wwPDB EM Validation Summary Report ⓘ

Dec 12, 2022 – 03:34 am GMT

PDB ID	:	6YAC
EMDB ID	:	EMD-10746
Title	:	Plant PSI-ferredoxin supercomplex
Authors	:	Caspy, I.; Nelson, N.; Shkolnisky, Y.; Klaiman, D.; Sheinker, A.
Deposited on	:	2020-03-12
Resolution	:	2.50 Å(reported)
Based on initial models	:	1A70, 5L8R

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

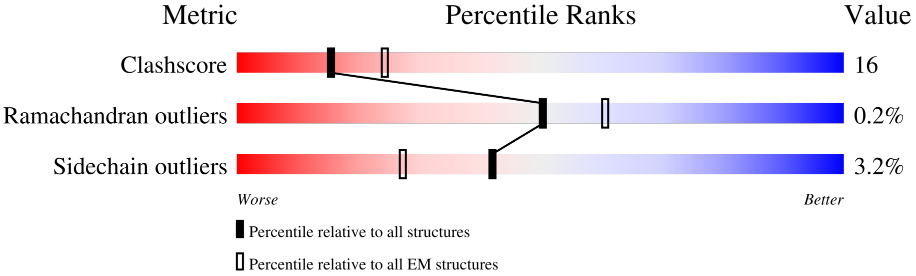
EMDB validation analysis	:	0.0.1.dev43
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)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

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 2.50 Å.

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



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

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

Mol	Chain	Length	Quality of chain
1	A	743	
2	B	733	
3	C	80	
4	D	143	
5	E	66	
6	F	154	
7	G	97	
8	H	88	

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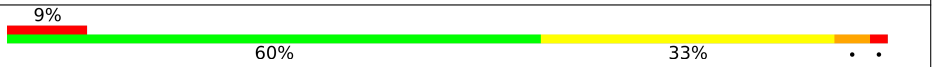
Mol	Chain	Length	Quality of chain
9	I	31	
10	J	42	
11	K	81	
12	L	157	
13	1	193	
14	2	208	
15	3	221	
16	4	198	
17	N	97	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
18	CL0	A	1011	X	-	-	-
19	CLA	1	601	X	-	-	-
19	CLA	1	602	X	-	-	-
19	CLA	1	603	X	-	-	-
19	CLA	1	604	X	-	-	-
19	CLA	1	605	X	-	-	-
19	CLA	1	606	X	-	-	-
19	CLA	1	607	X	-	-	-
19	CLA	1	608	X	-	-	-
19	CLA	1	611	X	-	-	-
19	CLA	1	613	X	-	-	-
19	CLA	1	614	X	-	-	-
19	CLA	2	601	X	-	-	-
19	CLA	2	602	X	-	-	-
19	CLA	2	603	X	-	-	-
19	CLA	2	604	X	-	-	-
19	CLA	2	605	X	-	-	-
19	CLA	2	606	X	-	-	-
19	CLA	2	607	X	-	-	-
19	CLA	2	608	X	-	-	-
19	CLA	2	612	X	-	-	-
19	CLA	3	601	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
19	CLA	3	602	X	-	-	-
19	CLA	3	603	X	-	-	-
19	CLA	3	606	X	-	-	-
19	CLA	3	608	X	-	-	-
19	CLA	3	610	X	-	-	-
19	CLA	3	612	X	-	-	-
19	CLA	3	613	X	-	-	-
19	CLA	3	614	X	-	-	-
19	CLA	3	617	X	-	-	-
19	CLA	4	601	X	-	-	-
19	CLA	4	602	X	-	-	-
19	CLA	4	603	X	-	-	-
19	CLA	4	604	X	-	-	-
19	CLA	4	606	X	-	-	-
19	CLA	4	607	X	-	-	-
19	CLA	4	608	X	-	-	-
19	CLA	4	609	X	-	-	-
19	CLA	4	612	X	-	-	-
19	CLA	4	617	X	-	-	-
19	CLA	A	1012	X	-	-	-
19	CLA	A	1013	X	-	-	-
19	CLA	A	1101	X	-	-	-
19	CLA	A	1102	X	-	-	-
19	CLA	A	1103	X	-	-	-
19	CLA	A	1104	X	-	-	-
19	CLA	A	1105	X	-	-	-
19	CLA	A	1106	X	-	-	-
19	CLA	A	1107	X	-	-	-
19	CLA	A	1108	X	-	-	-
19	CLA	A	1109	X	-	-	-
19	CLA	A	1110	X	-	-	-
19	CLA	A	1111	X	-	-	-
19	CLA	A	1112	X	-	-	-
19	CLA	A	1113	X	-	-	-
19	CLA	A	1114	X	-	-	-
19	CLA	A	1115	X	-	-	-
19	CLA	A	1116	X	-	-	-
19	CLA	A	1117	X	-	-	-
19	CLA	A	1118	X	-	-	-
19	CLA	A	1119	X	-	-	-
19	CLA	A	1120	X	-	-	-
19	CLA	A	1121	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
19	CLA	A	1122	X	-	-	-
19	CLA	A	1123	X	-	-	-
19	CLA	A	1124	X	-	-	-
19	CLA	A	1125	X	-	-	-
19	CLA	A	1126	X	-	-	-
19	CLA	A	1127	X	-	-	-
19	CLA	A	1128	X	-	-	-
19	CLA	A	1129	X	-	-	-
19	CLA	A	1130	X	-	-	-
19	CLA	A	1131	X	-	-	-
19	CLA	A	1132	X	-	-	-
19	CLA	A	1133	X	-	-	-
19	CLA	A	1134	X	-	-	-
19	CLA	A	1135	X	-	-	-
19	CLA	A	1136	X	-	-	-
19	CLA	A	1137	X	-	-	-
19	CLA	A	1138	X	-	-	-
19	CLA	A	1139	X	-	-	-
19	CLA	A	1140	X	-	-	-
19	CLA	A	1141	X	-	-	-
19	CLA	B	1021	X	-	-	-
19	CLA	B	1022	X	-	-	-
19	CLA	B	1023	X	-	-	-
19	CLA	B	1201	X	-	-	-
19	CLA	B	1202	X	-	-	-
19	CLA	B	1203	X	-	-	-
19	CLA	B	1204	X	-	-	-
19	CLA	B	1205	X	-	-	-
19	CLA	B	1206	X	-	-	-
19	CLA	B	1207	X	-	-	-
19	CLA	B	1208	X	-	-	-
19	CLA	B	1209	X	-	-	-
19	CLA	B	1210	X	-	-	-
19	CLA	B	1211	X	-	-	-
19	CLA	B	1212	X	-	-	-
19	CLA	B	1213	X	-	-	-
19	CLA	B	1214	X	-	-	-
19	CLA	B	1215	X	-	-	-
19	CLA	B	1216	X	-	-	-
19	CLA	B	1217	X	-	-	-
19	CLA	B	1218	X	-	-	-
19	CLA	B	1219	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
19	CLA	B	1220	X	-	-	-
19	CLA	B	1221	X	-	-	-
19	CLA	B	1222	X	-	-	-
19	CLA	B	1223	X	-	-	-
19	CLA	B	1224	X	-	-	-
19	CLA	B	1225	X	-	-	-
19	CLA	B	1226	X	-	-	-
19	CLA	B	1227	X	-	-	-
19	CLA	B	1228	X	-	-	-
19	CLA	B	1229	X	-	-	-
19	CLA	B	1230	X	-	-	-
19	CLA	B	1231	X	-	-	-
19	CLA	B	1232	X	-	-	-
19	CLA	B	1234	X	-	-	-
19	CLA	B	1235	X	-	-	-
19	CLA	B	1236	X	-	-	-
19	CLA	B	1237	X	-	-	-
19	CLA	B	1238	X	-	-	-
19	CLA	B	1239	X	-	-	-
19	CLA	B	1240	X	-	-	-
19	CLA	F	1301	X	-	-	-
19	CLA	F	1302	X	-	-	-
19	CLA	G	1601	X	-	-	-
19	CLA	G	1602	X	-	-	-
19	CLA	G	1603	X	-	-	-
19	CLA	G	1701	X	-	-	-
19	CLA	J	1901	X	-	-	-
19	CLA	K	1401	X	-	-	-
19	CLA	K	1402	X	-	-	-
19	CLA	K	1403	X	-	-	-
19	CLA	K	1404	X	-	-	-
19	CLA	L	1501	X	-	-	-
19	CLA	L	1502	X	-	-	-
19	CLA	L	1503	X	-	-	-
28	LUT	2	501	X	-	-	-
28	LUT	3	502	X	-	-	-
28	LUT	J	4013	X	-	-	-
29	CHL	1	609	X	-	-	-
29	CHL	1	610	X	-	-	-
29	CHL	1	612	X	-	-	-
29	CHL	2	609	X	-	-	-
29	CHL	2	610	X	-	-	-

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

2 Entry composition

There are 33 unique types of molecules in this entry. The entry contains 38469 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Photosystem I P700 chlorophyll a apoprotein A1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	743	5858	3839	998	1003	18	0	0

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

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

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

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

- Molecule 4 is a protein called PsaD.

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

- Molecule 5 is a protein called PsaE.

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

- Molecule 6 is a protein called PsaF.

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

- Molecule 7 is a protein called PsaG.

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

- Molecule 8 is a protein called PsaH.

Mol	Chain	Residues	Atoms	AltConf	Trace
8	H	88	Total C N O 673 442 106 125	0	0

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

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

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

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

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
J	32	PHE	LEU	conflict	UNP D5MAL3

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

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

There is a discrepancy between the modelled and reference sequences:

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

- Molecule 12 is a protein called PsaL.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
12	L	157	1174	772	189	212	1	0	0

- Molecule 13 is a protein called Lhca1.

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

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

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

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

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

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

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

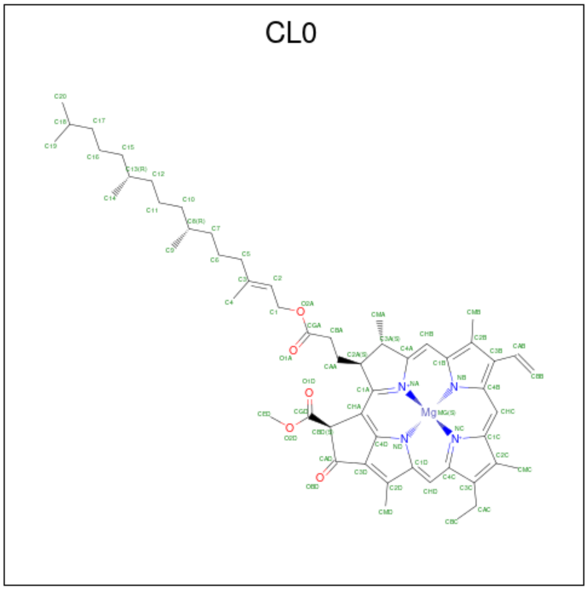
There are 3 discrepancies between the modelled and reference sequences:

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

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

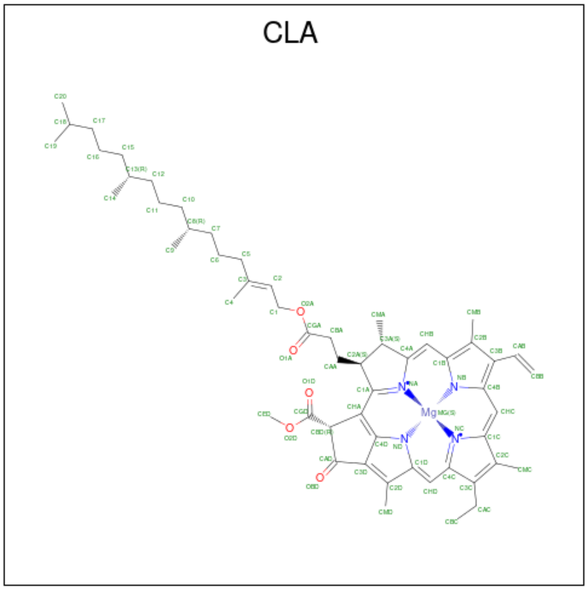
Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
17	N	97	724	448	111	160	5	0	0

- Molecule 18 is CHLOROPHYLL A ISOMER (three-letter code: CL0) (formula: $C_{55}H_{72}MgN_4O_5$).



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

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



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

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

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

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

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

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Mol	Chain	Residues	Atoms	AltConf
19	G	1	Total C Mg N O 226 186 4 16 20	0
19	G	1	Total C Mg N O 226 186 4 16 20	0
19	G	1	Total C Mg N O 226 186 4 16 20	0
19	G	1	Total C Mg N O 226 186 4 16 20	0
19	J	1	Total C Mg N O 50 40 1 4 5	0
19	K	1	Total C Mg N O 199 159 4 16 20	0
19	K	1	Total C Mg N O 199 159 4 16 20	0
19	K	1	Total C Mg N O 199 159 4 16 20	0
19	K	1	Total C Mg N O 199 159 4 16 20	0
19	L	1	Total C Mg N O 160 130 3 12 15	0
19	L	1	Total C Mg N O 160 130 3 12 15	0
19	L	1	Total C Mg N O 160 130 3 12 15	0
19	1	1	Total C Mg N O 608 498 11 44 55	0
19	1	1	Total C Mg N O 608 498 11 44 55	0
19	1	1	Total C Mg N O 608 498 11 44 55	0
19	1	1	Total C Mg N O 608 498 11 44 55	0
19	1	1	Total C Mg N O 608 498 11 44 55	0
19	1	1	Total C Mg N O 608 498 11 44 55	0
19	1	1	Total C Mg N O 608 498 11 44 55	0
19	1	1	Total C Mg N O 608 498 11 44 55	0
19	1	1	Total C Mg N O 608 498 11 44 55	0

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Mol	Chain	Residues	Atoms	AltConf
19	1	1	Total C Mg N O 608 498 11 44 55	0
19	1	1	Total C Mg N O 608 498 11 44 55	0
19	2	1	Total C Mg N O 522 432 9 36 45	0
19	2	1	Total C Mg N O 522 432 9 36 45	0
19	2	1	Total C Mg N O 522 432 9 36 45	0
19	2	1	Total C Mg N O 522 432 9 36 45	0
19	2	1	Total C Mg N O 522 432 9 36 45	0
19	2	1	Total C Mg N O 522 432 9 36 45	0
19	2	1	Total C Mg N O 522 432 9 36 45	0
19	2	1	Total C Mg N O 522 432 9 36 45	0
19	2	1	Total C Mg N O 522 432 9 36 45	0
19	3	1	Total C Mg N O 578 470 11 44 53	0
19	3	1	Total C Mg N O 578 470 11 44 53	0
19	3	1	Total C Mg N O 578 470 11 44 53	0
19	3	1	Total C Mg N O 578 470 11 44 53	0
19	3	1	Total C Mg N O 578 470 11 44 53	0
19	3	1	Total C Mg N O 578 470 11 44 53	0
19	3	1	Total C Mg N O 578 470 11 44 53	0
19	3	1	Total C Mg N O 578 470 11 44 53	0
19	3	1	Total C Mg N O 578 470 11 44 53	0
19	3	1	Total C Mg N O 578 470 11 44 53	0

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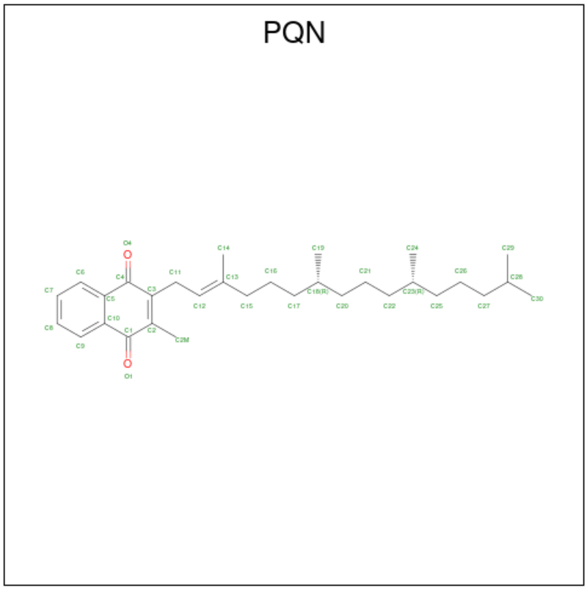
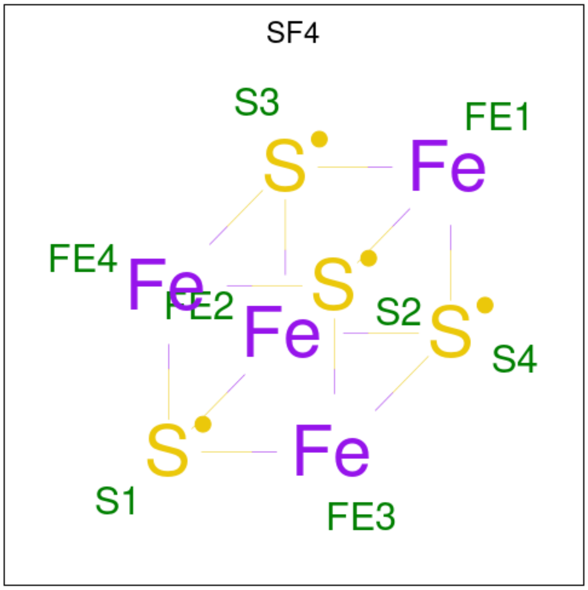
Mol	Chain	Residues	Atoms					AltConf
19	3	1	Total 578	C 470	Mg 11	N 44	O 53	0
19	4	1	Total 631	C 521	Mg 11	N 44	O 55	0
19	4	1	Total 631	C 521	Mg 11	N 44	O 55	0
19	4	1	Total 631	C 521	Mg 11	N 44	O 55	0
19	4	1	Total 631	C 521	Mg 11	N 44	O 55	0
19	4	1	Total 631	C 521	Mg 11	N 44	O 55	0
19	4	1	Total 631	C 521	Mg 11	N 44	O 55	0
19	4	1	Total 631	C 521	Mg 11	N 44	O 55	0
19	4	1	Total 631	C 521	Mg 11	N 44	O 55	0
19	4	1	Total 631	C 521	Mg 11	N 44	O 55	0
19	4	1	Total 631	C 521	Mg 11	N 44	O 55	0
19	4	1	Total 631	C 521	Mg 11	N 44	O 55	0

- Molecule 20 is PHYLLOQUINONE (three-letter code: PQN) (formula: $C_{31}H_{46}O_2$).



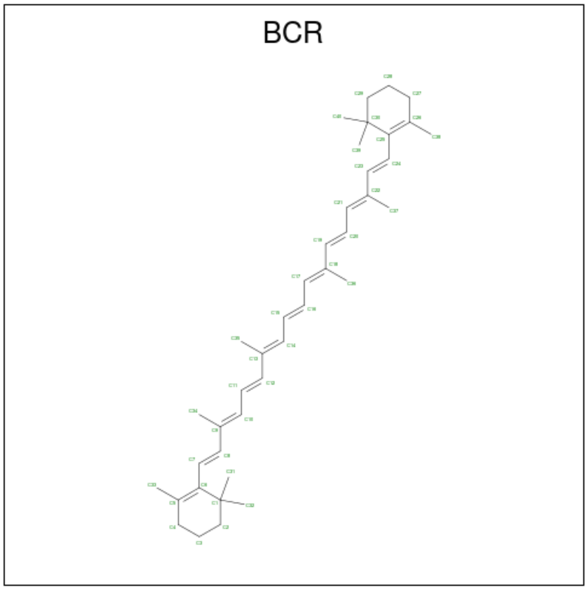
Mol	Chain	Residues	Atoms			AltConf
20	A	1	Total 33	C 31	O 2	0
20	B	1	Total 33	C 31	O 2	0

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



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

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



Mol	Chain	Residues	Atoms	AltConf
22	A	1	Total C 240 240	0
22	A	1	Total C 240 240	0
22	A	1	Total C 240 240	0
22	A	1	Total C 240 240	0
22	A	1	Total C 240 240	0
22	A	1	Total C 240 240	0
22	B	1	Total C 200 200	0
22	B	1	Total C 200 200	0
22	B	1	Total C 200 200	0
22	B	1	Total C 200 200	0
22	B	1	Total C 200 200	0
22	F	1	Total C 80 80	0
22	F	1	Total C 80 80	0
22	G	1	Total C 80 80	0

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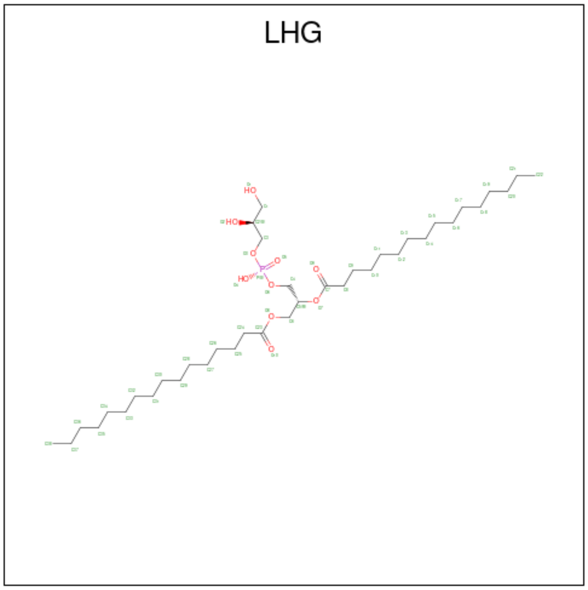
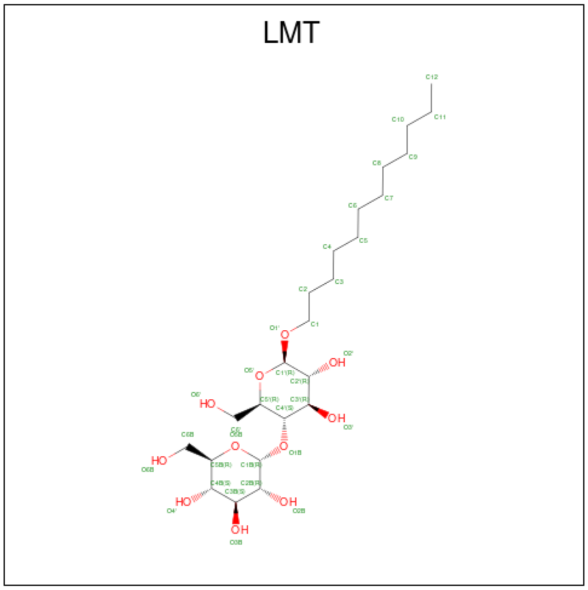
Mol	Chain	Residues	Atoms	AltConf
22	G	1	Total C 80 80	0
22	I	1	Total C 80 80	0
22	I	1	Total C 80 80	0
22	J	1	Total C 40 40	0
22	K	1	Total C 80 80	0
22	K	1	Total C 80 80	0
22	L	1	Total C 80 80	0
22	L	1	Total C 80 80	0
22	1	1	Total C 80 80	0
22	1	1	Total C 80 80	0
22	2	1	Total C 40 40	0
22	3	1	Total C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

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



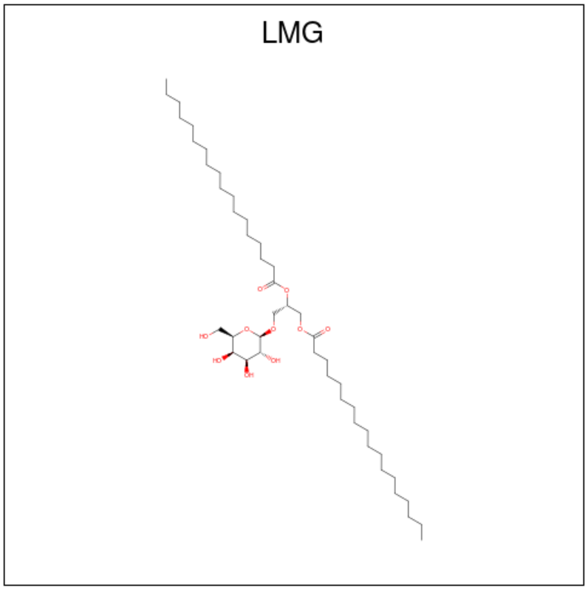
Mol	Chain	Residues	Atoms	AltConf
23	A	1	Total C O P 89 67 20 2	0
23	A	1	Total C O P 89 67 20 2	0
23	B	1	Total C O P 70 48 20 2	0
23	B	1	Total C O P 70 48 20 2	0
23	1	1	Total C O P 49 38 10 1	0
23	2	1	Total C O P 68 46 20 2	0
23	2	1	Total C O P 68 46 20 2	0
23	3	1	Total C O P 17 8 8 1	0

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



Mol	Chain	Residues	Atoms	AltConf
24	A	1	Total C O 35 24 11	0
24	B	1	Total C O 63 41 22	0
24	B	1	Total C O 63 41 22	0
24	G	1	Total C O 66 44 22	0
24	G	1	Total C O 66 44 22	0
24	J	1	Total C O 25 14 11	0

- Molecule 25 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (three-letter code: LMG) (formula: $C_{45}H_{86}O_{10}$).



Mol	Chain	Residues	Atoms	AltConf
25	A	1	Total C O 50 40 10	0
25	B	1	Total C O 102 72 30	0
25	B	1	Total C O 102 72 30	0
25	B	1	Total C O 102 72 30	0
25	F	1	Total C O 160 114 46	0
25	F	1	Total C O 160 114 46	0
25	F	1	Total C O 160 114 46	0
25	F	1	Total C O 160 114 46	0
25	F	1	Total C O 160 114 46	0
25	G	1	Total C O 124 94 30	0
25	G	1	Total C O 124 94 30	0
25	G	1	Total C O 124 94 30	0
25	1	1	Total C O 46 36 10	0
25	2	1	Total C O 117 75 42	0

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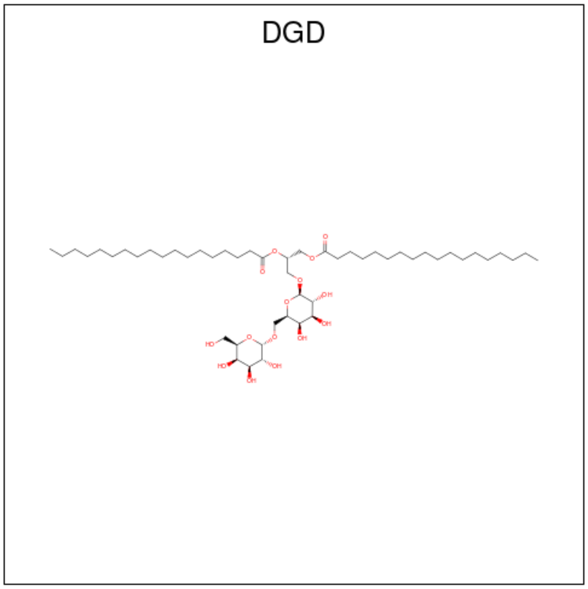
Mol	Chain	Residues	Atoms	AltConf
25	2	1	Total C O 117 75 42	0
25	2	1	Total C O 117 75 42	0
25	2	1	Total C O 117 75 42	0
25	2	1	Total C O 117 75 42	0
25	3	1	Total C O 30 20 10	0

- Molecule 26 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms	AltConf
26	A	1	Total Ca 1 1	0
26	B	1	Total Ca 1 1	0

- Molecule 27 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (three-letter code: DGD) (formula: $C_{51}H_{96}O_{15}$).



Mol	Chain	Residues	Atoms	AltConf
27	B	1	Total C O 61 46 15	0
27	F	1	Total C O 57 42 15	0

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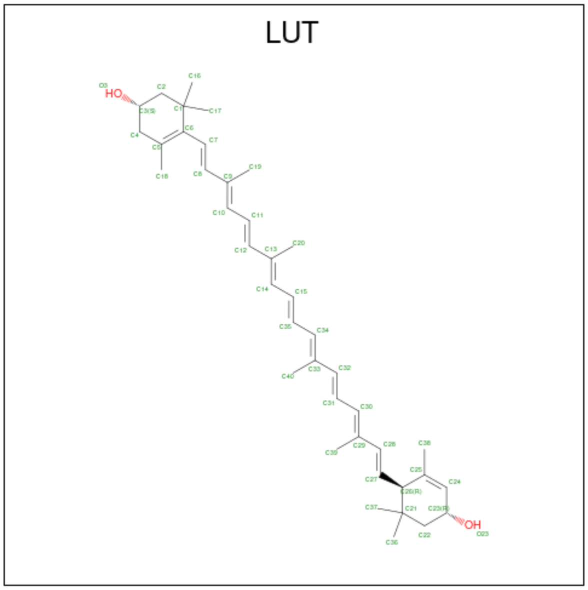
Mol	Chain	Residues	Atoms	AltConf
27	G	1	Total C O 47 32 15	0
27	J	1	Total C O 58 43 15	0
27	1	1	Total C O 41 26 15	0
27	3	1	Total C O 51 36 15	0
27	4	1	Total C O 102 72 30	0
27	4	1	Total C O 102 72 30	0

- Molecule 28 is (3R,3'R,6S)-4,5-DIDEHYDRO-5,6-DIHYDRO-BETA,BETA-CAROTENE-3,3'-DIOL (three-letter code: LUT) (formula: $C_{40}H_{56}O_2$).



Mol	Chain	Residues	Atoms	AltConf
28	J	1	Total C O 42 40 2	0
28	1	1	Total C O 84 80 4	0
28	1	1	Total C O 84 80 4	0
28	2	1	Total C O 42 40 2	0
28	3	1	Total C O 84 80 4	0

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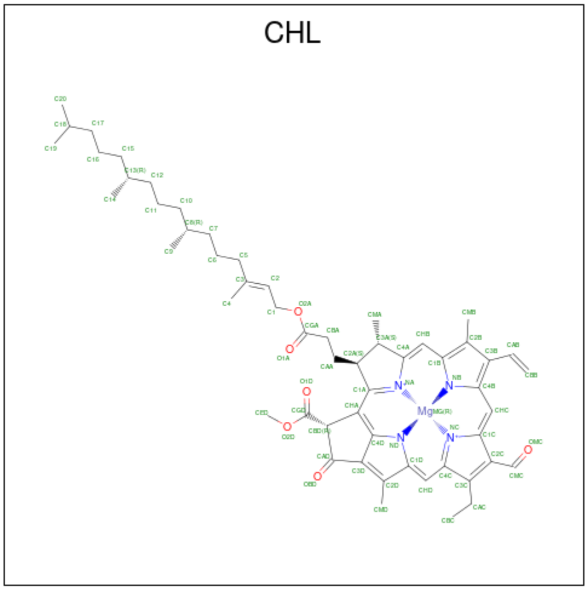
Mol	Chain	Residues	Atoms	AltConf
28	3	1	Total C O 84 80 4	0
28	4	1	Total C O 42 40 2	0

- Molecule 29 is CHLOROPHYLL B (three-letter code: CHL) (formula: $C_{55}H_{70}MgN_4O_6$).



Mol	Chain	Residues	Atoms	AltConf
29	1	1	Total C Mg N O 164 131 3 12 18	0
29	1	1	Total C Mg N O 164 131 3 12 18	0
29	1	1	Total C Mg N O 164 131 3 12 18	0
29	2	1	Total C Mg N O 272 217 5 20 30	0
29	2	1	Total C Mg N O 272 217 5 20 30	0
29	2	1	Total C Mg N O 272 217 5 20 30	0
29	2	1	Total C Mg N O 272 217 5 20 30	0
29	2	1	Total C Mg N O 272 217 5 20 30	0
29	3	1	Total C Mg N O 164 131 3 12 18	0

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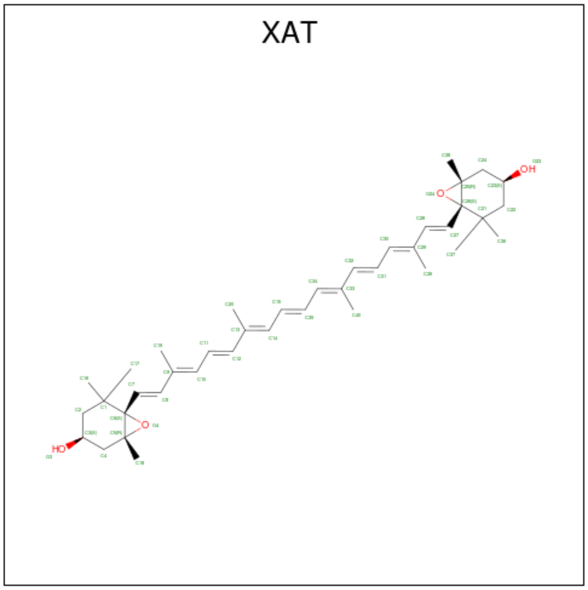
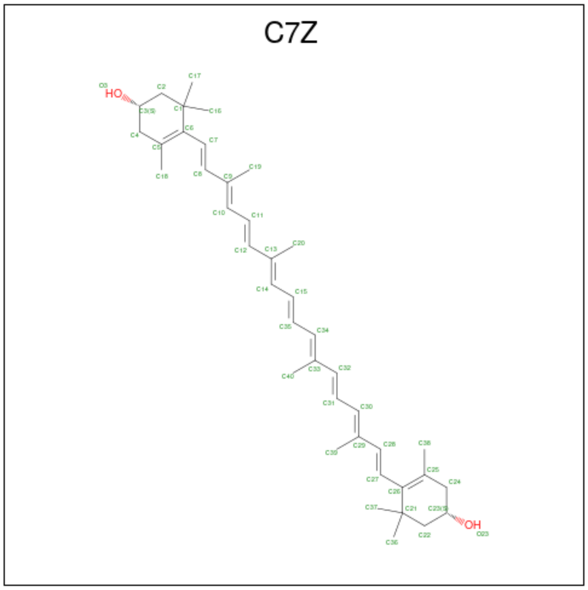
Mol	Chain	Residues	Atoms					AltConf
29	3	1	Total 164	C 131	Mg 3	N 12	O 18	0
29	3	1	Total 164	C 131	Mg 3	N 12	O 18	0
29	4	1	Total 202	C 160	Mg 4	N 16	O 22	0
29	4	1	Total 202	C 160	Mg 4	N 16	O 22	0
29	4	1	Total 202	C 160	Mg 4	N 16	O 22	0
29	4	1	Total 202	C 160	Mg 4	N 16	O 22	0

- Molecule 30 is (3S,5R,6S,3'S,5'R,6'S)-5,6,5',6'-DIEPOXY-5,6,5',6'- TETRAHYDRO-BETA ,BETA-CAROTENE-3,3'-DIOL (three-letter code: XAT) (formula: $C_{40}H_{56}O_4$).



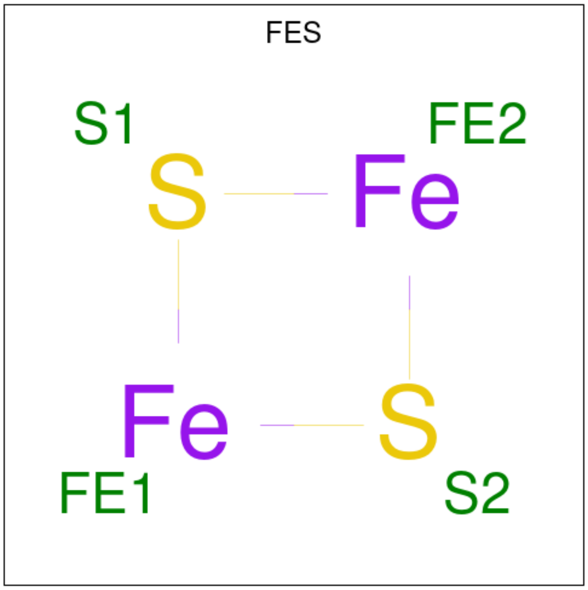
Mol	Chain	Residues	Atoms			AltConf
30	2	1	Total 44	C 40	O 4	0
30	4	1	Total 44	C 40	O 4	0

- Molecule 31 is (1 {S})-3,5,5-trimethyl-4-[(1 {E},3 {E},5 {E},7 {E},9 {E},11 {E},13 {E},15 {E},17 {E})-3,7,12,16-tetramethyl-18-[(4 {S})-2,6,6-trimethyl-4-oxidanyl-cyclohexen-1-yl]octadeca-1,3,5,7,9,11,13,15,17-nonaenyl]cyclohex-3-en-1-ol (three-letter code: C7Z) (formula: $C_{40}H_{56}O_2$).



Mol	Chain	Residues	Atoms	AltConf
31	4	1	Total C O 42 40 2	0

- Molecule 32 is FE2/S2 (INORGANIC) CLUSTER (three-letter code: FES) (formula: Fe_2S_2).



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

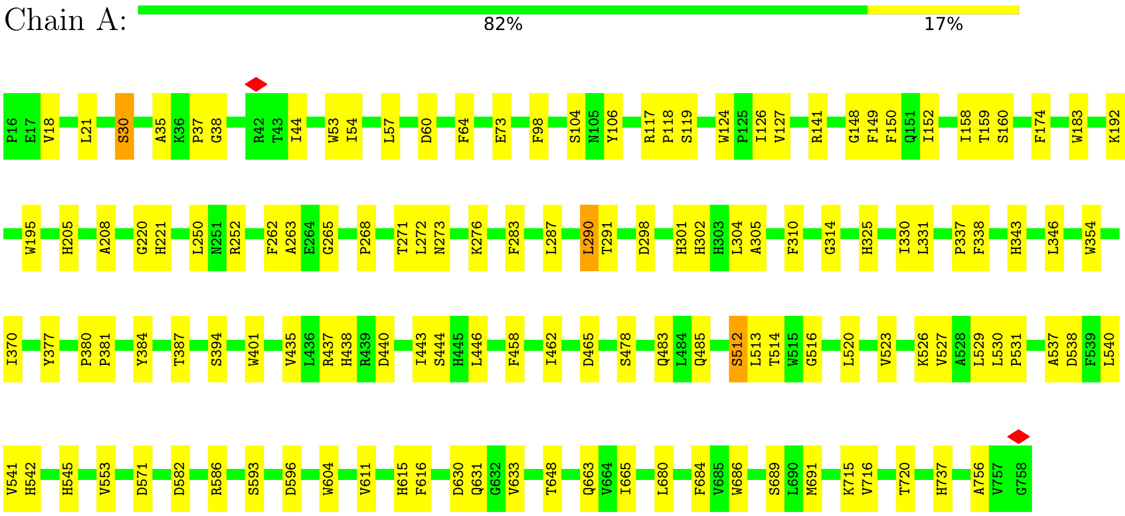
- Molecule 33 is water.

Mol	Chain	Residues	Atoms	AltConf
33	A	13	Total O 13 13	0
33	B	15	Total O 15 15	0
33	C	2	Total O 2 2	0
33	D	1	Total O 1 1	0
33	F	3	Total O 3 3	0
33	G	4	Total O 4 4	0
33	I	1	Total O 1 1	0
33	J	2	Total O 2 2	0
33	K	1	Total O 1 1	0
33	L	3	Total O 3 3	0
33	1	5	Total O 5 5	0
33	2	2	Total O 2 2	0
33	3	3	Total O 3 3	0
33	4	1	Total O 1 1	0

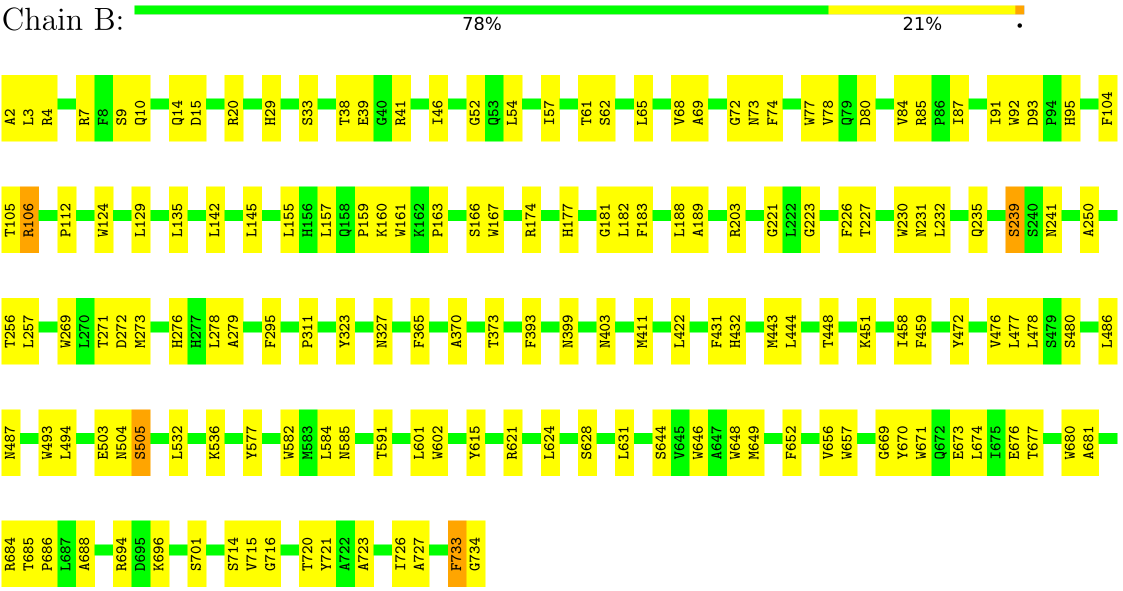
3 Residue-property plots ⓘ

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

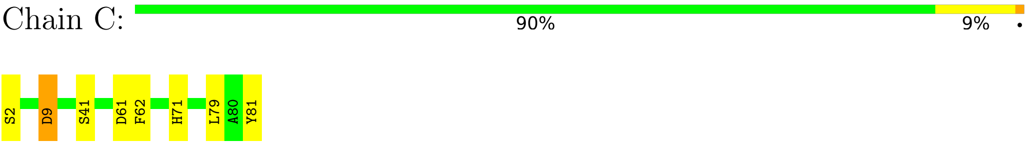
- Molecule 1: Photosystem I P700 chlorophyll a apoprotein A1



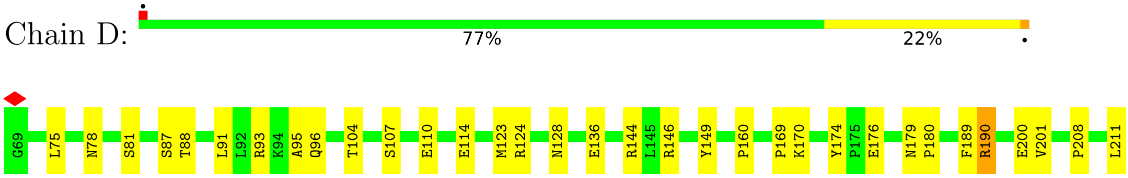
- Molecule 2: Photosystem I P700 chlorophyll a apoprotein A2



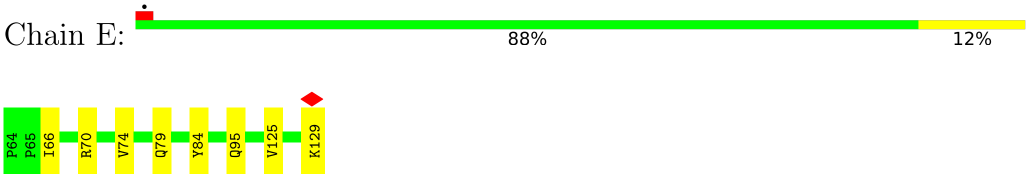
- Molecule 3: Photosystem I iron-sulfur center



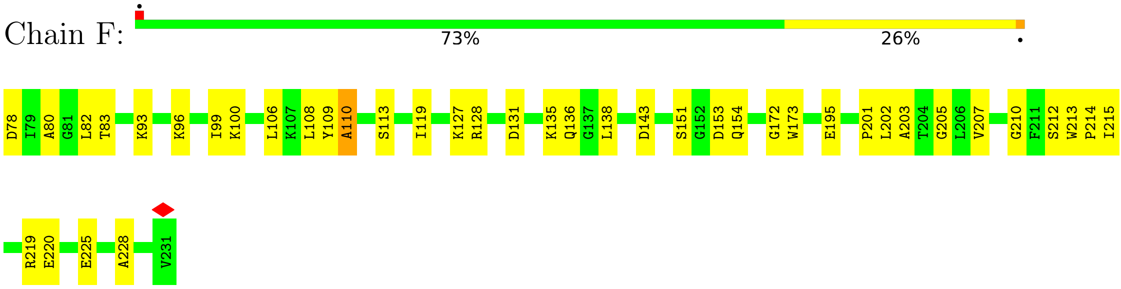
- Molecule 4: PsaD



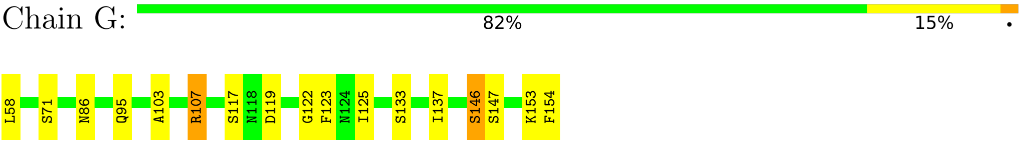
- Molecule 5: PsaE



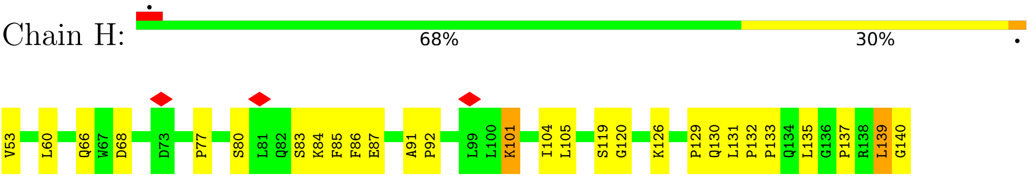
- Molecule 6: PsaF



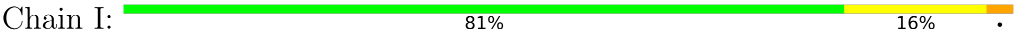
- Molecule 7: PsaG

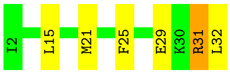


- Molecule 8: PsaH

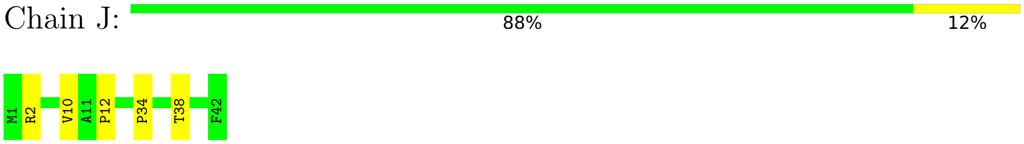


- Molecule 9: Photosystem I reaction center subunit VIII

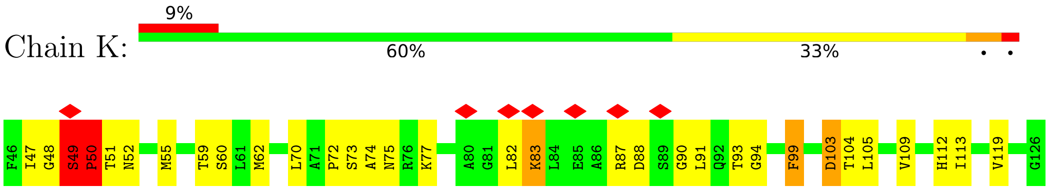




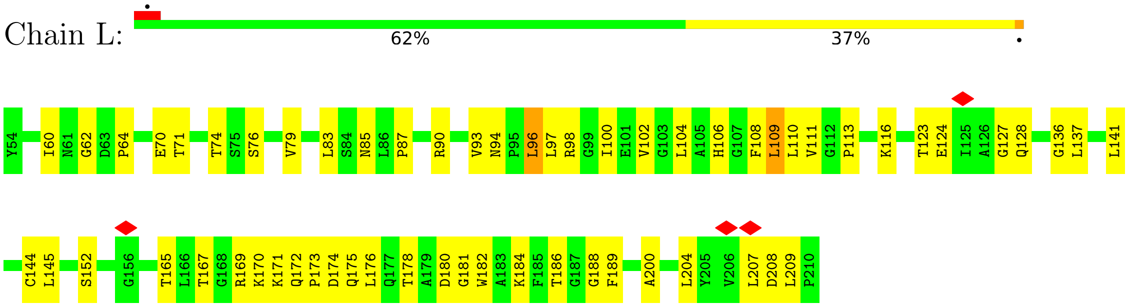
- Molecule 10: Photosystem I reaction center subunit IX



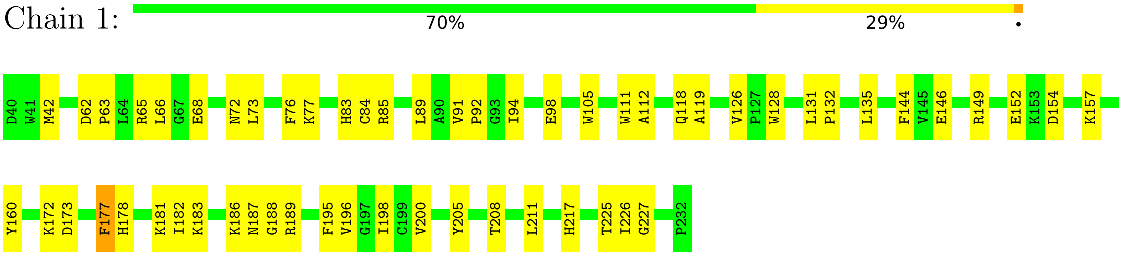
- Molecule 11: Photosystem I reaction center subunit X psaK



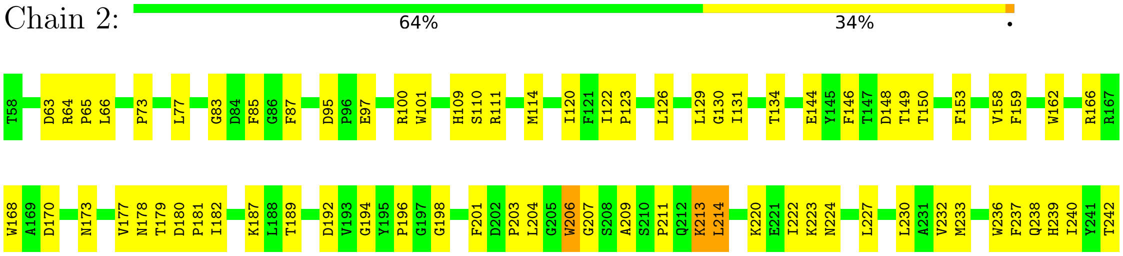
- Molecule 12: PsaL

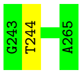


- Molecule 13: Lhca1



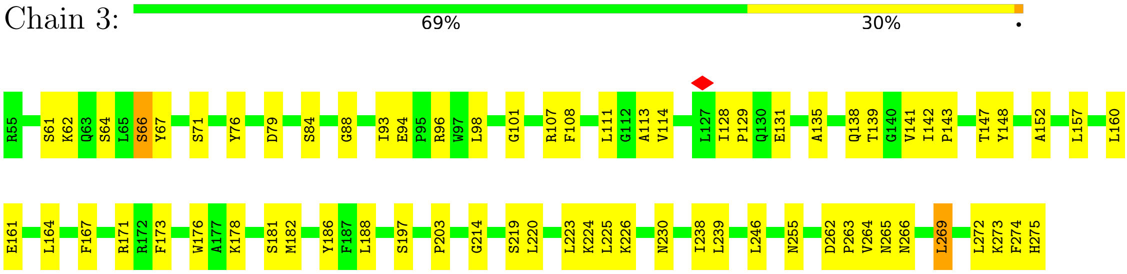
- Molecule 14: Chlorophyll a-b binding protein, chloroplastic





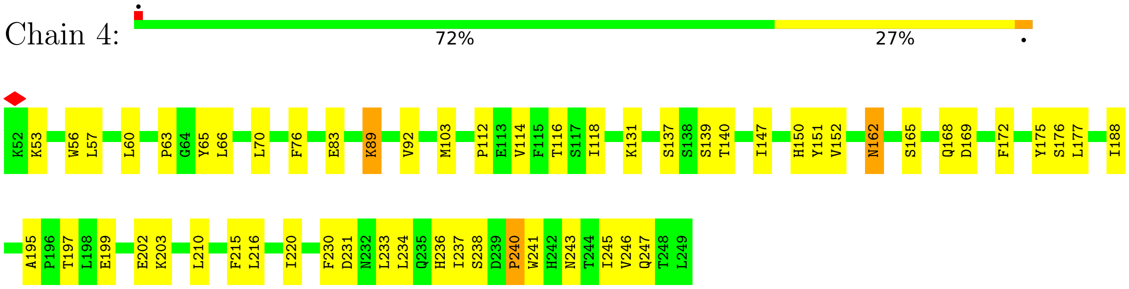
- Molecule 15: Chlorophyll a-b binding protein 3, chloroplastic

Chain 3:



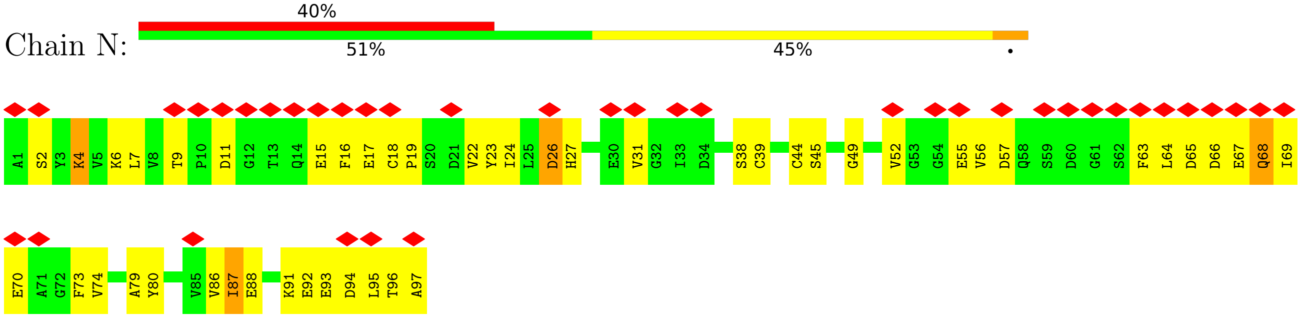
- Molecule 16: Chlorophyll a-b binding protein P4, chloroplastic

Chain 4:



- Molecule 17: Ferredoxin-1, chloroplastic

Chain N:



4 Experimental information ⓘ

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	269657	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose $(e^-/\text{Å}^2)$	1.075	Depositor
Minimum defocus (nm)	900	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.111	Depositor
Minimum map value	-0.059	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.004	Depositor
Recommended contour level	0.0131	Depositor
Map size (Å)	358.05002, 358.05002, 358.05002	wwPDB
Map dimensions	330, 330, 330	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.085, 1.085, 1.085	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, CLA, SF4, CA, LMT, LUT, LMG, BCR, XAT, CL0, FES, PQN, CHL, C7Z, DGD

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#|Z| > 5$	RMSZ	$\#|Z| > 5$
1	A	0.41	1/6057 (0.0%)	0.49	0/8264
2	B	0.38	0/6069	0.49	0/8286
3	C	0.36	0/625	0.51	0/846
4	D	0.38	0/1163	0.53	0/1572
5	E	0.39	0/540	0.48	0/734
6	F	0.49	1/1234 (0.1%)	0.57	0/1670
7	G	0.36	0/776	0.47	0/1054
8	H	0.36	0/693	0.57	0/942
9	I	0.36	0/246	0.49	0/335
10	J	0.34	0/349	0.43	0/476
11	K	0.71	2/576 (0.3%)	0.66	1/779 (0.1%)
12	L	0.35	0/1207	0.51	0/1651
13	1	0.34	0/1558	0.47	0/2125
14	2	0.38	0/1679	0.52	0/2302
15	3	0.35	0/1760	0.50	0/2390
16	4	0.37	0/1608	0.47	0/2191
17	N	0.42	0/736	0.60	0/1000
All	All	0.40	4/26876 (0.0%)	0.50	1/36617 (0.0%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	K	50	PRO	N-CA	13.71	1.70	1.47
1	A	117	ARG	C-N	8.93	1.51	1.34
6	F	83	THR	C-N	8.57	1.50	1.34
11	K	49	SER	C-N	6.03	1.45	1.34

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	K	50	PRO	CA-N-CD	-7.88	100.47	111.50

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5858	0	5719	108	0
2	B	5857	0	5653	140	0
3	C	612	0	591	5	0
4	D	1132	0	1141	24	0
5	E	528	0	528	4	0
6	F	1206	0	1231	33	0
7	G	757	0	743	17	0
8	H	673	0	667	27	0
9	I	240	0	264	12	0
10	J	338	0	345	6	0
11	K	569	0	596	37	0
12	L	1174	0	1183	52	0
13	1	1508	0	1489	54	0
14	2	1620	0	1557	70	0
15	3	1706	0	1661	60	0
16	4	1559	0	1527	55	0
17	N	724	0	672	73	0
18	A	65	0	72	6	0
19	1	608	0	565	49	0
19	2	522	0	503	46	0
19	3	578	0	497	37	0
19	4	631	0	600	46	0
19	A	2643	0	2751	183	0
19	B	2610	0	2750	180	0
19	F	130	0	144	8	0
19	G	226	0	212	14	0
19	J	50	0	39	0	0
19	K	199	0	158	19	0
19	L	160	0	136	13	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
20	A	33	0	46	0	0
20	B	33	0	46	4	0
21	A	8	0	0	0	0
21	C	16	0	0	0	0
22	1	80	0	105	8	0
22	2	40	0	53	10	0
22	3	80	0	105	6	0
22	A	240	0	316	17	0
22	B	200	0	264	14	0
22	F	80	0	104	5	0
22	G	80	0	105	8	0
22	I	80	0	105	6	0
22	J	40	0	53	1	0
22	K	80	0	106	12	0
22	L	80	0	106	7	0
23	1	49	0	74	8	0
23	2	68	0	76	4	0
23	3	17	0	12	0	0
23	A	89	0	127	5	0
23	B	70	0	86	9	0
24	A	35	0	45	3	0
24	B	63	0	69	4	0
24	G	66	0	77	2	0
24	J	25	0	22	0	0
25	1	46	0	65	3	0
25	2	117	0	114	9	0
25	3	30	0	30	0	0
25	A	50	0	73	5	0
25	B	102	0	114	5	0
25	F	160	0	188	13	0
25	G	124	0	161	8	0
26	A	1	0	0	0	0
26	B	1	0	0	0	0
27	1	41	0	40	1	0
27	3	51	0	60	3	0
27	4	102	0	120	6	0
27	B	61	0	83	7	0
27	F	57	0	75	7	0
27	G	47	0	52	4	0
27	J	58	0	77	4	0
28	1	84	0	110	16	0
28	2	42	0	55	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
28	3	84	0	110	4	0
28	4	42	0	55	6	0
28	J	42	0	55	4	0
29	1	164	0	133	19	0
29	2	272	0	226	21	0
29	3	164	0	137	18	0
29	4	202	0	151	13	0
30	2	44	0	56	10	0
30	4	44	0	56	6	0
31	4	42	0	0	0	0
32	N	4	0	0	1	0
33	1	5	0	0	2	0
33	2	2	0	0	0	0
33	3	3	0	0	0	0
33	4	1	0	0	0	0
33	A	13	0	0	1	0
33	B	15	0	0	0	0
33	C	2	0	0	0	0
33	D	1	0	0	0	0
33	F	3	0	0	0	0
33	G	4	0	0	1	0
33	I	1	0	0	0	0
33	J	2	0	0	0	0
33	K	1	0	0	0	0
33	L	3	0	0	1	0
All	All	38469	0	38492	1259	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 16.

The worst 5 of 1259 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)
11:K:50:PRO:N	11:K:50:PRO:CA	1.70	1.36
17:N:73:PHE:CG	17:N:95:LEU:HD23	1.75	1.19
17:N:64:LEU:CD2	17:N:69:ILE:HD11	1.80	1.12
14:2:182:ILE:HG12	19:4:607:CLA:HMB1	1.35	1.09
11:K:49:SER:H	11:K:50:PRO:CD	1.65	1.09

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	741/743 (100%)	715 (96%)	26 (4%)	0	100	100
2	B	731/733 (100%)	698 (96%)	33 (4%)	0	100	100
3	C	78/80 (98%)	74 (95%)	4 (5%)	0	100	100
4	D	141/143 (99%)	131 (93%)	10 (7%)	0	100	100
5	E	64/66 (97%)	61 (95%)	3 (5%)	0	100	100
6	F	152/154 (99%)	145 (95%)	6 (4%)	1 (1%)	22	39
7	G	95/97 (98%)	90 (95%)	5 (5%)	0	100	100
8	H	86/88 (98%)	78 (91%)	8 (9%)	0	100	100
9	I	29/31 (94%)	29 (100%)	0	0	100	100
10	J	40/42 (95%)	40 (100%)	0	0	100	100
11	K	79/81 (98%)	70 (89%)	6 (8%)	3 (4%)	3	4
12	L	155/157 (99%)	143 (92%)	12 (8%)	0	100	100
13	1	191/193 (99%)	175 (92%)	16 (8%)	0	100	100
14	2	206/208 (99%)	178 (86%)	26 (13%)	2 (1%)	15	28
15	3	219/221 (99%)	190 (87%)	29 (13%)	0	100	100
16	4	196/198 (99%)	181 (92%)	15 (8%)	0	100	100
17	N	95/97 (98%)	84 (88%)	9 (10%)	2 (2%)	7	11
All	All	3298/3332 (99%)	3082 (94%)	208 (6%)	8 (0%)	50	68

5 of 8 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
11	K	49	SER
11	K	50	PRO
17	N	66	ASP
14	2	149	THR
17	N	68	GLN

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	604/604 (100%)	590 (98%)	14 (2%)	50	76
2	B	598/598 (100%)	583 (98%)	15 (2%)	47	73
3	C	69/69 (100%)	67 (97%)	2 (3%)	42	69
4	D	122/122 (100%)	119 (98%)	3 (2%)	47	73
5	E	58/58 (100%)	57 (98%)	1 (2%)	60	82
6	F	125/126 (99%)	123 (98%)	2 (2%)	62	84
7	G	82/82 (100%)	76 (93%)	6 (7%)	14	27
8	H	71/71 (100%)	68 (96%)	3 (4%)	30	54
9	I	27/27 (100%)	26 (96%)	1 (4%)	34	60
10	J	35/35 (100%)	35 (100%)	0	100	100
11	K	59/59 (100%)	55 (93%)	4 (7%)	16	30
12	L	124/124 (100%)	119 (96%)	5 (4%)	31	56
13	1	158/158 (100%)	155 (98%)	3 (2%)	57	80
14	2	167/167 (100%)	157 (94%)	10 (6%)	19	37
15	3	171/172 (99%)	165 (96%)	6 (4%)	36	62
16	4	164/164 (100%)	158 (96%)	6 (4%)	34	60
17	N	82/82 (100%)	75 (92%)	7 (8%)	10	21
All	All	2716/2718 (100%)	2628 (97%)	88 (3%)	42	65

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

Mol	Chain	Res	Type
13	1	131	LEU
15	3	108	PHE
14	2	65	PRO
14	2	192	ASP
16	4	53	LYS

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

Mol	Chain	Res	Type
7	G	95	GLN

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 monosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 243 ligands modelled in this entry, 2 are monoatomic - leaving 241 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
19	CLA	4	617	-	65,73,73	1.36	7 (10%)	76,113,113	1.94	17 (22%)
19	CLA	A	1125	-	65,73,73	1.36	7 (10%)	76,113,113	1.96	16 (21%)
19	CLA	2	606	-	50,58,73	1.55	7 (14%)	58,95,113	2.33	17 (29%)
22	BCR	A	4003	-	41,41,41	1.83	4 (9%)	56,56,56	4.20	16 (28%)
19	CLA	A	1132	-	65,73,73	1.41	8 (12%)	76,113,113	2.03	18 (23%)
19	CLA	A	1124	33	55,63,73	1.47	8 (14%)	64,101,113	2.20	18 (28%)
19	CLA	B	1222	33	65,73,73	1.36	7 (10%)	76,113,113	2.13	16 (21%)
19	CLA	B	1224	-	65,73,73	1.38	7 (10%)	76,113,113	1.95	18 (23%)
19	CLA	2	603	-	65,73,73	1.38	8 (12%)	76,113,113	2.00	17 (22%)
27	DGD	F	5005	-	58,58,67	1.05	5 (8%)	72,72,81	1.17	5 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#|Z| > 2	Counts	RMSZ	#|Z| > 2
19	CLA	B	1211	-	65,73,73	1.34	6 (9%)	76,113,113	2.09	21 (27%)
25	LMG	F	5002	-	47,47,55	0.98	3 (6%)	55,55,63	1.22	4 (7%)
19	CLA	4	609	16	50,58,73	1.54	8 (16%)	58,95,113	2.28	16 (27%)
19	CLA	B	1210	-	65,73,73	1.33	7 (10%)	76,113,113	2.11	20 (26%)
19	CLA	B	1209	-	46,54,73	1.60	7 (15%)	53,90,113	2.20	14 (26%)
19	CLA	A	1102	-	65,73,73	1.34	8 (12%)	76,113,113	2.01	16 (21%)
22	BCR	B	4010	-	41,41,41	1.86	4 (9%)	56,56,56	4.17	13 (23%)
19	CLA	B	1205	-	65,73,73	1.40	7 (10%)	76,113,113	1.96	14 (18%)
19	CLA	2	607	-	60,68,73	1.42	8 (13%)	70,107,113	2.07	18 (25%)
23	LHG	1	801	-	48,48,48	0.40	0	51,54,54	1.14	4 (7%)
27	DGD	4	802	-	52,52,67	0.90	2 (3%)	66,66,81	1.02	2 (3%)
25	LMG	A	5006	-	50,50,55	1.06	5 (10%)	58,58,63	1.22	5 (8%)
18	CL0	A	1011	-	65,73,73	2.20	17 (26%)	76,113,113	2.43	21 (27%)
19	CLA	G	1602	7	46,54,73	1.59	8 (17%)	53,90,113	2.17	16 (30%)
19	CLA	K	1403	11	48,56,73	1.60	9 (18%)	55,92,113	2.35	17 (30%)
29	CHL	2	611	-	48,56,74	1.17	5 (10%)	51,92,114	1.39	10 (19%)
19	CLA	A	1116	-	56,64,73	1.49	7 (12%)	65,102,113	2.05	16 (24%)
19	CLA	G	1603	-	65,73,73	1.37	8 (12%)	76,113,113	2.02	16 (21%)
22	BCR	2	503	-	41,41,41	1.90	4 (9%)	56,56,56	4.98	24 (42%)
19	CLA	A	1126	-	65,73,73	1.39	7 (10%)	76,113,113	1.97	15 (19%)
25	LMG	1	802	-	46,46,55	0.94	3 (6%)	54,54,63	1.10	3 (5%)
19	CLA	A	1130	-	55,63,73	1.46	7 (12%)	64,101,113	2.15	18 (28%)
19	CLA	3	612	15	50,58,73	1.53	8 (16%)	58,95,113	2.28	15 (25%)
19	CLA	B	1207	-	65,73,73	1.39	8 (12%)	76,113,113	1.99	17 (22%)
23	LHG	B	5001	-	20,20,48	0.62	0	23,26,54	1.60	3 (13%)
19	CLA	A	1115	-	65,73,73	1.36	7 (10%)	76,113,113	1.96	13 (17%)
24	LMT	J	5003	-	26,26,36	1.34	5 (19%)	37,37,47	1.14	3 (8%)
19	CLA	A	1111	-	65,73,73	1.34	7 (10%)	76,113,113	2.05	17 (22%)
19	CLA	B	1226	-	65,73,73	1.37	8 (12%)	76,113,113	2.09	18 (23%)
22	BCR	F	4016	-	41,41,41	1.84	5 (12%)	56,56,56	4.19	12 (21%)
19	CLA	B	1218	-	65,73,73	1.39	9 (13%)	76,113,113	2.01	19 (25%)
19	CLA	3	610	15	65,73,73	1.34	8 (12%)	76,113,113	1.97	17 (22%)
19	CLA	A	1013	-	65,73,73	1.36	7 (10%)	76,113,113	1.87	18 (23%)
24	LMT	A	5004	-	36,36,36	1.19	6 (16%)	47,47,47	1.21	4 (8%)
29	CHL	2	615	-	56,64,74	0.93	3 (5%)	61,102,114	1.54	11 (18%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#|Z| > 2	Counts	RMSZ	#|Z| > 2
19	CLA	A	1139	-	65,73,73	1.37	7 (10%)	76,113,113	2.08	21 (27%)
22	BCR	L	4020	-	41,41,41	1.87	4 (9%)	56,56,56	4.27	17 (30%)
19	CLA	2	604	-	65,73,73	1.36	7 (10%)	76,113,113	2.08	19 (25%)
25	LMG	2	806	-	13,13,55	0.53	0	18,18,63	0.55	0
19	CLA	B	1234	-	55,63,73	1.50	8 (14%)	64,101,113	2.10	17 (26%)
19	CLA	B	1022	-	65,73,73	1.40	7 (10%)	76,113,113	1.96	16 (21%)
29	CHL	1	612	-	61,69,74	0.94	3 (4%)	67,108,114	1.27	11 (16%)
19	CLA	2	602	-	52,60,73	1.55	8 (15%)	60,97,113	2.10	18 (30%)
28	LUT	1	501	-	42,43,43	2.35	1 (2%)	51,60,60	1.81	10 (19%)
21	SF4	A	3001	1,2	0,12,12	-	-	-		
29	CHL	3	604	-	66,74,74	0.89	4 (6%)	73,114,114	1.41	10 (13%)
19	CLA	A	1012	-	65,73,73	1.41	7 (10%)	76,113,113	2.10	16 (21%)
19	CLA	B	1227	-	65,73,73	1.38	7 (10%)	76,113,113	1.98	14 (18%)
19	CLA	1	606	-	50,58,73	1.54	8 (16%)	58,95,113	2.23	18 (31%)
19	CLA	B	1223	-	65,73,73	1.38	7 (10%)	76,113,113	1.96	17 (22%)
19	CLA	L	1501	-	50,58,73	1.52	7 (14%)	58,95,113	2.32	19 (32%)
19	CLA	A	1127	-	65,73,73	1.36	8 (12%)	76,113,113	2.00	16 (21%)
19	CLA	L	1502	-	60,68,73	1.41	8 (13%)	70,107,113	2.05	17 (24%)
19	CLA	B	1237	-	65,73,73	1.35	7 (10%)	76,113,113	1.98	16 (21%)
23	LHG	A	5001	-	39,39,48	0.44	0	42,45,54	1.12	3 (7%)
19	CLA	3	606	-	50,58,73	1.56	8 (16%)	58,95,113	2.26	18 (31%)
27	DGD	G	5003	-	48,48,67	0.85	2 (4%)	62,62,81	1.14	3 (4%)
19	CLA	4	606	-	50,58,73	1.56	7 (14%)	58,95,113	2.17	16 (27%)
19	CLA	B	1235	-	65,73,73	1.33	8 (12%)	76,113,113	1.99	17 (22%)
19	CLA	3	602	-	52,60,73	1.53	8 (15%)	60,97,113	2.10	18 (30%)
19	CLA	J	1901	33	50,58,73	1.54	9 (18%)	58,95,113	2.12	16 (27%)
19	CLA	B	1215	-	65,73,73	1.35	7 (10%)	76,113,113	2.17	18 (23%)
27	DGD	4	801	-	52,52,67	0.95	4 (7%)	66,66,81	1.30	8 (12%)
20	PQN	A	2001	-	34,34,34	0.32	0	42,45,45	1.24	4 (9%)
19	CLA	B	1201	-	65,73,73	1.36	8 (12%)	76,113,113	2.05	18 (23%)
24	LMT	G	5005	-	32,32,36	1.29	6 (18%)	43,43,47	1.13	5 (11%)
25	LMG	F	5006	-	13,13,55	0.53	0	18,18,63	0.75	0
22	BCR	K	4001	-	41,41,41	1.85	4 (9%)	56,56,56	4.37	14 (25%)
19	CLA	A	1122	-	65,73,73	1.36	8 (12%)	76,113,113	1.94	16 (21%)
19	CLA	A	1140	-	65,73,73	1.37	7 (10%)	76,113,113	1.88	16 (21%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\lvert Z\rvert > 2$	Counts	RMSZ	$\#\lvert Z\rvert > 2$
19	CLA	A	1104	1	65,73,73	1.36	7 (10%)	76,113,113	2.02	18 (23%)
22	BCR	A	4011	-	41,41,41	1.83	4 (9%)	56,56,56	4.29	17 (30%)
25	LMG	2	802	-	25,25,55	0.58	0	33,33,63	1.22	3 (9%)
31	C7Z	4	505	-	43,43,43	5.44	17 (39%)	58,60,60	5.32	31 (53%)
19	CLA	A	1106	1	65,73,73	1.36	7 (10%)	76,113,113	2.02	16 (21%)
25	LMG	G	5002	-	50,50,55	1.05	5 (10%)	58,58,63	1.18	3 (5%)
22	BCR	3	503	-	41,41,41	1.86	4 (9%)	56,56,56	4.39	16 (28%)
25	LMG	F	5001	-	30,30,55	0.54	0	38,38,63	1.16	2 (5%)
22	BCR	1	503	-	41,41,41	1.86	4 (9%)	56,56,56	4.23	17 (30%)
29	CHL	4	615	-	43,51,74	1.06	2 (4%)	45,86,114	1.52	10 (22%)
25	LMG	B	5003	-	35,35,55	0.74	1 (2%)	43,43,63	1.17	5 (11%)
23	LHG	2	801	-	34,34,48	0.49	0	37,40,54	1.18	4 (10%)
19	CLA	B	1236	-	50,58,73	1.56	7 (14%)	58,95,113	2.24	17 (29%)
19	CLA	A	1107	1	65,73,73	1.36	6 (9%)	76,113,113	2.03	20 (26%)
19	CLA	1	611	-	65,73,73	1.34	7 (10%)	76,113,113	1.98	16 (21%)
22	BCR	B	4004	-	41,41,41	1.97	4 (9%)	56,56,56	5.07	22 (39%)
19	CLA	1	604	-	65,73,73	1.38	8 (12%)	76,113,113	1.94	18 (23%)
19	CLA	B	1219	-	65,73,73	1.36	7 (10%)	76,113,113	2.01	18 (23%)
19	CLA	B	1221	-	65,73,73	1.35	7 (10%)	76,113,113	2.06	16 (21%)
19	CLA	A	1133	-	65,73,73	1.35	7 (10%)	76,113,113	1.99	18 (23%)
22	BCR	I	4018	-	41,41,41	1.81	5 (12%)	56,56,56	4.24	21 (37%)
19	CLA	3	614	-	42,50,73	1.68	9 (21%)	48,85,113	2.19	16 (33%)
28	LUT	3	502	-	42,43,43	2.33	1 (2%)	51,60,60	1.99	13 (25%)
19	CLA	B	1206	-	65,73,73	1.34	8 (12%)	76,113,113	2.02	14 (18%)
19	CLA	B	1232	-	55,63,73	1.52	8 (14%)	64,101,113	2.17	18 (28%)
24	LMT	B	5006	-	33,33,36	1.23	5 (15%)	44,44,47	1.04	4 (9%)
22	BCR	J	4012	-	41,41,41	1.83	4 (9%)	56,56,56	4.23	17 (30%)
19	CLA	A	1108	-	50,58,73	1.57	7 (14%)	58,95,113	2.19	19 (32%)
19	CLA	G	1701	-	60,68,73	1.42	8 (13%)	70,107,113	2.04	15 (21%)
27	DGD	3	803	-	52,52,67	0.86	3 (5%)	66,66,81	1.11	3 (4%)
25	LMG	G	5001	-	49,49,55	0.99	4 (8%)	57,57,63	1.25	4 (7%)
29	CHL	4	613	-	61,69,74	1.00	3 (4%)	67,108,114	1.27	10 (14%)
19	CLA	A	1119	-	65,73,73	1.36	8 (12%)	76,113,113	1.94	15 (19%)
22	BCR	1	504	-	41,41,41	1.89	4 (9%)	56,56,56	4.63	22 (39%)
19	CLA	1	608	-	46,54,73	1.64	8 (17%)	53,90,113	2.27	13 (24%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#|Z| > 2	Counts	RMSZ	#|Z| > 2
19	CLA	B	1203	2	65,73,73	1.36	7 (10%)	76,113,113	1.87	17 (22%)
19	CLA	F	1302	6	65,73,73	1.34	7 (10%)	76,113,113	2.01	15 (19%)
19	CLA	B	1212	-	55,63,73	1.48	8 (14%)	64,101,113	2.21	19 (29%)
19	CLA	4	605	-	60,68,73	1.48	8 (13%)	70,107,113	2.05	20 (28%)
28	LUT	3	501	-	42,43,43	2.37	1 (2%)	51,60,60	2.04	14 (27%)
19	CLA	A	1120	-	60,68,73	1.40	7 (11%)	70,107,113	2.07	16 (22%)
19	CLA	A	1123	-	65,73,73	1.37	8 (12%)	76,113,113	2.01	16 (21%)
19	CLA	1	613	-	45,53,73	1.64	8 (17%)	52,89,113	2.06	14 (26%)
19	CLA	3	608	-	48,56,73	1.60	9 (18%)	55,92,113	2.21	16 (29%)
19	CLA	1	602	13	46,54,73	1.61	8 (17%)	53,90,113	2.16	13 (24%)
25	LMG	2	805	-	13,13,55	0.53	0	18,18,63	0.68	0
19	CLA	3	601	15	55,63,73	1.46	6 (10%)	64,101,113	2.14	17 (26%)
25	LMG	F	5003	-	36,36,55	0.71	1 (2%)	44,44,63	1.04	2 (4%)
22	BCR	F	4014	-	41,41,41	1.85	4 (9%)	56,56,56	4.28	13 (23%)
19	CLA	B	1240	-	65,73,73	1.36	7 (10%)	76,113,113	2.07	19 (25%)
19	CLA	2	605	-	65,73,73	1.36	7 (10%)	76,113,113	2.11	17 (22%)
30	XAT	4	502	-	39,47,47	0.80	1 (2%)	54,74,74	1.75	15 (27%)
19	CLA	4	602	-	50,58,73	1.53	8 (16%)	58,95,113	2.33	18 (31%)
22	BCR	B	4005	-	41,41,41	1.85	5 (12%)	56,56,56	4.27	16 (28%)
32	FES	N	101	17	0,4,4	-	-	-		
28	LUT	4	501	-	42,43,43	2.36	1 (2%)	51,60,60	2.02	16 (31%)
22	BCR	G	4021	-	41,41,41	1.89	4 (9%)	56,56,56	4.36	18 (32%)
29	CHL	3	607	-	51,59,74	1.00	3 (5%)	55,96,114	1.30	7 (12%)
19	CLA	B	1239	-	65,73,73	1.40	9 (13%)	76,113,113	1.99	15 (19%)
22	BCR	A	4017	-	41,41,41	1.86	5 (12%)	56,56,56	4.83	18 (32%)
25	LMG	2	804	-	30,30,55	0.52	0	38,38,63	1.20	3 (7%)
29	CHL	1	609	13	56,64,74	1.06	6 (10%)	61,102,114	1.31	9 (14%)
23	LHG	A	5002	-	48,48,48	0.41	0	51,54,54	1.10	3 (5%)
19	CLA	A	1128	-	65,73,73	1.37	7 (10%)	76,113,113	2.04	17 (22%)
19	CLA	A	1136	-	65,73,73	1.33	8 (12%)	76,113,113	2.02	16 (21%)
22	BCR	G	4011	-	41,41,41	1.85	4 (9%)	56,56,56	4.54	20 (35%)
19	CLA	A	1114	-	46,54,73	1.63	7 (15%)	53,90,113	2.18	14 (26%)
19	CLA	B	1214	-	65,73,73	1.37	7 (10%)	76,113,113	1.98	16 (21%)
19	CLA	A	1103	-	65,73,73	1.34	7 (10%)	76,113,113	2.05	19 (25%)
19	CLA	A	1129	-	65,73,73	1.37	8 (12%)	76,113,113	1.98	13 (17%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#|Z| > 2	Counts	RMSZ	#|Z| > 2
21	SF4	C	3003	3	0,12,12	-	-	-		
29	CHL	2	609	14	66,74,74	0.97	4 (6%)	73,114,114	1.31	10 (13%)
19	CLA	A	1109	-	65,73,73	1.36	8 (12%)	76,113,113	1.98	16 (21%)
19	CLA	3	605	15	55,63,73	1.53	9 (16%)	64,101,113	2.10	18 (28%)
19	CLA	B	1228	-	60,68,73	1.41	7 (11%)	70,107,113	2.04	14 (20%)
19	CLA	K	1402	-	60,68,73	1.44	9 (15%)	70,107,113	2.09	17 (24%)
19	CLA	B	1230	-	58,66,73	1.44	7 (12%)	67,104,113	2.14	18 (26%)
19	CLA	4	612	16	65,73,73	1.37	7 (10%)	76,113,113	1.98	18 (23%)
25	LMG	3	802	-	30,30,55	0.57	1 (3%)	38,38,63	1.16	4 (10%)
29	CHL	4	611	-	51,59,74	1.12	4 (7%)	55,96,114	1.74	13 (23%)
22	BCR	3	506	-	41,41,41	1.86	4 (9%)	56,56,56	4.43	16 (28%)
19	CLA	B	1208	-	60,68,73	1.42	7 (11%)	70,107,113	2.00	17 (24%)
19	CLA	A	1105	-	60,68,73	1.43	6 (10%)	70,107,113	2.07	16 (22%)
19	CLA	B	1023	-	65,73,73	1.40	7 (10%)	76,113,113	1.97	18 (23%)
19	CLA	2	601	-	60,68,73	1.42	9 (15%)	70,107,113	2.00	16 (22%)
22	BCR	I	4020	-	41,41,41	1.89	5 (12%)	56,56,56	4.45	15 (26%)
23	LHG	3	801	-	16,16,48	0.87	1 (6%)	17,20,54	0.67	0
19	CLA	B	1021	-	65,73,73	1.38	7 (10%)	76,113,113	2.01	18 (23%)
19	CLA	A	1110	-	55,63,73	1.48	8 (14%)	64,101,113	2.10	18 (28%)
19	CLA	4	604	-	60,68,73	1.41	7 (11%)	70,107,113	2.18	18 (25%)
22	BCR	B	4006	-	41,41,41	1.88	4 (9%)	56,56,56	4.18	25 (44%)
19	CLA	B	1220	-	55,63,73	1.51	7 (12%)	64,101,113	2.00	17 (26%)
22	BCR	A	4007	-	41,41,41	1.84	4 (9%)	56,56,56	4.41	19 (33%)
24	LMT	G	5004	-	36,36,36	1.21	6 (16%)	47,47,47	1.20	3 (6%)
19	CLA	B	1238	-	65,73,73	1.37	7 (10%)	76,113,113	2.06	18 (23%)
19	CLA	1	614	13	60,68,73	1.42	9 (15%)	70,107,113	2.11	19 (27%)
25	LMG	F	5004	-	34,34,55	0.46	0	42,42,63	1.13	2 (4%)
19	CLA	3	613	-	46,54,73	1.64	8 (17%)	53,90,113	2.18	13 (24%)
22	BCR	K	4002	-	41,41,41	1.85	4 (9%)	56,56,56	4.36	17 (30%)
28	LUT	1	502	-	42,43,43	2.24	1 (2%)	51,60,60	1.99	14 (27%)
19	CLA	F	1301	-	65,73,73	1.36	7 (10%)	76,113,113	1.99	16 (21%)
20	PQN	B	2002	-	34,34,34	0.32	0	42,45,45	1.18	2 (4%)
19	CLA	A	1131	-	65,73,73	1.40	7 (10%)	76,113,113	1.97	15 (19%)
25	LMG	B	5007	-	34,34,55	0.49	0	42,42,63	1.18	3 (7%)
19	CLA	A	1121	-	60,68,73	1.44	8 (13%)	70,107,113	1.99	18 (25%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
19	CLA	B	1204	-	65,73,73	1.40	7 (10%)	76,113,113	1.84	12 (15%)
25	LMG	2	803	-	36,36,55	0.68	2 (5%)	44,44,63	1.06	3 (6%)
29	CHL	2	613	-	46,54,74	1.08	3 (6%)	49,90,114	1.37	8 (16%)
19	CLA	B	1216	-	65,73,73	1.35	8 (12%)	76,113,113	1.95	17 (22%)
19	CLA	2	612	-	55,63,73	1.49	7 (12%)	64,101,113	2.12	14 (21%)
19	CLA	A	1112	-	65,73,73	1.36	8 (12%)	76,113,113	1.98	19 (25%)
19	CLA	A	1135	-	51,59,73	1.52	8 (15%)	59,96,113	2.25	18 (30%)
19	CLA	3	603	-	55,63,73	1.46	8 (14%)	64,101,113	2.12	17 (26%)
19	CLA	K	1404	-	46,54,73	1.65	9 (19%)	53,90,113	1.97	13 (24%)
19	CLA	1	603	-	55,63,73	1.50	8 (14%)	64,101,113	2.23	18 (28%)
19	CLA	B	1231	-	60,68,73	1.43	7 (11%)	70,107,113	2.00	16 (22%)
29	CHL	1	610	13	47,55,74	1.10	4 (8%)	50,91,114	1.54	9 (18%)
22	BCR	B	4009	-	41,41,41	1.83	4 (9%)	56,56,56	4.23	16 (28%)
19	CLA	4	603	-	65,73,73	1.38	7 (10%)	76,113,113	1.91	17 (22%)
22	BCR	A	4008	-	41,41,41	1.85	4 (9%)	56,56,56	4.13	17 (30%)
19	CLA	1	607	-	46,54,73	1.59	7 (15%)	53,90,113	2.12	13 (24%)
29	CHL	3	611	-	47,55,74	1.17	5 (10%)	50,91,114	1.50	9 (18%)
19	CLA	G	1601	-	55,63,73	1.48	8 (14%)	64,101,113	2.14	18 (28%)
23	LHG	B	5002	-	48,48,48	0.39	0	51,54,54	1.08	3 (5%)
29	CHL	4	610	-	47,55,74	1.04	3 (6%)	50,91,114	1.44	8 (16%)
19	CLA	B	1213	-	60,68,73	1.45	7 (11%)	70,107,113	2.06	17 (24%)
19	CLA	1	605	-	65,73,73	1.36	7 (10%)	76,113,113	2.08	17 (22%)
19	CLA	A	1118	-	50,58,73	1.56	8 (16%)	58,95,113	2.30	16 (27%)
22	BCR	A	4002	-	41,41,41	1.84	4 (9%)	56,56,56	4.24	22 (39%)
22	BCR	L	4019	-	41,41,41	1.85	4 (9%)	56,56,56	4.28	16 (28%)
19	CLA	B	1229	-	65,73,73	1.37	7 (10%)	76,113,113	2.01	15 (19%)
21	SF4	C	3002	3	0,12,12	-	-	-		
28	LUT	J	4013	-	42,43,43	2.27	1 (2%)	51,60,60	1.98	12 (23%)
23	LHG	2	807	-	32,32,48	0.45	0	35,38,54	1.22	2 (5%)
28	LUT	2	501	-	42,43,43	2.39	1 (2%)	51,60,60	2.20	15 (29%)
19	CLA	4	607	-	60,68,73	1.43	8 (13%)	70,107,113	1.88	15 (21%)
19	CLA	K	1401	-	45,53,73	1.61	10 (22%)	52,89,113	2.15	13 (25%)
19	CLA	4	608	-	46,54,73	1.61	8 (17%)	53,90,113	2.05	12 (22%)
27	DGD	1	803	-	42,42,67	0.87	1 (2%)	56,56,81	1.10	3 (5%)
29	CHL	2	610	-	56,64,74	0.88	2 (3%)	61,102,114	1.43	15 (24%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#|Z| > 2	Counts	RMSZ	#|Z| > 2
19	CLA	4	601	16	60,68,73	1.43	7 (11%)	70,107,113	2.08	17 (24%)
19	CLA	B	1217	-	46,54,73	1.65	8 (17%)	53,90,113	2.16	15 (28%)
19	CLA	A	1117	-	65,73,73	1.35	7 (10%)	76,113,113	1.96	16 (21%)
19	CLA	B	1225	-	65,73,73	1.38	8 (12%)	76,113,113	1.89	14 (18%)
19	CLA	2	608	-	50,58,73	1.54	8 (16%)	58,95,113	2.20	18 (31%)
25	LMG	B	5004	-	33,33,55	0.55	1 (3%)	41,41,63	1.23	4 (9%)
25	LMG	G	5006	-	25,25,55	0.56	0	33,33,63	1.32	2 (6%)
19	CLA	A	1101	-	65,73,73	1.36	8 (12%)	76,113,113	2.19	19 (25%)
19	CLA	B	1202	-	65,73,73	1.36	7 (10%)	76,113,113	1.84	18 (23%)
19	CLA	L	1503	33	50,58,73	1.54	9 (18%)	58,95,113	2.27	19 (32%)
19	CLA	A	1141	-	60,68,73	1.43	7 (11%)	70,107,113	2.16	18 (25%)
27	DGD	B	5005	-	62,62,67	1.10	6 (9%)	76,76,81	1.09	4 (5%)
19	CLA	1	601	-	65,73,73	1.38	7 (10%)	76,113,113	1.98	17 (22%)
30	XAT	2	502	-	39,47,47	0.75	1 (2%)	54,74,74	2.42	15 (27%)
24	LMT	B	5008	-	32,32,36	1.27	5 (15%)	43,43,47	0.96	2 (4%)
19	CLA	A	1138	-	65,73,73	1.35	8 (12%)	76,113,113	1.88	16 (21%)
19	CLA	A	1134	1	55,63,73	1.49	8 (14%)	64,101,113	2.18	16 (25%)
19	CLA	A	1113	-	45,53,73	1.65	8 (17%)	52,89,113	2.19	15 (28%)
19	CLA	A	1137	-	65,73,73	1.39	8 (12%)	76,113,113	1.92	16 (21%)
19	CLA	3	617	-	60,68,73	1.41	6 (10%)	70,107,113	1.98	18 (25%)
27	DGD	J	5001	-	59,59,67	1.04	5 (8%)	73,73,81	1.00	2 (2%)

