



wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 19, 2020 – 10:31 PM BST

PDB ID : 5OY0
Title : Structure of synechocystis photosystem I trimer at 2.5A resolution
Authors : Nelson, N.; Malavath, T.; Caspy, I.
Deposited on : 2017-09-07
Resolution : 2.50 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.13.1
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.13.1

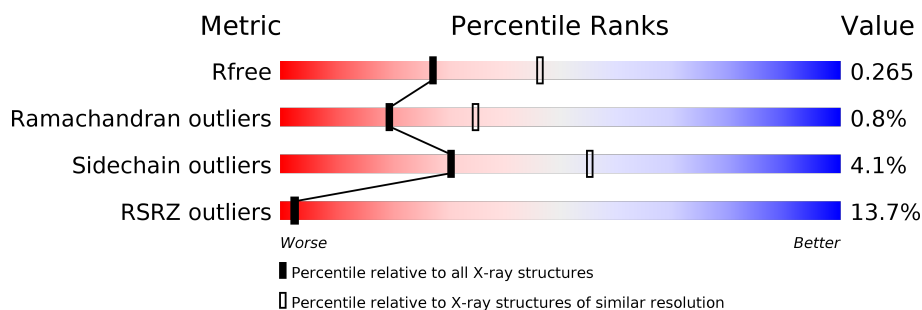
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	4661 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (2.50-2.50)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower 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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	751	<div> <div>3%</div> <div>97%</div> <div>.</div> </div>
1	a	751	<div> <div>19%</div> <div>97%</div> <div>.</div> </div>
2	2	731	<div> <div>18%</div> <div>97%</div> <div>.</div> </div>
2	B	731	<div> <div>6%</div> <div>96%</div> <div>.</div> </div>
3	3	80	<div> <div>29%</div> <div>98%</div> <div>.</div> </div>
3	C	80	<div> <div>%</div> <div>93%</div> <div>6% .</div> </div>
4	D	141	<div> <div>5%</div> <div>96%</div> <div>.</div> </div>

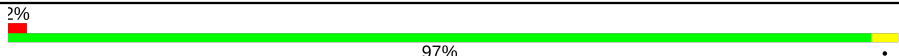
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Mol	Chain	Length	Quality of chain
4	d	141	
5	5	69	
5	E	69	
6	6	143	
6	F	143	
6	f	143	
7	I	40	
7	i	40	
8	7	40	
8	J	40	
8	j	40	
9	K	80	
10	L	157	
10	l	157	
11	9	31	
11	M	31	
11	m	31	
12	b	729	
13	c	81	
14	e	68	
15	k	78	
16	1	744	
17	4	140	
18	h	38	
19	8	79	

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Mol	Chain	Length	Quality of chain
20	0	154	

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
21	CLA	0	1501	X	-	-	-
21	CLA	0	1502	X	-	-	-
21	CLA	0	1503	X	-	-	-
21	CLA	1	1011	X	-	-	-
21	CLA	1	1012	X	-	-	-
21	CLA	1	1013	X	-	-	-
21	CLA	1	1101	X	-	-	-
21	CLA	1	1102	X	-	-	-
21	CLA	1	1103	X	-	-	-
21	CLA	1	1104	X	-	-	-
21	CLA	1	1105	X	-	-	-
21	CLA	1	1106	X	-	-	-
21	CLA	1	1107	X	-	-	-
21	CLA	1	1108	X	-	-	-
21	CLA	1	1109	X	-	-	-
21	CLA	1	1110	X	-	-	-
21	CLA	1	1111	X	-	-	-
21	CLA	1	1112	X	-	-	-
21	CLA	1	1113	X	-	-	-
21	CLA	1	1114	X	-	-	-
21	CLA	1	1115	X	-	-	-
21	CLA	1	1116	X	-	-	-
21	CLA	1	1117	X	-	-	-
21	CLA	1	1118	X	-	-	-
21	CLA	1	1119	X	-	-	-
21	CLA	1	1120	X	-	-	-
21	CLA	1	1121	X	-	-	-
21	CLA	1	1122	X	-	-	-
21	CLA	1	1123	X	-	-	-
21	CLA	1	1124	X	-	-	-
21	CLA	1	1125	X	-	-	-
21	CLA	1	1126	X	-	-	-
21	CLA	1	1127	X	-	-	-
21	CLA	1	1128	X	-	-	-
21	CLA	1	1129	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
21	CLA	1	1130	X	-	-	-
21	CLA	1	1131	X	-	-	-
21	CLA	1	1132	X	-	-	-
21	CLA	1	1133	X	-	-	-
21	CLA	1	1134	X	-	-	-
21	CLA	1	1135	X	-	-	-
21	CLA	1	1136	X	-	-	-
21	CLA	1	1137	X	-	-	-
21	CLA	1	1138	X	-	-	-
21	CLA	1	1139	X	-	-	-
21	CLA	1	1140	X	-	-	-
21	CLA	1	1801	X	-	-	-
21	CLA	2	1021	X	-	-	-
21	CLA	2	1022	X	-	-	-
21	CLA	2	1023	X	-	-	-
21	CLA	2	1201	X	-	-	-
21	CLA	2	1202	X	-	-	-
21	CLA	2	1203	X	-	-	-
21	CLA	2	1204	X	-	-	-
21	CLA	2	1205	X	-	-	-
21	CLA	2	1206	X	-	-	-
21	CLA	2	1207	X	-	-	-
21	CLA	2	1208	X	-	-	-
21	CLA	2	1209	X	-	-	-
21	CLA	2	1210	X	-	-	-
21	CLA	2	1211	X	-	-	-
21	CLA	2	1212	X	-	-	-
21	CLA	2	1213	X	-	-	-
21	CLA	2	1214	X	-	-	-
21	CLA	2	1215	X	-	-	-
21	CLA	2	1216	X	-	-	-
21	CLA	2	1217	X	-	-	-
21	CLA	2	1218	X	-	-	-
21	CLA	2	1219	X	-	-	-
21	CLA	2	1220	X	-	-	-
21	CLA	2	1221	X	-	-	-
21	CLA	2	1222	X	-	-	-
21	CLA	2	1223	X	-	-	-
21	CLA	2	1224	X	-	-	-
21	CLA	2	1225	X	-	-	-
21	CLA	2	1226	X	-	-	-
21	CLA	2	1227	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
21	CLA	2	1228	X	-	-	-
21	CLA	2	1229	X	-	-	-
21	CLA	2	1230	X	-	-	-
21	CLA	2	1231	X	-	-	-
21	CLA	2	1232	X	-	-	-
21	CLA	2	1234	X	-	-	-
21	CLA	2	1235	X	-	-	-
21	CLA	2	1236	X	-	-	-
21	CLA	2	1237	X	-	-	-
21	CLA	2	1238	X	-	-	-
21	CLA	2	1239	X	-	-	-
21	CLA	2	1240	X	-	-	X
21	CLA	6	1301	X	-	-	-
21	CLA	6	1302	X	-	-	X
21	CLA	7	1302	X	-	-	-
21	CLA	7	1303	X	-	-	-
21	CLA	8	1401	X	-	-	-
21	CLA	8	1402	X	-	-	-
21	CLA	A	1011	X	-	-	-
21	CLA	A	1012	X	-	-	-
21	CLA	A	1013	X	-	-	-
21	CLA	A	1101	X	-	-	-
21	CLA	A	1102	X	-	-	-
21	CLA	A	1103	X	-	-	-
21	CLA	A	1104	X	-	-	-
21	CLA	A	1105	X	-	-	-
21	CLA	A	1106	X	-	-	-
21	CLA	A	1107	X	-	-	-
21	CLA	A	1108	X	-	-	-
21	CLA	A	1109	X	-	-	-
21	CLA	A	1110	X	-	-	-
21	CLA	A	1111	X	-	-	-
21	CLA	A	1112	X	-	-	-
21	CLA	A	1113	X	-	-	-
21	CLA	A	1114	X	-	-	-
21	CLA	A	1115	X	-	-	-
21	CLA	A	1116	X	-	-	-
21	CLA	A	1117	X	-	-	-
21	CLA	A	1118	X	-	-	-
21	CLA	A	1119	X	-	-	-
21	CLA	A	1120	X	-	-	-
21	CLA	A	1121	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
21	CLA	A	1122	X	-	-	-
21	CLA	A	1123	X	-	-	-
21	CLA	A	1124	X	-	-	-
21	CLA	A	1125	X	-	-	-
21	CLA	A	1126	X	-	-	-
21	CLA	A	1127	X	-	-	-
21	CLA	A	1128	X	-	-	-
21	CLA	A	1129	X	-	-	-
21	CLA	A	1130	X	-	-	-
21	CLA	A	1131	X	-	-	-
21	CLA	A	1132	X	-	-	-
21	CLA	A	1133	X	-	-	-
21	CLA	A	1134	X	-	-	-
21	CLA	A	1135	X	-	-	-
21	CLA	A	1136	X	-	-	-
21	CLA	A	1137	X	-	-	-
21	CLA	A	1138	X	-	-	-
21	CLA	A	1139	X	-	-	-
21	CLA	A	1140	X	-	-	-
21	CLA	A	1801	X	-	-	-
21	CLA	B	1021	X	-	-	-
21	CLA	B	1022	X	-	-	-
21	CLA	B	1023	X	-	-	-
21	CLA	B	1201	X	-	-	-
21	CLA	B	1202	X	-	-	-
21	CLA	B	1203	X	-	-	-
21	CLA	B	1204	X	-	-	-
21	CLA	B	1205	X	-	-	-
21	CLA	B	1206	X	-	-	-
21	CLA	B	1207	X	-	-	-
21	CLA	B	1208	X	-	-	-
21	CLA	B	1209	X	-	-	-
21	CLA	B	1210	X	-	-	-
21	CLA	B	1211	X	-	-	-
21	CLA	B	1212	X	-	-	-
21	CLA	B	1213	X	-	-	-
21	CLA	B	1214	X	-	-	-
21	CLA	B	1215	X	-	-	-
21	CLA	B	1216	X	-	-	-
21	CLA	B	1217	X	-	-	-
21	CLA	B	1218	X	-	-	-
21	CLA	B	1219	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
21	CLA	B	1220	X	-	-	-
21	CLA	B	1221	X	-	-	-
21	CLA	B	1222	X	-	-	-
21	CLA	B	1223	X	-	-	-
21	CLA	B	1224	X	-	-	-
21	CLA	B	1225	X	-	-	-
21	CLA	B	1226	X	-	-	-
21	CLA	B	1227	X	-	-	-
21	CLA	B	1228	X	-	-	-
21	CLA	B	1229	X	-	-	-
21	CLA	B	1230	X	-	-	-
21	CLA	B	1231	X	-	-	-
21	CLA	B	1232	X	-	-	-
21	CLA	B	1234	X	-	-	-
21	CLA	B	1235	X	-	-	-
21	CLA	B	1236	X	-	-	-
21	CLA	B	1237	X	-	-	-
21	CLA	B	1238	X	-	-	-
21	CLA	B	1239	X	-	-	-
21	CLA	B	1240	X	-	-	-
21	CLA	F	1301	X	-	-	-
21	CLA	F	1302	X	-	-	-
21	CLA	J	1302	X	-	-	-
21	CLA	J	1303	X	-	-	-
21	CLA	K	1401	X	-	-	-
21	CLA	K	1402	X	-	-	-
21	CLA	L	1501	X	-	-	-
21	CLA	L	1502	X	-	-	-
21	CLA	L	1503	X	-	-	-
21	CLA	a	1011	X	-	-	-
21	CLA	a	1012	X	-	-	-
21	CLA	a	1013	X	-	-	-
21	CLA	a	1101	X	-	-	-
21	CLA	a	1102	X	-	-	-
21	CLA	a	1103	X	-	-	-
21	CLA	a	1104	X	-	-	-
21	CLA	a	1105	X	-	-	-
21	CLA	a	1106	X	-	-	-
21	CLA	a	1107	X	-	-	-
21	CLA	a	1108	X	-	-	-
21	CLA	a	1109	X	-	-	-
21	CLA	a	1110	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
21	CLA	a	1111	X	-	-	-
21	CLA	a	1112	X	-	-	-
21	CLA	a	1113	X	-	-	X
21	CLA	a	1114	X	-	-	-
21	CLA	a	1115	X	-	-	-
21	CLA	a	1116	X	-	-	-
21	CLA	a	1117	X	-	-	-
21	CLA	a	1118	X	-	-	-
21	CLA	a	1119	X	-	-	-
21	CLA	a	1120	X	-	-	-
21	CLA	a	1121	X	-	-	-
21	CLA	a	1122	X	-	-	-
21	CLA	a	1123	X	-	-	-
21	CLA	a	1124	X	-	-	-
21	CLA	a	1125	X	-	-	-
21	CLA	a	1126	X	-	-	-
21	CLA	a	1127	X	-	-	-
21	CLA	a	1128	X	-	-	-
21	CLA	a	1129	X	-	-	-
21	CLA	a	1130	X	-	-	-
21	CLA	a	1131	X	-	-	-
21	CLA	a	1132	X	-	-	-
21	CLA	a	1133	X	-	-	-
21	CLA	a	1134	X	-	-	-
21	CLA	a	1135	X	-	-	-
21	CLA	a	1136	X	-	-	-
21	CLA	a	1137	X	-	-	-
21	CLA	a	1138	X	-	-	-
21	CLA	a	1139	X	-	-	-
21	CLA	a	1140	X	-	-	-
21	CLA	a	1801	X	-	-	-
21	CLA	b	1021	X	-	-	-
21	CLA	b	1022	X	-	-	-
21	CLA	b	1023	X	-	-	-
21	CLA	b	1201	X	-	-	-
21	CLA	b	1202	X	-	-	-
21	CLA	b	1203	X	-	-	-
21	CLA	b	1204	X	-	-	-
21	CLA	b	1205	X	-	-	-
21	CLA	b	1206	X	-	-	-
21	CLA	b	1207	X	-	-	-
21	CLA	b	1208	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
21	CLA	b	1209	X	-	-	-
21	CLA	b	1210	X	-	-	-
21	CLA	b	1211	X	-	-	-
21	CLA	b	1212	X	-	-	-
21	CLA	b	1213	X	-	-	-
21	CLA	b	1214	X	-	-	-
21	CLA	b	1215	X	-	-	-
21	CLA	b	1216	X	-	-	-
21	CLA	b	1217	X	-	-	-
21	CLA	b	1218	X	-	-	-
21	CLA	b	1219	X	-	-	-
21	CLA	b	1220	X	-	-	-
21	CLA	b	1221	X	-	-	-
21	CLA	b	1222	X	-	-	-
21	CLA	b	1223	X	-	-	-
21	CLA	b	1224	X	-	-	-
21	CLA	b	1225	X	-	-	-
21	CLA	b	1226	X	-	-	-
21	CLA	b	1227	X	-	-	-
21	CLA	b	1228	X	-	-	-
21	CLA	b	1229	X	-	-	-
21	CLA	b	1230	X	-	-	-
21	CLA	b	1231	X	-	-	-
21	CLA	b	1232	X	-	-	-
21	CLA	b	1234	X	-	-	-
21	CLA	b	1235	X	-	-	-
21	CLA	b	1236	X	-	-	-
21	CLA	b	1237	X	-	-	-
21	CLA	b	1238	X	-	-	-
21	CLA	b	1239	X	-	-	-
21	CLA	b	1240	X	-	-	-
21	CLA	f	1301	X	-	-	-
21	CLA	f	1302	X	-	-	-
21	CLA	j	1302	X	-	-	-
21	CLA	j	1303	X	-	-	-
21	CLA	k	1401	X	-	-	-
21	CLA	k	1402	X	-	-	-
21	CLA	l	1501	X	-	-	-
21	CLA	l	1502	X	-	-	-
21	CLA	l	1503	X	-	-	-
24	BCR	1	4001	-	-	-	X
24	BCR	1	4019	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
24	BCR	2	4004	-	-	-	X
24	BCR	2	4018	-	-	-	X
24	BCR	6	4016	-	-	-	X
24	BCR	8	4001	-	-	-	X
24	BCR	A	4019	-	-	-	X
24	BCR	B	4018	-	-	-	X
24	BCR	a	4019	-	-	-	X
24	BCR	b	4018	-	-	-	X
24	BCR	k	4001	-	-	-	X
25	LHG	1	5007	-	-	-	X
25	LHG	2	5004	-	-	-	X
25	LHG	B	5006	-	-	-	X
25	LHG	F	5002	-	-	-	X
25	LHG	a	5007	-	-	-	X
26	LMG	2	5005	-	-	-	X
26	LMG	A	5008	-	-	-	X
26	LMG	b	5007	-	-	-	X
31	SQD	F	5001	-	-	-	X
34	ZEX	7	4015	-	-	-	X
34	ZEX	F	4016	X	-	-	-
35	LMT	1	6001	-	-	-	X

2 Entry composition

There are 38 unique types of molecules in this entry. The entry contains 77117 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, 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					ZeroOcc	AltConf	Trace
1	A	751	Total	C	N	O	S	0	0	0
			5878	3847	1000	1003	28			
1	a	751	Total	C	N	O	S	0	0	0
			5878	3847	1000	1003	28			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	731	Total	C	N	O	S	0	0	0
			5783	3806	969	992	16			
2	2	731	Total	C	N	O	S	0	0	0
			5783	3806	969	992	16			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	80	Total	C	N	O	S	0	0	0
			600	369	103	117	11			
3	3	80	Total	C	N	O	S	0	0	0
			600	369	103	117	11			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	141	Total	C	N	O	S	0	0	0
			1102	697	190	211	4			
4	d	141	Total	C	N	O	S	0	0	0
			1102	697	190	211	4			

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
5	E	69	Total	C	N	O	0	0	0
			543	340	96	107			
5	5	69	Total	C	N	O	0	0	0
			543	340	96	107			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	F	143	Total	C	N	O	S	0	0	0
			1113	718	185	205	5			
6	f	143	Total	C	N	O	S	0	0	0
			1113	718	185	205	5			
6	6	143	Total	C	N	O	S	0	0	0
			1113	718	185	205	5			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	I	40	Total	C	N	O	S	0	0	0
			311	209	44	55	3			
7	i	40	Total	C	N	O	S	0	0	0
			311	209	44	55	3			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	J	40	Total	C	N	O	S	0	0	0
			319	215	47	54	3			
8	j	40	Total	C	N	O	S	0	0	0
			319	215	47	54	3			
8	7	40	Total	C	N	O	S	0	0	0
			319	215	47	54	3			

- Molecule 9 is a protein called Photosystem I reaction center subunit Psak 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	K	80	Total	C	N	O	S	0	1	0
			579	378	93	102	6			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	L	157	Total	C	N	O	S	0	0	0
			1178	766	191	218	3			
10	l	157	Total	C	N	O	S	0	0	0
			1178	766	191	218	3			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	M	31	Total	C	N	O	S	0	0	0
			238	159	36	42	1			
11	m	31	Total	C	N	O	S	0	0	0
			238	159	36	42	1			
11	9	31	Total	C	N	O	S	0	0	0
			238	159	36	42	1			

- Molecule 12 is a protein called Photosystem I P700 chlorophyll a apoprotein A2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	b	729	Total	C	N	O	S	0	0	0
			5770	3798	967	990	15			

- Molecule 13 is a protein called Photosystem I iron-sulfur center.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	c	81	Total	C	N	O	S	0	0	0
			608	374	104	118	12			

- Molecule 14 is a protein called Photosystem I reaction center subunit IV.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
14	e	68	Total	C	N	O	0	0	0
			533	335	94	104			

- Molecule 15 is a protein called Photosystem I reaction center subunit PsaK 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
15	k	78	Total	C	N	O	S	0	0	0
			559	366	90	98	5			

- Molecule 16 is a protein called Photosystem I P700 chlorophyll a apoprotein A1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
16	1	744	Total	C	N	O	S	0	0	0
			5826	3814	993	992	27			

- Molecule 17 is a protein called Photosystem I reaction center subunit II.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
17	4	140	Total	C	N	O	S	0	0	0
			1094	692	189	210	3			

- Molecule 18 is a protein called Photosystem I reaction center subunit VIII.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
18	h	38	Total	C	N	O	S	0	0	0
			298	202	42	51	3			

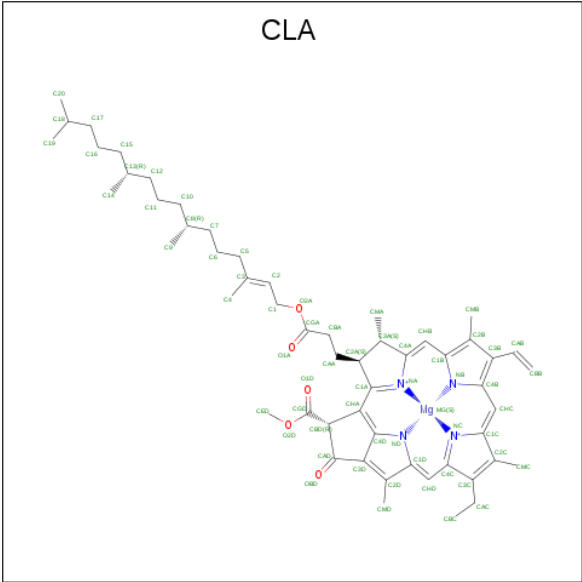
- Molecule 19 is a protein called Photosystem I reaction center subunit PsaK 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
19	8	79	Total	C	N	O	S	0	0	0
			565	369	91	100	5			

- Molecule 20 is a protein called Photosystem I reaction center subunit XI.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
20	0	154	Total	C	N	O	S	0	0	0
			1156	753	188	213	2			

- Molecule 21 is CHLOROPHYLL A (three-letter code: CLA) (formula: C₅₅H₇₂MgN₄O₅).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
21	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
21	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
21	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
21	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
21	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
21	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
21	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
21	A	1	Total	C	Mg	N	O	0	0
			53	43	1	4	5		
21	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
21	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
21	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
21	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
21	A	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
21	A	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
21	A	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
21	A	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
21	A	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
21	A	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
21	A	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
21	A	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
21	A	1	Total 60	C 50	Mg 1	N 4	O 5	0	0
21	A	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
21	A	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
21	A	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
21	A	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
21	A	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
21	A	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
21	A	1	Total 58	C 48	Mg 1	N 4	O 5	0	0
21	A	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
21	A	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
21	A	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
21	A	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
21	A	1	Total 65	C 55	Mg 1	N 4	O 5	0	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
21	A	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
21	A	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
21	A	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
21	A	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
21	A	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
21	A	1	Total 60	C 50	Mg 1	N 4	O 5	0	0
21	A	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
21	A	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
21	A	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
21	B	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
21	B	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
21	B	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
21	B	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
21	B	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
21	B	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
21	B	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
21	B	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
21	B	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
21	B	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
21	B	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
21	B	1	Total 65	C 55	Mg 1	N 4	O 5	0	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
21	B	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
21	B	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
21	B	1	Total 55	C 45	Mg 1	N 4	O 5	0	0
21	B	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
21	B	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
21	B	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
21	B	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
21	B	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
21	B	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
21	B	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
21	B	1	Total 57	C 47	Mg 1	N 4	O 5	0	0
21	B	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
21	B	1	Total 55	C 45	Mg 1	N 4	O 5	0	0
21	B	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
21	B	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
21	B	1	Total 55	C 45	Mg 1	N 4	O 5	0	0
21	B	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
21	B	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
21	B	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
21	B	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
21	B	1	Total 65	C 55	Mg 1	N 4	O 5	0	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
21	B	1	Total 50	C 40	Mg 1	N 4	O 5	0	0
21	B	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
21	B	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
21	B	1	Total 50	C 40	Mg 1	N 4	O 5	0	0
21	B	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
21	B	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
21	B	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
21	B	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
21	B	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
21	F	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
21	F	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
21	J	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
21	J	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
21	K	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
21	K	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
21	L	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
21	L	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
21	L	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
21	a	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
21	a	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
21	a	1	Total 65	C 55	Mg 1	N 4	O 5	0	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
21	a	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
21	a	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
21	a	1	Total	C	Mg	N	O	0	0
			58	48	1	4	5		
21	a	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
21	a	1	Total	C	Mg	N	O	0	0
			50	40	1	4	5		
21	a	1	Total	C	Mg	N	O	0	0
			57	47	1	4	5		
21	a	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
21	a	1	Total	C	Mg	N	O	0	0
			59	49	1	4	5		
21	a	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
21	a	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
21	a	1	Total	C	Mg	N	O	0	0
			50	40	1	4	5		
21	a	1	Total	C	Mg	N	O	0	0
			52	42	1	4	5		
21	a	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
21	a	1	Total	C	Mg	N	O	0	0
			60	50	1	4	5		
21	a	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
21	a	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
21	a	1	Total	C	Mg	N	O	0	0
			55	45	1	4	5		
21	a	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
21	a	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
21	a	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
21	a	1	Total	C	Mg	N	O	0	0
			55	45	1	4	5		
21	a	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
21	a	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
21	a	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
21	a	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
21	a	1	Total	C	Mg	N	O	0	0
			52	42	1	4	5		
21	a	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
21	a	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
21	a	1	Total	C	Mg	N	O	0	0
			49	39	1	4	5		
21	a	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
21	a	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
21	a	1	Total	C	Mg	N	O	0	0
			51	41	1	4	5		
21	a	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
21	a	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
21	a	1	Total	C	Mg	N	O	0	0
			55	45	1	4	5		
21	a	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
21	a	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
21	a	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
21	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
21	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
21	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
21	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
21	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
21	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
21	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
21	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
21	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
21	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
21	b	1	Total 60	C 50	Mg 1	N 4	O 5	0	0
21	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
21	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
21	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
21	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
21	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
21	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
21	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
21	b	1	Total 51	C 41	Mg 1	N 4	O 5	0	0
21	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
21	b	1	Total 60	C 50	Mg 1	N 4	O 5	0	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
21	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
21	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
21	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
21	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
21	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
21	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
21	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
21	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
21	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
21	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
21	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
21	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
21	b	1	Total 53	C 43	Mg 1	N 4	O 5	0	0
21	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
21	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
21	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
21	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
21	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
21	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
21	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
21	f	1	Total 50	C 40	Mg 1	N 4	O 5	0	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
21	f	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
21	j	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
21	j	1	Total 55	C 45	Mg 1	N 4	O 5	0	0
21	k	1	Total 50	C 40	Mg 1	N 4	O 5	0	0
21	k	1	Total 49	C 39	Mg 1	N 4	O 5	0	0
21	l	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
21	l	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
21	l	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
21	1	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
21	1	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
21	1	1	Total 55	C 45	Mg 1	N 4	O 5	0	0
21	1	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
21	1	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
21	1	1	Total 50	C 40	Mg 1	N 4	O 5	0	0
21	1	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
21	1	1	Total 51	C 41	Mg 1	N 4	O 5	0	0
21	1	1	Total 47	C 37	Mg 1	N 4	O 5	0	0
21	1	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
21	1	1	Total 50	C 40	Mg 1	N 4	O 5	0	0
21	1	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
21	1	1	Total 50	C 40	Mg 1	N 4	O 5	0	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
21	1	1	Total	C	Mg	N	O	0	0
			44	35	1	4	4		
21	1	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
21	1	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
21	1	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
21	1	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
21	1	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
21	1	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
21	1	1	Total	C	Mg	N	O	0	0
			55	45	1	4	5		
21	1	1	Total	C	Mg	N	O	0	0
			60	50	1	4	5		
21	1	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
21	1	1	Total	C	Mg	N	O	0	0
			56	46	1	4	5		
21	1	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
21	1	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
21	1	1	Total	C	Mg	N	O	0	0
			50	40	1	4	5		
21	1	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
21	1	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
21	1	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
21	1	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
21	1	1	Total	C	Mg	N	O	0	0
			52	42	1	4	5		
21	1	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
21	1	1	Total	C	Mg	N	O	0	0
			51	41	1	4	5		
21	1	1	Total	C	Mg	N	O	0	0
			60	50	1	4	5		
21	1	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
21	1	1	Total	C	Mg	N	O	0	0
			56	46	1	4	5		
21	1	1	Total	C	Mg	N	O	0	0
			55	45	1	4	5		
21	1	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
21	1	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
21	1	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
21	2	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
21	2	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
21	2	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
21	2	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
21	2	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
21	2	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
21	2	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
21	2	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
21	2	1	Total	C	Mg	N	O	0	0
			56	46	1	4	5		

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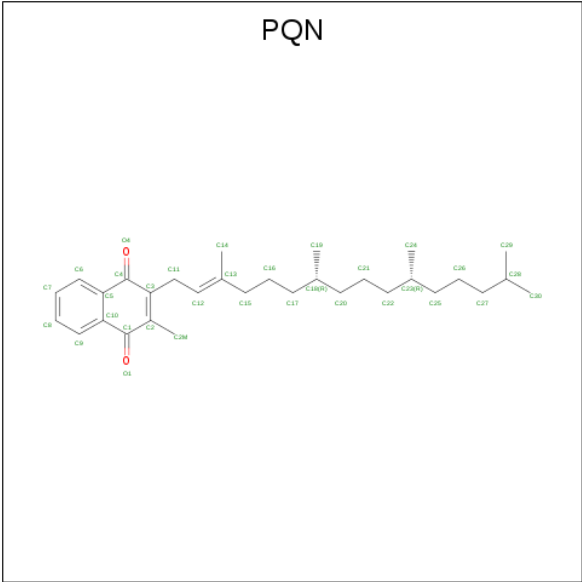
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
21	2	1	Total	C	Mg	N	O	0	0
			60	50	1	4	5		
21	2	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
21	2	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
21	2	1	Total	C	Mg	N	O	0	0
			50	40	1	4	5		
21	2	1	Total	C	Mg	N	O	0	0
			41	33	1	4	3		
21	2	1	Total	C	Mg	N	O	0	0
			50	40	1	4	5		
21	2	1	Total	C	Mg	N	O	0	0
			59	49	1	4	5		
21	2	1	Total	C	Mg	N	O	0	0
			60	50	1	4	5		
21	2	1	Total	C	Mg	N	O	0	0
			50	40	1	4	5		
21	2	1	Total	C	Mg	N	O	0	0
			52	42	1	4	5		
21	2	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
21	2	1	Total	C	Mg	N	O	0	0
			53	43	1	4	5		
21	2	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
21	2	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
21	2	1	Total	C	Mg	N	O	0	0
			50	40	1	4	5		
21	2	1	Total	C	Mg	N	O	0	0
			55	45	1	4	5		
21	2	1	Total	C	Mg	N	O	0	0
			55	45	1	4	5		
21	2	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
21	2	1	Total	C	Mg	N	O	0	0
			55	45	1	4	5		
21	2	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
21	2	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
21	2	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
21	2	1	Total	C	Mg	N	O	0	0
			46	36	1	4	5		
21	2	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
21	2	1	Total	C	Mg	N	O	0	0
			50	40	1	4	5		
21	2	1	Total	C	Mg	N	O	0	0
			53	43	1	4	5		
21	2	1	Total	C	Mg	N	O	0	0
			50	40	1	4	5		
21	2	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
21	2	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
21	2	1	Total	C	Mg	N	O	0	0
			41	33	1	4	3		
21	2	1	Total	C	Mg	N	O	0	0
			47	37	1	4	5		
21	6	1	Total	C	Mg	N	O	0	0
			47	37	1	4	5		
21	6	1	Total	C	Mg	N	O	0	0
			43	35	1	4	3		
21	7	1	Total	C	Mg	N	O	0	0
			41	33	1	4	3		
21	7	1	Total	C	Mg	N	O	0	0
			41	33	1	4	3		
21	8	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
21	8	1	Total	C	Mg	N	O	0	0
			46	36	1	4	5		
21	0	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
21	0	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
21	0	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		

- Molecule 22 is PHYLLOQUINONE (three-letter code: PQN) (formula: C₃₁H₄₆O₂).



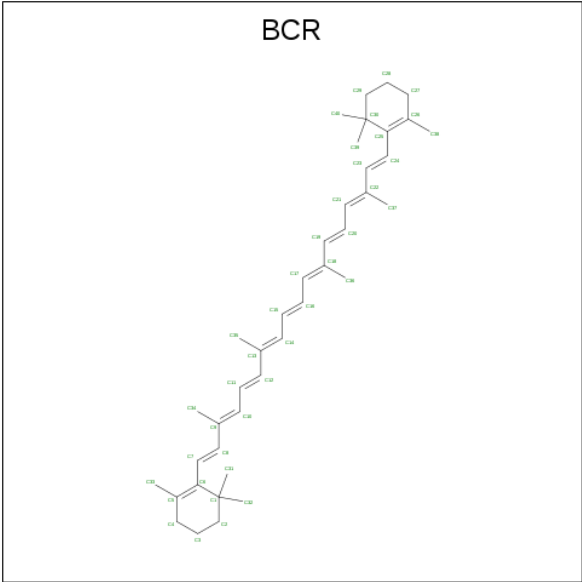
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
22	A	1	Total	C	O	0	0
			33	31	2		
22	B	1	Total	C	O	0	0
			33	31	2		
22	a	1	Total	C	O	0	0
			33	31	2		
22	b	1	Total	C	O	0	0
			33	31	2		
22	1	1	Total	C	O	0	0
			33	31	2		
22	2	1	Total	C	O	0	0
			33	31	2		

- Molecule 23 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe₄S₄).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
23	A	1	Total	Fe	S	0	0
			8	4	4		
23	C	1	Total	Fe	S		
			8	4	4		
23	C	1	Total	Fe	S		
			8	4	4		
23	a	1	Total	Fe	S		
			8	4	4		
23	c	1	Total	Fe	S		
			8	4	4		
23	c	1	Total	Fe	S	0	0
			8	4	4		
23	1	1	Total	Fe	S	0	0
			8	4	4		
23	3	1	Total	Fe	S	0	0
			8	4	4		
23	3	1	Total	Fe	S	0	0
			8	4	4		

- Molecule 24 is BETA-CAROTENE (three-letter code: BCR) (formula: C₄₀H₅₆).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
24	A	1	Total C 40 40	0	0
24	A	1	Total C 40 40	0	0
24	A	1	Total C 40 40	0	0
24	A	1	Total C 40 40	0	0
24	A	1	Total C 40 40	0	0
24	A	1	Total C 40 40	0	0
24	A	1	Total C 40 40	0	0
24	B	1	Total C 40 40	0	0
24	B	1	Total C 40 40	0	0
24	B	1	Total C 40 40	0	0
24	B	1	Total C 40 40	0	0
24	B	1	Total C 40 40	0	0
24	B	1	Total C 40 40	0	0
24	I	1	Total C 40 40	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
24	J	1	Total C 40 40	0	0
24	K	1	Total C 40 40	0	0
24	L	1	Total C 40 40	0	0
24	L	1	Total C 40 40	0	0
24	a	1	Total C 40 40	0	0
24	a	1	Total C 40 40	0	0
24	a	1	Total C 40 40	0	0
24	a	1	Total C 40 40	0	0
24	a	1	Total C 40 40	0	0
24	a	1	Total C 40 40	0	0
24	a	1	Total C 40 40	0	0
24	a	1	Total C 40 40	0	0
24	b	1	Total C 40 40	0	0
24	b	1	Total C 40 40	0	0
24	b	1	Total C 40 40	0	0
24	b	1	Total C 40 40	0	0
24	b	1	Total C 40 40	0	0
24	b	1	Total C 40 40	0	0
24	f	1	Total C 40 40	0	0
24	i	1	Total C 40 40	0	0
24	j	1	Total C 40 40	0	0
24	k	1	Total C 40 40	0	0

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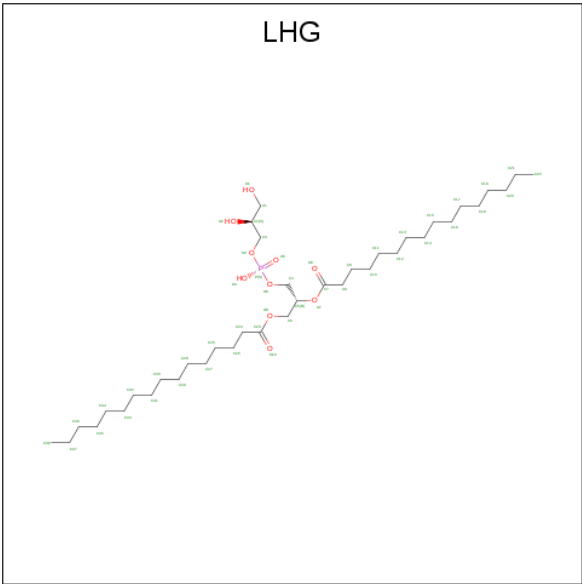
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
24	1	1	Total C 40 40	0	0
24	1	1	Total C 40 40	0	0
24	1	1	Total C 40 40	0	0
24	1	1	Total C 40 40	0	0
24	1	1	Total C 40 40	0	0
24	1	1	Total C 40 40	0	0
24	1	1	Total C 40 40	0	0
24	1	1	Total C 40 40	0	0
24	1	1	Total C 40 40	0	0
24	2	1	Total C 40 40	0	0
24	2	1	Total C 40 40	0	0
24	2	1	Total C 40 40	0	0
24	2	1	Total C 40 40	0	0
24	2	1	Total C 40 40	0	0
24	2	1	Total C 40 40	0	0
24	2	1	Total C 40 40	0	0
24	6	1	Total C 40 40	0	0
24	h	1	Total C 40 40	0	0
24	7	1	Total C 40 40	0	0
24	8	1	Total C 40 40	0	0
24	0	1	Total C 40 40	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
24	0	1	Total C 40 40	0	0
24	9	1	Total C 40 40	0	0

- Molecule 25 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (three-letter code: LHG) (formula: C₃₈H₇₅O₁₀P).



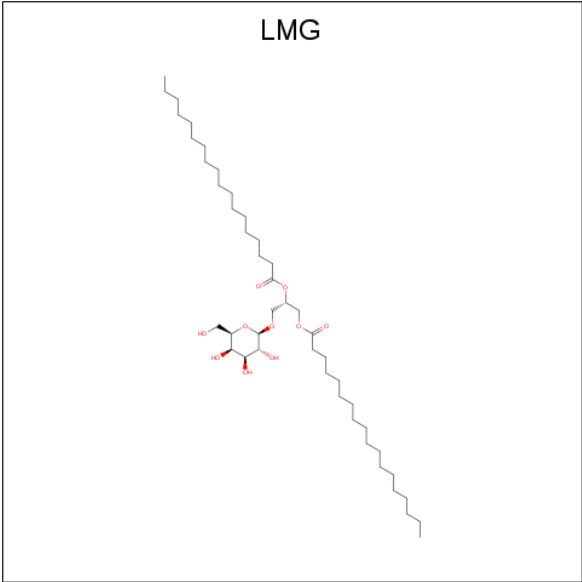
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
25	A	1	Total C O P 49 38 10 1	0	0
25	A	1	Total C O P 49 38 10 1	0	0
25	A	1	Total C O P 49 38 10 1	0	0
25	A	1	Total C O P 49 38 10 1	0	0
25	A	1	Total C O P 49 38 10 1	0	0
25	B	1	Total C O P 49 38 10 1	0	0
25	B	1	Total C O P 49 38 10 1	0	0
25	F	1	Total C O P 49 38 10 1	0	0
25	L	1	Total C O P 49 38 10 1	0	0

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
25	M	1	Total	C	O	P	0	0
			49	38	10	1		
25	a	1	Total	C	O	P	0	0
			49	38	10	1		
25	a	1	Total	C	O	P	0	0
			49	38	10	1		
25	a	1	Total	C	O	P	0	0
			49	38	10	1		
25	a	1	Total	C	O	P	0	0
			49	38	10	1		
25	b	1	Total	C	O	P	0	0
			49	38	10	1		
25	l	1	Total	C	O	P	0	0
			49	38	10	1		
25	l	1	Total	C	O	P	0	0
			49	38	10	1		
25	l	1	Total	C	O	P	0	0
			49	38	10	1		
25	l	1	Total	C	O	P	0	0
			49	38	10	1		
25	1	1	Total	C	O	P	0	0
			49	38	10	1		
25	1	1	Total	C	O	P	0	0
			49	38	10	1		
25	1	1	Total	C	O	P	0	0
			49	38	10	1		
25	1	1	Total	C	O	P	0	0
			49	38	10	1		
25	2	1	Total	C	O	P	0	0
			49	38	10	1		
25	6	1	Total	C	O	P	0	0
			12	5	6	1		
25	0	1	Total	C	O	P	0	0
			49	38	10	1		
25	0	1	Total	C	O	P	0	0
			49	38	10	1		

- Molecule 26 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (three-letter code: LMG) (formula: C₄₅H₈₆O₁₀).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
26	A	1	Total	C	O	0	0
			50	40	10		
26	A	1	Total	C	O	0	0
			48	38	10		
26	A	1	Total	C	O	0	0
			55	45	10		
26	B	1	Total	C	O	0	0
			55	45	10		
26	B	1	Total	C	O	0	0
			55	45	10		
26	K	1	Total	C	O	0	0
			55	45	10		
26	a	1	Total	C	O	0	0
			50	40	10		
26	a	1	Total	C	O	0	0
			55	45	10		
26	b	1	Total	C	O	0	0
			55	45	10		
26	b	1	Total	C	O	0	0
			55	45	10		
26	b	1	Total	C	O	0	0
			55	45	10		
26	1	1	Total	C	O	0	0
			50	40	10		
26	1	1	Total	C	O	0	0
			55	45	10		
26	2	1	Total	C	O	0	0
			55	45	10		

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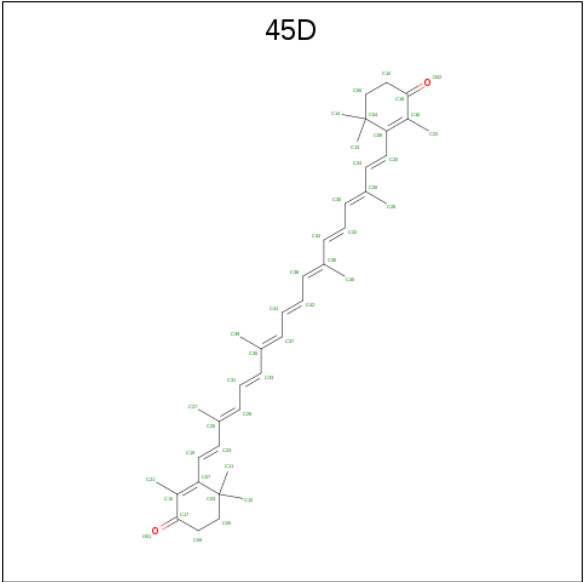
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
26	2	1	Total	C	O	0	0
			55	45	10		
26	0	1	Total	C	O	0	0
			55	45	10		

- Molecule 27 is ACETATE ION (three-letter code: ACT) (formula: $C_2H_3O_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
27	A	1	Total	C	O	0	0
			4	2	2		
27	B	1	Total	C	O	0	0
			4	2	2		
27	B	1	Total	C	O	0	0
			4	2	2		
27	a	1	Total	C	O	0	0
			4	2	2		

- Molecule 28 is beta,beta-carotene-4,4'-dione (three-letter code: 45D) (formula: $C_{40}H_{52}O_2$).

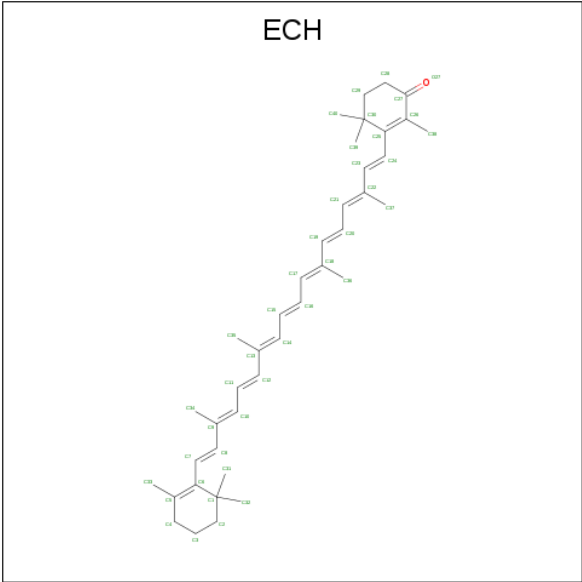


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
28	B	1	Total	C	O	0	0
			42	40	2		
28	h	1	Total	C	O	0	0
			42	40	2		

- Molecule 29 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

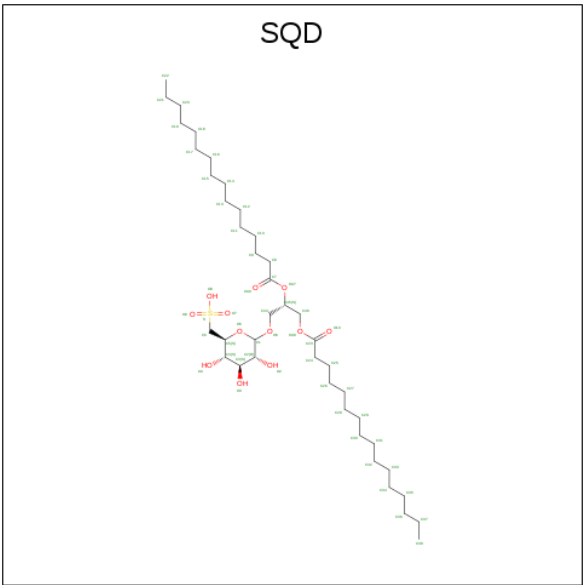
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
29	B	1	Total	Cl	0	0
			1	1		
29	b	1	Total	Cl	0	0
			1	1		
29	2	1	Total	Cl	0	0
			1	1		

- Molecule 30 is beta,beta-caroten-4-one (three-letter code: ECH) (formula: C₄₀H₅₄O).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
30	B	1	Total	C	O	0	0
			41	40	1		
30	M	1	Total	C	O	0	0
			41	40	1		
30	b	1	Total	C	O	0	0
			41	40	1		
30	b	1	Total	C	O	0	0
			41	40	1		
30	i	1	Total	C	O	0	0
			41	40	1		
30	m	1	Total	C	O	0	0
			41	40	1		
30	2	1	Total	C	O	0	0
			41	40	1		

- Molecule 31 is 1,2-DI-O-ACYL-3-O-[6-DEOXY-6-SULFO-ALPHA-D-GLUCOPYRANOSYL]-SN-GLYCEROL (three-letter code: SQD) (formula: C₄₁H₇₈O₁₂S).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
31	B	1	Total	C	O	S	0	0
			54	41	12	1		
31	F	1	Total	C	O	S	0	0
			54	41	12	1		
31	L	1	Total	C	O	S	0	0
			51	38	12	1		
31	L	1	Total	C	O	S	0	0
			54	41	12	1		
31	b	1	Total	C	O	S	0	0
			54	41	12	1		
31	f	1	Total	C	O	S	0	0
			54	41	12	1		
31	0	1	Total	C	O	S	0	0
			54	41	12	1		

- Molecule 32 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
32	0	1	Total	Ca	0	0
			1	1		
32	L	1	Total	Ca	0	0
			1	1		
32	B	1	Total	Ca	0	0
			1	1		
32	2	1	Total	Ca	0	0
			1	1		
32	l	1	Total	Ca	0	0
			1	1		

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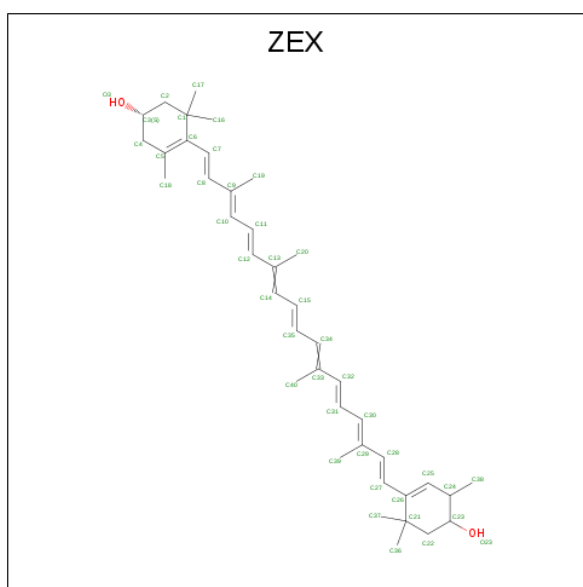
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
32	b	1	Total	Ca	0	0
			1	1		

- Molecule 33 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

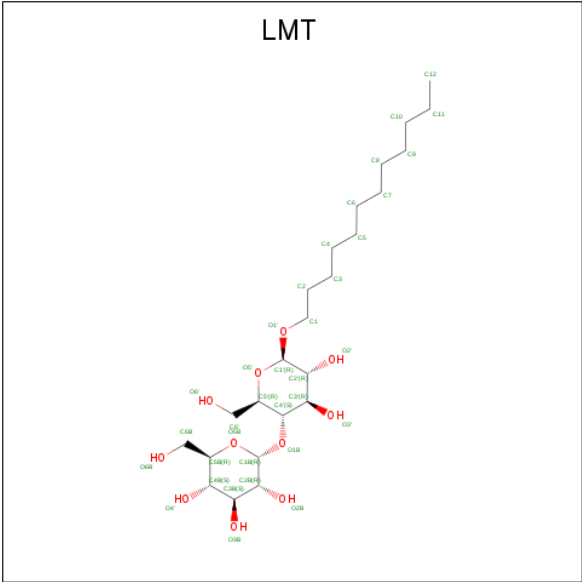
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
33	B	1	Total	Mg	0	0
			1	1		
33	b	1	Total	Mg	0	0
			1	1		

- Molecule 34 is (1R,2S)-4-[(1E,3E,5E,7E,9E,11E,13E,15E,17E)-18-[(4S)-4-hydroxy-2,6,6-trimethylcyclohex-1-en-1-yl]-3,7,12,16-tetramethyloctadeca-1,3,5,7,9,11,13,15,17-nonaen-1-yl]-2,5,5-trimethylcyclohex-3-en-1-ol (three-letter code: ZEX) (formula: C₄₀H₅₆O₂).



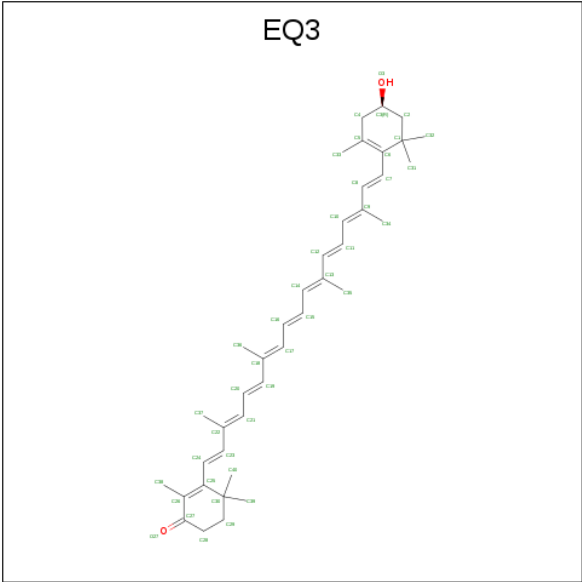
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
34	F	1	Total	C	O	0	0
			42	40	2		
34	J	1	Total	C	O	0	0
			42	40	2		
34	j	1	Total	C	O	0	0
			42	40	2		
34	7	1	Total	C	O	0	0
			42	40	2		

- Molecule 35 is DODECYL-BETA-D-MALTOSIDE (three-letter code: LMT) (formula: C₂₄H₄₆O₁₁).



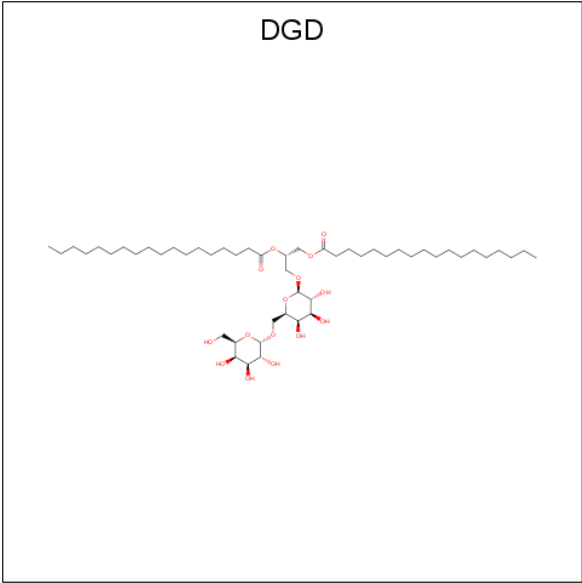
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
35	F	1	Total	C	O	0	0
			35	24	11		
35	L	1	Total	C	O	0	0
			35	24	11		
35	1	1	Total	C	O	0	0
			35	24	11		
35	1	1	Total	C	O	0	0
			35	24	11		
35	0	1	Total	C	O	0	0
			35	24	11		

- Molecule 36 is (3'R)-3'-hydroxy-beta,beta-caroten-4-one (three-letter code: EQ3) (formula: C₄₀H₅₄O₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
36	I	1	Total	C	O	0	0
			42	40	2		

- Molecule 37 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (three-letter code: DGD) (formula: C₅₁H₉₆O₁₅).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
37	L	1	Total	C	O	0	0
			66	51	15		

- Molecule 38 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
38	A	186	Total 186	O 186	0	0
38	B	114	Total 114	O 114	0	0
38	C	48	Total 48	O 48	0	0
38	D	57	Total 57	O 57	0	0
38	E	16	Total 16	O 16	0	0
38	F	8	Total 8	O 8	0	0
38	I	6	Total 6	O 6	0	0
38	J	4	Total 4	O 4	0	0
38	K	9	Total 9	O 9	0	0
38	L	46	Total 46	O 46	0	0
38	M	3	Total 3	O 3	0	0
38	a	39	Total 39	O 39	0	0
38	b	141	Total 141	O 141	0	0
38	c	13	Total 13	O 13	0	0
38	d	15	Total 15	O 15	0	0
38	e	4	Total 4	O 4	0	0
38	f	10	Total 10	O 10	0	0
38	i	7	Total 7	O 7	0	0
38	j	5	Total 5	O 5	0	0
38	l	20	Total 20	O 20	0	0
38	m	8	Total 8	O 8	0	0
38	1	37	Total 37	O 37	0	0

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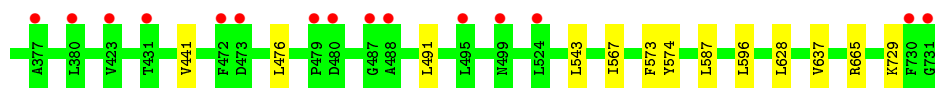
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
38	2	24	Total 24	O 24	0	0
38	3	11	Total 11	O 11	0	0
38	4	13	Total 13	O 13	0	0
38	5	4	Total 4	O 4	0	0
38	6	1	Total 1	O 1	0	0
38	h	3	Total 3	O 3	0	0
38	7	1	Total 1	O 1	0	0
38	8	2	Total 2	O 2	0	0
38	0	33	Total 33	O 33	0	0
38	9	1	Total 1	O 1	0	0

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 electron 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 dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). 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.

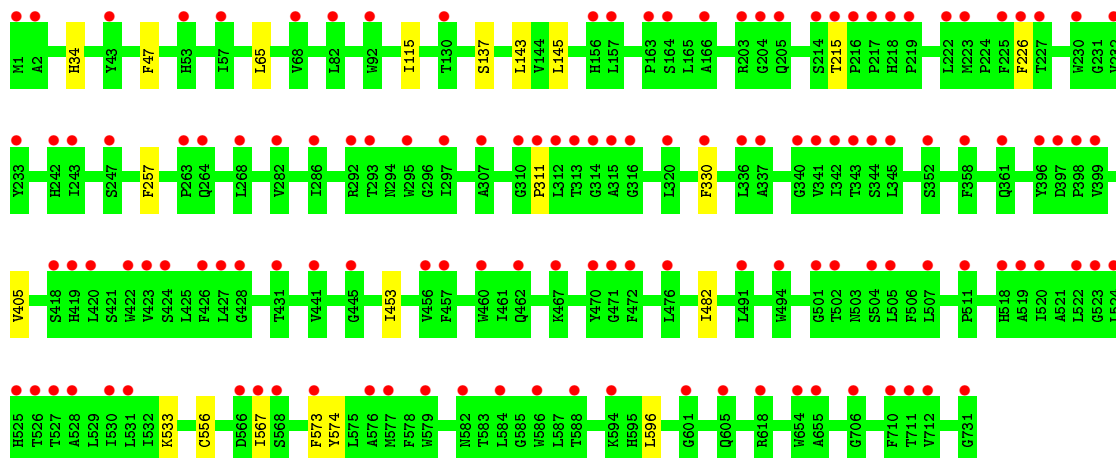
- Chain A:
-
- | Position | Amino Acid | Conservation (bits) |
|----------|------------|---------------------|
| 1 | Met | 0.14 |
| 2 | Met | 0.14 |
| 3 | Met | 0.14 |
| 4 | Met | 0.14 |
| 5 | Met | 0.14 |
| 6 | Met | 0.14 |
| 7 | Met | 0.14 |
| 8 | Met | 0.14 |
| 9 | Met | 0.14 |
| 10 | Met | 0.14 |
| 11 | Met | 0.14 |
| 12 | Met | 0.14 |
| 13 | Met | 0.14 |
| 14 | Met | 0.14 |
| 15 | Met | 0.14 |
| 16 | Met | 0.14 |
| 17 | Met | 0.14 |
| 18 | Met | 0.14 |
| 19 | Met | 0.14 |
| 20 | Met | 0.14 |
| 21 | Met | 0.14 |
| 22 | Met | 0.14 |
| 23 | Met | 0.14 |
| 24 | Met | 0.14 |
| 25 | Met | 0.14 |
| 26 | Met | 0.14 |
| 27 | Met | 0.14 |
| 28 | Met | 0.14 |
| 29 | Met | 0.14 |
| 30 | Met | 0.14 |
| 31 | Met | 0.14 |
| 32 | Met | 0.14 |
| 33 | Met | 0.14 |
| 34 | Met | 0.14 |
| 35 | Met | 0.14 |
| 36 | Met | 0.14 |
| 37 | Met | 0.14 |
| 38 | Met | 0.14 |
| 39 | Met | 0.14 |
| 40 | Met | 0.14 |
| 41 | Met | 0.14 |
| 42 | Met | 0.14 |
| 43 | Met | 0.14 |
| 44 | Met | 0.14 |
| 45 | Met | 0.14 |
| 46 | Met | 0.14 |
| 47 | Met | 0.14 |
| 48 | Met | 0.14 |
| 49 | Met | 0.14 |
| 50 | Met | 0.14 |
| 51 | Met | 0.14 |
| 52 | Met | 0.14 |
| 53 | Met | 0.14 |
| 54 | Met | 0.14 |
| 55 | Met | 0.14 |
| 56 | Met | 0.14 |
| 57 | Met | 0.14 |
| 58 | Met | 0.14 |
| 59 | Met | 0.14 |
| 60 | Met | 0.14 |
| 61 | Met | 0.14 |
| 62 | Met | 0.14 |
| 63 | Met | 0.14 |
| 64 | Met | 0.14 |
| 65 | Met | 0.14 |
| 66 | Met | 0.14 |
| | | |

- Chain a:
-
- | Category | 19% | 97% |
|----------|-----|-----|
| A521 | | |
| I548 | | |
| L561 | | |
| L593 | | |
| W611 | | |
| K612 | | |
| M613 | | |
| D616 | | |
| V617 | | |
| W618 | | |
| G619 | | |
| T620 | | |
| V621 | | |
| S622 | | |
| P623 | | |
| D624 | | |
| V630 | | |
| F635 | | |
| A636 | | |
| Q637 | | |
| Y668 | | |
| G675 | | |
| H676 | | |
| F677 | | |
| V678 | | |
| Y684 | | |
| V709 | | |
| G723 | | |
| V726 | | |
| A729 | | |
| L733 | | |
| G734 | | |
| S747 | | |
| L748 | | |
| S749 | | |
| I750 | | |
| G751 | | |
| T276 | | |
| F277 | | |
| P283 | | |
| V284 | | |
| T285 | | |
| G286 | | |
| I300 | | |
| A301 | | |
| V302 | | |
| L303 | | |
| F304 | | |
| I305 | | |
| L306 | | |
| A307 | | |
| G308 | | |
| H319 | | |
| E323 | | |
| T333 | | |
| G334 | | |
| K338 | | |
| G339 | | |
| L340 | | |
| L362 | | |
| T363 | | |
| V366 | | |
| A367 | | |
| Q368 | | |
| H369 | | |
| H370 | | |
| Y371 | | |
| V378 | | |
| I381 | | |
| D382 | | |
| Y383 | | |
| I396 | | |
| F411 | | |
| I431 | | |
| L492 | | |
| H500 | | |
| T513 | | |
| G518 | | |
| K519 | | |
| H520 | | |
| F174 | | |
| V182 | | |
| W197 | | |
| H198 | | |
| H199 | | |
| H200 | | |
| L201 | | |
| A202 | | |
| G203 | | |
| L204 | | |
| L205 | | |
| G206 | | |
| L207 | | |
| G208 | | |
| S209 | | |
| F222 | | |
| A229 | | |
| G230 | | |
| V231 | | |
| A232 | | |
| T233 | | |
| K234 | | |
| D235 | | |
| F242 | | |
| L243 | | |
| L244 | | |
| S247 | | |
| K248 | | |
| K249 | | |
| A250 | | |
| Y253 | | |
| P254 | | |
| S255 | | |
| F256 | | |
| A257 | | |
| Q258 | | |
| G259 | | |
| L260 | | |
| T261 | | |
| P262 | | |
| F263 | | |
| T264 | | |
| T265 | | |
| L266 | | |
| I267 | | |
| V268 | | |
| G269 | | |
| V270 | | |
| Y271 | | |
| S272 | | |
| D273 | | |
| T274 | | |
| L275 | | |
| M1 | | |
| T2 | | |
| I3 | | |
| S4 | | |
| P5 | | |
| F6 | | |
| E7 | | |
| R8 | | |
| A10 | | |
| K11 | | |
| A12 | | |
| S24 | | |
| F25 | | |
| E26 | | |
| K27 | | |
| F31 | | |
| F34 | | |
| D35 | | |
| K36 | | |
| T37 | | |
| L38 | | |
| A39 | | |
| R40 | | |
| Q41 | | |
| P42 | | |
| K43 | | |
| W47 | | |
| V68 | | |
| S74 | | |
| F92 | | |
| K96 | | |
| A105 | | |
| D106 | | |
| P107 | | |
| T108 | | |
| Q115 | | |
| V121 | | |
| D129 | | |
| Y145 | | |
| Y156 | | |
| Y159 | | |
| I163 | | |

- Chain B:
-
- 96%
- 6%
- M1 A2 T3 R50 R65 V113 V120 L143 L182 G204 N211 F212 S214 T215 F216 T227 G228 T239 A240 L243 F244 T252 F257 L258 G259 Q264 T295 G296 L297 G298 E299 L312 T313 S338 G340 T341 L342 T343 S344 L345 L346



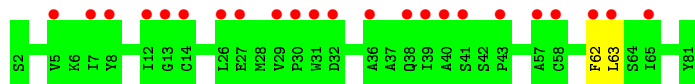
- Molecule 2: Photosystem I P700 chlorophyll a apoprotein A2



- Molecule 3: Photosystem I iron-sulfur center



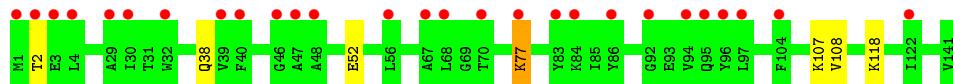
- Molecule 3: Photosystem I iron-sulfur center



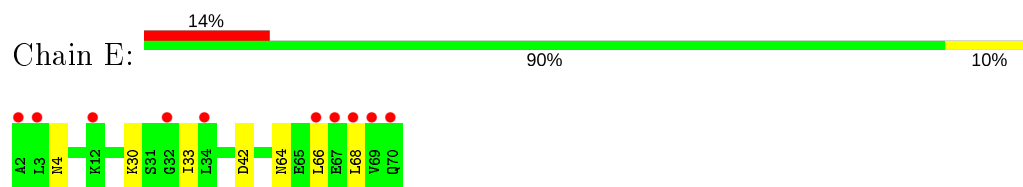
- Molecule 4: Photosystem I reaction center subunit II



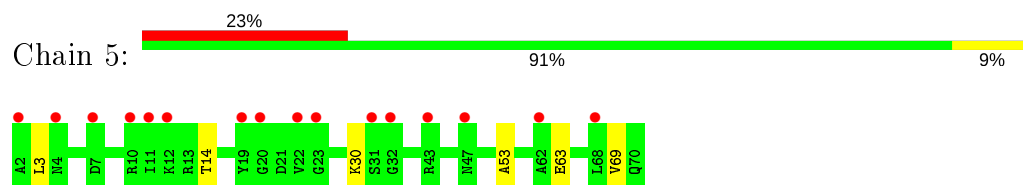
- Molecule 4: Photosystem I reaction center subunit II



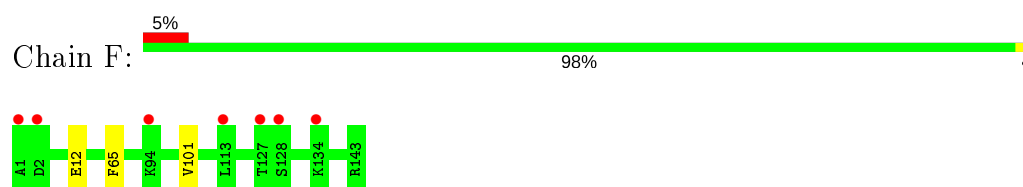
- Molecule 5: Photosystem I reaction center subunit IV



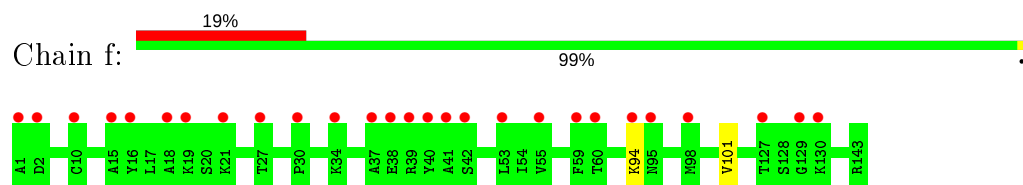
- Molecule 5: Photosystem I reaction center subunit IV



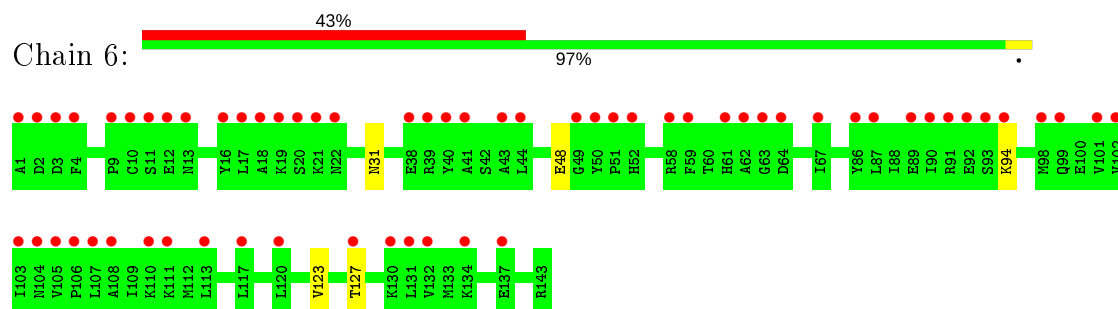
- Molecule 6: Photosystem I reaction center subunit III



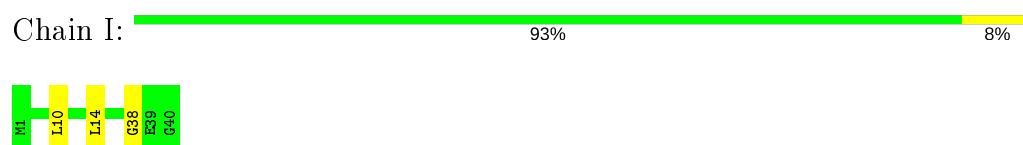
- Molecule 6: Photosystem I reaction center subunit III



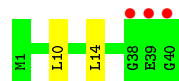
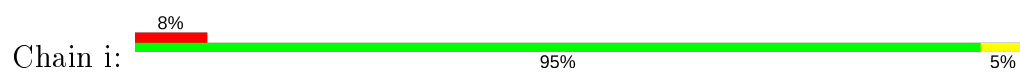
- Molecule 6: Photosystem I reaction center subunit III



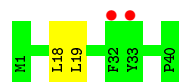
- Molecule 7: Photosystem I reaction center subunit VIII



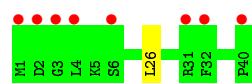
- Molecule 7: Photosystem I reaction center subunit VIII



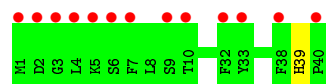
- Molecule 8: Photosystem I reaction center subunit IX



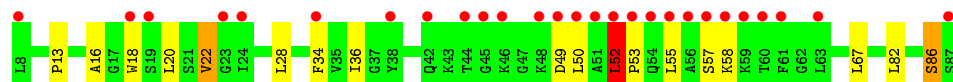
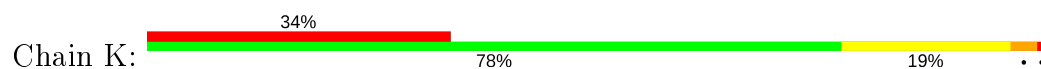
- Molecule 8: Photosystem I reaction center subunit IX



- Molecule 8: Photosystem I reaction center subunit IX



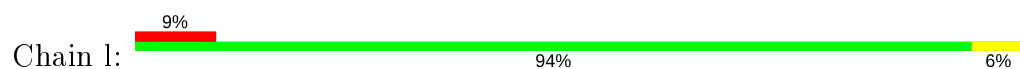
- Molecule 9: Photosystem I reaction center subunit PsaK 2



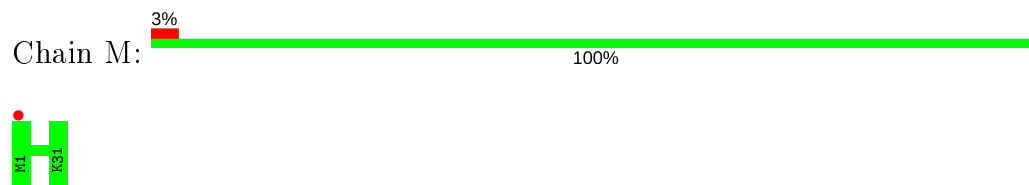
- Molecule 10: Photosystem I reaction center subunit XI



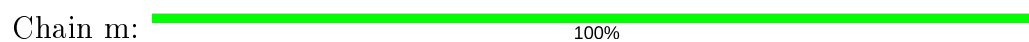
- Molecule 10: Photosystem I reaction center subunit XI



- Molecule 11: Photosystem I reaction center subunit XII

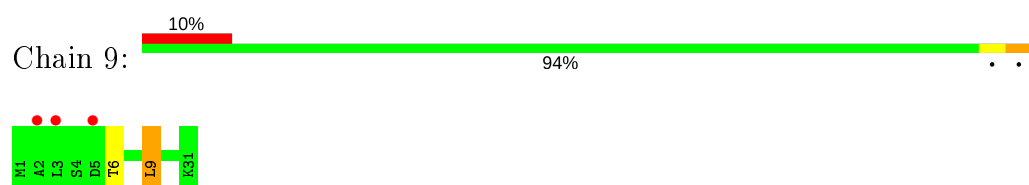


- Molecule 11: Photosystem I reaction center subunit XII

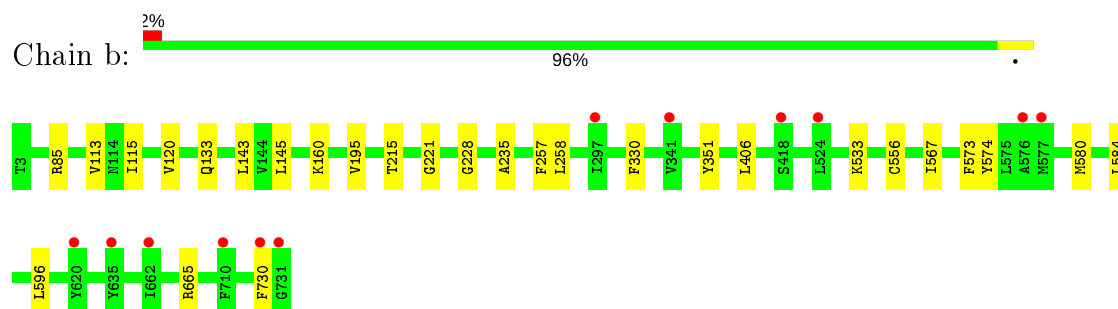


There are no outlier residues recorded for this chain.

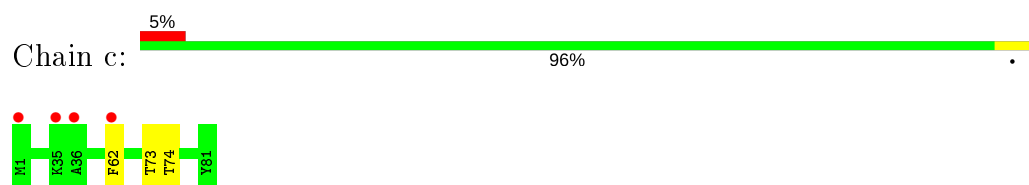
- Molecule 11: Photosystem I reaction center subunit XII



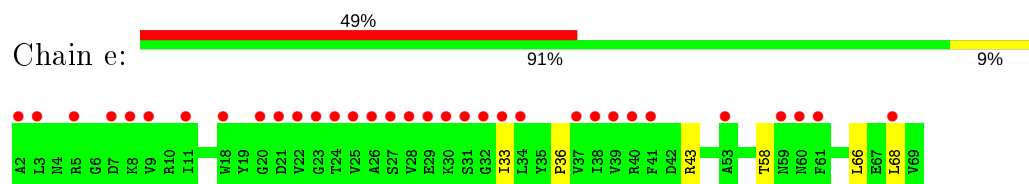
- Molecule 12: Photosystem I P700 chlorophyll a apoprotein A2



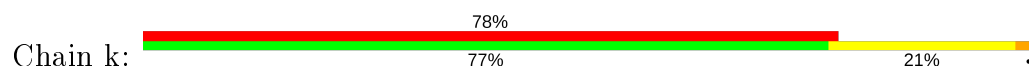
- Molecule 13: Photosystem I iron-sulfur center

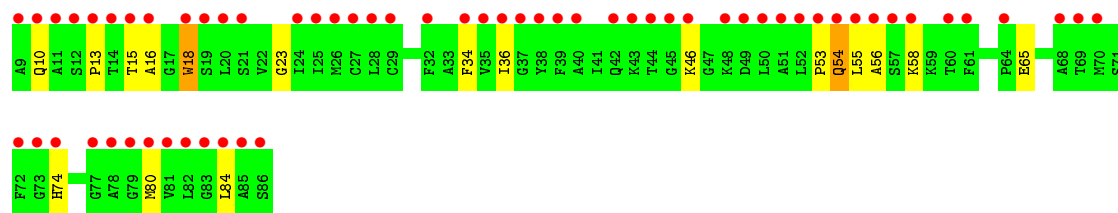


- Molecule 14: Photosystem I reaction center subunit IV

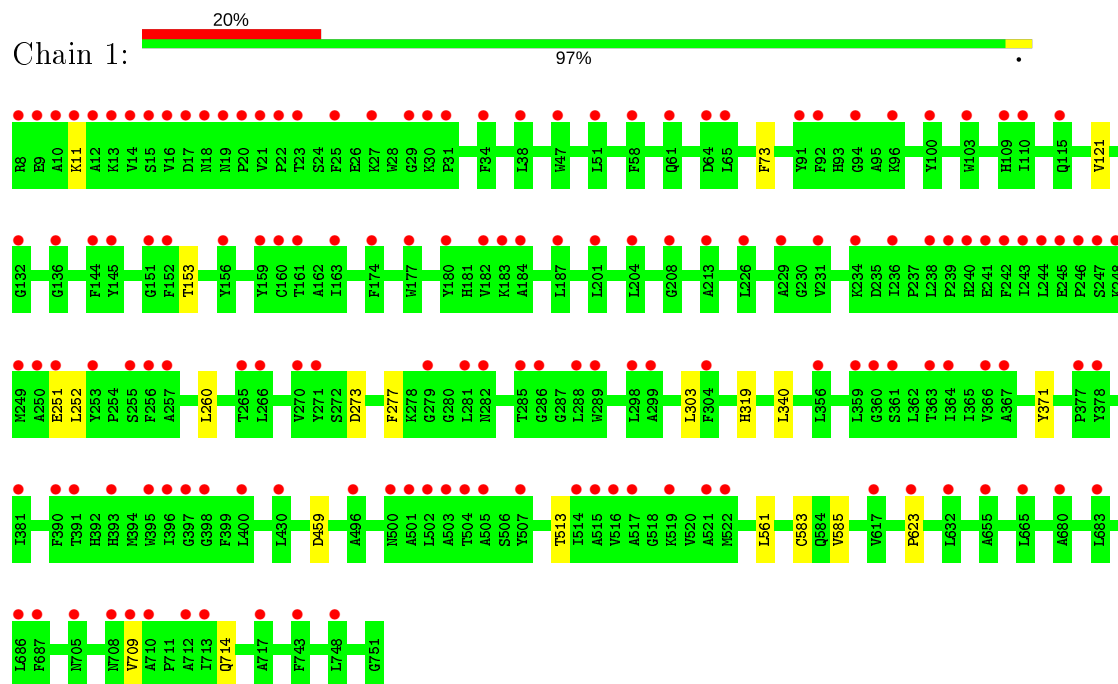


- Molecule 15: Photosystem I reaction center subunit PsaK 2

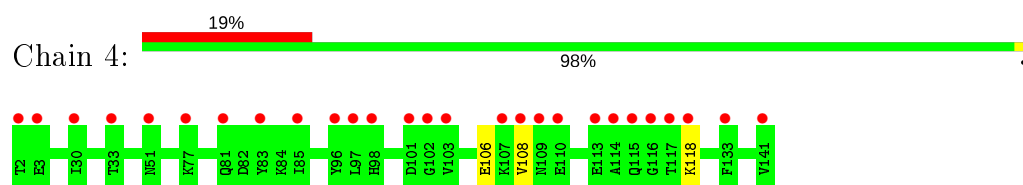




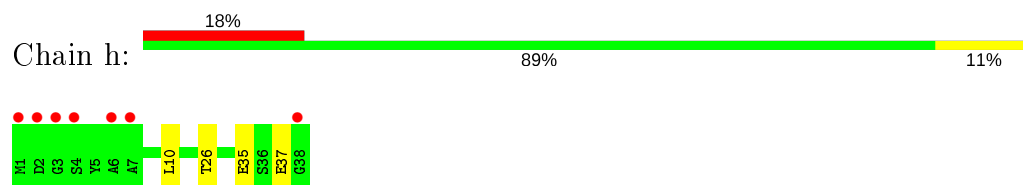
• Molecule 16: Photosystem I P700 chlorophyll a apoprotein A1



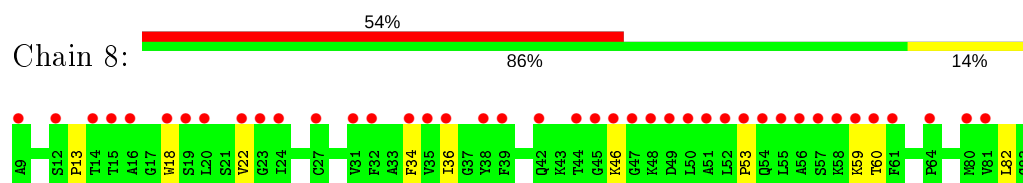
• Molecule 17: Photosystem I reaction center subunit II



• Molecule 18: Photosystem I reaction center subunit VIII

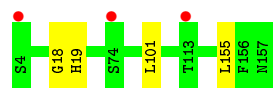


• Molecule 19: Photosystem I reaction center subunit PsaK 2



- Molecule 20: Photosystem I reaction center subunit XI

Chain 0:  2% 97%



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	212.17Å 137.62Å 225.09Å 90.00° 116.74° 90.00°	Depositor
Resolution (Å)	49.48 – 2.50 49.48 – 2.50	Depositor EDS
% Data completeness (in resolution range)	99.4 (49.48-2.50) 99.4 (49.48-2.50)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.10 (at 2.51Å)	Xtriage
Refinement program	PHENIX (dev_2947: ???)	Depositor
R, R_{free}	0.228 , 0.264 0.228 , 0.265	Depositor DCC
R_{free} test set	7881 reflections (1.99%)	wwPDB-VP
Wilson B-factor (Å ²)	58.1	Xtriage
Anisotropy	0.086	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 66.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.008 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	77117	wwPDB-VP
Average B, all atoms (Å ²)	77.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.13% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: LHG, MG, DGD, CL, SF4, LMT, CLA, PQN, ECH, BCR, ACT, ZEX, LMG, 45D, EQ3, CA, SQD

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	0.31	0/6078	0.46	0/8284
1	a	0.27	0/6078	0.42	0/8284
2	2	0.26	0/5994	0.41	0/8195
2	B	0.33	0/5994	0.45	2/8195 (0.0%)
3	3	0.24	0/610	0.45	0/826
3	C	0.37	1/610 (0.2%)	0.56	1/826 (0.1%)
4	D	0.29	0/1126	0.49	0/1517
4	d	0.26	0/1126	0.48	0/1517
5	5	0.25	0/552	0.39	0/745
5	E	0.26	0/552	0.44	0/745
6	6	0.25	0/1143	0.40	0/1553
6	F	0.26	0/1143	0.43	0/1553
6	f	0.25	0/1143	0.40	0/1553
7	I	0.26	0/322	0.43	0/438
7	i	0.26	0/322	0.44	0/438
8	7	0.27	0/328	0.42	0/443
8	J	0.28	0/328	0.46	0/443
8	j	0.26	0/328	0.42	0/443
9	K	0.29	0/590	0.53	0/797
10	L	0.28	0/1208	0.47	0/1640
10	l	0.27	0/1208	0.43	0/1640
11	9	0.25	0/241	0.55	1/326 (0.3%)
11	M	0.27	0/241	0.41	0/326
11	m	0.27	0/241	0.39	0/326
12	b	0.31	0/5981	0.46	1/8178 (0.0%)
13	c	0.26	0/618	0.49	0/836
14	e	0.26	0/542	0.42	0/733
15	k	0.28	0/570	0.45	0/770
16	1	0.26	0/6024	0.41	0/8209
17	4	0.26	0/1118	0.45	0/1507
18	h	0.26	0/309	0.43	0/421
19	8	0.27	0/576	0.46	0/778

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
20	0	0.28	0/1186	0.43	0/1611
All	All	0.29	1/54430 (0.0%)	0.44	5/74096 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
9	K	0	1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	17	CYS	CB-SG	5.38	1.91	1.82

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	b	665	ARG	N-CA-C	7.42	131.03	111.00
2	B	587	LEU	CA-CB-CG	6.99	131.38	115.30
2	B	665	ARG	N-CA-C	6.41	128.31	111.00
11	9	9	LEU	CA-CB-CG	6.23	129.62	115.30
3	C	17	CYS	CA-CB-SG	5.76	124.37	114.00

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
9	K	52	LEU	Peptide

5.2 Too-close contacts [i](#)

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 X-ray entries followed by that with respect to entries of similar resolution.

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	749/751 (100%)	719 (96%)	28 (4%)	2 (0%)	41	61
1	a	749/751 (100%)	712 (95%)	31 (4%)	6 (1%)	19	35
2	2	729/731 (100%)	694 (95%)	33 (4%)	2 (0%)	41	61
2	B	729/731 (100%)	697 (96%)	28 (4%)	4 (0%)	29	48
3	3	78/80 (98%)	72 (92%)	5 (6%)	1 (1%)	12	21
3	C	78/80 (98%)	72 (92%)	4 (5%)	2 (3%)	5	8
4	D	139/141 (99%)	135 (97%)	4 (3%)	0	100	100
4	d	139/141 (99%)	134 (96%)	4 (3%)	1 (1%)	22	39
5	5	67/69 (97%)	59 (88%)	6 (9%)	2 (3%)	4	6
5	E	67/69 (97%)	61 (91%)	6 (9%)	0	100	100
6	6	141/143 (99%)	134 (95%)	6 (4%)	1 (1%)	22	39
6	F	141/143 (99%)	135 (96%)	5 (4%)	1 (1%)	22	39
6	f	141/143 (99%)	134 (95%)	7 (5%)	0	100	100
7	I	38/40 (95%)	36 (95%)	1 (3%)	1 (3%)	5	8
7	i	38/40 (95%)	37 (97%)	1 (3%)	0	100	100
8	7	38/40 (95%)	38 (100%)	0	0	100	100
8	J	38/40 (95%)	37 (97%)	1 (3%)	0	100	100
8	j	38/40 (95%)	38 (100%)	0	0	100	100
9	K	79/80 (99%)	66 (84%)	6 (8%)	7 (9%)	1	0
10	L	155/157 (99%)	148 (96%)	7 (4%)	0	100	100
10	l	155/157 (99%)	150 (97%)	3 (2%)	2 (1%)	12	21
11	9	29/31 (94%)	27 (93%)	2 (7%)	0	100	100
11	M	29/31 (94%)	29 (100%)	0	0	100	100
11	m	29/31 (94%)	29 (100%)	0	0	100	100
12	b	727/729 (100%)	701 (96%)	22 (3%)	4 (1%)	25	43

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
13	c	79/81 (98%)	75 (95%)	3 (4%)	1 (1%)	12	21
14	e	66/68 (97%)	62 (94%)	3 (4%)	1 (2%)	10	18
15	k	76/78 (97%)	60 (79%)	7 (9%)	9 (12%)	0	0
16	1	742/744 (100%)	706 (95%)	34 (5%)	2 (0%)	41	61
17	4	138/140 (99%)	133 (96%)	5 (4%)	0	100	100
18	h	36/38 (95%)	32 (89%)	3 (8%)	1 (3%)	5	7
19	8	77/79 (98%)	64 (83%)	9 (12%)	4 (5%)	2	2
20	0	152/154 (99%)	148 (97%)	3 (2%)	1 (1%)	22	39
All	All	6706/6771 (99%)	6374 (95%)	277 (4%)	55 (1%)	19	35

5 of 55 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	C	62	PHE
9	K	16	ALA
9	K	52	LEU
13	c	62	PHE
15	k	13	PRO

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 X-ray entries followed by that with respect to entries of similar resolution.

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	603/603 (100%)	585 (97%)	18 (3%)	41	68
1	a	603/603 (100%)	588 (98%)	15 (2%)	47	73
2	2	583/583 (100%)	564 (97%)	19 (3%)	38	64
2	B	583/583 (100%)	563 (97%)	20 (3%)	37	63
3	3	68/68 (100%)	67 (98%)	1 (2%)	65	85
3	C	68/68 (100%)	64 (94%)	4 (6%)	19	37
4	D	116/116 (100%)	111 (96%)	5 (4%)	29	53
4	d	116/116 (100%)	109 (94%)	7 (6%)	19	37

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
5	5	58/58 (100%)	54 (93%)	4 (7%)	15	30
5	E	58/58 (100%)	51 (88%)	7 (12%)	5	9
6	6	119/119 (100%)	115 (97%)	4 (3%)	37	63
6	F	119/119 (100%)	117 (98%)	2 (2%)	60	82
6	f	119/119 (100%)	117 (98%)	2 (2%)	60	82
7	I	32/32 (100%)	30 (94%)	2 (6%)	18	34
7	i	32/32 (100%)	30 (94%)	2 (6%)	18	34
8	7	35/35 (100%)	34 (97%)	1 (3%)	42	69
8	J	35/35 (100%)	33 (94%)	2 (6%)	20	39
8	j	35/35 (100%)	34 (97%)	1 (3%)	42	69
9	K	60/60 (100%)	46 (77%)	14 (23%)	1	1
10	L	118/118 (100%)	110 (93%)	8 (7%)	16	30
10	l	118/118 (100%)	111 (94%)	7 (6%)	19	37
11	9	25/25 (100%)	23 (92%)	2 (8%)	12	23
11	M	25/25 (100%)	25 (100%)	0	100	100
11	m	25/25 (100%)	25 (100%)	0	100	100
12	b	582/582 (100%)	559 (96%)	23 (4%)	31	56
13	c	69/69 (100%)	67 (97%)	2 (3%)	42	69
14	e	57/57 (100%)	52 (91%)	5 (9%)	10	19
15	k	57/58 (98%)	46 (81%)	11 (19%)	1	2
16	1	596/596 (100%)	577 (97%)	19 (3%)	39	65
17	4	115/115 (100%)	112 (97%)	3 (3%)	46	72
18	h	31/31 (100%)	28 (90%)	3 (10%)	8	16
19	8	58/59 (98%)	51 (88%)	7 (12%)	5	9
20	0	116/116 (100%)	113 (97%)	3 (3%)	46	72
All	All	5434/5436 (100%)	5211 (96%)	223 (4%)	30	55

5 of 223 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
12	b	120	VAL
4	d	52	GLU
6	6	127	THR

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Mol	Chain	Res	Type
12	b	145	LEU
12	b	567	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	276	HIS
2	2	277	HIS
2	2	518	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 443 ligands modelled in this entry, 11 are monoatomic - leaving 432 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$
21	CLA	A	1012	38	59,73,73	1.27	7 (11%)	67,113,113	1.85	8 (11%)
21	CLA	2	1220	-	36,53,73	1.62	9 (25%)	39,89,113	2.04	6 (15%)
26	LMG	0	5001	-	55,55,55	1.14	6 (10%)	63,63,63	1.28	6 (9%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
21	CLA	B	1214	-	59,73,73	1.27	9 (15%)	67,113,113	1.63	6 (8%)
21	CLA	1	1112	-	44,58,73	1.47	9 (20%)	49,95,113	2.10	7 (14%)
21	CLA	1	1139	-	59,73,73	1.27	9 (15%)	67,113,113	1.78	6 (8%)
21	CLA	1	1122	-	54,68,73	1.32	9 (16%)	61,107,113	1.80	5 (8%)
21	CLA	1	1011	-	59,73,73	1.26	7 (11%)	67,113,113	1.84	8 (11%)
24	BCR	a	4001	-	41,41,41	0.70	0	56,56,56	3.44	14 (25%)
37	DGD	L	5004	-	67,67,67	1.07	6 (8%)	81,81,81	1.02	2 (2%)
21	CLA	2	1231	38	40,54,73	1.50	8 (20%)	44,90,113	1.91	5 (11%)
21	CLA	b	1220	-	59,73,73	1.26	8 (13%)	67,113,113	1.77	7 (10%)
21	CLA	2	1213	-	44,58,73	1.45	8 (18%)	49,95,113	2.09	5 (10%)
21	CLA	B	1204	-	59,73,73	1.27	8 (13%)	67,113,113	1.64	6 (8%)
21	CLA	2	1229	-	59,73,73	1.28	8 (13%)	67,113,113	1.67	6 (8%)
21	CLA	2	1214	-	53,67,73	1.34	9 (16%)	59,105,113	1.75	9 (15%)
21	CLA	a	1102	-	59,73,73	1.25	8 (13%)	67,113,113	1.85	7 (10%)
27	ACT	a	7001	-	1,3,3	6.51	1 (100%)	0,3,3	0.00	-
21	CLA	B	1220	-	51,65,73	1.36	7 (13%)	57,103,113	1.87	7 (12%)
35	LMT	F	6001	-	36,36,36	1.15	5 (13%)	47,47,47	0.99	1 (2%)
21	CLA	1	1131	-	59,73,73	1.26	8 (13%)	67,113,113	1.64	5 (7%)
21	CLA	A	1801	25	59,73,73	1.24	7 (11%)	67,113,113	1.80	7 (10%)
21	CLA	j	1302	-	59,73,73	1.27	8 (13%)	67,113,113	1.79	5 (7%)
25	LHG	l	5002	-	48,48,48	0.39	0	51,54,54	1.09	3 (5%)
24	BCR	1	4001	-	41,41,41	0.70	0	56,56,56	3.27	10 (17%)
23	SF4	C	3003	3	0,12,12	0.00	-	-		
24	BCR	6	4016	-	41,41,41	0.70	0	56,56,56	3.42	13 (23%)
21	CLA	b	1225	-	59,73,73	1.24	7 (11%)	67,113,113	1.65	7 (10%)
21	CLA	2	1023	-	59,73,73	1.25	8 (13%)	67,113,113	1.91	7 (10%)
26	LMG	A	5004	-	48,48,55	0.98	4 (8%)	56,56,63	1.09	3 (5%)
25	LHG	2	5004	-	48,48,48	0.39	0	51,54,54	1.02	3 (5%)
21	CLA	b	1202	-	59,73,73	1.23	7 (11%)	67,113,113	1.83	7 (10%)
21	CLA	A	1114	38	59,73,73	1.29	8 (13%)	67,113,113	1.64	6 (8%)
24	BCR	B	4010	-	41,41,41	0.65	0	56,56,56	3.18	11 (19%)
21	CLA	a	1116	-	54,68,73	1.33	8 (14%)	61,107,113	1.82	7 (11%)
34	ZEX	7	4015	-	42,43,43	5.79	4 (9%)	55,60,60	6.95	12 (21%)
34	ZEX	j	4015	-	42,43,43	5.77	3 (7%)	55,60,60	7.02	13 (23%)
21	CLA	b	1216	38	59,73,73	1.27	9 (15%)	67,113,113	1.71	5 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
21	CLA	b	1211	-	59,73,73	1.25	9 (15%)	67,113,113	1.69	3 (4%)
28	45D	B	4011	-	43,43,43	3.44	15 (34%)	54,60,60	2.24	18 (33%)
21	CLA	A	1101	-	59,73,73	1.29	9 (15%)	67,113,113	1.77	9 (13%)
21	CLA	B	1213	-	59,73,73	1.28	9 (15%)	67,113,113	1.81	9 (13%)
21	CLA	2	1236	-	44,58,73	1.48	8 (18%)	49,95,113	1.86	7 (14%)
21	CLA	B	1216	38	59,73,73	1.30	9 (15%)	67,113,113	1.71	6 (8%)
21	CLA	B	1237	38	59,73,73	1.23	7 (11%)	67,113,113	1.71	8 (11%)
25	LHG	B	5004	-	48,48,48	0.37	0	51,54,54	1.12	3 (5%)
21	CLA	1	1013	-	59,73,73	1.26	7 (11%)	67,113,113	1.89	9 (13%)
21	CLA	2	1206	2	59,73,73	1.26	8 (13%)	67,113,113	1.84	7 (10%)
24	BCR	1	4007	-	41,41,41	0.64	0	56,56,56	3.27	10 (17%)
21	CLA	2	1022	38	59,73,73	1.26	7 (11%)	67,113,113	1.82	8 (11%)
21	CLA	a	1101	-	59,73,73	1.29	9 (15%)	67,113,113	1.83	9 (13%)
24	BCR	A	4008	-	41,41,41	0.64	0	56,56,56	2.91	9 (16%)
21	CLA	a	1121	-	59,73,73	1.27	9 (15%)	67,113,113	1.72	8 (11%)
21	CLA	B	1219	-	59,73,73	1.28	7 (11%)	67,113,113	1.71	6 (8%)
21	CLA	A	1126	-	59,73,73	1.25	6 (10%)	67,113,113	1.75	5 (7%)
21	CLA	B	1240	-	59,73,73	1.29	9 (15%)	67,113,113	1.73	8 (11%)
21	CLA	b	1214	-	59,73,73	1.27	8 (13%)	67,113,113	1.67	7 (10%)
21	CLA	b	1235	-	59,73,73	1.25	8 (13%)	67,113,113	1.73	6 (8%)
21	CLA	2	1230	-	41,55,73	1.52	8 (19%)	45,91,113	2.02	7 (15%)
21	CLA	B	1217	-	59,73,73	1.28	9 (15%)	67,113,113	1.82	9 (13%)
21	CLA	A	1116	-	59,73,73	1.28	9 (15%)	67,113,113	1.67	6 (8%)
21	CLA	f	1301	38	44,58,73	1.47	7 (15%)	49,95,113	1.87	7 (14%)
21	CLA	a	1115	-	59,73,73	1.27	7 (11%)	67,113,113	1.74	6 (8%)
21	CLA	b	1227	-	59,73,73	1.24	8 (13%)	67,113,113	1.69	7 (10%)
21	CLA	2	1234	-	44,58,73	1.49	8 (18%)	49,95,113	1.99	8 (16%)
21	CLA	b	1208	-	54,68,73	1.30	7 (12%)	61,107,113	1.66	5 (8%)
24	BCR	A	4012	-	41,41,41	0.71	0	56,56,56	3.11	10 (17%)
24	BCR	1	4003	-	41,41,41	0.69	0	56,56,56	3.25	11 (19%)
21	CLA	b	1230	-	59,73,73	1.25	8 (13%)	67,113,113	1.80	7 (10%)
21	CLA	b	1203	-	59,73,73	1.25	8 (13%)	67,113,113	1.70	6 (8%)
21	CLA	B	1207	-	59,73,73	1.31	8 (13%)	67,113,113	1.86	9 (13%)
21	CLA	a	1011	-	59,73,73	1.26	7 (11%)	67,113,113	1.88	9 (13%)
21	CLA	2	1237	38	59,73,73	1.24	8 (13%)	67,113,113	1.72	7 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
24	BCR	f	4016	-	41,41,41	0.73	0	56,56,56	3.28	12 (21%)
21	CLA	2	1210	-	59,73,73	1.28	9 (15%)	67,113,113	1.71	7 (10%)
21	CLA	k	1401	-	44,58,73	1.47	8 (18%)	49,95,113	2.03	7 (14%)
22	PQN	A	2001	-	34,34,34	0.41	0	42,45,45	1.21	4 (9%)
24	BCR	l	4022	-	41,41,41	0.69	0	56,56,56	3.22	12 (21%)
21	CLA	1	1134	16	59,73,73	1.27	9 (15%)	67,113,113	1.72	6 (8%)
24	BCR	k	4001	-	41,41,41	0.67	0	56,56,56	3.16	10 (17%)
24	BCR	2	4018	-	41,41,41	0.76	0	56,56,56	3.24	19 (33%)
21	CLA	A	1110	-	59,73,73	1.28	8 (13%)	67,113,113	1.65	4 (5%)
21	CLA	1	1124	-	50,64,73	1.38	9 (18%)	56,102,113	1.79	7 (12%)
21	CLA	2	1201	-	59,73,73	1.25	8 (13%)	67,113,113	1.85	7 (10%)
25	LHG	a	5007	-	48,48,48	0.40	0	51,54,54	1.02	3 (5%)
21	CLA	2	1216	-	44,58,73	1.44	8 (18%)	49,95,113	2.02	5 (10%)
21	CLA	A	1113	-	59,73,73	1.28	8 (13%)	67,113,113	1.72	8 (11%)
21	CLA	B	1231	38	59,73,73	1.25	9 (15%)	67,113,113	1.78	8 (11%)
21	CLA	A	1011	-	59,73,73	1.26	8 (13%)	67,113,113	2.26	14 (20%)
25	LHG	1	5001	-	48,48,48	0.39	0	51,54,54	1.06	3 (5%)
27	ACT	B	7001	-	1,3,3	6.52	1 (100%)	0,3,3	0.00	-
21	CLA	b	1240	-	59,73,73	1.28	8 (13%)	67,113,113	1.77	7 (10%)
24	BCR	0	4022	-	41,41,41	0.71	0	56,56,56	3.25	14 (25%)
21	CLA	b	1222	38	59,73,73	1.24	8 (13%)	67,113,113	1.75	9 (13%)
21	CLA	a	1133	-	59,73,73	1.29	9 (15%)	67,113,113	1.67	6 (8%)
21	CLA	b	1229	-	59,73,73	1.28	8 (13%)	67,113,113	1.66	7 (10%)
21	CLA	2	1235	-	47,61,73	1.42	9 (19%)	52,98,113	1.92	5 (9%)
21	CLA	1	1115	-	59,73,73	1.27	8 (13%)	67,113,113	1.68	6 (8%)
23	SF4	3	3003	-	0,12,12	0.00	-	-	-	-
21	CLA	1	1106	16	59,73,73	1.24	7 (11%)	67,113,113	1.75	5 (7%)
21	CLA	2	1211	-	44,58,73	1.47	9 (20%)	49,95,113	1.99	7 (14%)
21	CLA	1	1113	-	38,52,73	1.57	8 (21%)	40,87,113	2.05	5 (12%)
21	CLA	A	1123	38	59,73,73	1.27	8 (13%)	67,113,113	1.82	7 (10%)
21	CLA	a	1013	-	59,73,73	1.22	8 (13%)	67,113,113	1.79	6 (8%)
27	ACT	A	7001	-	1,3,3	7.80	1 (100%)	0,3,3	0.00	-
24	BCR	B	4014	-	41,41,41	0.71	0	56,56,56	3.12	12 (21%)
21	CLA	2	1226	-	49,63,73	1.40	8 (16%)	55,101,113	1.88	8 (14%)
21	CLA	B	1023	-	59,73,73	1.26	8 (13%)	67,113,113	1.83	8 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
21	CLA	b	1224	-	59,73,73	1.25	9 (15%)	67,113,113	1.72	7 (10%)
24	BCR	h	4018	-	41,41,41	0.69	0	56,56,56	3.34	10 (17%)
21	CLA	1	1111	-	59,73,73	1.27	8 (13%)	67,113,113	1.72	9 (13%)
25	LHG	6	5001	-	11,11,48	0.48	0	12,14,54	0.52	0
22	PQN	B	2002	-	34,34,34	0.88	2 (5%)	42,45,45	1.27	3 (7%)
25	LHG	F	5002	-	48,48,48	0.37	0	51,54,54	0.96	2 (3%)
21	CLA	2	1225	-	59,73,73	1.28	8 (13%)	67,113,113	1.66	6 (8%)
21	CLA	b	1022	-	59,73,73	1.25	7 (11%)	67,113,113	1.74	8 (11%)
21	CLA	1	1116	-	59,73,73	1.27	9 (15%)	67,113,113	1.76	7 (10%)
21	CLA	a	1131	-	59,73,73	1.27	9 (15%)	67,113,113	1.62	5 (7%)
21	CLA	1	1119	38	59,73,73	1.24	7 (11%)	67,113,113	1.85	7 (10%)
31	SQD	F	5001	-	53,54,54	0.80	0	62,65,65	0.92	2 (3%)
21	CLA	F	1302	6	59,73,73	1.28	8 (13%)	67,113,113	1.73	6 (8%)
21	CLA	2	1223	-	49,63,73	1.40	8 (16%)	55,101,113	1.89	6 (10%)
21	CLA	a	1123	1	59,73,73	1.28	9 (15%)	67,113,113	1.73	6 (8%)
24	BCR	J	4013	-	41,41,41	0.69	0	56,56,56	3.22	12 (21%)
21	CLA	A	1112	-	59,73,73	1.26	8 (13%)	67,113,113	1.82	7 (10%)
21	CLA	A	1103	-	59,73,73	1.22	8 (13%)	67,113,113	1.73	5 (7%)
21	CLA	a	1107	1	44,58,73	1.47	8 (18%)	49,95,113	2.02	9 (18%)
23	SF4	3	3002	-	0,12,12	0.00	-	-	-	-
21	CLA	a	1122	-	59,73,73	1.26	9 (15%)	67,113,113	1.80	7 (10%)
21	CLA	B	1211	-	59,73,73	1.27	7 (11%)	67,113,113	1.75	7 (10%)
21	CLA	B	1239	-	59,73,73	1.29	8 (13%)	67,113,113	1.80	7 (10%)
21	CLA	B	1236	-	44,58,73	1.48	8 (18%)	49,95,113	1.85	6 (12%)
24	BCR	A	4001	-	41,41,41	0.68	0	56,56,56	3.06	12 (21%)
21	CLA	8	1402	-	40,54,73	1.53	7 (17%)	44,90,113	1.89	5 (11%)
21	CLA	7	1302	8	35,49,73	1.65	9 (25%)	38,84,113	2.08	5 (13%)
21	CLA	L	1503	38	59,73,73	1.26	9 (15%)	67,113,113	1.75	9 (13%)
24	BCR	1	4002	-	41,41,41	0.64	0	56,56,56	3.26	11 (19%)
21	CLA	B	1224	-	59,73,73	1.25	8 (13%)	67,113,113	1.71	6 (8%)
21	CLA	a	1127	-	59,73,73	1.28	9 (15%)	67,113,113	1.72	6 (8%)
23	SF4	1	3001	2,16	0,12,12	0.00	-	-	-	-
21	CLA	a	1105	-	52,66,73	1.36	8 (15%)	58,104,113	1.83	7 (12%)
21	CLA	a	1132	-	59,73,73	1.25	7 (11%)	67,113,113	1.71	8 (11%)
21	CLA	K	1401	38	59,73,73	1.26	6 (10%)	67,113,113	1.81	10 (14%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
25	LHG	A	5007	-	48,48,48	0.40	0	51,54,54	1.11	3 (5%)
21	CLA	1	1137	-	45,59,73	1.47	9 (20%)	50,96,113	1.94	7 (14%)
21	CLA	2	1238	38	59,73,73	1.27	7 (11%)	67,113,113	1.66	7 (10%)
24	BCR	b	4010	-	41,41,41	0.64	0	56,56,56	3.06	7 (12%)
24	BCR	b	4017	-	41,41,41	0.63	0	56,56,56	3.28	10 (17%)
24	BCR	2	4011	-	41,41,41	0.68	0	56,56,56	2.94	9 (16%)
21	CLA	a	1128	-	59,73,73	1.25	7 (11%)	67,113,113	1.86	9 (13%)
21	CLA	B	1208	-	59,73,73	1.25	7 (11%)	67,113,113	1.71	7 (10%)
21	CLA	1	1107	-	45,59,73	1.45	7 (15%)	50,96,113	1.99	8 (16%)
21	CLA	a	1106	-	59,73,73	1.24	9 (15%)	67,113,113	1.79	6 (8%)
21	CLA	b	1212	-	59,73,73	1.30	9 (15%)	67,113,113	1.61	6 (8%)
21	CLA	1	1101	-	59,73,73	1.29	9 (15%)	67,113,113	1.78	7 (10%)
34	ZEX	J	4015	-	42,43,43	5.80	3 (7%)	55,60,60	6.94	10 (18%)
25	LHG	l	5001	-	48,48,48	0.39	0	51,54,54	1.09	3 (5%)
26	LMG	1	5004	-	55,55,55	1.14	6 (10%)	63,63,63	1.04	2 (3%)
21	CLA	a	1103	-	59,73,73	1.22	8 (13%)	67,113,113	1.73	7 (10%)
26	LMG	b	5005	-	55,55,55	1.14	6 (10%)	63,63,63	1.30	4 (6%)
21	CLA	1	1132	-	59,73,73	1.26	8 (13%)	67,113,113	1.78	8 (11%)
21	CLA	B	1226	-	59,73,73	1.24	7 (11%)	67,113,113	1.76	9 (13%)
26	LMG	B	5002	-	55,55,55	1.14	6 (10%)	63,63,63	1.07	5 (7%)
21	CLA	A	1105	-	59,73,73	1.30	8 (13%)	67,113,113	1.62	6 (8%)
21	CLA	b	1228	-	59,73,73	1.28	9 (15%)	67,113,113	1.68	6 (8%)
21	CLA	b	1206	12	59,73,73	1.25	8 (13%)	67,113,113	1.80	9 (13%)
21	CLA	B	1215	-	59,73,73	1.24	8 (13%)	67,113,113	1.76	8 (11%)
21	CLA	0	1502	28	59,73,73	1.27	7 (11%)	67,113,113	1.77	6 (8%)
25	LHG	A	5001	-	48,48,48	0.41	0	51,54,54	1.11	3 (5%)
21	CLA	A	1102	21	59,73,73	1.25	8 (13%)	67,113,113	1.79	8 (11%)
21	CLA	1	1103	-	59,73,73	1.22	9 (15%)	67,113,113	1.78	3 (4%)
24	BCR	I	4018	-	41,41,41	0.60	0	56,56,56	3.10	14 (25%)
23	SF4	a	3001	1,12	0,12,12	0.00	-	-	-	-
21	CLA	k	1402	-	43,57,73	1.48	9 (20%)	46,93,113	2.13	7 (15%)
21	CLA	1	1118	-	59,73,73	1.25	7 (11%)	67,113,113	1.74	8 (11%)
21	CLA	B	1202	-	59,73,73	1.25	8 (13%)	67,113,113	1.75	7 (10%)
21	CLA	L	1502	-	59,73,73	1.23	6 (10%)	67,113,113	1.75	8 (11%)
26	LMG	1	5002	-	50,50,55	1.03	5 (10%)	58,58,63	1.06	2 (3%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
25	LHG	b	5004	-	48,48,48	0.39	0	51,54,54	1.08	3 (5%)
21	CLA	B	1222	38	49,63,73	1.34	7 (14%)	55,101,113	1.93	8 (14%)
24	BCR	B	4005	-	41,41,41	0.67	0	56,56,56	3.22	10 (17%)
21	CLA	B	1230	-	59,73,73	1.26	9 (15%)	67,113,113	1.68	4 (5%)
21	CLA	b	1234	-	47,61,73	1.42	6 (12%)	52,98,113	1.93	9 (17%)
21	CLA	1	1129	-	44,58,73	1.46	7 (15%)	49,95,113	2.00	8 (16%)
24	BCR	2	4005	-	41,41,41	0.73	0	56,56,56	3.34	10 (17%)
23	SF4	c	3003	13	0,12,12	0.00	-	-		
24	BCR	0	4019	-	41,41,41	0.67	0	56,56,56	3.10	11 (19%)
26	LMG	2	5005	-	55,55,55	1.14	6 (10%)	63,63,63	1.07	2 (3%)
21	CLA	B	1212	-	49,63,73	1.41	8 (16%)	55,101,113	1.83	6 (10%)
21	CLA	A	1122	-	54,68,73	1.32	8 (14%)	61,107,113	1.75	8 (13%)
25	LHG	a	5005	-	48,48,48	0.38	0	51,54,54	1.10	3 (5%)
21	CLA	B	1238	38	59,73,73	1.30	8 (13%)	67,113,113	1.50	6 (8%)
24	BCR	a	4008	-	41,41,41	0.65	0	56,56,56	3.28	12 (21%)
21	CLA	A	1121	-	59,73,73	1.25	8 (13%)	67,113,113	1.74	6 (8%)
21	CLA	B	1209	-	59,73,73	1.29	8 (13%)	67,113,113	1.79	7 (10%)
21	CLA	a	1111	-	59,73,73	1.27	9 (15%)	67,113,113	1.67	6 (8%)
21	CLA	1	1130	-	49,63,73	1.37	8 (16%)	55,101,113	1.83	7 (12%)
21	CLA	l	1501	10	59,73,73	1.25	8 (13%)	67,113,113	1.78	10 (14%)
21	CLA	a	1113	-	44,58,73	1.47	9 (20%)	49,95,113	1.99	8 (16%)
21	CLA	F	1301	38	59,73,73	1.27	8 (13%)	67,113,113	1.69	7 (10%)
21	CLA	B	1228	-	59,73,73	1.24	7 (11%)	67,113,113	1.71	7 (10%)
21	CLA	A	1106	1	59,73,73	1.23	6 (10%)	67,113,113	1.74	7 (10%)
21	CLA	A	1138	-	59,73,73	1.26	9 (15%)	67,113,113	1.79	7 (10%)
21	CLA	b	1239	-	59,73,73	1.29	9 (15%)	67,113,113	1.77	6 (8%)
21	CLA	a	1129	-	46,60,73	1.44	8 (17%)	51,97,113	1.91	8 (15%)
23	SF4	C	3002	3	0,12,12	0.00	-	-		
21	CLA	A	1136	-	59,73,73	1.30	8 (13%)	67,113,113	1.66	7 (10%)
21	CLA	b	1021	-	59,73,73	1.25	8 (13%)	67,113,113	1.71	6 (8%)
24	BCR	K	4001	-	41,41,41	0.58	0	56,56,56	3.17	16 (28%)
30	ECH	M	4021	-	42,42,42	0.65	0	55,58,58	1.68	11 (20%)
21	CLA	1	1105	-	44,58,73	1.50	9 (20%)	49,95,113	1.92	6 (12%)
21	CLA	B	1210	-	59,73,73	1.28	8 (13%)	67,113,113	1.73	8 (11%)
24	BCR	9	4021	-	41,41,41	0.67	0	56,56,56	3.27	17 (30%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
21	CLA	2	1207	-	50,64,73	1.38	8 (16%)	56,102,113	1.85	8 (14%)
30	ECH	b	4011	-	42,42,42	0.82	1 (2%)	55,58,58	2.42	15 (27%)
21	CLA	b	1226	-	59,73,73	1.29	8 (13%)	67,113,113	1.60	8 (11%)
21	CLA	b	1205	-	59,73,73	1.24	7 (11%)	67,113,113	1.73	6 (8%)
21	CLA	B	1234	-	59,73,73	1.27	7 (11%)	67,113,113	1.74	7 (10%)
21	CLA	2	1208	-	54,68,73	1.34	8 (14%)	61,107,113	1.72	6 (9%)
21	CLA	1	1123	-	59,73,73	1.27	9 (15%)	67,113,113	1.75	7 (10%)
35	LMT	1	6001	-	36,36,36	1.15	4 (11%)	47,47,47	0.98	3 (6%)
26	LMG	K	5009	-	55,55,55	1.17	7 (12%)	63,63,63	1.26	5 (7%)
21	CLA	a	1130	-	59,73,73	1.27	9 (15%)	67,113,113	1.67	5 (7%)
21	CLA	B	1223	-	59,73,73	1.29	8 (13%)	67,113,113	1.71	6 (8%)
21	CLA	a	1140	-	59,73,73	1.26	8 (13%)	67,113,113	1.76	7 (10%)
24	BCR	b	4014	-	41,41,41	0.71	0	56,56,56	3.19	12 (21%)
21	CLA	2	1021	-	59,73,73	1.23	7 (11%)	67,113,113	1.77	6 (8%)
21	CLA	1	1135	-	46,60,73	1.45	8 (17%)	51,97,113	1.93	8 (15%)
21	CLA	b	1201	-	59,73,73	1.26	9 (15%)	67,113,113	1.66	6 (8%)
26	LMG	b	5002	-	55,55,55	1.13	6 (10%)	63,63,63	1.18	6 (9%)
21	CLA	a	1109	-	59,73,73	1.23	7 (11%)	67,113,113	1.87	7 (10%)
21	CLA	2	1204	-	59,73,73	1.26	8 (13%)	67,113,113	1.74	6 (8%)
21	CLA	A	1135	-	59,73,73	1.26	9 (15%)	67,113,113	1.76	7 (10%)
35	LMT	L	6001	-	36,36,36	1.15	5 (13%)	47,47,47	1.16	4 (8%)
21	CLA	A	1104	-	59,73,73	1.26	7 (11%)	67,113,113	1.73	9 (13%)
24	BCR	A	4002	-	41,41,41	0.66	0	56,56,56	3.14	17 (30%)
24	BCR	A	4003	-	41,41,41	0.69	0	56,56,56	3.15	13 (23%)
22	PQN	1	2001	-	34,34,34	0.44	0	42,45,45	1.09	3 (7%)
21	CLA	2	1227	-	36,53,73	1.63	9 (25%)	39,89,113	1.94	4 (10%)
21	CLA	b	1217	-	45,59,73	1.47	9 (20%)	50,96,113	1.87	7 (14%)
21	CLA	a	1112	-	59,73,73	1.26	9 (15%)	67,113,113	1.83	7 (10%)
21	CLA	J	1303	-	59,73,73	1.27	9 (15%)	67,113,113	1.77	7 (10%)
21	CLA	b	1236	-	59,73,73	1.28	8 (13%)	67,113,113	1.68	6 (8%)
21	CLA	1	1133	-	59,73,73	1.28	8 (13%)	67,113,113	1.75	6 (8%)
21	CLA	2	1205	-	59,73,73	1.25	9 (15%)	67,113,113	1.82	6 (8%)
26	LMG	A	5008	-	55,55,55	1.14	6 (10%)	63,63,63	1.04	2 (3%)
21	CLA	a	1801	25	49,63,73	1.40	9 (18%)	55,101,113	1.89	5 (9%)
21	CLA	0	1501	20	59,73,73	1.25	9 (15%)	67,113,113	1.70	6 (8%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
21	CLA	1	1801	25	50,64,73	1.39	9 (18%)	56,102,113	1.91	8 (14%)
21	CLA	2	1219	-	47,61,73	1.43	8 (17%)	52,98,113	1.97	9 (17%)
21	CLA	a	1012	38	59,73,73	1.25	7 (11%)	67,113,113	1.80	10 (14%)
24	BCR	2	4010	-	41,41,41	0.74	0	56,56,56	3.62	14 (25%)
31	SQD	B	5008	-	53,54,54	0.80	0	62,65,65	0.91	3 (4%)
21	CLA	2	1217	-	46,60,73	1.45	8 (17%)	51,97,113	1.91	7 (13%)
34	ZEX	F	4016	-	42,43,43	5.85	2 (4%)	55,60,60	7.03	13 (23%)
24	BCR	1	4008	-	41,41,41	0.62	0	56,56,56	3.19	10 (17%)
21	CLA	1	1121	-	49,63,73	1.39	9 (18%)	55,101,113	1.90	7 (12%)
25	LHG	1	5003	21	48,48,48	0.40	0	51,54,54	1.09	3 (5%)
24	BCR	8	4001	-	41,41,41	0.66	0	56,56,56	3.23	10 (17%)
21	CLA	A	1137	-	59,73,73	1.28	9 (15%)	67,113,113	1.64	6 (8%)
21	CLA	B	1201	-	59,73,73	1.24	8 (13%)	67,113,113	1.67	7 (10%)
21	CLA	A	1132	-	59,73,73	1.27	7 (11%)	67,113,113	1.66	6 (8%)
21	CLA	B	1229	-	59,73,73	1.27	8 (13%)	67,113,113	1.72	5 (7%)
21	CLA	b	1218	-	59,73,73	1.26	7 (11%)	67,113,113	1.72	8 (11%)
21	CLA	a	1104	-	59,73,73	1.24	7 (11%)	67,113,113	1.70	7 (10%)
21	CLA	1	1125	-	59,73,73	1.28	8 (13%)	67,113,113	1.81	7 (10%)
30	ECH	B	4006	-	42,42,42	0.91	2 (4%)	55,58,58	2.52	15 (27%)
21	CLA	b	1231	38	59,73,73	1.25	9 (15%)	67,113,113	1.85	6 (8%)
21	CLA	A	1129	-	52,66,73	1.32	8 (15%)	58,104,113	1.83	9 (15%)
24	BCR	j	4013	-	41,41,41	0.74	0	56,56,56	3.24	13 (23%)
25	LHG	a	5003	21	48,48,48	0.39	0	51,54,54	1.05	3 (5%)
22	PQN	a	2001	-	34,34,34	0.47	0	42,45,45	1.01	2 (4%)
21	CLA	A	1111	-	59,73,73	1.26	8 (13%)	67,113,113	1.78	8 (11%)
21	CLA	b	1215	-	59,73,73	1.25	8 (13%)	67,113,113	1.82	8 (11%)
21	CLA	L	1501	10	59,73,73	1.26	7 (11%)	67,113,113	1.73	6 (8%)
21	CLA	A	1134	1	59,73,73	1.27	9 (15%)	67,113,113	1.74	7 (10%)
21	CLA	1	1110	-	44,58,73	1.48	9 (20%)	49,95,113	1.96	5 (10%)
21	CLA	0	1503	38	59,73,73	1.26	8 (13%)	67,113,113	1.69	5 (7%)
24	BCR	B	4017	-	41,41,41	0.65	0	56,56,56	3.27	12 (21%)
21	CLA	f	1302	-	59,73,73	1.27	9 (15%)	67,113,113	1.69	7 (10%)
21	CLA	2	1202	-	59,73,73	1.25	7 (11%)	67,113,113	1.78	8 (11%)
21	CLA	b	1204	-	59,73,73	1.27	8 (13%)	67,113,113	1.62	7 (10%)
21	CLA	A	1130	-	54,68,73	1.31	8 (14%)	61,107,113	1.91	10 (16%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
31	SQD	b	5006	-	53,54,54	0.79	0	62,65,65	0.90	3 (4%)
21	CLA	6	1302	6	37,51,73	1.59	8 (21%)	40,86,113	2.36	7 (17%)
21	CLA	A	1107	1	59,73,73	1.26	7 (11%)	67,113,113	1.80	8 (11%)
21	CLA	b	1237	38	59,73,73	1.23	6 (10%)	67,113,113	1.76	10 (14%)
21	CLA	2	1215	-	54,68,73	1.32	9 (16%)	61,107,113	1.86	8 (13%)
21	CLA	B	1235	-	59,73,73	1.23	7 (11%)	67,113,113	1.85	5 (7%)
21	CLA	A	1133	-	59,73,73	1.26	8 (13%)	67,113,113	1.60	4 (5%)
21	CLA	2	1232	-	36,53,73	1.60	9 (25%)	39,89,113	2.05	5 (12%)
21	CLA	a	1139	38	59,73,73	1.28	9 (15%)	67,113,113	1.75	6 (8%)
22	PQN	2	2002	-	34,34,34	0.38	0	42,45,45	1.27	3 (7%)
21	CLA	B	1221	-	59,73,73	1.24	9 (15%)	67,113,113	1.73	7 (10%)
21	CLA	1	1126	-	59,73,73	1.25	7 (11%)	67,113,113	1.80	7 (10%)
21	CLA	a	1124	-	49,63,73	1.36	8 (16%)	55,101,113	1.90	8 (14%)
24	BCR	b	4005	-	41,41,41	0.64	0	56,56,56	3.15	12 (21%)
25	LHG	M	5001	-	48,48,48	0.41	0	51,54,54	1.11	3 (5%)
21	CLA	A	1115	-	59,73,73	1.25	7 (11%)	67,113,113	1.68	7 (10%)
21	CLA	2	1222	-	44,58,73	1.46	7 (15%)	49,95,113	2.04	8 (16%)
21	CLA	B	1218	-	59,73,73	1.27	9 (15%)	67,113,113	1.75	9 (13%)
24	BCR	a	4003	-	41,41,41	0.73	0	56,56,56	3.31	11 (19%)
21	CLA	a	1117	-	59,73,73	1.27	8 (13%)	67,113,113	1.70	5 (7%)
21	CLA	7	1303	-	35,49,73	1.62	8 (22%)	38,84,113	2.10	6 (15%)
26	LMG	b	5007	-	55,55,55	1.14	6 (10%)	63,63,63	1.14	3 (4%)
25	LHG	A	5003	21	48,48,48	0.40	0	51,54,54	1.02	4 (7%)
21	CLA	1	1104	-	59,73,73	1.25	9 (15%)	67,113,113	1.72	7 (10%)
36	EQ3	I	4020	-	43,43,43	4.12	25 (58%)	56,60,60	2.21	22 (39%)
21	CLA	b	1207	-	59,73,73	1.27	8 (13%)	67,113,113	1.70	7 (10%)
21	CLA	1	1109	16	59,73,73	1.26	9 (15%)	67,113,113	1.77	7 (10%)
21	CLA	2	1212	-	35,49,73	1.62	8 (22%)	38,84,113	2.16	6 (15%)
21	CLA	2	1218	-	59,73,73	1.27	8 (13%)	67,113,113	1.74	9 (13%)
21	CLA	B	1021	-	59,73,73	1.24	8 (13%)	67,113,113	1.80	6 (8%)
21	CLA	B	1227	-	49,63,73	1.41	8 (16%)	55,101,113	1.80	5 (9%)
21	CLA	A	1131	-	59,73,73	1.28	8 (13%)	67,113,113	1.64	5 (7%)
24	BCR	a	4019	-	41,41,41	0.71	0	56,56,56	3.49	12 (21%)
30	ECH	b	4006	-	42,42,42	0.72	1 (2%)	55,58,58	2.25	15 (27%)
21	CLA	j	1303	-	49,63,73	1.41	9 (18%)	55,101,113	1.86	7 (12%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
31	SQD	f	5001	-	53,54,54	0.79	0	62,65,65	0.90	2 (3%)
21	CLA	A	1117	-	59,73,73	1.28	8 (13%)	67,113,113	1.68	6 (8%)
24	BCR	B	4018	-	41,41,41	0.72	0	56,56,56	3.45	14 (25%)
21	CLA	A	1128	-	59,73,73	1.25	7 (11%)	67,113,113	1.88	9 (13%)
25	LHG	1	5007	-	48,48,48	0.40	0	51,54,54	1.02	2 (3%)
21	CLA	b	1238	38	59,73,73	1.27	7 (11%)	67,113,113	1.69	7 (10%)
24	BCR	l	4019	-	41,41,41	0.63	0	56,56,56	2.88	12 (21%)
21	CLA	l	1502	-	59,73,73	1.26	7 (11%)	67,113,113	1.70	6 (8%)
21	CLA	B	1022	38	59,73,73	1.29	7 (11%)	67,113,113	1.68	7 (10%)
21	CLA	2	1240	-	35,49,73	1.65	9 (25%)	38,84,113	2.07	5 (13%)
21	CLA	K	1402	-	59,73,73	1.27	9 (15%)	67,113,113	1.68	6 (8%)
25	LHG	L	5005	-	48,48,48	0.40	0	51,54,54	0.95	2 (3%)
24	BCR	2	4017	-	41,41,41	0.65	0	56,56,56	3.23	12 (21%)
21	CLA	a	1110	-	53,67,73	1.36	9 (16%)	59,105,113	1.83	6 (10%)
28	45D	h	4020	21	43,43,43	3.51	17 (39%)	54,60,60	3.40	23 (42%)
24	BCR	2	4014	-	41,41,41	0.72	0	56,56,56	3.32	13 (23%)
24	BCR	1	4012	-	41,41,41	0.68	0	56,56,56	3.22	9 (16%)
21	CLA	b	1221	38	59,73,73	1.25	8 (13%)	67,113,113	1.89	8 (11%)
31	SQD	L	5002	-	53,54,54	0.80	0	62,65,65	0.89	3 (4%)
21	CLA	b	1210	-	59,73,73	1.26	9 (15%)	67,113,113	1.70	7 (10%)
26	LMG	a	5002	-	50,50,55	1.04	4 (8%)	58,58,63	1.09	2 (3%)
24	BCR	L	4019	-	41,41,41	0.69	0	56,56,56	2.85	14 (25%)
21	CLA	B	1203	-	59,73,73	1.25	8 (13%)	67,113,113	1.69	5 (7%)
30	ECH	2	4006	-	42,42,42	0.80	1 (2%)	55,58,58	2.53	16 (29%)
21	CLA	A	1119	38	59,73,73	1.22	6 (10%)	67,113,113	1.65	6 (8%)
21	CLA	1	1140	-	59,73,73	1.27	8 (13%)	67,113,113	1.74	7 (10%)
21	CLA	1	1114	-	36,53,73	1.62	9 (25%)	39,89,113	1.93	5 (12%)
25	LHG	B	5006	-	48,48,48	0.39	0	51,54,54	1.06	3 (5%)
35	LMT	l	6001	-	36,36,36	1.11	4 (11%)	47,47,47	1.20	3 (6%)
21	CLA	b	1209	-	59,73,73	1.27	8 (13%)	67,113,113	1.84	9 (13%)
21	CLA	A	1139	38	59,73,73	1.25	9 (15%)	67,113,113	1.74	4 (5%)
24	BCR	a	4007	-	41,41,41	0.65	0	56,56,56	3.09	12 (21%)
24	BCR	b	4004	-	41,41,41	0.67	0	56,56,56	3.29	14 (25%)
21	CLA	a	1118	-	59,73,73	1.26	8 (13%)	67,113,113	1.63	7 (10%)
21	CLA	1	1102	-	49,63,73	1.36	8 (16%)	55,101,113	2.03	10 (18%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
24	BCR	7	4013	-	41,41,41	0.71	0	56,56,56	3.29	15 (26%)
21	CLA	A	1125	-	59,73,73	1.26	6 (10%)	67,113,113	1.80	10 (14%)
21	CLA	6	1301	38	41,55,73	1.51	9 (21%)	45,91,113	1.92	8 (17%)
21	CLA	B	1232	-	44,58,73	1.49	9 (20%)	49,95,113	1.99	6 (12%)
24	BCR	A	4019	-	41,41,41	0.71	0	56,56,56	3.60	14 (25%)
21	CLA	2	1228	-	36,53,73	1.59	9 (25%)	39,89,113	2.12	5 (12%)
23	SF4	c	3002	-	0,12,12	0.00	-	-		
21	CLA	a	1136	-	59,73,73	1.28	9 (15%)	67,113,113	1.89	10 (14%)
25	LHG	A	5006	-	48,48,48	0.40	0	51,54,54	1.03	3 (5%)
21	CLA	A	1140	-	59,73,73	1.27	9 (15%)	67,113,113	1.71	7 (10%)
26	LMG	a	5004	-	55,55,55	1.14	7 (12%)	63,63,63	1.21	4 (6%)
21	CLA	1	1136	-	59,73,73	1.29	8 (13%)	67,113,113	1.71	7 (10%)
21	CLA	2	1209	-	36,53,73	1.64	9 (25%)	39,89,113	2.08	5 (12%)
21	CLA	2	1203	-	59,73,73	1.27	9 (15%)	67,113,113	1.67	7 (10%)
21	CLA	8	1401	-	36,53,73	1.61	8 (22%)	39,89,113	2.08	7 (17%)
21	CLA	A	1108	-	47,61,73	1.41	9 (19%)	52,98,113	1.91	5 (9%)
21	CLA	2	1239	-	59,73,73	1.29	9 (15%)	67,113,113	1.79	9 (13%)
21	CLA	1	1108	-	40,54,73	1.54	9 (22%)	44,90,113	1.89	4 (9%)
21	CLA	A	1013	-	59,73,73	1.25	9 (15%)	67,113,113	1.79	9 (13%)
21	CLA	1	1138	-	54,68,73	1.35	9 (16%)	61,107,113	1.78	6 (9%)
21	CLA	b	1223	-	59,73,73	1.25	7 (11%)	67,113,113	1.72	8 (11%)
30	ECH	m	4021	-	42,42,42	0.65	0	55,58,58	1.68	10 (18%)
25	LHG	0	5002	-	48,48,48	0.39	0	51,54,54	1.04	2 (3%)
24	BCR	b	4018	-	41,41,41	0.70	0	56,56,56	3.35	8 (14%)
21	CLA	2	1221	-	59,73,73	1.26	9 (15%)	67,113,113	1.79	8 (11%)
21	CLA	A	1120	-	59,73,73	1.26	7 (11%)	67,113,113	1.74	10 (14%)
21	CLA	B	1205	-	59,73,73	1.23	6 (10%)	67,113,113	1.77	6 (8%)
24	BCR	L	4022	-	41,41,41	0.61	0	56,56,56	3.06	10 (17%)
21	CLA	1	1012	38	59,73,73	1.25	7 (11%)	67,113,113	1.90	9 (13%)
21	CLA	b	1023	-	59,73,73	1.24	8 (13%)	67,113,113	1.89	8 (11%)
21	CLA	B	1225	-	59,73,73	1.30	8 (13%)	67,113,113	1.67	5 (7%)
25	LHG	A	5005	-	48,48,48	0.40	0	51,54,54	1.09	4 (7%)
21	CLA	1	1127	-	59,73,73	1.30	8 (13%)	67,113,113	1.64	6 (8%)
21	CLA	a	1137	-	44,58,73	1.49	9 (20%)	49,95,113	1.94	6 (12%)
26	LMG	A	5002	-	50,50,55	1.06	5 (10%)	58,58,63	1.17	4 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
26	LMG	B	5005	-	55,55,55	1.13	6 (10%)	63,63,63	1.09	3 (4%)
21	CLA	l	1503	-	59,73,73	1.23	7 (11%)	67,113,113	1.69	8 (11%)
25	LHG	l	5004	-	48,48,48	0.39	0	51,54,54	1.04	3 (5%)
30	ECH	i	4020	-	42,42,42	0.81	1 (2%)	55,58,58	2.40	17 (30%)
25	LHG	l	5005	-	48,48,48	0.40	0	51,54,54	1.03	3 (5%)
21	CLA	b	1219	-	54,68,73	1.34	8 (14%)	61,107,113	1.80	7 (11%)
24	BCR	A	4007	-	41,41,41	0.63	0	56,56,56	2.90	13 (23%)
24	BCR	a	4002	-	41,41,41	0.65	0	56,56,56	3.53	12 (21%)
21	CLA	a	1134	1	43,57,73	1.50	9 (20%)	46,93,113	2.07	7 (15%)
21	CLA	l	1120	-	59,73,73	1.28	8 (13%)	67,113,113	1.76	6 (8%)
25	LHG	l	5003	-	48,48,48	0.40	0	51,54,54	1.00	3 (5%)
21	CLA	b	1232	-	59,73,73	1.27	9 (15%)	67,113,113	1.71	7 (10%)
25	LHG	a	5001	-	48,48,48	0.41	0	51,54,54	1.11	3 (5%)
21	CLA	A	1124	38	59,73,73	1.25	7 (11%)	67,113,113	1.72	9 (13%)
25	LHG	0	5004	-	48,48,48	0.39	0	51,54,54	1.03	3 (5%)
21	CLA	2	1224	-	49,63,73	1.36	8 (16%)	55,101,113	1.89	7 (12%)
35	LMT	0	6001	-	36,36,36	1.13	4 (11%)	47,47,47	1.17	3 (6%)
21	CLA	A	1109	21	59,73,73	1.25	7 (11%)	67,113,113	1.77	7 (10%)
21	CLA	J	1302	8	59,73,73	1.27	8 (13%)	67,113,113	1.86	7 (10%)
21	CLA	a	1135	-	59,73,73	1.29	8 (13%)	67,113,113	1.63	6 (8%)
21	CLA	a	1138	-	59,73,73	1.27	8 (13%)	67,113,113	1.80	5 (7%)
26	LMG	2	5002	-	55,55,55	1.14	6 (10%)	63,63,63	1.08	2 (3%)
21	CLA	b	1213	-	59,73,73	1.26	9 (15%)	67,113,113	1.79	8 (11%)
24	BCR	l	4019	-	41,41,41	0.67	0	56,56,56	3.36	8 (14%)
21	CLA	l	1117	-	59,73,73	1.26	7 (11%)	67,113,113	1.69	6 (8%)
24	BCR	a	4012	-	41,41,41	0.69	0	56,56,56	3.12	14 (25%)
21	CLA	a	1114	-	46,60,73	1.44	9 (19%)	51,97,113	1.98	8 (15%)
21	CLA	B	1206	2	59,73,73	1.26	8 (13%)	67,113,113	1.84	8 (11%)
31	SQD	L	5001	-	50,51,54	0.80	0	59,62,65	0.93	4 (6%)
27	ACT	B	7002	-	1,3,3	6.86	1 (100%)	0,3,3	0.00	-
21	CLA	A	1127	-	59,73,73	1.28	7 (11%)	67,113,113	1.63	8 (11%)
24	BCR	i	4018	-	41,41,41	0.70	0	56,56,56	3.39	12 (21%)
23	SF4	A	3001	1,2	0,12,12	0.00	-	-	-	-
21	CLA	l	1128	-	59,73,73	1.26	8 (13%)	67,113,113	1.83	8 (11%)
21	CLA	a	1126	-	59,73,73	1.25	7 (11%)	67,113,113	1.88	6 (8%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
31	SQD	0	5005	-	53,54,54	0.80	0	62,65,65	0.89	3 (4%)
24	BCR	B	4004	-	41,41,41	0.68	0	56,56,56	3.19	12 (21%)
21	CLA	A	1118	-	59,73,73	1.27	8 (13%)	67,113,113	1.66	6 (8%)
21	CLA	a	1108	-	51,65,73	1.38	9 (17%)	57,103,113	1.88	7 (12%)
22	PQN	b	2002	-	34,34,34	0.77	2 (5%)	42,45,45	1.27	5 (11%)
21	CLA	a	1125	-	59,73,73	1.27	8 (13%)	67,113,113	1.84	9 (13%)
21	CLA	a	1120	-	49,63,73	1.40	9 (18%)	55,101,113	1.90	7 (12%)
24	BCR	2	4004	-	41,41,41	0.68	0	56,56,56	3.26	9 (16%)
21	CLA	a	1119	-	59,73,73	1.25	8 (13%)	67,113,113	1.68	8 (11%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
21	CLA	A	1012	38	2/2/20/25	22/37/135/135	-
21	CLA	2	1220	-	3/3/16/25	5/11/111/135	-
26	LMG	0	5001	-	-	24/50/70/70	0/1/1/1
21	CLA	B	1214	-	3/3/20/25	17/37/135/135	-
21	CLA	1	1112	-	3/3/17/25	8/19/117/135	-
21	CLA	1	1139	-	3/3/20/25	14/37/135/135	-
21	CLA	b	1235	-	3/3/20/25	17/37/135/135	-
21	CLA	1	1011	-	3/3/20/25	13/37/135/135	-
24	BCR	a	4001	-	-	16/29/63/63	0/2/2/2
37	DGD	L	5004	-	-	23/55/95/95	0/2/2/2
21	CLA	2	1231	38	3/3/16/25	4/15/113/135	-
21	CLA	b	1220	-	3/3/20/25	12/37/135/135	-
21	CLA	2	1213	-	3/3/17/25	8/19/117/135	-
21	CLA	B	1204	-	2/2/20/25	17/37/135/135	-
21	CLA	2	1229	-	3/3/20/25	21/37/135/135	-
21	CLA	2	1214	-	3/3/18/25	16/30/128/135	-
23	SF4	A	3001	1,2	-	-	0/6/5/5
21	CLA	a	1102	-	3/3/20/25	11/37/135/135	-
21	CLA	B	1220	-	3/3/18/25	15/28/126/135	-
35	LMT	F	6001	-	-	8/21/61/61	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
21	CLA	1	1131	-	3/3/20/25	12/37/135/135	-
21	CLA	A	1801	25	3/3/20/25	20/37/135/135	-
21	CLA	j	1302	-	3/3/20/25	19/37/135/135	-
25	LHG	l	5002	-	-	32/53/53/53	-
24	BCR	1	4001	-	-	10/29/63/63	0/2/2/2
23	SF4	C	3003	3	-	-	0/6/5/5
24	BCR	6	4016	-	-	13/29/63/63	0/2/2/2
21	CLA	b	1225	-	3/3/20/25	13/37/135/135	-
25	LHG	M	5001	-	-	31/53/53/53	-
26	LMG	A	5004	-	-	18/43/63/70	0/1/1/1
25	LHG	2	5004	-	-	25/53/53/53	-
21	CLA	b	1202	-	2/2/20/25	18/37/135/135	-
21	CLA	A	1114	38	3/3/20/25	21/37/135/135	-
24	BCR	B	4010	-	-	10/29/63/63	0/2/2/2
21	CLA	a	1116	-	2/2/19/25	10/31/129/135	-
34	ZEX	7	4015	-	-	7/29/67/67	0/2/2/2
34	ZEX	j	4015	-	-	7/29/67/67	0/2/2/2
21	CLA	b	1216	38	3/3/20/25	21/37/135/135	-
21	CLA	b	1211	-	3/3/20/25	17/37/135/135	-
28	45D	B	4011	-	-	11/29/69/69	0/2/2/2
21	CLA	A	1101	-	1/1/20/25	8/37/135/135	-
21	CLA	B	1213	-	3/3/20/25	14/37/135/135	-
21	CLA	2	1236	-	3/3/17/25	9/19/117/135	-
21	CLA	B	1216	38	3/3/20/25	23/37/135/135	-
21	CLA	B	1237	38	3/3/20/25	12/37/135/135	-
25	LHG	B	5004	-	-	28/53/53/53	-
21	CLA	1	1013	-	3/3/20/25	17/37/135/135	-
21	CLA	2	1206	2	3/3/20/25	14/37/135/135	-
24	BCR	1	4007	-	-	16/29/63/63	0/2/2/2
21	CLA	2	1022	38	3/3/20/25	7/37/135/135	-
21	CLA	a	1101	-	2/2/20/25	11/37/135/135	-
24	BCR	A	4008	-	-	5/29/63/63	0/2/2/2
21	CLA	a	1121	-	3/3/20/25	24/37/135/135	-
21	CLA	B	1219	-	2/2/20/25	17/37/135/135	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
21	CLA	A	1126	-	3/3/20/25	18/37/135/135	-
21	CLA	B	1240	-	3/3/20/25	17/37/135/135	-
21	CLA	b	1214	-	3/3/20/25	17/37/135/135	-
21	CLA	1	1122	-	3/3/19/25	14/31/129/135	-
21	CLA	2	1230	-	3/3/16/25	11/16/114/135	-
21	CLA	B	1217	-	3/3/20/25	16/37/135/135	-
21	CLA	A	1116	-	3/3/20/25	21/37/135/135	-
21	CLA	f	1301	38	3/3/17/25	5/19/117/135	-
21	CLA	a	1115	-	2/2/20/25	8/37/135/135	-
21	CLA	b	1227	-	3/3/20/25	13/37/135/135	-
21	CLA	2	1234	-	3/3/17/25	9/19/117/135	-
21	CLA	b	1208	-	3/3/19/25	15/31/129/135	-
24	BCR	A	4012	-	-	11/29/63/63	0/2/2/2
24	BCR	1	4003	-	-	13/29/63/63	0/2/2/2
21	CLA	1	1127	-	3/3/20/25	21/37/135/135	-
21	CLA	b	1203	-	3/3/20/25	18/37/135/135	-
21	CLA	B	1207	-	2/2/20/25	11/37/135/135	-
21	CLA	a	1011	-	3/3/20/25	20/37/135/135	-
21	CLA	2	1237	38	3/3/20/25	14/37/135/135	-
24	BCR	f	4016	-	-	11/29/63/63	0/2/2/2
21	CLA	2	1210	-	2/2/20/25	22/37/135/135	-
21	CLA	k	1401	-	3/3/17/25	5/19/117/135	-
21	CLA	1	1104	-	3/3/20/25	15/37/135/135	-
24	BCR	l	4022	-	-	14/29/63/63	0/2/2/2
21	CLA	1	1134	16	3/3/20/25	22/37/135/135	-
24	BCR	k	4001	-	-	10/29/63/63	0/2/2/2
24	BCR	2	4018	-	-	14/29/63/63	0/2/2/2
21	CLA	A	1110	-	3/3/20/25	19/37/135/135	-
21	CLA	1	1124	-	3/3/18/25	11/27/125/135	-
21	CLA	2	1201	-	3/3/20/25	12/37/135/135	-
25	LHG	a	5007	-	-	34/53/53/53	-
21	CLA	2	1216	-	3/3/17/25	6/19/117/135	-
21	CLA	A	1113	-	3/3/20/25	22/37/135/135	-
21	CLA	B	1231	38	1/1/20/25	20/37/135/135	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
25	LHG	1	5001	-	-	27/53/53/53	-
21	CLA	b	1240	-	3/3/20/25	20/37/135/135	-
24	BCR	0	4022	-	-	9/29/63/63	0/2/2/2
21	CLA	b	1222	38	3/3/20/25	15/37/135/135	-
21	CLA	a	1133	-	2/2/20/25	18/37/135/135	-
21	CLA	b	1229	-	3/3/20/25	14/37/135/135	-
21	CLA	2	1235	-	3/3/17/25	9/23/121/135	-
21	CLA	1	1115	-	3/3/20/25	9/37/135/135	-
23	SF4	3	3003	-	-	-	0/6/5/5
21	CLA	1	1106	16	3/3/20/25	17/37/135/135	-
21	CLA	2	1211	-	3/3/17/25	10/19/117/135	-
21	CLA	1	1113	-	3/3/15/25	7/11/110/135	-
21	CLA	A	1123	38	2/2/20/25	12/37/135/135	-
21	CLA	a	1013	-	3/3/20/25	12/37/135/135	-
24	BCR	B	4014	-	-	8/29/63/63	0/2/2/2
21	CLA	2	1226	-	3/3/18/25	15/25/123/135	-
21	CLA	B	1023	-	3/3/20/25	5/37/135/135	-
21	CLA	b	1224	-	3/3/20/25	12/37/135/135	-
24	BCR	h	4018	-	-	13/29/63/63	0/2/2/2
21	CLA	1	1111	-	3/3/20/25	15/37/135/135	-
25	LHG	6	5001	-	-	6/12/12/53	-
22	PQN	B	2002	-	-	10/23/43/43	0/2/2/2
25	LHG	F	5002	-	-	40/53/53/53	-
21	CLA	2	1225	-	3/3/20/25	15/37/135/135	-
21	CLA	b	1022	-	2/2/20/25	10/37/135/135	-
21	CLA	1	1116	-	3/3/20/25	17/37/135/135	-
21	CLA	a	1131	-	3/3/20/25	14/37/135/135	-
21	CLA	1	1119	38	3/3/20/25	15/37/135/135	-
31	SQD	F	5001	-	-	23/49/69/69	0/1/1/1
21	CLA	F	1302	6	3/3/20/25	19/37/135/135	-
21	CLA	2	1223	-	2/2/18/25	8/25/123/135	-
21	CLA	a	1123	1	2/2/20/25	16/37/135/135	-
24	BCR	J	4013	-	-	14/29/63/63	0/2/2/2
21	CLA	A	1112	-	3/3/20/25	19/37/135/135	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
21	CLA	A	1103	-	3/3/20/25	19/37/135/135	-
21	CLA	a	1107	1	3/3/17/25	7/19/117/135	-
25	LHG	L	5005	-	-	24/53/53/53	-
21	CLA	a	1122	-	3/3/20/25	24/37/135/135	-
21	CLA	B	1211	-	3/3/20/25	19/37/135/135	-
21	CLA	B	1239	-	3/3/20/25	17/37/135/135	-
21	CLA	B	1236	-	3/3/17/25	5/19/117/135	-
24	BCR	A	4001	-	-	5/29/63/63	0/2/2/2
21	CLA	8	1402	-	3/3/16/25	11/15/113/135	-
21	CLA	7	1302	8	2/2/15/25	3/8/106/135	-
21	CLA	L	1503	38	2/2/20/25	20/37/135/135	-
24	BCR	1	4002	-	-	14/29/63/63	0/2/2/2
21	CLA	B	1224	-	3/3/20/25	21/37/135/135	-
21	CLA	a	1127	-	3/3/20/25	23/37/135/135	-
21	CLA	b	1023	-	3/3/20/25	11/37/135/135	-
21	CLA	a	1105	-	3/3/18/25	8/29/127/135	-
21	CLA	a	1132	-	3/3/20/25	13/37/135/135	-
21	CLA	K	1401	38	3/3/20/25	15/37/135/135	-
25	LHG	A	5007	-	-	29/53/53/53	-
21	CLA	1	1137	-	3/3/17/25	9/21/119/135	-
21	CLA	2	1238	38	3/3/20/25	11/37/135/135	-
24	BCR	b	4010	-	-	9/29/63/63	0/2/2/2
24	BCR	b	4017	-	-	11/29/63/63	0/2/2/2
24	BCR	2	4011	-	-	15/29/63/63	0/2/2/2
21	CLA	a	1128	-	3/3/20/25	23/37/135/135	-
21	CLA	B	1208	-	3/3/20/25	17/37/135/135	-
21	CLA	1	1107	-	3/3/17/25	9/21/119/135	-
21	CLA	a	1106	-	3/3/20/25	17/37/135/135	-
21	CLA	b	1212	-	2/2/20/25	16/37/135/135	-
21	CLA	1	1101	-	1/1/20/25	15/37/135/135	-
21	CLA	j	1303	-	3/3/18/25	11/25/123/135	-
25	LHG	l	5001	-	-	31/53/53/53	-
26	LMG	1	5004	-	-	20/50/70/70	0/1/1/1
21	CLA	a	1103	-	2/2/20/25	22/37/135/135	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
26	LMG	b	5005	-	-	17/50/70/70	0/1/1/1
21	CLA	1	1132	-	3/3/20/25	13/37/135/135	-
21	CLA	B	1226	-	3/3/20/25	22/37/135/135	-
26	LMG	B	5002	-	-	10/50/70/70	0/1/1/1
21	CLA	A	1105	-	3/3/20/25	15/37/135/135	-
21	CLA	b	1228	-	3/3/20/25	15/37/135/135	-
21	CLA	b	1206	12	3/3/20/25	18/37/135/135	-
21	CLA	B	1215	-	3/3/20/25	17/37/135/135	-
21	CLA	0	1502	28	3/3/20/25	12/37/135/135	-
25	LHG	A	5001	-	-	35/53/53/53	-
21	CLA	A	1102	21	3/3/20/25	18/37/135/135	-
21	CLA	1	1103	-	2/2/20/25	26/37/135/135	-
24	BCR	I	4018	-	-	10/29/63/63	0/2/2/2
23	SF4	a	3001	1,12	-	-	0/6/5/5
21	CLA	k	1402	-	3/3/16/25	13/18/116/135	-
21	CLA	1	1118	-	3/3/20/25	16/37/135/135	-
21	CLA	B	1202	-	2/2/20/25	19/37/135/135	-
21	CLA	L	1502	-	3/3/20/25	13/37/135/135	-
26	LMG	1	5002	-	-	20/45/65/70	0/1/1/1
25	LHG	b	5004	-	-	25/53/53/53	-
21	CLA	B	1222	38	3/3/18/25	8/25/123/135	-
24	BCR	B	4005	-	-	13/29/63/63	0/2/2/2
21	CLA	B	1230	-	3/3/20/25	20/37/135/135	-
21	CLA	b	1234	-	3/3/17/25	4/23/121/135	-
21	CLA	1	1129	-	3/3/17/25	7/19/117/135	-
24	BCR	2	4005	-	-	11/29/63/63	0/2/2/2
23	SF4	c	3003	13	-	-	0/6/5/5
24	BCR	0	4019	-	-	10/29/63/63	0/2/2/2
26	LMG	2	5005	-	-	17/50/70/70	0/1/1/1
21	CLA	B	1212	-	3/3/18/25	12/25/123/135	-
21	CLA	A	1122	-	3/3/19/25	13/31/129/135	-
25	LHG	a	5005	-	-	30/53/53/53	-
21	CLA	B	1238	38	3/3/20/25	8/37/135/135	-
24	BCR	a	4008	-	-	13/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
21	CLA	A	1121	-	3/3/20/25	19/37/135/135	-
21	CLA	B	1209	-	2/2/20/25	19/37/135/135	-
21	CLA	a	1111	-	3/3/20/25	19/37/135/135	-
21	CLA	1	1130	-	3/3/18/25	9/25/123/135	-
21	CLA	l	1501	10	3/3/20/25	21/37/135/135	-
21	CLA	a	1113	-	3/3/17/25	9/19/117/135	-
21	CLA	F	1301	38	3/3/20/25	15/37/135/135	-
21	CLA	B	1228	-	3/3/20/25	17/37/135/135	-
21	CLA	A	1106	1	3/3/20/25	19/37/135/135	-
21	CLA	A	1138	-	3/3/20/25	14/37/135/135	-
21	CLA	b	1239	-	3/3/20/25	12/37/135/135	-
21	CLA	a	1129	-	3/3/17/25	10/22/120/135	-
23	SF4	C	3002	3	-	-	0/6/5/5
21	CLA	A	1136	-	3/3/20/25	19/37/135/135	-
21	CLA	b	1021	-	3/3/20/25	22/37/135/135	-
24	BCR	K	4001	-	-	12/29/63/63	0/2/2/2
30	ECH	M	4021	-	-	8/29/66/66	0/2/2/2
21	CLA	1	1105	-	3/3/17/25	4/19/117/135	-
21	CLA	B	1210	-	2/2/20/25	17/37/135/135	-
24	BCR	9	4021	-	-	13/29/63/63	0/2/2/2
21	CLA	2	1207	-	2/2/18/25	14/27/125/135	-
30	ECH	b	4011	-	-	11/29/66/66	0/2/2/2
21	CLA	b	1226	-	3/3/20/25	15/37/135/135	-
21	CLA	b	1205	-	3/3/20/25	11/37/135/135	-
21	CLA	B	1234	-	1/1/20/25	11/37/135/135	-
21	CLA	2	1208	-	3/3/19/25	13/31/129/135	-
21	CLA	1	1123	-	1/1/20/25	15/37/135/135	-
35	LMT	1	6001	-	-	8/21/61/61	0/2/2/2
26	LMG	K	5009	-	-	17/50/70/70	0/1/1/1
21	CLA	a	1130	-	3/3/20/25	15/37/135/135	-
21	CLA	B	1223	-	3/3/20/25	10/37/135/135	-
21	CLA	a	1140	-	3/3/20/25	12/37/135/135	-
24	BCR	b	4014	-	-	10/29/63/63	0/2/2/2
21	CLA	2	1021	-	3/3/20/25	14/37/135/135	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
21	CLA	1	1135	-	1/1/17/25	12/22/120/135	-
21	CLA	b	1201	-	3/3/20/25	13/37/135/135	-
26	LMG	b	5002	-	-	12/50/70/70	0/1/1/1
21	CLA	a	1109	-	3/3/20/25	18/37/135/135	-
21	CLA	2	1204	-	3/3/20/25	15/37/135/135	-
21	CLA	A	1135	-	1/1/20/25	17/37/135/135	-
35	LMT	L	6001	-	-	9/21/61/61	0/2/2/2
21	CLA	A	1104	-	2/2/20/25	16/37/135/135	-
24	BCR	A	4002	-	-	7/29/63/63	0/2/2/2
24	BCR	A	4003	-	-	15/29/63/63	0/2/2/2
22	PQN	1	2001	-	-	3/23/43/43	0/2/2/2
21	CLA	2	1227	-	3/3/16/25	2/11/111/135	-
21	CLA	b	1217	-	3/3/17/25	10/21/119/135	-
21	CLA	a	1112	-	3/3/20/25	17/37/135/135	-
21	CLA	J	1303	-	3/3/20/25	22/37/135/135	-
21	CLA	1	1121	-	3/3/18/25	12/25/123/135	-
21	CLA	1	1133	-	3/3/20/25	18/37/135/135	-
21	CLA	2	1205	-	3/3/20/25	19/37/135/135	-
26	LMG	A	5008	-	-	24/50/70/70	0/1/1/1
21	CLA	a	1801	25	3/3/18/25	13/25/123/135	-
21	CLA	0	1501	20	3/3/20/25	16/37/135/135	-
21	CLA	1	1801	25	3/3/18/25	11/27/125/135	-
21	CLA	2	1219	-	2/2/17/25	9/23/121/135	-
21	CLA	a	1012	38	3/3/20/25	19/37/135/135	-
24	BCR	2	4010	-	-	12/29/63/63	0/2/2/2
31	SQD	B	5008	-	-	23/49/69/69	0/1/1/1
21	CLA	2	1217	-	3/3/17/25	12/22/120/135	-
34	ZEX	F	4016	-	1/1/12/27	7/29/67/67	0/2/2/2
24	BCR	1	4008	-	-	9/29/63/63	0/2/2/2
21	CLA	b	1236	-	3/3/20/25	13/37/135/135	-
25	LHG	1	5003	21	-	32/53/53/53	-
24	BCR	8	4001	-	-	10/29/63/63	0/2/2/2
21	CLA	A	1137	-	3/3/20/25	16/37/135/135	-
21	CLA	B	1201	-	3/3/20/25	15/37/135/135	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
21	CLA	A	1132	-	3/3/20/25	13/37/135/135	-
21	CLA	B	1229	-	3/3/20/25	16/37/135/135	-
21	CLA	b	1218	-	3/3/20/25	18/37/135/135	-
21	CLA	a	1104	-	3/3/20/25	25/37/135/135	-
21	CLA	b	1232	-	3/3/20/25	18/37/135/135	-
30	ECH	B	4006	-	-	7/29/66/66	0/2/2/2
21	CLA	b	1231	38	3/3/20/25	22/37/135/135	-
21	CLA	A	1129	-	2/2/18/25	11/29/127/135	-
24	BCR	j	4013	-	-	9/29/63/63	0/2/2/2
25	LHG	a	5003	21	-	39/53/53/53	-
22	PQN	a	2001	-	-	7/23/43/43	0/2/2/2
21	CLA	A	1111	-	3/3/20/25	16/37/135/135	-
21	CLA	b	1215	-	3/3/20/25	17/37/135/135	-
21	CLA	L	1501	10	3/3/20/25	17/37/135/135	-
21	CLA	A	1134	1	3/3/20/25	19/37/135/135	-
21	CLA	1	1110	-	3/3/17/25	8/19/117/135	-
21	CLA	0	1503	38	3/3/20/25	20/37/135/135	-
24	BCR	B	4017	-	-	9/29/63/63	0/2/2/2
21	CLA	f	1302	-	3/3/20/25	23/37/135/135	-
21	CLA	2	1202	-	2/2/20/25	21/37/135/135	-
21	CLA	b	1204	-	3/3/20/25	12/37/135/135	-
21	CLA	A	1130	-	3/3/19/25	6/31/129/135	-
31	SQD	b	5006	-	-	27/49/69/69	0/1/1/1
21	CLA	6	1302	6	3/3/15/25	5/11/109/135	-
21	CLA	A	1107	1	3/3/20/25	19/37/135/135	-
21	CLA	b	1237	38	3/3/20/25	14/37/135/135	-
21	CLA	2	1215	-	3/3/19/25	16/31/129/135	-
21	CLA	B	1235	-	3/3/20/25	14/37/135/135	-
21	CLA	A	1133	-	3/3/20/25	11/37/135/135	-
21	CLA	a	1139	38	3/3/20/25	13/37/135/135	-
22	PQN	2	2002	-	-	8/23/43/43	0/2/2/2
21	CLA	B	1221	-	3/3/20/25	12/37/135/135	-
21	CLA	1	1126	-	3/3/20/25	20/37/135/135	-
21	CLA	a	1124	-	3/3/18/25	9/25/123/135	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	BCR	b	4005	-	-	12/29/63/63	0/2/2/2
21	CLA	2	1023	-	3/3/20/25	16/37/135/135	-
21	CLA	A	1115	-	3/3/20/25	7/37/135/135	-
21	CLA	2	1222	-	3/3/17/25	6/19/117/135	-
21	CLA	B	1218	-	3/3/20/25	21/37/135/135	-
24	BCR	a	4003	-	-	12/29/63/63	0/2/2/2
21	CLA	a	1117	-	3/3/20/25	20/37/135/135	-
21	CLA	7	1303	-	3/3/15/25	3/8/106/135	-
26	LMG	b	5007	-	-	18/50/70/70	0/1/1/1
25	LHG	A	5003	21	-	27/53/53/53	-
22	PQN	A	2001	-	-	10/23/43/43	0/2/2/2
36	EQ3	I	4020	-	-	8/29/68/68	0/2/2/2
21	CLA	b	1207	-	2/2/20/25	13/37/135/135	-
21	CLA	1	1109	16	3/3/20/25	17/37/135/135	-
21	CLA	2	1212	-	3/3/15/25	5/8/106/135	-
21	CLA	2	1218	-	3/3/20/25	18/37/135/135	-
21	CLA	B	1021	-	3/3/20/25	10/37/135/135	-
21	CLA	B	1227	-	2/2/18/25	13/25/123/135	-
21	CLA	A	1131	-	3/3/20/25	17/37/135/135	-
24	BCR	a	4019	-	-	9/29/63/63	0/2/2/2
30	ECH	b	4006	-	-	7/29/66/66	0/2/2/2
34	ZEX	J	4015	-	-	3/29/67/67	0/2/2/2
31	SQD	f	5001	-	-	19/49/69/69	0/1/1/1
21	CLA	A	1117	-	3/3/20/25	16/37/135/135	-
24	BCR	B	4018	-	-	13/29/63/63	0/2/2/2
21	CLA	A	1128	-	3/3/20/25	16/37/135/135	-
25	LHG	1	5007	-	-	30/53/53/53	-
21	CLA	b	1238	38	3/3/20/25	7/37/135/135	-
24	BCR	l	4019	-	-	7/29/63/63	0/2/2/2
21	CLA	l	1502	-	3/3/20/25	15/37/135/135	-
21	CLA	B	1022	38	3/3/20/25	6/37/135/135	-
23	SF4	1	3001	2,16	-	-	0/6/5/5
21	CLA	2	1240	-	2/2/15/25	4/8/106/135	-
21	CLA	K	1402	-	1/1/20/25	17/37/135/135	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
23	SF4	3	3002	-	-	-	0/6/5/5
24	BCR	2	4017	-	-	12/29/63/63	0/2/2/2
21	CLA	a	1110	-	3/3/18/25	17/30/128/135	-
28	45D	h	4020	21	-	15/29/69/69	0/2/2/2
24	BCR	2	4014	-	-	7/29/63/63	0/2/2/2
24	BCR	1	4012	-	-	14/29/63/63	0/2/2/2
21	CLA	b	1221	38	3/3/20/25	13/37/135/135	-
31	SQD	L	5002	-	-	18/49/69/69	0/1/1/1
21	CLA	b	1210	-	2/2/20/25	20/37/135/135	-
26	LMG	a	5002	-	-	18/45/65/70	0/1/1/1
24	BCR	L	4019	-	-	6/29/63/63	0/2/2/2
21	CLA	B	1203	-	2/2/20/25	15/37/135/135	-
30	ECH	2	4006	-	-	11/29/66/66	0/2/2/2
21	CLA	A	1119	38	3/3/20/25	18/37/135/135	-
21	CLA	1	1140	-	3/3/20/25	14/37/135/135	-
21	CLA	1	1114	-	3/3/16/25	5/11/111/135	-
25	LHG	B	5006	-	-	34/53/53/53	-
35	LMT	l	6001	-	-	6/21/61/61	0/2/2/2
21	CLA	b	1209	-	2/2/20/25	18/37/135/135	-
21	CLA	A	1139	38	3/3/20/25	15/37/135/135	-
24	BCR	a	4007	-	-	9/29/63/63	0/2/2/2
24	BCR	b	4004	-	-	13/29/63/63	0/2/2/2
21	CLA	a	1118	-	3/3/20/25	19/37/135/135	-
21	CLA	1	1102	-	3/3/18/25	11/25/123/135	-
24	BCR	7	4013	-	-	12/29/63/63	0/2/2/2
21	CLA	A	1125	-	2/2/20/25	21/37/135/135	-
21	CLA	6	1301	38	3/3/16/25	6/16/114/135	-
21	CLA	B	1232	-	3/3/17/25	4/19/117/135	-
24	BCR	A	4019	-	-	11/29/63/63	0/2/2/2
21	CLA	2	1228	-	3/3/16/25	7/11/111/135	-
23	SF4	c	3002	-	-	-	0/6/5/5
21	CLA	a	1136	-	3/3/20/25	17/37/135/135	-
25	LHG	A	5006	-	-	29/53/53/53	-
21	CLA	A	1140	-	3/3/20/25	17/37/135/135	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
26	LMG	a	5004	-	-	15/50/70/70	0/1/1/1
21	CLA	1	1136	-	3/3/20/25	18/37/135/135	-
21	CLA	2	1209	-	1/1/16/25	6/11/111/135	-
21	CLA	2	1203	-	3/3/20/25	20/37/135/135	-
21	CLA	8	1401	-	3/3/16/25	4/11/111/135	-
21	CLA	A	1108	-	3/3/17/25	11/23/121/135	-
21	CLA	2	1239	-	3/3/20/25	17/37/135/135	-
21	CLA	1	1108	-	3/3/16/25	10/15/113/135	-
21	CLA	A	1013	-	3/3/20/25	15/37/135/135	-
21	CLA	1	1138	-	3/3/19/25	13/31/129/135	-
21	CLA	b	1223	-	2/2/20/25	13/37/135/135	-
30	ECH	m	4021	-	-	7/29/66/66	0/2/2/2
25	LHG	0	5002	-	-	24/53/53/53	-
24	BCR	b	4018	-	-	10/29/63/63	0/2/2/2
21	CLA	2	1221	-	3/3/20/25	15/37/135/135	-
21	CLA	A	1120	-	3/3/20/25	17/37/135/135	-
21	CLA	B	1205	-	3/3/20/25	16/37/135/135	-
24	BCR	L	4022	-	-	10/29/63/63	0/2/2/2
21	CLA	1	1012	38	2/2/20/25	21/37/135/135	-
21	CLA	A	1011	-	3/3/20/25	11/37/135/135	-
21	CLA	B	1225	-	3/3/20/25	13/37/135/135	-
25	LHG	A	5005	-	-	36/53/53/53	-
21	CLA	b	1230	-	3/3/20/25	21/37/135/135	-
21	CLA	a	1137	-	3/3/17/25	7/19/117/135	-
26	LMG	A	5002	-	-	21/45/65/70	0/1/1/1
26	LMG	B	5005	-	-	11/50/70/70	0/1/1/1
21	CLA	l	1503	-	3/3/20/25	23/37/135/135	-
25	LHG	l	5004	-	-	28/53/53/53	-
30	ECH	i	4020	-	-	10/29/66/66	0/2/2/2
25	LHG	1	5005	-	-	36/53/53/53	-
21	CLA	b	1219	-	3/3/19/25	18/31/129/135	-
24	BCR	A	4007	-	-	9/29/63/63	0/2/2/2
24	BCR	a	4002	-	-	15/29/63/63	0/2/2/2
21	CLA	a	1134	1	3/3/16/25	10/18/116/135	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
21	CLA	1	1120	-	3/3/20/25	19/37/135/135	-
25	LHG	l	5003	-	-	33/53/53/53	-
21	CLA	1	1125	-	3/3/20/25	15/37/135/135	-
25	LHG	a	5001	-	-	27/53/53/53	-
21	CLA	A	1124	38	3/3/20/25	10/37/135/135	-
25	LHG	0	5004	-	-	32/53/53/53	-
21	CLA	2	1224	-	3/3/18/25	17/25/123/135	-
35	LMT	0	6001	-	-	14/21/61/61	0/2/2/2
21	CLA	A	1109	21	3/3/20/25	15/37/135/135	-
21	CLA	J	1302	8	3/3/20/25	13/37/135/135	-
21	CLA	a	1135	-	2/2/20/25	23/37/135/135	-
21	CLA	a	1138	-	3/3/20/25	13/37/135/135	-
26	LMG	2	5002	-	-	11/50/70/70	0/1/1/1
21	CLA	b	1213	-	3/3/20/25	17/37/135/135	-
24	BCR	1	4019	-	-	14/29/63/63	0/2/2/2
21	CLA	1	1117	-	3/3/20/25	16/37/135/135	-
24	BCR	a	4012	-	-	7/29/63/63	0/2/2/2
21	CLA	a	1114	-	3/3/17/25	8/22/120/135	-
21	CLA	B	1206	2	3/3/20/25	17/37/135/135	-
31	SQD	L	5001	-	-	21/46/66/69	0/1/1/1
21	CLA	A	1127	-	3/3/20/25	17/37/135/135	-
24	BCR	i	4018	-	-	12/29/63/63	0/2/2/2
21	CLA	2	1232	-	2/2/16/25	5/11/111/135	-
21	CLA	1	1128	-	3/3/20/25	18/37/135/135	-
21	CLA	a	1126	-	3/3/20/25	21/37/135/135	-
31	SQD	0	5005	-	-	27/49/69/69	0/1/1/1
24	BCR	B	4004	-	-	15/29/63/63	0/2/2/2
21	CLA	A	1118	-	3/3/20/25	17/37/135/135	-
21	CLA	a	1108	-	3/3/18/25	13/28/126/135	-
22	PQN	b	2002	-	-	8/23/43/43	0/2/2/2
21	CLA	a	1125	-	3/3/20/25	11/37/135/135	-
21	CLA	a	1120	-	2/2/18/25	10/25/123/135	-
24	BCR	2	4004	-	-	13/29/63/63	0/2/2/2
21	CLA	a	1119	-	3/3/20/25	17/37/135/135	-

The worst 5 of 2502 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
34	F	4016	ZEX	C38-C24	37.43	2.55	1.53
34	J	4015	ZEX	C38-C24	37.01	2.54	1.53
34	j	4015	ZEX	C38-C24	36.94	2.54	1.53
34	7	4015	ZEX	C38-C24	36.93	2.54	1.53
28	h	4020	45D	C08-C16	13.47	1.54	1.35

The worst 5 of 3060 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	F	4016	ZEX	C38-C24-C25	-50.09	31.10	110.87
34	J	4015	ZEX	C38-C24-C25	-49.79	31.58	110.87
34	j	4015	ZEX	C38-C24-C25	-49.78	31.59	110.87
34	7	4015	ZEX	C38-C24-C25	-49.71	31.71	110.87
24	a	4019	BCR	C16-C15-C14	16.68	157.64	123.47

5 of 799 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
21	A	1012	CLA	NA
21	A	1012	CLA	ND
21	2	1220	CLA	NC
21	2	1220	CLA	ND
21	2	1220	CLA	NA

5 of 6201 torsion outliers are listed below:

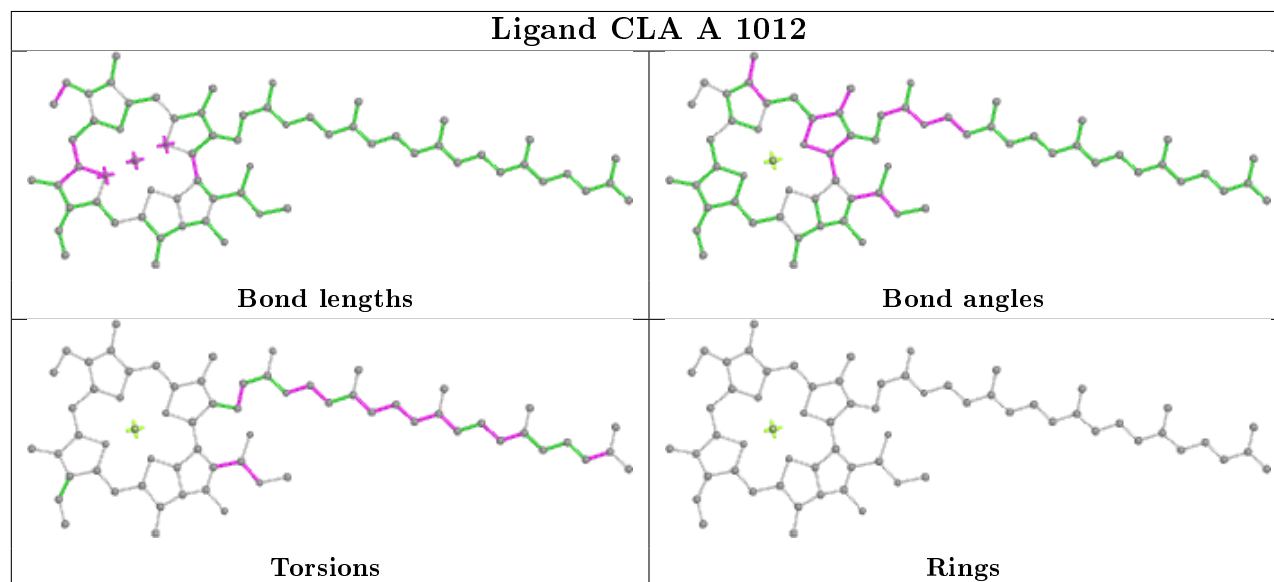
Mol	Chain	Res	Type	Atoms
21	A	1012	CLA	CHA-CBD-CGD-O1D
21	A	1012	CLA	CHA-CBD-CGD-O2D
21	A	1012	CLA	CAD-CBD-CGD-O1D
21	A	1012	CLA	CAD-CBD-CGD-O2D
21	A	1012	CLA	C2-C3-C5-C6

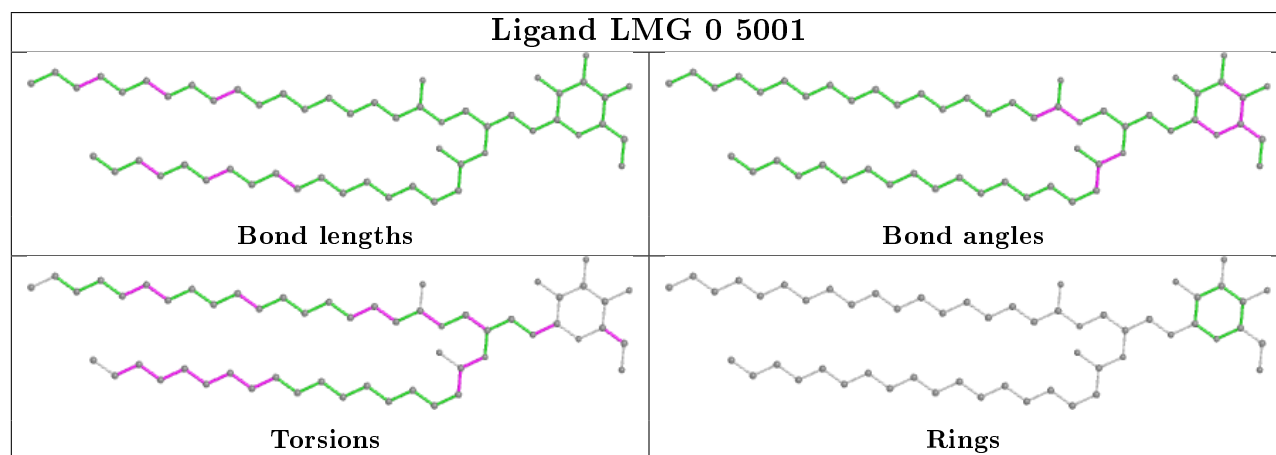
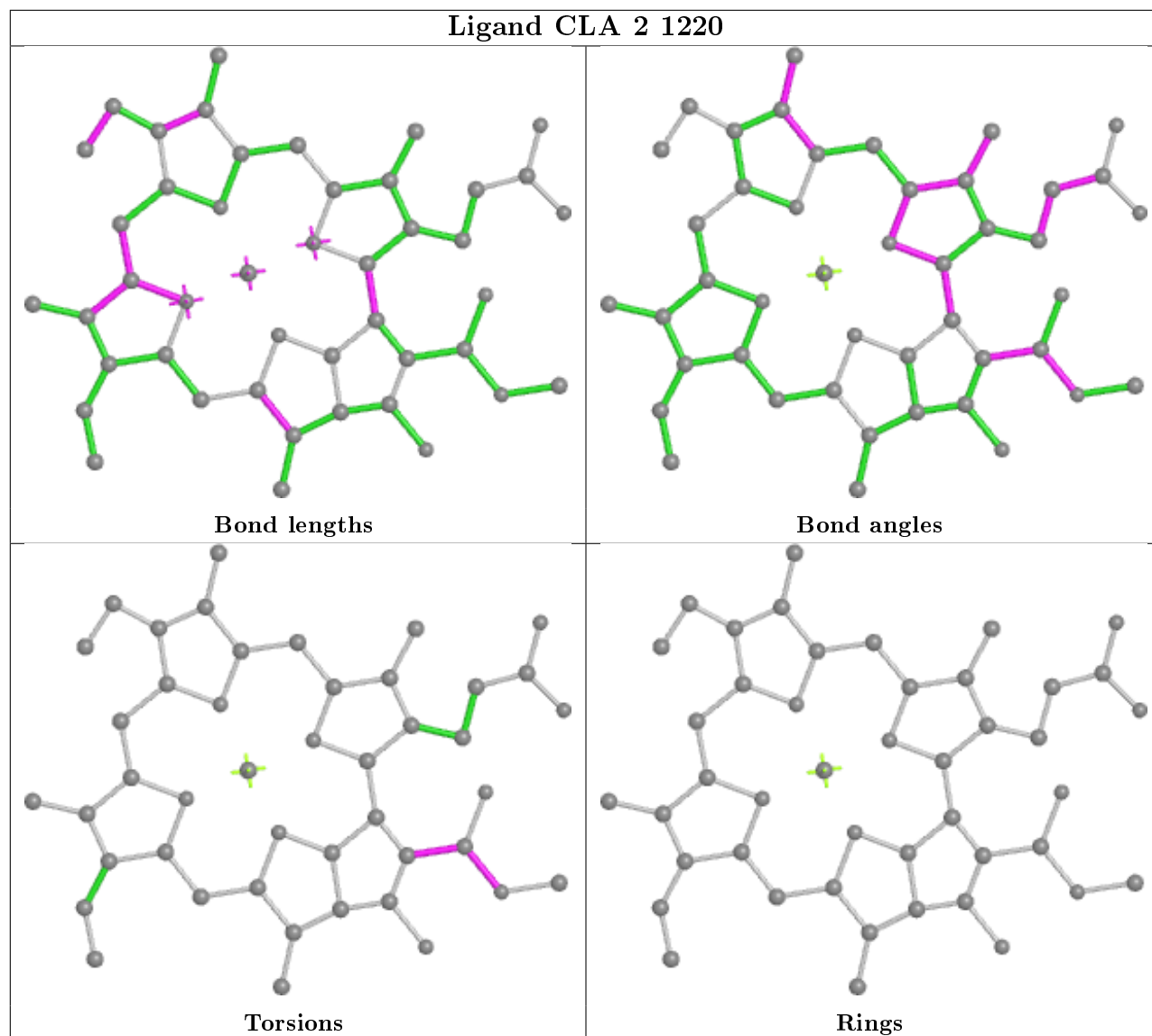
There are no ring outliers.

