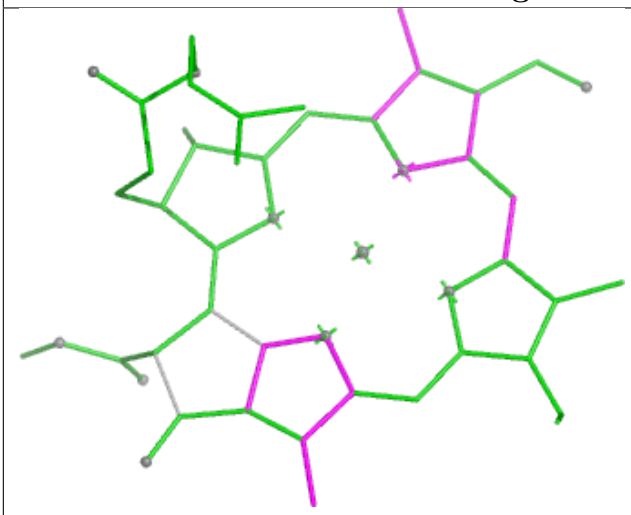


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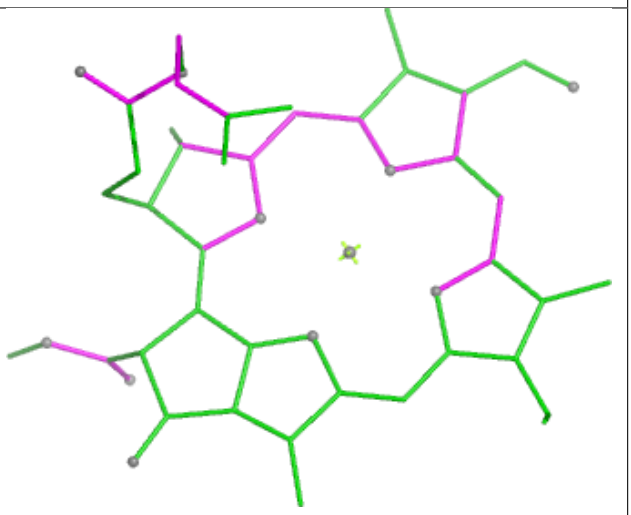


Rings

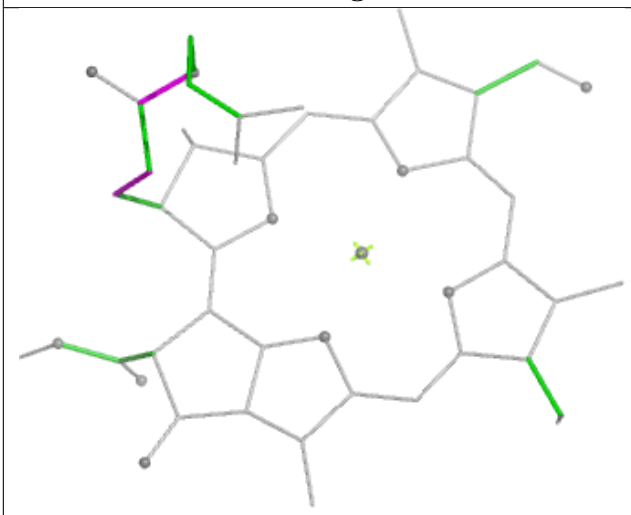
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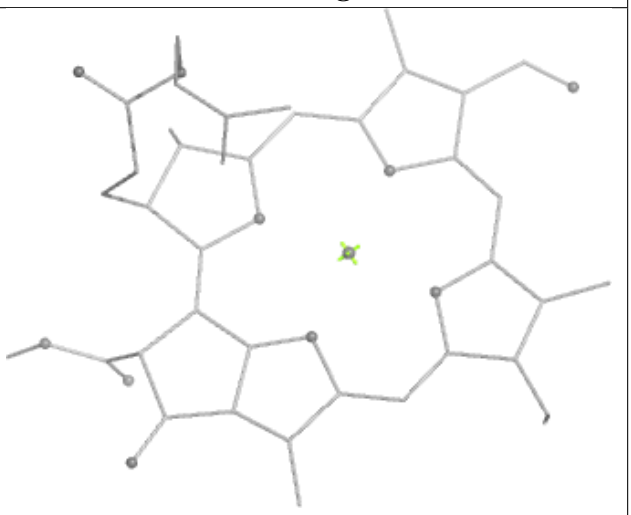
Bond lengths



Bond angles

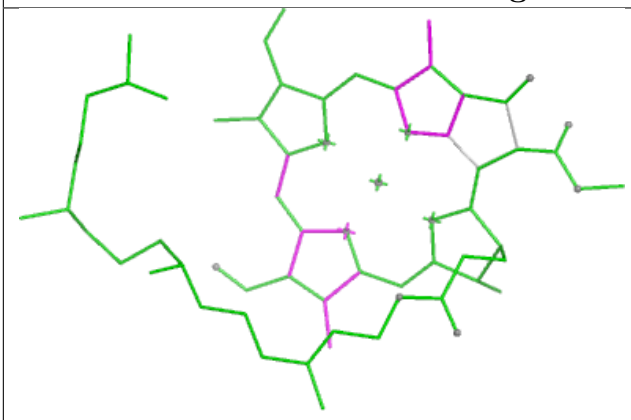


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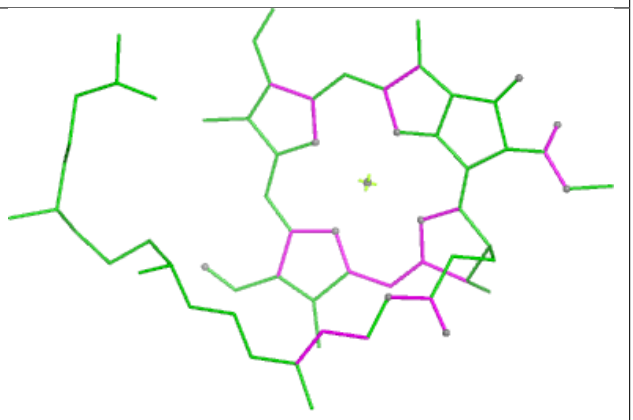


Rings

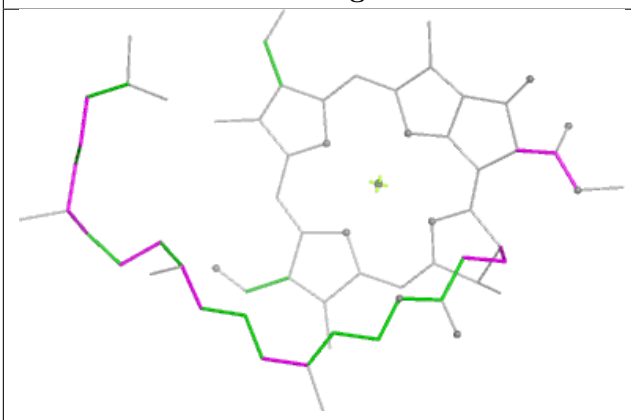
Ligand CL7 bA 1117



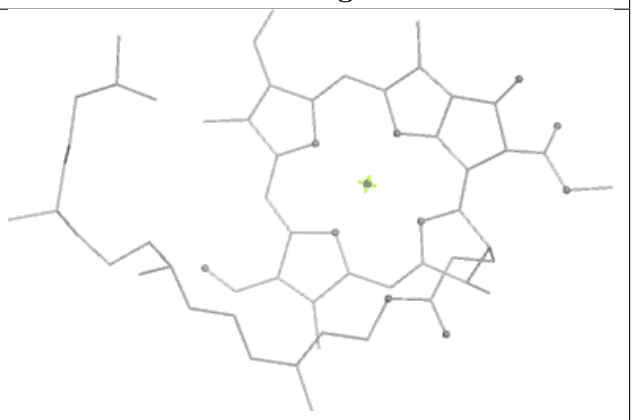
Bond lengths



Bond angles



Torsions



Rings

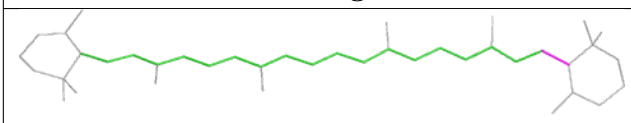
Ligand A1JPJ bA 4003



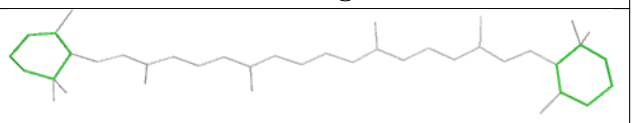
Bond lengths



Bond angles

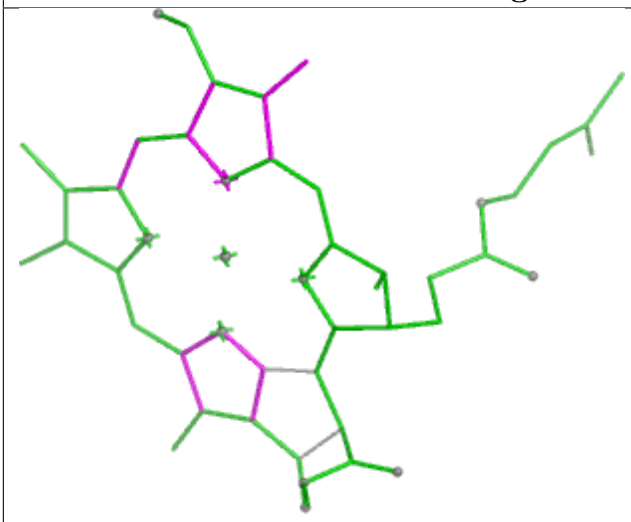


Torsions

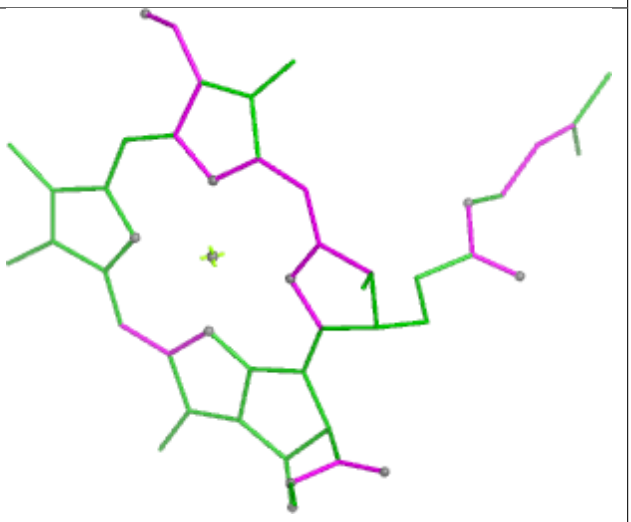


Rings

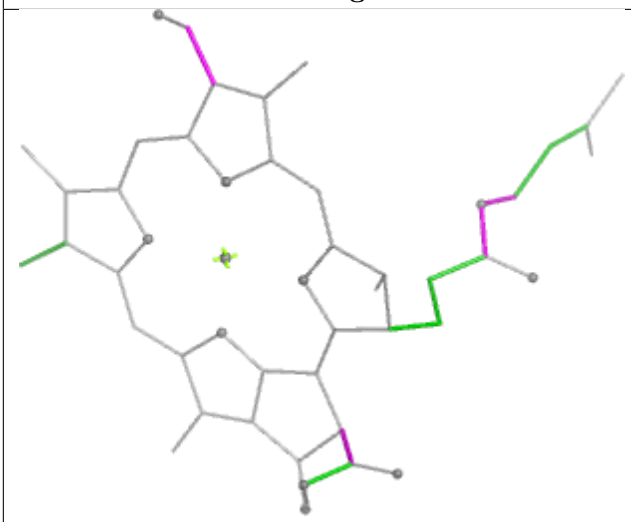
Ligand CL7 aA 1129



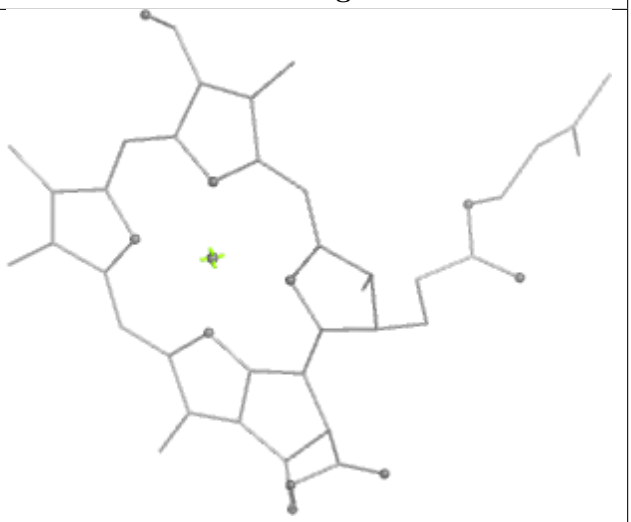
Bond lengths



Bond angles

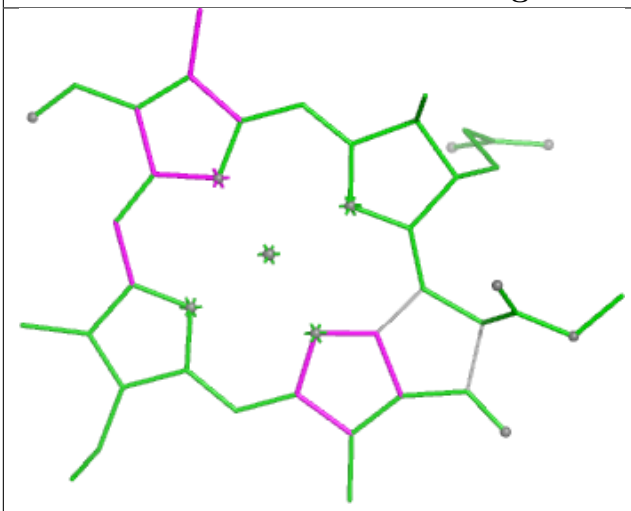


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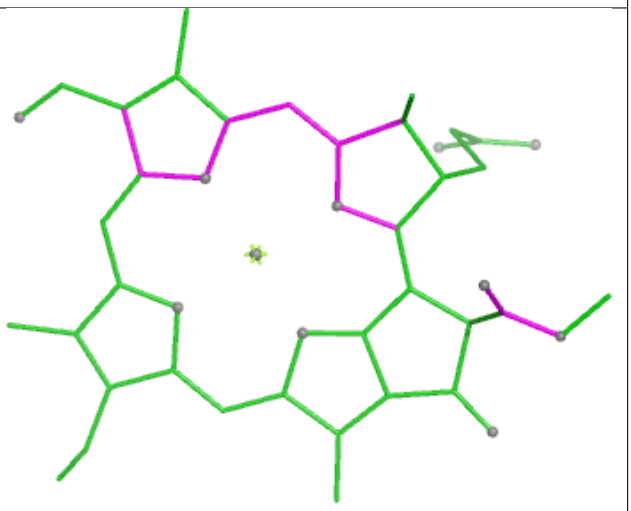


Rings

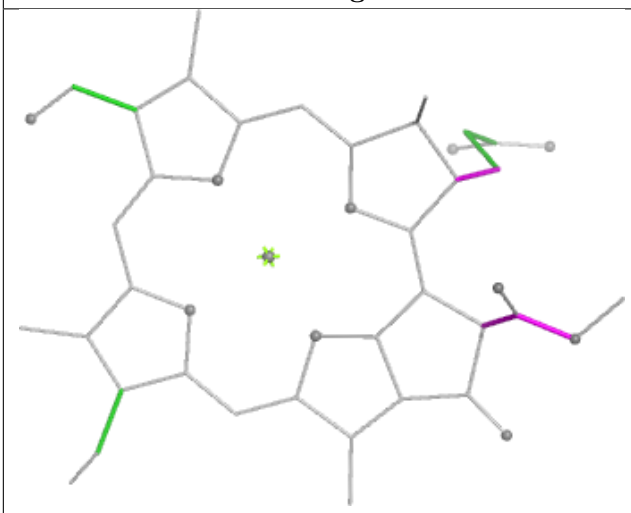
Ligand CL7 aB 1216



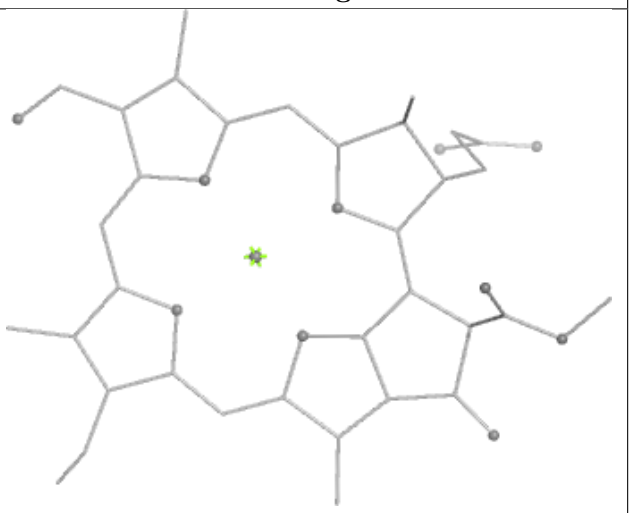
Bond lengths



Bond angles

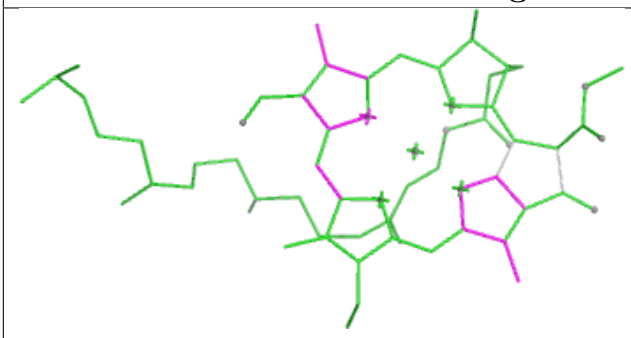


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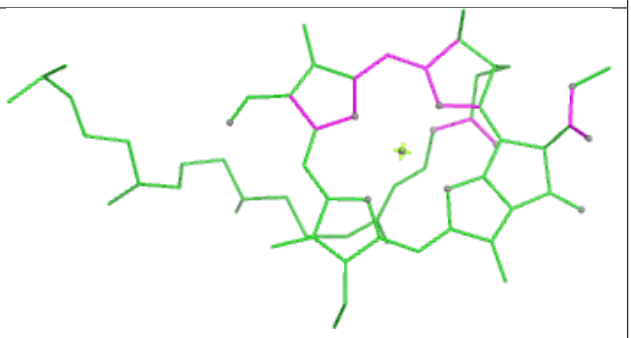


Rings

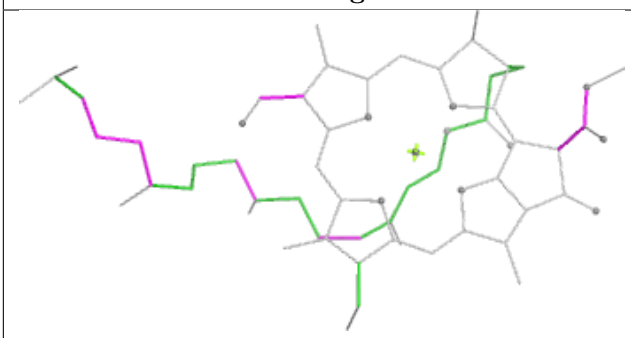
Ligand CL7 bA 1138



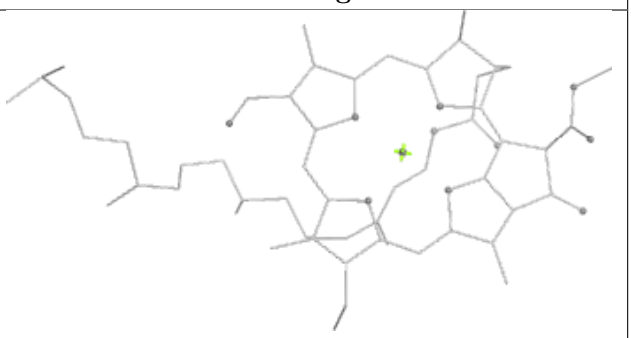
Bond lengths



Bond angles

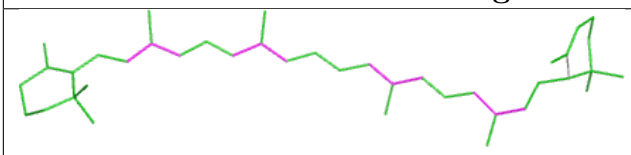


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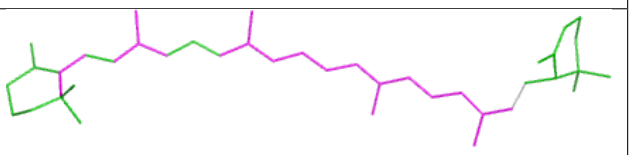


Rings

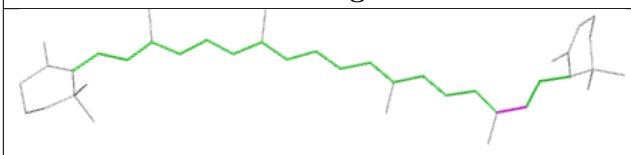
Ligand A1JPJ aL 4023



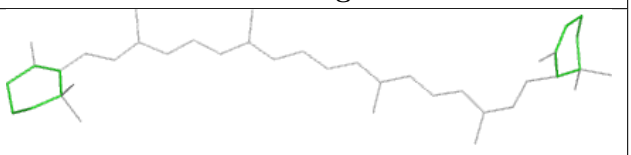
Bond lengths



Bond angles

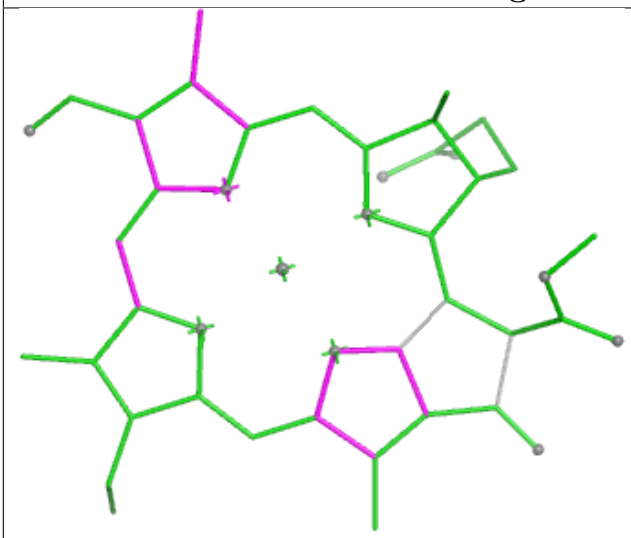


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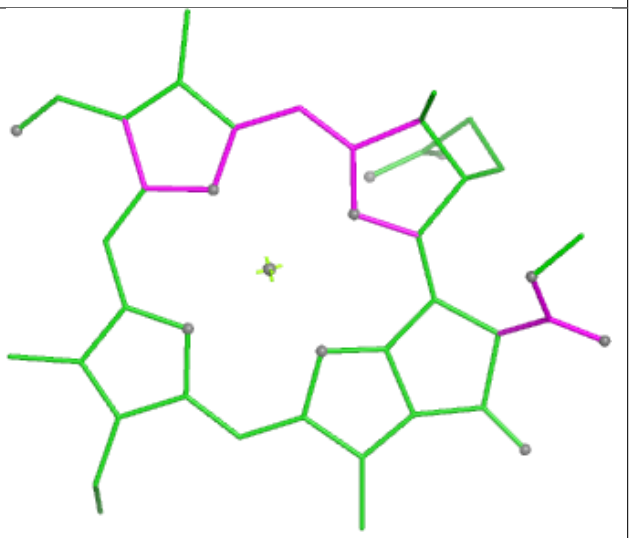


Rings

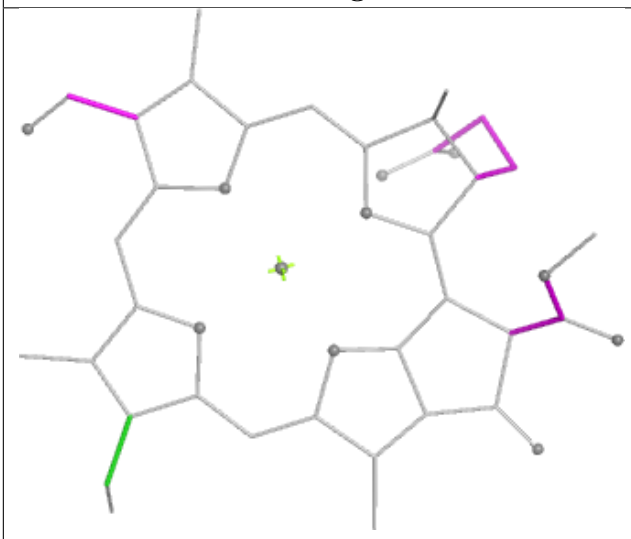
Ligand CL7 bA 1110



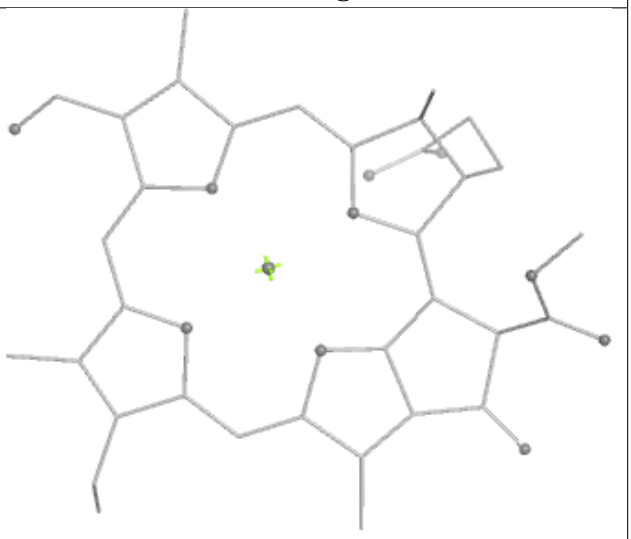
Bond lengths



Bond angles

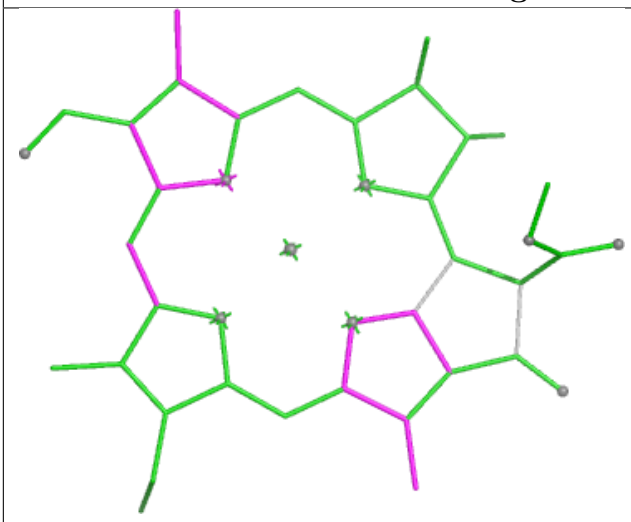


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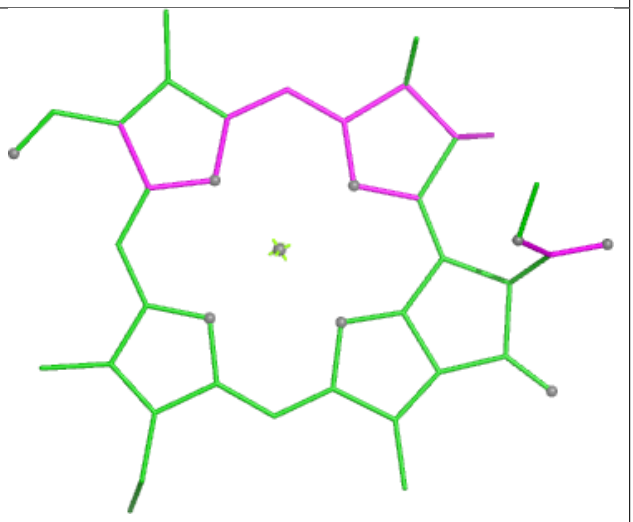