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
19	CLA	4	617	-	1/1/15/20	17/37/115/115	-
19	CLA	A	1125	-	1/1/15/20	17/37/115/115	-
19	CLA	2	606	-	1/1/12/20	6/19/97/115	-
22	BCR	A	4003	-	-	8/29/63/63	0/2/2/2
19	CLA	A	1132	-	1/1/15/20	14/37/115/115	-
19	CLA	A	1124	33	1/1/13/20	8/25/103/115	-
19	CLA	B	1222	33	1/1/15/20	18/37/115/115	-
19	CLA	B	1224	-	1/1/15/20	15/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
19	CLA	2	603	-	1/1/15/20	17/37/115/115	-
27	DGD	F	5005	-	-	20/46/86/95	0/2/2/2
19	CLA	B	1211	-	1/1/15/20	19/37/115/115	-
25	LMG	F	5002	-	-	10/42/62/70	0/1/1/1
19	CLA	4	609	16	1/1/12/20	10/19/97/115	-
19	CLA	B	1210	-	1/1/15/20	16/37/115/115	-
19	CLA	B	1209	-	1/1/11/20	6/15/93/115	-
19	CLA	A	1102	-	1/1/15/20	25/37/115/115	-
22	BCR	B	4010	-	-	12/29/63/63	0/2/2/2
19	CLA	B	1205	-	1/1/15/20	10/37/115/115	-
19	CLA	2	607	-	1/1/14/20	14/31/109/115	-
23	LHG	1	801	-	-	30/53/53/53	-
27	DGD	4	802	-	-	16/40/80/95	0/2/2/2
25	LMG	A	5006	-	-	16/45/65/70	0/1/1/1
18	CL0	A	1011	-	3/3/20/25	8/37/135/135	-
19	CLA	G	1602	7	1/1/11/20	8/15/93/115	-
19	CLA	K	1403	11	1/1/11/20	9/17/95/115	-
29	CHL	2	611	-	3/3/16/26	5/18/116/137	-
19	CLA	A	1116	-	1/1/13/20	15/27/105/115	-
19	CLA	G	1603	-	1/1/15/20	17/37/115/115	-
22	BCR	2	503	-	-	14/29/63/63	0/2/2/2
19	CLA	A	1126	-	1/1/15/20	21/37/115/115	-
25	LMG	1	802	-	-	13/41/61/70	0/1/1/1
19	CLA	A	1130	-	1/1/13/20	14/25/103/115	-
19	CLA	3	612	15	1/1/12/20	9/19/97/115	-
19	CLA	B	1207	-	1/1/15/20	19/37/115/115	-
23	LHG	B	5001	-	-	12/23/23/53	-
19	CLA	A	1115	-	1/1/15/20	23/37/115/115	-
24	LMT	J	5003	-	-	6/11/51/61	0/2/2/2
19	CLA	A	1111	-	1/1/15/20	17/37/115/115	-
19	CLA	B	1226	-	1/1/15/20	24/37/115/115	-
22	BCR	F	4016	-	-	14/29/63/63	0/2/2/2
19	CLA	B	1218	-	1/1/15/20	13/37/115/115	-
19	CLA	3	610	15	1/1/15/20	20/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
19	CLA	A	1013	-	1/1/15/20	22/37/115/115	-
24	LMT	A	5004	-	-	7/21/61/61	0/2/2/2
29	CHL	2	615	-	4/4/18/26	8/27/125/137	-
19	CLA	A	1139	-	1/1/15/20	17/37/115/115	-
22	BCR	L	4020	-	-	9/29/63/63	0/2/2/2
19	CLA	2	604	-	1/1/15/20	15/37/115/115	-
25	LMG	2	806	-	-	1/4/24/70	0/1/1/1
19	CLA	B	1234	-	1/1/13/20	12/25/103/115	-
19	CLA	B	1022	-	1/1/15/20	10/37/115/115	-
29	CHL	1	612	-	4/4/19/26	6/33/131/137	-
19	CLA	2	602	-	1/1/12/20	8/22/100/115	-
28	LUT	1	501	-	-	2/29/67/67	0/2/2/2
29	CHL	3	604	-	4/4/20/26	11/39/137/137	-
21	SF4	A	3001	1,2	-	-	0/6/5/5
19	CLA	A	1012	-	1/1/15/20	19/37/115/115	-
19	CLA	B	1227	-	1/1/15/20	14/37/115/115	-
19	CLA	1	606	-	1/1/12/20	7/19/97/115	-
19	CLA	B	1223	-	1/1/15/20	16/37/115/115	-
19	CLA	L	1501	-	1/1/12/20	6/19/97/115	-
19	CLA	A	1127	-	1/1/15/20	19/37/115/115	-
19	CLA	L	1502	-	1/1/14/20	15/31/109/115	-
19	CLA	B	1237	-	1/1/15/20	20/37/115/115	-
23	LHG	A	5001	-	-	24/44/44/53	-
19	CLA	3	606	-	1/1/12/20	11/19/97/115	-
27	DGD	G	5003	-	-	11/36/76/95	0/2/2/2
19	CLA	4	606	-	1/1/12/20	7/19/97/115	-
19	CLA	B	1235	-	1/1/15/20	17/37/115/115	-
19	CLA	3	602	-	1/1/12/20	9/22/100/115	-
19	CLA	J	1901	33	1/1/12/20	7/19/97/115	-
19	CLA	B	1215	-	1/1/15/20	18/37/115/115	-
27	DGD	4	801	-	-	17/40/80/95	0/2/2/2
20	PQN	A	2001	-	-	4/23/43/43	0/2/2/2
19	CLA	B	1201	-	1/1/15/20	18/37/115/115	-
24	LMT	G	5005	-	-	7/17/57/61	0/2/2/2
25	LMG	F	5006	-	-	1/4/24/70	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	BCR	K	4001	-	-	9/29/63/63	0/2/2/2
19	CLA	A	1122	-	1/1/15/20	17/37/115/115	-
19	CLA	A	1140	-	1/1/15/20	9/37/115/115	-
19	CLA	A	1104	1	1/1/15/20	17/37/115/115	-
22	BCR	A	4011	-	-	11/29/63/63	0/2/2/2
25	LMG	2	802	-	-	8/20/40/70	0/1/1/1
31	C7Z	4	505	-	-	17/29/67/67	0/2/2/2
19	CLA	A	1106	1	1/1/15/20	17/37/115/115	-
25	LMG	G	5002	-	-	20/45/65/70	0/1/1/1
22	BCR	3	503	-	-	12/29/63/63	0/2/2/2
25	LMG	F	5001	-	-	9/25/45/70	0/1/1/1
22	BCR	1	503	-	-	17/29/63/63	0/2/2/2
29	CHL	4	615	-	3/3/15/26	0/12/110/137	-
25	LMG	B	5003	-	-	9/30/50/70	0/1/1/1
23	LHG	2	801	-	-	21/39/39/53	-
19	CLA	B	1236	-	1/1/12/20	10/19/97/115	-
19	CLA	A	1107	1	1/1/15/20	18/37/115/115	-
19	CLA	1	611	-	1/1/15/20	14/37/115/115	-
22	BCR	B	4004	-	-	8/29/63/63	0/2/2/2
19	CLA	1	604	-	1/1/15/20	16/37/115/115	-
19	CLA	B	1219	-	1/1/15/20	20/37/115/115	-
19	CLA	B	1221	-	1/1/15/20	19/37/115/115	-
19	CLA	A	1133	-	1/1/15/20	21/37/115/115	-
22	BCR	I	4018	-	-	13/29/63/63	0/2/2/2
19	CLA	3	614	-	1/1/10/20	3/10/88/115	-
28	LUT	3	502	-	1/1/12/27	8/29/67/67	0/2/2/2
19	CLA	B	1206	-	1/1/15/20	18/37/115/115	-
19	CLA	B	1232	-	1/1/13/20	13/25/103/115	-
24	LMT	B	5006	-	-	9/18/58/61	0/2/2/2
22	BCR	J	4012	-	-	11/29/63/63	0/2/2/2
19	CLA	A	1108	-	1/1/12/20	7/19/97/115	-
19	CLA	G	1701	-	1/1/14/20	12/31/109/115	-
29	CHL	4	613	-	4/4/19/26	8/33/131/137	-
25	LMG	G	5001	-	-	21/44/64/70	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
27	DGD	3	803	-	-	10/40/80/95	0/2/2/2
19	CLA	A	1119	-	1/1/15/20	14/37/115/115	-
22	BCR	1	504	-	-	14/29/63/63	0/2/2/2
19	CLA	1	608	-	1/1/11/20	7/15/93/115	-
19	CLA	B	1203	2	1/1/15/20	15/37/115/115	-
19	CLA	F	1302	6	1/1/15/20	19/37/115/115	-
19	CLA	B	1212	-	1/1/13/20	12/25/103/115	-
19	CLA	4	605	-	-	15/31/109/115	-
28	LUT	3	501	-	-	4/29/67/67	0/2/2/2
19	CLA	A	1120	-	1/1/14/20	12/31/109/115	-
19	CLA	A	1123	-	1/1/15/20	16/37/115/115	-
19	CLA	1	613	-	1/1/11/20	4/13/91/115	-
19	CLA	3	608	-	1/1/11/20	6/17/95/115	-
19	CLA	1	602	13	1/1/11/20	6/15/93/115	-
25	LMG	2	805	-	-	2/4/24/70	0/1/1/1
19	CLA	3	601	15	1/1/13/20	10/25/103/115	-
25	LMG	F	5003	-	-	13/31/51/70	0/1/1/1
22	BCR	F	4014	-	-	10/29/63/63	0/2/2/2
19	CLA	B	1240	-	1/1/15/20	18/37/115/115	-
19	CLA	2	605	-	1/1/15/20	20/37/115/115	-
30	XAT	4	502	-	2/2/12/26	6/31/93/93	0/4/4/4
19	CLA	4	602	-	1/1/12/20	8/19/97/115	-
22	BCR	B	4005	-	-	9/29/63/63	0/2/2/2
32	FES	N	101	17	-	-	0/1/1/1
28	LUT	4	501	-	-	5/29/67/67	0/2/2/2
29	CHL	3	607	-	3/3/17/26	6/21/119/137	-
22	BCR	G	4021	-	-	14/29/63/63	0/2/2/2
19	CLA	B	1239	-	1/1/15/20	19/37/115/115	-
22	BCR	A	4017	-	-	8/29/63/63	0/2/2/2
25	LMG	2	804	-	-	9/25/45/70	0/1/1/1
29	CHL	1	609	13	4/4/18/26	4/27/125/137	-
23	LHG	A	5002	-	-	39/53/53/53	-
19	CLA	A	1128	-	1/1/15/20	13/37/115/115	-
19	CLA	A	1136	-	1/1/15/20	19/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	BCR	G	4011	-	-	10/29/63/63	0/2/2/2
19	CLA	A	1114	-	1/1/11/20	9/15/93/115	-
19	CLA	B	1214	-	1/1/15/20	14/37/115/115	-
19	CLA	A	1103	-	1/1/15/20	26/37/115/115	-
19	CLA	A	1129	-	1/1/15/20	18/37/115/115	-
21	SF4	C	3003	3	-	-	0/6/5/5
29	CHL	2	609	14	4/4/20/26	8/39/137/137	-
19	CLA	A	1109	-	1/1/15/20	10/37/115/115	-
19	CLA	3	605	15	-	10/25/103/115	-
19	CLA	B	1228	-	1/1/14/20	14/31/109/115	-
19	CLA	K	1402	-	1/1/14/20	24/31/109/115	-
19	CLA	B	1230	-	1/1/13/20	11/29/107/115	-
19	CLA	4	612	16	1/1/15/20	14/37/115/115	-
29	CHL	4	611	-	3/3/17/26	0/21/119/137	-
25	LMG	3	802	-	-	9/25/45/70	0/1/1/1
22	BCR	3	506	-	-	14/29/63/63	0/2/2/2
19	CLA	B	1208	-	1/1/14/20	12/31/109/115	-
19	CLA	A	1105	-	1/1/14/20	18/31/109/115	-
19	CLA	B	1023	-	1/1/15/20	10/37/115/115	-
19	CLA	2	601	-	1/1/14/20	13/31/109/115	-
22	BCR	I	4020	-	-	11/29/63/63	0/2/2/2
23	LHG	3	801	-	-	7/19/19/53	-
19	CLA	B	1021	-	1/1/15/20	10/37/115/115	-
19	CLA	A	1110	-	1/1/13/20	7/25/103/115	-
19	CLA	4	604	-	1/1/14/20	13/31/109/115	-
22	BCR	B	4006	-	-	12/29/63/63	0/2/2/2
19	CLA	B	1220	-	1/1/13/20	9/25/103/115	-
22	BCR	A	4007	-	-	4/29/63/63	0/2/2/2
24	LMT	G	5004	-	-	11/21/61/61	0/2/2/2
19	CLA	B	1238	-	1/1/15/20	24/37/115/115	-
19	CLA	1	614	13	1/1/14/20	15/31/109/115	-
25	LMG	F	5004	-	-	9/29/49/70	0/1/1/1
19	CLA	3	613	-	1/1/11/20	6/15/93/115	-
22	BCR	K	4002	-	-	11/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
28	LUT	1	502	-	-	2/29/67/67	0/2/2/2
19	CLA	F	1301	-	1/1/15/20	18/37/115/115	-
20	PQN	B	2002	-	-	11/23/43/43	0/2/2/2
19	CLA	A	1131	-	1/1/15/20	14/37/115/115	-
25	LMG	B	5007	-	-	9/29/49/70	0/1/1/1
19	CLA	A	1121	-	1/1/14/20	13/31/109/115	-
19	CLA	B	1204	-	1/1/15/20	20/37/115/115	-
25	LMG	2	803	-	-	14/31/51/70	0/1/1/1
29	CHL	2	613	-	3/3/16/26	4/15/113/137	-
19	CLA	B	1216	-	1/1/15/20	16/37/115/115	-
19	CLA	2	612	-	1/1/13/20	11/25/103/115	-
19	CLA	A	1112	-	1/1/15/20	22/37/115/115	-
19	CLA	A	1135	-	1/1/12/20	10/21/99/115	-
19	CLA	3	603	-	1/1/13/20	13/25/103/115	-
19	CLA	K	1404	-	1/1/11/20	6/15/93/115	-
19	CLA	1	603	-	1/1/13/20	7/25/103/115	-
19	CLA	B	1231	-	1/1/14/20	11/31/109/115	-
29	CHL	1	610	13	3/3/16/26	2/17/115/137	-
22	BCR	B	4009	-	-	8/29/63/63	0/2/2/2
19	CLA	4	603	-	1/1/15/20	15/37/115/115	-
22	BCR	A	4008	-	-	13/29/63/63	0/2/2/2
19	CLA	1	607	-	1/1/11/20	4/15/93/115	-
29	CHL	3	611	-	3/3/16/26	1/17/115/137	-
19	CLA	G	1601	-	1/1/13/20	8/25/103/115	-
23	LHG	B	5002	-	-	31/53/53/53	-
19	CLA	B	1213	-	1/1/14/20	6/31/109/115	-
19	CLA	1	605	-	1/1/15/20	16/37/115/115	-
19	CLA	A	1118	-	1/1/12/20	4/19/97/115	-
29	CHL	4	610	-	3/3/16/26	7/17/115/137	-
22	BCR	A	4002	-	-	12/29/63/63	0/2/2/2
19	CLA	B	1229	-	1/1/15/20	13/37/115/115	-
28	LUT	J	4013	-	1/1/12/27	4/29/67/67	0/2/2/2
28	LUT	2	501	-	1/1/12/27	5/29/67/67	0/2/2/2
22	BCR	L	4019	-	-	12/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
23	LHG	2	807	-	-	19/37/37/53	-
19	CLA	4	607	-	1/1/14/20	16/31/109/115	-
21	SF4	C	3002	3	-	-	0/6/5/5
19	CLA	K	1401	-	1/1/11/20	6/13/91/115	-
19	CLA	4	608	-	1/1/11/20	8/15/93/115	-
29	CHL	2	610	-	4/4/18/26	3/27/125/137	-
27	DGD	1	803	-	-	12/30/70/95	0/2/2/2
19	CLA	4	601	16	1/1/14/20	16/31/109/115	-
19	CLA	B	1217	-	1/1/11/20	7/15/93/115	-
19	CLA	A	1117	-	1/1/15/20	19/37/115/115	-
19	CLA	B	1225	-	1/1/15/20	18/37/115/115	-
19	CLA	2	608	-	1/1/12/20	10/19/97/115	-
25	LMG	B	5004	-	-	16/28/48/70	0/1/1/1
25	LMG	G	5006	-	-	10/20/40/70	0/1/1/1
19	CLA	A	1101	-	1/1/15/20	21/37/115/115	-
19	CLA	B	1202	-	1/1/15/20	15/37/115/115	-
19	CLA	L	1503	33	1/1/12/20	6/19/97/115	-
19	CLA	A	1141	-	1/1/14/20	11/31/109/115	-
27	DGD	B	5005	-	-	25/50/90/95	0/2/2/2
19	CLA	1	601	-	1/1/15/20	15/37/115/115	-
30	XAT	2	502	-	1/1/12/26	5/31/93/93	0/4/4/4
24	LMT	B	5008	-	-	7/17/57/61	0/2/2/2
19	CLA	A	1138	-	1/1/15/20	14/37/115/115	-
19	CLA	A	1134	1	1/1/13/20	13/25/103/115	-
19	CLA	A	1113	-	1/1/11/20	7/13/91/115	-
19	CLA	A	1137	-	1/1/15/20	17/37/115/115	-
19	CLA	3	617	-	1/1/14/20	14/31/109/115	-
27	DGD	J	5001	-	-	12/47/87/95	0/2/2/2

The worst 5 of 1364 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	4	505	C7Z	C10-C9	14.87	1.55	1.35
31	4	505	C7Z	C34-C33	14.83	1.55	1.35
31	4	505	C7Z	C14-C13	14.73	1.55	1.35
31	4	505	C7Z	C30-C29	14.67	1.55	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	3	501	LUT	C24-C25	14.53	1.51	1.33

The worst 5 of 3279 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	B	4004	BCR	C11-C10-C9	19.37	154.96	127.31
22	A	4017	BCR	C16-C15-C14	18.15	160.66	123.47
22	1	504	BCR	C10-C11-C12	17.64	178.27	123.22
22	G	4021	BCR	C10-C11-C12	17.50	177.83	123.22
22	I	4018	BCR	C10-C11-C12	17.47	177.72	123.22

5 of 200 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
18	A	1011	CL0	NC
18	A	1011	CL0	NA
18	A	1011	CL0	ND
19	A	1012	CLA	ND
19	A	1013	CLA	ND

5 of 2925 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
19	A	1012	CLA	C2-C3-C5-C6
19	A	1012	CLA	C4-C3-C5-C6
19	A	1013	CLA	C2-C1-O2A-CGA
19	A	1013	CLA	C2-C3-C5-C6
19	A	1013	CLA	C4-C3-C5-C6

There are no ring outliers.

222 monomers are involved in 798 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
19	4	617	CLA	3	0
19	A	1125	CLA	4	0
19	2	606	CLA	5	0
22	A	4003	BCR	2	0
19	A	1132	CLA	2	0
19	A	1124	CLA	3	0
19	B	1222	CLA	9	0
19	B	1224	CLA	7	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
19	2	603	CLA	10	0
27	F	5005	DGD	7	0
19	B	1211	CLA	4	0
25	F	5002	LMG	8	0
19	4	609	CLA	3	0
19	B	1210	CLA	7	0
19	B	1209	CLA	3	0
19	A	1102	CLA	7	0
22	B	4010	BCR	1	0
19	B	1205	CLA	4	0
19	2	607	CLA	2	0
23	1	801	LHG	8	0
27	4	802	DGD	3	0
25	A	5006	LMG	5	0
18	A	1011	CL0	6	0
19	G	1602	CLA	3	0
19	K	1403	CLA	2	0
29	2	611	CHL	5	0
19	A	1116	CLA	9	0
19	G	1603	CLA	4	0
22	2	503	BCR	10	0
19	A	1126	CLA	7	0
25	1	802	LMG	3	0
19	A	1130	CLA	2	0
19	3	612	CLA	4	0
19	B	1207	CLA	10	0
23	B	5001	LHG	4	0
19	A	1115	CLA	9	0
19	A	1111	CLA	9	0
19	B	1226	CLA	5	0
22	F	4016	BCR	5	0
19	B	1218	CLA	5	0
19	3	610	CLA	6	0
19	A	1013	CLA	9	0
24	A	5004	LMT	3	0
29	2	615	CHL	5	0
19	A	1139	CLA	3	0
19	2	604	CLA	12	0
25	2	806	LMG	1	0
19	B	1234	CLA	7	0
19	B	1022	CLA	4	0
29	1	612	CHL	6	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
19	2	602	CLA	3	0
28	1	501	LUT	9	0
29	3	604	CHL	8	0
19	A	1012	CLA	8	0
19	B	1227	CLA	5	0
19	1	606	CLA	1	0
19	B	1223	CLA	5	0
19	L	1501	CLA	4	0
19	A	1127	CLA	1	0
19	L	1502	CLA	5	0
19	B	1237	CLA	7	0
23	A	5001	LHG	3	0
19	3	606	CLA	2	0
27	G	5003	DGD	4	0
19	4	606	CLA	3	0
19	B	1235	CLA	6	0
19	3	602	CLA	5	0
19	B	1215	CLA	2	0
27	4	801	DGD	3	0
19	B	1201	CLA	5	0
25	F	5006	LMG	1	0
22	K	4001	BCR	5	0
19	A	1122	CLA	6	0
19	A	1140	CLA	3	0
19	A	1104	CLA	4	0
22	A	4011	BCR	3	0
25	2	802	LMG	2	0
19	A	1106	CLA	6	0
25	G	5002	LMG	5	0
22	3	503	BCR	3	0
25	F	5001	LMG	1	0
22	1	503	BCR	6	0
29	4	615	CHL	3	0
25	B	5003	LMG	3	0
23	2	801	LHG	2	0
19	B	1236	CLA	1	0
19	A	1107	CLA	4	0
19	1	611	CLA	4	0
22	B	4004	BCR	4	0
19	1	604	CLA	8	0
19	B	1219	CLA	9	0
19	B	1221	CLA	4	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
19	A	1133	CLA	3	0
22	I	4018	BCR	3	0
19	3	614	CLA	2	0
28	3	502	LUT	2	0
19	B	1206	CLA	5	0
19	B	1232	CLA	3	0
24	B	5006	LMT	3	0
22	J	4012	BCR	1	0
19	A	1108	CLA	2	0
19	G	1701	CLA	4	0
27	3	803	DGD	3	0
25	G	5001	LMG	3	0
29	4	613	CHL	8	0
19	A	1119	CLA	7	0
22	1	504	BCR	2	0
19	B	1203	CLA	3	0
19	F	1302	CLA	4	0
19	B	1212	CLA	2	0
19	4	605	CLA	9	0
28	3	501	LUT	2	0
19	A	1120	CLA	4	0
19	A	1123	CLA	5	0
19	1	613	CLA	6	0
19	3	608	CLA	1	0
19	1	602	CLA	4	0
19	3	601	CLA	9	0
25	F	5003	LMG	1	0
19	B	1240	CLA	12	0
19	2	605	CLA	6	0
30	4	502	XAT	6	0
19	4	602	CLA	3	0
22	B	4005	BCR	1	0
32	N	101	FES	1	0
28	4	501	LUT	6	0
22	G	4021	BCR	4	0
29	3	607	CHL	6	0
19	B	1239	CLA	7	0
22	A	4017	BCR	5	0
29	1	609	CHL	6	0
23	A	5002	LHG	2	0
19	A	1128	CLA	3	0
19	A	1136	CLA	9	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
22	G	4011	BCR	4	0
19	A	1114	CLA	3	0
19	B	1214	CLA	6	0
19	A	1103	CLA	8	0
19	A	1129	CLA	2	0
29	2	609	CHL	3	0
19	A	1109	CLA	10	0
19	3	605	CLA	4	0
19	B	1228	CLA	1	0
19	K	1402	CLA	2	0
19	B	1230	CLA	6	0
19	4	612	CLA	5	0
29	4	611	CHL	1	0
22	3	506	BCR	3	0
19	B	1208	CLA	5	0
19	A	1105	CLA	8	0
19	B	1023	CLA	5	0
19	2	601	CLA	7	0
22	I	4020	BCR	3	0
19	B	1021	CLA	4	0
19	A	1110	CLA	5	0
19	4	604	CLA	5	0
22	B	4006	BCR	5	0
19	B	1220	CLA	3	0
22	A	4007	BCR	4	0
24	G	5004	LMT	2	0
19	B	1238	CLA	7	0
19	1	614	CLA	3	0
25	F	5004	LMG	2	0
19	3	613	CLA	3	0
22	K	4002	BCR	7	0
28	1	502	LUT	7	0
19	F	1301	CLA	4	0
20	B	2002	PQN	4	0
19	A	1131	CLA	3	0
25	B	5007	LMG	2	0
19	A	1121	CLA	7	0
19	B	1204	CLA	6	0
25	2	803	LMG	6	0
29	2	613	CHL	1	0
19	B	1216	CLA	2	0
19	2	612	CLA	5	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
19	A	1112	CLA	8	0
19	A	1135	CLA	6	0
19	3	603	CLA	3	0
19	K	1404	CLA	4	0
19	1	603	CLA	6	0
19	B	1231	CLA	2	0
29	1	610	CHL	7	0
22	B	4009	BCR	3	0
19	4	603	CLA	7	0
22	A	4008	BCR	2	0
19	1	607	CLA	4	0
29	3	611	CHL	4	0
19	G	1601	CLA	3	0
23	B	5002	LHG	5	0
29	4	610	CHL	3	0
19	B	1213	CLA	5	0
19	1	605	CLA	5	0
22	A	4002	BCR	3	0
22	L	4019	BCR	7	0
19	B	1229	CLA	5	0
28	J	4013	LUT	4	0
23	2	807	LHG	2	0
28	2	501	LUT	4	0
19	4	607	CLA	7	0
19	K	1401	CLA	11	0
19	4	608	CLA	2	0
27	1	803	DGD	1	0
29	2	610	CHL	7	0
19	4	601	CLA	3	0
19	A	1117	CLA	2	0
19	B	1225	CLA	5	0
19	2	608	CLA	2	0
19	A	1101	CLA	4	0
19	B	1202	CLA	6	0
19	L	1503	CLA	5	0
19	A	1141	CLA	4	0
27	B	5005	DGD	7	0
19	1	601	CLA	12	0
30	2	502	XAT	10	0
24	B	5008	LMT	1	0
19	A	1138	CLA	3	0
19	A	1134	CLA	3	0

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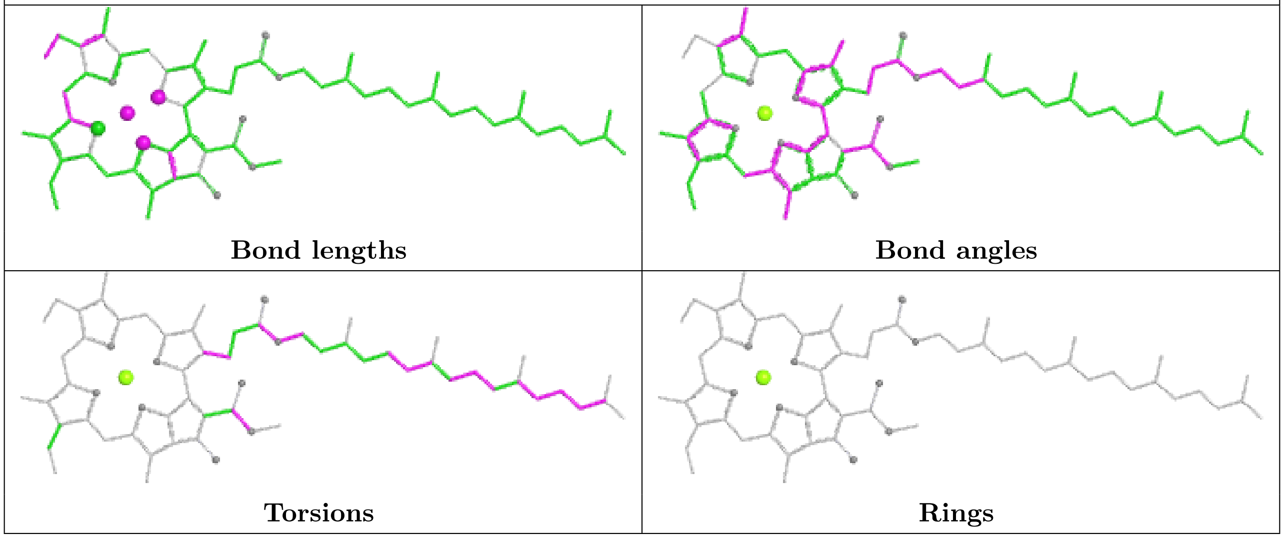
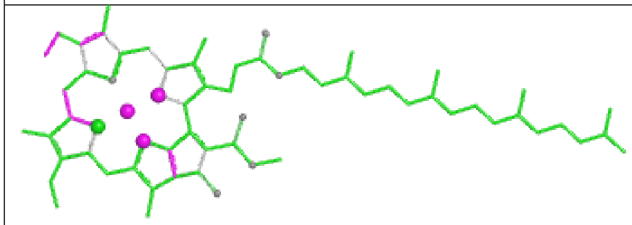
Mol	Chain	Res	Type	Clashes	Symm-Clashes
19	A	1113	CLA	6	0
19	A	1137	CLA	4	0
19	3	617	CLA	3	0
27	J	5001	DGD	4	0

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

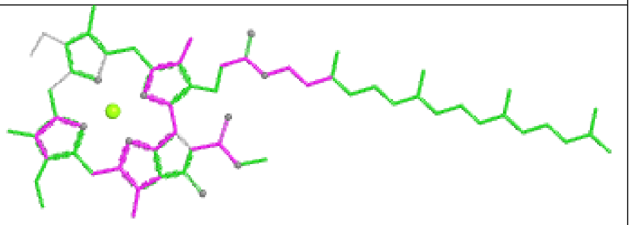
Ligand CLA 4 617



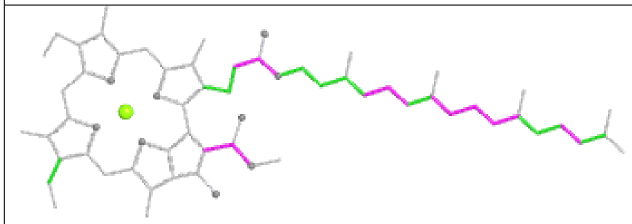
Ligand CLA A 1125



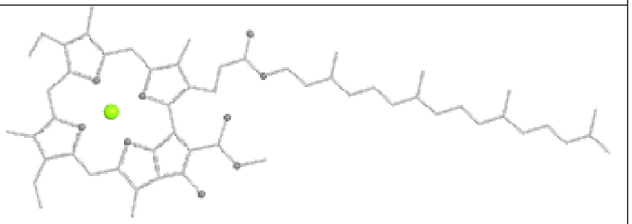
Bond lengths



Bond angles

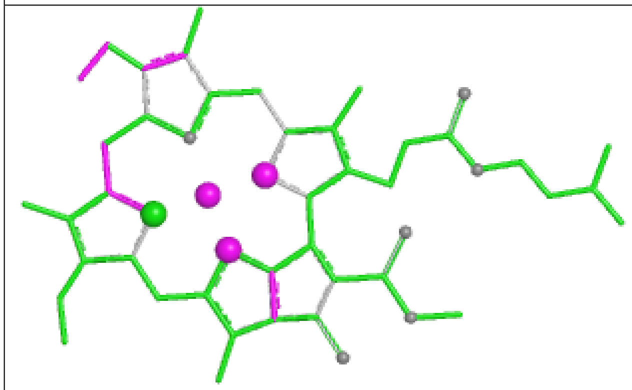


Torsions

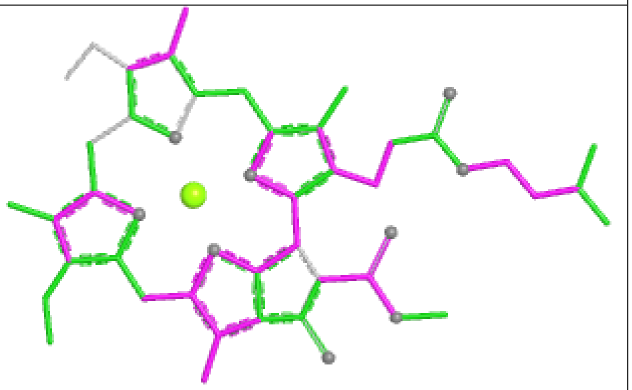


Rings

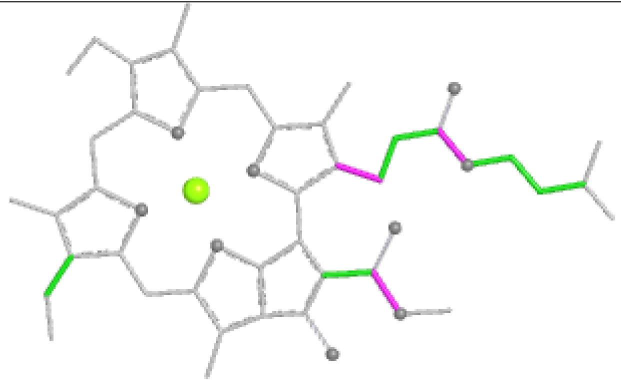
Ligand CLA 2 606



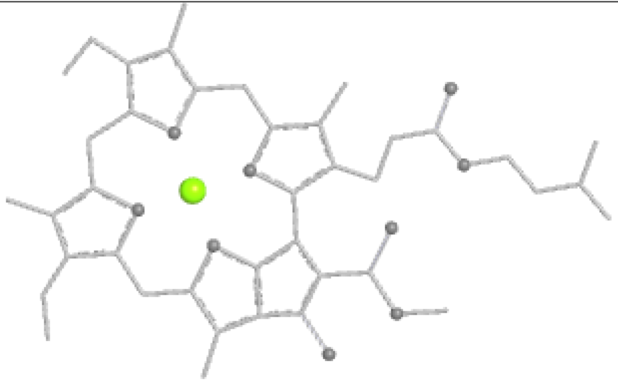
Bond lengths



Bond angles

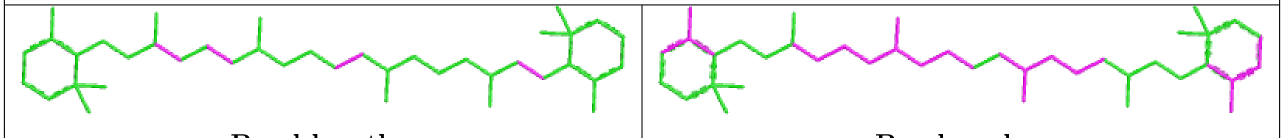


Torsions

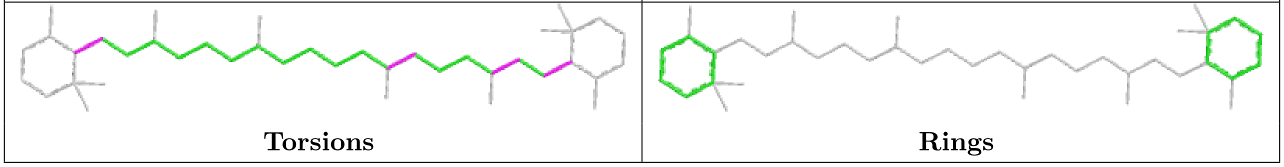


Rings

Ligand BCR A 4003

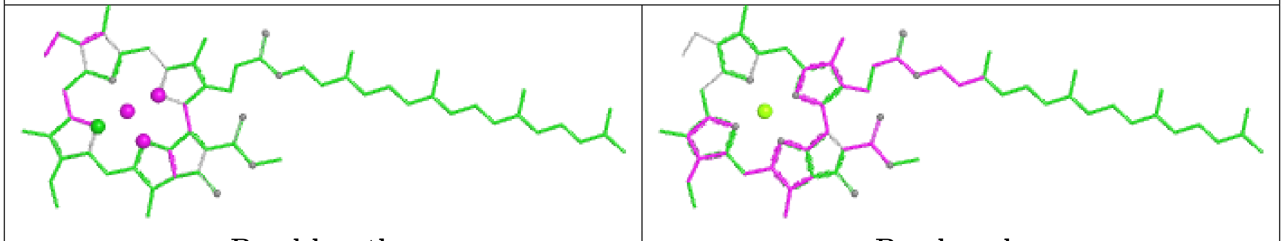


Bond lengths Bond angles

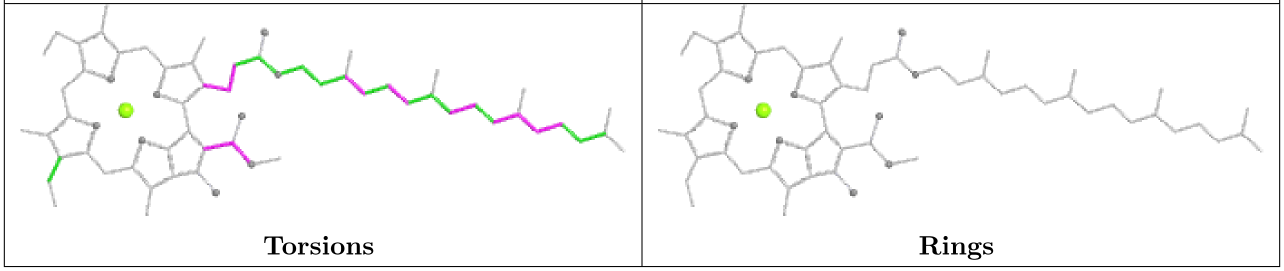


Torsions Rings

Ligand CLA A 1132

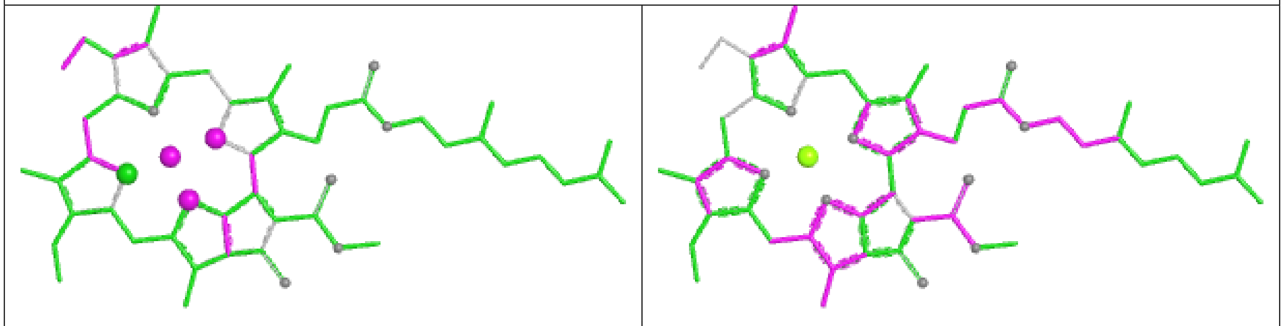


Bond lengths Bond angles

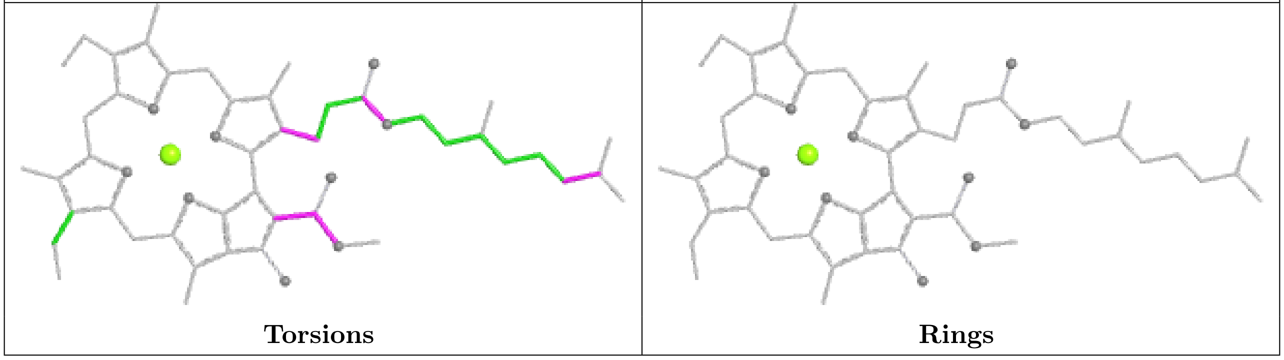


Torsions Rings

Ligand CLA A 1124

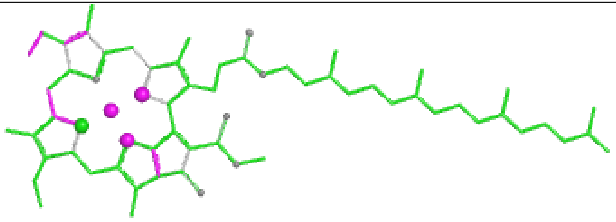
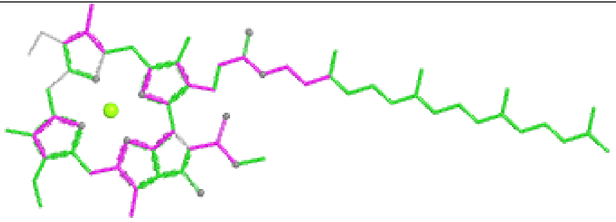
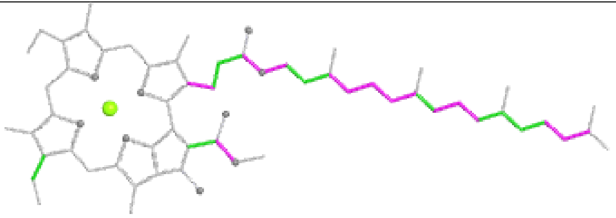
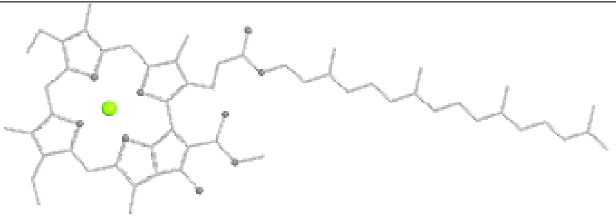


Bond lengths Bond angles

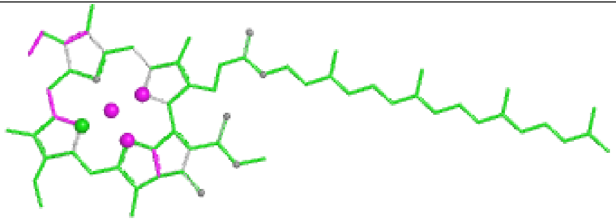
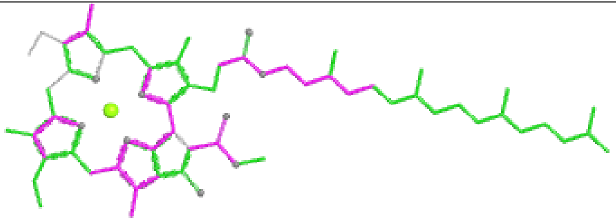
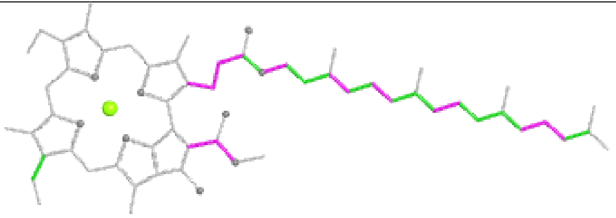
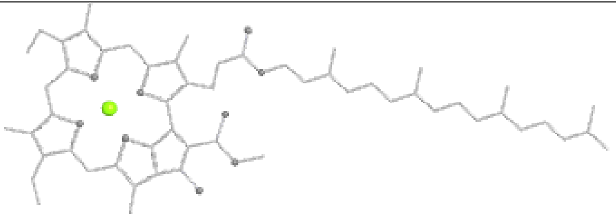


Torsions Rings

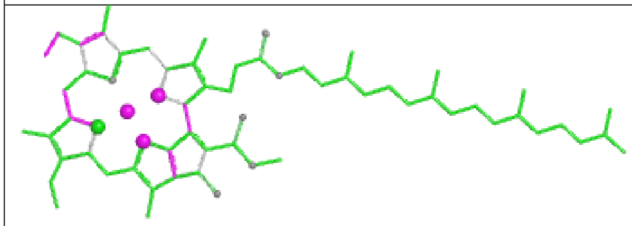
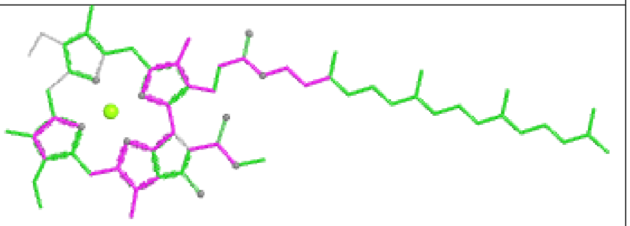
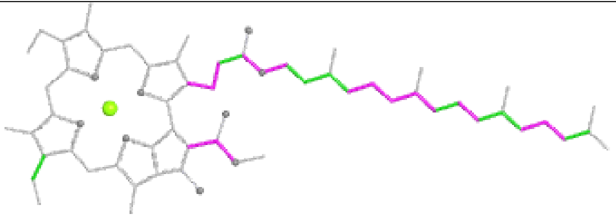
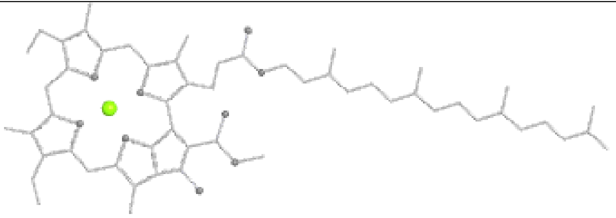
Ligand CLA B 1222

 **Bond lengths**	 **Bond angles**
 **Torsions**	 **Rings**

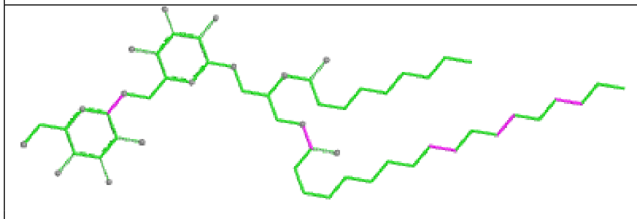
Ligand CLA B 1224

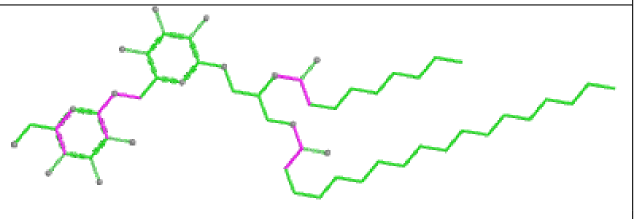
 **Bond lengths**	 **Bond angles**
 **Torsions**	 **Rings**

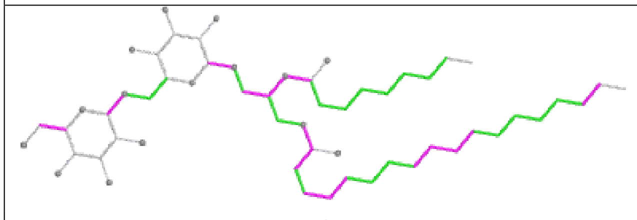
Ligand CLA 2 603

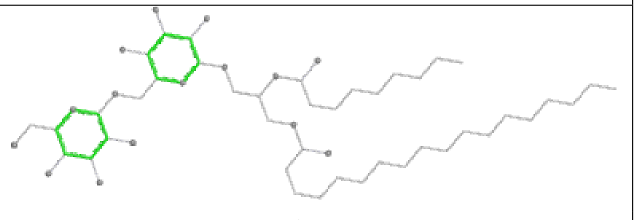
 **Bond lengths**	 **Bond angles**
 **Torsions**	 **Rings**

Ligand DGD F 5005

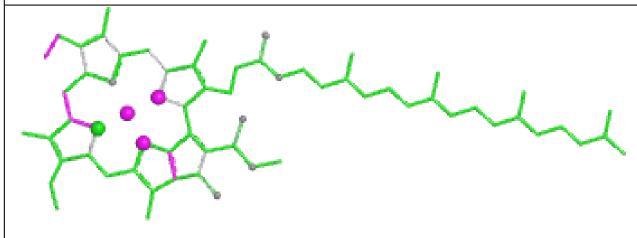

Bond lengths

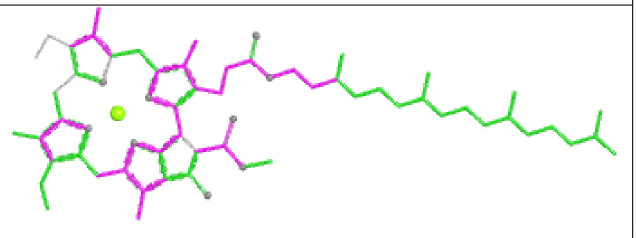

Bond angles

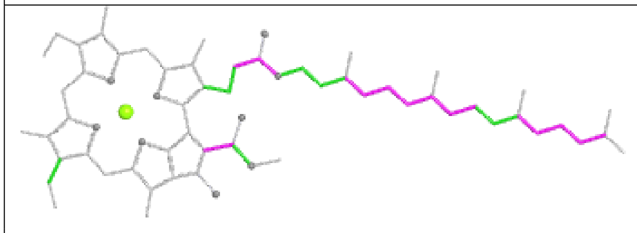

Torsions


Rings

Ligand CLA B 1211


Bond lengths


Bond angles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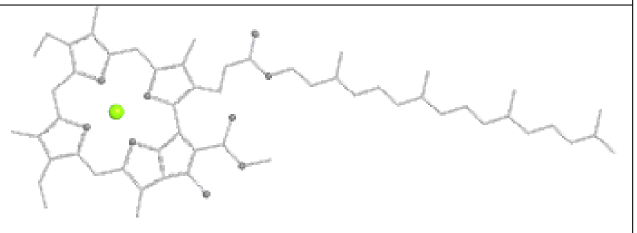
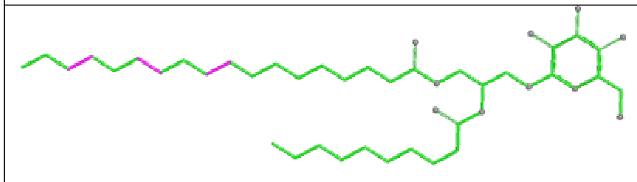

Rings

Ligand LMG F 5002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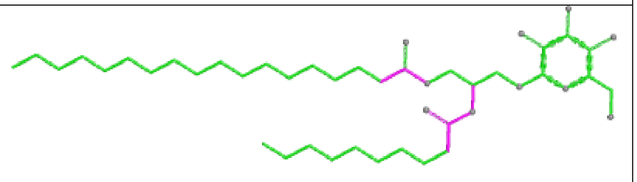
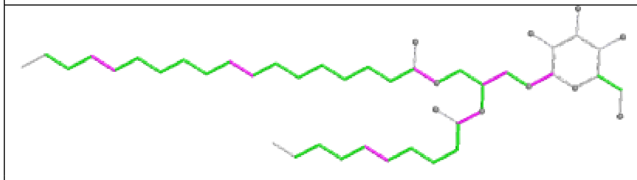

Bond angles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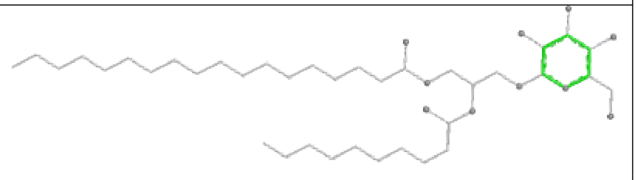
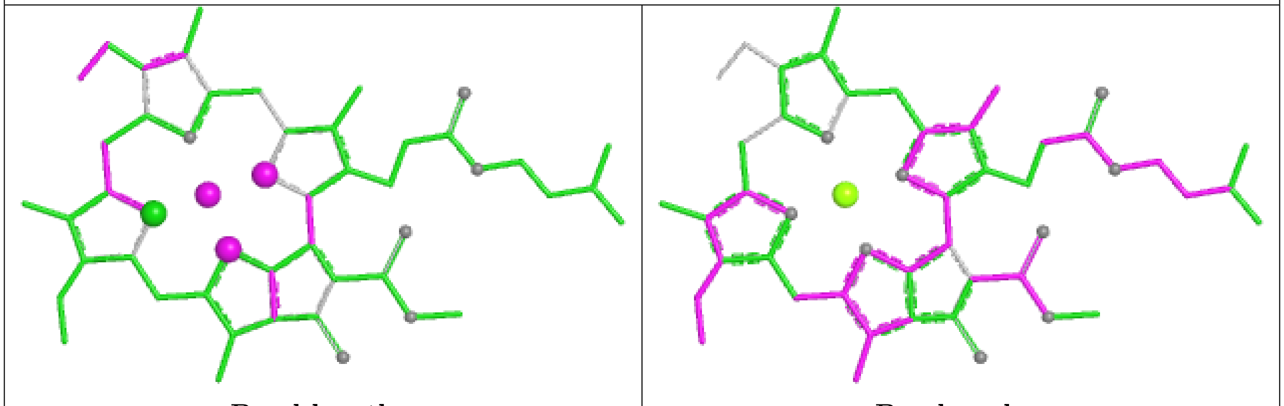
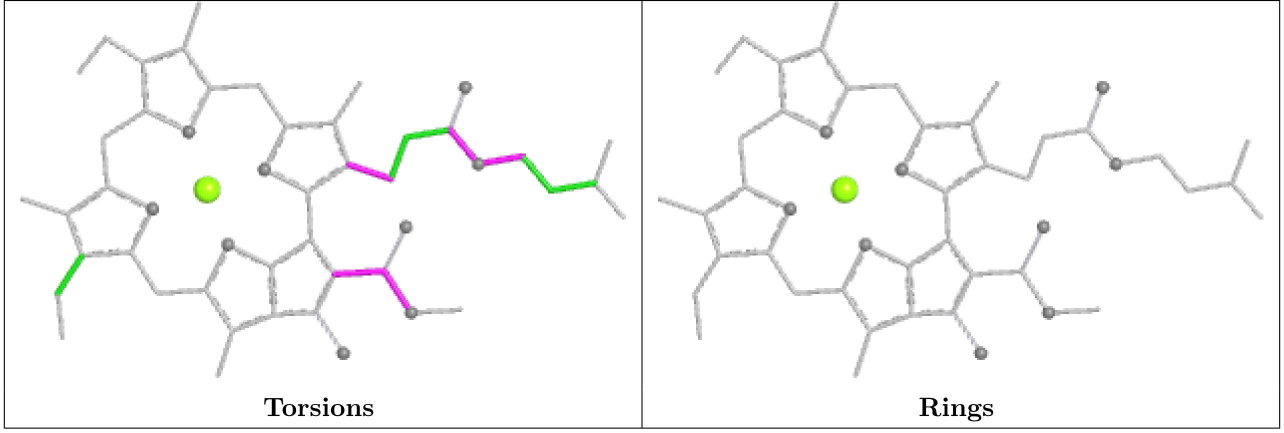

Rings

Ligand CLA 4 609



Bond lengths

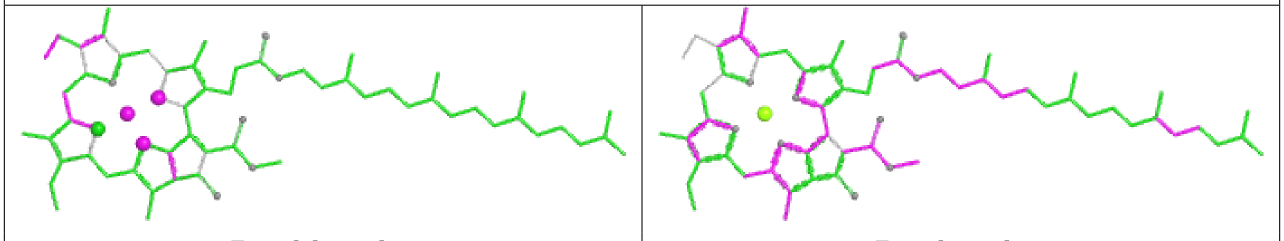
Bond angles



Torsions

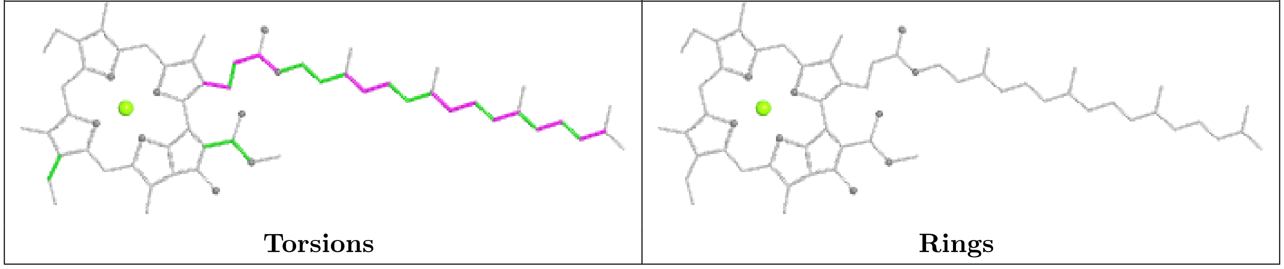
Rings

Ligand CLA B 1210



Bond lengths

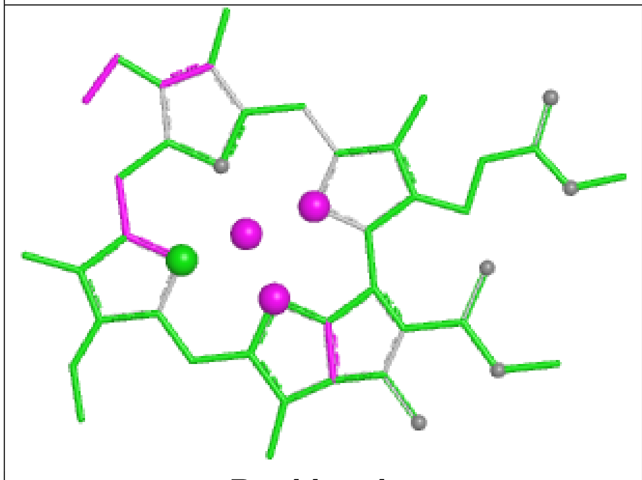
Bond angles



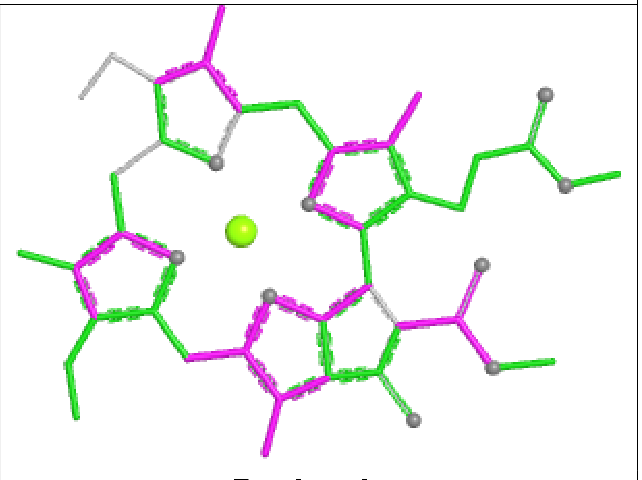
Torsions

Rings

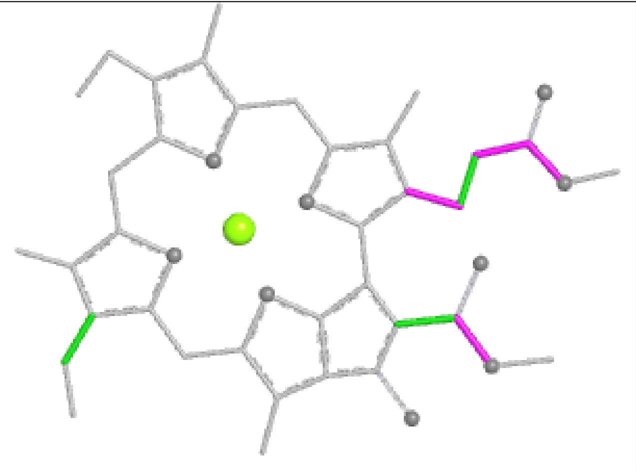
Ligand CLA B 1209



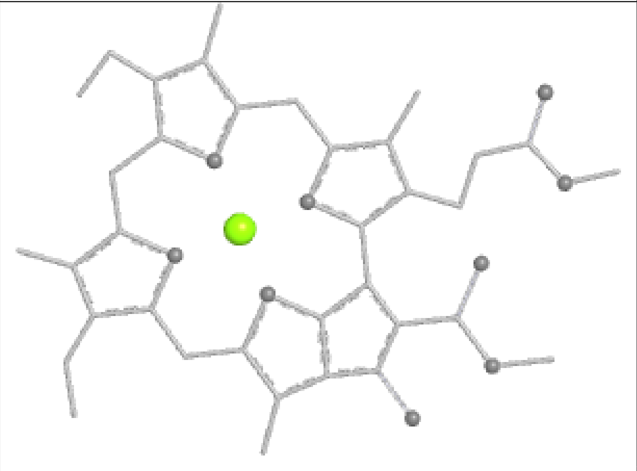
Bond lengths



Bond angles

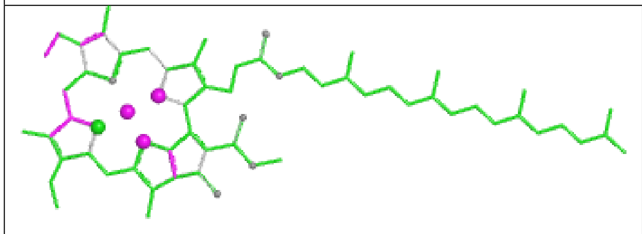


Torsions

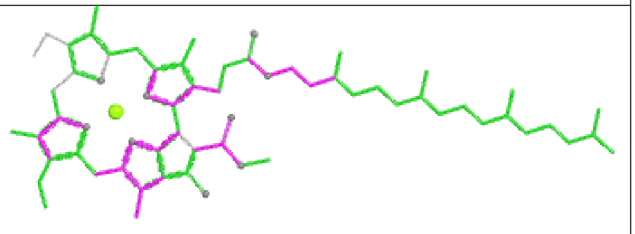


Rings

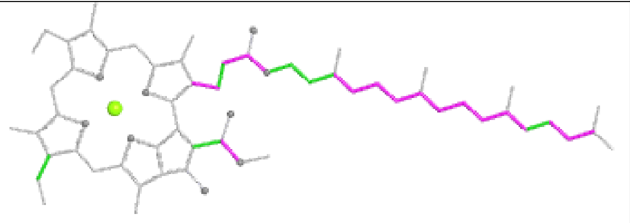
Ligand CLA A 1102



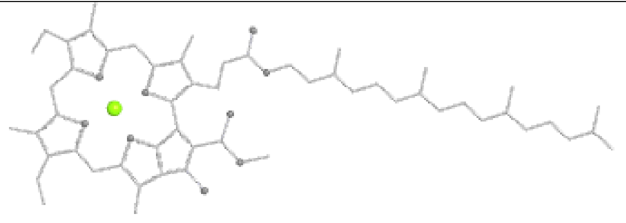
Bond lengths



Bond angles

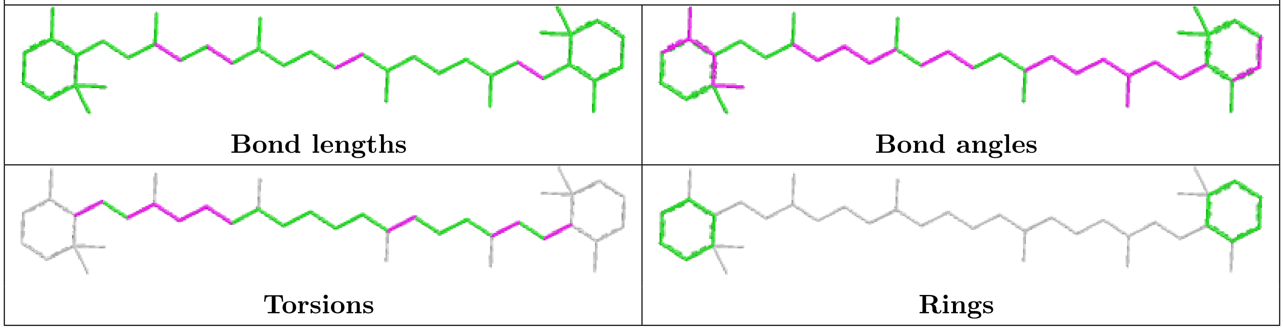


Torsions



Rings

Ligand BCR B 4010



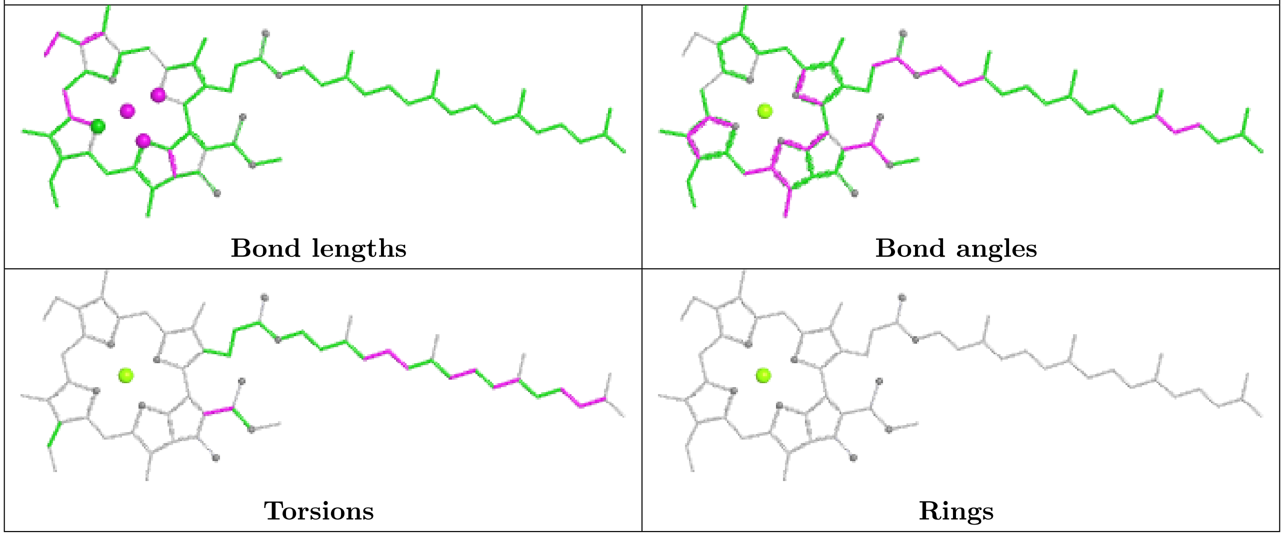
Bond lengths

Bond angles

Torsions

Rings

Ligand CLA B 1205



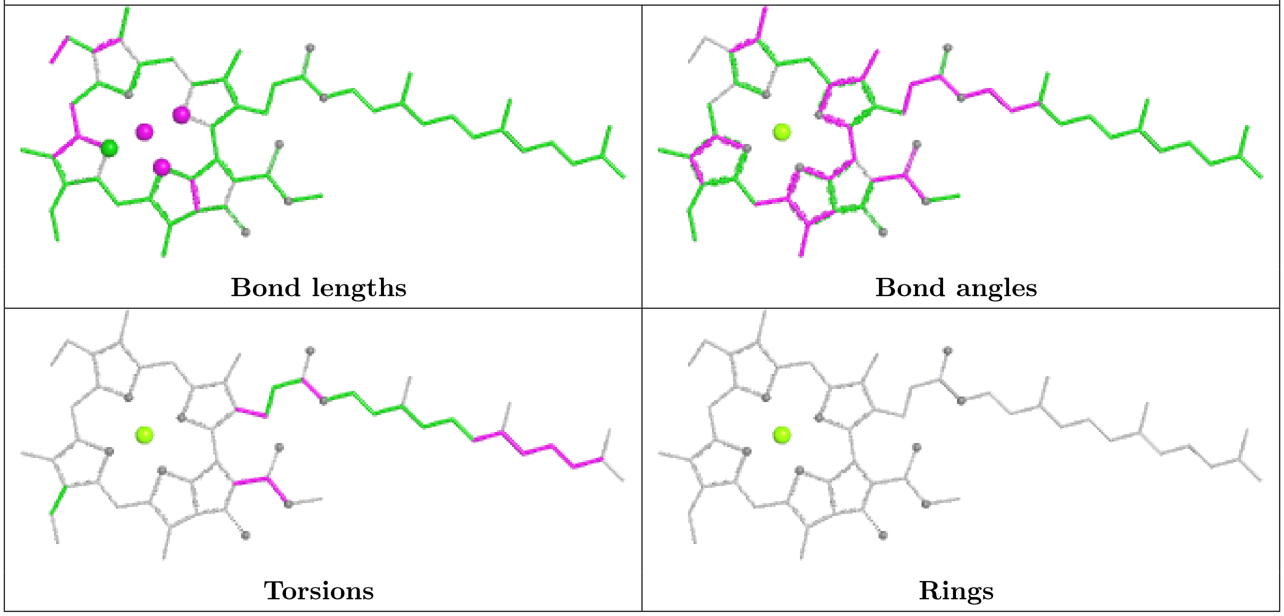
Bond lengths

Bond angles

Torsions

Rings

Ligand CLA 2 607



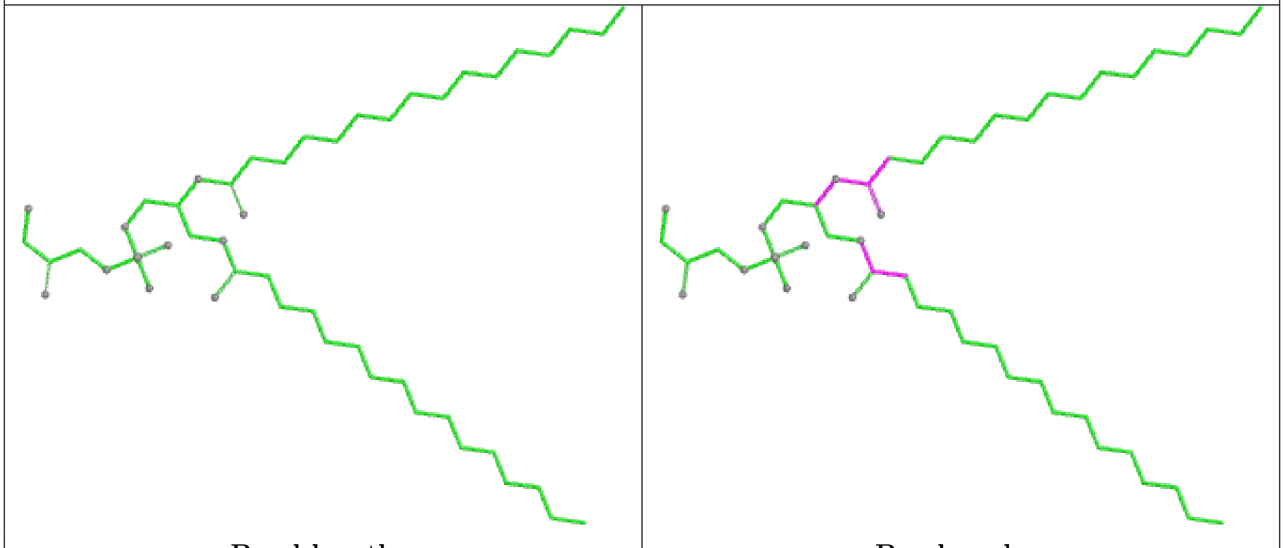
Bond lengths

Bond angles

Torsions

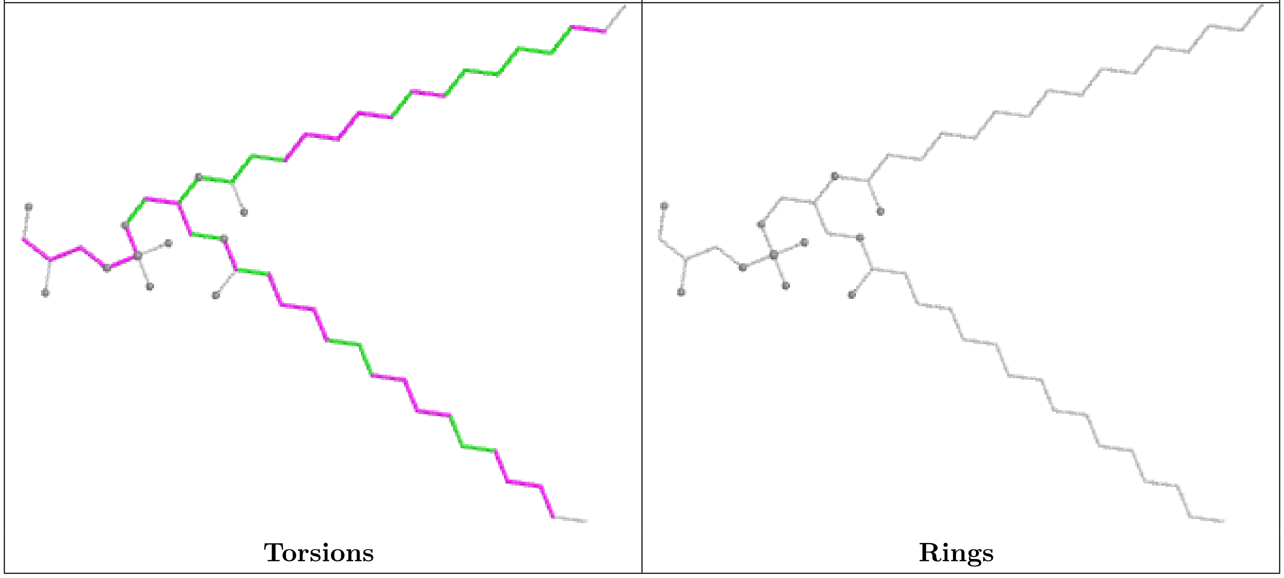
Rings

Ligand LHG 1 801



Bond lengths

Bond angles



Torsions

Rings

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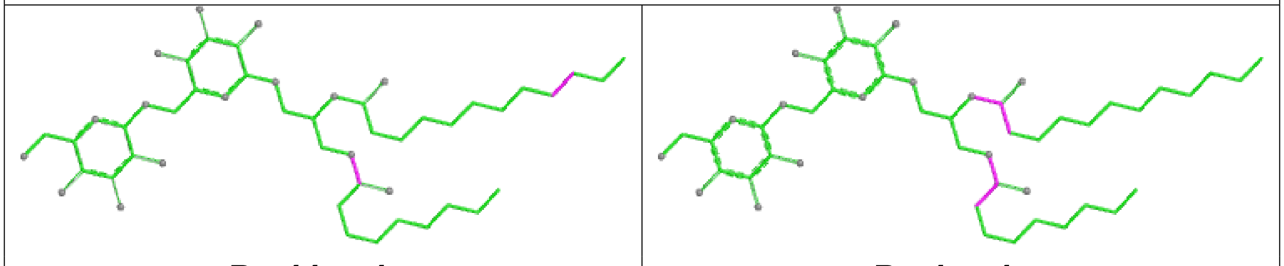
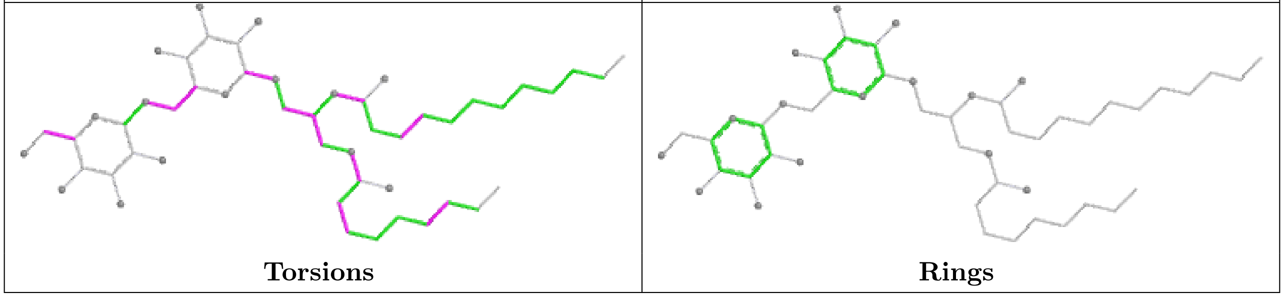


Bond lengths

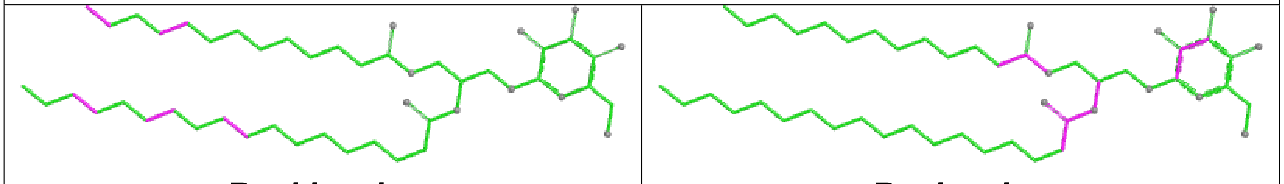
Bond angles



Torsions

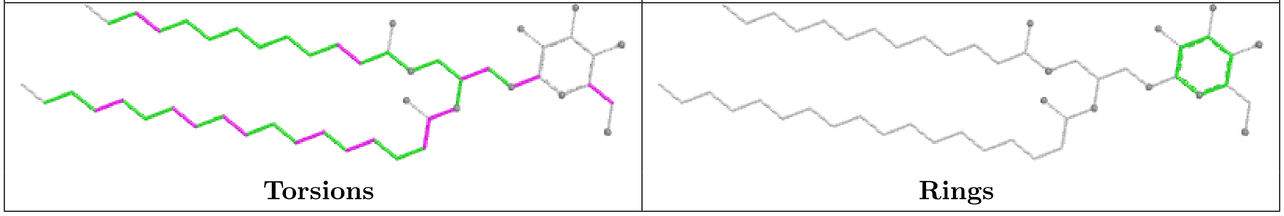
Rings

Ligand LMG A 5006



Bond lengths

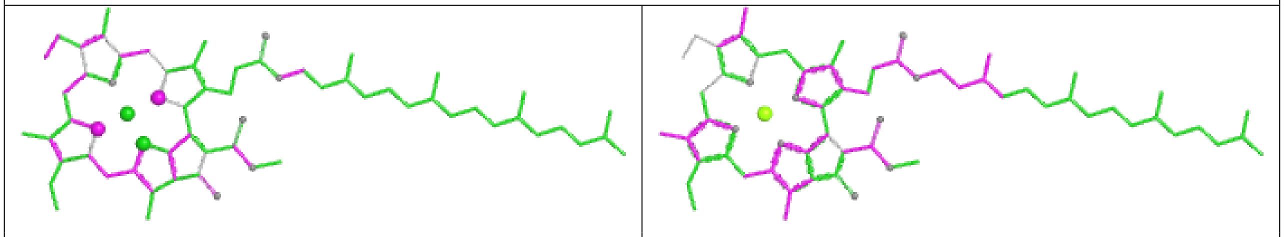
Bond angles



Torsions

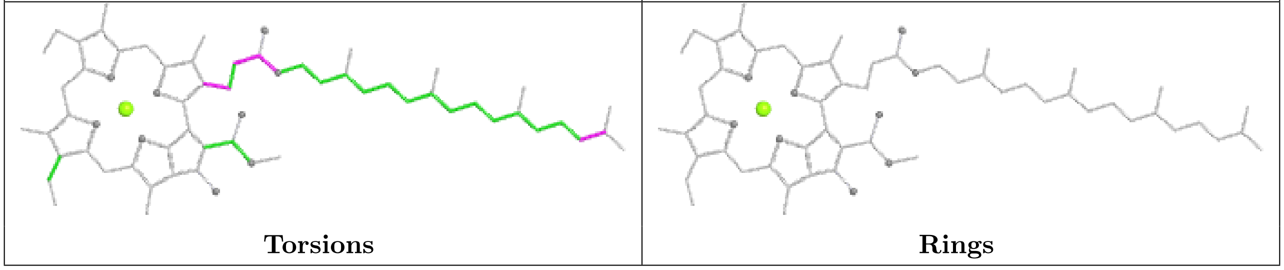
Rings

Ligand CL0 A 1011



Bond lengths

Bond angles



Torsions

Rings

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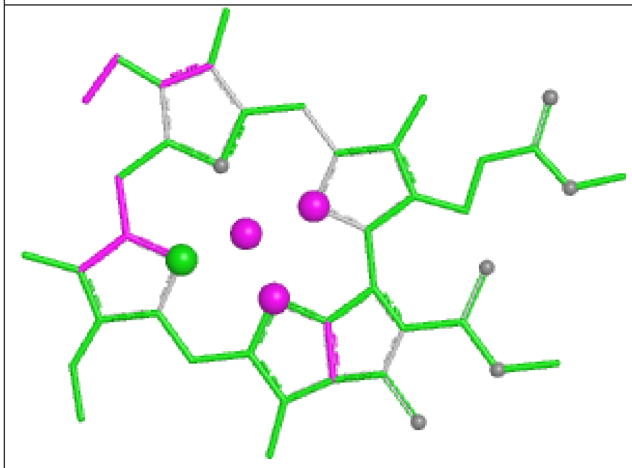
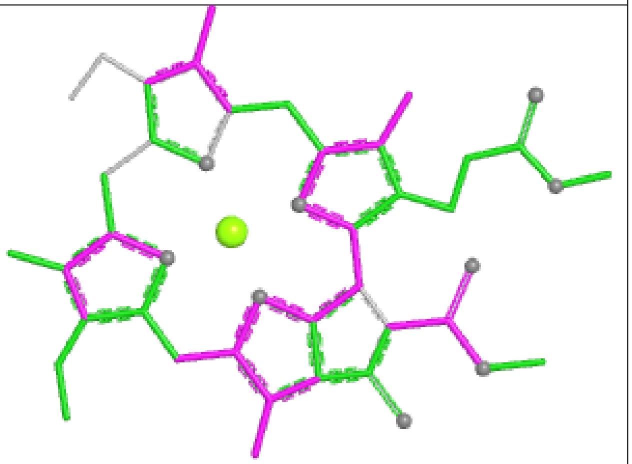
<tr><td>
Bond lengths</td><td>
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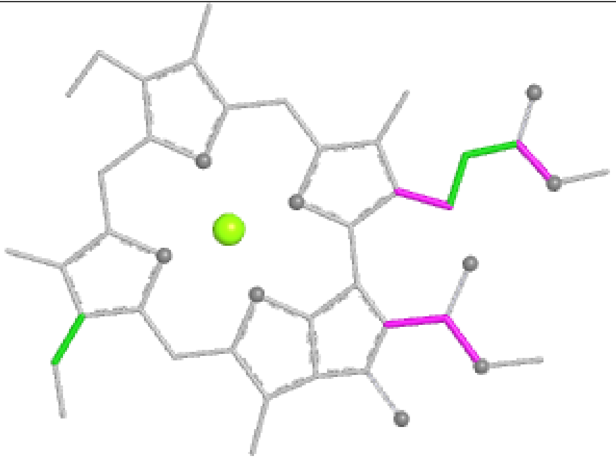
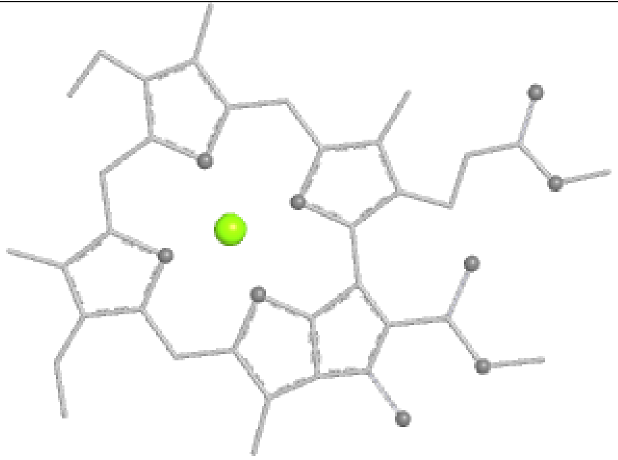
<tr><td>
Torsions</td><td>
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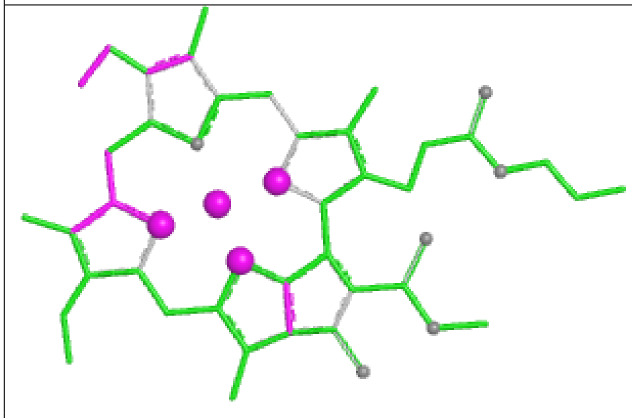
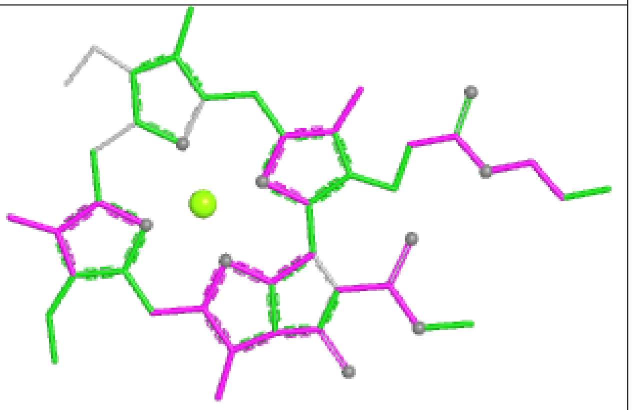
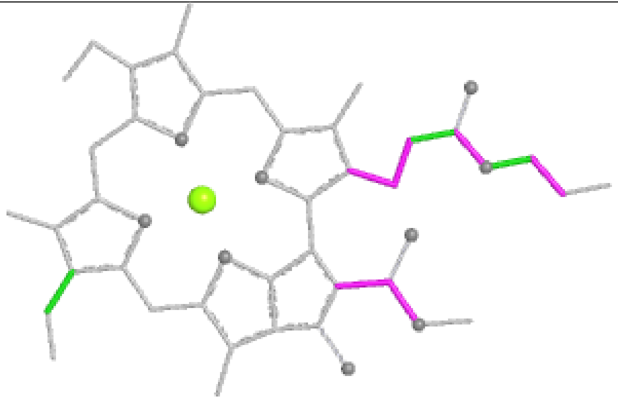
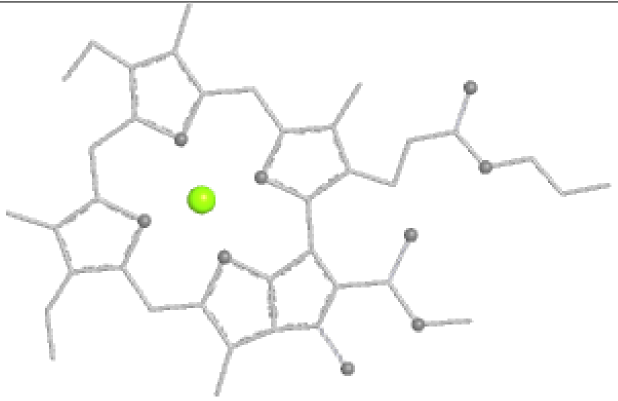
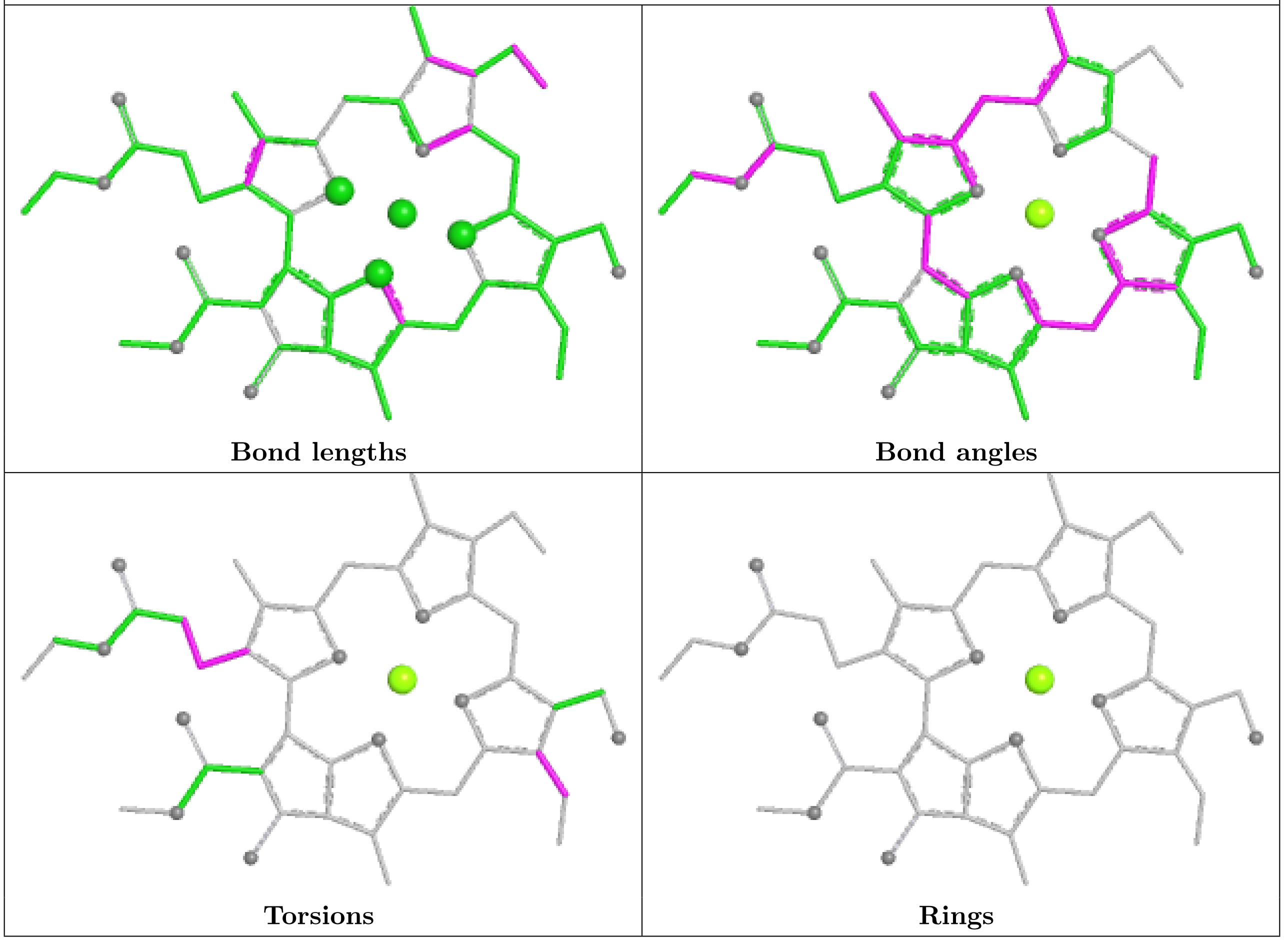
 **Bond lengths**	 **Bond angles**
 **Torsions**	 **Rings**

