wwPDB EM Validation Summary Report ⓘ

Nov 19, 2022 – 11:38 PM EST

PDB ID	:	7LX0
EMDB ID	:	EMD-23563
Title	:	Quantitative assessment of chlorophyll types in cryo-EM maps of photosystem I acclimated to far-red light
Authors	:	Gisriel, C.J.; Wang, J.
Deposited on	:	2021-03-02
Resolution	:	2.96 Å(reported)

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

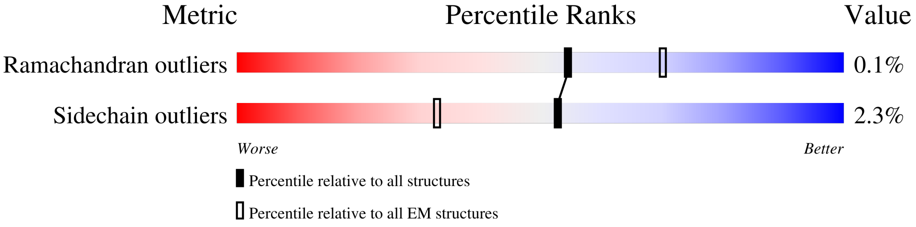
EMDB validation analysis	:	0.0.1.dev43
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.2

1 Overall quality at a glance

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

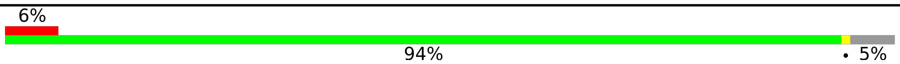
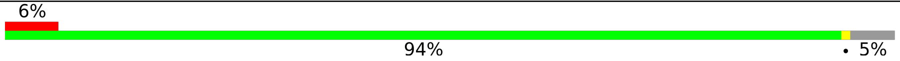
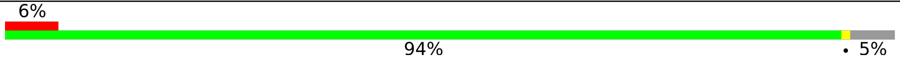
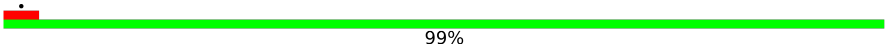
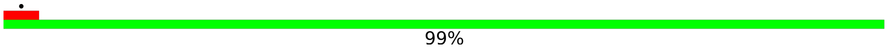
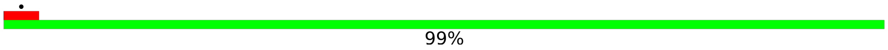
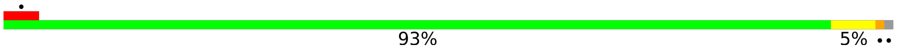
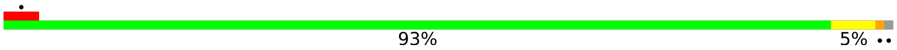
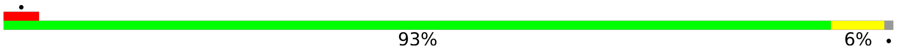
The reported resolution of this entry is 2.96 Å.

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)
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	788	
1	G	788	
1	a	788	
2	B	741	
2	H	741	
2	b	741	
3	C	81	
3	N	81	
3	c	81	

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Mol	Chain	Length	Quality of chain
4	D	159	13% 84% • • 13%
4	O	159	16% 84% • • 13%
4	d	159	15% 84% • • 13%
5	E	72	26% 82% • 14%
5	P	72	24% 82% • 14%
5	e	72	29% 82% • 14%
6	F	159	46% 77% 6% •• 15%
6	Q	159	44% 77% 6% •• 15%
6	f	159	44% 77% 6% •• 15%
7	I	67	6% 63% 37%
7	R	67	6% 63% 37%
7	i	67	7% 63% 37%
8	J	48	40% 79% 8% • 10%
8	S	48	33% 79% 8% • 10%
8	j	48	38% 79% 8% • 10%
9	K	49	88% 88% • 10%
9	T	49	88% 88% • 10%
9	k	49	84% 88% • 10%
10	L	174	6% 92% •• 6%
10	U	174	5% 92% •• 6%
10	l	174	5% 92% •• 6%
11	M	31	6% 97% •
11	V	31	6% 97% •
11	m	31	• 97% •
12	W	101	9% 29% 71%

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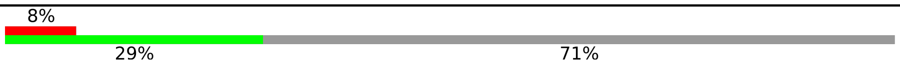
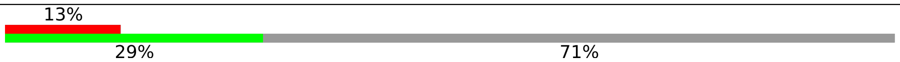
Mol	Chain	Length	Quality of chain
12	X	101	
12	x	101	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
13	CL0	A	1011	X	-	-	-
13	CL0	G	1011	X	-	-	-
13	CL0	a	1011	X	-	-	-
14	CLA	A	1012	X	-	-	-
14	CLA	A	1013	X	-	-	-
14	CLA	A	1101	X	-	-	-
14	CLA	A	1102	X	-	-	-
14	CLA	A	1103	X	-	-	-
14	CLA	A	1104	X	-	-	-
14	CLA	A	1105	X	-	-	-
14	CLA	A	1106	X	-	-	-
14	CLA	A	1107	X	-	-	-
14	CLA	A	1108	X	-	-	-
14	CLA	A	1109	X	-	-	-
14	CLA	A	1110	X	-	-	-
14	CLA	A	1111	X	-	-	-
14	CLA	A	1112	X	-	-	-
14	CLA	A	1113	X	-	-	-
14	CLA	A	1114	X	-	-	-
14	CLA	A	1115	X	-	-	-
14	CLA	A	1116	X	-	-	-
14	CLA	A	1117	X	-	-	-
14	CLA	A	1118	X	-	-	-
14	CLA	A	1119	X	-	-	-
14	CLA	A	1120	X	-	-	-
14	CLA	A	1122	X	-	-	-
14	CLA	A	1123	X	-	-	-
14	CLA	A	1124	X	-	-	-
14	CLA	A	1125	X	-	-	-
14	CLA	A	1126	X	-	-	-
14	CLA	A	1127	X	-	-	-
14	CLA	A	1128	X	-	-	-
14	CLA	A	1129	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
14	CLA	A	1130	X	-	-	-
14	CLA	A	1131	X	-	-	-
14	CLA	A	1132	X	-	-	-
14	CLA	A	1133	X	-	-	-
14	CLA	A	1134	X	-	-	-
14	CLA	A	1135	X	-	-	-
14	CLA	A	1136	X	-	-	-
14	CLA	A	1137	X	-	-	-
14	CLA	A	1138	X	-	-	-
14	CLA	A	1139	X	-	-	-
14	CLA	A	1140	X	-	-	-
14	CLA	B	1021	X	-	-	-
14	CLA	B	1022	X	-	-	-
14	CLA	B	1023	X	-	-	-
14	CLA	B	1201	X	-	-	-
14	CLA	B	1202	X	-	-	-
14	CLA	B	1203	X	-	-	-
14	CLA	B	1204	X	-	-	-
14	CLA	B	1205	X	-	-	-
14	CLA	B	1206	X	-	-	-
14	CLA	B	1208	X	-	-	-
14	CLA	B	1209	X	-	-	-
14	CLA	B	1210	X	-	-	-
14	CLA	B	1211	X	-	-	-
14	CLA	B	1212	X	-	-	-
14	CLA	B	1213	X	-	-	-
14	CLA	B	1214	X	-	-	-
14	CLA	B	1215	X	-	-	-
14	CLA	B	1216	X	-	-	-
14	CLA	B	1217	X	-	-	-
14	CLA	B	1218	X	-	-	-
14	CLA	B	1219	X	-	-	-
14	CLA	B	1220	X	-	-	-
14	CLA	B	1221	X	-	-	-
14	CLA	B	1222	X	-	-	-
14	CLA	B	1223	X	-	-	-
14	CLA	B	1224	X	-	-	-
14	CLA	B	1225	X	-	-	-
14	CLA	B	1226	X	-	-	-
14	CLA	B	1227	X	-	-	-
14	CLA	B	1228	X	-	-	-
14	CLA	B	1229	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
14	CLA	B	1231	X	-	-	-
14	CLA	B	1232	X	-	-	-
14	CLA	B	1233	X	-	-	-
14	CLA	B	1234	X	-	-	-
14	CLA	B	1235	X	-	-	-
14	CLA	B	1236	X	-	-	-
14	CLA	B	1239	X	-	-	-
14	CLA	G	1012	X	-	-	-
14	CLA	G	1013	X	-	-	-
14	CLA	G	1101	X	-	-	-
14	CLA	G	1102	X	-	-	-
14	CLA	G	1103	X	-	-	-
14	CLA	G	1104	X	-	-	-
14	CLA	G	1105	X	-	-	-
14	CLA	G	1106	X	-	-	-
14	CLA	G	1107	X	-	-	-
14	CLA	G	1108	X	-	-	-
14	CLA	G	1109	X	-	-	-
14	CLA	G	1110	X	-	-	-
14	CLA	G	1111	X	-	-	-
14	CLA	G	1112	X	-	-	-
14	CLA	G	1113	X	-	-	-
14	CLA	G	1114	X	-	-	-
14	CLA	G	1115	X	-	-	-
14	CLA	G	1116	X	-	-	-
14	CLA	G	1117	X	-	-	-
14	CLA	G	1118	X	-	-	-
14	CLA	G	1119	X	-	-	-
14	CLA	G	1120	X	-	-	-
14	CLA	G	1122	X	-	-	-
14	CLA	G	1123	X	-	-	-
14	CLA	G	1124	X	-	-	-
14	CLA	G	1125	X	-	-	-
14	CLA	G	1126	X	-	-	-
14	CLA	G	1127	X	-	-	-
14	CLA	G	1128	X	-	-	-
14	CLA	G	1129	X	-	-	-
14	CLA	G	1130	X	-	-	-
14	CLA	G	1131	X	-	-	-
14	CLA	G	1132	X	-	-	-
14	CLA	G	1133	X	-	-	-
14	CLA	G	1134	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
14	CLA	G	1135	X	-	-	-
14	CLA	G	1136	X	-	-	-
14	CLA	G	1137	X	-	-	-
14	CLA	G	1138	X	-	-	-
14	CLA	G	1139	X	-	-	-
14	CLA	G	1140	X	-	-	-
14	CLA	H	1021	X	-	-	-
14	CLA	H	1022	X	-	-	-
14	CLA	H	1023	X	-	-	-
14	CLA	H	1201	X	-	-	-
14	CLA	H	1202	X	-	-	-
14	CLA	H	1203	X	-	-	-
14	CLA	H	1204	X	-	-	-
14	CLA	H	1205	X	-	-	-
14	CLA	H	1206	X	-	-	-
14	CLA	H	1208	X	-	-	-
14	CLA	H	1209	X	-	-	-
14	CLA	H	1210	X	-	-	-
14	CLA	H	1211	X	-	-	-
14	CLA	H	1212	X	-	-	-
14	CLA	H	1213	X	-	-	-
14	CLA	H	1214	X	-	-	-
14	CLA	H	1215	X	-	-	-
14	CLA	H	1216	X	-	-	-
14	CLA	H	1217	X	-	-	-
14	CLA	H	1218	X	-	-	-
14	CLA	H	1219	X	-	-	-
14	CLA	H	1220	X	-	-	-
14	CLA	H	1221	X	-	-	-
14	CLA	H	1222	X	-	-	-
14	CLA	H	1223	X	-	-	-
14	CLA	H	1224	X	-	-	-
14	CLA	H	1225	X	-	-	-
14	CLA	H	1226	X	-	-	-
14	CLA	H	1227	X	-	-	-
14	CLA	H	1228	X	-	-	-
14	CLA	H	1229	X	-	-	-
14	CLA	H	1231	X	-	-	-
14	CLA	H	1232	X	-	-	-
14	CLA	H	1233	X	-	-	-
14	CLA	H	1234	X	-	-	-
14	CLA	H	1235	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
14	CLA	H	1236	X	-	-	-
14	CLA	H	1239	X	-	-	-
14	CLA	K	1401	X	-	-	-
14	CLA	L	1501	X	-	-	-
14	CLA	L	1502	X	-	-	-
14	CLA	L	1503	X	-	-	-
14	CLA	T	1401	X	-	-	-
14	CLA	U	1501	X	-	-	-
14	CLA	U	1502	X	-	-	-
14	CLA	U	1503	X	-	-	-
14	CLA	W	1701	X	-	-	-
14	CLA	X	1701	X	-	-	-
14	CLA	a	1012	X	-	-	-
14	CLA	a	1013	X	-	-	-
14	CLA	a	1101	X	-	-	-
14	CLA	a	1102	X	-	-	-
14	CLA	a	1103	X	-	-	-
14	CLA	a	1104	X	-	-	-
14	CLA	a	1105	X	-	-	-
14	CLA	a	1106	X	-	-	-
14	CLA	a	1107	X	-	-	-
14	CLA	a	1108	X	-	-	-
14	CLA	a	1109	X	-	-	-
14	CLA	a	1110	X	-	-	-
14	CLA	a	1111	X	-	-	-
14	CLA	a	1112	X	-	-	-
14	CLA	a	1113	X	-	-	-
14	CLA	a	1114	X	-	-	-
14	CLA	a	1115	X	-	-	-
14	CLA	a	1116	X	-	-	-
14	CLA	a	1117	X	-	-	-
14	CLA	a	1118	X	-	-	-
14	CLA	a	1119	X	-	-	-
14	CLA	a	1120	X	-	-	-
14	CLA	a	1122	X	-	-	-
14	CLA	a	1123	X	-	-	-
14	CLA	a	1124	X	-	-	-
14	CLA	a	1125	X	-	-	-
14	CLA	a	1126	X	-	-	-
14	CLA	a	1127	X	-	-	-
14	CLA	a	1128	X	-	-	-
14	CLA	a	1129	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
14	CLA	a	1130	X	-	-	-
14	CLA	a	1131	X	-	-	-
14	CLA	a	1132	X	-	-	-
14	CLA	a	1133	X	-	-	-
14	CLA	a	1134	X	-	-	-
14	CLA	a	1135	X	-	-	-
14	CLA	a	1136	X	-	-	-
14	CLA	a	1137	X	-	-	-
14	CLA	a	1138	X	-	-	-
14	CLA	a	1139	X	-	-	-
14	CLA	a	1140	X	-	-	-
14	CLA	b	1021	X	-	-	-
14	CLA	b	1022	X	-	-	-
14	CLA	b	1023	X	-	-	-
14	CLA	b	1201	X	-	-	-
14	CLA	b	1202	X	-	-	-
14	CLA	b	1203	X	-	-	-
14	CLA	b	1204	X	-	-	-
14	CLA	b	1205	X	-	-	-
14	CLA	b	1206	X	-	-	-
14	CLA	b	1208	X	-	-	-
14	CLA	b	1209	X	-	-	-
14	CLA	b	1210	X	-	-	-
14	CLA	b	1211	X	-	-	-
14	CLA	b	1212	X	-	-	-
14	CLA	b	1213	X	-	-	-
14	CLA	b	1214	X	-	-	-
14	CLA	b	1215	X	-	-	-
14	CLA	b	1216	X	-	-	-
14	CLA	b	1217	X	-	-	-
14	CLA	b	1218	X	-	-	-
14	CLA	b	1219	X	-	-	-
14	CLA	b	1220	X	-	-	-
14	CLA	b	1221	X	-	-	-
14	CLA	b	1222	X	-	-	-
14	CLA	b	1223	X	-	-	-
14	CLA	b	1224	X	-	-	-
14	CLA	b	1225	X	-	-	-
14	CLA	b	1226	X	-	-	-
14	CLA	b	1227	X	-	-	-
14	CLA	b	1228	X	-	-	-
14	CLA	b	1229	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
14	CLA	b	1231	X	-	-	-
14	CLA	b	1232	X	-	-	-
14	CLA	b	1233	X	-	-	-
14	CLA	b	1234	X	-	-	-
14	CLA	b	1235	X	-	-	-
14	CLA	b	1236	X	-	-	-
14	CLA	b	1239	X	-	-	-
14	CLA	k	1401	X	-	-	-
14	CLA	l	1501	X	-	-	-
14	CLA	l	1502	X	-	-	-
14	CLA	l	1503	X	-	-	-
14	CLA	x	1701	X	-	-	-

2 Entry composition (i)

There are 22 unique types of molecules in this entry. The entry contains 72462 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
1	G	751	Total 5931	C 3892	N 1013	O 993	S 33	0	0
1	a	751	Total 5931	C 3892	N 1013	O 993	S 33	0	0
1	A	751	Total 5931	C 3892	N 1013	O 993	S 33	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	H	739	Total 5913	C 3896	N 997	O 1002	S 18	0	0
2	b	739	Total 5913	C 3896	N 997	O 1002	S 18	0	0
2	B	739	Total 5913	C 3896	N 997	O 1002	S 18	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
3	N	80	Total 601	C 367	N 105	O 118	S 11	0	0
3	c	80	Total 601	C 367	N 105	O 118	S 11	0	0
3	C	80	Total 601	C 367	N 105	O 118	S 11	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
4	O	139	Total 1092	C 694	N 192	O 203	S 3	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
4	d	139	Total 1092	C 694	N 192	O 203	S 3	0	0
4	D	139	Total 1092	C 694	N 192	O 203	S 3	0	0

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

Mol	Chain	Residues	Atoms				AltConf	Trace
5	P	62	Total 497	C 313	N 88	O 96	0	0
5	e	62	Total 497	C 313	N 88	O 96	0	0
5	E	62	Total 497	C 313	N 88	O 96	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
6	Q	135	Total 1060	C 694	N 167	O 192	S 7	0	0
6	f	135	Total 1060	C 694	N 167	O 192	S 7	0	0
6	F	135	Total 1060	C 694	N 167	O 192	S 7	0	0

- Molecule 7 is a protein called photosystem I subunit VIII.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	R	42	Total 350	C 246	N 48	O 54	S 2	0	0
7	i	42	Total 350	C 246	N 48	O 54	S 2	0	0
7	I	42	Total 350	C 246	N 48	O 54	S 2	0	0

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
R	1	MET	-	initiating methionine	UNP A0A2N6MR25
i	1	MET	-	initiating methionine	UNP A0A2N6MR25
I	1	MET	-	initiating methionine	UNP A0A2N6MR25

- Molecule 8 is a protein called Photosystem I reaction centre subunit IX / PsaJ.

Mol	Chain	Residues	Atoms				AltConf	Trace
8	S	43	Total 344	C 238	N 51	O 55	0	0
8	j	43	Total 344	C 238	N 51	O 55	0	0
8	J	43	Total 344	C 238	N 51	O 55	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
9	T	44	Total 253	C 161	N 46	O 45	S 1	0	0
9	k	44	Total 253	C 161	N 46	O 45	S 1	0	0
9	K	44	Total 253	C 161	N 46	O 45	S 1	0	0

- Molecule 10 is a protein called PSI subunit V.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	U	163	Total 1227	C 792	N 207	O 223	S 5	0	0
10	l	163	Total 1227	C 792	N 207	O 223	S 5	0	0
10	L	163	Total 1227	C 792	N 207	O 223	S 5	0	0

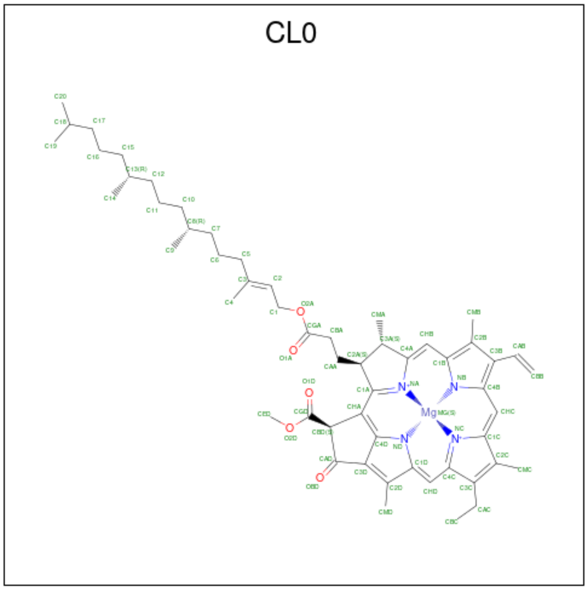
- Molecule 11 is a protein called Photosystem I reaction center subunit XII.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	V	31	Total 245	C 164	N 37	O 43	S 1	0	0
11	m	31	Total 245	C 164	N 37	O 43	S 1	0	0
11	M	31	Total 245	C 164	N 37	O 43	S 1	0	0

- Molecule 12 is a protein called Photosystem one PsaX.

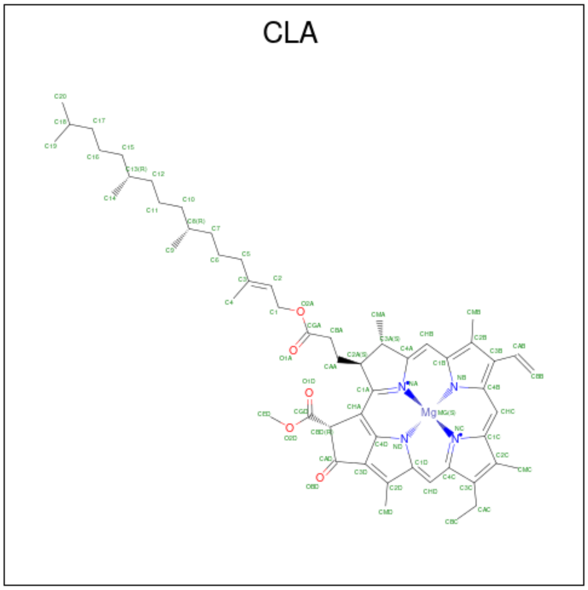
Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
12	W	29	246	172	36	38	0	0
12	x	29	246	172	36	38	0	0
12	X	29	246	172	36	38	0	0

- Molecule 13 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	
13	G	1	65	55	1	4	5	0
13	a	1	65	55	1	4	5	0
13	A	1	65	55	1	4	5	0

- Molecule 14 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	
14	G	1	Total 2315	C 1905	Mg 41	N 164	O 205	0
14	G	1	Total 2315	C 1905	Mg 41	N 164	O 205	0
14	G	1	Total 2315	C 1905	Mg 41	N 164	O 205	0
14	G	1	Total 2315	C 1905	Mg 41	N 164	O 205	0
14	G	1	Total 2315	C 1905	Mg 41	N 164	O 205	0
14	G	1	Total 2315	C 1905	Mg 41	N 164	O 205	0
14	G	1	Total 2315	C 1905	Mg 41	N 164	O 205	0
14	G	1	Total 2315	C 1905	Mg 41	N 164	O 205	0
14	G	1	Total 2315	C 1905	Mg 41	N 164	O 205	0
14	G	1	Total 2315	C 1905	Mg 41	N 164	O 205	0
14	G	1	Total 2315	C 1905	Mg 41	N 164	O 205	0
14	G	1	Total 2315	C 1905	Mg 41	N 164	O 205	0
14	G	1	Total 2315	C 1905	Mg 41	N 164	O 205	0
14	G	1	Total 2315	C 1905	Mg 41	N 164	O 205	0

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Mol	Chain	Residues	Atoms					AltConf
14	G	1	Total 2315	C 1905	Mg 41	N 164	O 205	0
14	G	1	Total 2315	C 1905	Mg 41	N 164	O 205	0
14	G	1	Total 2315	C 1905	Mg 41	N 164	O 205	0
14	G	1	Total 2315	C 1905	Mg 41	N 164	O 205	0
14	G	1	Total 2315	C 1905	Mg 41	N 164	O 205	0
14	G	1	Total 2315	C 1905	Mg 41	N 164	O 205	0
14	G	1	Total 2315	C 1905	Mg 41	N 164	O 205	0
14	G	1	Total 2315	C 1905	Mg 41	N 164	O 205	0
14	G	1	Total 2315	C 1905	Mg 41	N 164	O 205	0
14	G	1	Total 2315	C 1905	Mg 41	N 164	O 205	0
14	G	1	Total 2315	C 1905	Mg 41	N 164	O 205	0
14	G	1	Total 2315	C 1905	Mg 41	N 164	O 205	0
14	G	1	Total 2315	C 1905	Mg 41	N 164	O 205	0
14	G	1	Total 2315	C 1905	Mg 41	N 164	O 205	0
14	G	1	Total 2315	C 1905	Mg 41	N 164	O 205	0
14	G	1	Total 2315	C 1905	Mg 41	N 164	O 205	0
14	G	1	Total 2315	C 1905	Mg 41	N 164	O 205	0
14	G	1	Total 2315	C 1905	Mg 41	N 164	O 205	0
14	G	1	Total 2315	C 1905	Mg 41	N 164	O 205	0
14	G	1	Total 2315	C 1905	Mg 41	N 164	O 205	0
14	G	1	Total 2315	C 1905	Mg 41	N 164	O 205	0

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Mol	Chain	Residues	Atoms	AltConf
14	G	1	Total C Mg N O 2315 1905 41 164 205	0
14	G	1	Total C Mg N O 2315 1905 41 164 205	0
14	G	1	Total C Mg N O 2315 1905 41 164 205	0
14	G	1	Total C Mg N O 2315 1905 41 164 205	0
14	G	1	Total C Mg N O 2315 1905 41 164 205	0
14	G	1	Total C Mg N O 2315 1905 41 164 205	0
14	H	1	Total C Mg N O 2220 1840 38 152 190	0
14	H	1	Total C Mg N O 2220 1840 38 152 190	0
14	H	1	Total C Mg N O 2220 1840 38 152 190	0
14	H	1	Total C Mg N O 2220 1840 38 152 190	0
14	H	1	Total C Mg N O 2220 1840 38 152 190	0
14	H	1	Total C Mg N O 2220 1840 38 152 190	0
14	H	1	Total C Mg N O 2220 1840 38 152 190	0
14	H	1	Total C Mg N O 2220 1840 38 152 190	0
14	H	1	Total C Mg N O 2220 1840 38 152 190	0
14	H	1	Total C Mg N O 2220 1840 38 152 190	0
14	H	1	Total C Mg N O 2220 1840 38 152 190	0
14	H	1	Total C Mg N O 2220 1840 38 152 190	0
14	H	1	Total C Mg N O 2220 1840 38 152 190	0
14	H	1	Total C Mg N O 2220 1840 38 152 190	0
14	H	1	Total C Mg N O 2220 1840 38 152 190	0

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Mol	Chain	Residues	Atoms					AltConf
14	H	1	Total 2220	C 1840	Mg 38	N 152	O 190	0
14	H	1	Total 2220	C 1840	Mg 38	N 152	O 190	0
14	H	1	Total 2220	C 1840	Mg 38	N 152	O 190	0
14	H	1	Total 2220	C 1840	Mg 38	N 152	O 190	0
14	H	1	Total 2220	C 1840	Mg 38	N 152	O 190	0
14	H	1	Total 2220	C 1840	Mg 38	N 152	O 190	0
14	H	1	Total 2220	C 1840	Mg 38	N 152	O 190	0
14	H	1	Total 2220	C 1840	Mg 38	N 152	O 190	0
14	H	1	Total 2220	C 1840	Mg 38	N 152	O 190	0
14	H	1	Total 2220	C 1840	Mg 38	N 152	O 190	0
14	H	1	Total 2220	C 1840	Mg 38	N 152	O 190	0
14	H	1	Total 2220	C 1840	Mg 38	N 152	O 190	0
14	H	1	Total 2220	C 1840	Mg 38	N 152	O 190	0
14	H	1	Total 2220	C 1840	Mg 38	N 152	O 190	0
14	H	1	Total 2220	C 1840	Mg 38	N 152	O 190	0
14	H	1	Total 2220	C 1840	Mg 38	N 152	O 190	0
14	H	1	Total 2220	C 1840	Mg 38	N 152	O 190	0
14	H	1	Total 2220	C 1840	Mg 38	N 152	O 190	0
14	H	1	Total 2220	C 1840	Mg 38	N 152	O 190	0
14	H	1	Total 2220	C 1840	Mg 38	N 152	O 190	0
14	H	1	Total 2220	C 1840	Mg 38	N 152	O 190	0

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Mol	Chain	Residues	Atoms	AltConf
14	H	1	Total C Mg N O 2220 1840 38 152 190	0
14	H	1	Total C Mg N O 2220 1840 38 152 190	0
14	T	1	Total C Mg N O 45 35 1 4 5	0
14	U	1	Total C Mg N O 190 160 3 12 15	0
14	U	1	Total C Mg N O 190 160 3 12 15	0
14	U	1	Total C Mg N O 190 160 3 12 15	0
14	W	1	Total C Mg N O 55 45 1 4 5	0
14	a	1	Total C Mg N O 2315 1905 41 164 205	0
14	a	1	Total C Mg N O 2315 1905 41 164 205	0
14	a	1	Total C Mg N O 2315 1905 41 164 205	0
14	a	1	Total C Mg N O 2315 1905 41 164 205	0
14	a	1	Total C Mg N O 2315 1905 41 164 205	0
14	a	1	Total C Mg N O 2315 1905 41 164 205	0
14	a	1	Total C Mg N O 2315 1905 41 164 205	0
14	a	1	Total C Mg N O 2315 1905 41 164 205	0
14	a	1	Total C Mg N O 2315 1905 41 164 205	0
14	a	1	Total C Mg N O 2315 1905 41 164 205	0
14	a	1	Total C Mg N O 2315 1905 41 164 205	0
14	a	1	Total C Mg N O 2315 1905 41 164 205	0
14	a	1	Total C Mg N O 2315 1905 41 164 205	0
14	a	1	Total C Mg N O 2315 1905 41 164 205	0

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Mol	Chain	Residues	Atoms	AltConf
14	a	1	Total C Mg N O 2315 1905 41 164 205	0
14	a	1	Total C Mg N O 2315 1905 41 164 205	0
14	a	1	Total C Mg N O 2315 1905 41 164 205	0
14	a	1	Total C Mg N O 2315 1905 41 164 205	0
14	a	1	Total C Mg N O 2315 1905 41 164 205	0
14	a	1	Total C Mg N O 2315 1905 41 164 205	0
14	a	1	Total C Mg N O 2315 1905 41 164 205	0
14	a	1	Total C Mg N O 2315 1905 41 164 205	0
14	a	1	Total C Mg N O 2315 1905 41 164 205	0
14	a	1	Total C Mg N O 2315 1905 41 164 205	0
14	a	1	Total C Mg N O 2315 1905 41 164 205	0
14	a	1	Total C Mg N O 2315 1905 41 164 205	0
14	a	1	Total C Mg N O 2315 1905 41 164 205	0
14	a	1	Total C Mg N O 2315 1905 41 164 205	0
14	a	1	Total C Mg N O 2315 1905 41 164 205	0
14	a	1	Total C Mg N O 2315 1905 41 164 205	0
14	a	1	Total C Mg N O 2315 1905 41 164 205	0
14	a	1	Total C Mg N O 2315 1905 41 164 205	0
14	a	1	Total C Mg N O 2315 1905 41 164 205	0
14	a	1	Total C Mg N O 2315 1905 41 164 205	0
14	a	1	Total C Mg N O 2315 1905 41 164 205	0

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Mol	Chain	Residues	Atoms	AltConf
14	a	1	Total C Mg N O 2315 1905 41 164 205	0
14	a	1	Total C Mg N O 2315 1905 41 164 205	0
14	a	1	Total C Mg N O 2315 1905 41 164 205	0
14	a	1	Total C Mg N O 2315 1905 41 164 205	0
14	a	1	Total C Mg N O 2315 1905 41 164 205	0
14	a	1	Total C Mg N O 2315 1905 41 164 205	0
14	b	1	Total C Mg N O 2220 1840 38 152 190	0
14	b	1	Total C Mg N O 2220 1840 38 152 190	0
14	b	1	Total C Mg N O 2220 1840 38 152 190	0
14	b	1	Total C Mg N O 2220 1840 38 152 190	0
14	b	1	Total C Mg N O 2220 1840 38 152 190	0
14	b	1	Total C Mg N O 2220 1840 38 152 190	0
14	b	1	Total C Mg N O 2220 1840 38 152 190	0
14	b	1	Total C Mg N O 2220 1840 38 152 190	0
14	b	1	Total C Mg N O 2220 1840 38 152 190	0
14	b	1	Total C Mg N O 2220 1840 38 152 190	0
14	b	1	Total C Mg N O 2220 1840 38 152 190	0
14	b	1	Total C Mg N O 2220 1840 38 152 190	0
14	b	1	Total C Mg N O 2220 1840 38 152 190	0
14	b	1	Total C Mg N O 2220 1840 38 152 190	0
14	b	1	Total C Mg N O 2220 1840 38 152 190	0

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Mol	Chain	Residues	Atoms	AltConf
14	b	1	Total C Mg N O 2220 1840 38 152 190	0
14	b	1	Total C Mg N O 2220 1840 38 152 190	0
14	b	1	Total C Mg N O 2220 1840 38 152 190	0
14	b	1	Total C Mg N O 2220 1840 38 152 190	0
14	b	1	Total C Mg N O 2220 1840 38 152 190	0
14	b	1	Total C Mg N O 2220 1840 38 152 190	0
14	b	1	Total C Mg N O 2220 1840 38 152 190	0
14	b	1	Total C Mg N O 2220 1840 38 152 190	0
14	b	1	Total C Mg N O 2220 1840 38 152 190	0
14	b	1	Total C Mg N O 2220 1840 38 152 190	0
14	b	1	Total C Mg N O 2220 1840 38 152 190	0
14	b	1	Total C Mg N O 2220 1840 38 152 190	0
14	b	1	Total C Mg N O 2220 1840 38 152 190	0
14	b	1	Total C Mg N O 2220 1840 38 152 190	0
14	b	1	Total C Mg N O 2220 1840 38 152 190	0
14	b	1	Total C Mg N O 2220 1840 38 152 190	0
14	b	1	Total C Mg N O 2220 1840 38 152 190	0
14	b	1	Total C Mg N O 2220 1840 38 152 190	0
14	b	1	Total C Mg N O 2220 1840 38 152 190	0
14	b	1	Total C Mg N O 2220 1840 38 152 190	0
14	b	1	Total C Mg N O 2220 1840 38 152 190	0

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Mol	Chain	Residues	Atoms	AltConf
14	b	1	Total C Mg N O 2220 1840 38 152 190	0
14	b	1	Total C Mg N O 2220 1840 38 152 190	0
14	k	1	Total C Mg N O 45 35 1 4 5	0
14	l	1	Total C Mg N O 190 160 3 12 15	0
14	l	1	Total C Mg N O 190 160 3 12 15	0
14	l	1	Total C Mg N O 190 160 3 12 15	0
14	x	1	Total C Mg N O 55 45 1 4 5	0
14	A	1	Total C Mg N O 2315 1905 41 164 205	0
14	A	1	Total C Mg N O 2315 1905 41 164 205	0
14	A	1	Total C Mg N O 2315 1905 41 164 205	0
14	A	1	Total C Mg N O 2315 1905 41 164 205	0
14	A	1	Total C Mg N O 2315 1905 41 164 205	0
14	A	1	Total C Mg N O 2315 1905 41 164 205	0
14	A	1	Total C Mg N O 2315 1905 41 164 205	0
14	A	1	Total C Mg N O 2315 1905 41 164 205	0
14	A	1	Total C Mg N O 2315 1905 41 164 205	0
14	A	1	Total C Mg N O 2315 1905 41 164 205	0
14	A	1	Total C Mg N O 2315 1905 41 164 205	0
14	A	1	Total C Mg N O 2315 1905 41 164 205	0
14	A	1	Total C Mg N O 2315 1905 41 164 205	0
14	A	1	Total C Mg N O 2315 1905 41 164 205	0

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Mol	Chain	Residues	Atoms	AltConf
14	A	1	Total C Mg N O 2315 1905 41 164 205	0
14	A	1	Total C Mg N O 2315 1905 41 164 205	0
14	A	1	Total C Mg N O 2315 1905 41 164 205	0
14	A	1	Total C Mg N O 2315 1905 41 164 205	0
14	A	1	Total C Mg N O 2315 1905 41 164 205	0
14	A	1	Total C Mg N O 2315 1905 41 164 205	0
14	A	1	Total C Mg N O 2315 1905 41 164 205	0
14	A	1	Total C Mg N O 2315 1905 41 164 205	0
14	A	1	Total C Mg N O 2315 1905 41 164 205	0
14	A	1	Total C Mg N O 2315 1905 41 164 205	0
14	A	1	Total C Mg N O 2315 1905 41 164 205	0
14	A	1	Total C Mg N O 2315 1905 41 164 205	0
14	A	1	Total C Mg N O 2315 1905 41 164 205	0
14	A	1	Total C Mg N O 2315 1905 41 164 205	0
14	A	1	Total C Mg N O 2315 1905 41 164 205	0
14	A	1	Total C Mg N O 2315 1905 41 164 205	0
14	A	1	Total C Mg N O 2315 1905 41 164 205	0
14	A	1	Total C Mg N O 2315 1905 41 164 205	0
14	A	1	Total C Mg N O 2315 1905 41 164 205	0
14	A	1	Total C Mg N O 2315 1905 41 164 205	0
14	A	1	Total C Mg N O 2315 1905 41 164 205	0

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Mol	Chain	Residues	Atoms	AltConf
14	A	1	Total C Mg N O 2315 1905 41 164 205	0
14	A	1	Total C Mg N O 2315 1905 41 164 205	0
14	A	1	Total C Mg N O 2315 1905 41 164 205	0
14	A	1	Total C Mg N O 2315 1905 41 164 205	0
14	A	1	Total C Mg N O 2315 1905 41 164 205	0
14	A	1	Total C Mg N O 2315 1905 41 164 205	0
14	B	1	Total C Mg N O 2220 1840 38 152 190	0
14	B	1	Total C Mg N O 2220 1840 38 152 190	0
14	B	1	Total C Mg N O 2220 1840 38 152 190	0
14	B	1	Total C Mg N O 2220 1840 38 152 190	0
14	B	1	Total C Mg N O 2220 1840 38 152 190	0
14	B	1	Total C Mg N O 2220 1840 38 152 190	0
14	B	1	Total C Mg N O 2220 1840 38 152 190	0
14	B	1	Total C Mg N O 2220 1840 38 152 190	0
14	B	1	Total C Mg N O 2220 1840 38 152 190	0
14	B	1	Total C Mg N O 2220 1840 38 152 190	0
14	B	1	Total C Mg N O 2220 1840 38 152 190	0
14	B	1	Total C Mg N O 2220 1840 38 152 190	0
14	B	1	Total C Mg N O 2220 1840 38 152 190	0
14	B	1	Total C Mg N O 2220 1840 38 152 190	0
14	B	1	Total C Mg N O 2220 1840 38 152 190	0

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Mol	Chain	Residues	Atoms	AltConf
14	B	1	Total C Mg N O 2220 1840 38 152 190	0
14	B	1	Total C Mg N O 2220 1840 38 152 190	0
14	B	1	Total C Mg N O 2220 1840 38 152 190	0
14	B	1	Total C Mg N O 2220 1840 38 152 190	0
14	B	1	Total C Mg N O 2220 1840 38 152 190	0
14	B	1	Total C Mg N O 2220 1840 38 152 190	0
14	B	1	Total C Mg N O 2220 1840 38 152 190	0
14	B	1	Total C Mg N O 2220 1840 38 152 190	0
14	B	1	Total C Mg N O 2220 1840 38 152 190	0
14	B	1	Total C Mg N O 2220 1840 38 152 190	0
14	B	1	Total C Mg N O 2220 1840 38 152 190	0
14	B	1	Total C Mg N O 2220 1840 38 152 190	0
14	B	1	Total C Mg N O 2220 1840 38 152 190	0
14	B	1	Total C Mg N O 2220 1840 38 152 190	0
14	B	1	Total C Mg N O 2220 1840 38 152 190	0
14	B	1	Total C Mg N O 2220 1840 38 152 190	0
14	B	1	Total C Mg N O 2220 1840 38 152 190	0
14	B	1	Total C Mg N O 2220 1840 38 152 190	0
14	B	1	Total C Mg N O 2220 1840 38 152 190	0
14	B	1	Total C Mg N O 2220 1840 38 152 190	0
14	B	1	Total C Mg N O 2220 1840 38 152 190	0

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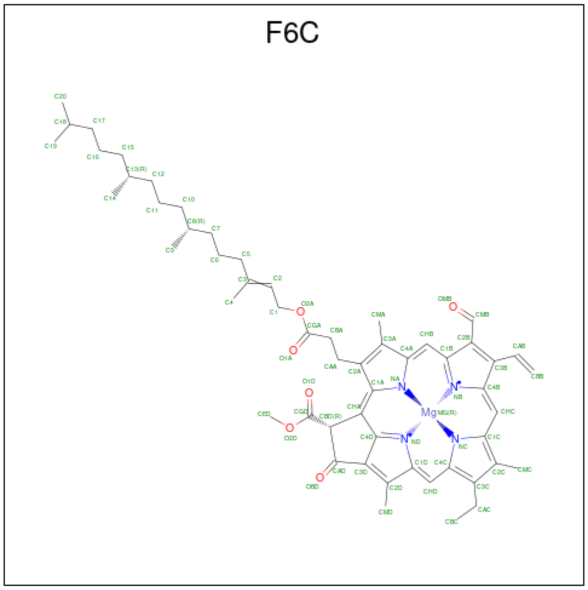
Mol	Chain	Residues	Atoms	AltConf
14	B	1	Total C Mg N O 2220 1840 38 152 190	0
14	B	1	Total C Mg N O 2220 1840 38 152 190	0
14	K	1	Total C Mg N O 45 35 1 4 5	0
14	L	1	Total C Mg N O 190 160 3 12 15	0
14	L	1	Total C Mg N O 190 160 3 12 15	0
14	L	1	Total C Mg N O 190 160 3 12 15	0
14	X	1	Total C Mg N O 55 45 1 4 5	0

- Molecule 15 is Chlorophyll F (three-letter code: F6C) (formula: $C_{55}H_{68}MgN_4O_6$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	AltConf
15	G	1	Total C Mg N O 46 35 1 4 6	0
15	H	1	Total C Mg N O 244 200 4 16 24	0
15	H	1	Total C Mg N O 244 200 4 16 24	0
15	H	1	Total C Mg N O 244 200 4 16 24	0

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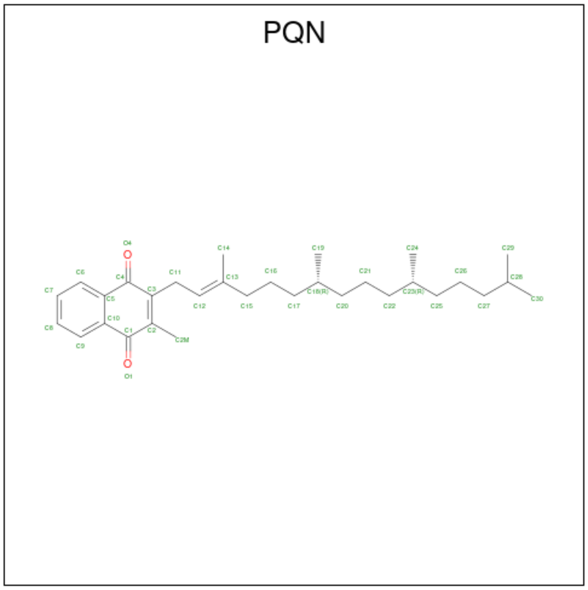
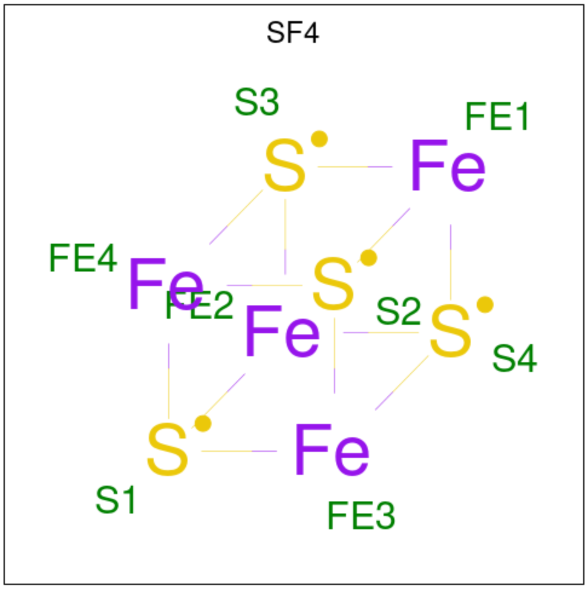
Mol	Chain	Residues	Atoms	AltConf
15	H	1	Total C Mg N O 244 200 4 16 24	0
15	a	1	Total C Mg N O 46 35 1 4 6	0
15	b	1	Total C Mg N O 244 200 4 16 24	0
15	b	1	Total C Mg N O 244 200 4 16 24	0
15	b	1	Total C Mg N O 244 200 4 16 24	0
15	b	1	Total C Mg N O 244 200 4 16 24	0
15	A	1	Total C Mg N O 46 35 1 4 6	0
15	B	1	Total C Mg N O 244 200 4 16 24	0
15	B	1	Total C Mg N O 244 200 4 16 24	0
15	B	1	Total C Mg N O 244 200 4 16 24	0
15	B	1	Total C Mg N O 244 200 4 16 24	0

- Molecule 16 is PHYLLOQUINONE (three-letter code: PQN) (formula: $C_{31}H_{46}O_2$).



Mol	Chain	Residues	Atoms	AltConf
16	G	1	Total C O 33 31 2	0
16	H	1	Total C O 33 31 2	0
16	a	1	Total C O 33 31 2	0
16	b	1	Total C O 33 31 2	0
16	A	1	Total C O 33 31 2	0
16	B	1	Total C O 33 31 2	0

- Molecule 17 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe_4S_4).



Mol	Chain	Residues	Atoms	AltConf
17	G	1	Total Fe S 8 4 4	0
17	N	1	Total Fe S 16 8 8	0
17	N	1	Total Fe S 16 8 8	0
17	a	1	Total Fe S 8 4 4	0
17	c	1	Total Fe S 16 8 8	0
17	c	1	Total Fe S 16 8 8	0

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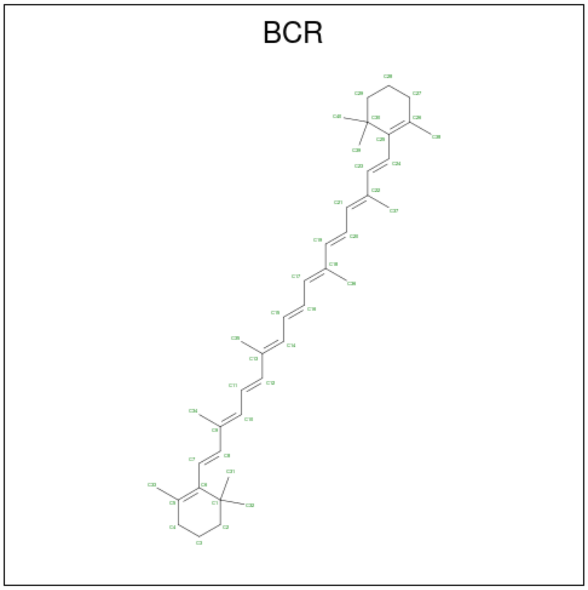
Mol	Chain	Residues	Atoms	AltConf
17	A	1	Total Fe S 8 4 4	0
17	C	1	Total Fe S 16 8 8	0
17	C	1	Total Fe S 16 8 8	0

- Molecule 18 is BETA-CAROTENE (three-letter code: BCR) (formula: $C_{40}H_{56}$).



Mol	Chain	Residues	Atoms	AltConf
18	G	1	Total C 240 240	0
18	G	1	Total C 240 240	0
18	G	1	Total C 240 240	0
18	G	1	Total C 240 240	0
18	G	1	Total C 240 240	0
18	G	1	Total C 240 240	0
18	H	1	Total C 360 360	0
18	H	1	Total C 360 360	0

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Mol	Chain	Residues	Atoms	AltConf
18	H	1	Total C 360 360	0
18	H	1	Total C 360 360	0
18	H	1	Total C 360 360	0
18	H	1	Total C 360 360	0
18	H	1	Total C 360 360	0
18	H	1	Total C 360 360	0
18	H	1	Total C 360 360	0
18	R	1	Total C 80 80	0
18	R	1	Total C 80 80	0
18	U	1	Total C 80 80	0
18	U	1	Total C 80 80	0
18	V	1	Total C 40 40	0
18	a	1	Total C 240 240	0
18	a	1	Total C 240 240	0
18	a	1	Total C 240 240	0
18	a	1	Total C 240 240	0
18	a	1	Total C 240 240	0
18	a	1	Total C 240 240	0
18	b	1	Total C 360 360	0
18	b	1	Total C 360 360	0
18	b	1	Total C 360 360	0

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Mol	Chain	Residues	Atoms	AltConf
18	b	1	Total C 360 360	0
18	b	1	Total C 360 360	0
18	b	1	Total C 360 360	0
18	b	1	Total C 360 360	0
18	b	1	Total C 360 360	0
18	b	1	Total C 360 360	0
18	i	1	Total C 80 80	0
18	i	1	Total C 80 80	0
18	l	1	Total C 80 80	0
18	l	1	Total C 80 80	0
18	m	1	Total C 40 40	0
18	A	1	Total C 240 240	0
18	A	1	Total C 240 240	0
18	A	1	Total C 240 240	0
18	A	1	Total C 240 240	0
18	A	1	Total C 240 240	0
18	A	1	Total C 240 240	0
18	B	1	Total C 360 360	0
18	B	1	Total C 360 360	0
18	B	1	Total C 360 360	0
18	B	1	Total C 360 360	0

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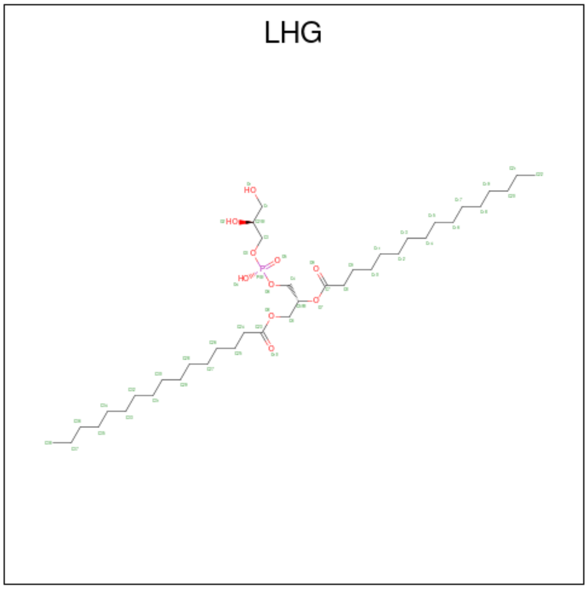
Mol	Chain	Residues	Atoms	AltConf
18	B	1	Total C 360 360	0
18	B	1	Total C 360 360	0
18	B	1	Total C 360 360	0
18	B	1	Total C 360 360	0
18	B	1	Total C 360 360	0
18	I	1	Total C 80 80	0
18	I	1	Total C 80 80	0
18	L	1	Total C 80 80	0
18	L	1	Total C 80 80	0
18	M	1	Total C 40 40	0

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



Mol	Chain	Residues	Atoms	AltConf
19	G	1	Total C O P 42 31 10 1	0

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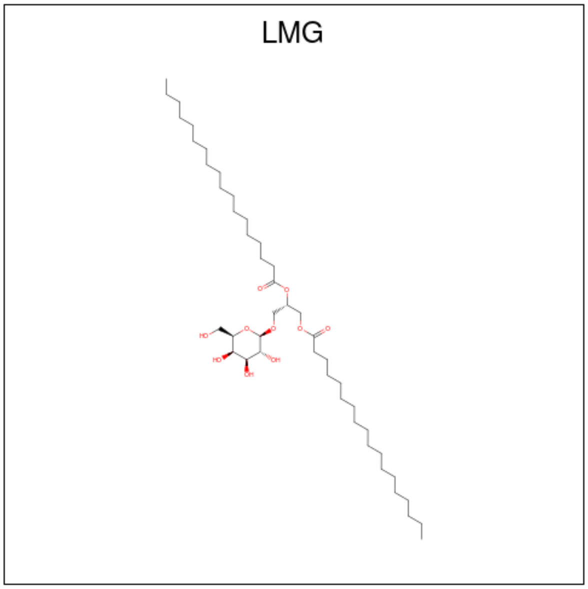
Mol	Chain	Residues	Atoms	AltConf
19	H	1	Total C O P 44 33 10 1	0
19	a	1	Total C O P 42 31 10 1	0
19	b	1	Total C O P 44 33 10 1	0
19	A	1	Total C O P 42 31 10 1	0
19	B	1	Total C O P 44 33 10 1	0

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



Mol	Chain	Residues	Atoms	AltConf
20	G	1	Total C O 46 36 10	0
20	H	1	Total C O 46 36 10	0
20	R	1	Total C O 37 27 10	0
20	U	1	Total C O 50 40 10	0
20	a	1	Total C O 46 36 10	0
20	b	1	Total C O 46 36 10	0

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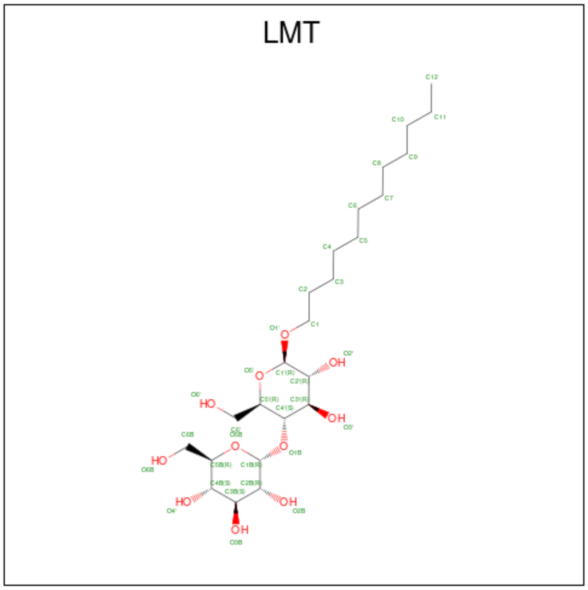
Mol	Chain	Residues	Atoms	AltConf
20	i	1	Total C O 37 27 10	0
20	l	1	Total C O 50 40 10	0
20	A	1	Total C O 46 36 10	0
20	B	1	Total C O 46 36 10	0
20	I	1	Total C O 37 27 10	0
20	L	1	Total C O 50 40 10	0

- Molecule 21 is DODECYL-BETA-D-MALTOSIDE (three-letter code: LMT) (formula: $C_{24}H_{46}O_{11}$).



Mol	Chain	Residues	Atoms	AltConf
21	G	1	Total C O 59 37 22	0
21	G	1	Total C O 59 37 22	0
21	a	1	Total C O 59 37 22	0
21	a	1	Total C O 59 37 22	0
21	A	1	Total C O 59 37 22	0

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Mol	Chain	Residues	Atoms	AltConf
21	A	1	Total C O 59 37 22	0

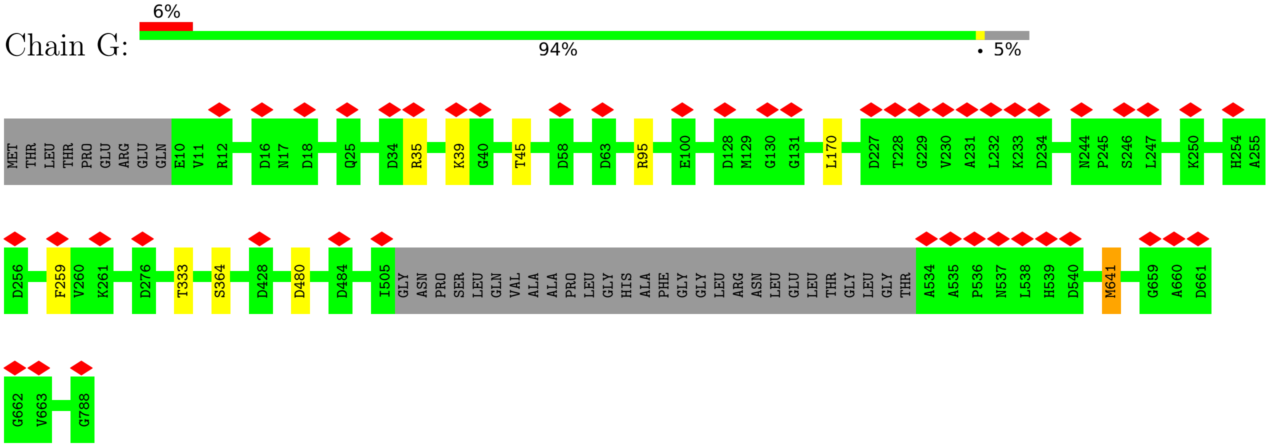
- Molecule 22 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms	AltConf
22	U	1	Total Ca 1 1	0
22	l	1	Total Ca 1 1	0
22	L	1	Total Ca 1 1	0

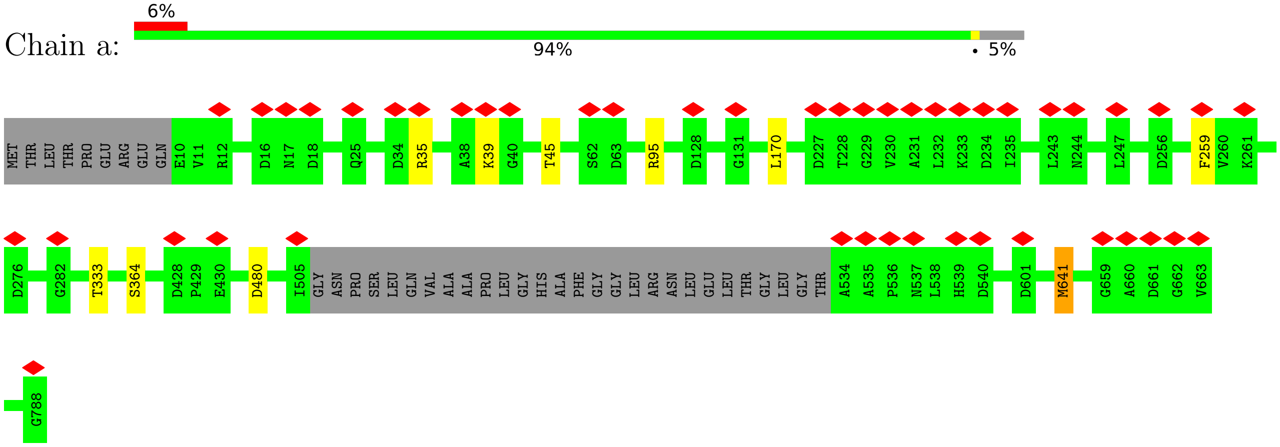
3 Residue-property plots ⓘ

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.

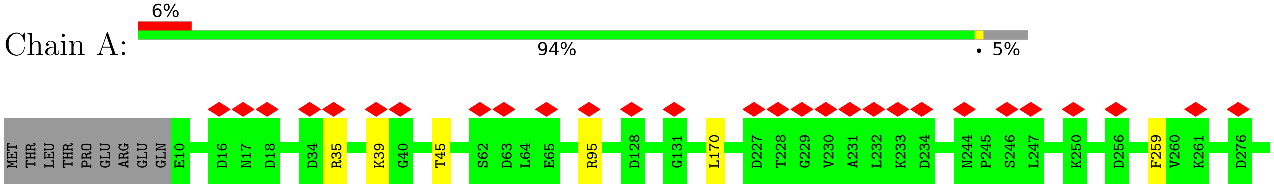
- Molecule 1: Photosystem I P700 chlorophyll a apoprotein A1

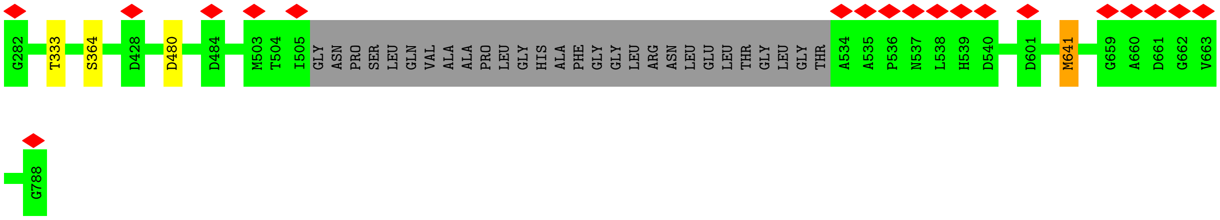


- Molecule 1: Photosystem I P700 chlorophyll a apoprotein A1



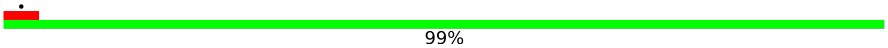
- Molecule 1: Photosystem I P700 chlorophyll a apoprotein A1

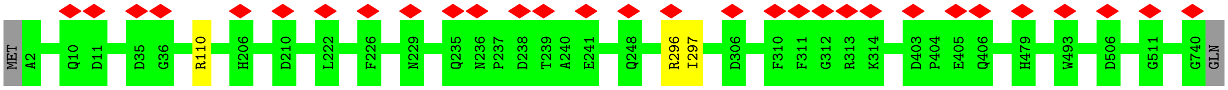




- Molecule 2: Photosystem I P700 chlorophyll a apoprotein A2

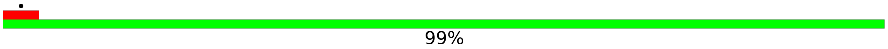
Chain H:

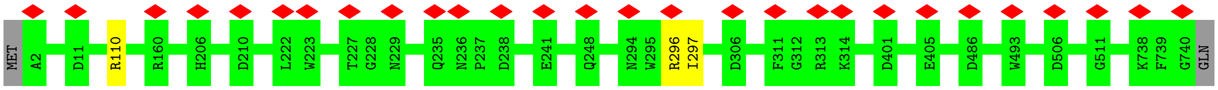




- Molecule 2: Photosystem I P700 chlorophyll a apoprotein A2

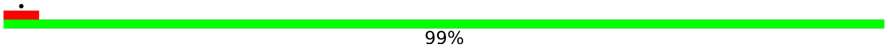
Chain b:

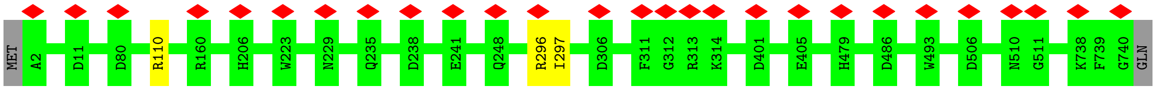




- Molecule 2: Photosystem I P700 chlorophyll a apoprotein A2

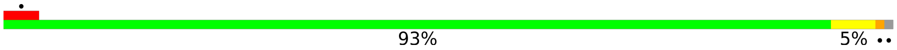
Chain B:

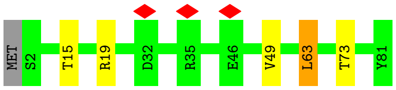




- Molecule 3: Photosystem I iron-sulfur center

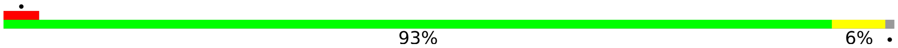
Chain N:

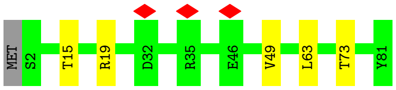




- Molecule 3: Photosystem I iron-sulfur center

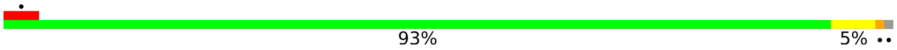
Chain c:

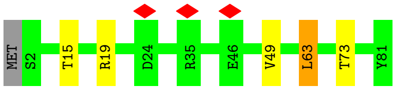




- Molecule 3: Photosystem I iron-sulfur center

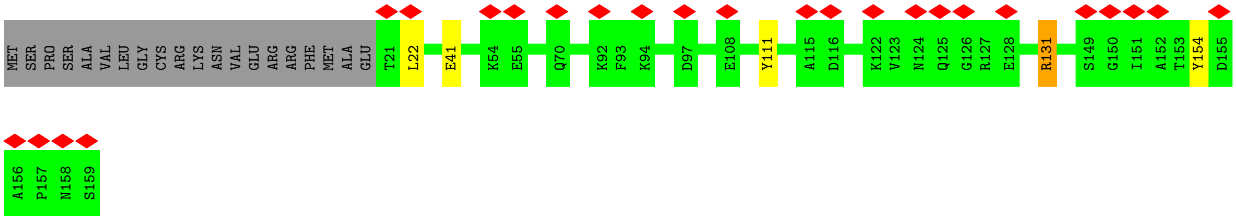
Chain C:





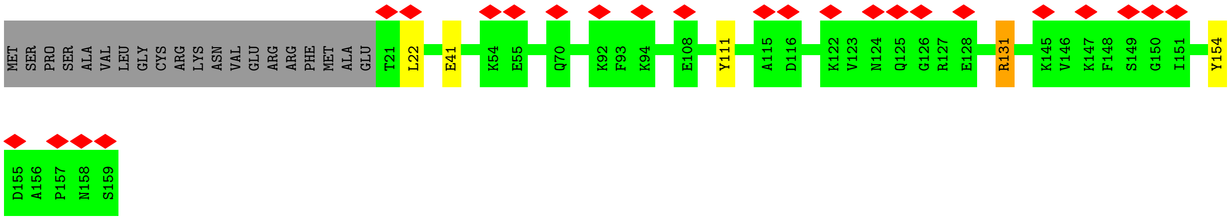
- Molecule 4: Photosystem I protein PsaD

Chain O:



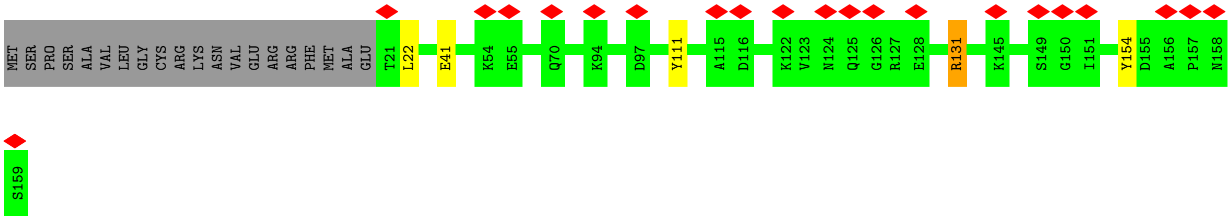
- Molecule 4: Photosystem I protein PsaD

Chain d:



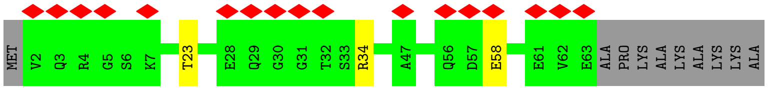
- Molecule 4: Photosystem I protein PsaD

Chain D:



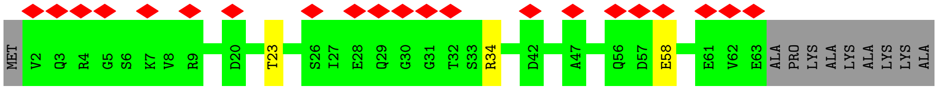
- Molecule 5: Photosystem I reaction center subunit IV

Chain P:



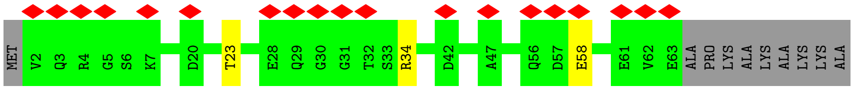
- Molecule 5: Photosystem I reaction center subunit IV

Chain e:



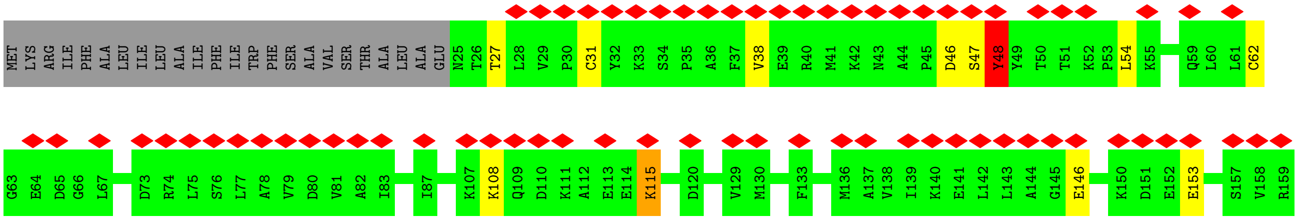
- Molecule 5: Photosystem I reaction center subunit IV

Chain E:



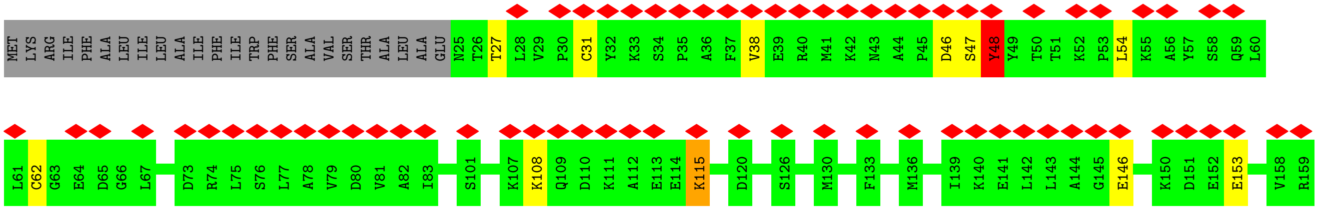
- Molecule 6: Photosystem I reaction center protein PsaF subunit III

Chain Q:



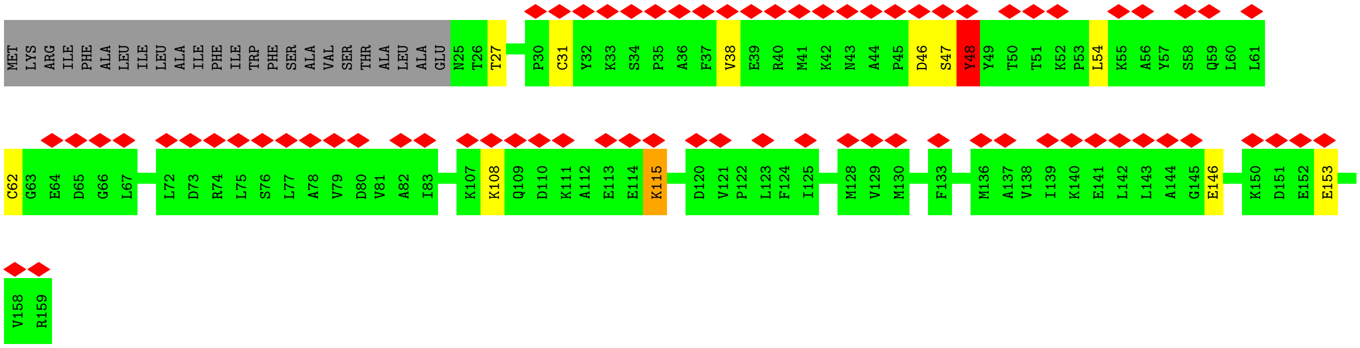
- Molecule 6: Photosystem I reaction center protein PsaF subunit III

Chain f:

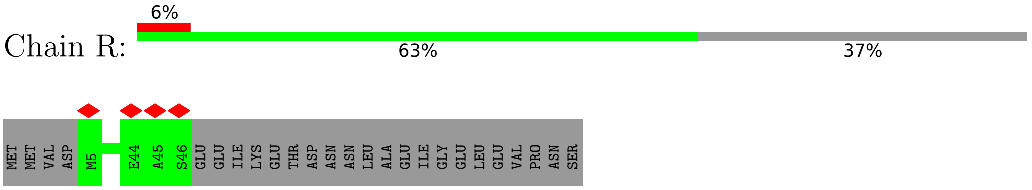


- Molecule 6: Photosystem I reaction center protein PsaF subunit III

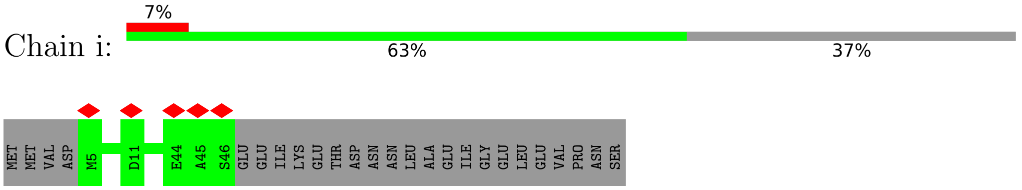
Chain F:



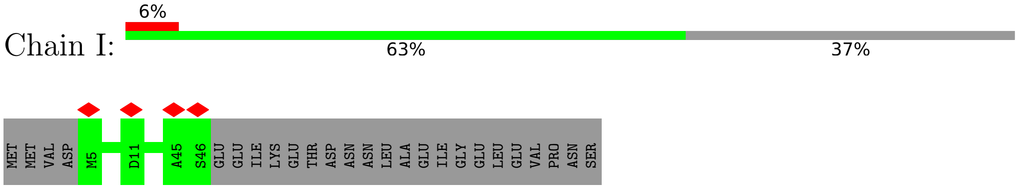
- Molecule 7: photosystem I subunit VIII



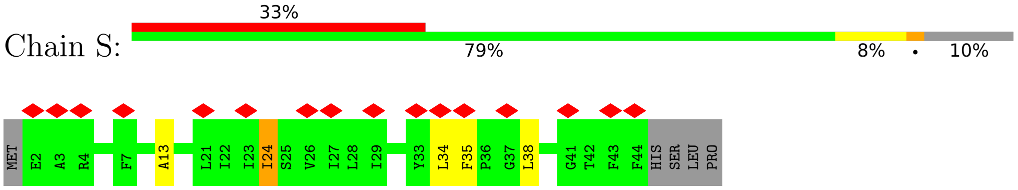
- Molecule 7: photosystem I subunit VIII



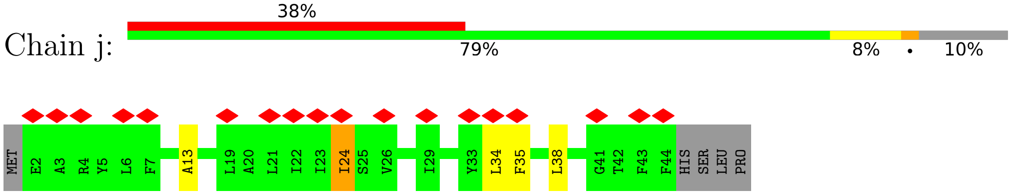
- Molecule 7: photosystem I subunit VIII



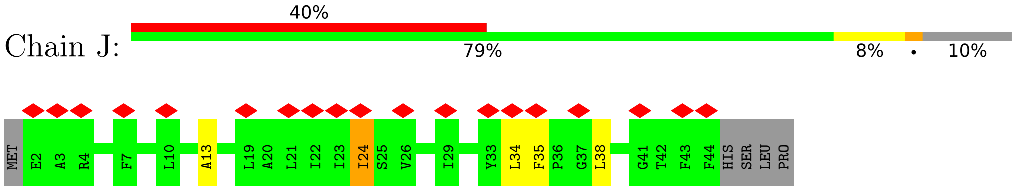
- Molecule 8: Photosystem I reaction centre subunit IX / PsaJ



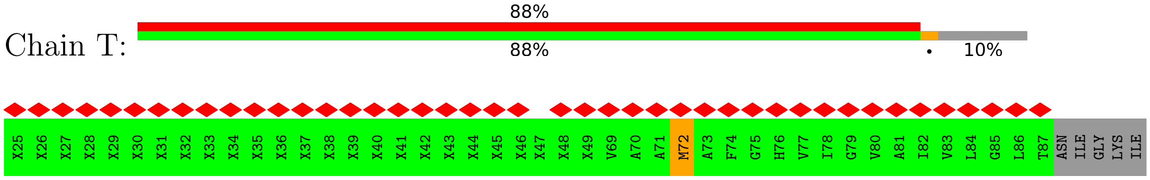
- Molecule 8: Photosystem I reaction centre subunit IX / PsaJ



- Molecule 8: Photosystem I reaction centre subunit IX / PsaJ

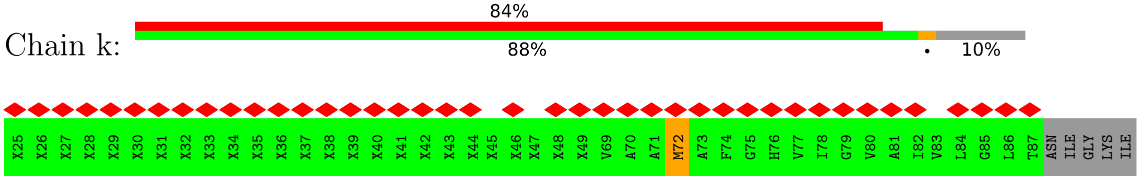


- Molecule 9: Photosystem I reaction center subunit PsaK



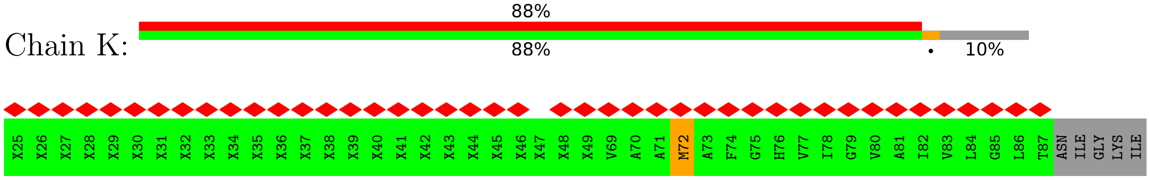
- Molecule 9: Photosystem I reaction center subunit PsaK

Chain k:



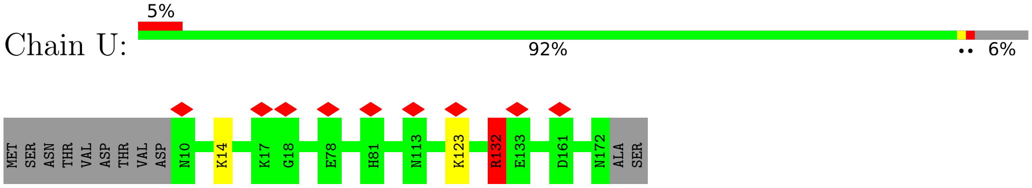
- Molecule 9: Photosystem I reaction center subunit PsaK

Chain K:



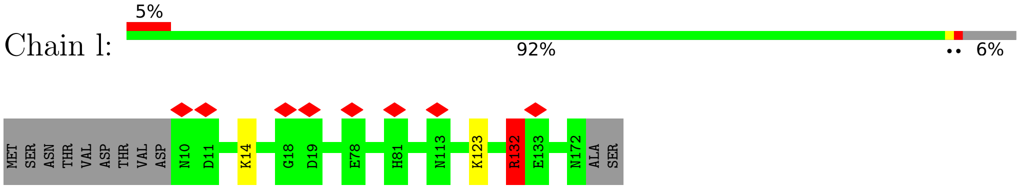
- Molecule 10: PSI subunit V

Chain U:



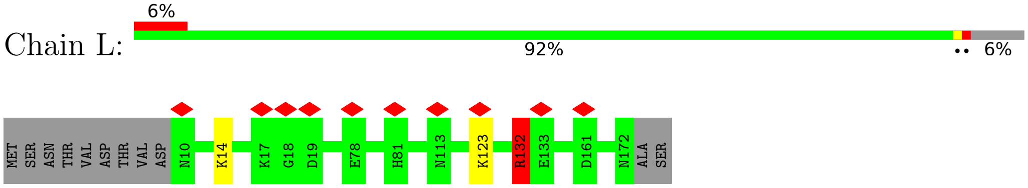
- Molecule 10: PSI subunit V

Chain l:



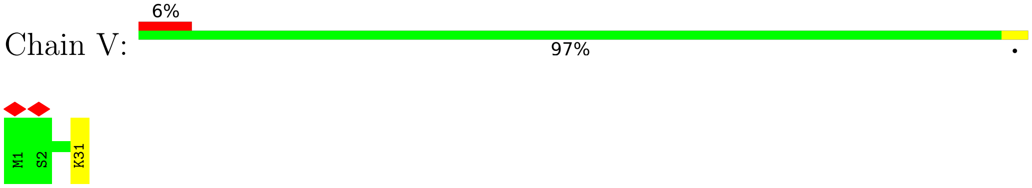
- Molecule 10: PSI subunit V

Chain L:



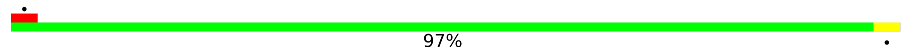
- Molecule 11: Photosystem I reaction center subunit XII

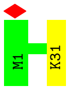
Chain V:



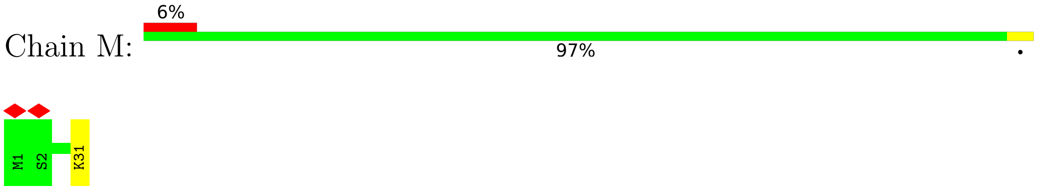
- Molecule 11: Photosystem I reaction center subunit XII

Chain m:

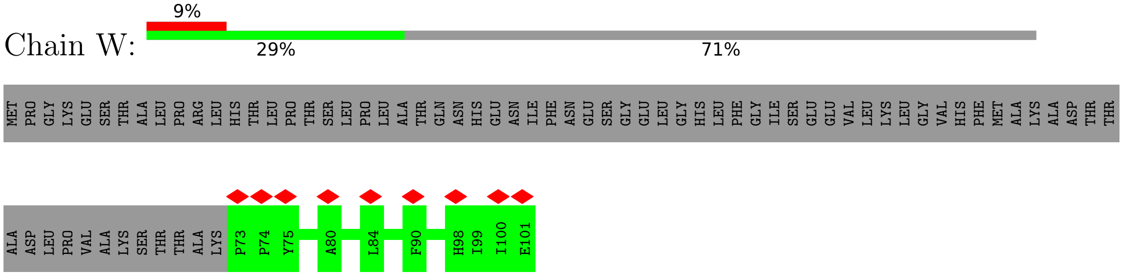




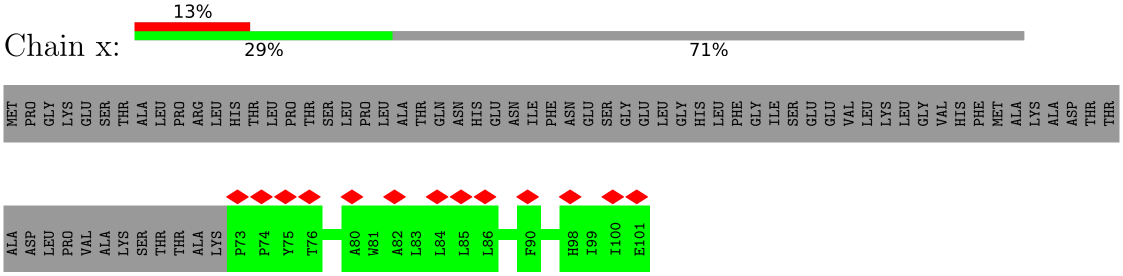
- Molecule 11: Photosystem I reaction center subunit XII



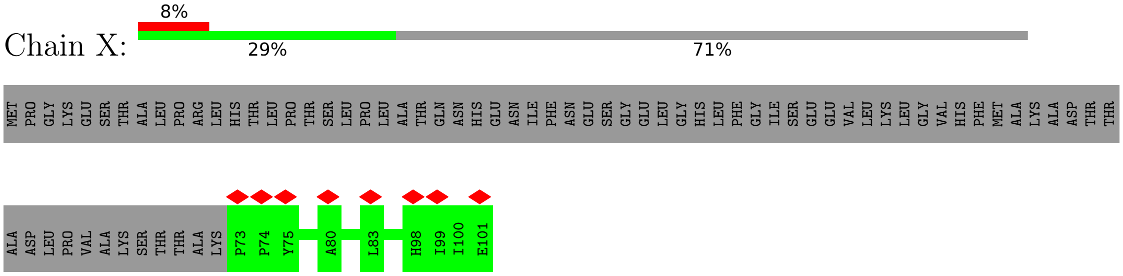
- Molecule 12: Photosystem one PsaX



- Molecule 12: Photosystem one PsaX



- Molecule 12: Photosystem one PsaX



4 Experimental information ⓘ

Property	**Value**	**Source**
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	201104	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose $(e^-/\text{Å}^2)$	57.328	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.324	Depositor
Minimum map value	-0.155	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.011	Depositor
Recommended contour level	0.055	Depositor
Map size (Å)	381.6013, 381.6013, 381.6013	wwPDB
Map dimensions	256, 256, 256	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.49063, 1.49063, 1.49063	Depositor

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: LMG, CA, CL0, PQN, F6C, BCR, SF4, LHG, LMT, CLA

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	0.54	0/6138	0.55	1/8362 (0.0%)
1	G	0.54	0/6138	0.55	1/8362 (0.0%)
1	a	0.54	0/6138	0.55	1/8362 (0.0%)
2	B	0.57	0/6135	0.54	0/8385
2	H	0.57	0/6135	0.54	0/8385
2	b	0.57	0/6135	0.54	0/8385
3	C	0.62	0/611	0.77	1/828 (0.1%)
3	N	0.62	0/611	0.77	1/828 (0.1%)
3	c	0.62	0/611	0.77	1/828 (0.1%)
4	D	0.49	0/1116	0.64	1/1505 (0.1%)
4	O	0.49	0/1116	0.64	1/1505 (0.1%)
4	d	0.49	0/1116	0.64	1/1505 (0.1%)
5	E	0.48	0/506	0.59	0/686
5	P	0.48	0/506	0.59	0/686
5	e	0.48	0/506	0.59	0/686
6	F	0.45	0/1084	0.74	2/1470 (0.1%)
6	Q	0.45	0/1084	0.74	2/1470 (0.1%)
6	f	0.45	0/1084	0.74	2/1470 (0.1%)
7	I	0.59	0/365	0.72	0/502
7	R	0.59	0/365	0.72	0/502
7	i	0.59	0/365	0.72	0/502
8	J	0.37	0/353	0.78	1/482 (0.2%)
8	S	0.36	0/353	0.78	1/482 (0.2%)
8	j	0.37	0/353	0.78	1/482 (0.2%)
9	K	0.31	0/129	1.21	3/175 (1.7%)
9	T	0.31	0/129	1.21	3/175 (1.7%)
9	k	0.31	0/129	1.21	3/175 (1.7%)
10	L	0.56	0/1255	0.84	5/1702 (0.3%)
10	U	0.56	0/1255	0.84	5/1702 (0.3%)
10	l	0.56	0/1255	0.84	5/1702 (0.3%)
11	M	0.45	0/250	0.64	0/340
11	V	0.45	0/250	0.64	0/340

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
11	m	0.45	0/250	0.64	0/340
12	W	0.40	0/256	0.47	0/350
12	X	0.40	0/256	0.47	0/350
12	x	0.39	0/256	0.47	0/350
All	All	0.54	0/54594	0.61	42/74361 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	G	0	1
1	a	0	1
6	F	0	2
6	Q	0	2
6	f	0	2
8	J	0	1
8	S	0	1
8	j	0	1
10	L	0	1
10	U	0	1
10	l	0	1
All	All	0	15

There are no bond length outliers.

The worst 5 of 42 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
10	U	132	ARG	CG-CD-NE	12.77	138.61	111.80
10	L	132	ARG	CG-CD-NE	12.75	138.57	111.80
10	l	132	ARG	CG-CD-NE	12.74	138.55	111.80
10	l	132	ARG	NE-CZ-NH2	-12.23	114.18	120.30
10	L	132	ARG	NE-CZ-NH2	-12.18	114.21	120.30

There are no chirality outliers.

5 of 15 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	G	333	THR	Peptide

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Mol	Chain	Res	Type	Group
6	Q	47	SER	Peptide
6	Q	48	TYR	Peptide
8	S	35	PHE	Peptide
10	U	132	ARG	Peptide

5.2 Too-close contacts ⓘ

Due to software issues we are unable to calculate clashes - this section is therefore empty.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	747/788 (95%)	707 (95%)	40 (5%)	0	100	100
1	G	747/788 (95%)	707 (95%)	40 (5%)	0	100	100
1	a	747/788 (95%)	707 (95%)	40 (5%)	0	100	100
2	B	737/741 (100%)	707 (96%)	30 (4%)	0	100	100
2	H	737/741 (100%)	707 (96%)	30 (4%)	0	100	100
2	b	737/741 (100%)	707 (96%)	30 (4%)	0	100	100
3	C	78/81 (96%)	72 (92%)	5 (6%)	1 (1%)	12	41
3	N	78/81 (96%)	72 (92%)	5 (6%)	1 (1%)	12	41
3	c	78/81 (96%)	72 (92%)	6 (8%)	0	100	100
4	D	137/159 (86%)	129 (94%)	8 (6%)	0	100	100
4	O	137/159 (86%)	129 (94%)	8 (6%)	0	100	100
4	d	137/159 (86%)	129 (94%)	8 (6%)	0	100	100
5	E	60/72 (83%)	57 (95%)	3 (5%)	0	100	100
5	P	60/72 (83%)	57 (95%)	3 (5%)	0	100	100
5	e	60/72 (83%)	57 (95%)	3 (5%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
6	F	133/159 (84%)	118 (89%)	14 (10%)	1 (1%)	19	53
6	Q	133/159 (84%)	118 (89%)	14 (10%)	1 (1%)	19	53
6	f	133/159 (84%)	118 (89%)	14 (10%)	1 (1%)	19	53
7	I	40/67 (60%)	36 (90%)	4 (10%)	0	100	100
7	R	40/67 (60%)	36 (90%)	4 (10%)	0	100	100
7	i	40/67 (60%)	36 (90%)	4 (10%)	0	100	100
8	J	41/48 (85%)	32 (78%)	8 (20%)	1 (2%)	6	26
8	S	41/48 (85%)	32 (78%)	8 (20%)	1 (2%)	6	26
8	j	41/48 (85%)	32 (78%)	8 (20%)	1 (2%)	6	26
9	K	17/49 (35%)	17 (100%)	0	0	100	100
9	T	17/49 (35%)	17 (100%)	0	0	100	100
9	k	17/49 (35%)	17 (100%)	0	0	100	100
10	L	161/174 (92%)	150 (93%)	11 (7%)	0	100	100
10	U	161/174 (92%)	150 (93%)	11 (7%)	0	100	100
10	l	161/174 (92%)	150 (93%)	11 (7%)	0	100	100
11	M	29/31 (94%)	28 (97%)	1 (3%)	0	100	100
11	V	29/31 (94%)	28 (97%)	1 (3%)	0	100	100
11	m	29/31 (94%)	28 (97%)	1 (3%)	0	100	100
12	W	27/101 (27%)	27 (100%)	0	0	100	100
12	X	27/101 (27%)	27 (100%)	0	0	100	100
12	x	27/101 (27%)	27 (100%)	0	0	100	100
All	All	6621/7410 (89%)	6240 (94%)	373 (6%)	8 (0%)	54	83

5 of 8 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
6	Q	48	TYR
6	f	48	TYR
6	F	48	TYR
3	N	63	LEU
8	S	13	ALA

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	613/641 (96%)	604 (98%)	9 (2%)	65 85
1	G	613/641 (96%)	604 (98%)	9 (2%)	65 85
1	a	613/641 (96%)	604 (98%)	9 (2%)	65 85
2	B	595/597 (100%)	592 (100%)	3 (0%)	88 95
2	H	595/597 (100%)	592 (100%)	3 (0%)	88 95
2	b	595/597 (100%)	592 (100%)	3 (0%)	88 95
3	C	68/69 (99%)	64 (94%)	4 (6%)	19 50
3	N	68/69 (99%)	64 (94%)	4 (6%)	19 50
3	c	68/69 (99%)	64 (94%)	4 (6%)	19 50
4	D	115/132 (87%)	110 (96%)	5 (4%)	29 62
4	O	115/132 (87%)	110 (96%)	5 (4%)	29 62
4	d	115/132 (87%)	110 (96%)	5 (4%)	29 62
5	E	54/60 (90%)	51 (94%)	3 (6%)	21 53
5	P	54/60 (90%)	51 (94%)	3 (6%)	21 53
5	e	54/60 (90%)	51 (94%)	3 (6%)	21 53
6	F	115/134 (86%)	105 (91%)	10 (9%)	10 33
6	Q	115/134 (86%)	105 (91%)	10 (9%)	10 33
6	f	115/134 (86%)	105 (91%)	10 (9%)	10 33
7	I	37/60 (62%)	37 (100%)	0	100 100
7	R	37/60 (62%)	37 (100%)	0	100 100
7	i	37/60 (62%)	37 (100%)	0	100 100
8	J	36/42 (86%)	33 (92%)	3 (8%)	11 35
8	S	36/42 (86%)	33 (92%)	3 (8%)	11 35
8	j	36/42 (86%)	33 (92%)	3 (8%)	11 35
9	K	12/16 (75%)	11 (92%)	1 (8%)	11 35
9	T	12/16 (75%)	11 (92%)	1 (8%)	11 35

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
9	k	12/16 (75%)	11 (92%)	1 (8%)	11	35
10	L	128/138 (93%)	125 (98%)	3 (2%)	50	78
10	U	128/138 (93%)	125 (98%)	3 (2%)	50	78
10	l	128/138 (93%)	125 (98%)	3 (2%)	50	78
11	M	26/26 (100%)	25 (96%)	1 (4%)	33	66
11	V	26/26 (100%)	25 (96%)	1 (4%)	33	66
11	m	26/26 (100%)	25 (96%)	1 (4%)	33	66
12	W	24/84 (29%)	24 (100%)	0	100	100
12	X	24/84 (29%)	24 (100%)	0	100	100
12	x	24/84 (29%)	24 (100%)	0	100	100
All	All	5469/5997 (91%)	5343 (98%)	126 (2%)	53	78

5 of 126 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	c	73	THR
6	F	46	ASP
6	f	62	CYS
6	F	38	VAL
8	J	24	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 71 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	731	GLN
2	B	34	HIS
2	B	444	ASN
1	a	144	GLN
1	a	105	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no monosaccharides in this entry.

5.6 Ligand geometry

Of 372 ligands modelled in this entry, 3 are monoatomic - leaving 369 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	$\#\|Z\| > 2$
17	SF4	N	3003	3	0,12,12	-	-	-		
18	BCR	L	4019	-	41,41,41	2.98	7 (17%)	56,56,56	7.02	29 (51%)
14	CLA	U	1501	10	65,73,73	2.19	19 (29%)	76,113,113	2.52	24 (31%)
14	CLA	U	1503	-	65,73,73	2.20	18 (27%)	76,113,113	2.60	25 (32%)
18	BCR	B	4014	-	41,41,41	3.05	7 (17%)	56,56,56	6.44	24 (42%)
18	BCR	H	4004	-	41,41,41	2.85	7 (17%)	56,56,56	6.49	25 (44%)
14	CLA	G	1109	-	65,73,73	2.18	18 (27%)	76,113,113	2.63	25 (32%)
14	CLA	b	1239	-	65,73,73	2.22	18 (27%)	76,113,113	2.71	32 (42%)
14	CLA	H	1022	-	65,73,73	2.16	18 (27%)	76,113,113	2.63	26 (34%)
18	BCR	b	4013	-	41,41,41	2.81	6 (14%)	56,56,56	6.71	22 (39%)
18	BCR	b	4005	-	41,41,41	2.99	7 (17%)	56,56,56	6.59	24 (42%)
18	BCR	I	4020	-	41,41,41	3.22	10 (24%)	56,56,56	6.75	23 (41%)
14	CLA	a	1103	-	60,68,73	2.25	19 (31%)	70,107,113	2.72	25 (35%)
18	BCR	b	4016	-	41,41,41	2.97	6 (14%)	56,56,56	6.64	20 (35%)
14	CLA	H	1204	-	65,73,73	2.21	17 (26%)	76,113,113	2.54	27 (35%)
16	PQN	A	2001	-	34,34,34	1.44	2 (5%)	42,45,45	1.25	5 (11%)
14	CLA	G	1124	-	55,63,73	2.37	18 (32%)	64,101,113	2.88	24 (37%)
14	CLA	A	1129	-	50,58,73	2.49	19 (38%)	58,95,113	2.88	23 (39%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#|Z| > 2	Counts	RMSZ	#|Z| > 2
14	CLA	B	1217	-	55,63,73	2.35	18 (32%)	64,101,113	2.82	22 (34%)
20	LMG	i	5006	-	37,37,55	1.11	3 (8%)	45,45,63	1.20	3 (6%)
20	LMG	A	5005	-	46,46,55	1.29	5 (10%)	54,54,63	1.09	2 (3%)
13	CL0	G	1011	-	65,73,73	2.17	20 (30%)	76,113,113	2.61	23 (30%)
14	CLA	H	1221	-	65,73,73	2.18	19 (29%)	76,113,113	2.54	24 (31%)
14	CLA	l	1503	-	65,73,73	2.20	19 (29%)	76,113,113	2.59	25 (32%)
14	CLA	H	1209	-	45,53,73	2.51	18 (40%)	52,89,113	2.98	21 (40%)
14	CLA	b	1236	-	45,53,73	2.47	17 (37%)	52,89,113	2.92	19 (36%)
14	CLA	U	1502	-	60,68,73	2.23	18 (30%)	70,107,113	2.75	23 (32%)
14	CLA	H	1217	-	55,63,73	2.35	18 (32%)	64,101,113	2.81	22 (34%)
14	CLA	a	1118	-	55,63,73	2.38	18 (32%)	64,101,113	2.79	27 (42%)
14	CLA	G	1115	-	65,73,73	2.21	18 (27%)	76,113,113	2.72	26 (34%)
15	F6C	b	1237	-	69,74,74	2.67	24 (34%)	70,114,114	3.21	27 (38%)
14	CLA	A	1135	-	60,68,73	2.28	18 (30%)	70,107,113	2.68	24 (34%)
14	CLA	a	1119	-	65,73,73	2.21	19 (29%)	76,113,113	2.63	24 (31%)
14	CLA	A	1117	-	65,73,73	2.17	18 (27%)	76,113,113	2.63	27 (35%)
14	CLA	a	1116	-	55,63,73	2.39	18 (32%)	64,101,113	2.80	27 (42%)
15	F6C	A	1121	-	49,54,74	3.14	23 (46%)	46,90,114	3.85	28 (60%)
14	CLA	G	1130	-	55,63,73	2.40	18 (32%)	64,101,113	2.75	25 (39%)
14	CLA	A	1138	-	60,68,73	2.31	18 (30%)	70,107,113	2.59	23 (32%)
20	LMG	l	5007	-	50,50,55	1.34	7 (14%)	58,58,63	1.09	2 (3%)
14	CLA	G	1101	-	45,53,73	2.45	17 (37%)	52,89,113	2.94	20 (38%)
14	CLA	a	1013	-	60,68,73	2.28	18 (30%)	70,107,113	2.77	24 (34%)
14	CLA	A	1125	-	65,73,73	2.16	19 (29%)	76,113,113	2.67	22 (28%)
14	CLA	G	1123	-	60,68,73	2.31	19 (31%)	70,107,113	2.65	25 (35%)
14	CLA	l	1501	10	65,73,73	2.19	19 (29%)	76,113,113	2.52	24 (31%)
14	CLA	G	1113	-	45,53,73	2.49	17 (37%)	52,89,113	2.89	22 (42%)
14	CLA	b	1226	-	65,73,73	2.24	19 (29%)	76,113,113	2.52	23 (30%)
20	LMG	B	5002	-	46,46,55	1.25	5 (10%)	54,54,63	1.26	4 (7%)
14	CLA	B	1213	-	65,73,73	2.20	18 (27%)	76,113,113	2.62	23 (30%)
14	CLA	A	1119	-	65,73,73	2.21	19 (29%)	76,113,113	2.62	24 (31%)
14	CLA	B	1225	-	65,73,73	2.24	19 (29%)	76,113,113	2.49	21 (27%)
21	LMT	a	6001	-	32,32,36	1.27	6 (18%)	43,43,47	1.05	2 (4%)
14	CLA	A	1128	-	60,68,73	2.32	19 (31%)	70,107,113	2.71	23 (32%)
14	CLA	A	1118	-	55,63,73	2.38	18 (32%)	64,101,113	2.78	27 (42%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#|Z| > 2	Counts	RMSZ	#|Z| > 2
14	CLA	a	1109	-	65,73,73	2.18	18 (27%)	76,113,113	2.63	25 (32%)
14	CLA	A	1114	-	45,53,73	2.54	19 (42%)	52,89,113	2.87	20 (38%)
14	CLA	G	1140	-	65,73,73	2.18	18 (27%)	76,113,113	2.52	24 (31%)
14	CLA	b	1216	-	65,73,73	2.18	18 (27%)	76,113,113	2.50	24 (31%)
14	CLA	B	1231	2	55,63,73	2.38	18 (32%)	64,101,113	2.76	22 (34%)
14	CLA	A	1137	-	50,58,73	2.50	19 (38%)	58,95,113	3.04	25 (43%)
18	BCR	B	4016	-	41,41,41	2.97	6 (14%)	56,56,56	6.64	20 (35%)
14	CLA	B	1224	-	65,73,73	2.20	19 (29%)	76,113,113	2.57	22 (28%)
14	CLA	a	1124	-	55,63,73	2.37	18 (32%)	64,101,113	2.87	24 (37%)
14	CLA	G	1012	-	65,73,73	2.18	18 (27%)	76,113,113	2.63	26 (34%)
14	CLA	H	1023	-	65,73,73	2.19	19 (29%)	76,113,113	2.74	26 (34%)
14	CLA	b	1206	2	45,53,73	2.52	16 (35%)	52,89,113	2.79	20 (38%)
14	CLA	A	1109	-	65,73,73	2.18	18 (27%)	76,113,113	2.63	25 (32%)
14	CLA	B	1021	-	65,73,73	2.17	20 (30%)	76,113,113	2.55	25 (32%)
14	CLA	G	1125	-	65,73,73	2.16	20 (30%)	76,113,113	2.67	22 (28%)
18	BCR	A	4001	-	41,41,41	2.95	6 (14%)	56,56,56	6.60	23 (41%)
14	CLA	a	1131	-	60,68,73	2.28	18 (30%)	70,107,113	2.65	21 (30%)
15	F6C	B	1237	-	69,74,74	2.68	23 (33%)	70,114,114	3.22	27 (38%)
16	PQN	B	2002	-	34,34,34	1.47	2 (5%)	42,45,45	1.26	2 (4%)
18	BCR	i	4018	-	41,41,41	3.05	8 (19%)	56,56,56	6.57	24 (42%)
14	CLA	H	1224	-	65,73,73	2.19	18 (27%)	76,113,113	2.56	22 (28%)
18	BCR	H	4005	-	41,41,41	2.99	7 (17%)	56,56,56	6.59	24 (42%)
14	CLA	H	1205	-	65,73,73	2.16	18 (27%)	76,113,113	2.60	23 (30%)
14	CLA	a	1139	-	45,53,73	2.50	17 (37%)	52,89,113	2.85	22 (42%)
18	BCR	H	4010	-	41,41,41	3.11	7 (17%)	56,56,56	6.68	21 (37%)
13	CL0	a	1011	-	65,73,73	2.16	20 (30%)	76,113,113	2.61	23 (30%)
14	CLA	b	1213	-	65,73,73	2.20	18 (27%)	76,113,113	2.62	23 (30%)
14	CLA	k	1401	-	45,53,73	2.55	19 (42%)	52,89,113	2.94	21 (40%)
14	CLA	b	1211	-	65,73,73	2.20	20 (30%)	76,113,113	2.64	23 (30%)
14	CLA	B	1212	-	45,53,73	2.49	17 (37%)	52,89,113	2.89	19 (36%)
14	CLA	b	1021	-	65,73,73	2.17	20 (30%)	76,113,113	2.55	25 (32%)
18	BCR	G	4003	-	41,41,41	2.89	6 (14%)	56,56,56	6.55	22 (39%)
14	CLA	B	1218	-	45,53,73	2.59	18 (40%)	52,89,113	2.83	18 (34%)
14	CLA	X	1701	-	55,63,73	2.39	18 (32%)	64,101,113	2.78	23 (35%)
14	CLA	G	1132	-	65,73,73	2.17	17 (26%)	76,113,113	2.69	24 (31%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#$\|Z\|>2$	Counts	RMSZ	#$\|Z\|>2$
18	BCR	a	4002	-	41,41,41	3.05	7 (17%)	56,56,56	6.29	28 (50%)
14	CLA	H	1208	-	65,73,73	2.20	18 (27%)	76,113,113	2.56	22 (28%)
18	BCR	G	4001	-	41,41,41	2.95	6 (14%)	56,56,56	6.60	23 (41%)
18	BCR	G	4011	-	41,41,41	3.03	8 (19%)	56,56,56	6.53	27 (48%)
14	CLA	a	1123	-	60,68,73	2.31	19 (31%)	70,107,113	2.64	25 (35%)
14	CLA	b	1201	-	55,63,73	2.39	17 (30%)	64,101,113	2.86	23 (35%)
14	CLA	B	1219	-	45,53,73	2.53	19 (42%)	52,89,113	2.86	21 (40%)
20	LMG	a	5005	-	46,46,55	1.30	5 (10%)	54,54,63	1.09	2 (3%)
20	LMG	H	5002	-	46,46,55	1.26	5 (10%)	54,54,63	1.25	4 (7%)
14	CLA	B	1202	-	60,68,73	2.19	19 (31%)	70,107,113	2.69	24 (34%)
14	CLA	H	1239	-	65,73,73	2.22	18 (27%)	76,113,113	2.71	32 (42%)
14	CLA	A	1122	-	55,63,73	2.36	18 (32%)	64,101,113	2.77	26 (40%)
20	LMG	R	5006	-	37,37,55	1.12	3 (8%)	45,45,63	1.20	3 (6%)
14	CLA	b	1222	-	65,73,73	2.22	19 (29%)	76,113,113	2.65	27 (35%)
14	CLA	A	1106	-	60,68,73	2.27	19 (31%)	70,107,113	2.78	24 (34%)
18	BCR	b	4006	-	41,41,41	2.87	6 (14%)	56,56,56	6.61	21 (37%)
21	LMT	G	6002	-	29,29,36	1.40	6 (20%)	40,40,47	1.16	4 (10%)
14	CLA	A	1139	-	45,53,73	2.49	17 (37%)	52,89,113	2.85	22 (42%)
20	LMG	L	5007	-	50,50,55	1.34	7 (14%)	58,58,63	1.09	2 (3%)
14	CLA	b	1215	-	60,68,73	2.24	18 (30%)	70,107,113	2.60	21 (30%)
14	CLA	a	1125	-	65,73,73	2.17	20 (30%)	76,113,113	2.68	22 (28%)
14	CLA	G	1103	-	60,68,73	2.25	19 (31%)	70,107,113	2.72	24 (34%)
14	CLA	A	1101	-	45,53,73	2.45	17 (37%)	52,89,113	2.94	20 (38%)
14	CLA	L	1501	10	65,73,73	2.19	19 (29%)	76,113,113	2.52	23 (30%)
14	CLA	B	1210	-	65,73,73	2.21	19 (29%)	76,113,113	2.76	26 (34%)
18	BCR	b	4004	-	41,41,41	2.85	7 (17%)	56,56,56	6.49	25 (44%)
18	BCR	L	4022	-	41,41,41	3.10	9 (21%)	56,56,56	6.48	23 (41%)
21	LMT	A	6001	-	32,32,36	1.28	6 (18%)	43,43,47	1.05	2 (4%)
14	CLA	H	1218	-	45,53,73	2.58	18 (40%)	52,89,113	2.83	18 (34%)
14	CLA	A	1136	-	65,73,73	2.17	18 (27%)	76,113,113	2.59	22 (28%)
18	BCR	B	4006	-	41,41,41	2.86	6 (14%)	56,56,56	6.61	21 (37%)
14	CLA	B	1211	-	65,73,73	2.20	19 (29%)	76,113,113	2.64	23 (30%)
17	SF4	C	3002	3	0,12,12	-	-	-		
18	BCR	U	4022	-	41,41,41	3.09	9 (21%)	56,56,56	6.48	23 (41%)
14	CLA	H	1219	-	45,53,73	2.53	19 (42%)	52,89,113	2.85	21 (40%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#|Z| > 2	Counts	RMSZ	#|Z| > 2
14	CLA	B	1220	-	55,63,73	2.38	18 (32%)	64,101,113	2.92	25 (39%)
14	CLA	B	1232	-	45,53,73	2.54	18 (40%)	52,89,113	2.86	20 (38%)
14	CLA	G	1137	-	50,58,73	2.50	19 (38%)	58,95,113	3.04	25 (43%)
18	BCR	A	4002	-	41,41,41	3.06	7 (17%)	56,56,56	6.30	28 (50%)
14	CLA	H	1226	-	65,73,73	2.24	19 (29%)	76,113,113	2.52	23 (30%)
17	SF4	C	3003	3	0,12,12	-	-	-		
18	BCR	R	4018	-	41,41,41	3.05	8 (19%)	56,56,56	6.57	24 (42%)
14	CLA	a	1138	-	60,68,73	2.31	18 (30%)	70,107,113	2.58	23 (32%)
18	BCR	a	4011	-	41,41,41	3.03	8 (19%)	56,56,56	6.53	27 (48%)
16	PQN	a	2001	-	34,34,34	1.43	2 (5%)	42,45,45	1.25	5 (11%)
14	CLA	b	1235	-	60,68,73	2.29	18 (30%)	70,107,113	2.67	22 (31%)
14	CLA	b	1221	-	65,73,73	2.18	19 (29%)	76,113,113	2.54	24 (31%)
18	BCR	M	4021	-	41,41,41	2.98	7 (17%)	56,56,56	6.66	19 (33%)
14	CLA	b	1209	-	45,53,73	2.51	18 (40%)	52,89,113	2.97	21 (40%)
14	CLA	B	1239	-	65,73,73	2.21	18 (27%)	76,113,113	2.71	31 (40%)
14	CLA	A	1124	-	55,63,73	2.37	18 (32%)	64,101,113	2.88	24 (37%)
14	CLA	a	1110	-	45,53,73	2.50	17 (37%)	52,89,113	2.87	20 (38%)
14	CLA	b	1217	-	55,63,73	2.35	18 (32%)	64,101,113	2.81	22 (34%)
14	CLA	G	1105	-	45,53,73	2.54	18 (40%)	52,89,113	2.94	21 (40%)
14	CLA	H	1212	-	45,53,73	2.49	17 (37%)	52,89,113	2.90	19 (36%)
14	CLA	A	1116	-	55,63,73	2.39	18 (32%)	64,101,113	2.81	27 (42%)
14	CLA	B	1223	-	65,73,73	2.18	19 (29%)	76,113,113	2.66	27 (35%)
18	BCR	A	4003	-	41,41,41	2.89	6 (14%)	56,56,56	6.55	22 (39%)
14	CLA	G	1128	-	60,68,73	2.31	19 (31%)	70,107,113	2.71	23 (32%)
14	CLA	b	1227	-	45,53,73	2.57	19 (42%)	52,89,113	2.81	22 (42%)
14	CLA	G	1133	-	60,68,73	2.30	18 (30%)	70,107,113	2.77	25 (35%)
18	BCR	H	4017	-	41,41,41	3.03	9 (21%)	56,56,56	6.74	20 (35%)
14	CLA	H	1201	-	55,63,73	2.38	18 (32%)	64,101,113	2.88	23 (35%)
18	BCR	H	4016	-	41,41,41	2.98	6 (14%)	56,56,56	6.64	20 (35%)
17	SF4	a	3001	2,1	0,12,12	-	-	-		
14	CLA	A	1130	-	55,63,73	2.41	18 (32%)	64,101,113	2.75	25 (39%)
15	F6C	a	1121	-	49,54,74	3.14	23 (46%)	46,90,114	3.85	28 (60%)
18	BCR	m	4021	-	41,41,41	2.98	7 (17%)	56,56,56	6.65	19 (33%)
14	CLA	B	1234	-	65,73,73	2.14	19 (29%)	76,113,113	2.57	22 (28%)
18	BCR	R	4020	-	41,41,41	3.22	10 (24%)	56,56,56	6.75	22 (39%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
14	CLA	H	1213	-	65,73,73	2.20	18 (27%)	76,113,113	2.62	23 (30%)
14	CLA	B	1022	-	65,73,73	2.15	19 (29%)	76,113,113	2.63	26 (34%)
15	F6C	H	1207	-	69,74,74	2.73	24 (34%)	70,114,114	3.44	28 (40%)
14	CLA	H	1220	-	55,63,73	2.38	18 (32%)	64,101,113	2.92	26 (40%)
18	BCR	B	4010	-	41,41,41	3.12	7 (17%)	56,56,56	6.68	21 (37%)
18	BCR	B	4005	-	41,41,41	2.99	7 (17%)	56,56,56	6.59	24 (42%)
14	CLA	b	1023	-	65,73,73	2.18	19 (29%)	76,113,113	2.74	25 (32%)
17	SF4	c	3002	3	0,12,12	-	-	-		
14	CLA	G	1139	-	45,53,73	2.50	17 (37%)	52,89,113	2.84	22 (42%)
14	CLA	T	1401	-	45,53,73	2.55	19 (42%)	52,89,113	2.95	21 (40%)
14	CLA	A	1108	-	45,53,73	2.55	18 (40%)	52,89,113	2.87	21 (40%)
14	CLA	H	1206	2	45,53,73	2.52	16 (35%)	52,89,113	2.79	19 (36%)
14	CLA	b	1228	-	55,63,73	2.39	20 (36%)	64,101,113	2.81	26 (40%)
14	CLA	A	1140	-	65,73,73	2.17	18 (27%)	76,113,113	2.52	23 (30%)
14	CLA	B	1216	-	65,73,73	2.18	18 (27%)	76,113,113	2.50	25 (32%)
14	CLA	a	1101	-	45,53,73	2.45	17 (37%)	52,89,113	2.95	20 (38%)
14	CLA	a	1107	1	45,53,73	2.50	17 (37%)	52,89,113	2.81	21 (40%)
14	CLA	A	1123	-	60,68,73	2.31	19 (31%)	70,107,113	2.65	25 (35%)
14	CLA	H	1229	-	60,68,73	2.29	19 (31%)	70,107,113	2.73	24 (34%)
14	CLA	b	1224	-	65,73,73	2.19	19 (29%)	76,113,113	2.56	22 (28%)
20	LMG	G	5005	-	46,46,55	1.29	5 (10%)	54,54,63	1.09	2 (3%)
15	F6C	B	1230	-	49,54,74	3.15	26 (53%)	46,90,114	3.82	25 (54%)
18	BCR	H	4006	-	41,41,41	2.87	6 (14%)	56,56,56	6.61	21 (37%)
14	CLA	H	1234	-	65,73,73	2.15	19 (29%)	76,113,113	2.58	22 (28%)
18	BCR	B	4013	-	41,41,41	2.80	6 (14%)	56,56,56	6.71	22 (39%)
14	CLA	H	1232	-	45,53,73	2.53	18 (40%)	52,89,113	2.86	20 (38%)
14	CLA	B	1214	-	65,73,73	2.20	20 (30%)	76,113,113	2.55	26 (34%)
18	BCR	H	4014	-	41,41,41	3.05	7 (17%)	56,56,56	6.43	24 (42%)
18	BCR	G	4007	-	41,41,41	3.13	9 (21%)	56,56,56	6.55	24 (42%)
14	CLA	W	1701	-	55,63,73	2.39	18 (32%)	64,101,113	2.78	23 (35%)
18	BCR	H	4009	-	41,41,41	2.96	7 (17%)	56,56,56	6.43	23 (41%)
18	BCR	U	4019	-	41,41,41	2.98	7 (17%)	56,56,56	7.03	29 (51%)
14	CLA	H	1235	-	60,68,73	2.29	18 (30%)	70,107,113	2.68	22 (31%)
18	BCR	l	4019	-	41,41,41	2.99	7 (17%)	56,56,56	7.03	29 (51%)
14	CLA	b	1208	-	65,73,73	2.20	18 (27%)	76,113,113	2.56	23 (30%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\lvert Z\rvert > 2$	Counts	RMSZ	$\#\lvert Z\rvert > 2$
14	CLA	b	1229	-	60,68,73	2.29	19 (31%)	70,107,113	2.74	24 (34%)
14	CLA	G	1134	-	45,53,73	2.61	19 (42%)	52,89,113	2.93	21 (40%)
18	BCR	a	4003	-	41,41,41	2.89	6 (14%)	56,56,56	6.55	22 (39%)
14	CLA	x	1701	-	55,63,73	2.39	18 (32%)	64,101,113	2.77	23 (35%)
19	LHG	B	5004	-	43,43,48	0.96	2 (4%)	46,49,54	1.12	3 (6%)
14	CLA	A	1105	-	45,53,73	2.55	18 (40%)	52,89,113	2.95	21 (40%)
14	CLA	A	1102	-	60,68,73	2.30	18 (30%)	70,107,113	2.69	23 (32%)
14	CLA	G	1108	-	45,53,73	2.55	18 (40%)	52,89,113	2.86	21 (40%)
19	LHG	a	5001	-	41,41,48	0.99	2 (4%)	44,47,54	1.10	3 (6%)
18	BCR	G	4002	-	41,41,41	3.05	7 (17%)	56,56,56	6.30	28 (50%)
14	CLA	A	1111	-	60,68,73	2.27	19 (31%)	70,107,113	4.78	27 (38%)
14	CLA	a	1130	-	55,63,73	2.40	18 (32%)	64,101,113	2.75	25 (39%)
18	BCR	V	4021	-	41,41,41	2.99	7 (17%)	56,56,56	6.66	19 (33%)
14	CLA	A	1131	-	60,68,73	2.28	17 (28%)	70,107,113	2.66	21 (30%)
14	CLA	a	1104	-	65,73,73	2.15	19 (29%)	76,113,113	2.76	26 (34%)
14	CLA	G	1126	-	60,68,73	2.30	19 (31%)	70,107,113	2.62	25 (35%)
14	CLA	B	1204	-	65,73,73	2.21	18 (27%)	76,113,113	2.53	27 (35%)
14	CLA	B	1226	-	65,73,73	2.23	19 (29%)	76,113,113	2.52	23 (30%)
14	CLA	A	1110	-	45,53,73	2.50	17 (37%)	52,89,113	2.87	20 (38%)
14	CLA	B	1203	-	65,73,73	2.16	19 (29%)	76,113,113	2.66	21 (27%)
15	F6C	b	1230	-	49,54,74	3.15	26 (53%)	46,90,114	3.82	25 (54%)
14	CLA	b	1218	-	45,53,73	2.58	18 (40%)	52,89,113	2.82	18 (34%)
14	CLA	A	1115	-	65,73,73	2.21	18 (27%)	76,113,113	2.72	26 (34%)
14	CLA	b	1231	2	55,63,73	2.38	18 (32%)	64,101,113	2.76	22 (34%)
14	CLA	B	1205	-	65,73,73	2.16	18 (27%)	76,113,113	2.60	22 (28%)
14	CLA	G	1111	-	60,68,73	2.27	19 (31%)	70,107,113	4.78	27 (38%)
14	CLA	B	1215	-	60,68,73	2.24	18 (30%)	70,107,113	2.60	21 (30%)
14	CLA	H	1227	-	45,53,73	2.57	19 (42%)	52,89,113	2.81	22 (42%)
14	CLA	a	1117	-	65,73,73	2.17	18 (27%)	76,113,113	2.62	27 (35%)
14	CLA	A	1133	-	60,68,73	2.30	18 (30%)	70,107,113	2.77	25 (35%)
14	CLA	H	1203	-	65,73,73	2.16	19 (29%)	76,113,113	2.66	21 (27%)
18	BCR	b	4014	-	41,41,41	3.05	8 (19%)	56,56,56	6.44	24 (42%)
17	SF4	c	3003	3	0,12,12	-	-	-		
14	CLA	G	1112	-	55,63,73	2.39	18 (32%)	64,101,113	2.78	24 (37%)
14	CLA	B	1206	2	45,53,73	2.51	16 (35%)	52,89,113	2.78	19 (36%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\lvert Z\rvert > 2$	Counts	RMSZ	$\#\lvert Z\rvert > 2$
14	CLA	K	1401	-	45,53,73	2.56	19 (42%)	52,89,113	2.95	21 (40%)
14	CLA	a	1140	-	65,73,73	2.17	18 (27%)	76,113,113	2.53	24 (31%)
14	CLA	A	1013	-	60,68,73	2.29	18 (30%)	70,107,113	2.77	25 (35%)
14	CLA	G	1013	-	60,68,73	2.28	18 (30%)	70,107,113	2.77	24 (34%)
14	CLA	b	1234	-	65,73,73	2.15	19 (29%)	76,113,113	2.57	22 (28%)
19	LHG	H	5004	-	43,43,48	0.96	2 (4%)	46,49,54	1.12	3 (6%)
14	CLA	b	1205	-	65,73,73	2.16	18 (27%)	76,113,113	2.59	23 (30%)
14	CLA	G	1131	-	60,68,73	2.28	17 (28%)	70,107,113	2.66	22 (31%)
20	LMG	I	5006	-	37,37,55	1.11	3 (8%)	45,45,63	1.20	3 (6%)
18	BCR	G	4008	-	41,41,41	3.18	9 (21%)	56,56,56	6.46	21 (37%)
14	CLA	A	1112	-	55,63,73	2.38	18 (32%)	64,101,113	2.77	24 (37%)
14	CLA	A	1107	1	45,53,73	2.50	17 (37%)	52,89,113	2.81	21 (40%)
19	LHG	A	5001	-	41,41,48	0.99	2 (4%)	44,47,54	1.10	3 (6%)
14	CLA	a	1127	-	65,73,73	2.20	19 (29%)	76,113,113	2.60	21 (27%)
14	CLA	a	1113	-	45,53,73	2.49	17 (37%)	52,89,113	2.89	22 (42%)
14	CLA	A	1012	-	65,73,73	2.18	18 (27%)	76,113,113	2.63	26 (34%)
14	CLA	G	1138	-	60,68,73	2.31	18 (30%)	70,107,113	2.59	23 (32%)
18	BCR	b	4017	-	41,41,41	3.02	9 (21%)	56,56,56	6.73	20 (35%)
18	BCR	A	4007	-	41,41,41	3.13	9 (21%)	56,56,56	6.55	24 (42%)
17	SF4	A	3001	2,1	0,12,12	-	-	-		
14	CLA	B	1221	-	65,73,73	2.19	19 (29%)	76,113,113	2.55	24 (31%)
14	CLA	b	1219	-	45,53,73	2.52	18 (40%)	52,89,113	2.86	21 (40%)
14	CLA	a	1108	-	45,53,73	2.55	18 (40%)	52,89,113	2.86	21 (40%)
14	CLA	H	1202	-	60,68,73	2.19	19 (31%)	70,107,113	2.69	24 (34%)
14	CLA	B	1236	-	45,53,73	2.47	18 (40%)	52,89,113	2.93	19 (36%)
18	BCR	i	4020	-	41,41,41	3.22	10 (24%)	56,56,56	6.75	23 (41%)
14	CLA	B	1233	-	45,53,73	2.53	18 (40%)	52,89,113	2.89	20 (38%)
14	CLA	H	1216	-	65,73,73	2.18	18 (27%)	76,113,113	2.50	24 (31%)
14	CLA	H	1225	-	65,73,73	2.24	19 (29%)	76,113,113	2.48	21 (27%)
14	CLA	G	1106	-	60,68,73	2.27	18 (30%)	70,107,113	2.77	24 (34%)
14	CLA	G	1116	-	55,63,73	2.39	18 (32%)	64,101,113	2.79	27 (42%)
14	CLA	A	1127	-	65,73,73	2.20	19 (29%)	76,113,113	2.60	21 (27%)
14	CLA	G	1114	-	45,53,73	2.54	20 (44%)	52,89,113	2.86	20 (38%)
14	CLA	a	1122	-	55,63,73	2.36	18 (32%)	64,101,113	2.77	26 (40%)
14	CLA	H	1233	-	45,53,73	2.53	18 (40%)	52,89,113	2.90	19 (36%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#|Z| > 2	Counts	RMSZ	#|Z| > 2
14	CLA	G	1107	1	45,53,73	2.50	17 (37%)	52,89,113	2.81	21 (40%)
18	BCR	l	4022	-	41,41,41	3.10	9 (21%)	56,56,56	6.49	23 (41%)
14	CLA	H	1210	-	65,73,73	2.22	20 (30%)	76,113,113	2.76	26 (34%)
14	CLA	B	1023	-	65,73,73	2.19	19 (29%)	76,113,113	2.75	26 (34%)
14	CLA	a	1112	-	55,63,73	2.39	19 (34%)	64,101,113	2.78	24 (37%)
21	LMT	a	6002	-	29,29,36	1.40	6 (20%)	40,40,47	1.16	4 (10%)
14	CLA	A	1104	-	65,73,73	2.15	19 (29%)	76,113,113	2.76	26 (34%)
14	CLA	B	1228	-	55,63,73	2.39	20 (36%)	64,101,113	2.82	26 (40%)
15	F6C	B	1207	-	69,74,74	2.73	24 (34%)	70,114,114	3.44	28 (40%)
14	CLA	G	1135	-	60,68,73	2.29	20 (33%)	70,107,113	2.68	24 (34%)
14	CLA	A	1120	-	45,53,73	2.46	17 (37%)	52,89,113	2.98	20 (38%)
14	CLA	H	1021	-	65,73,73	2.18	20 (30%)	76,113,113	2.55	25 (32%)
20	LMG	U	5007	-	50,50,55	1.34	7 (14%)	58,58,63	1.09	2 (3%)
16	PQN	b	2002	-	34,34,34	1.47	2 (5%)	42,45,45	1.26	2 (4%)
18	BCR	a	4008	-	41,41,41	3.18	9 (21%)	56,56,56	6.45	20 (35%)
14	CLA	a	1111	-	60,68,73	2.27	19 (31%)	70,107,113	4.78	27 (38%)
14	CLA	a	1012	-	65,73,73	2.18	18 (27%)	76,113,113	2.63	26 (34%)
14	CLA	B	1208	-	65,73,73	2.20	18 (27%)	76,113,113	2.56	22 (28%)
15	F6C	b	1207	-	69,74,74	2.73	24 (34%)	70,114,114	3.44	28 (40%)
14	CLA	B	1222	-	65,73,73	2.22	19 (29%)	76,113,113	2.65	27 (35%)
14	CLA	A	1103	-	60,68,73	2.24	19 (31%)	70,107,113	2.72	23 (32%)
15	F6C	H	1230	-	49,54,74	3.15	26 (53%)	46,90,114	3.82	25 (54%)
14	CLA	a	1106	-	60,68,73	2.27	19 (31%)	70,107,113	2.77	24 (34%)
14	CLA	H	1231	2	55,63,73	2.38	18 (32%)	64,101,113	2.76	23 (35%)
18	BCR	H	4013	-	41,41,41	2.81	6 (14%)	56,56,56	6.71	22 (39%)
13	CL0	A	1011	-	65,73,73	2.16	20 (30%)	76,113,113	2.60	22 (28%)
14	CLA	a	1114	-	45,53,73	2.54	20 (44%)	52,89,113	2.87	20 (38%)
14	CLA	b	1212	-	45,53,73	2.49	17 (37%)	52,89,113	2.90	19 (36%)
18	BCR	A	4011	-	41,41,41	3.02	8 (19%)	56,56,56	6.53	27 (48%)
14	CLA	a	1105	-	45,53,73	2.54	18 (40%)	52,89,113	2.94	21 (40%)
14	CLA	a	1115	-	65,73,73	2.20	18 (27%)	76,113,113	2.72	26 (34%)
14	CLA	G	1102	-	60,68,73	2.30	18 (30%)	70,107,113	2.68	23 (32%)
14	CLA	G	1120	-	45,53,73	2.47	17 (37%)	52,89,113	2.99	20 (38%)
14	CLA	b	1214	-	65,73,73	2.21	20 (30%)	76,113,113	2.55	26 (34%)
14	CLA	a	1133	-	60,68,73	2.30	19 (31%)	70,107,113	2.77	25 (35%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
14	CLA	G	1117	-	65,73,73	2.18	18 (27%)	76,113,113	2.63	27 (35%)
18	BCR	a	4007	-	41,41,41	3.13	8 (19%)	56,56,56	6.56	24 (42%)
14	CLA	a	1102	-	60,68,73	2.30	18 (30%)	70,107,113	2.69	23 (32%)
14	CLA	B	1201	-	55,63,73	2.38	18 (32%)	64,101,113	2.87	23 (35%)
14	CLA	H	1236	-	45,53,73	2.48	18 (40%)	52,89,113	2.93	19 (36%)
20	LMG	b	5002	-	46,46,55	1.25	5 (10%)	54,54,63	1.25	4 (7%)
15	F6C	b	1238	-	69,74,74	2.70	23 (33%)	70,114,114	3.26	29 (41%)
14	CLA	b	1233	-	45,53,73	2.53	18 (40%)	52,89,113	2.89	18 (34%)
16	PQN	G	2001	-	34,34,34	1.44	2 (5%)	42,45,45	1.25	5 (11%)
15	F6C	H	1237	-	69,74,74	2.68	23 (33%)	70,114,114	3.22	27 (38%)
14	CLA	B	1229	-	60,68,73	2.29	19 (31%)	70,107,113	2.73	24 (34%)
14	CLA	G	1136	-	65,73,73	2.17	18 (27%)	76,113,113	2.58	22 (28%)
14	CLA	a	1137	-	50,58,73	2.50	19 (38%)	58,95,113	3.05	25 (43%)
14	CLA	A	1113	-	45,53,73	2.49	17 (37%)	52,89,113	2.89	23 (44%)
14	CLA	A	1134	-	45,53,73	2.62	19 (42%)	52,89,113	2.93	21 (40%)
14	CLA	G	1129	-	50,58,73	2.50	19 (38%)	58,95,113	2.89	23 (39%)
17	SF4	N	3002	3	0,12,12	-	-	-		
14	CLA	a	1135	-	60,68,73	2.29	20 (33%)	70,107,113	2.68	24 (34%)
14	CLA	L	1503	-	65,73,73	2.20	18 (27%)	76,113,113	2.60	24 (31%)
14	CLA	b	1203	-	65,73,73	2.16	20 (30%)	76,113,113	2.66	21 (27%)
14	CLA	G	1119	-	65,73,73	2.20	19 (29%)	76,113,113	2.62	24 (31%)
18	BCR	B	4009	-	41,41,41	2.96	7 (17%)	56,56,56	6.43	23 (41%)
14	CLA	a	1126	-	60,68,73	2.30	19 (31%)	70,107,113	2.61	25 (35%)
15	F6C	B	1238	-	69,74,74	2.71	23 (33%)	70,114,114	3.26	29 (41%)
14	CLA	G	1127	-	65,73,73	2.20	19 (29%)	76,113,113	2.59	22 (28%)
19	LHG	b	5004	-	43,43,48	0.97	2 (4%)	46,49,54	1.12	3 (6%)
21	LMT	G	6001	-	32,32,36	1.28	6 (18%)	43,43,47	1.05	2 (4%)
14	CLA	a	1128	-	60,68,73	2.32	19 (31%)	70,107,113	2.72	23 (32%)
14	CLA	b	1204	-	65,73,73	2.21	18 (27%)	76,113,113	2.54	27 (35%)
14	CLA	b	1220	-	55,63,73	2.38	17 (30%)	64,101,113	2.92	26 (40%)
14	CLA	b	1232	-	45,53,73	2.53	18 (40%)	52,89,113	2.86	20 (38%)
19	LHG	G	5001	-	41,41,48	0.99	2 (4%)	44,47,54	1.10	3 (6%)
16	PQN	H	2002	-	34,34,34	1.48	2 (5%)	42,45,45	1.26	2 (4%)
18	BCR	b	4009	-	41,41,41	2.96	7 (17%)	56,56,56	6.43	22 (39%)
15	F6C	H	1238	-	69,74,74	2.70	23 (33%)	70,114,114	3.26	29 (41%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
14	CLA	a	1120	-	45,53,73	2.47	17 (37%)	52,89,113	2.99	20 (38%)
14	CLA	G	1122	-	55,63,73	2.37	18 (32%)	64,101,113	2.77	26 (40%)
14	CLA	A	1126	-	60,68,73	2.30	19 (31%)	70,107,113	2.62	25 (35%)
18	BCR	B	4017	-	41,41,41	3.03	8 (19%)	56,56,56	6.74	20 (35%)
21	LMT	A	6002	-	29,29,36	1.40	6 (20%)	40,40,47	1.16	4 (10%)
14	CLA	G	1118	-	55,63,73	2.38	18 (32%)	64,101,113	2.78	27 (42%)
14	CLA	G	1110	-	45,53,73	2.51	17 (37%)	52,89,113	2.88	20 (38%)
14	CLA	L	1502	-	60,68,73	2.23	18 (30%)	70,107,113	2.75	23 (32%)
14	CLA	G	1104	-	65,73,73	2.14	19 (29%)	76,113,113	2.76	25 (32%)
14	CLA	B	1235	-	60,68,73	2.30	18 (30%)	70,107,113	2.68	22 (31%)
14	CLA	b	1202	-	60,68,73	2.19	18 (30%)	70,107,113	2.69	24 (34%)
18	BCR	A	4008	-	41,41,41	3.18	9 (21%)	56,56,56	6.45	21 (37%)
14	CLA	B	1209	-	45,53,73	2.51	18 (40%)	52,89,113	2.97	21 (40%)
14	CLA	b	1225	-	65,73,73	2.24	19 (29%)	76,113,113	2.48	21 (27%)
14	CLA	a	1134	-	45,53,73	2.61	19 (42%)	52,89,113	2.93	21 (40%)
14	CLA	H	1223	-	65,73,73	2.18	19 (29%)	76,113,113	2.67	26 (34%)
14	CLA	H	1211	-	65,73,73	2.20	20 (30%)	76,113,113	2.65	22 (28%)
15	F6C	G	1121	-	49,54,74	3.13	23 (46%)	46,90,114	3.86	28 (60%)
18	BCR	B	4004	-	41,41,41	2.85	7 (17%)	56,56,56	6.49	25 (44%)
14	CLA	H	1214	-	65,73,73	2.21	20 (30%)	76,113,113	2.55	27 (35%)
17	SF4	G	3001	2,1	0,12,12	-	-	-		
14	CLA	B	1227	-	45,53,73	2.57	19 (42%)	52,89,113	2.81	23 (44%)
14	CLA	a	1129	-	50,58,73	2.50	19 (38%)	58,95,113	2.89	23 (39%)
14	CLA	b	1022	-	65,73,73	2.15	18 (27%)	76,113,113	2.62	26 (34%)
14	CLA	H	1228	-	55,63,73	2.39	20 (36%)	64,101,113	2.83	26 (40%)
14	CLA	b	1210	-	65,73,73	2.22	20 (30%)	76,113,113	2.76	26 (34%)
18	BCR	I	4018	-	41,41,41	3.05	8 (19%)	56,56,56	6.57	24 (42%)
14	CLA	A	1132	-	65,73,73	2.16	17 (26%)	76,113,113	2.69	24 (31%)
14	CLA	b	1223	-	65,73,73	2.17	19 (29%)	76,113,113	2.65	26 (34%)
14	CLA	H	1222	-	65,73,73	2.21	19 (29%)	76,113,113	2.64	27 (35%)
14	CLA	a	1132	-	65,73,73	2.16	17 (26%)	76,113,113	2.69	24 (31%)
18	BCR	a	4001	-	41,41,41	2.95	6 (14%)	56,56,56	6.60	24 (42%)
14	CLA	a	1136	-	65,73,73	2.17	18 (27%)	76,113,113	2.58	22 (28%)
14	CLA	l	1502	-	60,68,73	2.23	18 (30%)	70,107,113	2.74	23 (32%)
18	BCR	b	4010	-	41,41,41	3.11	7 (17%)	56,56,56	6.68	21 (37%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#|Z| > 2	Counts	RMSZ	#|Z| > 2
14	CLA	H	1215	-	60,68,73	2.24	18 (30%)	70,107,113	2.59	21 (30%)