No monomer is involved in short contacts.

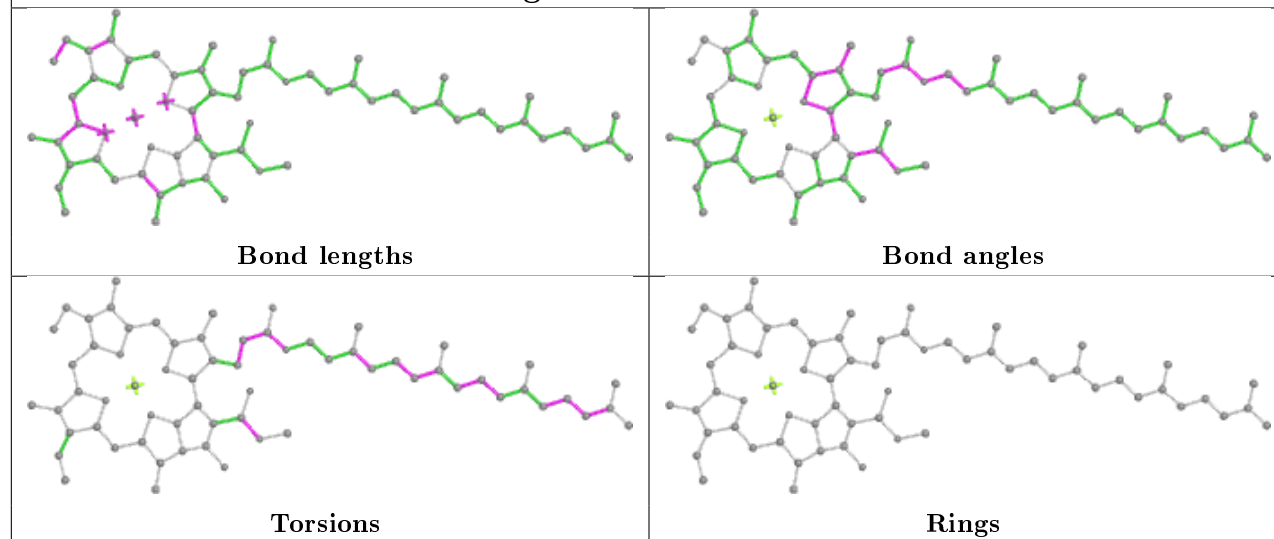
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier.

Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

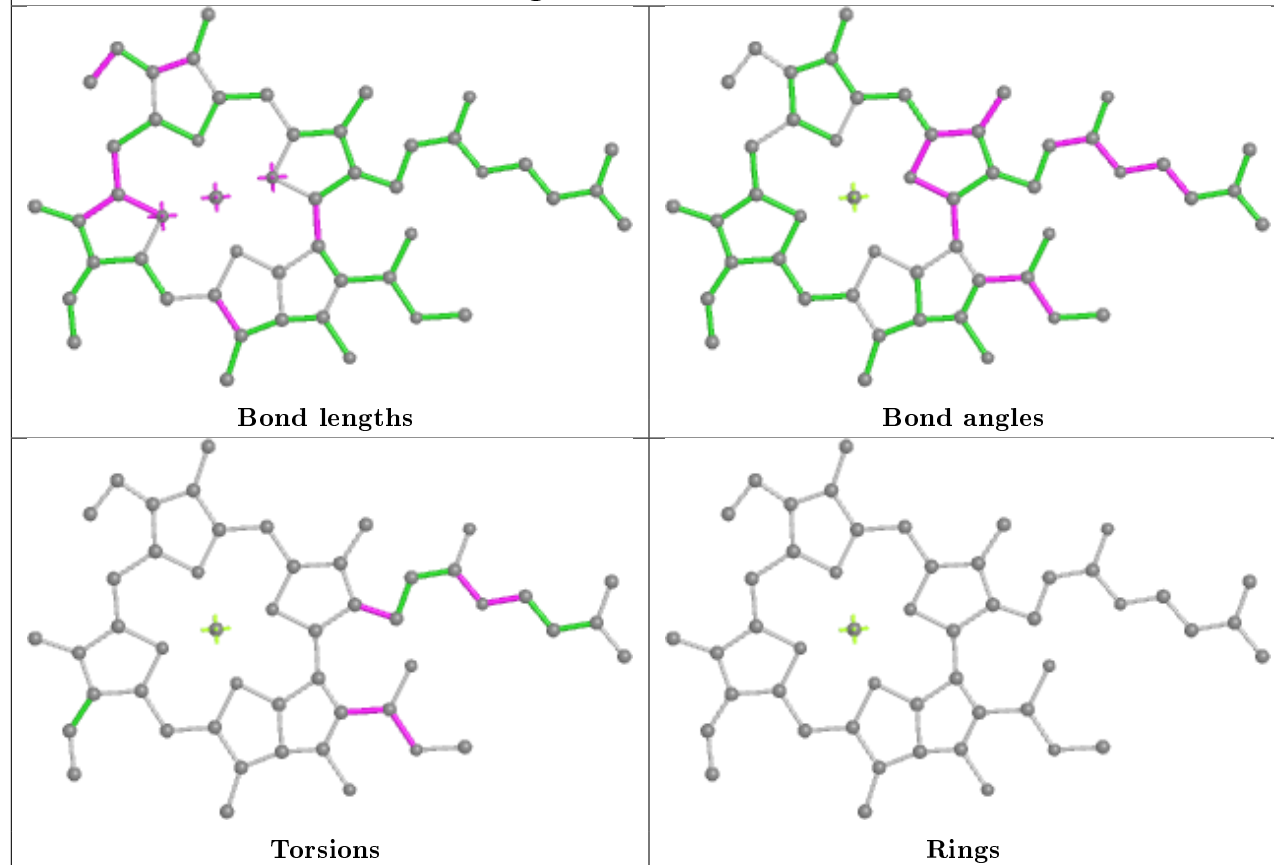


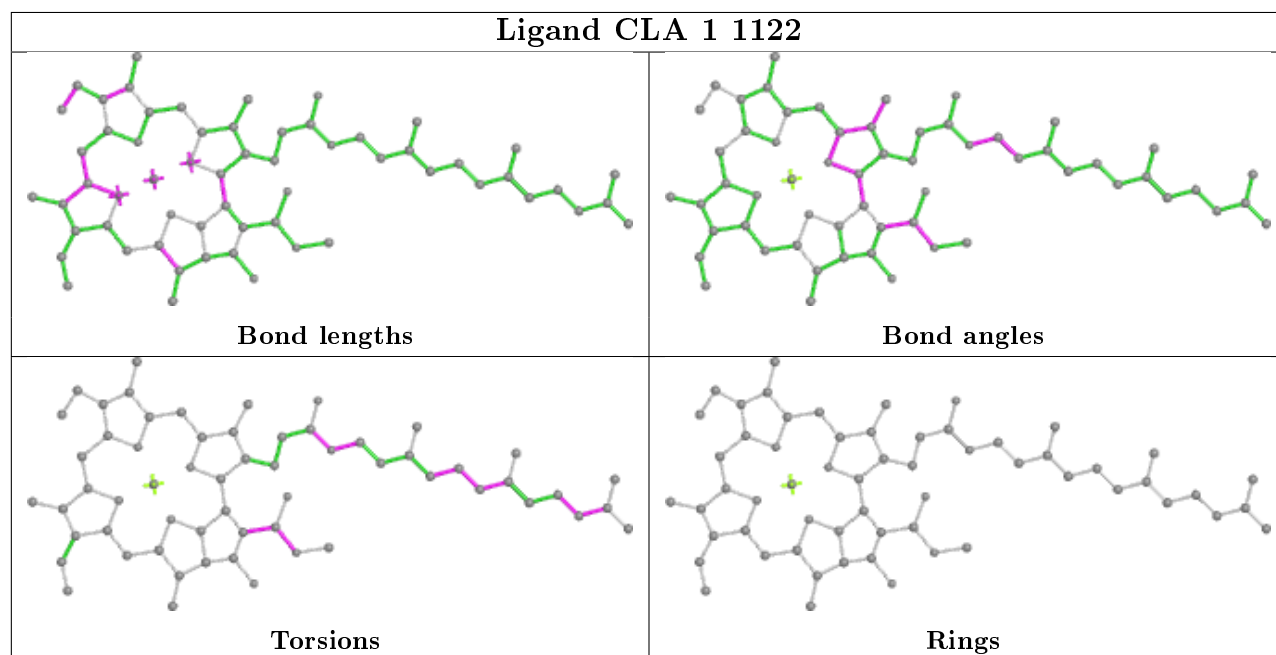
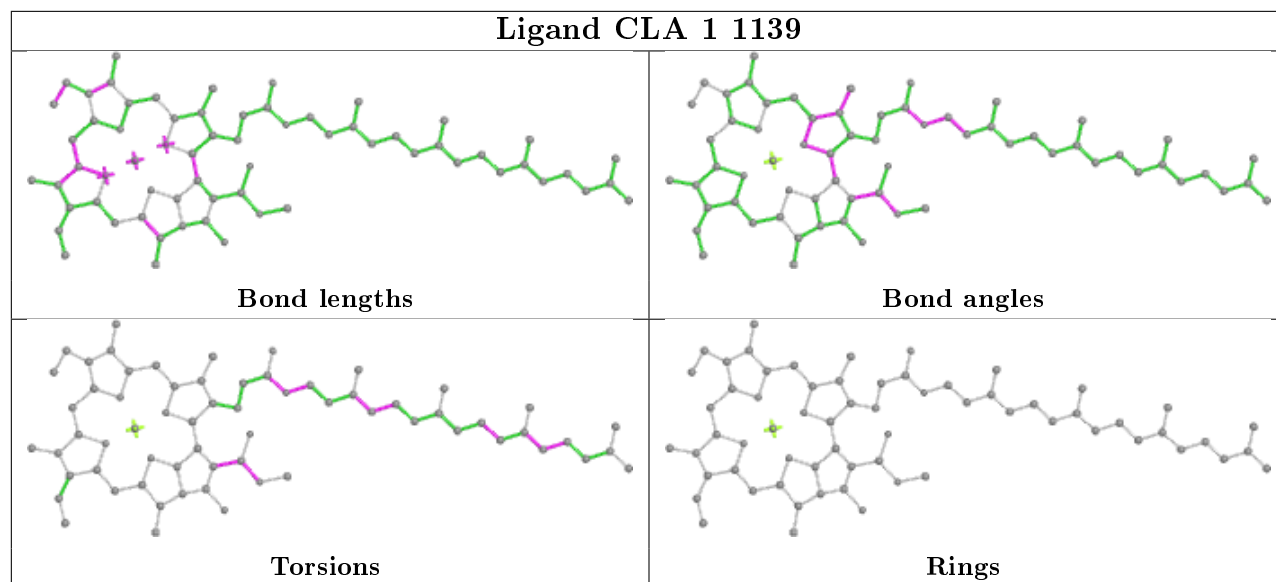


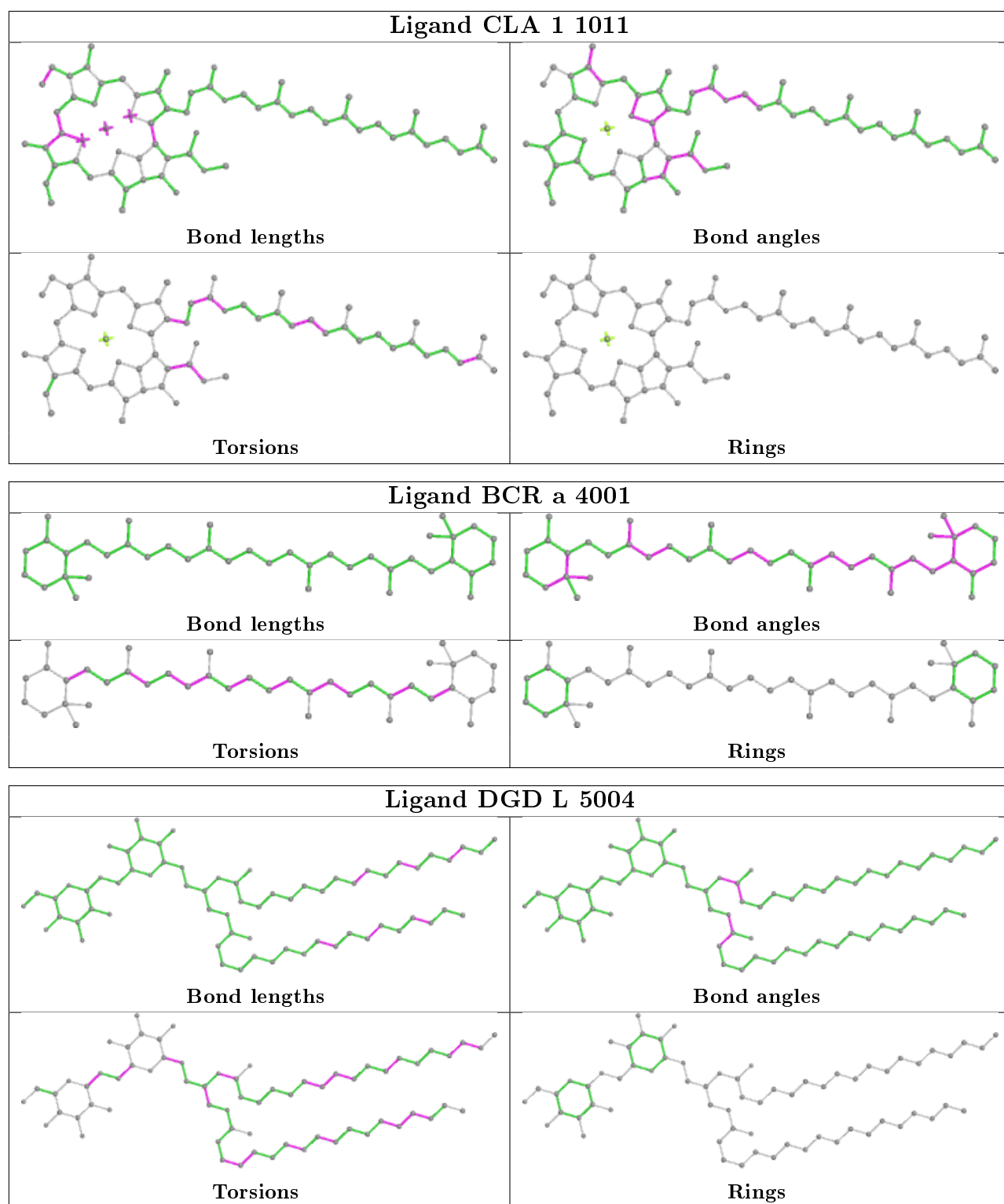
Ligand CLA B 1214

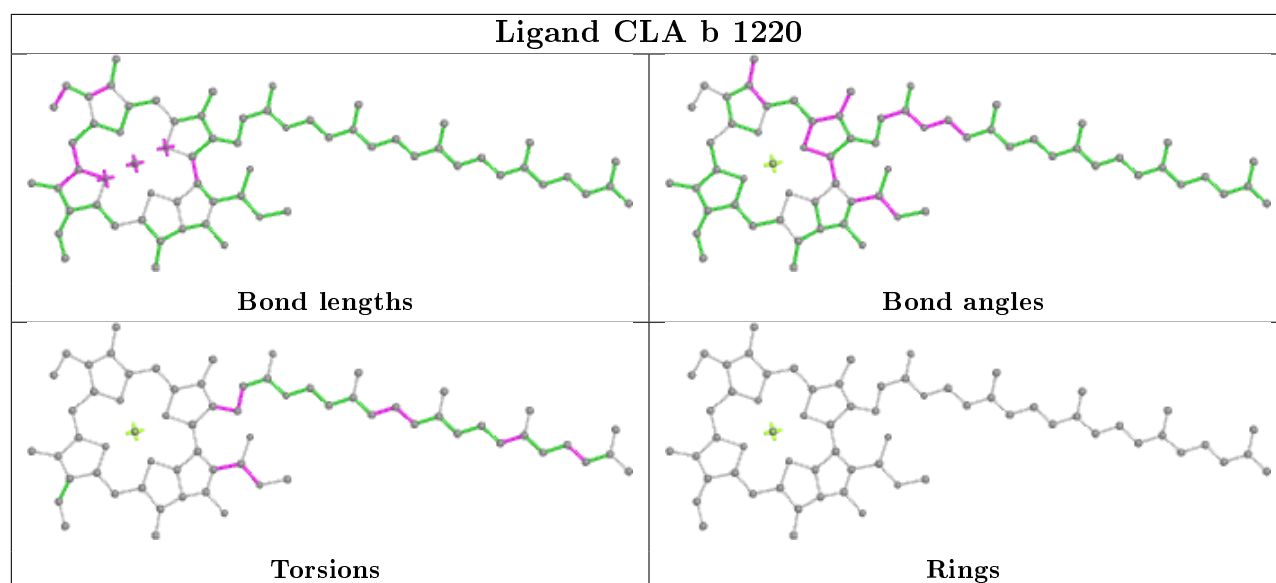
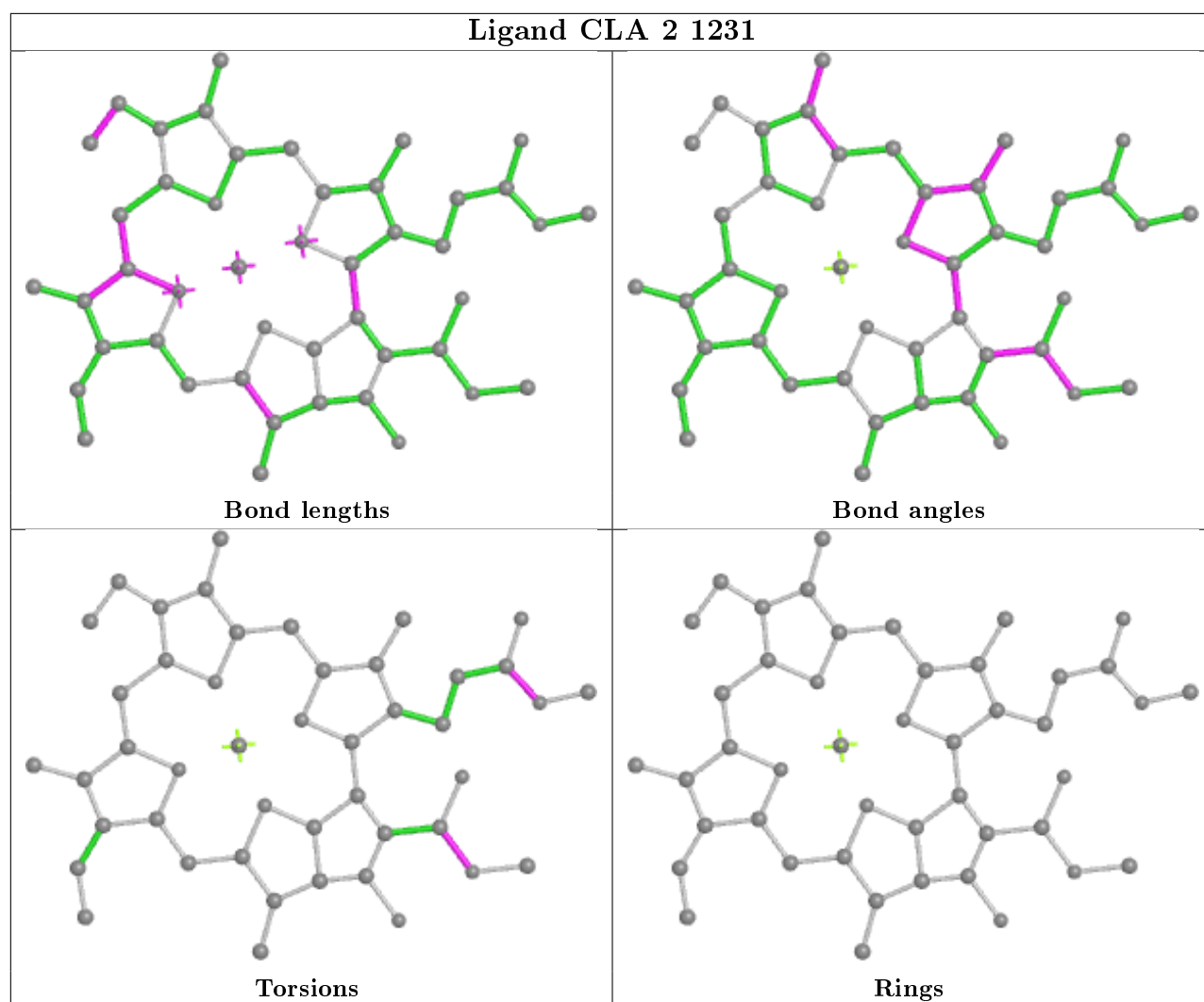


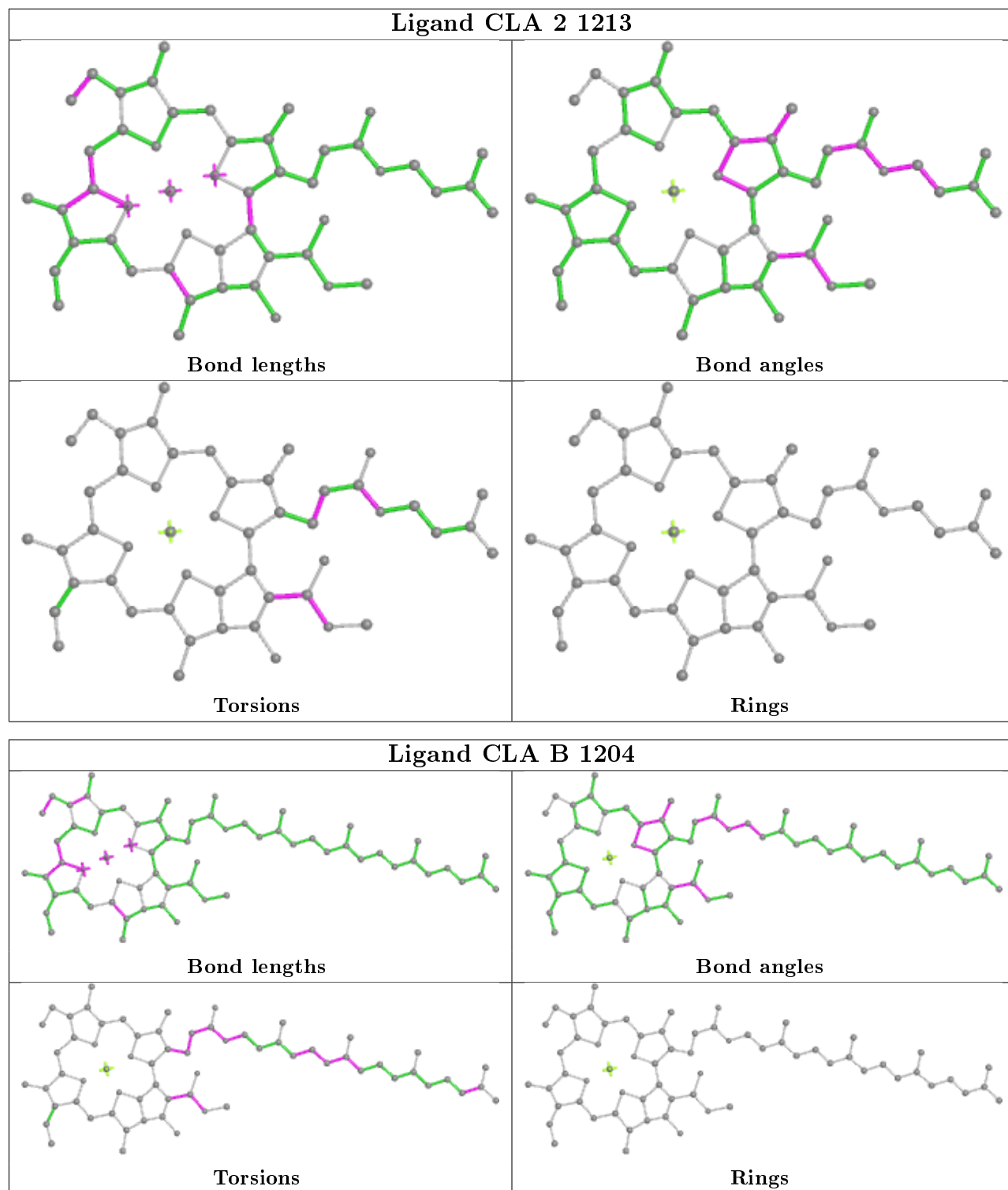
Ligand CLA 1 1112

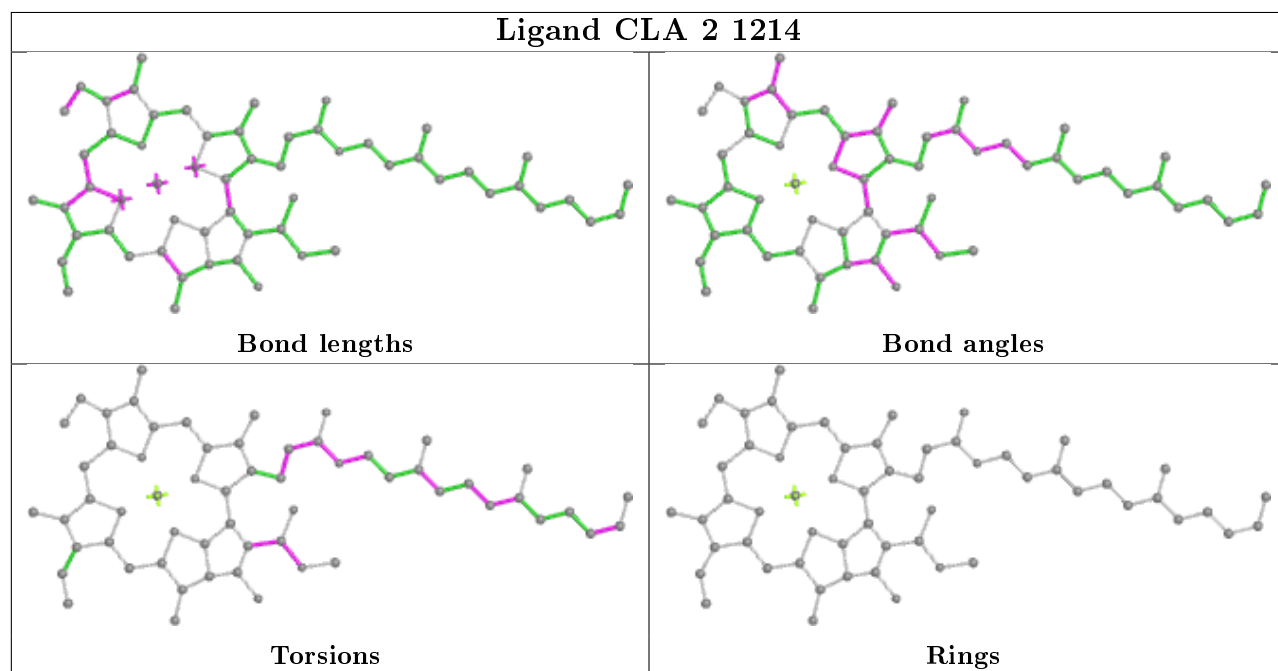
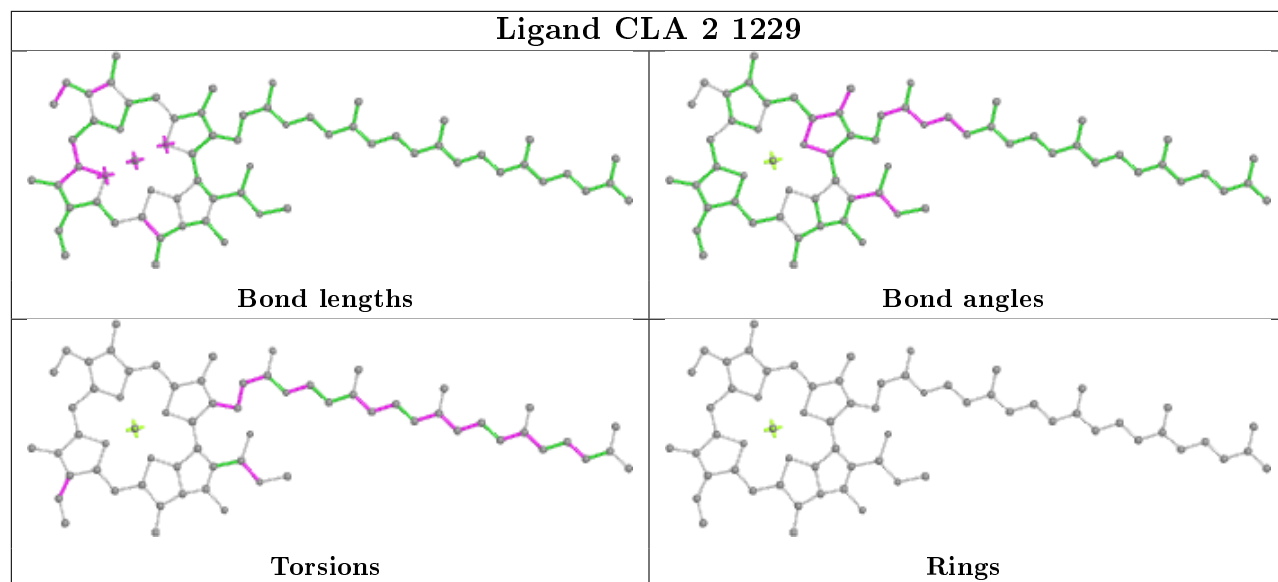


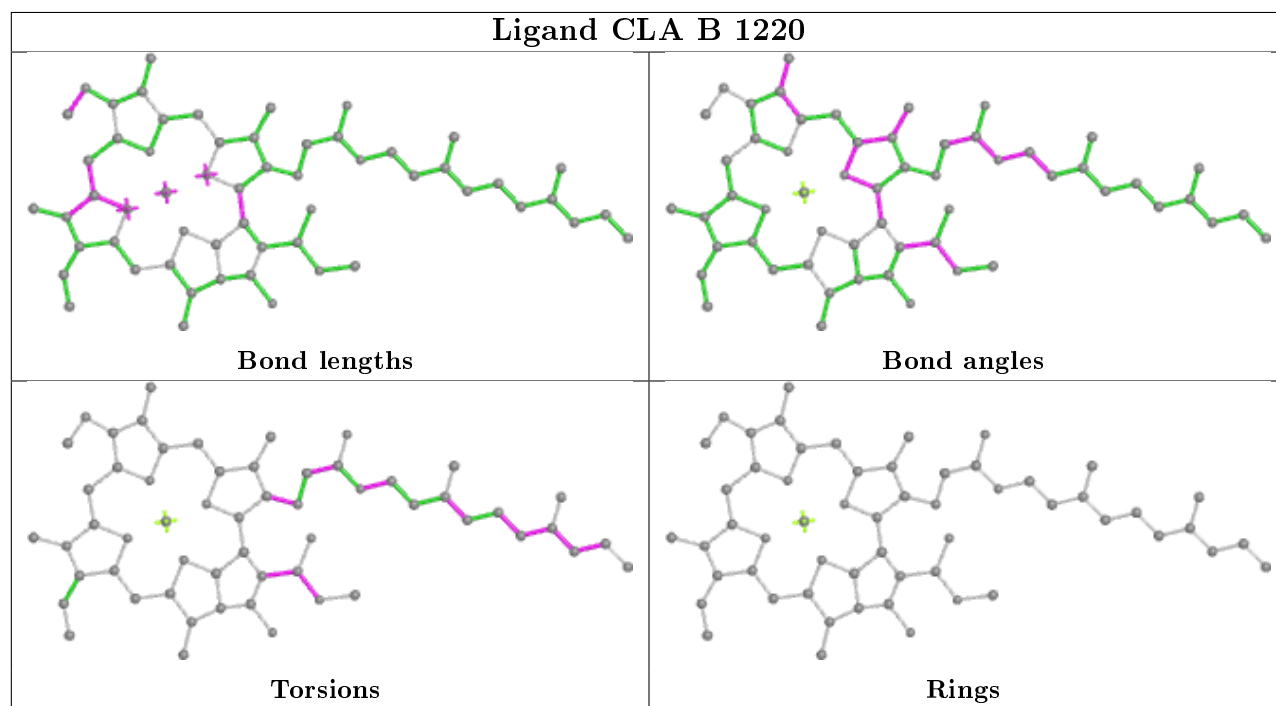
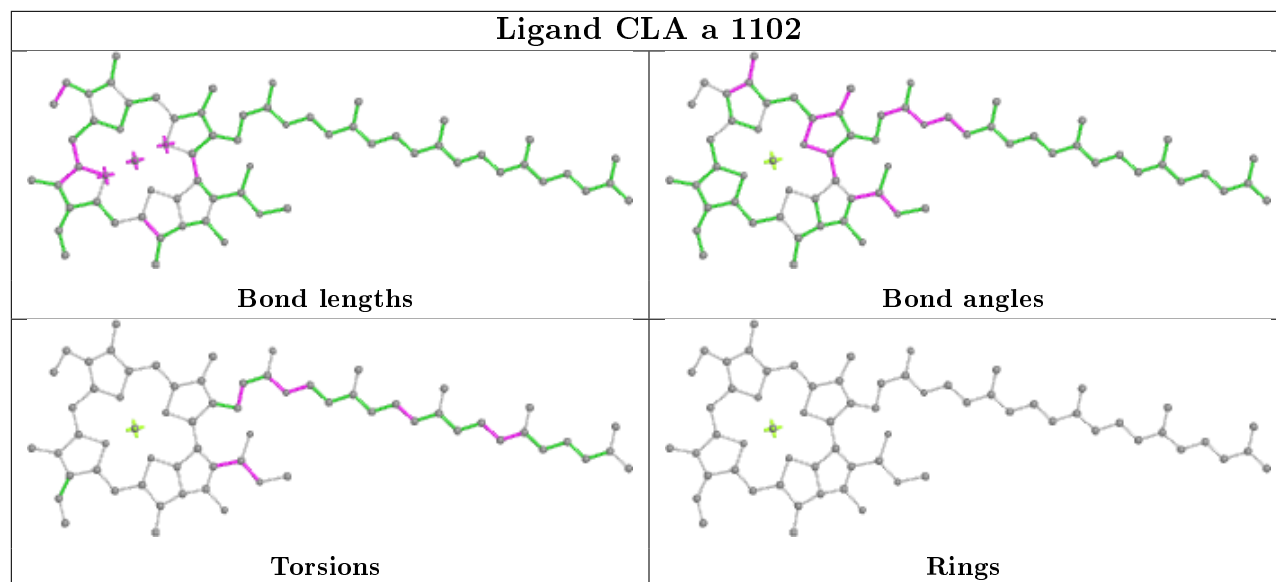


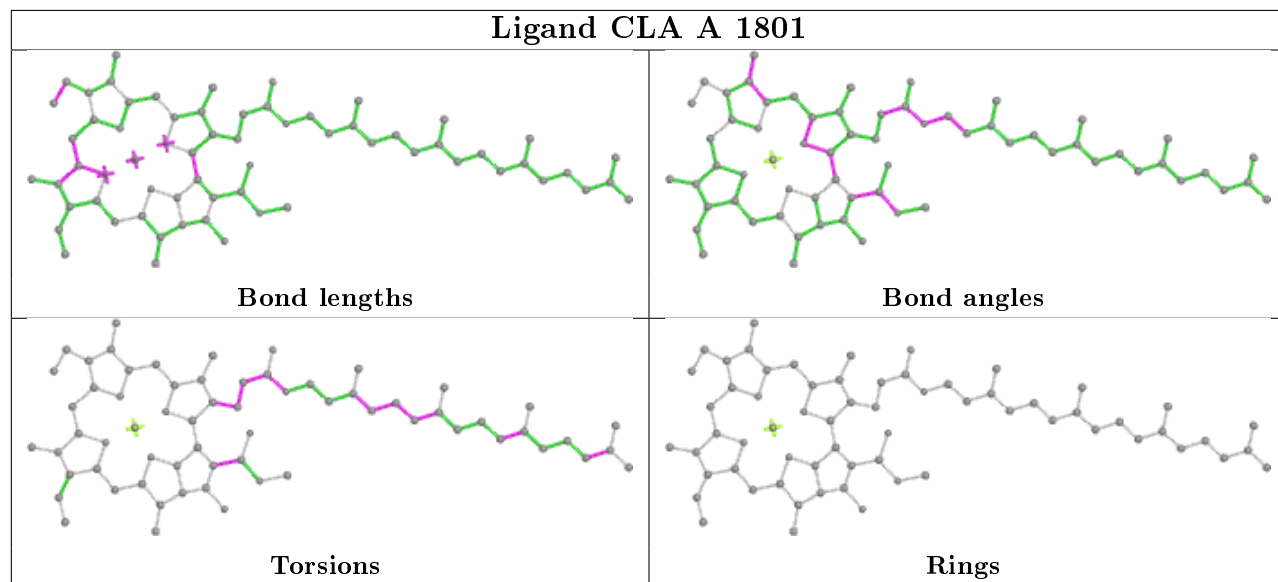
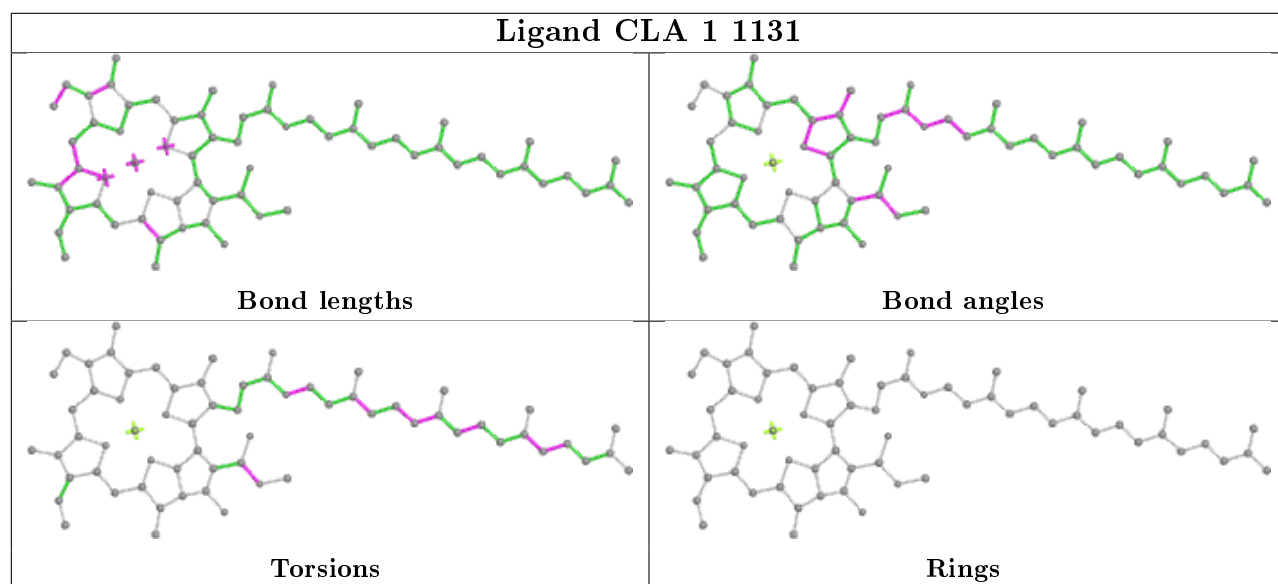
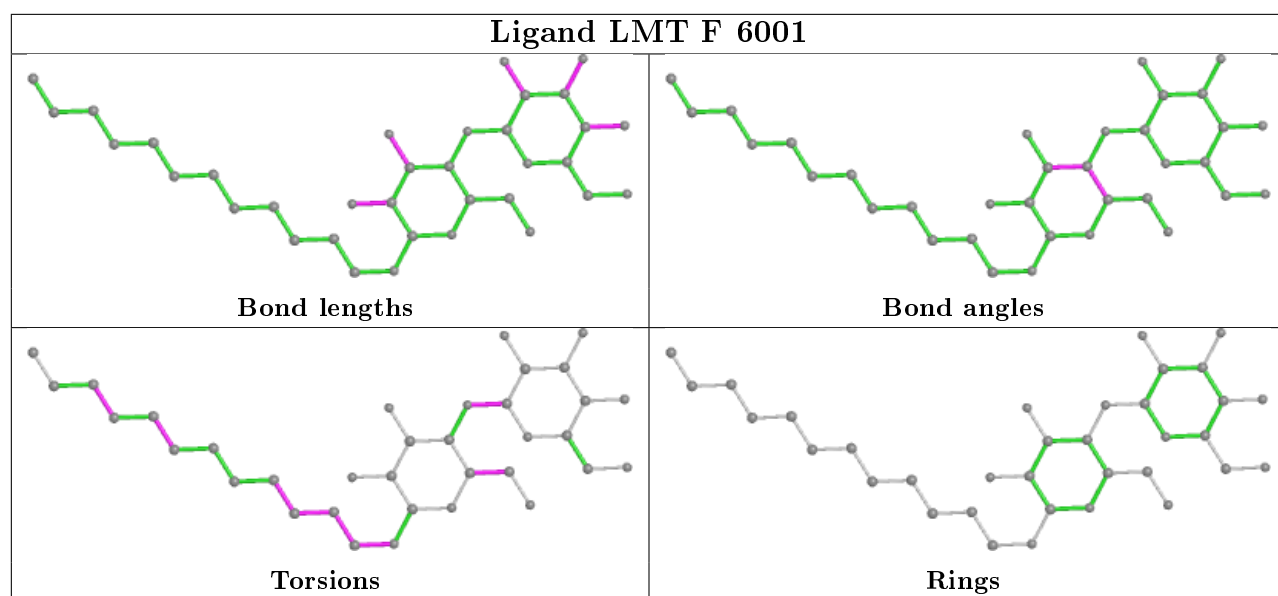


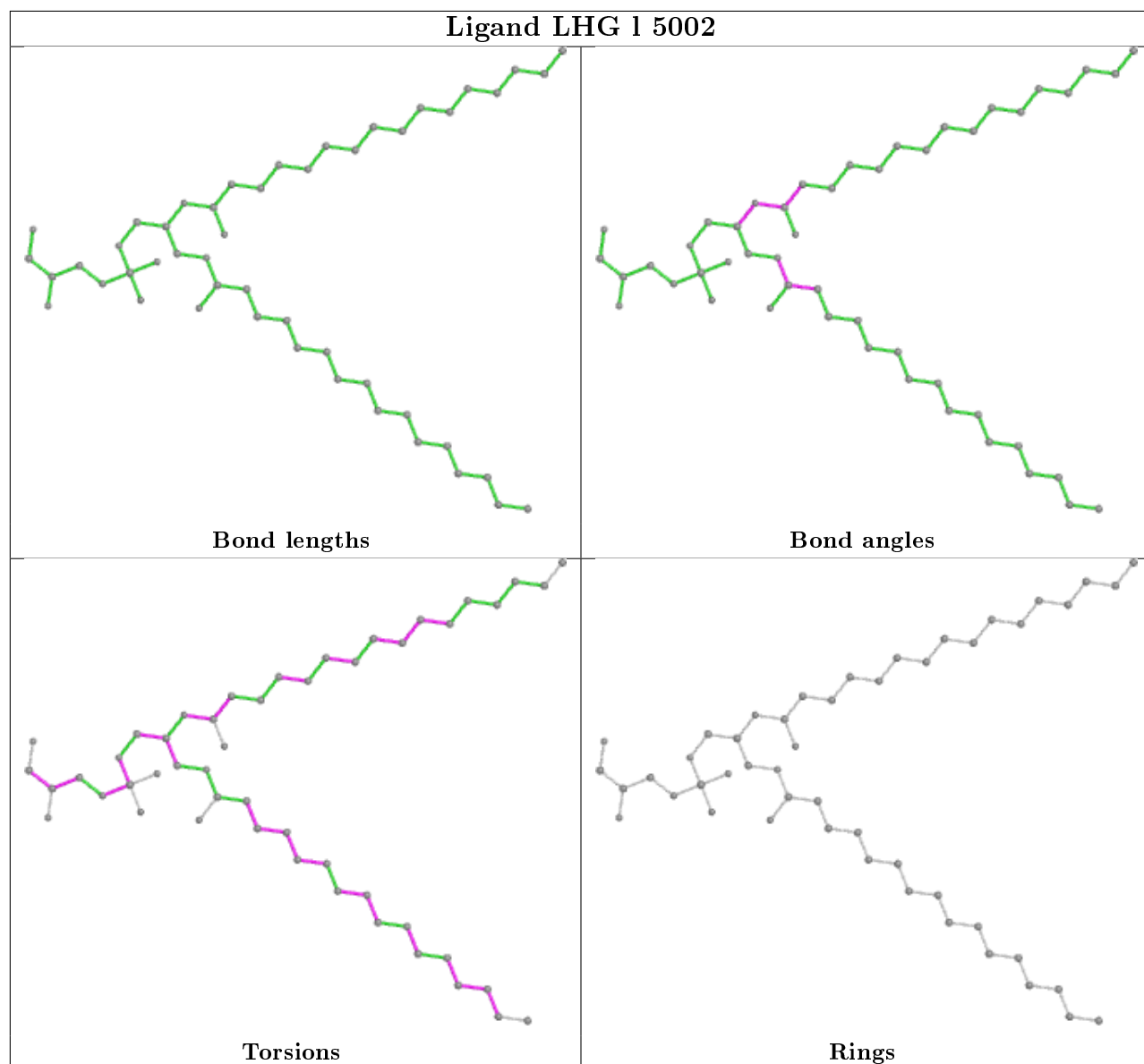
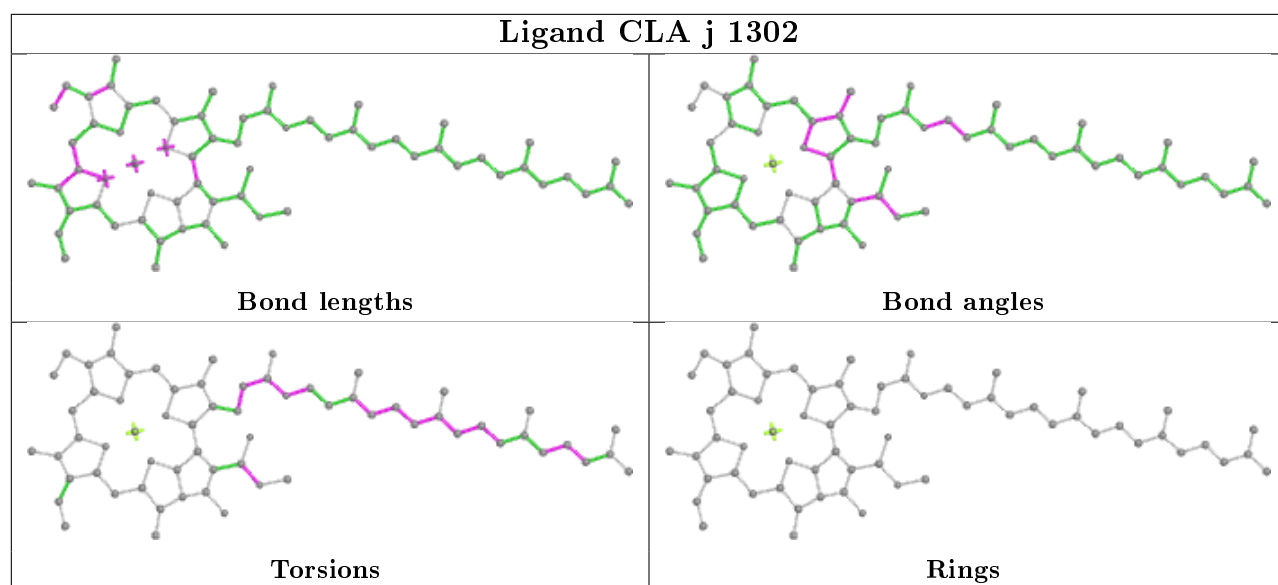


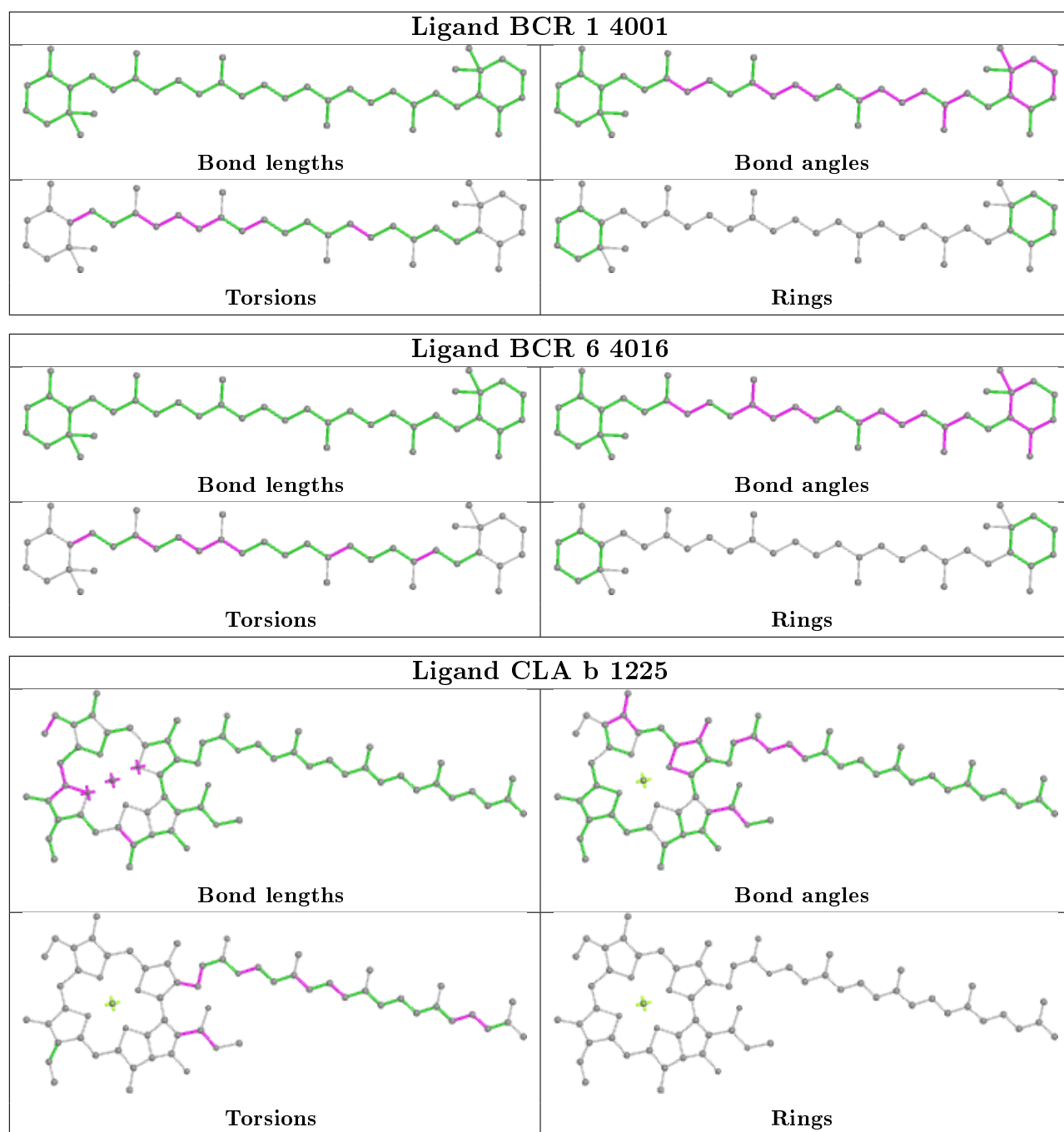


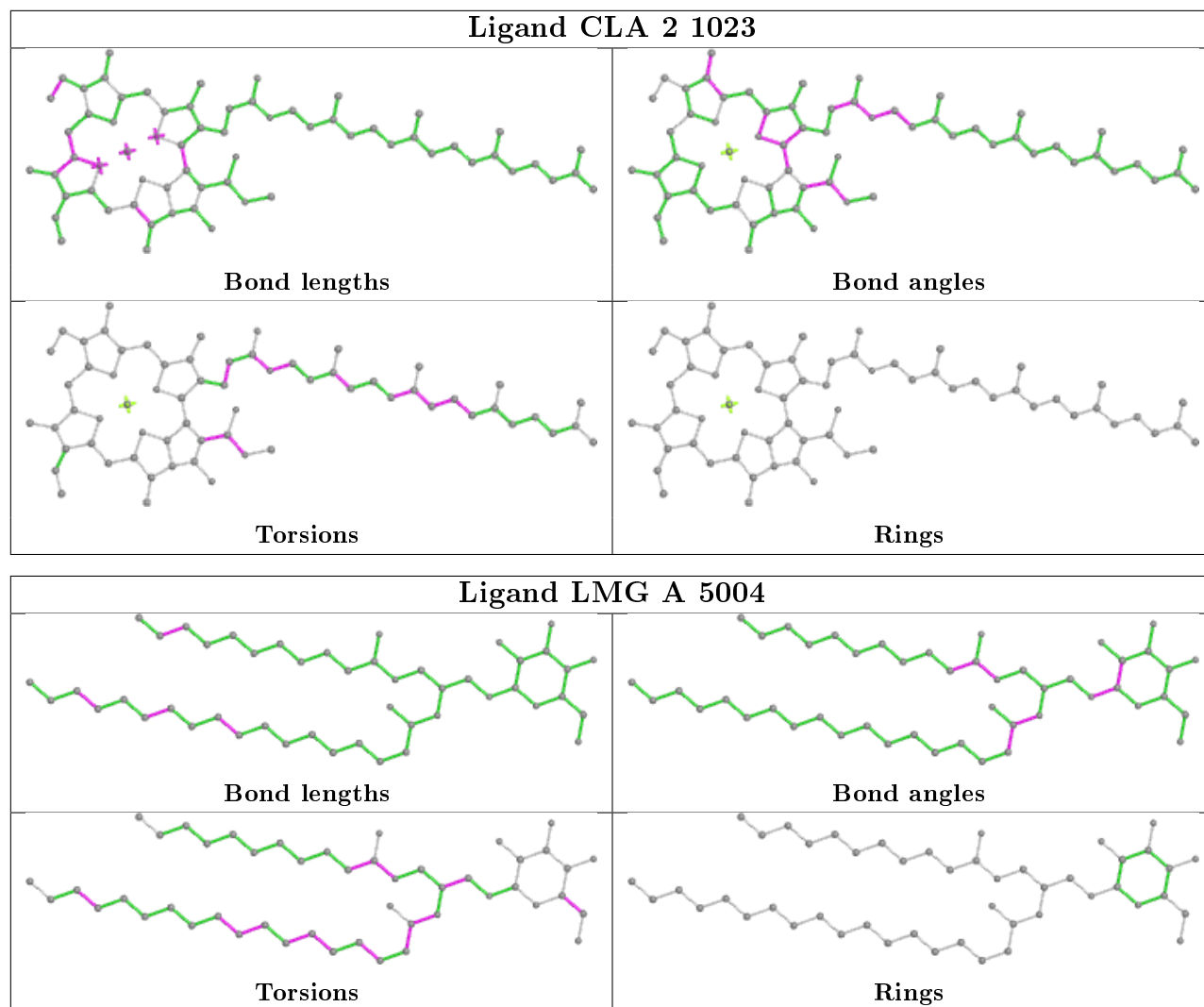


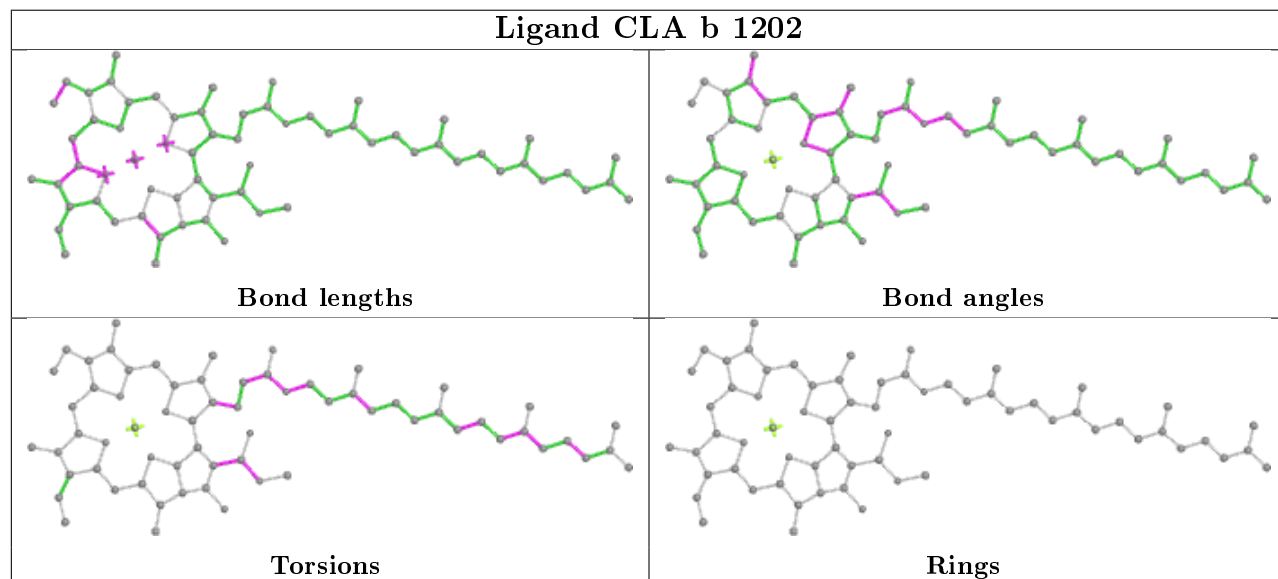
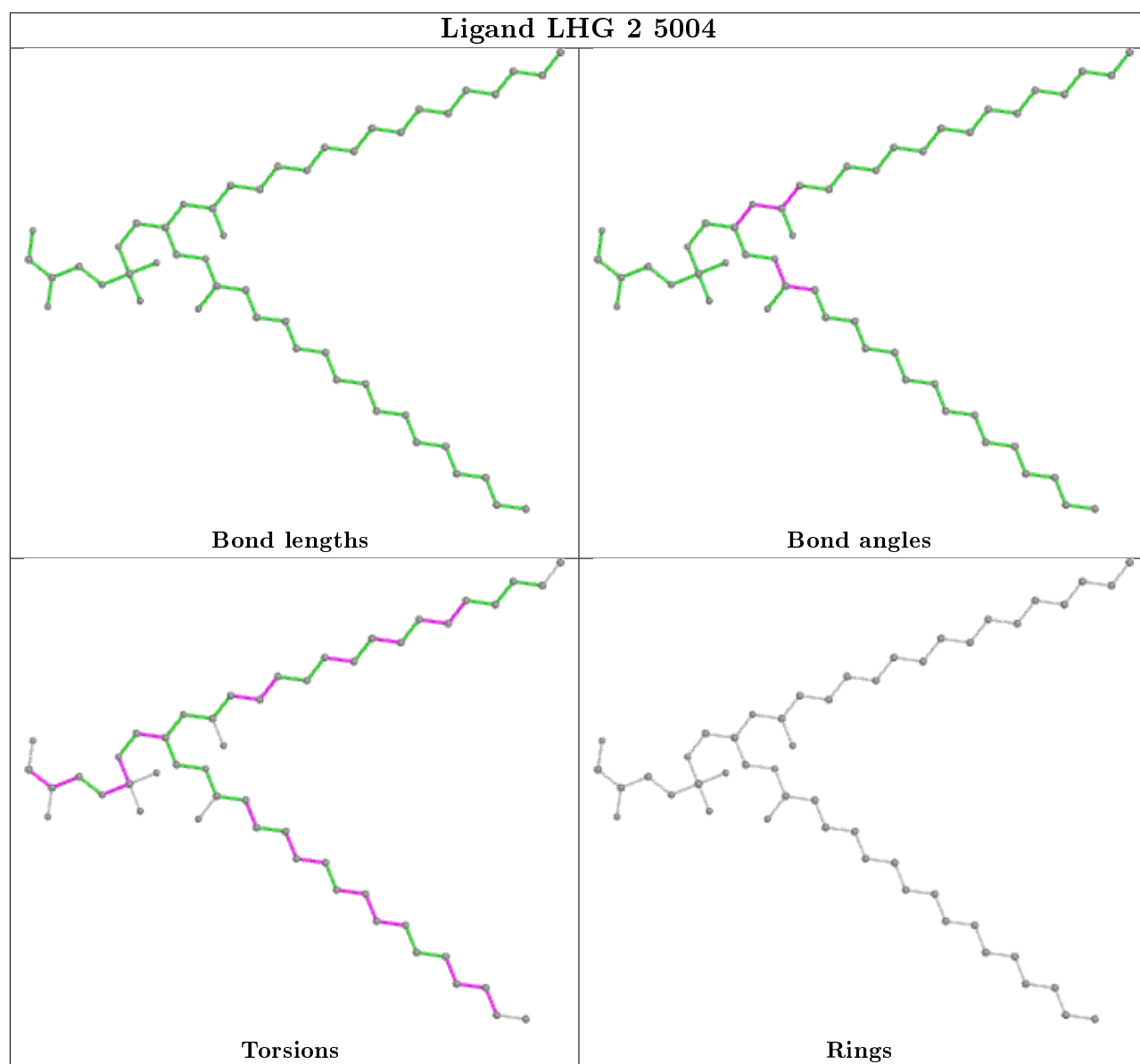


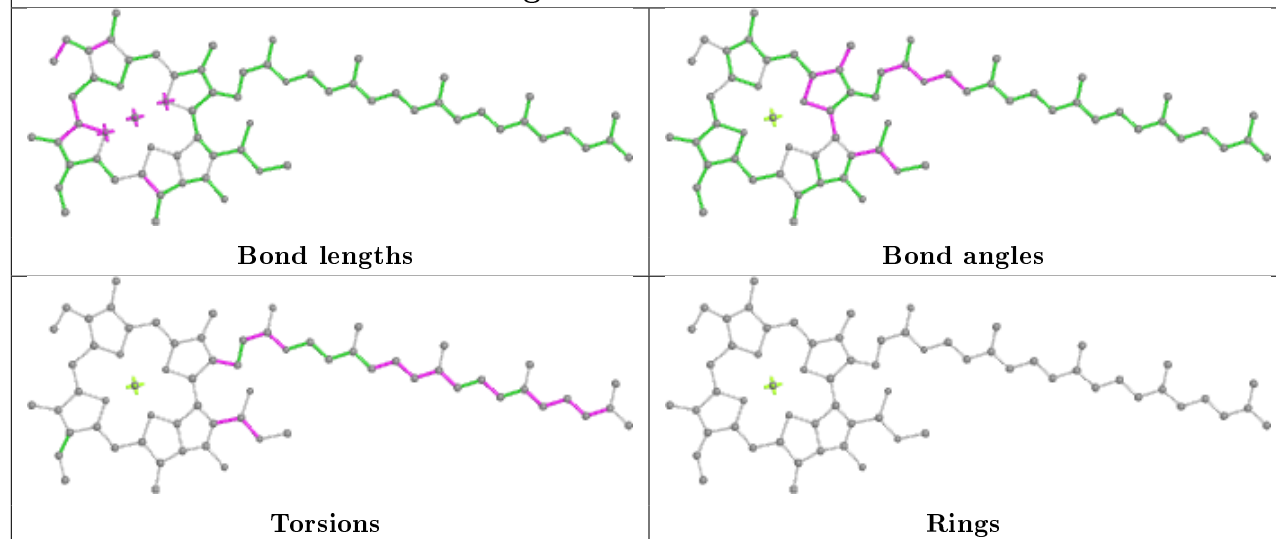
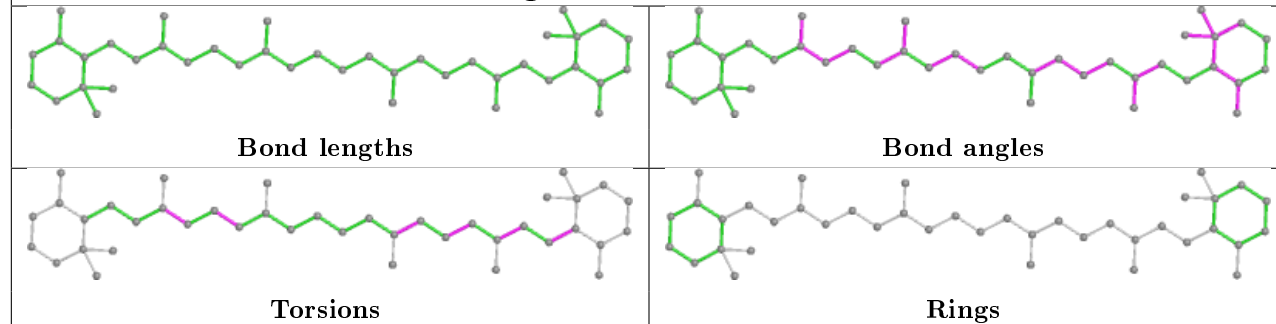
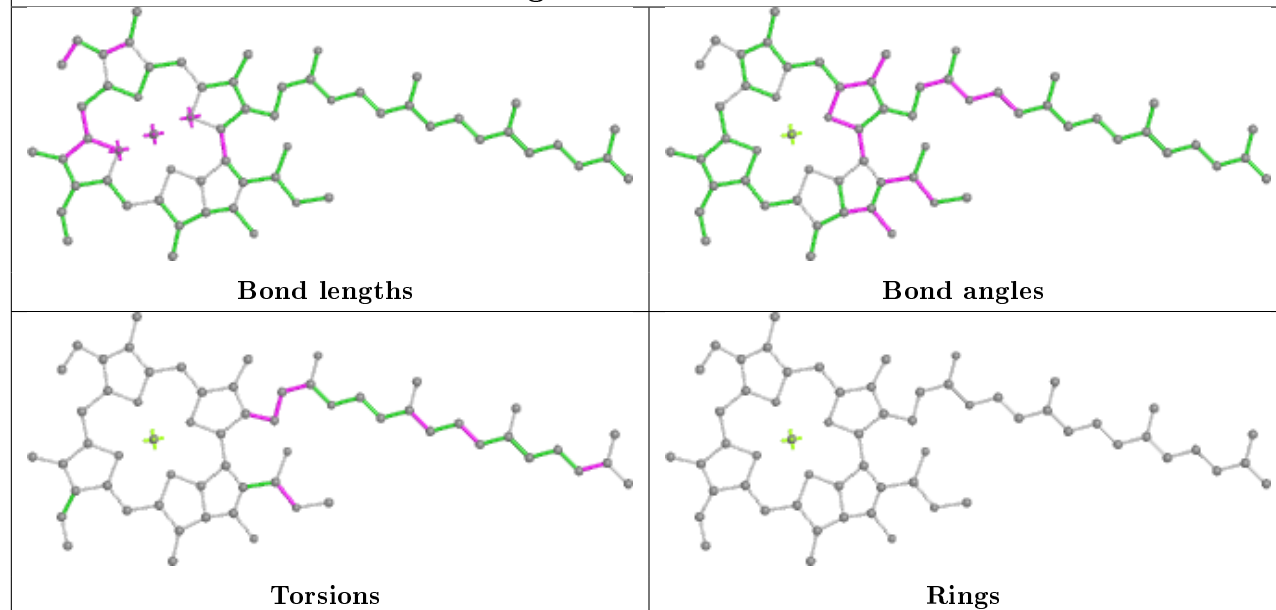


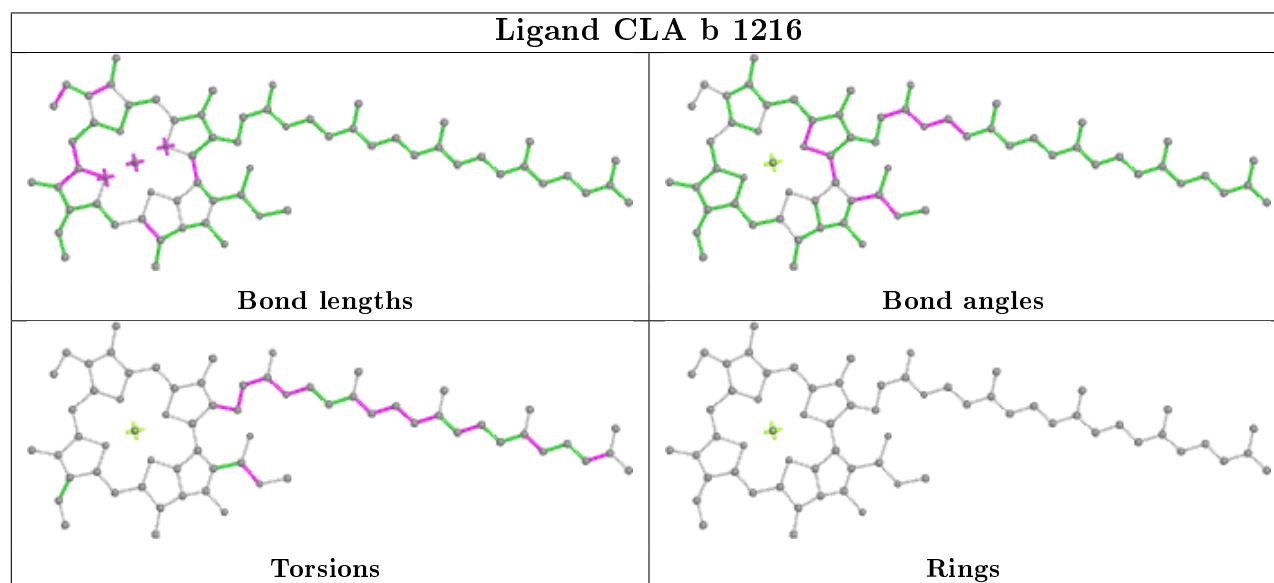
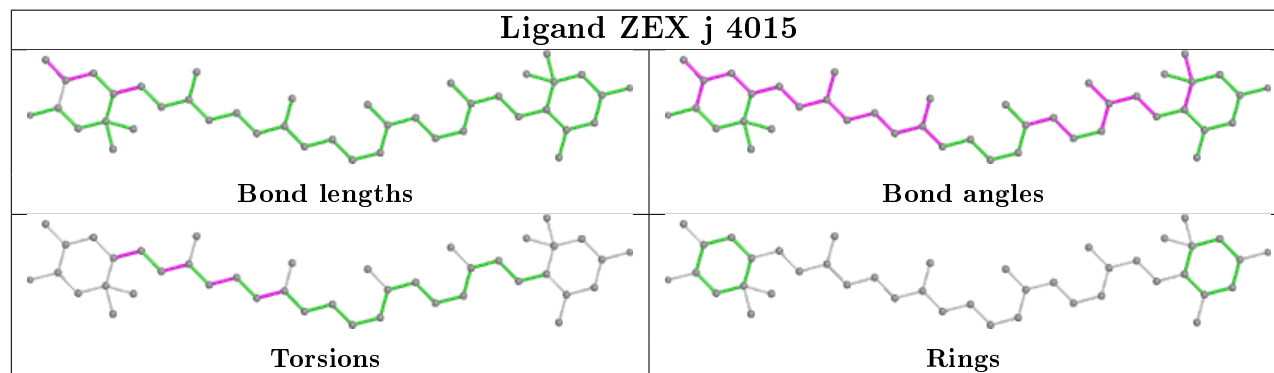
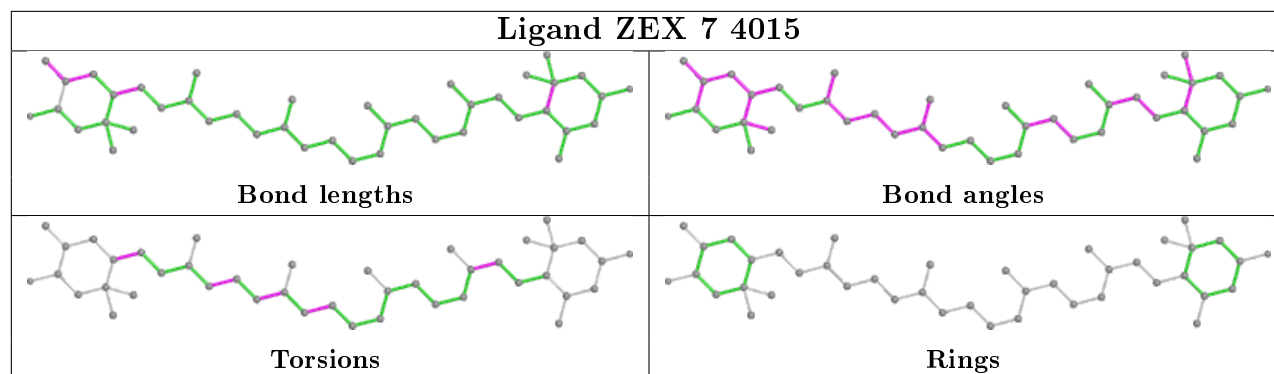


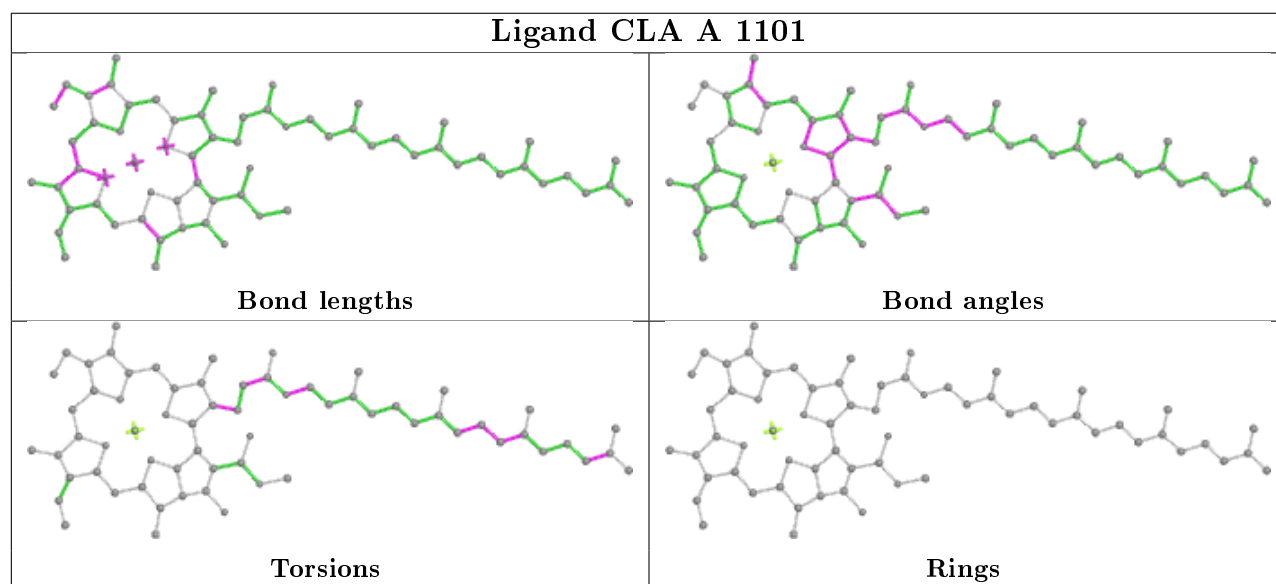
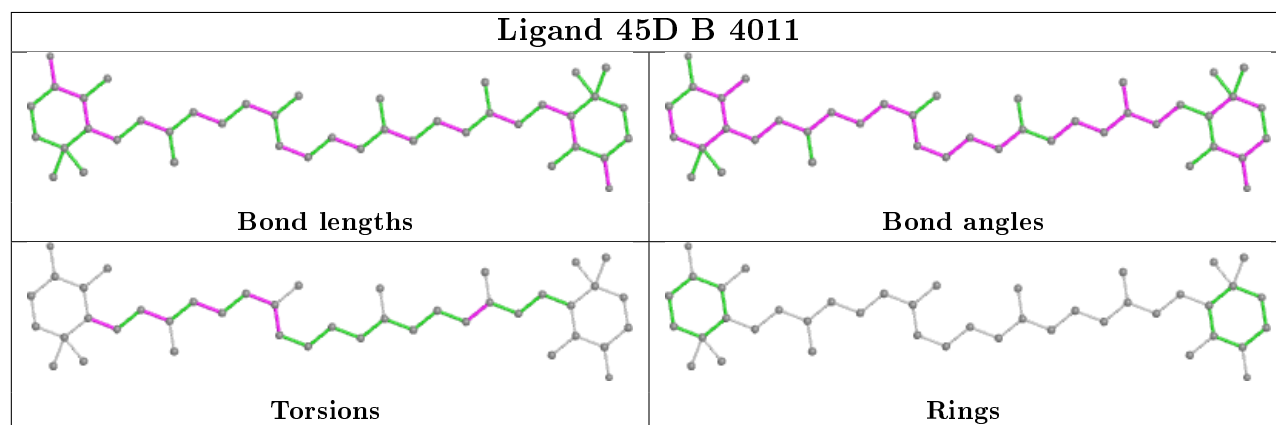
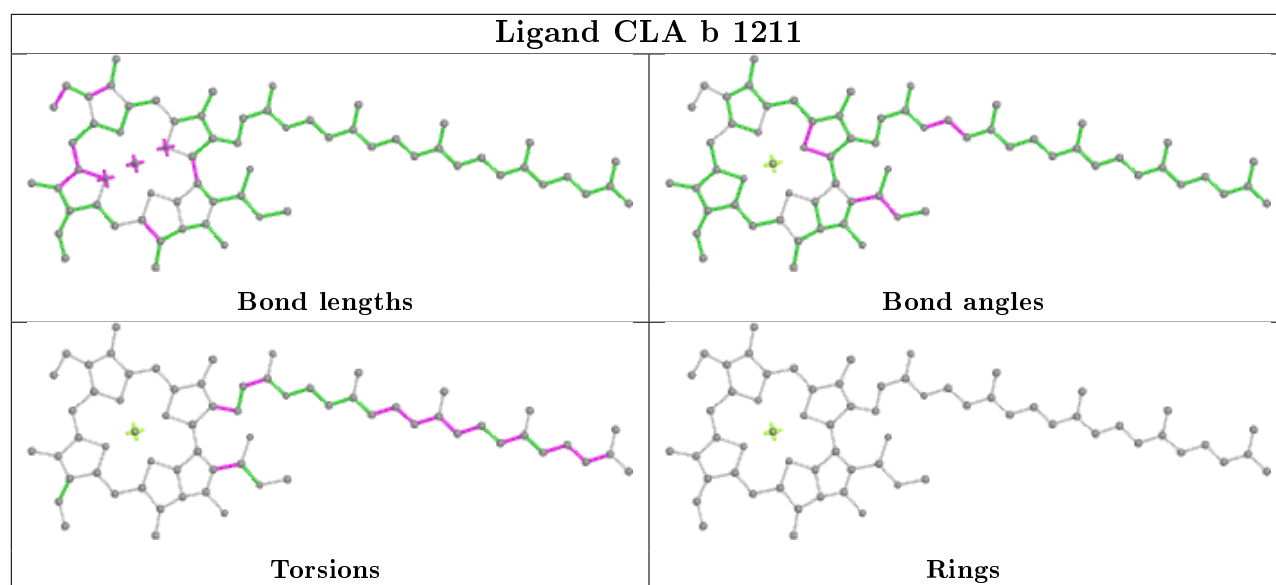


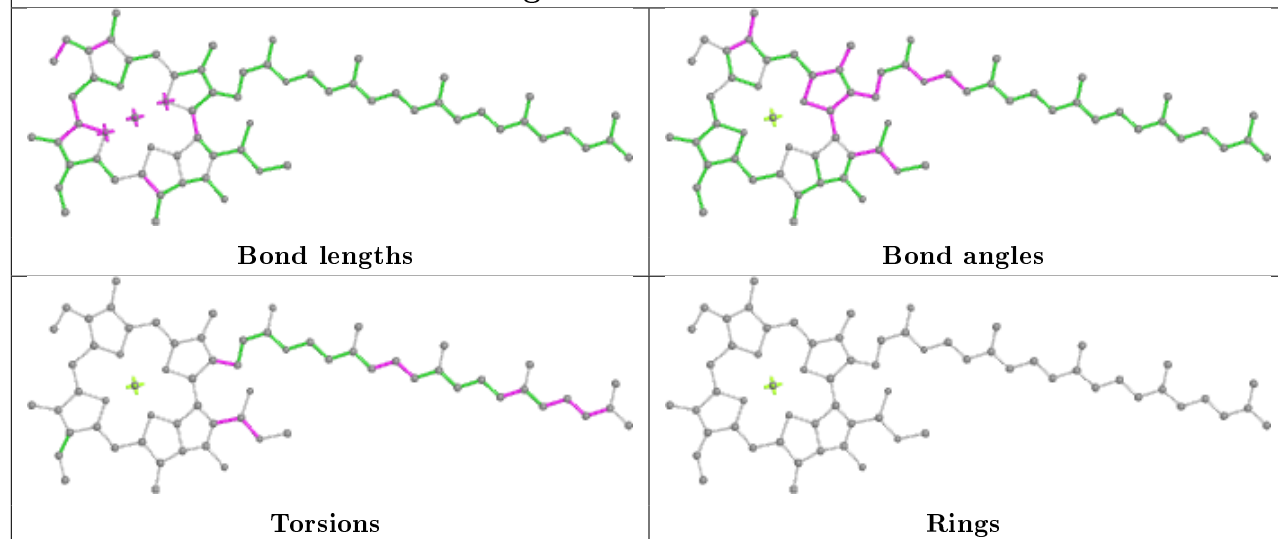
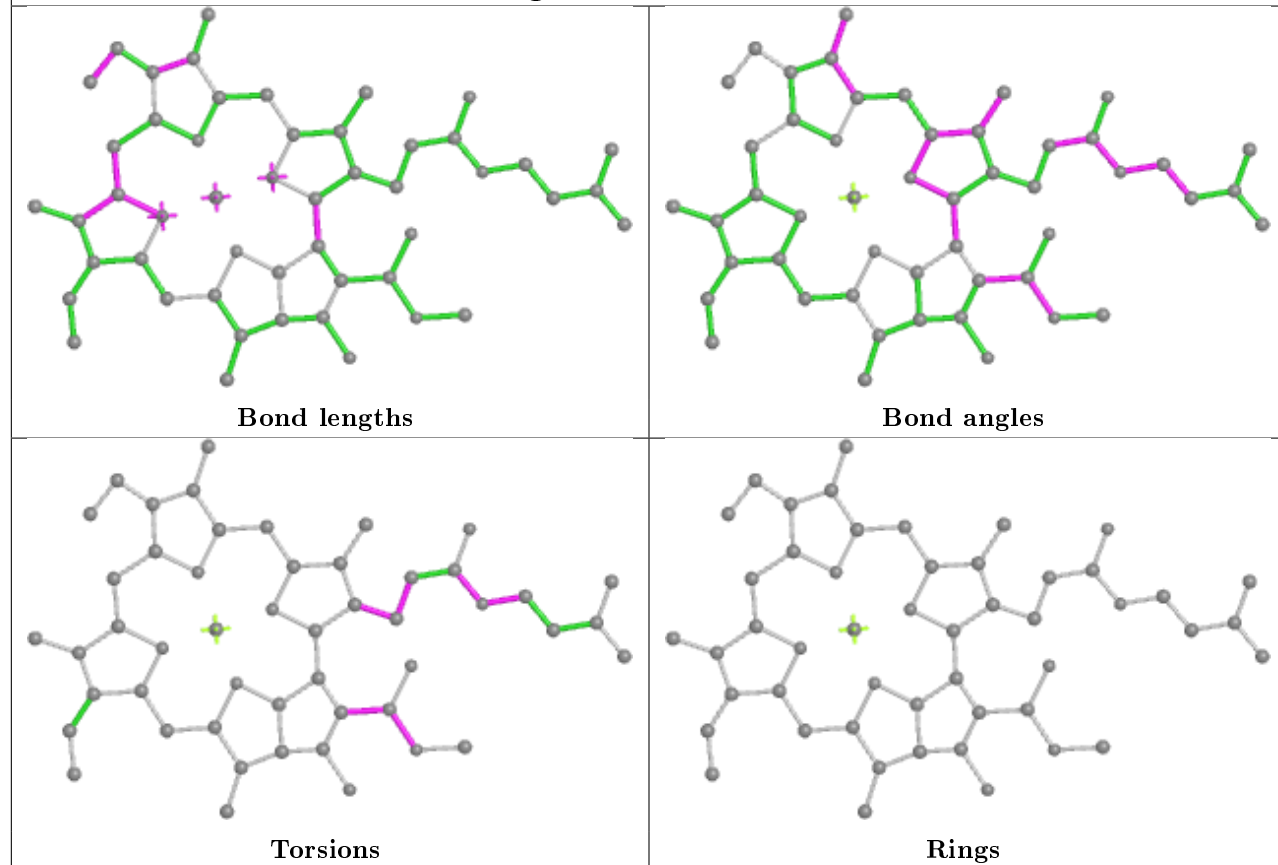


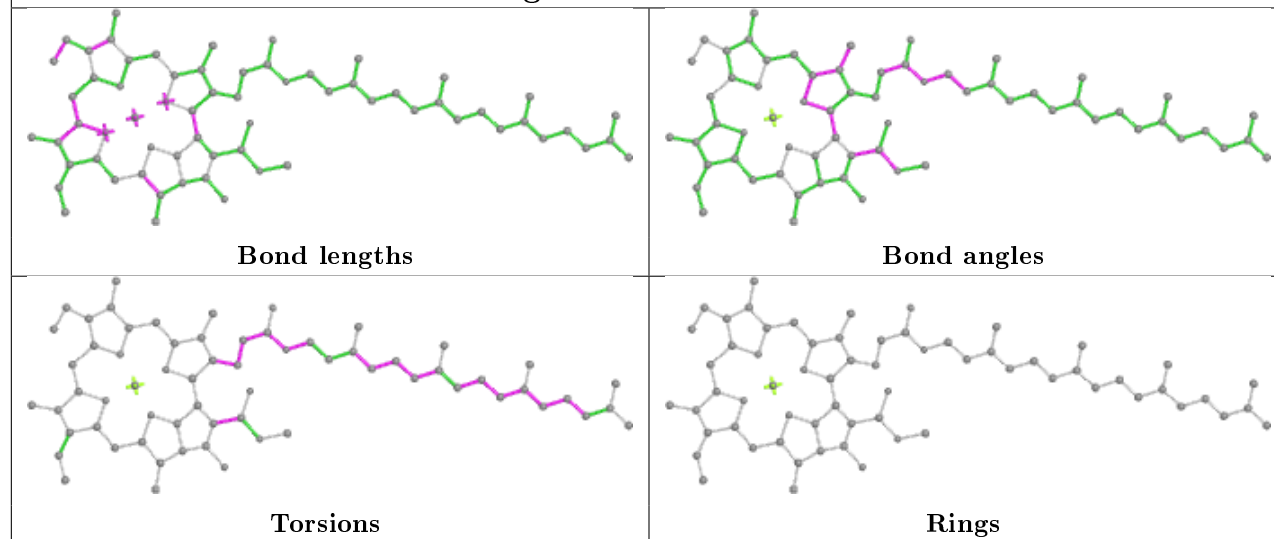
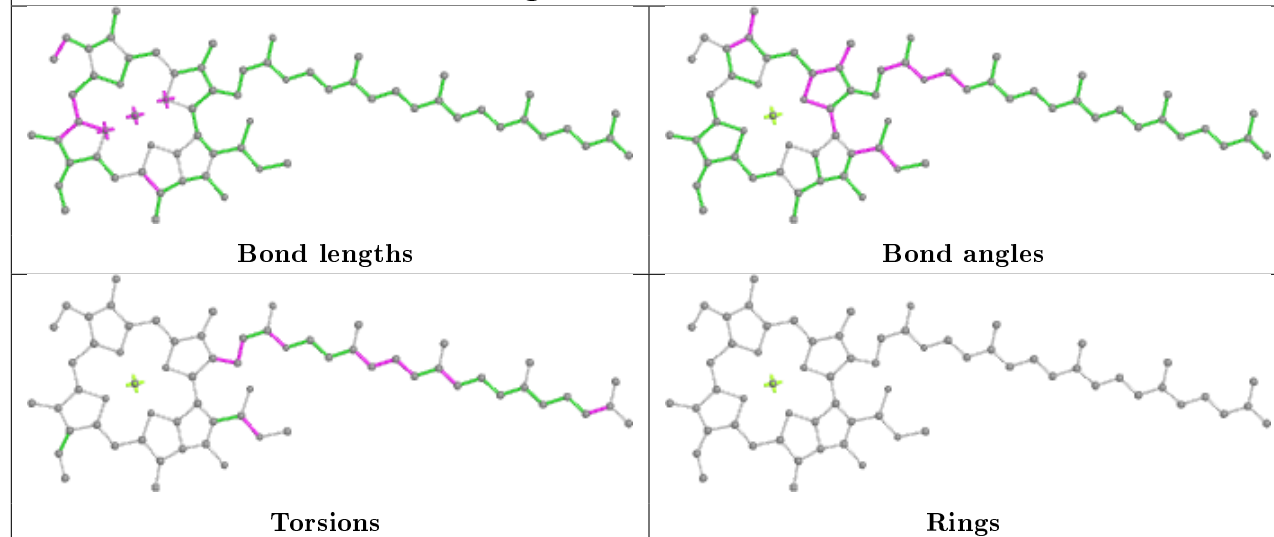


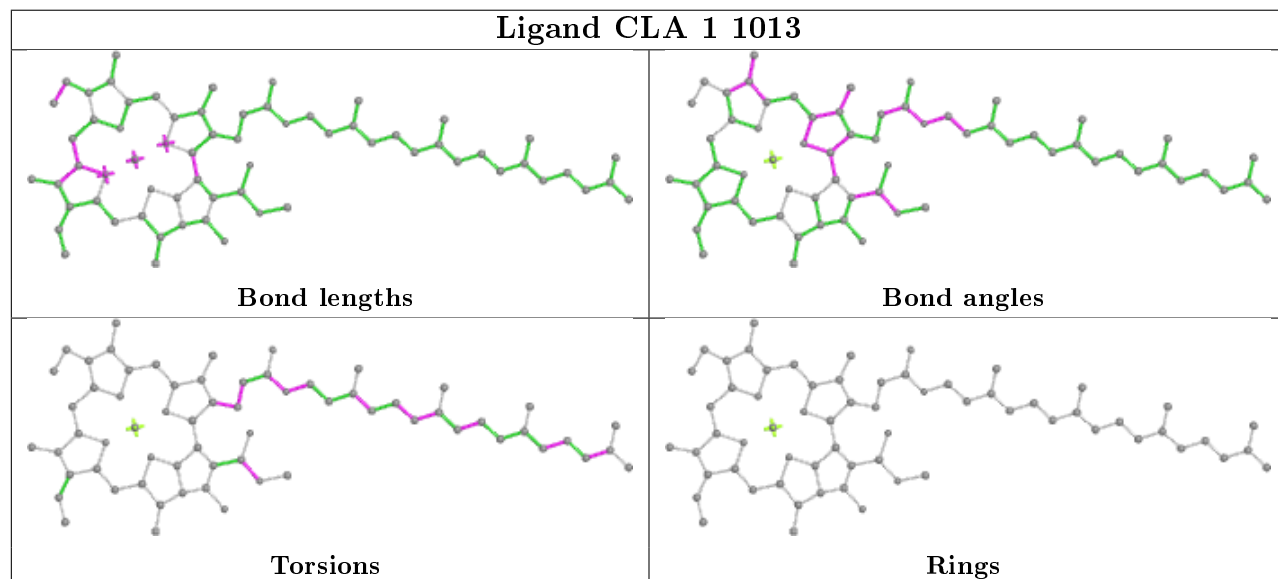
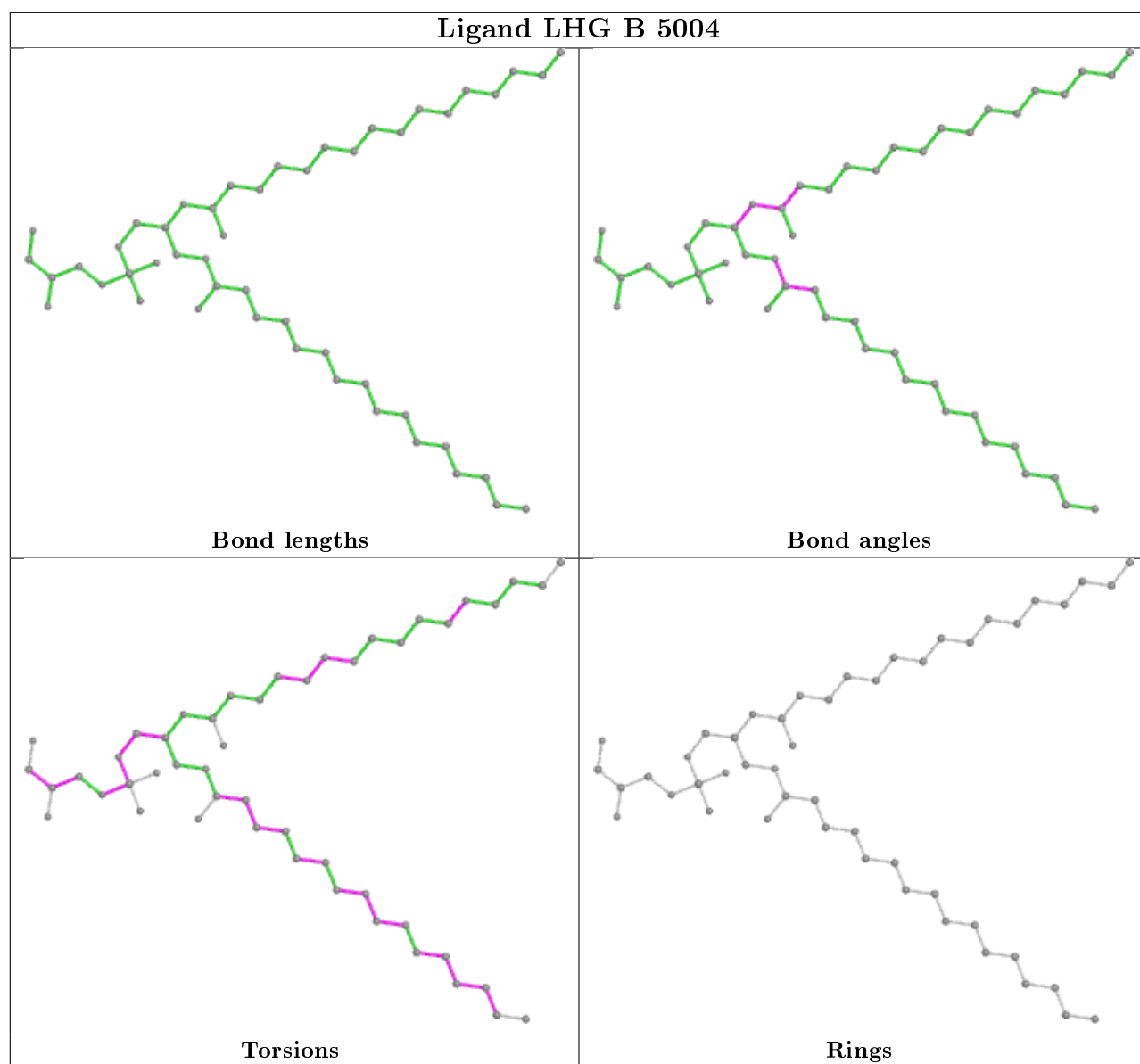
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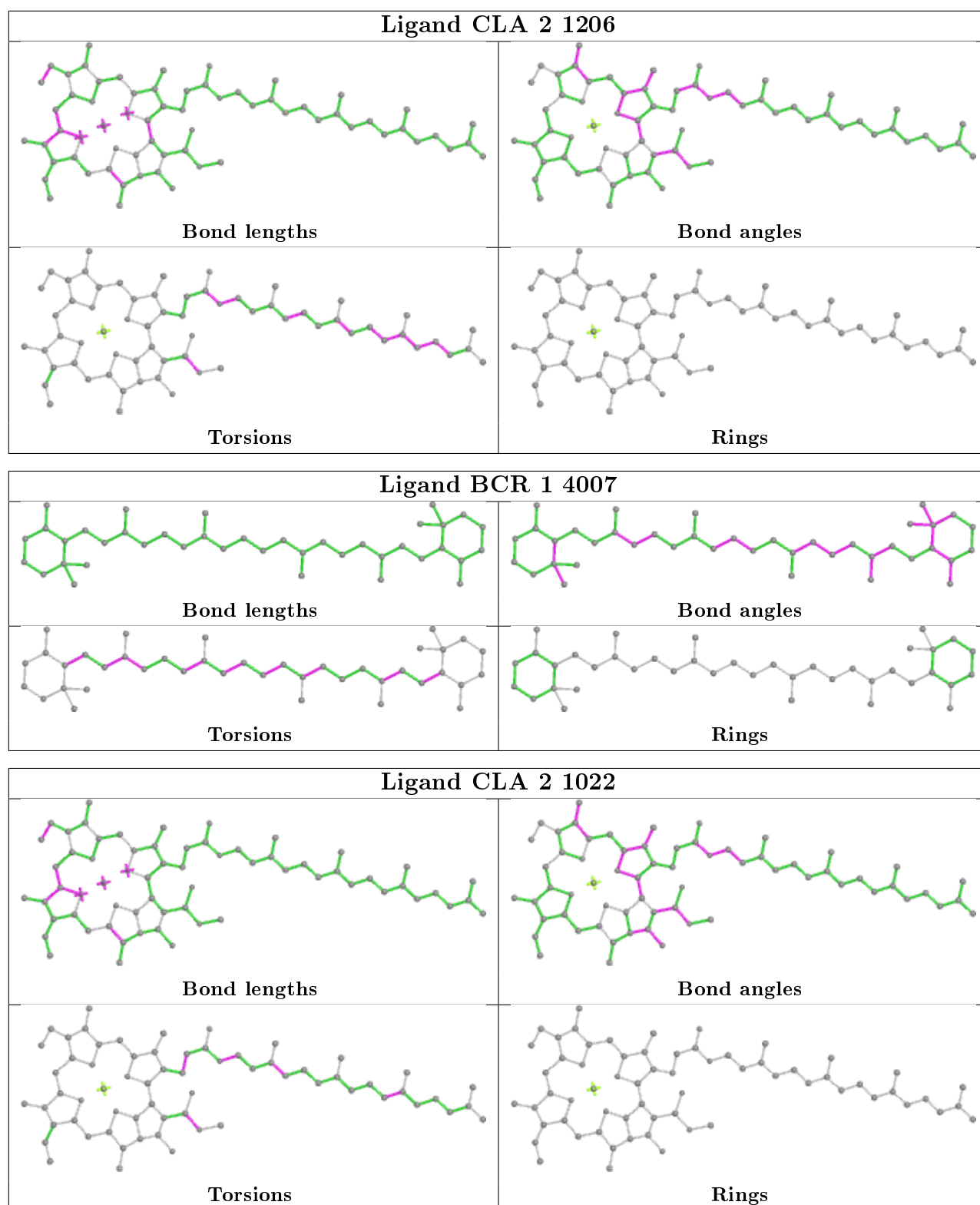


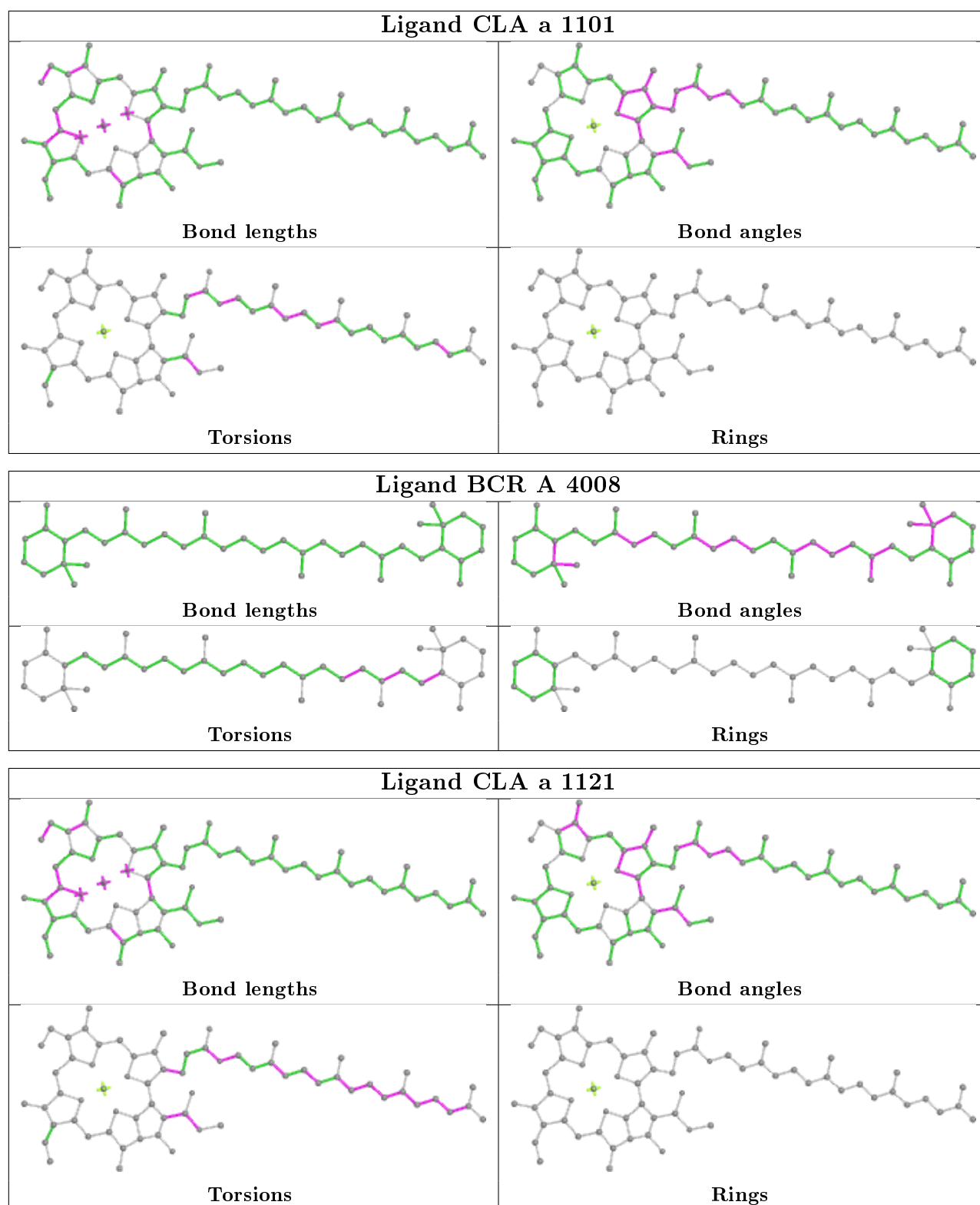


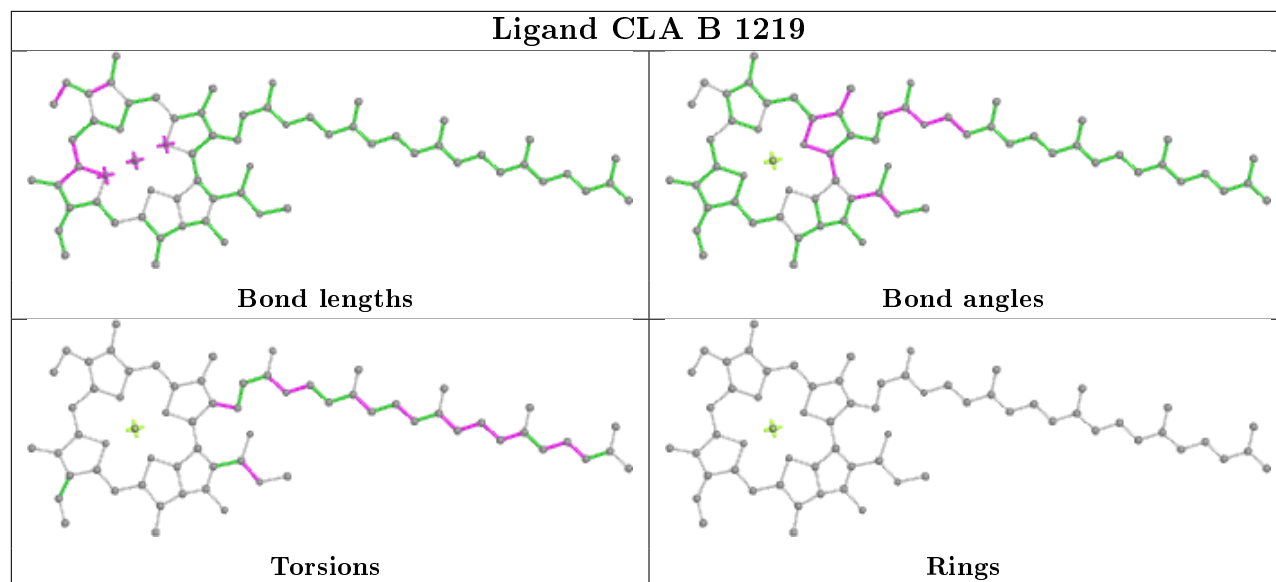
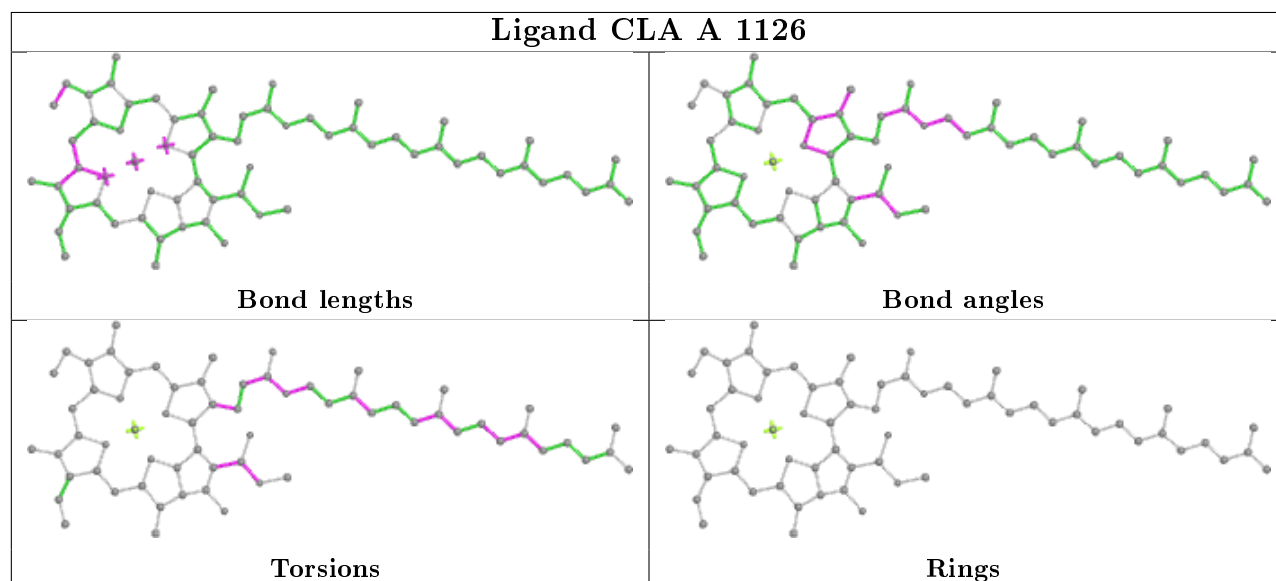
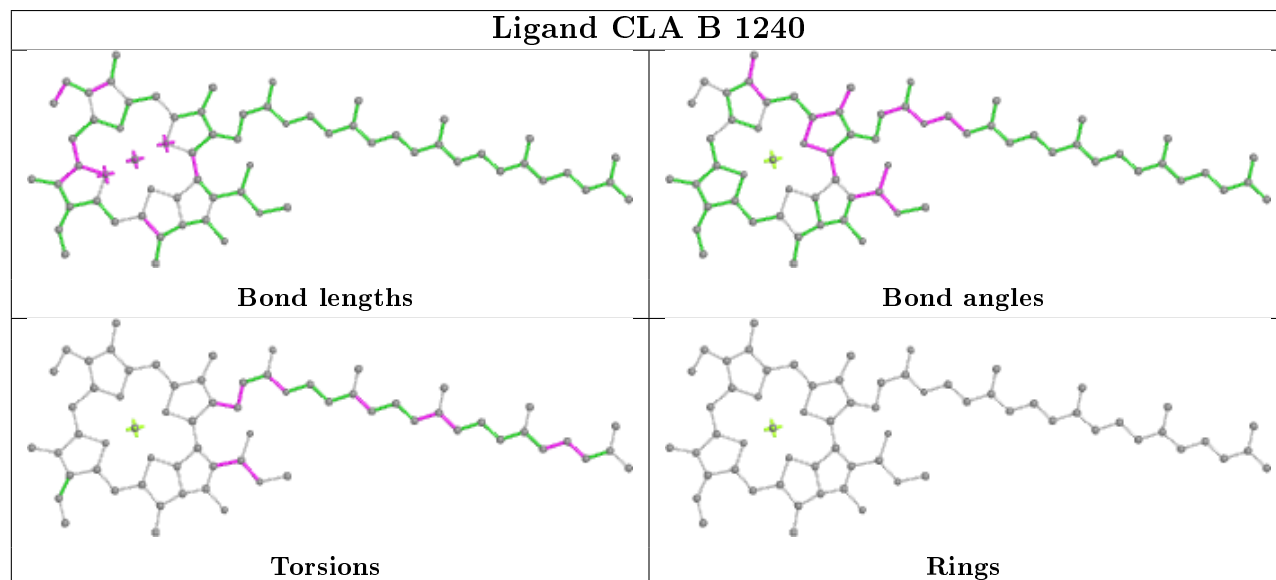
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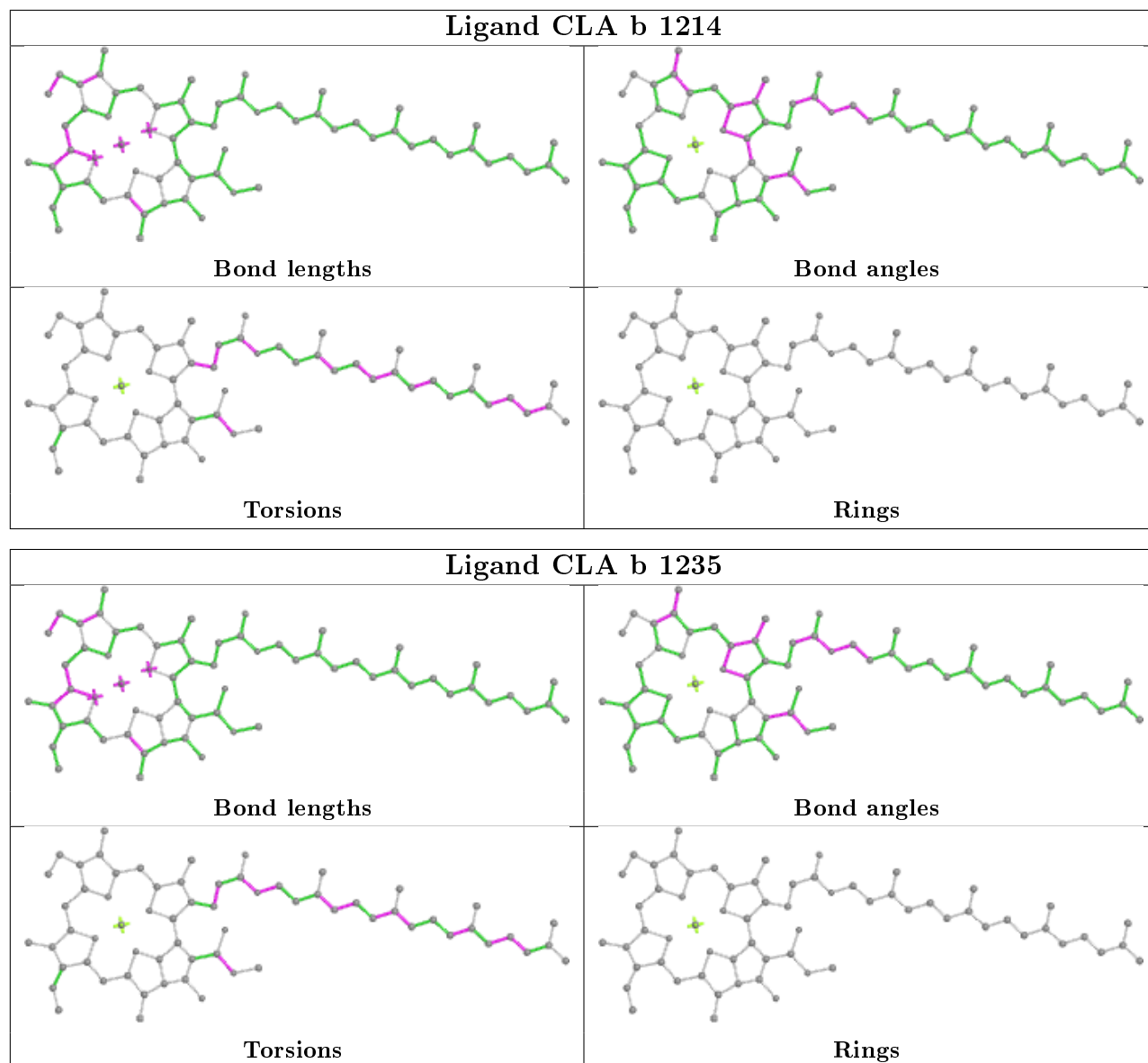
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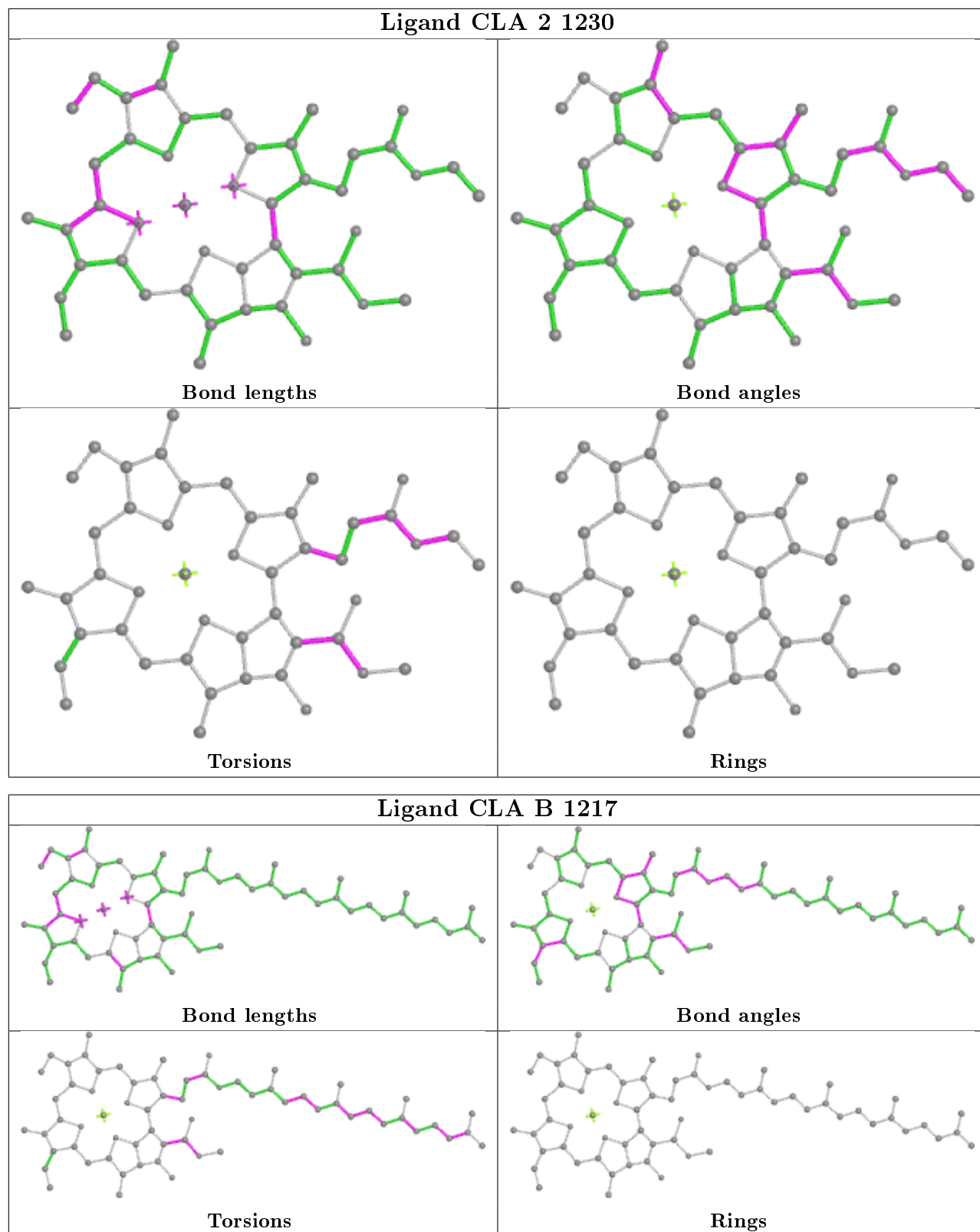




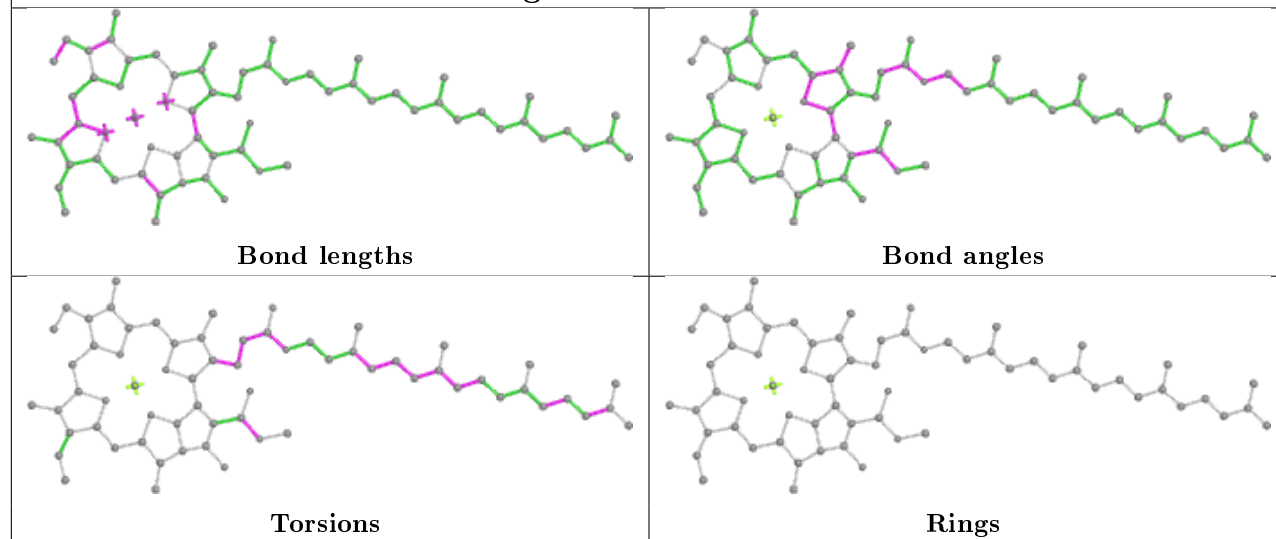


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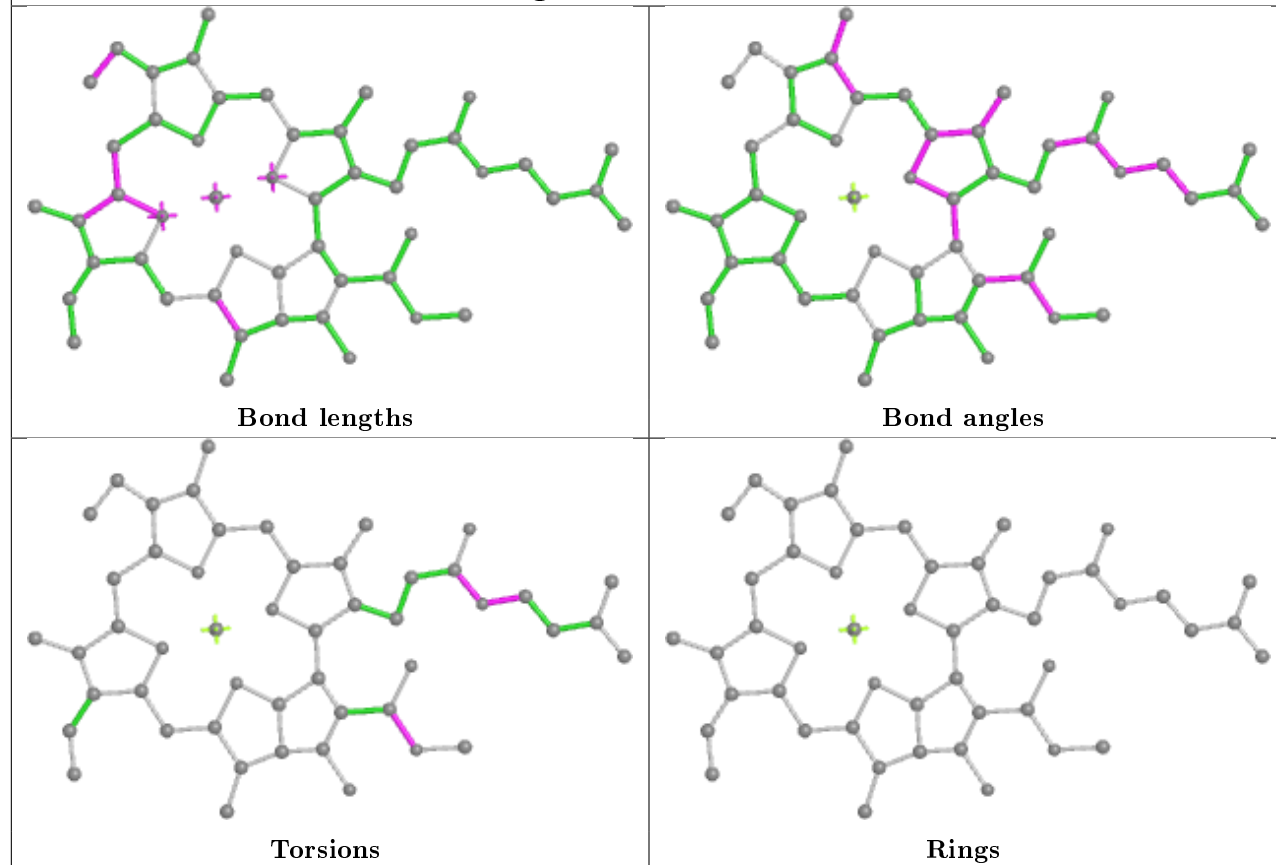


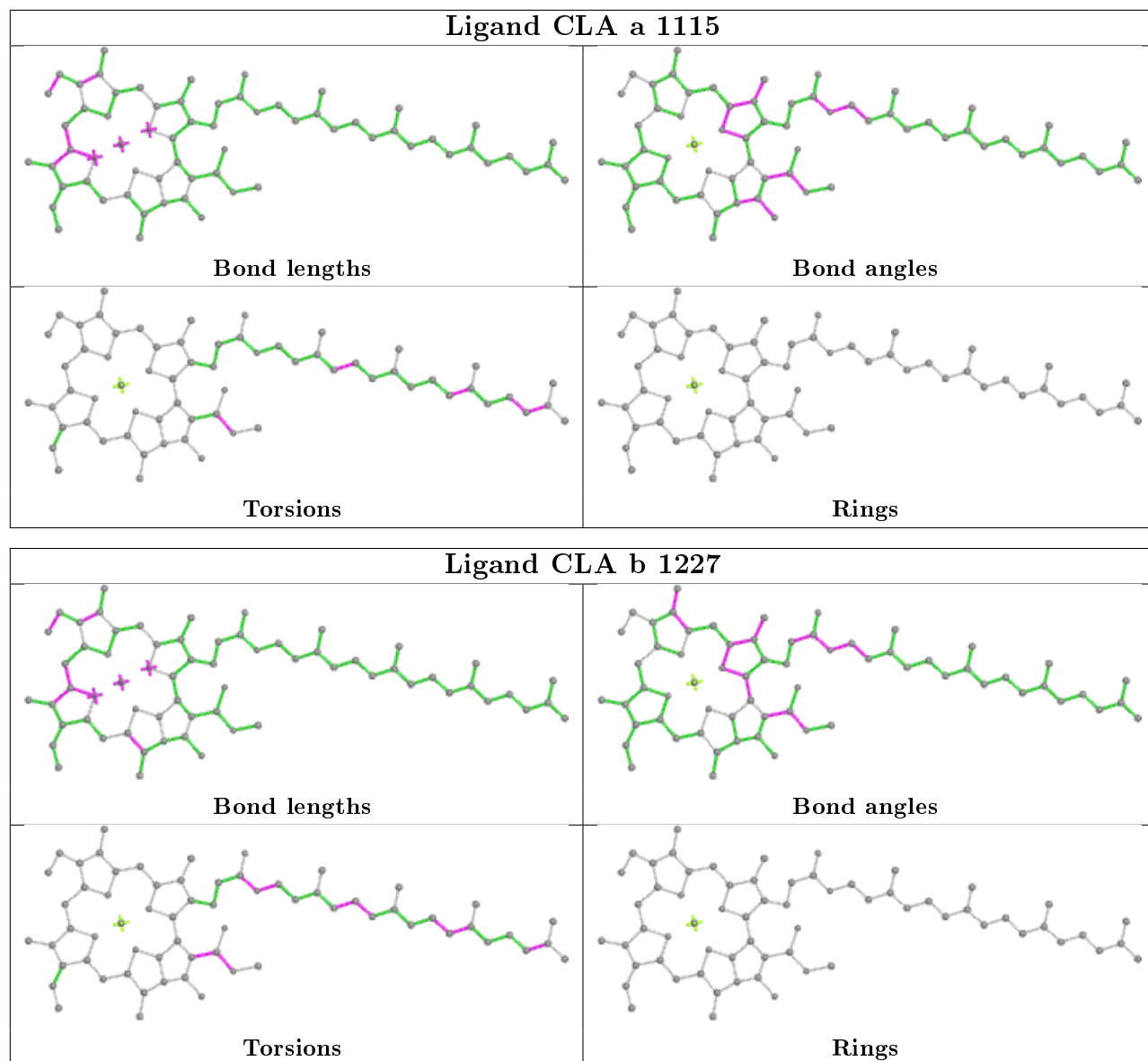


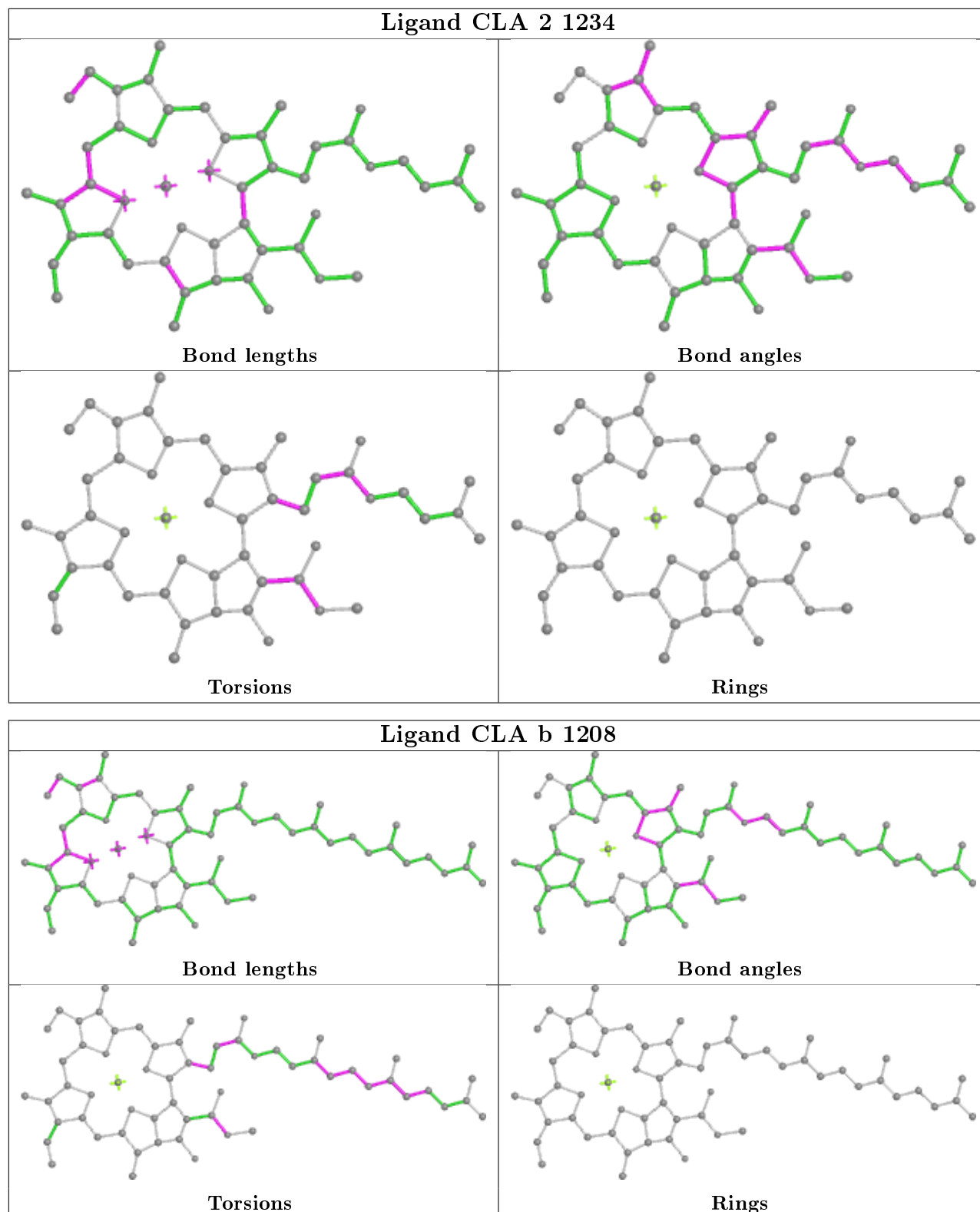
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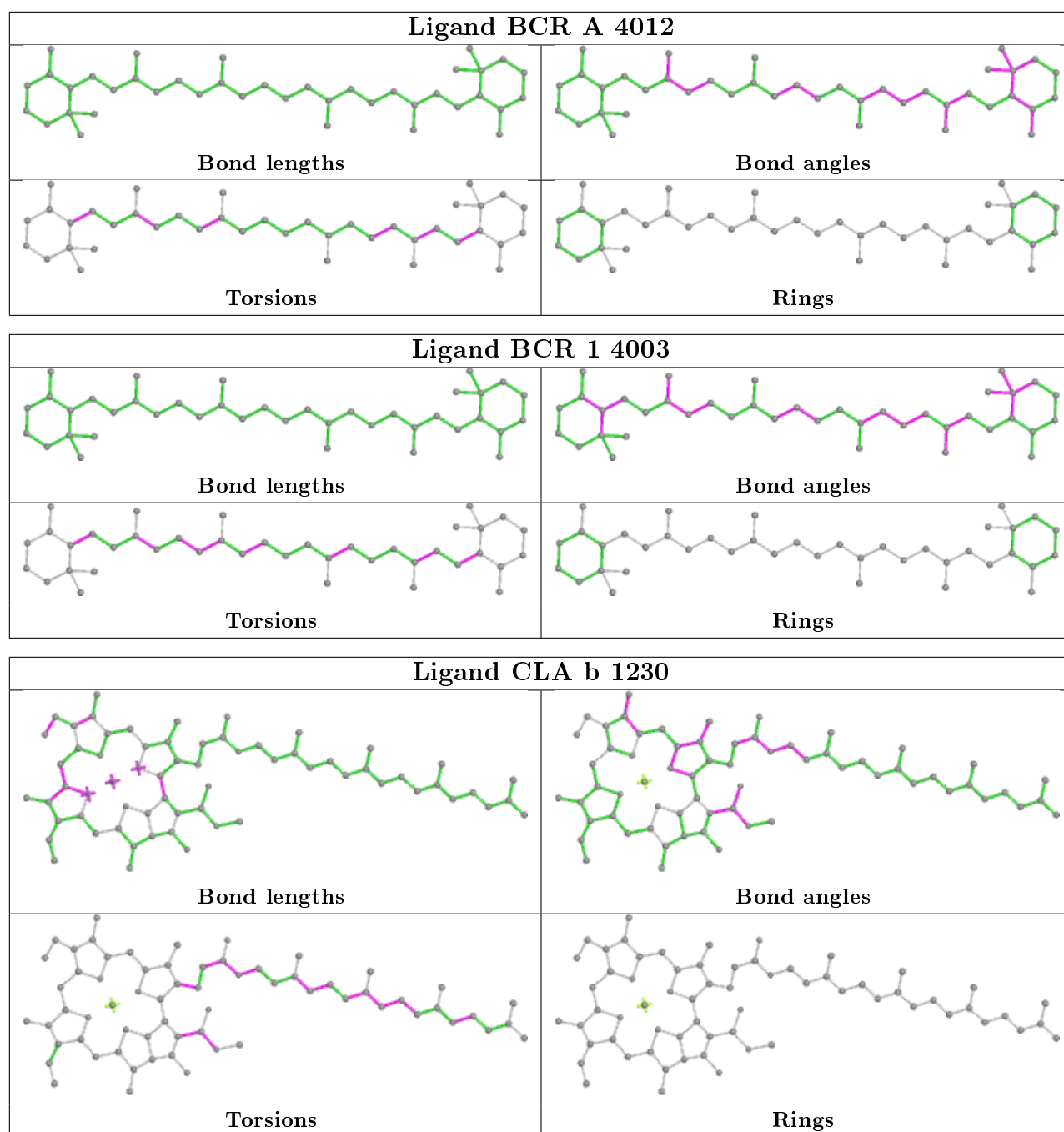


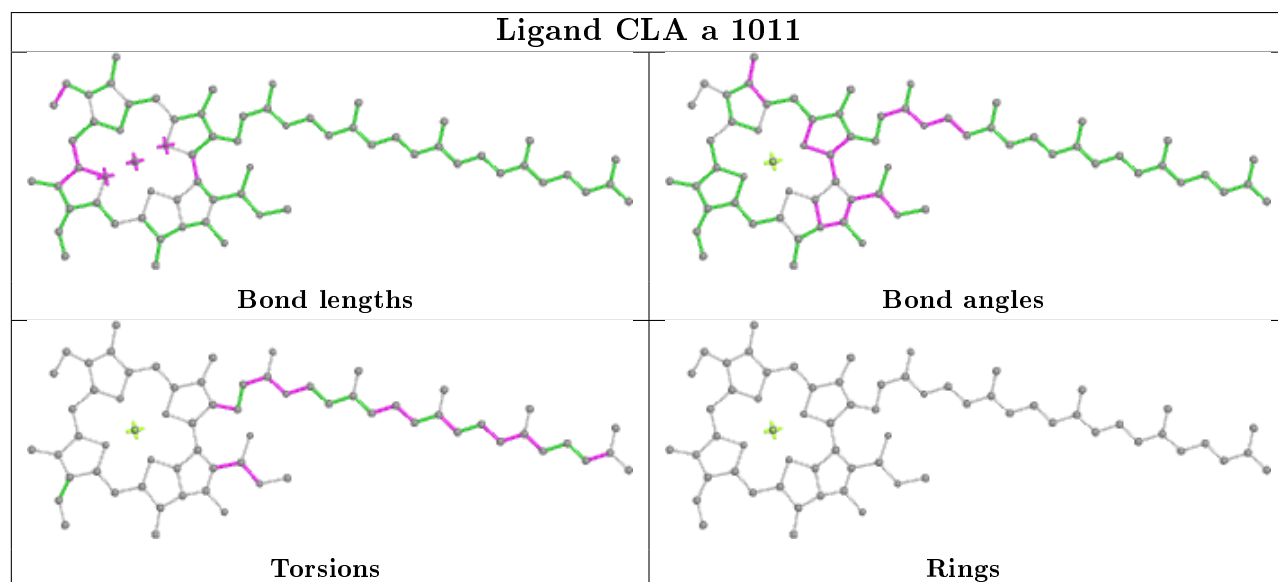
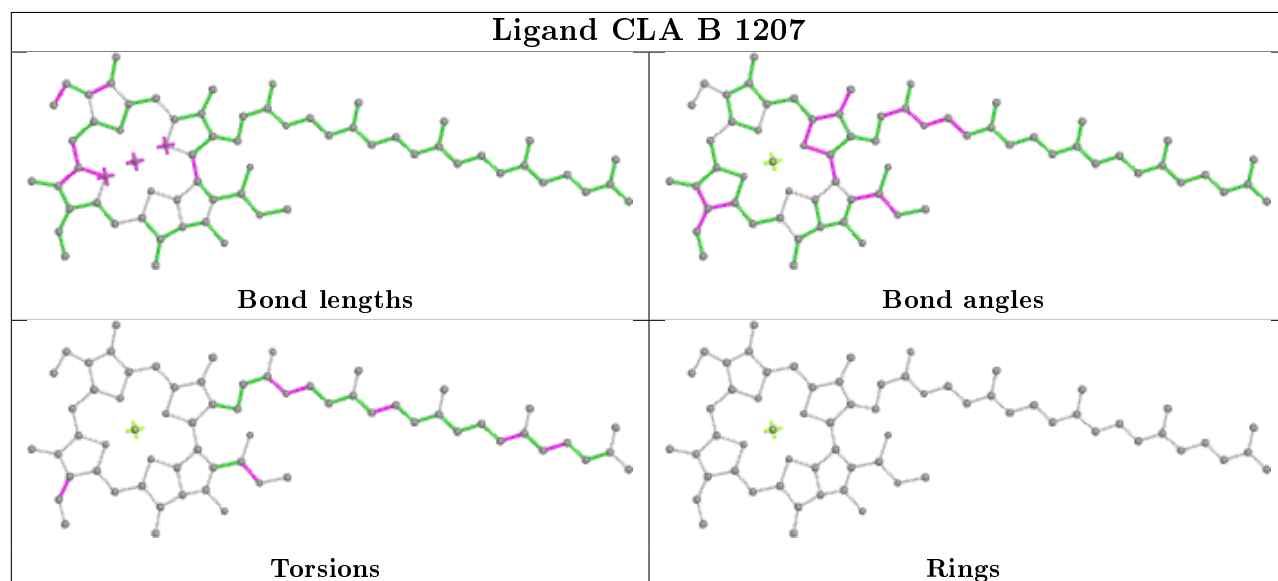
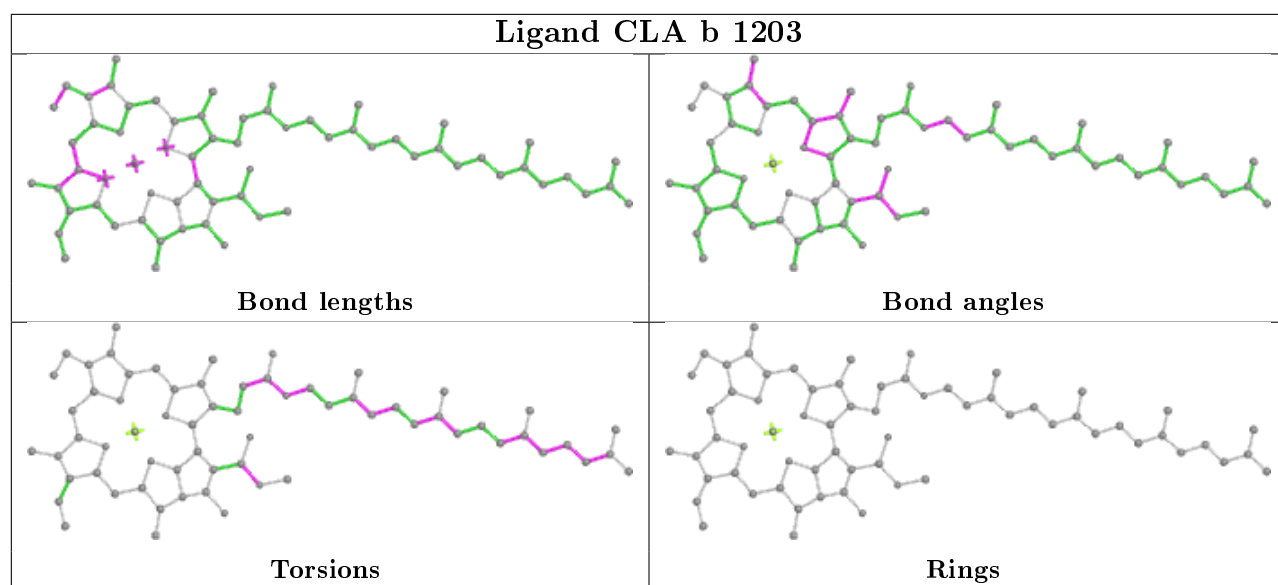
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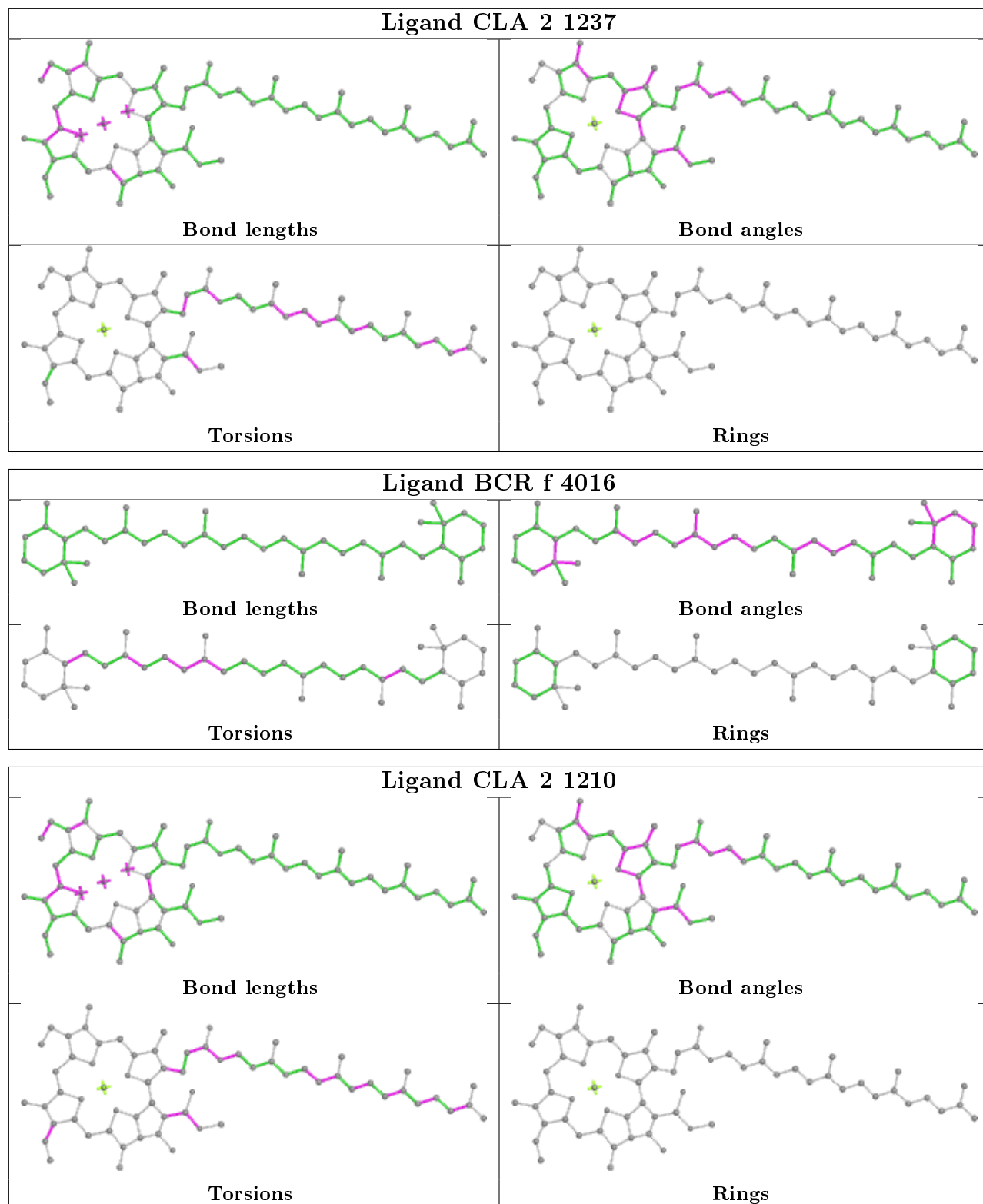


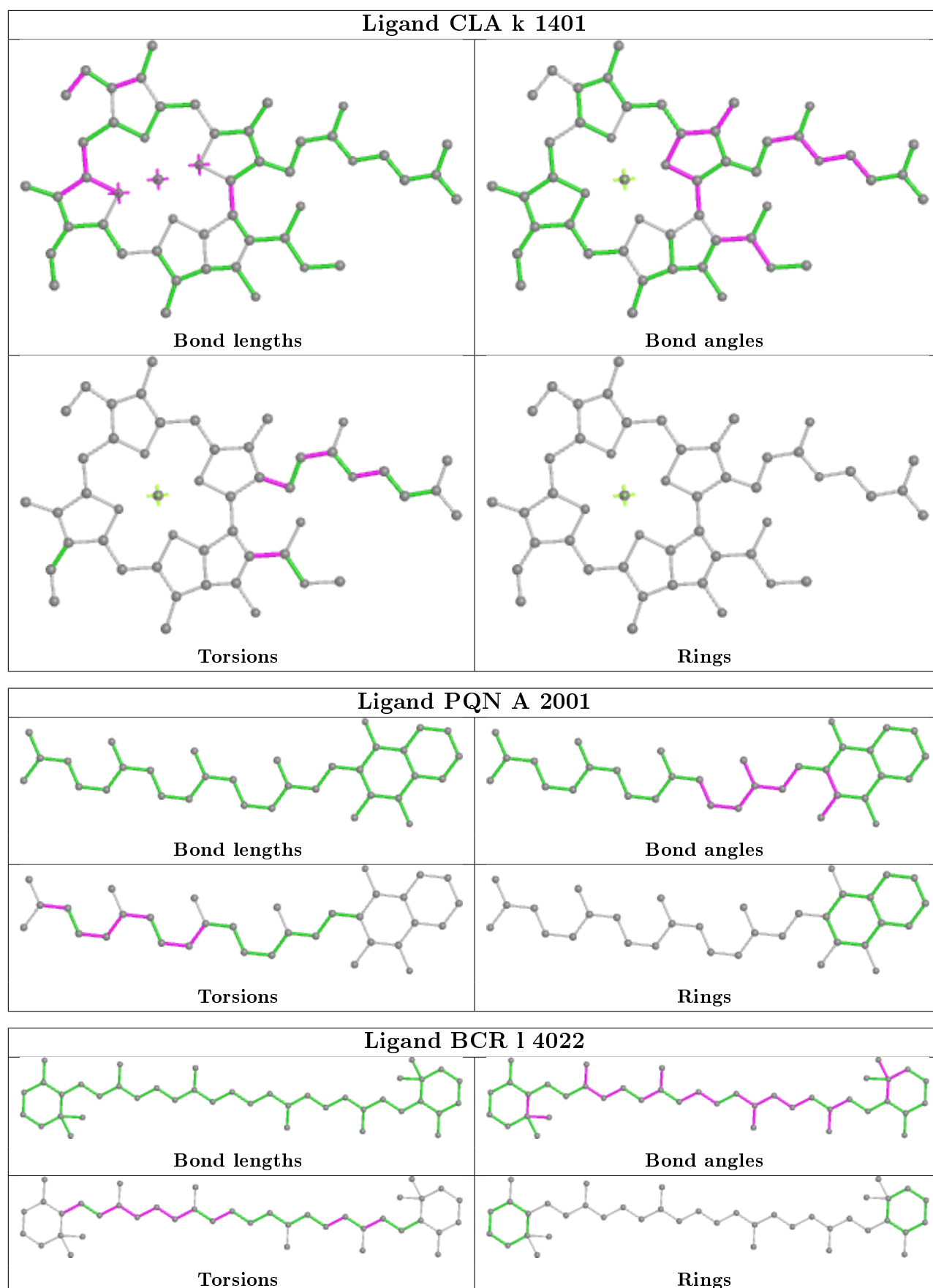


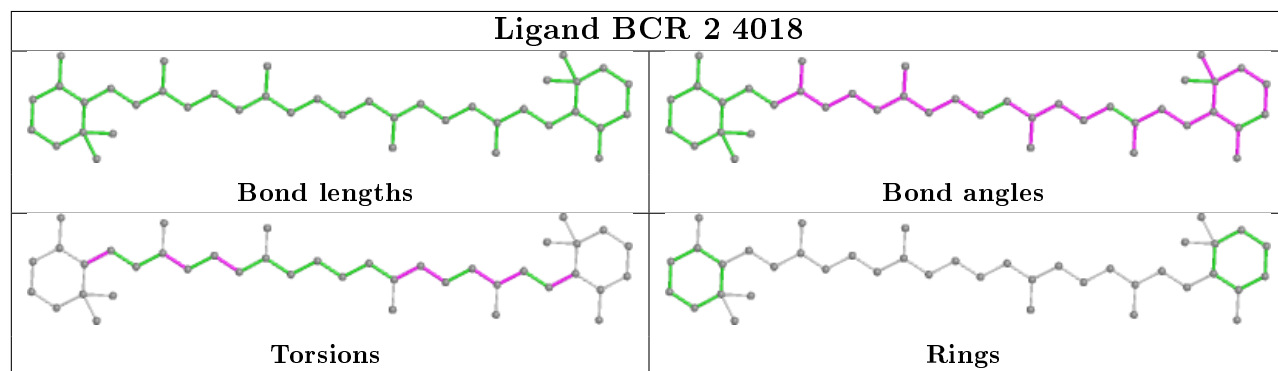
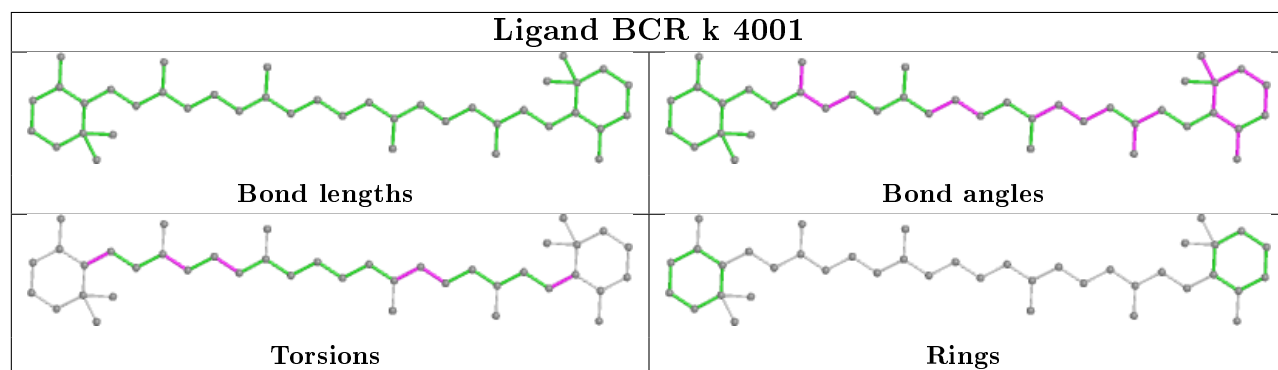
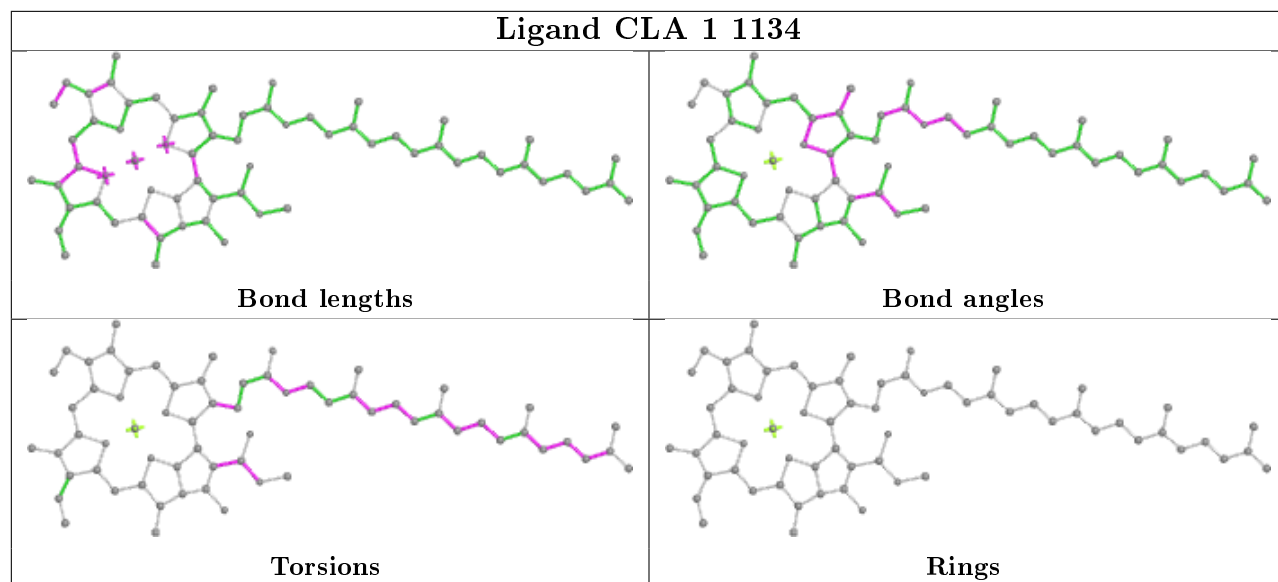


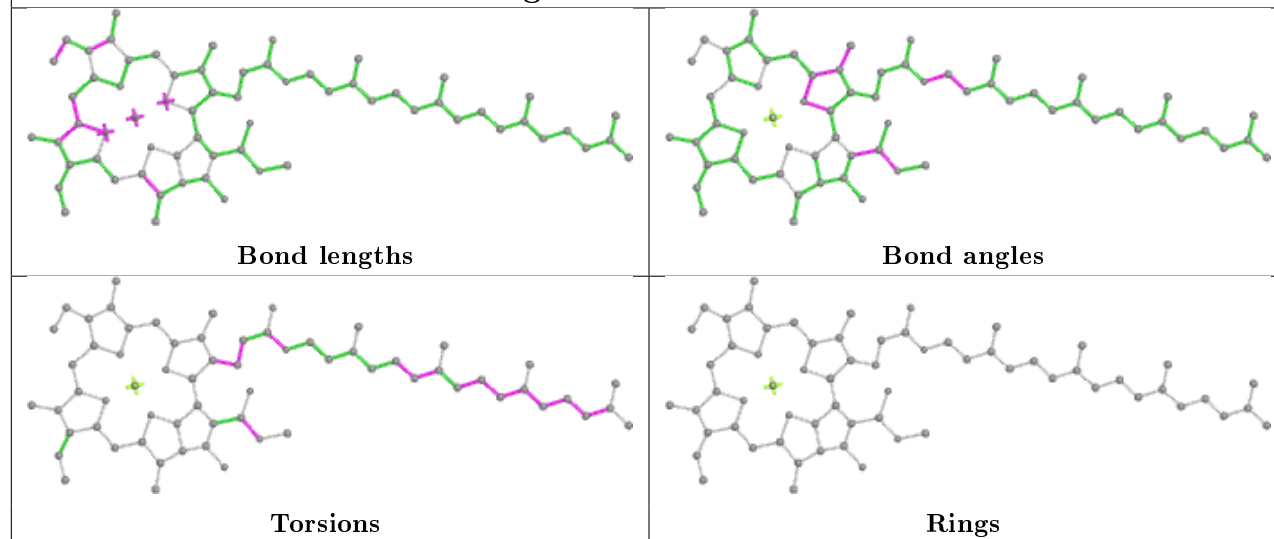
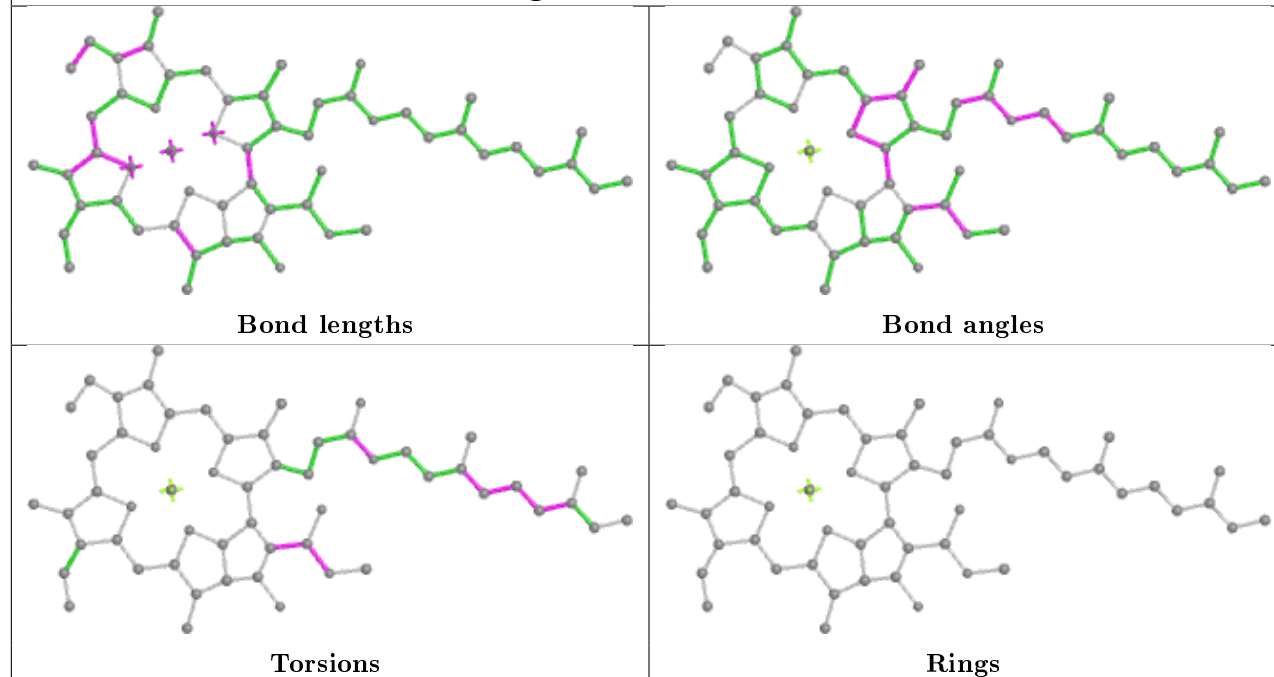


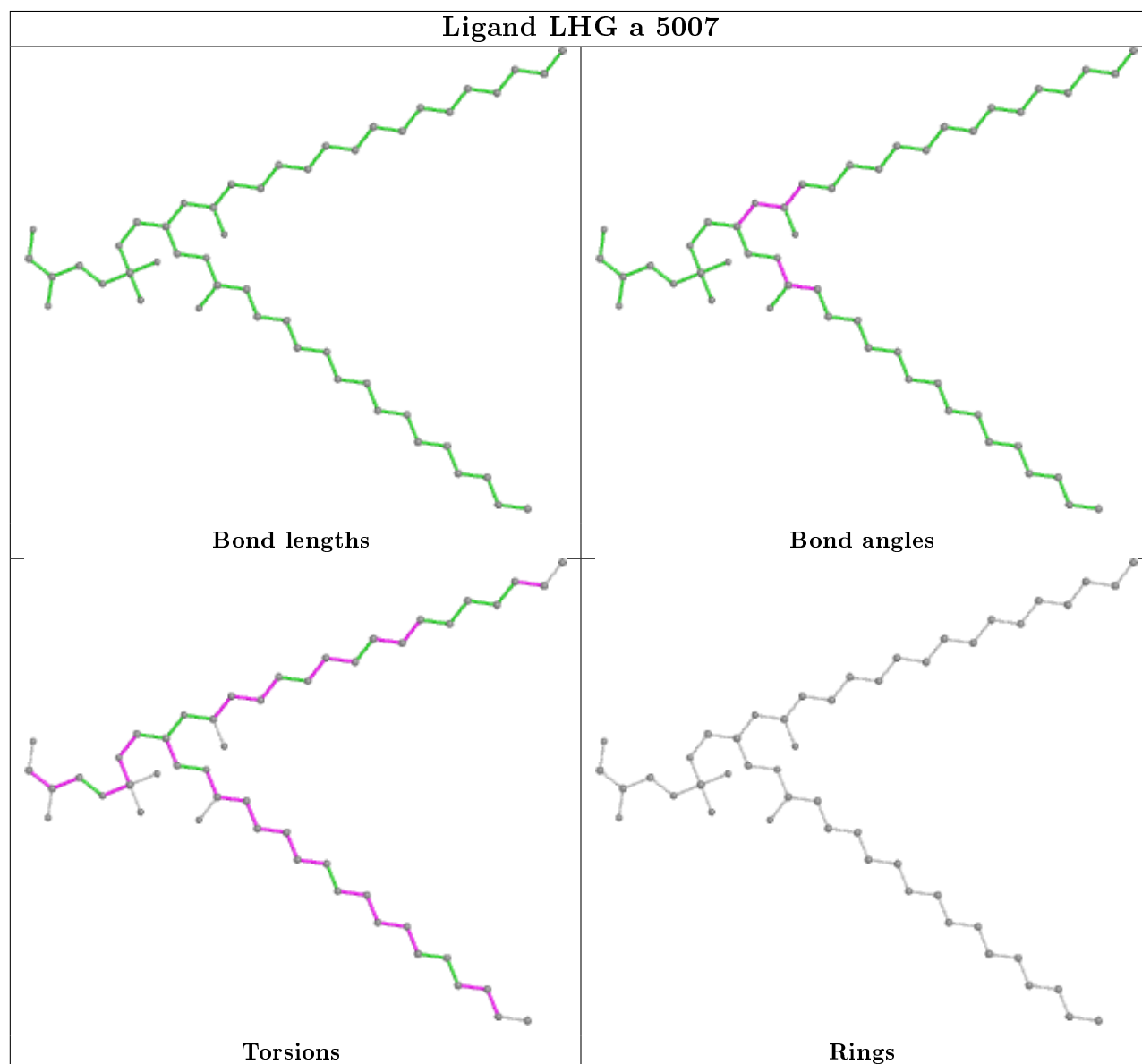
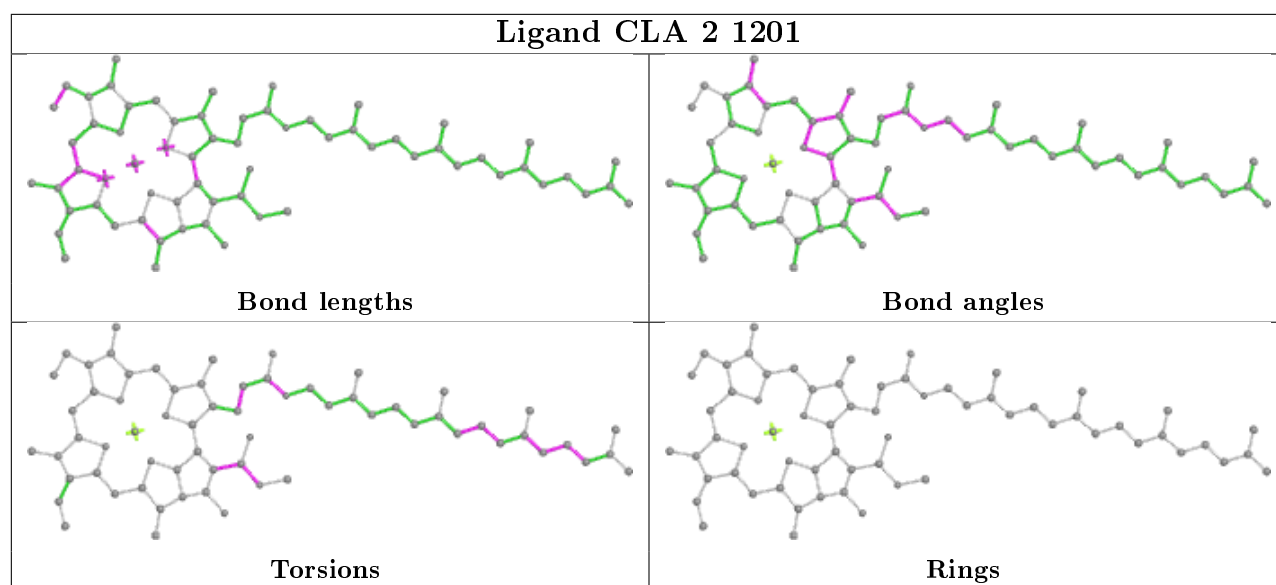


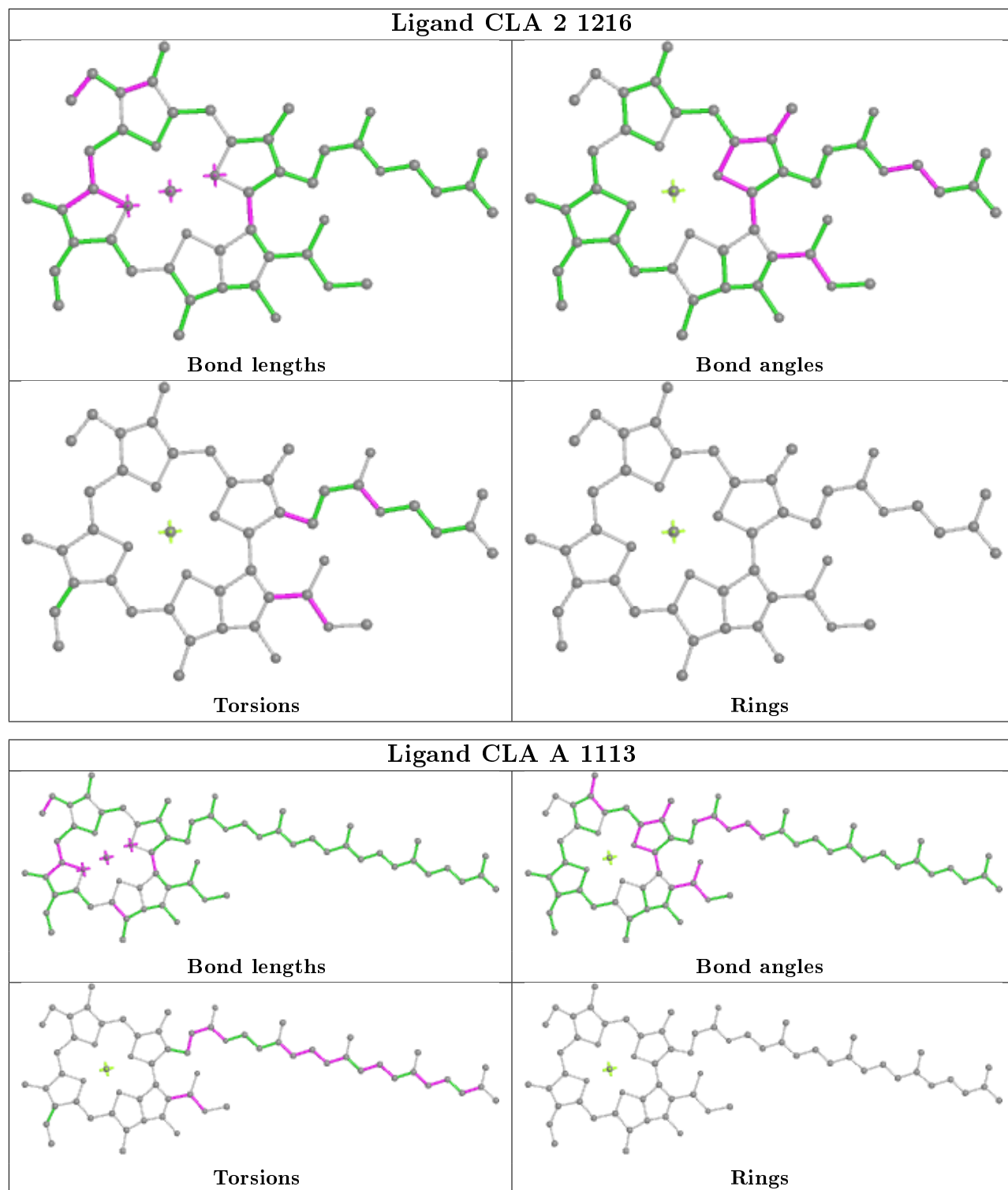


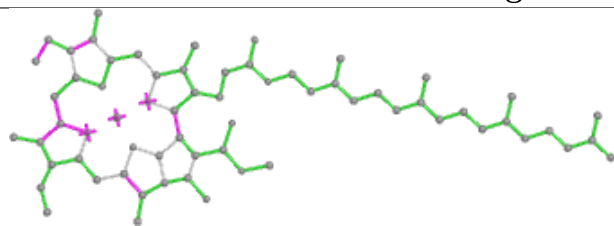
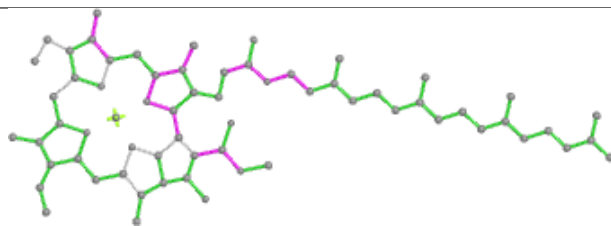
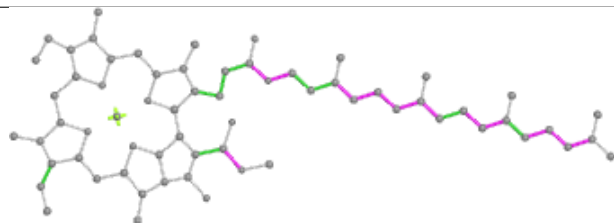
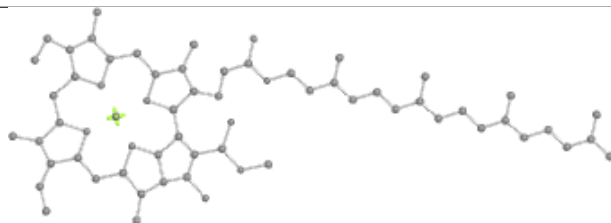
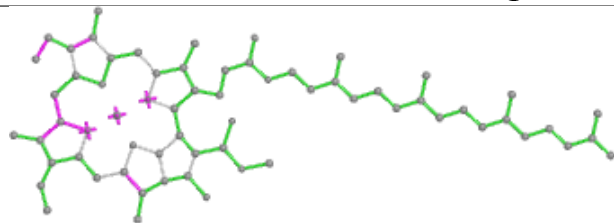
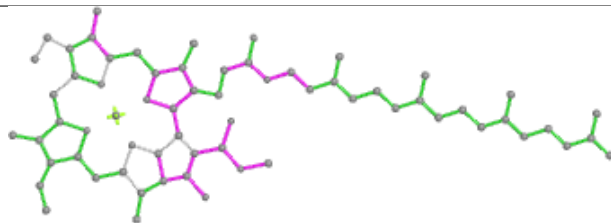
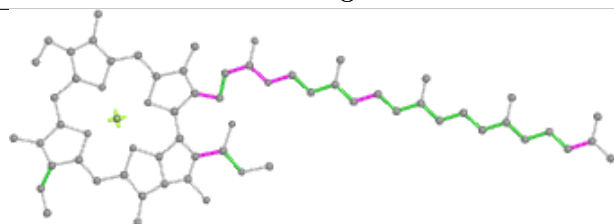
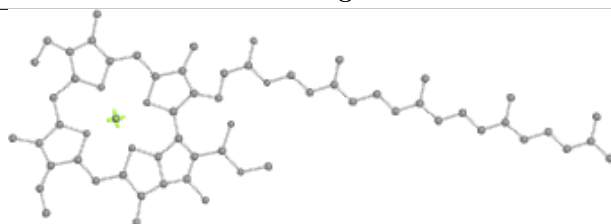