Rings

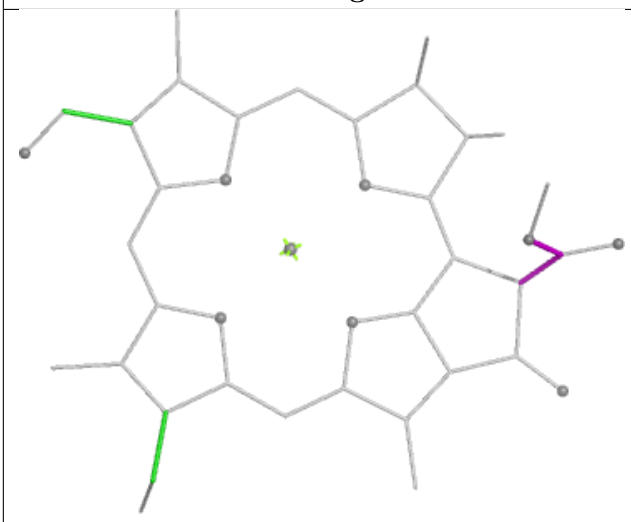
Ligand CL7 bB 1218



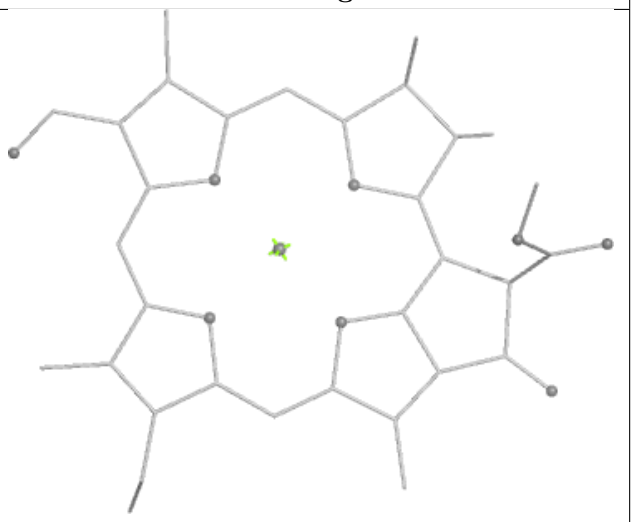
Bond lengths



Bond angles

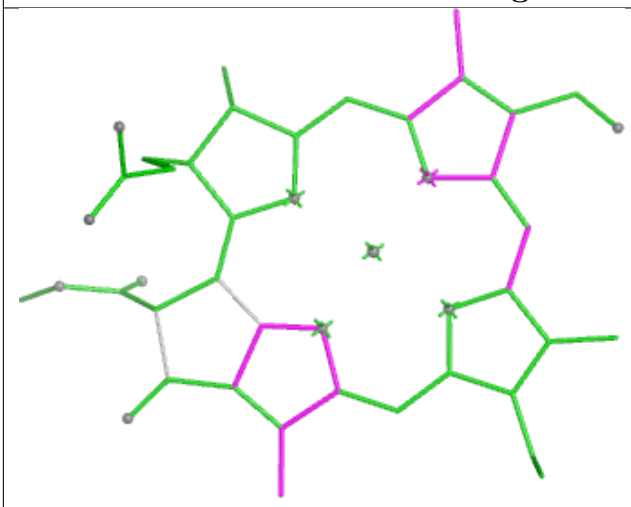


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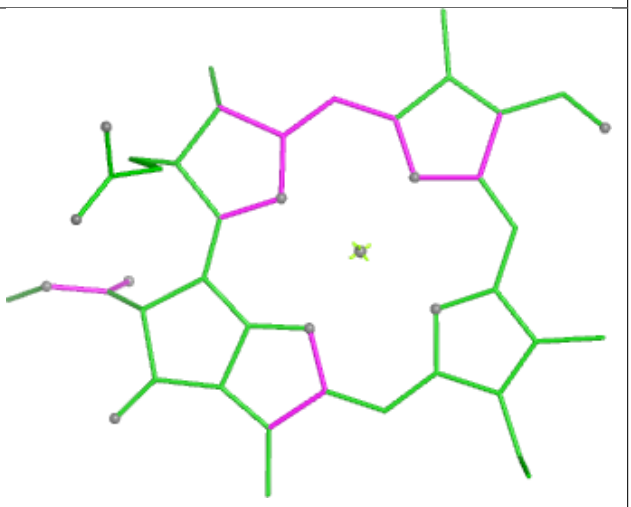


Rings

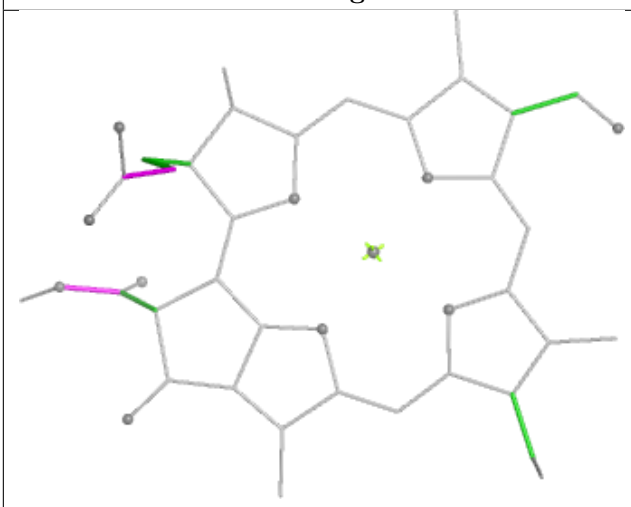
Ligand CL7 cA 1107



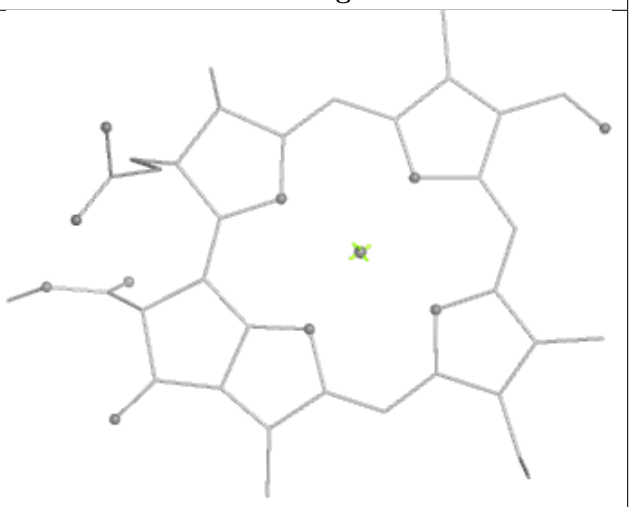
Bond lengths



Bond angles

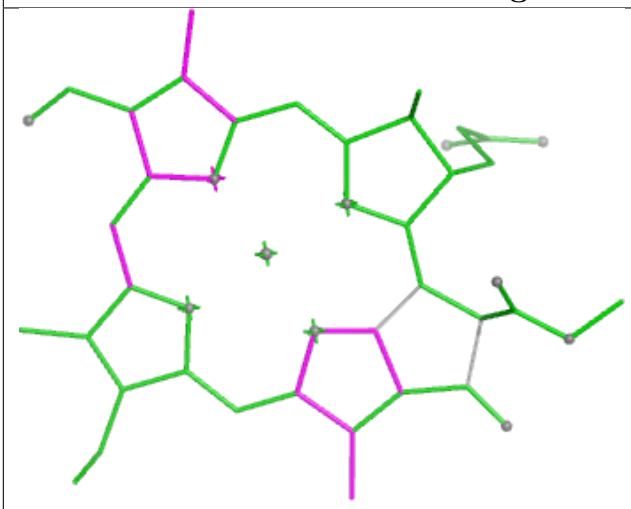


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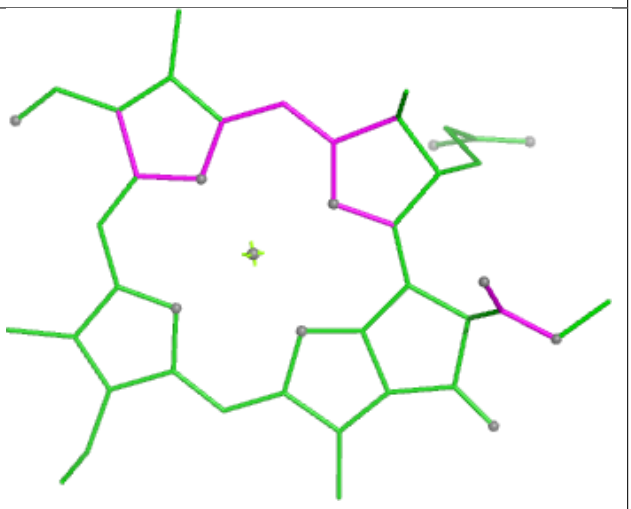


Rings

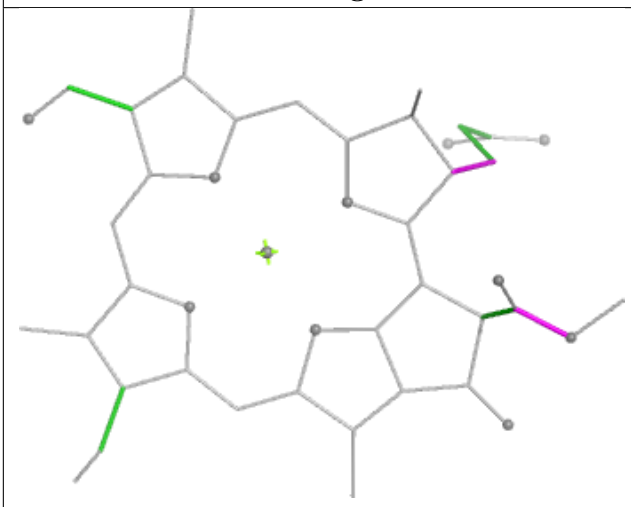
Ligand CL7 bB 1216



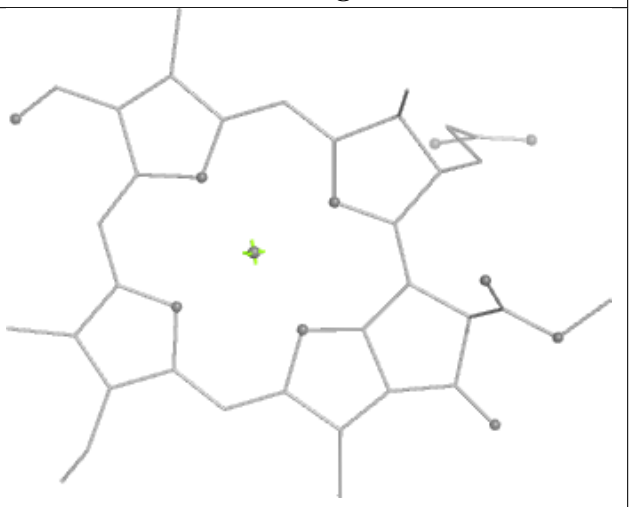
Bond lengths



Bond angles

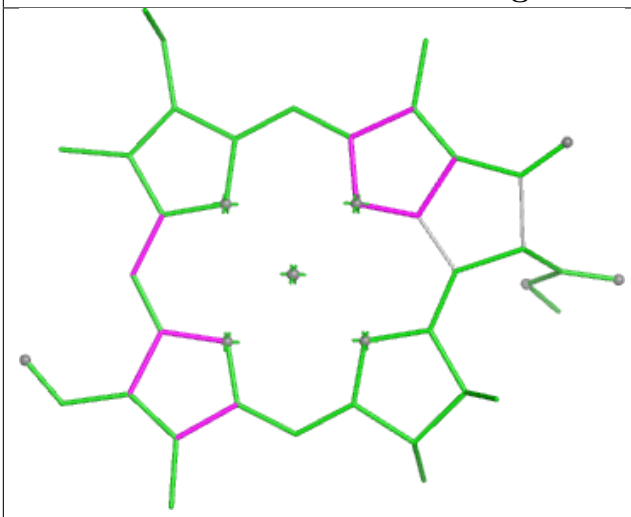


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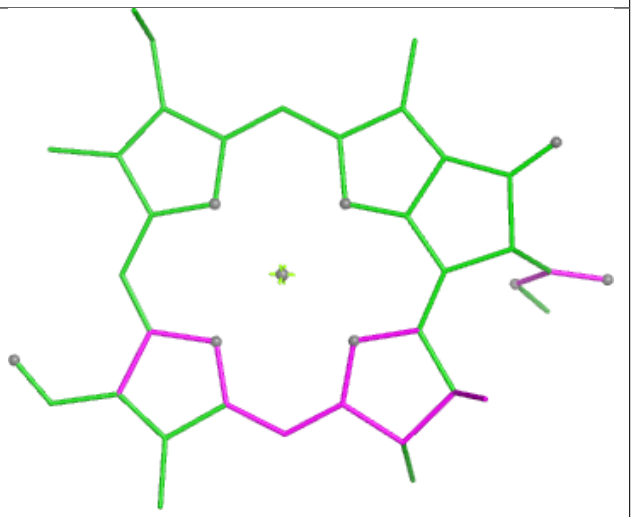


Rings

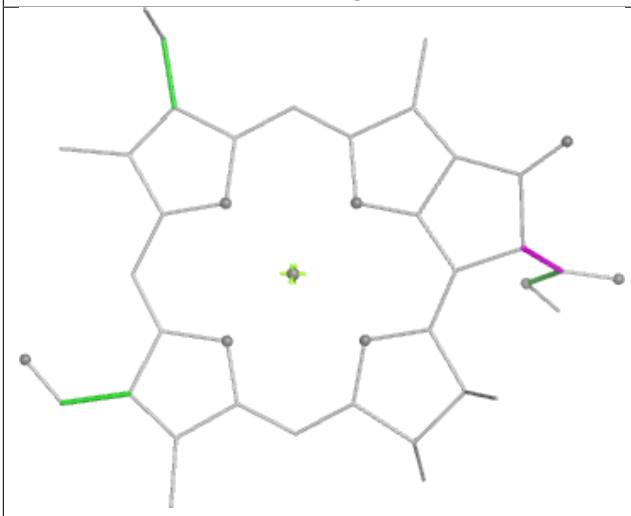
Ligand CL7 aB 1217



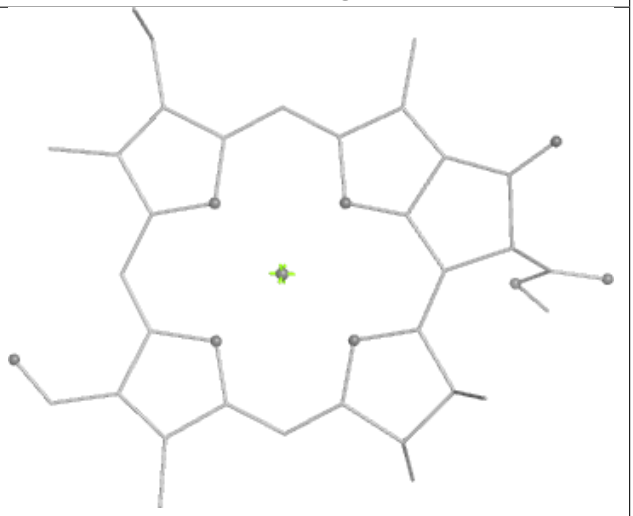
Bond lengths



Bond angles

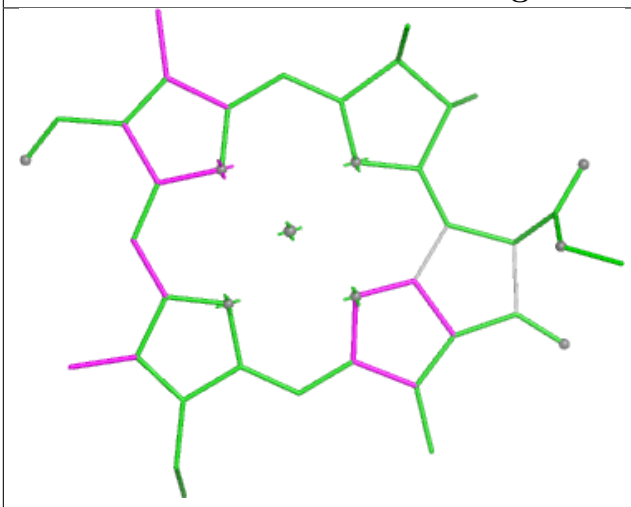


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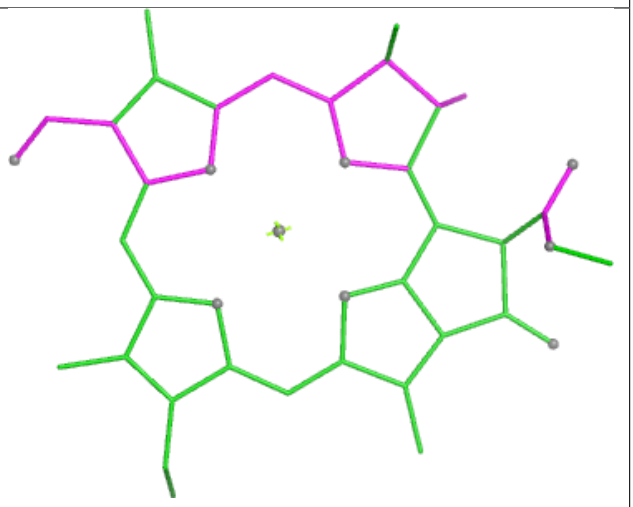


Rings

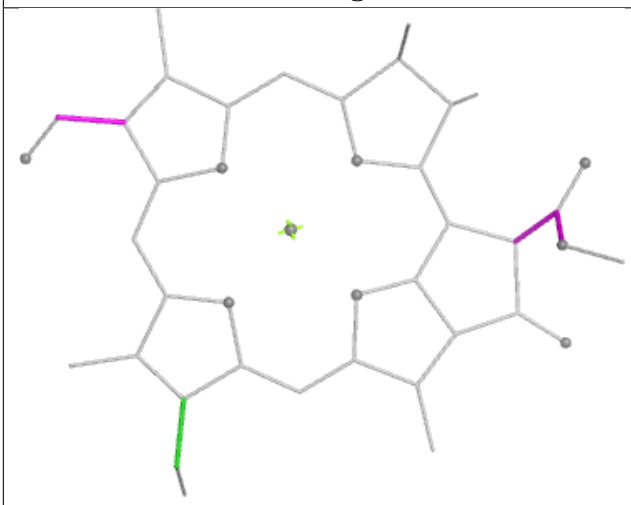
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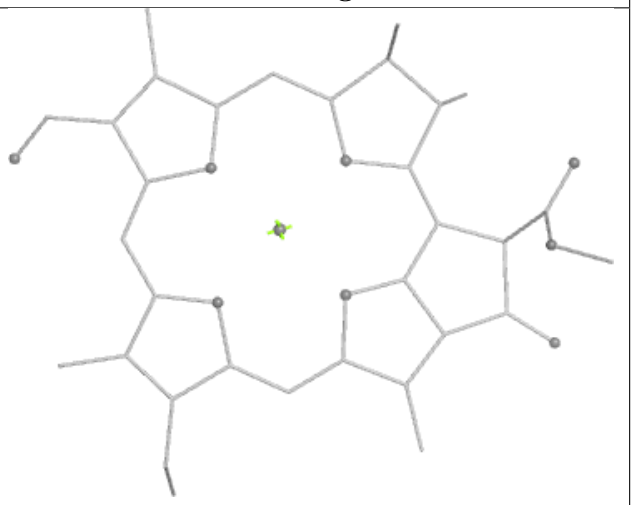
Bond lengths



Bond angles

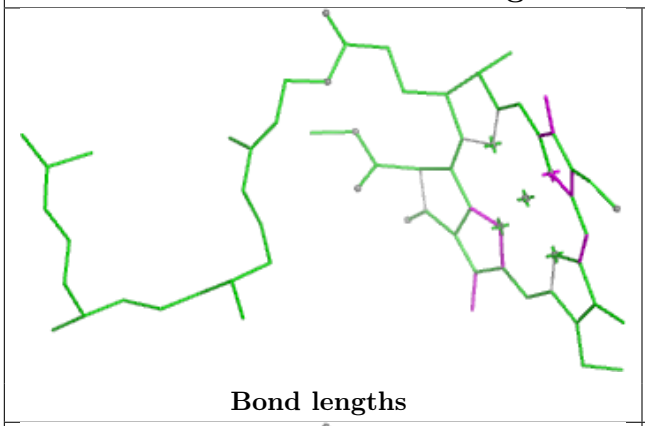


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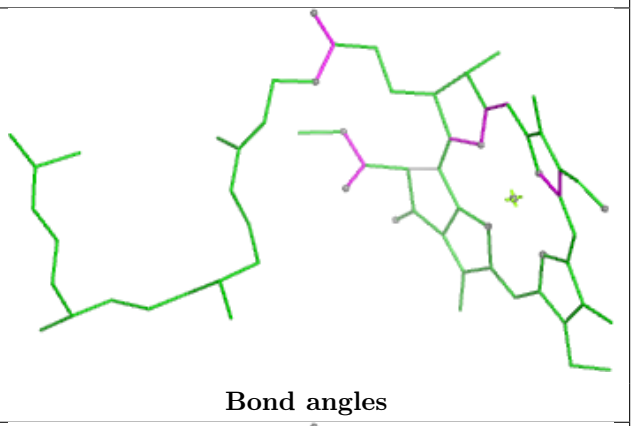


Rings

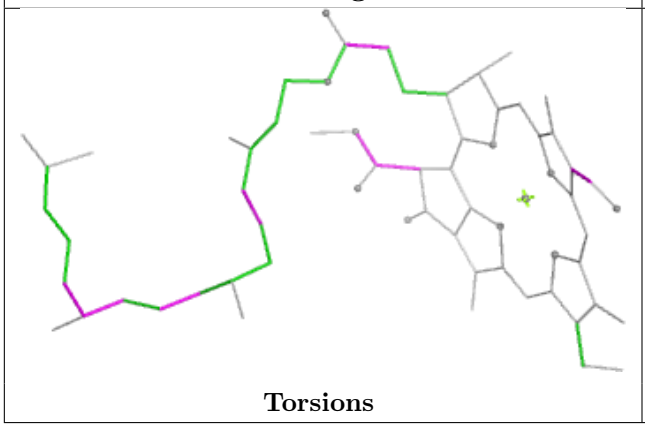
Ligand G9R bA 1011



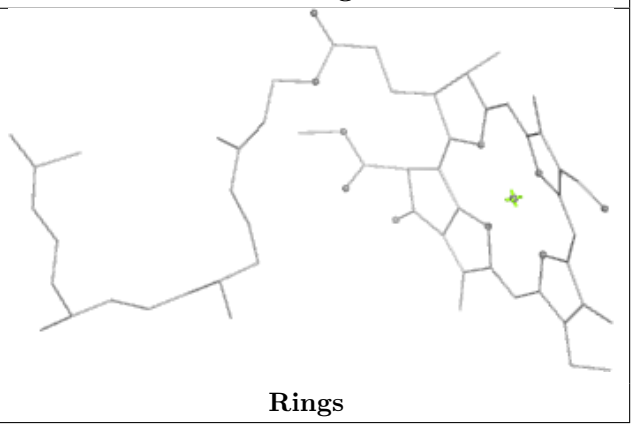
Bond lengths



Bond angles

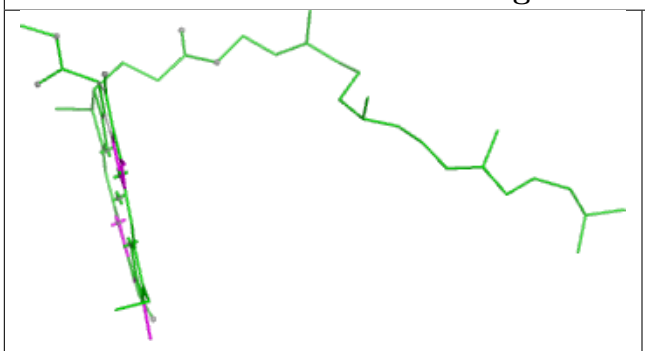


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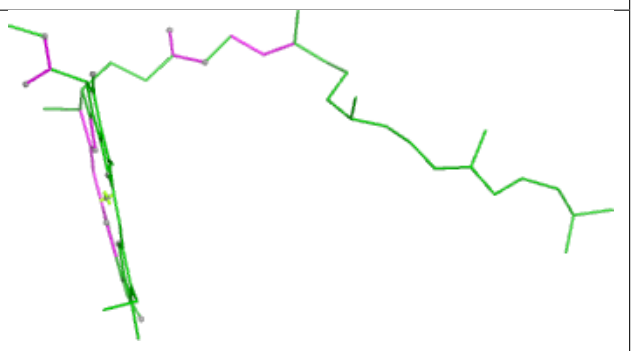


Rings

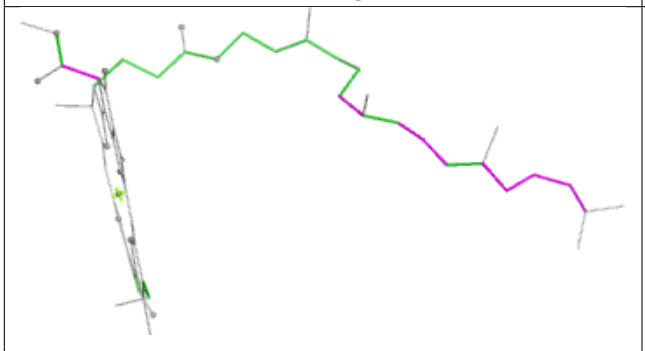
Ligand CL7 cB 1239



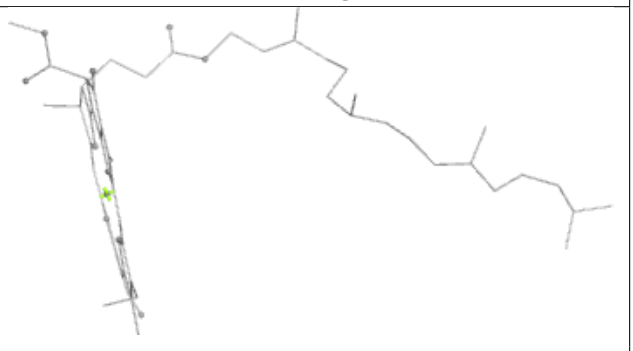
Bond lengths



Bond angles



Torsions

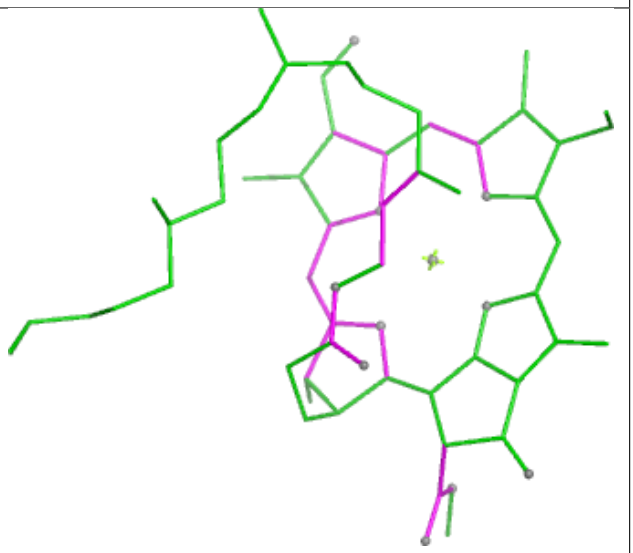


Rings

Ligand CL7 aB 1205



Bond lengths



Bond angles



Torsions



Rings

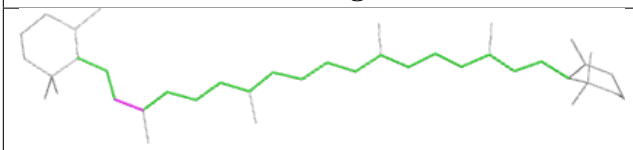
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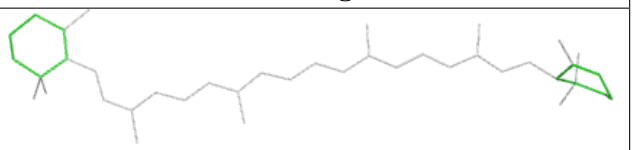
Bond lengths