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
18	BCR	L	4019	-	-	12/29/63/63	0/2/2/2
17	SF4	N	3003	3	-	-	0/6/5/5
14	CLA	U	1501	10	1/1/15/20	14/37/115/115	-
14	CLA	U	1503	-	1/1/15/20	14/37/115/115	-
18	BCR	B	4014	-	-	7/29/63/63	0/2/2/2
18	BCR	H	4004	-	-	7/29/63/63	0/2/2/2
14	CLA	G	1109	-	1/1/15/20	19/37/115/115	-
14	CLA	b	1239	-	1/1/15/20	20/37/115/115	-
14	CLA	H	1022	-	1/1/15/20	19/37/115/115	-
18	BCR	b	4013	-	-	11/29/63/63	0/2/2/2
18	BCR	b	4005	-	-	6/29/63/63	0/2/2/2
18	BCR	I	4020	-	-	13/29/63/63	0/2/2/2
14	CLA	a	1103	-	1/1/14/20	15/31/109/115	-
18	BCR	b	4016	-	-	12/29/63/63	0/2/2/2
14	CLA	H	1204	-	1/1/15/20	16/37/115/115	-
16	PQN	A	2001	-	-	9/23/43/43	0/2/2/2
14	CLA	G	1124	-	1/1/13/20	9/25/103/115	-
14	CLA	A	1129	-	1/1/12/20	6/19/97/115	-
14	CLA	B	1217	-	1/1/13/20	13/25/103/115	-
20	LMG	i	5006	-	-	10/32/52/70	0/1/1/1
20	LMG	A	5005	-	-	19/41/61/70	0/1/1/1
13	CL0	G	1011	-	3/3/20/25	11/37/135/135	-
14	CLA	H	1221	-	1/1/15/20	12/37/115/115	-
14	CLA	l	1503	-	1/1/15/20	14/37/115/115	-
14	CLA	H	1209	-	1/1/11/20	3/13/91/115	-
14	CLA	b	1236	-	1/1/11/20	3/13/91/115	-
14	CLA	U	1502	-	1/1/14/20	13/31/109/115	-
14	CLA	H	1217	-	1/1/13/20	13/25/103/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
14	CLA	a	1118	-	1/1/13/20	11/25/103/115	-
14	CLA	G	1115	-	1/1/15/20	20/37/115/115	-
15	F6C	b	1237	-	-	21/41/97/97	-
14	CLA	A	1135	-	1/1/14/20	12/31/109/115	-
14	CLA	a	1119	-	1/1/15/20	11/37/115/115	-
14	CLA	A	1117	-	1/1/15/20	19/37/115/115	-
14	CLA	a	1116	-	1/1/13/20	10/25/103/115	-
15	F6C	A	1121	-	-	9/17/73/97	-
14	CLA	G	1130	-	1/1/13/20	9/25/103/115	-
14	CLA	A	1138	-	1/1/14/20	20/31/109/115	-
20	LMG	l	5007	-	-	15/45/65/70	0/1/1/1
14	CLA	G	1101	-	1/1/11/20	6/13/91/115	-
14	CLA	a	1013	-	1/1/14/20	13/31/109/115	-
14	CLA	A	1125	-	1/1/15/20	19/37/115/115	-
14	CLA	G	1123	-	1/1/14/20	14/31/109/115	-
14	CLA	l	1501	10	1/1/15/20	14/37/115/115	-
14	CLA	G	1113	-	1/1/11/20	8/13/91/115	-
14	CLA	b	1226	-	1/1/15/20	12/37/115/115	-
20	LMG	B	5002	-	-	13/41/61/70	0/1/1/1
14	CLA	B	1213	-	1/1/15/20	17/37/115/115	-
14	CLA	A	1119	-	1/1/15/20	11/37/115/115	-
14	CLA	B	1225	-	1/1/15/20	18/37/115/115	-
21	LMT	a	6001	-	-	7/17/57/61	0/2/2/2
14	CLA	A	1128	-	1/1/14/20	15/31/109/115	-
14	CLA	A	1118	-	1/1/13/20	11/25/103/115	-
14	CLA	a	1109	-	1/1/15/20	19/37/115/115	-
14	CLA	A	1114	-	1/1/11/20	9/13/91/115	-
14	CLA	G	1140	-	1/1/15/20	21/37/115/115	-
14	CLA	b	1216	-	1/1/15/20	21/37/115/115	-
14	CLA	B	1231	2	1/1/13/20	5/25/103/115	-
14	CLA	A	1137	-	1/1/12/20	5/19/97/115	-
18	BCR	B	4016	-	-	12/29/63/63	0/2/2/2
14	CLA	B	1224	-	1/1/15/20	17/37/115/115	-
14	CLA	a	1124	-	1/1/13/20	9/25/103/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
14	CLA	G	1012	-	1/1/15/20	10/37/115/115	-
14	CLA	H	1023	-	1/1/15/20	15/37/115/115	-
14	CLA	b	1206	2	1/1/11/20	7/13/91/115	-
14	CLA	A	1109	-	1/1/15/20	19/37/115/115	-
14	CLA	B	1021	-	1/1/15/20	22/37/115/115	-
14	CLA	G	1125	-	1/1/15/20	19/37/115/115	-
18	BCR	A	4001	-	-	14/29/63/63	0/2/2/2
14	CLA	a	1131	-	1/1/14/20	12/31/109/115	-
15	F6C	B	1237	-	-	21/41/97/97	-
16	PQN	B	2002	-	-	12/23/43/43	0/2/2/2
18	BCR	i	4018	-	-	8/29/63/63	0/2/2/2
14	CLA	H	1224	-	1/1/15/20	17/37/115/115	-
18	BCR	H	4005	-	-	6/29/63/63	0/2/2/2
14	CLA	H	1205	-	1/1/15/20	10/37/115/115	-
14	CLA	a	1139	-	1/1/11/20	3/13/91/115	-
18	BCR	H	4010	-	-	10/29/63/63	0/2/2/2
13	CL0	a	1011	-	3/3/20/25	11/37/135/135	-
14	CLA	b	1213	-	1/1/15/20	17/37/115/115	-
14	CLA	k	1401	-	1/1/11/20	7/13/91/115	-
14	CLA	b	1211	-	1/1/15/20	20/37/115/115	-
14	CLA	B	1212	-	1/1/11/20	4/13/91/115	-
14	CLA	b	1021	-	1/1/15/20	22/37/115/115	-
18	BCR	G	4003	-	-	14/29/63/63	0/2/2/2
14	CLA	B	1218	-	1/1/11/20	6/13/91/115	-
14	CLA	X	1701	-	1/1/13/20	11/25/103/115	-
14	CLA	G	1132	-	1/1/15/20	12/37/115/115	-
18	BCR	a	4002	-	-	6/29/63/63	0/2/2/2
14	CLA	H	1208	-	1/1/15/20	16/37/115/115	-
18	BCR	G	4001	-	-	14/29/63/63	0/2/2/2
18	BCR	G	4011	-	-	17/29/63/63	0/2/2/2
14	CLA	a	1123	-	1/1/14/20	14/31/109/115	-
14	CLA	b	1201	-	1/1/13/20	7/25/103/115	-
14	CLA	B	1219	-	1/1/11/20	4/13/91/115	-
20	LMG	a	5005	-	-	19/41/61/70	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
20	LMG	H	5002	-	-	13/41/61/70	0/1/1/1
14	CLA	B	1202	-	1/1/14/20	13/31/109/115	-
14	CLA	H	1239	-	1/1/15/20	20/37/115/115	-
14	CLA	A	1122	-	1/1/13/20	13/25/103/115	-
20	LMG	R	5006	-	-	10/32/52/70	0/1/1/1
14	CLA	b	1222	-	1/1/15/20	17/37/115/115	-
14	CLA	A	1106	-	1/1/14/20	13/31/109/115	-
18	BCR	b	4006	-	-	10/29/63/63	0/2/2/2
21	LMT	G	6002	-	-	7/14/54/61	0/2/2/2
14	CLA	A	1139	-	1/1/11/20	3/13/91/115	-
20	LMG	L	5007	-	-	15/45/65/70	0/1/1/1
14	CLA	b	1215	-	1/1/14/20	18/31/109/115	-
14	CLA	a	1125	-	1/1/15/20	19/37/115/115	-
14	CLA	G	1103	-	1/1/14/20	15/31/109/115	-
14	CLA	A	1101	-	1/1/11/20	6/13/91/115	-
14	CLA	L	1501	10	1/1/15/20	14/37/115/115	-
14	CLA	B	1210	-	1/1/15/20	19/37/115/115	-
18	BCR	b	4004	-	-	7/29/63/63	0/2/2/2
18	BCR	L	4022	-	-	6/29/63/63	0/2/2/2
21	LMT	A	6001	-	-	7/17/57/61	0/2/2/2
14	CLA	H	1218	-	1/1/11/20	6/13/91/115	-
14	CLA	A	1136	-	1/1/15/20	17/37/115/115	-
18	BCR	B	4006	-	-	10/29/63/63	0/2/2/2
14	CLA	B	1211	-	1/1/15/20	20/37/115/115	-
18	BCR	U	4022	-	-	6/29/63/63	0/2/2/2
17	SF4	C	3002	3	-	-	0/6/5/5
14	CLA	H	1219	-	1/1/11/20	4/13/91/115	-
14	CLA	B	1220	-	1/1/13/20	12/25/103/115	-
14	CLA	B	1232	-	1/1/11/20	2/13/91/115	-
14	CLA	G	1137	-	1/1/12/20	5/19/97/115	-
18	BCR	A	4002	-	-	6/29/63/63	0/2/2/2
14	CLA	H	1226	-	1/1/15/20	12/37/115/115	-
18	BCR	R	4018	-	-	8/29/63/63	0/2/2/2
17	SF4	C	3003	3	-	-	0/6/5/5

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
14	CLA	a	1138	-	1/1/14/20	20/31/109/115	-
18	BCR	a	4011	-	-	17/29/63/63	0/2/2/2
16	PQN	a	2001	-	-	9/23/43/43	0/2/2/2
14	CLA	b	1235	-	1/1/14/20	14/31/109/115	-
14	CLA	b	1221	-	1/1/15/20	12/37/115/115	-
18	BCR	M	4021	-	-	18/29/63/63	0/2/2/2
14	CLA	b	1209	-	1/1/11/20	3/13/91/115	-
14	CLA	B	1239	-	1/1/15/20	20/37/115/115	-
14	CLA	A	1124	-	1/1/13/20	9/25/103/115	-
14	CLA	a	1110	-	1/1/11/20	5/13/91/115	-
14	CLA	b	1217	-	1/1/13/20	13/25/103/115	-
14	CLA	G	1105	-	1/1/11/20	4/13/91/115	-
14	CLA	H	1212	-	1/1/11/20	4/13/91/115	-
14	CLA	A	1116	-	1/1/13/20	10/25/103/115	-
14	CLA	B	1223	-	1/1/15/20	18/37/115/115	-
18	BCR	A	4003	-	-	14/29/63/63	0/2/2/2
14	CLA	G	1128	-	1/1/14/20	15/31/109/115	-
14	CLA	b	1227	-	1/1/11/20	5/13/91/115	-
14	CLA	G	1133	-	1/1/14/20	9/31/109/115	-
18	BCR	H	4017	-	-	15/29/63/63	0/2/2/2
14	CLA	H	1201	-	1/1/13/20	7/25/103/115	-
18	BCR	H	4016	-	-	12/29/63/63	0/2/2/2
17	SF4	a	3001	2,1	-	-	0/6/5/5
14	CLA	A	1130	-	1/1/13/20	9/25/103/115	-
15	F6C	a	1121	-	-	9/17/73/97	-
18	BCR	m	4021	-	-	18/29/63/63	0/2/2/2
14	CLA	B	1234	-	1/1/15/20	16/37/115/115	-
18	BCR	R	4020	-	-	13/29/63/63	0/2/2/2
14	CLA	H	1213	-	1/1/15/20	17/37/115/115	-
14	CLA	B	1022	-	1/1/15/20	19/37/115/115	-
15	F6C	H	1207	-	-	20/41/97/97	-
14	CLA	H	1220	-	1/1/13/20	12/25/103/115	-
18	BCR	B	4010	-	-	10/29/63/63	0/2/2/2
18	BCR	B	4005	-	-	6/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
14	CLA	b	1023	-	1/1/15/20	15/37/115/115	-
17	SF4	c	3002	3	-	-	0/6/5/5
14	CLA	G	1139	-	1/1/11/20	3/13/91/115	-
14	CLA	T	1401	-	1/1/11/20	7/13/91/115	-
14	CLA	A	1108	-	1/1/11/20	6/13/91/115	-
14	CLA	H	1206	2	1/1/11/20	7/13/91/115	-
14	CLA	b	1228	-	1/1/13/20	16/25/103/115	-
14	CLA	A	1140	-	1/1/15/20	21/37/115/115	-
14	CLA	B	1216	-	1/1/15/20	21/37/115/115	-
14	CLA	a	1101	-	1/1/11/20	6/13/91/115	-
14	CLA	a	1107	1	1/1/11/20	3/13/91/115	-
14	CLA	A	1123	-	1/1/14/20	14/31/109/115	-
14	CLA	H	1229	-	1/1/14/20	14/31/109/115	-
14	CLA	b	1224	-	1/1/15/20	17/37/115/115	-
20	LMG	G	5005	-	-	19/41/61/70	0/1/1/1
15	F6C	B	1230	-	-	8/17/73/97	-
18	BCR	H	4006	-	-	10/29/63/63	0/2/2/2
14	CLA	H	1234	-	1/1/15/20	16/37/115/115	-
18	BCR	B	4013	-	-	11/29/63/63	0/2/2/2
14	CLA	H	1232	-	1/1/11/20	2/13/91/115	-
14	CLA	B	1214	-	1/1/15/20	15/37/115/115	-
18	BCR	H	4014	-	-	7/29/63/63	0/2/2/2
18	BCR	G	4007	-	-	12/29/63/63	0/2/2/2
14	CLA	W	1701	-	1/1/13/20	11/25/103/115	-
18	BCR	H	4009	-	-	9/29/63/63	0/2/2/2
18	BCR	U	4019	-	-	12/29/63/63	0/2/2/2
14	CLA	H	1235	-	1/1/14/20	14/31/109/115	-
18	BCR	l	4019	-	-	12/29/63/63	0/2/2/2
14	CLA	b	1208	-	1/1/15/20	16/37/115/115	-
14	CLA	b	1229	-	1/1/14/20	14/31/109/115	-
14	CLA	G	1134	-	1/1/11/20	8/13/91/115	-
18	BCR	a	4003	-	-	14/29/63/63	0/2/2/2
14	CLA	x	1701	-	1/1/13/20	11/25/103/115	-
19	LHG	B	5004	-	-	25/48/48/53	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
14	CLA	A	1105	-	1/1/11/20	4/13/91/115	-
14	CLA	A	1102	-	1/1/14/20	16/31/109/115	-
14	CLA	G	1108	-	1/1/11/20	6/13/91/115	-
19	LHG	a	5001	-	-	23/46/46/53	-
18	BCR	G	4002	-	-	6/29/63/63	0/2/2/2
14	CLA	A	1111	-	1/1/14/20	15/31/109/115	-
14	CLA	a	1130	-	1/1/13/20	9/25/103/115	-
18	BCR	V	4021	-	-	18/29/63/63	0/2/2/2
14	CLA	A	1131	-	1/1/14/20	12/31/109/115	-
14	CLA	a	1104	-	1/1/15/20	10/37/115/115	-
14	CLA	G	1126	-	1/1/14/20	21/31/109/115	-
14	CLA	B	1204	-	1/1/15/20	16/37/115/115	-
14	CLA	B	1226	-	1/1/15/20	12/37/115/115	-
14	CLA	A	1110	-	1/1/11/20	5/13/91/115	-
14	CLA	B	1203	-	1/1/15/20	16/37/115/115	-
15	F6C	b	1230	-	-	8/17/73/97	-
14	CLA	b	1218	-	1/1/11/20	6/13/91/115	-
14	CLA	A	1115	-	1/1/15/20	20/37/115/115	-
14	CLA	b	1231	2	1/1/13/20	5/25/103/115	-
14	CLA	B	1205	-	1/1/15/20	10/37/115/115	-
14	CLA	G	1111	-	1/1/14/20	15/31/109/115	-
14	CLA	B	1215	-	1/1/14/20	18/31/109/115	-
14	CLA	H	1227	-	1/1/11/20	5/13/91/115	-
14	CLA	a	1117	-	1/1/15/20	19/37/115/115	-
14	CLA	A	1133	-	1/1/14/20	9/31/109/115	-
14	CLA	H	1203	-	1/1/15/20	16/37/115/115	-
18	BCR	b	4014	-	-	7/29/63/63	0/2/2/2
17	SF4	c	3003	3	-	-	0/6/5/5
14	CLA	G	1112	-	1/1/13/20	13/25/103/115	-
14	CLA	B	1206	2	1/1/11/20	7/13/91/115	-
14	CLA	K	1401	-	1/1/11/20	7/13/91/115	-
14	CLA	a	1140	-	1/1/15/20	21/37/115/115	-
14	CLA	A	1013	-	1/1/14/20	13/31/109/115	-
14	CLA	G	1013	-	1/1/14/20	13/31/109/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
14	CLA	b	1234	-	1/1/15/20	16/37/115/115	-
19	LHG	H	5004	-	-	25/48/48/53	-
14	CLA	b	1205	-	1/1/15/20	10/37/115/115	-
14	CLA	G	1131	-	1/1/14/20	12/31/109/115	-
20	LMG	I	5006	-	-	10/32/52/70	0/1/1/1
18	BCR	G	4008	-	-	12/29/63/63	0/2/2/2
14	CLA	A	1112	-	1/1/13/20	13/25/103/115	-
14	CLA	A	1107	1	1/1/11/20	3/13/91/115	-
19	LHG	A	5001	-	-	23/46/46/53	-
14	CLA	a	1127	-	1/1/15/20	15/37/115/115	-
14	CLA	a	1113	-	1/1/11/20	8/13/91/115	-
14	CLA	A	1012	-	1/1/15/20	10/37/115/115	-
14	CLA	G	1138	-	1/1/14/20	20/31/109/115	-
18	BCR	b	4017	-	-	15/29/63/63	0/2/2/2
18	BCR	A	4007	-	-	12/29/63/63	0/2/2/2
17	SF4	A	3001	2,1	-	-	0/6/5/5
14	CLA	B	1221	-	1/1/15/20	12/37/115/115	-
14	CLA	b	1219	-	1/1/11/20	4/13/91/115	-
14	CLA	a	1108	-	1/1/11/20	6/13/91/115	-
14	CLA	H	1202	-	1/1/14/20	13/31/109/115	-
14	CLA	B	1236	-	1/1/11/20	3/13/91/115	-
18	BCR	i	4020	-	-	13/29/63/63	0/2/2/2
14	CLA	B	1233	-	1/1/11/20	7/13/91/115	-
14	CLA	H	1216	-	1/1/15/20	21/37/115/115	-
14	CLA	H	1225	-	1/1/15/20	18/37/115/115	-
14	CLA	G	1106	-	1/1/14/20	13/31/109/115	-
14	CLA	G	1116	-	1/1/13/20	10/25/103/115	-
14	CLA	A	1127	-	1/1/15/20	15/37/115/115	-
14	CLA	G	1114	-	1/1/11/20	9/13/91/115	-
14	CLA	a	1122	-	1/1/13/20	13/25/103/115	-
14	CLA	H	1233	-	1/1/11/20	7/13/91/115	-
14	CLA	G	1107	1	1/1/11/20	3/13/91/115	-
18	BCR	l	4022	-	-	6/29/63/63	0/2/2/2
14	CLA	H	1210	-	1/1/15/20	19/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
14	CLA	B	1023	-	1/1/15/20	15/37/115/115	-
14	CLA	a	1112	-	1/1/13/20	13/25/103/115	-
21	LMT	a	6002	-	-	7/14/54/61	0/2/2/2
14	CLA	A	1104	-	1/1/15/20	10/37/115/115	-
14	CLA	B	1228	-	1/1/13/20	16/25/103/115	-
15	F6C	B	1207	-	-	20/41/97/97	-
14	CLA	G	1135	-	1/1/14/20	13/31/109/115	-
14	CLA	A	1120	-	1/1/11/20	7/13/91/115	-
14	CLA	H	1021	-	1/1/15/20	22/37/115/115	-
20	LMG	U	5007	-	-	15/45/65/70	0/1/1/1
16	PQN	b	2002	-	-	12/23/43/43	0/2/2/2
18	BCR	a	4008	-	-	12/29/63/63	0/2/2/2
14	CLA	a	1111	-	1/1/14/20	15/31/109/115	-
14	CLA	a	1012	-	1/1/15/20	10/37/115/115	-
14	CLA	B	1208	-	1/1/15/20	16/37/115/115	-
15	F6C	b	1207	-	-	20/41/97/97	-
14	CLA	B	1222	-	1/1/15/20	17/37/115/115	-
14	CLA	A	1103	-	1/1/14/20	15/31/109/115	-
15	F6C	H	1230	-	-	8/17/73/97	-
14	CLA	a	1106	-	1/1/14/20	13/31/109/115	-
14	CLA	H	1231	2	1/1/13/20	5/25/103/115	-
18	BCR	H	4013	-	-	11/29/63/63	0/2/2/2
13	CL0	A	1011	-	3/3/20/25	11/37/135/135	-
14	CLA	a	1114	-	1/1/11/20	9/13/91/115	-
14	CLA	b	1212	-	1/1/11/20	4/13/91/115	-
18	BCR	A	4011	-	-	17/29/63/63	0/2/2/2
14	CLA	a	1105	-	1/1/11/20	4/13/91/115	-
14	CLA	a	1115	-	1/1/15/20	20/37/115/115	-
14	CLA	G	1102	-	1/1/14/20	16/31/109/115	-
14	CLA	G	1120	-	1/1/11/20	7/13/91/115	-
14	CLA	b	1214	-	1/1/15/20	15/37/115/115	-
14	CLA	a	1133	-	1/1/14/20	9/31/109/115	-
14	CLA	G	1117	-	1/1/15/20	19/37/115/115	-
18	BCR	a	4007	-	-	12/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
14	CLA	a	1102	-	1/1/14/20	16/31/109/115	-
14	CLA	B	1201	-	1/1/13/20	7/25/103/115	-
14	CLA	H	1236	-	1/1/11/20	3/13/91/115	-
20	LMG	b	5002	-	-	13/41/61/70	0/1/1/1
15	F6C	b	1238	-	-	16/41/97/97	-
14	CLA	b	1233	-	1/1/11/20	7/13/91/115	-
16	PQN	G	2001	-	-	9/23/43/43	0/2/2/2
15	F6C	H	1237	-	-	21/41/97/97	-
14	CLA	B	1229	-	1/1/14/20	14/31/109/115	-
14	CLA	G	1136	-	1/1/15/20	17/37/115/115	-
14	CLA	a	1137	-	1/1/12/20	5/19/97/115	-
14	CLA	A	1113	-	1/1/11/20	8/13/91/115	-
14	CLA	A	1134	-	1/1/11/20	8/13/91/115	-
14	CLA	G	1129	-	1/1/12/20	6/19/97/115	-
17	SF4	N	3002	3	-	-	0/6/5/5
14	CLA	a	1135	-	1/1/14/20	12/31/109/115	-
14	CLA	L	1503	-	1/1/15/20	14/37/115/115	-
14	CLA	b	1203	-	1/1/15/20	16/37/115/115	-
14	CLA	G	1119	-	1/1/15/20	11/37/115/115	-
18	BCR	B	4009	-	-	9/29/63/63	0/2/2/2
14	CLA	a	1126	-	1/1/14/20	21/31/109/115	-
15	F6C	B	1238	-	-	16/41/97/97	-
14	CLA	G	1127	-	1/1/15/20	15/37/115/115	-
19	LHG	b	5004	-	-	25/48/48/53	-
21	LMT	G	6001	-	-	7/17/57/61	0/2/2/2
14	CLA	a	1128	-	1/1/14/20	15/31/109/115	-
14	CLA	b	1204	-	1/1/15/20	16/37/115/115	-
14	CLA	b	1220	-	1/1/13/20	12/25/103/115	-
14	CLA	b	1232	-	1/1/11/20	2/13/91/115	-
19	LHG	G	5001	-	-	23/46/46/53	-
16	PQN	H	2002	-	-	12/23/43/43	0/2/2/2
18	BCR	b	4009	-	-	9/29/63/63	0/2/2/2
15	F6C	H	1238	-	-	16/41/97/97	-
14	CLA	a	1120	-	1/1/11/20	7/13/91/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
14	CLA	G	1122	-	1/1/13/20	13/25/103/115	-
14	CLA	A	1126	-	1/1/14/20	21/31/109/115	-
18	BCR	B	4017	-	-	15/29/63/63	0/2/2/2
21	LMT	A	6002	-	-	7/14/54/61	0/2/2/2
14	CLA	G	1118	-	1/1/13/20	11/25/103/115	-
14	CLA	G	1110	-	1/1/11/20	5/13/91/115	-
14	CLA	L	1502	-	1/1/14/20	13/31/109/115	-
14	CLA	G	1104	-	1/1/15/20	10/37/115/115	-
14	CLA	B	1235	-	1/1/14/20	14/31/109/115	-
14	CLA	b	1202	-	1/1/14/20	13/31/109/115	-
18	BCR	A	4008	-	-	12/29/63/63	0/2/2/2
14	CLA	B	1209	-	1/1/11/20	3/13/91/115	-
14	CLA	b	1225	-	1/1/15/20	18/37/115/115	-
14	CLA	a	1134	-	1/1/11/20	8/13/91/115	-
14	CLA	H	1223	-	1/1/15/20	18/37/115/115	-
14	CLA	H	1211	-	1/1/15/20	20/37/115/115	-
15	F6C	G	1121	-	-	9/17/73/97	-
18	BCR	B	4004	-	-	7/29/63/63	0/2/2/2
14	CLA	H	1214	-	1/1/15/20	15/37/115/115	-
17	SF4	G	3001	2,1	-	-	0/6/5/5
14	CLA	B	1227	-	1/1/11/20	5/13/91/115	-
14	CLA	a	1129	-	1/1/12/20	6/19/97/115	-
14	CLA	b	1022	-	1/1/15/20	19/37/115/115	-
14	CLA	H	1228	-	1/1/13/20	16/25/103/115	-
14	CLA	b	1210	-	1/1/15/20	19/37/115/115	-
18	BCR	I	4018	-	-	8/29/63/63	0/2/2/2
14	CLA	A	1132	-	1/1/15/20	12/37/115/115	-
14	CLA	b	1223	-	1/1/15/20	18/37/115/115	-
14	CLA	H	1222	-	1/1/15/20	17/37/115/115	-
14	CLA	a	1132	-	1/1/15/20	12/37/115/115	-
18	BCR	a	4001	-	-	14/29/63/63	0/2/2/2
14	CLA	a	1136	-	1/1/15/20	17/37/115/115	-
14	CLA	l	1502	-	1/1/14/20	13/31/109/115	-
18	BCR	b	4010	-	-	10/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
14	CLA	H	1215	-	1/1/14/20	19/31/109/115	-

The worst 5 of 5605 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	A	4002	BCR	C10-C9	-9.91	1.22	1.35
18	G	4002	BCR	C10-C9	-9.90	1.22	1.35
18	a	4002	BCR	C10-C9	-9.85	1.22	1.35
18	A	4007	BCR	C10-C9	-9.09	1.23	1.35
18	G	4008	BCR	C10-C9	-9.08	1.23	1.35

The worst 5 of 7829 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
18	H	4010	BCR	C16-C17-C18	25.75	164.06	127.31
18	b	4010	BCR	C16-C17-C18	25.71	164.00	127.31
18	B	4010	BCR	C16-C17-C18	25.69	163.97	127.31
18	H	4017	BCR	C20-C21-C22	24.30	161.99	127.31
18	B	4017	BCR	C20-C21-C22	24.30	161.99	127.31

5 of 261 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
13	G	1011	CL0	NC
13	G	1011	CL0	ND
13	G	1011	CL0	NA
13	a	1011	CL0	NC
13	a	1011	CL0	ND

5 of 4427 torsion outliers are listed below:

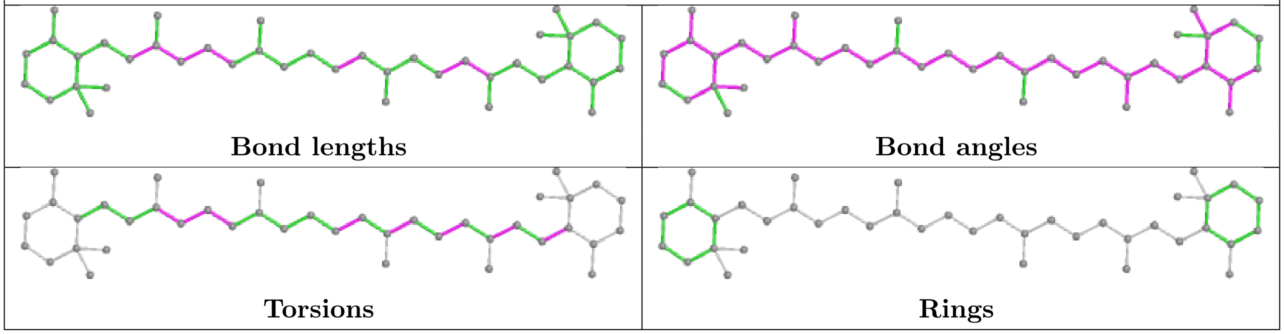
Mol	Chain	Res	Type	Atoms
14	G	1013	CLA	C1A-C2A-CAA-CBA
14	G	1013	CLA	C3A-C2A-CAA-CBA
14	G	1013	CLA	C11-C10-C8-C9
14	G	1101	CLA	CHA-CBD-CGD-O2D
14	G	1102	CLA	C1A-C2A-CAA-CBA

There are no ring outliers.

No monomer is involved in short contacts.

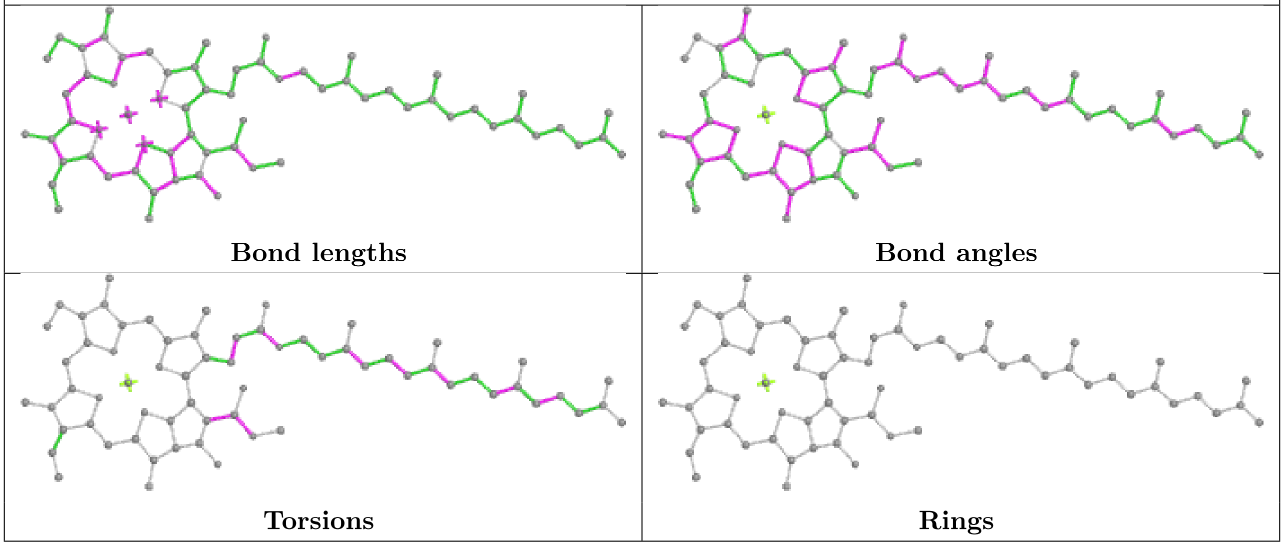
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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 BCR L 4019



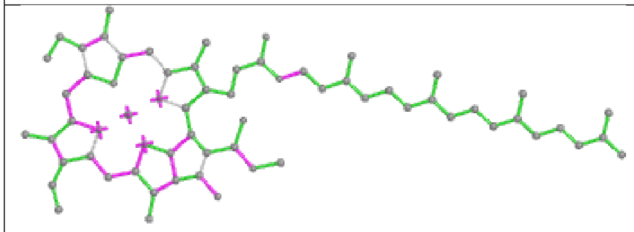
Bond lengths **Bond angles** **Torsions** **Rings**

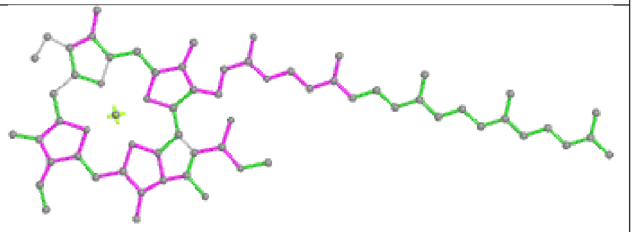
Ligand CLA U 1501

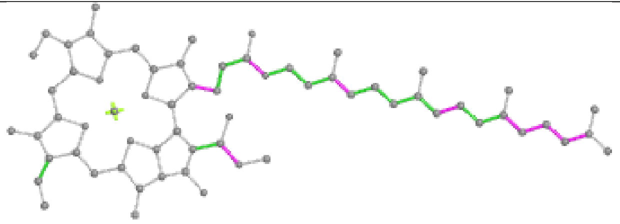


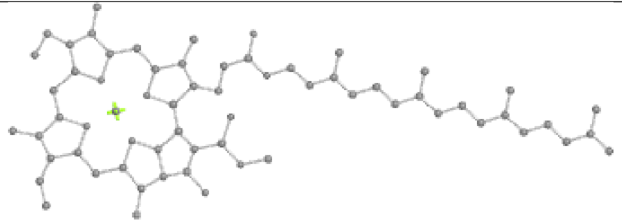
Bond lengths **Bond angles** **Torsions** **Rings**

Ligand CLA U 1503

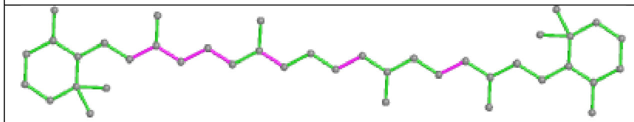

Bond lengths


Bond angles


Torsions


Rings

Ligand BCR B 4014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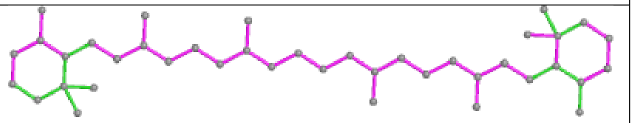
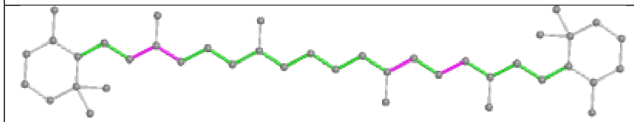

Bond angles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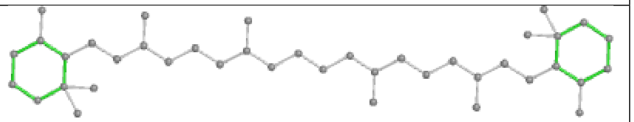
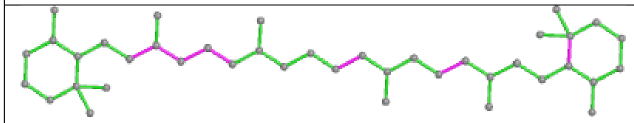
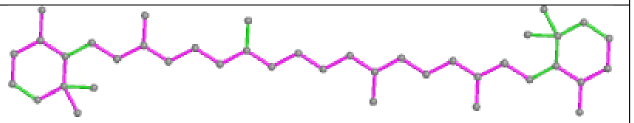
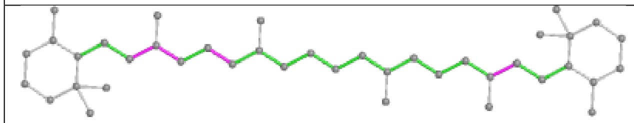

Rings

Ligand BCR H 4004


Bond lengths


Bond angles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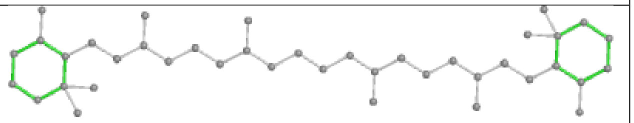
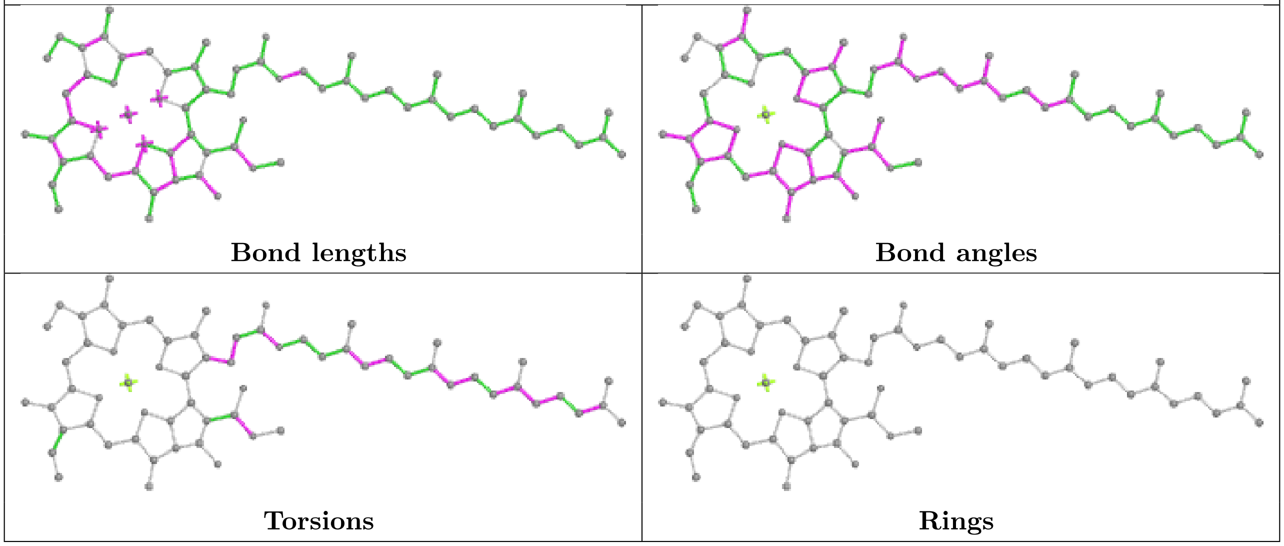

Rings

Ligand CLA G 1109



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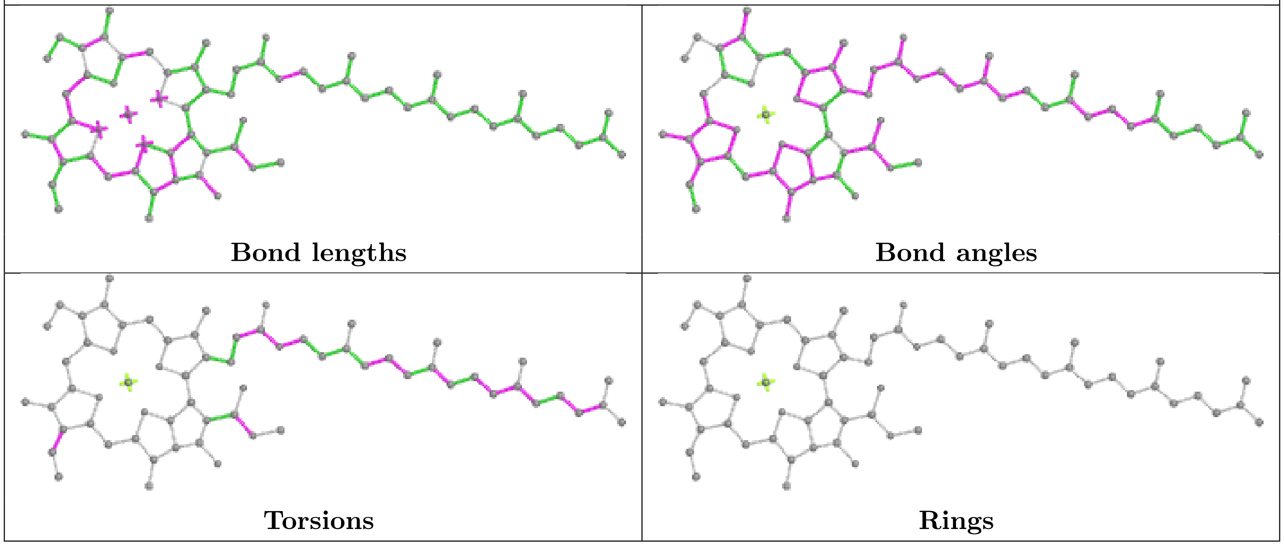

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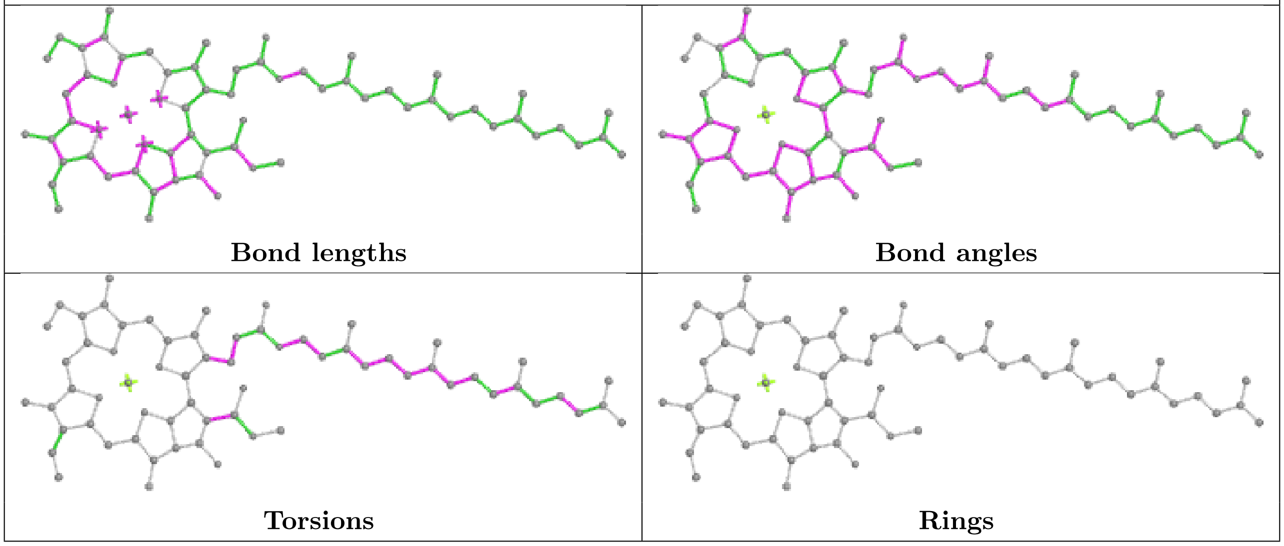

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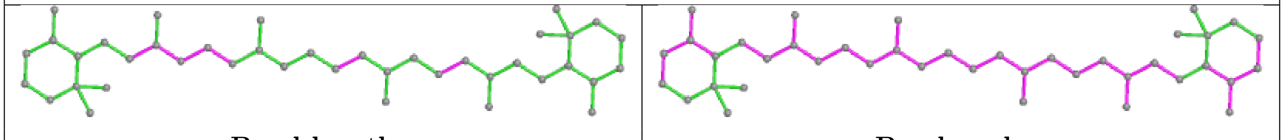
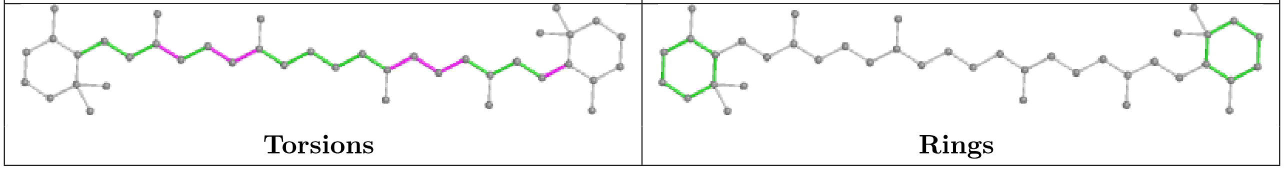
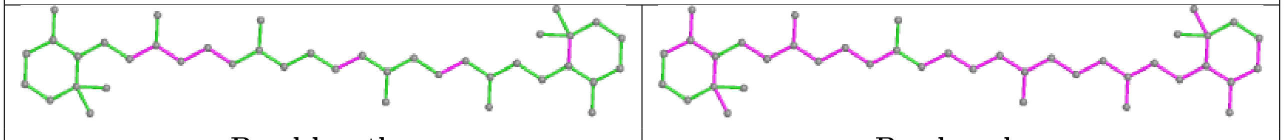


Bond lengths Bond angles

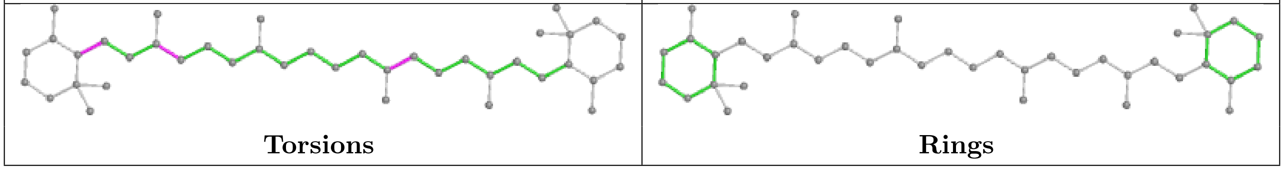


Torsions Rings

Ligand BCR b 4005

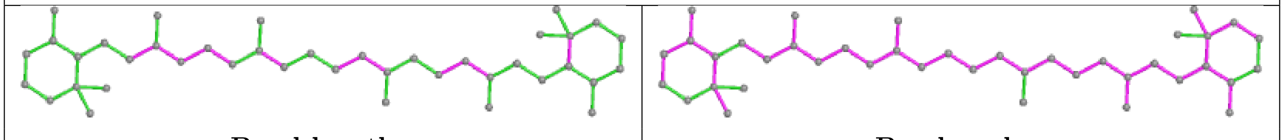


Bond lengths Bond angles

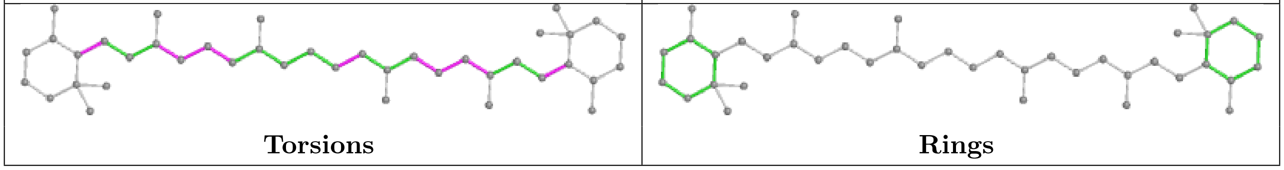


Torsions Rings

Ligand BCR I 4020

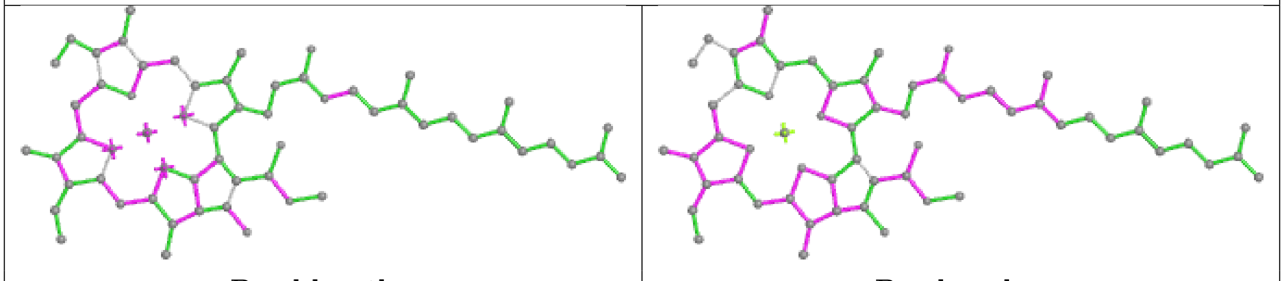


Bond lengths Bond angles

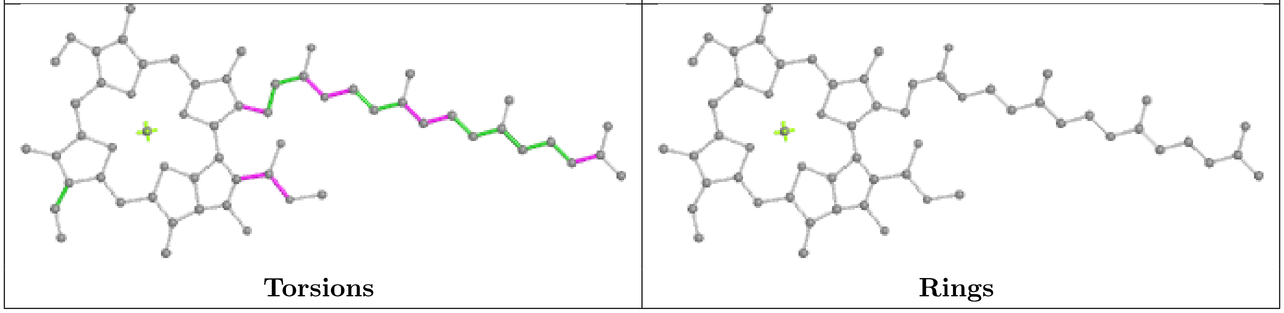


Torsions Rings

Ligand CLA a 1103

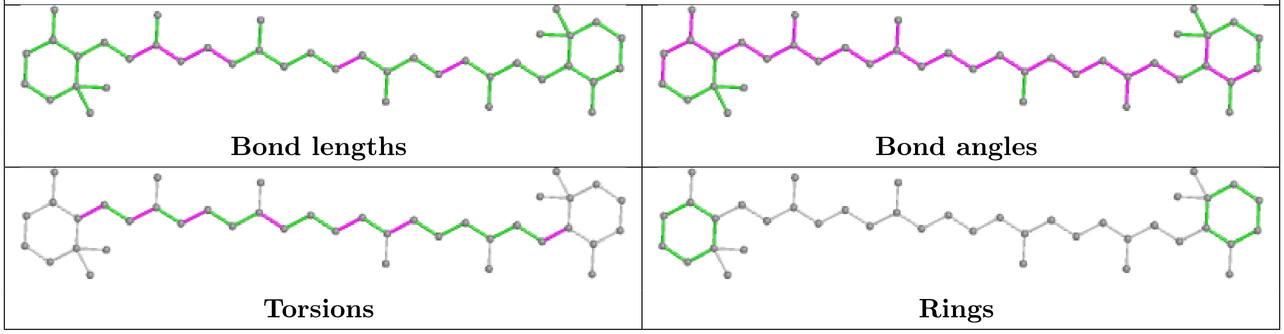


Bond lengths Bond angles



Torsions Rings

Ligand BCR b 4016



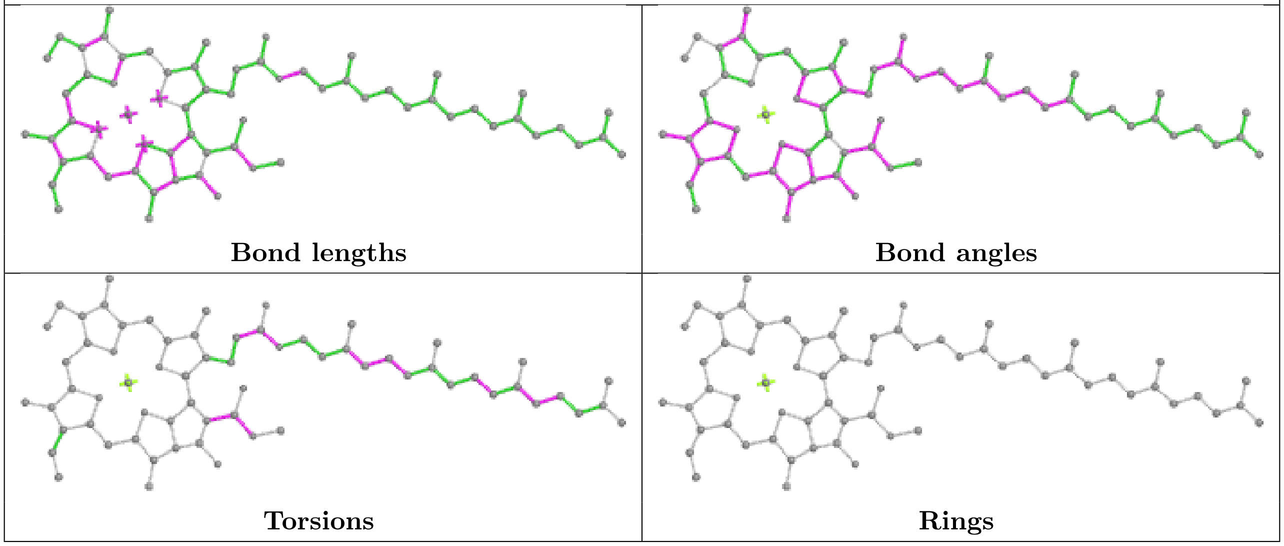
Bond lengths

Bond angles

Torsions

Rings

Ligand CLA H 1204



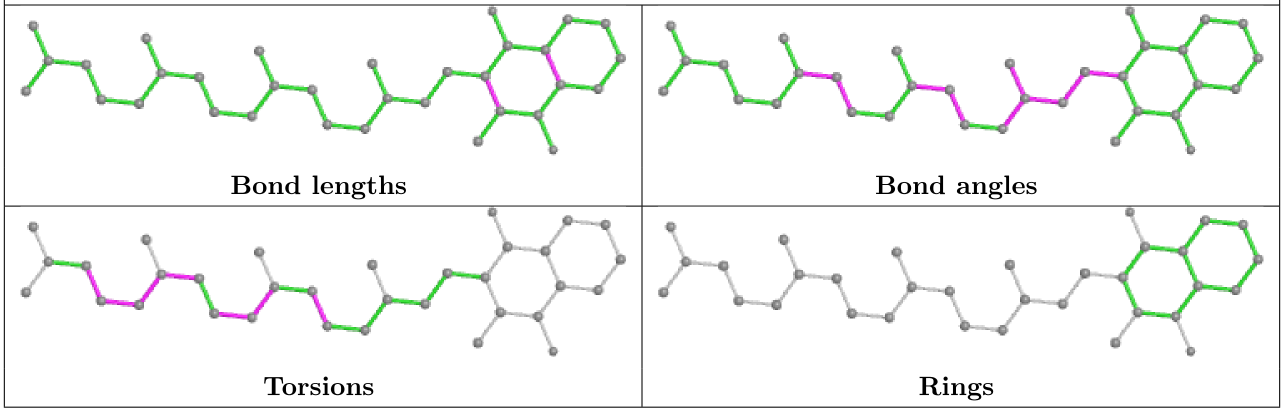
Bond lengths

Bond angles

Torsions

Rings

Ligand PQN A 2001



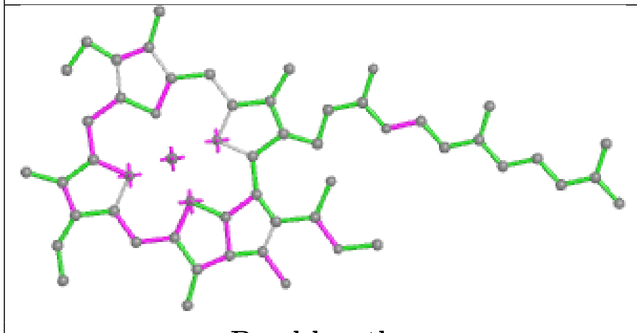
Bond lengths

Bond angles

Torsions

Rings

Ligand CLA G 1124



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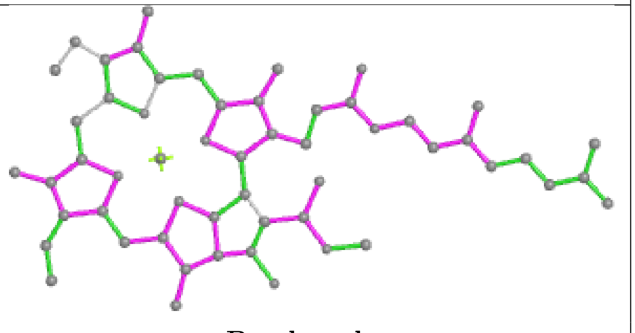
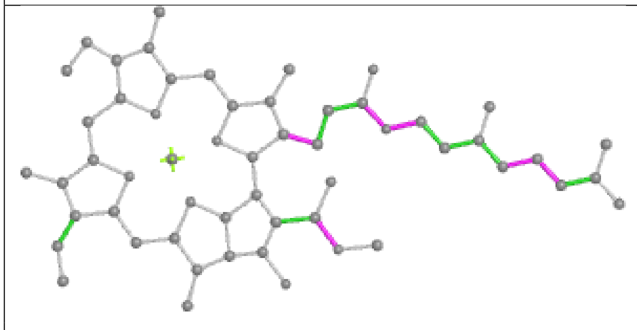
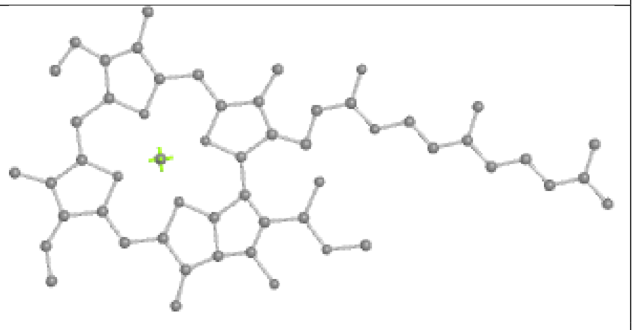


Bond angles

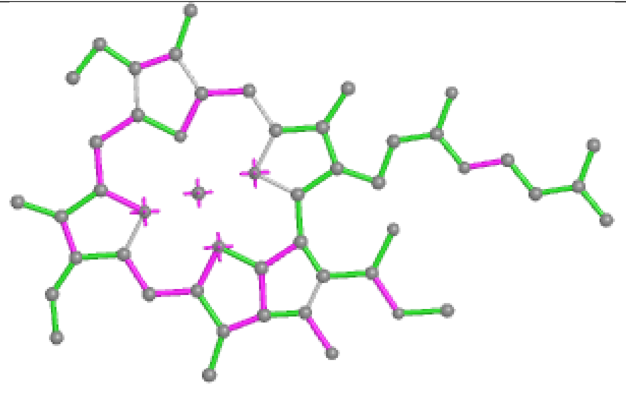


Torsions

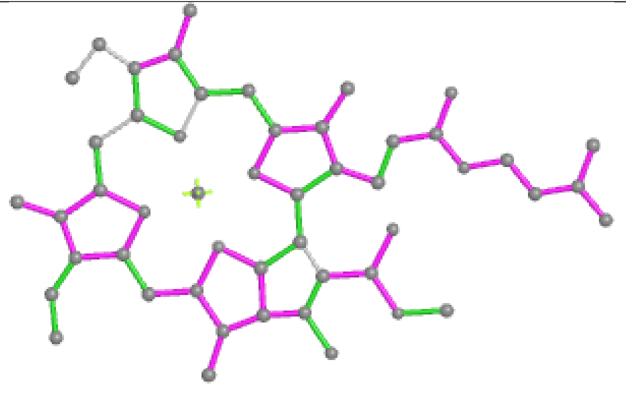


Rings

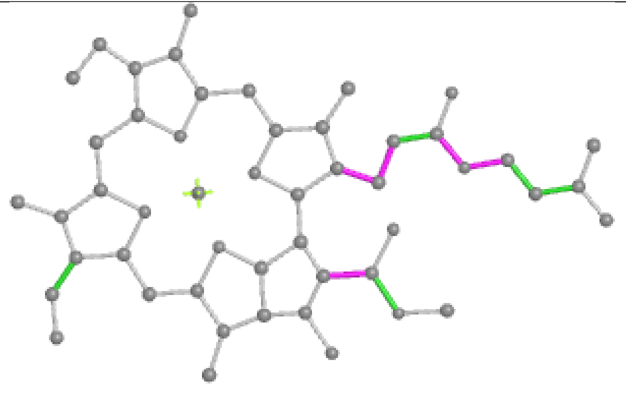
Ligand CLA A 1129



Bond lengths



Bond angles



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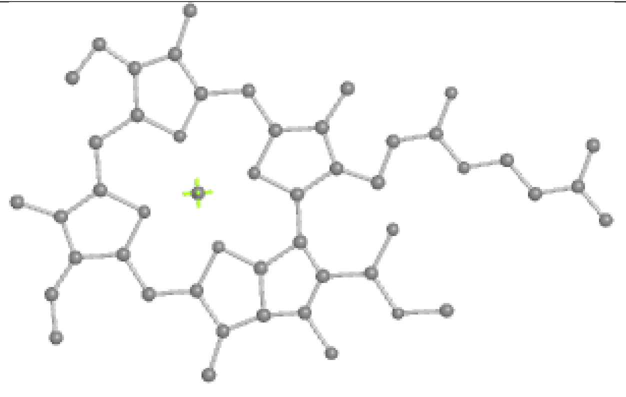
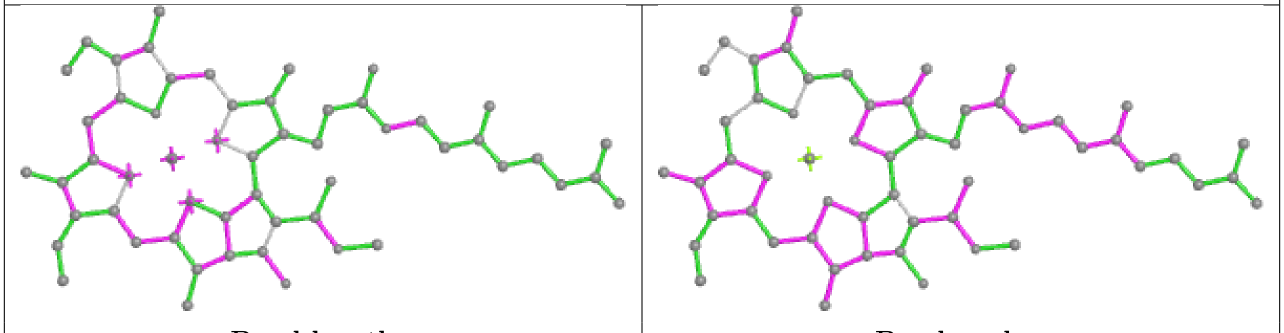
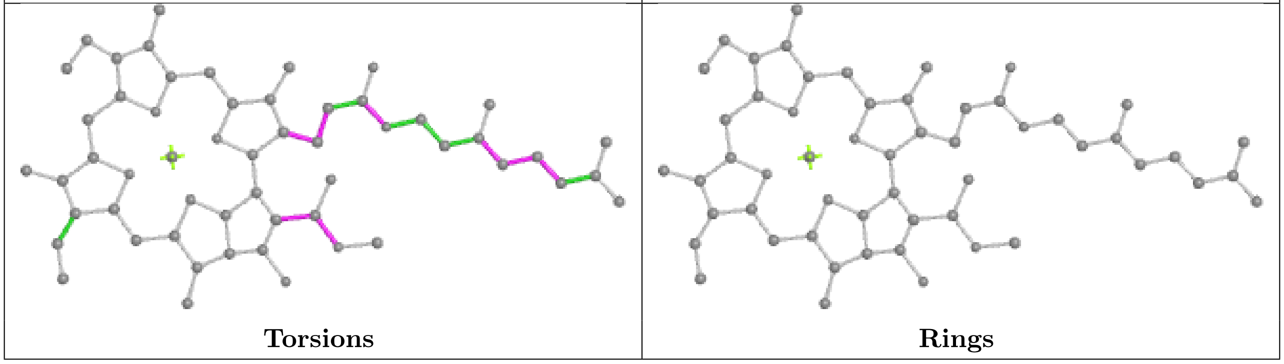


Rings

Ligand CLA B 1217

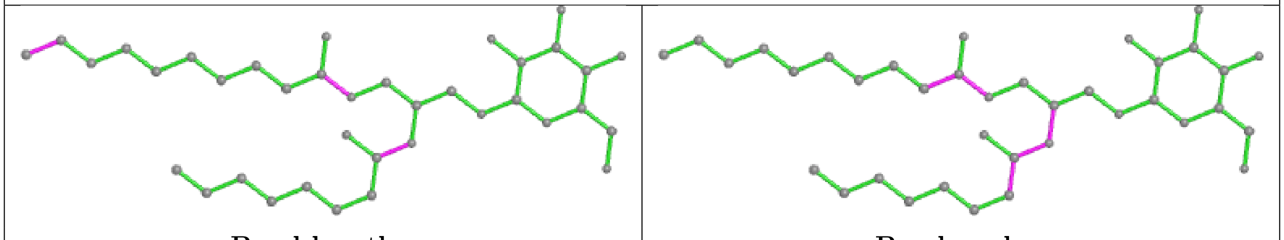


Bond lengths Bond angles

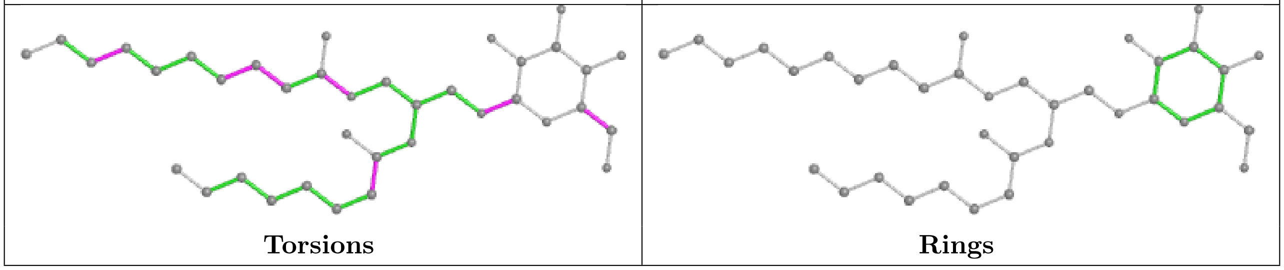


Torsions Rings

Ligand LMG i 5006

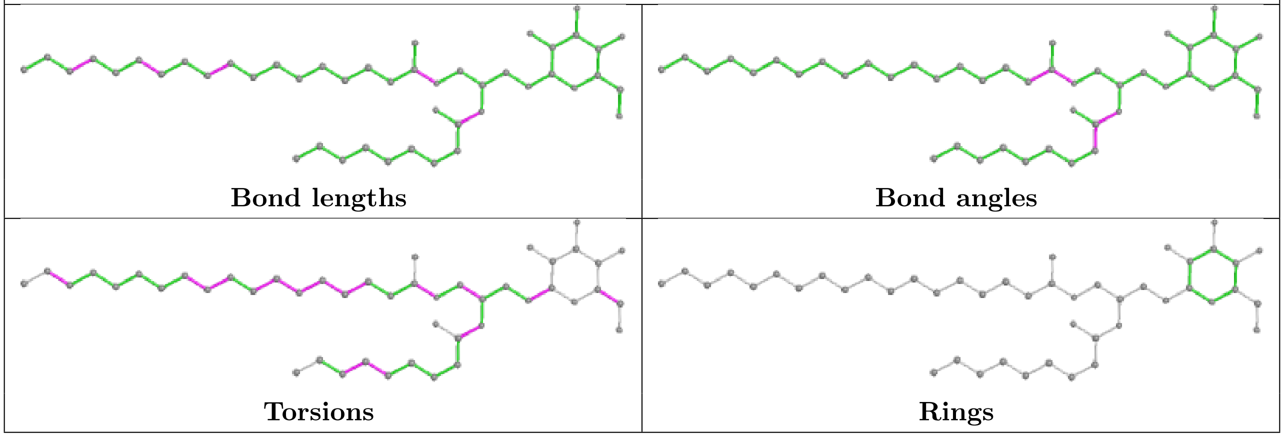


Bond lengths Bond angles

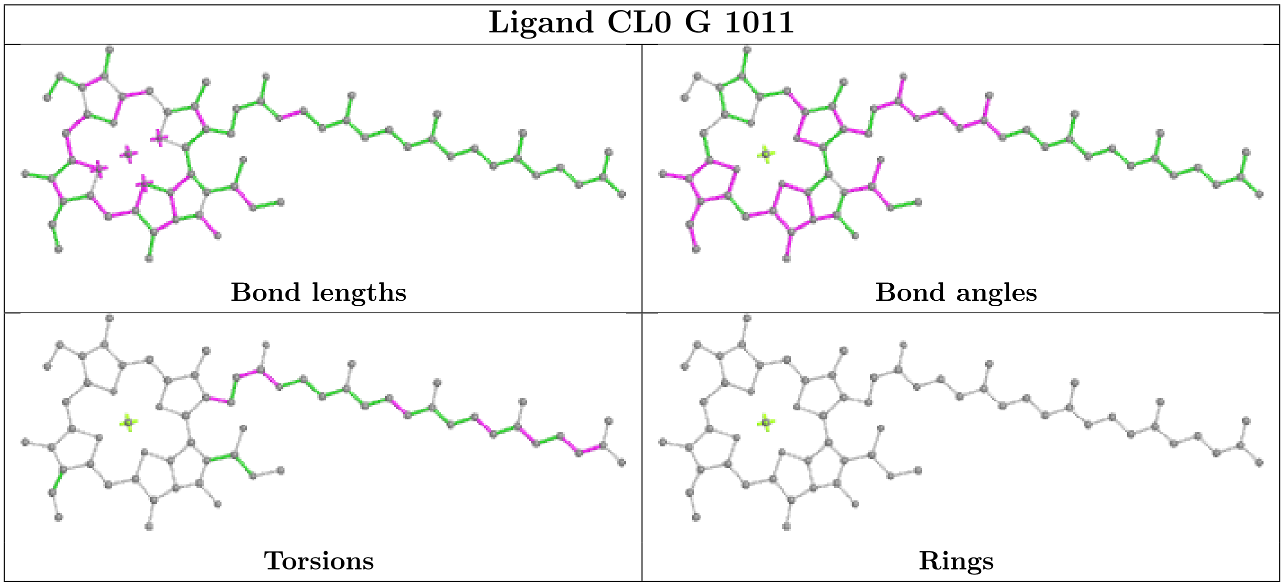


Torsions Rings

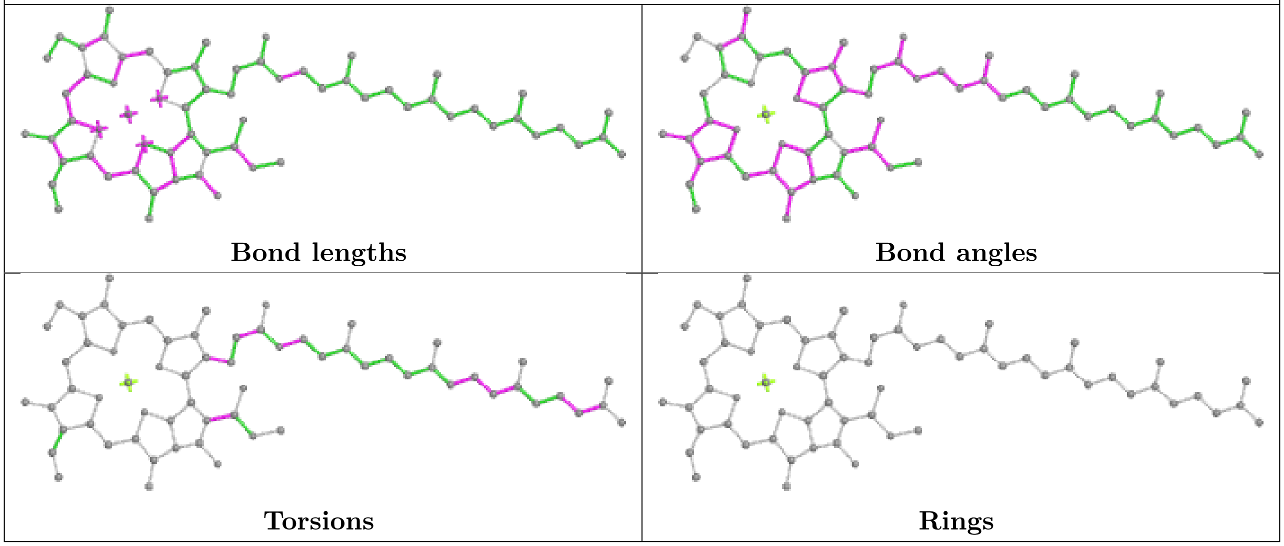
Ligand LMG A 5005



Ligand CL0 G 1011



Ligand CLA H 1221



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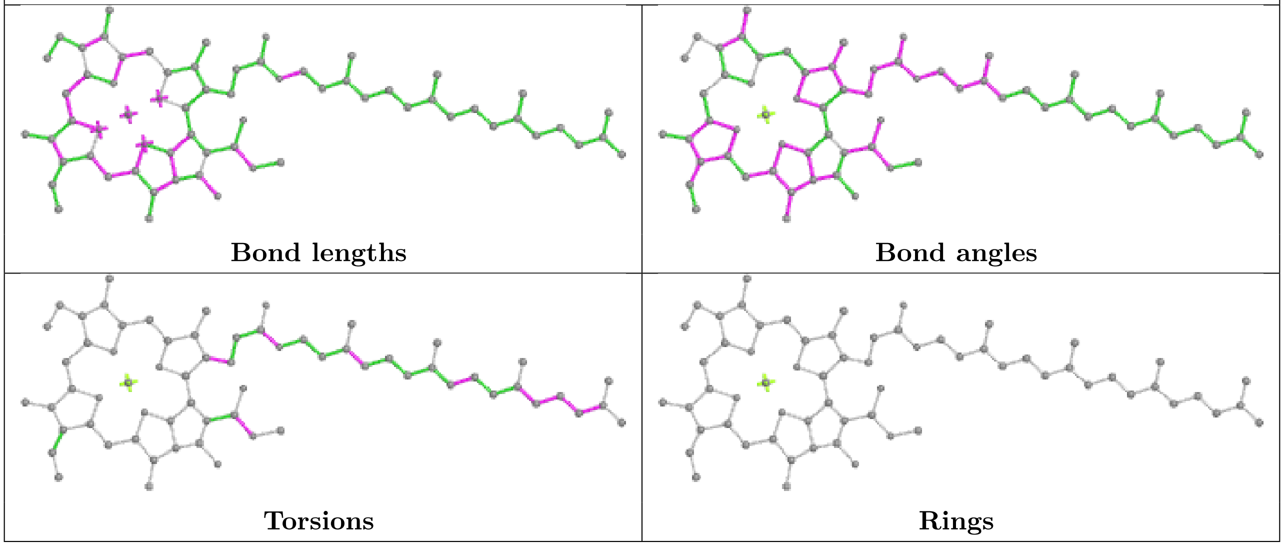