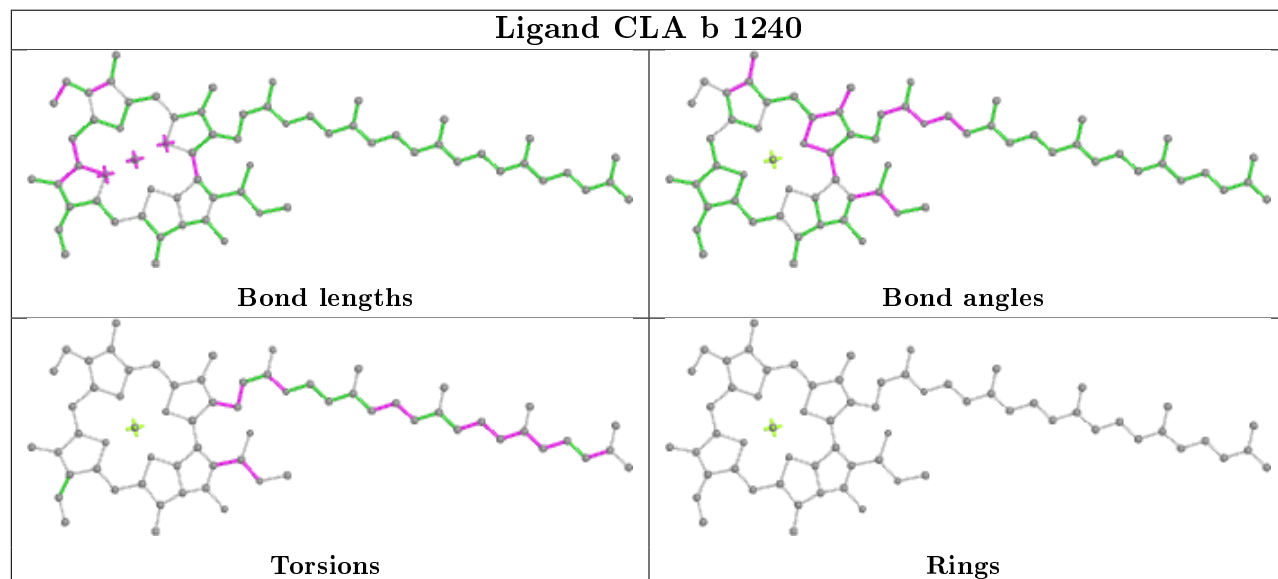
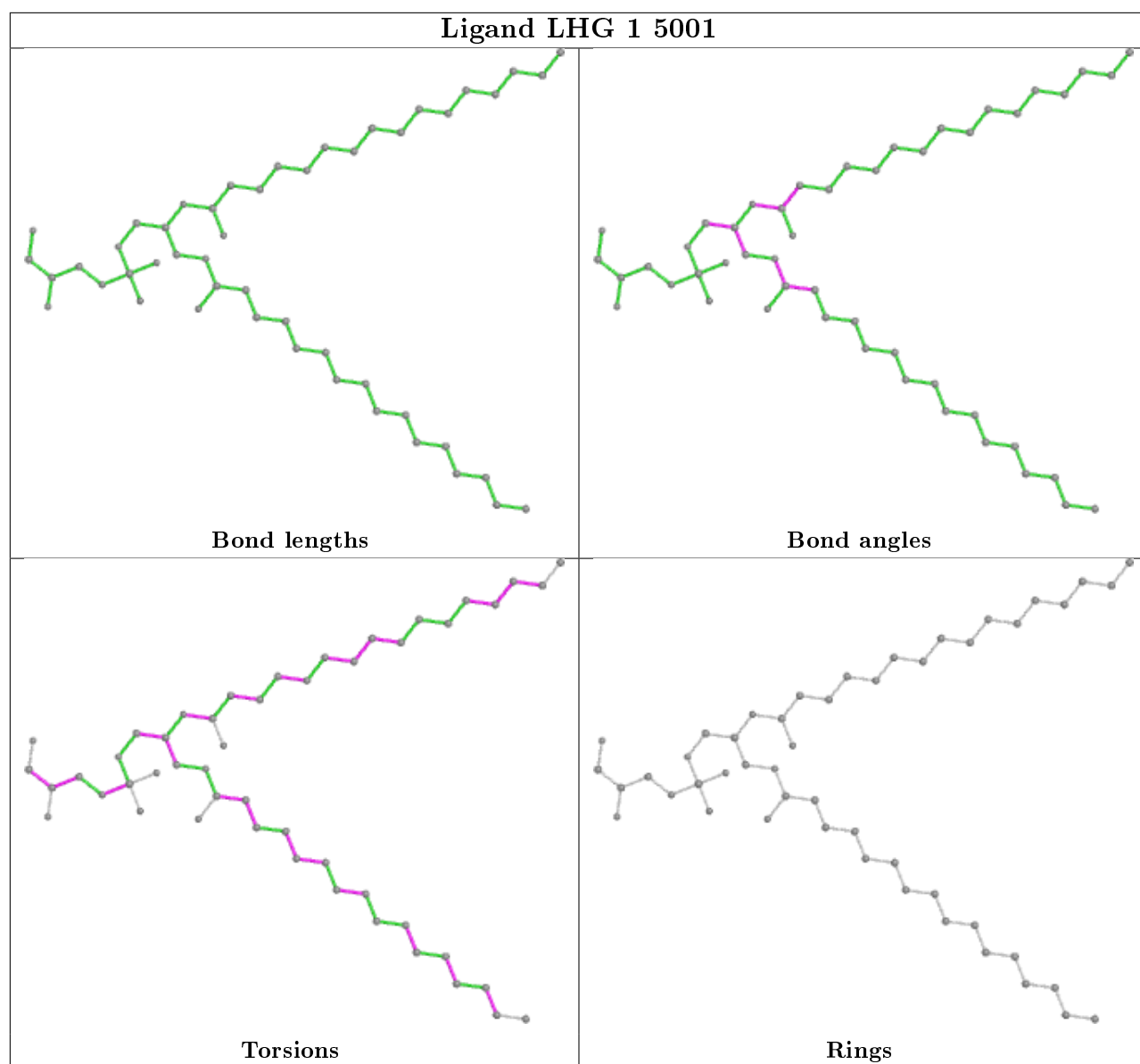


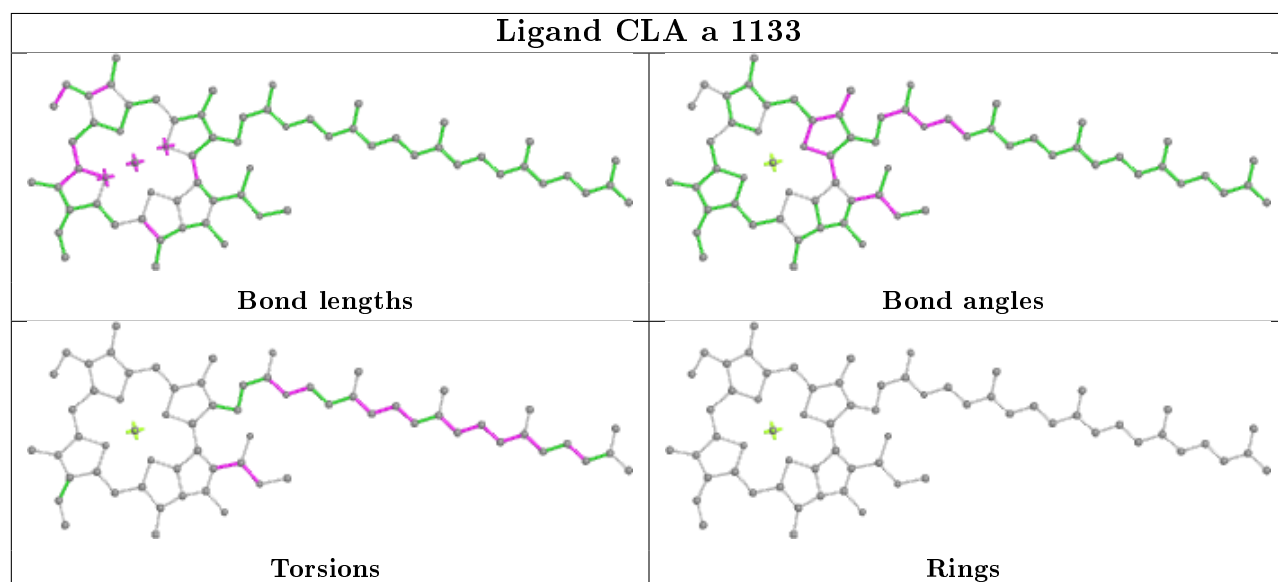
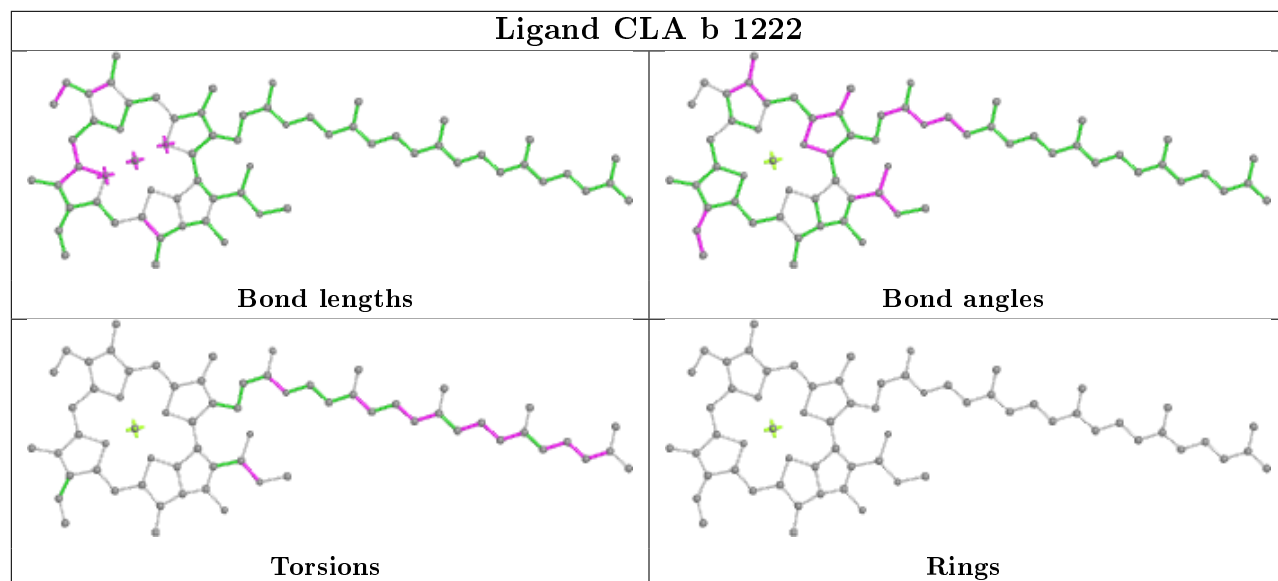
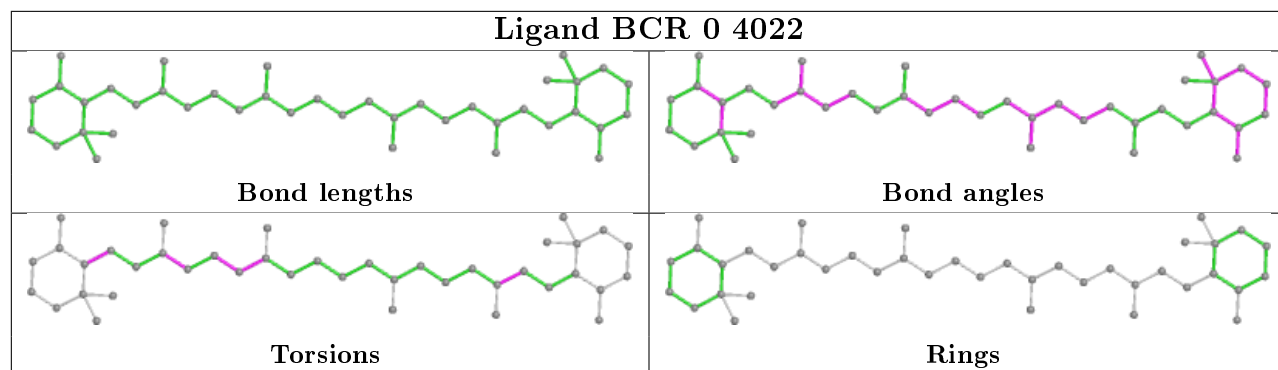
Ligand CLA A 1110**Ligand CLA 1 1124**

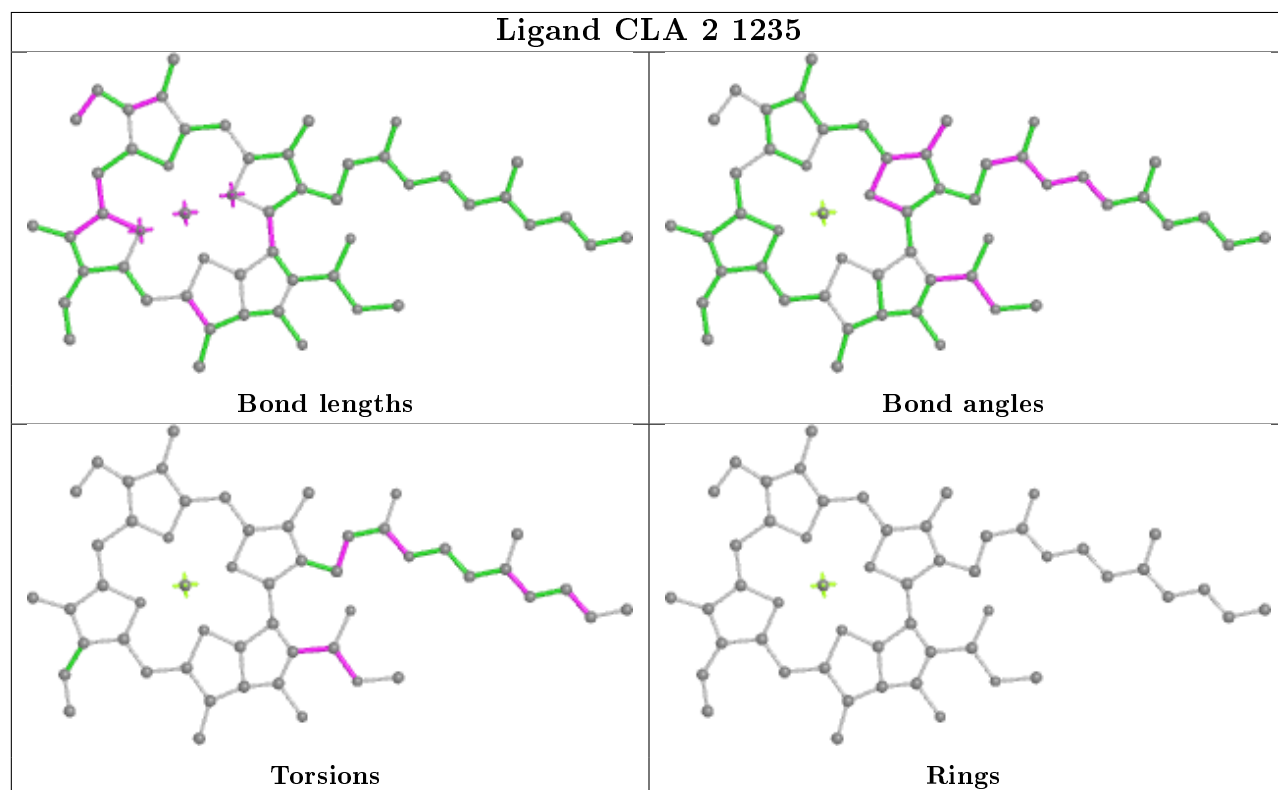
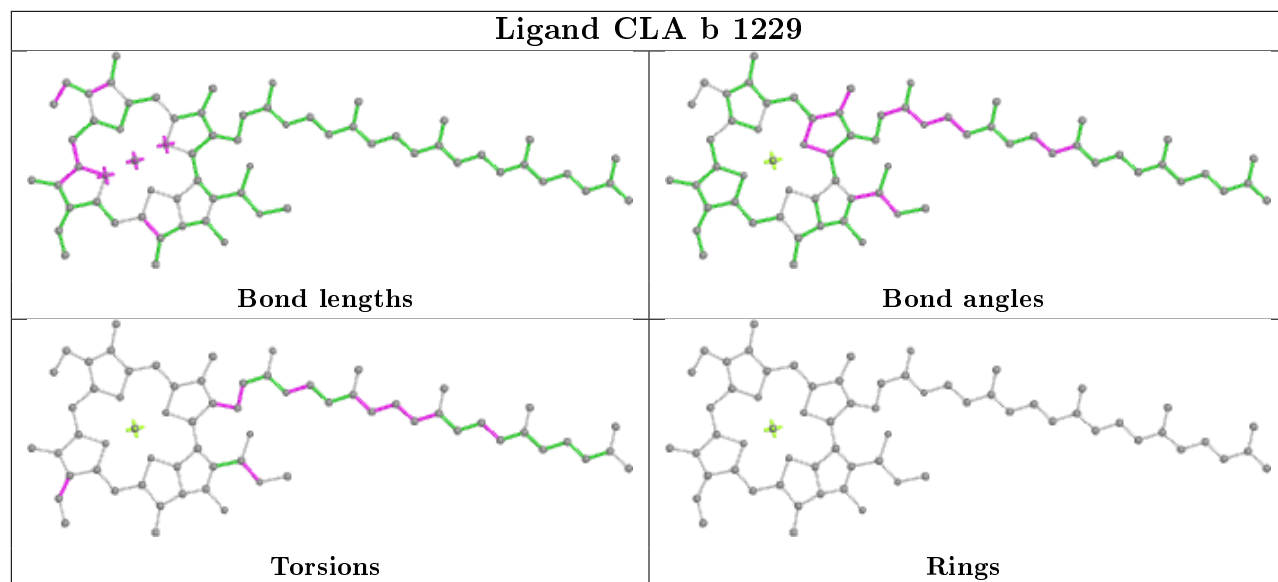


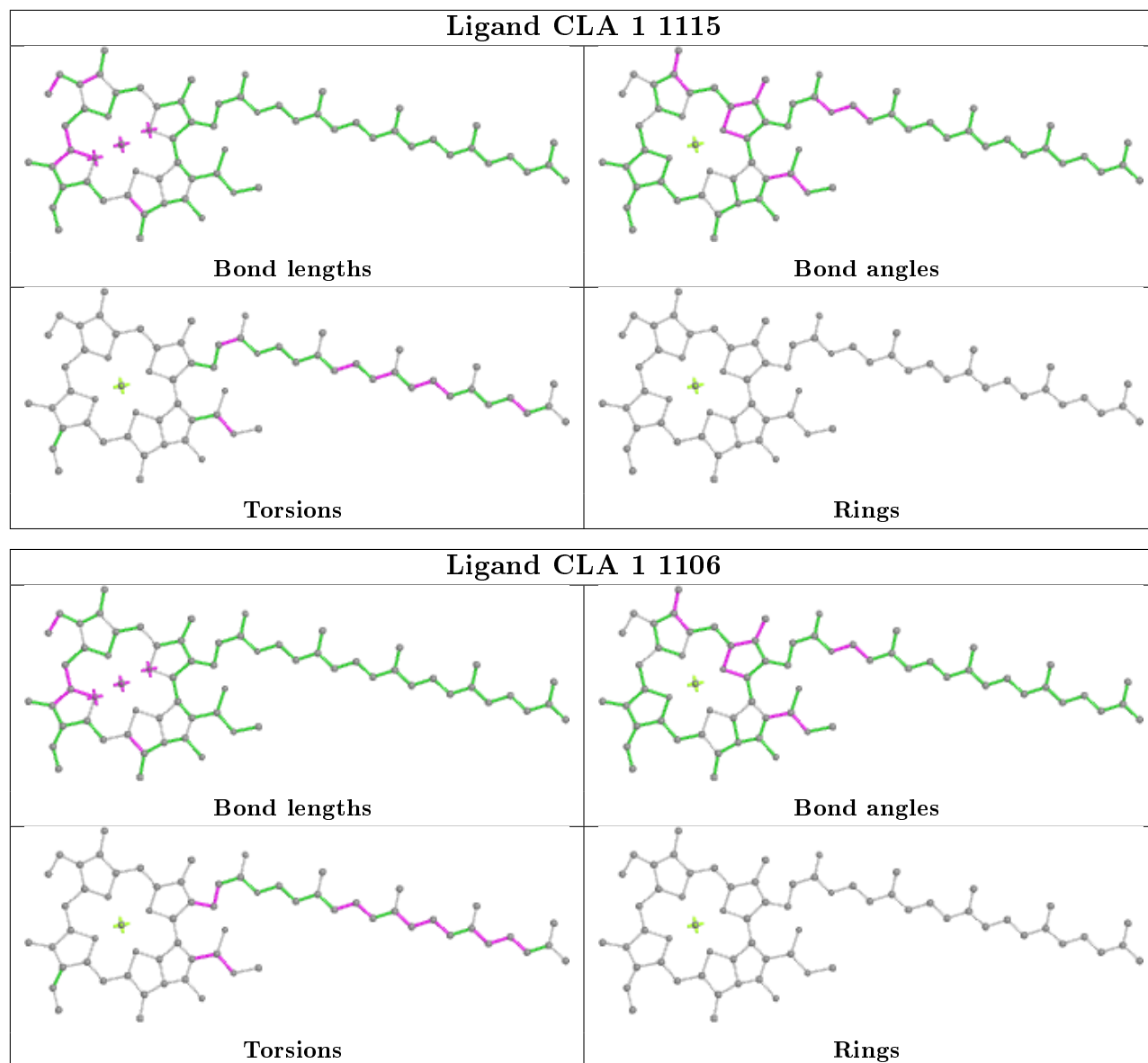


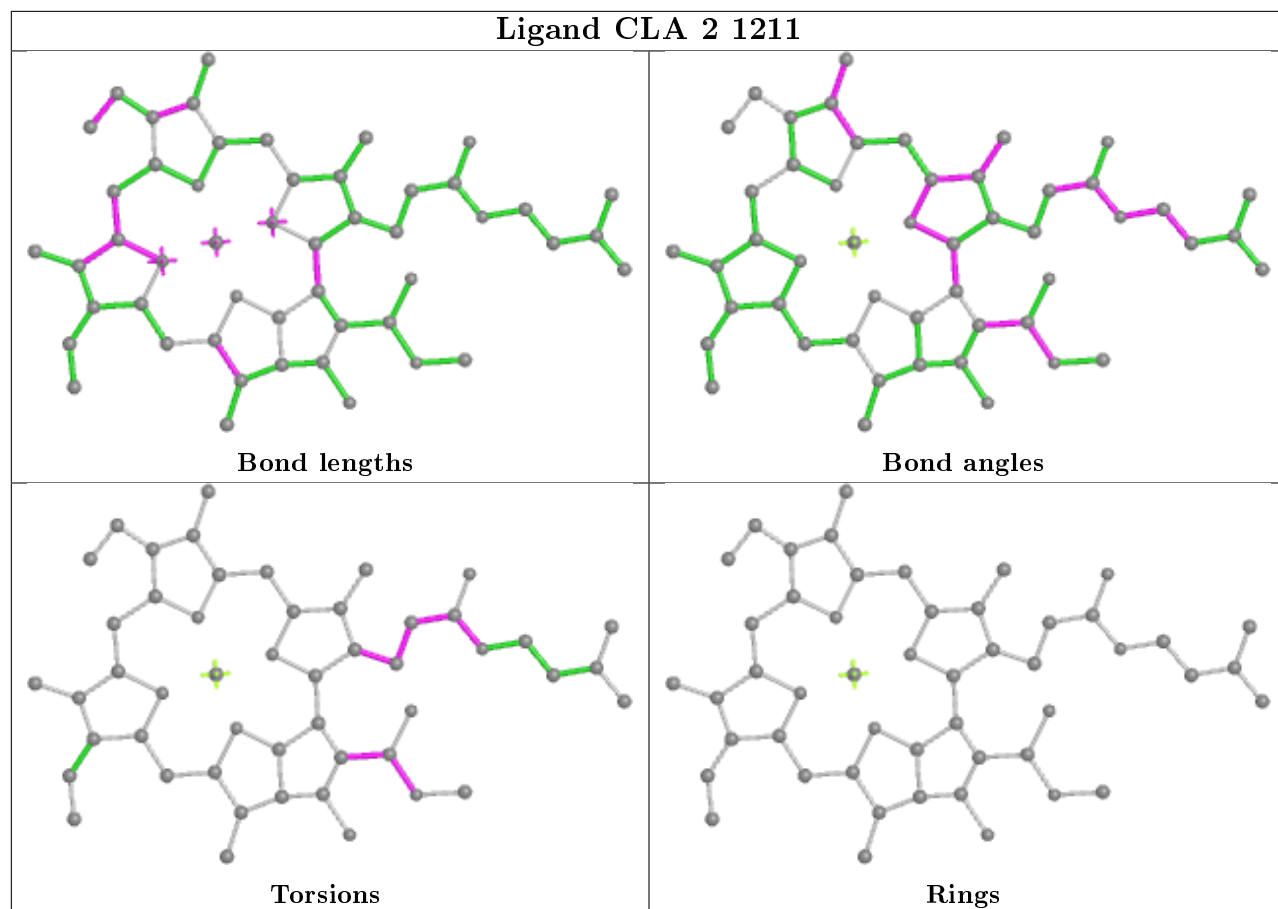
Ligand CLA B 1231**Bond lengths****Bond angles****Torsions****Rings****Ligand CLA A 1011****Bond lengths****Bond angles****Torsions****Rings**

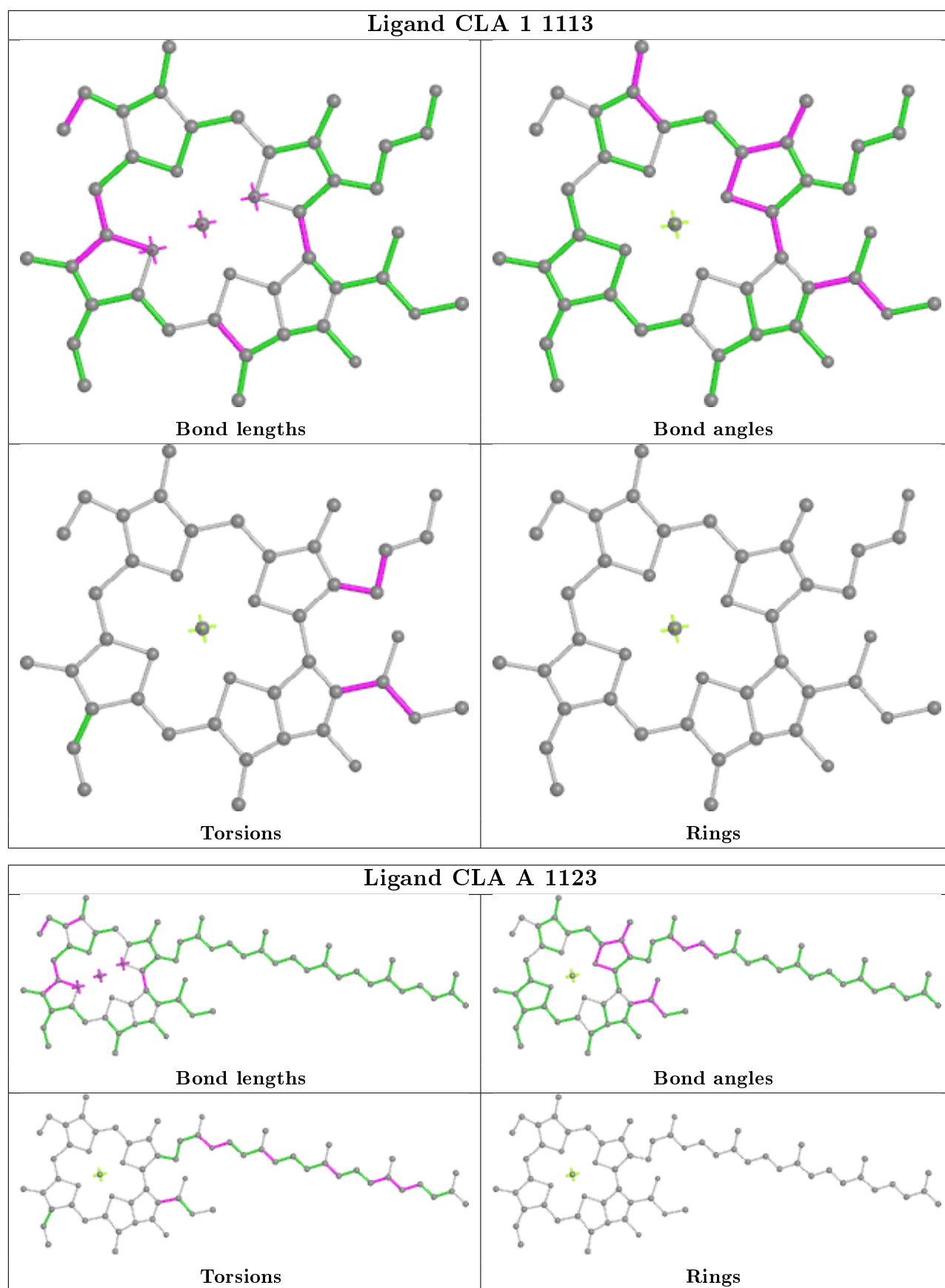


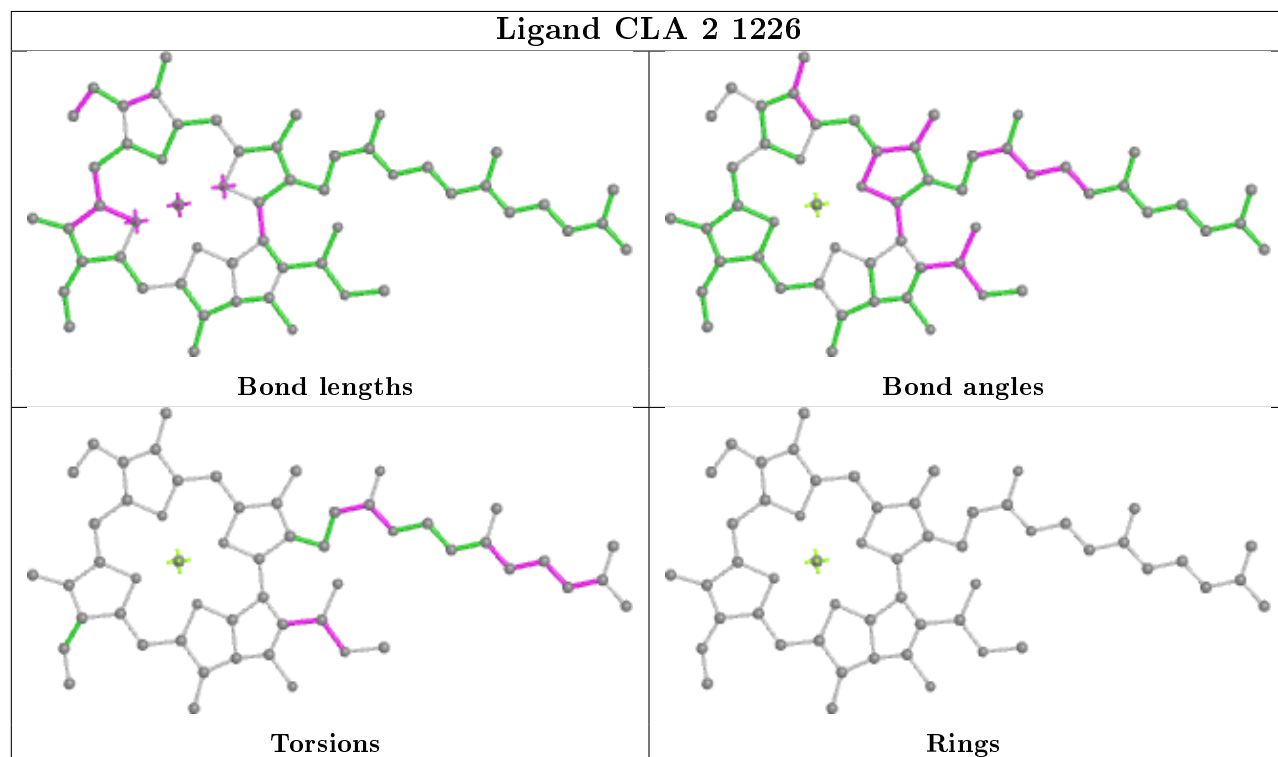
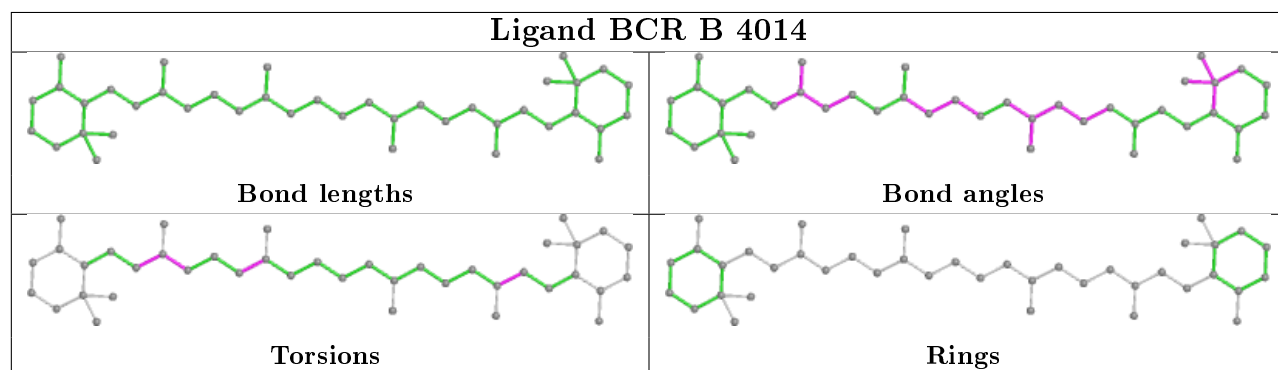
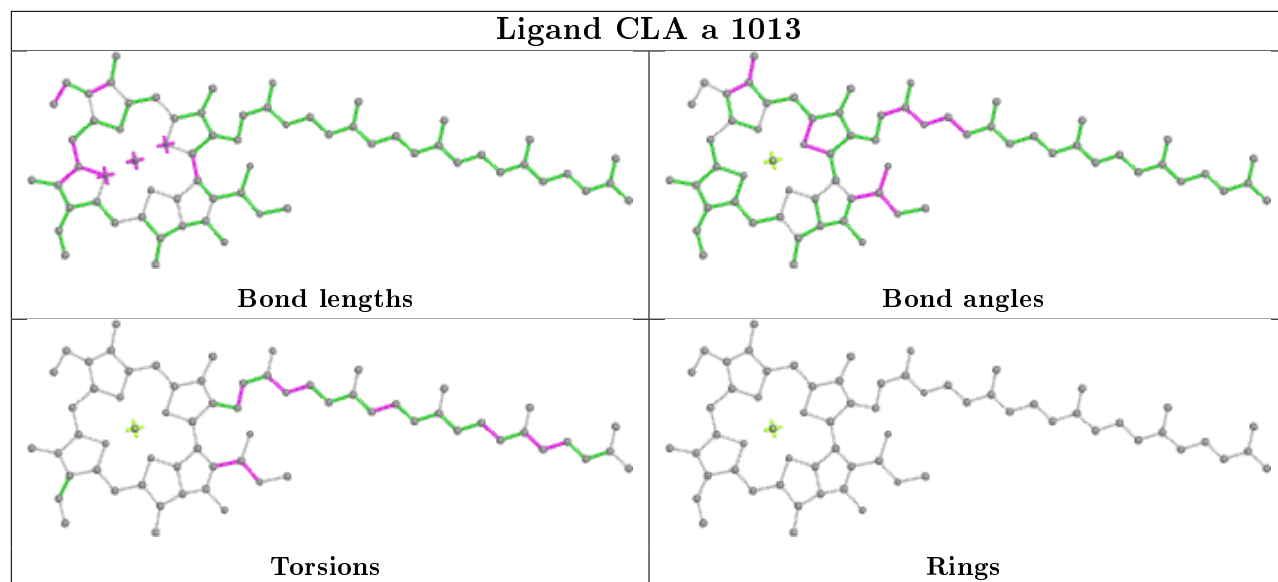


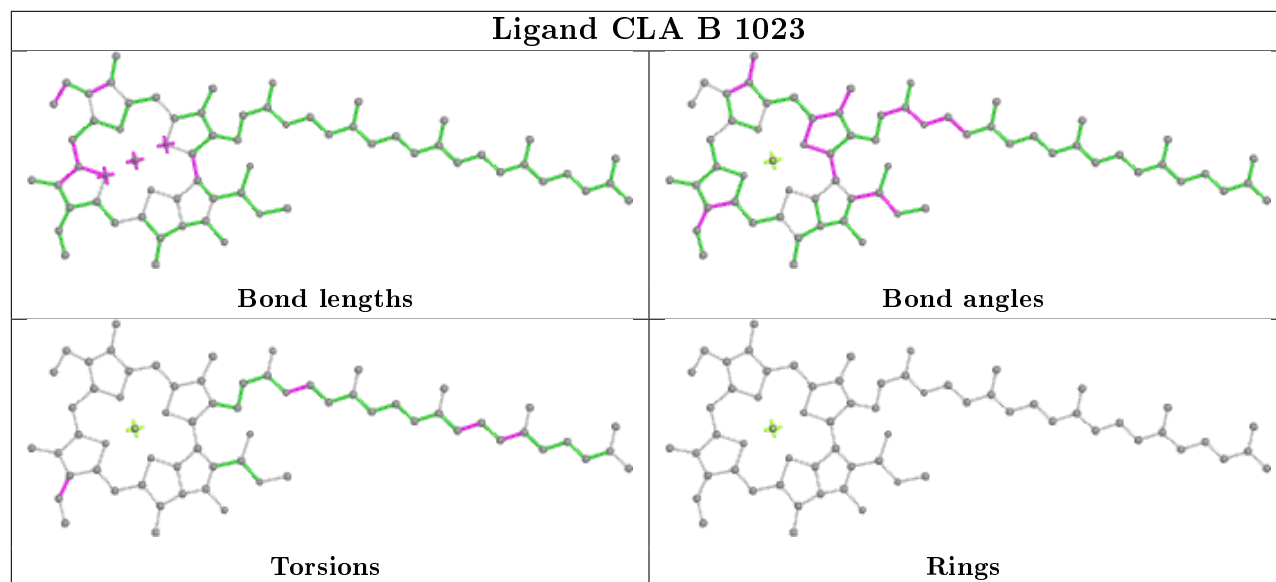
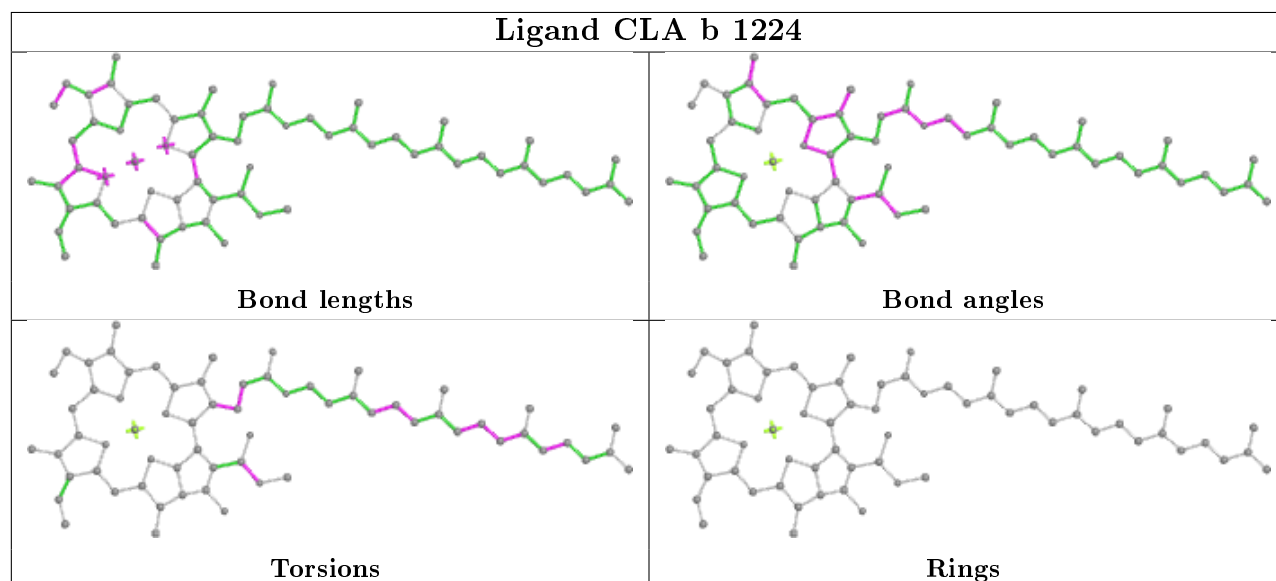
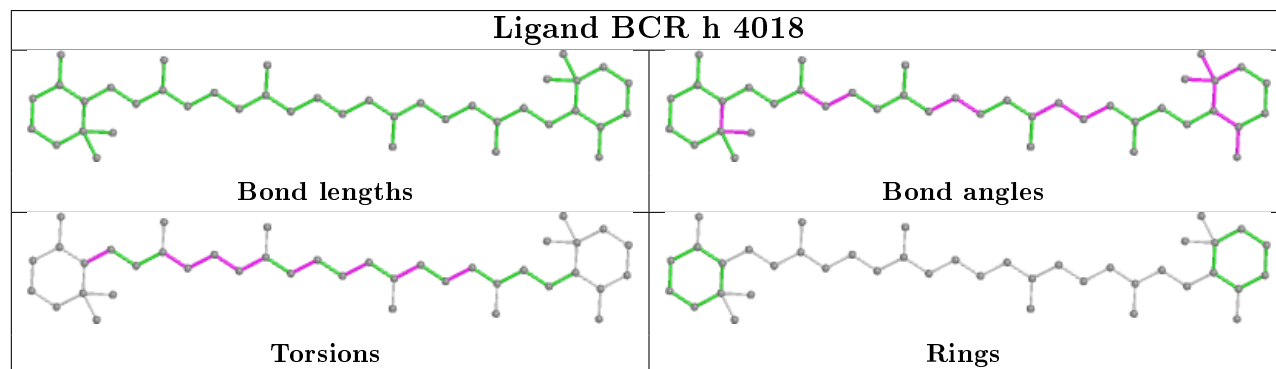


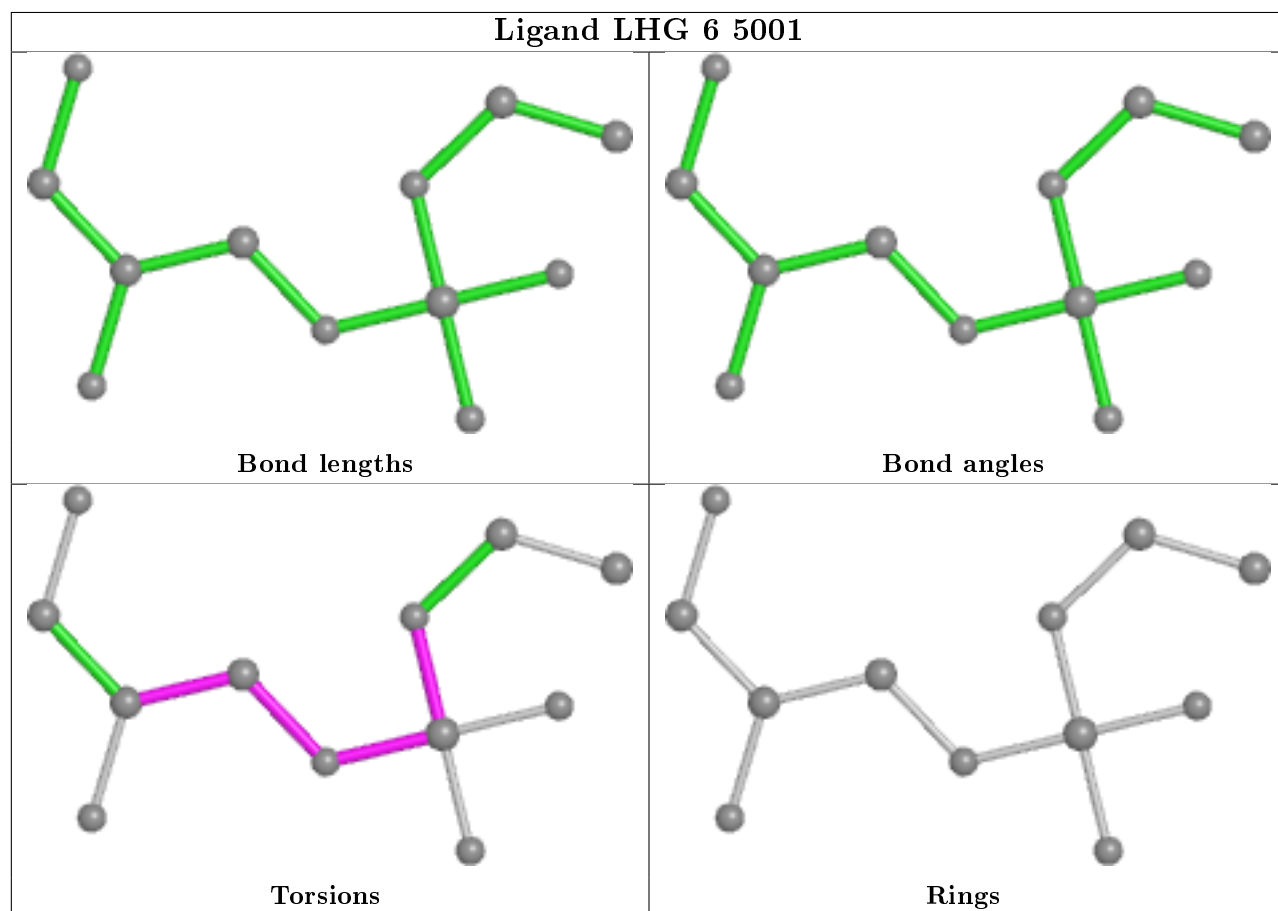
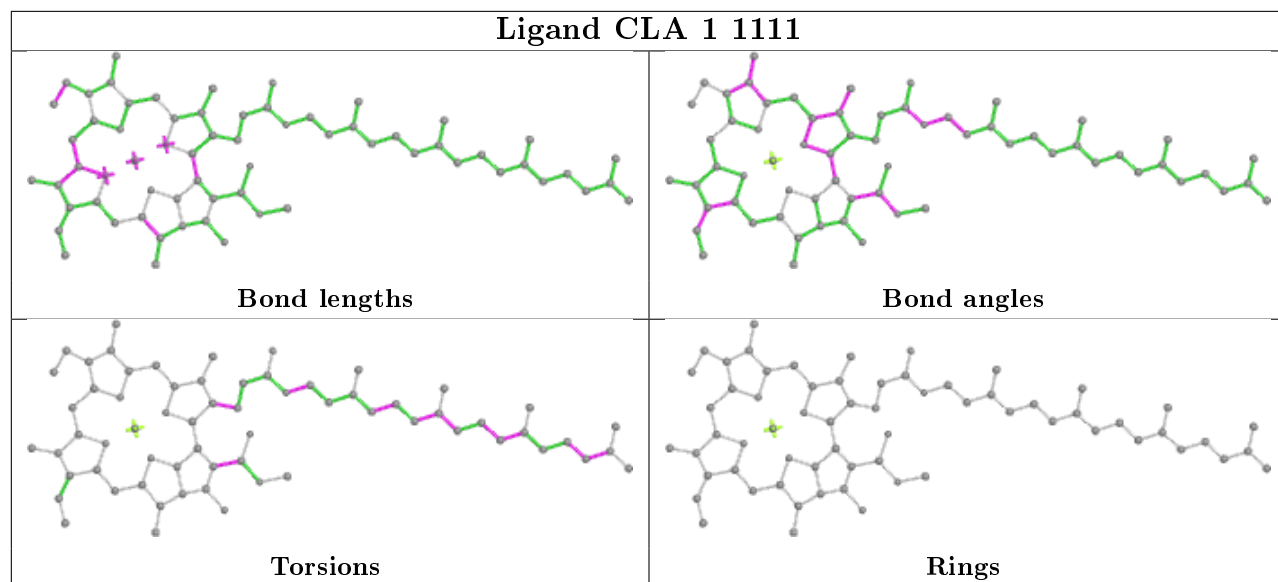


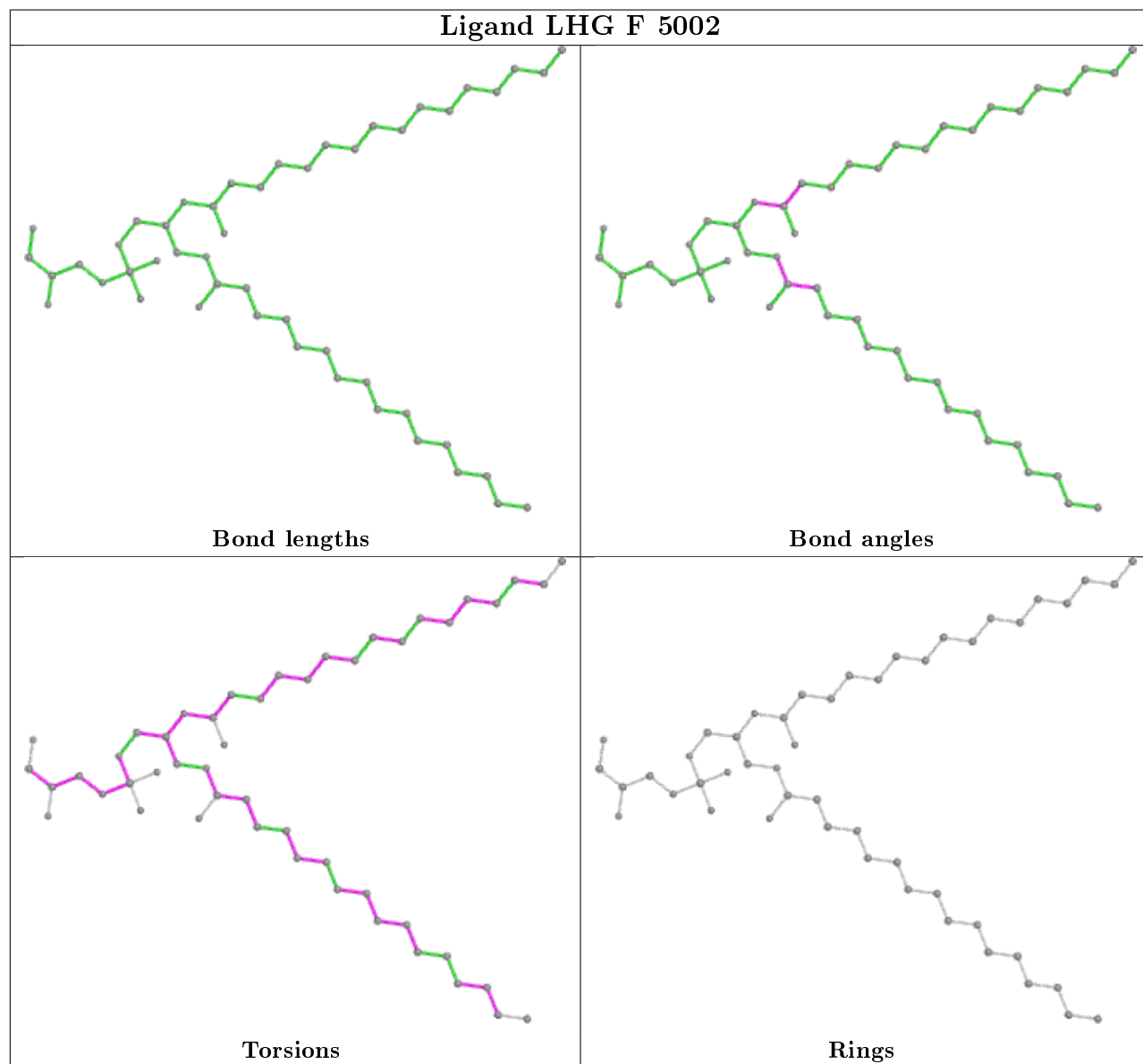
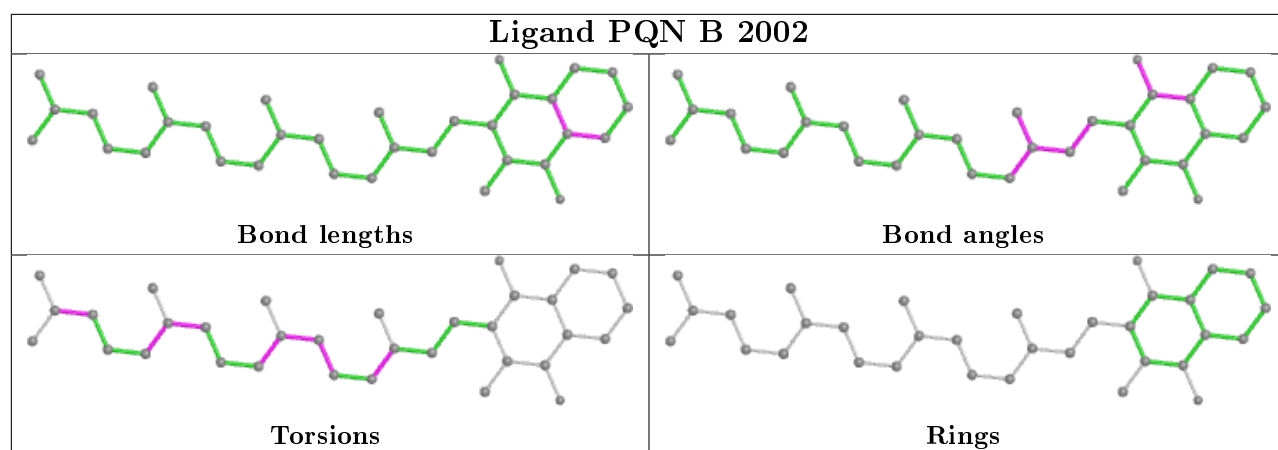


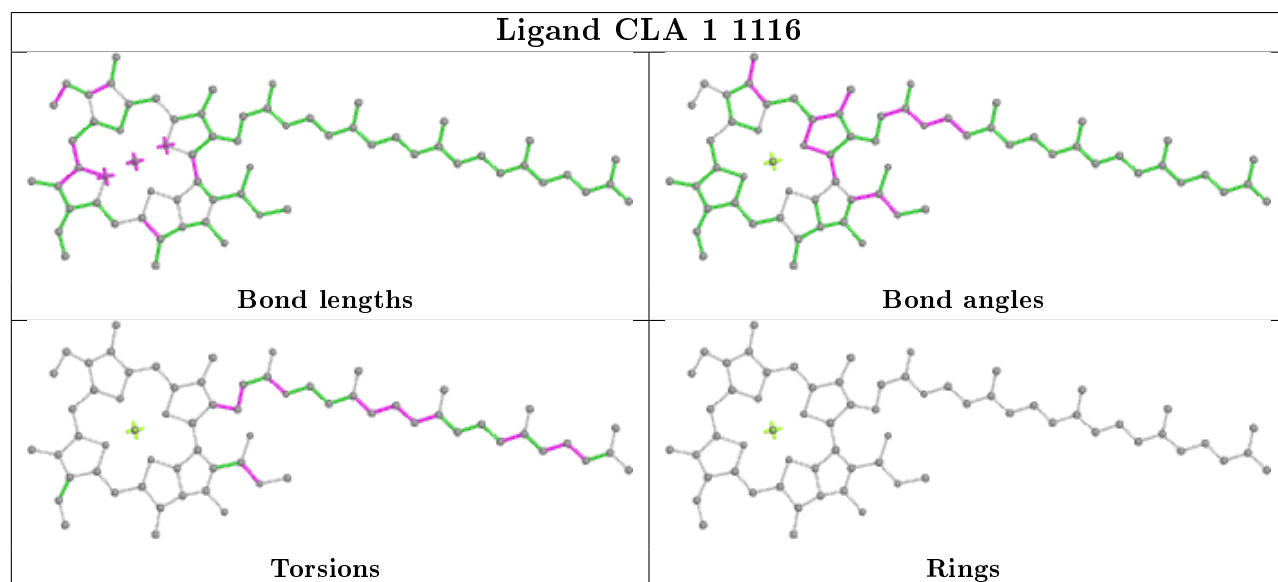
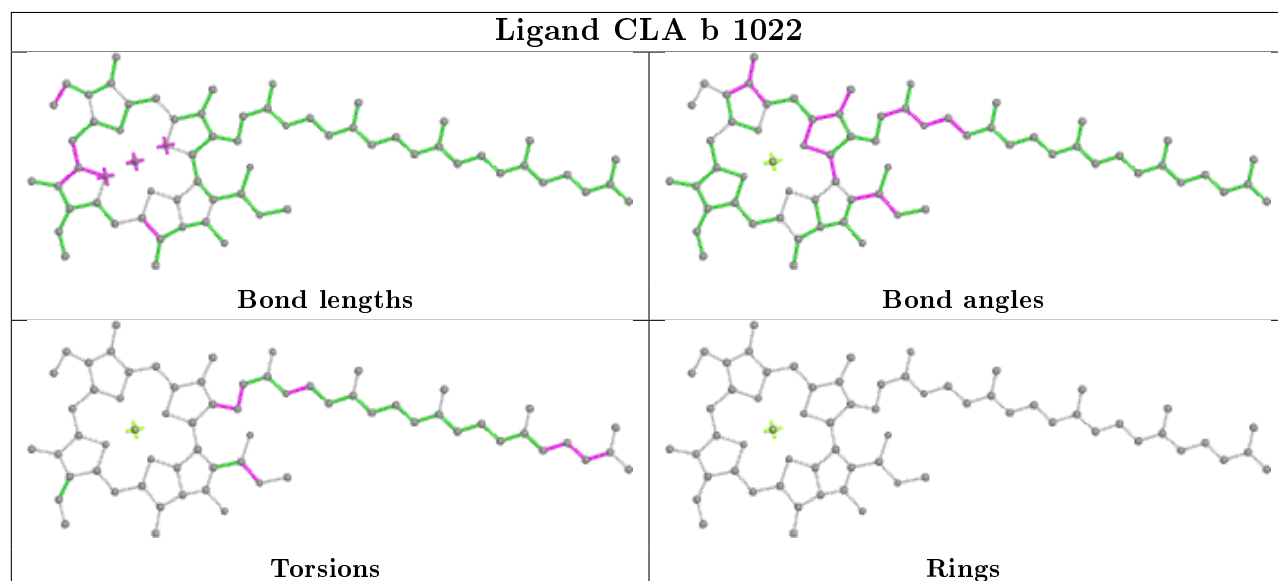
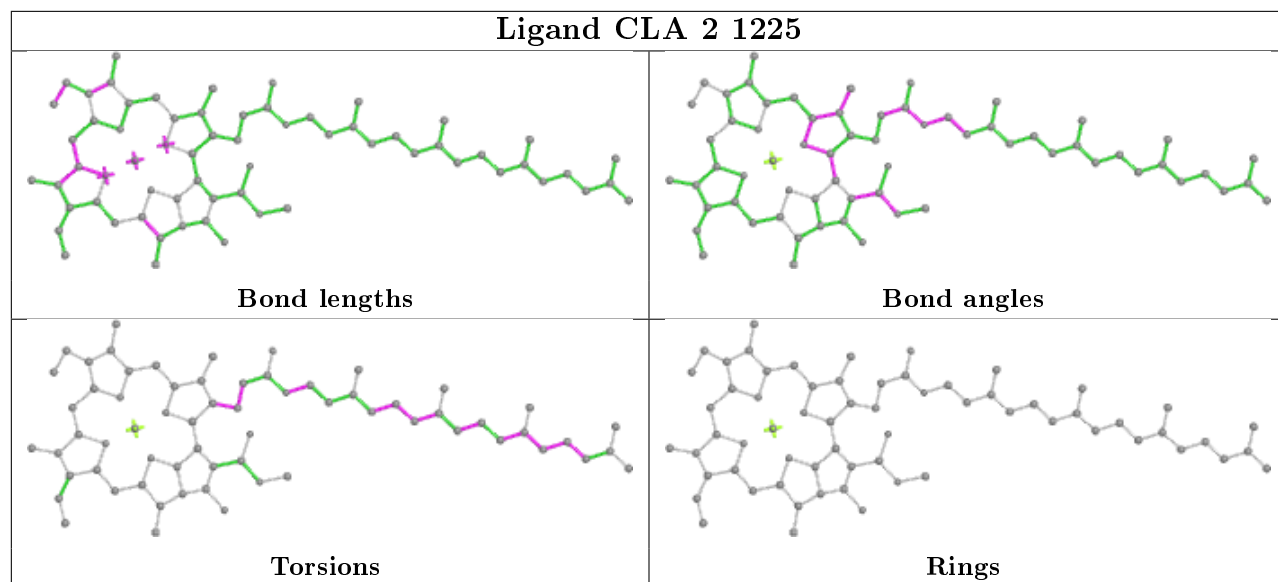


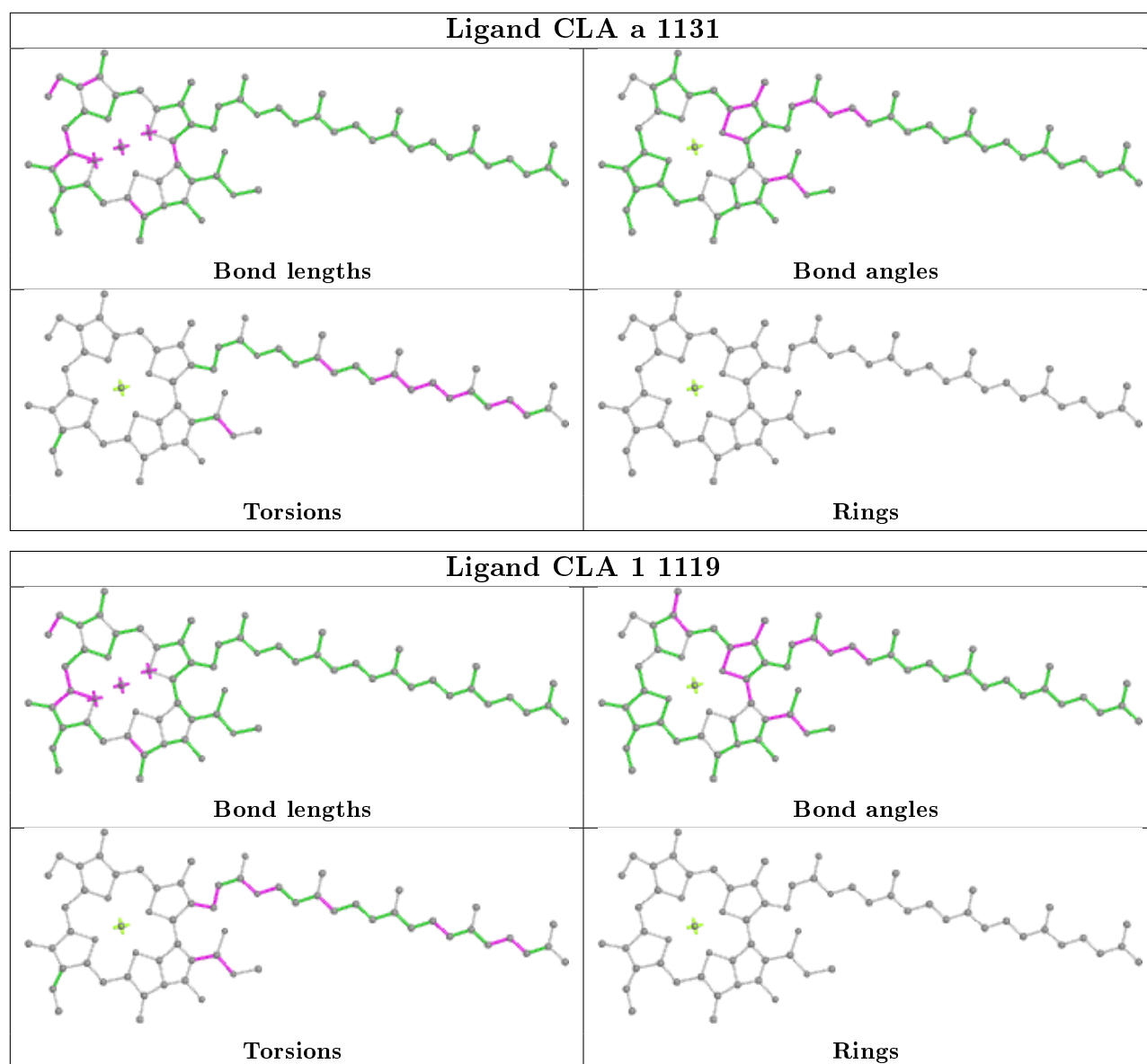


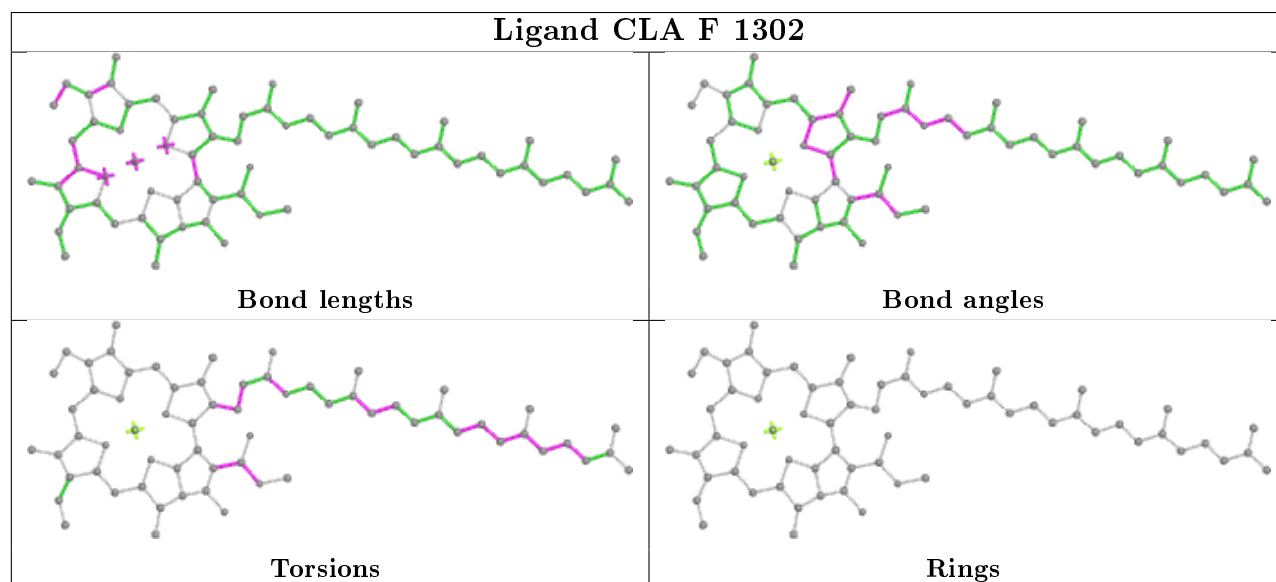
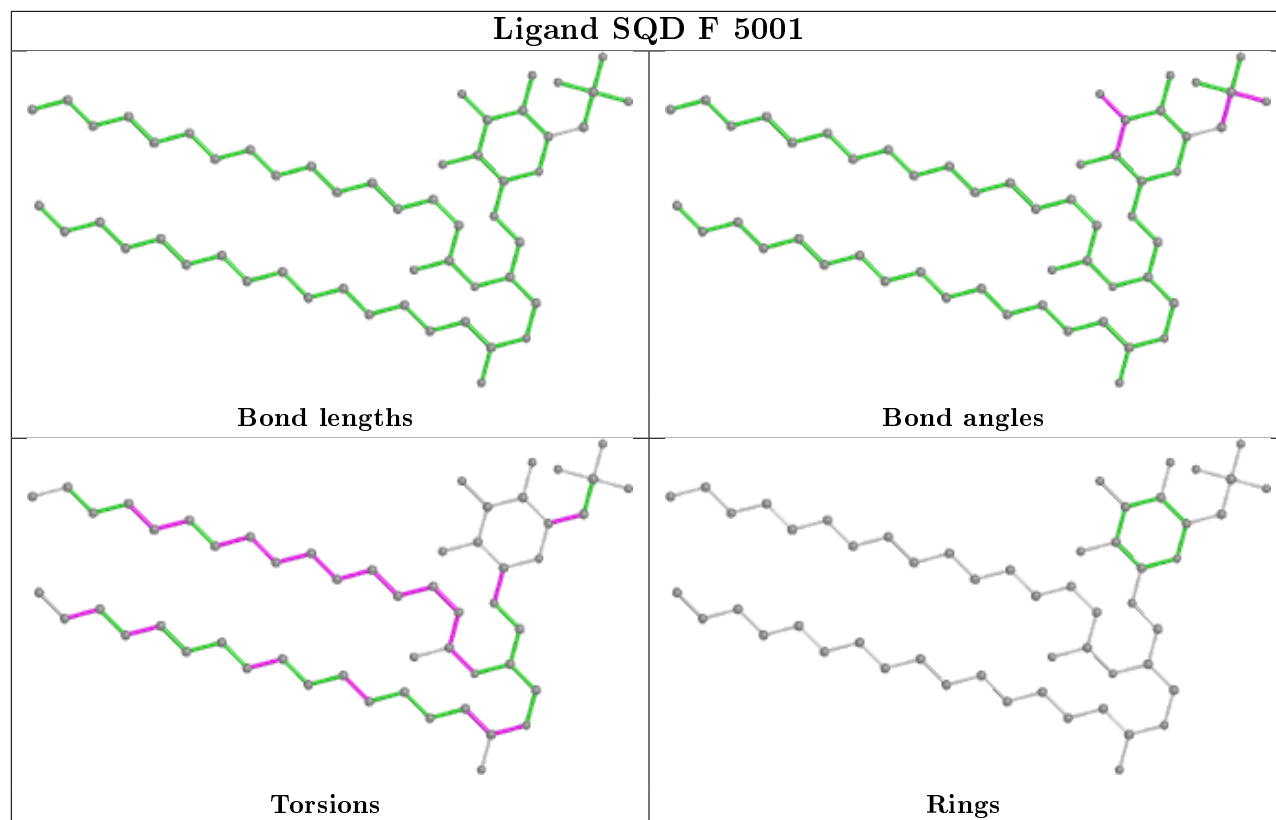
Ligand CLA B 1023**Ligand CLA b 1224****Ligand BCR h 4018**

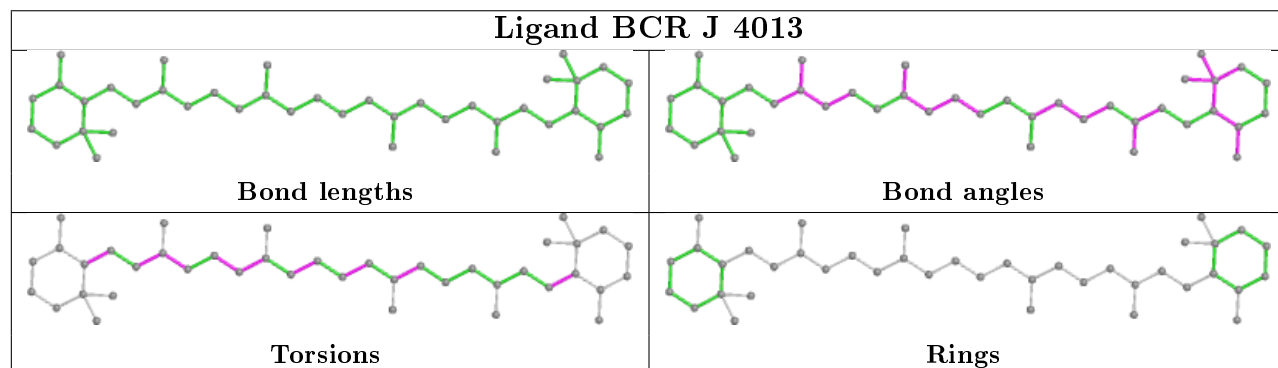
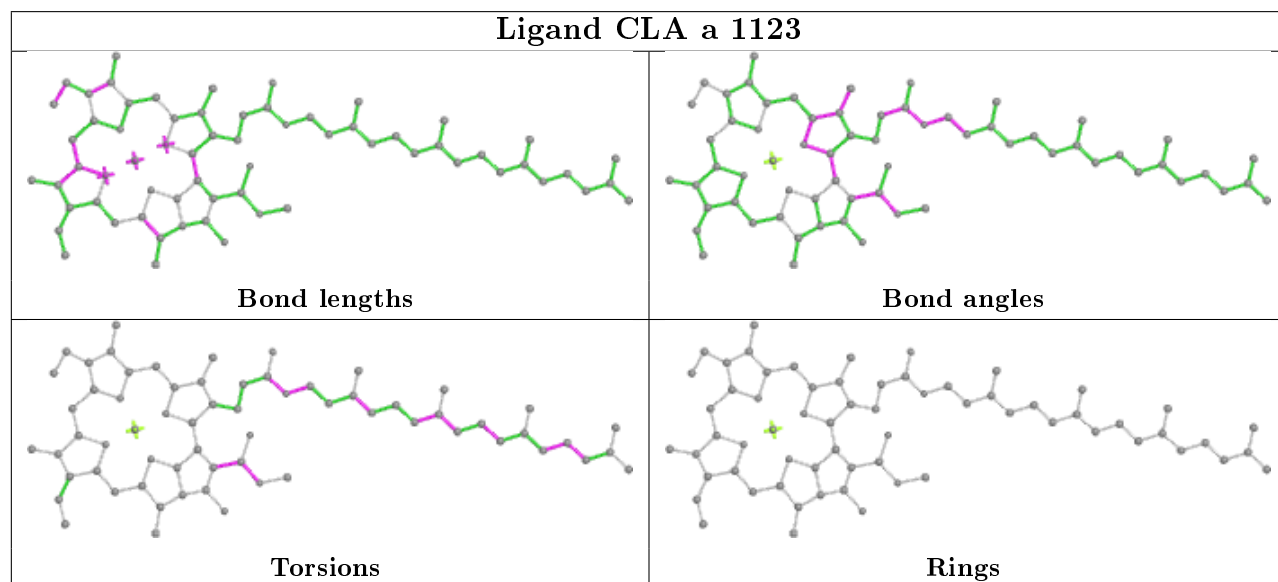
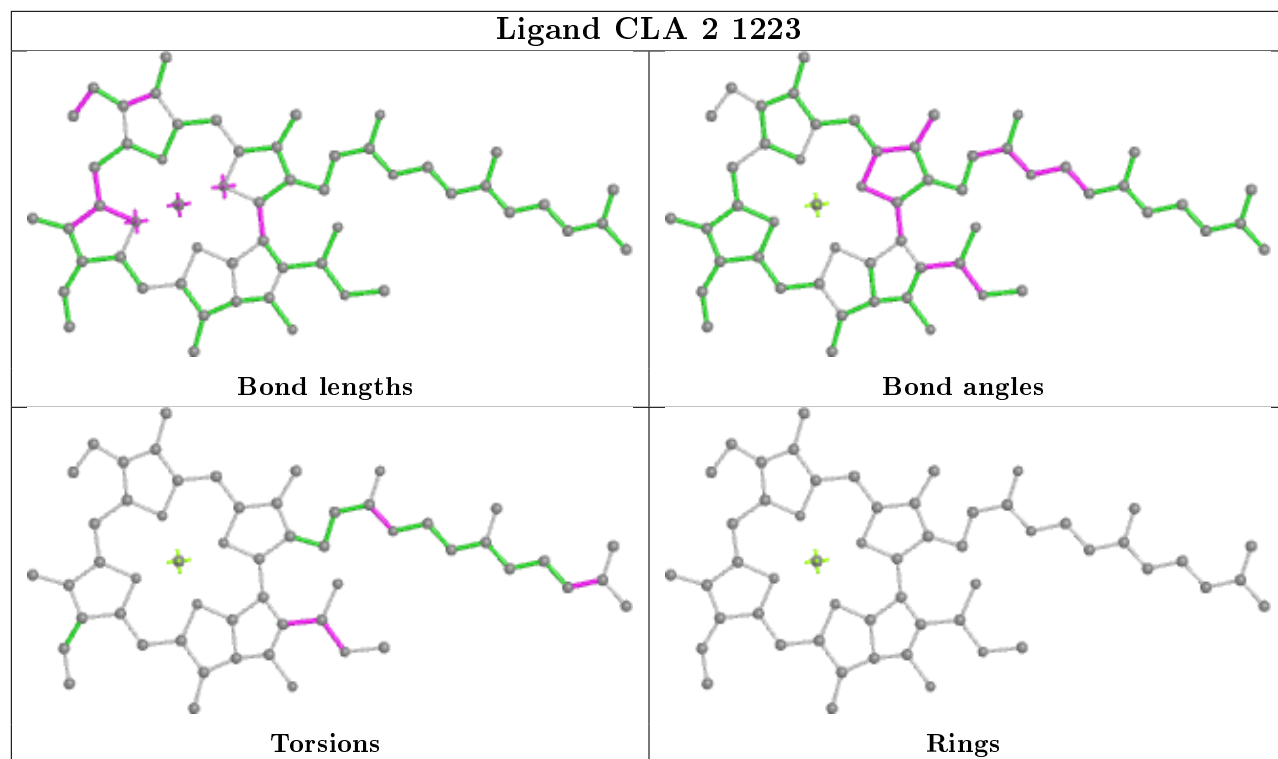


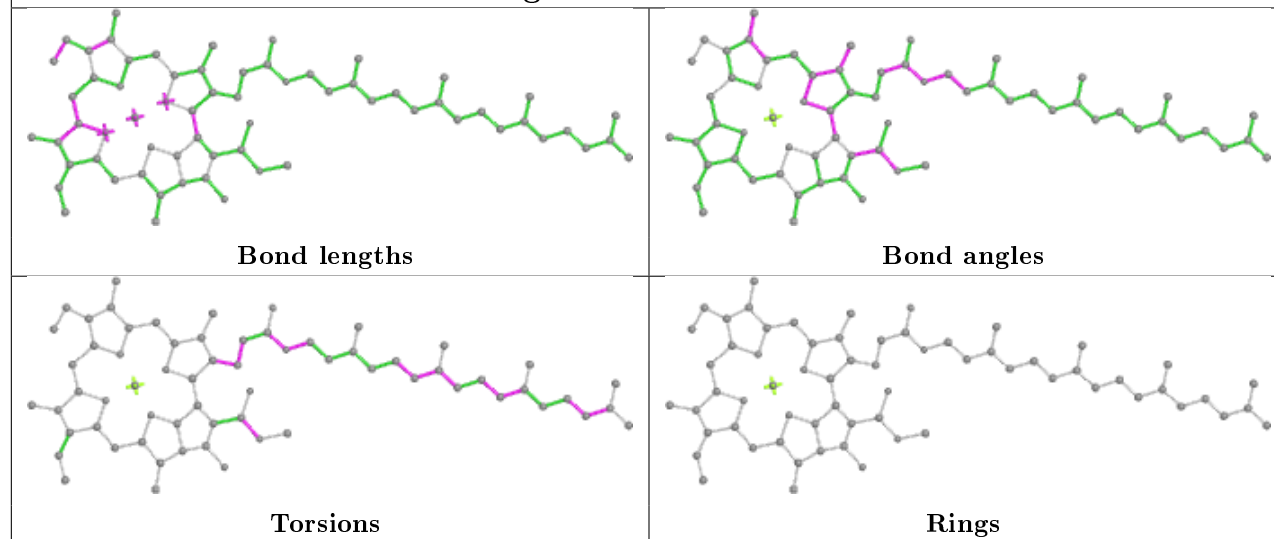
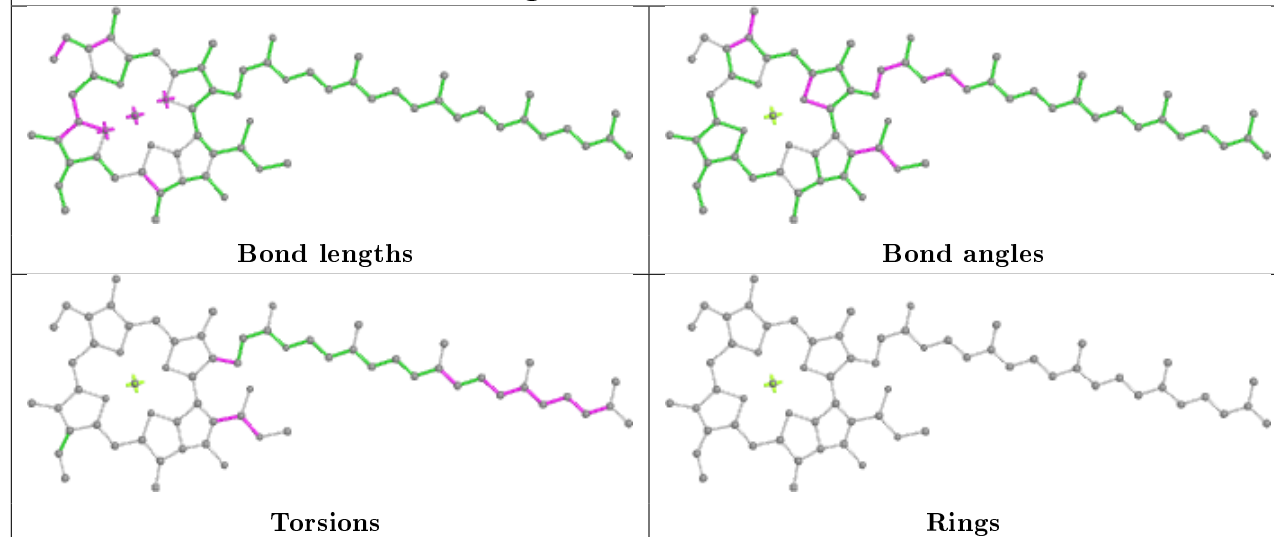


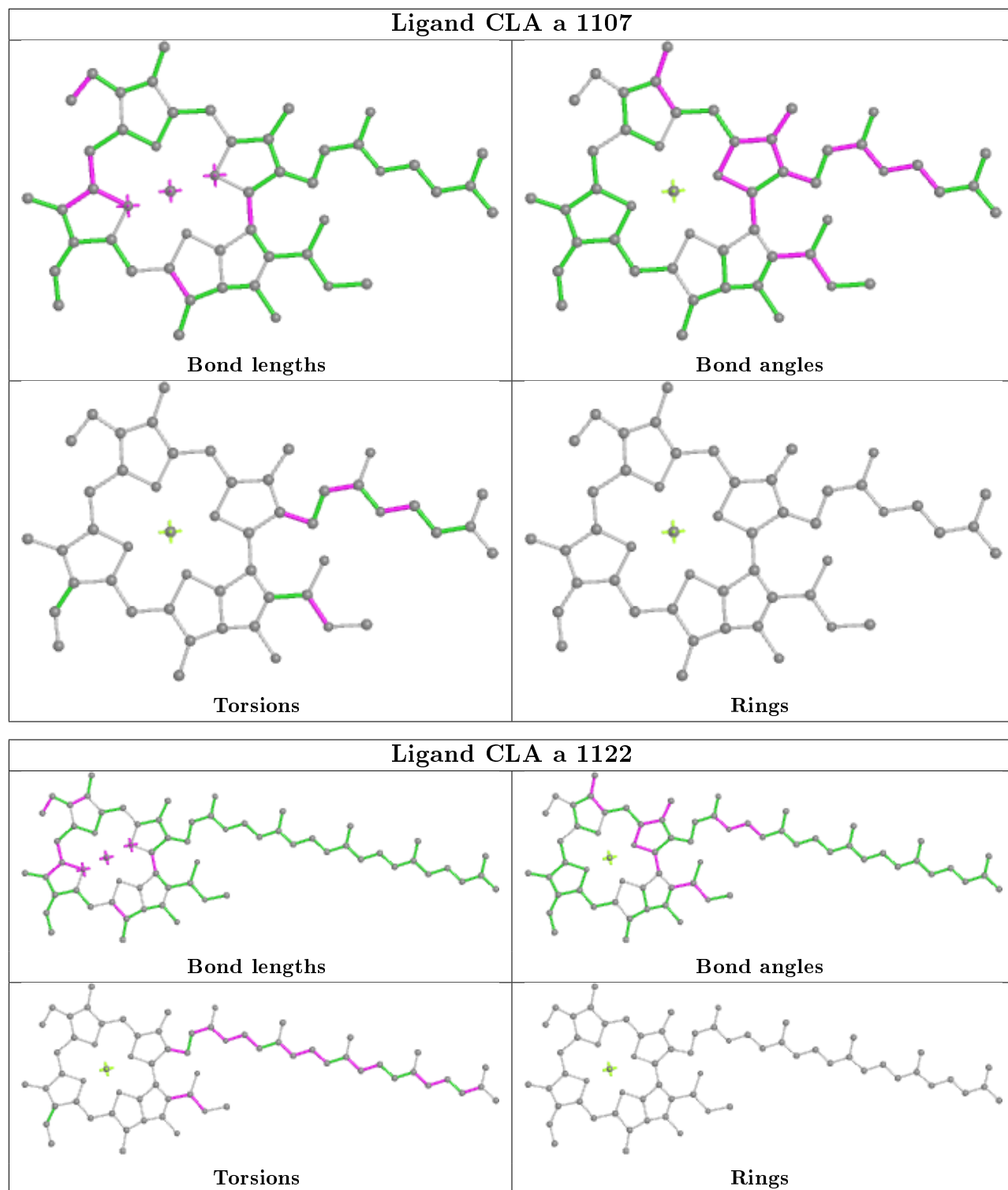


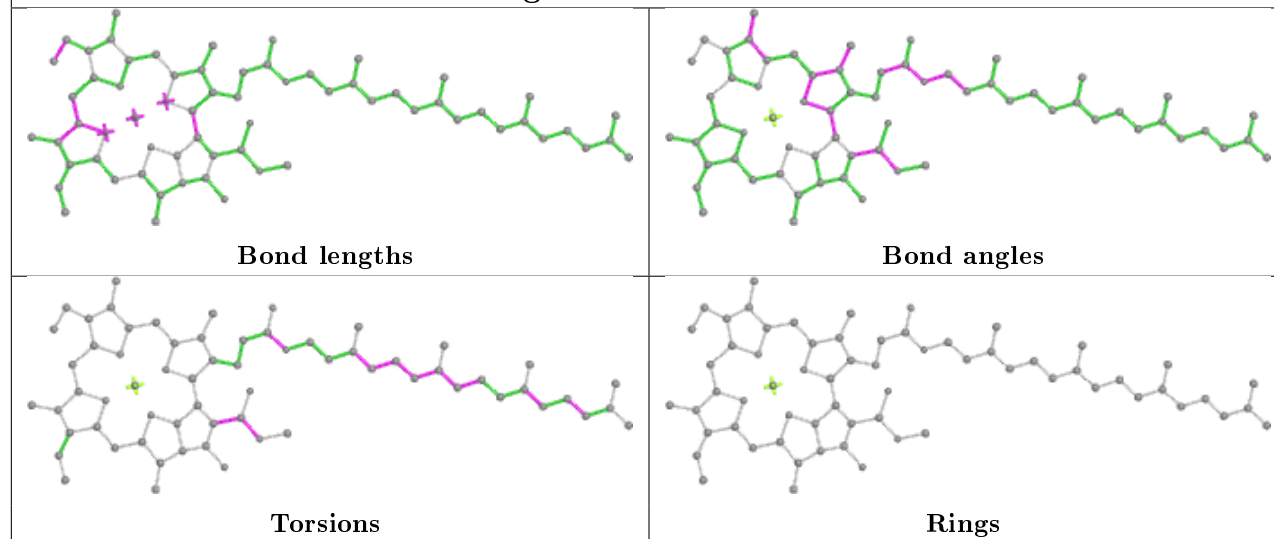
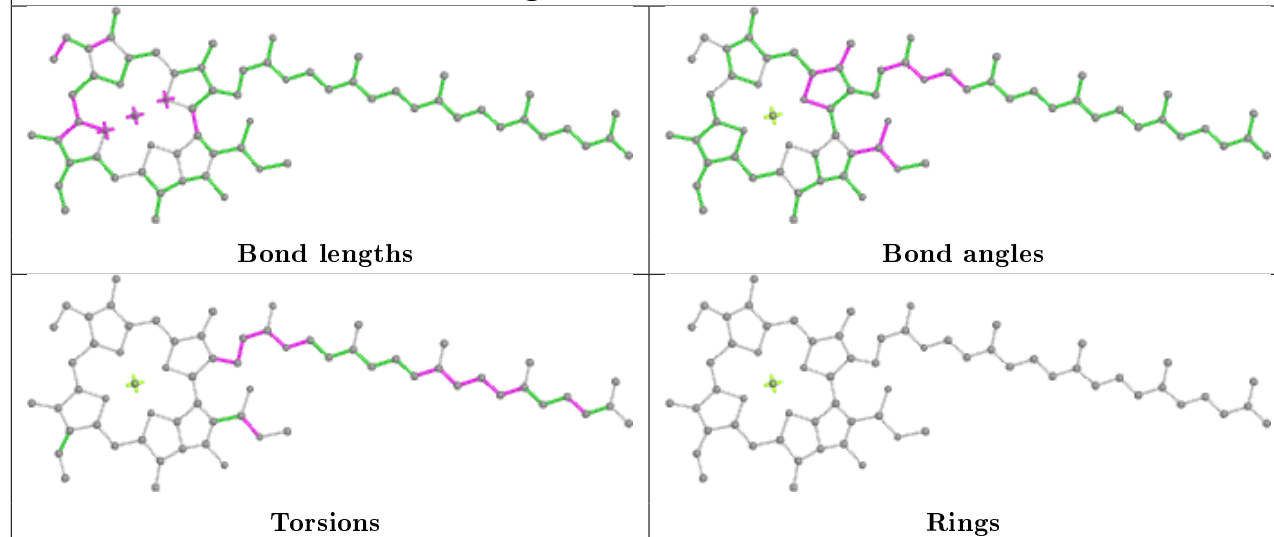


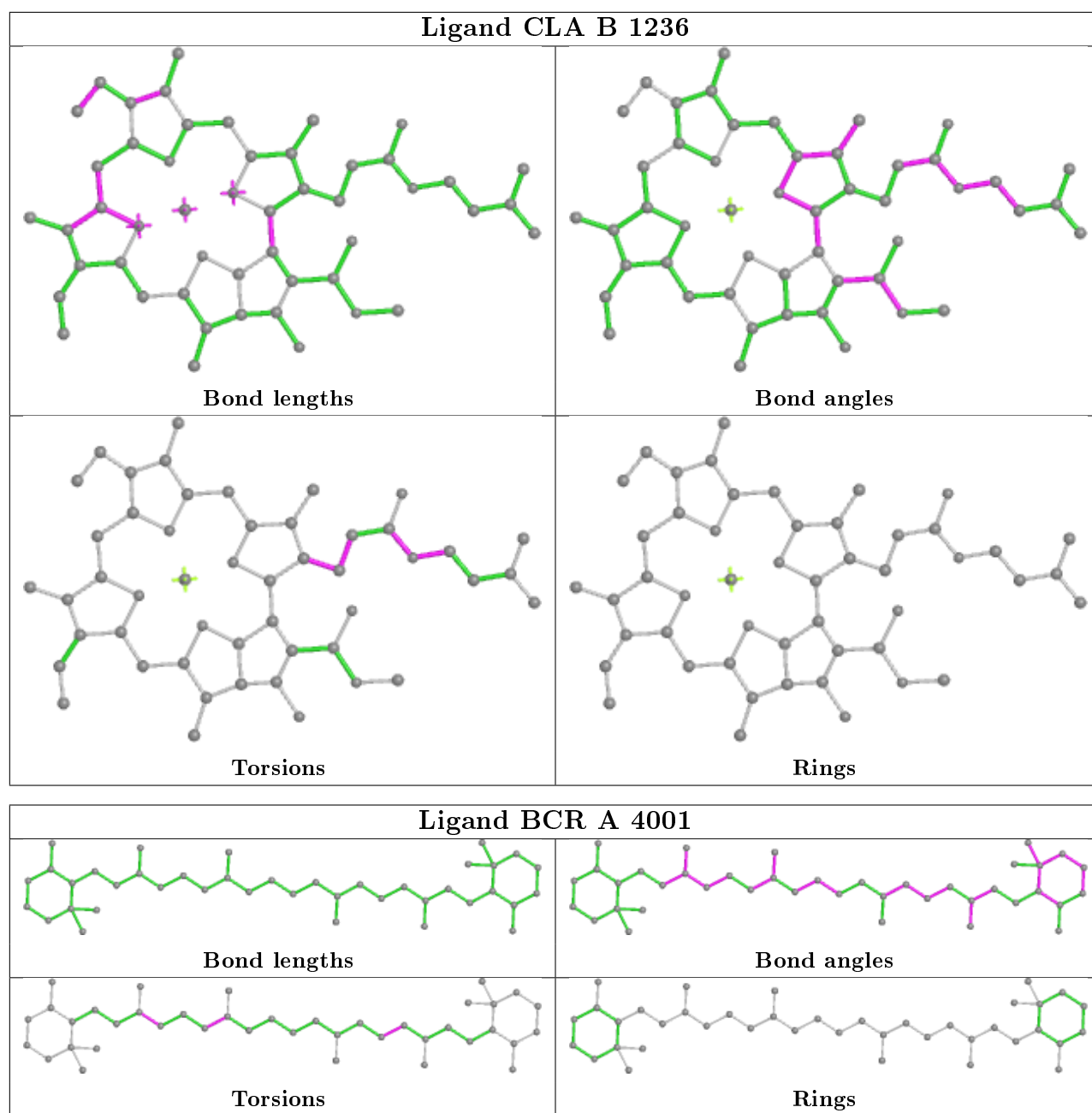


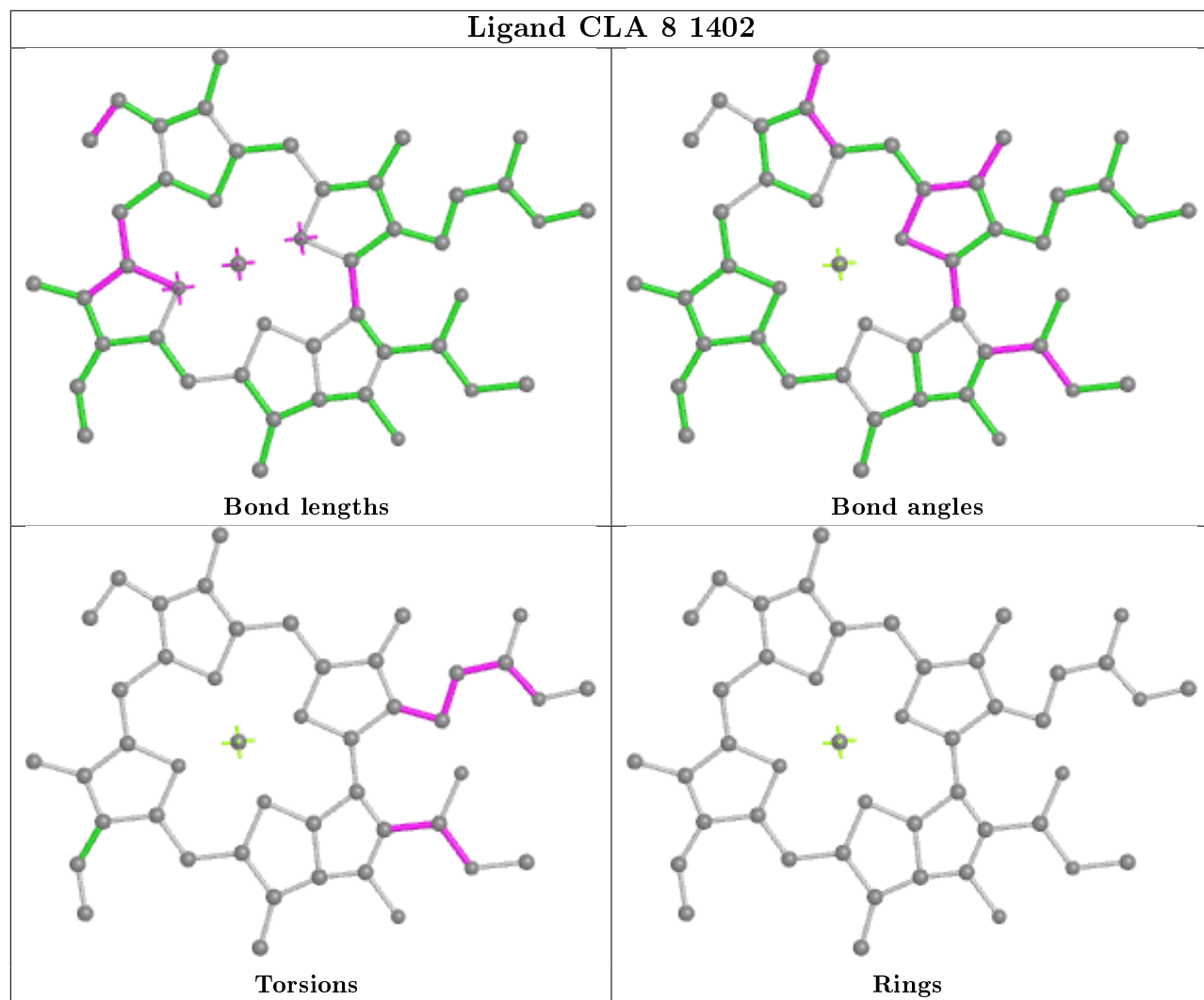


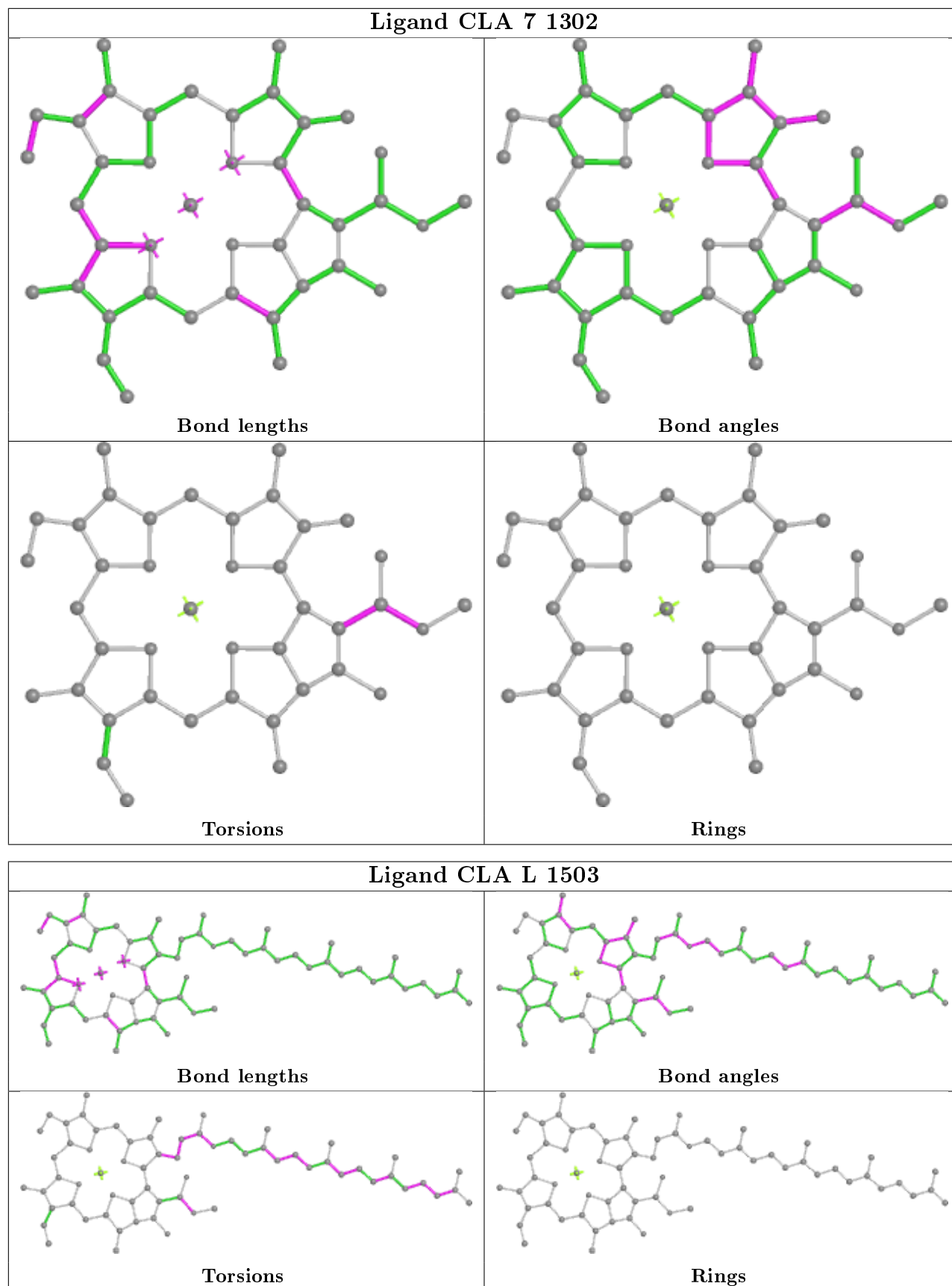
Ligand CLA A 1112**Ligand CLA A 1103**

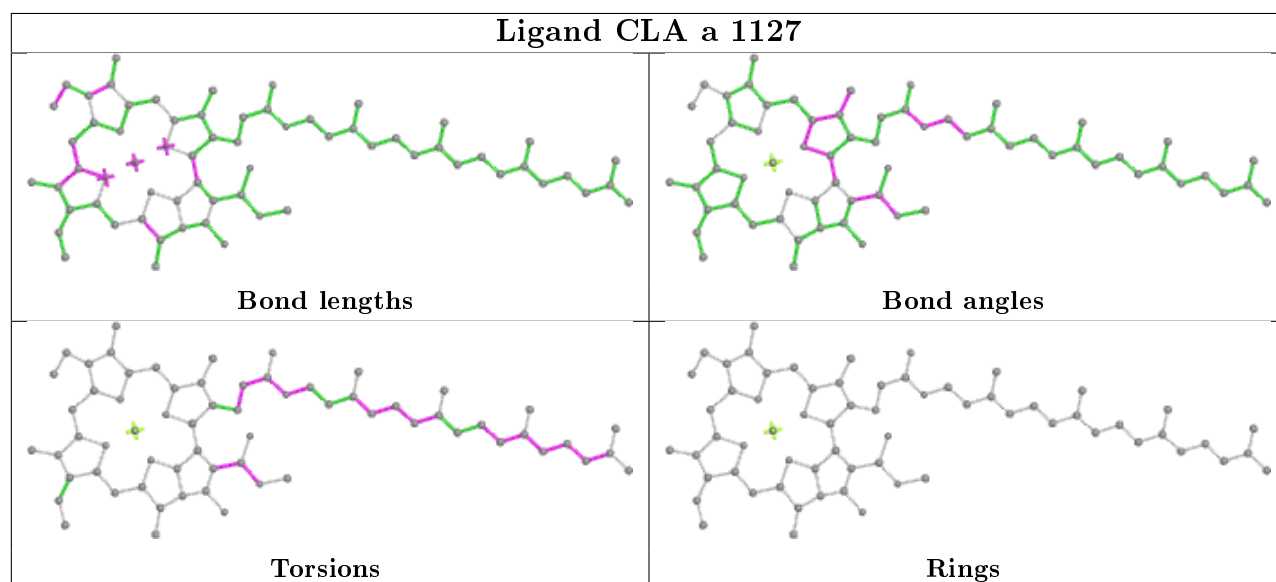
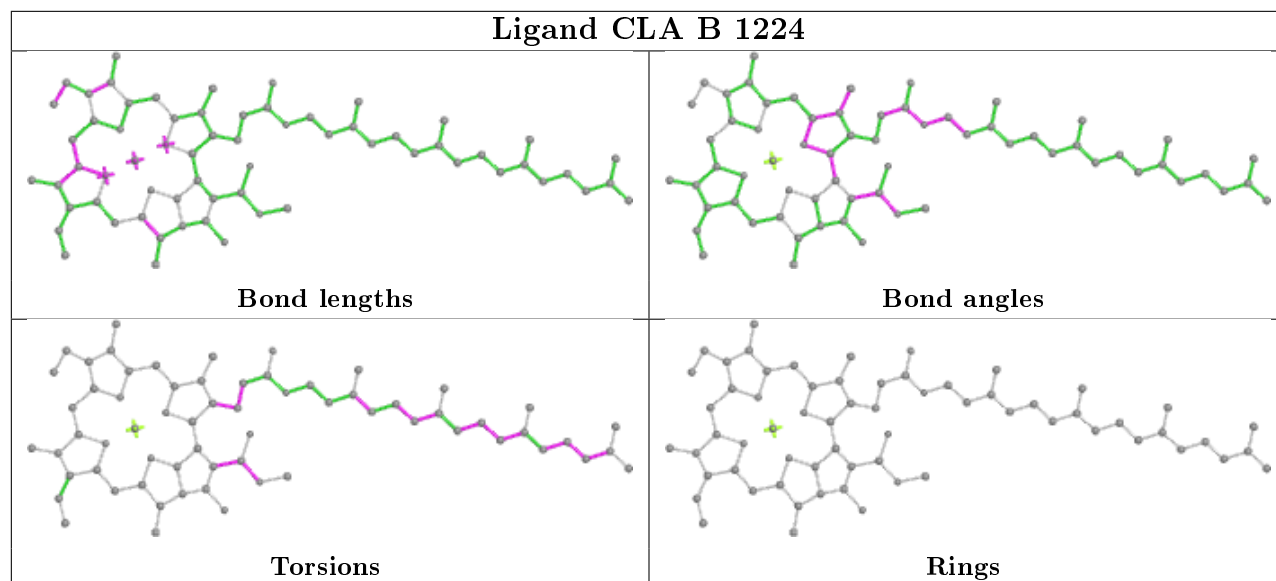
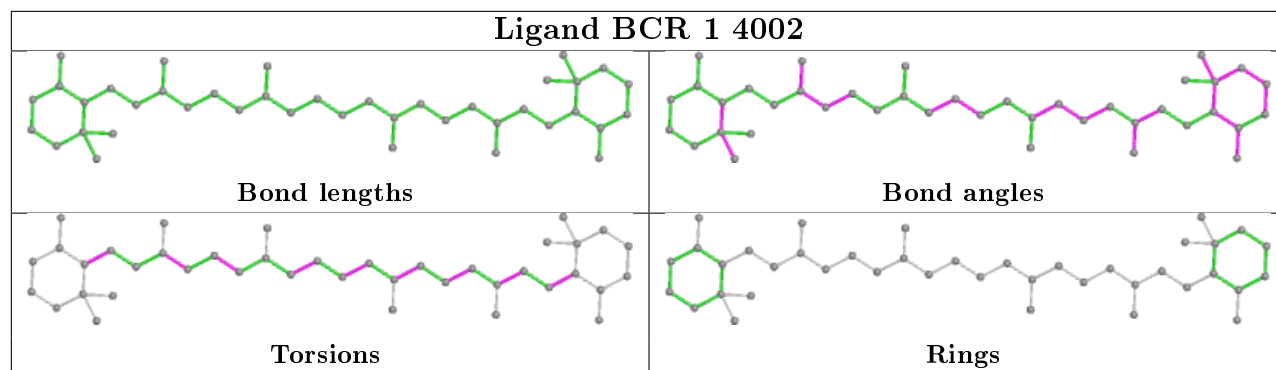


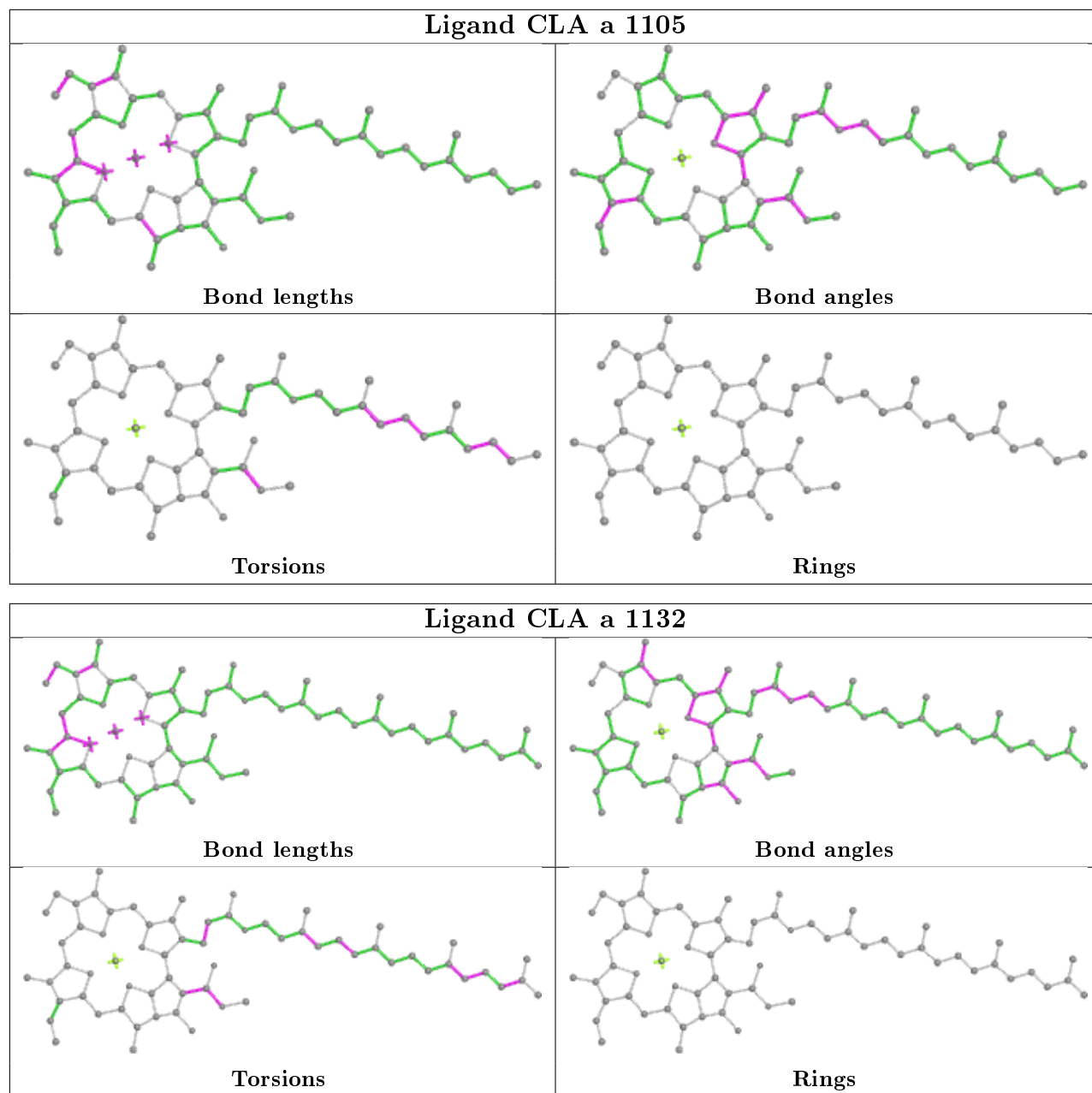
Ligand CLA B 1211**Ligand CLA B 1239**

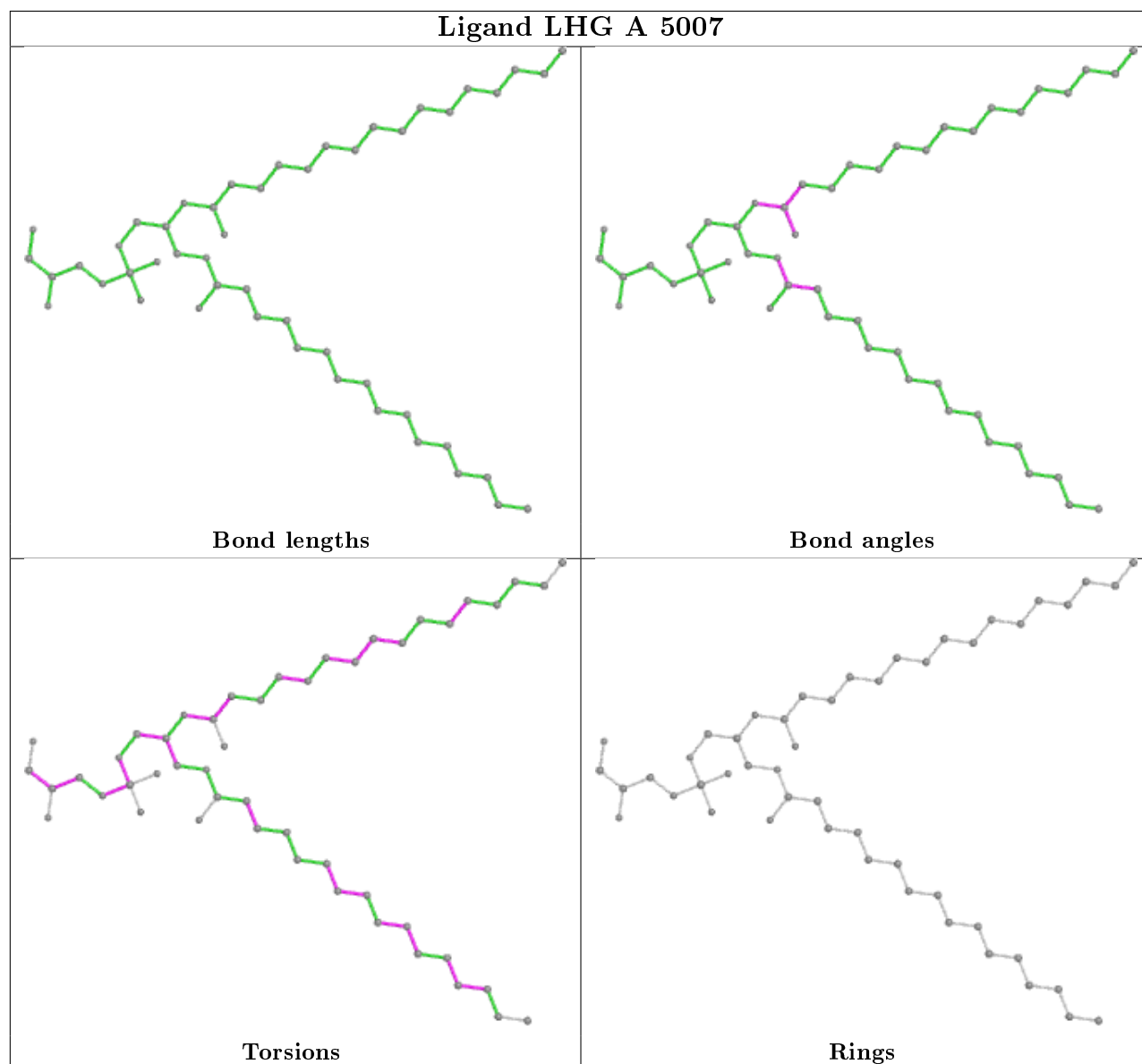
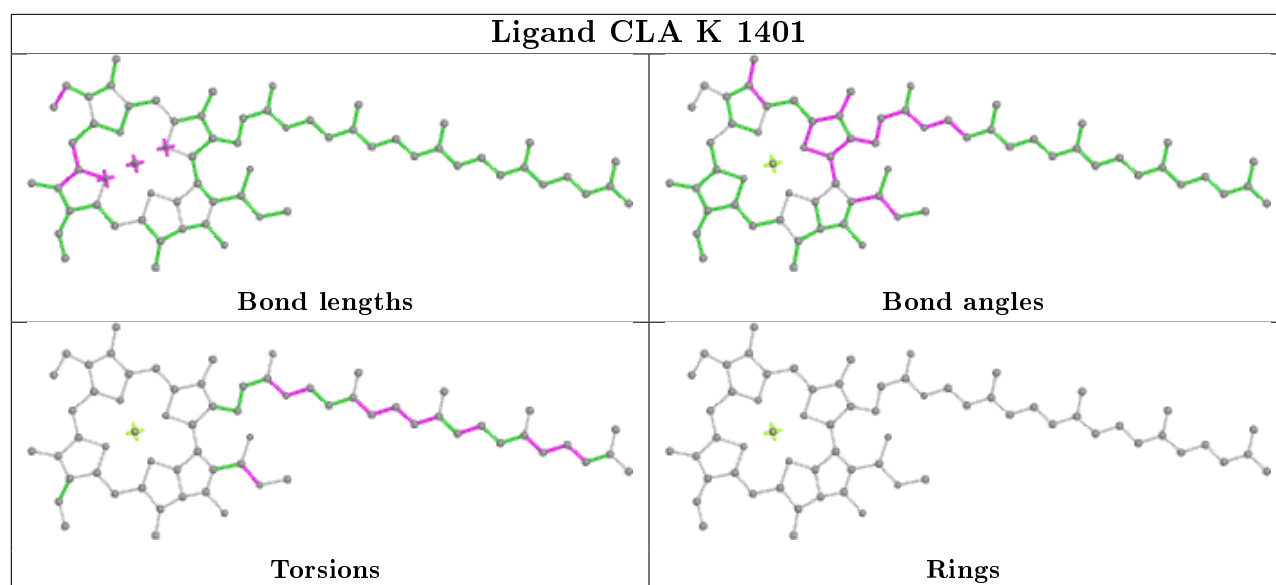


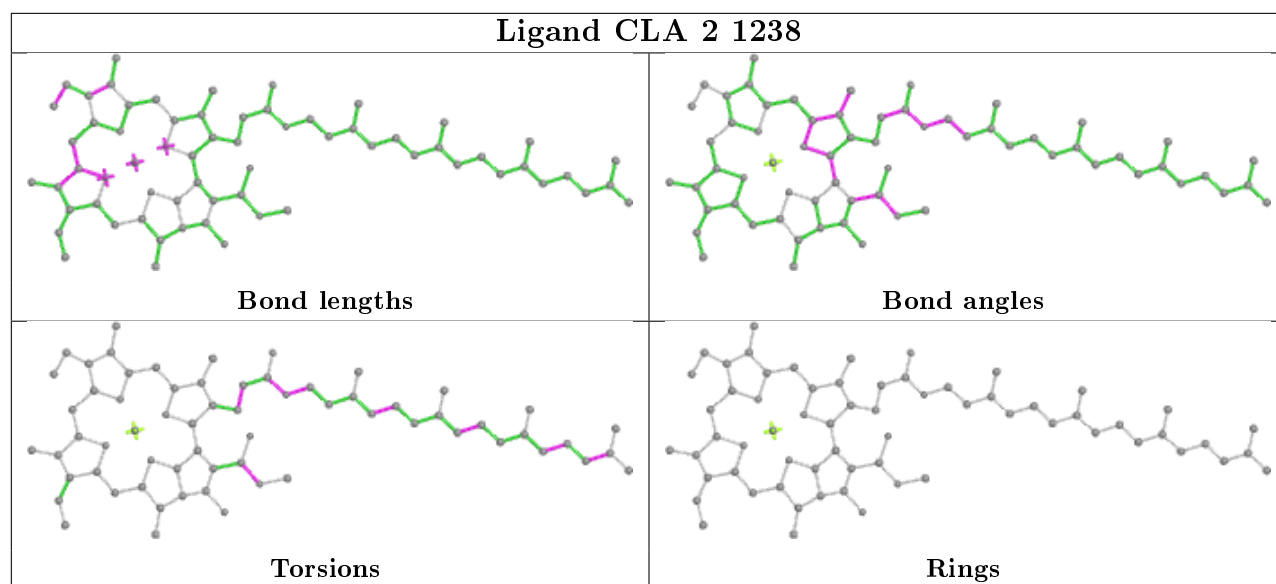
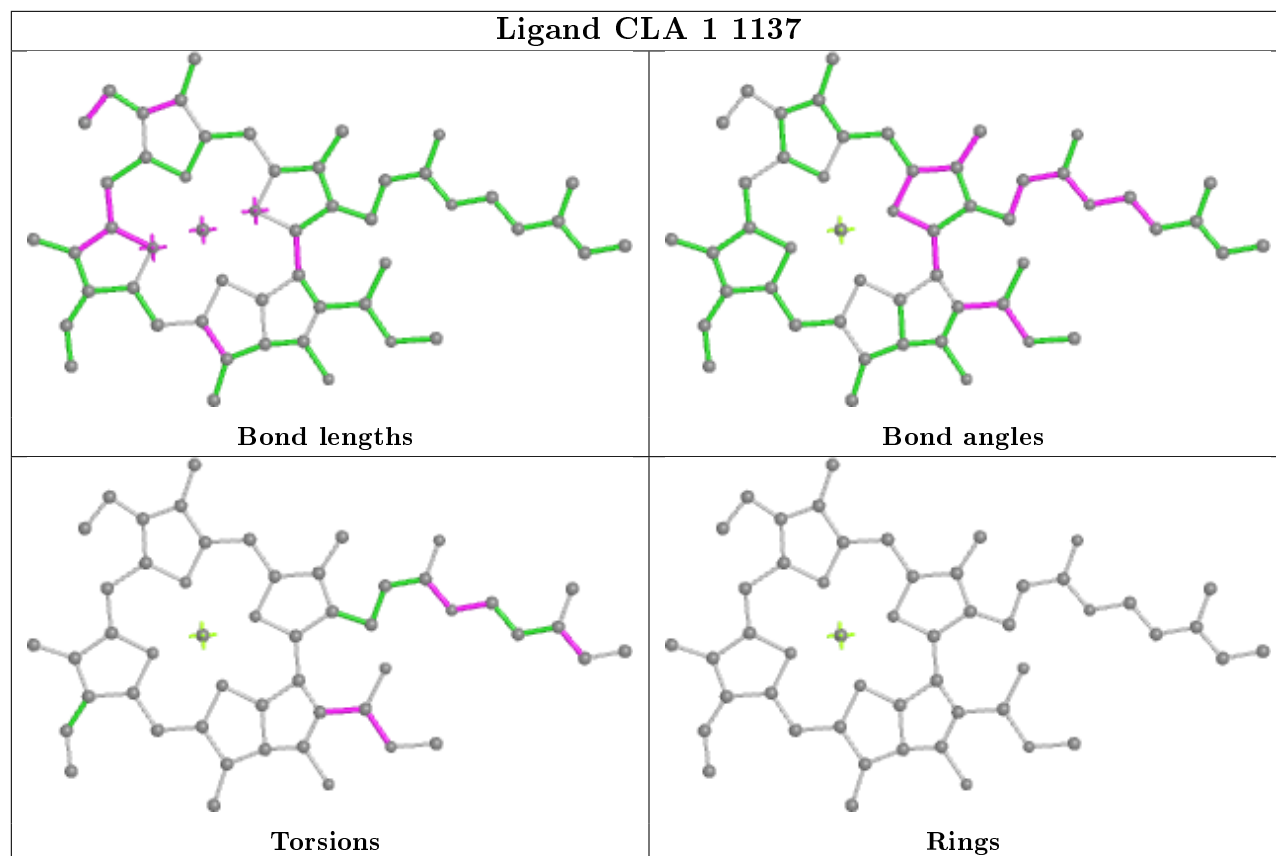


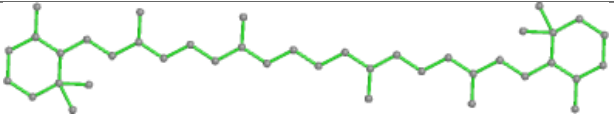
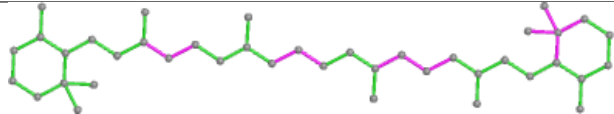
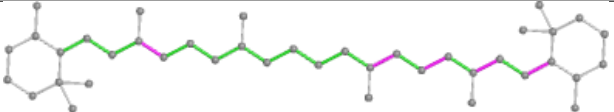
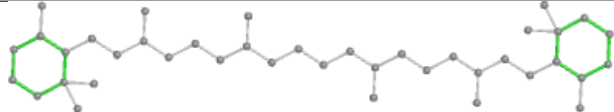


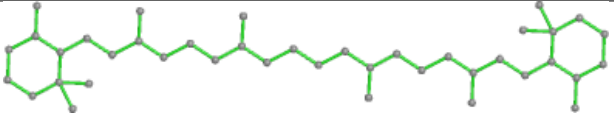
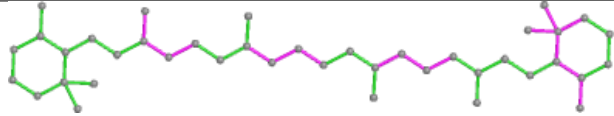
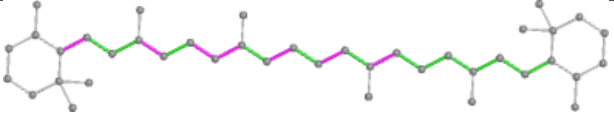
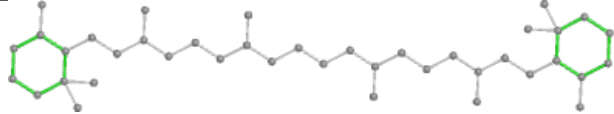


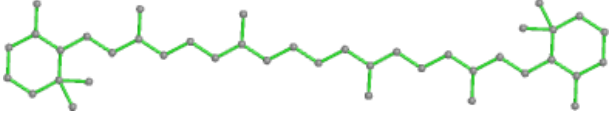
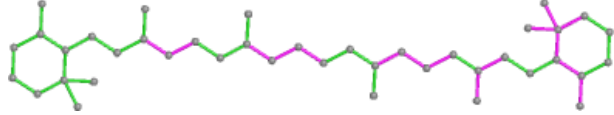
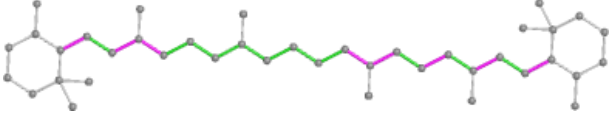
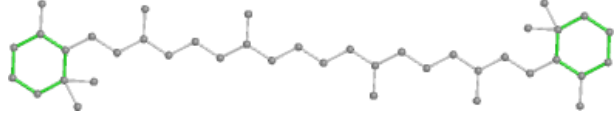


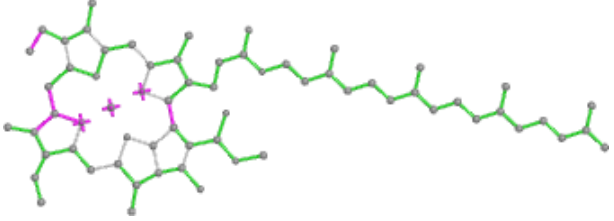
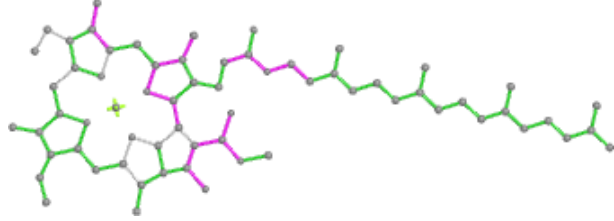
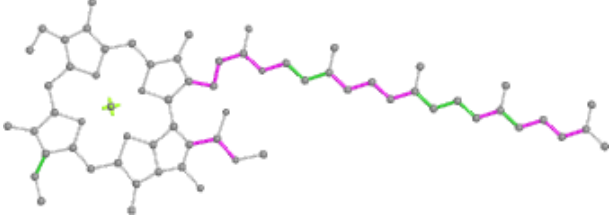
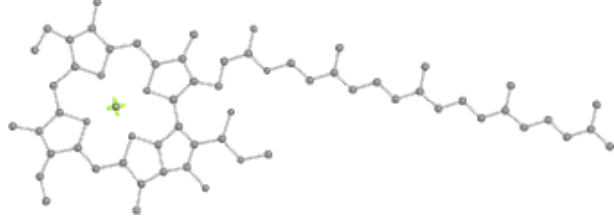




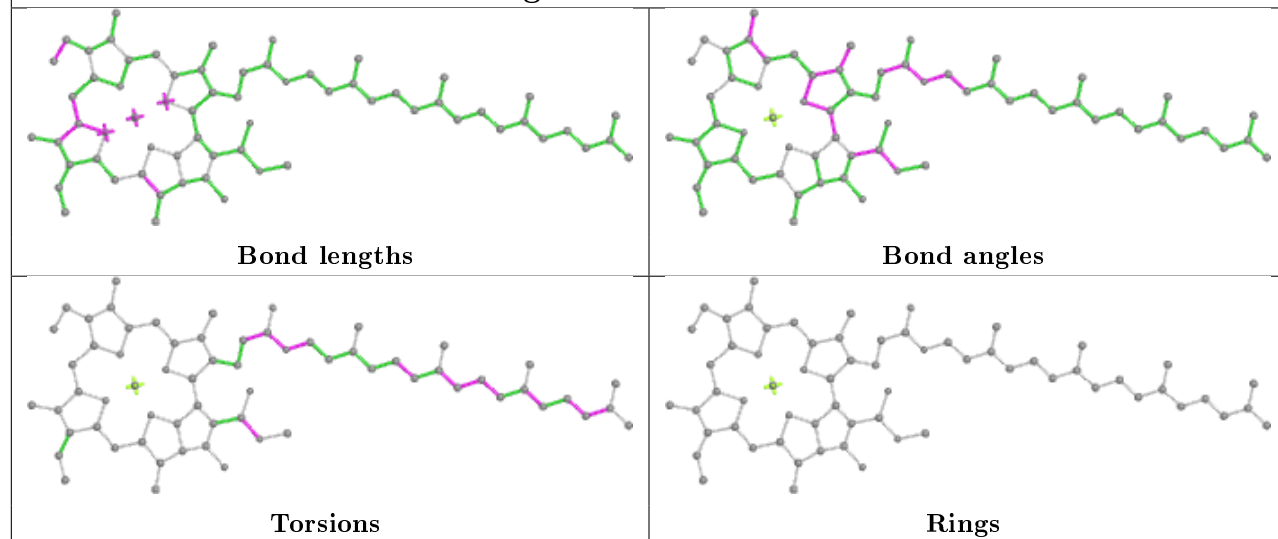
Ligand BCR b 4010	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand BCR b 4017	
	
Bond lengths	Bond angles
	
Torsions	Rings

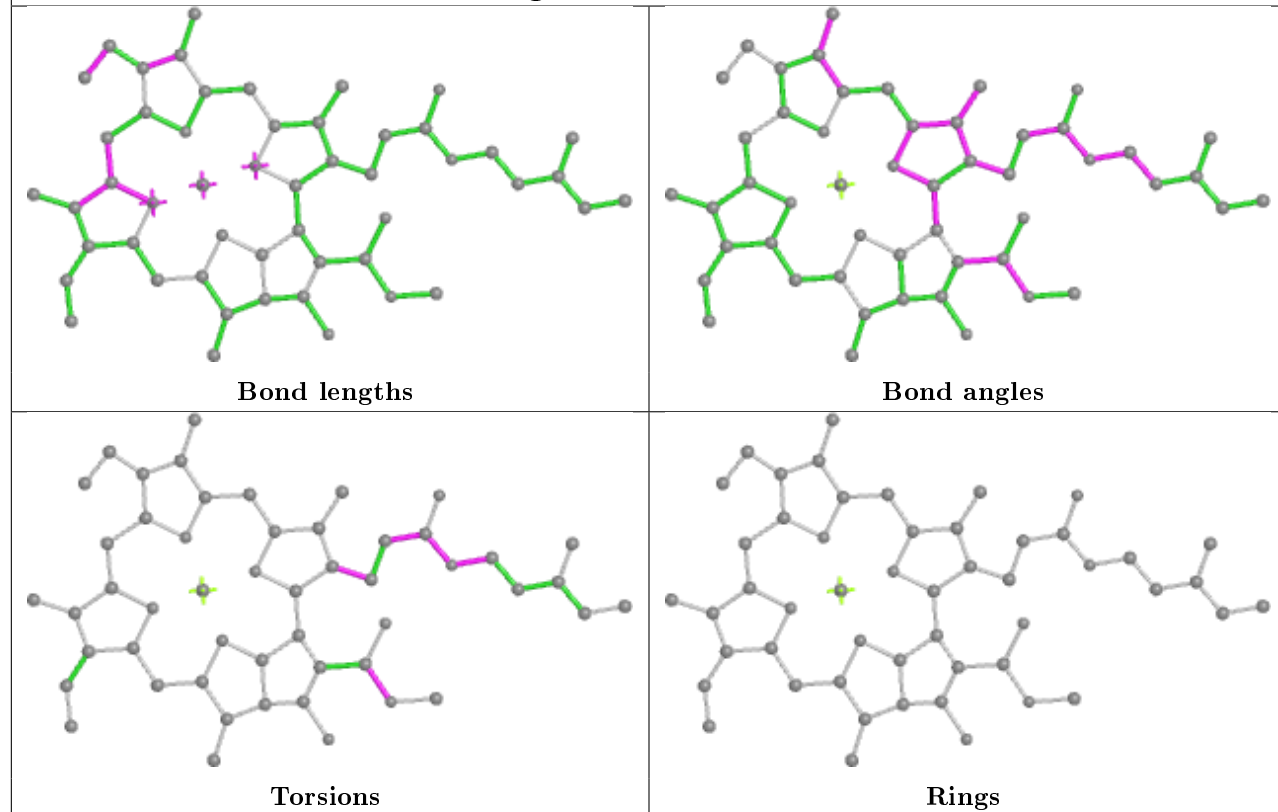
Ligand BCR 2 4011	
	
Bond lengths	Bond angles
	
Torsions	Rings

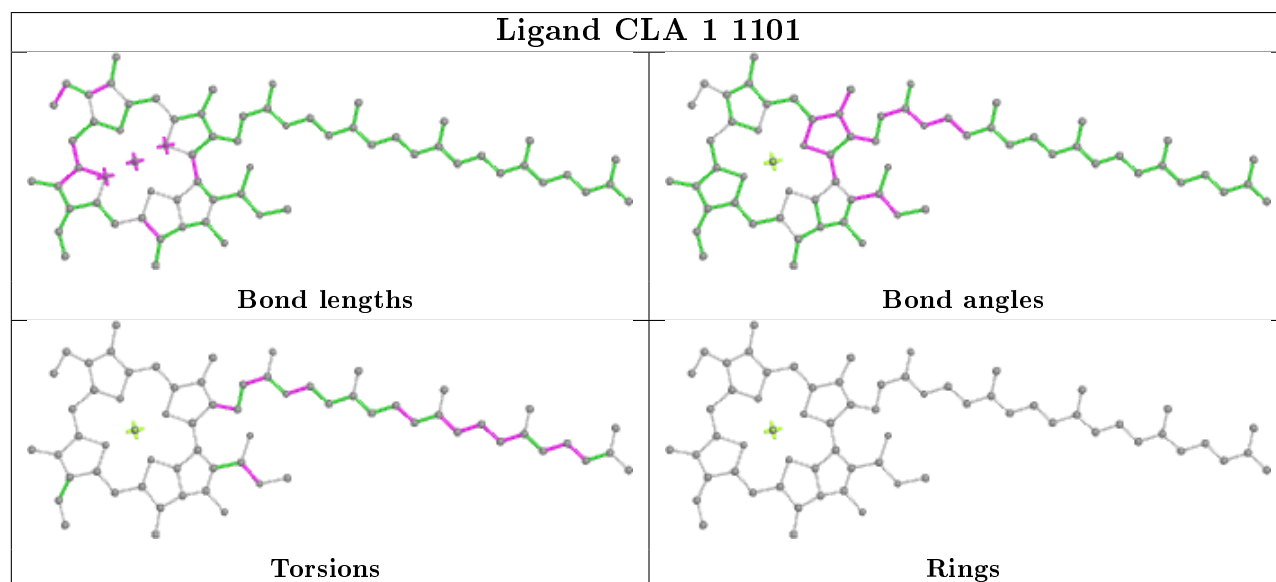
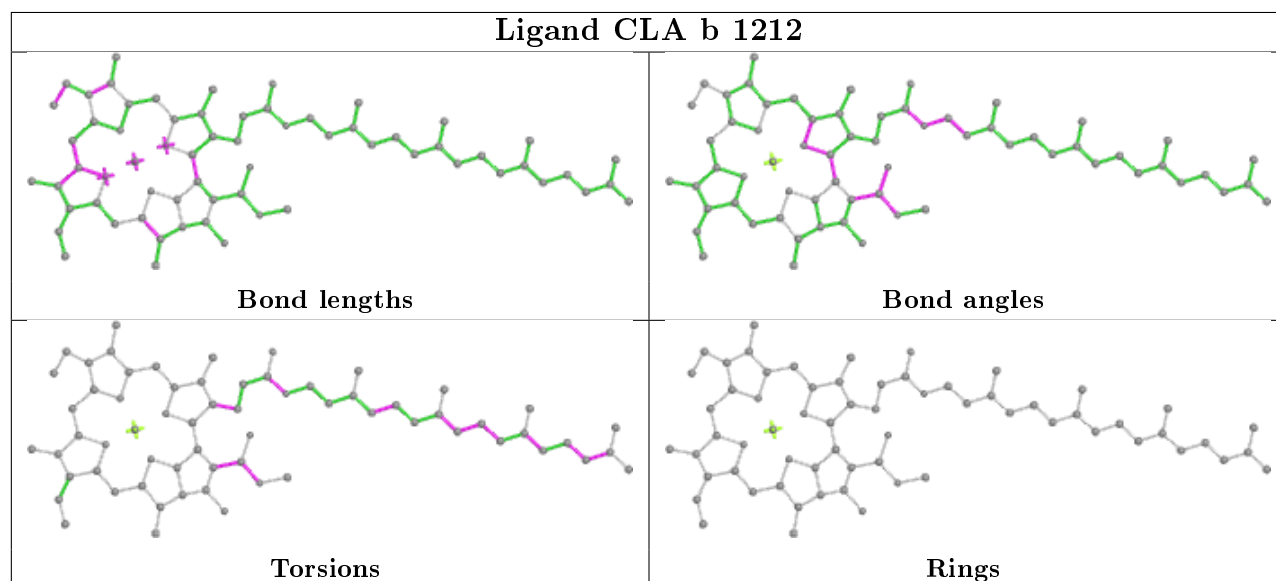
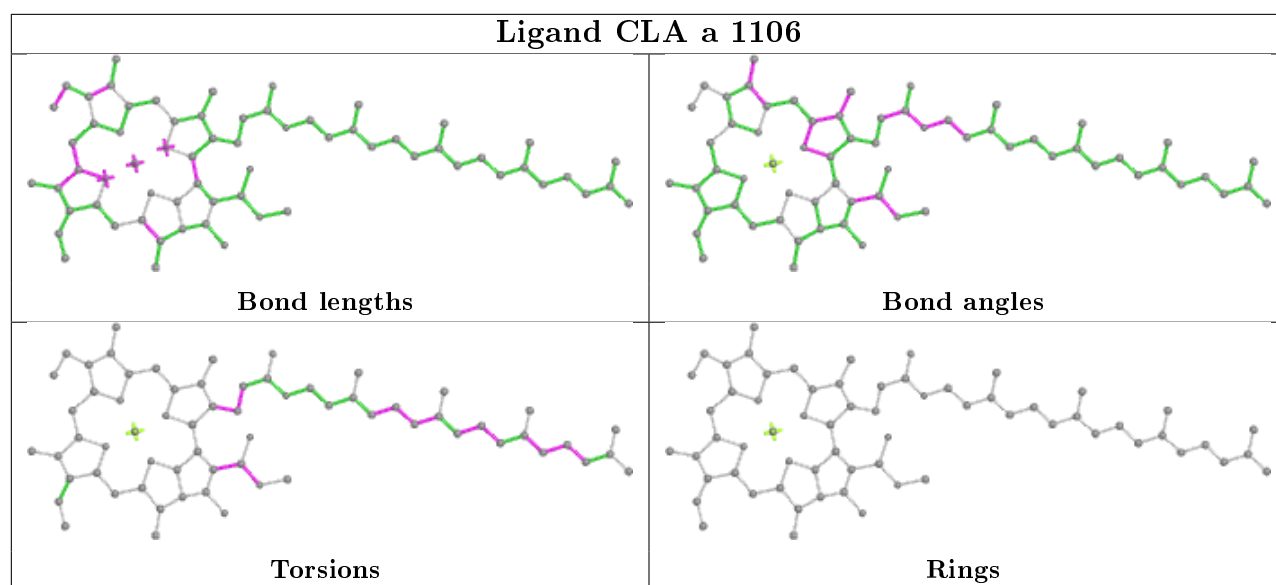
Ligand CLA a 1128	
	
Bond lengths	Bond angles
	
Torsions	Rings

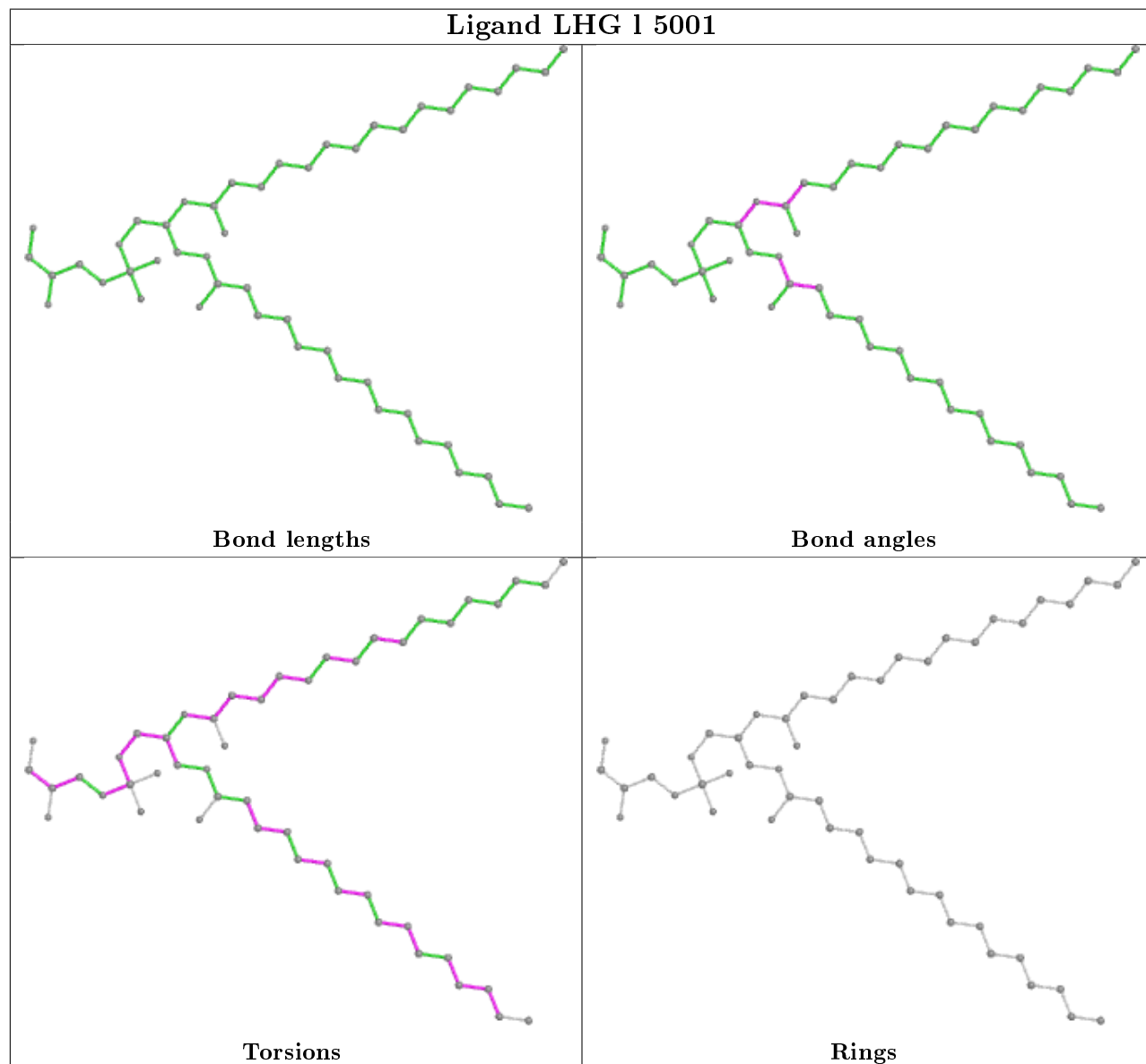
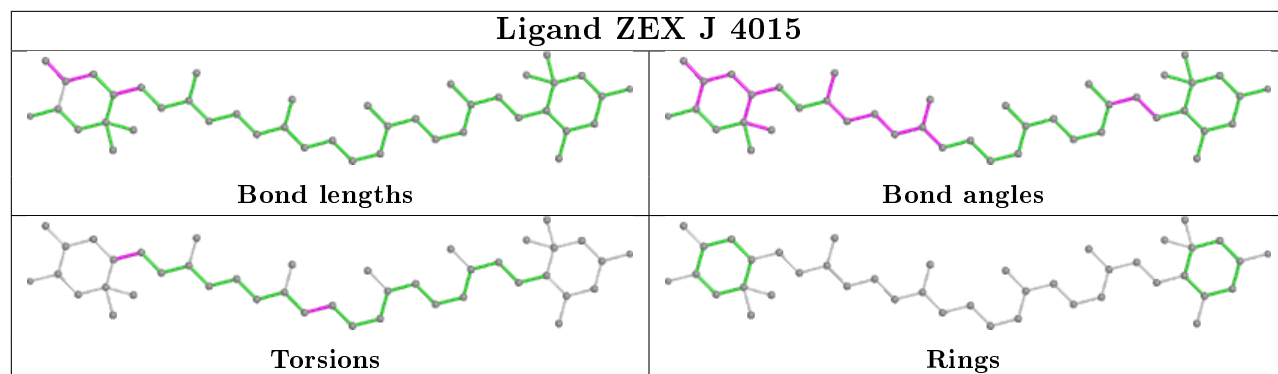
Ligand CLA B 1208

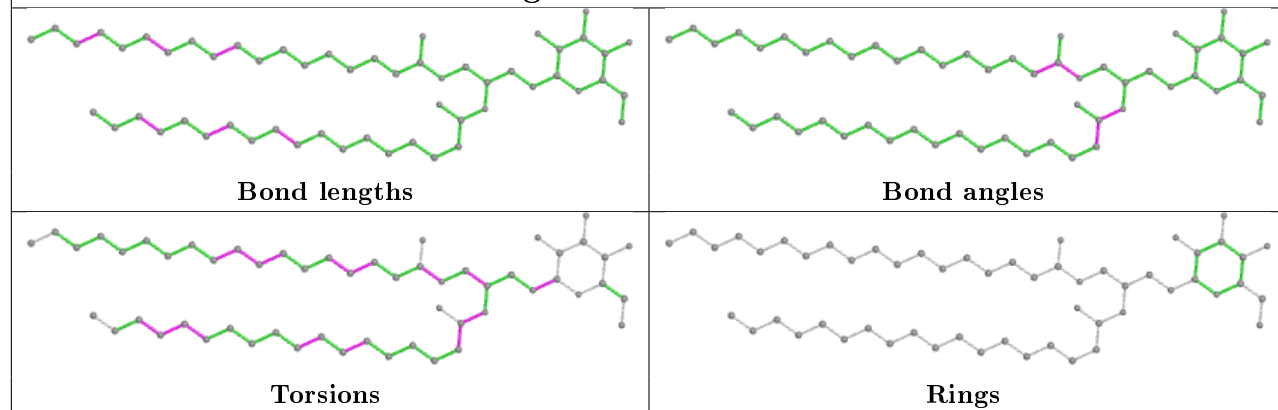
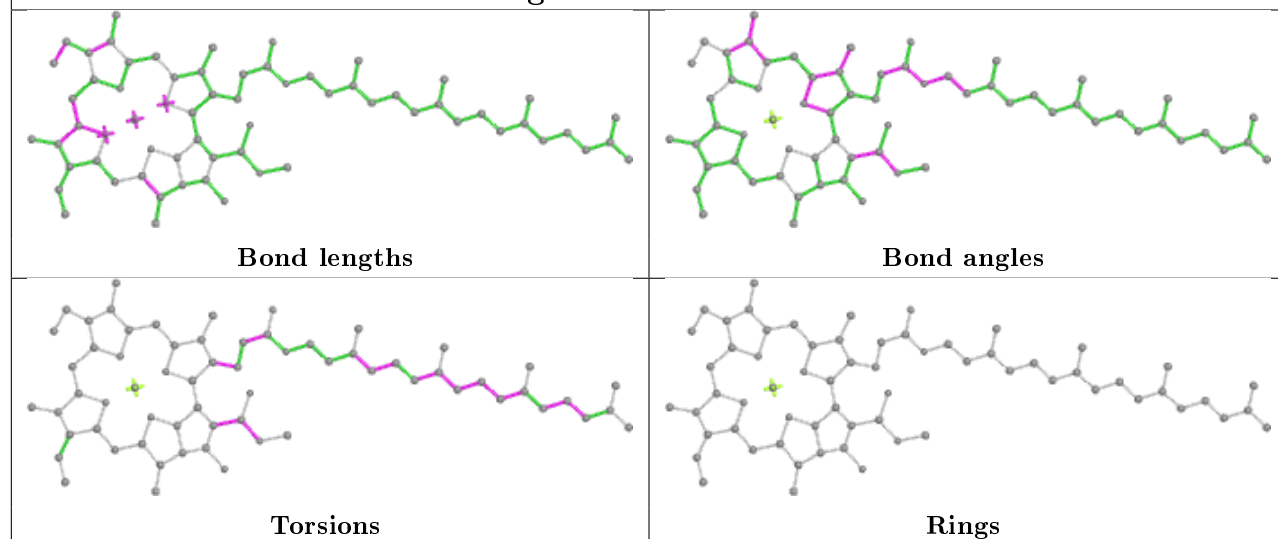
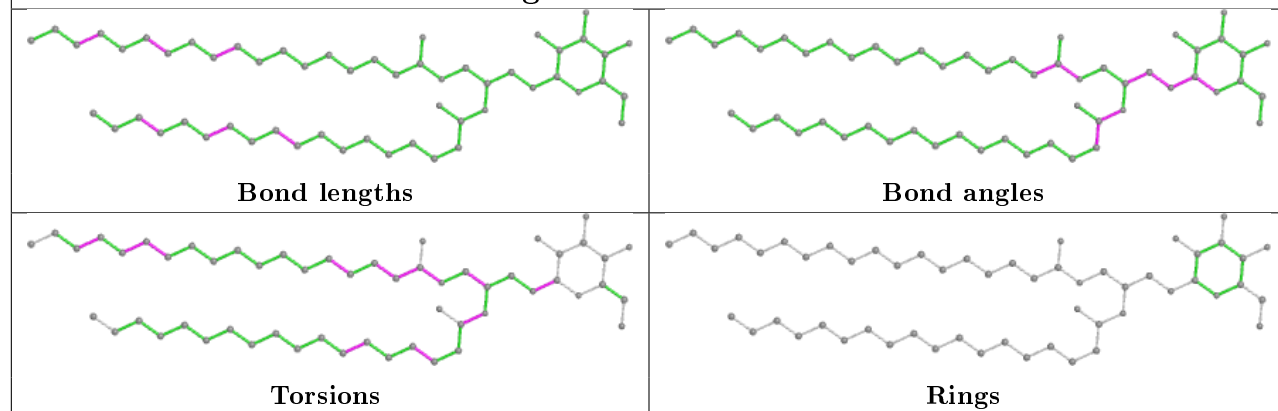


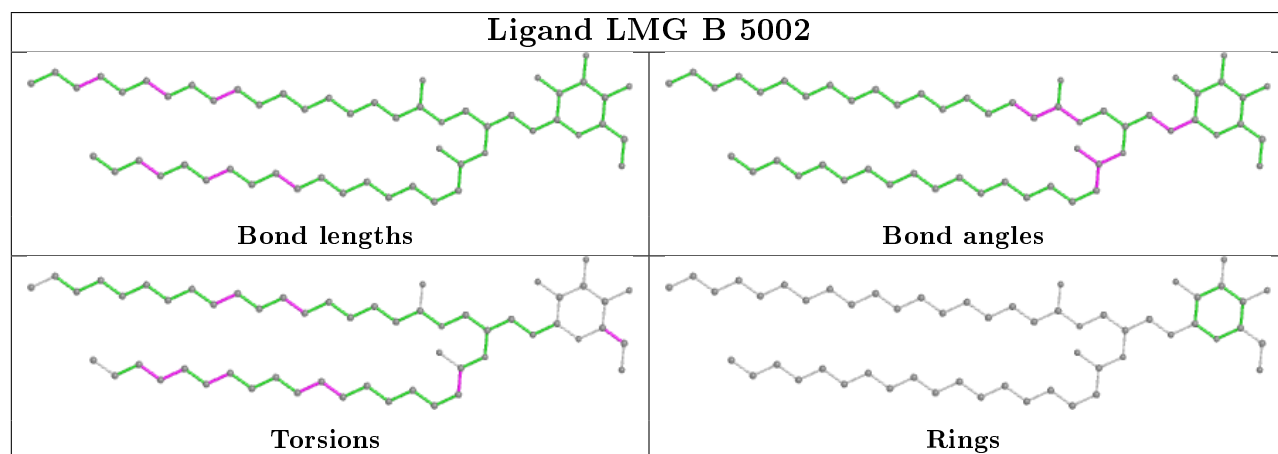
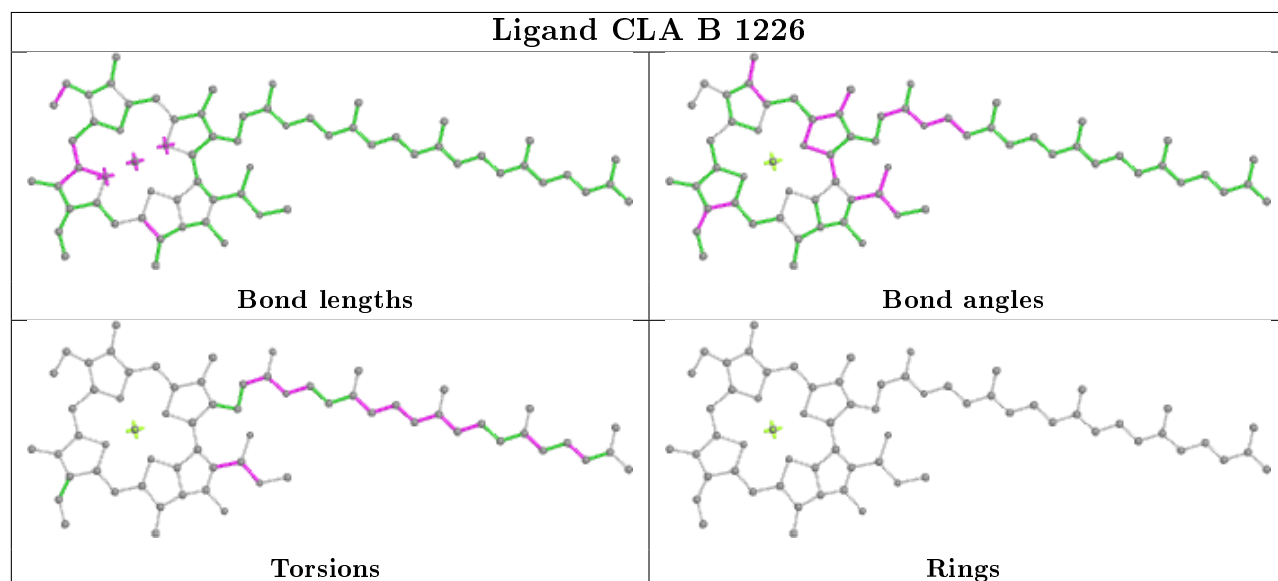
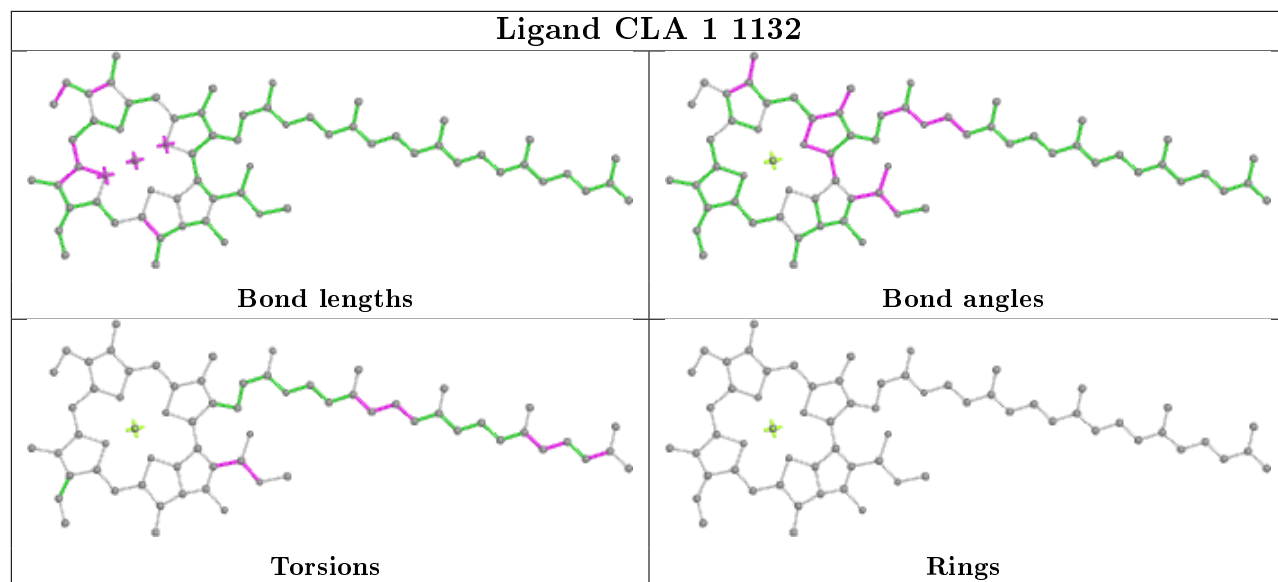
Ligand CLA 1 1107



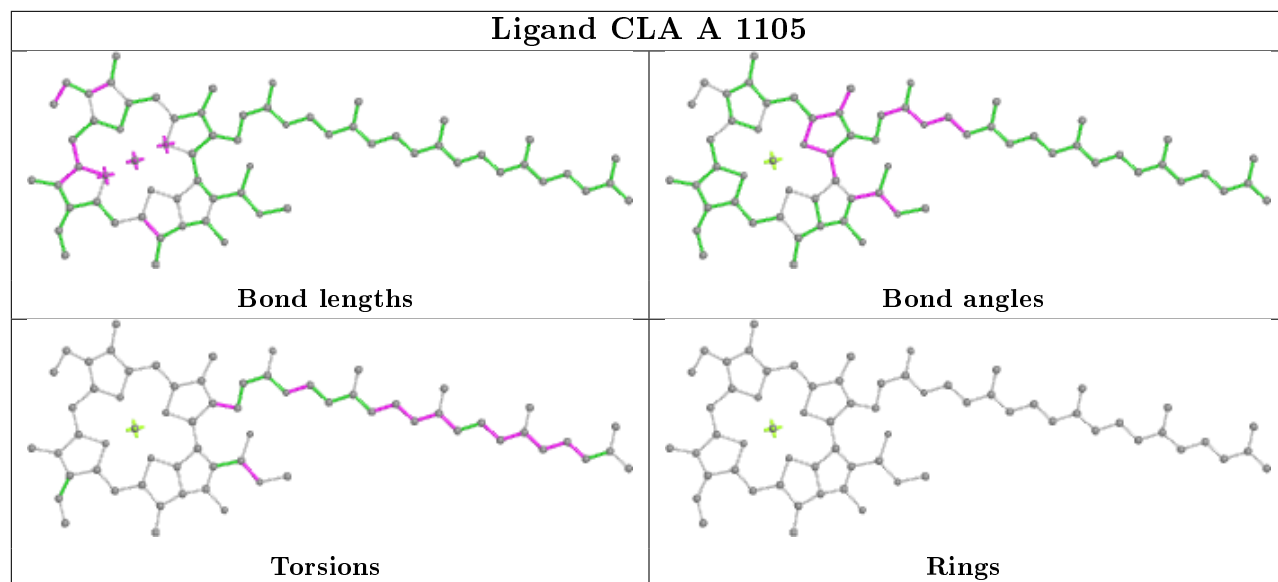




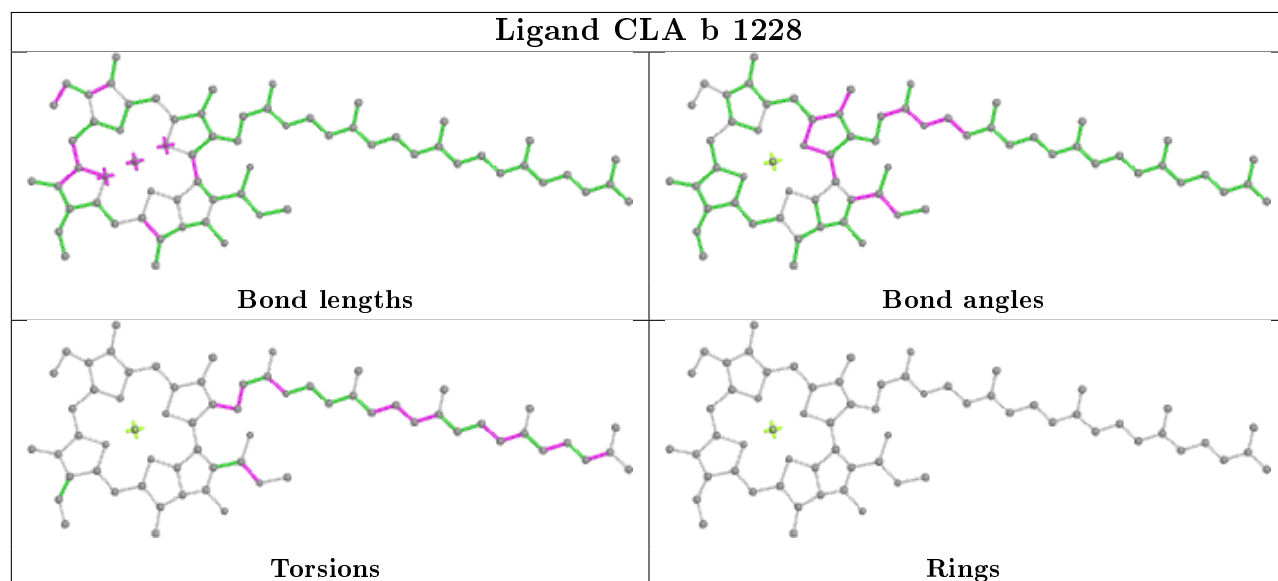
Ligand LMG 1 5004**Ligand CLA a 1103****Ligand LMG b 5005**



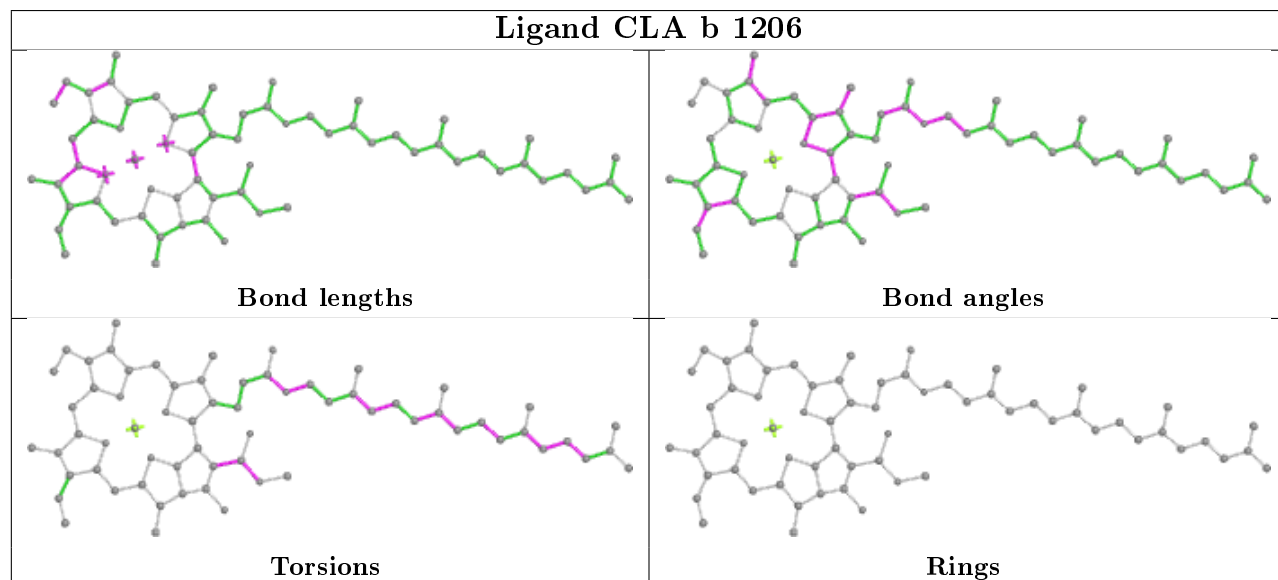
Ligand CLA A 1105

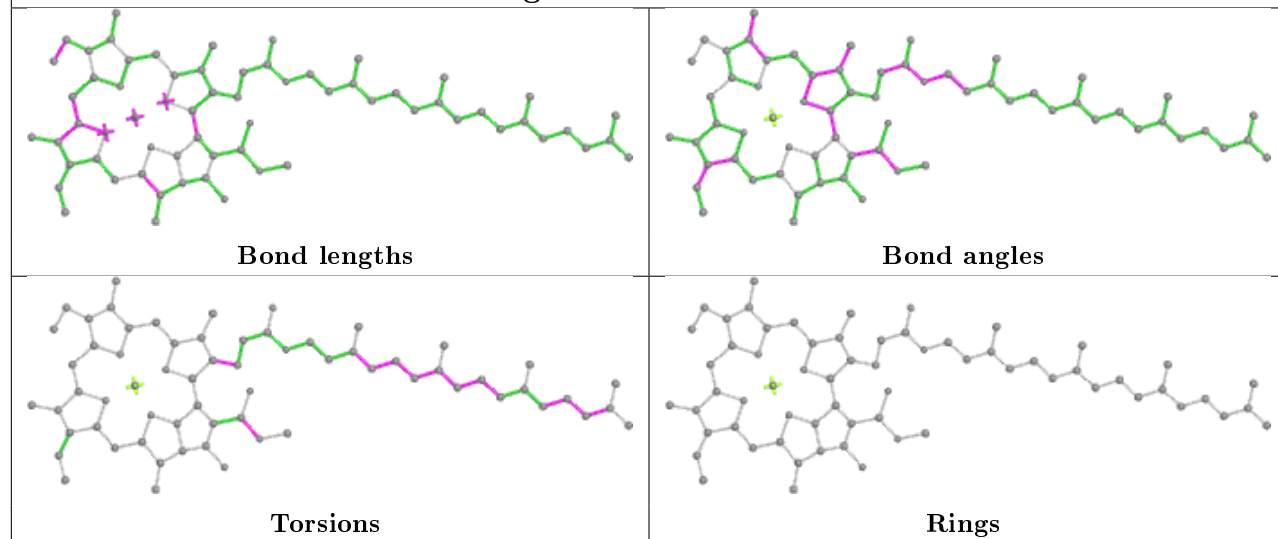
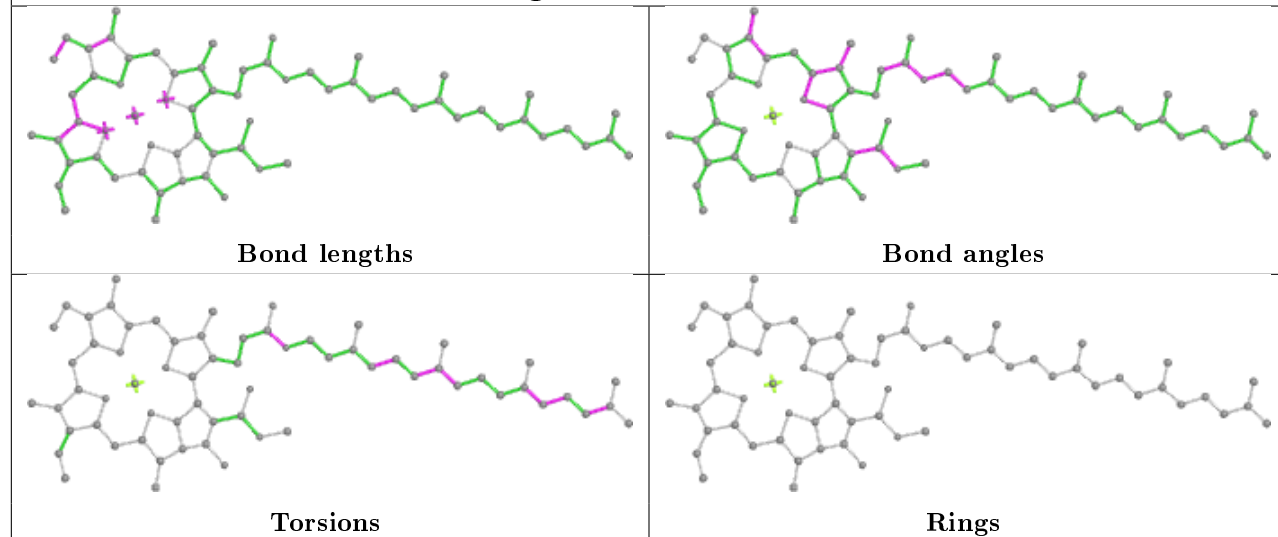


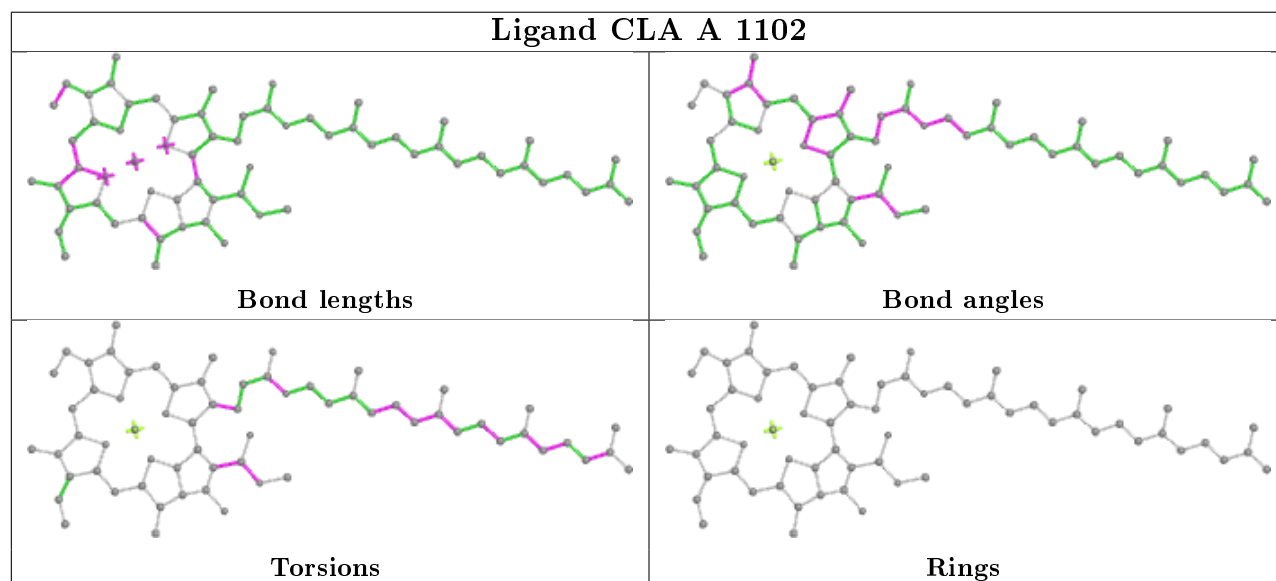
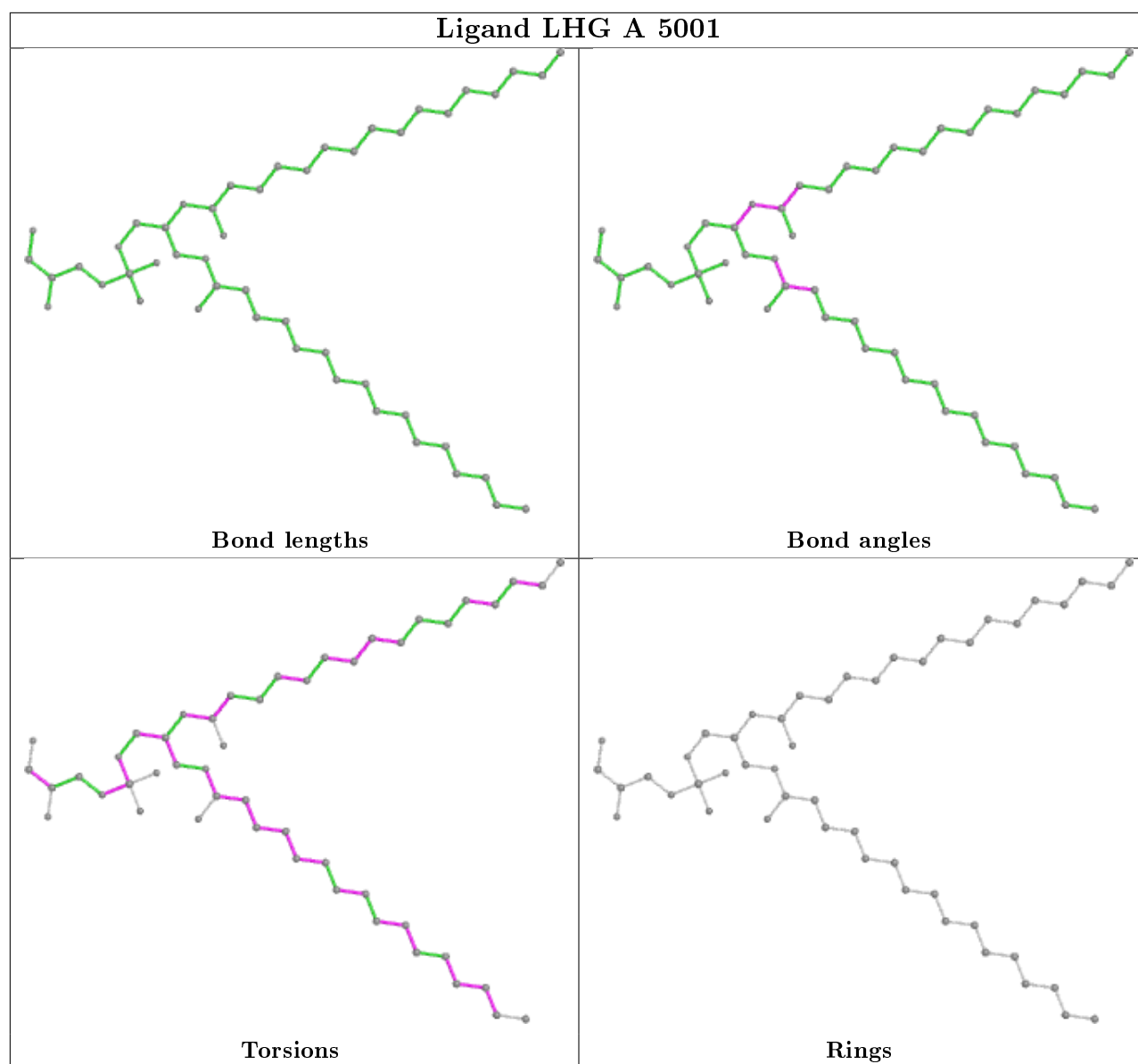
Ligand CLA b 1228