Ligand CHL 2 611



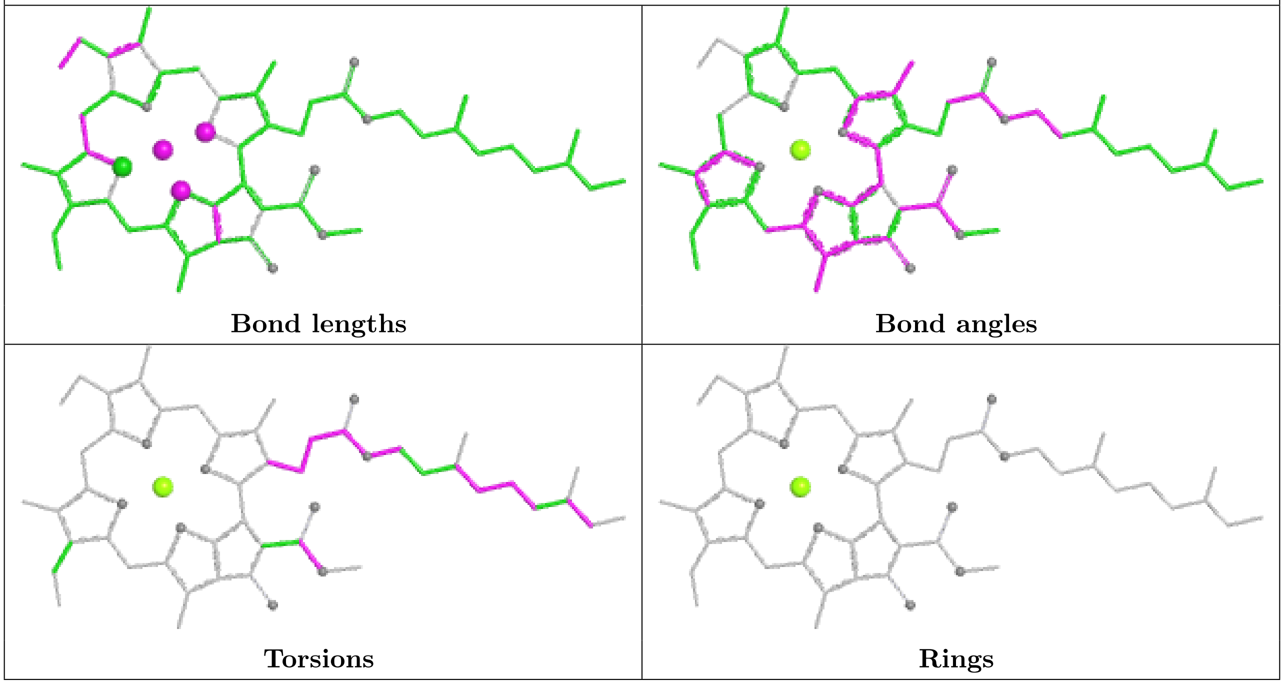
Bond lengths

Bond angles

Torsions

Rings

Ligand CLA A 1116



Bond lengths

Bond angles

Torsions

Rings

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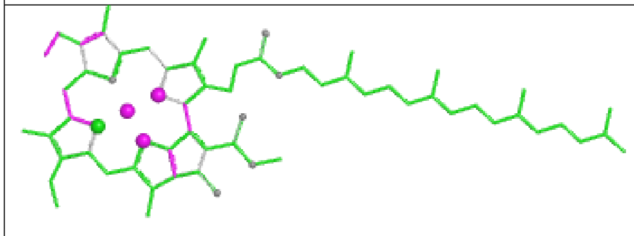

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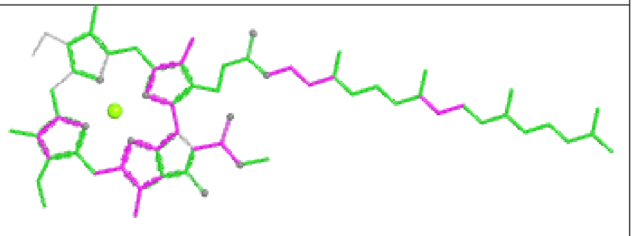

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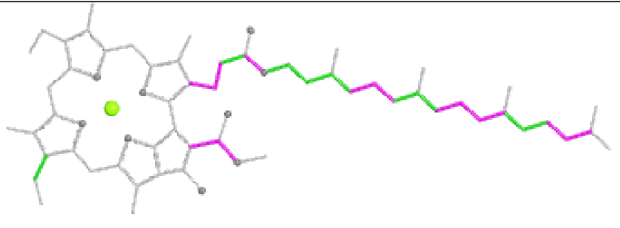

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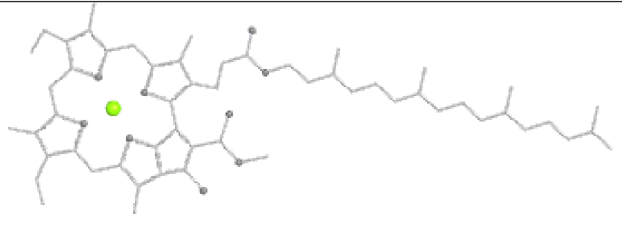
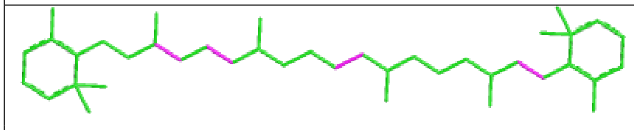


Rings

Ligand BCR 2 503



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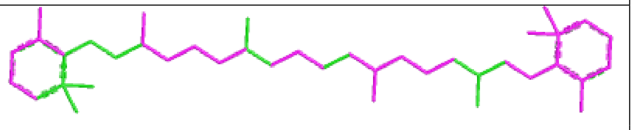

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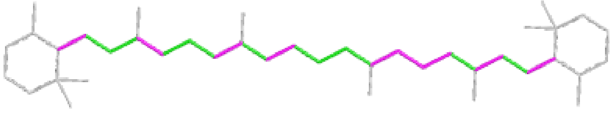

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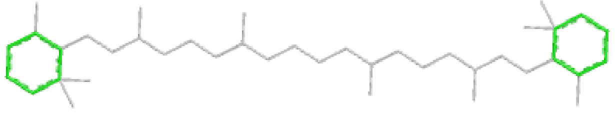
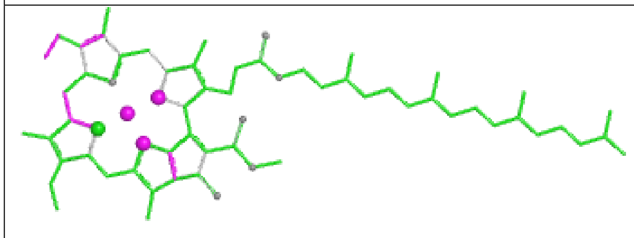


Rings

Ligand CLA A 1126



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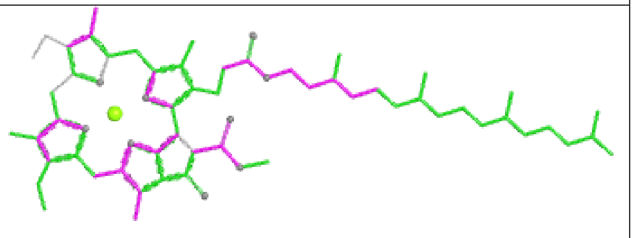

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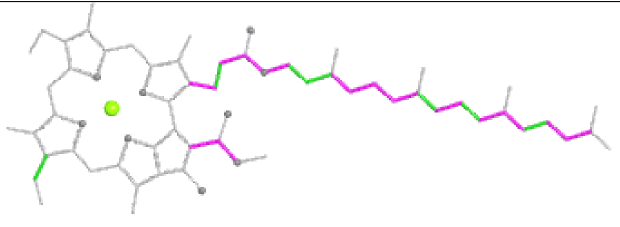

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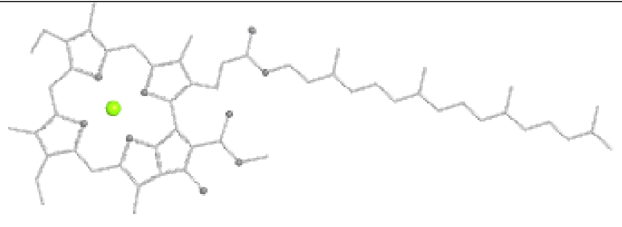
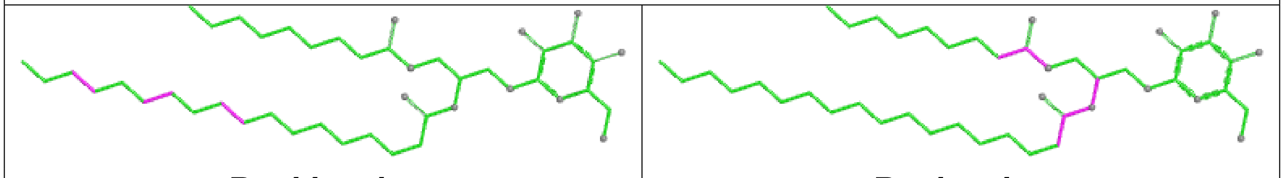


Rings

Ligand LMG 1 802



Bond lengths

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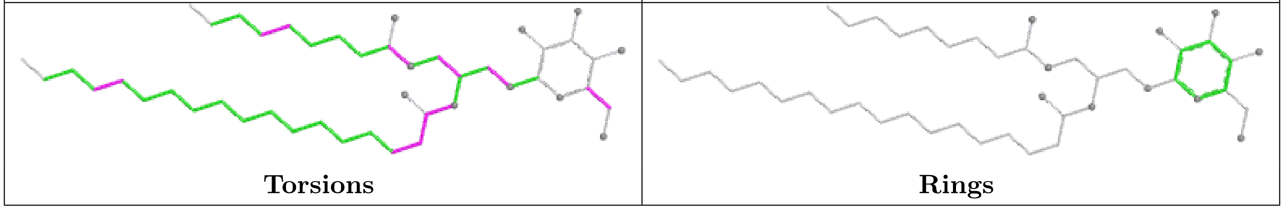

Torsions

Rings

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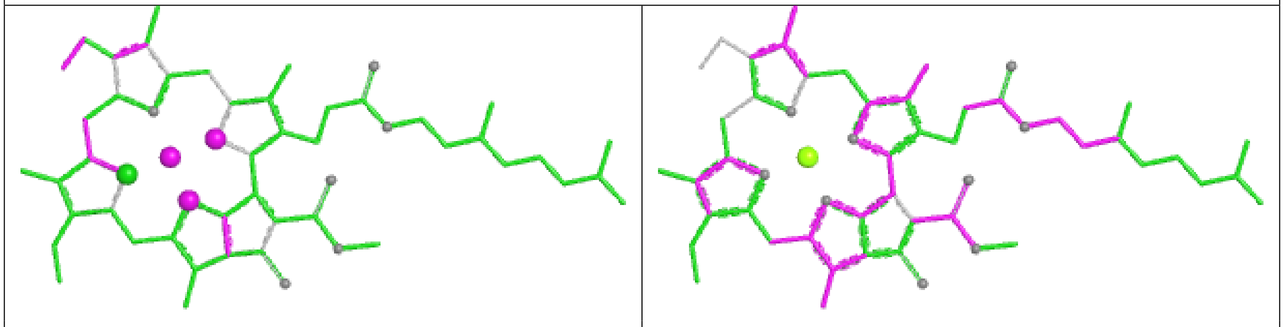
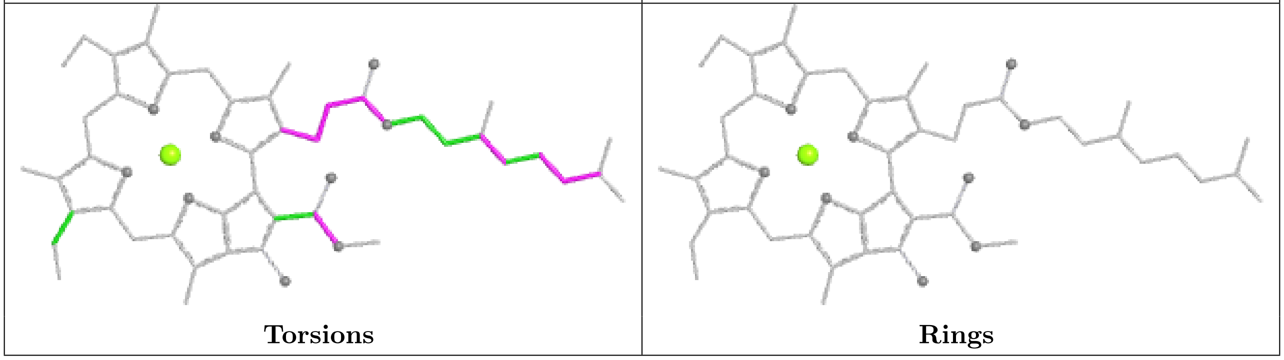


Bond lengths

Bond angles



Torsions

Rings

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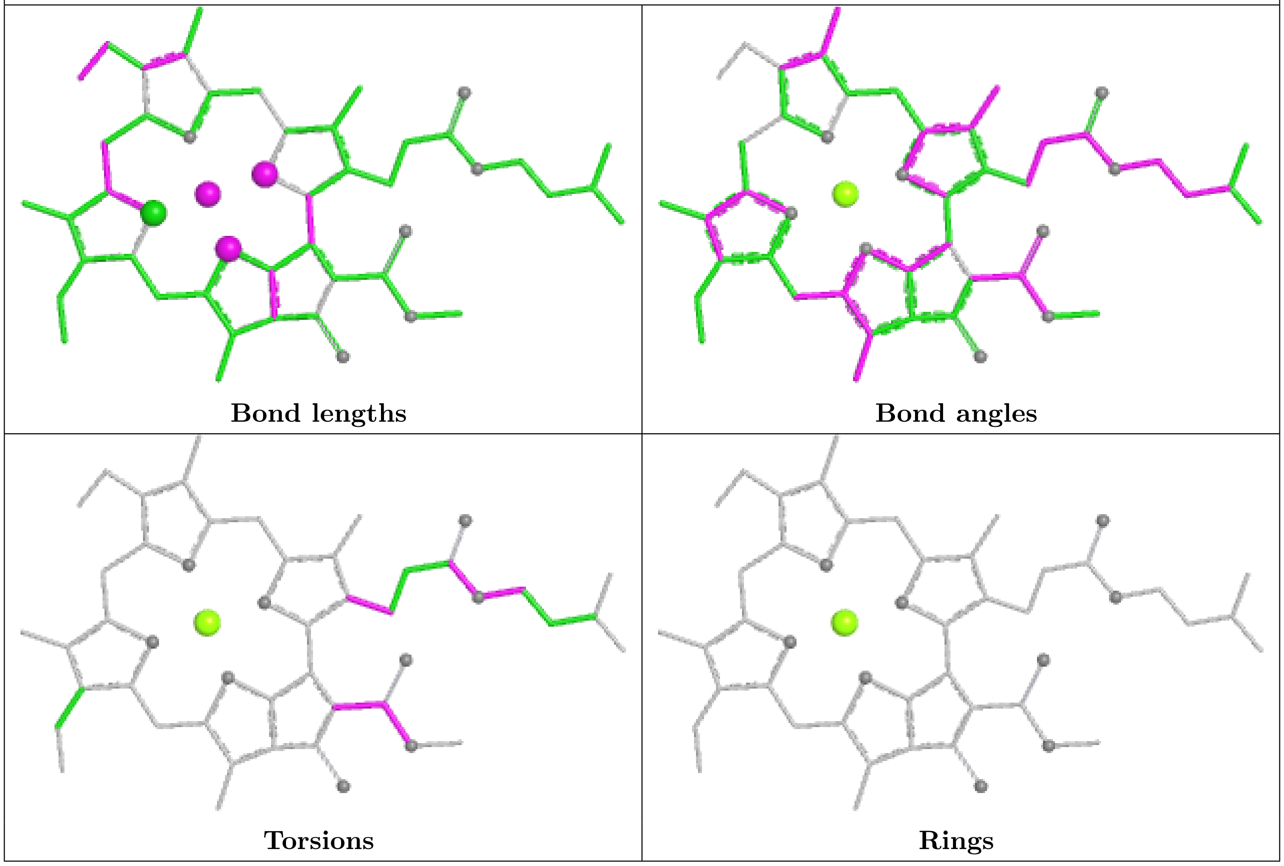

Bond lengths

Bond angles

Torsions

Rings

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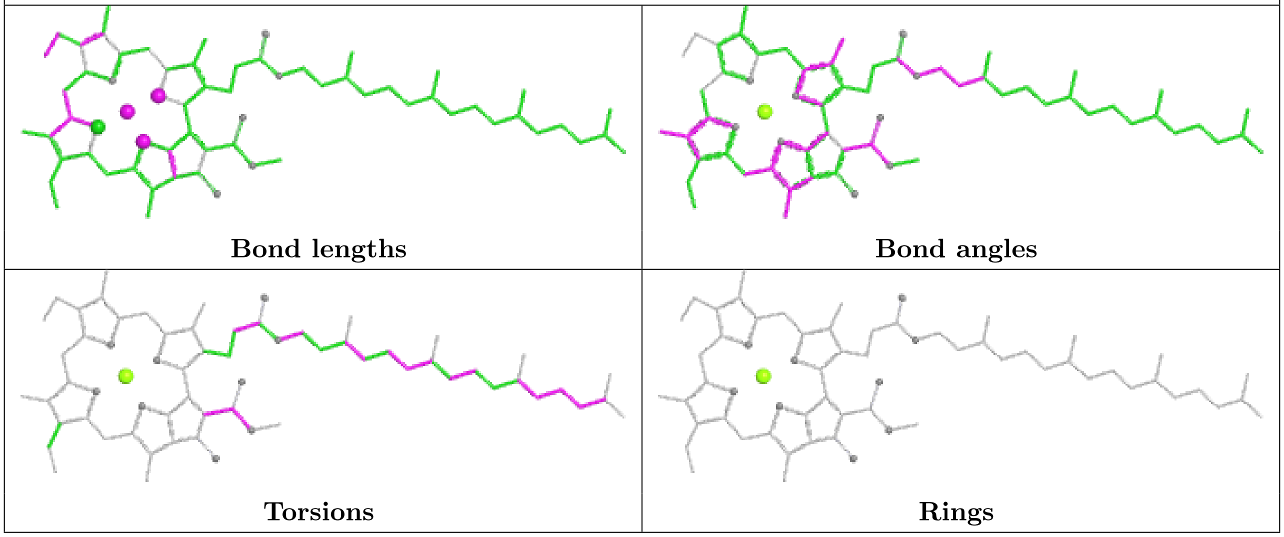

Bond lengths

Bond angles

Torsions

Rings

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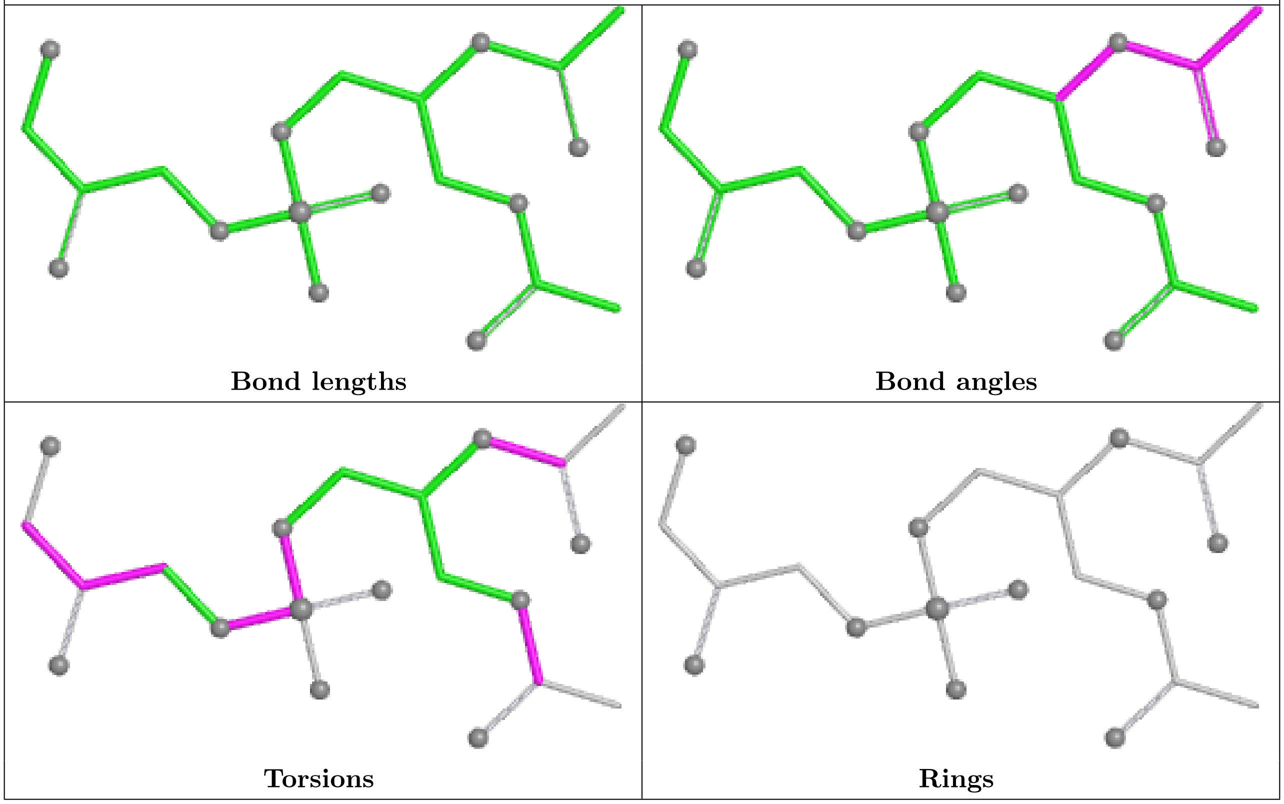

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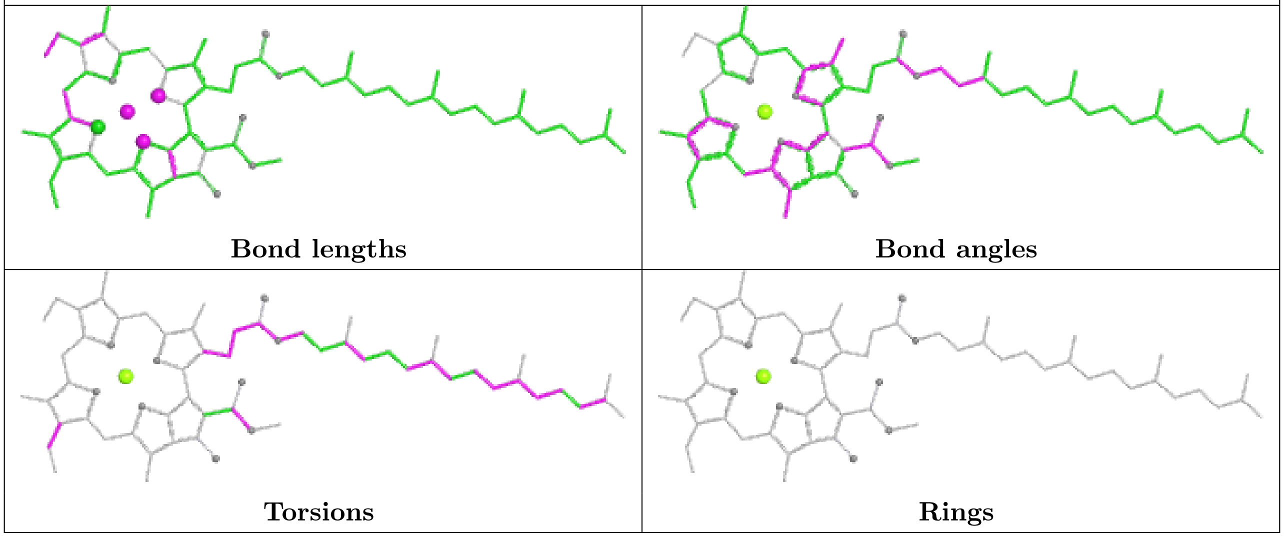

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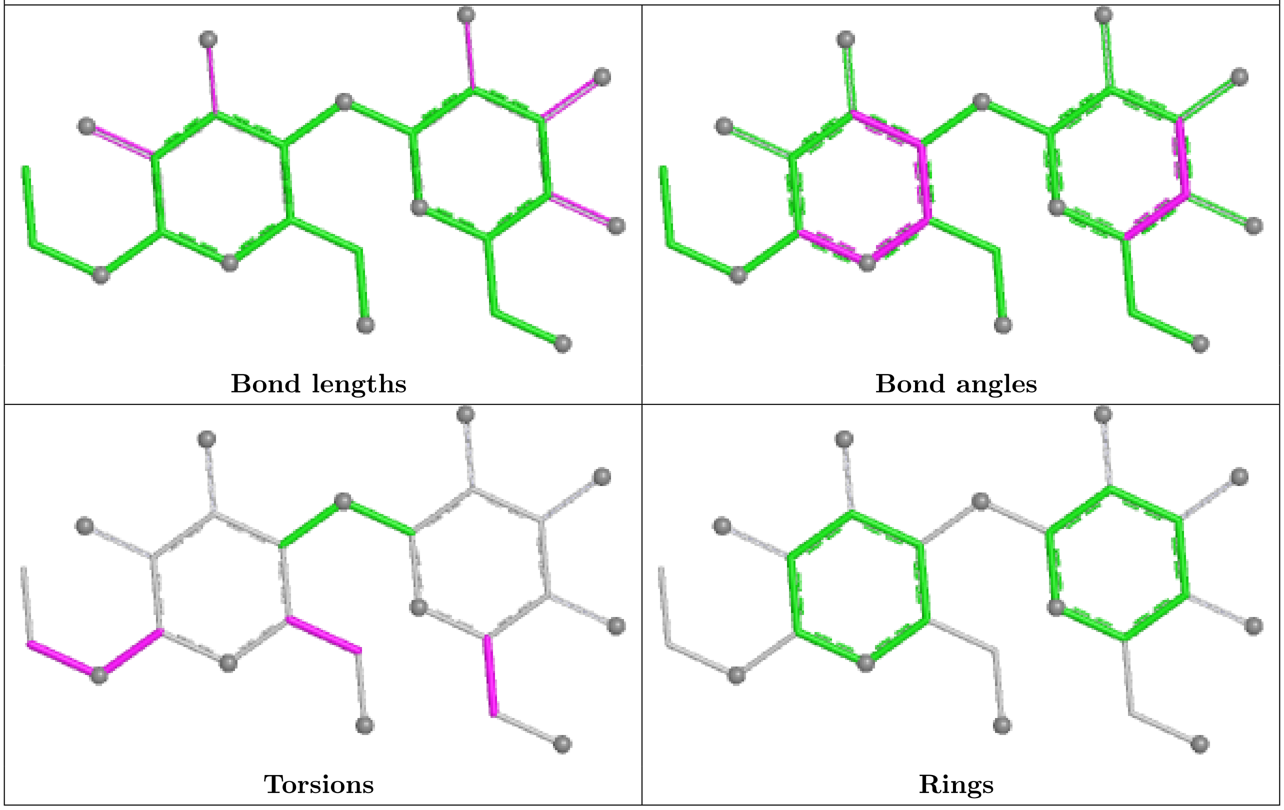

Bond lengths

Bond angles

Torsions

Rings

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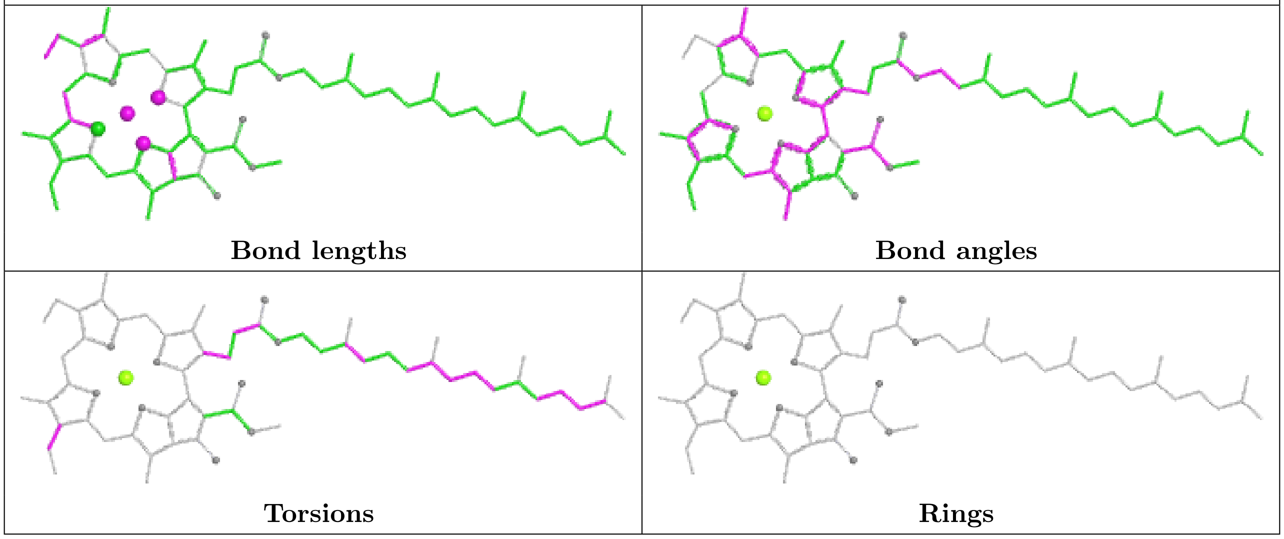

Bond lengths

Bond angles

Torsions

Rings

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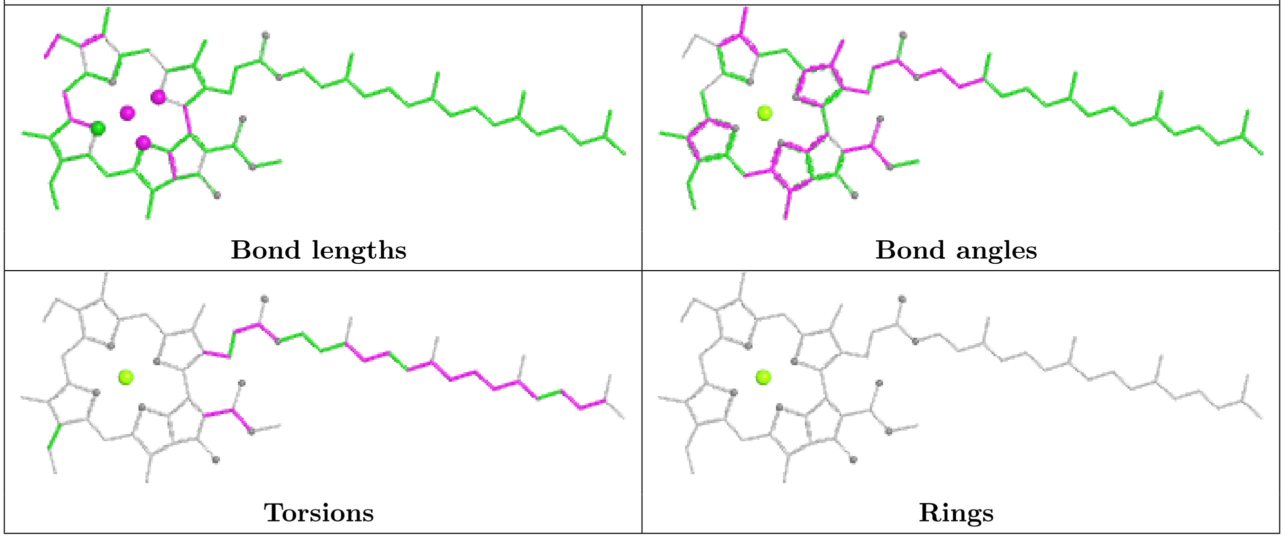

Bond lengths

Bond angles

Torsions

Rings

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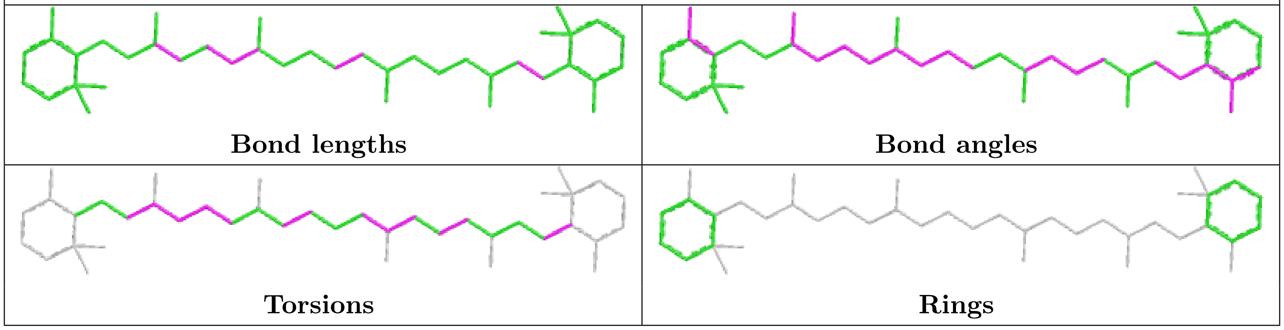

Bond lengths

Bond angles

Torsions

Rings

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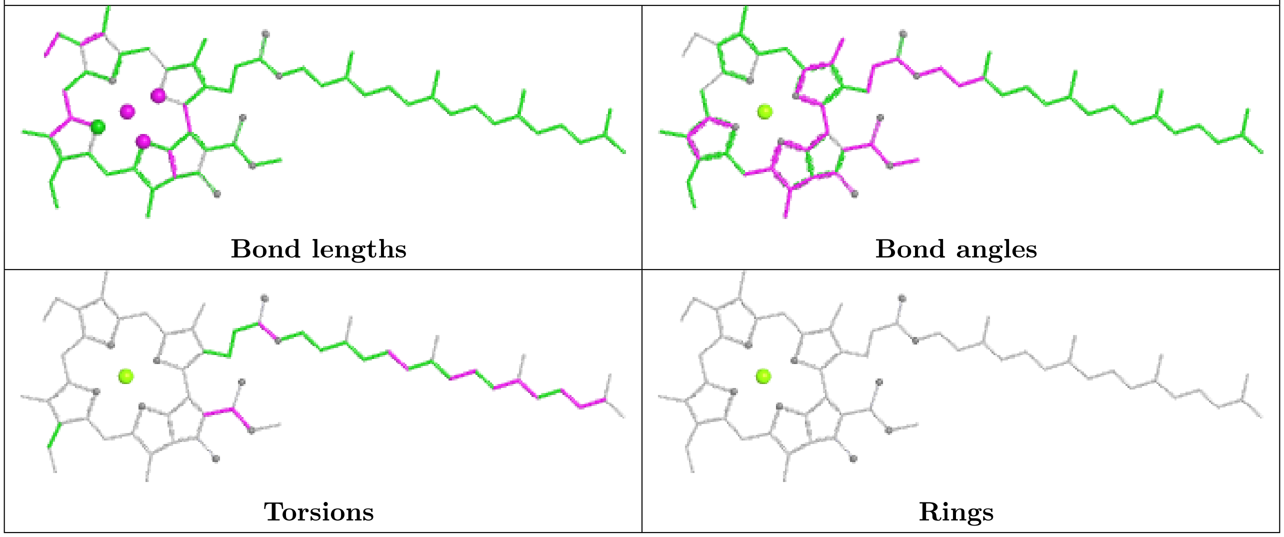

Bond lengths

Bond angles

Torsions

Rings

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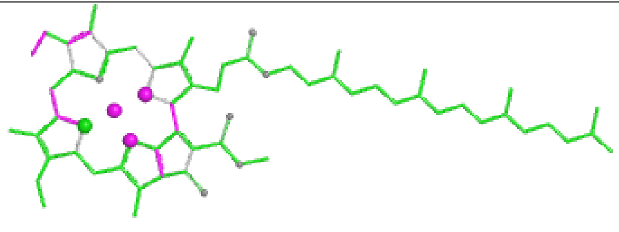

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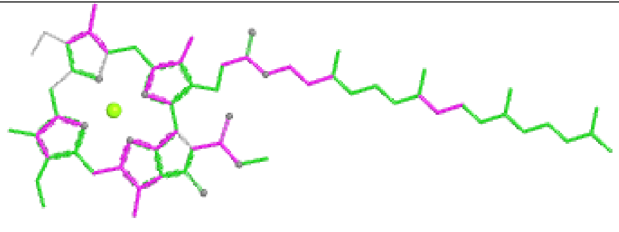

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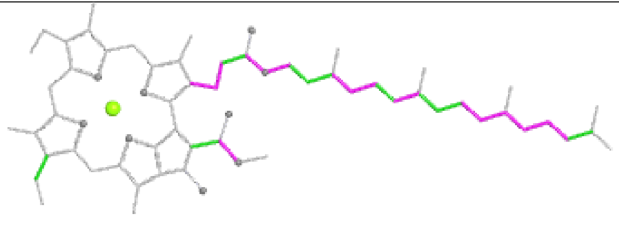

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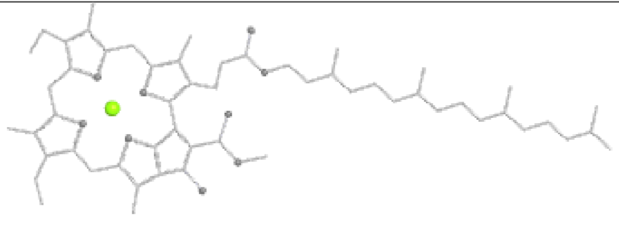

Rings

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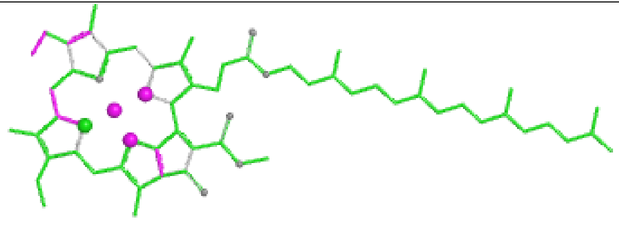

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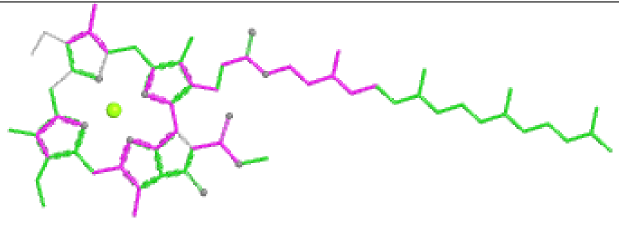

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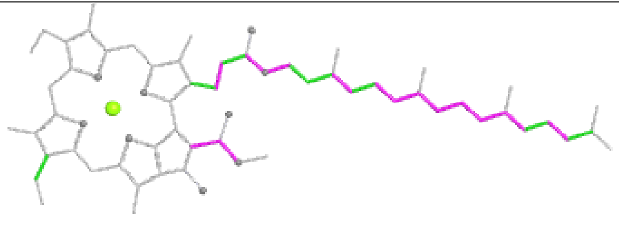

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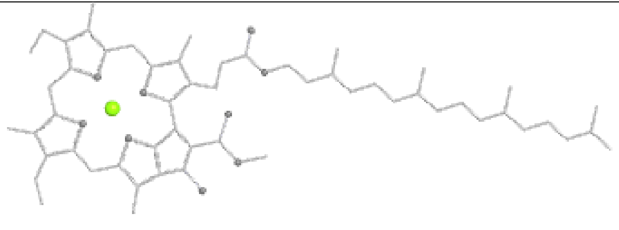

Rings

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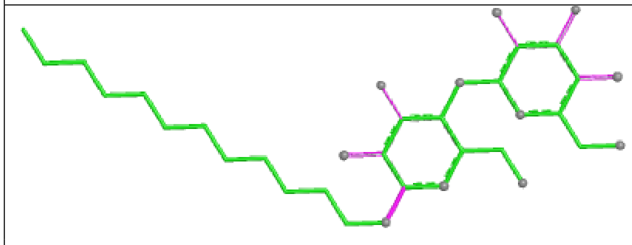

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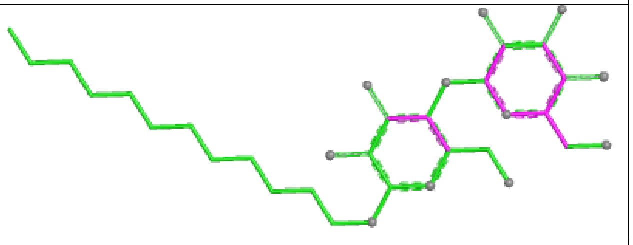

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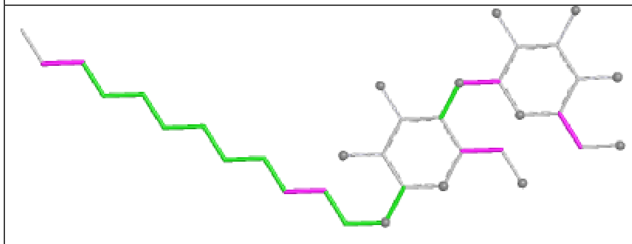

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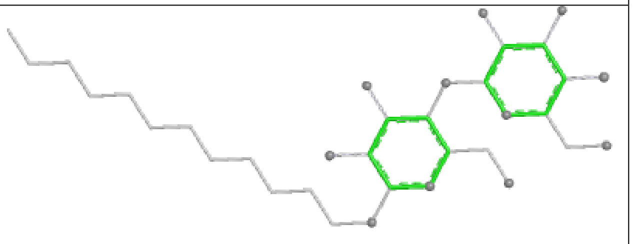
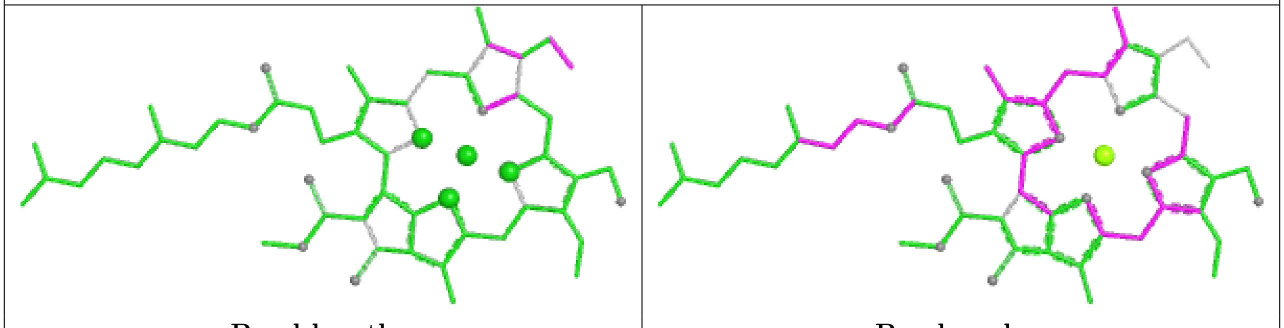
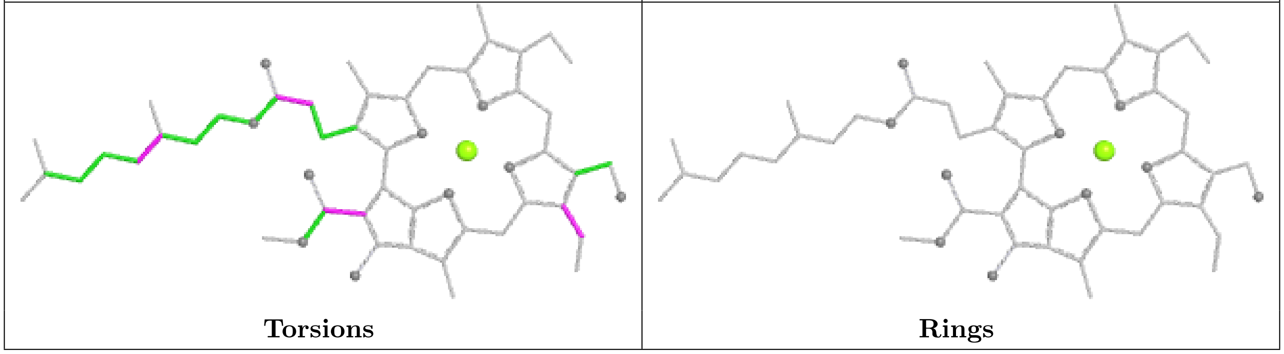


Rings

Ligand CHL 2 615



Bond lengths Bond angles



Torsions Rings

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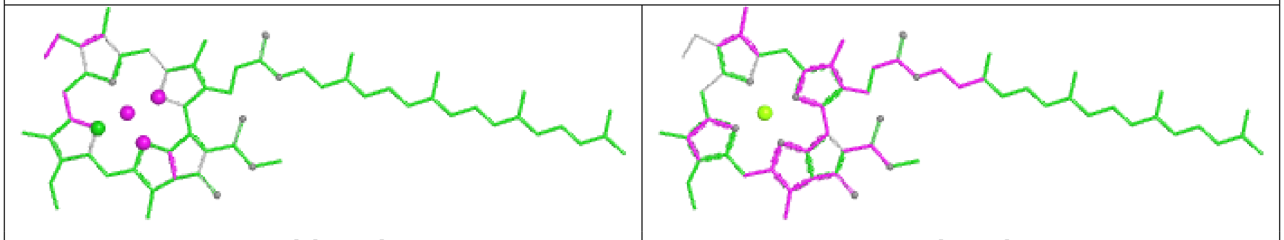
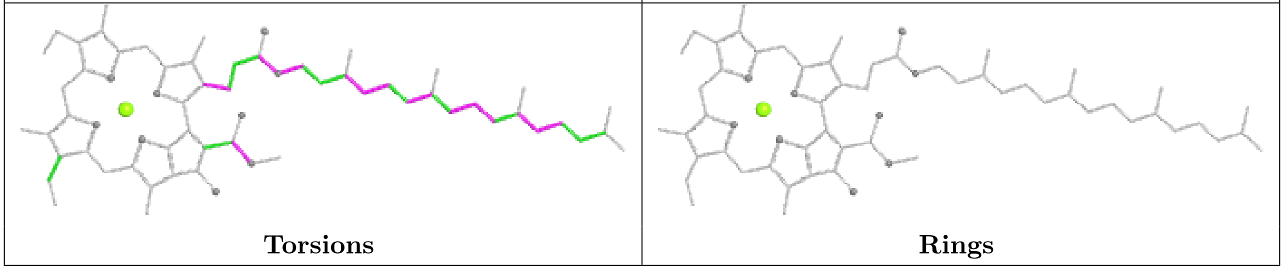


Bond lengths Bond angles



Torsions Rings

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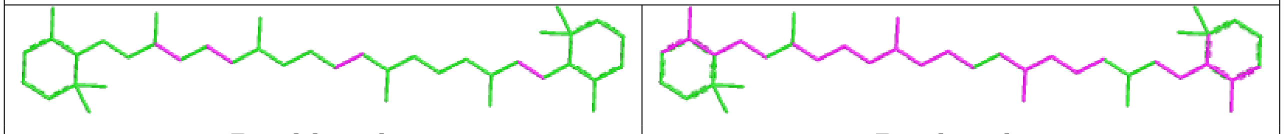

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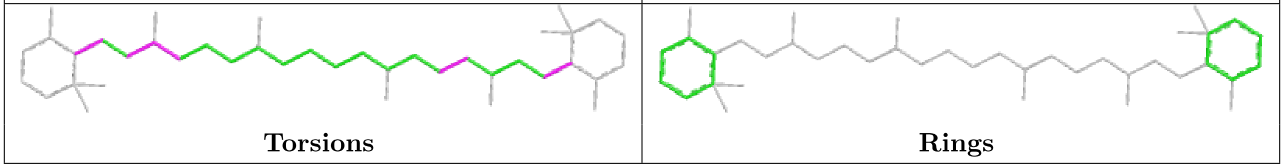

Torsions Rings

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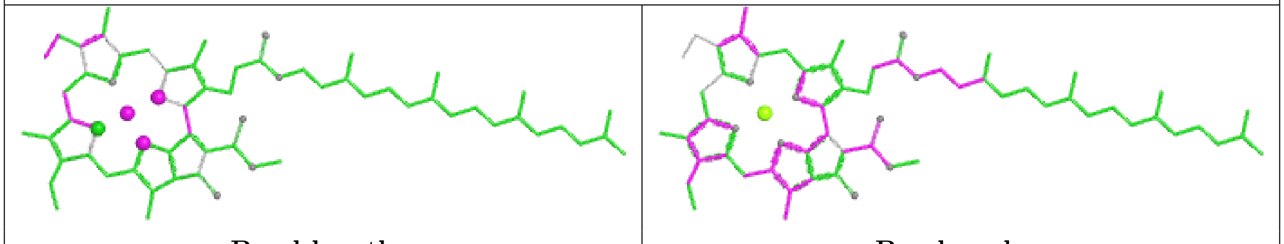
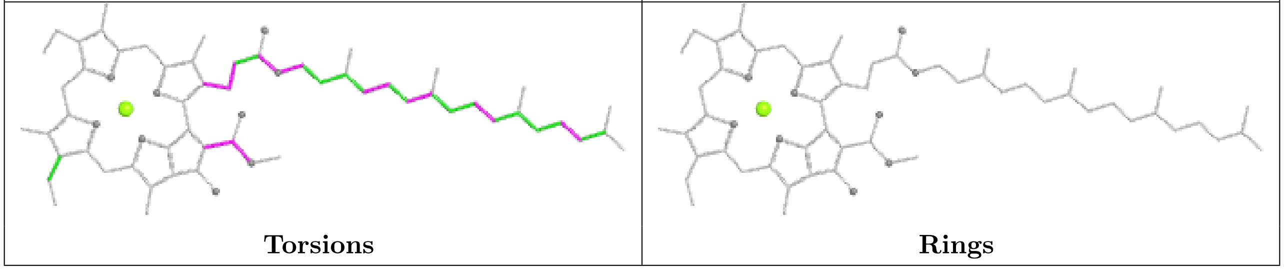


Bond lengths

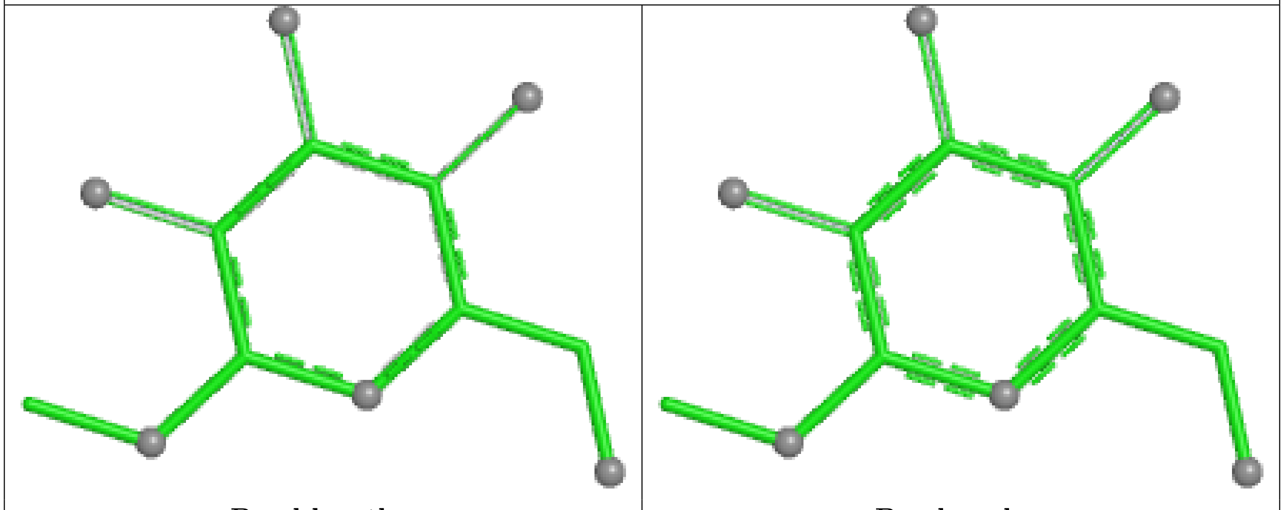
Bond angles



Torsions

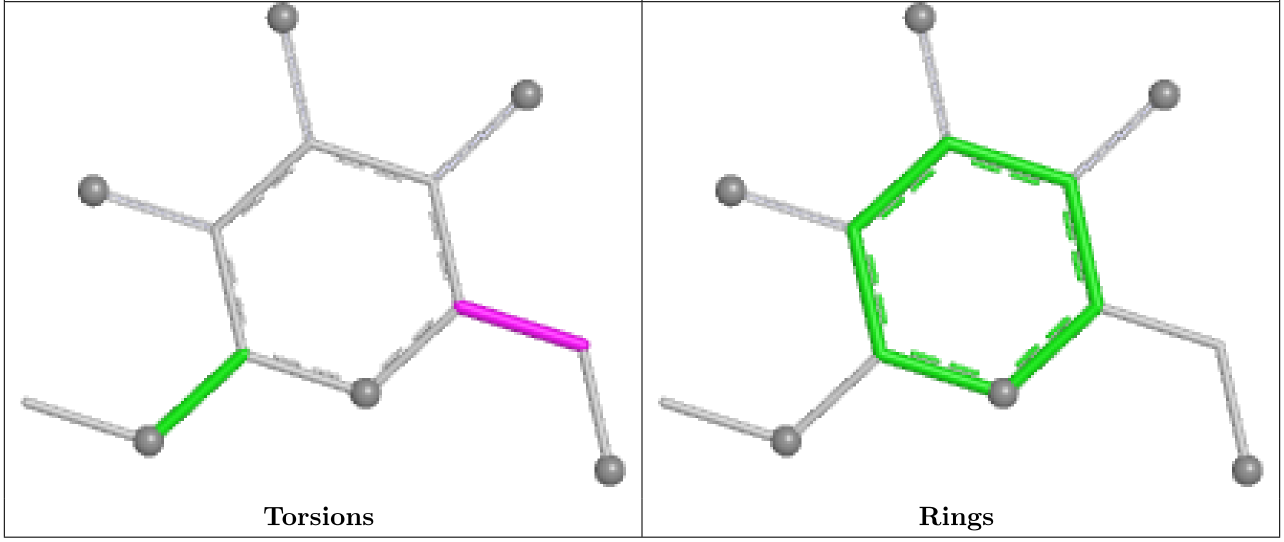
Rings

Ligand LMG 2 806



Bond lengths

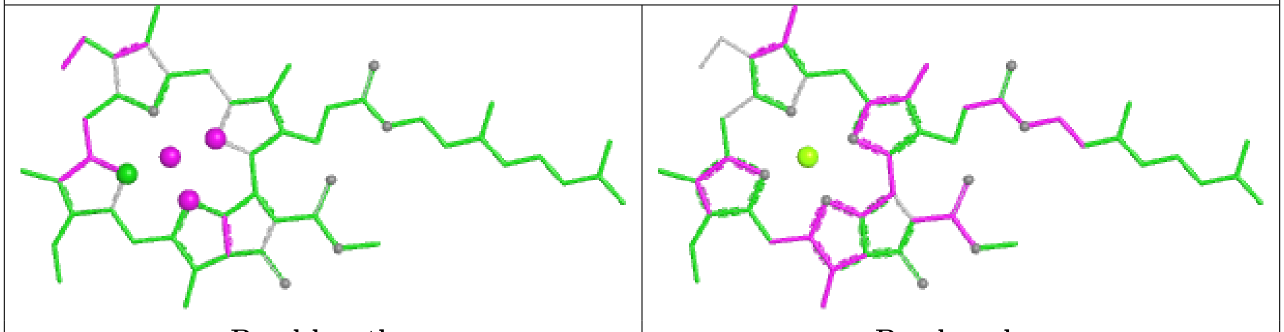
Bond angles



Torsions

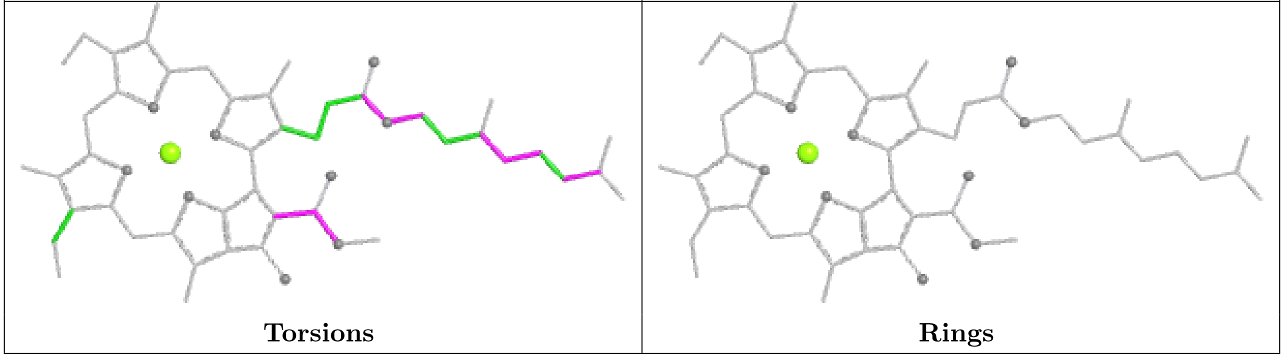
Rings

Ligand CLA B 1234



Bond lengths

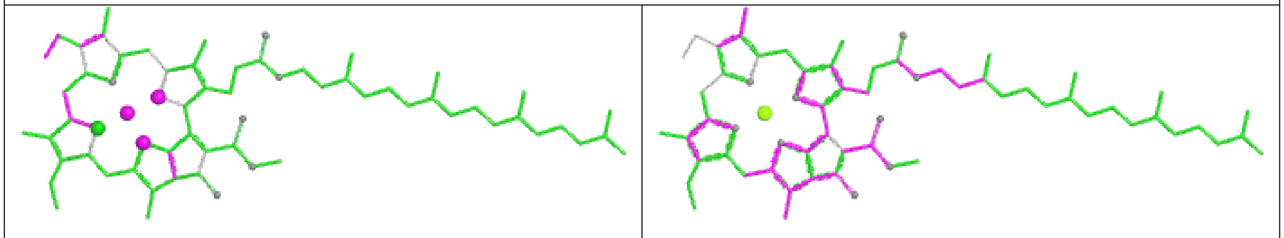
Bond angles



Torsions

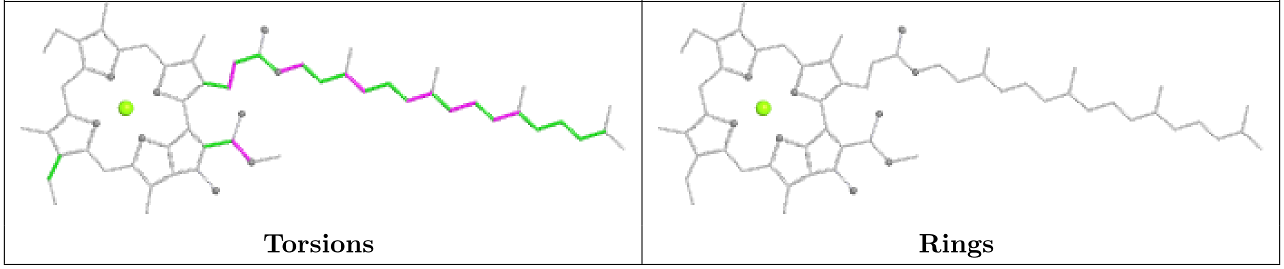
Rings

Ligand CLA B 1022



Bond lengths

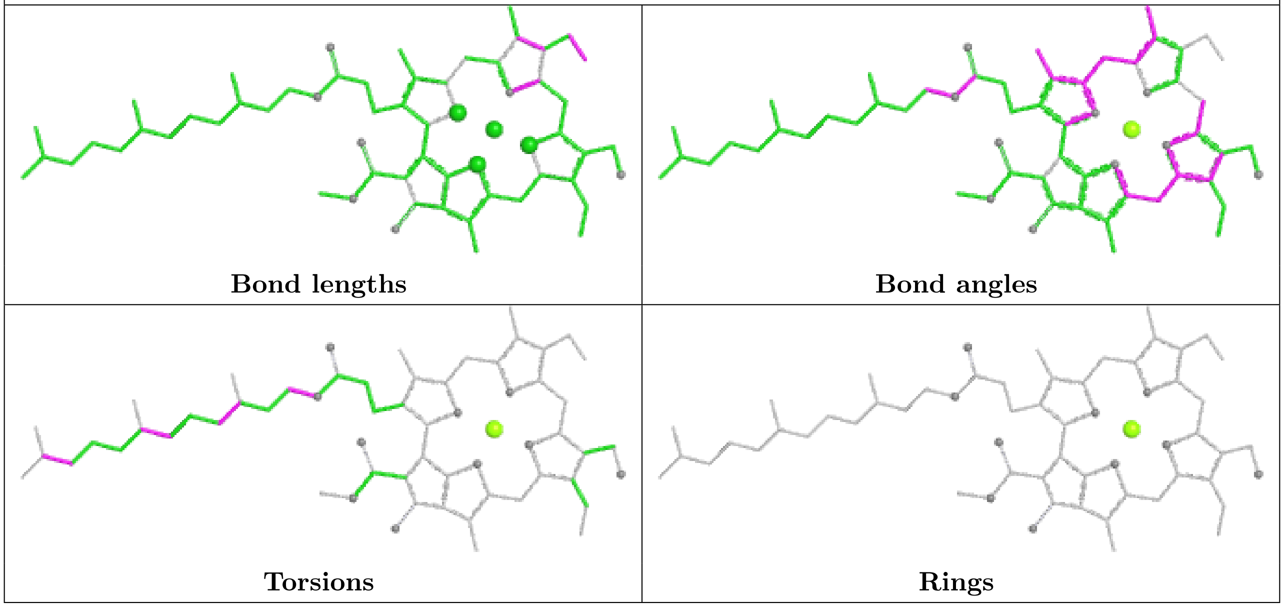
Bond angles



Torsions

Rings

Ligand CHL 1 612



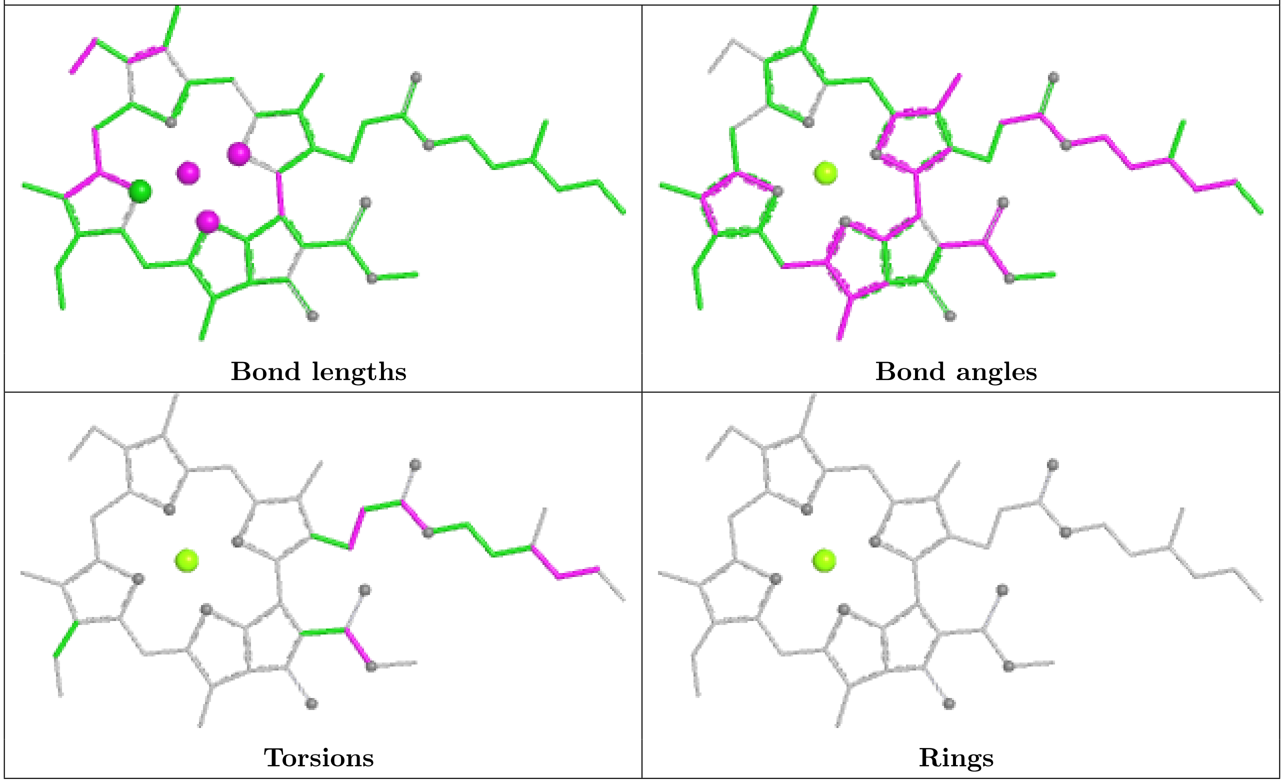
Bond lengths

Bond angles

Torsions

Rings

Ligand CLA 2 602



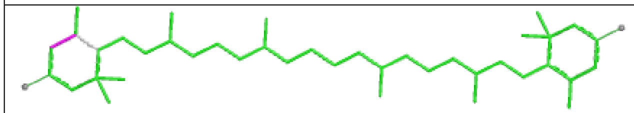
Bond lengths

Bond angles

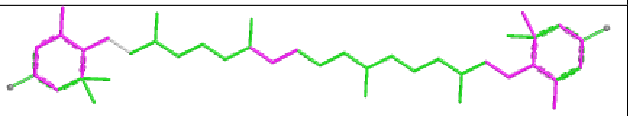
Torsions

Rings

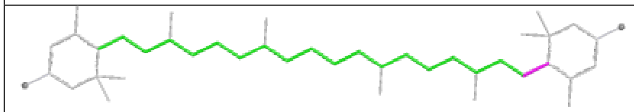
Ligand LUT 1 501



Bond lengths



Bond angles



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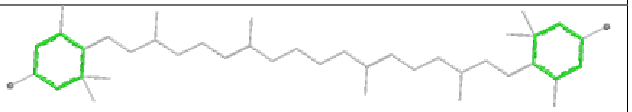
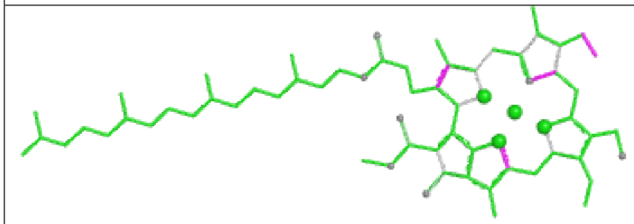
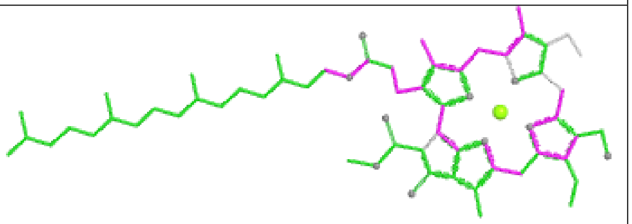


Rings

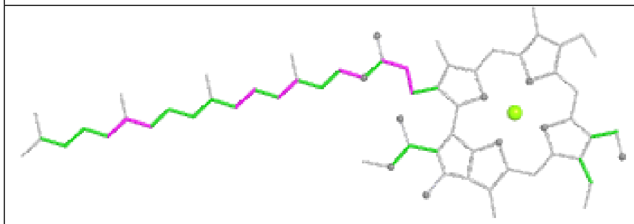
Ligand CHL 3 604



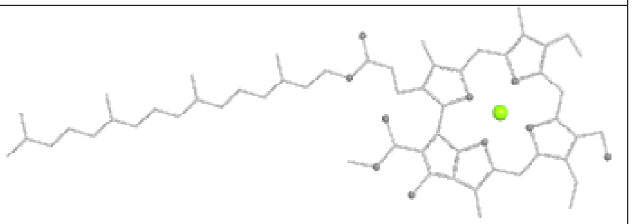
Bond lengths



Bond angles

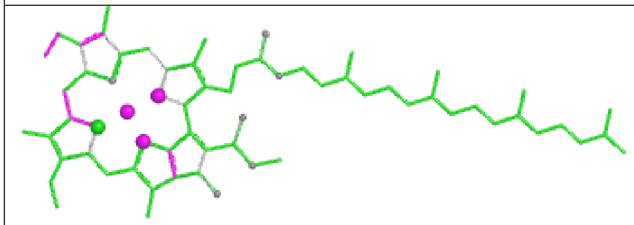


Torsions

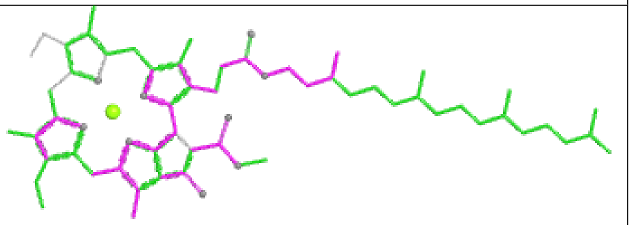


Rings

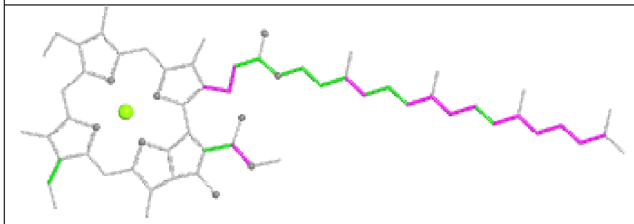
Ligand CLA A 1012



Bond lengths



Bond angles



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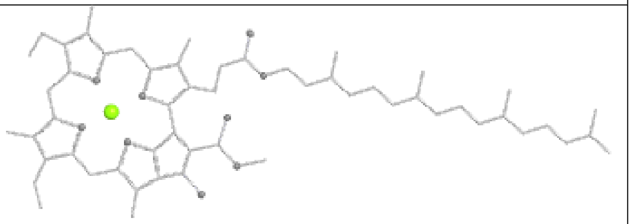
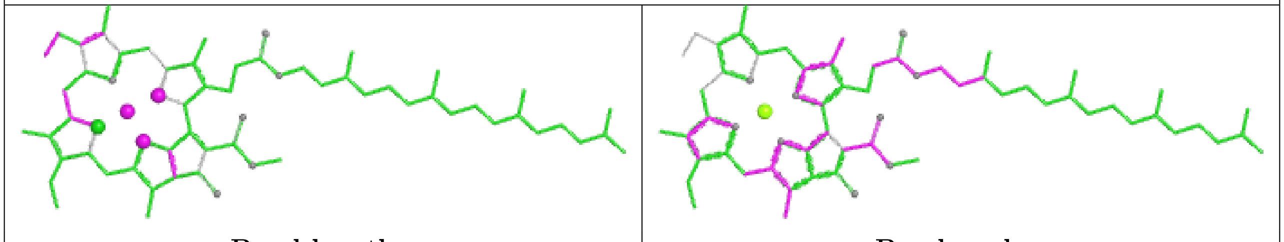
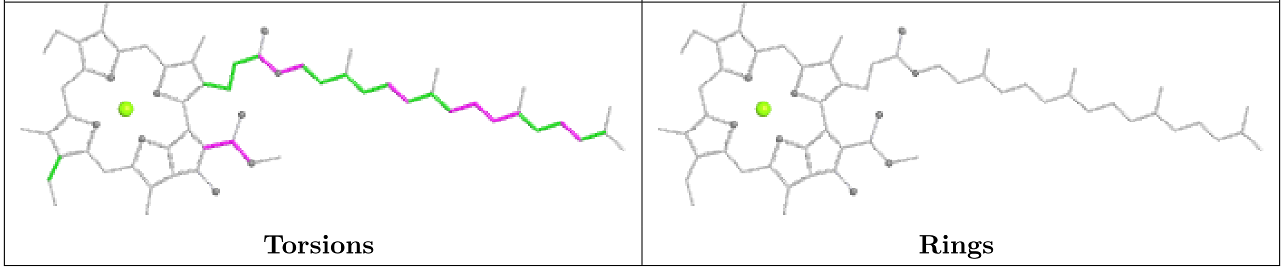


Rings

Ligand CLA B 1227

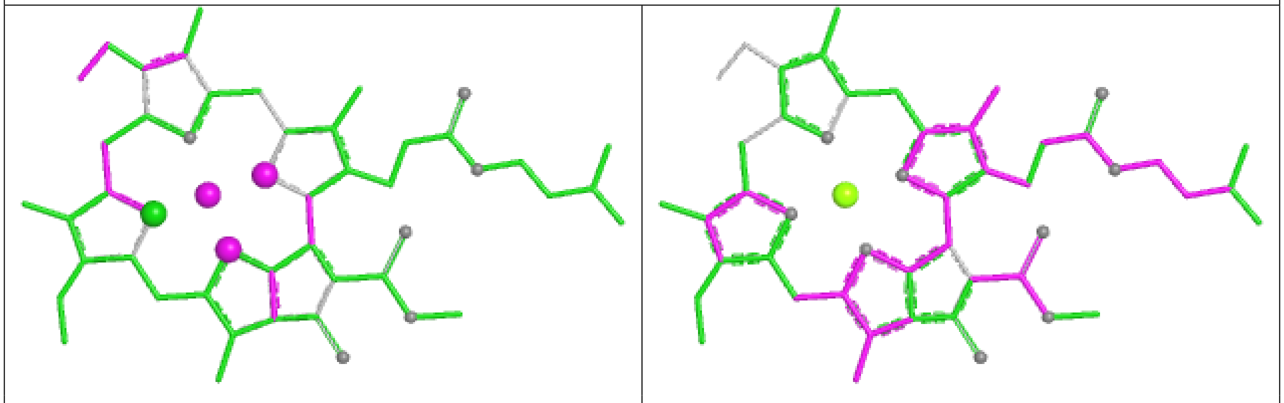


Bond lengths **Bond angles**

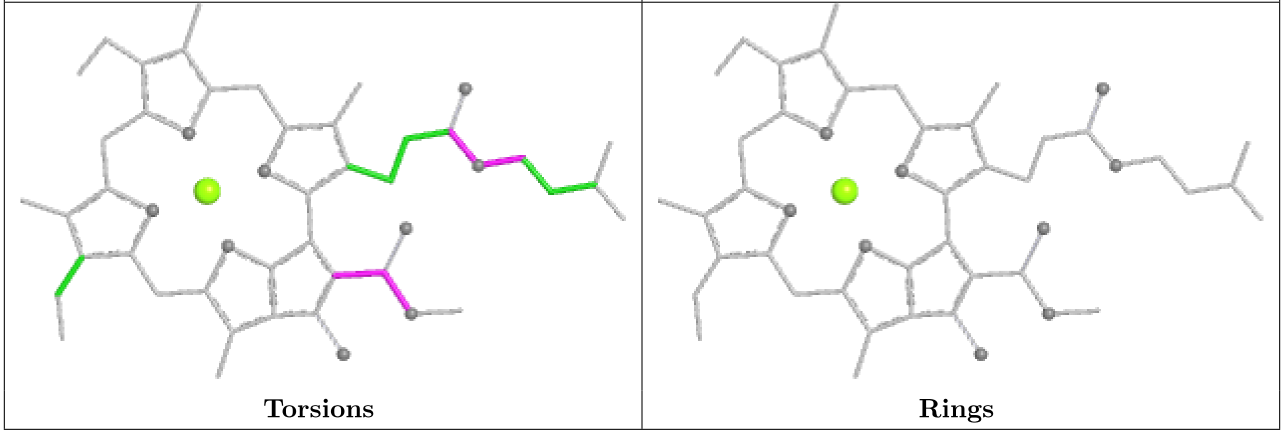


Torsions **Rings**

Ligand CLA 1 606

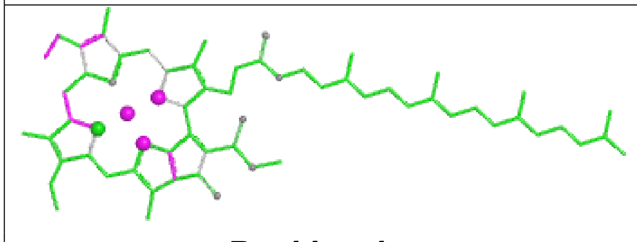


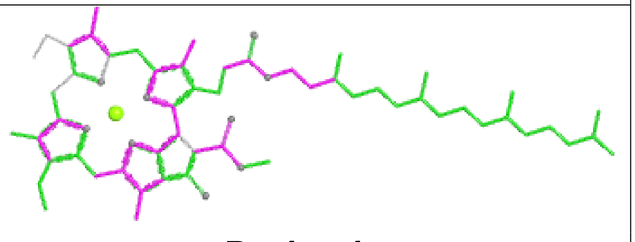
Bond lengths **Bond angles**

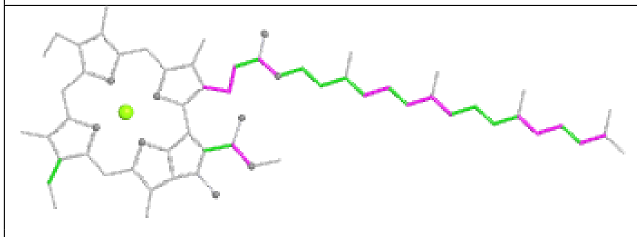


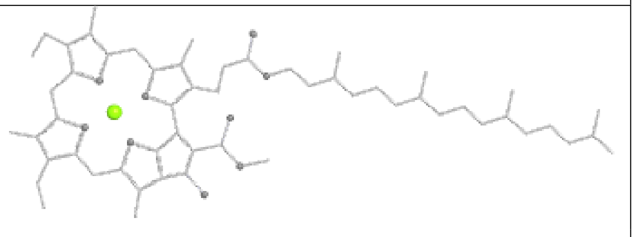
Torsions **Rings**

Ligand CLA B 1223

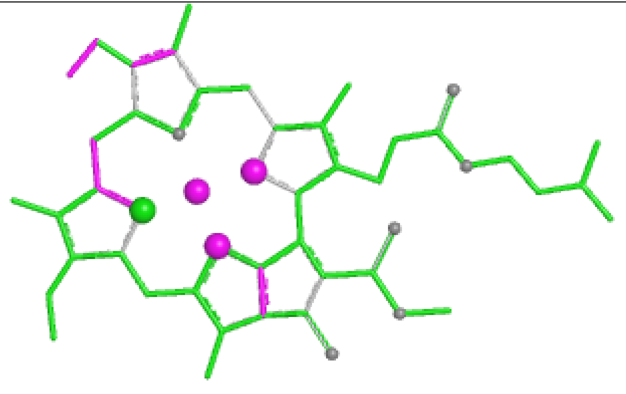

Bond lengths

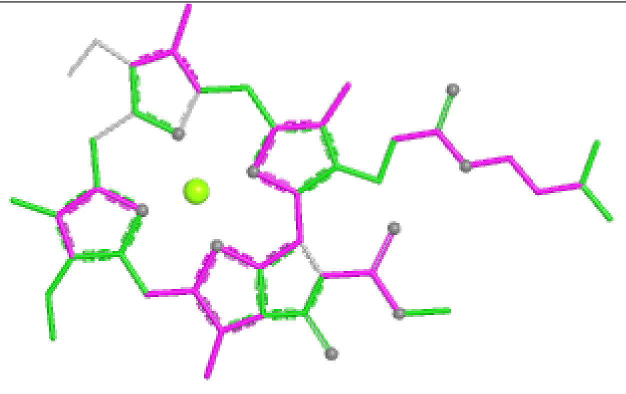

Bond angles

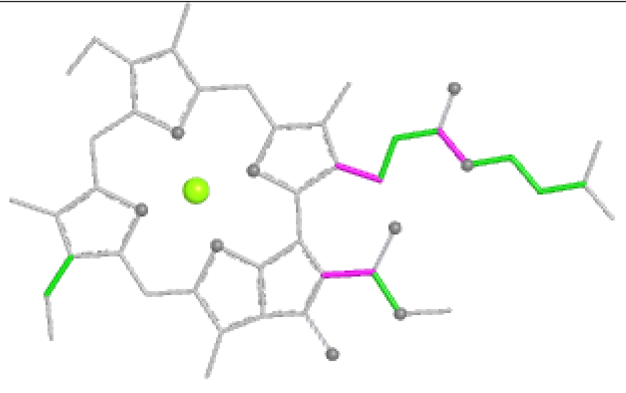

Torsions


Rings

Ligand CLA L 1501


Bond lengths


Bond angles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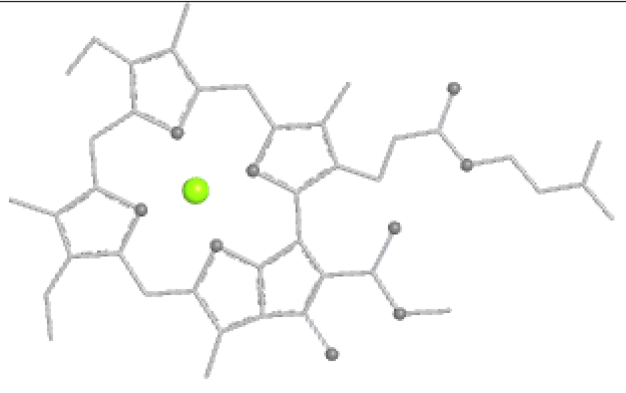
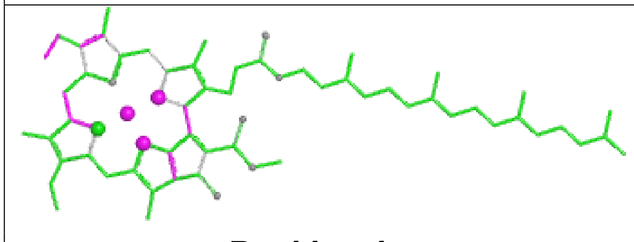
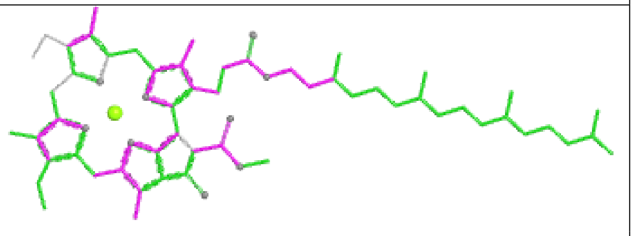

Rings

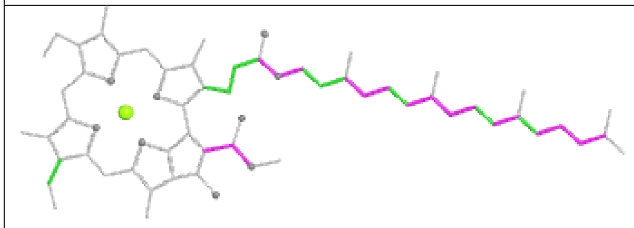
Ligand CLA A 1127



Bond lengths



Bond angles



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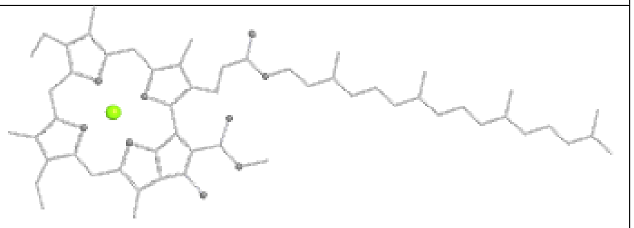
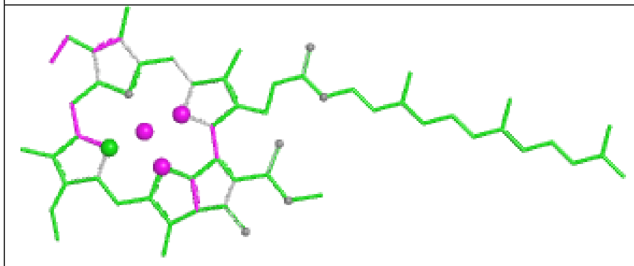
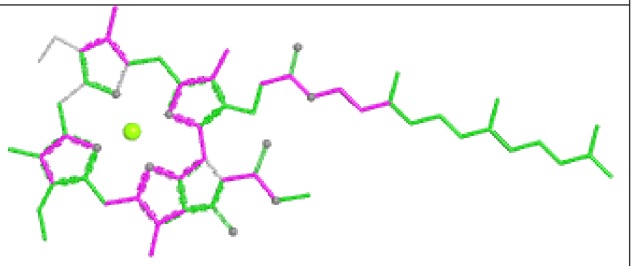


Rings

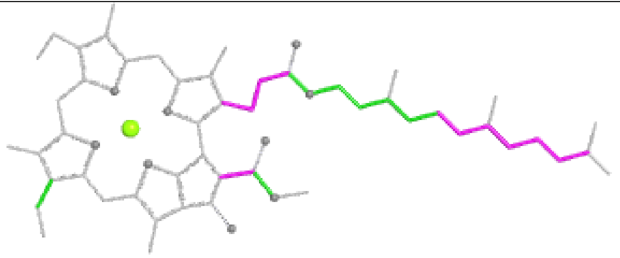
Ligand CLA L 1502



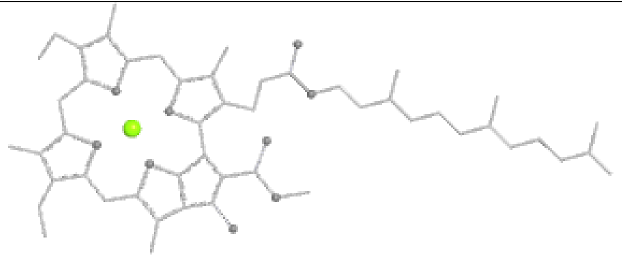
Bond lengths



Bond angles

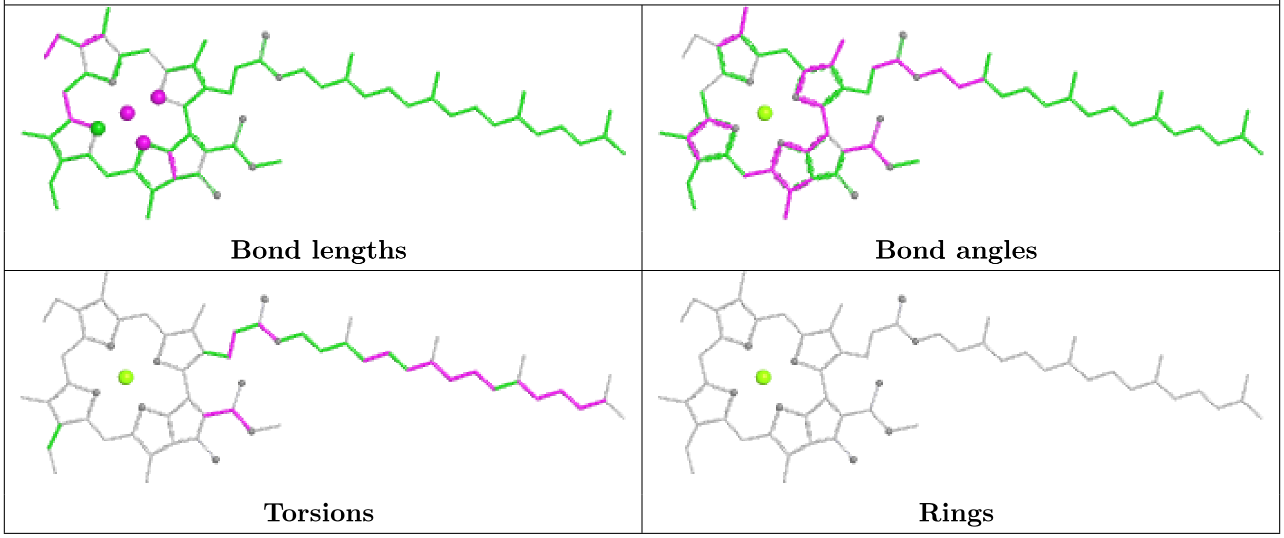


Torsions



Rings

Ligand CLA B 1237



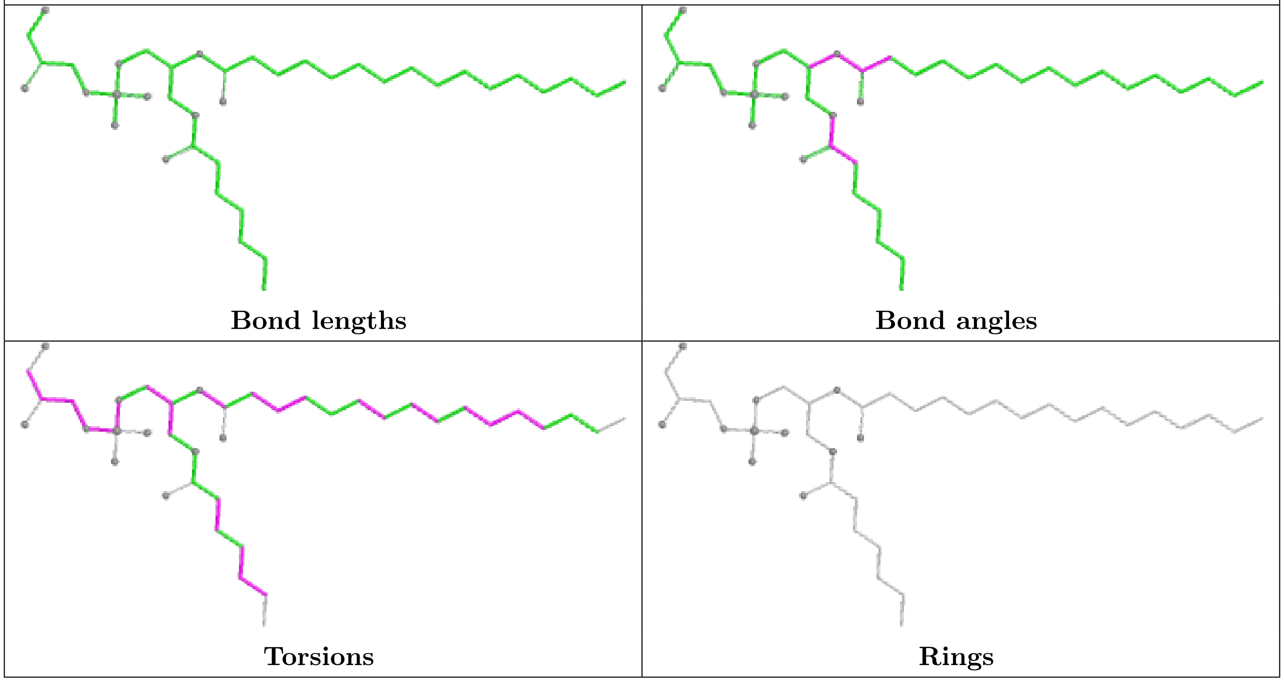
Bond lengths

Bond angles

Torsions

Rings

Ligand LHG A 5001



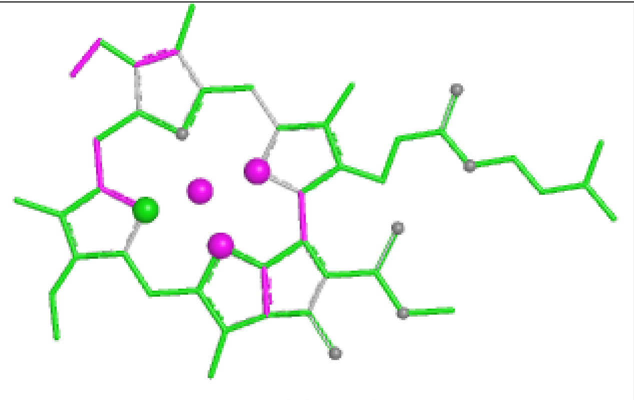
Bond lengths

Bond angles

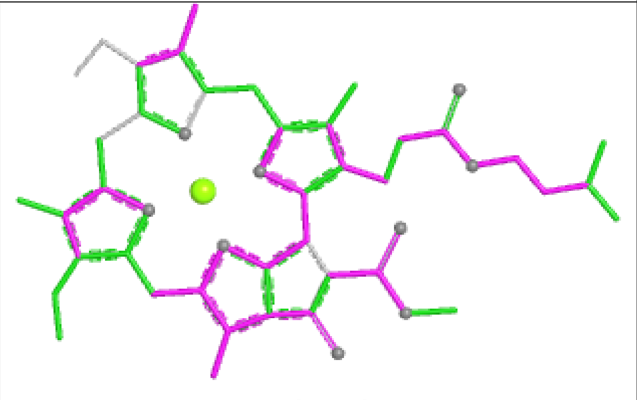
Torsions

Rings

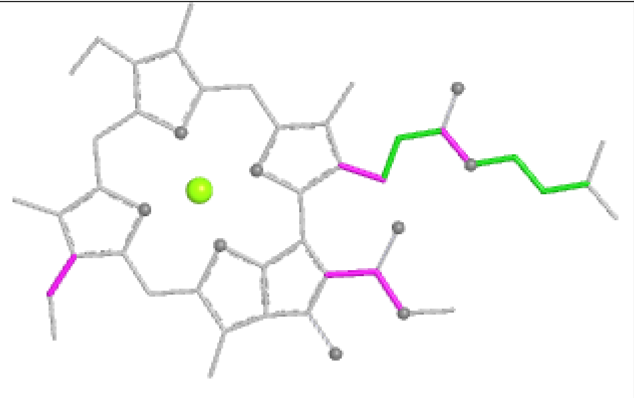
Ligand CLA 3 606



Bond lengths



Bond angles



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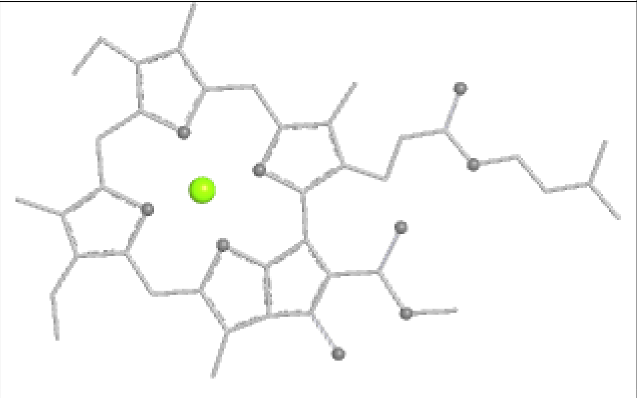
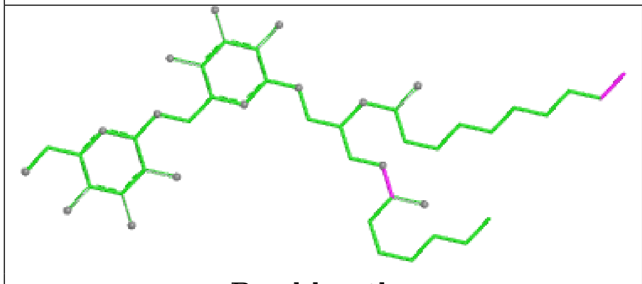