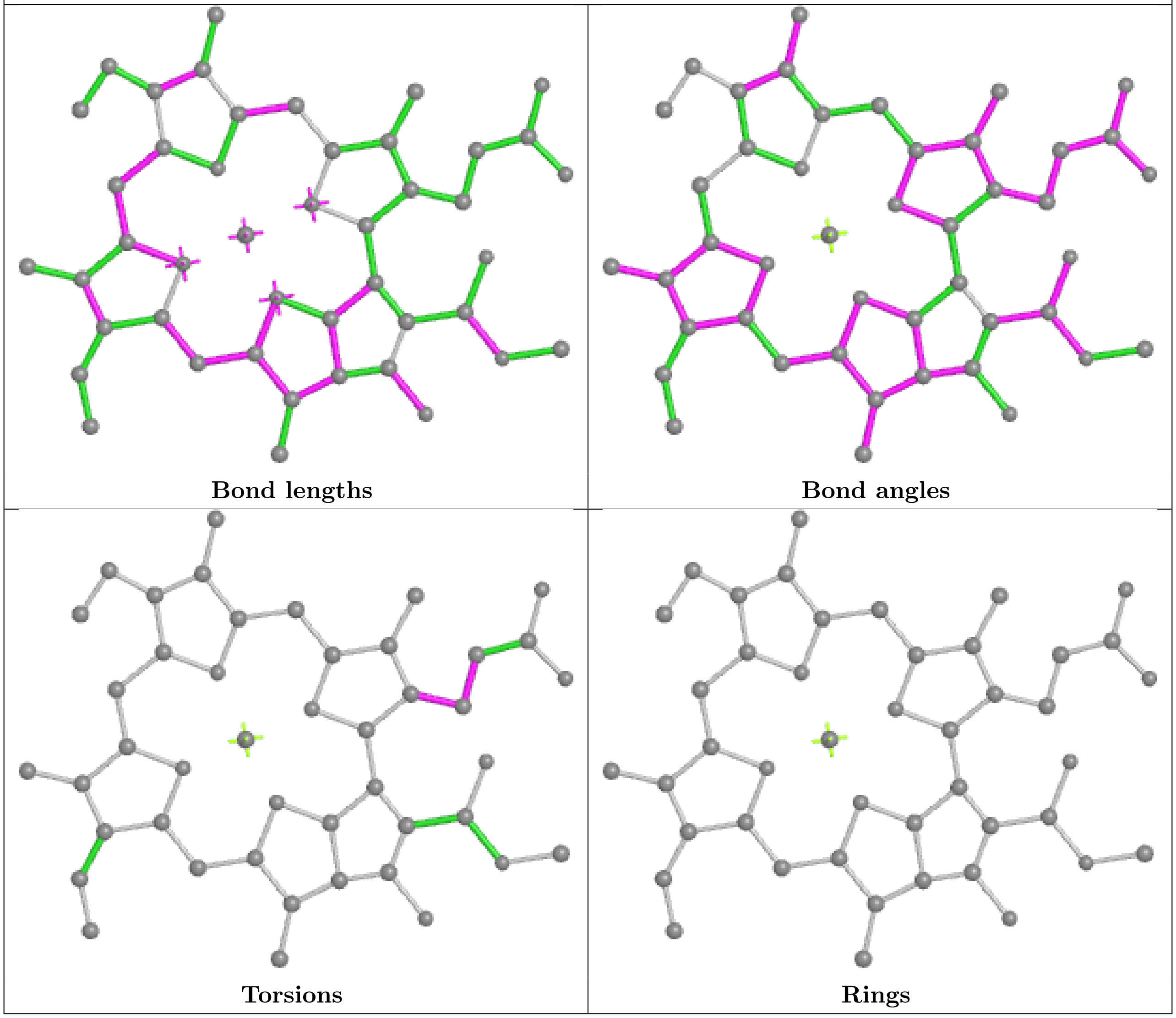
Bond lengths

Bond angles

Torsions

Rings

Ligand CLA H 1209

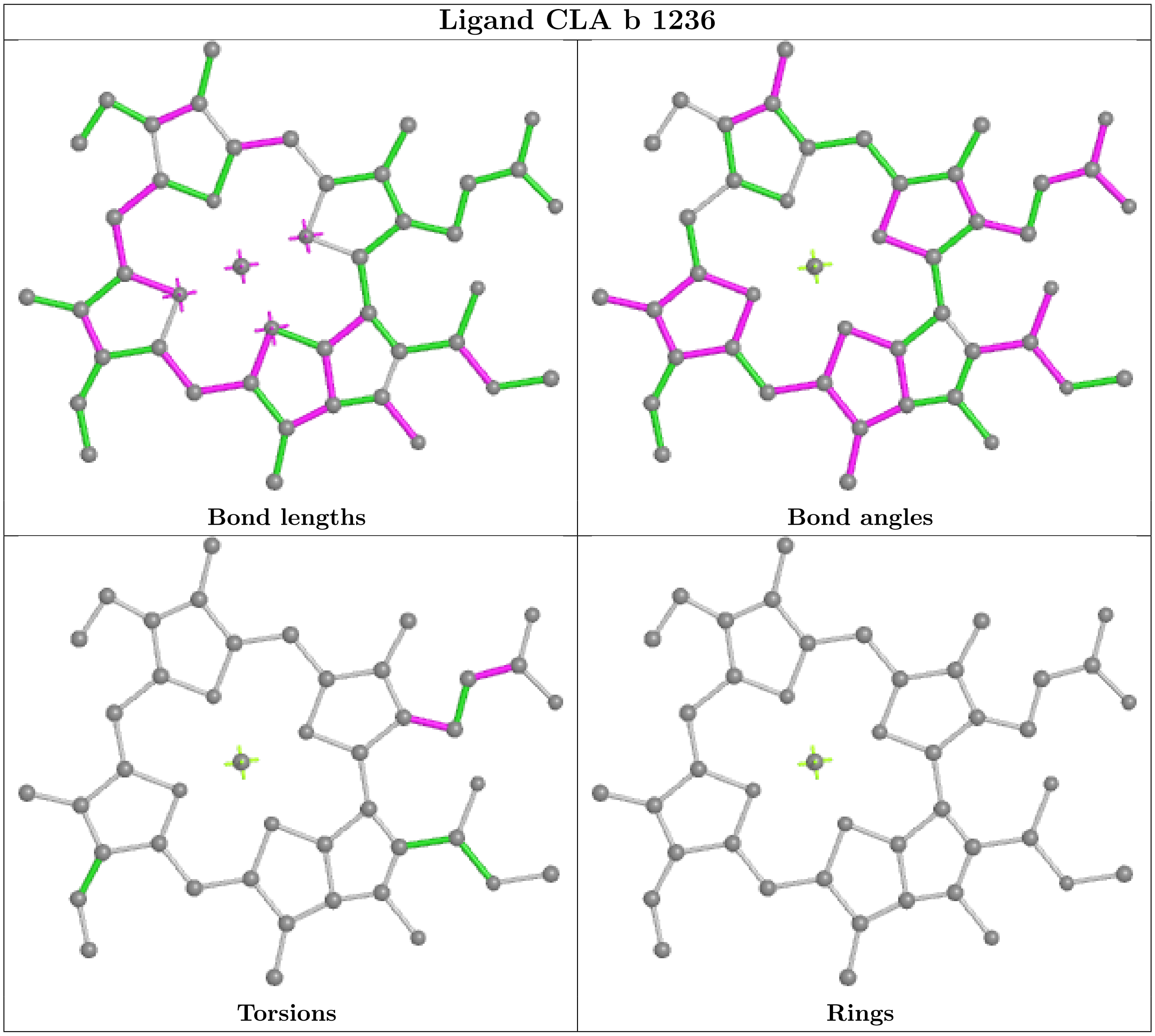


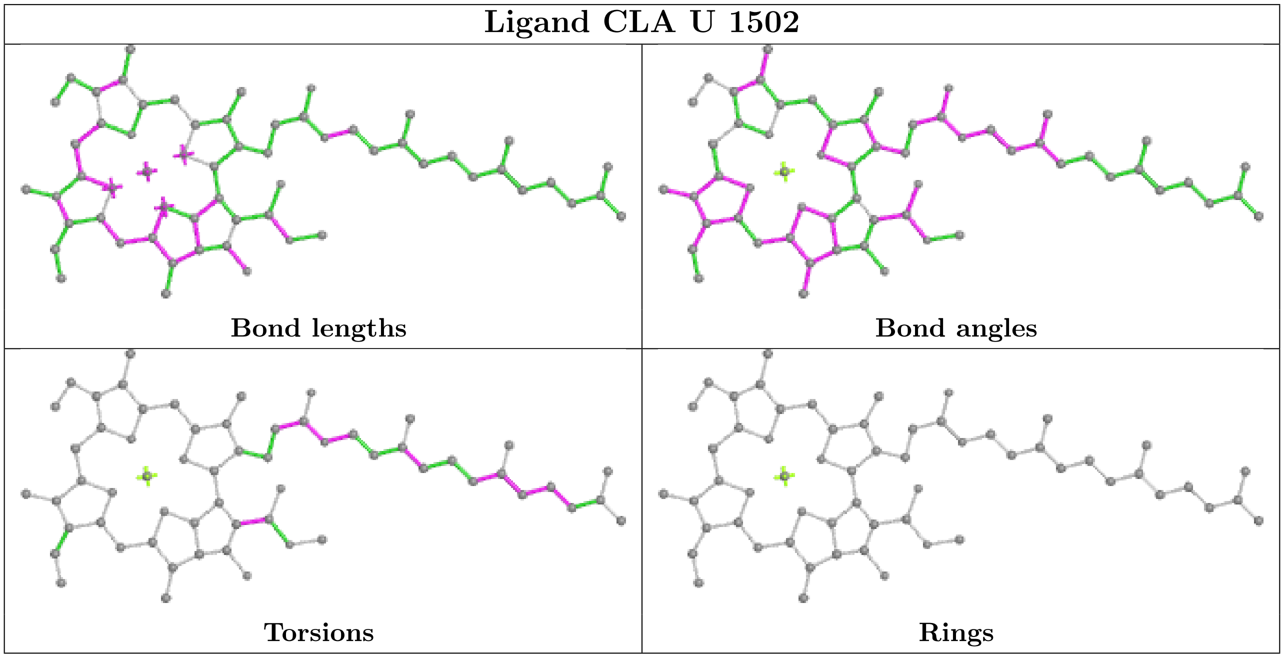
Bond lengths

Bond angles

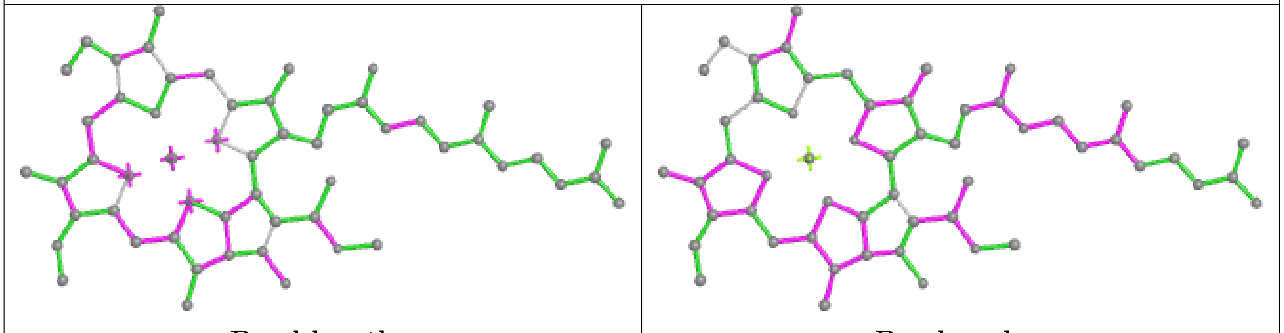
Torsions

Rings

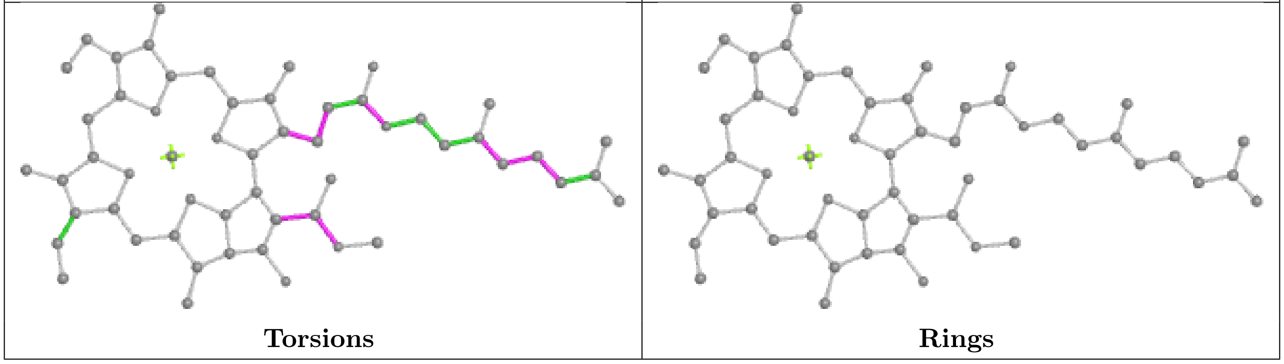

Ligand CLA b 1236
Bond lengths
Bond angles
Torsions
Rings


Ligand CLA U 1502
Bond lengths
Bond angles
Torsions
Rings

Ligand CLA H 1217

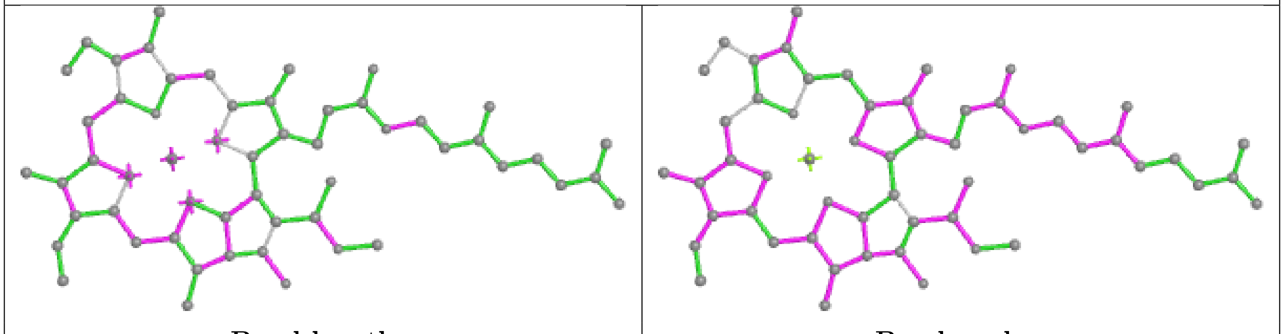


Bond lengths **Bond angles**

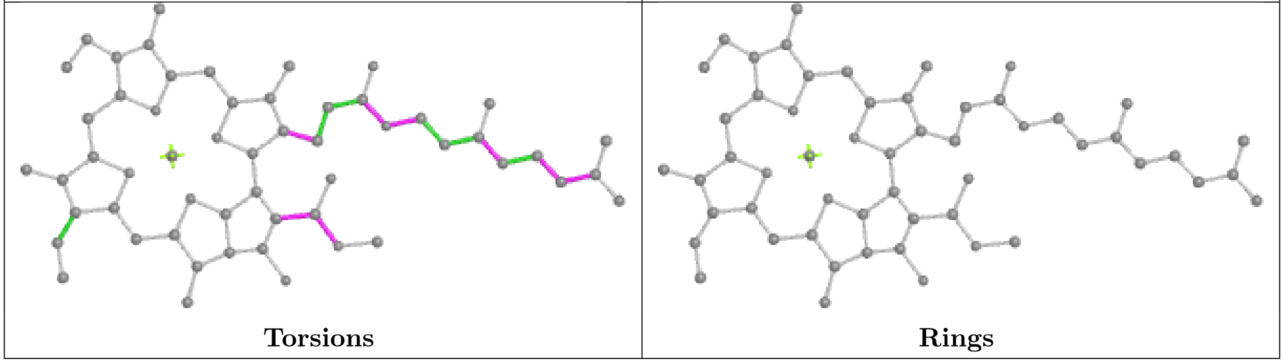


Torsions **Rings**

Ligand CLA a 1118

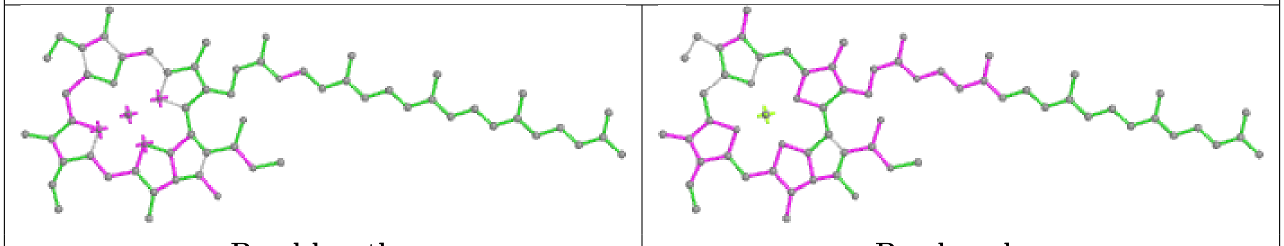


Bond lengths **Bond angles**

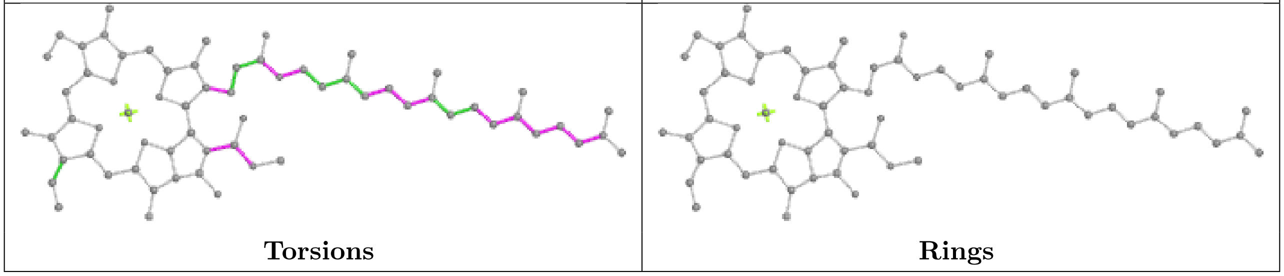


Torsions **Rings**

Ligand CLA G 1115

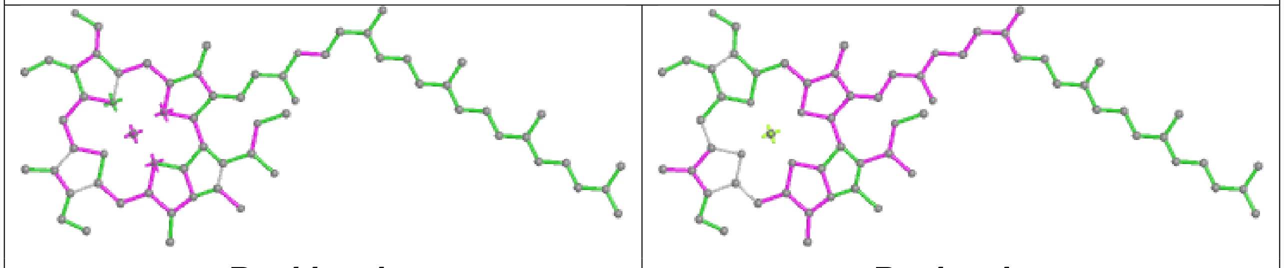


Bond lengths Bond angles

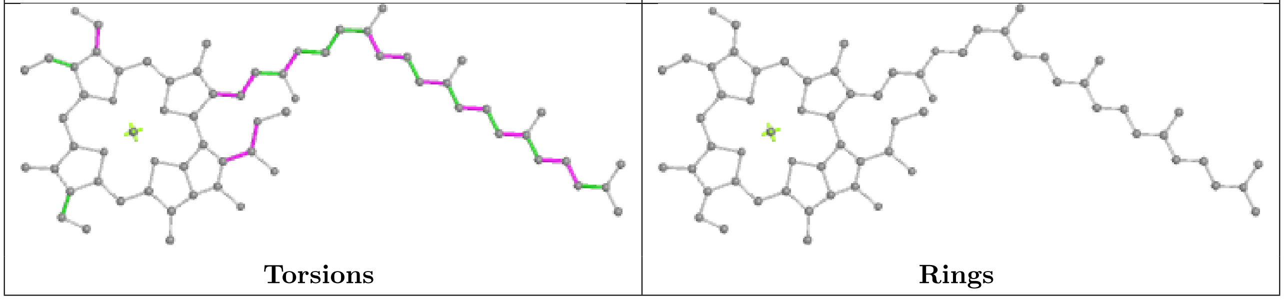


Torsions Rings

Ligand F6C b 1237

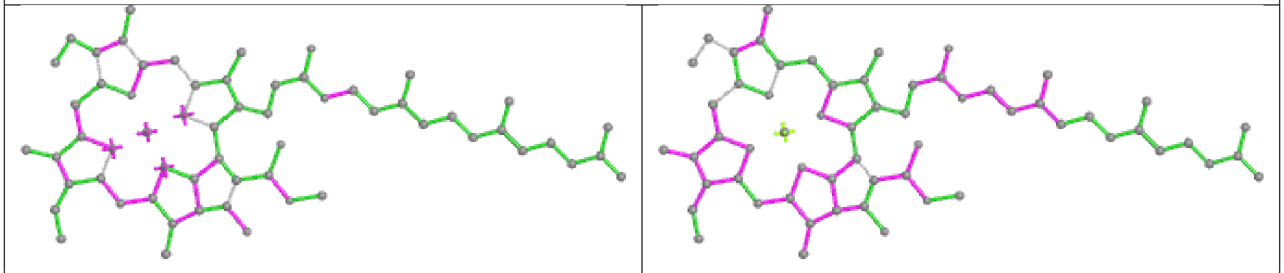


Bond lengths Bond angles



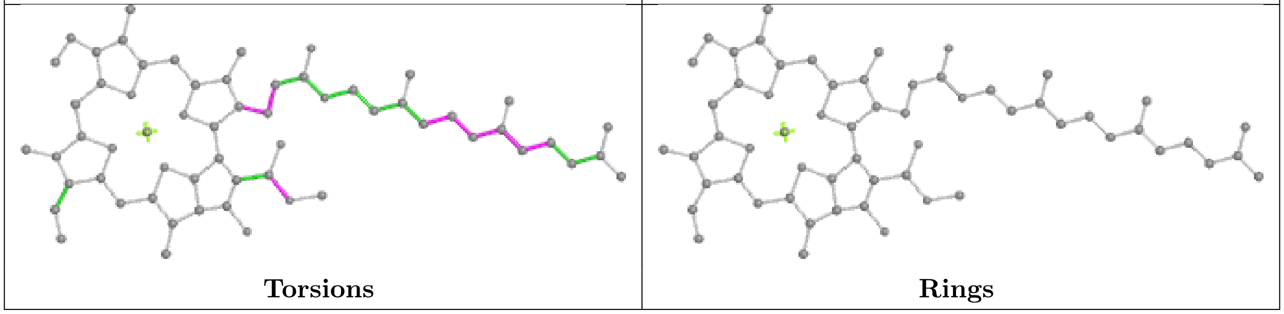
Torsions Rings

Ligand CLA A 1135



Bond lengths

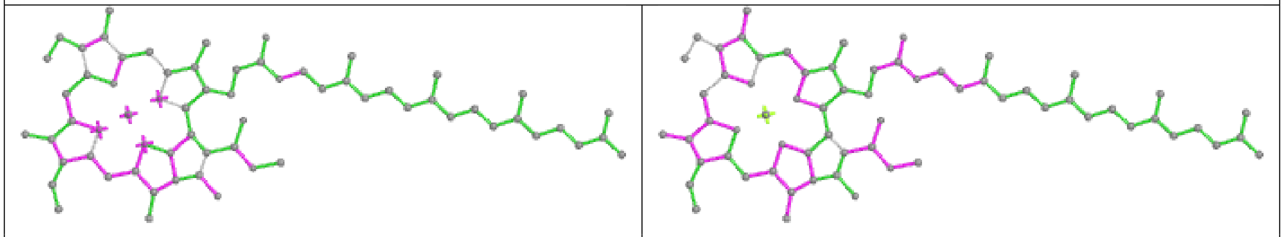
Bond angles



Torsions

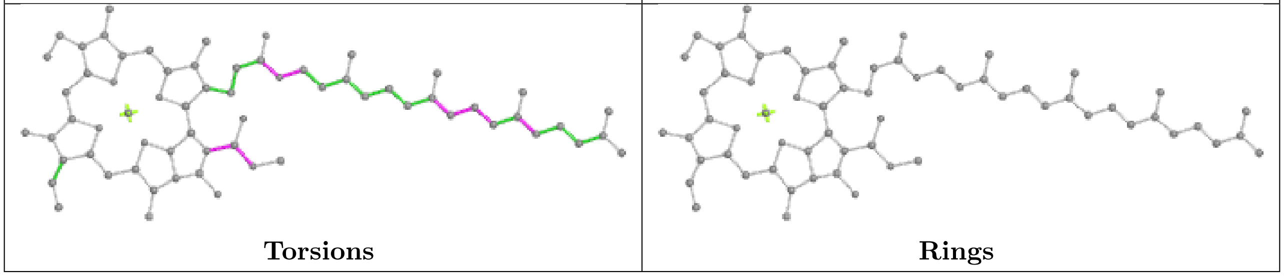
Rings

Ligand CLA a 1119



Bond lengths

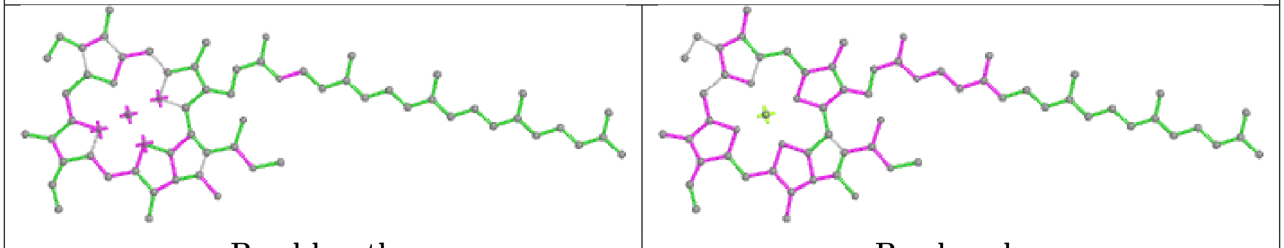
Bond angles



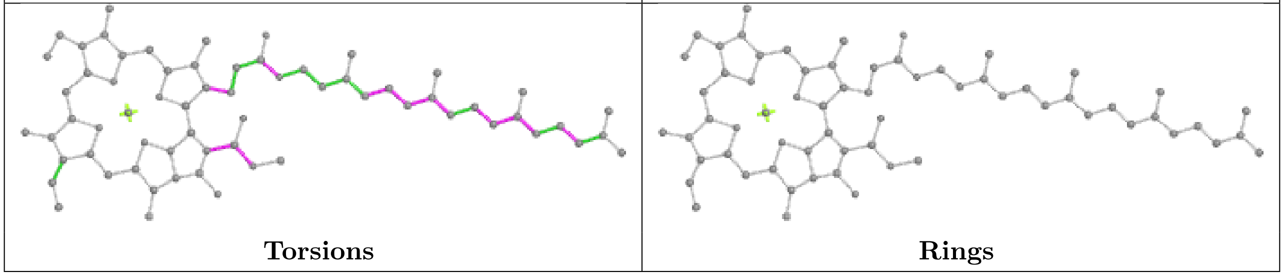
Torsions

Rings

Ligand CLA A 1117

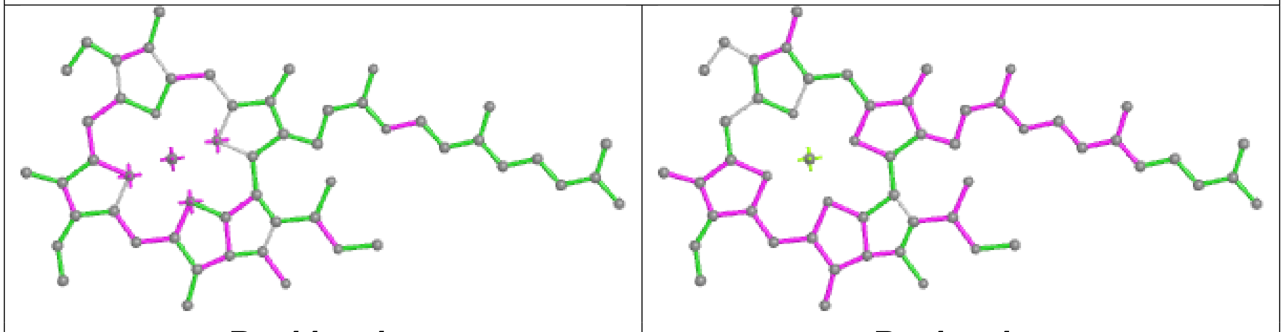


Bond lengths Bond angles

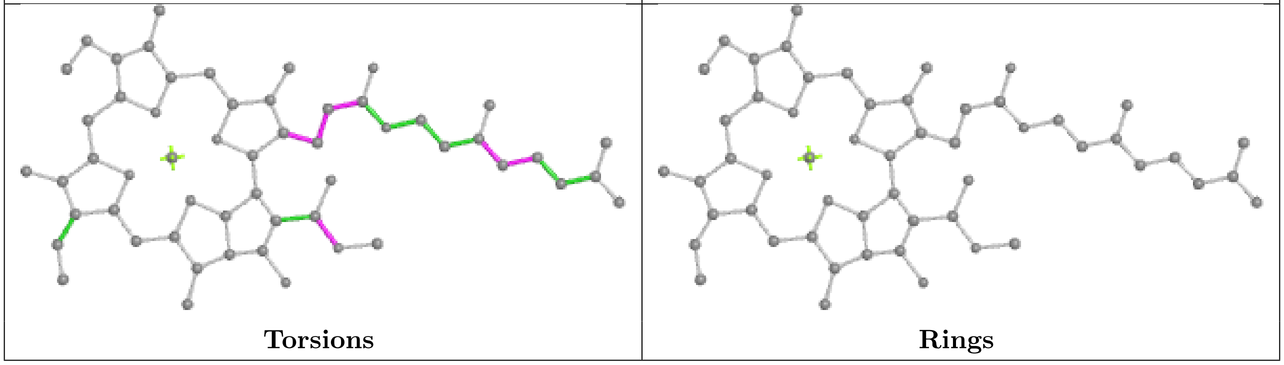


Torsions Rings

Ligand CLA a 1116

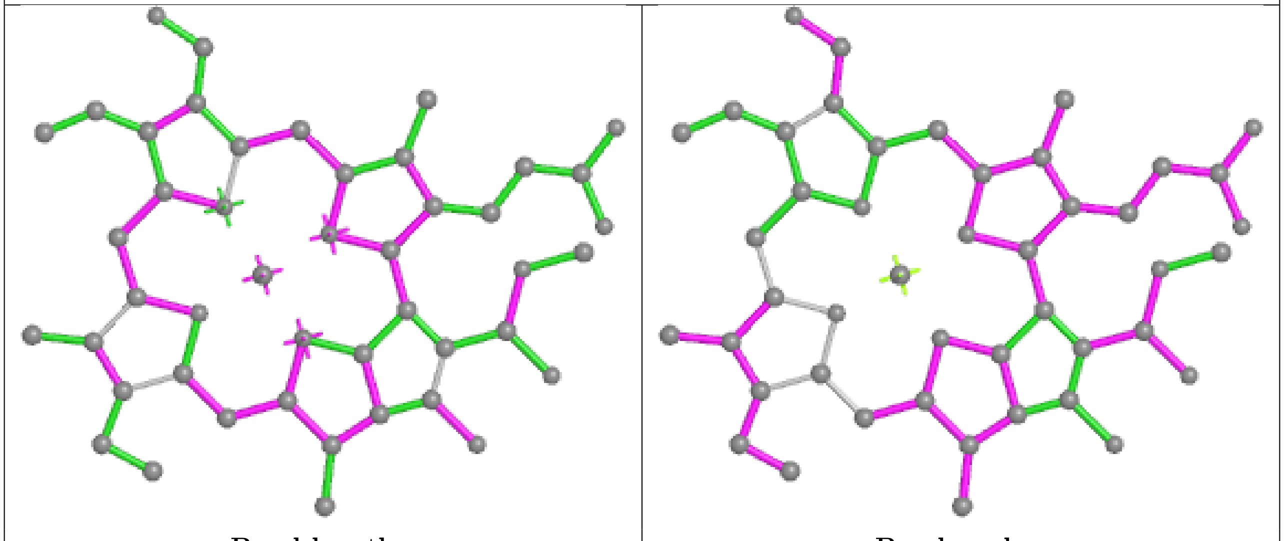


Bond lengths Bond angles

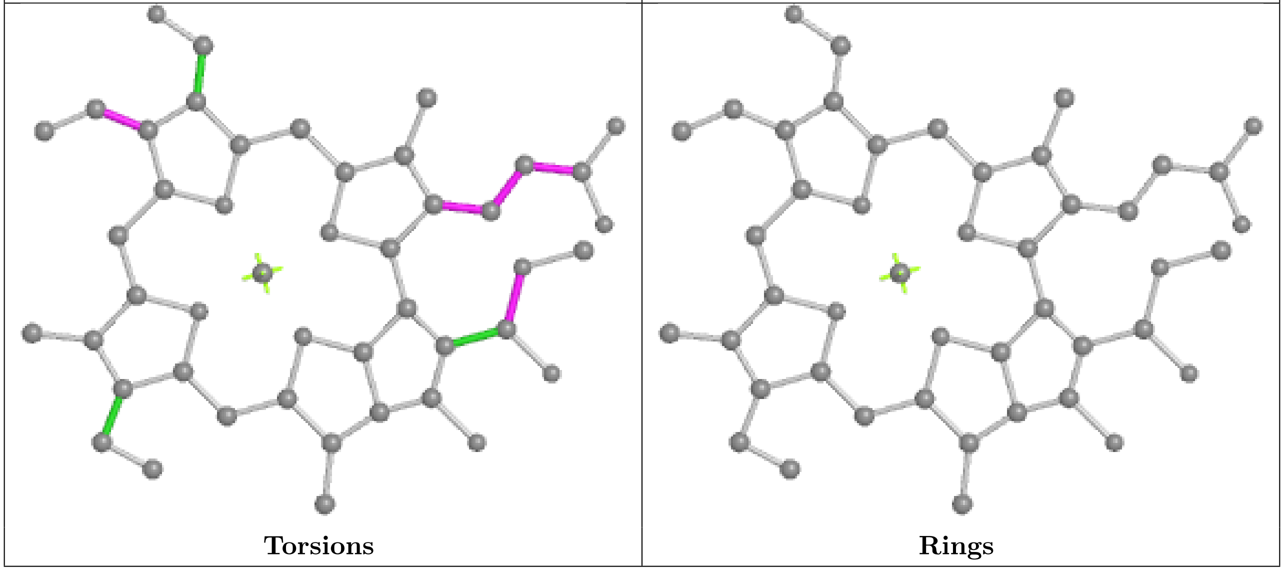


Torsions Rings

Ligand F6C A 1121

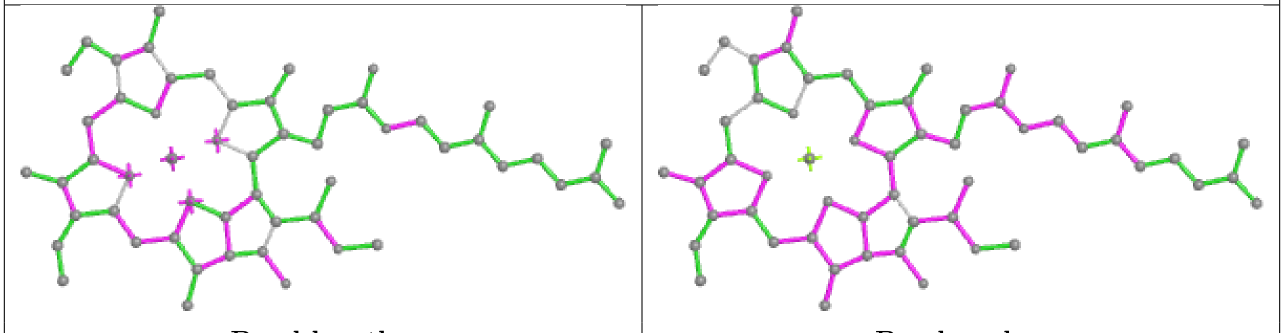


Bond lengths **Bond angles**



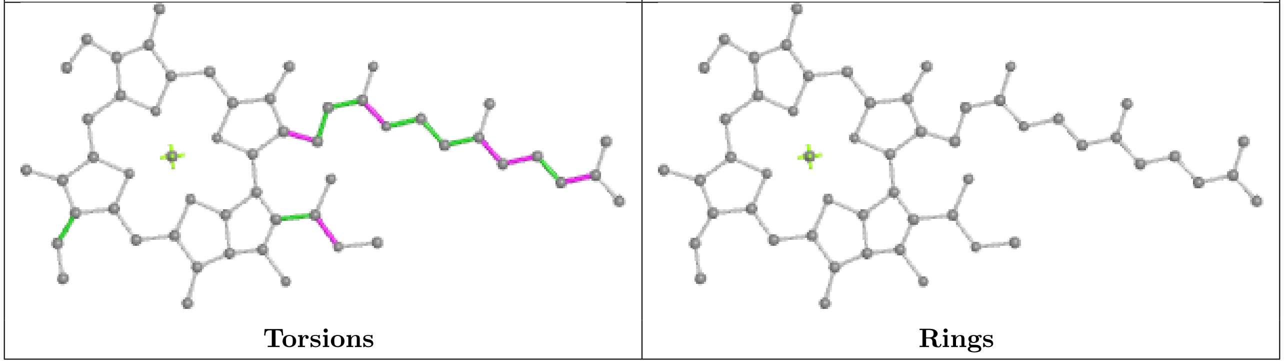
Torsions **Rings**

Ligand CLA G 1130



Bond lengths

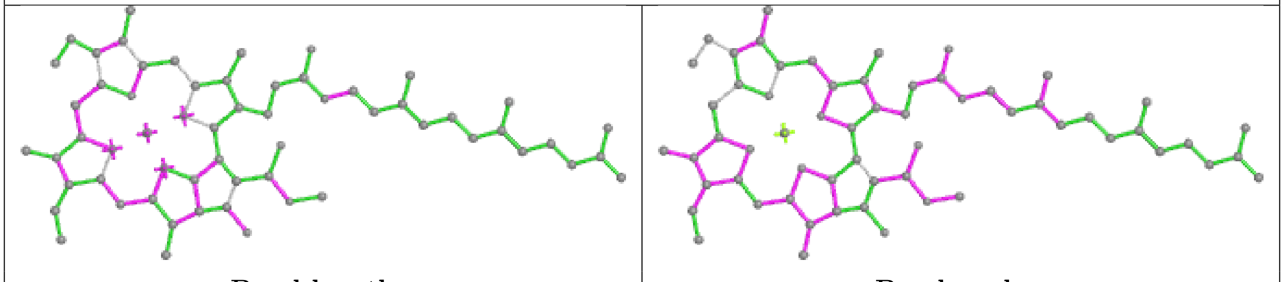
Bond angles



Torsions

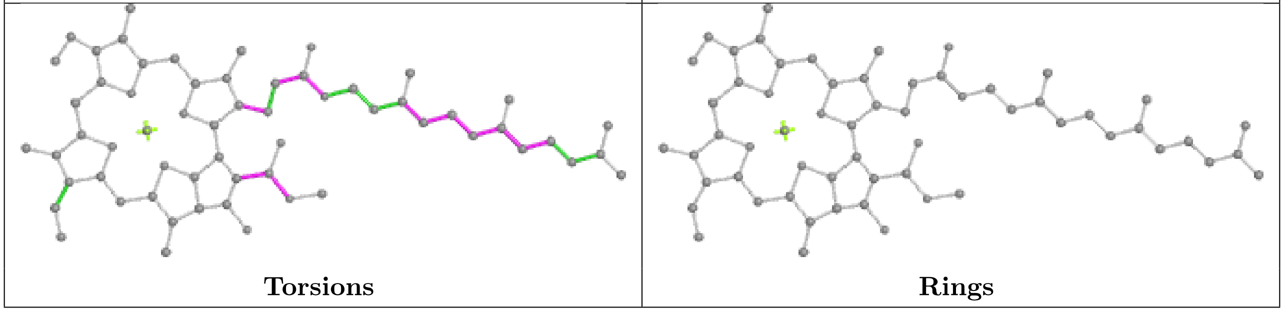
Rings

Ligand CLA A 1138



Bond lengths

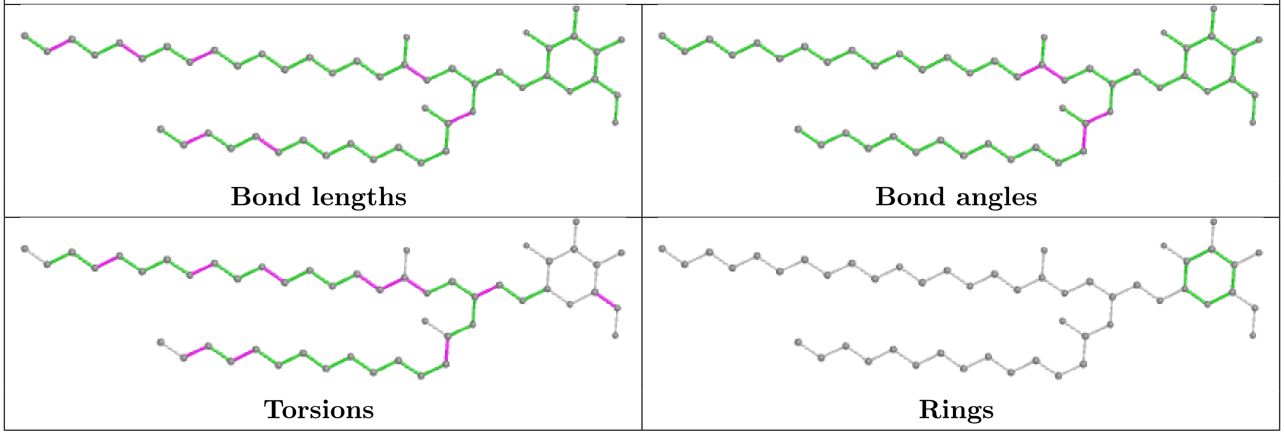
Bond angles



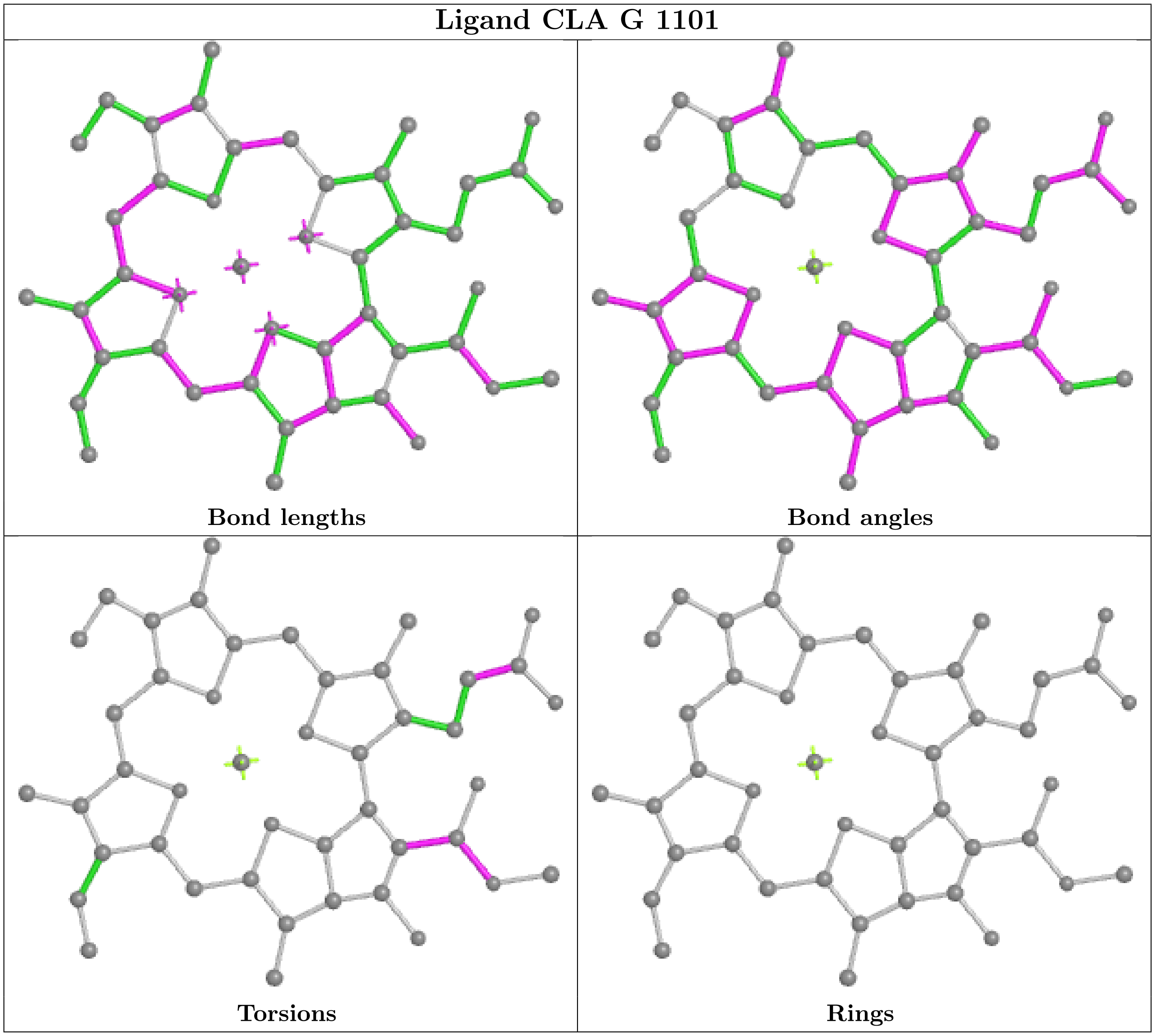
Torsions

Rings

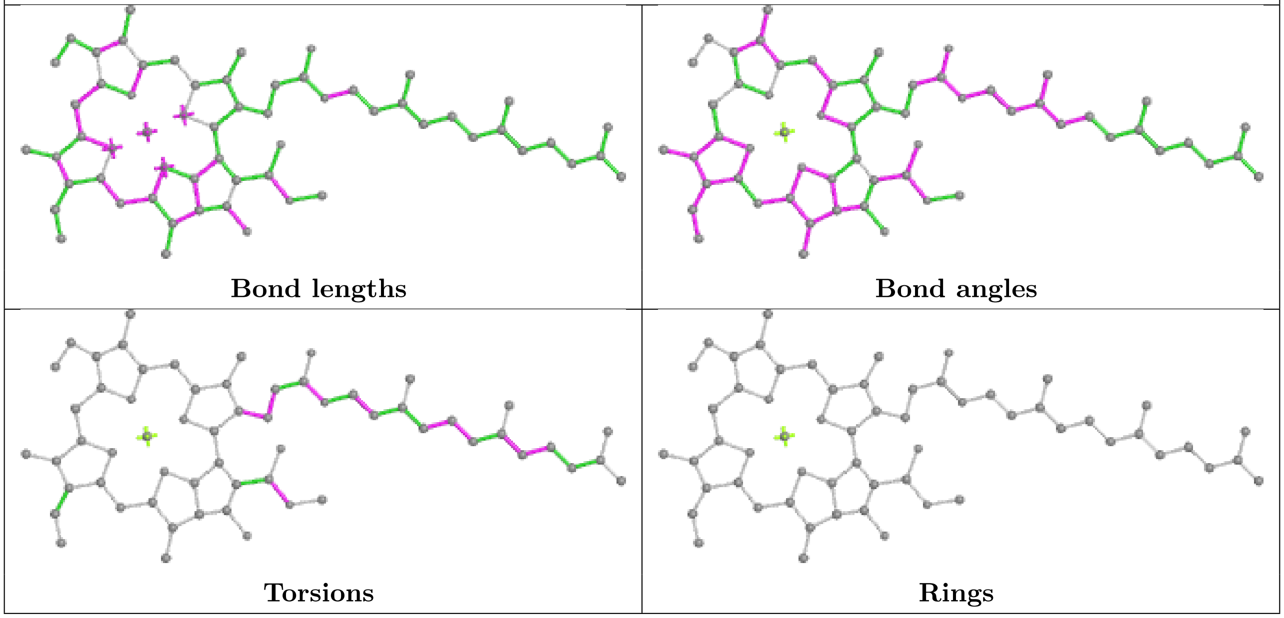
Ligand LMG l 5007



Ligand CLA G 1101



Ligand CLA a 1013



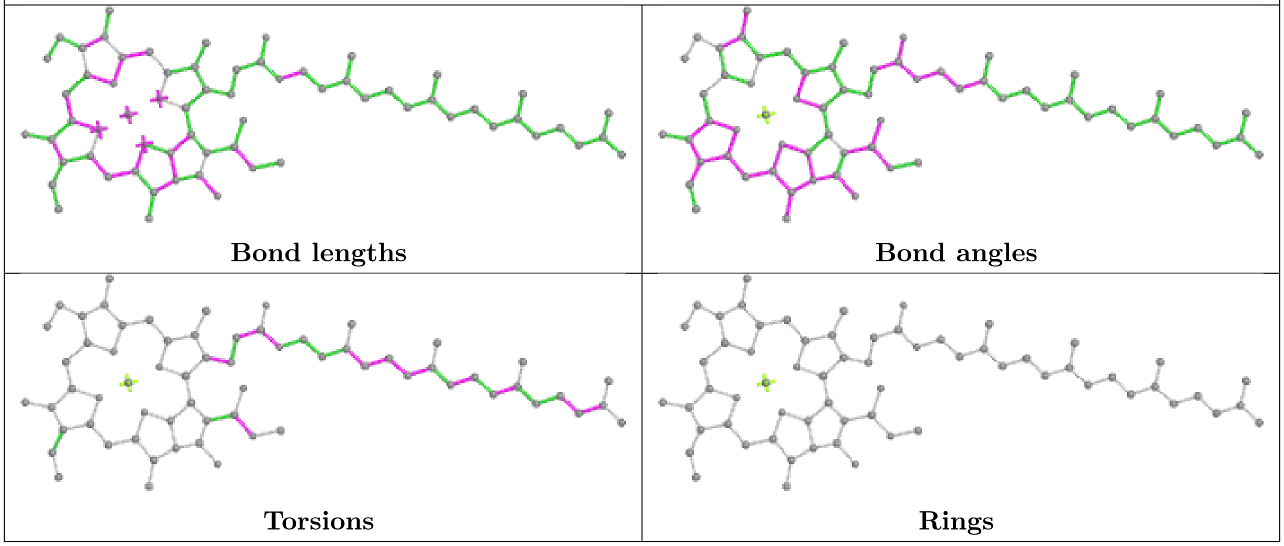
Bond lengths

Bond angles

Torsions

Rings

Ligand CLA A 1125



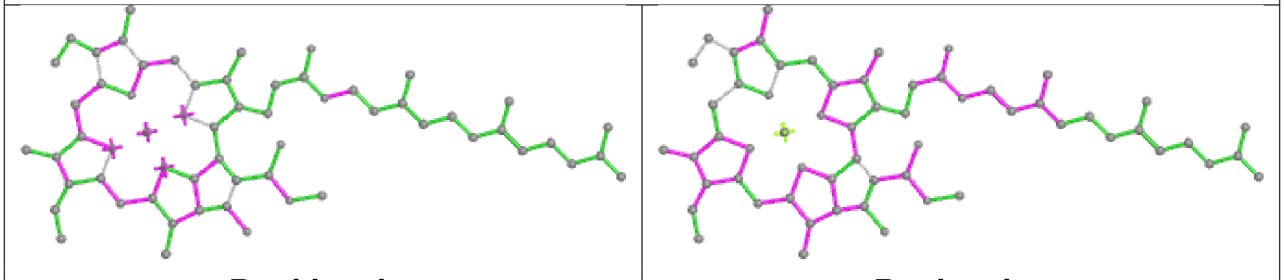
Bond lengths

Bond angles

Torsions

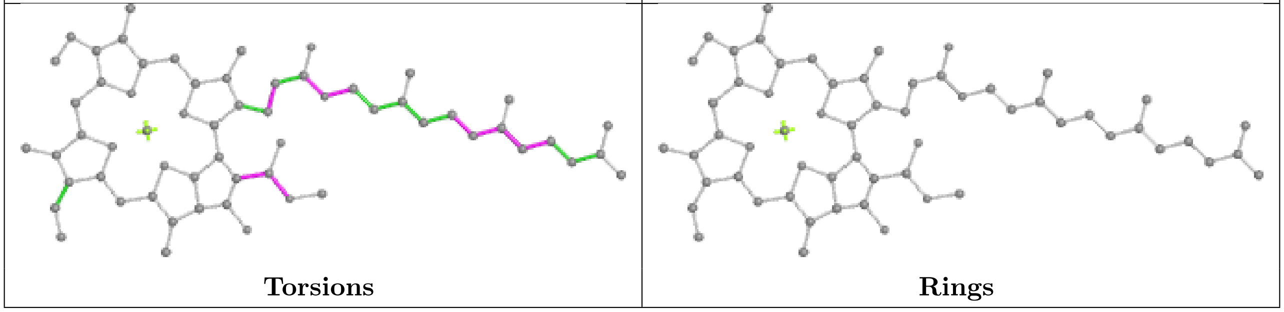
Rings

Ligand CLA G 1123



Bond lengths

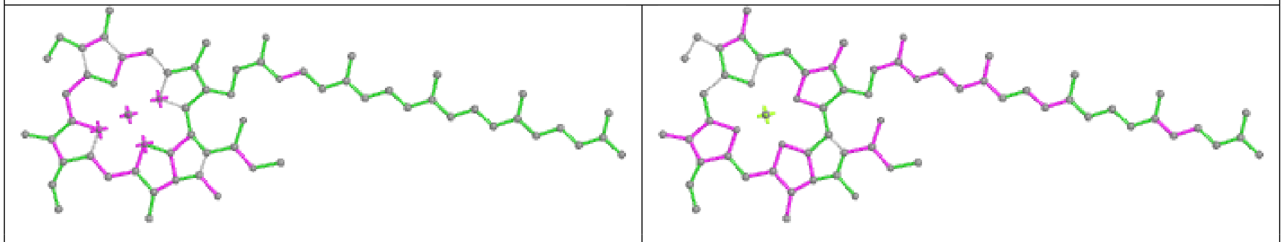
Bond angles



Torsions

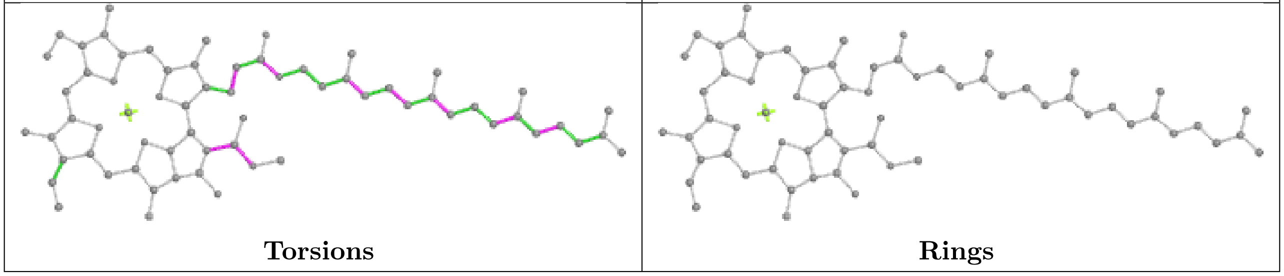
Rings

Ligand CLA l 1501



Bond lengths

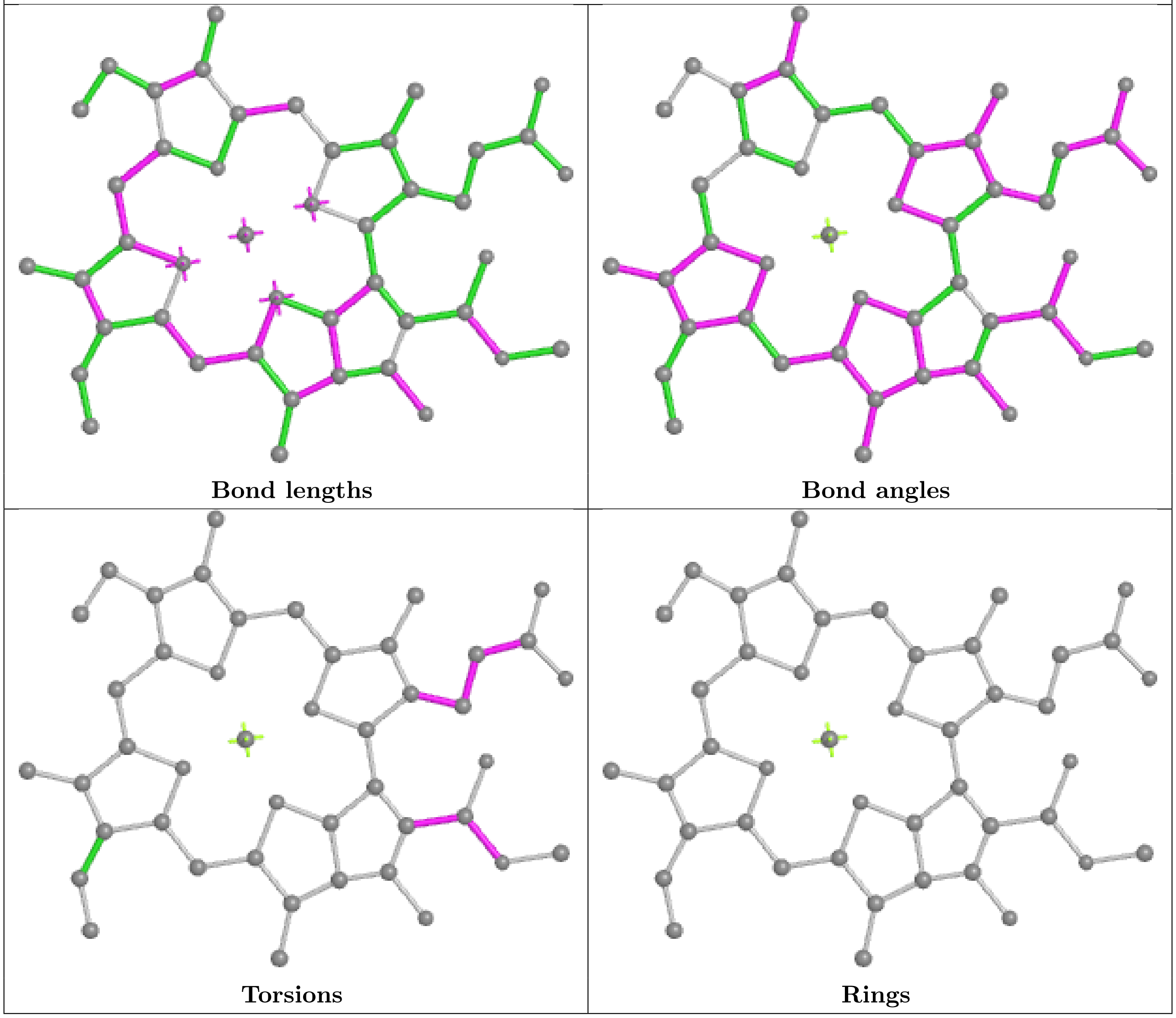
Bond angles



Torsions

Rings

Ligand CLA G 1113



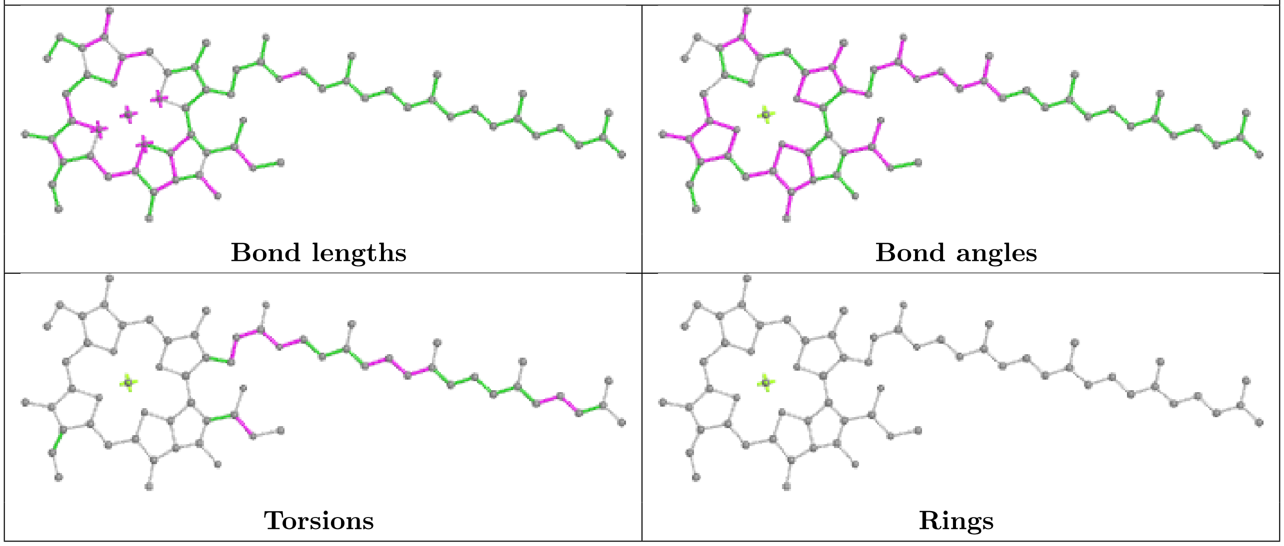
Bond lengths

Bond angles

Torsions

Rings

Ligand CLA b 1226



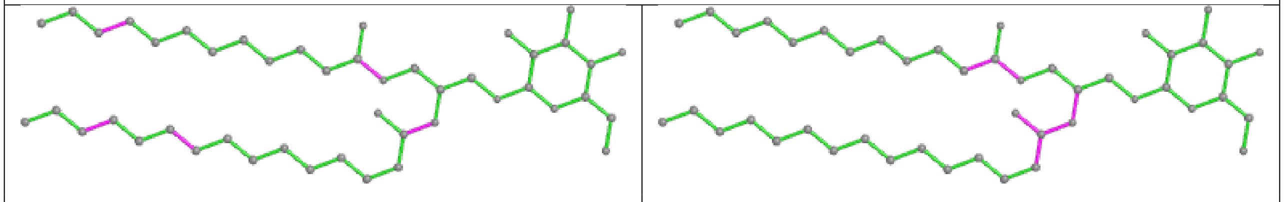
Bond lengths

Bond angles

Torsions

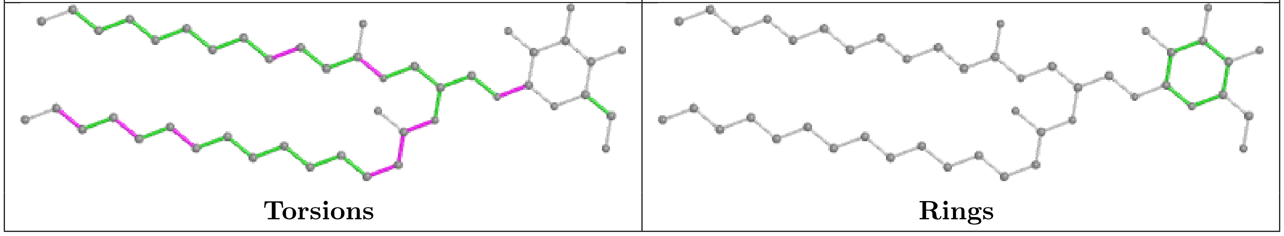
Rings

Ligand LMG B 5002



Bond lengths

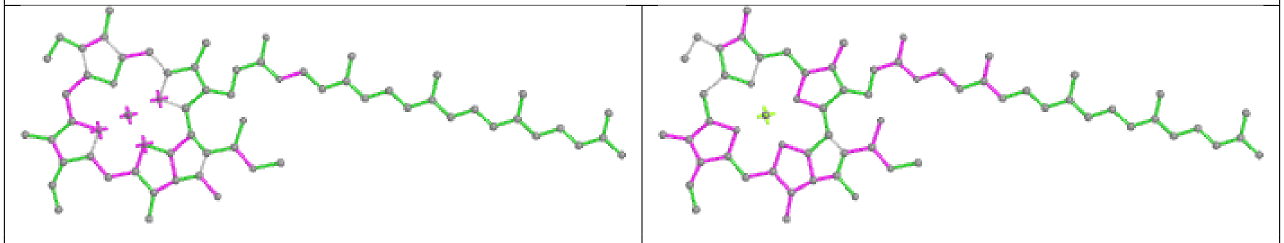
Bond angles



Torsions

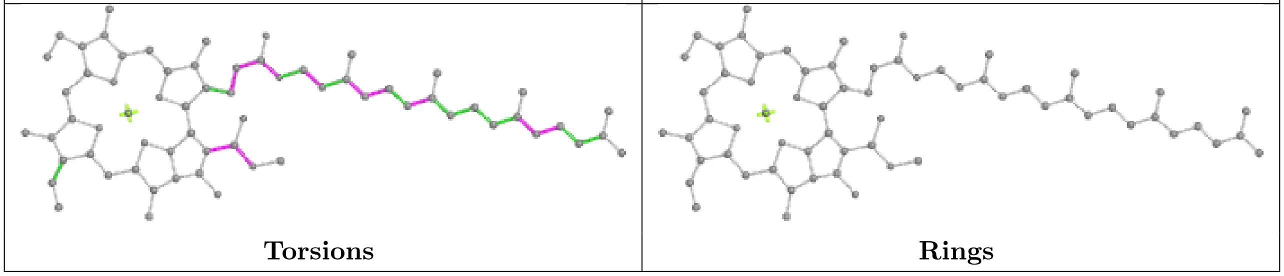
Rings

Ligand CLA B 1213



Bond lengths

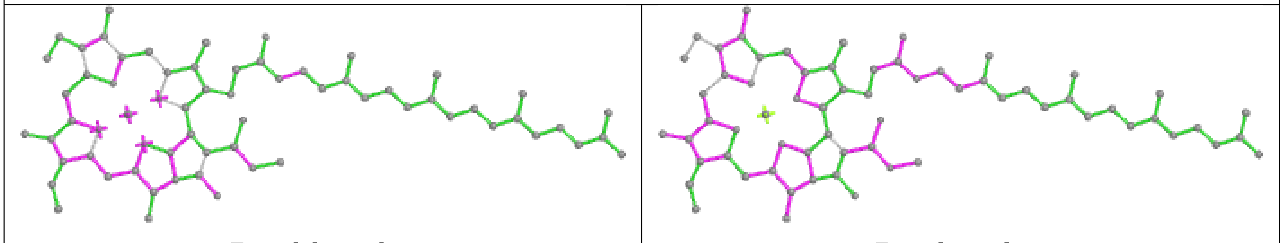
Bond angles



Torsions

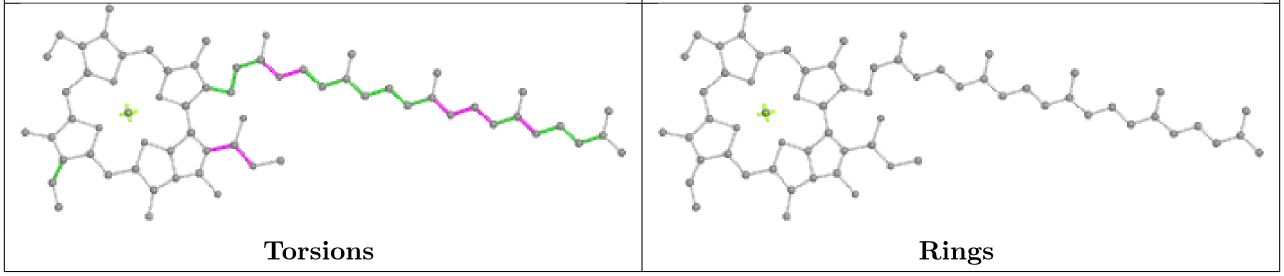
Rings

Ligand CLA A 1119



Bond lengths

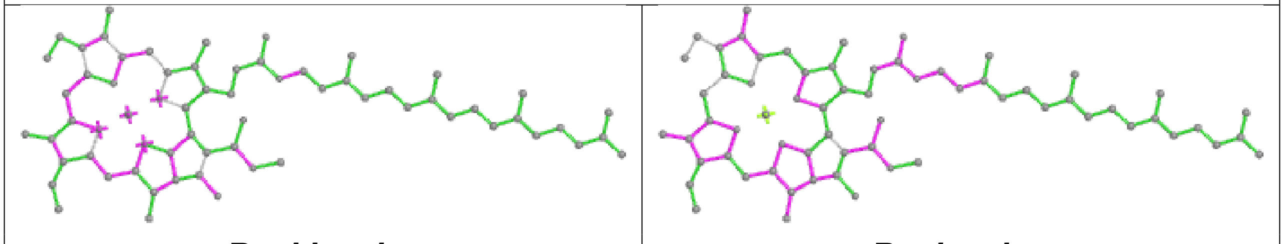
Bond angles



Torsions

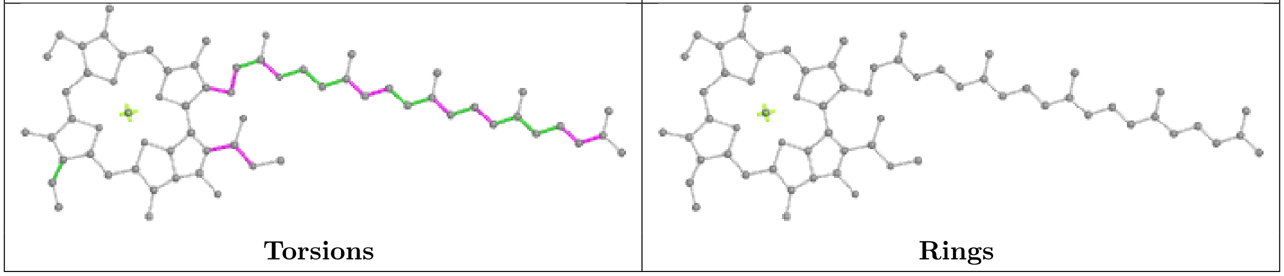
Rings

Ligand CLA B 1225



Bond lengths

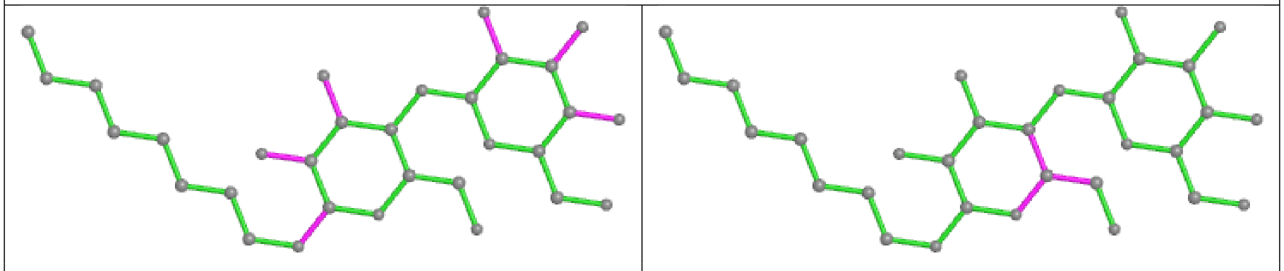
Bond angles



Torsions

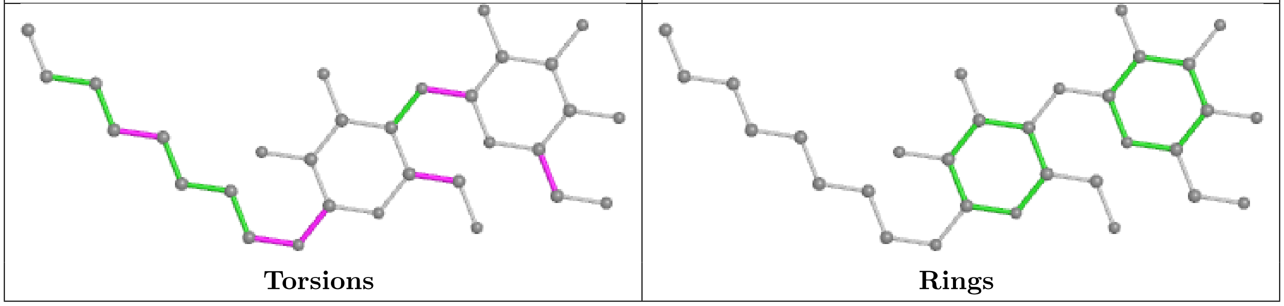
Rings

Ligand LMT a 6001



Bond lengths

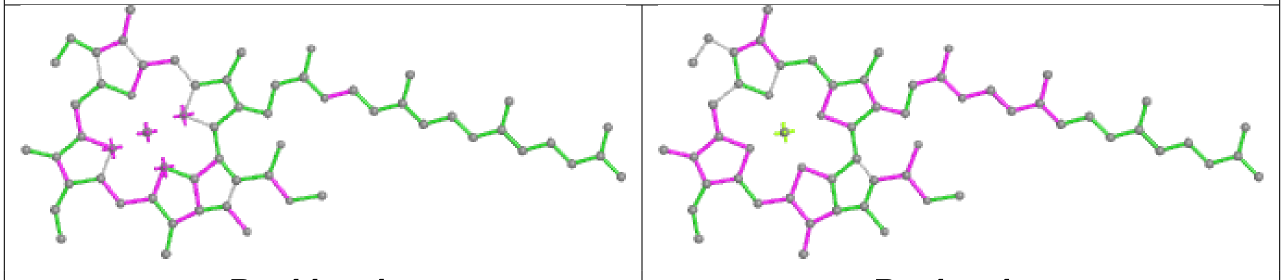
Bond angles



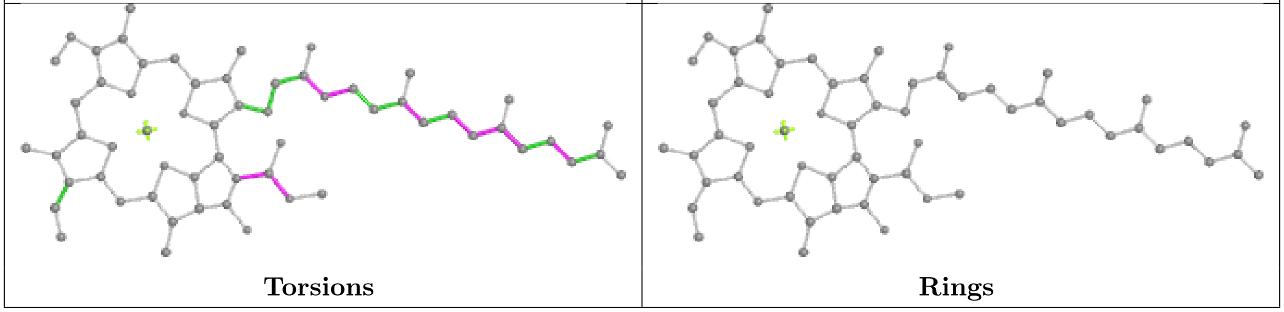
Torsions

Rings

Ligand CLA A 1128

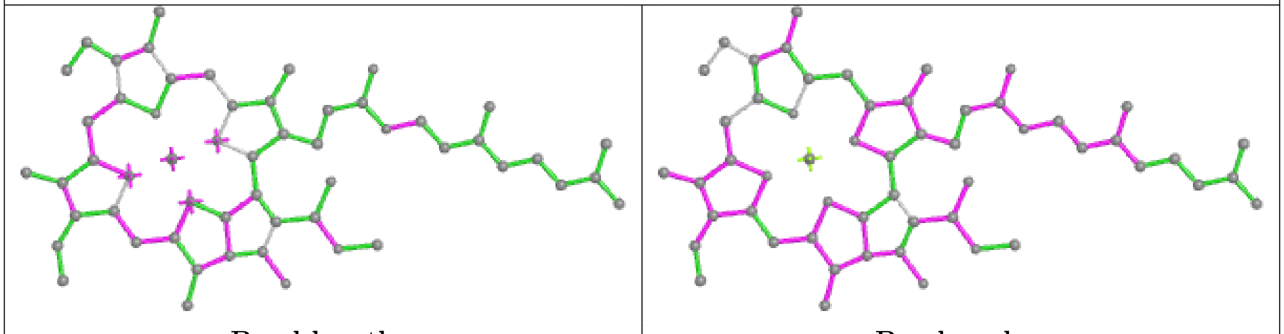


Bond lengths Bond angles

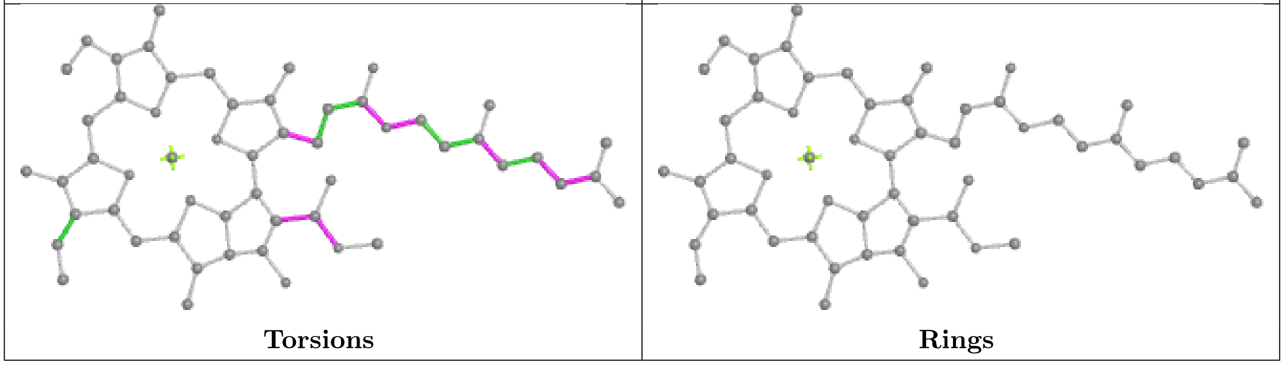


Torsions Rings

Ligand CLA A 1118

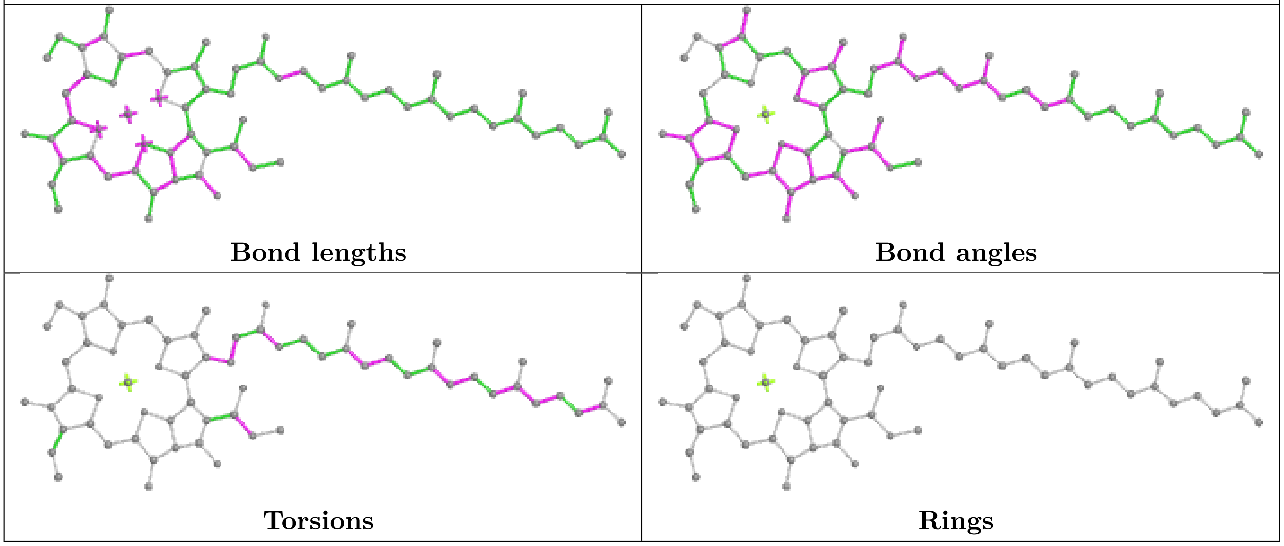


Bond lengths Bond angles



Torsions Rings

Ligand CLA a 1109



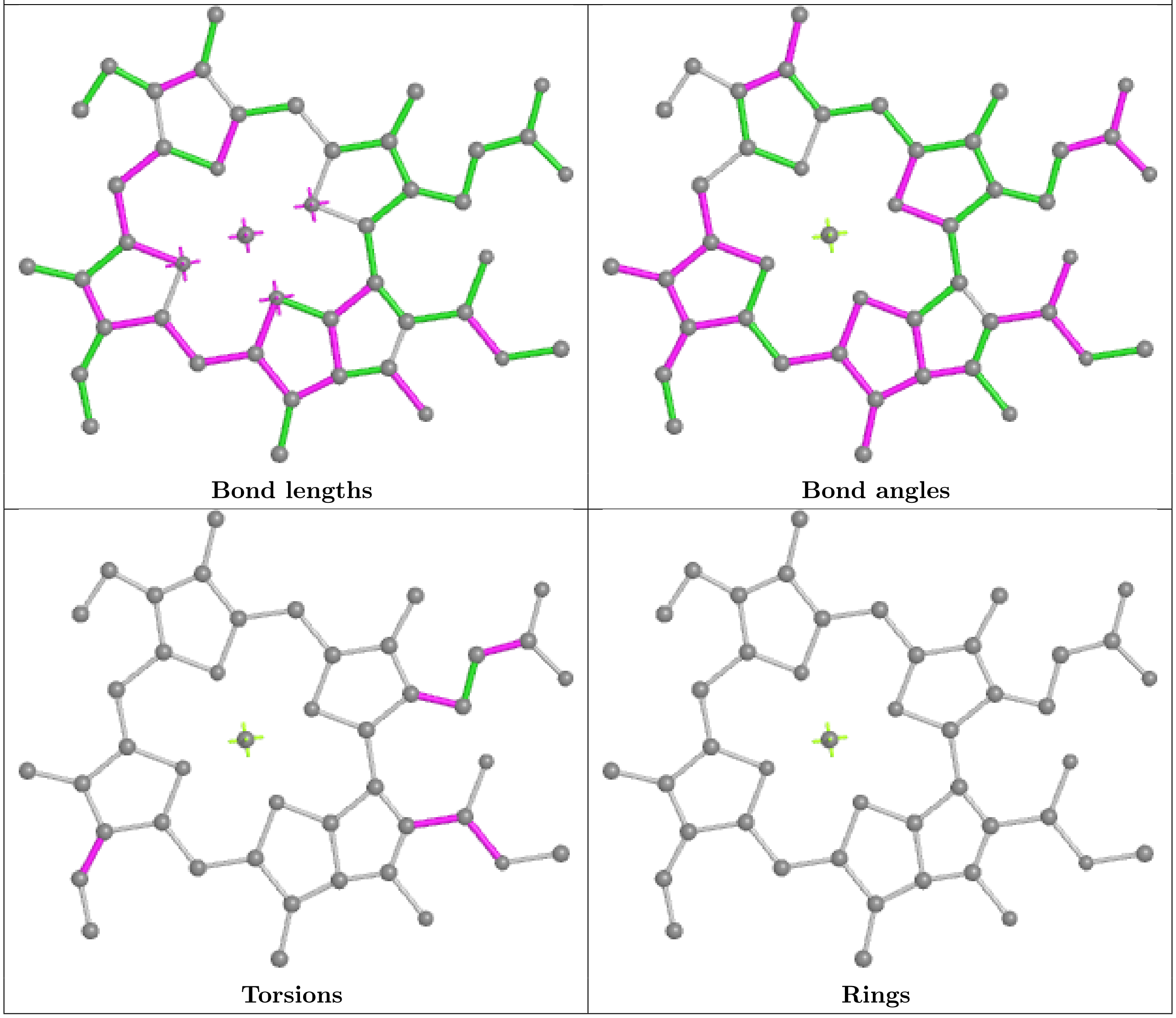
Bond lengths

Bond angles

Torsions

Rings

Ligand CLA A 1114



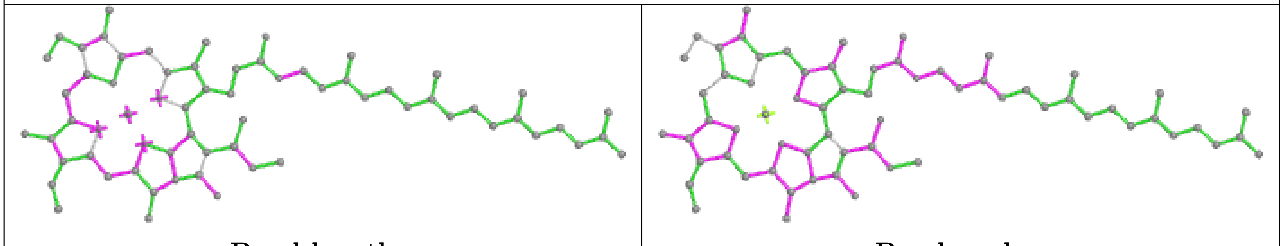
Bond lengths

Bond angles

Torsions

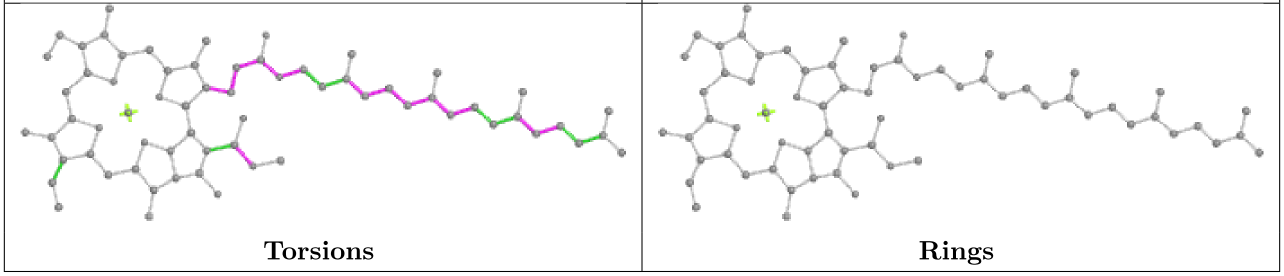
Rings

Ligand CLA G 1140



Bond lengths

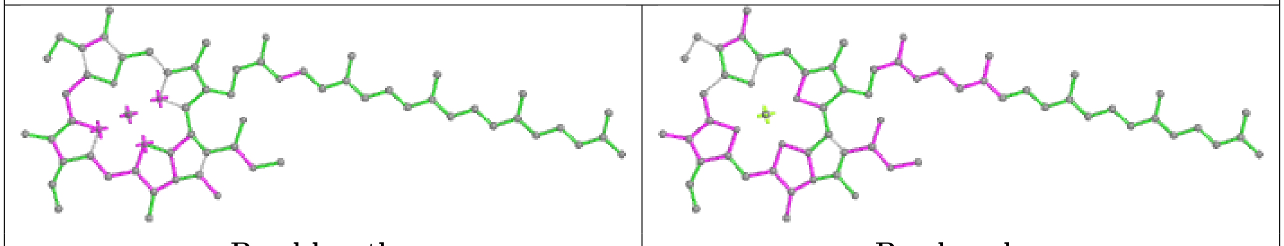
Bond angles



Torsions

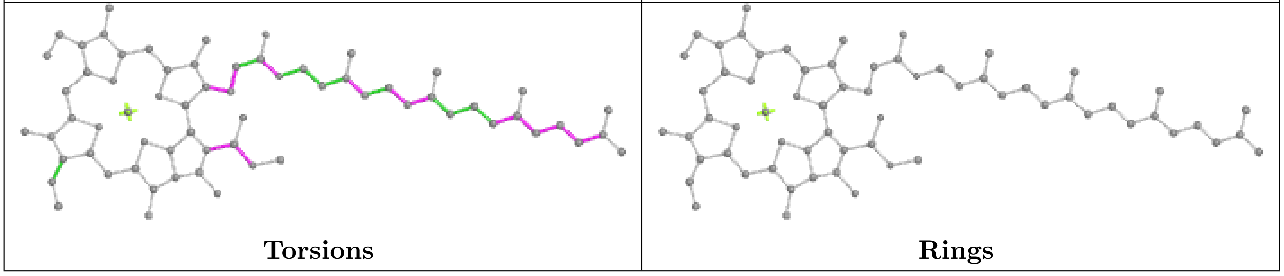
Rings

Ligand CLA b 1216



Bond lengths

Bond angles



Torsions

Rings

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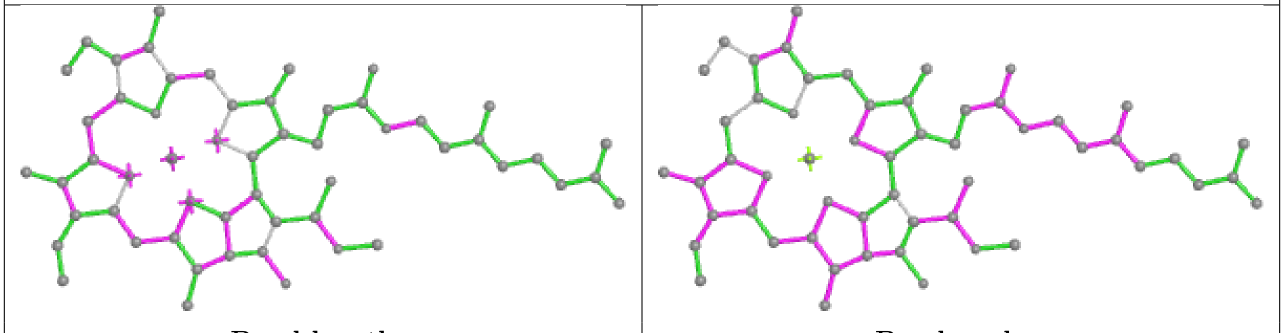
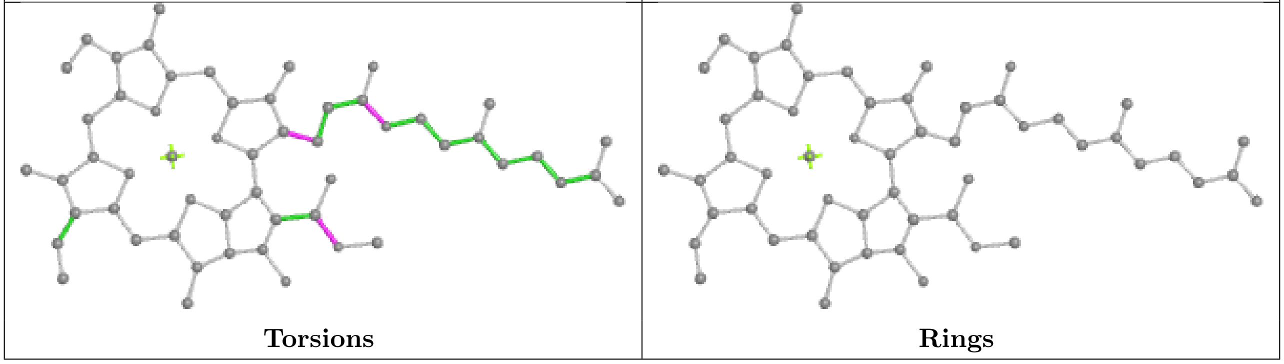


Bond lengths

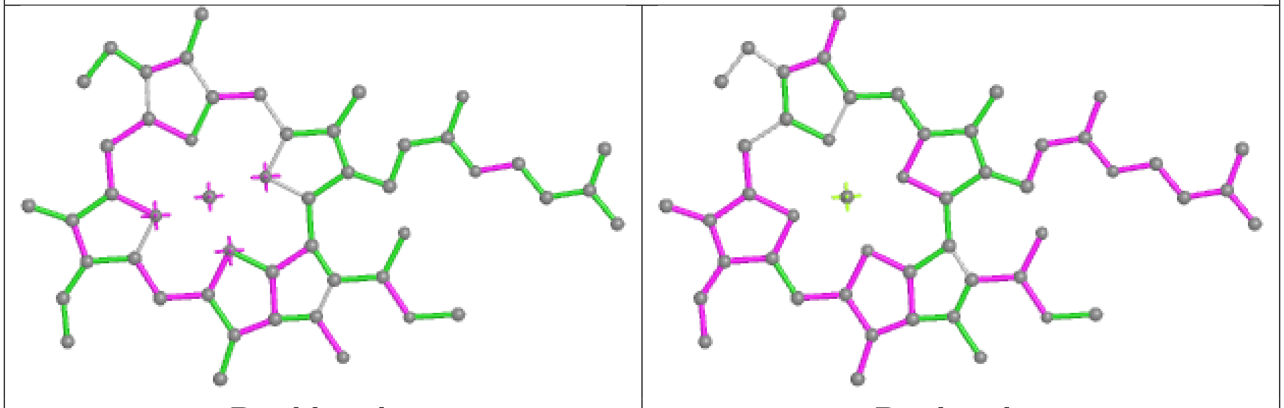
Bond angles



Torsions

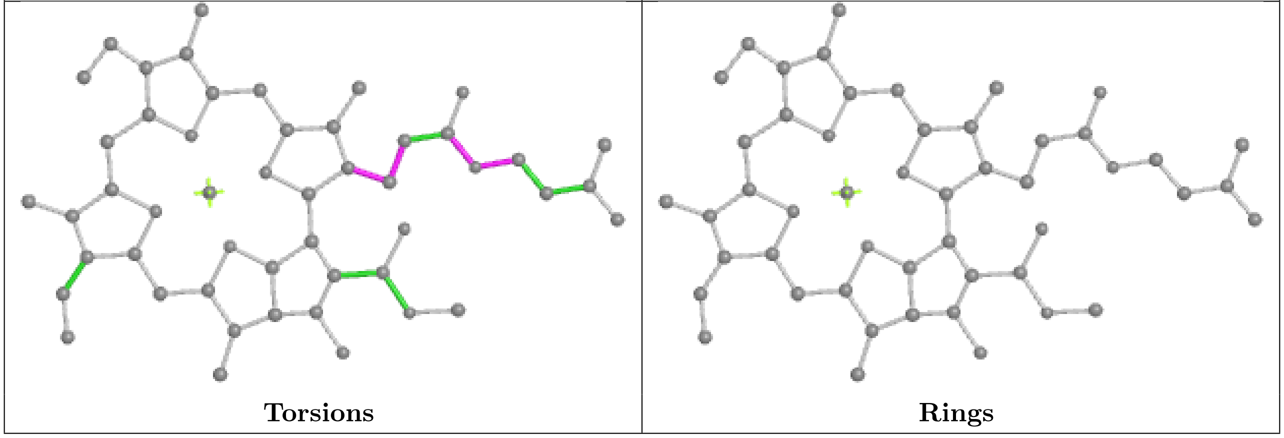
Rings

Ligand CLA A 1137



Bond lengths

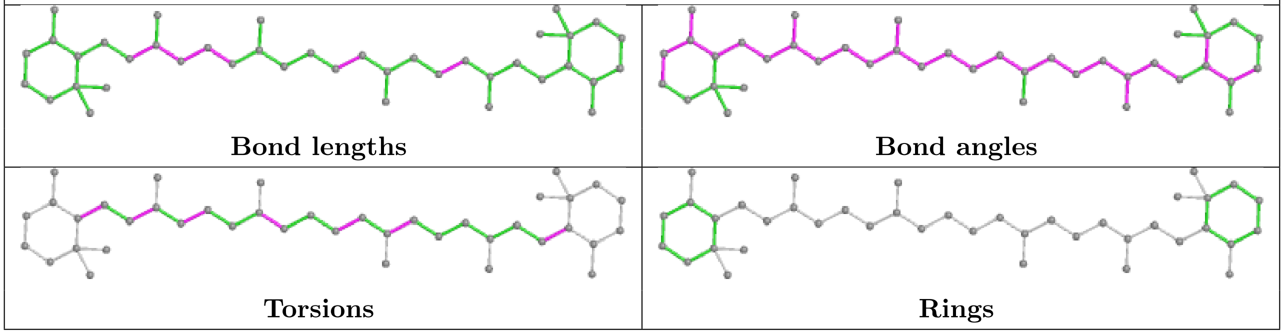
Bond angles



Torsions

Rings

Ligand BCR B 4016



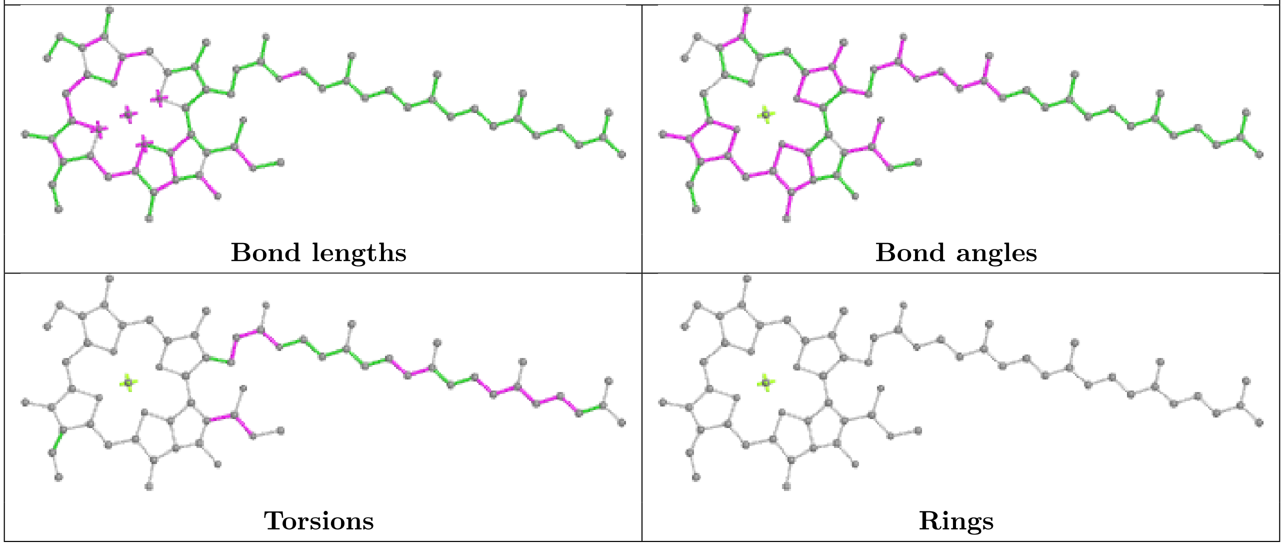
Bond lengths

Bond angles

Torsions

Rings

Ligand CLA B 1224



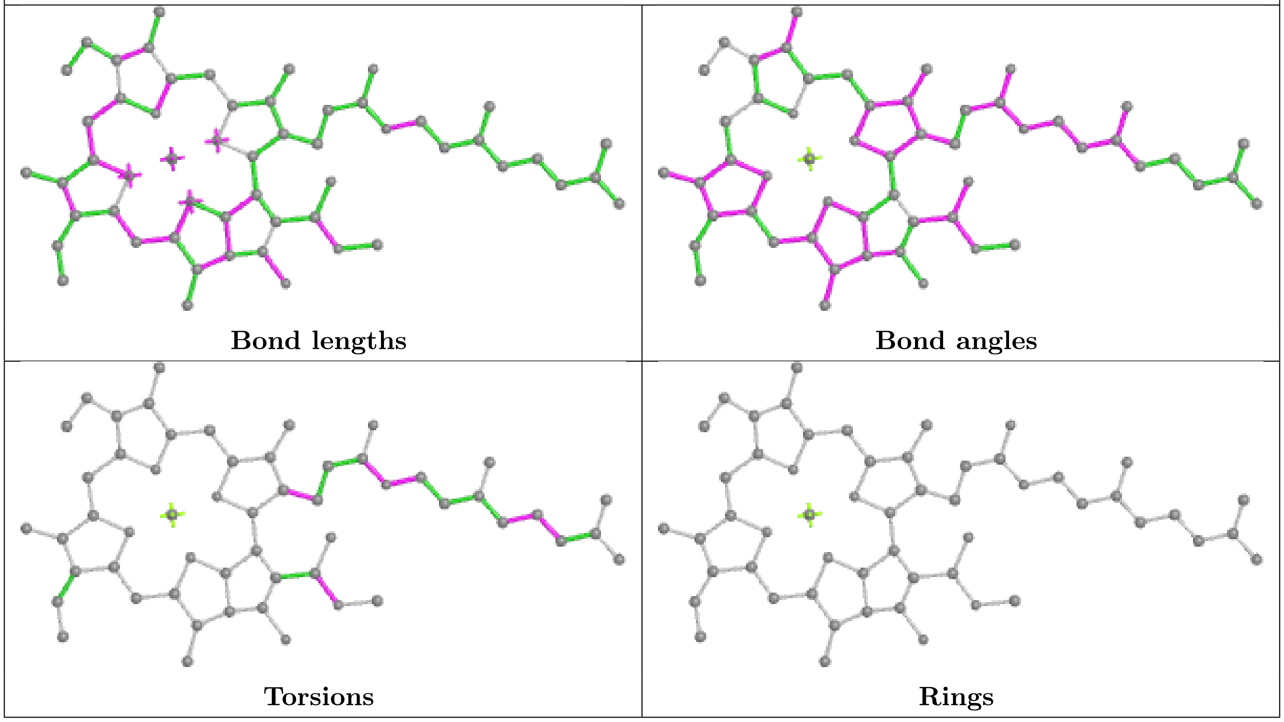
Bond lengths

Bond angles

Torsions

Rings

Ligand CLA a 1124



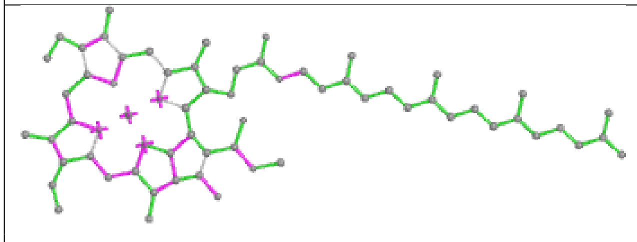
Bond lengths

Bond angles

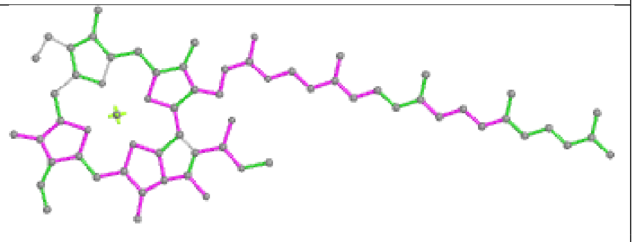
Torsions

Rings

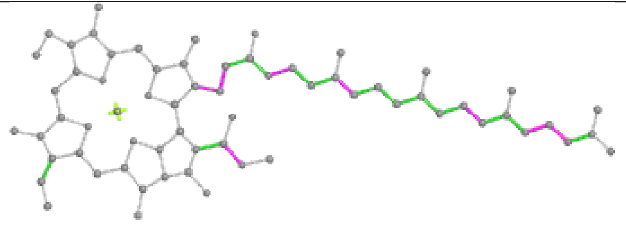
Ligand CLA G 1012



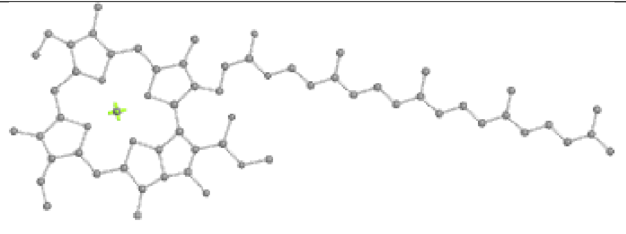
Bond lengths



Bond angles

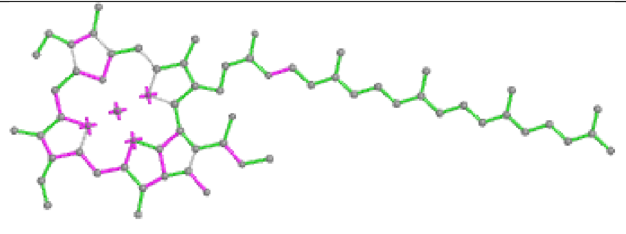


Torsions

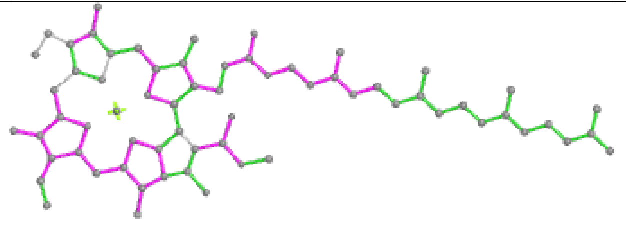


Rings

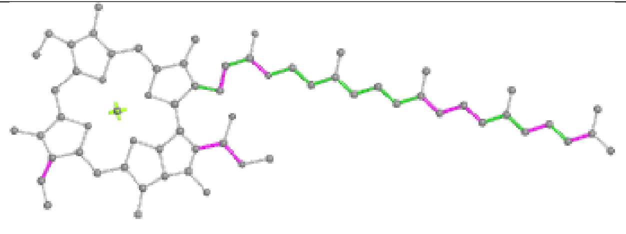
Ligand CLA H 1023



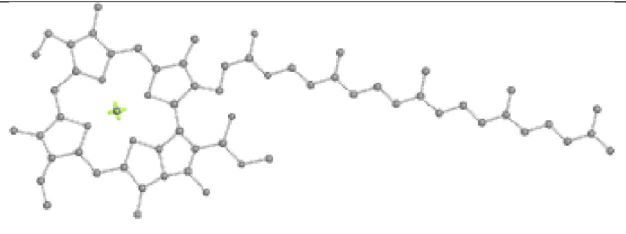
Bond lengths



Bond angles

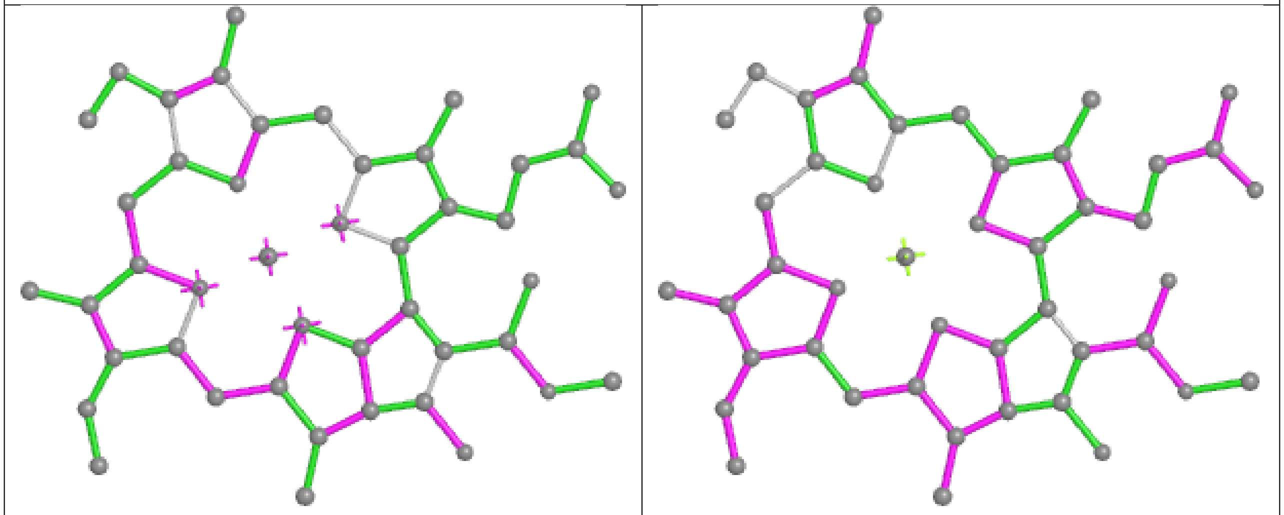


Torsions



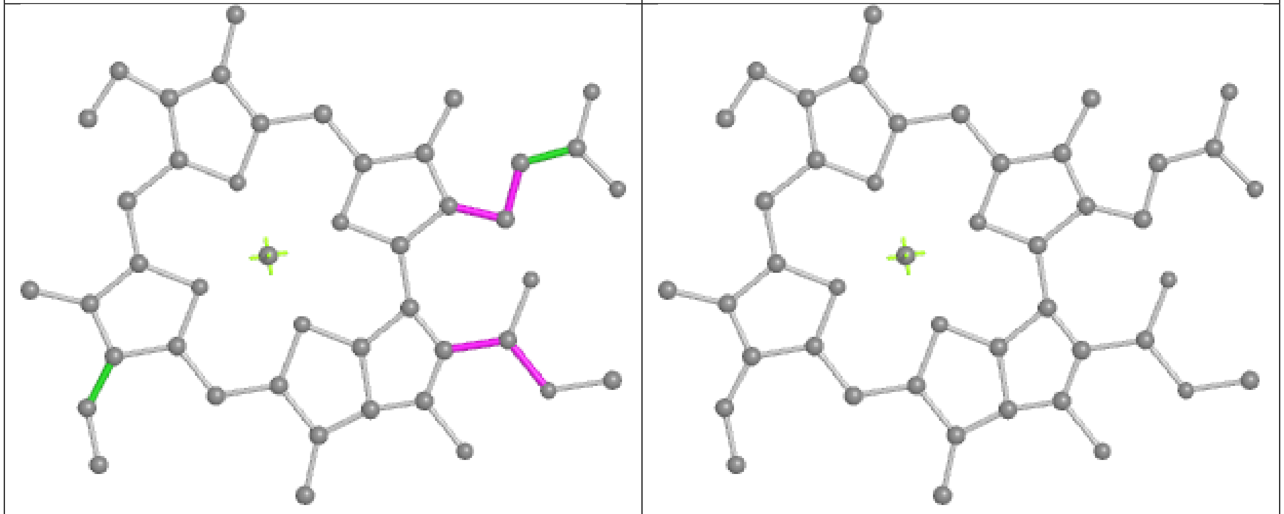
Rings

Ligand CLA b 1206



Bond lengths

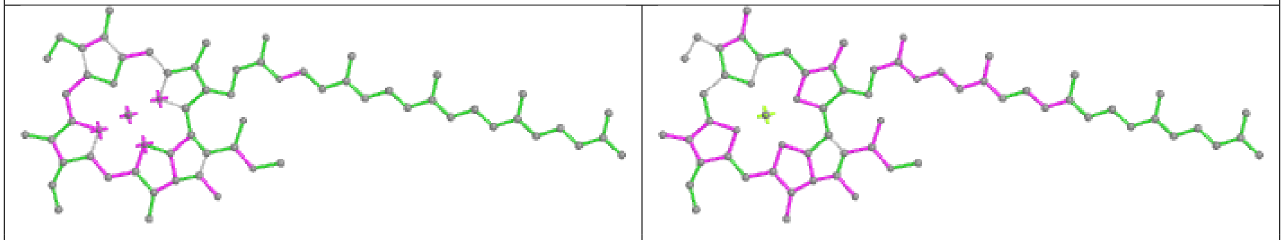
Bond angles



Torsions

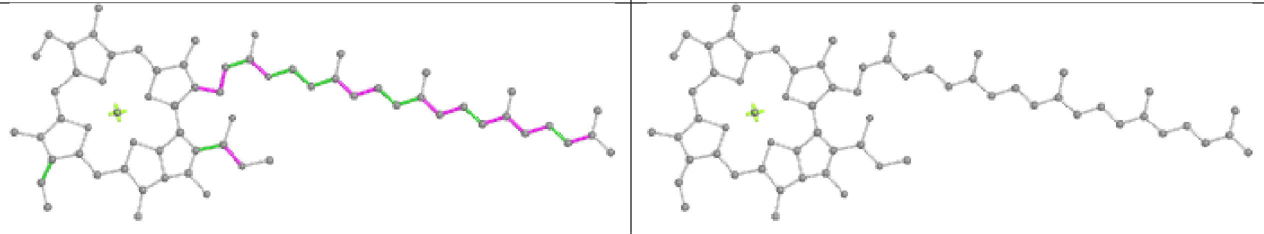
Rings

Ligand CLA A 1109



Bond lengths

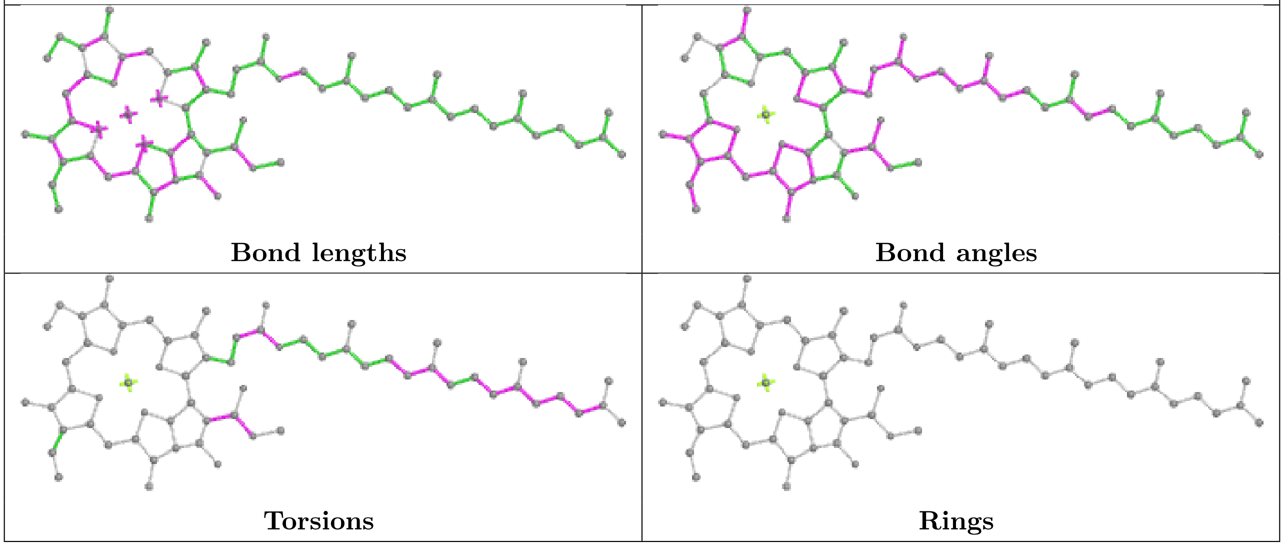
Bond angles



Torsions

Rings

Ligand CLA B 1021



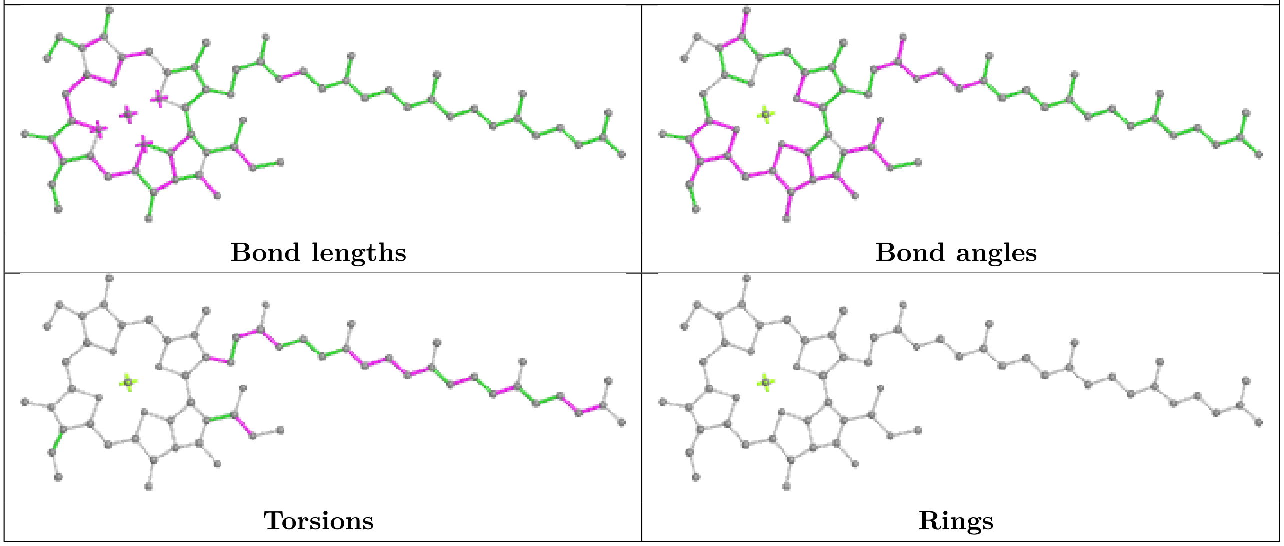
Bond lengths

Bond angles

Torsions

Rings

Ligand CLA G 1125



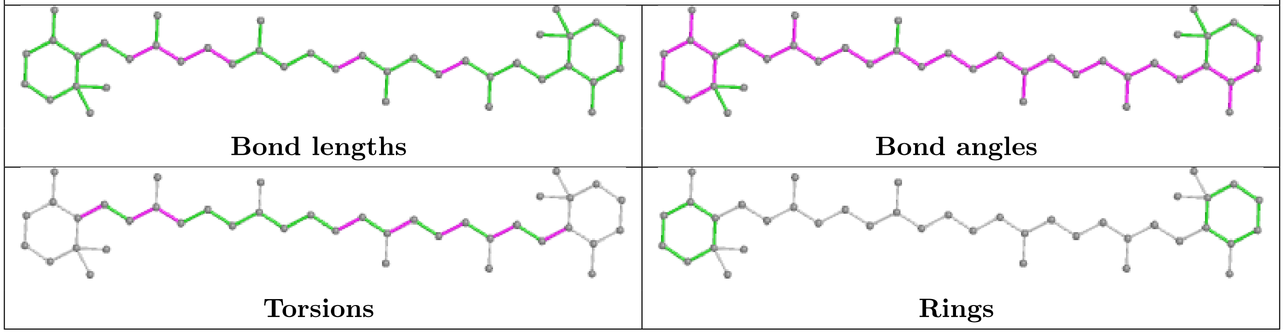
Bond lengths

Bond angles

Torsions

Rings

Ligand BCR A 4001



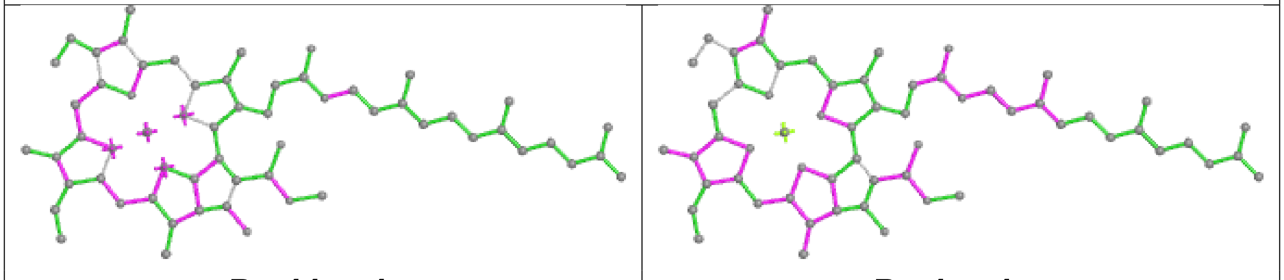
Bond lengths

Bond angles

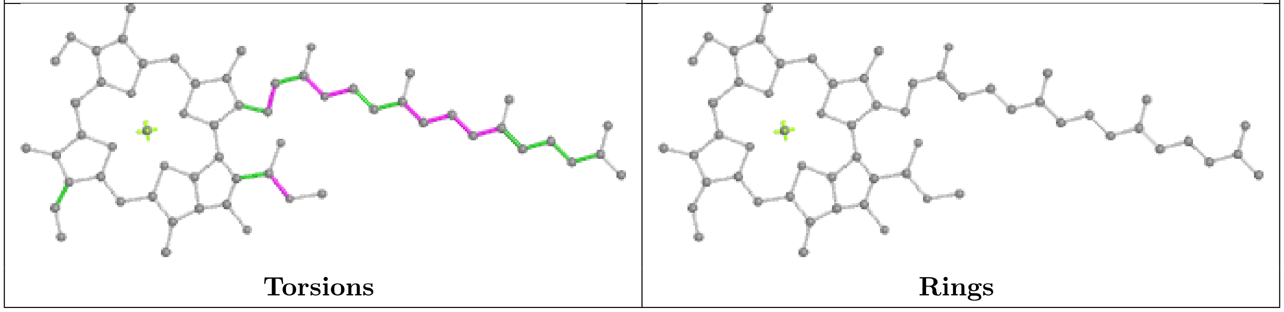
Torsions

Rings

Ligand CLA a 1131

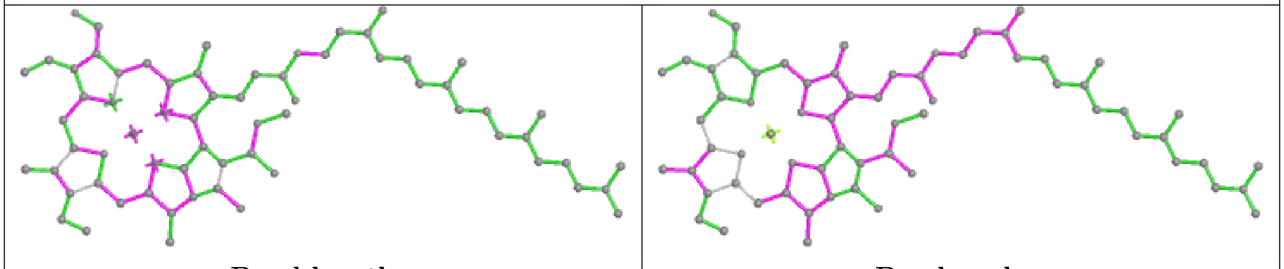


Bond lengths Bond angles

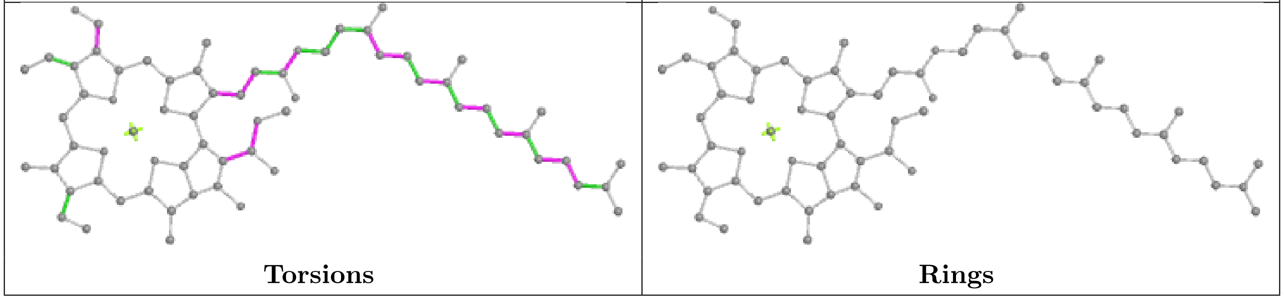


Torsions Rings

Ligand F6C B 1237

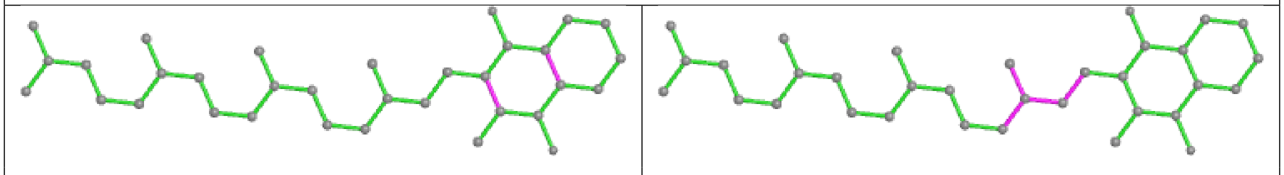


Bond lengths Bond angles

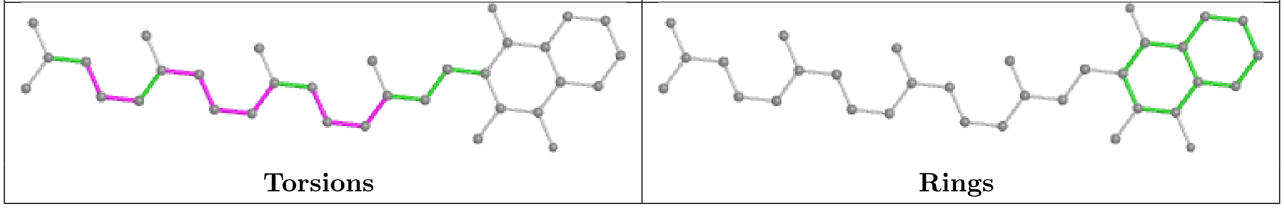


Torsions Rings

Ligand PQN B 2002

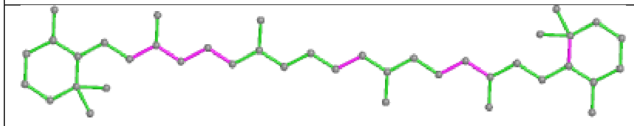


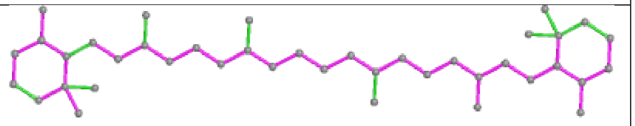
Bond lengths Bond angles

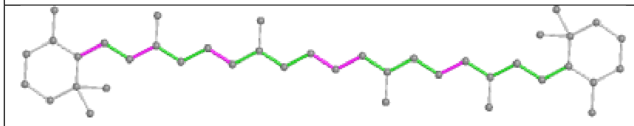


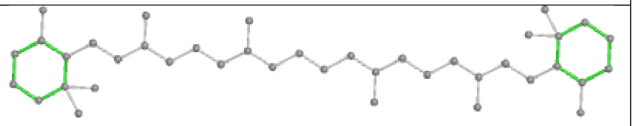
Torsions Rings

Ligand BCR i 4018

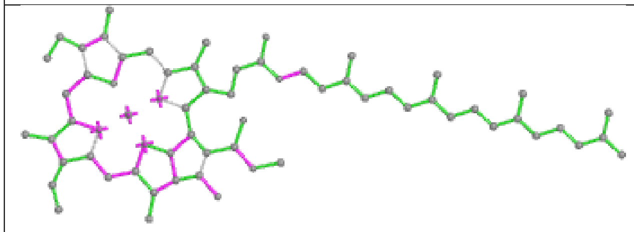

Bond lengths

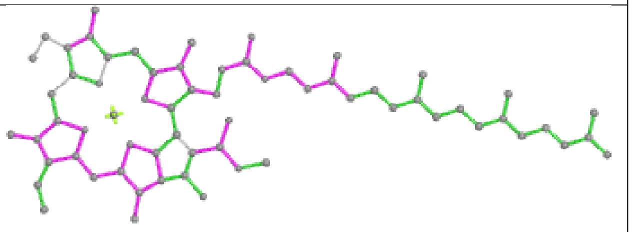

Bond angles

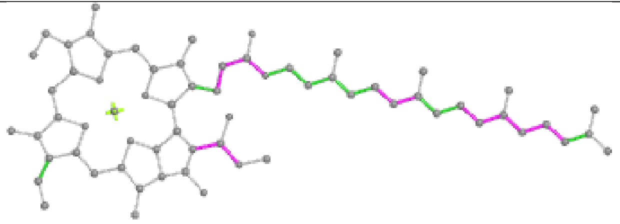

Torsions

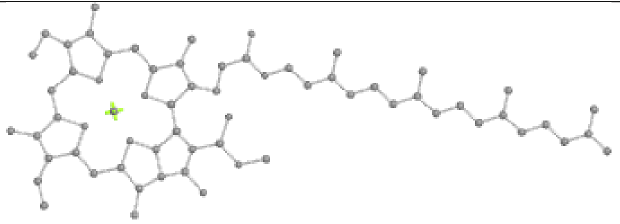

Rings

Ligand CLA H 1224

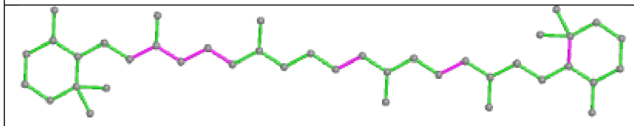

Bond lengths

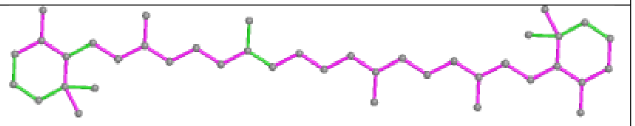

Bond angles

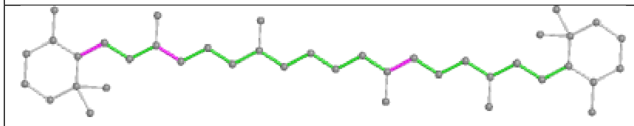

Torsions

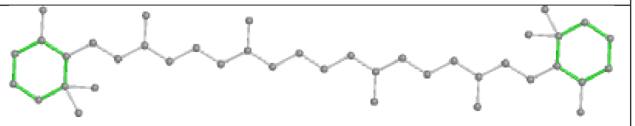

Rings

Ligand BCR H 4005

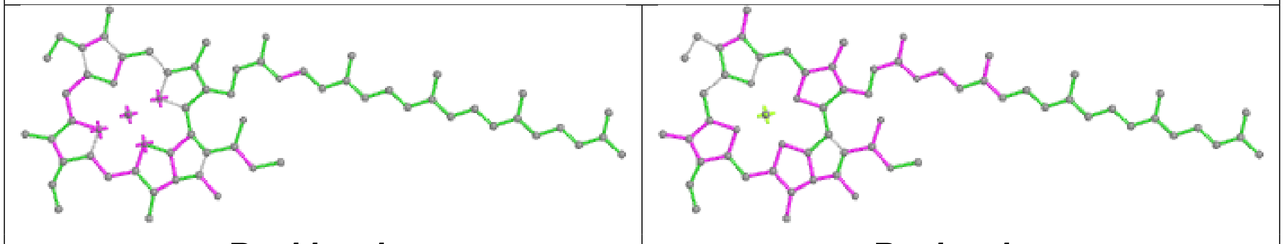

Bond lengths


Bond angles


Torsions

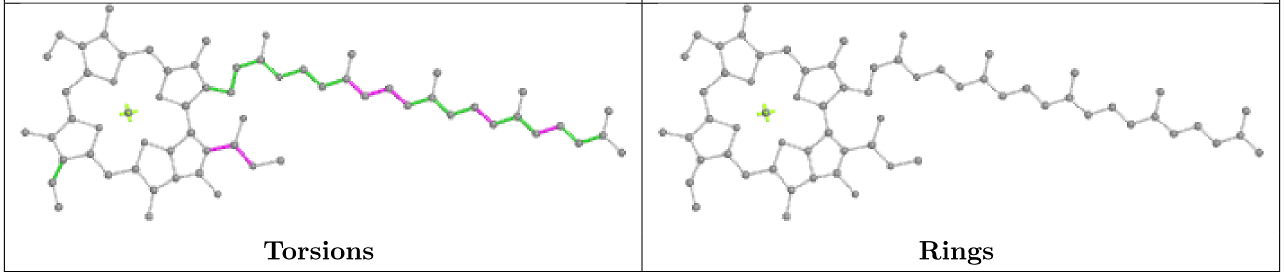

Rings

Ligand CLA H 1205



Bond lengths

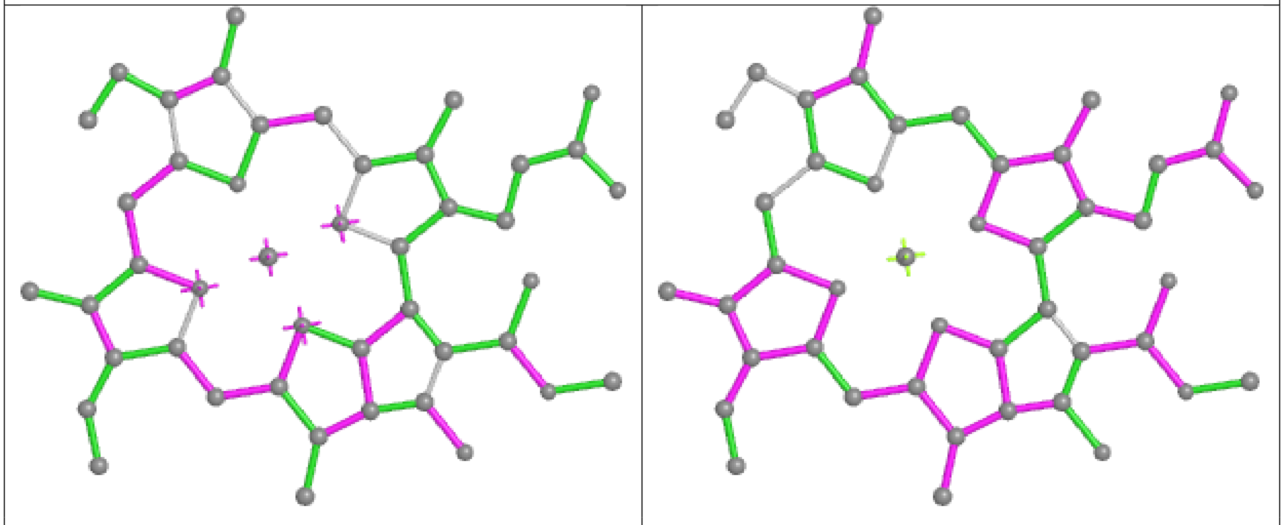
Bond angles



Torsions

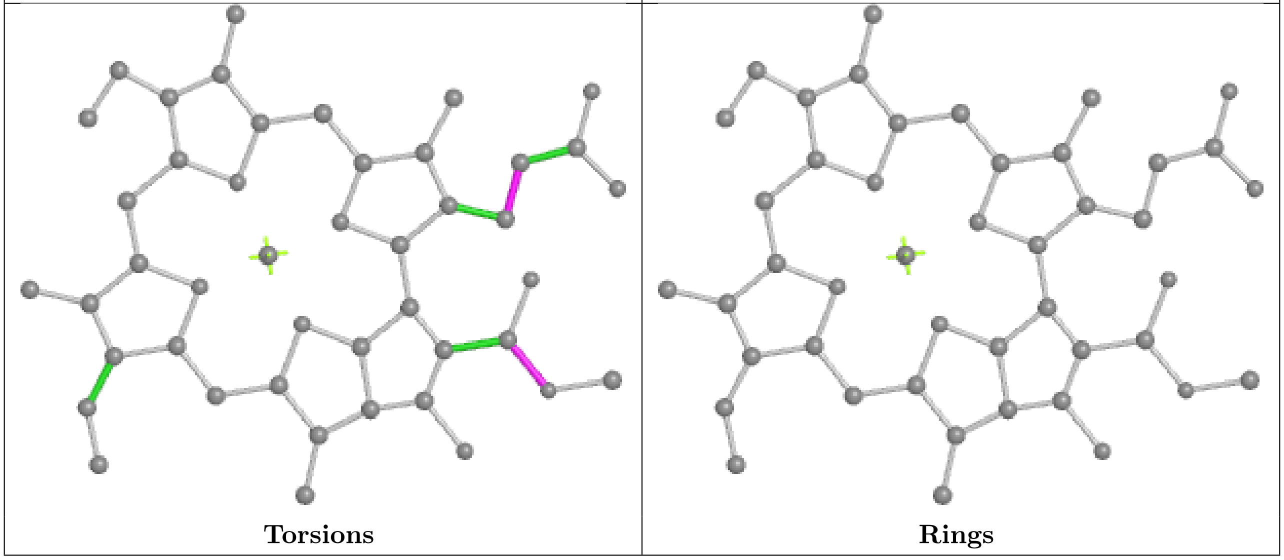
Rings

Ligand CLA a 1139



Bond lengths

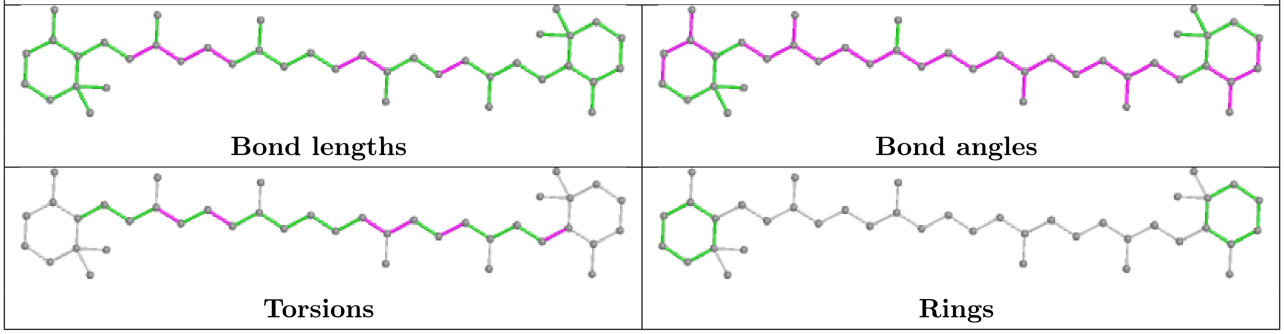
Bond angles



Torsions

Rings

Ligand BCR H 4010



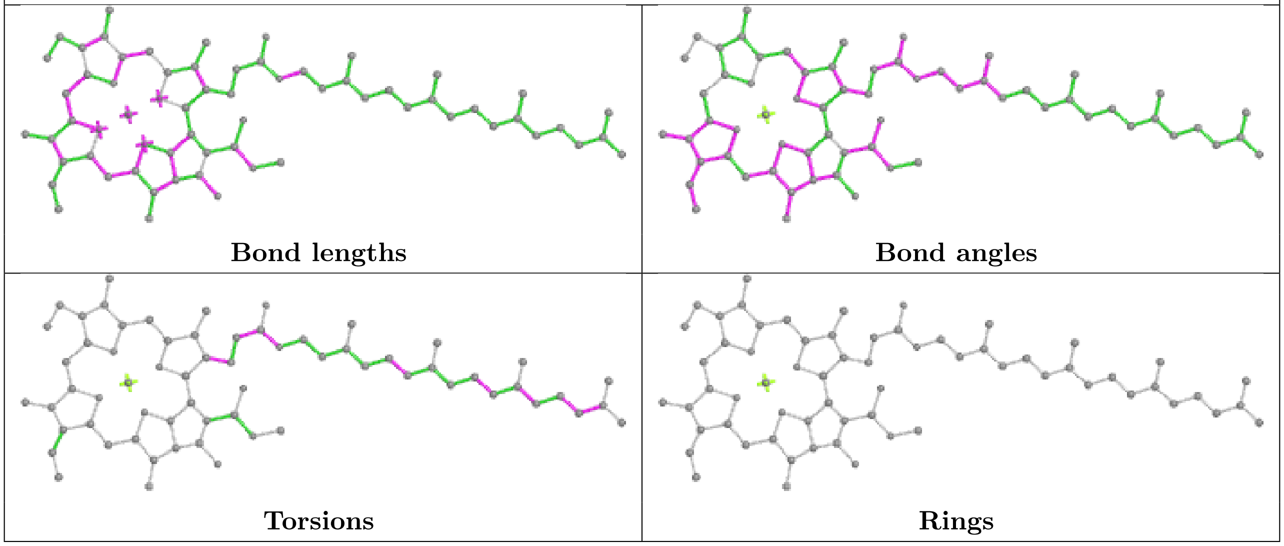
Bond lengths

Bond angles

Torsions

Rings

Ligand CL0 a 1011



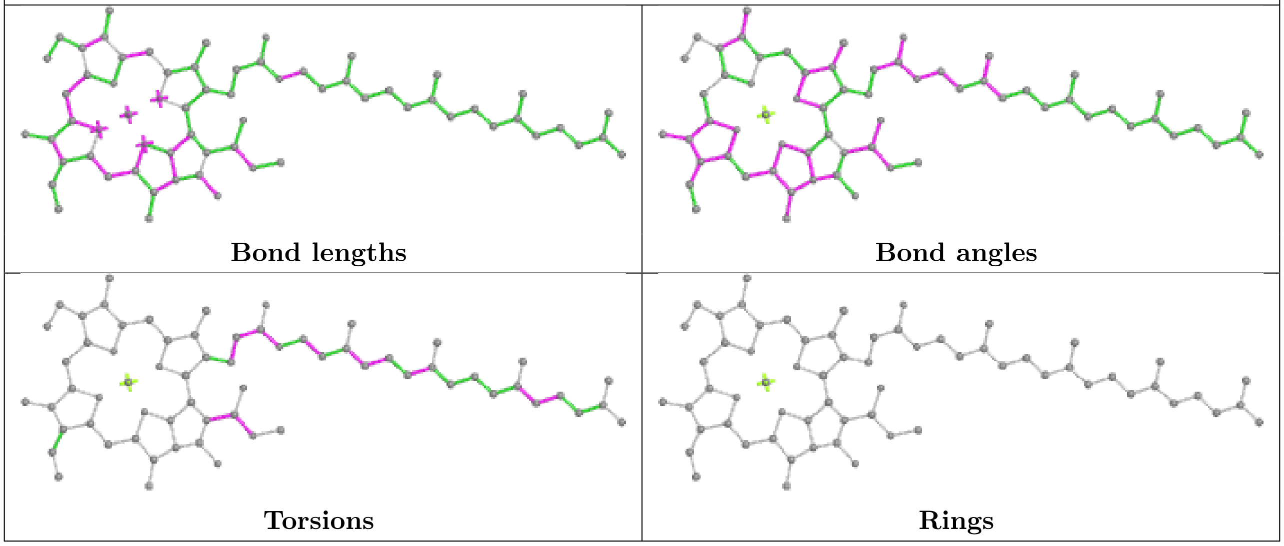
Bond lengths

Bond angles

Torsions

Rings

Ligand CLA b 1213



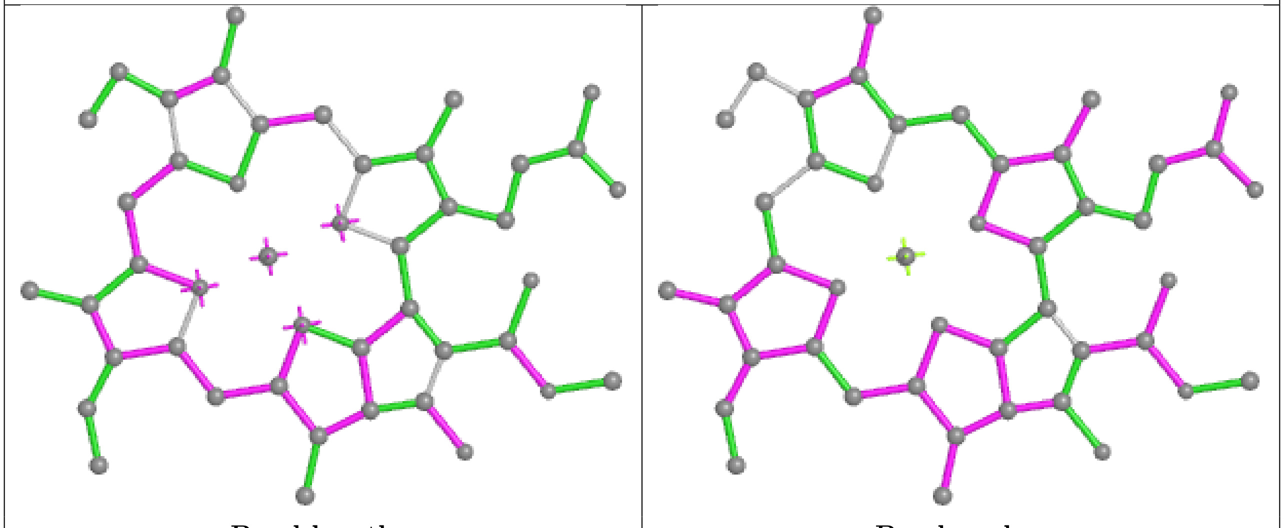
Bond lengths

Bond angles

Torsions

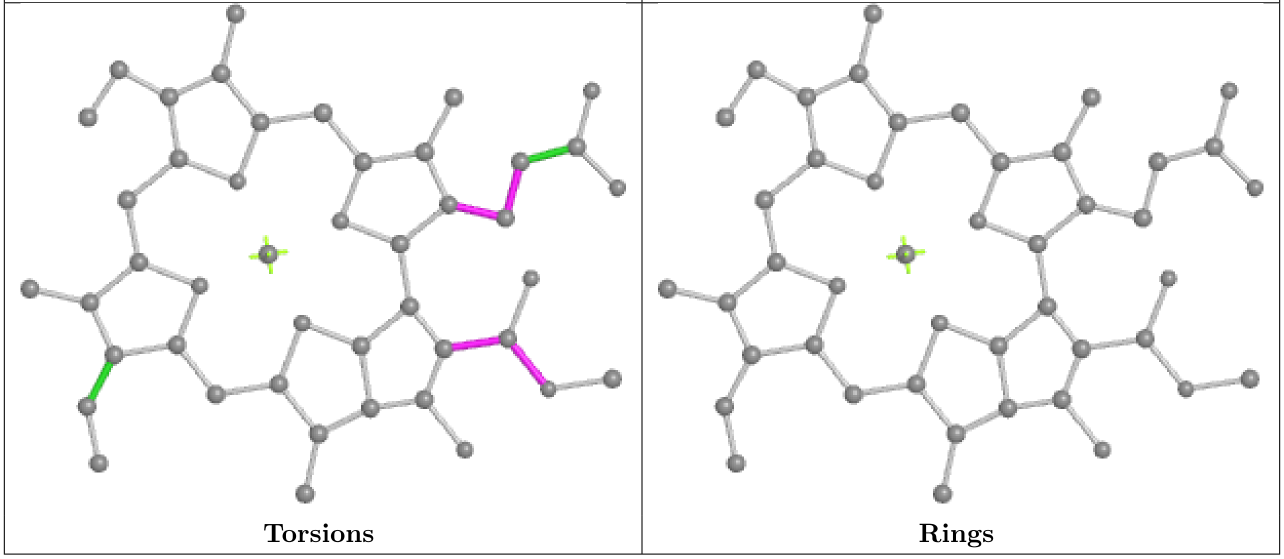
Rings

Ligand CLA k 1401



Bond lengths

Bond angles



Torsions

Rings

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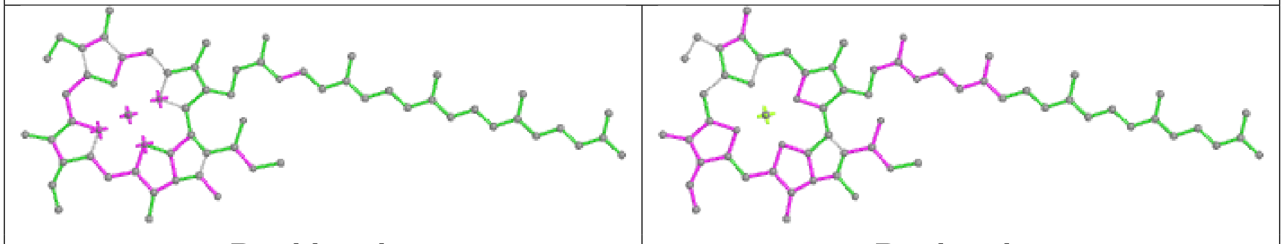
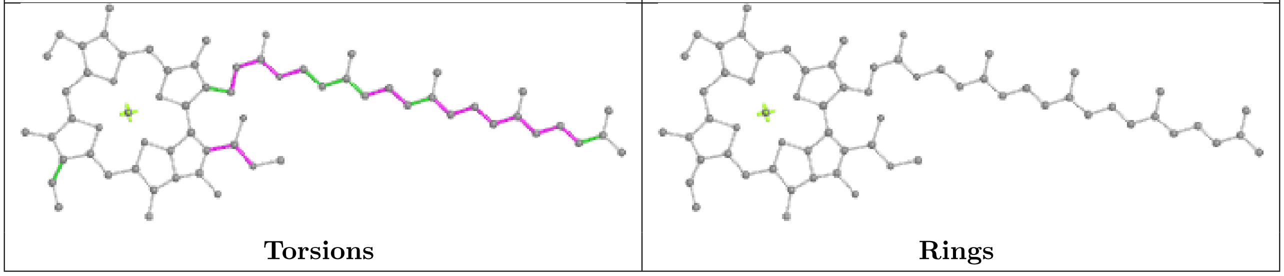


Bond lengths

Bond angles



Torsions

Rings

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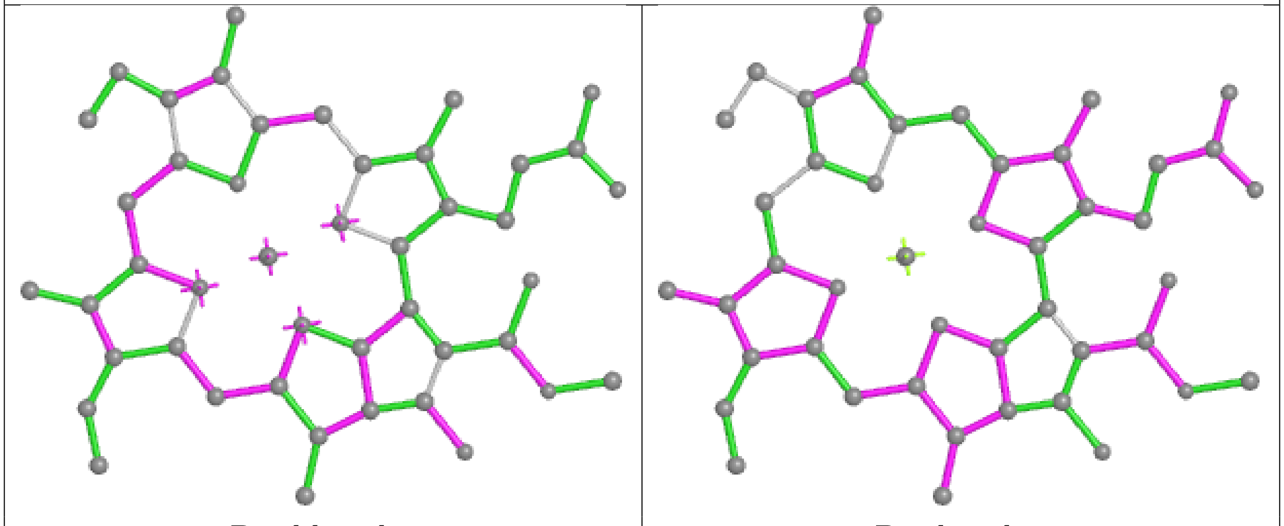
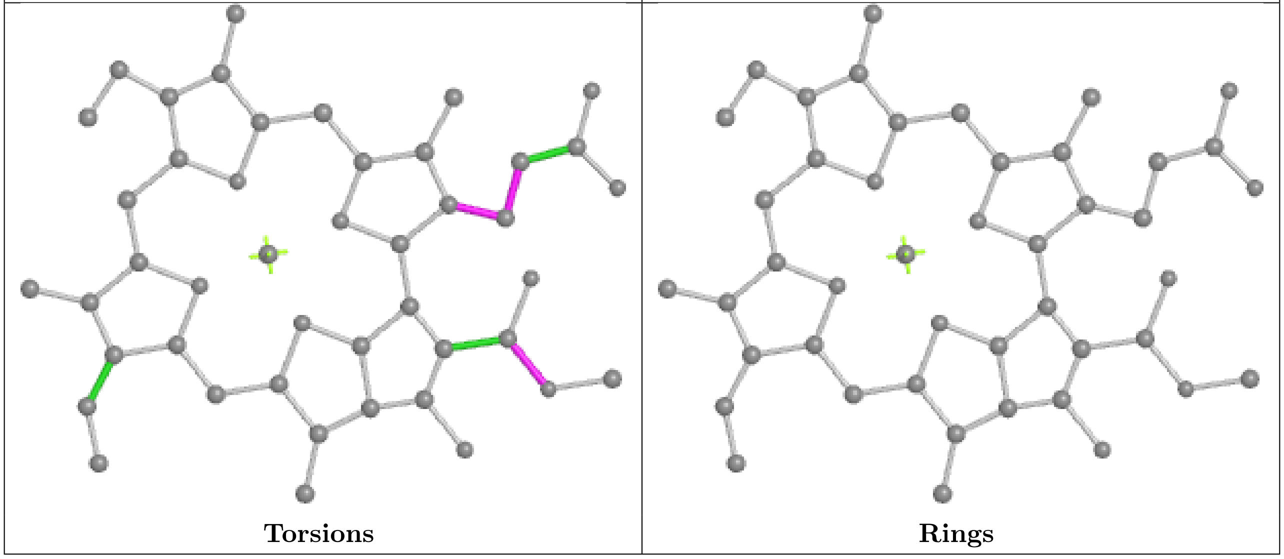


Bond lengths

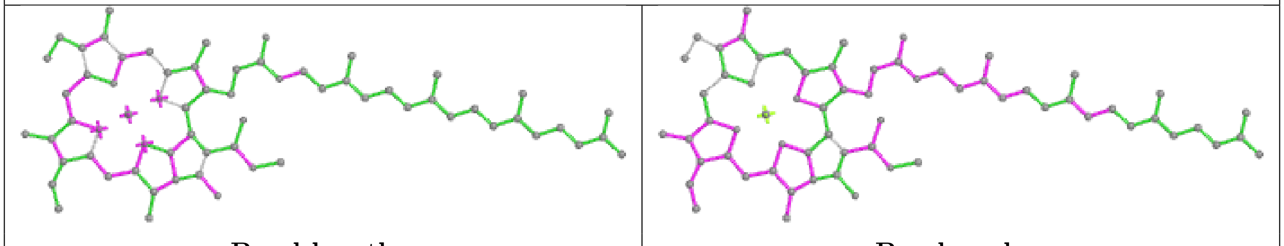
Bond angles



Torsions

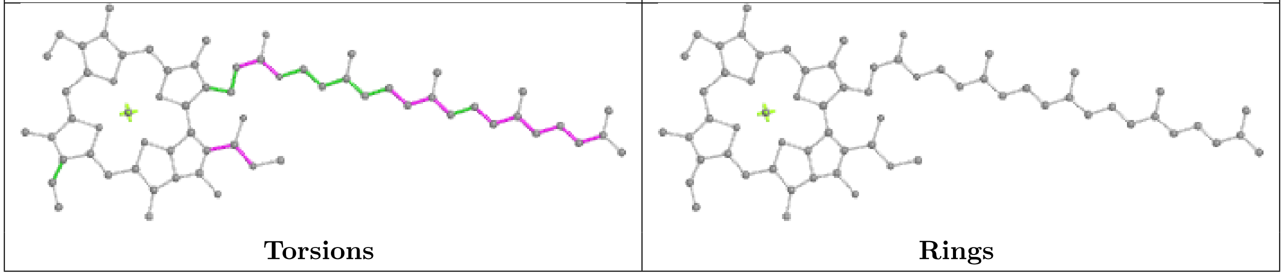
Rings

Ligand CLA b 1021



Bond lengths

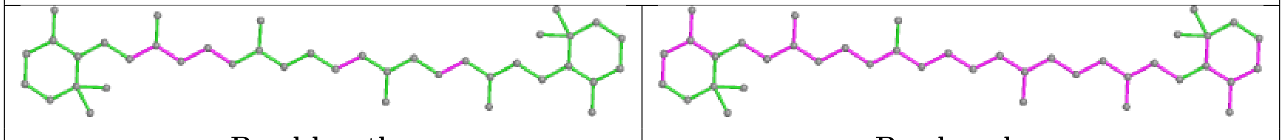
Bond angles



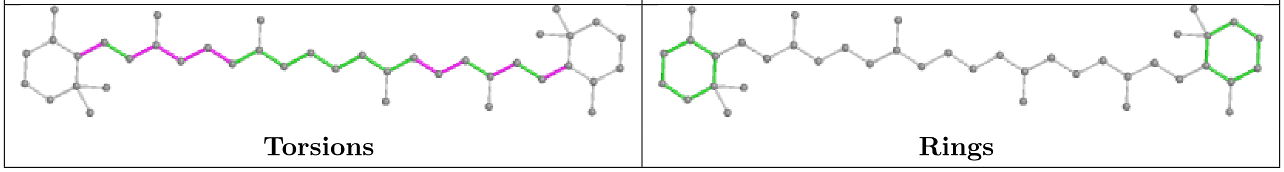
Torsions

Rings

Ligand BCR G 4003

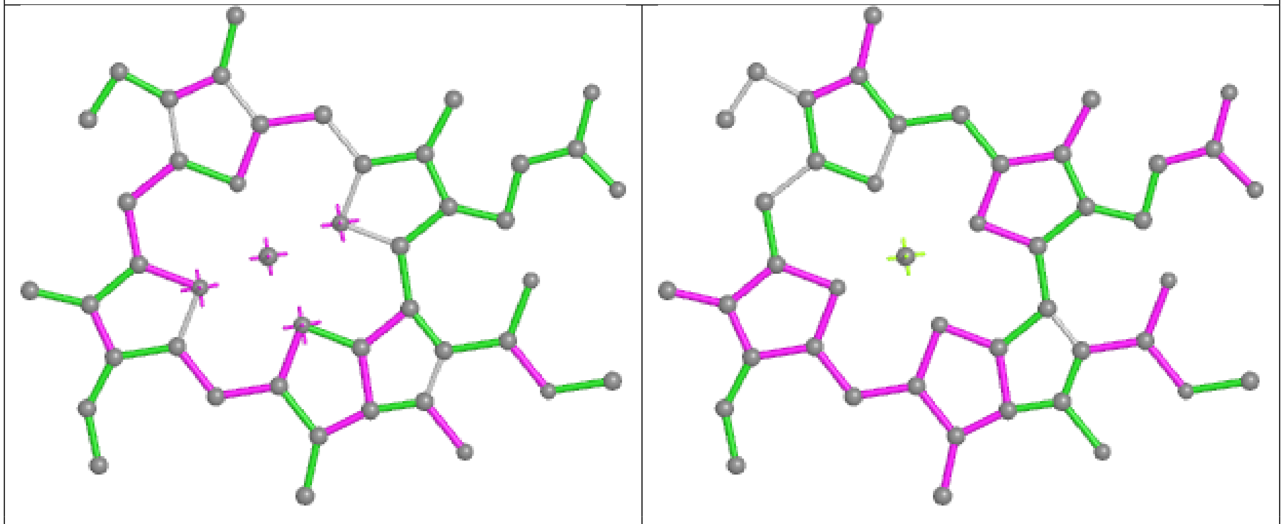


Bond lengths Bond angles

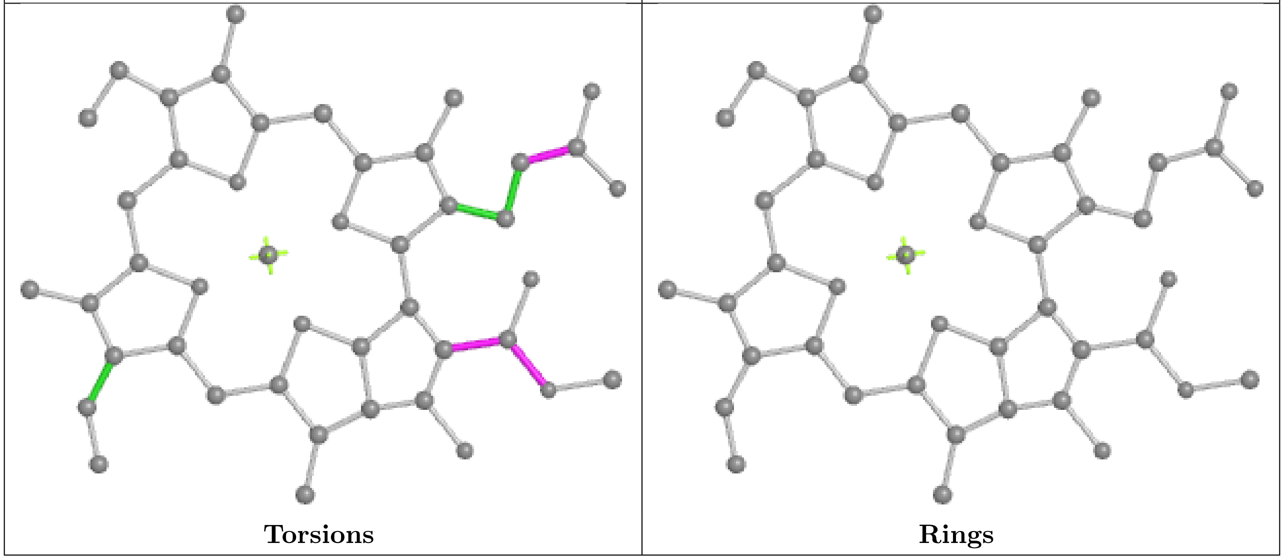


Torsions Rings

Ligand CLA B 1218

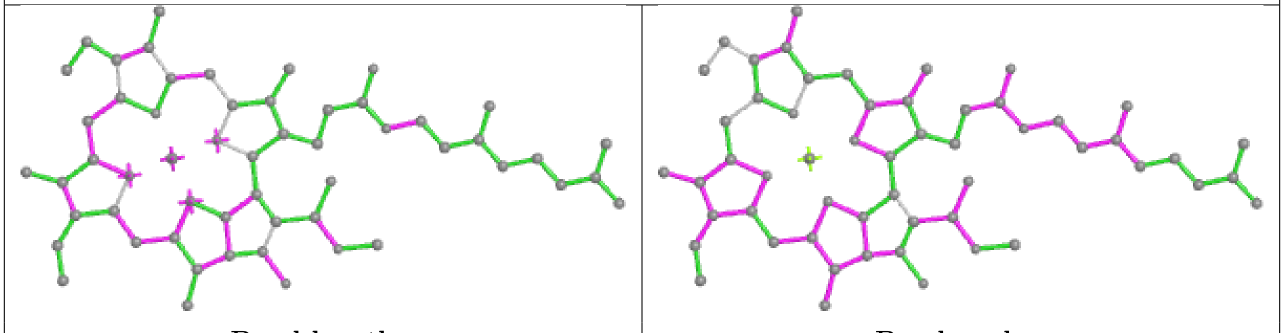


Bond lengths Bond angles

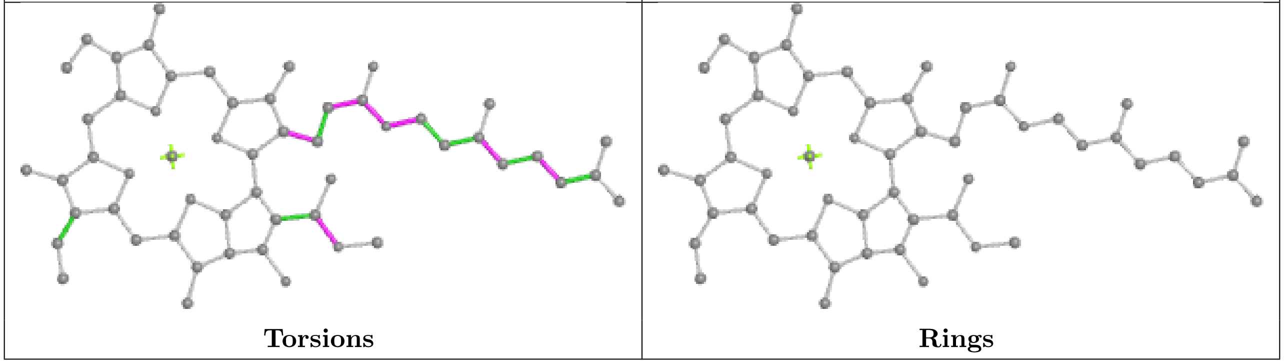


Torsions Rings

Ligand CLA X 1701

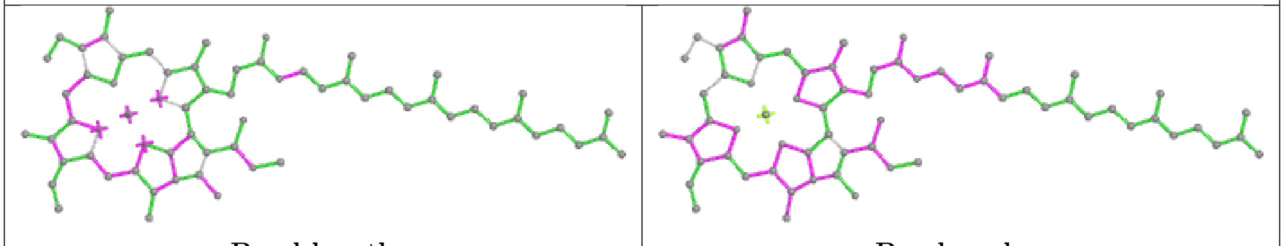


Bond lengths Bond angles

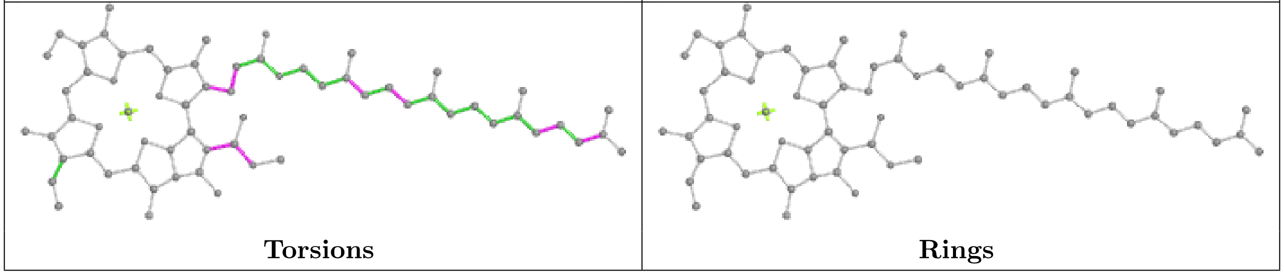


Torsions Rings

Ligand CLA G 1132

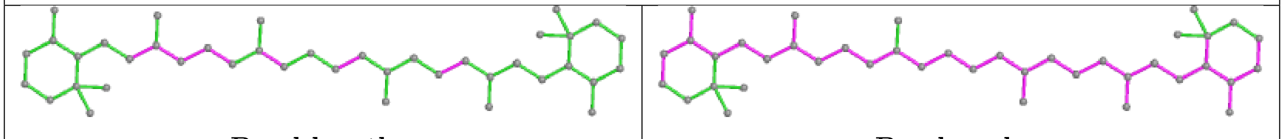


Bond lengths Bond angles

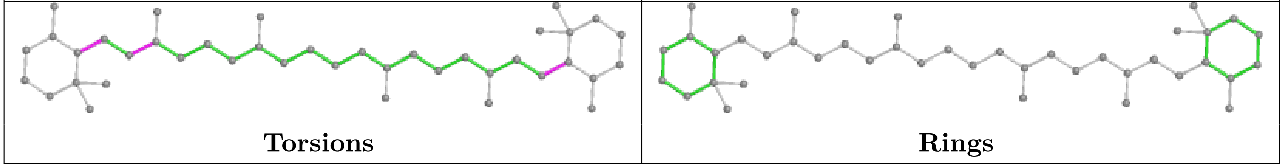


Torsions Rings

Ligand BCR a 4002

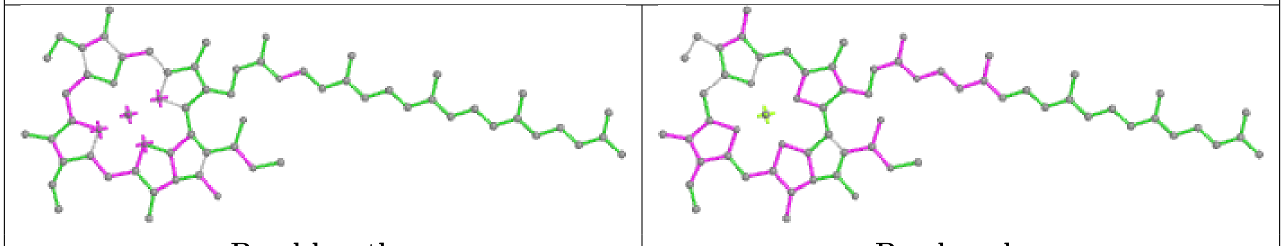


Bond lengths Bond angles



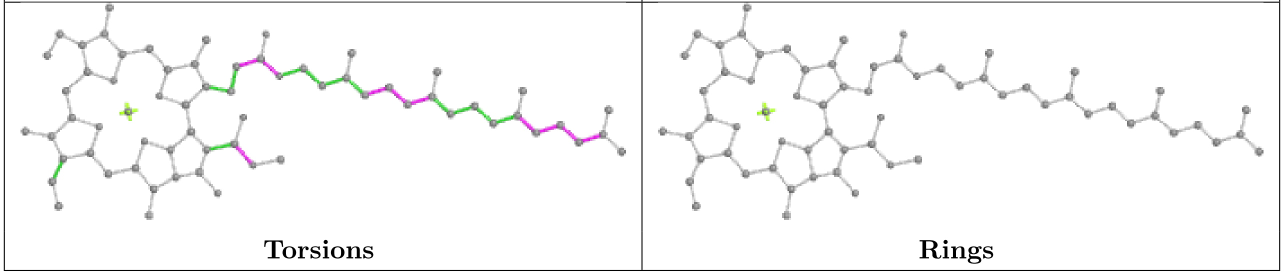
Torsions Rings

Ligand CLA H 1208



Bond lengths

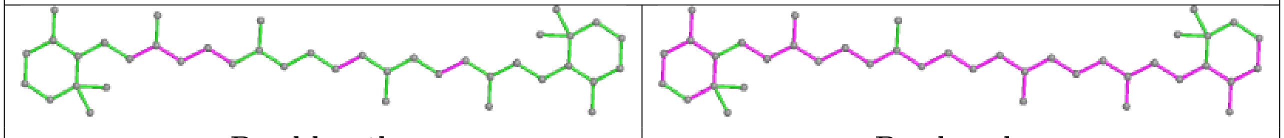
Bond angles



Torsions

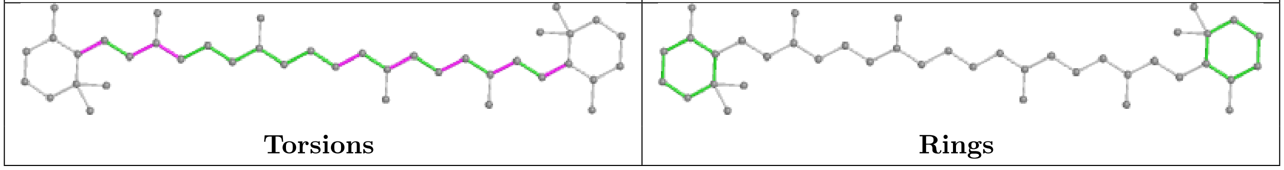
Rings

Ligand BCR G 4001



Bond lengths

Bond angles



Torsions

Rings

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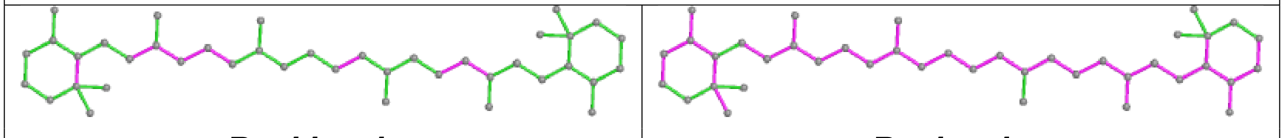
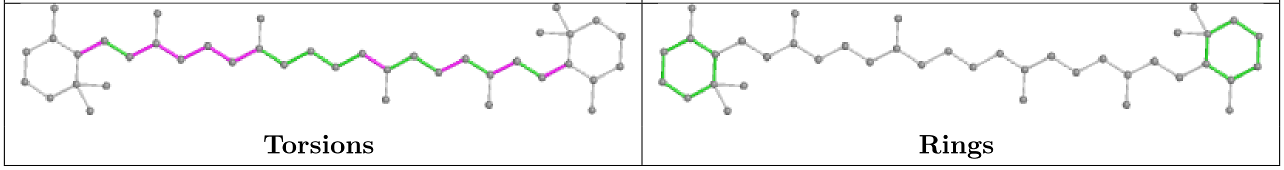