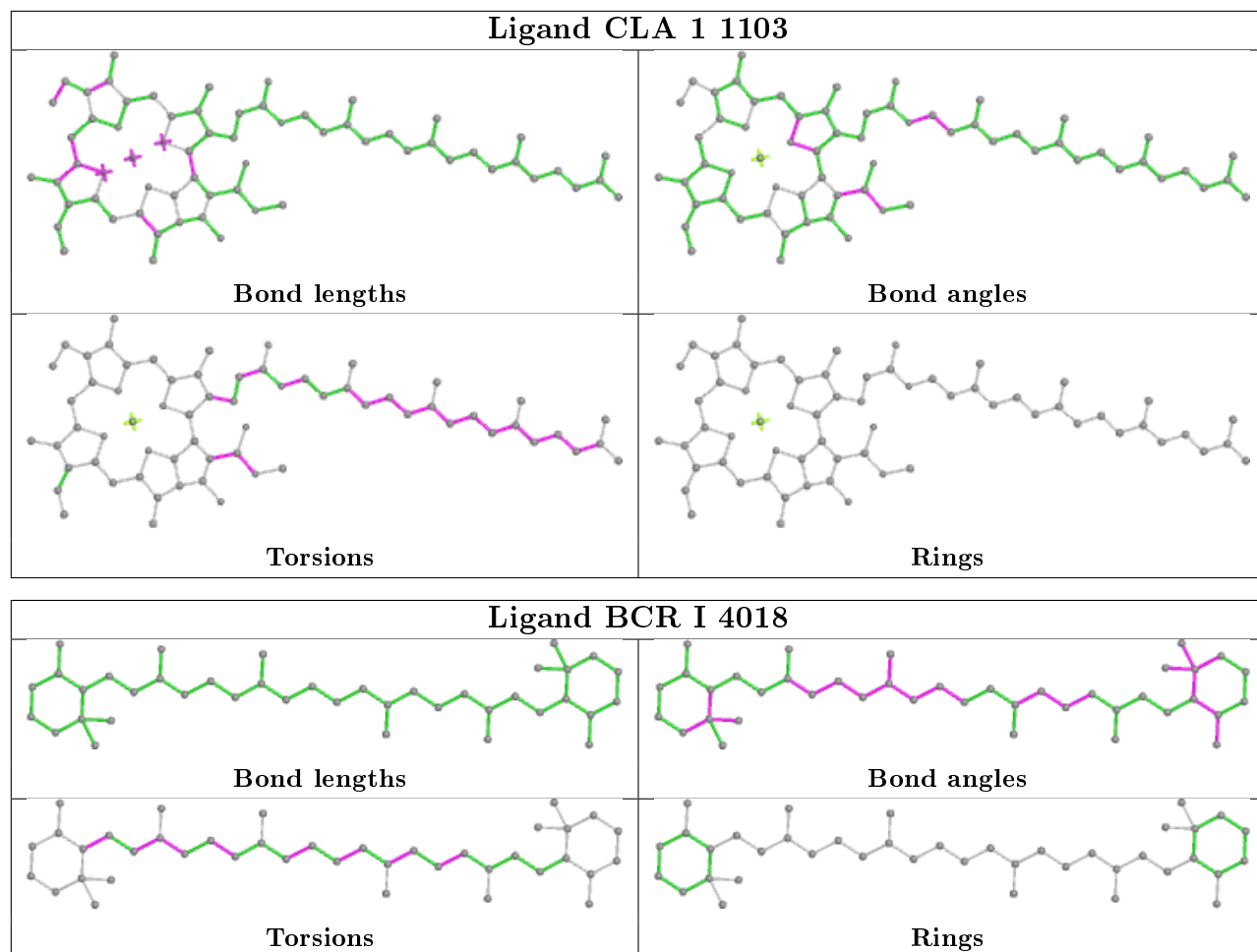


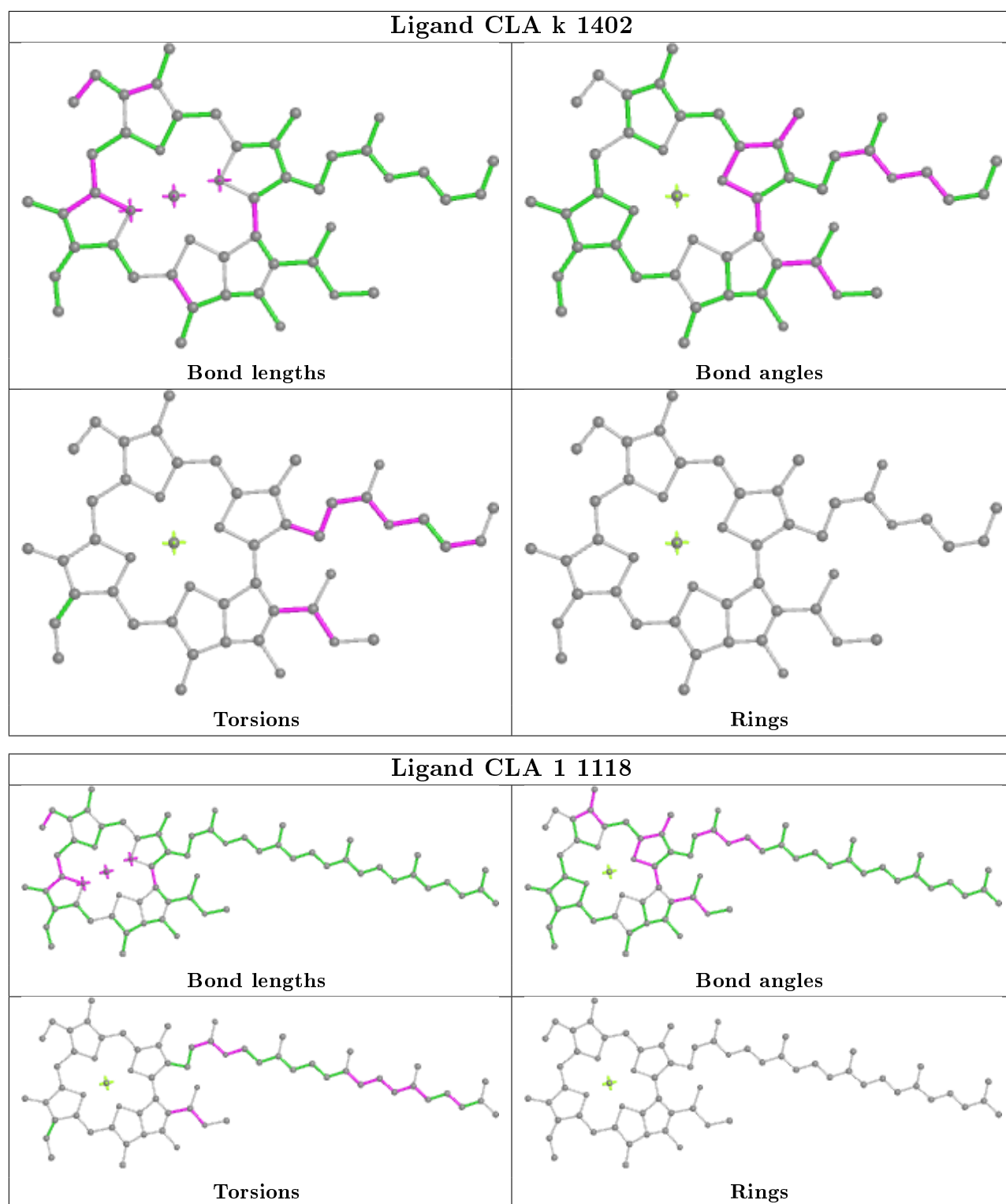
Ligand CLA b 1206

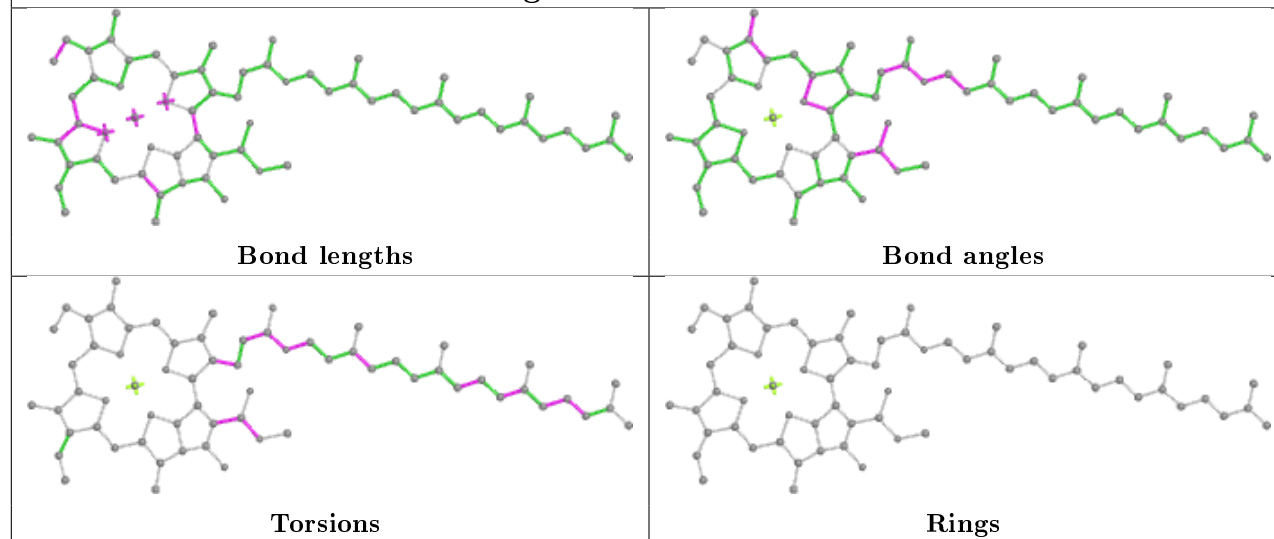
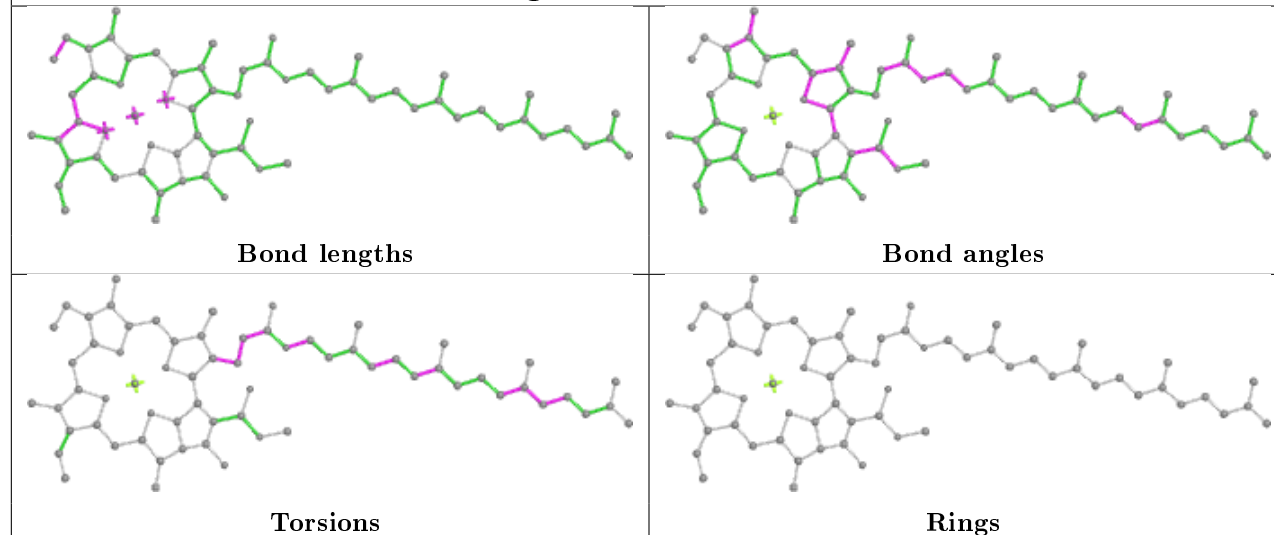
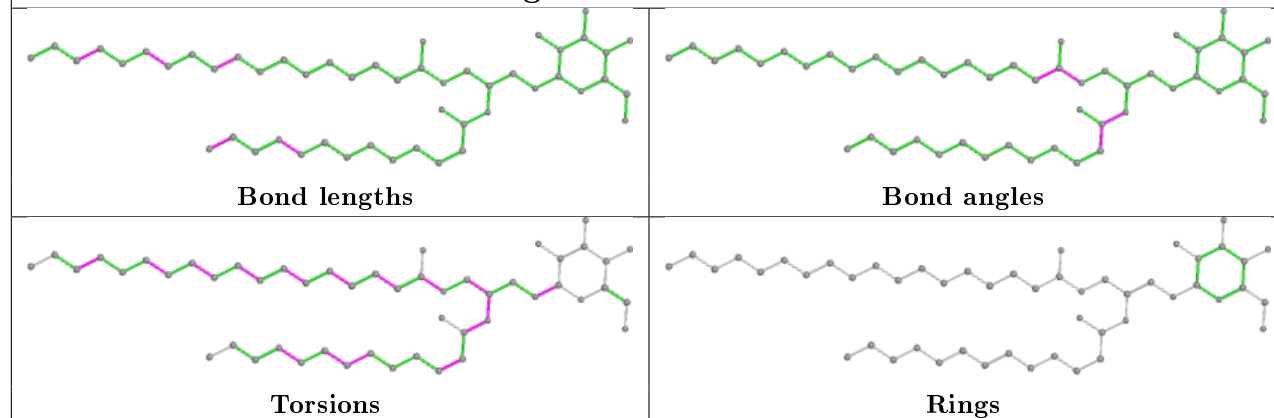


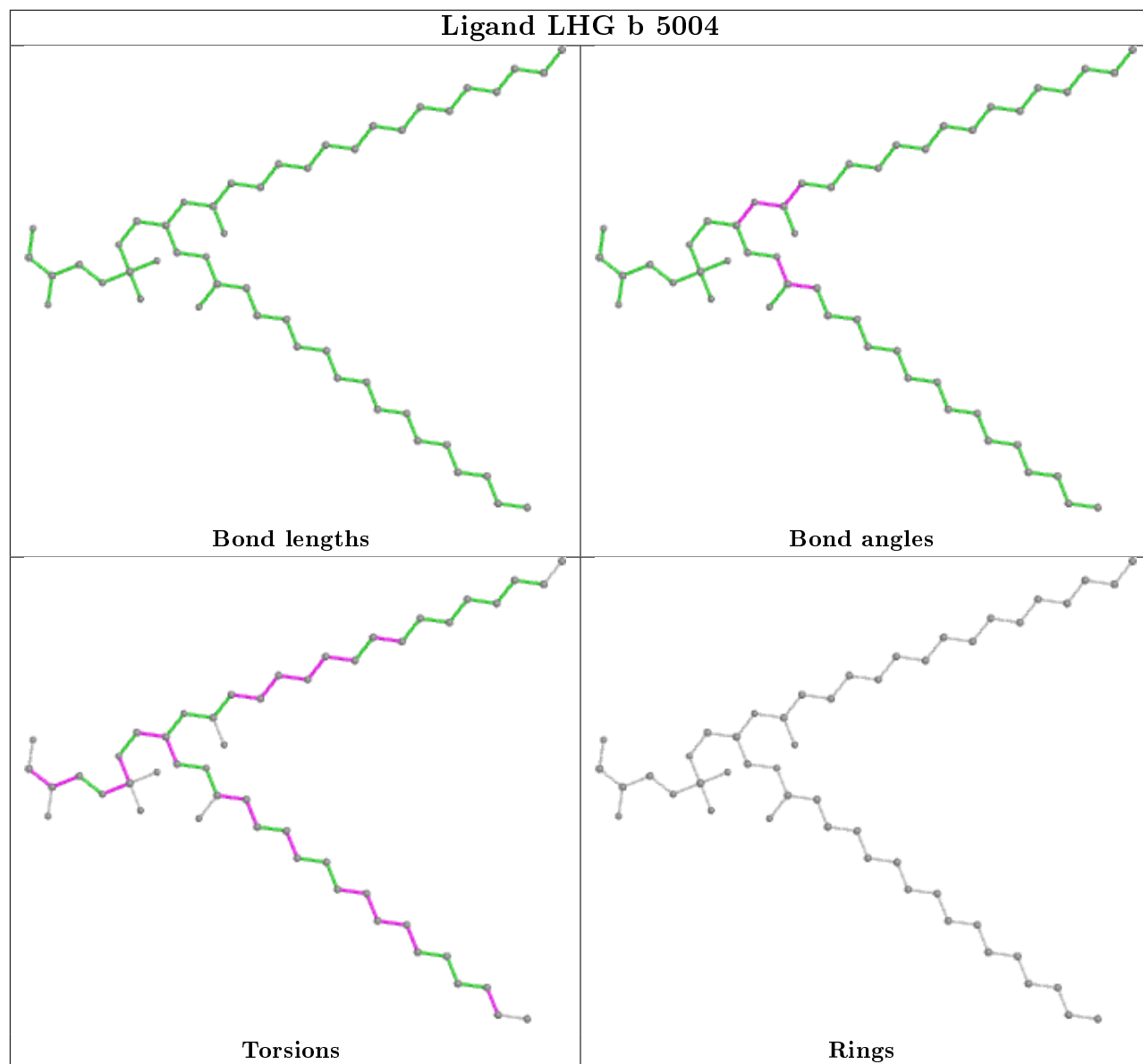
Ligand CLA B 1215**Ligand CLA 0 1502**

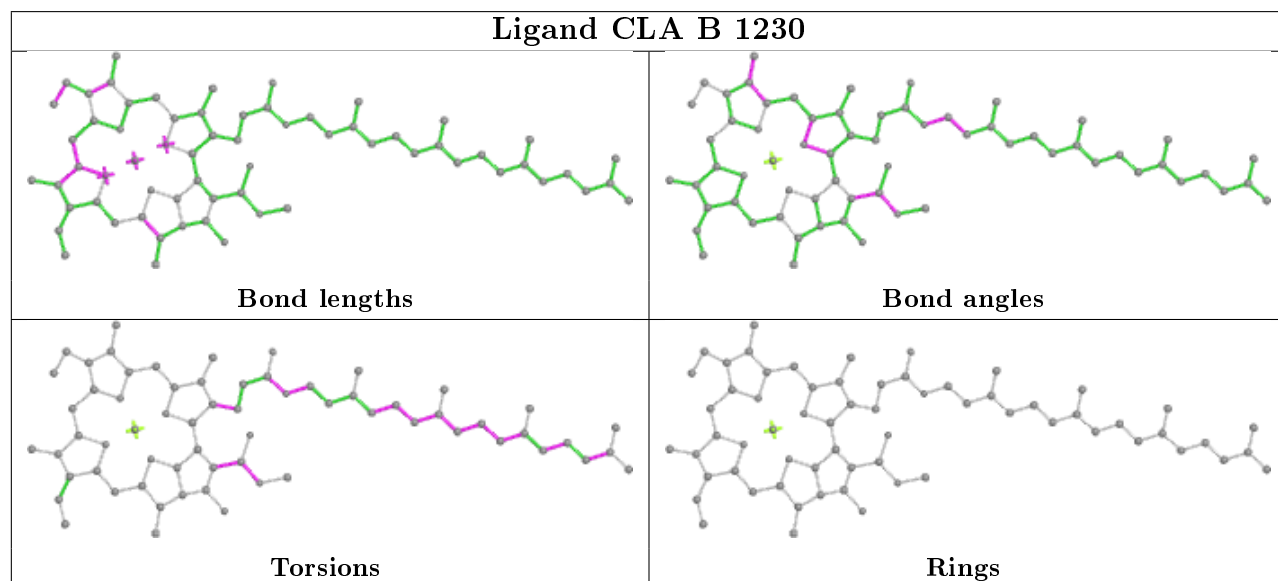
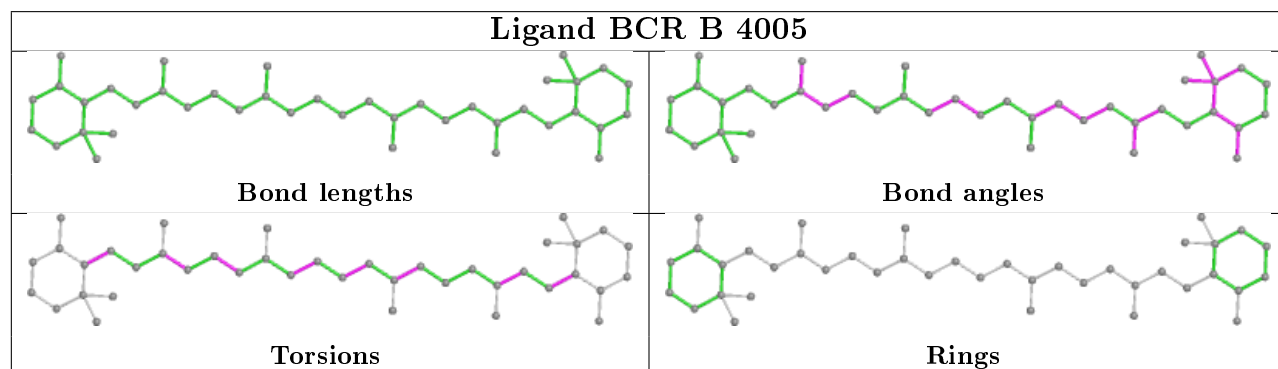
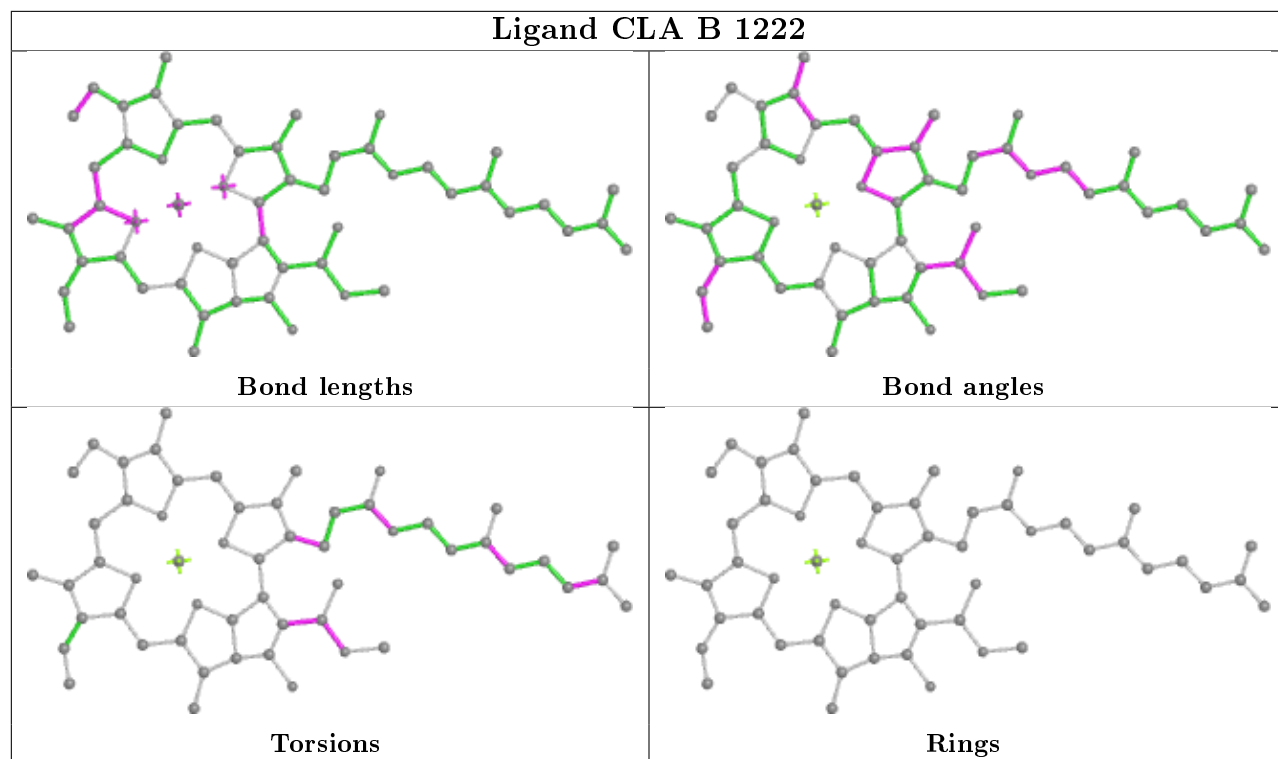


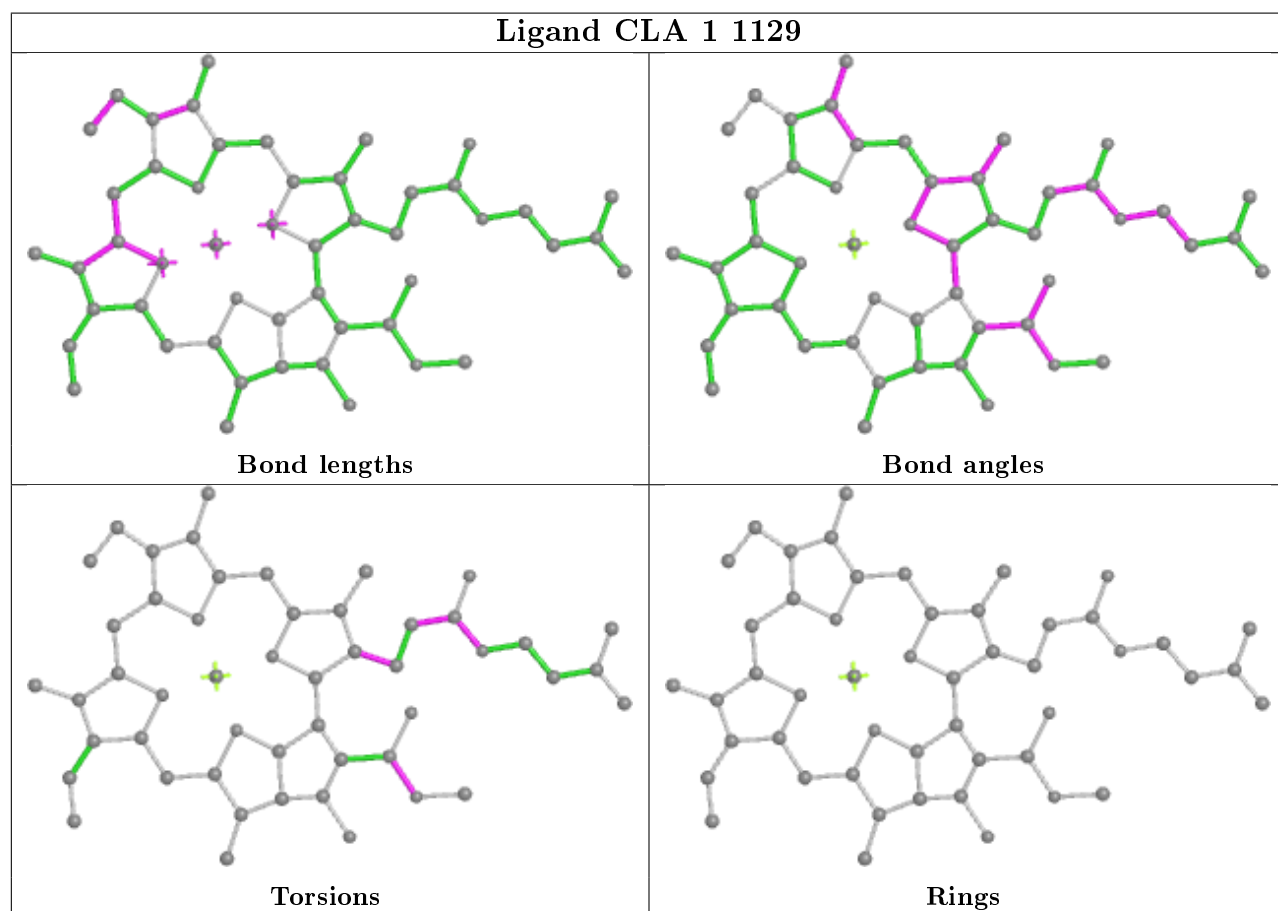
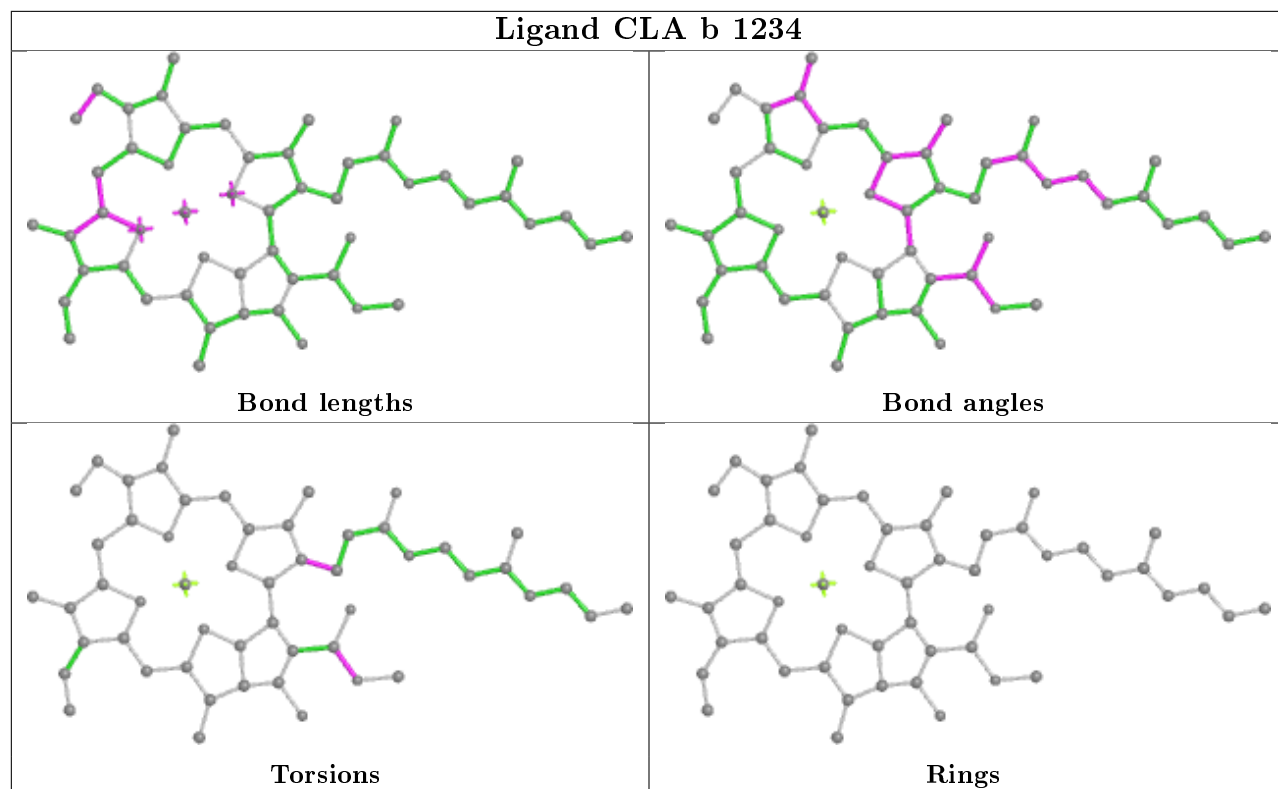


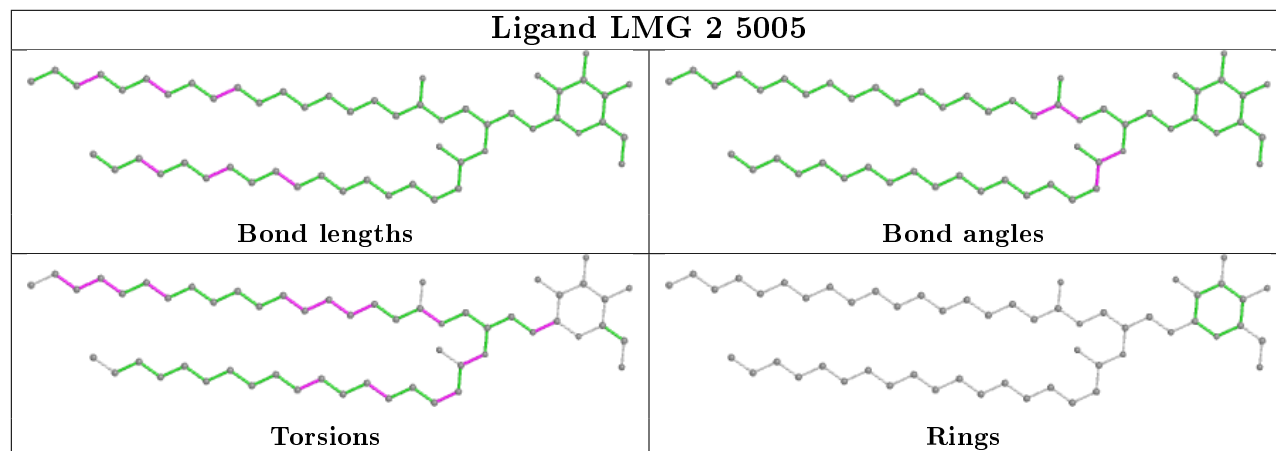
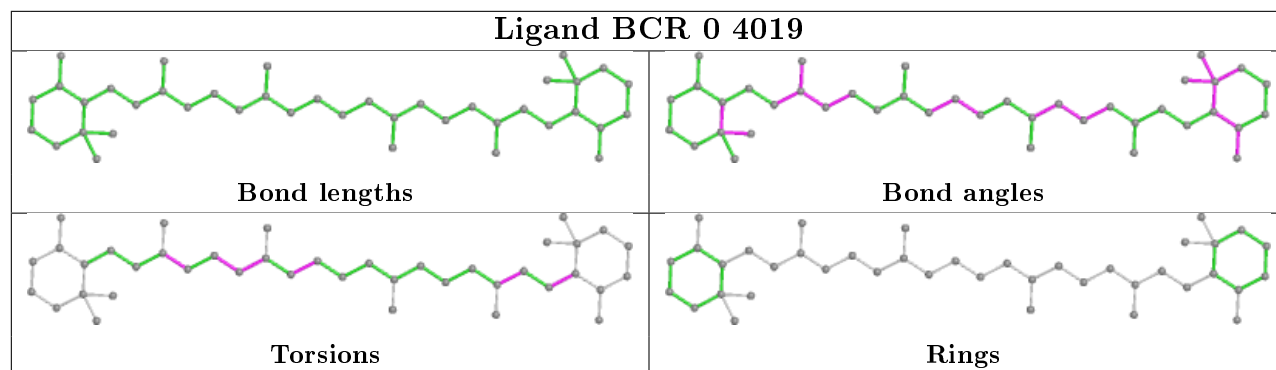
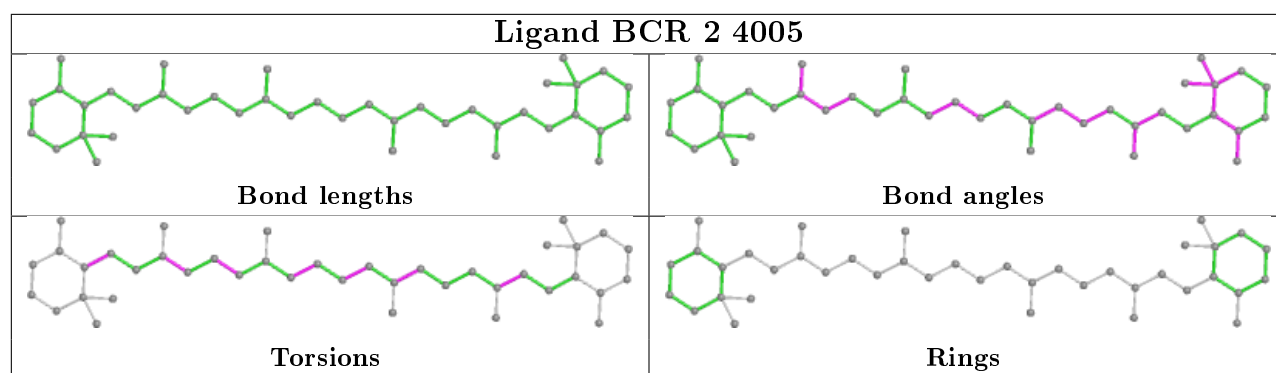


Ligand CLA B 1202**Ligand CLA L 1502****Ligand LMG 1 5002**

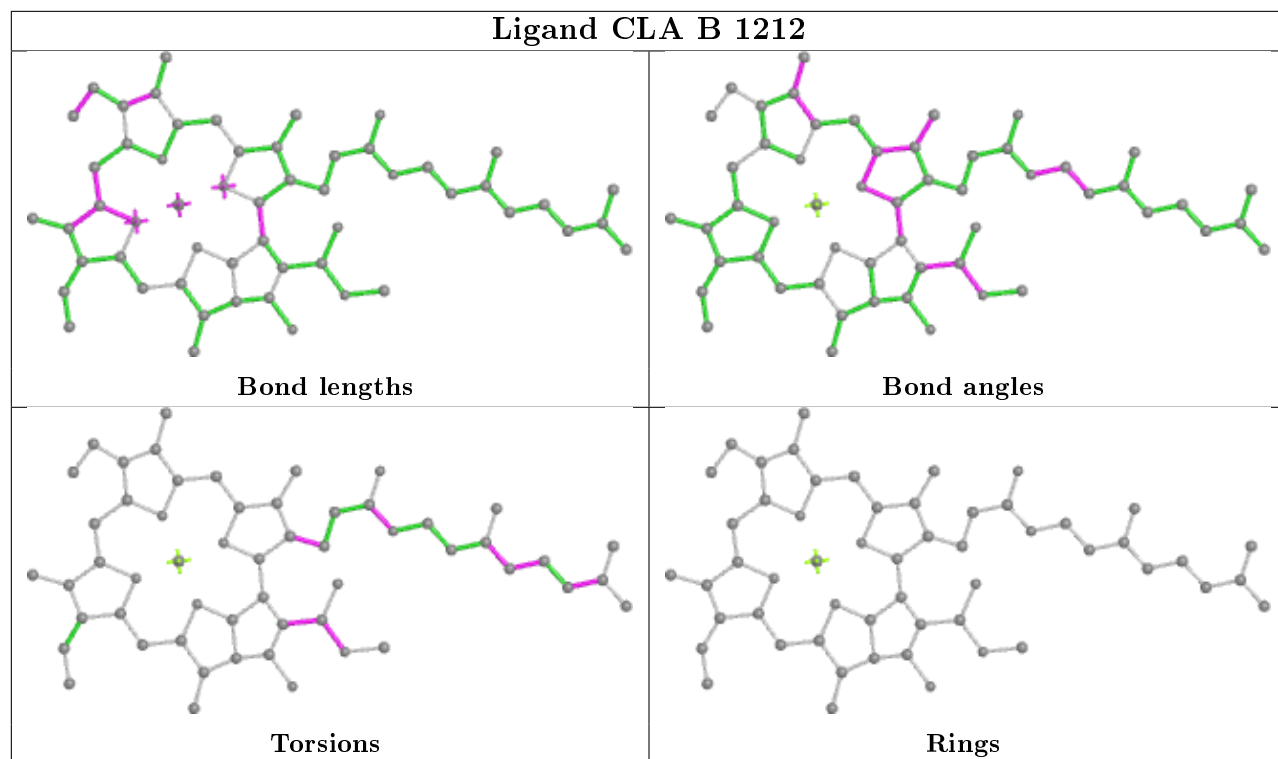




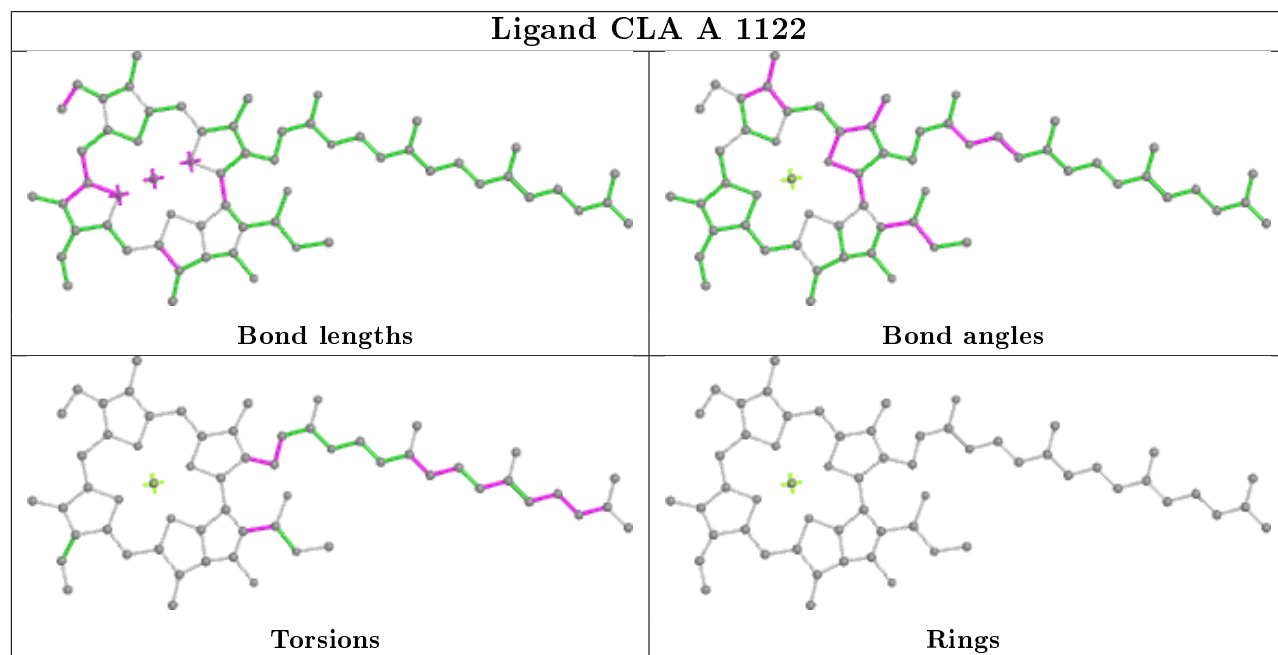


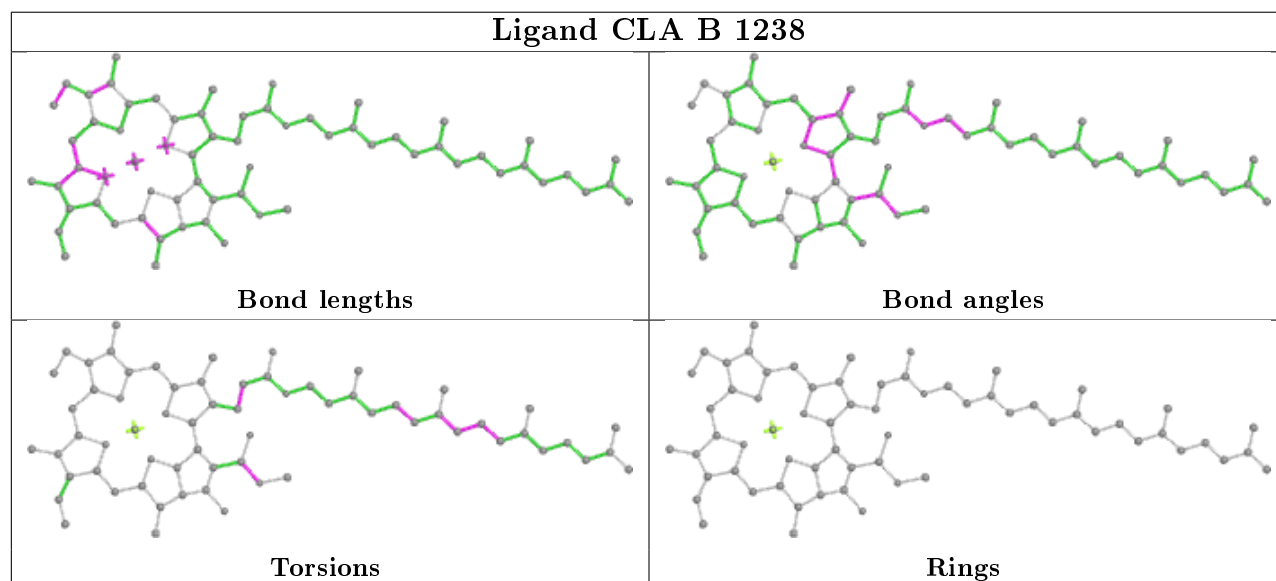
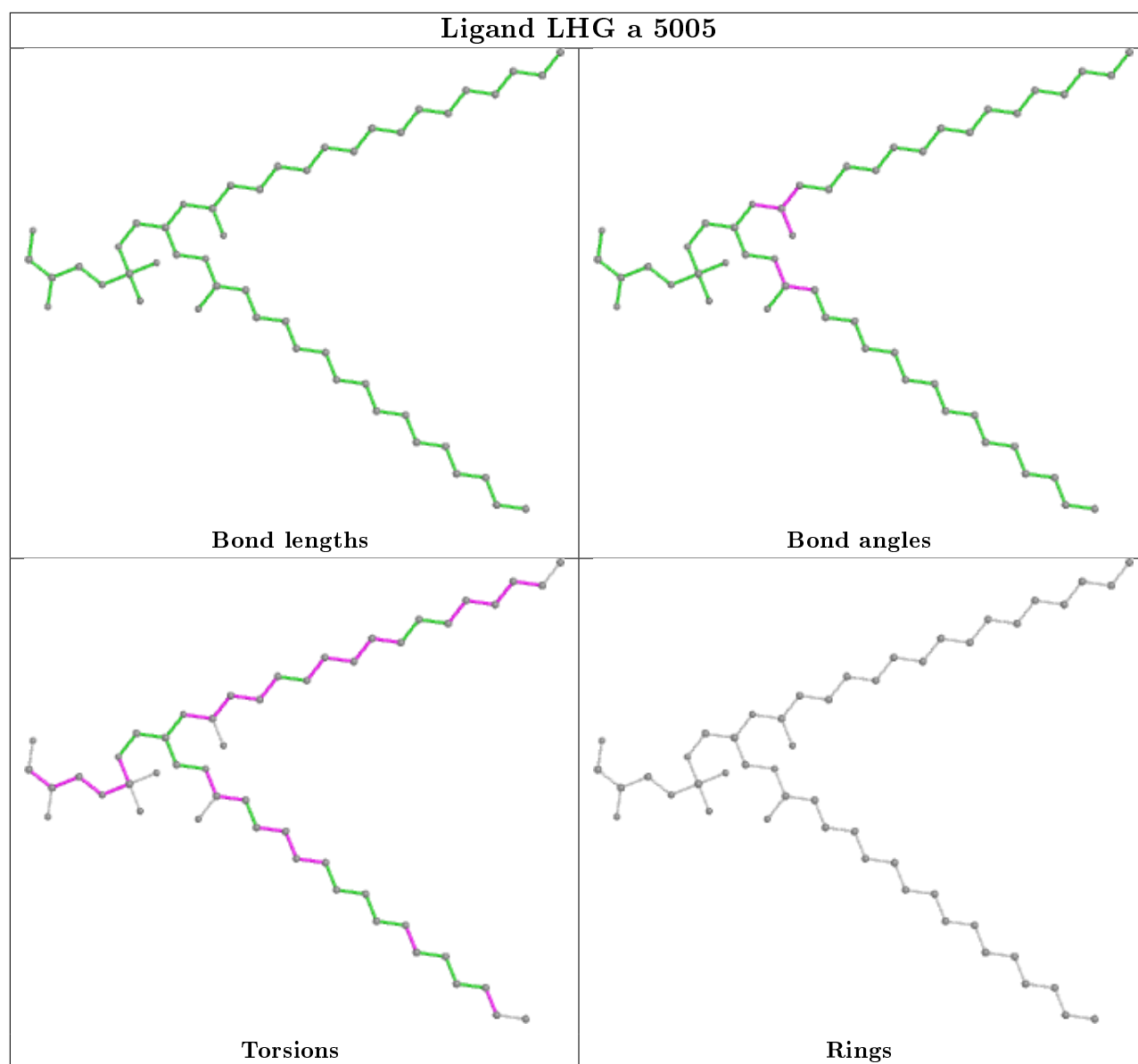


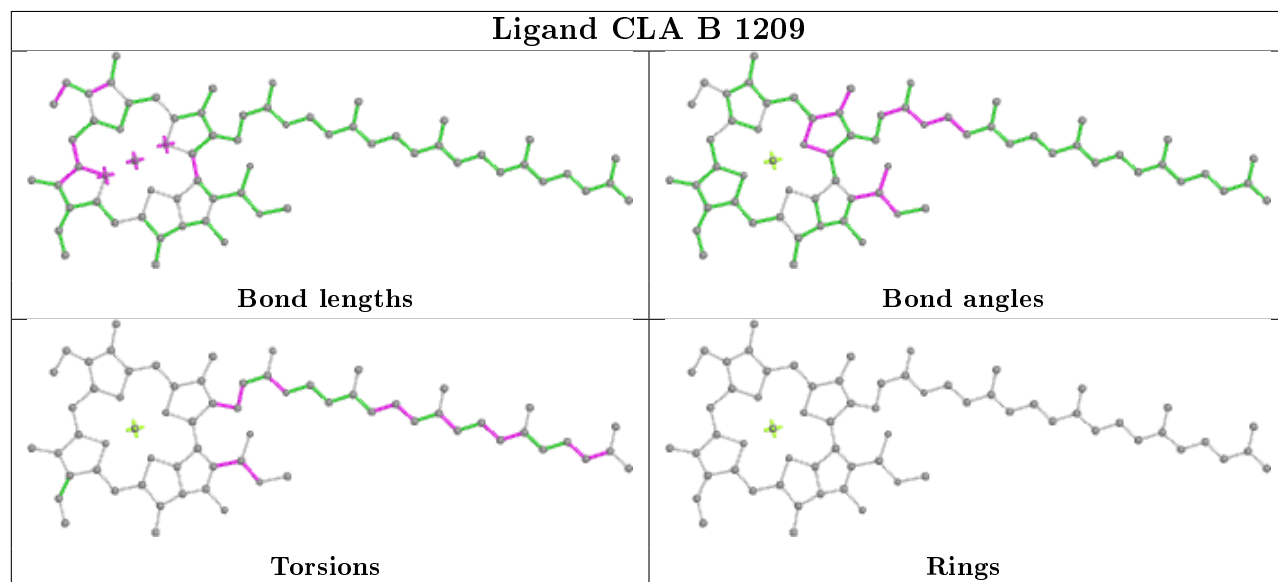
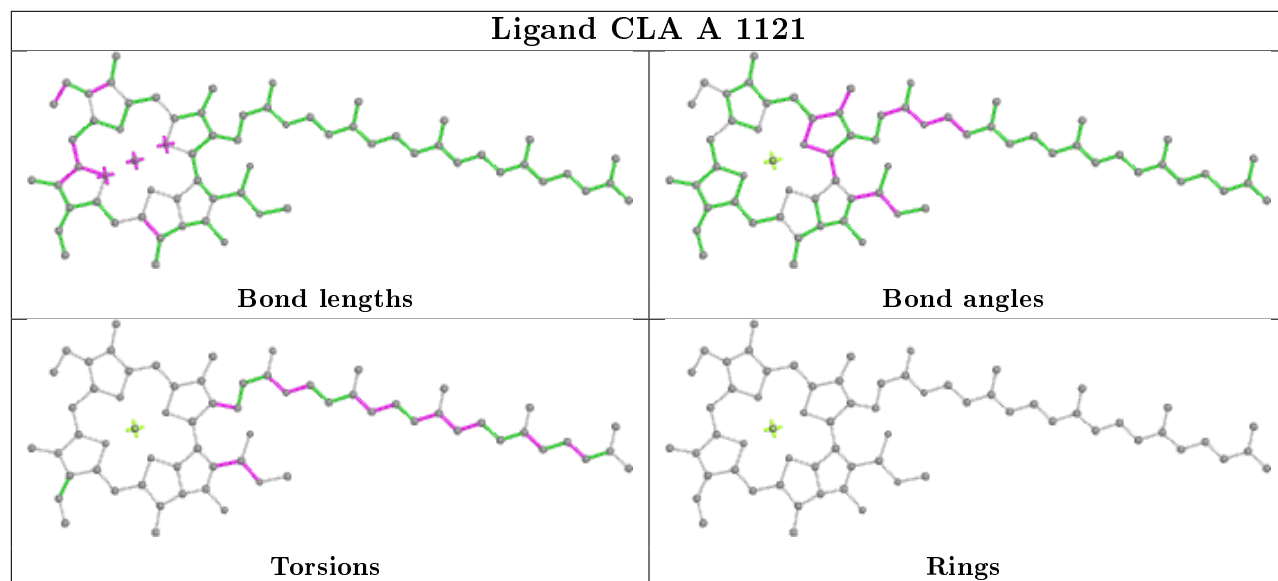
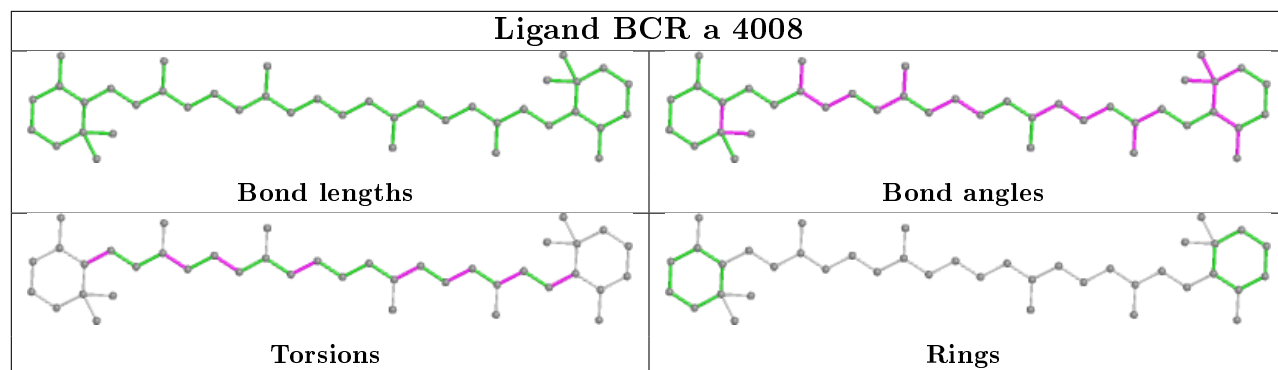
Ligand CLA B 1212

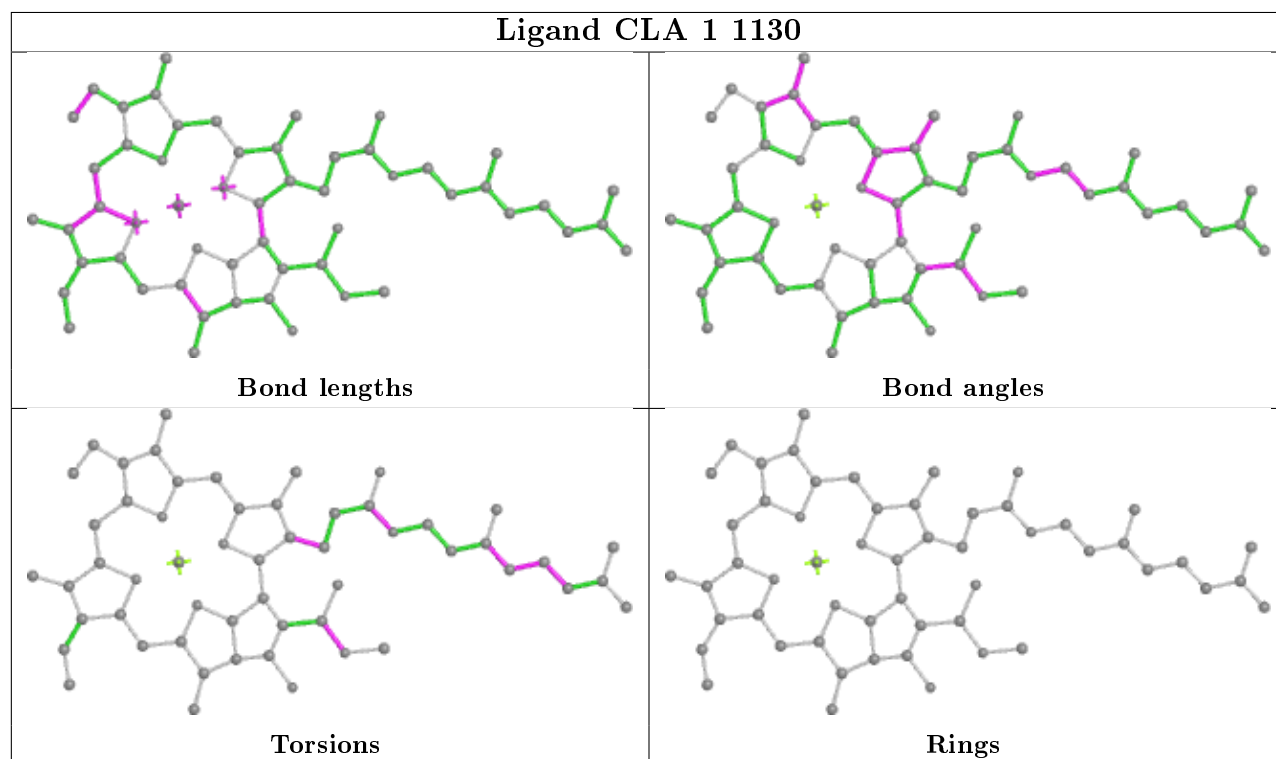
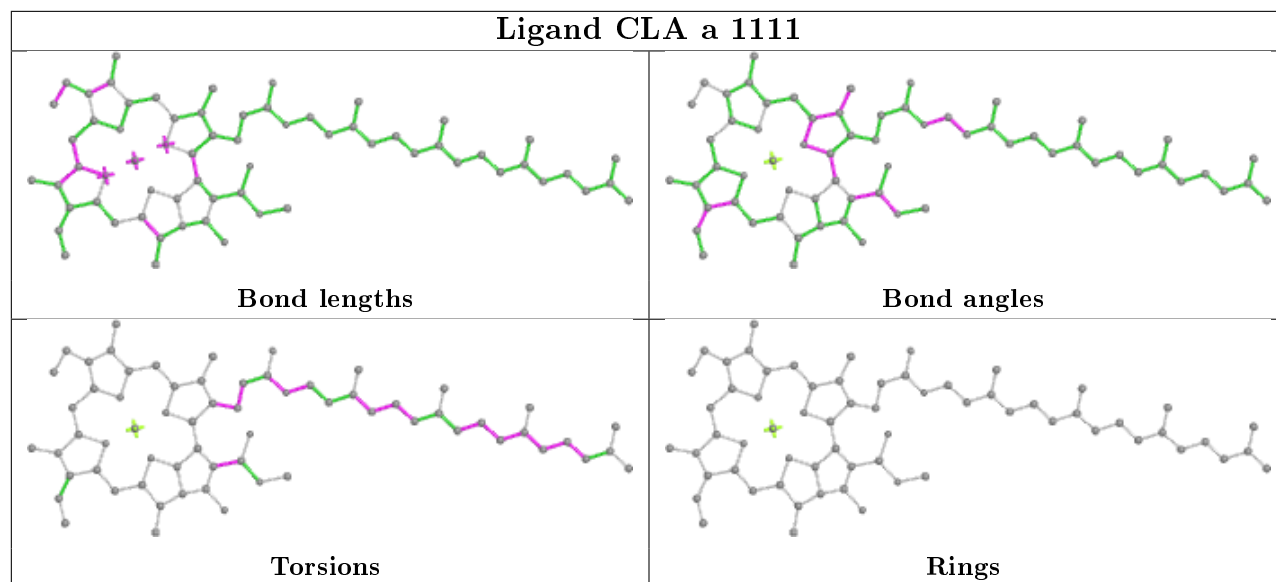


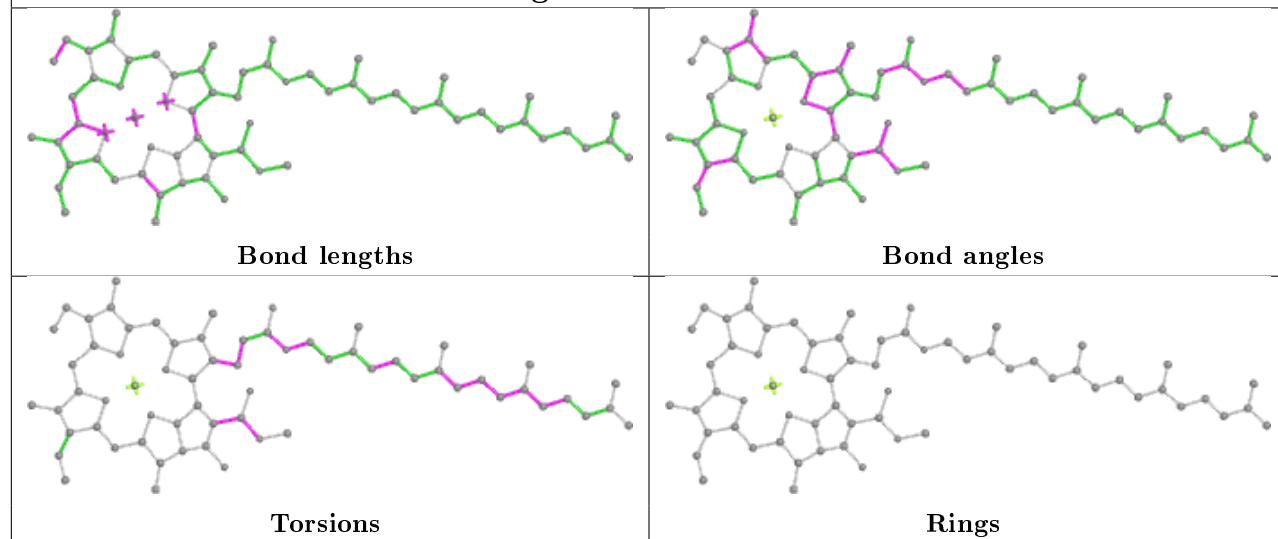
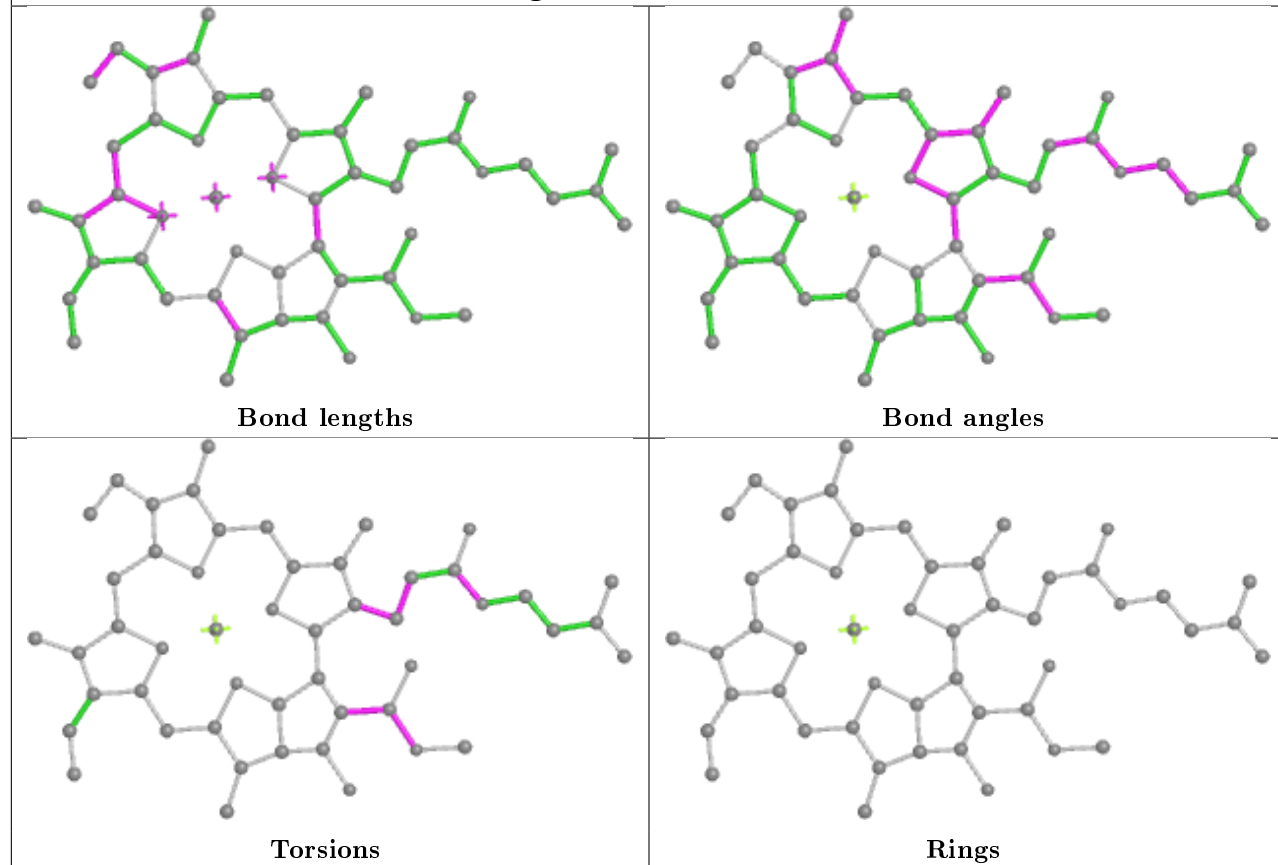
Ligand CLA A 1122

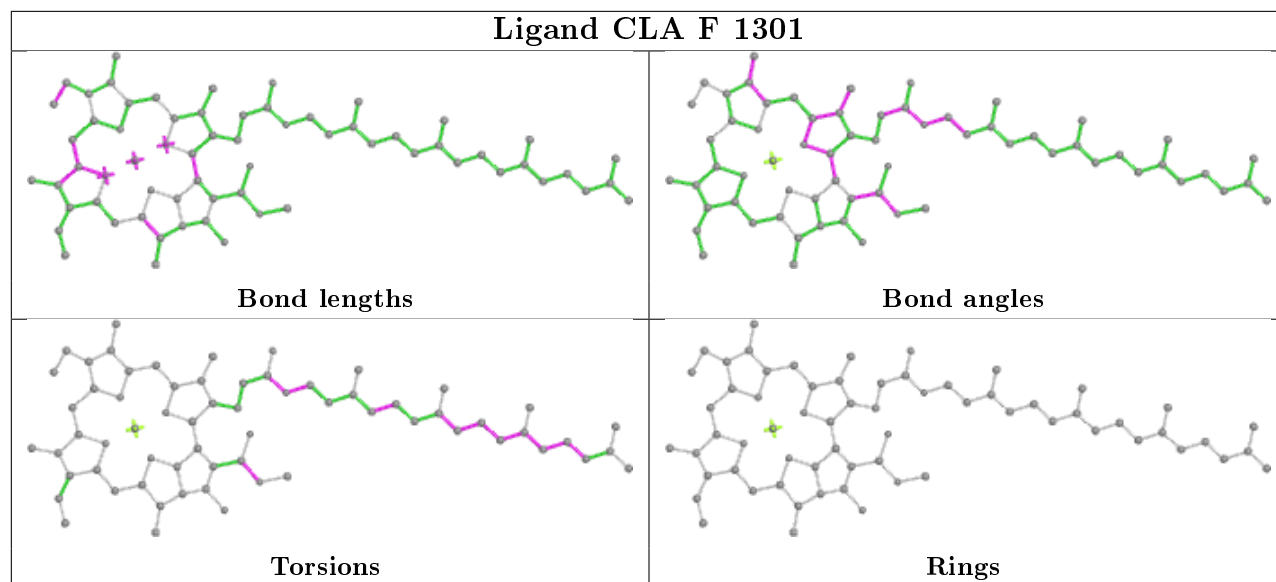
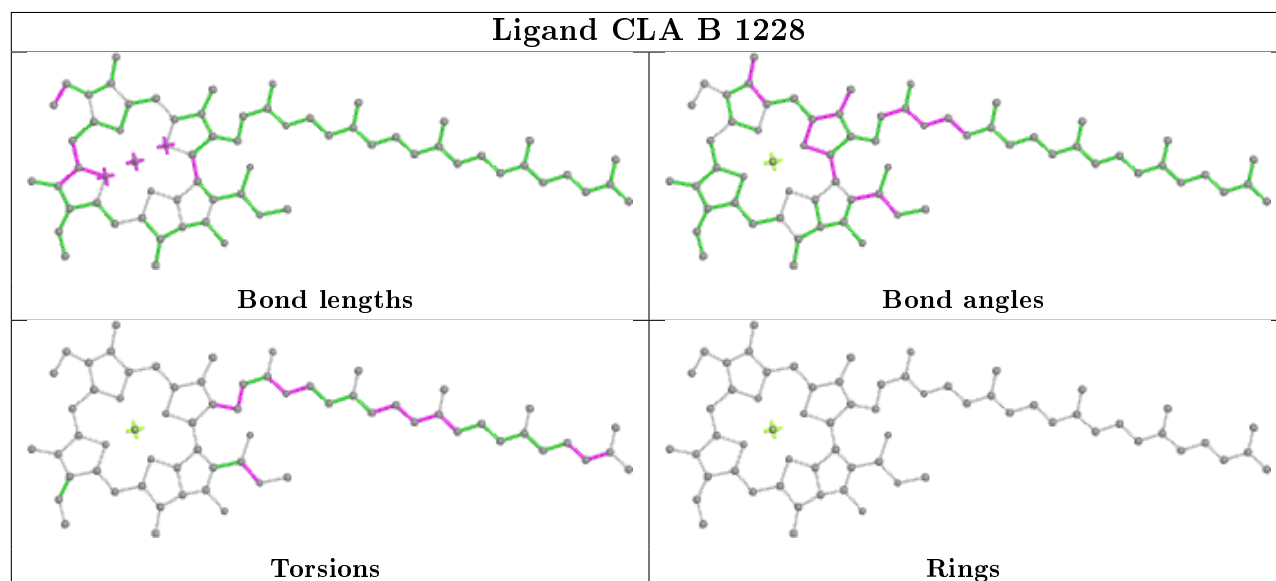
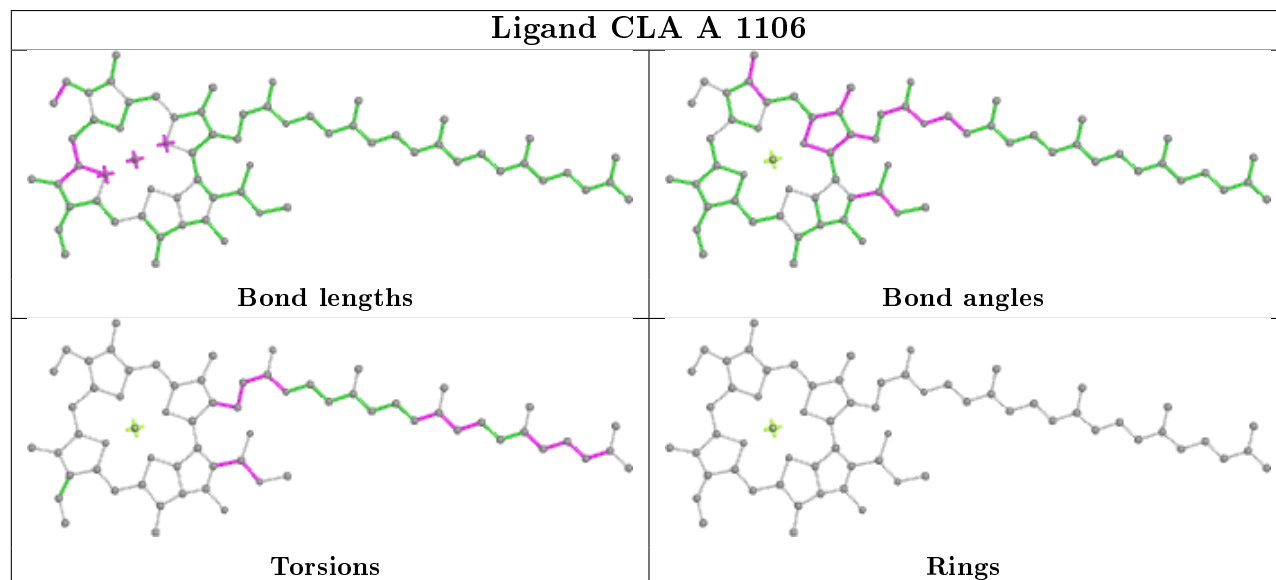


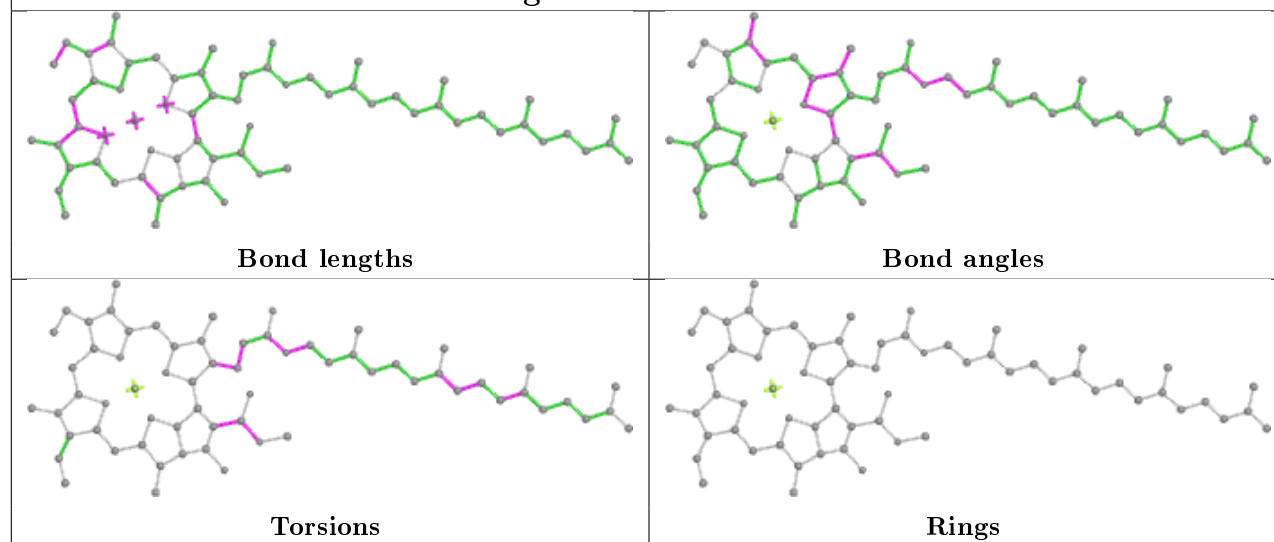
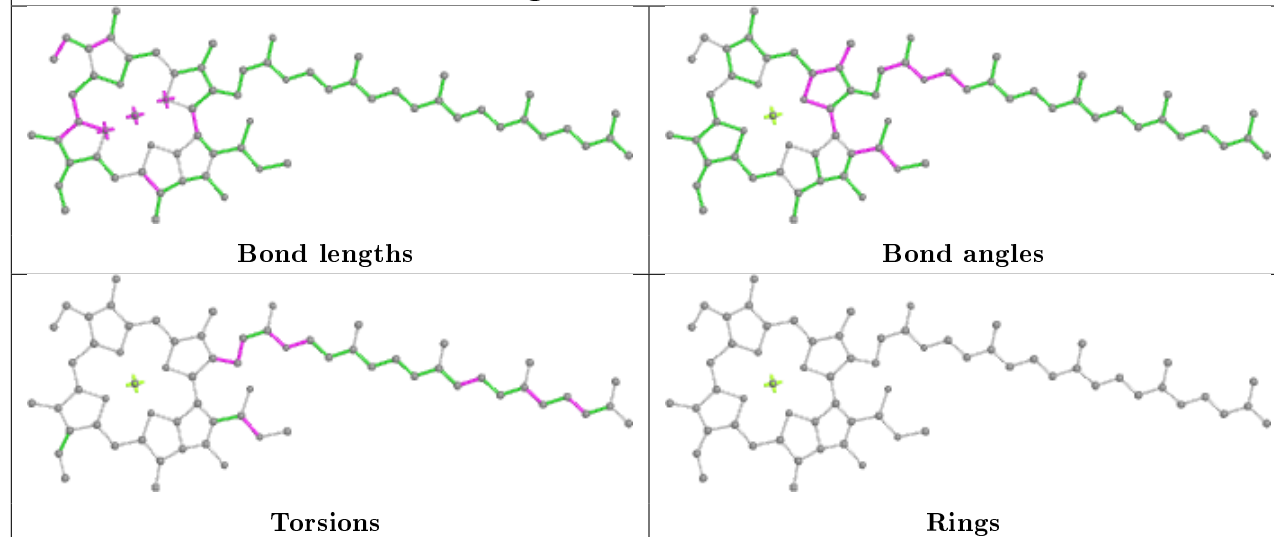


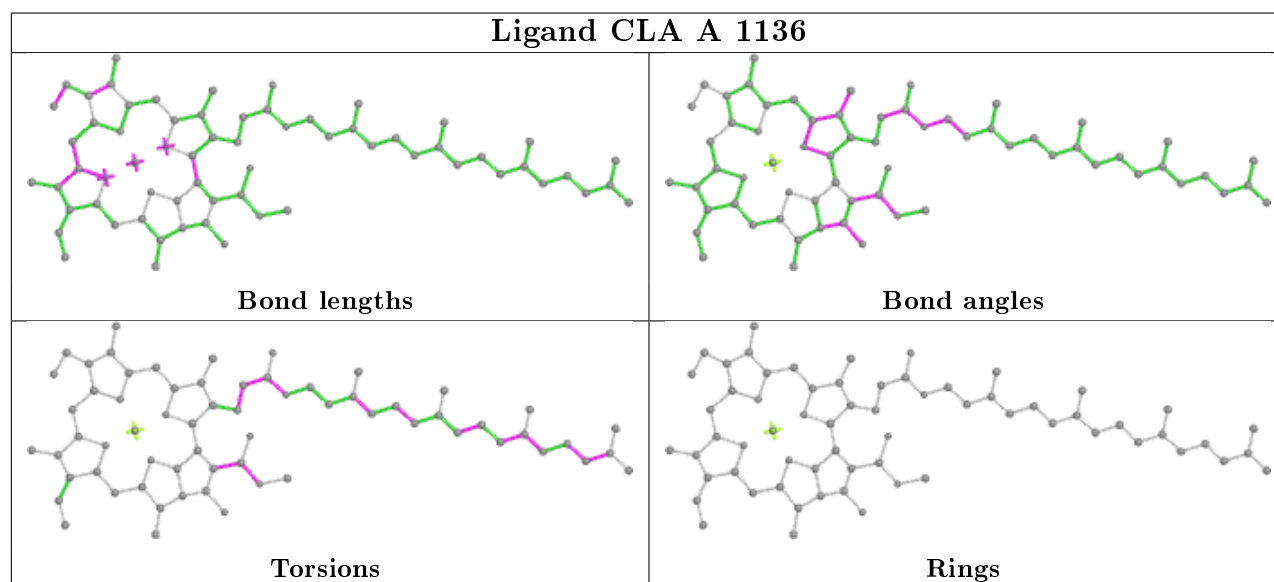
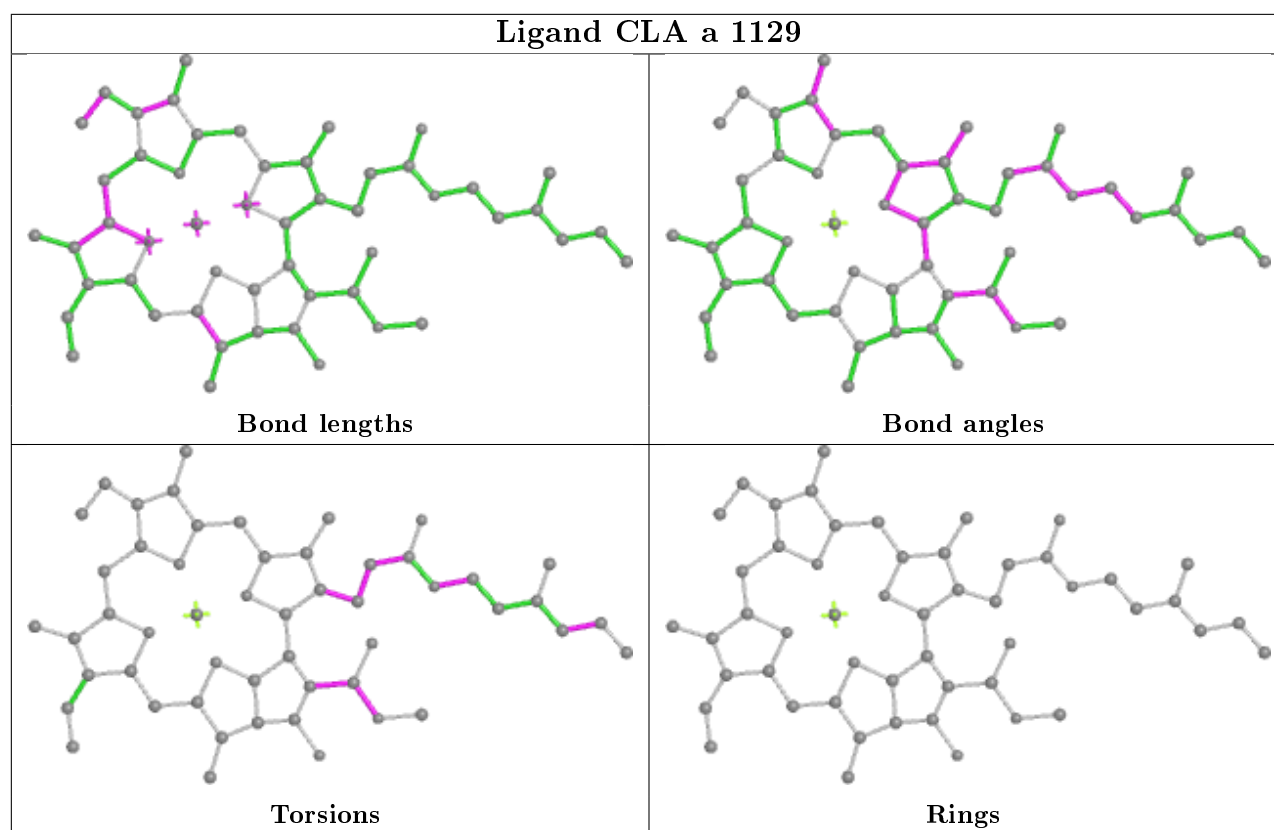


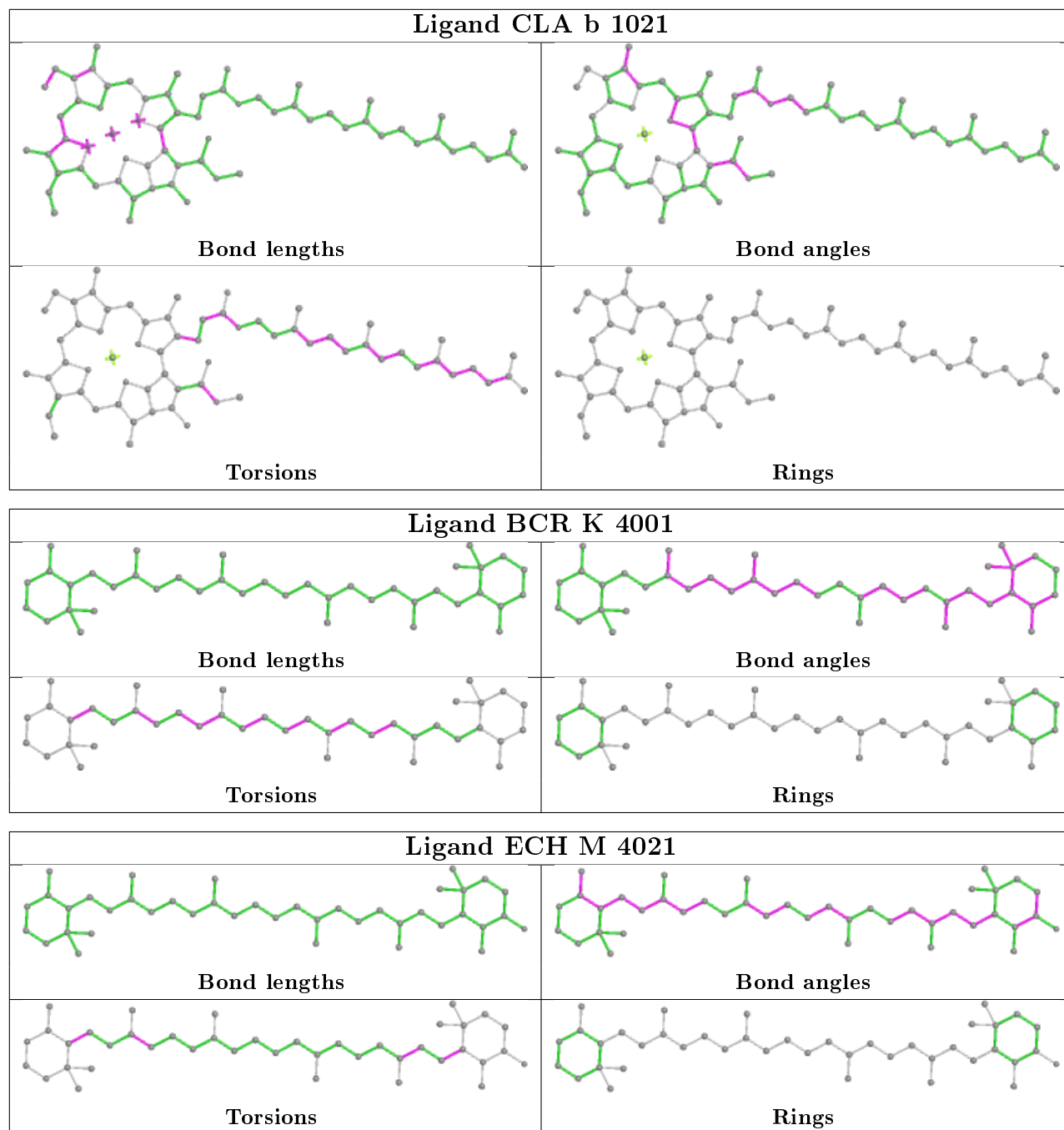


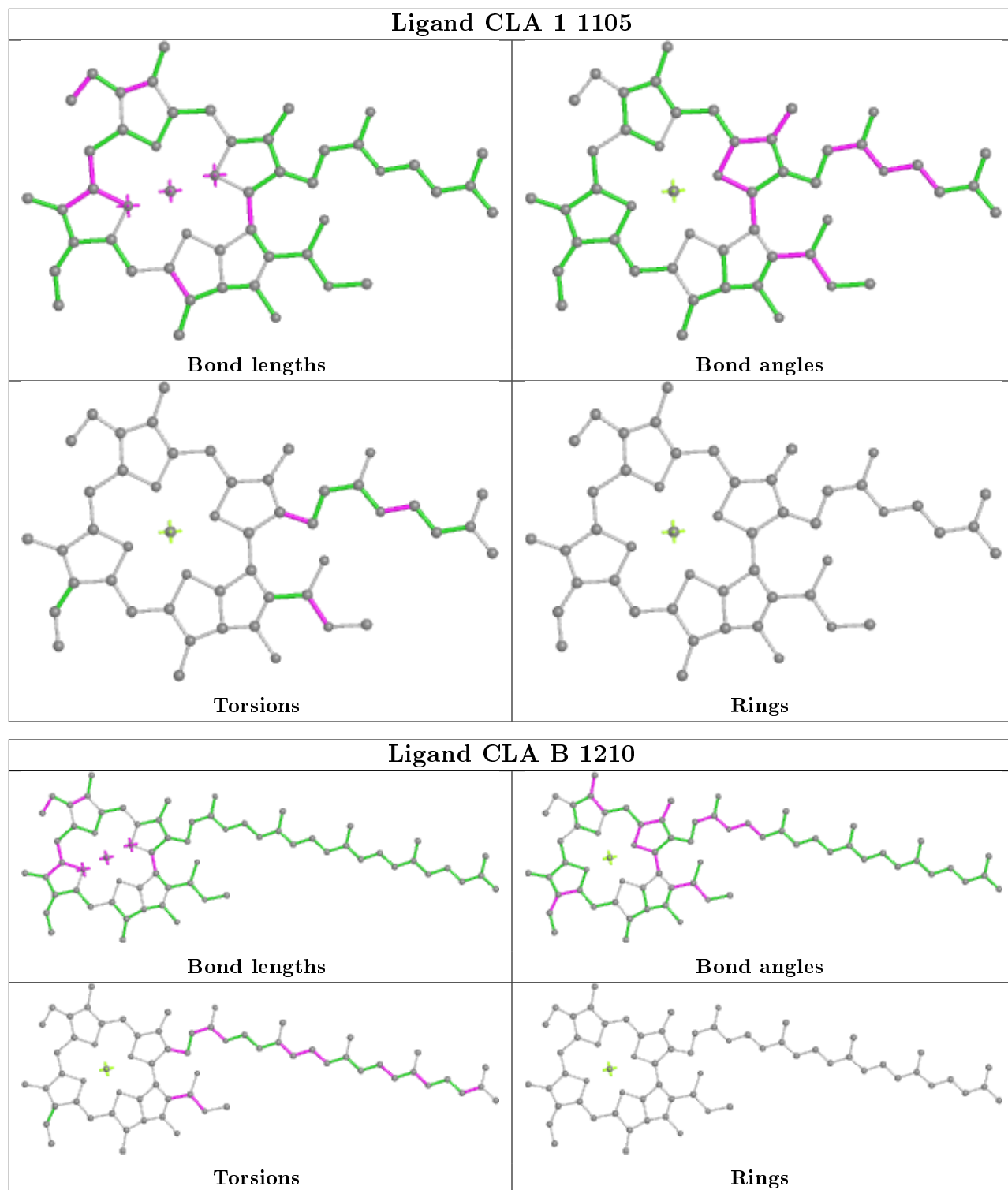
Ligand CLA 1 1501**Ligand CLA a 1113**

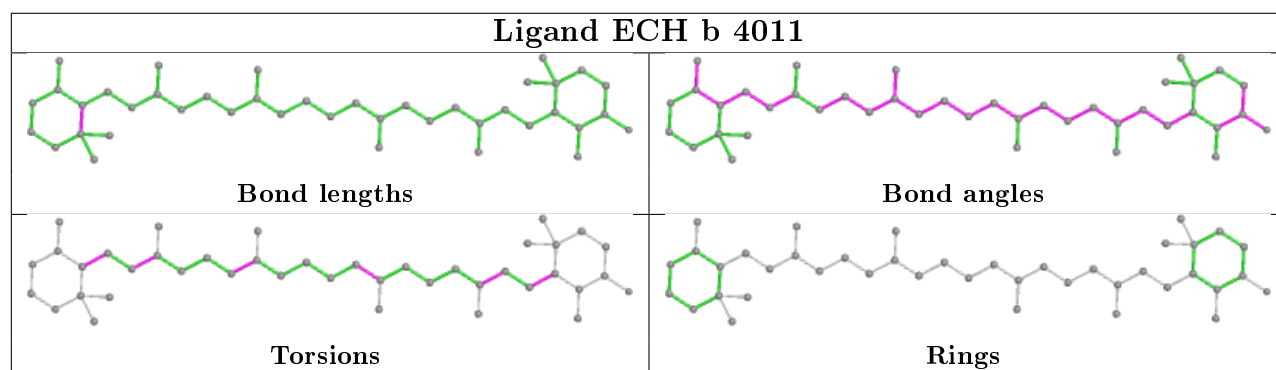
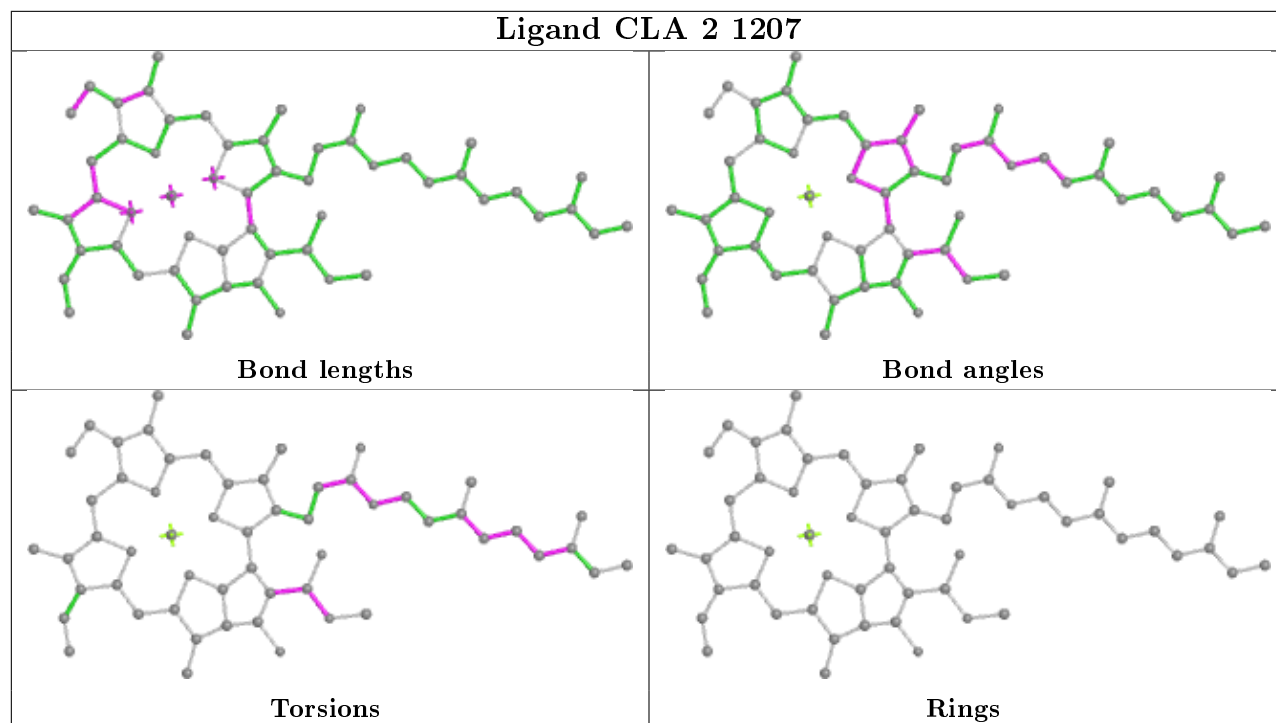
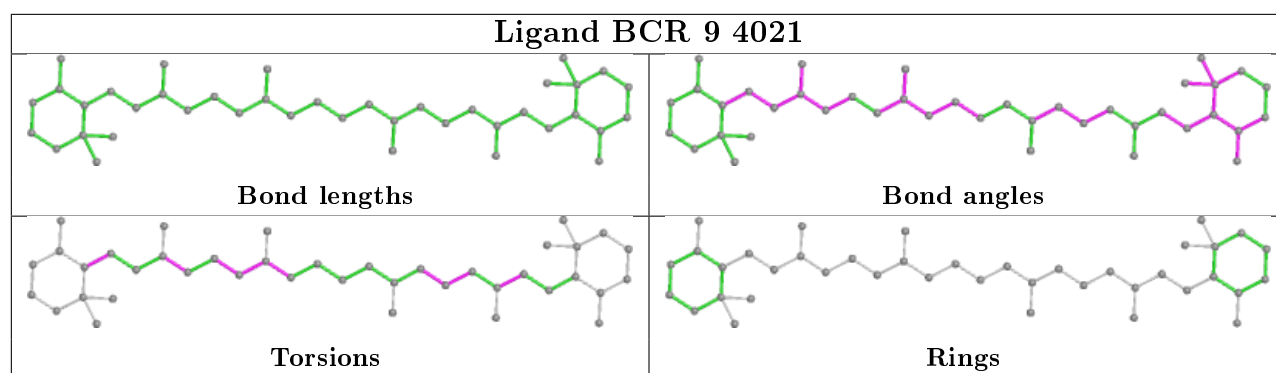
Ligand CLA F 1301**Ligand CLA B 1228****Ligand CLA A 1106**

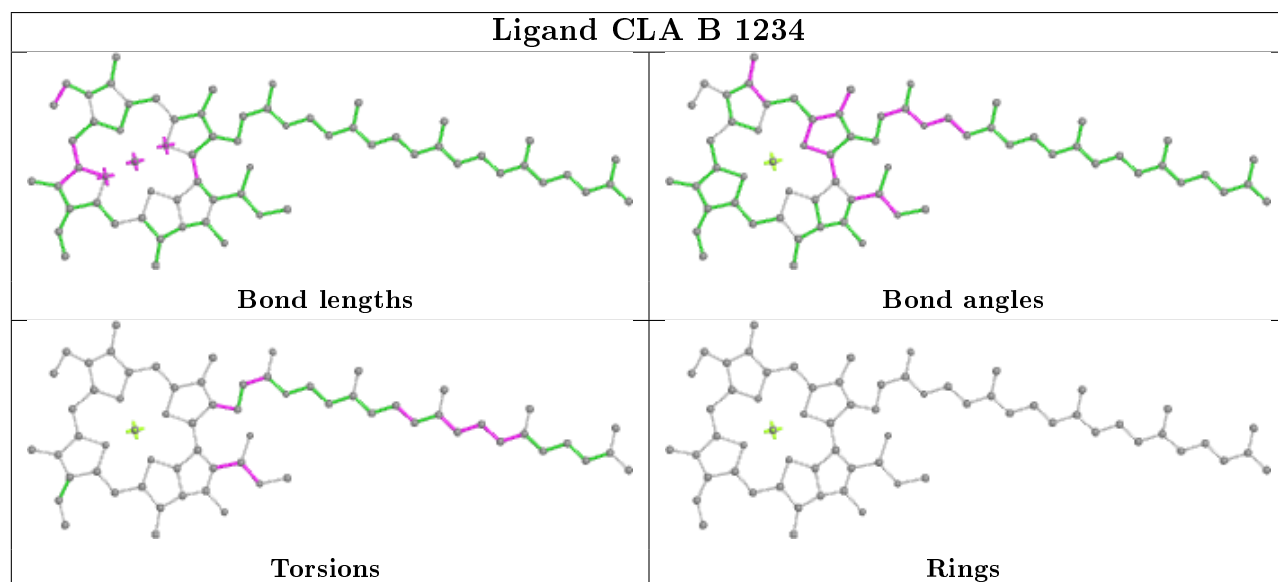
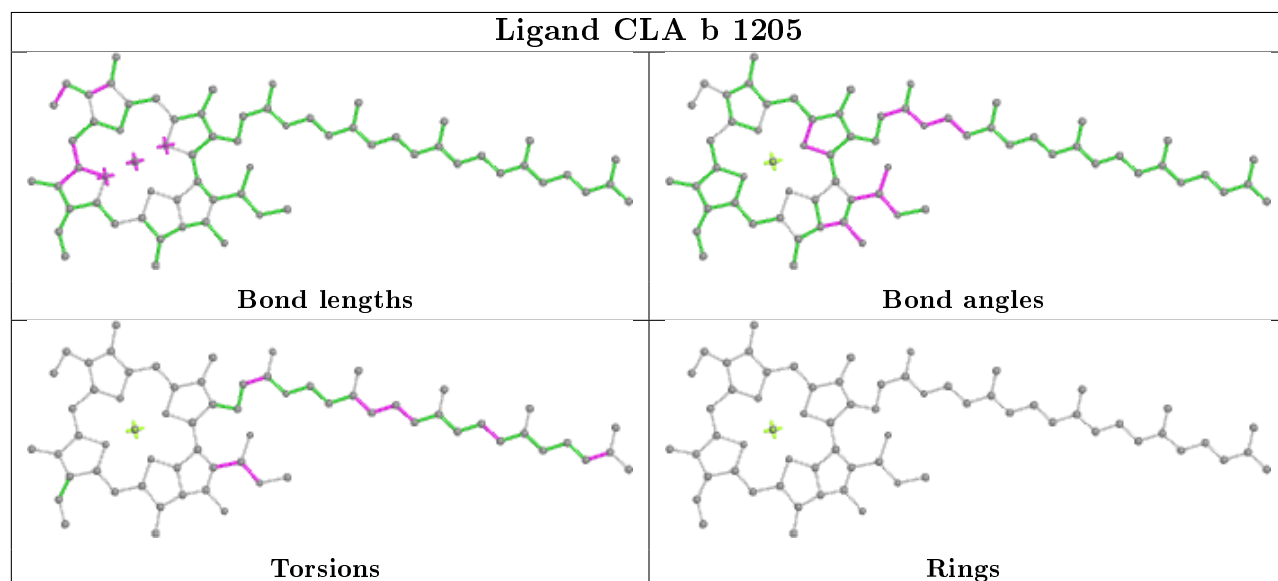
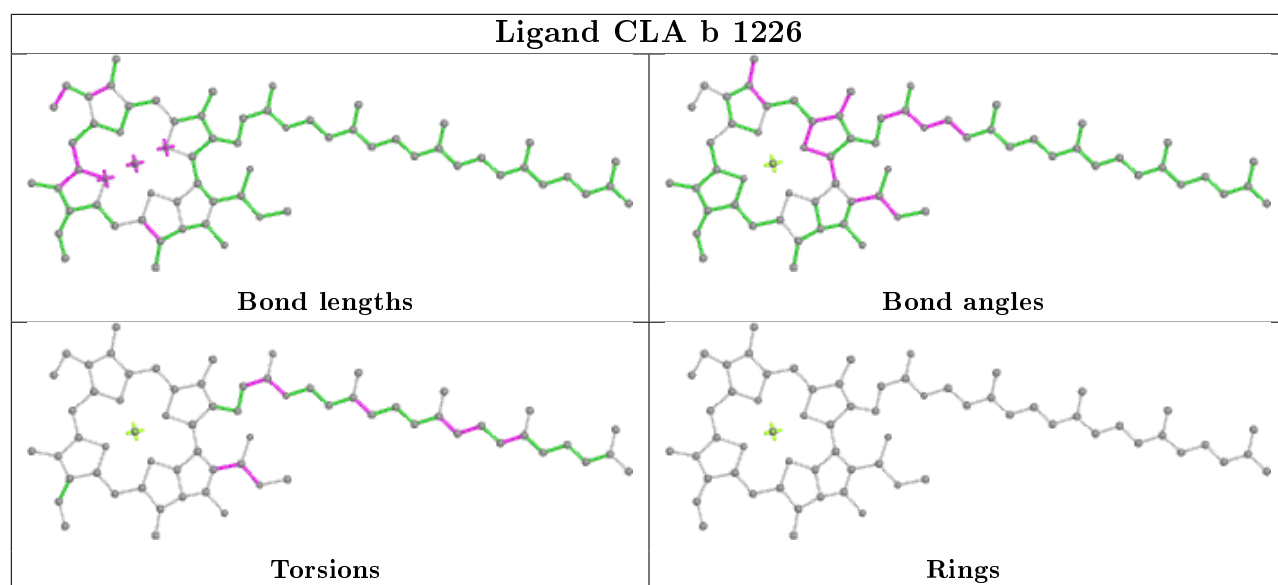
Ligand CLA A 1138**Ligand CLA b 1239**

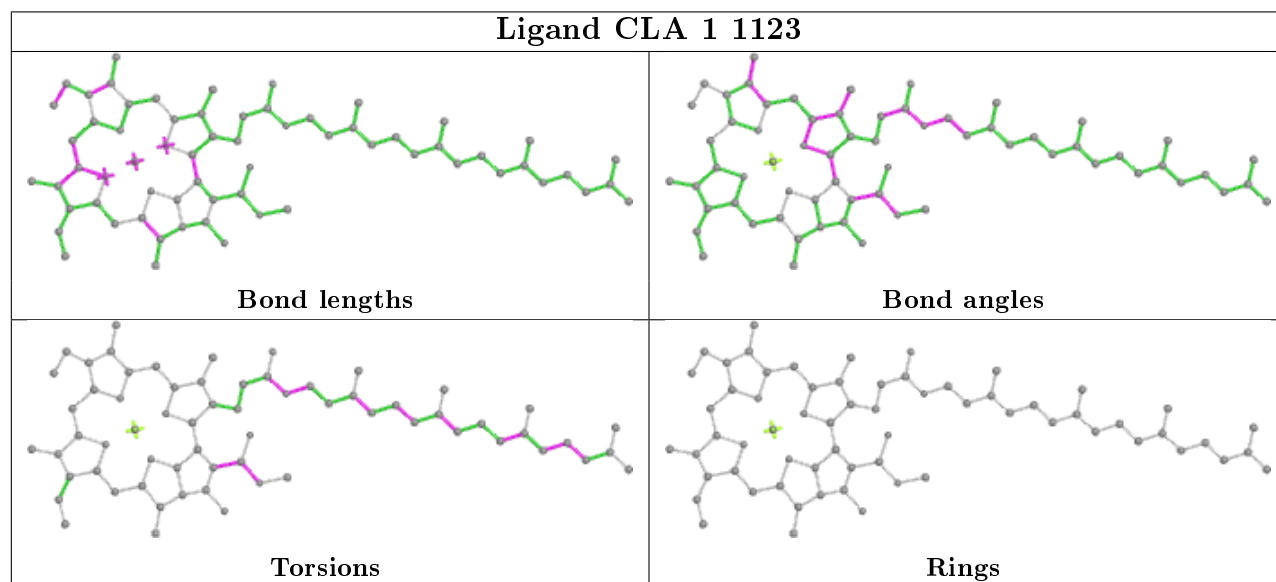
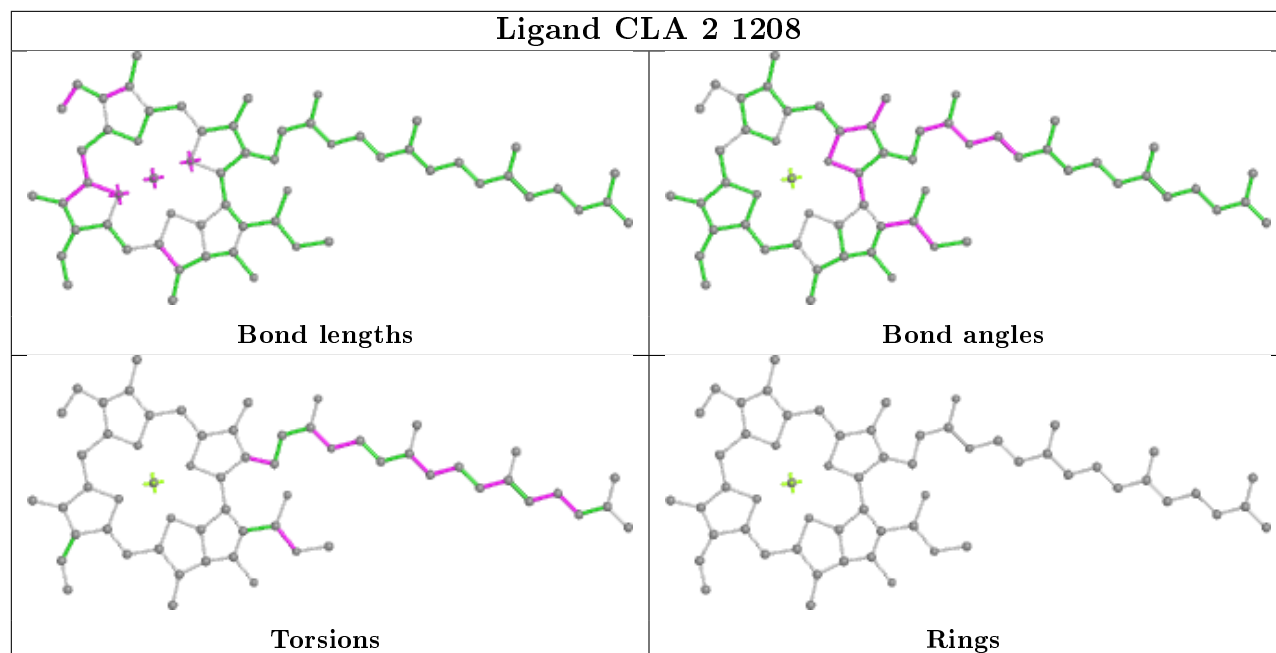


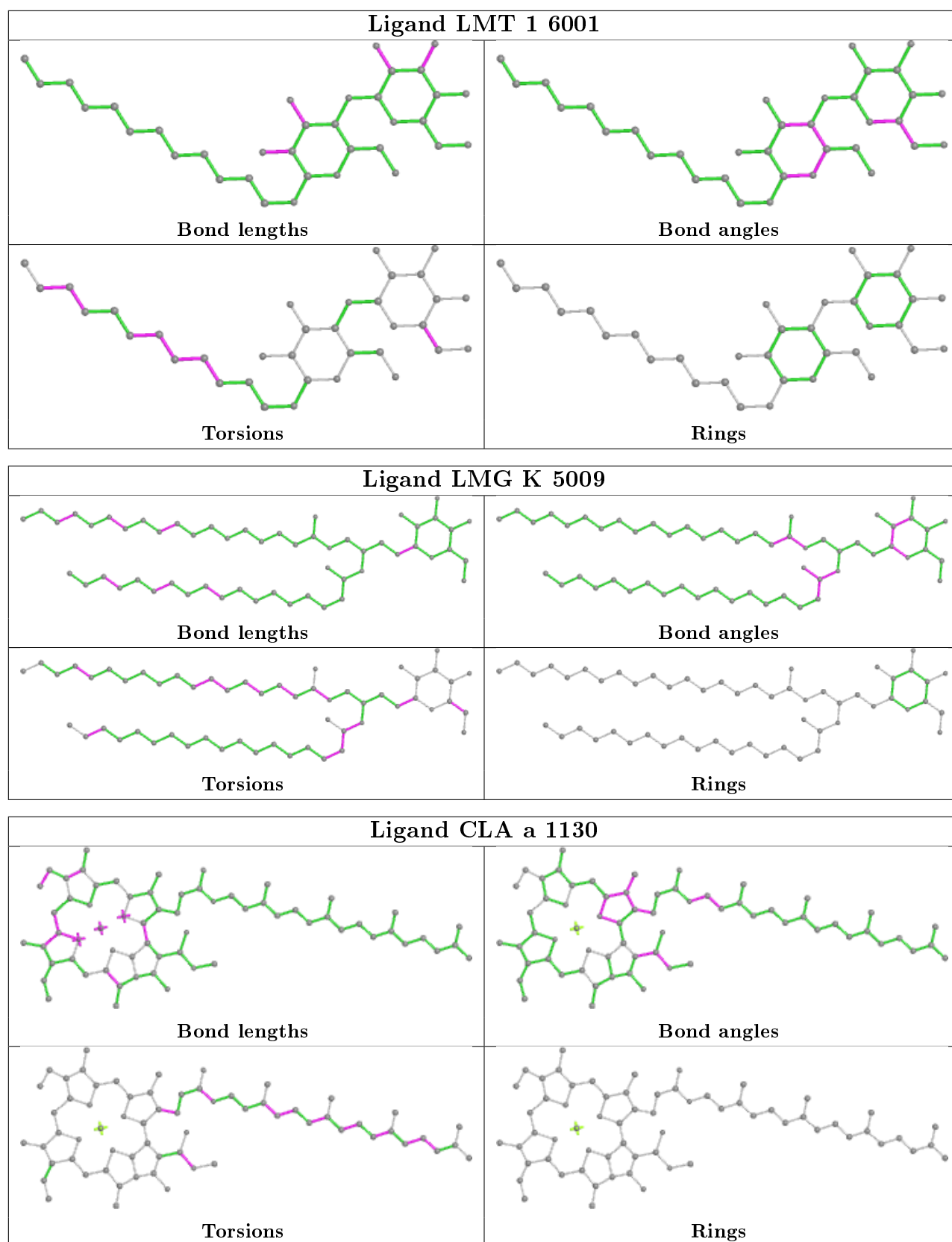


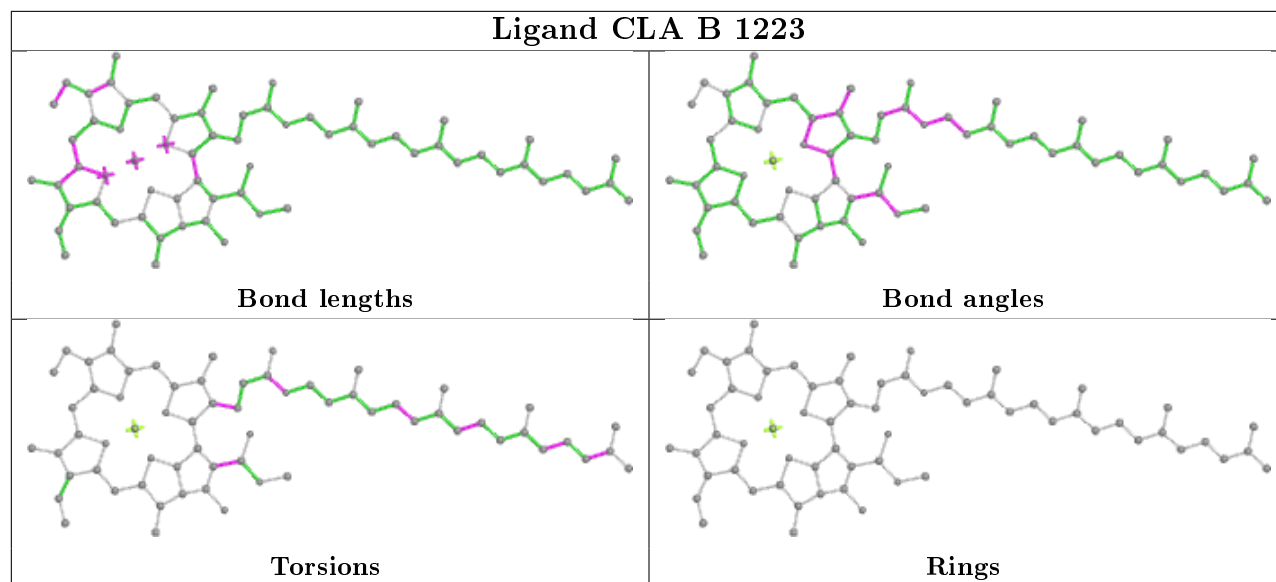
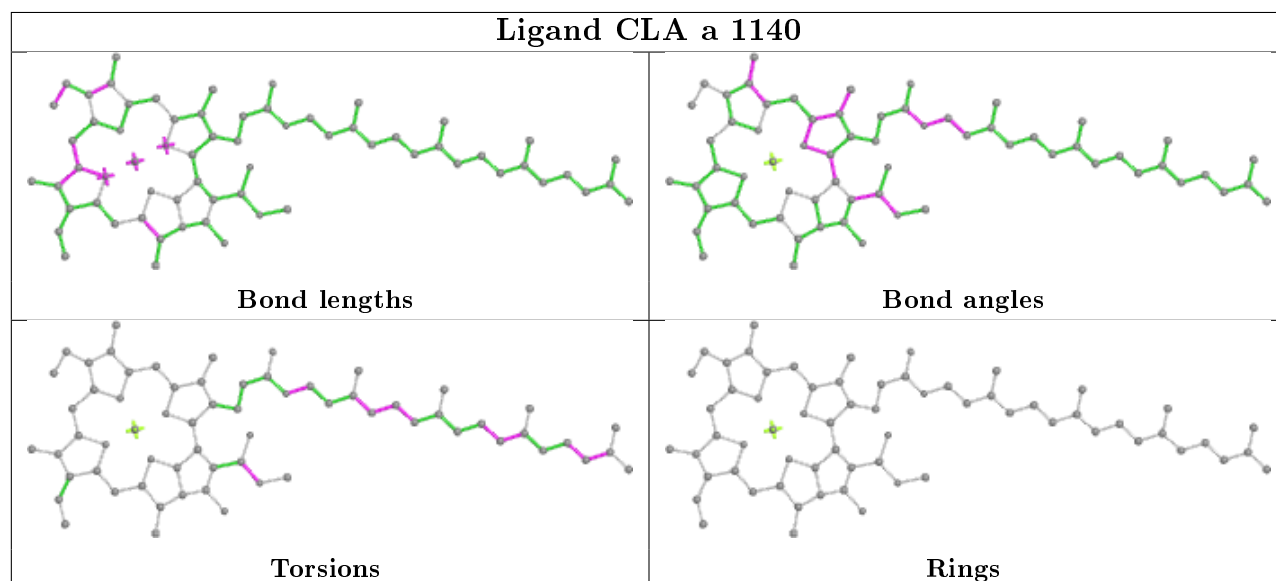
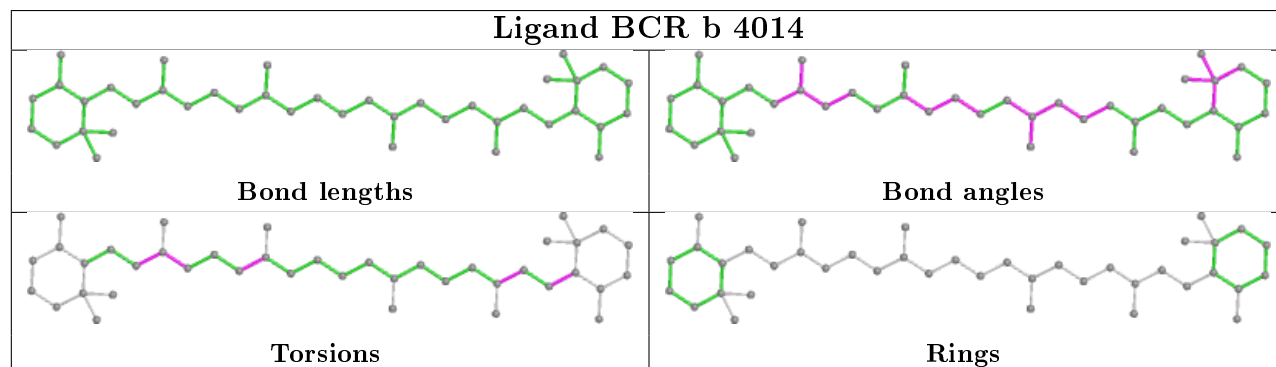


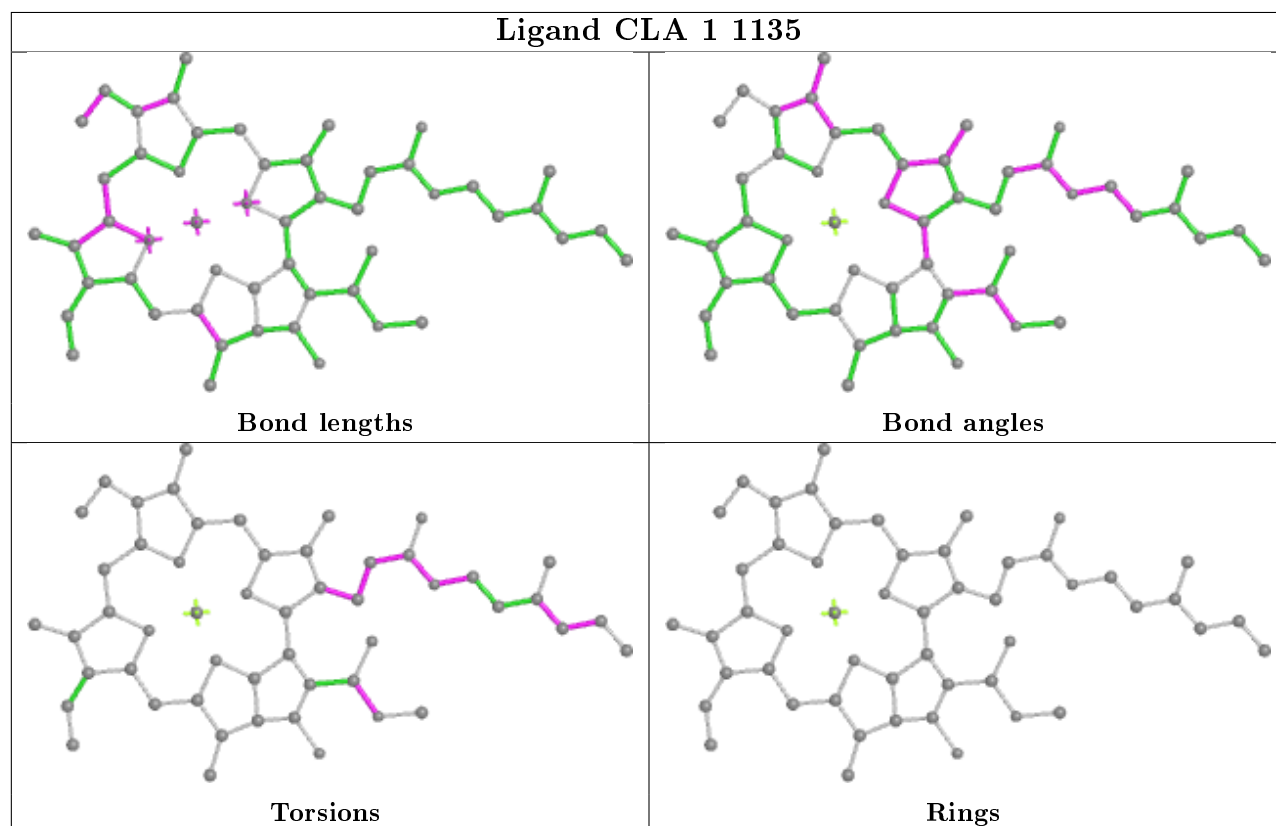
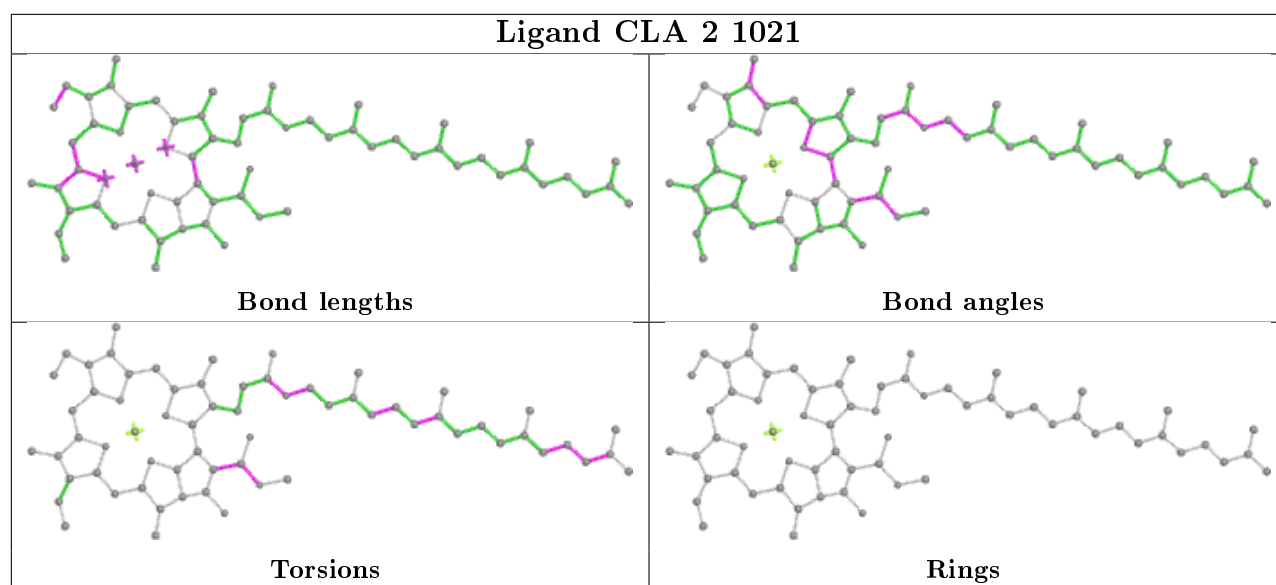


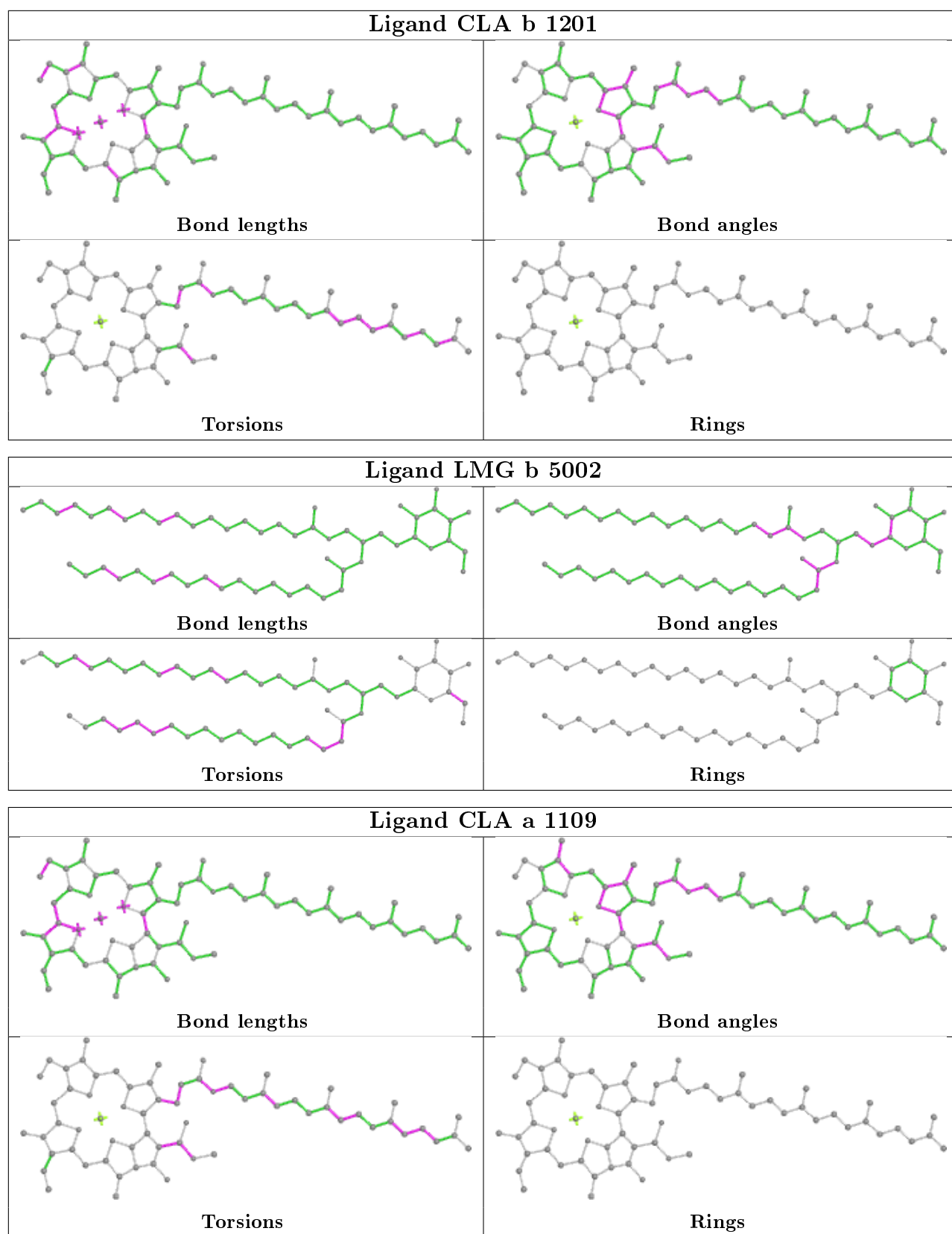


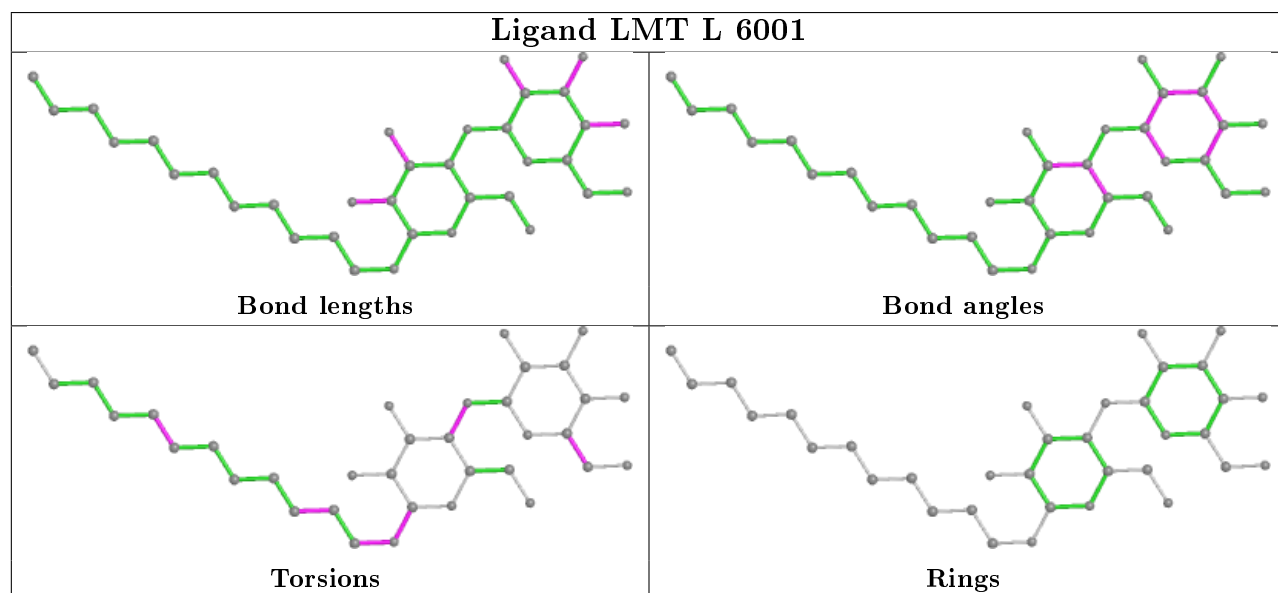
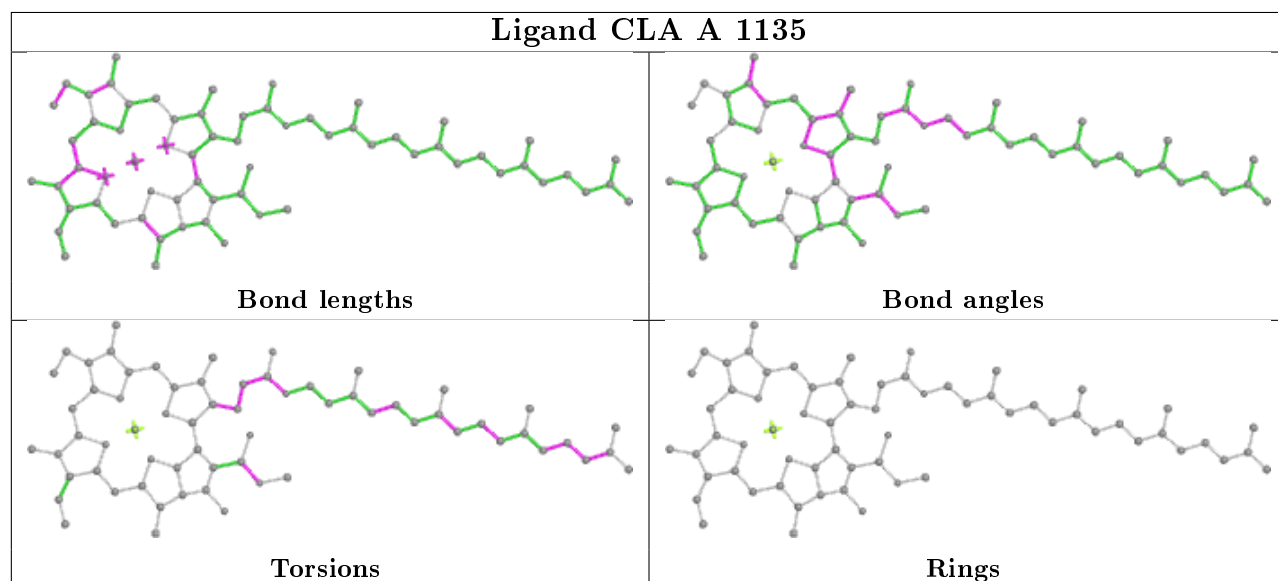
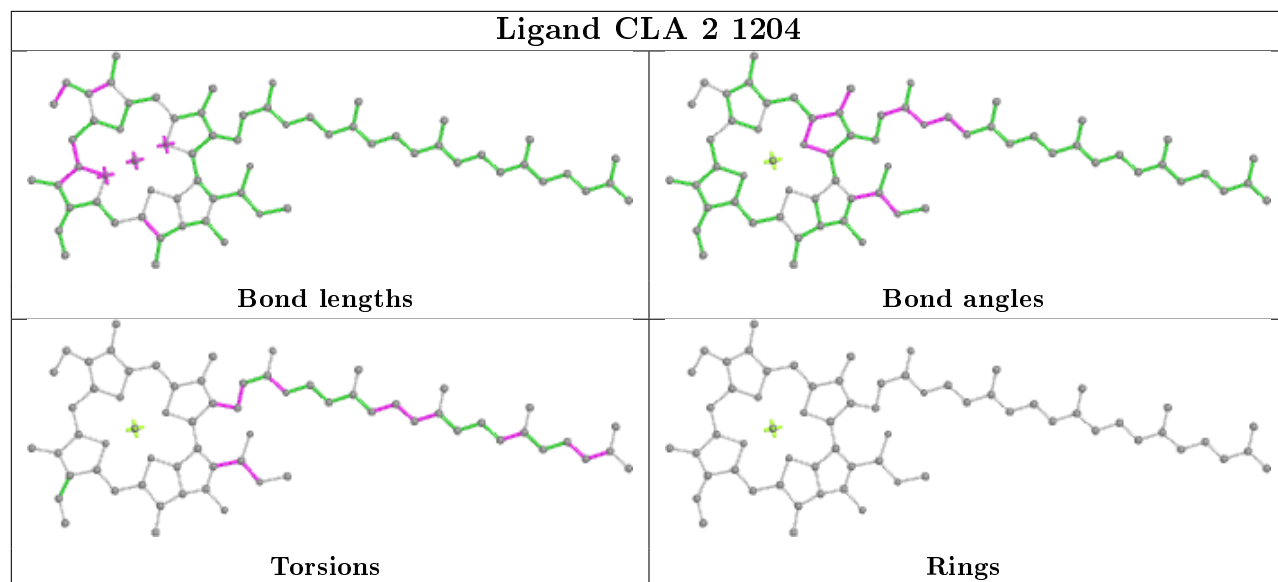


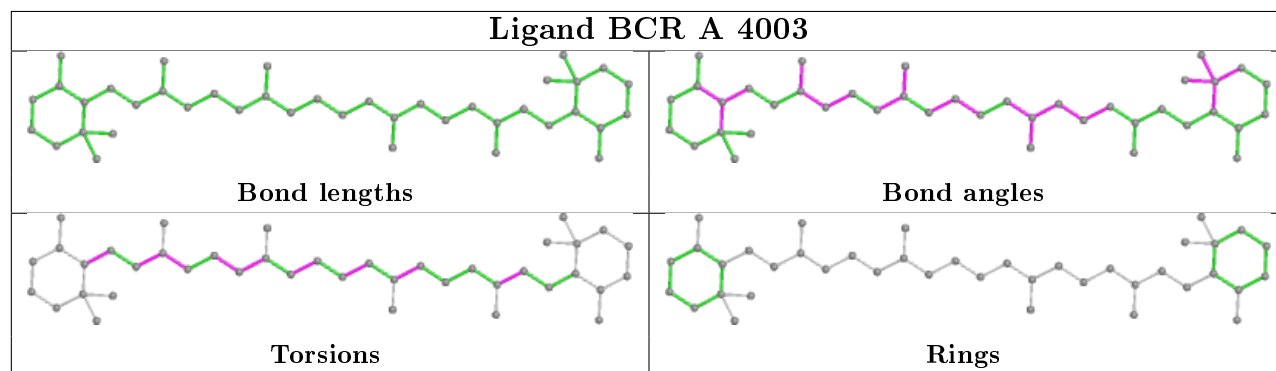
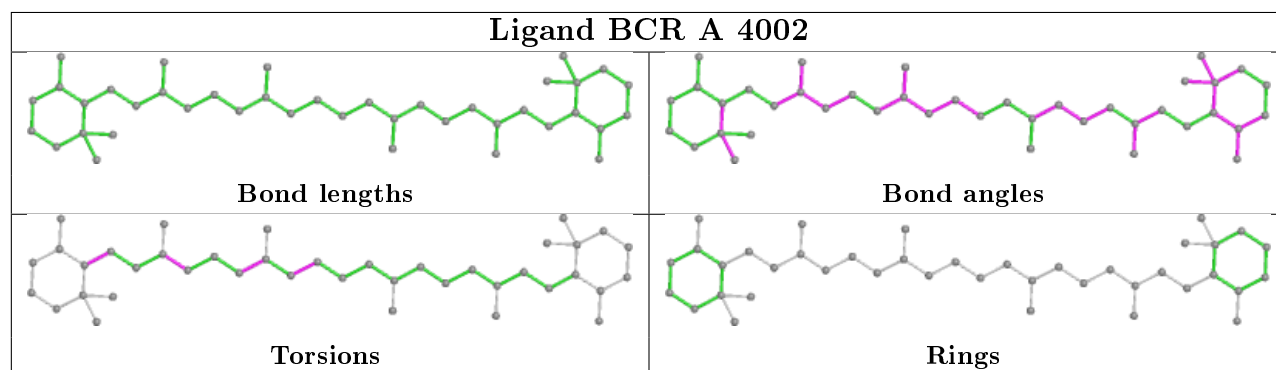
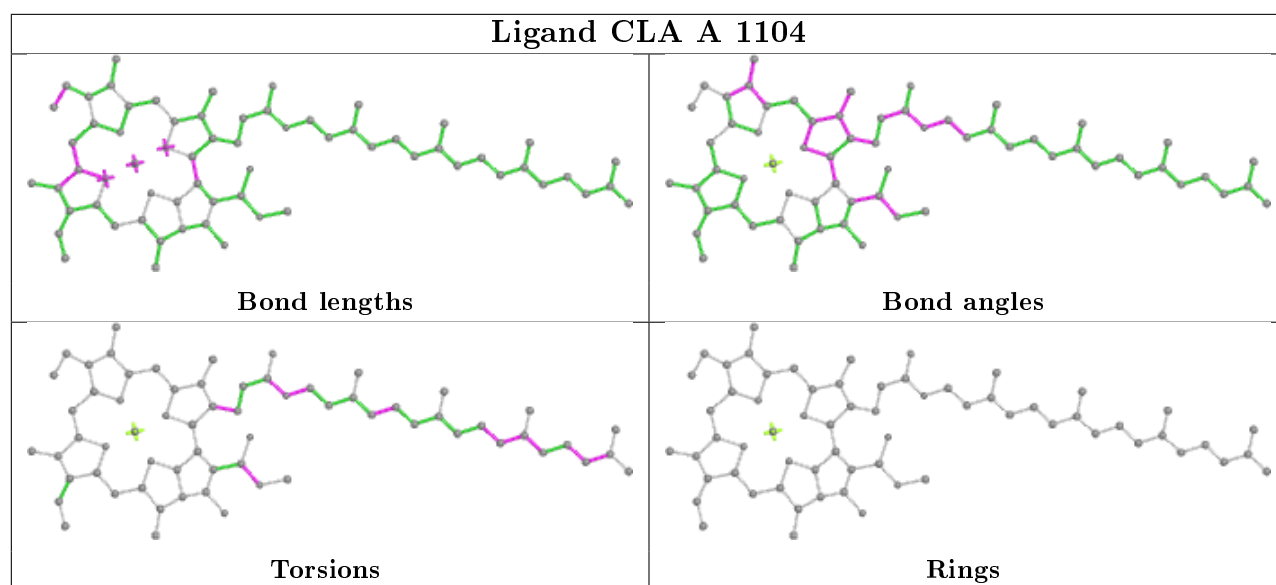


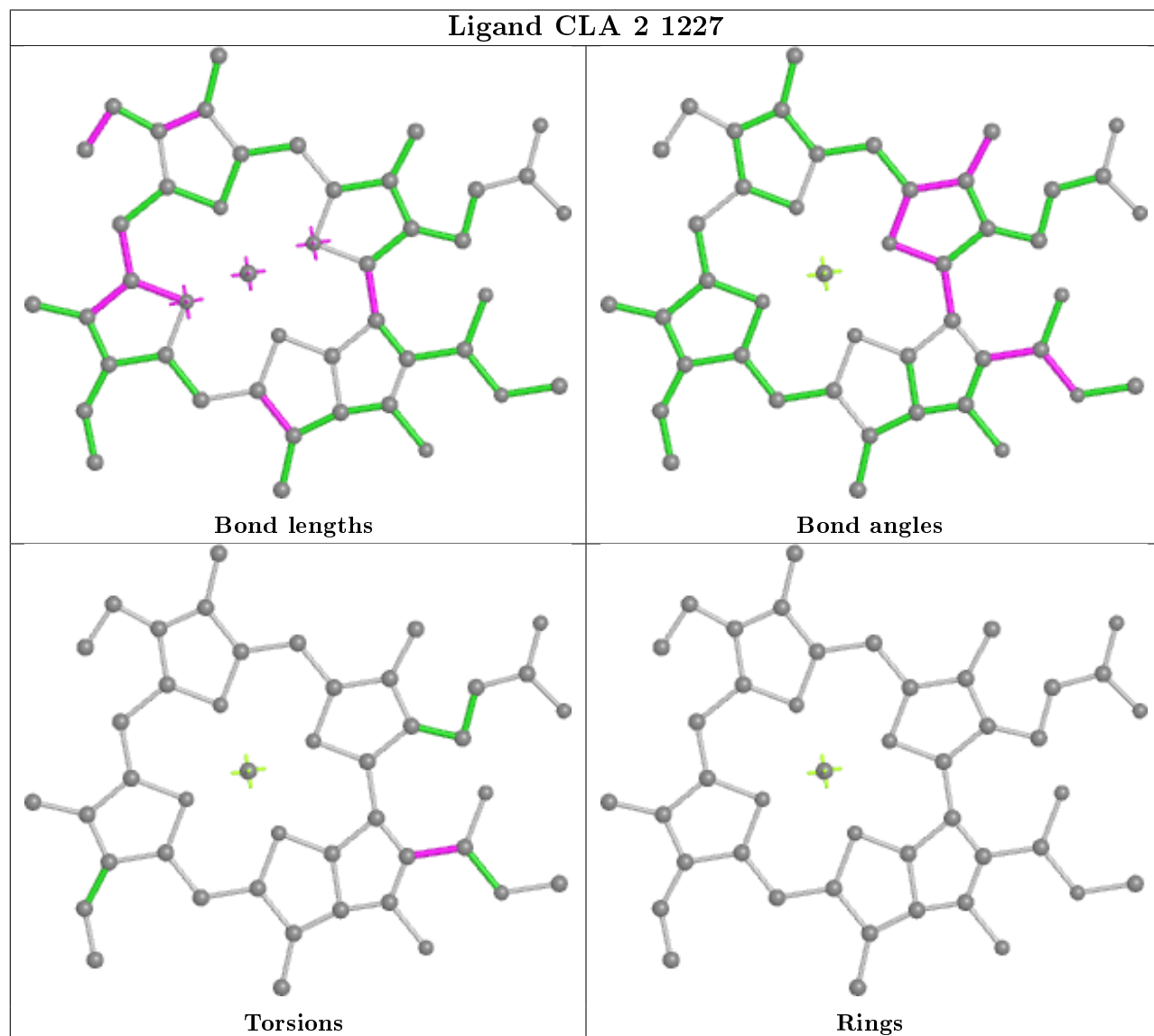
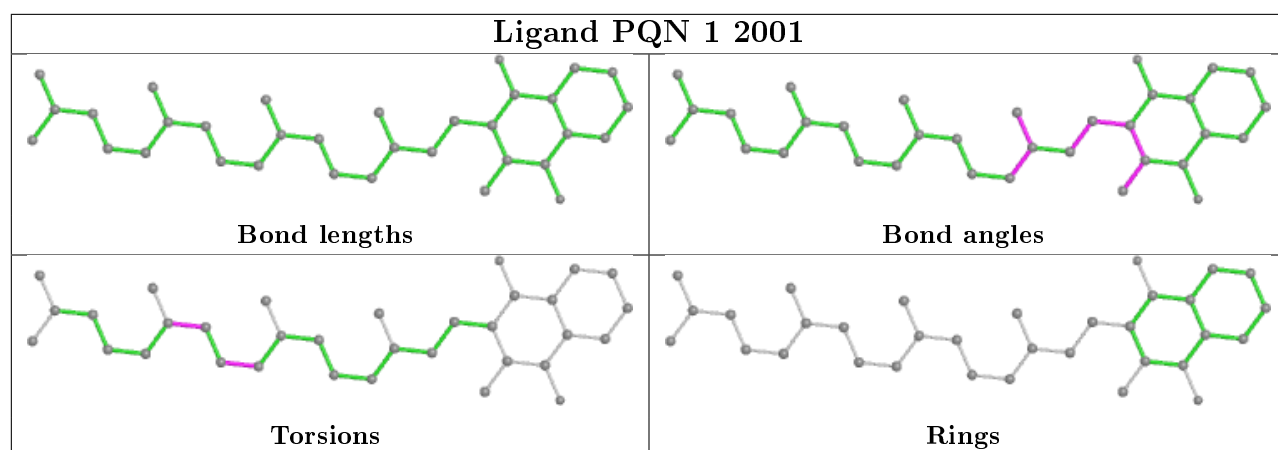
Ligand CLA B 1223**Ligand CLA a 1140****Ligand BCR b 4014**

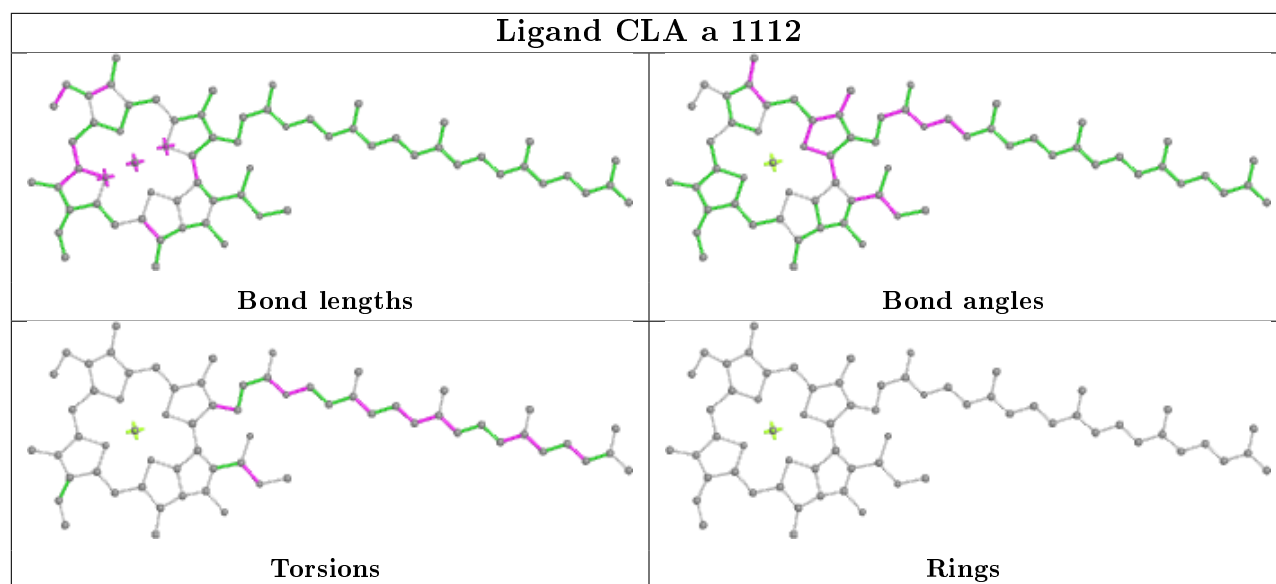
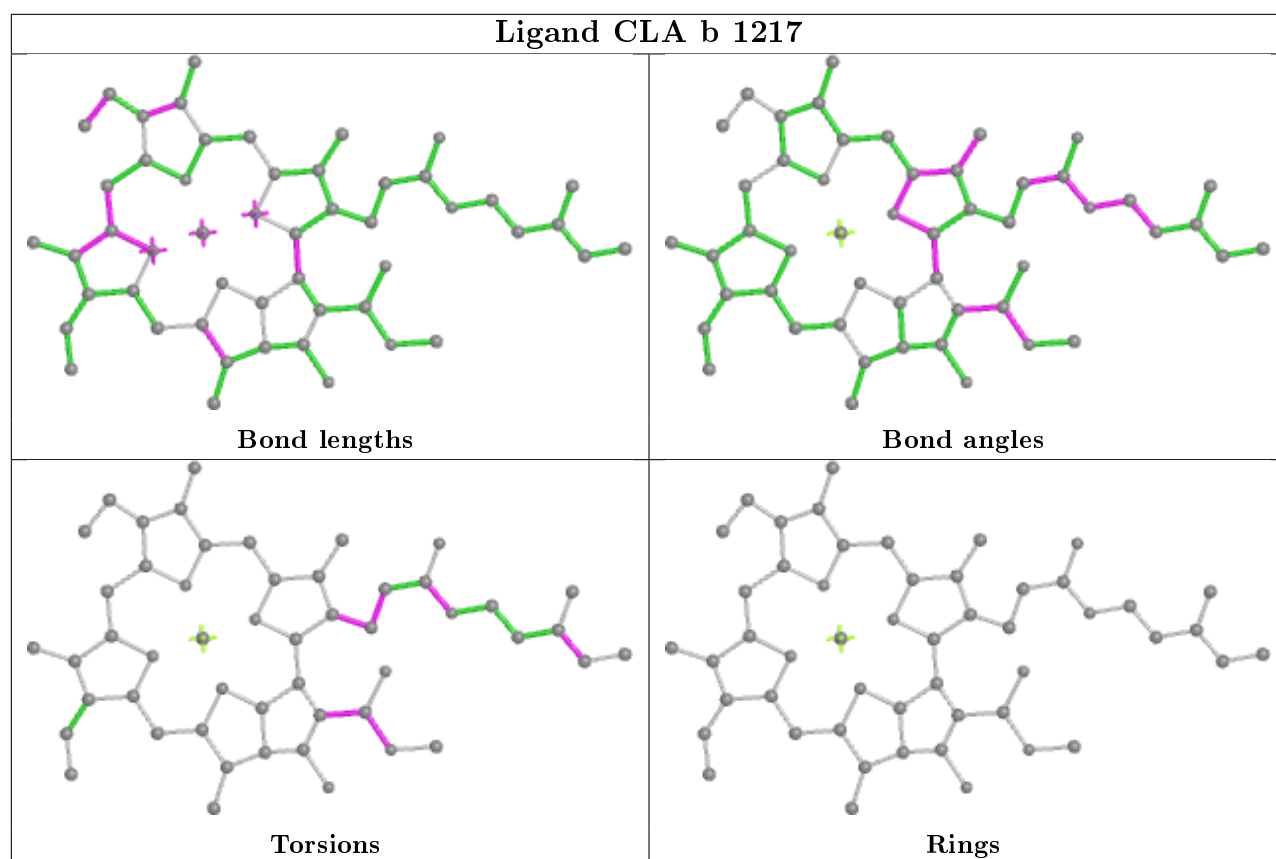


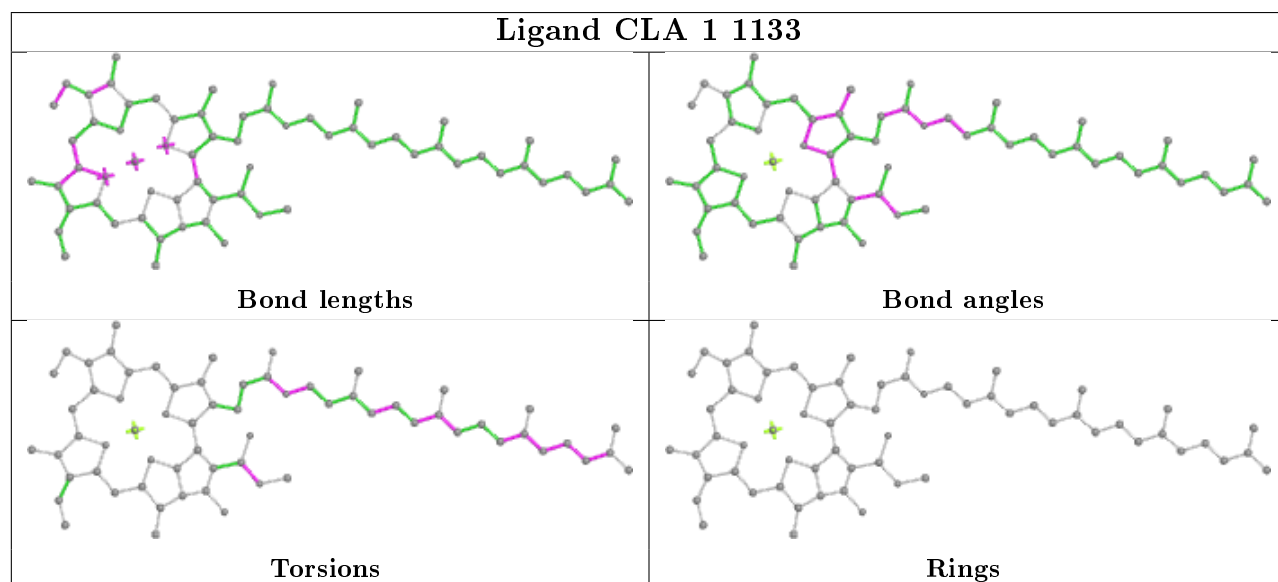
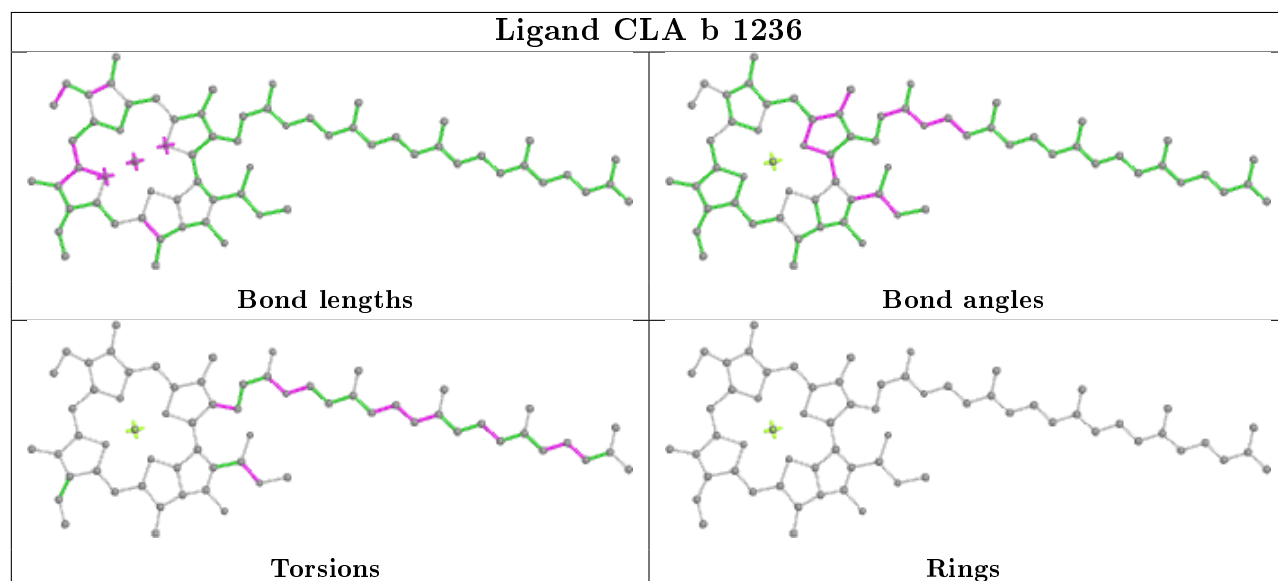
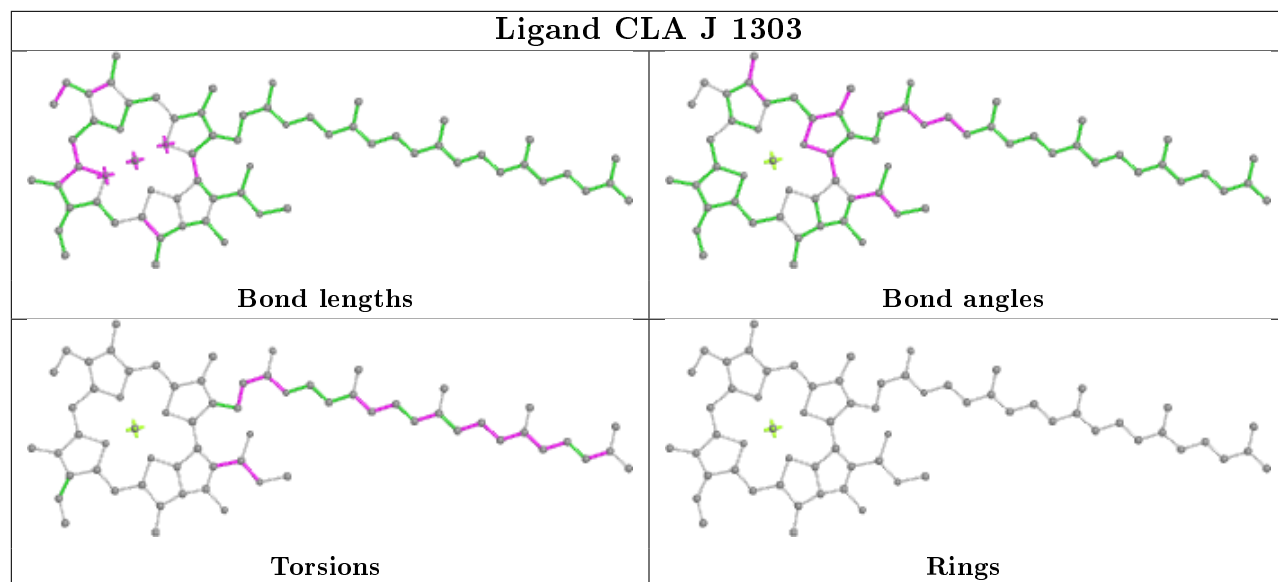


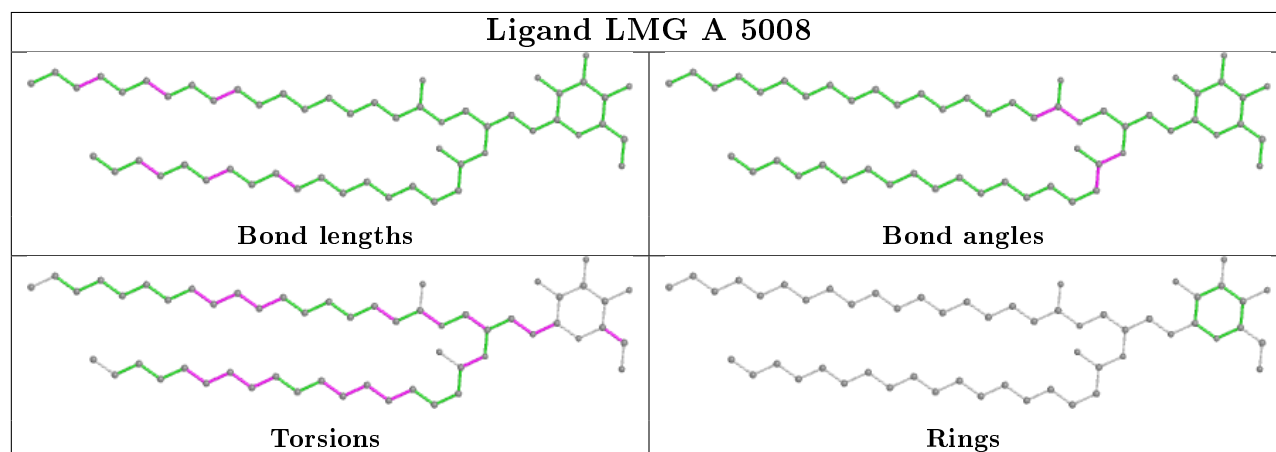
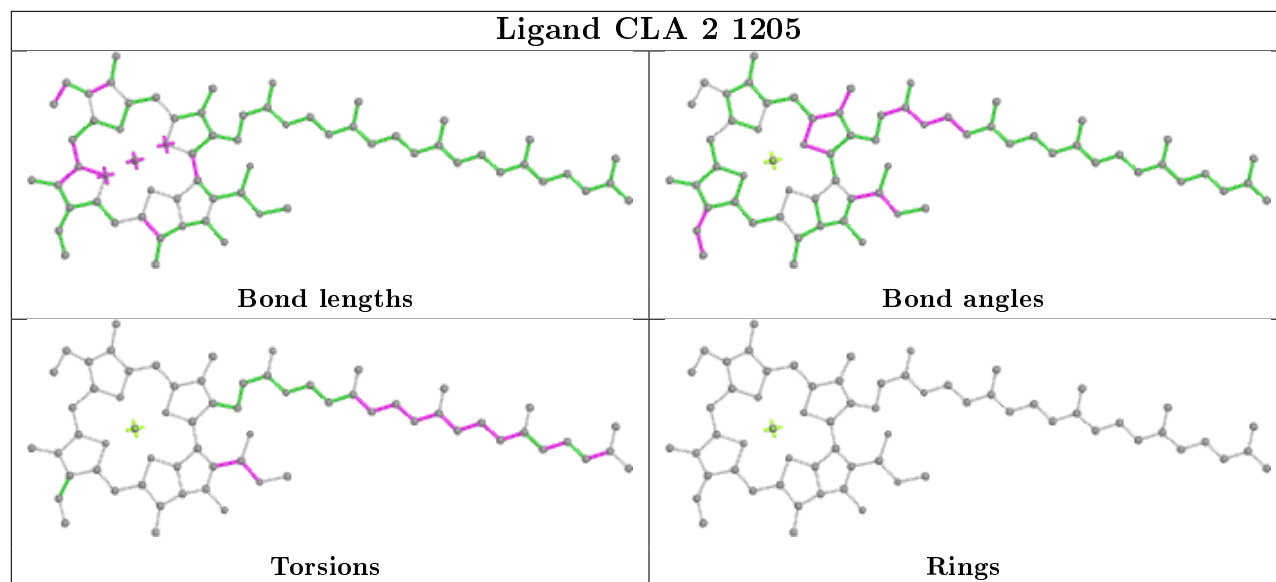


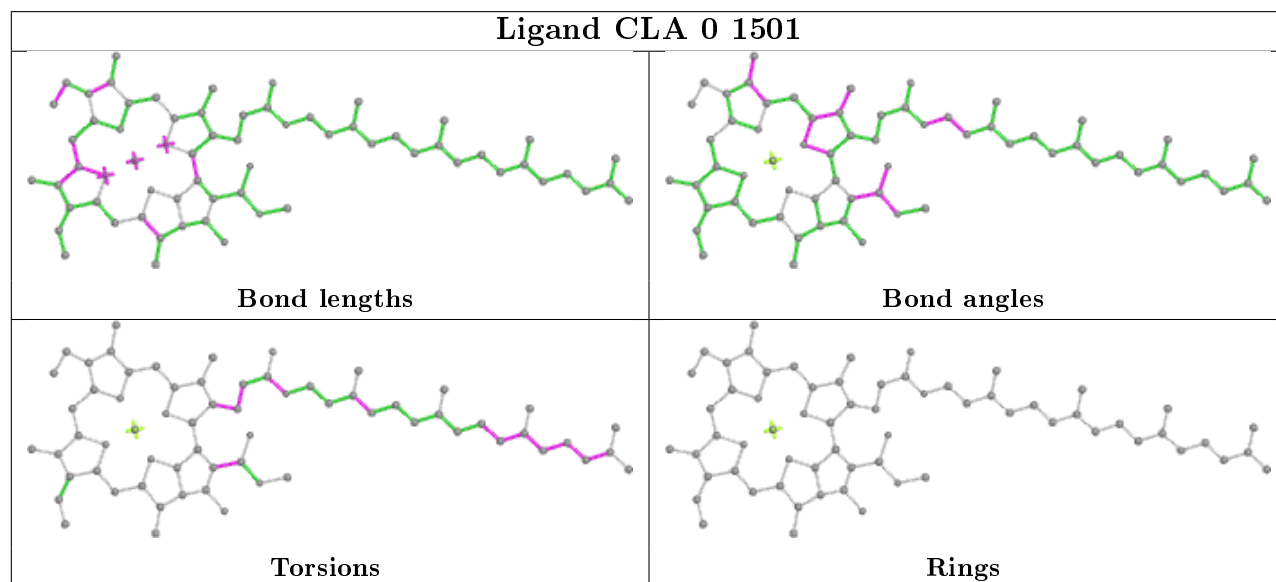
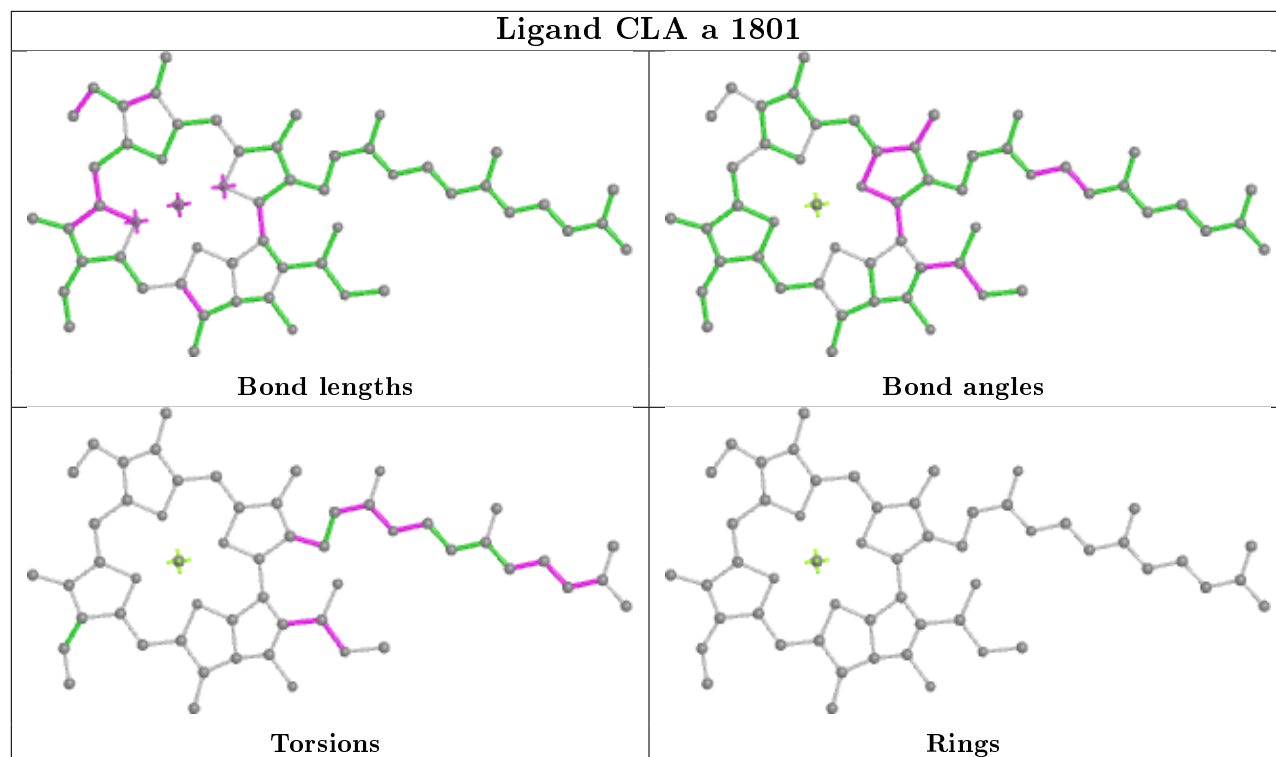


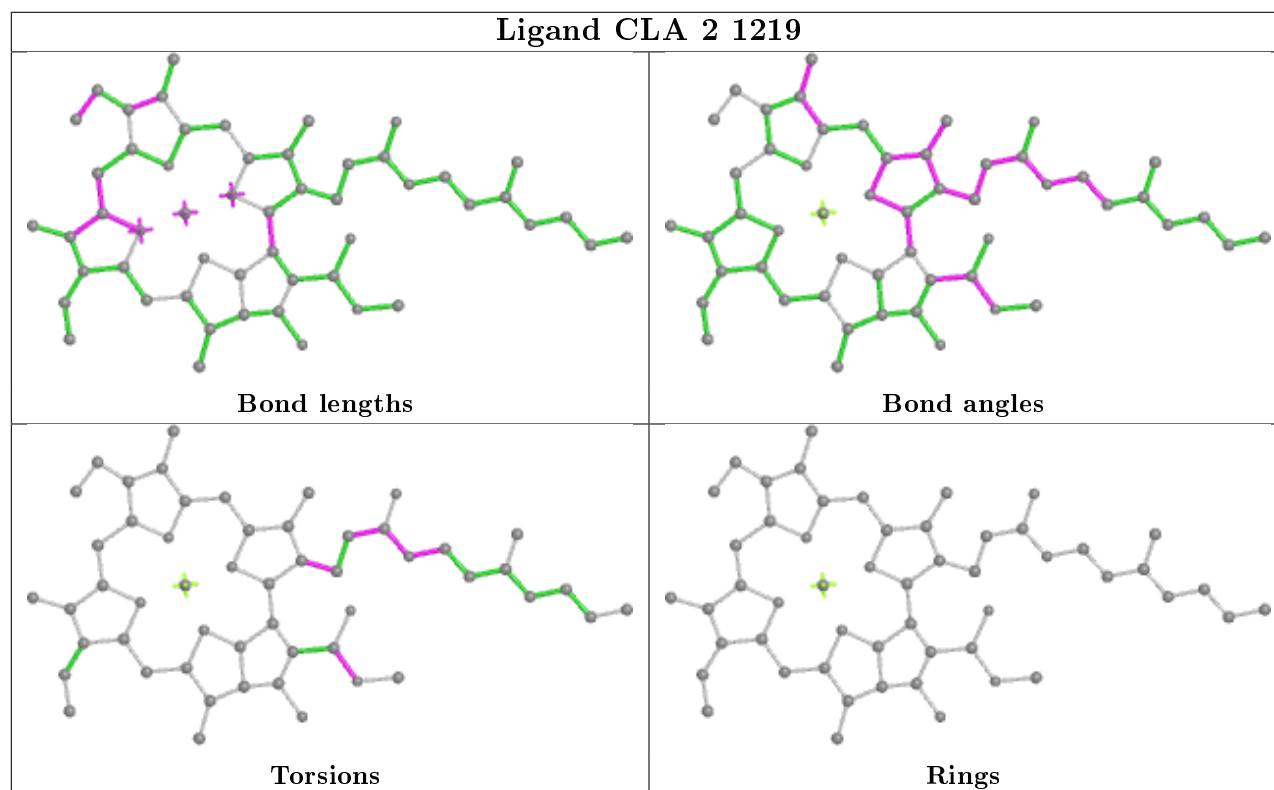
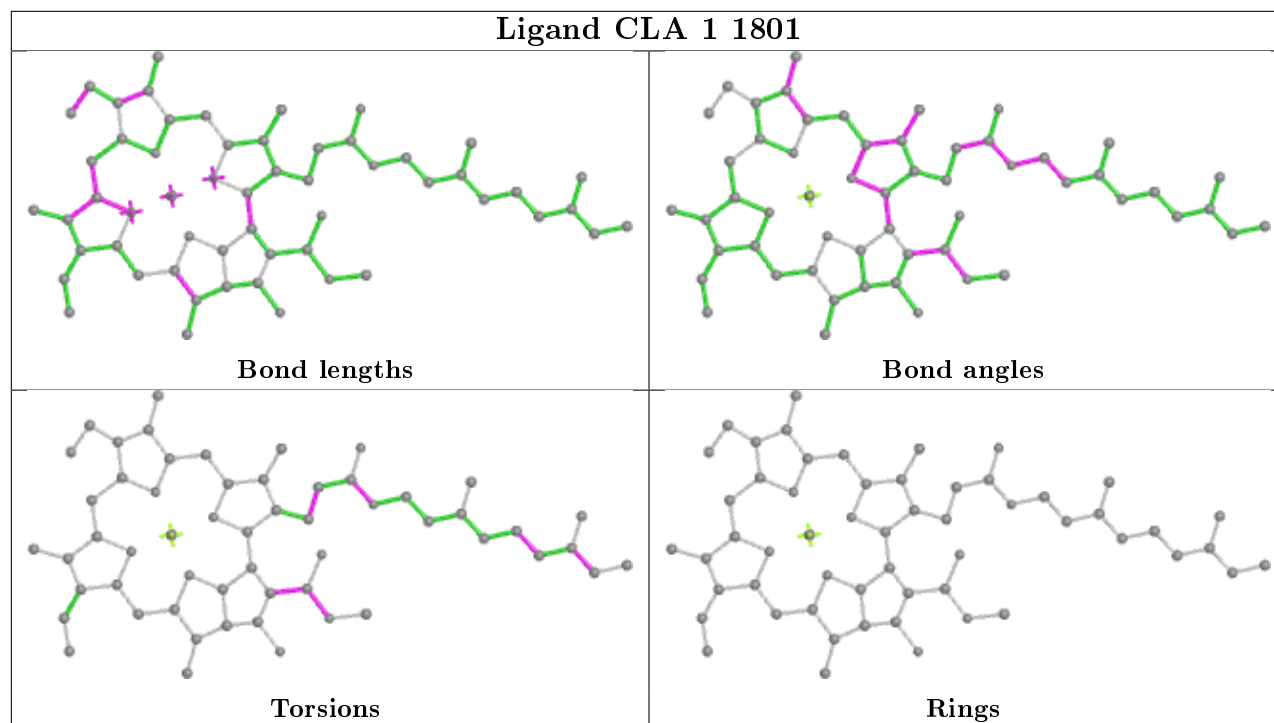