Rings

Ligand DGD G 5003



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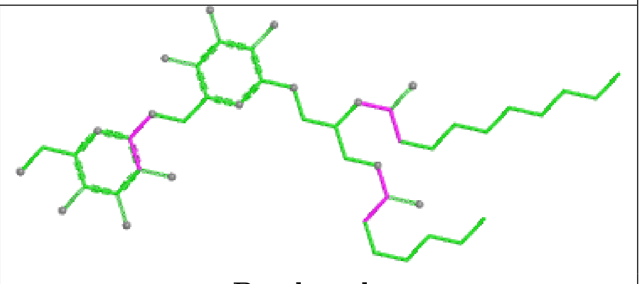
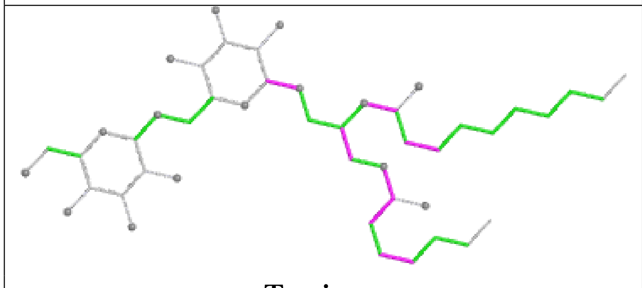
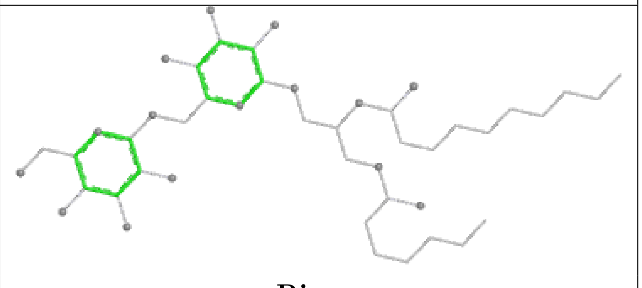


Bond angles

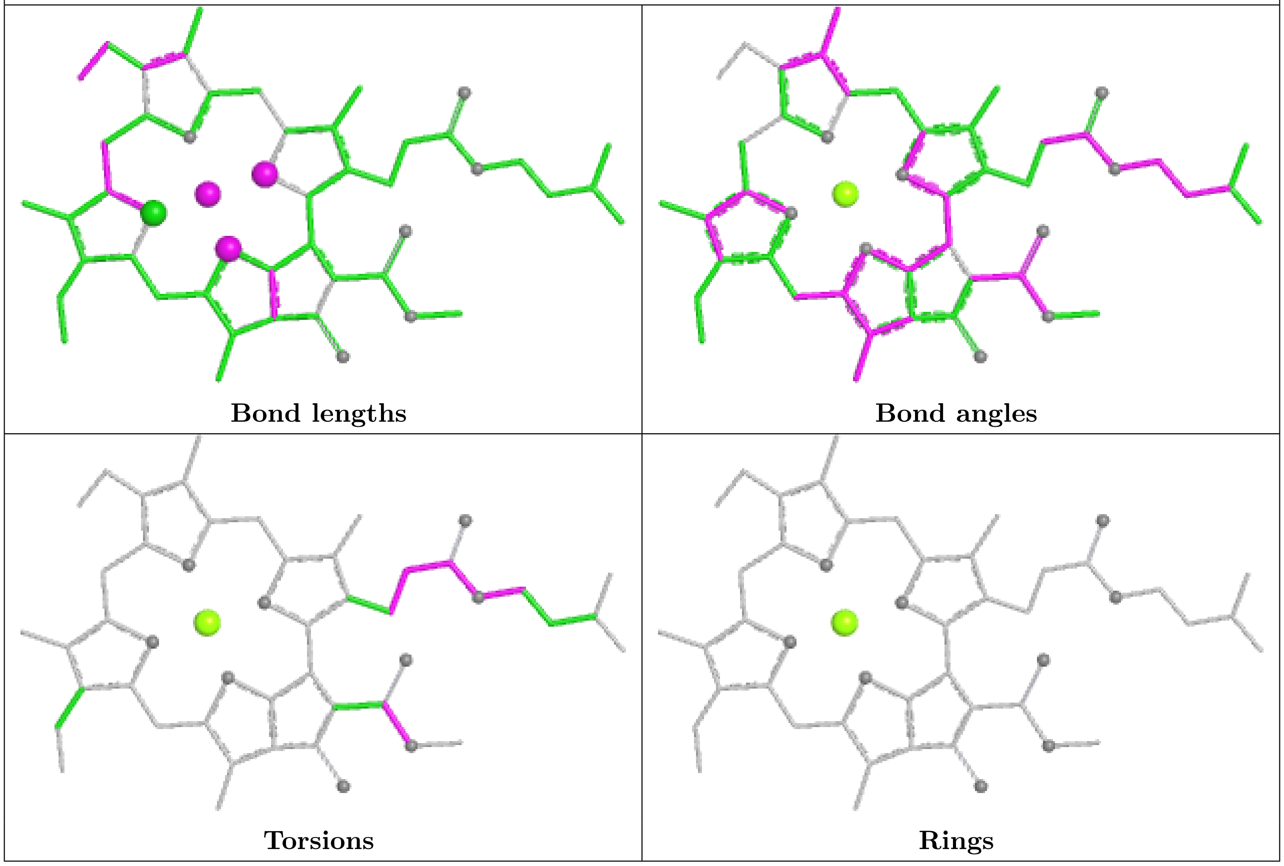


Torsions



Rings

Ligand CLA 4 606



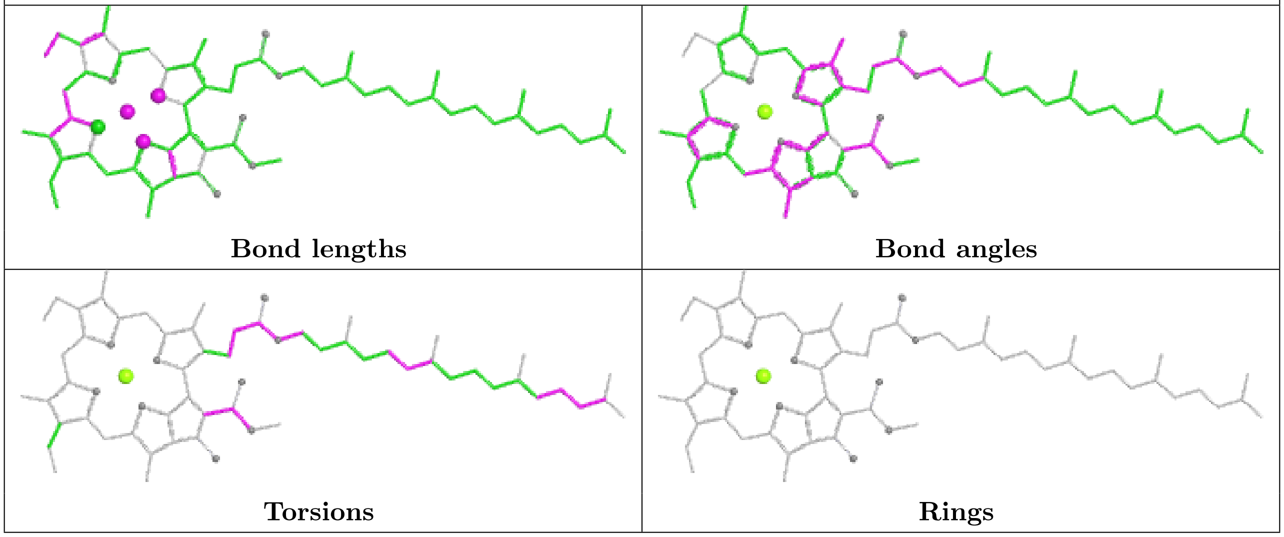
Bond lengths

Bond angles

Torsions

Rings

Ligand CLA B 1235



Bond lengths

Bond angles

Torsions

Rings

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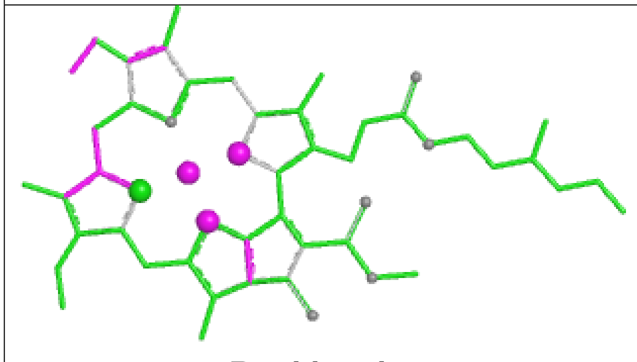
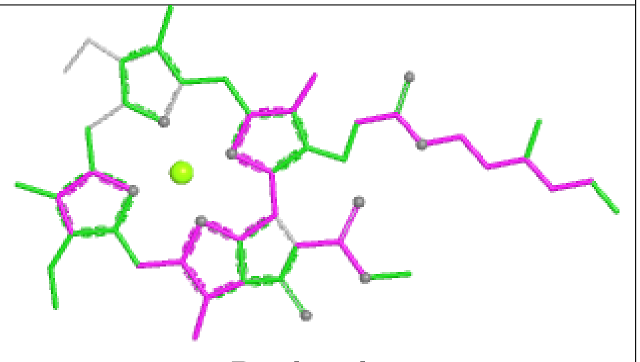
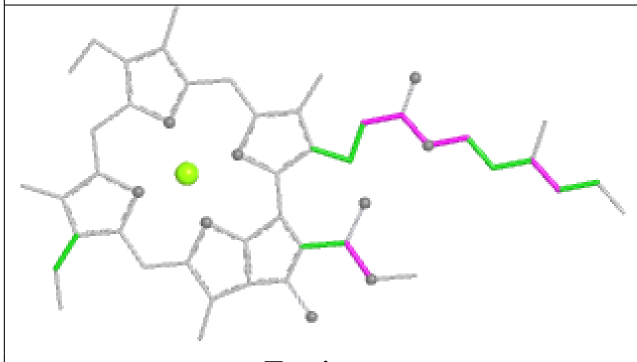

Bond lengths


Bond angles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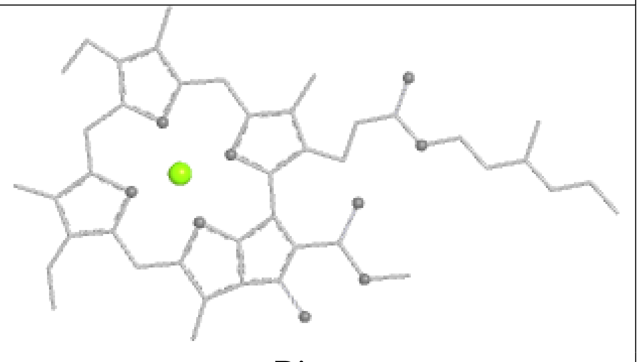
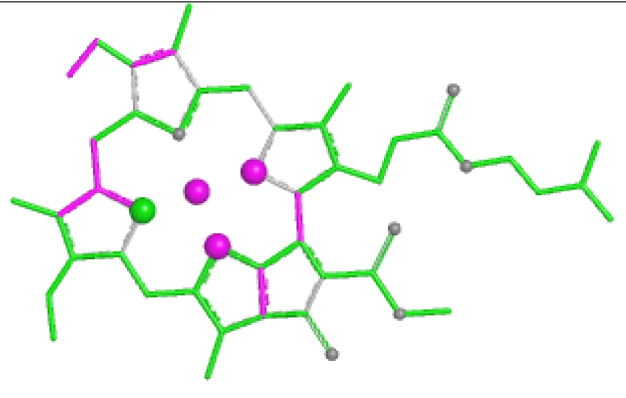
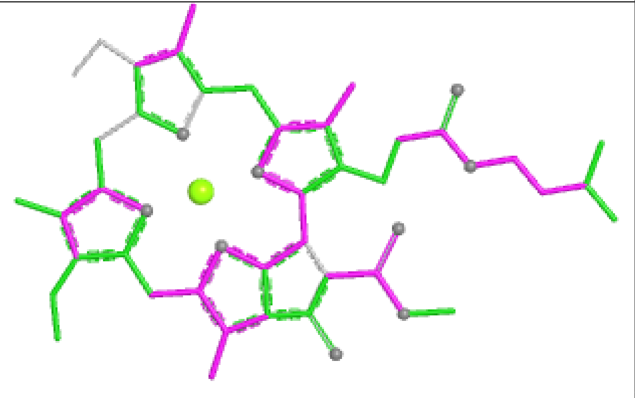
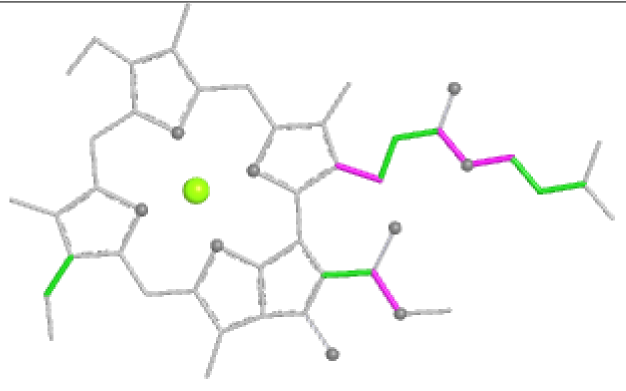
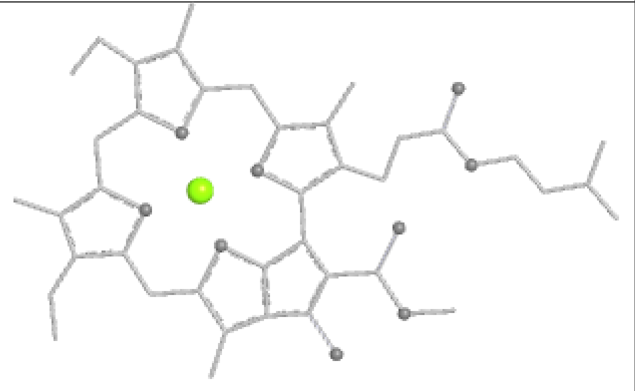

Rings

Ligand CLA J 1901

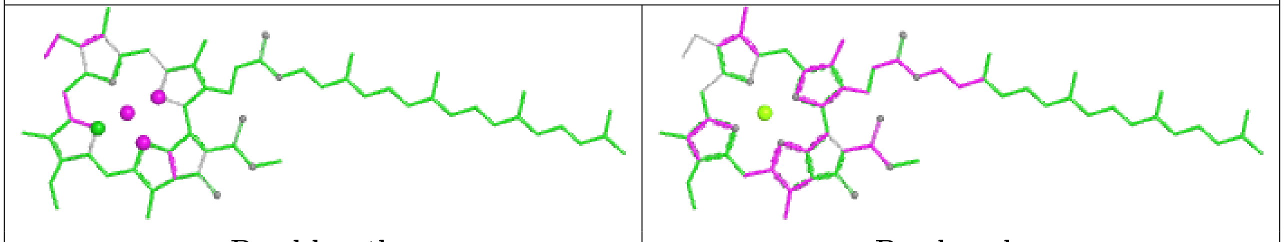

Bond lengths


Bond angles

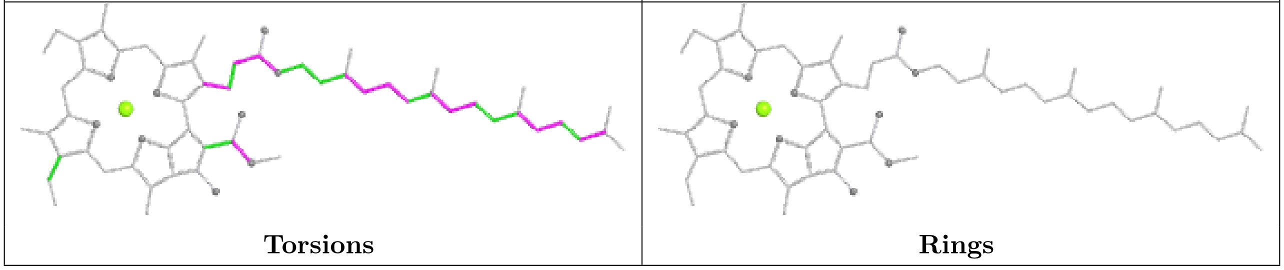

Torsions


Rings

Ligand CLA B 1215

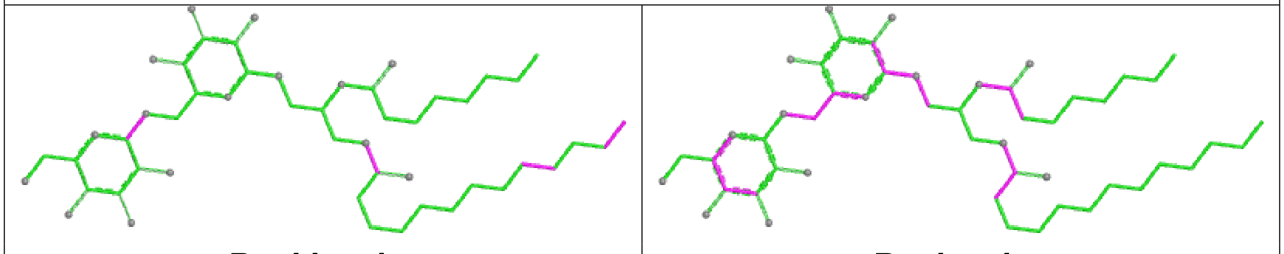


Bond lengths **Bond angles**

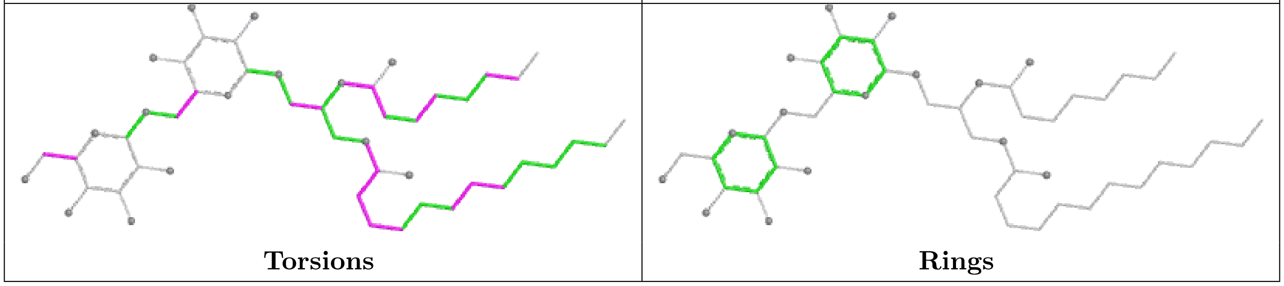


Torsions **Rings**

Ligand DGD 4 801

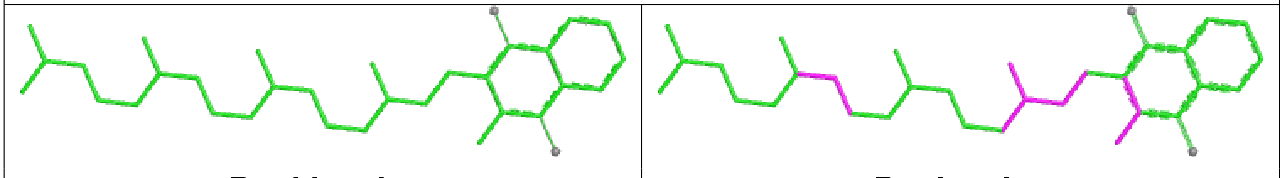


Bond lengths **Bond angles**

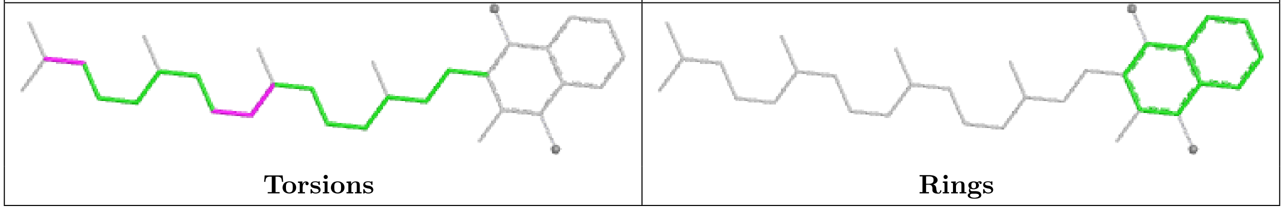


Torsions **Rings**

Ligand PQN A 2001

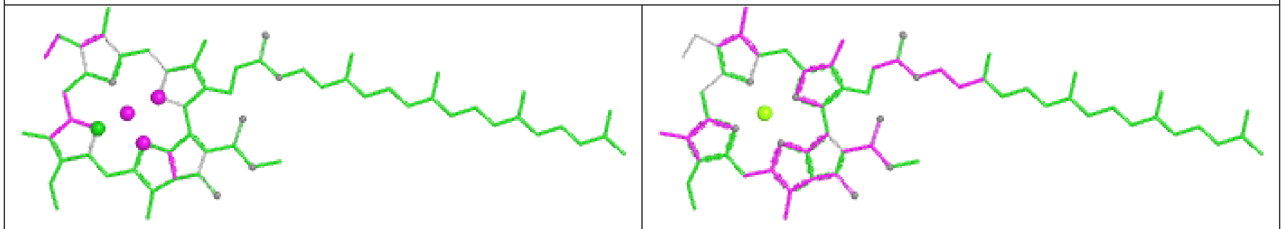


Bond lengths **Bond angles**



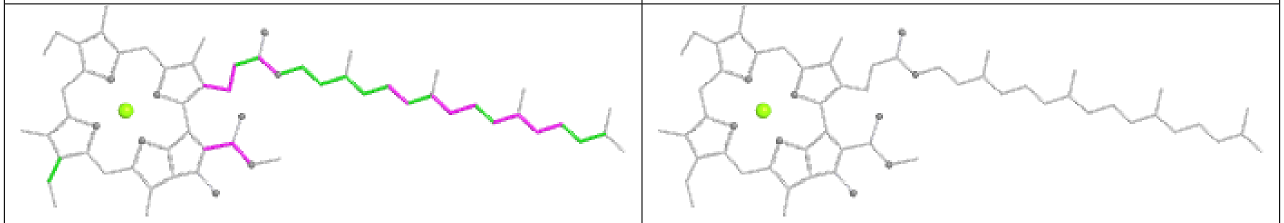
Torsions **Rings**

Ligand CLA B 1201



Bond lengths

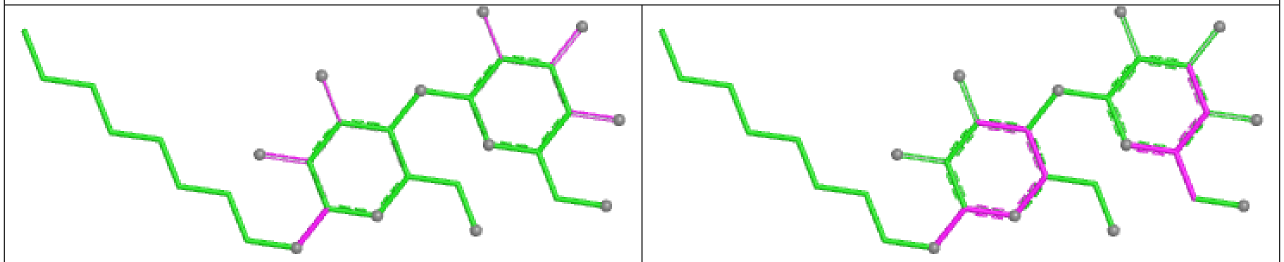
Bond angles



Torsions

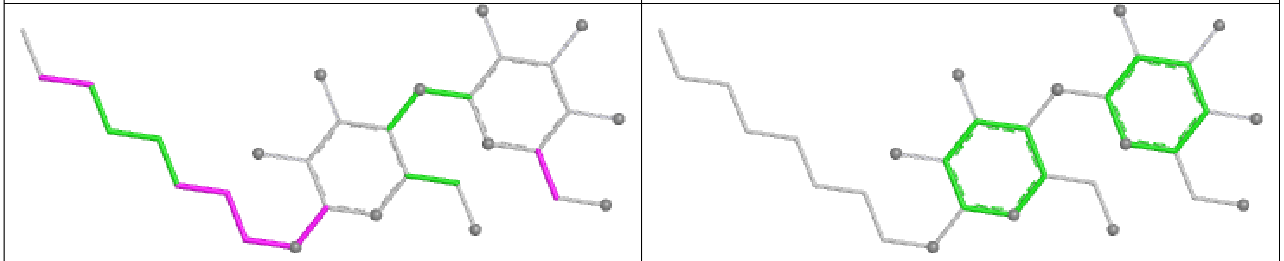
Rings

Ligand LMT G 5005



Bond lengths

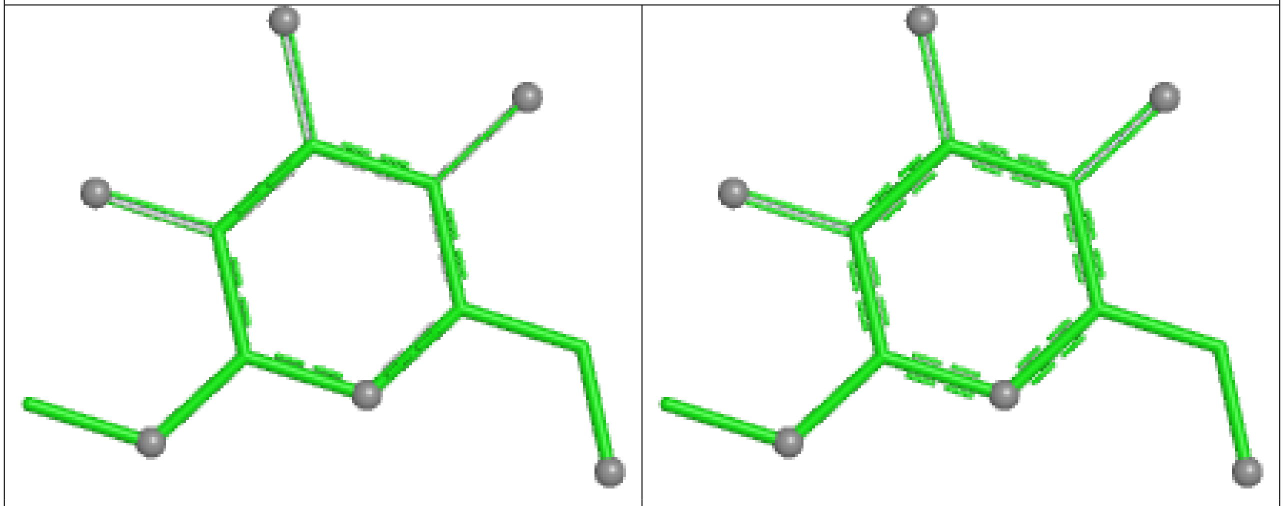
Bond angles



Torsions

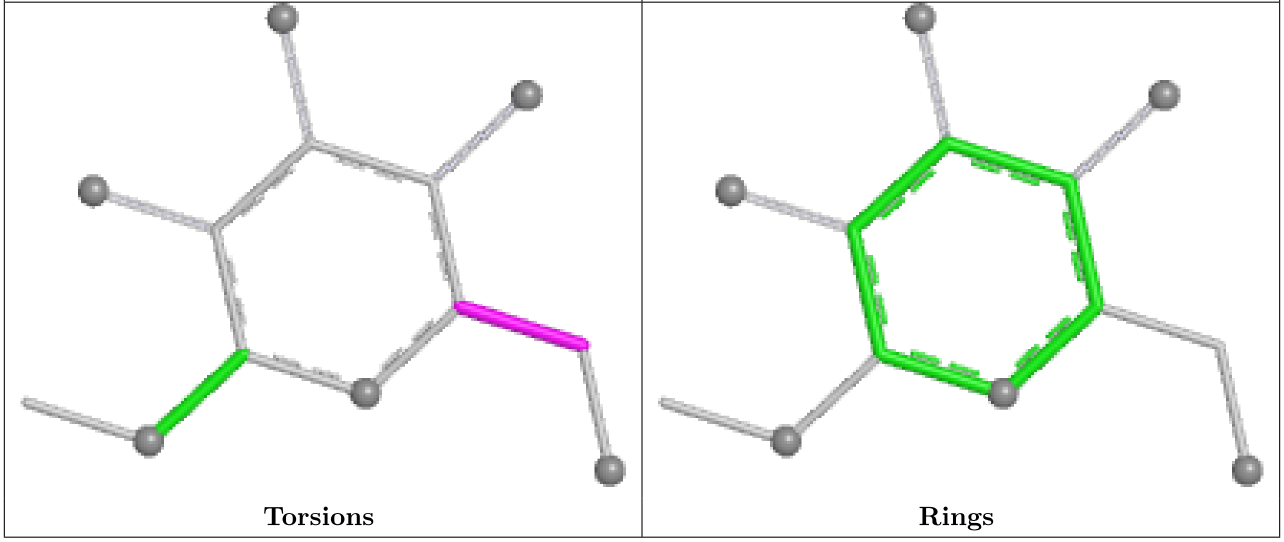
Rings

Ligand LMG F 5006



Bond lengths

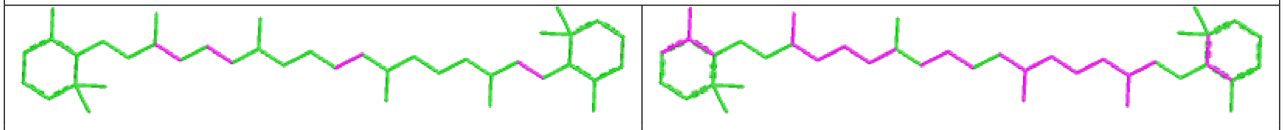
Bond angles



Torsions

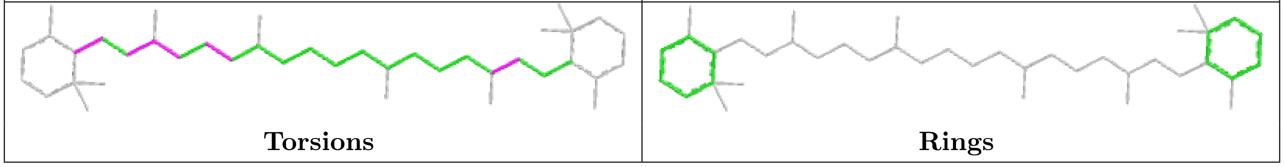
Rings

Ligand BCR K 4001



Bond lengths

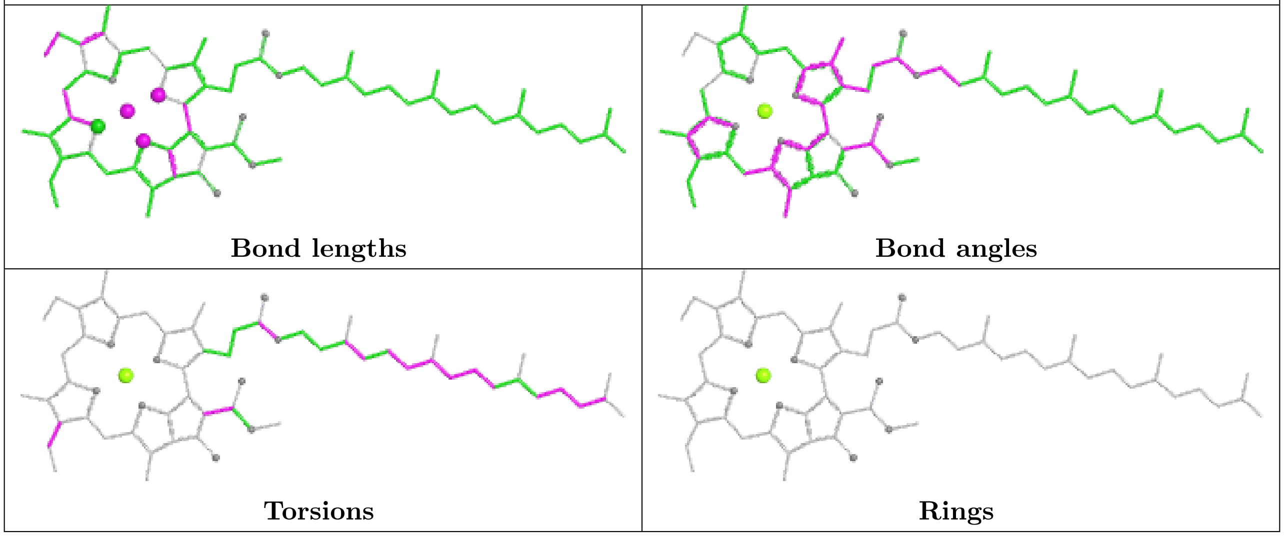
Bond angles



Torsions

Rings

Ligand CLA A 1122



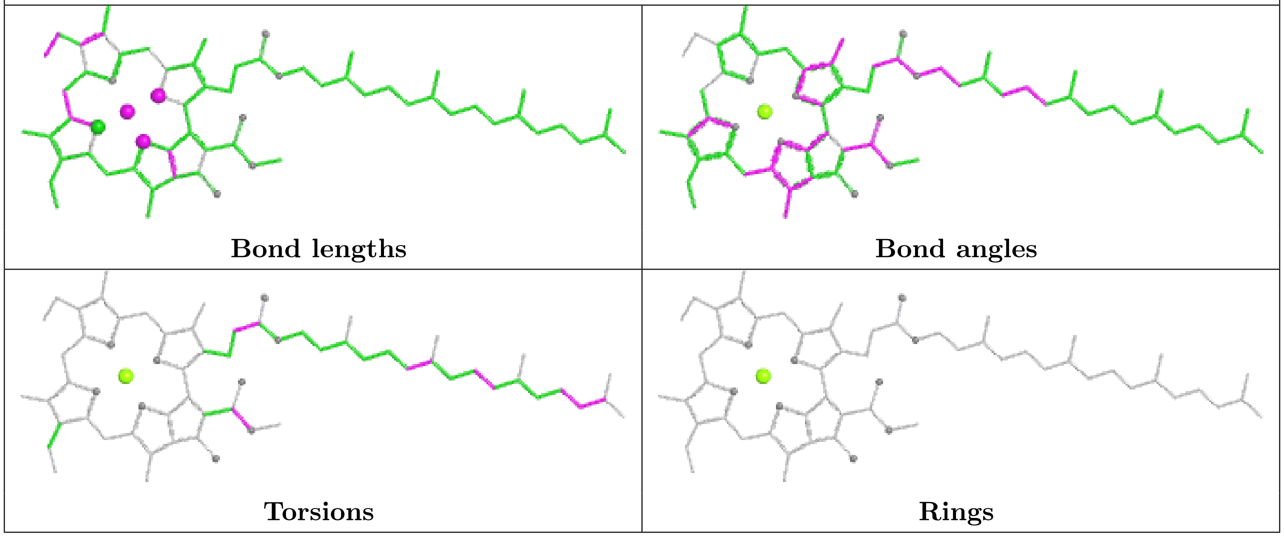
Bond lengths

Bond angles

Torsions

Rings

Ligand CLA A 1140



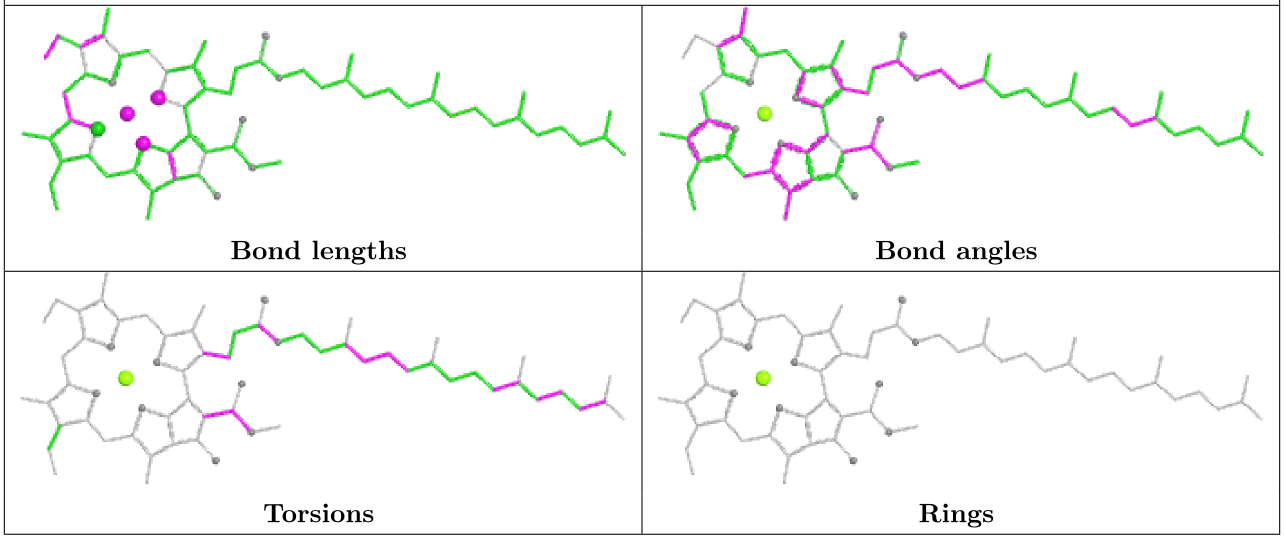
Bond lengths

Bond angles

Torsions

Rings

Ligand CLA A 1104



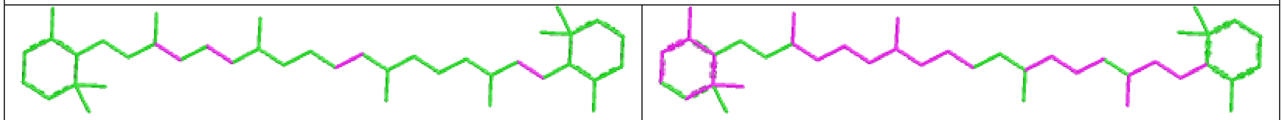
Bond lengths

Bond angles

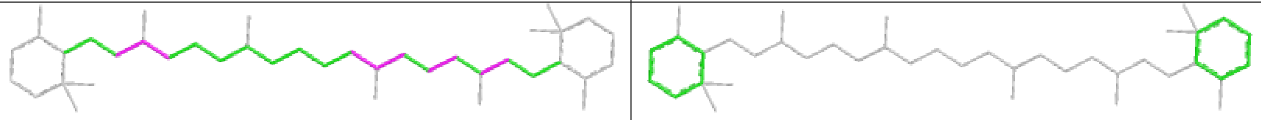
Torsions

Rings

Ligand BCR A 4011

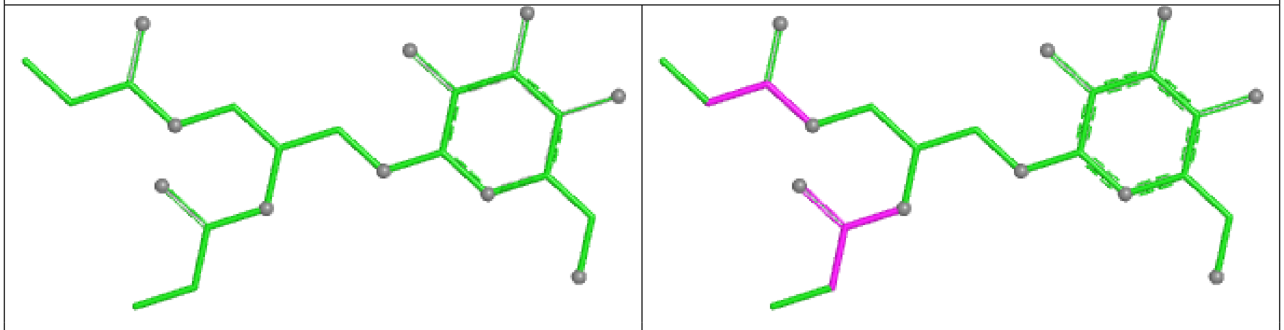


Bond lengths **Bond angles**

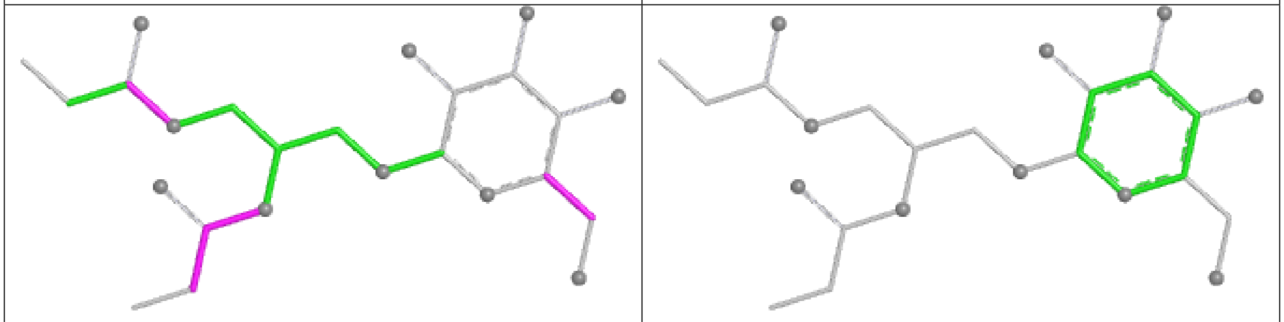


Torsions **Rings**

Ligand LMG 2 802

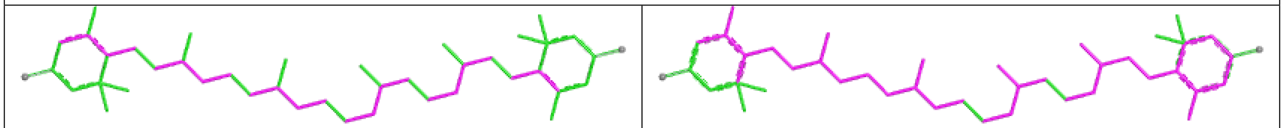


Bond lengths **Bond angles**

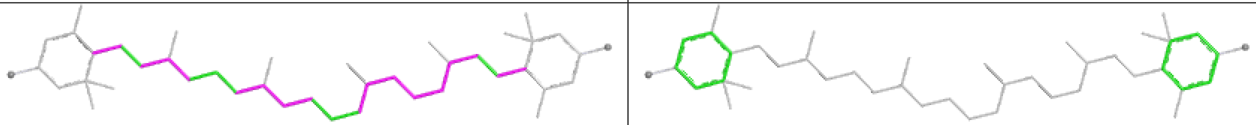


Torsions **Rings**

Ligand C7Z 4 505

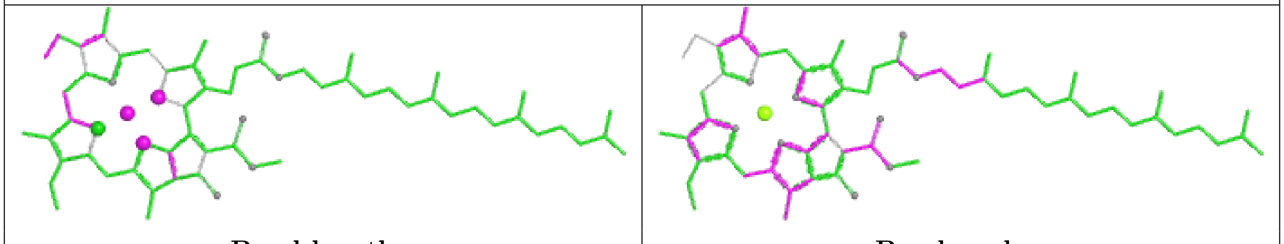


Bond lengths **Bond angles**



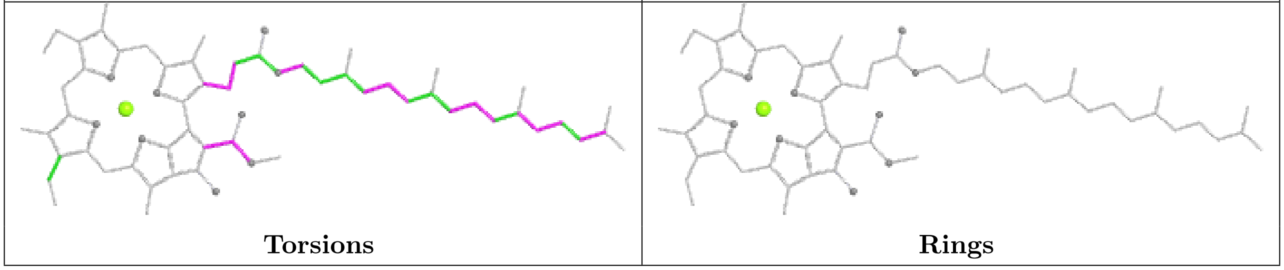
Torsions **Rings**

Ligand CLA A 1106



Bond lengths

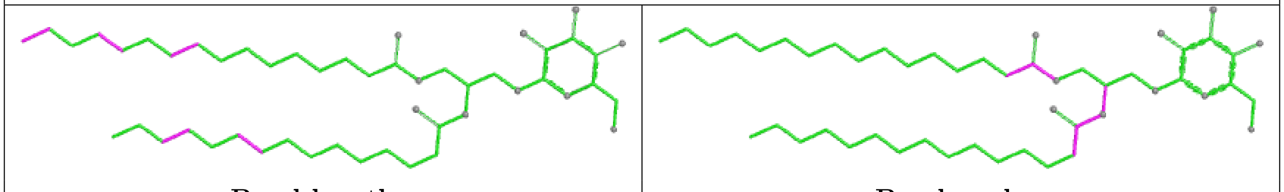
Bond angles



Torsions

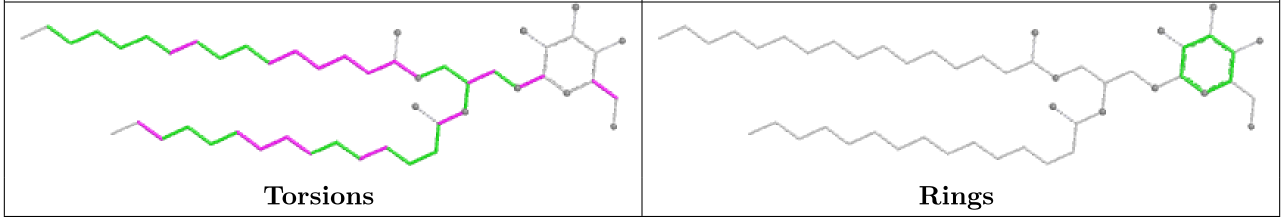
Rings

Ligand LMG G 5002



Bond lengths

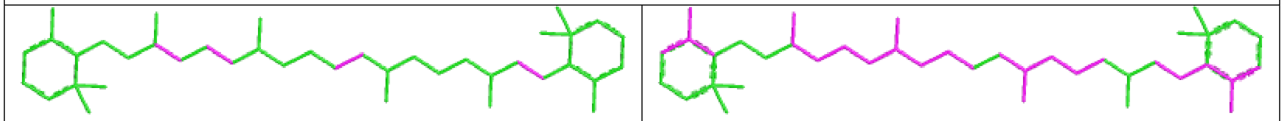
Bond angles



Torsions

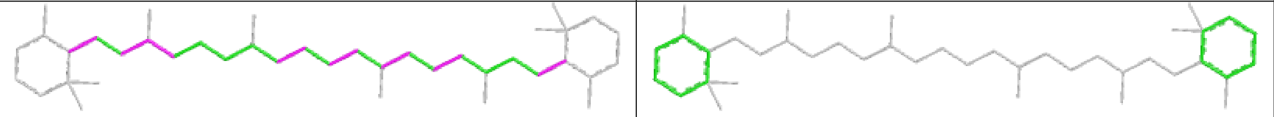
Rings

Ligand BCR 3 503



Bond lengths

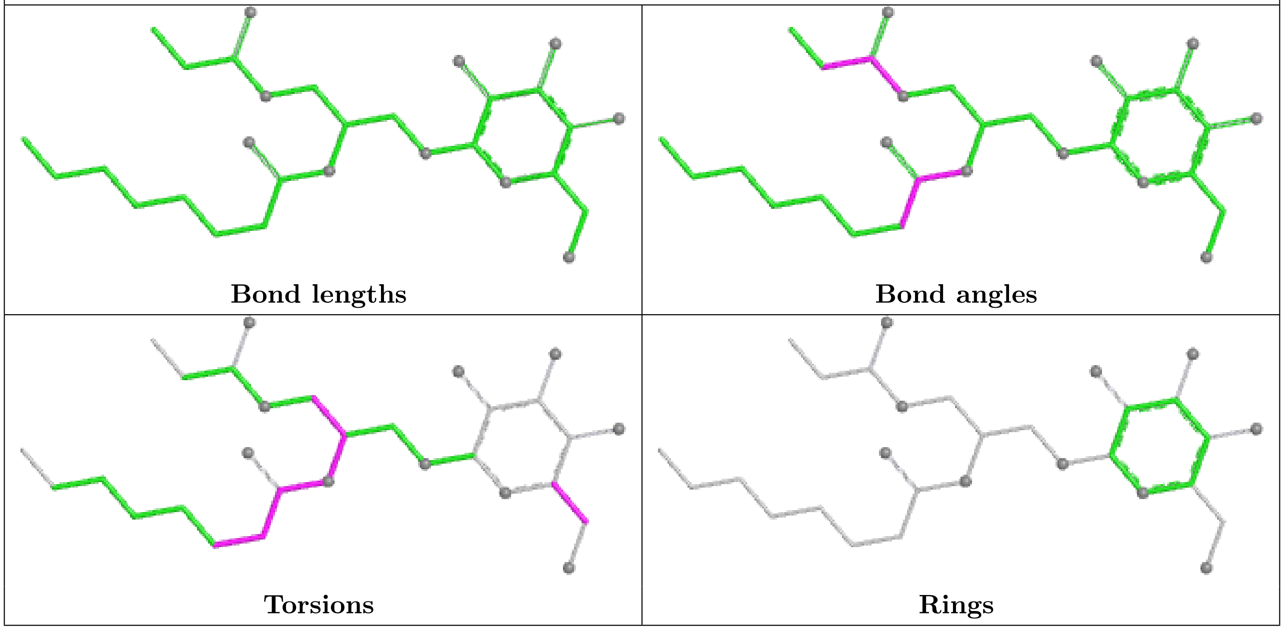
Bond angles



Torsions

Rings

Ligand LMG F 5001



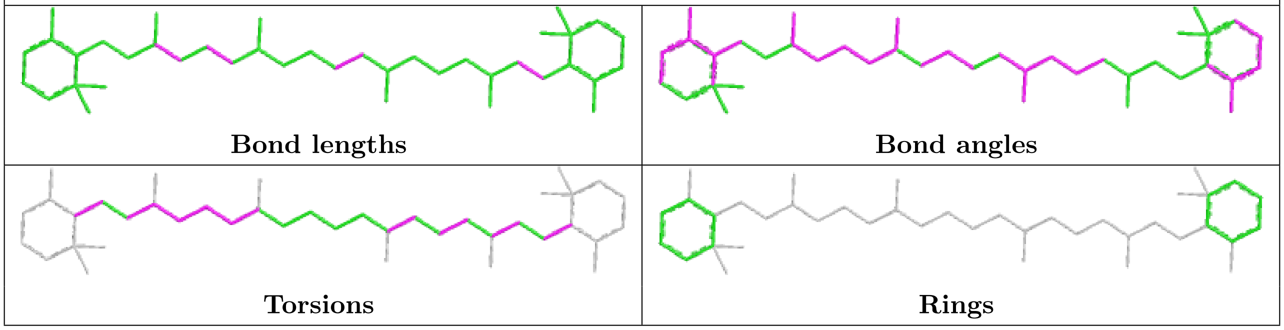
Bond lengths

Bond angles

Torsions

Rings

Ligand BCR 1 503



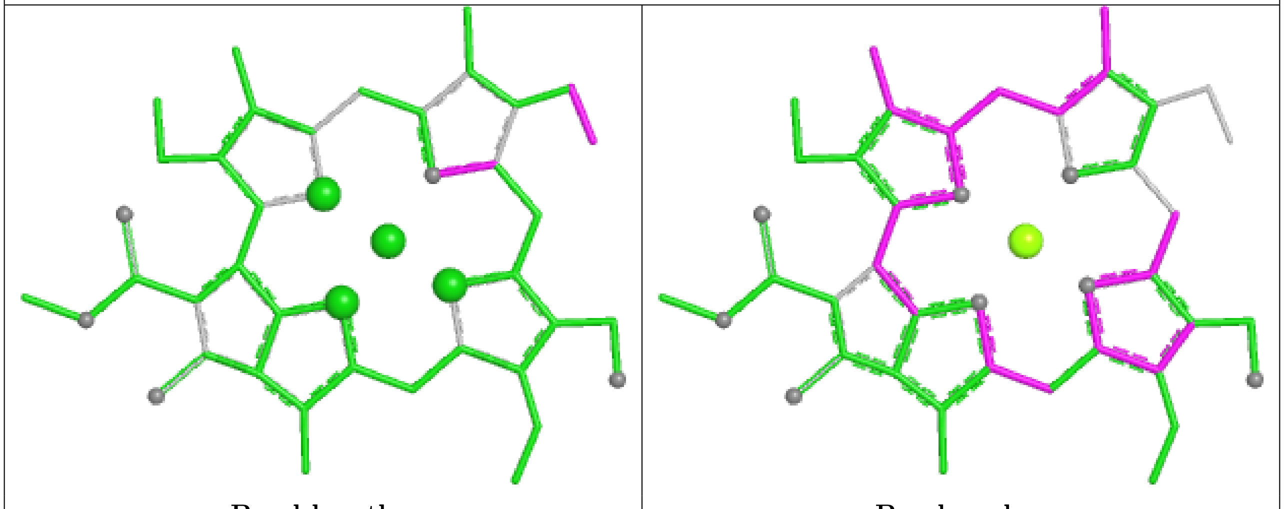
Bond lengths

Bond angles

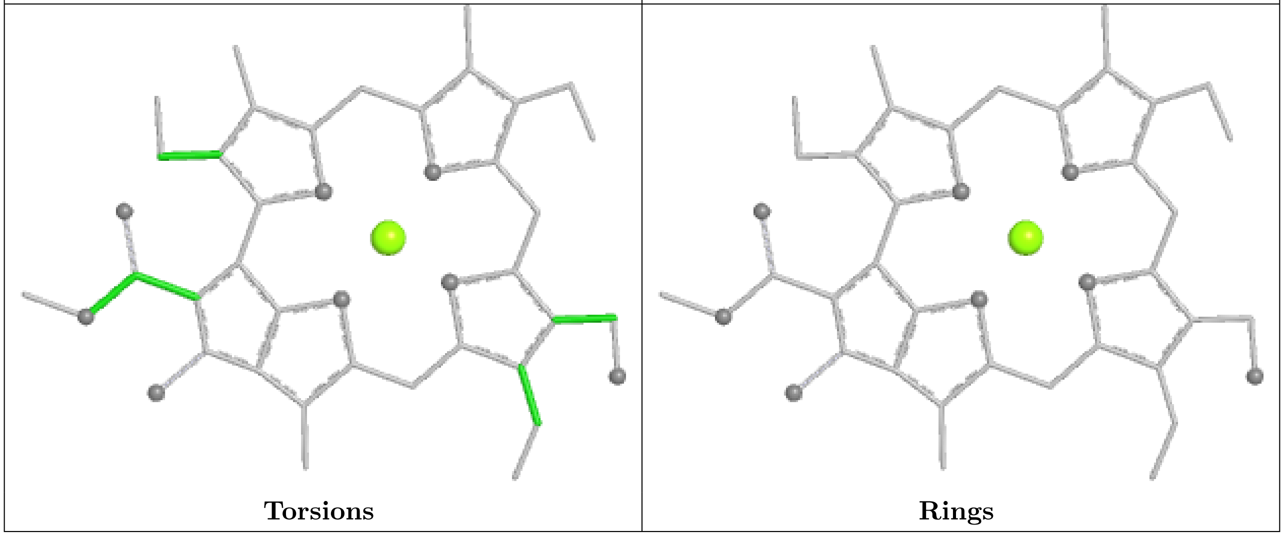
Torsions

Rings

Ligand CHL 4 615

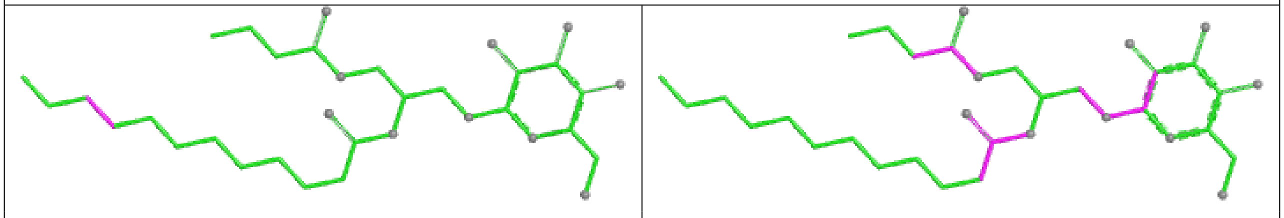


Bond lengths Bond angles

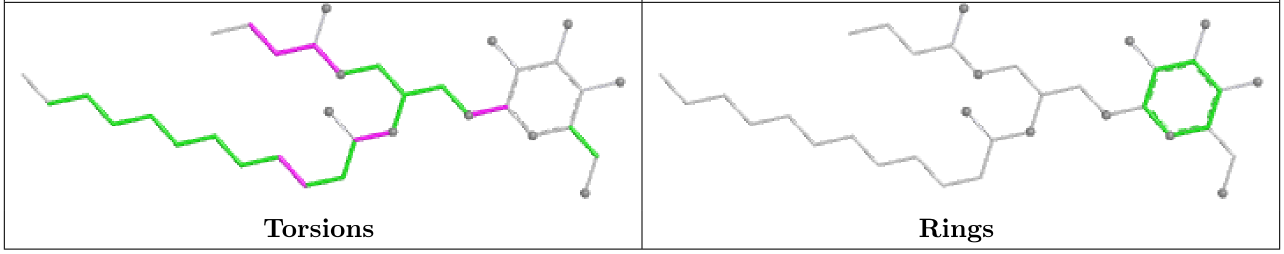


Torsions Rings

Ligand LMG B 5003

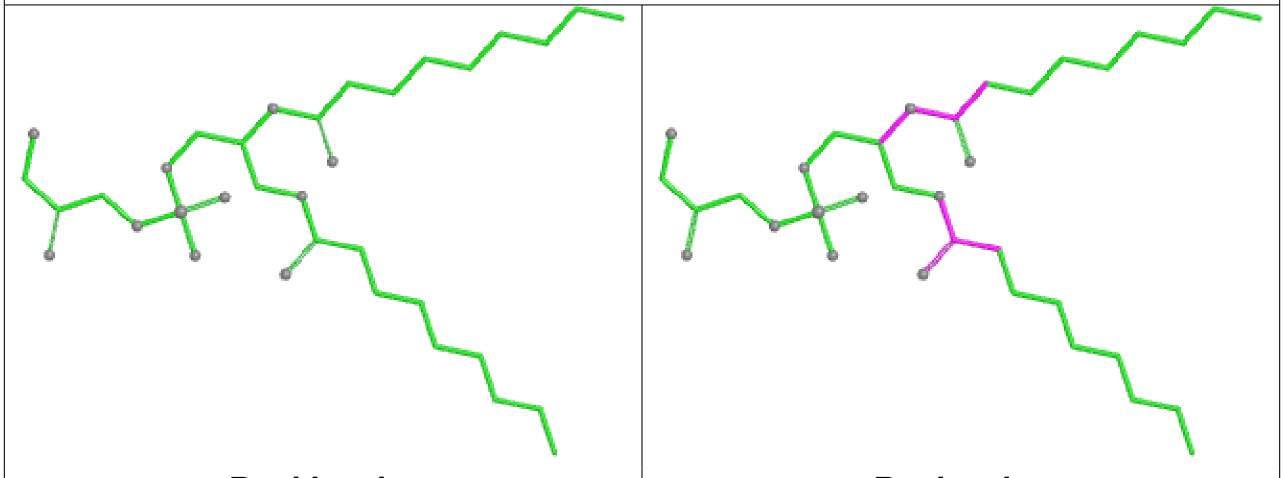


Bond lengths Bond angles

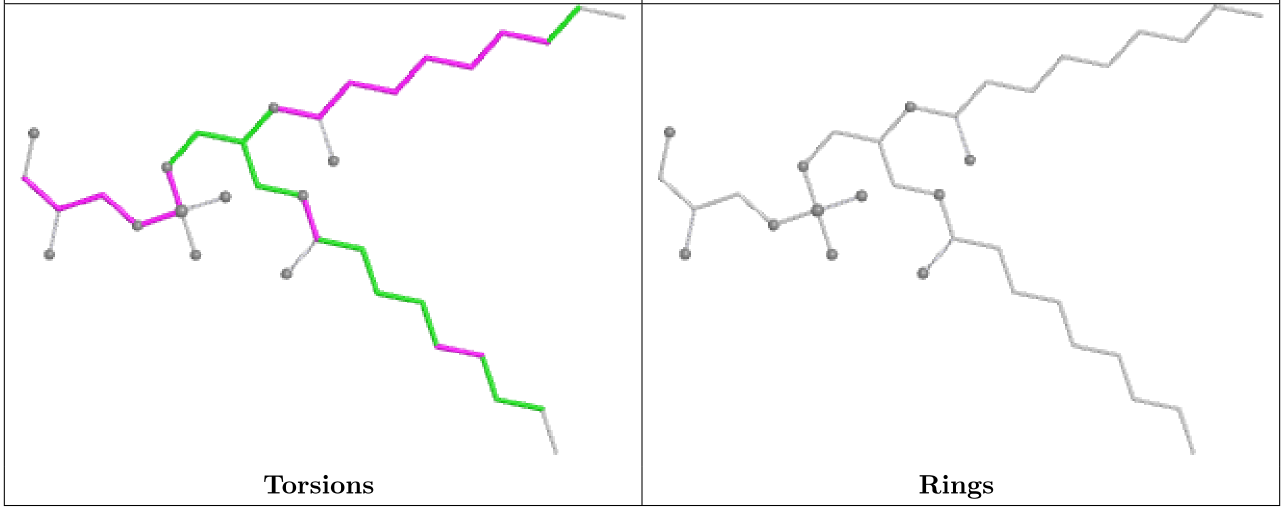


Torsions Rings

Ligand LHG 2 801

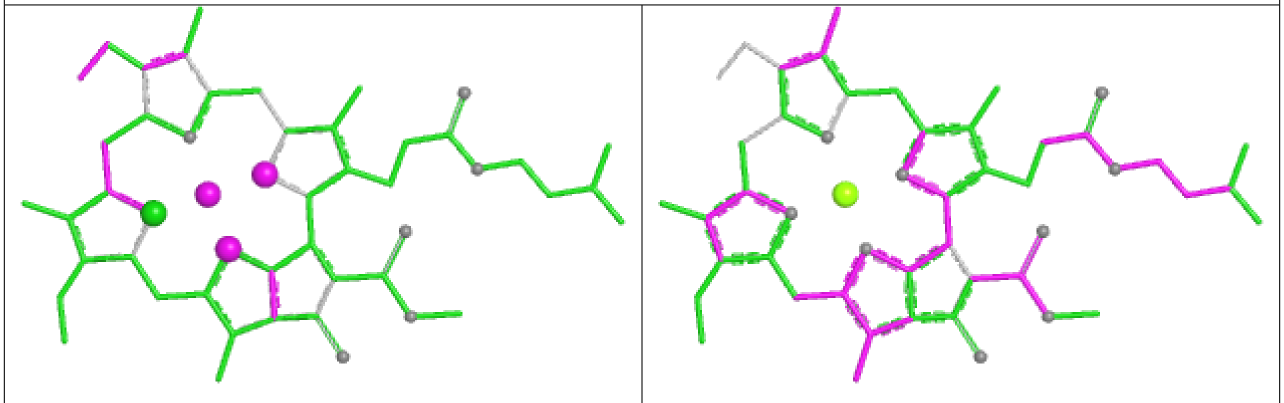


Bond lengths **Bond angles**

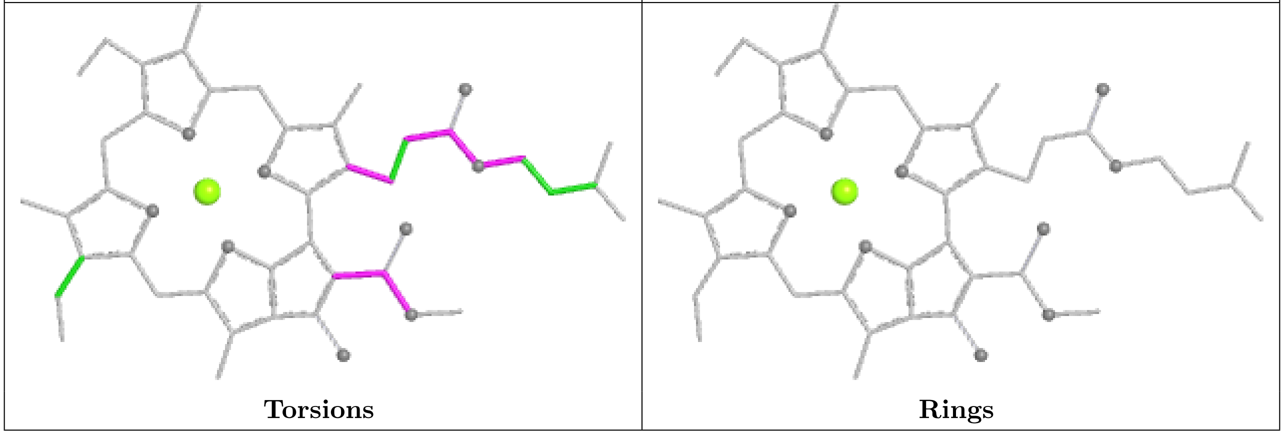


Torsions **Rings**

Ligand CLA B 1236

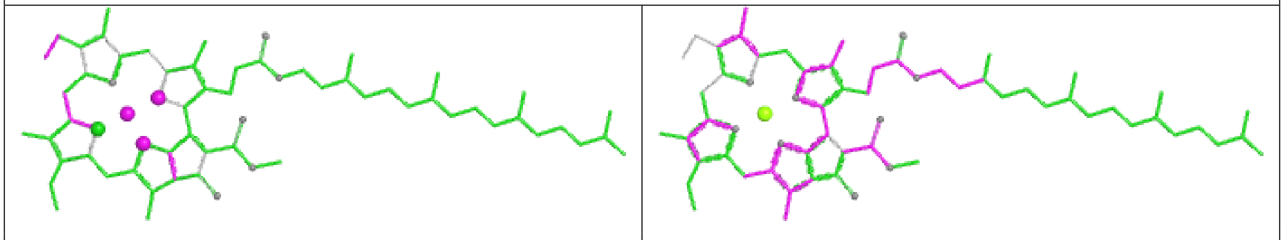


Bond lengths Bond angles

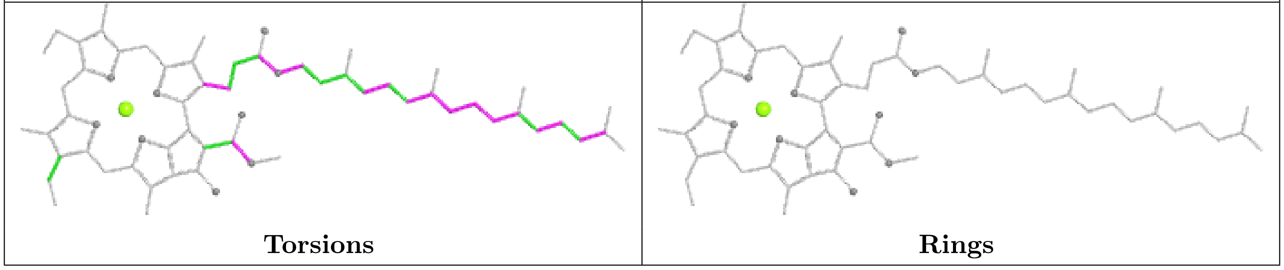


Torsions Rings

Ligand CLA A 1107

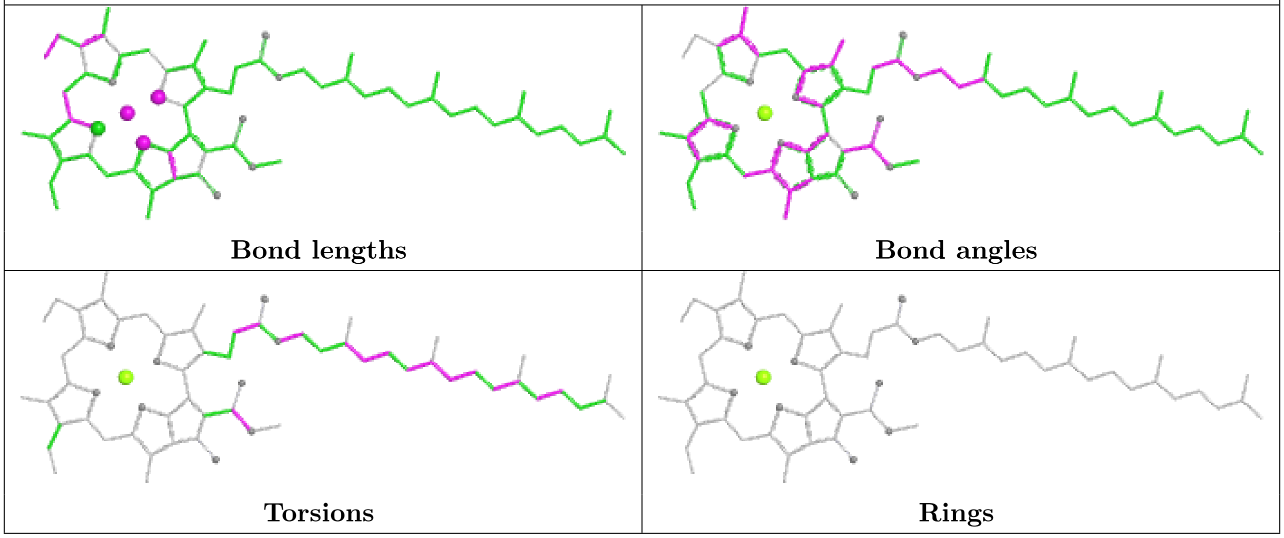


Bond lengths Bond angles

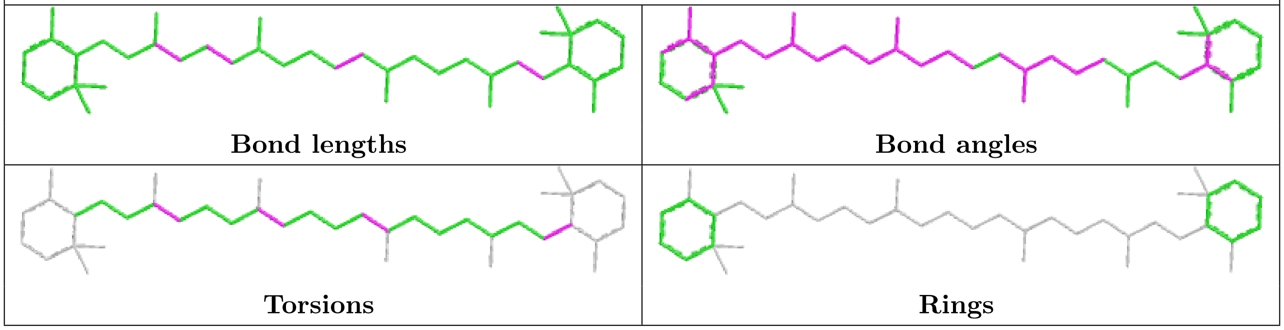


Torsions Rings

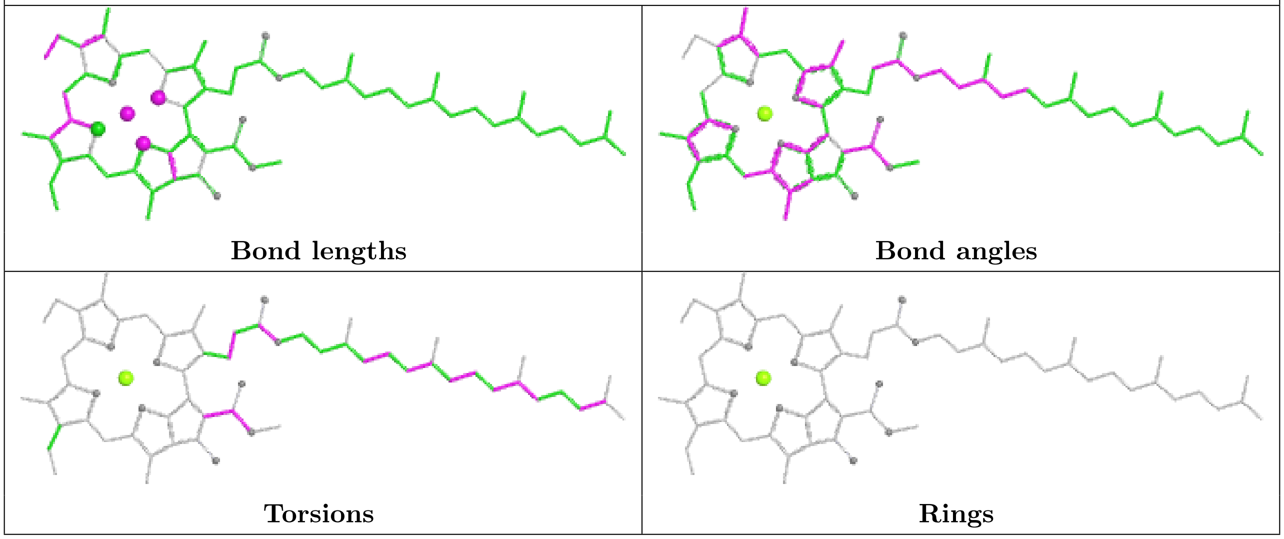
Ligand CLA 1 611



Ligand BCR B 4004



Ligand CLA 1 604



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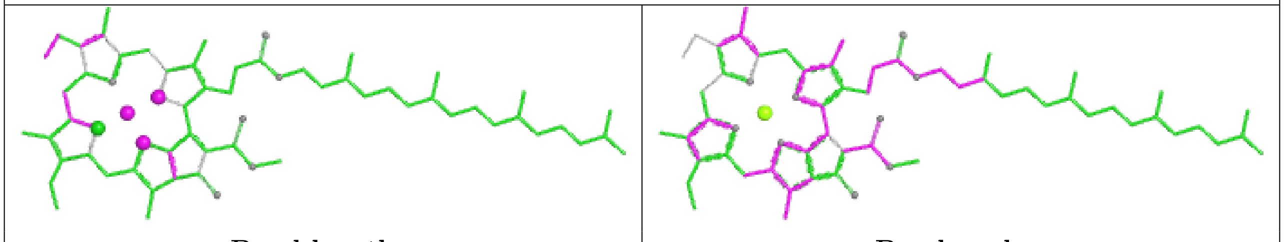
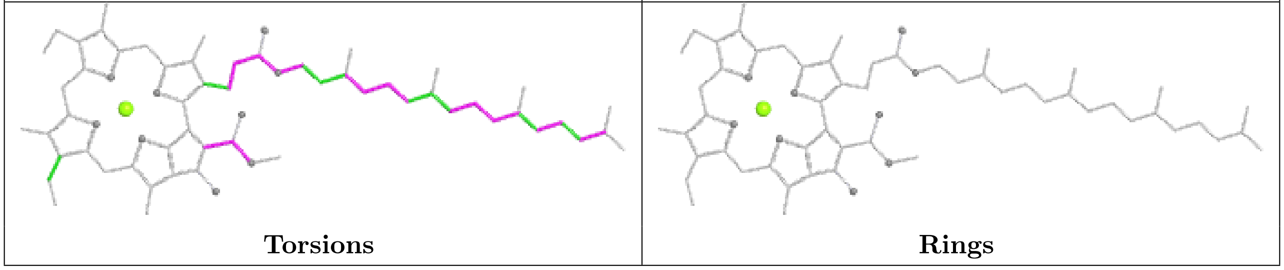


Bond lengths Bond angles



Torsions Rings

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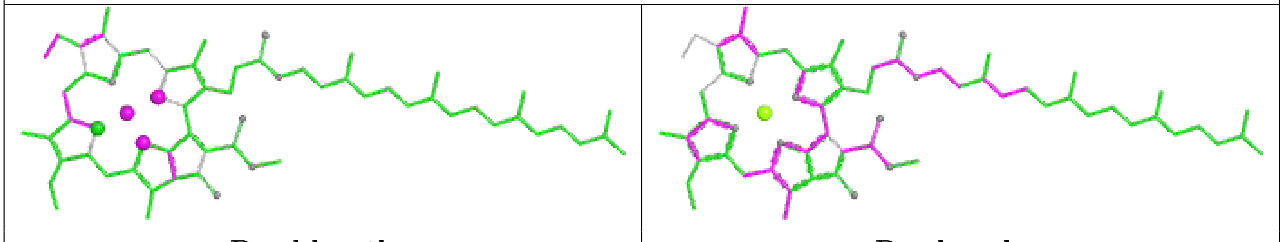
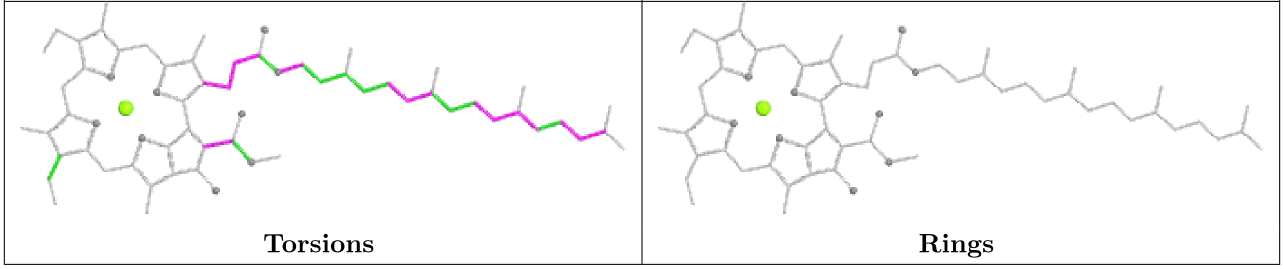
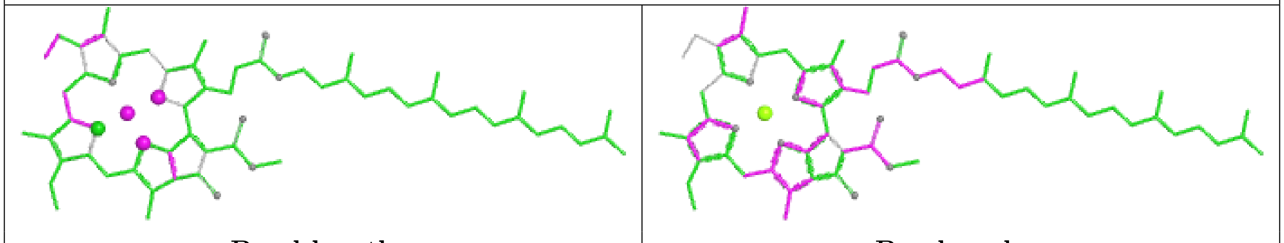


Bond lengths Bond angles

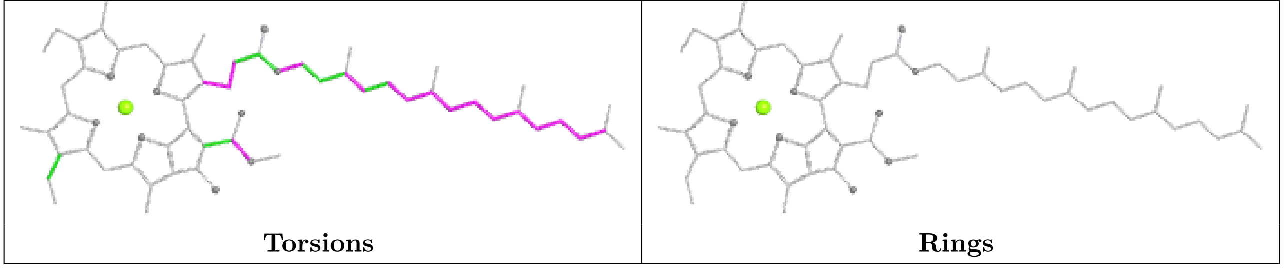


Torsions Rings

Ligand CLA A 1133

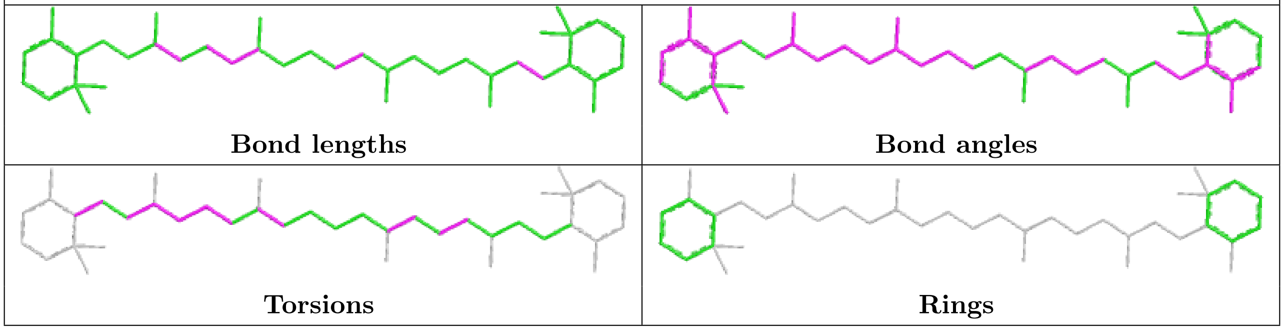


Bond lengths Bond angles



Torsions Rings

Ligand BCR I 4018



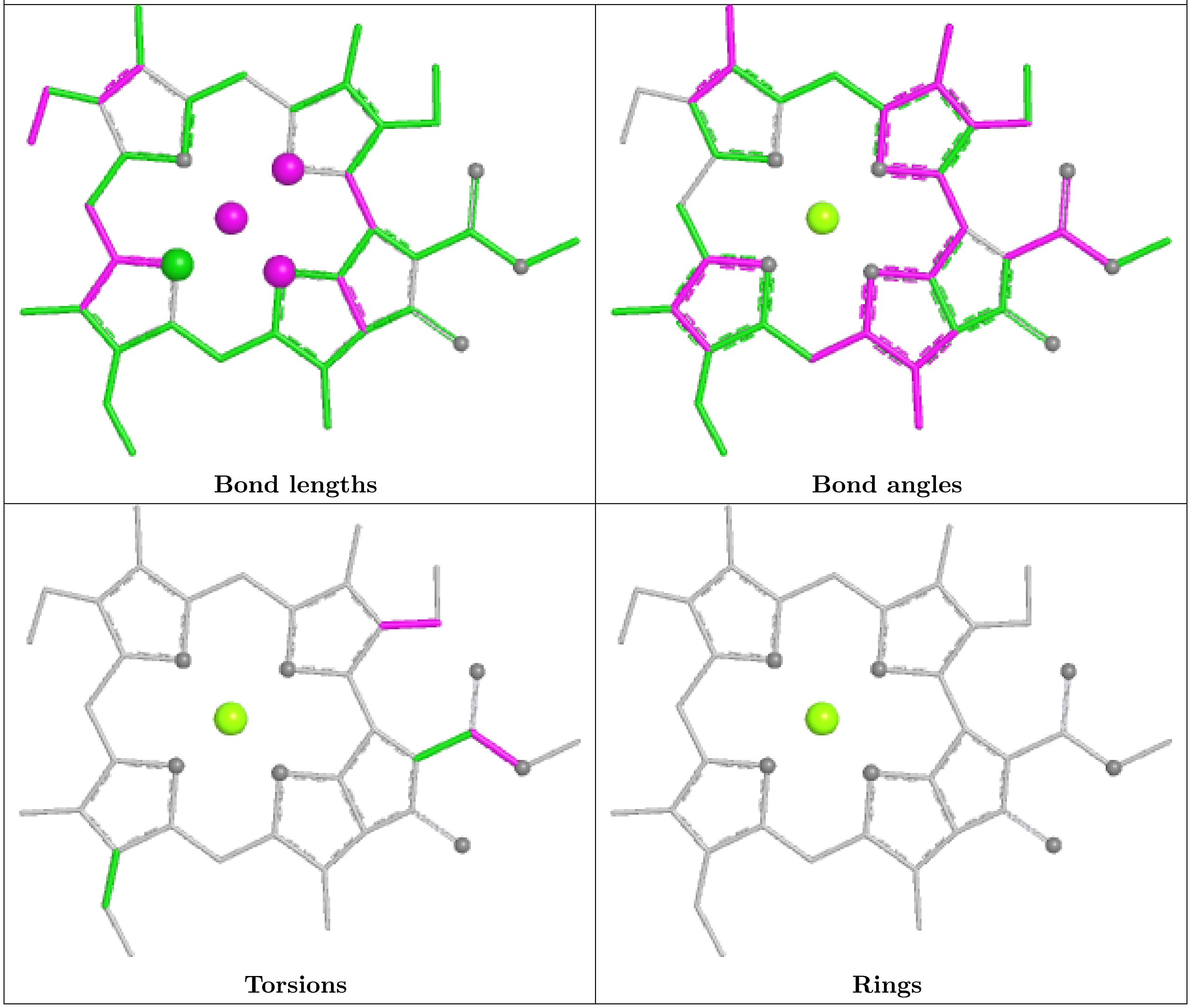
Bond lengths

Bond angles

Torsions

Rings

Ligand CLA 3 614



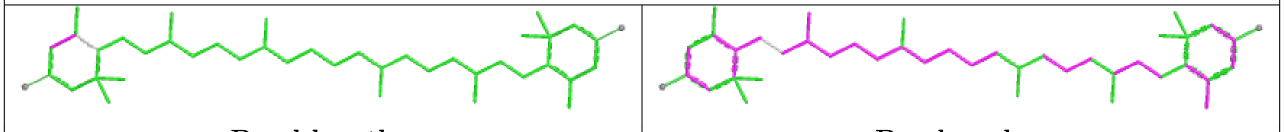
Bond lengths

Bond angles

Torsions

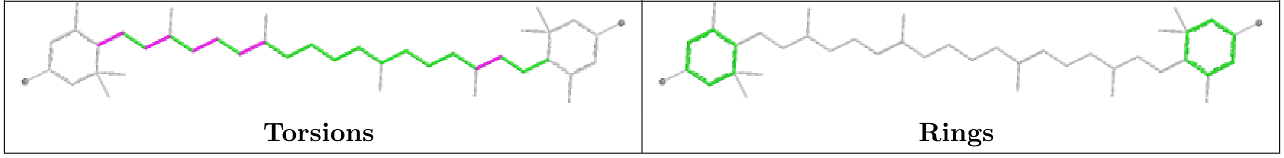
Rings

Ligand LUT 3 502



Bond lengths

Bond angles



Torsions

Rings

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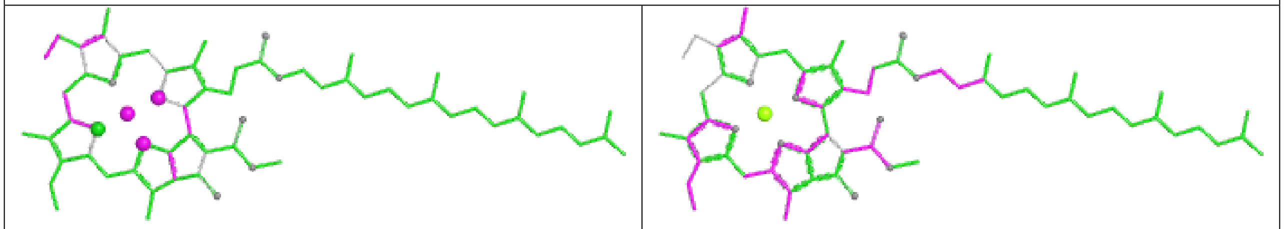
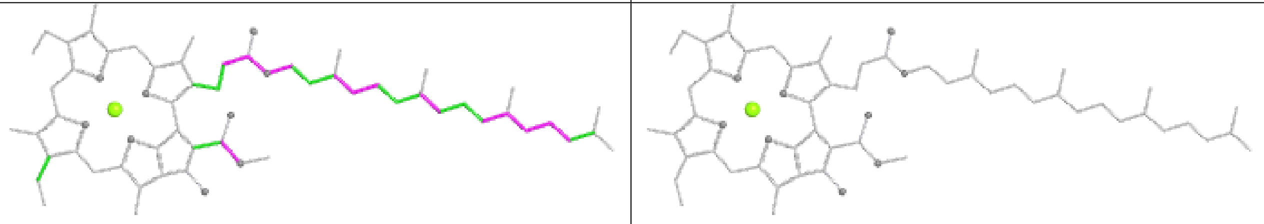