Bond lengths

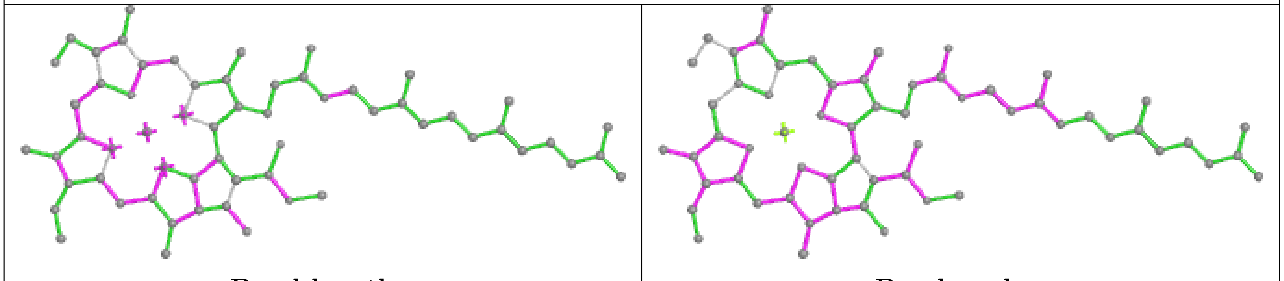
Bond angles



Torsions

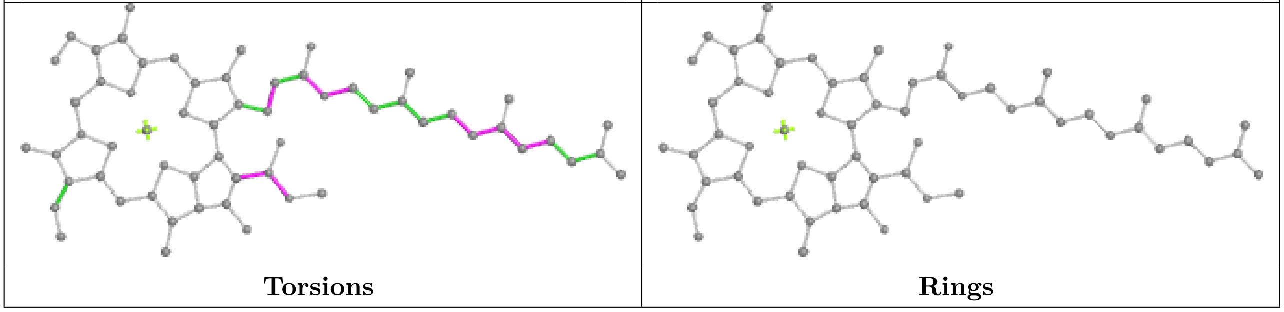
Rings

Ligand CLA a 1123



Bond lengths

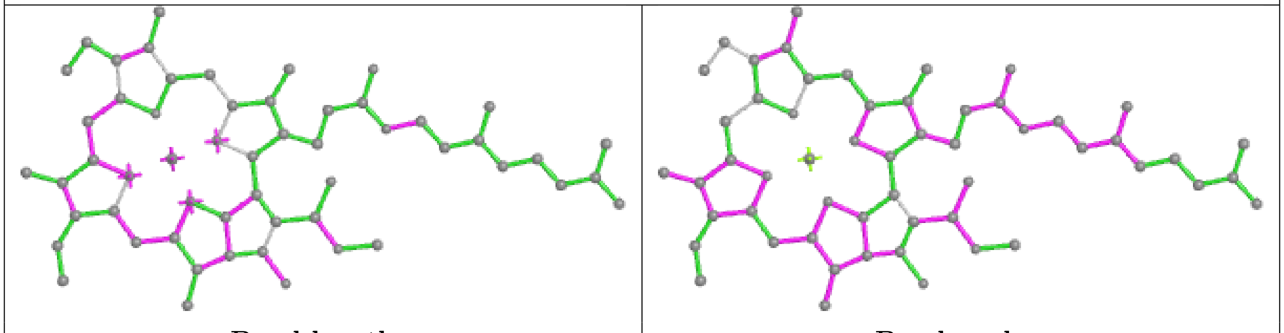
Bond angles



Torsions

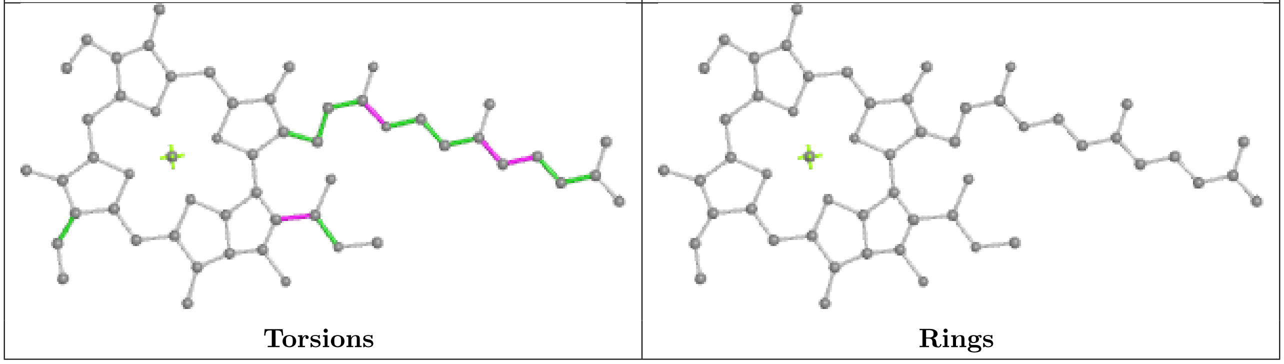
Rings

Ligand CLA b 1201



Bond lengths

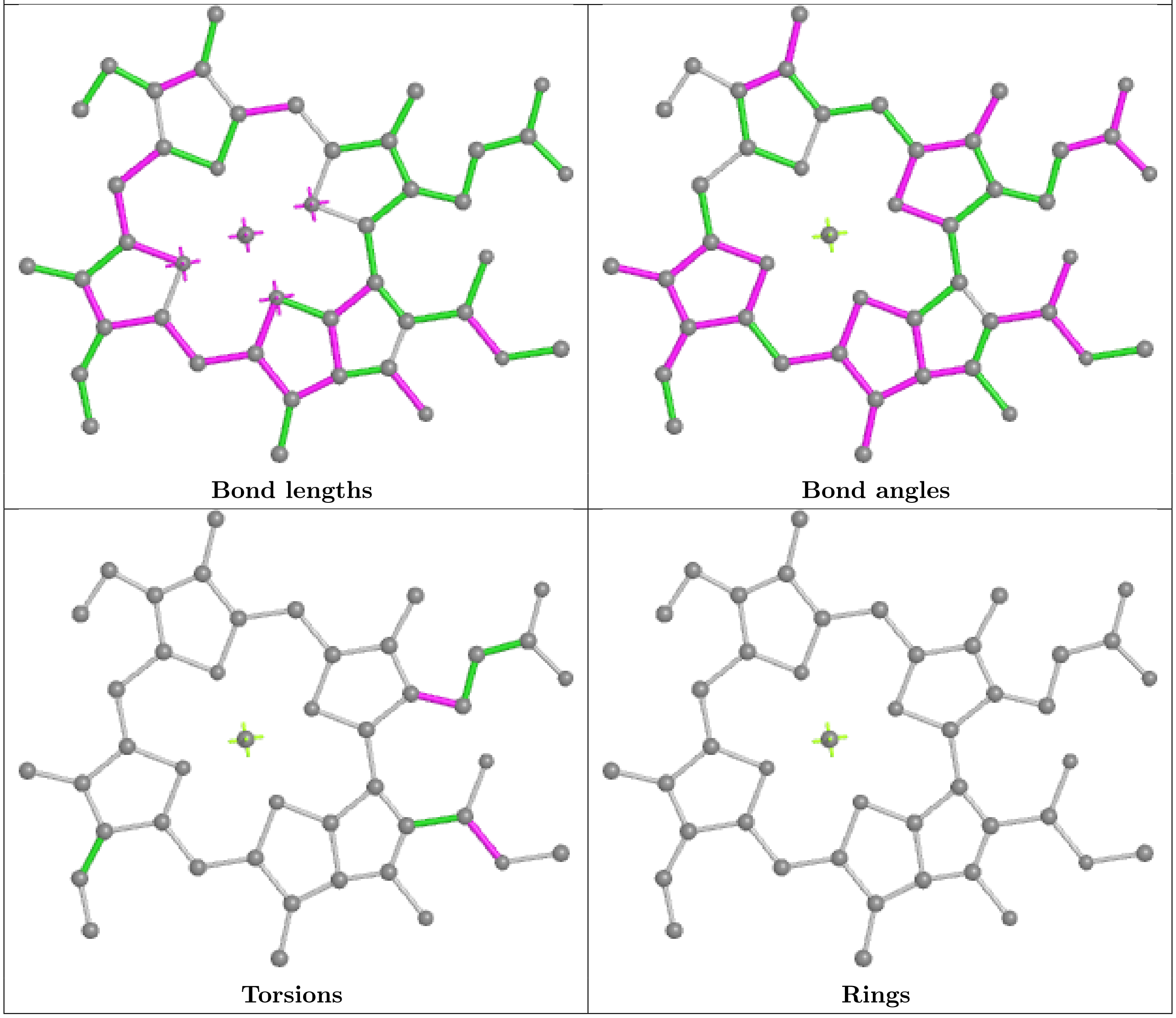
Bond angles



Torsions

Rings

Ligand CLA B 1219



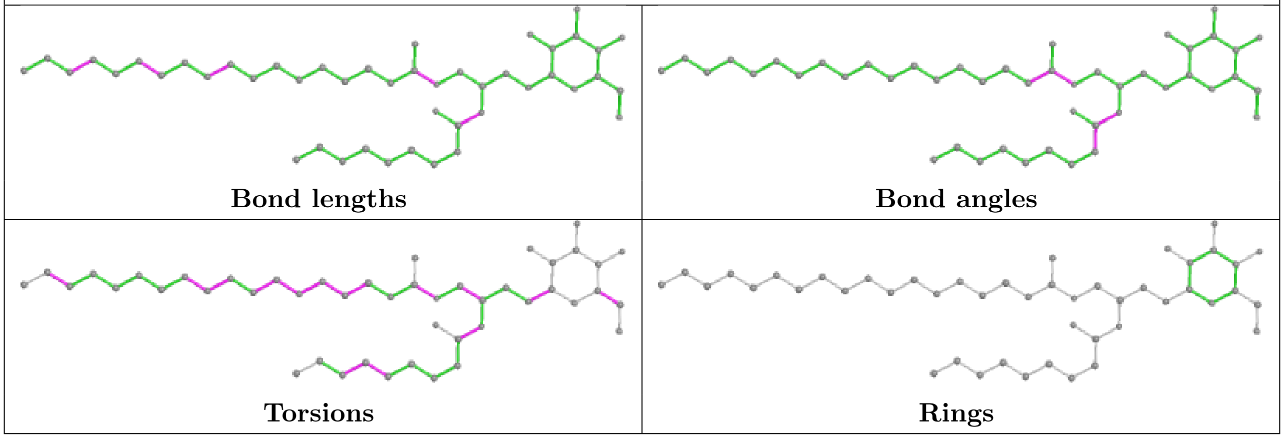
Bond lengths

Bond angles

Torsions

Rings

Ligand LMG a 5005



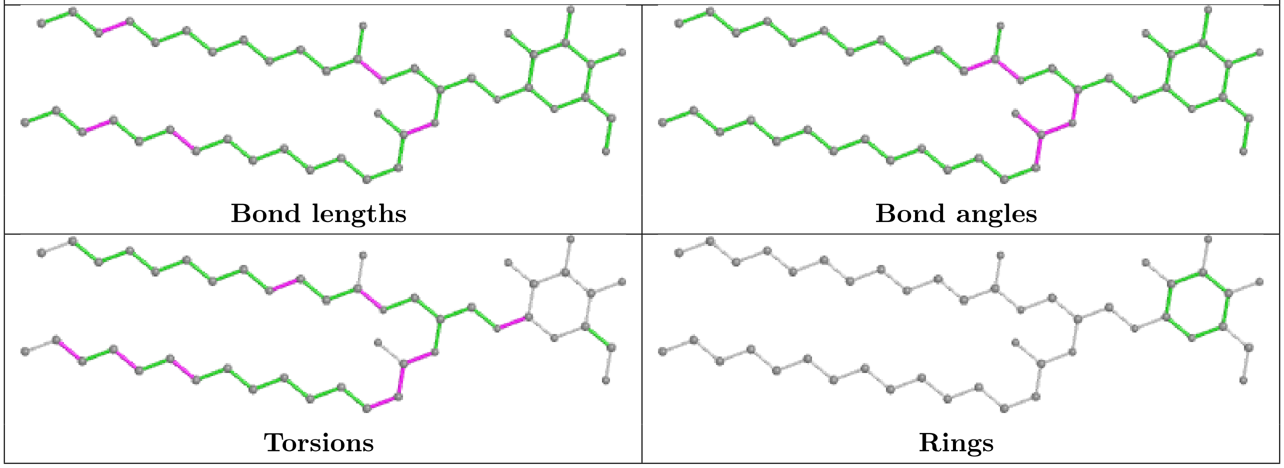
Bond lengths

Bond angles

Torsions

Rings

Ligand LMG H 5002



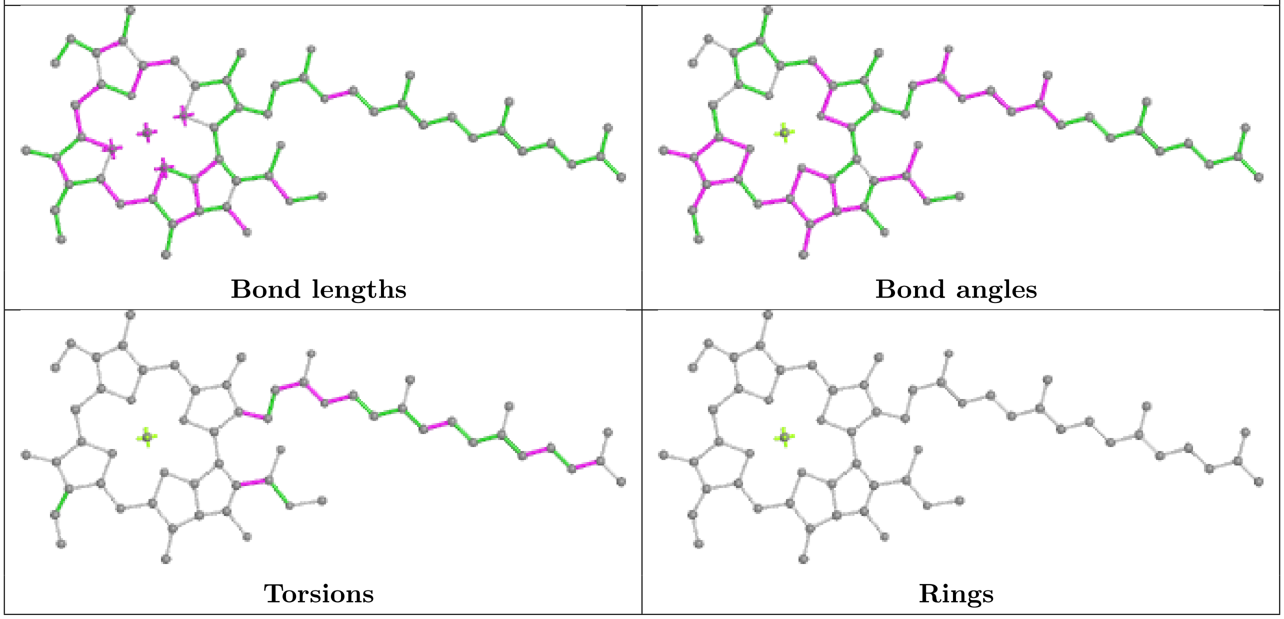
Bond lengths

Bond angles

Torsions

Rings

Ligand CLA B 1202



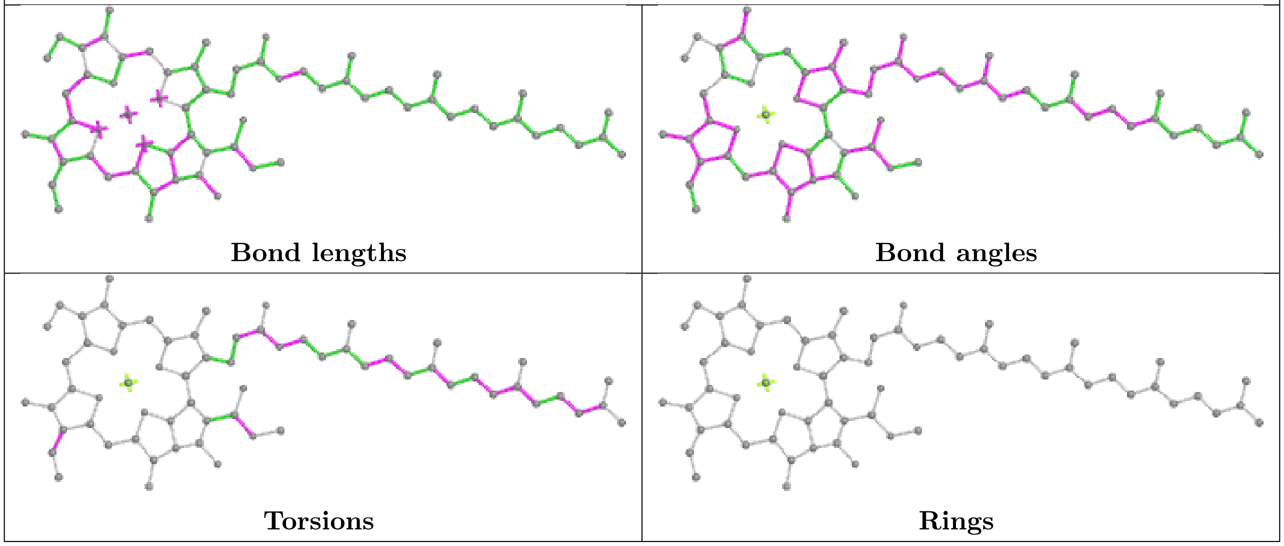
Bond lengths

Bond angles

Torsions

Rings

Ligand CLA H 1239



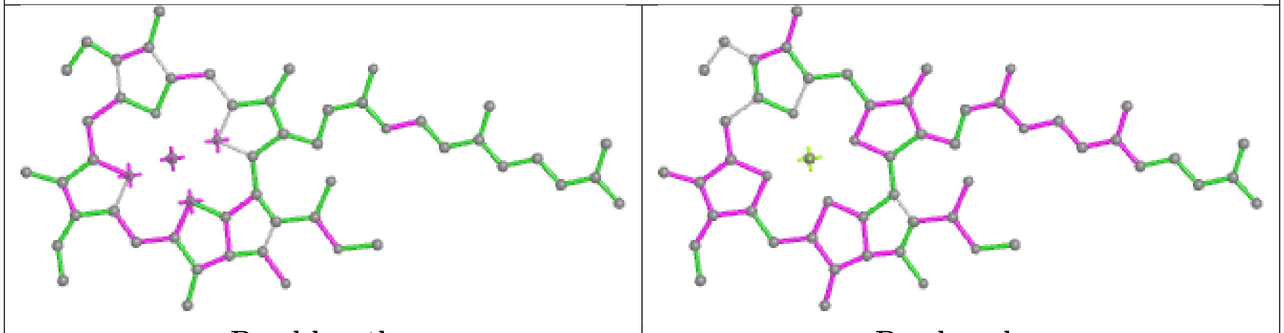
Bond lengths

Bond angles

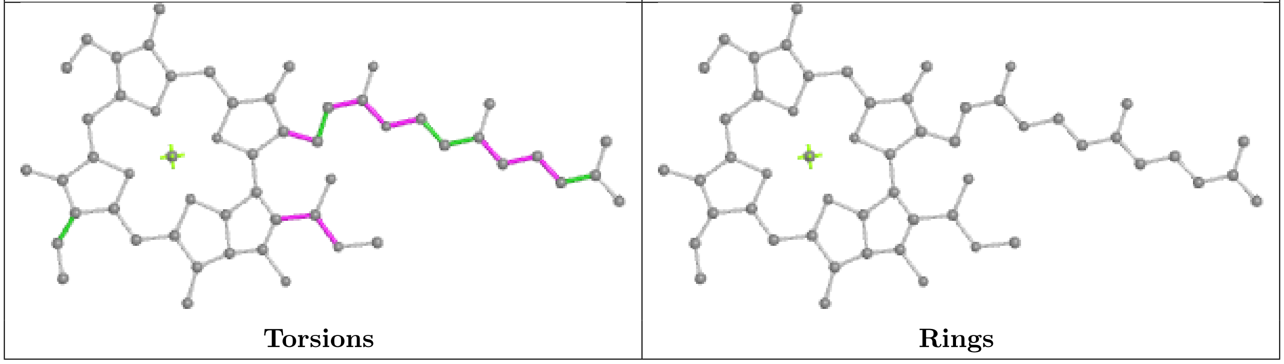
Torsions

Rings

Ligand CLA A 1122

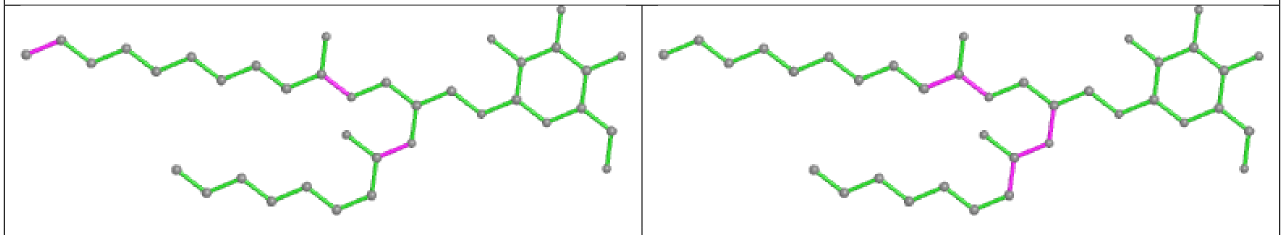


Bond lengths | Bond angles

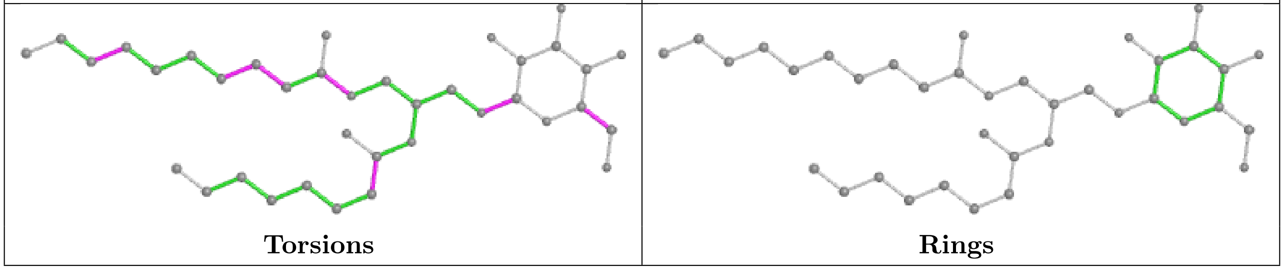


Torsions | Rings

Ligand LMG R 5006

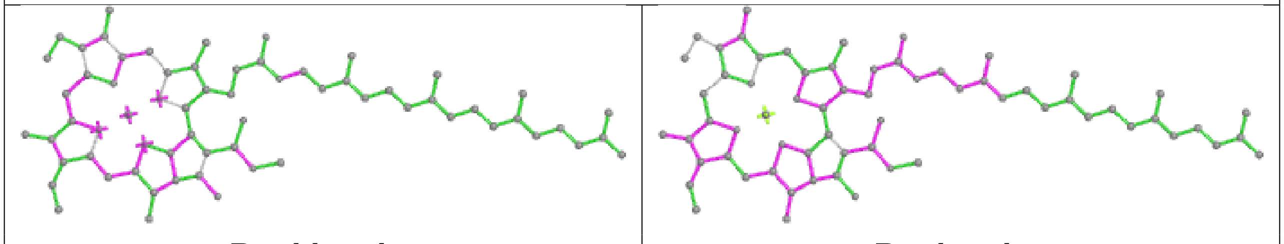


Bond lengths | Bond angles



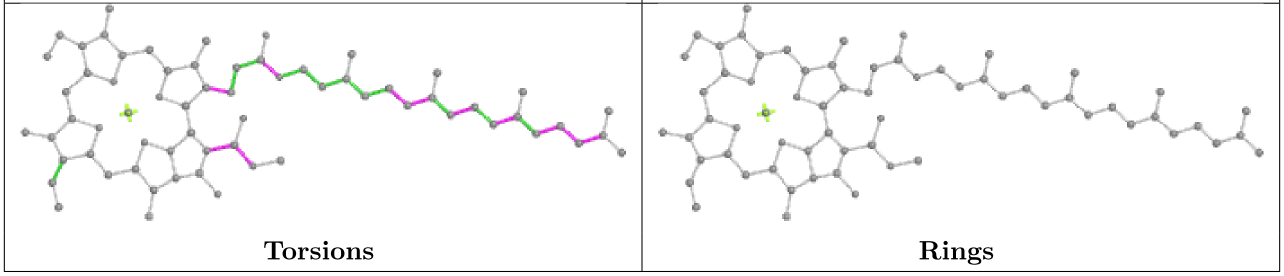
Torsions | Rings

Ligand CLA b 1222



Bond lengths

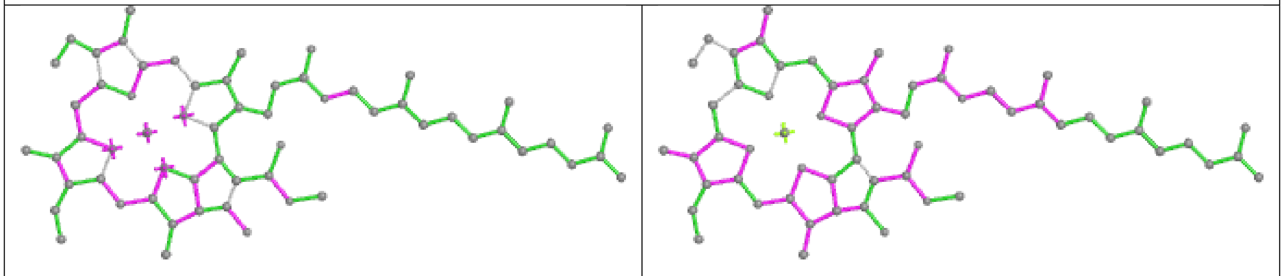
Bond angles



Torsions

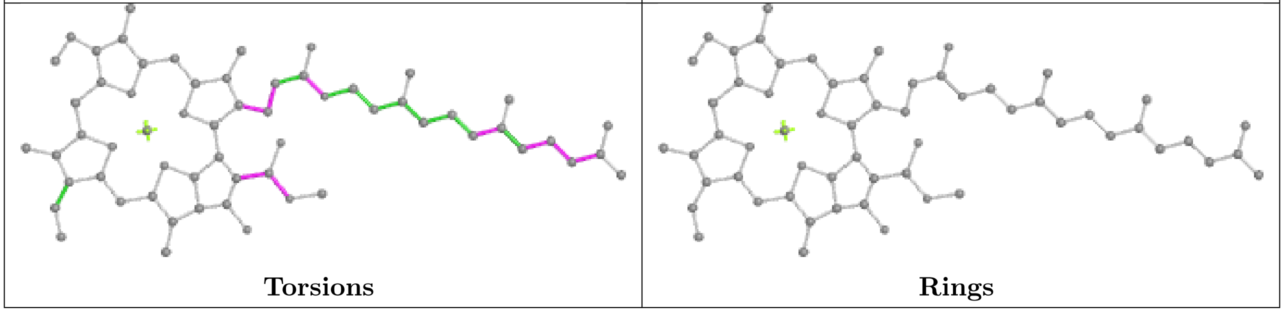
Rings

Ligand CLA A 1106



Bond lengths

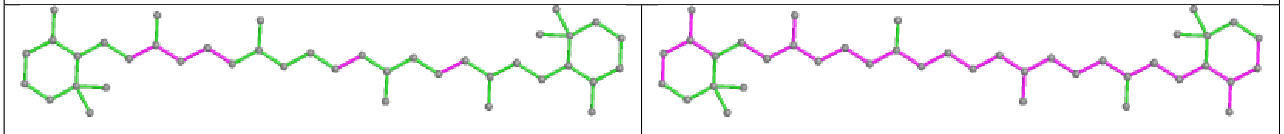
Bond angles



Torsions

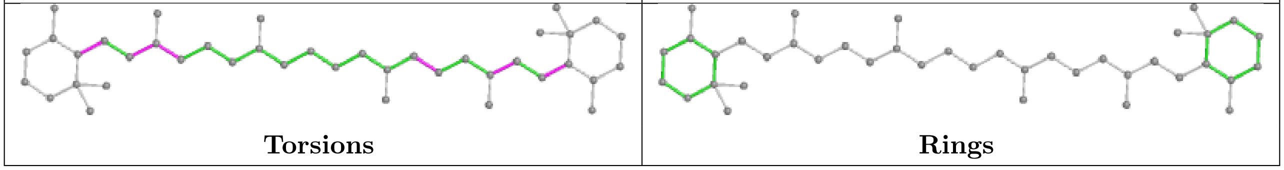
Rings

Ligand BCR b 4006



Bond lengths

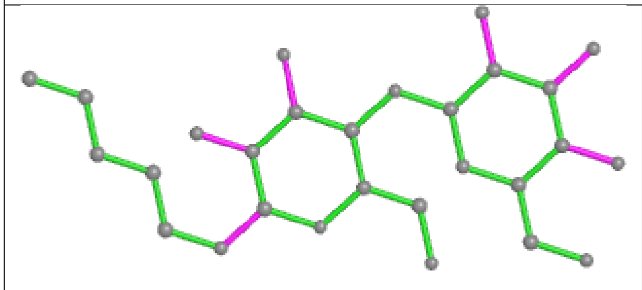
Bond angles



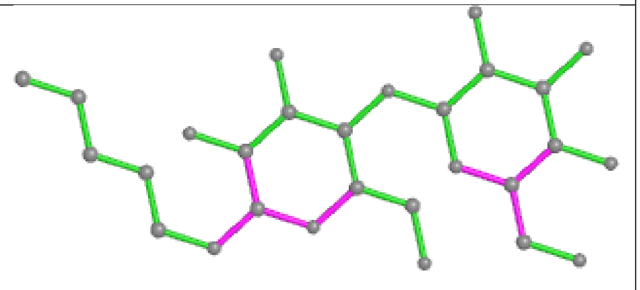
Torsions

Rings

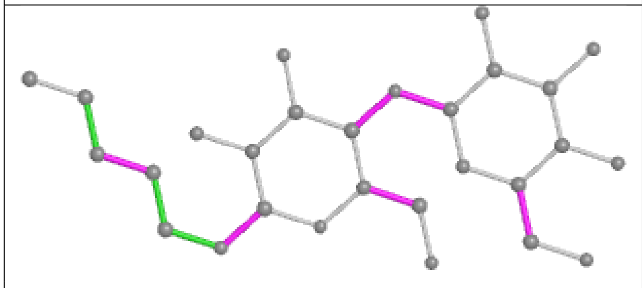
Ligand LMT G 6002



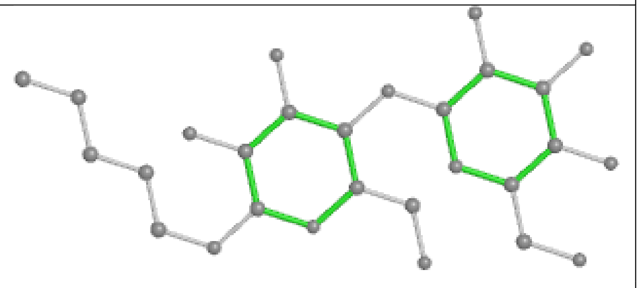
Bond lengths



Bond angles

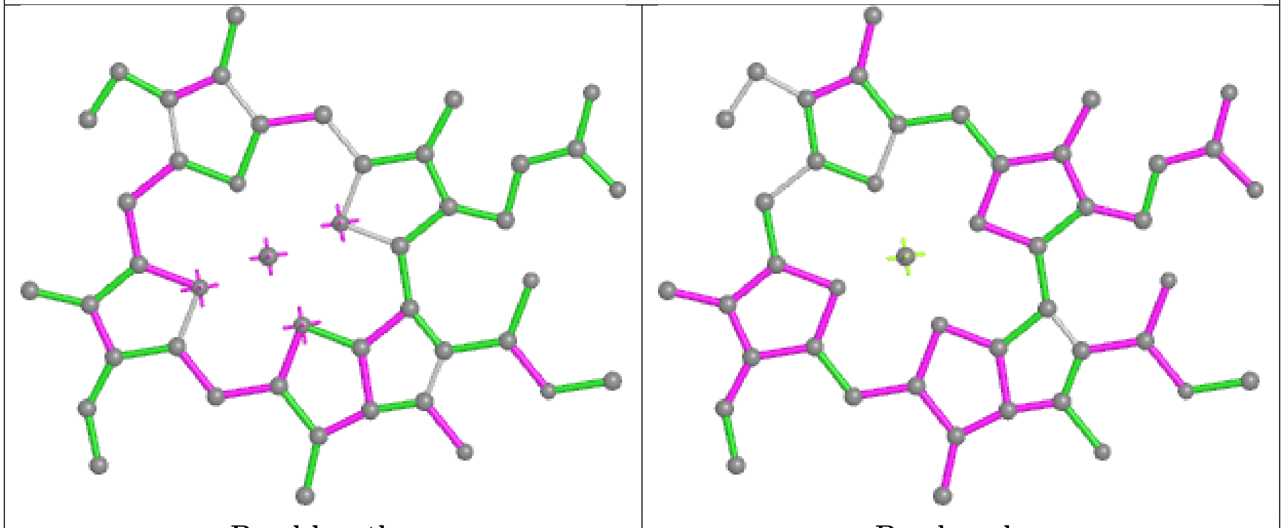


Torsions



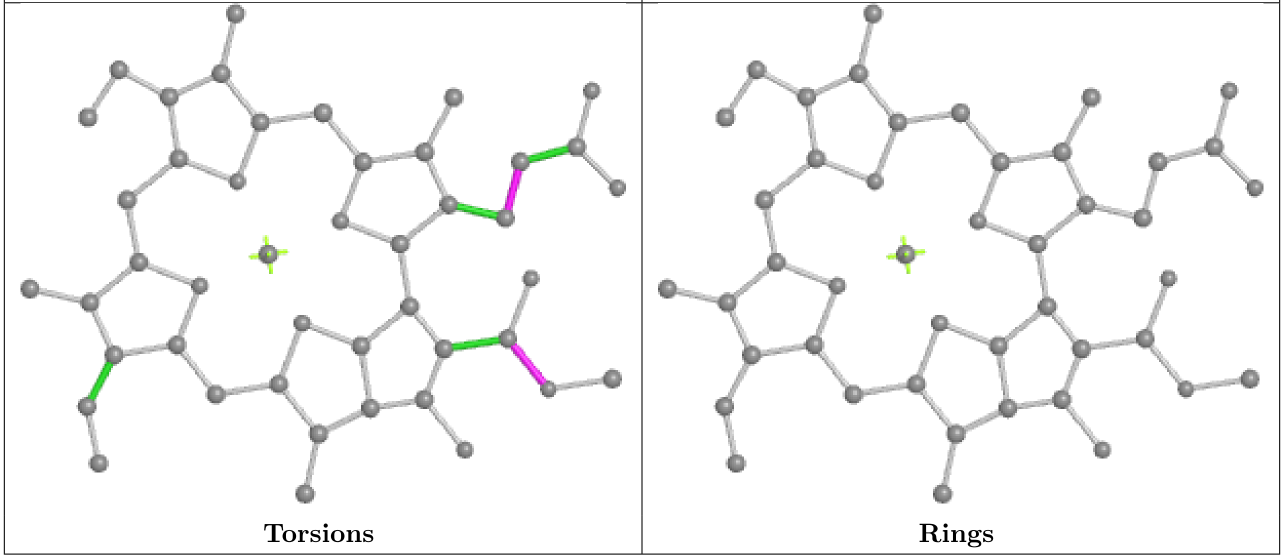
Rings

Ligand CLA A 1139



Bond lengths

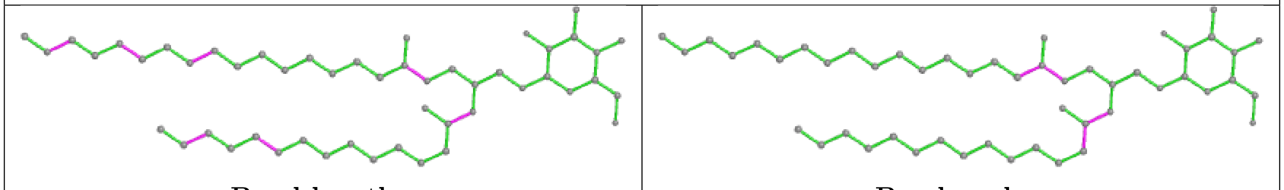
Bond angles



Torsions

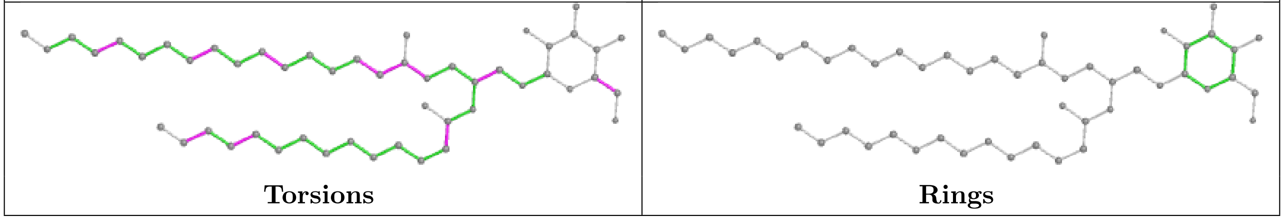
Rings

Ligand LMG L 5007



Bond lengths

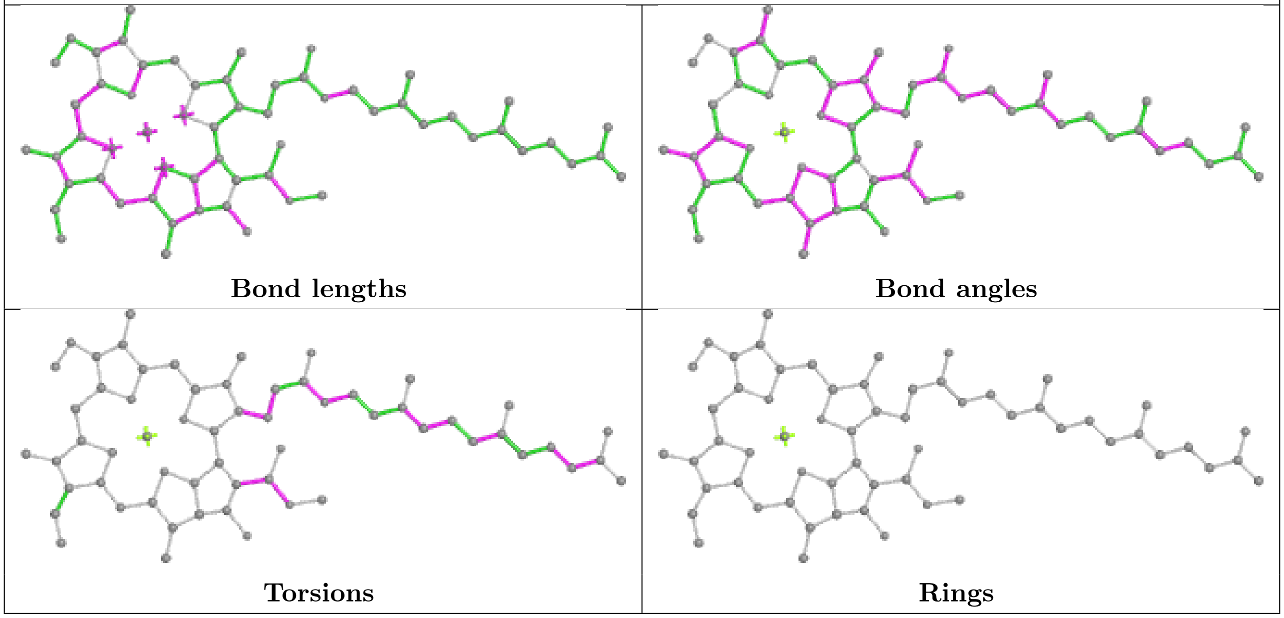
Bond angles



Torsions

Rings

Ligand CLA b 1215



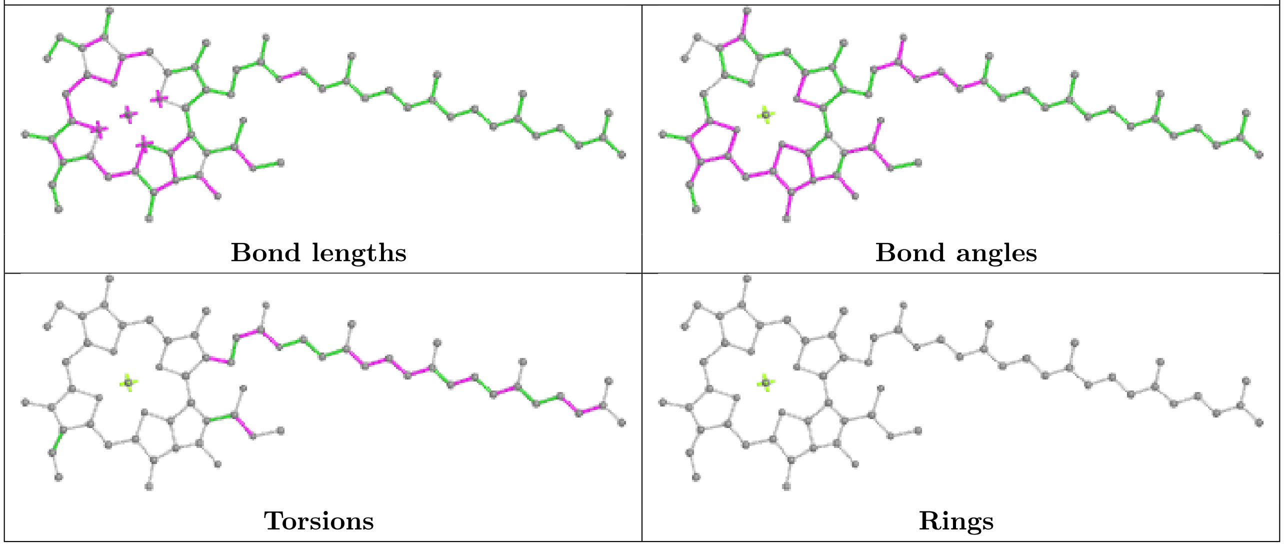
Bond lengths

Bond angles

Torsions

Rings

Ligand CLA a 1125



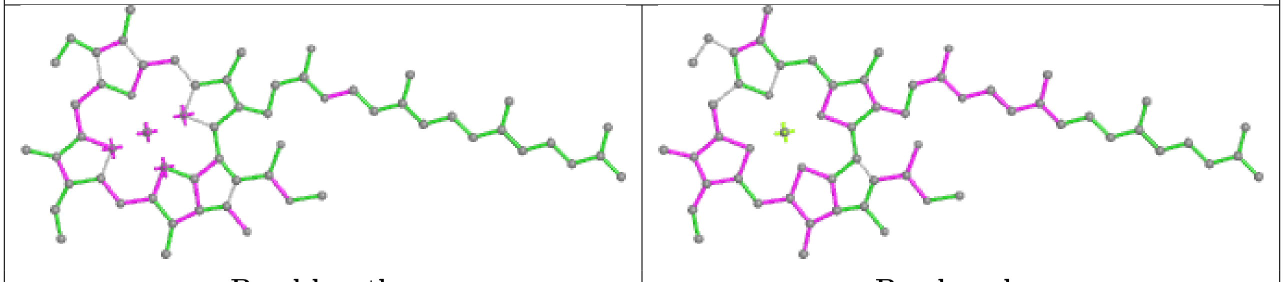
Bond lengths

Bond angles

Torsions

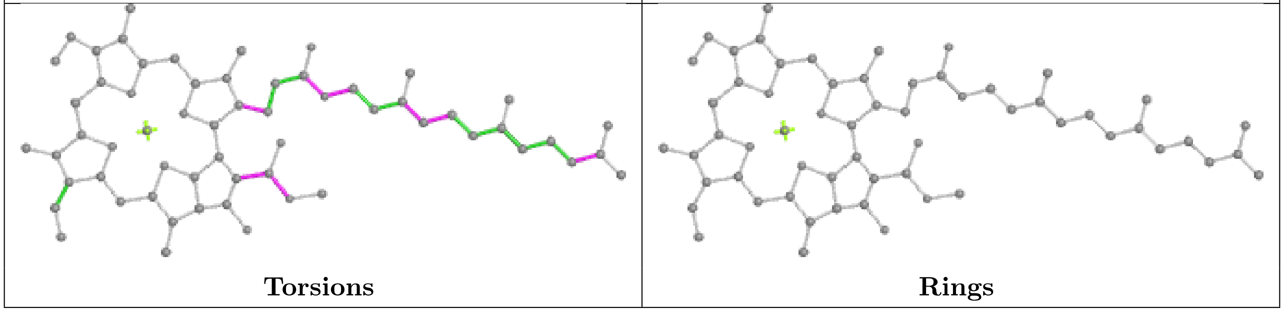
Rings

Ligand CLA G 1103



Bond lengths

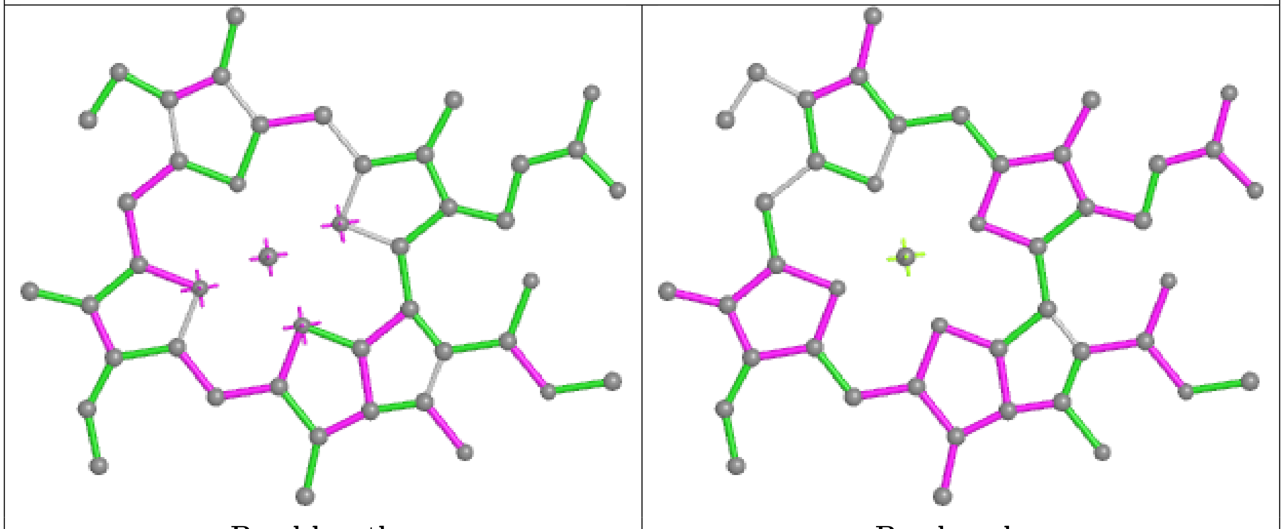
Bond angles



Torsions

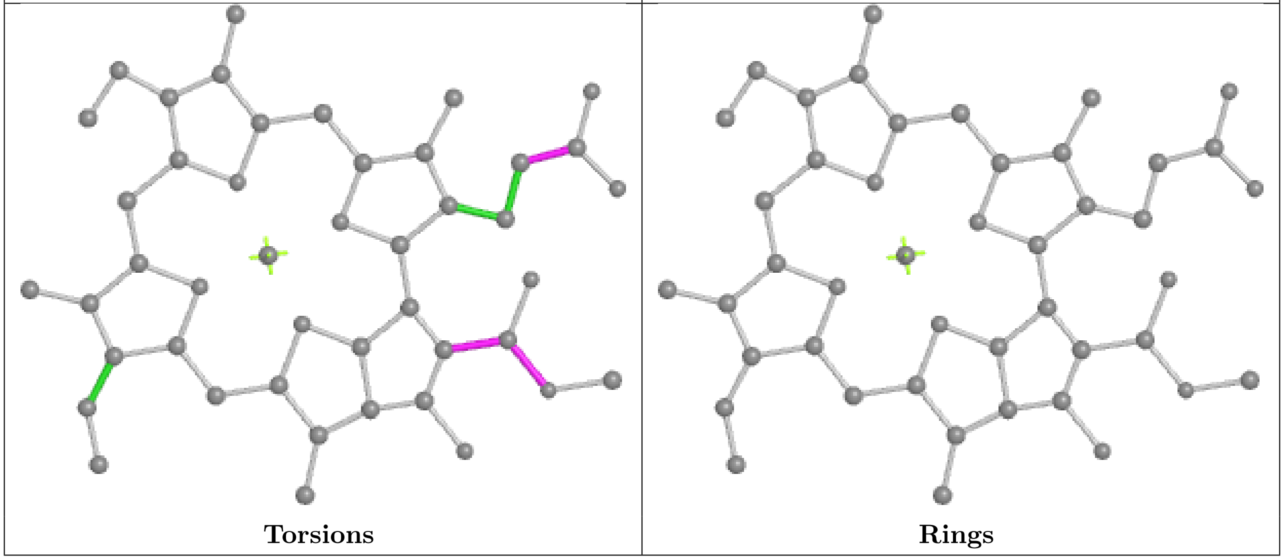
Rings

Ligand CLA A 1101



Bond lengths

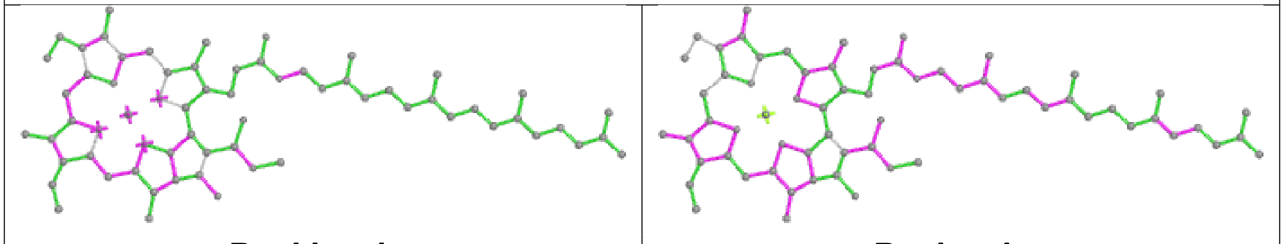
Bond angles



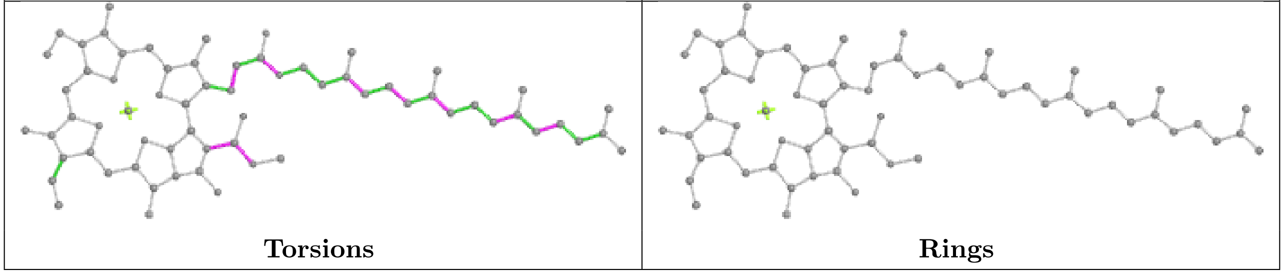
Torsions

Rings

Ligand CLA L 1501

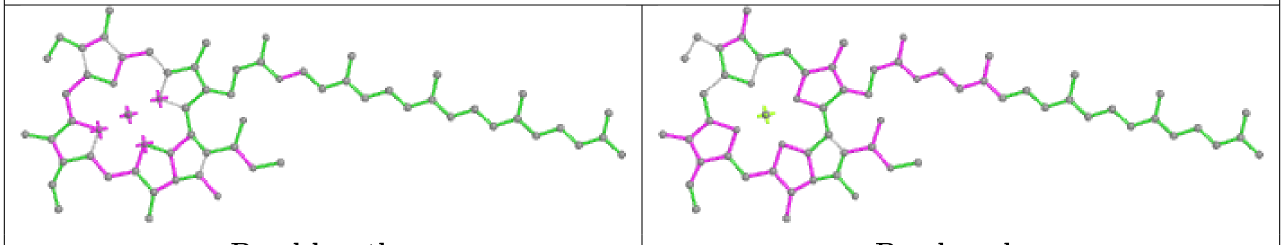


Bond lengths Bond angles

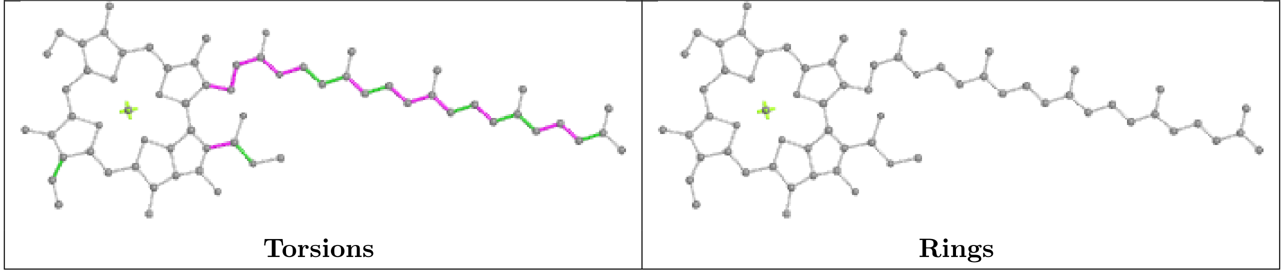


Torsions Rings

Ligand CLA B 1210

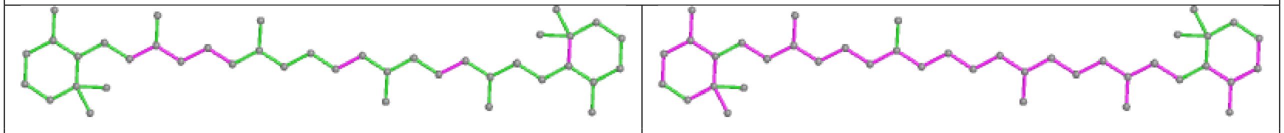


Bond lengths Bond angles

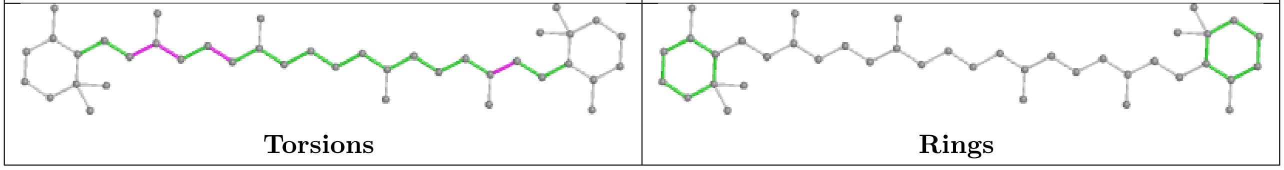


Torsions Rings

Ligand BCR b 4004

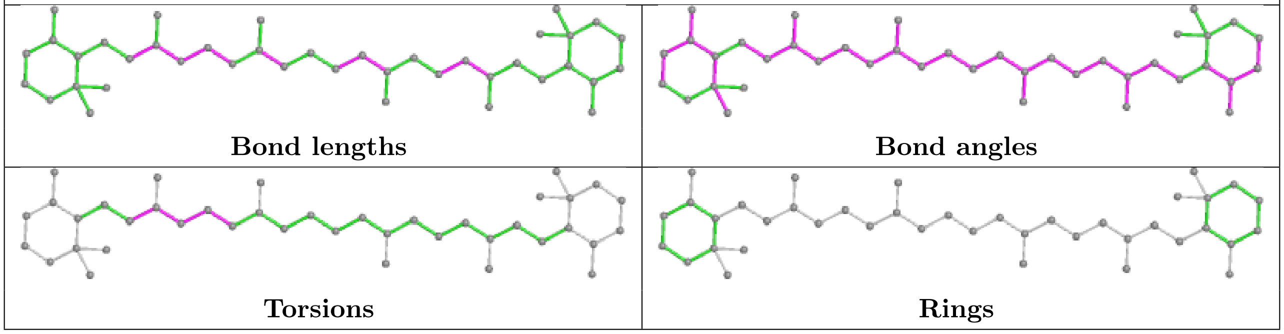


Bond lengths Bond angles



Torsions Rings

Ligand BCR L 4022



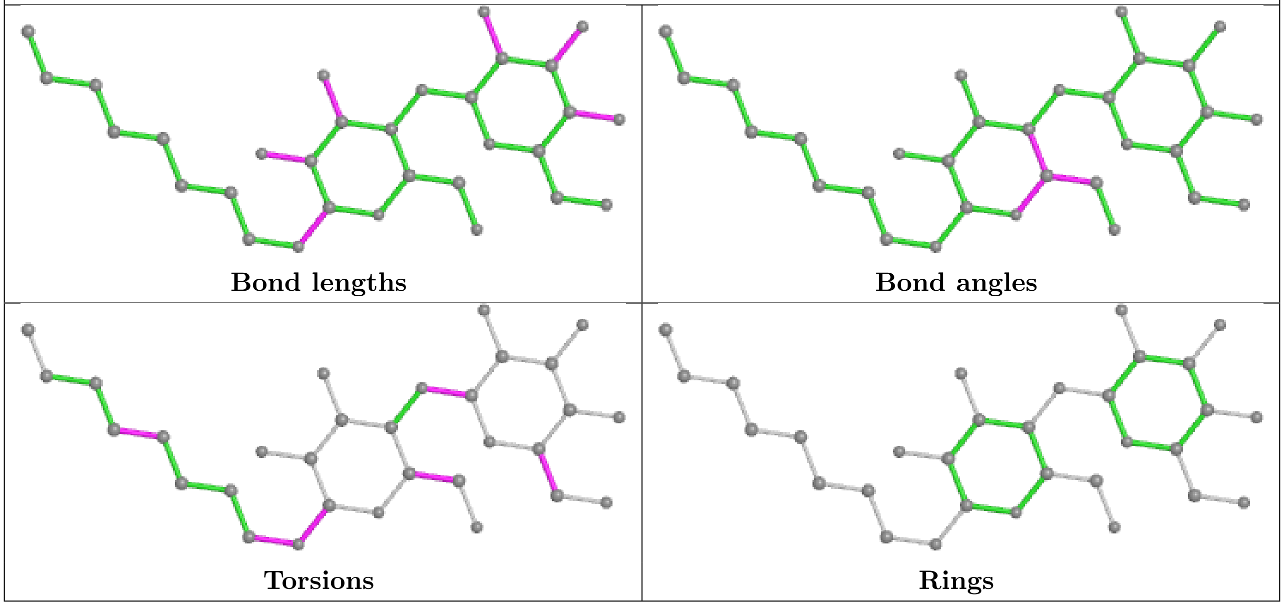
Bond lengths

Bond angles

Torsions

Rings

Ligand LMT A 6001



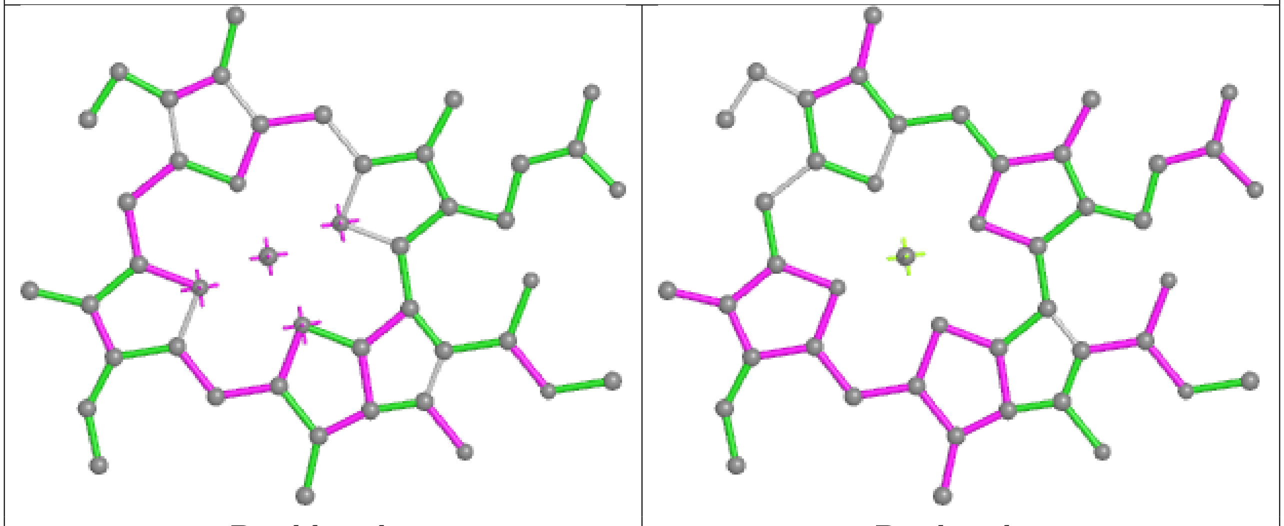
Bond lengths

Bond angles

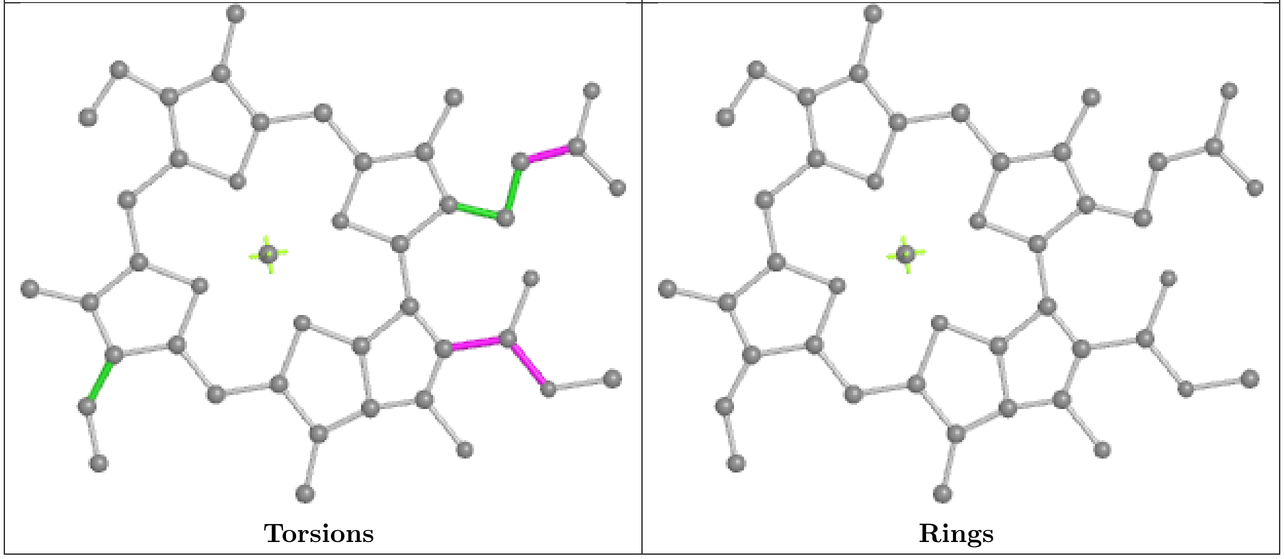
Torsions

Rings

Ligand CLA H 1218

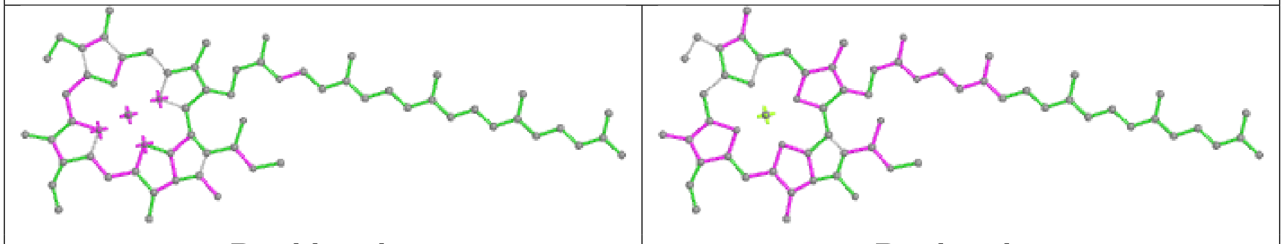


Bond lengths **Bond angles**

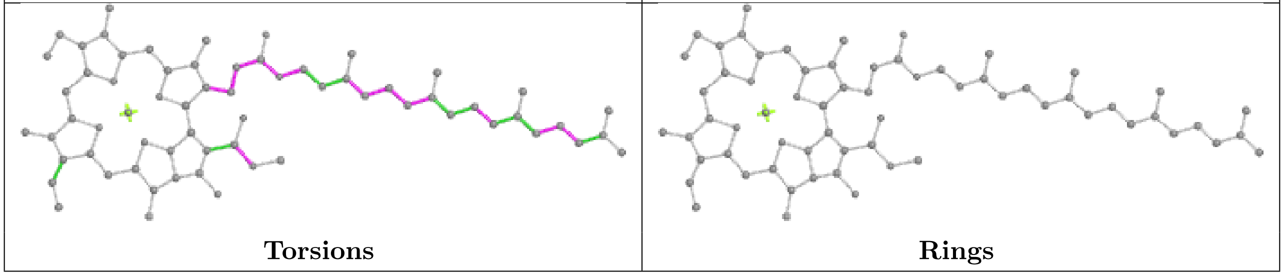


Torsions **Rings**

Ligand CLA A 1136

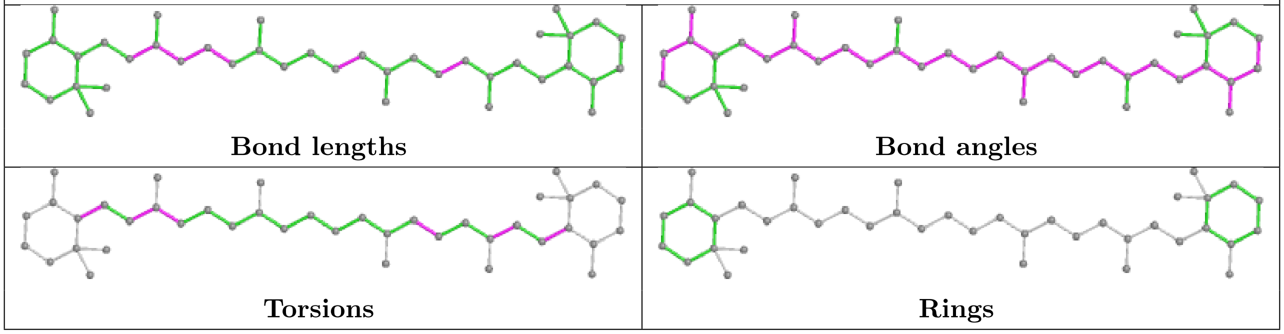


Bond lengths **Bond angles**



Torsions **Rings**

Ligand BCR B 4006



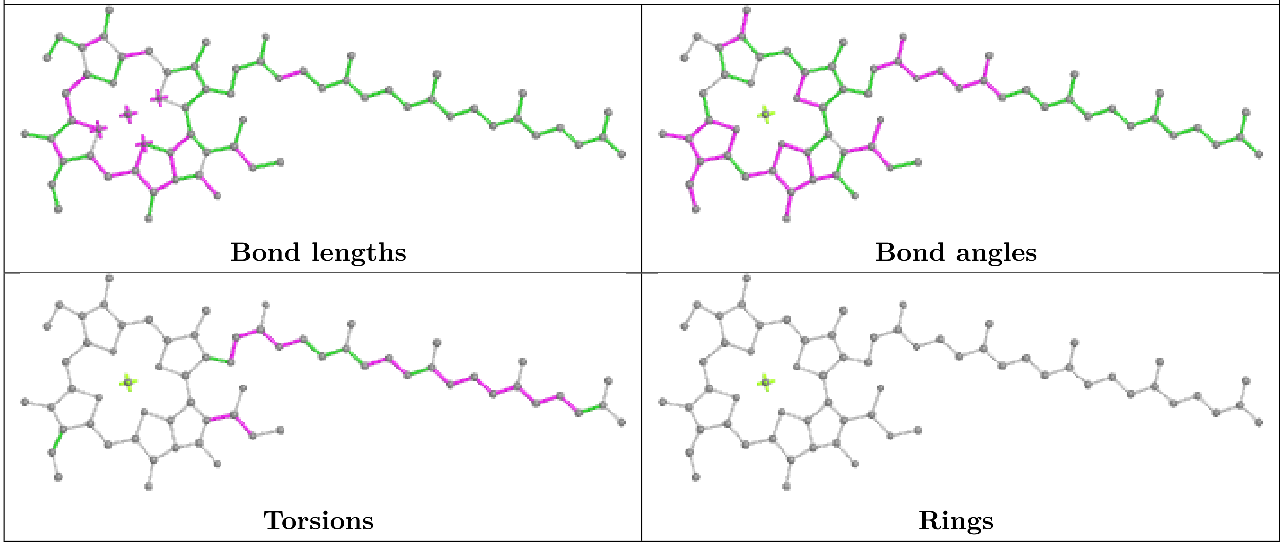
Bond lengths

Bond angles

Torsions

Rings

Ligand CLA B 1211



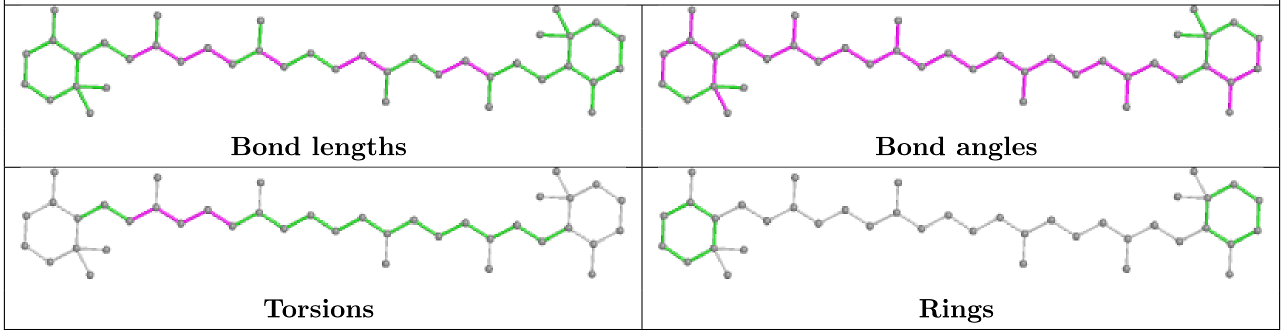
Bond lengths

Bond angles

Torsions

Rings

Ligand BCR U 4022



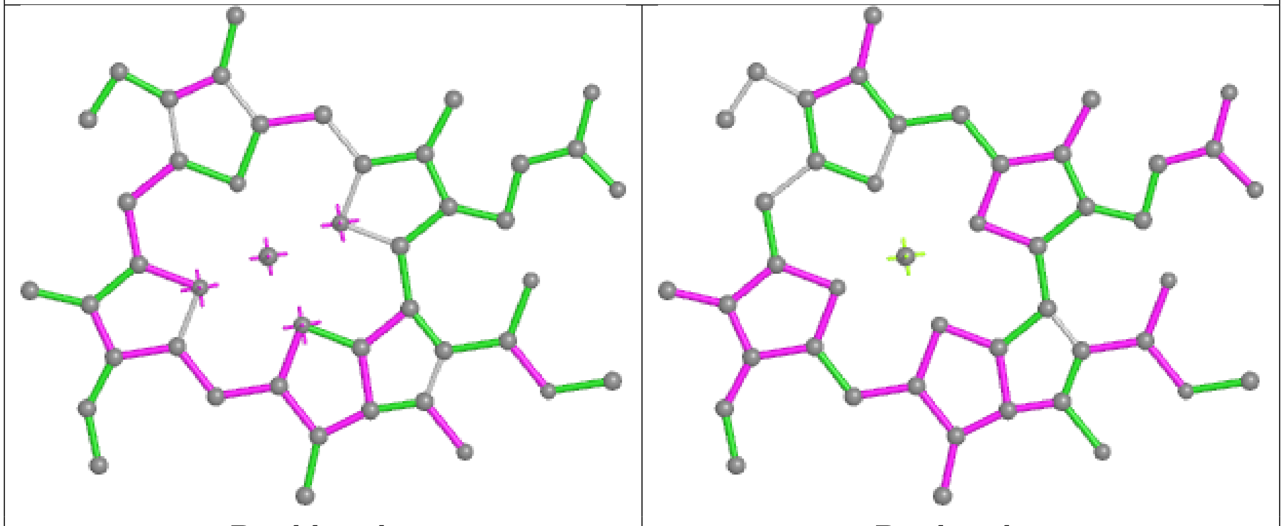
Bond lengths

Bond angles

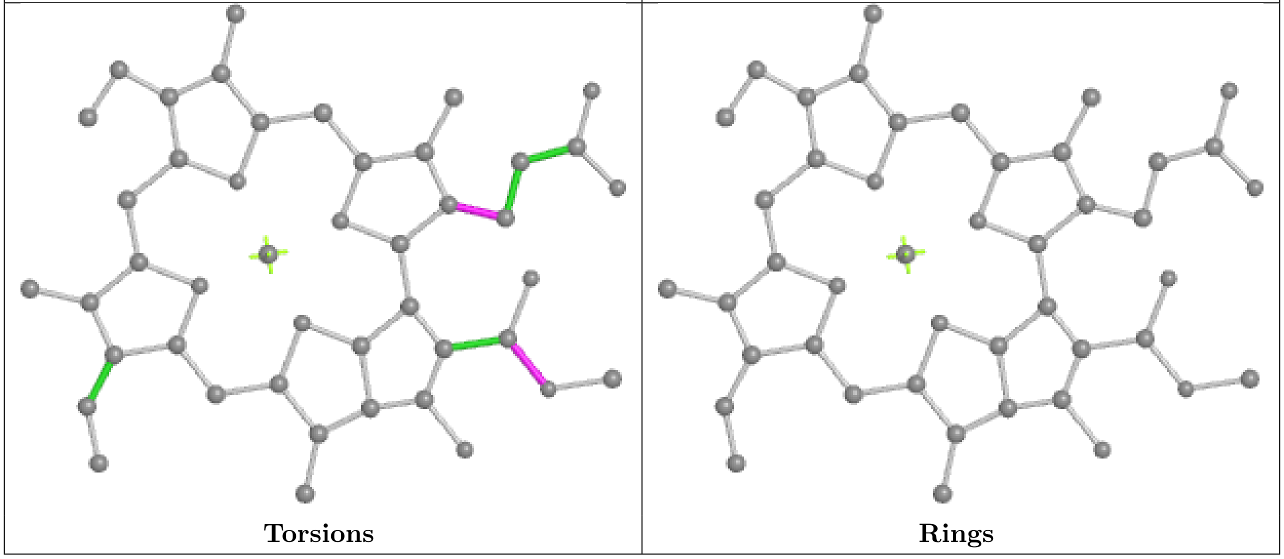
Torsions

Rings

Ligand CLA H 1219

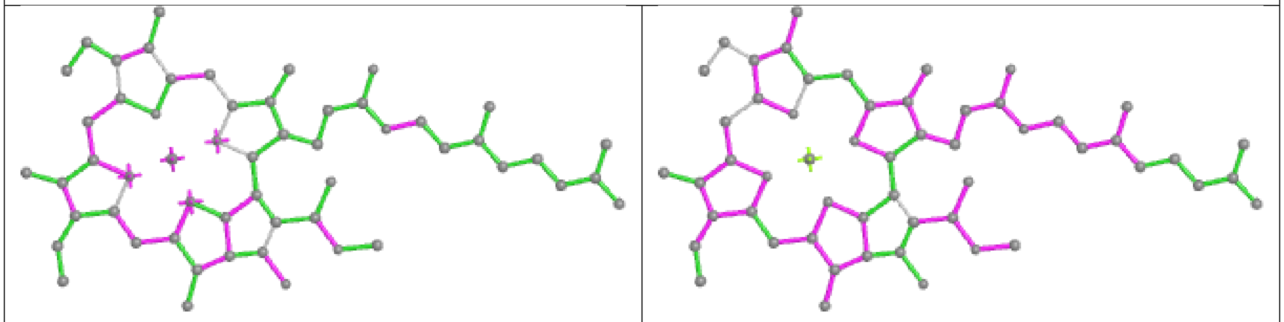


Bond lengths **Bond angles**



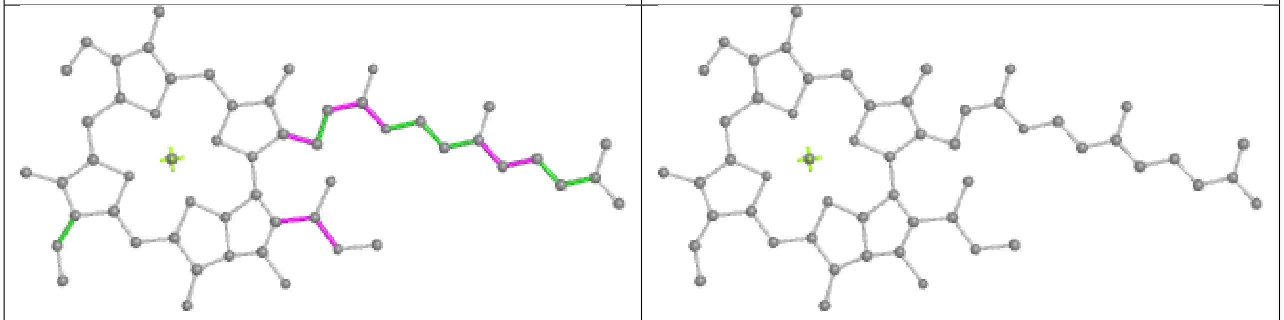
Torsions **Rings**

Ligand CLA B 1220



Bond lengths

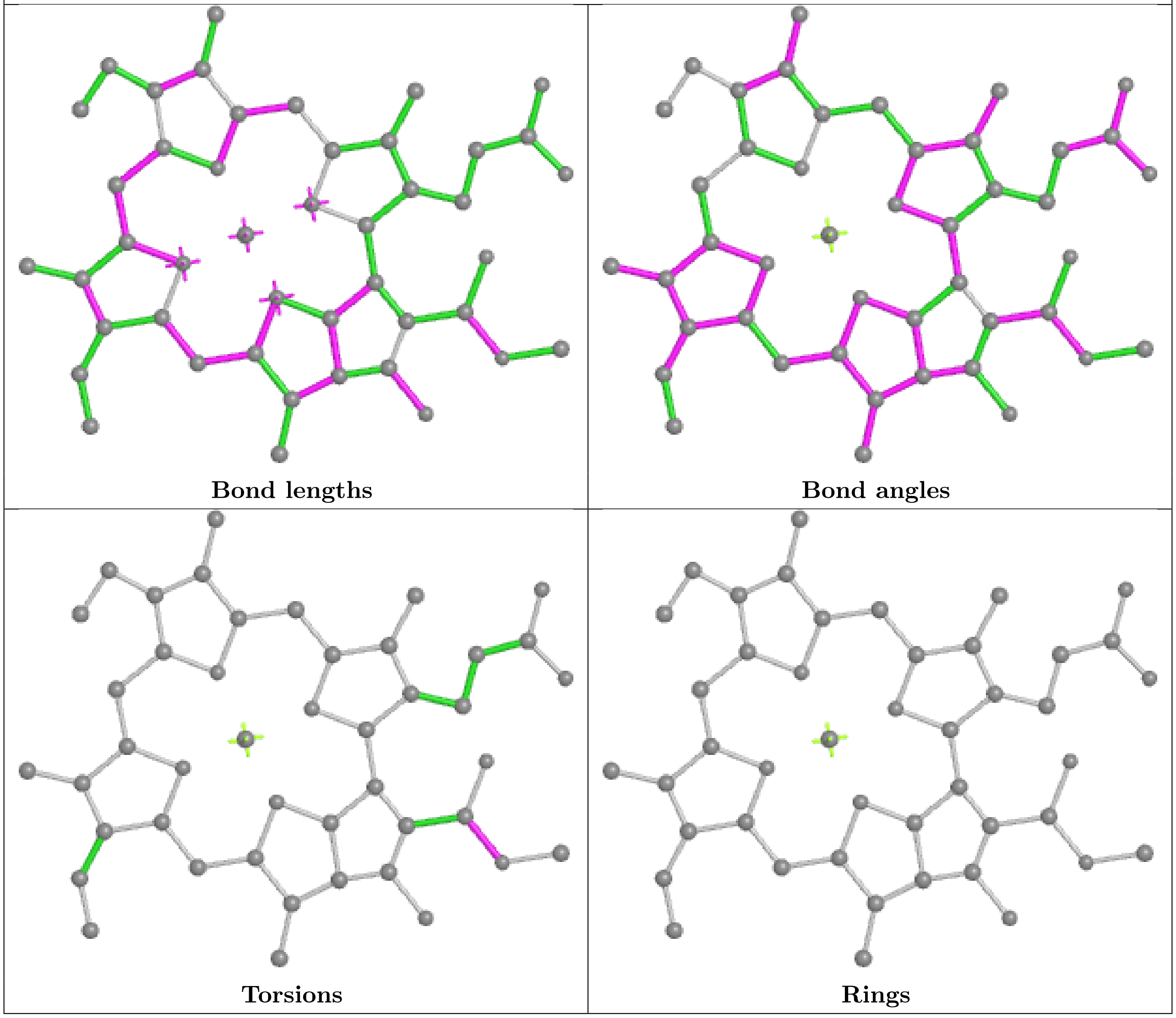
Bond angles



Torsions

Rings

Ligand CLA B 1232



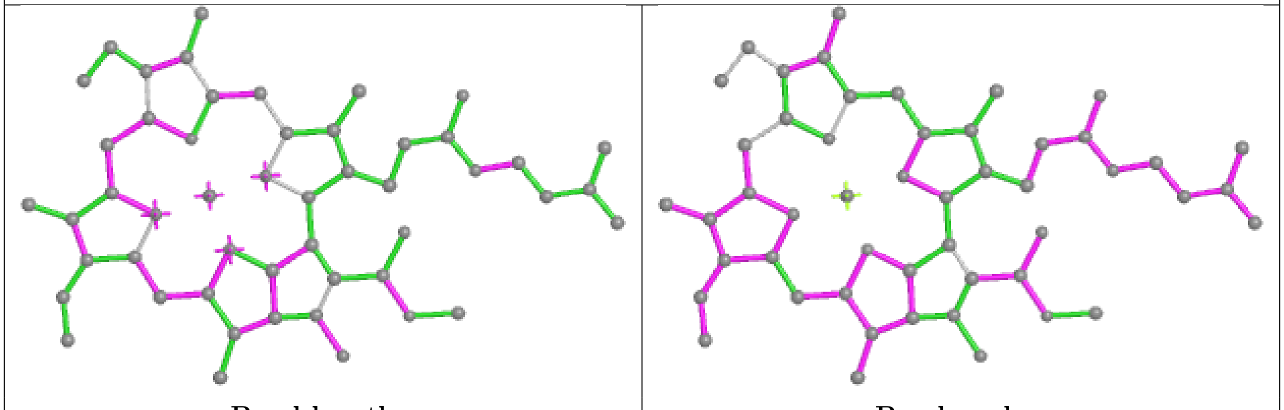
Bond lengths

Bond angles

Torsions

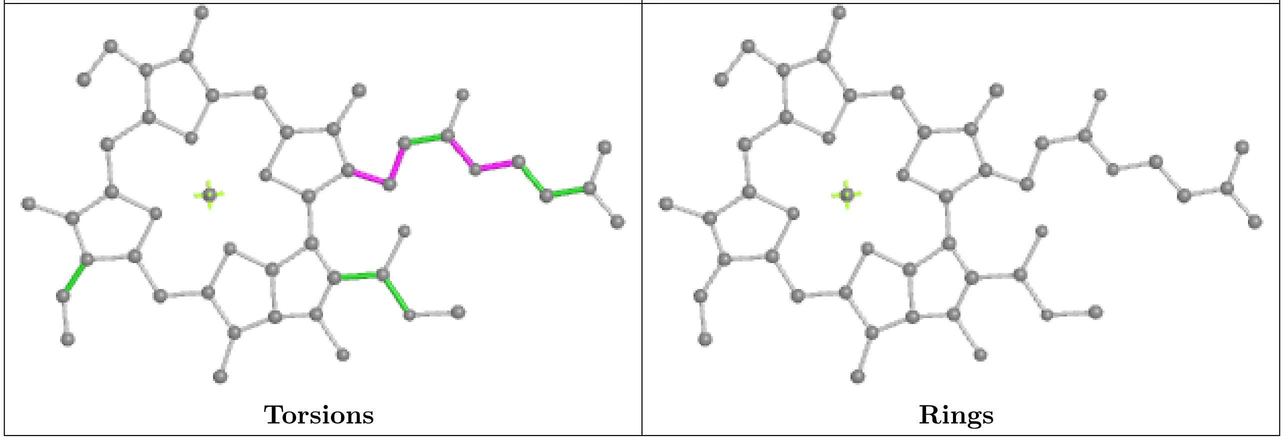
Rings

Ligand CLA G 1137



Bond lengths

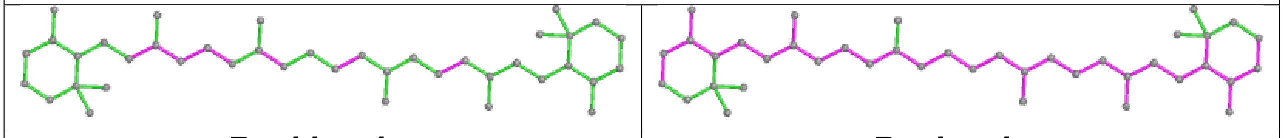
Bond angles



Torsions

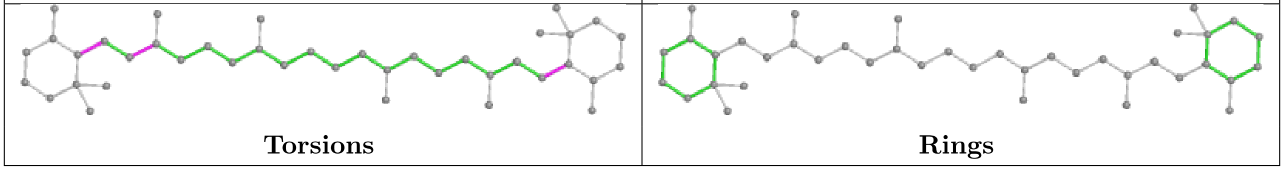
Rings

Ligand BCR A 4002



Bond lengths

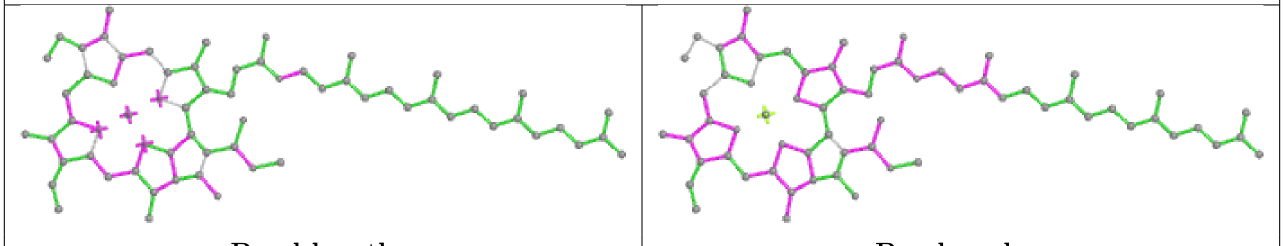
Bond angles



Torsions

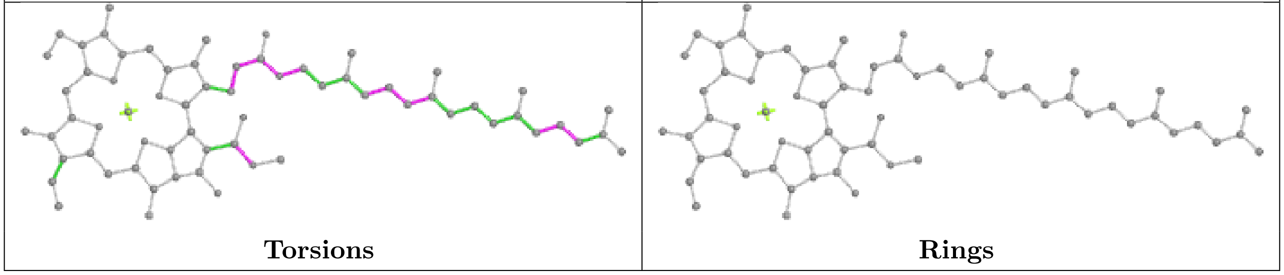
Rings

Ligand CLA H 1226



Bond lengths

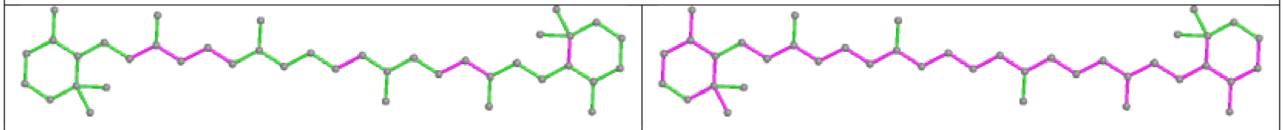
Bond angles



Torsions

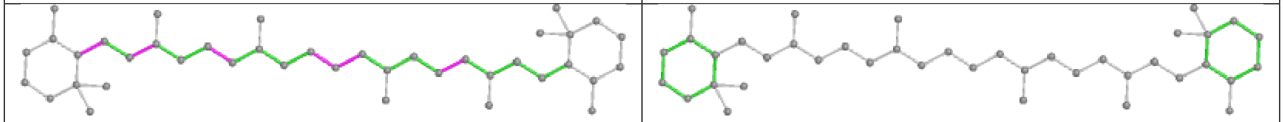
Rings

Ligand BCR R 4018



Bond lengths

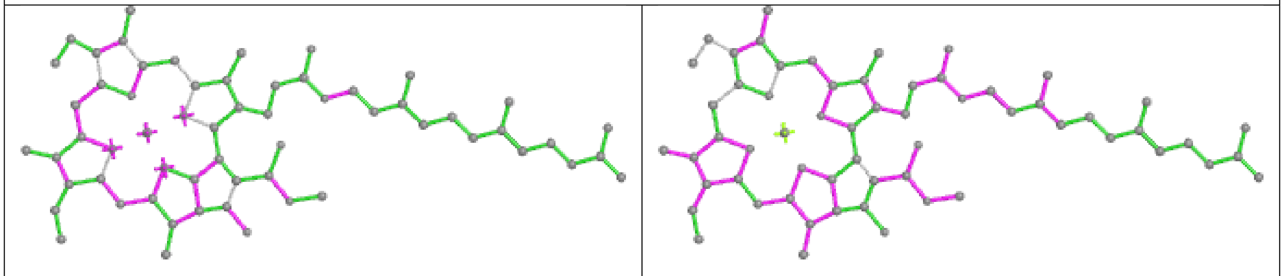
Bond angles



Torsions

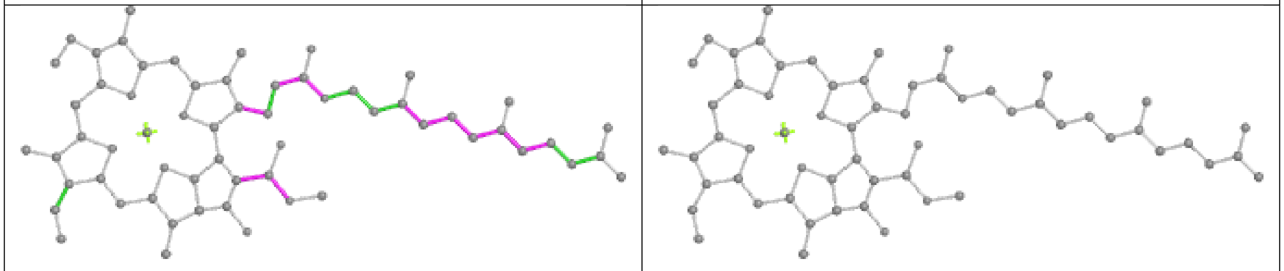
Rings

Ligand CLA a 1138



Bond lengths

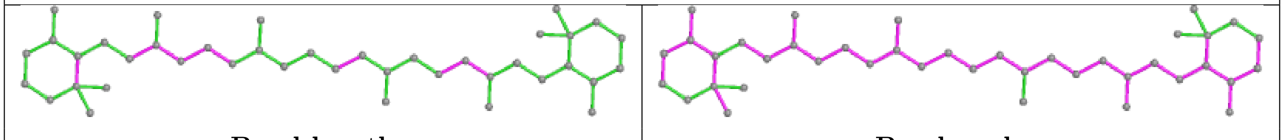
Bond angles



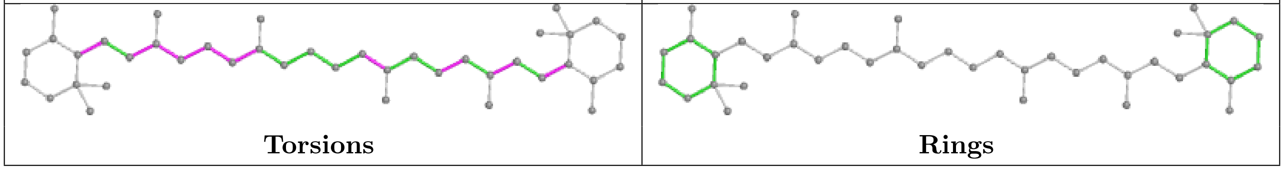
Torsions

Rings

Ligand BCR a 4011

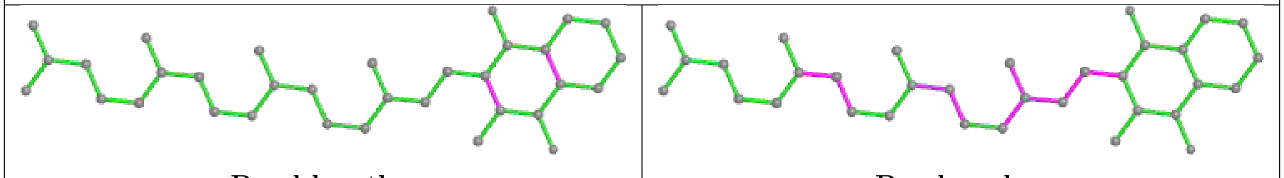


Bond lengths | Bond angles

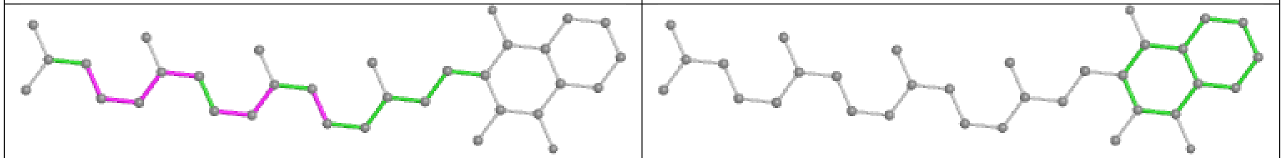


Torsions | Rings

Ligand PQN a 2001

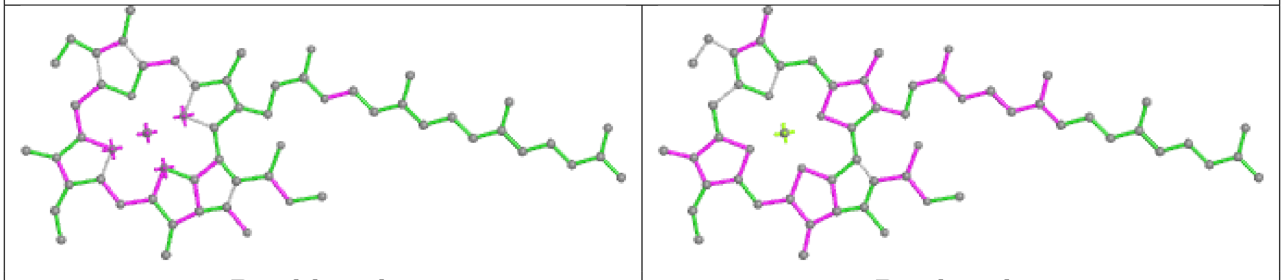


Bond lengths | Bond angles

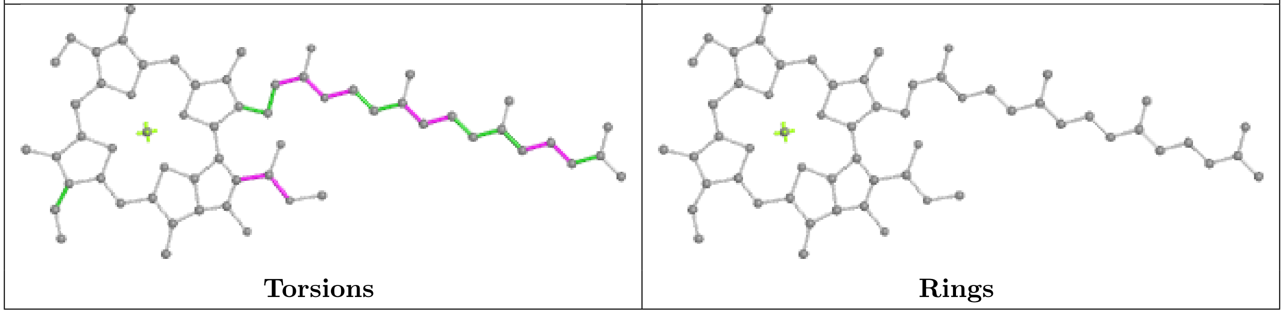


Torsions | Rings

Ligand CLA b 1235

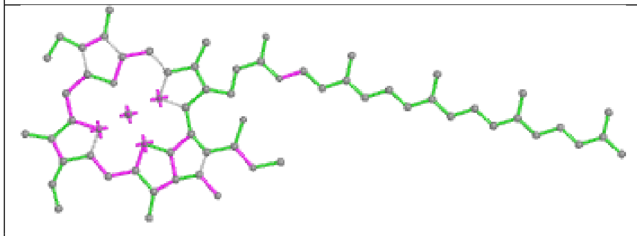


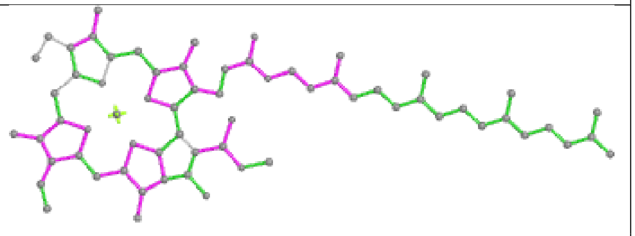
Bond lengths | Bond angles

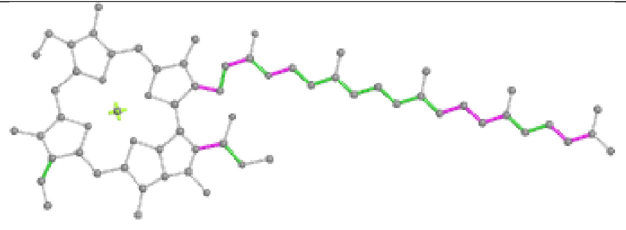


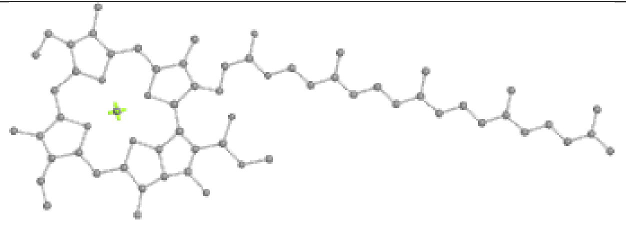
Torsions | Rings

Ligand CLA b 1221

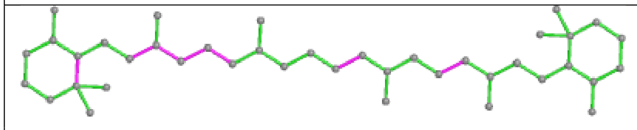

Bond lengths


Bond angles


Torsions


Rings

Ligand BCR M 4021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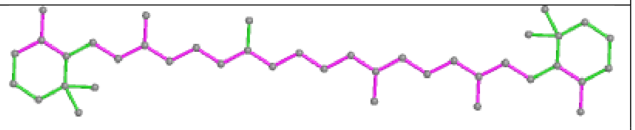
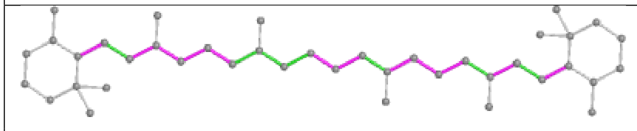
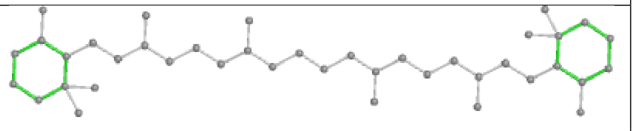
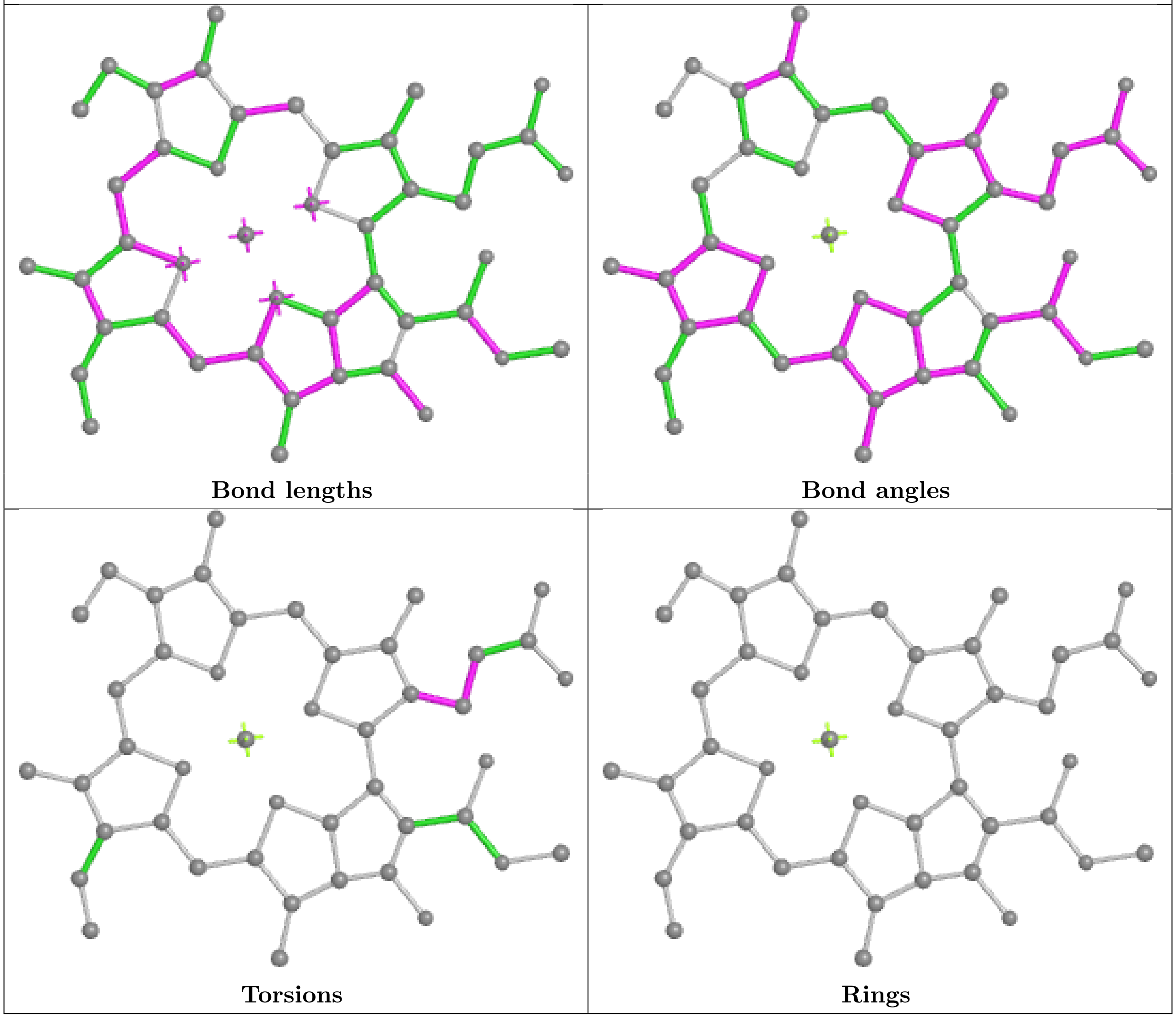

Bond angles


Torsions


Rings

Ligand CLA b 1209



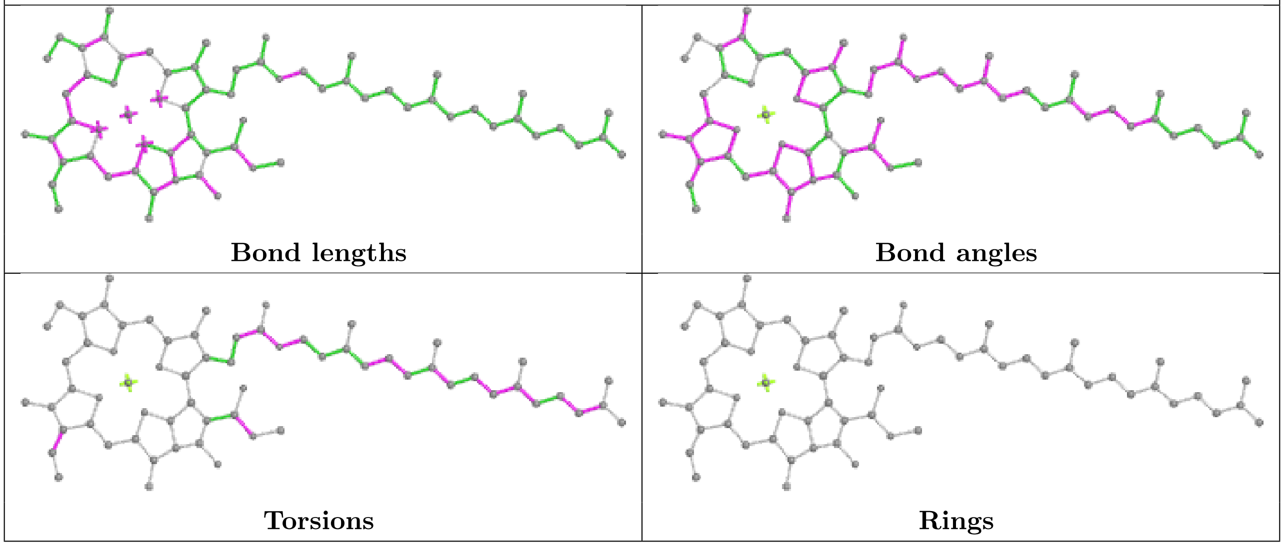
Bond lengths

Bond angles

Torsions

Rings

Ligand CLA B 1239

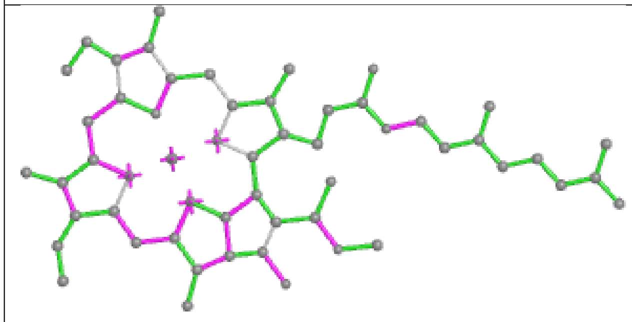
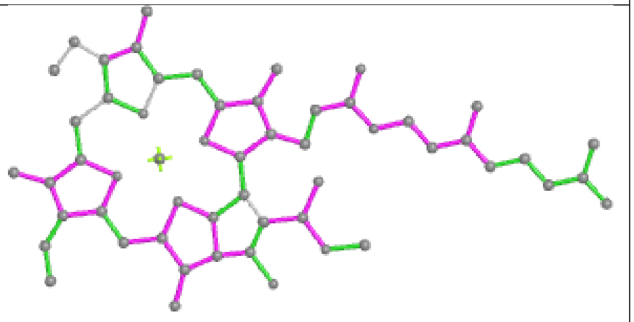
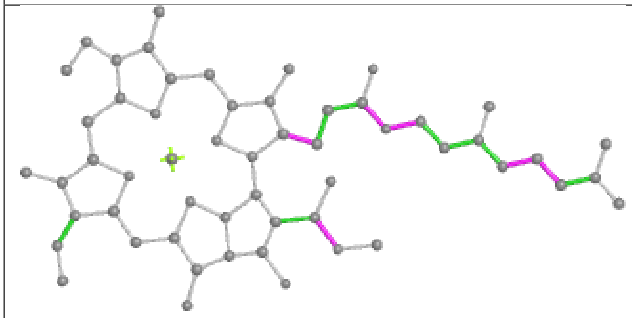
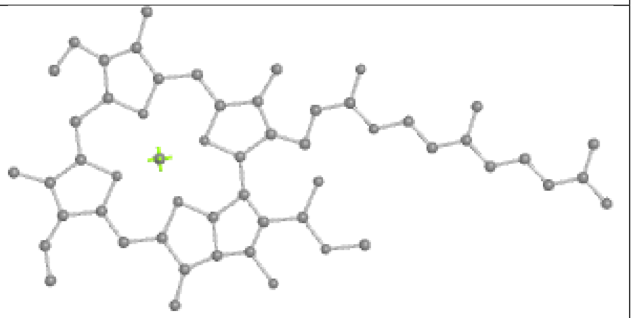