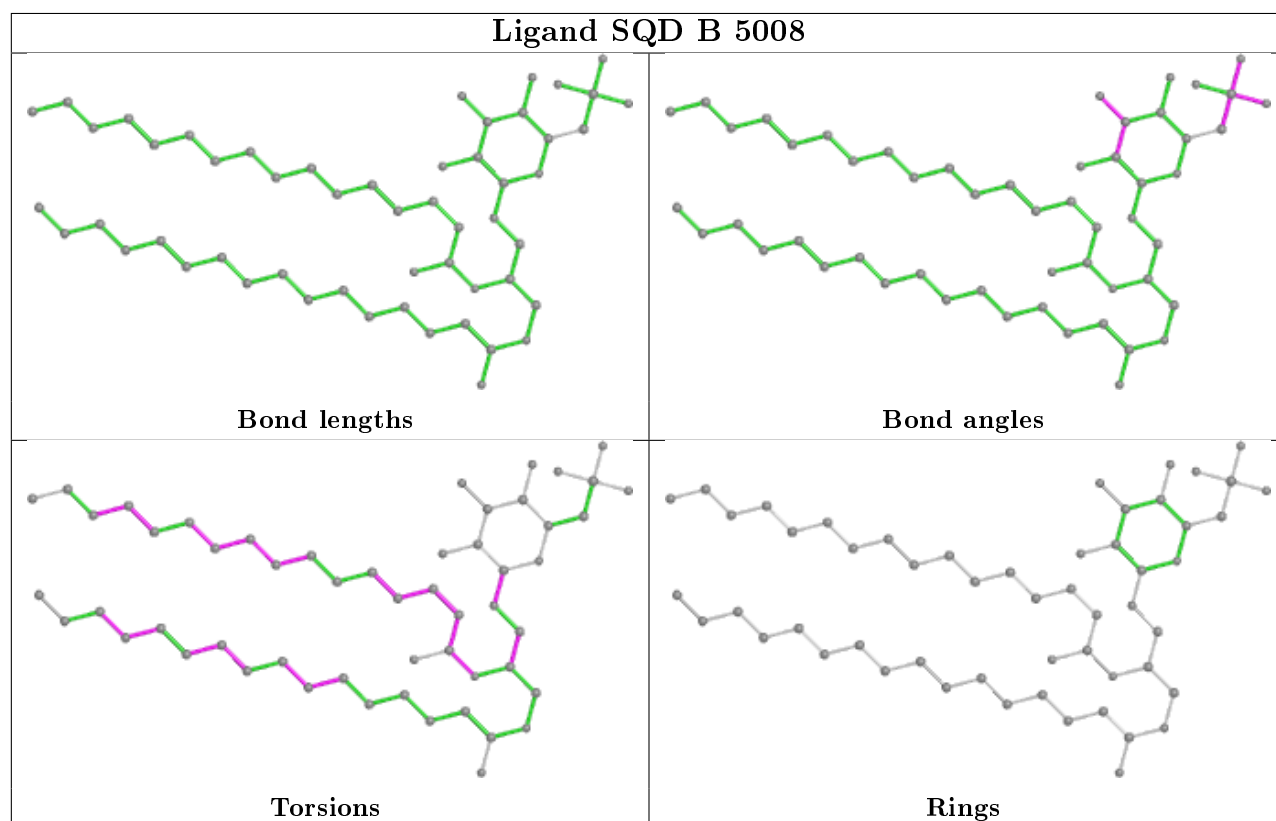
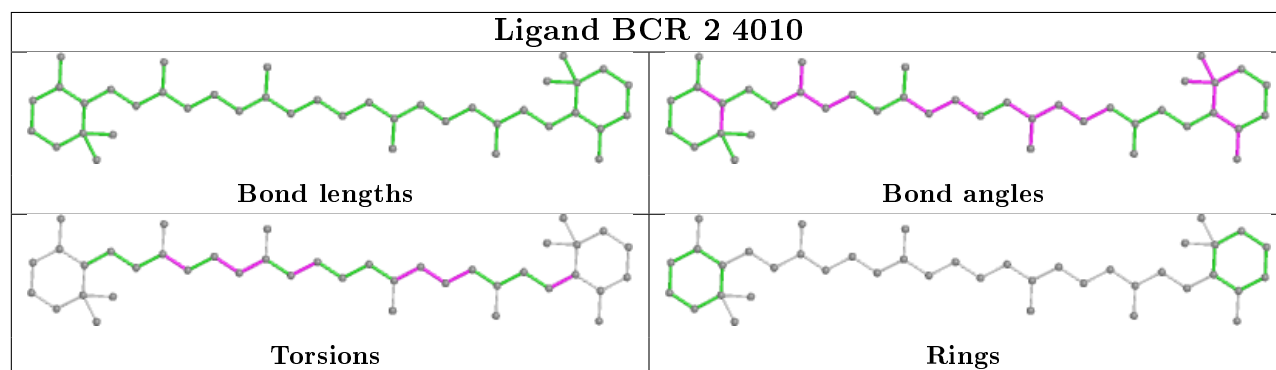
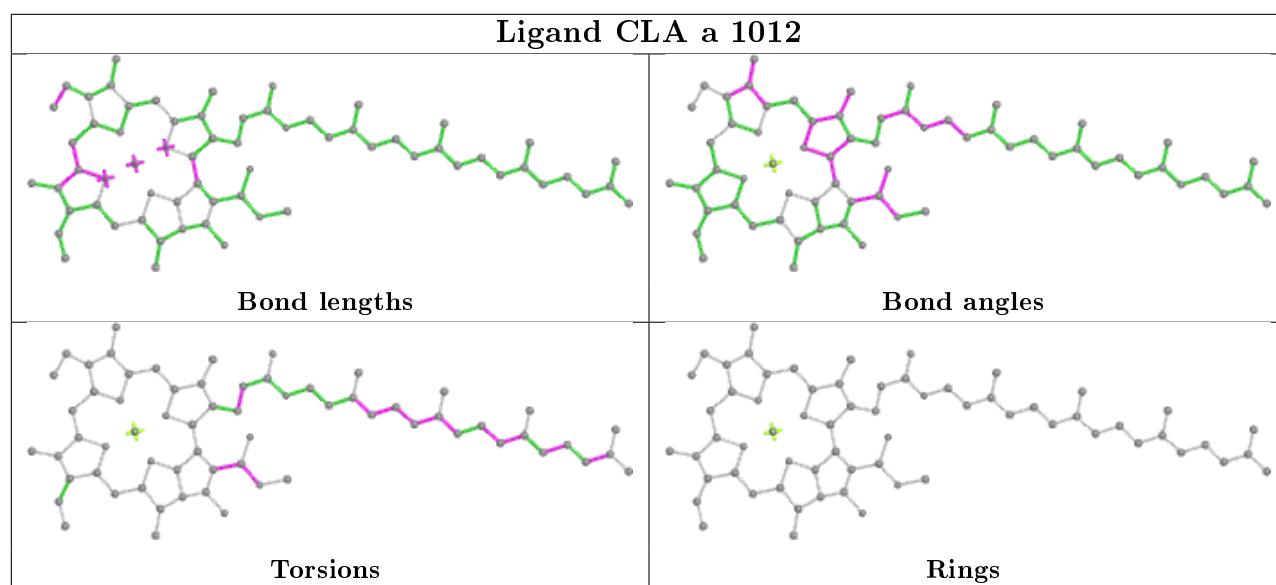


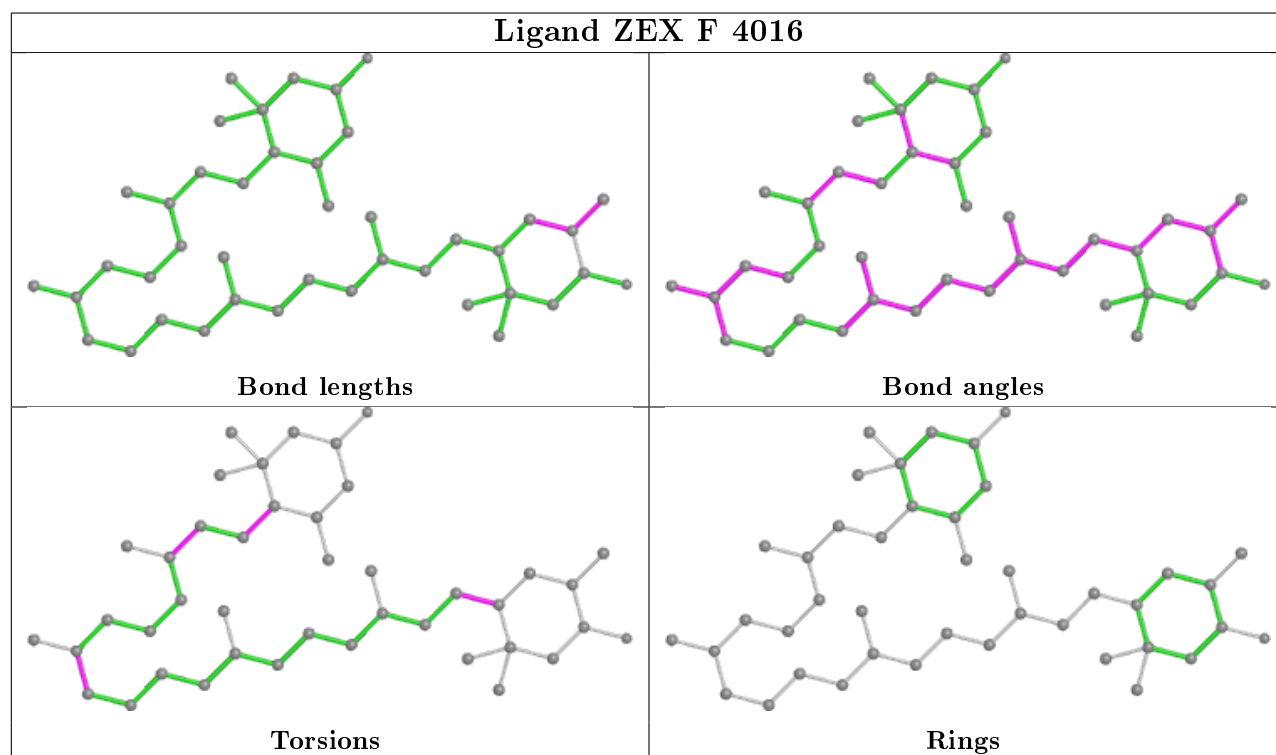
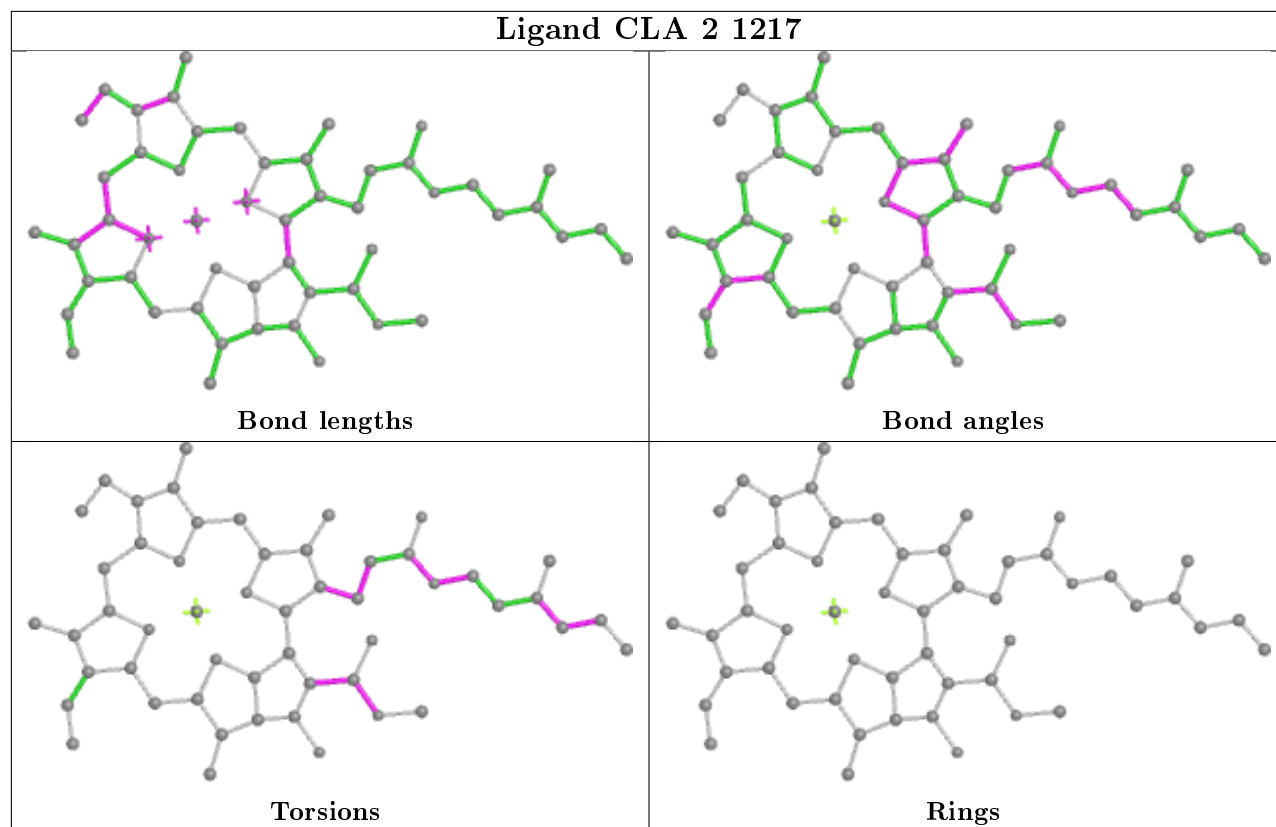


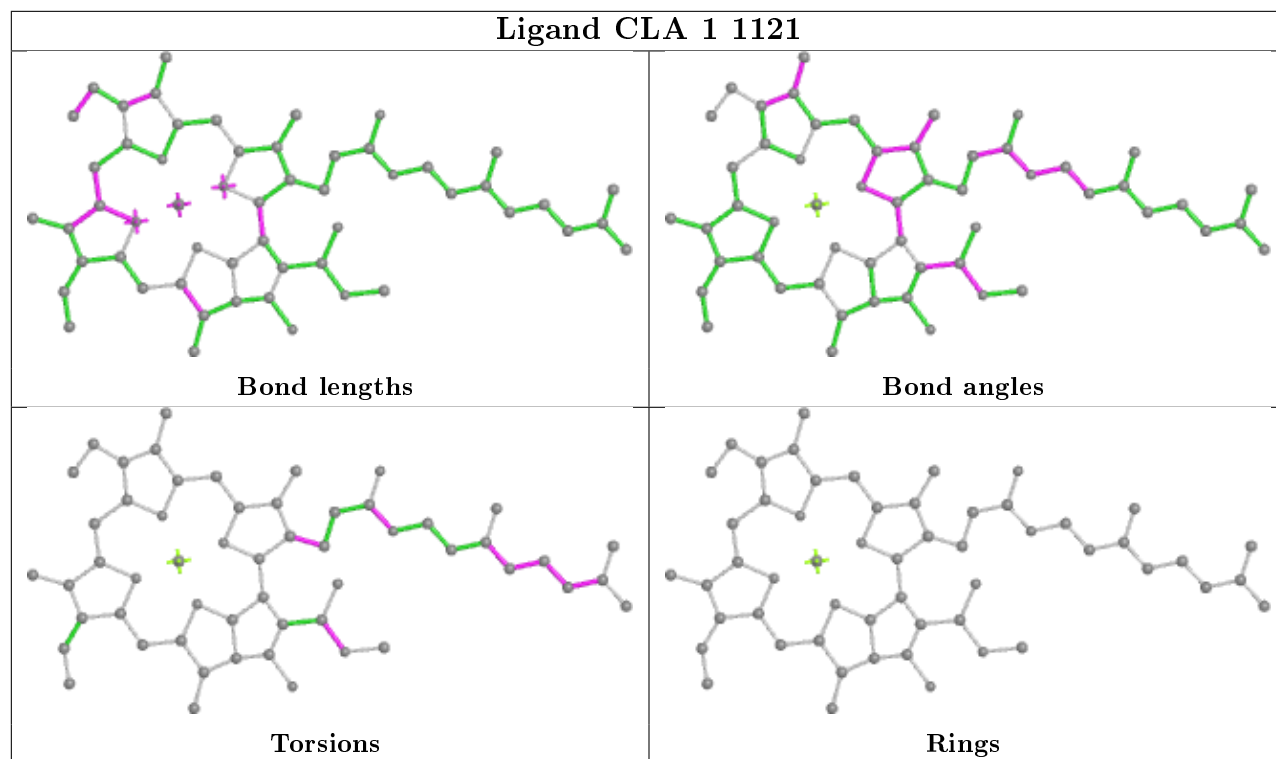
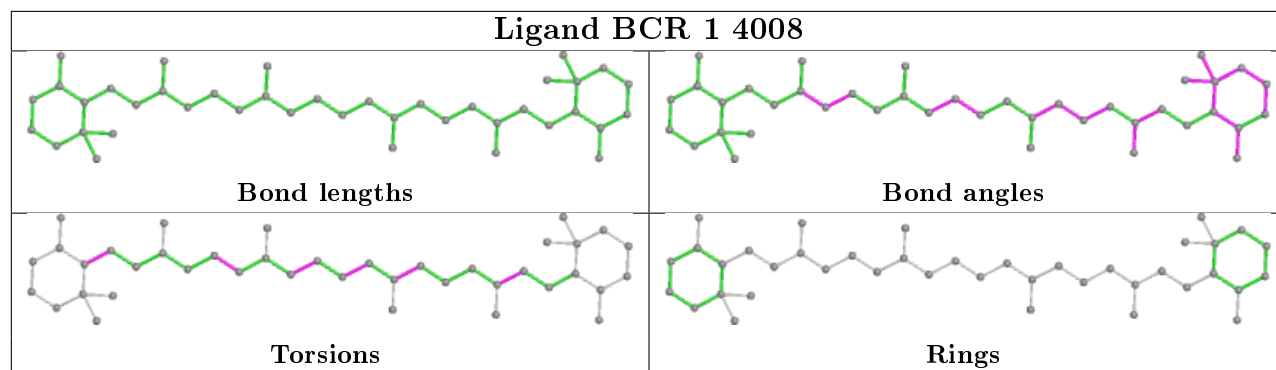


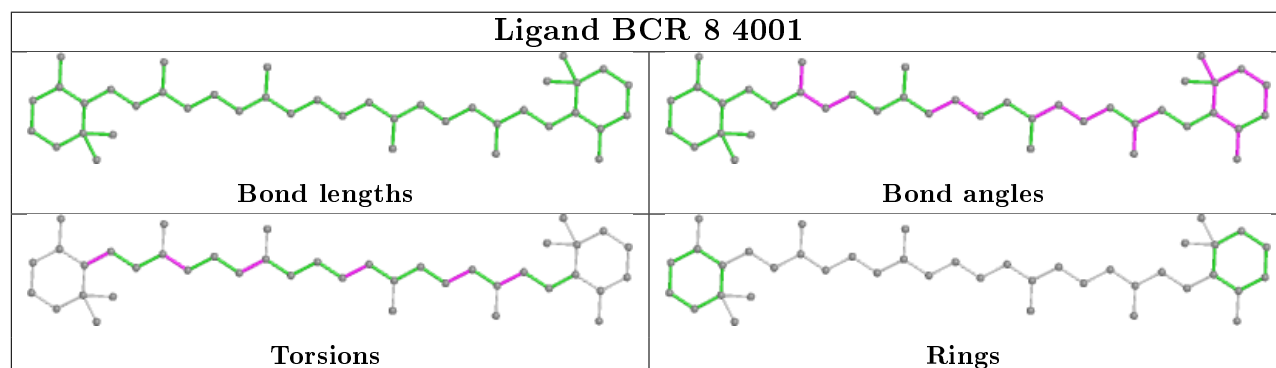
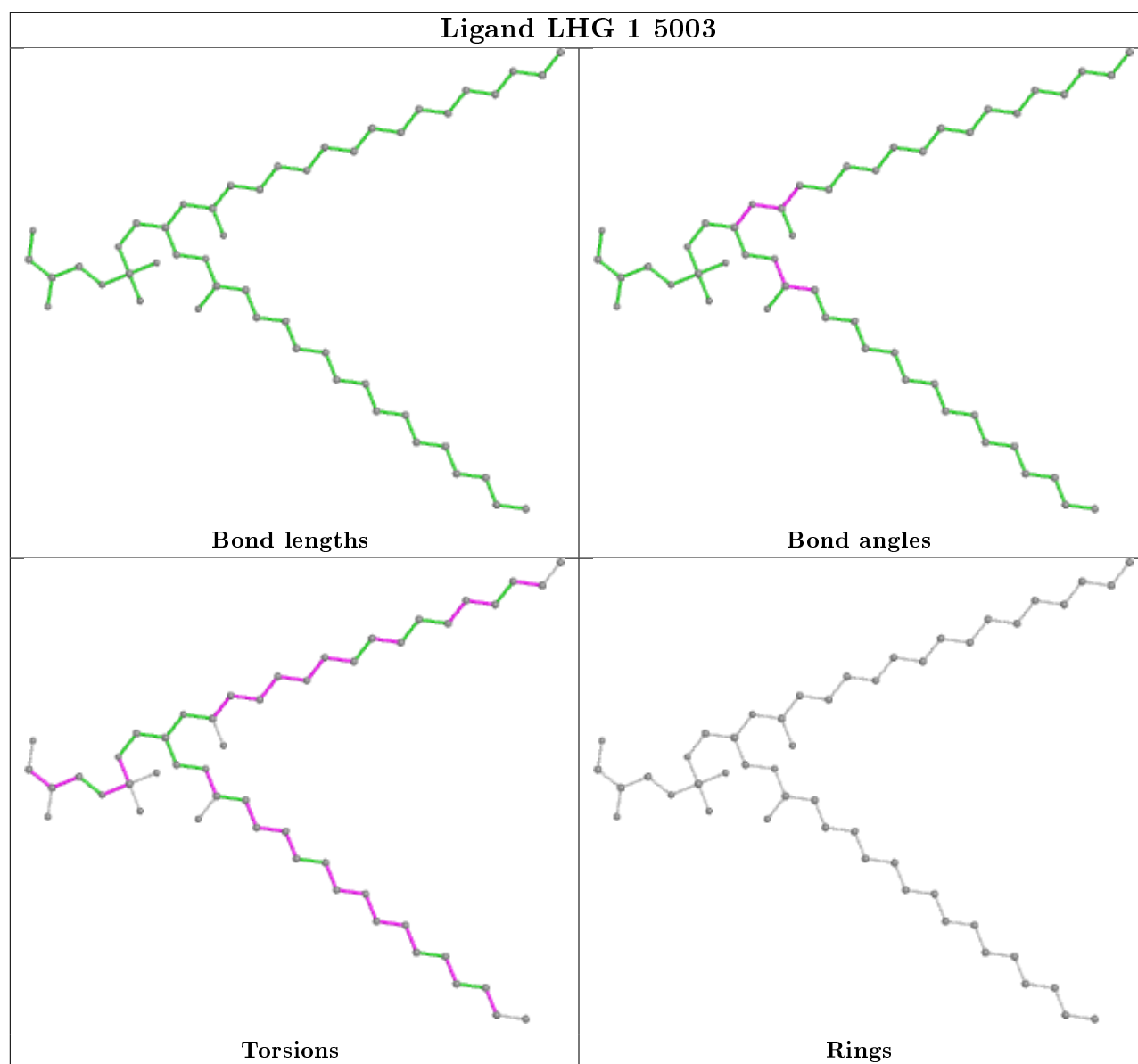




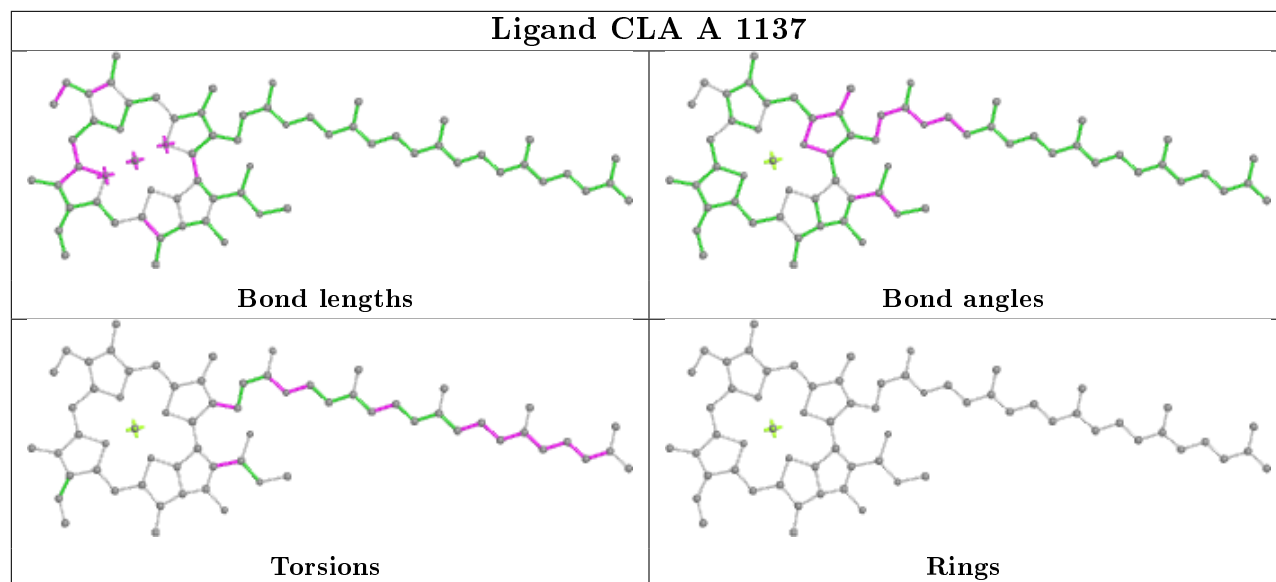




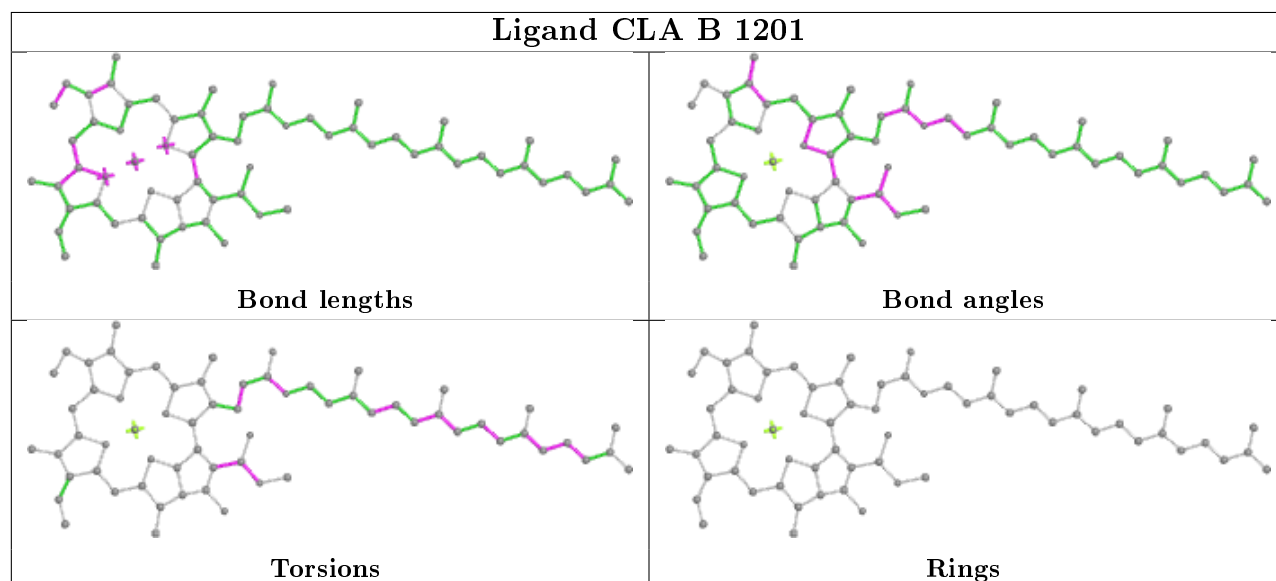




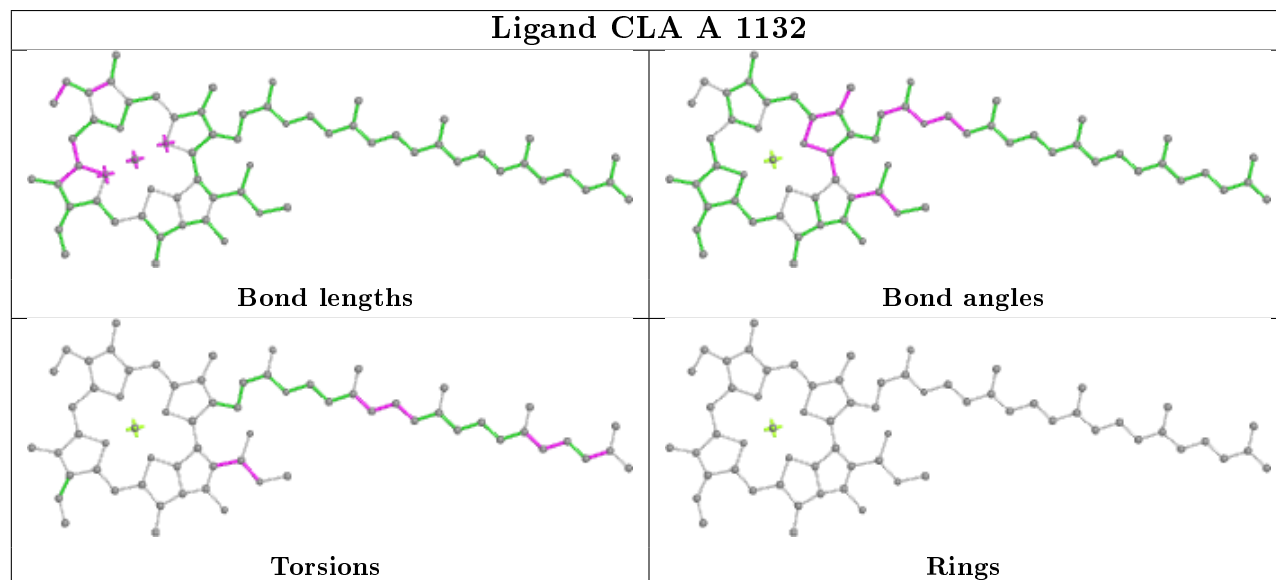
Ligand CLA A 1137

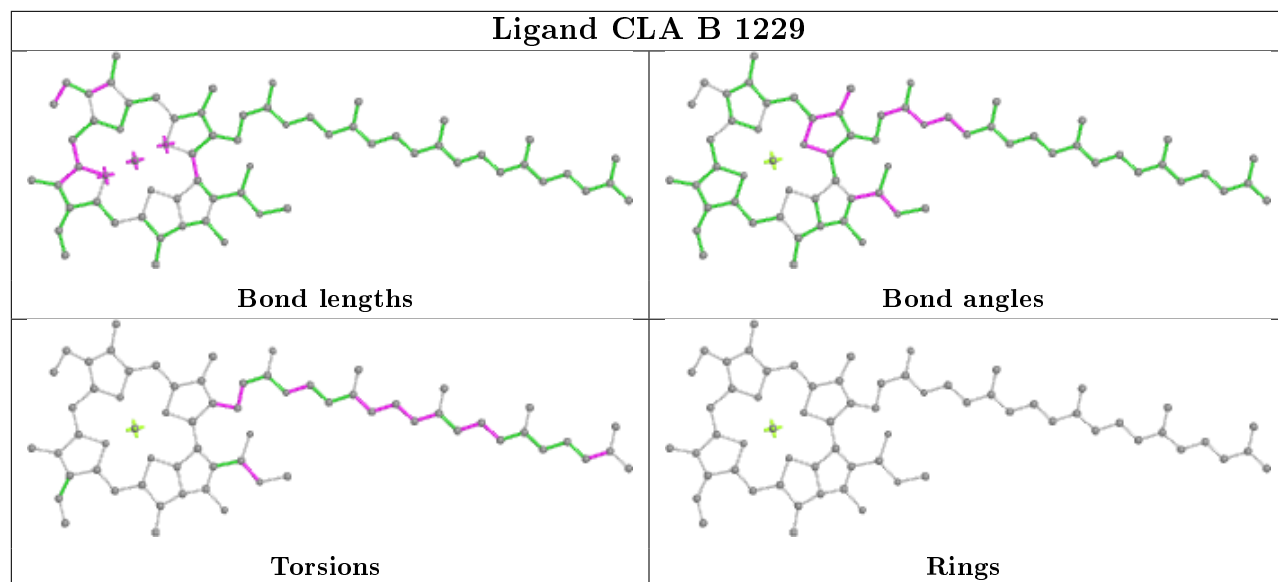
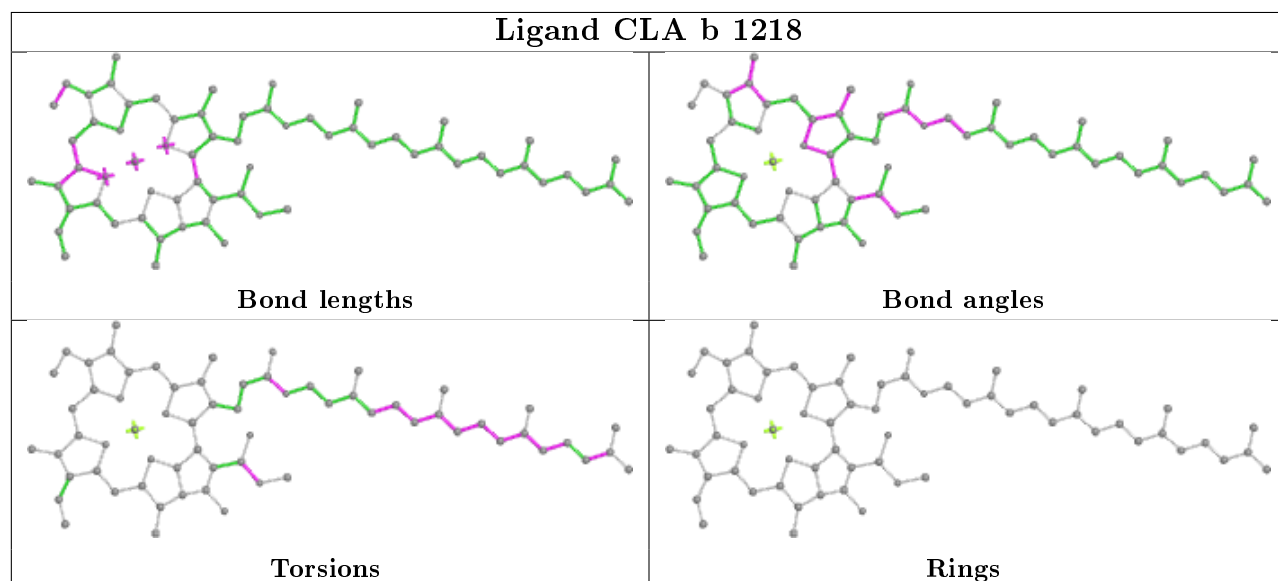
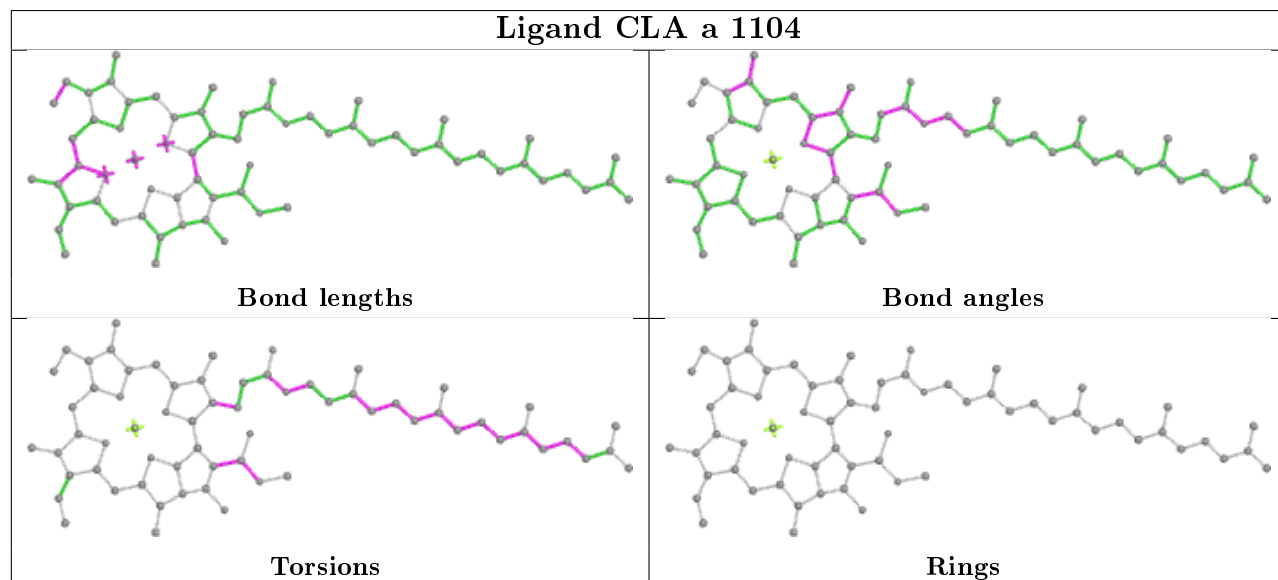


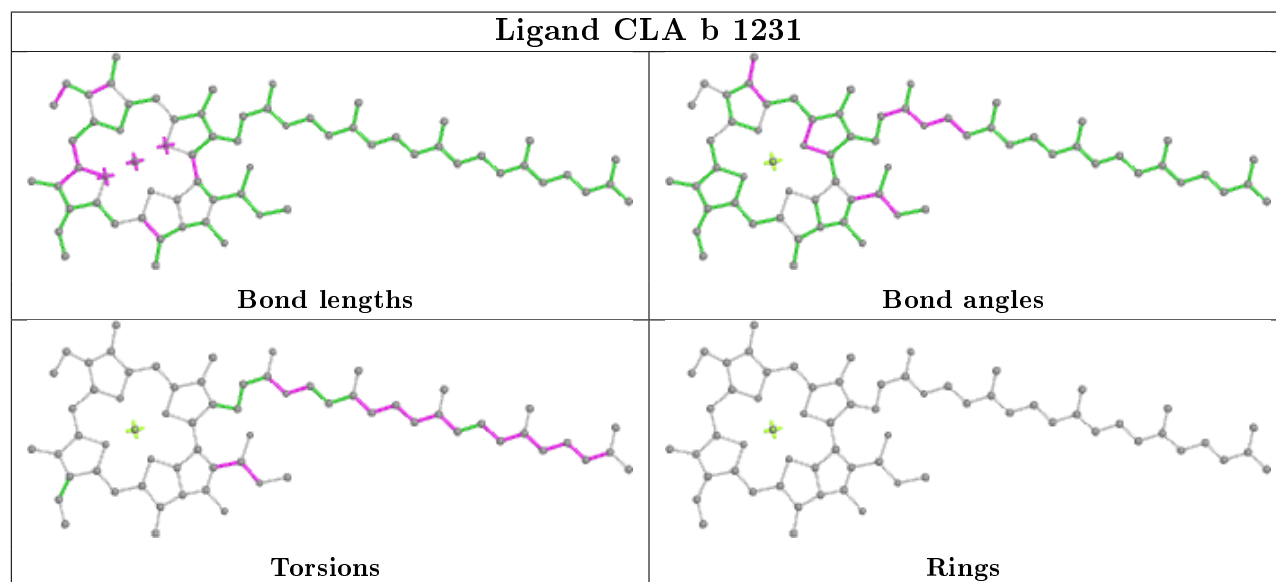
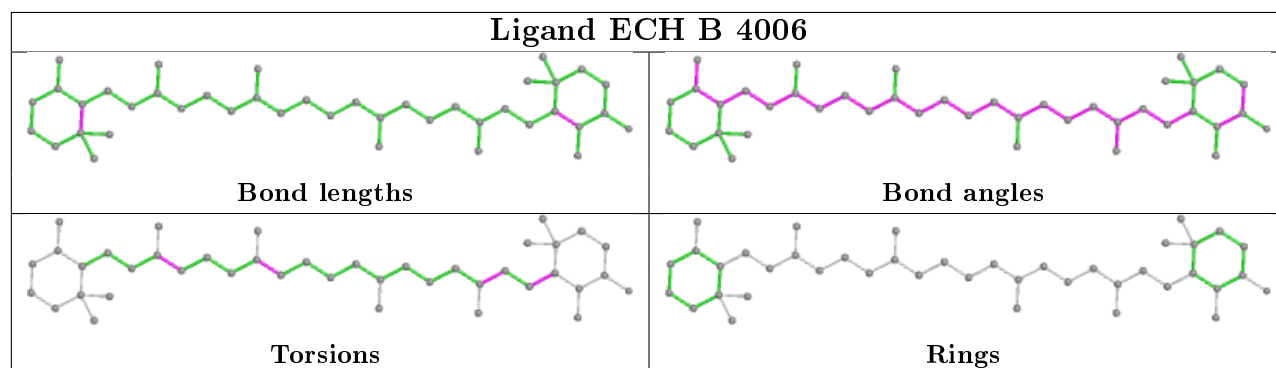
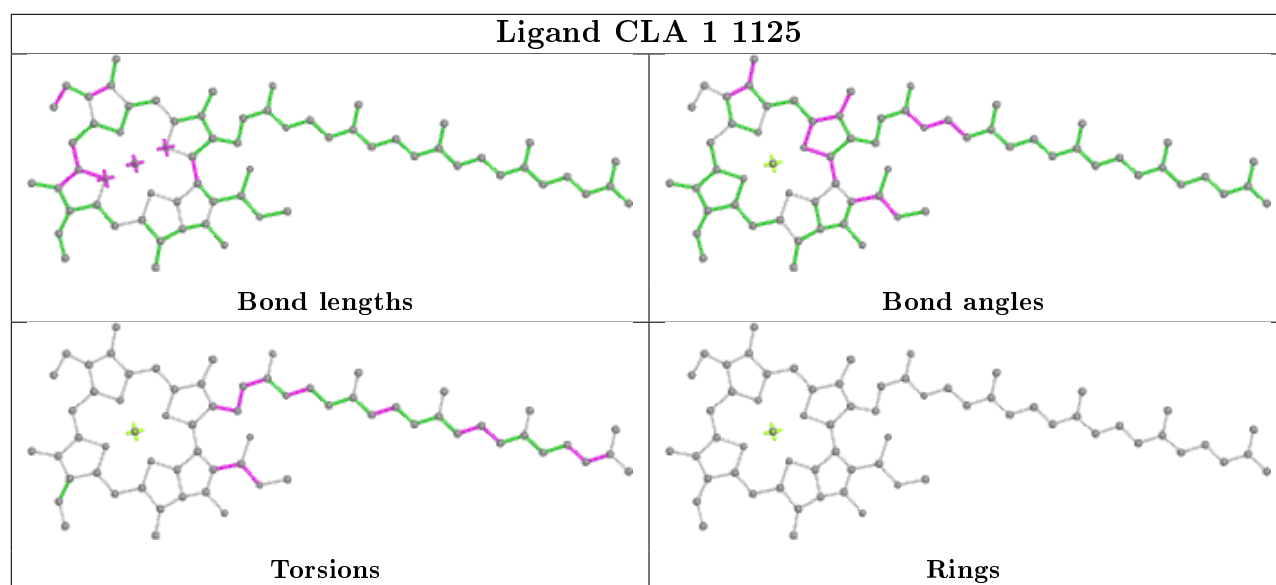
Ligand CLA B 1201

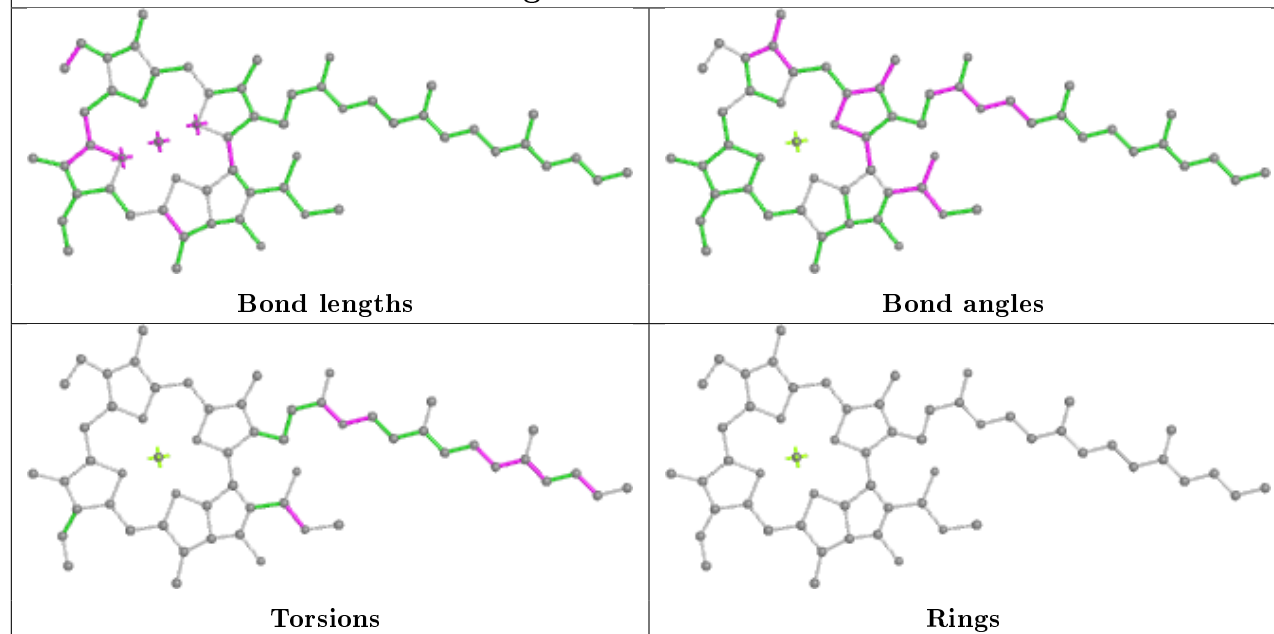
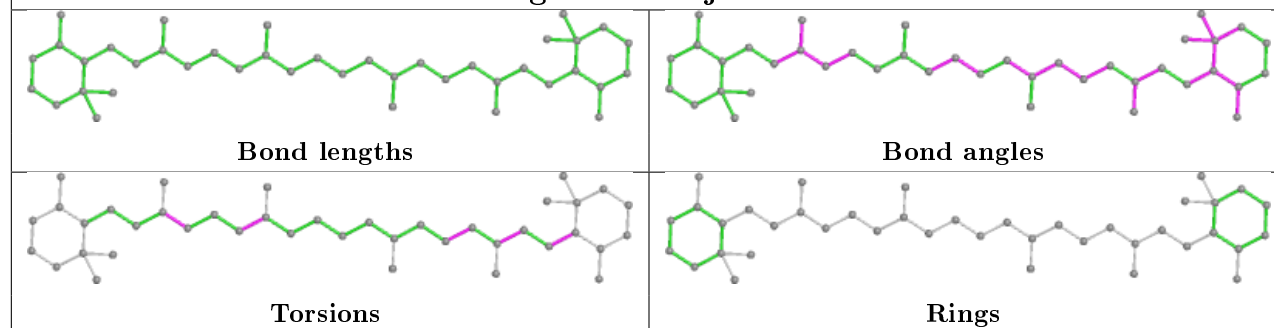


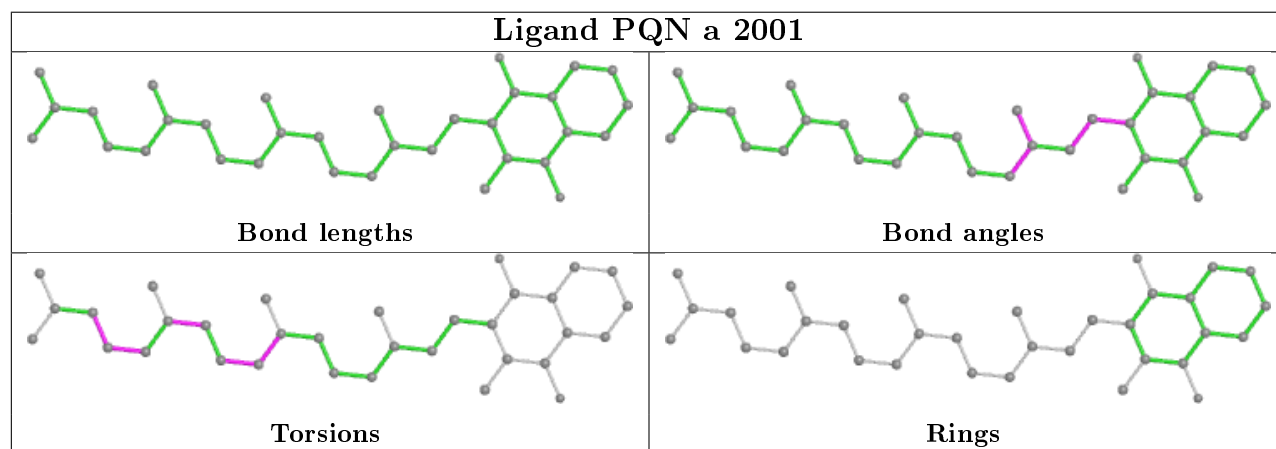
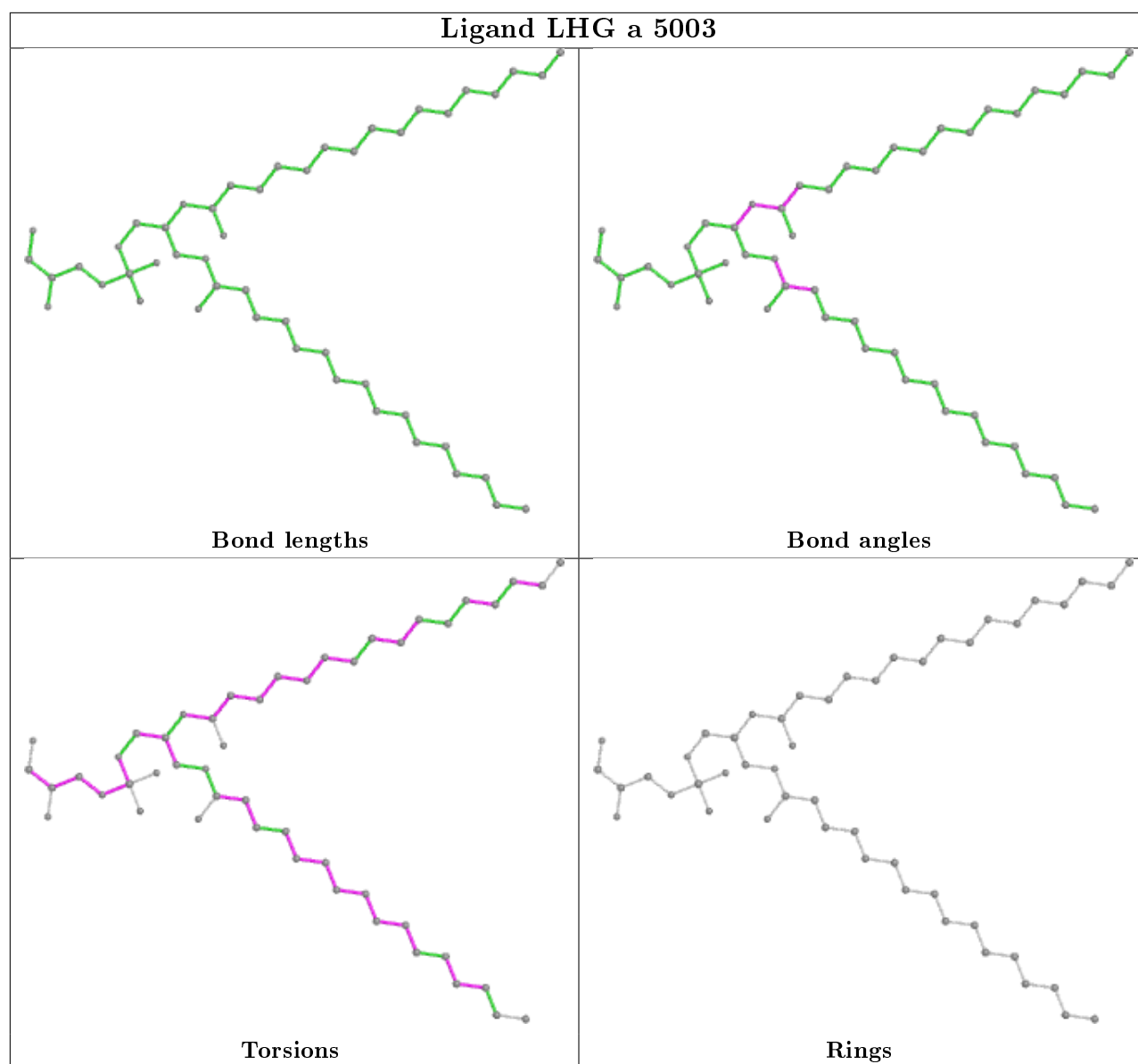
Ligand CLA A 1132

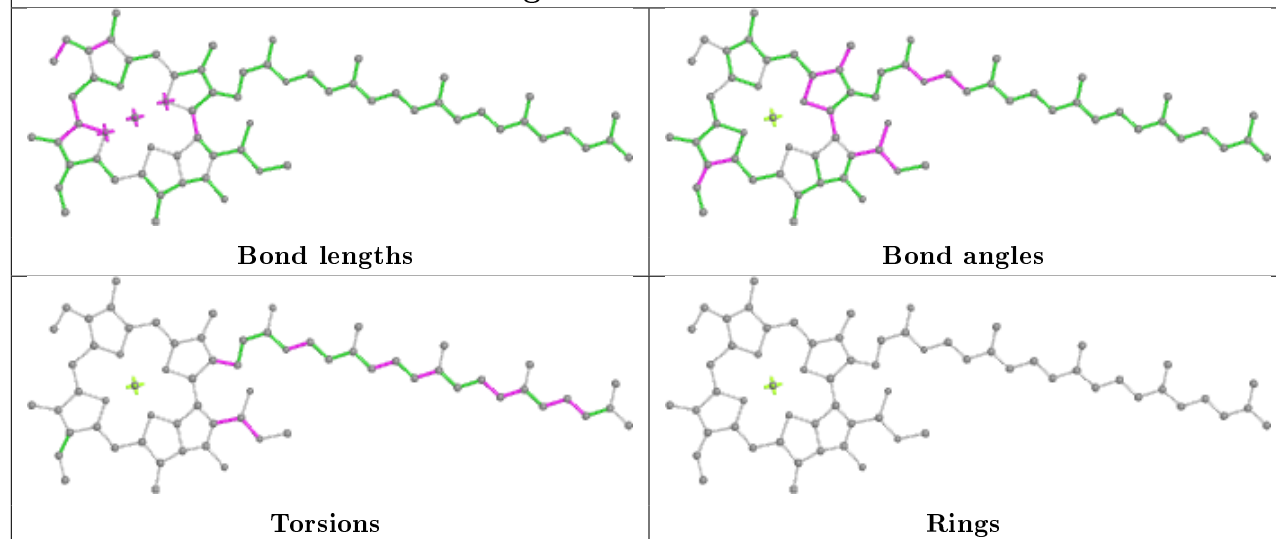
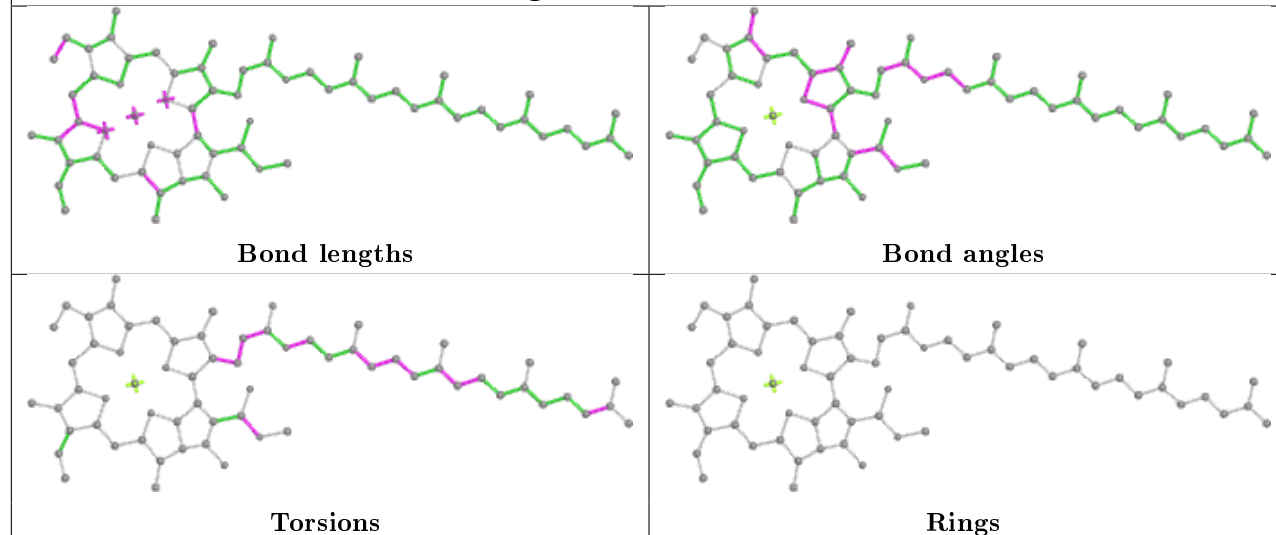
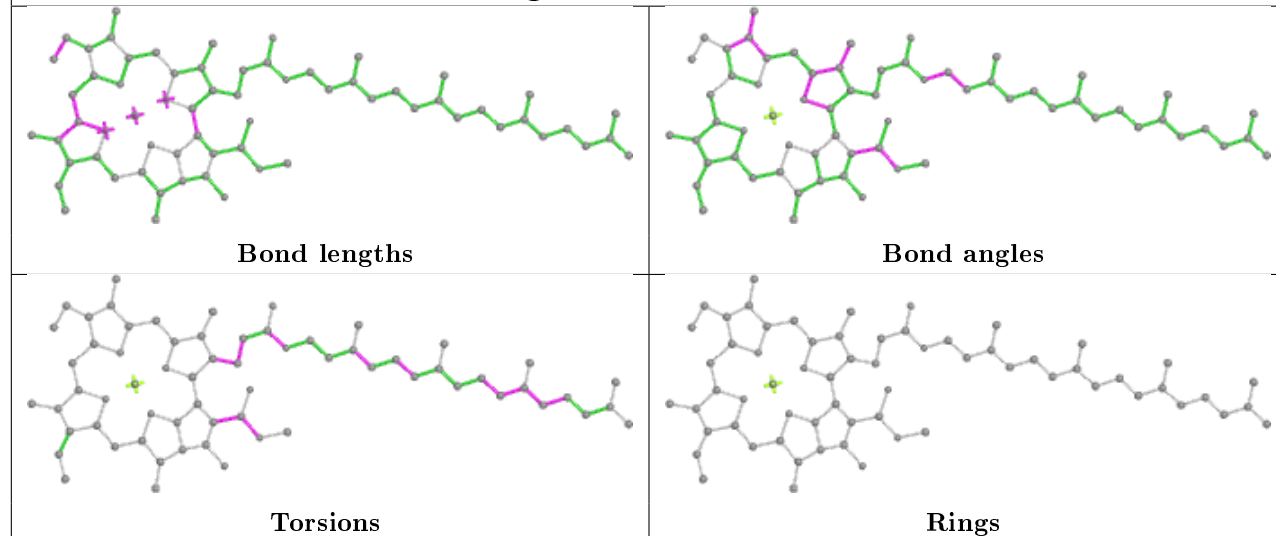


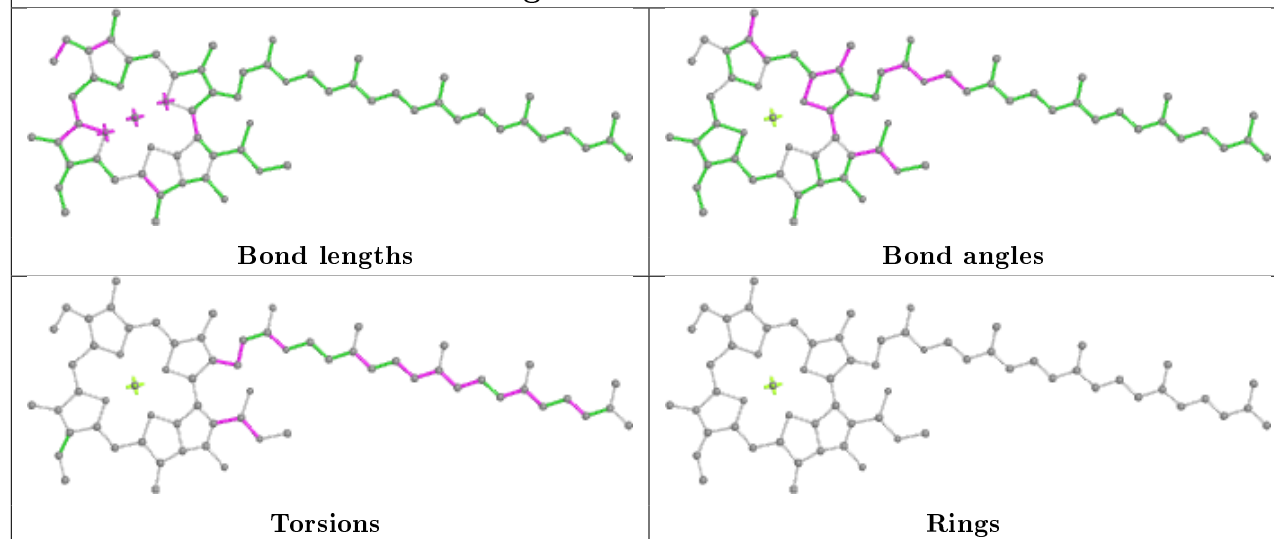
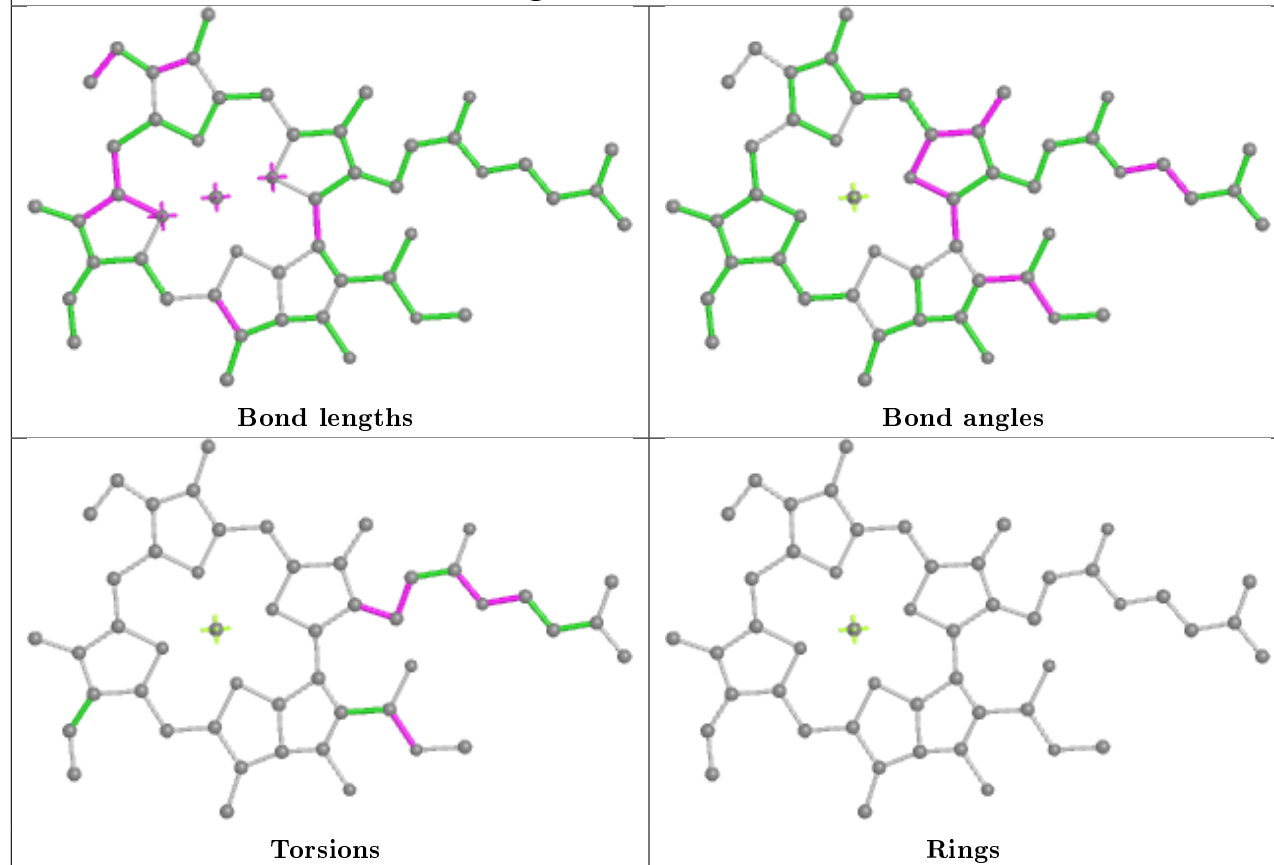
Ligand CLA B 1229**Ligand CLA b 1218****Ligand CLA a 1104**

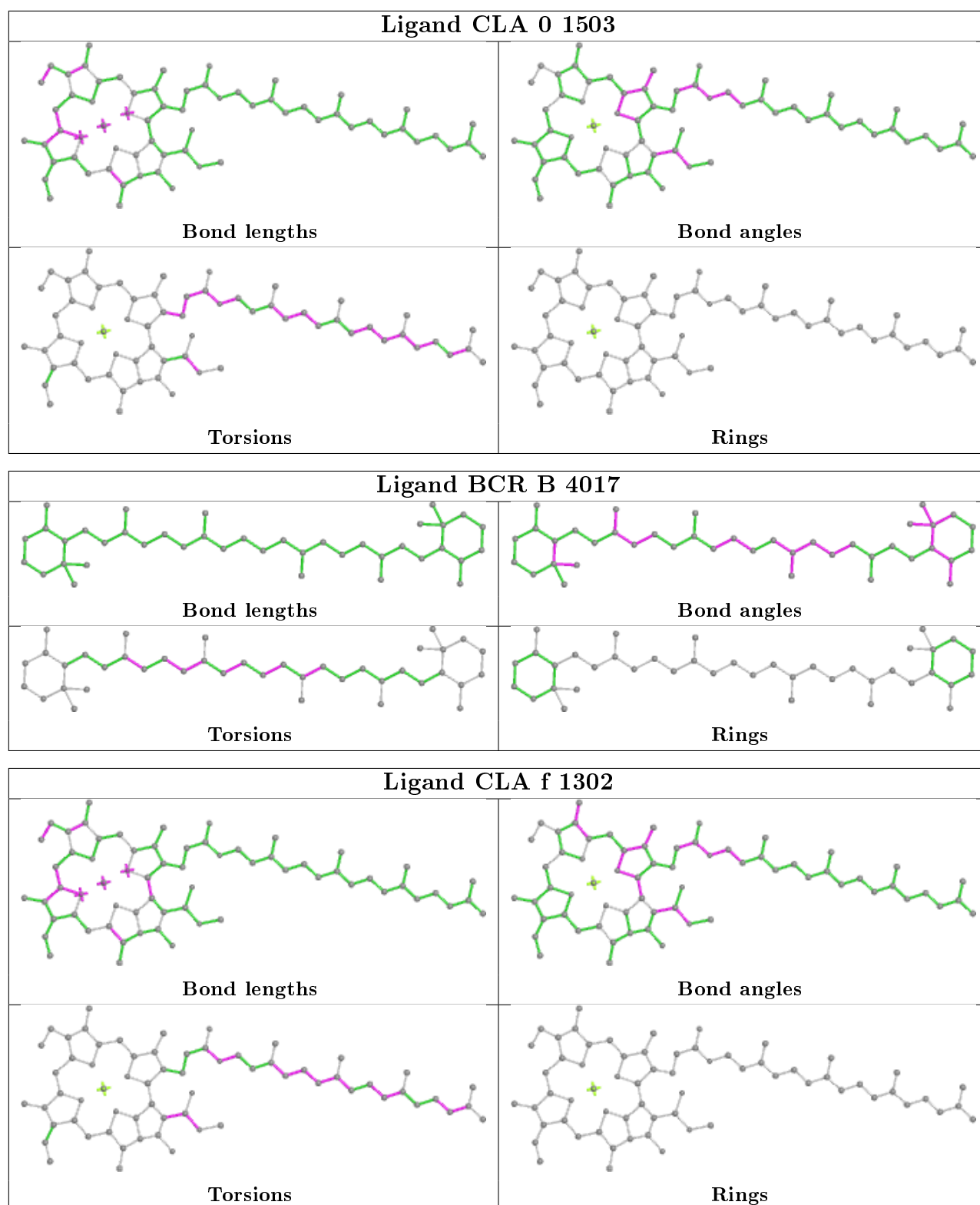


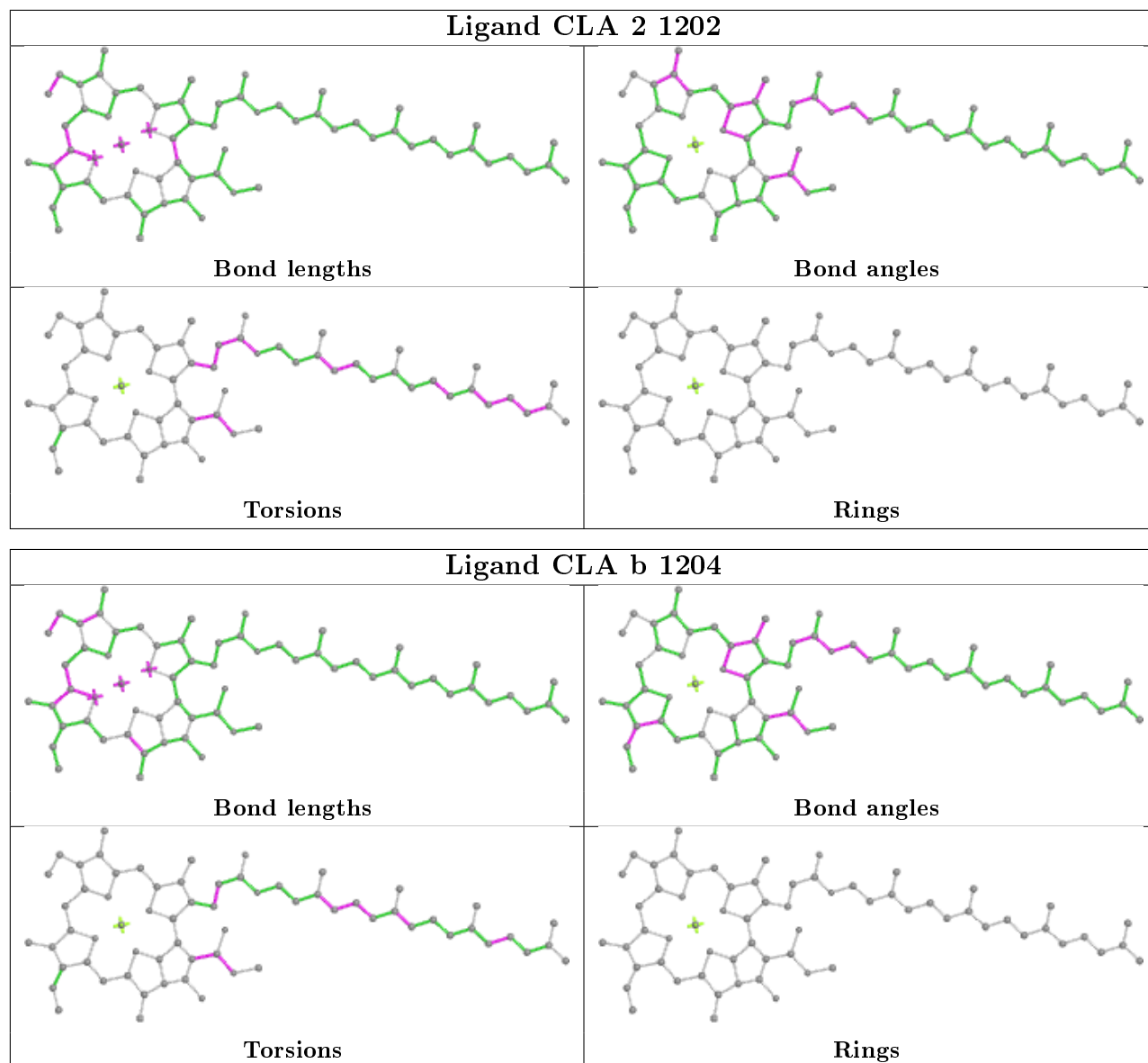
Ligand CLA A 1129**Ligand BCR j 4013**

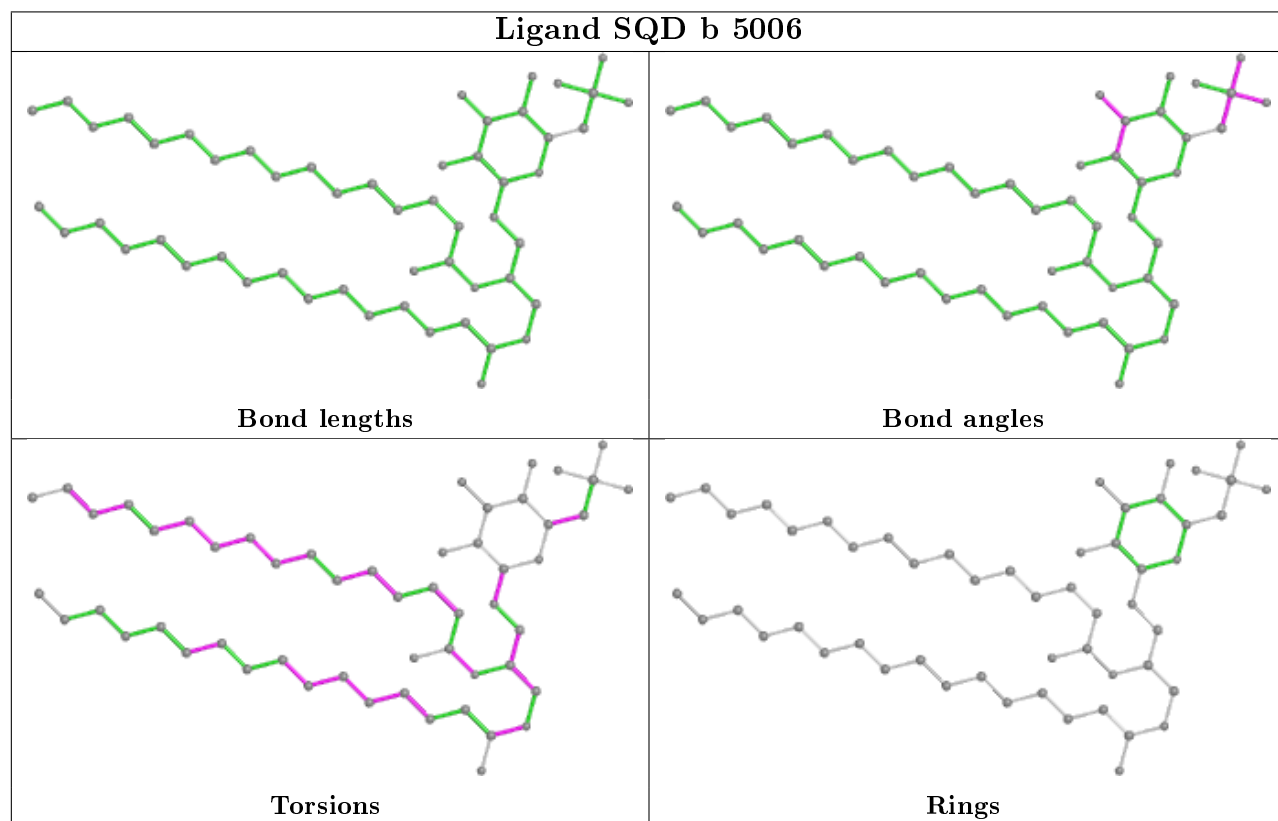
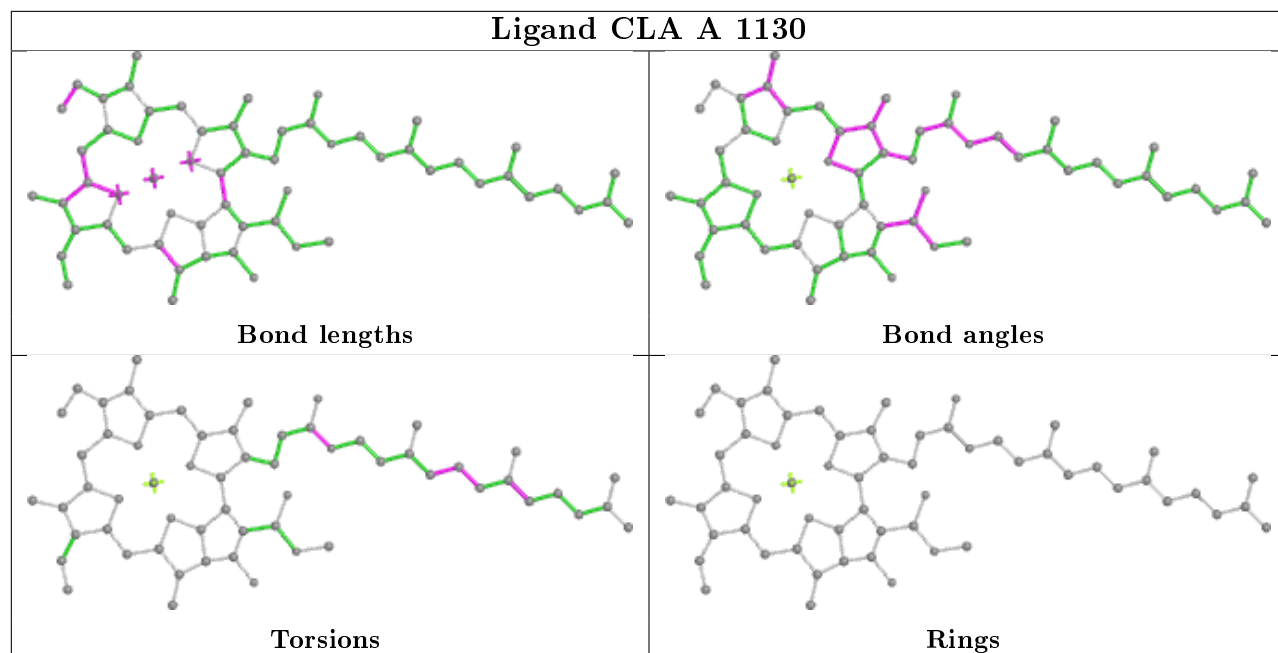


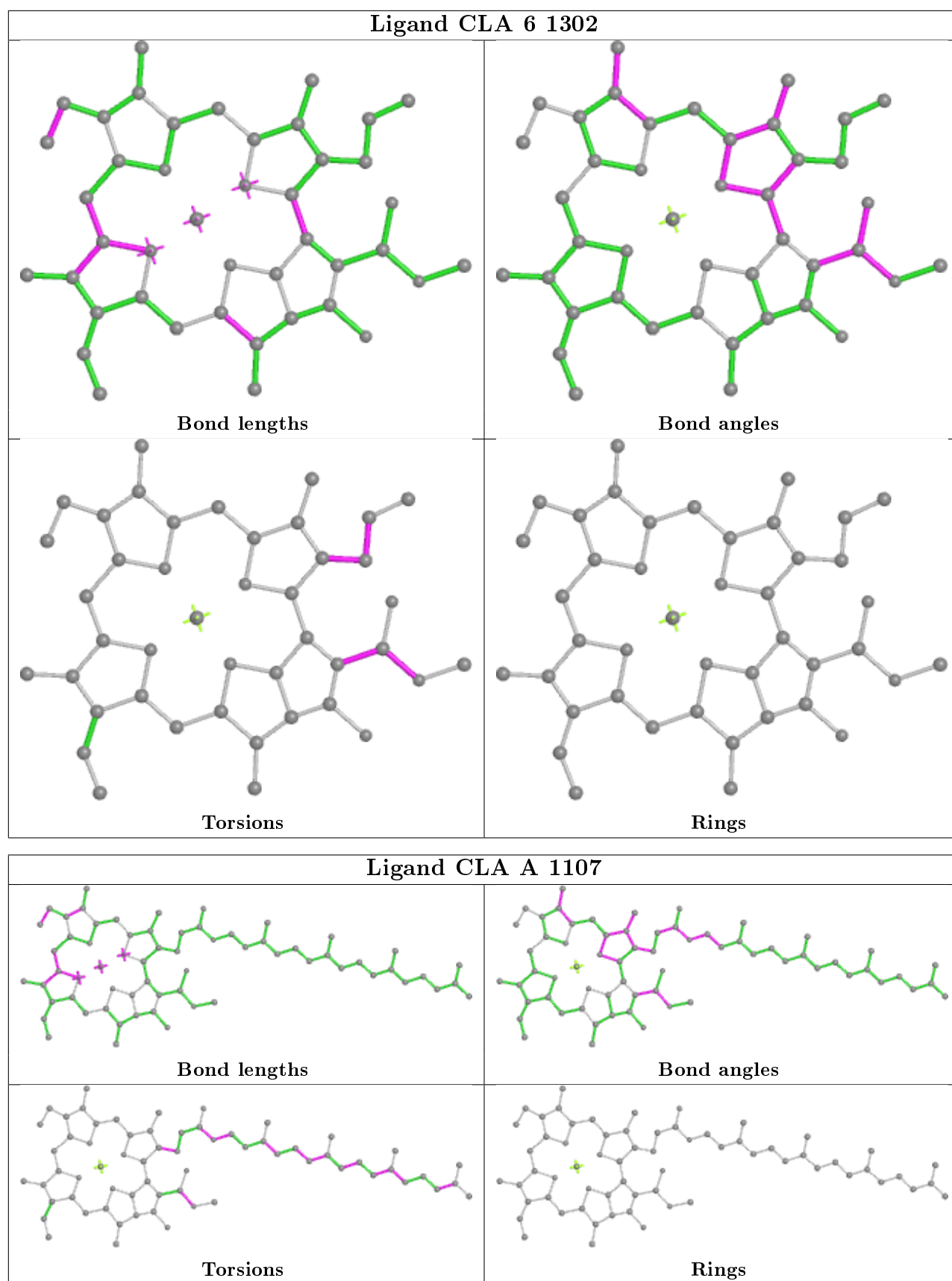
Ligand CLA A 1111**Ligand CLA b 1215****Ligand CLA L 1501**

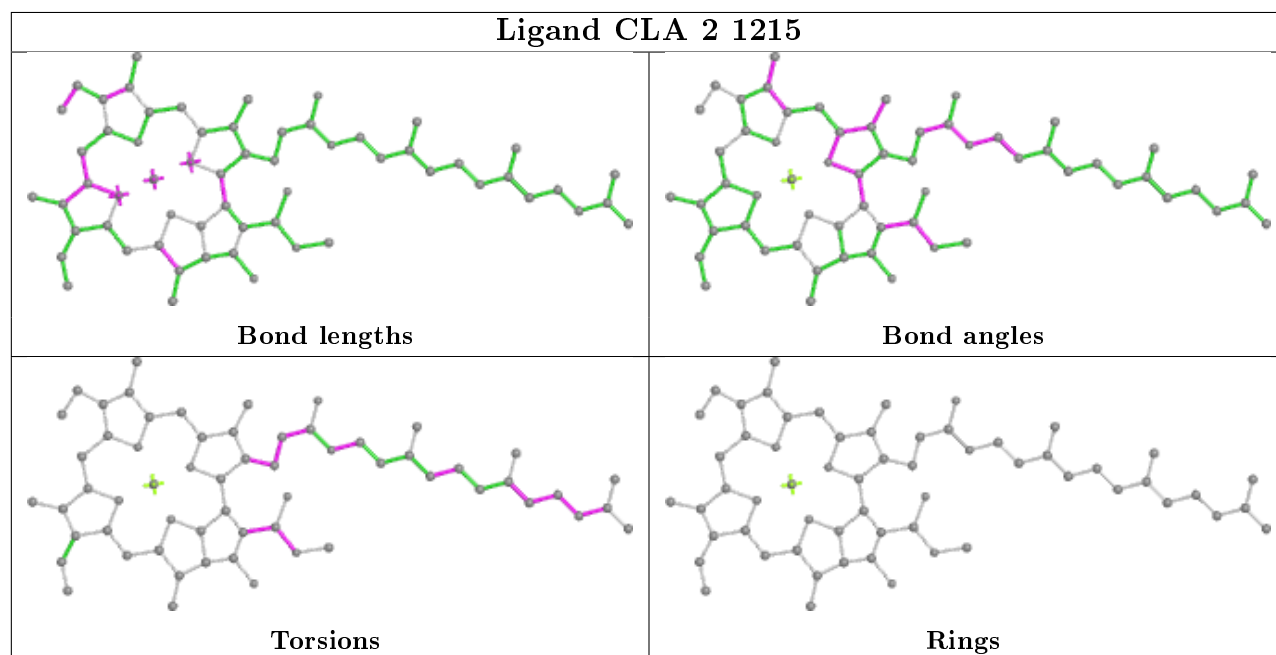
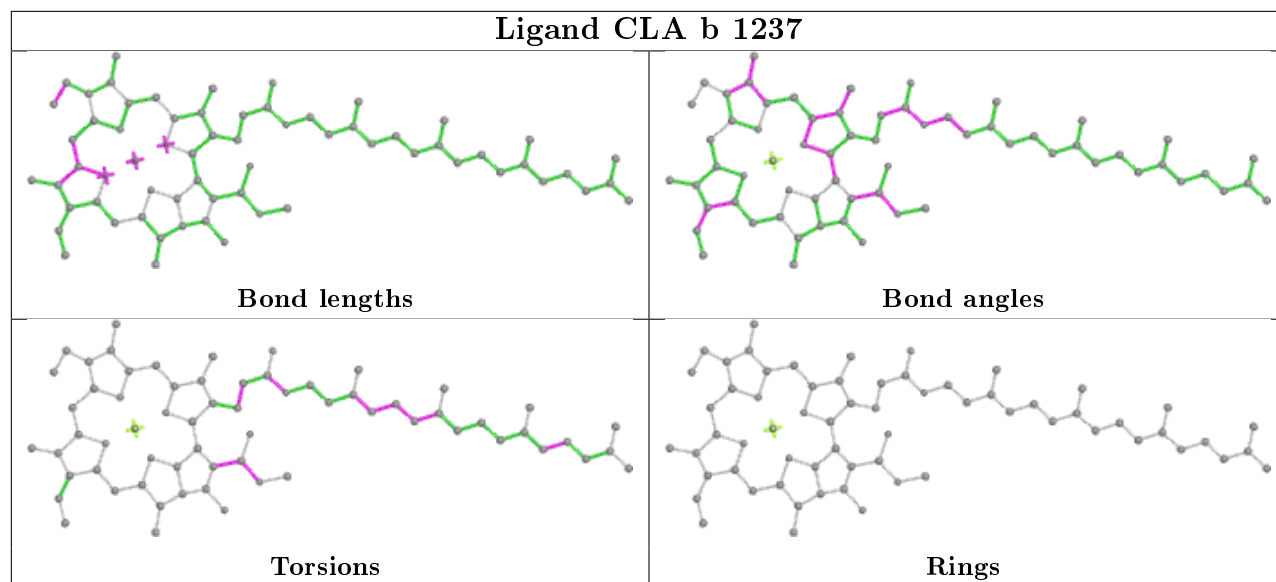
Ligand CLA A 1134**Ligand CLA 1 1110**

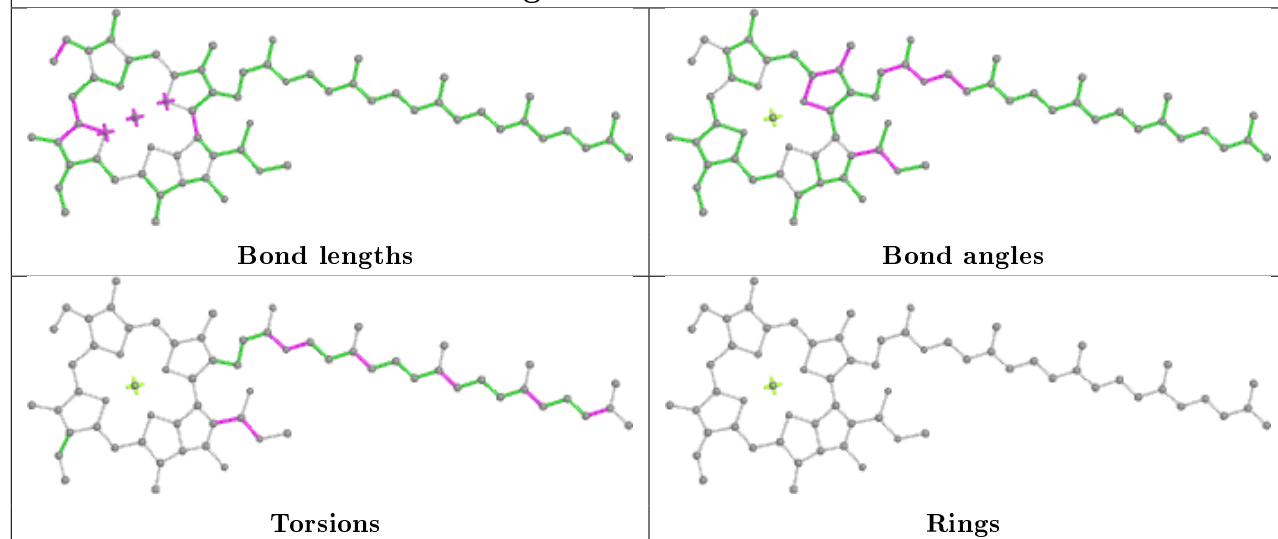
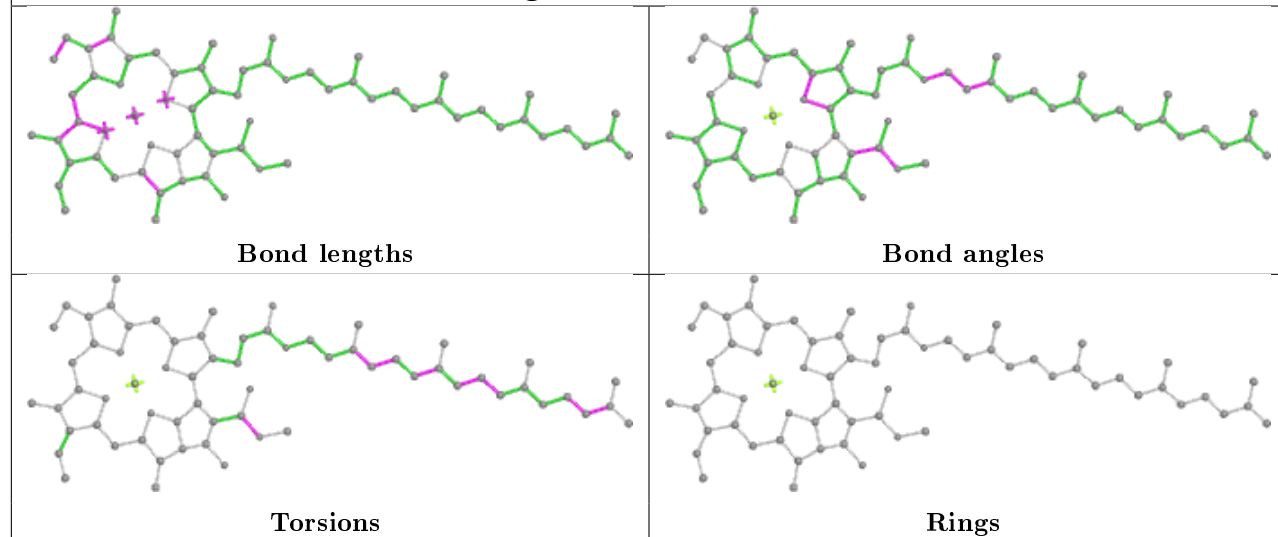


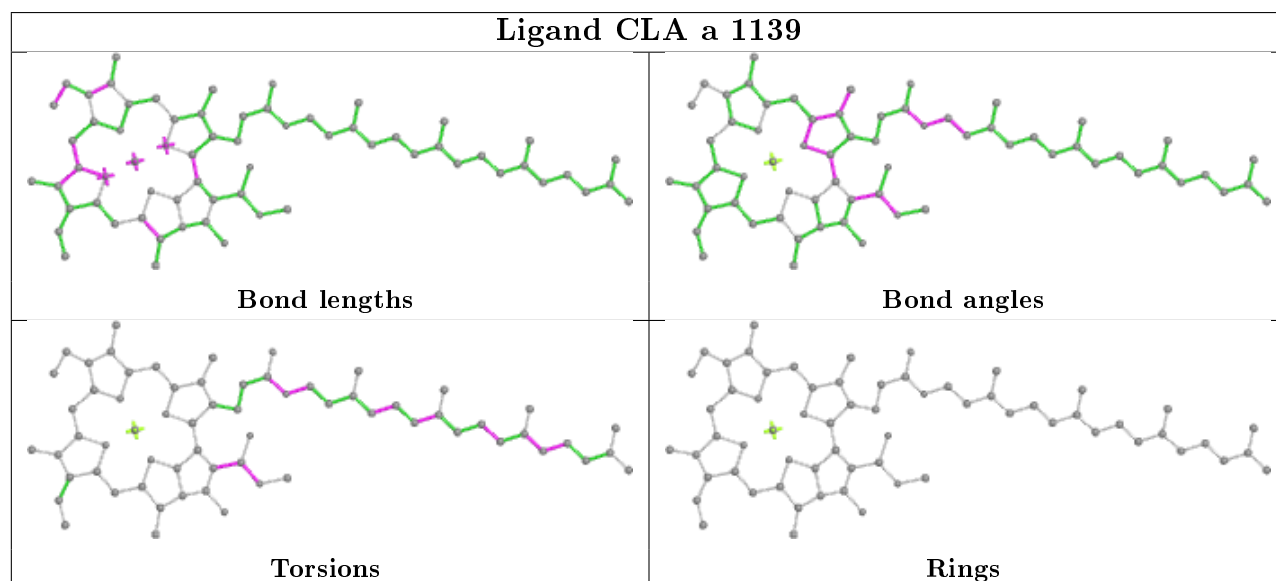
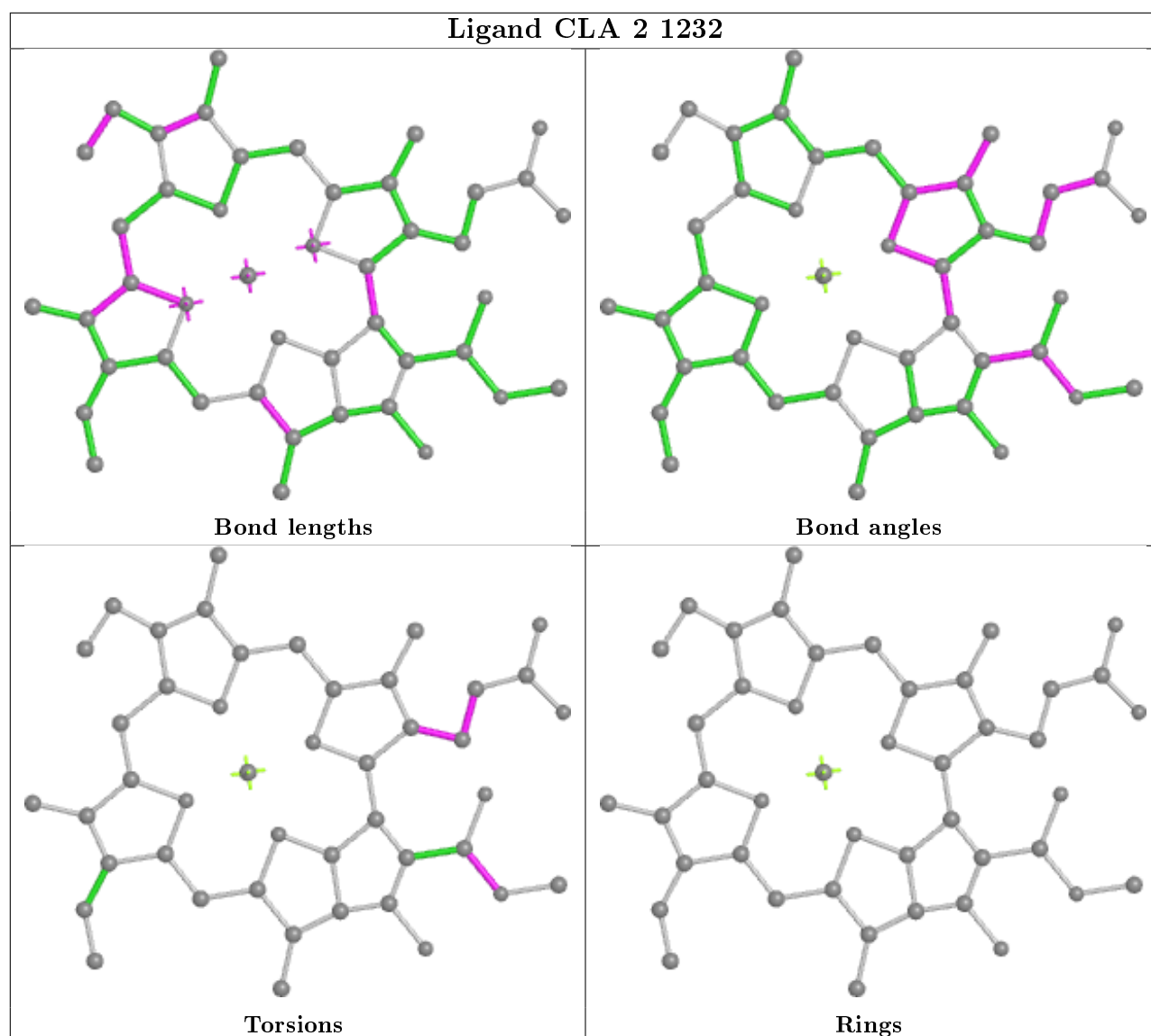


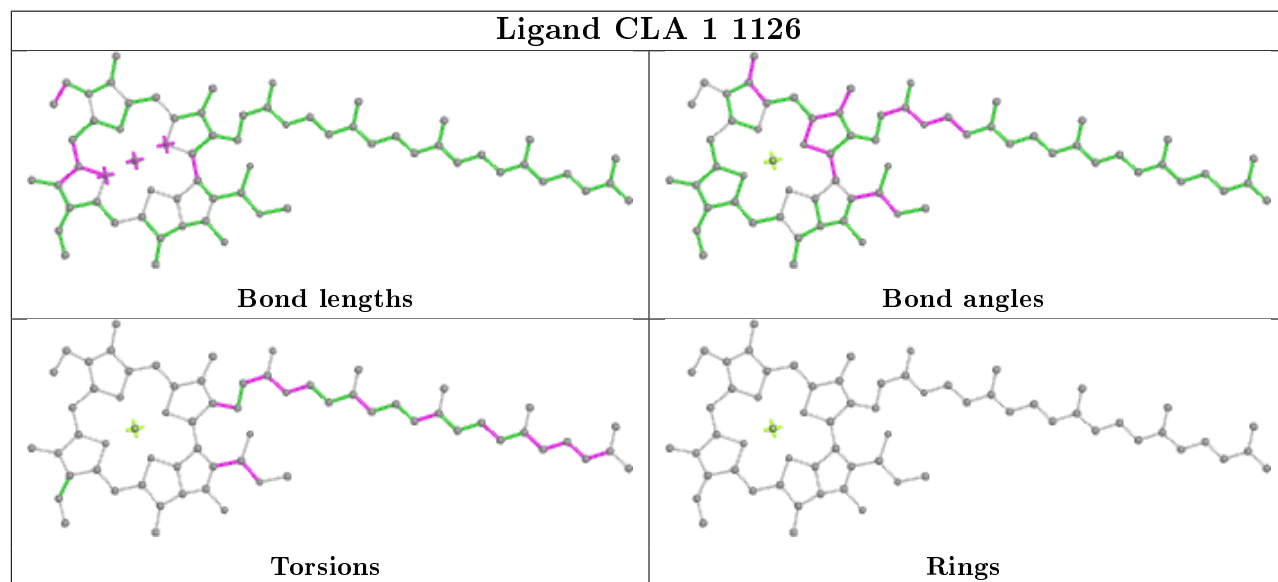
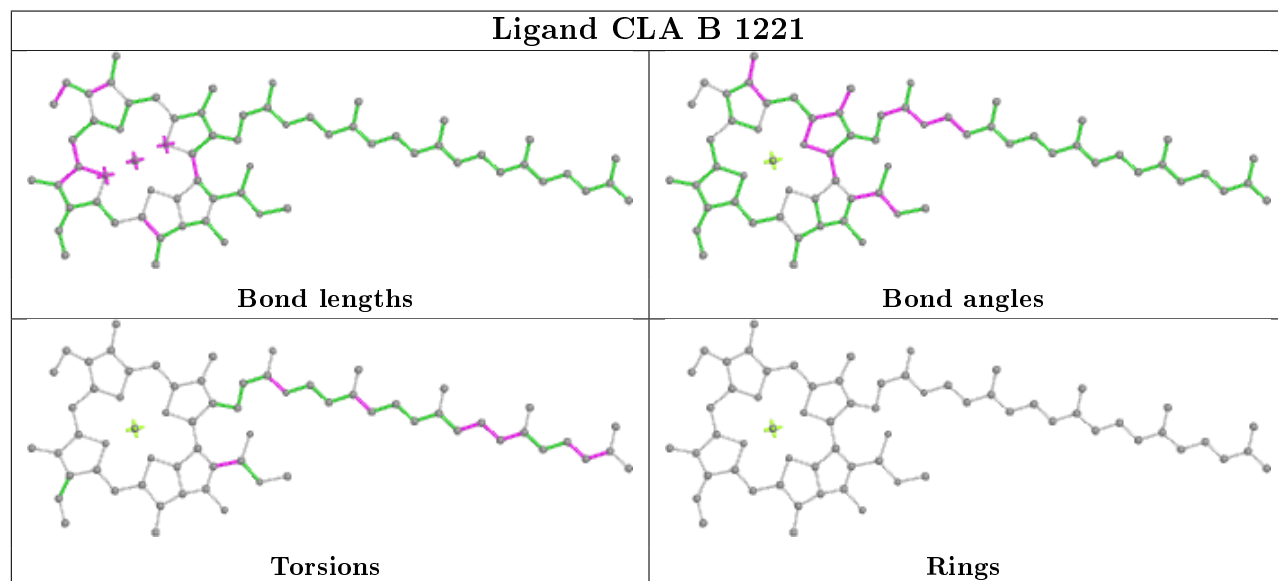
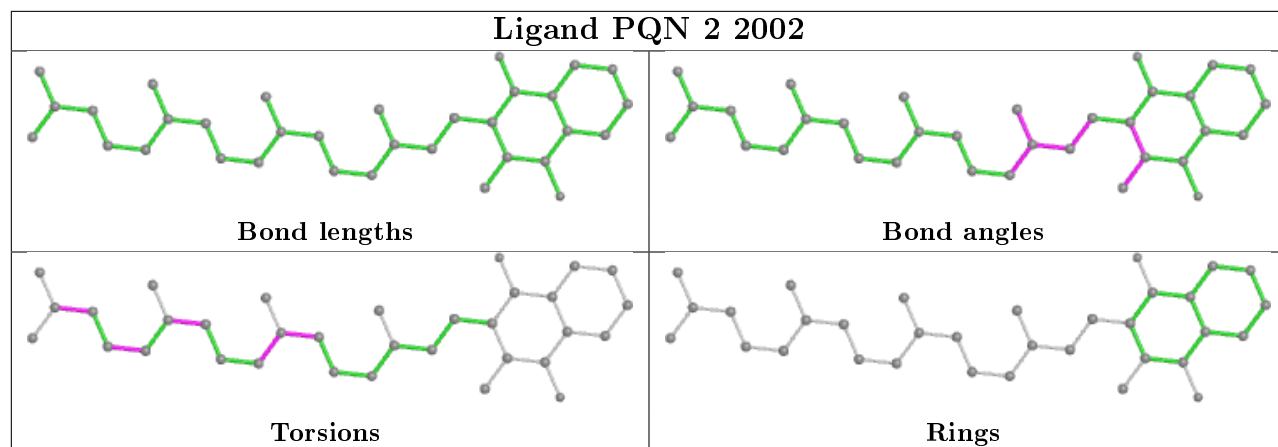


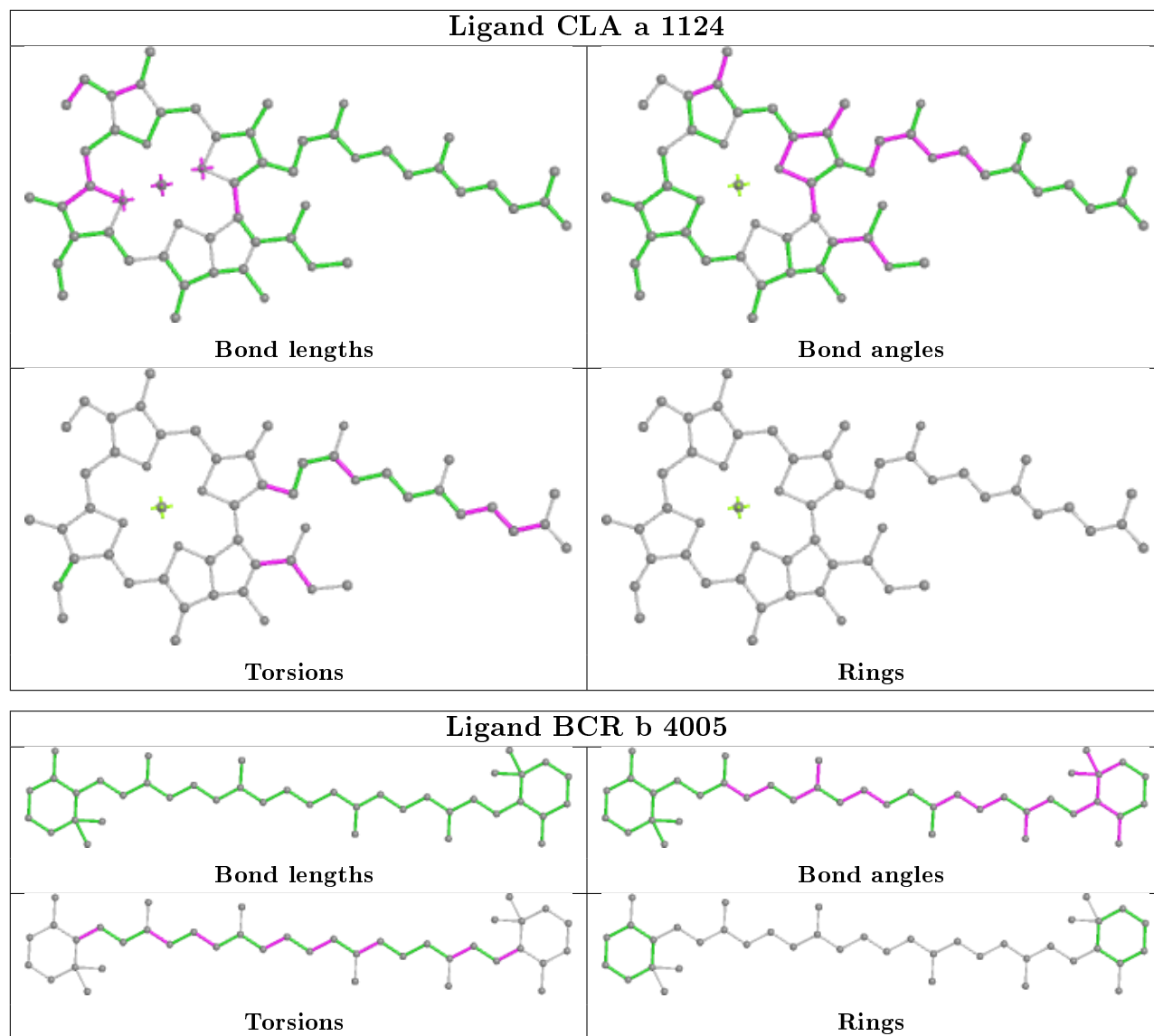




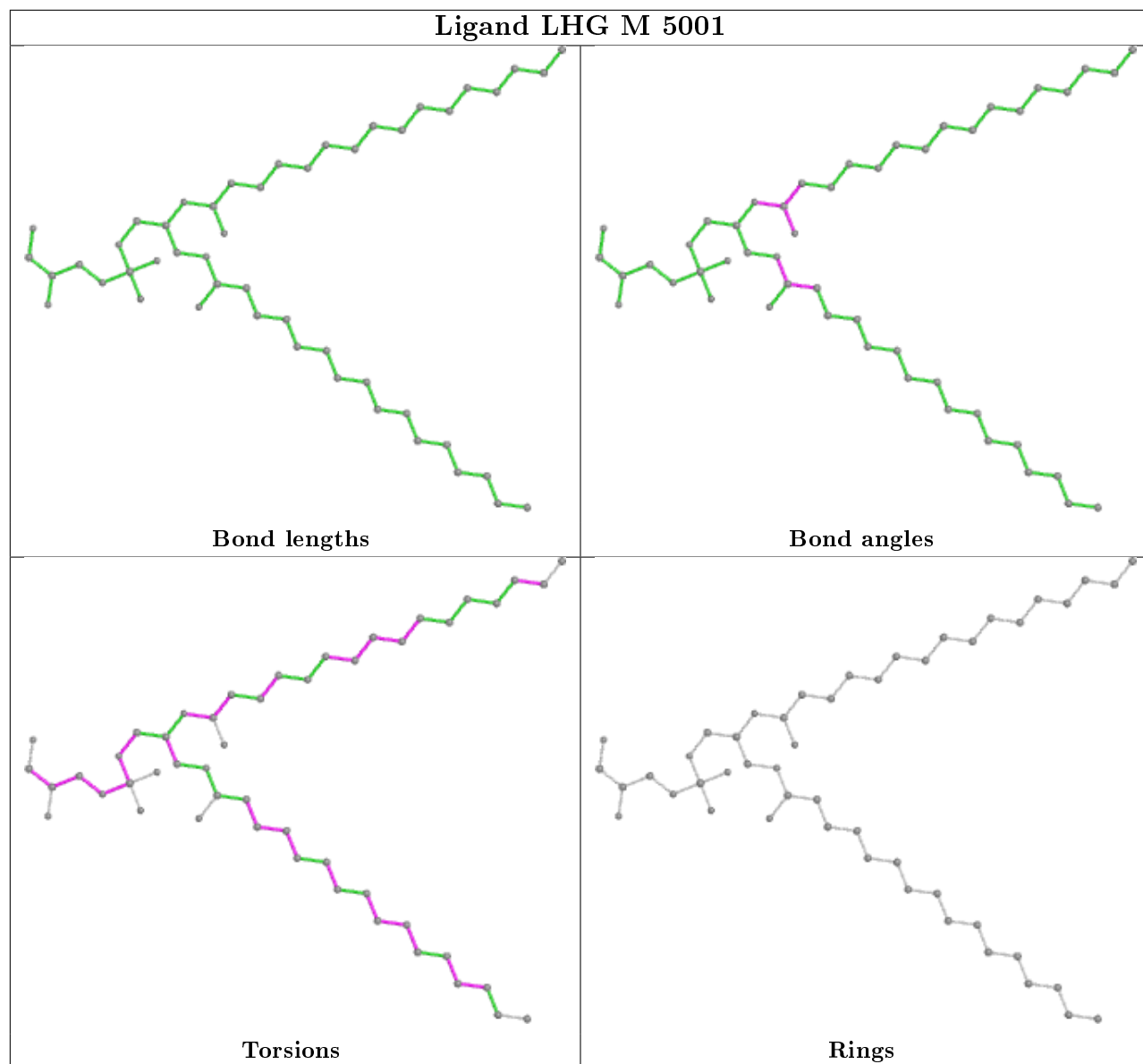
Ligand CLA B 1235**Ligand CLA A 1133**



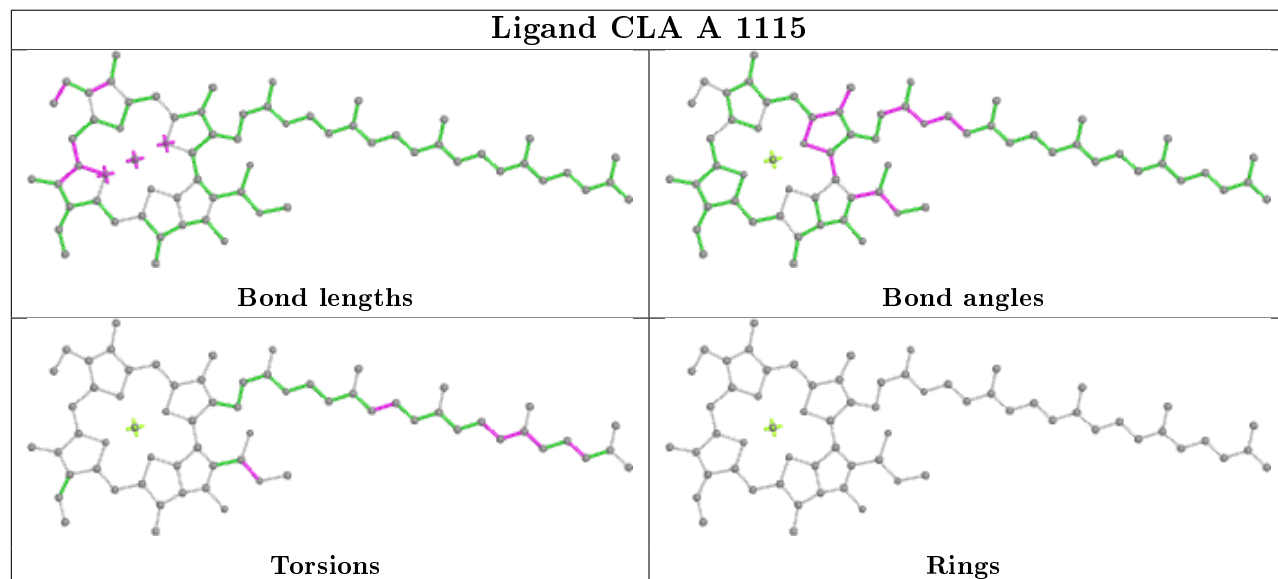


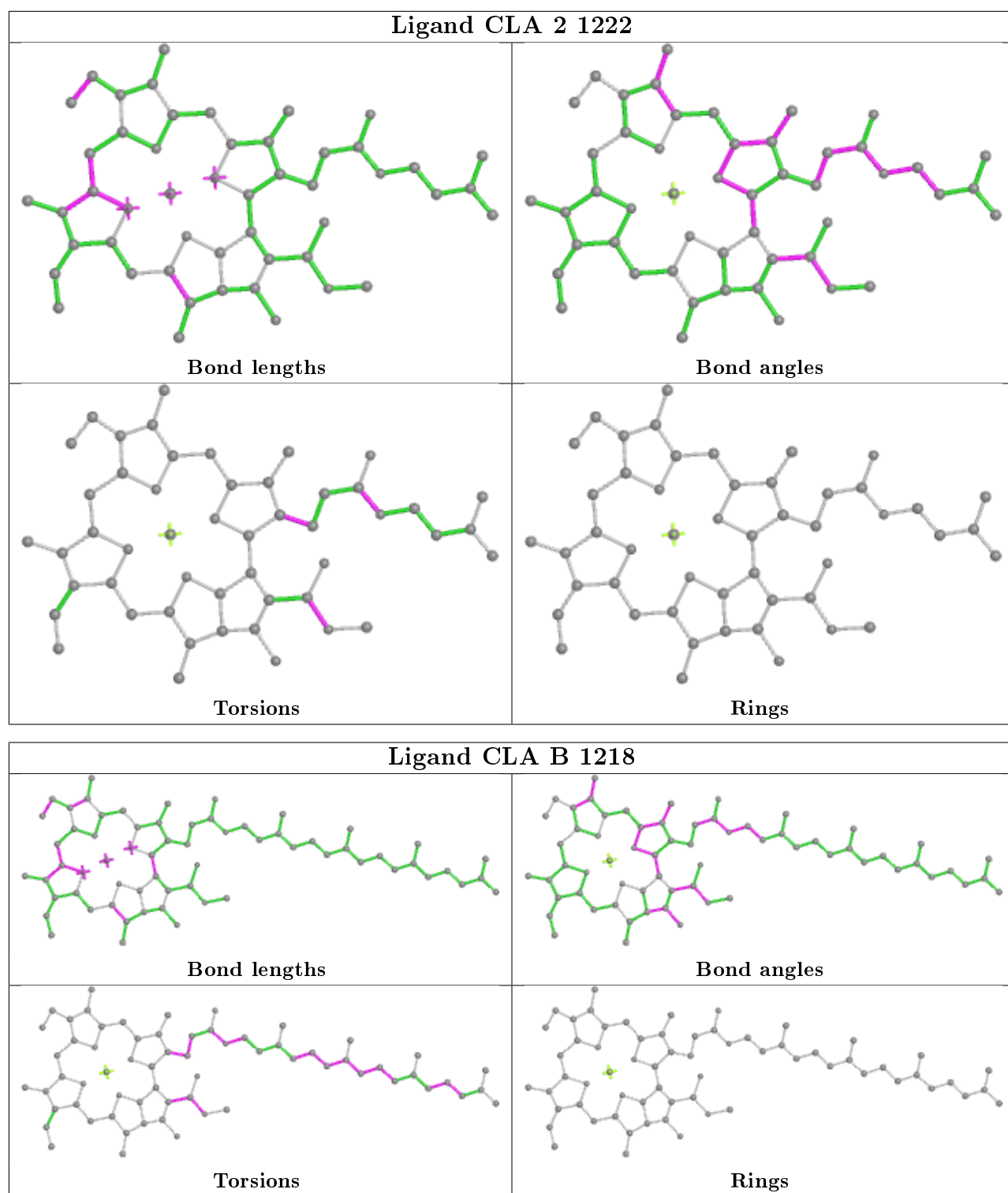


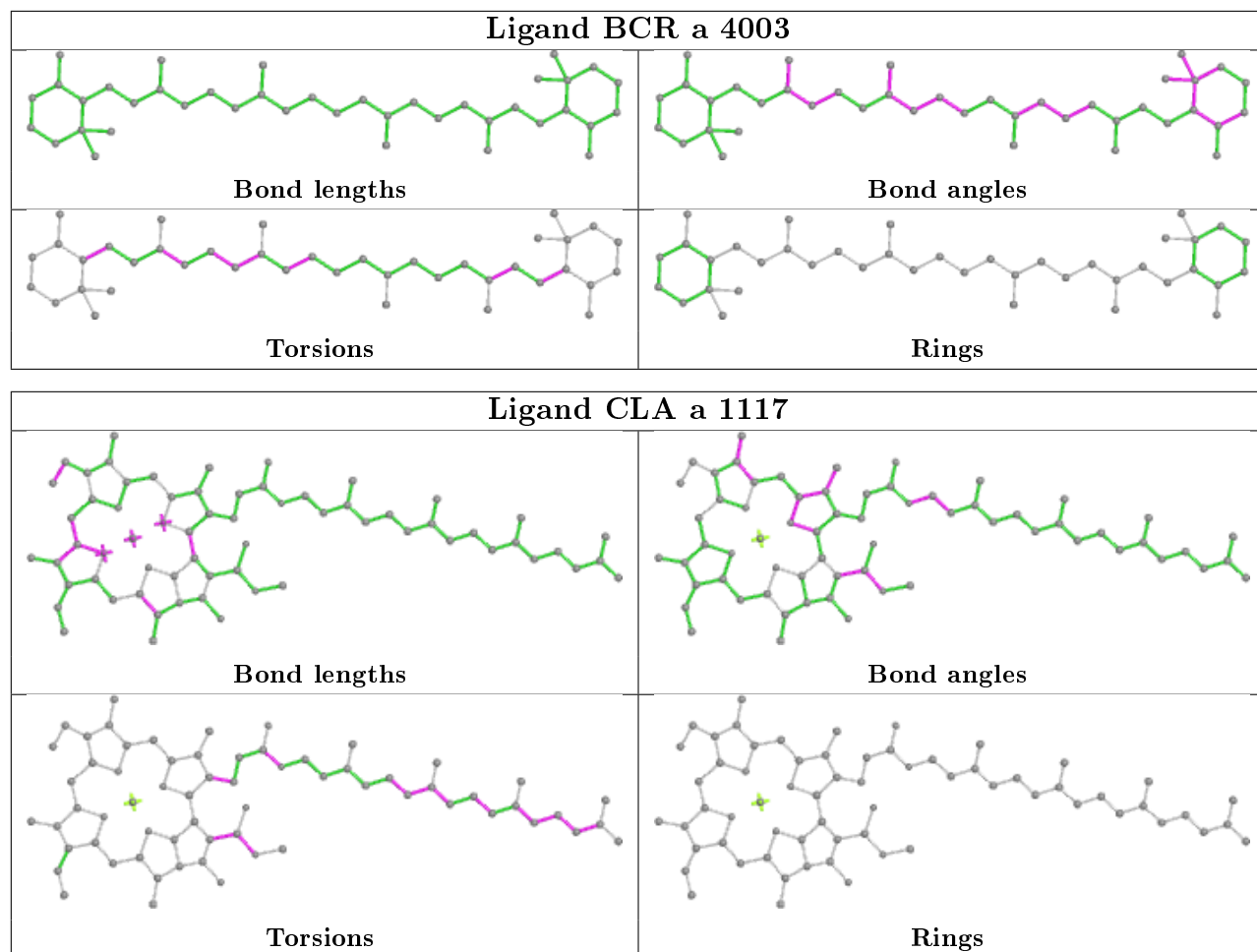
Ligand LHG M 5001

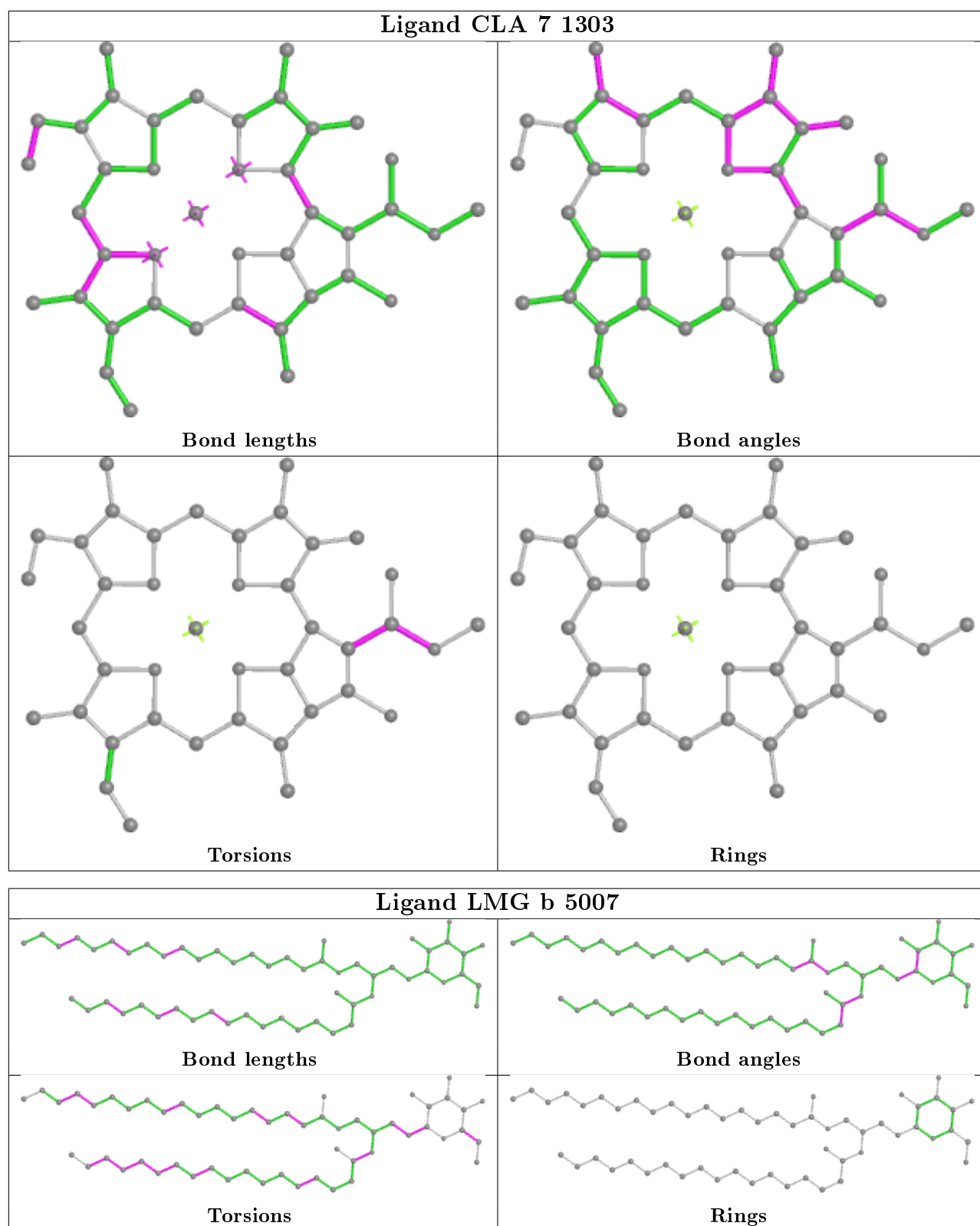


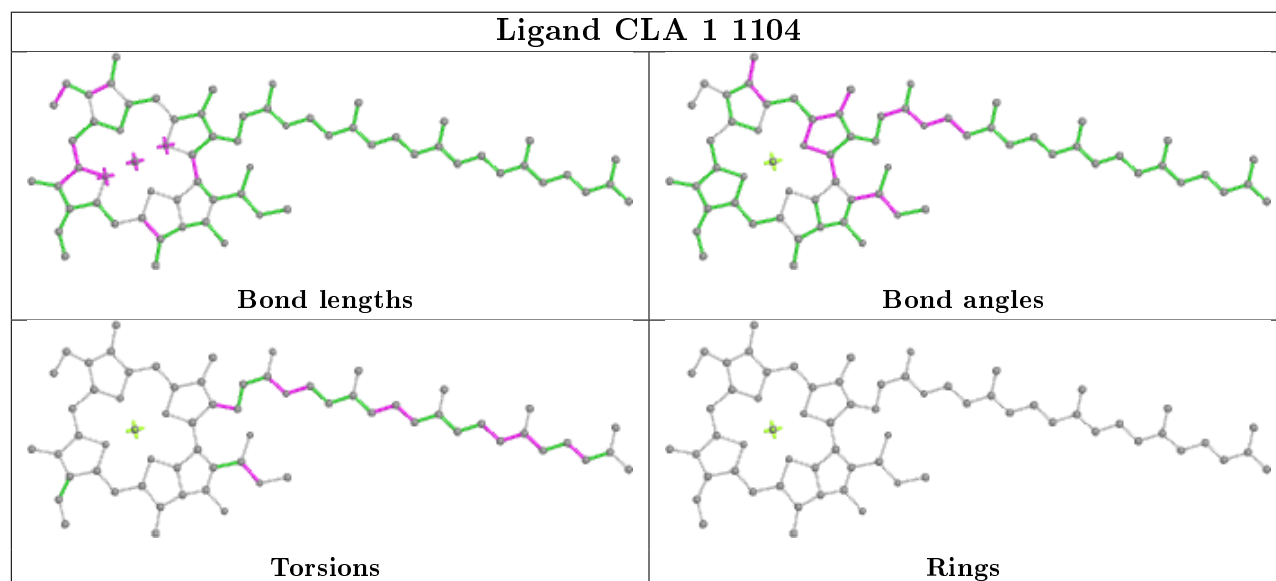
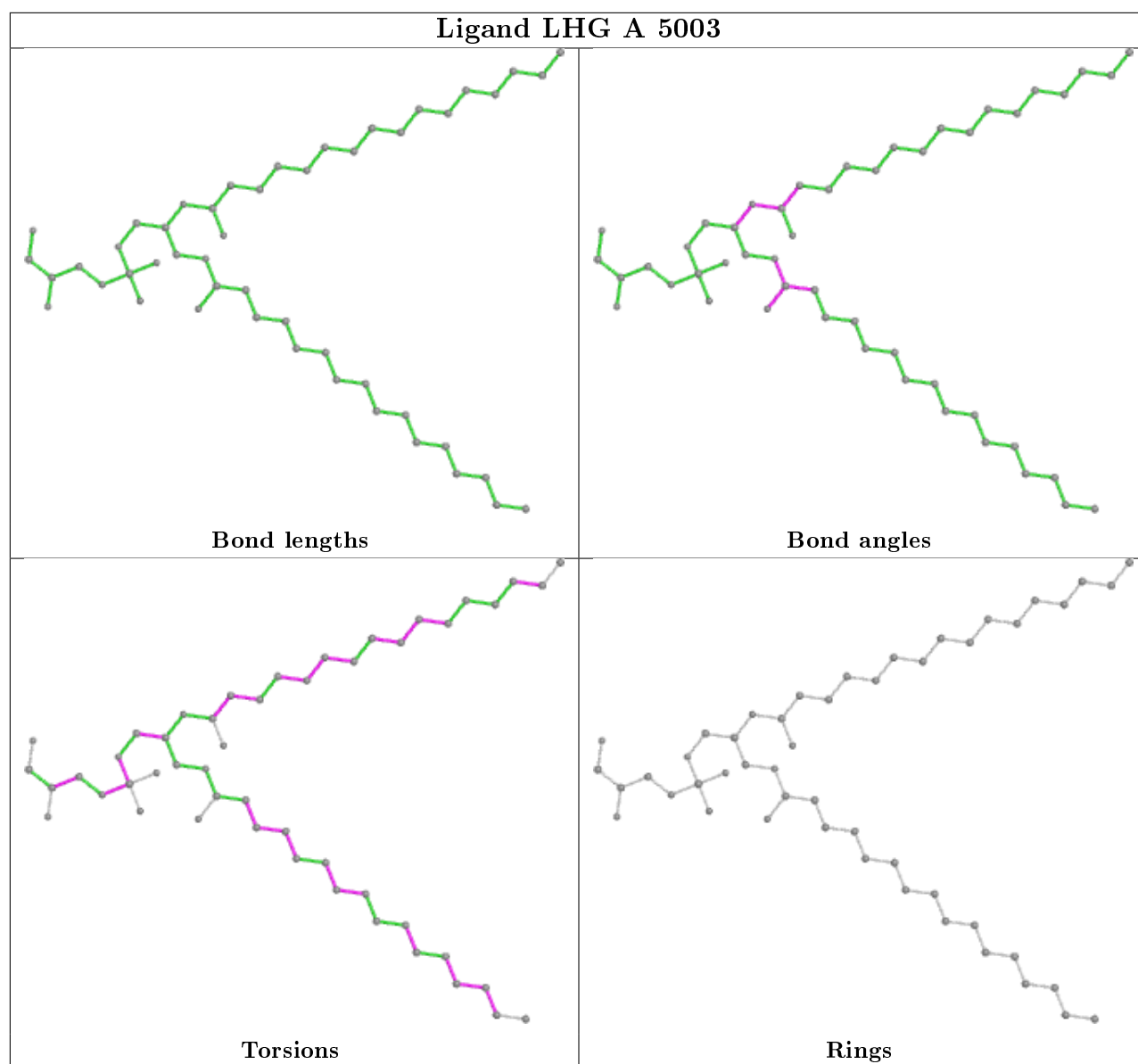
Ligand CLA A 1115

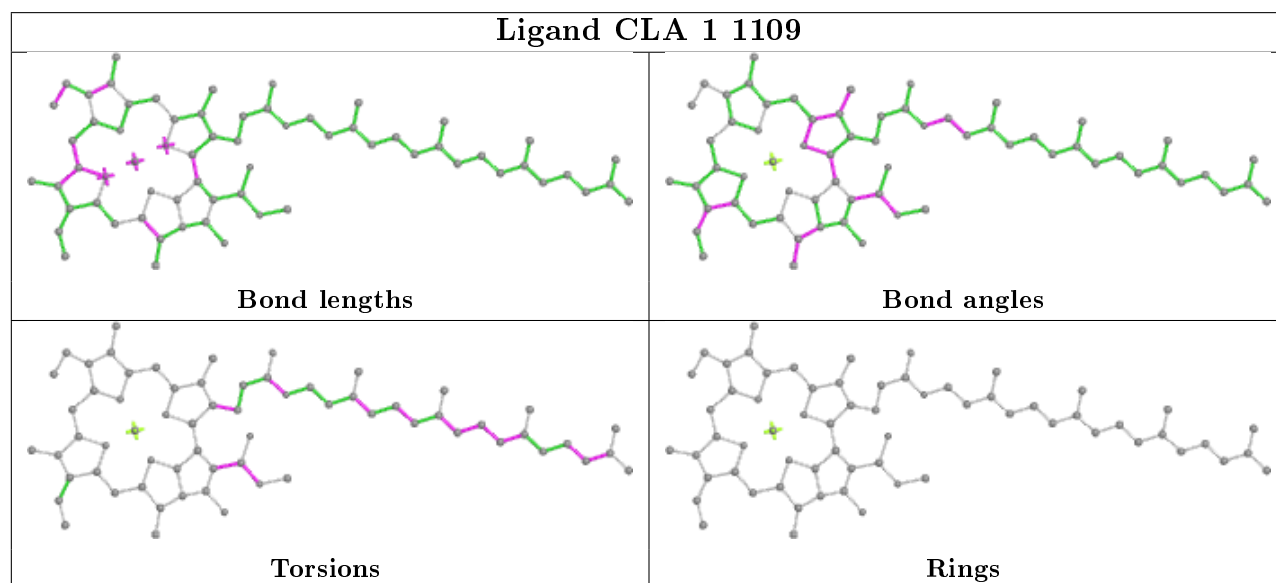
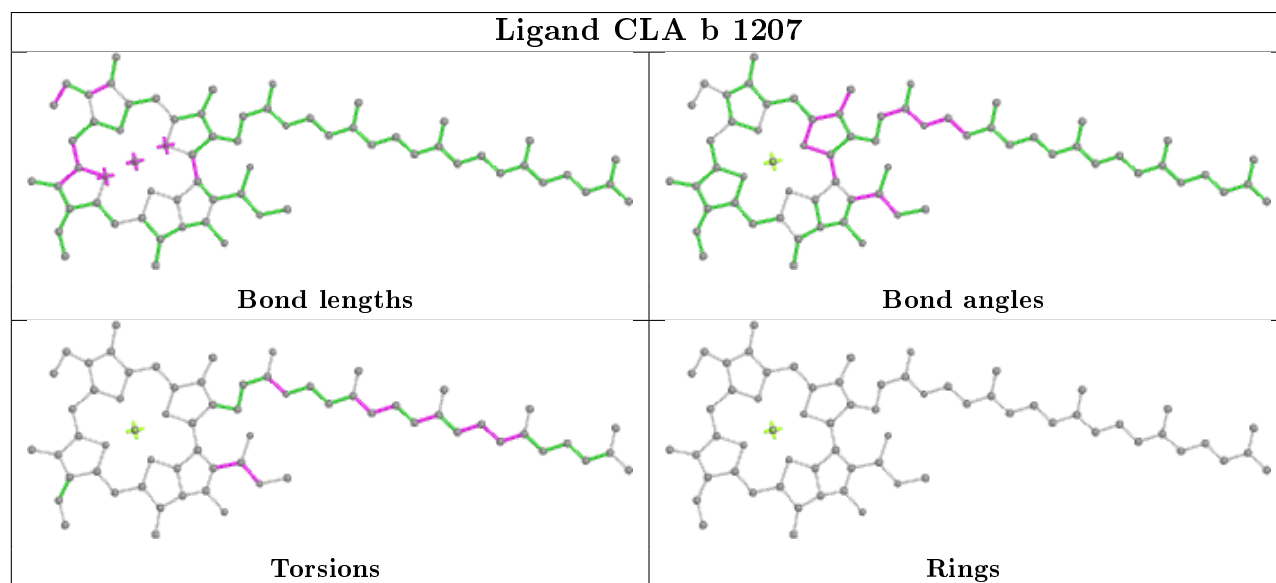
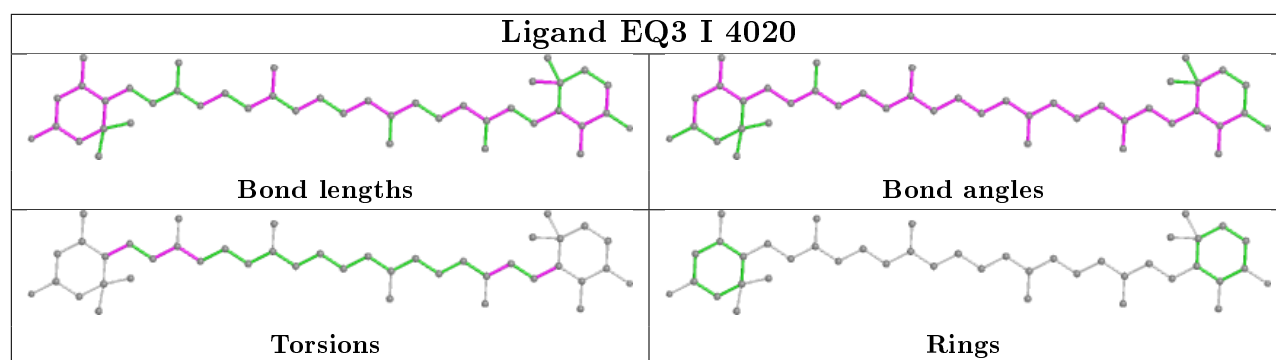


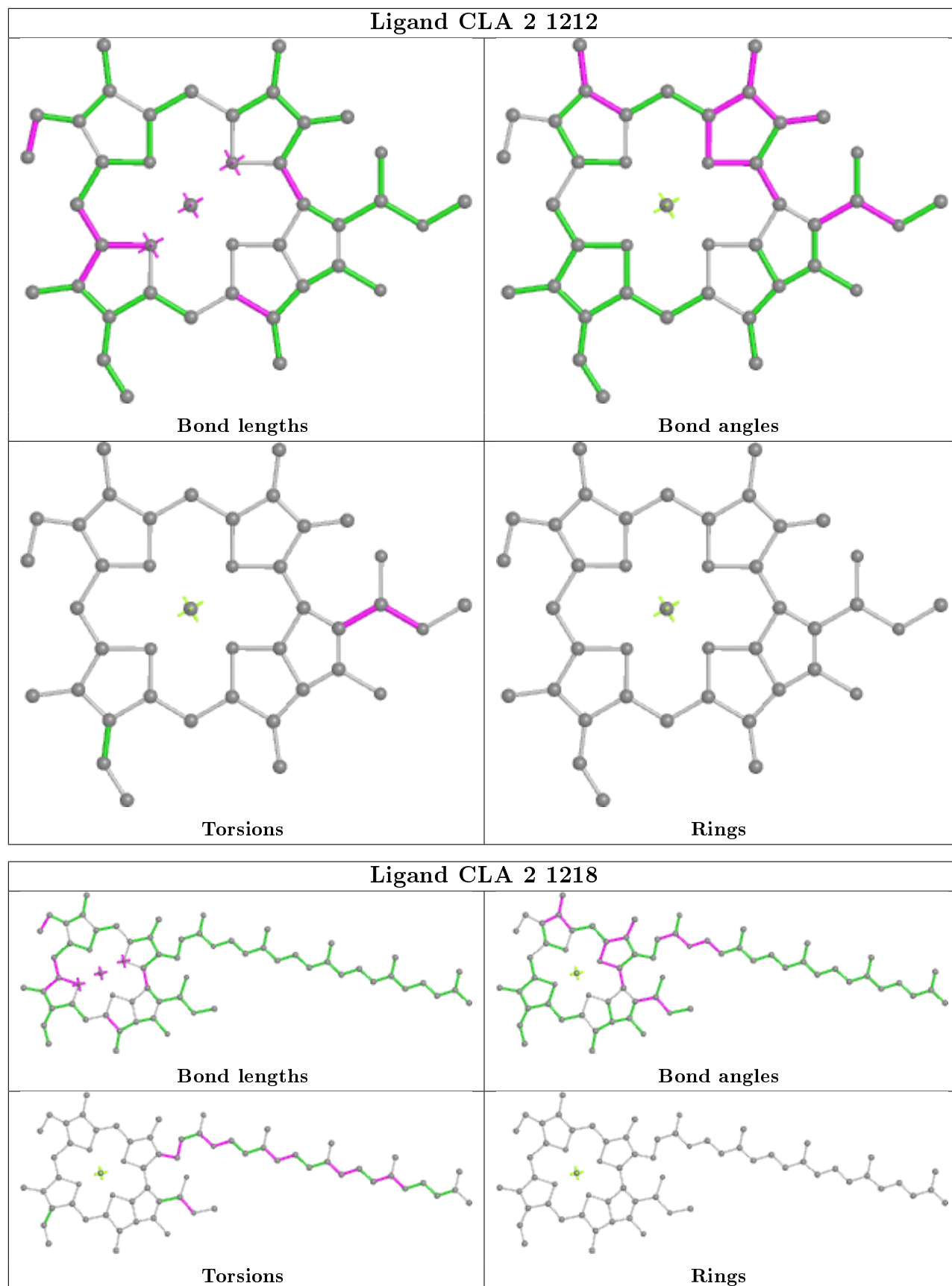




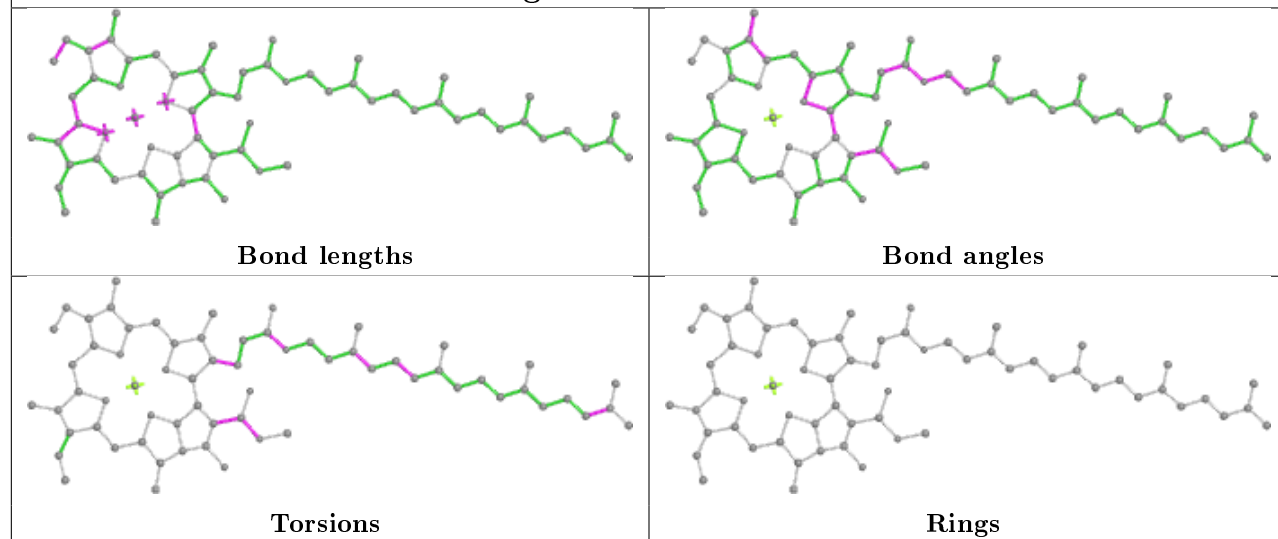




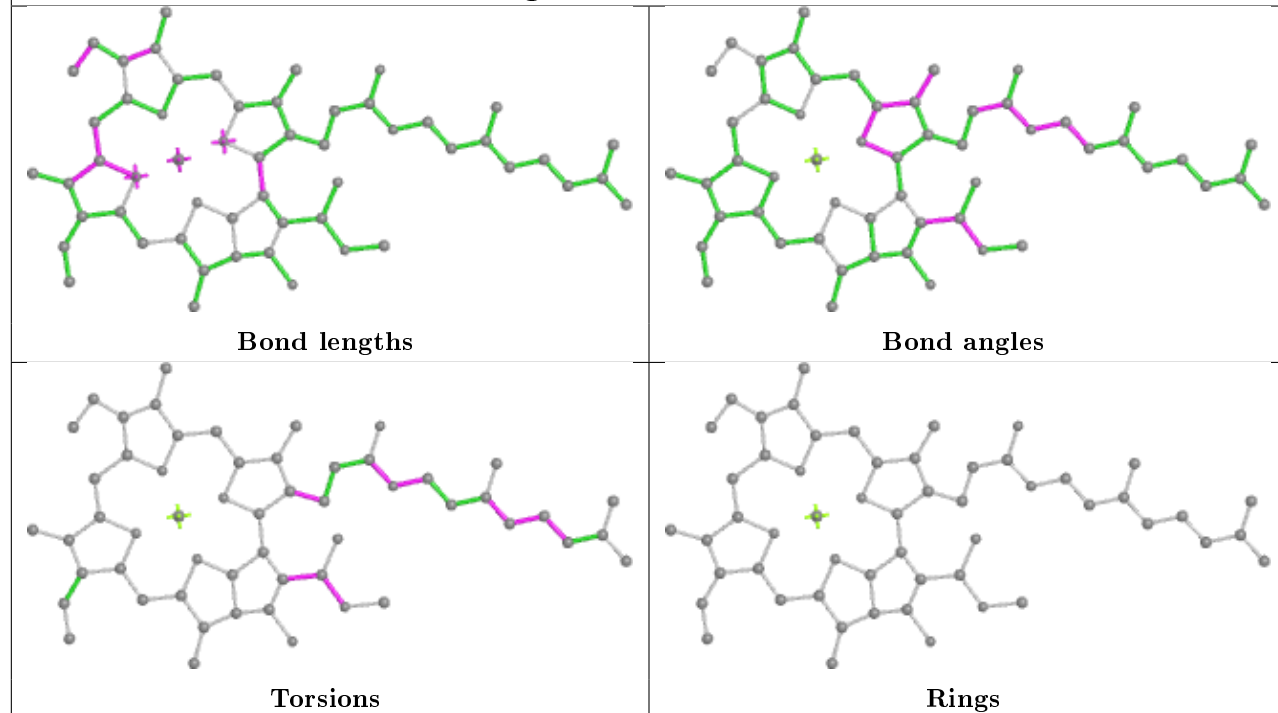


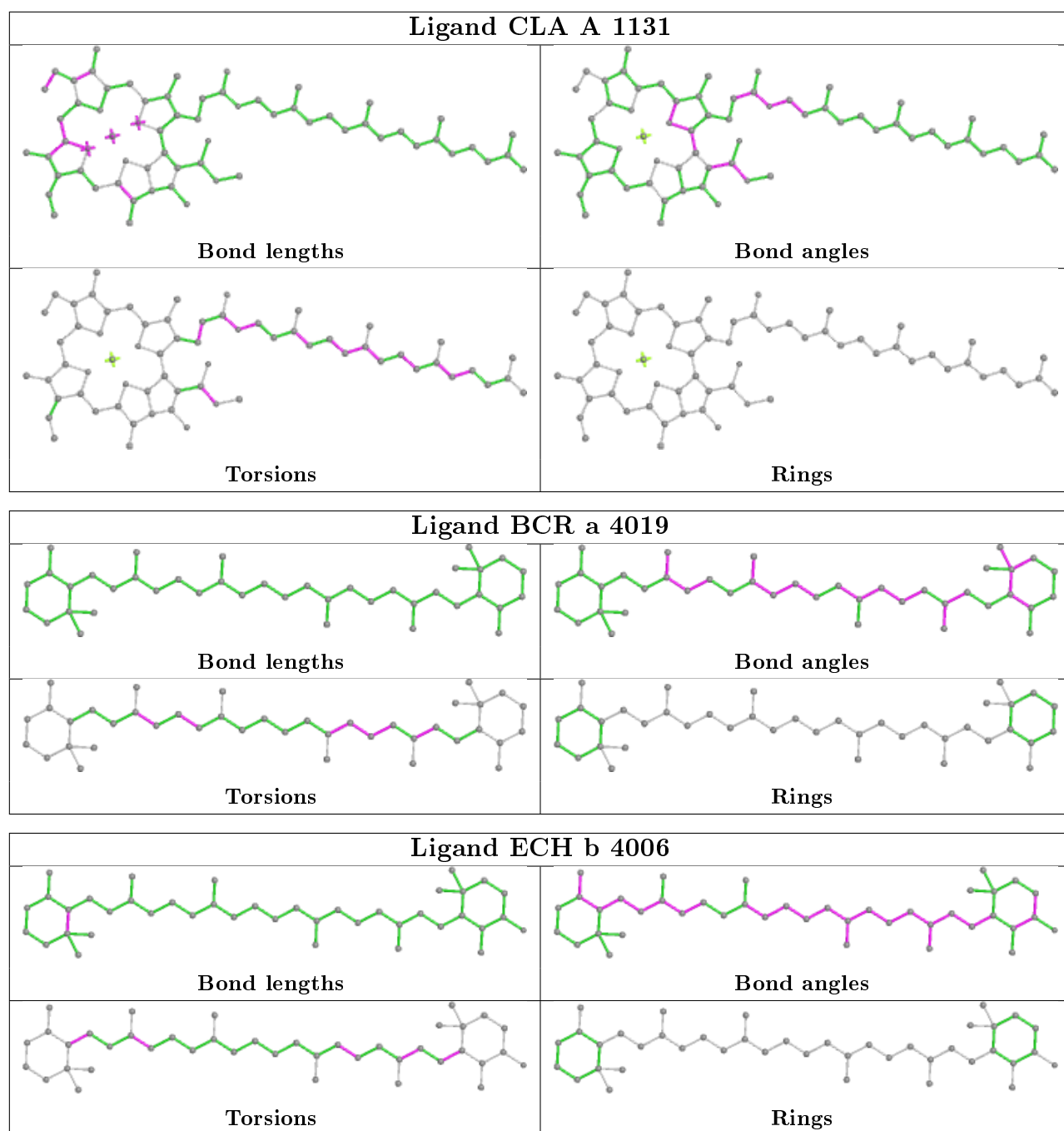


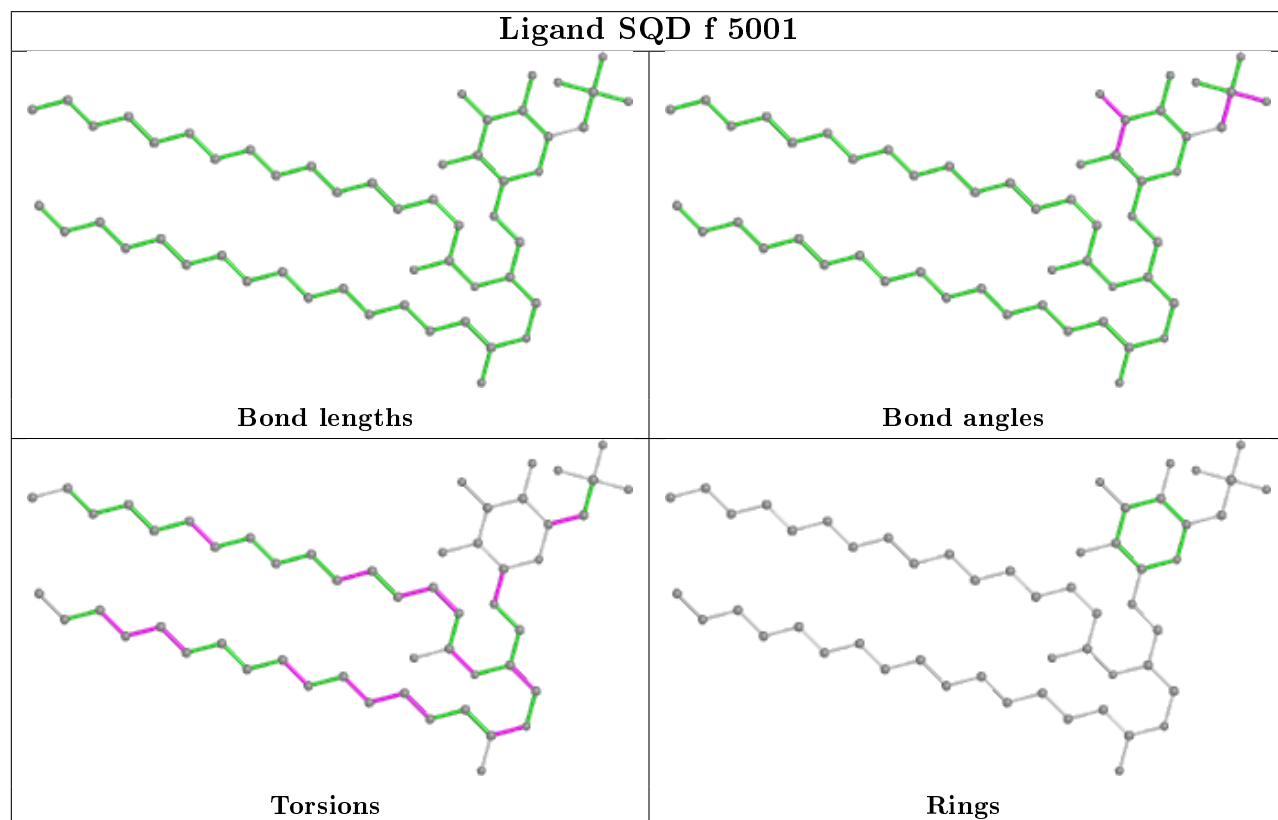
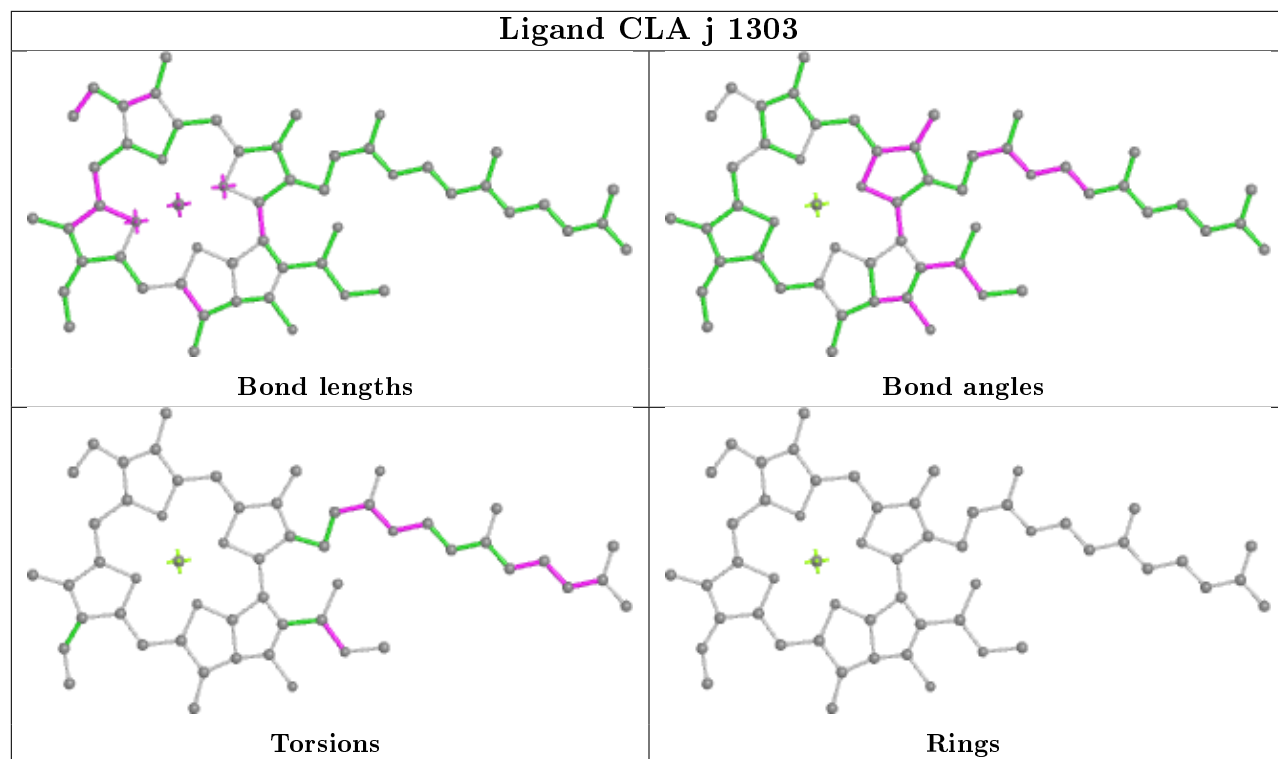
Ligand CLA B 1021

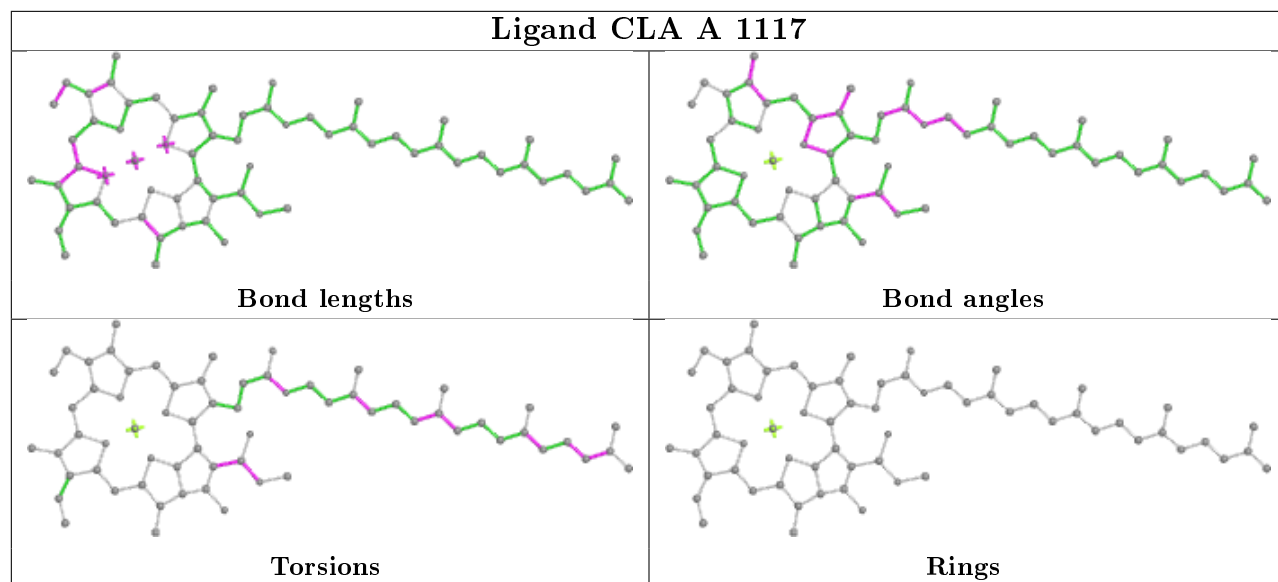
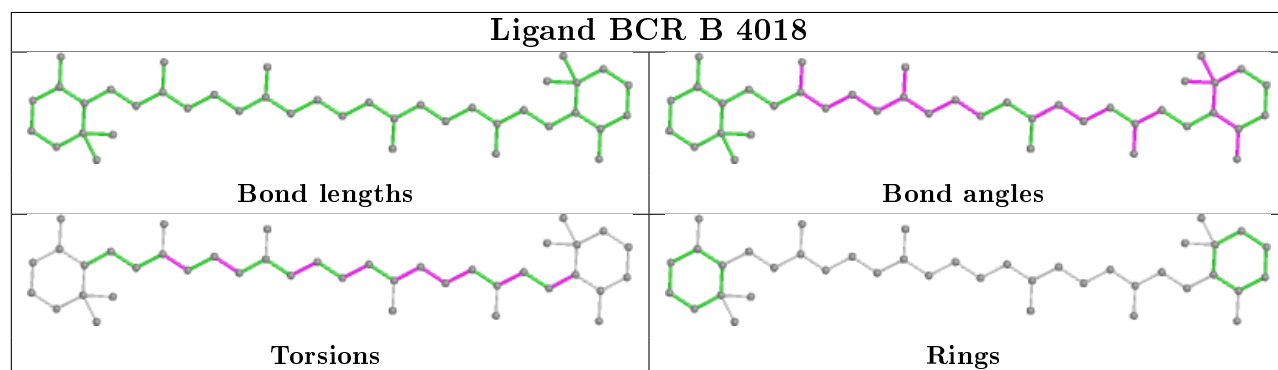
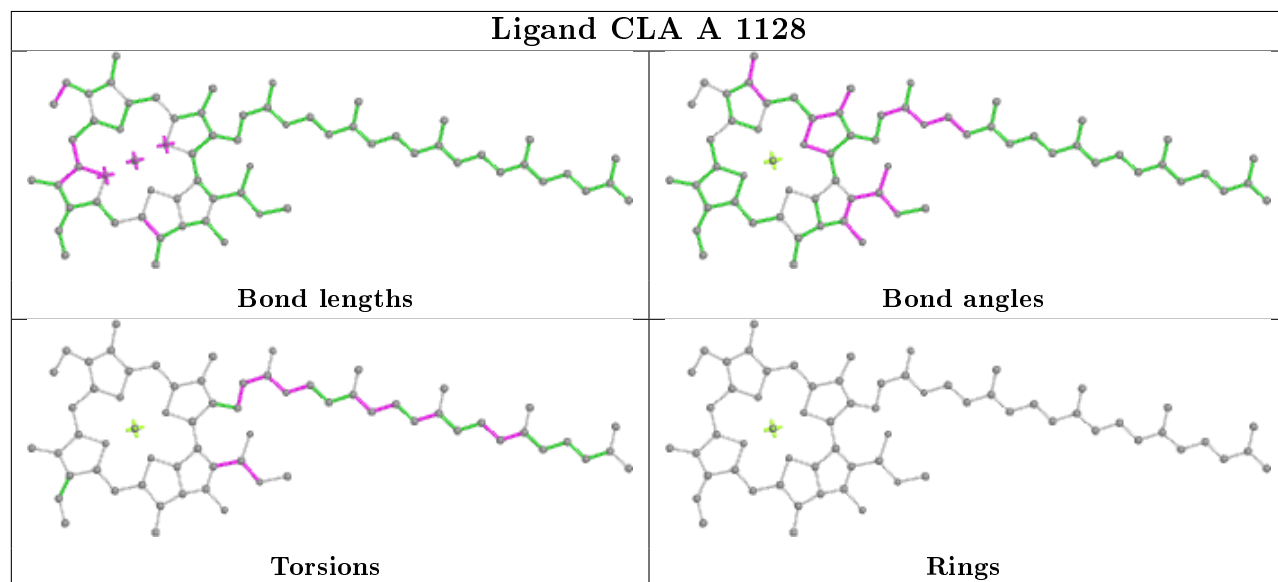


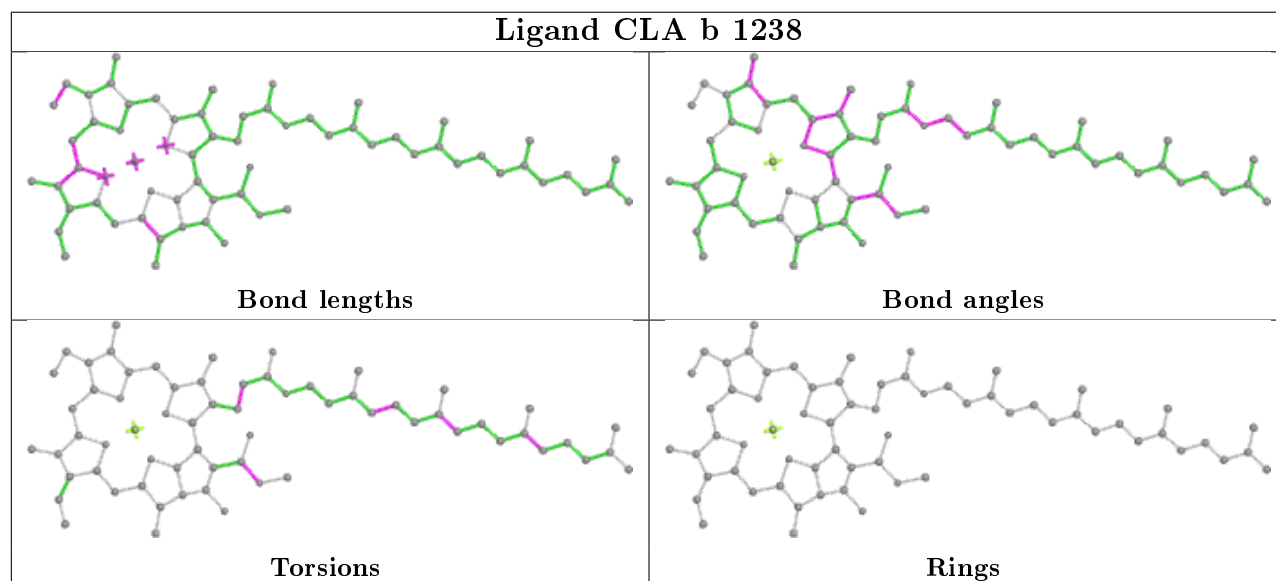
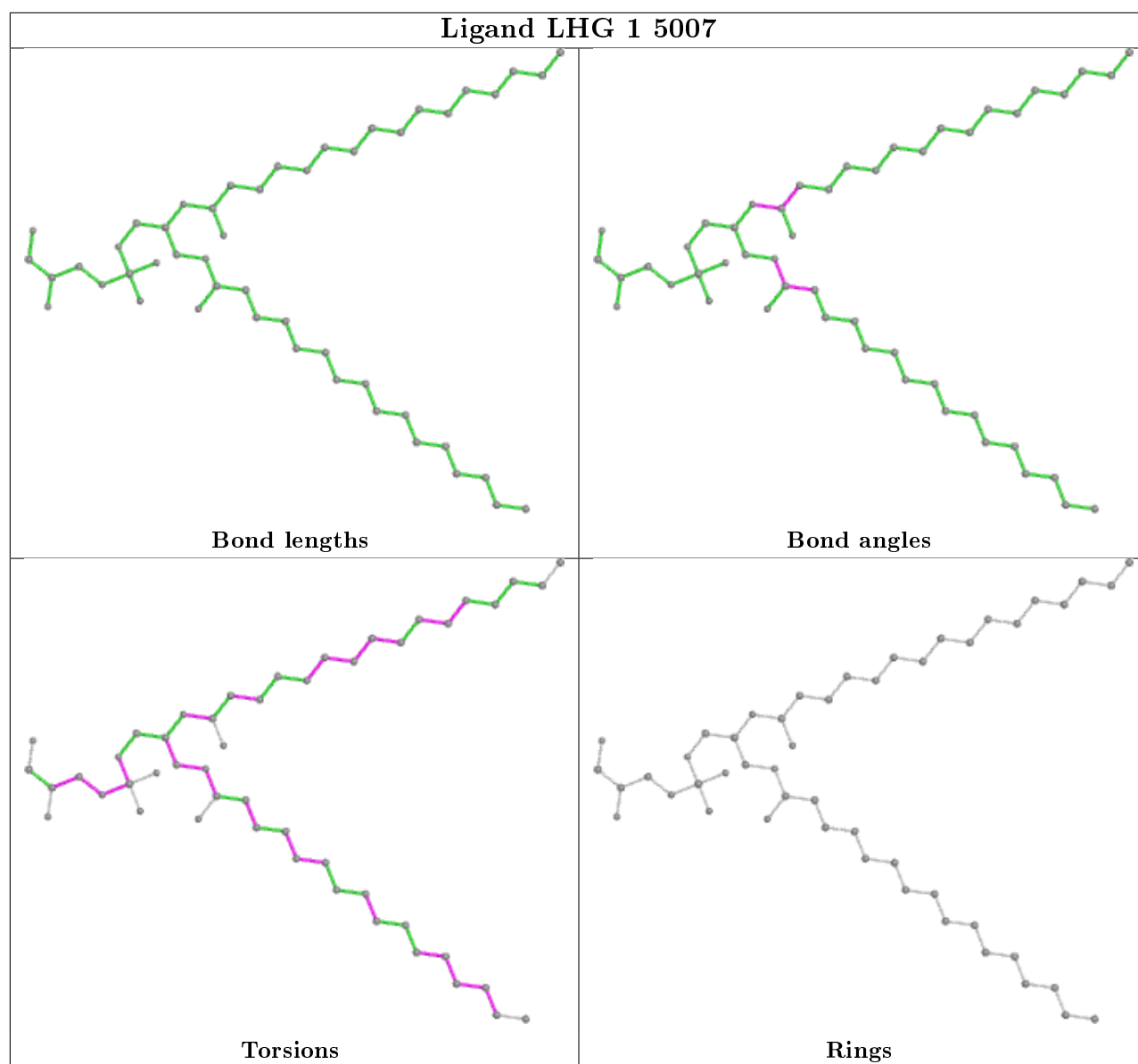
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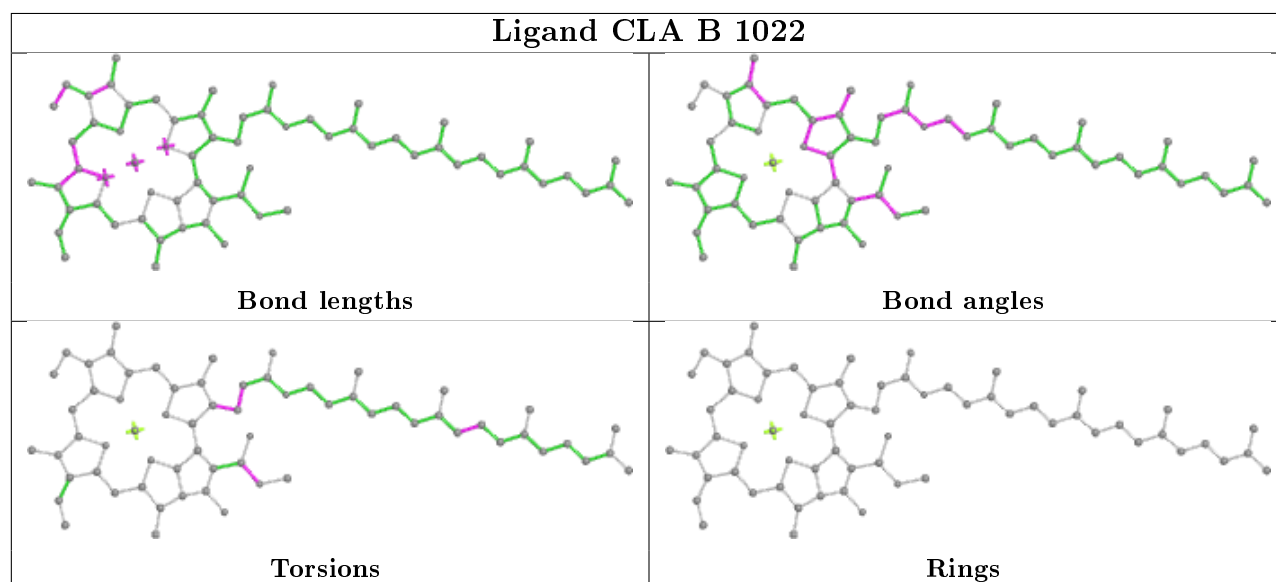
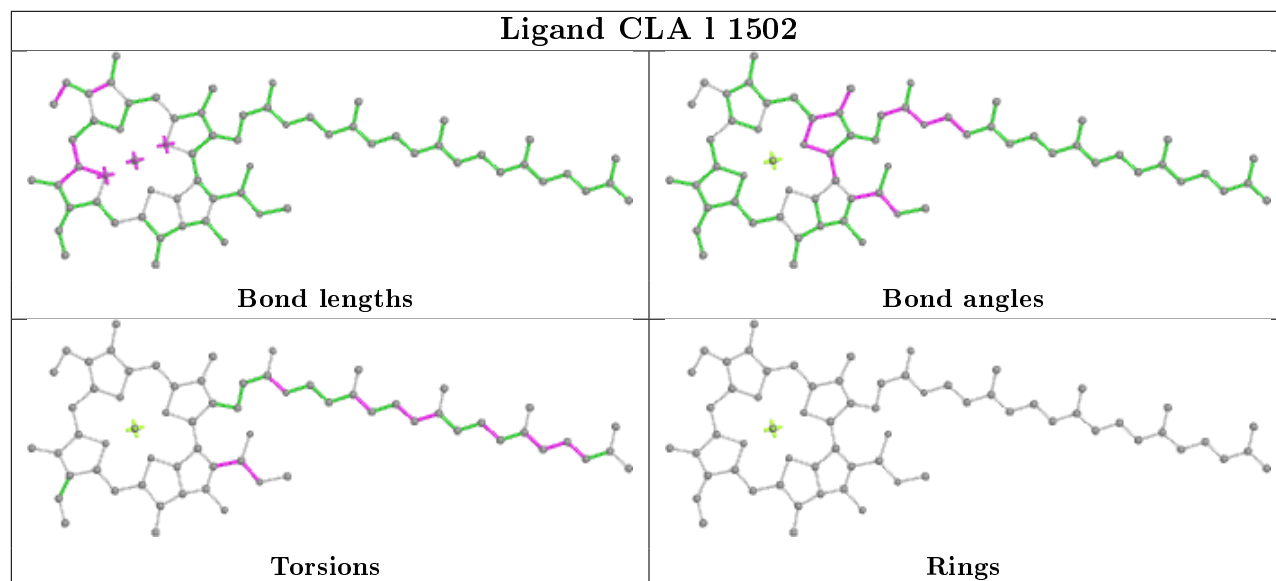
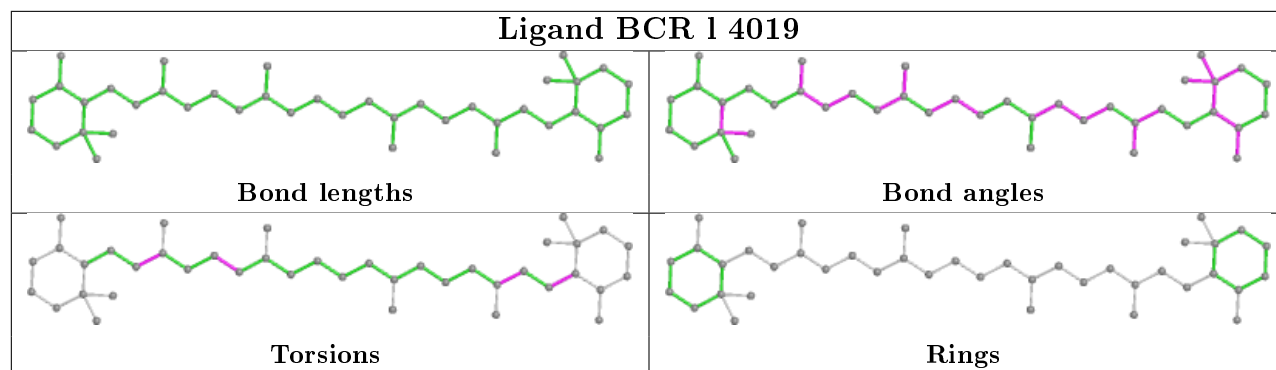