Bond angles

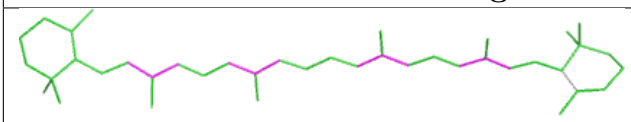


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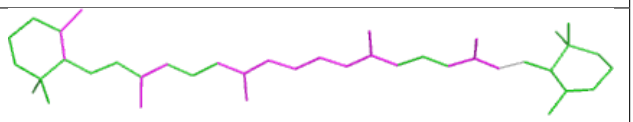


Rings

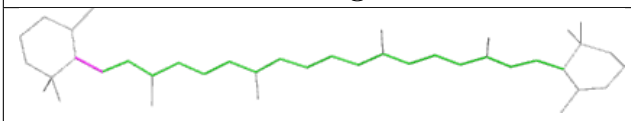
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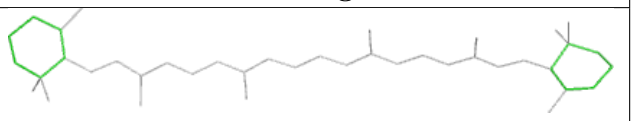
Bond lengths



Bond angles

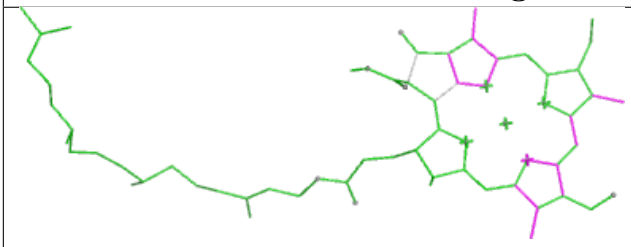


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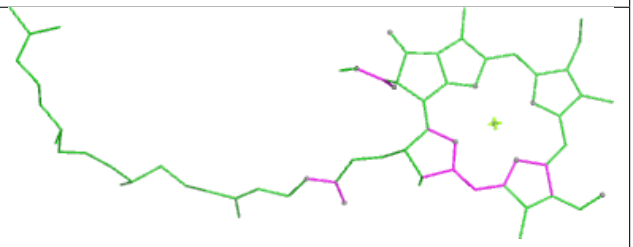


Rings

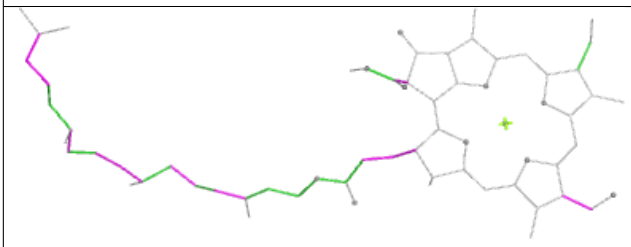
Ligand CL7 bB 1223



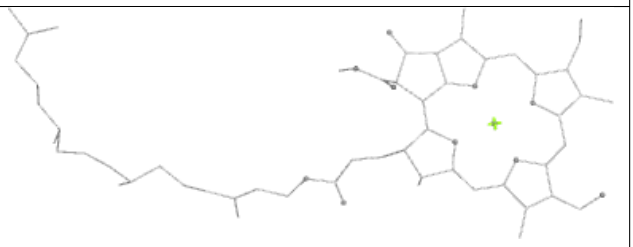
Bond lengths



Bond angles

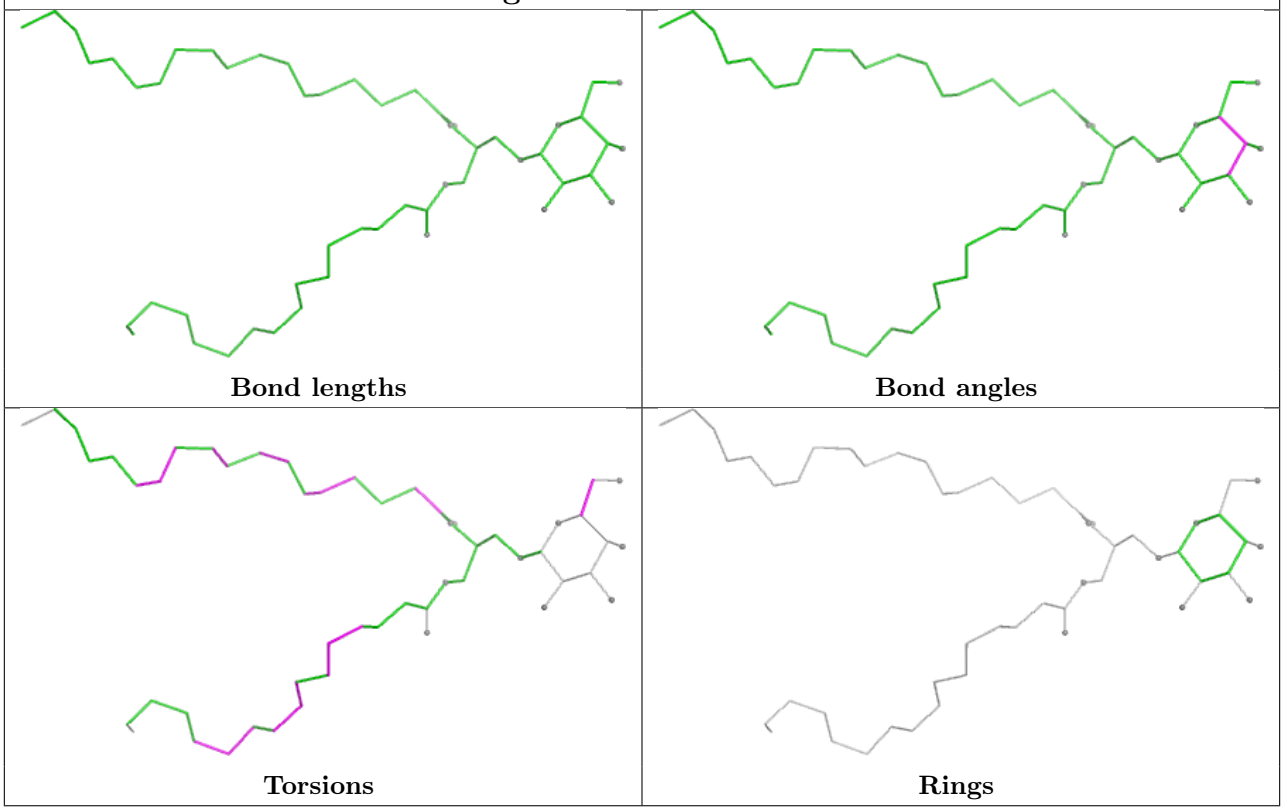


Torsions

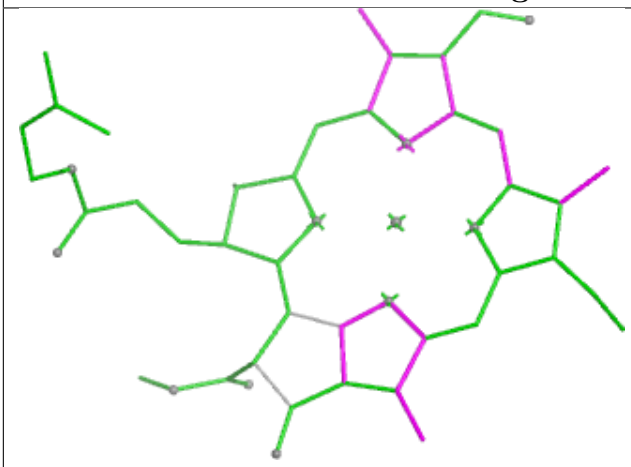


Rings

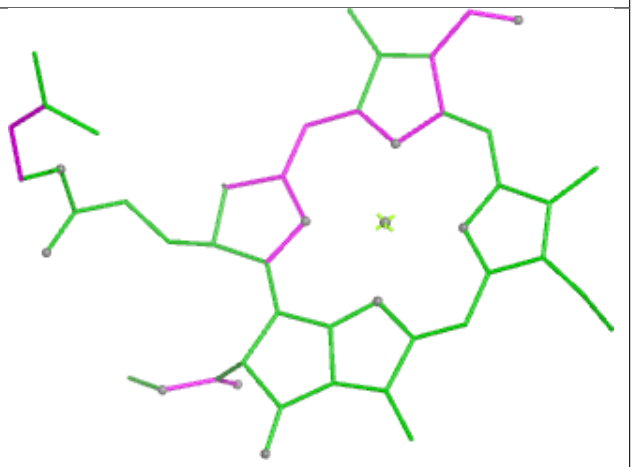
Ligand LMG aB 5002



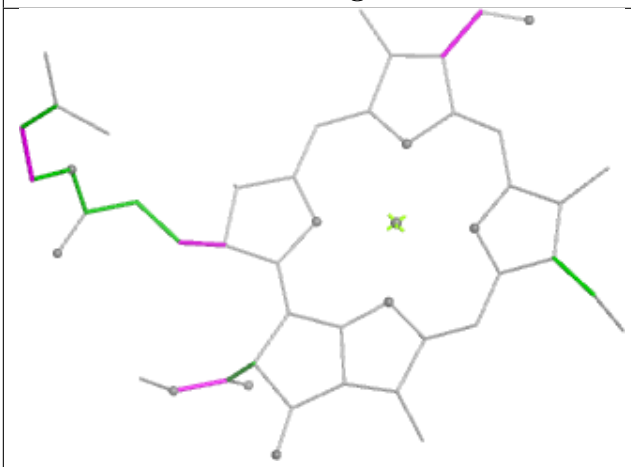
Ligand CL7 aB 1206



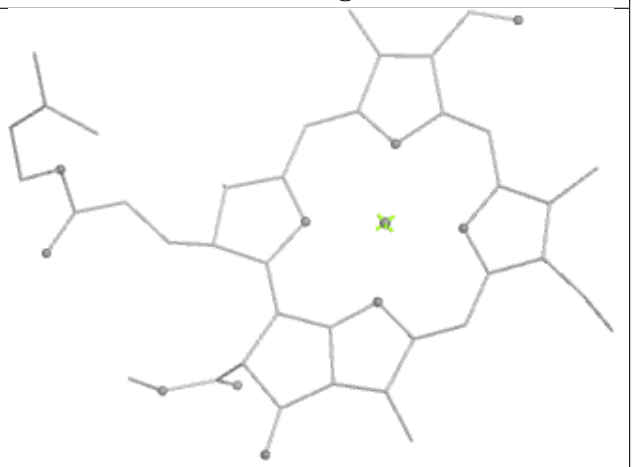
Bond lengths



Bond angles

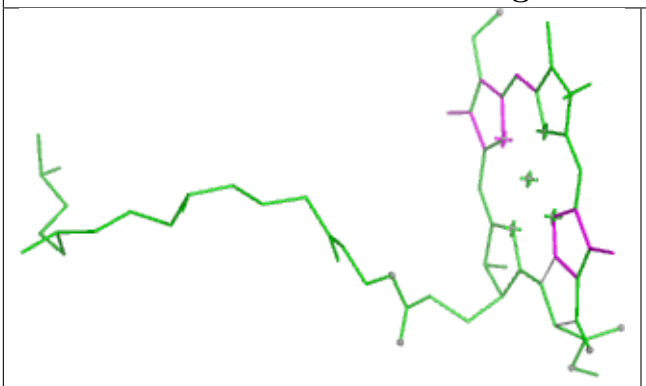


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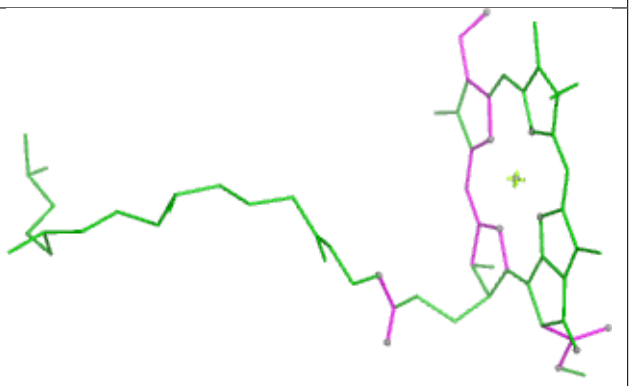


Rings

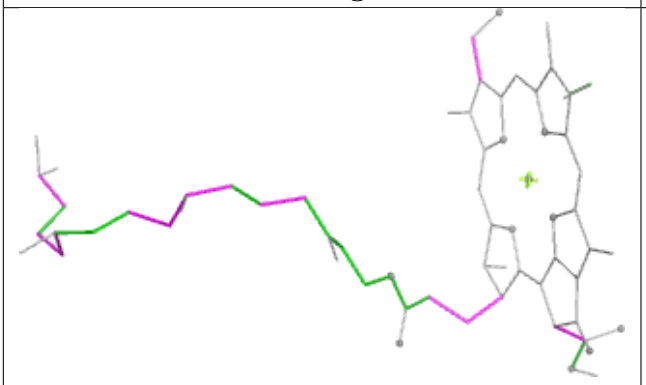
Ligand CL7 bL 1502



Bond lengths



Bond angles

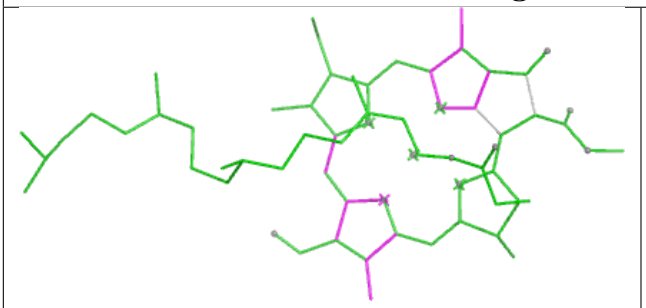


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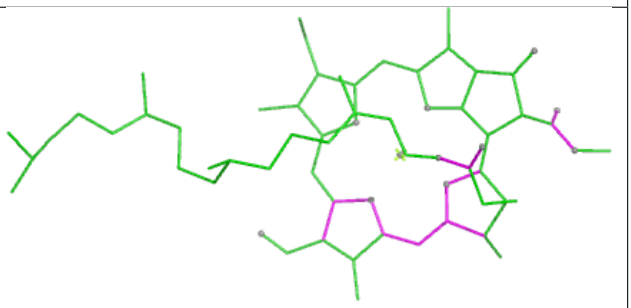


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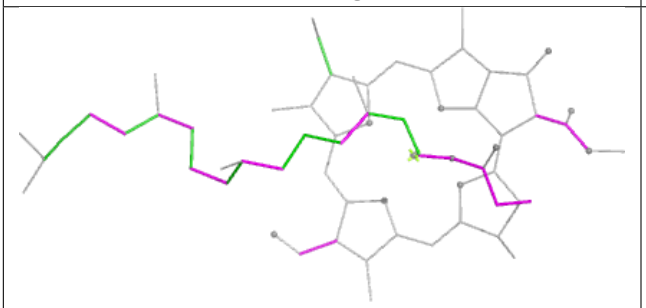
Ligand CL7 aA 1136



Bond lengths



Bond angles

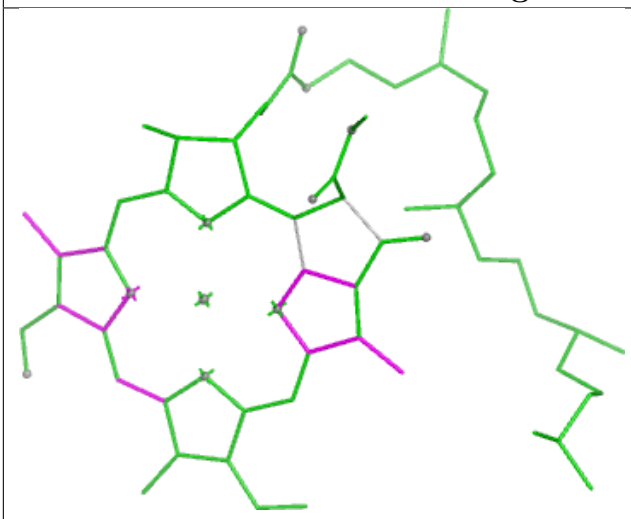


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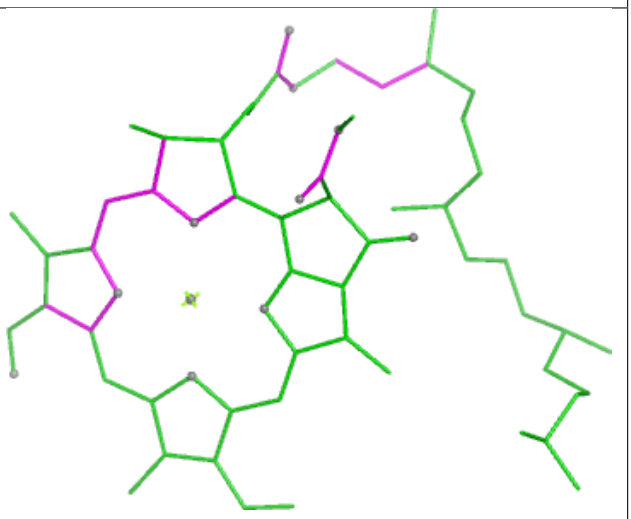


Rings

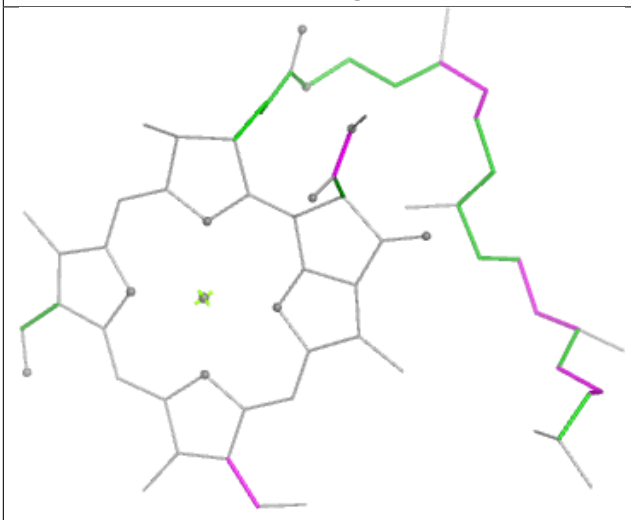
Ligand CL7 aB 1229



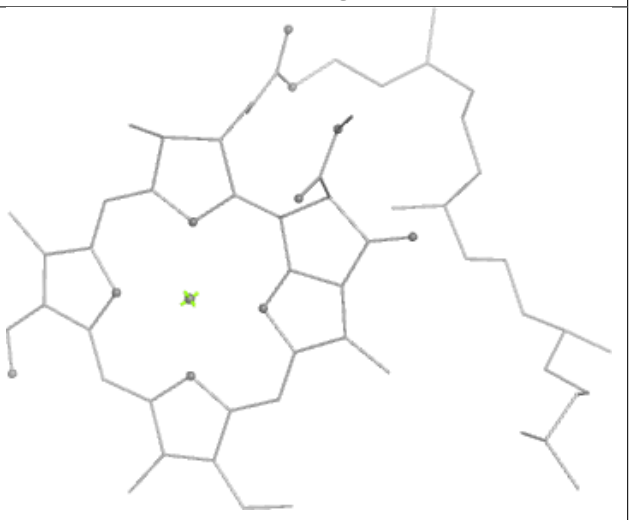
Bond lengths



Bond angles

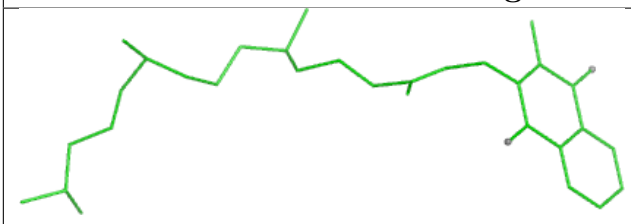


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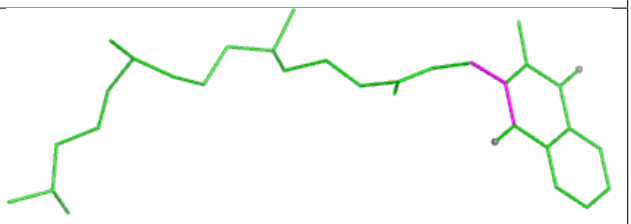


Rings

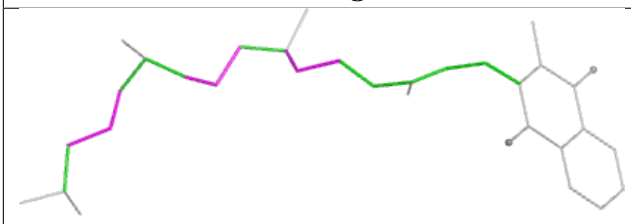
Ligand PQN aB 2002



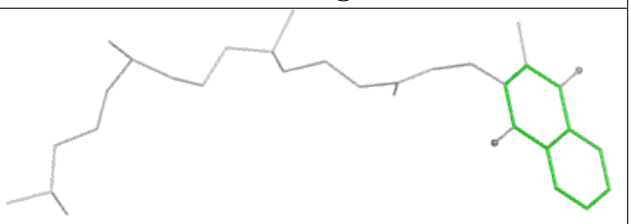
Bond lengths



Bond angles

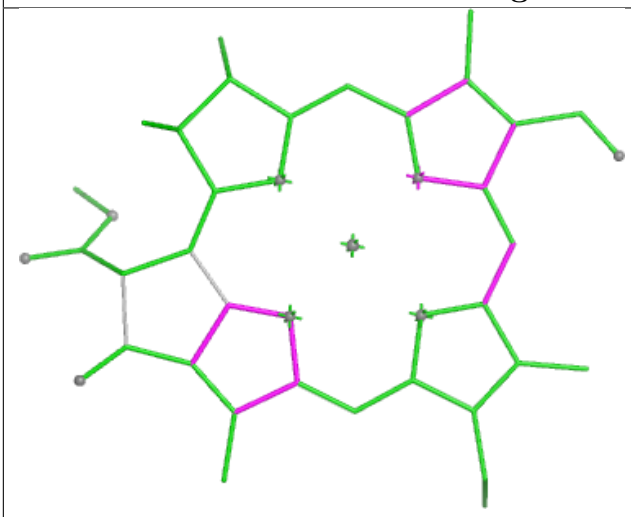


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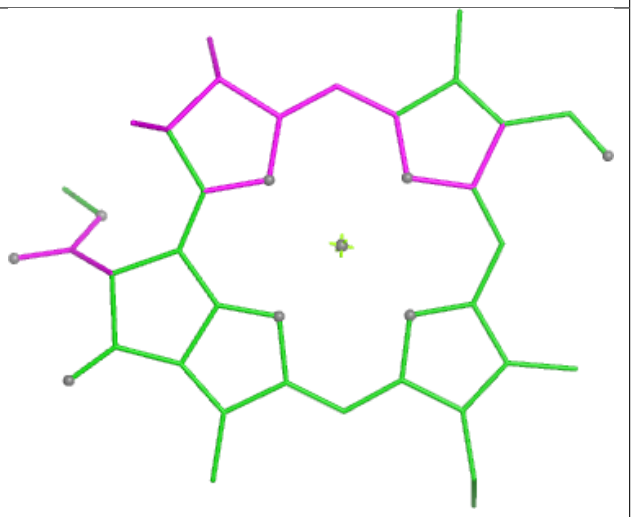


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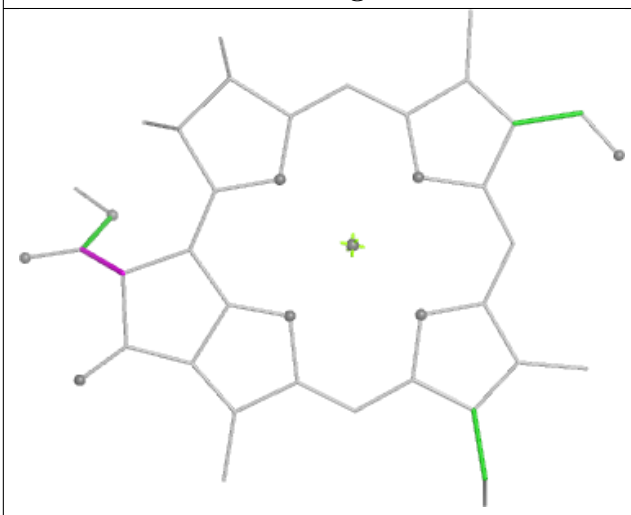
Ligand CL7 aA 1101



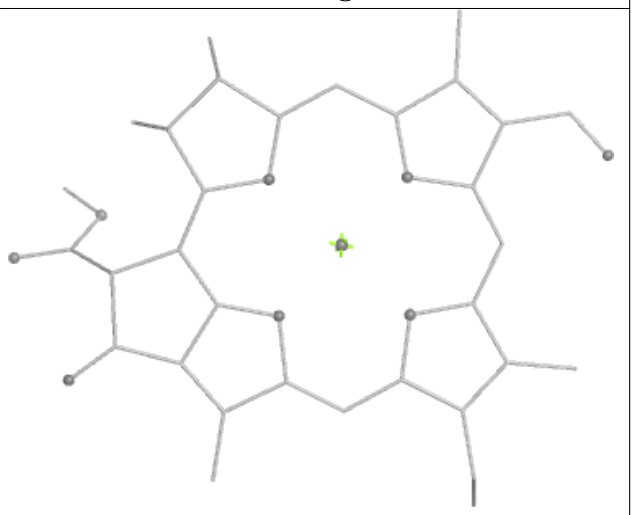
Bond lengths



Bond angles



Torsions



Rings

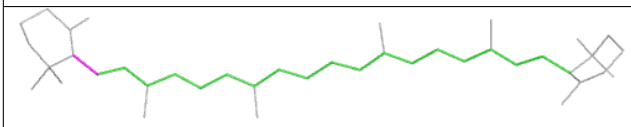
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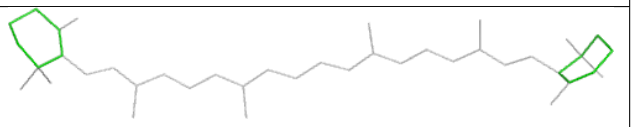
Bond lengths