Bond lengths

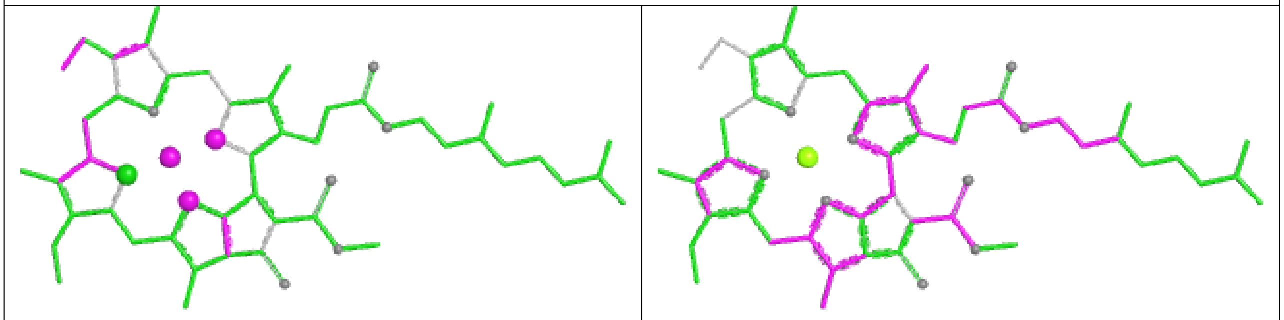
Bond angles



Torsions

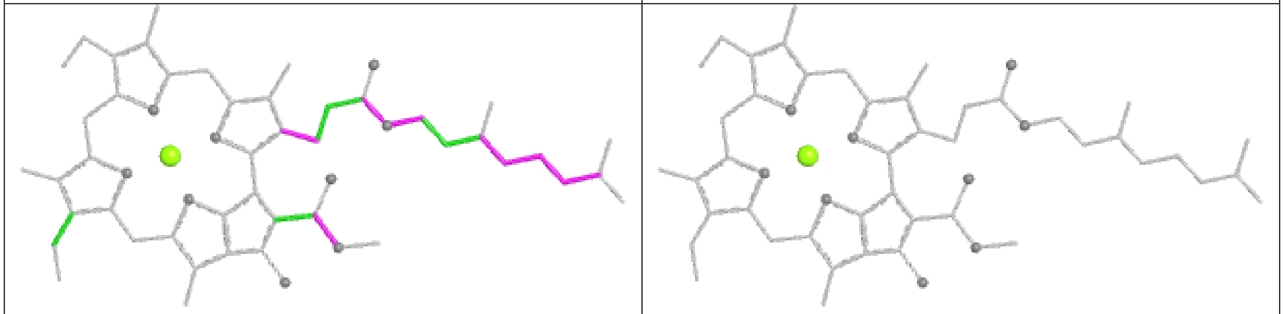
Rings

Ligand CLA B 1232



Bond lengths

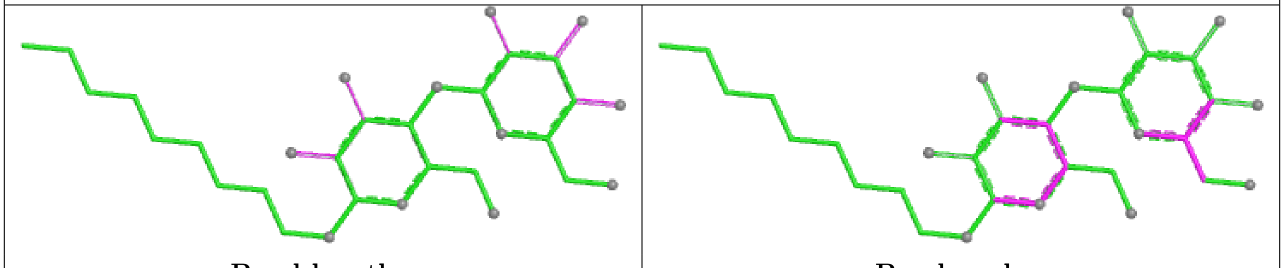
Bond angles



Torsions

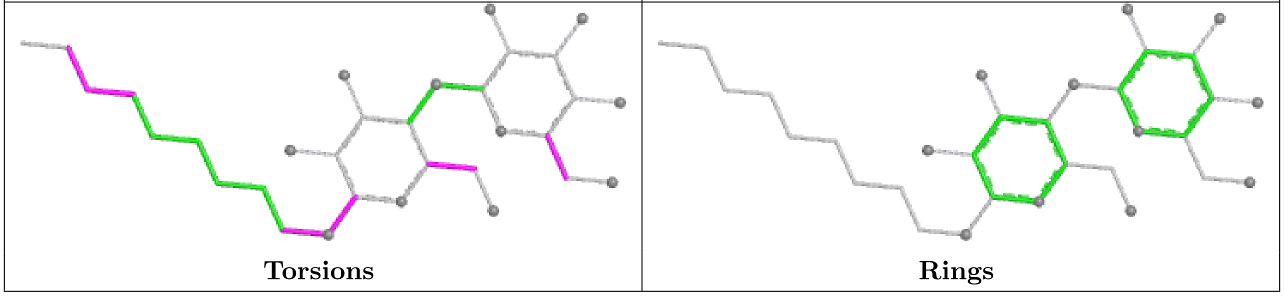
Rings

Ligand LMT B 5006



Bond lengths

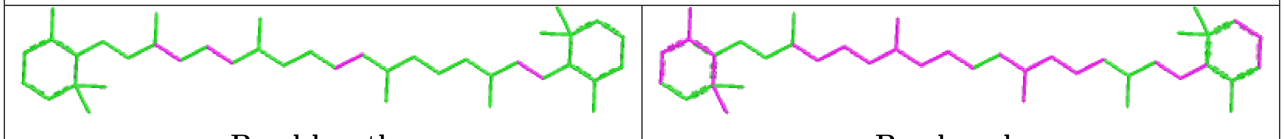
Bond angles



Torsions

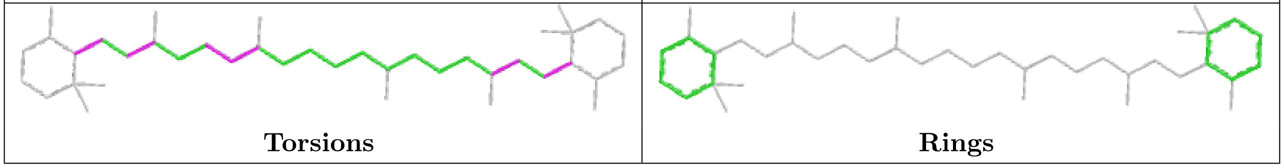
Rings

Ligand BCR J 4012



Bond lengths

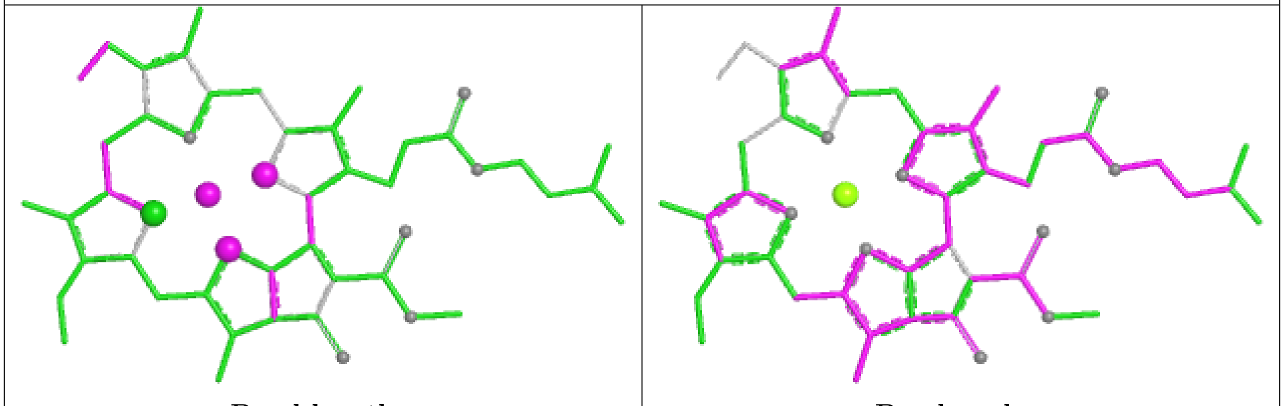
Bond angles



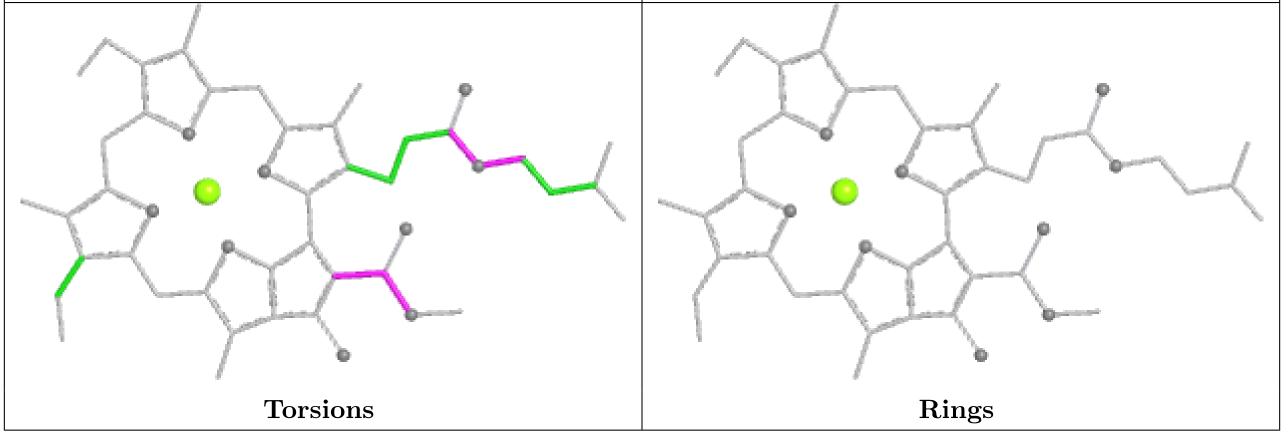
Torsions

Rings

Ligand CLA A 1108

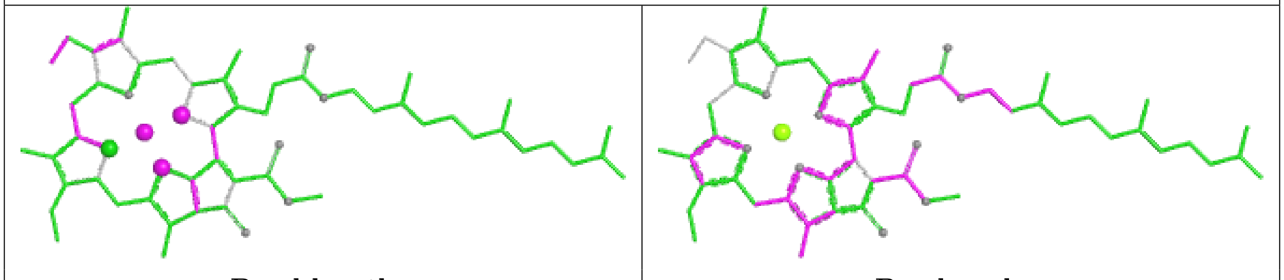


Bond lengths | Bond angles

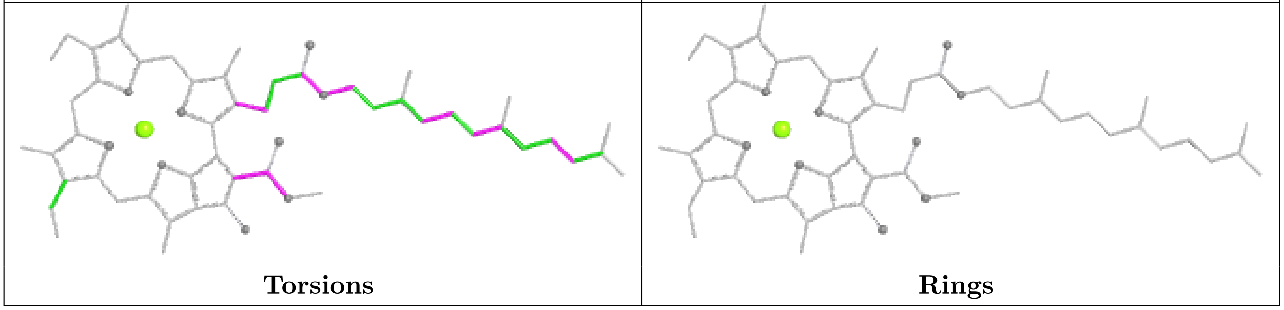


Torsions | Rings

Ligand CLA G 1701

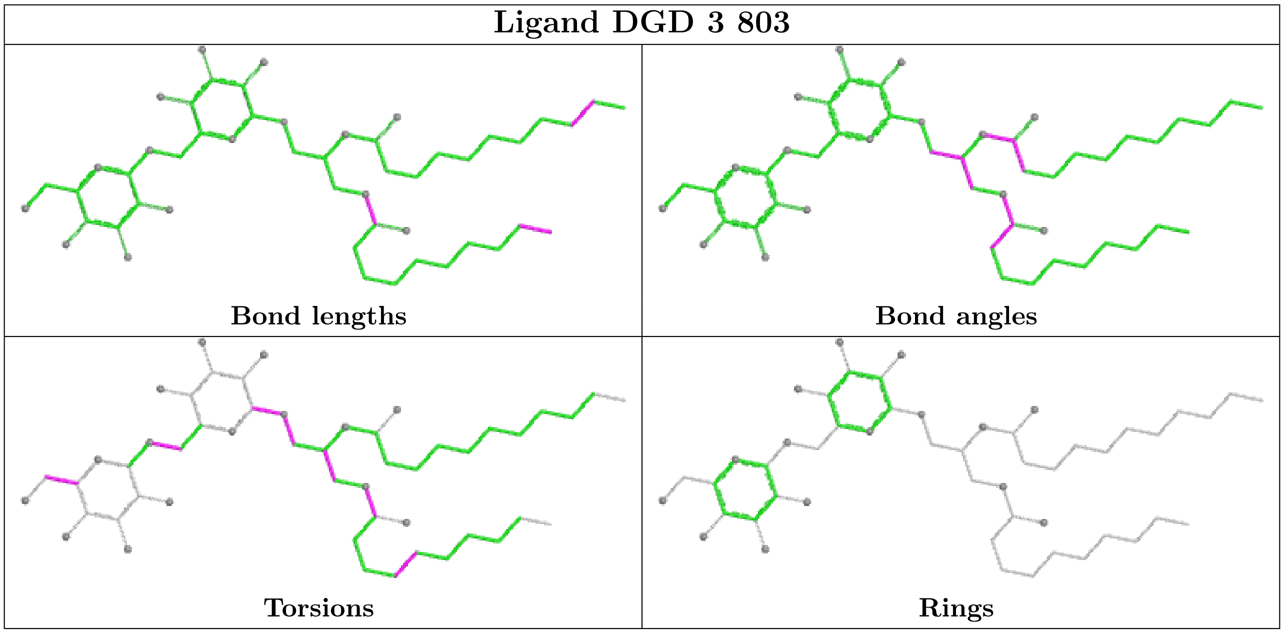


Bond lengths | Bond angles

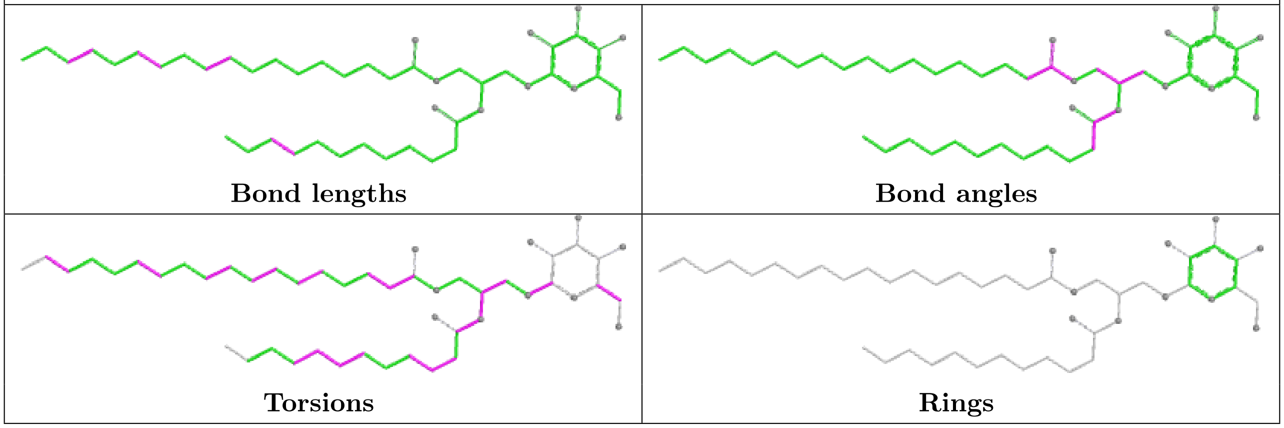


Torsions | Rings

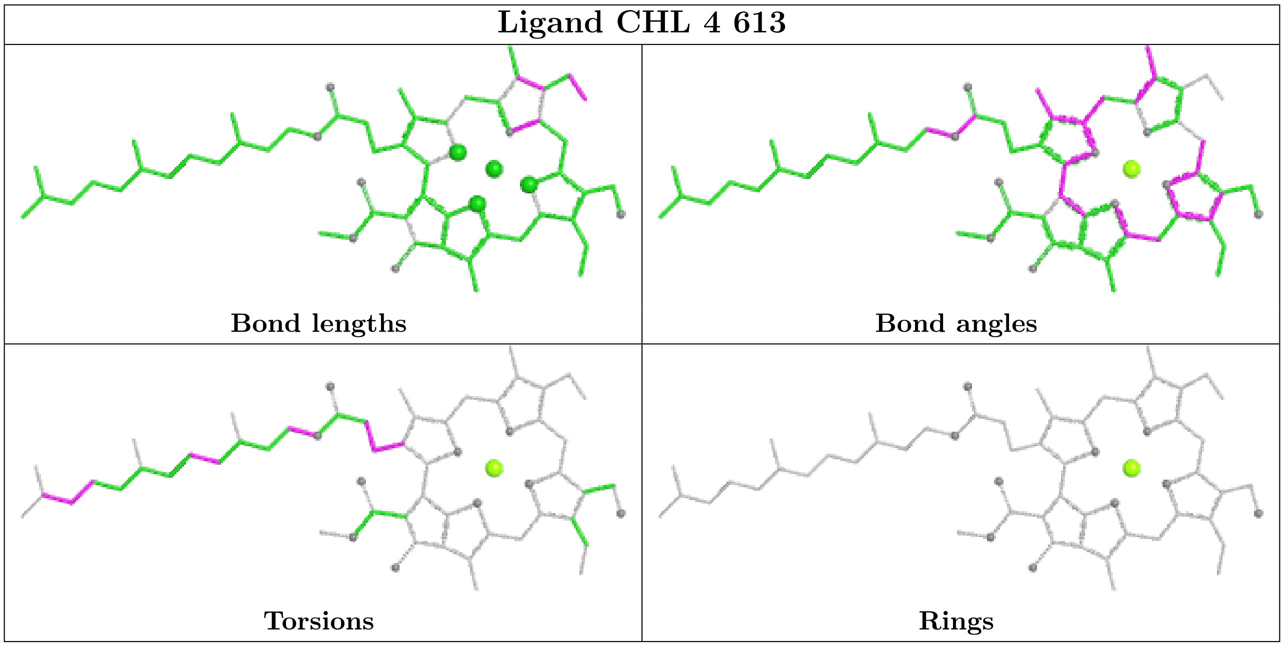
Ligand DGD 3 803



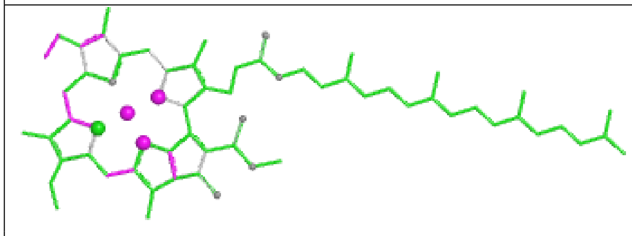
Ligand LMG G 5001



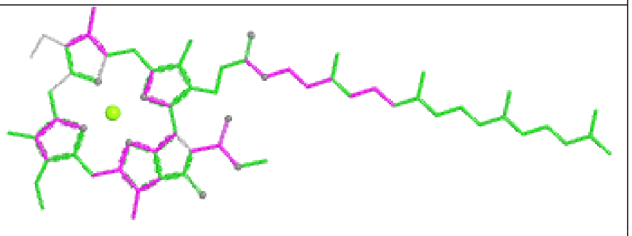
Ligand CHL 4 613



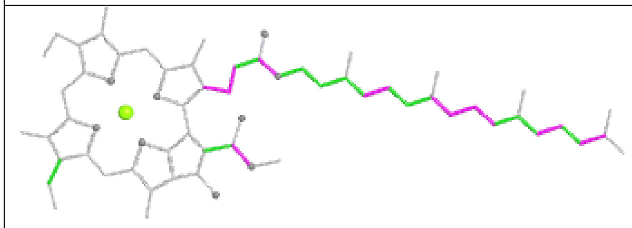
Ligand CLA A 1119



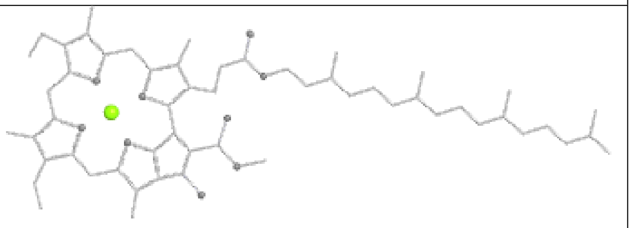
Bond lengths



Bond angles

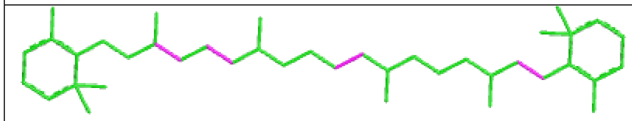


Torsions

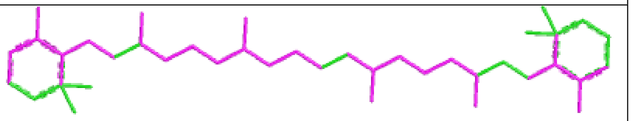


Rings

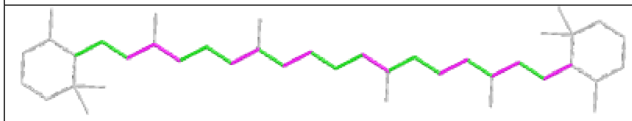
Ligand BCR 1 504



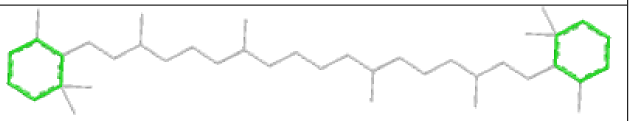
Bond lengths



Bond angles

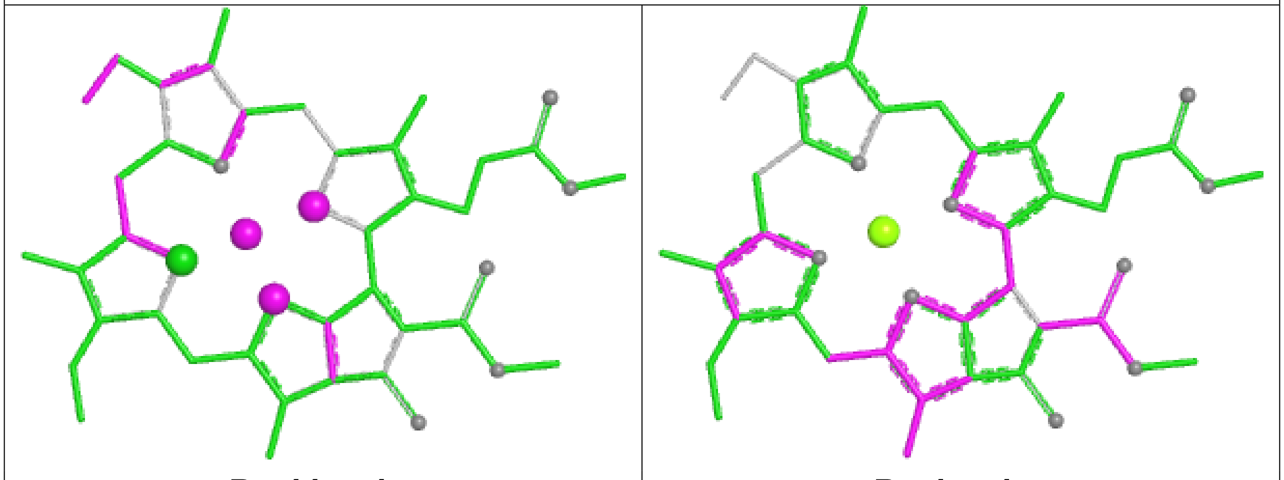


Torsions



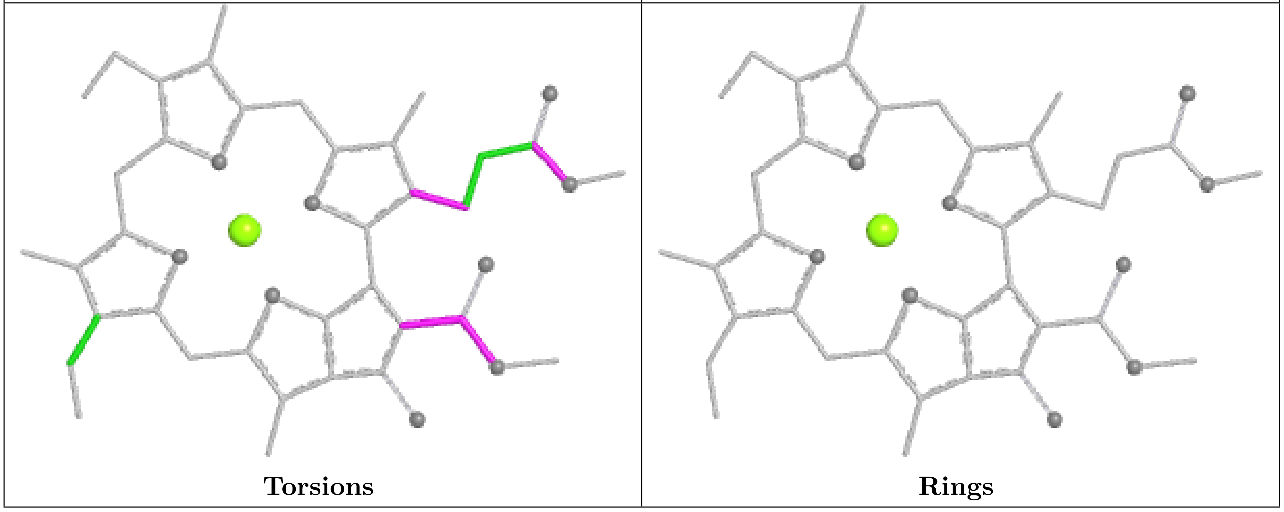
Rings

Ligand CLA 1 608



Bond lengths

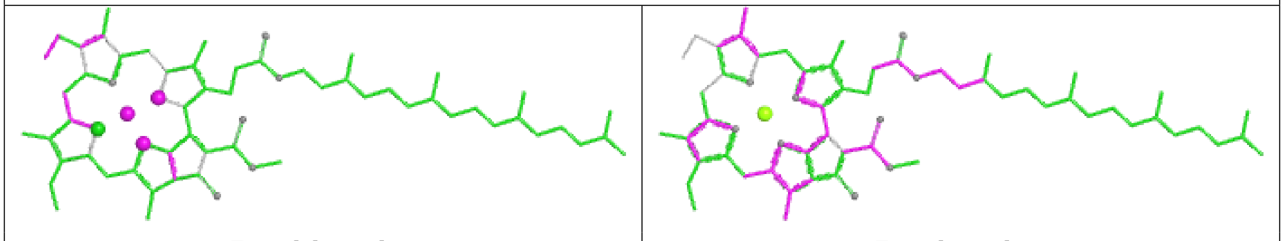
Bond angles



Torsions

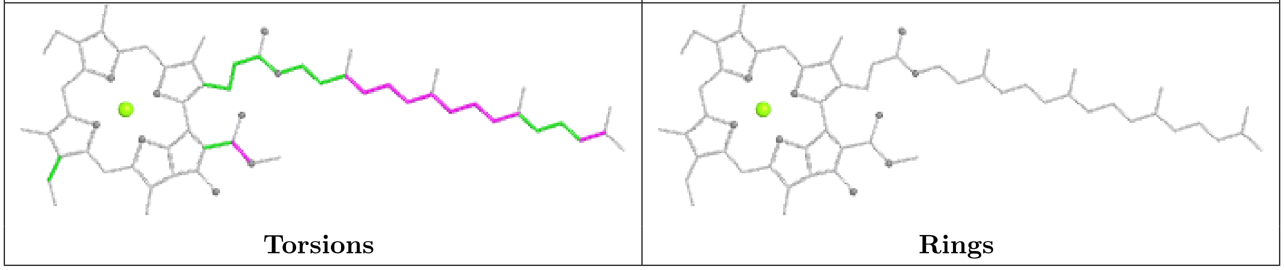
Rings

Ligand CLA B 1203



Bond lengths

Bond angles



Torsions

Rings

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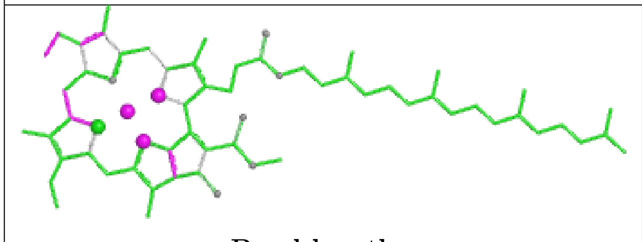

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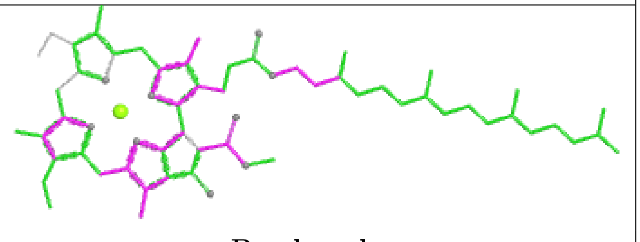

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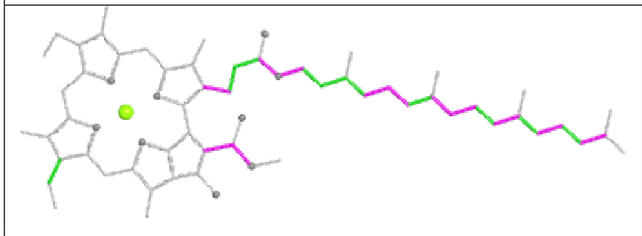

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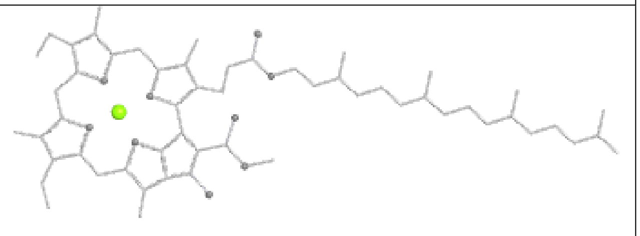

Rings

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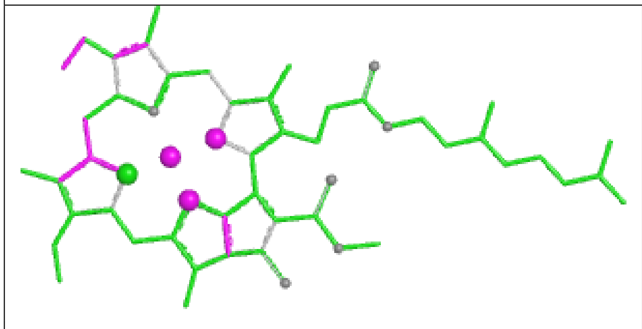

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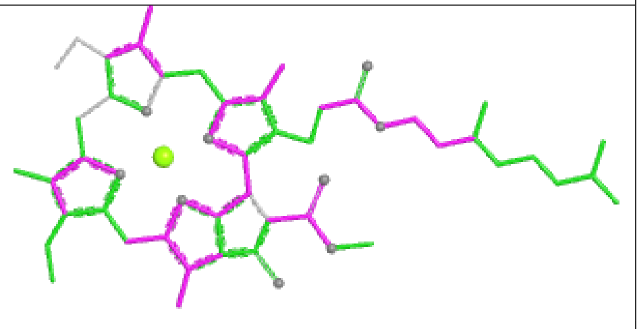

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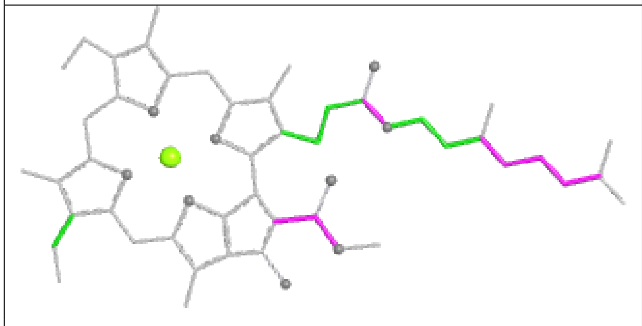

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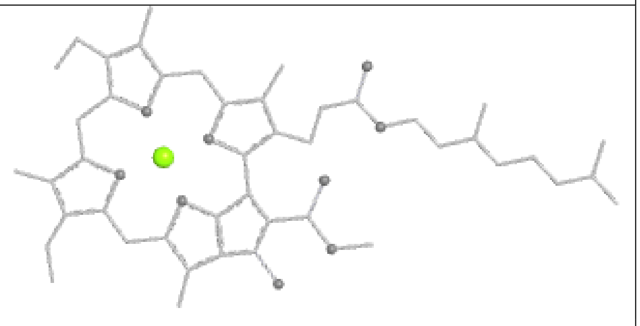

Rings

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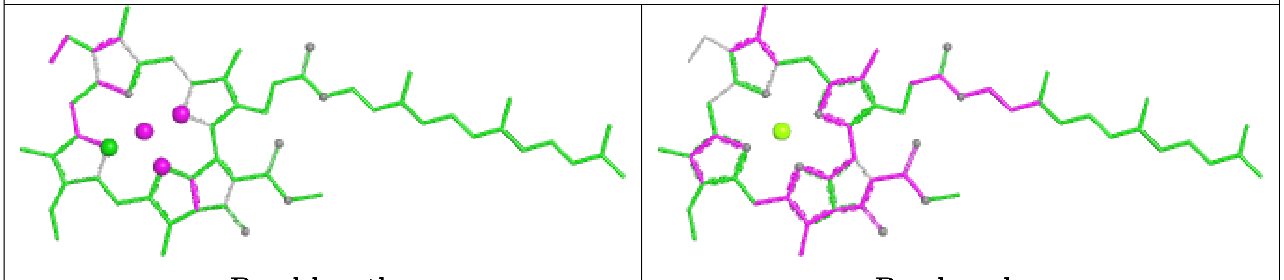
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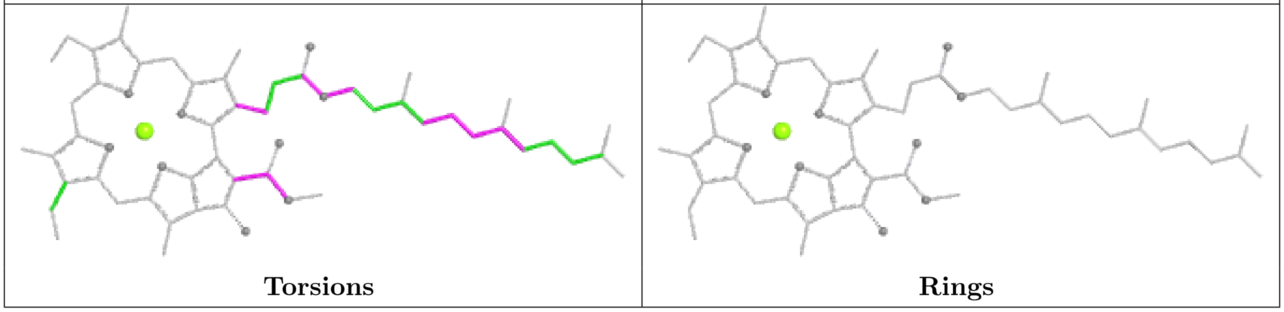
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Rings

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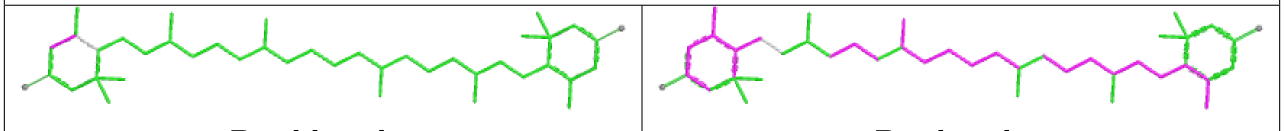
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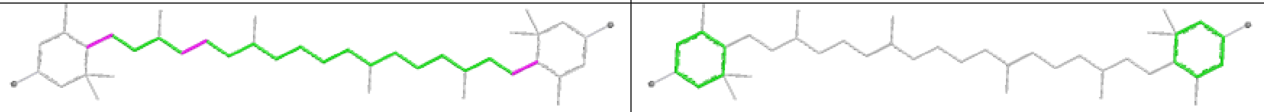
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Rings

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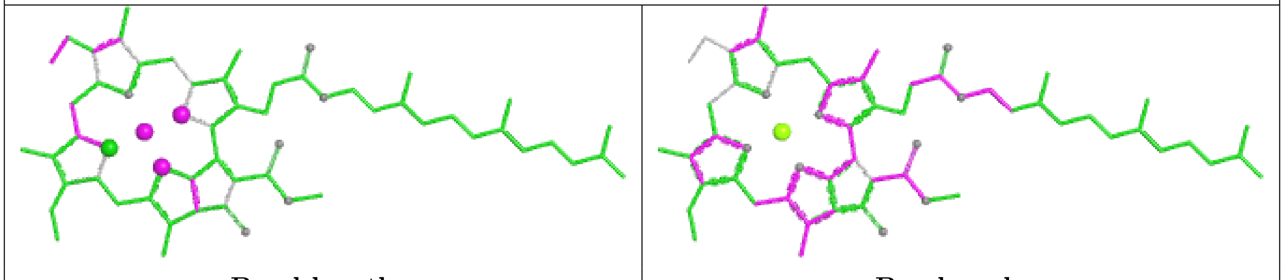
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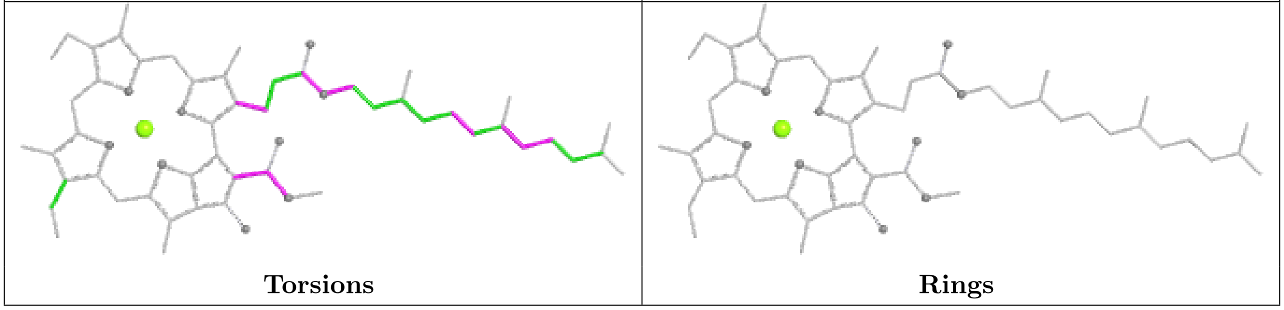
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Rings

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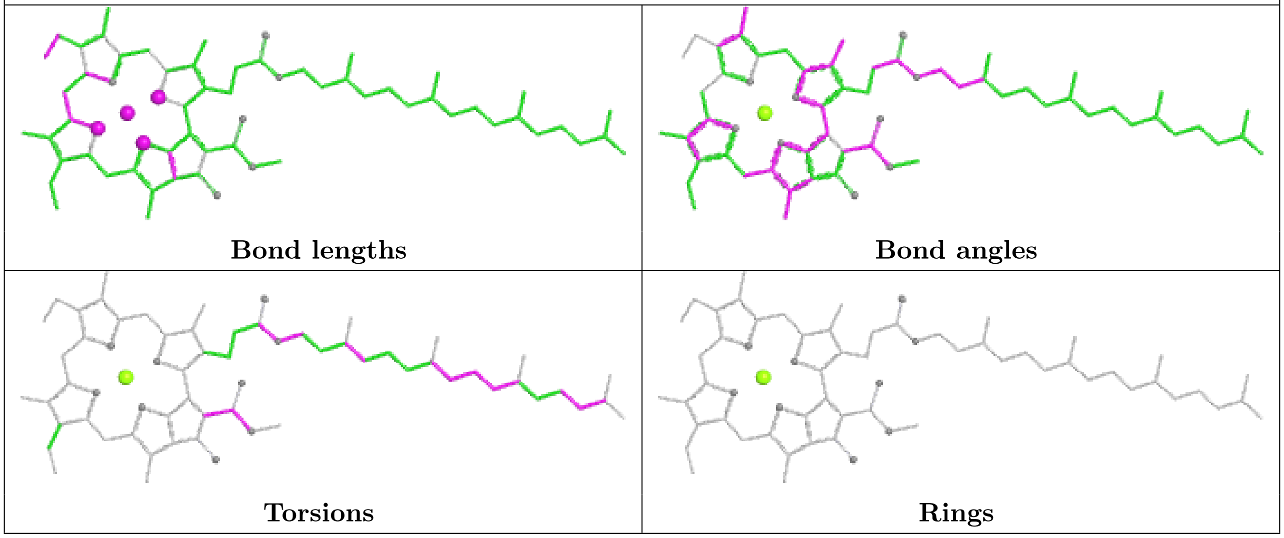

Bond lengths

Bond angles

Torsions

Rings

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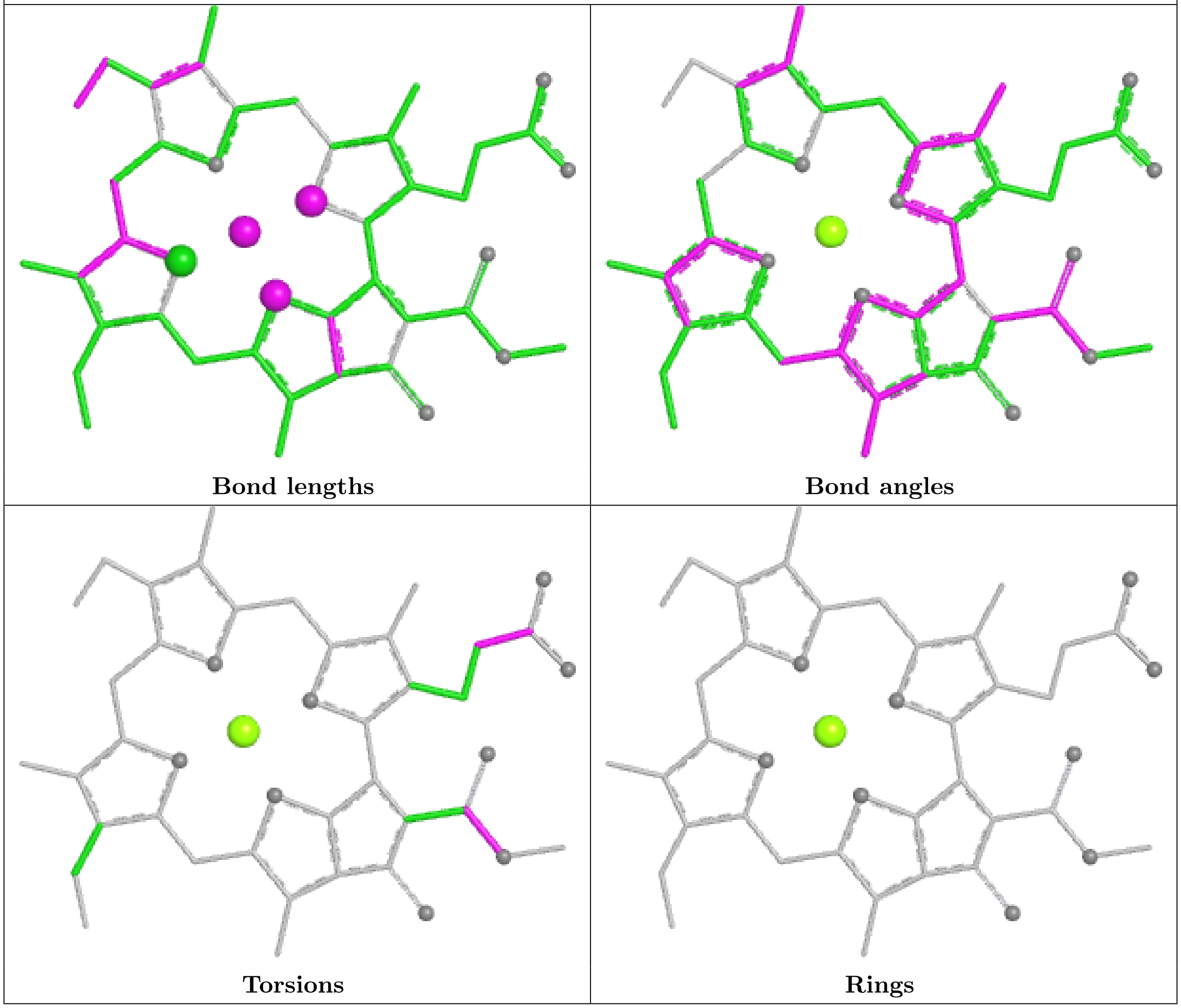

Bond lengths

Bond angles

Torsions

Rings

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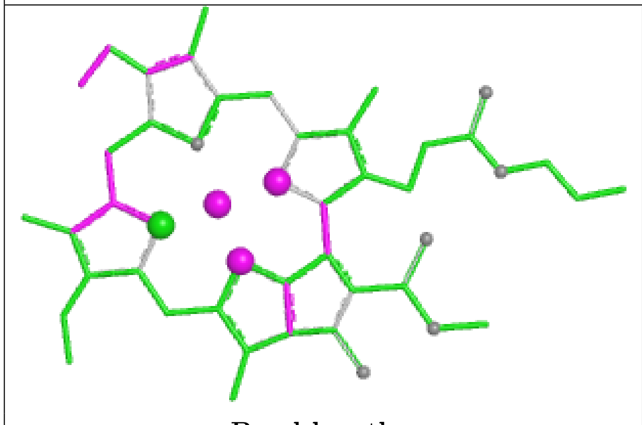
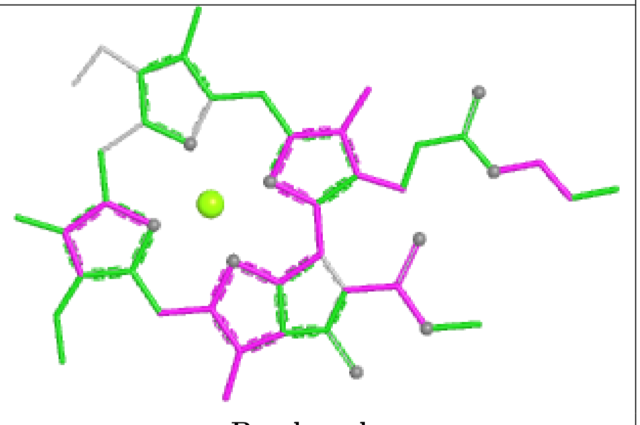
<tr><td>
Bond lengths</td><td>
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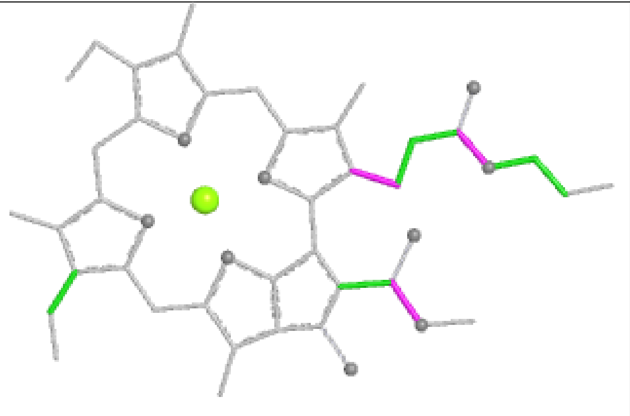
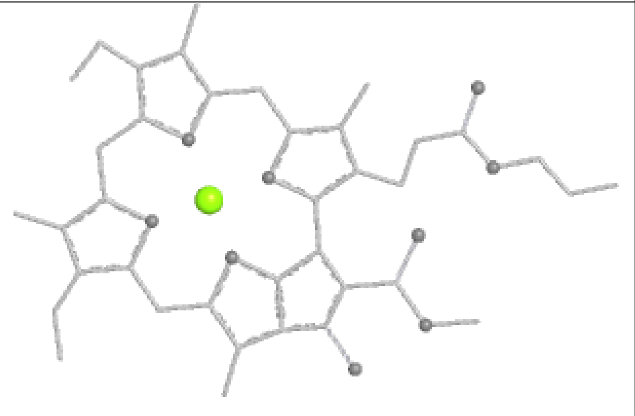
<tr><td>
Torsions</td><td>
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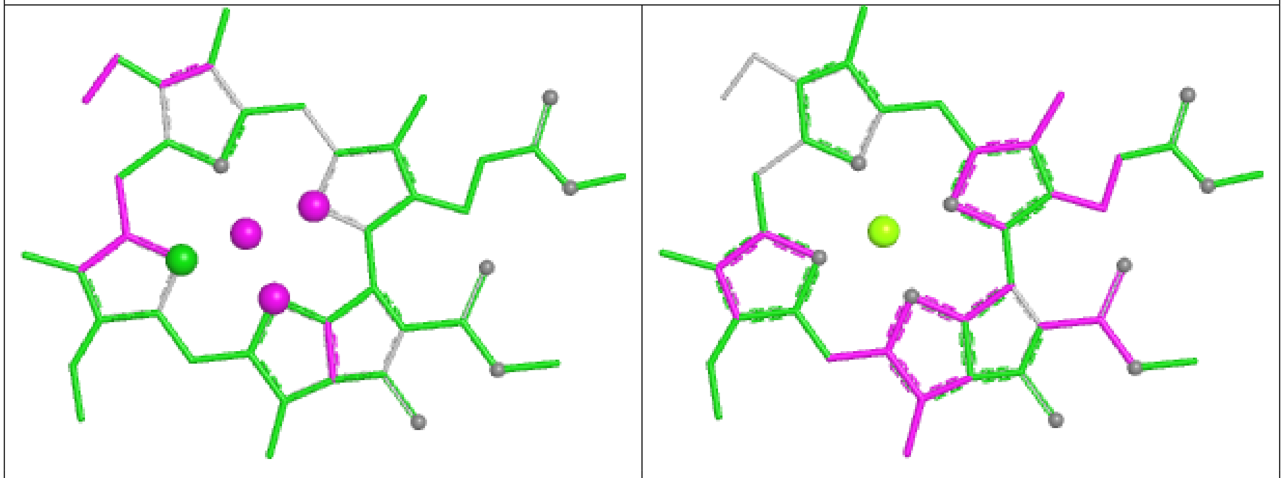

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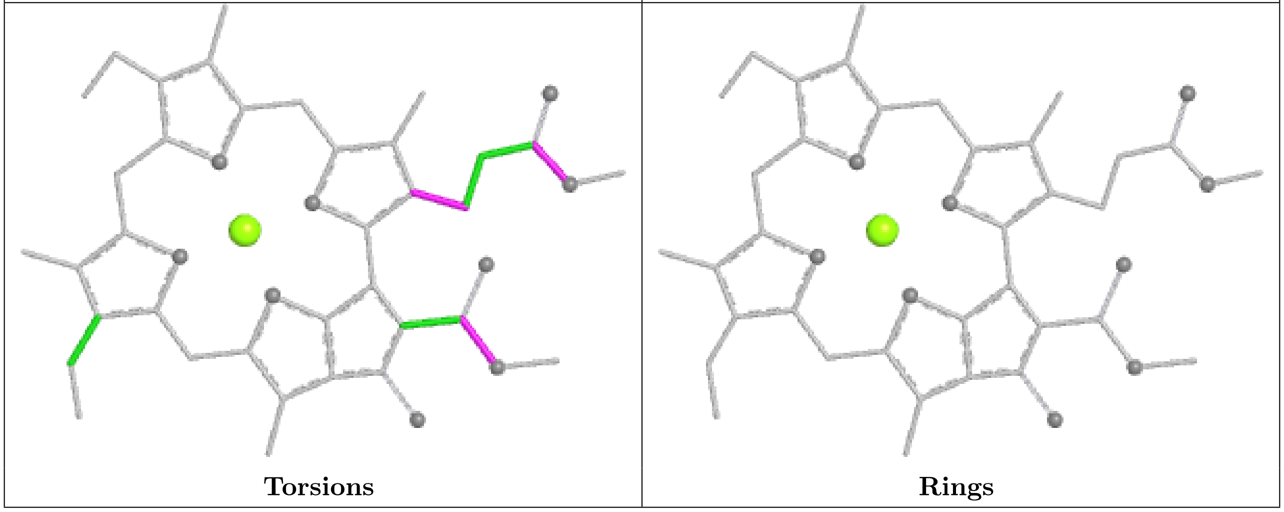

Torsions

Rings

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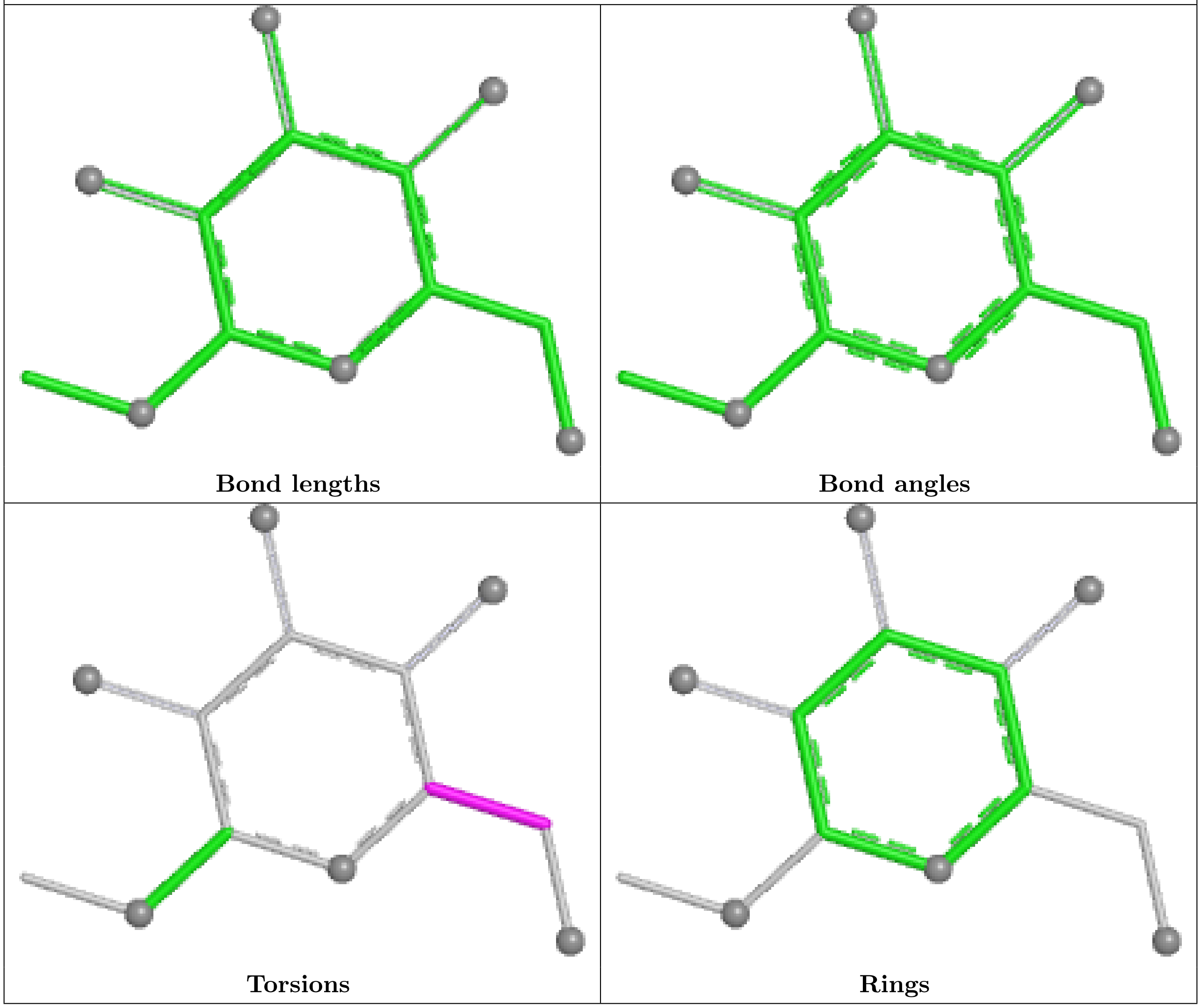

Bond lengths

Bond angles

Torsions

Rings

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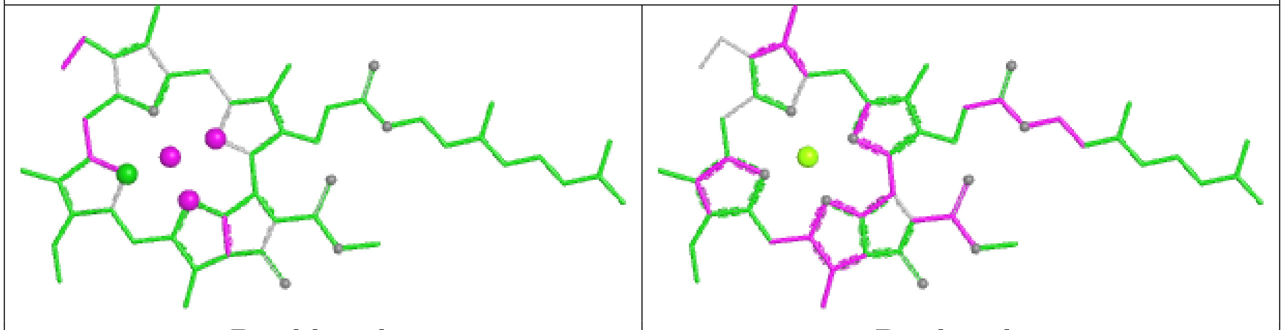

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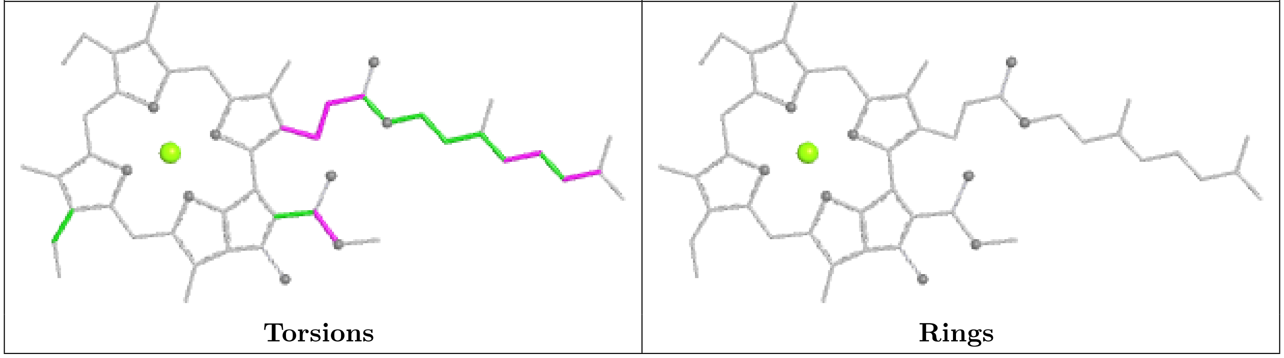

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Rings

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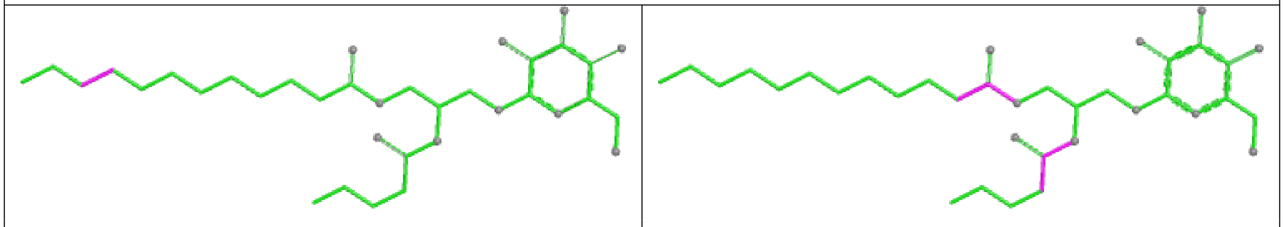

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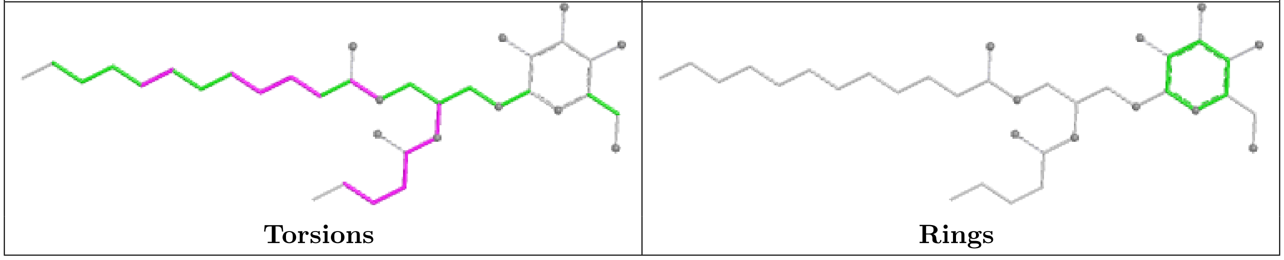

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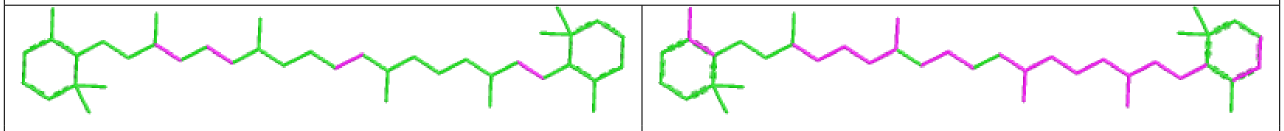

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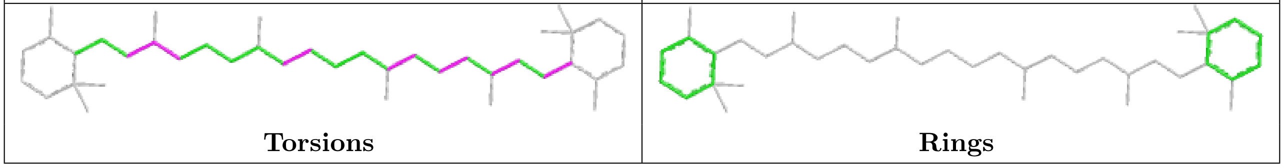

Torsions

Rings

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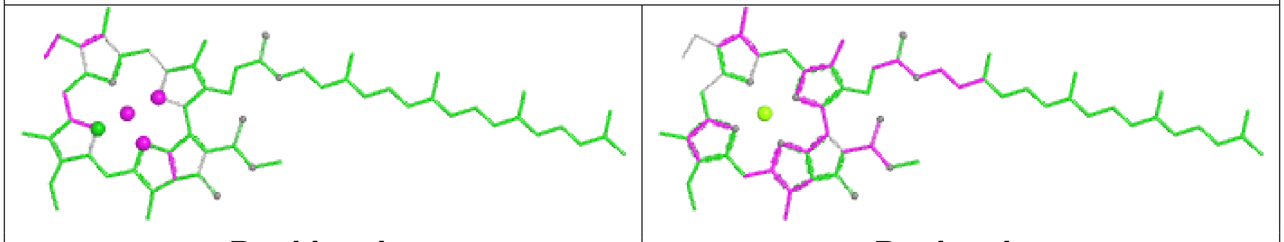

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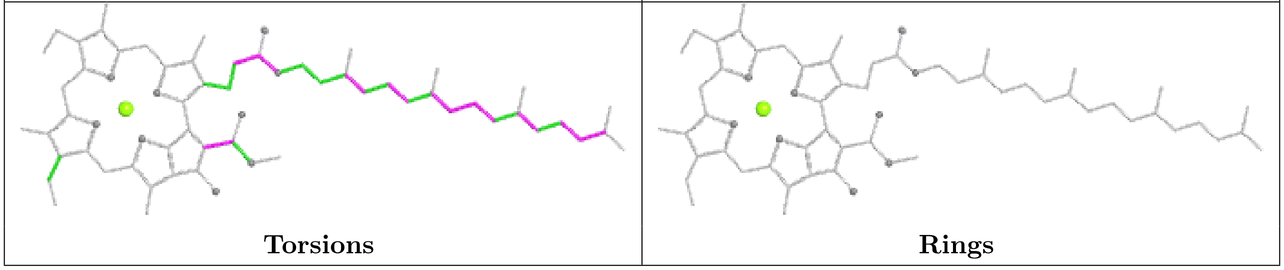

Torsions Rings

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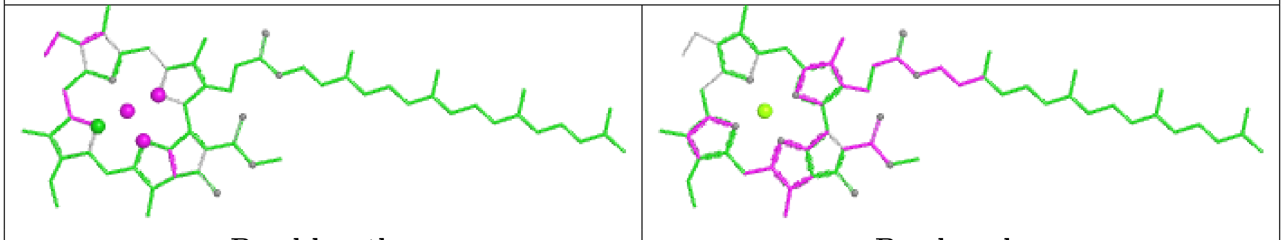

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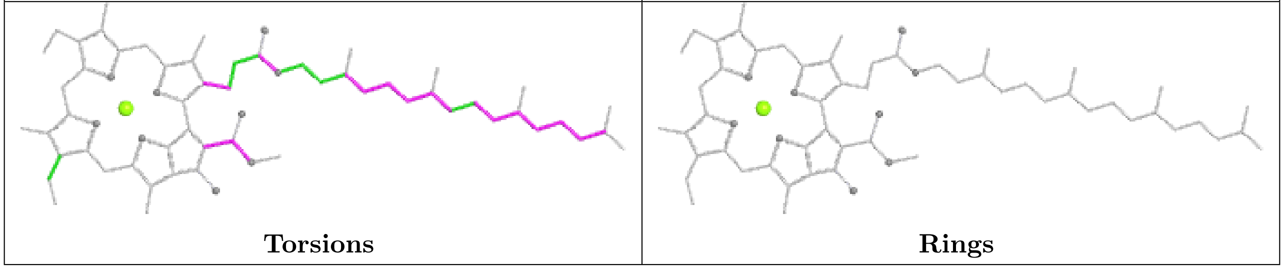

Torsions Rings

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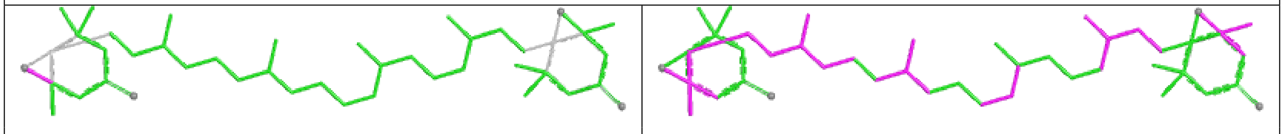

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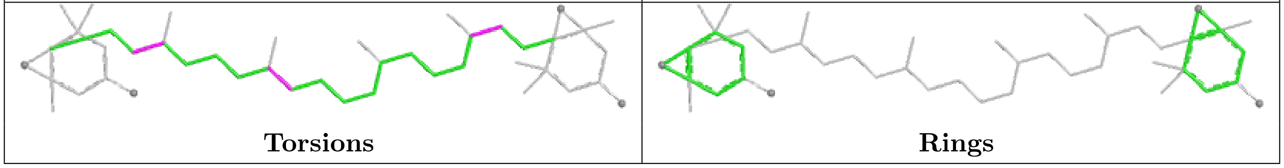

Torsions Rings

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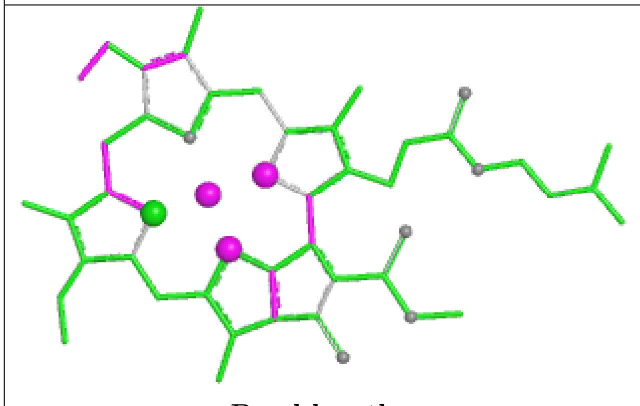
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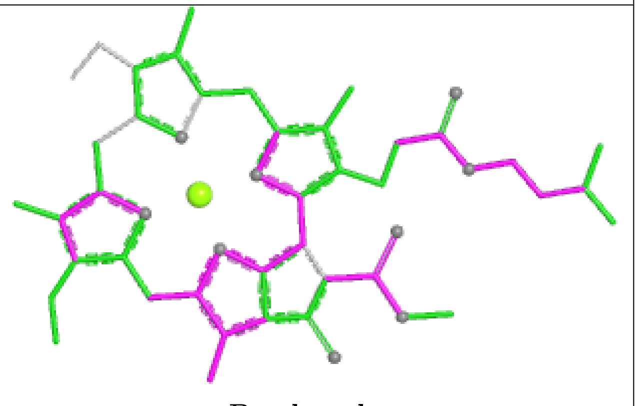
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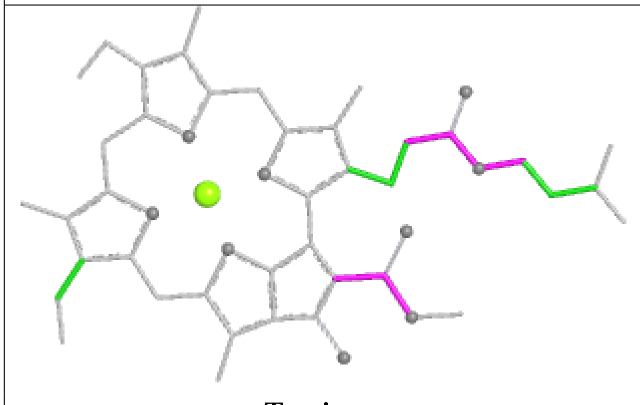
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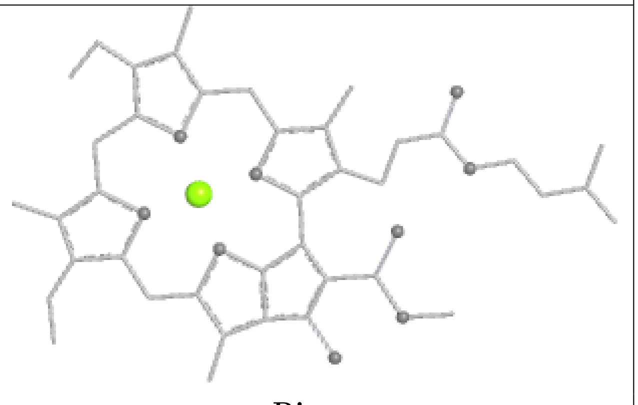
Rings

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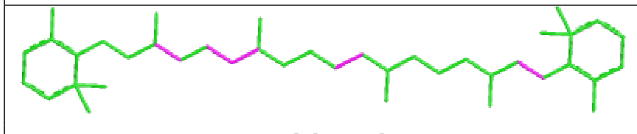
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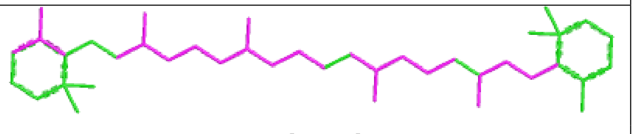
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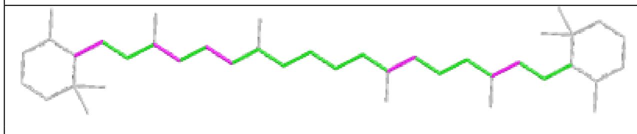
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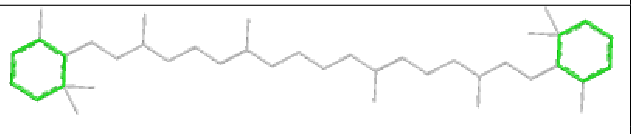
Rings

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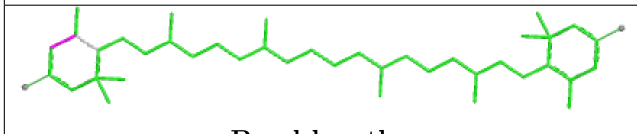
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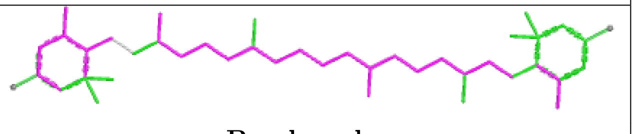
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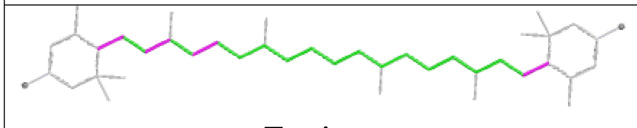
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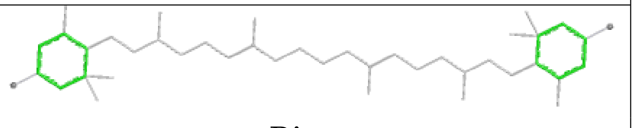
Rings

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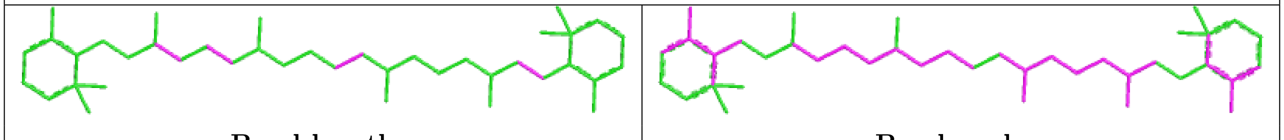
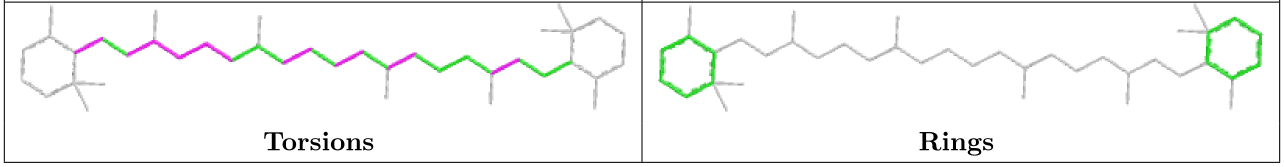


Bond lengths

Bond angles



Torsions

Rings

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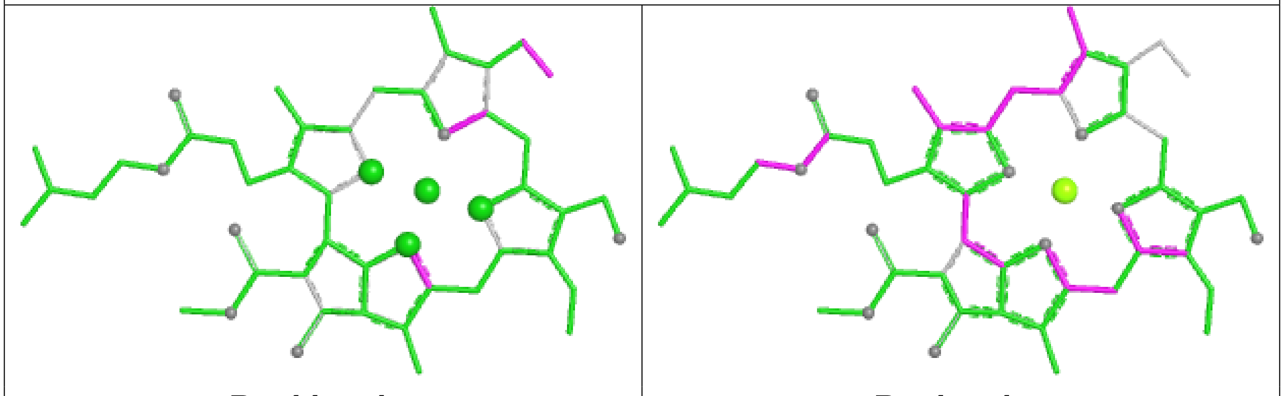
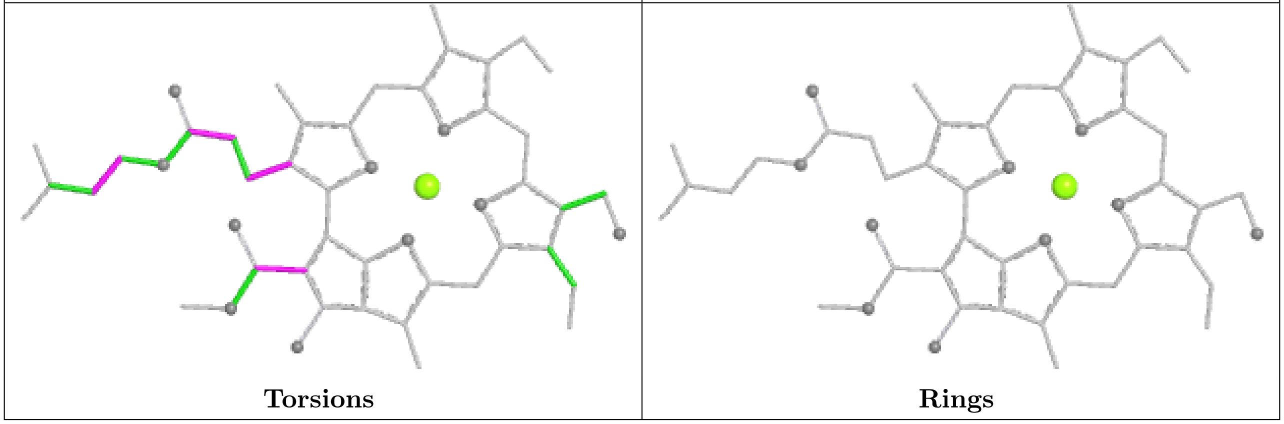


Bond lengths

Bond angles



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Rings

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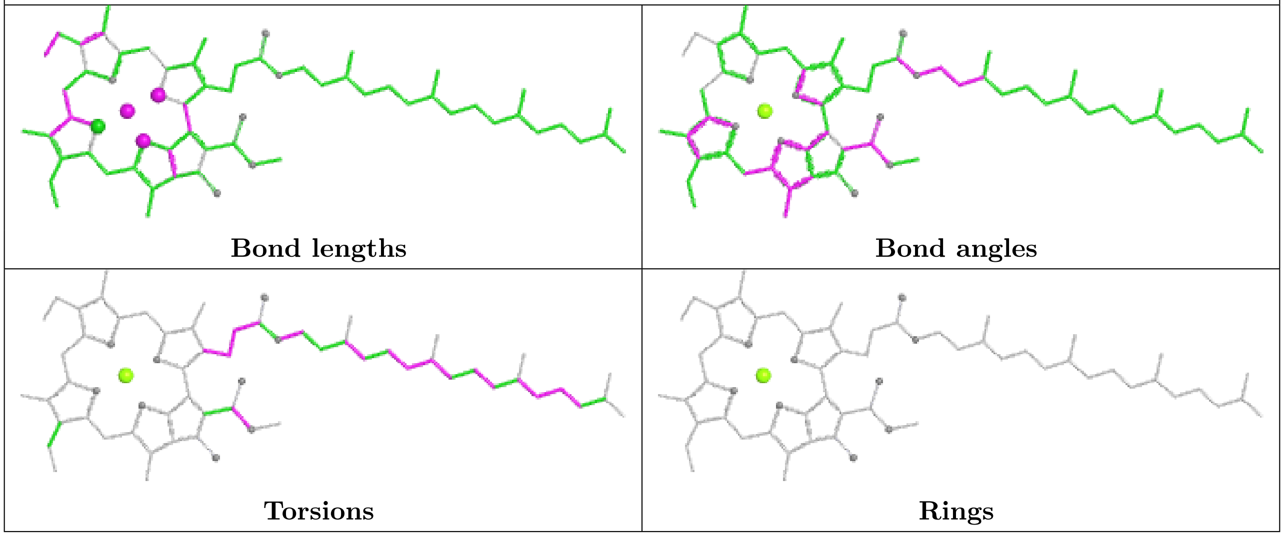

Bond lengths

Bond angles

Torsions

Rings

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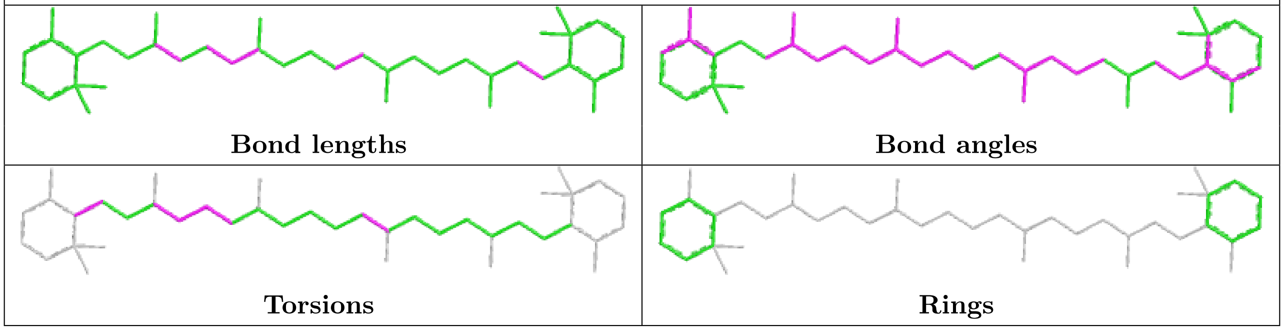

Bond lengths

Bond angles

Torsions

Rings

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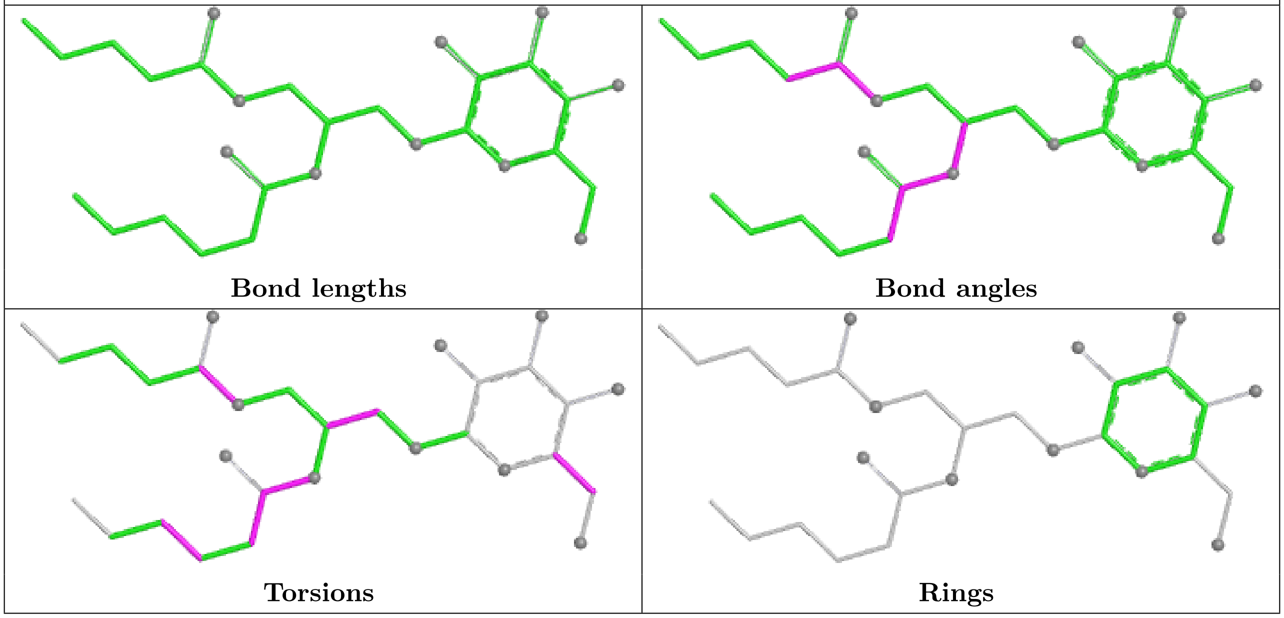

Bond lengths

Bond angles

Torsions

Rings

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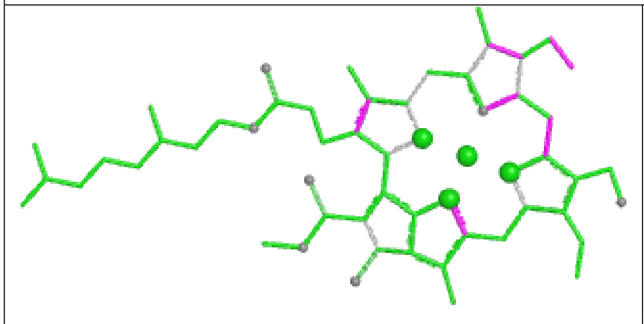
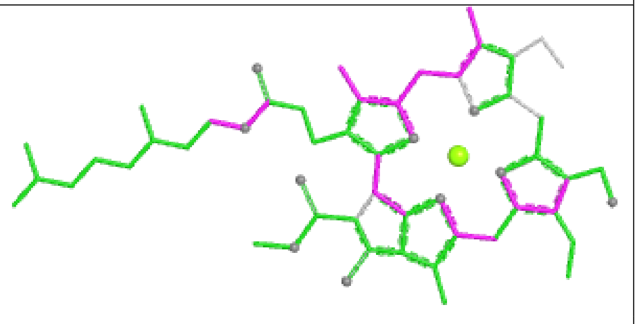
<tr><td>
Bond lengths</td><td>
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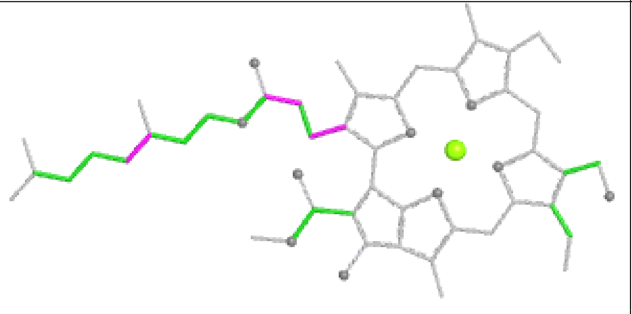
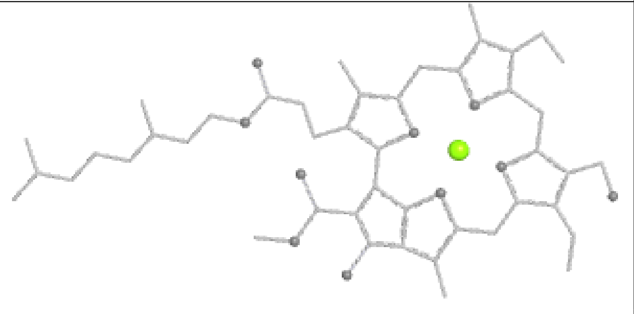
<tr><td>
Torsions</td><td>
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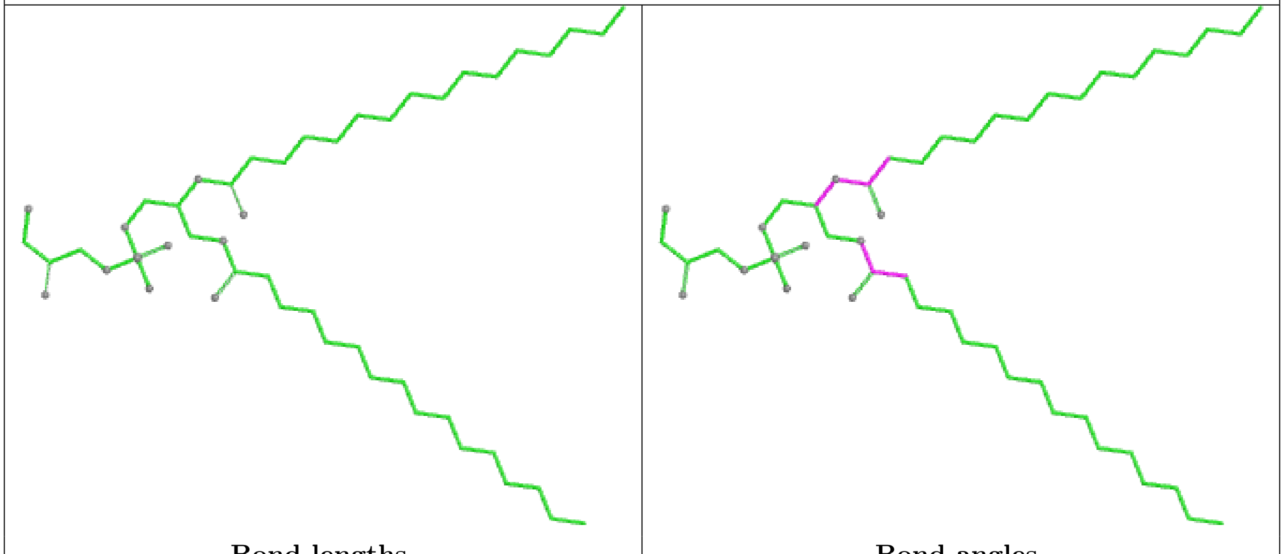
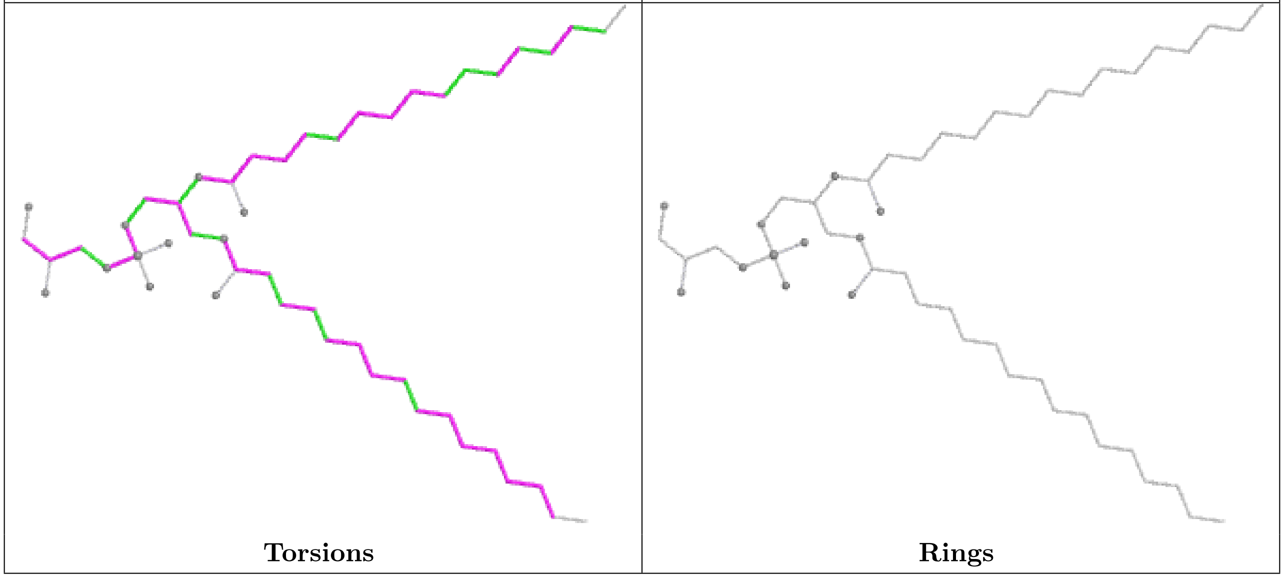