Bond lengths

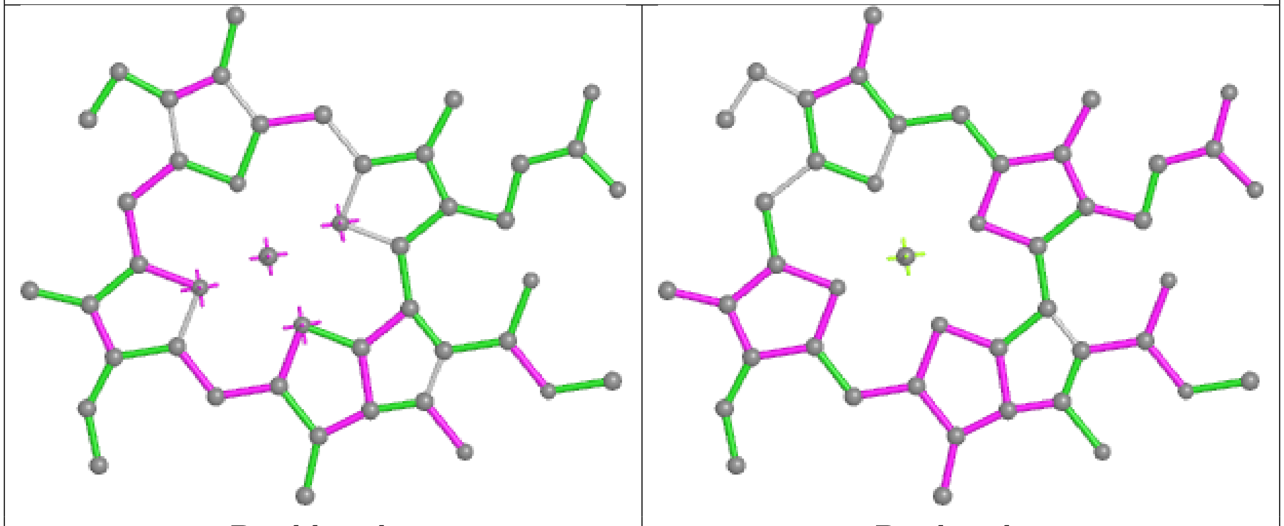
Bond angles

Torsions

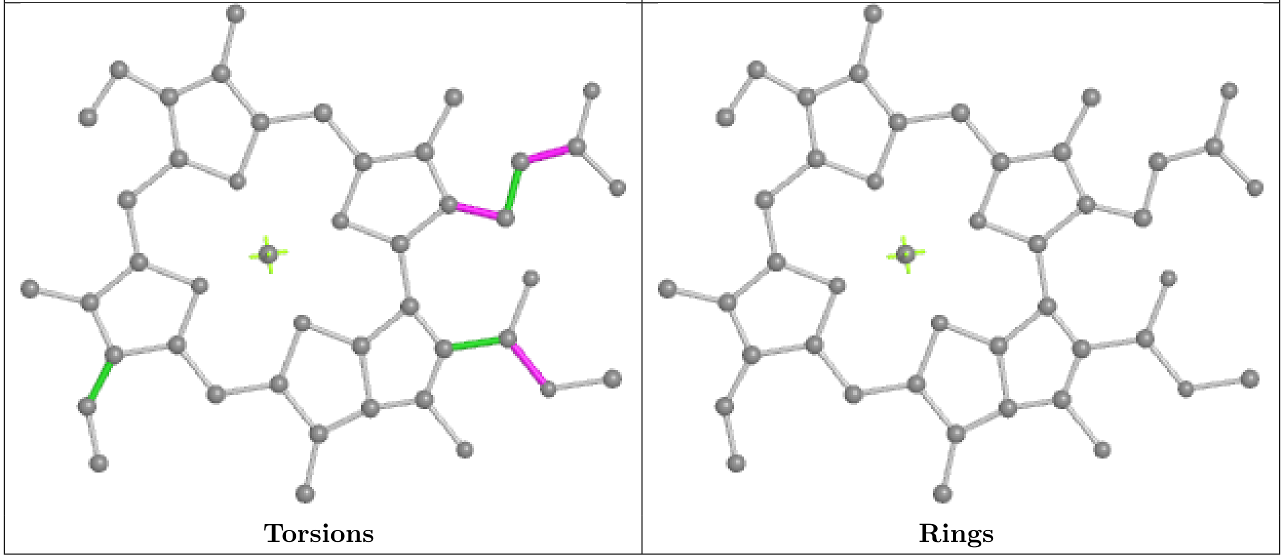
Rings

Ligand CLA A 1124	
 **Bond lengths**	 **Bond angles**
 **Torsions**	 **Rings**

Ligand CLA a 1110

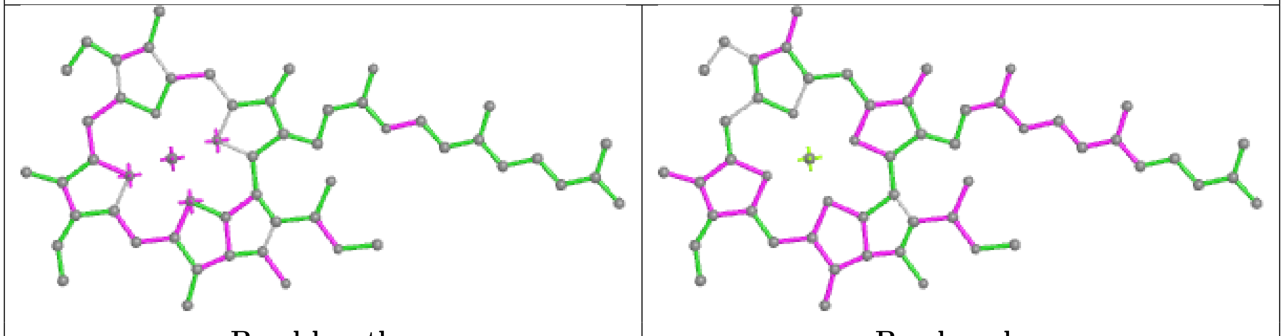


Bond lengths **Bond angles**

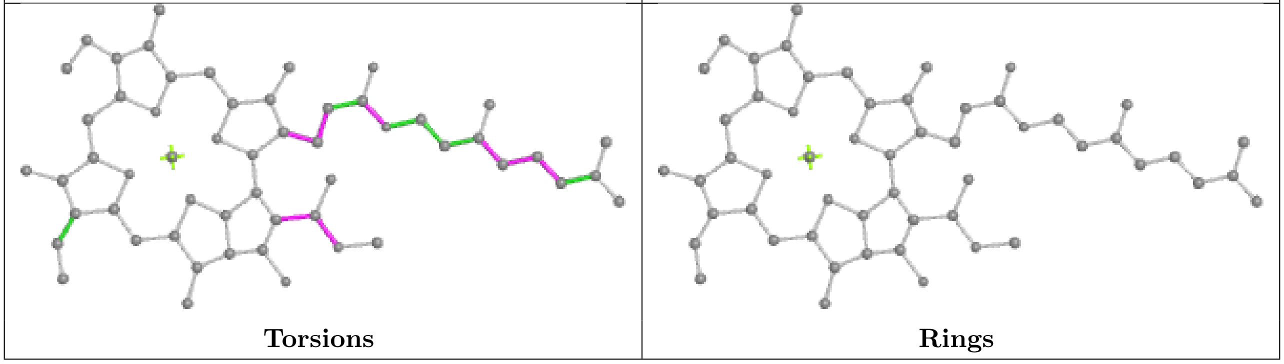


Torsions **Rings**

Ligand CLA b 1217

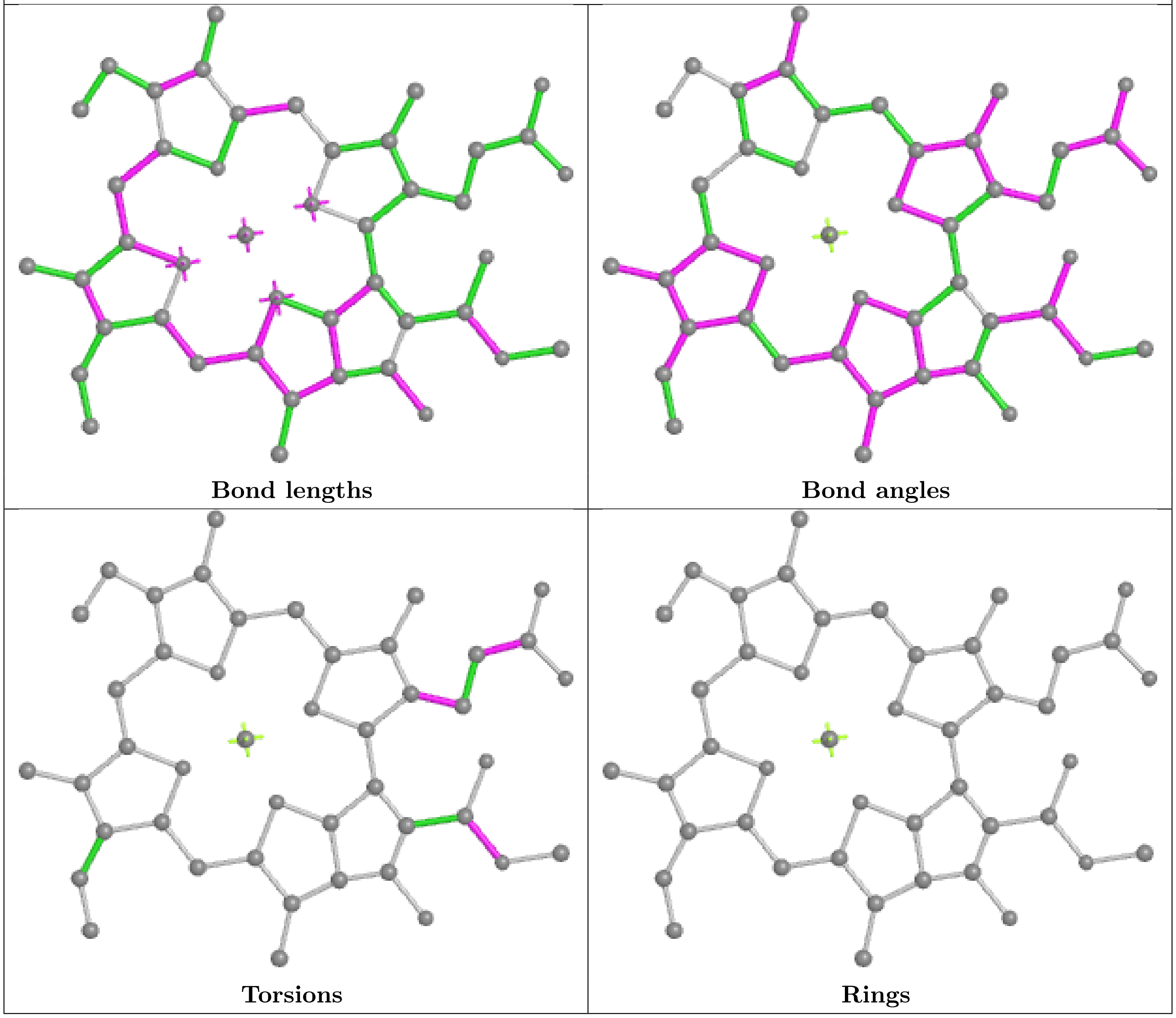


Bond lengths **Bond angles**



Torsions **Rings**

Ligand CLA G 1105



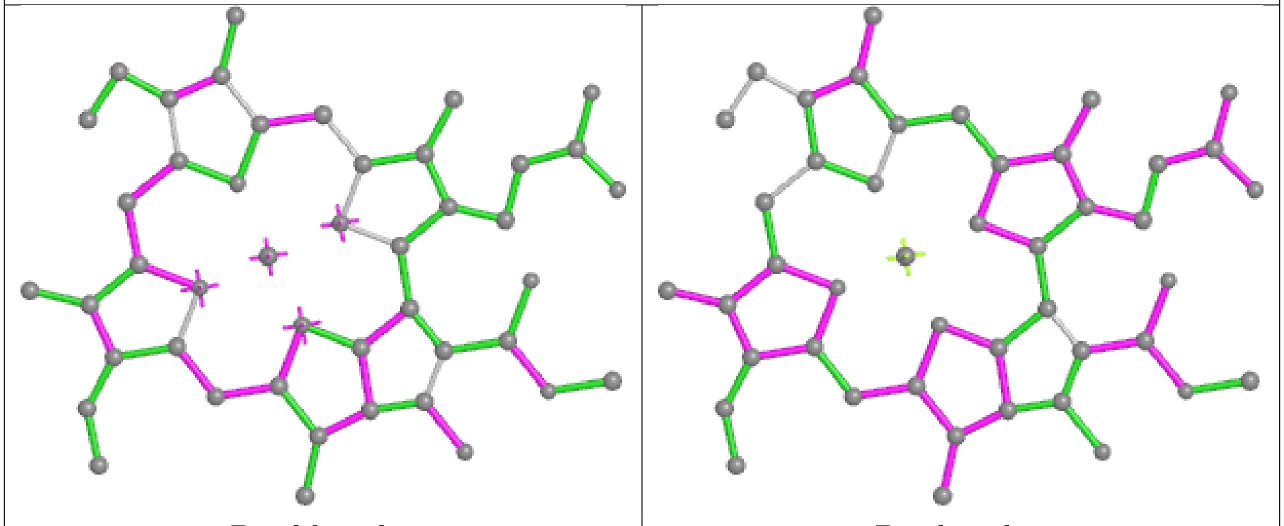
Bond lengths

Bond angles

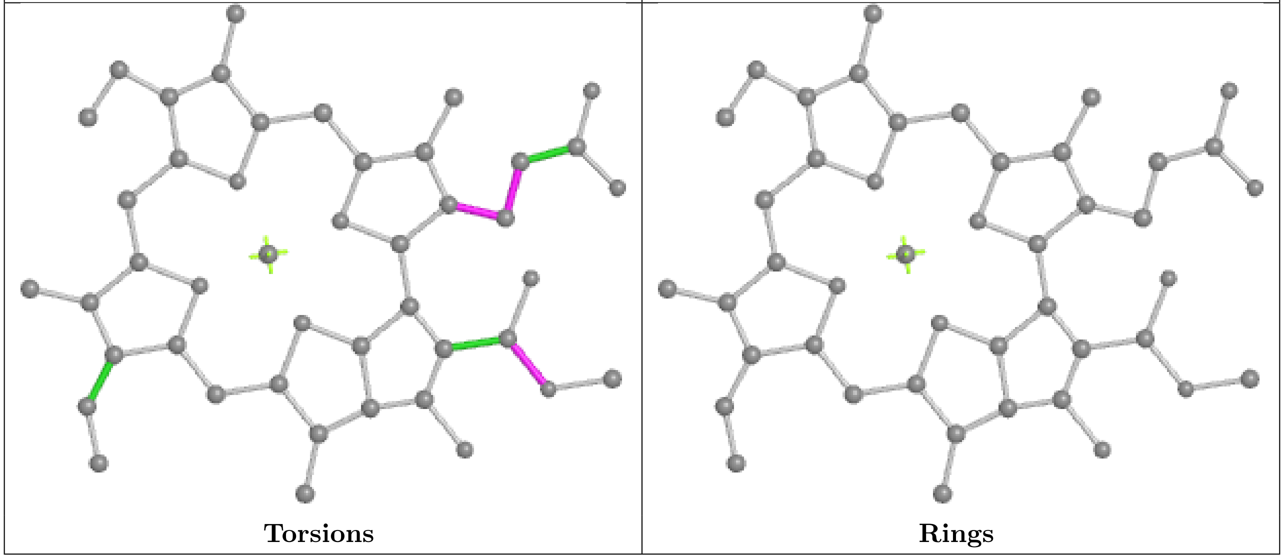
Torsions

Rings

Ligand CLA H 1212

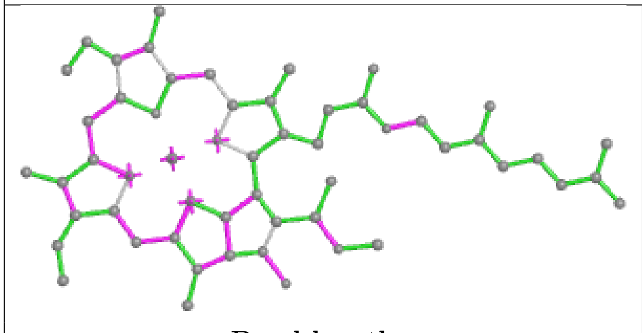


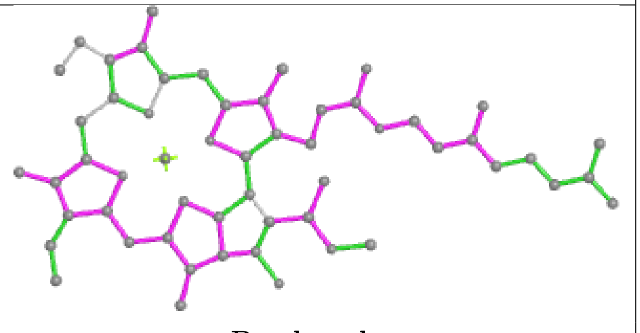
Bond lengths **Bond angles**

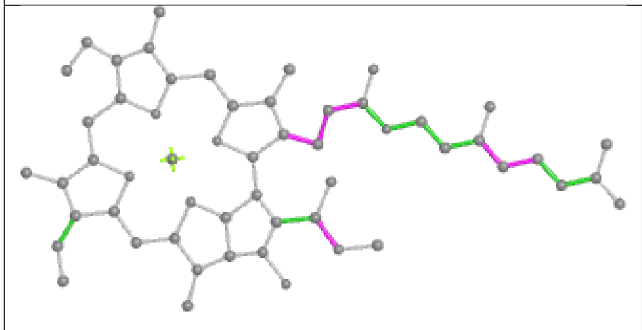


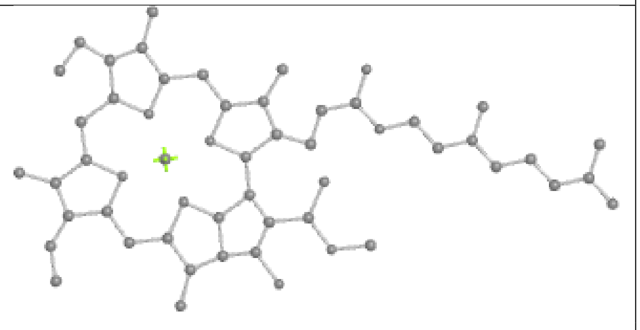
Torsions **Rings**

Ligand CLA A 1116

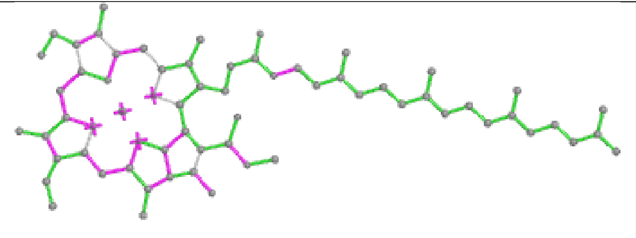

Bond lengths

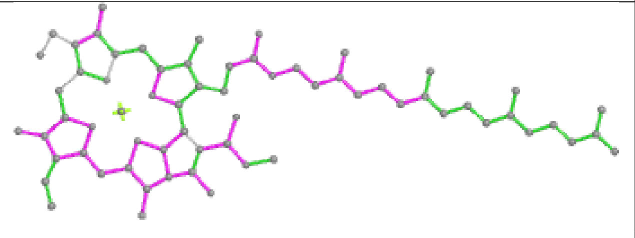

Bond angles

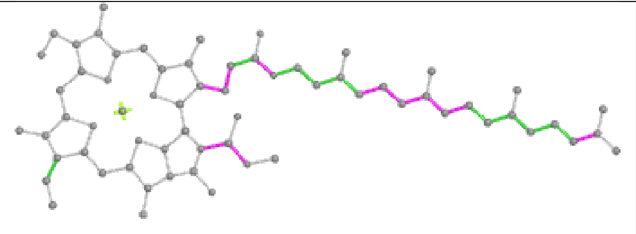

Torsions

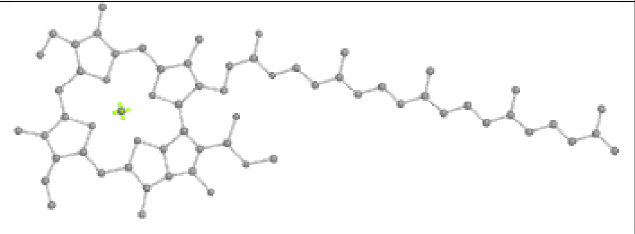

Rings

Ligand CLA B 1223


Bond lengths

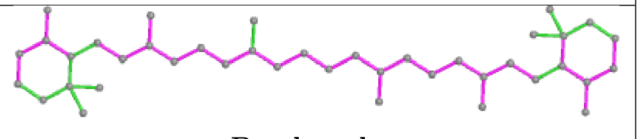

Bond angles

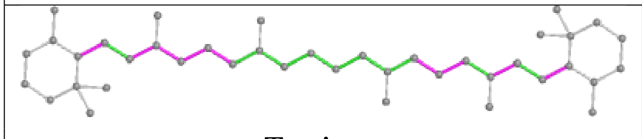

Torsions

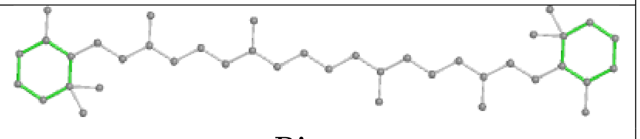

Rings

Ligand BCR A 4003

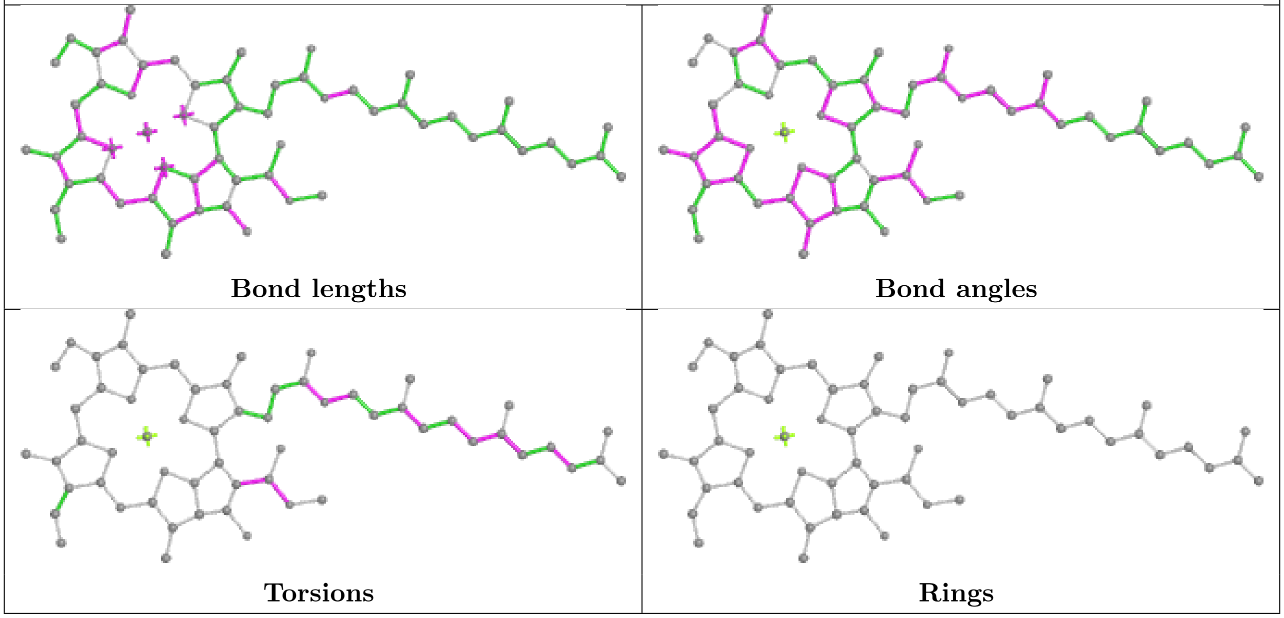

Bond lengths


Bond angles


Torsions


Rings

Ligand CLA G 1128



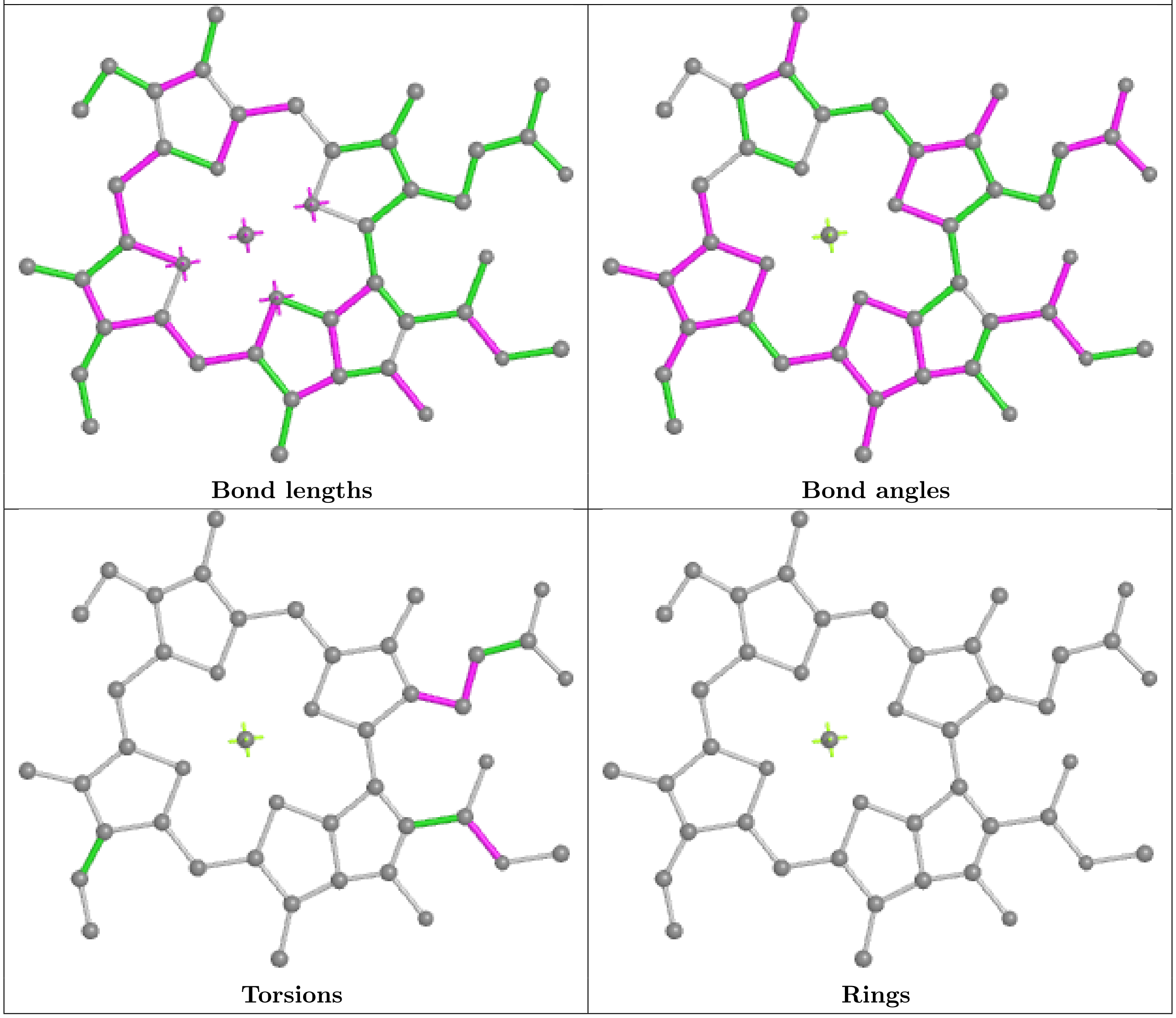
Bond lengths

Bond angles

Torsions

Rings

Ligand CLA b 1227



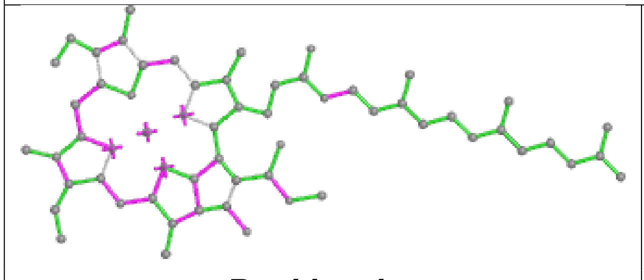
Bond lengths

Bond angles

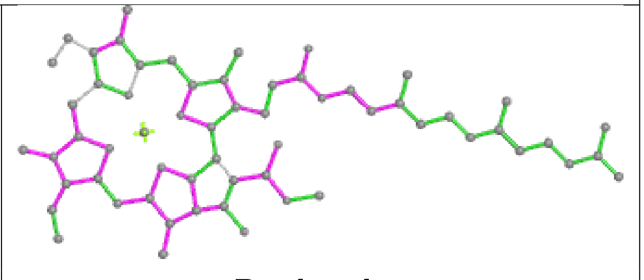
Torsions

Rings

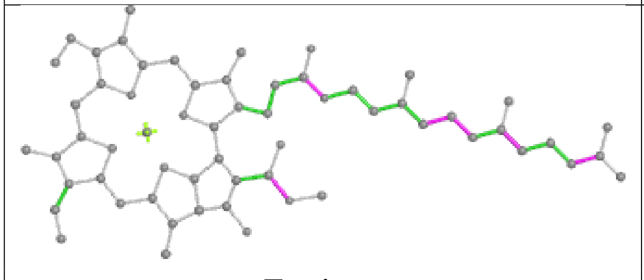
Ligand CLA G 1133



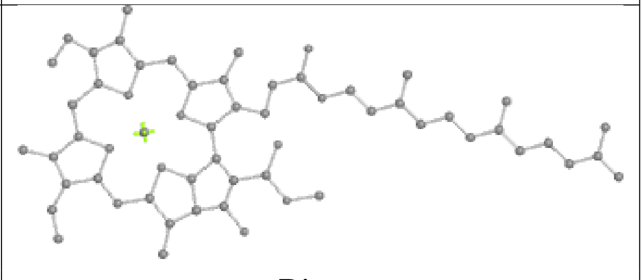
Bond lengths



Bond angles

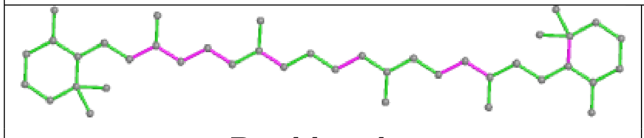


Torsions

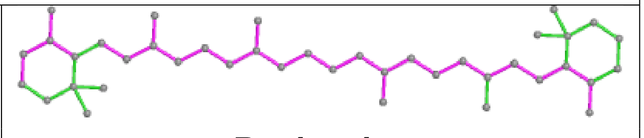


Rings

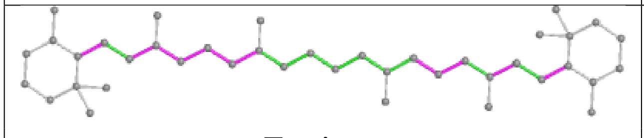
Ligand BCR H 4017



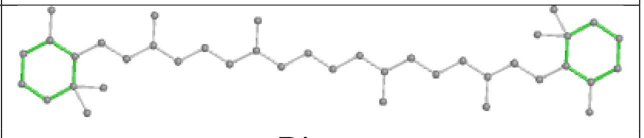
Bond lengths



Bond angles

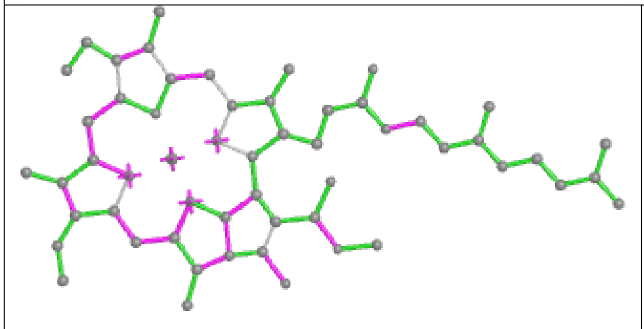


Torsions

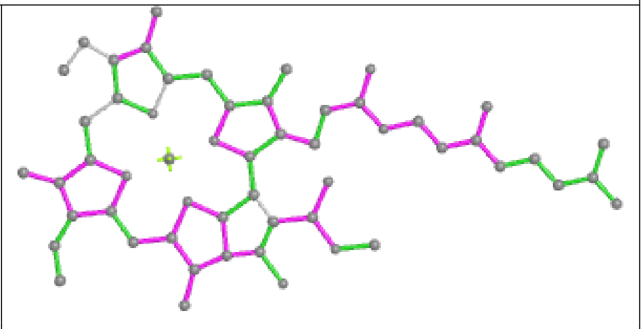


Rings

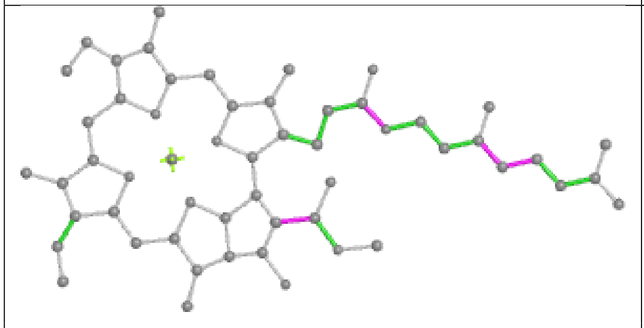
Ligand CLA H 1201



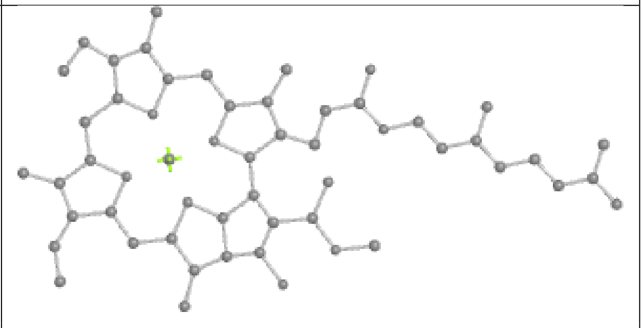
Bond lengths



Bond angles

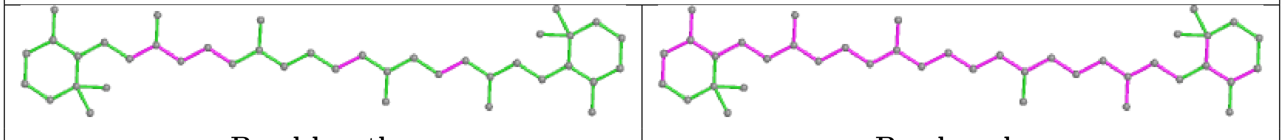


Torsions



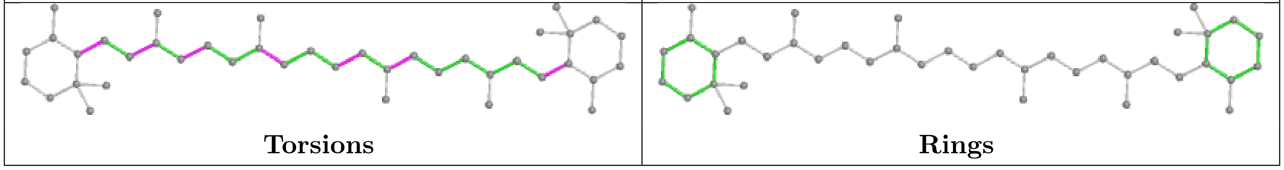
Rings

Ligand BCR H 4016



Bond lengths

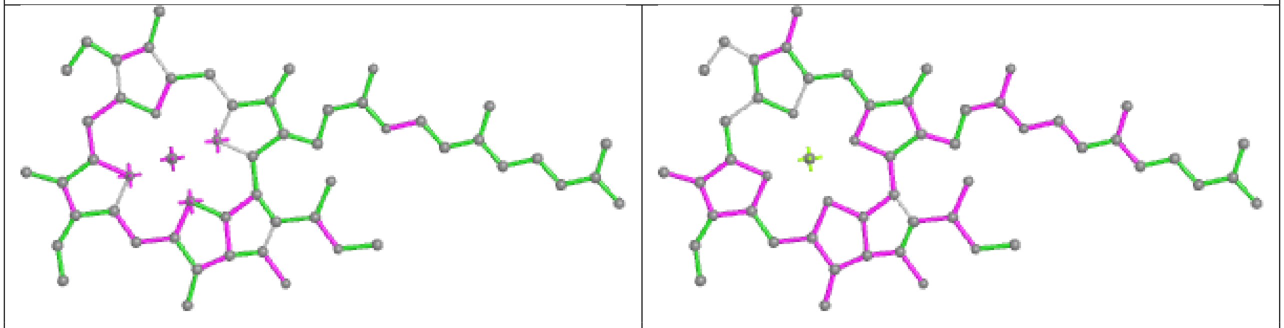
Bond angles



Torsions

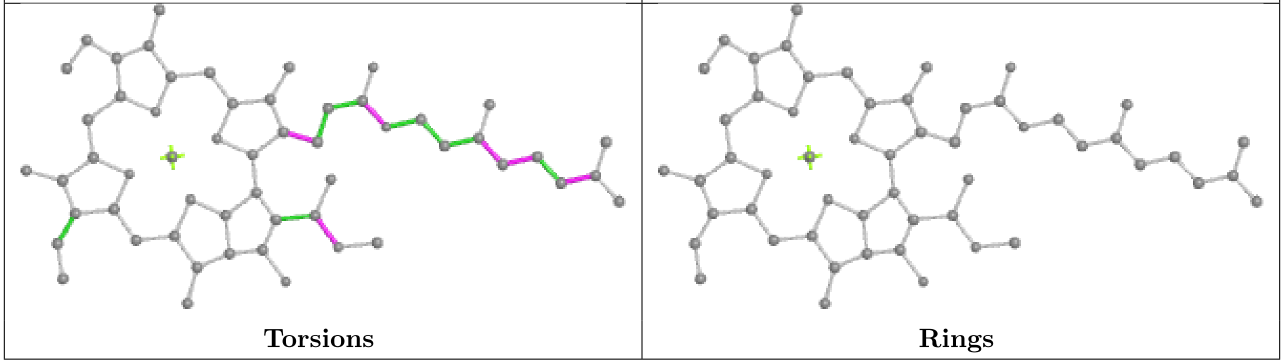
Rings

Ligand CLA A 1130



Bond lengths

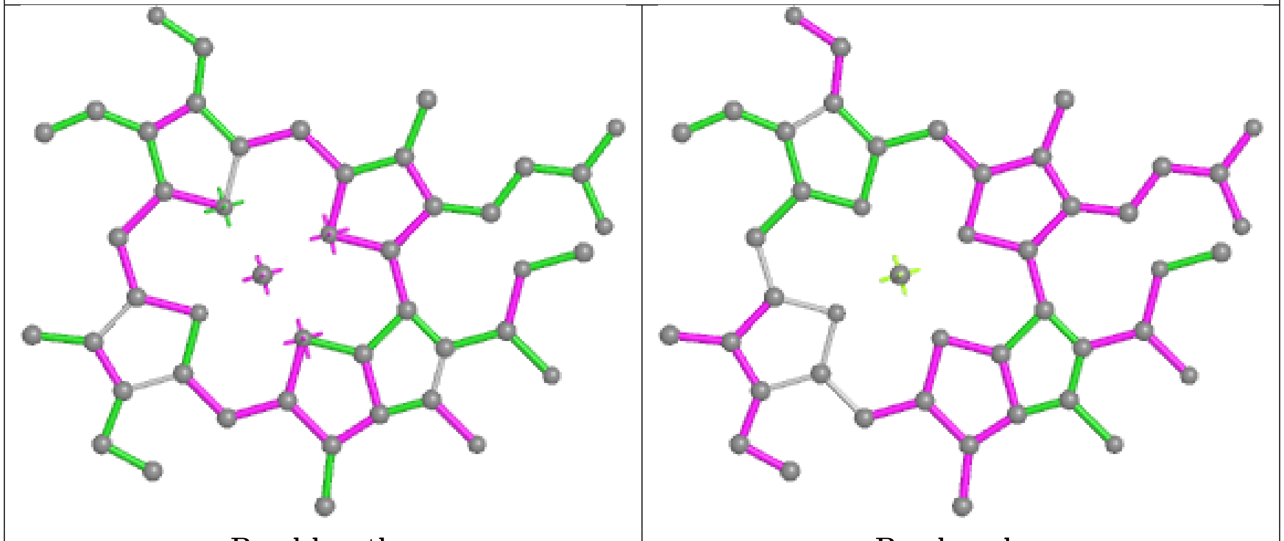
Bond angles



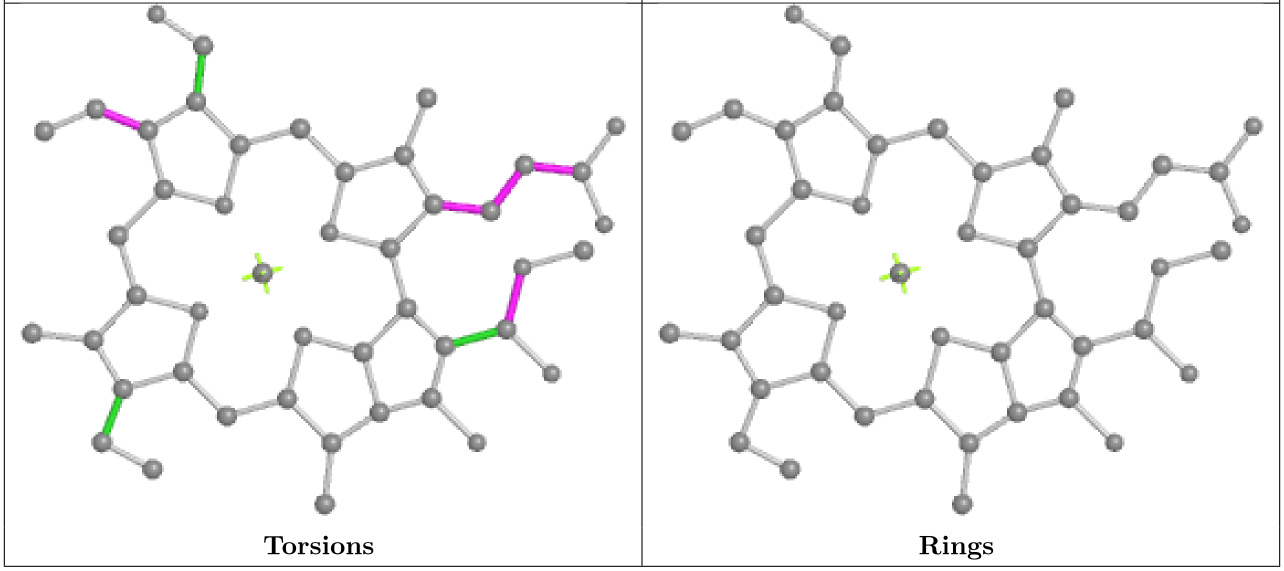
Torsions

Rings

Ligand F6C a 1121

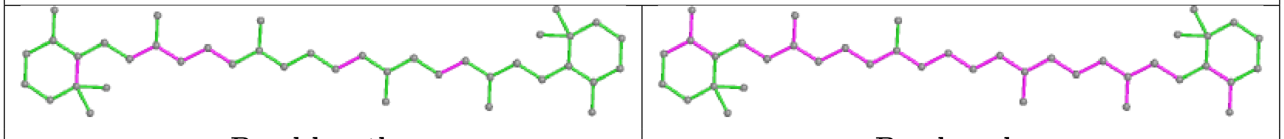


Bond lengths Bond angles

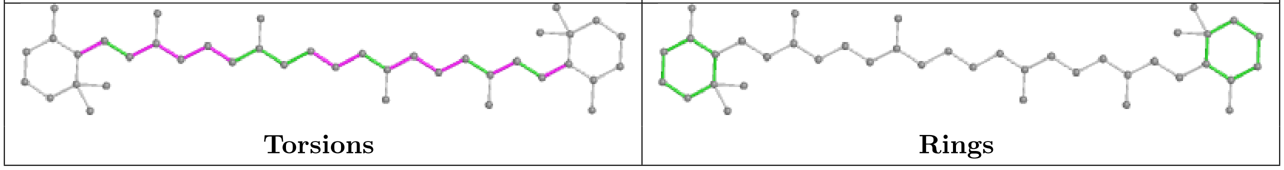


Torsions Rings

Ligand BCR m 4021

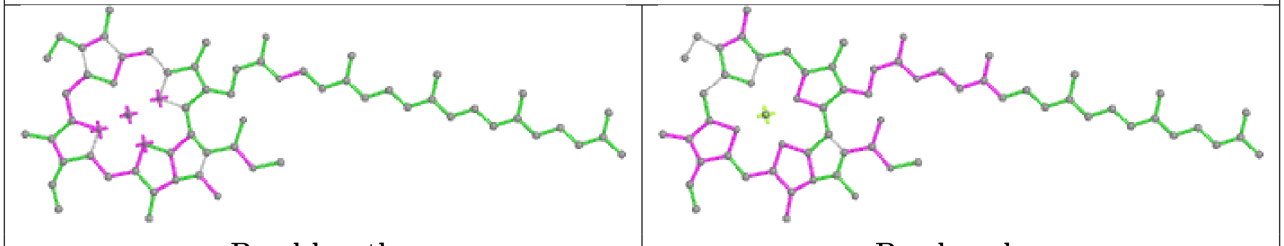


Bond lengths Bond angles

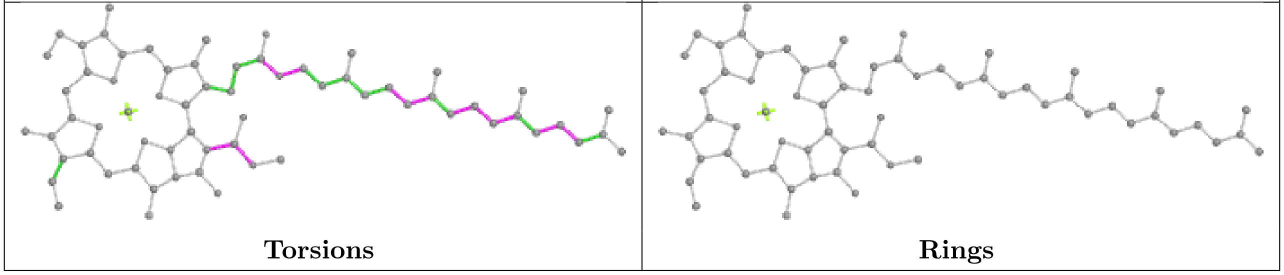


Torsions Rings

Ligand CLA B 1234

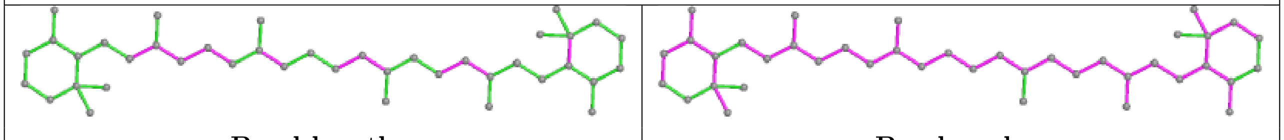


Bond lengths Bond angles

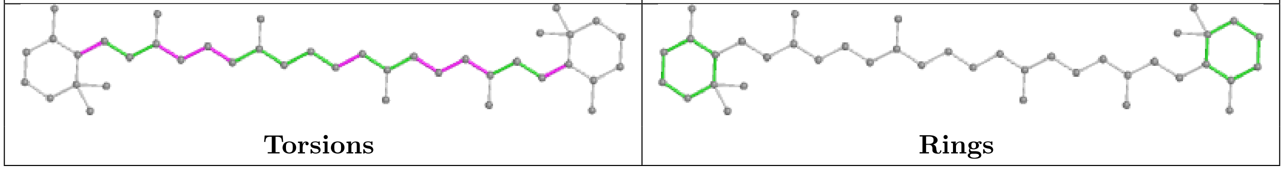


Torsions Rings

Ligand BCR R 4020

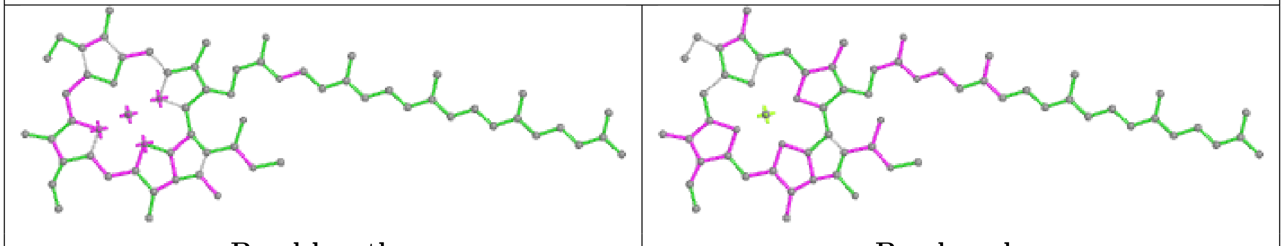


Bond lengths Bond angles

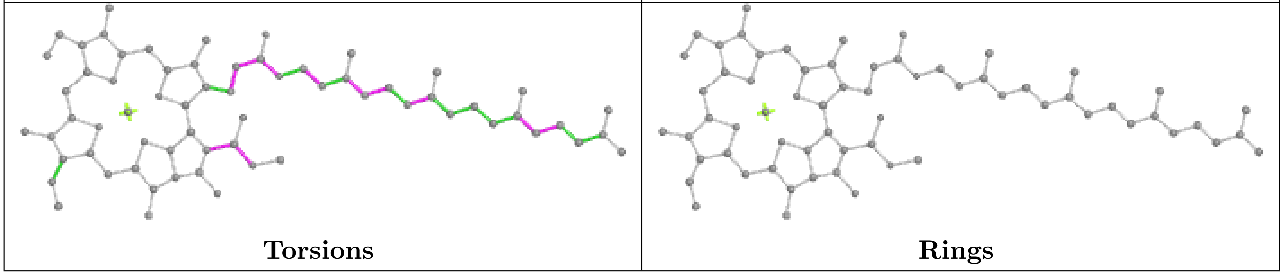


Torsions Rings

Ligand CLA H 1213

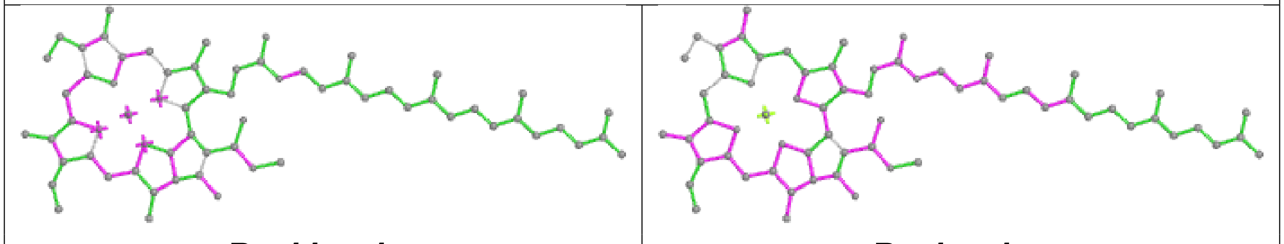


Bond lengths Bond angles



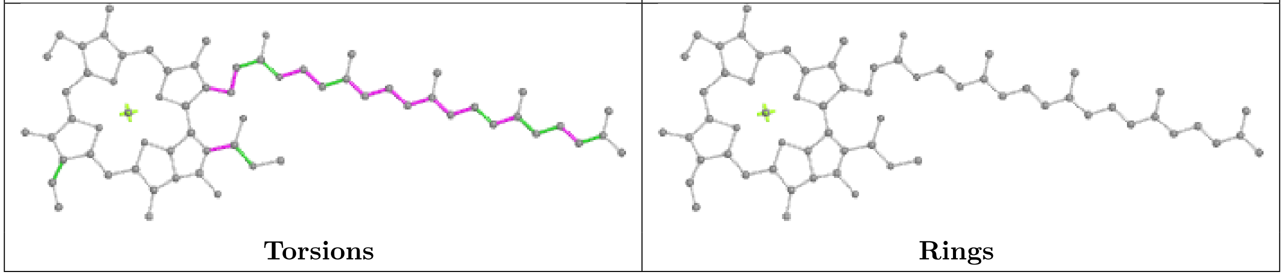
Torsions Rings

Ligand CLA B 1022



Bond lengths

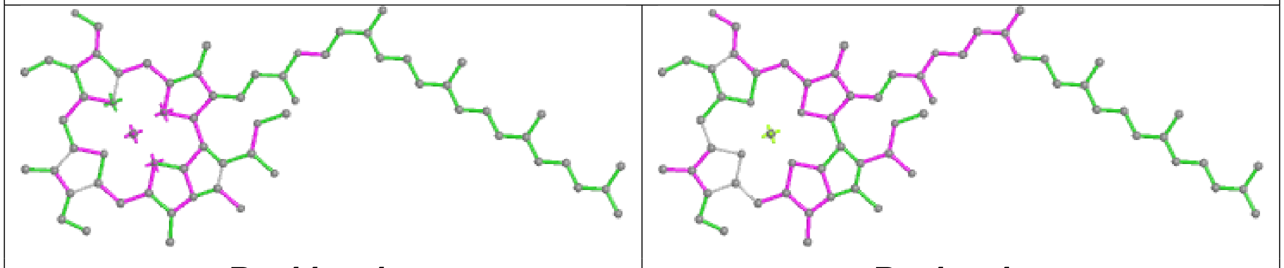
Bond angles



Torsions

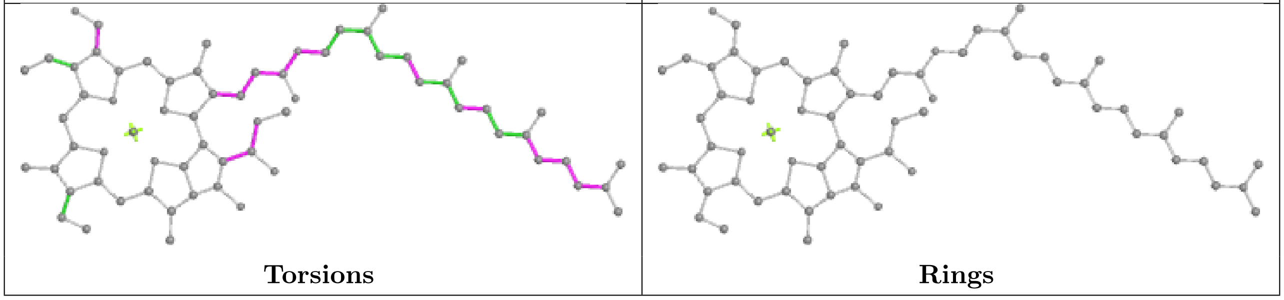
Rings

Ligand F6C H 1207



Bond lengths

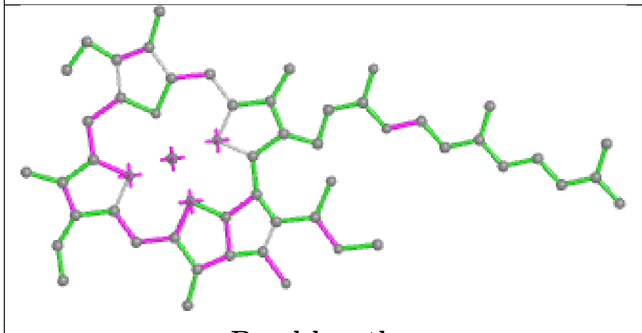
Bond angles



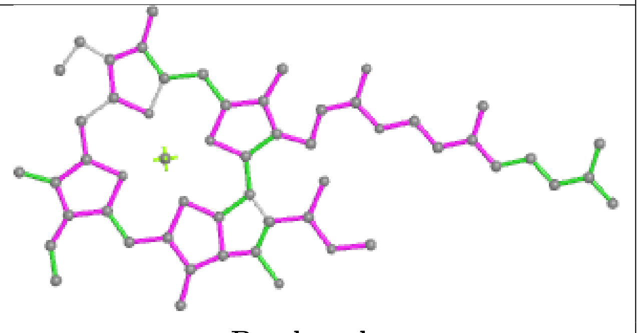
Torsions

Rings

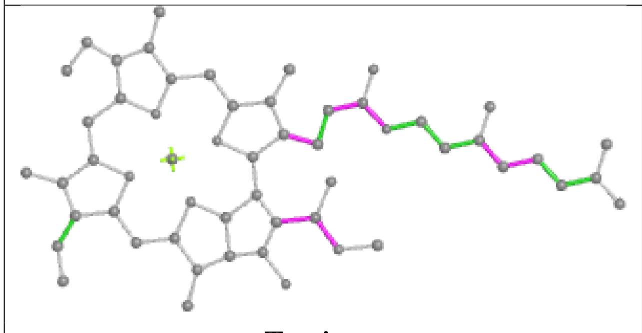
Ligand CLA H 1220



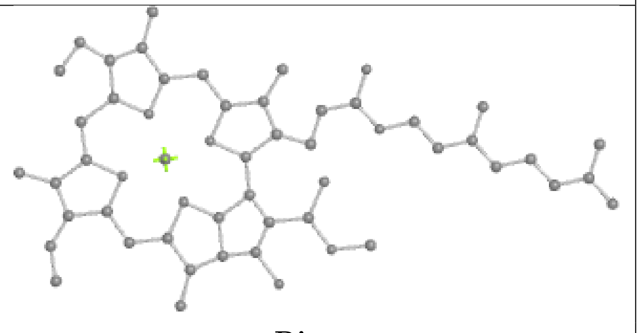
Bond lengths



Bond angles

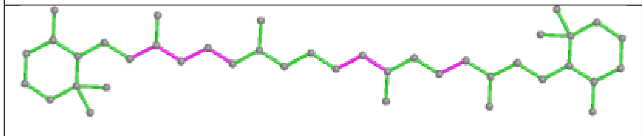


Torsions

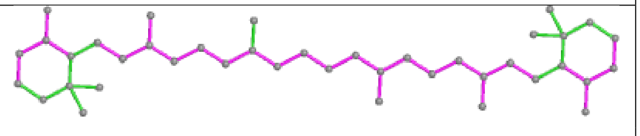


Rings

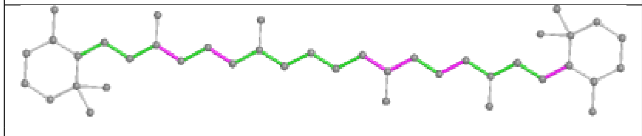
Ligand BCR B 4010



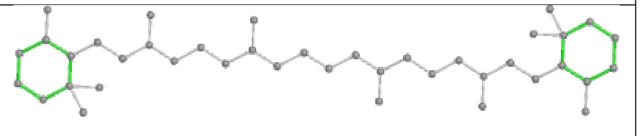
Bond lengths



Bond angles

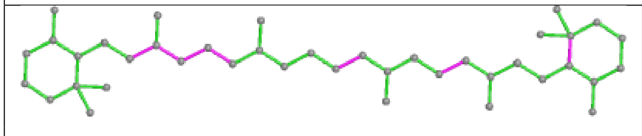


Torsions

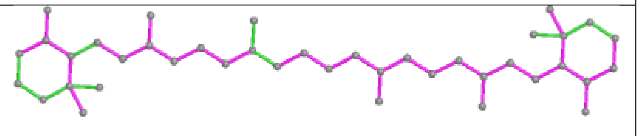


Rings

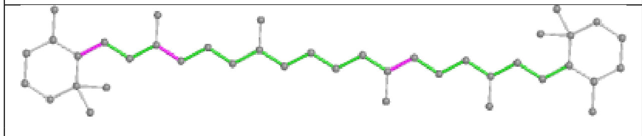
Ligand BCR B 4005



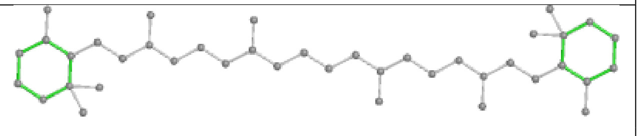
Bond lengths



Bond angles

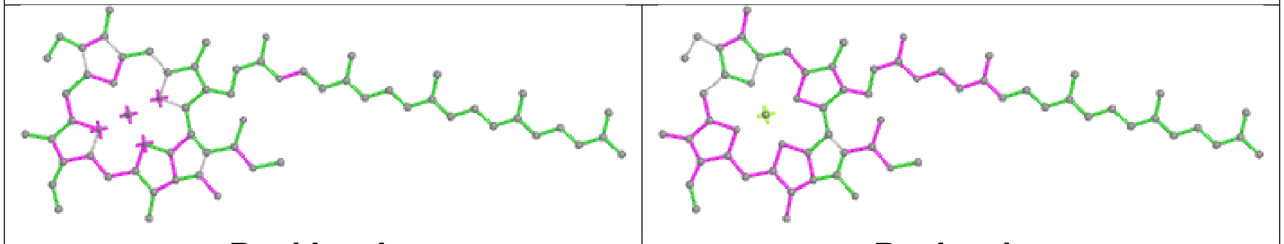


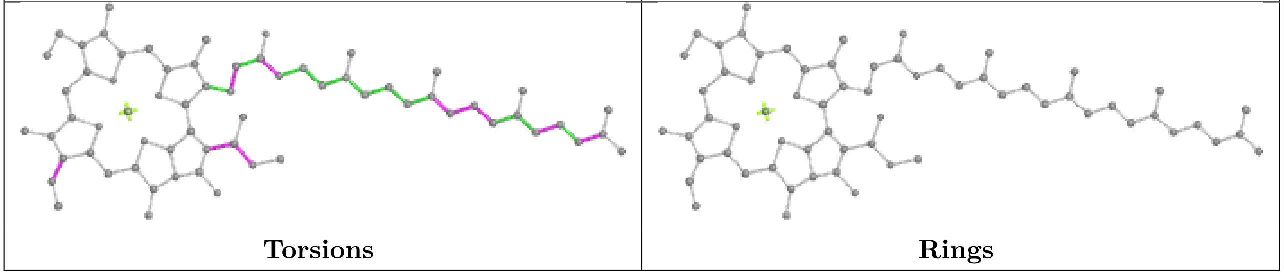
Torsions



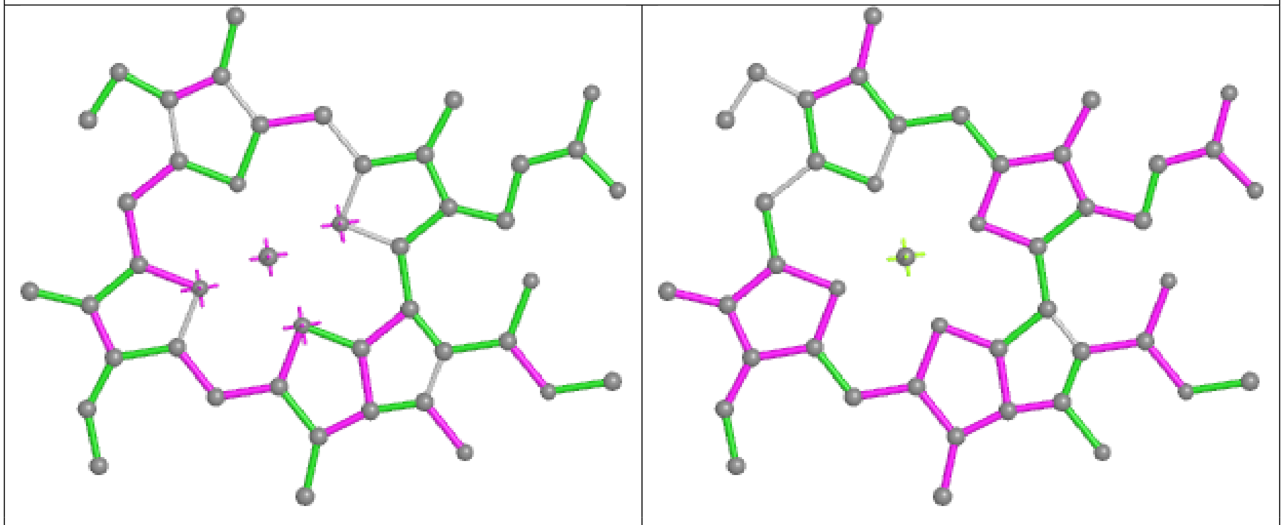
Rings

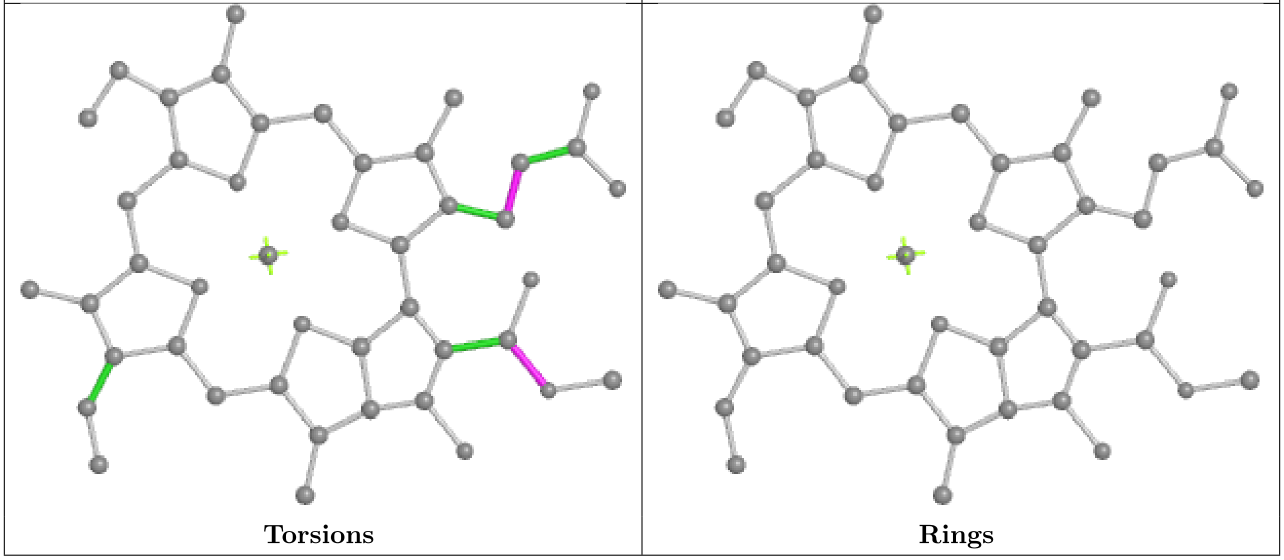
Ligand CLA b 1023


Bond lengths Bond angles

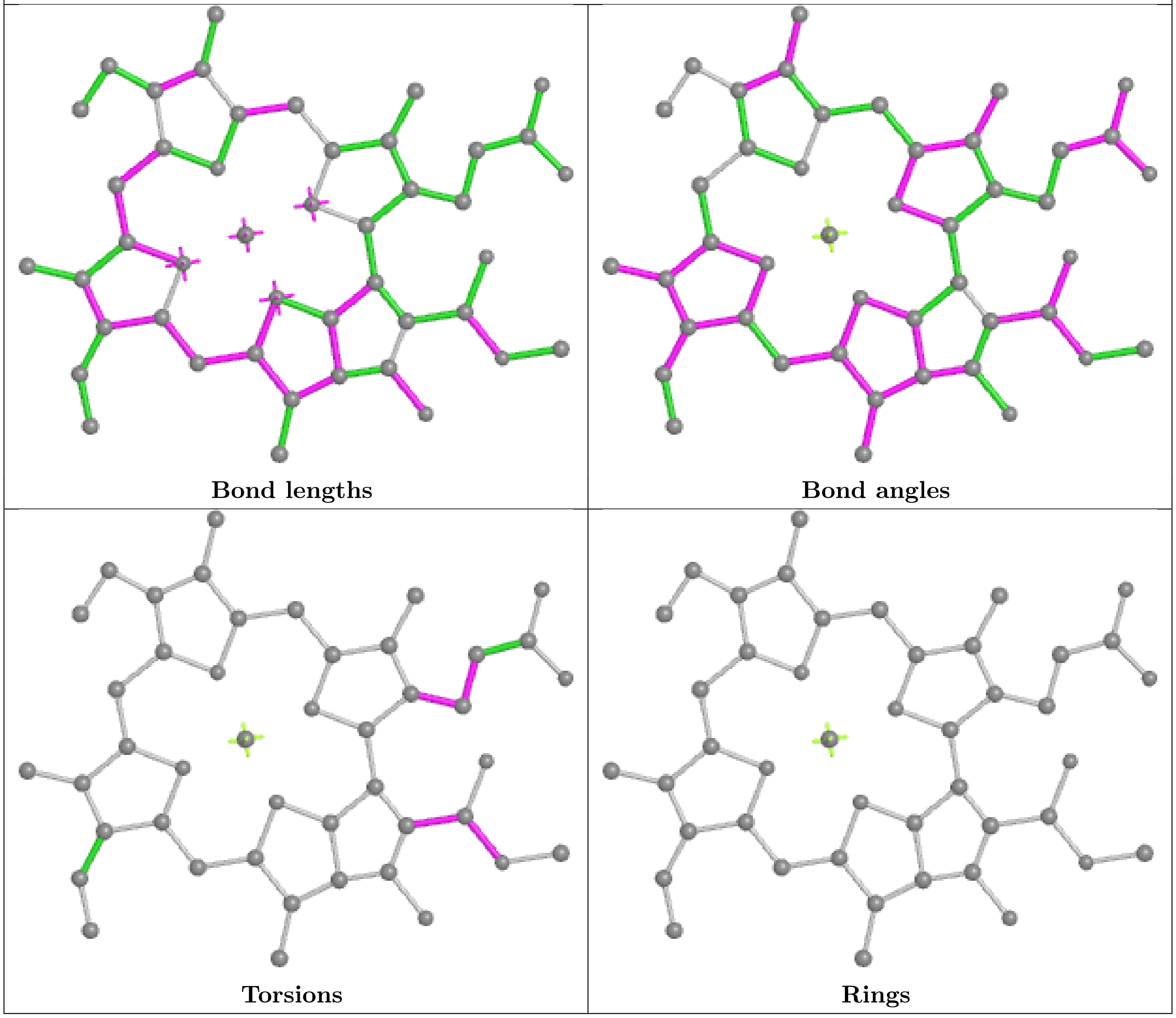

Torsions Rings

Ligand CLA G 1139


Bond lengths Bond angles


Torsions Rings

Ligand CLA T 1401



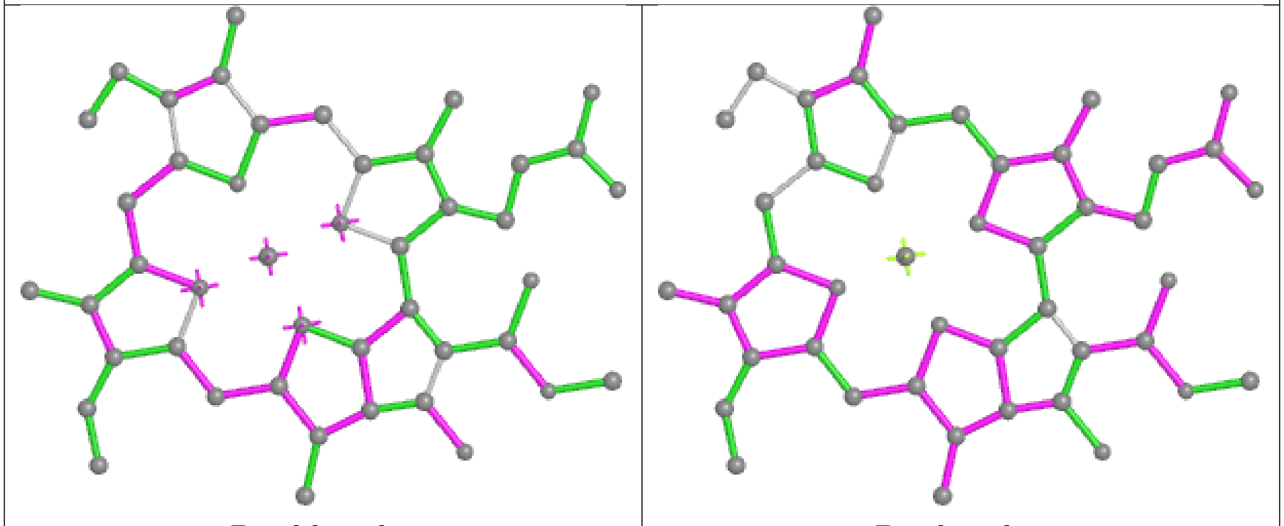
Bond lengths

Bond angles

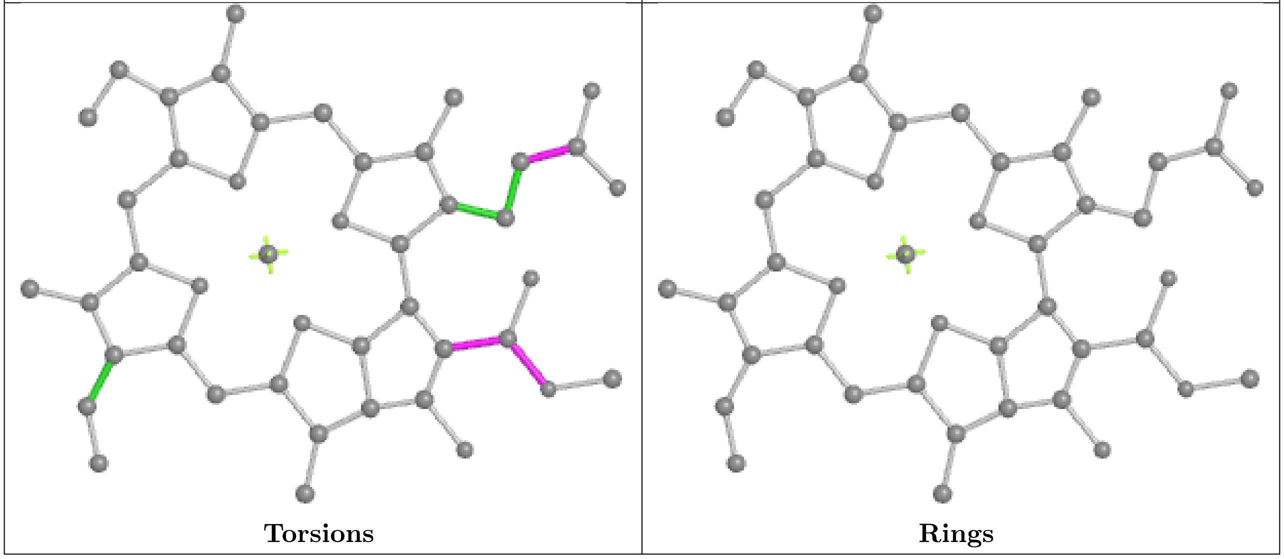
Torsions

Rings

Ligand CLA A 1108

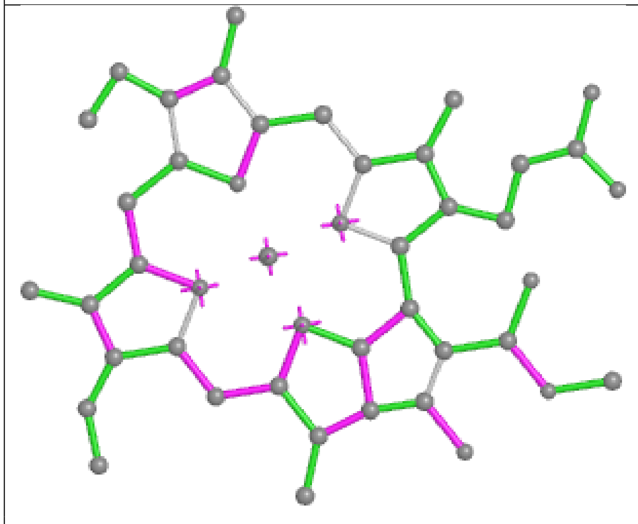


Bond lengths **Bond angles**

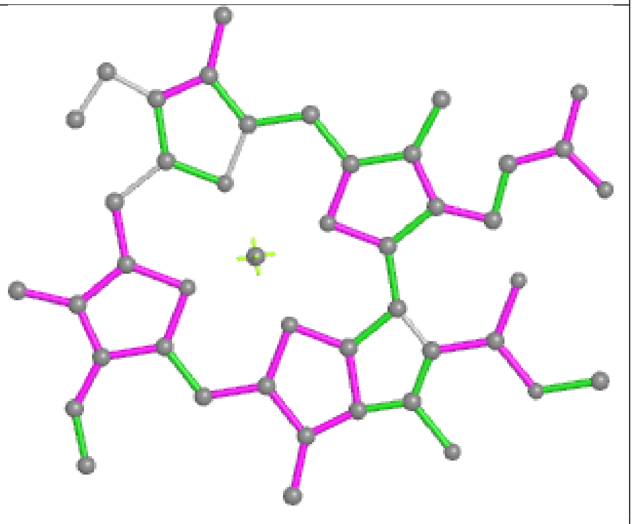


Torsions **Rings**

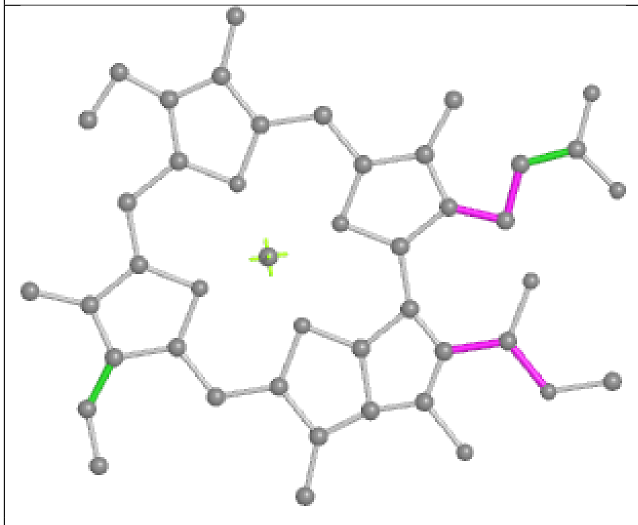
Ligand CLA H 1206



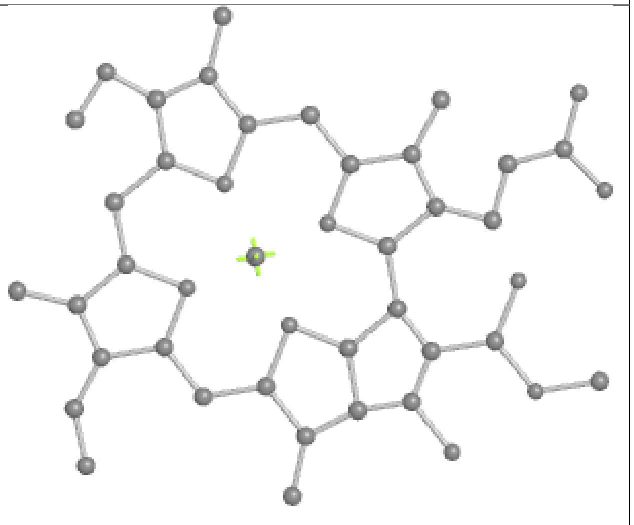
Bond lengths



Bond angles

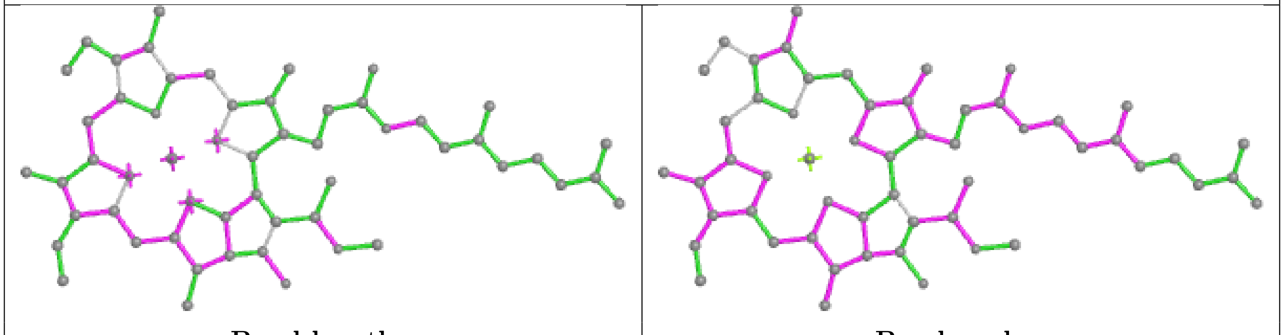


Torsions

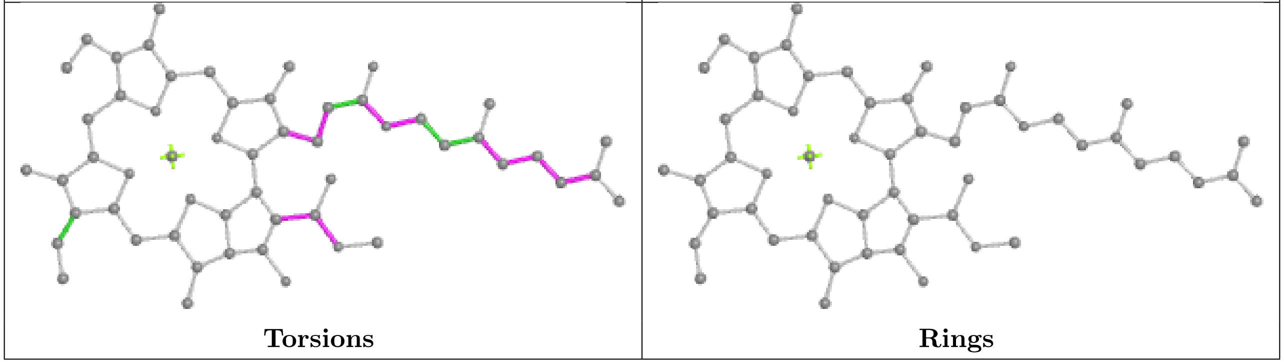


Rings

Ligand CLA b 1228

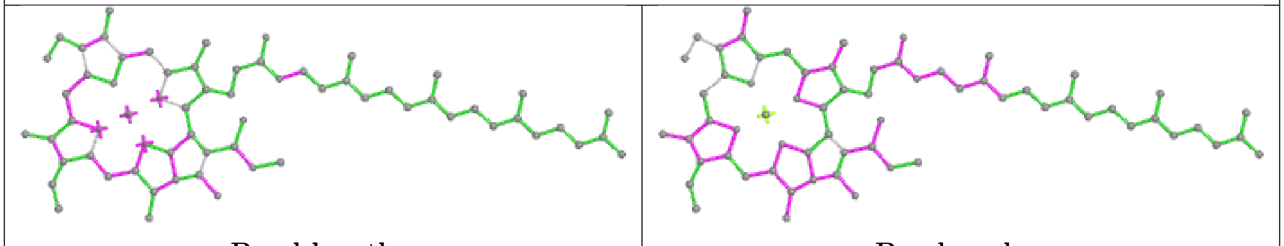


Bond lengths Bond angles

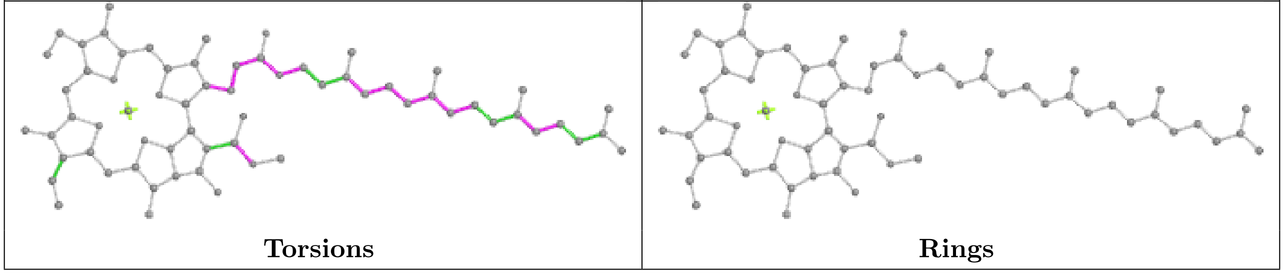


Torsions Rings

Ligand CLA A 1140

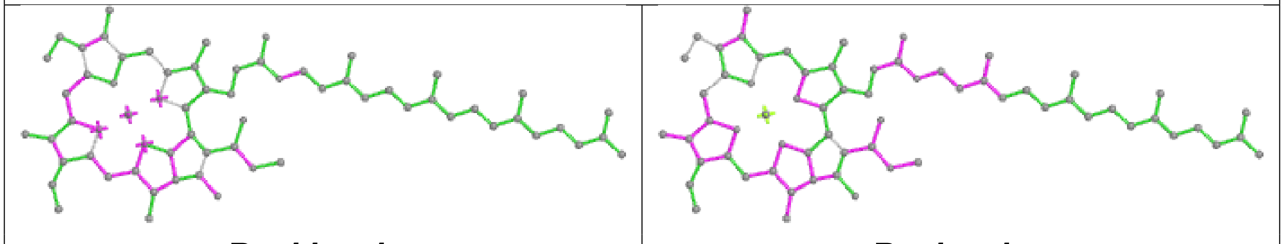


Bond lengths Bond angles



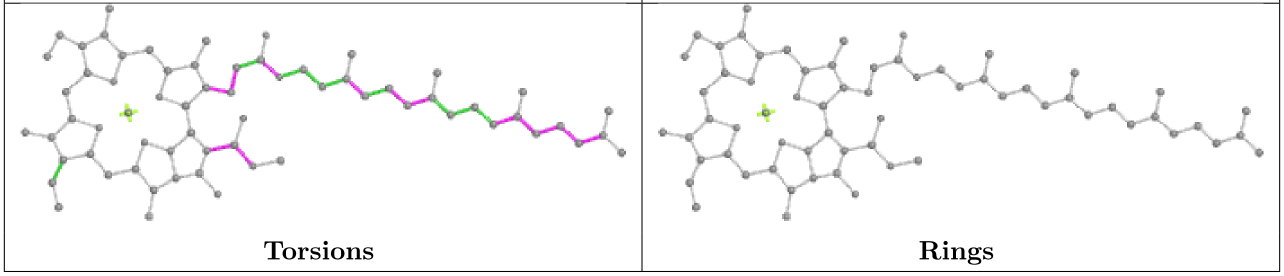
Torsions Rings

Ligand CLA B 1216



Bond lengths

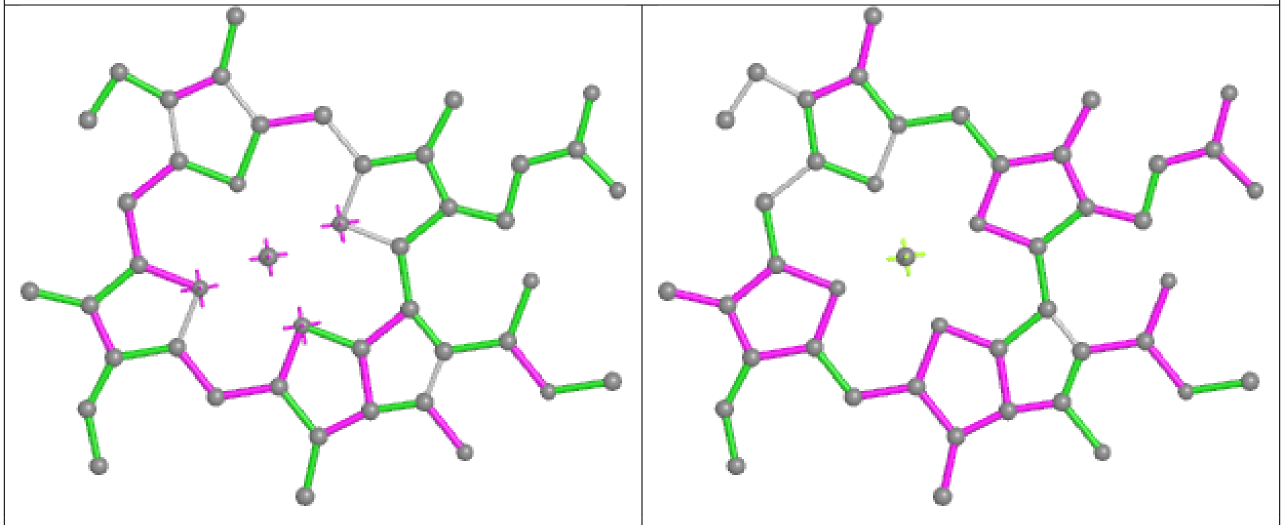
Bond angles



Torsions

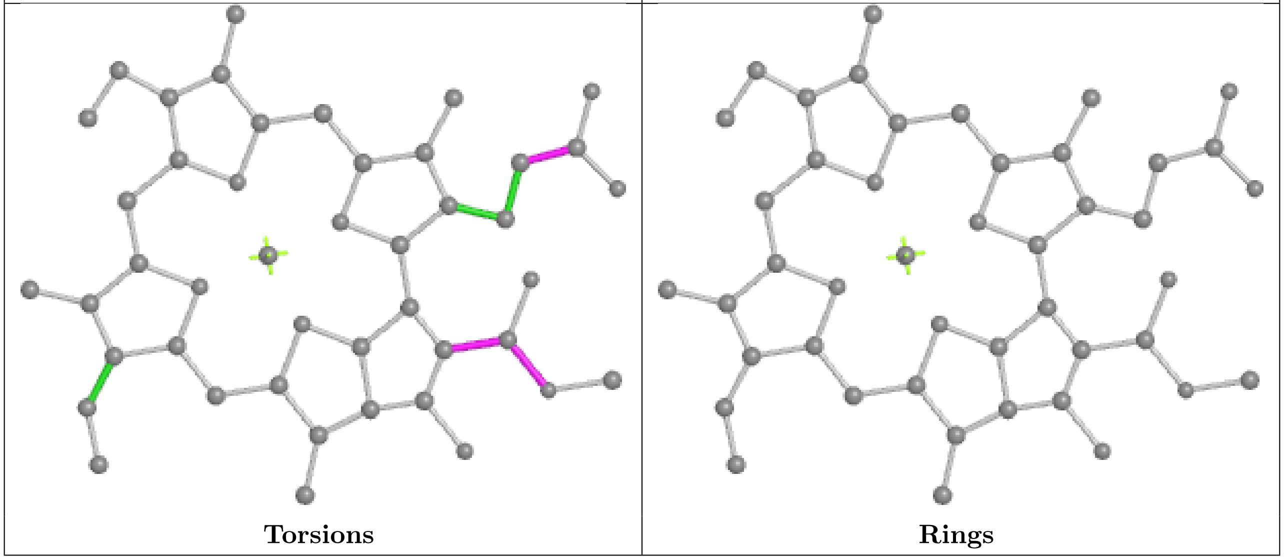
Rings

Ligand CLA a 1101



Bond lengths

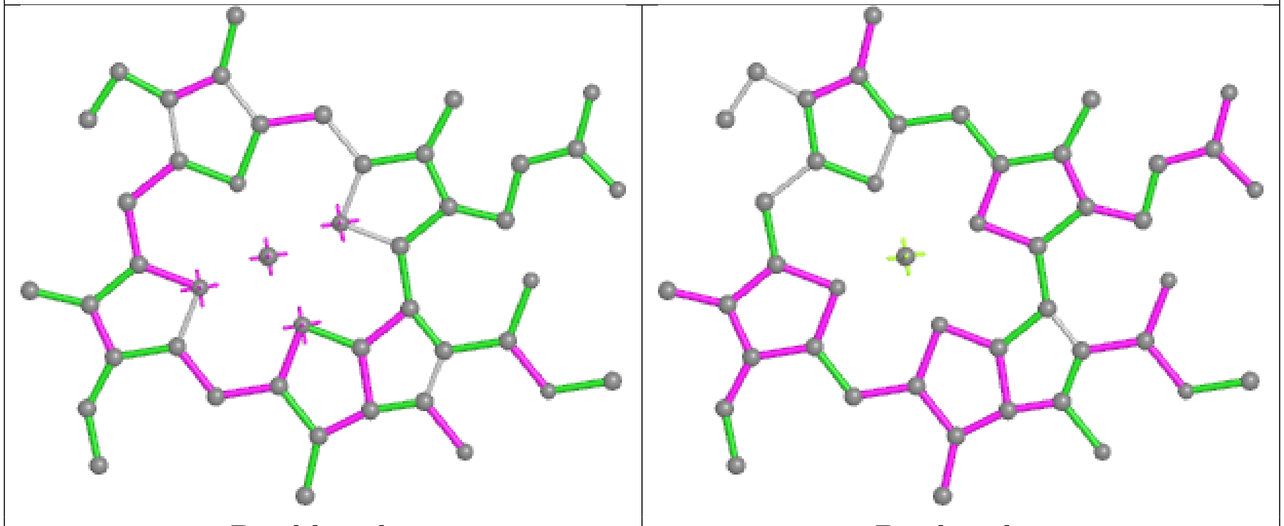
Bond angles



Torsions

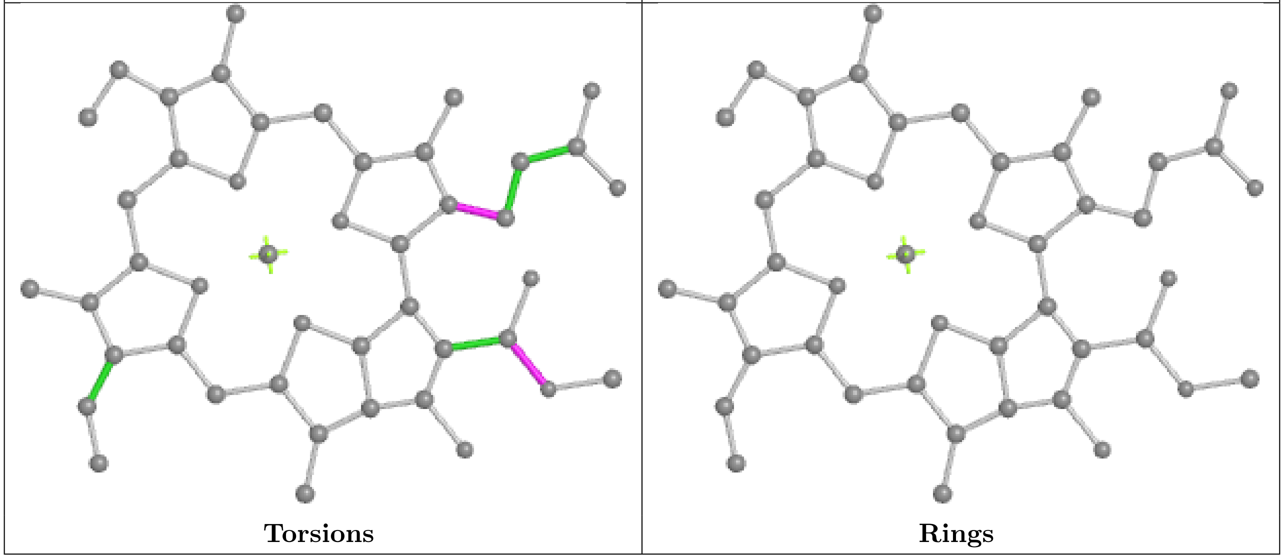
Rings

Ligand CLA a 1107



Bond lengths

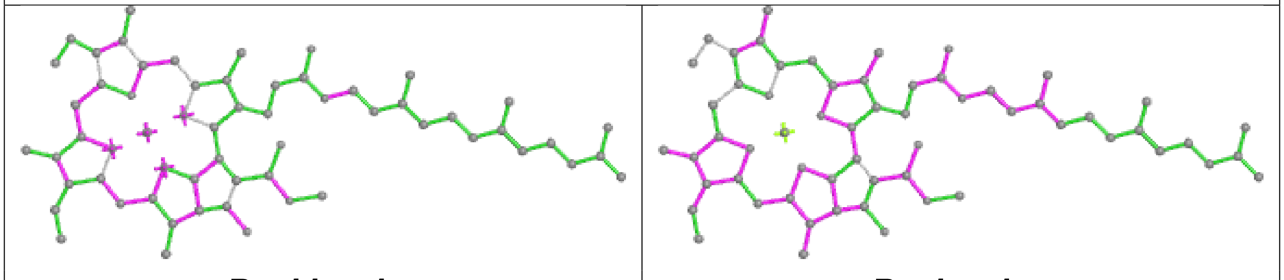
Bond angles



Torsions

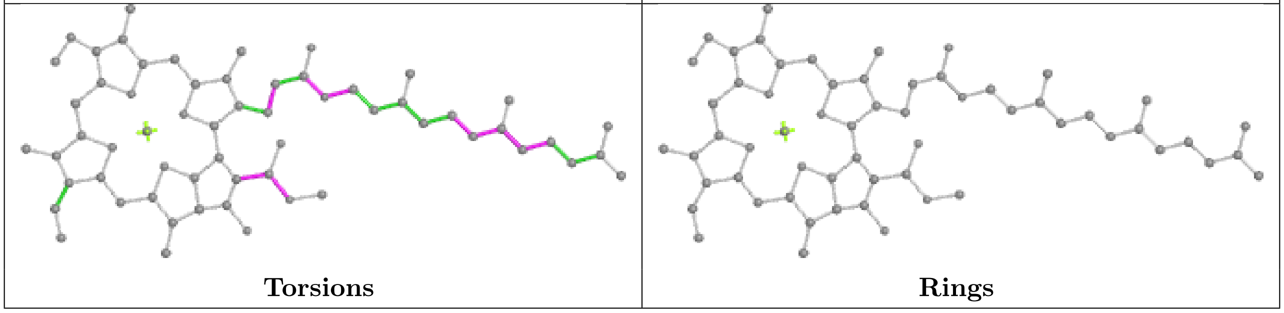
Rings

Ligand CLA A 1123



Bond lengths

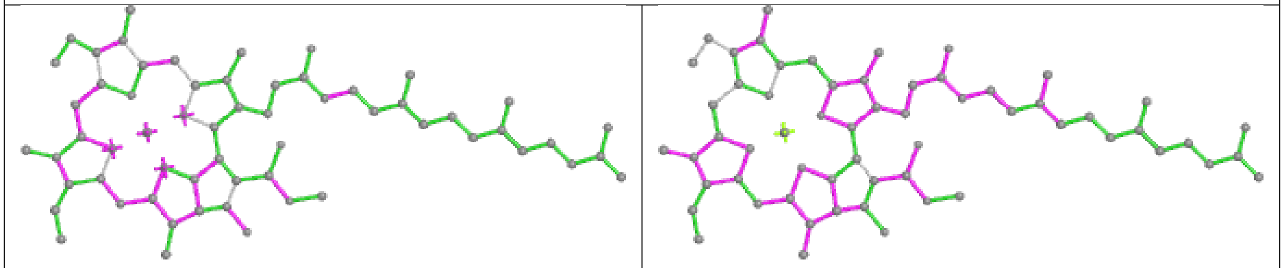
Bond angles



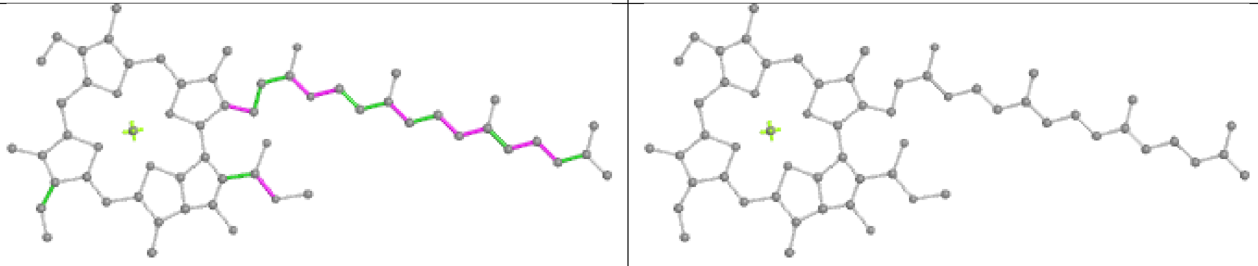
Torsions

Rings

Ligand CLA H 1229

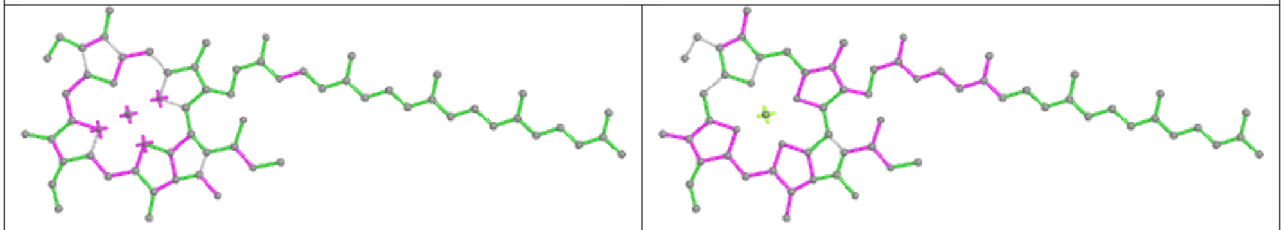


Bond lengths Bond angles

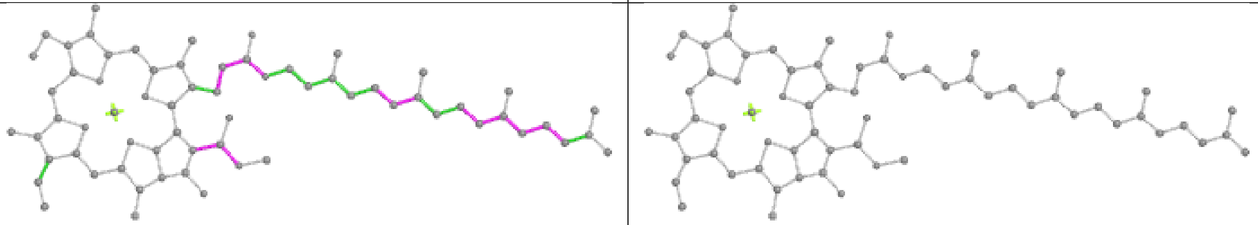


Torsions Rings

Ligand CLA b 1224

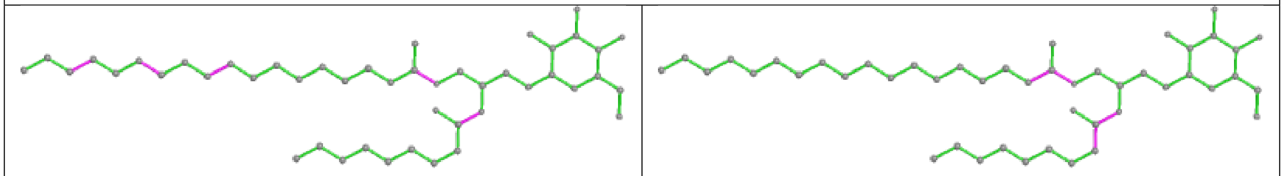


Bond lengths Bond angles

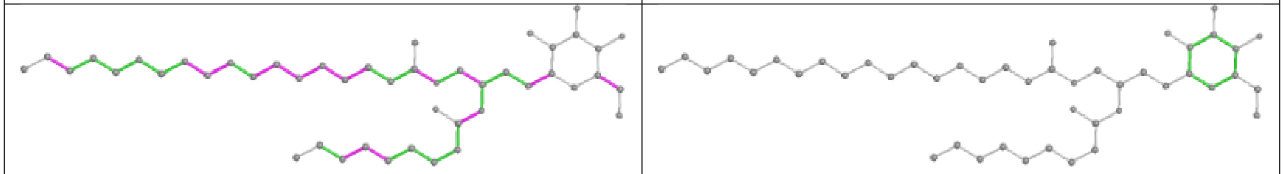


Torsions Rings

Ligand LMG G 5005

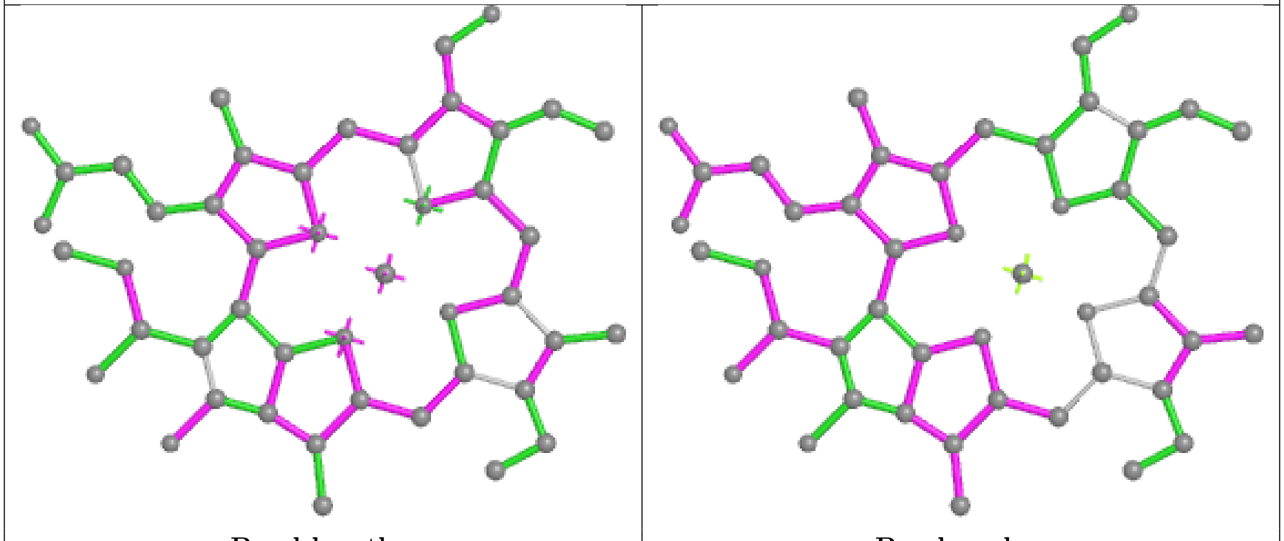


Bond lengths Bond angles



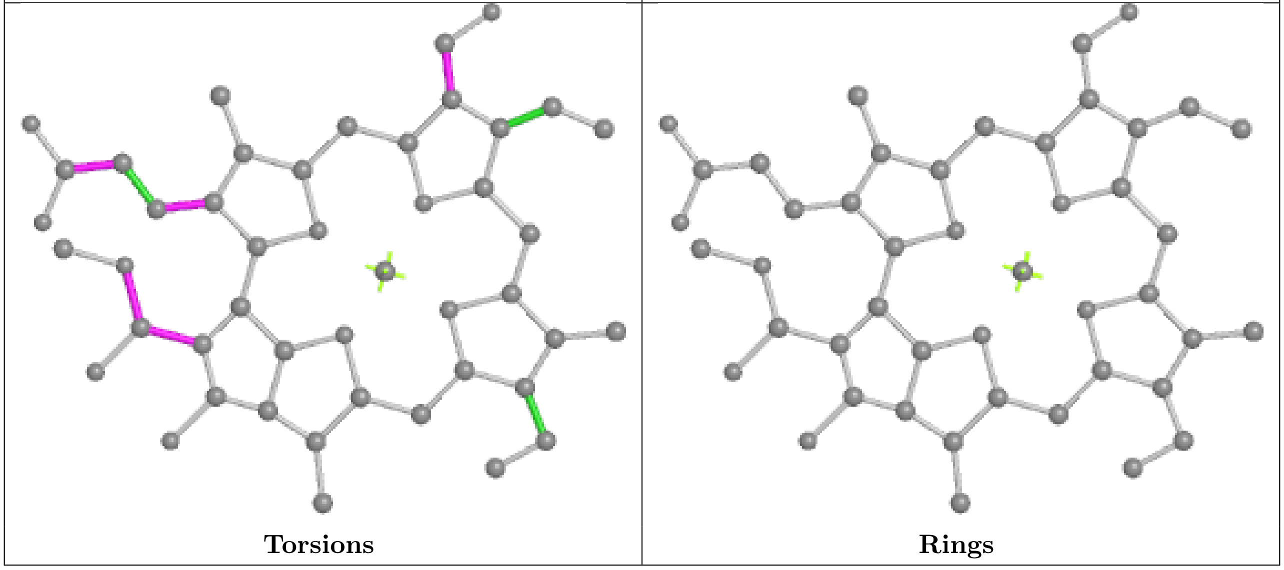
Torsions Rings

Ligand F6C B 1230



Bond lengths

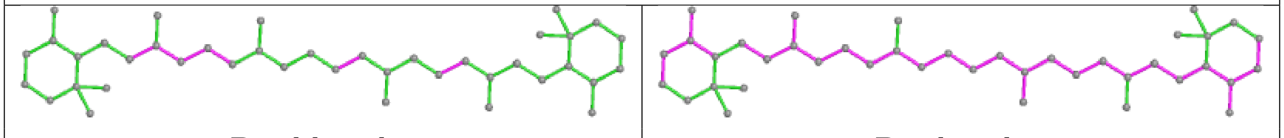
Bond angles



Torsions

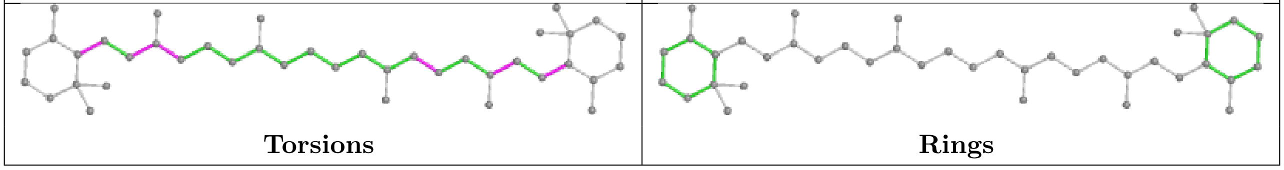
Rings

Ligand BCR H 4006



Bond lengths

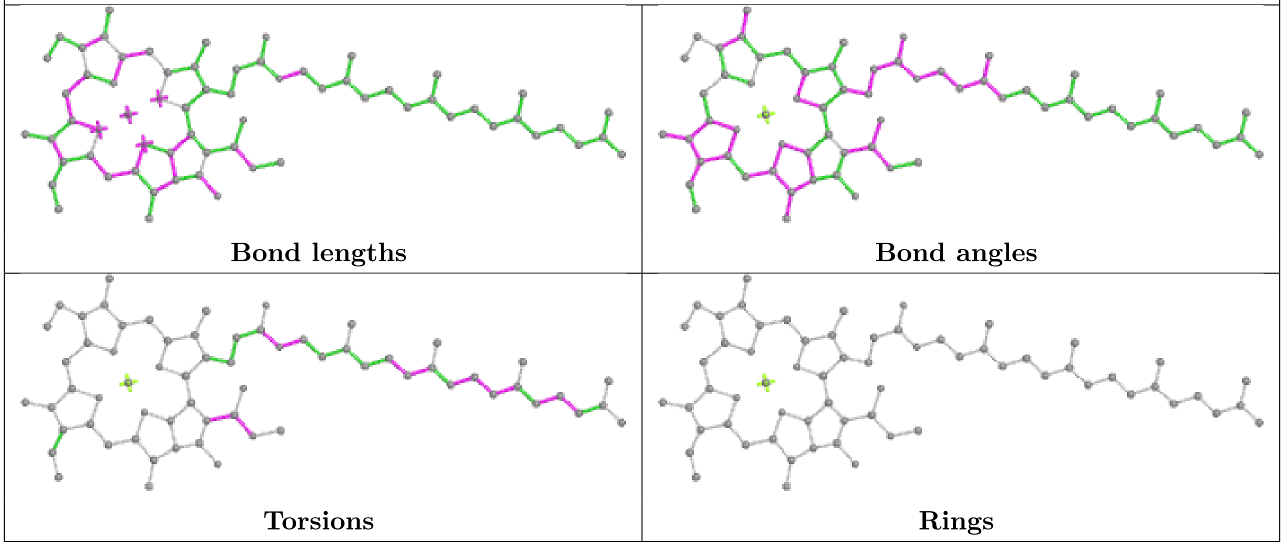
Bond angles



Torsions

Rings

Ligand CLA H 1234



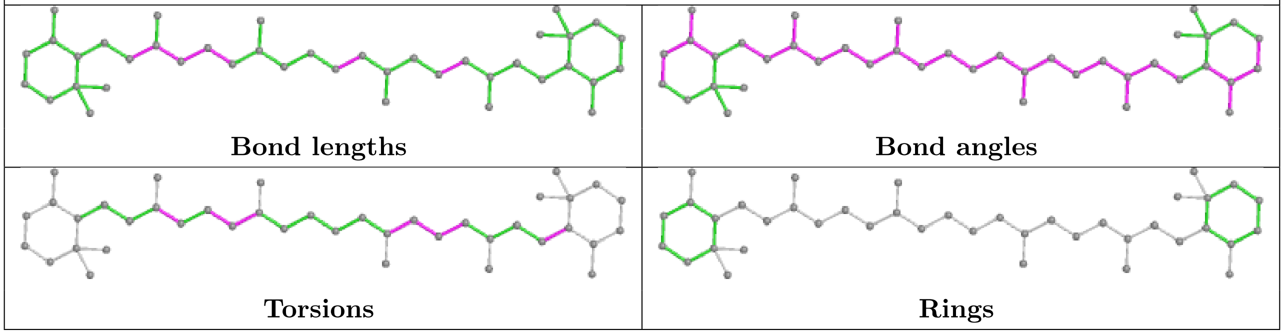
Bond lengths

Bond angles

Torsions

Rings

Ligand BCR B 4013



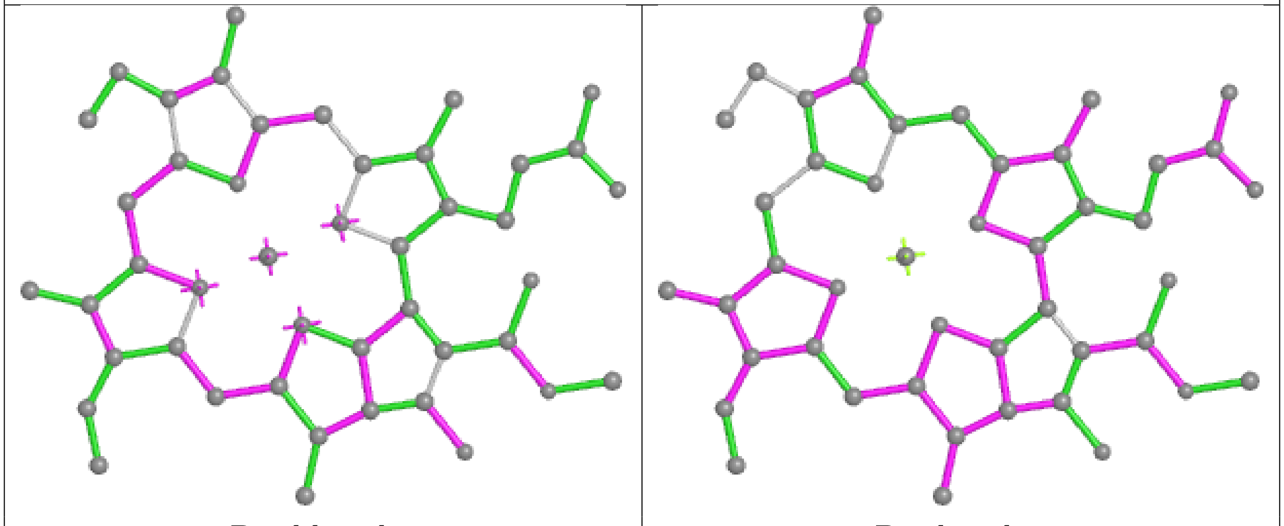
Bond lengths

Bond angles

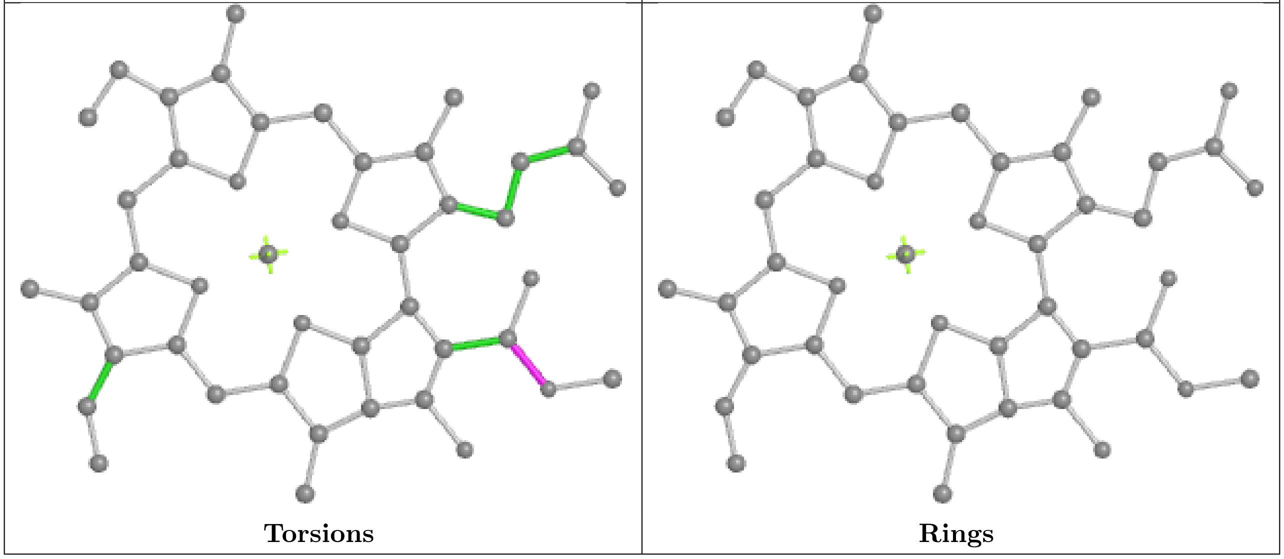
Torsions

Rings

Ligand CLA H 1232

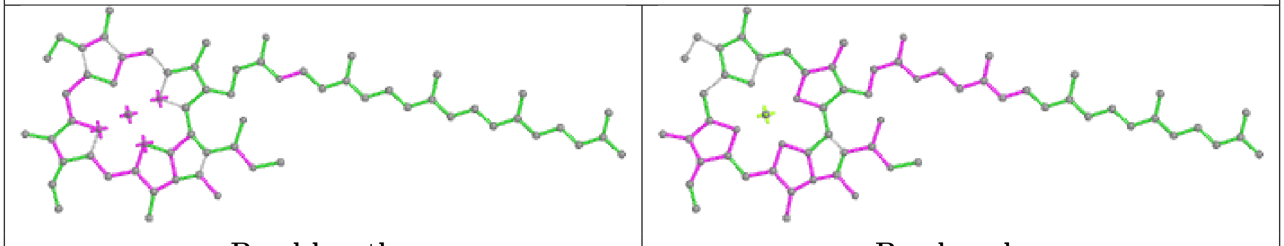


Bond lengths **Bond angles**

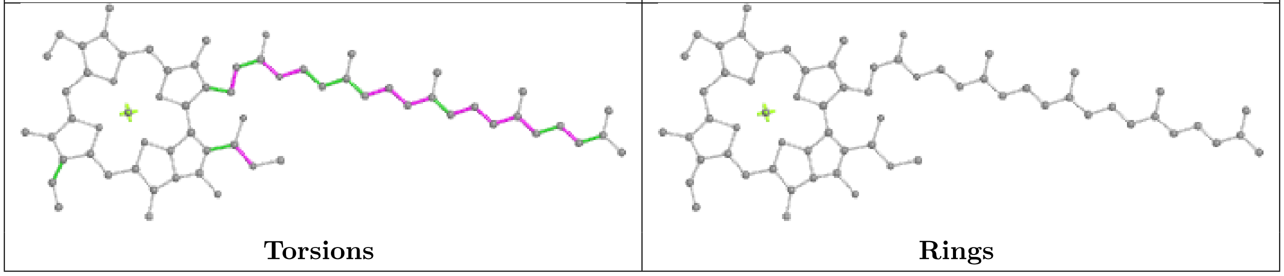


Torsions **Rings**

Ligand CLA B 1214

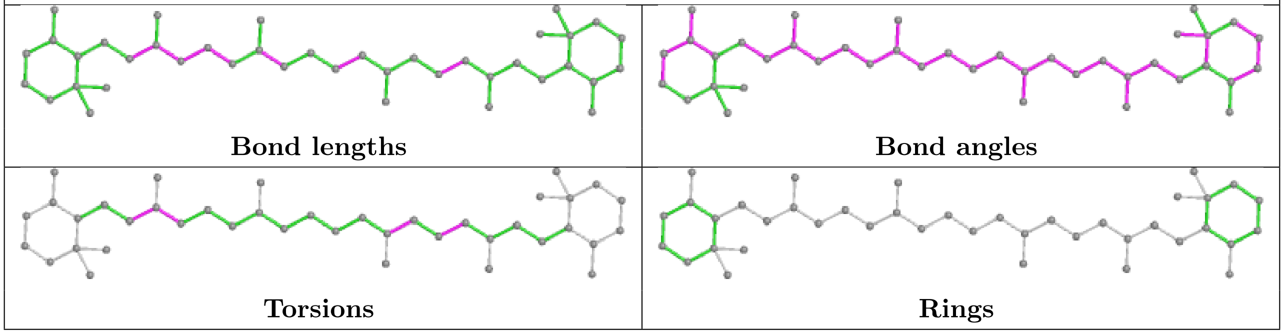


Bond lengths **Bond angles**

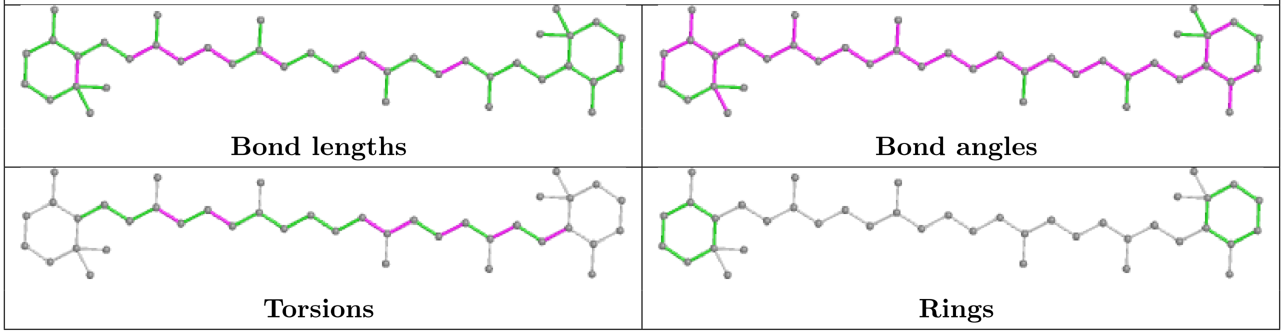


Torsions **Rings**

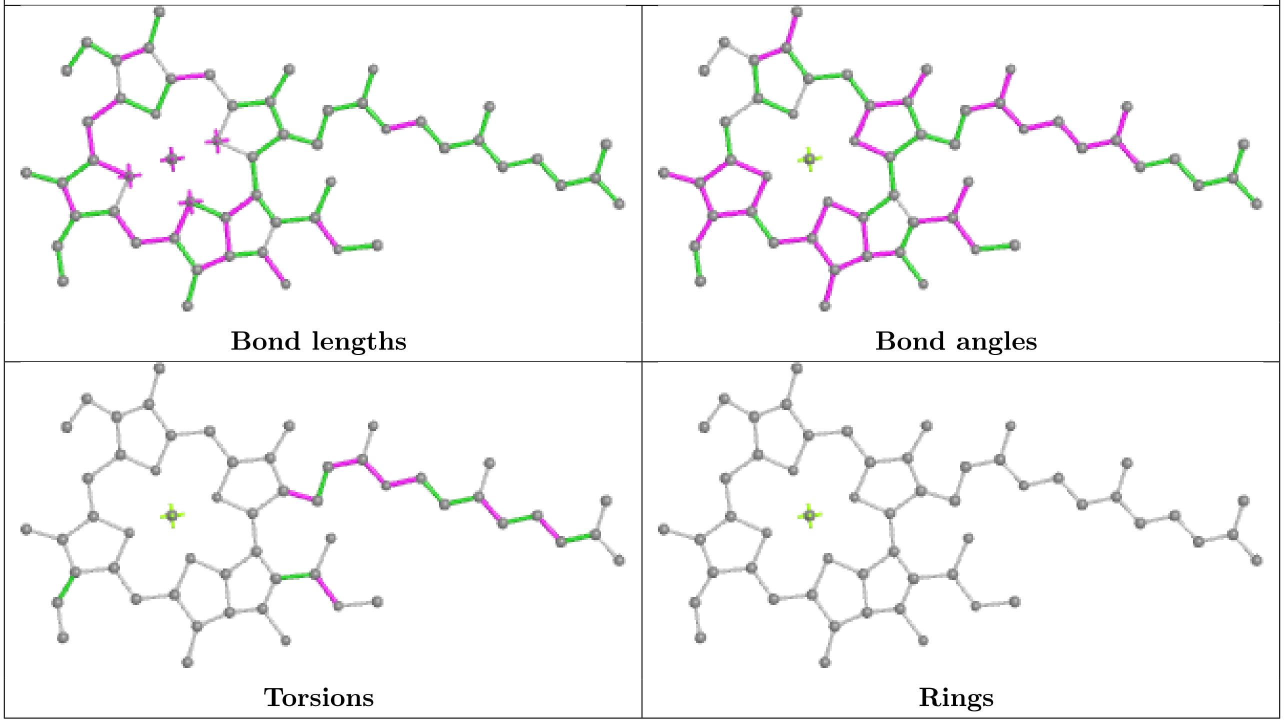
Ligand BCR H 4014



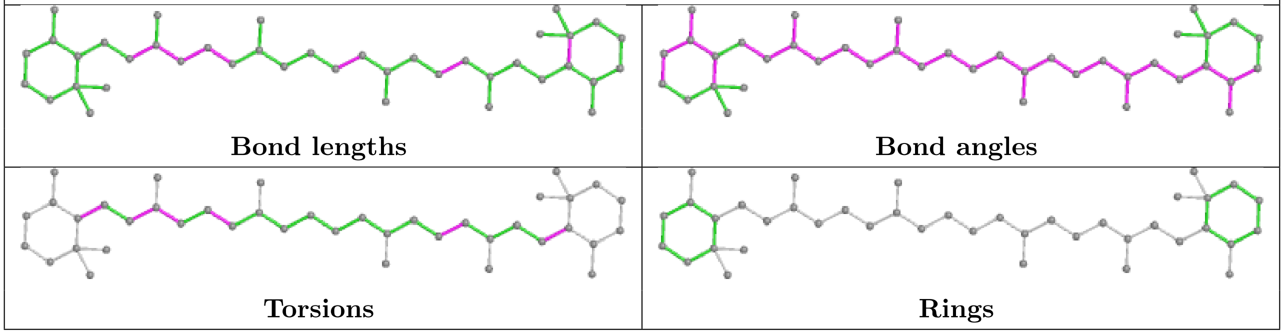
Ligand BCR G 4007



Ligand CLA W 1701



Ligand BCR H 4009



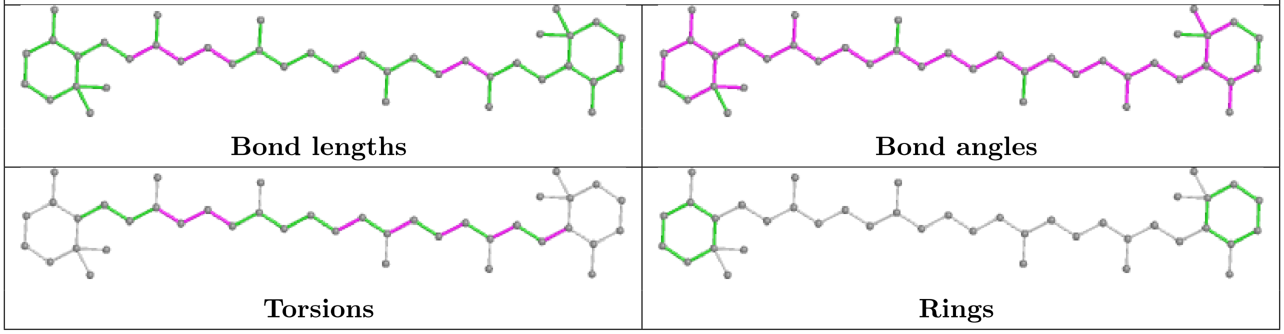
Bond lengths

Bond angles

Torsions

Rings

Ligand BCR U 4019



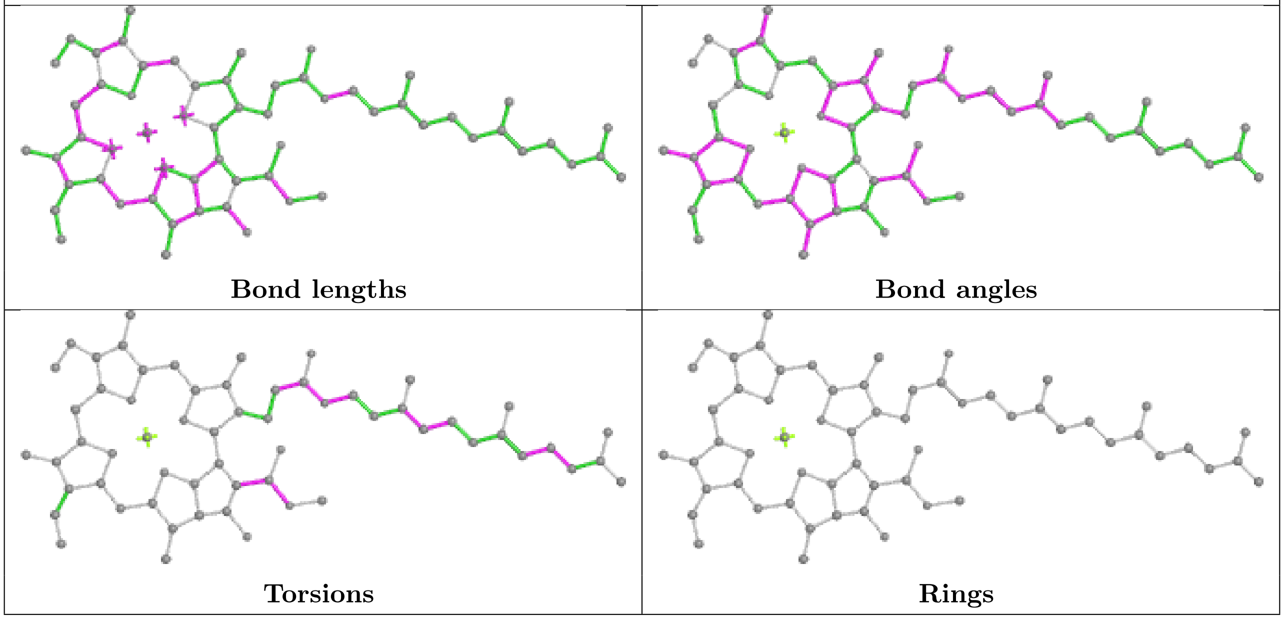
Bond lengths

Bond angles

Torsions

Rings

Ligand CLA H 1235



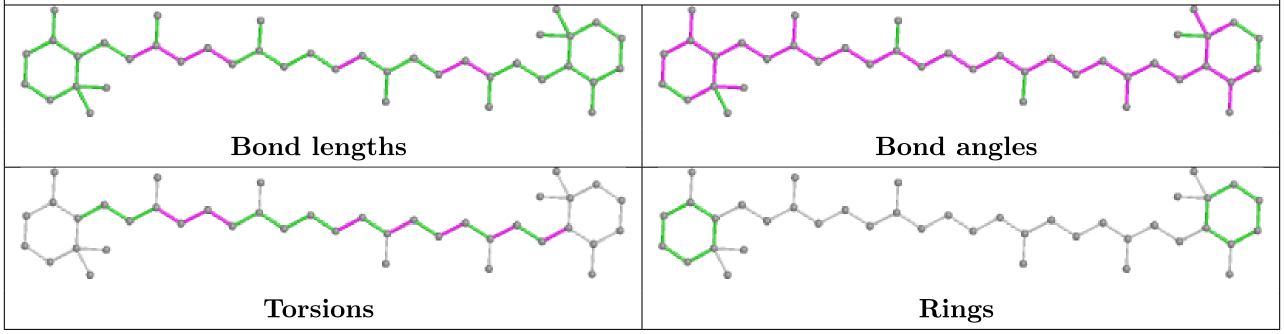
Bond lengths

Bond angles

Torsions

Rings

Ligand BCR l 4019



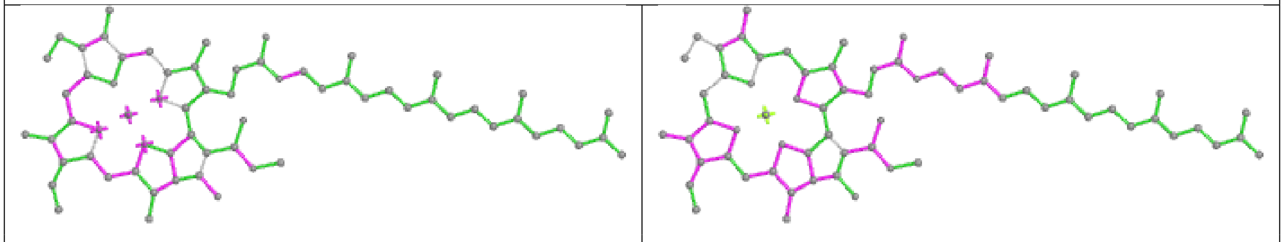
Bond lengths

Bond angles

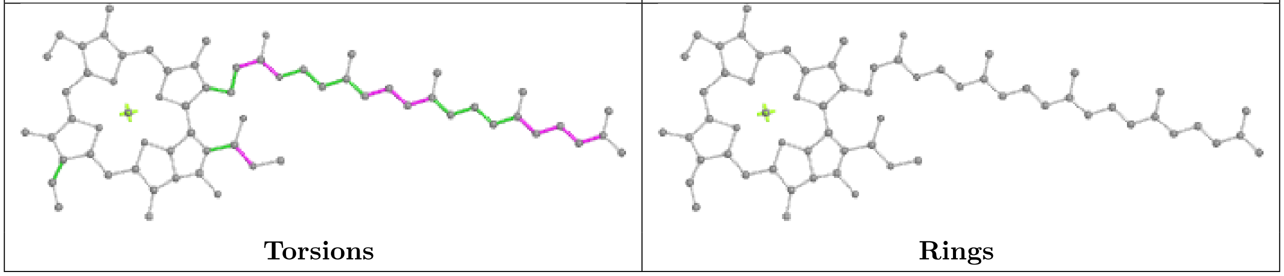
Torsions

Rings

Ligand CLA b 1208

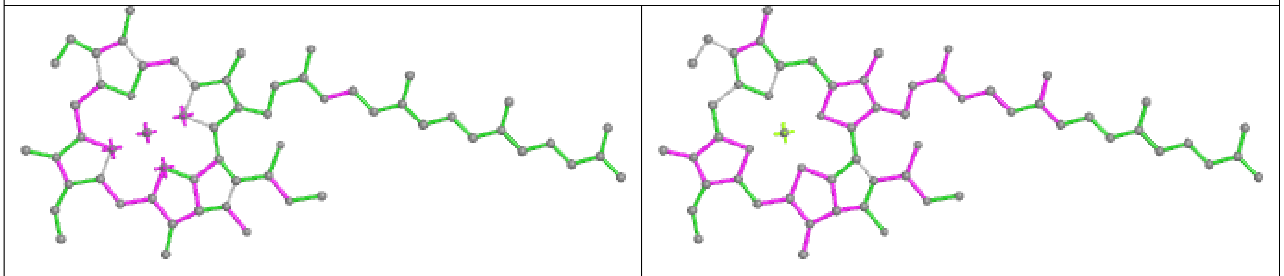


Bond lengths Bond angles

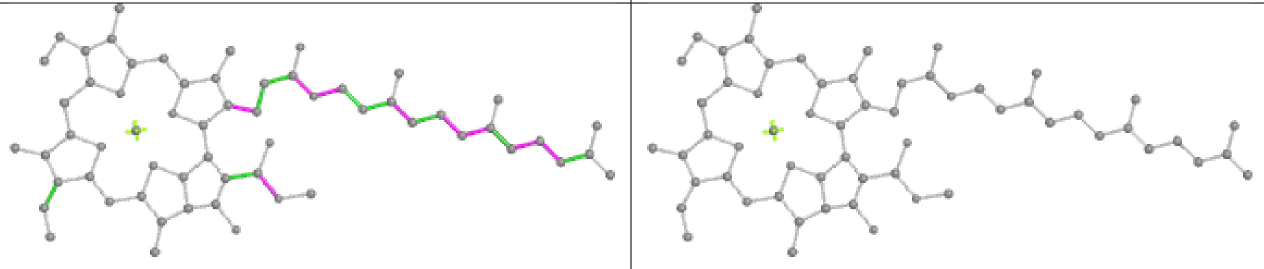


Torsions Rings

Ligand CLA b 1229

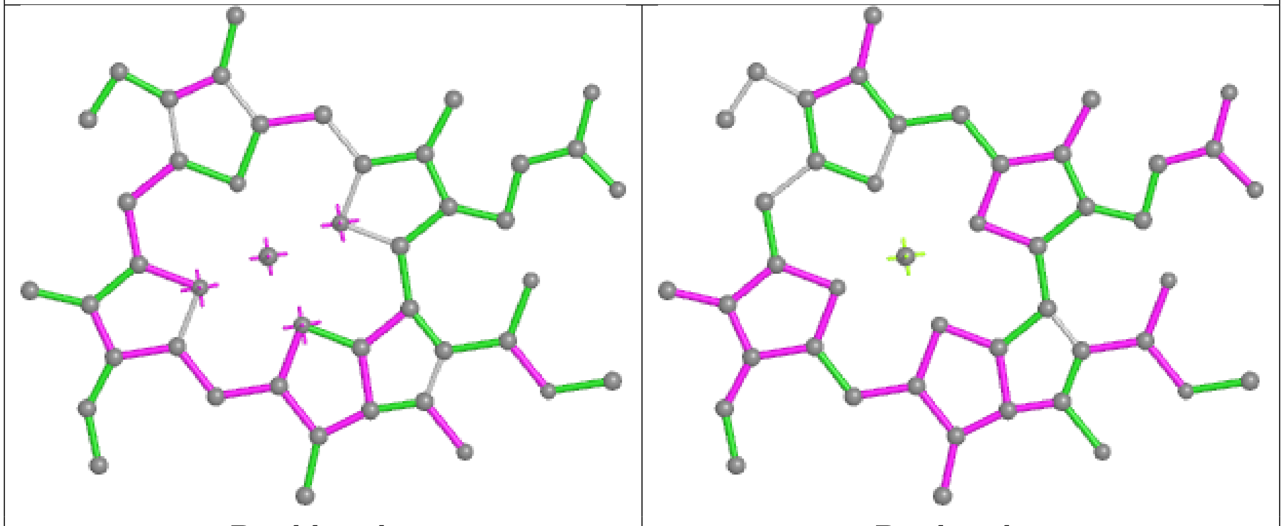


Bond lengths Bond angles



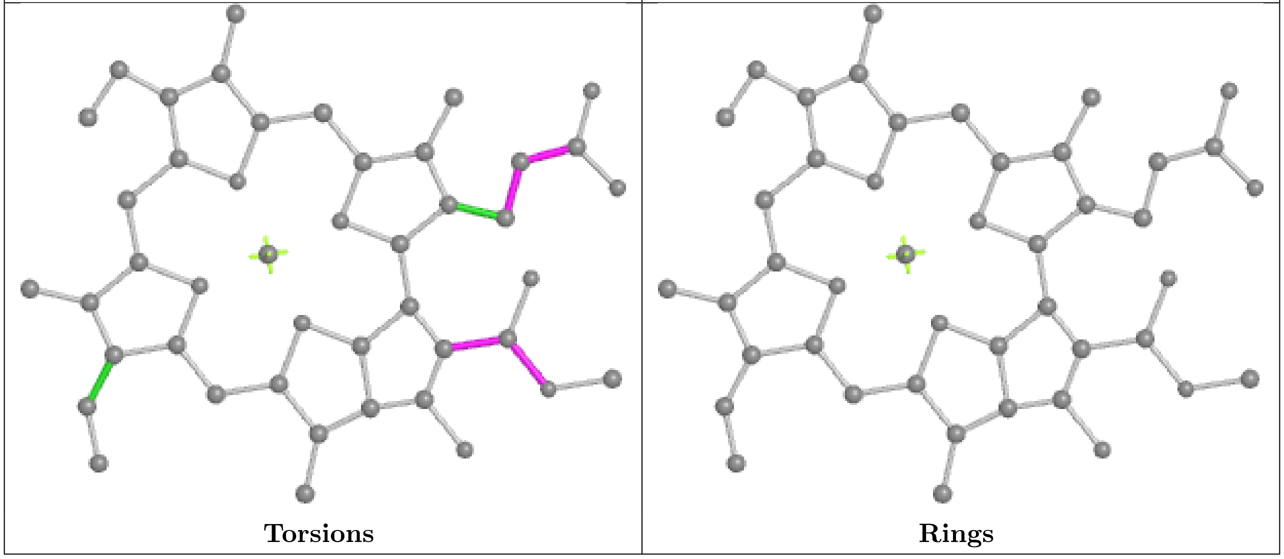
Torsions Rings

Ligand CLA G 1134



Bond lengths

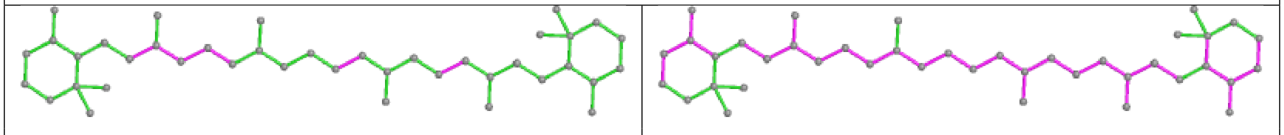
Bond angles



Torsions

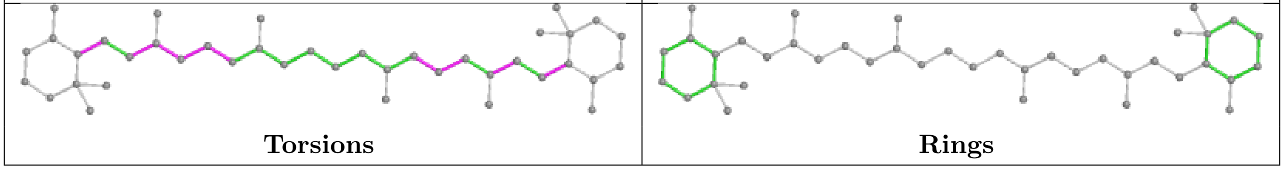
Rings

Ligand BCR a 4003



Bond lengths

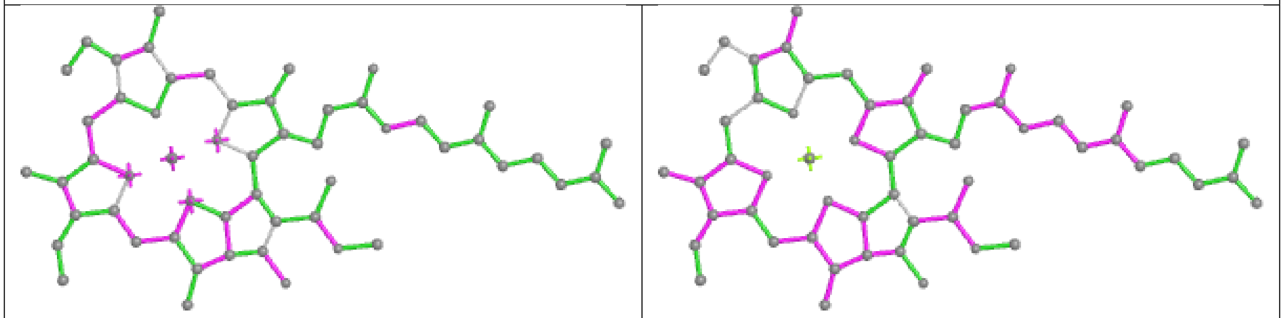
Bond angles



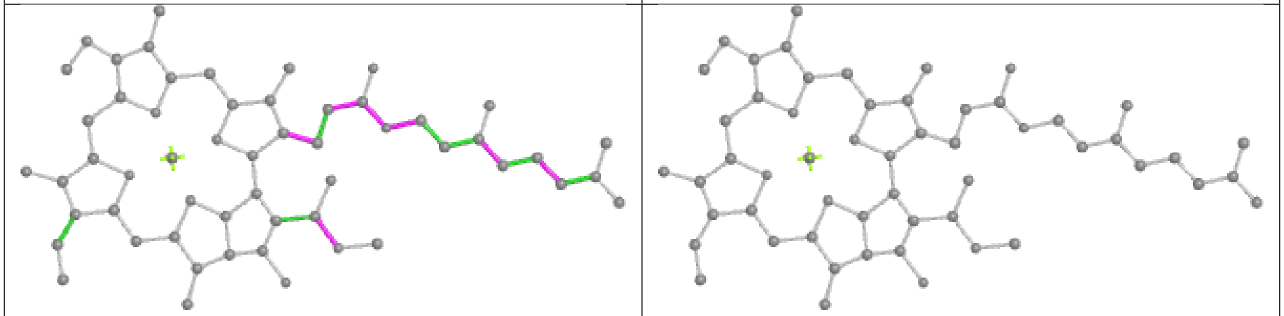
Torsions

Rings

Ligand CLA x 1701

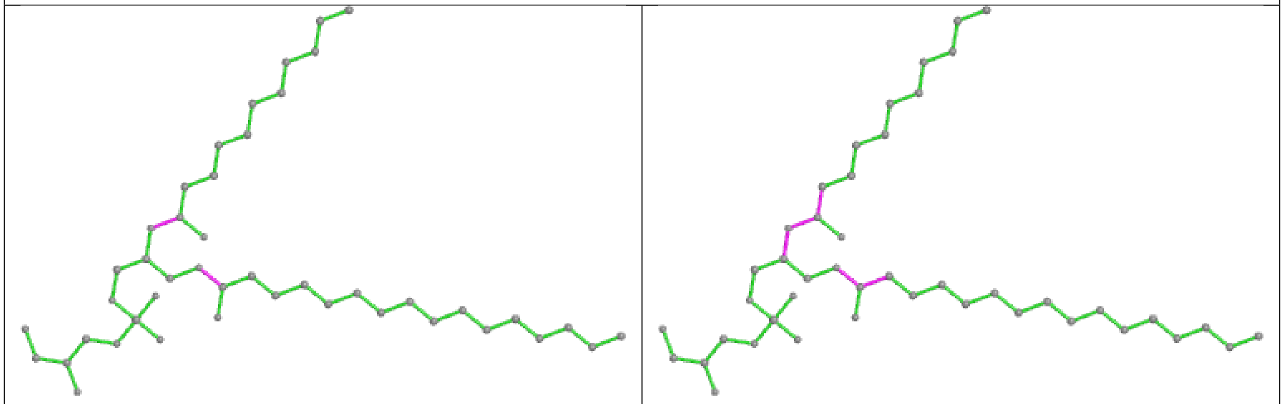


Bond lengths Bond angles

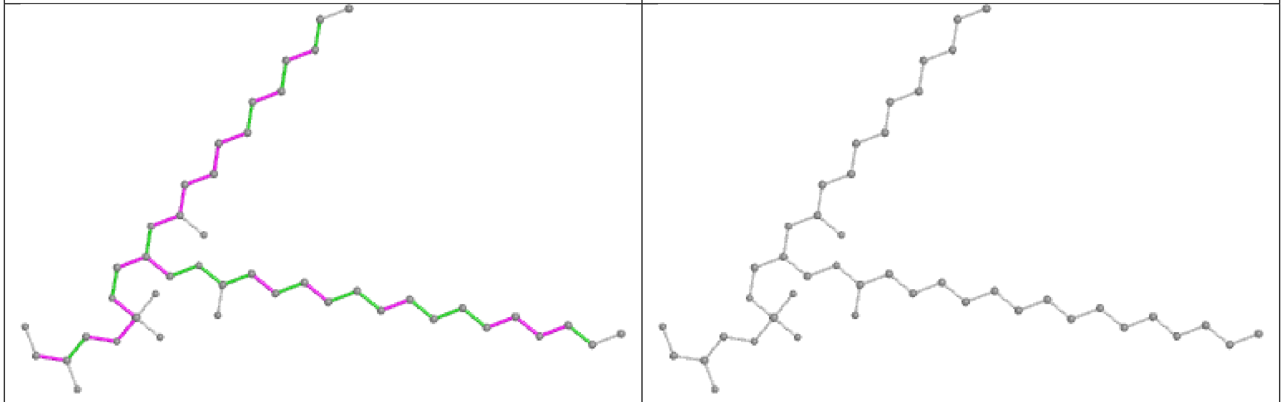


Torsions Rings

Ligand LHG B 5004

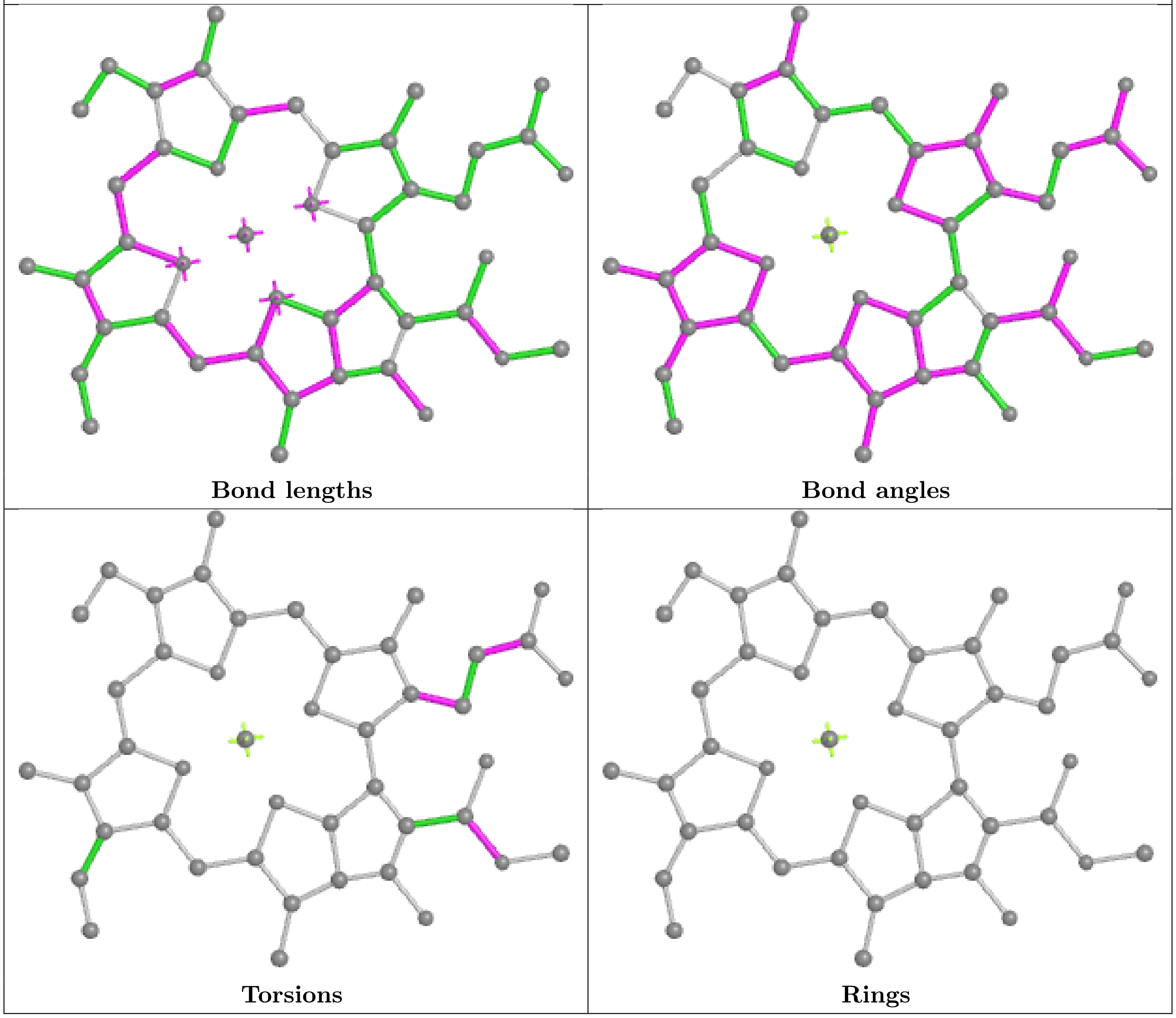


Bond lengths Bond angles



Torsions Rings

Ligand CLA A 1105



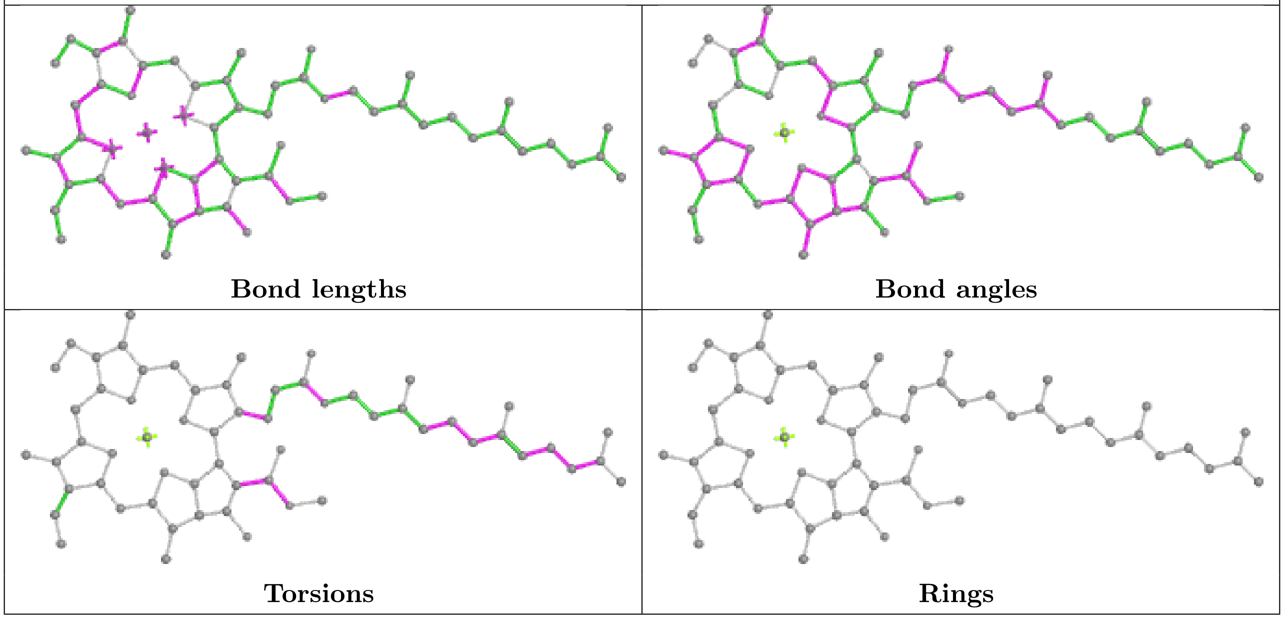
Bond lengths

Bond angles

Torsions

Rings

Ligand CLA A 1102



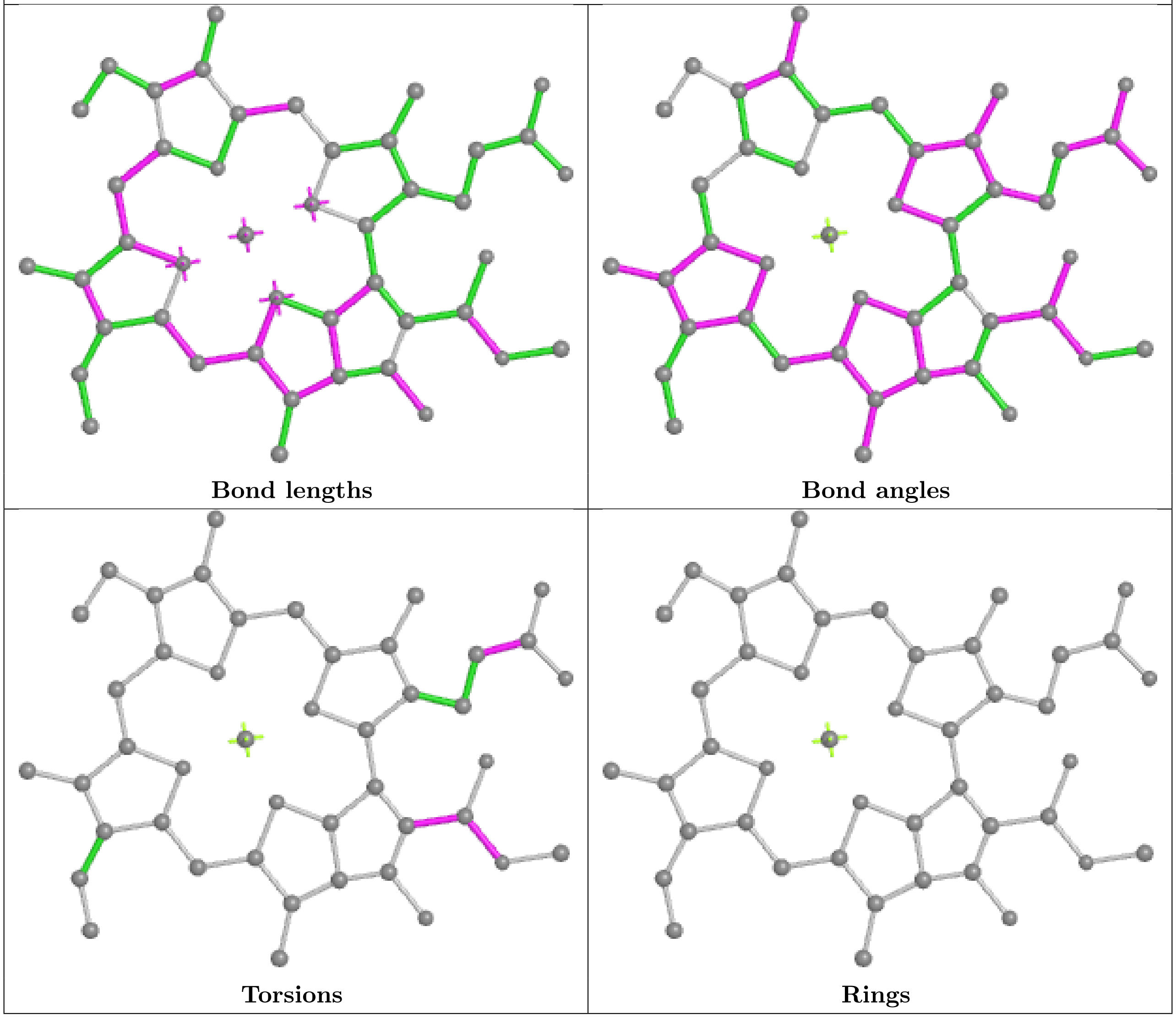
Bond lengths

Bond angles

Torsions

Rings

Ligand CLA G 1108



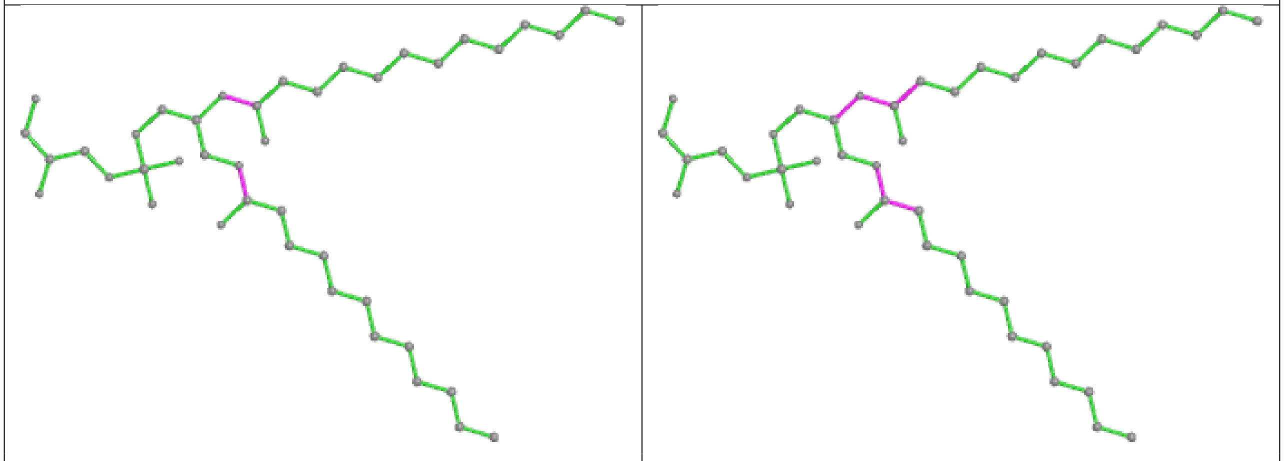
Bond lengths

Bond angles

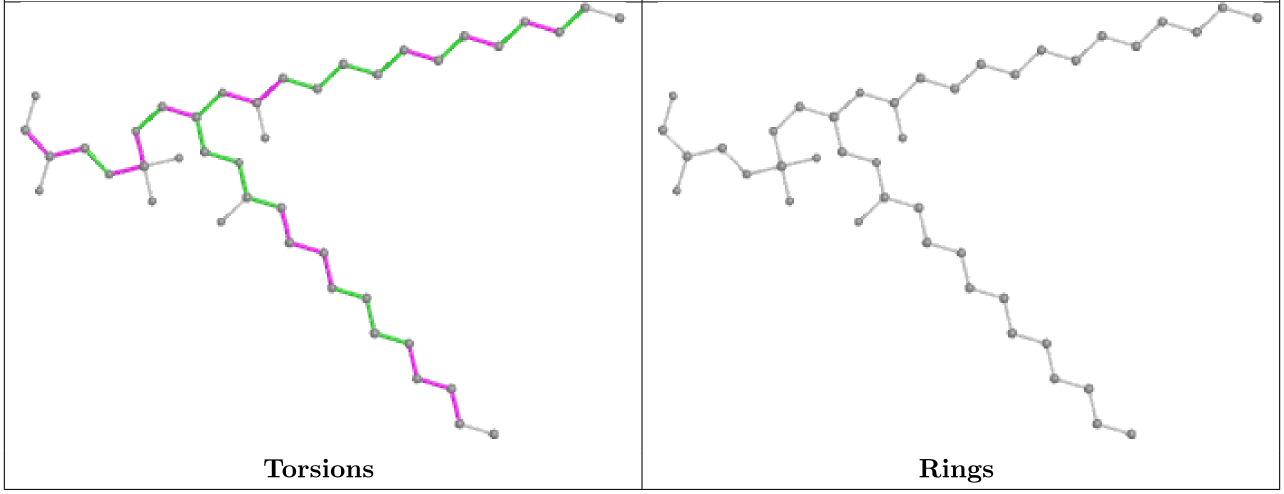
Torsions

Rings

Ligand LHG a 5001

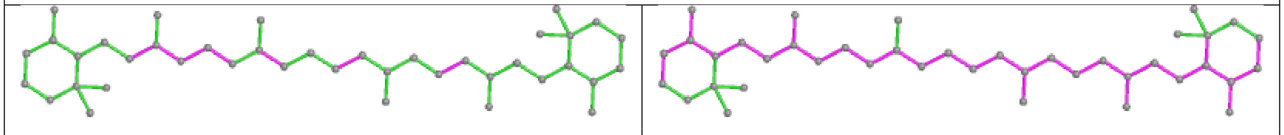


Bond lengths Bond angles

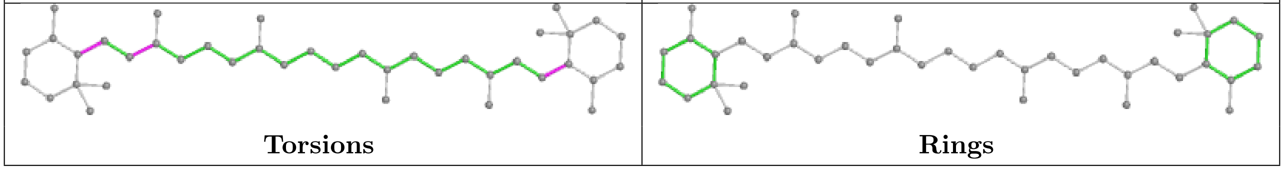


Torsions Rings

Ligand BCR G 4002

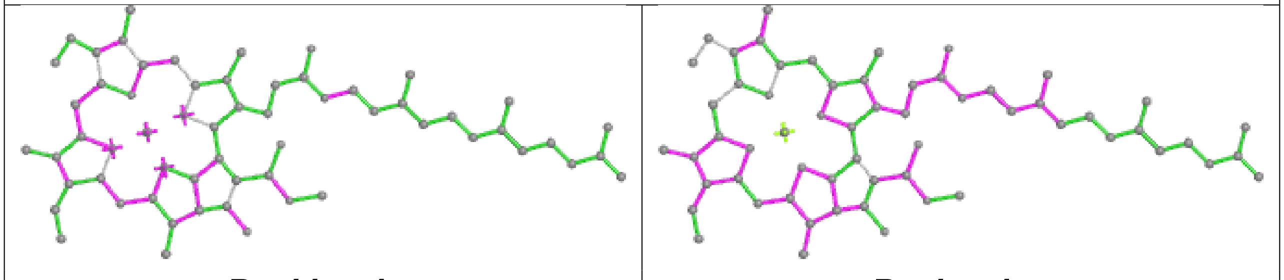


Bond lengths Bond angles



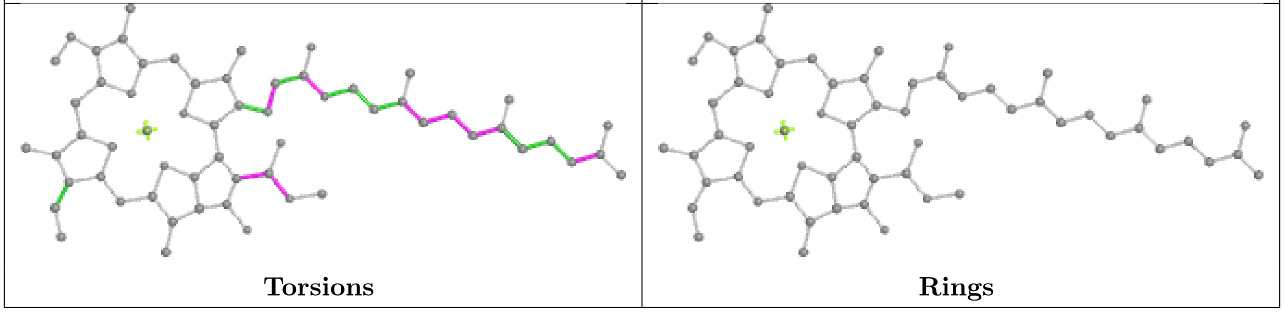
Torsions Rings