Bond angles

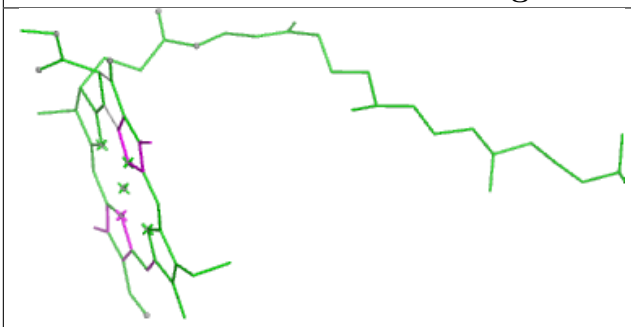


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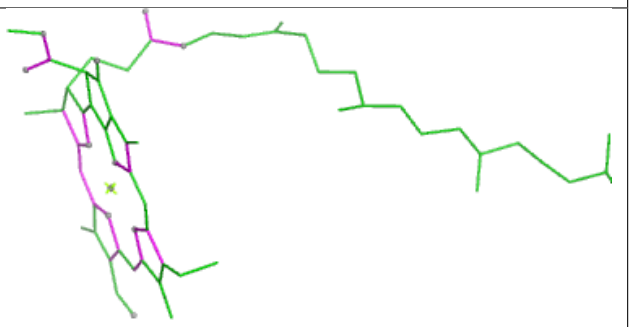


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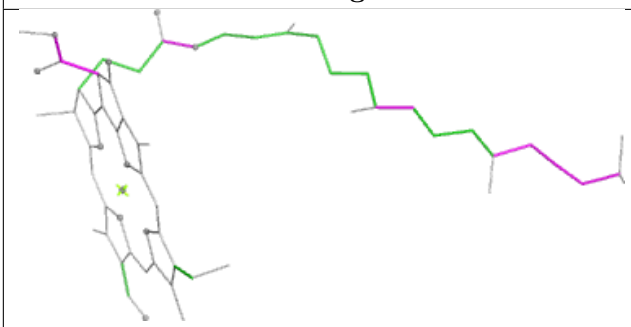
Ligand CL7 aB 1226



Bond lengths



Bond angles

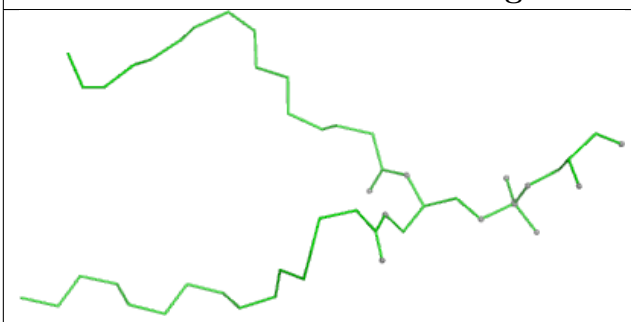


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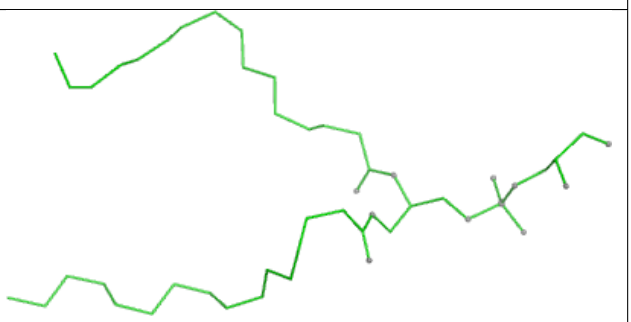


Rings

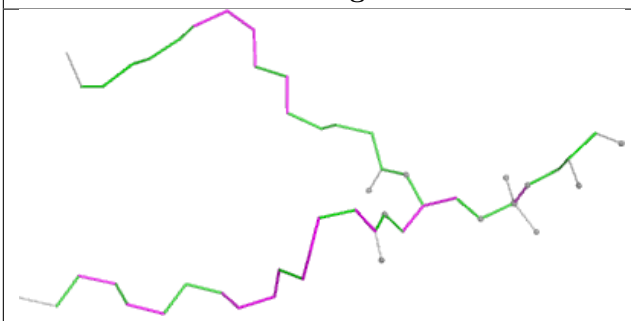
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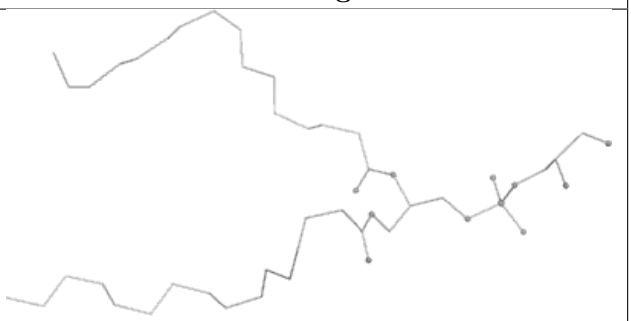
Bond lengths



Bond angles

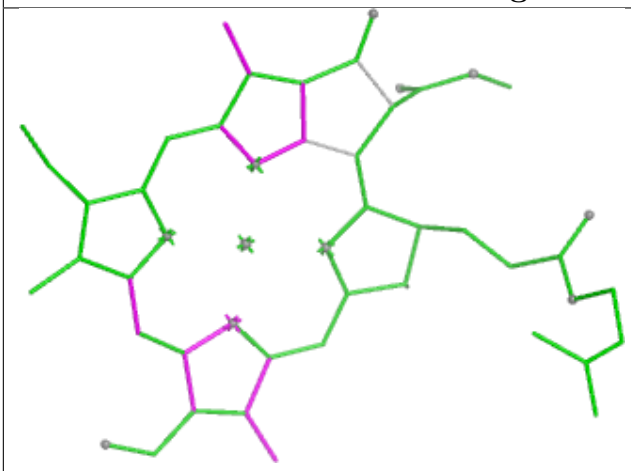


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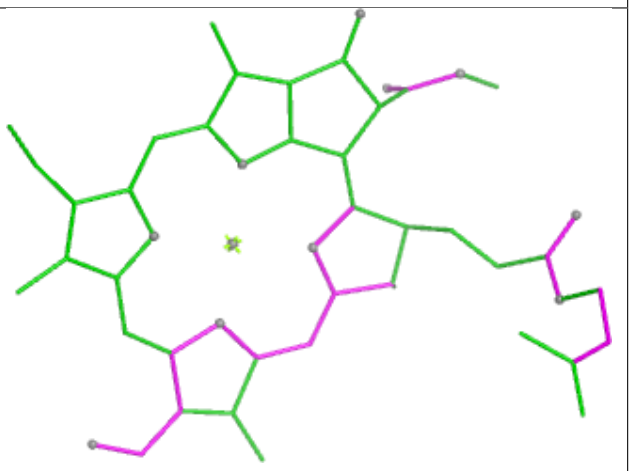


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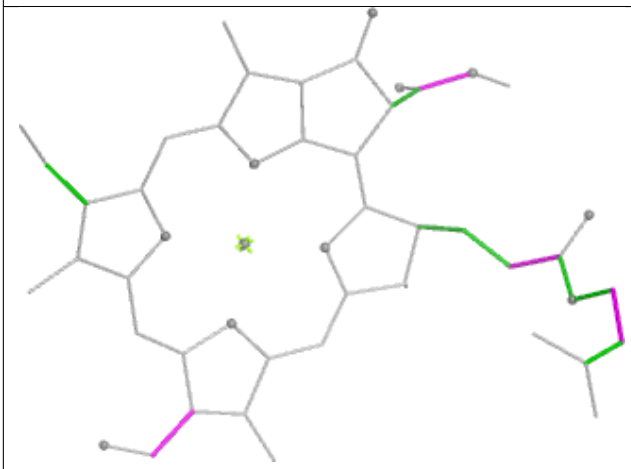
Ligand CL7 bB 1206



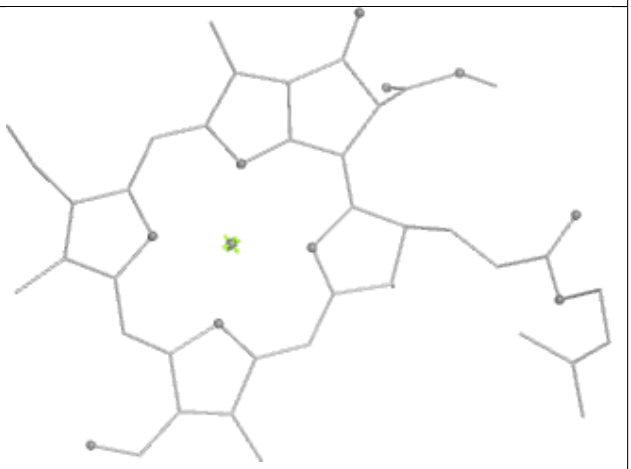
Bond lengths



Bond angles

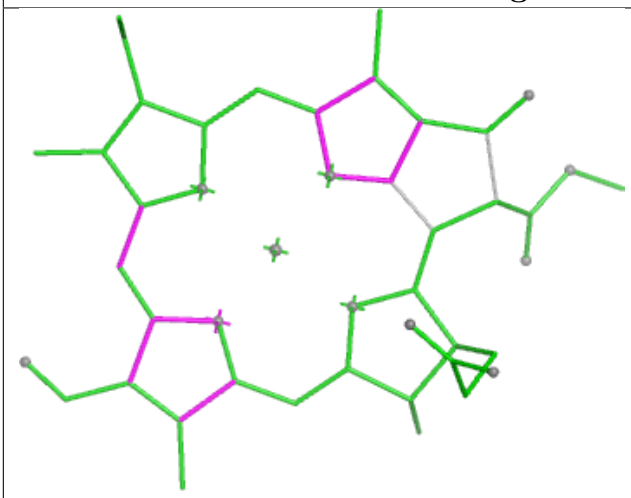


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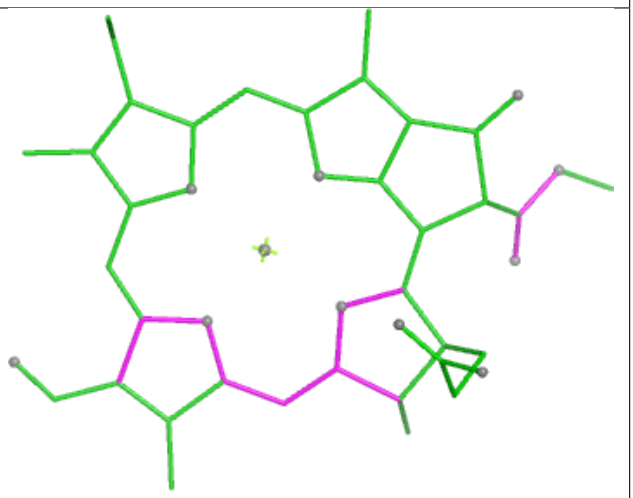


Rings

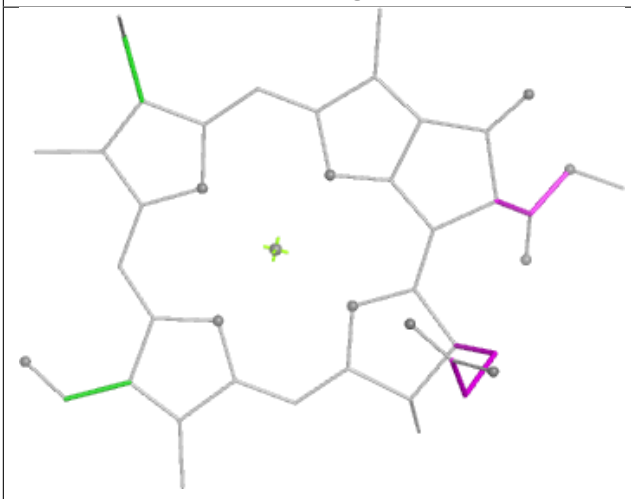
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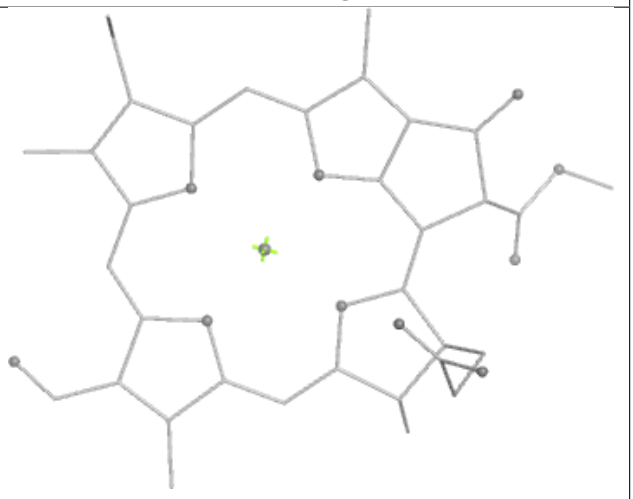
Bond lengths



Bond angles

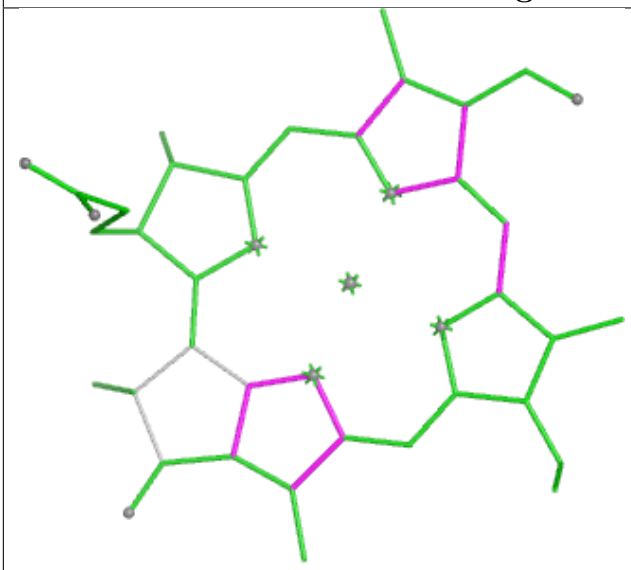


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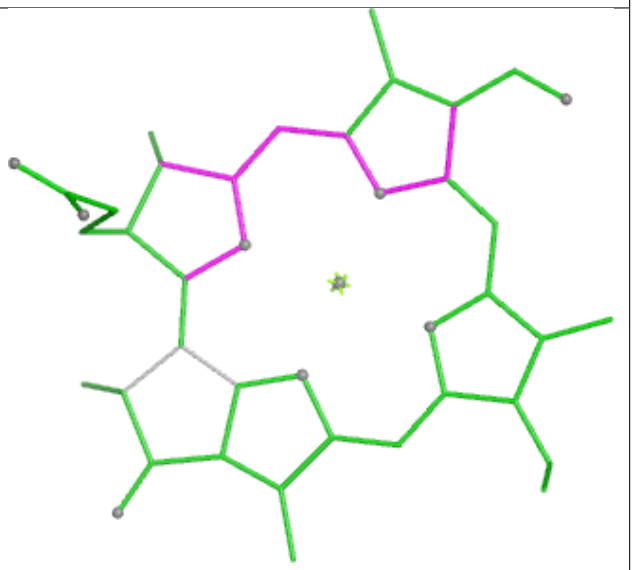


Rings

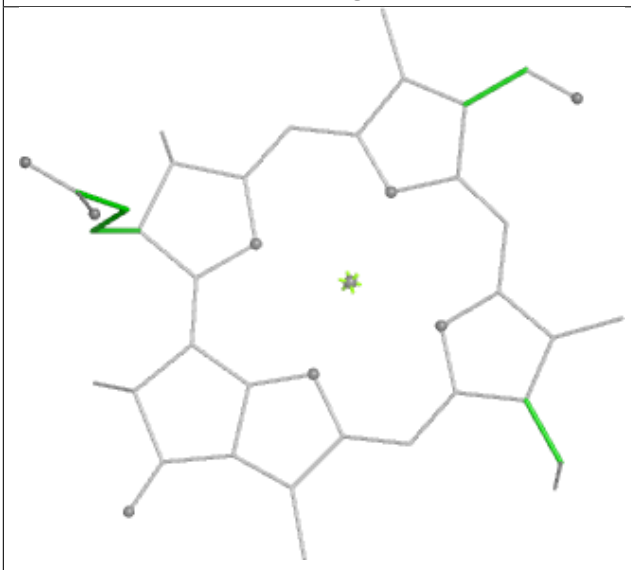
Ligand CL7 cJ 1302



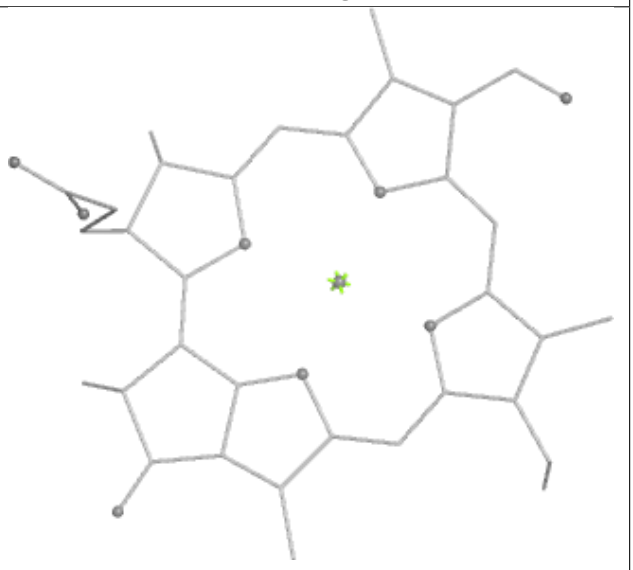
Bond lengths



Bond angles

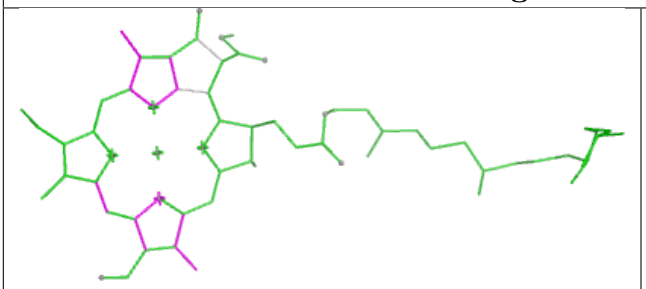


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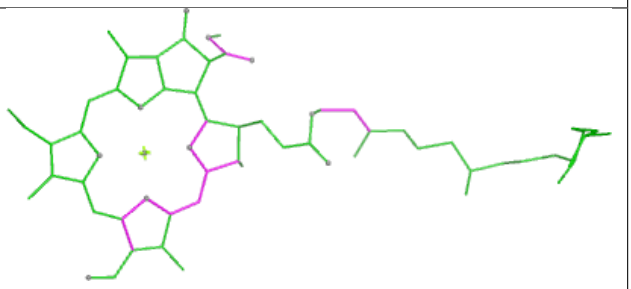


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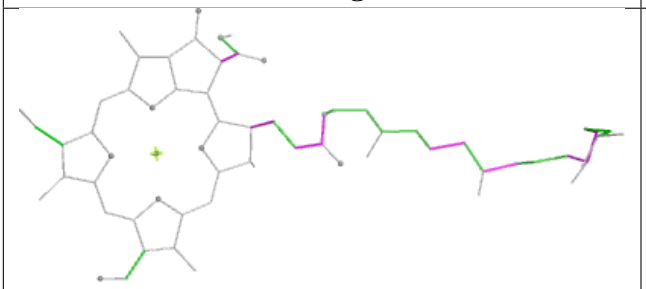
Ligand CL7 aA 1103



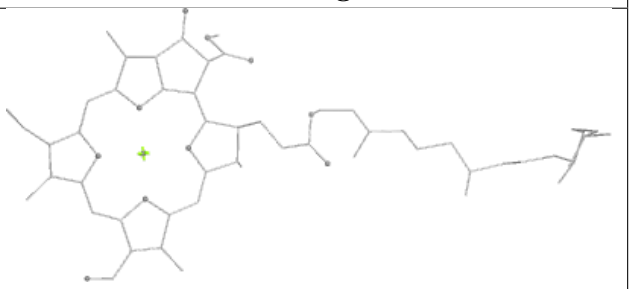
Bond lengths



Bond angles

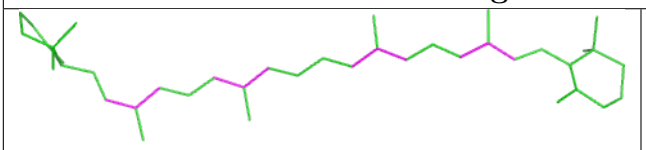


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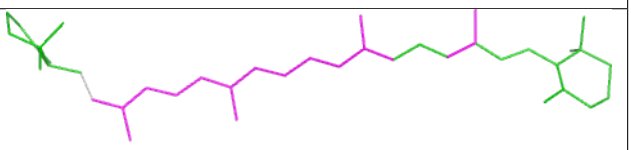


Rings

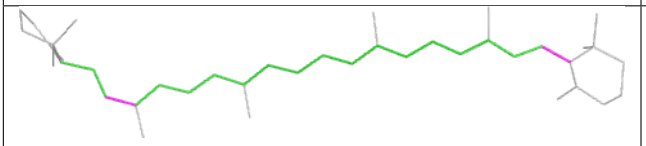
Ligand A1JPJ aB 4017



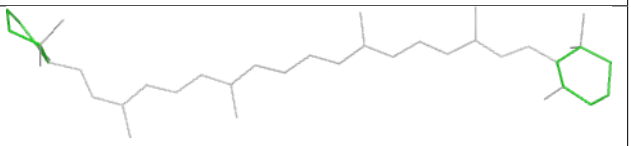
Bond lengths



Bond angles

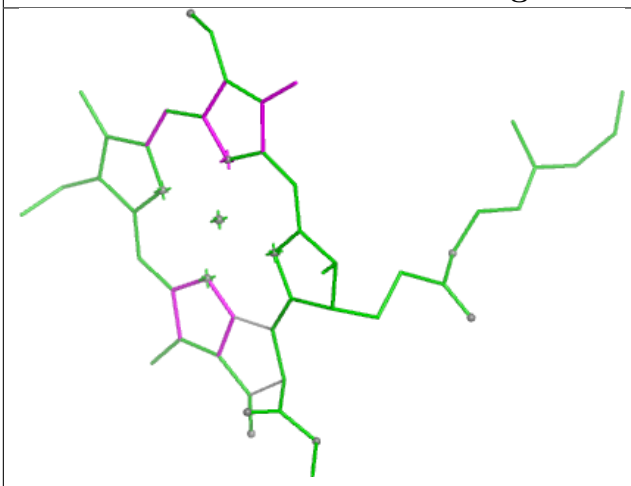


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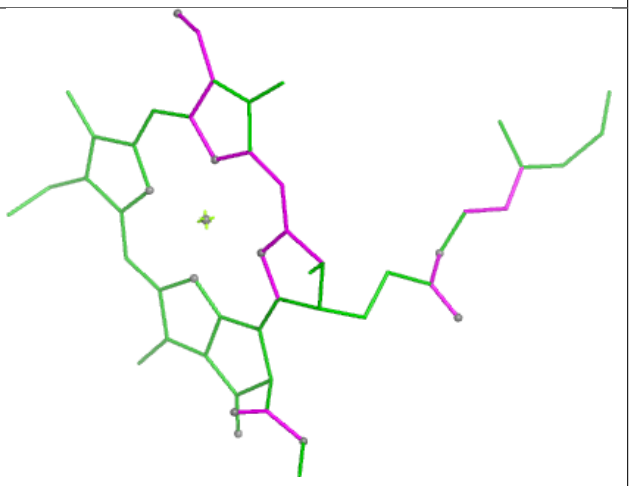