Bond lengths

Bond angles



Torsions

Rings

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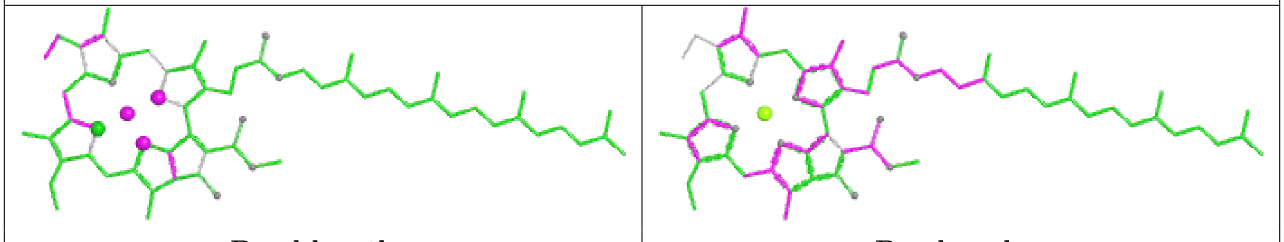
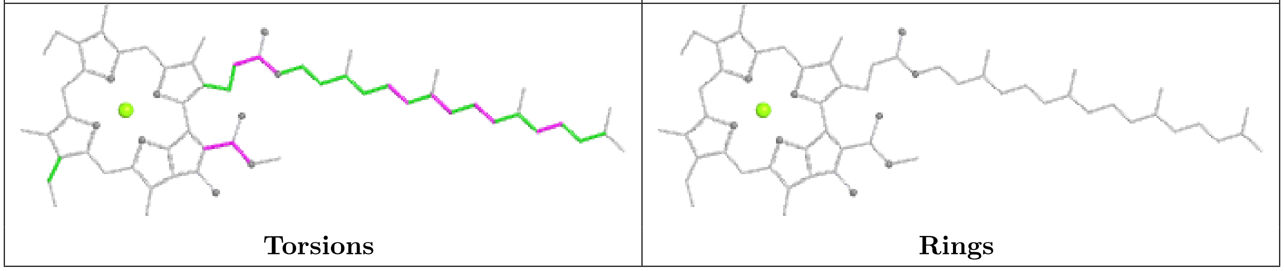


Bond lengths

Bond angles



Torsions

Rings

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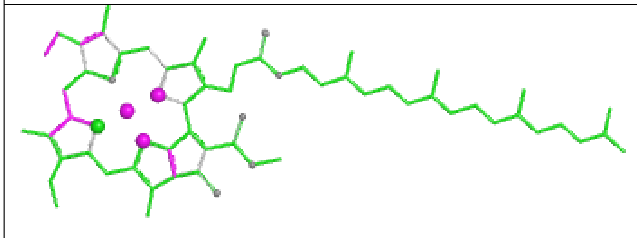
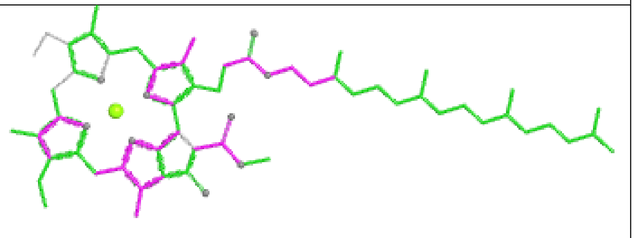
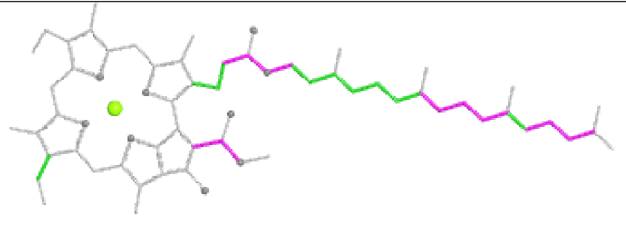
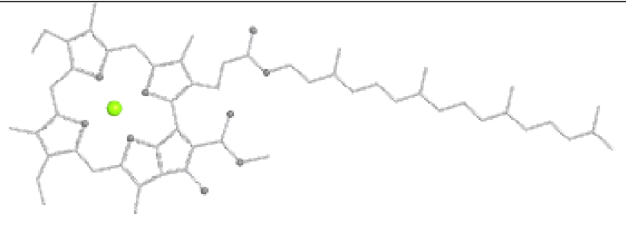
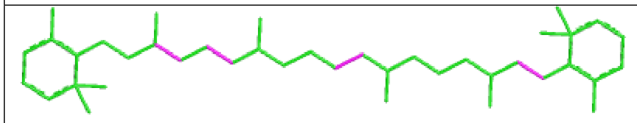
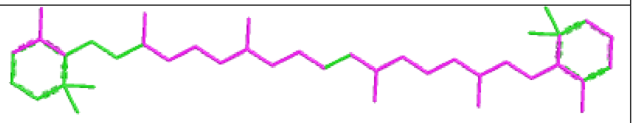
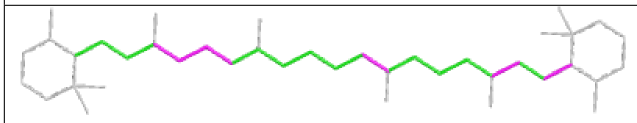
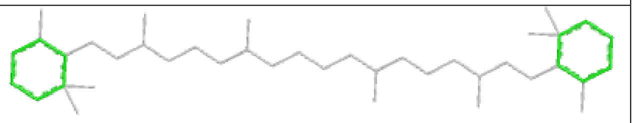
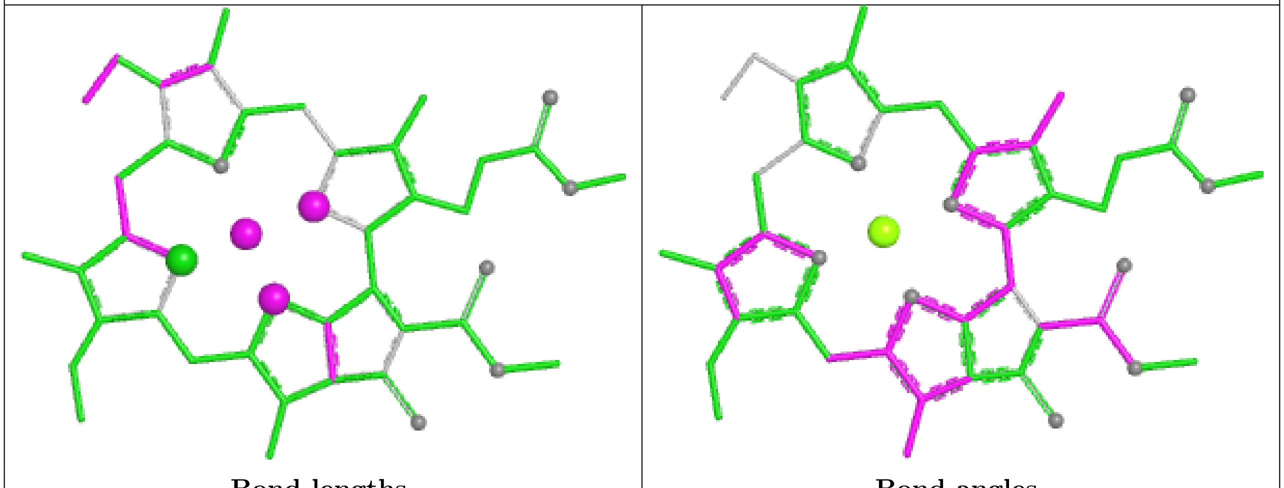
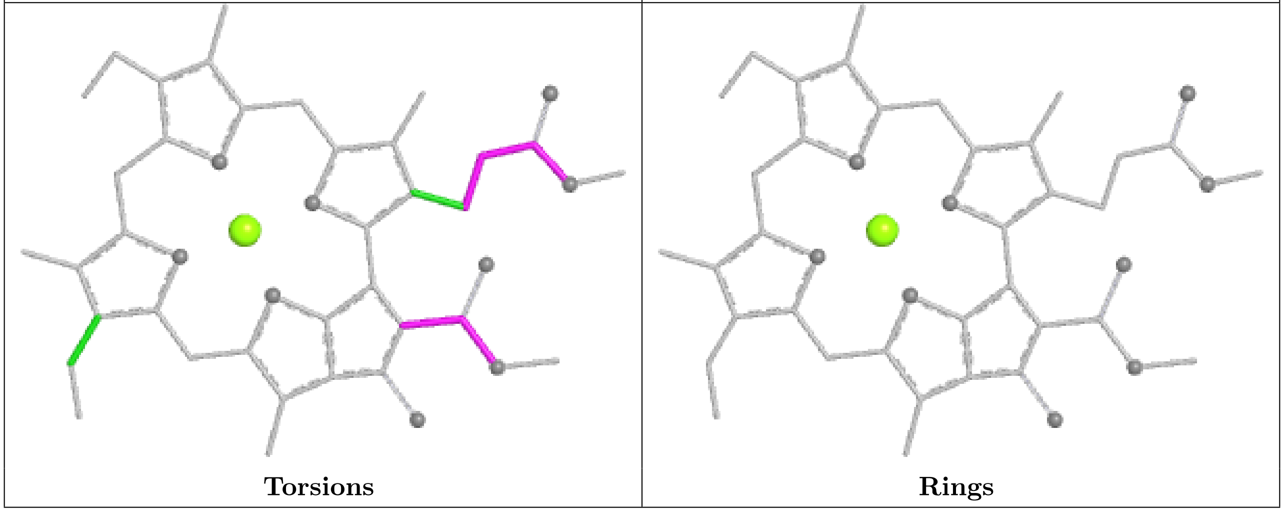
 **Bond lengths**	 **Bond angles**
 **Torsions**	 **Rings**

Ligand BCR G 4011	
 **Bond lengths**	 **Bond angles**
 **Torsions**	 **Rings**

Ligand CLA A 1114

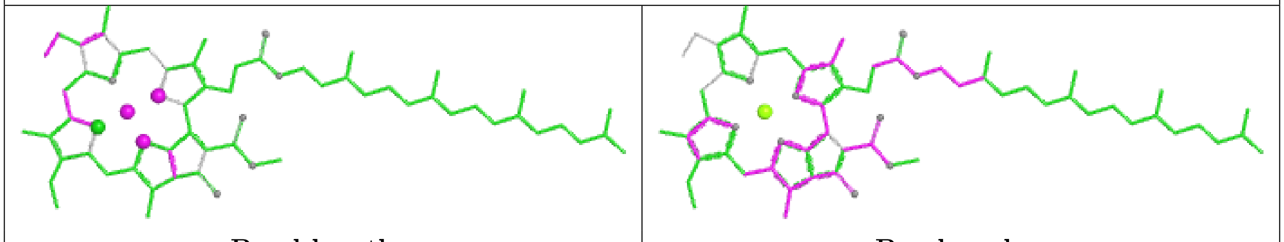


Bond lengths Bond angles

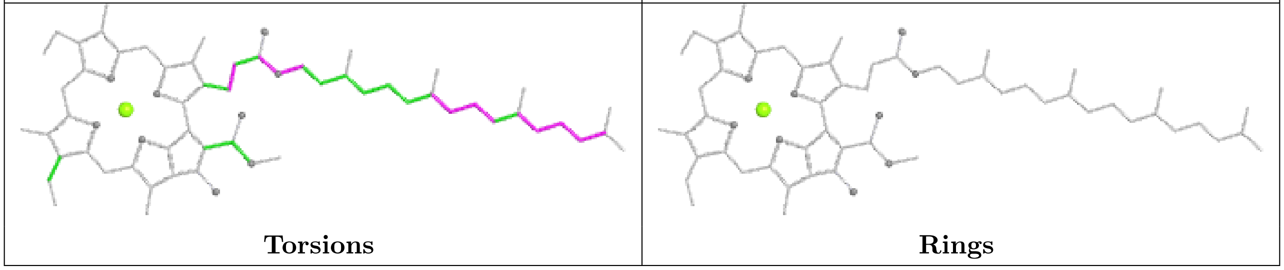


Torsions Rings

Ligand CLA B 1214

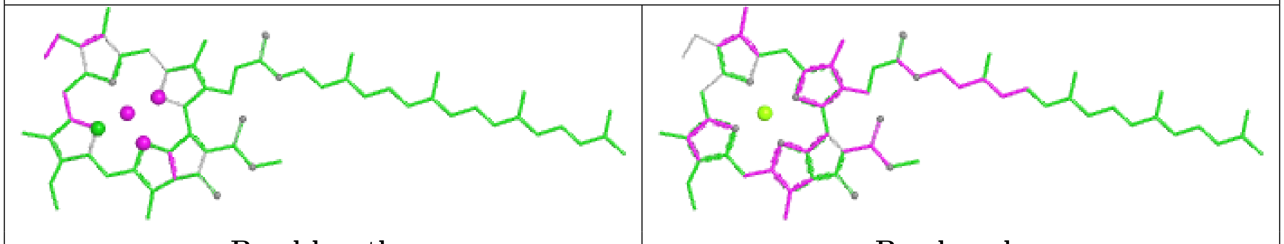


Bond lengths Bond angles



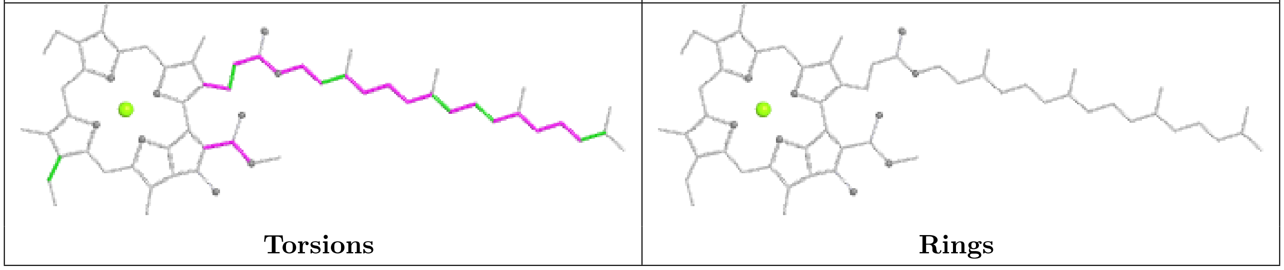
Torsions Rings

Ligand CLA A 1103



Bond lengths

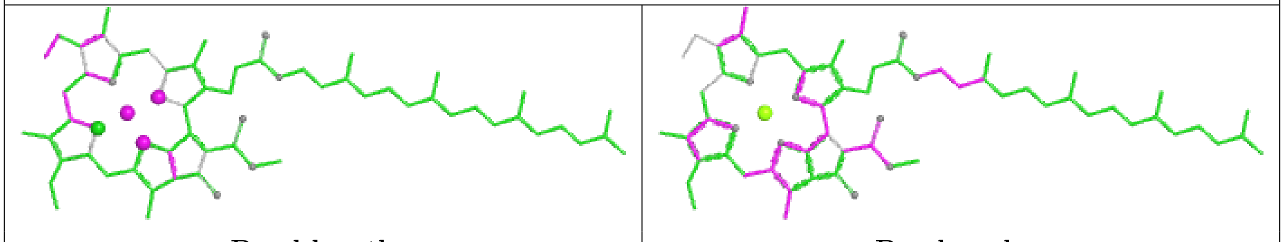
Bond angles



Torsions

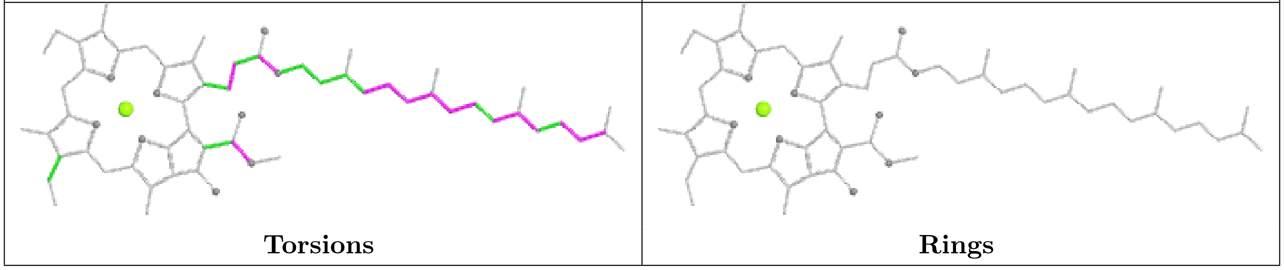
Rings

Ligand CLA A 1129



Bond lengths

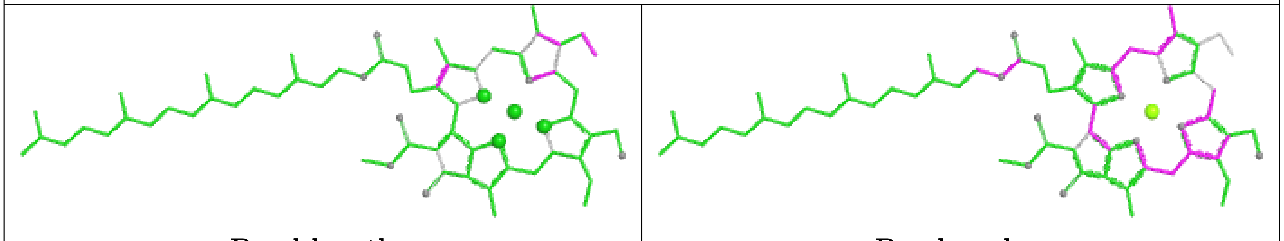
Bond angles



Torsions

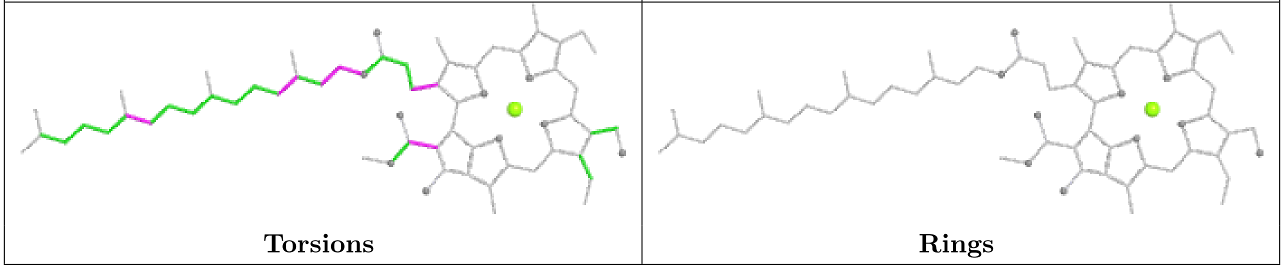
Rings

Ligand CHL 2 609



Bond lengths

Bond angles



Torsions

Rings

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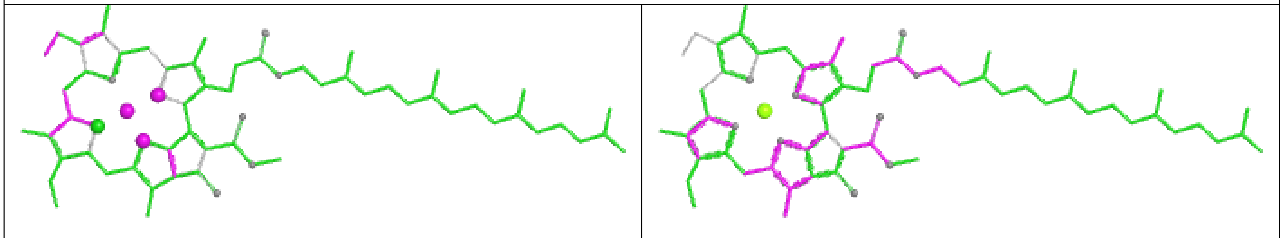
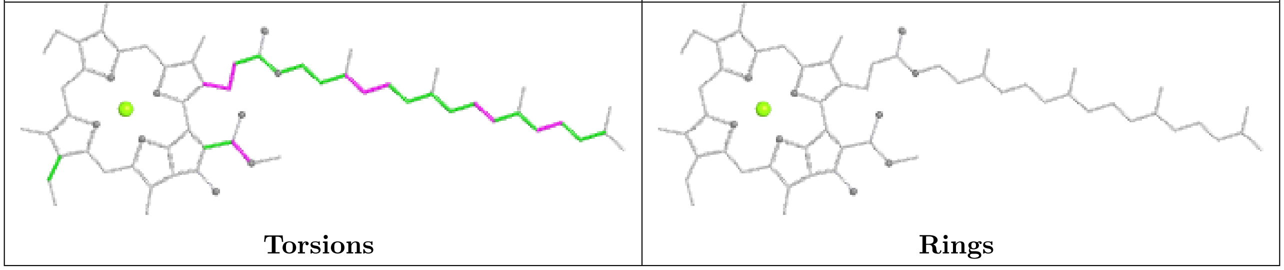


Bond lengths

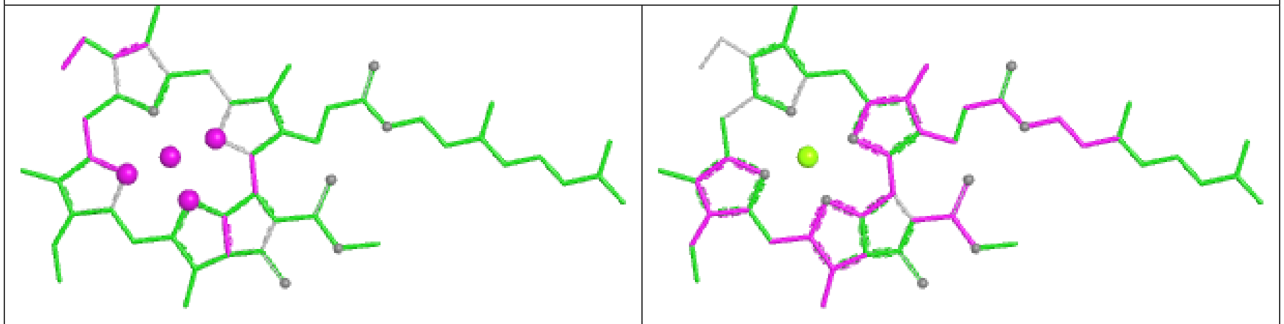
Bond angles



Torsions

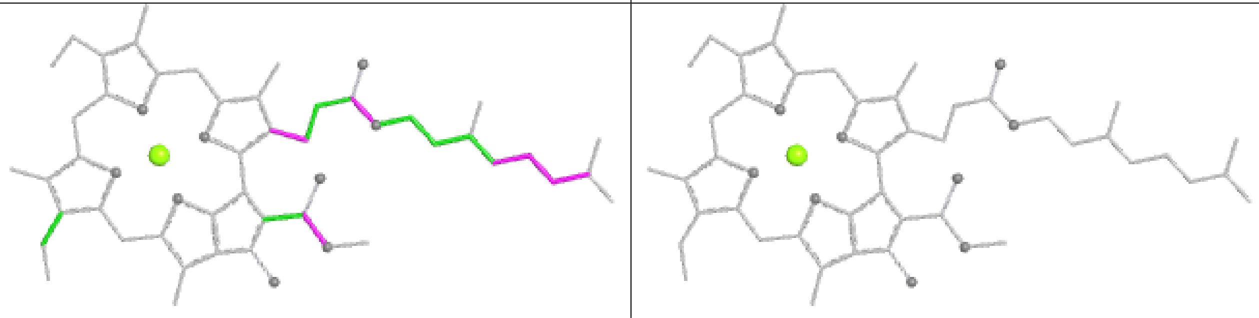
Rings

Ligand CLA 3 605



Bond lengths

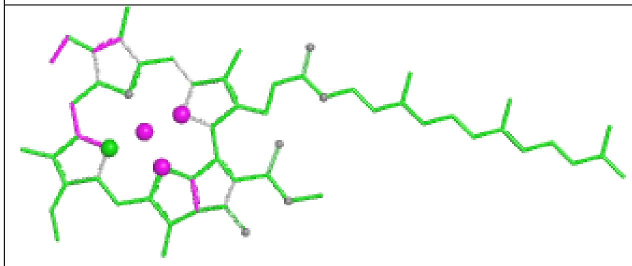
Bond angles



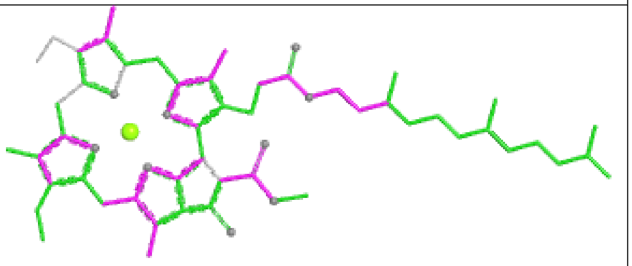
Torsions

Rings

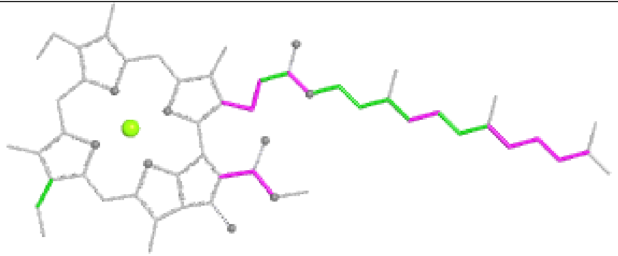
Ligand CLA B 1228



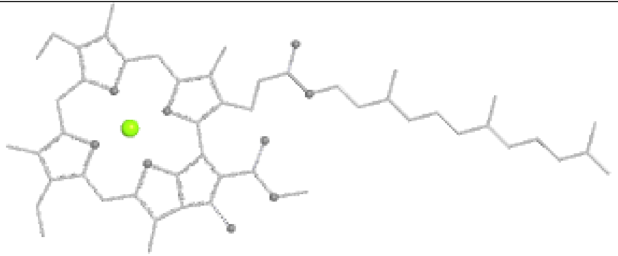
Bond lengths



Bond angles

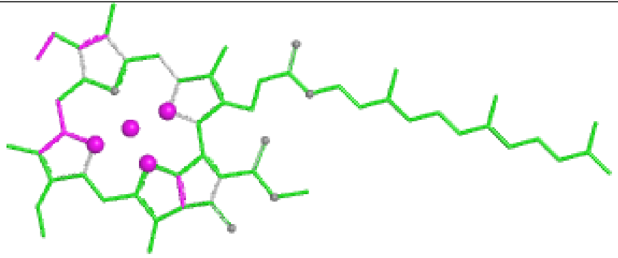


Torsions

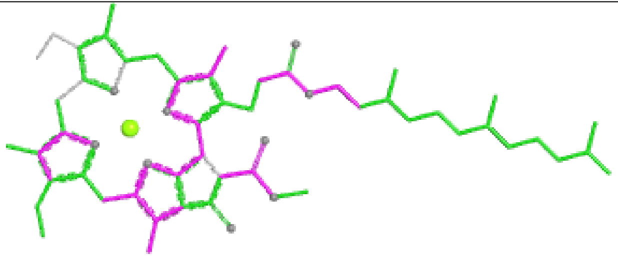


Rings

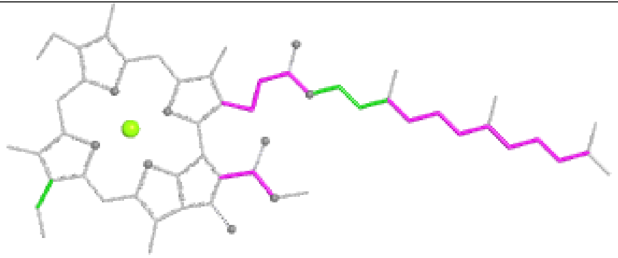
Ligand CLA K 1402



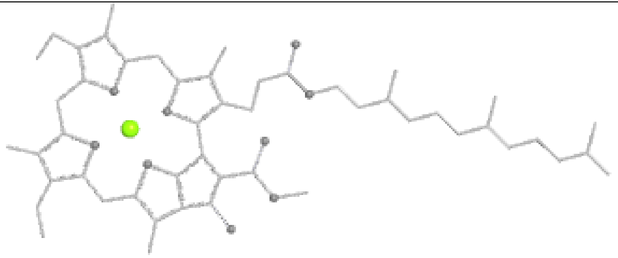
Bond lengths



Bond angles

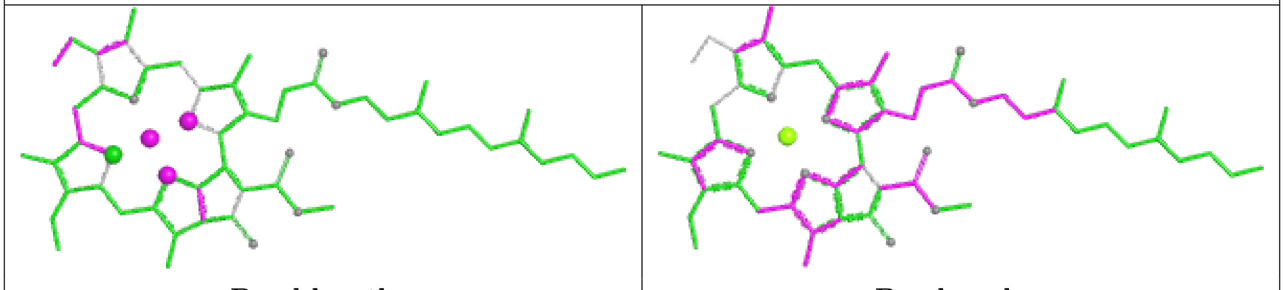


Torsions

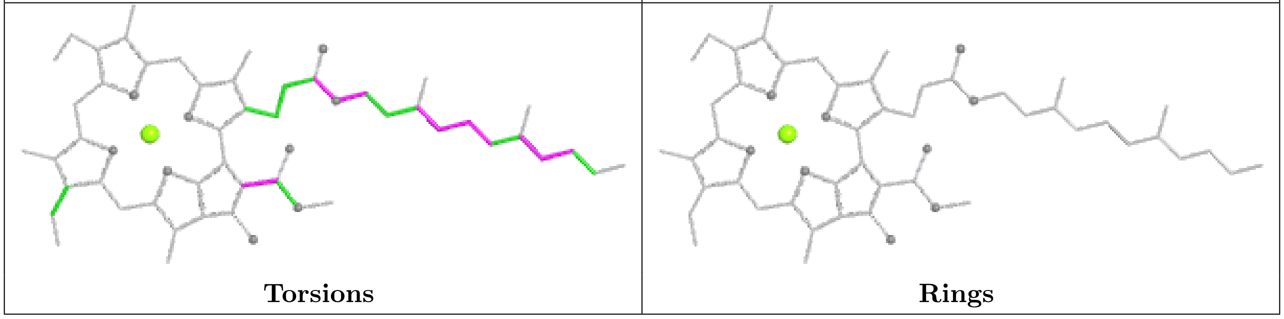


Rings

Ligand CLA B 1230

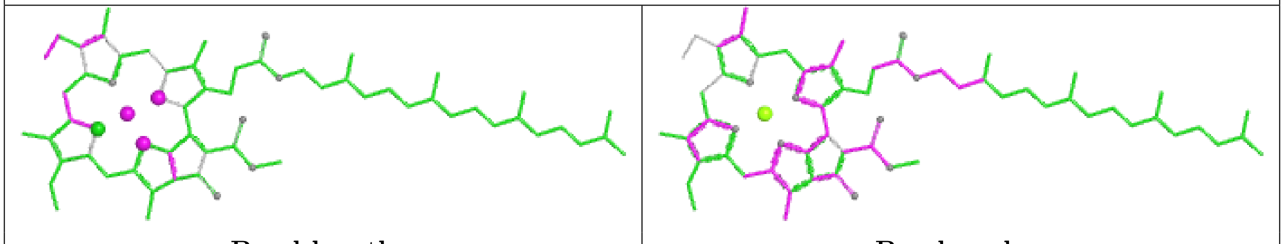


Bond lengths **Bond angles**

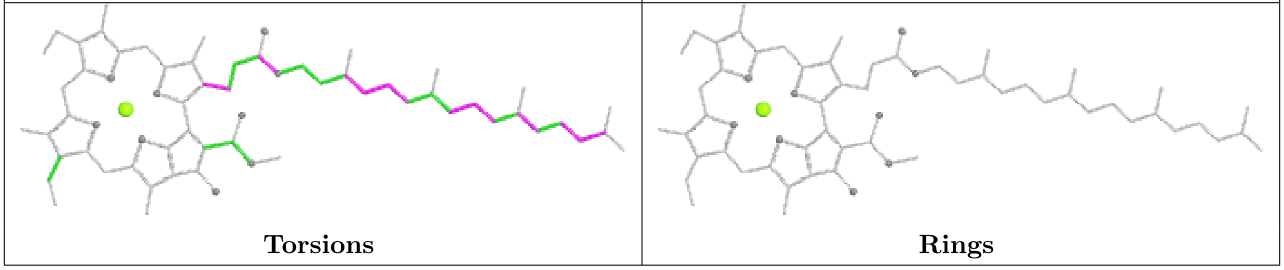


Torsions **Rings**

Ligand CLA 4 612

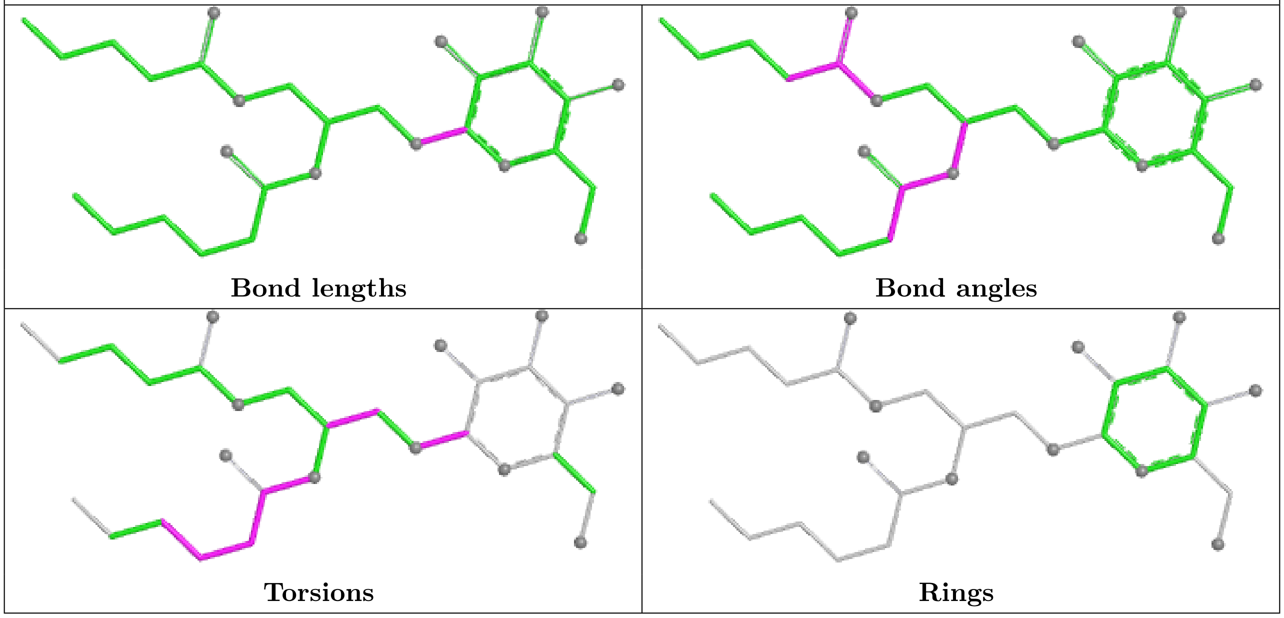


Bond lengths **Bond angles**



Torsions **Rings**

Ligand LMG 3 802



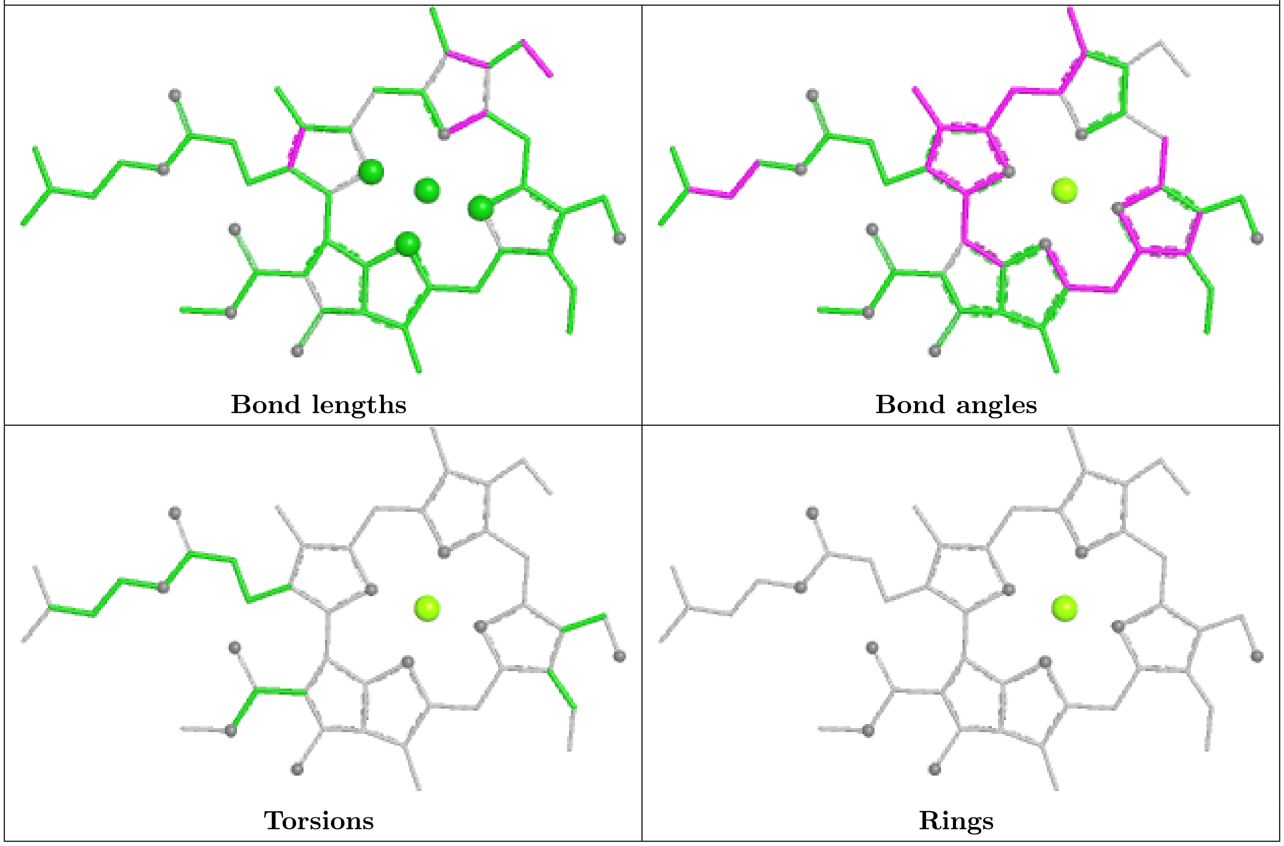
Bond lengths

Bond angles

Torsions

Rings

Ligand CHL 4 611



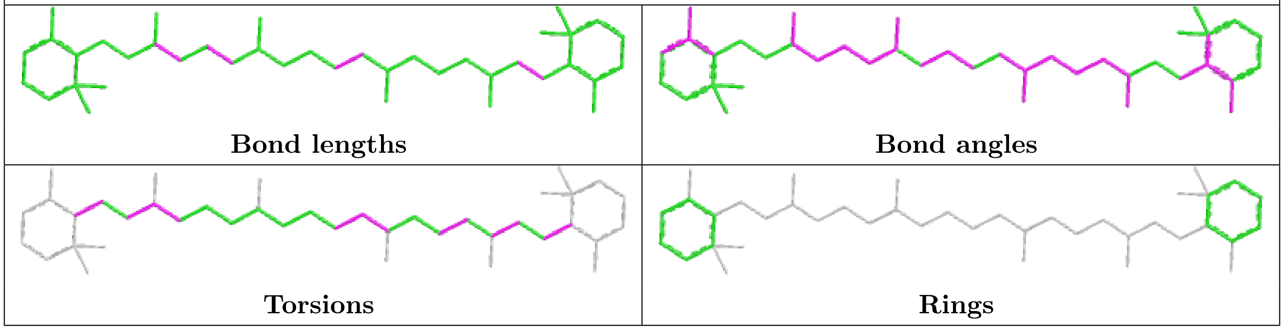
Bond lengths

Bond angles

Torsions

Rings

Ligand BCR 3 506



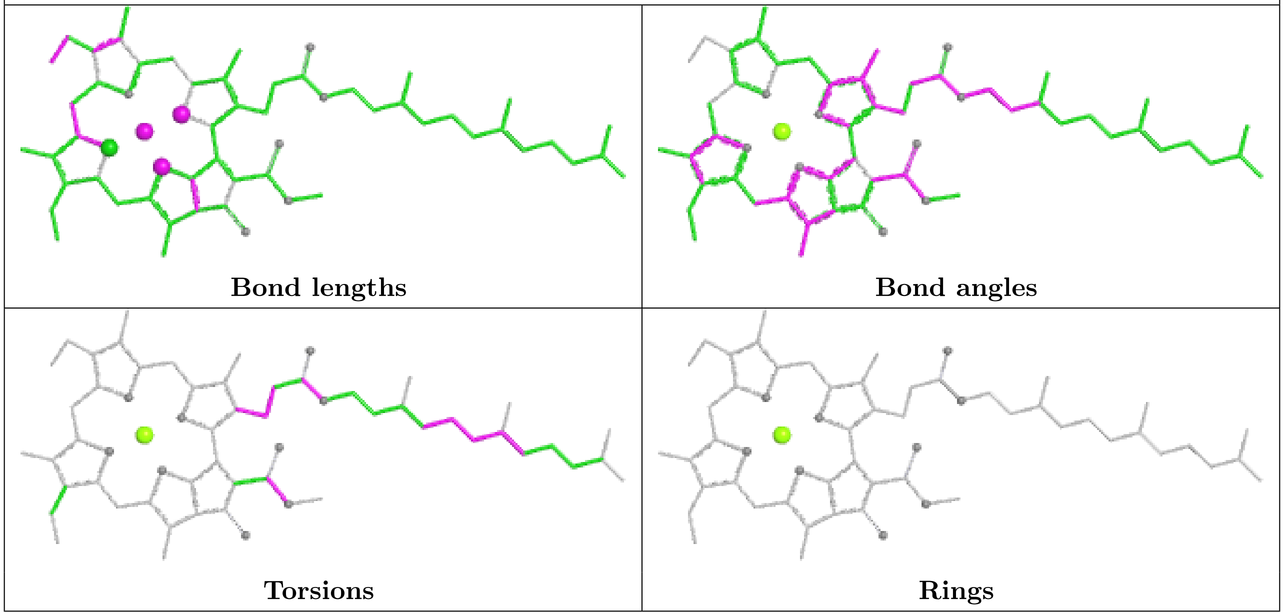
Bond lengths

Bond angles

Torsions

Rings

Ligand CLA B 1208



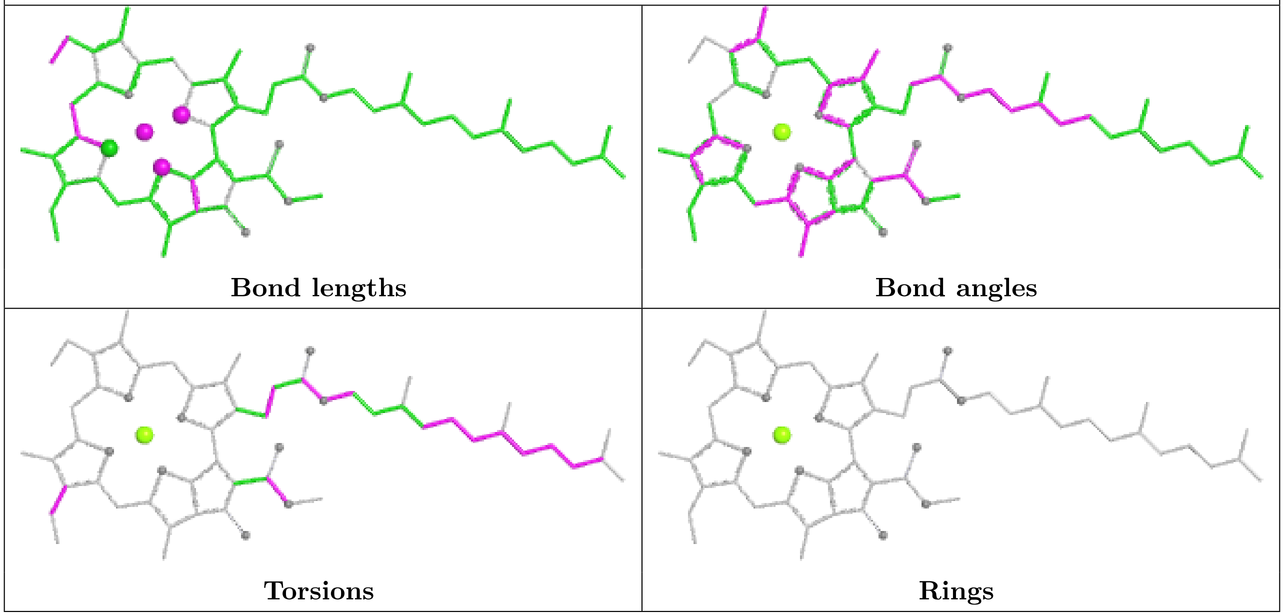
Bond lengths

Bond angles

Torsions

Rings

Ligand CLA A 1105



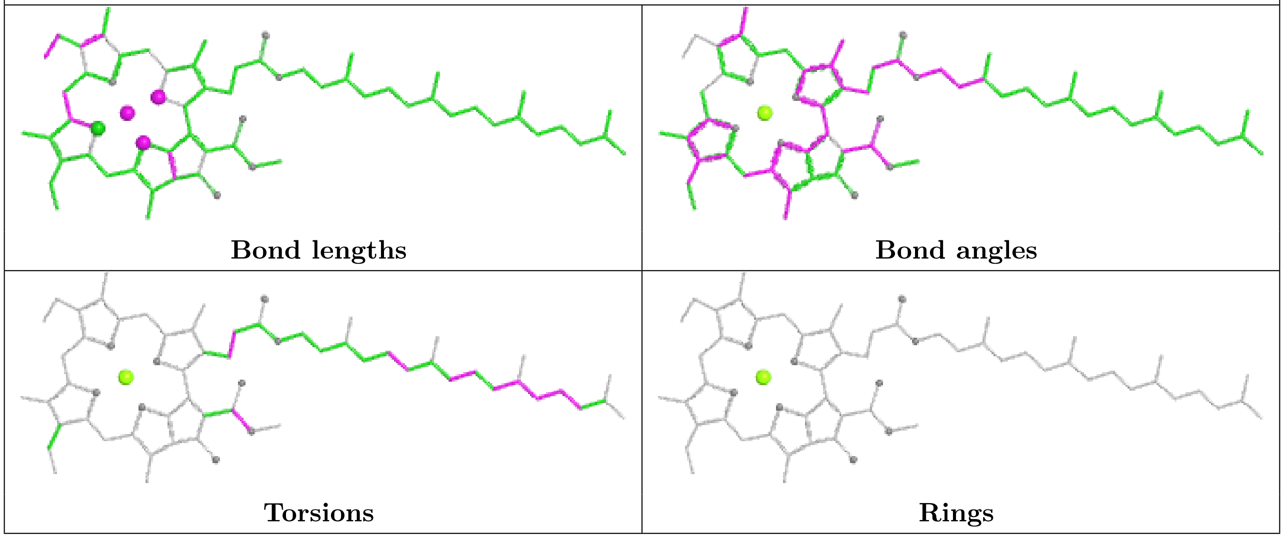
Bond lengths

Bond angles

Torsions

Rings

Ligand CLA B 1023



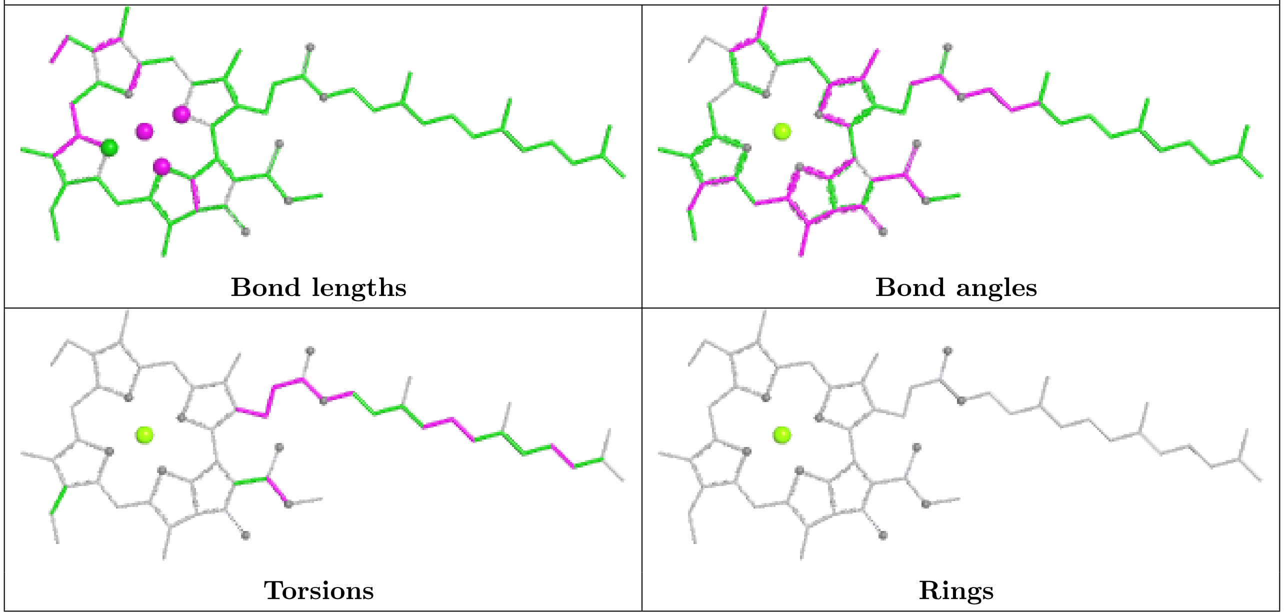
Bond lengths

Bond angles

Torsions

Rings

Ligand CLA 2 601



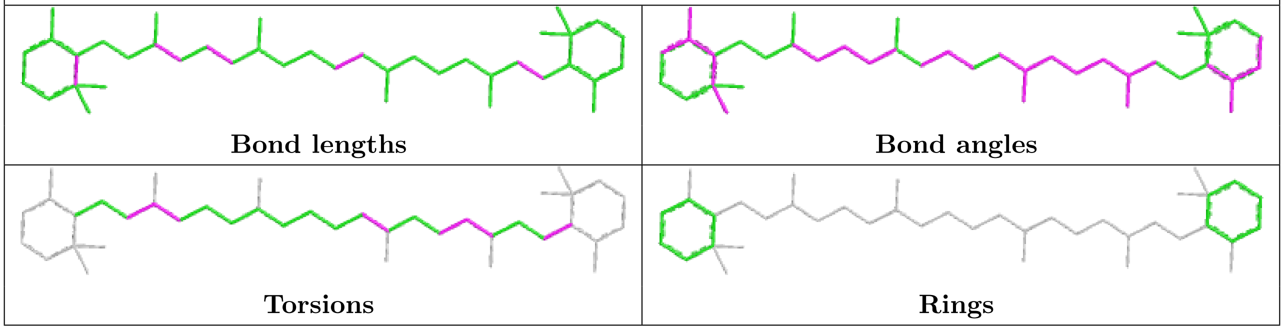
Bond lengths

Bond angles

Torsions

Rings

Ligand BCR I 4020



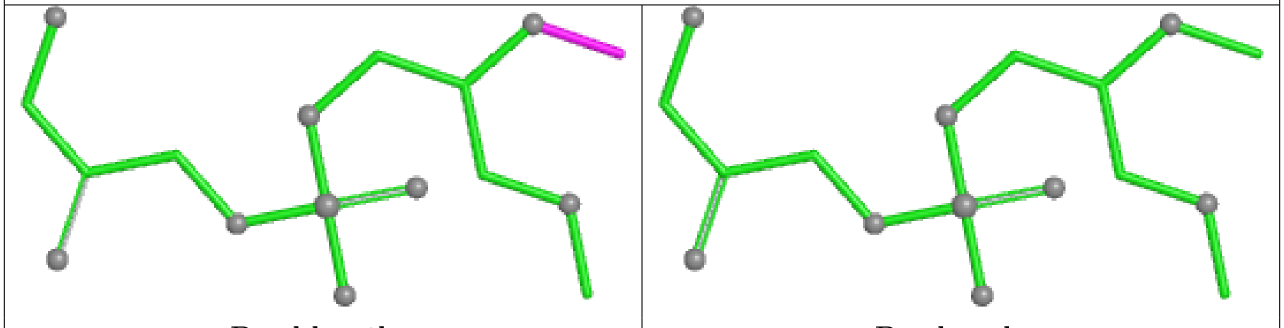
Bond lengths

Bond angles

Torsions

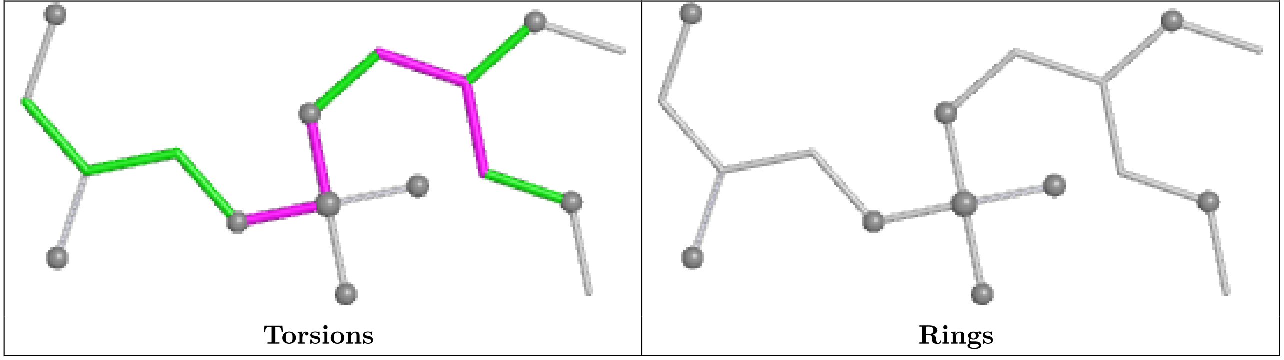
Rings

Ligand LHG 3 801



Bond lengths

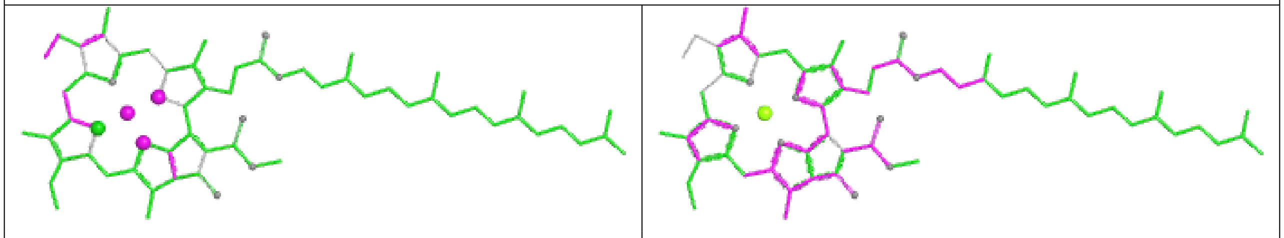
Bond angles



Torsions

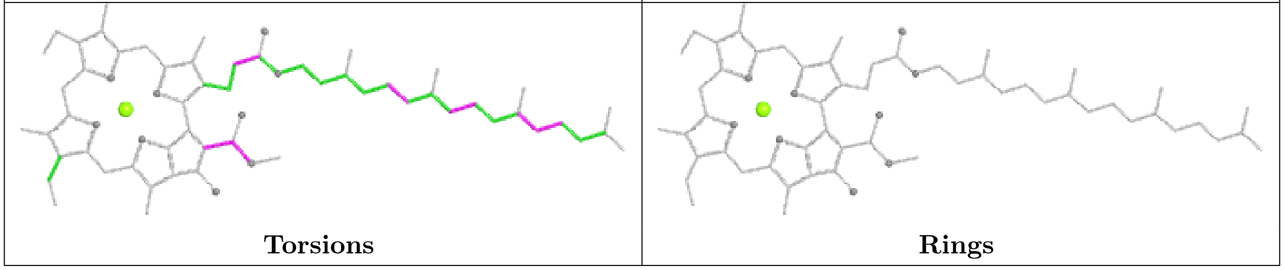
Rings

Ligand CLA B 1021



Bond lengths

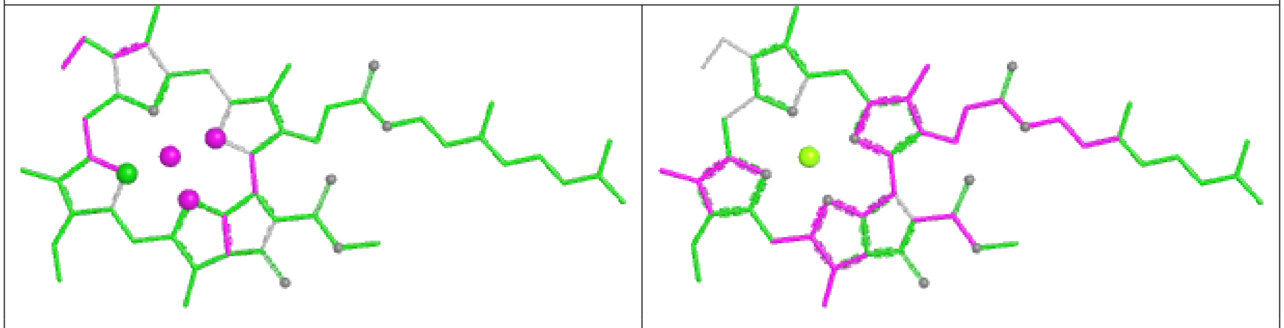
Bond angles



Torsions

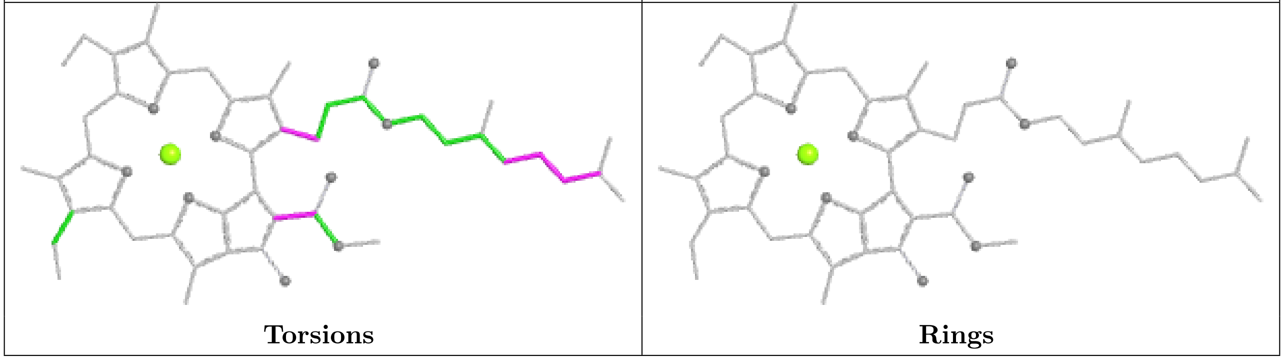
Rings

Ligand CLA A 1110



Bond lengths

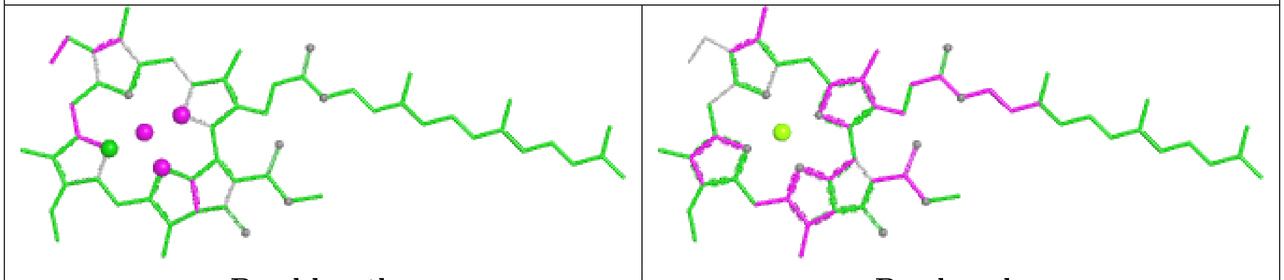
Bond angles



Torsions

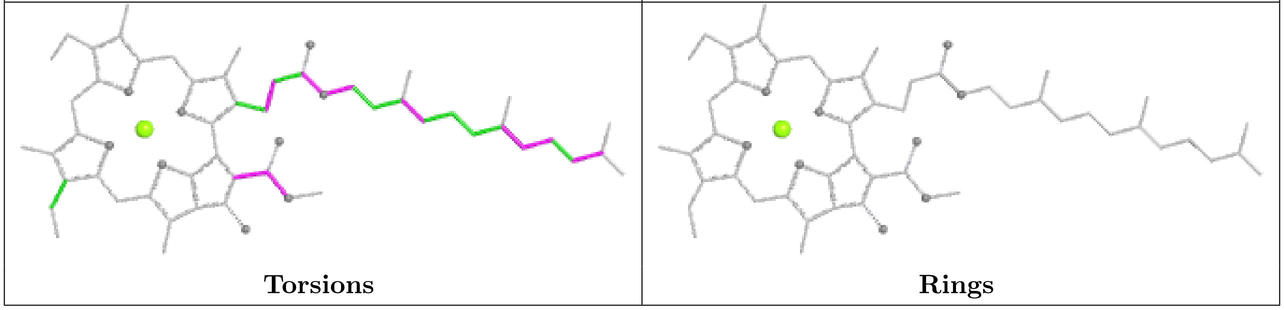
Rings

Ligand CLA 4 604



Bond lengths

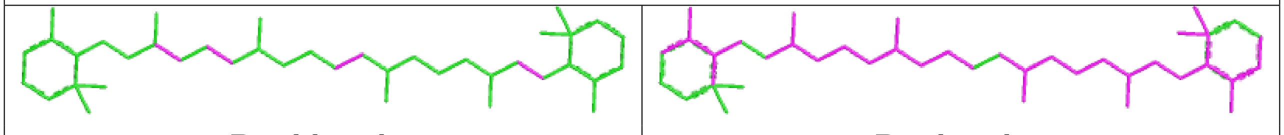
Bond angles



Torsions

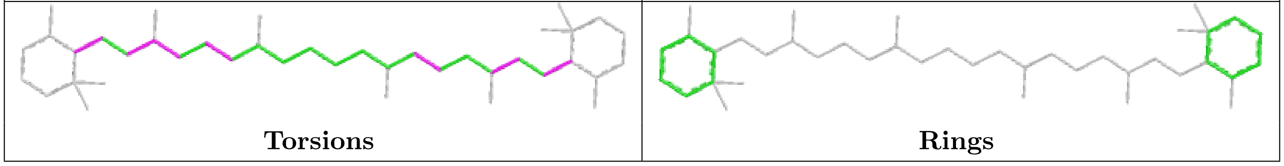
Rings

Ligand BCR B 4006



Bond lengths

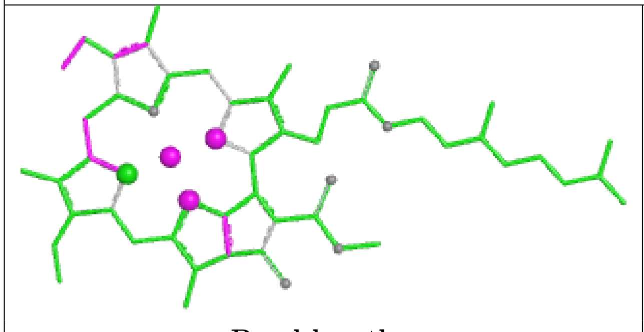
Bond angles



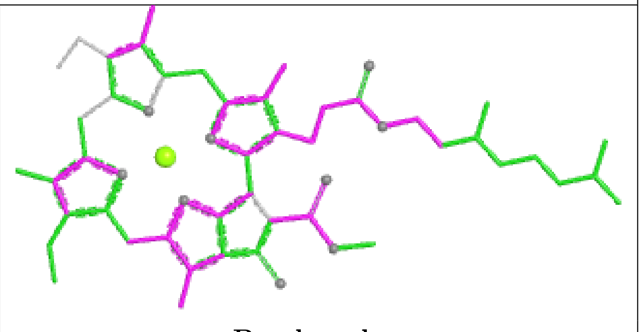
Torsions

Rings

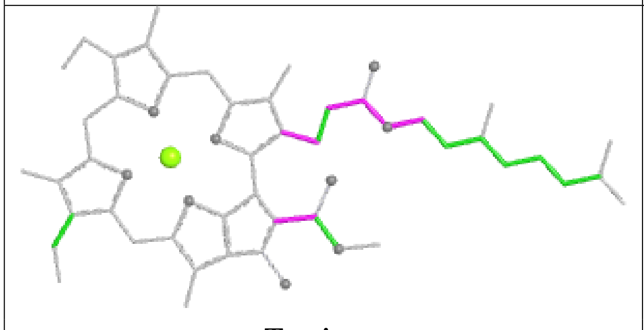
Ligand CLA B 1220



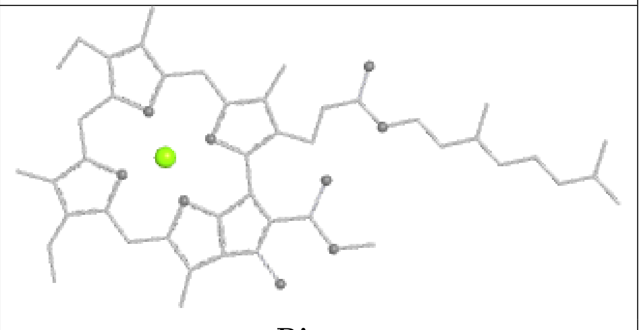
Bond lengths



Bond angles



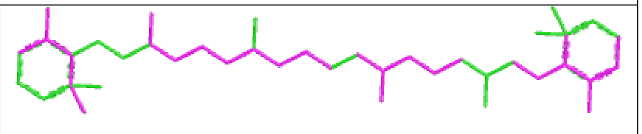
Torsions



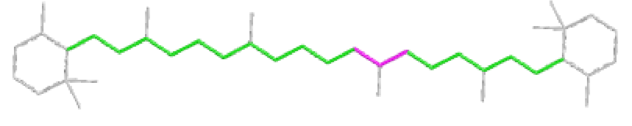
Rings

Ligand BCR A 4007

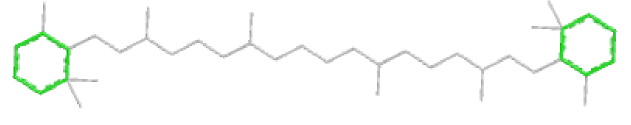
Bond lengths



Bond angles

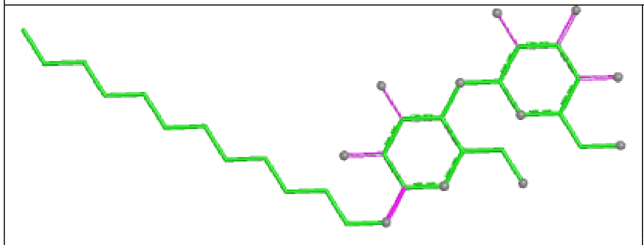


Torsions

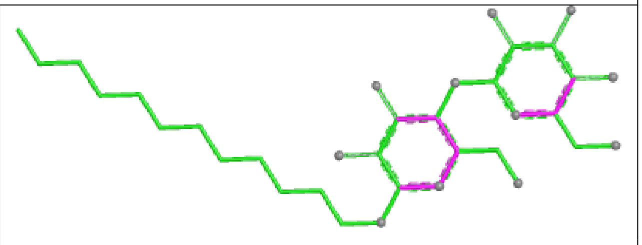


Rings

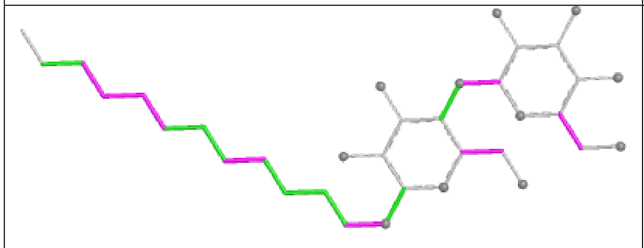
Ligand LMT G 5004



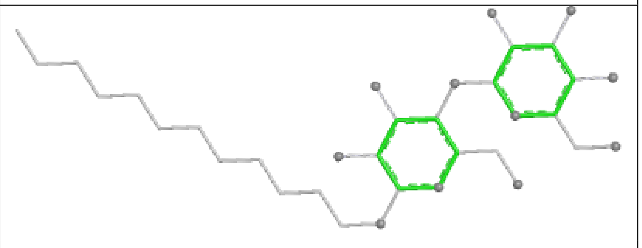
Bond lengths



Bond angles

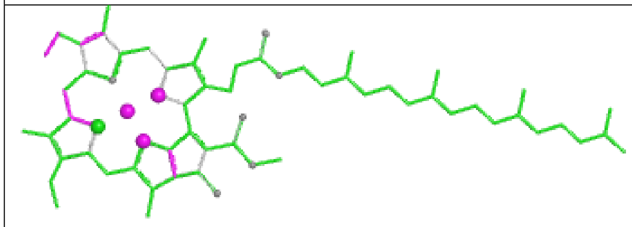


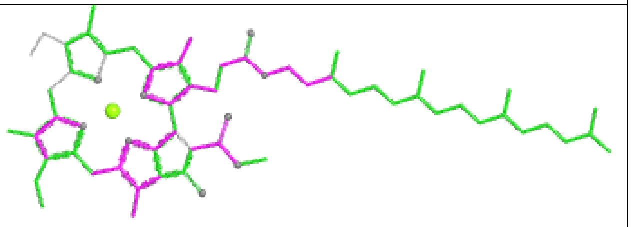
Torsions

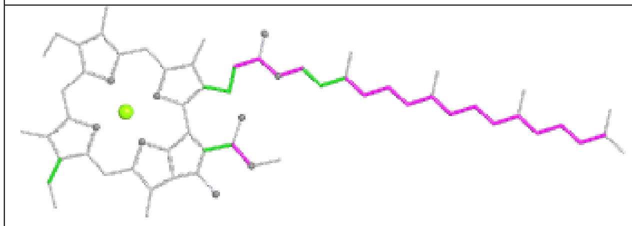


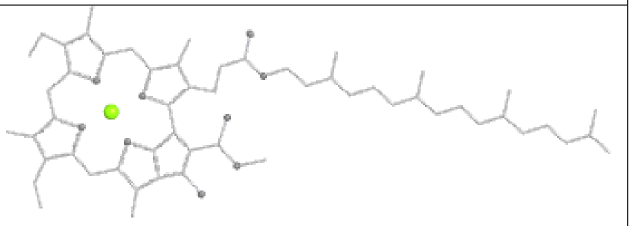
Rings

Ligand CLA B 1238

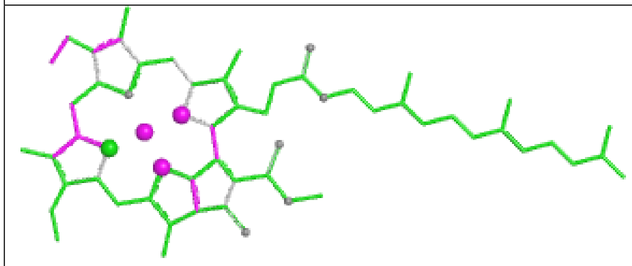

Bond lengths


Bond angles


Torsions


Rings

Ligand CLA 1 614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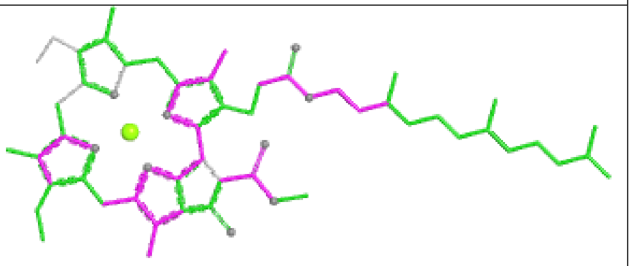
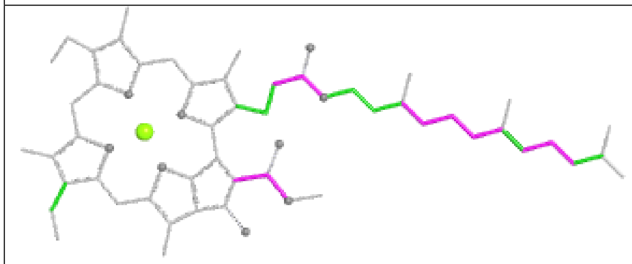
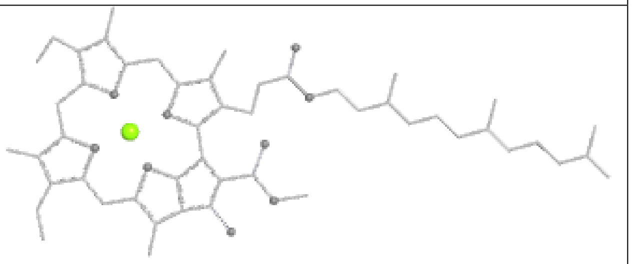
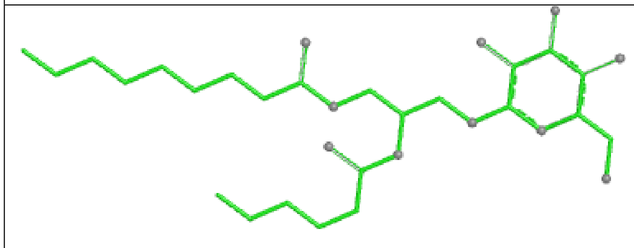
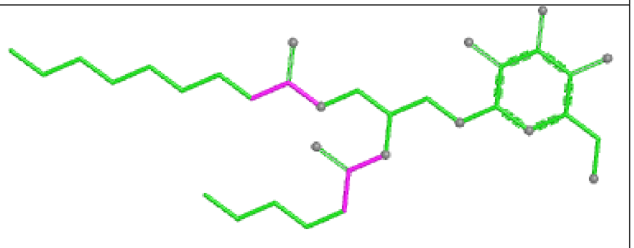
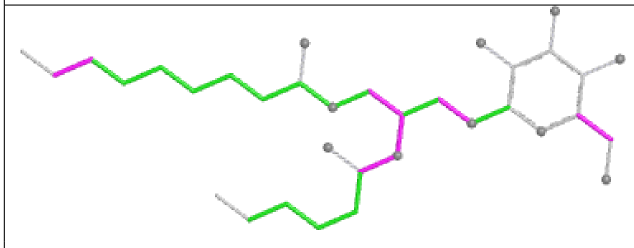
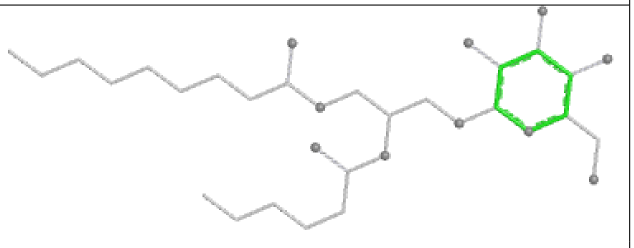
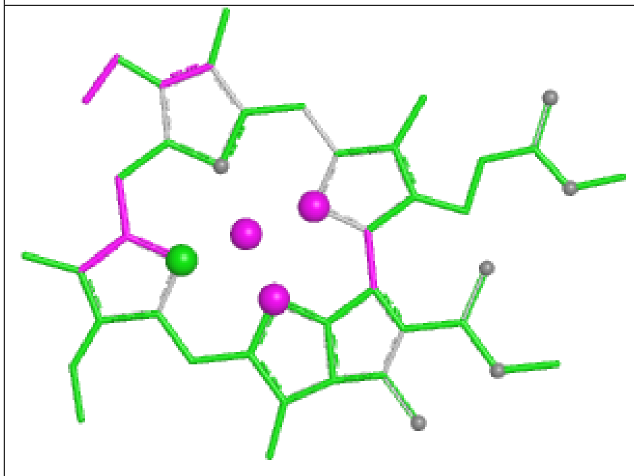
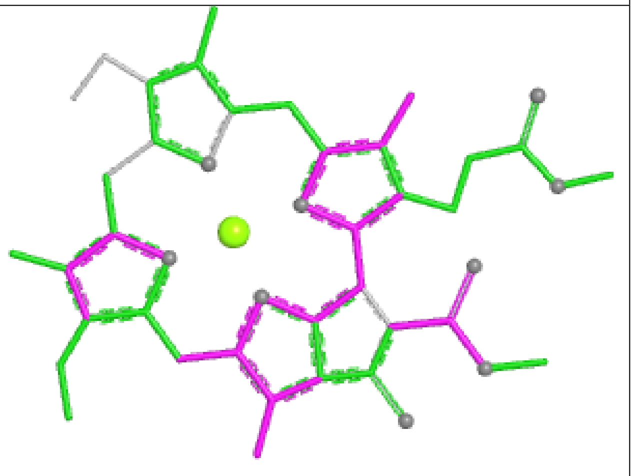
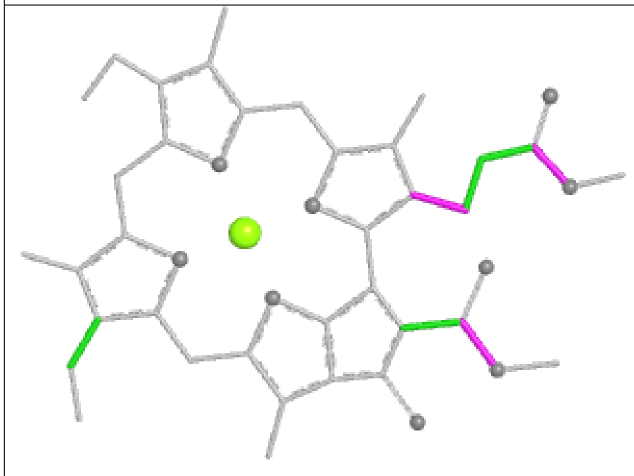
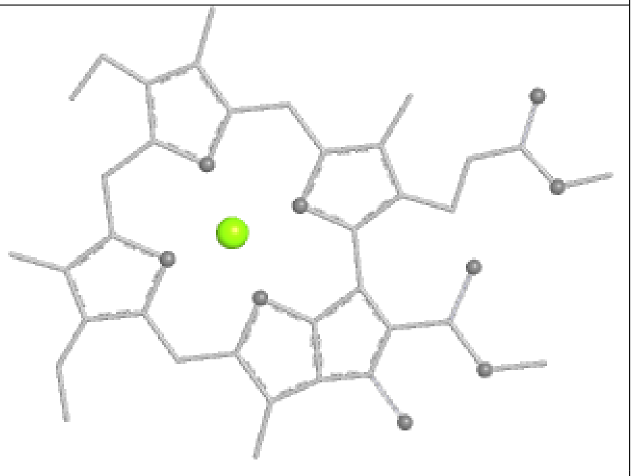

Bond angles

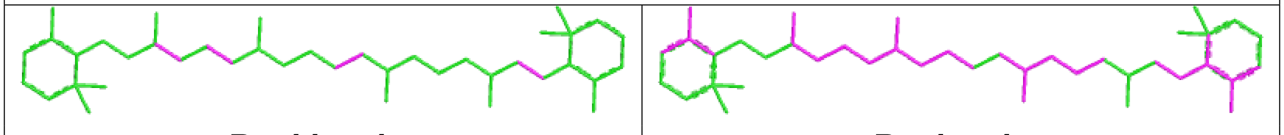

Torsions


Rings

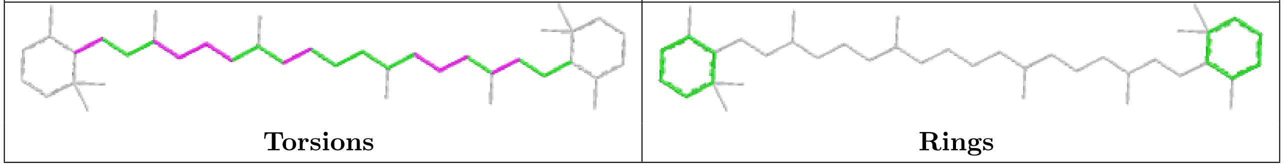
Ligand LMG F 5004	
 **Bond lengths**	 **Bond angles**
 **Torsions**	 **Rings**

Ligand CLA 3 613	
 **Bond lengths**	 **Bond angles**
 **Torsions**	 **Rings**

Ligand BCR K 4002

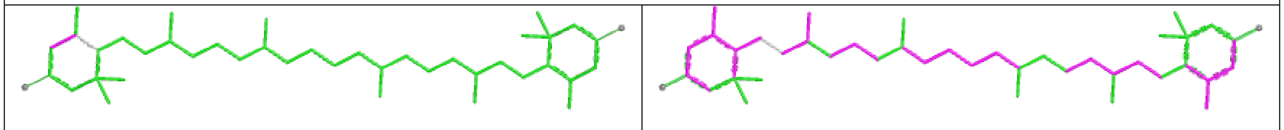


Bond lengths Bond angles

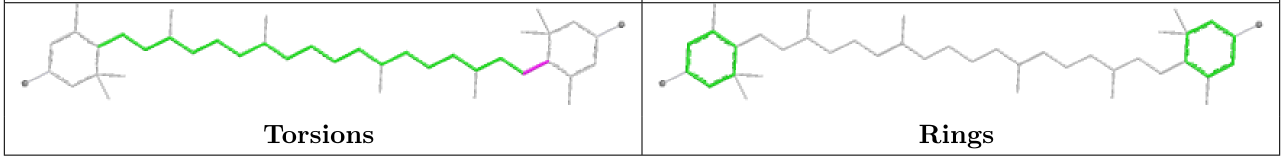


Torsions Rings

Ligand LUT 1 502

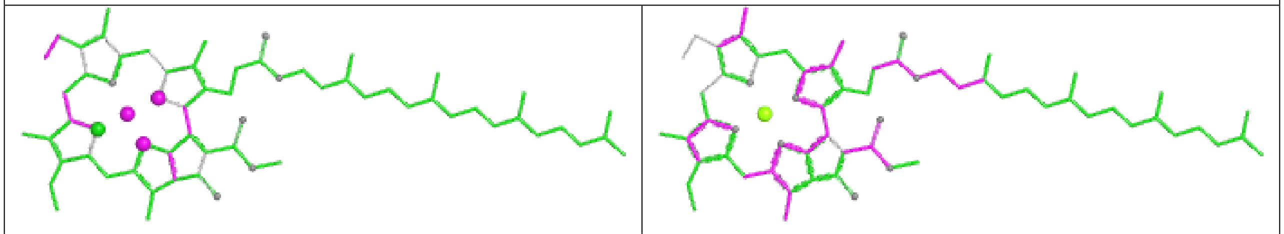


Bond lengths Bond angles

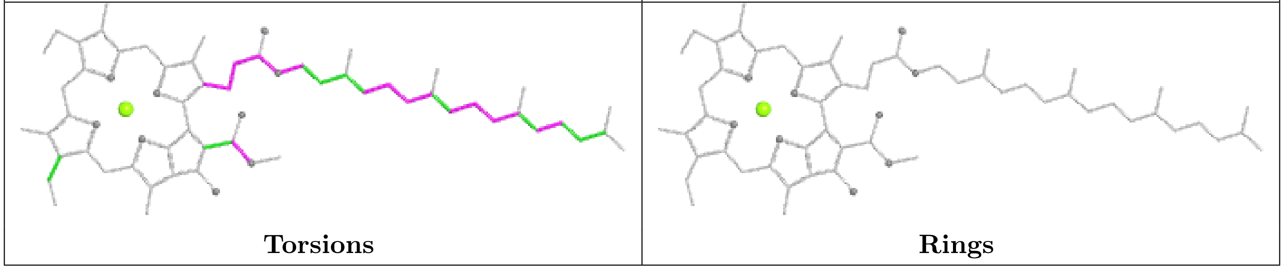


Torsions Rings

Ligand CLA F 1301

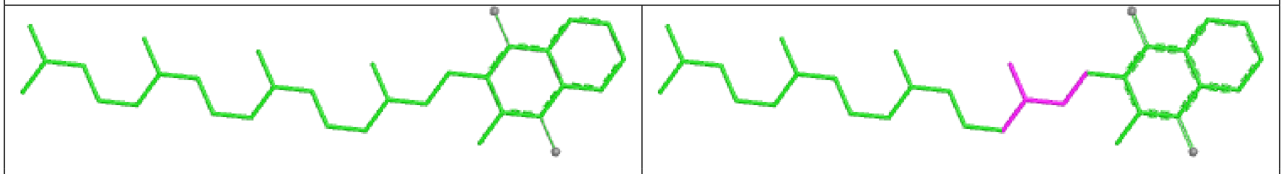


Bond lengths Bond angles

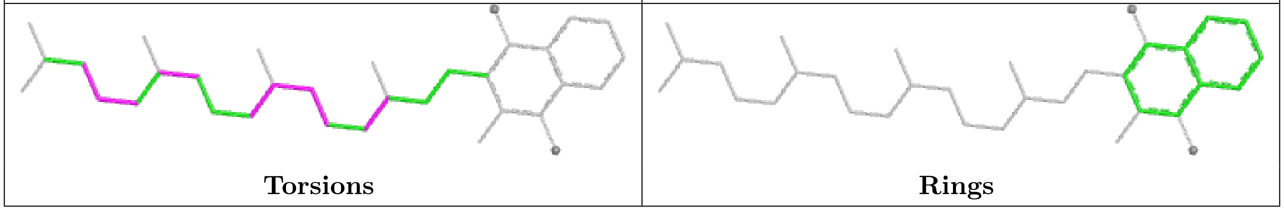


Torsions Rings

Ligand PQN B 2002

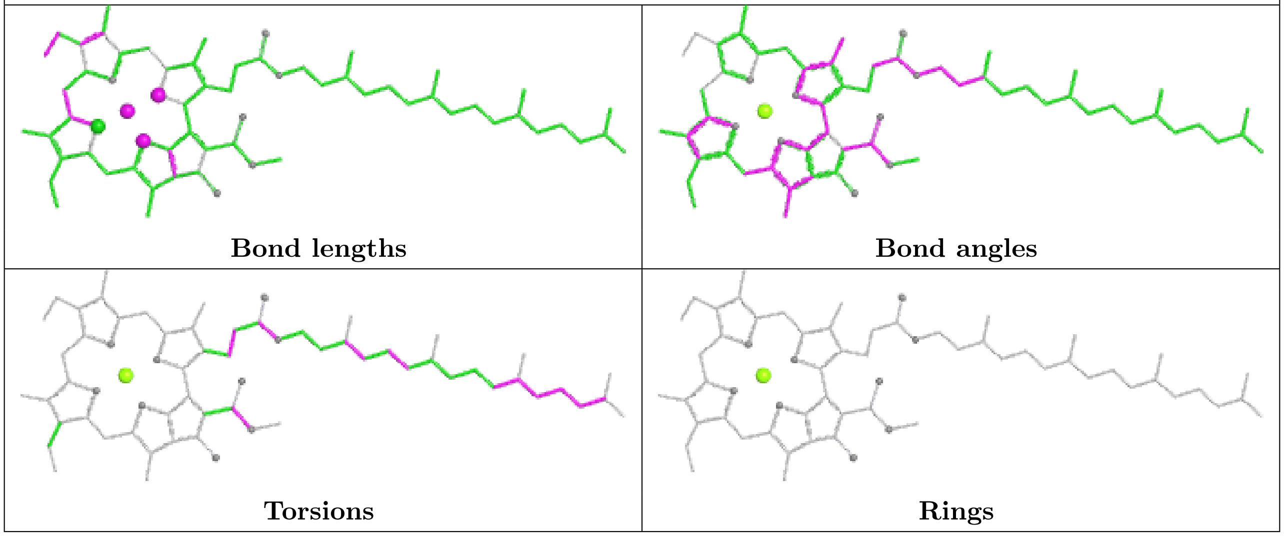


Bond lengths Bond angles



Torsions Rings

Ligand CLA A 1131



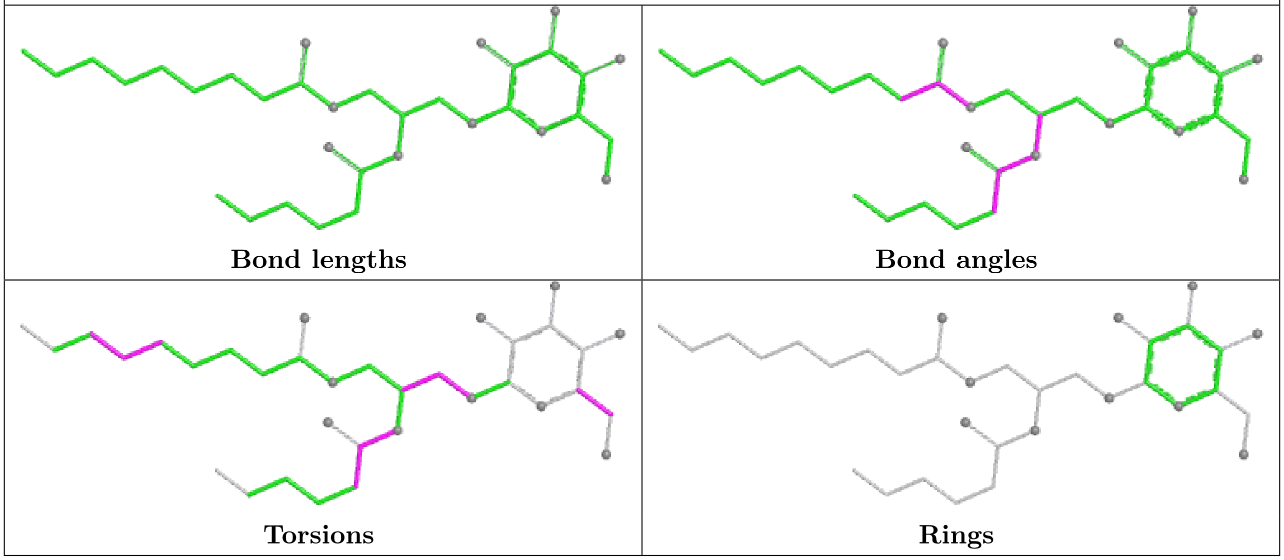
Bond lengths

Bond angles

Torsions

Rings

Ligand LMG B 5007



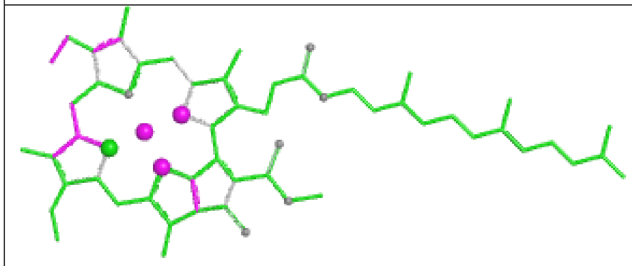
Bond lengths

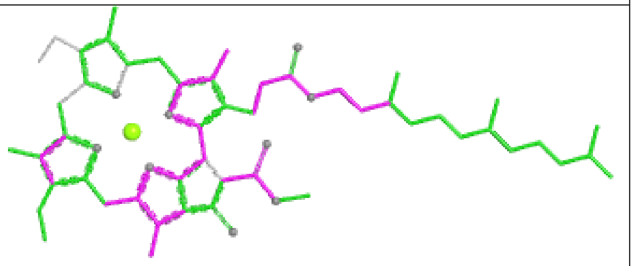
Bond angles

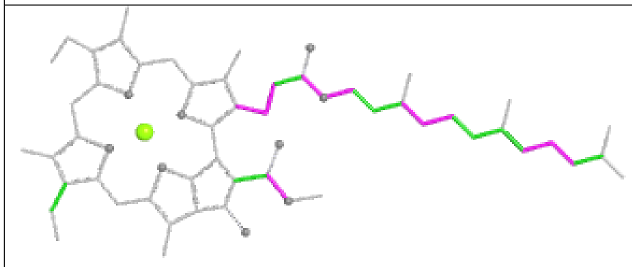
Torsions

Rings

Ligand CLA A 1121


Bond lengths


Bond angles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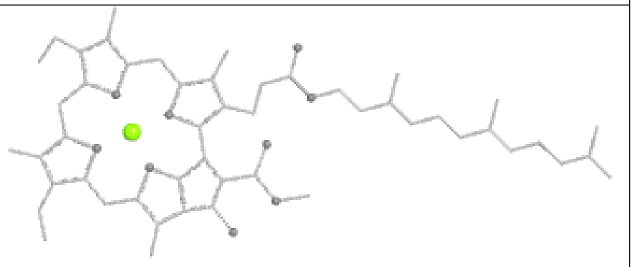
Rings