Ligand CLA A 1111



Bond lengths

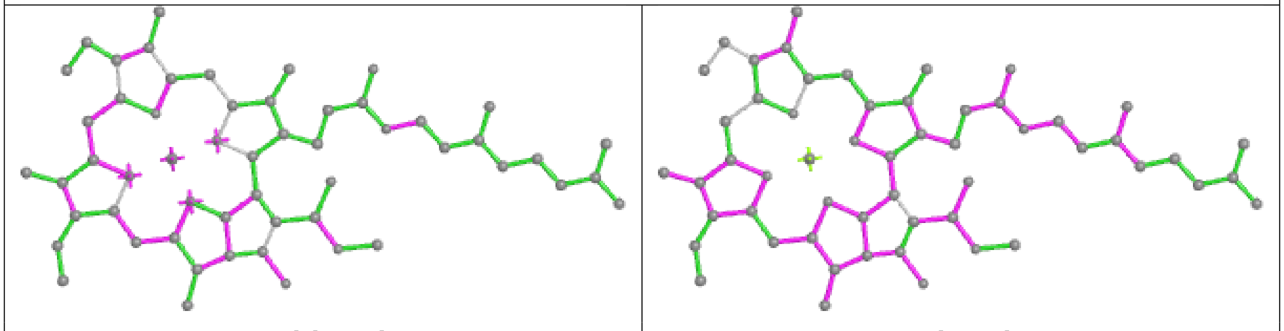
Bond angles



Torsions

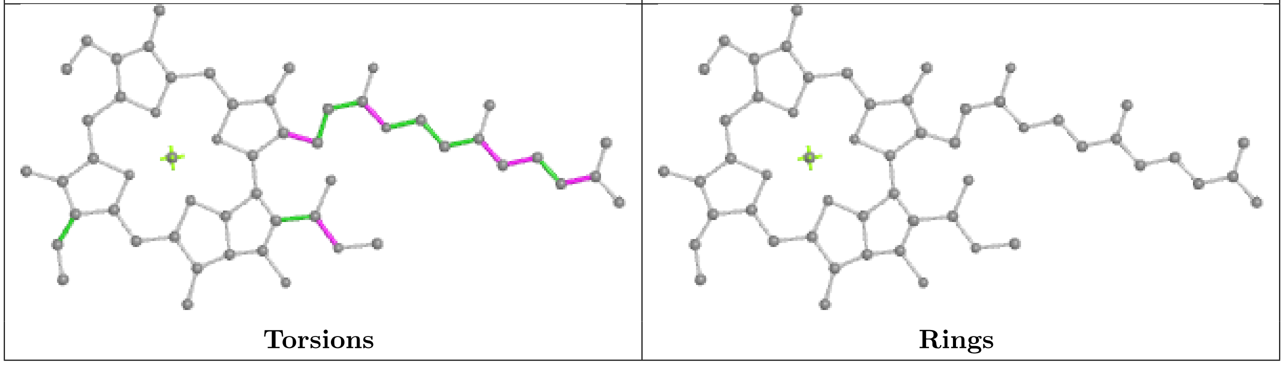
Rings

Ligand CLA a 1130



Bond lengths

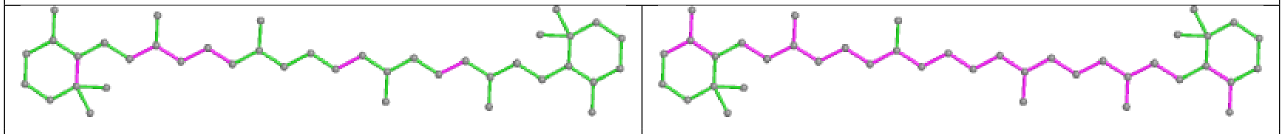
Bond angles



Torsions

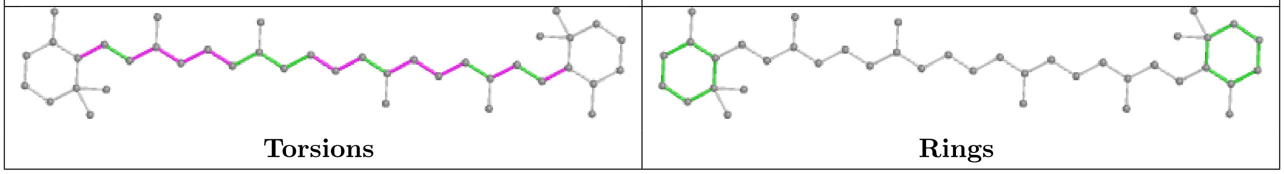
Rings

Ligand BCR V 4021



Bond lengths

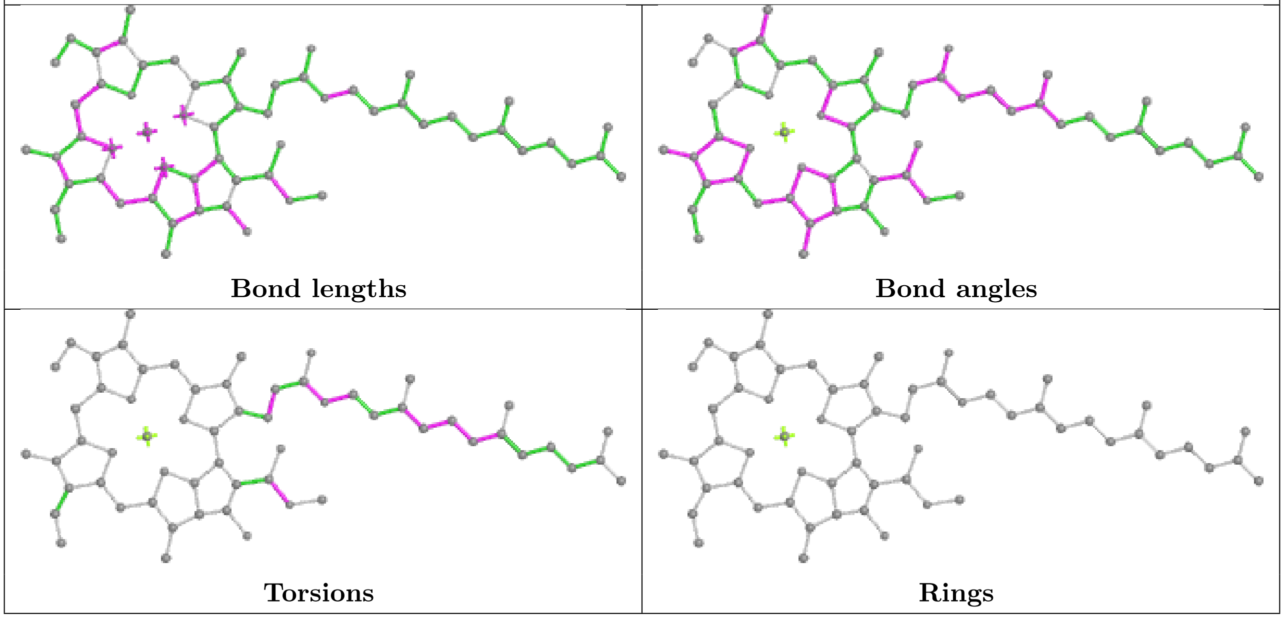
Bond angles



Torsions

Rings

Ligand CLA A 1131



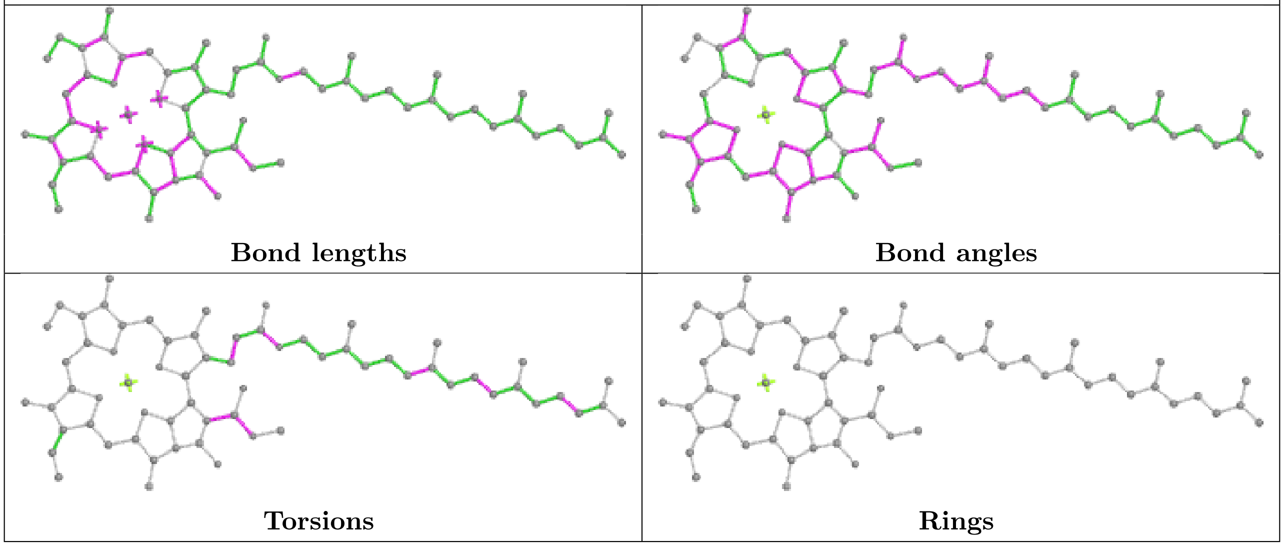
Bond lengths

Bond angles

Torsions

Rings

Ligand CLA a 1104



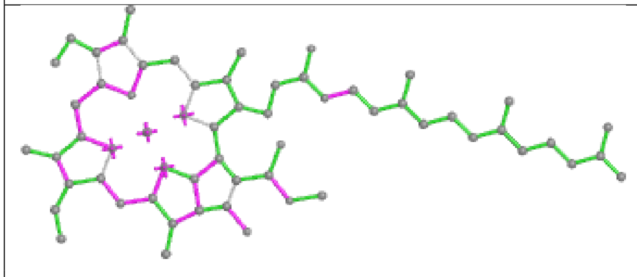
Bond lengths

Bond angles

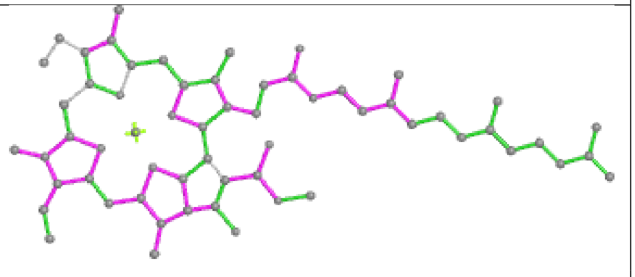
Torsions

Rings

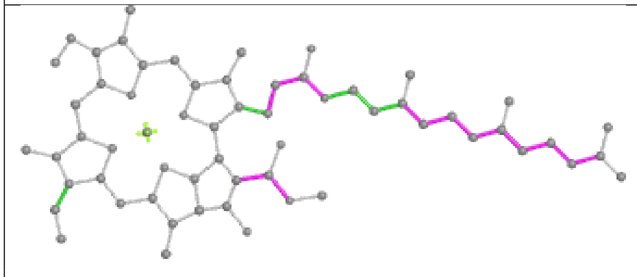
Ligand CLA G 1126



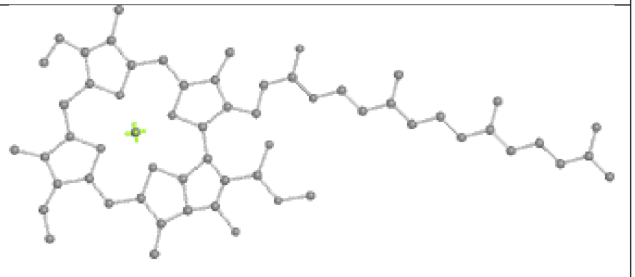
Bond lengths



Bond angles

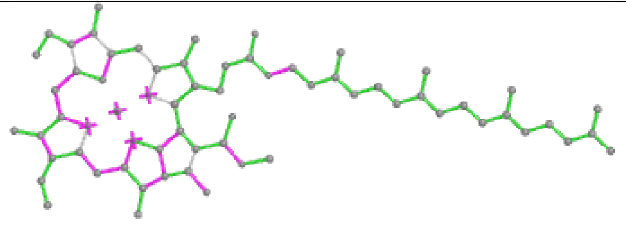


Torsions

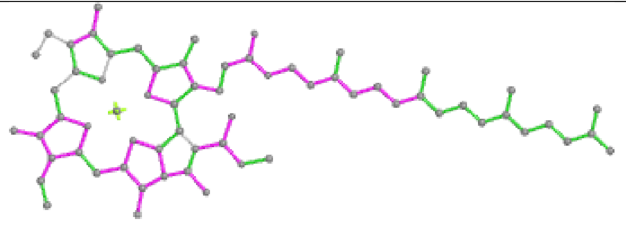


Rings

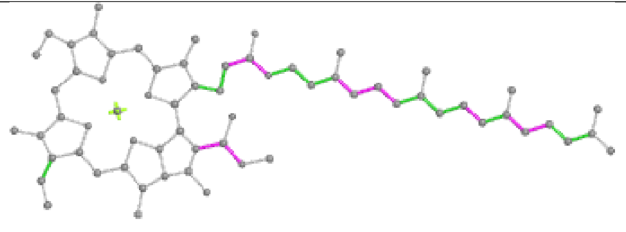
Ligand CLA B 1204



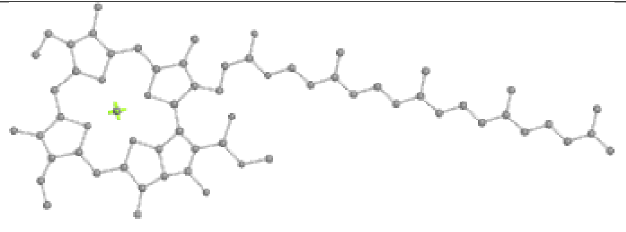
Bond lengths



Bond angles

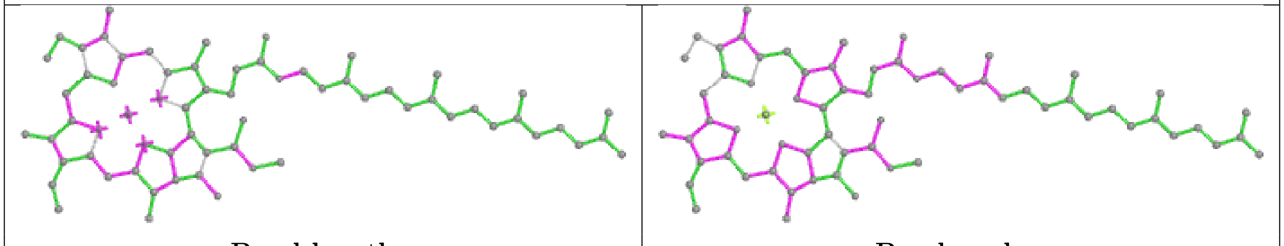


Torsions



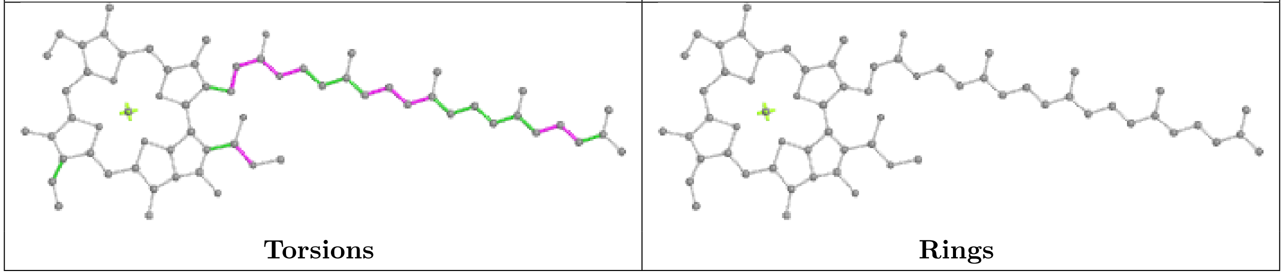
Rings

Ligand CLA B 1226



Bond lengths

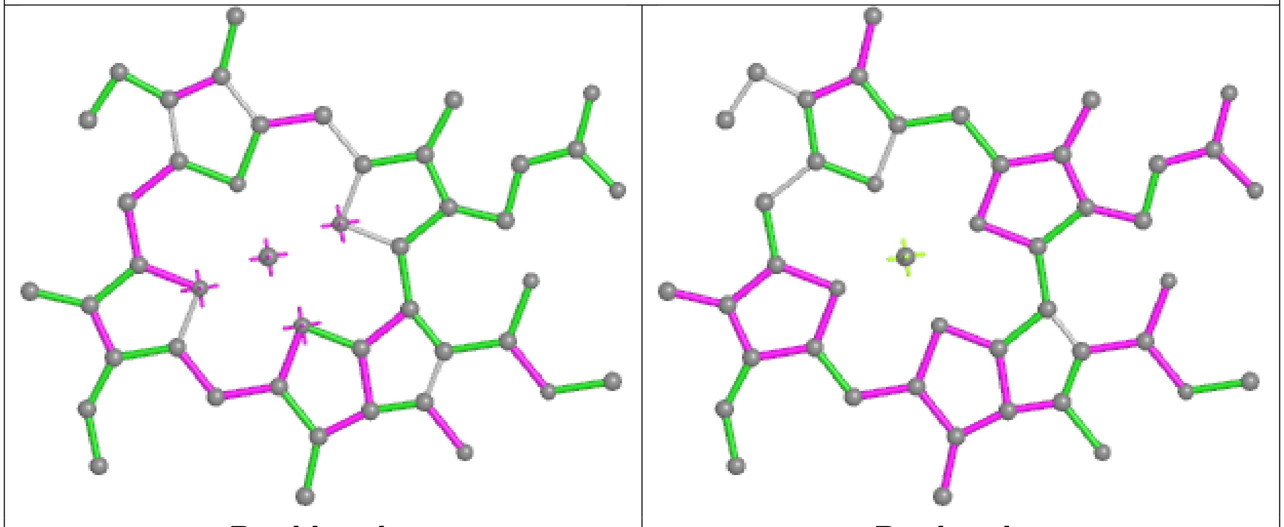
Bond angles



Torsions

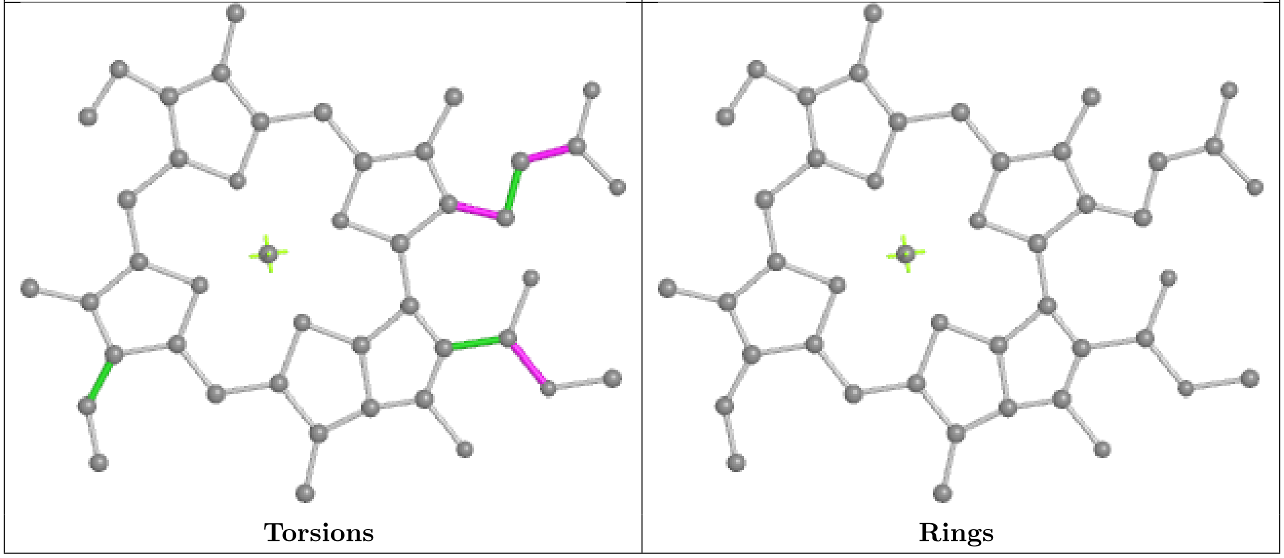
Rings

Ligand CLA A 1110



Bond lengths

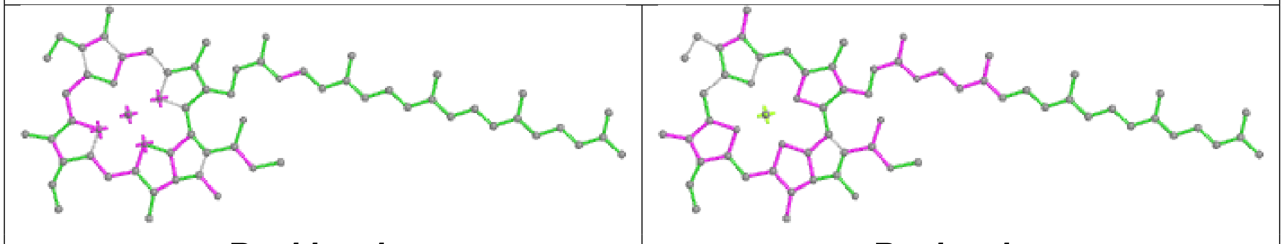
Bond angles



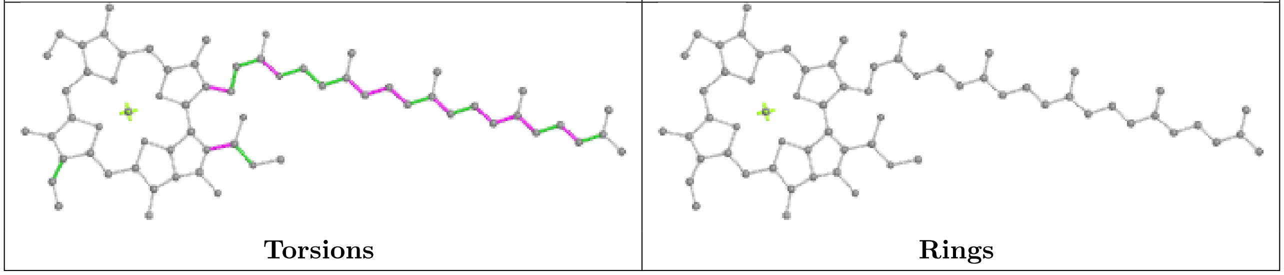
Torsions

Rings

Ligand CLA B 1203

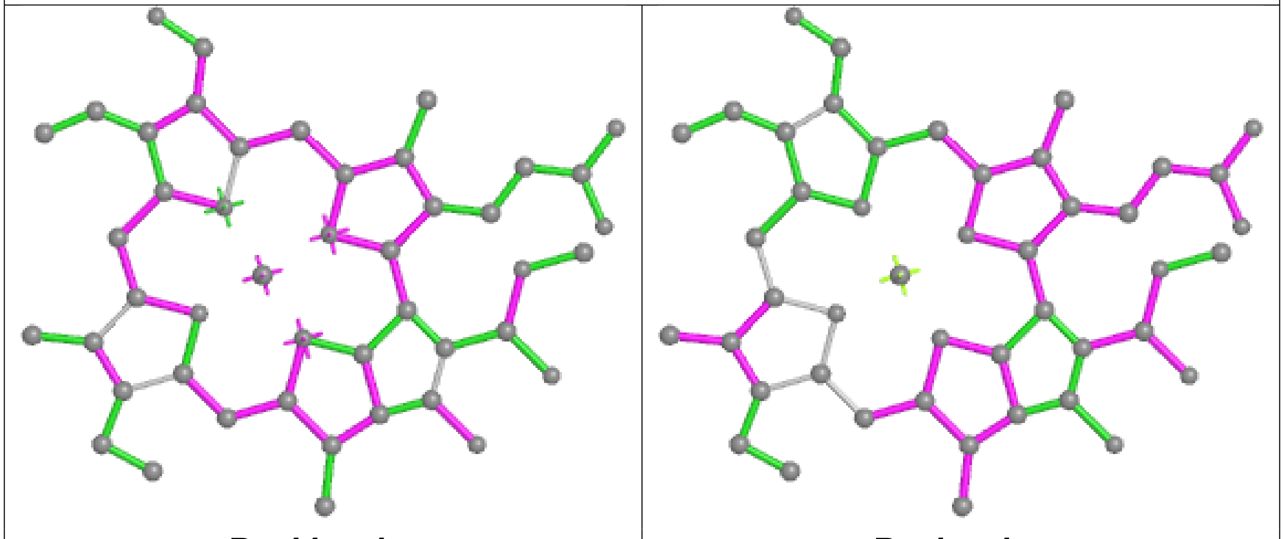


Bond lengths Bond angles

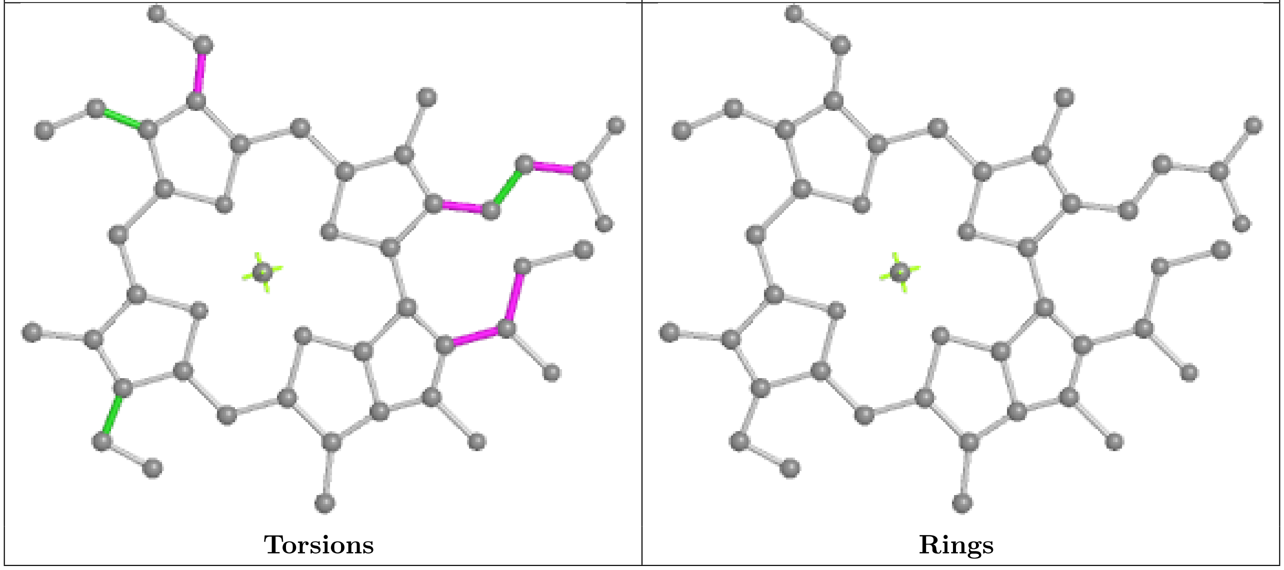


Torsions Rings

Ligand F6C b 1230

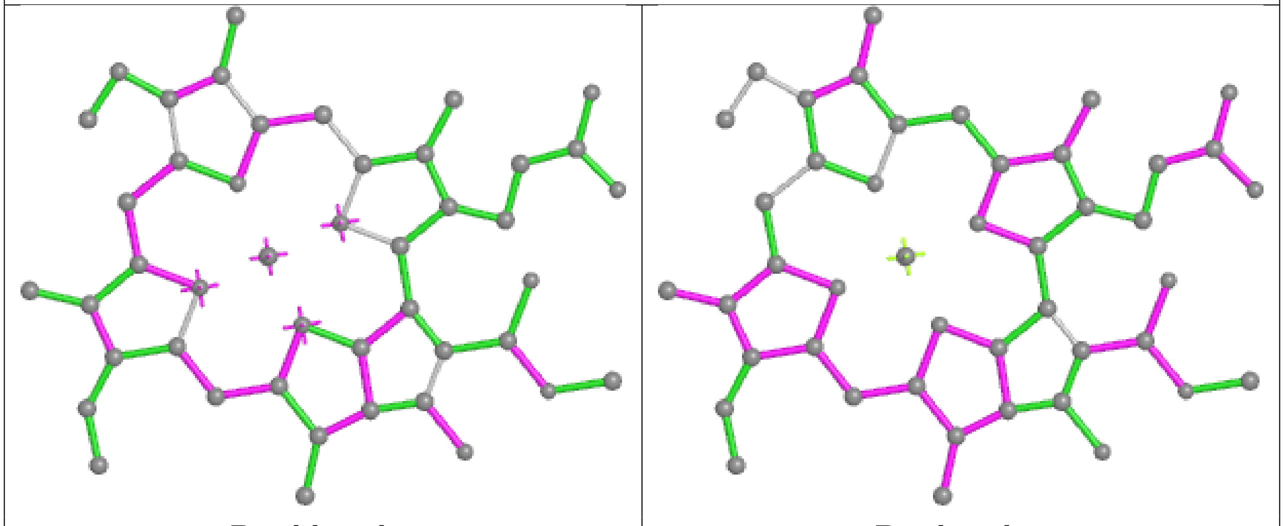


Bond lengths Bond angles

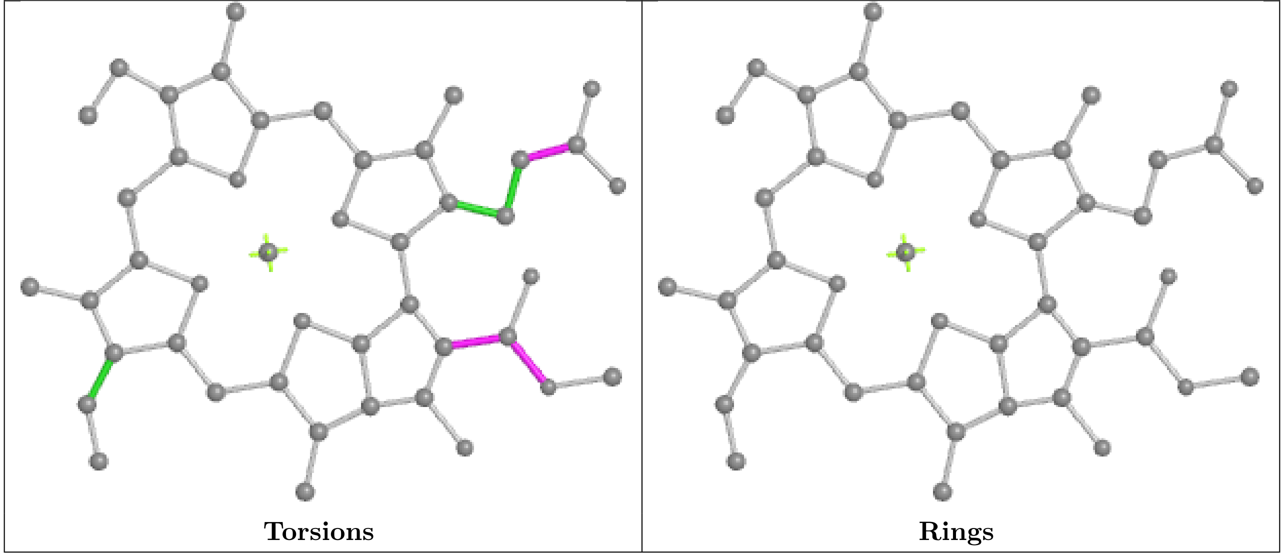


Torsions Rings

Ligand CLA b 1218

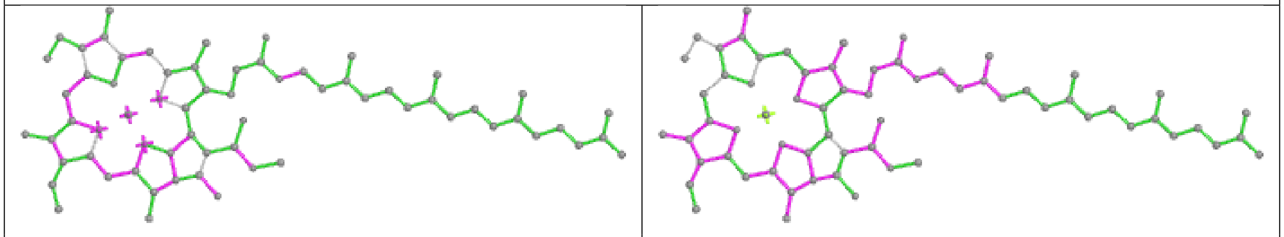


Bond lengths Bond angles

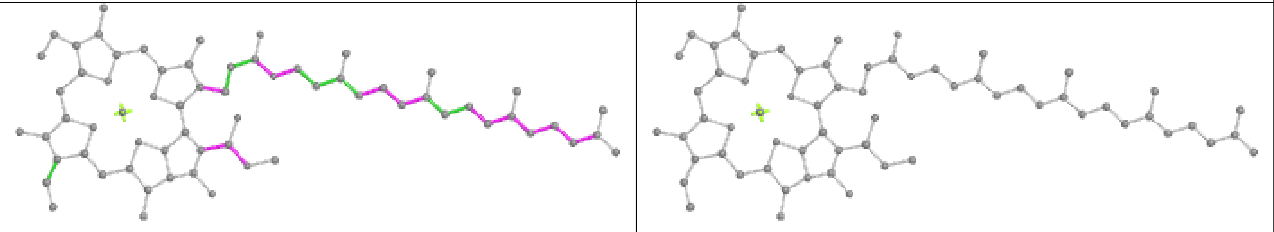


Torsions Rings

Ligand CLA A 1115

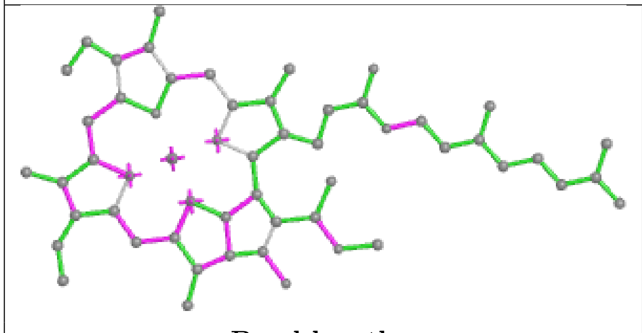


Bond lengths Bond angles

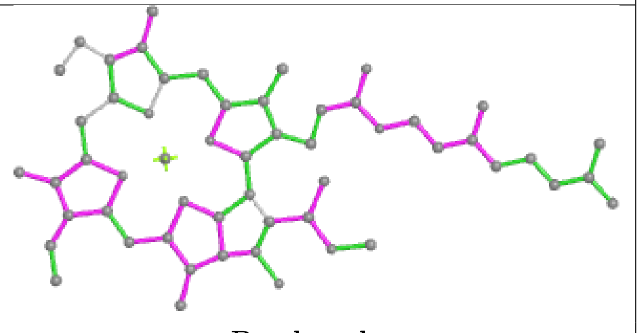


Torsions Rings

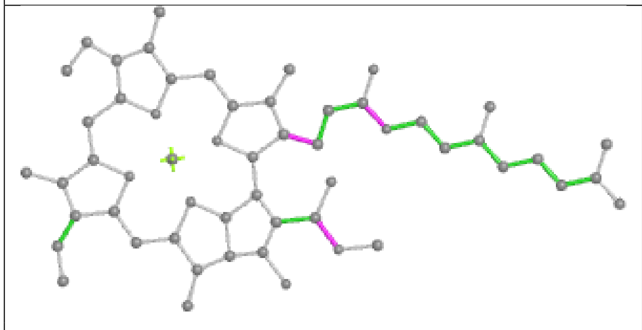
Ligand CLA b 1231



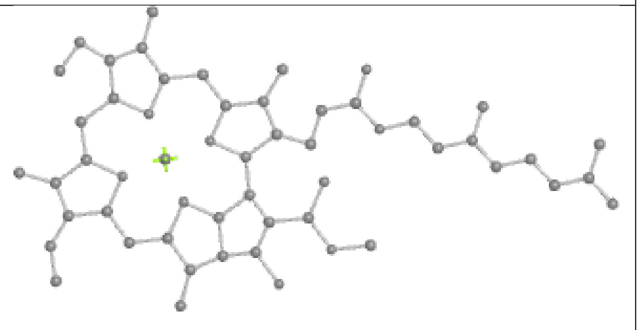
Bond lengths



Bond angles

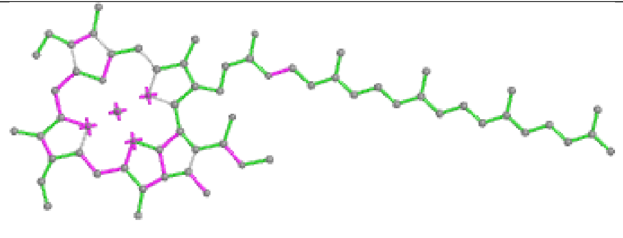


Torsions

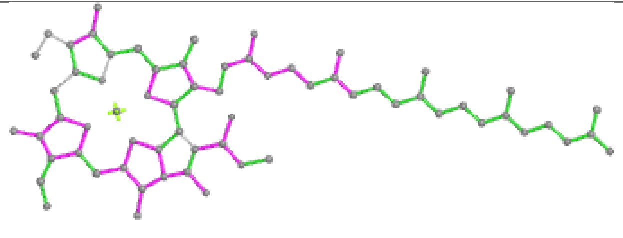


Rings

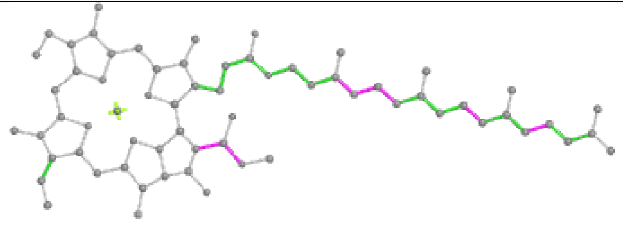
Ligand CLA B 1205



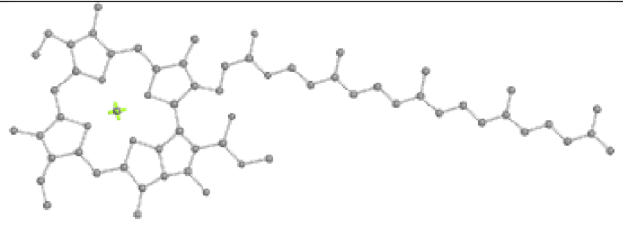
Bond lengths



Bond angles

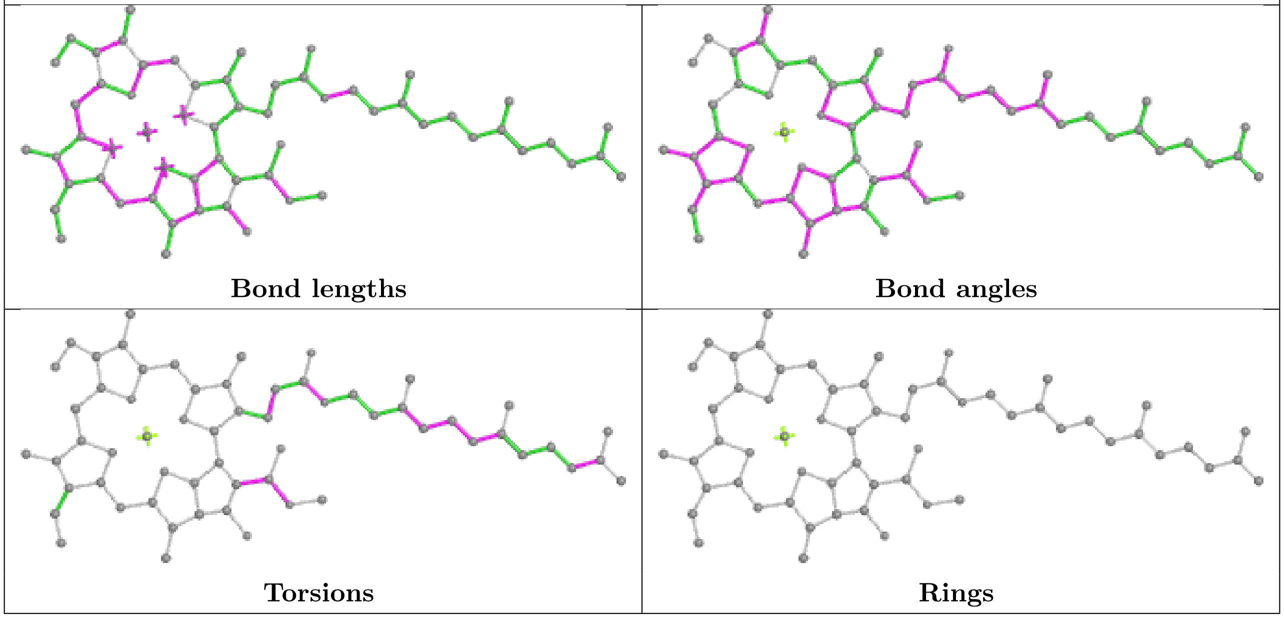


Torsions



Rings

Ligand CLA G 1111



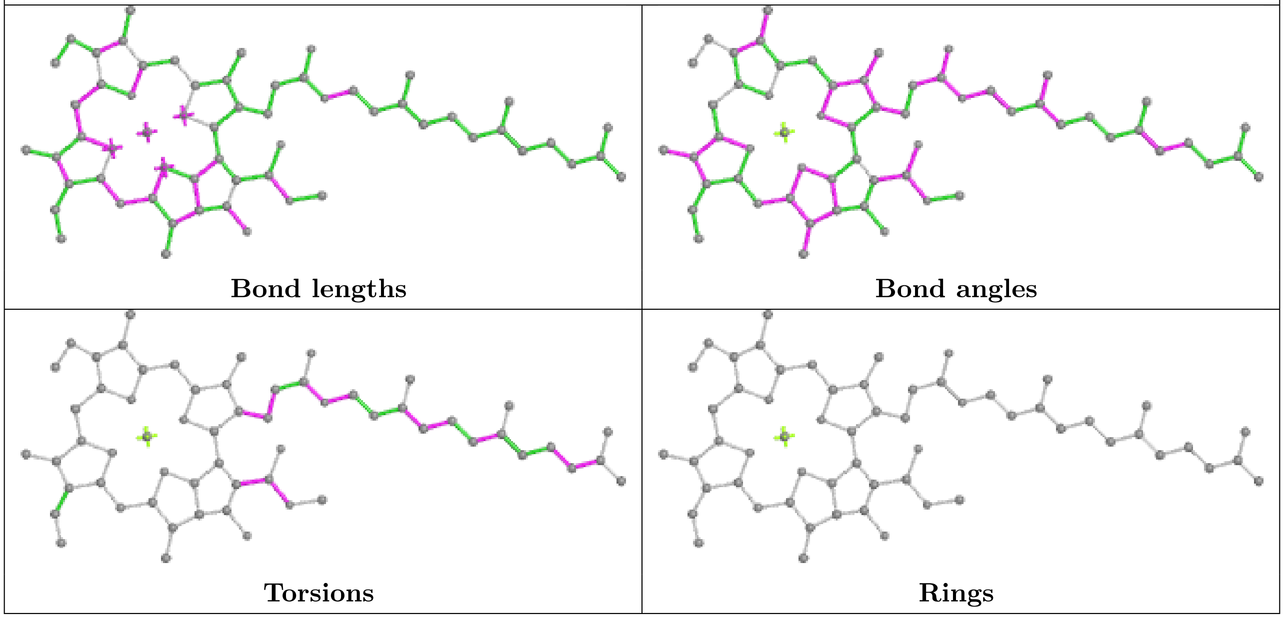
Bond lengths

Bond angles

Torsions

Rings

Ligand CLA B 1215



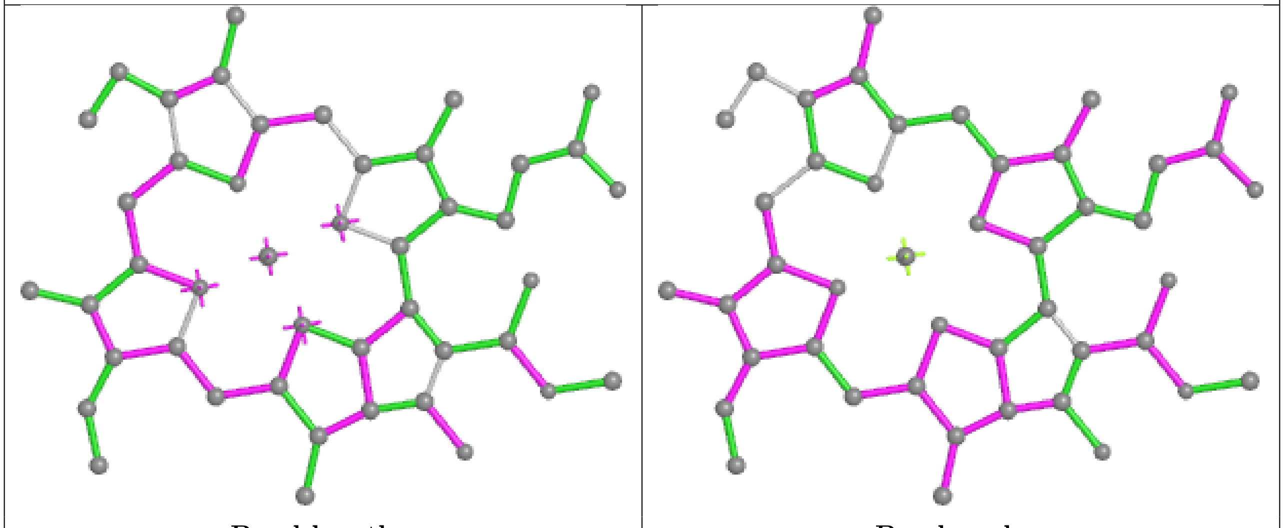
Bond lengths

Bond angles

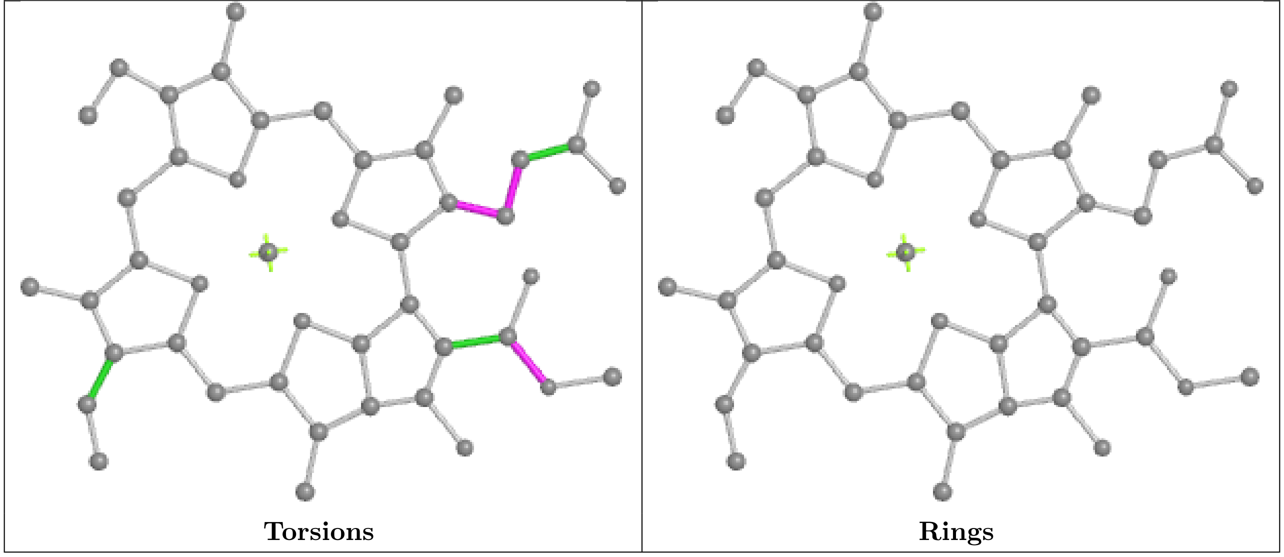
Torsions

Rings

Ligand CLA H 1227

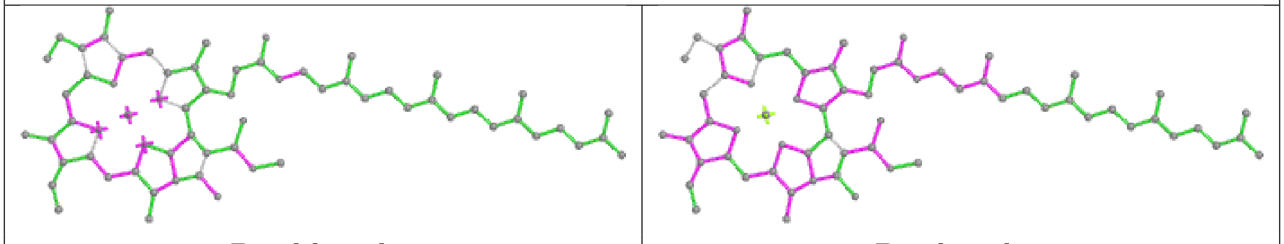


Bond lengths Bond angles

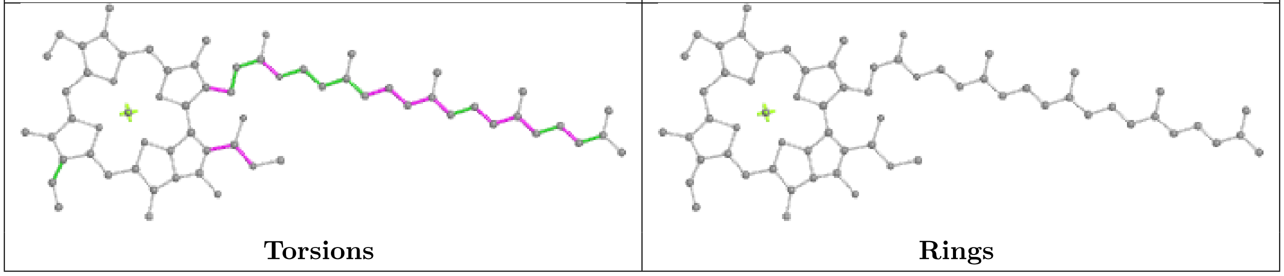


Torsions Rings

Ligand CLA a 1117

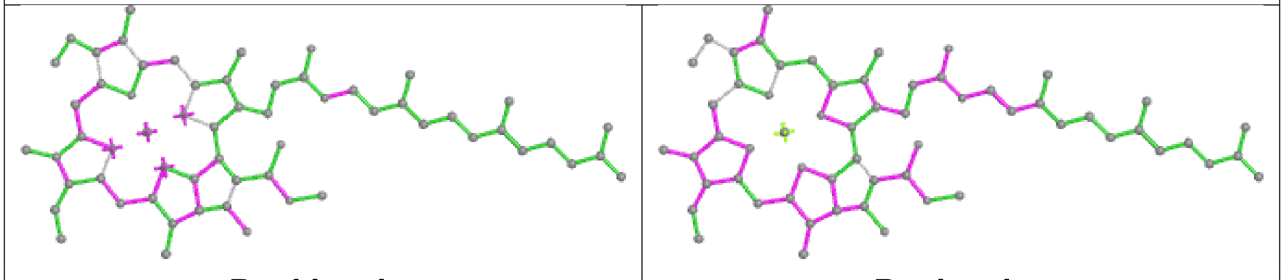


Bond lengths Bond angles



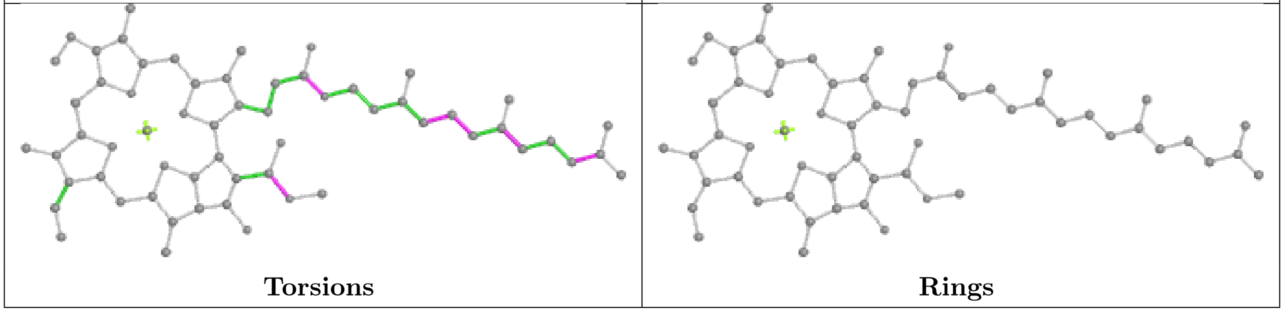
Torsions Rings

Ligand CLA A 1133



Bond lengths

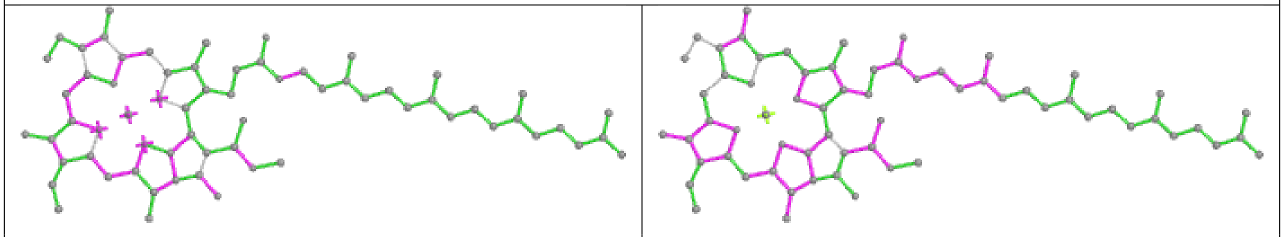
Bond angles



Torsions

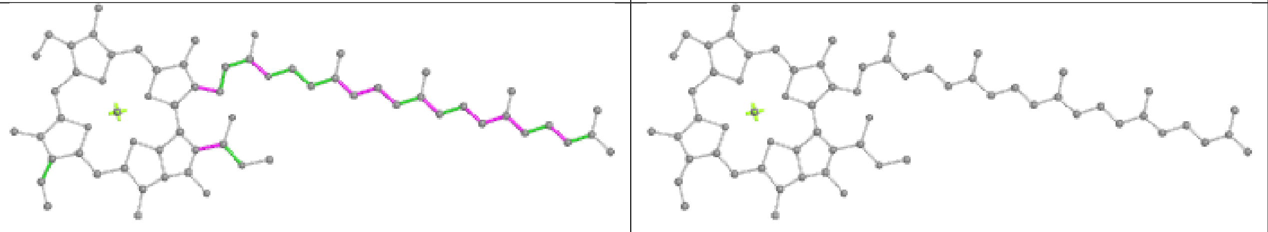
Rings

Ligand CLA H 1203



Bond lengths

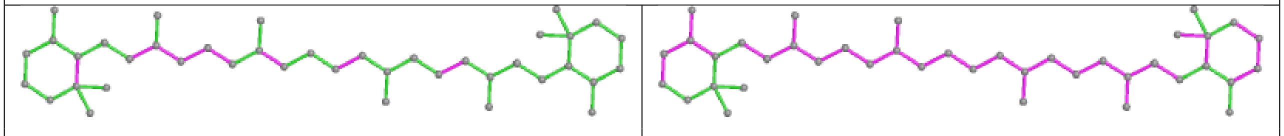
Bond angles



Torsions

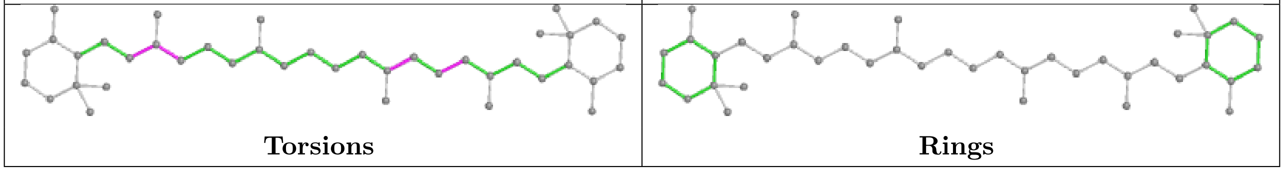
Rings

Ligand BCR b 4014



Bond lengths

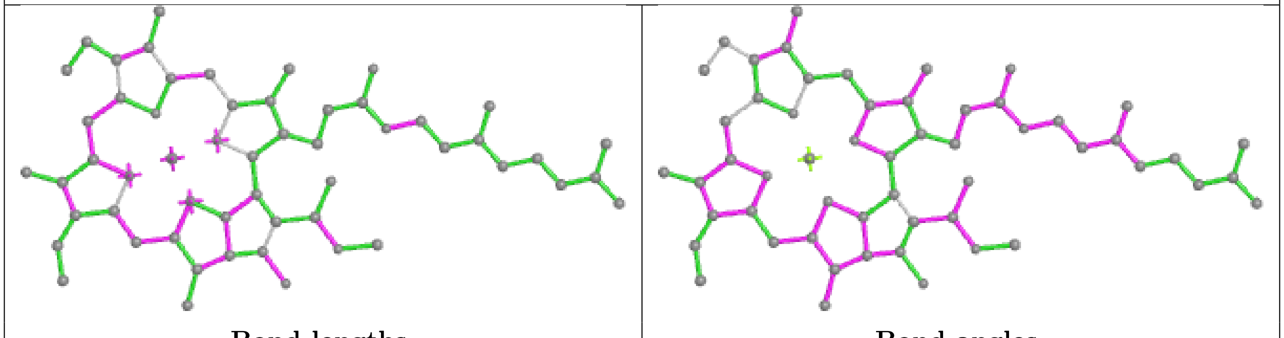
Bond angles



Torsions

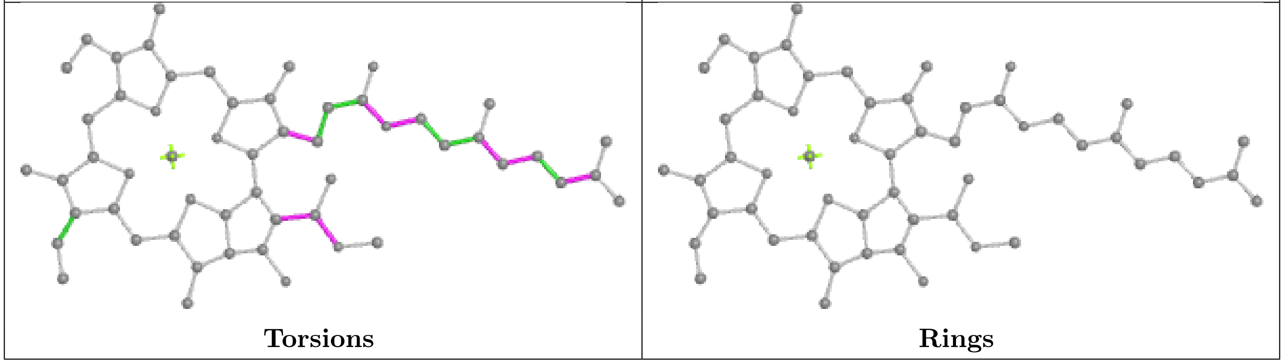
Rings

Ligand CLA G 1112



Bond lengths

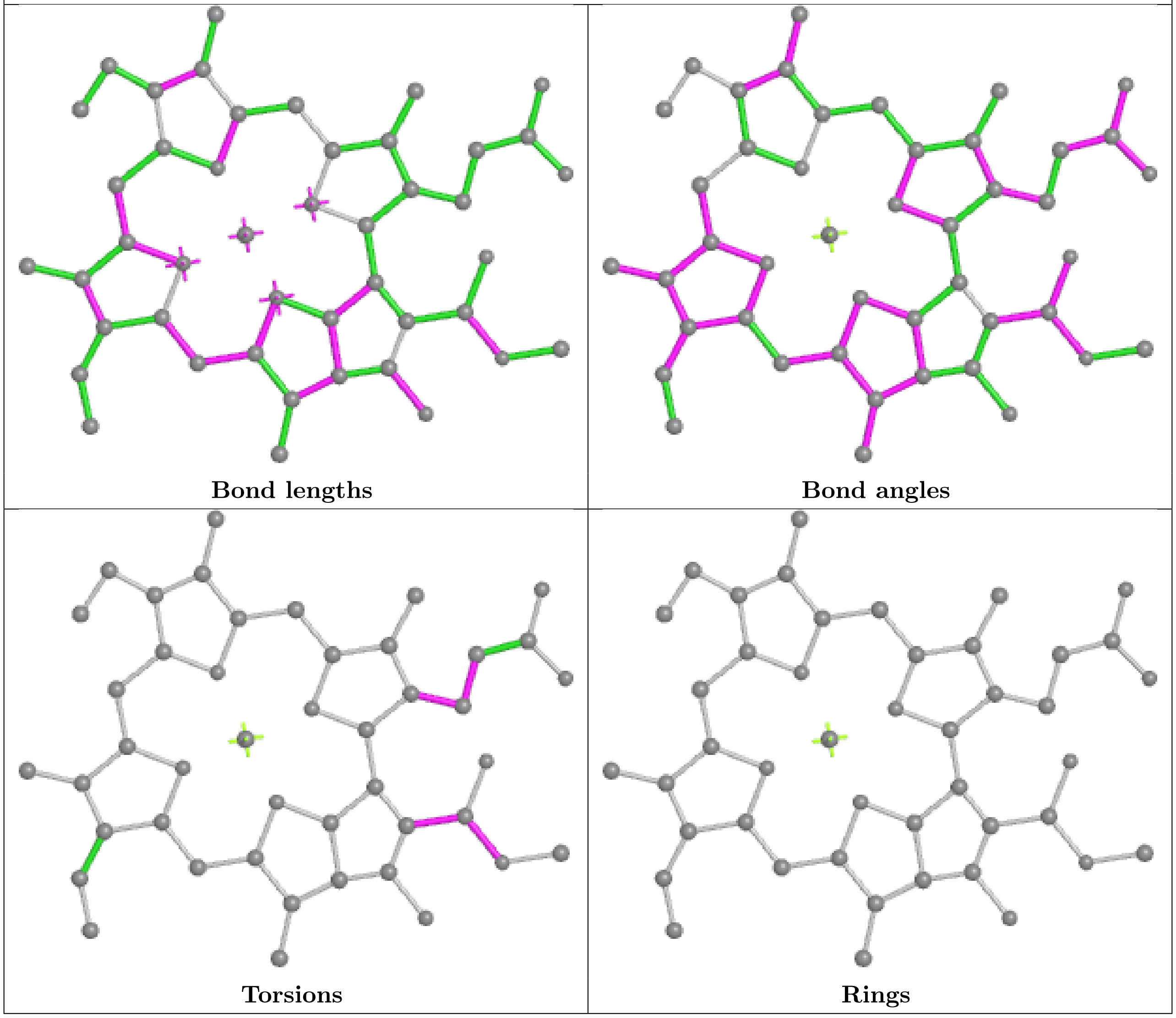
Bond angles



Torsions

Rings

Ligand CLA B 1206



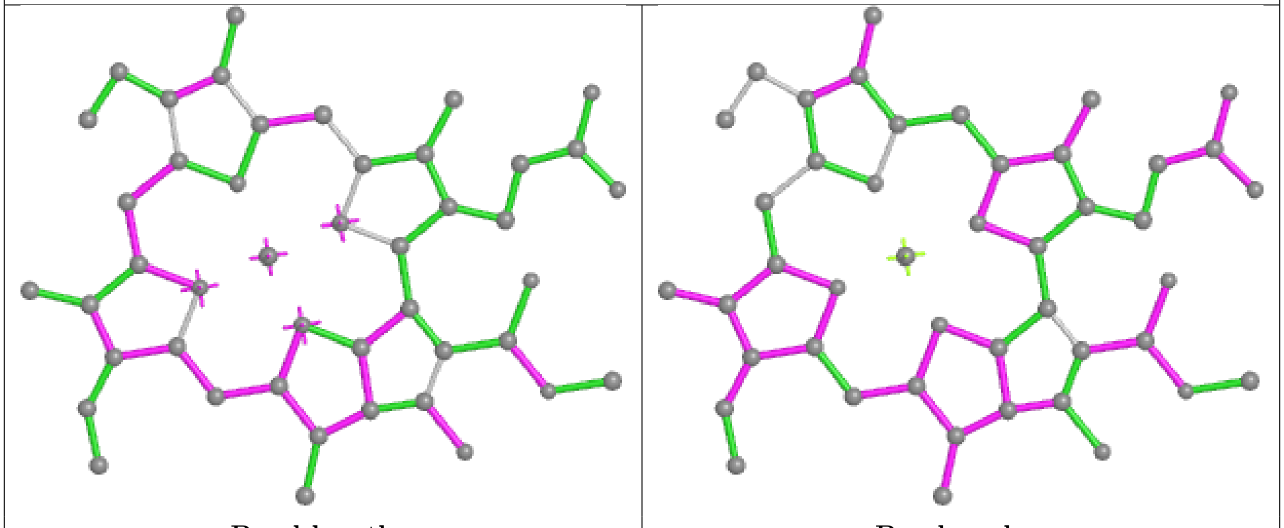
Bond lengths

Bond angles

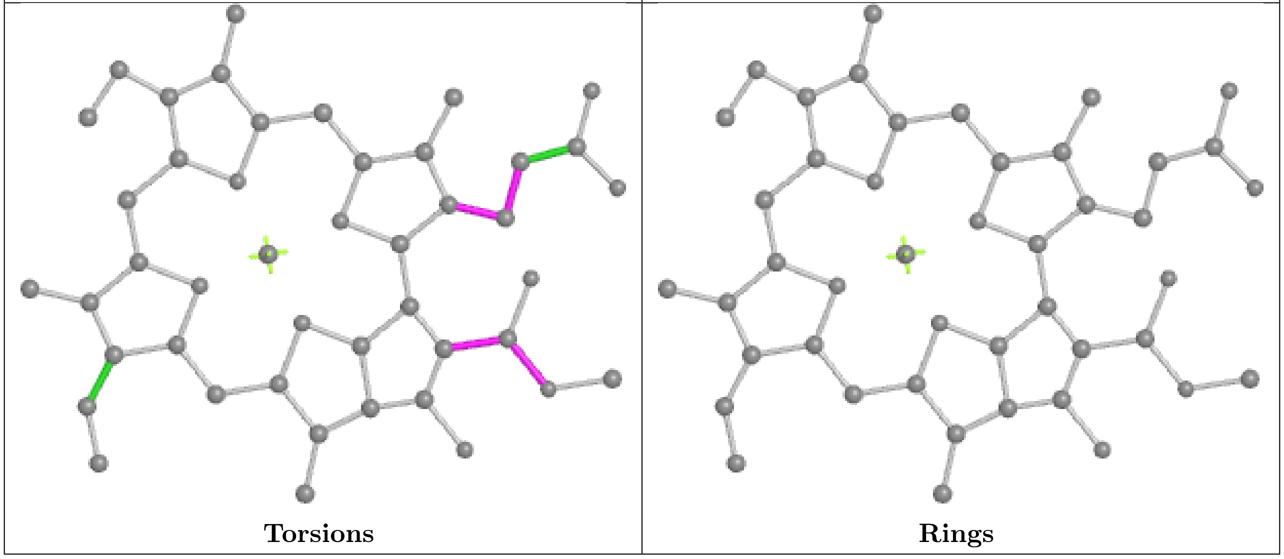
Torsions

Rings

Ligand CLA K 1401

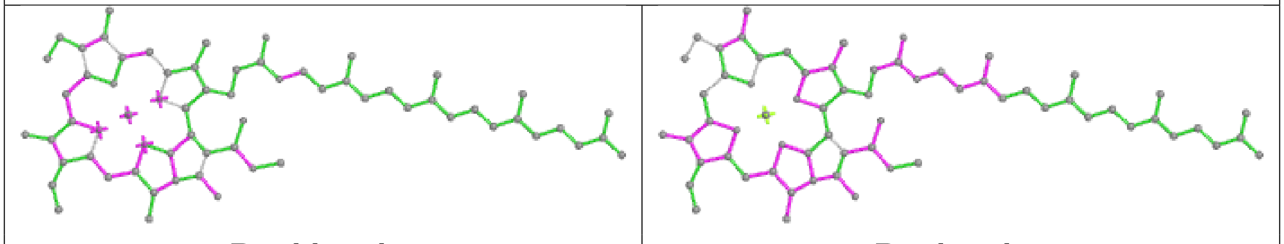


Bond lengths **Bond angles**

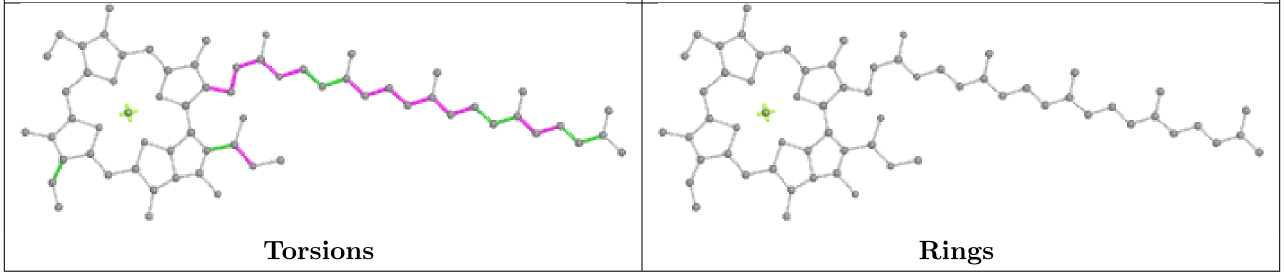


Torsions **Rings**

Ligand CLA a 1140

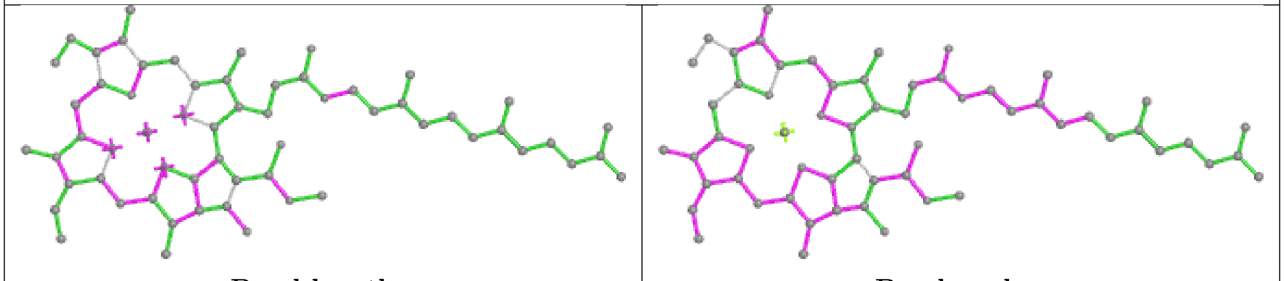


Bond lengths **Bond angles**

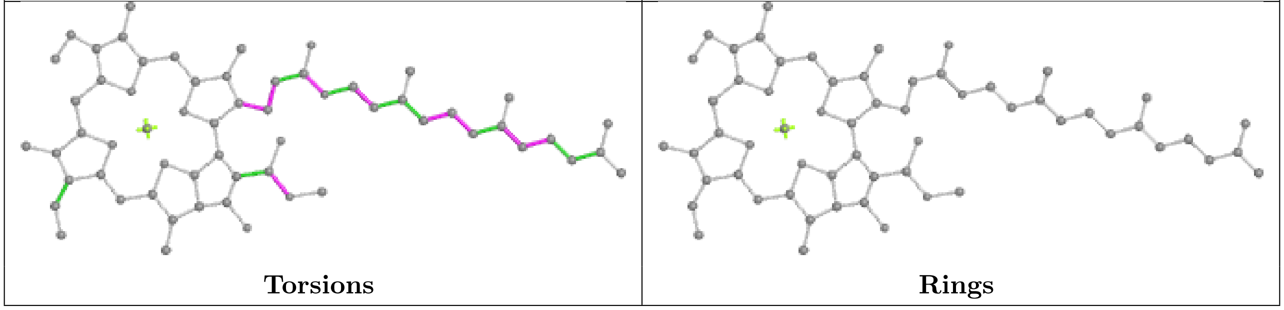


Torsions **Rings**

Ligand CLA A 1013

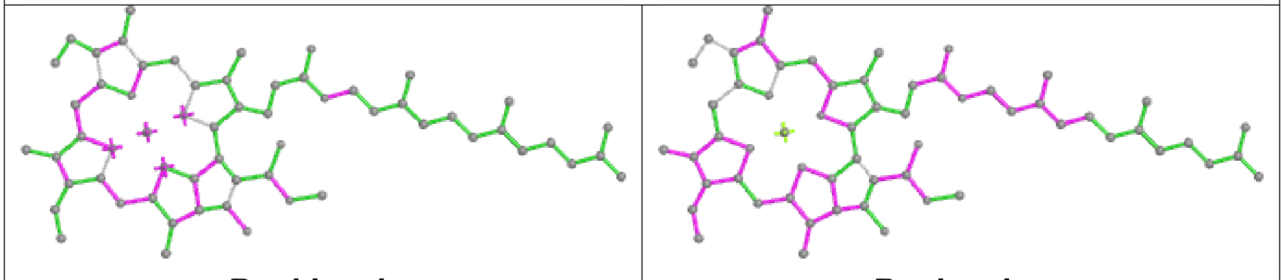


Bond lengths **Bond angles**

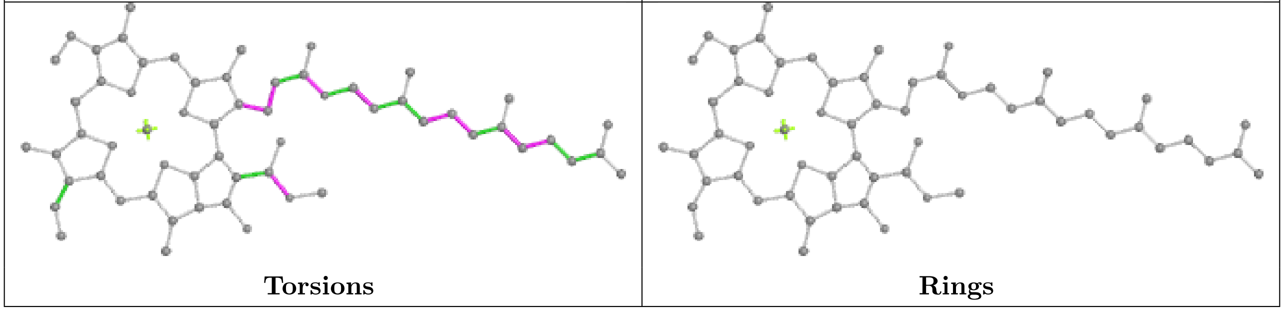


Torsions **Rings**

Ligand CLA G 1013

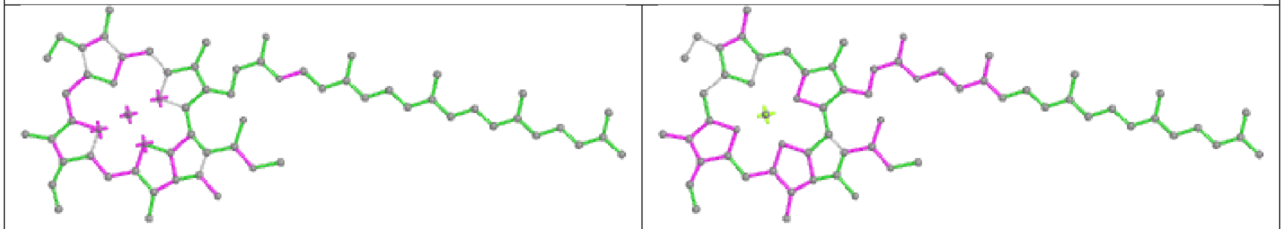


Bond lengths **Bond angles**



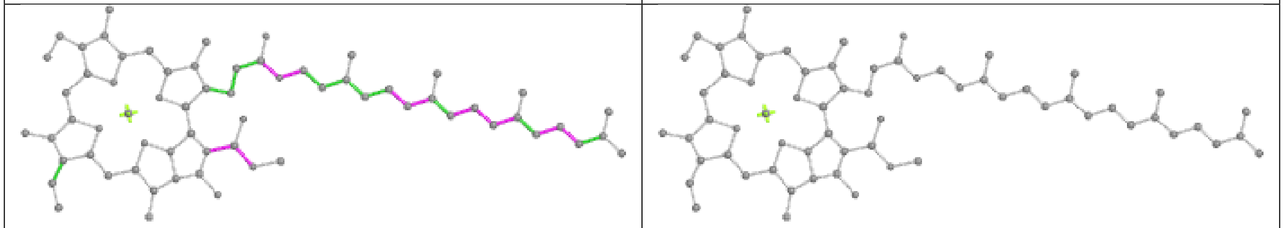
Torsions **Rings**

Ligand CLA b 1234



Bond lengths

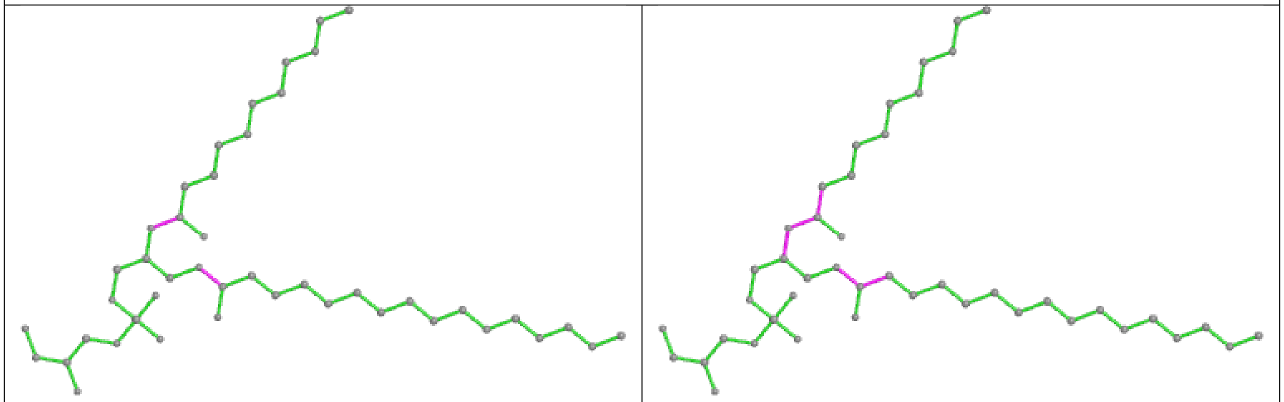
Bond angles



Torsions

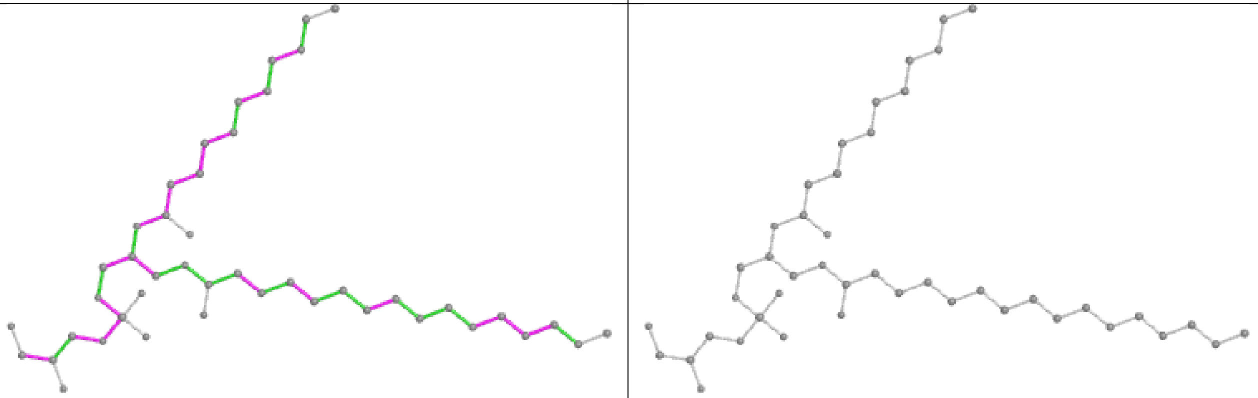
Rings

Ligand LHG H 5004



Bond lengths

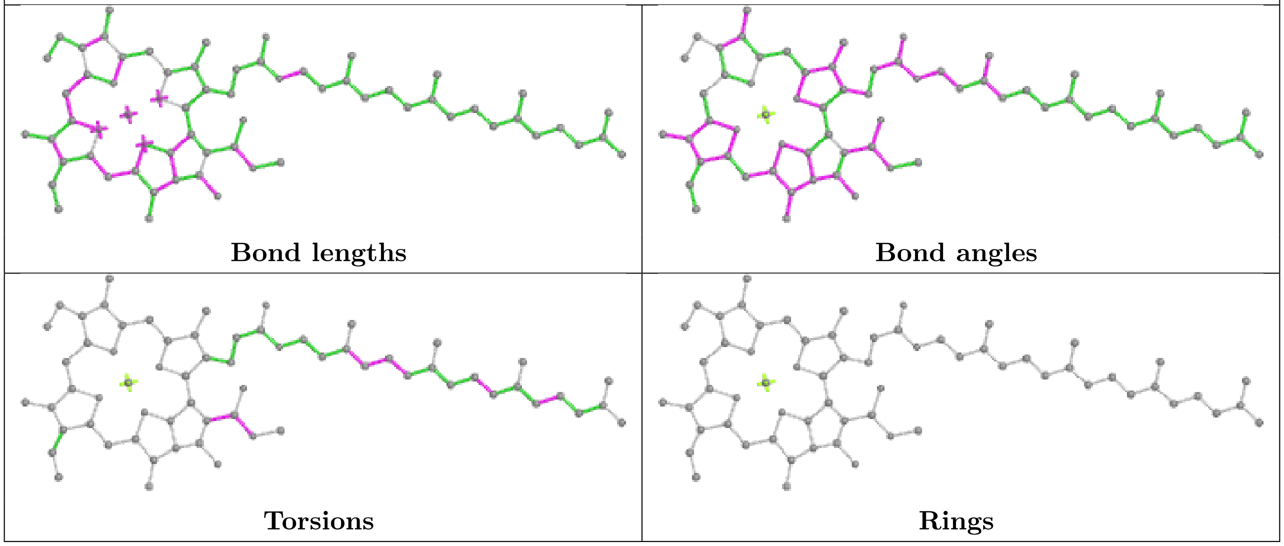
Bond angles



Torsions

Rings

Ligand CLA b 1205



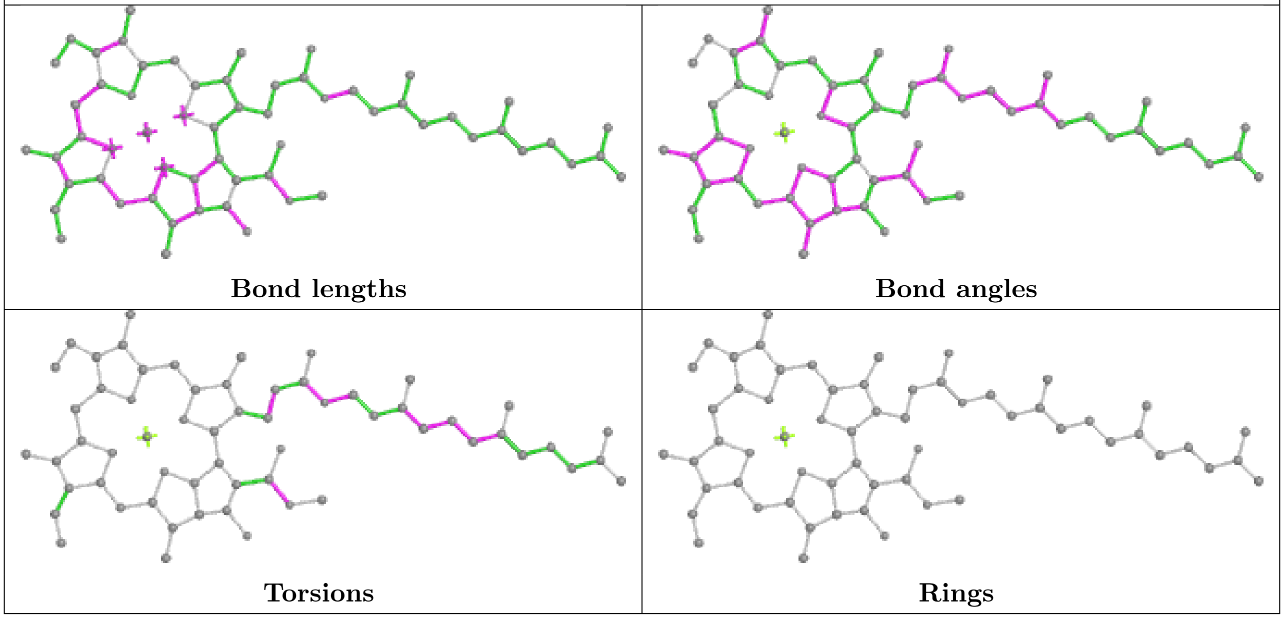
Bond lengths

Bond angles

Torsions

Rings

Ligand CLA G 1131



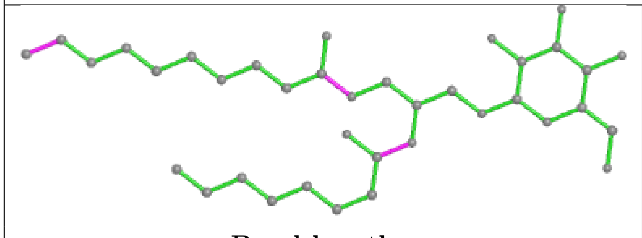
Bond lengths

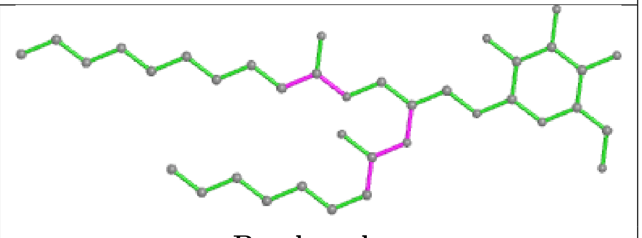
Bond angles

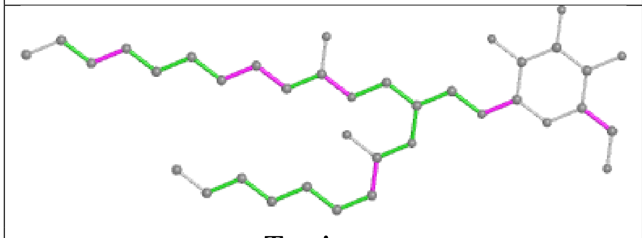
Torsions

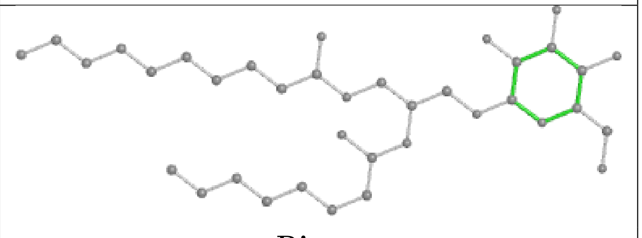
Rings

Ligand LMG I 5006

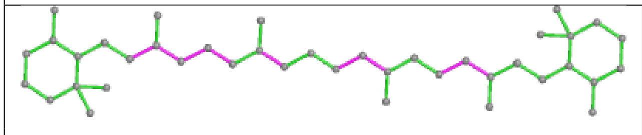

Bond lengths

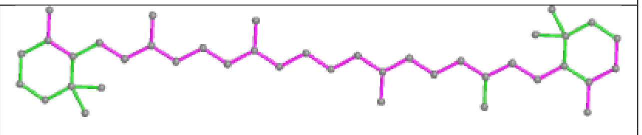

Bond angles

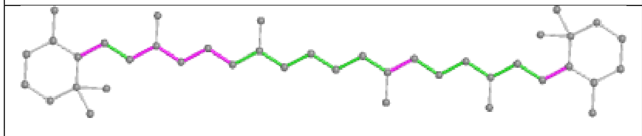

Torsions


Rings

Ligand BCR G 4008


Bond lengths


Bond angles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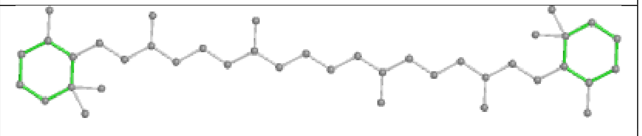
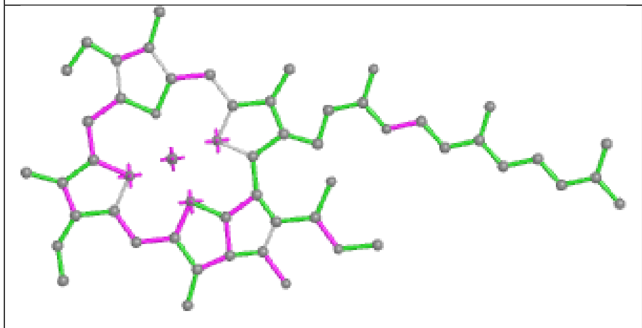
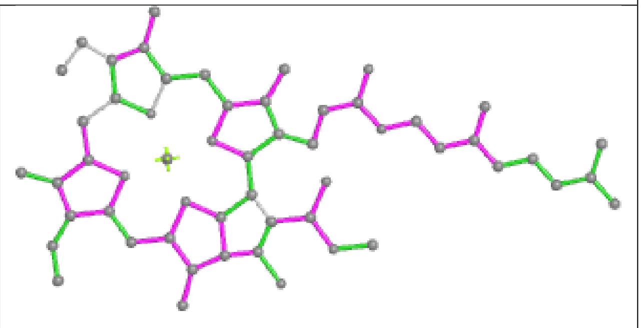
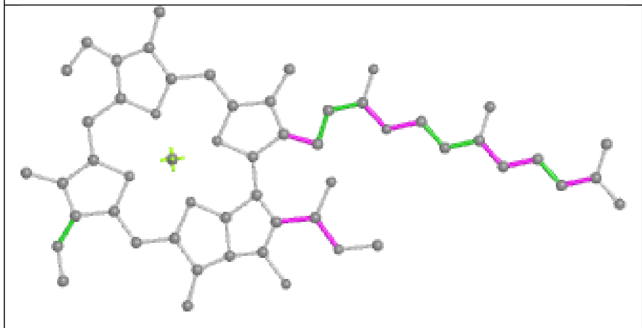

Rings

Ligand CLA A 1112


Bond lengths


Bond angles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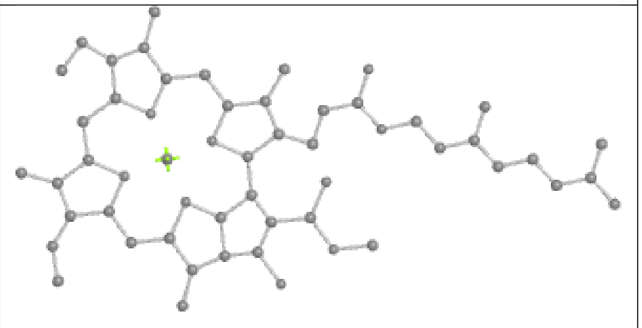
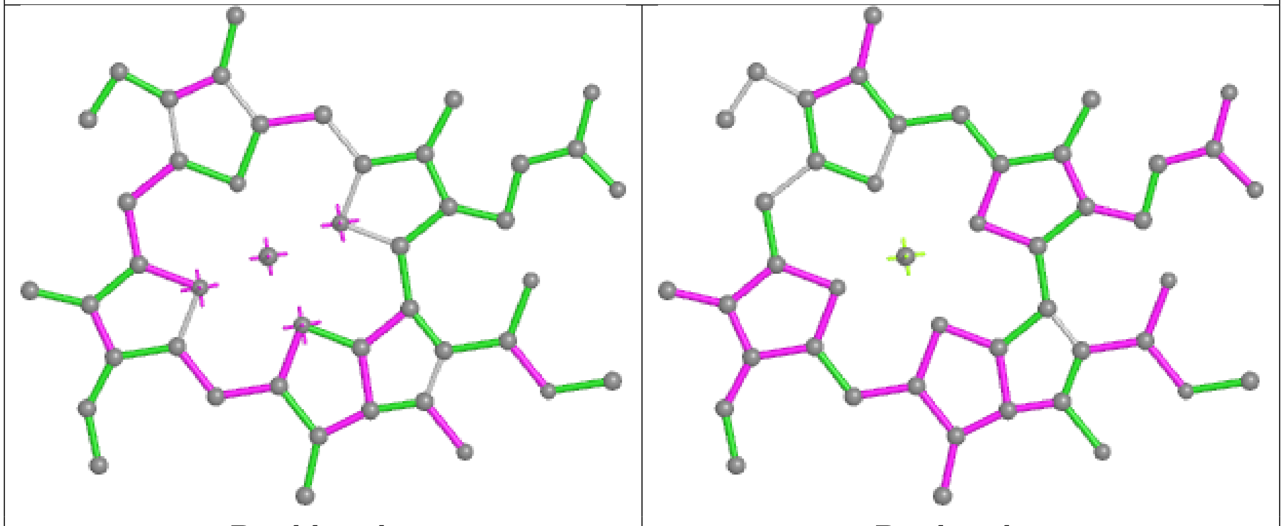
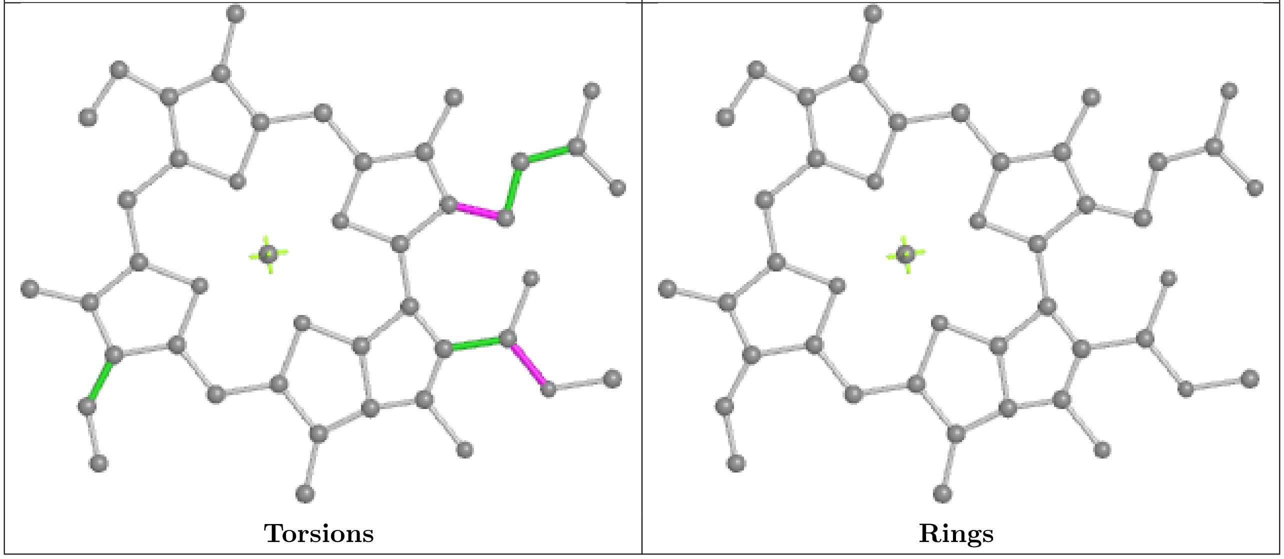

Rings

Ligand CLA A 1107

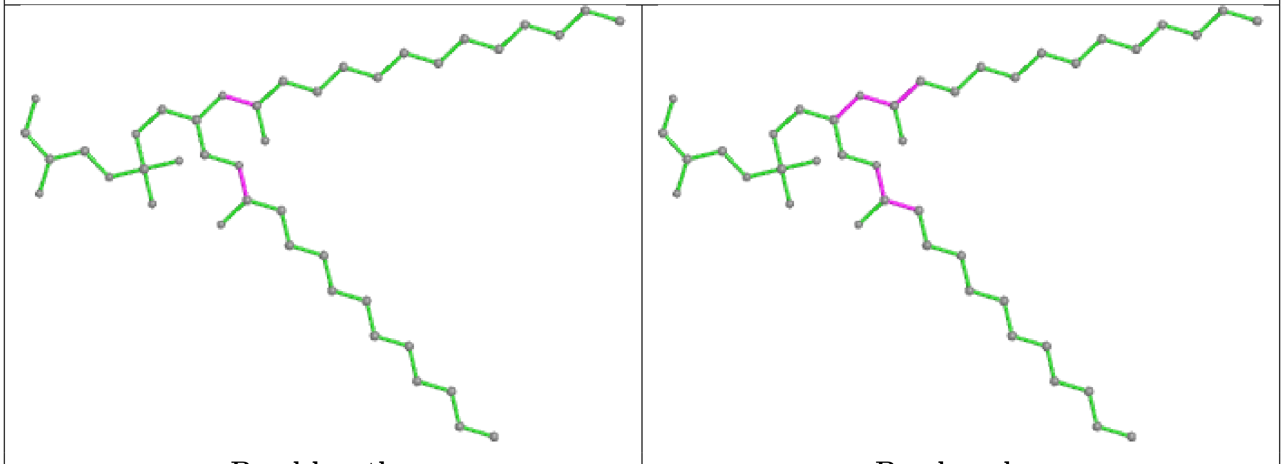


Bond lengths Bond angles

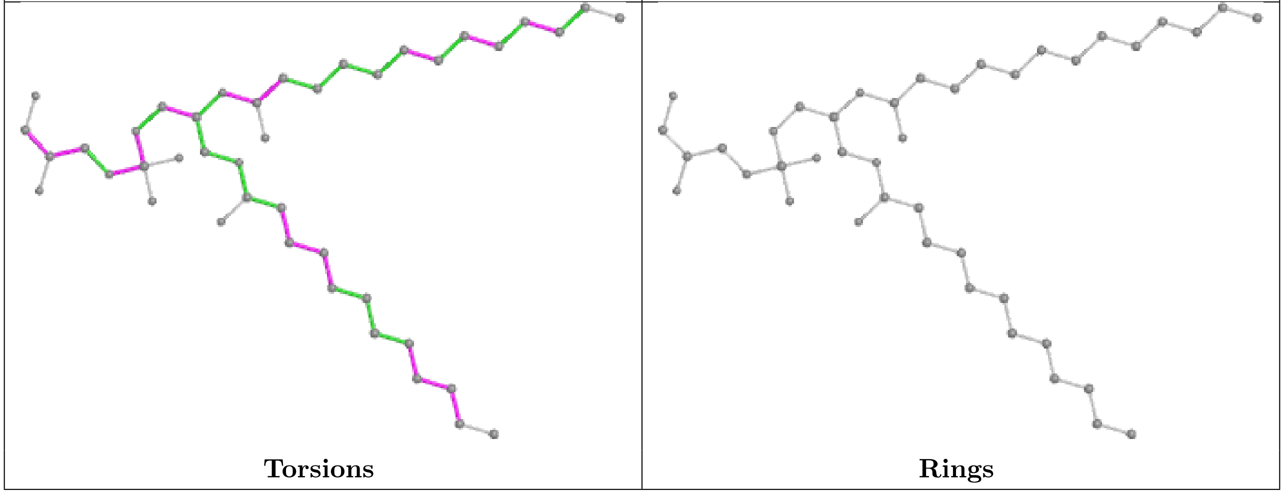


Torsions Rings

Ligand LHG A 5001

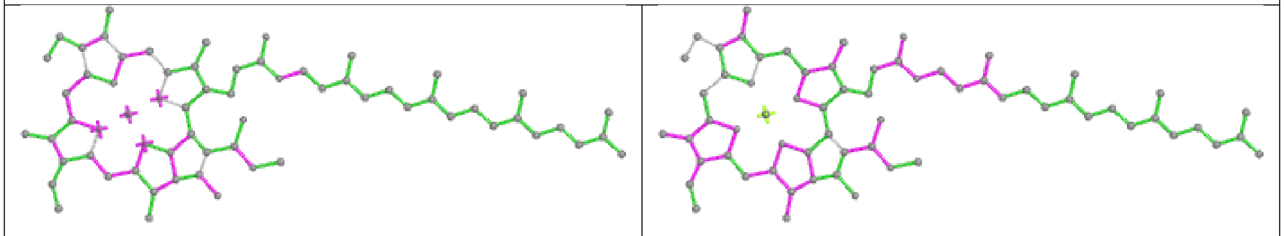


Bond lengths **Bond angles**

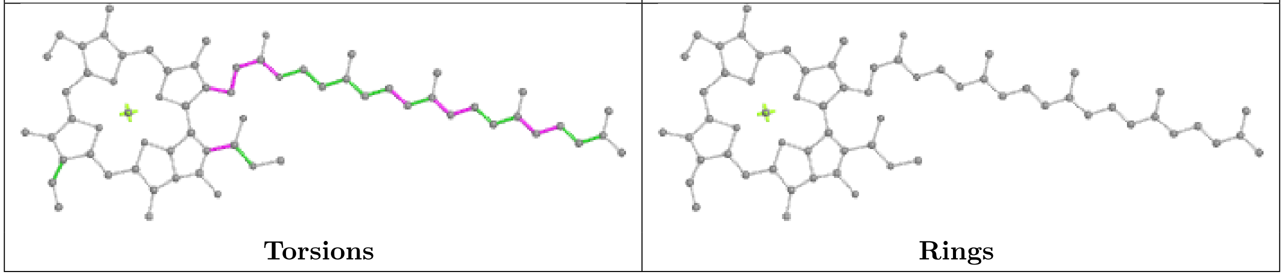


Torsions **Rings**

Ligand CLA a 1127

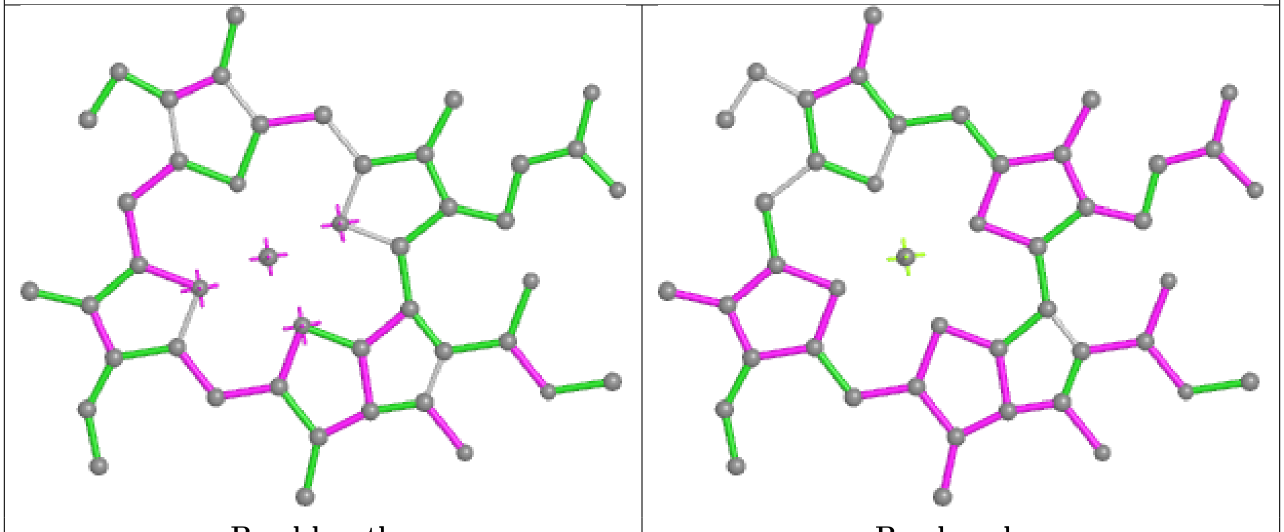


Bond lengths **Bond angles**

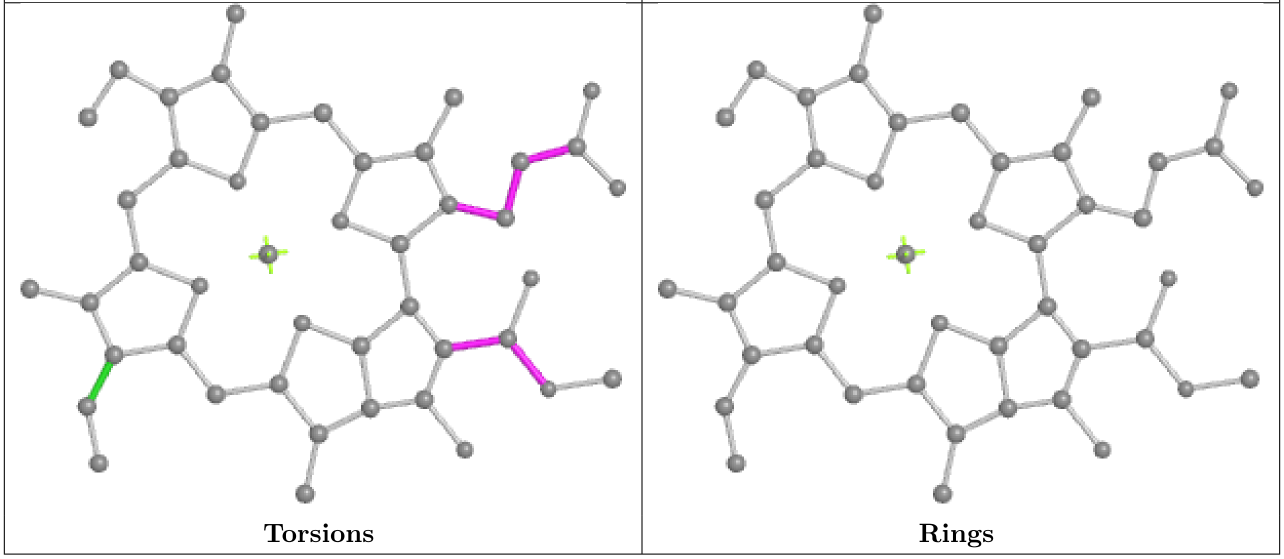


Torsions **Rings**

Ligand CLA a 1113

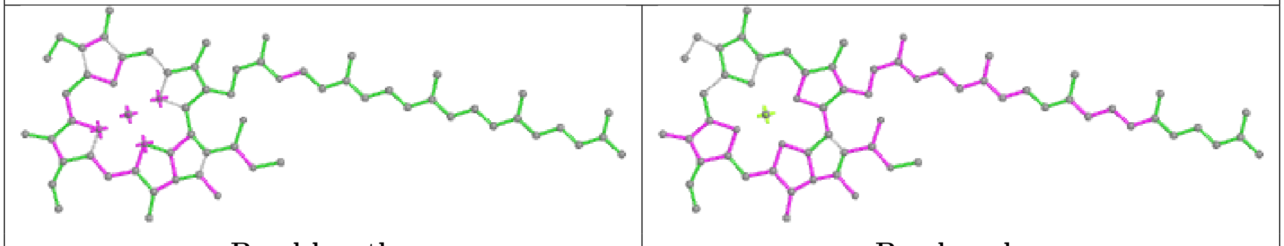


Bond lengths **Bond angles**

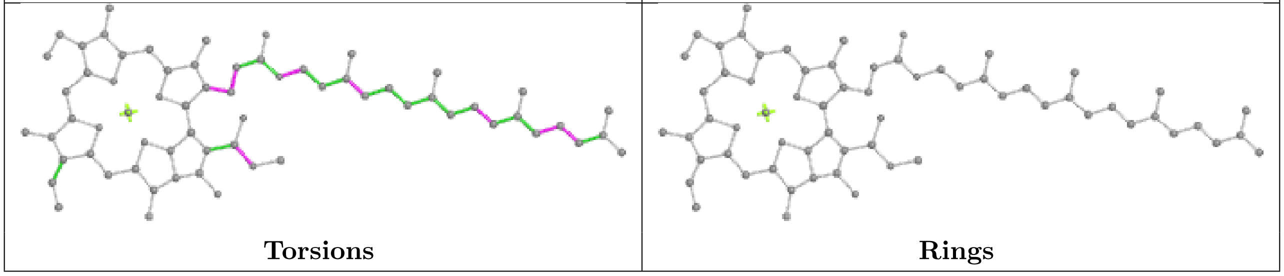


Torsions **Rings**

Ligand CLA A 1012

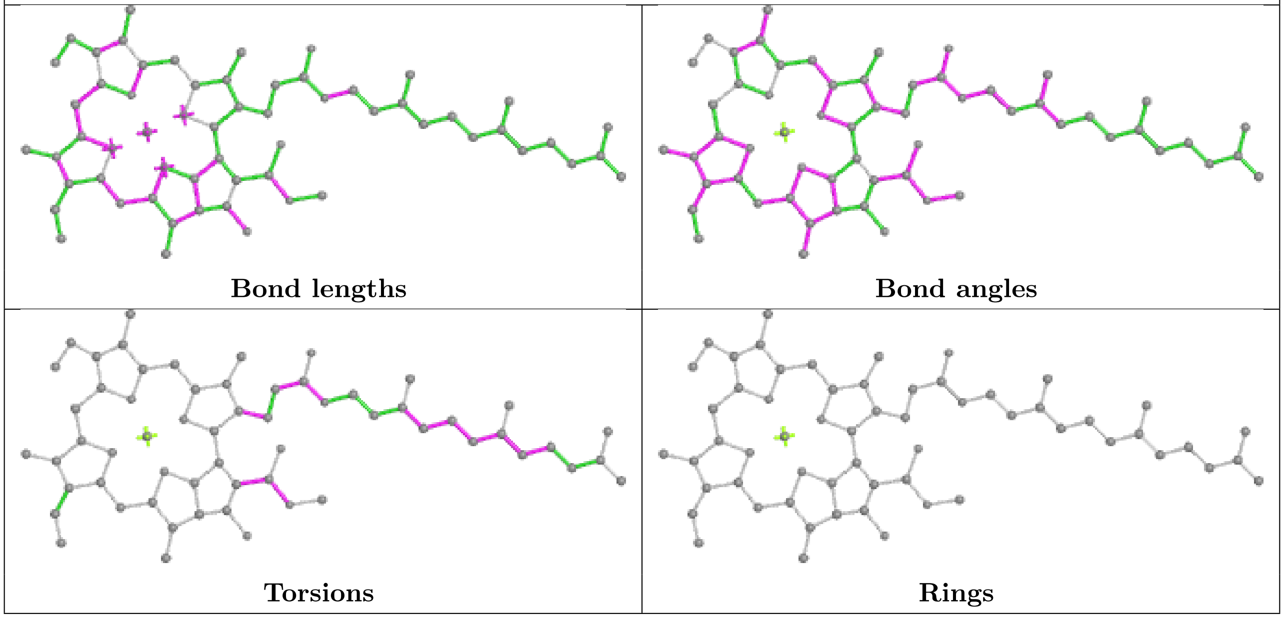


Bond lengths **Bond angles**



Torsions **Rings**

Ligand CLA G 1138



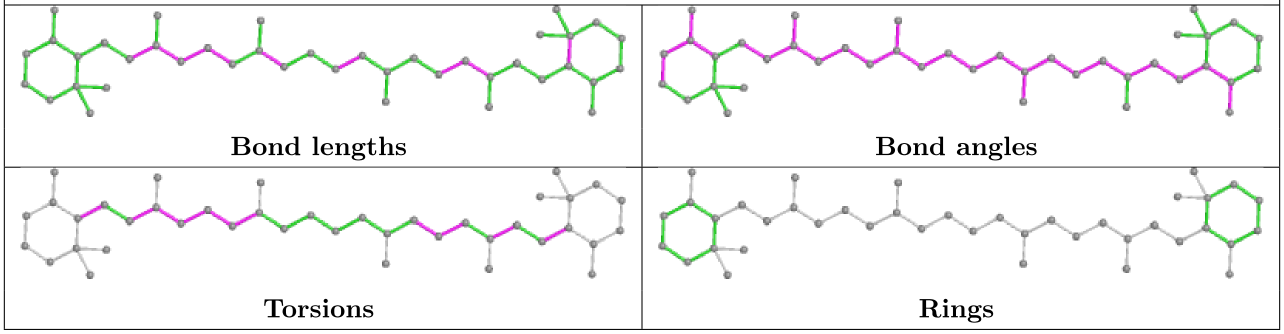
Bond lengths

Bond angles

Torsions

Rings

Ligand BCR b 4017



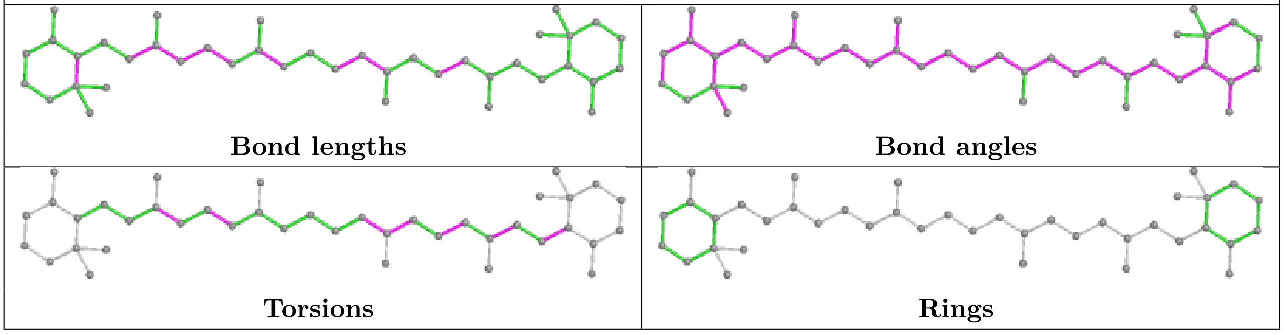
Bond lengths

Bond angles

Torsions

Rings

Ligand BCR A 4007



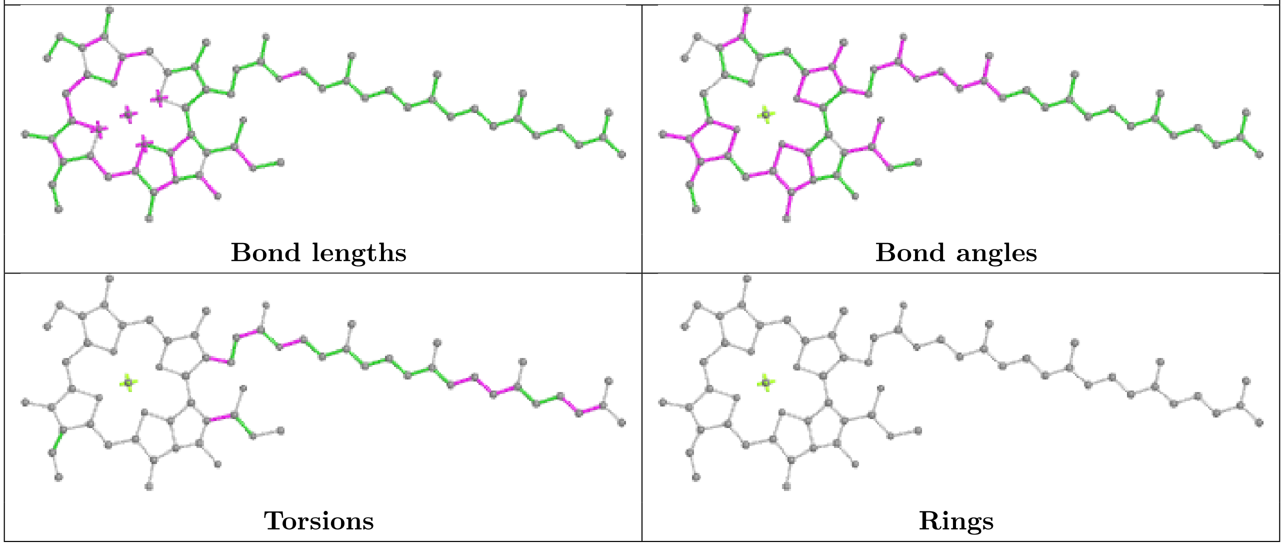
Bond lengths

Bond angles

Torsions

Rings

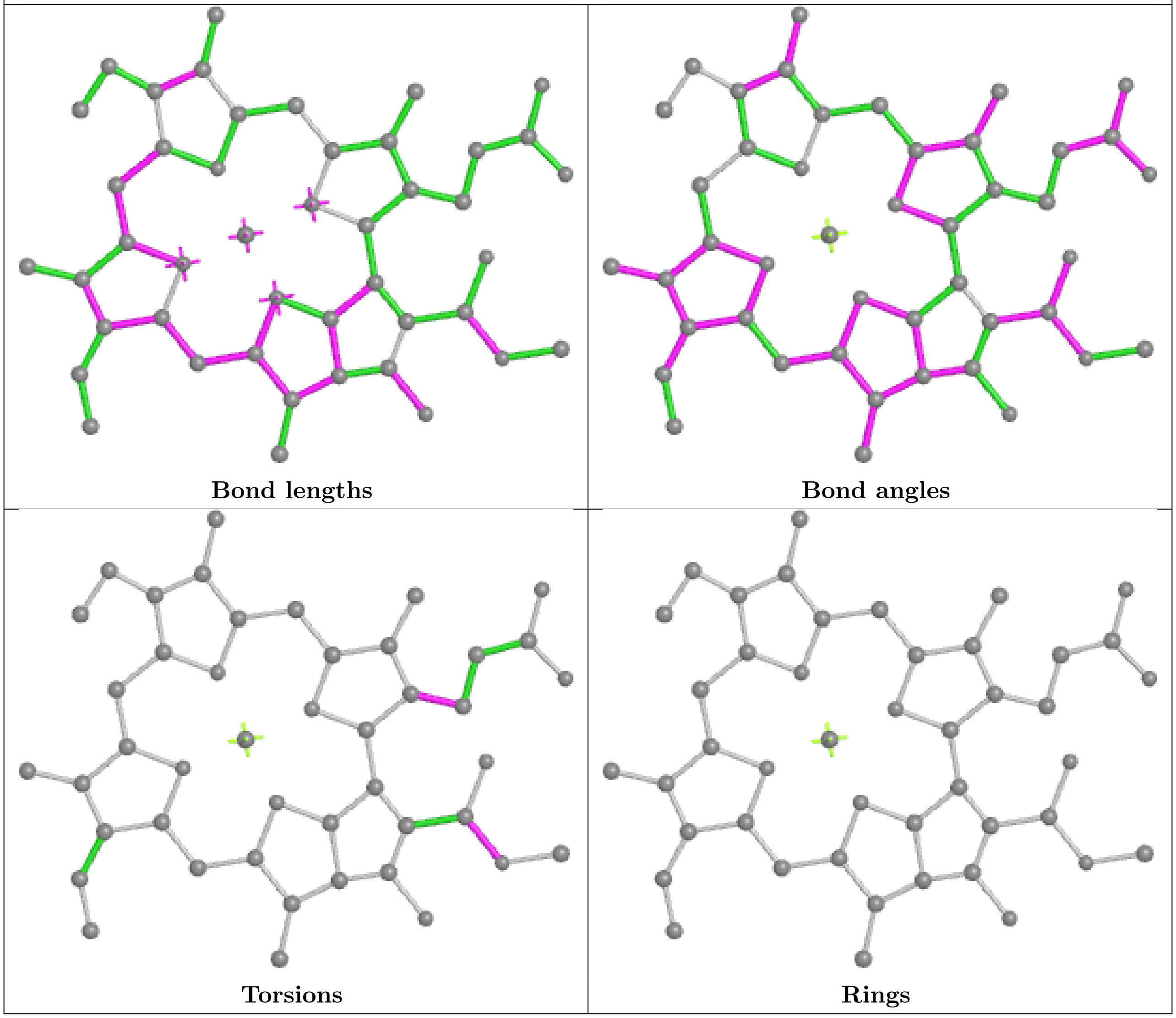
Ligand CLA B 1221



Bond lengths Bond angles

Torsions Rings

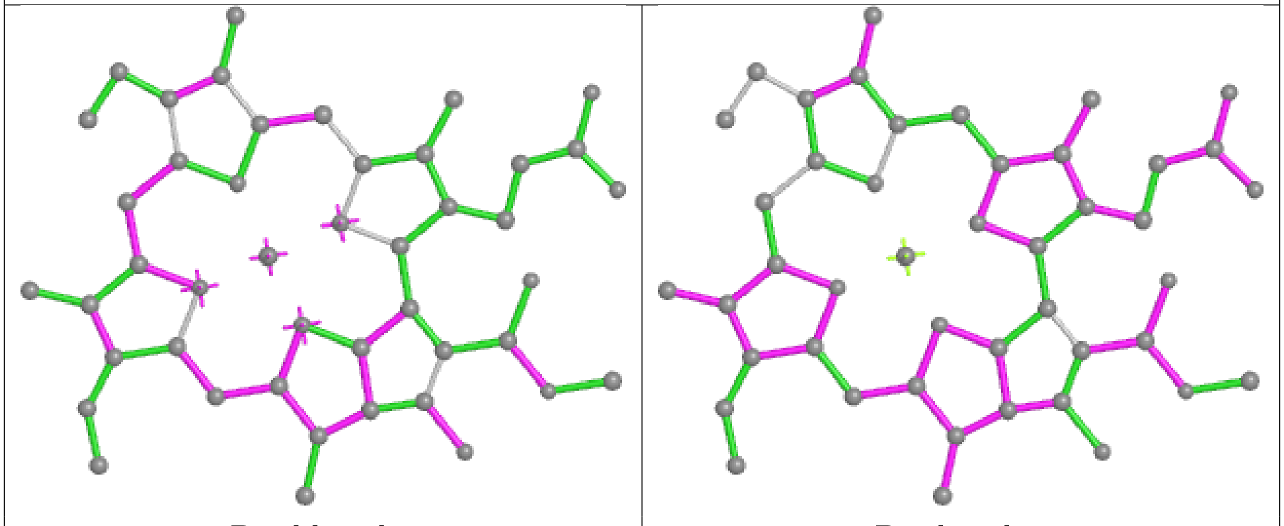
Ligand CLA b 1219



Bond lengths Bond angles

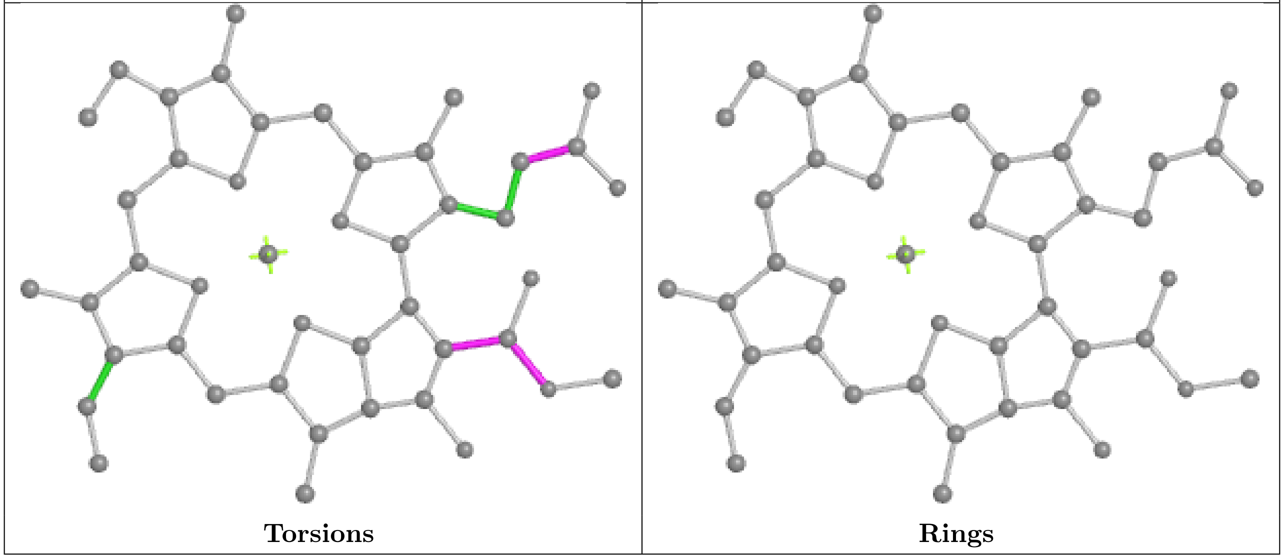
Torsions Rings

Ligand CLA a 1108



Bond lengths

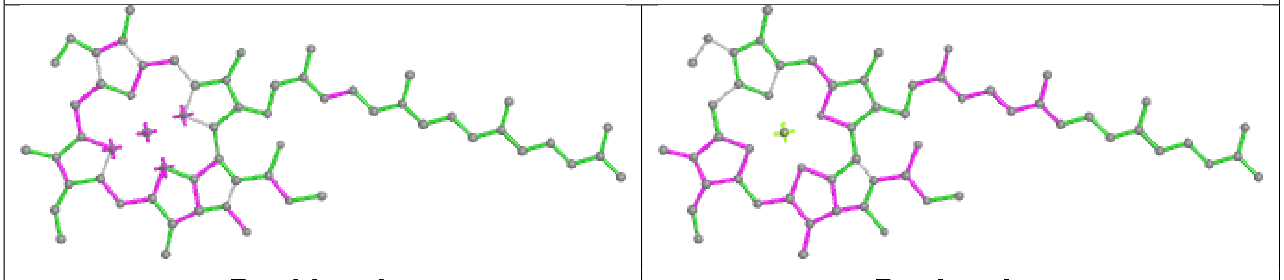
Bond angles



Torsions

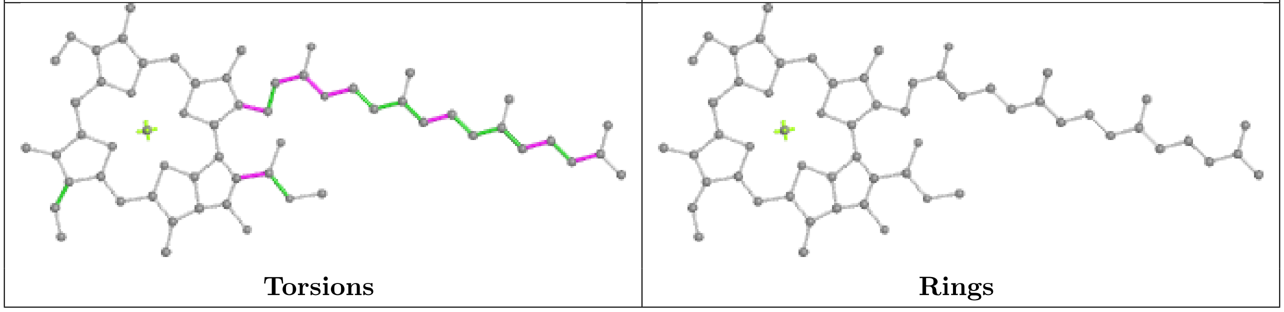
Rings

Ligand CLA H 1202



Bond lengths

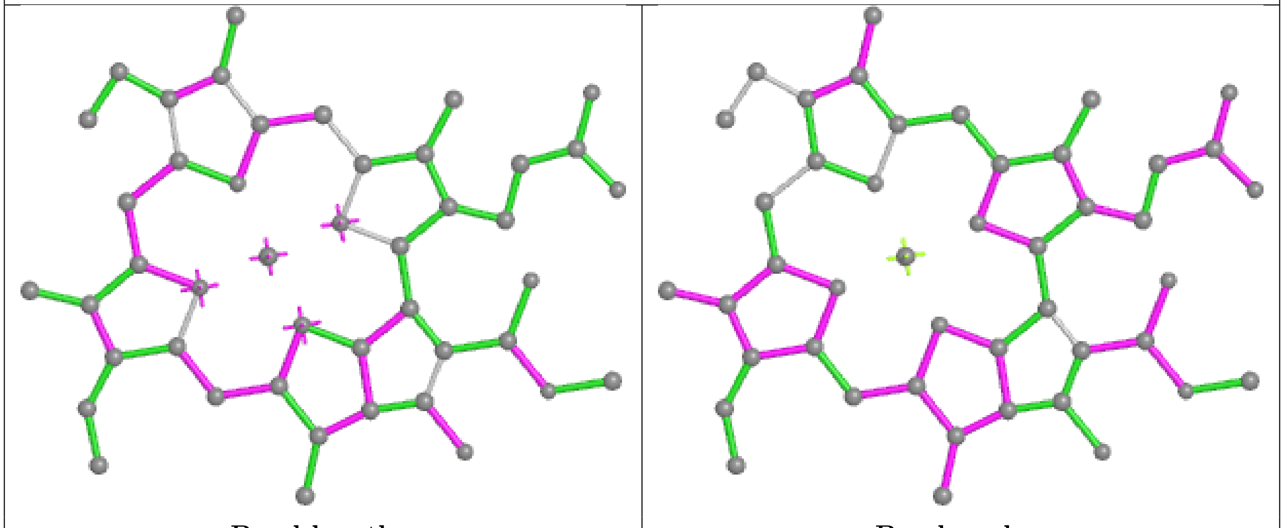
Bond angles



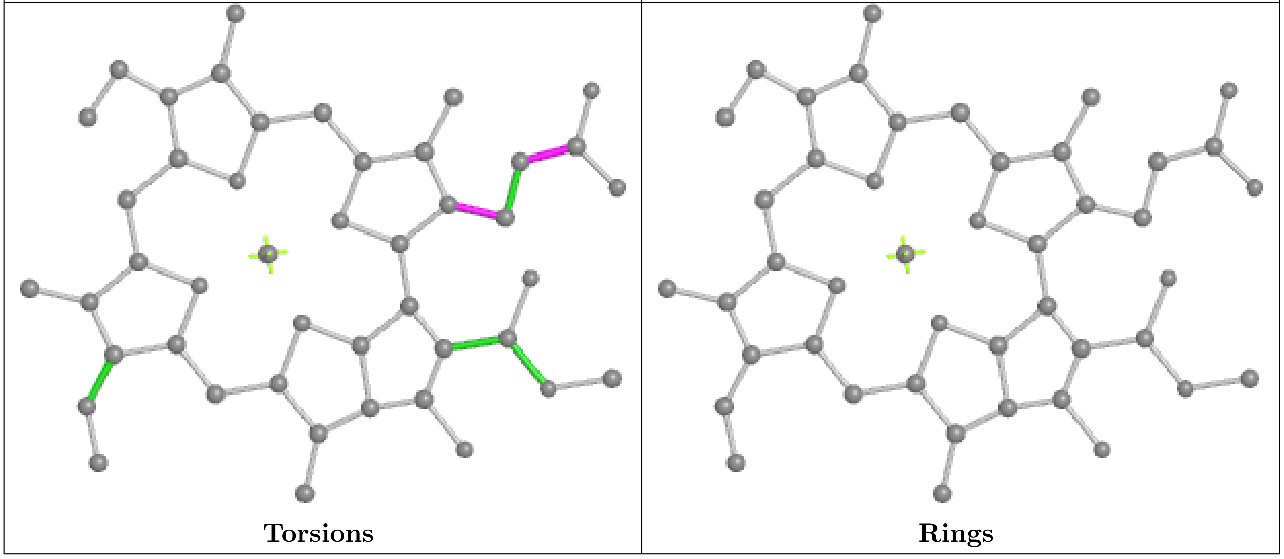
Torsions

Rings

Ligand CLA B 1236

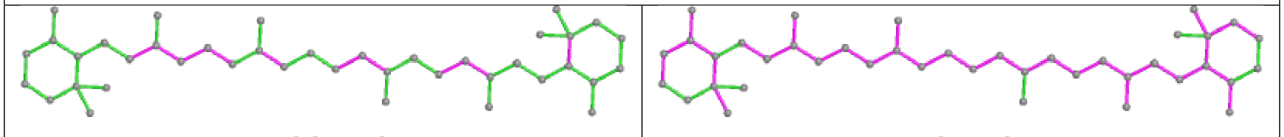


Bond lengths Bond angles

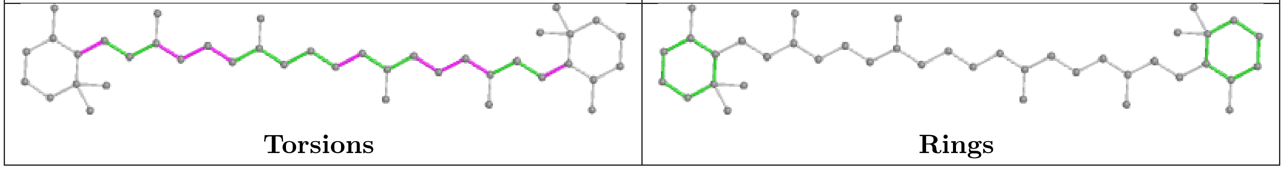


Torsions Rings

Ligand BCR i 4020

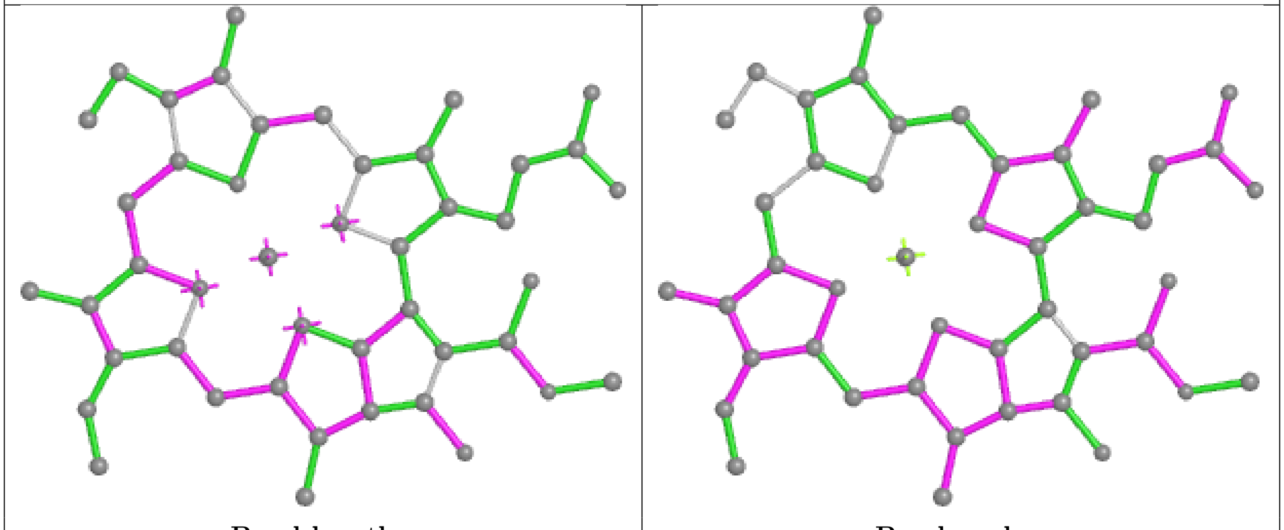


Bond lengths Bond angles

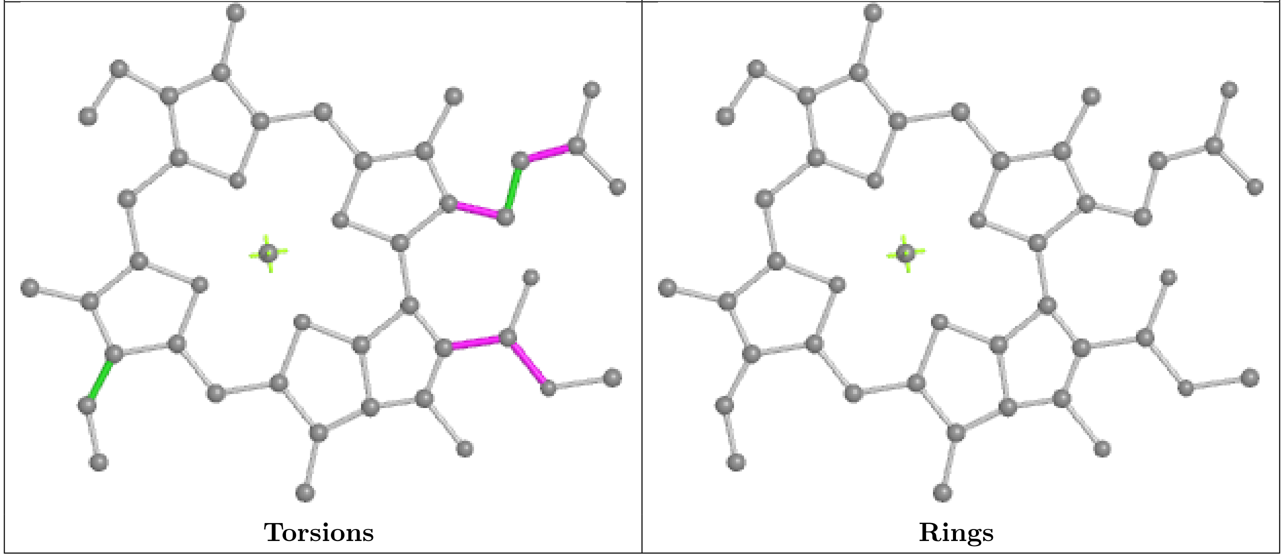


Torsions Rings

Ligand CLA B 1233

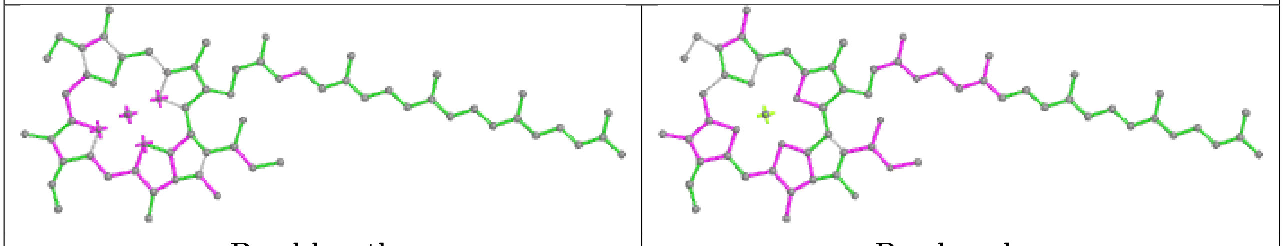


Bond lengths Bond angles

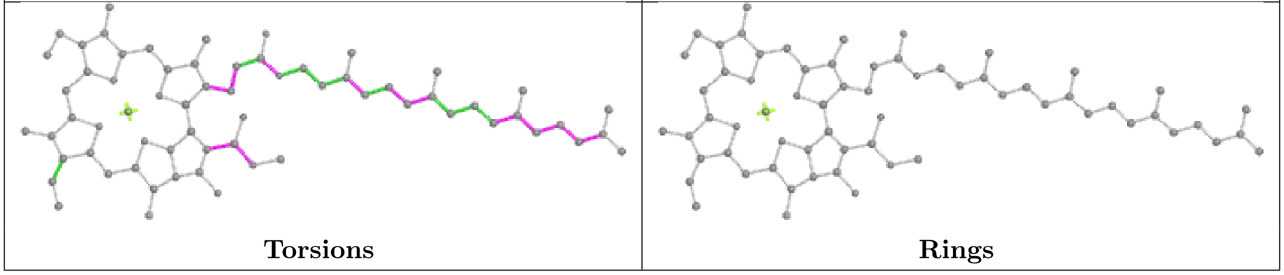


Torsions Rings

Ligand CLA H 1216

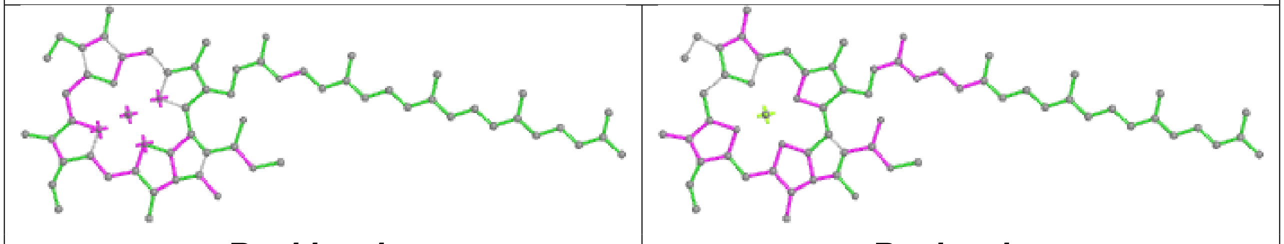


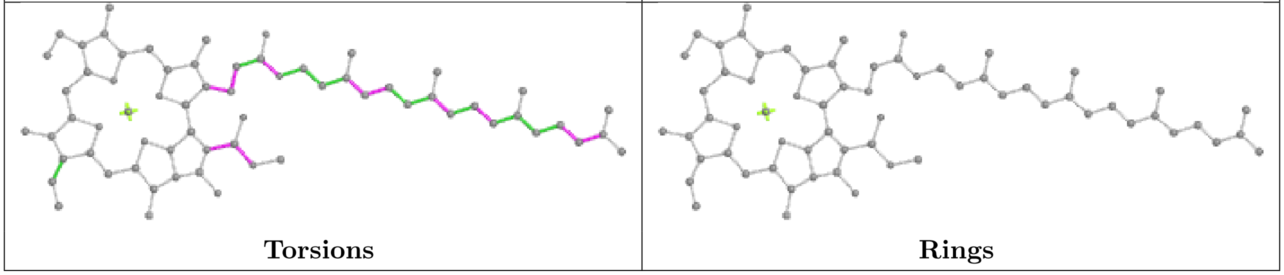
Bond lengths Bond angles



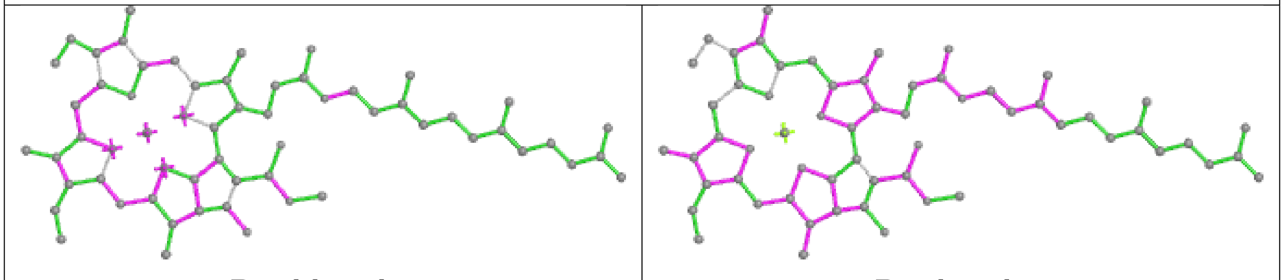
Torsions Rings

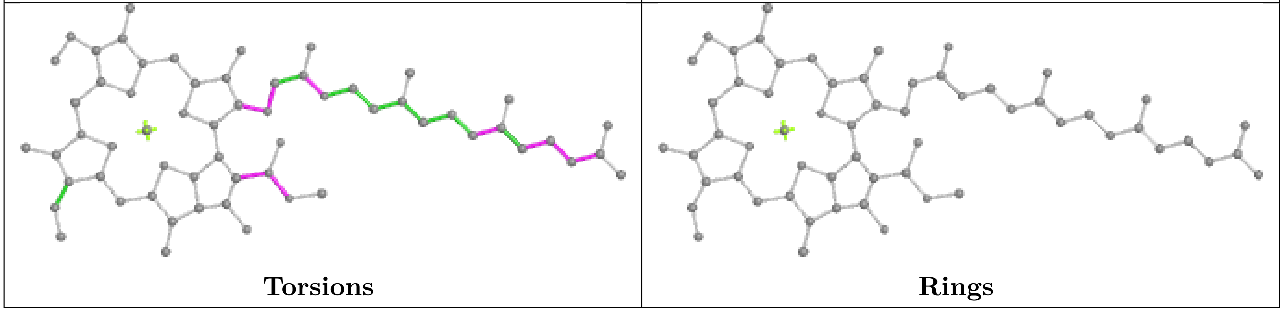
Ligand CLA H 1225


Bond lengths Bond angles

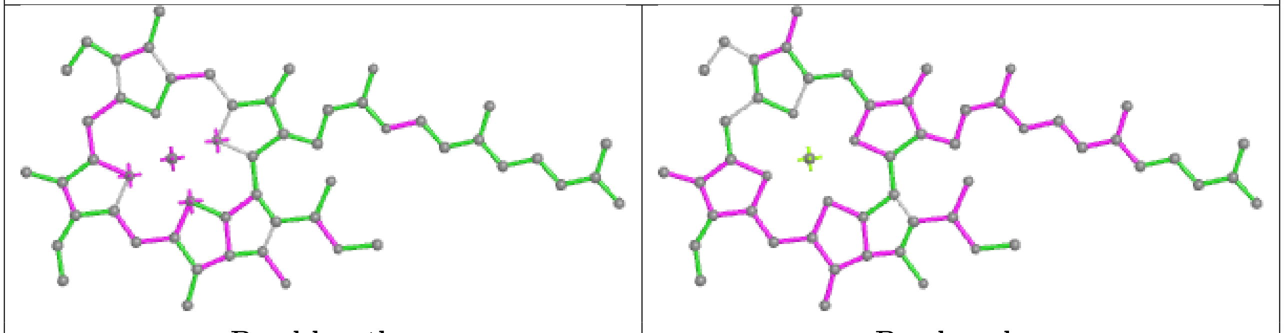

Torsions Rings

Ligand CLA G 1106

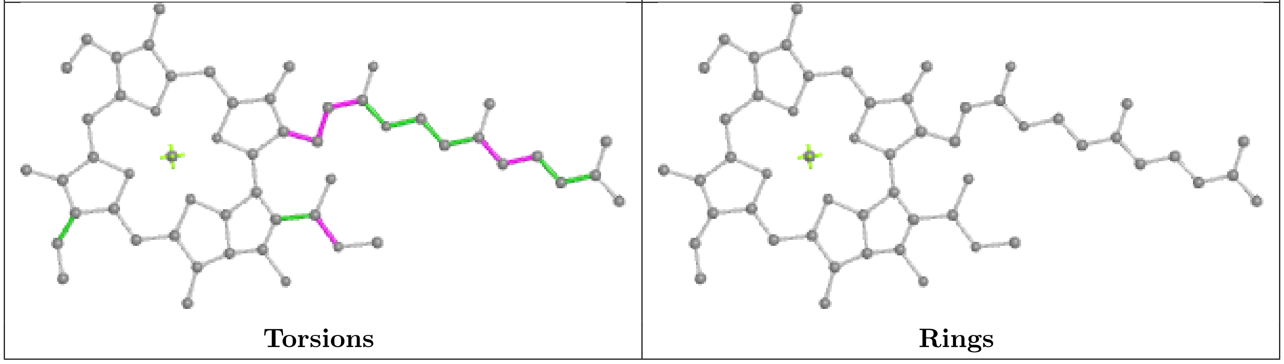

Bond lengths Bond angles


Torsions Rings

Ligand CLA G 1116

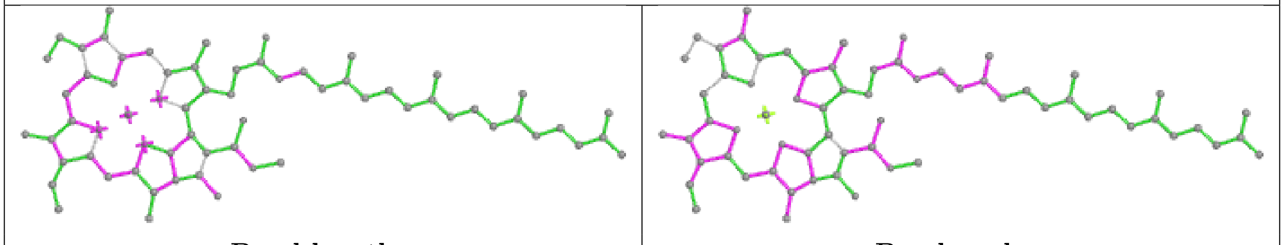


Bond lengths Bond angles

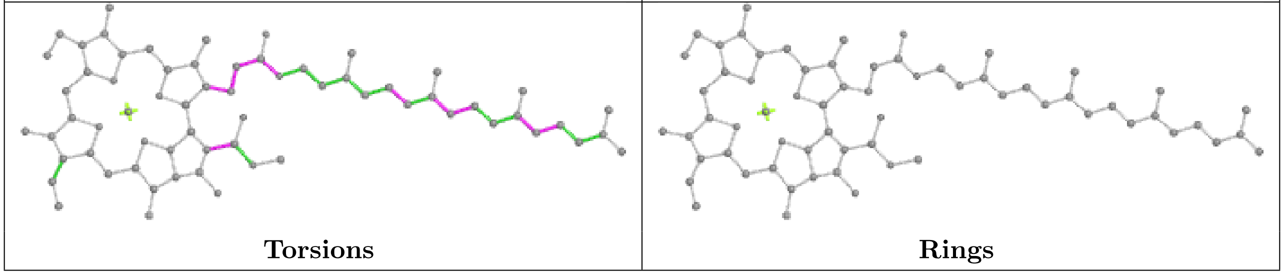


Torsions Rings

Ligand CLA A 1127

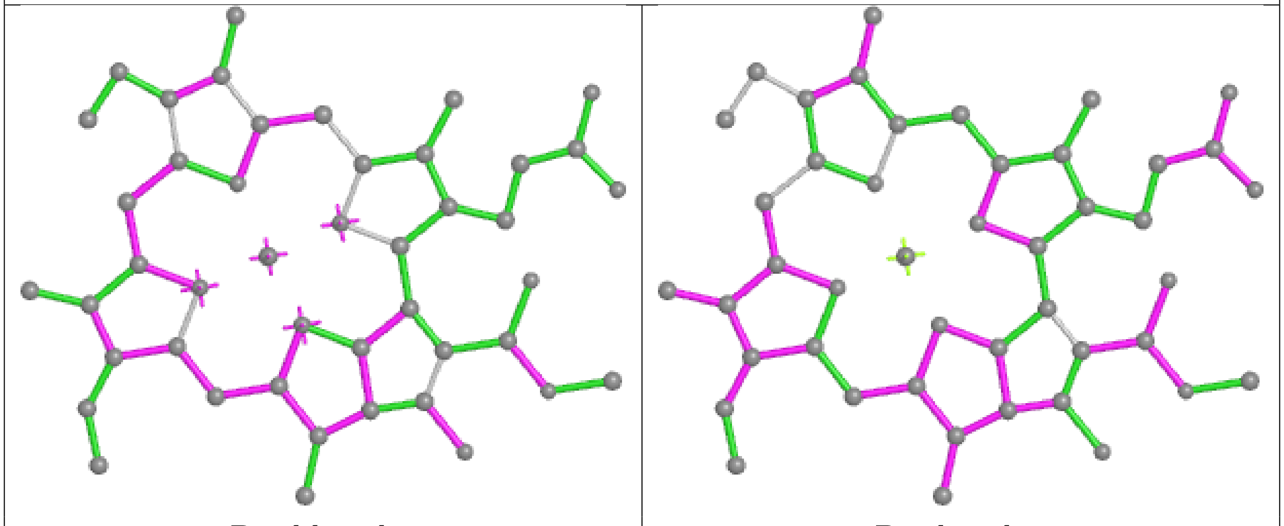


Bond lengths Bond angles



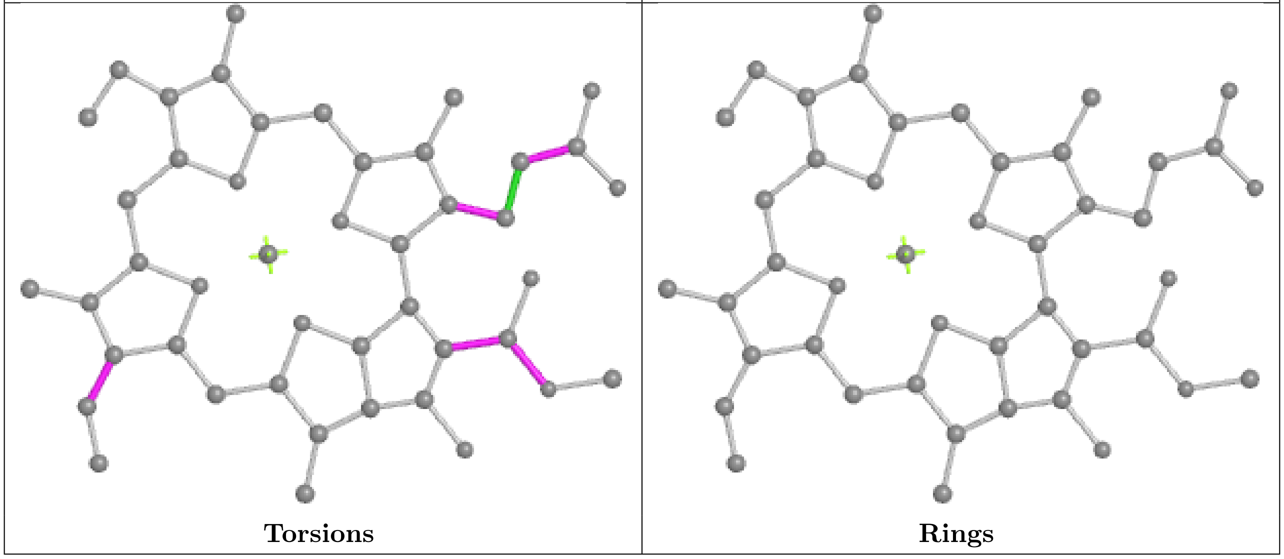
Torsions Rings

Ligand CLA G 1114



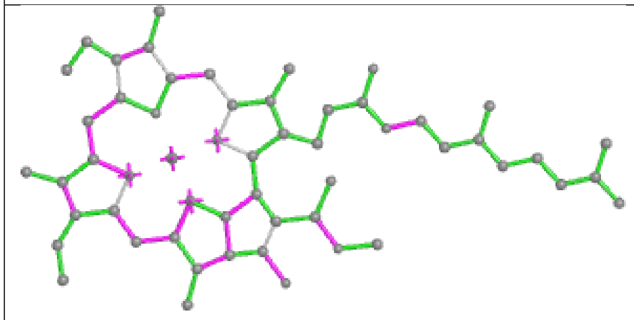
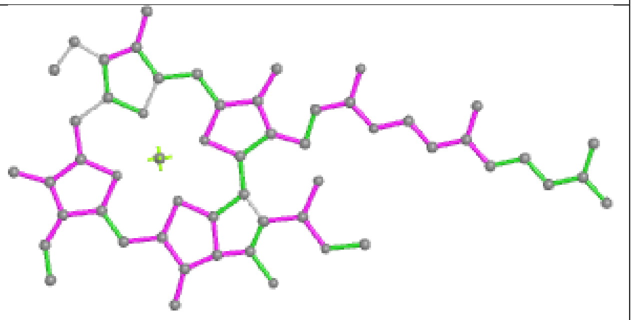
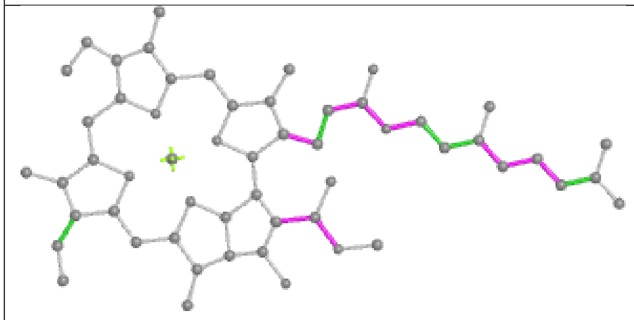
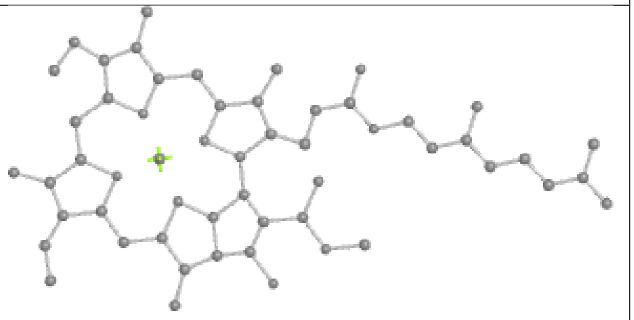
Bond lengths

Bond angles

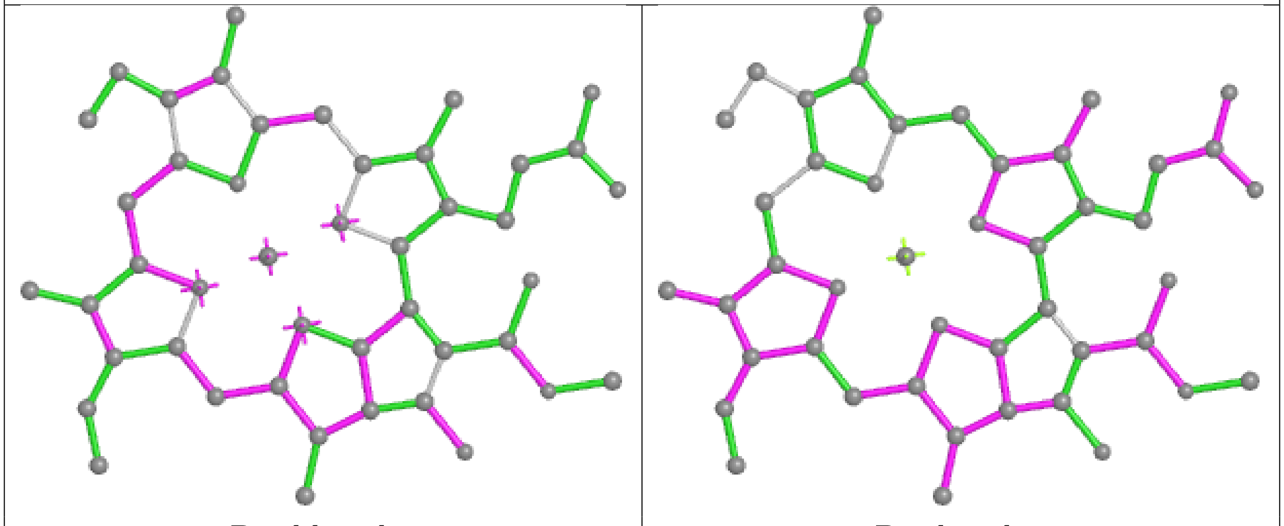


Torsions

Rings

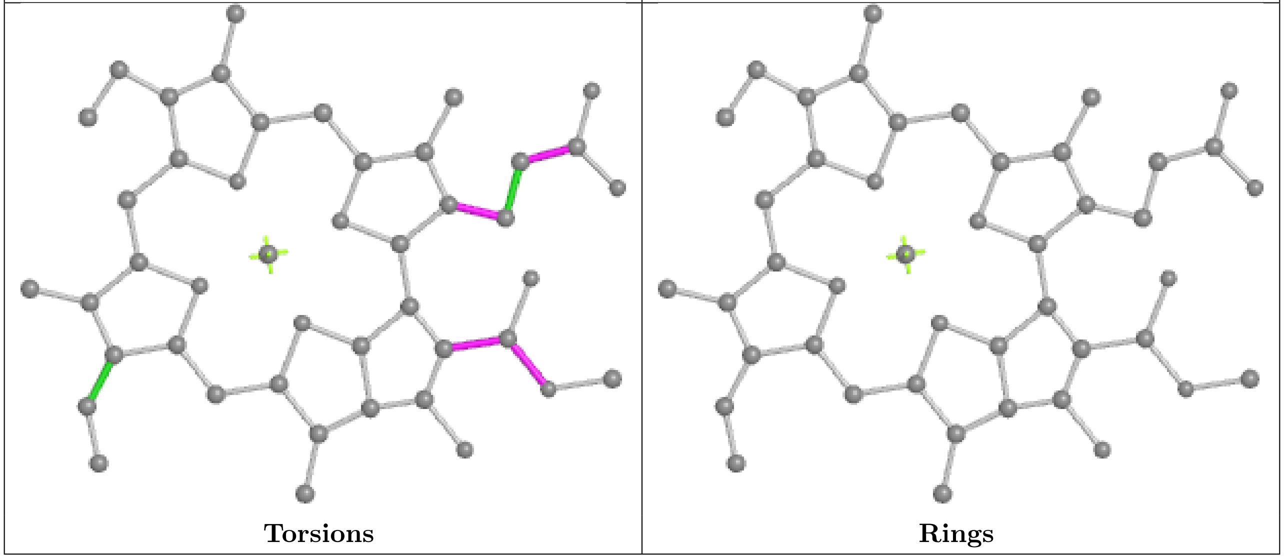
Ligand CLA a 1122	
 **Bond lengths**	 **Bond angles**
 **Torsions**	 **Rings**

Ligand CLA H 1233



Bond lengths

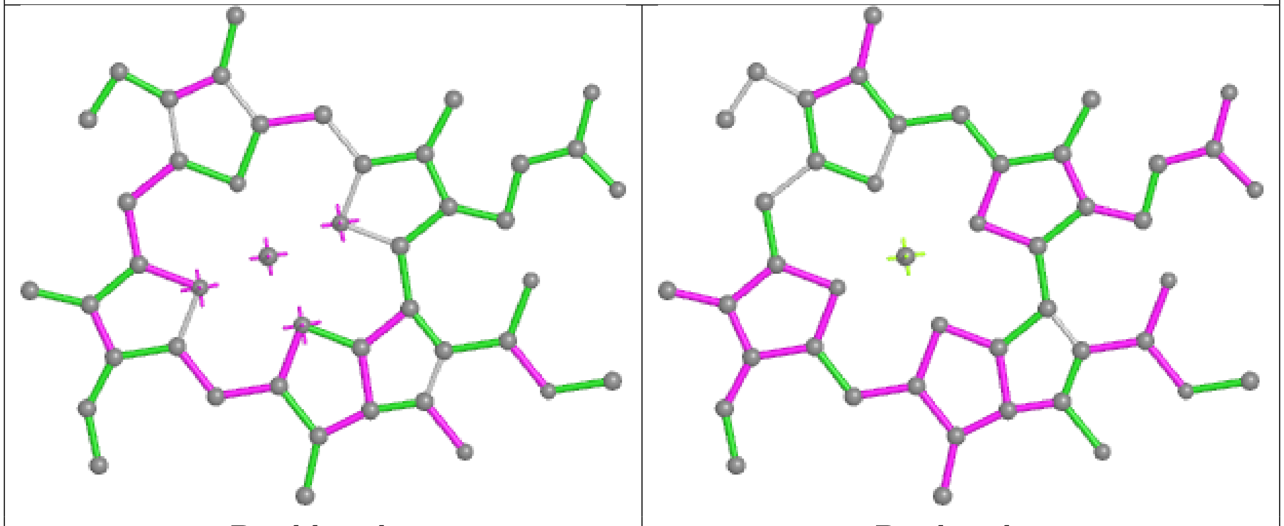
Bond angles



Torsions

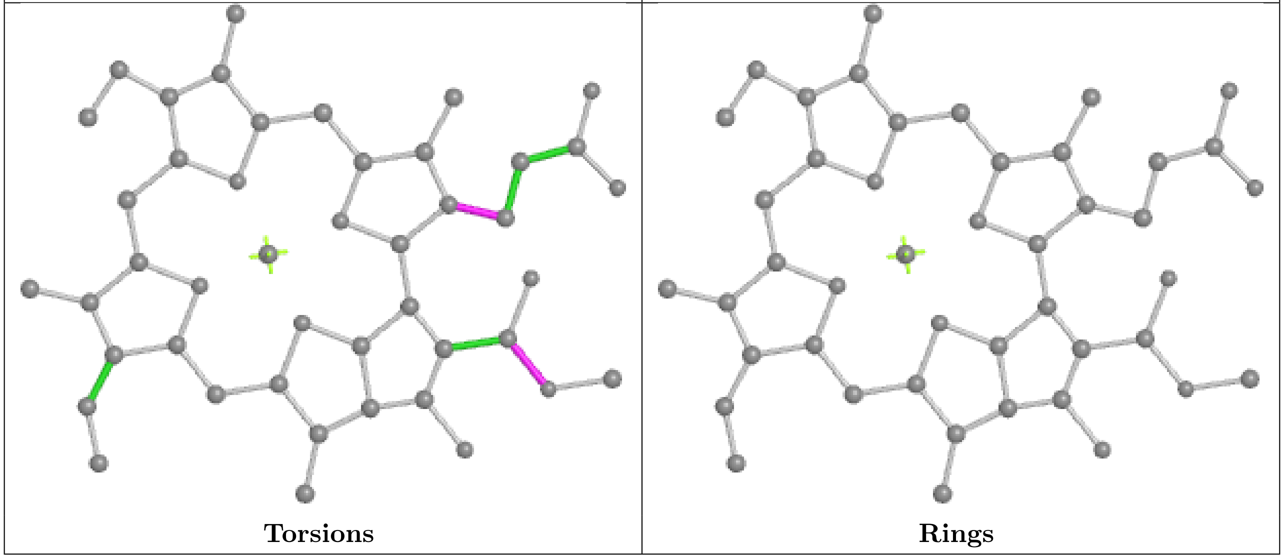
Rings

Ligand CLA G 1107



Bond lengths

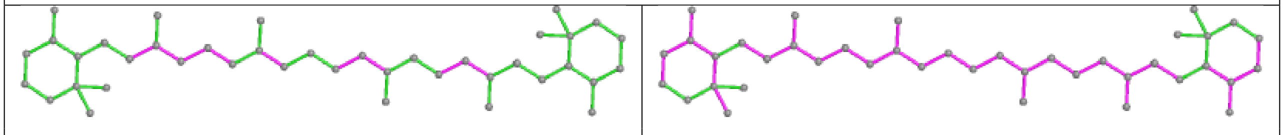
Bond angles



Torsions

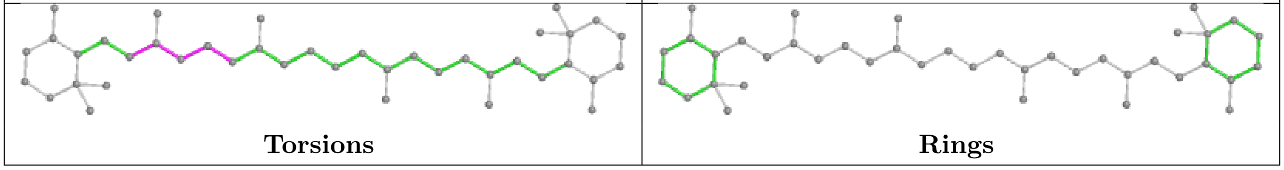
Rings

Ligand BCR l 4022



Bond lengths

Bond angles



Torsions

Rings

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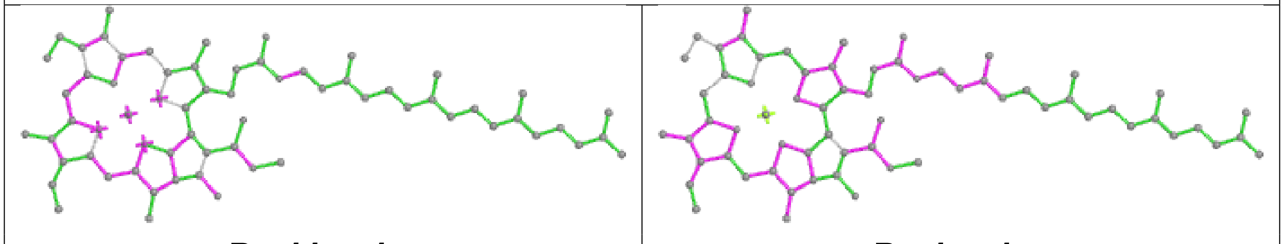
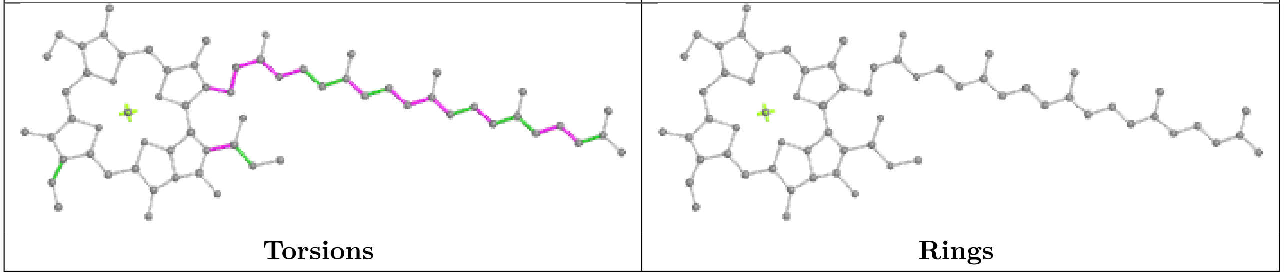


Bond lengths

Bond angles



Torsions

Rings

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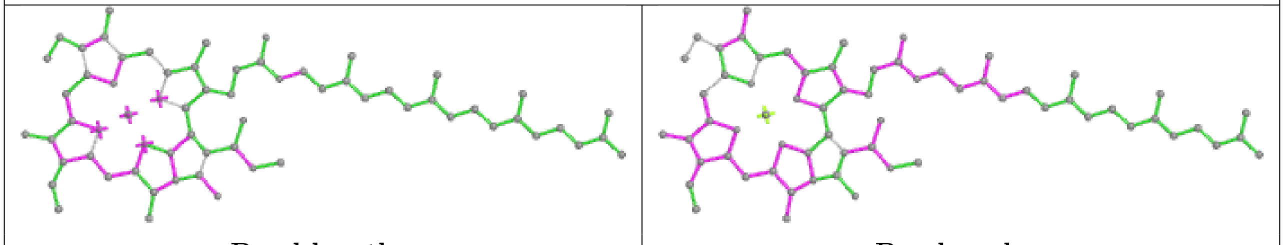
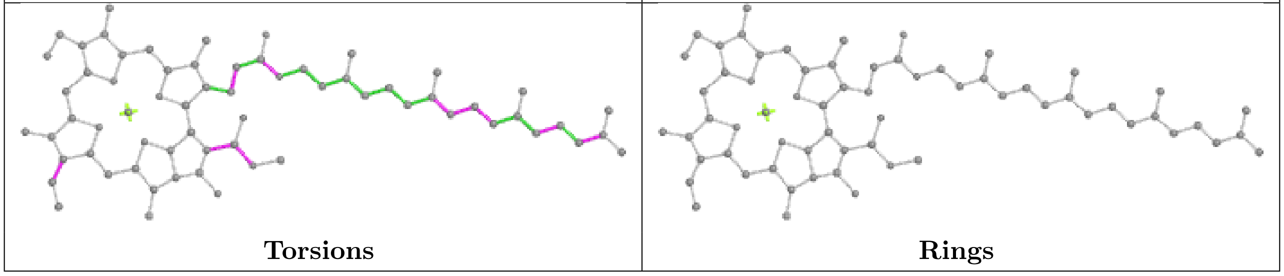