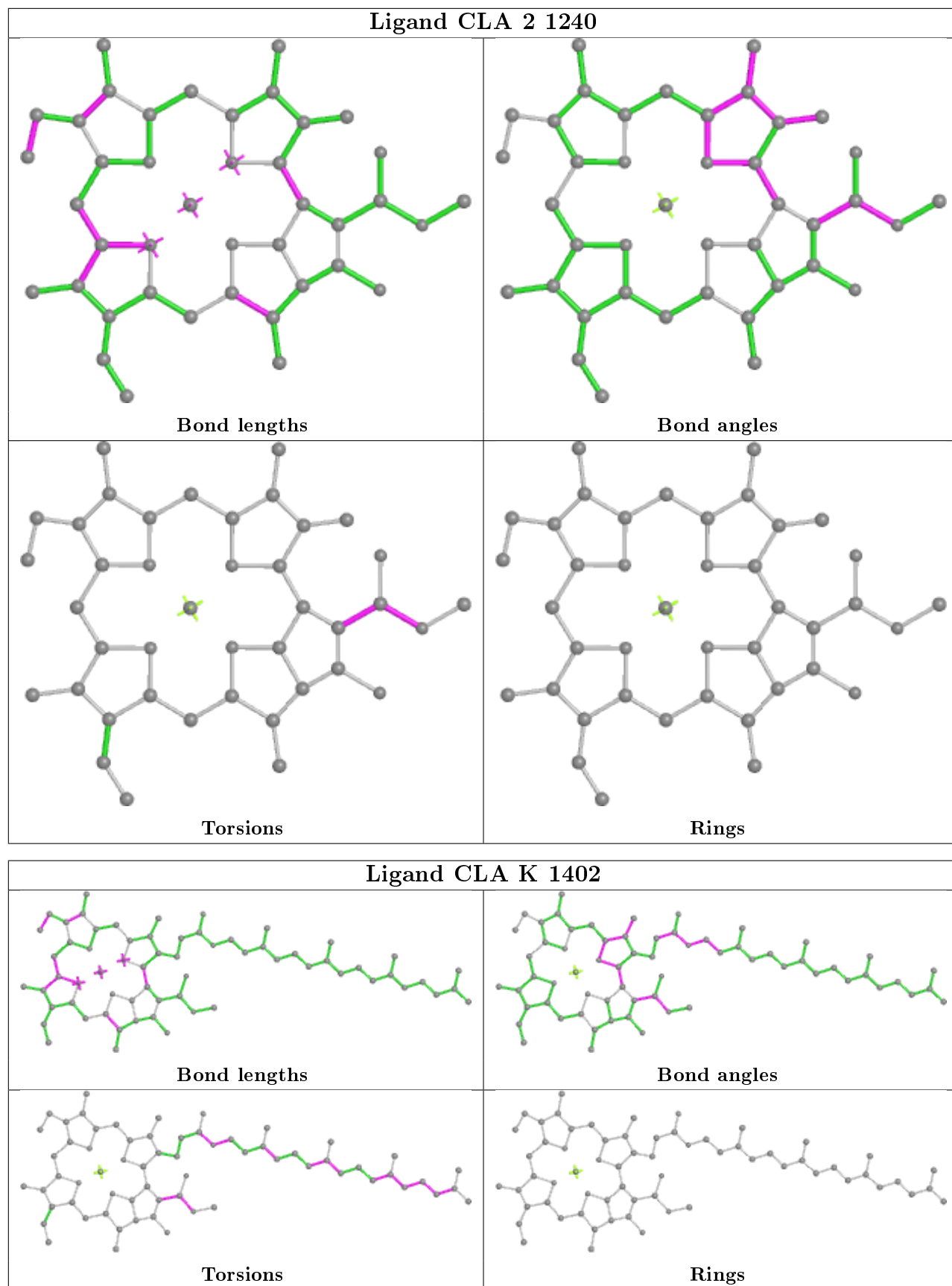


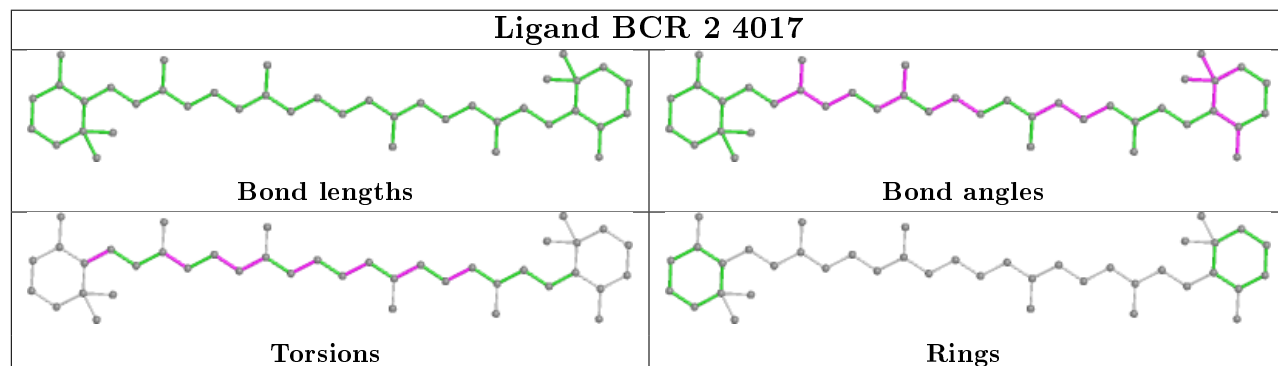
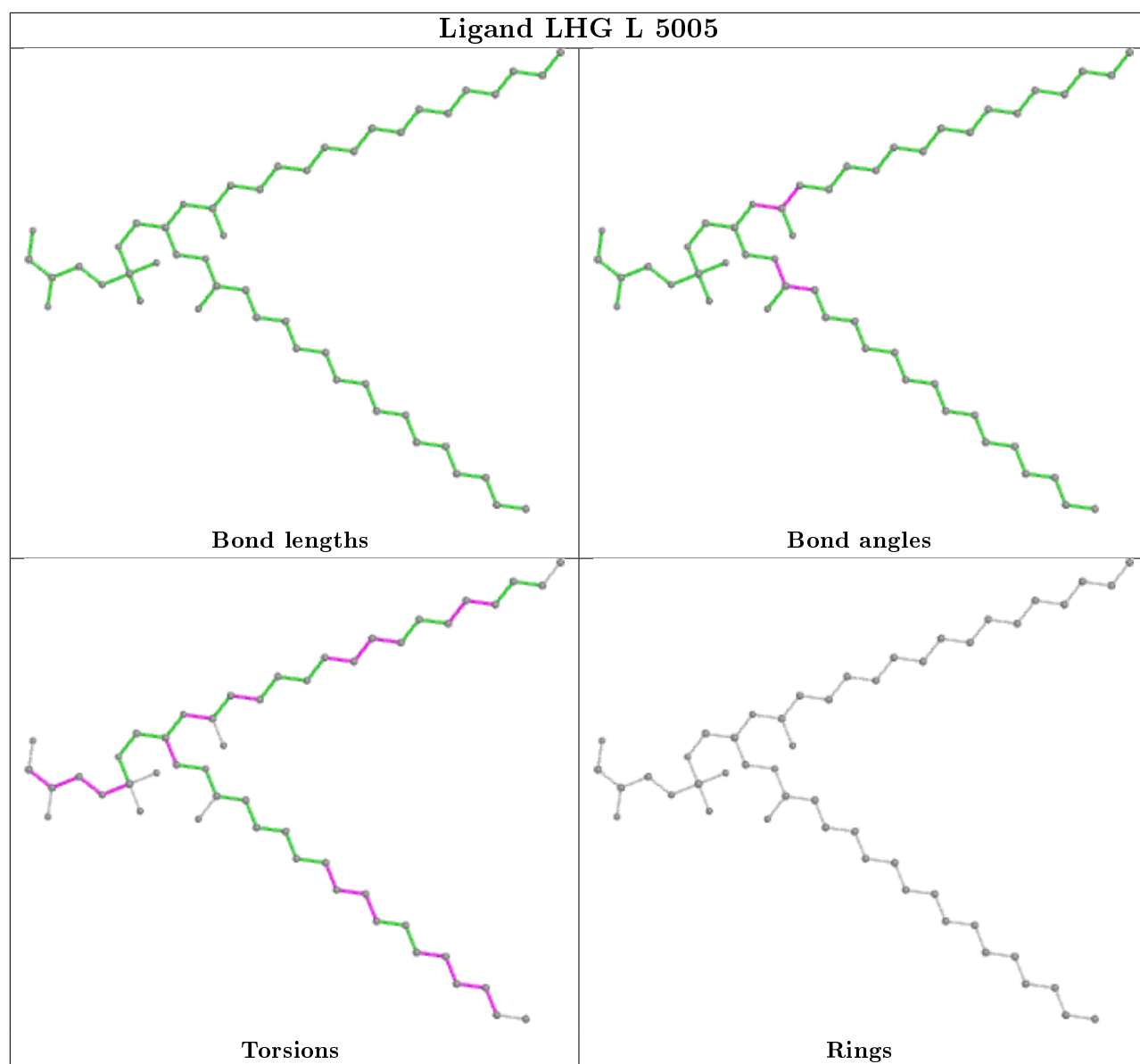


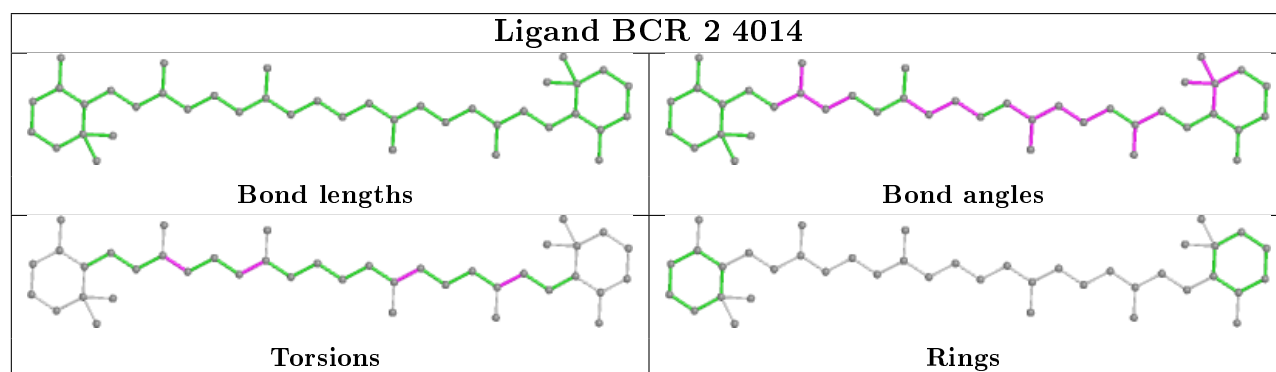
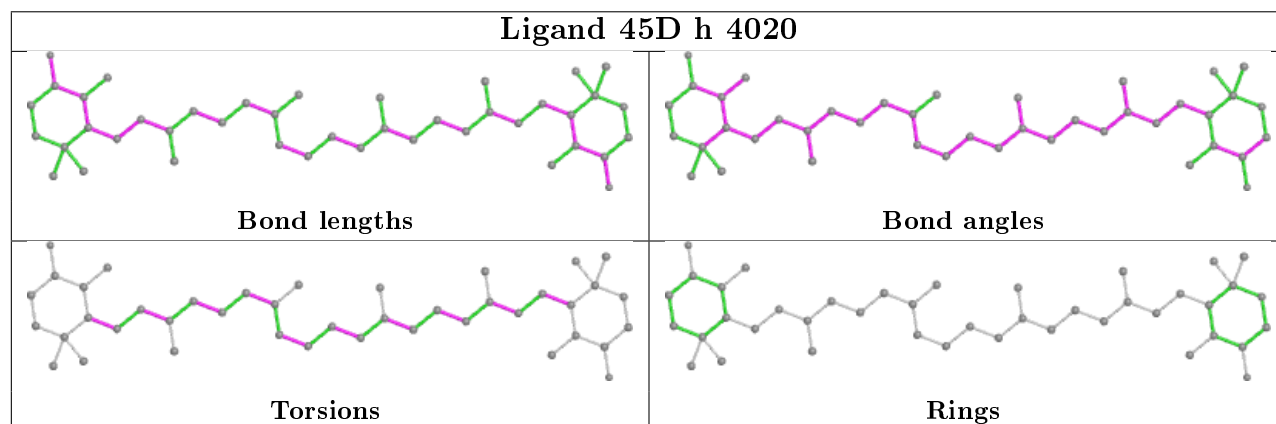
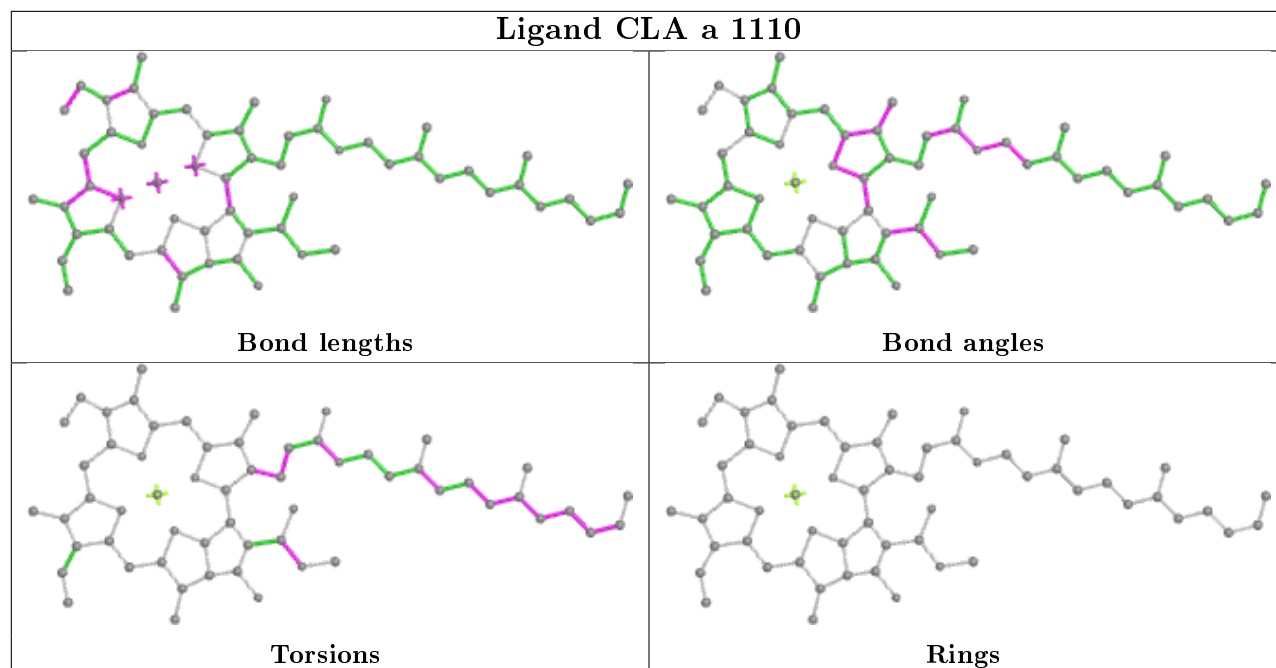
Ligand CLA A 1117**Ligand BCR B 4018****Ligand CLA A 1128**

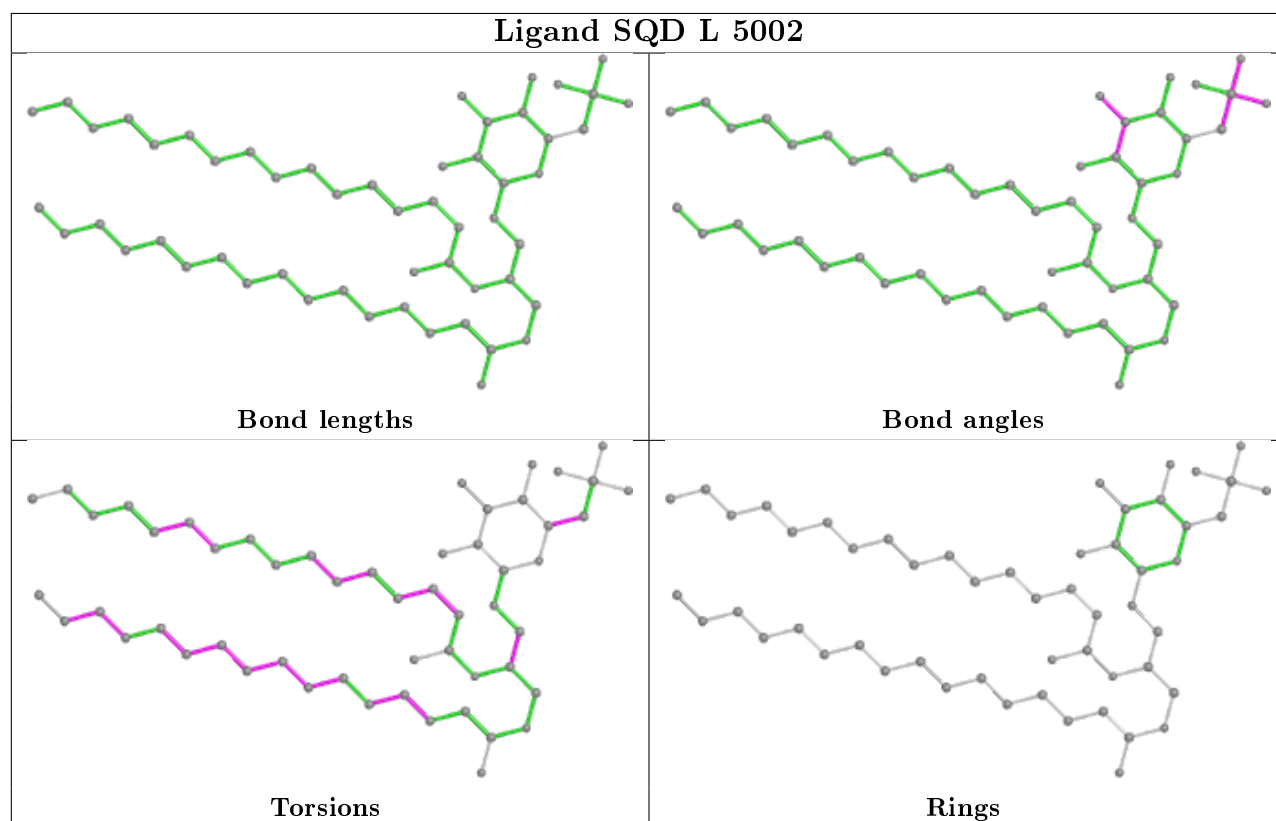
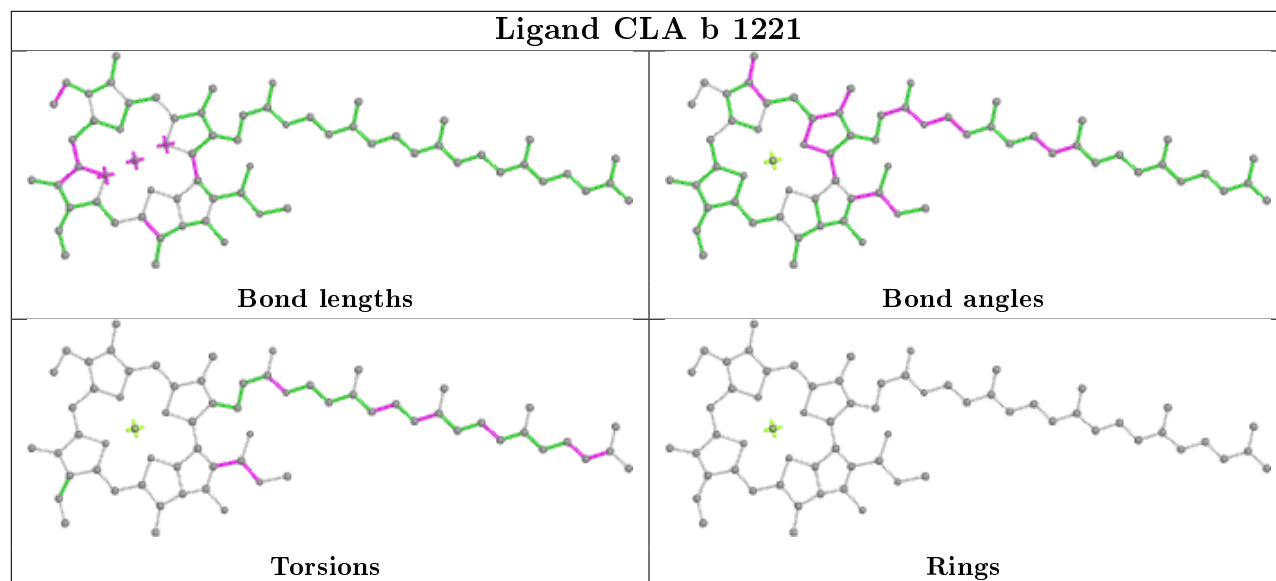
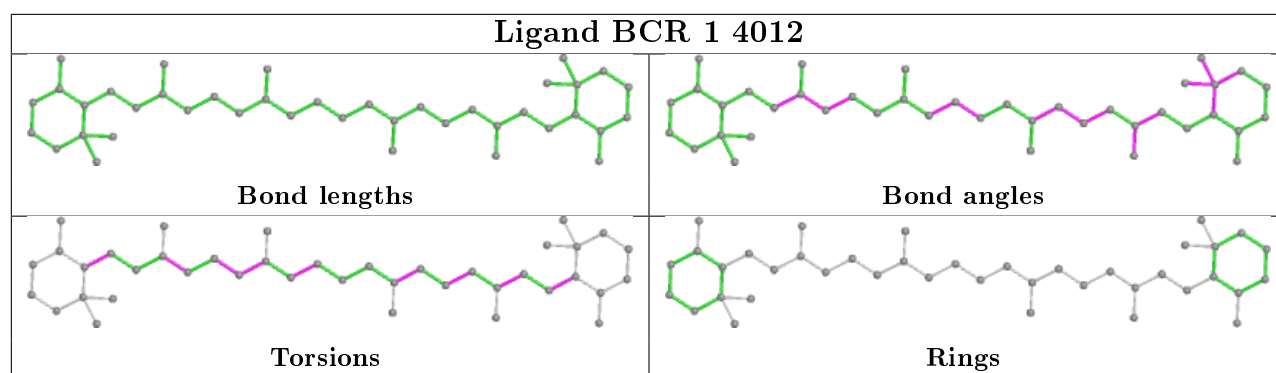


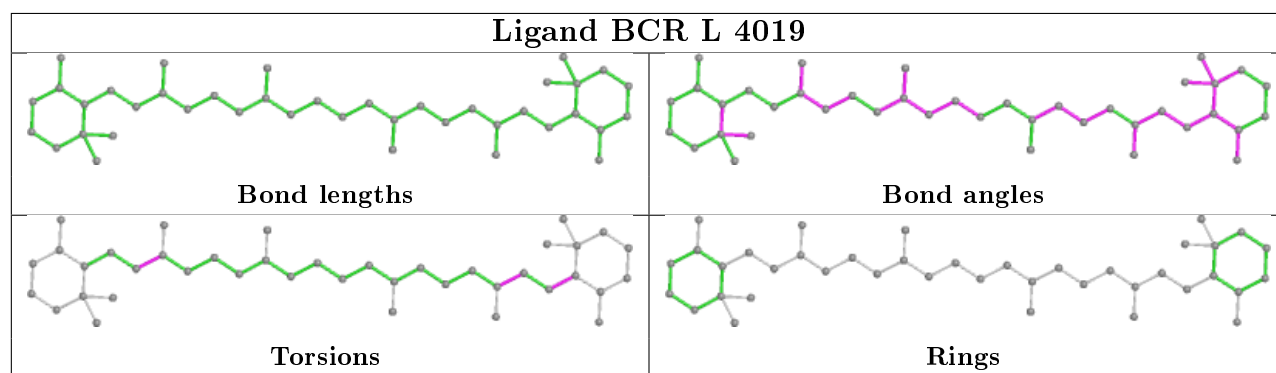
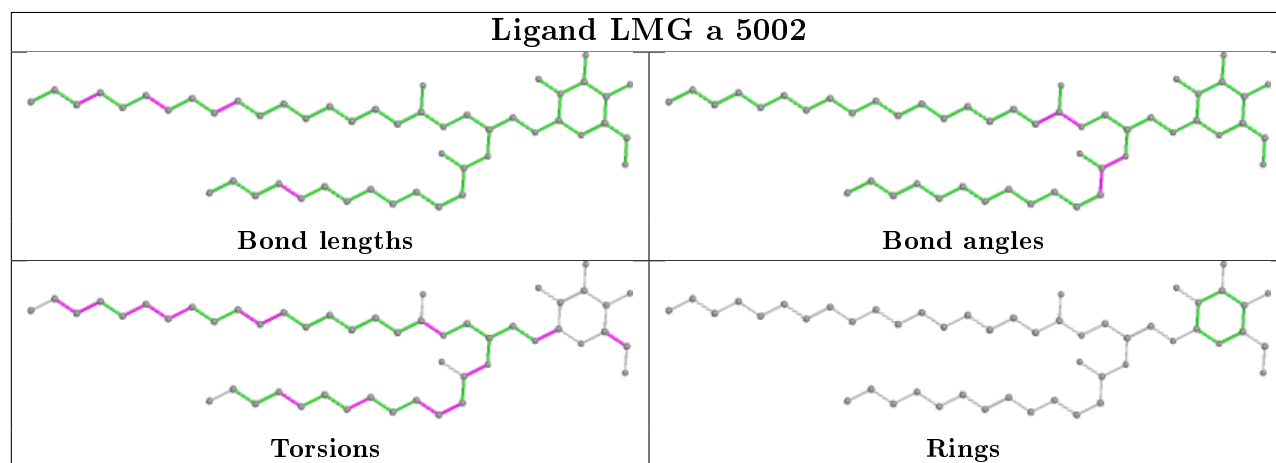
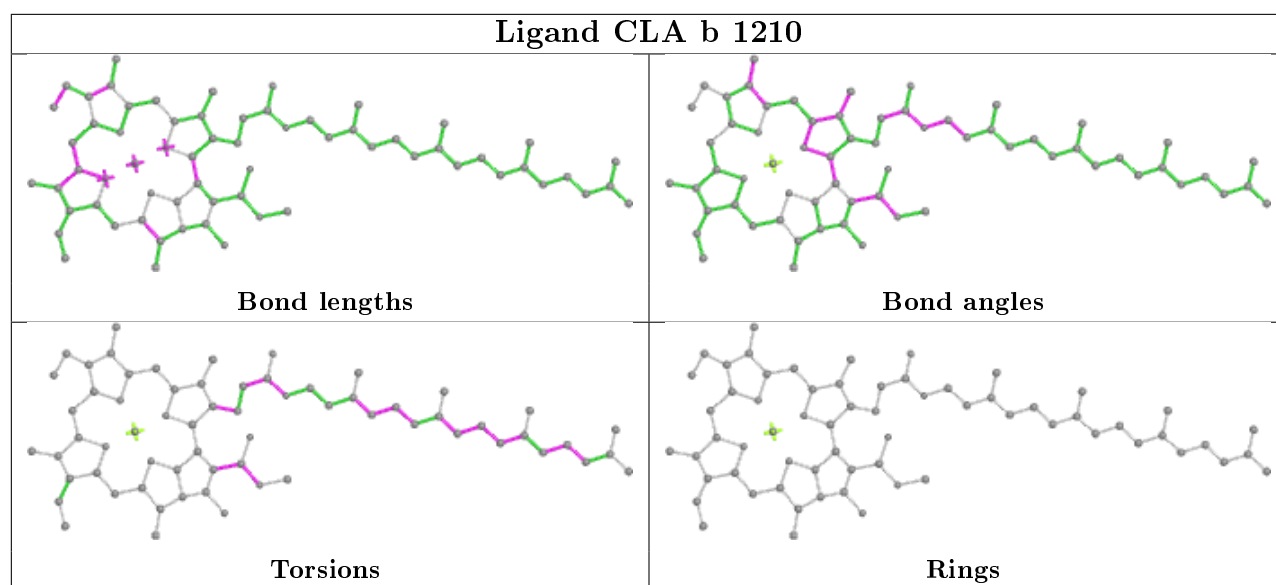


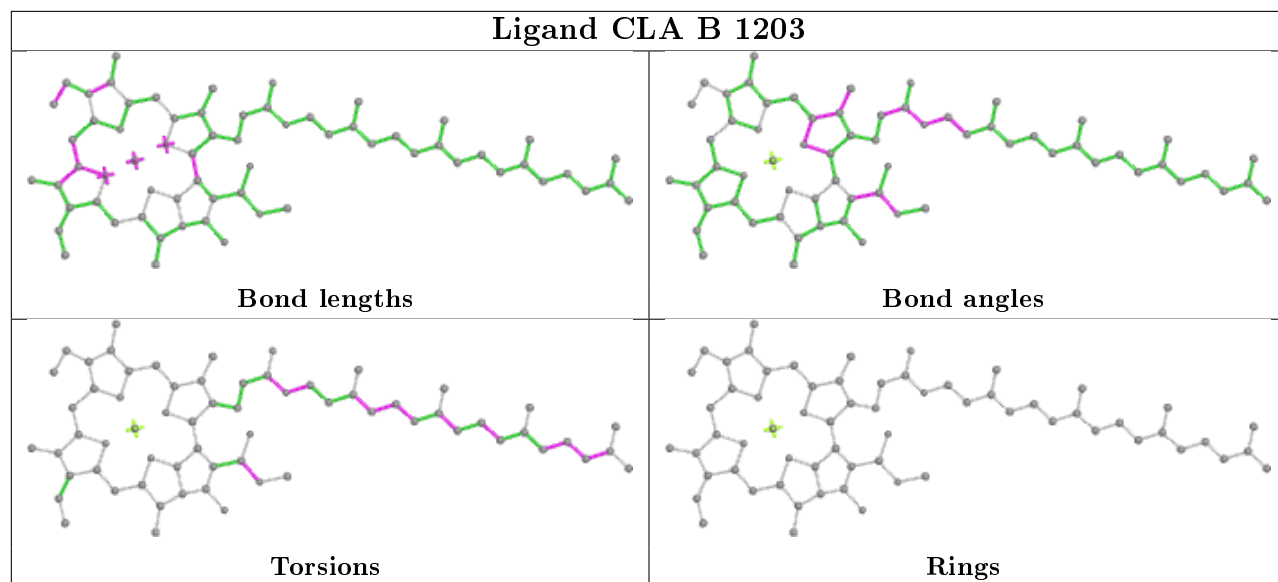
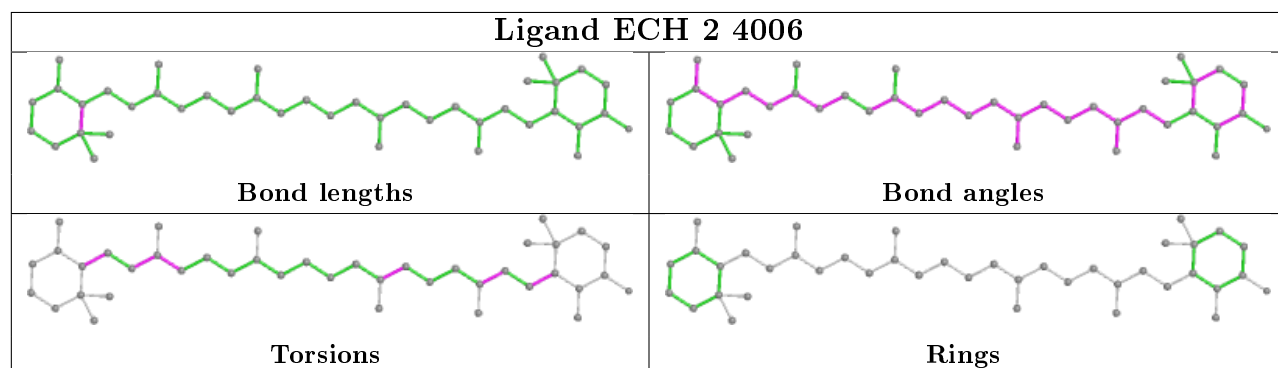
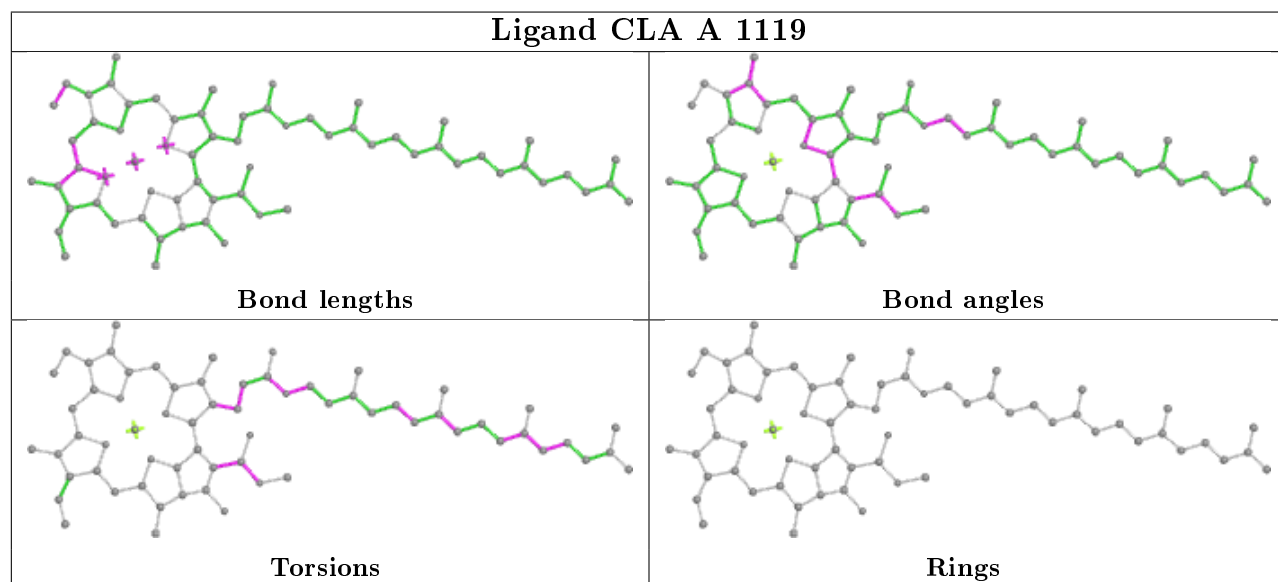


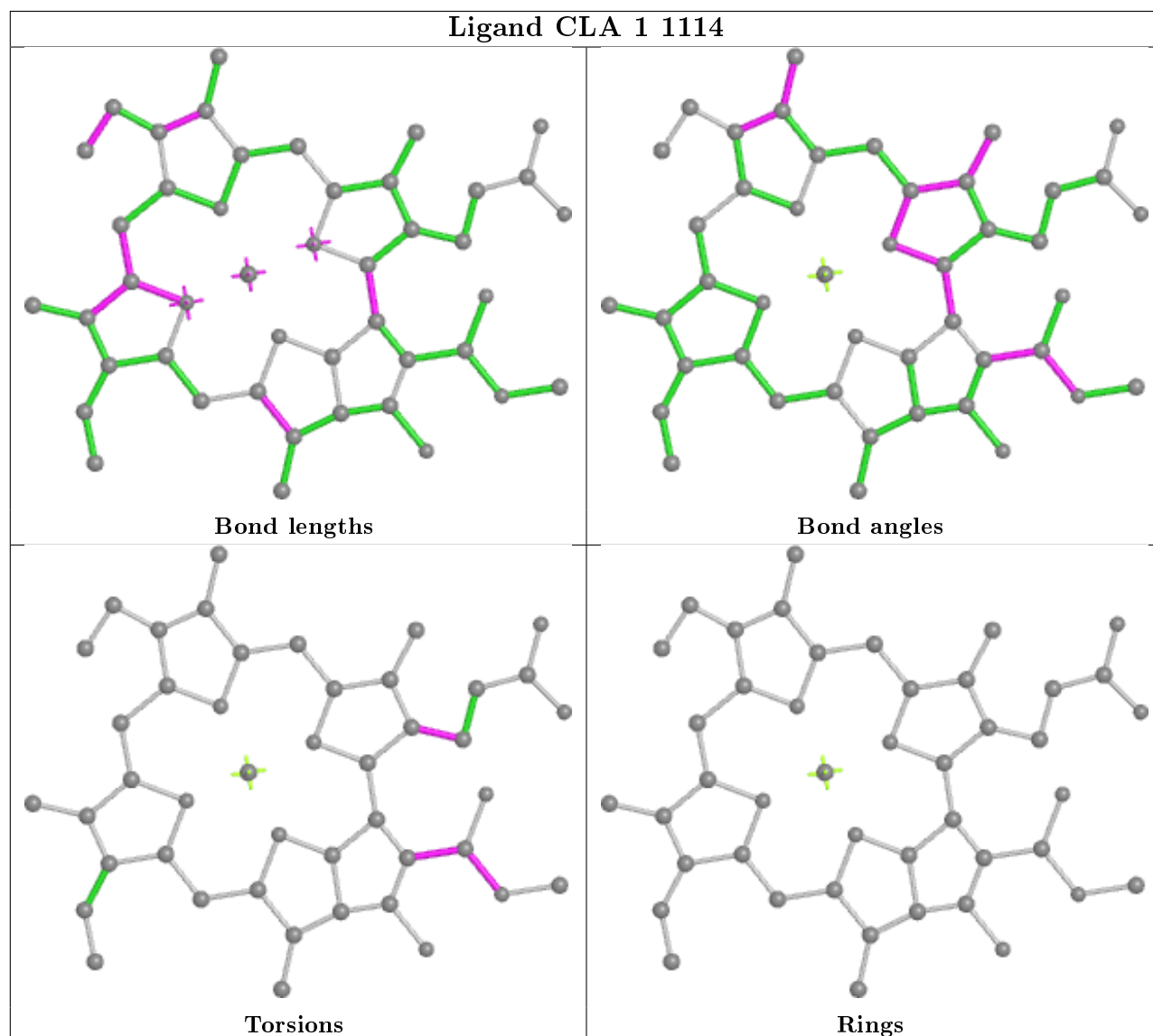
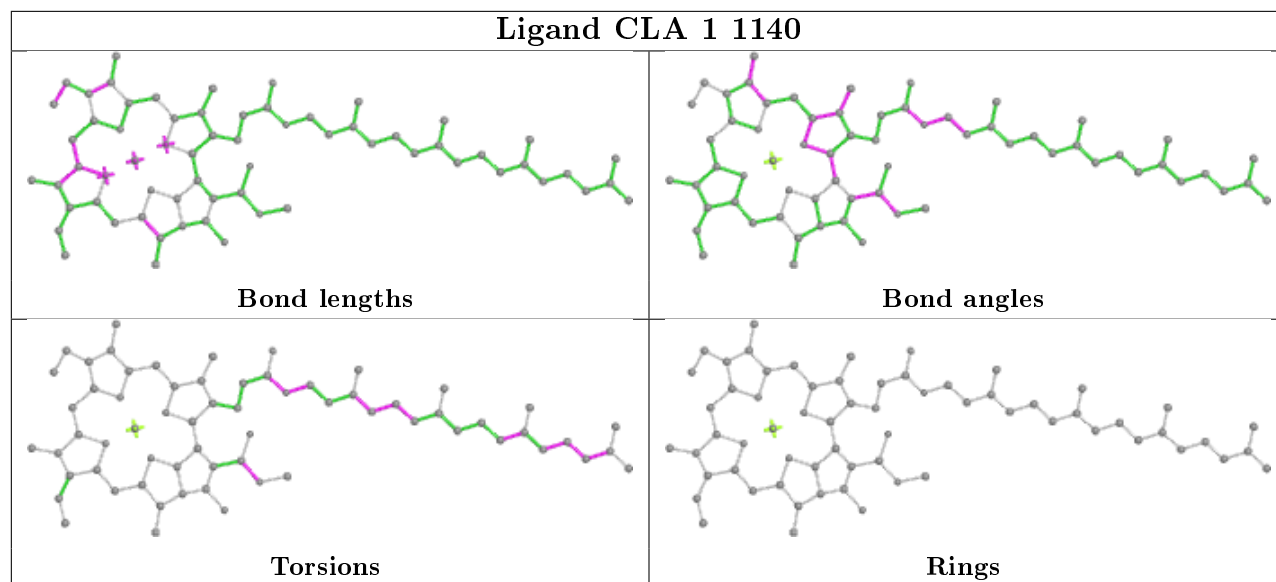


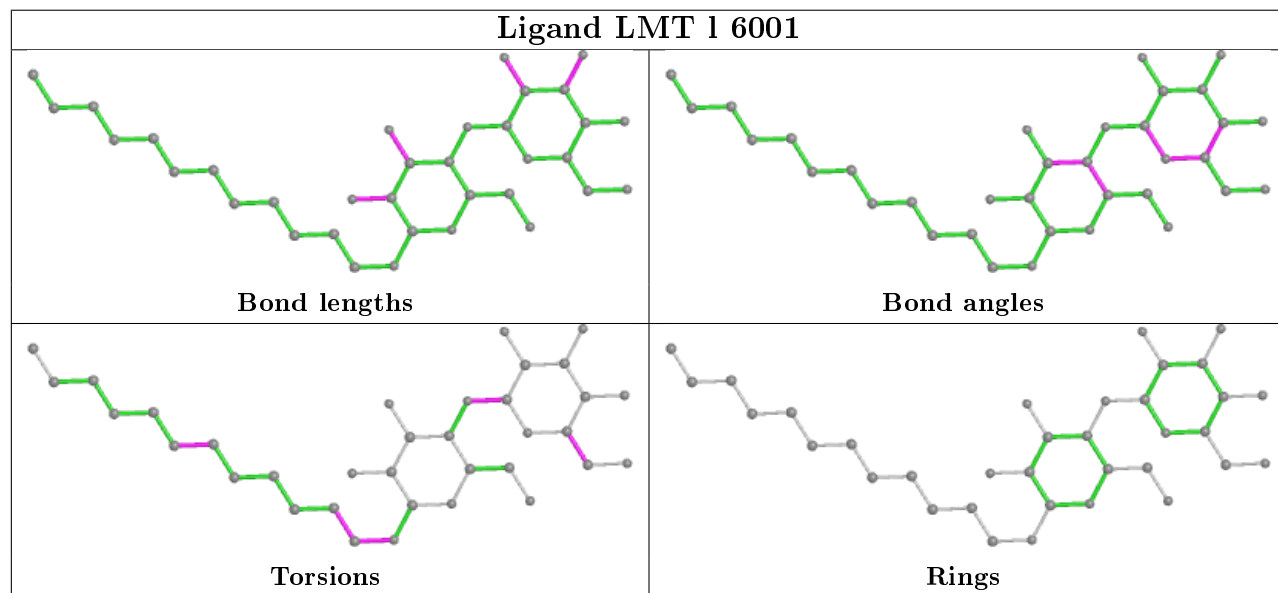
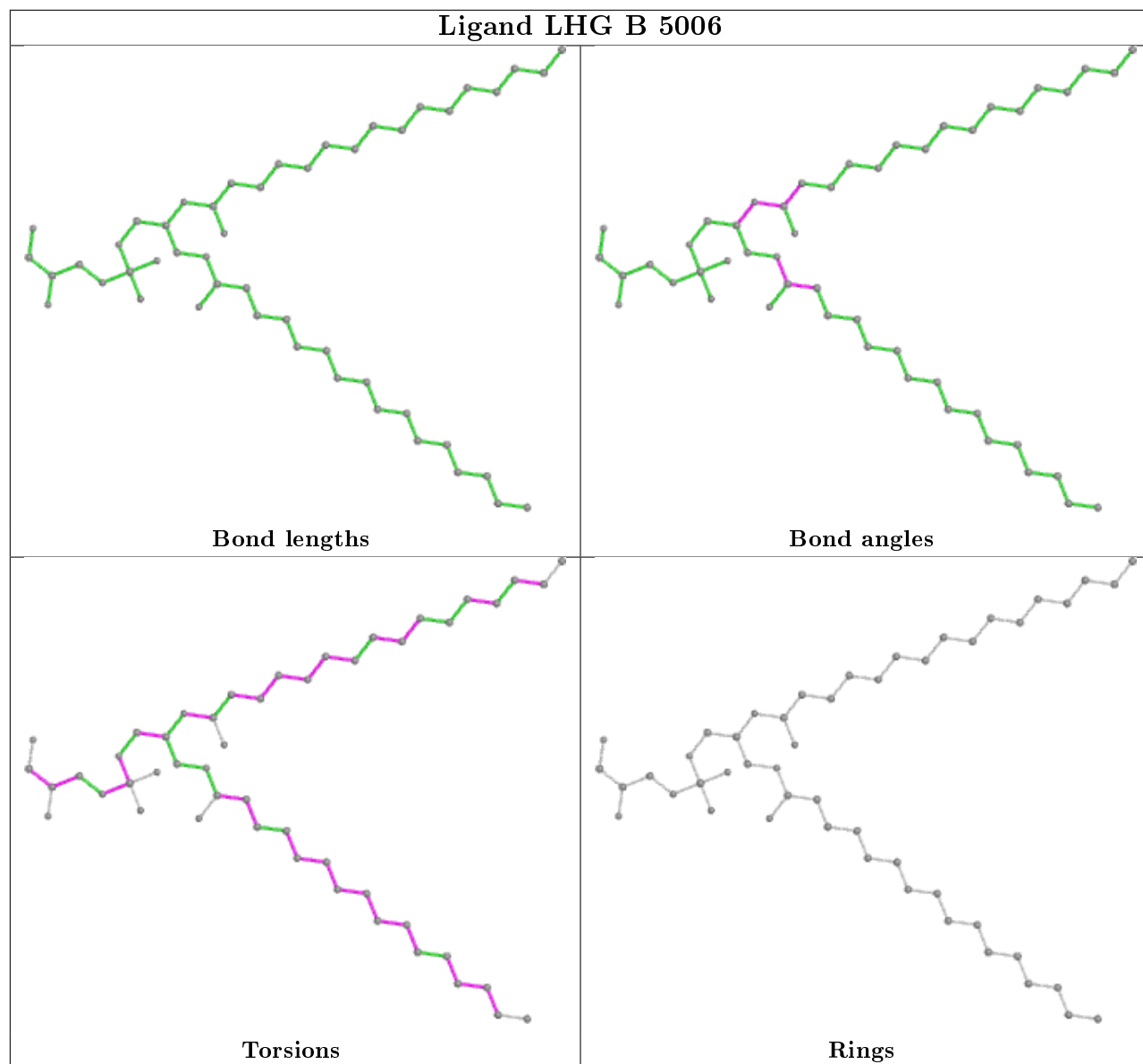


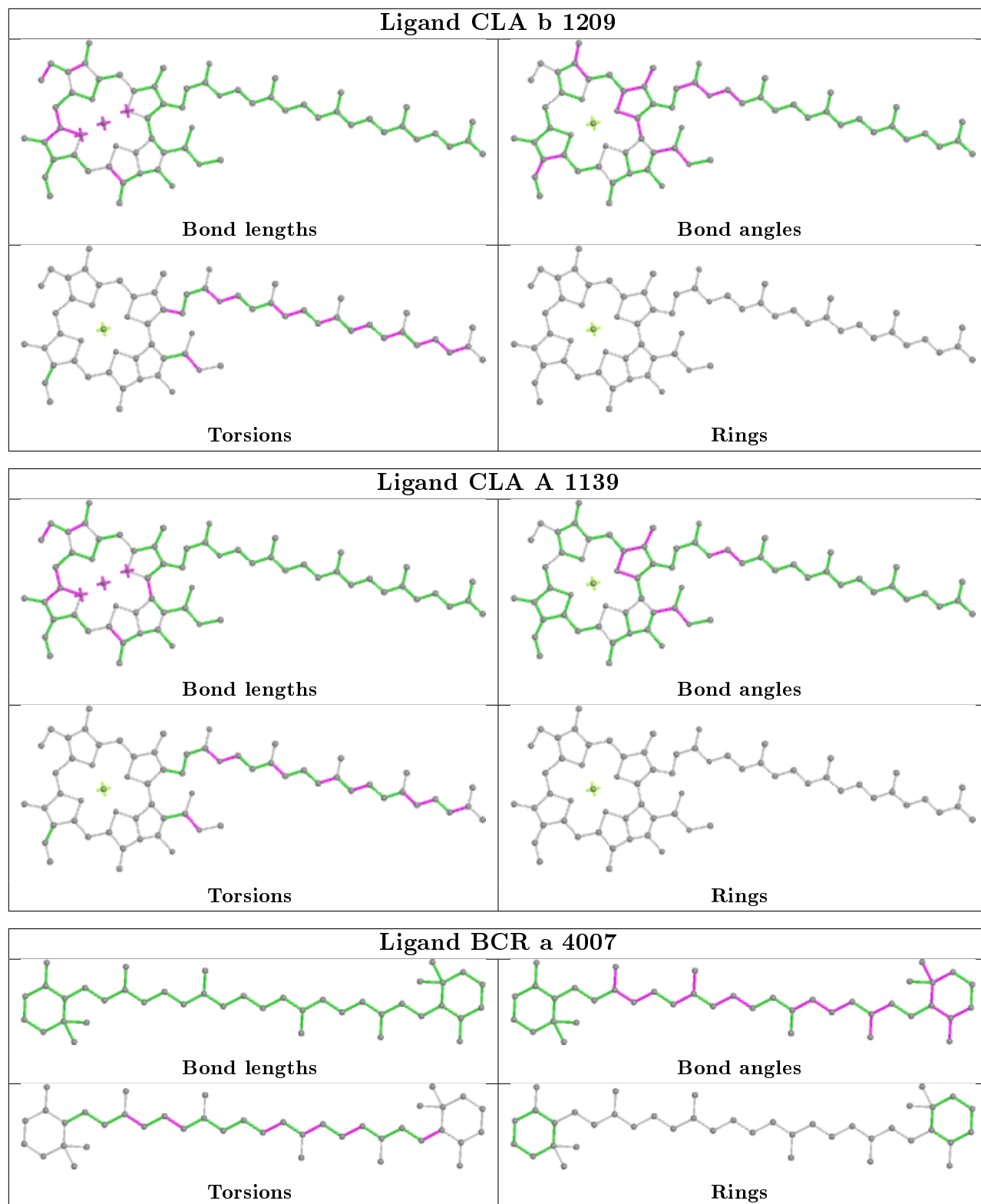


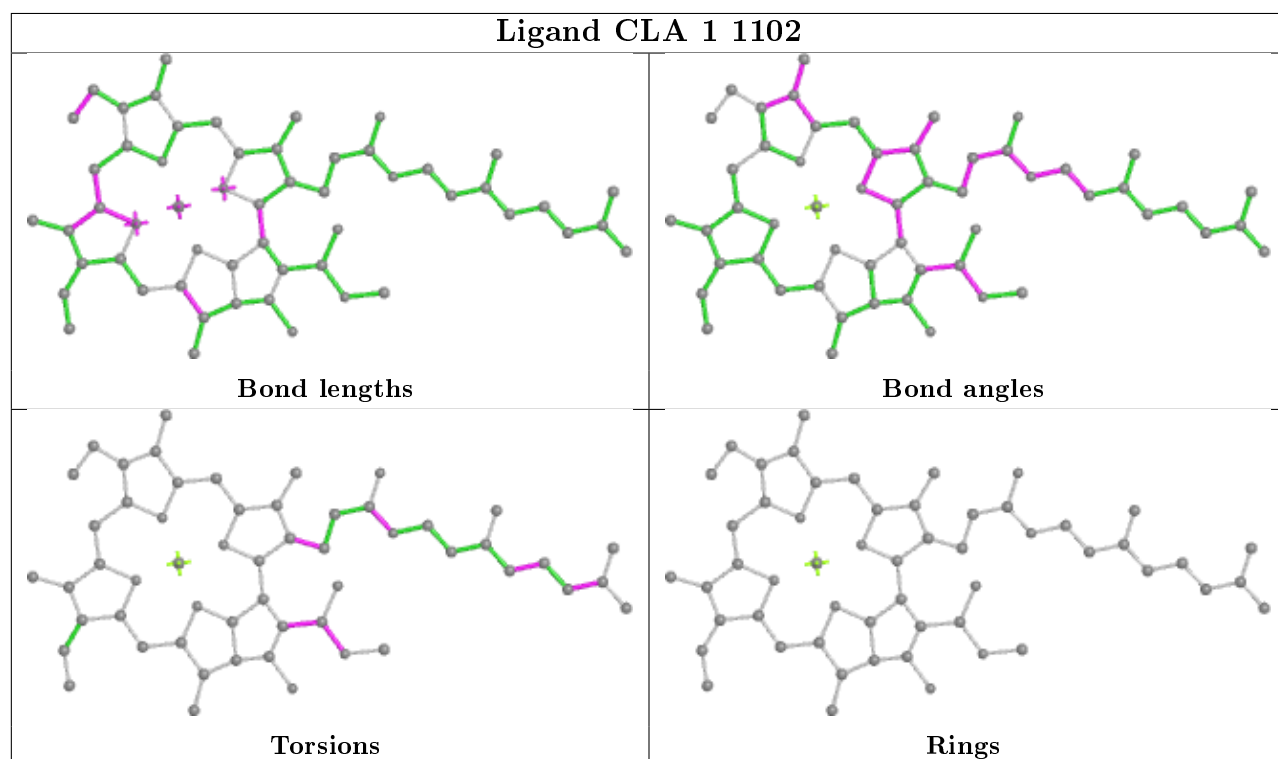
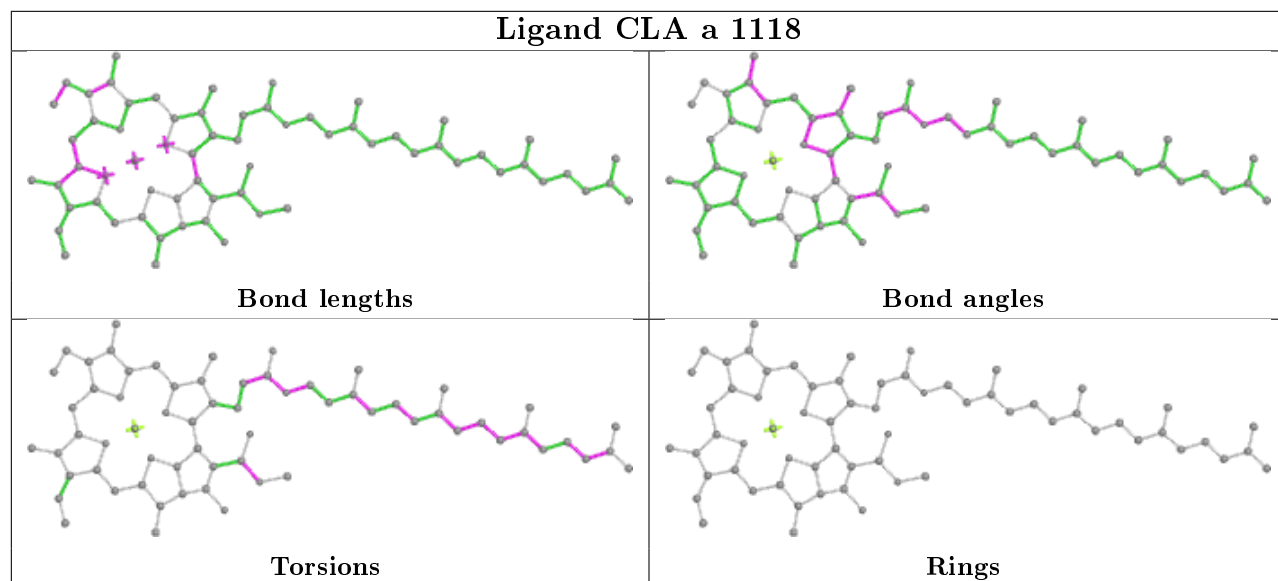
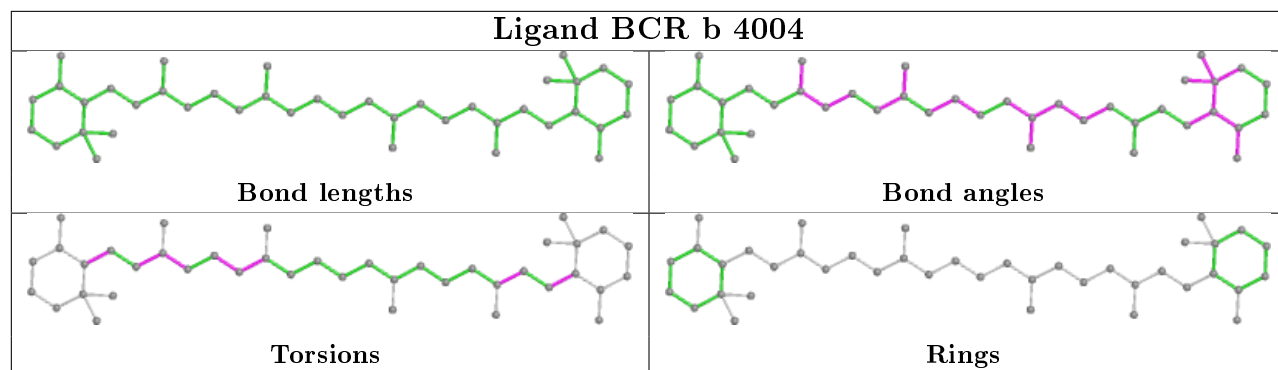


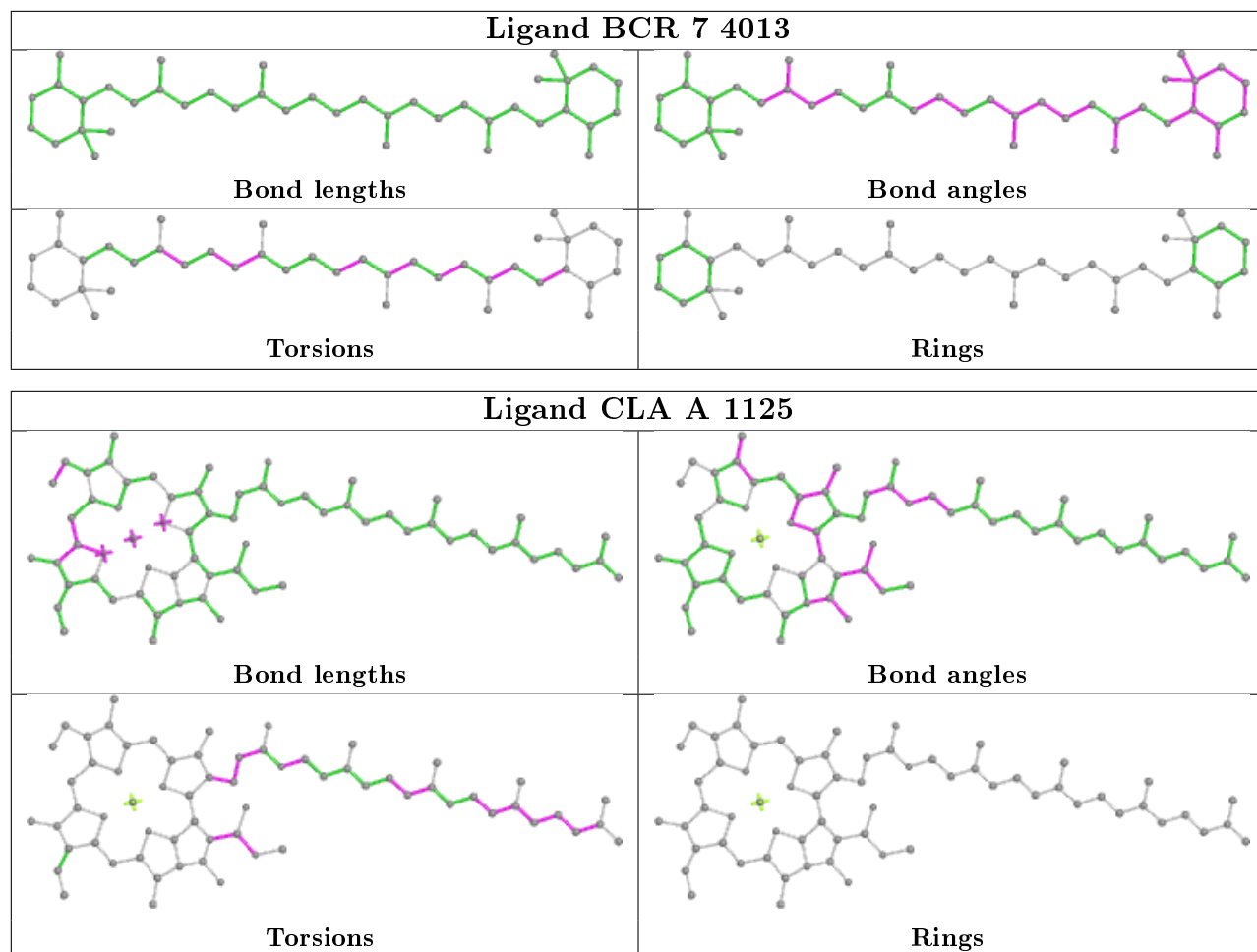
Ligand CLA B 1203**Ligand ECH 2 4006****Ligand CLA A 1119**

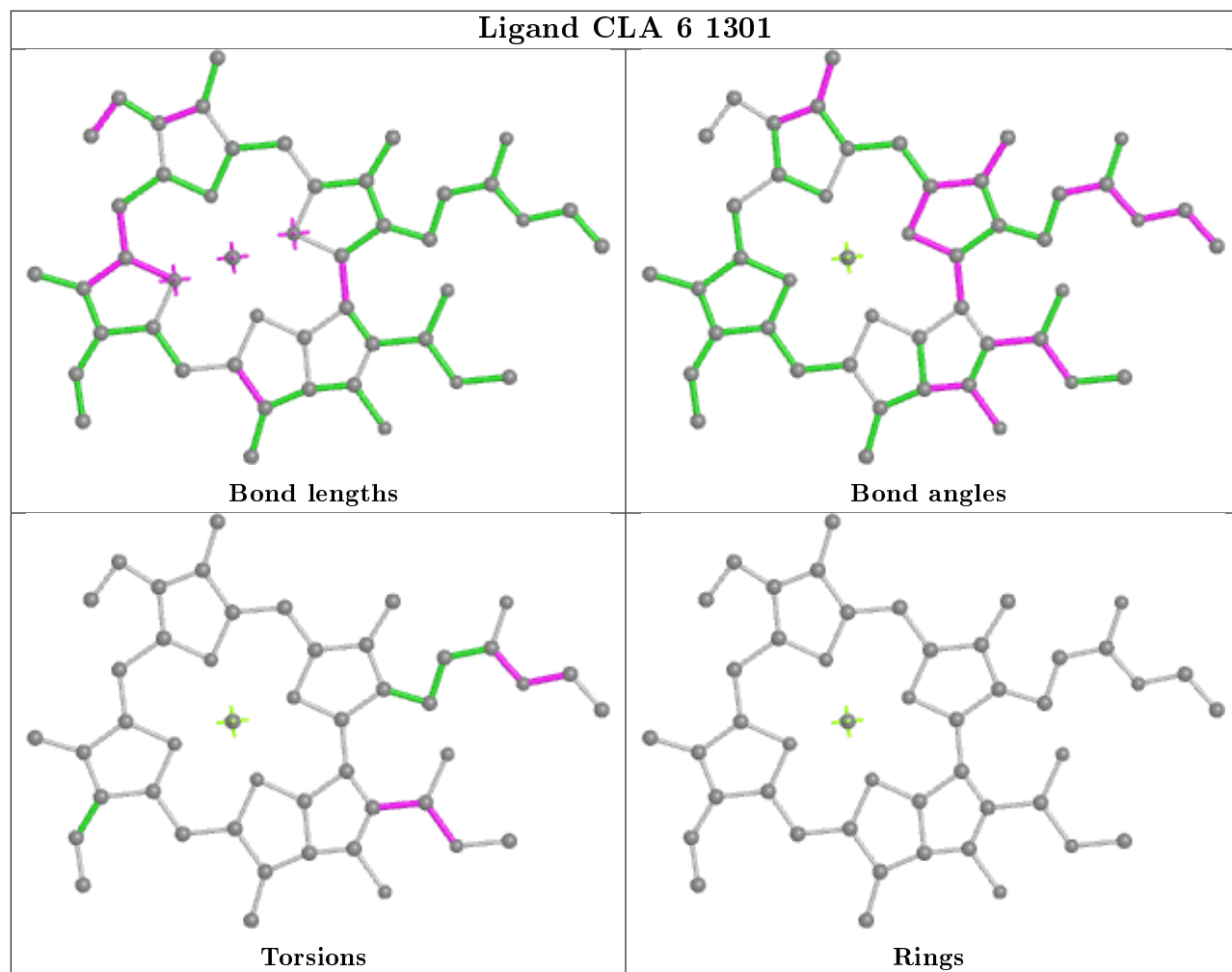


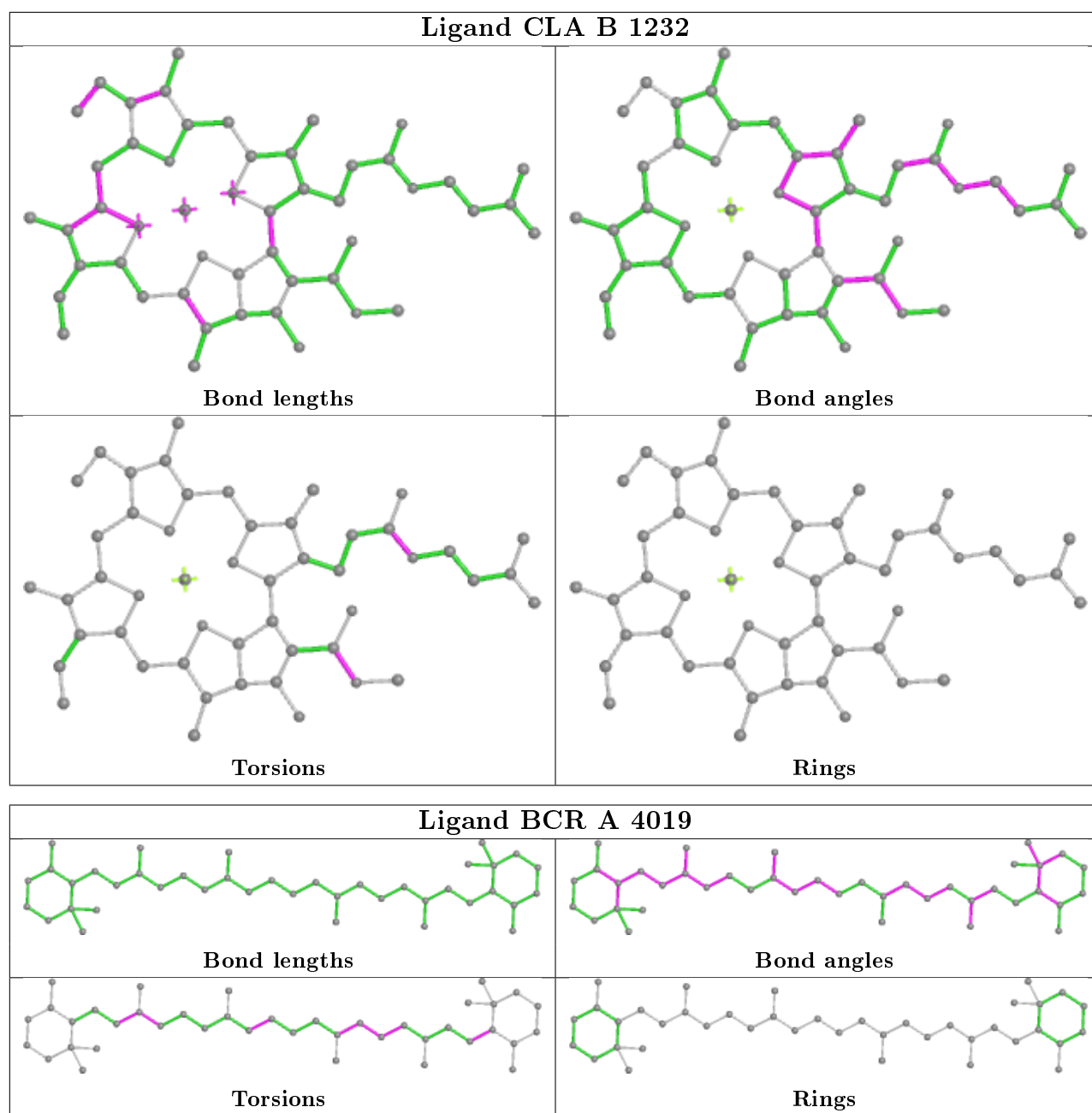


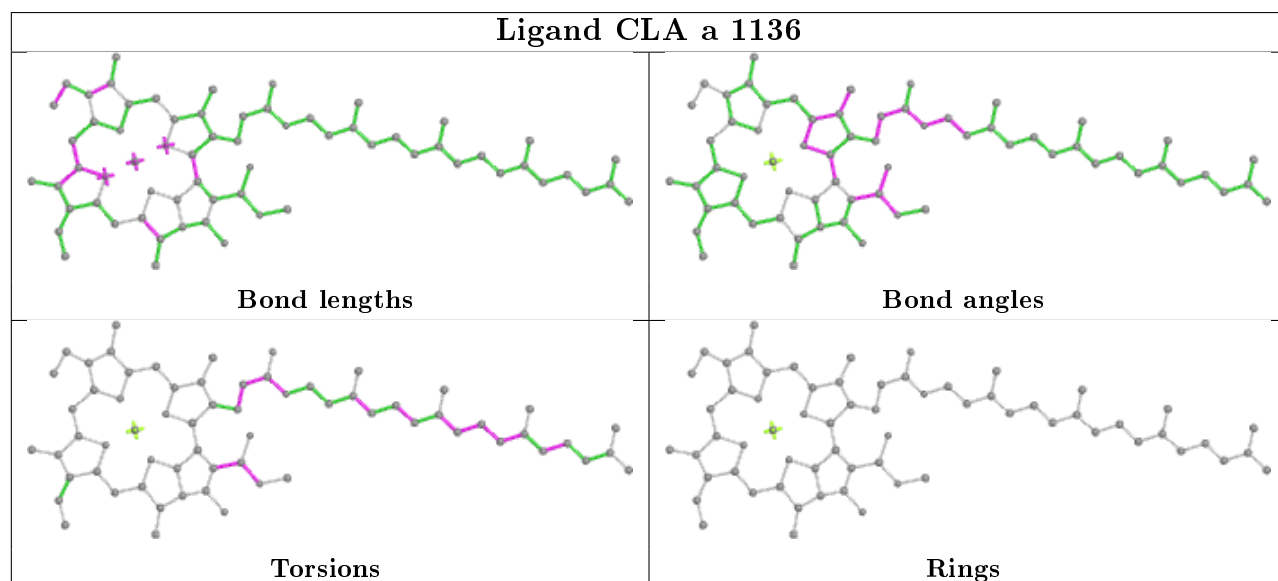
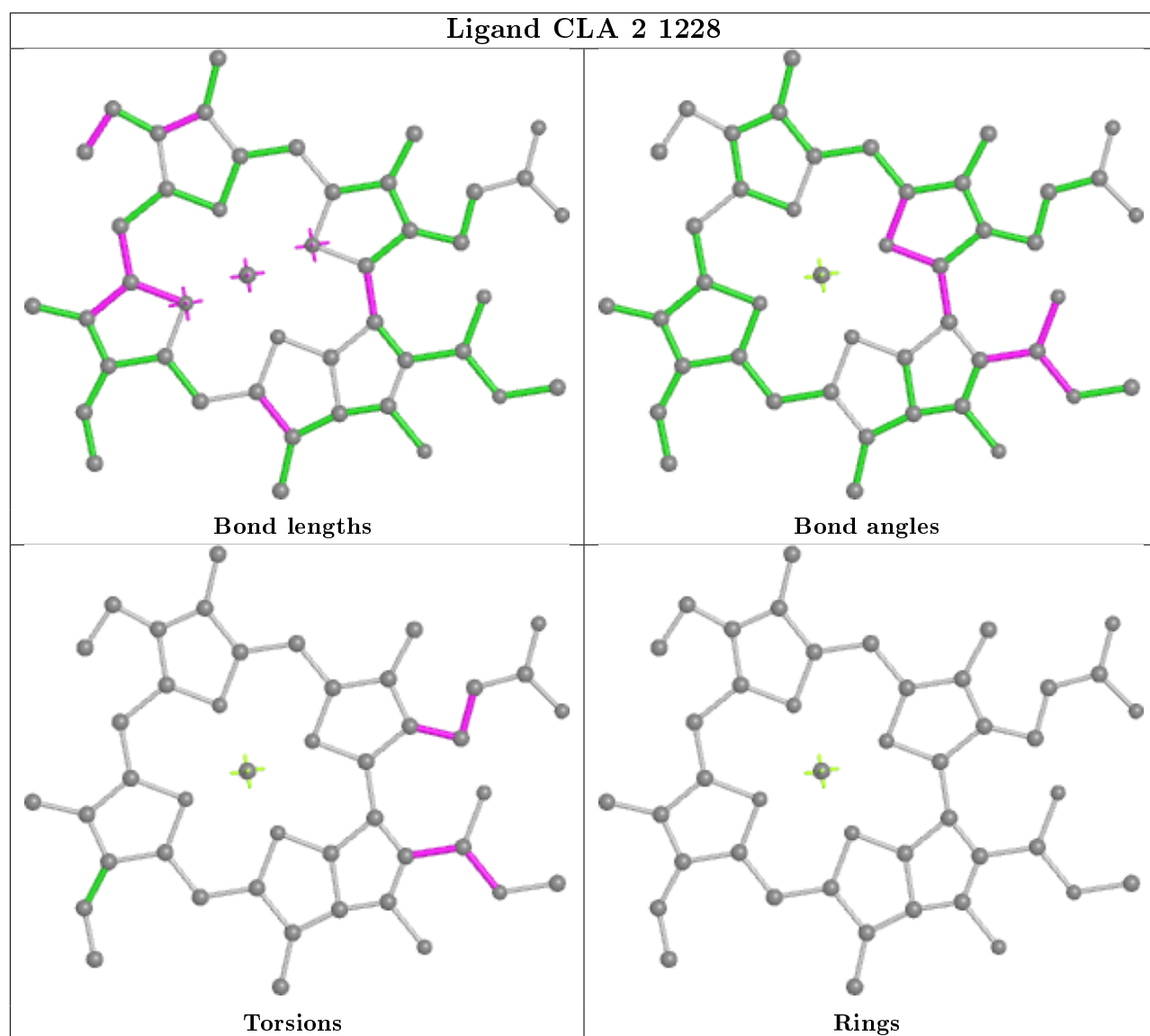


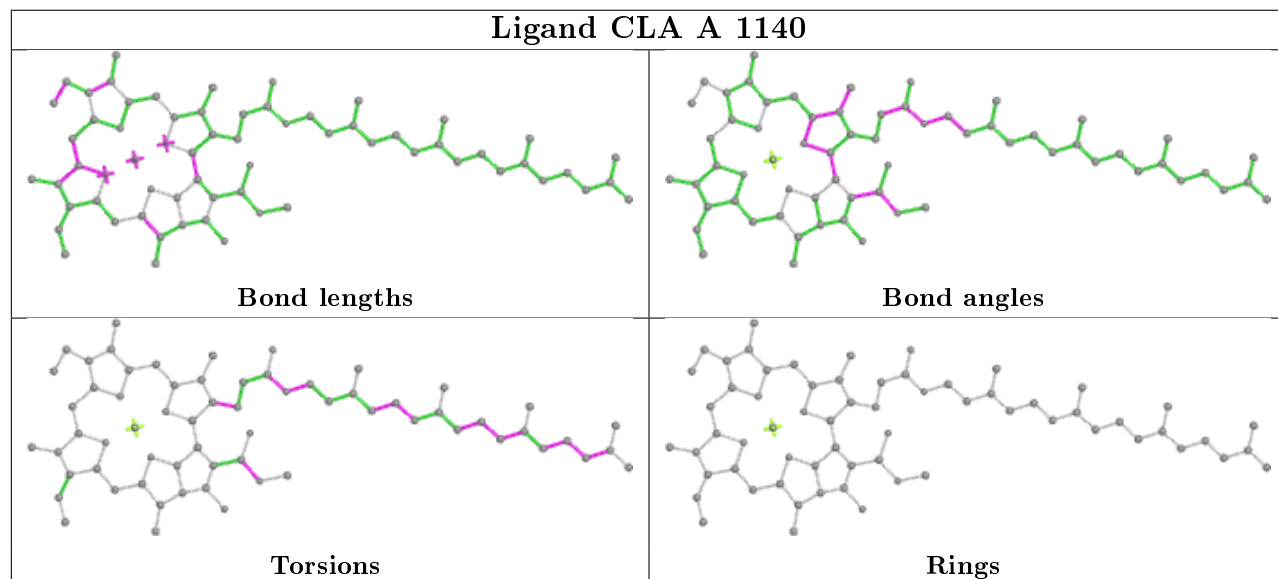
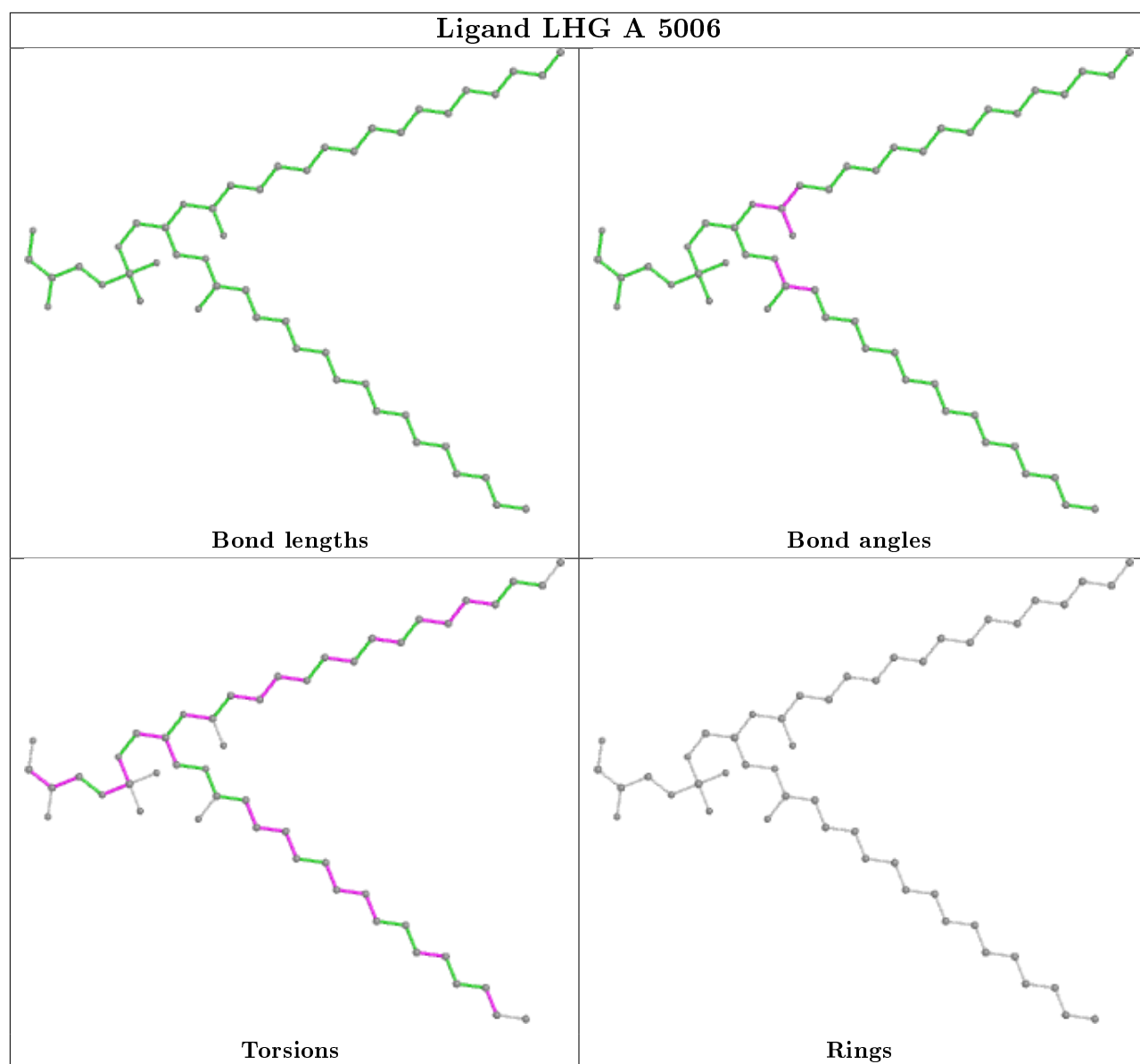


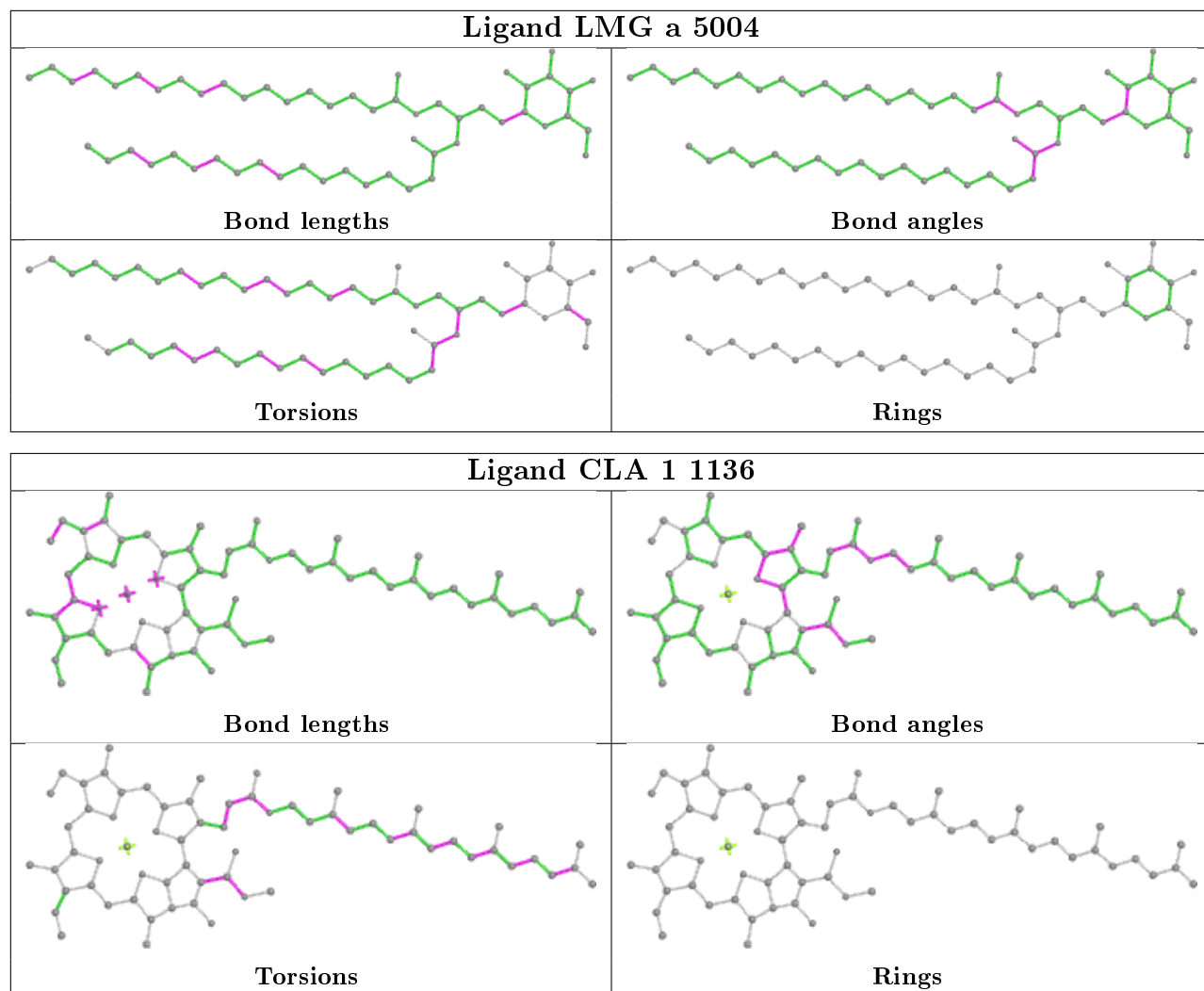


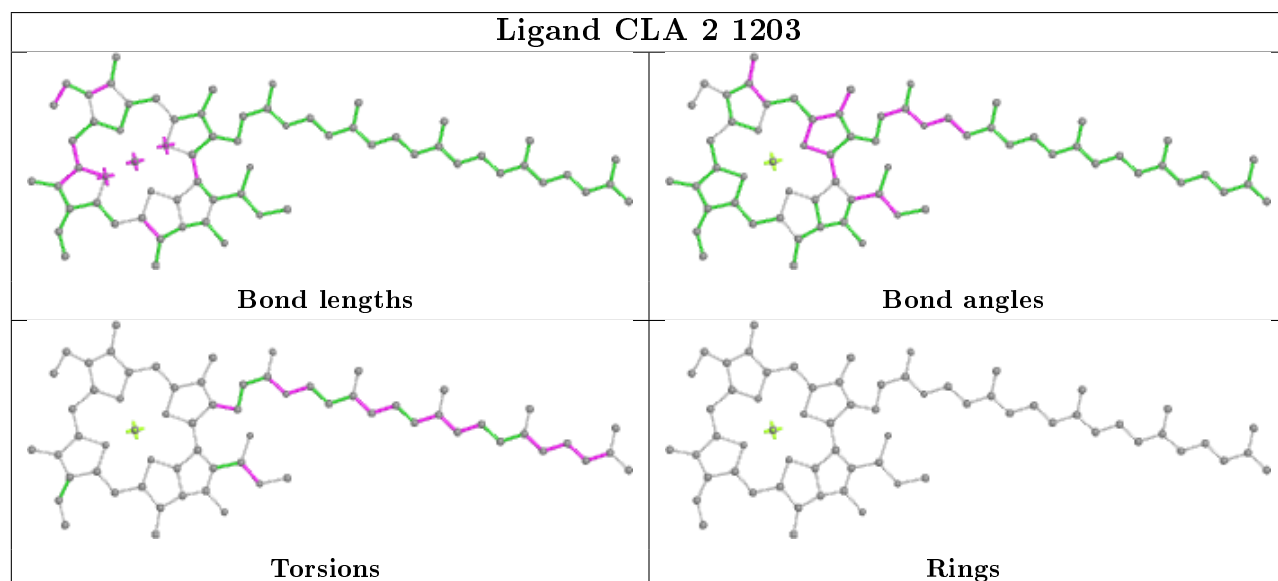
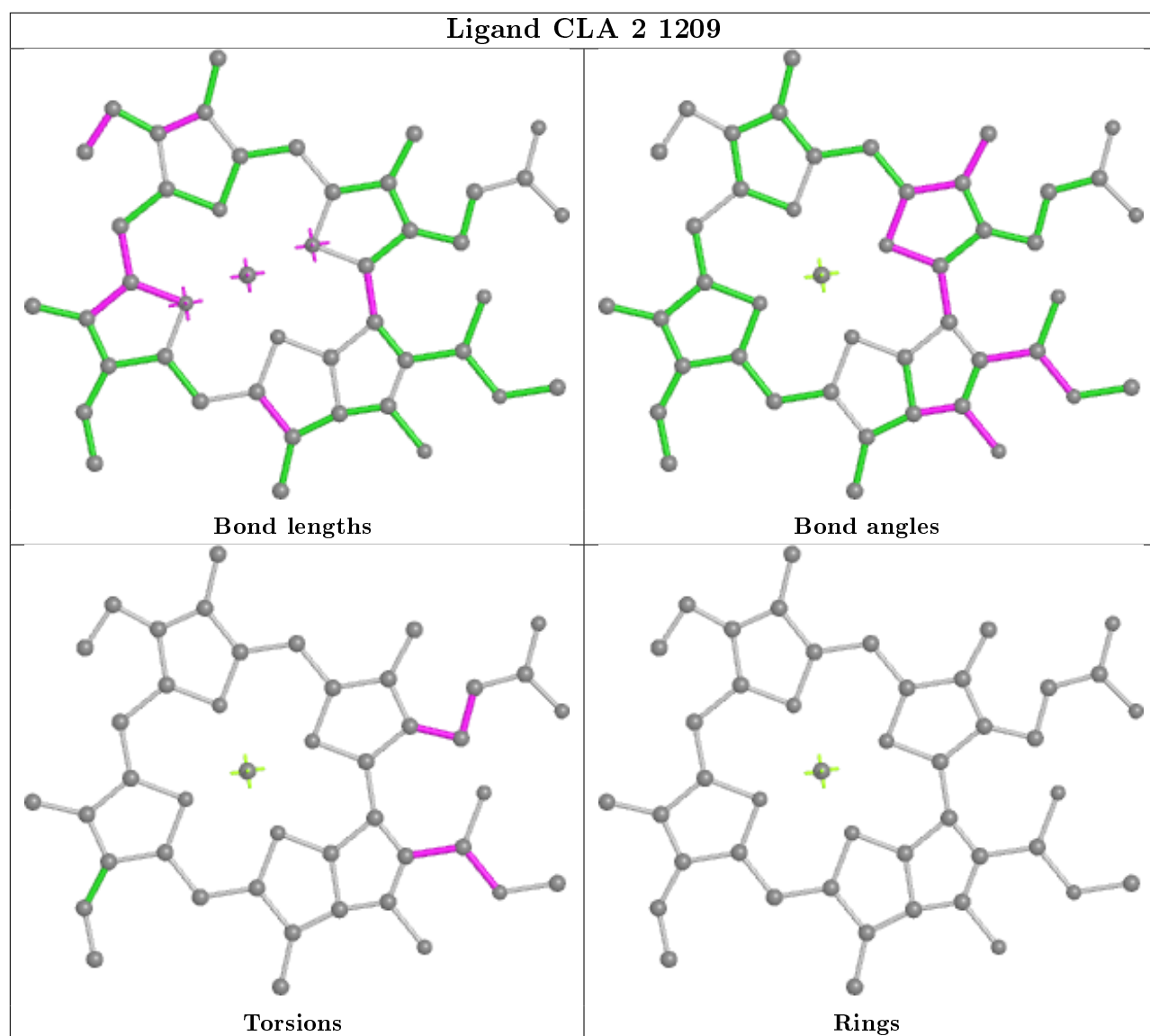


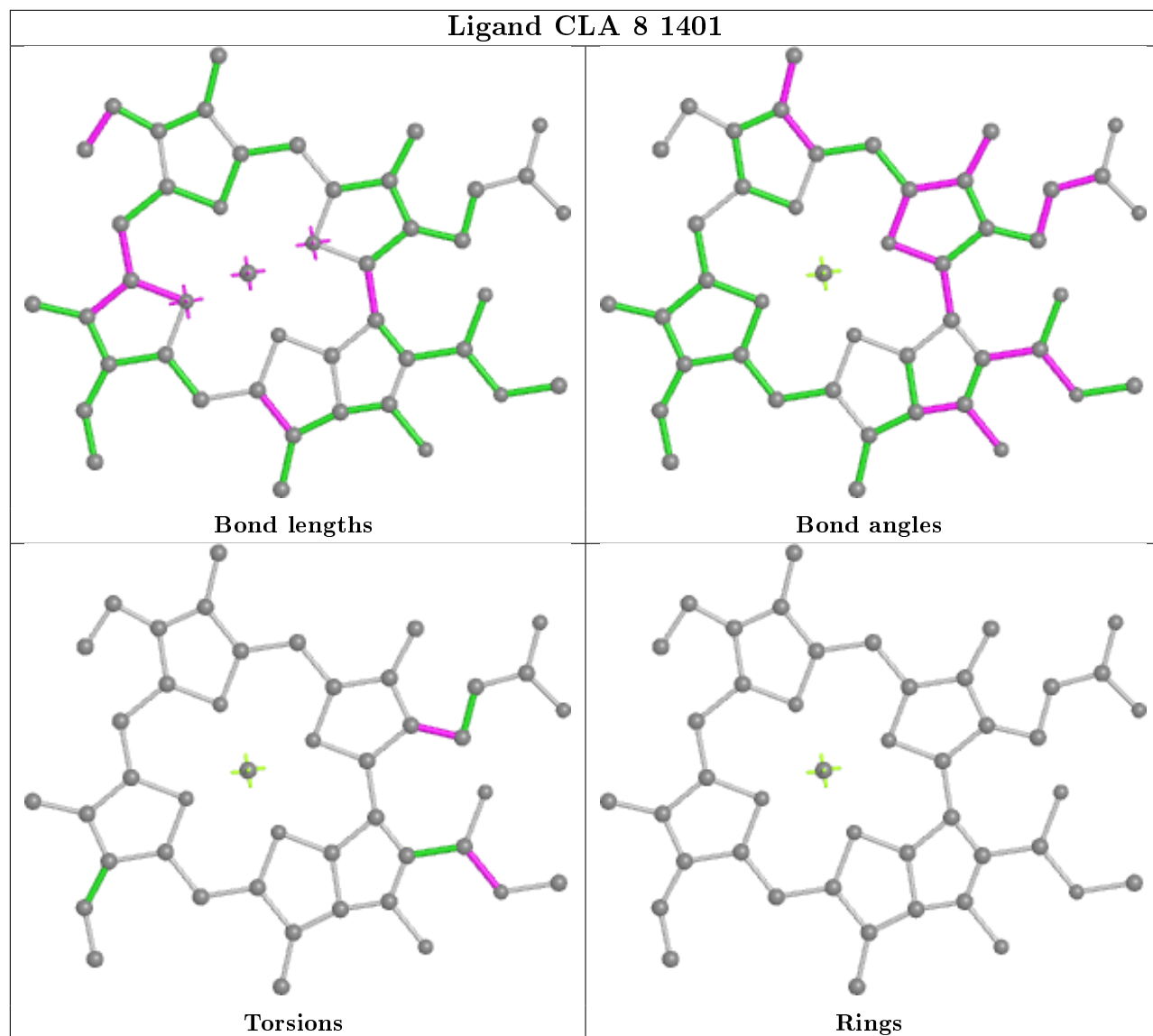




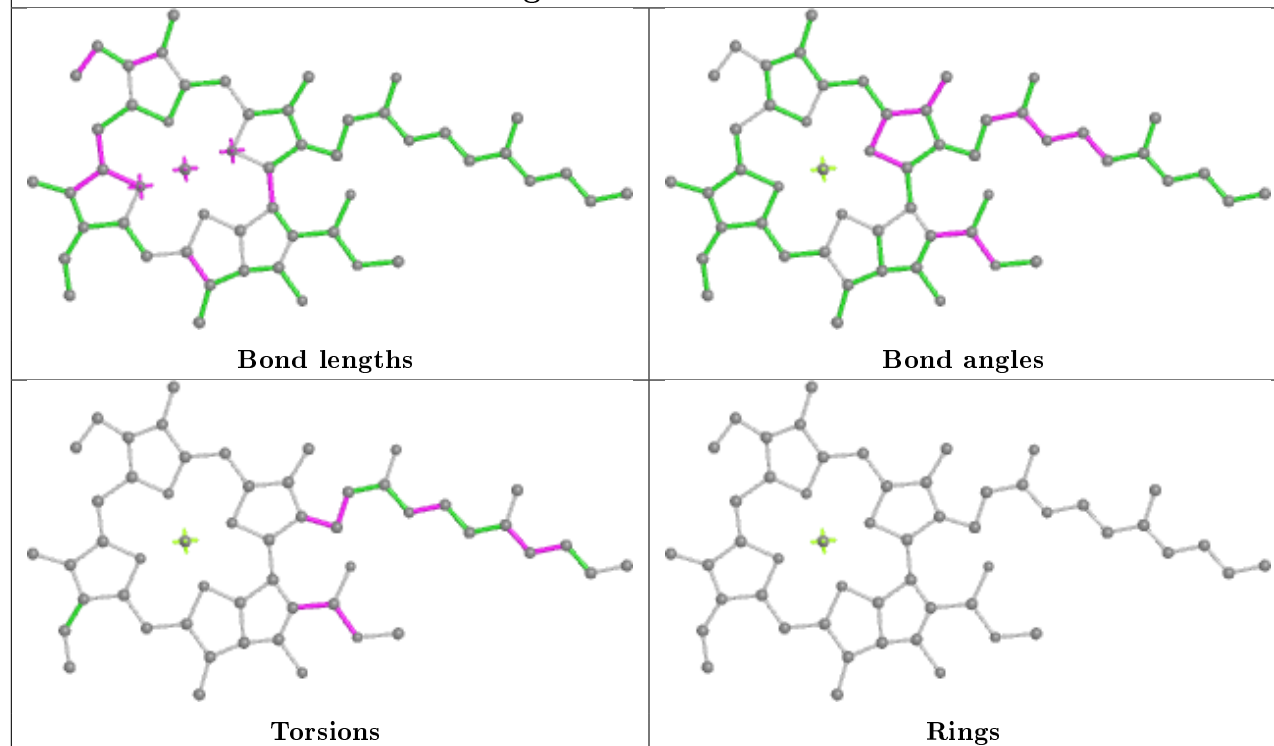




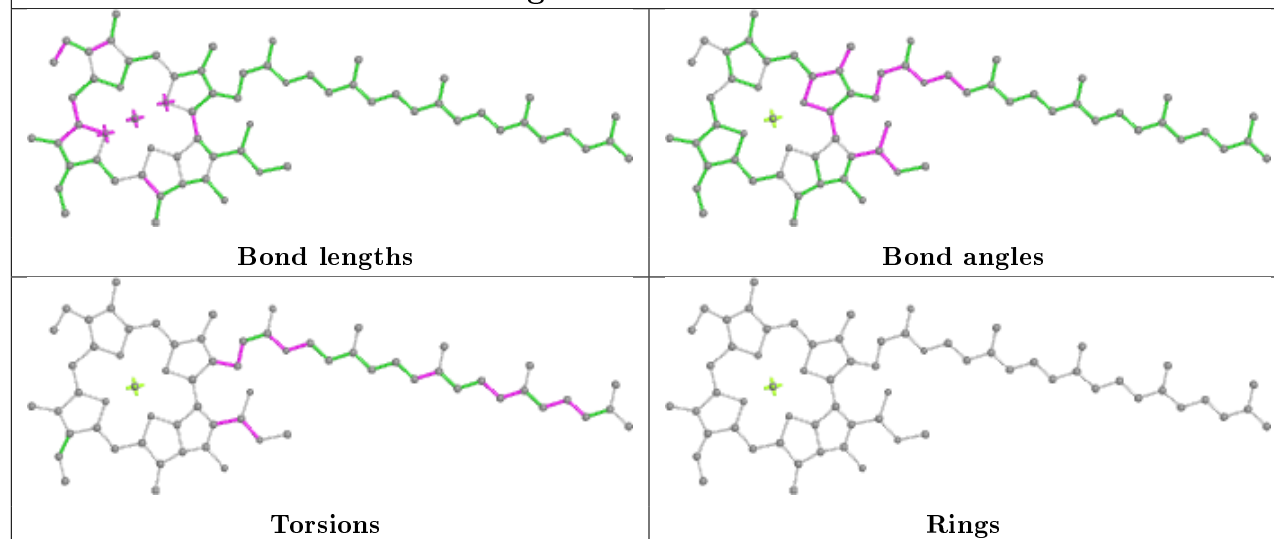


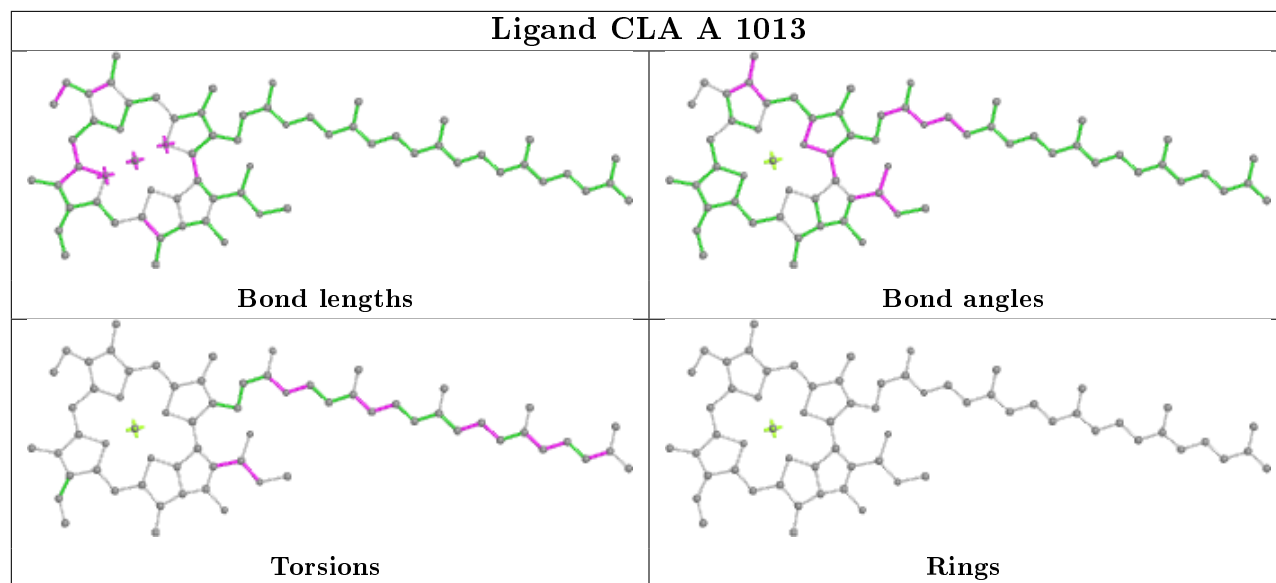
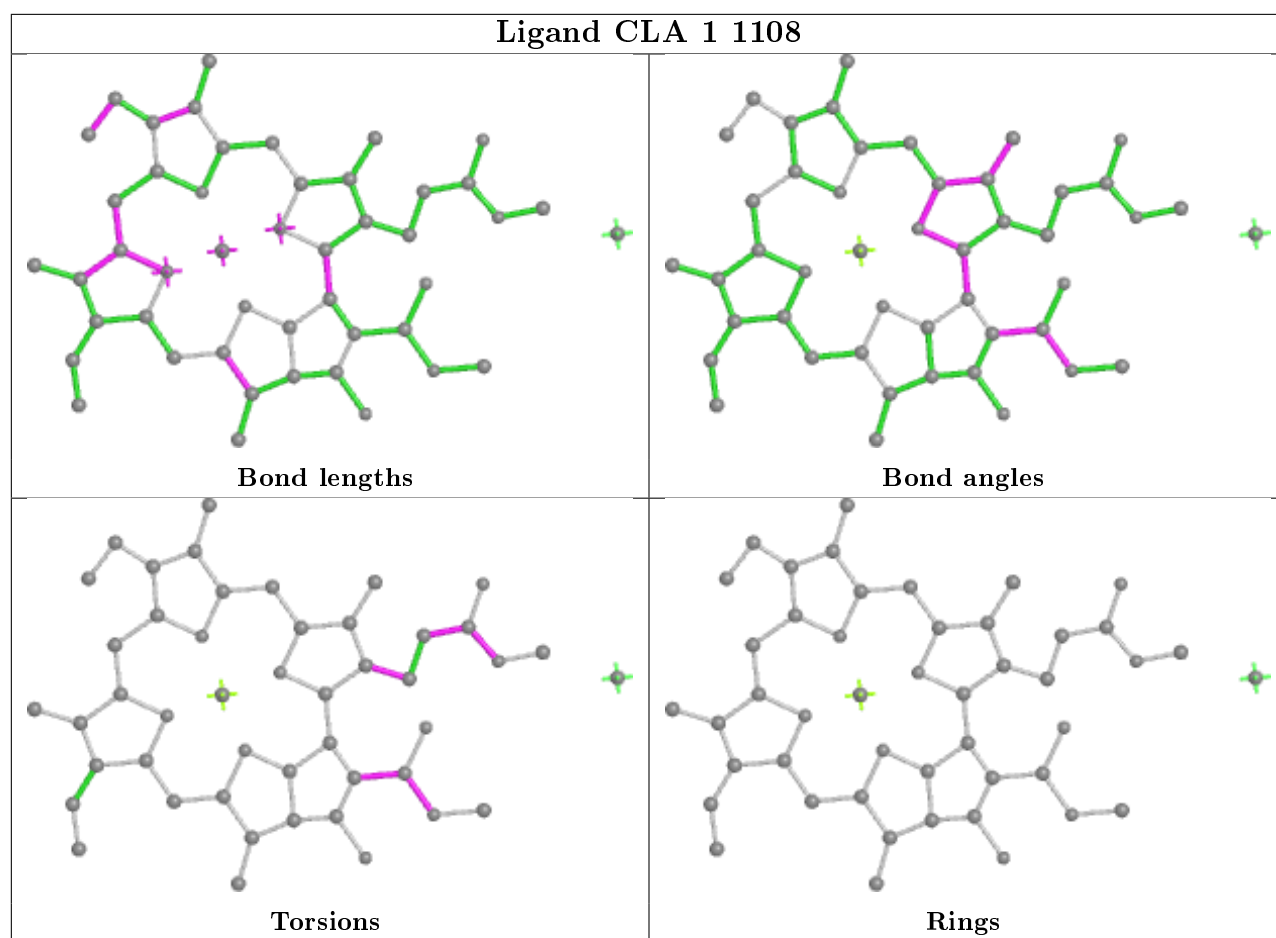


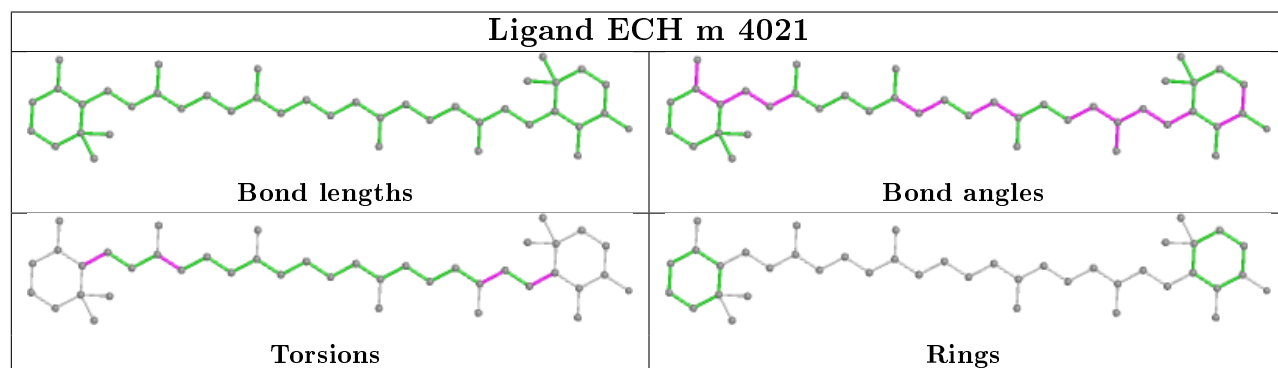
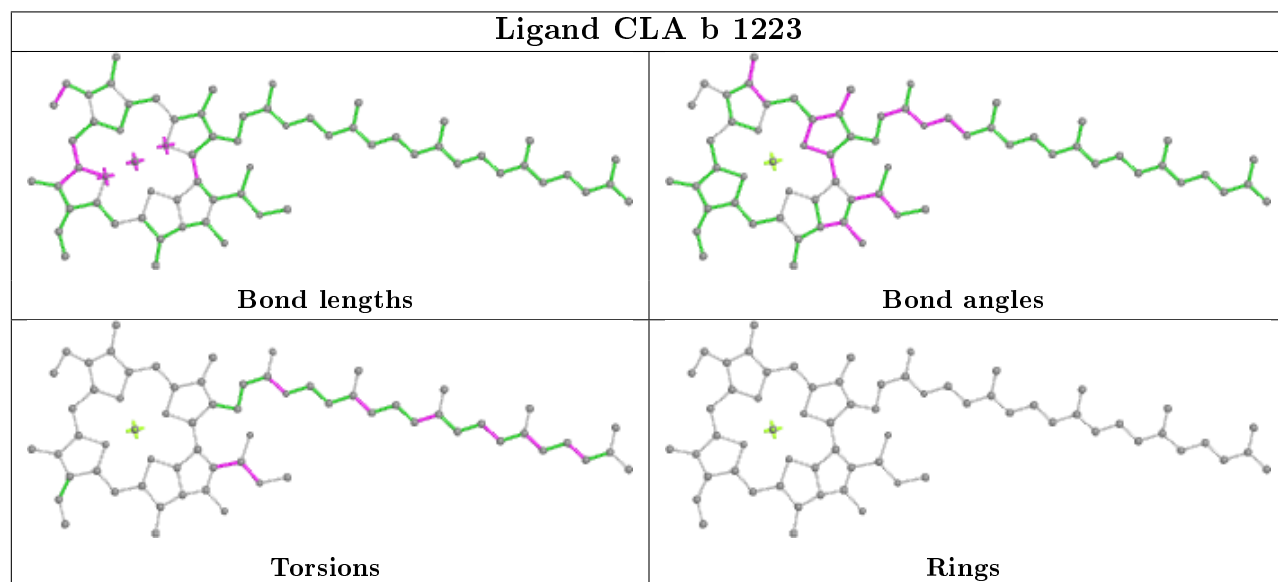
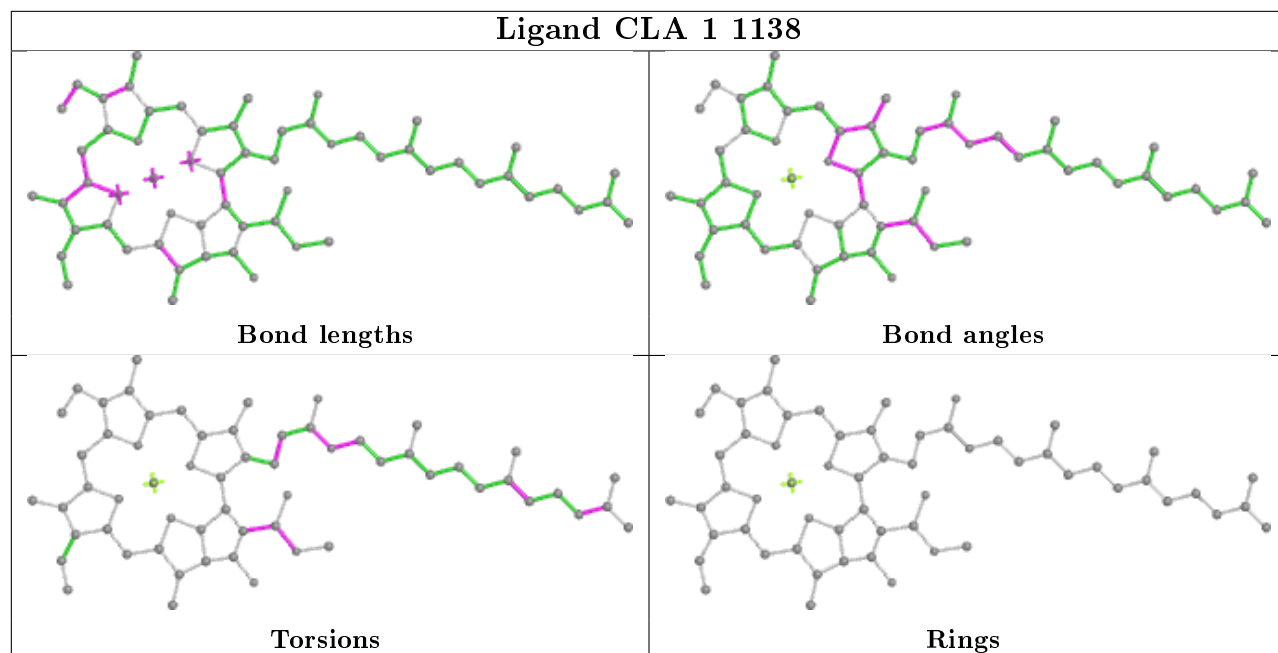
Ligand CLA A 1108

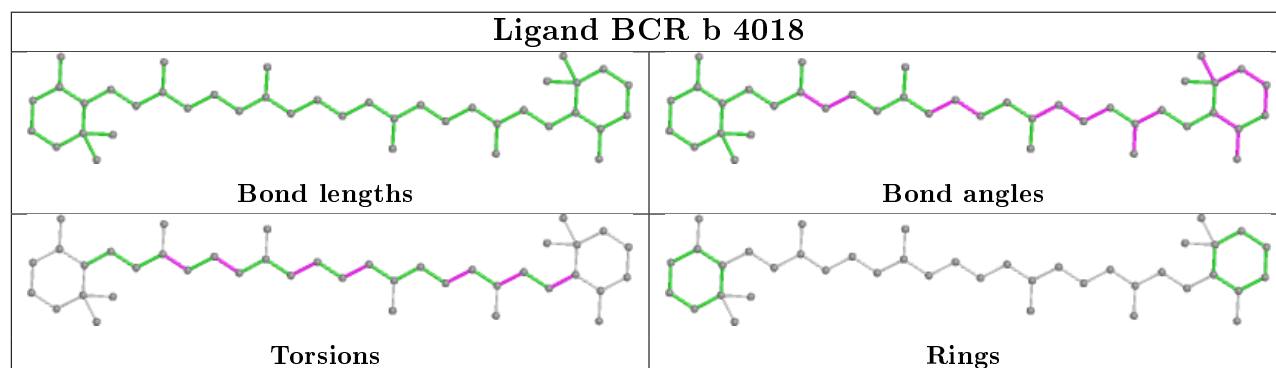
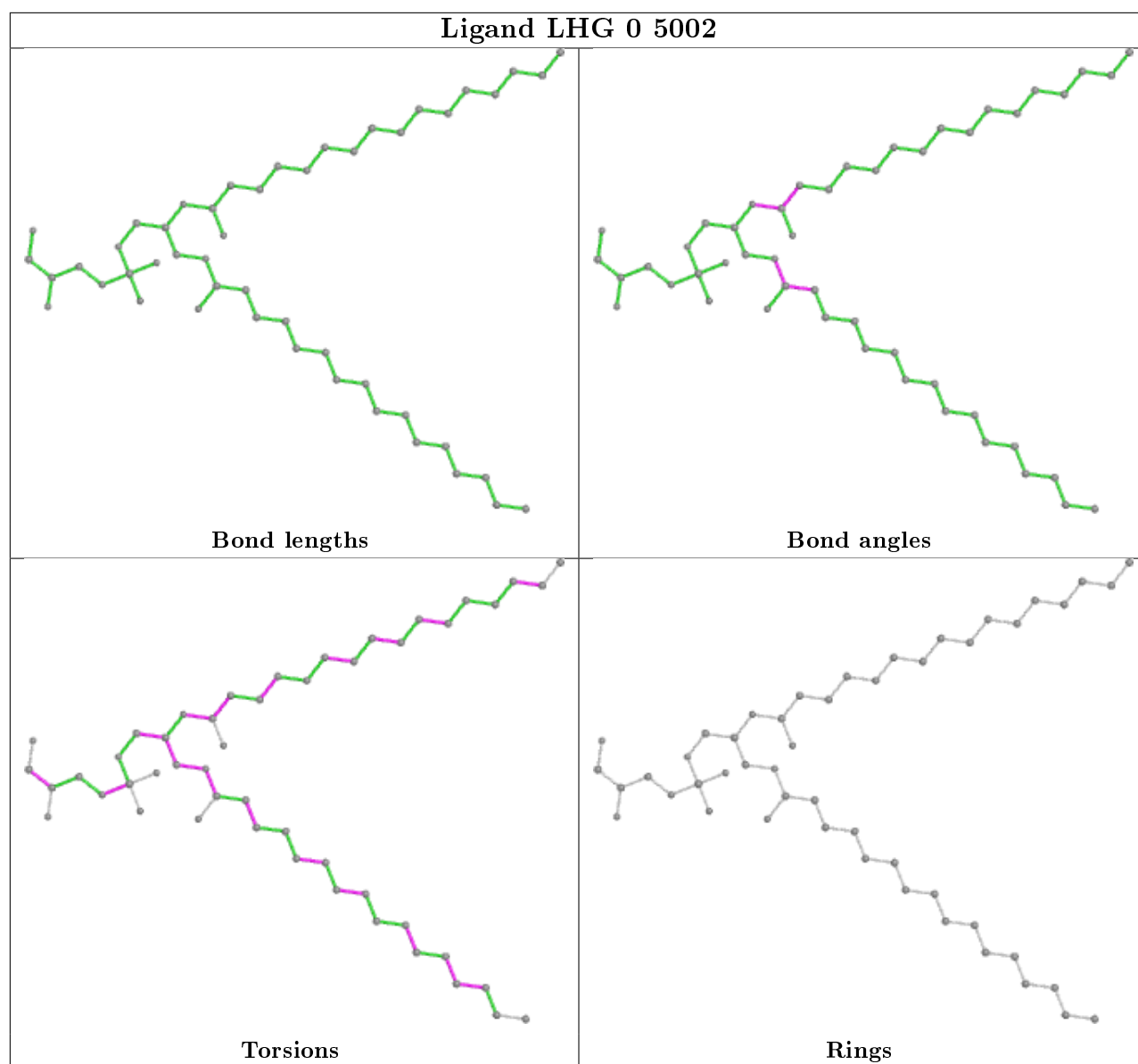


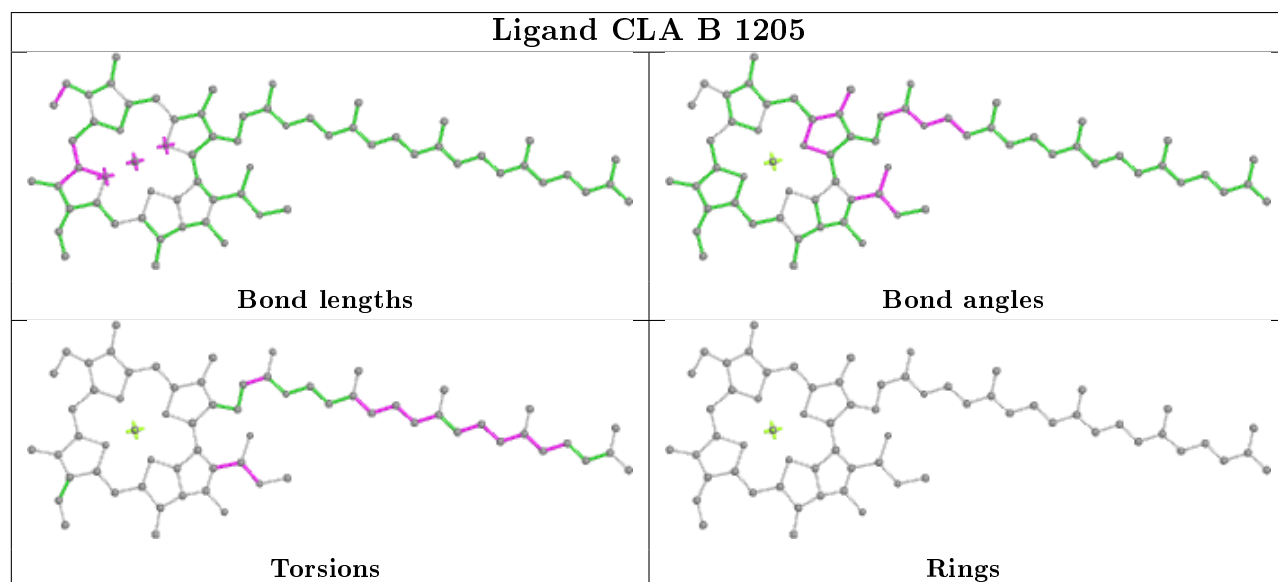
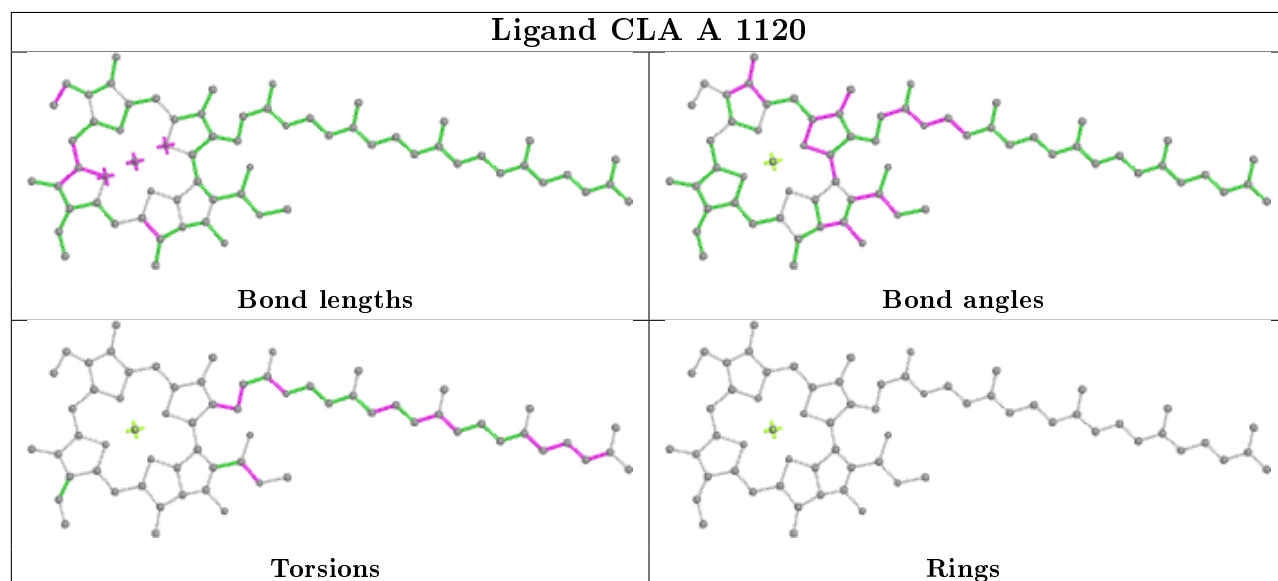
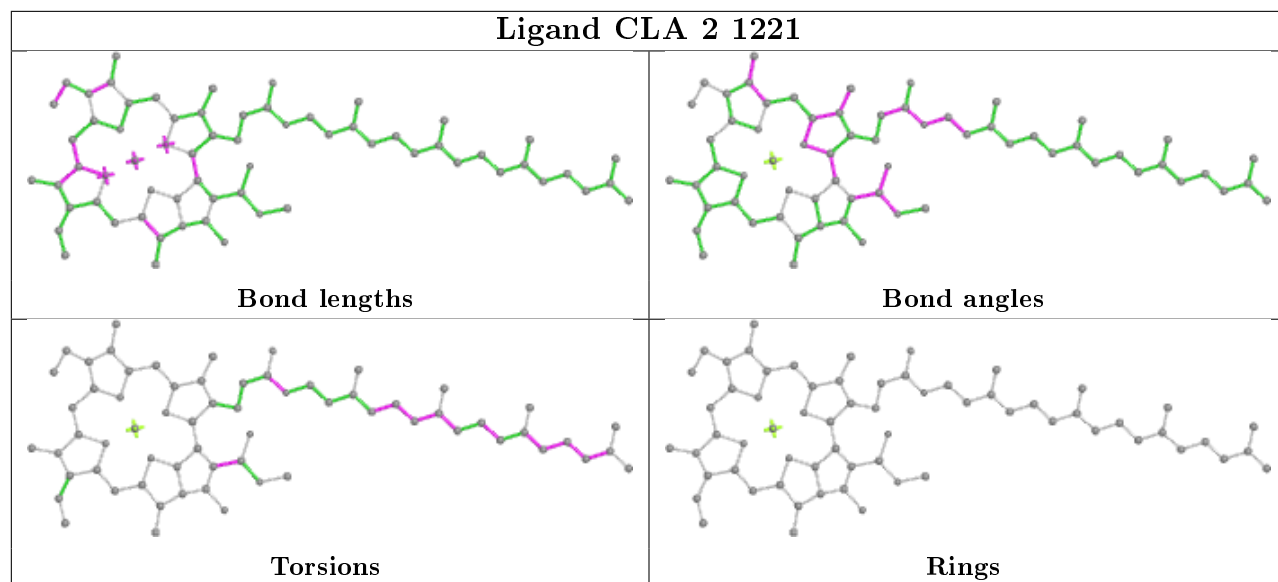
Ligand CLA 2 1239

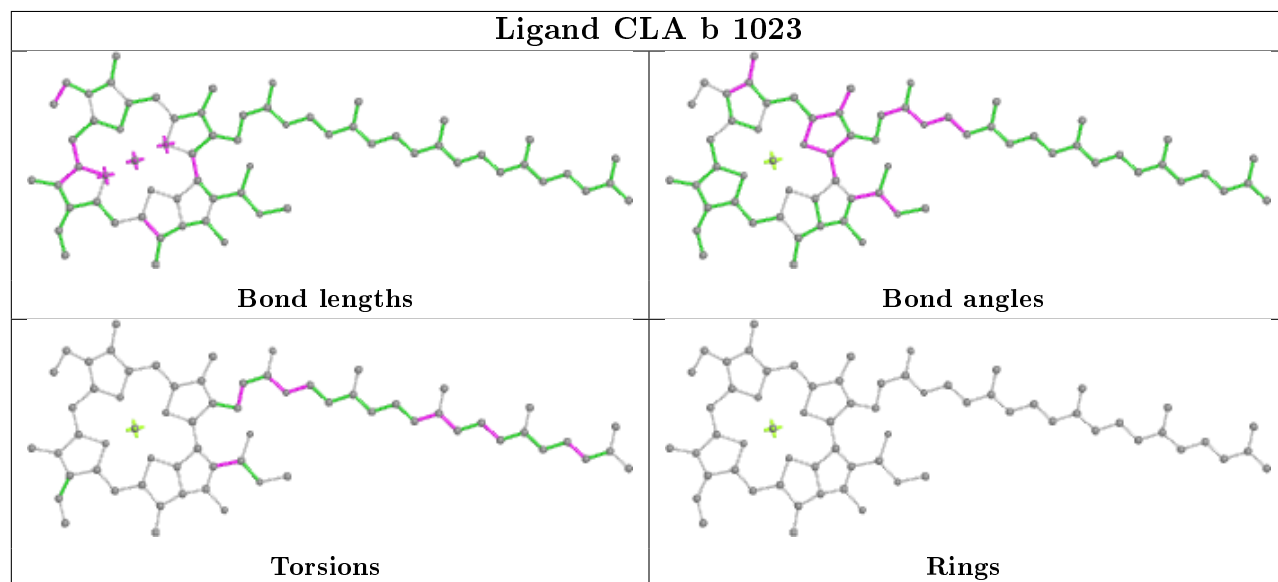
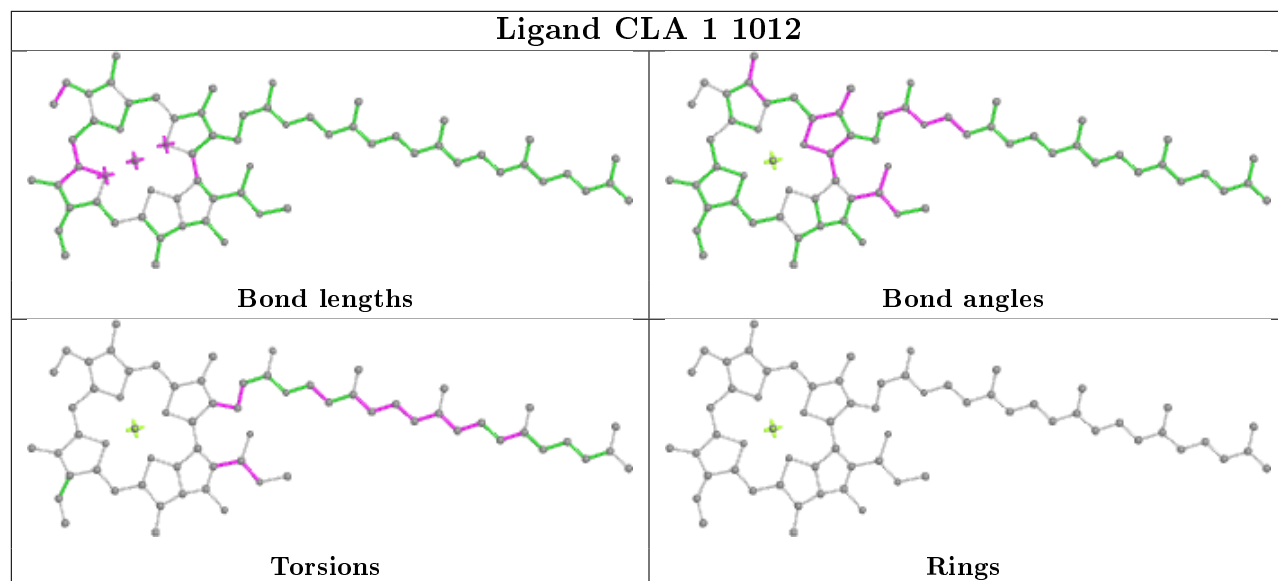
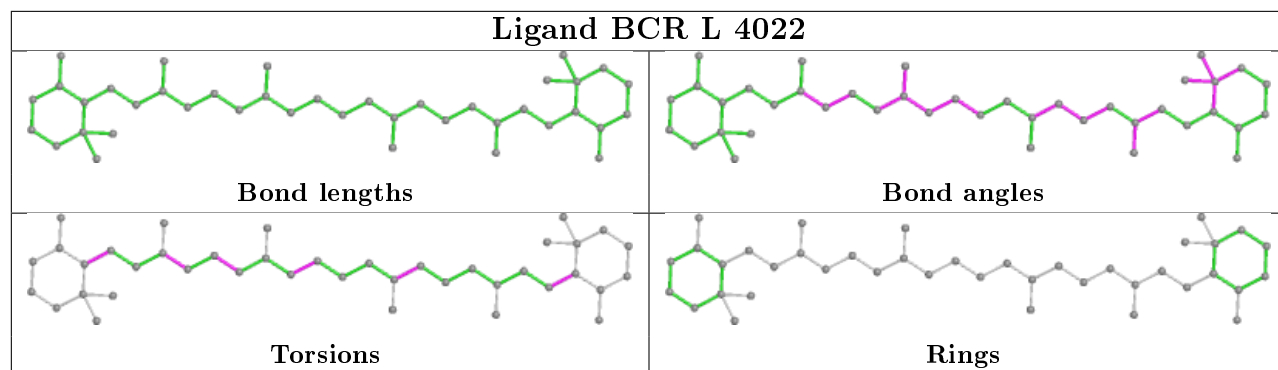


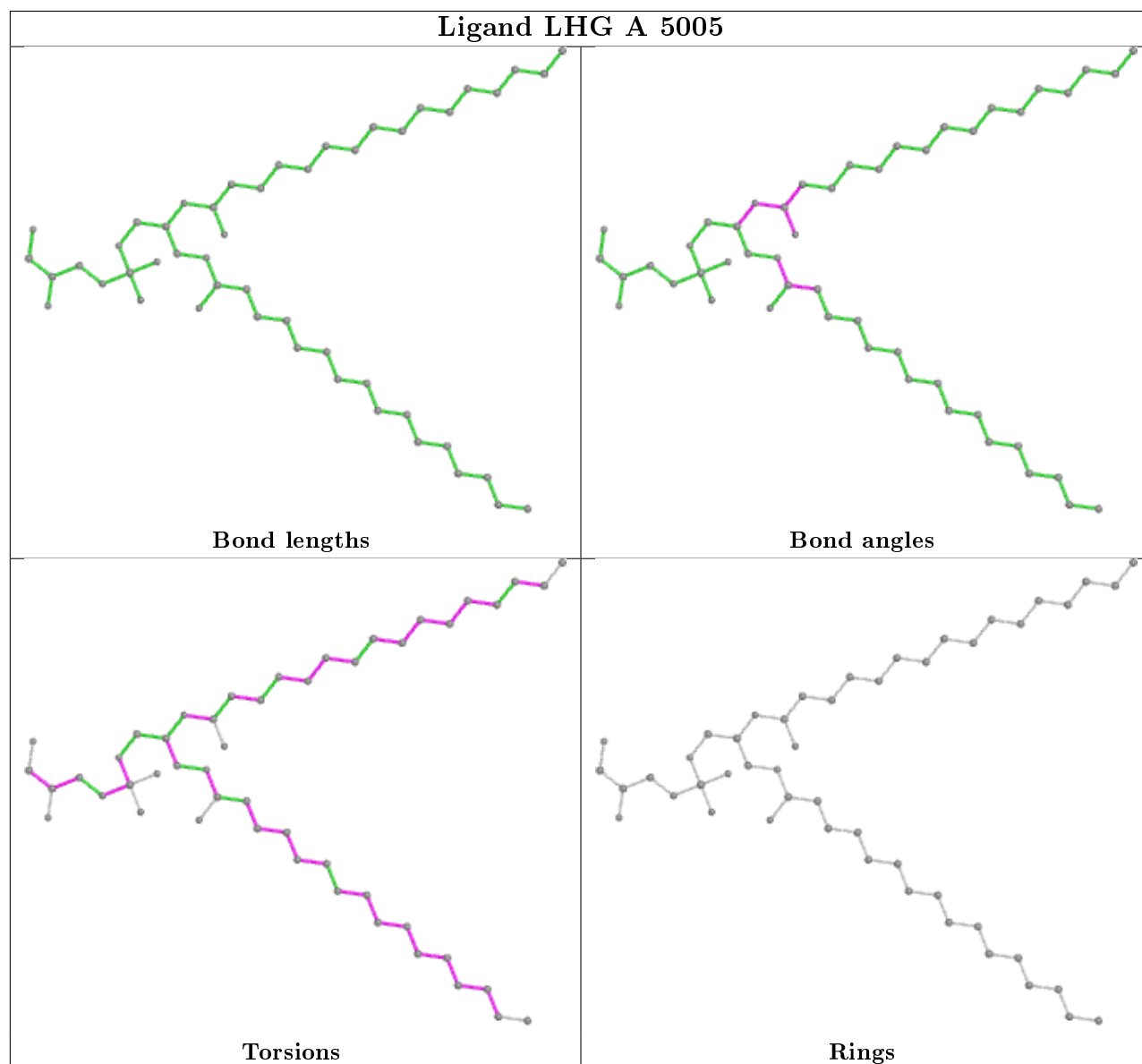
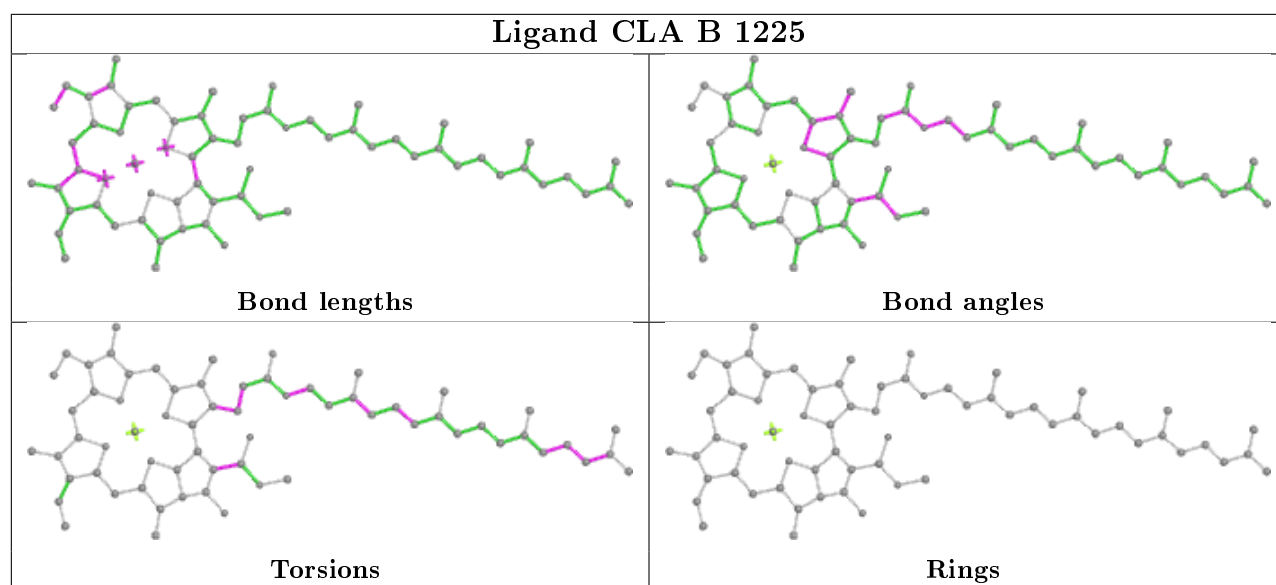


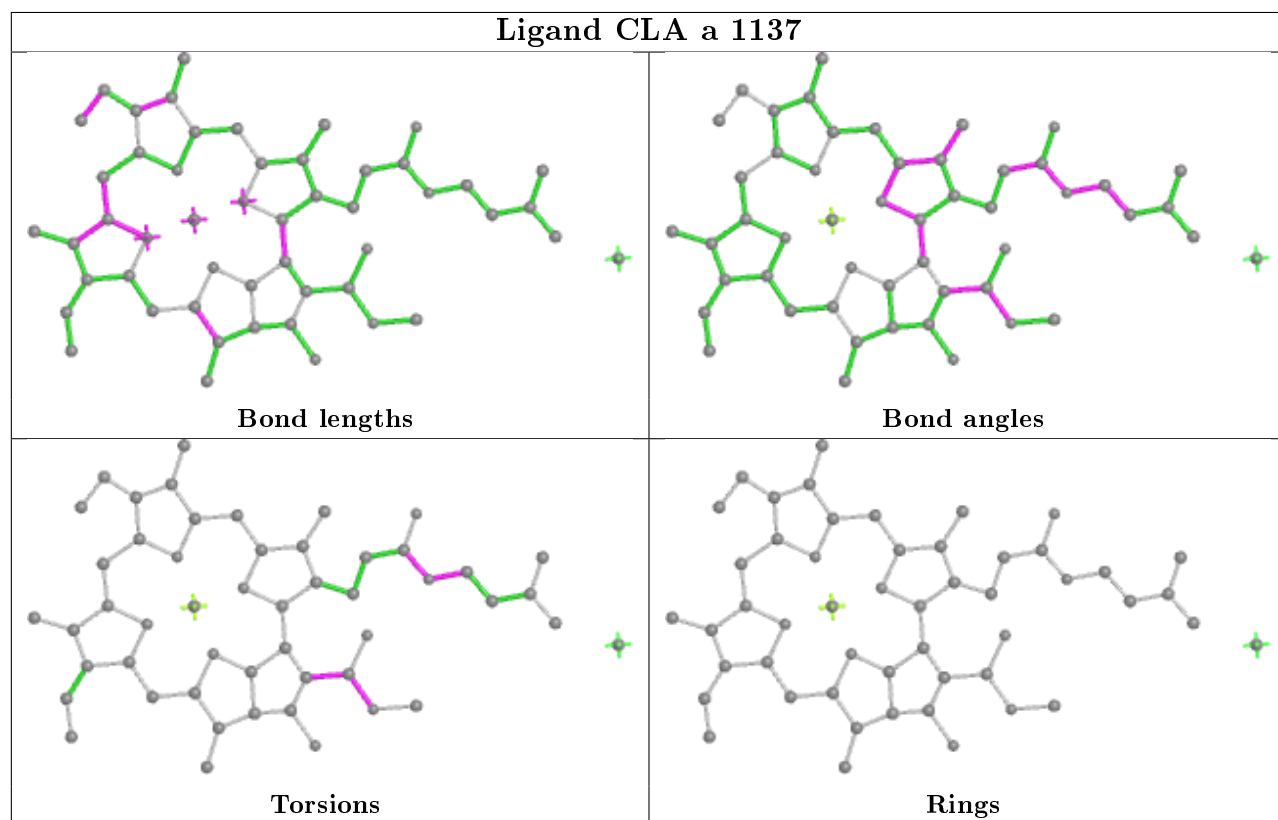
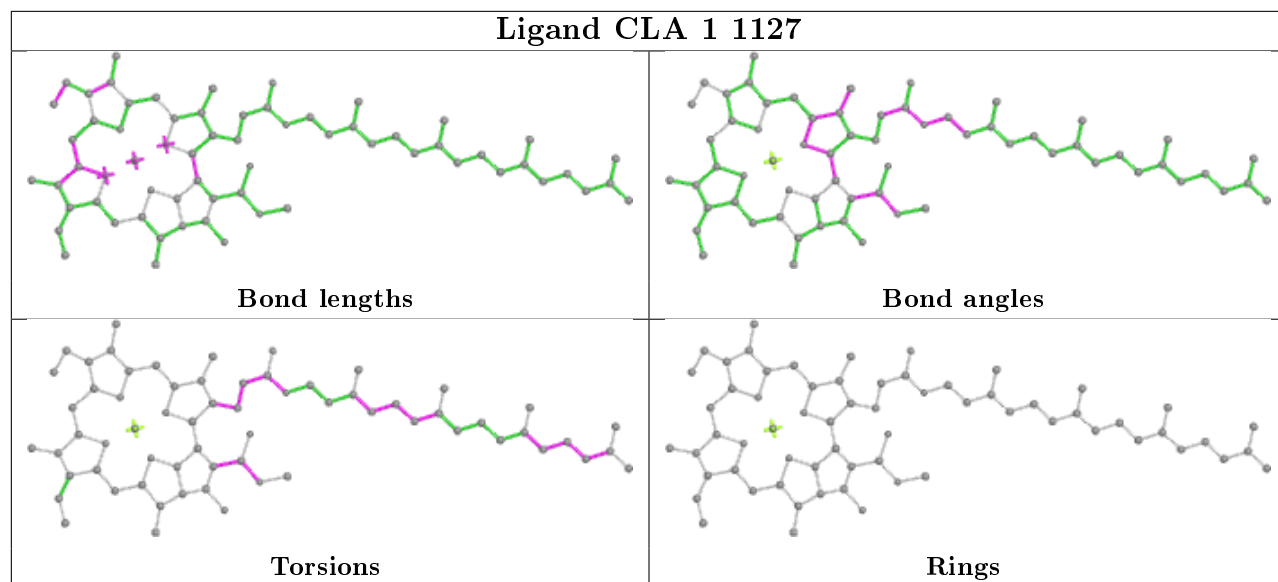


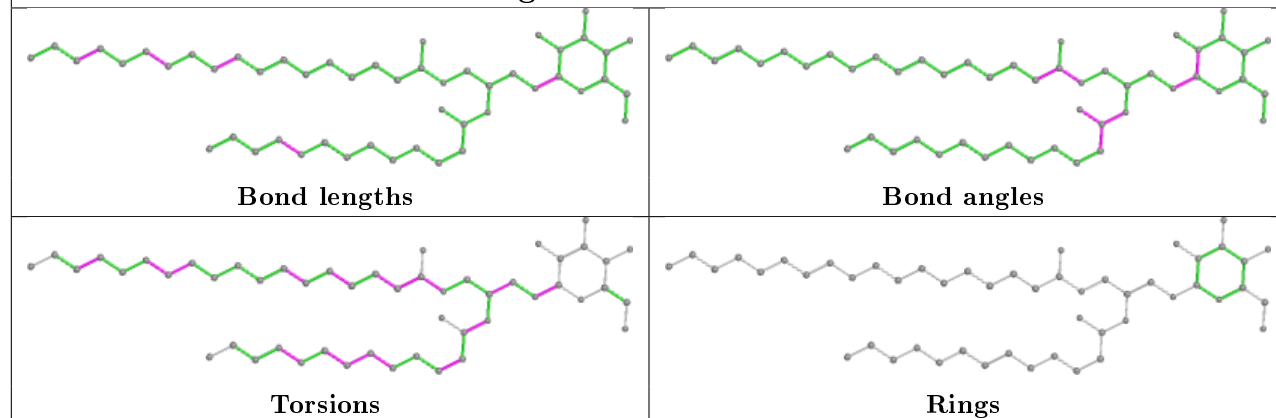
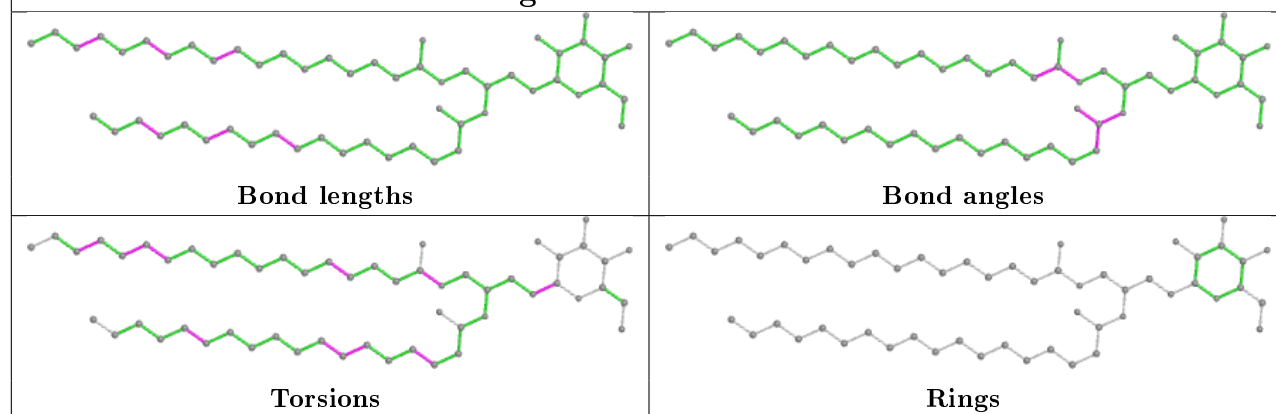
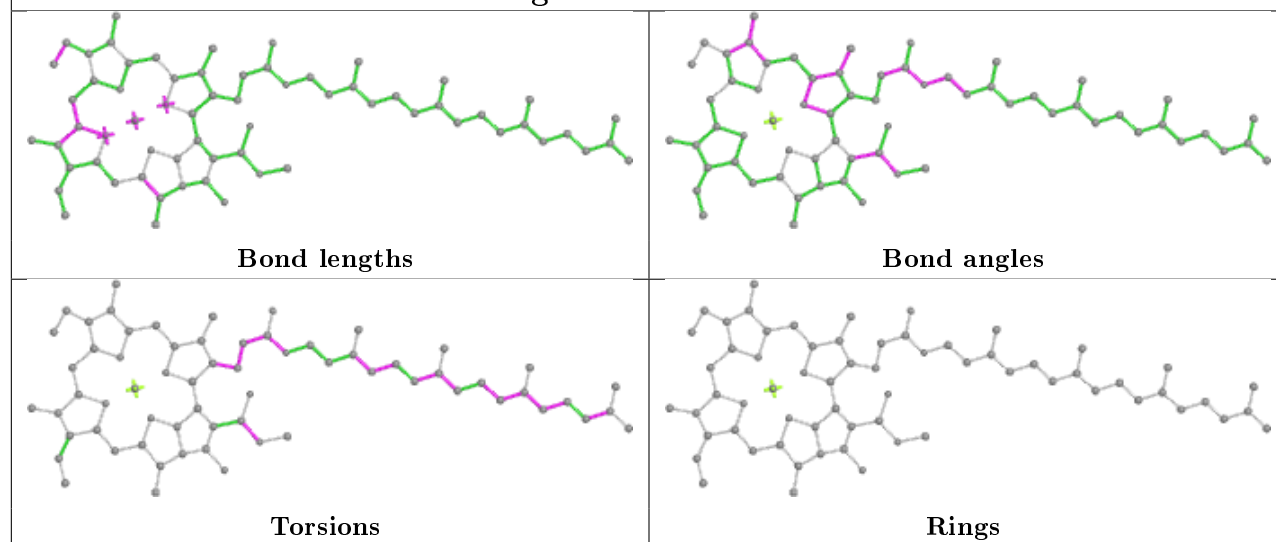


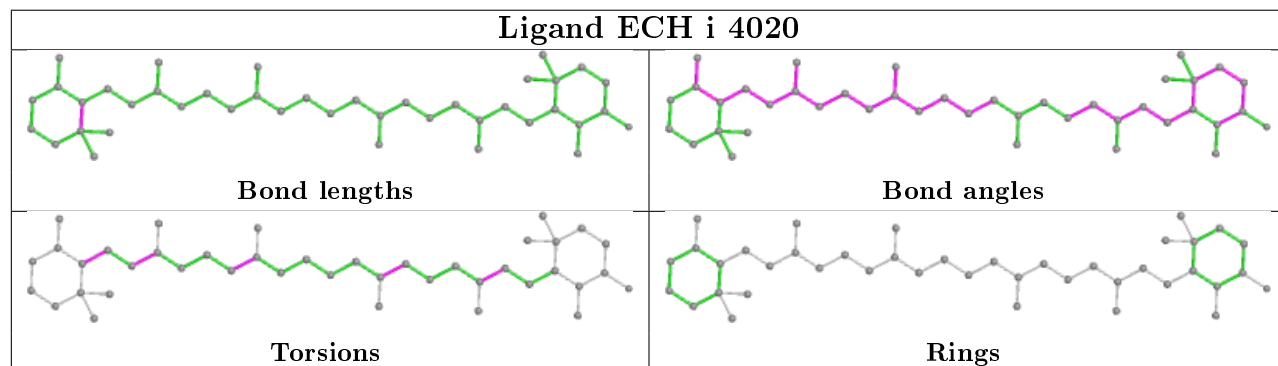
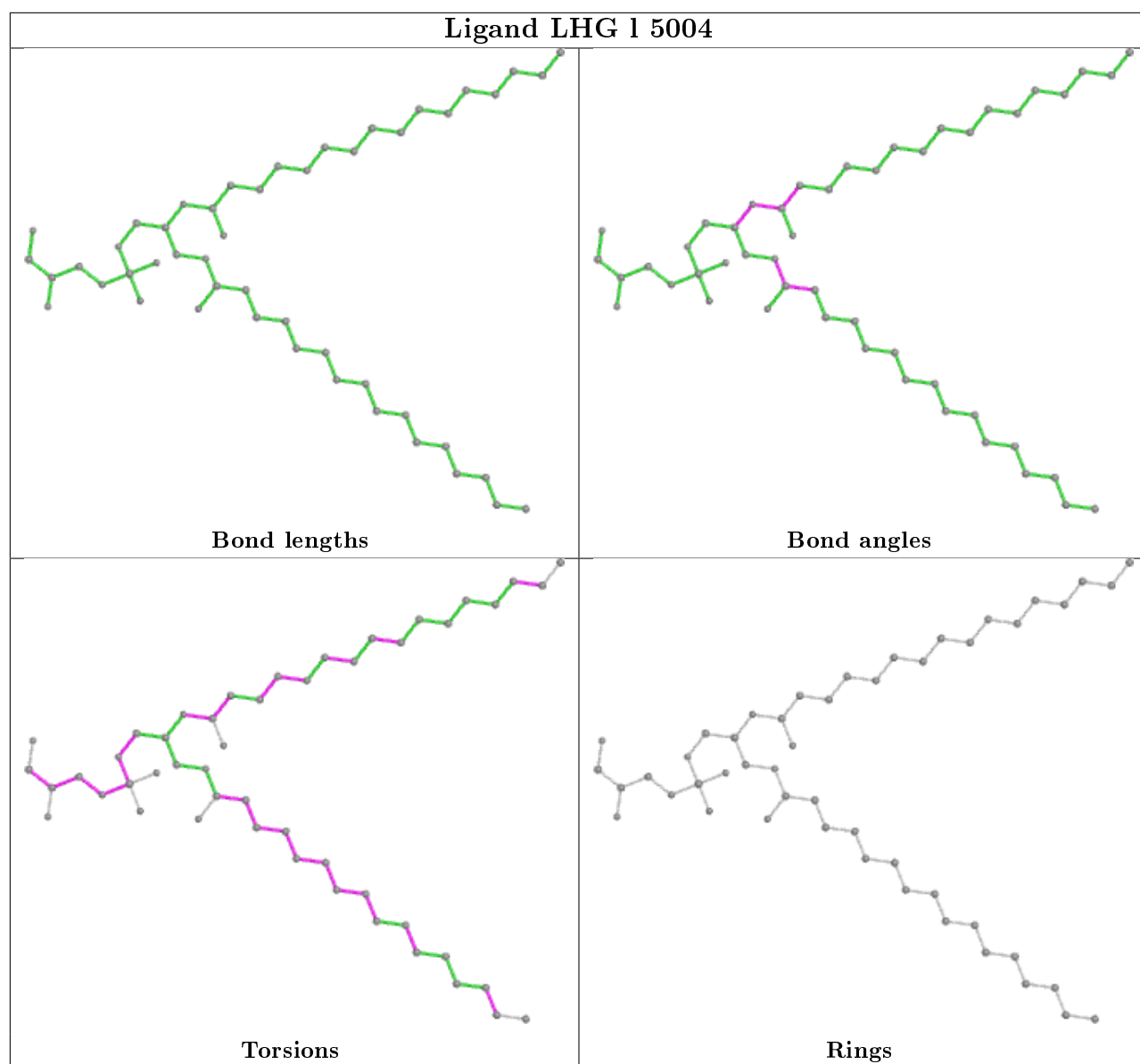


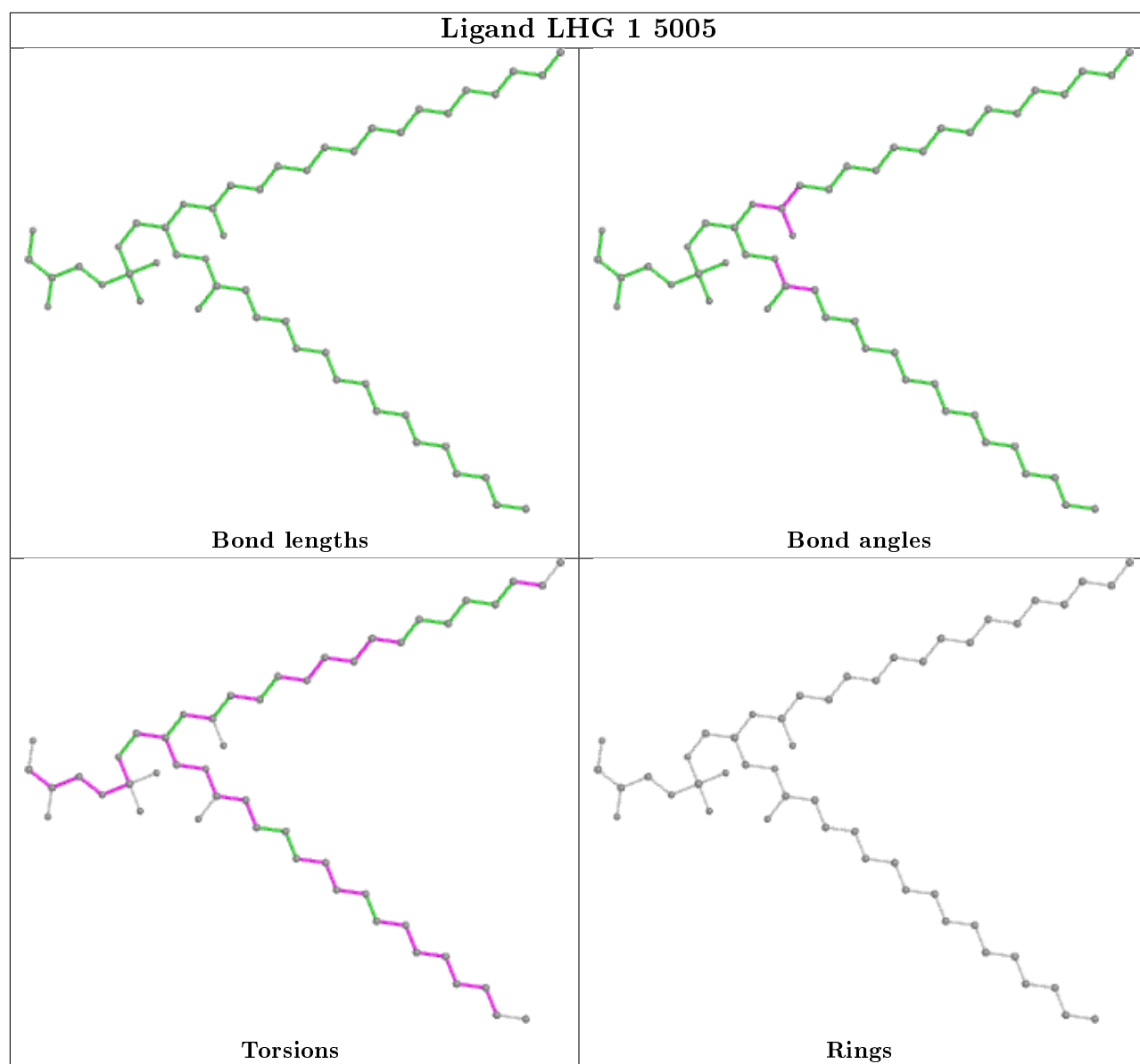


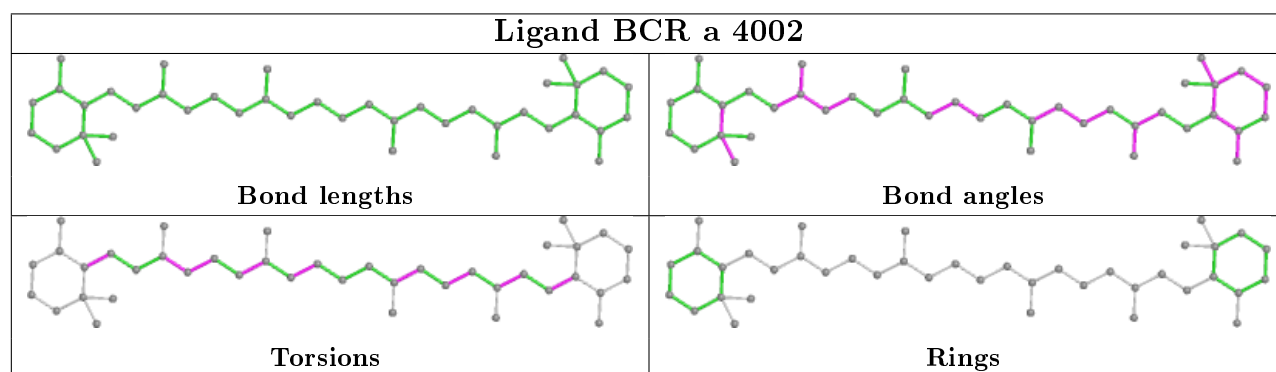
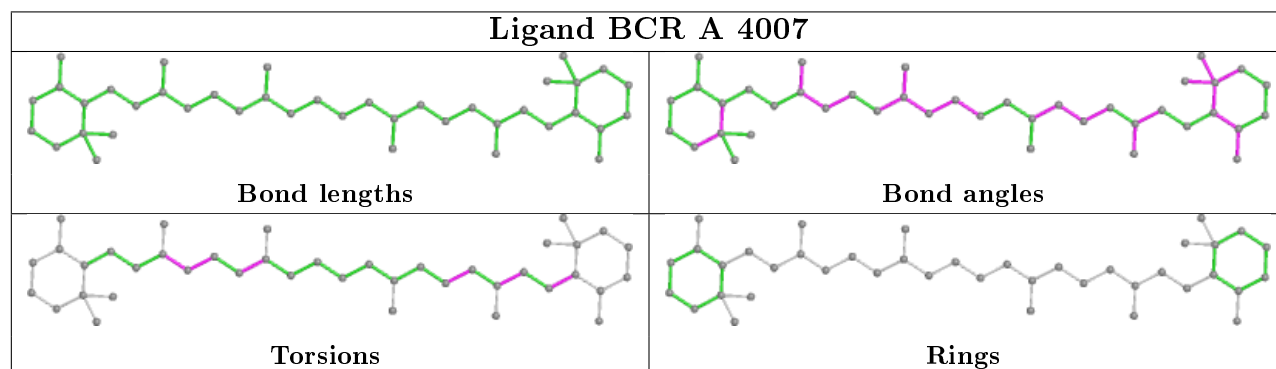
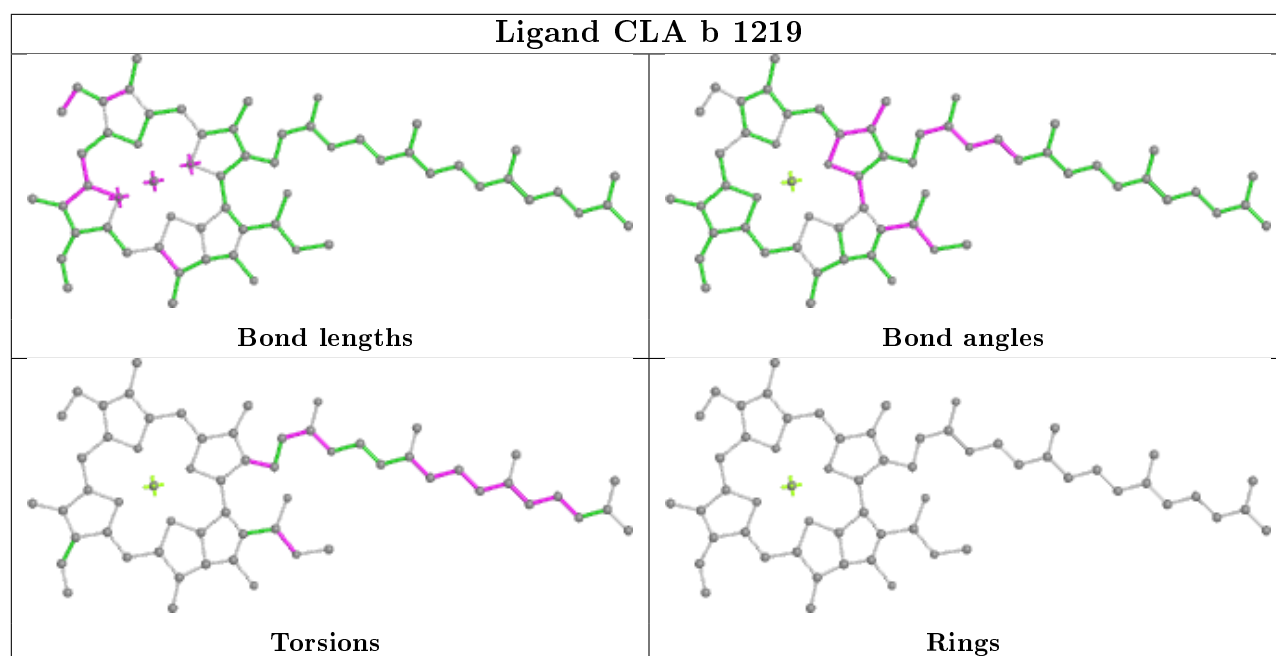


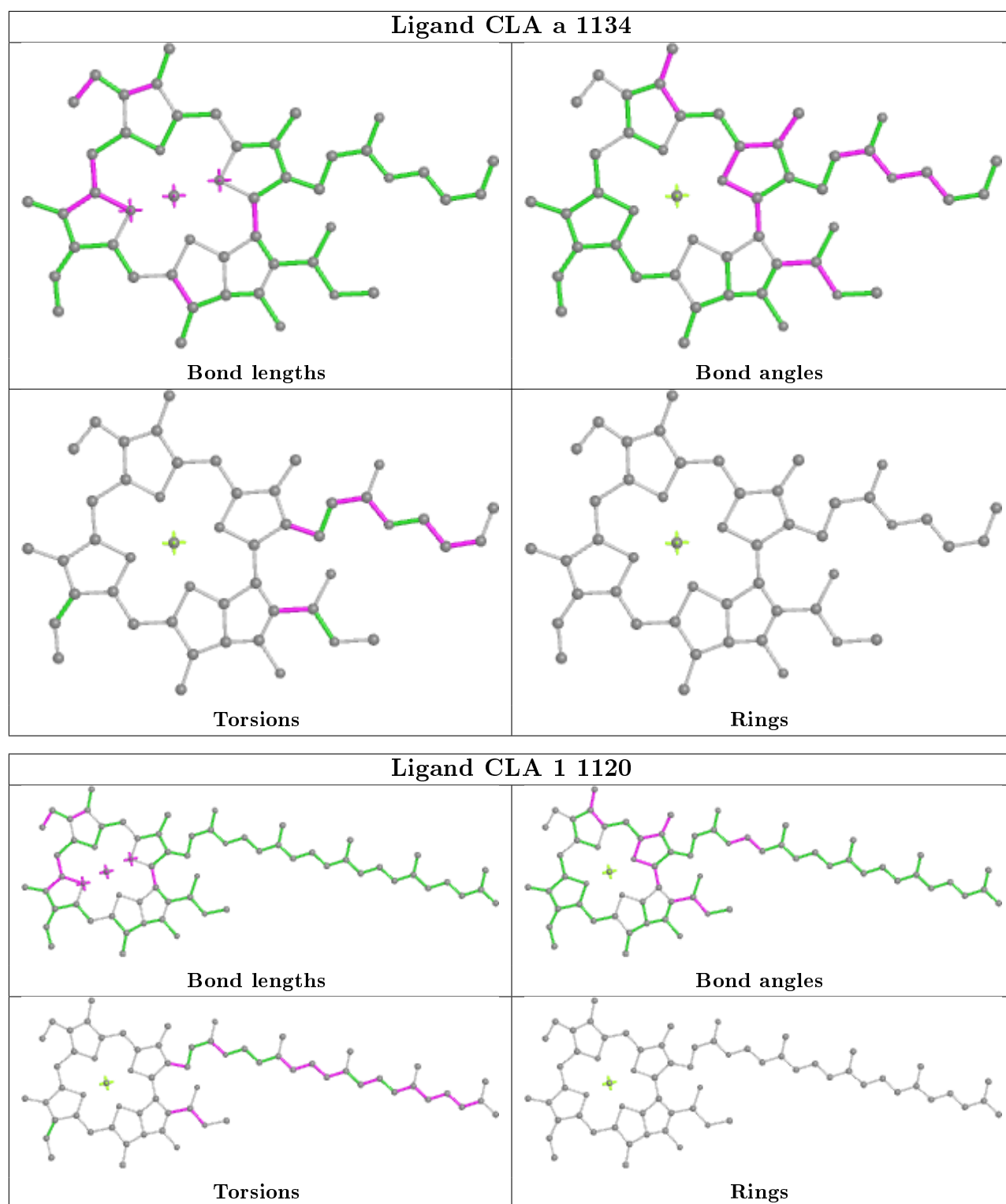


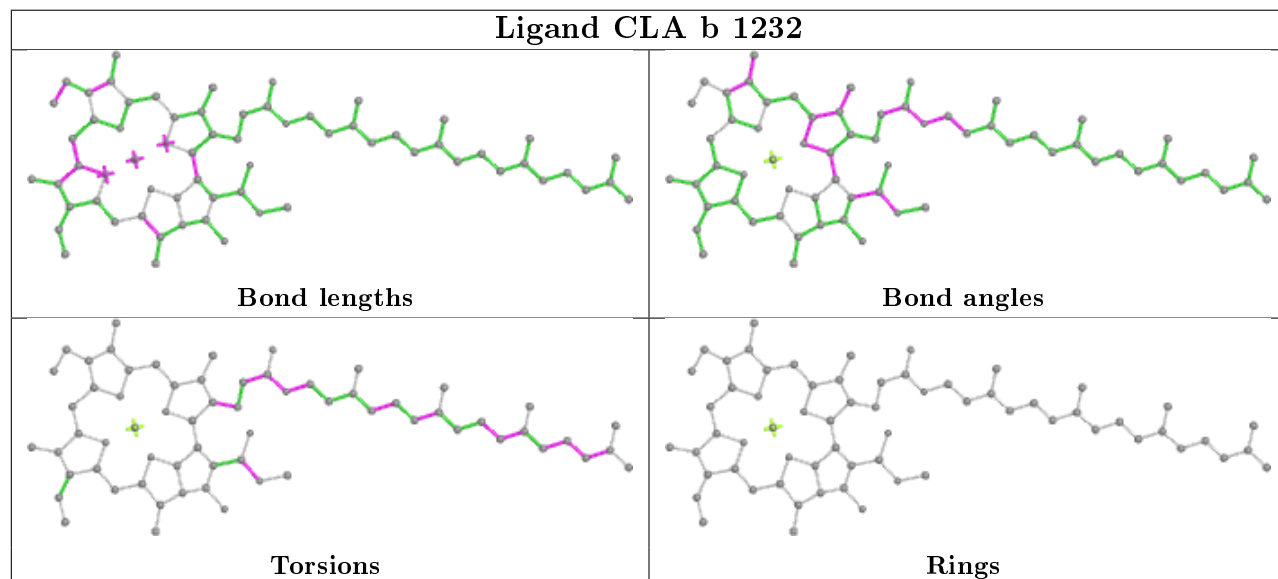
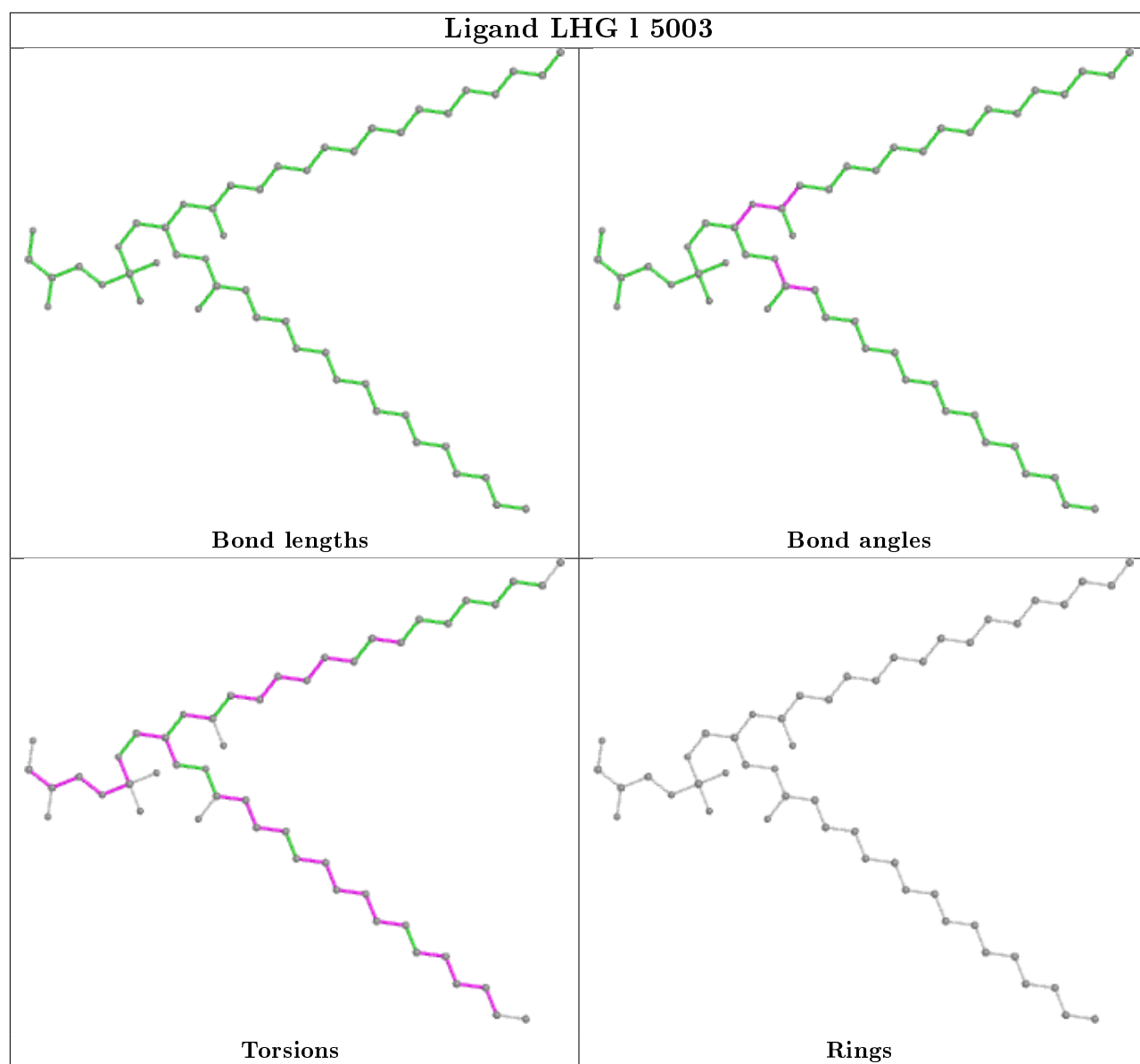
Ligand LMG A 5002**Ligand LMG B 5005****Ligand CLA 1 1503**