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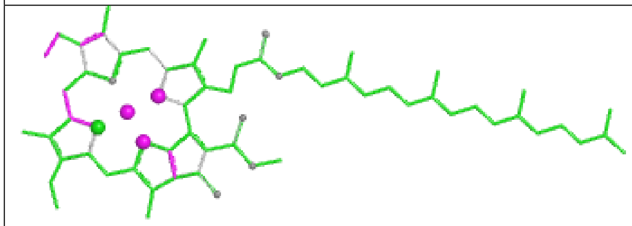
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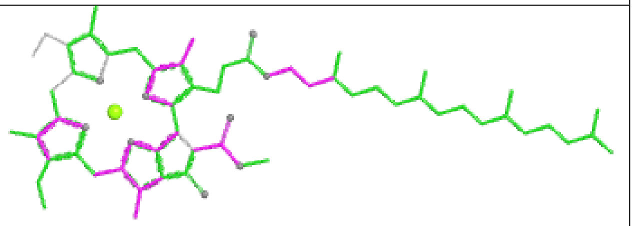
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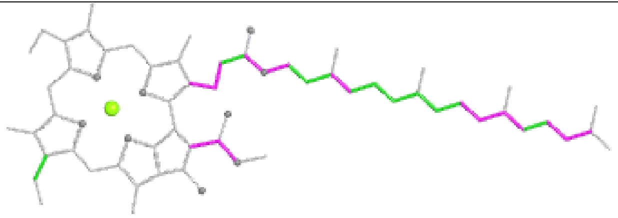
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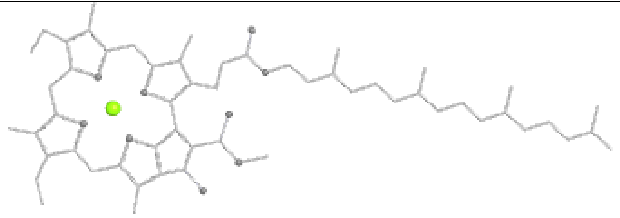
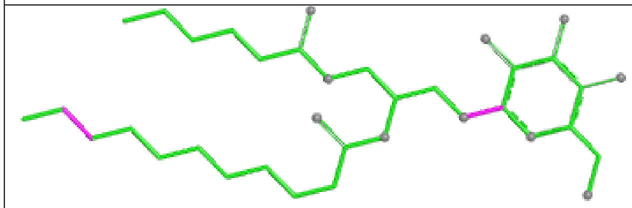

Rings

Ligand LMG 2 803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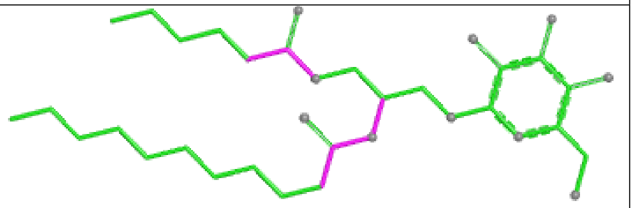
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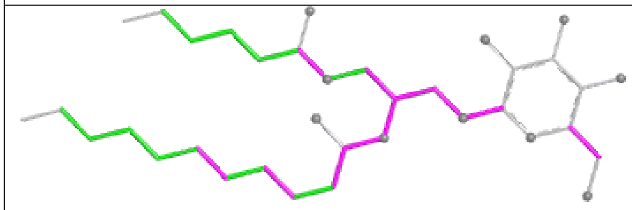
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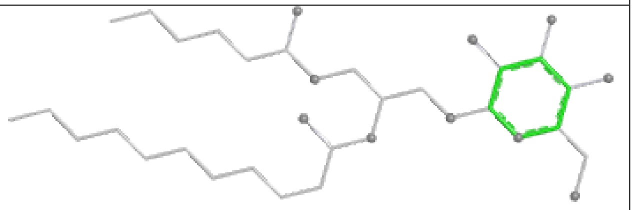
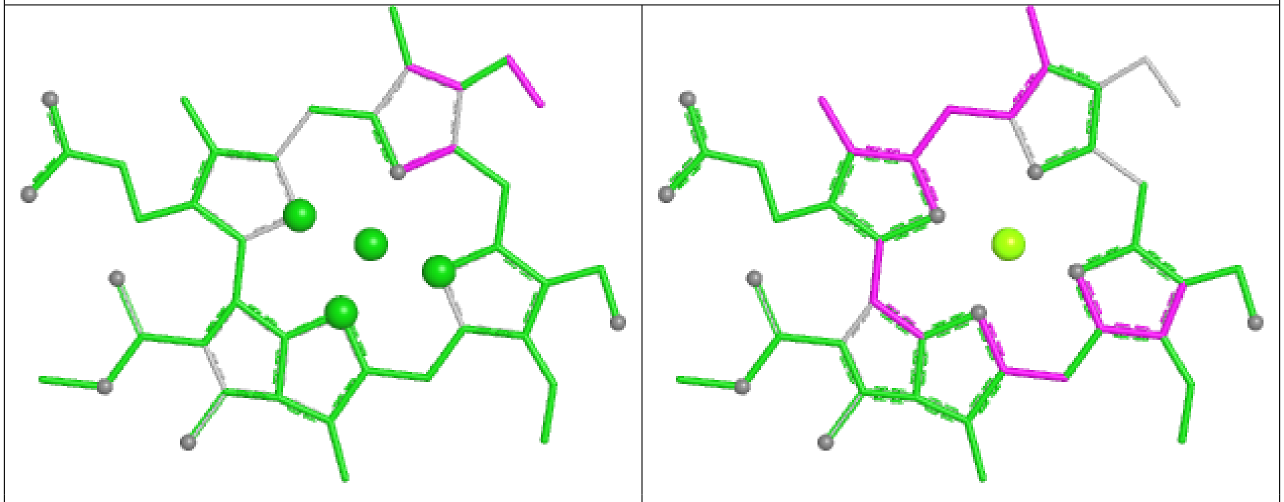
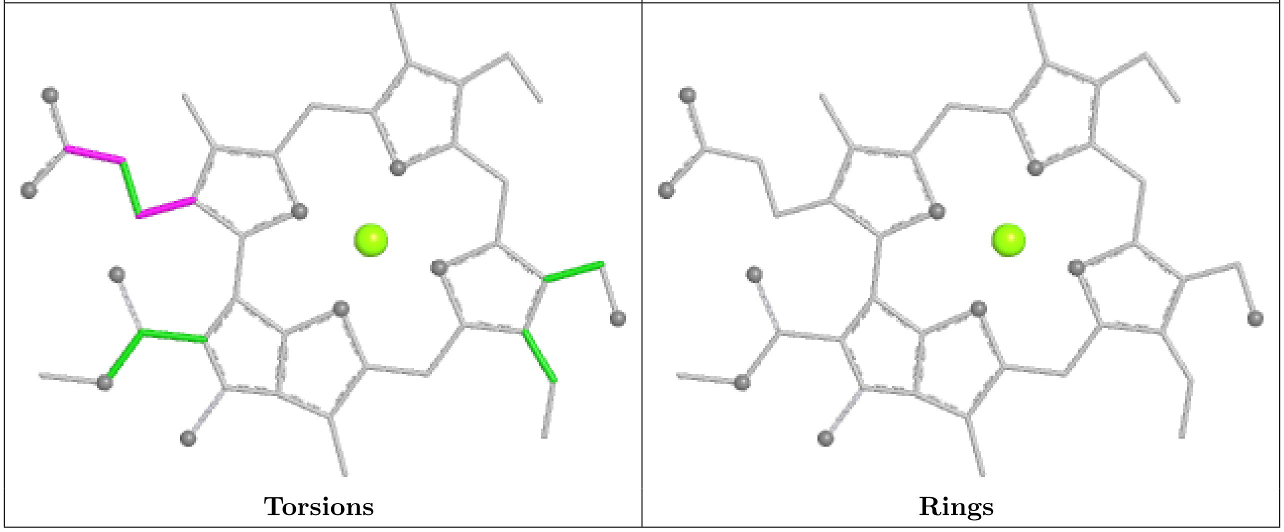

Rings

Ligand CHL 2 613



Bond lengths Bond angles



Torsions Rings

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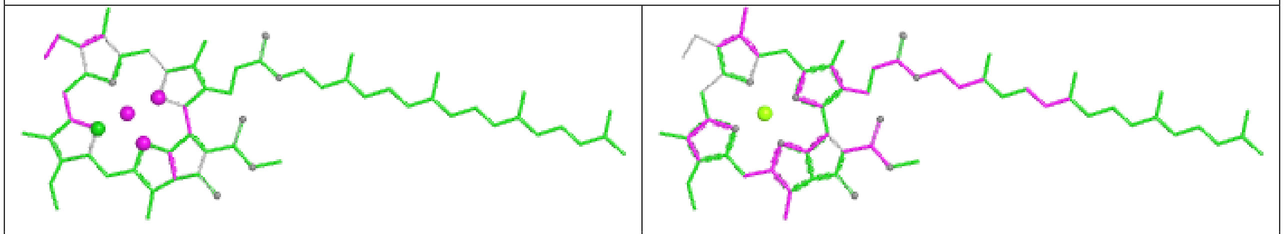
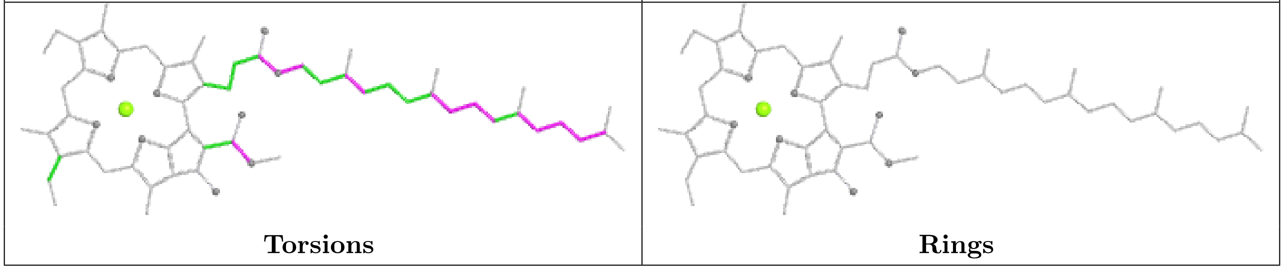


Bond lengths Bond angles



Torsions Rings

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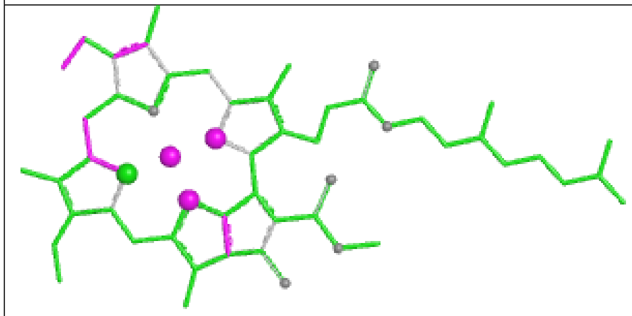
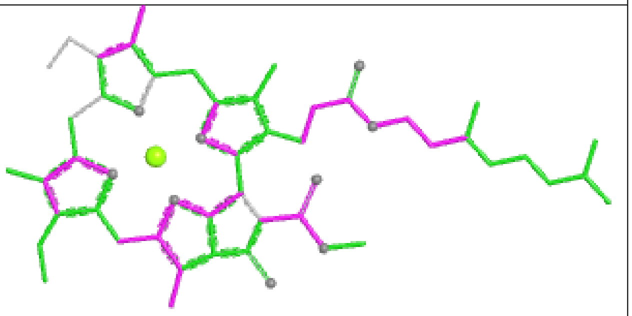
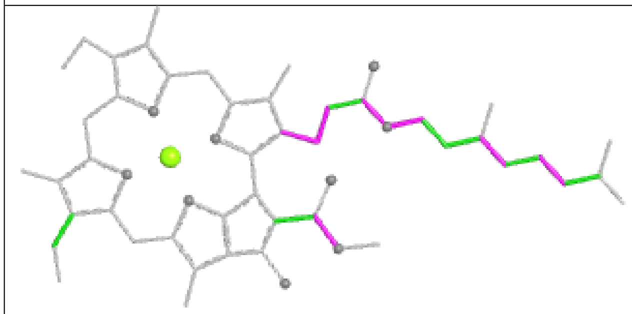


Bond lengths



Bond angles



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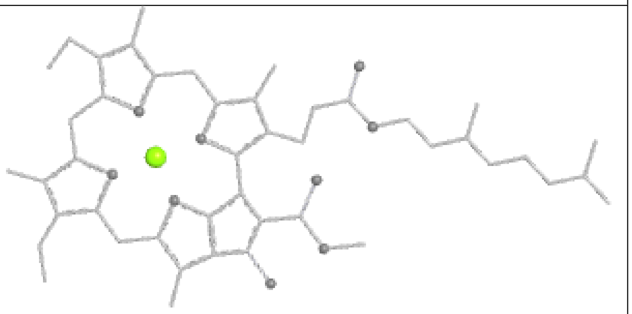
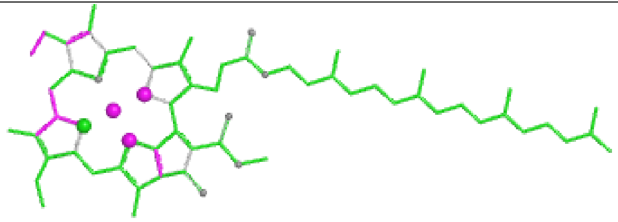


Rings

Ligand CLA A 1112



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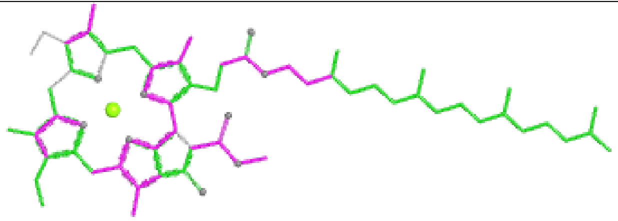
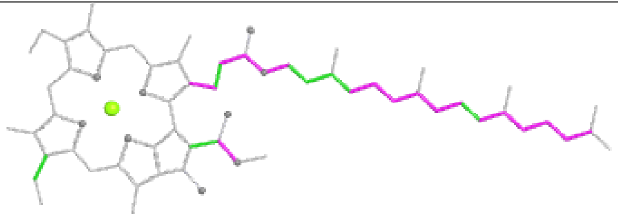


Bond angles



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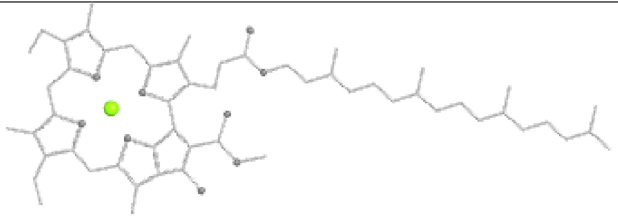

Rings

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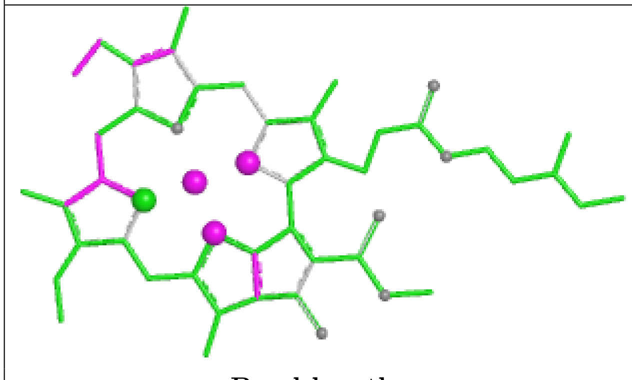

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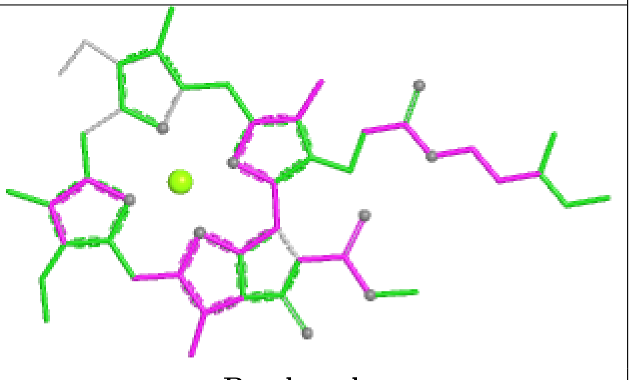
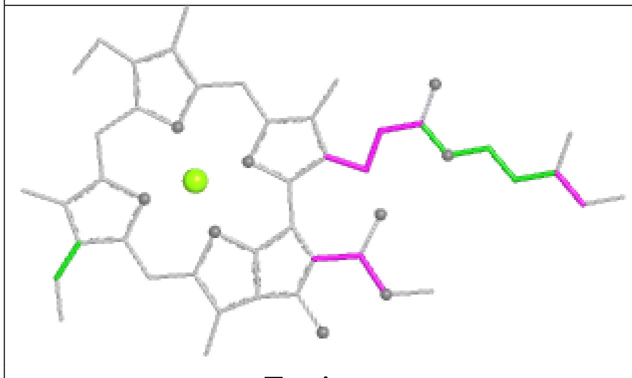


Bond angles



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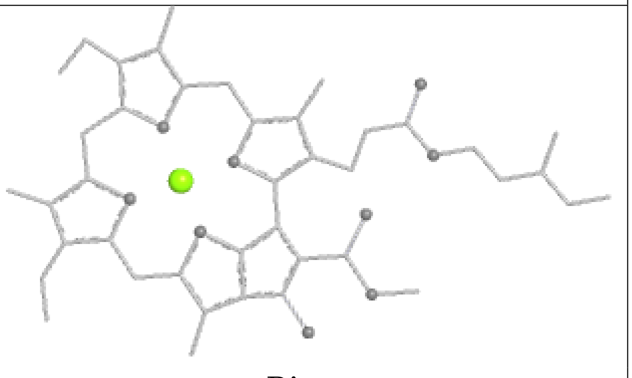
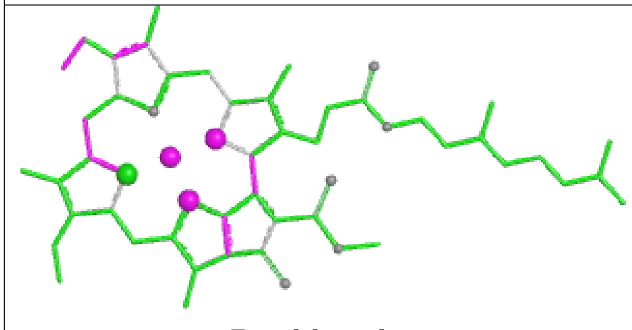


Rings

Ligand CLA 3 603



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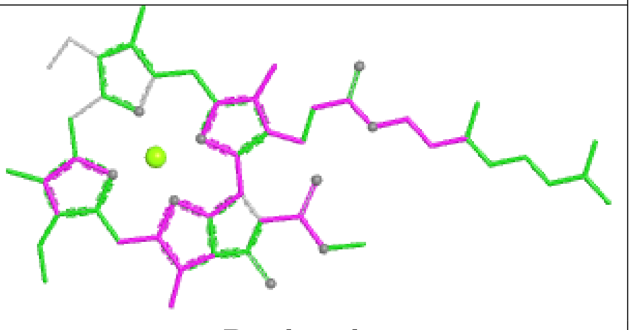
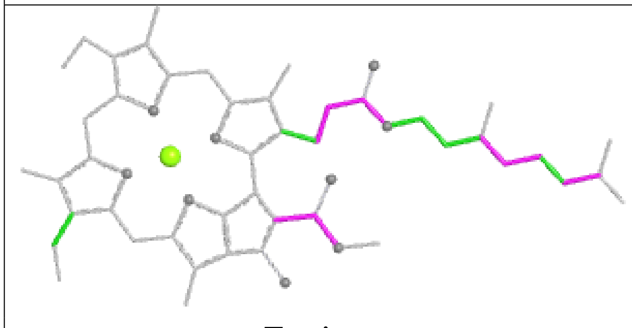


Bond angles



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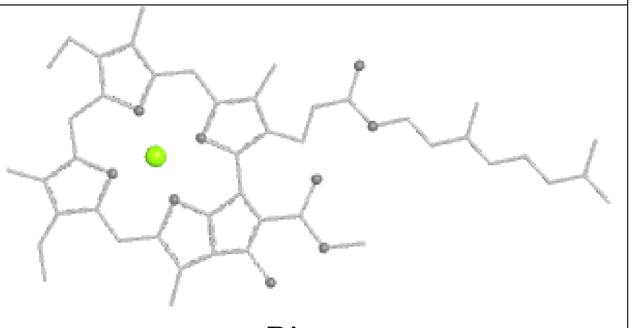
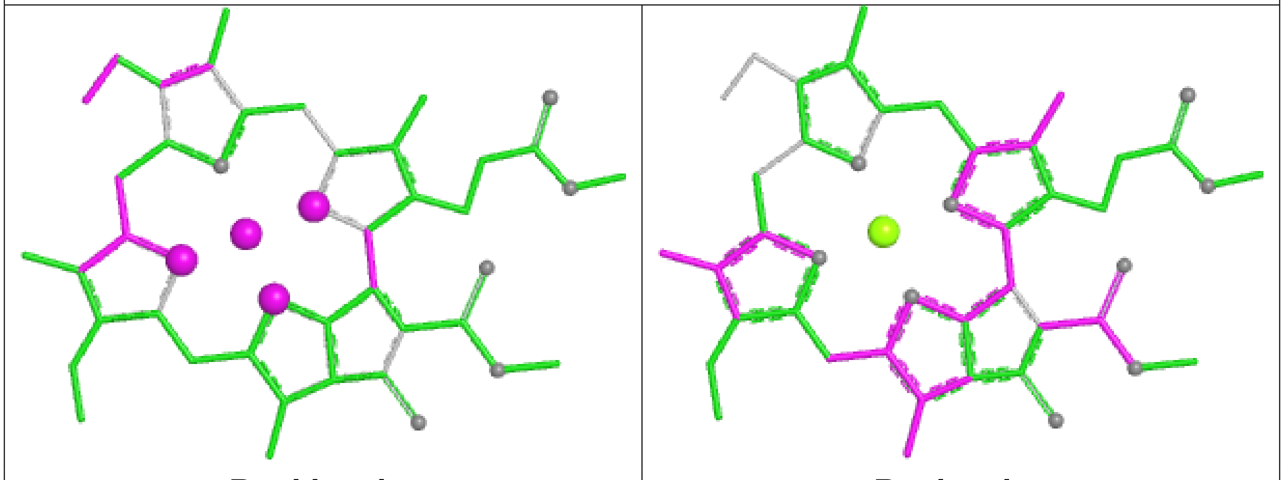
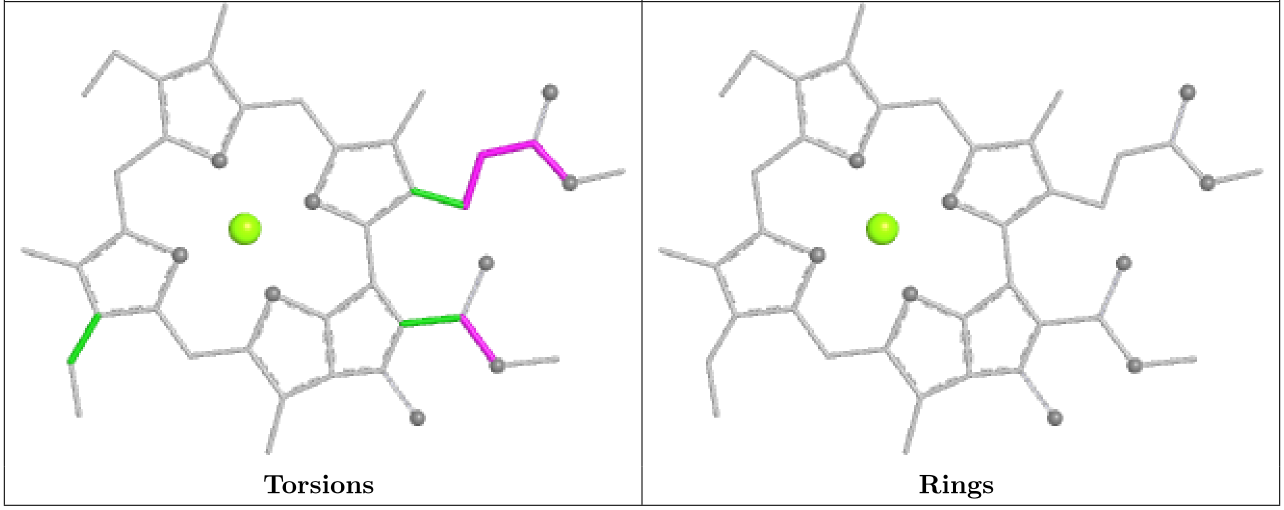


Rings

Ligand CLA K 1404

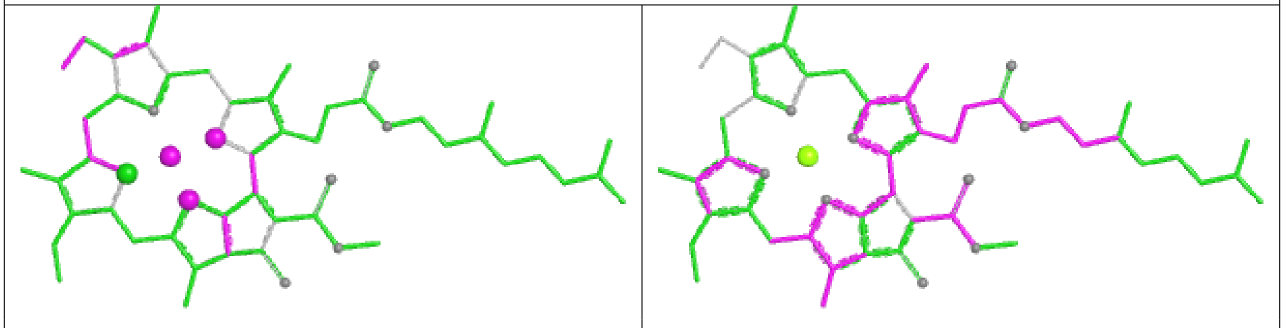


Bond lengths **Bond angles**

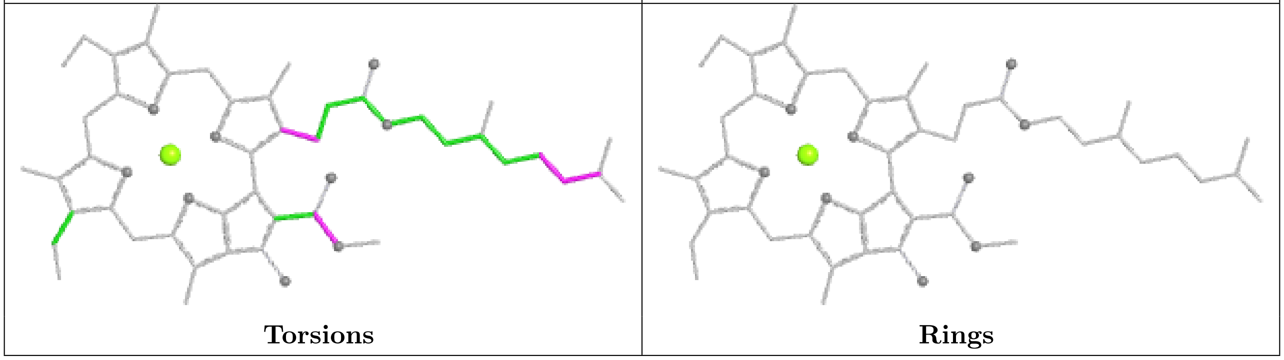


Torsions **Rings**

Ligand CLA 1 603

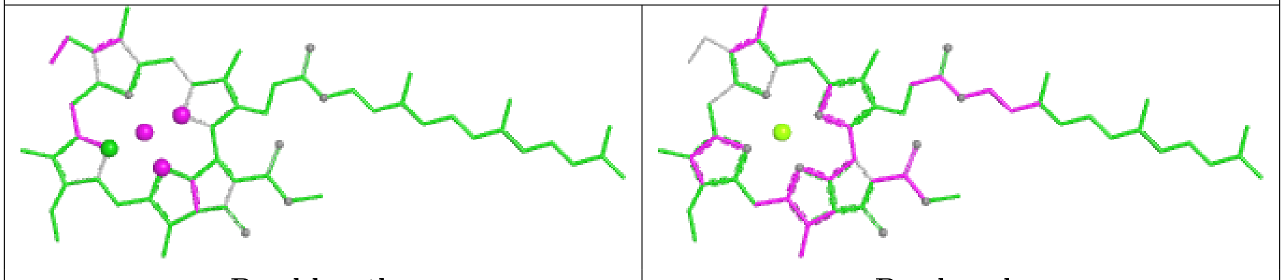


Bond lengths **Bond angles**

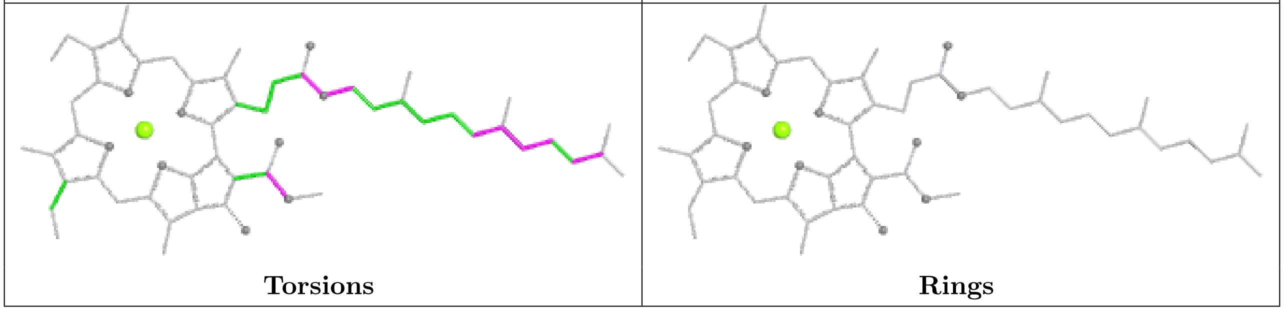


Torsions **Rings**

Ligand CLA B 1231

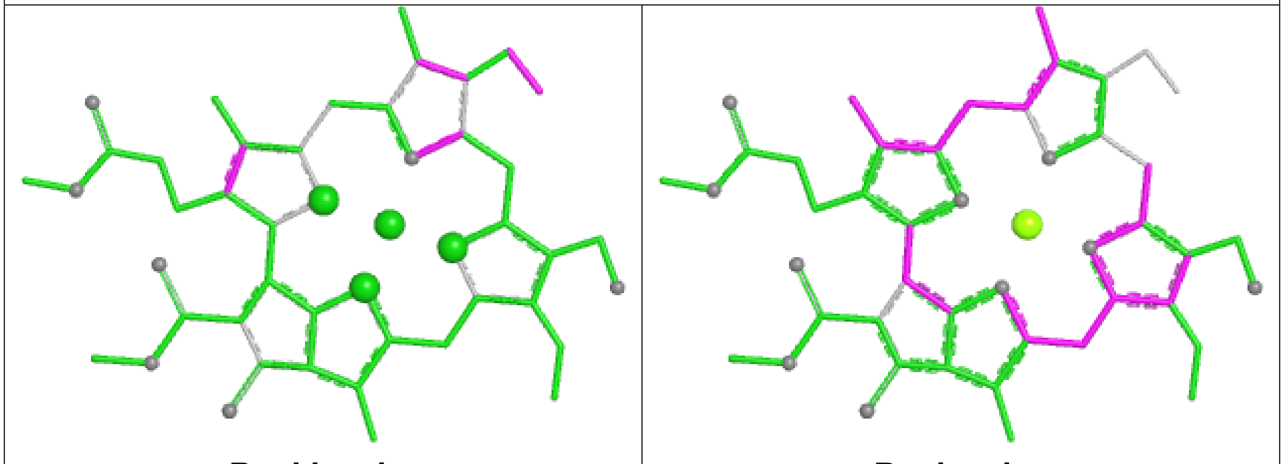


Bond lengths **Bond angles**



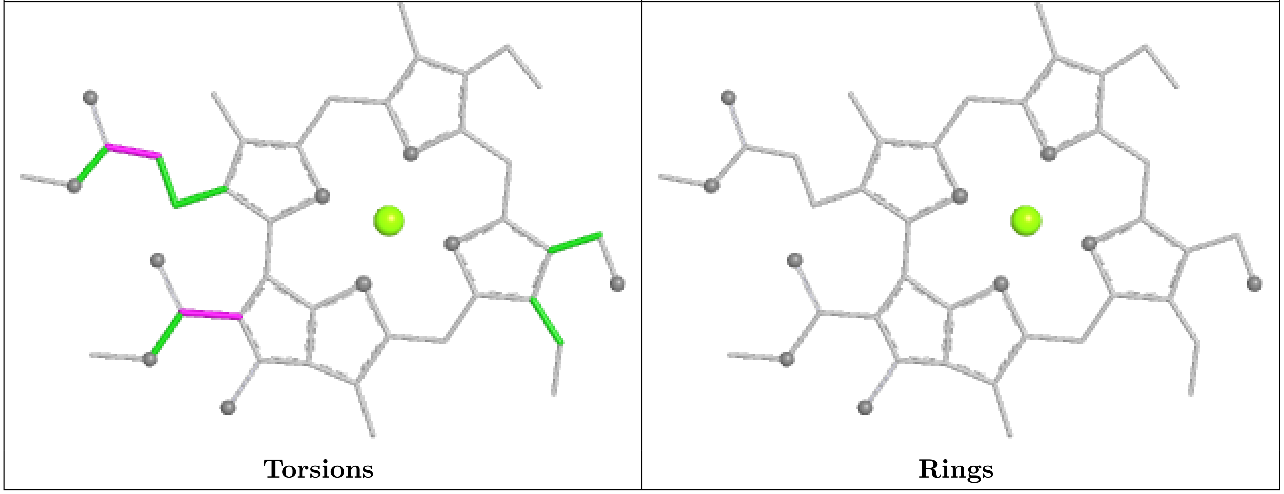
Torsions **Rings**

Ligand CHL 1 610



Bond lengths

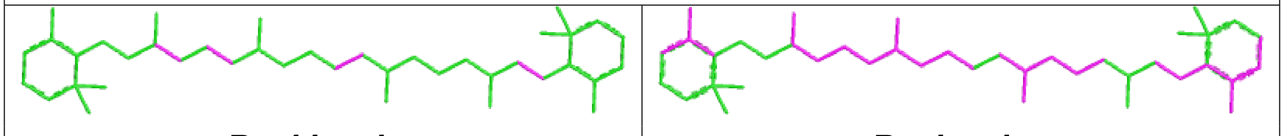
Bond angles



Torsions

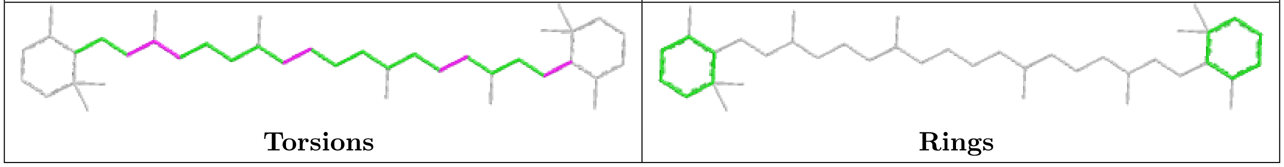
Rings

Ligand BCR B 4009



Bond lengths

Bond angles



Torsions

Rings

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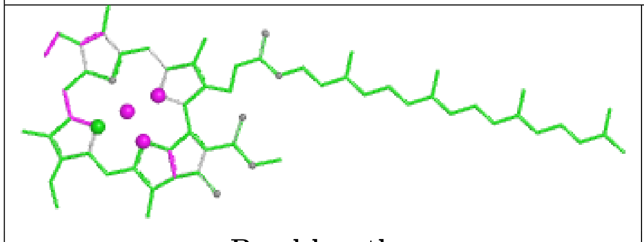
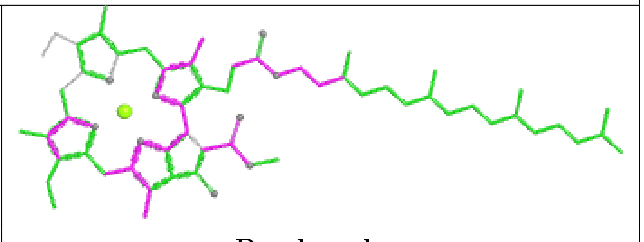
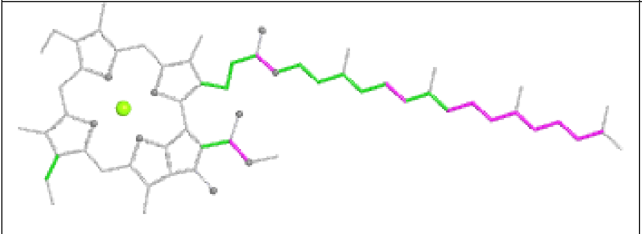
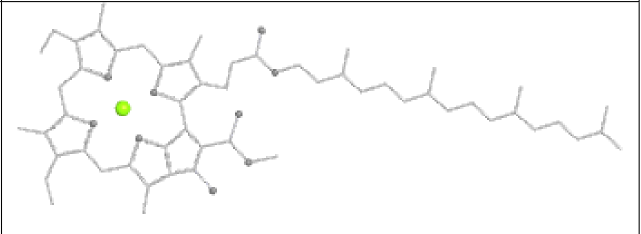
 Bond lengths	 Bond angles
 Torsions	 Rings

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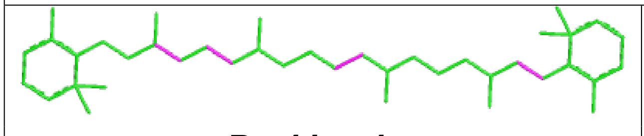
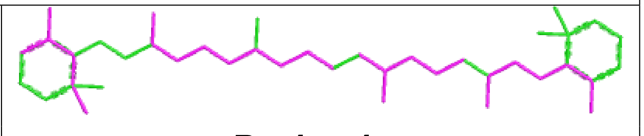
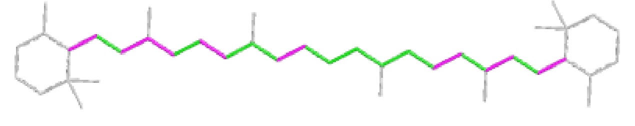
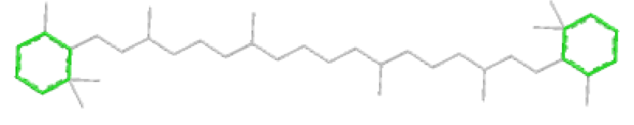
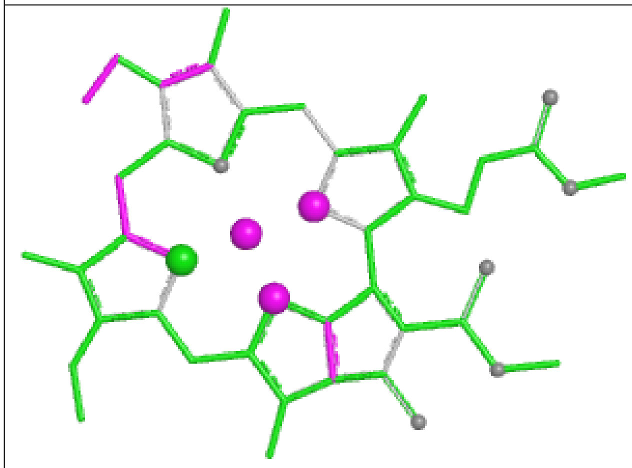
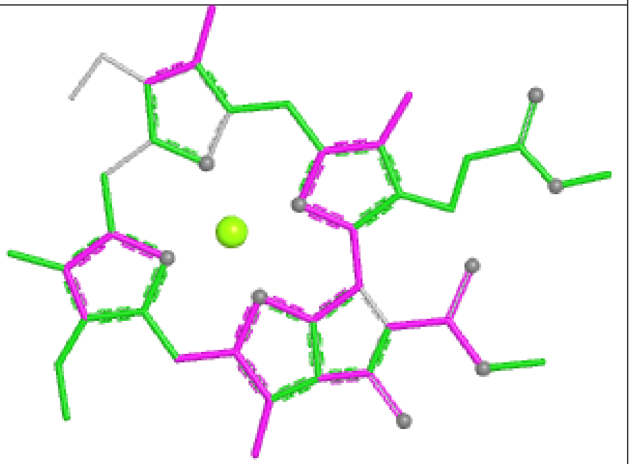
 Bond lengths	 Bond angles
 Torsions	 Rings

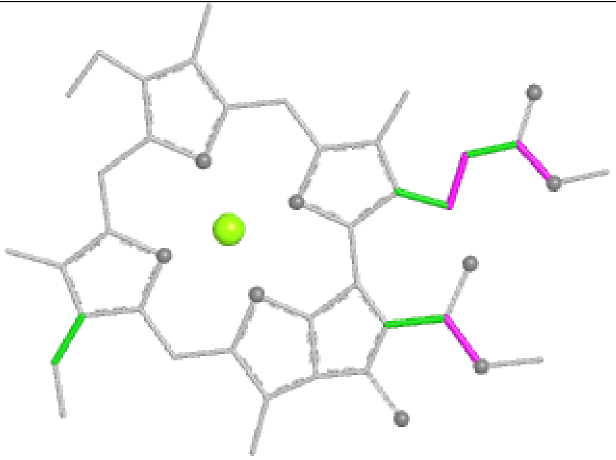
Ligand CLA 1 607



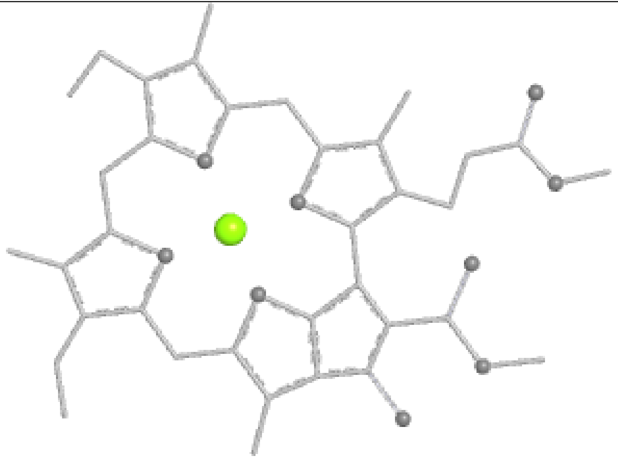
Bond lengths



Bond angles

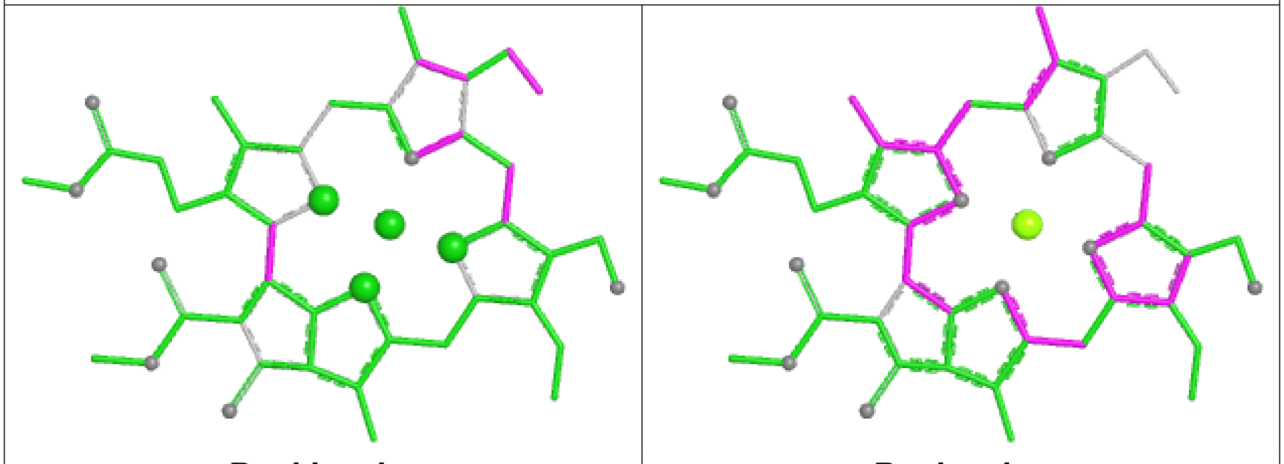


Torsions



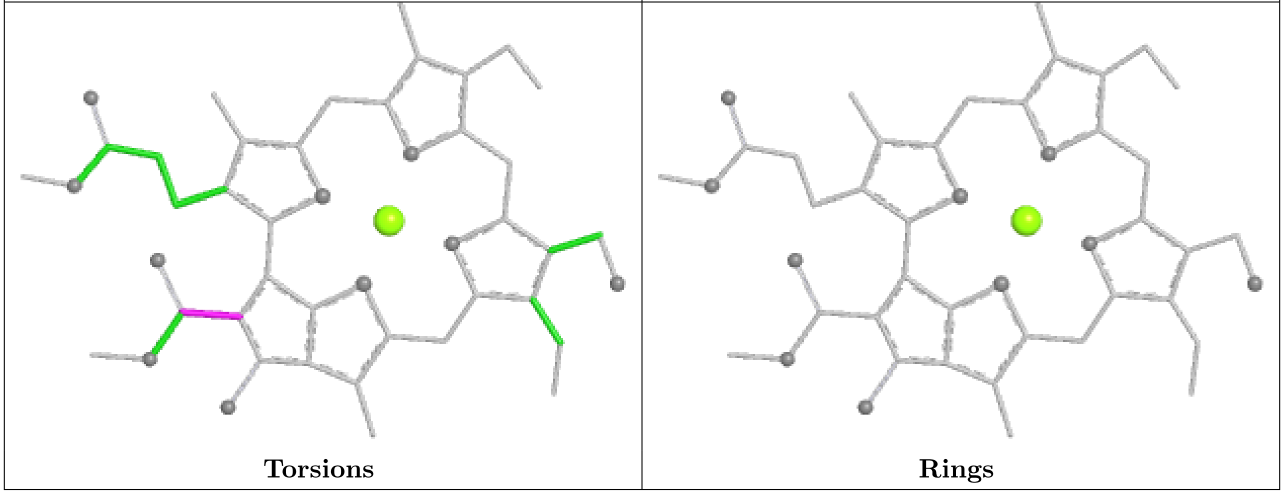
Rings

Ligand CHL 3 611



Bond lengths

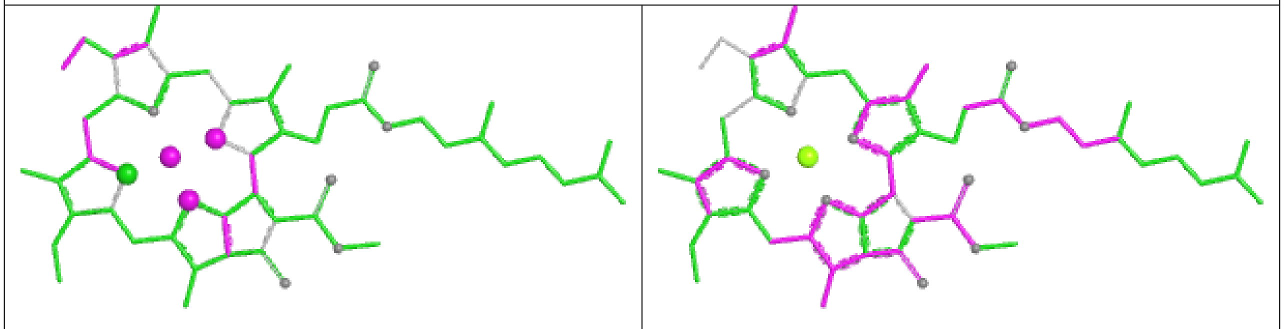
Bond angles



Torsions

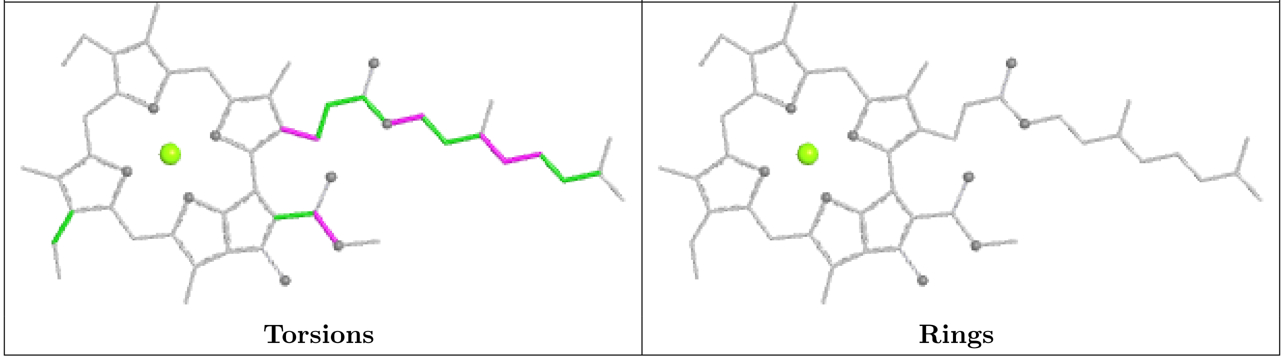
Rings

Ligand CLA G 1601



Bond lengths

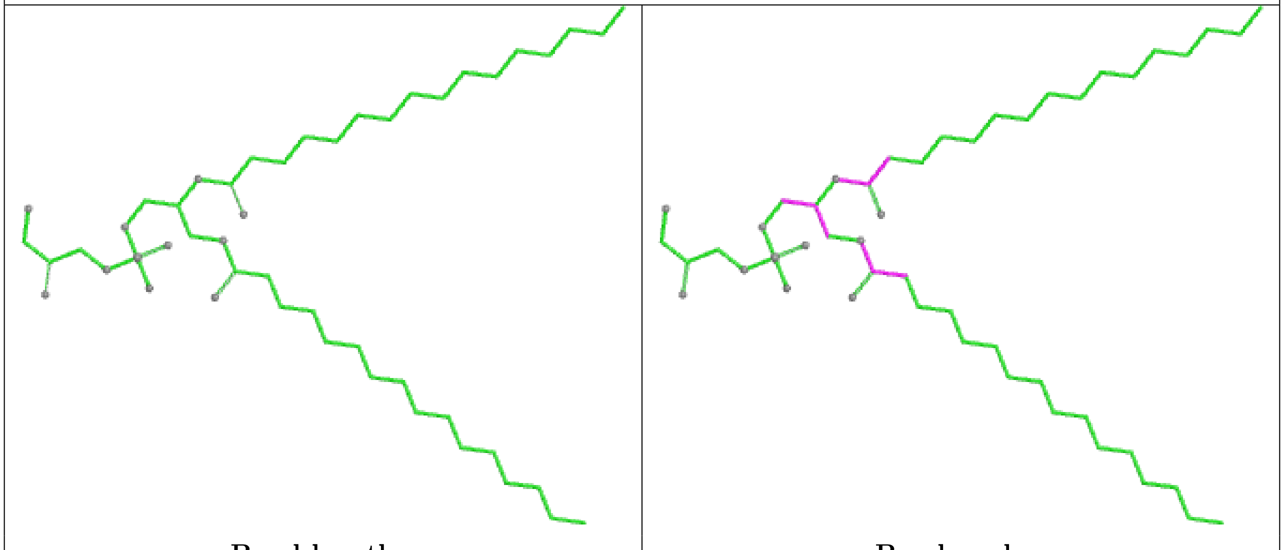
Bond angles



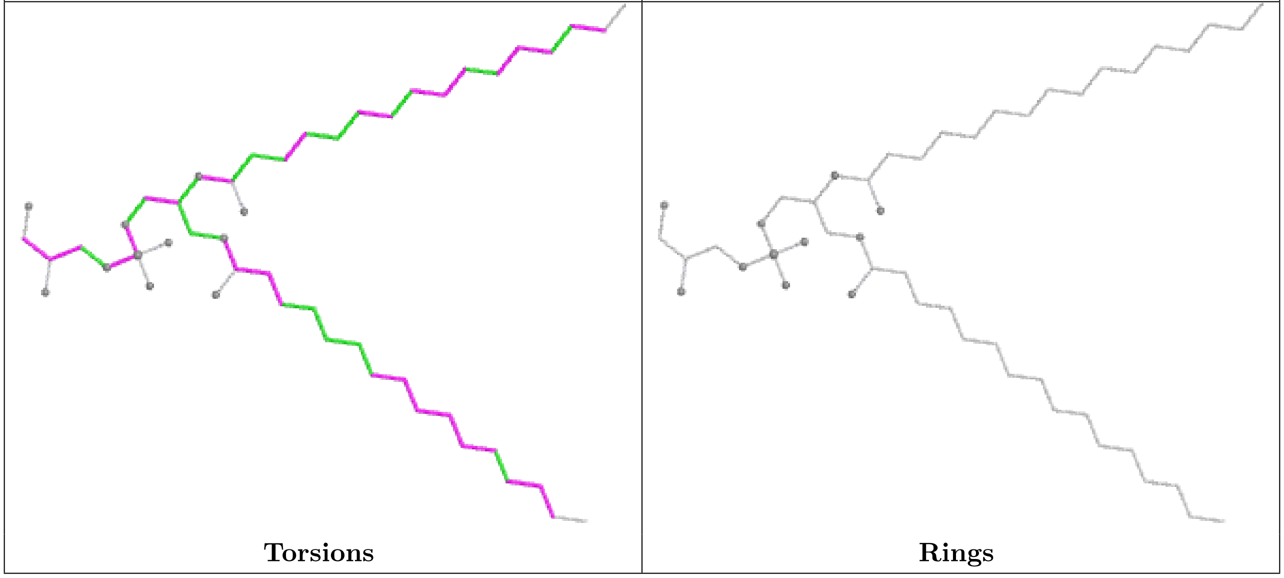
Torsions

Rings

Ligand LHG B 5002

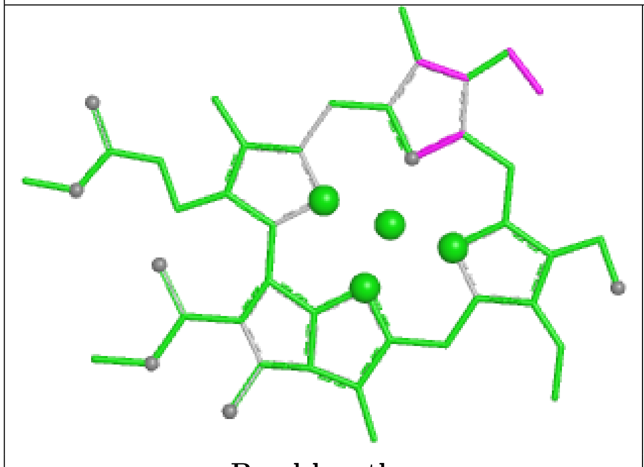


Bond lengths **Bond angles**

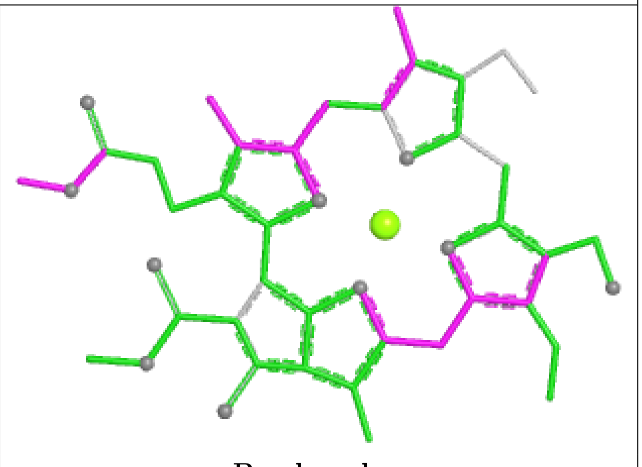


Torsions **Rings**

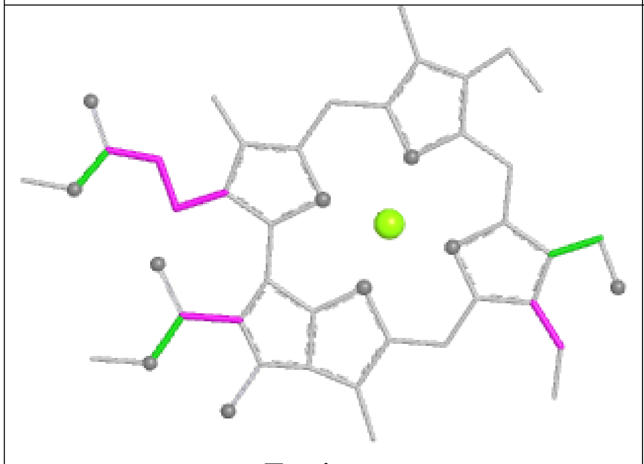
Ligand CHL 4 610



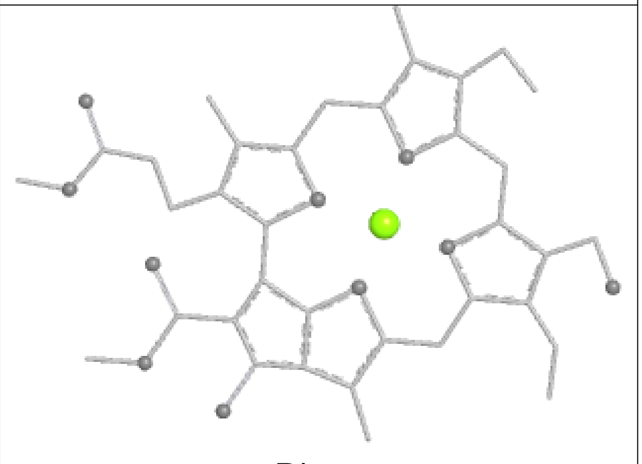
Bond lengths



Bond angles

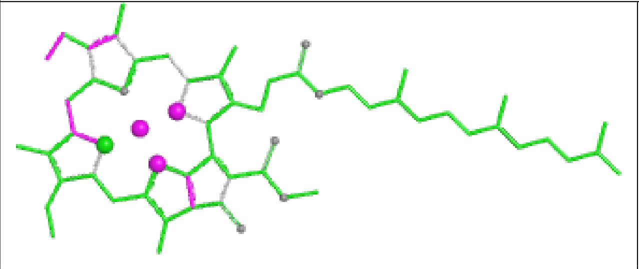


Torsions

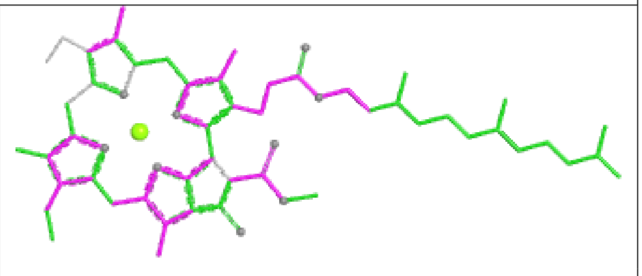


Rings

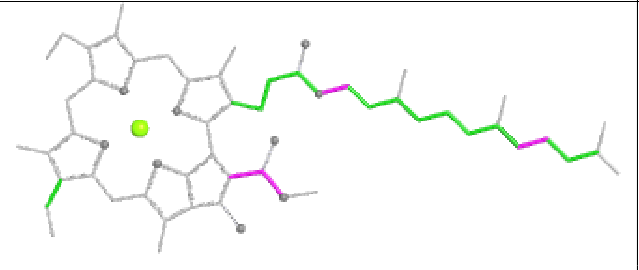
Ligand CLA B 1213



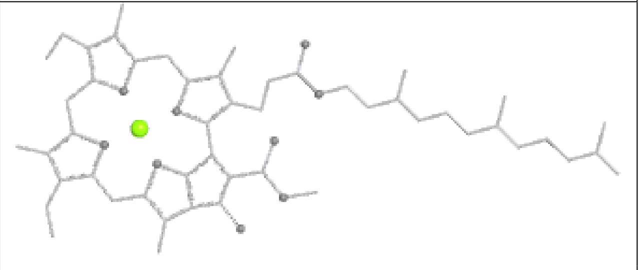
Bond lengths



Bond angles

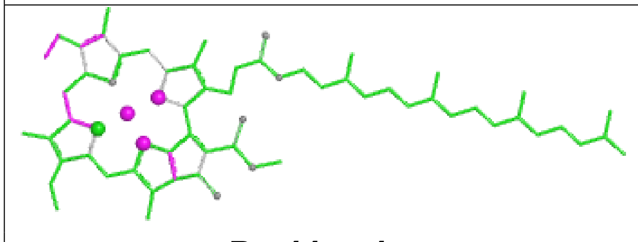


Torsions

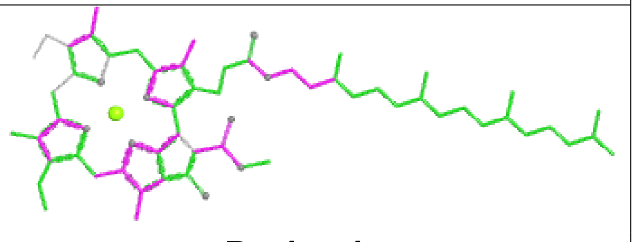


Rings

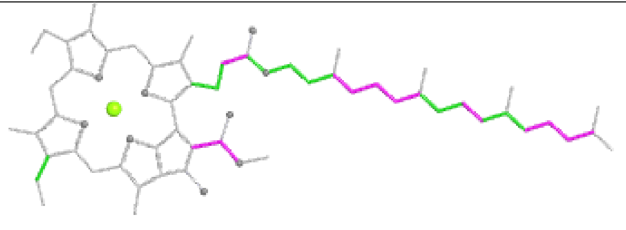
Ligand CLA 1 605



Bond lengths



Bond angles



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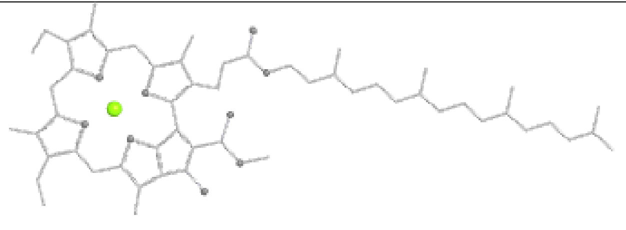
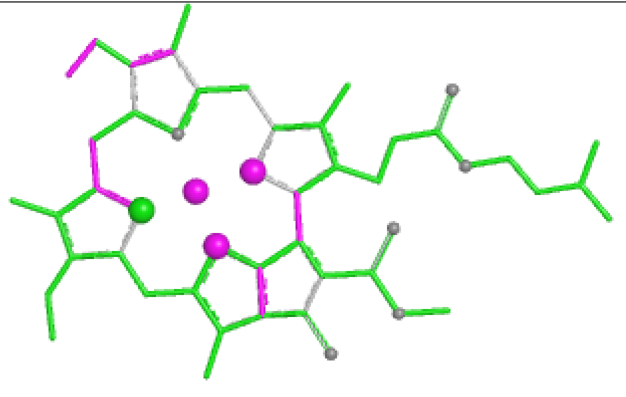
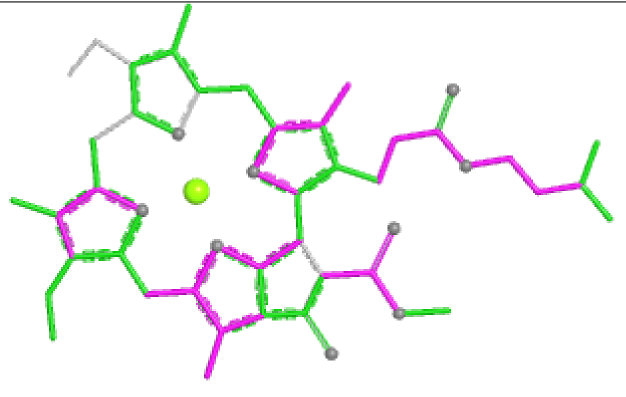


Rings

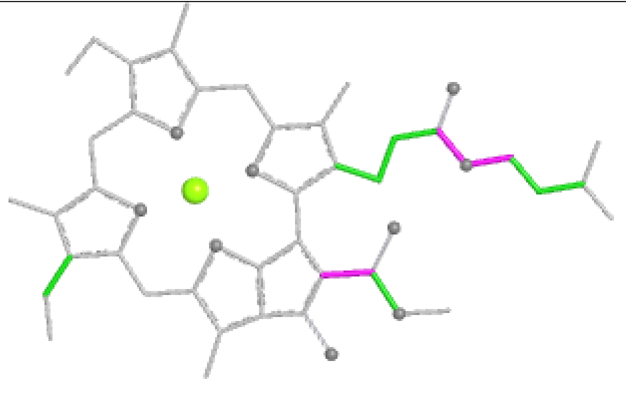
Ligand CLA A 1118



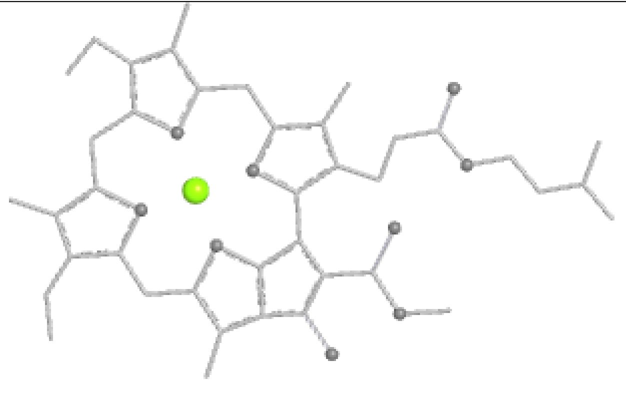
Bond lengths



Bond angles

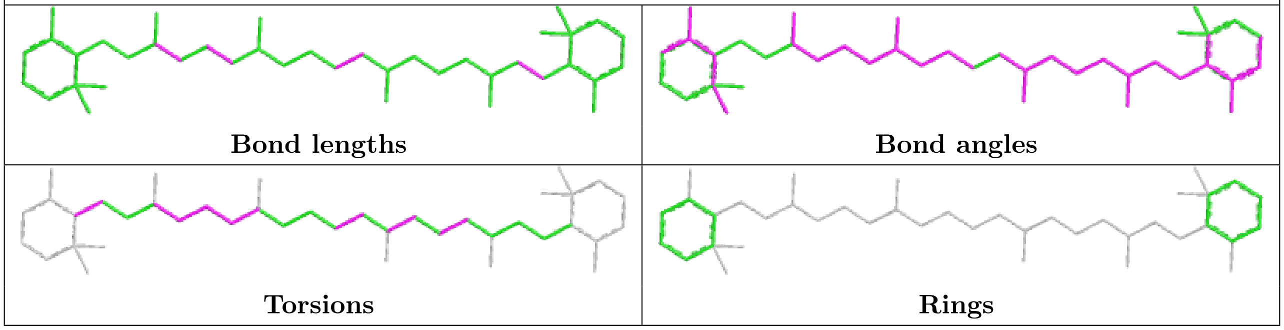


Torsions



Rings

Ligand BCR A 4002



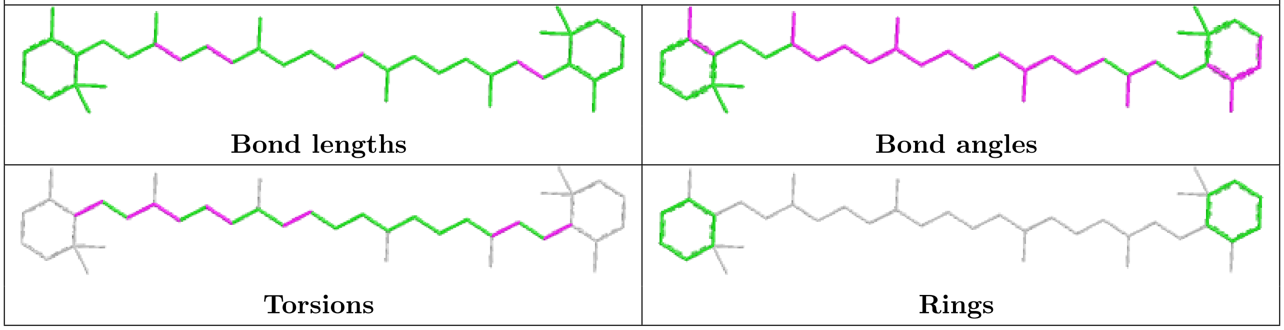
Bond lengths

Bond angles

Torsions

Rings

Ligand BCR L 4019



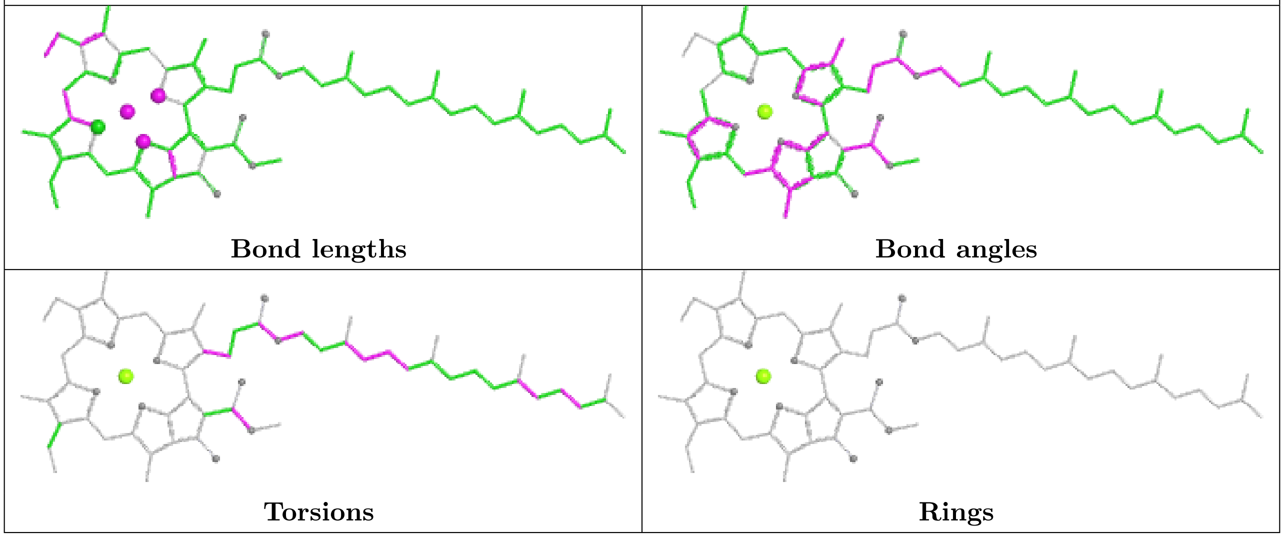
Bond lengths

Bond angles

Torsions

Rings

Ligand CLA B 1229



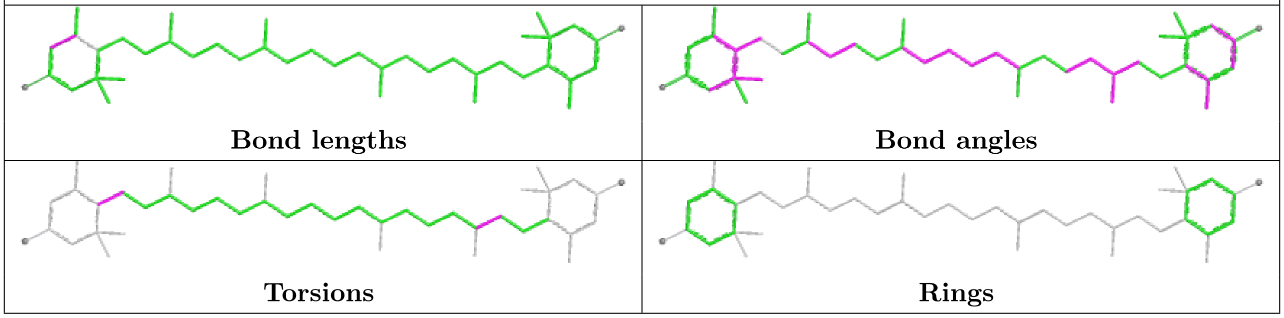
Bond lengths

Bond angles

Torsions

Rings

Ligand LUT J 4013

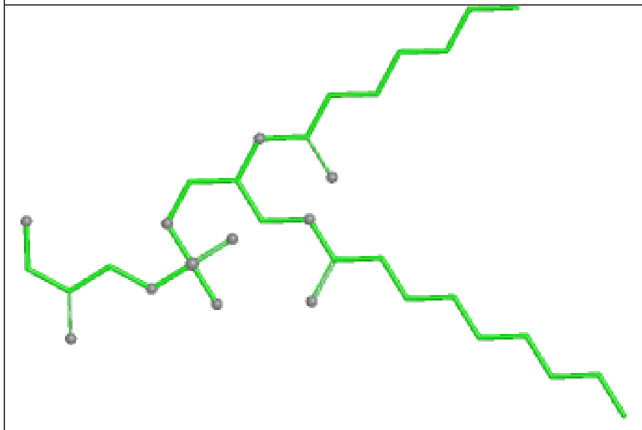
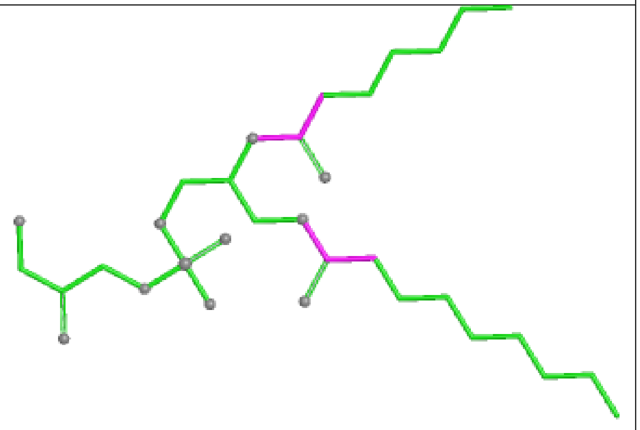
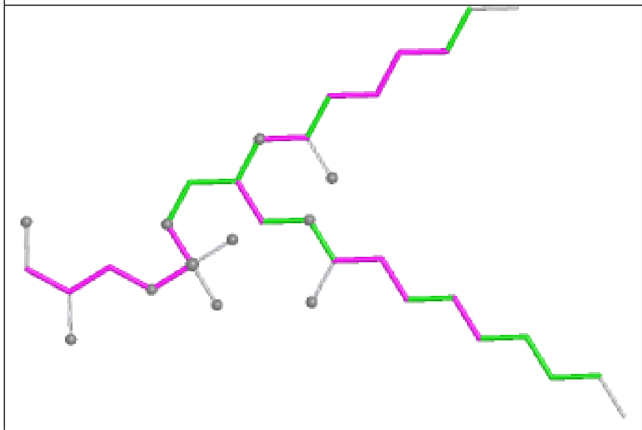
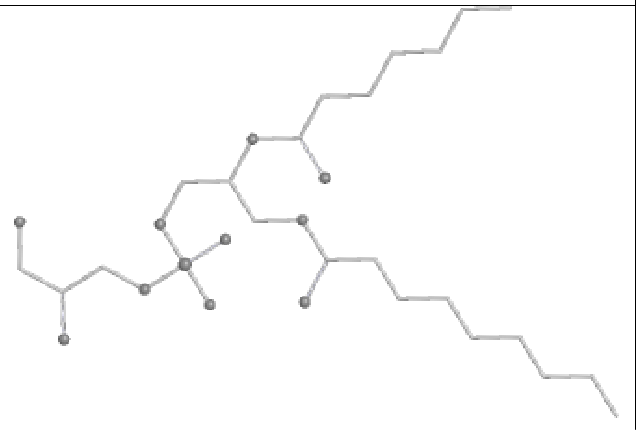


Bond lengths

Bond angles

Torsions

Rings

Ligand LHG 2 807	
 Bond lengths	 Bond angles
 Torsions	 Rings

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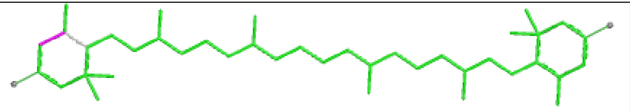
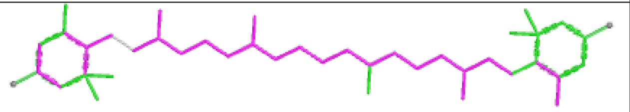
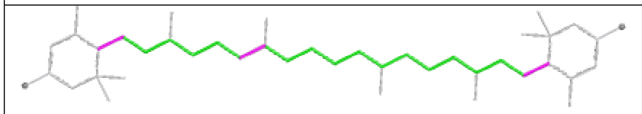
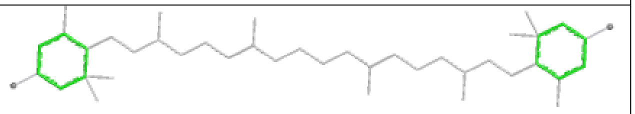
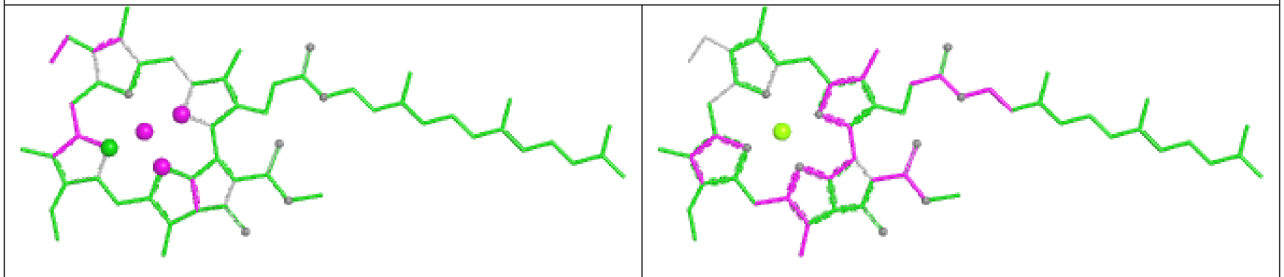
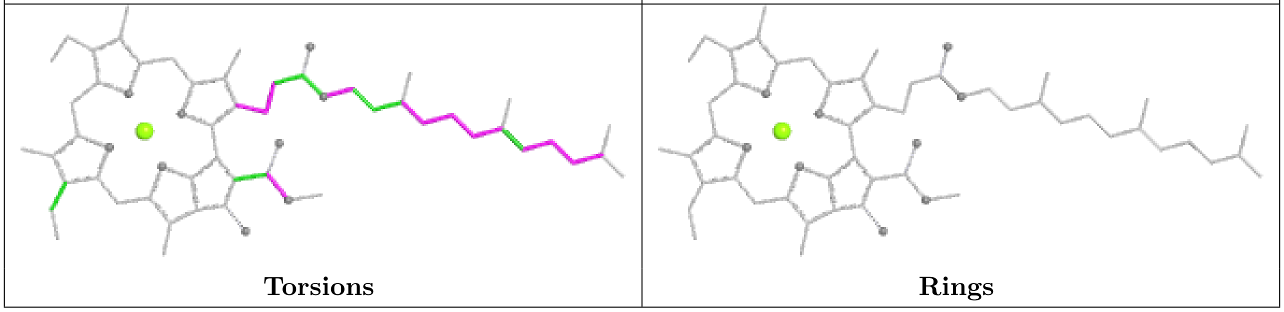
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA 4 607