Rings

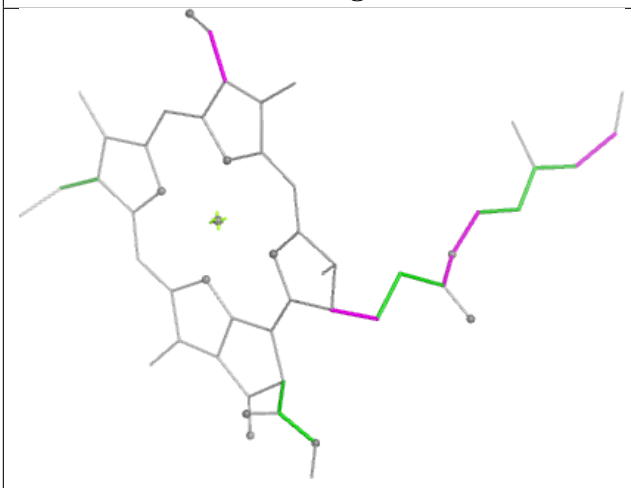
Ligand CL7 aA 1102



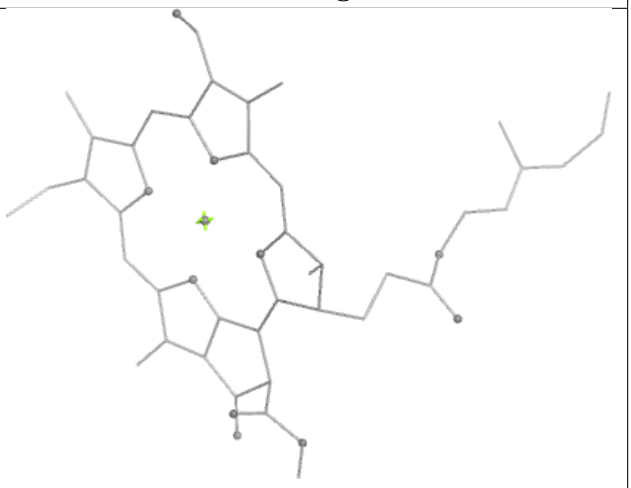
Bond lengths



Bond angles

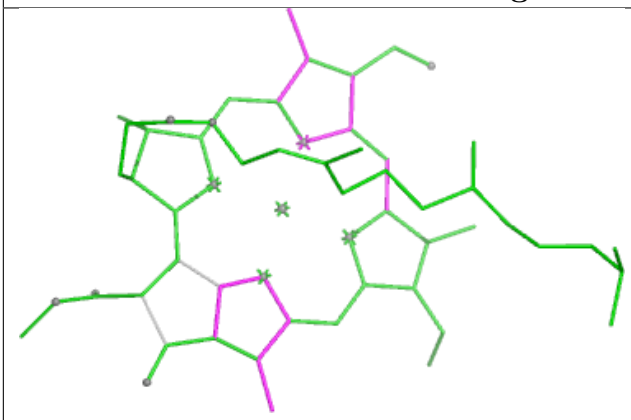


Torsions

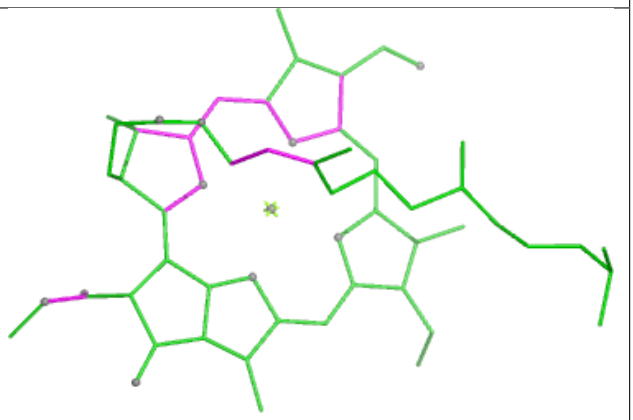


Rings

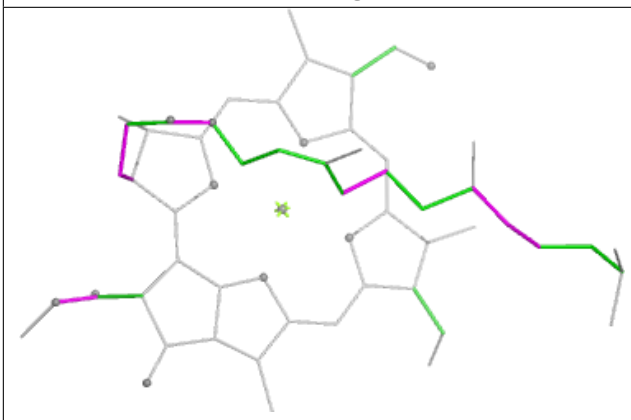
Ligand CL7 aA 1116



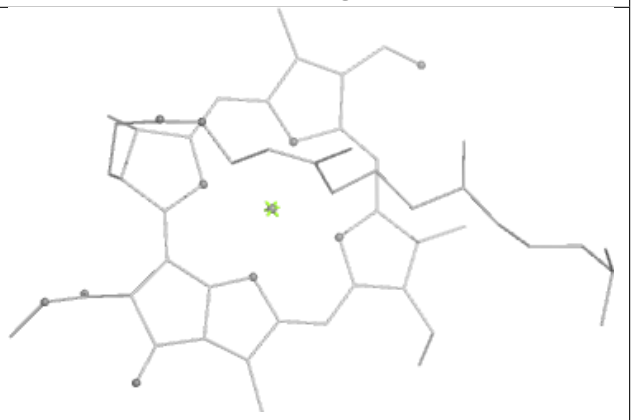
Bond lengths



Bond angles

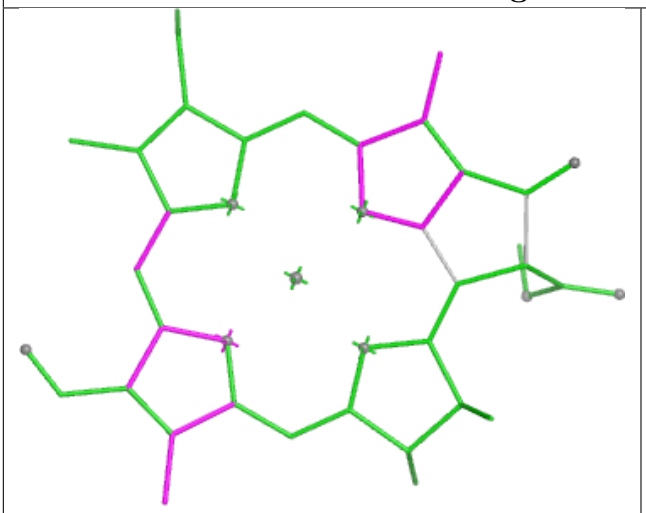


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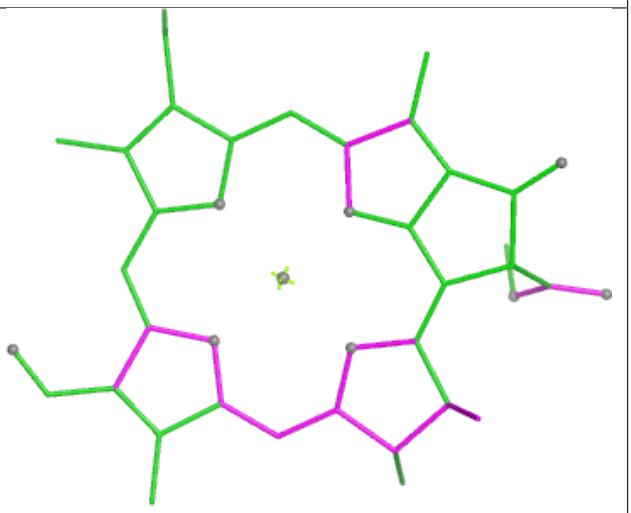


Rings

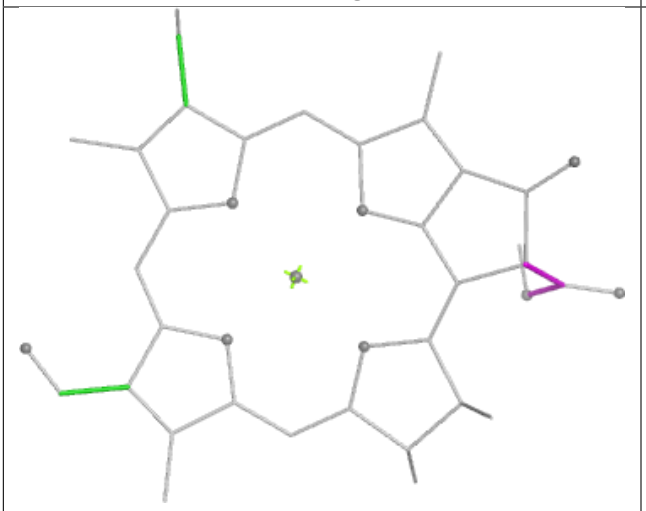
Ligand CL7 bB 1232



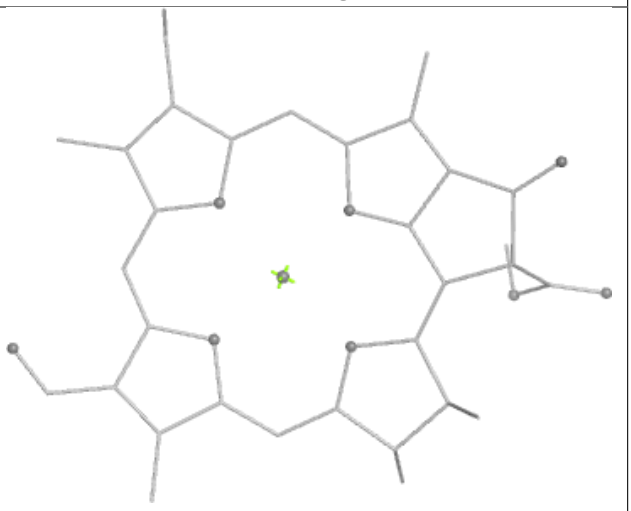
Bond lengths



Bond angles

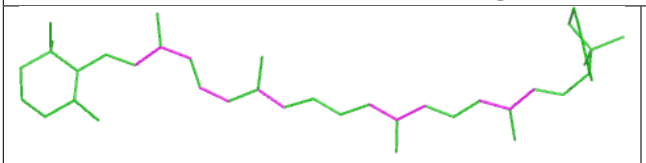


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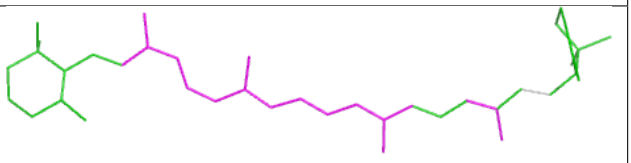


Rings

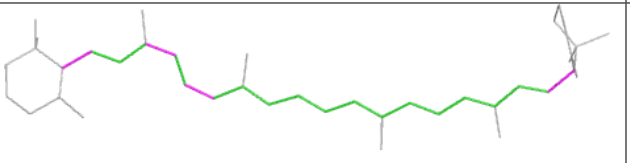
Ligand A1JPJ cB 4010



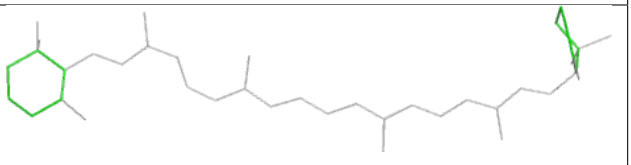
Bond lengths



Bond angles

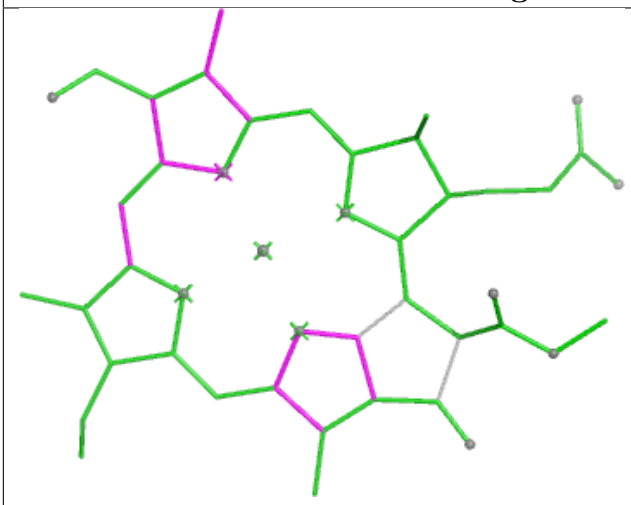


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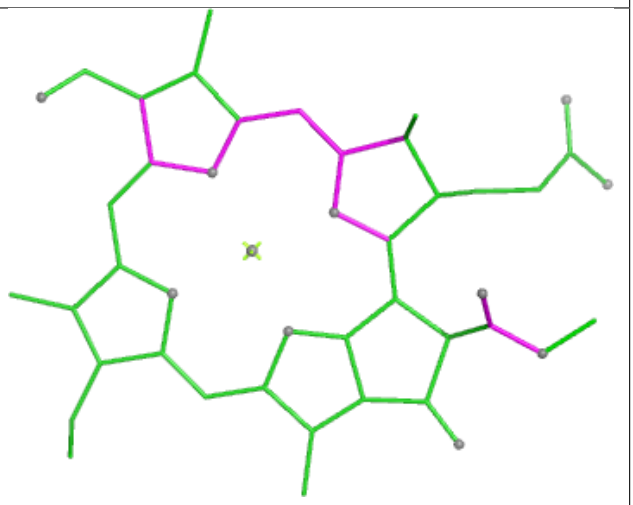


Rings

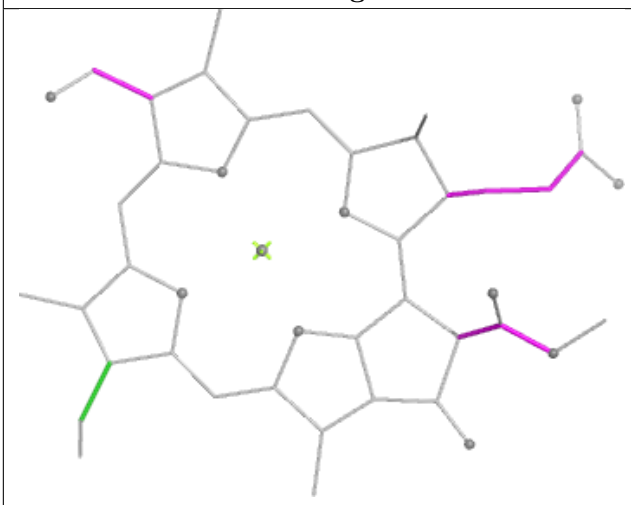
Ligand CL7 aA 1139



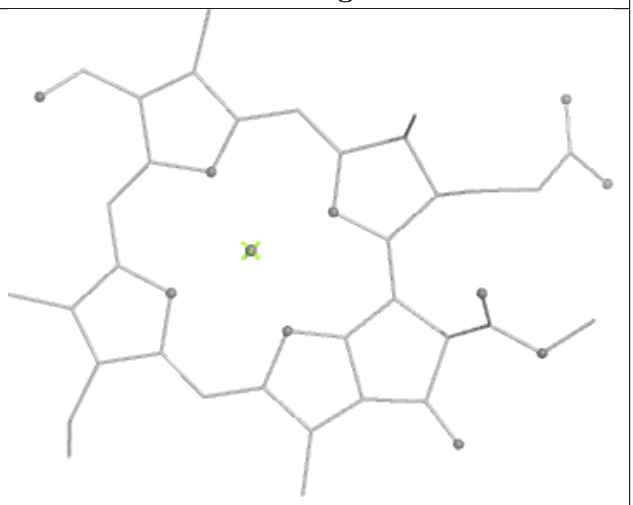
Bond lengths



Bond angles

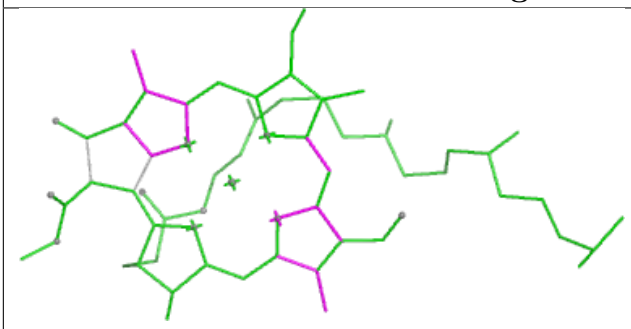


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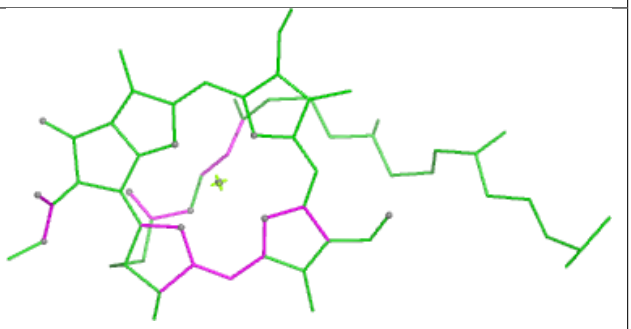


Rings

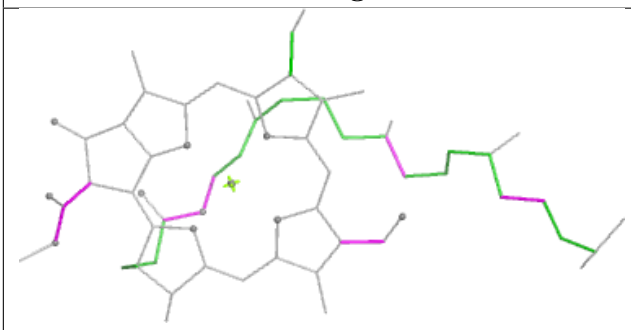
Ligand CL7 aA 1138



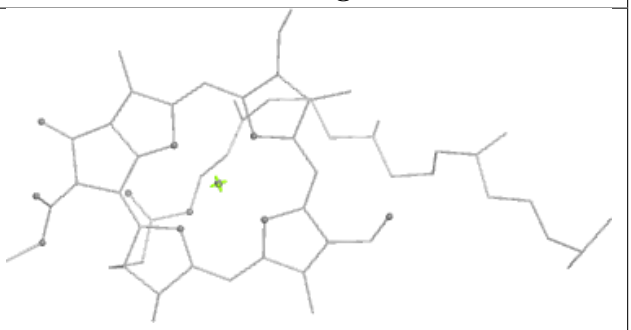
Bond lengths



Bond angles

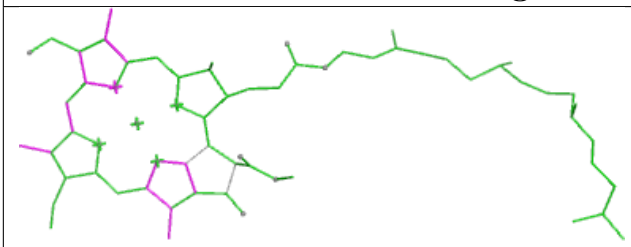


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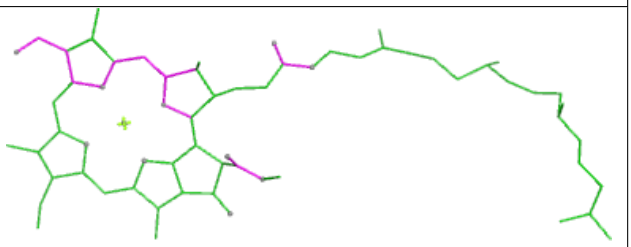


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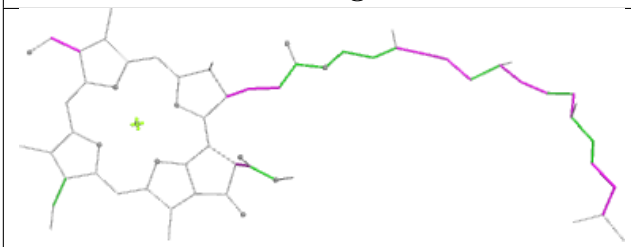
Ligand CL7 aB 1223



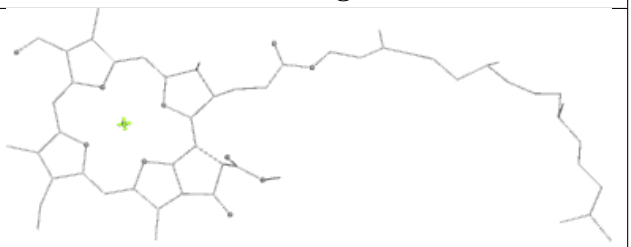
Bond lengths



Bond angles

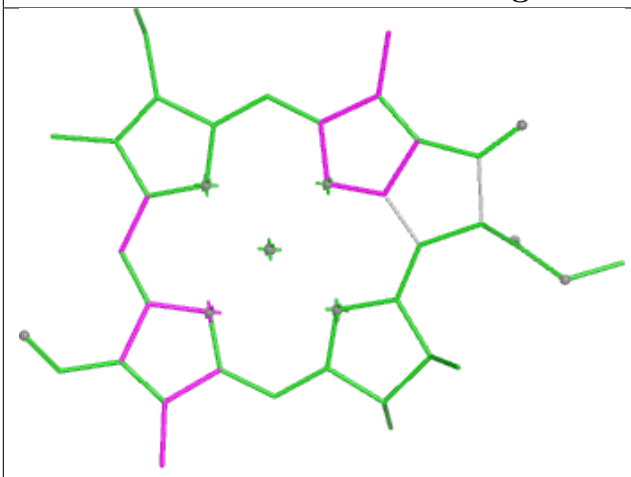


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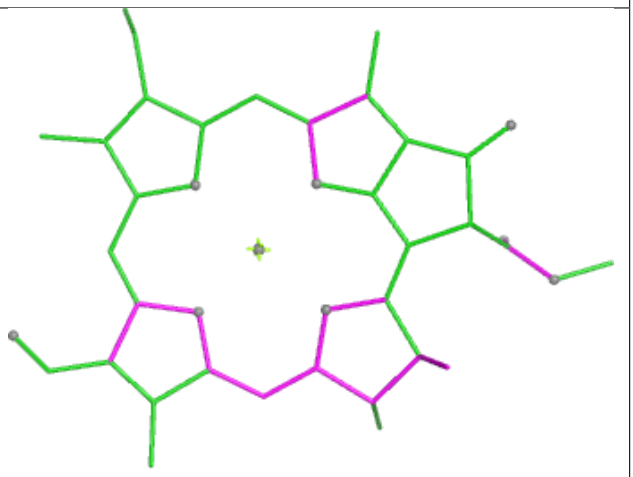


Rings

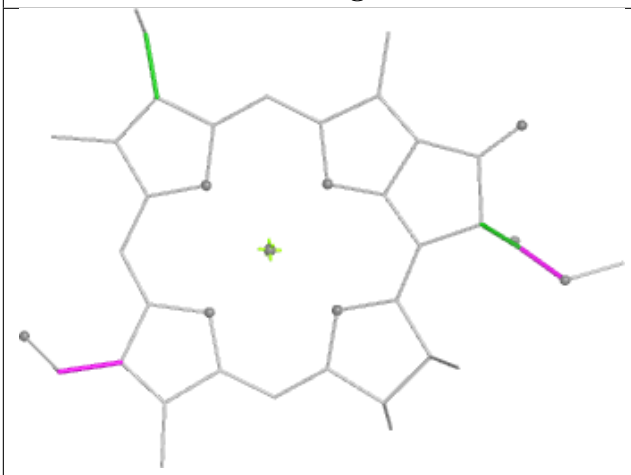
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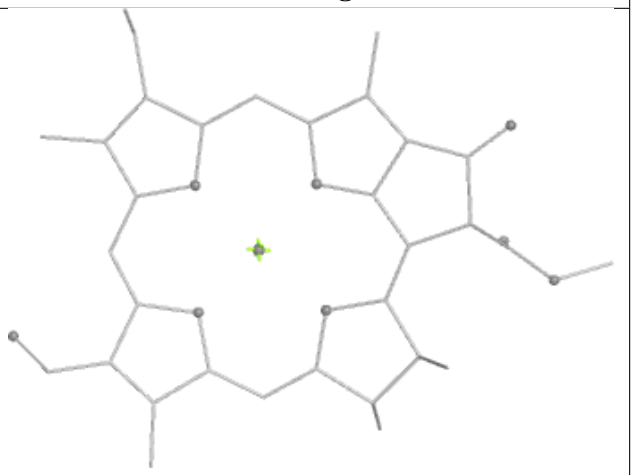
Bond lengths



Bond angles

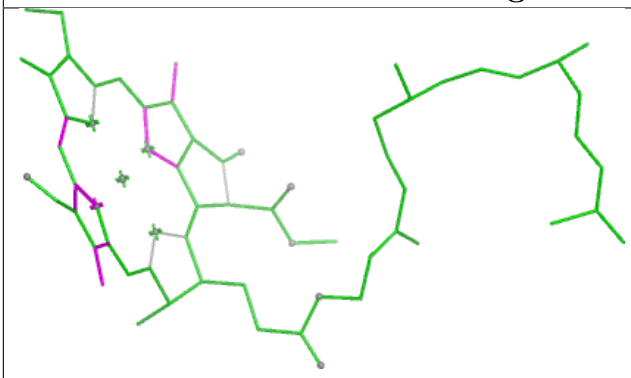


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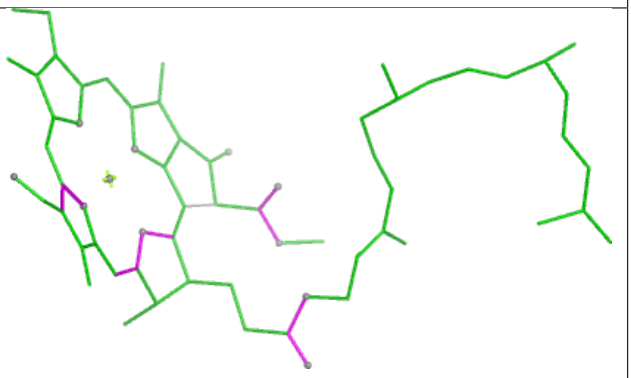


Rings

Ligand G9R cA 1011



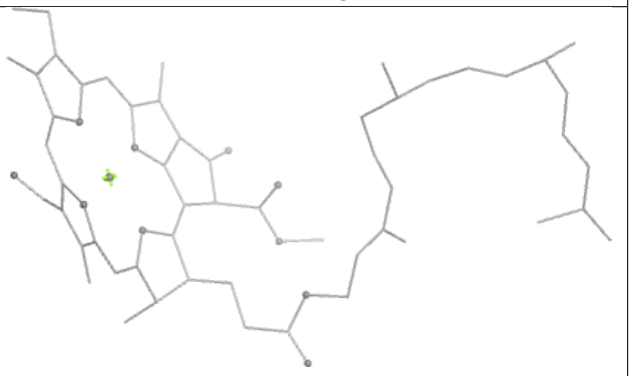
Bond lengths



Bond angles

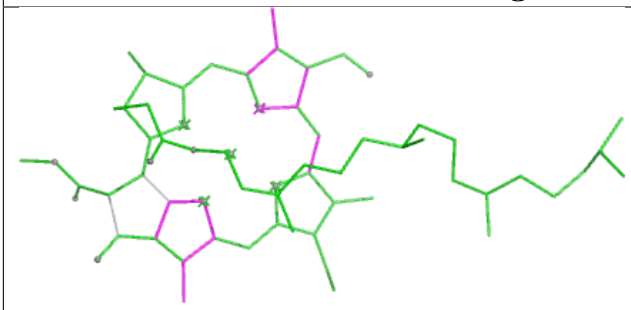


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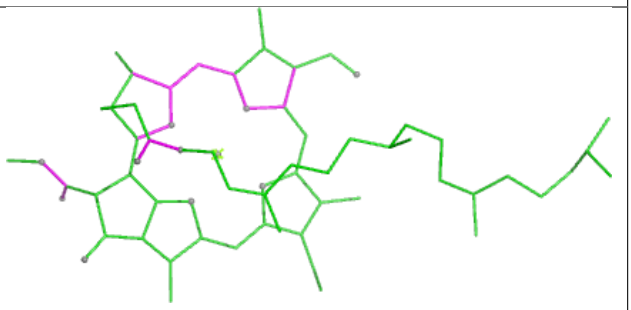


Rings

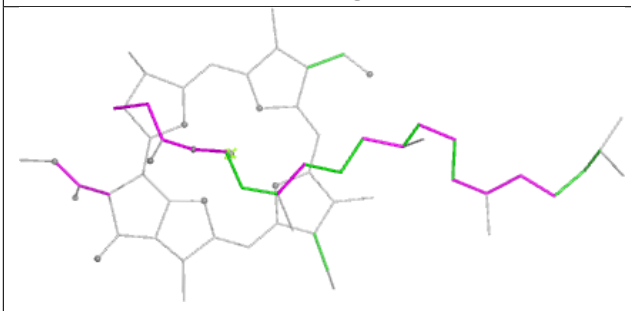
Ligand CL7 bA 1136



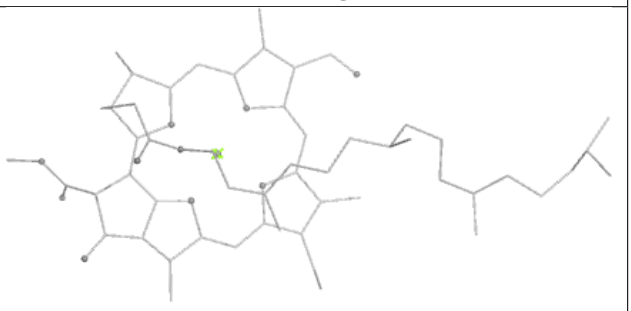
Bond lengths



Bond angles

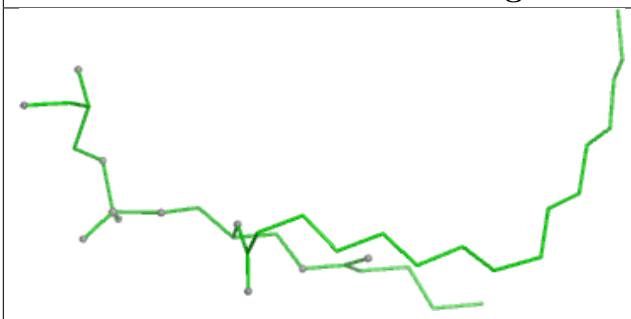


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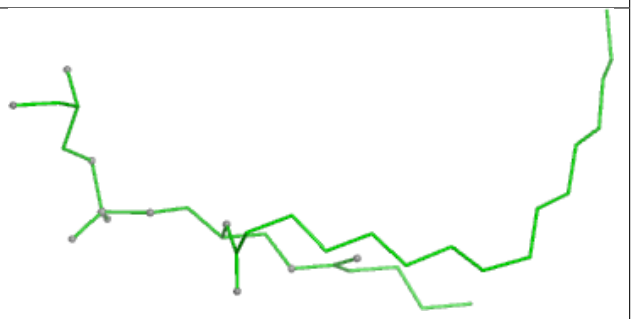