Bond lengths

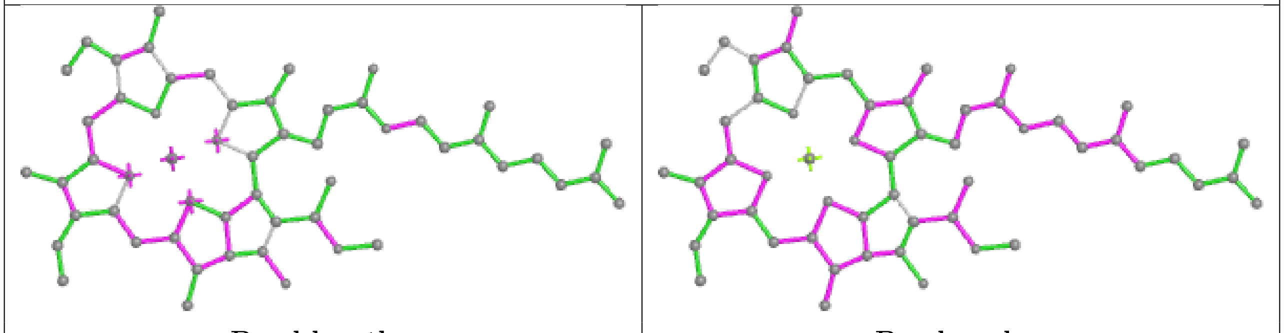
Bond angles



Torsions

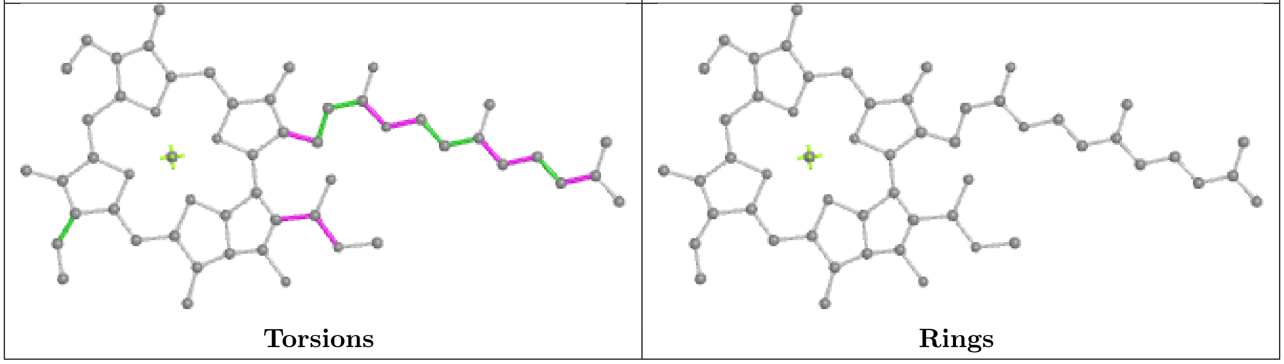
Rings

Ligand CLA a 1112



Bond lengths

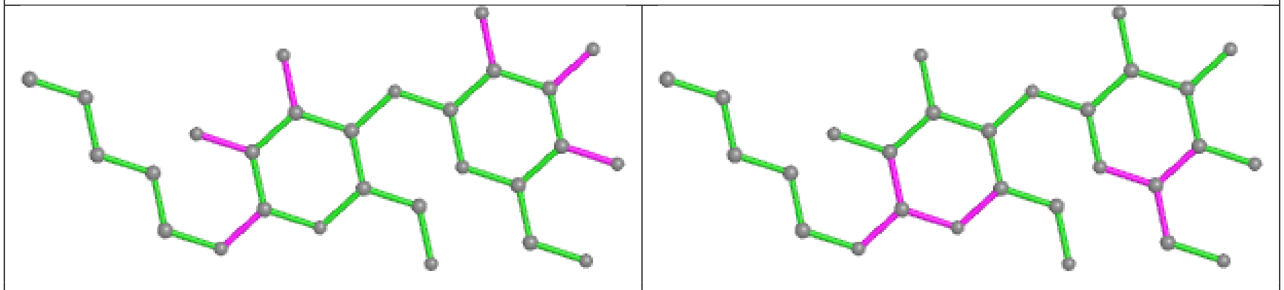
Bond angles



Torsions

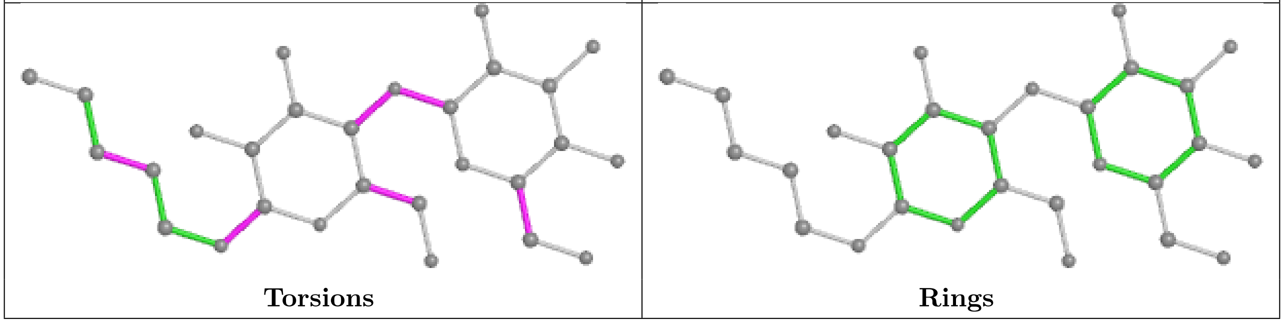
Rings

Ligand LMT a 6002



Bond lengths

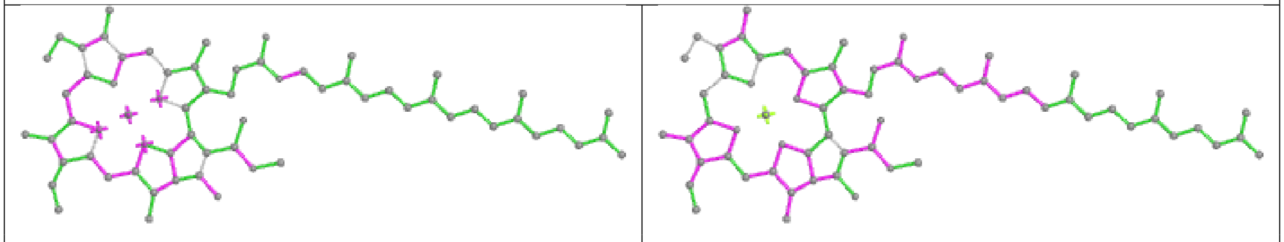
Bond angles



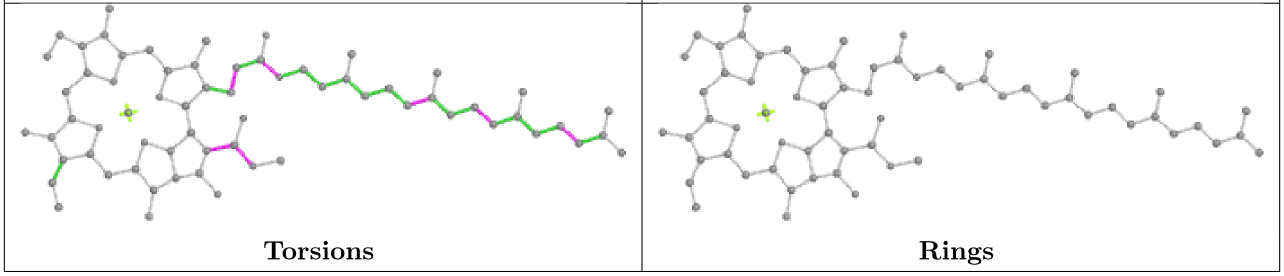
Torsions

Rings

Ligand CLA A 1104

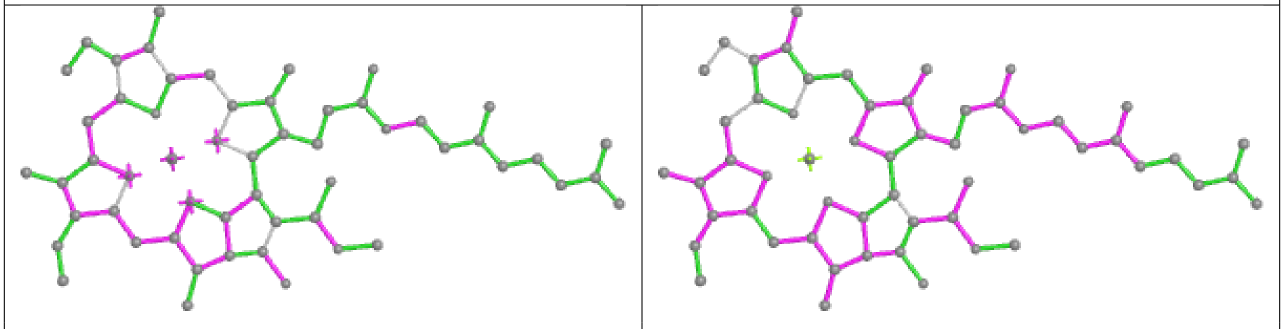


Bond lengths **Bond angles**

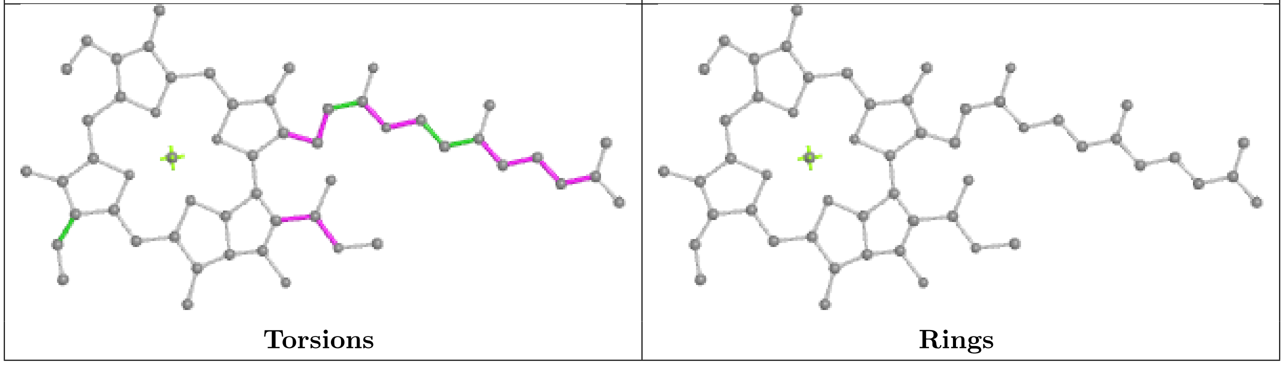


Torsions **Rings**

Ligand CLA B 1228

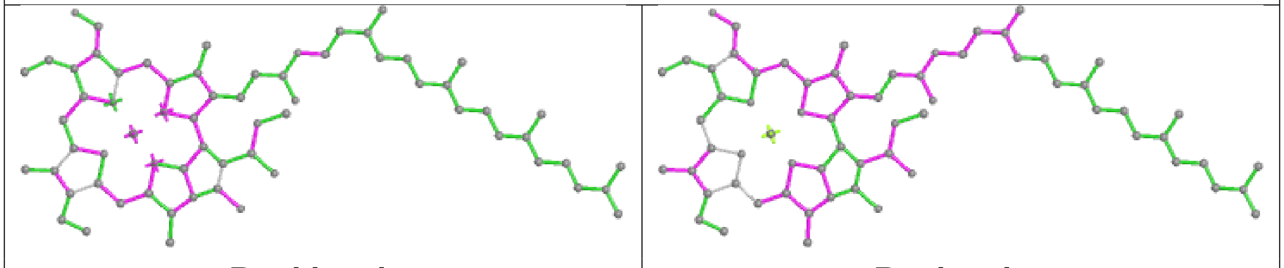


Bond lengths **Bond angles**

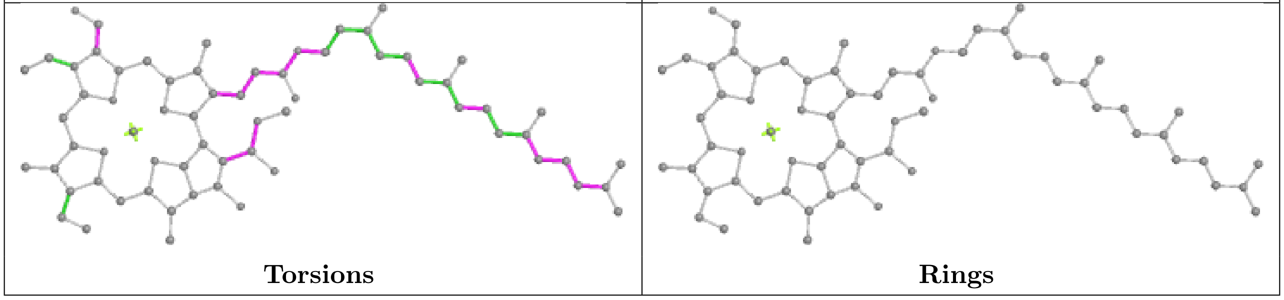


Torsions **Rings**

Ligand F6C B 1207

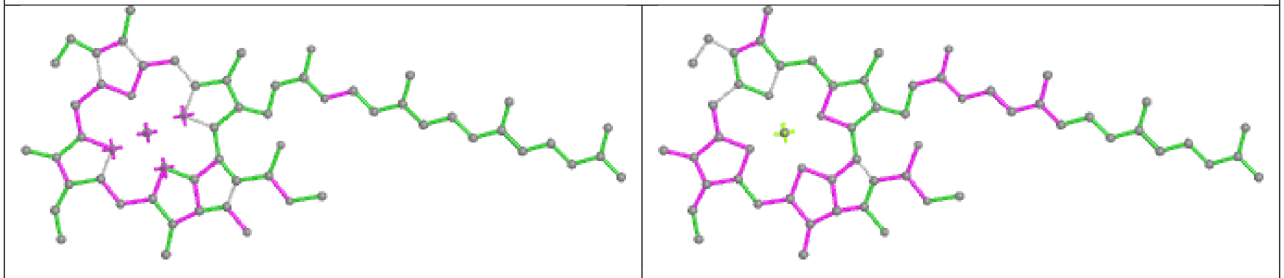


Bond lengths Bond angles

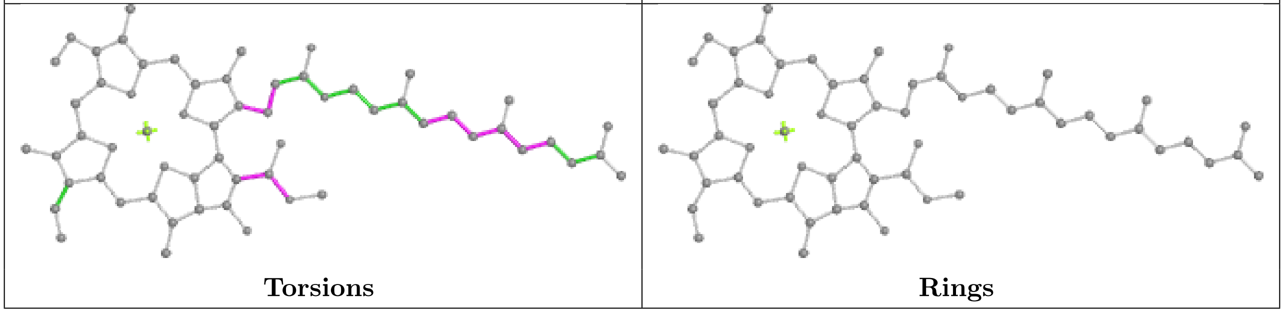


Torsions Rings

Ligand CLA G 1135

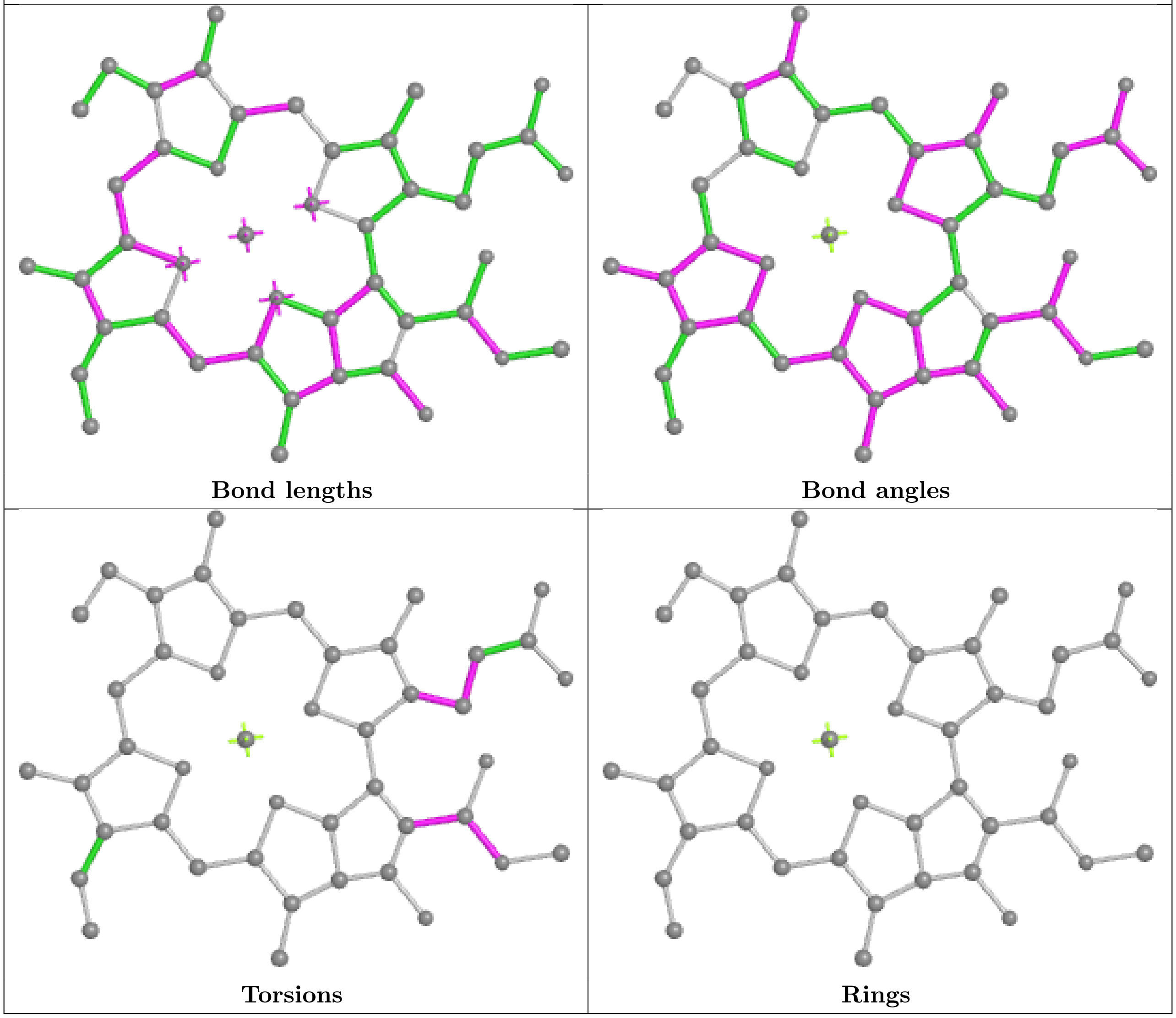


Bond lengths Bond angles



Torsions Rings

Ligand CLA A 1120



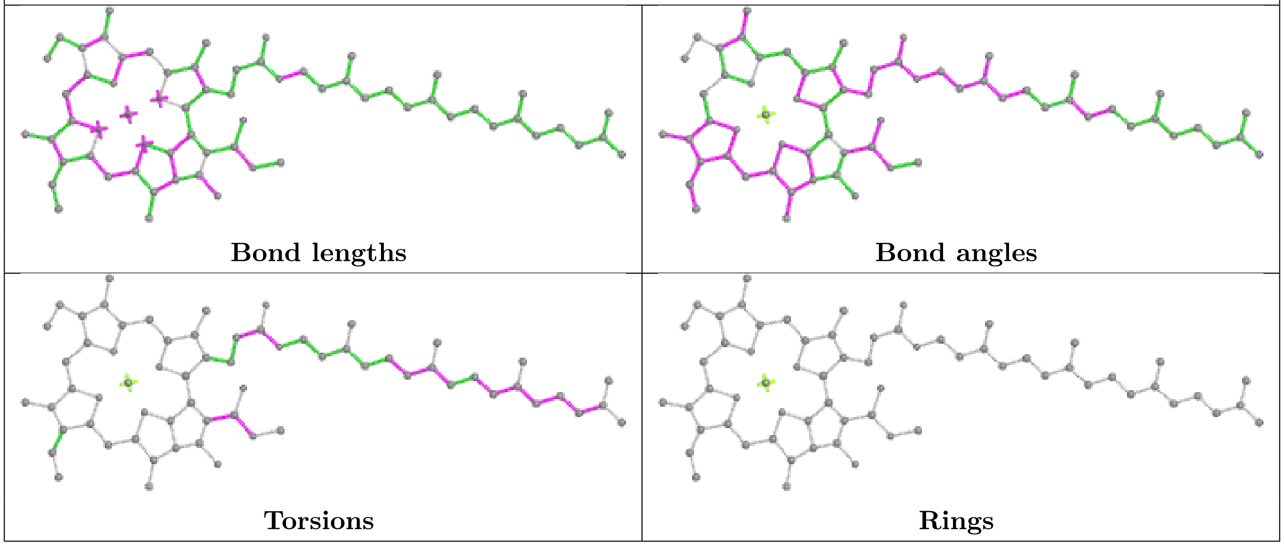
Bond lengths

Bond angles

Torsions

Rings

Ligand CLA H 1021



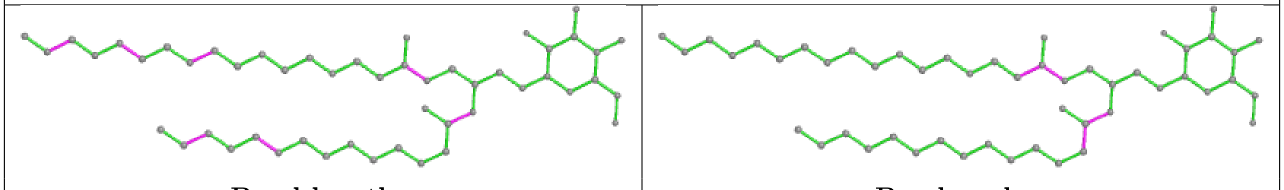
Bond lengths

Bond angles

Torsions

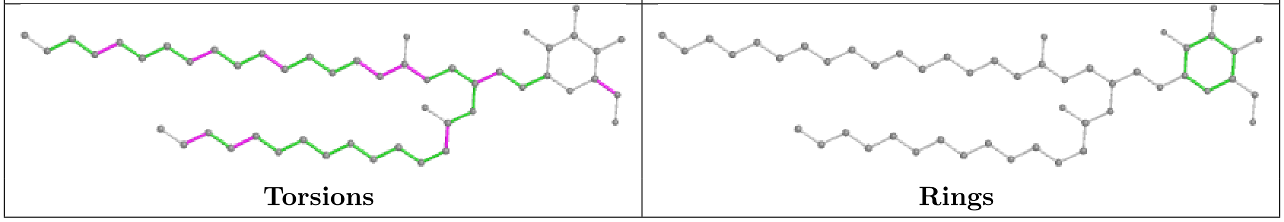
Rings

Ligand LMG U 5007



Bond lengths

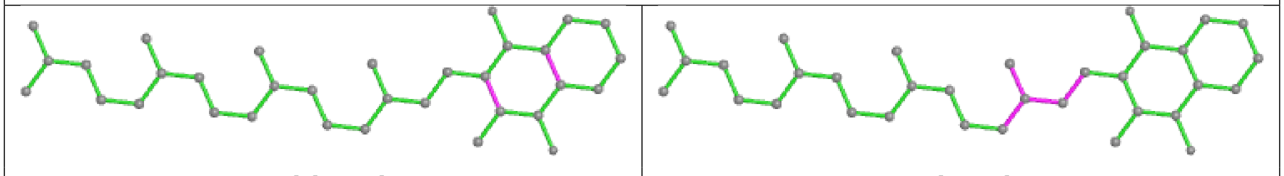
Bond angles



Torsions

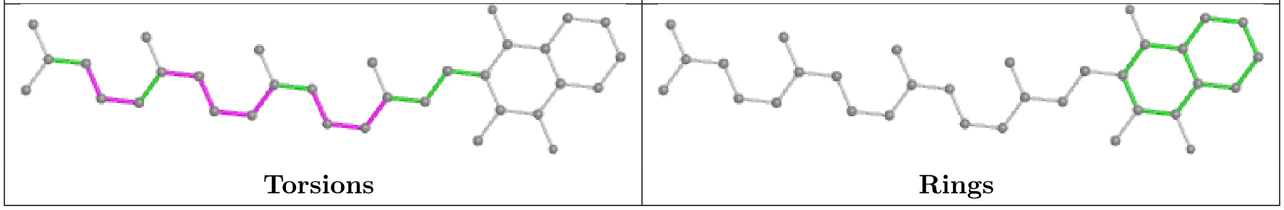
Rings

Ligand PQN b 2002



Bond lengths

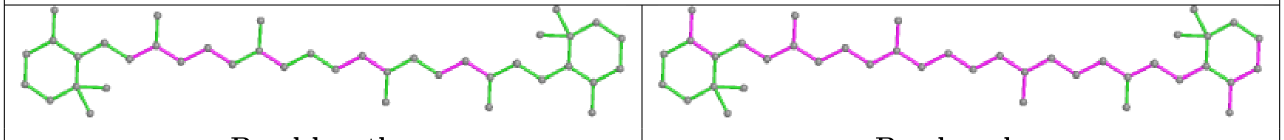
Bond angles



Torsions

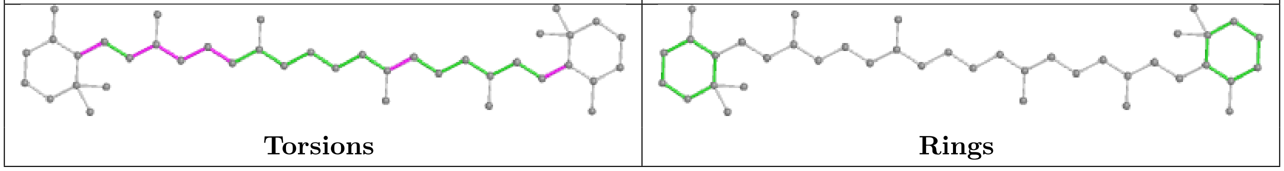
Rings

Ligand BCR a 4008



Bond lengths

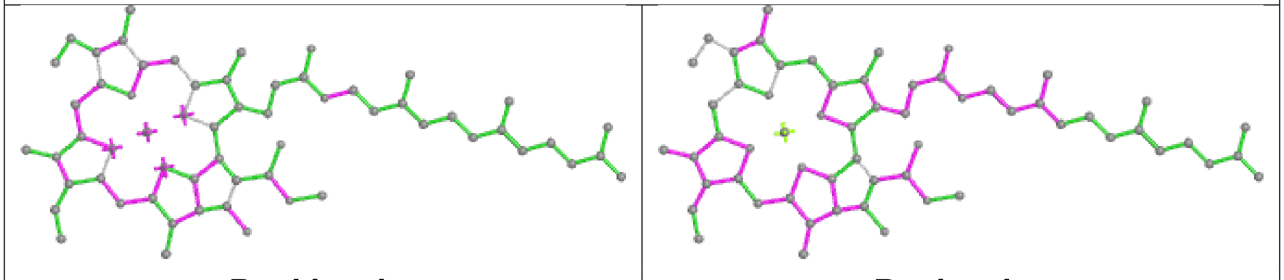
Bond angles



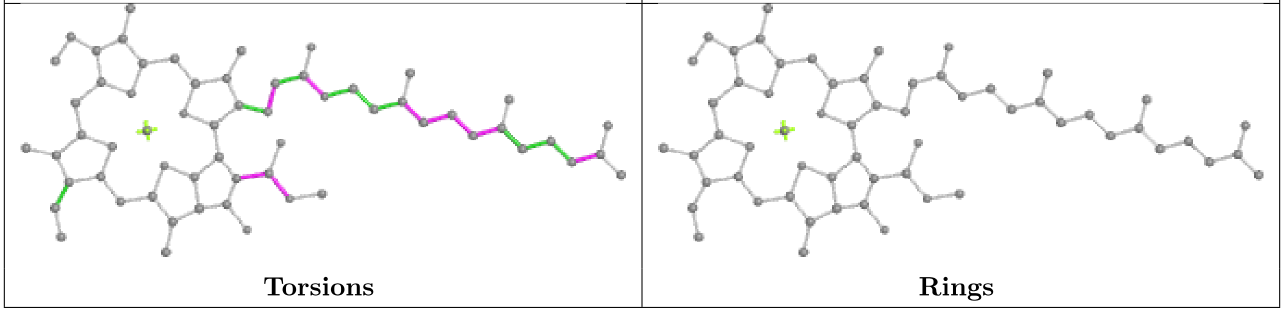
Torsions

Rings

Ligand CLA a 1111

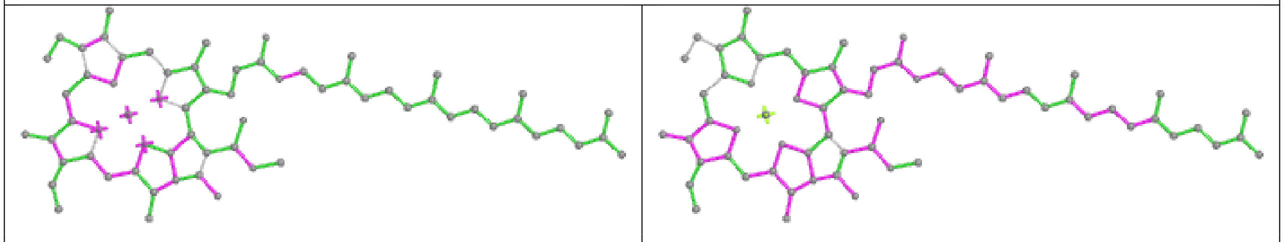


Bond lengths **Bond angles**

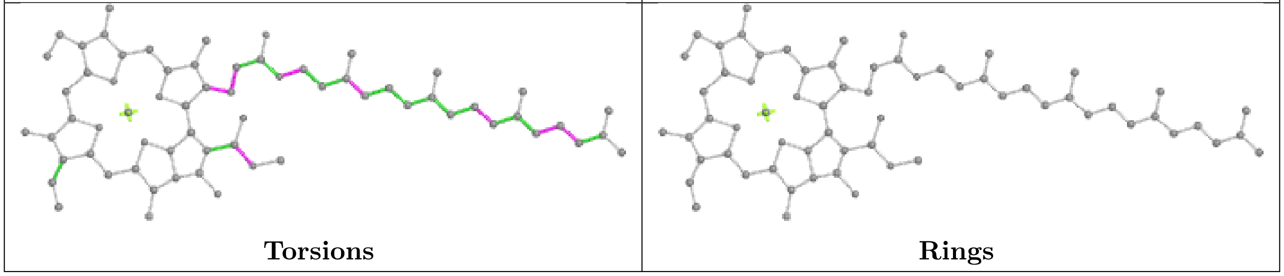


Torsions **Rings**

Ligand CLA a 1012

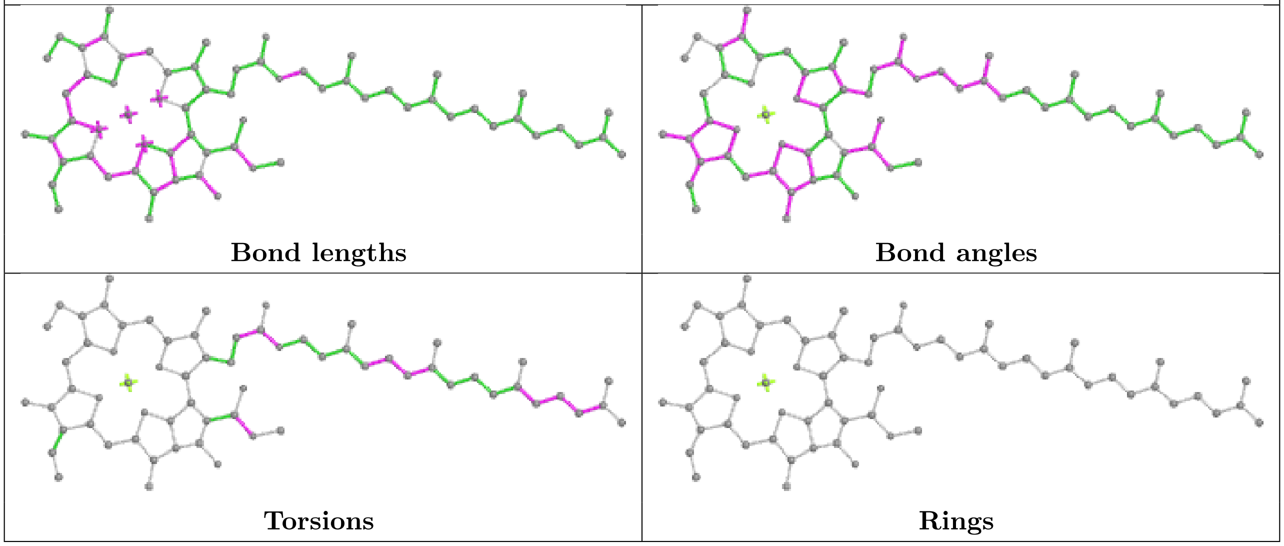


Bond lengths **Bond angles**



Torsions **Rings**

Ligand CLA B 1208



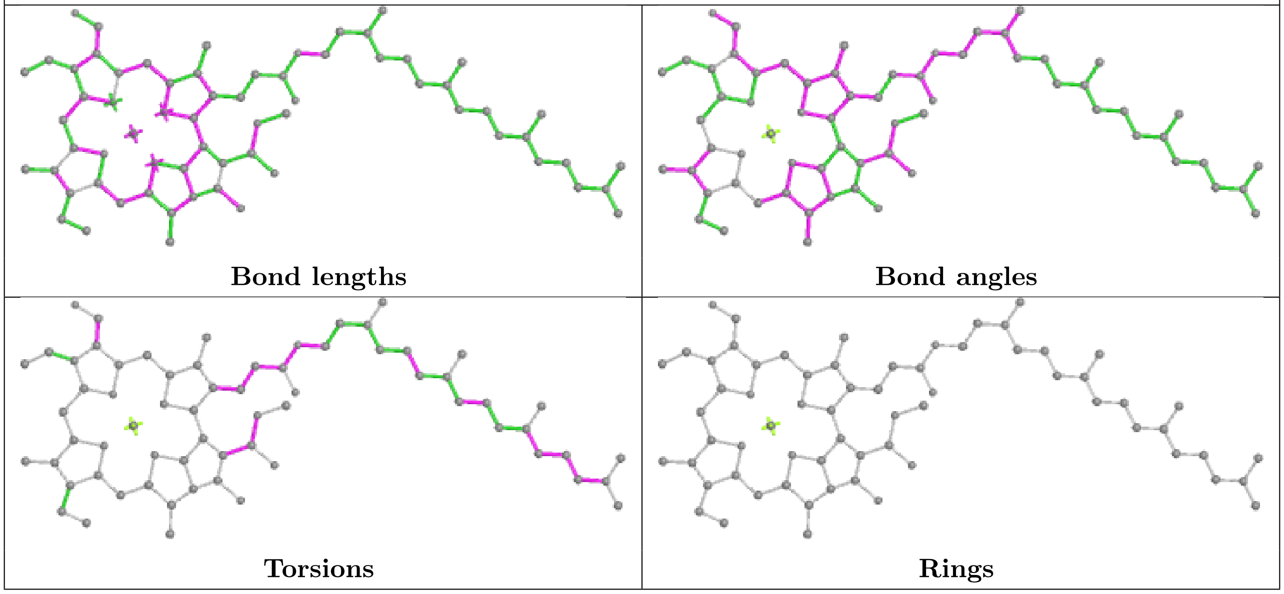
Bond lengths

Bond angles

Torsions

Rings

Ligand F6C b 1207



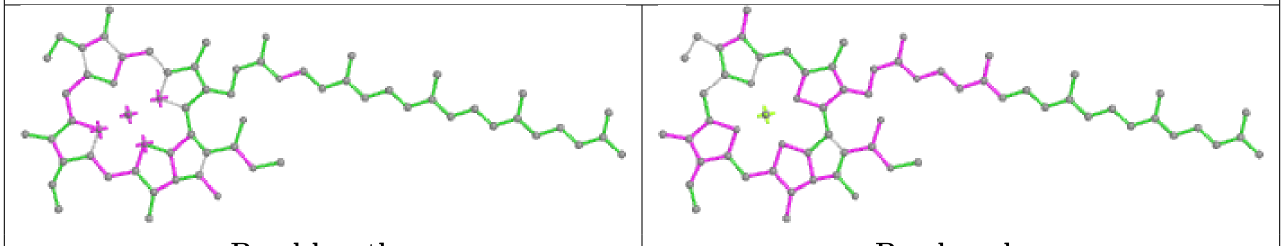
Bond lengths

Bond angles

Torsions

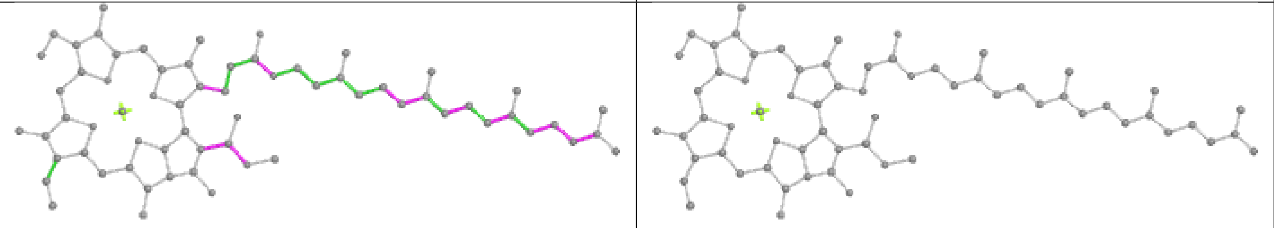
Rings

Ligand CLA B 1222



Bond lengths

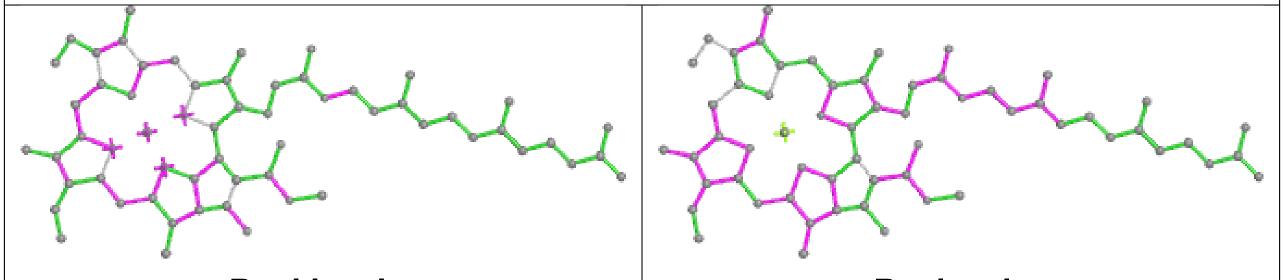
Bond angles



Torsions

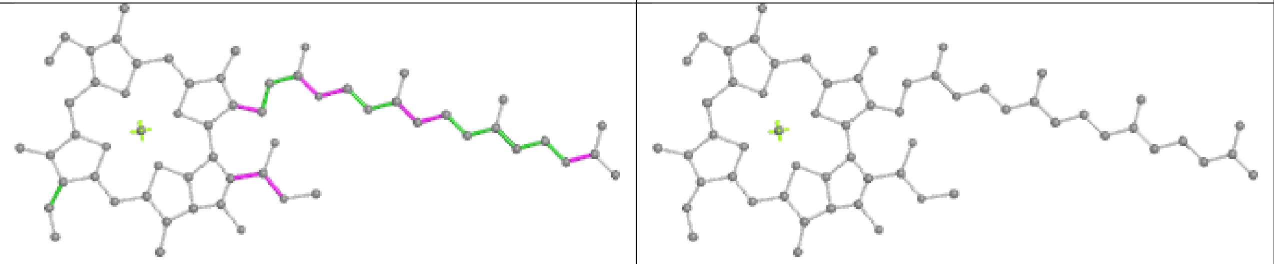
Rings

Ligand CLA A 1103



Bond lengths

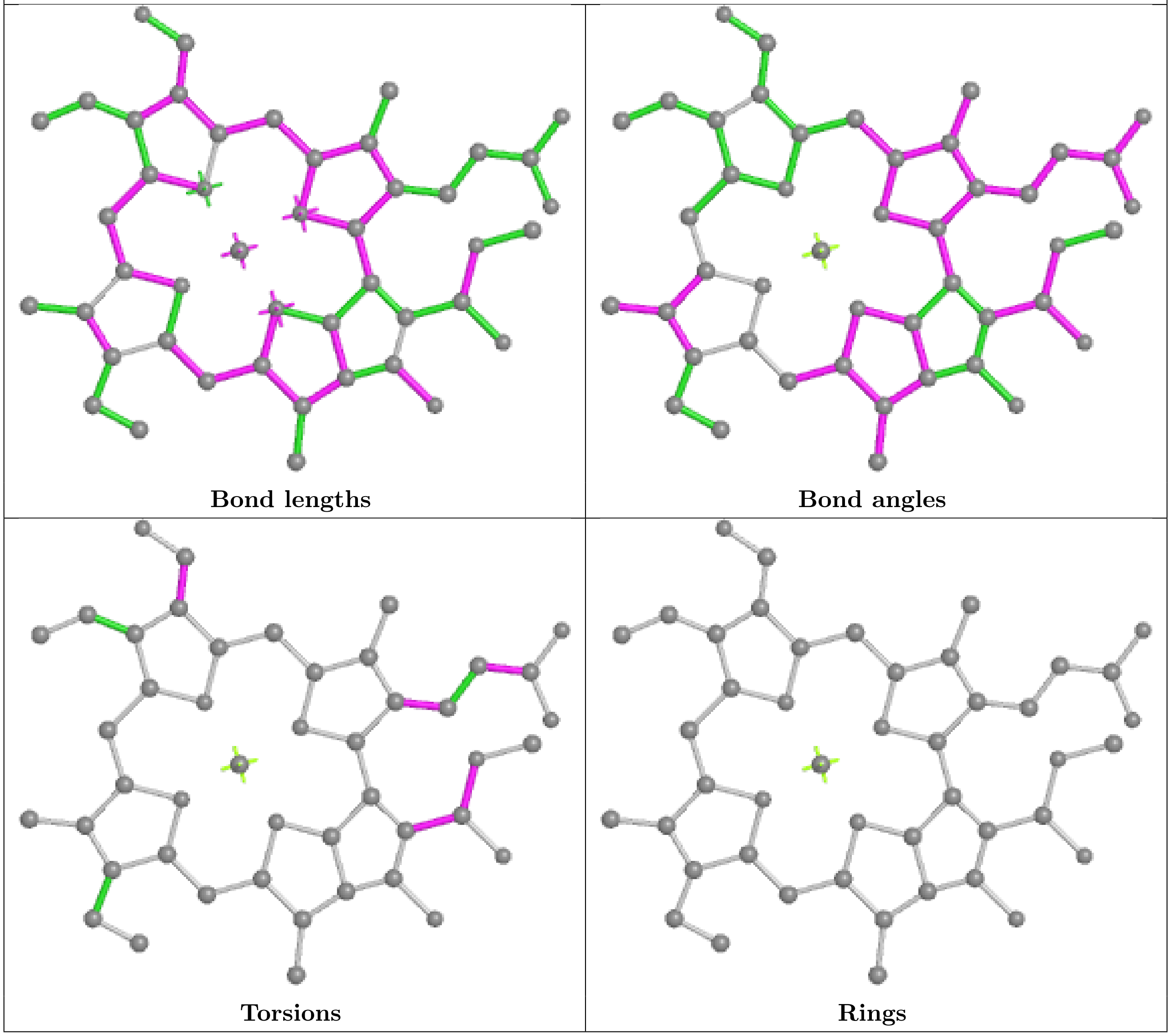
Bond angles



Torsions

Rings

Ligand F6C H 1230



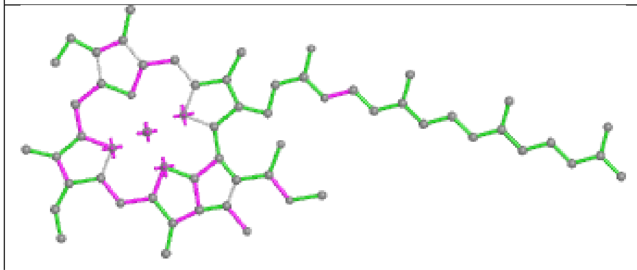
Bond lengths

Bond angles

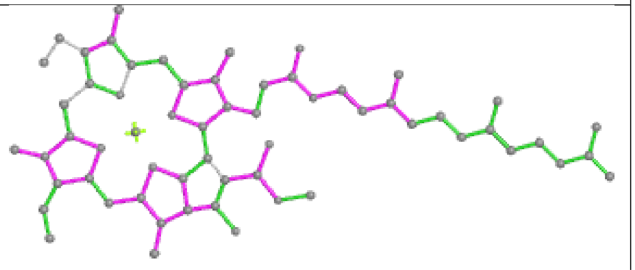
Torsions

Rings

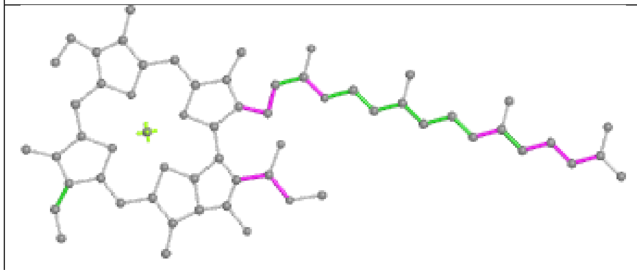
Ligand CLA a 1106



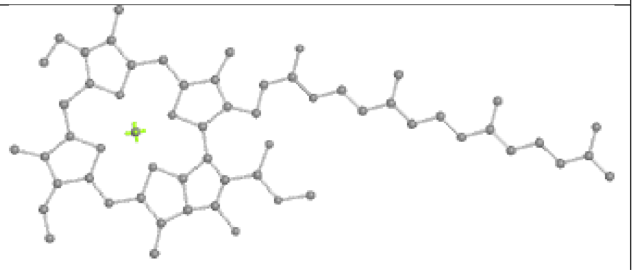
Bond lengths



Bond angles

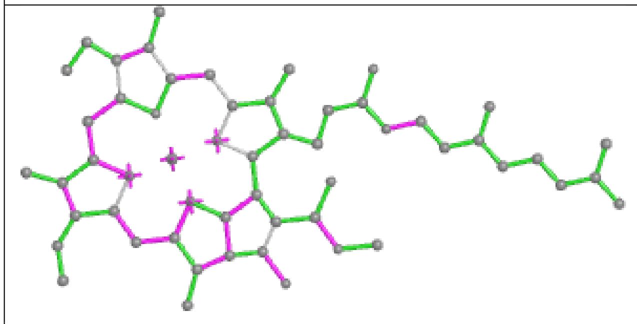


Torsions

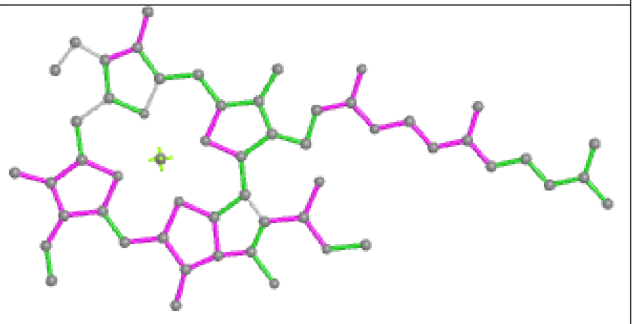


Rings

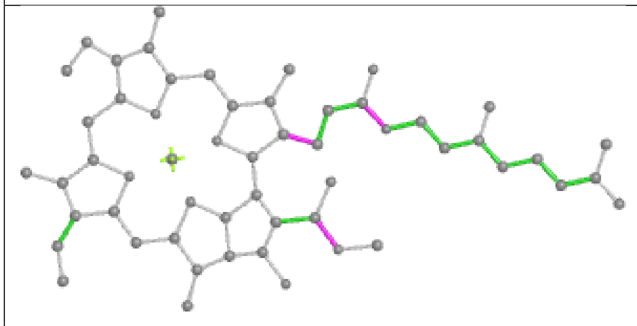
Ligand CLA H 1231



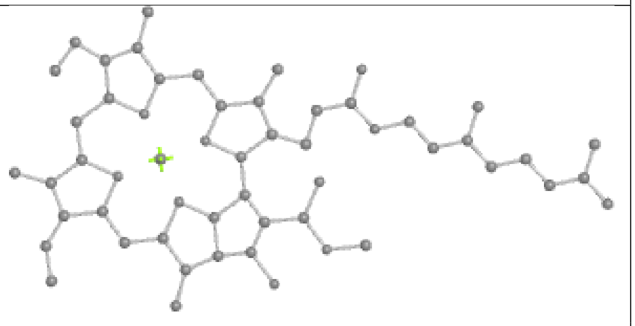
Bond lengths



Bond angles

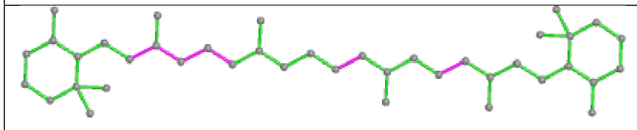


Torsions

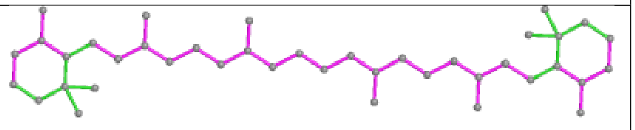


Rings

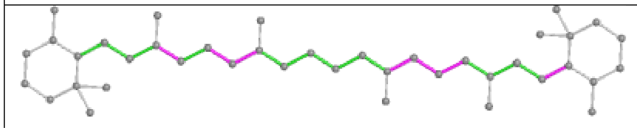
Ligand BCR H 4013



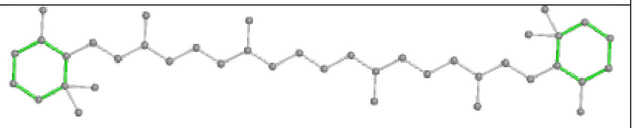
Bond lengths



Bond angles

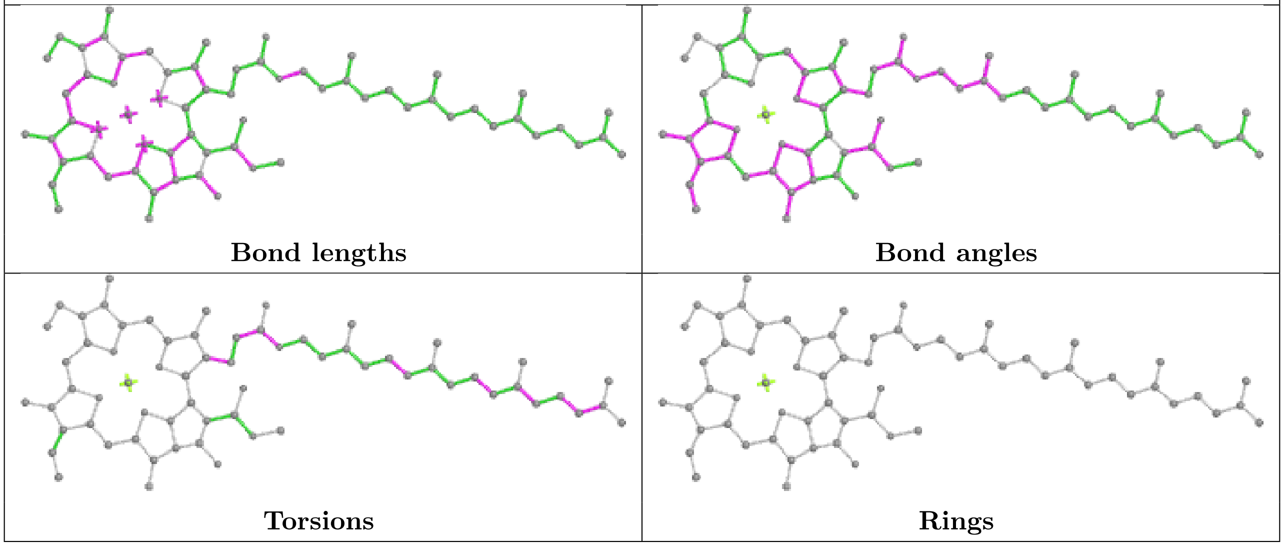


Torsions

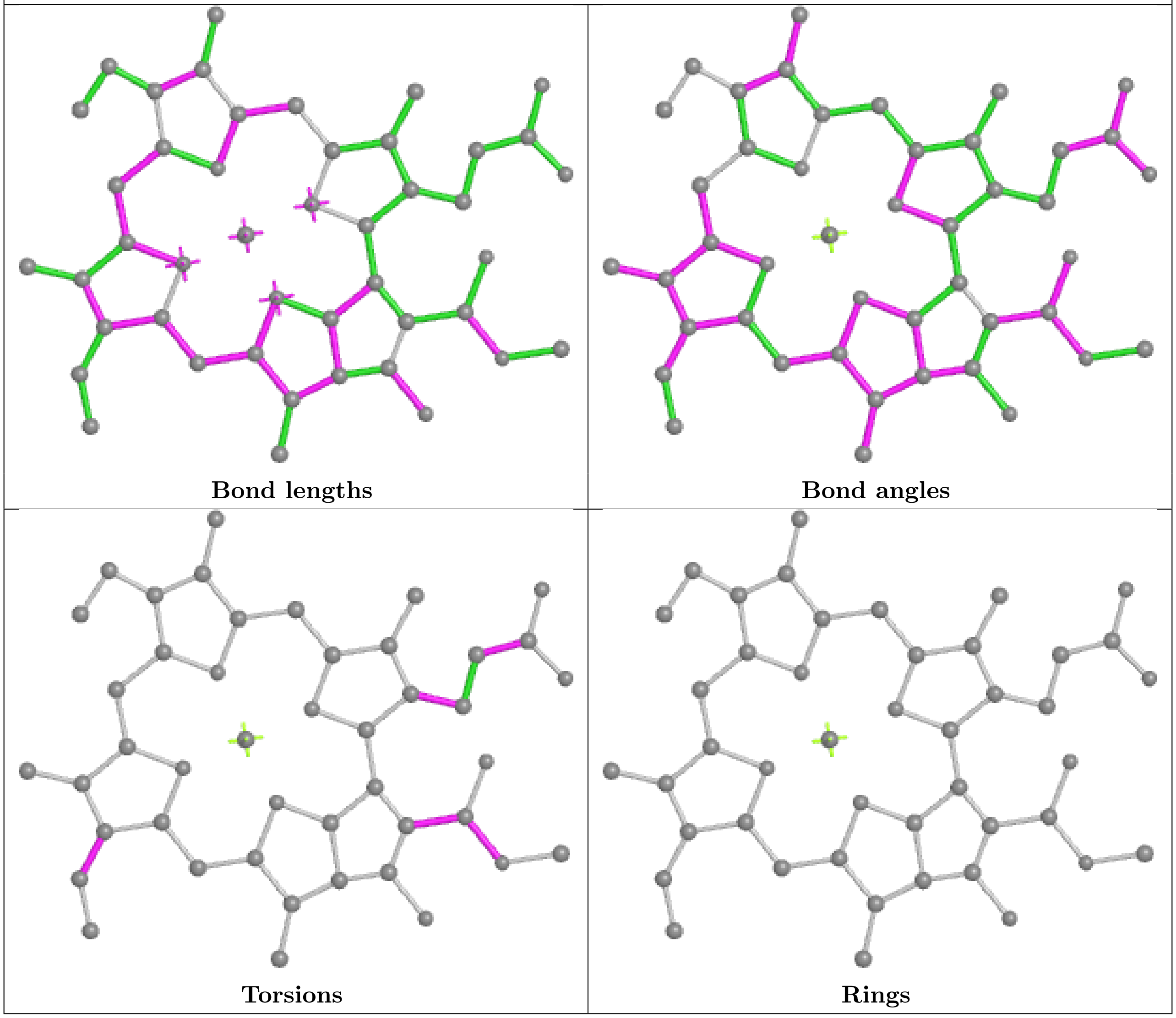


Rings

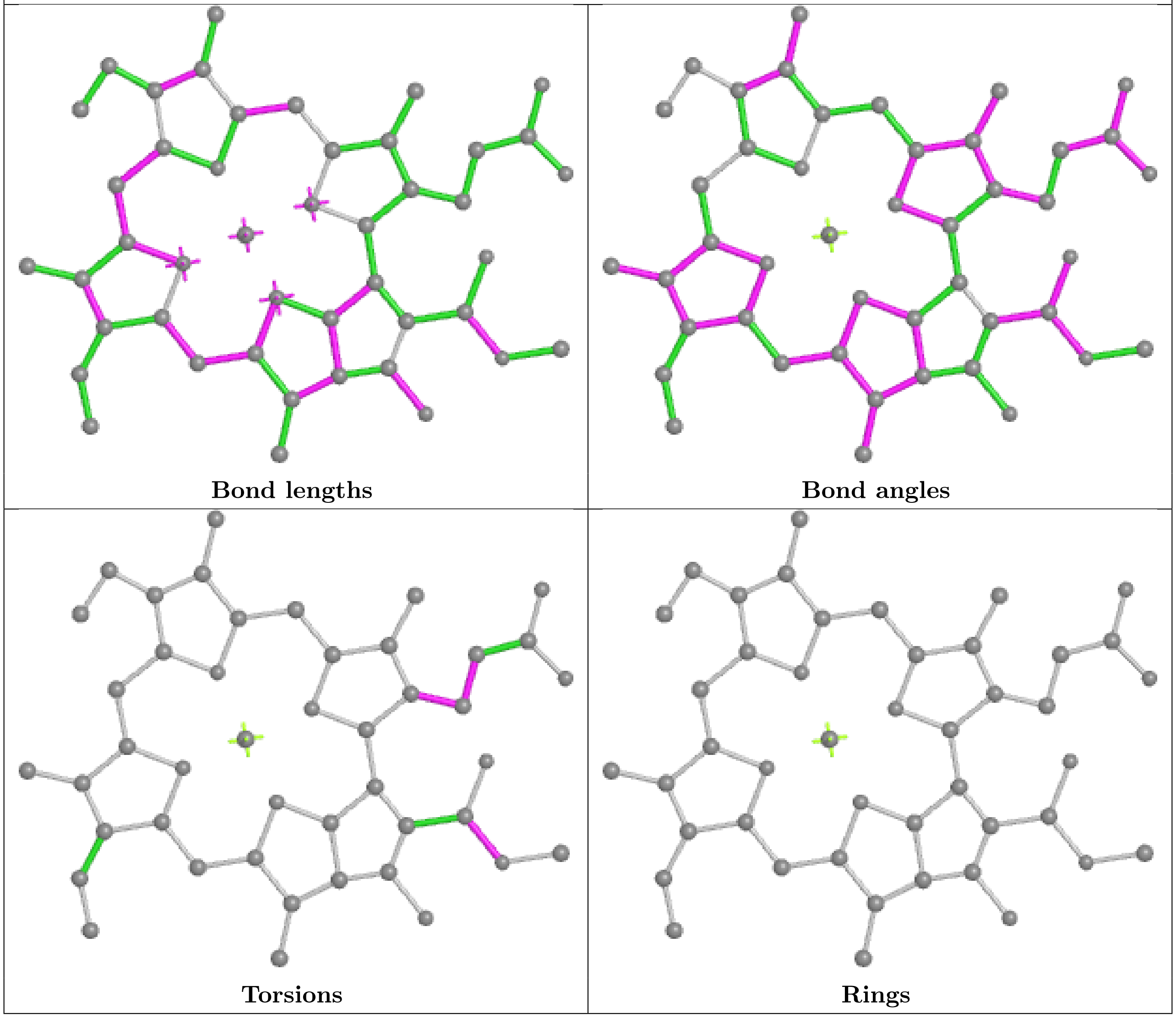
Ligand CL0 A 1011



Ligand CLA a 1114



Ligand CLA b 1212



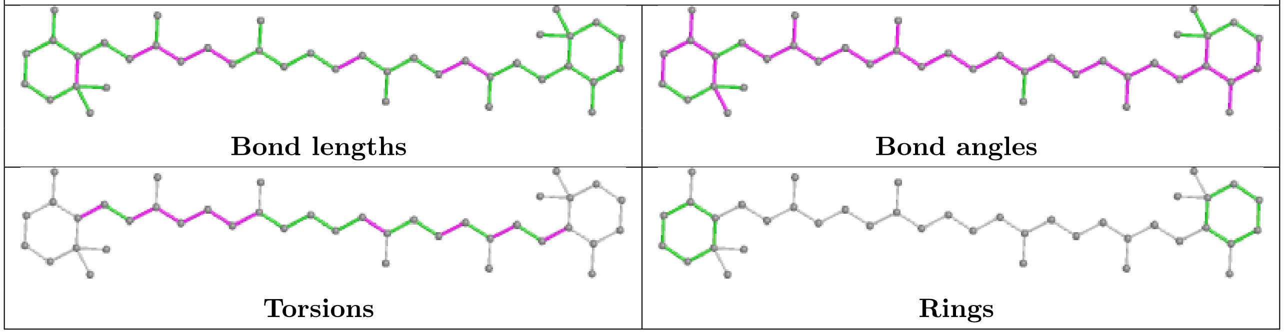
Bond lengths

Bond angles

Torsions

Rings

Ligand BCR A 4011



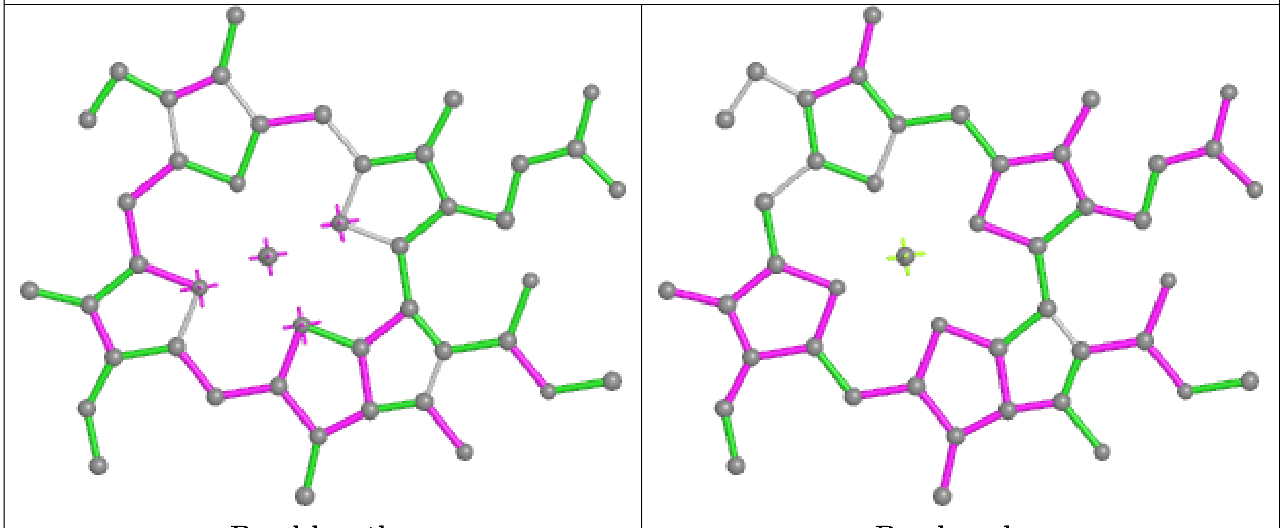
Bond lengths

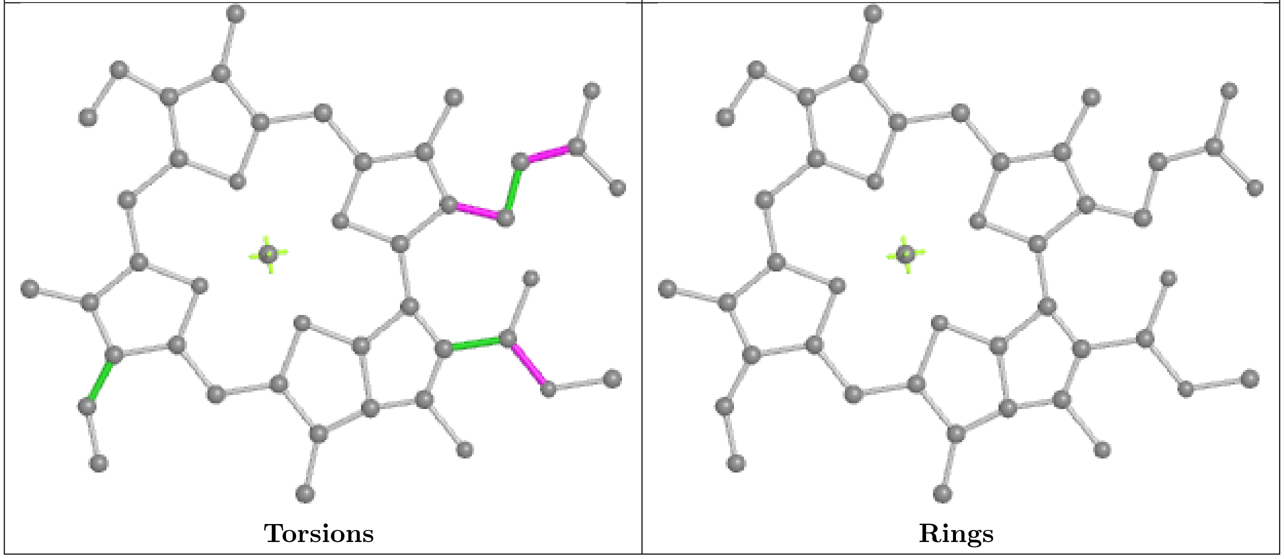
Bond angles

Torsions

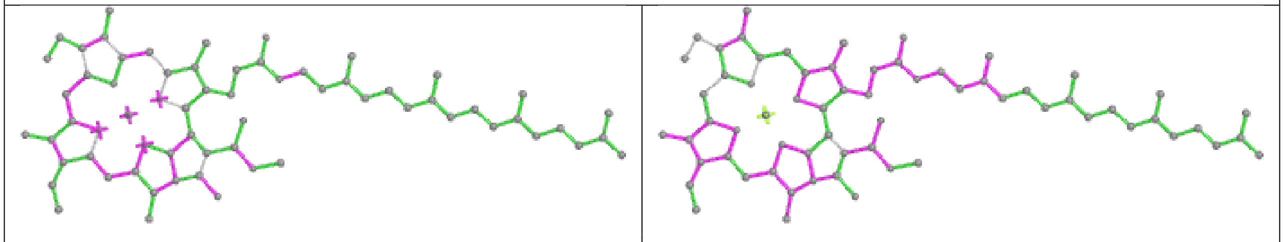
Rings

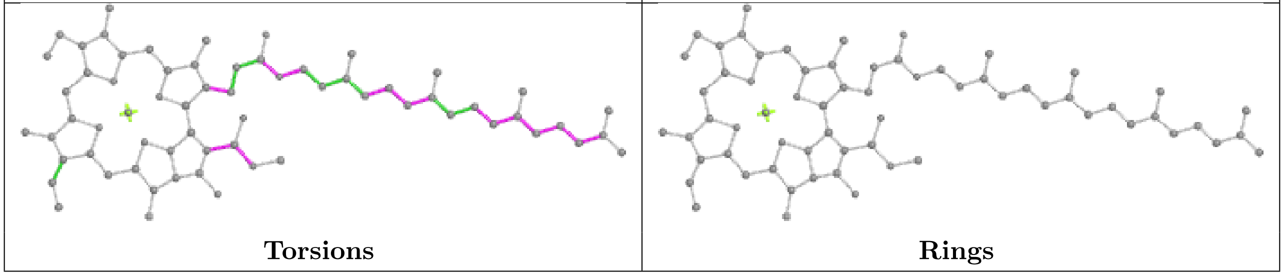
Ligand CLA a 1105


Bond lengths Bond angles

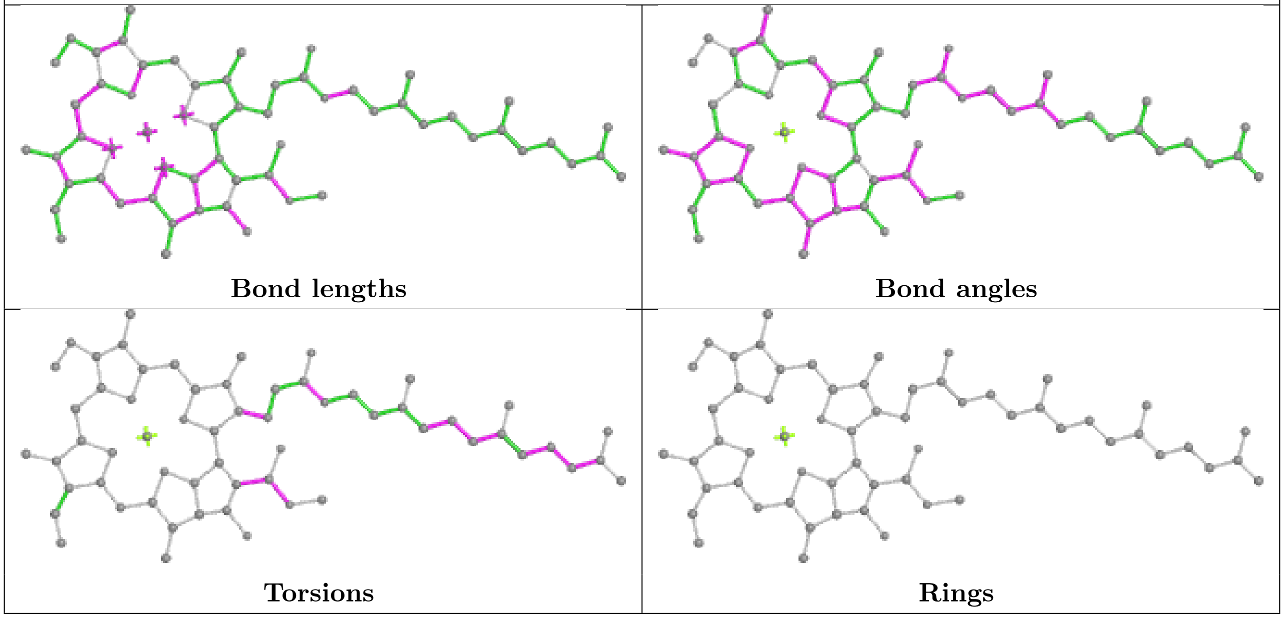

Torsions Rings

Ligand CLA a 1115


Bond lengths Bond angles


Torsions Rings

Ligand CLA G 1102



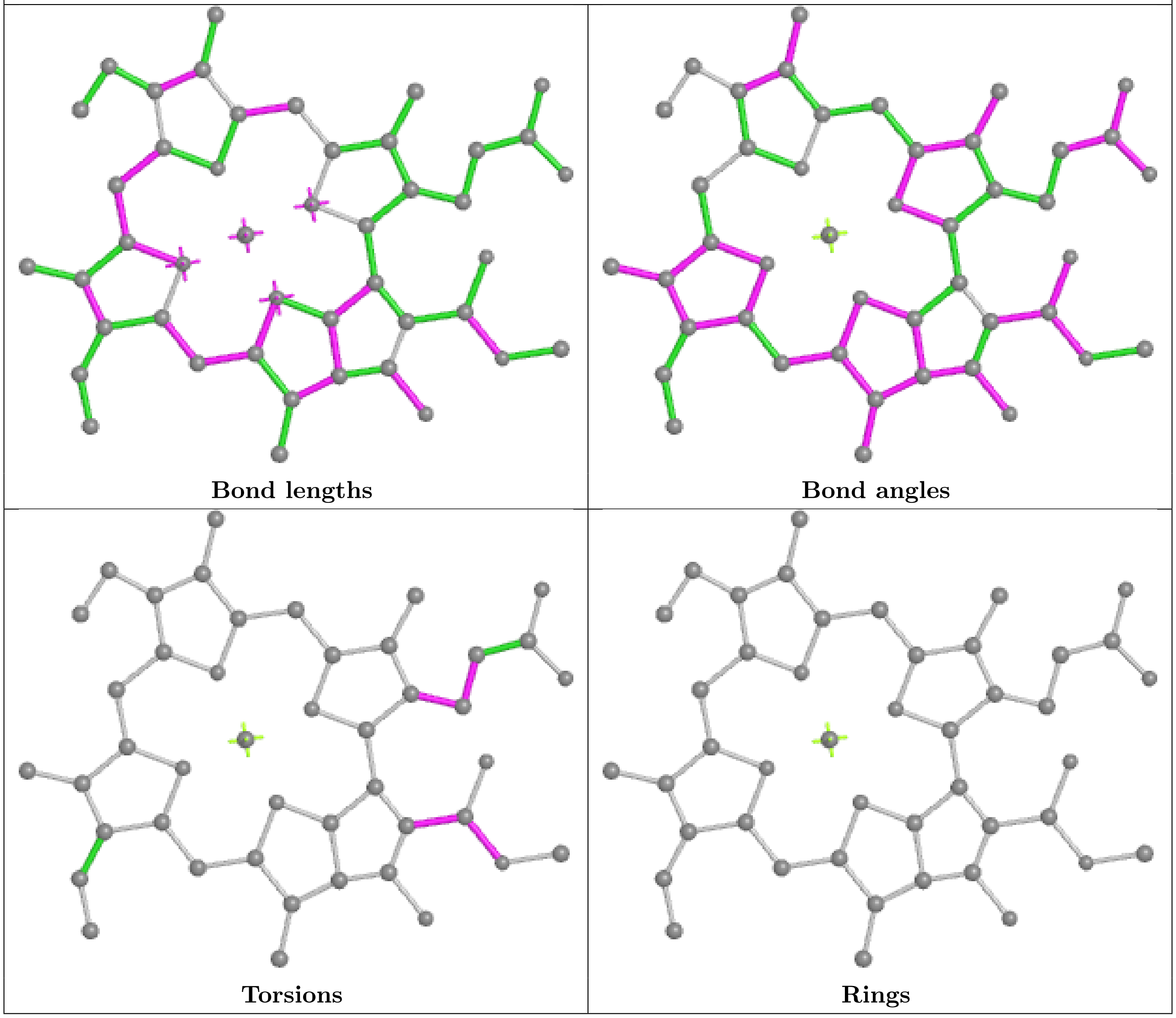
Bond lengths

Bond angles

Torsions

Rings

Ligand CLA G 1120



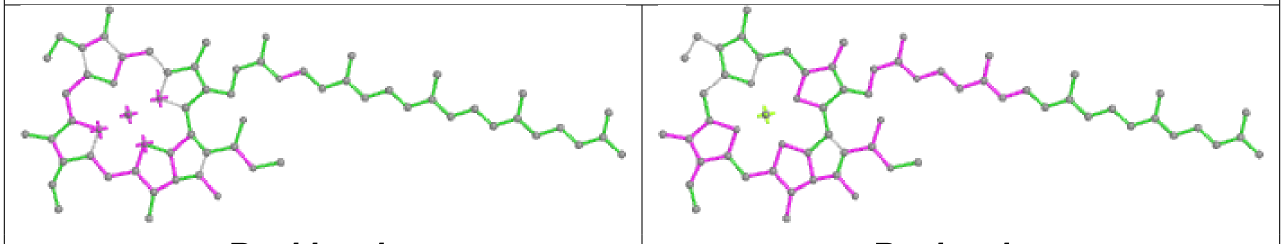
Bond lengths

Bond angles

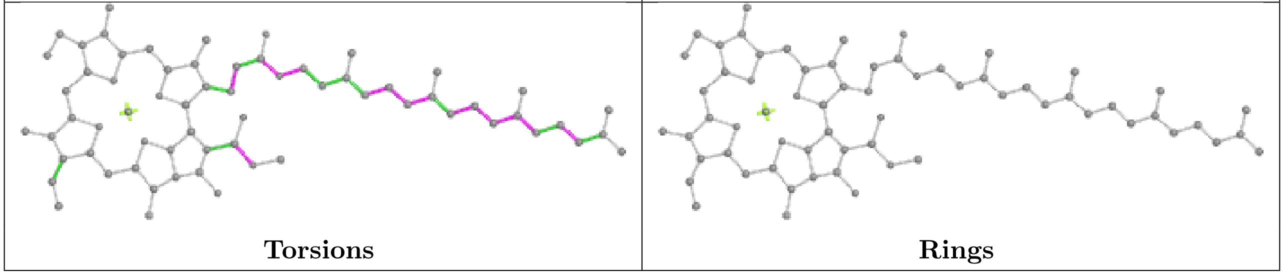
Torsions

Rings

Ligand CLA b 1214

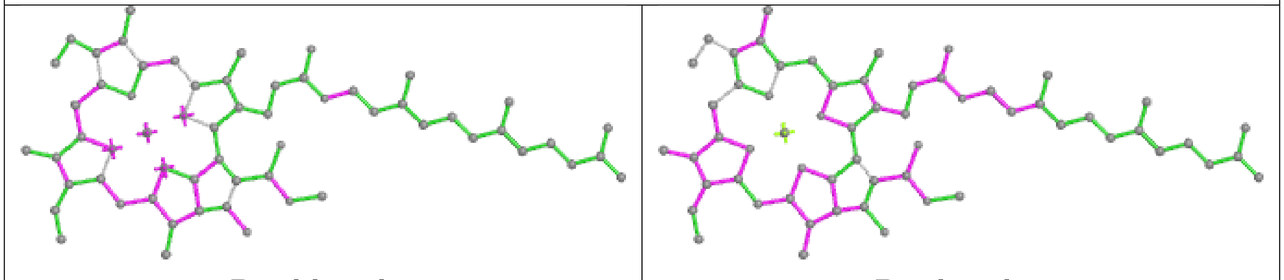


Bond lengths Bond angles

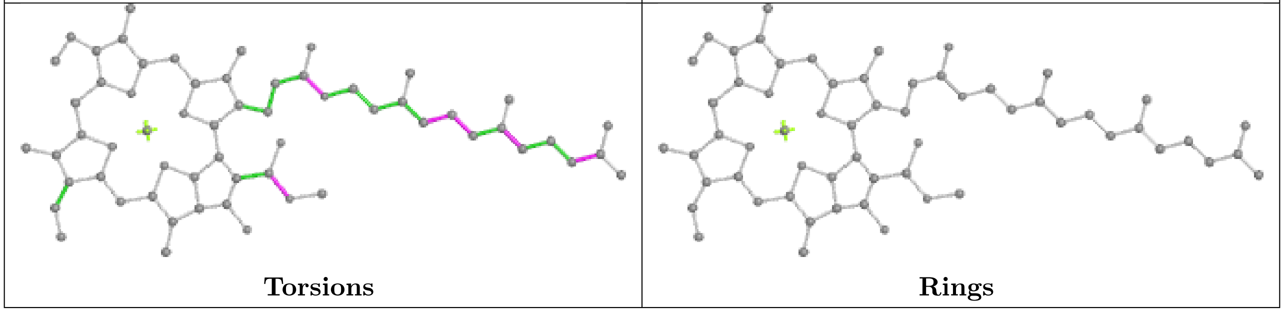


Torsions Rings

Ligand CLA a 1133

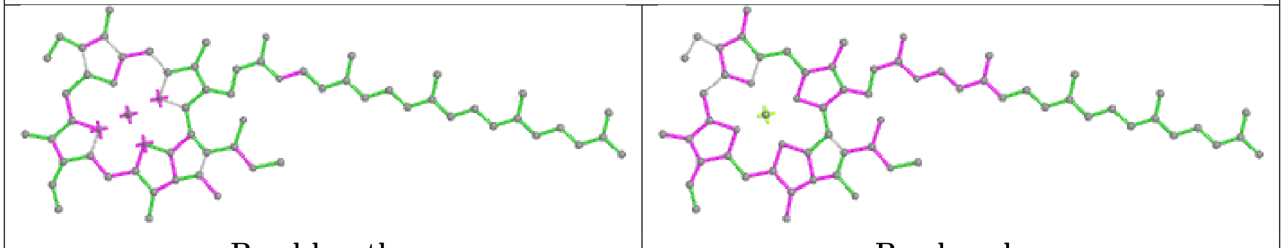


Bond lengths Bond angles



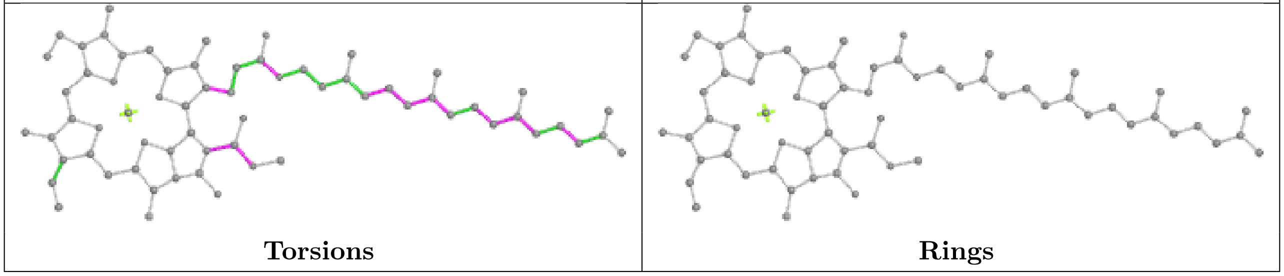
Torsions Rings

Ligand CLA G 1117



Bond lengths

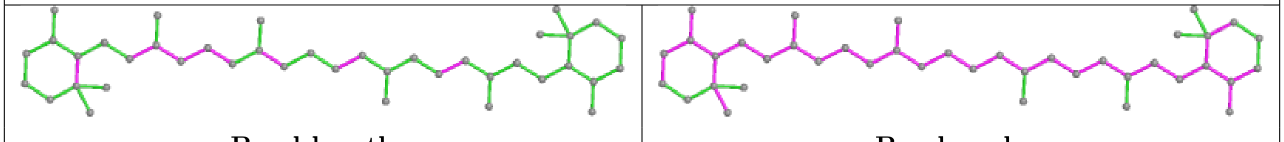
Bond angles



Torsions

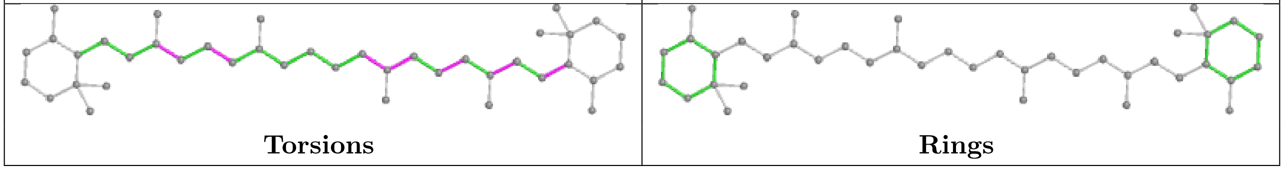
Rings

Ligand BCR a 4007



Bond lengths

Bond angles



Torsions

Rings

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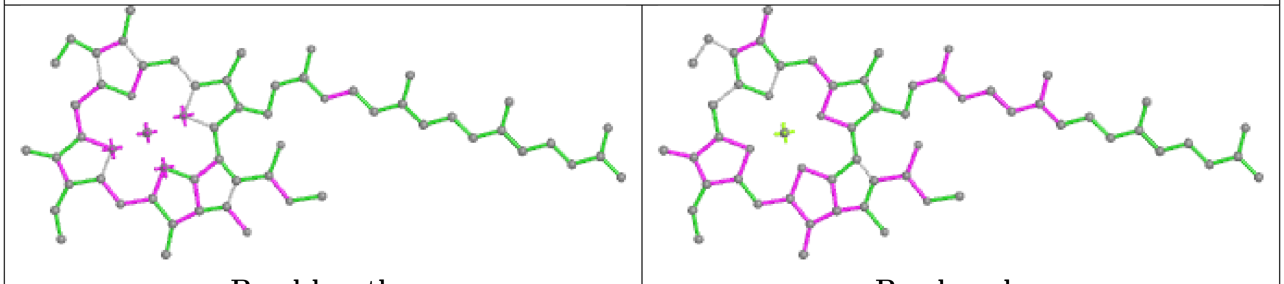
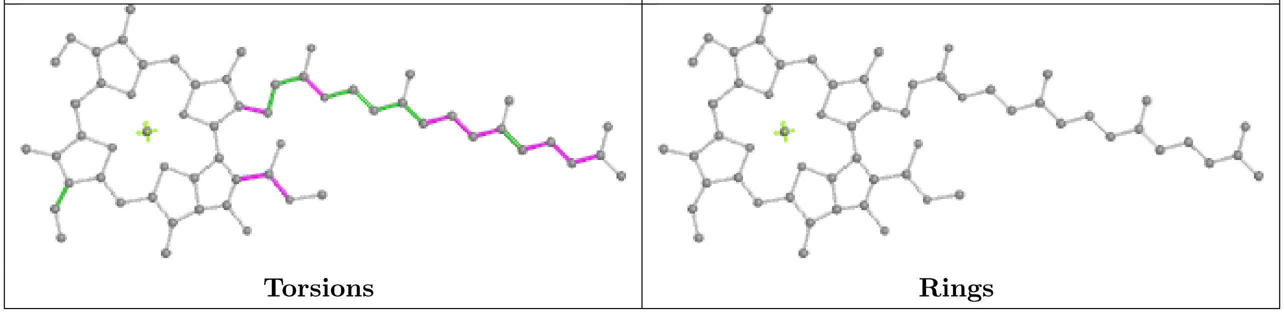


Bond lengths

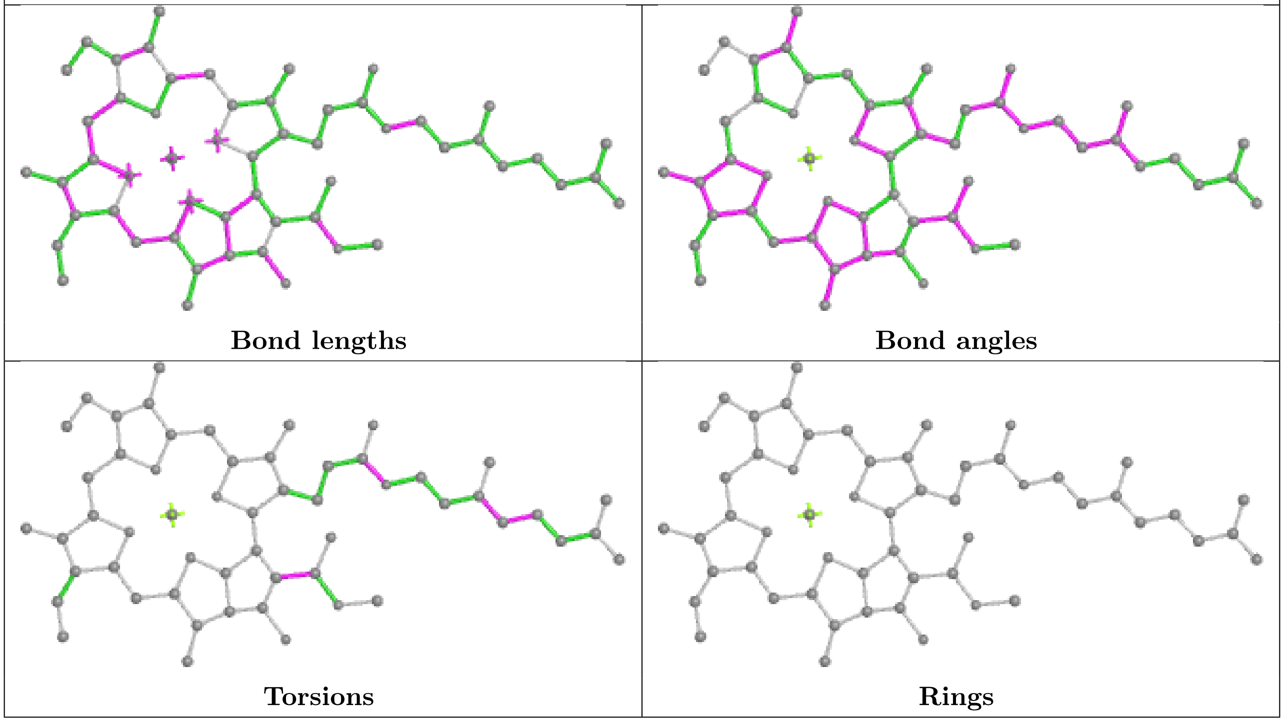
Bond angles



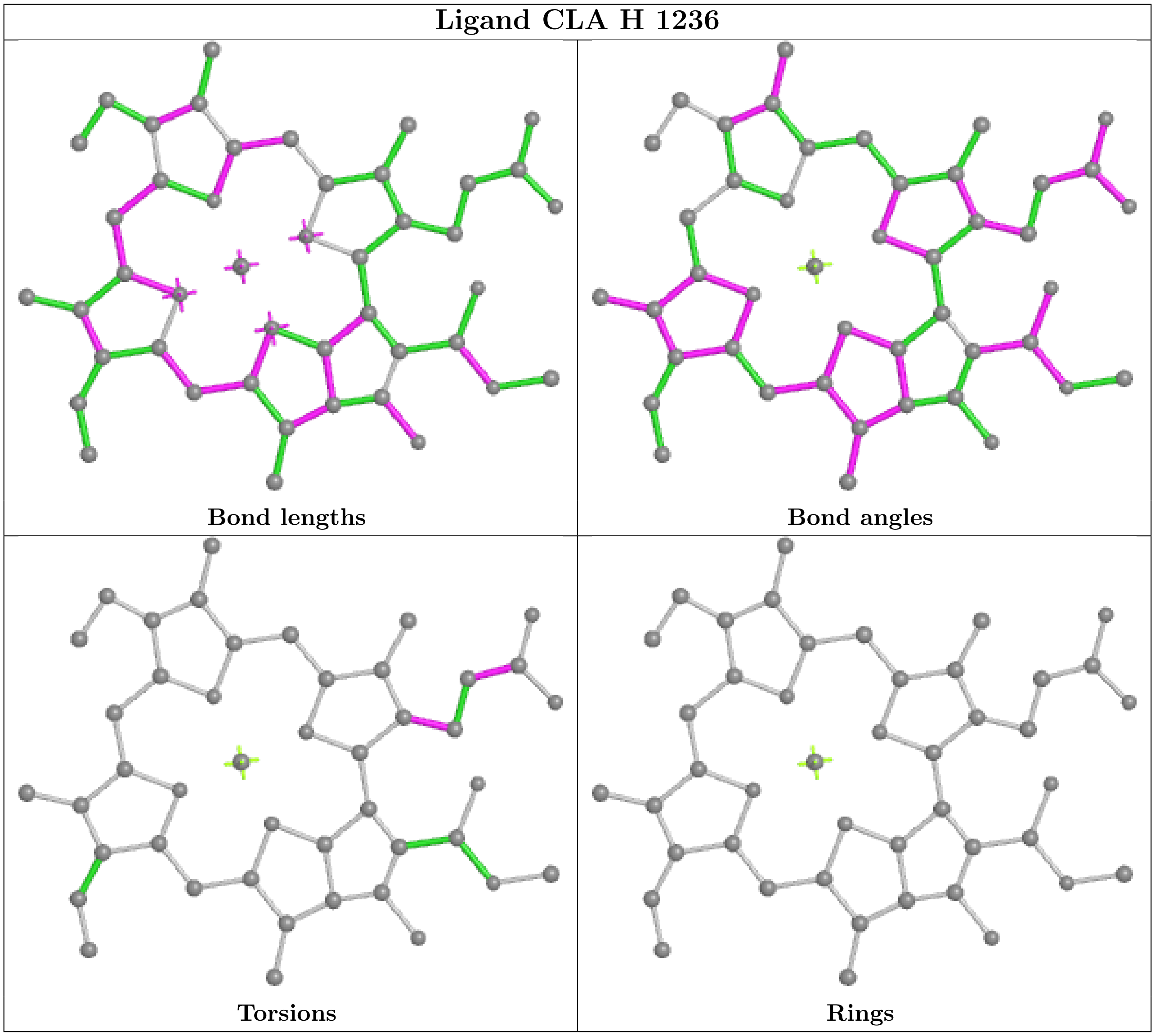
Torsions

Rings

Ligand CLA B 1201



Ligand CLA H 1236



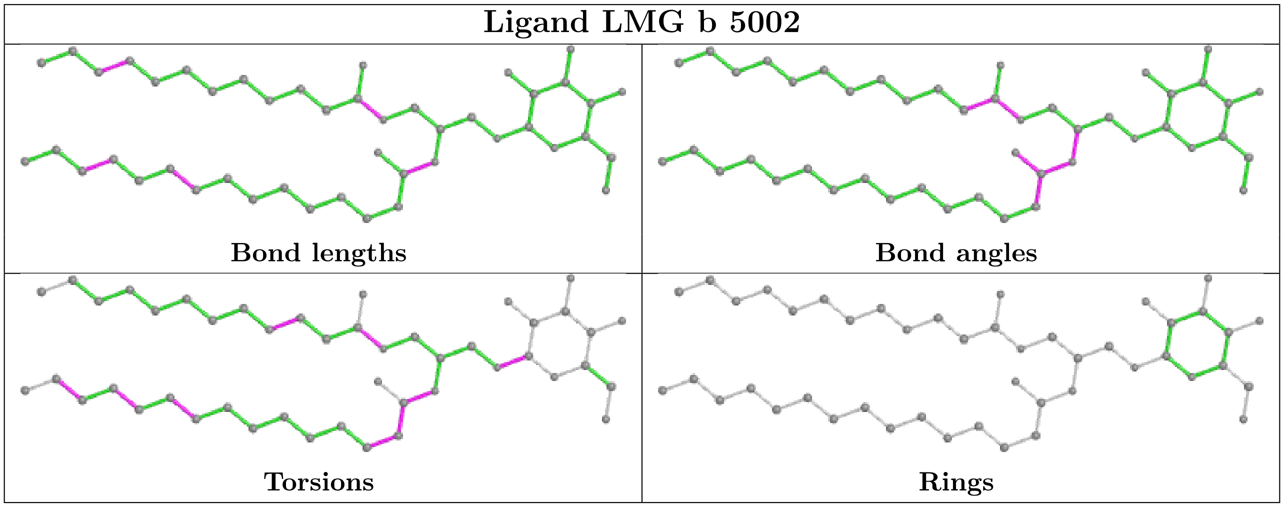
Bond lengths

Bond angles

Torsions

Rings

Ligand LMG b 5002



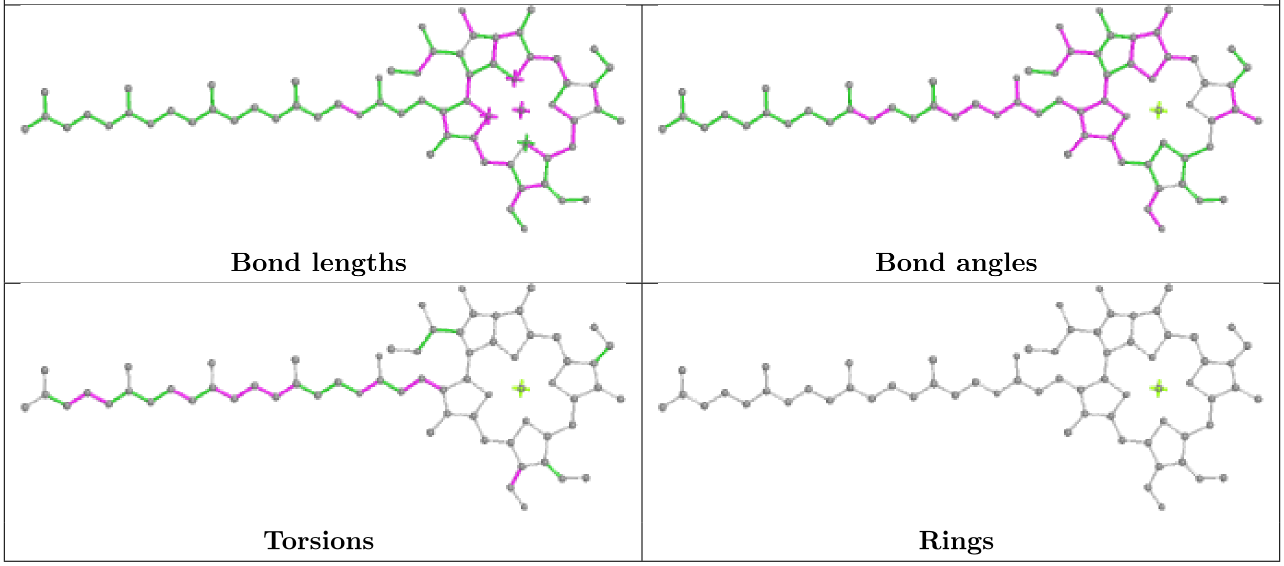
Bond lengths

Bond angles

Torsions

Rings

Ligand F6C b 1238



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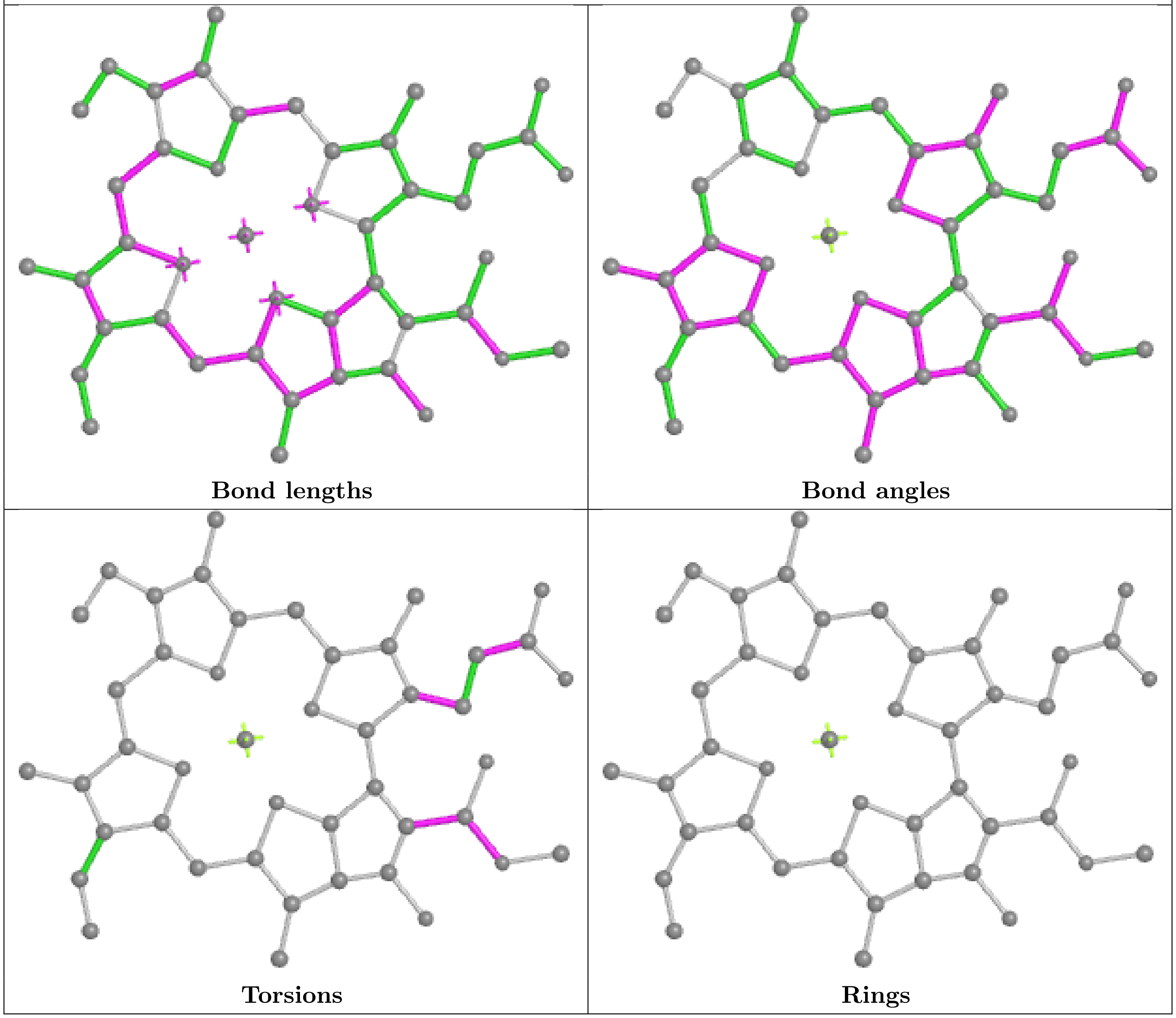

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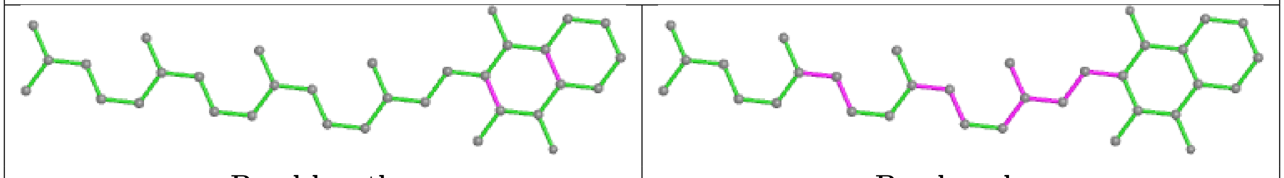
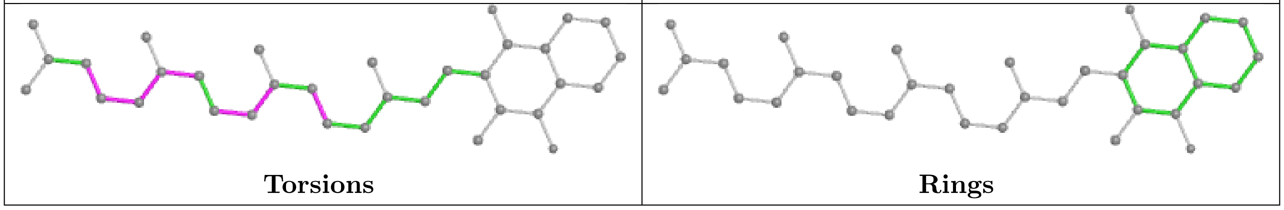