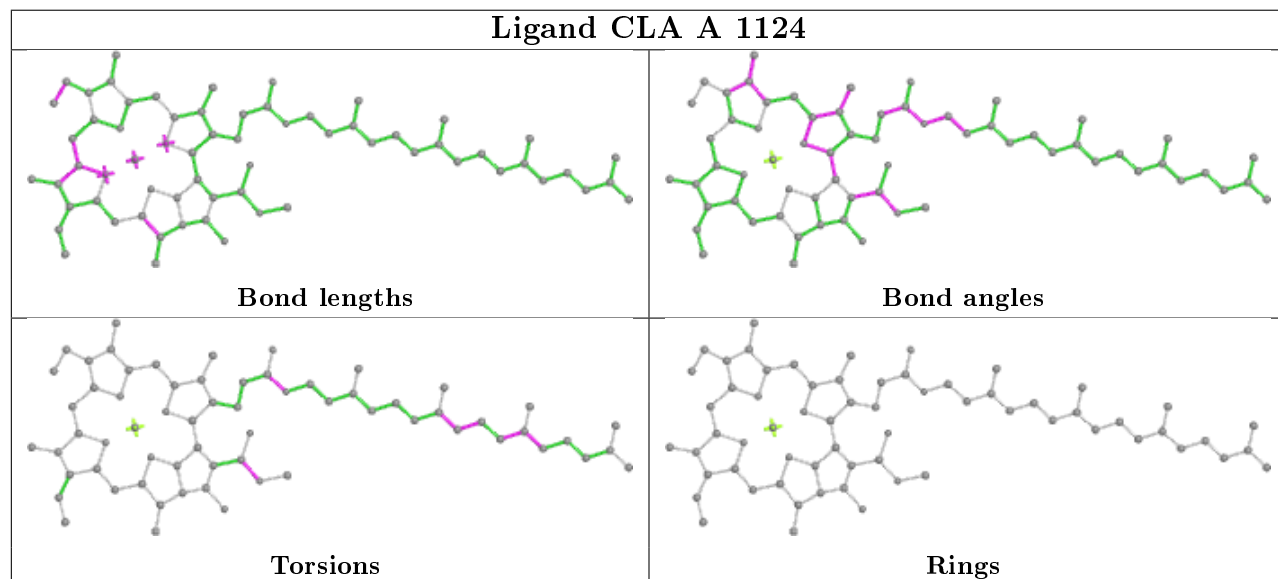
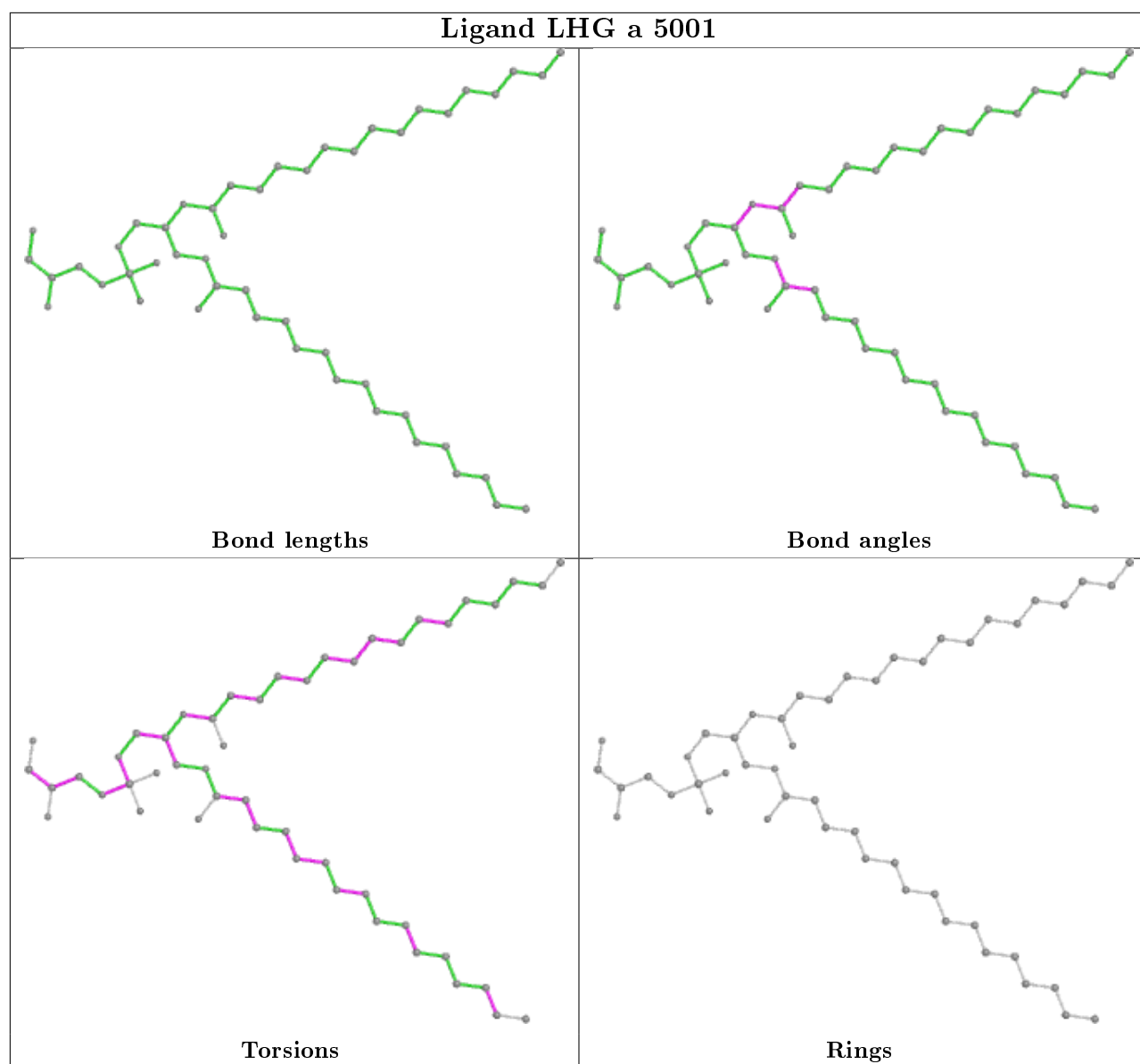


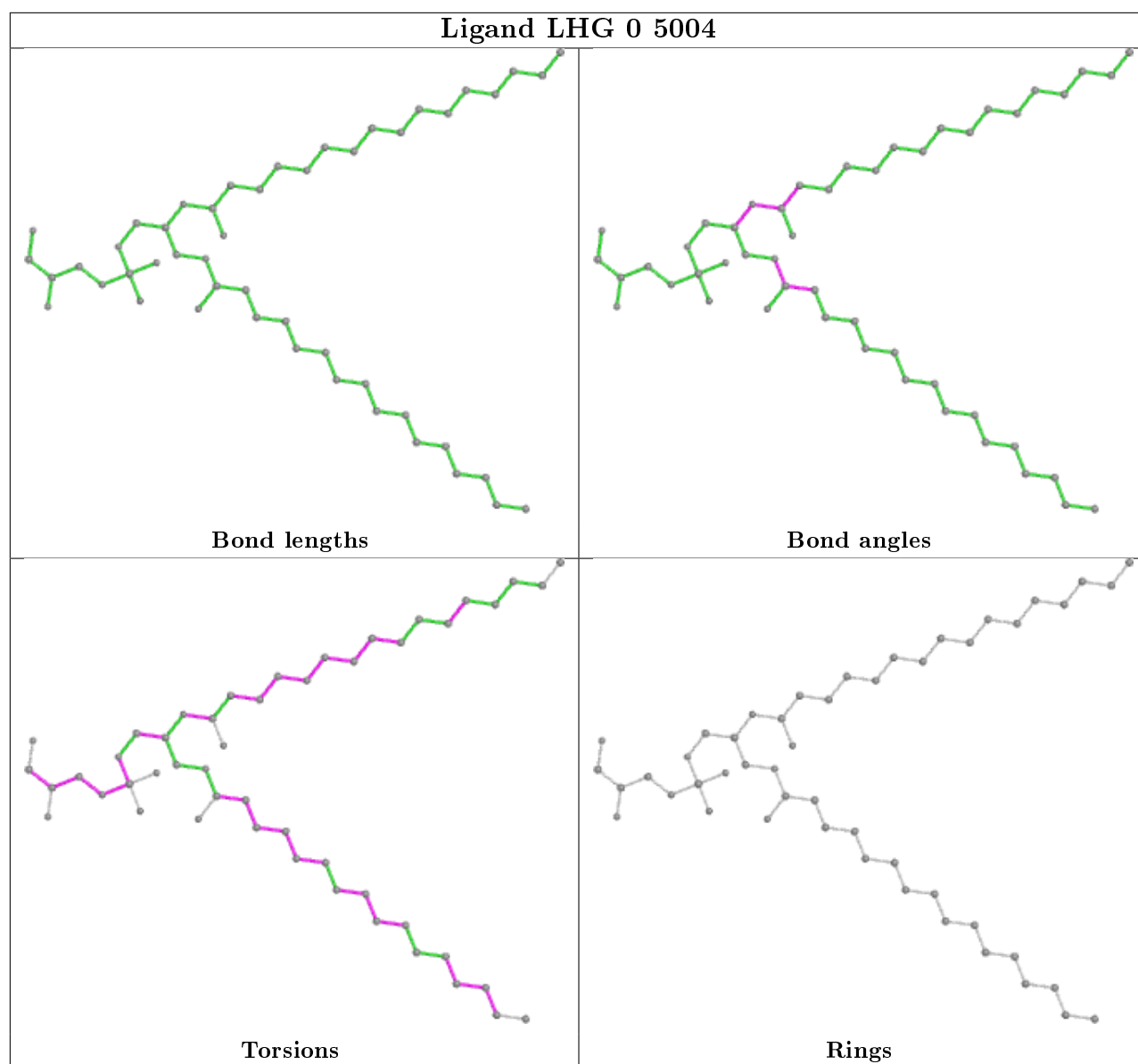


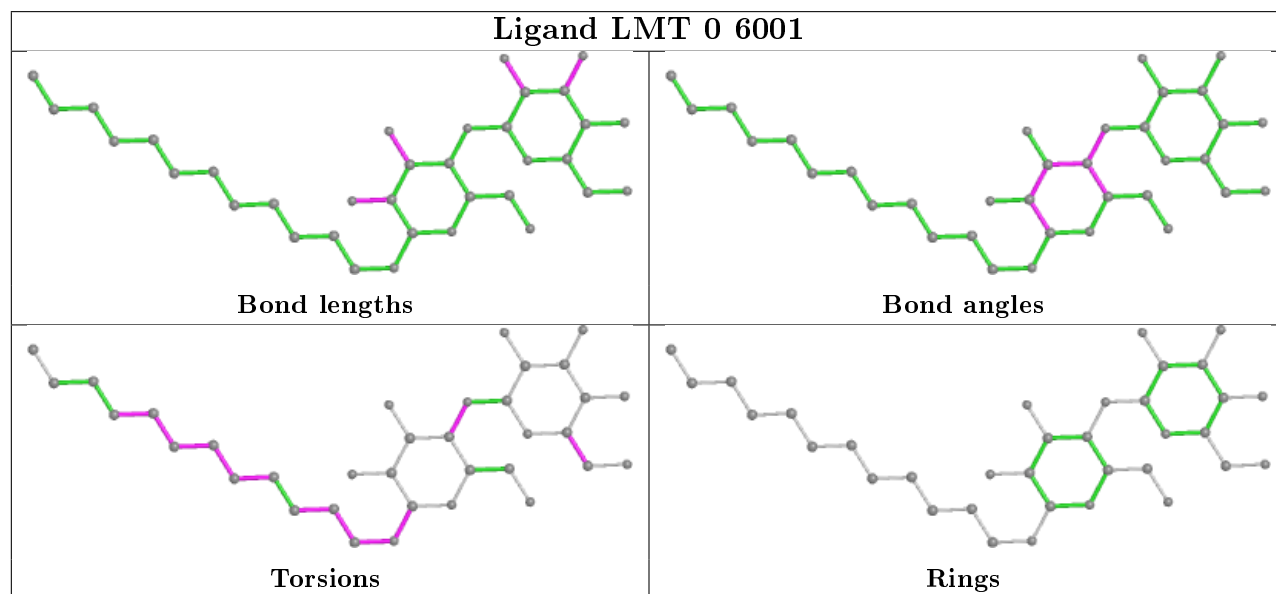
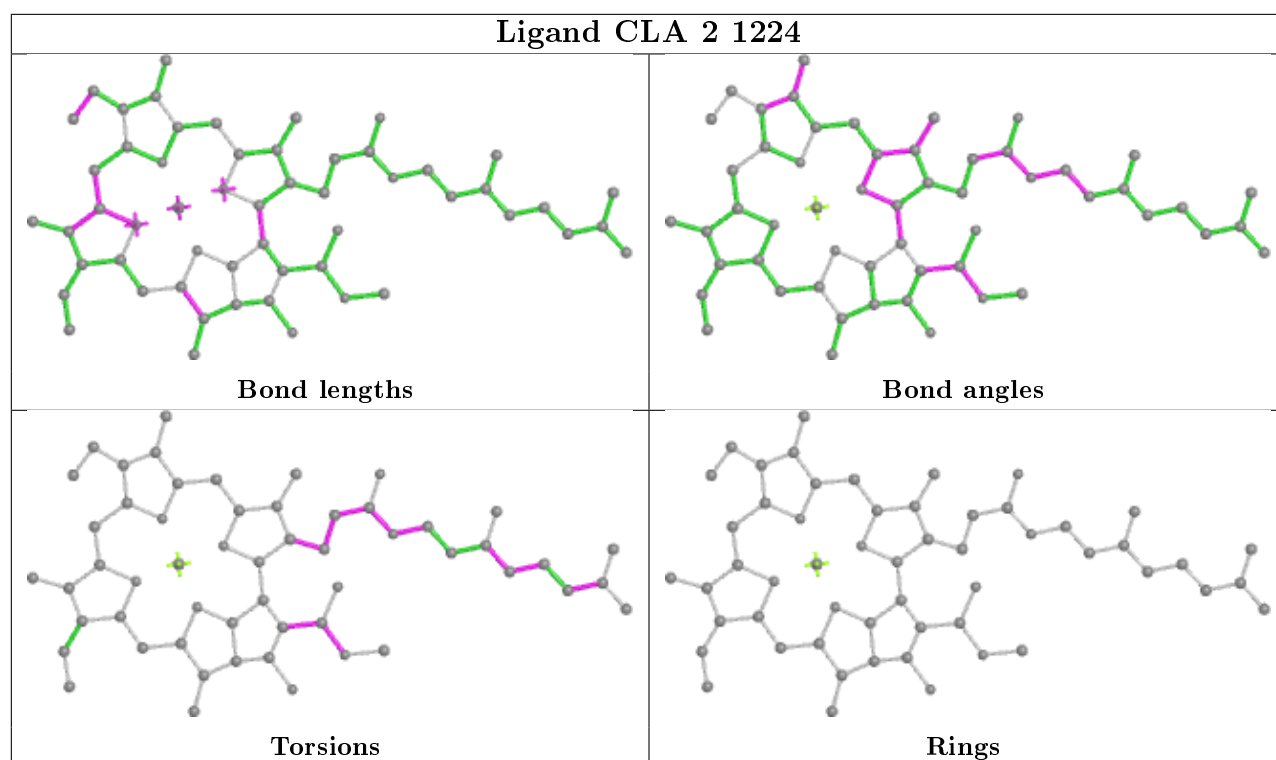


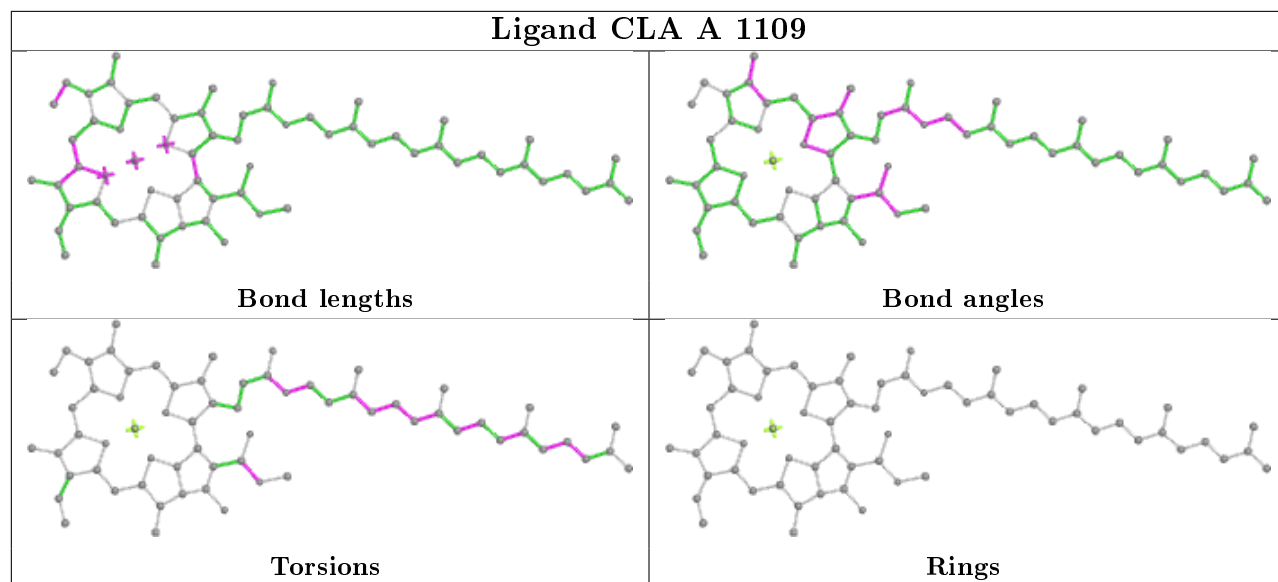
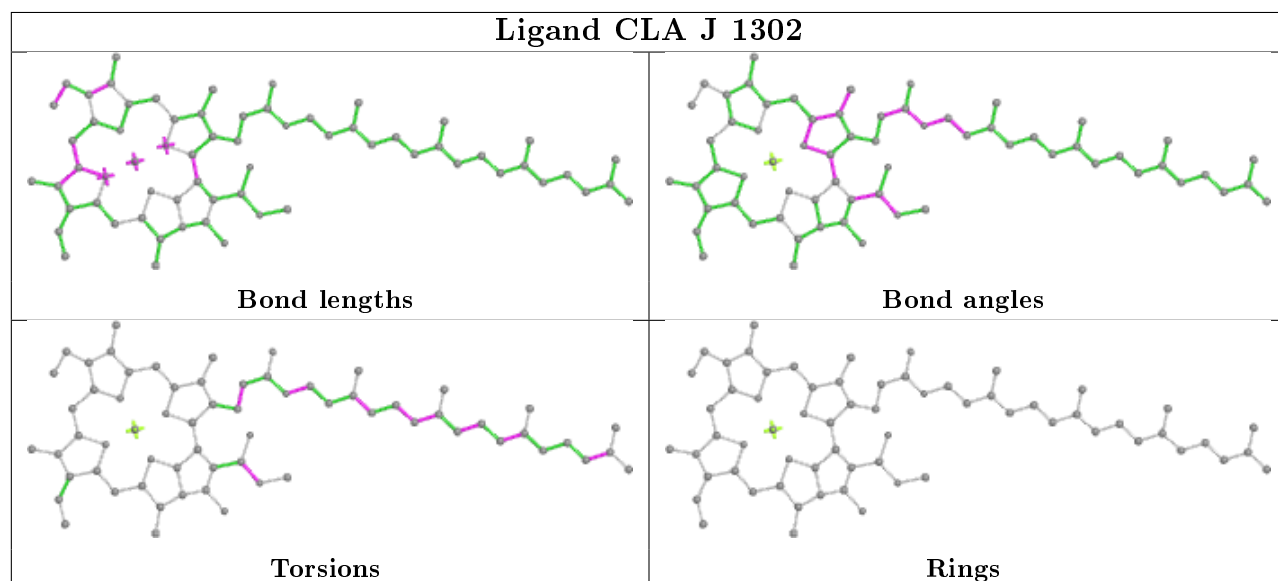
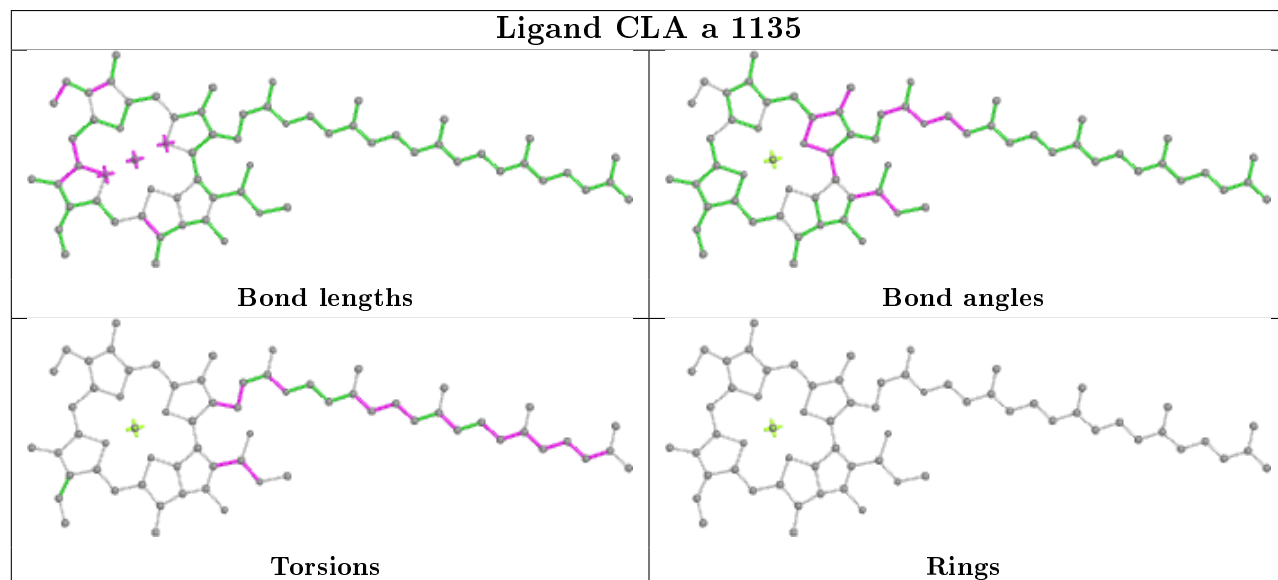


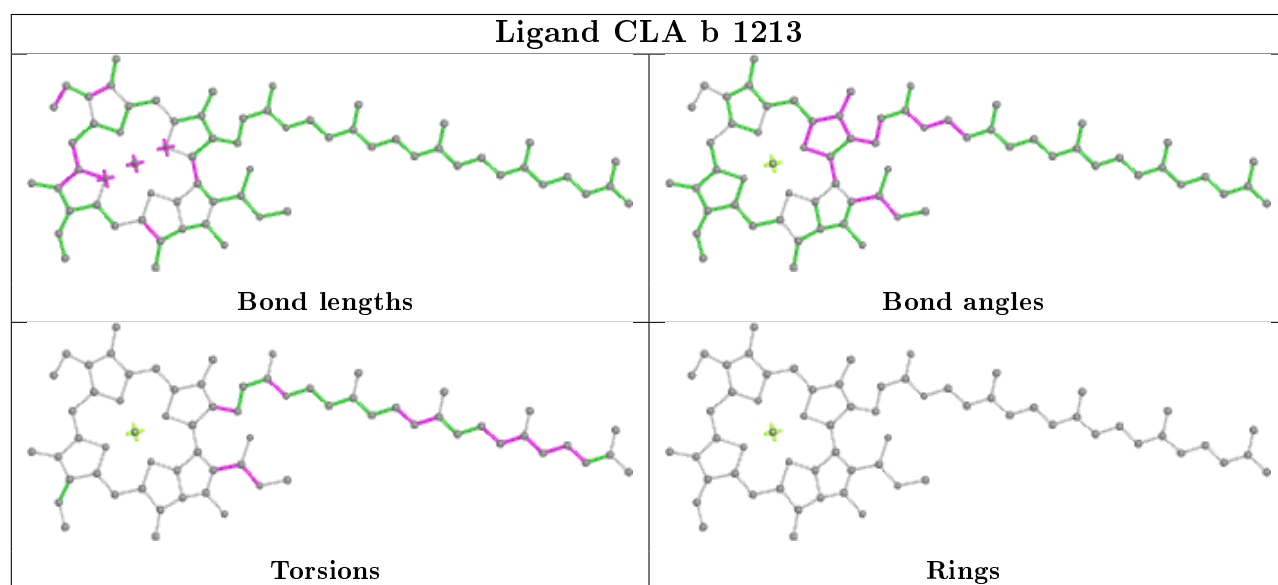
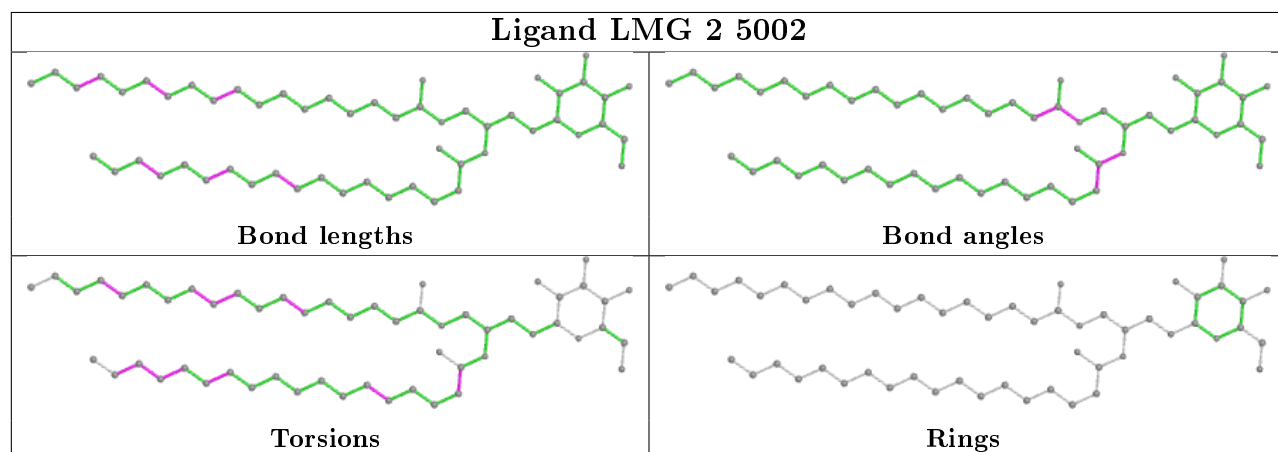
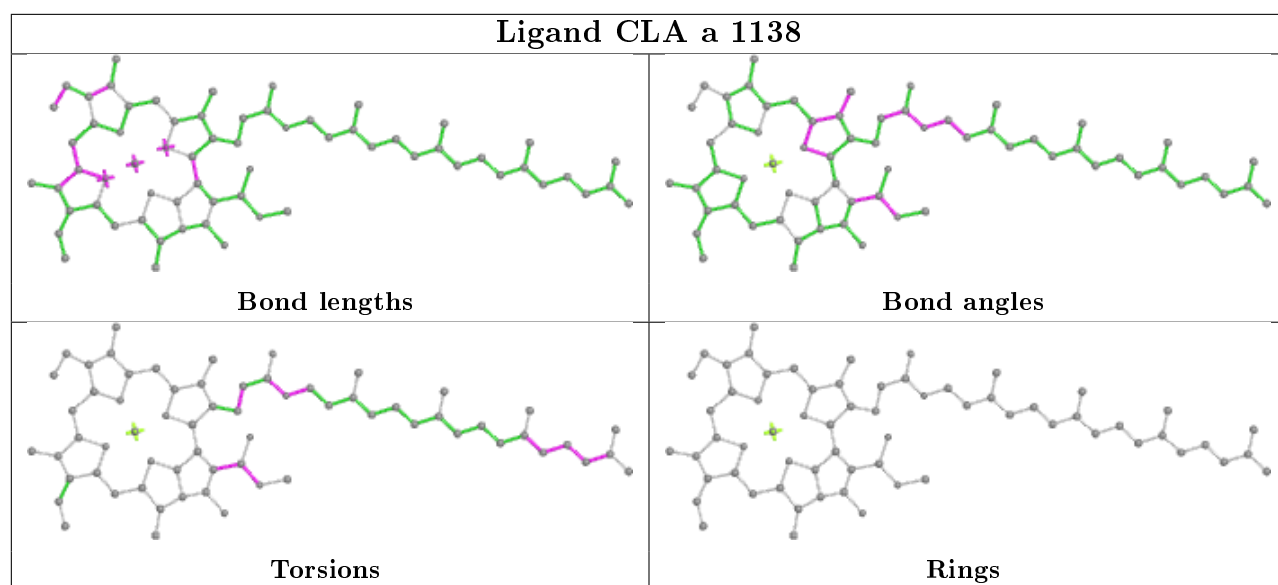


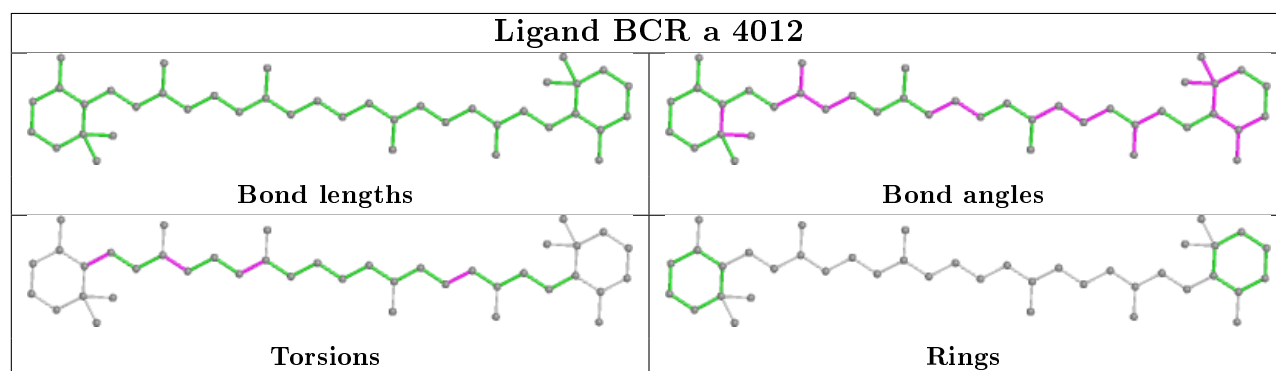
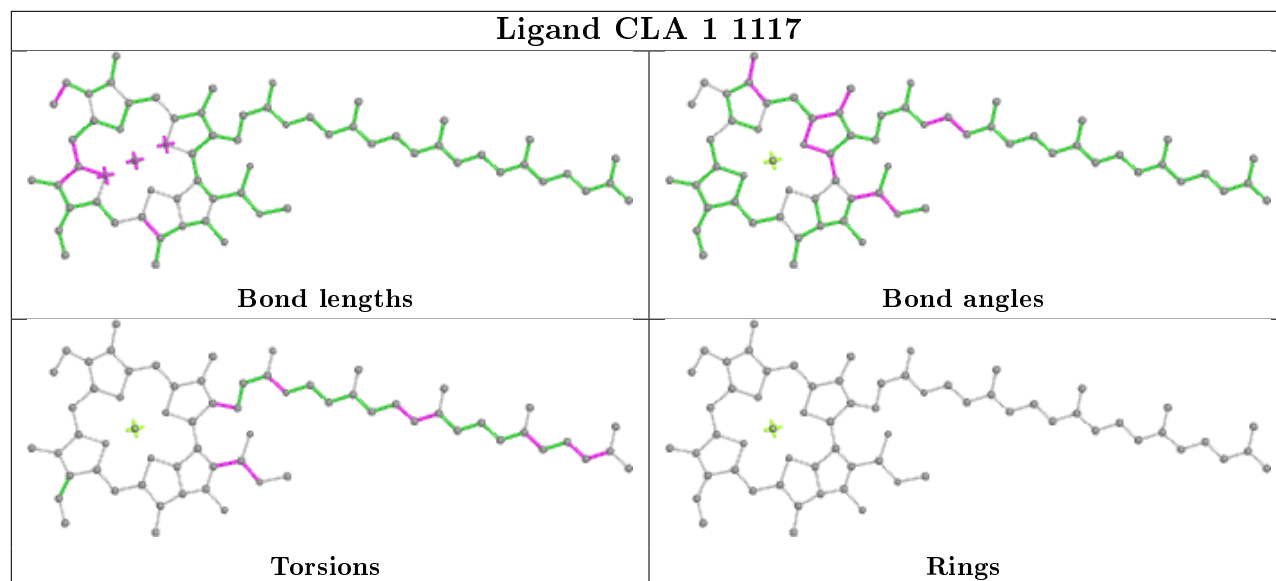
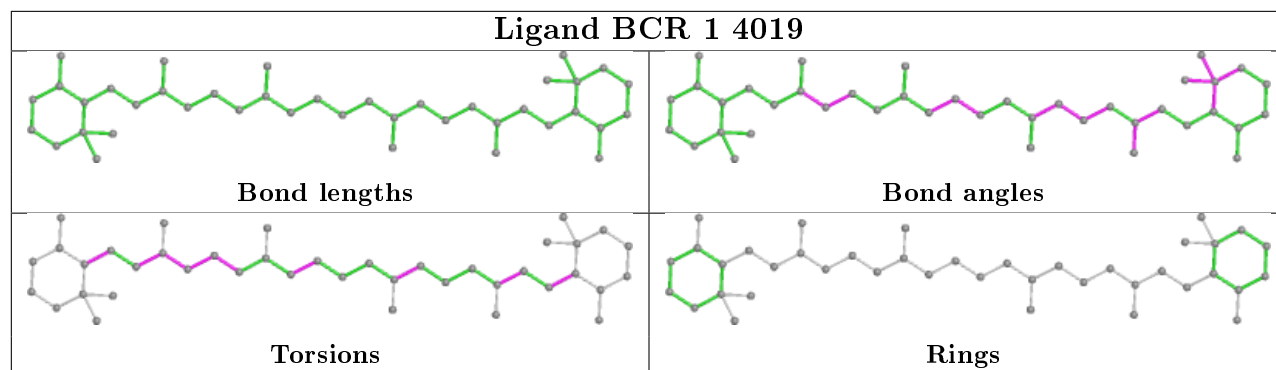


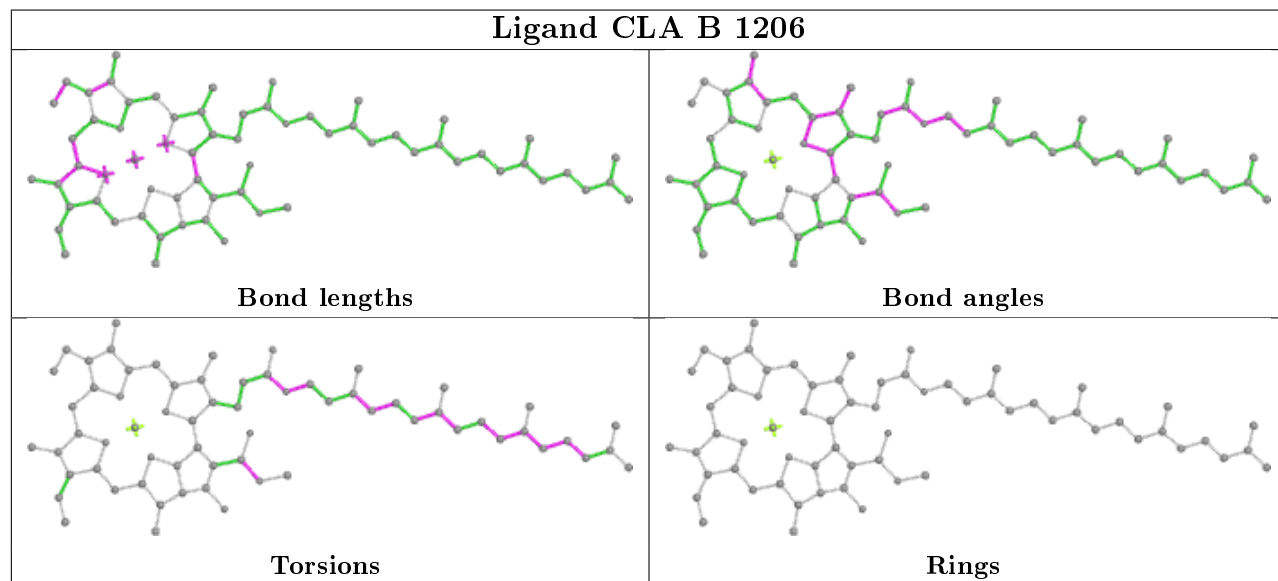
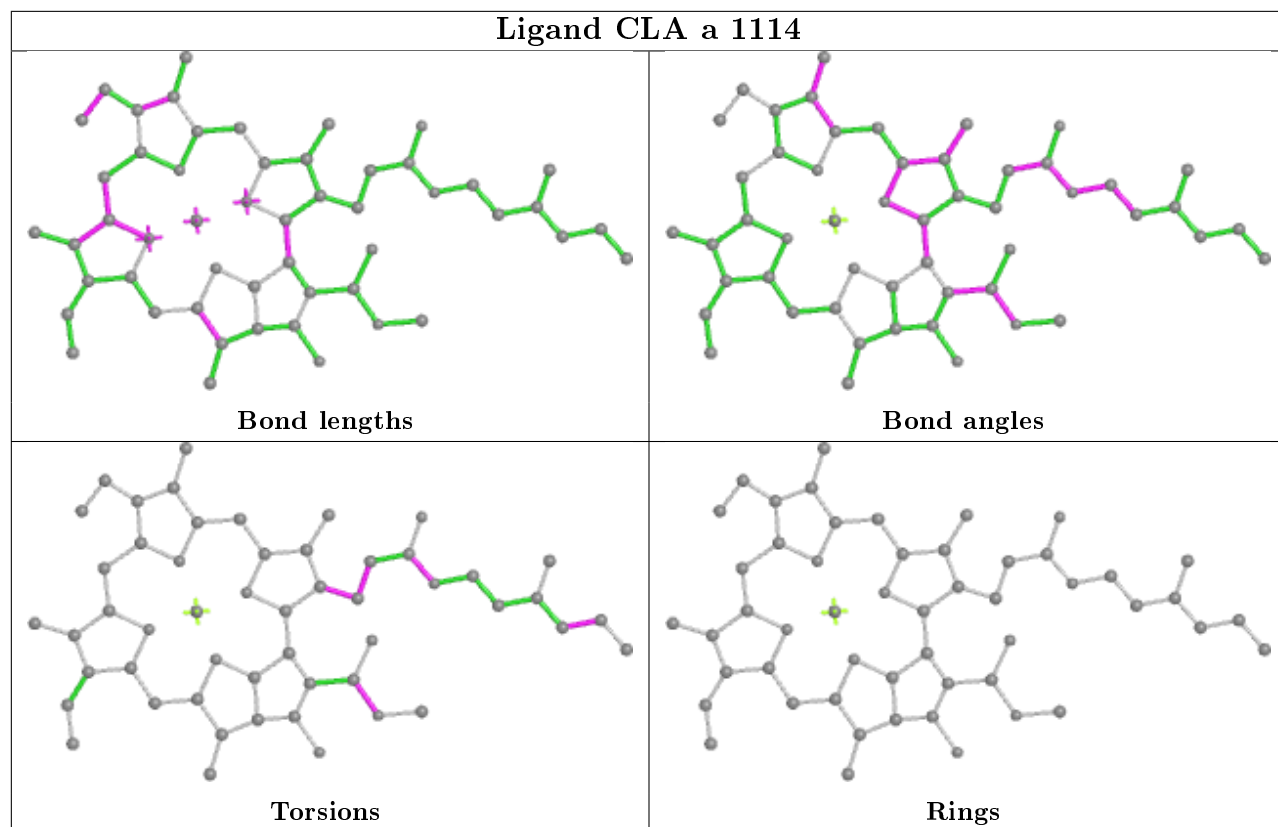


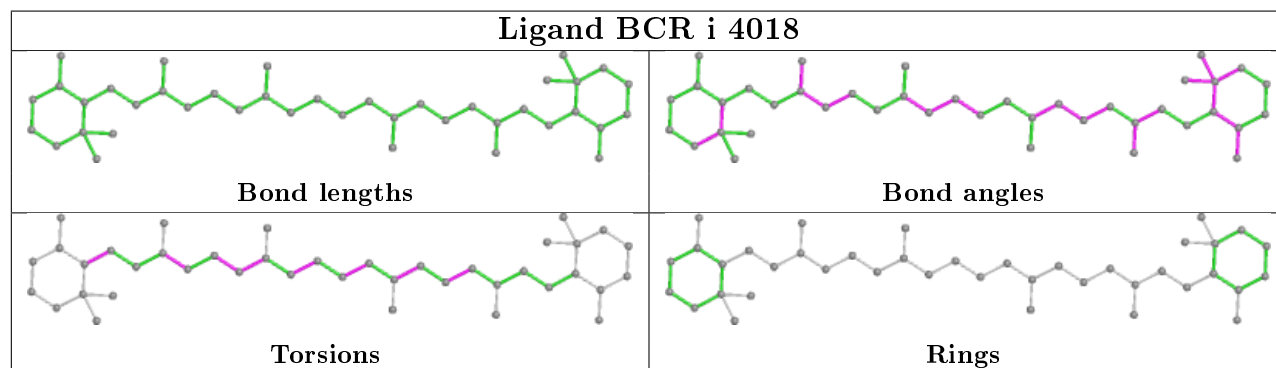
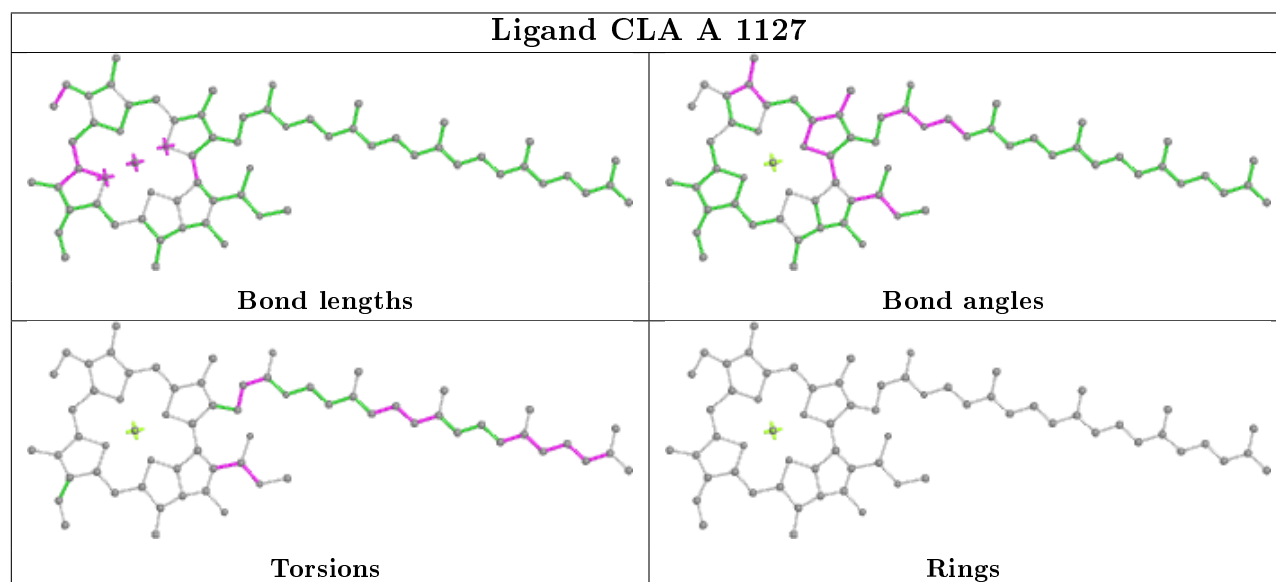
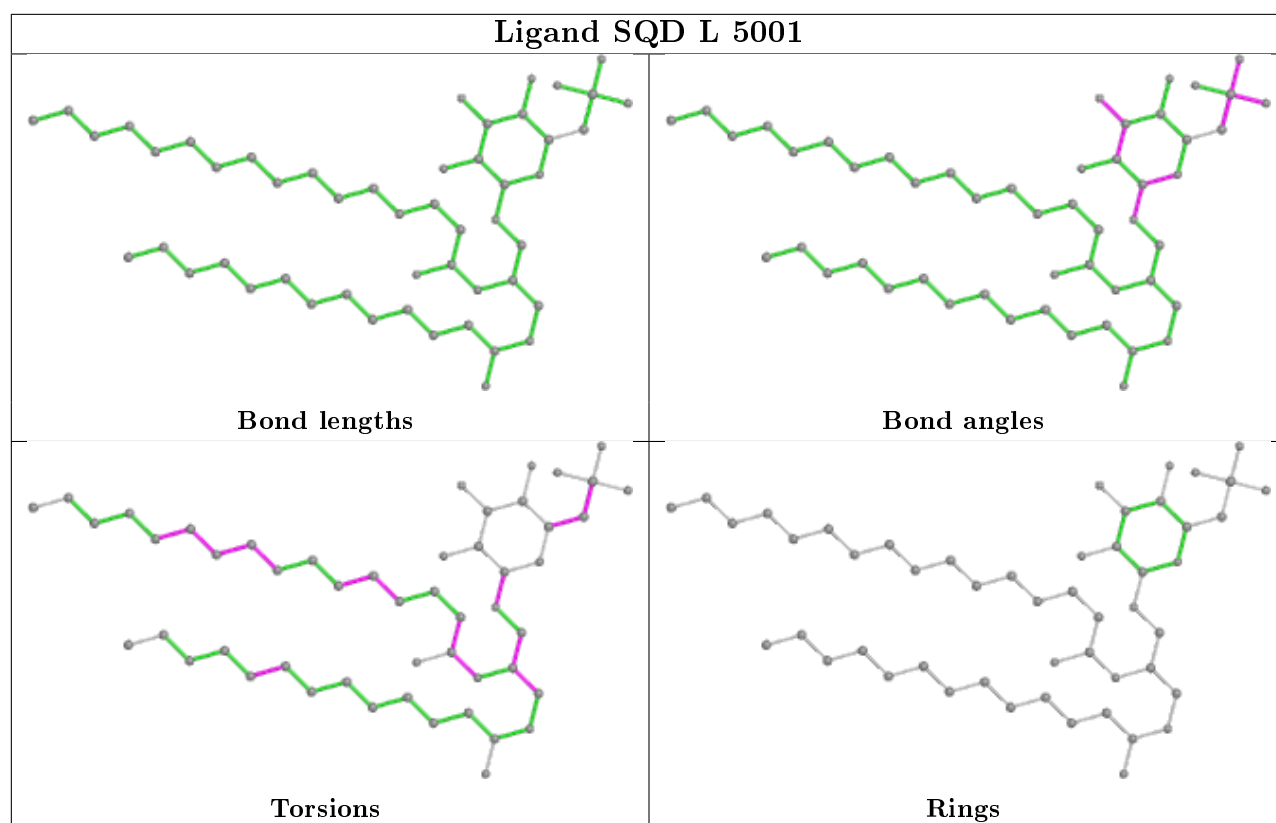


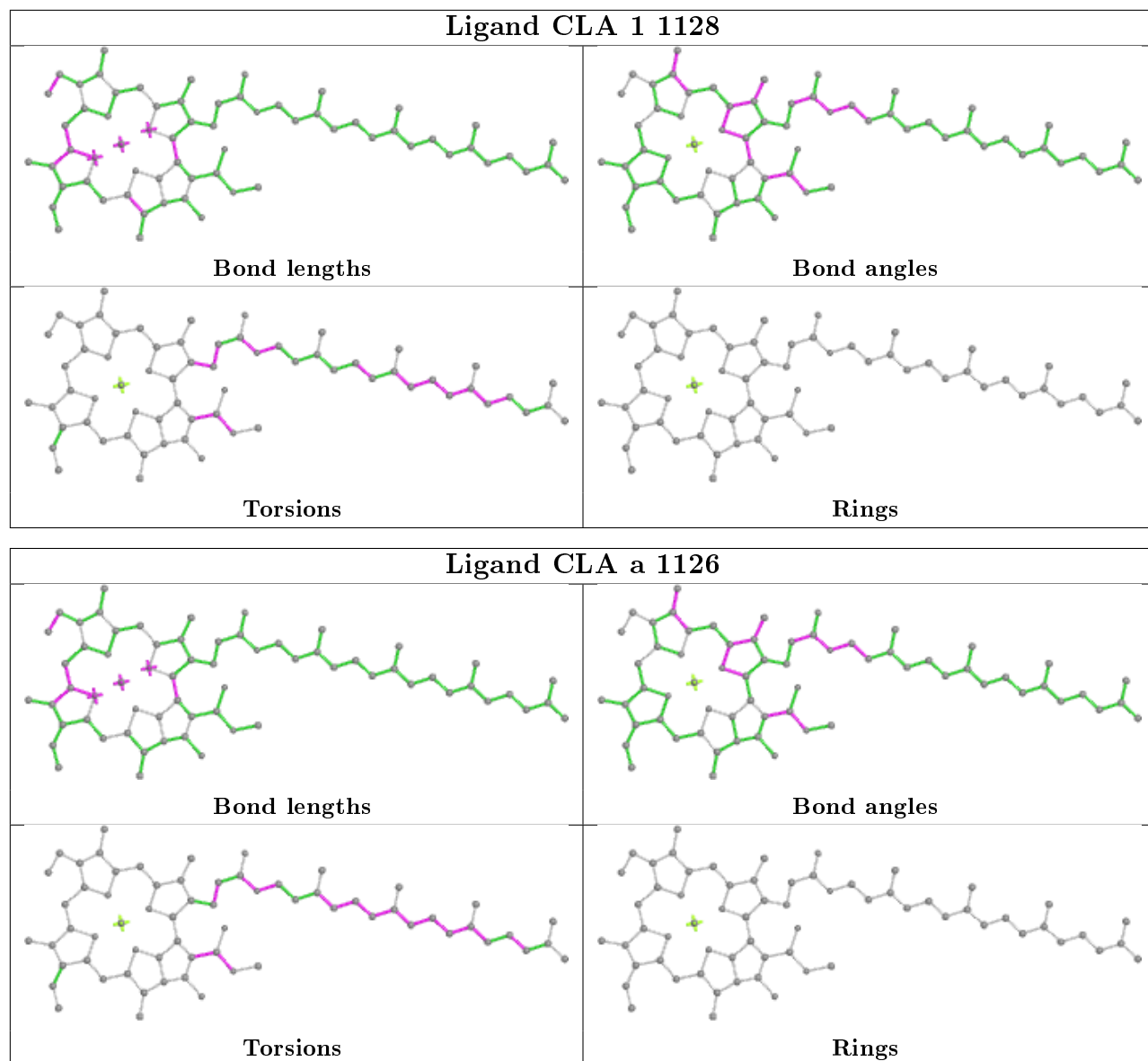
Ligand CLA A 1109**Ligand CLA J 1302****Ligand CLA a 1135**

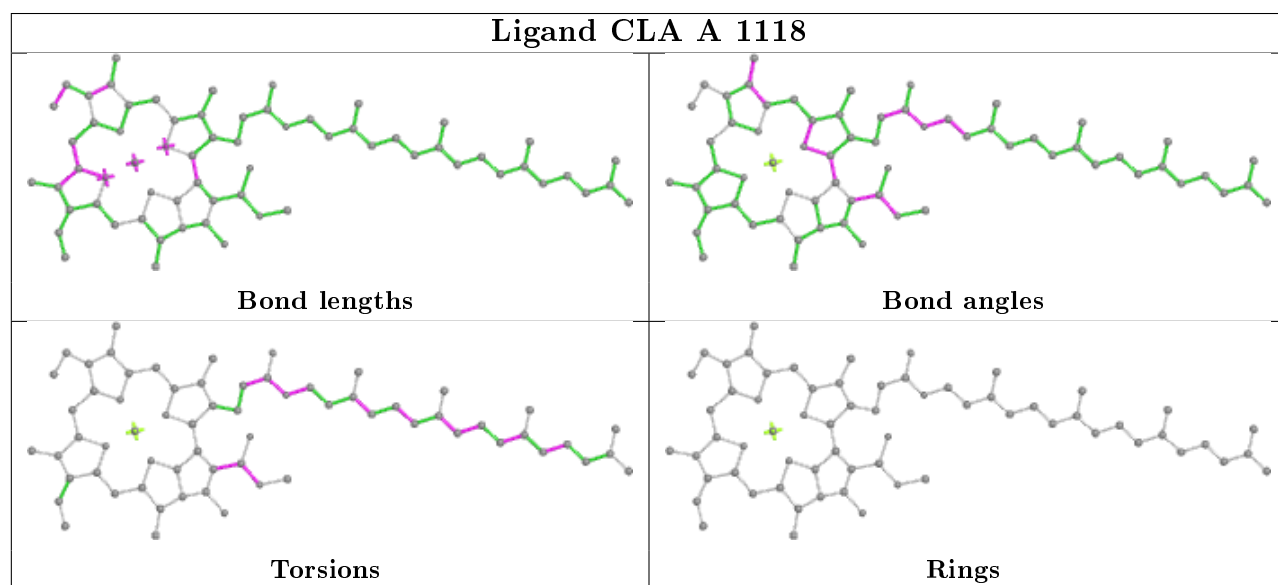
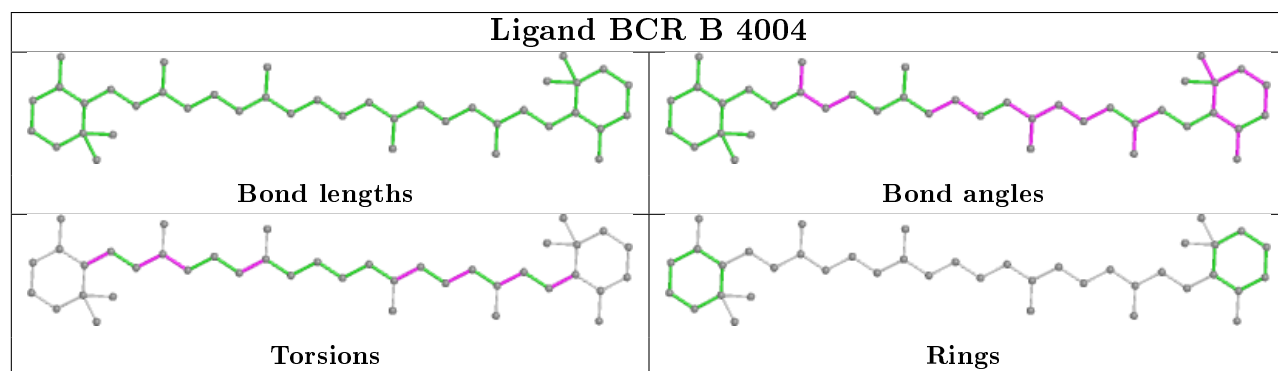
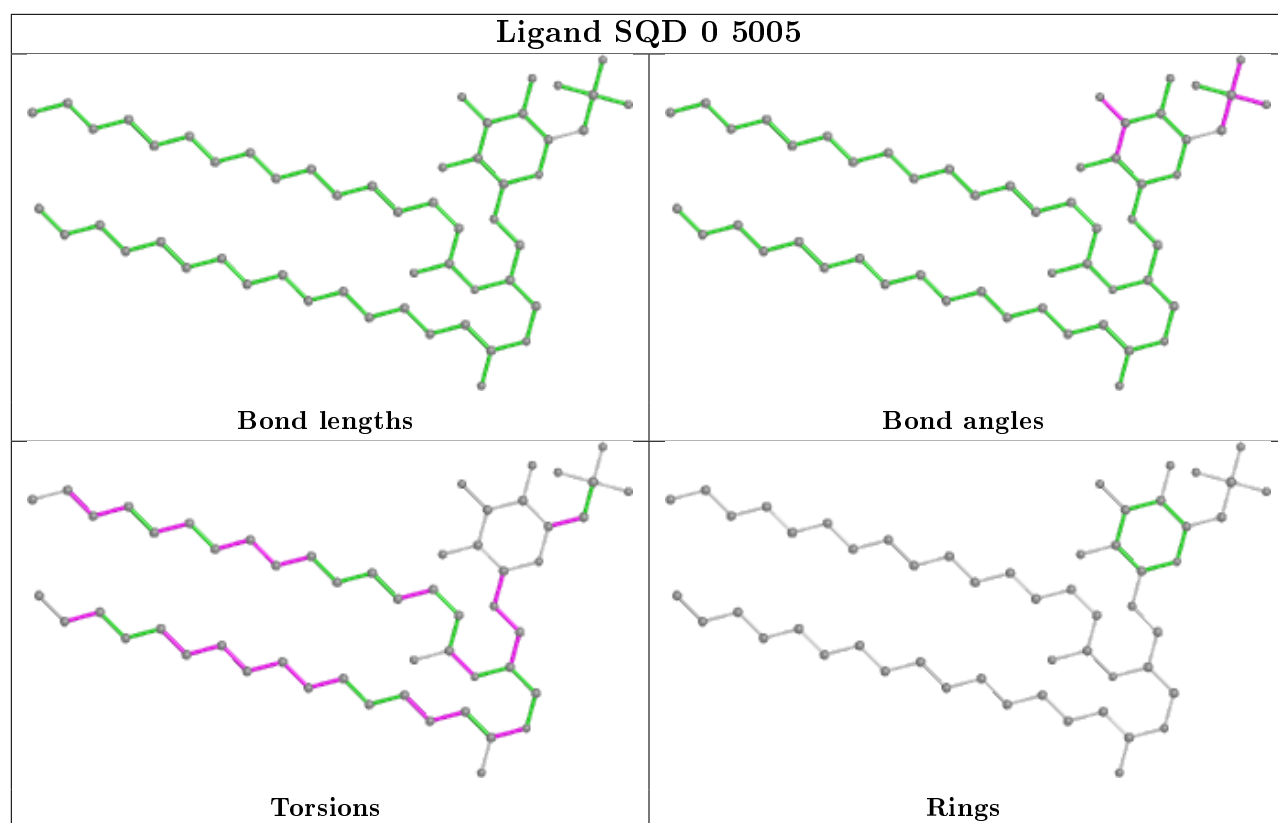


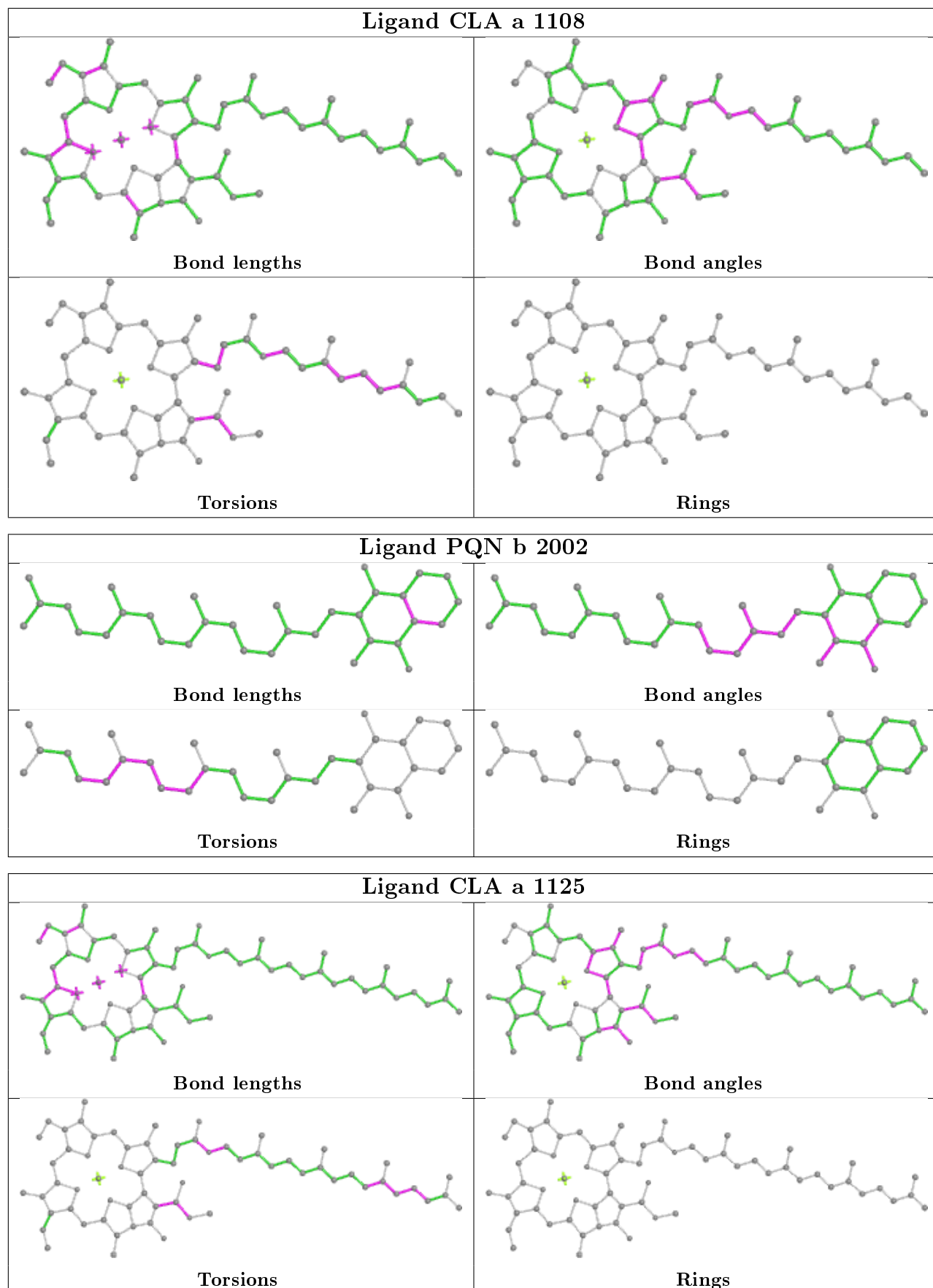


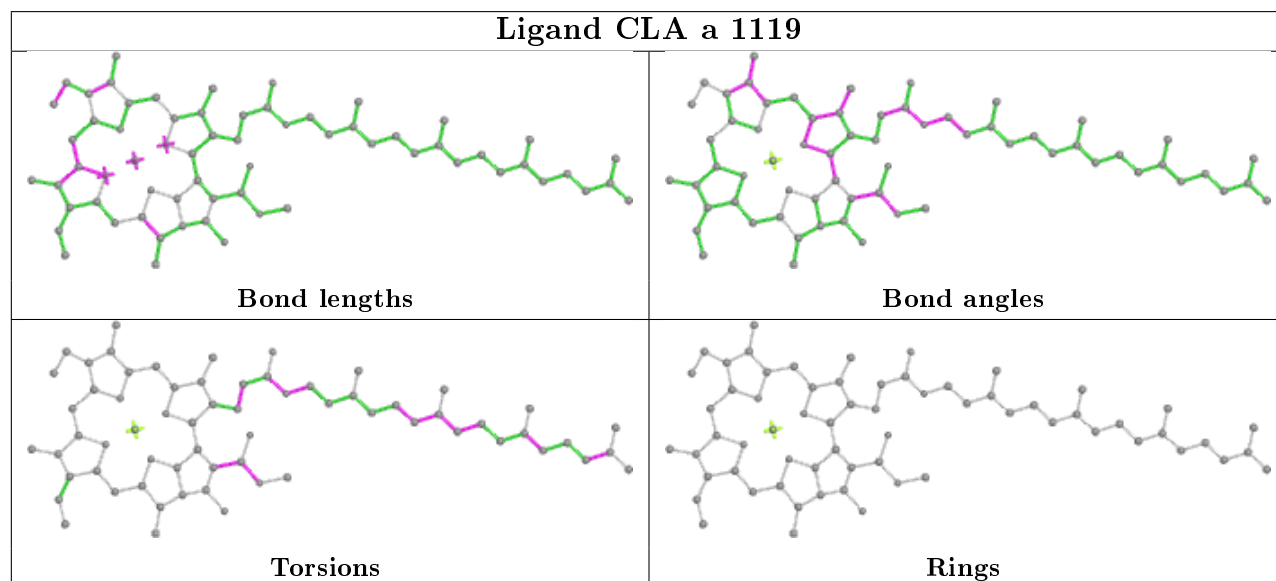
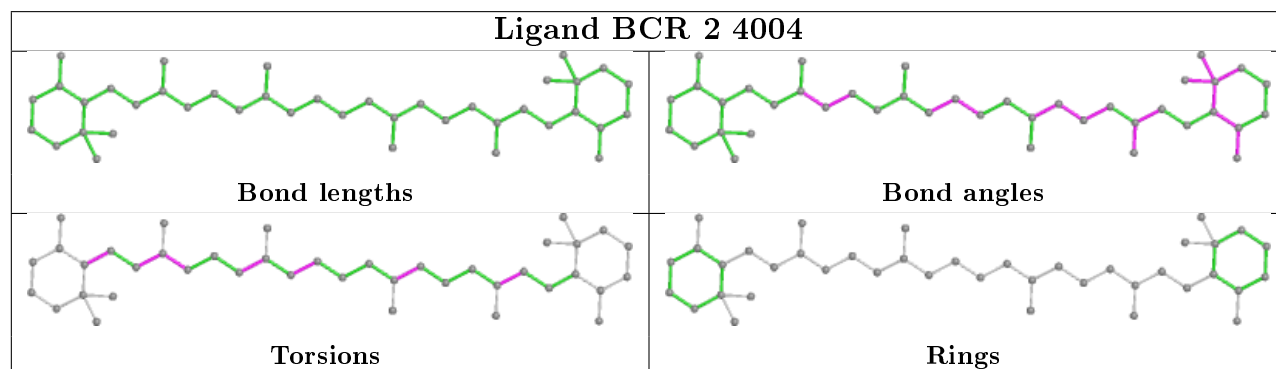
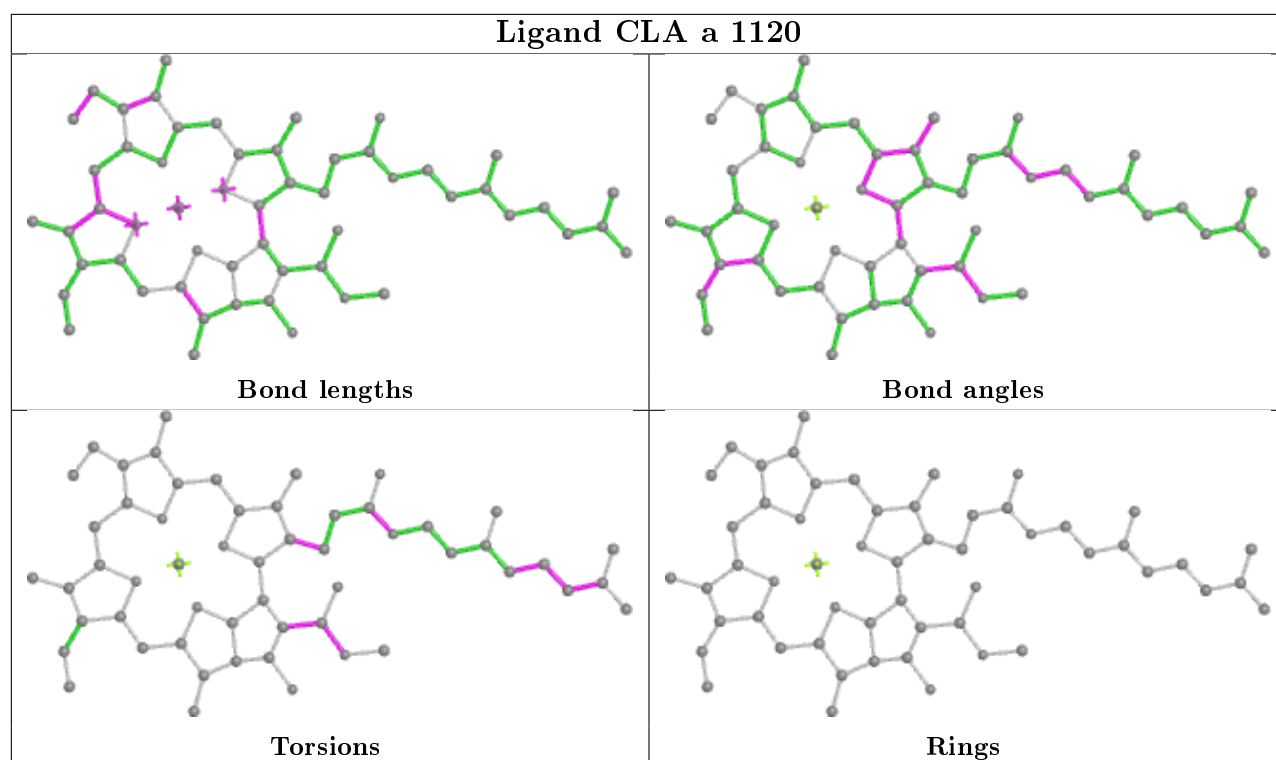












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	751/751 (100%)	-0.19	20 (2%) 54 58	29, 47, 72, 134	0
1	a	751/751 (100%)	0.97	140 (18%) 1 1	48, 95, 149, 209	0
2	2	731/731 (100%)	0.85	131 (17%) 1 1	43, 101, 146, 169	0
2	B	731/731 (100%)	0.06	42 (5%) 23 25	29, 56, 90, 152	0
3	3	80/80 (100%)	1.51	23 (28%) 0 0	54, 84, 110, 119	0
3	C	80/80 (100%)	-0.47	1 (1%) 77 79	33, 45, 59, 81	0
4	D	141/141 (100%)	-0.24	7 (4%) 28 30	30, 44, 70, 120	0
4	d	141/141 (100%)	0.81	27 (19%) 1 1	56, 82, 106, 136	0
5	5	69/69 (100%)	1.53	16 (23%) 0 0	75, 109, 122, 128	0
5	E	69/69 (100%)	0.59	10 (14%) 2 2	45, 62, 91, 97	0
6	6	143/143 (100%)	2.13	62 (43%) 0 0	114, 141, 158, 189	0
6	F	143/143 (100%)	-0.03	7 (4%) 29 31	56, 78, 94, 130	0
6	f	143/143 (100%)	0.86	27 (18%) 1 1	60, 97, 112, 132	0
7	I	40/40 (100%)	-0.02	0 100 100	36, 49, 87, 107	0
7	i	40/40 (100%)	0.48	3 (7%) 14 14	41, 49, 103, 132	0
8	7	40/40 (100%)	1.29	13 (32%) 0 0	109, 128, 152, 165	0
8	J	40/40 (100%)	-0.13	2 (5%) 28 30	54, 69, 95, 101	0
8	j	40/40 (100%)	0.81	8 (20%) 1 0	87, 98, 117, 132	0
9	K	80/80 (100%)	1.71	27 (33%) 0 0	53, 72, 127, 146	38 (47%)
10	L	157/157 (100%)	-0.03	6 (3%) 40 43	36, 43, 64, 131	0
10	l	157/157 (100%)	0.36	14 (8%) 9 9	45, 60, 107, 184	0
11	9	31/31 (100%)	0.30	3 (9%) 7 7	78, 86, 98, 111	0
11	M	31/31 (100%)	-0.30	1 (3%) 47 51	49, 58, 66, 96	0
11	m	31/31 (100%)	-0.58	0 100 100	38, 43, 55, 67	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
12	b	729/729 (100%)	-0.11	12 (1%) 72 74	39, 54, 75, 93	0
13	c	81/81 (100%)	0.25	4 (4%) 29 31	54, 69, 83, 96	0
14	e	68/68 (100%)	2.09	33 (48%) 0 0	63, 79, 100, 108	0
15	k	78/78 (100%)	4.54	61 (78%) 0 0	140, 160, 200, 208	38 (48%)
16	1	744/744 (100%)	1.09	150 (20%) 1 0	42, 90, 121, 151	0
17	4	140/140 (100%)	0.68	27 (19%) 1 1	51, 76, 105, 120	0
18	h	38/38 (100%)	0.60	7 (18%) 1 1	54, 68, 95, 96	0
19	8	79/79 (100%)	3.23	43 (54%) 0 0	103, 127, 168, 172	39 (49%)
20	0	154/154 (100%)	-0.26	3 (1%) 66 69	38, 51, 73, 108	0
All	All	6771/6771 (100%)	0.57	930 (13%) 3 2	29, 70, 138, 209	115 (1%)

The worst 5 of 930 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	a	4	SER	15.3
15	k	81	VAL	14.4
15	k	15	THR	13.7
1	a	6	PRO	12.8
1	a	5	PRO	12.1

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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

6.3 Carbohydrates ⓘ

There are no monosaccharides in this entry.

6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
24	BCR	k	4001	40/40	0.22	0.61	119,152,167,168	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
24	BCR	8	4001	40/40	0.53	0.54	105,124,139,140	0
34	ZEX	7	4015	42/42	0.54	0.43	100,131,150,152	0
27	ACT	a	7001	4/4	0.55	0.18	128,130,130,131	0
24	BCR	2	4004	40/40	0.56	0.86	105,125,145,147	0
25	LHG	B	5006	49/49	0.60	0.90	84,117,143,146	0
26	LMG	A	5008	55/55	0.60	0.65	72,119,146,146	0
26	LMG	b	5007	55/55	0.62	0.61	76,97,115,116	0
24	BCR	B	4018	40/40	0.62	0.61	64,85,115,121	0
21	CLA	a	1113	50/65	0.62	0.47	116,145,155,159	0
24	BCR	K	4001	40/40	0.62	0.38	40,73,103,106	0
25	LHG	1	5005	49/49	0.63	0.38	90,126,165,169	0
25	LHG	F	5002	49/49	0.64	0.41	73,110,175,181	0
24	BCR	1	4001	40/40	0.65	0.50	90,109,136,137	0
24	BCR	1	4019	40/40	0.66	0.63	106,122,142,143	0
24	BCR	b	4018	40/40	0.67	0.45	53,76,95,100	0
24	BCR	2	4018	40/40	0.67	0.81	83,136,143,144	0
24	BCR	2	4005	40/40	0.68	0.34	81,113,134,136	0
21	CLA	6	1302	43/65	0.68	0.56	116,141,171,178	0
26	LMG	B	5005	55/55	0.68	0.40	71,110,133,137	0
34	ZEX	j	4015	42/42	0.69	0.37	51,97,113,117	0
24	BCR	7	4013	40/40	0.69	0.39	78,113,122,124	0
25	LHG	l	5004	49/49	0.69	0.26	48,75,159,163	0
25	LHG	a	5007	49/49	0.70	0.70	100,139,169,175	0
25	LHG	l	5002	49/49	0.70	0.29	65,87,148,157	0
21	CLA	2	1217	52/65	0.71	0.34	99,130,138,139	0
25	LHG	a	5005	49/49	0.71	0.25	51,107,175,183	0
25	LHG	1	5007	49/49	0.72	0.46	80,102,149,154	0
26	LMG	2	5005	55/55	0.72	0.54	105,127,150,153	0
37	DGD	L	5004	66/66	0.72	0.33	42,87,116,121	0
31	SQD	b	5006	54/54	0.72	0.32	46,81,138,143	0
27	ACT	B	7001	4/4	0.72	0.38	57,71,71,74	0
24	BCR	a	4003	40/40	0.72	0.39	81,121,142,146	0
24	BCR	a	4001	40/40	0.72	0.34	89,142,156,156	0
35	LMT	1	6001	35/35	0.72	0.40	76,127,136,141	0
25	LHG	M	5001	49/49	0.72	0.24	51,97,144,149	0
25	LHG	0	5004	49/49	0.73	0.30	55,96,124,136	0
26	LMG	a	5002	50/55	0.73	0.23	54,78,109,110	0
25	LHG	A	5006	49/49	0.73	0.36	44,81,137,147	0
24	BCR	a	4019	40/40	0.74	0.53	98,114,155,155	0
24	BCR	a	4002	40/40	0.74	0.27	108,123,141,142	0
25	LHG	2	5004	49/49	0.74	0.41	92,108,152,153	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
24	BCR	A	4019	40/40	0.74	0.55	72,84,114,114	0
21	CLA	2	1209	45/65	0.75	0.36	104,130,139,142	0
23	SF4	C	3002	8/8	0.75	0.23	43,65,114,208	0
31	SQD	f	5001	54/54	0.75	0.36	42,100,123,132	0
25	LHG	6	5001	12/49	0.75	0.23	80,131,152,159	0
26	LMG	A	5002	50/55	0.76	0.23	40,72,99,106	0
24	BCR	1	4003	40/40	0.76	0.32	71,105,134,138	0
34	ZEX	J	4015	42/42	0.76	0.30	55,68,112,116	0
35	LMT	l	6001	35/35	0.76	0.36	55,95,118,120	0
21	CLA	1	1108	47/65	0.76	0.33	50,112,123,128	0
21	CLA	2	1240	41/65	0.76	0.48	131,137,146,150	0
31	SQD	0	5005	54/54	0.76	0.23	59,91,141,148	0
25	LHG	A	5005	49/49	0.76	0.27	48,72,132,139	0
25	LHG	l	5001	49/49	0.77	0.37	64,92,141,144	0
21	CLA	k	1402	49/65	0.77	0.26	134,158,161,161	8
24	BCR	6	4016	40/40	0.77	0.42	59,91,128,129	0
21	CLA	2	1216	50/65	0.77	0.32	91,127,138,139	0
25	LHG	l	5003	49/49	0.77	0.36	81,111,137,138	0
25	LHG	A	5007	49/49	0.77	0.32	46,85,113,121	0
21	CLA	B	1240	65/65	0.77	0.40	76,105,133,136	0
30	ECH	2	4006	41/41	0.77	0.34	65,122,132,133	0
21	CLA	2	1212	41/65	0.77	0.34	100,132,137,144	0
24	BCR	j	4013	40/40	0.78	0.32	72,90,121,123	0
21	CLA	2	1231	46/65	0.78	0.27	84,122,128,129	0
21	CLA	a	1114	52/65	0.78	0.34	119,138,150,152	0
26	LMG	1	5002	50/55	0.78	0.31	44,94,119,120	0
24	BCR	B	4004	40/40	0.78	0.31	63,93,109,110	0
26	LMG	K	5009	55/55	0.78	0.24	41,80,106,107	0
21	CLA	J	1302	65/65	0.79	0.32	75,95,121,137	0
24	BCR	1	4012	40/40	0.79	0.33	100,112,124,125	0
31	SQD	F	5001	54/54	0.79	0.42	66,93,129,134	0
21	CLA	a	1112	65/65	0.80	0.26	74,129,135,137	0
26	LMG	b	5005	55/55	0.80	0.36	54,79,114,116	0
21	CLA	1	1105	50/65	0.80	0.28	96,116,123,126	0
21	CLA	a	1118	65/65	0.80	0.24	102,119,142,150	0
21	CLA	1	1139	65/65	0.80	0.28	75,115,124,125	0
21	CLA	k	1401	50/65	0.80	0.24	84,137,147,152	5
21	CLA	a	1115	65/65	0.80	0.28	89,133,152,154	0
21	CLA	a	1120	55/65	0.80	0.27	98,124,129,138	0
26	LMG	a	5004	55/55	0.80	0.26	85,112,130,136	0
21	CLA	2	1234	50/65	0.81	0.25	90,107,111,113	0
21	CLA	2	1213	50/65	0.81	0.35	99,122,130,139	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
21	CLA	J	1303	65/65	0.81	0.34	93,112,125,127	0
21	CLA	2	1232	45/65	0.81	0.25	101,128,147,151	0
26	LMG	1	5004	55/55	0.81	0.36	83,97,112,118	0
21	CLA	2	1219	53/65	0.81	0.24	108,125,148,156	0
21	CLA	1	1138	60/65	0.81	0.28	84,118,134,136	0
24	BCR	2	4010	40/40	0.81	0.32	66,101,136,136	0
21	CLA	a	1102	65/65	0.81	0.33	68,92,118,128	0
21	CLA	a	1108	57/65	0.81	0.22	91,124,129,130	0
21	CLA	2	1218	65/65	0.81	0.31	91,133,158,162	0
21	CLA	1	1134	65/65	0.81	0.24	89,105,120,125	0
21	CLA	j	1302	65/65	0.82	0.35	77,110,125,133	0
24	BCR	B	4005	40/40	0.82	0.27	45,78,102,103	0
21	CLA	7	1303	41/65	0.82	0.39	133,150,155,157	0
21	CLA	1	1113	44/65	0.82	0.31	83,124,133,135	0
27	ACT	A	7001	4/4	0.82	0.33	28,55,63,71	0
21	CLA	1	1109	65/65	0.82	0.45	72,109,120,122	0
24	BCR	b	4014	40/40	0.82	0.29	59,79,88,92	0
31	SQD	L	5002	54/54	0.83	0.23	33,61,95,99	0
21	CLA	2	1202	65/65	0.83	0.26	56,94,106,108	0
21	CLA	2	1235	53/65	0.83	0.24	82,112,122,123	0
23	SF4	A	3001	8/8	0.83	0.27	40,87,137,173	0
26	LMG	0	5001	55/55	0.83	0.28	34,74,99,107	0
21	CLA	a	1123	65/65	0.83	0.30	55,105,117,121	0
21	CLA	1	1120	65/65	0.83	0.20	85,102,126,128	0
24	BCR	2	4014	40/40	0.83	0.35	78,113,132,136	0
21	CLA	j	1303	55/65	0.83	0.42	97,117,130,137	0
21	CLA	2	1214	59/65	0.84	0.25	70,109,135,159	0
21	CLA	1	1123	65/65	0.84	0.28	49,86,107,115	0
21	CLA	6	1301	47/65	0.84	0.22	99,128,135,136	0
31	SQD	B	5008	54/54	0.84	0.32	61,86,107,113	0
21	CLA	1	1103	65/65	0.84	0.25	63,87,101,103	0
21	CLA	1	1114	45/65	0.84	0.36	107,117,125,129	0
26	LMG	A	5004	48/55	0.84	0.31	37,84,102,107	0
21	CLA	a	1801	55/65	0.84	0.24	83,118,128,133	0
24	BCR	a	4007	40/40	0.84	0.37	69,87,144,147	0
24	BCR	A	4003	40/40	0.85	0.26	32,53,89,91	0
24	BCR	1	4002	40/40	0.85	0.24	89,100,119,123	0
24	BCR	1	4007	40/40	0.85	0.32	55,73,127,132	0
21	CLA	1	1013	65/65	0.85	0.28	73,91,97,104	0
24	BCR	a	4008	40/40	0.85	0.28	51,82,109,118	0
24	BCR	l	4022	40/40	0.85	0.25	57,74,97,100	0
24	BCR	9	4021	40/40	0.85	0.29	58,80,116,118	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
21	CLA	7	1302	41/65	0.85	0.42	120,130,140,143	0
21	CLA	2	1229	65/65	0.86	0.26	83,109,124,136	0
22	PQN	1	2001	33/33	0.86	0.29	67,88,108,108	0
24	BCR	b	4004	40/40	0.86	0.21	36,60,76,87	0
21	CLA	2	1230	47/65	0.86	0.18	89,114,127,129	0
21	CLA	1	1115	65/65	0.86	0.23	78,119,130,131	0
25	LHG	B	5004	49/49	0.86	0.25	73,87,96,101	0
21	CLA	B	1232	50/65	0.86	0.23	81,92,105,108	0
21	CLA	2	1222	50/65	0.86	0.32	69,105,119,122	0
26	LMG	2	5002	55/55	0.86	0.26	55,72,93,107	0
33	MG	B	6002	1/1	0.86	0.23	69,69,69,69	0
21	CLA	1	1117	65/65	0.86	0.31	57,99,112,123	0
21	CLA	a	1116	60/65	0.86	0.27	79,99,109,110	0
31	SQD	L	5001	51/54	0.86	0.21	42,80,104,107	0
21	CLA	2	1220	45/65	0.86	0.27	114,124,128,132	0
21	CLA	a	1011	65/65	0.86	0.20	40,58,71,96	0
21	CLA	1	1116	65/65	0.86	0.22	75,95,118,121	0
25	LHG	0	5002	49/49	0.86	0.17	44,63,131,140	0
21	CLA	a	1111	65/65	0.86	0.28	76,106,131,133	0
21	CLA	b	1231	65/65	0.86	0.20	50,69,93,98	0
21	CLA	2	1215	60/65	0.87	0.23	73,100,112,118	0
21	CLA	F	1302	65/65	0.87	0.22	70,93,105,114	0
21	CLA	a	1139	65/65	0.87	0.20	64,86,103,105	0
25	LHG	L	5005	49/49	0.87	0.22	46,75,102,104	0
21	CLA	B	1231	65/65	0.87	0.22	66,84,101,104	0
35	LMT	L	6001	35/35	0.87	0.27	55,79,90,97	0
21	CLA	1	1104	65/65	0.87	0.27	65,91,99,106	0
21	CLA	a	1101	65/65	0.87	0.21	50,83,91,100	0
21	CLA	1	1118	65/65	0.87	0.22	79,103,130,134	0
21	CLA	2	1236	50/65	0.87	0.27	75,110,117,124	0
25	LHG	a	5003	49/49	0.87	0.36	76,96,106,109	0
21	CLA	2	1221	65/65	0.87	0.25	84,95,132,137	0
21	CLA	f	1302	65/65	0.87	0.35	67,99,109,115	0
21	CLA	b	1236	65/65	0.87	0.25	48,74,118,122	0
21	CLA	B	1209	65/65	0.87	0.23	67,88,123,127	0
21	CLA	A	1113	65/65	0.87	0.31	41,64,105,111	0
21	CLA	2	1225	65/65	0.88	0.22	52,92,111,114	0
21	CLA	2	1227	45/65	0.88	0.18	81,94,127,131	0
21	CLA	a	1105	58/65	0.88	0.25	78,110,122,129	0
30	ECH	b	4011	41/41	0.88	0.28	60,81,90,94	0
21	CLA	2	1208	60/65	0.88	0.18	63,88,138,142	0
21	CLA	1	1133	65/65	0.88	0.20	73,87,99,107	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
21	CLA	a	1121	65/65	0.88	0.28	94,117,142,146	0
24	BCR	a	4012	40/40	0.88	0.26	66,95,106,110	0
21	CLA	B	1219	65/65	0.88	0.19	73,94,125,126	0
24	BCR	2	4011	40/40	0.88	0.26	60,93,104,109	0
24	BCR	f	4016	40/40	0.88	0.22	66,81,104,107	0
21	CLA	2	1210	65/65	0.88	0.23	75,107,116,119	0
24	BCR	B	4010	40/40	0.88	0.32	51,66,81,84	0
25	LHG	1	5003	49/49	0.88	0.33	62,83,96,99	0
21	CLA	a	1125	65/65	0.88	0.24	64,91,106,111	0
21	CLA	a	1110	59/65	0.88	0.23	77,109,156,159	0
21	CLA	a	1134	49/65	0.88	0.17	73,118,128,132	0
21	CLA	a	1119	65/65	0.88	0.27	54,82,128,133	0
21	CLA	a	1107	50/65	0.89	0.18	68,88,108,112	0
21	CLA	a	1122	65/65	0.89	0.23	61,95,108,113	0
24	BCR	0	4022	40/40	0.89	0.24	41,60,87,92	0
32	CA	2	6001	1/1	0.89	0.06	112,112,112,112	0
21	CLA	B	1216	65/65	0.89	0.24	65,85,101,106	0
21	CLA	a	1109	65/65	0.89	0.20	65,102,118,124	0
21	CLA	F	1301	65/65	0.89	0.22	53,77,121,124	0
21	CLA	a	1117	65/65	0.89	0.38	64,89,103,112	0
24	BCR	1	4008	40/40	0.89	0.24	49,69,93,95	0
24	BCR	A	4002	40/40	0.89	0.24	33,60,75,82	0
21	CLA	1	1112	50/65	0.89	0.23	83,109,122,126	0
24	BCR	L	4022	40/40	0.89	0.21	41,57,81,86	0
30	ECH	B	4006	41/41	0.89	0.19	45,86,105,108	0
21	CLA	1	1127	65/65	0.89	0.28	64,86,112,118	0
21	CLA	b	1227	65/65	0.89	0.25	58,73,120,124	0
24	BCR	b	4010	40/40	0.89	0.21	41,58,68,71	0
21	CLA	b	1240	65/65	0.89	0.23	60,88,134,154	0
21	CLA	1	1107	51/65	0.89	0.17	83,102,117,121	0
21	CLA	2	1211	50/65	0.90	0.16	80,110,117,123	0
25	LHG	1	5001	49/49	0.90	0.24	64,84,101,104	0
21	CLA	a	1128	65/65	0.90	0.20	59,86,97,102	0
21	CLA	1	1102	55/65	0.90	0.21	50,81,117,120	0
21	CLA	1	1121	55/65	0.90	0.20	58,96,124,128	0
21	CLA	1	1126	65/65	0.90	0.23	58,94,108,115	0
21	CLA	b	1232	65/65	0.90	0.22	64,79,121,123	0
24	BCR	l	4019	40/40	0.90	0.23	29,44,54,56	0
24	BCR	b	4005	40/40	0.90	0.19	30,47,90,91	0
21	CLA	b	1222	65/65	0.90	0.25	38,54,114,118	0
21	CLA	B	1218	65/65	0.90	0.25	62,91,123,125	0
28	45D	h	4020	42/42	0.90	0.19	33,55,68,75	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
21	CLA	2	1203	65/65	0.90	0.26	57,88,101,105	0
21	CLA	a	1106	65/65	0.90	0.24	58,95,106,112	0
25	LHG	b	5004	49/49	0.90	0.23	63,80,101,105	0
21	CLA	a	1133	65/65	0.90	0.19	70,95,114,117	0
21	CLA	1	1128	65/65	0.90	0.21	62,79,99,113	0
21	CLA	2	1205	65/65	0.90	0.20	54,77,89,91	0
21	CLA	a	1129	52/65	0.90	0.17	64,85,95,98	0
21	CLA	B	1217	65/65	0.90	0.23	64,93,113,116	0
21	CLA	1	1012	65/65	0.90	0.26	72,88,98,101	0
21	CLA	b	1021	65/65	0.90	0.18	36,52,66,72	0
21	CLA	b	1230	65/65	0.90	0.22	53,86,120,125	0
35	LMT	F	6001	35/35	0.90	0.28	57,88,112,115	0
21	CLA	1	1101	65/65	0.91	0.22	58,88,120,123	0
21	CLA	B	1234	65/65	0.91	0.22	39,73,95,100	0
21	CLA	B	1214	65/65	0.91	0.22	48,81,89,92	0
21	CLA	B	1213	65/65	0.91	0.18	58,80,112,120	0
21	CLA	b	1208	60/65	0.91	0.15	36,53,91,103	0
21	CLA	b	1220	65/65	0.91	0.20	48,64,100,103	0
21	CLA	l	1501	65/65	0.91	0.21	48,69,110,117	0
30	ECH	i	4020	41/41	0.91	0.22	38,53,83,90	0
26	LMG	b	5002	55/55	0.91	0.20	36,55,84,89	0
26	LMG	B	5002	55/55	0.91	0.19	36,52,81,89	0
21	CLA	b	1228	65/65	0.91	0.18	58,73,117,121	0
29	CL	2	6000	1/1	0.91	0.31	74,74,74,74	0
21	CLA	1	1125	65/65	0.91	0.28	56,78,91,94	0
25	LHG	a	5001	49/49	0.91	0.25	57,72,117,128	0
21	CLA	B	1228	65/65	0.91	0.20	44,66,113,122	0
21	CLA	2	1223	55/65	0.91	0.26	64,99,141,145	0
21	CLA	B	1227	55/65	0.91	0.26	67,76,102,107	0
21	CLA	1	1111	65/65	0.91	0.19	63,85,113,118	0
30	ECH	b	4006	41/41	0.91	0.16	32,47,97,99	0
21	CLA	2	1228	45/65	0.91	0.16	53,67,126,132	0
24	BCR	J	4013	40/40	0.91	0.19	48,69,89,91	0
22	PQN	a	2001	33/33	0.91	0.24	39,65,84,87	0
27	ACT	B	7002	4/4	0.91	0.11	78,82,83,84	0
24	BCR	B	4017	40/40	0.91	0.25	22,44,56,57	0
21	CLA	A	1112	65/65	0.91	0.17	39,62,94,98	0
21	CLA	a	1126	65/65	0.91	0.24	71,91,104,105	0
21	CLA	8	1401	45/65	0.91	0.12	83,101,137,143	3
21	CLA	f	1301	50/65	0.91	0.15	74,93,114,116	0
21	CLA	2	1206	65/65	0.91	0.17	44,66,80,88	0
30	ECH	m	4021	41/41	0.91	0.19	23,49,80,80	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
21	CLA	K	1402	65/65	0.91	0.20	50,71,111,115	10
21	CLA	B	1210	65/65	0.91	0.16	38,67,90,92	0
21	CLA	B	1211	65/65	0.91	0.17	45,76,102,107	0
21	CLA	B	1212	55/65	0.92	0.17	70,82,128,132	0
21	CLA	2	1023	65/65	0.92	0.20	46,60,68,82	0
21	CLA	A	1122	60/65	0.92	0.16	25,42,70,83	0
34	ZEX	F	4016	42/42	0.92	0.16	46,72,98,103	0
21	CLA	1	1119	65/65	0.92	0.27	53,75,92,112	0
21	CLA	A	1123	65/65	0.92	0.18	25,38,52,60	0
21	CLA	b	1229	65/65	0.92	0.22	54,68,97,108	0
21	CLA	2	1021	65/65	0.92	0.24	45,67,114,117	0
24	BCR	B	4014	40/40	0.92	0.21	35,57,80,84	0
21	CLA	2	1226	55/65	0.92	0.20	55,70,91,97	0
21	CLA	A	1125	65/65	0.92	0.21	22,46,61,65	0
21	CLA	b	1206	65/65	0.92	0.17	28,48,62,80	0
35	LMT	0	6001	35/35	0.92	0.21	51,72,84,90	0
24	BCR	h	4018	40/40	0.92	0.21	36,60,75,79	0
21	CLA	a	1135	65/65	0.92	0.22	42,69,151,157	0
21	CLA	a	1138	65/65	0.92	0.16	50,77,85,90	0
24	BCR	b	4017	40/40	0.92	0.22	35,52,61,64	0
21	CLA	b	1213	65/65	0.92	0.28	39,64,89,93	0
21	CLA	b	1235	65/65	0.92	0.19	45,80,93,97	0
21	CLA	a	1136	65/65	0.92	0.19	44,73,87,100	0
21	CLA	B	1202	65/65	0.92	0.17	32,54,66,69	0
21	CLA	A	1134	65/65	0.92	0.19	25,57,107,111	0
21	CLA	1	1110	50/65	0.92	0.15	70,91,137,157	0
23	SF4	C	3003	8/8	0.92	0.14	53,74,78,84	0
24	BCR	i	4018	40/40	0.92	0.22	29,52,63,69	0
21	CLA	1	1106	65/65	0.92	0.21	49,91,119,122	0
21	CLA	B	1222	55/65	0.92	0.32	50,68,84,89	0
30	ECH	M	4021	41/41	0.92	0.15	45,61,74,81	0
21	CLA	1	1124	56/65	0.92	0.22	44,66,87,93	0
21	CLA	B	1230	65/65	0.92	0.21	29,68,110,114	0
21	CLA	B	1235	65/65	0.92	0.26	45,66,92,94	0
21	CLA	A	1133	65/65	0.92	0.19	28,48,78,81	0
24	BCR	A	4012	40/40	0.92	0.19	43,60,73,73	0
24	BCR	0	4019	40/40	0.92	0.17	35,57,67,69	0
21	CLA	L	1503	65/65	0.92	0.18	35,54,82,87	0
21	CLA	A	1107	65/65	0.93	0.17	42,56,121,124	0
21	CLA	A	1120	65/65	0.93	0.13	30,53,102,104	0
21	CLA	b	1237	65/65	0.93	0.16	36,55,71,76	0
24	BCR	2	4017	40/40	0.93	0.19	31,56,72,76	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
21	CLA	B	1225	65/65	0.93	0.25	41,61,70,76	0
21	CLA	8	1402	46/65	0.93	0.18	103,119,135,139	5
21	CLA	b	1234	53/65	0.93	0.19	40,57,75,91	0
21	CLA	b	1212	65/65	0.93	0.17	41,53,87,97	0
21	CLA	B	1220	57/65	0.93	0.17	53,78,101,108	0
21	CLA	b	1226	65/65	0.93	0.17	26,50,71,76	0
21	CLA	B	1221	65/65	0.93	0.18	50,62,95,98	0
21	CLA	2	1201	65/65	0.93	0.16	61,77,86,90	0
21	CLA	b	1219	60/65	0.93	0.22	33,66,132,132	0
21	CLA	A	1119	65/65	0.93	0.18	27,39,52,56	0
21	CLA	1	1140	65/65	0.93	0.20	60,77,119,120	0
21	CLA	a	1124	55/65	0.93	0.20	45,59,117,127	0
21	CLA	b	1214	65/65	0.93	0.20	33,49,89,98	0
21	CLA	b	1224	65/65	0.93	0.19	33,48,83,87	0
21	CLA	b	1209	65/65	0.93	0.14	40,57,100,107	0
21	CLA	2	1224	55/65	0.93	0.21	53,70,95,110	0
21	CLA	A	1139	65/65	0.93	0.17	43,59,83,91	0
21	CLA	A	1109	65/65	0.93	0.17	36,54,65,74	0
21	CLA	A	1115	65/65	0.93	0.21	41,57,69,72	0
21	CLA	B	1224	65/65	0.93	0.20	28,52,78,87	0
21	CLA	B	1226	65/65	0.93	0.18	31,51,70,79	0
21	CLA	A	1121	65/65	0.93	0.17	28,48,130,132	0
21	CLA	1	1122	60/65	0.93	0.18	47,75,101,106	0
21	CLA	1	1135	52/65	0.93	0.17	53,69,89,108	0
21	CLA	b	1218	65/65	0.93	0.19	46,66,101,102	0
25	LHG	A	5003	49/49	0.93	0.21	29,62,101,107	0
21	CLA	A	1105	65/65	0.93	0.16	44,68,92,95	0
21	CLA	b	1216	65/65	0.93	0.16	41,57,91,102	0
21	CLA	2	1204	65/65	0.93	0.17	35,67,89,91	0
21	CLA	A	1127	65/65	0.93	0.24	22,42,59,64	0
21	CLA	K	1401	65/65	0.93	0.22	33,63,97,102	15
21	CLA	A	1104	65/65	0.93	0.21	19,41,62,64	0
21	CLA	1	1011	65/65	0.93	0.18	38,62,88,103	0
21	CLA	1	1137	51/65	0.93	0.18	48,65,76,87	0
21	CLA	A	1114	65/65	0.93	0.18	56,75,111,116	0
21	CLA	A	1108	53/65	0.93	0.20	30,57,91,92	0
21	CLA	A	1126	65/65	0.93	0.15	28,48,62,75	0
21	CLA	2	1237	65/65	0.93	0.18	30,51,61,76	0
21	CLA	B	1236	50/65	0.93	0.27	44,63,96,101	0
21	CLA	B	1208	65/65	0.93	0.16	53,76,108,111	0
24	BCR	A	4001	40/40	0.93	0.15	35,52,68,68	0
36	EQ3	I	4020	42/42	0.94	0.22	24,37,48,66	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
21	CLA	0	1503	65/65	0.94	0.15	43,56,82,99	0
24	BCR	A	4007	40/40	0.94	0.19	31,46,106,108	0
21	CLA	b	1202	65/65	0.94	0.16	26,43,52,57	0
21	CLA	A	1116	65/65	0.94	0.26	36,53,86,90	0
21	CLA	b	1211	65/65	0.94	0.14	29,46,98,103	0
21	CLA	B	1215	65/65	0.94	0.26	33,57,92,99	0
21	CLA	B	1207	65/65	0.94	0.17	28,39,61,68	0
21	CLA	1	1801	56/65	0.94	0.15	62,76,106,112	0
21	CLA	l	1503	65/65	0.94	0.20	31,54,99,101	0
21	CLA	A	1128	65/65	0.94	0.17	29,43,62,86	0
21	CLA	2	1022	65/65	0.94	0.18	34,62,74,74	0
21	CLA	b	1238	65/65	0.94	0.17	30,52,63,69	0
21	CLA	a	1130	65/65	0.94	0.15	52,68,111,119	0
23	SF4	1	3001	8/8	0.94	0.17	57,66,94,130	0
21	CLA	B	1223	65/65	0.94	0.27	54,67,78,95	0
24	BCR	I	4018	40/40	0.94	0.21	24,45,59,67	0
21	CLA	A	1103	65/65	0.94	0.20	25,41,61,66	0
21	CLA	2	1239	65/65	0.94	0.18	39,57,93,104	0
22	PQN	2	2002	33/33	0.94	0.18	42,57,70,78	0
21	CLA	0	1502	65/65	0.94	0.16	32,49,77,84	0
21	CLA	a	1127	65/65	0.94	0.31	50,80,108,110	0
21	CLA	A	1011	65/65	0.94	0.15	20,37,61,79	0
21	CLA	A	1138	65/65	0.94	0.16	46,61,68,73	0
21	CLA	A	1135	65/65	0.94	0.17	25,42,100,107	0
21	CLA	b	1210	65/65	0.94	0.14	31,43,63,68	0
21	CLA	a	1104	65/65	0.94	0.23	40,68,105,111	0
28	45D	B	4011	42/42	0.94	0.18	31,49,61,69	0
23	SF4	3	3002	8/8	0.94	0.13	65,73,110,240	0
24	BCR	A	4008	40/40	0.94	0.25	17,46,78,82	0
21	CLA	A	1118	65/65	0.94	0.19	38,52,84,89	0
21	CLA	A	1129	58/65	0.94	0.17	20,42,92,96	0
22	PQN	b	2002	33/33	0.94	0.24	36,51,69,69	0
21	CLA	a	1103	65/65	0.94	0.26	49,67,130,133	0
21	CLA	a	1013	65/65	0.94	0.25	34,53,90,92	0
21	CLA	1	1132	65/65	0.94	0.14	23,48,63,71	0
21	CLA	A	1801	65/65	0.94	0.14	22,47,108,110	0
21	CLA	A	1102	65/65	0.95	0.14	32,49,106,120	0
21	CLA	b	1022	65/65	0.95	0.21	37,49,59,65	0
21	CLA	L	1502	65/65	0.95	0.20	21,36,98,103	0
21	CLA	b	1201	65/65	0.95	0.15	30,44,81,84	0
33	MG	b	6002	1/1	0.95	0.12	54,54,54,54	0
21	CLA	A	1117	65/65	0.95	0.29	31,46,56,59	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
25	LHG	A	5001	49/49	0.95	0.18	31,47,61,64	0
21	CLA	0	1501	65/65	0.95	0.18	37,47,74,82	0
21	CLA	A	1106	65/65	0.95	0.14	26,45,71,87	0
21	CLA	B	1204	65/65	0.95	0.16	32,50,67,83	0
21	CLA	B	1238	65/65	0.95	0.19	17,35,46,56	0
21	CLA	A	1124	65/65	0.95	0.19	23,35,118,122	0
21	CLA	l	1502	65/65	0.95	0.19	30,55,103,110	0
21	CLA	A	1111	65/65	0.95	0.17	31,48,81,86	0
21	CLA	b	1215	65/65	0.95	0.17	28,48,68,83	0
21	CLA	A	1140	65/65	0.95	0.18	25,43,66,76	0
21	CLA	L	1501	65/65	0.95	0.18	33,51,91,94	0
21	CLA	1	1136	65/65	0.95	0.13	46,66,77,83	0
21	CLA	b	1239	65/65	0.95	0.23	36,51,62,84	0
21	CLA	1	1131	65/65	0.95	0.17	35,47,69,74	0
21	CLA	B	1237	65/65	0.95	0.21	21,34,54,61	0
21	CLA	b	1225	65/65	0.95	0.21	23,41,59,63	0
21	CLA	A	1012	65/65	0.95	0.17	31,44,63,73	0
21	CLA	b	1217	51/65	0.95	0.11	32,56,86,95	0
21	CLA	A	1013	65/65	0.95	0.21	23,47,57,65	0
21	CLA	b	1221	65/65	0.95	0.15	31,50,85,99	0
21	CLA	b	1204	65/65	0.95	0.15	26,40,78,108	0
22	PQN	A	2001	33/33	0.95	0.18	30,46,57,64	0
21	CLA	A	1130	60/65	0.95	0.17	21,39,93,95	0
24	BCR	L	4019	40/40	0.95	0.17	24,38,45,52	0
21	CLA	B	1203	65/65	0.95	0.21	33,50,69,75	0
21	CLA	B	1205	65/65	0.95	0.15	34,43,69,74	0
21	CLA	b	1207	65/65	0.95	0.16	32,50,71,81	0
21	CLA	a	1140	65/65	0.95	0.21	48,70,93,95	0
21	CLA	b	1023	65/65	0.95	0.23	34,51,66,80	0
21	CLA	1	1130	55/65	0.95	0.14	29,53,83,95	0
21	CLA	B	1201	65/65	0.95	0.14	37,48,80,91	0
21	CLA	B	1021	65/65	0.95	0.14	30,42,53,61	0
21	CLA	a	1137	51/65	0.95	0.17	43,63,109,113	0
21	CLA	B	1229	65/65	0.95	0.19	40,60,80,85	0
21	CLA	A	1131	65/65	0.95	0.21	27,38,59,76	0
21	CLA	A	1101	65/65	0.96	0.15	32,50,68,74	0
21	CLA	2	1207	56/65	0.96	0.14	29,46,78,86	0
21	CLA	a	1012	65/65	0.96	0.22	25,57,101,103	0
21	CLA	B	1206	65/65	0.96	0.15	31,43,60,72	0
21	CLA	B	1023	65/65	0.96	0.22	21,33,45,55	0
21	CLA	B	1022	65/65	0.96	0.19	19,36,44,51	0
21	CLA	a	1131	65/65	0.96	0.17	36,58,68,71	0

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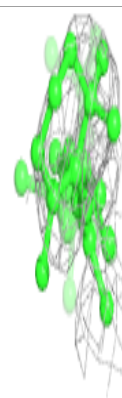
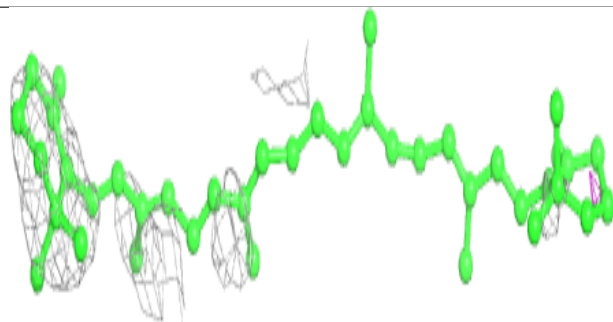
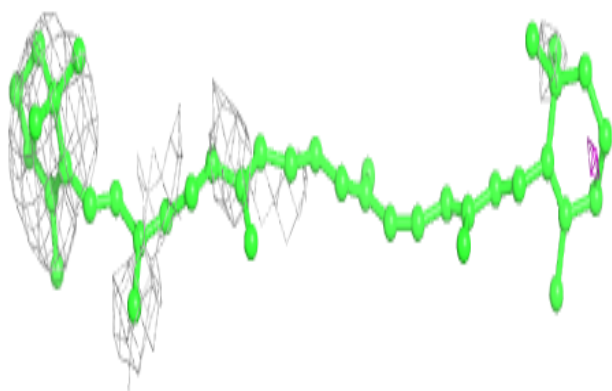
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
21	CLA	b	1205	65/65	0.96	0.13	28,43,59,65	0
21	CLA	2	1238	65/65	0.96	0.15	36,52,61,75	0
32	CA	l	1001	1/1	0.96	0.04	55,55,55,55	0
21	CLA	A	1136	65/65	0.96	0.13	21,42,68,77	0
21	CLA	A	1110	65/65	0.96	0.22	30,47,124,127	0
21	CLA	b	1203	65/65	0.96	0.19	25,45,60,64	0
21	CLA	a	1132	65/65	0.96	0.14	37,57,66,71	0
21	CLA	B	1239	65/65	0.96	0.24	11,39,59,85	0
21	CLA	A	1137	65/65	0.96	0.20	24,38,111,116	0
21	CLA	l	1129	50/65	0.96	0.15	49,63,76,78	0
32	CA	b	6001	1/1	0.96	0.06	61,61,61,61	0
21	CLA	A	1132	65/65	0.96	0.15	21,35,44,51	0
21	CLA	b	1223	65/65	0.96	0.18	33,55,83,86	0
29	CL	b	6000	1/1	0.97	0.11	53,53,53,53	0
22	PQN	B	2002	33/33	0.97	0.17	24,35,39,48	0
23	SF4	c	3003	8/8	0.98	0.09	57,78,82,85	0
32	CA	0	1001	1/1	0.98	0.04	56,56,56,56	0
32	CA	L	1001	1/1	0.98	0.08	44,44,44,44	0
23	SF4	3	3003	8/8	0.98	0.07	75,88,175,321	0
23	SF4	c	3002	8/8	0.98	0.11	53,57,64,76	0
32	CA	B	6001	1/1	0.98	0.10	80,80,80,80	0
23	SF4	a	3001	8/8	0.99	0.16	61,65,75,77	0
29	CL	B	6000	1/1	0.99	0.04	36,36,36,36	0

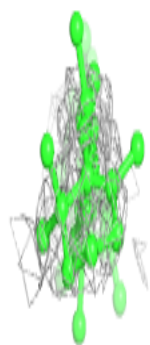
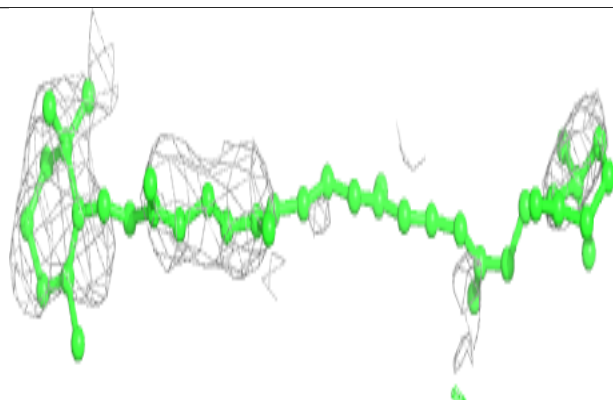
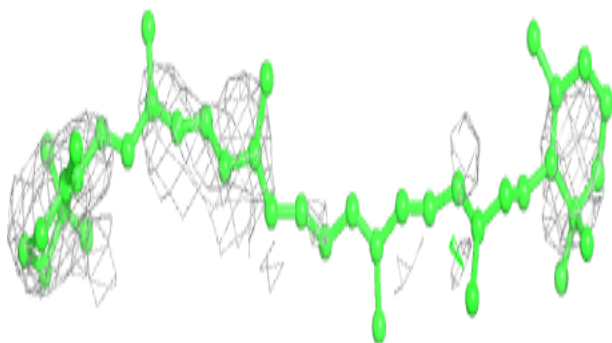
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around BCR k 4001:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

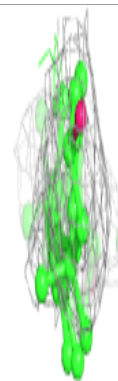
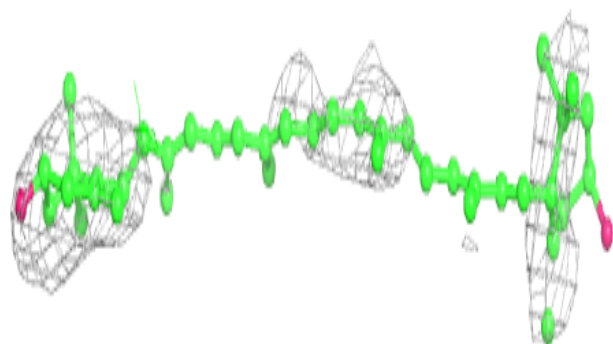
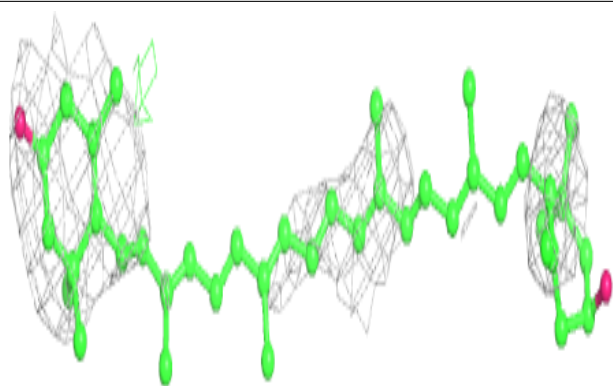
**Electron density around BCR 8 4001:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

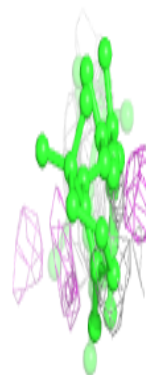
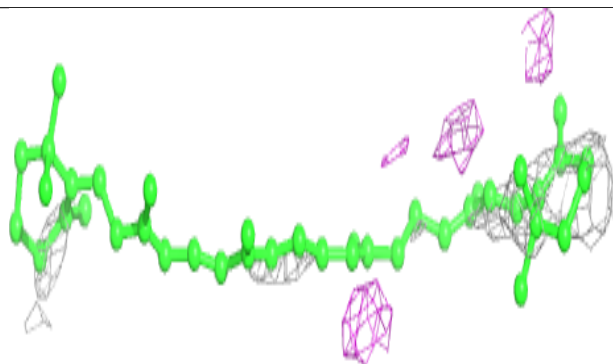
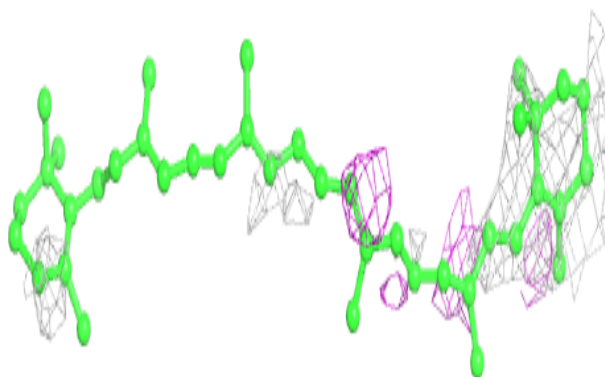


Electron density around ZEX 7 4015:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

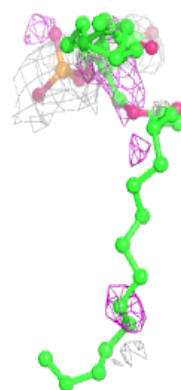
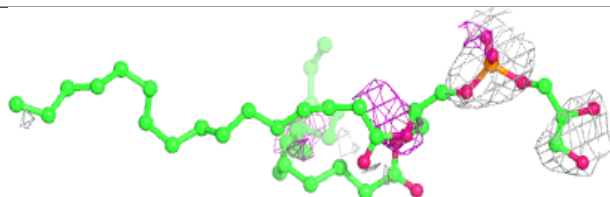
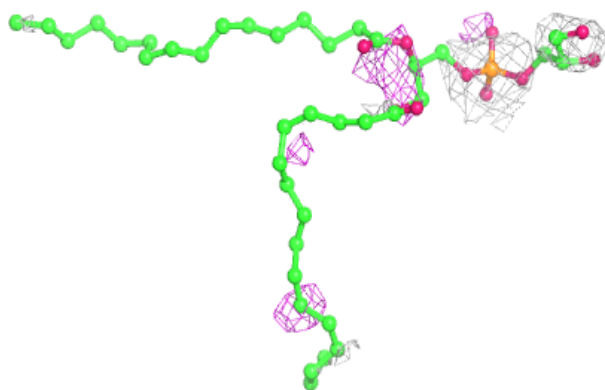
**Electron density around BCR 2 4004:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

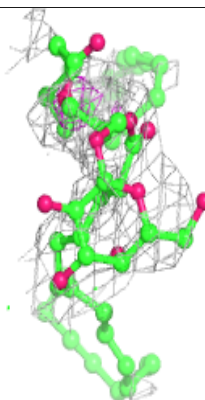
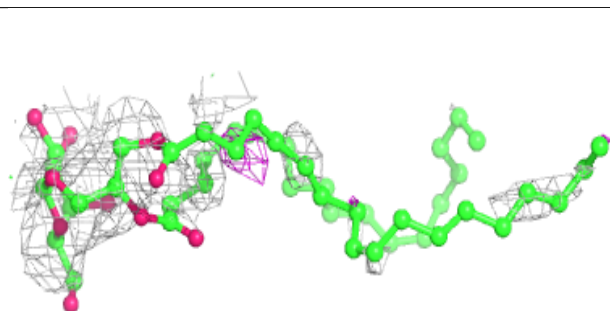
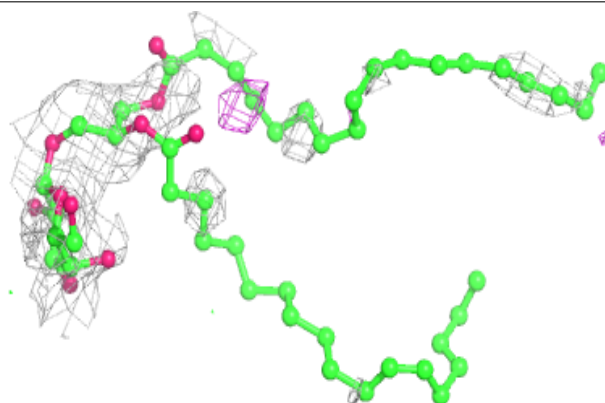


Electron density around LHG B 5006:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

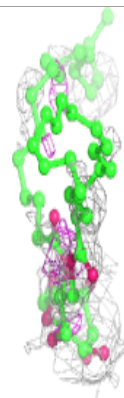
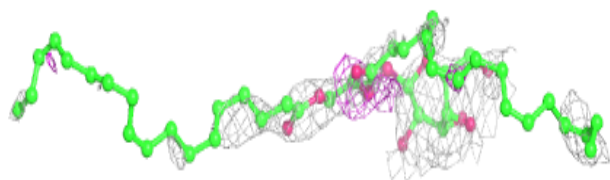
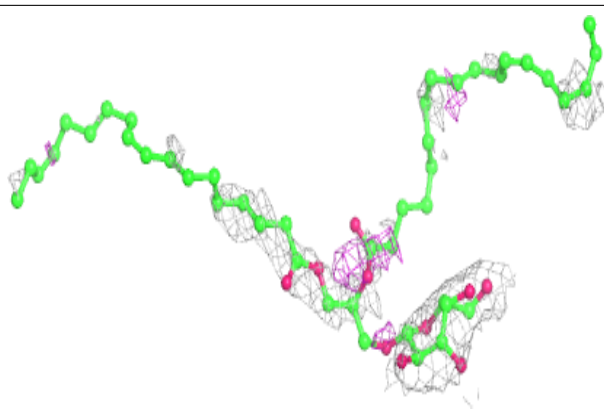
**Electron density around LMG A 5008:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

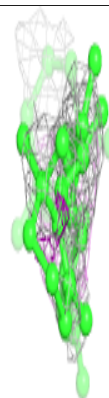
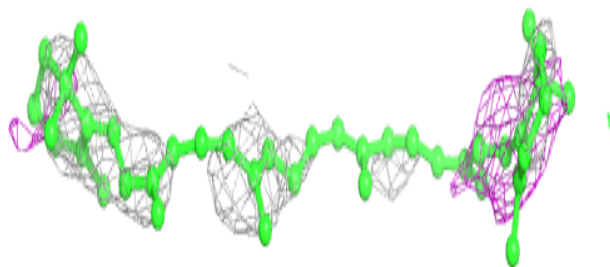
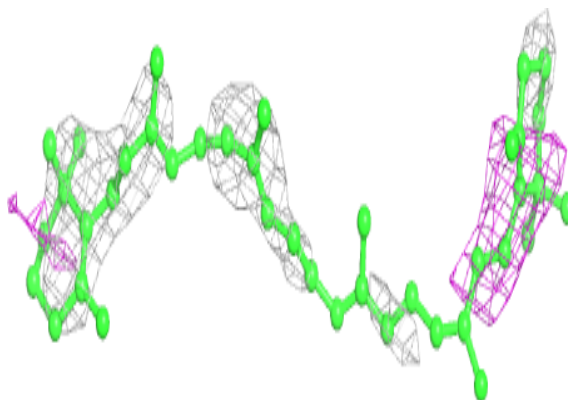


Electron density around LMG b 5007:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

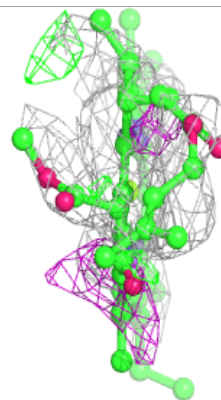
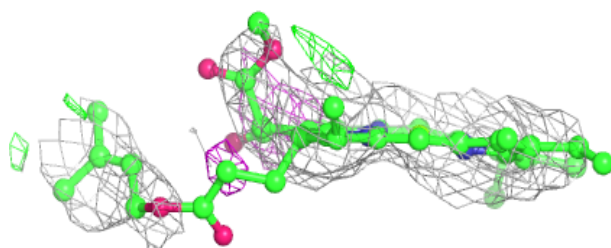
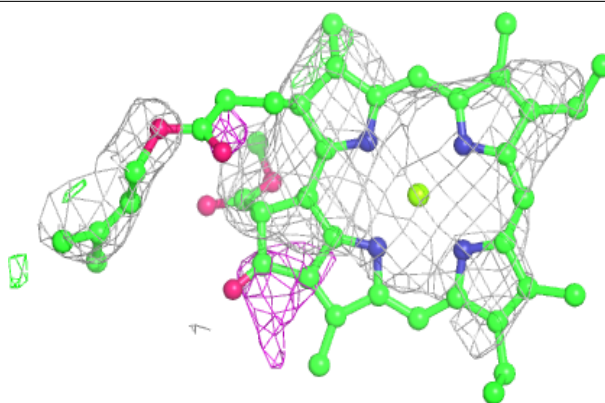
**Electron density around BCR B 4018:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

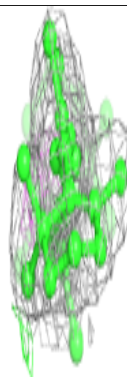
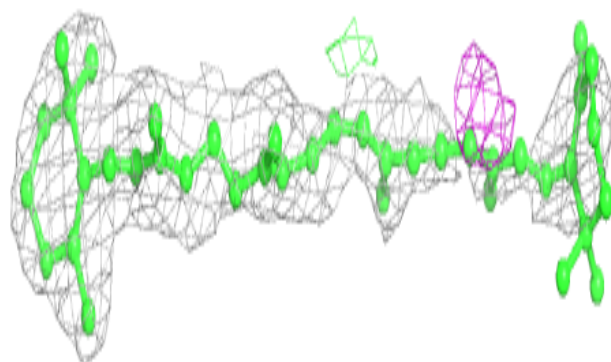
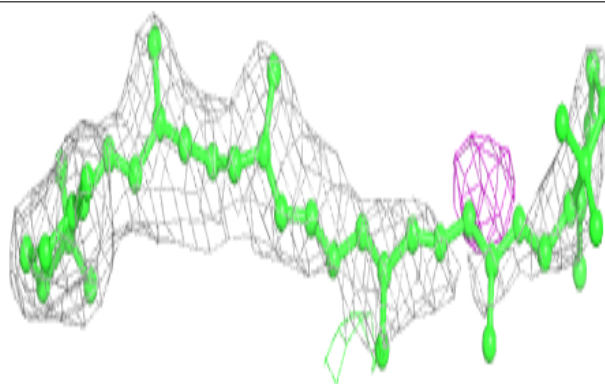


Electron density around CLA a 1113:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

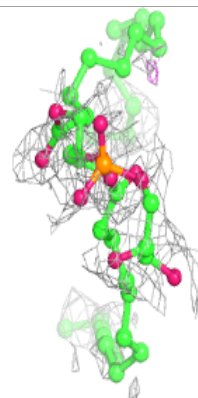
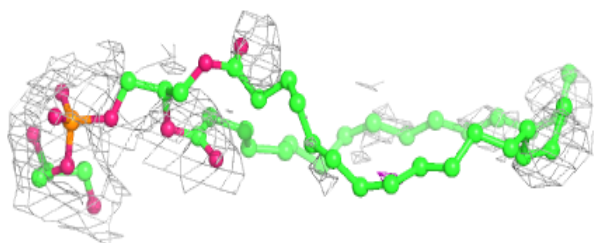
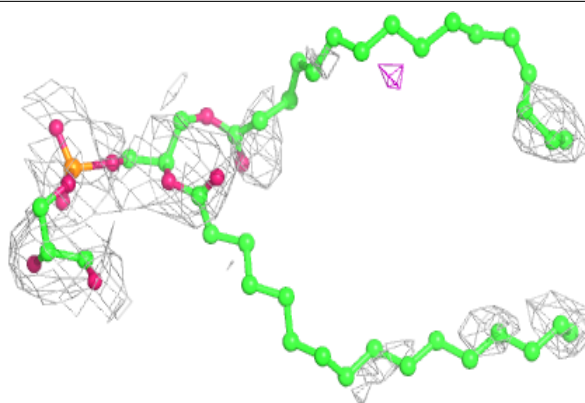
**Electron density around BCR K 4001:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

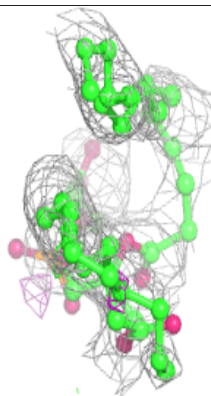
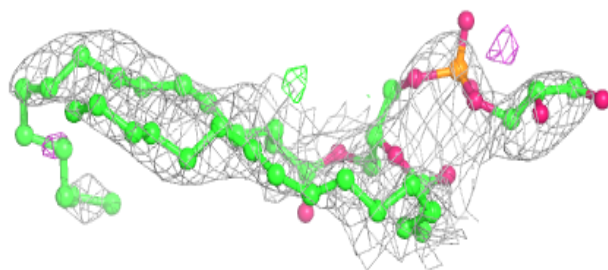
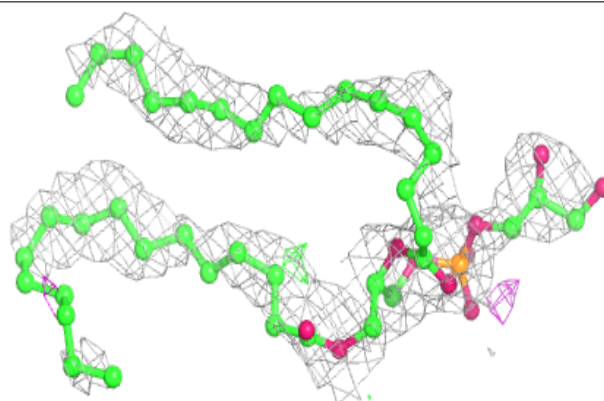


Electron density around LHG 1 5005:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

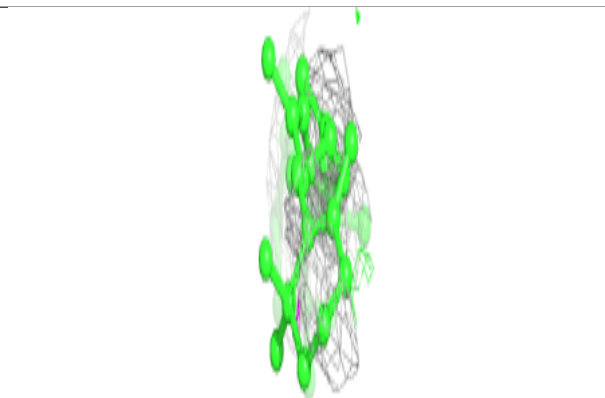
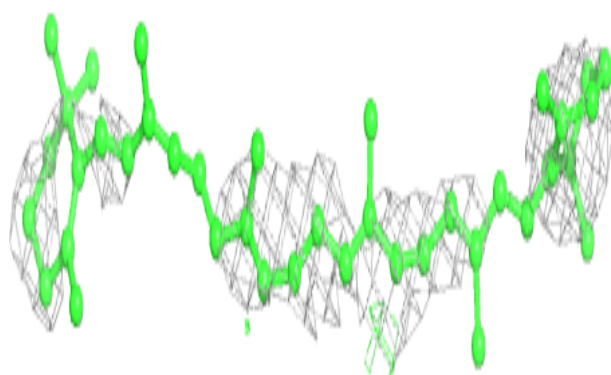
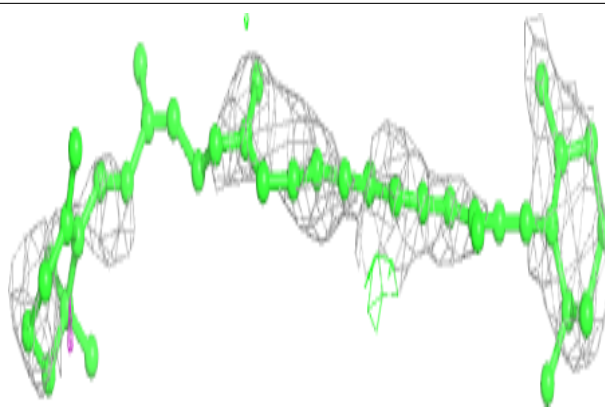
**Electron density around LHG F 5002:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

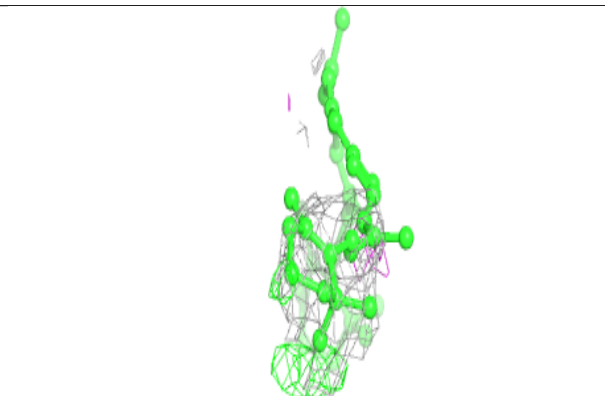
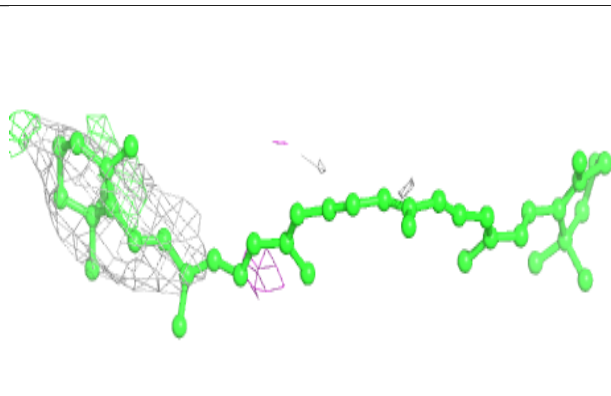
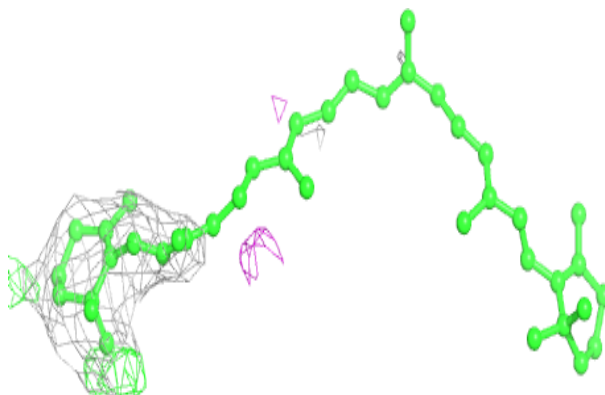


Electron density around BCR 1 4001:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

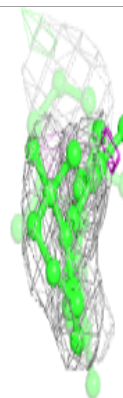
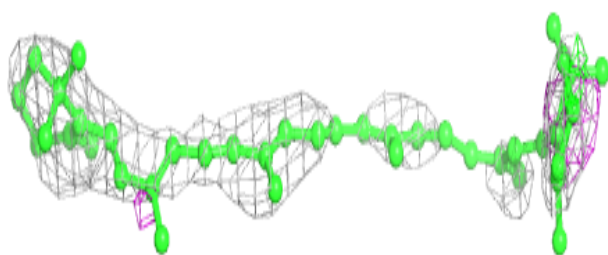
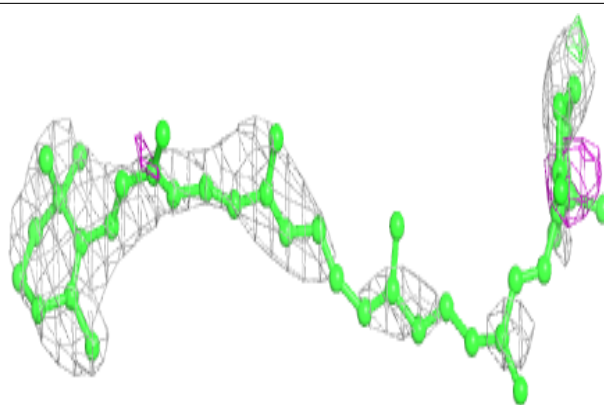
**Electron density around BCR 1 4019:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

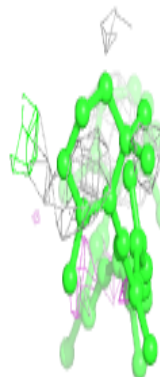
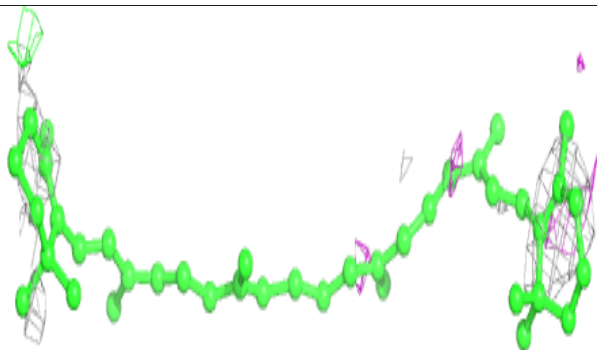
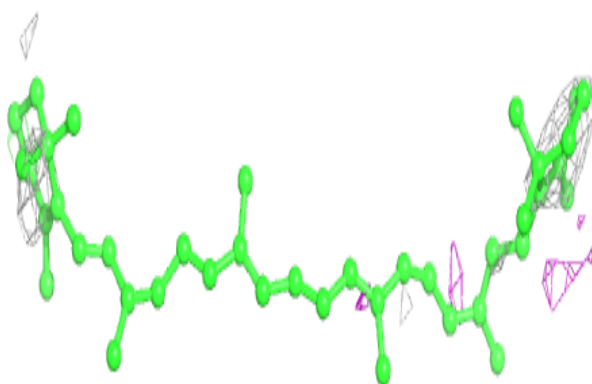


Electron density around BCR b 4018:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

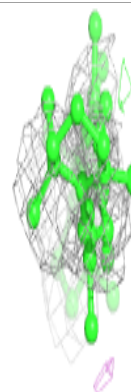
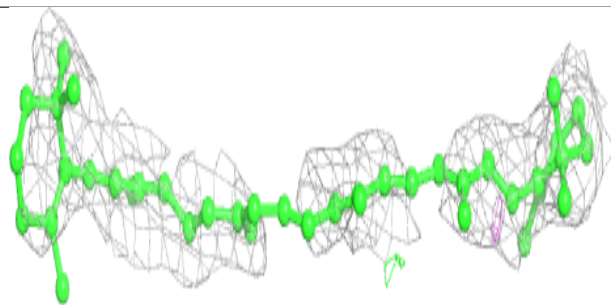
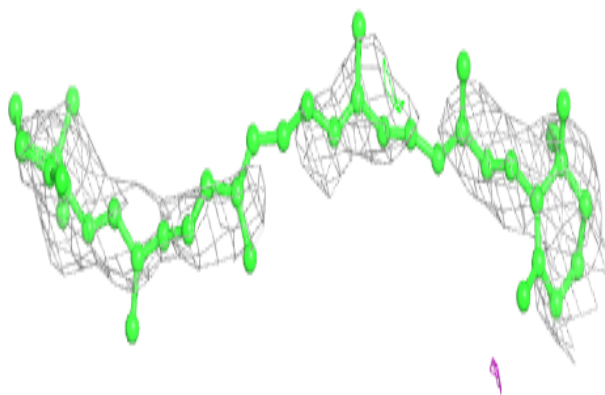
**Electron density around BCR 2 4018:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



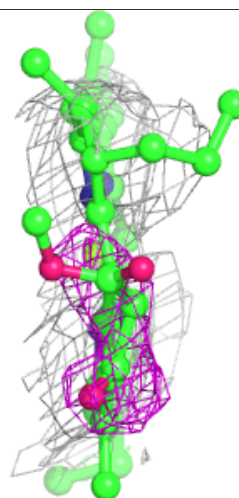
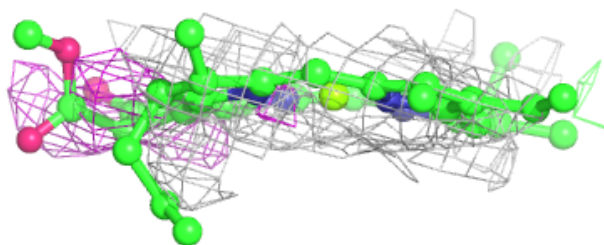
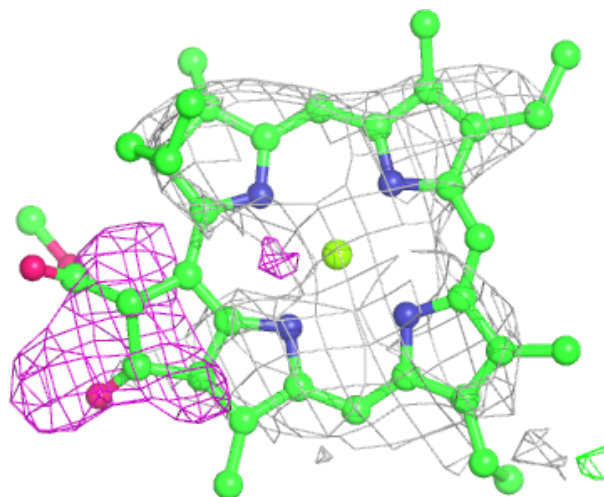
Electron density around BCR 2 4005:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



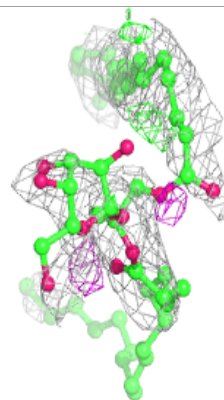
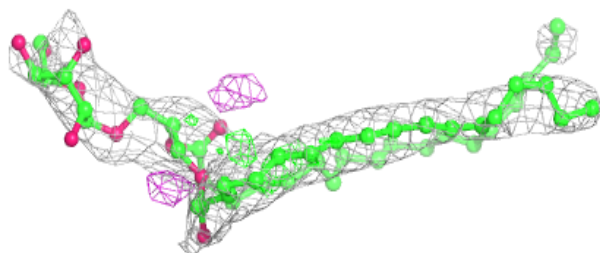
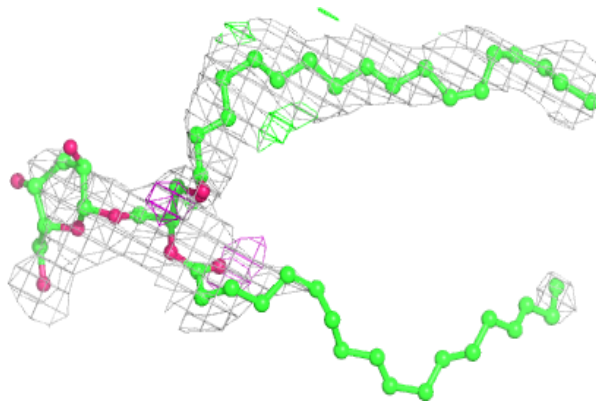
Electron density around CLA 6 1302:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

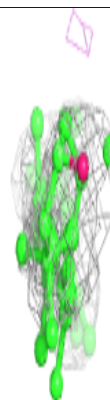
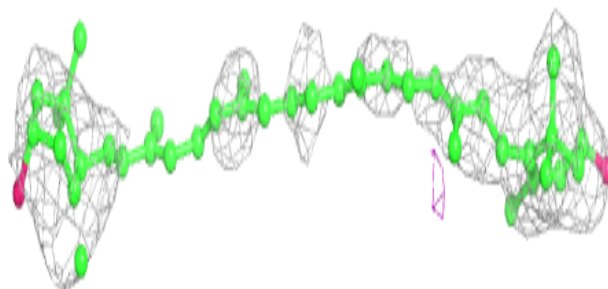
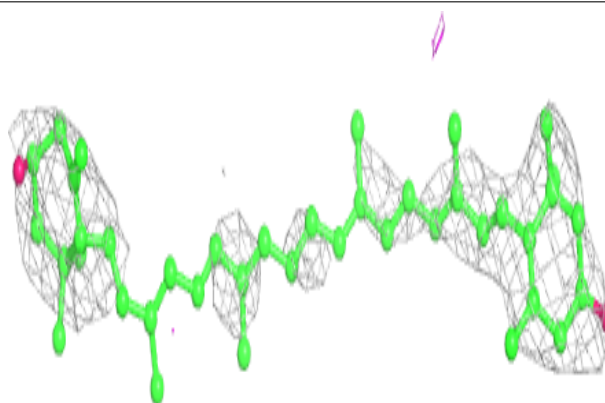


Electron density around LMG B 5005:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

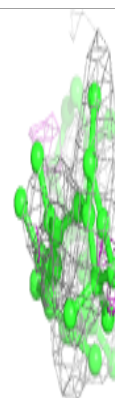
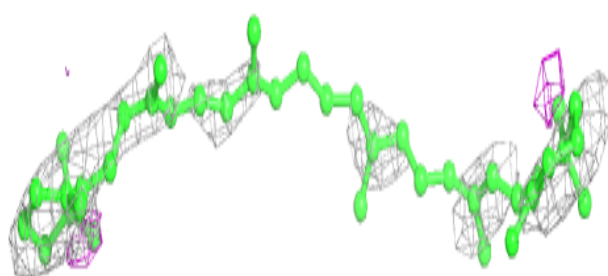
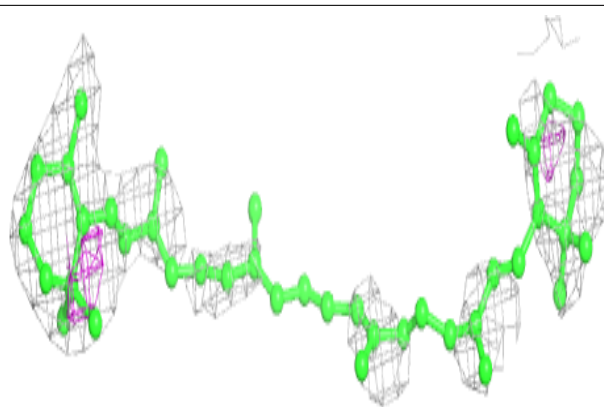
**Electron density around ZEX j 4015:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

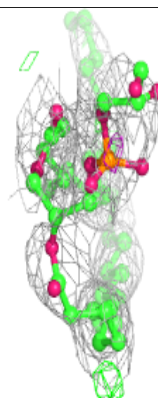
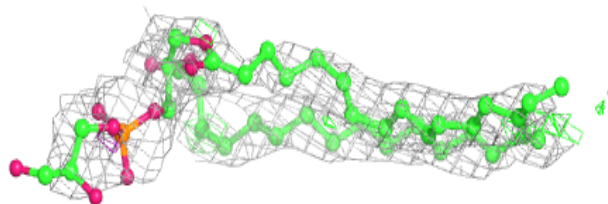
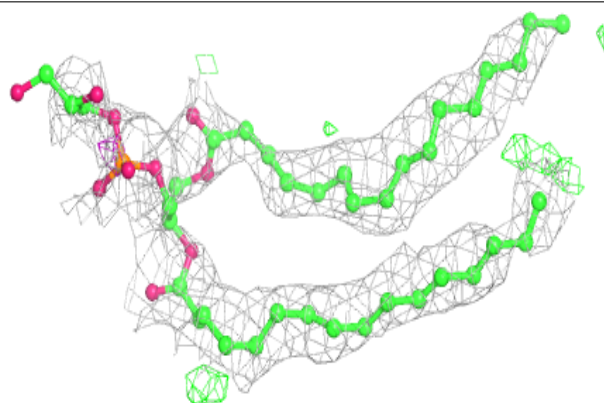


Electron density around BCR 7 4013:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

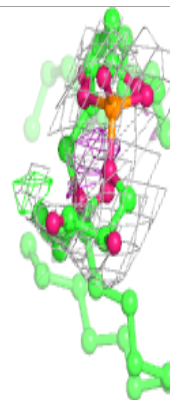
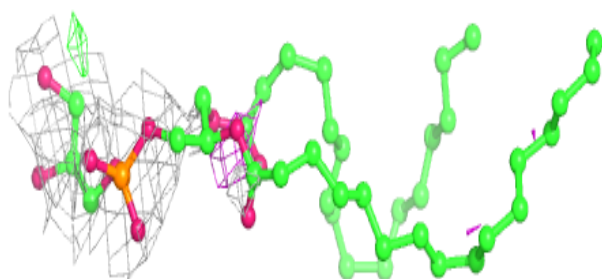
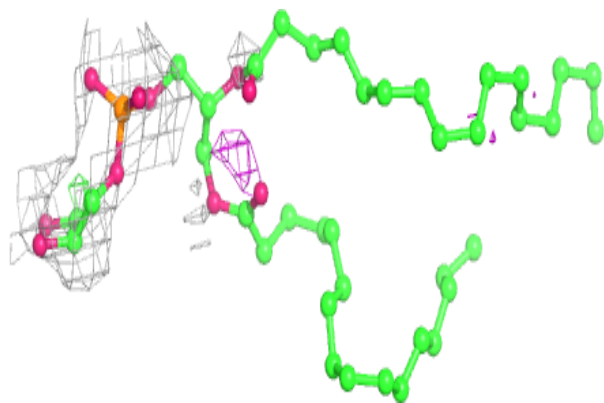
**Electron density around LHG 1 5004:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

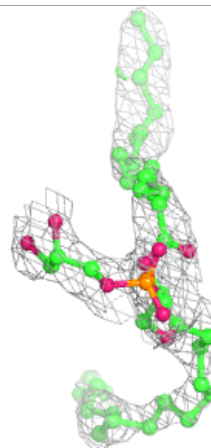
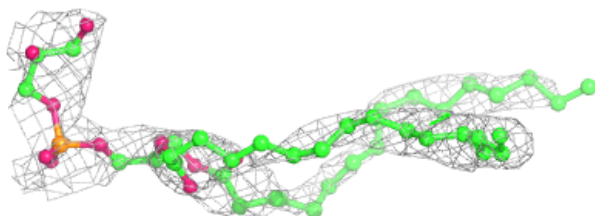
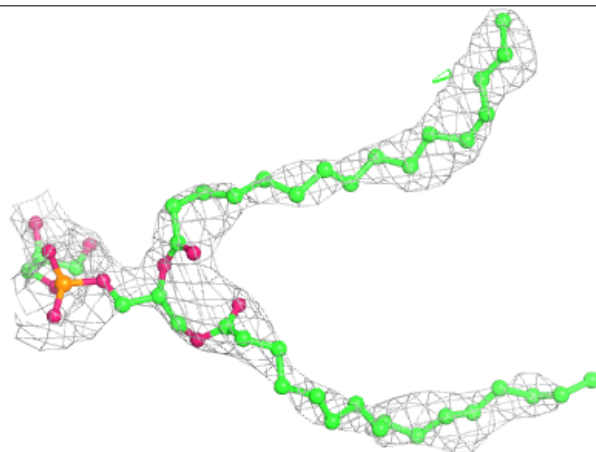


Electron density around LHG a 5007:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

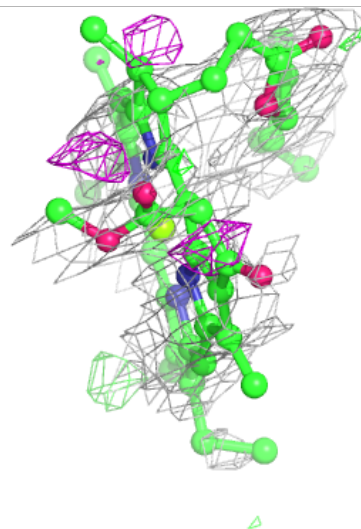
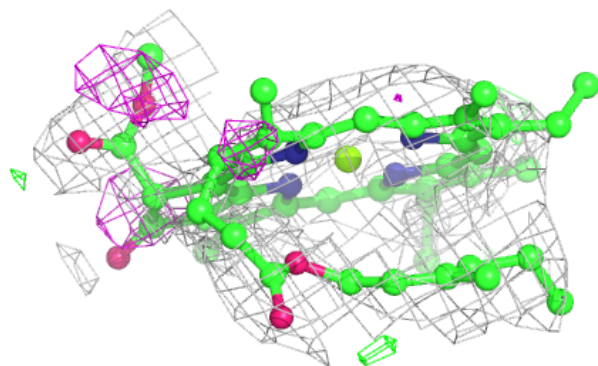
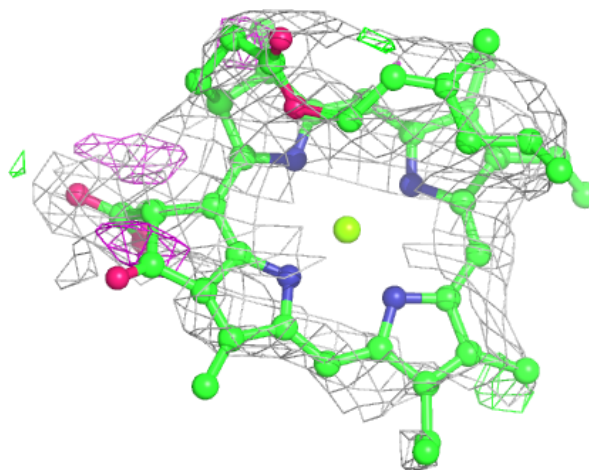
**Electron density around LHG 1 5002:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



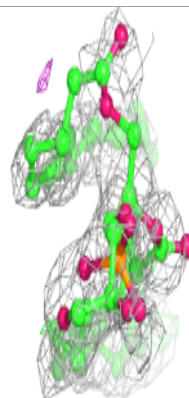
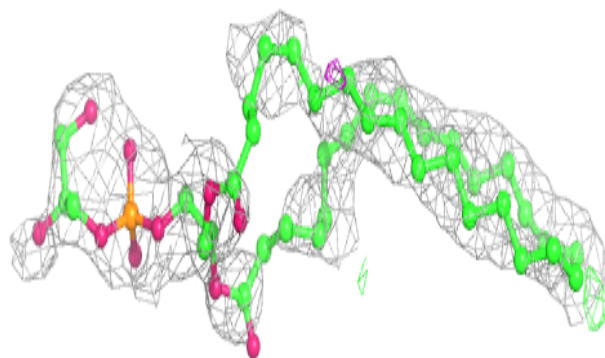
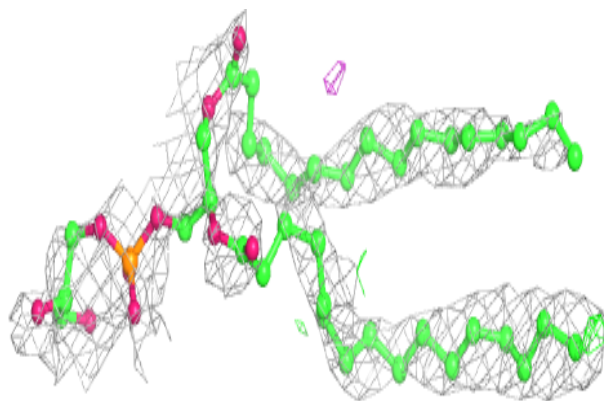
Electron density around CLA 2 1217:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

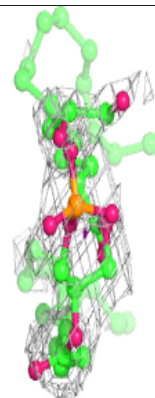
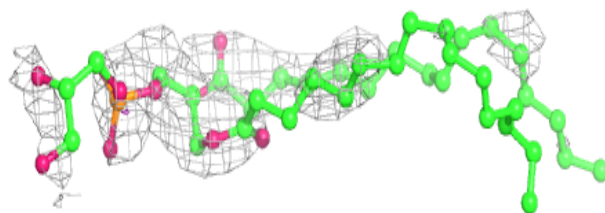
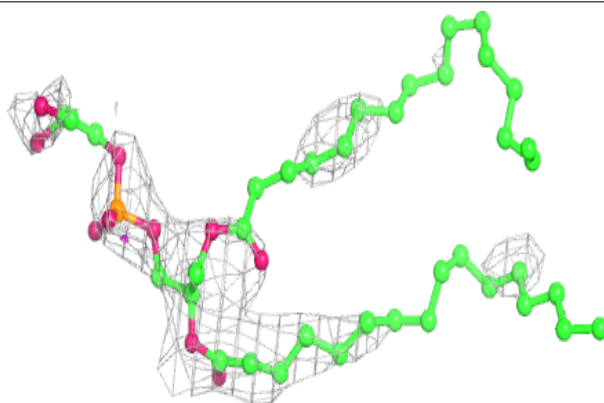


Electron density around LHG a 5005:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

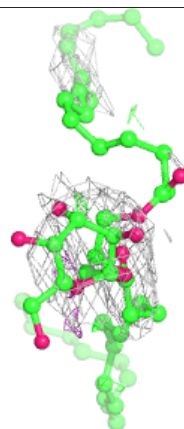
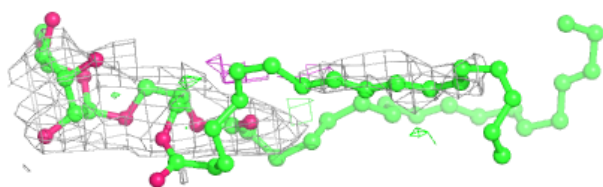
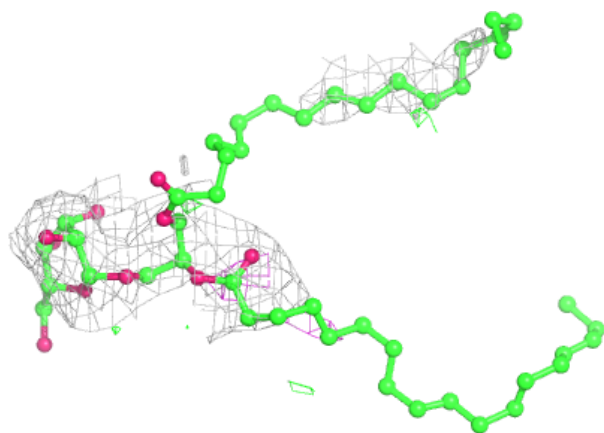
**Electron density around LHG 1 5007:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

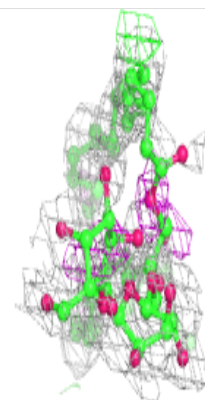
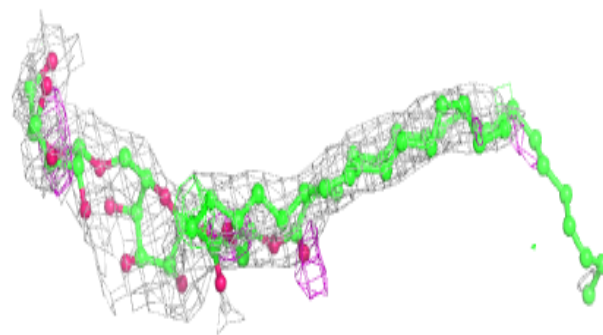
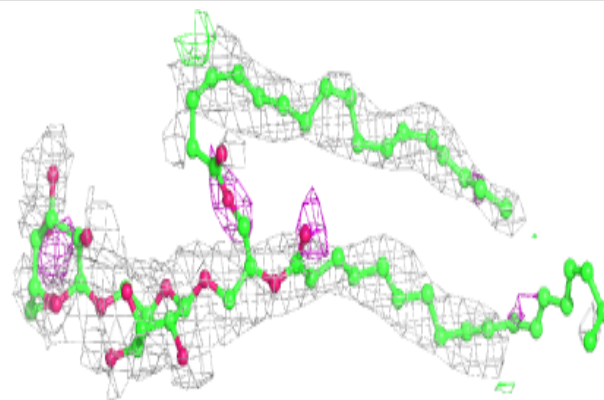


Electron density around LMG 2 5005:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

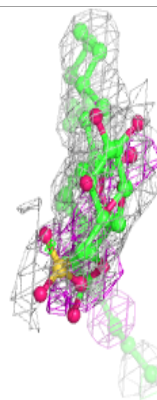
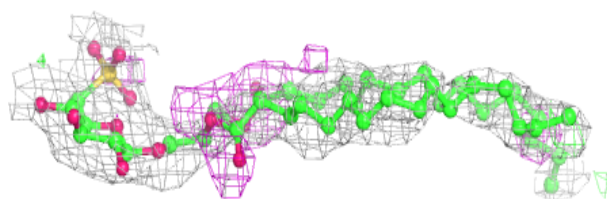
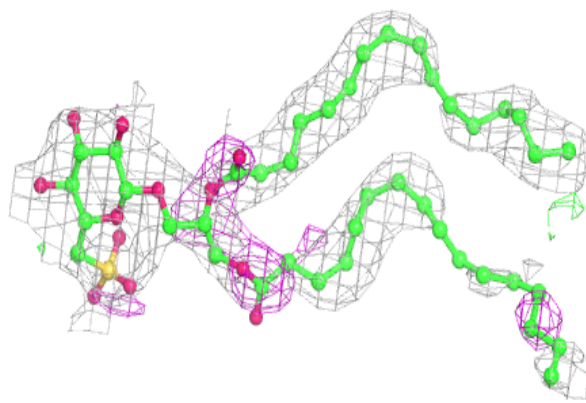
**Electron density around DGD L 5004:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

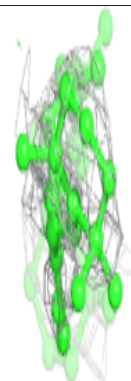
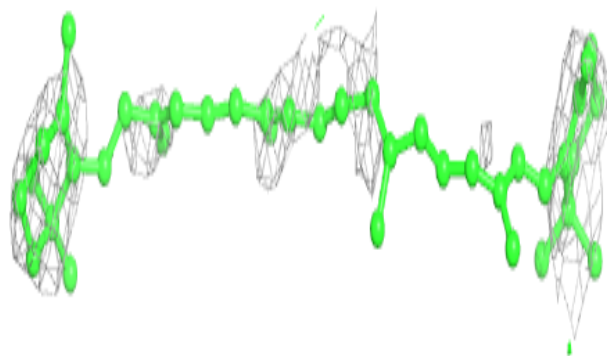
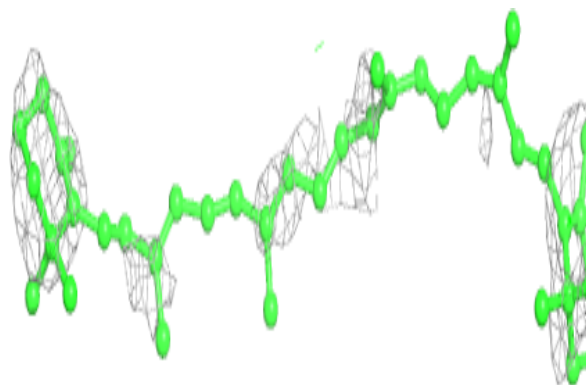


Electron density around SQD b 5006:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

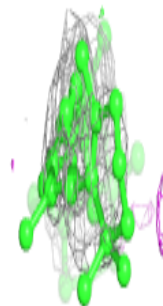
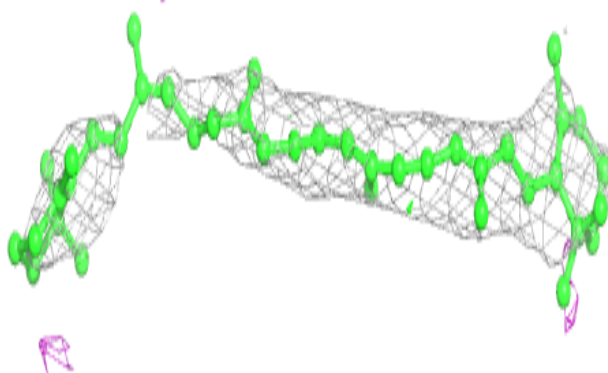
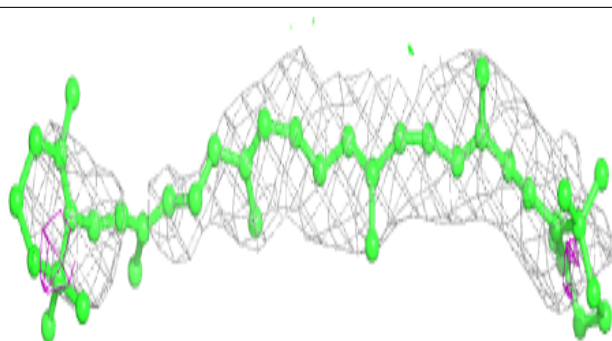
**Electron density around BCR a 4003:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

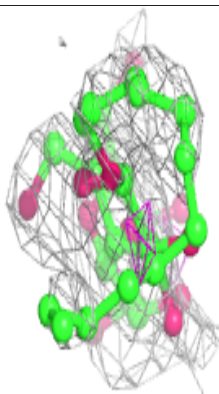
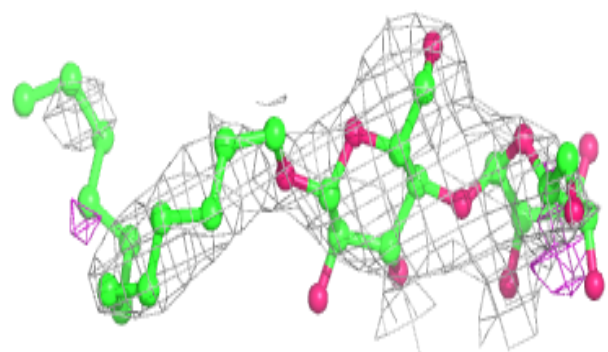
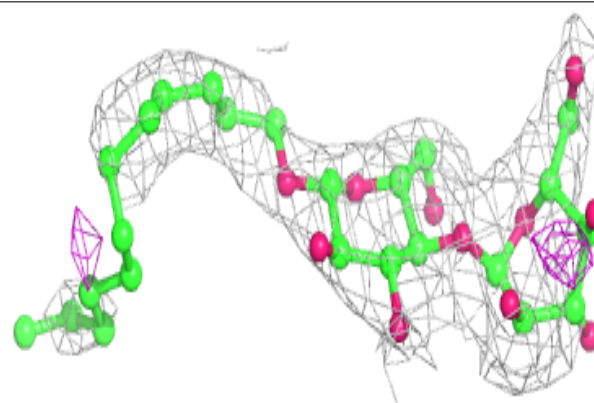


Electron density around BCR a 4001:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

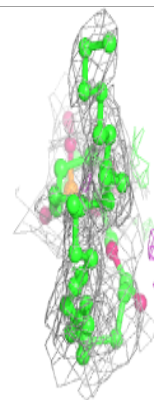
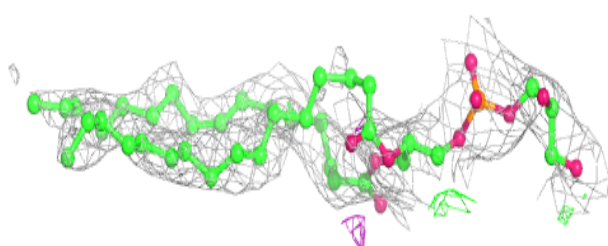
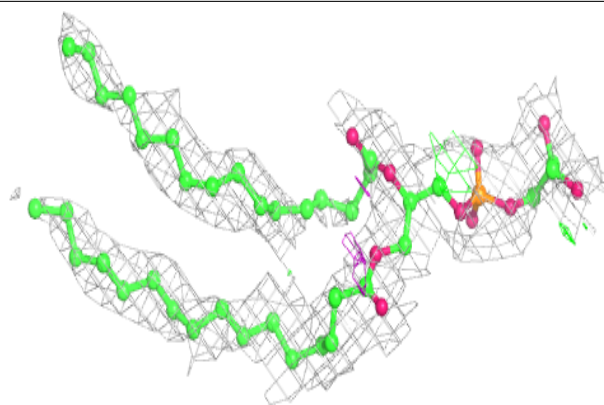
**Electron density around LMT 1 6001:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

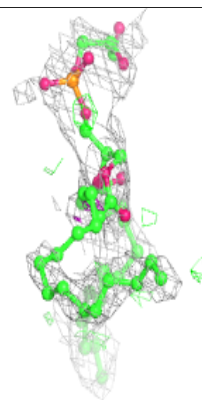
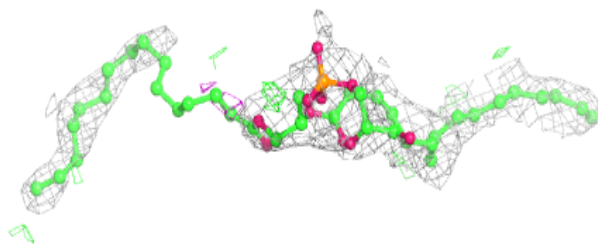
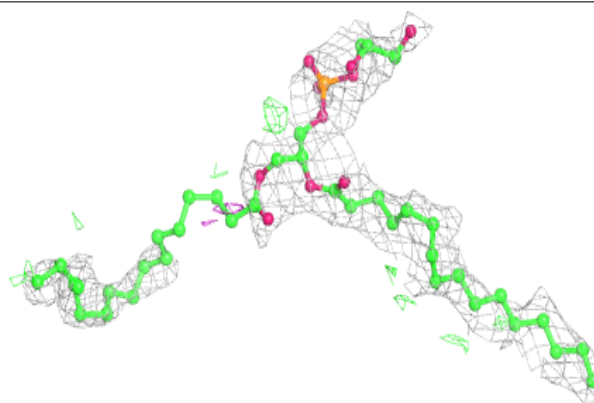


Electron density around LHG M 5001:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

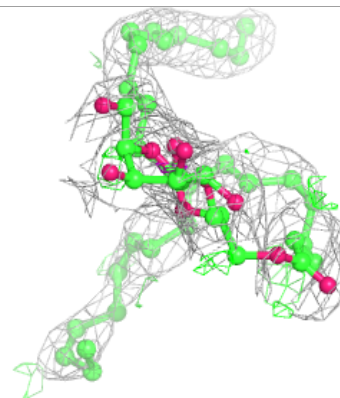
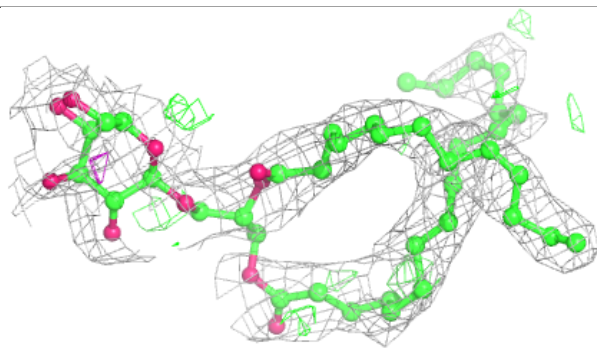
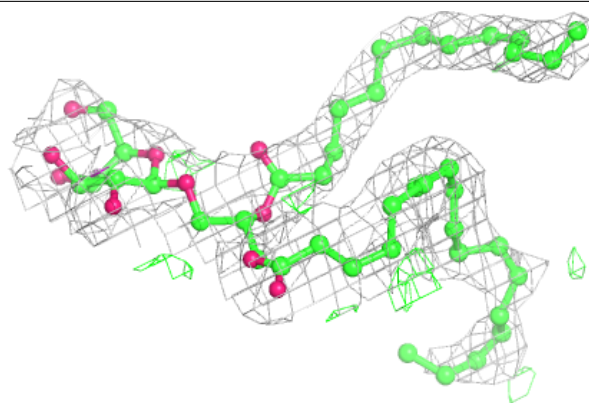
**Electron density around LHG 0 5004:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

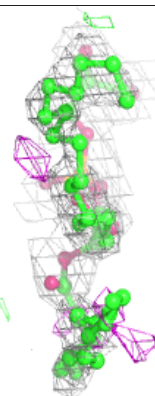
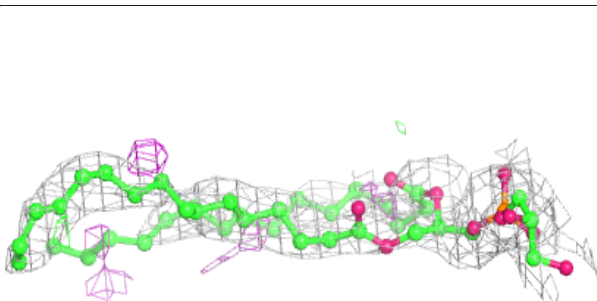
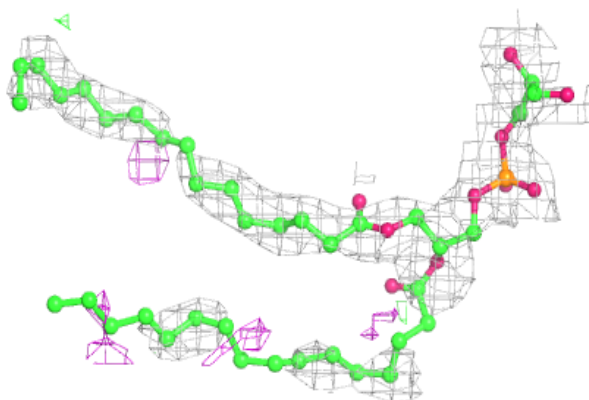


Electron density around LMG a 5002:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

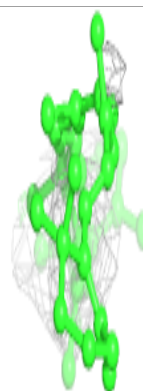
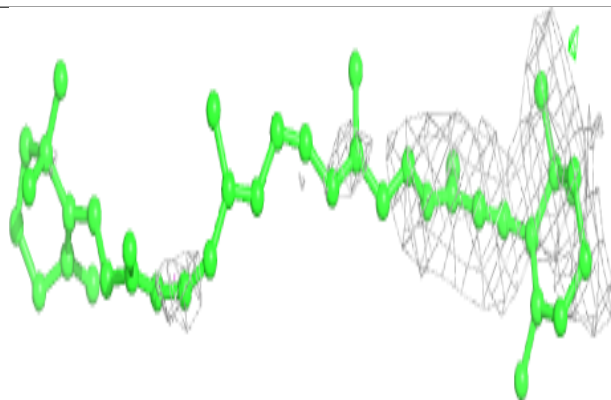
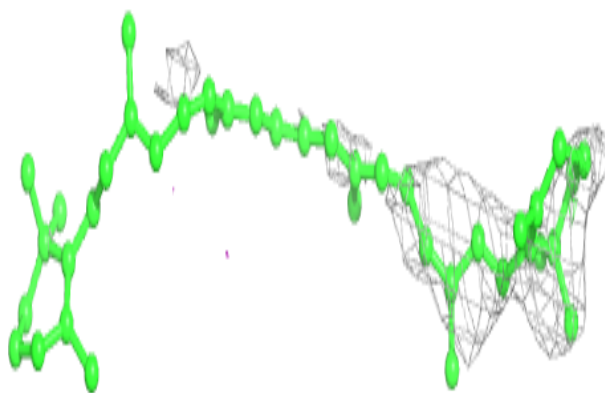
**Electron density around LHG A 5006:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

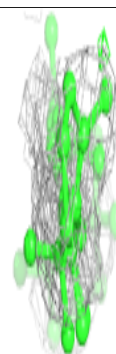
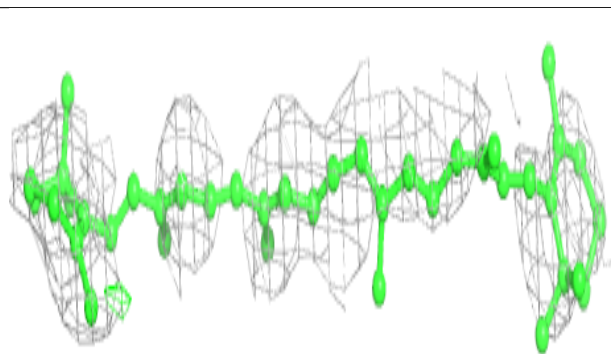
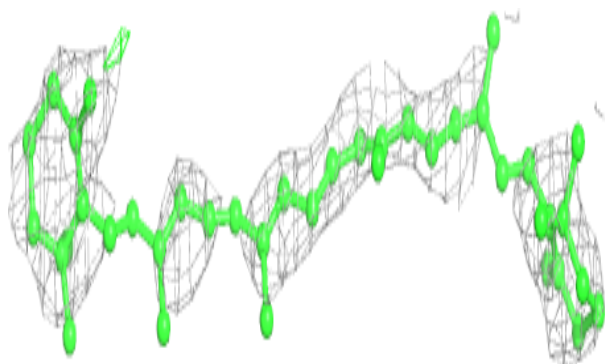


Electron density around BCR a 4019:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

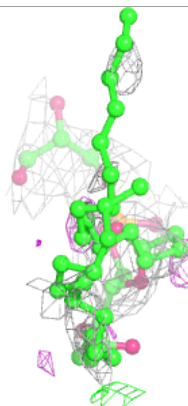
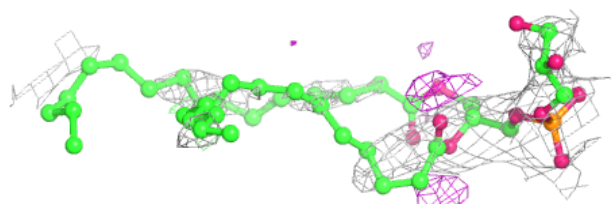
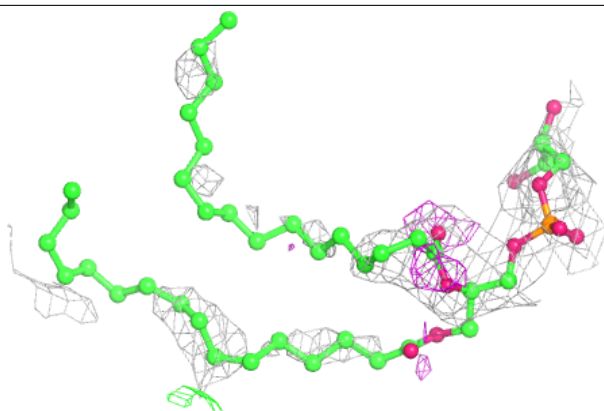
**Electron density around BCR a 4002:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

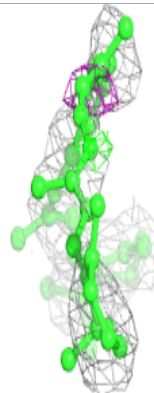
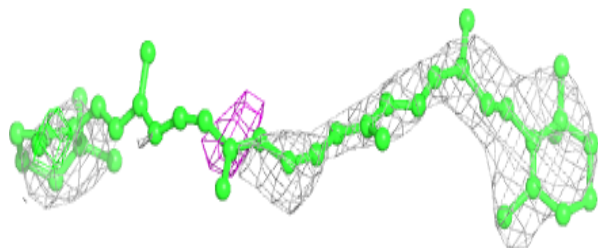
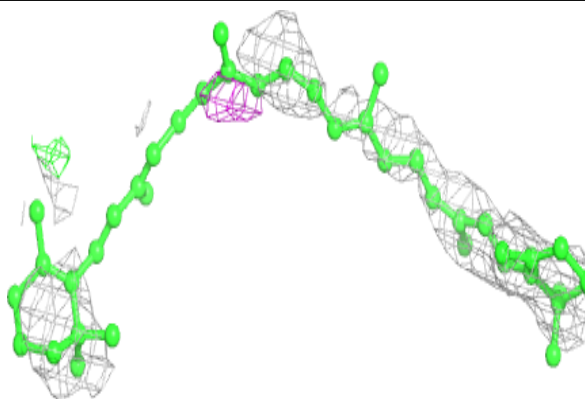