Rings

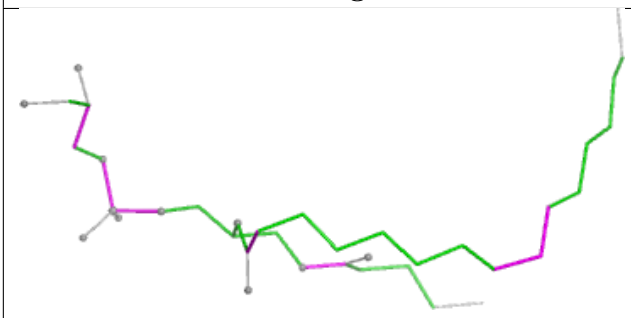
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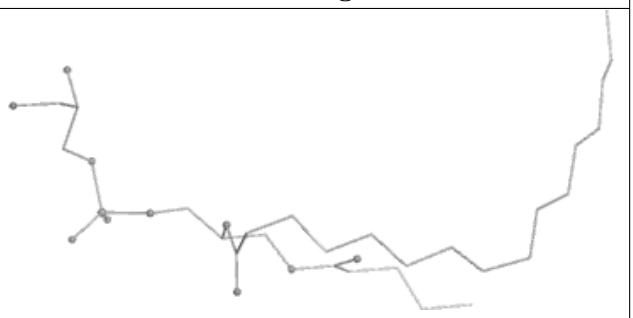
Bond lengths



Bond angles

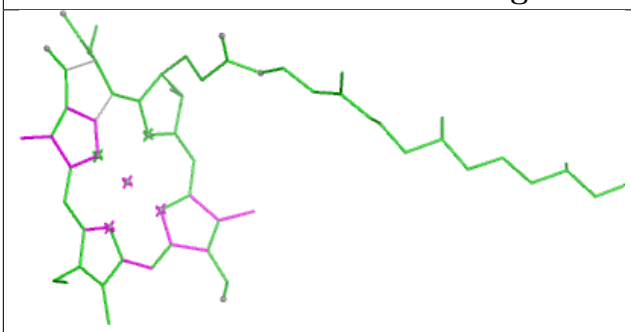


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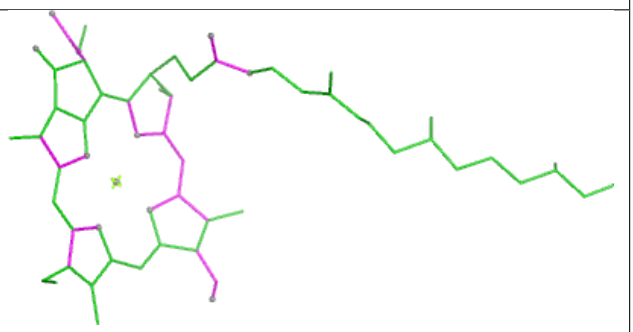


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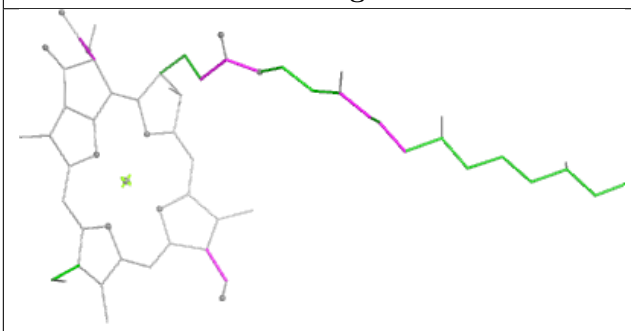
Ligand CL7 aA 1132



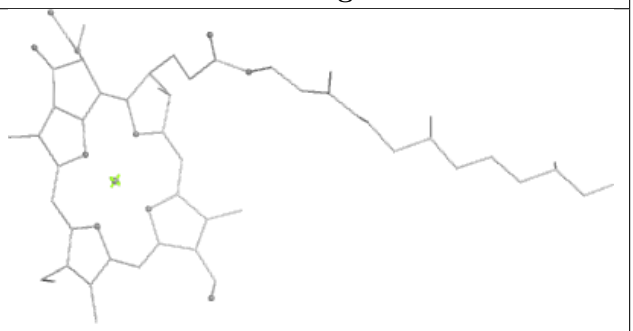
Bond lengths



Bond angles

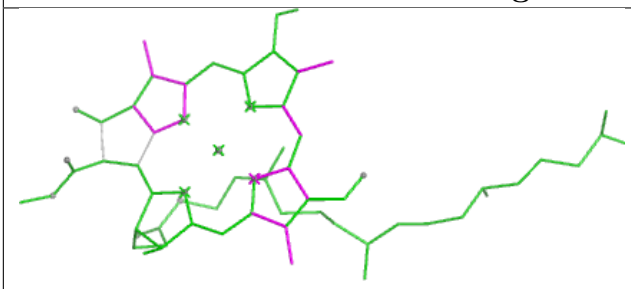


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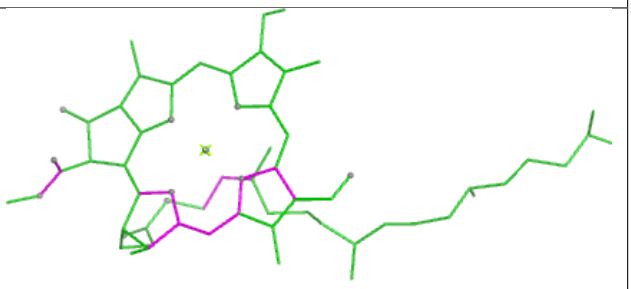


Rings

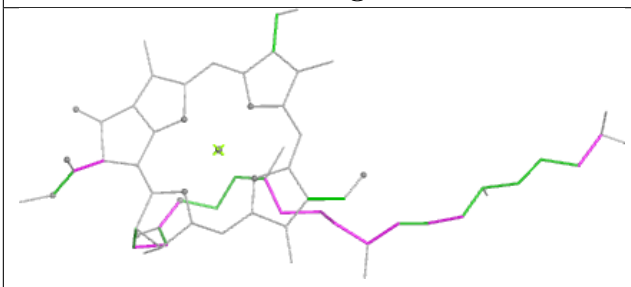
Ligand CL7 cB 1237



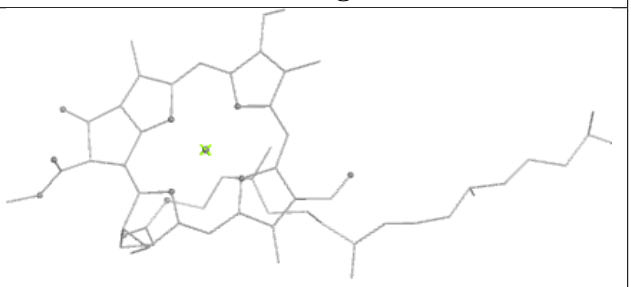
Bond lengths



Bond angles

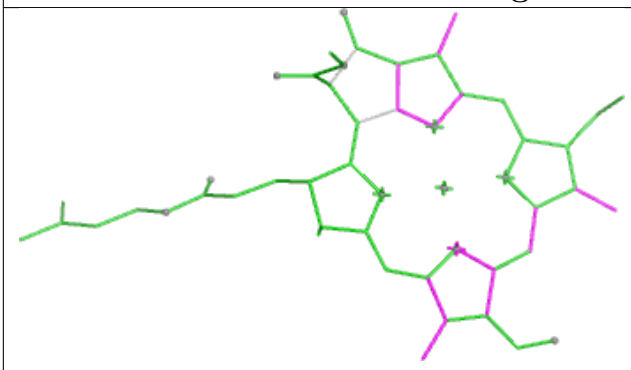


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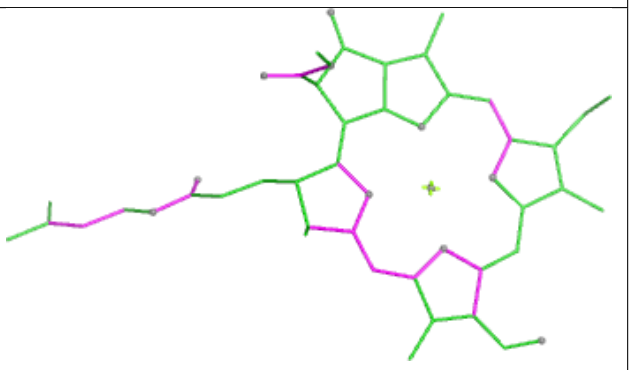


Rings

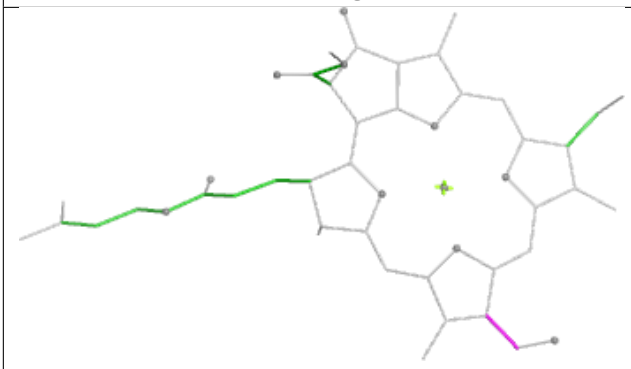
Ligand CL7 cA 1125



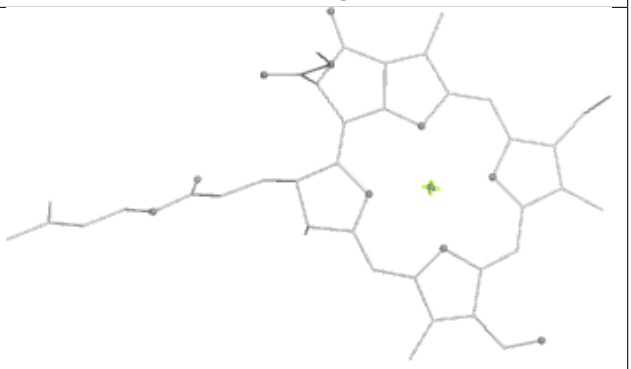
Bond lengths



Bond angles



Torsions

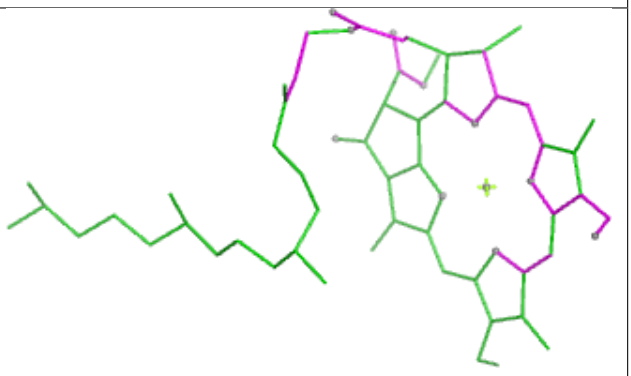


Rings

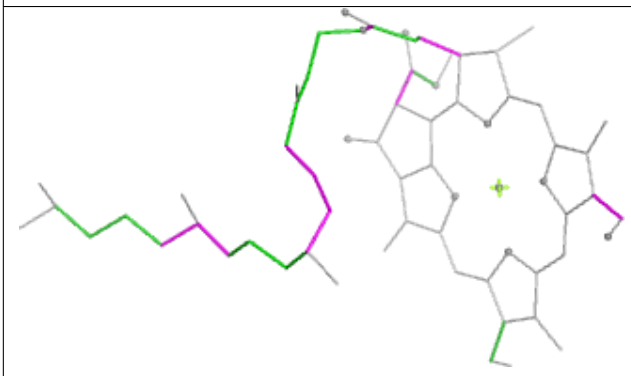
Ligand CL7 cA 1112



Bond lengths



Bond angles

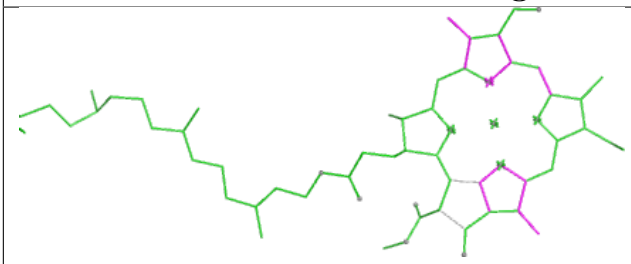


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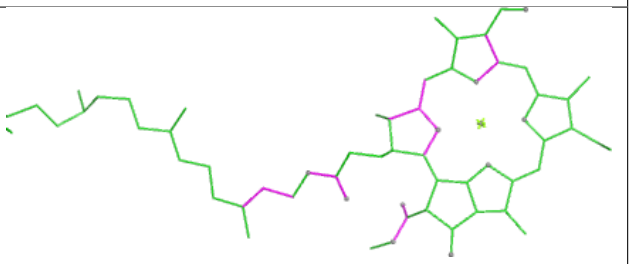


Rings

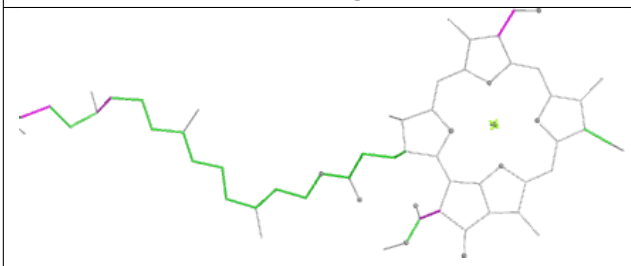
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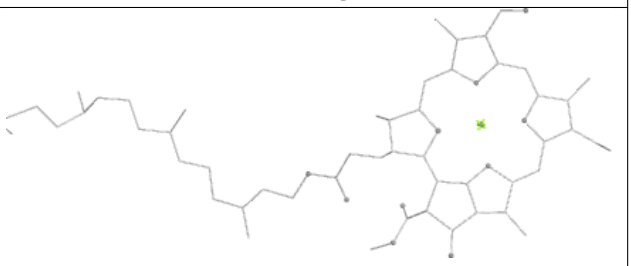
Bond lengths



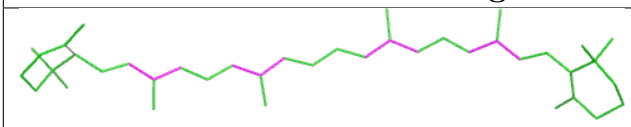
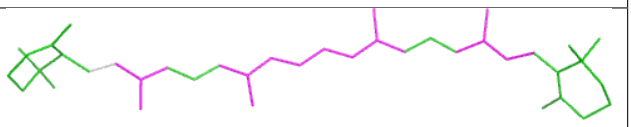
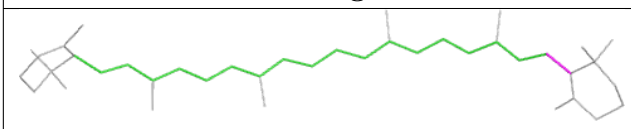
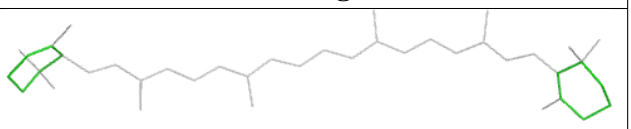
Bond angles

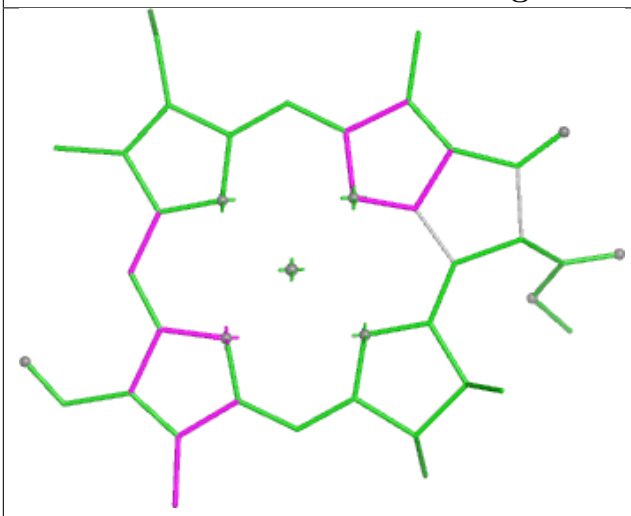
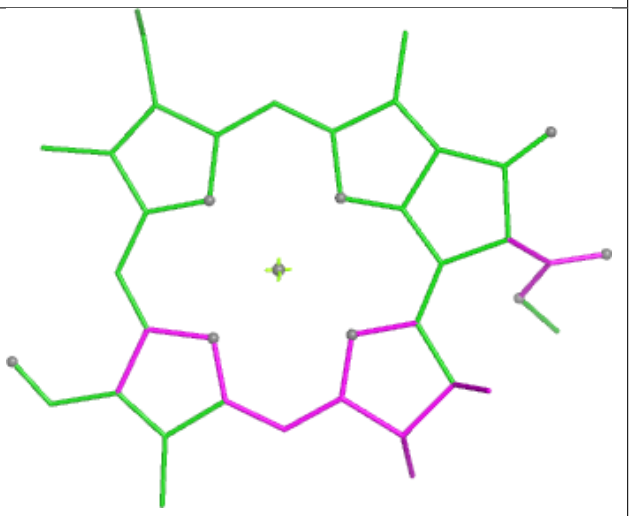
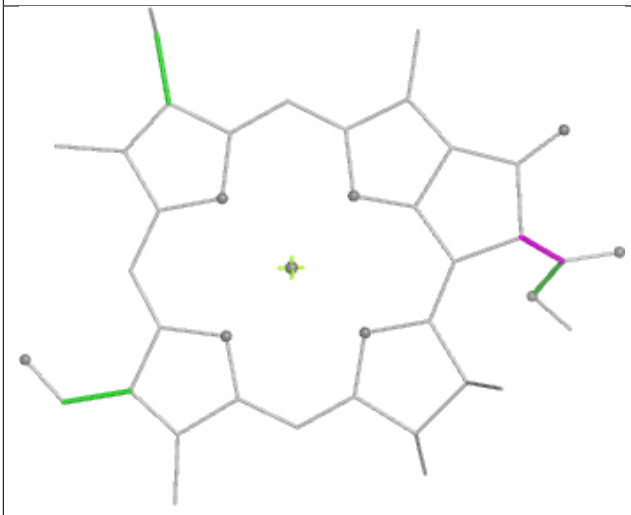
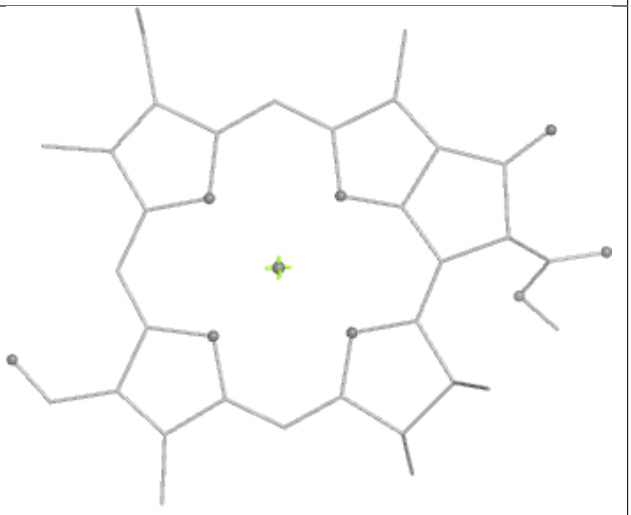


Torsions

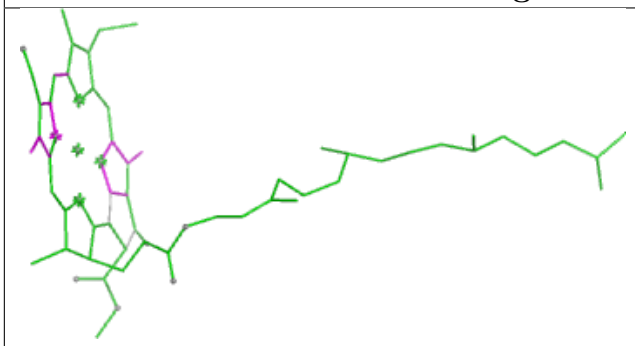


Rings

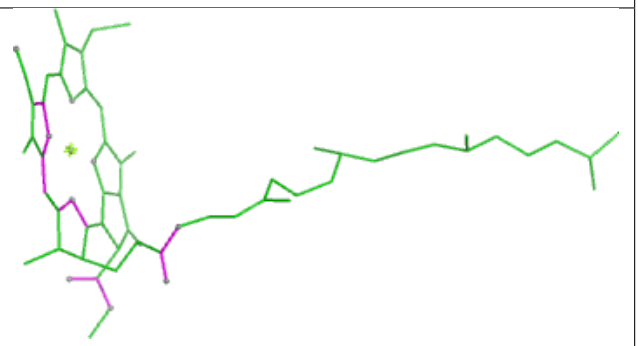
Ligand A1JPJ bA 4007	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CL7 cA 1101	
 Bond lengths	 Bond angles
 Torsions	 Rings