Bond lengths

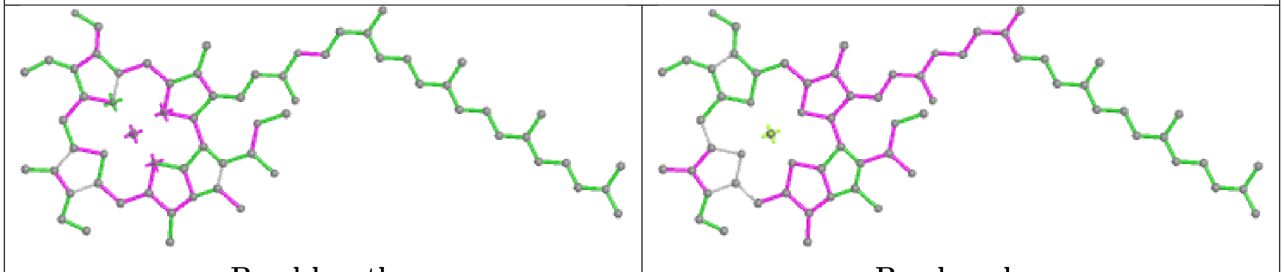
Bond angles



Torsions

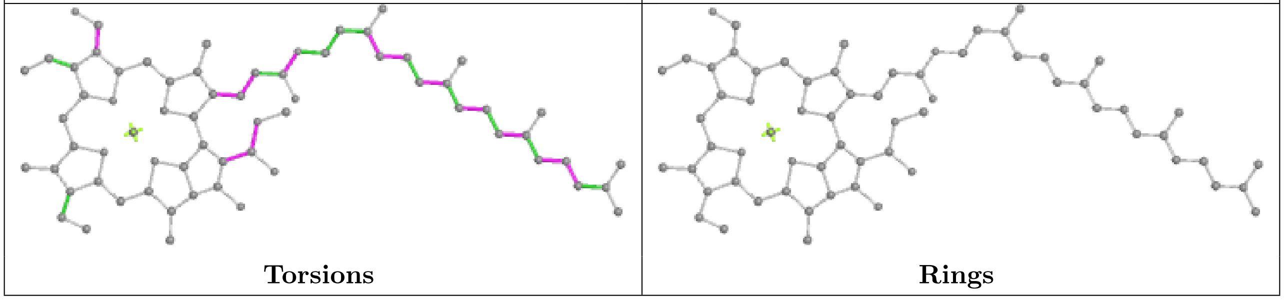
Rings

Ligand F6C H 1237



Bond lengths

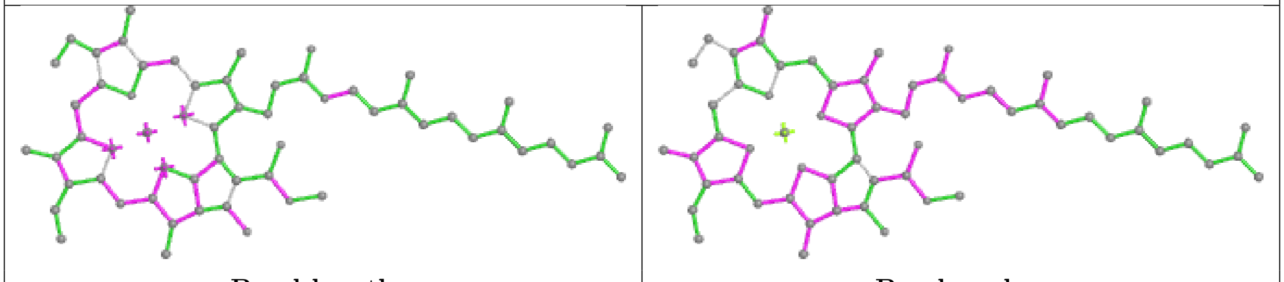
Bond angles



Torsions

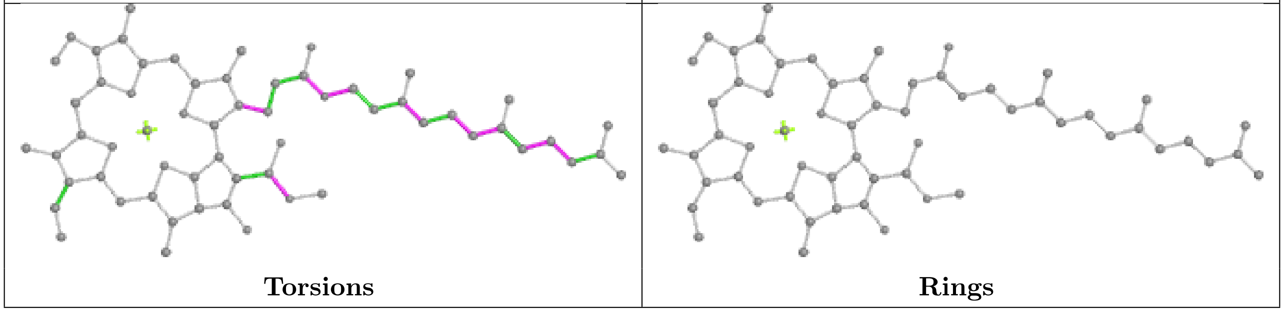
Rings

Ligand CLA B 1229



Bond lengths

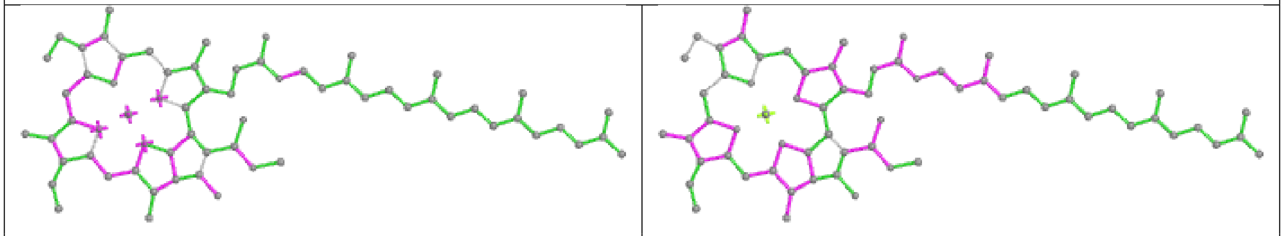
Bond angles



Torsions

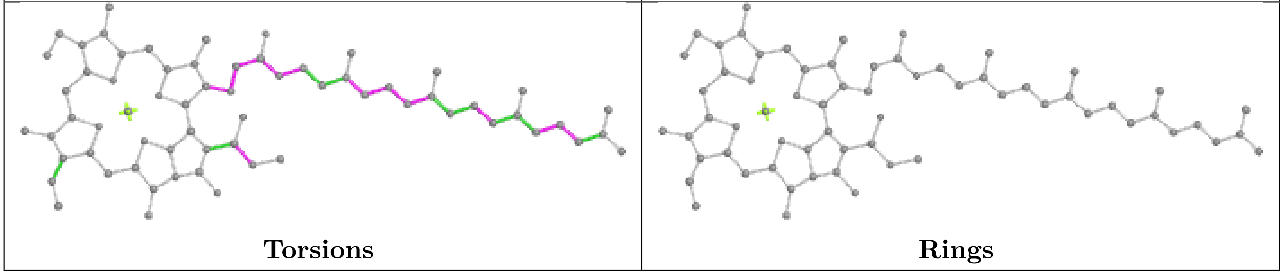
Rings

Ligand CLA G 1136



Bond lengths

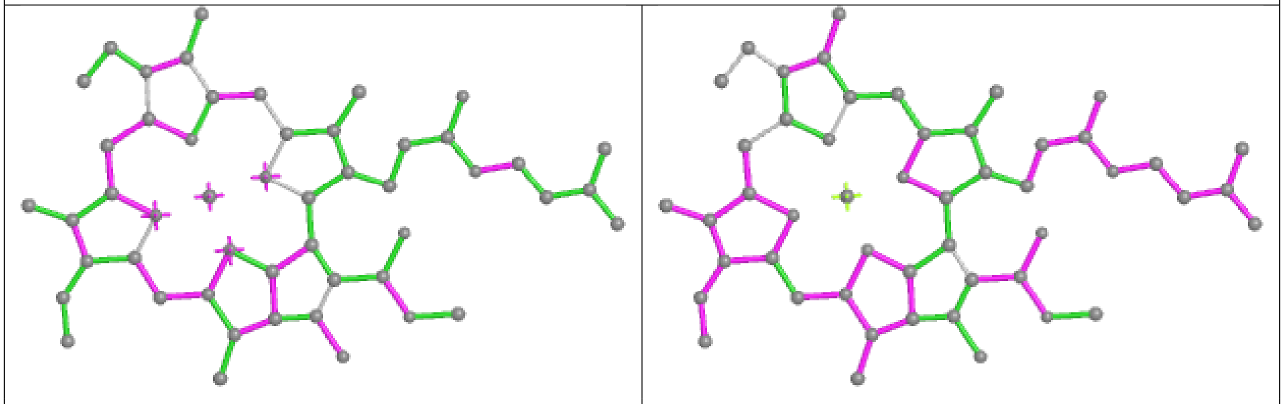
Bond angles



Torsions

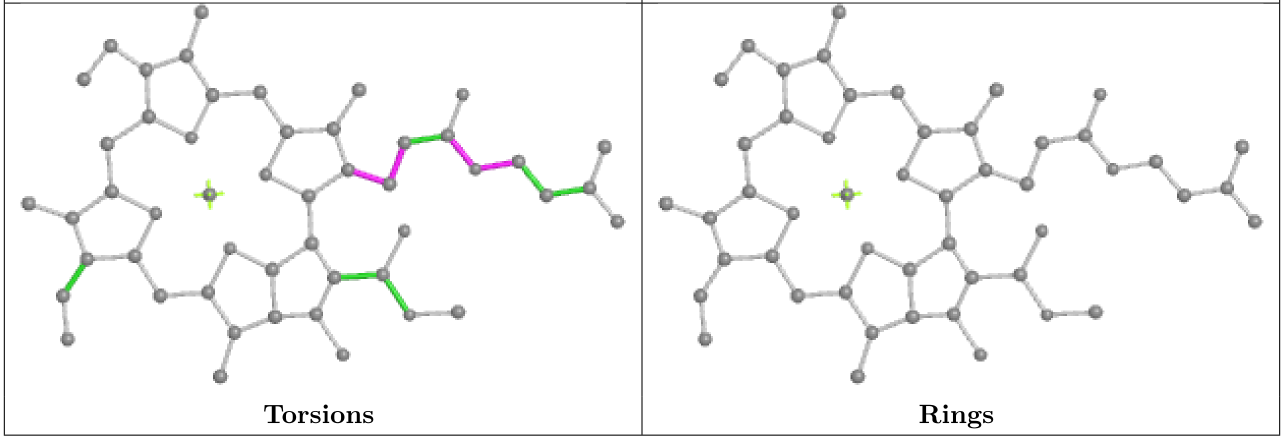
Rings

Ligand CLA a 1137



Bond lengths

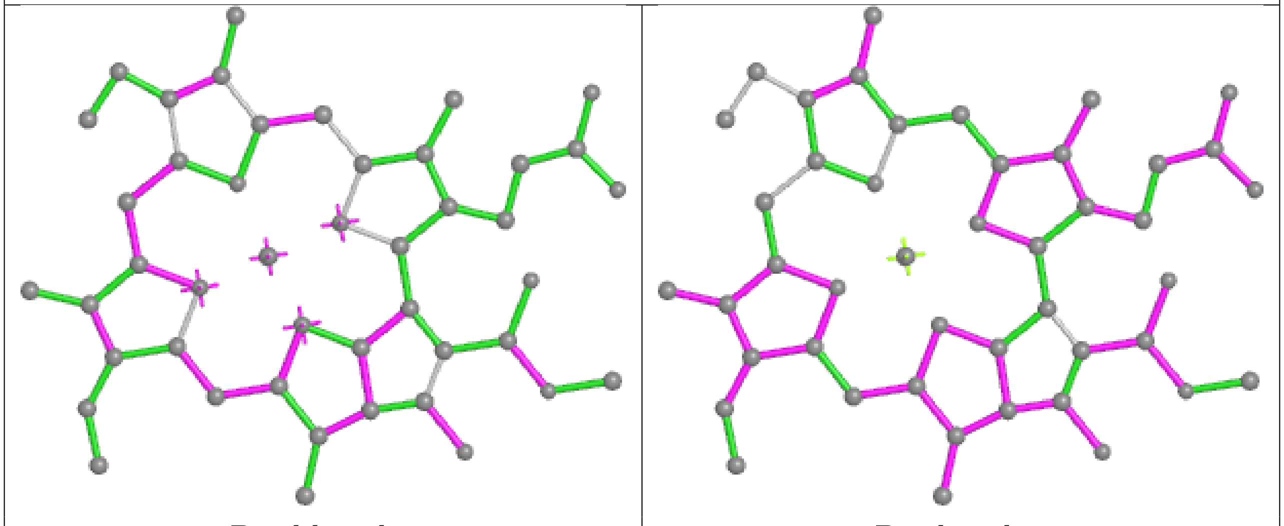
Bond angles



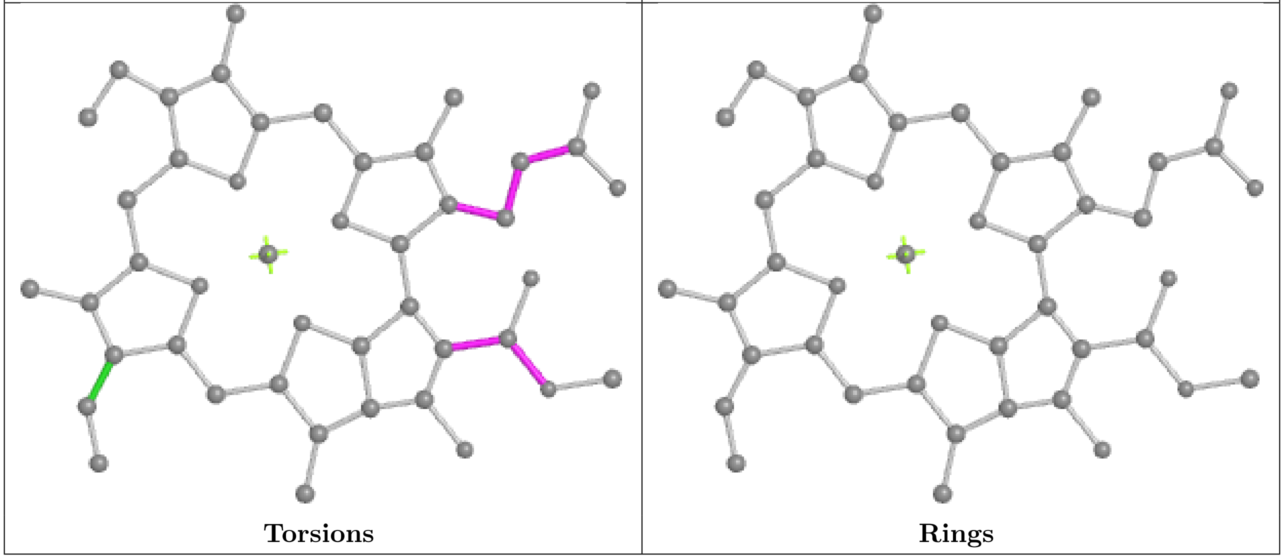
Torsions

Rings

Ligand CLA A 1113

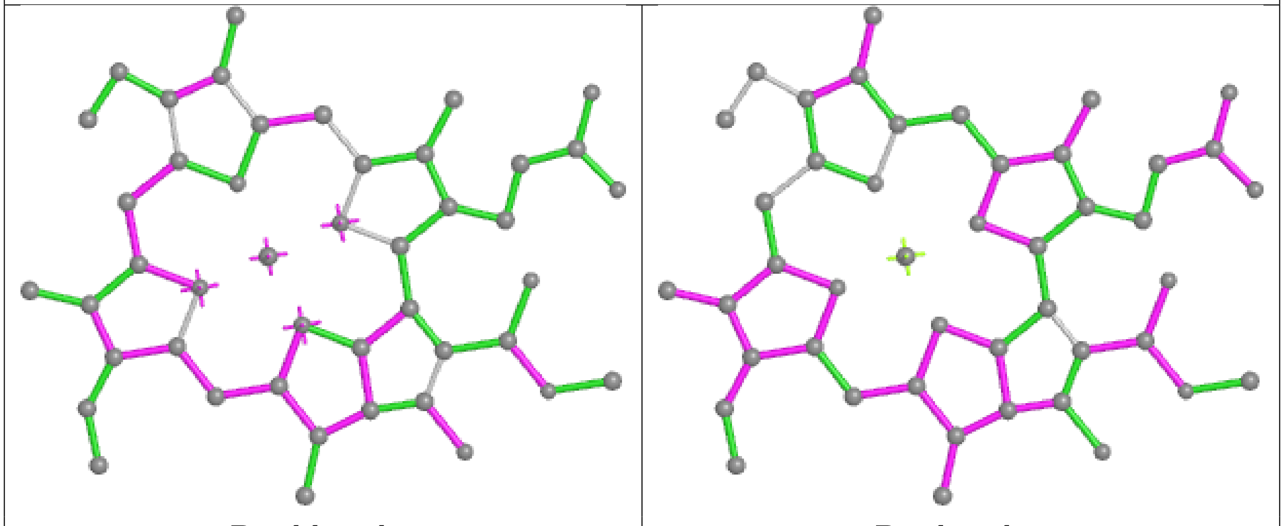


Bond lengths **Bond angles**



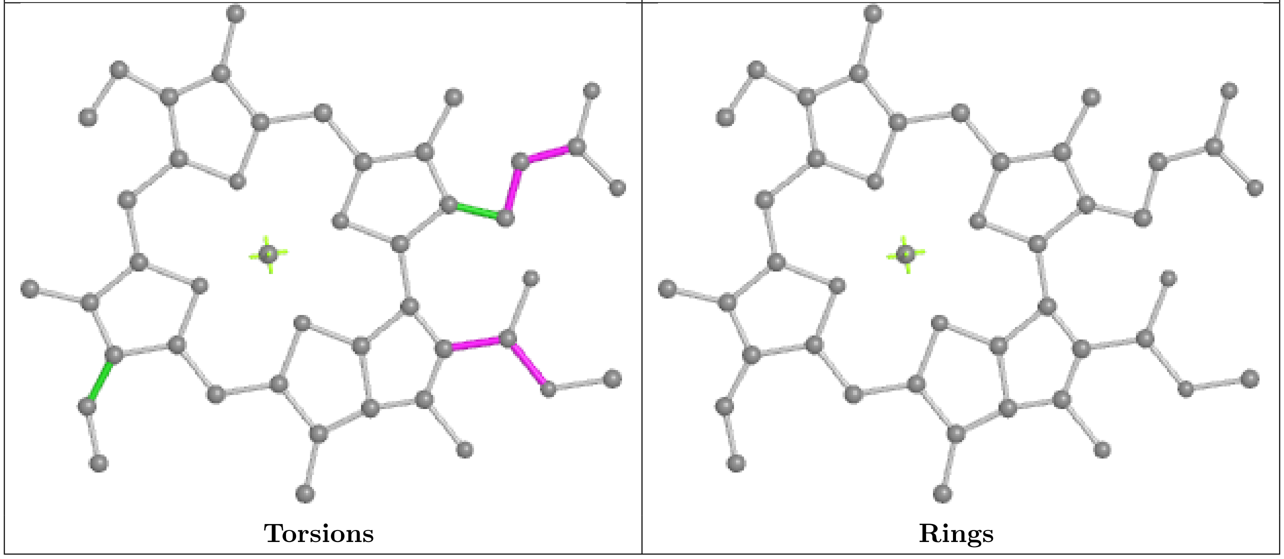
Torsions **Rings**

Ligand CLA A 1134



Bond lengths

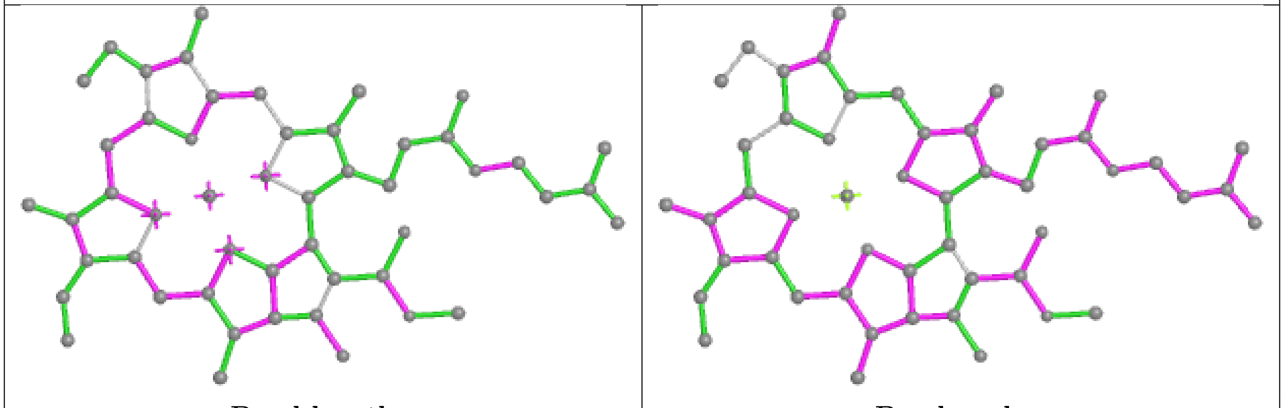
Bond angles



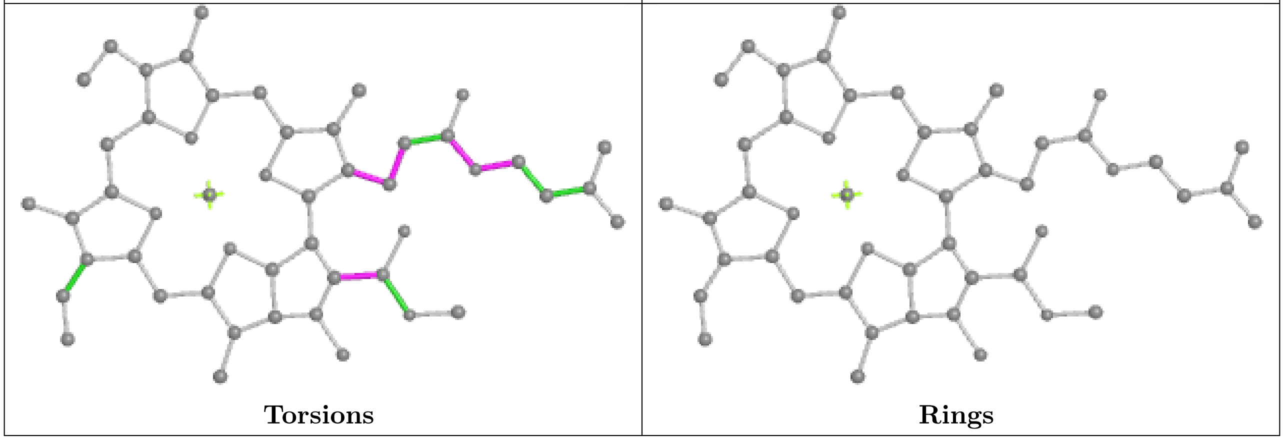
Torsions

Rings

Ligand CLA G 1129

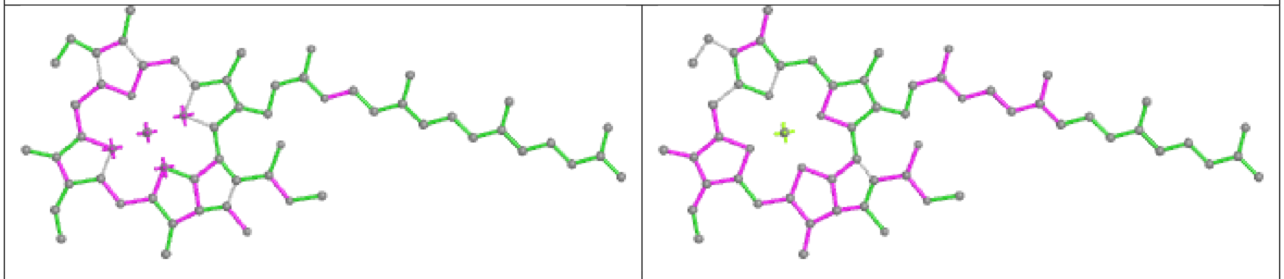


Bond lengths Bond angles

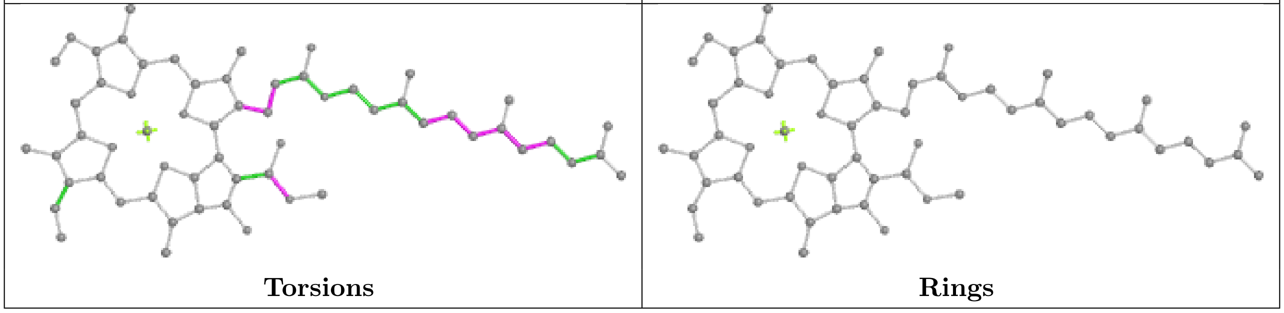


Torsions Rings

Ligand CLA a 1135

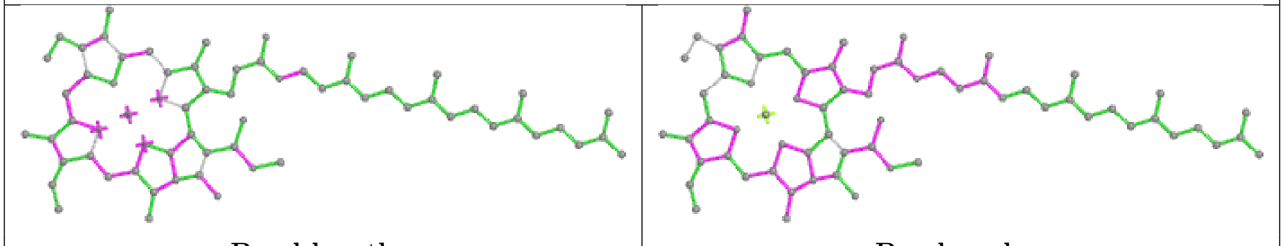


Bond lengths Bond angles

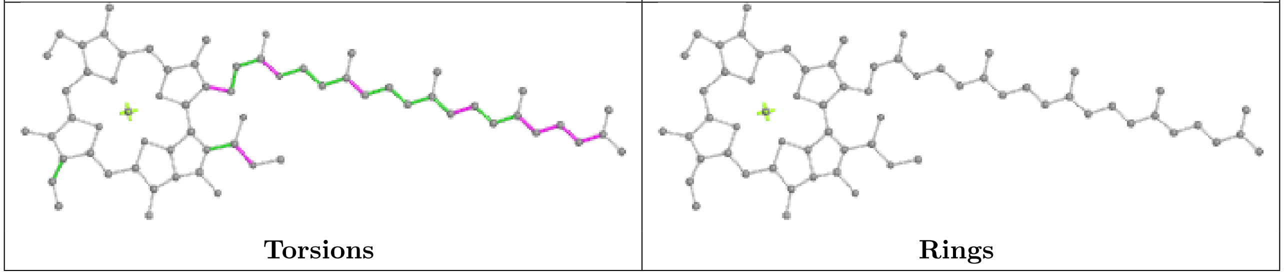


Torsions Rings

Ligand CLA L 1503

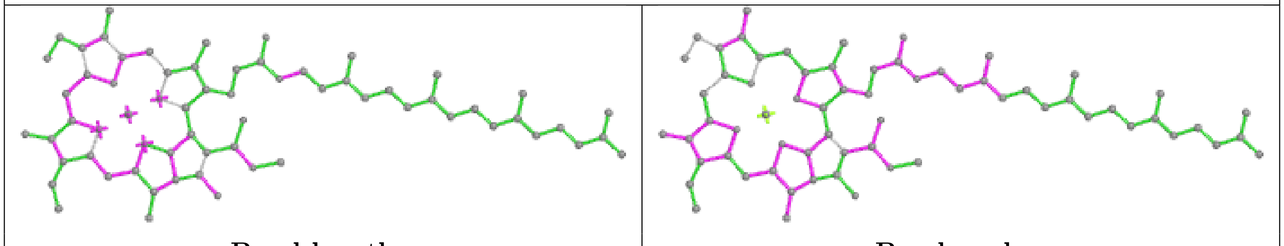


Bond lengths Bond angles

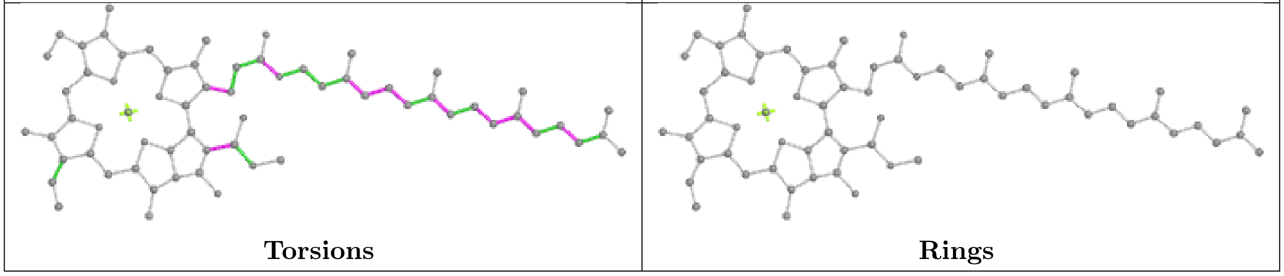


Torsions Rings

Ligand CLA b 1203

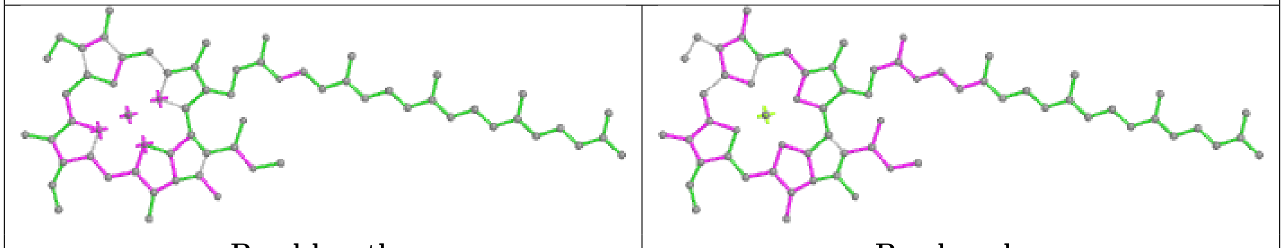


Bond lengths Bond angles

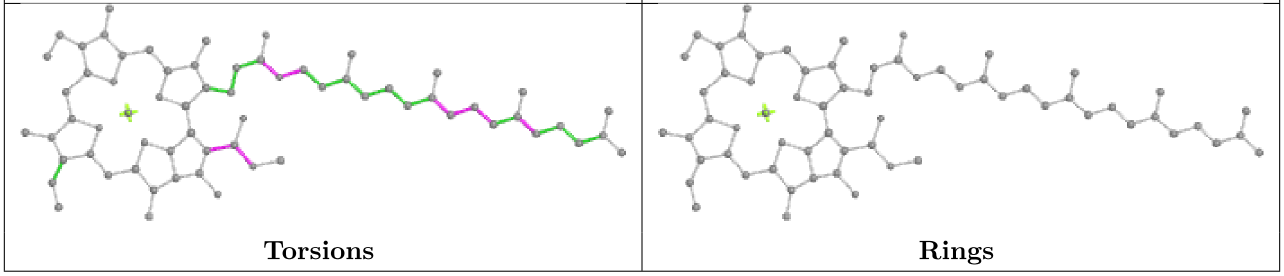


Torsions Rings

Ligand CLA G 1119

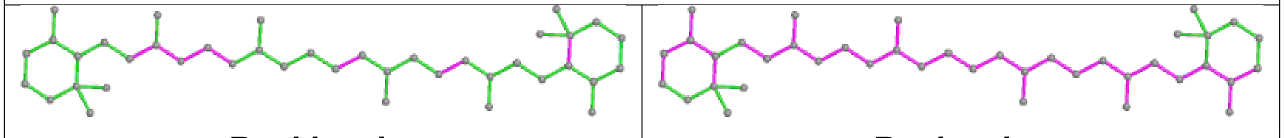


Bond lengths Bond angles

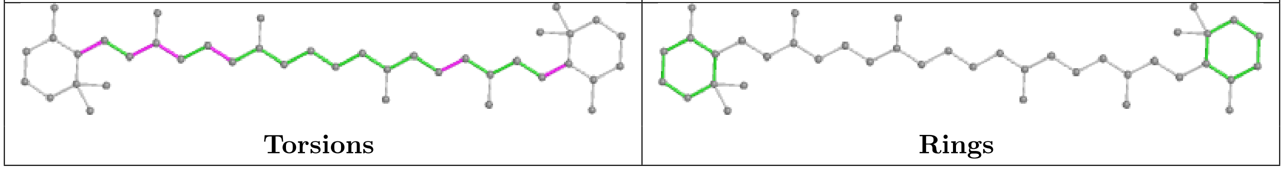


Torsions Rings

Ligand BCR B 4009

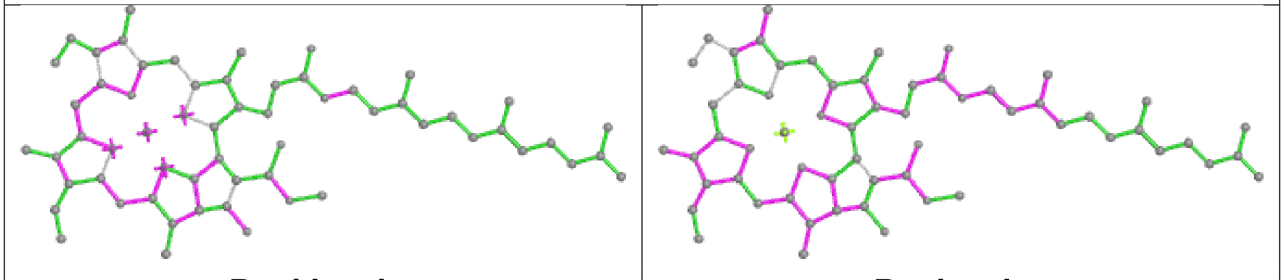

Bond lengths

Bond angles

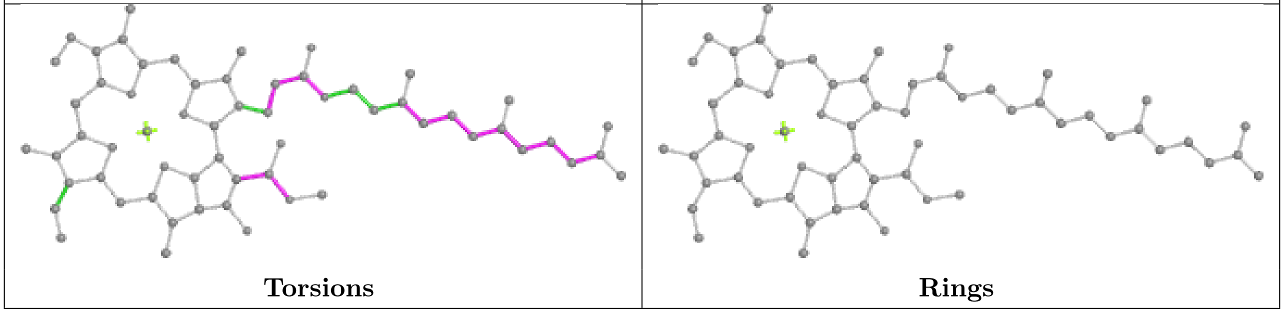

Torsions

Rings

Ligand CLA a 1126

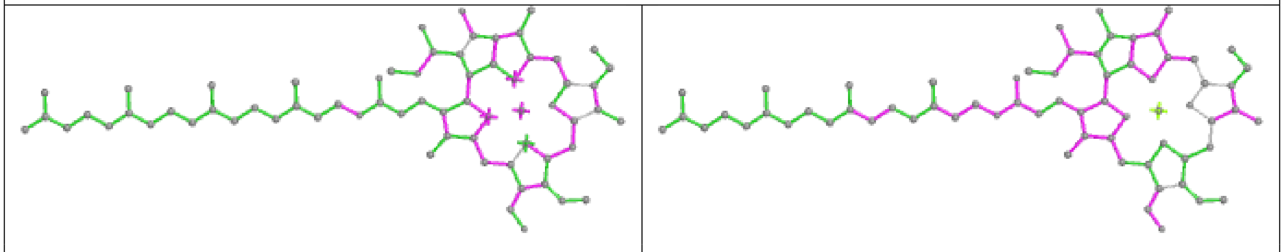

Bond lengths

Bond angles

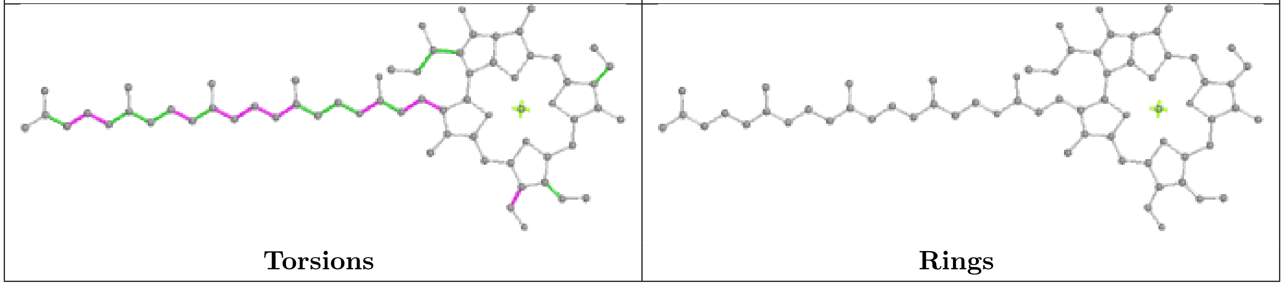

Torsions

Rings

Ligand F6C B 1238

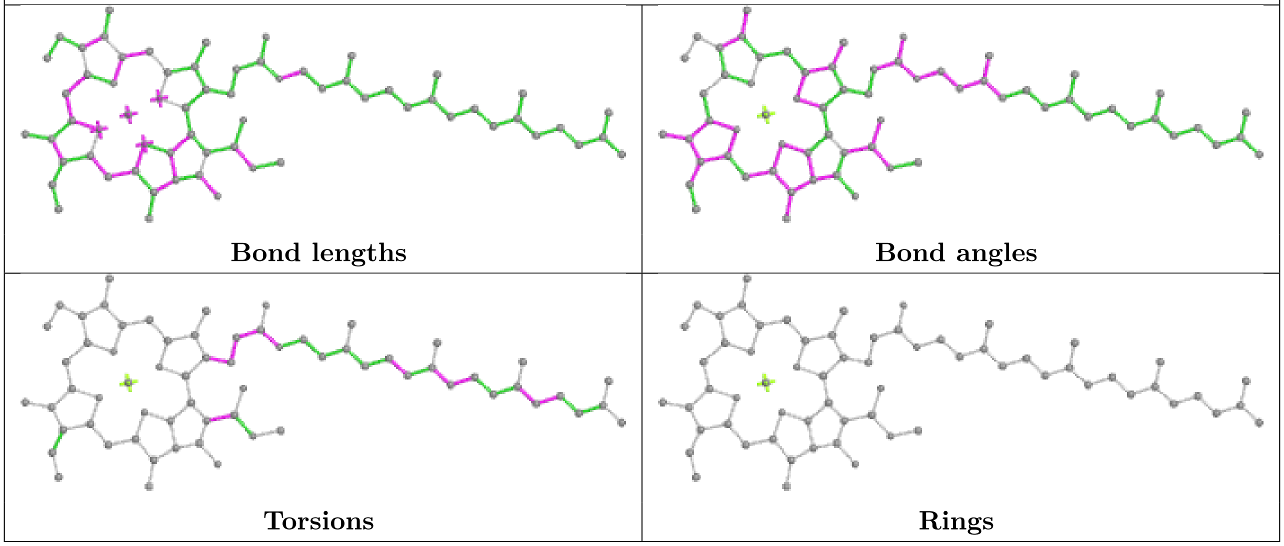

Bond lengths

Bond angles

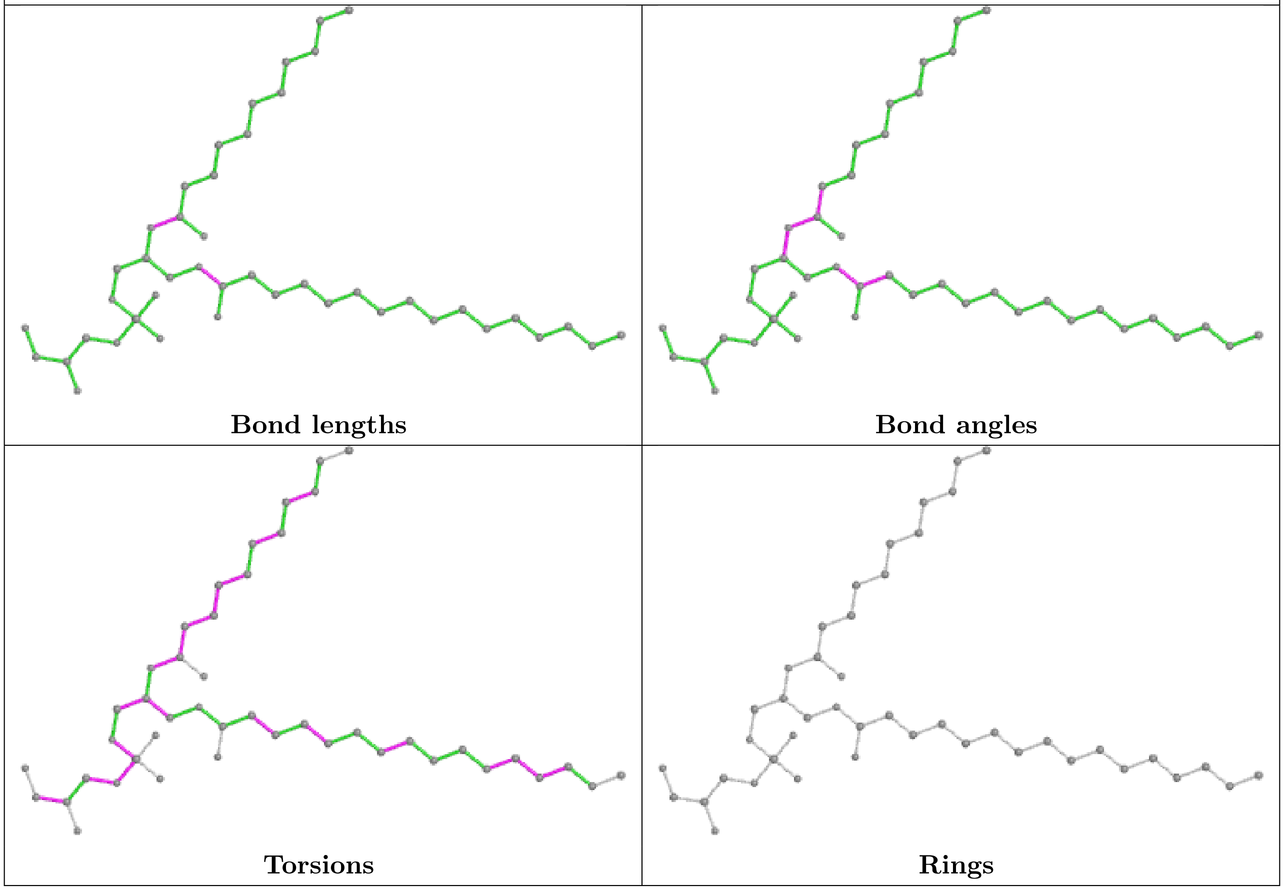

Torsions

Rings

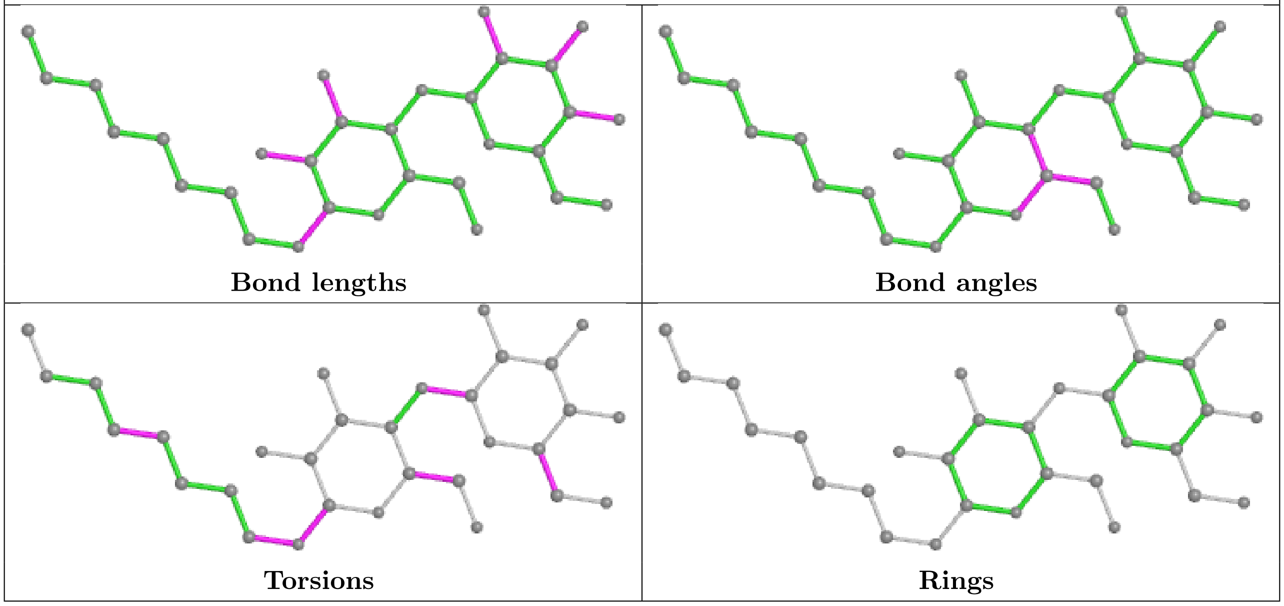
Ligand CLA G 1127



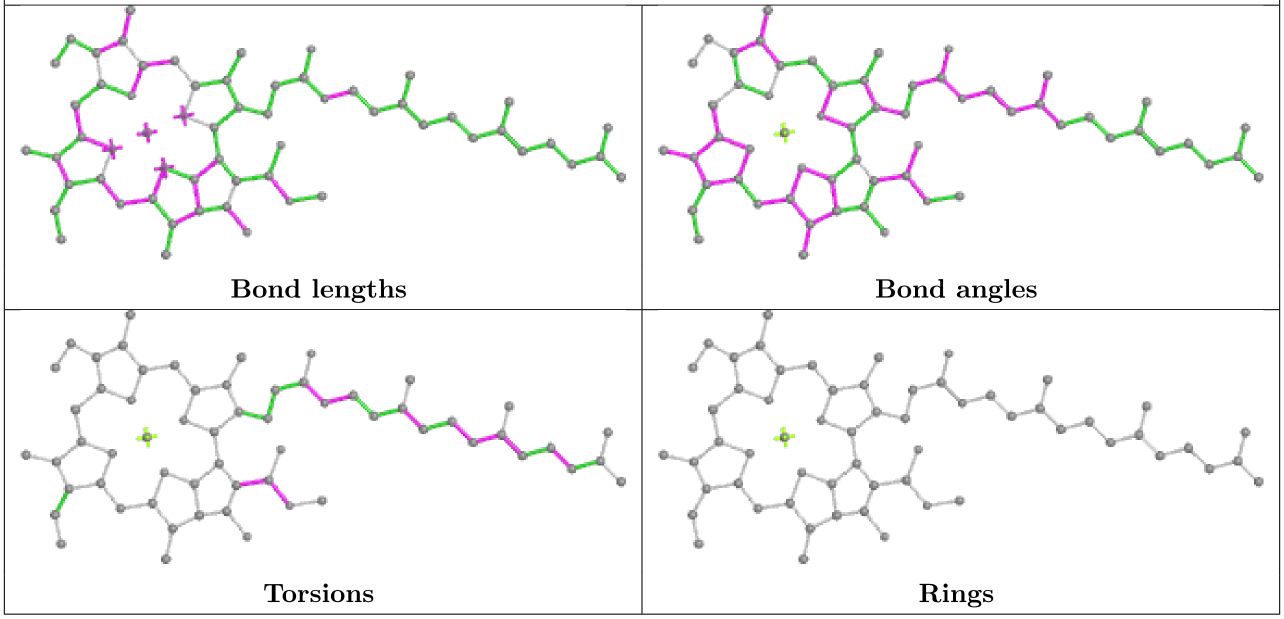
Ligand LHG b 5004



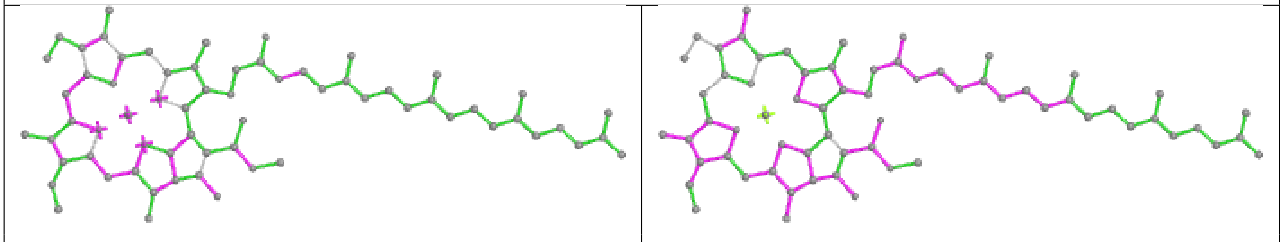
Ligand LMT G 6001



Ligand CLA a 1128

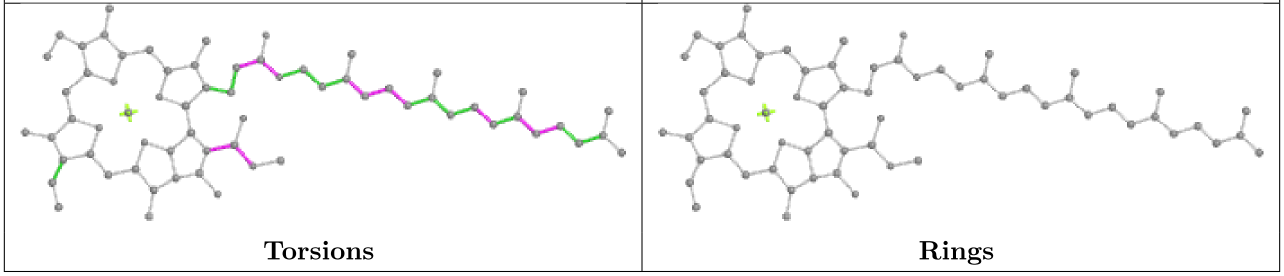


Ligand CLA b 1204



Bond lengths

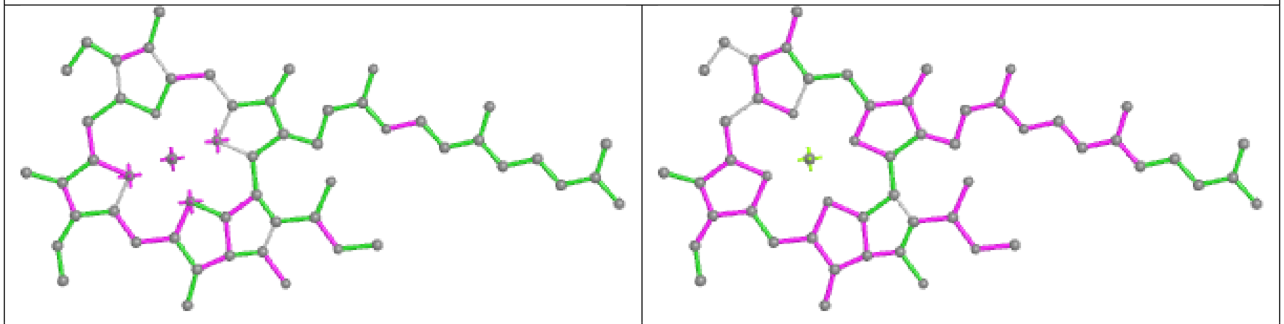
Bond angles



Torsions

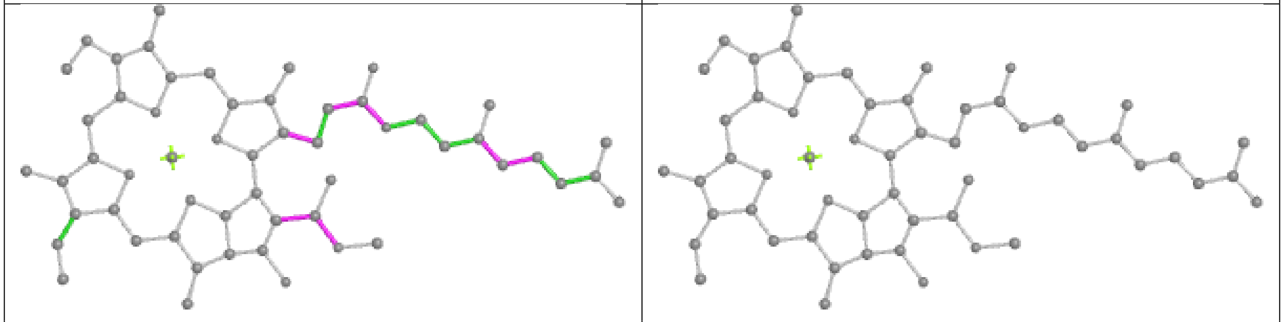
Rings

Ligand CLA b 1220



Bond lengths

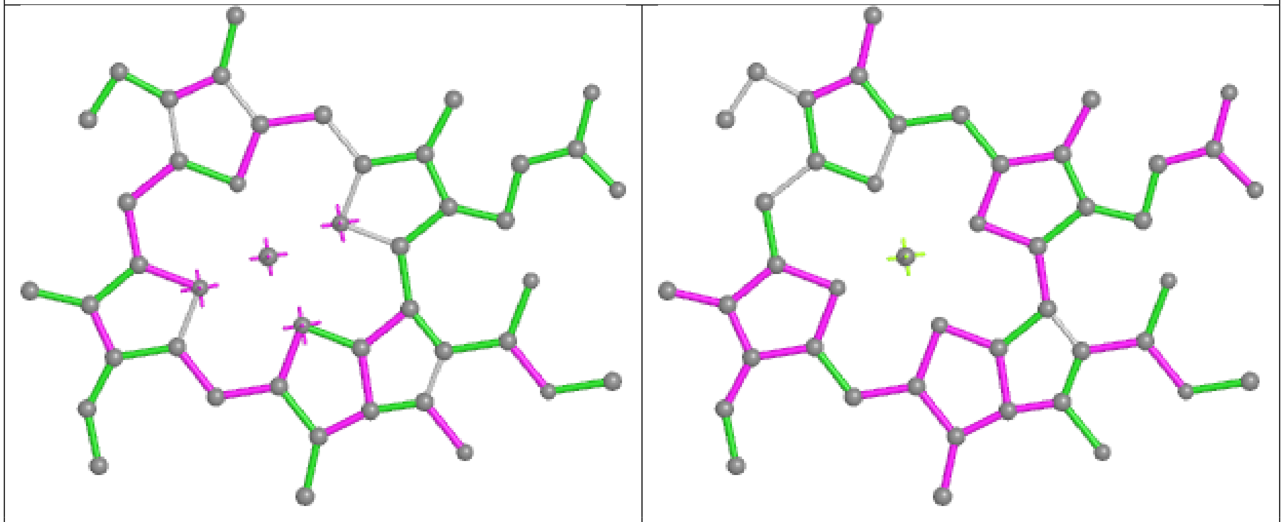
Bond angles



Torsions

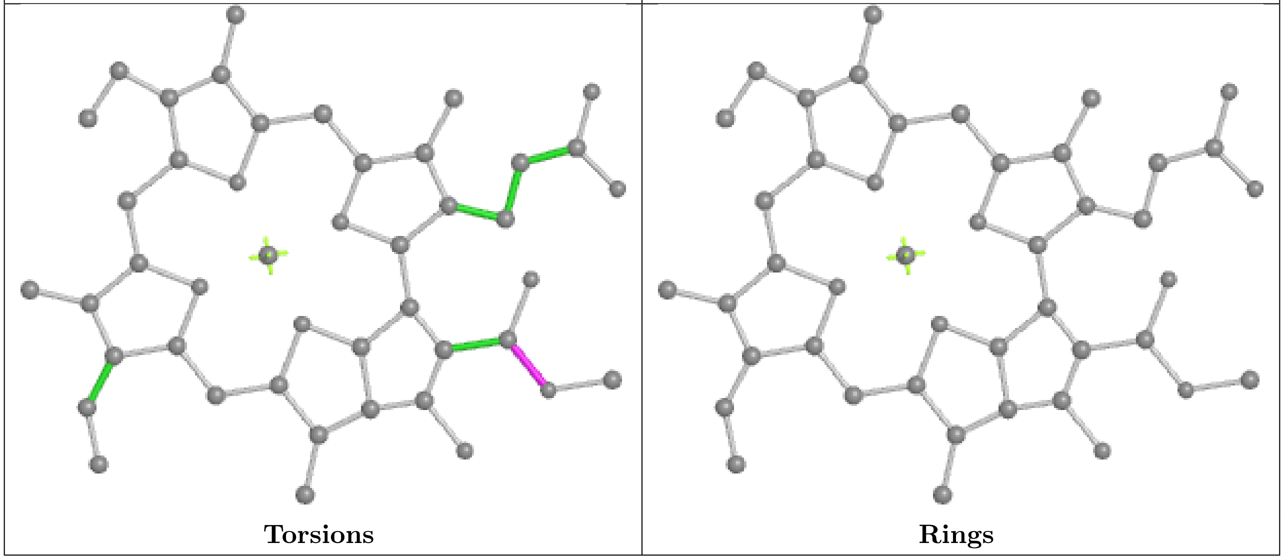
Rings

Ligand CLA b 1232



Bond lengths

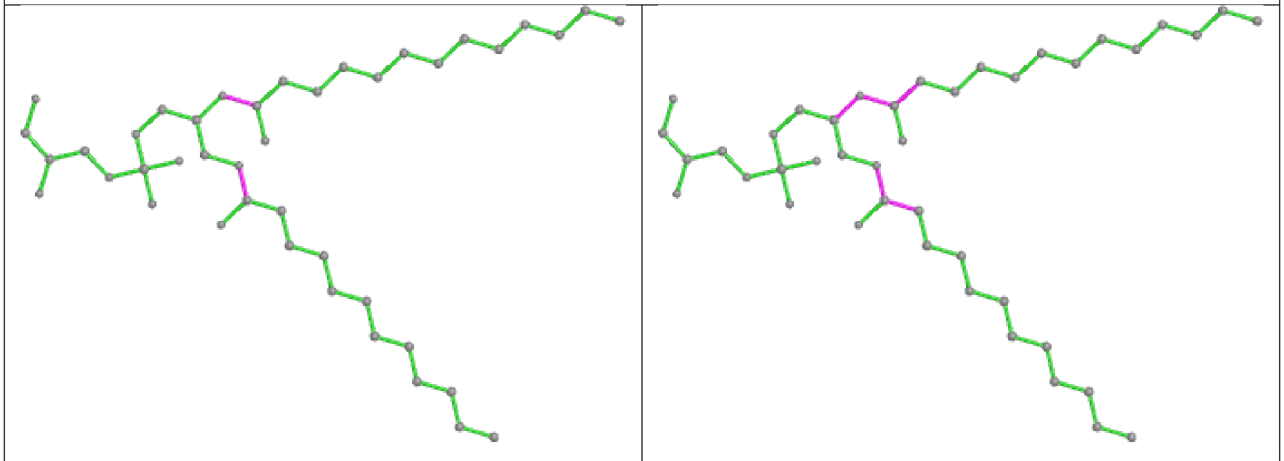
Bond angles



Torsions

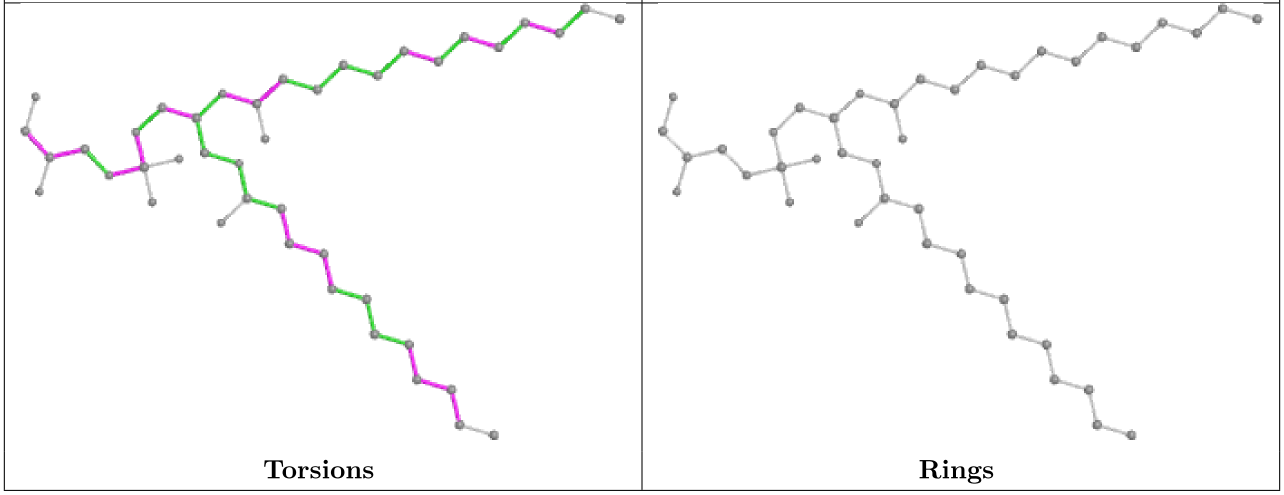
Rings

Ligand LHG G 5001



Bond lengths

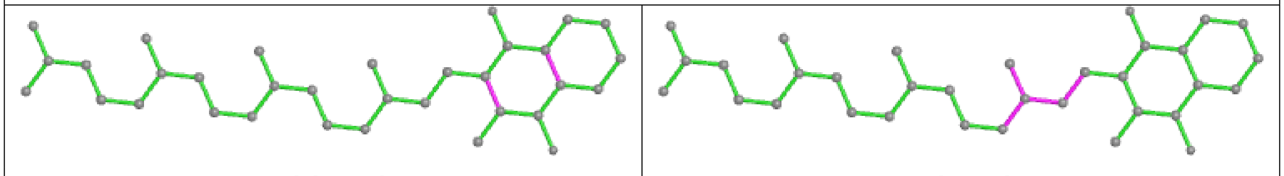
Bond angles



Torsions

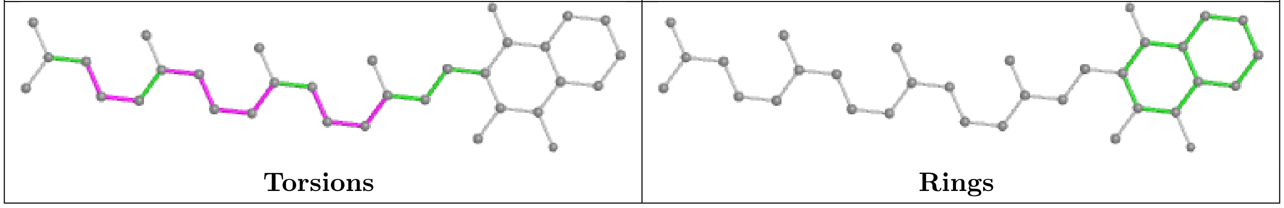
Rings

Ligand PQN H 2002



Bond lengths

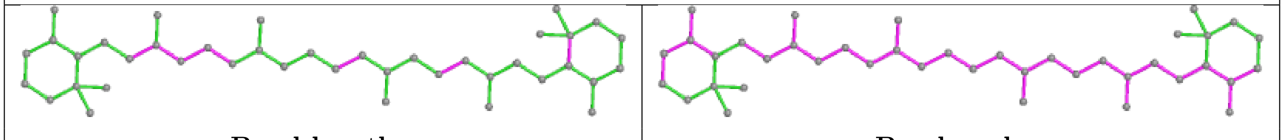
Bond angles



Torsions

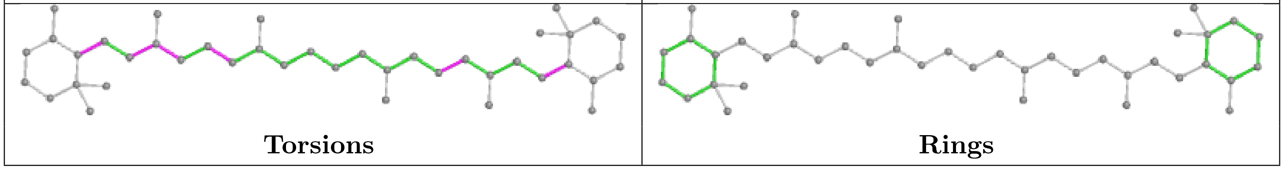
Rings

Ligand BCR b 4009



Bond lengths

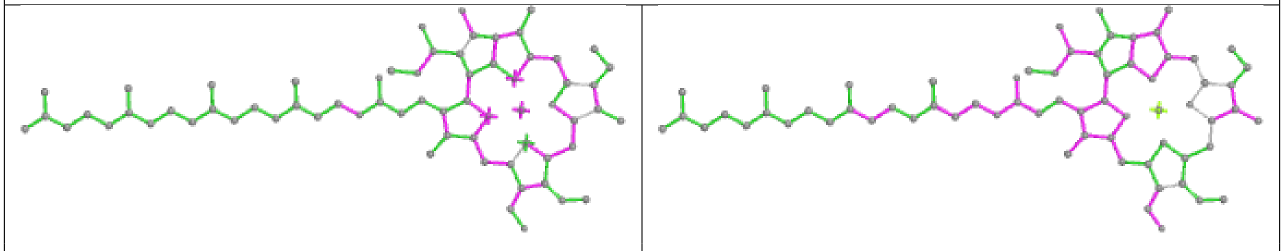
Bond angles



Torsions

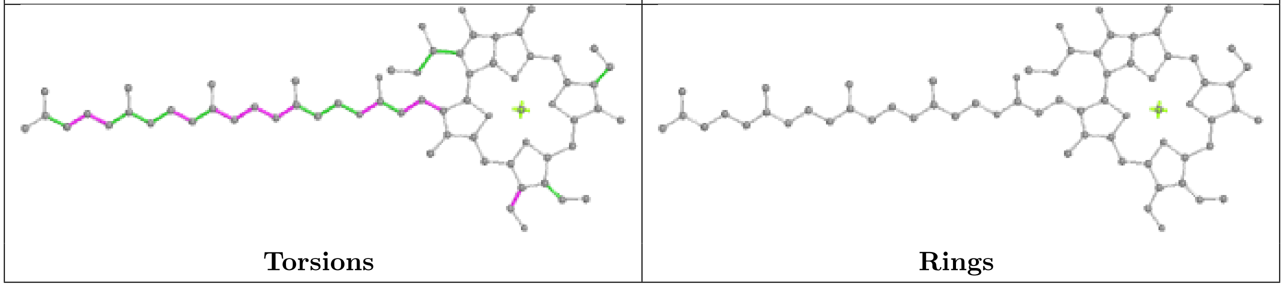
Rings

Ligand F6C H 1238



Bond lengths

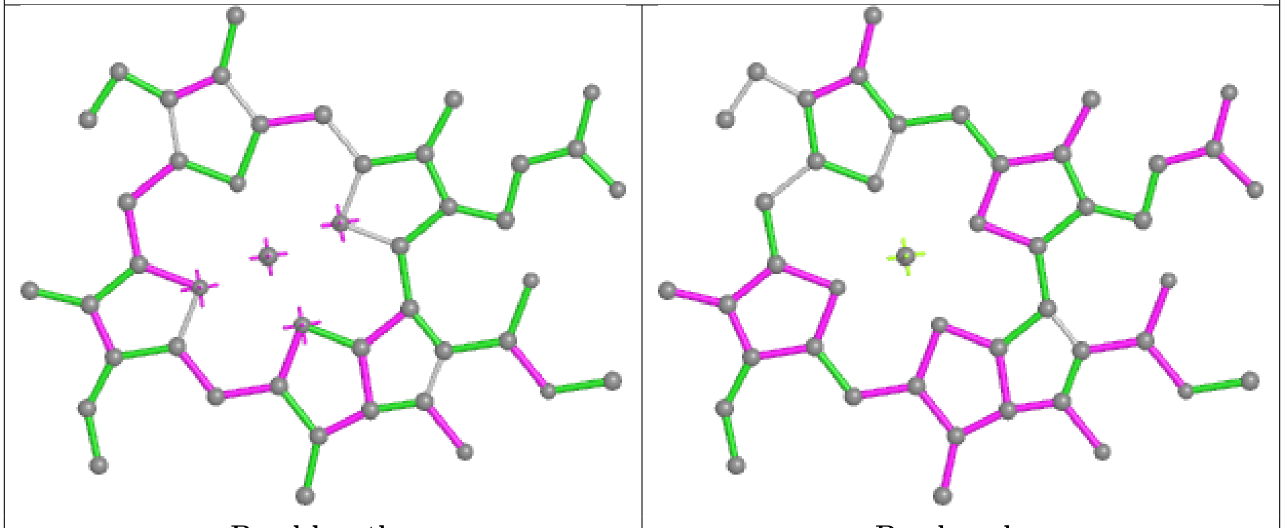
Bond angles



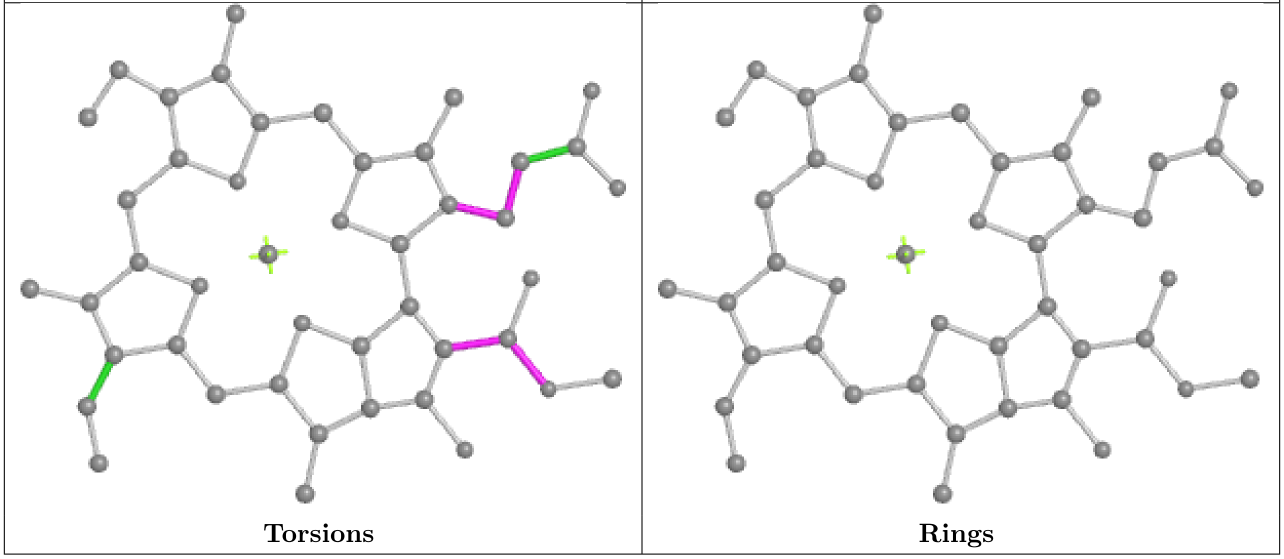
Torsions

Rings

Ligand CLA a 1120

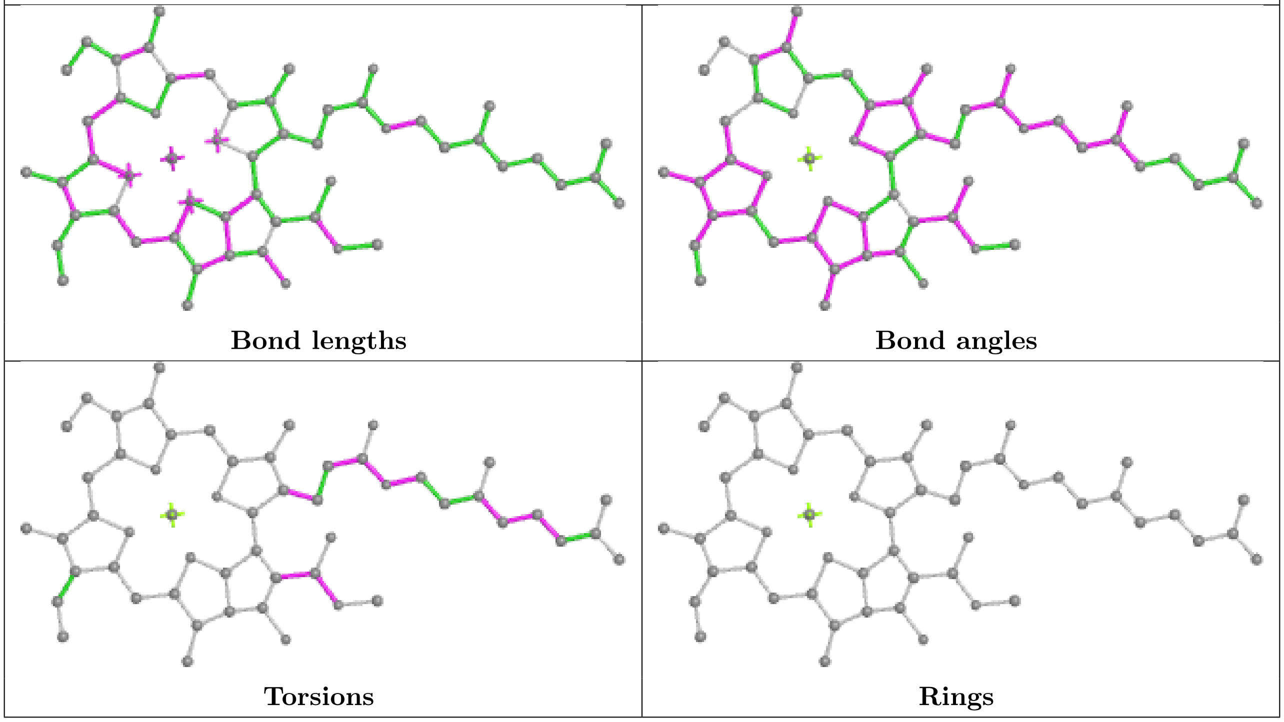


Bond lengths **Bond angles**

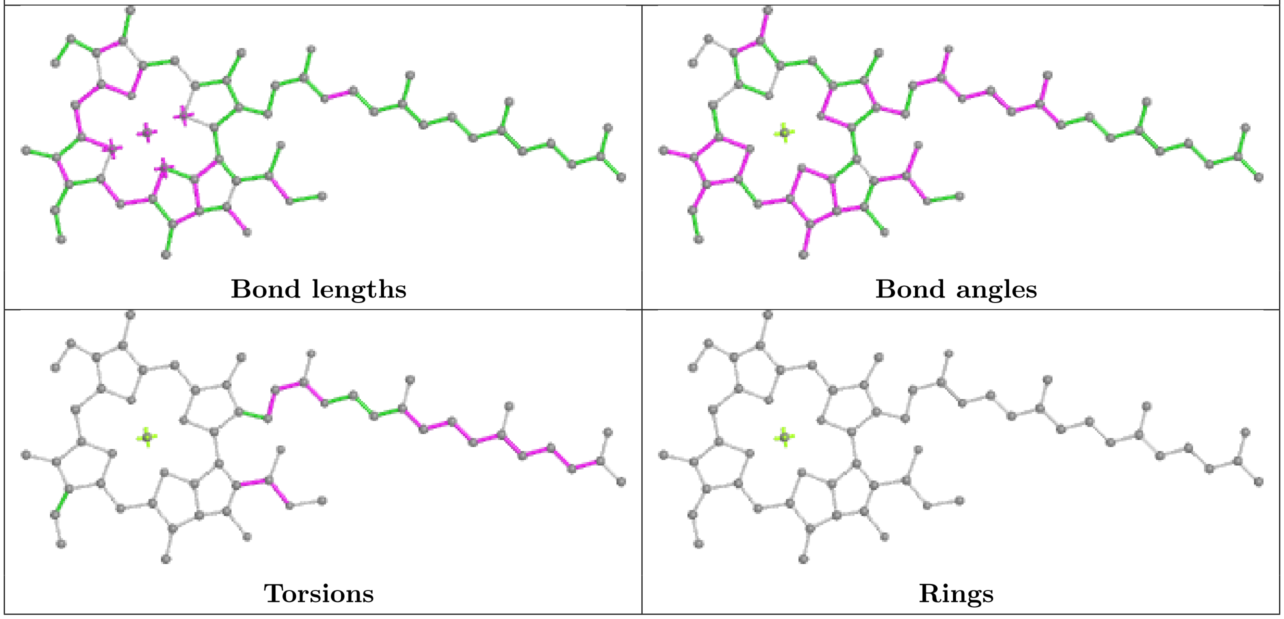


Torsions **Rings**

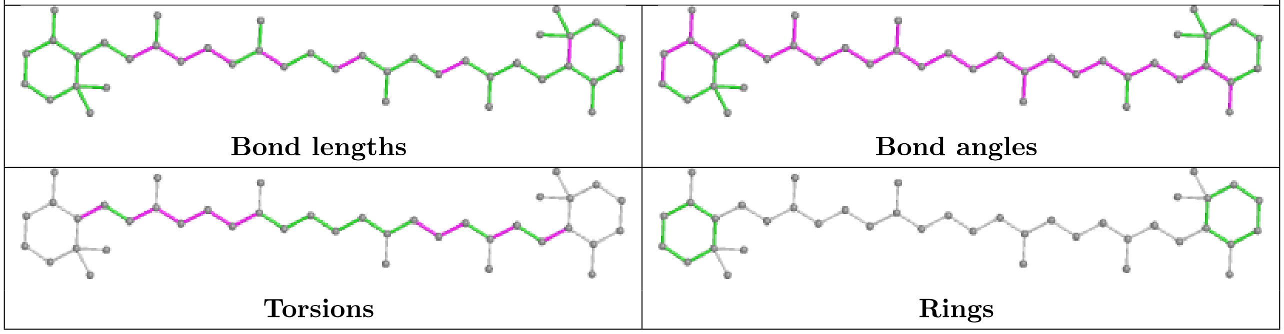
Ligand CLA G 1122



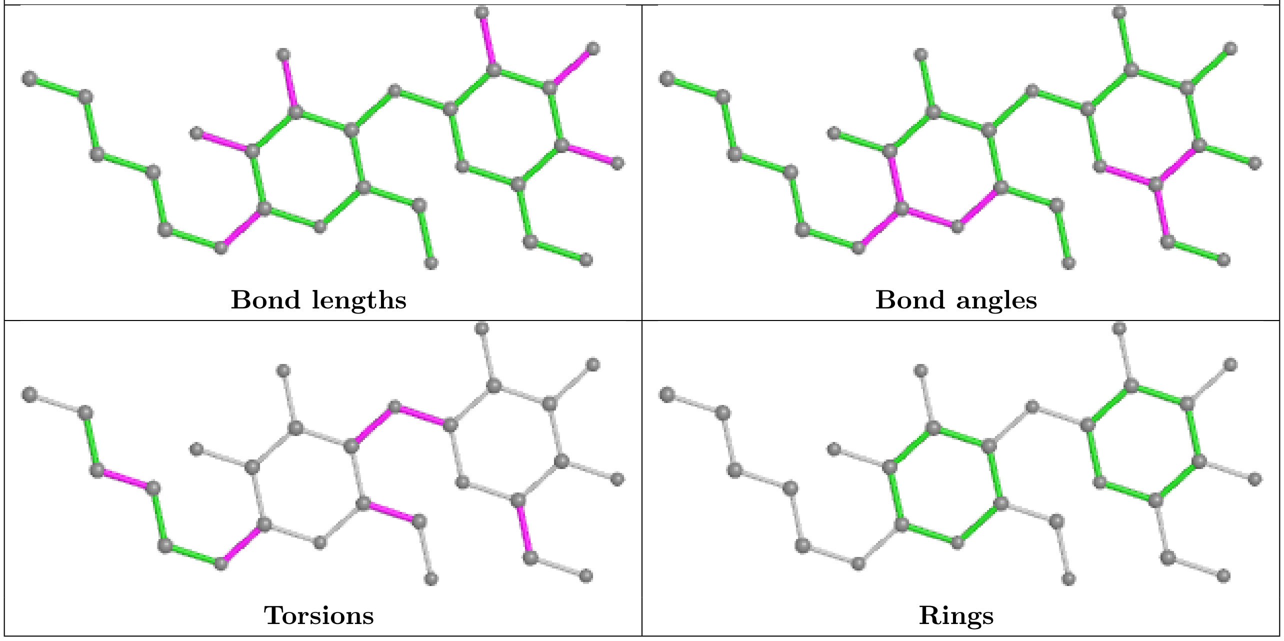
Ligand CLA A 1126



Ligand BCR B 4017



Ligand LMT A 6002



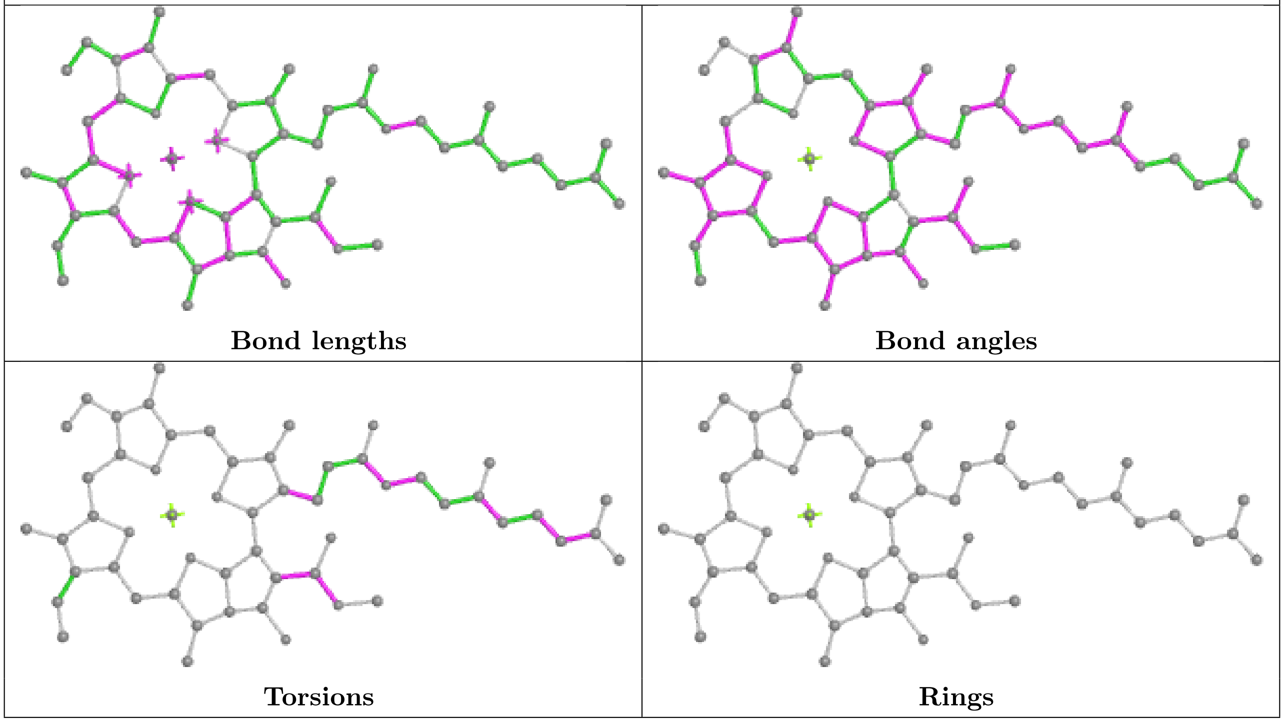
Bond lengths

Bond angles

Torsions

Rings

Ligand CLA G 1118



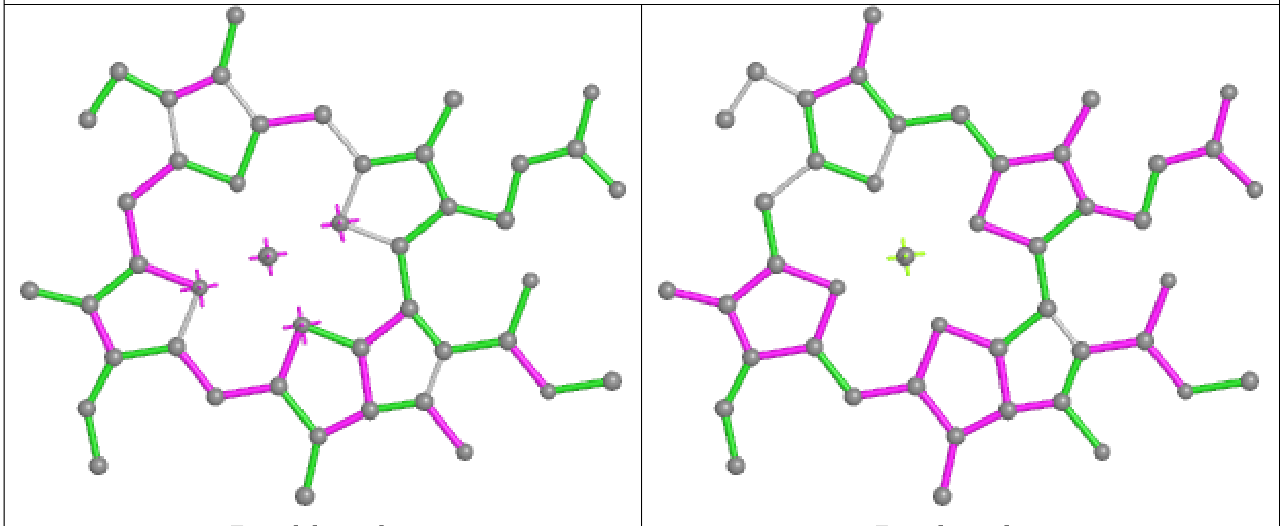
Bond lengths

Bond angles

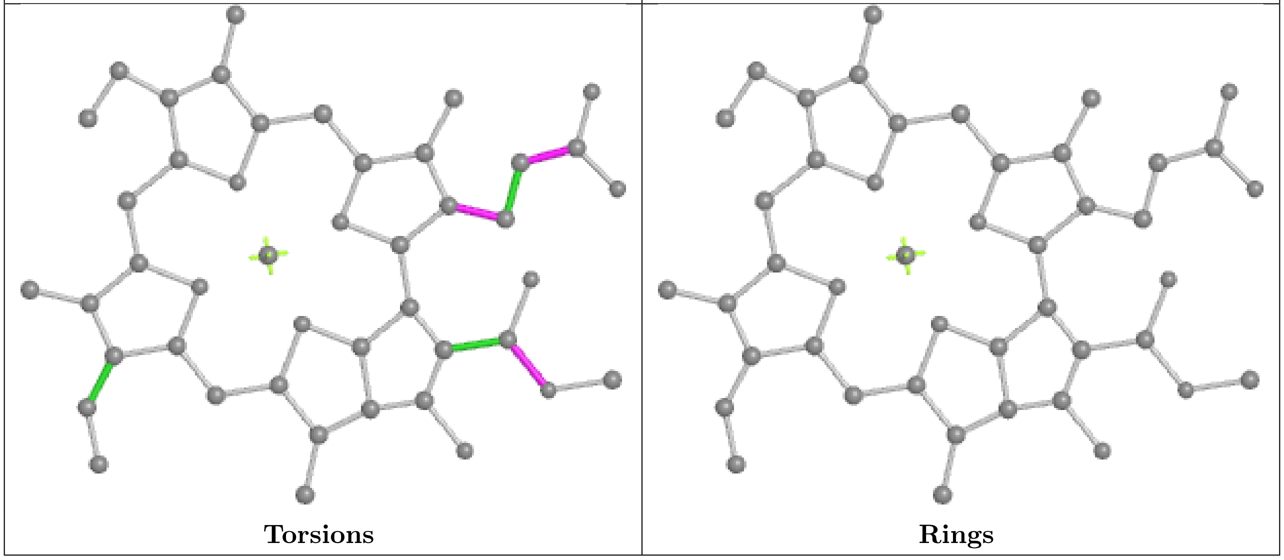
Torsions

Rings

Ligand CLA G 1110

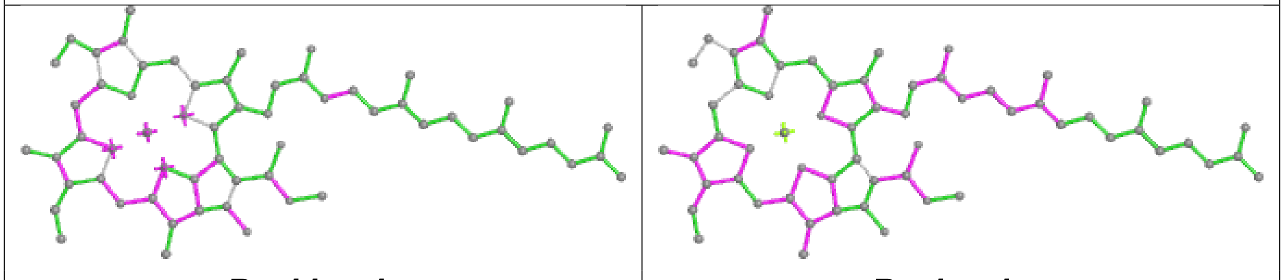


Bond lengths Bond angles

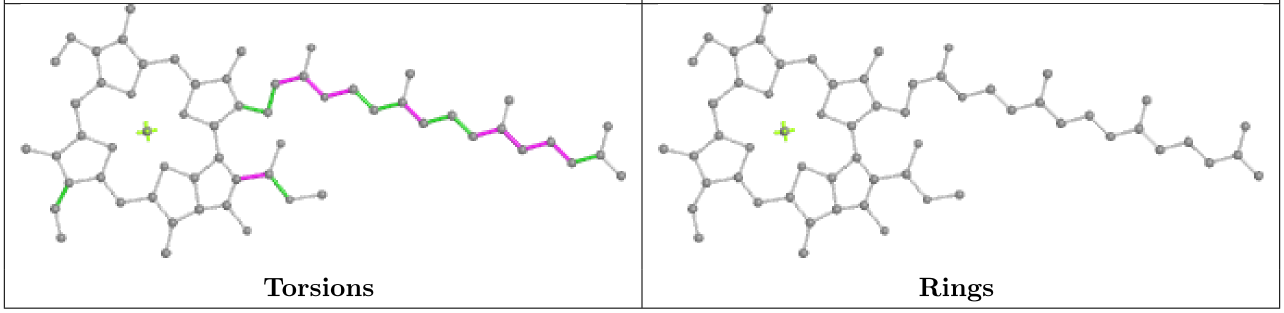


Torsions Rings

Ligand CLA L 1502

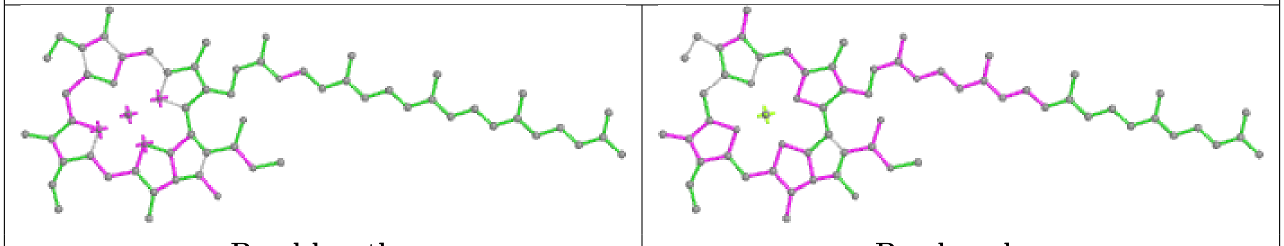


Bond lengths Bond angles



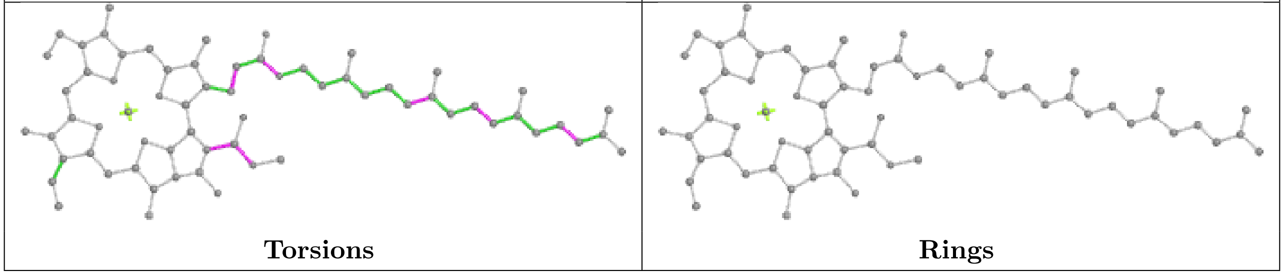
Torsions Rings

Ligand CLA G 1104



Bond lengths

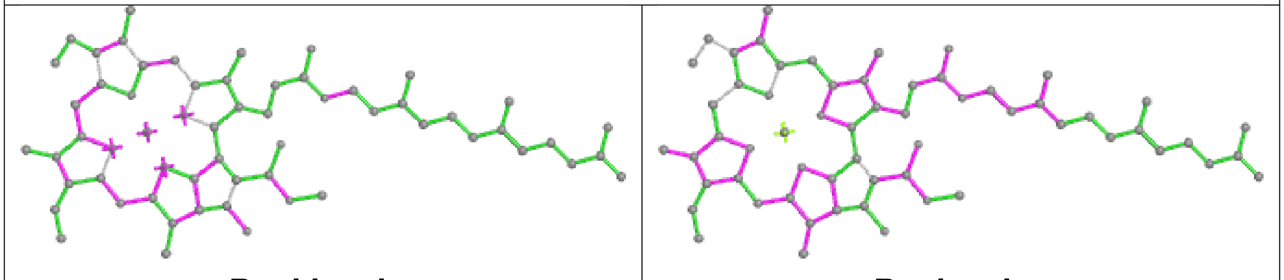
Bond angles



Torsions

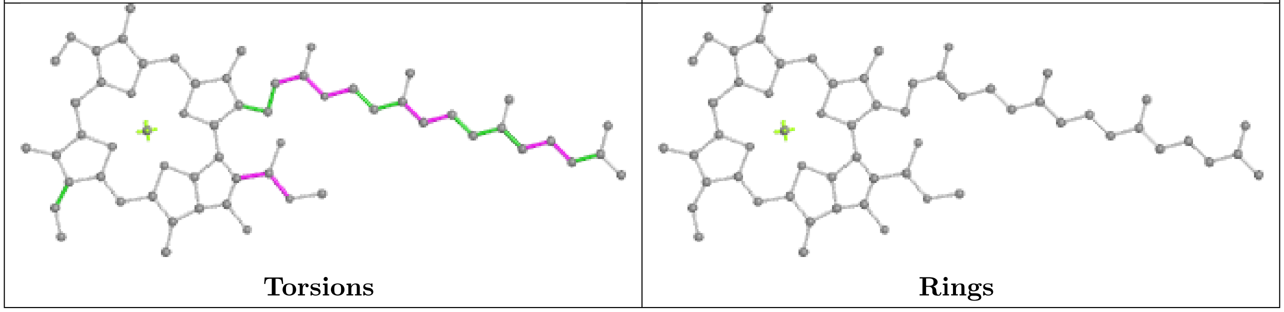
Rings

Ligand CLA B 1235



Bond lengths

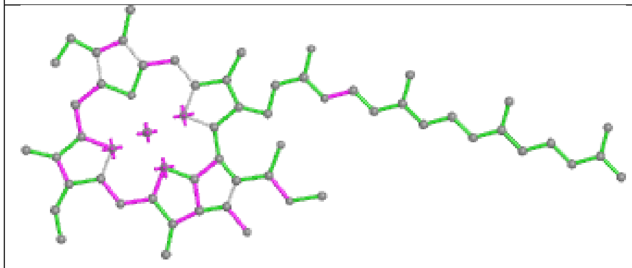
Bond angles



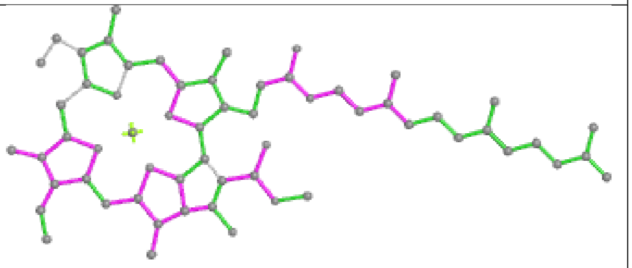
Torsions

Rings

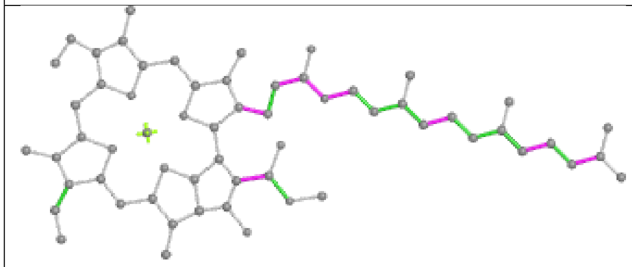
Ligand CLA b 1202



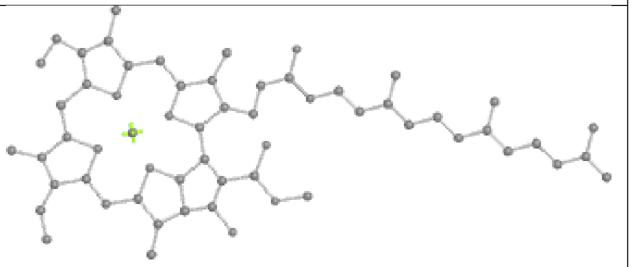
Bond lengths



Bond angles

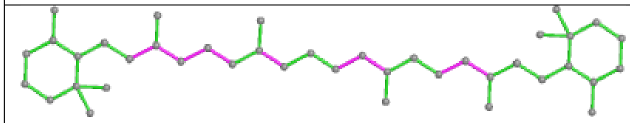


Torsions

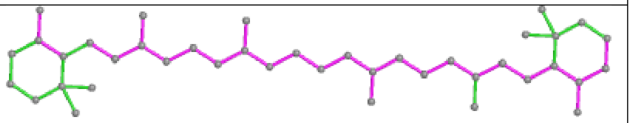


Rings

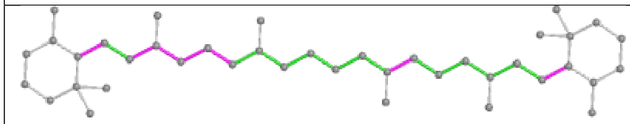
Ligand BCR A 4008



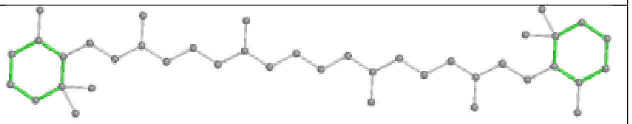
Bond lengths



Bond angles

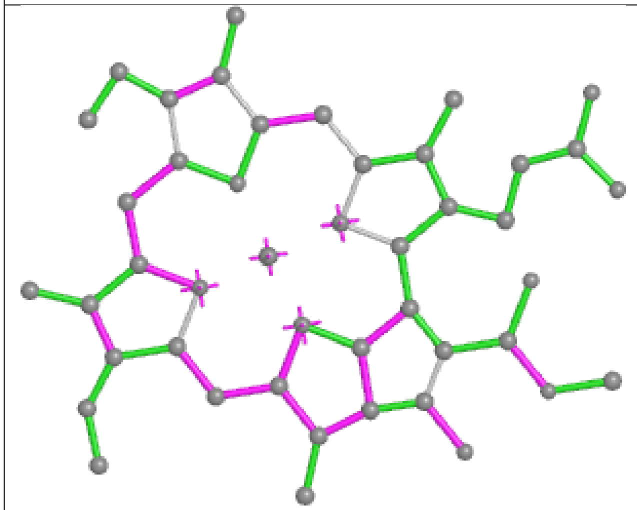


Torsions

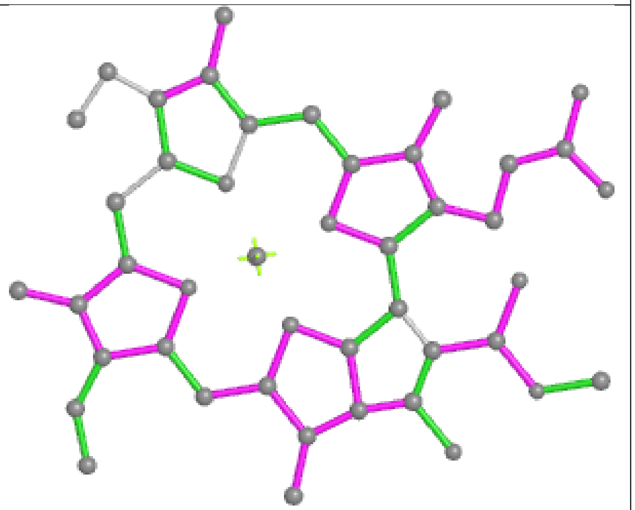


Rings

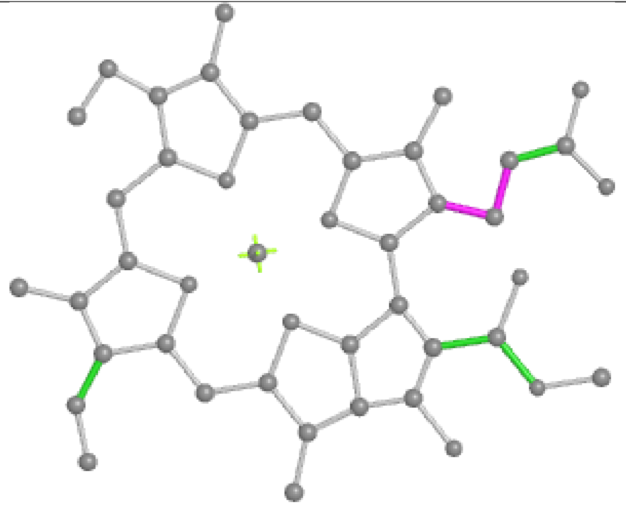
Ligand CLA B 1209



Bond lengths



Bond angles



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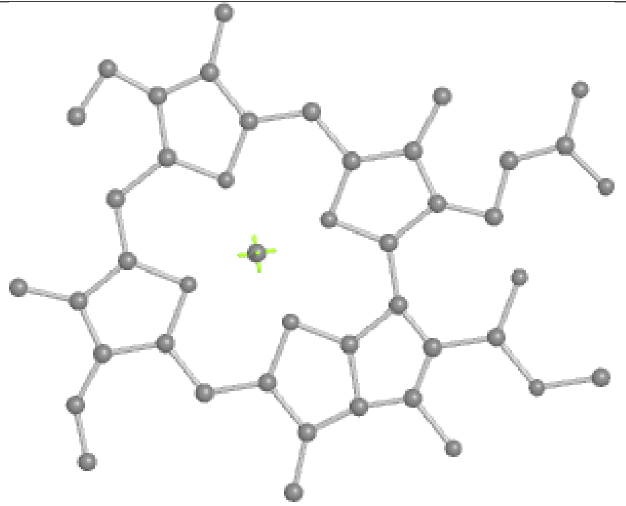
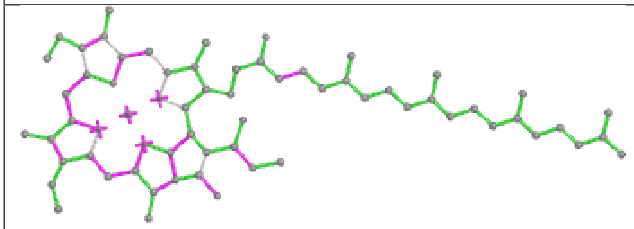


Rings

Ligand CLA b 1225



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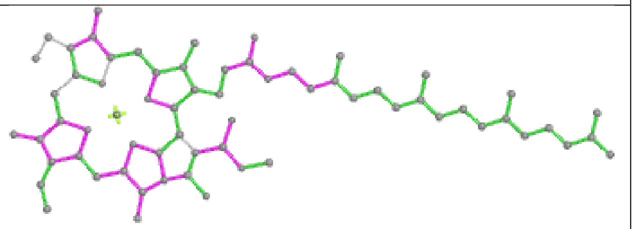
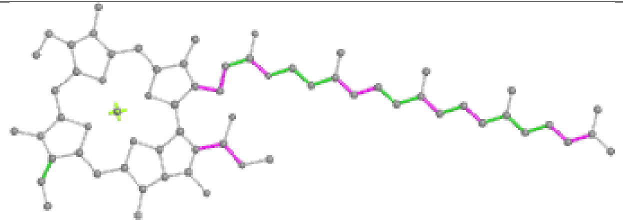
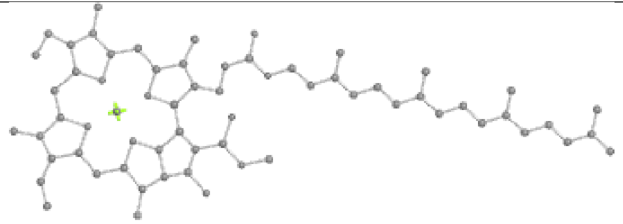


Bond angles

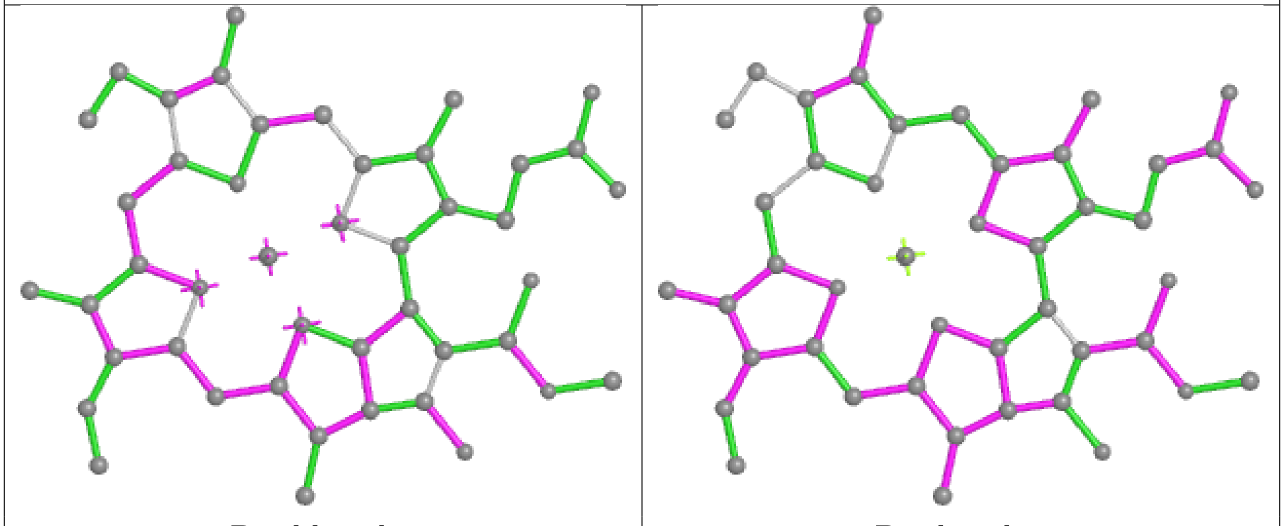


Torsions

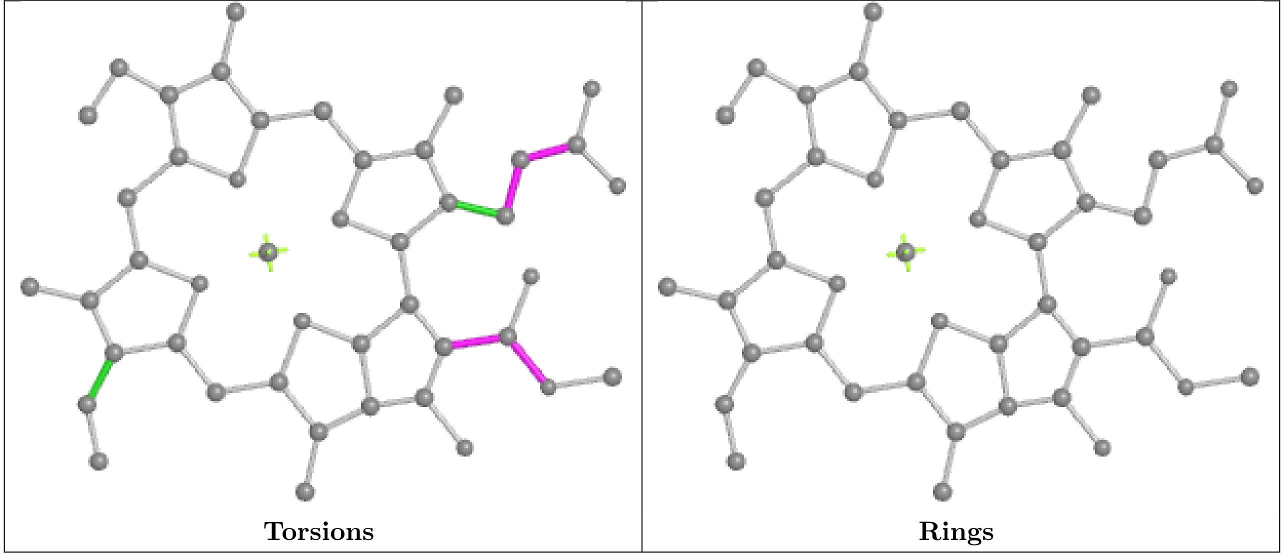


Rings

Ligand CLA a 1134

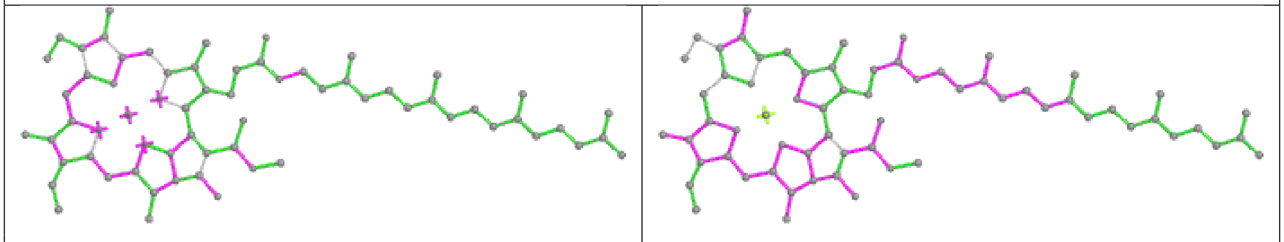

Bond lengths

Bond angles

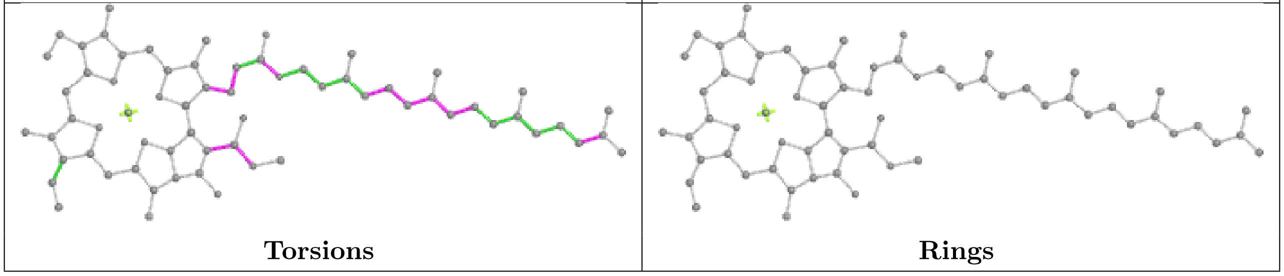

Torsions

Rings

Ligand CLA H 1223

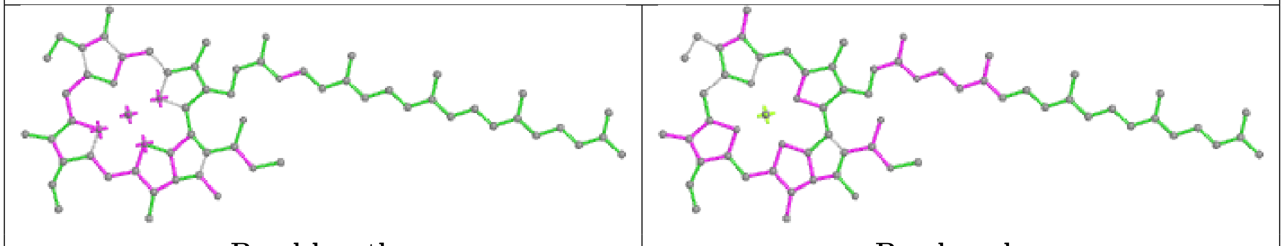

Bond lengths

Bond angles

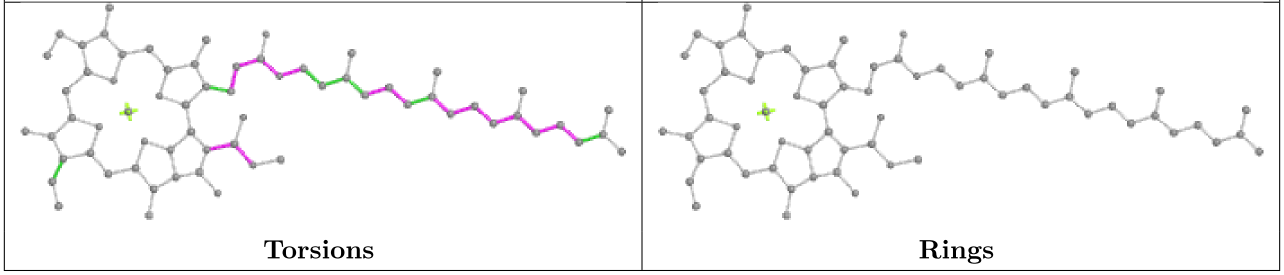

Torsions

Rings

Ligand CLA H 1211

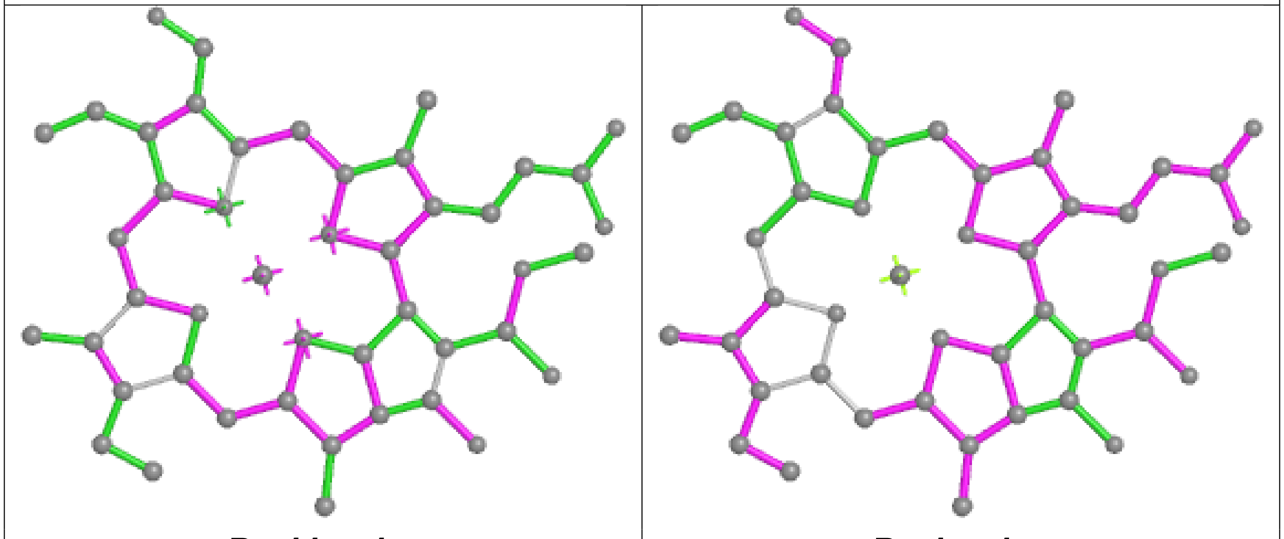


Bond lengths **Bond angles**

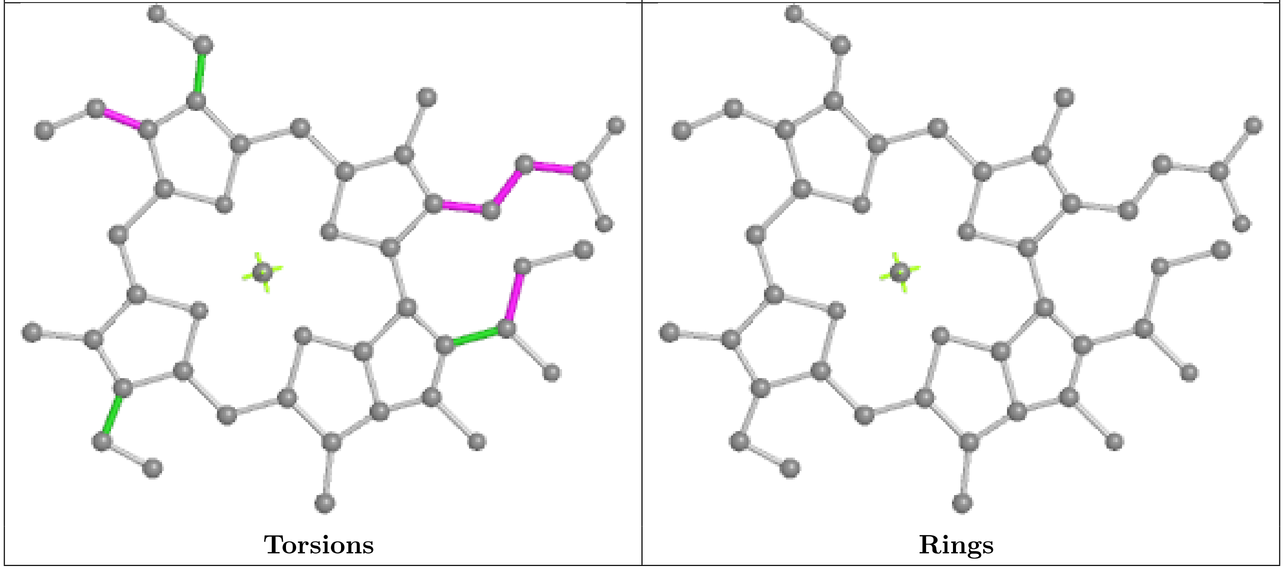


Torsions **Rings**

Ligand F6C G 1121

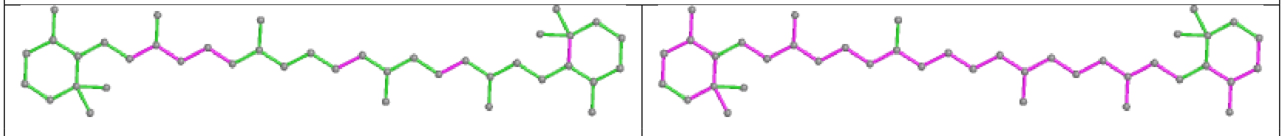


Bond lengths **Bond angles**



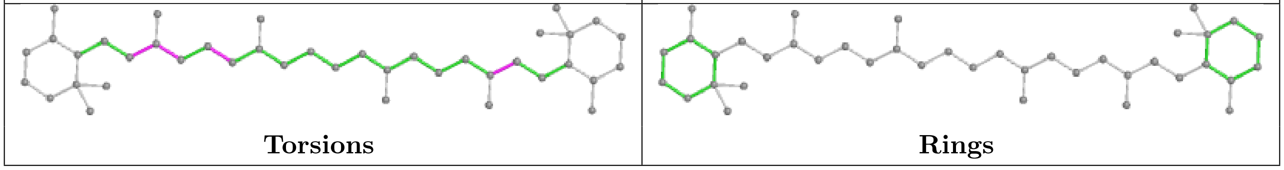
Torsions **Rings**

Ligand BCR B 4004



Bond lengths

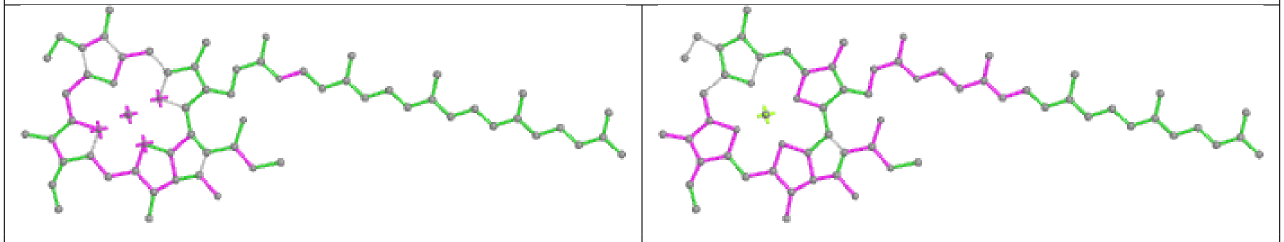
Bond angles



Torsions

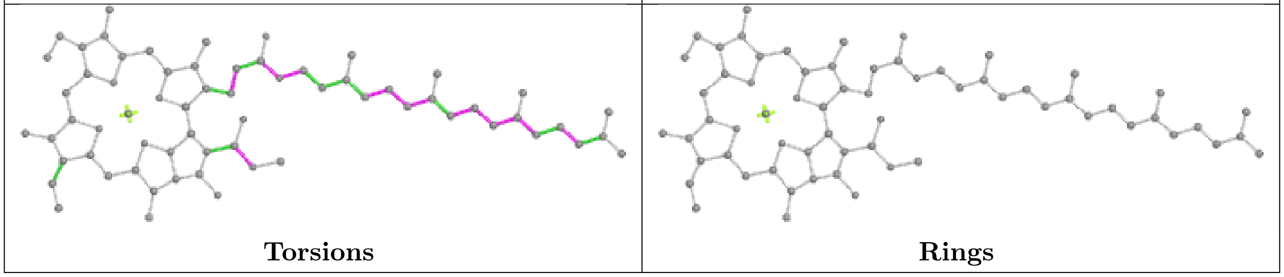
Rings

Ligand CLA H 1214



Bond lengths

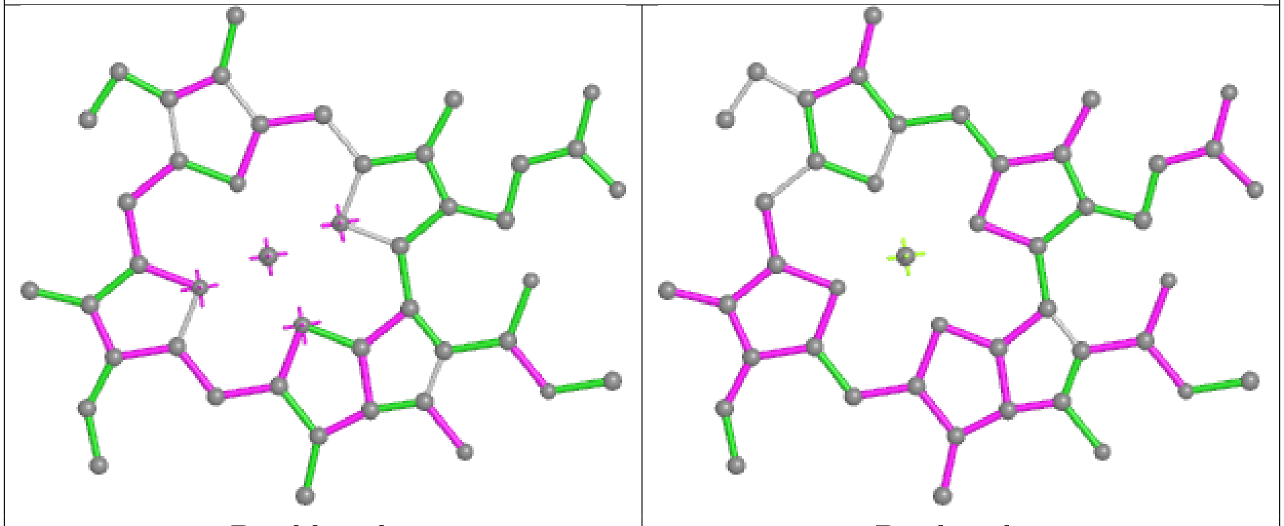
Bond angles



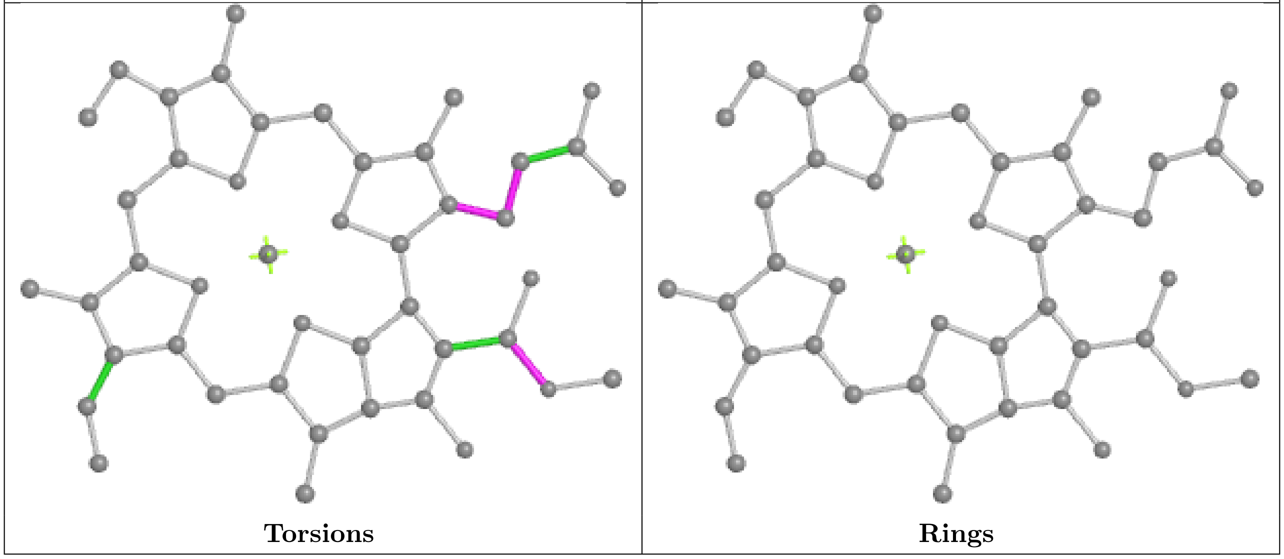
Torsions

Rings

Ligand CLA B 1227

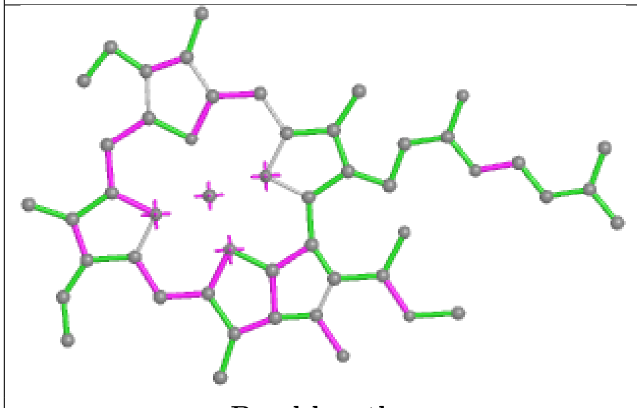


Bond lengths **Bond angles**

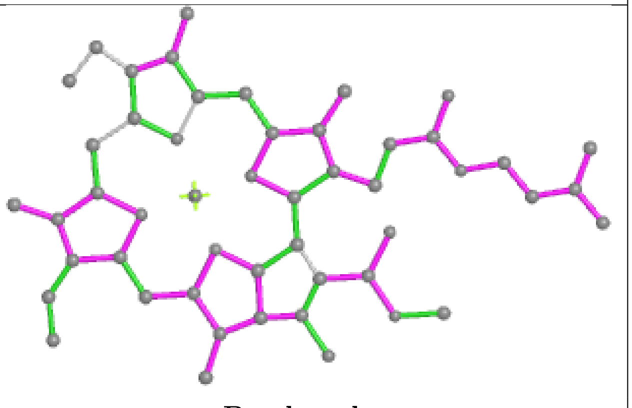


Torsions **Rings**

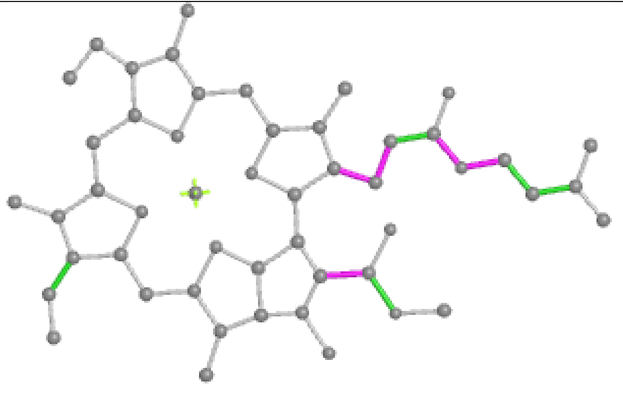
Ligand CLA a 1129



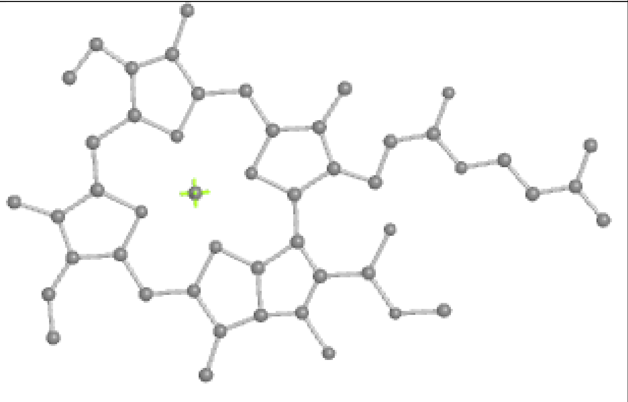
Bond lengths



Bond angles

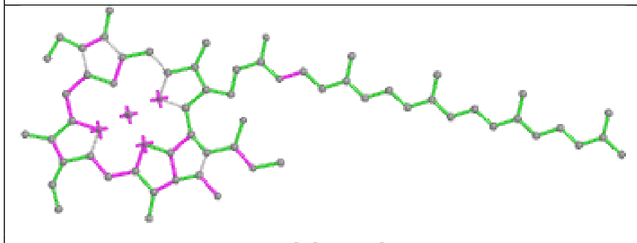


Torsions

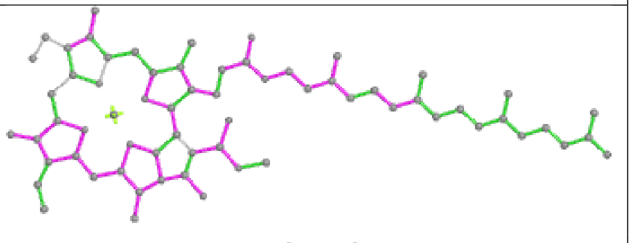


Rings

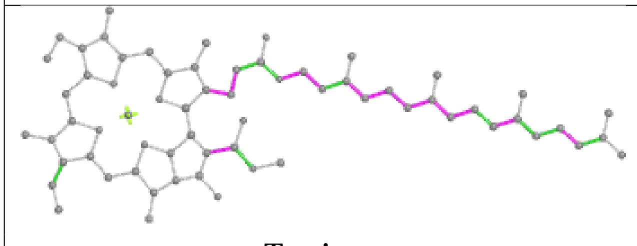
Ligand CLA b 1022



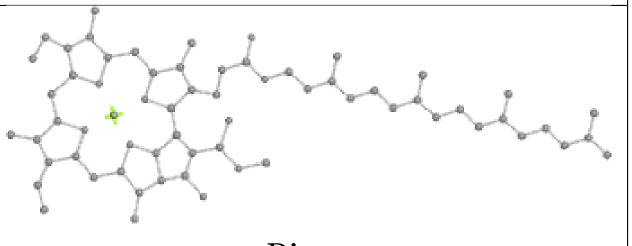
Bond lengths



Bond angles

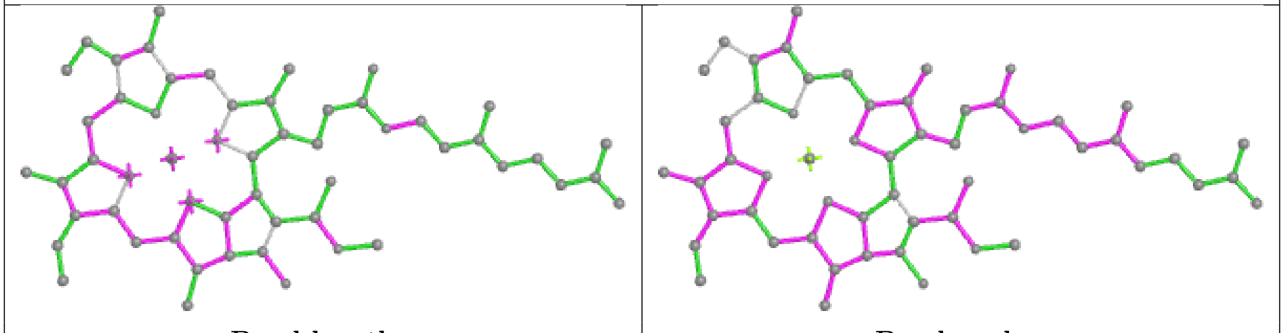


Torsions

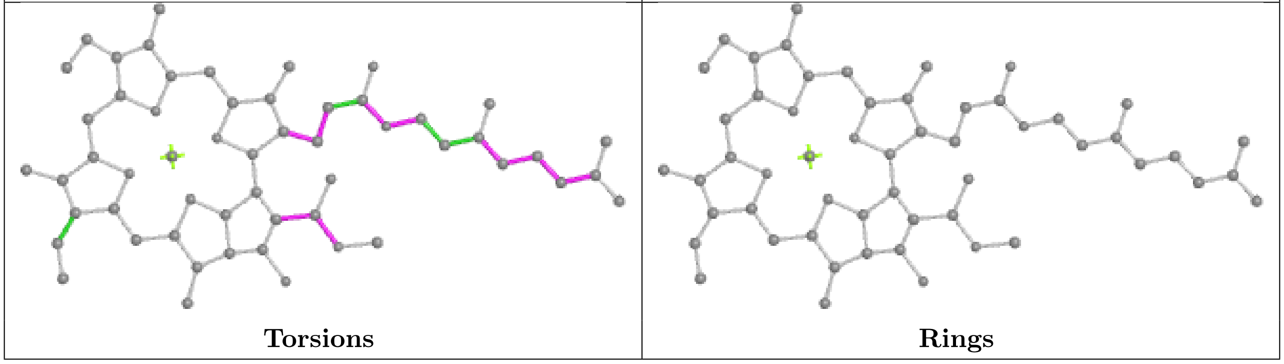


Rings

Ligand CLA H 1228

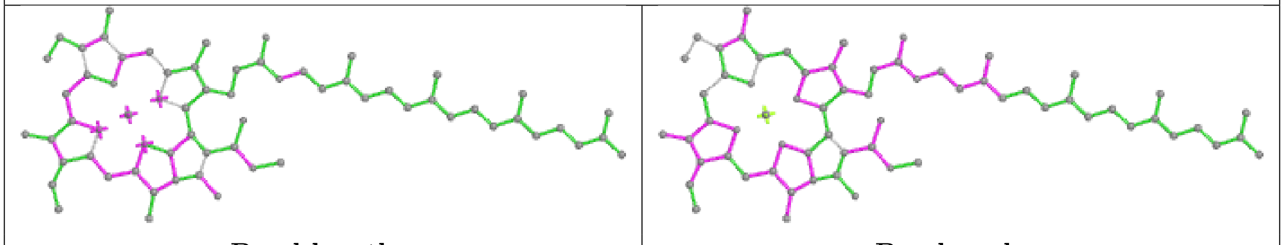


Bond lengths Bond angles

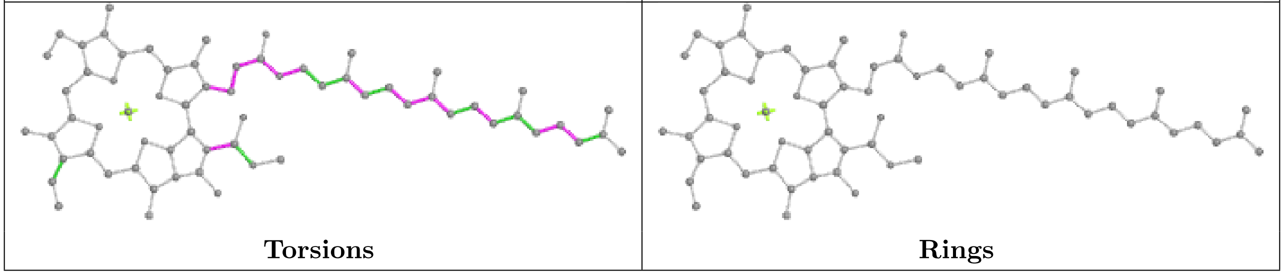


Torsions Rings

Ligand CLA b 1210

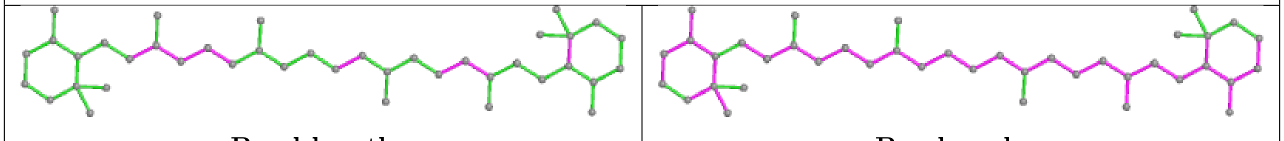


Bond lengths Bond angles

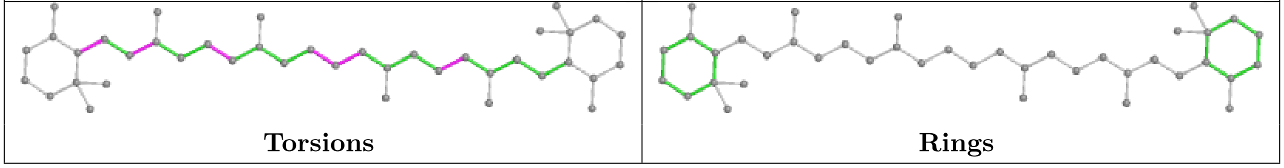


Torsions Rings

Ligand BCR I 4018

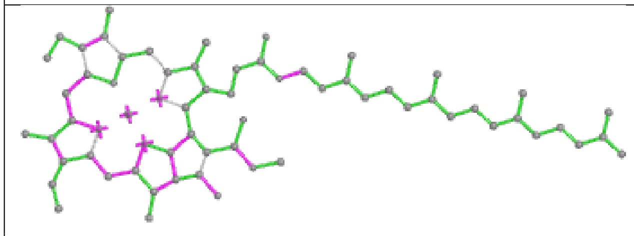


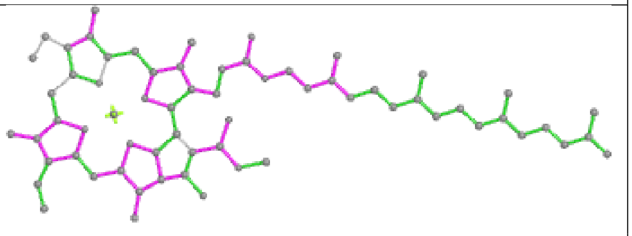
Bond lengths Bond angles

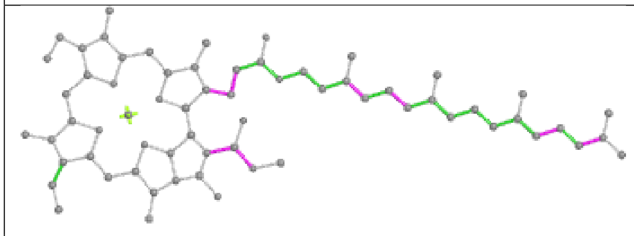


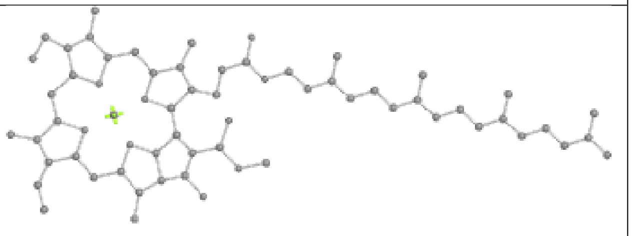
Torsions Rings

Ligand CLA A 1132

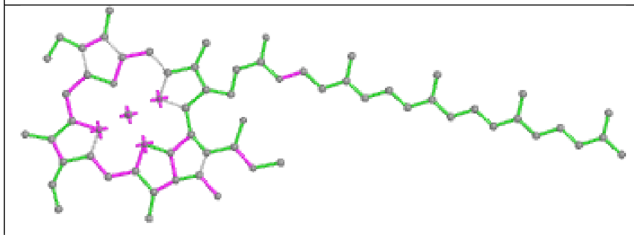

Bond lengths

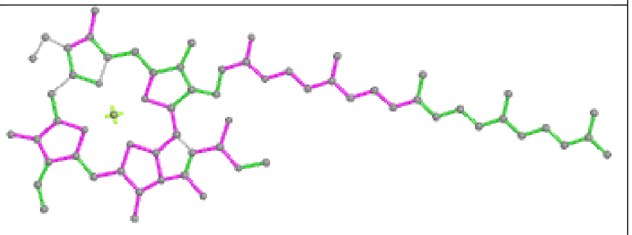

Bond angles

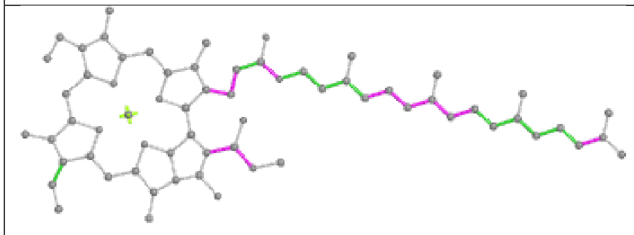

Torsions

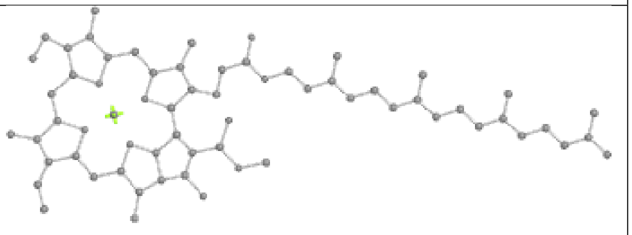

Rings

Ligand CLA b 1223

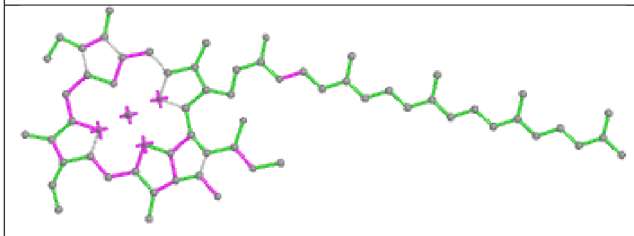

Bond lengths

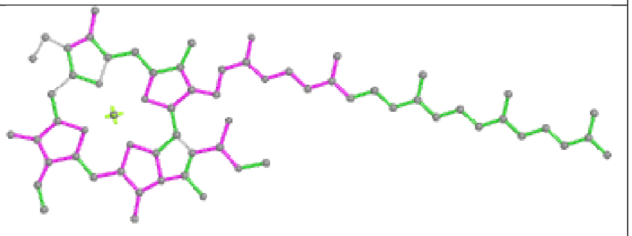

Bond angles

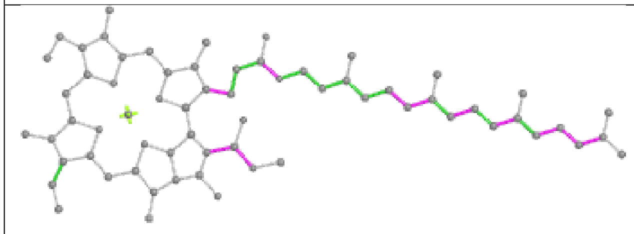

Torsions

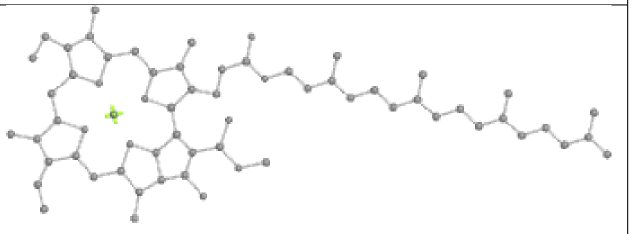

Rings

Ligand CLA H 1222

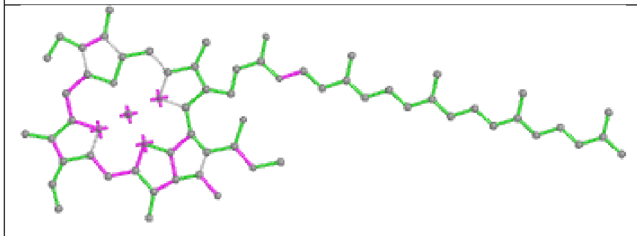

Bond lengths


Bond angles

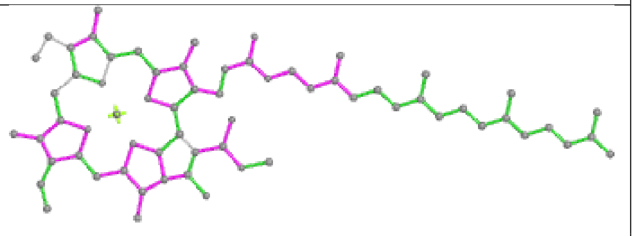

Torsions


Rings

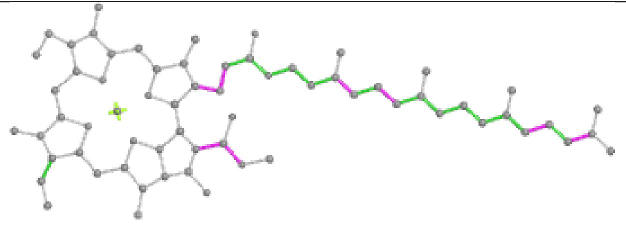
Ligand CLA a 1132



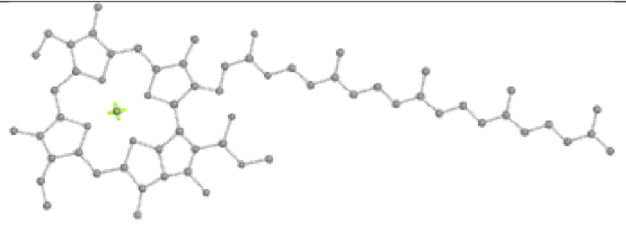
Bond lengths



Bond angles

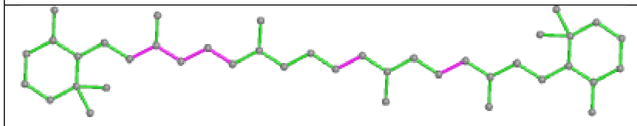


Torsions

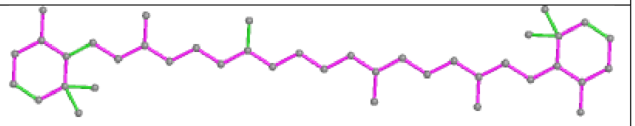


Rings

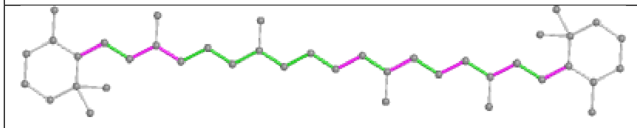
Ligand BCR a 4001



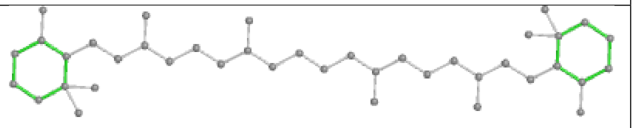
Bond lengths



Bond angles

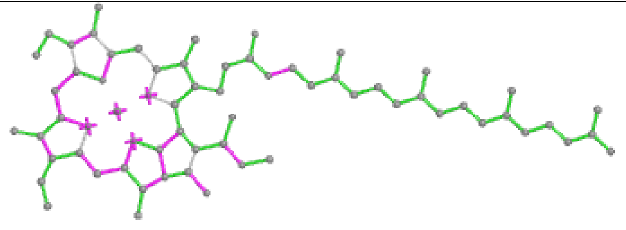


Torsions

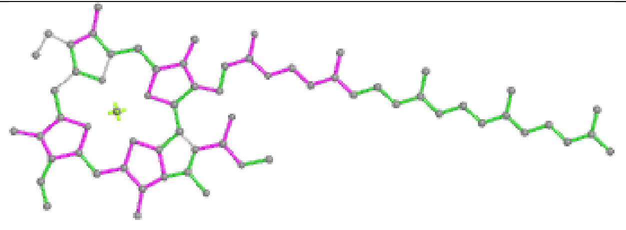


Rings

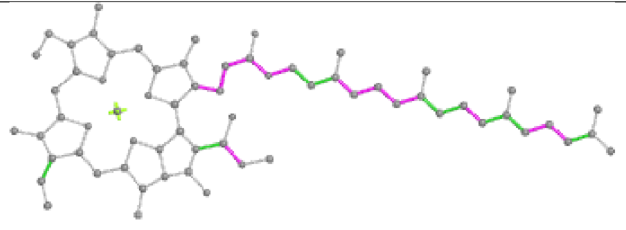
Ligand CLA a 1136



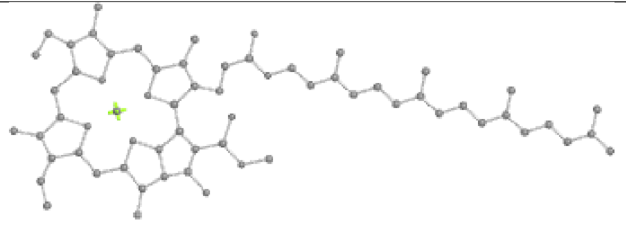
Bond lengths



Bond angles

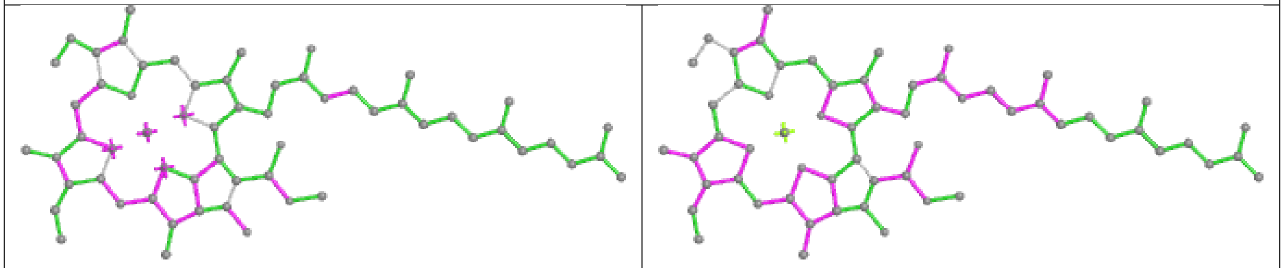


Torsions

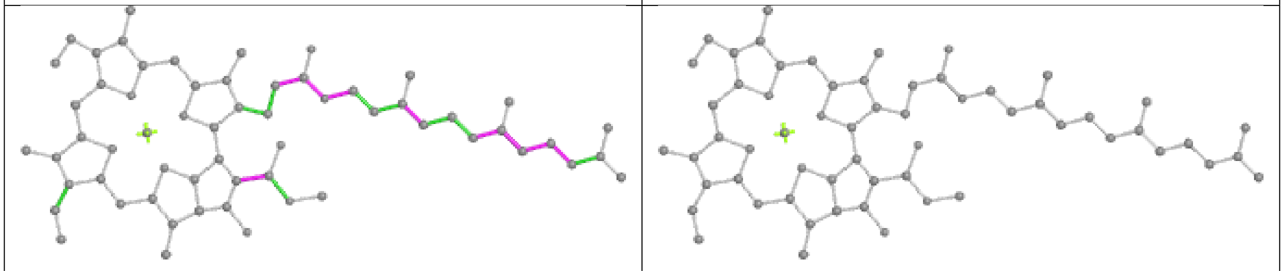


Rings

Ligand CLA l 1502

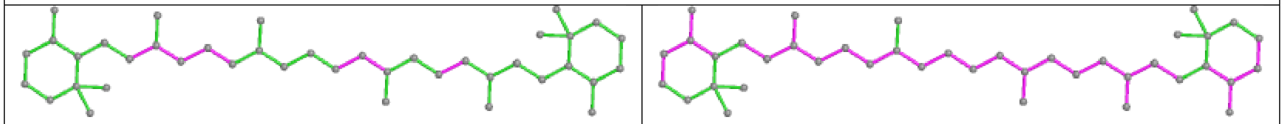


Bond lengths Bond angles

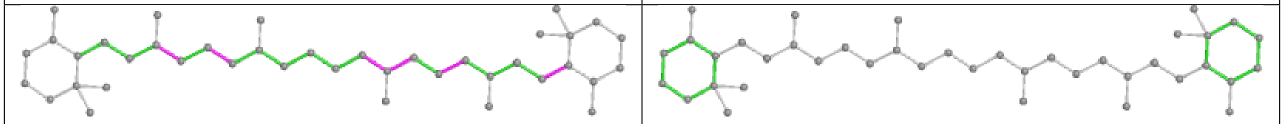


Torsions Rings

Ligand BCR b 4010

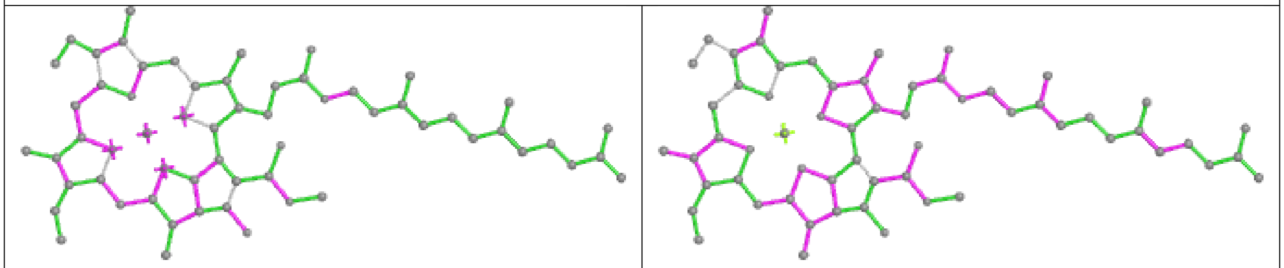


Bond lengths Bond angles

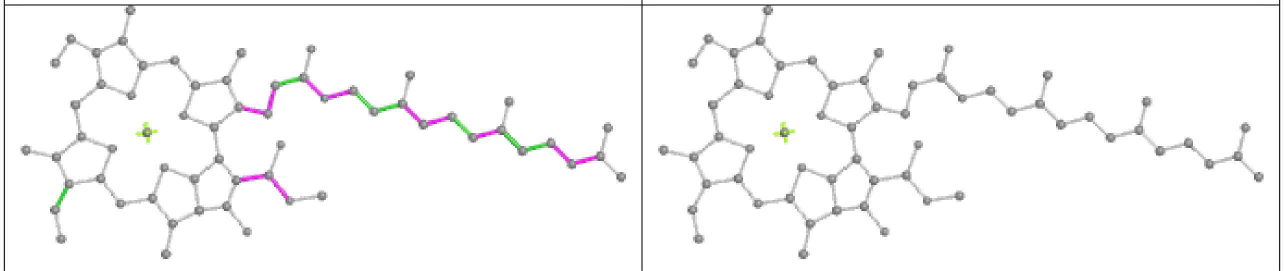


Torsions Rings

Ligand CLA H 1215



Bond lengths Bond angles



Torsions Rings

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

The following chains have linkage breaks:

Mol	Chain	Number of breaks
9	T	1
9	k	1
9	K	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	T	49:UNK	C	69:VAL	N	9.76
1	k	49:UNK	C	69:VAL	N	9.75
1	K	49:UNK	C	69:VAL	N	9.75

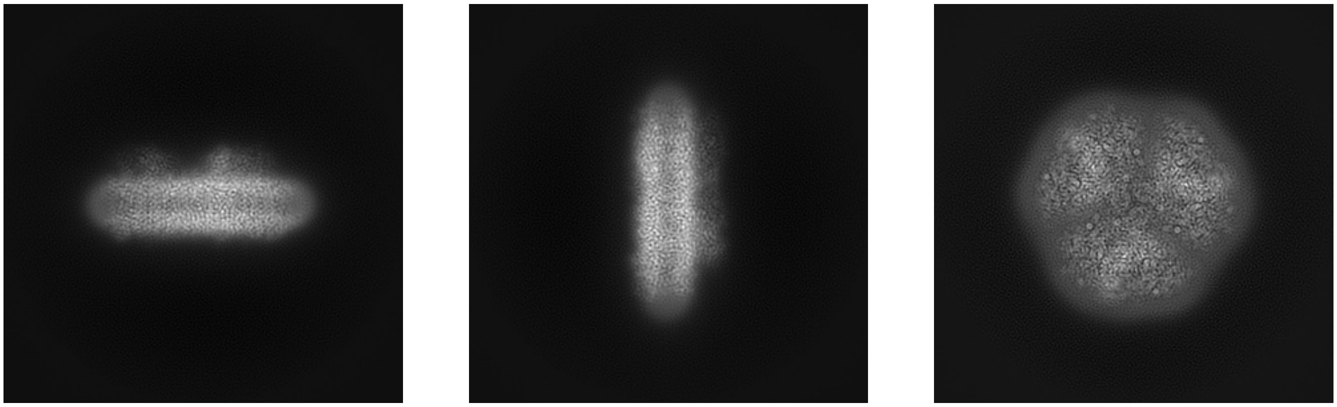
6 Map visualisation ⓘ

This section contains visualisations of the EMDB entry EMD-23563. 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 ⓘ

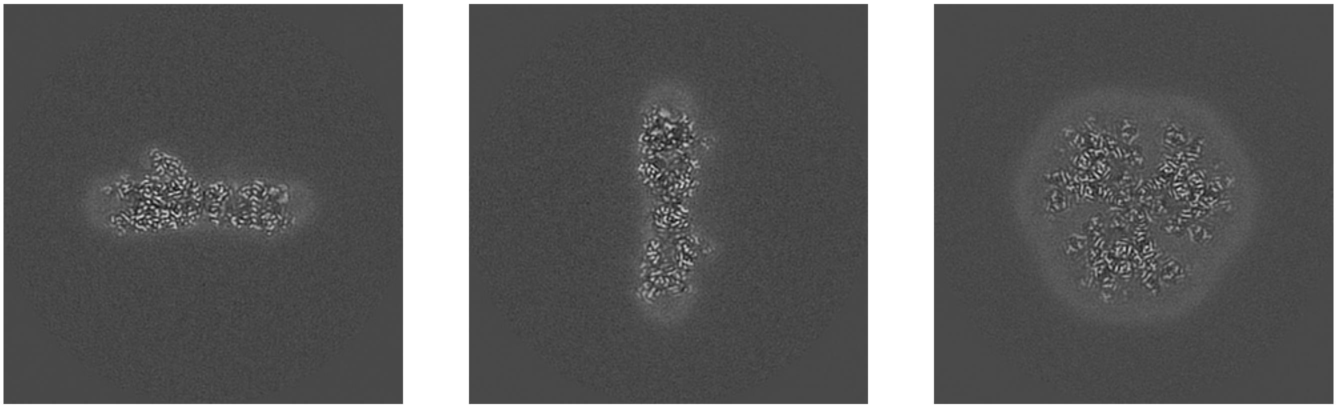
6.1.1 Primary map


X Y Z

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

6.2 Central slices ⓘ

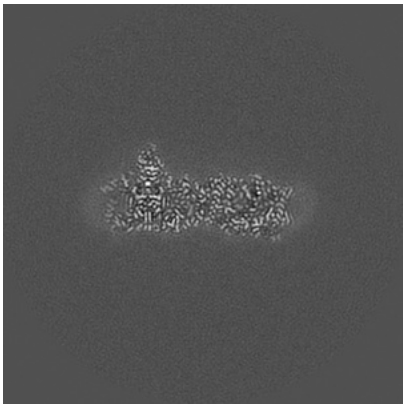
6.2.1 Primary map


X Index: 128 Y Index: 128 Z Index: 128

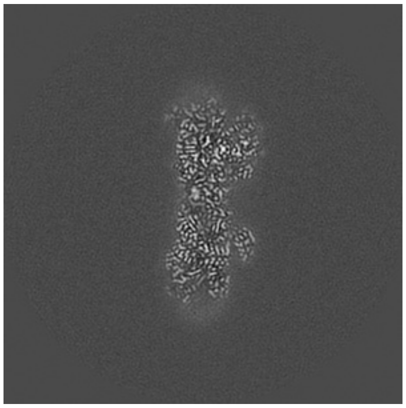
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices

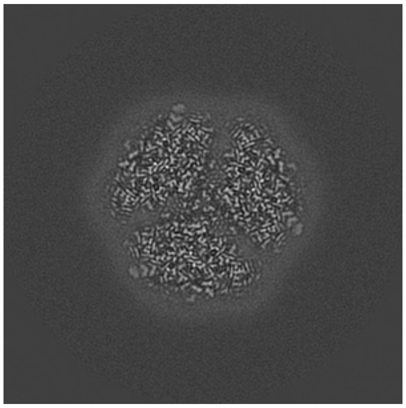
6.3.1 Primary map



X Index: 121



Y Index: 140

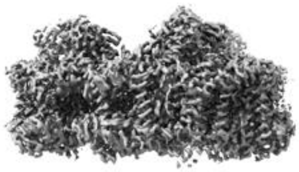


Z Index: 120

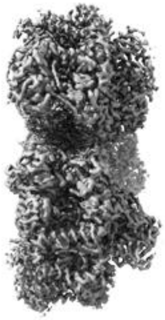
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal surface views

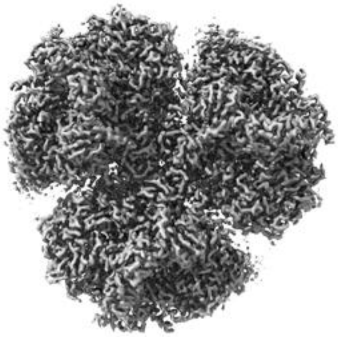
6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.055. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

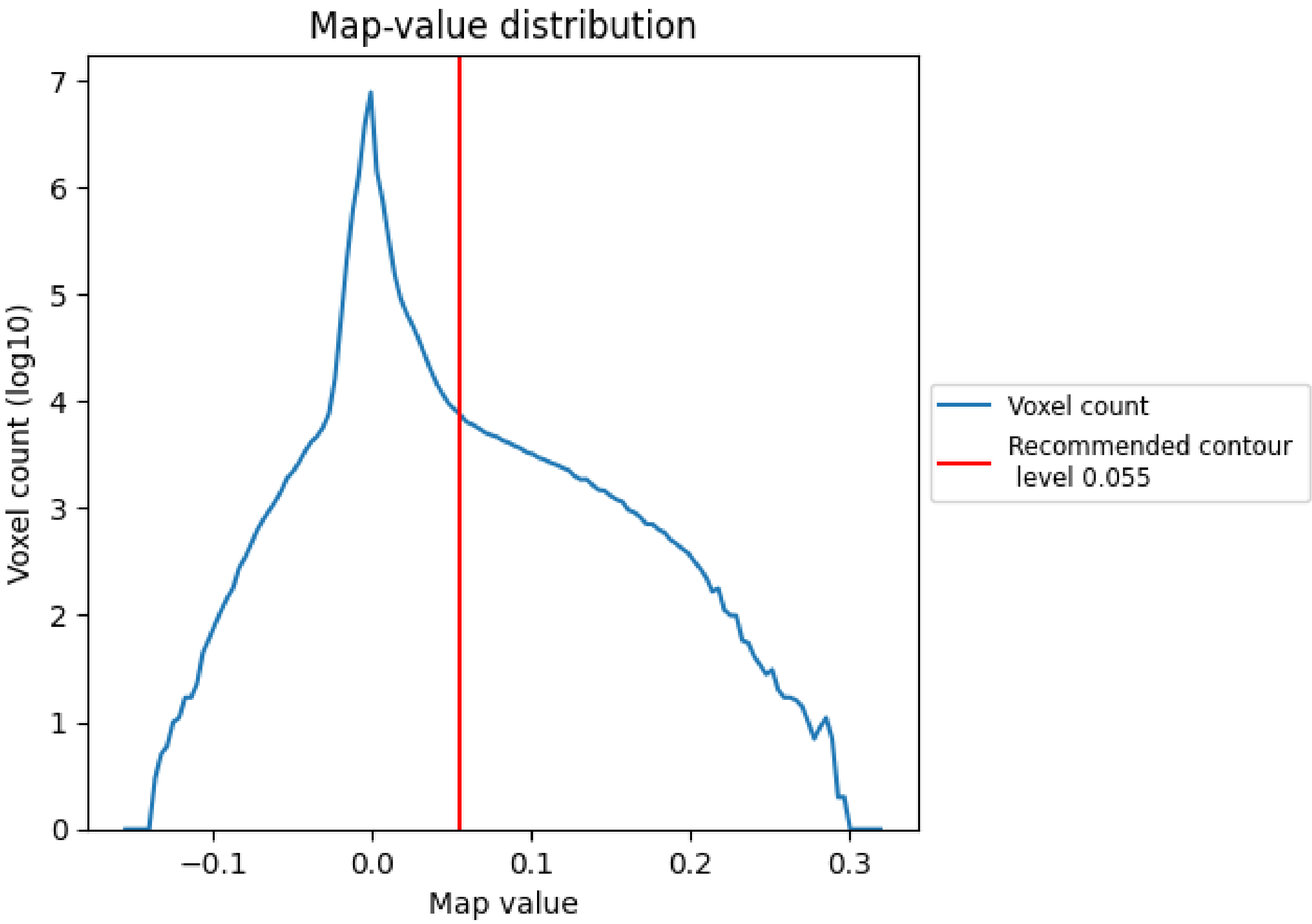
6.5 Mask visualisation

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

7 Map analysis ⓘ

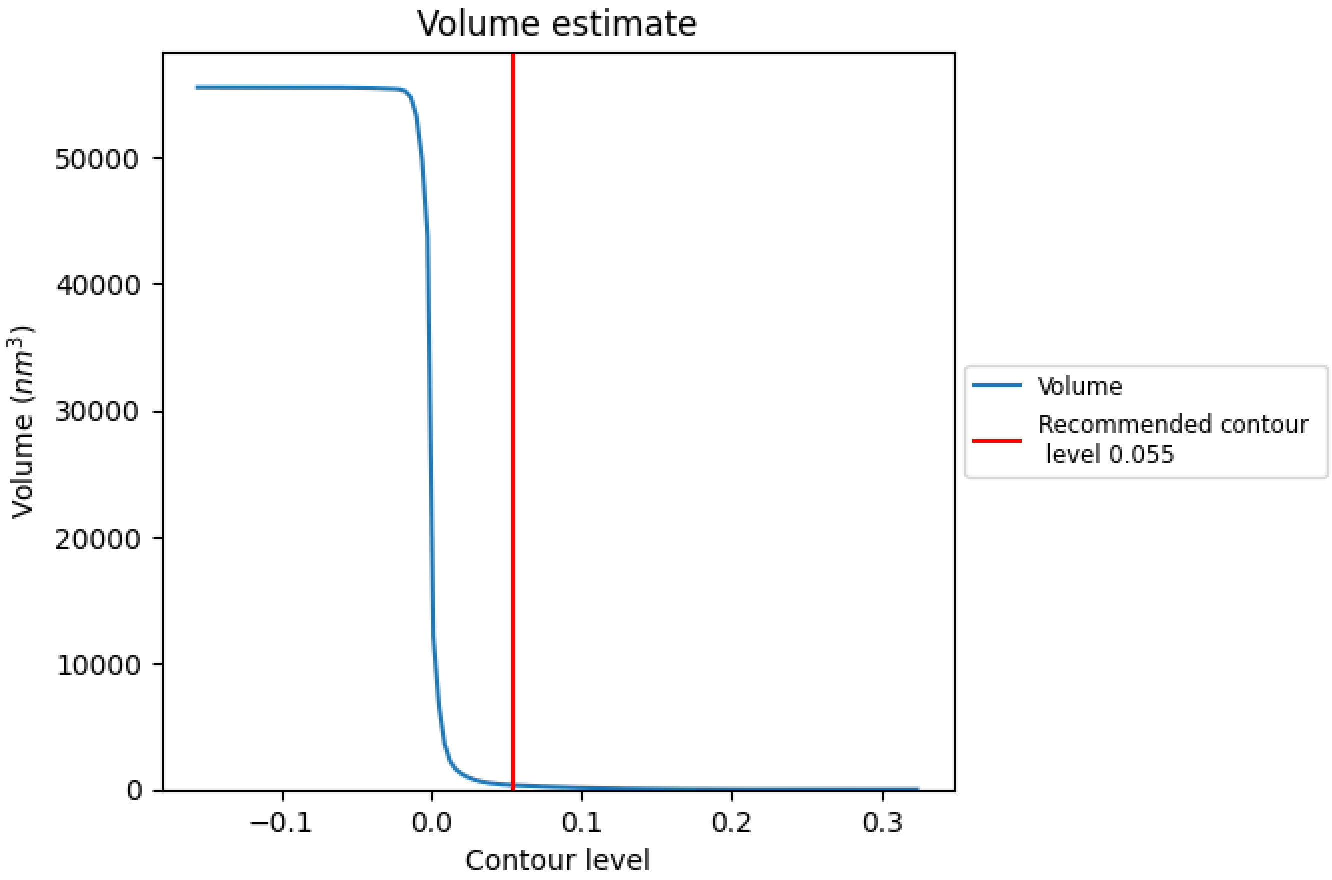
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution ⓘ



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

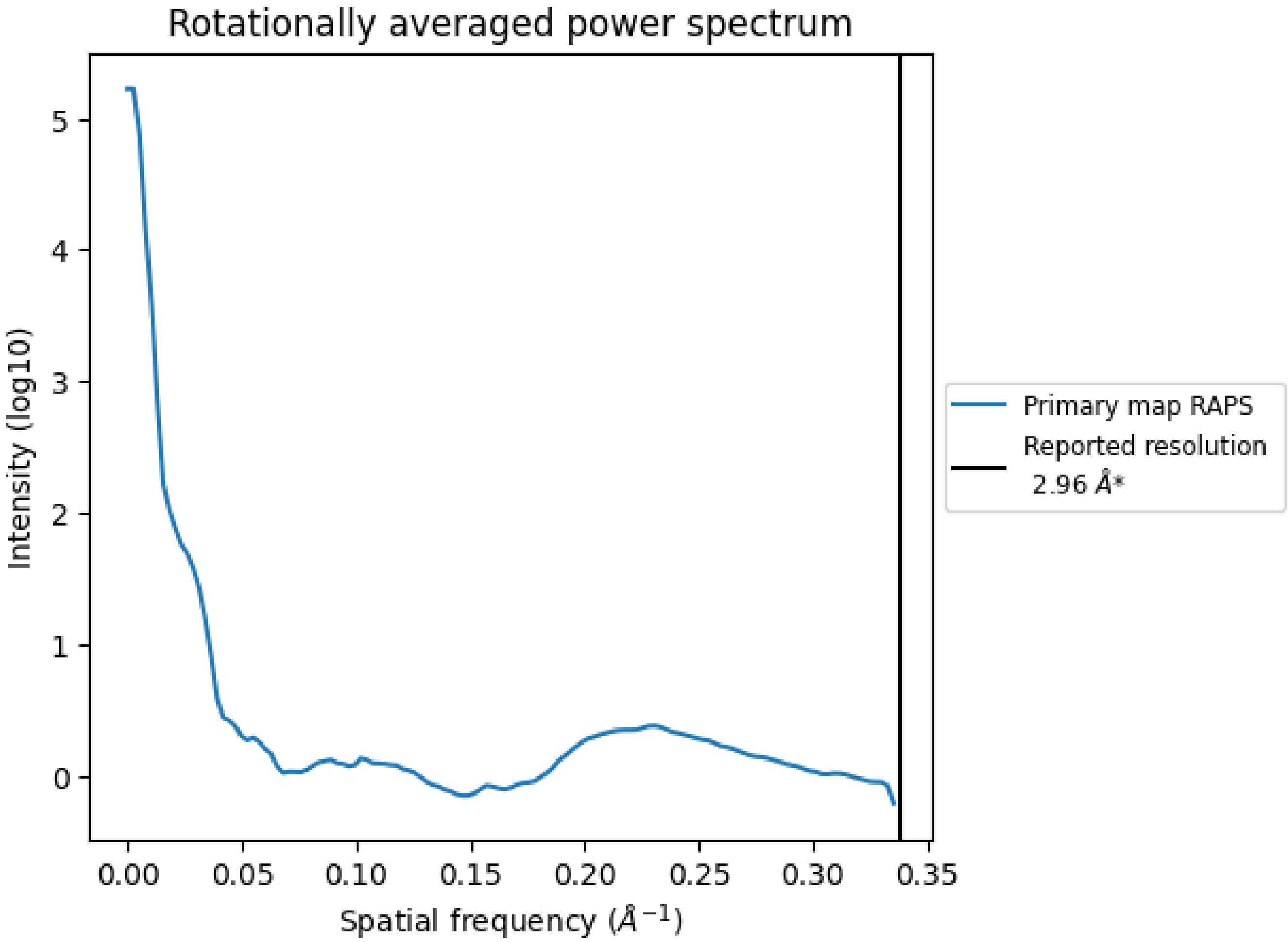
7.2 Volume estimate ⓘ



The volume at the recommended contour level is 339 nm^3; this corresponds to an approximate mass of 306 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 ⓘ

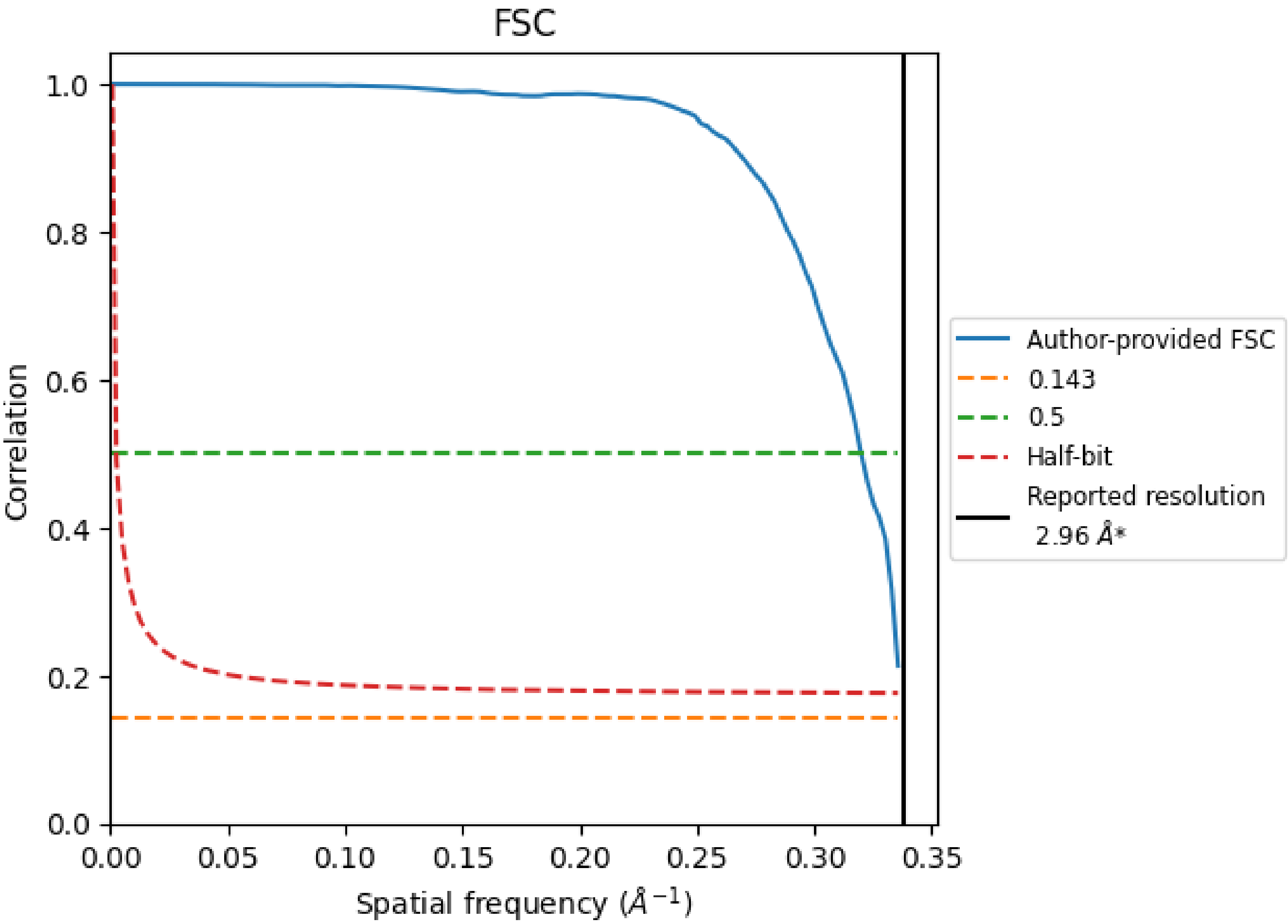


*Reported resolution corresponds to spatial frequency of 0.338 Å^{-1}

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 0.338 Å^{-1}

8.2 Resolution estimates ⓘ

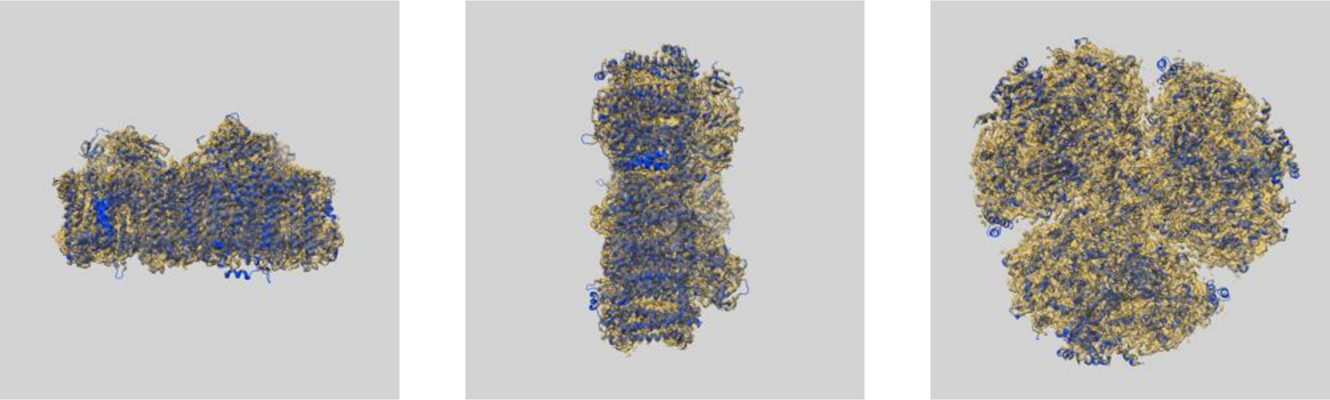
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.96	-	-
Author-provided FSC curve	-	3.13	-
Unmasked-calculated*	-	-	-

*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-23563 and PDB model 7LX0. Per-residue inclusion information can be found in section 3 on page 37.

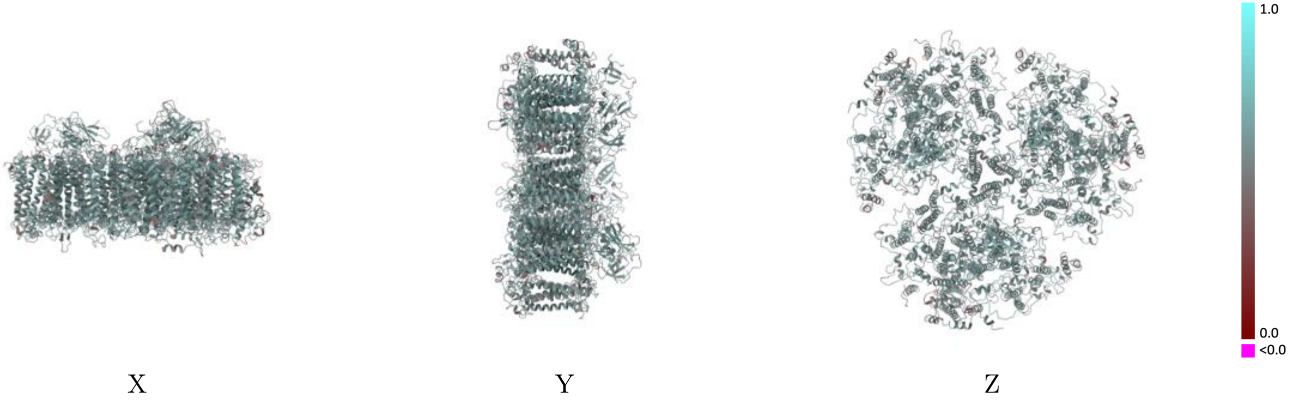
9.1 Map-model overlay ⓘ



X Y Z

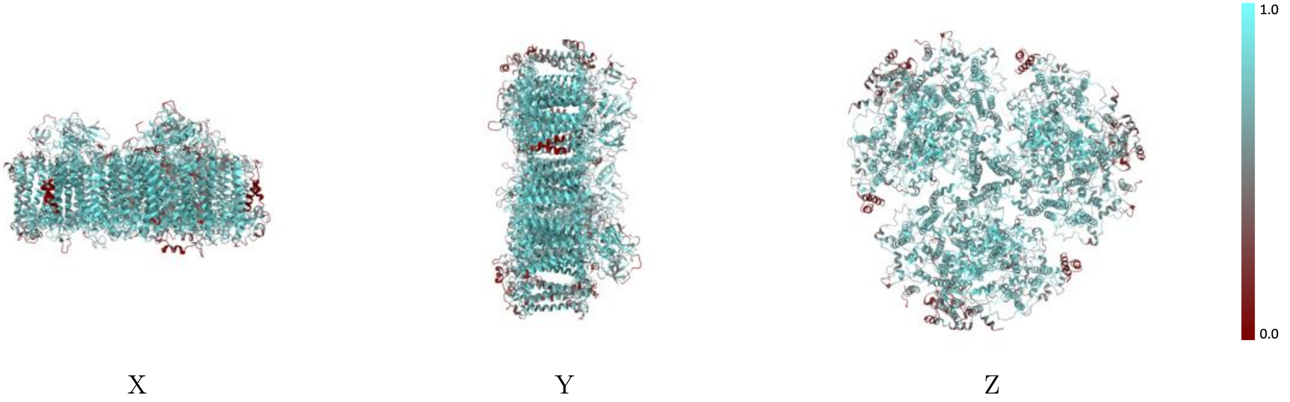
The images above show the 3D surface view of the map at the recommended contour level 0.055 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model ⓘ



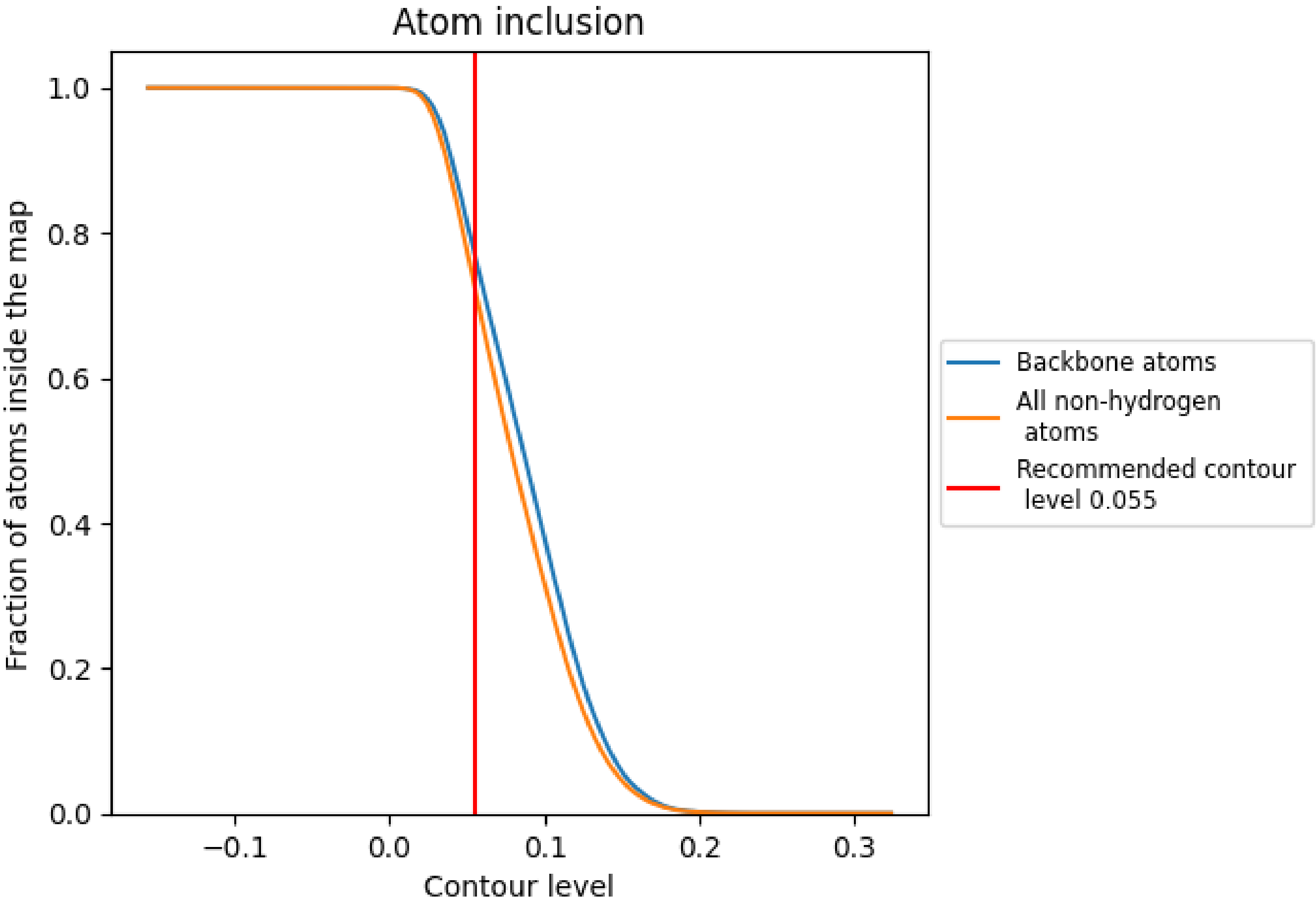
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.055).

9.4 Atom inclusion ⓘ



At the recommended contour level, 77% of all backbone atoms, 73% 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 (0.055) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7260	0.5650
A	0.7678	0.5740
B	0.7701	0.5740
C	0.7787	0.5640
D	0.6532	0.5490
E	0.5631	0.5200
F	0.3944	0.4990
G	0.7697	0.5750
H	0.7684	0.5770
I	0.7965	0.5720
J	0.4494	0.4770
K	0.0918	0.4640
L	0.7762	0.5720
M	0.7000	0.5480
N	0.7854	0.5550
O	0.6523	0.5470
P	0.5611	0.5160
Q	0.3973	0.5010
R	0.7835	0.5670
S	0.4583	0.4730
T	0.0714	0.4560
U	0.7795	0.5690
V	0.7107	0.5530
W	0.4914	0.4970
X	0.4811	0.4960
a	0.7691	0.5770
b	0.7654	0.5770
c	0.7870	0.5610
d	0.6448	0.5480
e	0.5404	0.5100
f	0.3964	0.4930
i	0.7922	0.5750
j	0.4405	0.4730
k	0.1054	0.4620
l	0.7703	0.5720

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Chain	Atom inclusion	Q-score
m	▬ 0.7000	▬ 0.5570
x	▬ 0.4777	▬ 0.4930