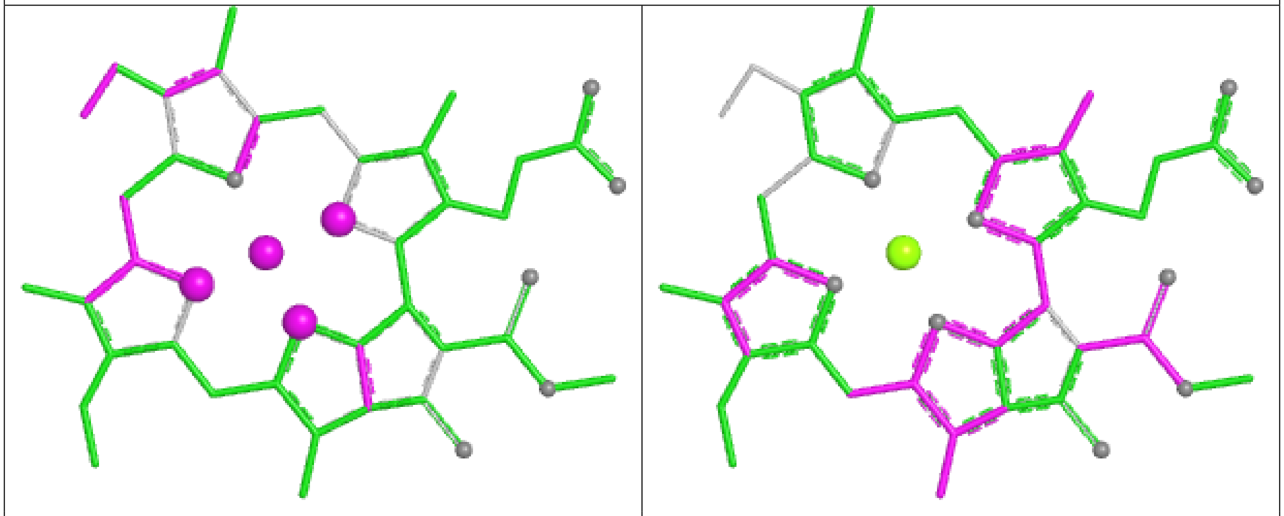


Bond lengths Bond angles

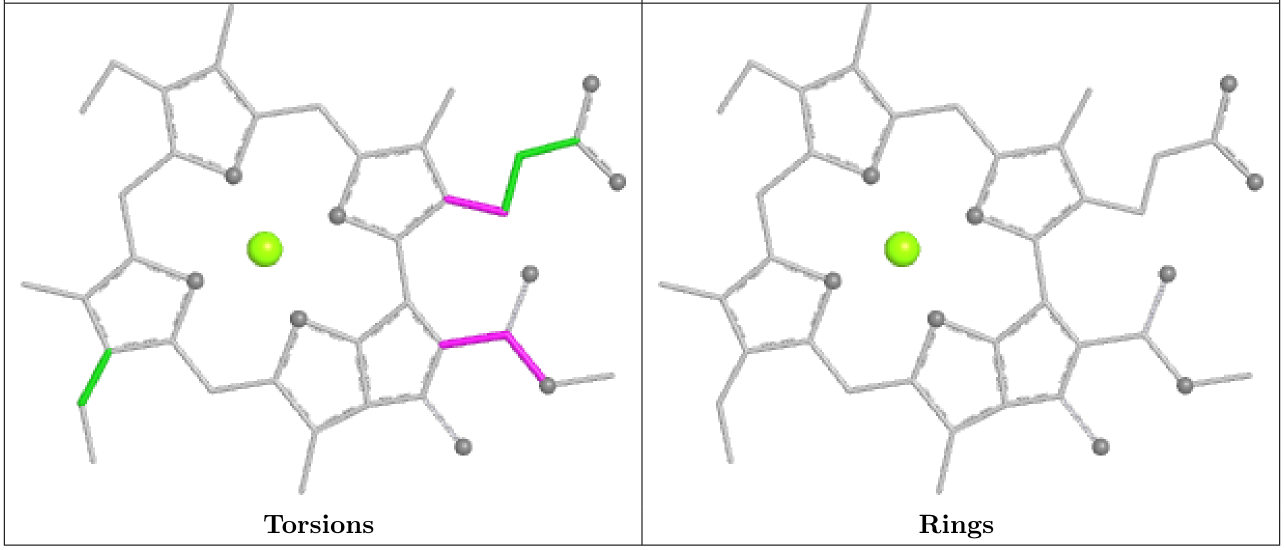


Torsions Rings

Ligand CLA K 1401

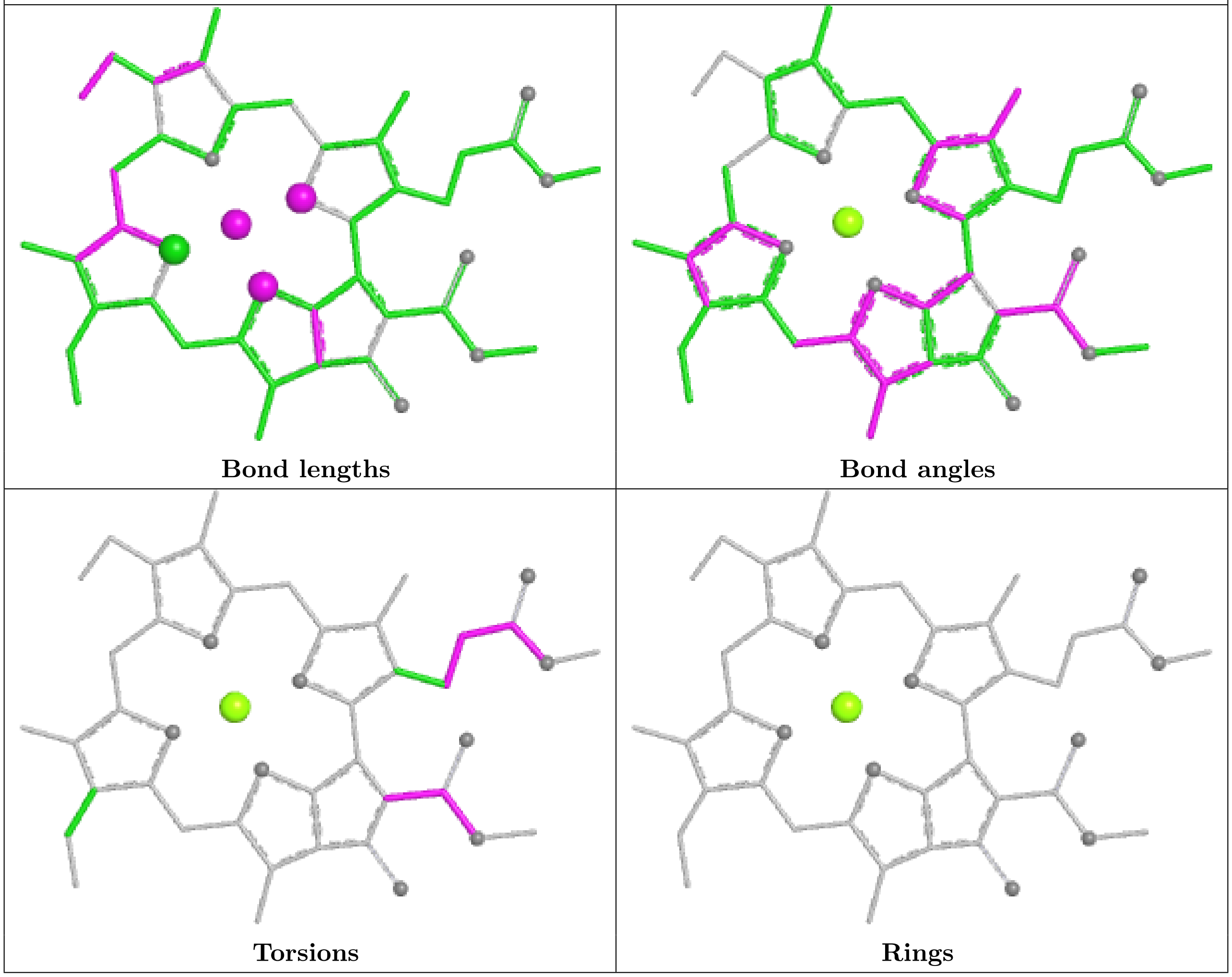


Bond lengths Bond angles

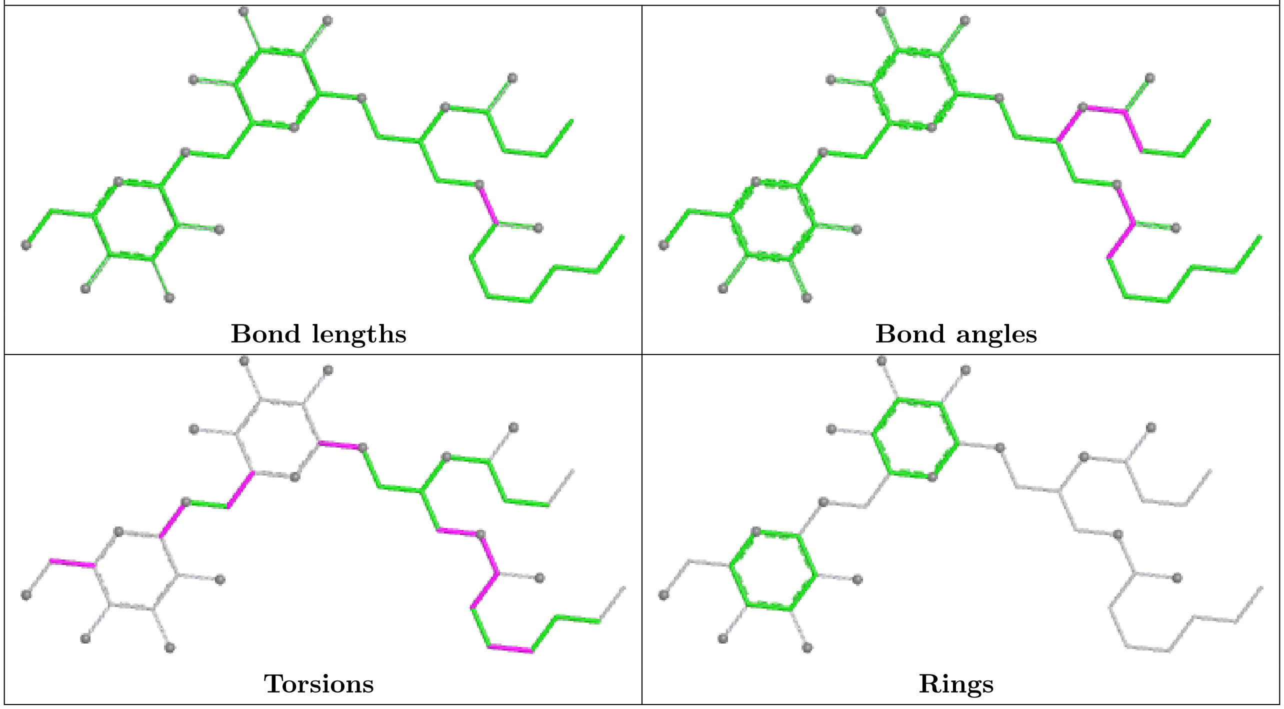


Torsions Rings

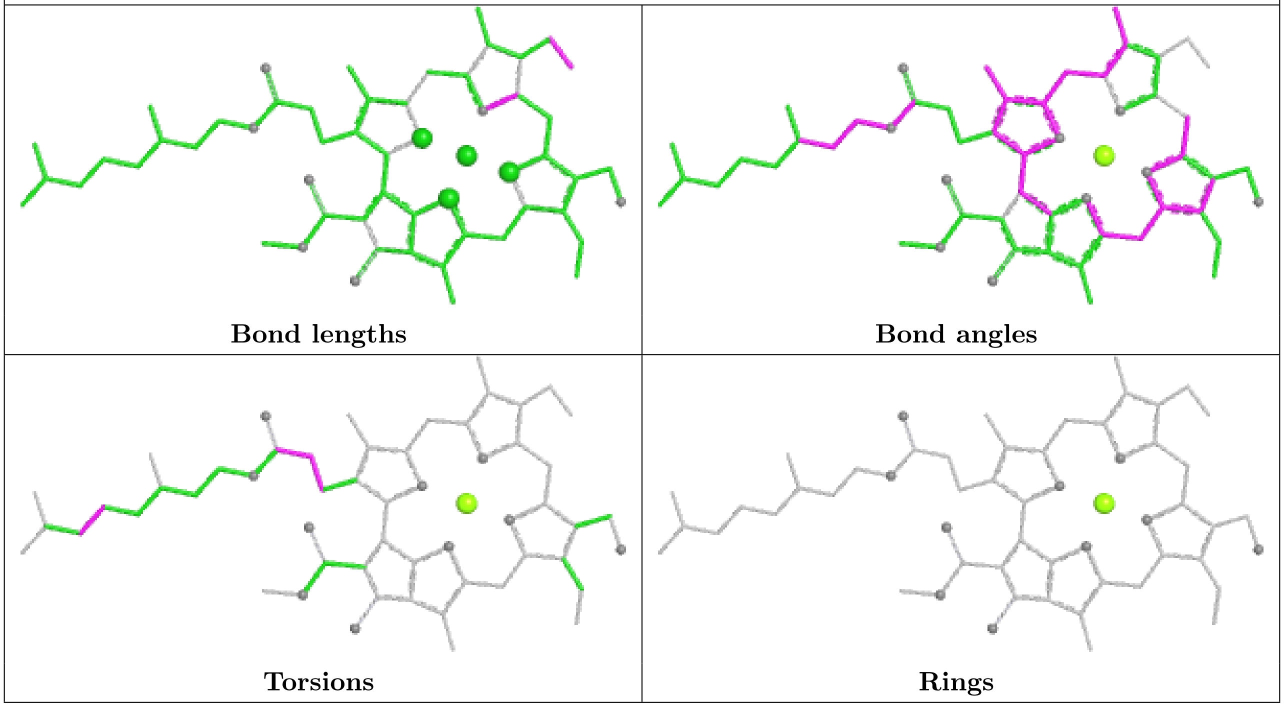
Ligand CLA 4 608



Ligand DGD 1 803



Ligand CHL 2 610



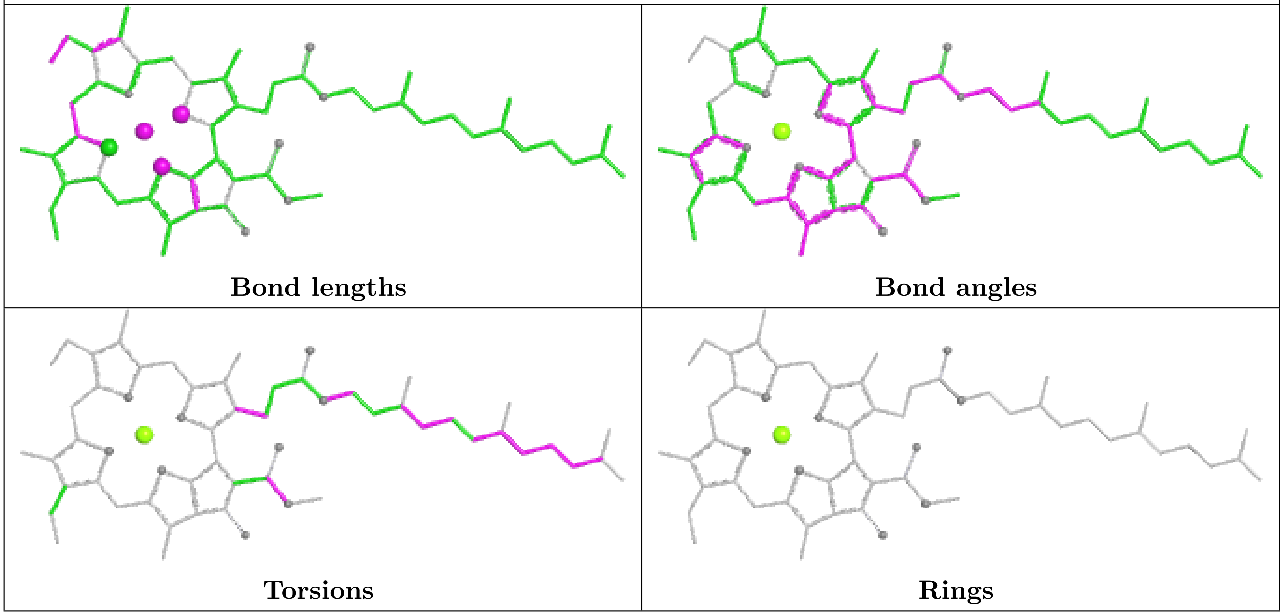
Bond lengths

Bond angles

Torsions

Rings

Ligand CLA 4 601



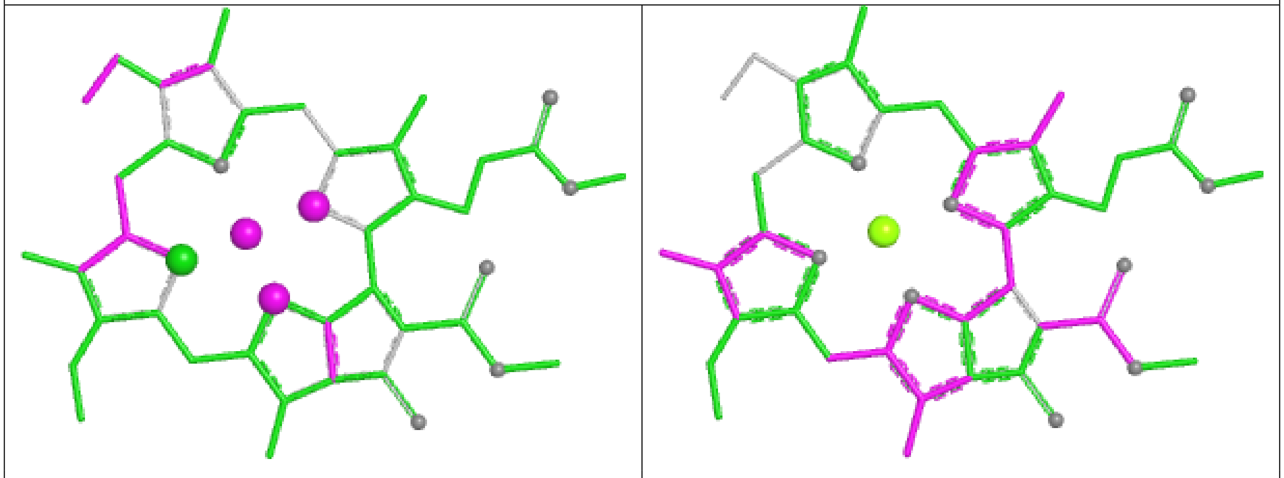
Bond lengths

Bond angles

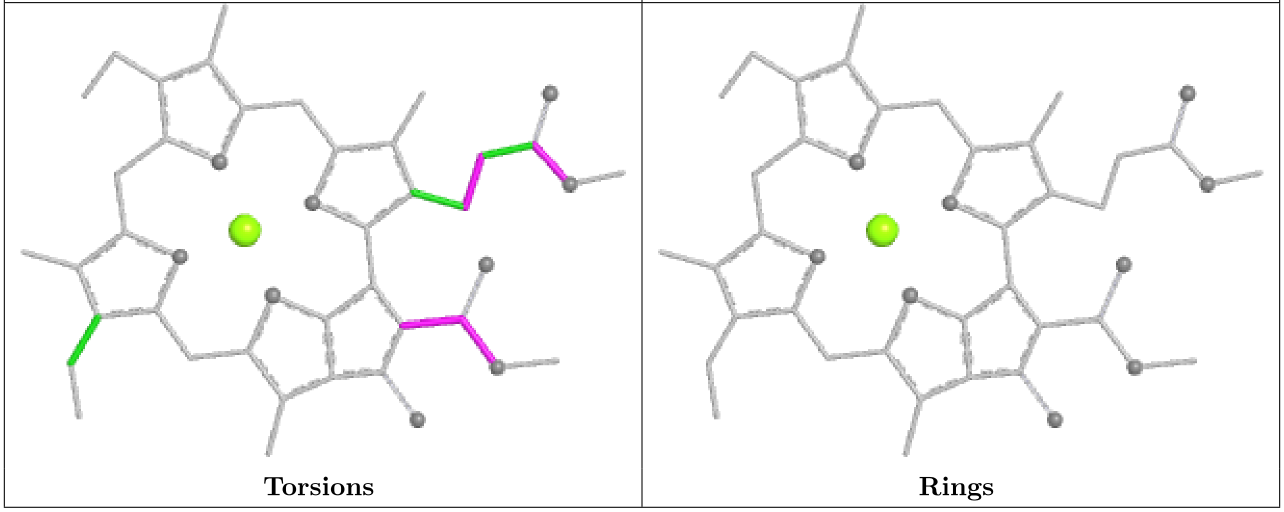
Torsions

Rings

Ligand CLA B 1217

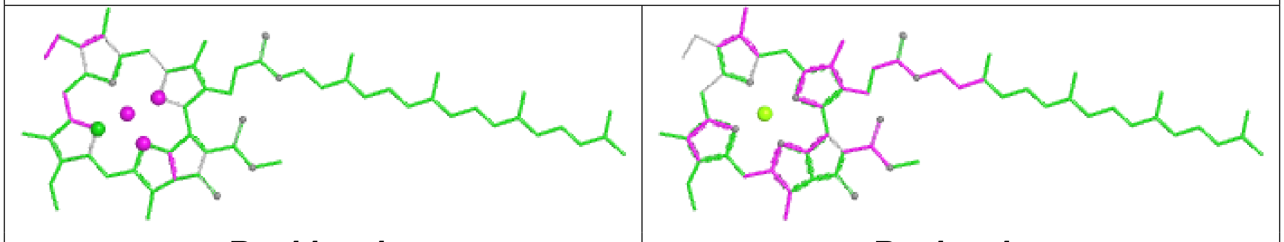


Bond lengths Bond angles

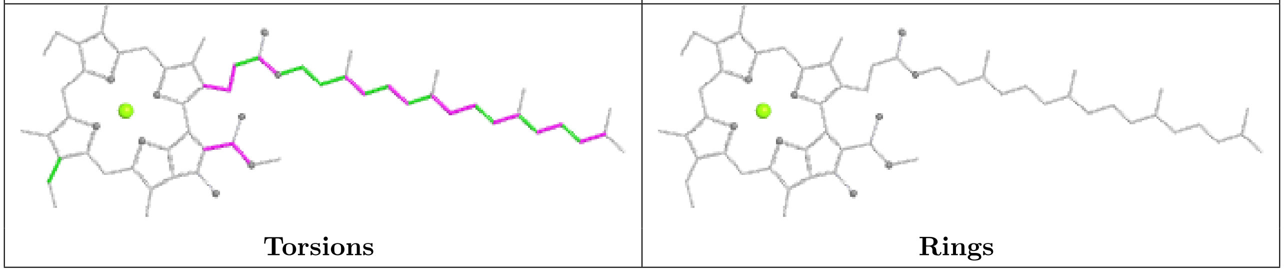


Torsions Rings

Ligand CLA A 1117

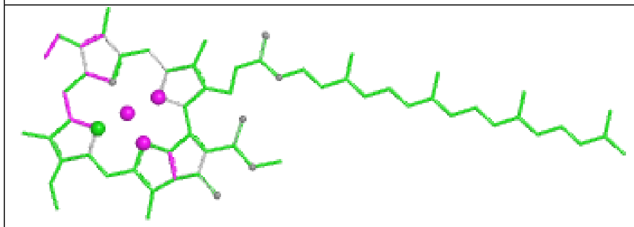


Bond lengths Bond angles

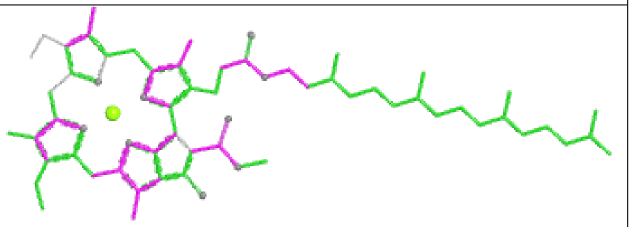


Torsions Rings

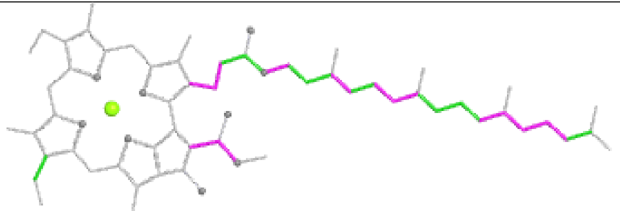
Ligand CLA B 1225



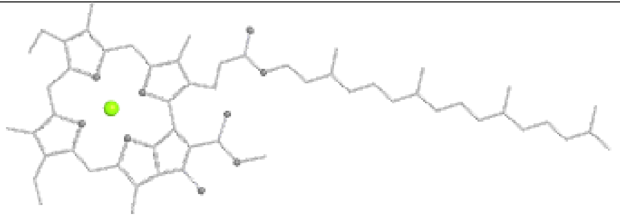
Bond lengths



Bond angles

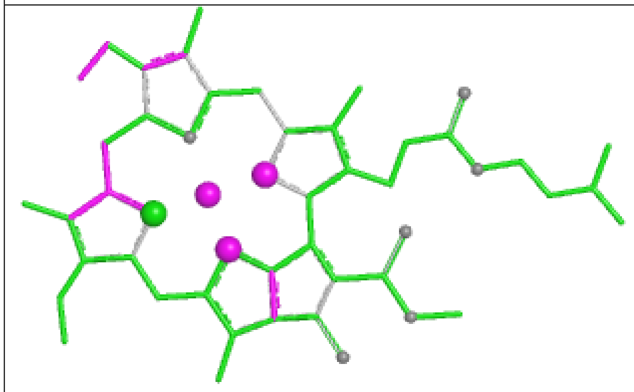


Torsions

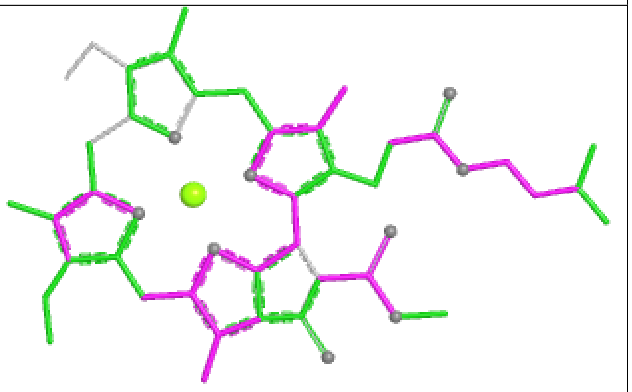


Rings

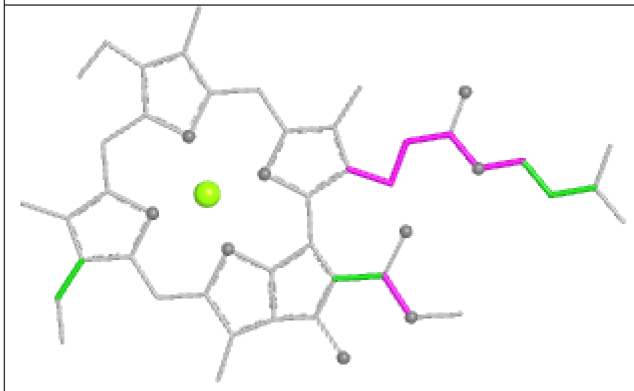
Ligand CLA 2 608



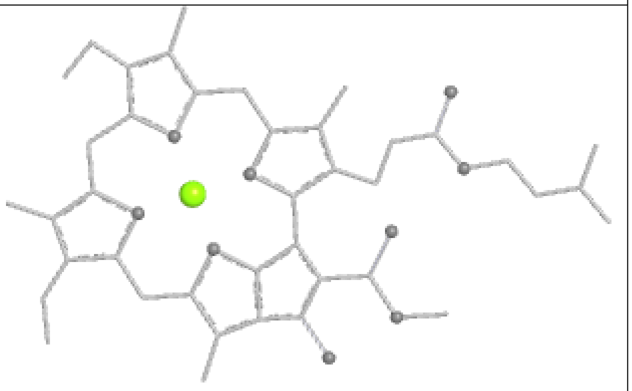
Bond lengths



Bond angles

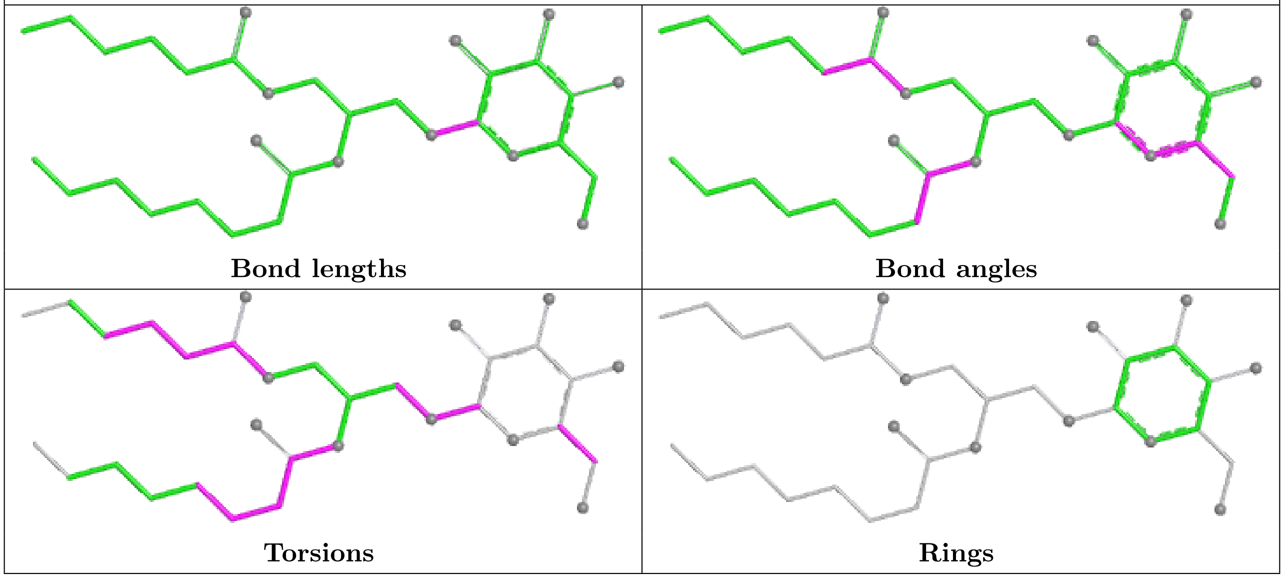


Torsions



Rings

Ligand LMG B 5004



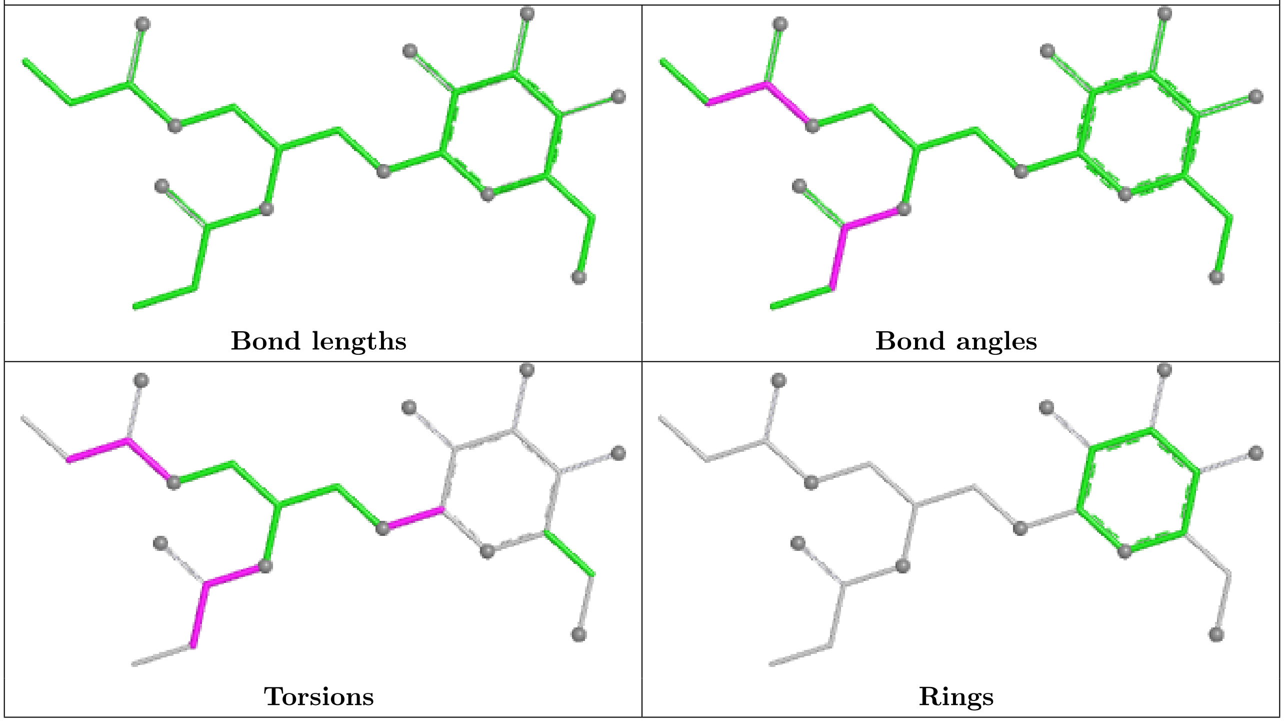
Bond lengths

Bond angles

Torsions

Rings

Ligand LMG G 5006



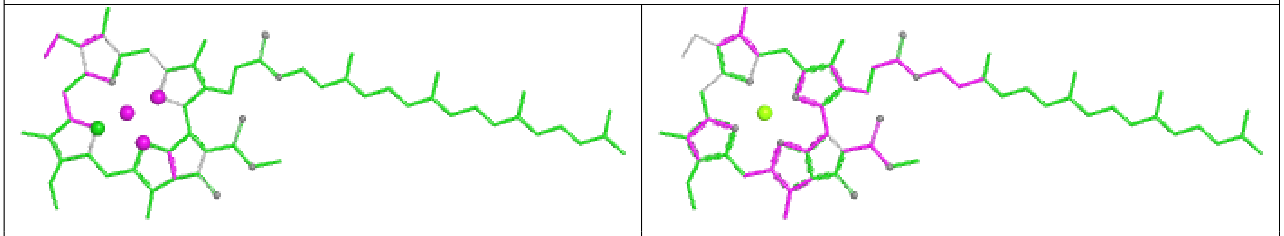
Bond lengths

Bond angles

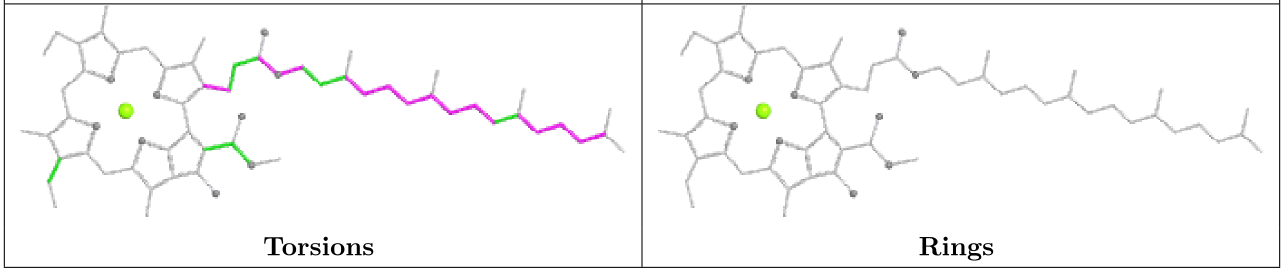
Torsions

Rings

Ligand CLA A 1101

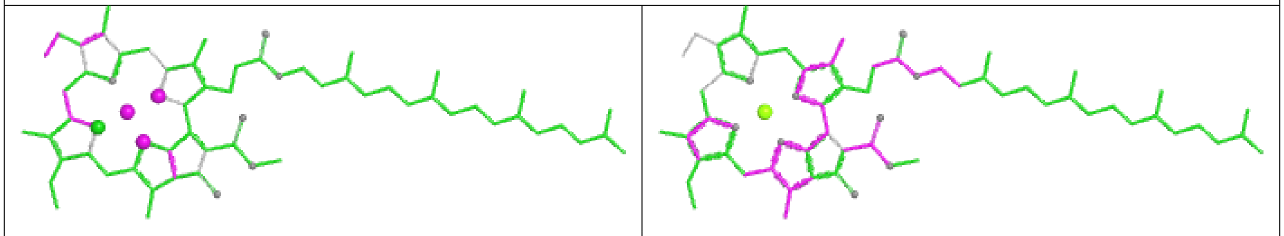


Bond lengths Bond angles

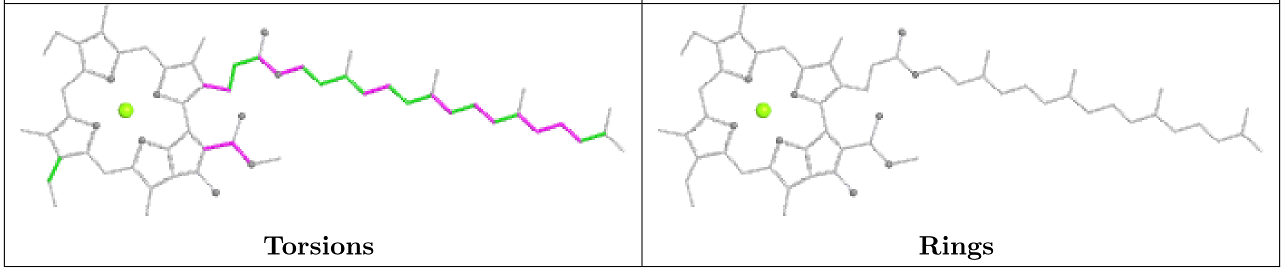


Torsions Rings

Ligand CLA B 1202

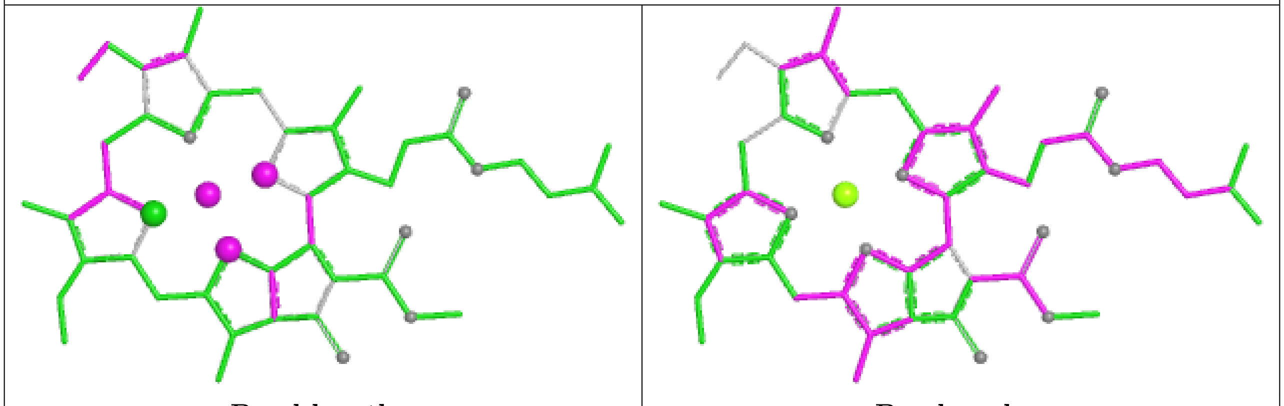


Bond lengths Bond angles



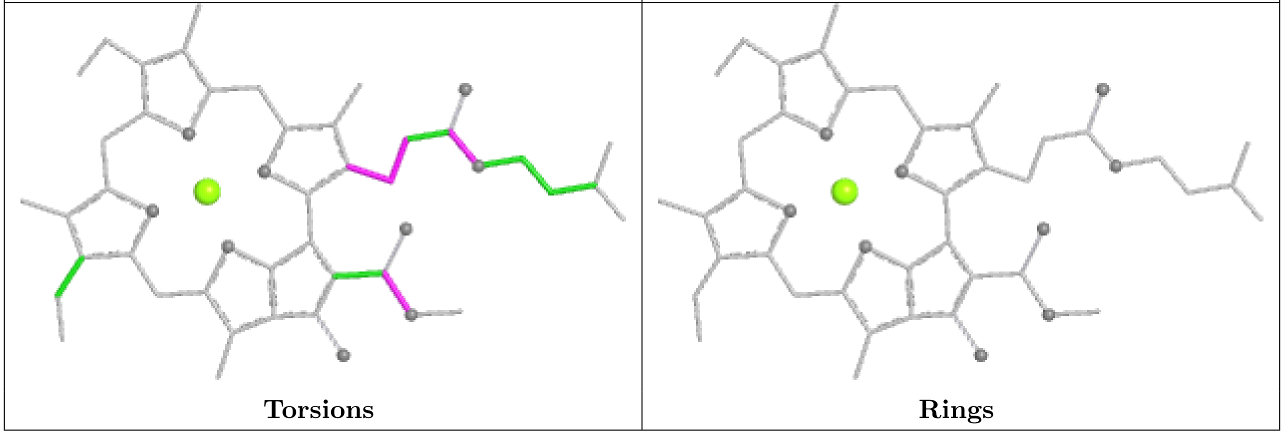
Torsions Rings

Ligand CLA L 1503



Bond lengths

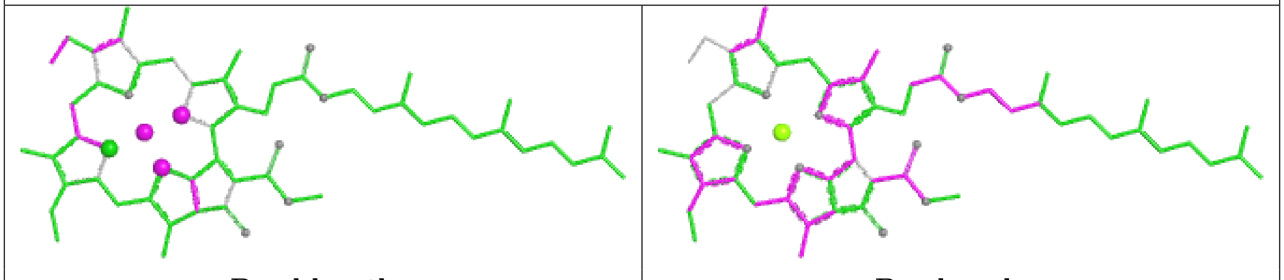
Bond angles



Torsions

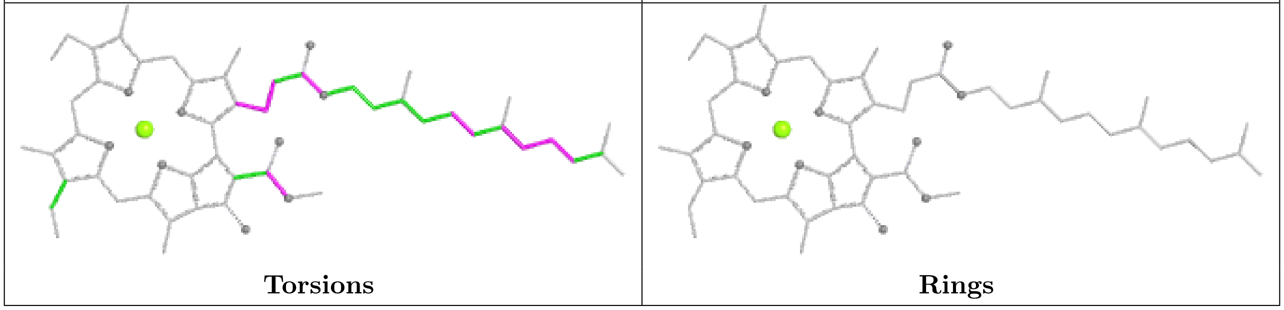
Rings

Ligand CLA A 1141



Bond lengths

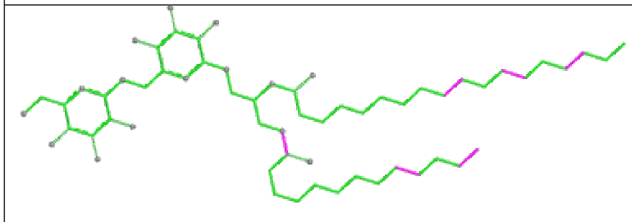
Bond angles



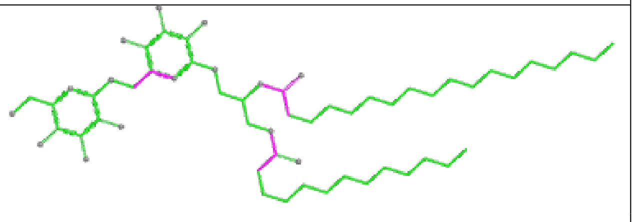
Torsions

Rings

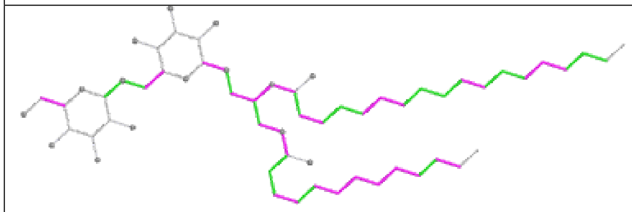
Ligand DGD B 5005



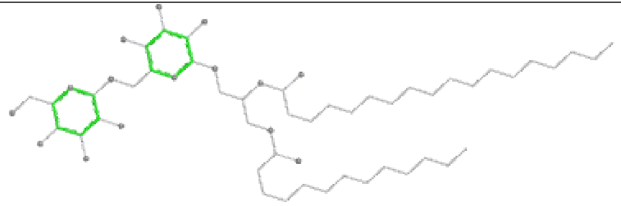
Bond lengths



Bond angles

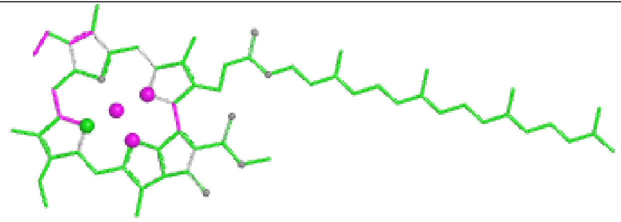


Torsions

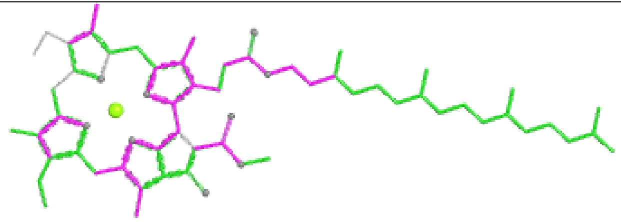


Rings

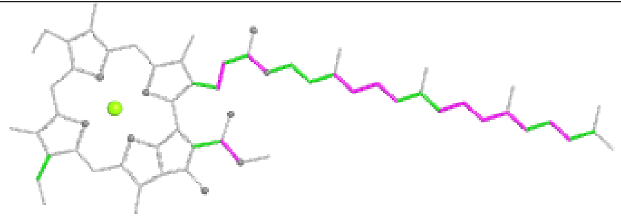
Ligand CLA 1 601



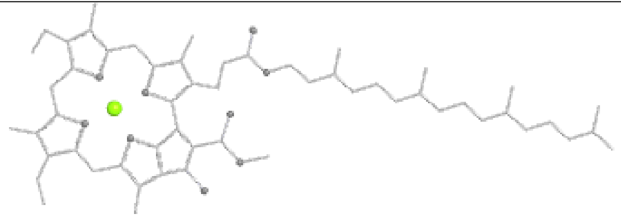
Bond lengths



Bond angles

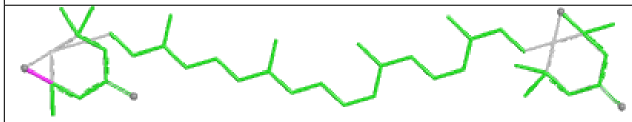


Torsions

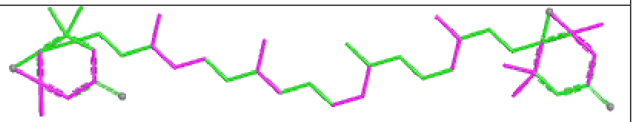


Rings

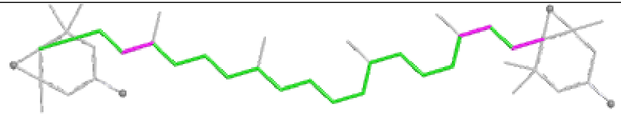
Ligand XAT 2 502



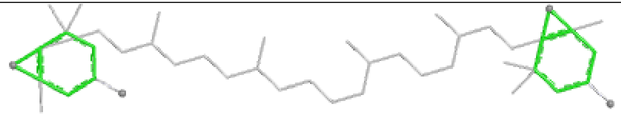
Bond lengths



Bond angles

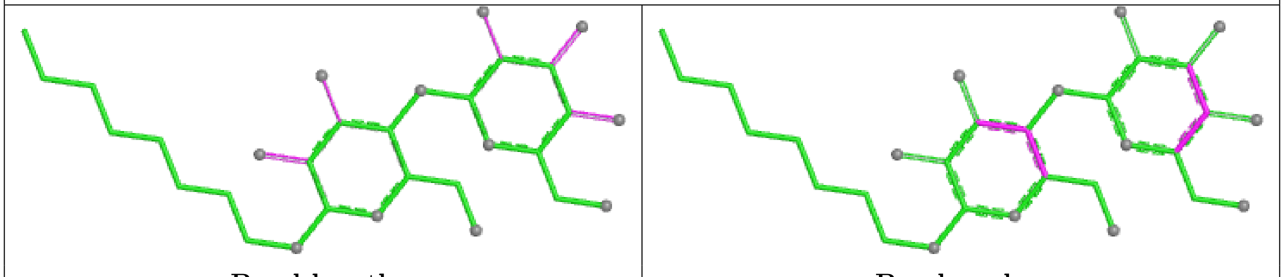


Torsions

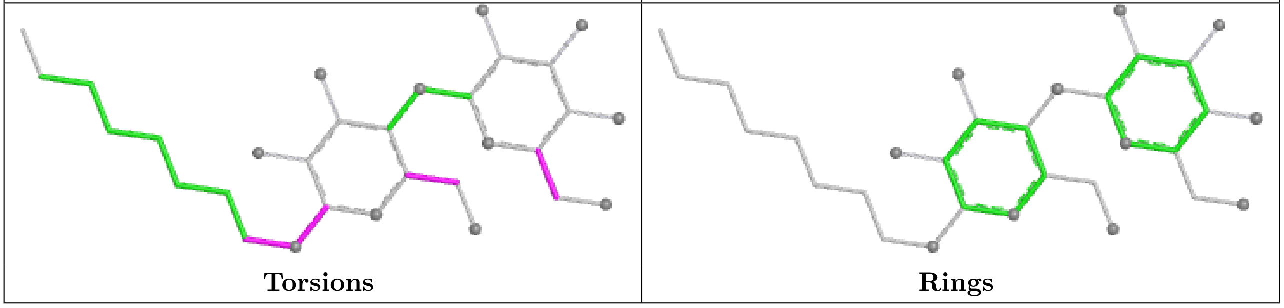


Rings

Ligand LMT B 5008

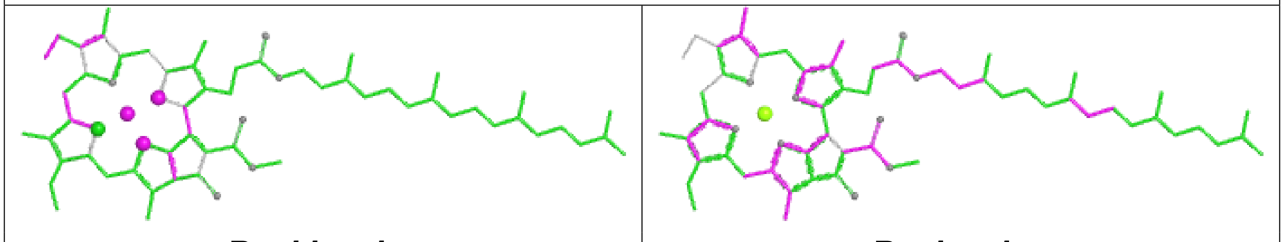


Bond lengths Bond angles

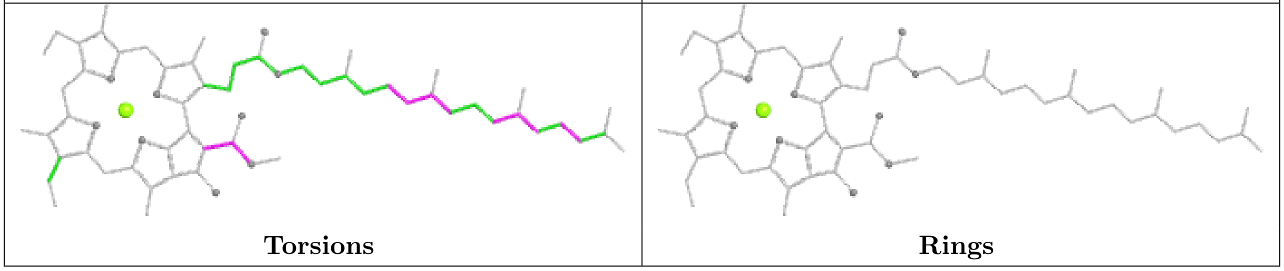


Torsions Rings

Ligand CLA A 1138

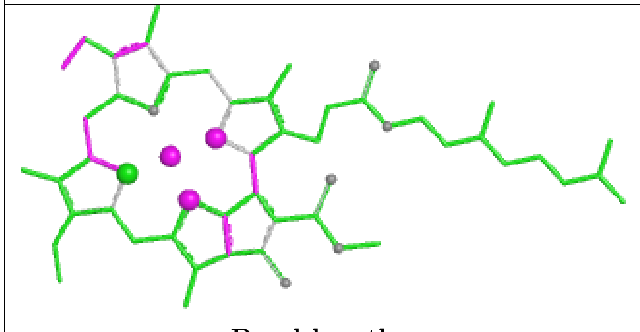


Bond lengths Bond angles

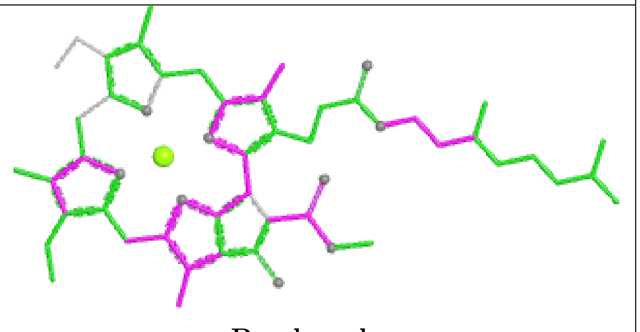


Torsions Rings

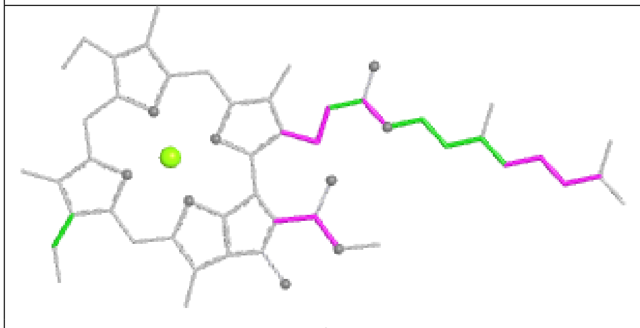
Ligand CLA A 1134



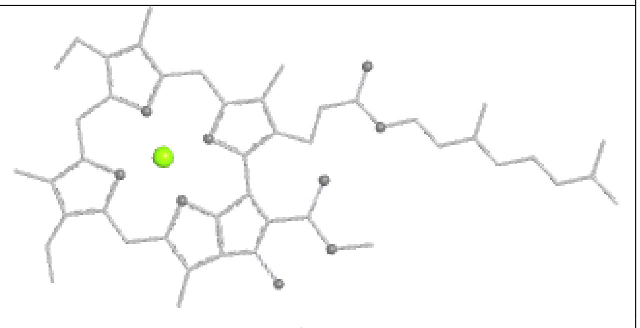
Bond lengths



Bond angles

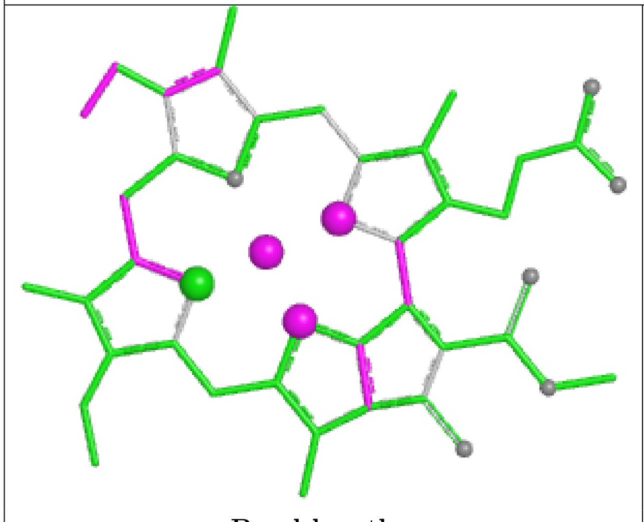


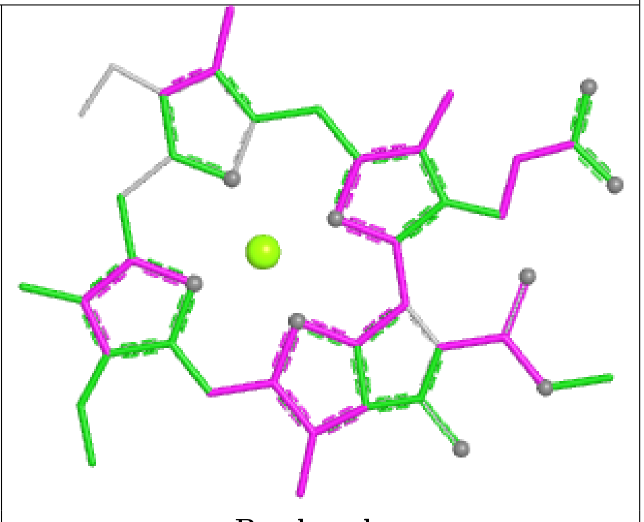
Torsions

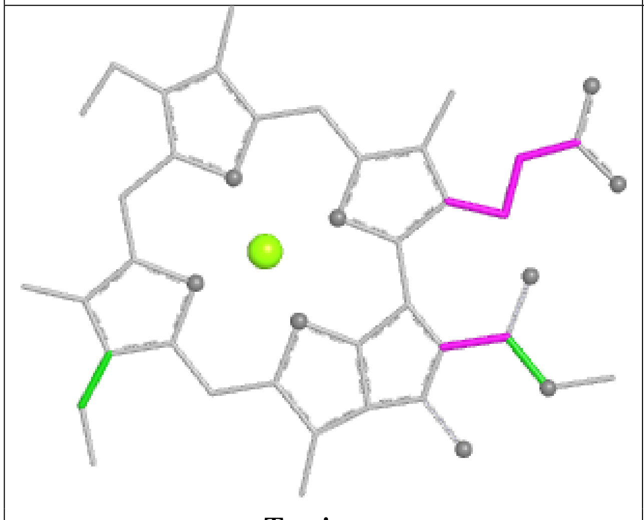


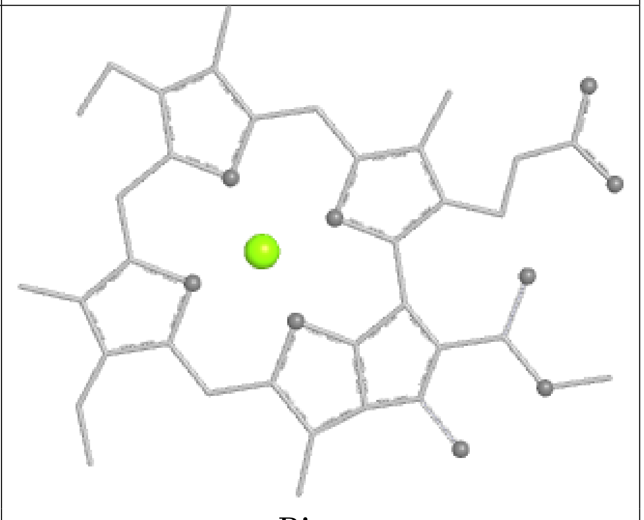
Rings

Ligand CLA A 1113

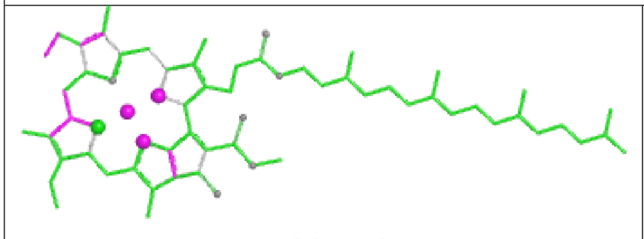

Bond lengths

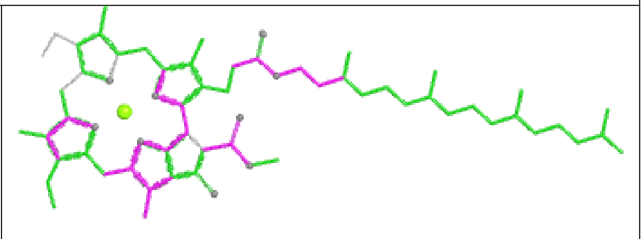

Bond angles

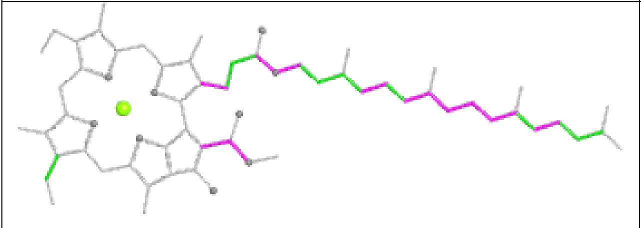

Torsions

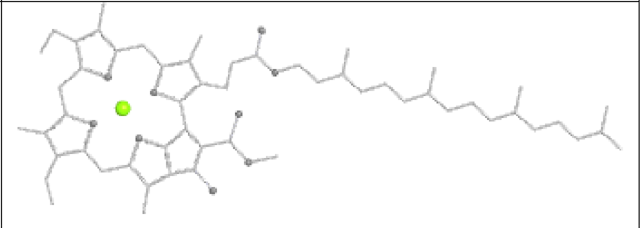

Rings

Ligand CLA A 1137

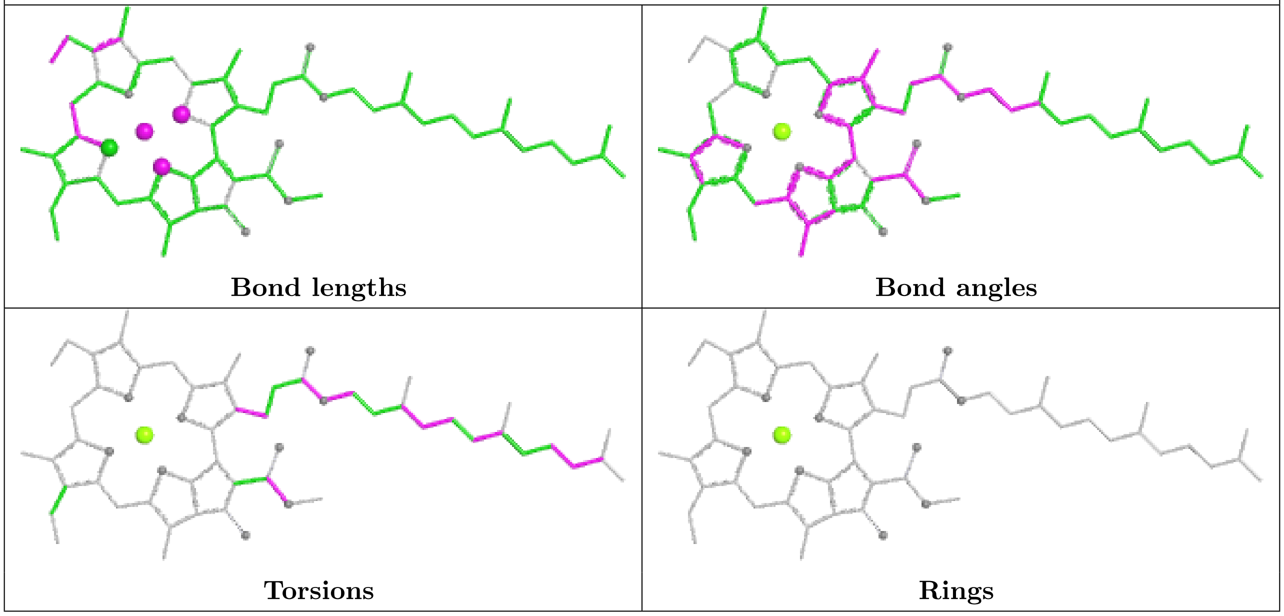

Bond lengths


Bond angles


Torsions


Rings

Ligand CLA 3 617



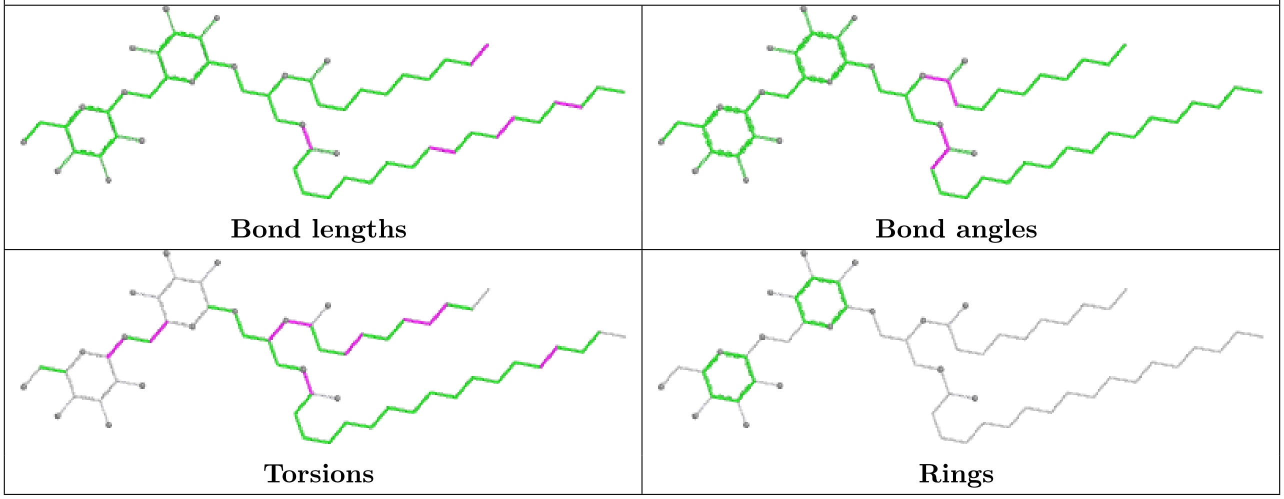
Bond lengths

Bond angles

Torsions

Rings

Ligand DGD J 5001



Bond lengths

Bond angles

Torsions

Rings

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

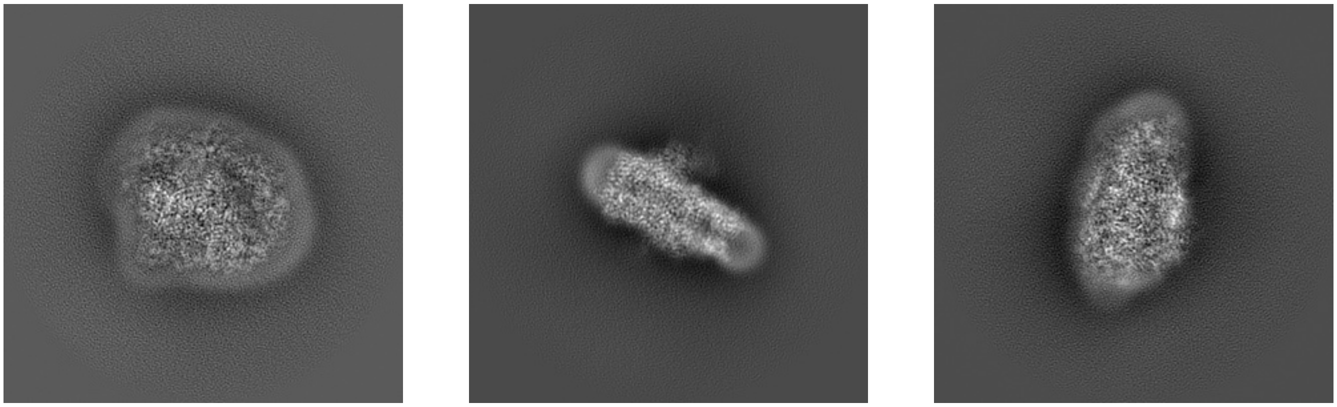
6 Map visualisation ⓘ

This section contains visualisations of the EMDB entry EMD-10746. These allow visual inspection of the internal detail of the map and identification of artifacts.

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

6.1 Orthogonal projections ⓘ

6.1.1 Primary map

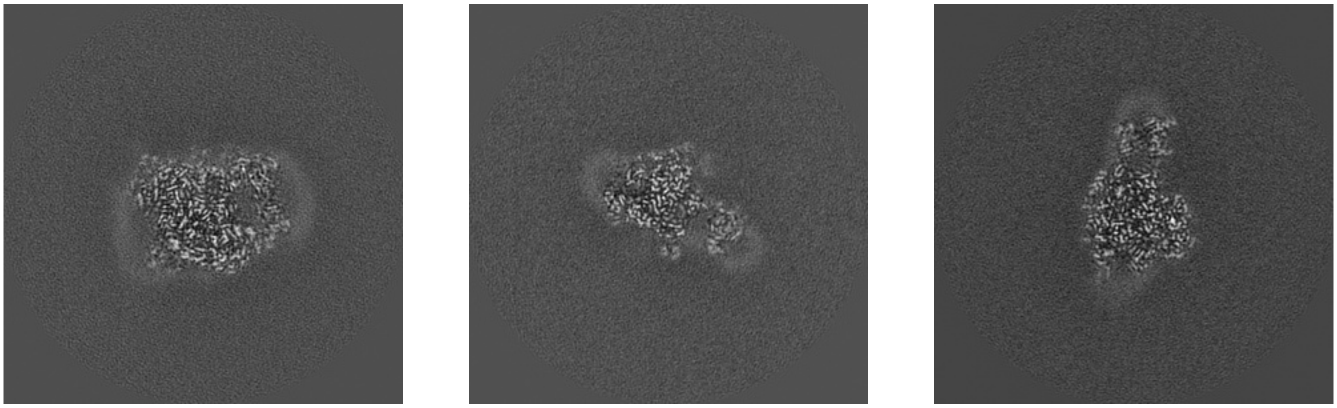


X Y Z

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

6.2 Central slices ⓘ

6.2.1 Primary map

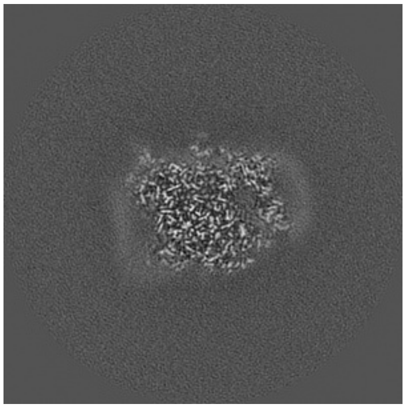


X Index: 165 Y Index: 165 Z Index: 165

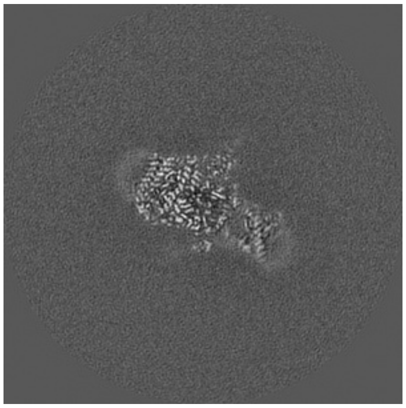
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices ⓘ

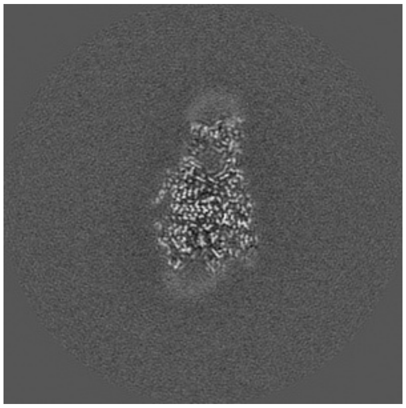
6.3.1 Primary map



X Index: 163



Y Index: 172

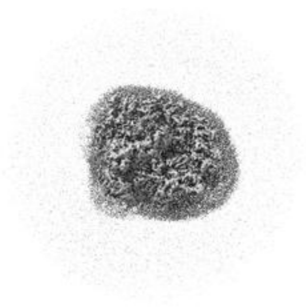


Z Index: 159

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

6.4 Orthogonal surface views ⓘ

6.4.1 Primary map



X

Y

Z

The images above show the 3D surface view of the map at the recommended contour level 0.0131. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

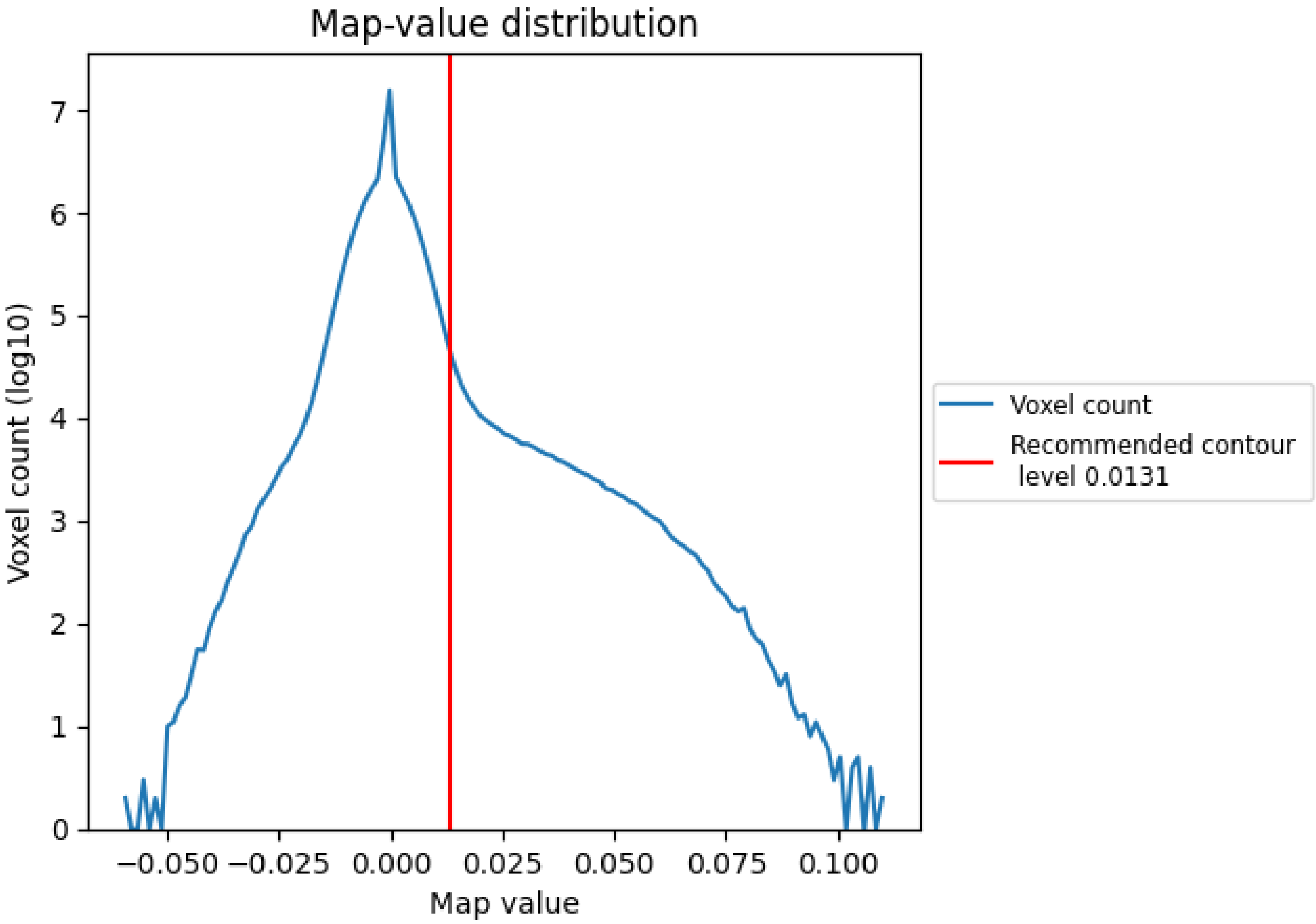
6.5 Mask visualisation ⓘ

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

7 Map analysis (i)

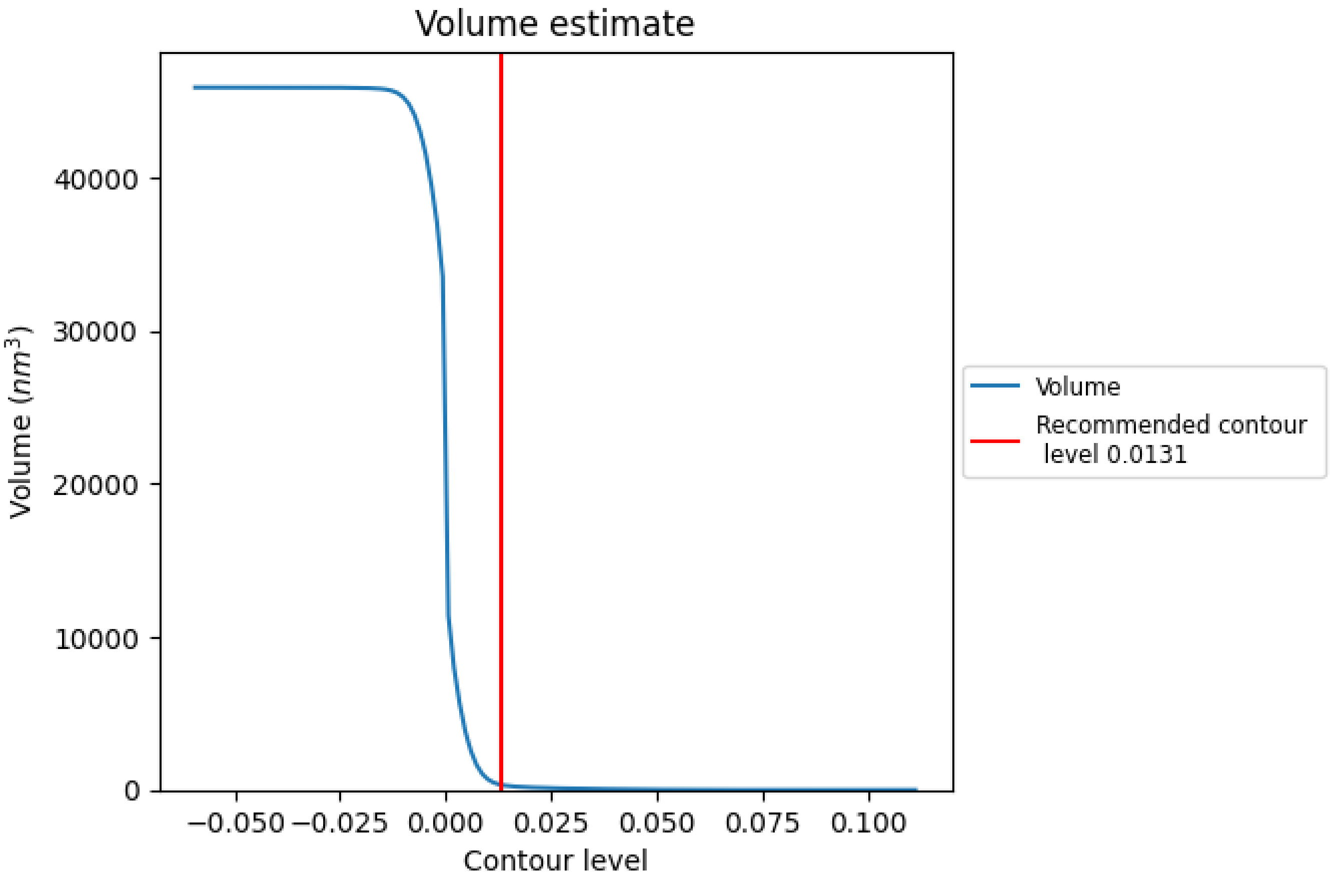
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution (i)



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

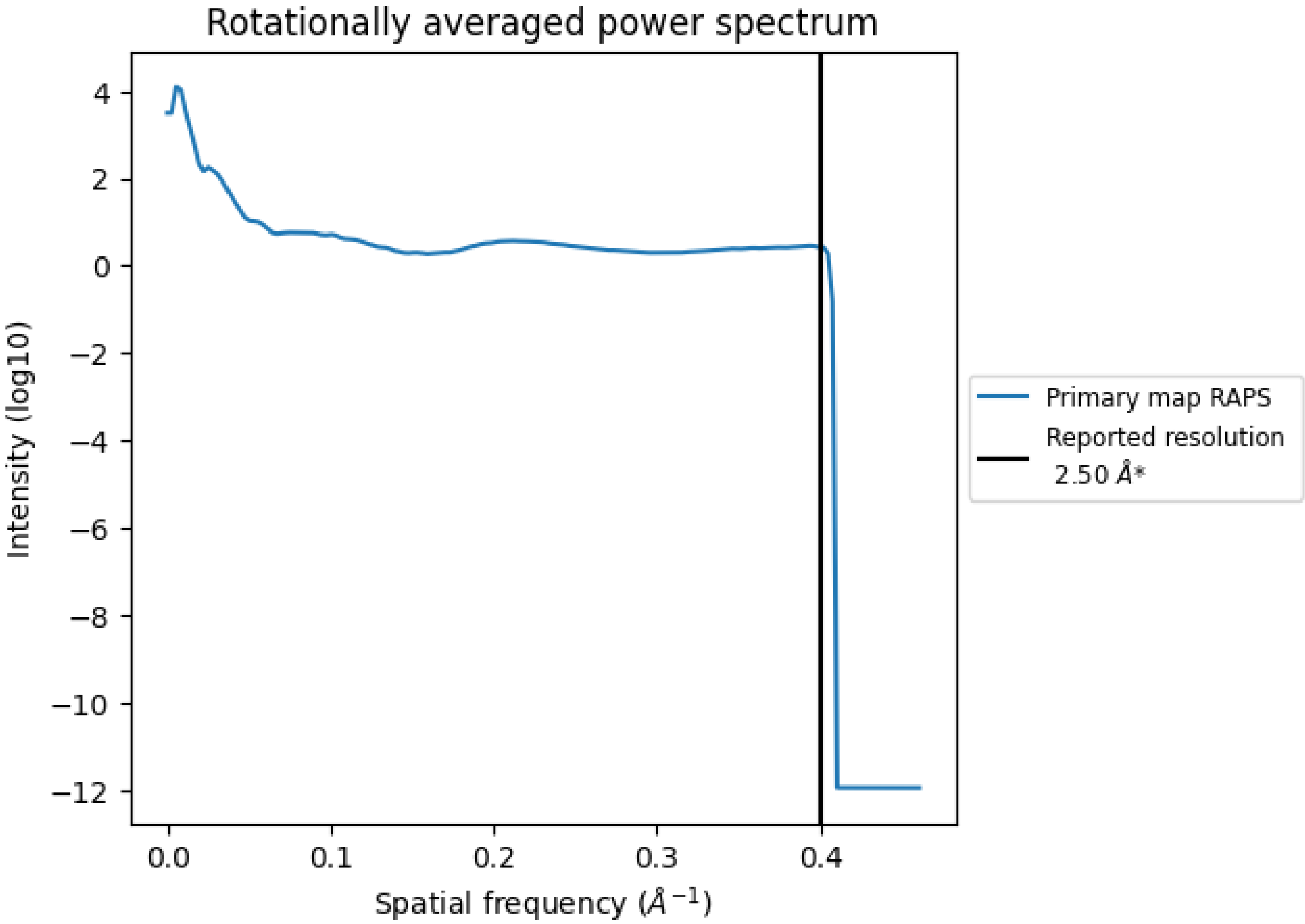
7.2 Volume estimate ⓘ



The volume at the recommended contour level is 338 nm^3; this corresponds to an approximate mass of 305 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 ⓘ

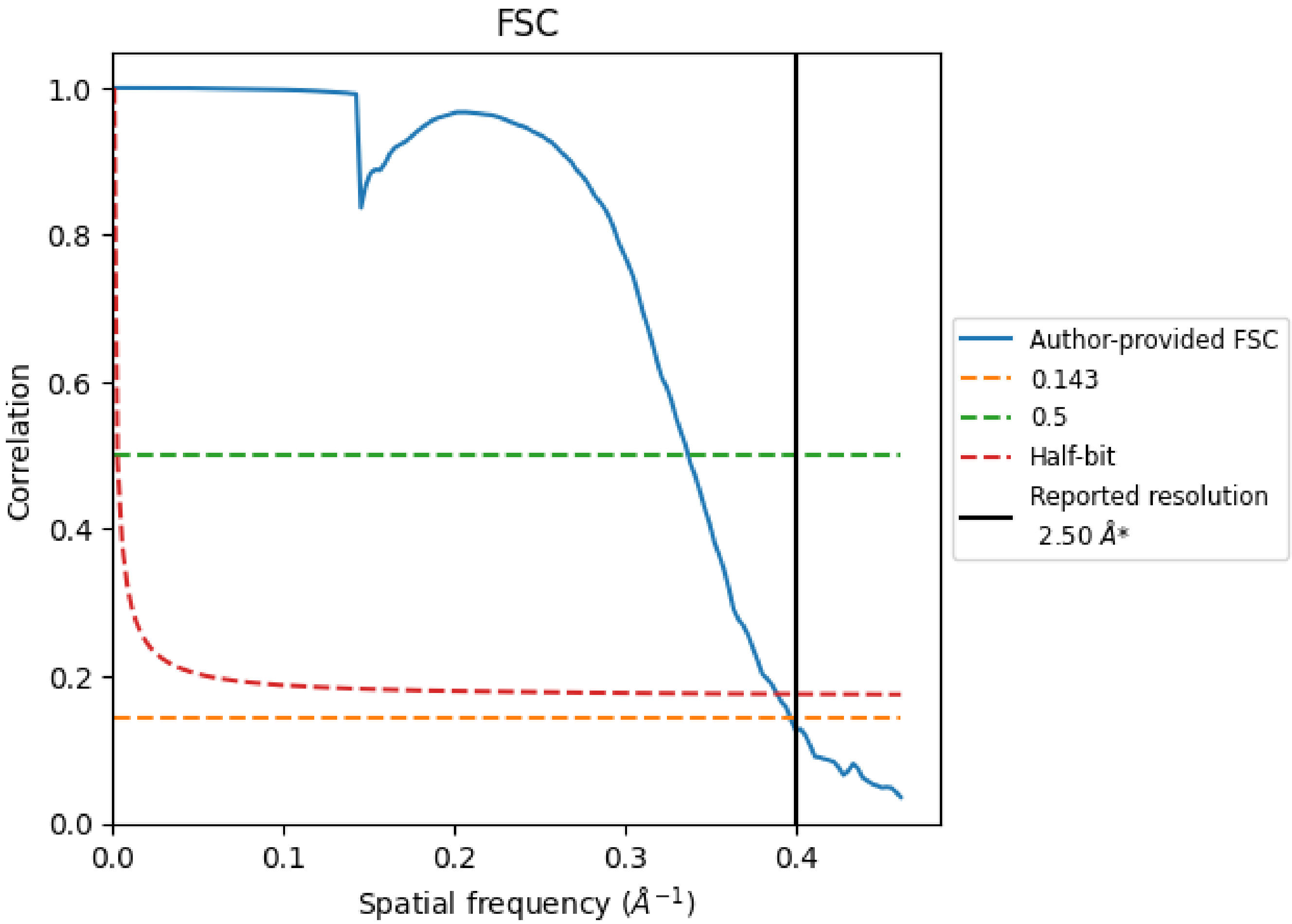


*Reported resolution corresponds to spatial frequency of 0.400 $Å^{-1}$

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 0.400 $\AA^{-1}$

8.2 Resolution estimates ⓘ

Resolution estimate (Å)	**Estimation criterion (FSC cut-off)**		
	0.143	0.5	Half-bit
Reported by author	2.50	-	-
Author-provided FSC curve	2.52	2.97	2.57
Unmasked-calculated*	-	-	-

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

9 Map-model fit ⓘ

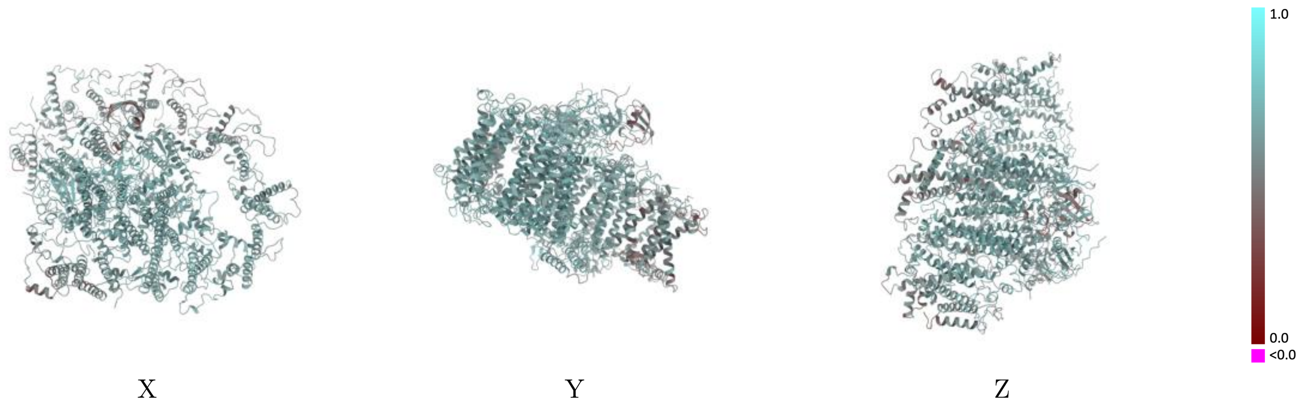
This section contains information regarding the fit between EMDB map EMD-10746 and PDB model 6YAC. Per-residue inclusion information can be found in section 3 on page 31.

9.1 Map-model overlay ⓘ

X Y Z

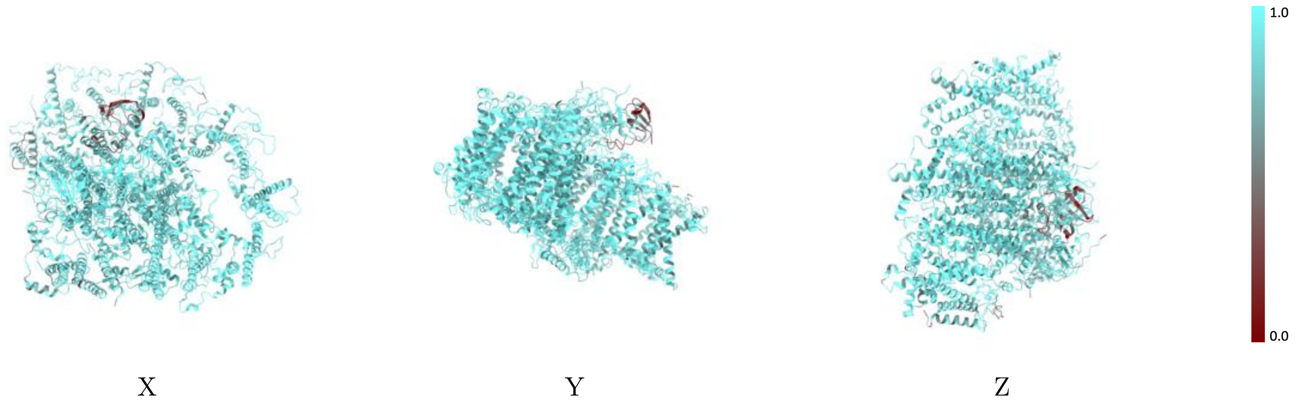
The images above show the 3D surface view of the map at the recommended contour level 0.0131 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model ⓘ



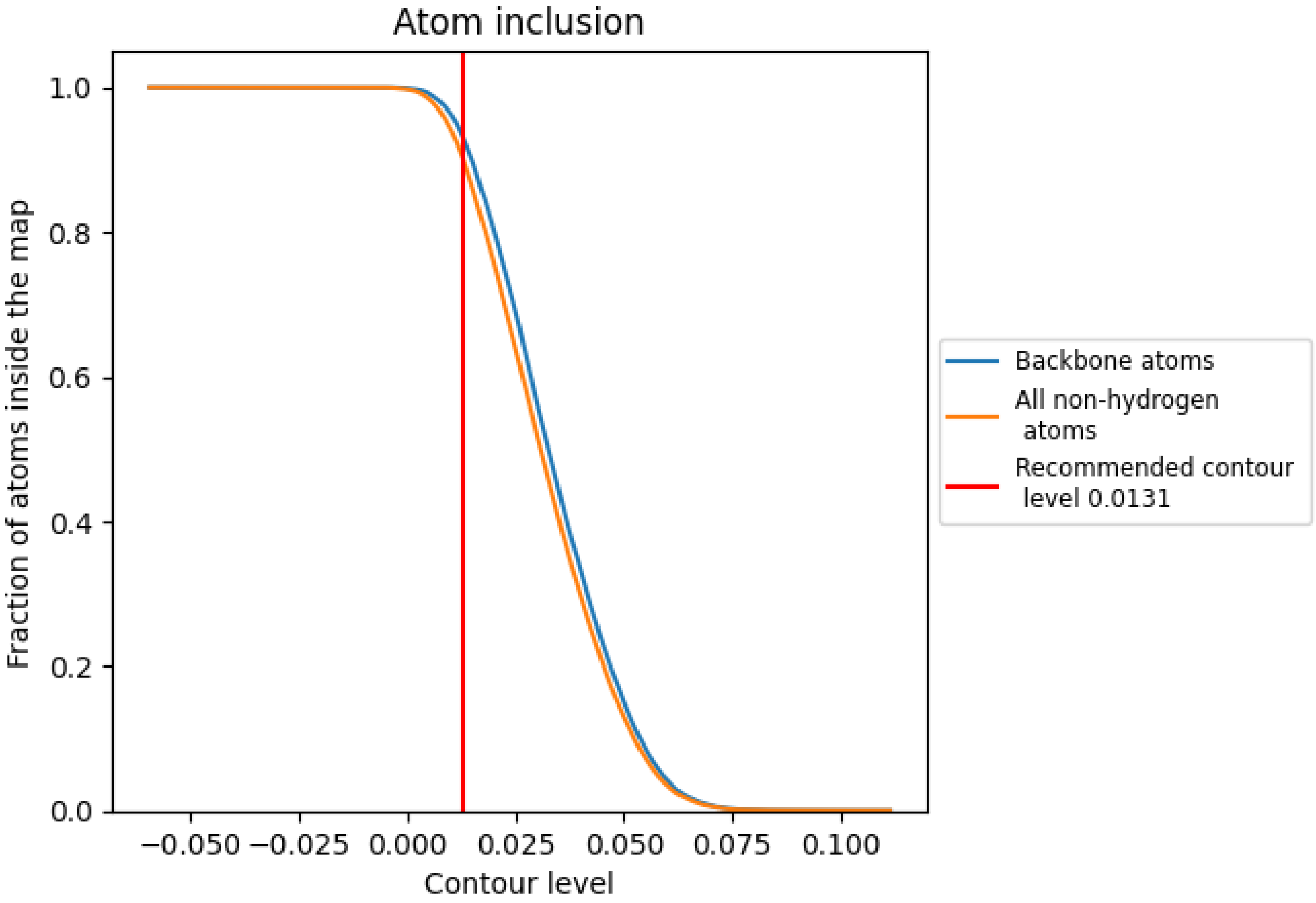
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 ⓘ



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 (0.0131).

9.4 Atom inclusion ⓘ



At the recommended contour level, 93% of all backbone atoms, 90% 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 (0.0131) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	▬ 0.8979	▬ 0.6010
1	▬ 0.8916	▬ 0.5840
2	▬ 0.8360	▬ 0.5290
3	▬ 0.8599	▬ 0.5540
4	▬ 0.8745	▬ 0.5560
A	▬ 0.9432	▬ 0.6420
B	▬ 0.9479	▬ 0.6440
C	▬ 0.9935	▬ 0.6600
D	▬ 0.9468	▬ 0.6240
E	▬ 0.9086	▬ 0.6250
F	▬ 0.8755	▬ 0.6040
G	▬ 0.8350	▬ 0.5770
H	▬ 0.8313	▬ 0.5350
I	▬ 0.8679	▬ 0.5780
J	▬ 0.8524	▬ 0.5930
K	▬ 0.7143	▬ 0.5190
L	▬ 0.8557	▬ 0.5440
N	▬ 0.4972	▬ 0.4580