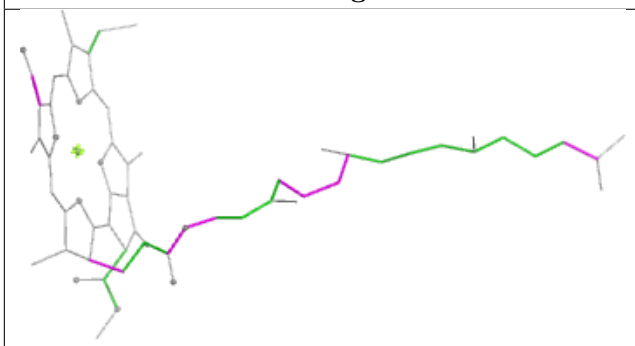
Ligand CL7 cB 1225



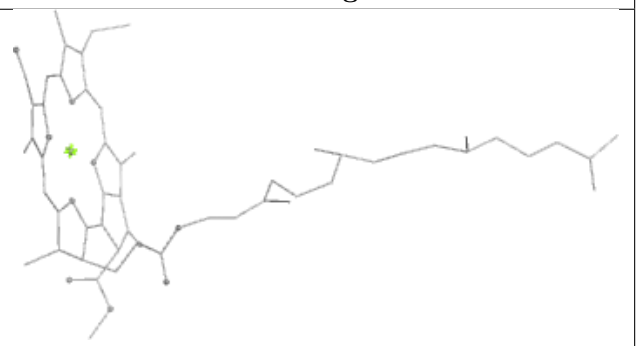
Bond lengths



Bond angles

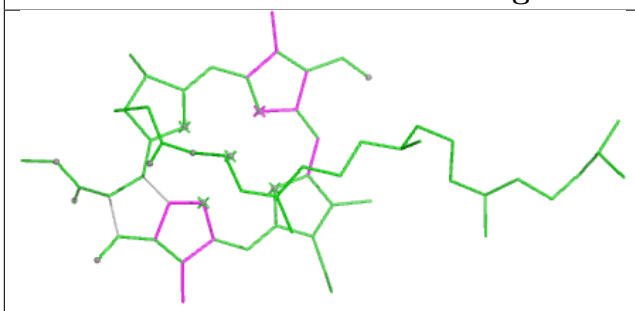


Torsions

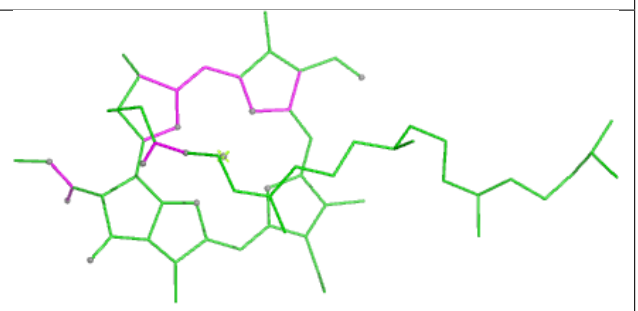


Rings

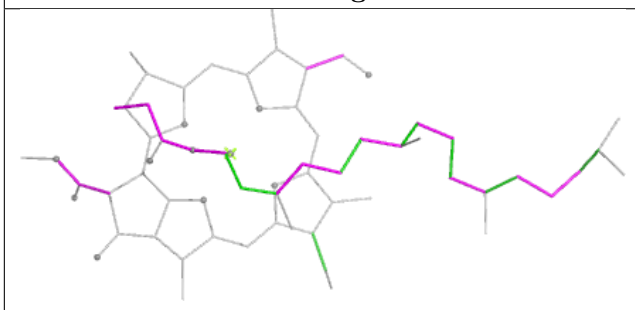
Ligand CL7 cA 1136



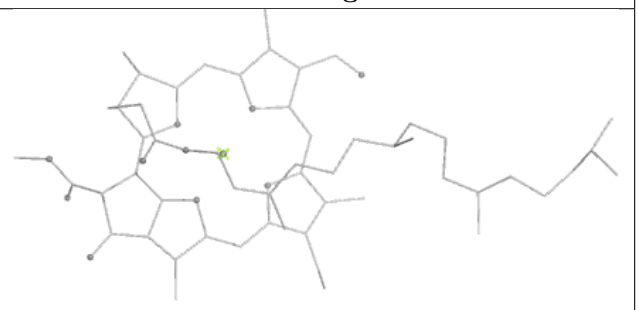
Bond lengths



Bond angles

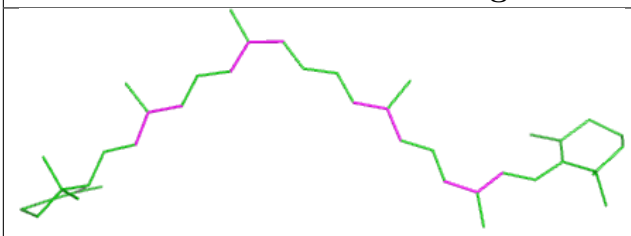


Torsions

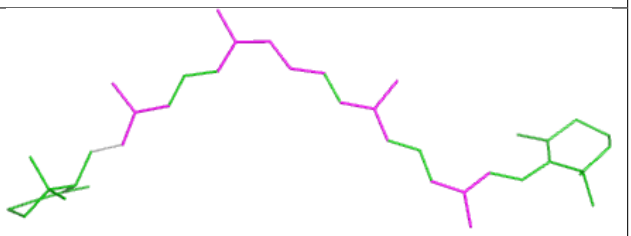


Rings

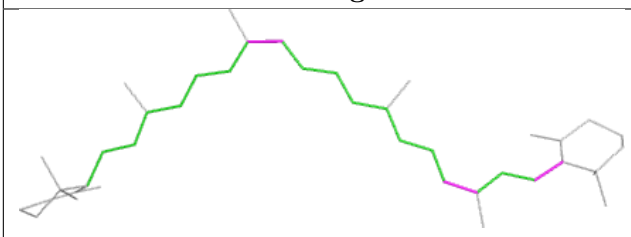
Ligand A1JPJ aA 4011



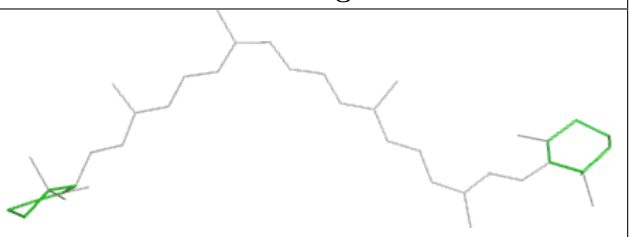
Bond lengths



Bond angles

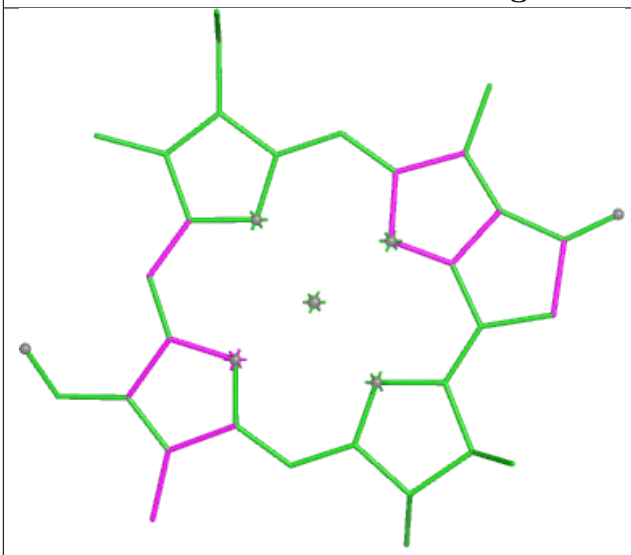


Torsions

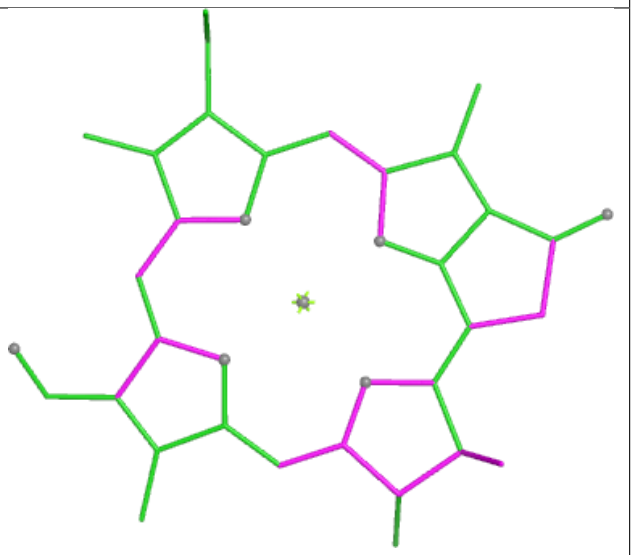


Rings

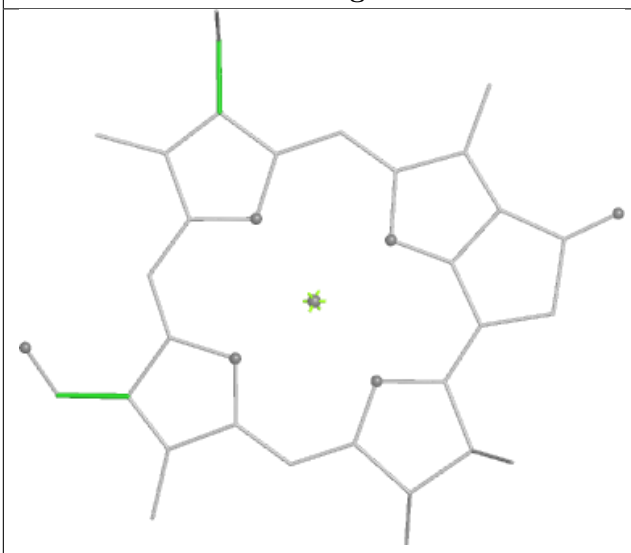
Ligand CL7 aK 1402



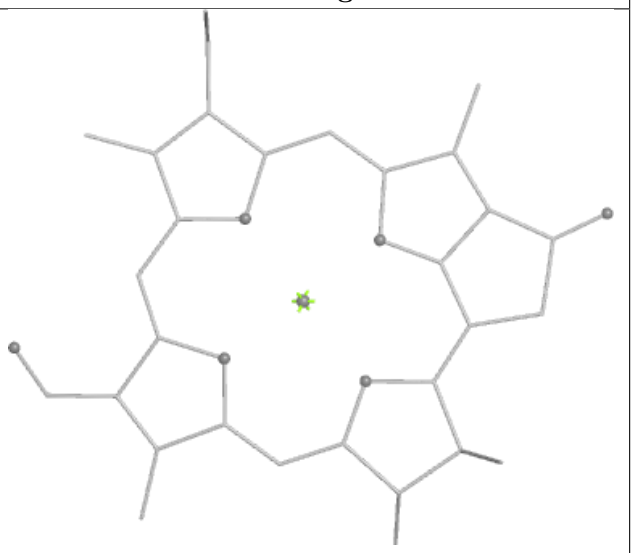
Bond lengths



Bond angles

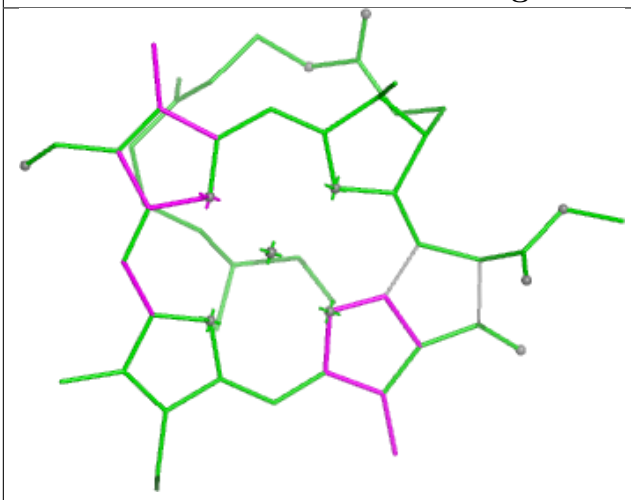


Torsions

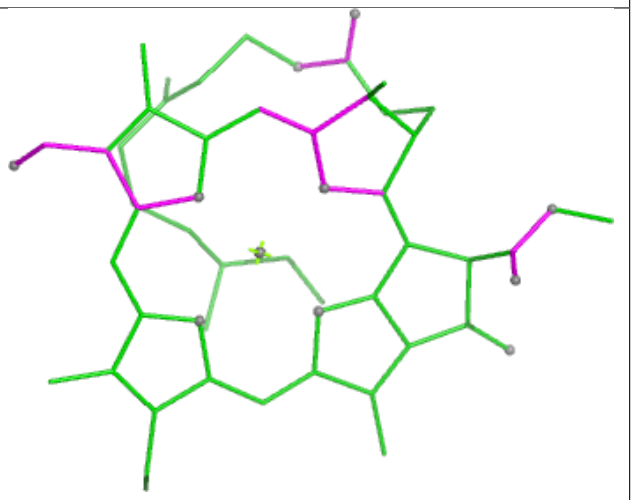


Rings

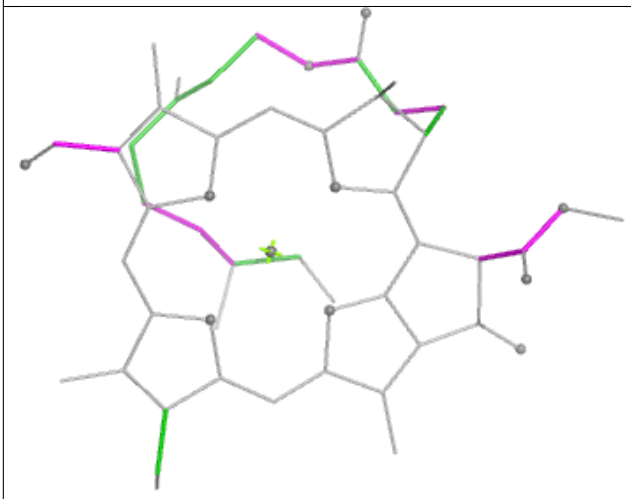
Ligand CL7 aB 1224



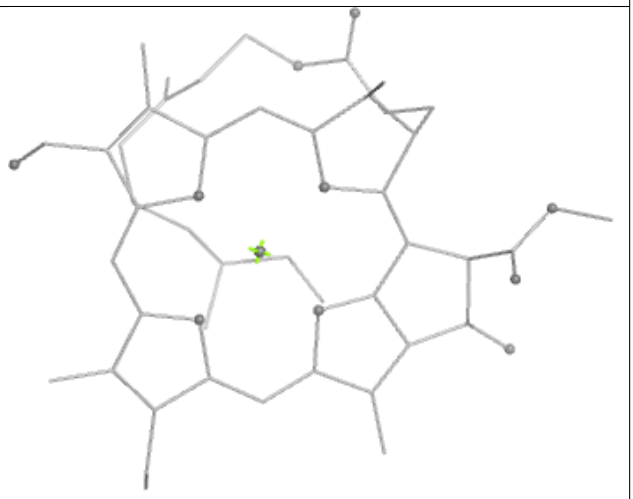
Bond lengths



Bond angles

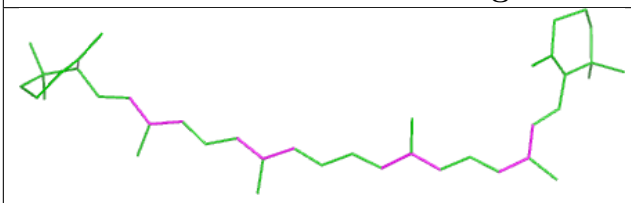


Torsions

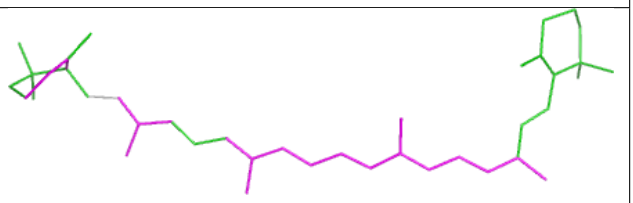


Rings

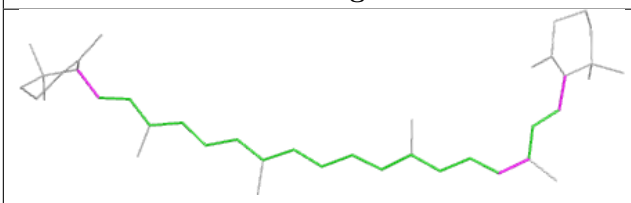
Ligand A1JPJ cB 4005



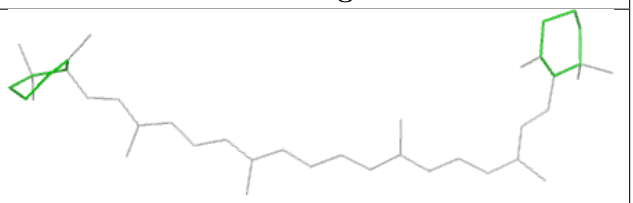
Bond lengths



Bond angles

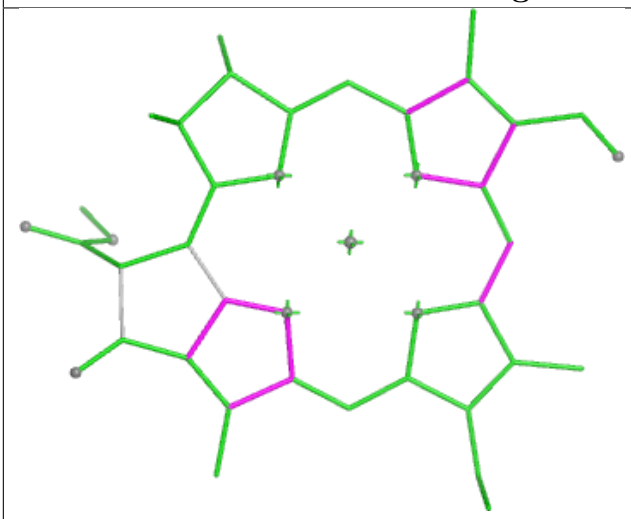


Torsions

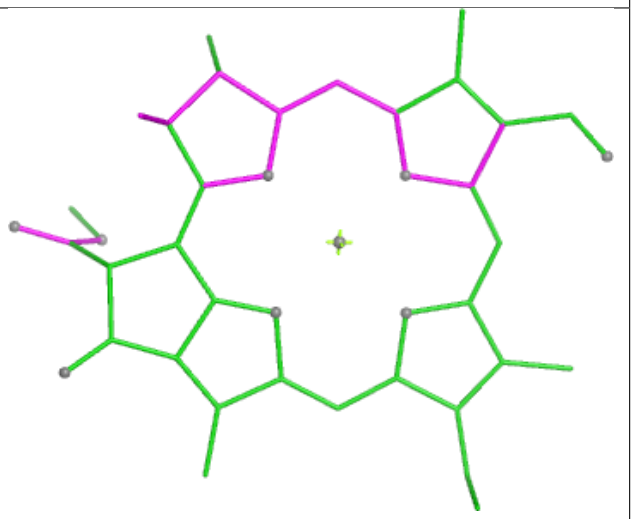


Rings

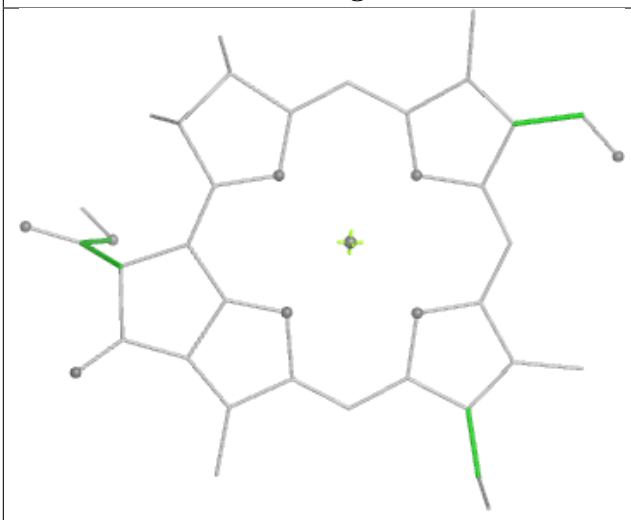
Ligand CL7 cB 1217



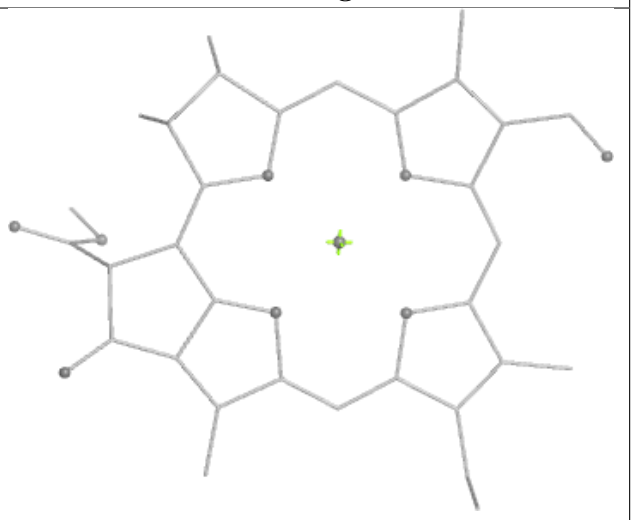
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

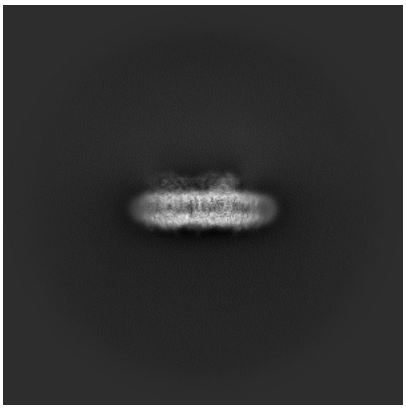
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-54956. These allow visual inspection of the internal detail of the map and identification of artifacts.

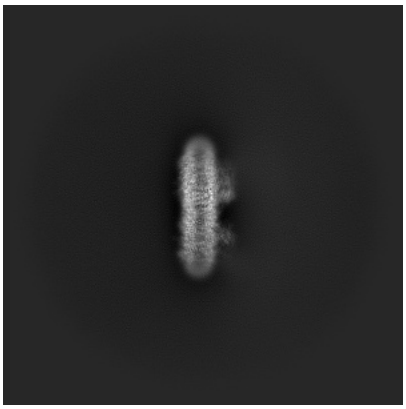
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

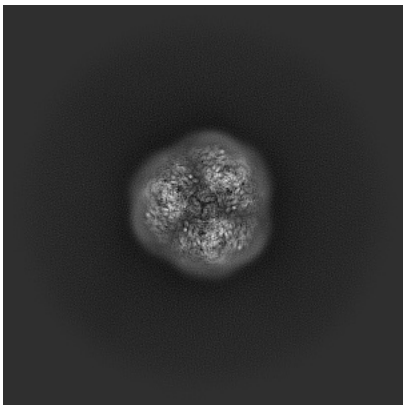
6.1.1 Primary map



X

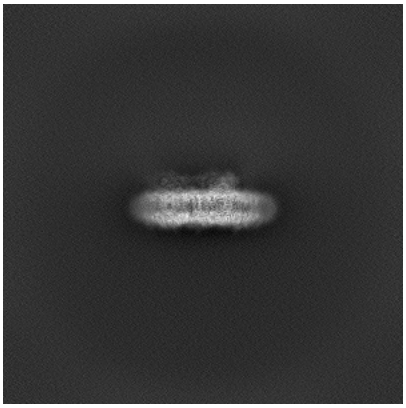


Y

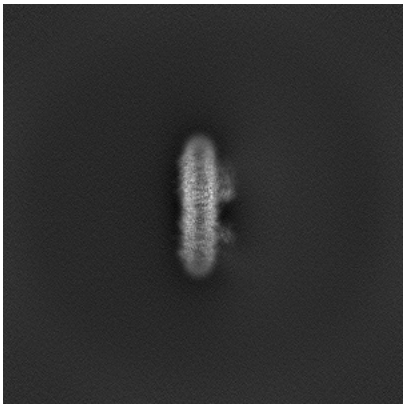


Z

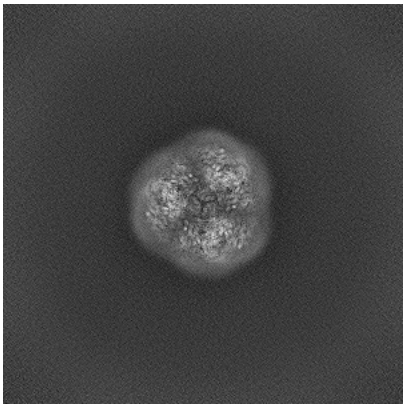
6.1.2 Raw map



X



Y

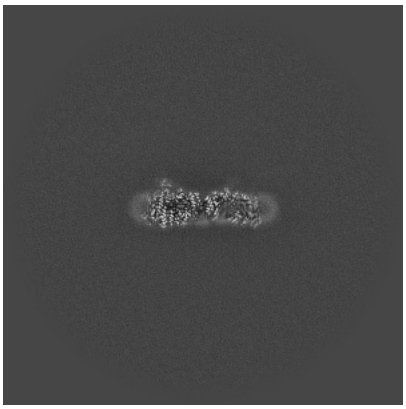


Z

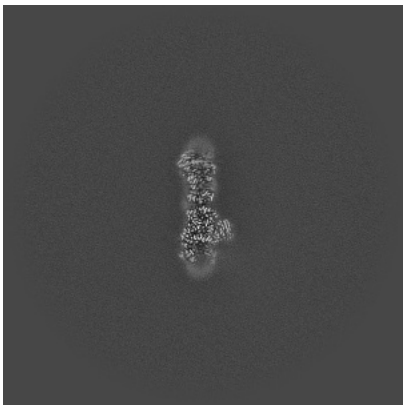
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

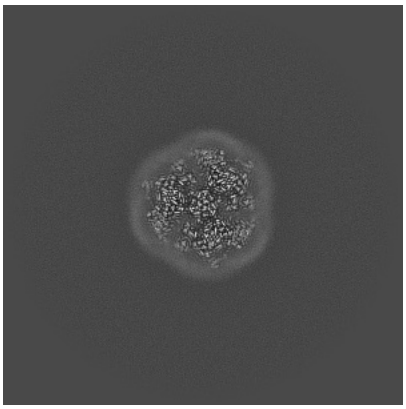
6.2.1 Primary map



X Index: 300

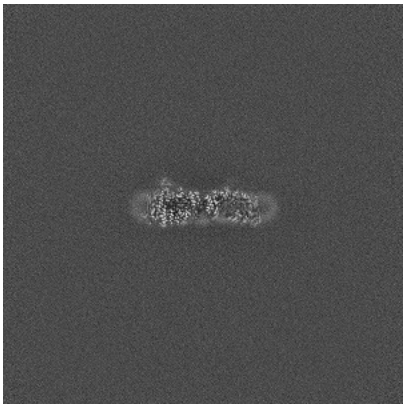


Y Index: 300

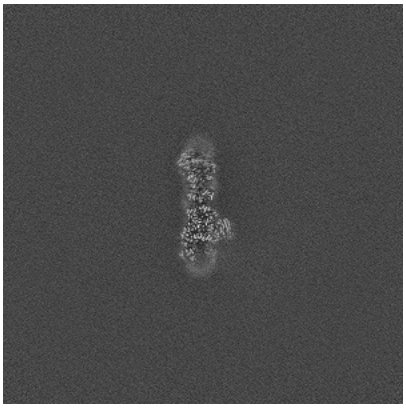


Z Index: 300

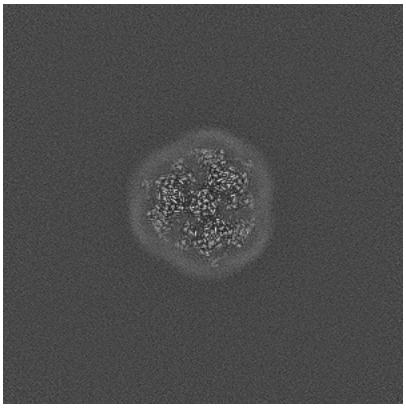
6.2.2 Raw map



X Index: 300



Y Index: 300

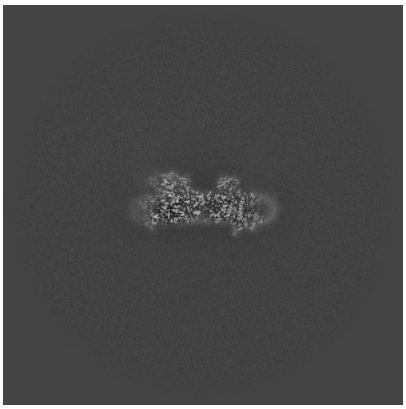


Z Index: 300

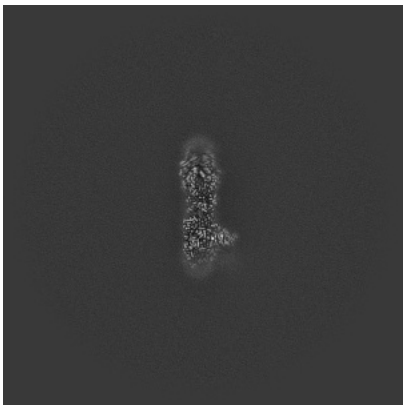
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

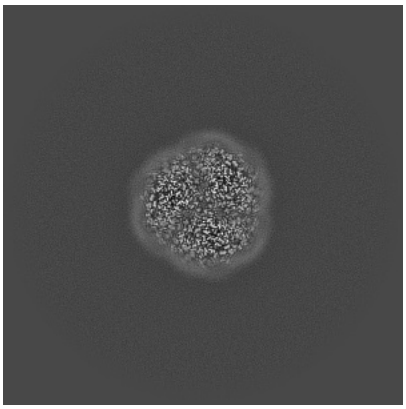
6.3.1 Primary map



X Index: 316

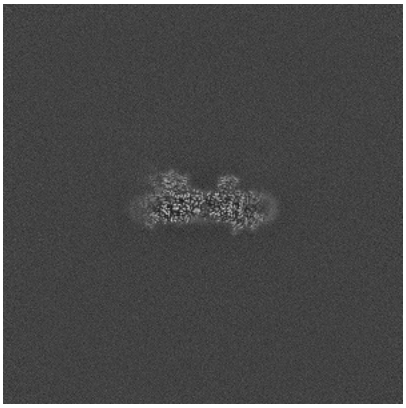


Y Index: 312

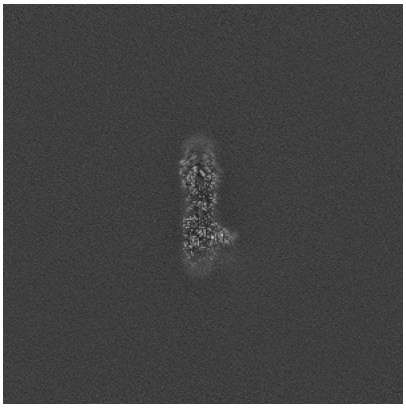


Z Index: 284

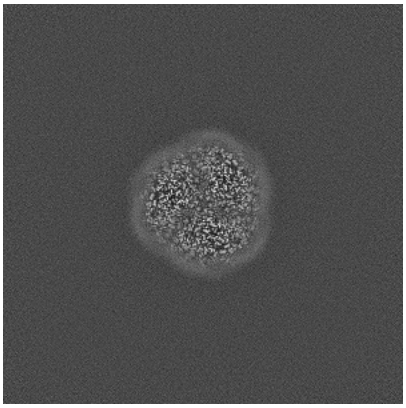
6.3.2 Raw map



X Index: 317



Y Index: 312

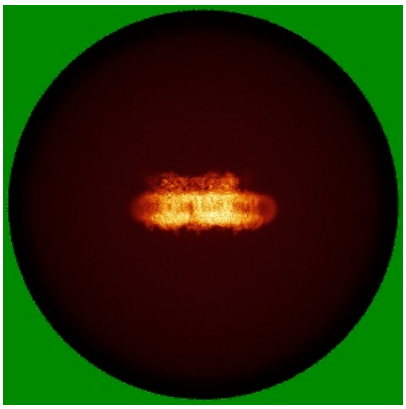


Z Index: 284

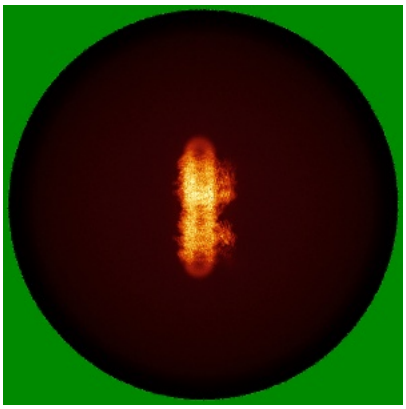
The images above show the largest variance slices of the map in three orthogonal directions.

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

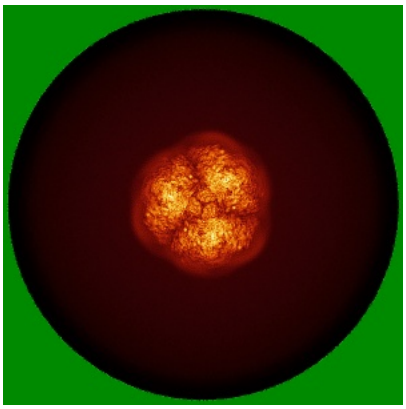
6.4.1 Primary map



X

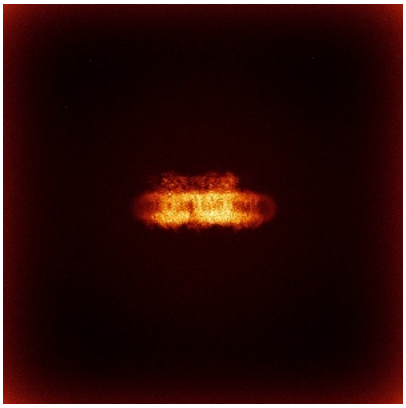


Y

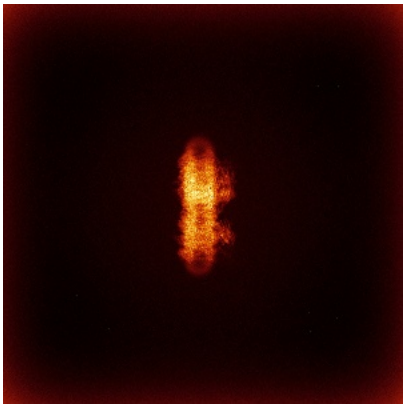


Z

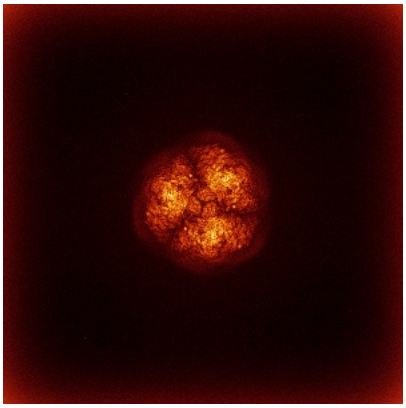
6.4.2 Raw map



X



Y



Z

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

6.5 Orthogonal surface views (i)

6.5.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.1. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



X Y Z

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

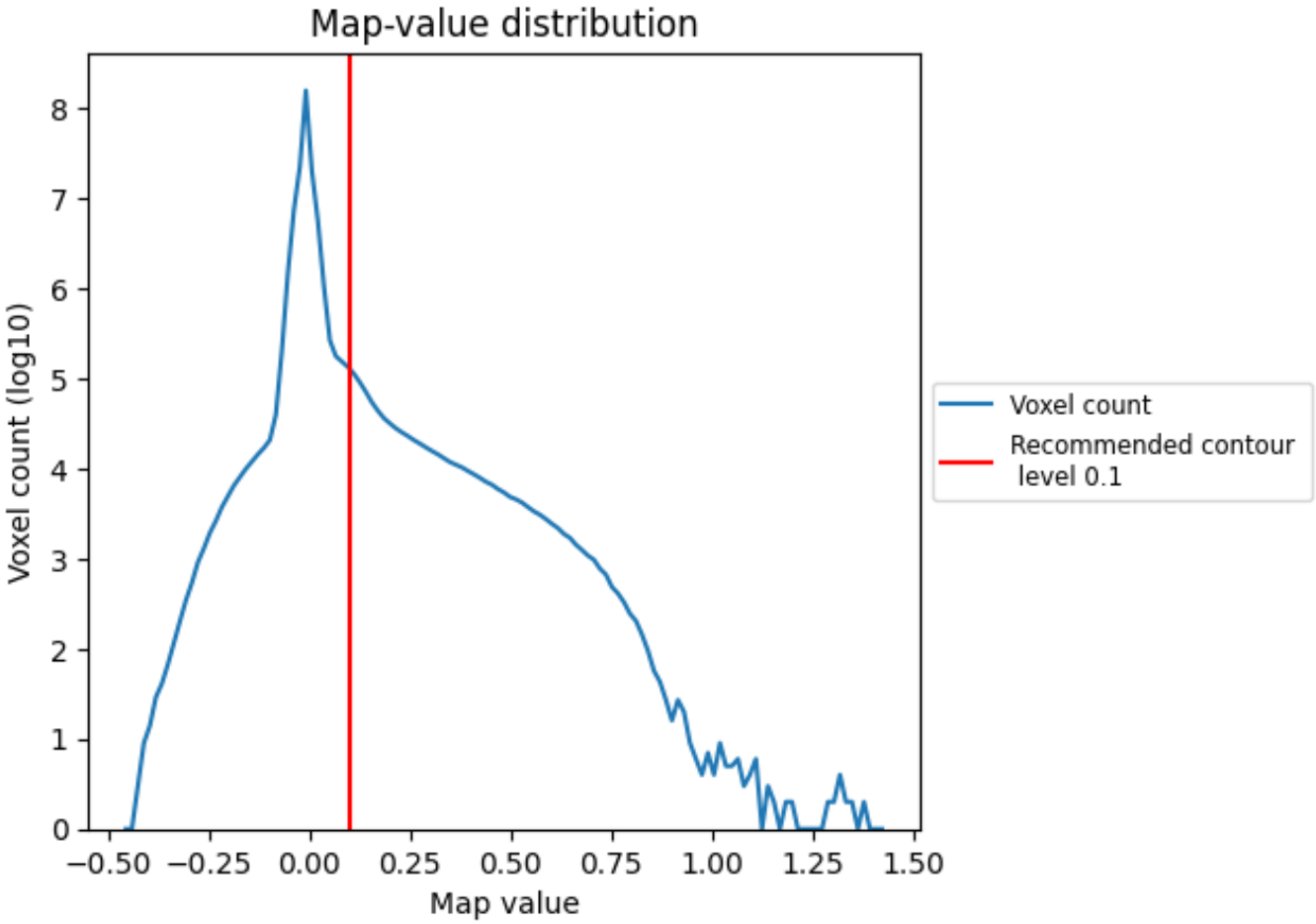
6.6 Mask visualisation (i)

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

7 Map analysis

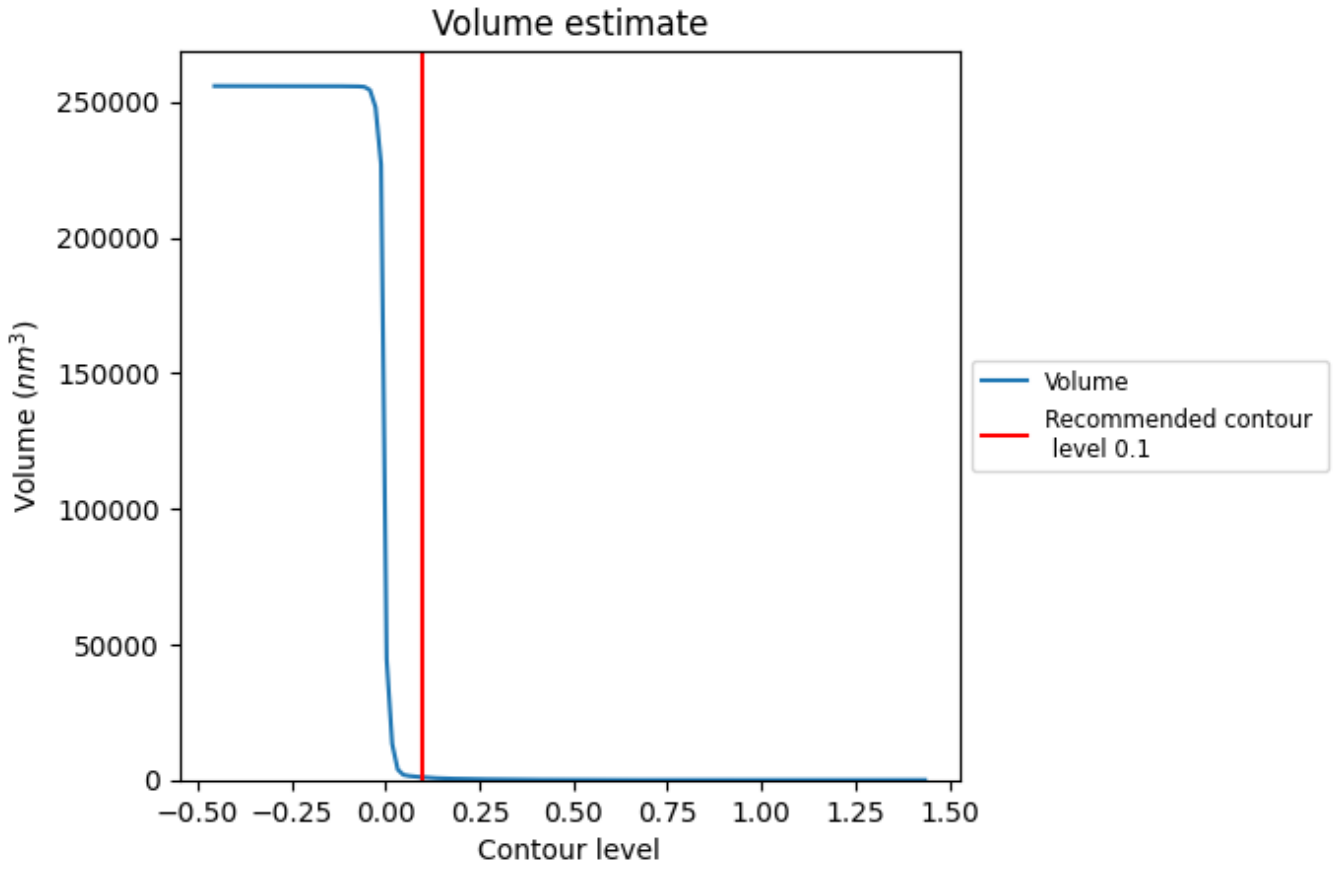
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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

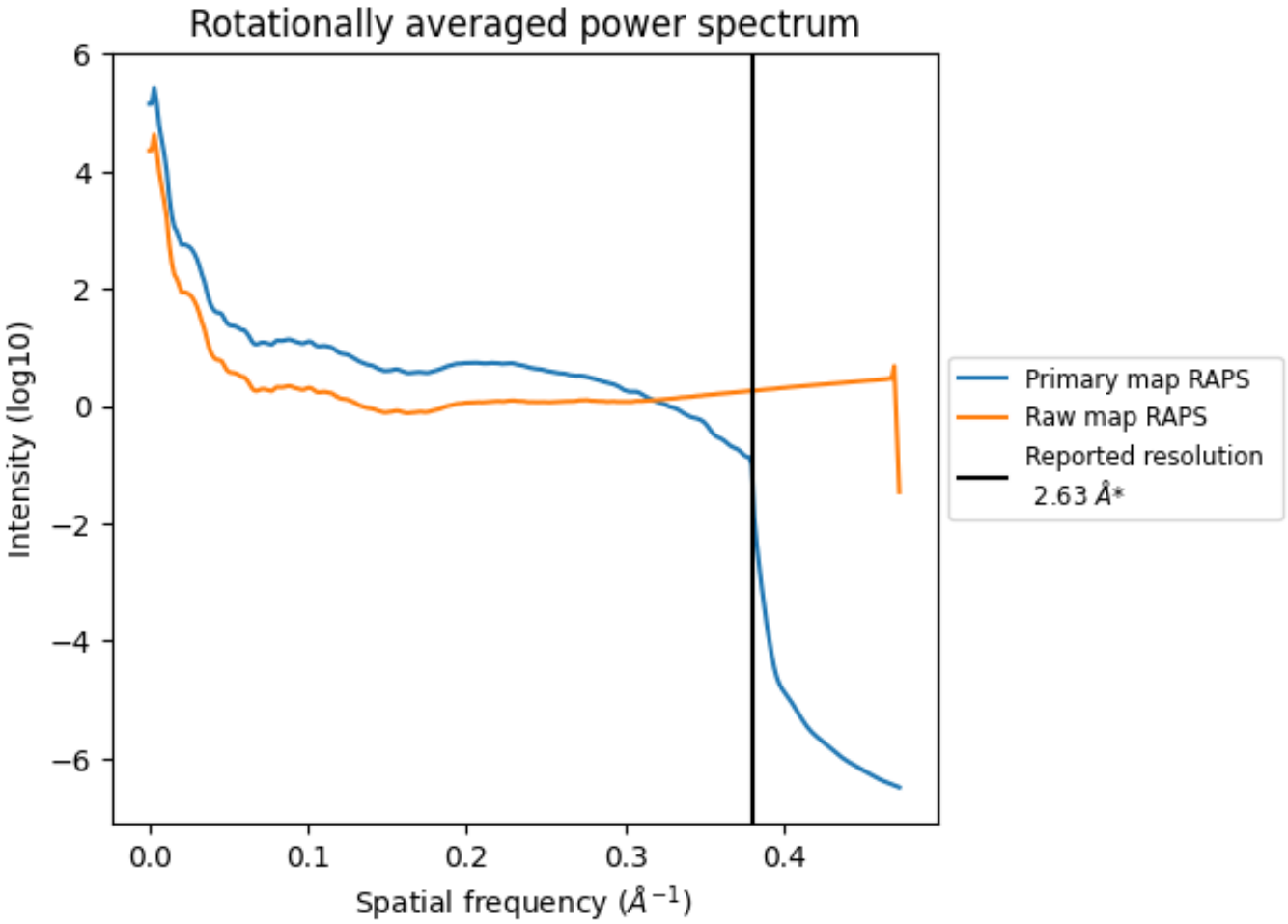
7.2 Volume estimate (i)



The volume at the recommended contour level is 992 nm^3; this corresponds to an approximate mass of 896 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)

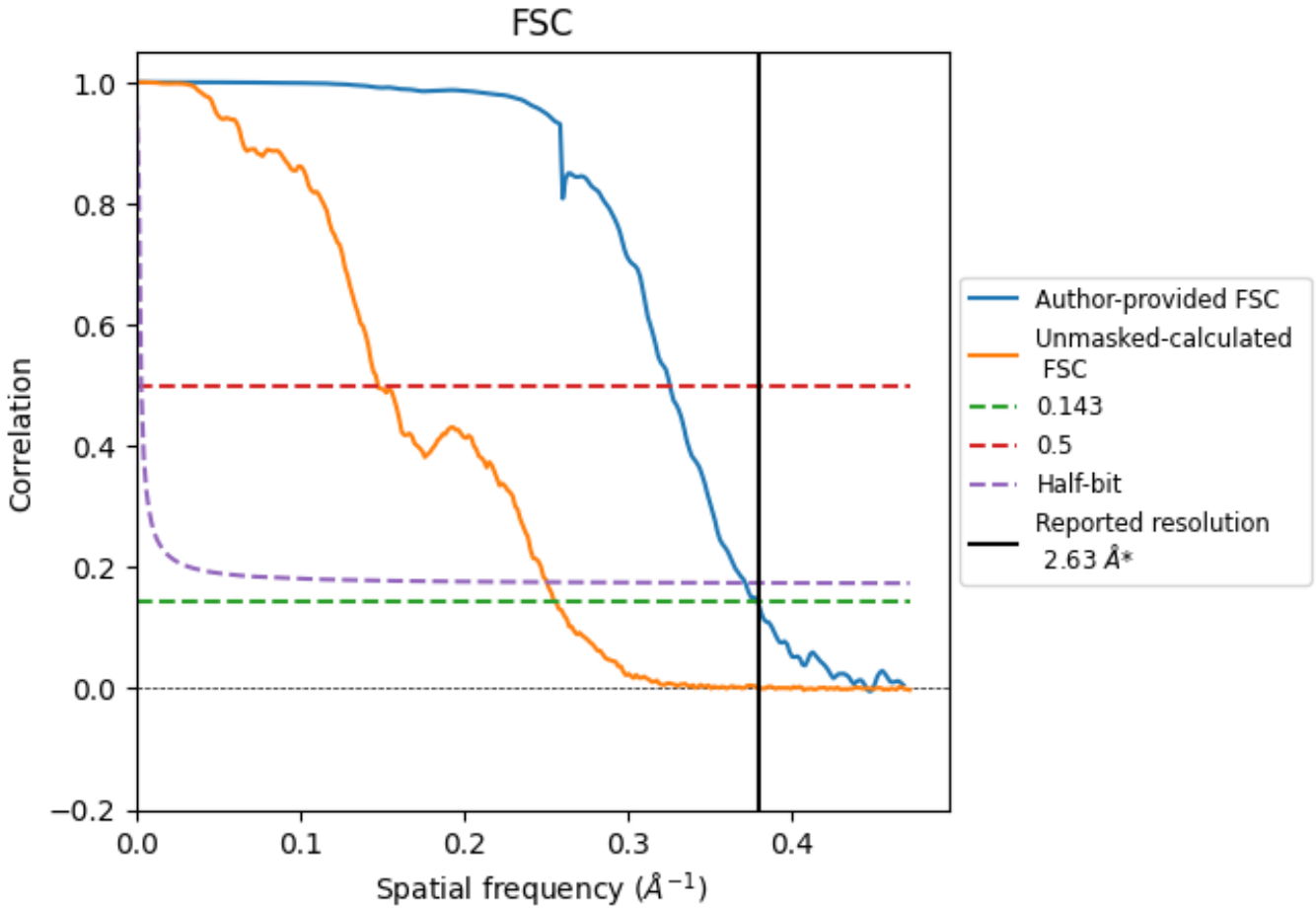


*Reported resolution corresponds to spatial frequency of 0.380 Å^{-1}

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 0.380 Å^{-1}

8.2 Resolution estimates (i)

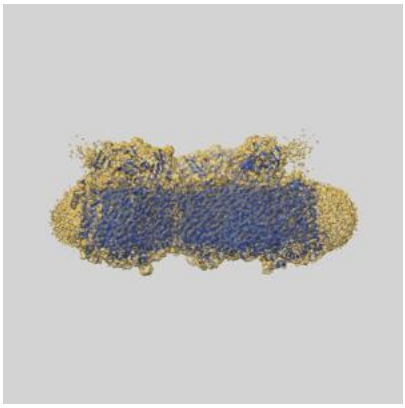
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.63	-	-
Author-provided FSC curve	2.63	3.07	2.69
Unmasked-calculated*	3.90	6.77	3.99

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.90 differs from the reported value 2.63 by more than 10 %

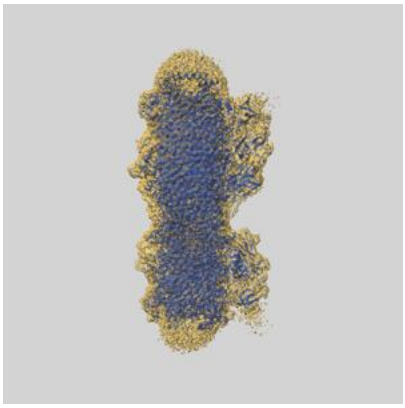
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-54956 and PDB model 9SK3. Per-residue inclusion information can be found in section 3 on page 38.

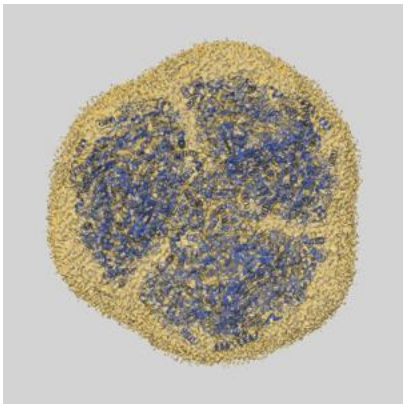
9.1 Map-model overlay



X



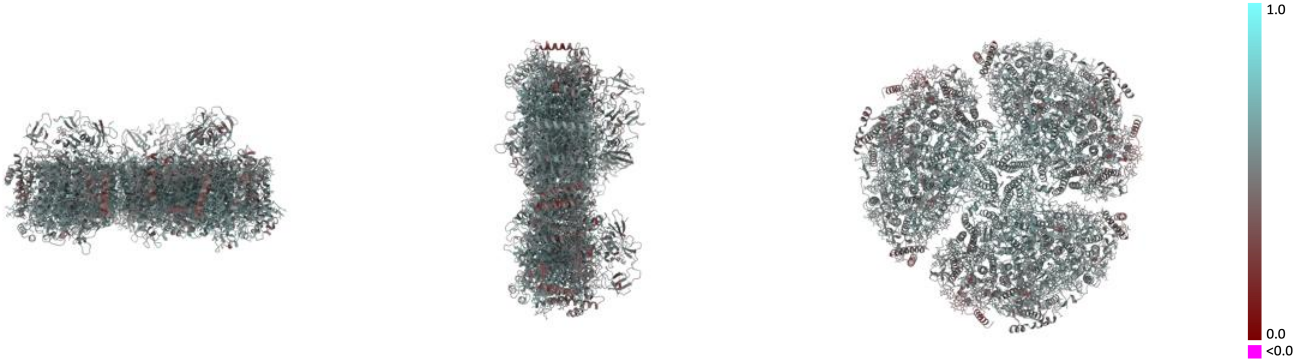
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.1 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.

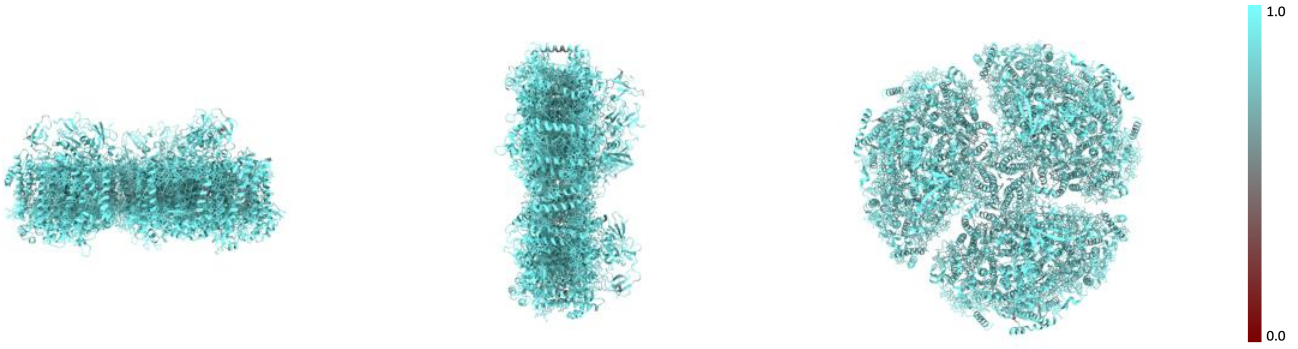
9.2 Q-score mapped to coordinate model (i)



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.

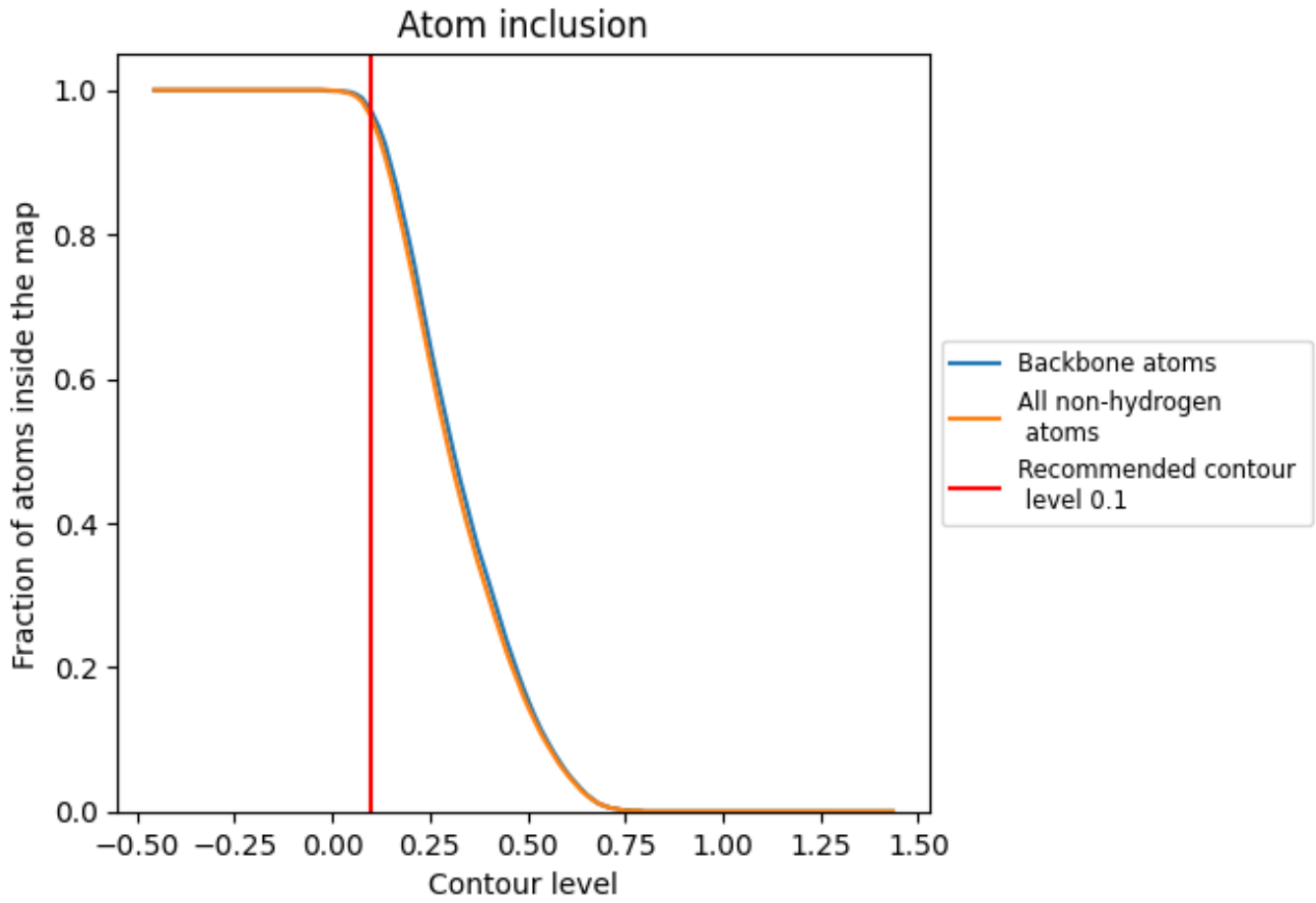
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.1).

9.4 Atom inclusion (i)



At the recommended contour level, 97% of all backbone atoms, 96% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.1) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.9630	0.5330
aA	0.9710	0.5490
aB	0.9700	0.5390
aC	0.9930	0.5120
aD	0.9740	0.5010
aE	0.8520	0.4920
aF	0.9290	0.4970
aI	0.9690	0.5670
aJ	0.9230	0.4930
aK	0.9160	0.3890
aL	0.9850	0.5740
aM	0.9240	0.4880
aX	0.8370	0.3300
bA	0.9680	0.5480
bB	0.9700	0.5400
bC	0.9870	0.5060
bD	0.9730	0.5030
bE	0.8480	0.4790
bF	0.9300	0.4950
bI	0.9720	0.5660
bJ	0.9010	0.4920
bK	0.9060	0.3900
bL	0.9860	0.5740
bM	0.9370	0.4990
bX	0.8210	0.3380
cA	0.9690	0.5500
cB	0.9700	0.5390
cC	0.9880	0.5060
cD	0.9700	0.5030
cE	0.8460	0.4790
cF	0.9260	0.4910
cI	0.9610	0.5660
cJ	0.9130	0.4890
cK	0.8990	0.3840
cL	0.9850	0.5780



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Chain	Atom inclusion	Q-score
cM	0.9330	0.5080
cX	0.8260	0.3420