Electron density around LHG 2 5004:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

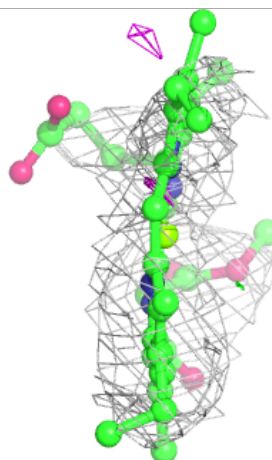
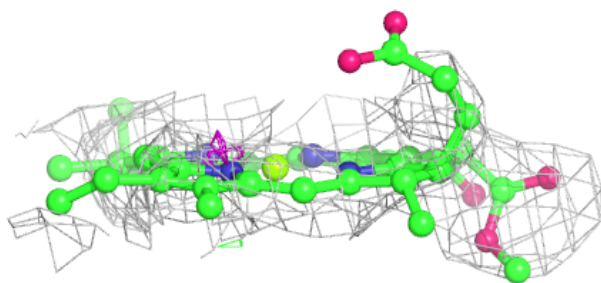
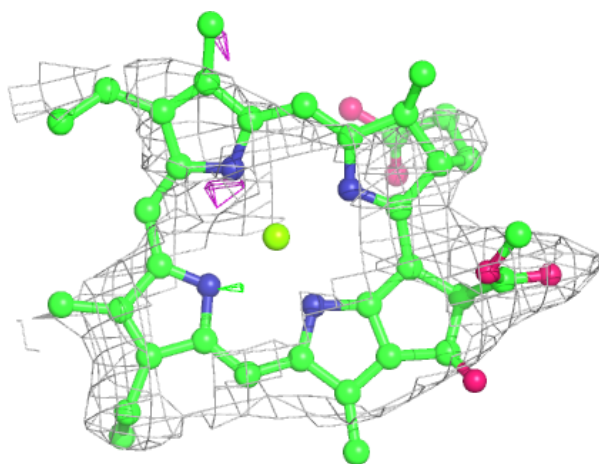
**Electron density around BCR A 4019:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



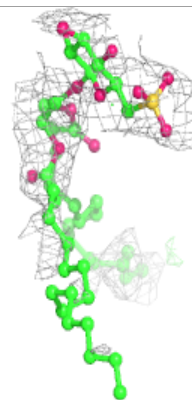
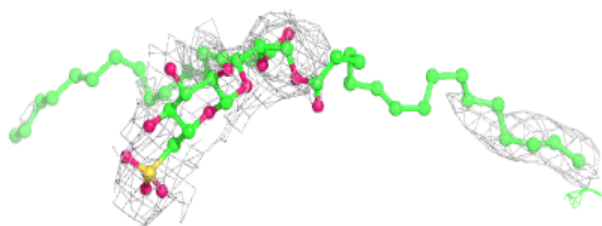
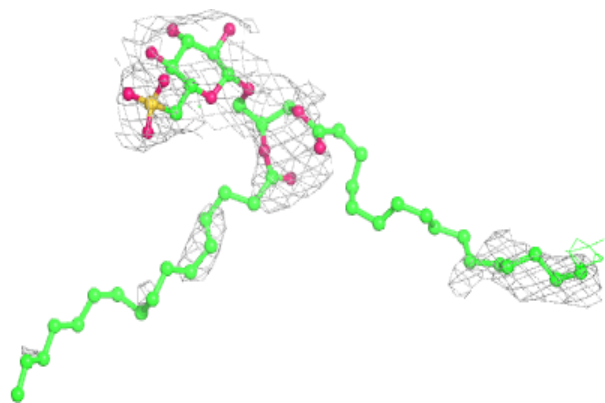
Electron density around CLA 2 1209:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

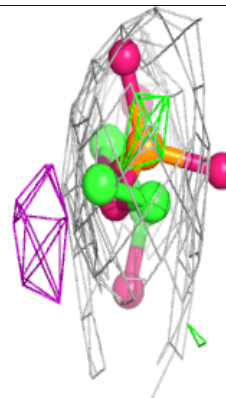
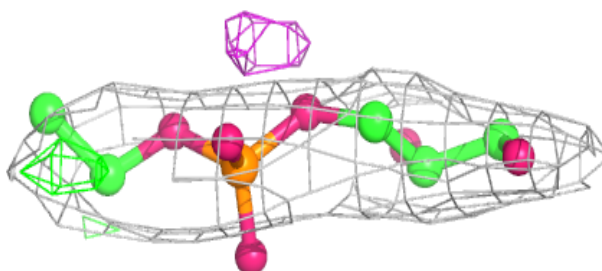
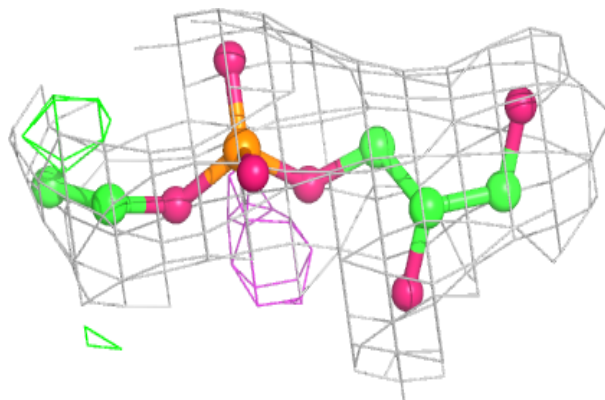


Electron density around SQD f 5001:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

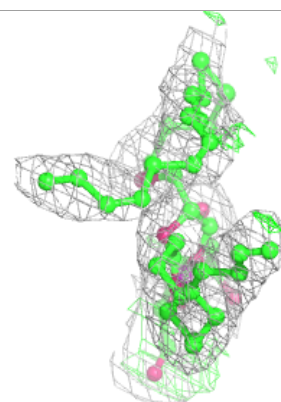
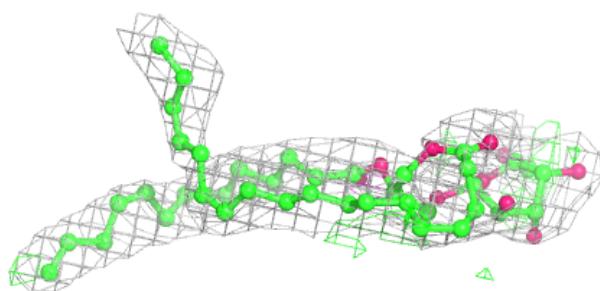
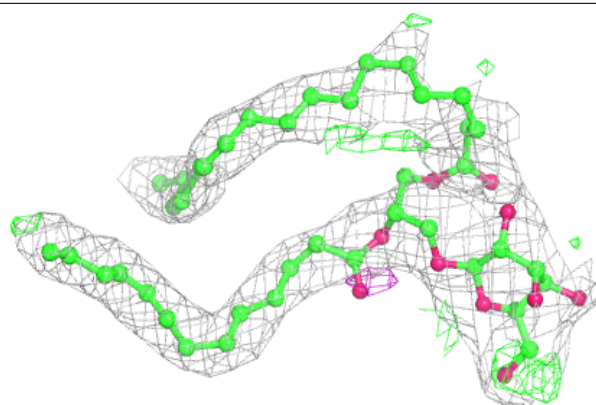
**Electron density around LHG 6 5001:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

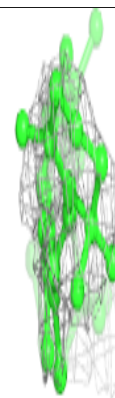
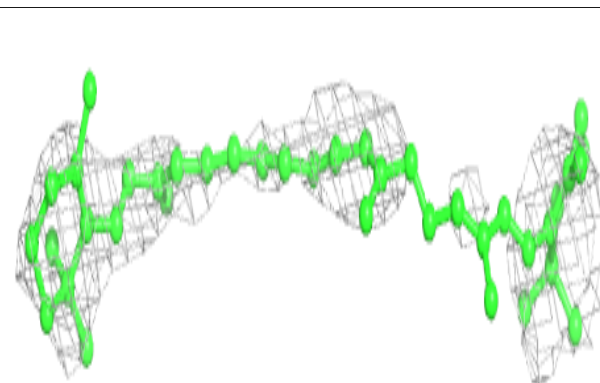
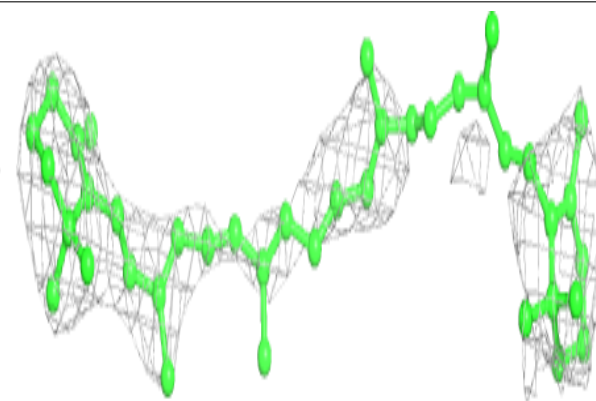


Electron density around LMG A 5002:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

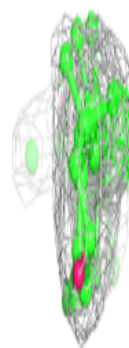
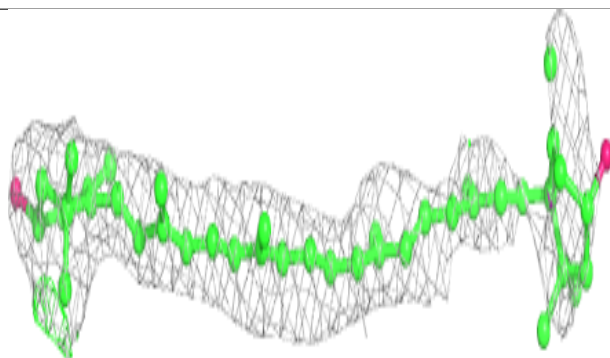
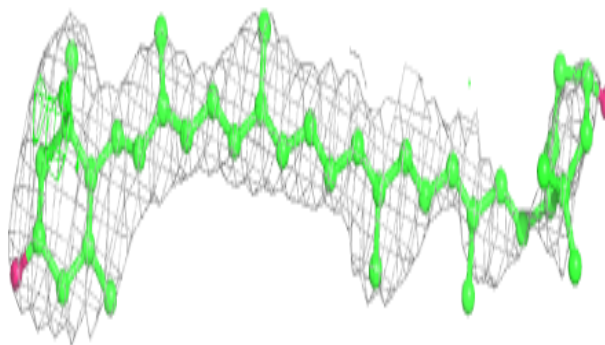
**Electron density around BCR 1 4003:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

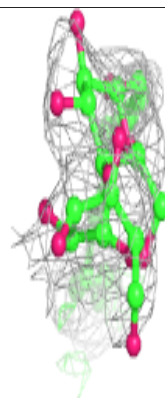
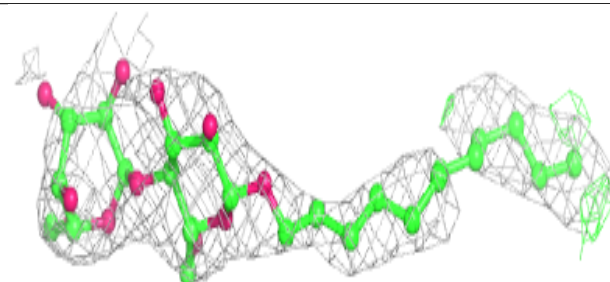
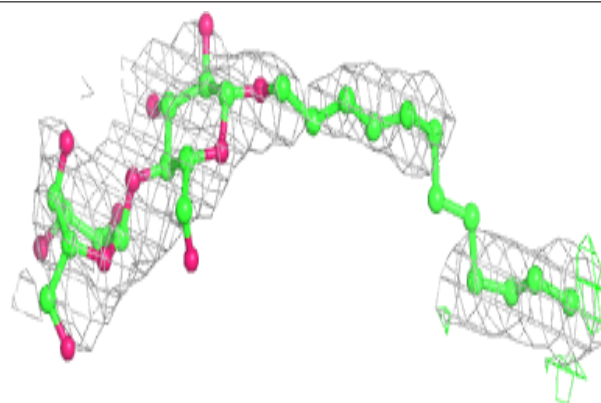


Electron density around ZEX J 4015:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

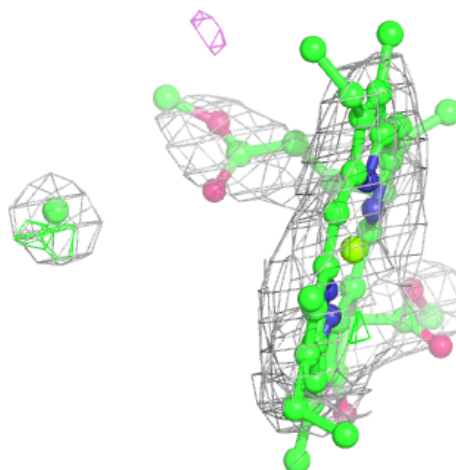
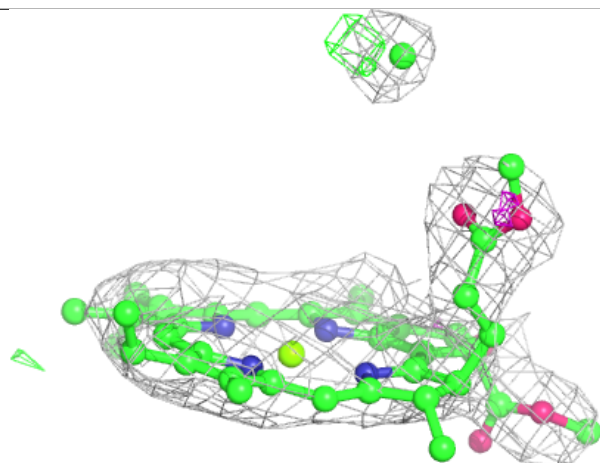
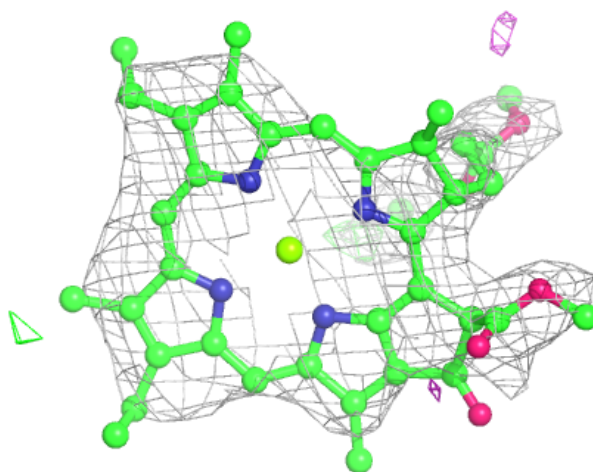
**Electron density around LMT 1 6001:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



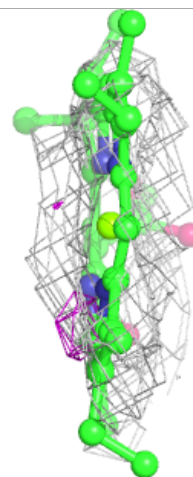
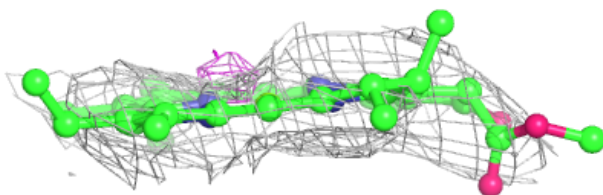
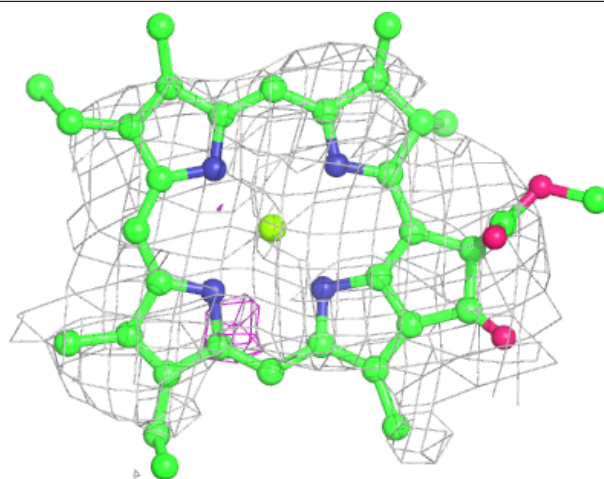
Electron density around CLA 1 1108:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



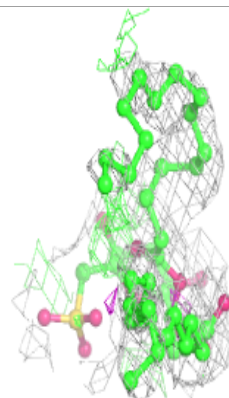
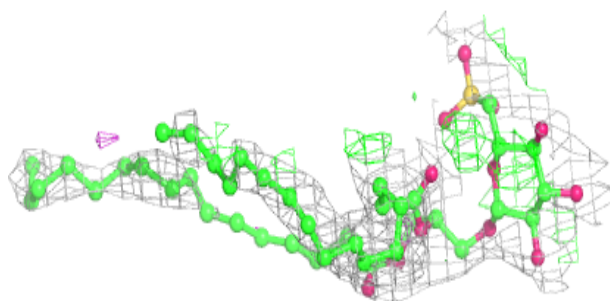
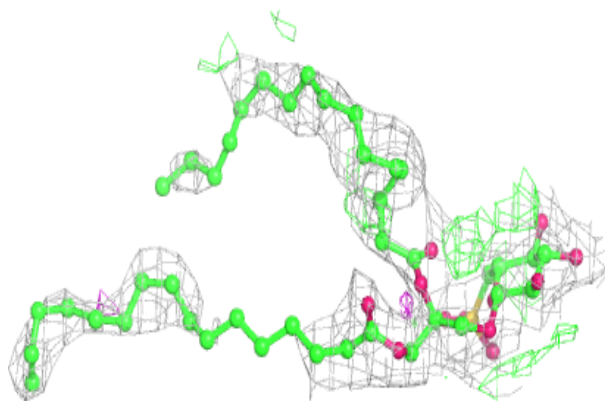
Electron density around CLA 2 1240:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

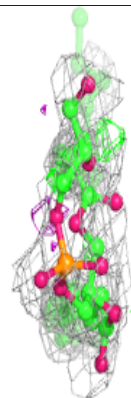
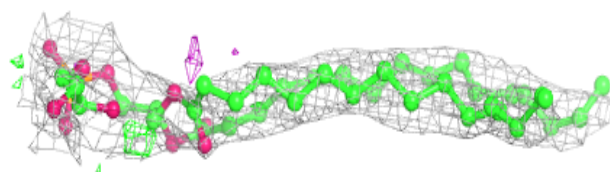
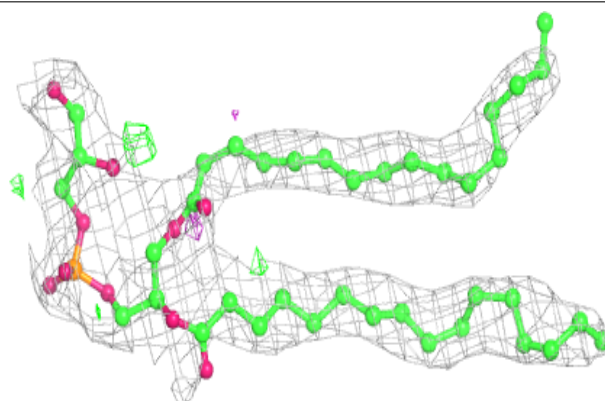


Electron density around SQD 0 5005:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

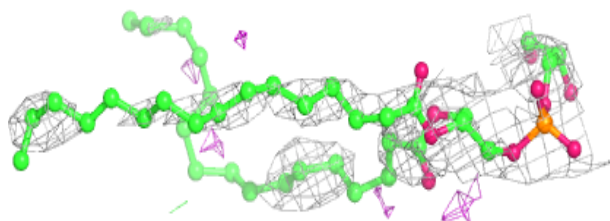
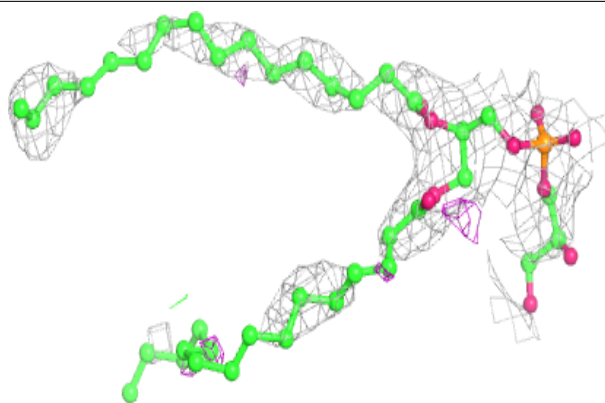
**Electron density around LHG A 5005:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

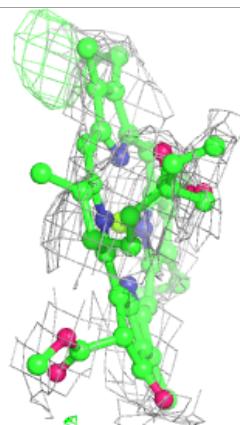
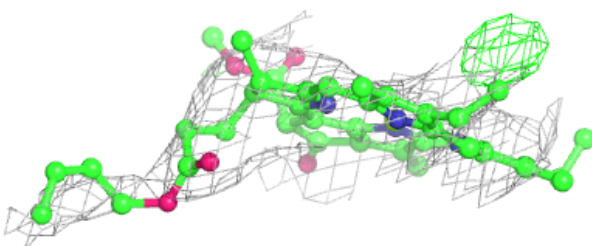
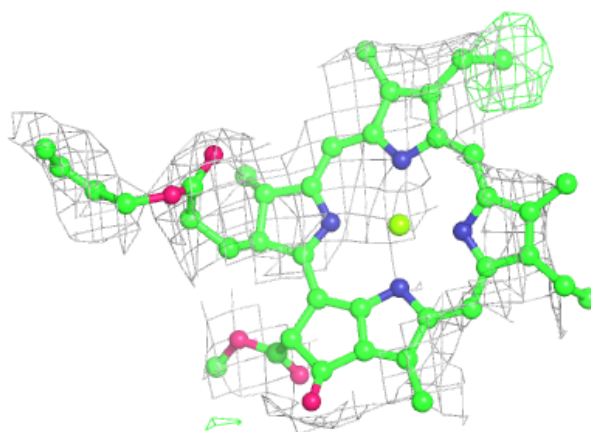


Electron density around LHG 1 5001:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

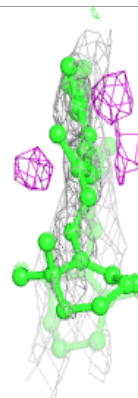
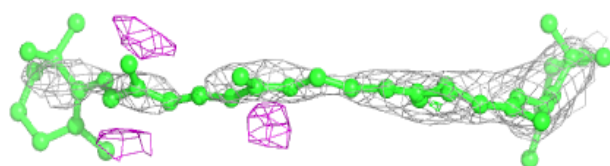
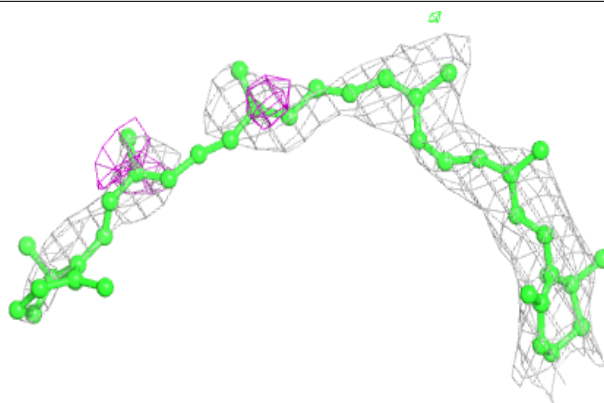
**Electron density around CLA k 1402:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



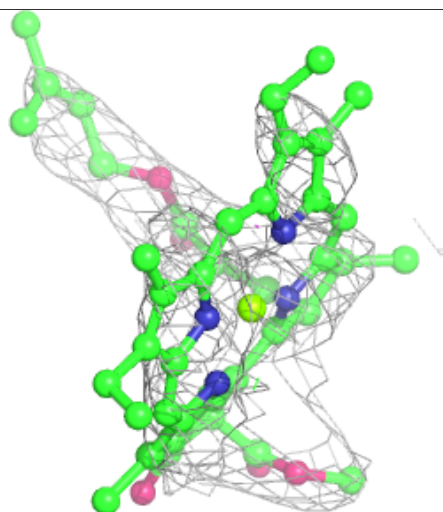
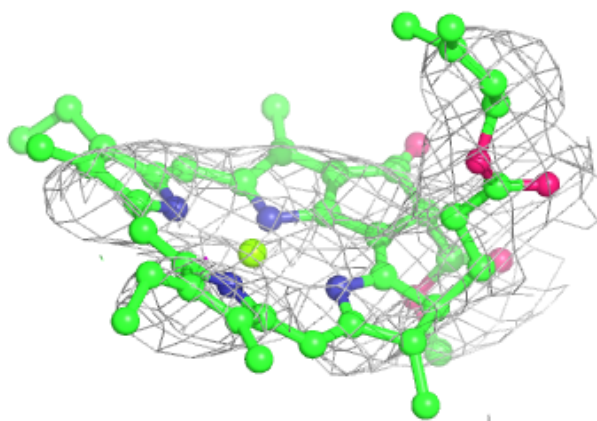
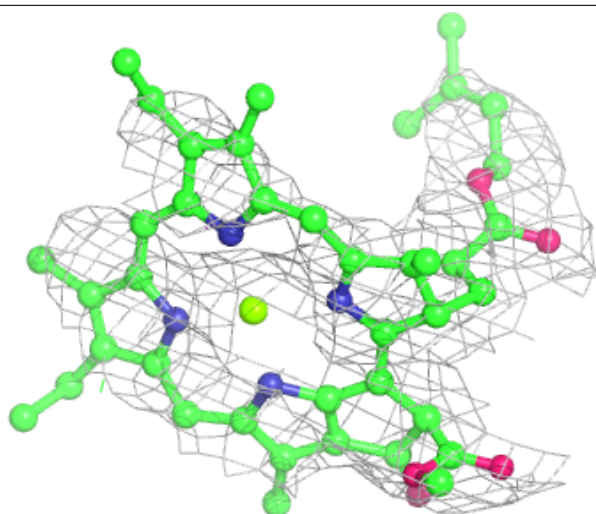
Electron density around BCR 6 4016:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



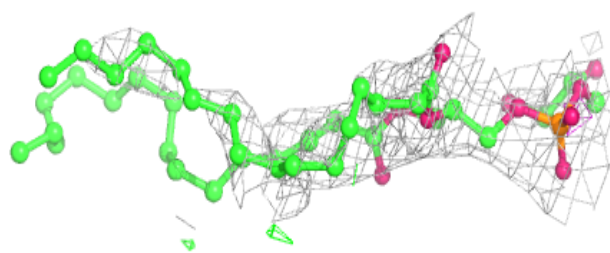
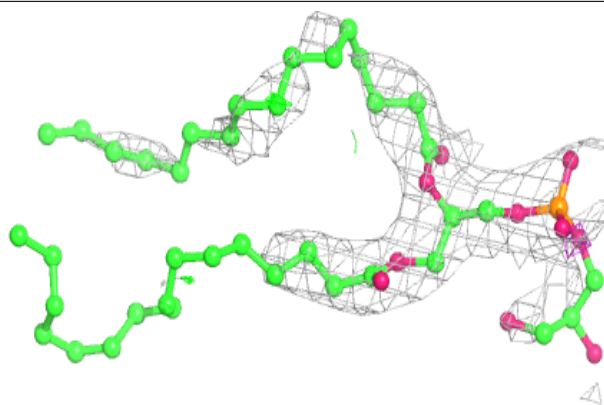
Electron density around CLA 2 1216:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



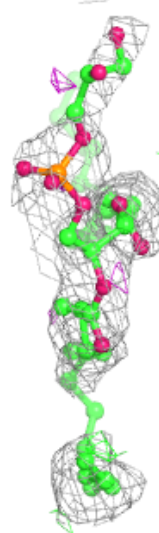
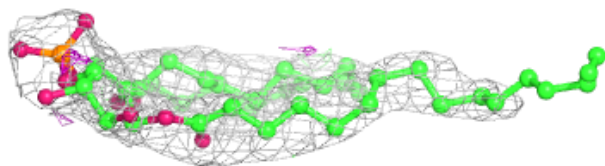
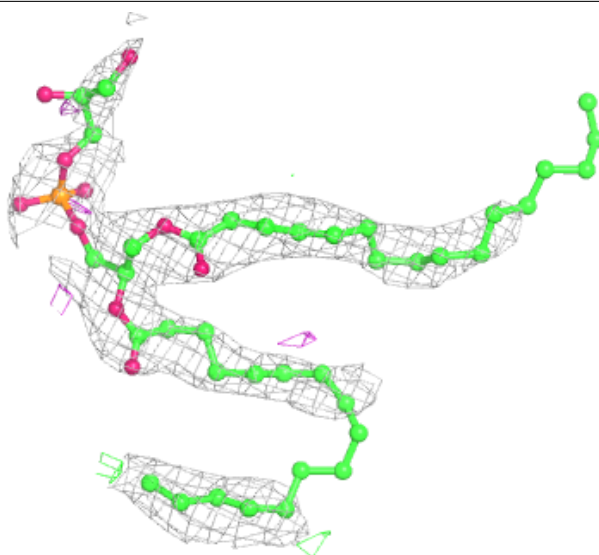
Electron density around LHG 1 5003:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



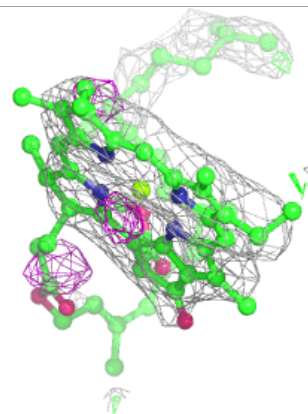
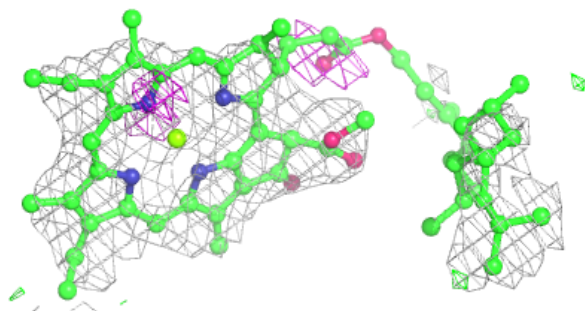
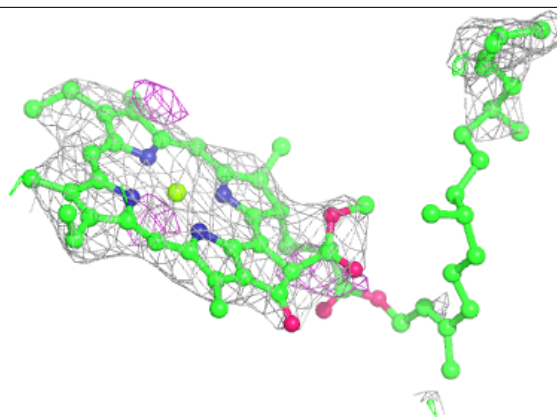
Electron density around LHG A 5007:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

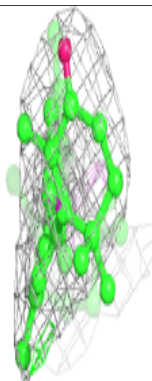
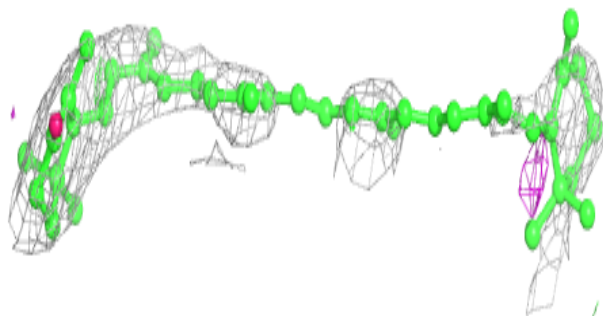
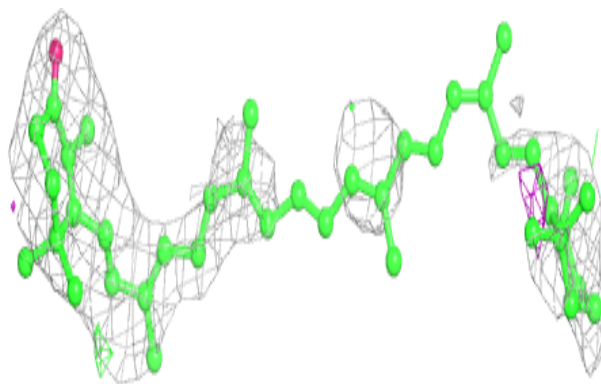


Electron density around CLA B 1240:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

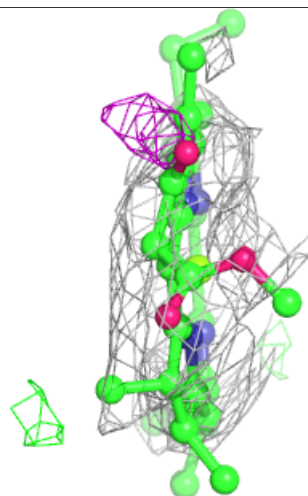
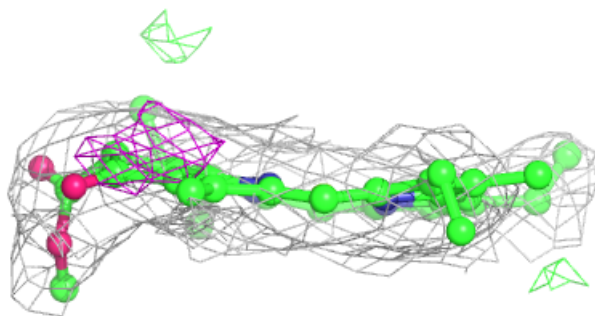
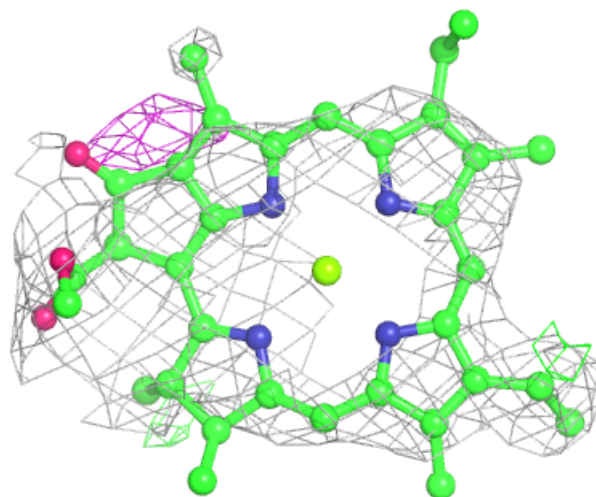
**Electron density around ECH 2 4006:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



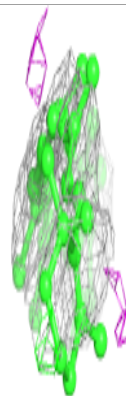
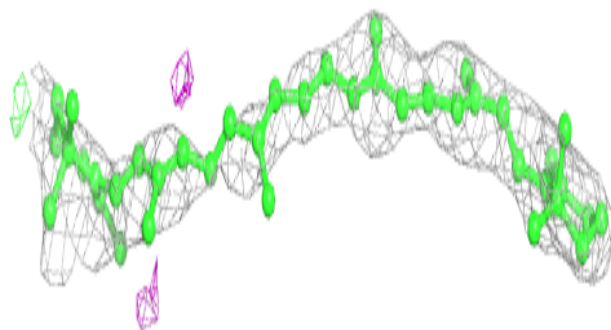
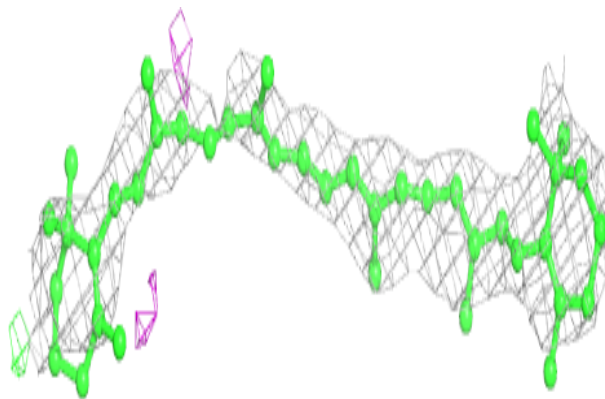
Electron density around CLA 2 1212:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



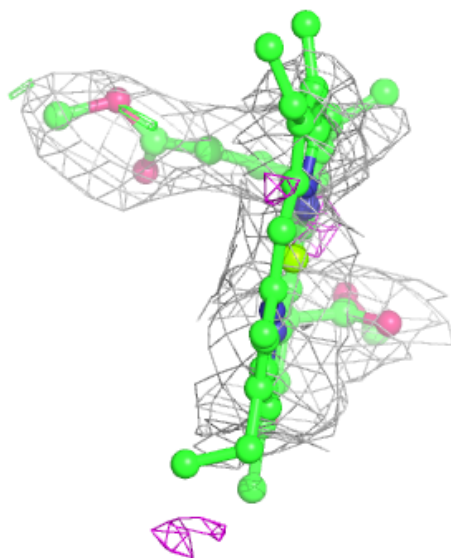
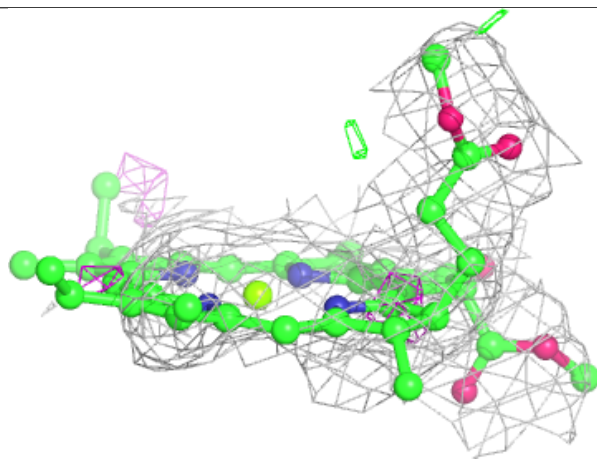
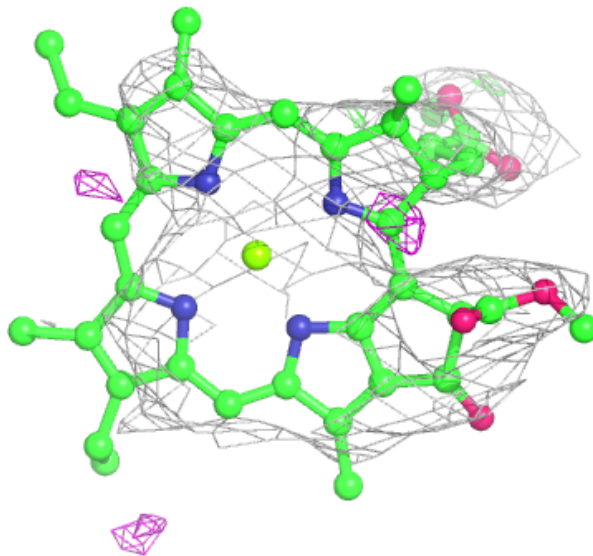
Electron density around BCR j 4013:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



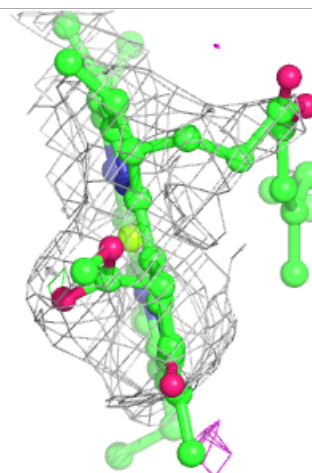
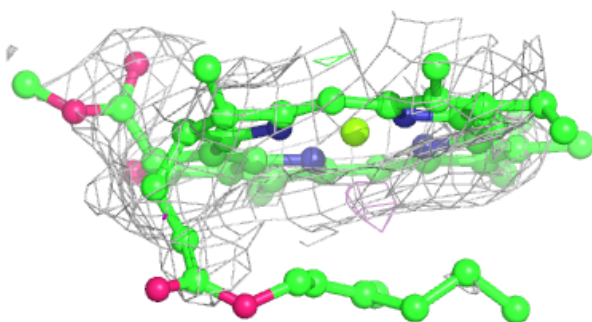
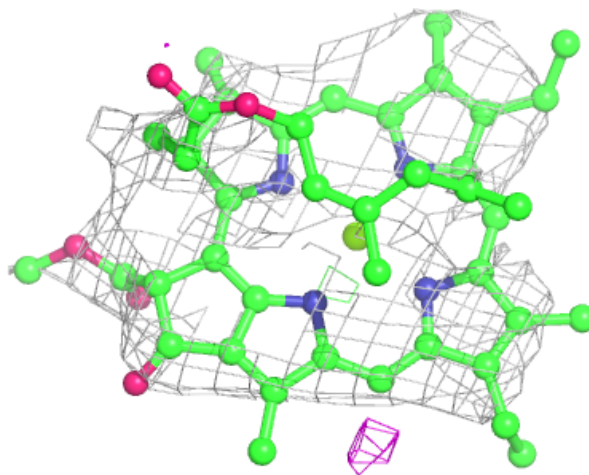
Electron density around CLA 2 1231:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



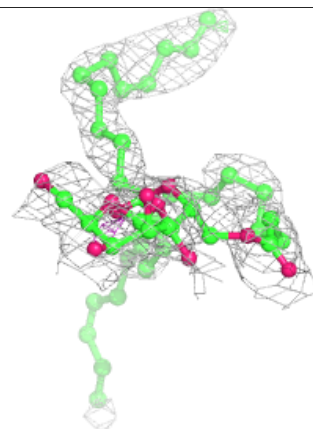
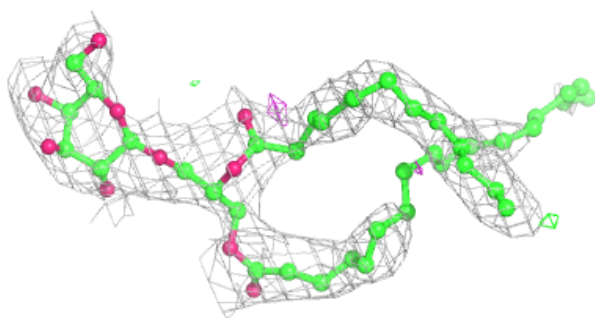
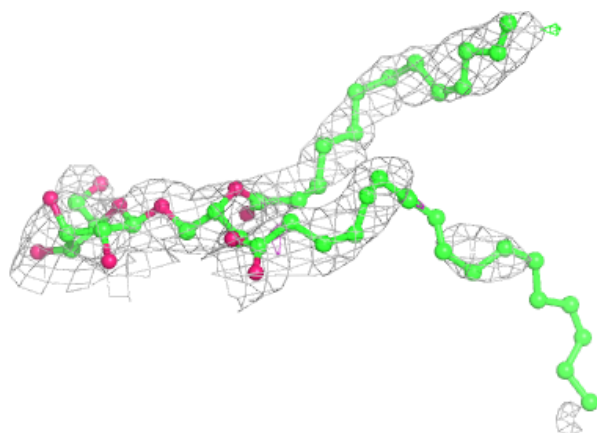
Electron density around CLA a 1114:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

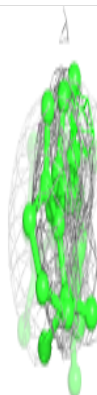
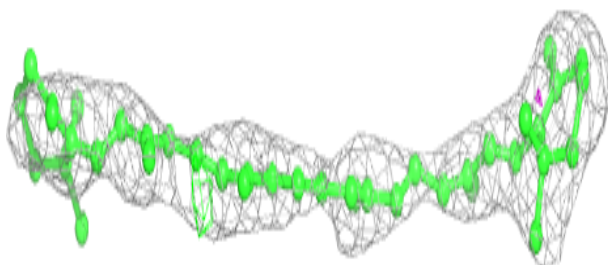
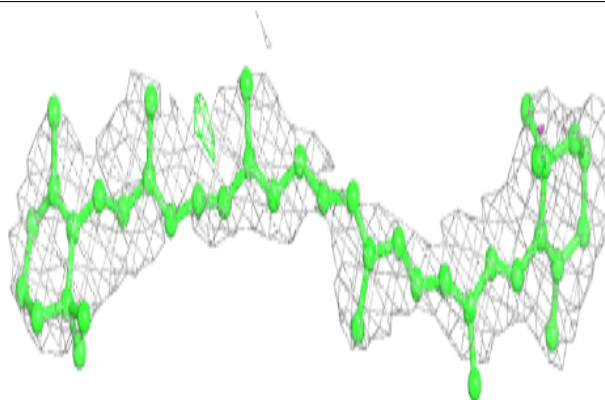


Electron density around LMG 1 5002:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

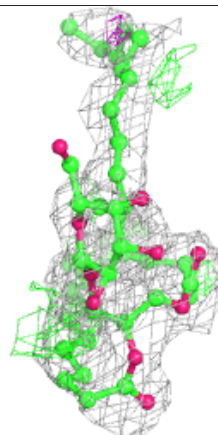
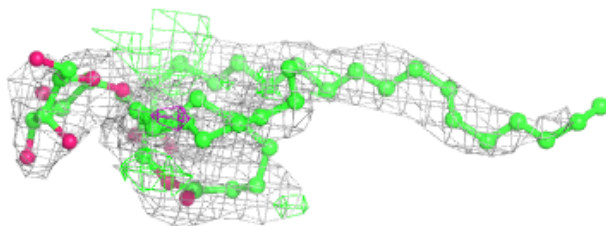
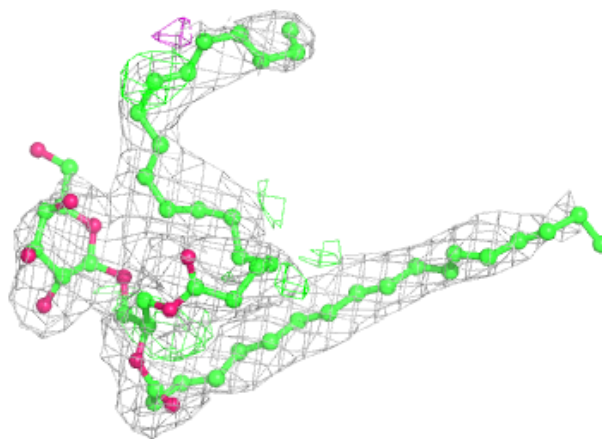
**Electron density around BCR B 4004:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

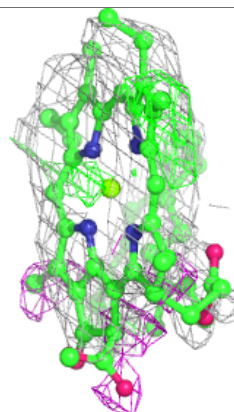
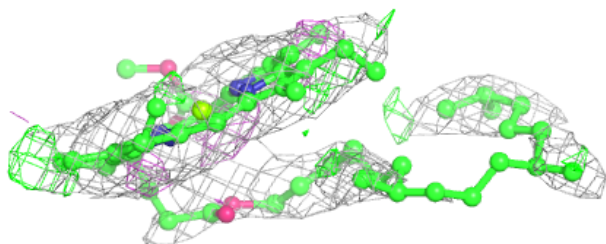
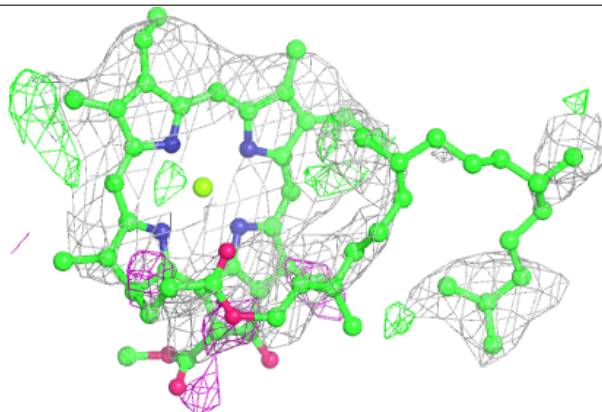


Electron density around LMG K 5009:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

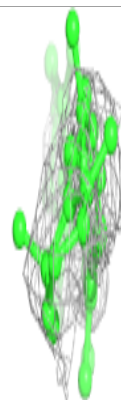
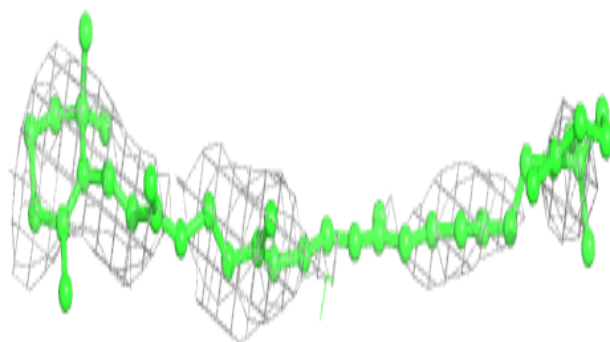
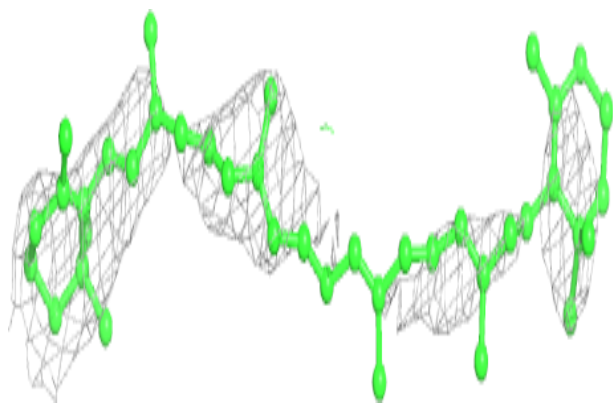
**Electron density around CLA J 1302:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

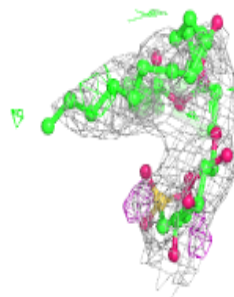
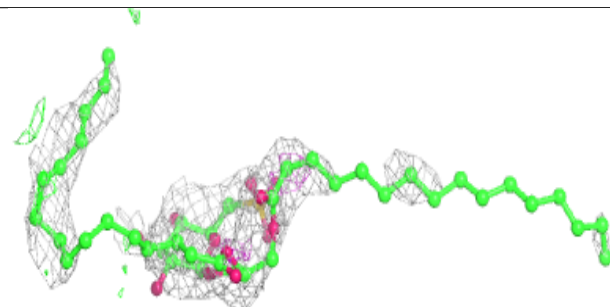
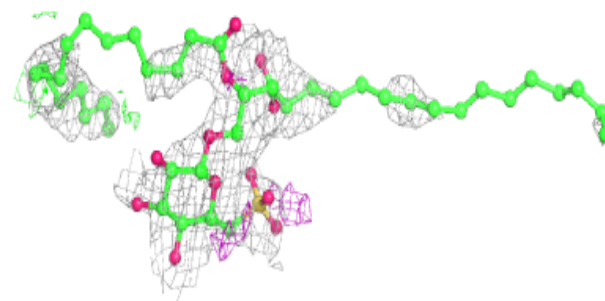


Electron density around BCR 1 4012:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

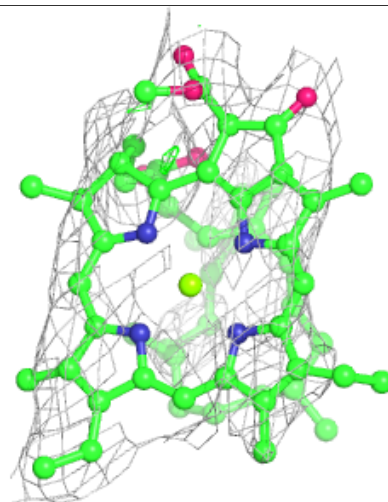
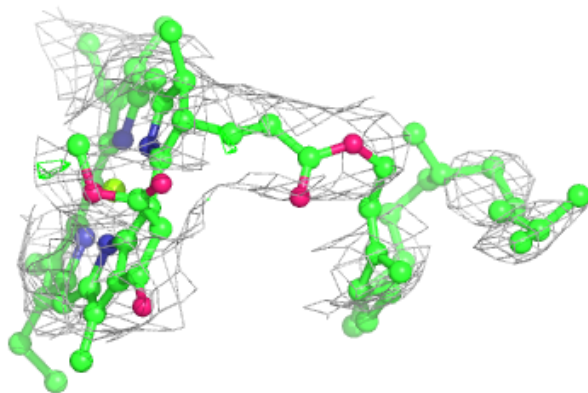
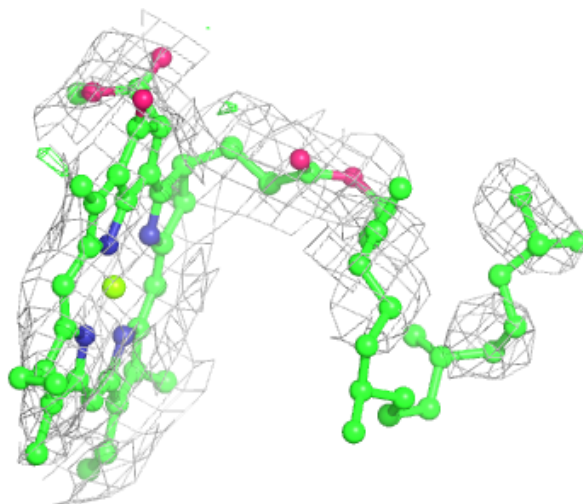
**Electron density around SQD F 5001:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



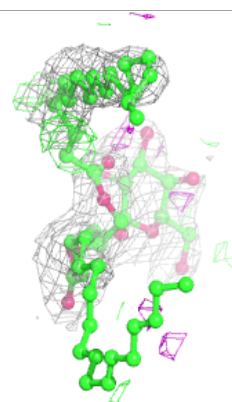
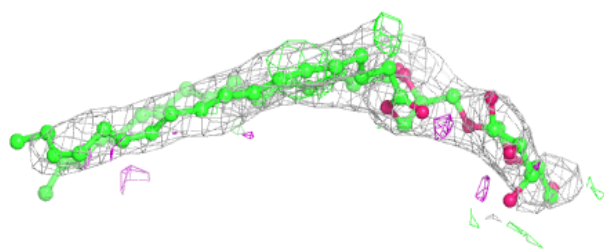
Electron density around CLA a 1112:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



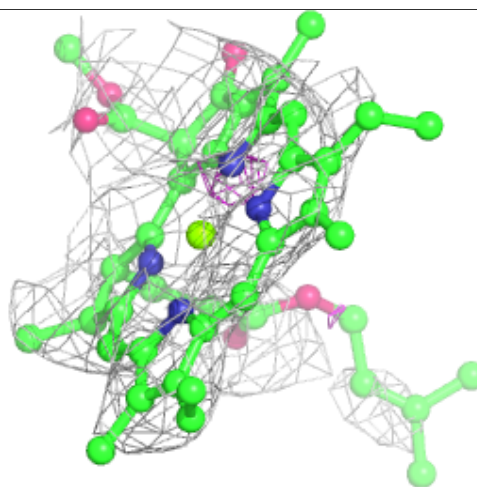
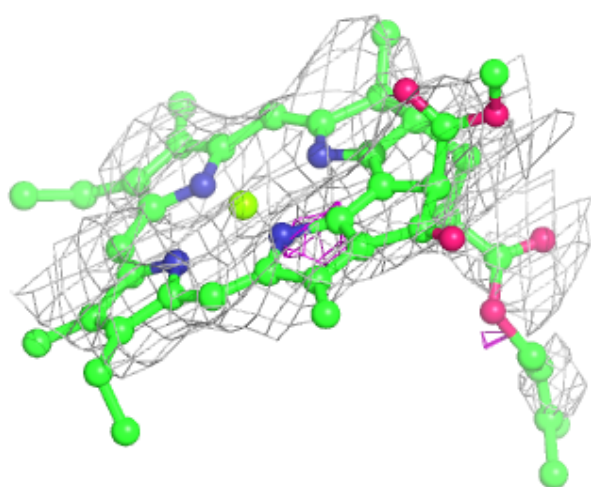
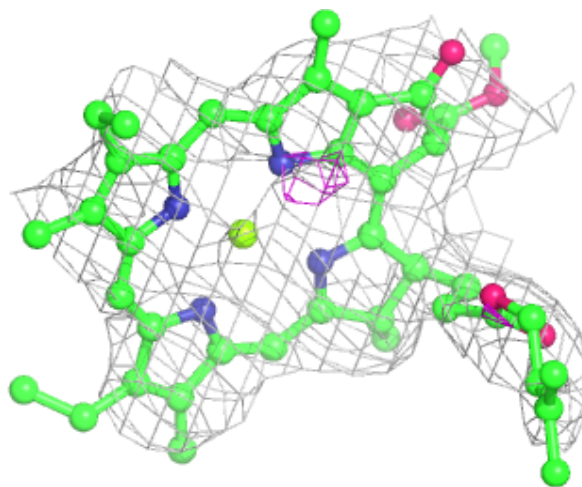
Electron density around LMG b 5005:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



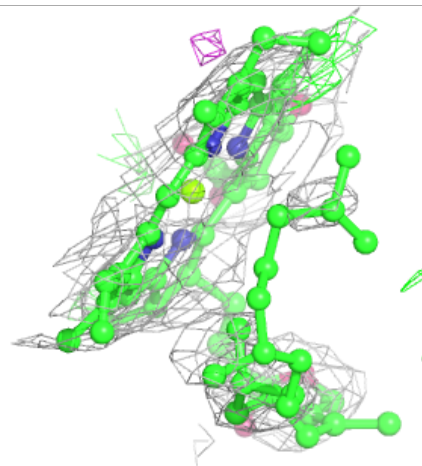
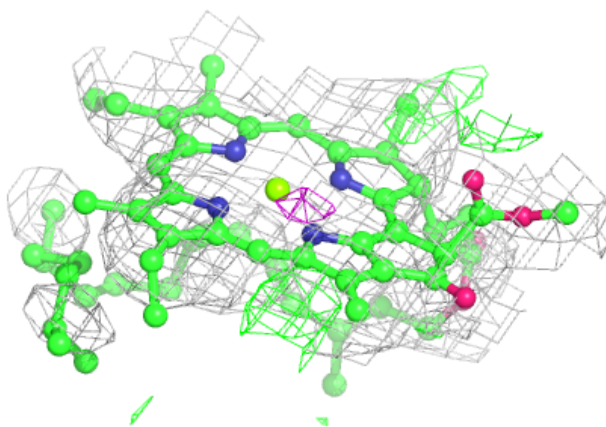
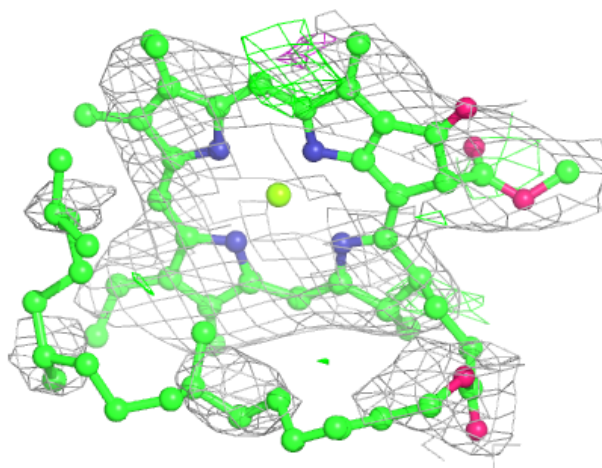
Electron density around CLA 1 1105:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



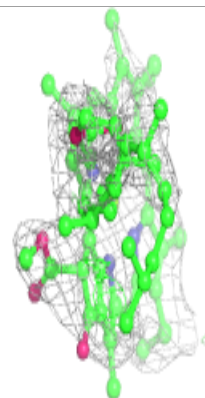
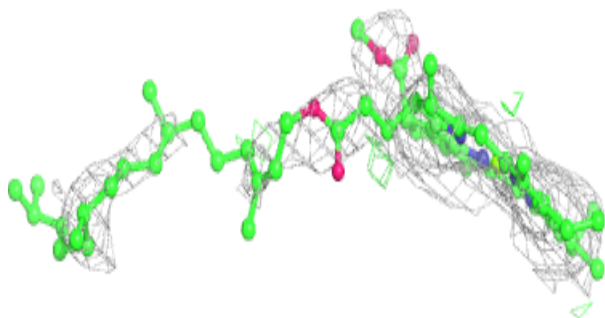
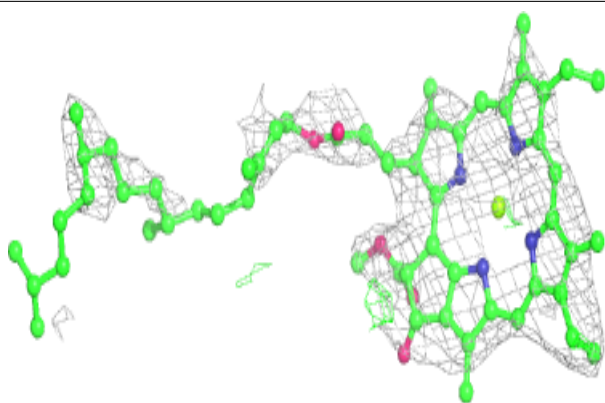
Electron density around CLA a 1118:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

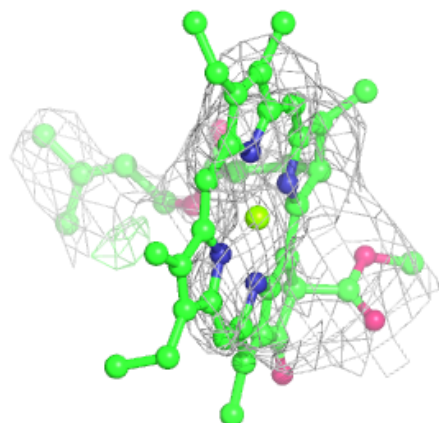
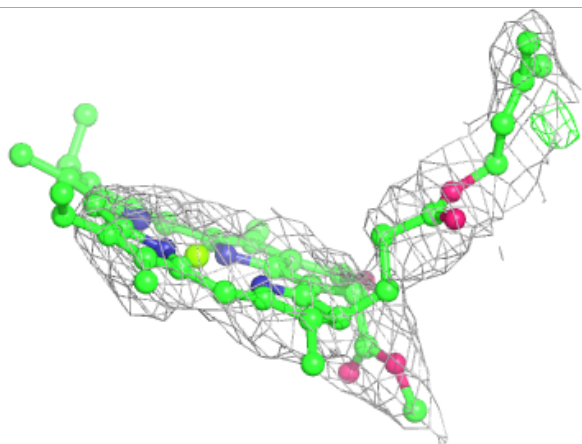
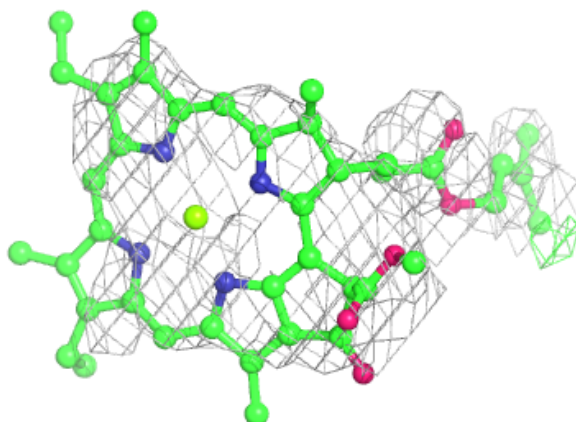


Electron density around CLA 1 1139:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

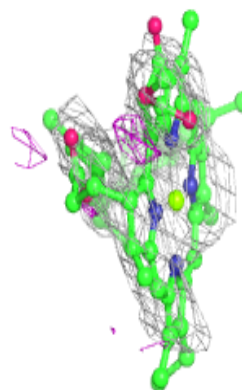
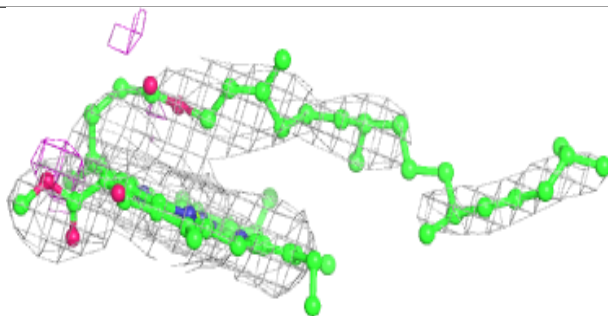
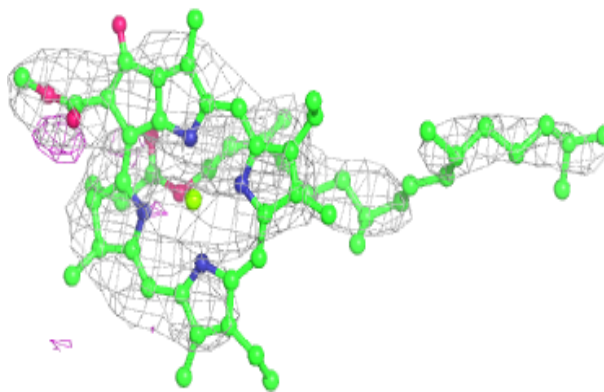
**Electron density around CLA k 1401:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



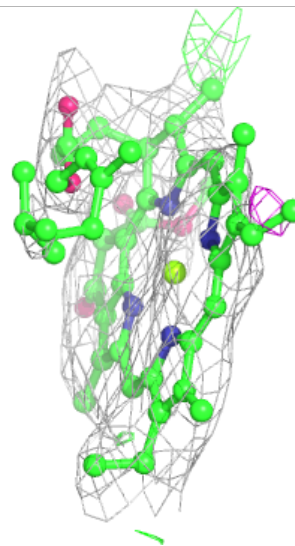
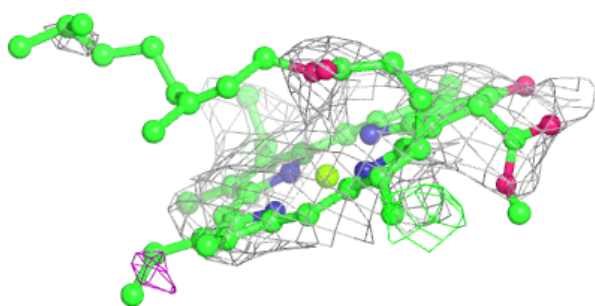
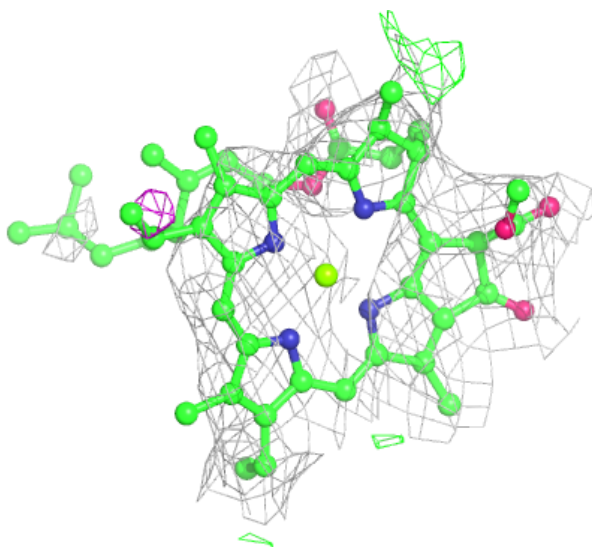
Electron density around CLA a 1115:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



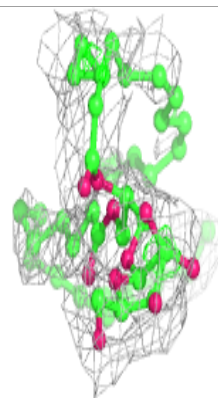
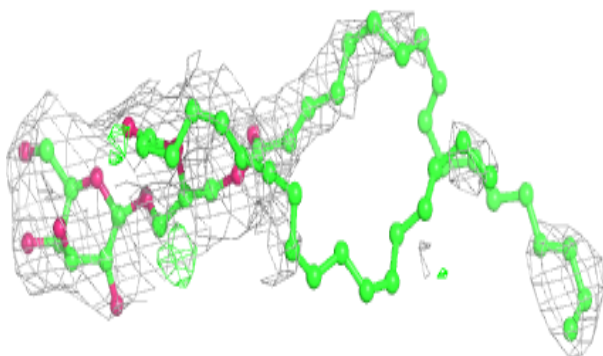
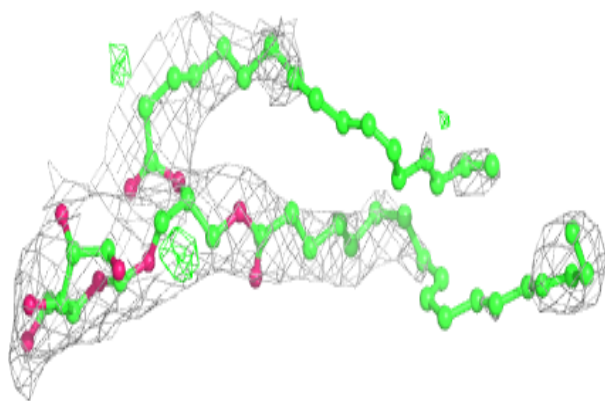
Electron density around CLA a 1120:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

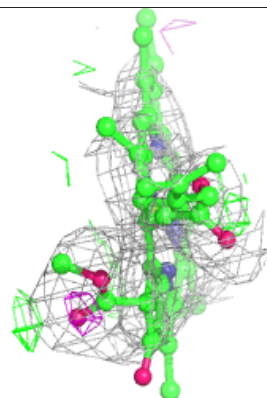
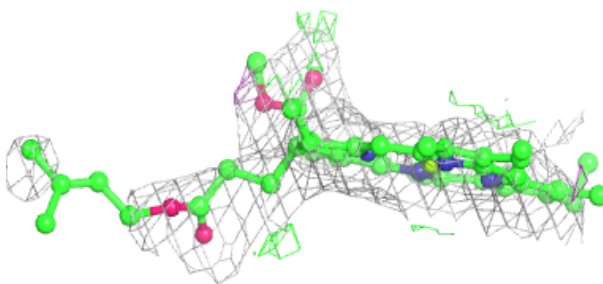
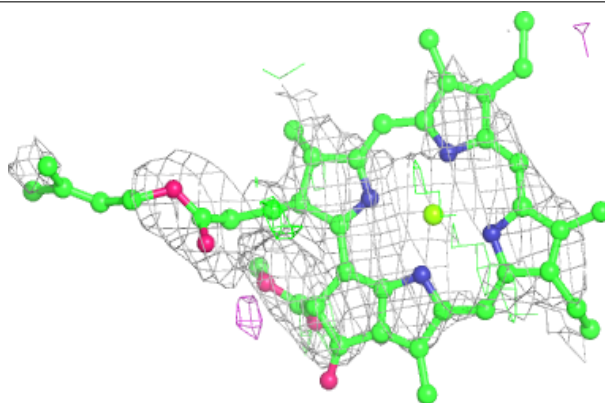


Electron density around LMG a 5004:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

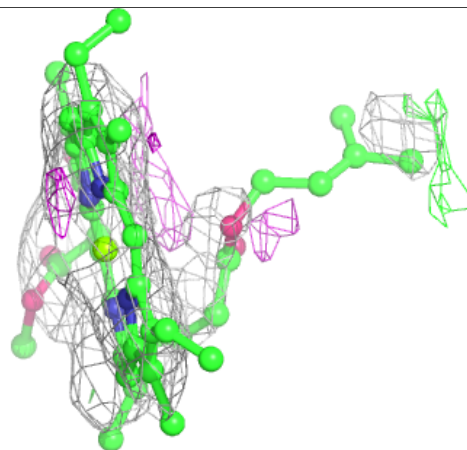
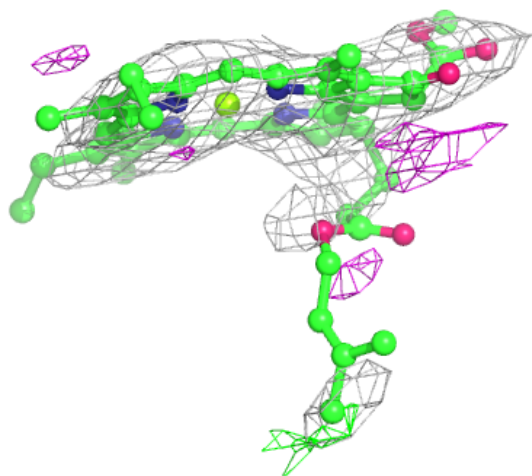
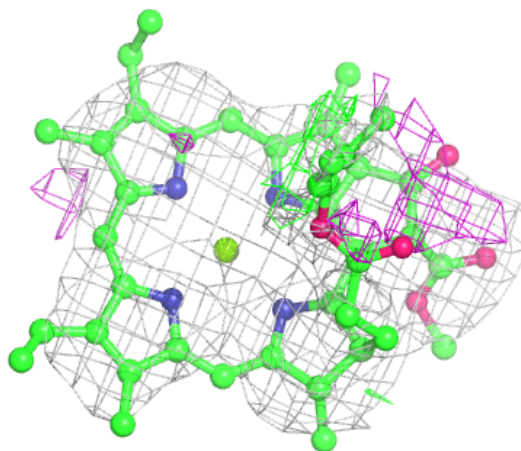
**Electron density around CLA 2 1234:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



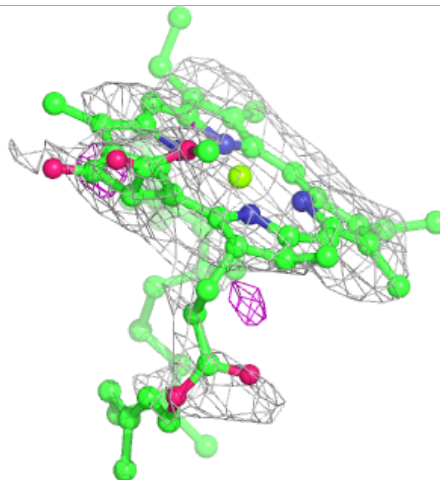
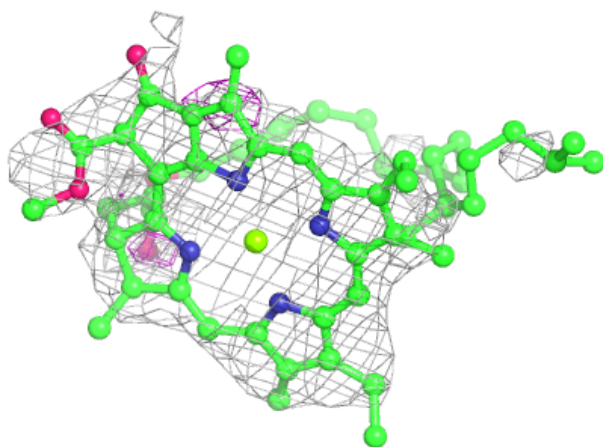
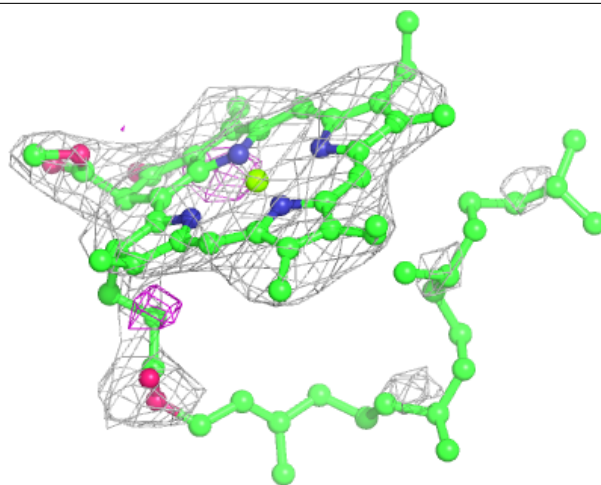
Electron density around CLA 2 1213:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



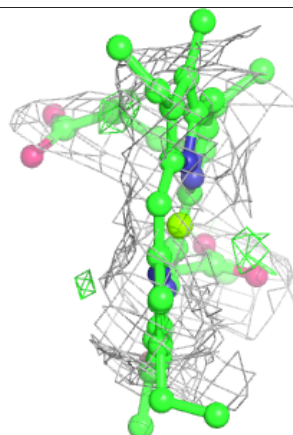
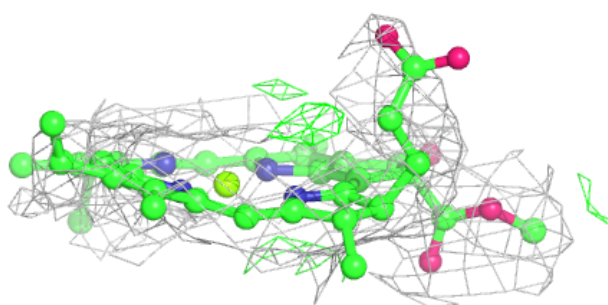
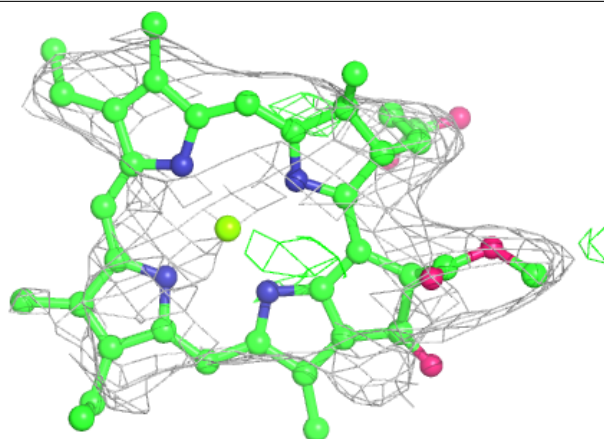
Electron density around CLA J 1303:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

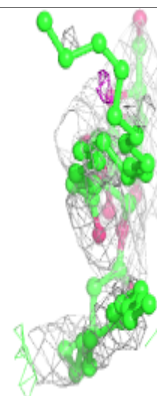
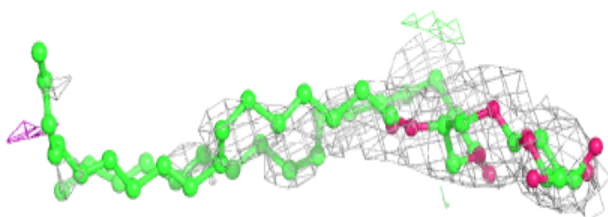
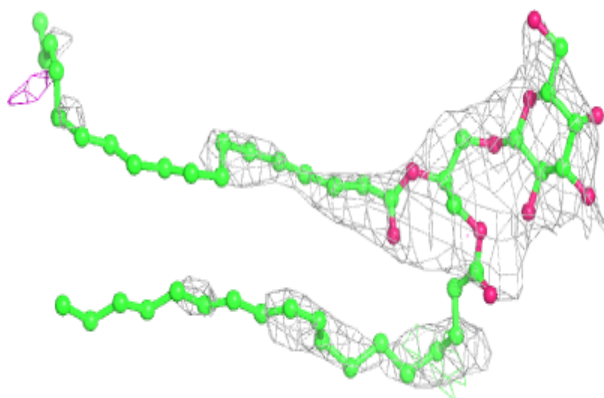


Electron density around CLA 2 1232:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

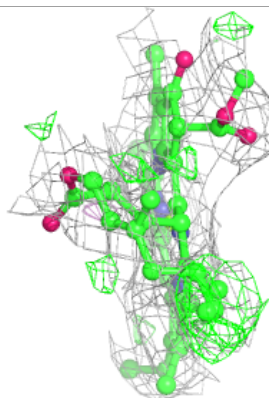
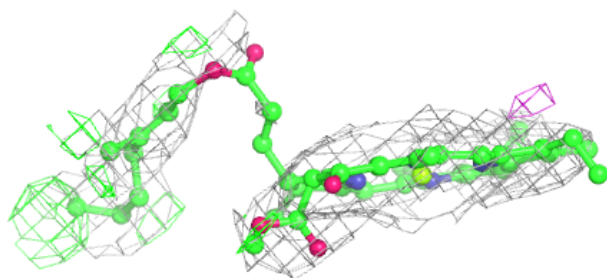
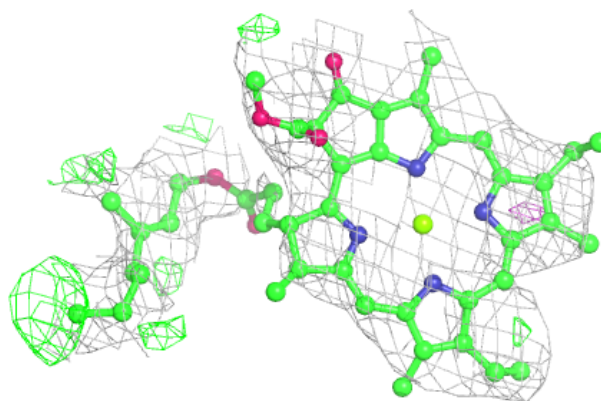
**Electron density around LMG 1 5004:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

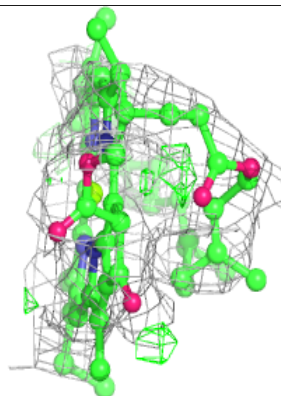
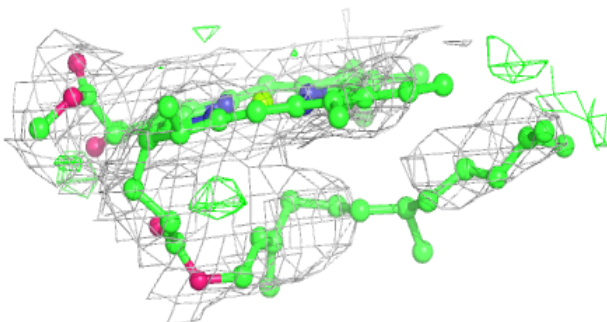
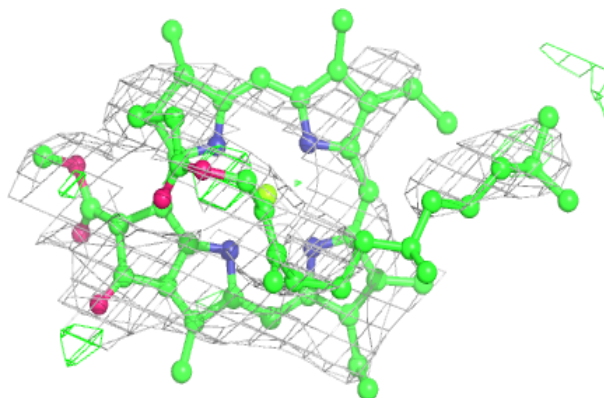


Electron density around CLA 2 1219:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

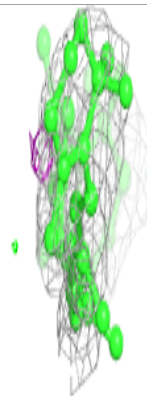
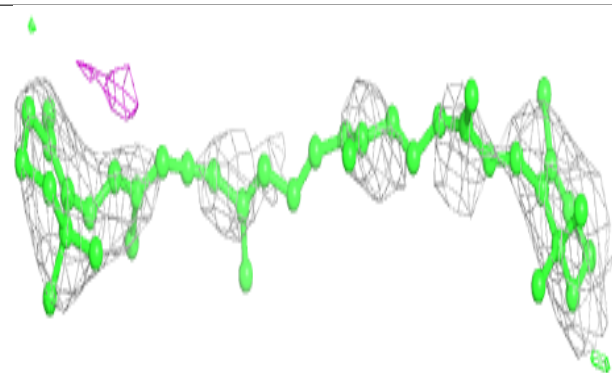
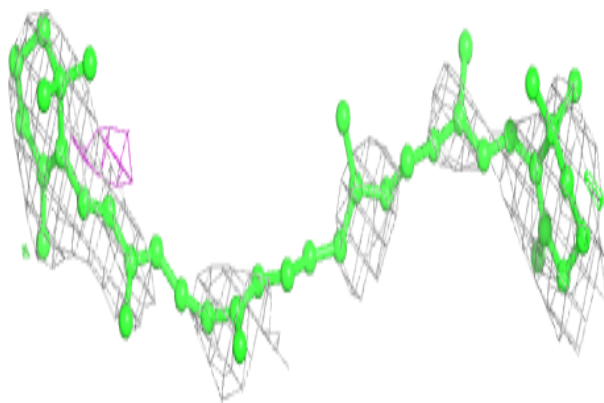
**Electron density around CLA 1 1138:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



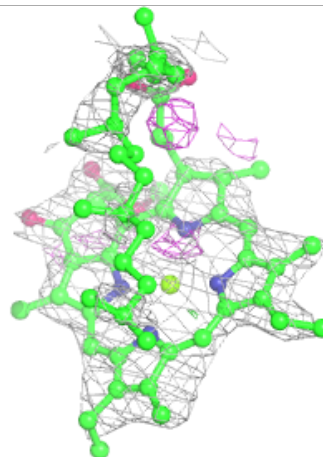
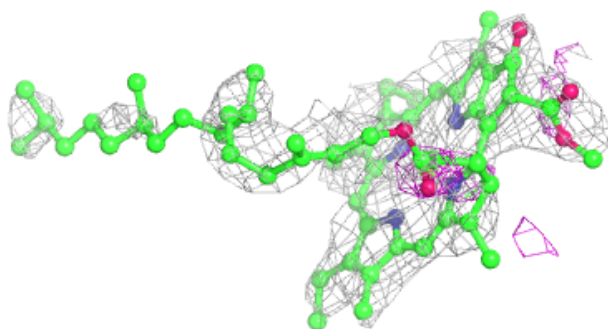
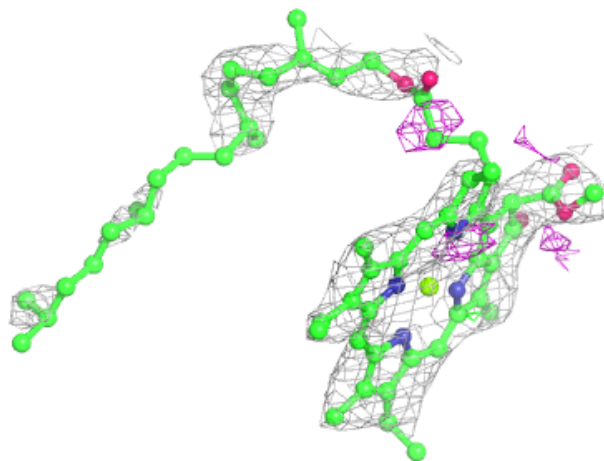
Electron density around BCR 2 4010:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



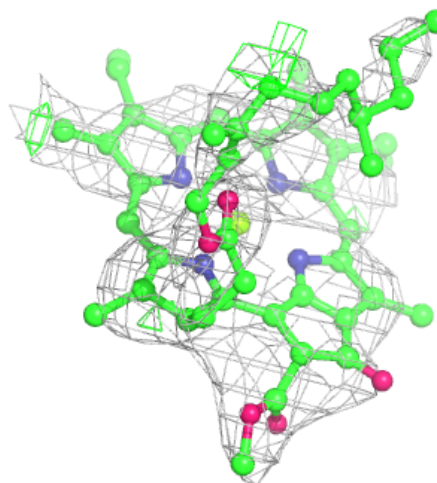
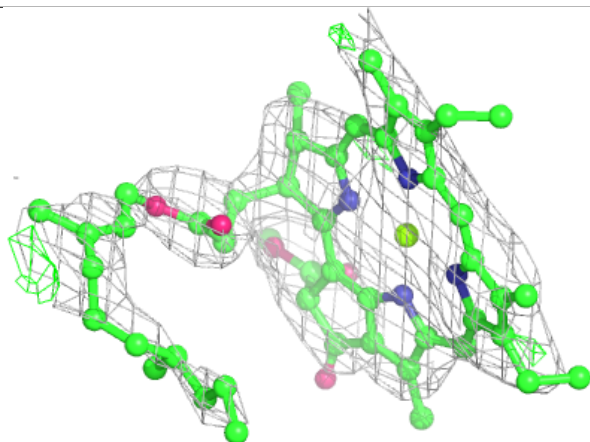
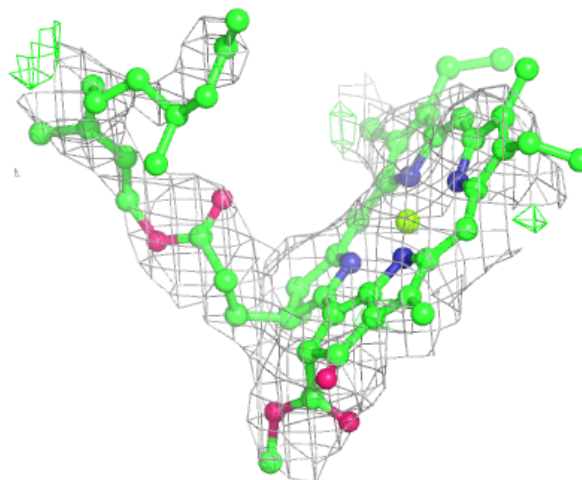
Electron density around CLA a 1102:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



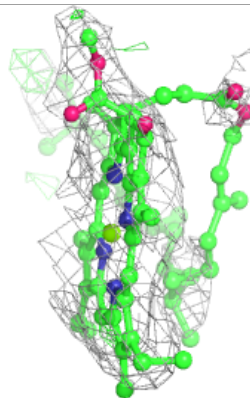
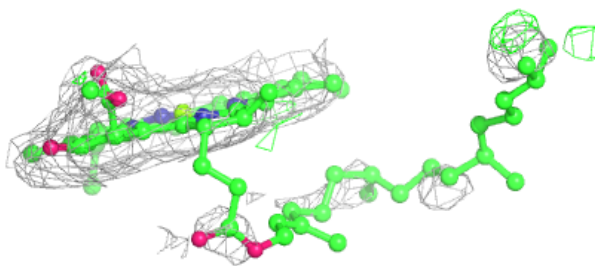
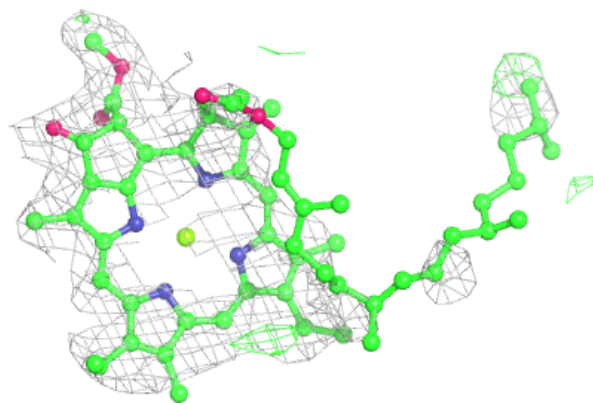
Electron density around CLA a 1108:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

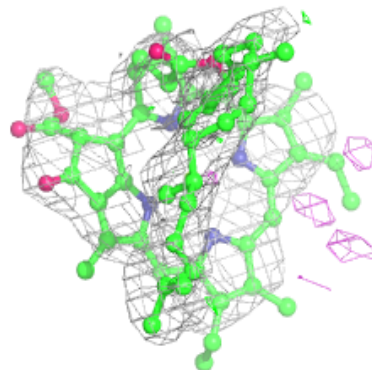
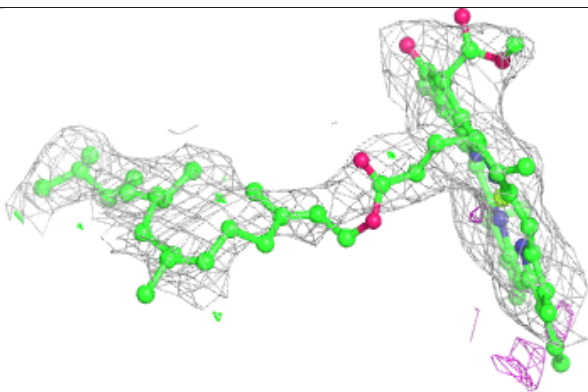
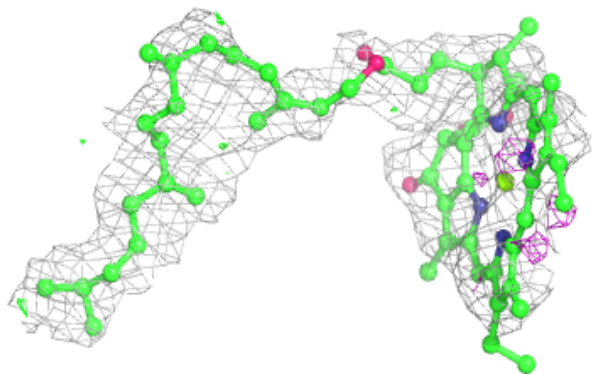


Electron density around CLA 2 1218:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

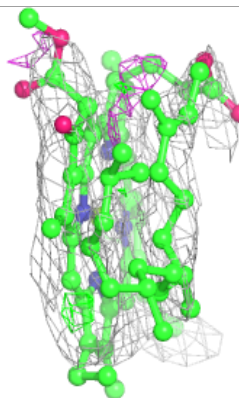
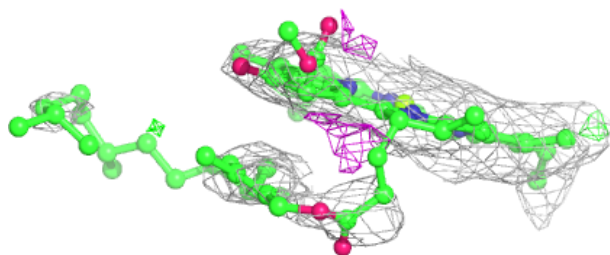
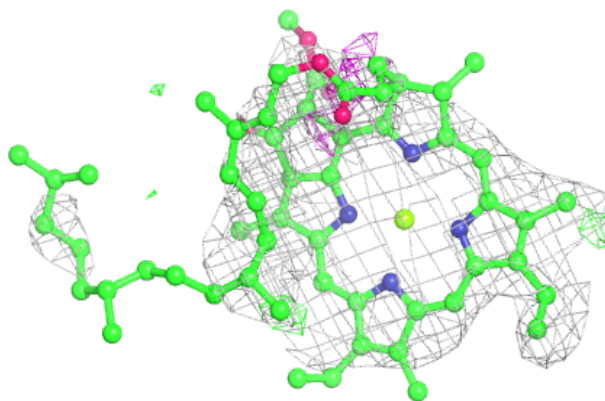
**Electron density around CLA 1 1134:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

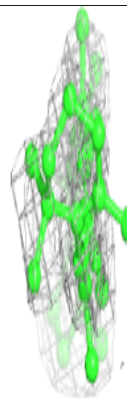
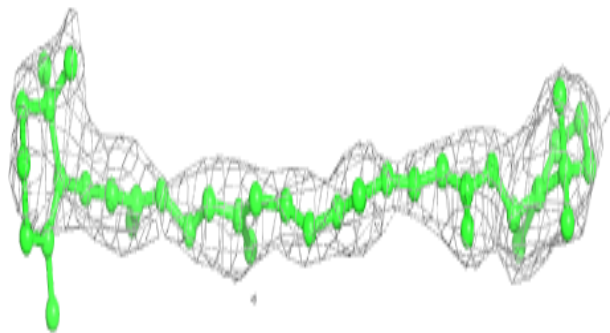
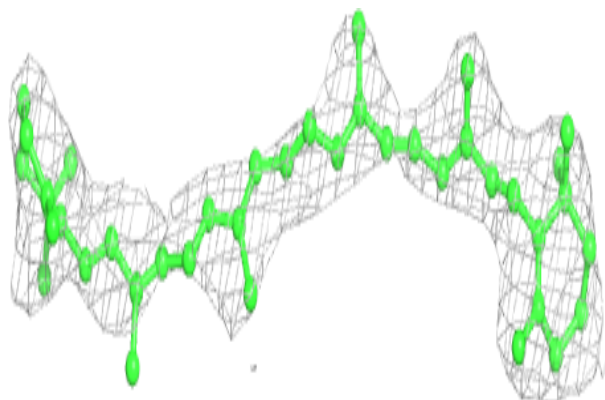


Electron density around CLA j 1302:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

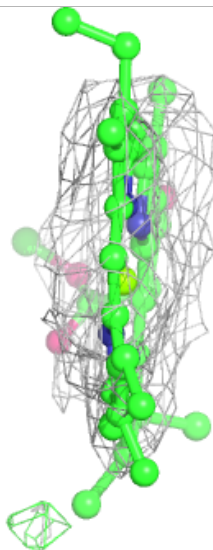
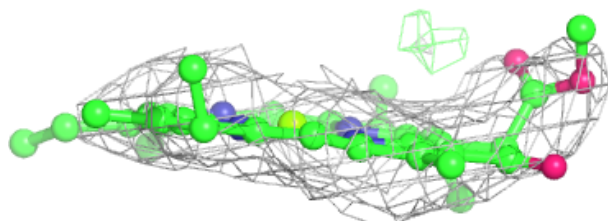
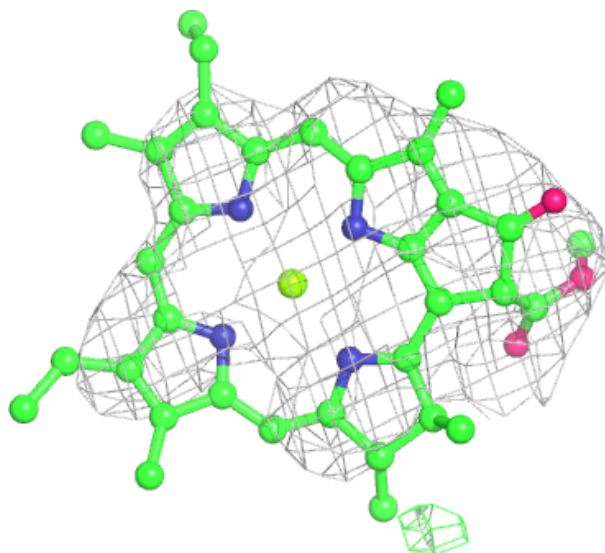
**Electron density around BCR B 4005:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



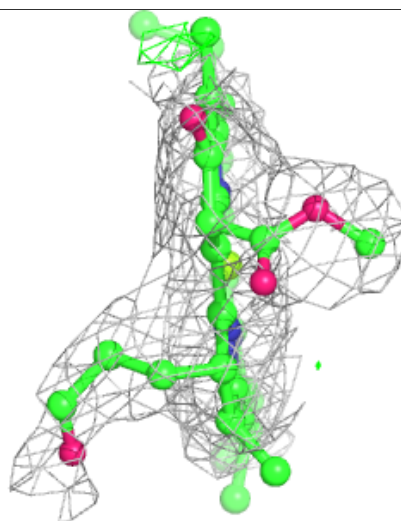
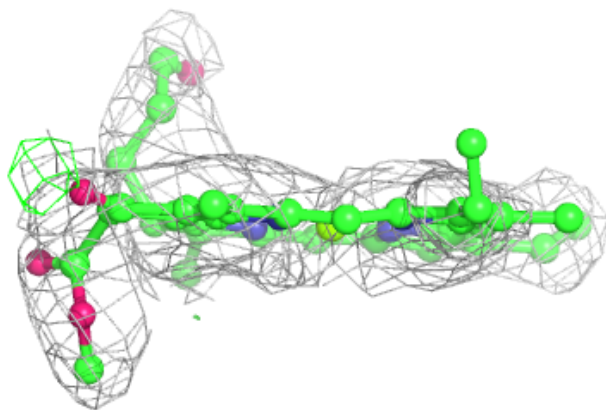
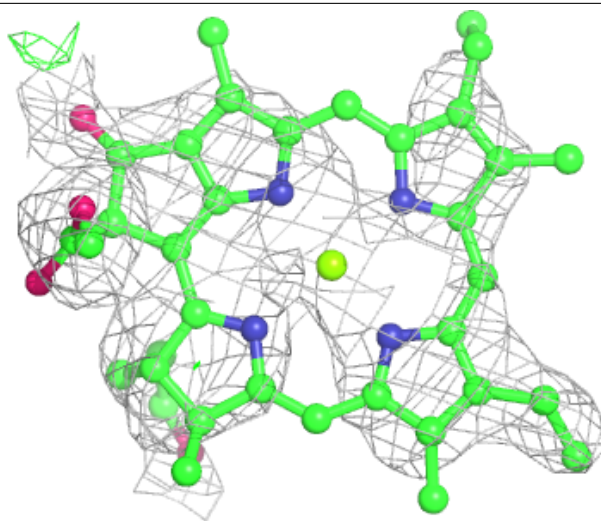
Electron density around CLA 7 1303:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



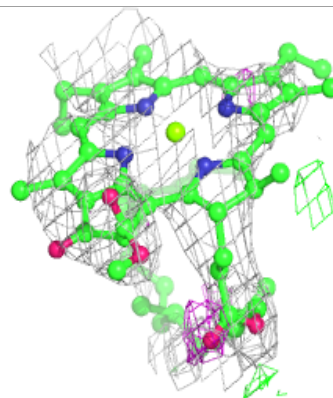
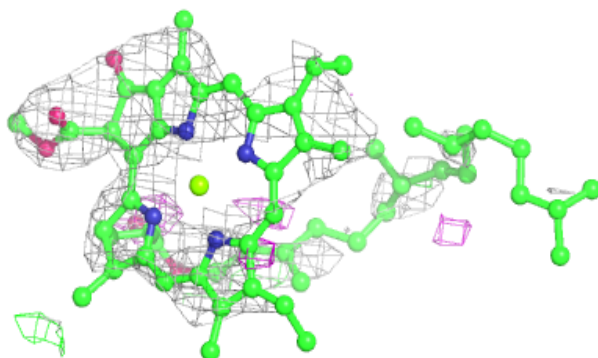
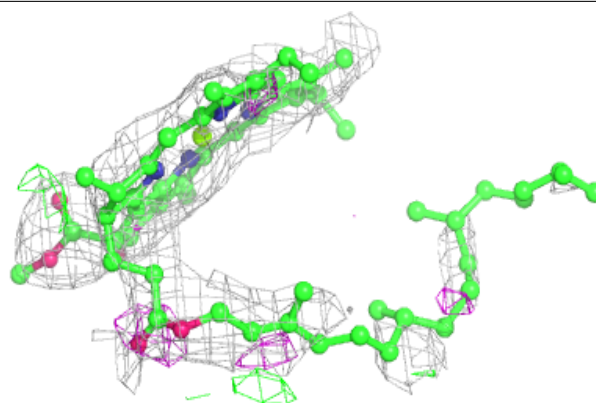
Electron density around CLA 1 1113:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

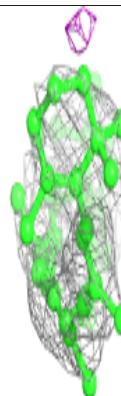
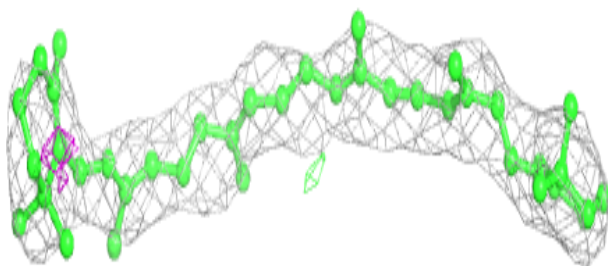
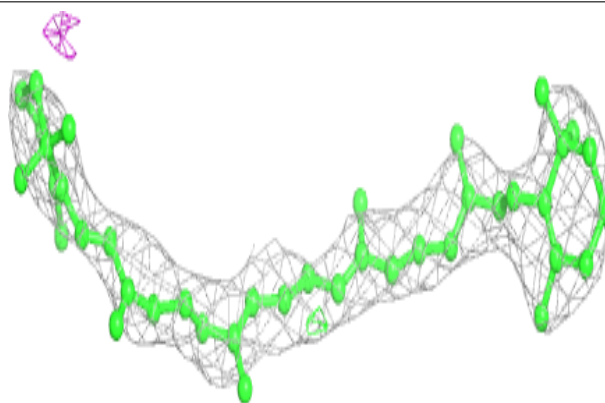


Electron density around CLA 1 1109:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

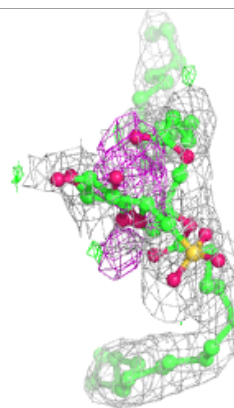
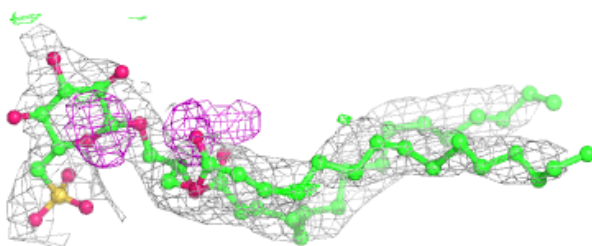
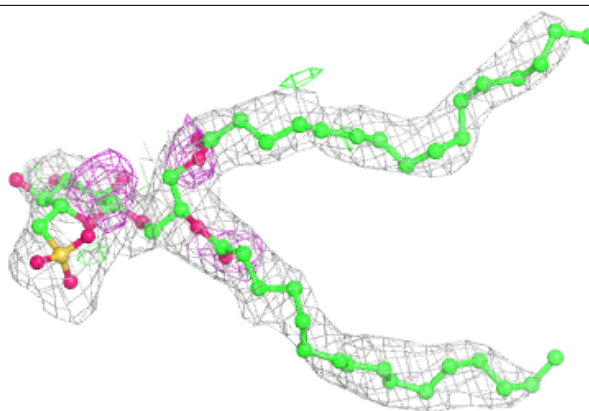
**Electron density around BCR b 4014:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



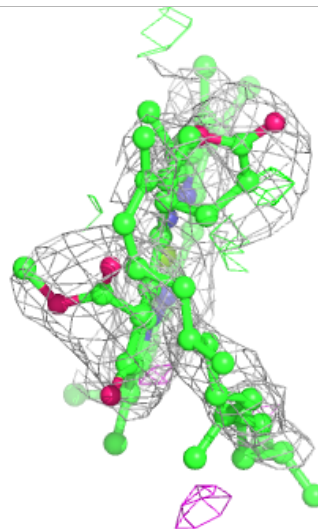
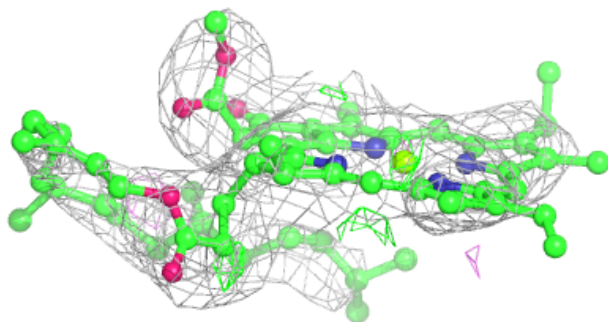
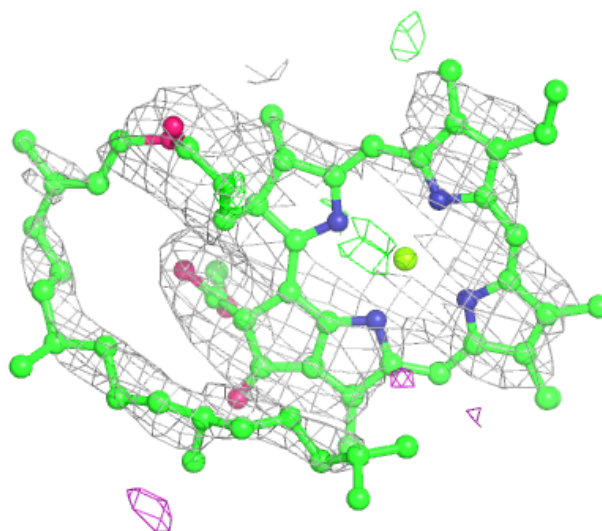
Electron density around SQD L 5002:

$2mF_o - DF_c$ (at 0.7 rmsd) in gray
 $mF_o - DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)



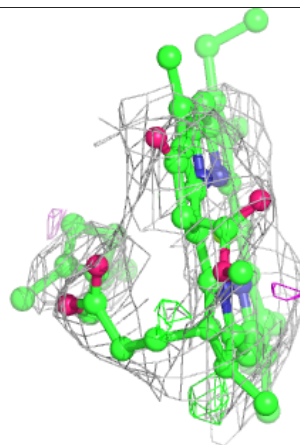
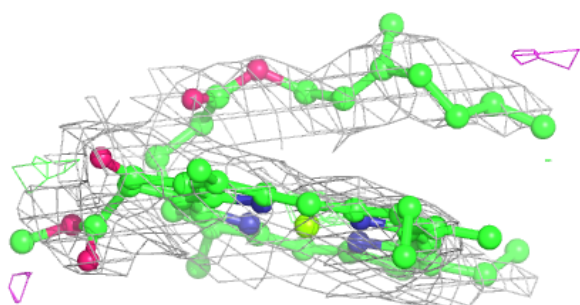
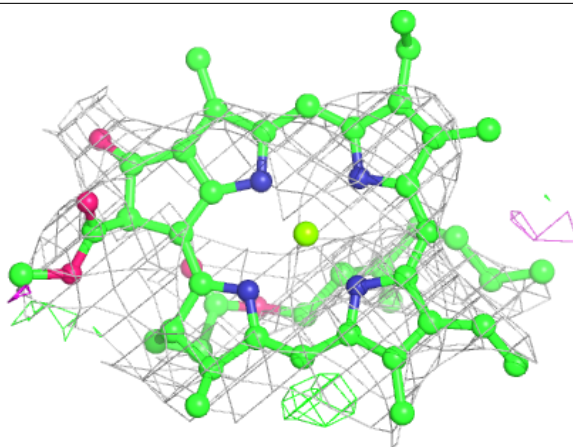
Electron density around CLA 2 1202:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



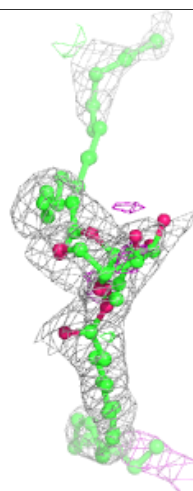
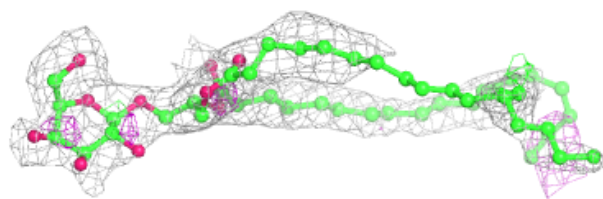
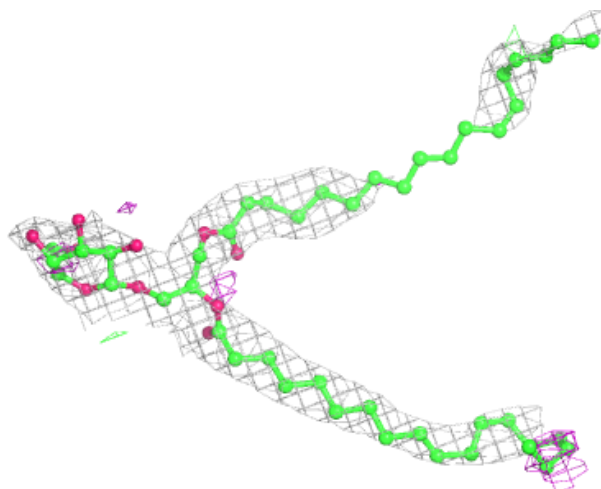
Electron density around CLA 2 1235:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



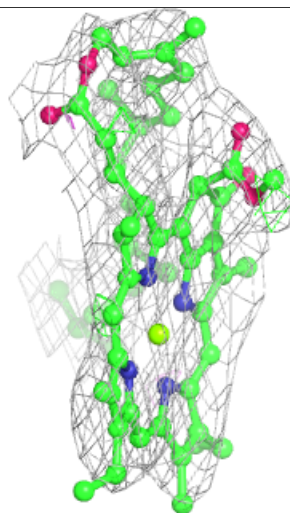
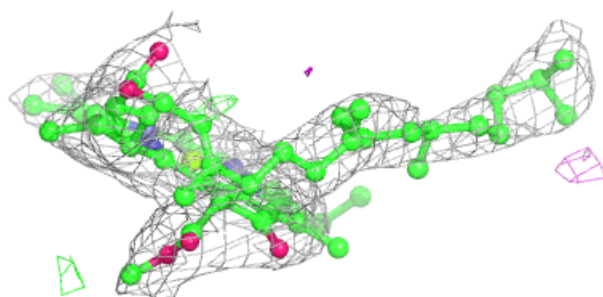
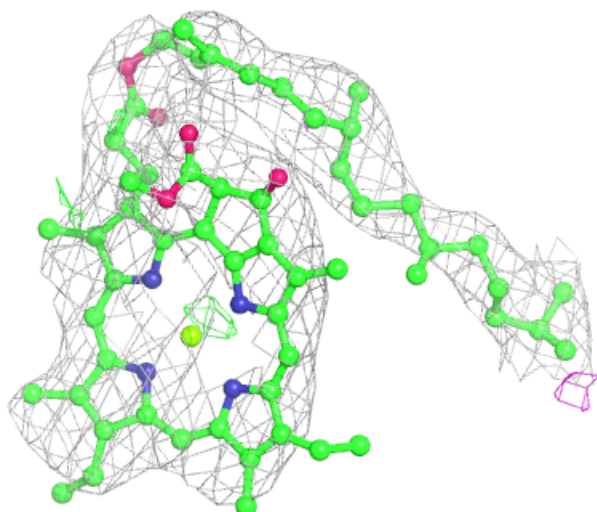
Electron density around LMG 0 5001:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



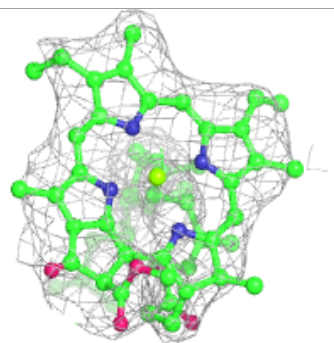
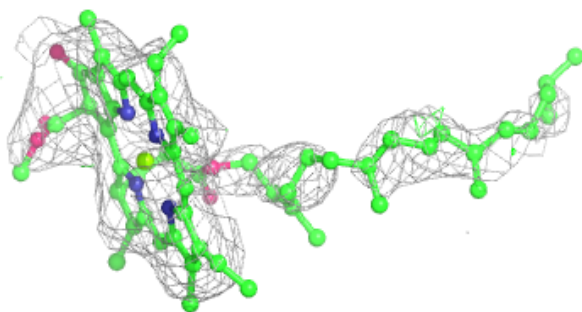
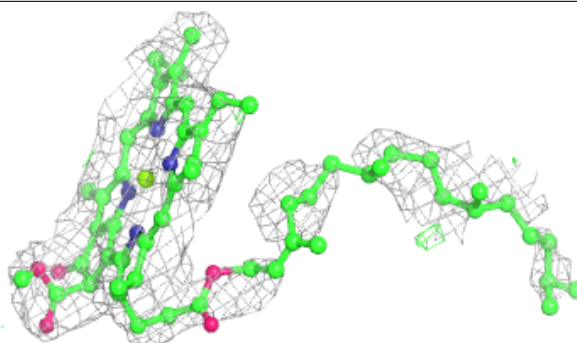
Electron density around CLA a 1123:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

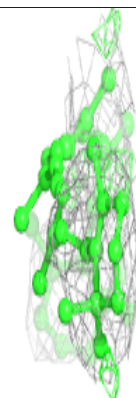
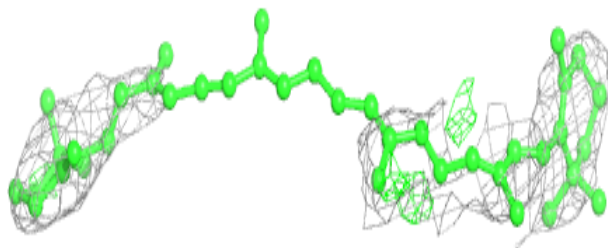
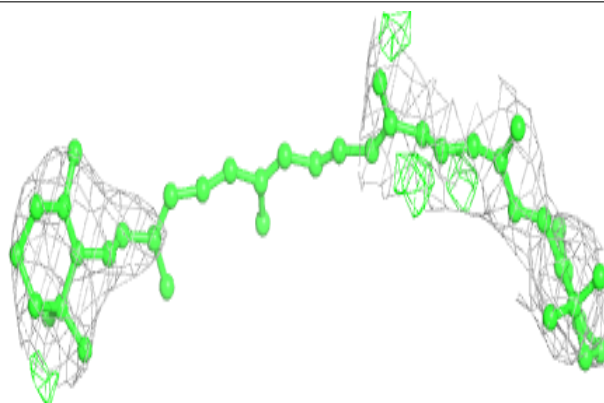


Electron density around CLA 1 1120:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

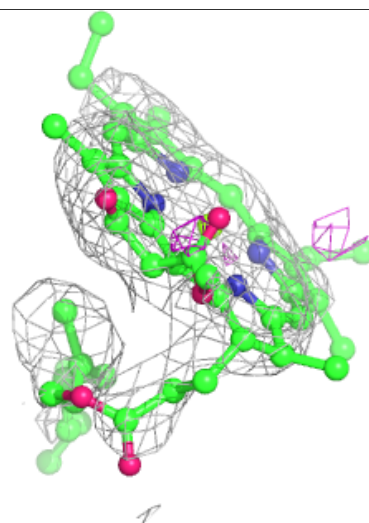
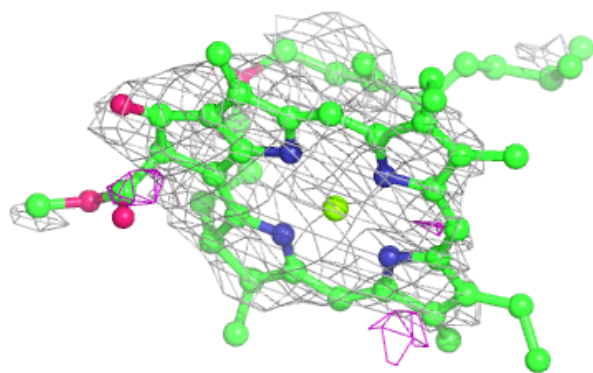
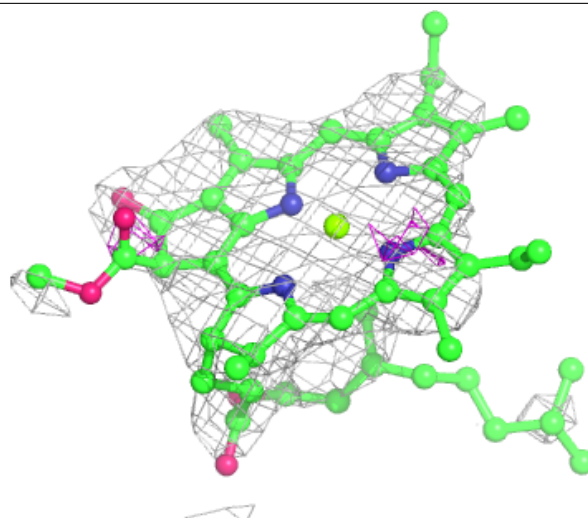
**Electron density around BCR 2 4014:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



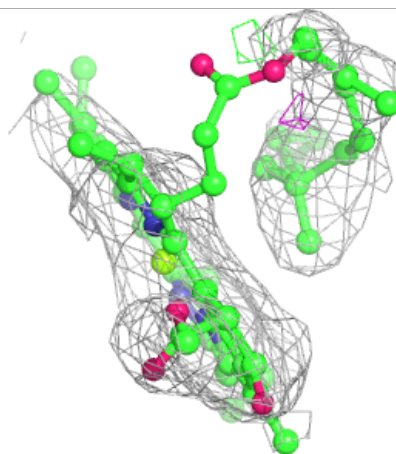
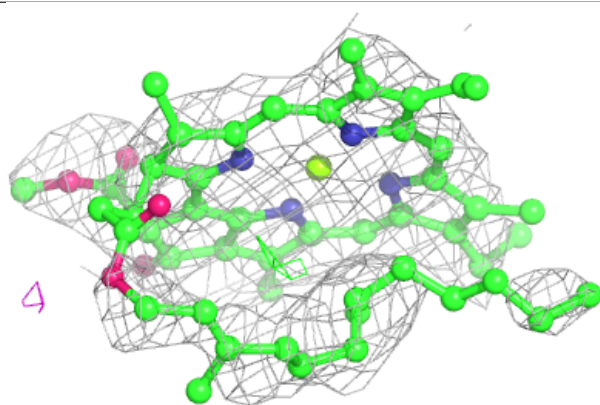
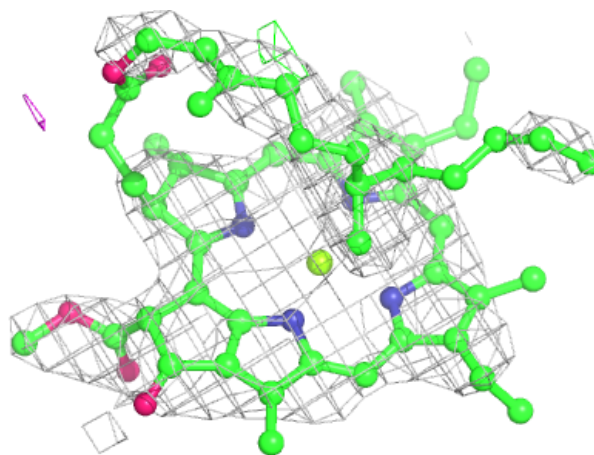
Electron density around CLA j 1303:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



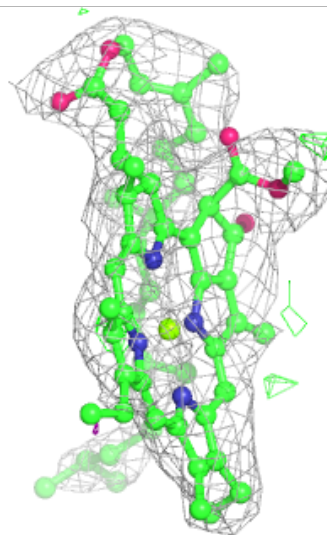
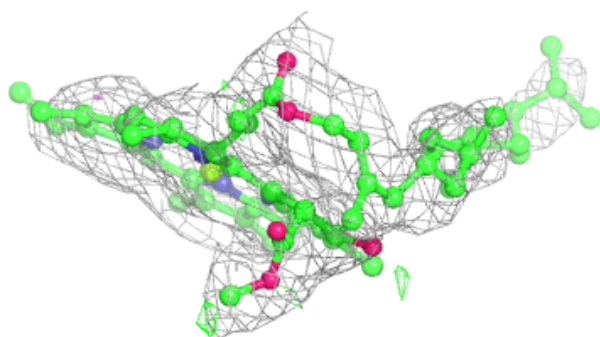
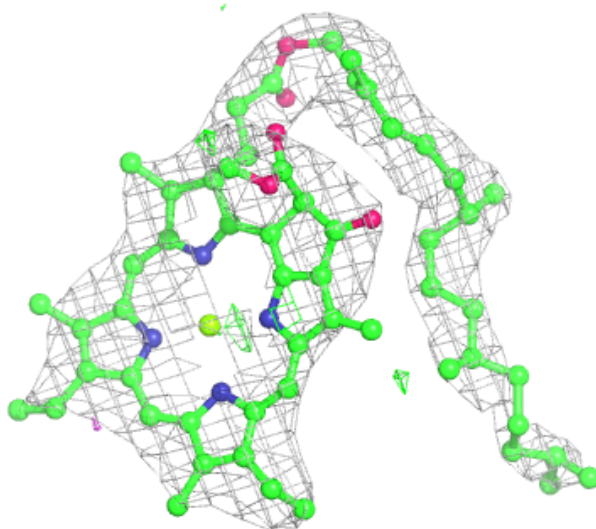
Electron density around CLA 2 1214:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



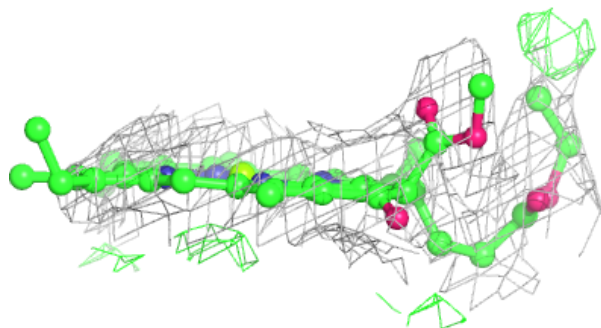
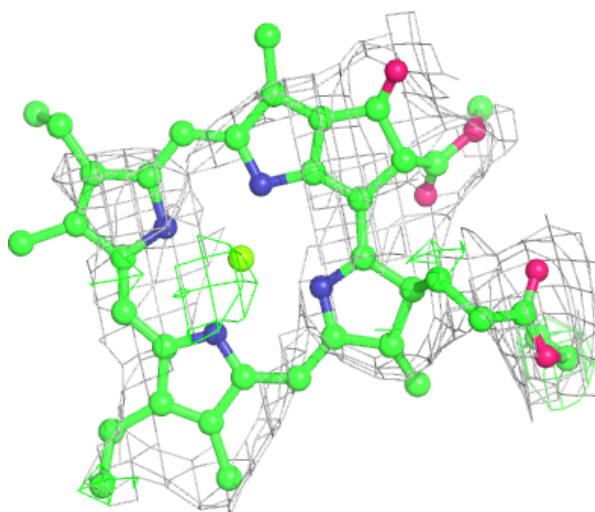
Electron density around CLA 1 1123:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



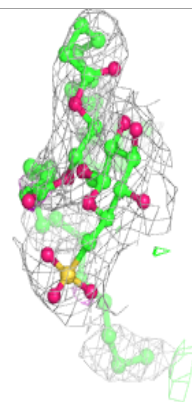
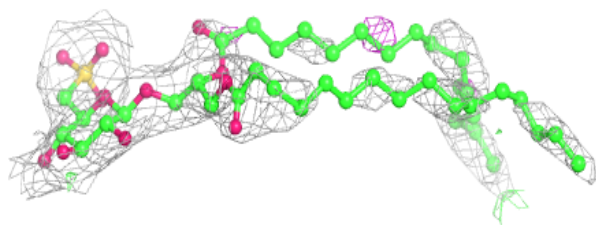
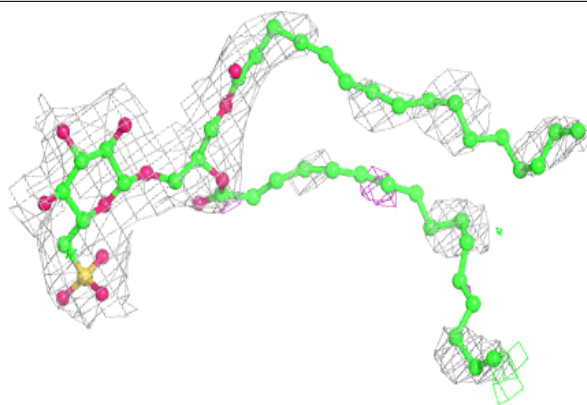
Electron density around CLA 6 1301:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

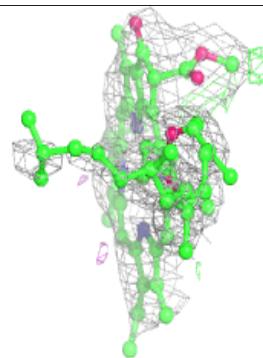
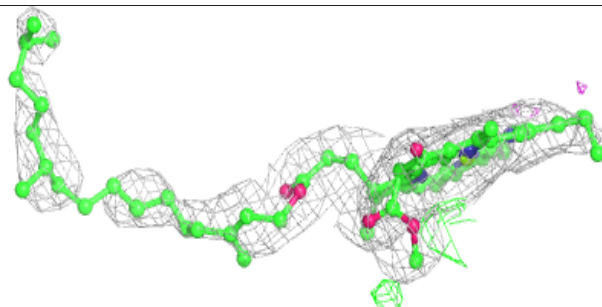
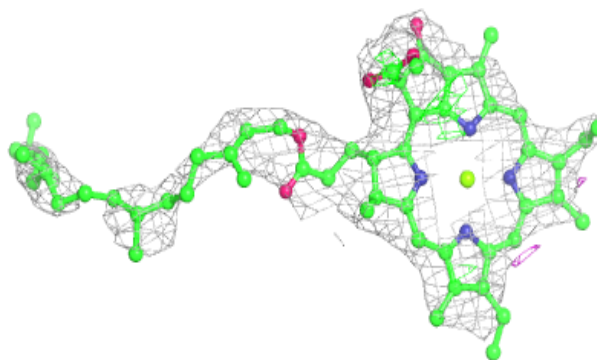


Electron density around SQD B 5008:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

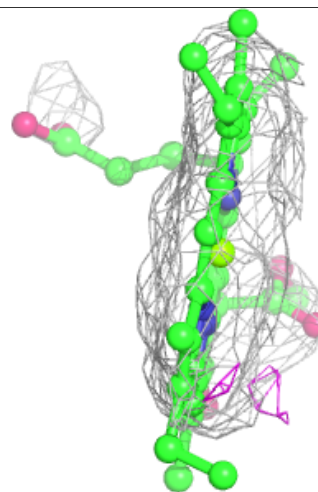
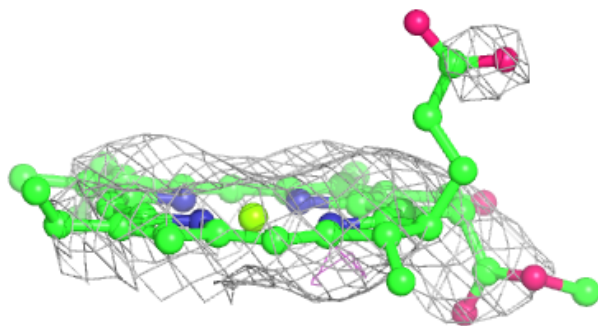
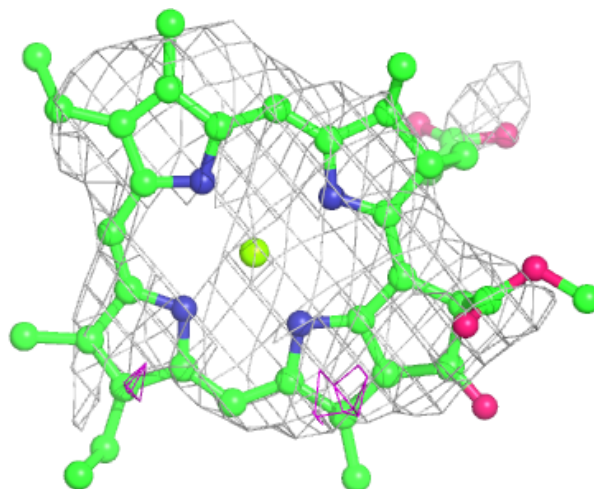
**Electron density around CLA 1 1103:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



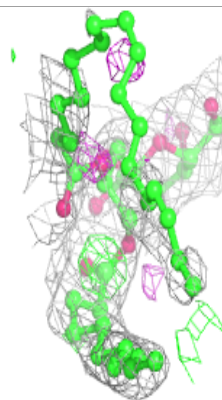
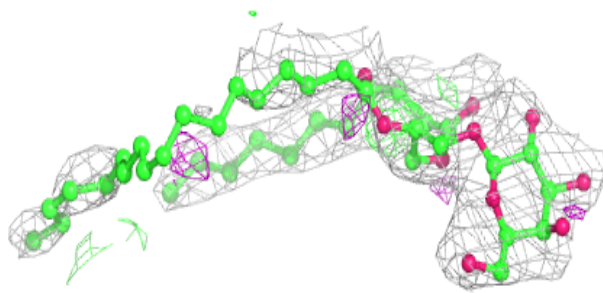
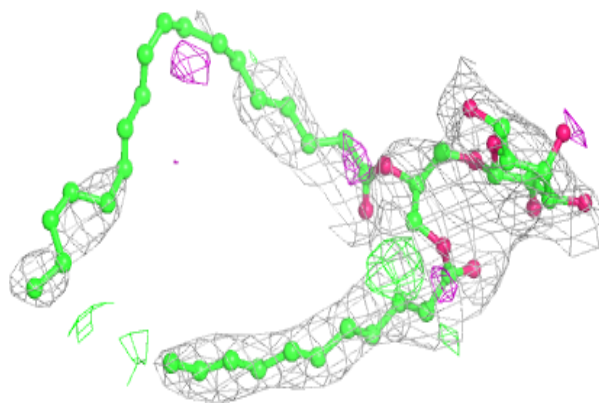
Electron density around CLA 1 1114:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



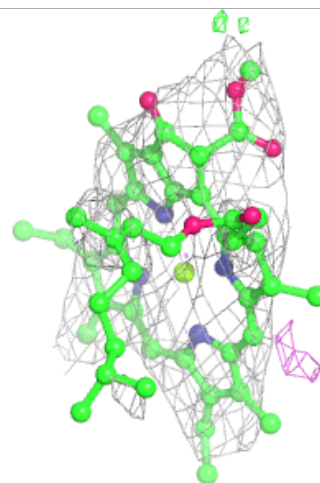
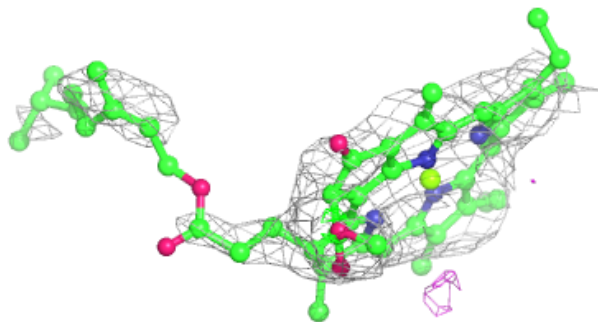
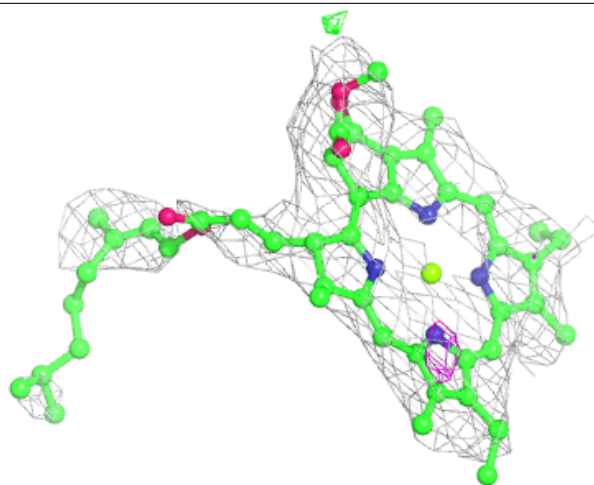
Electron density around LMG A 5004:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



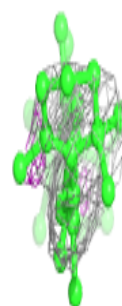
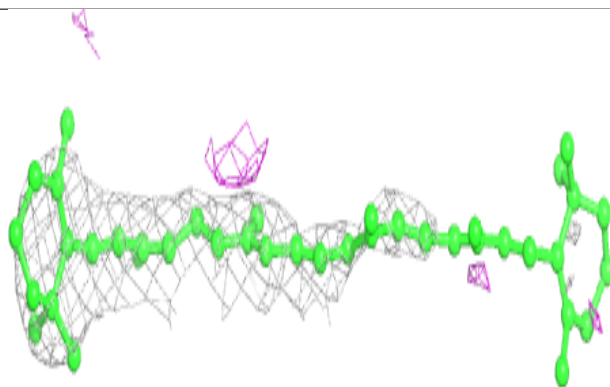
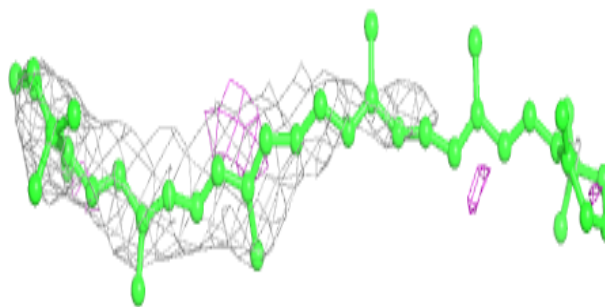
Electron density around CLA a 1801:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

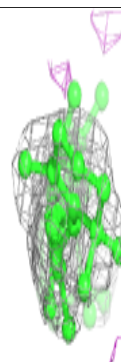
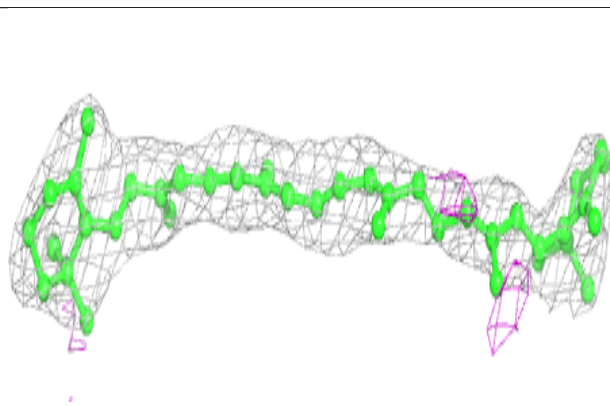
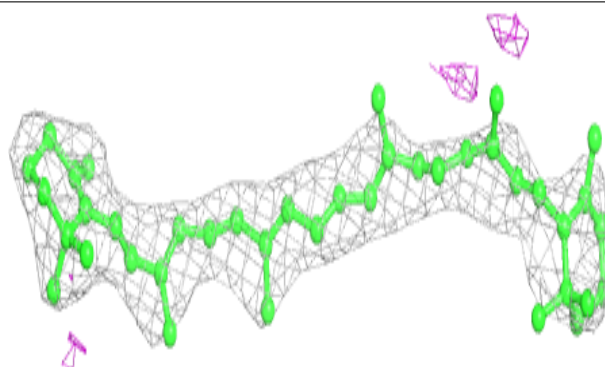


Electron density around BCR a 4007:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

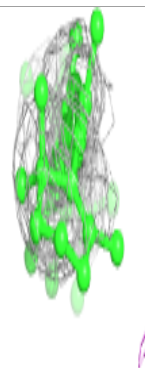
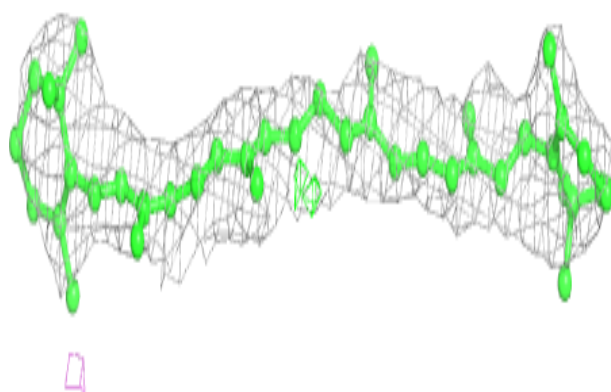
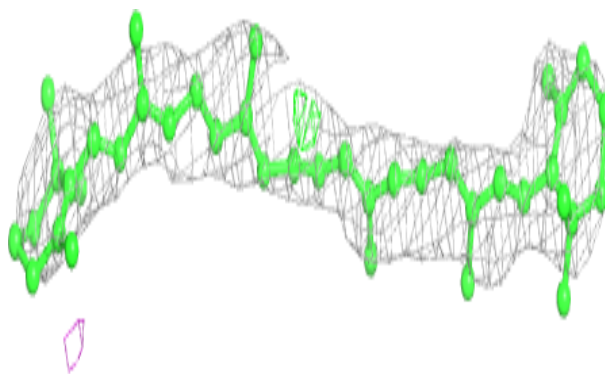
**Electron density around BCR A 4003:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

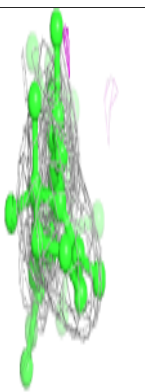
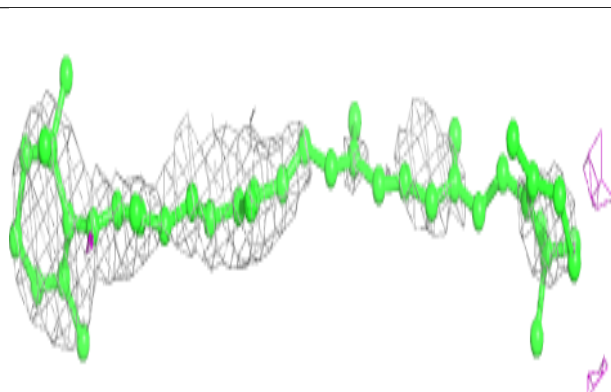
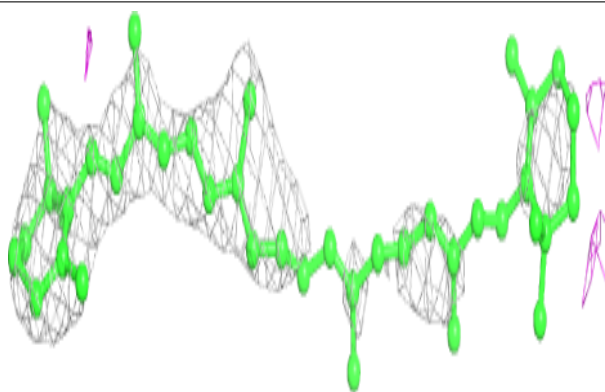


Electron density around BCR 1 4002:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

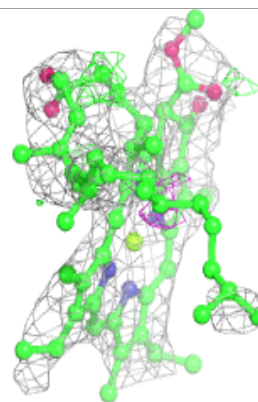
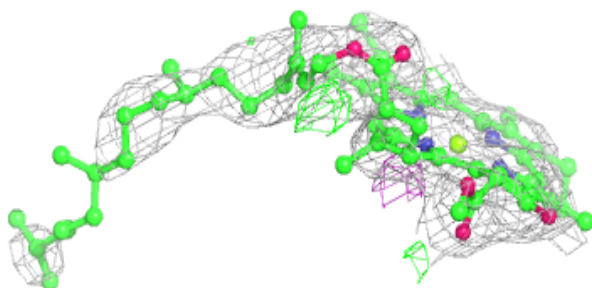
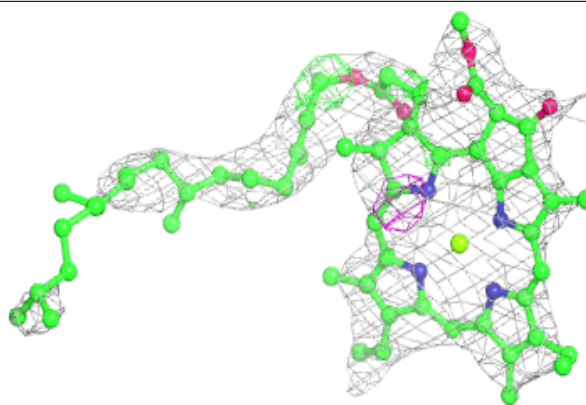
**Electron density around BCR 1 4007:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

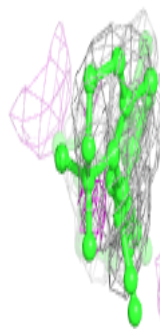
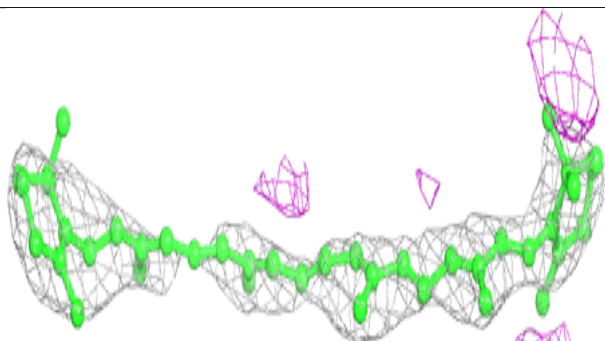
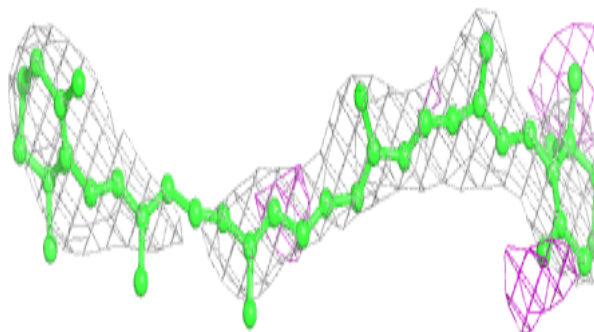


Electron density around CLA 1 1013:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

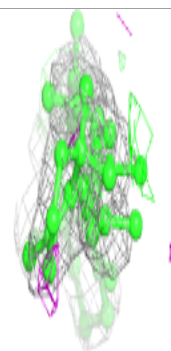
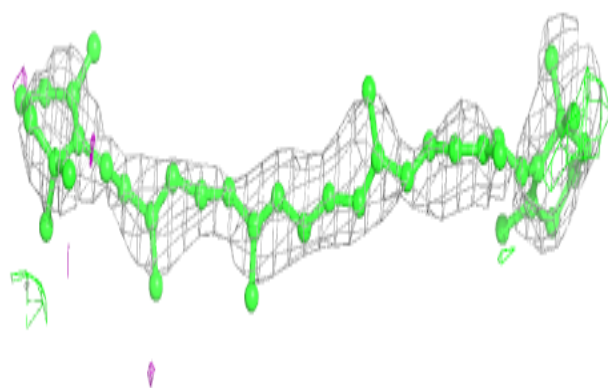
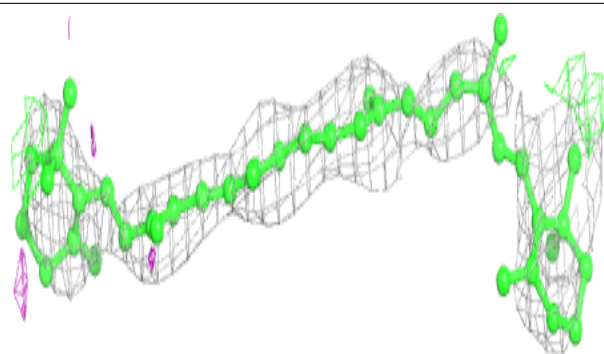
**Electron density around BCR a 4008:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

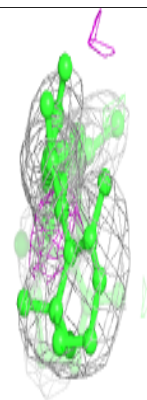
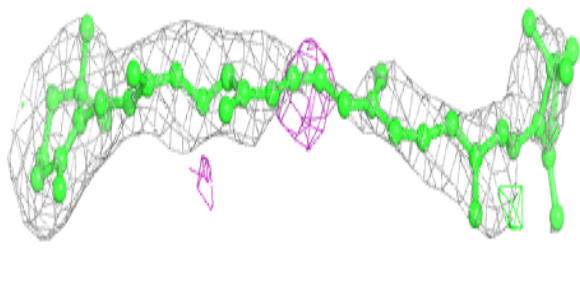
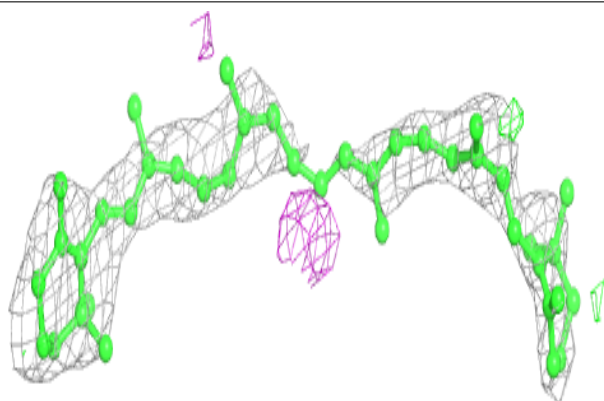


Electron density around BCR 1 4022:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

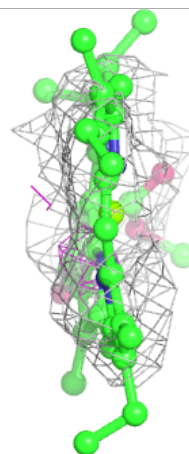
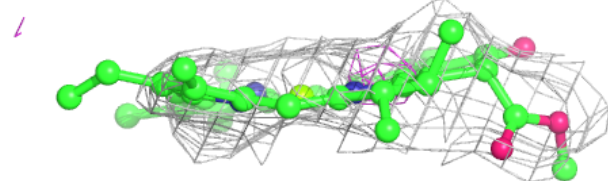
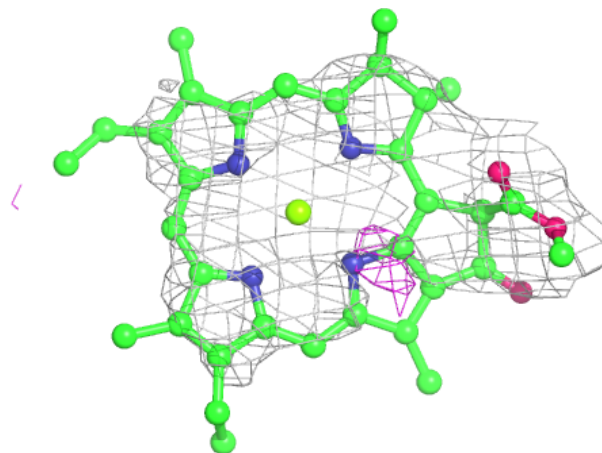
**Electron density around BCR 9 4021:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



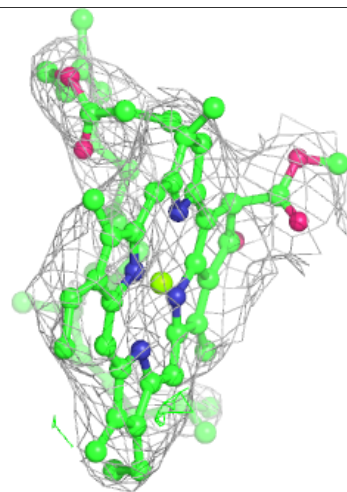
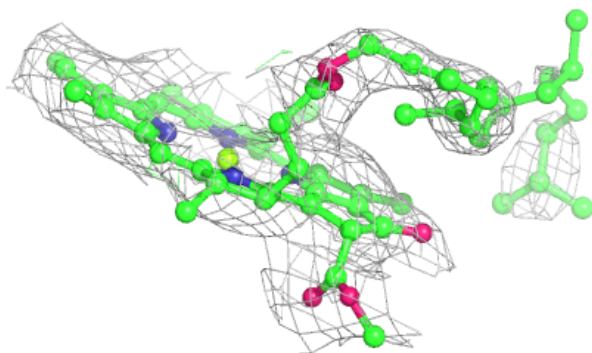
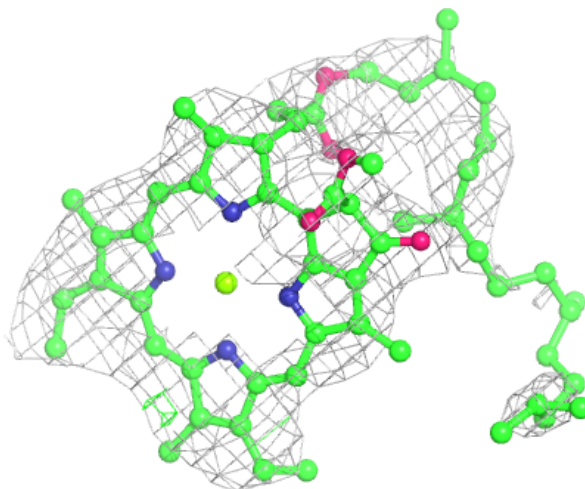
Electron density around CLA 7 1302:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



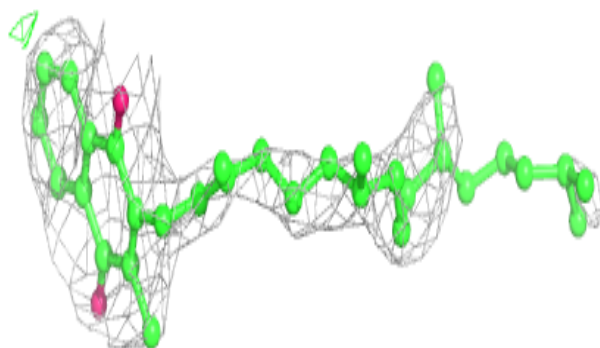
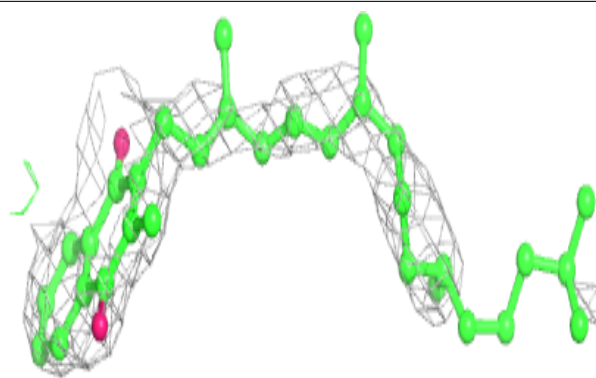
Electron density around CLA 2 1229:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

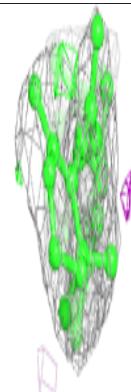
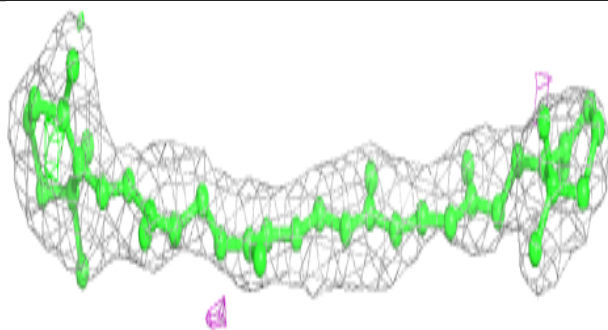
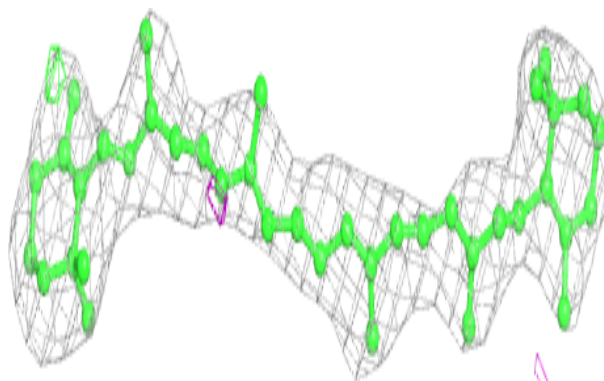


Electron density around PQN 1 2001:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

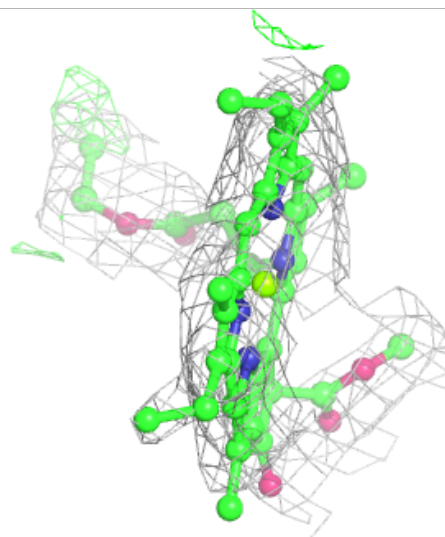
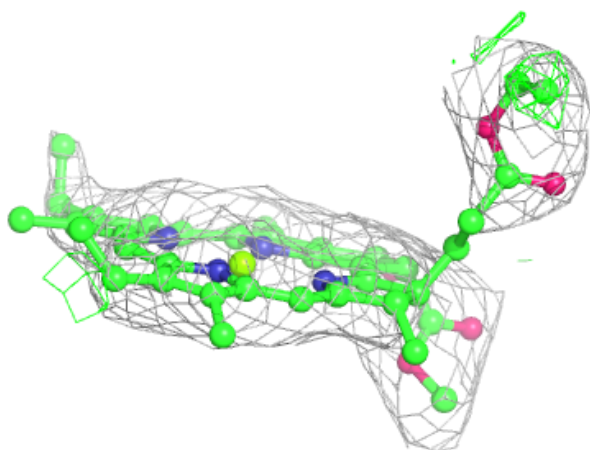
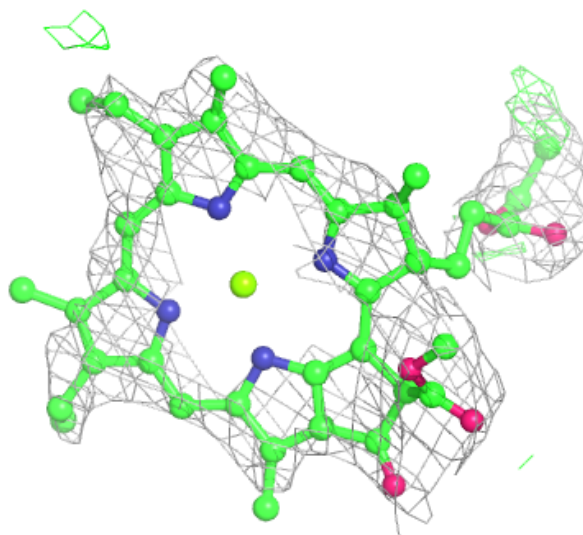
**Electron density around BCR b 4004:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



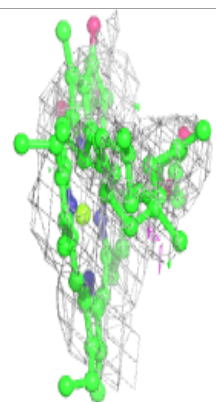
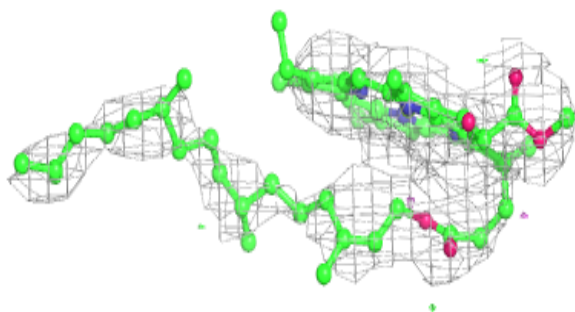
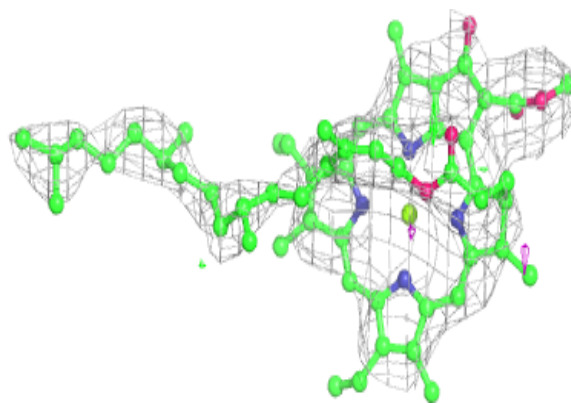
Electron density around CLA 2 1230:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

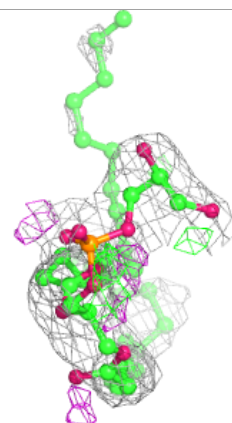
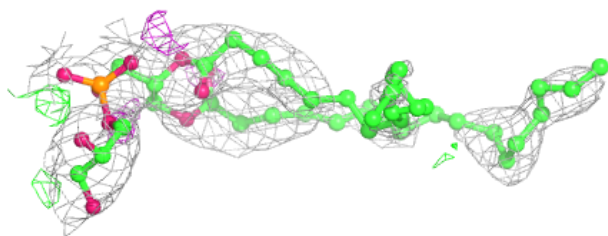
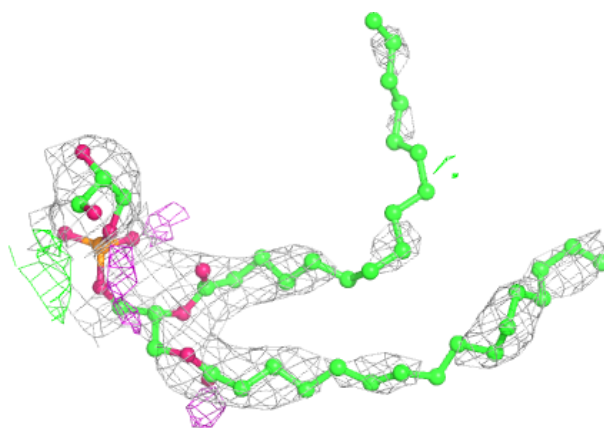


Electron density around CLA 1 1115:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

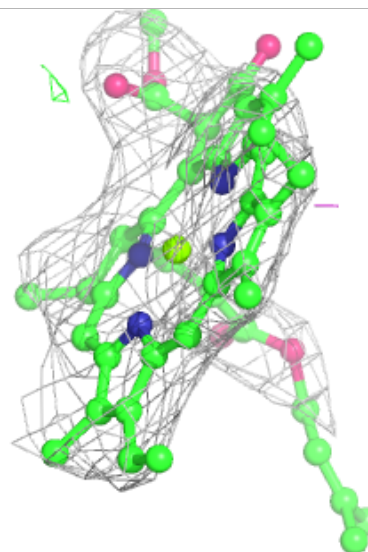
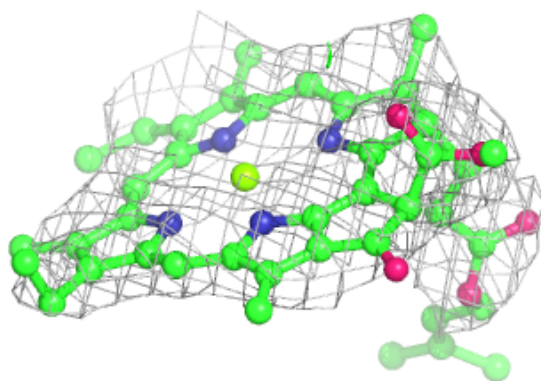
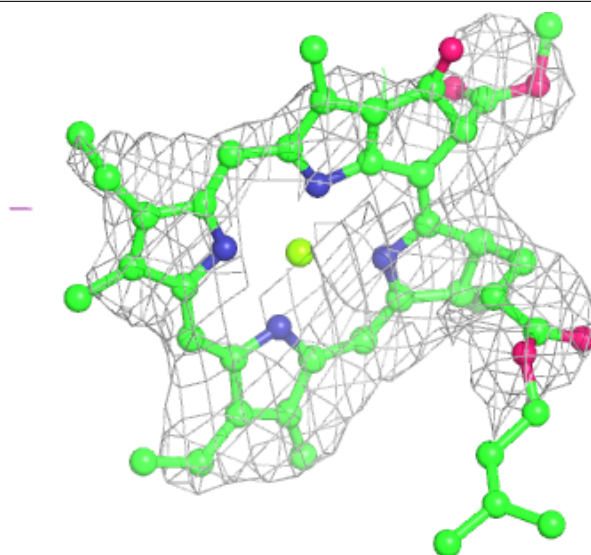
**Electron density around LHG B 5004:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



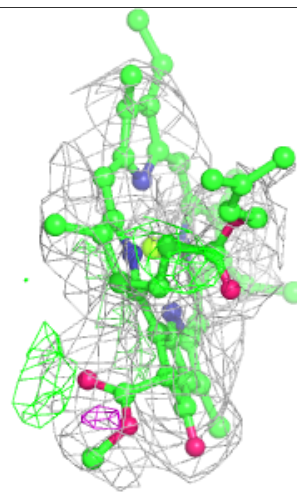
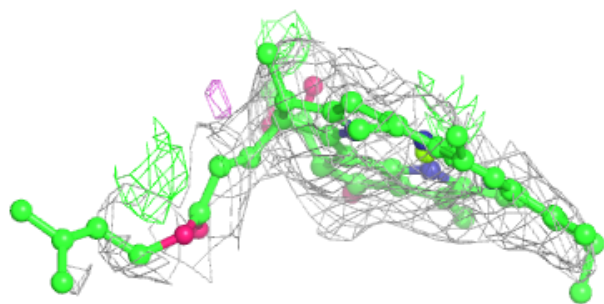
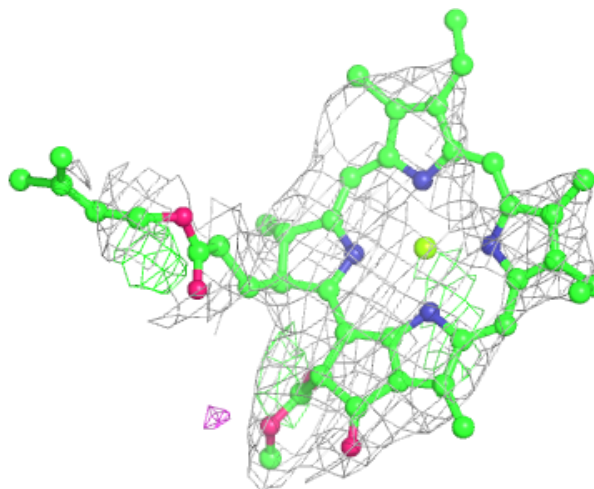
Electron density around CLA B 1232:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



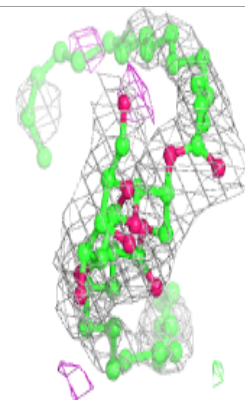
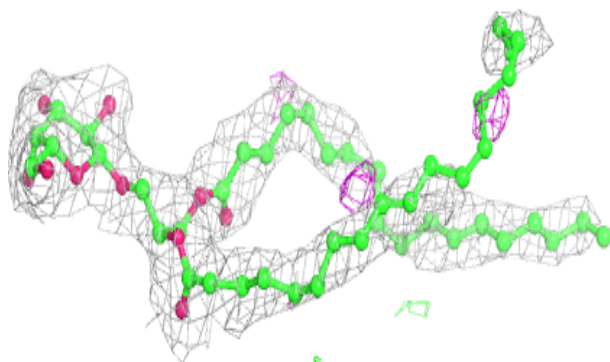
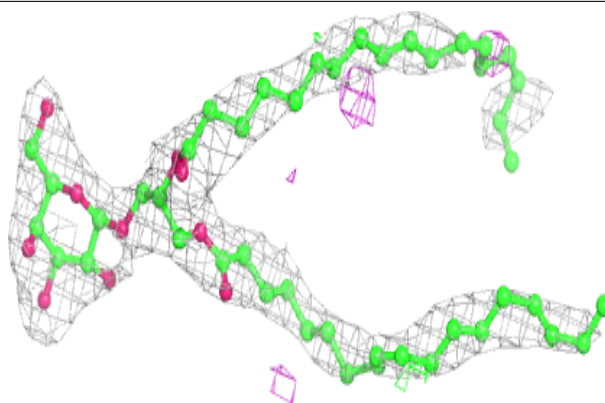
Electron density around CLA 2 1222:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

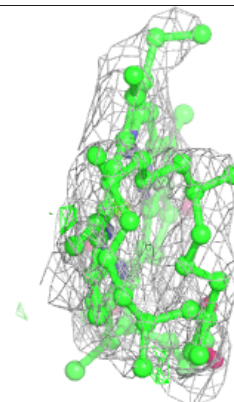
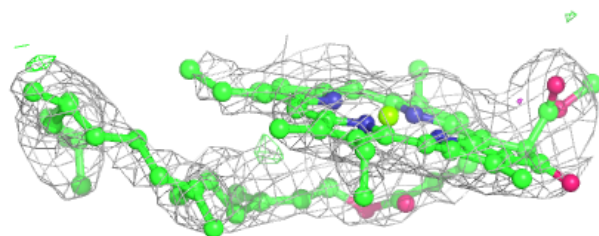
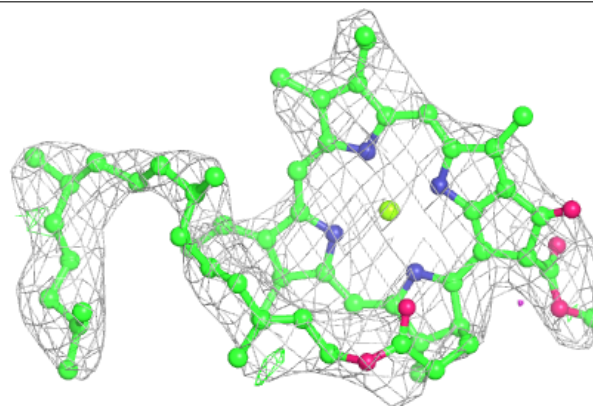


Electron density around LMG 2 5002:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

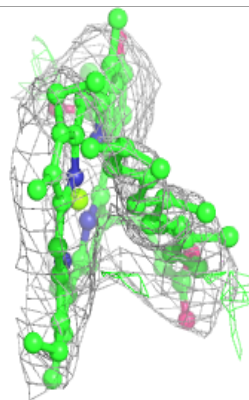
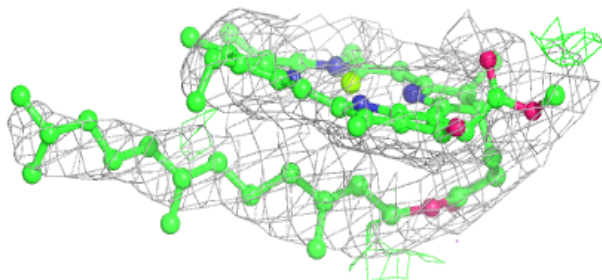
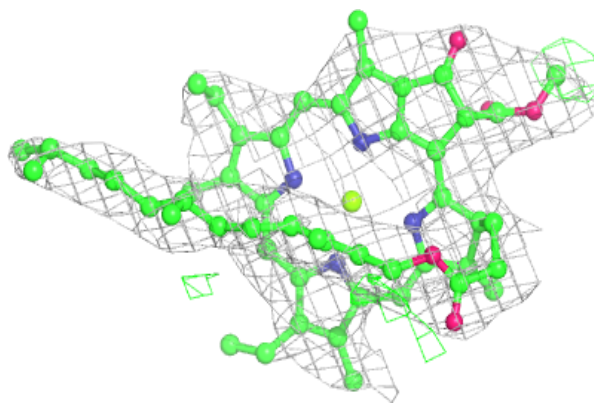
**Electron density around CLA 1 1117:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

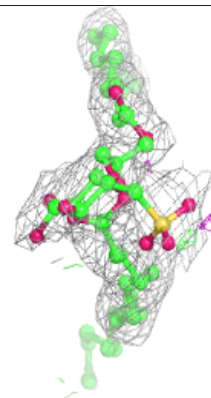
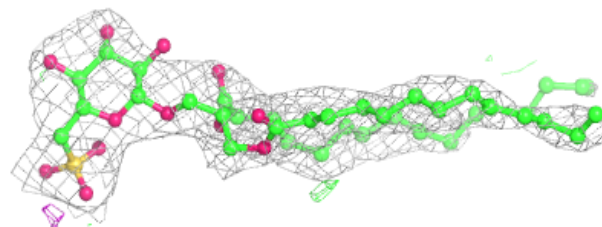
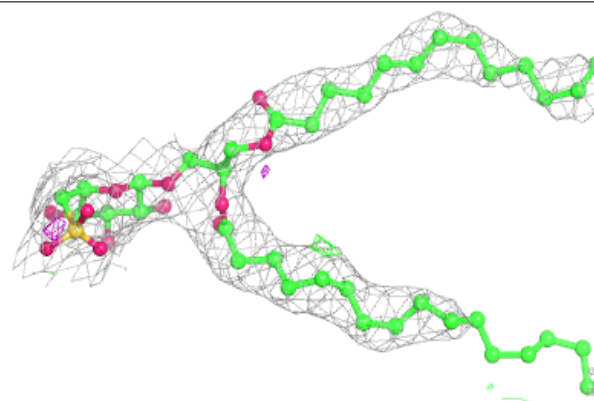


Electron density around CLA a 1116:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

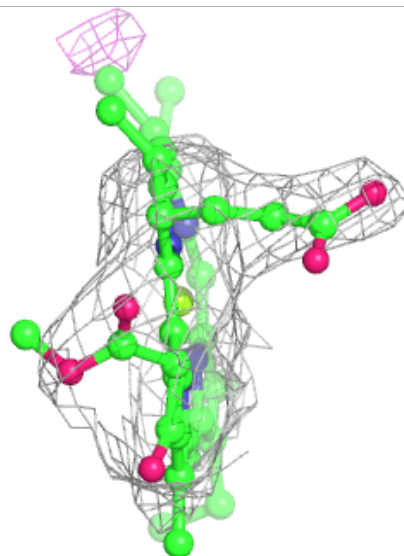
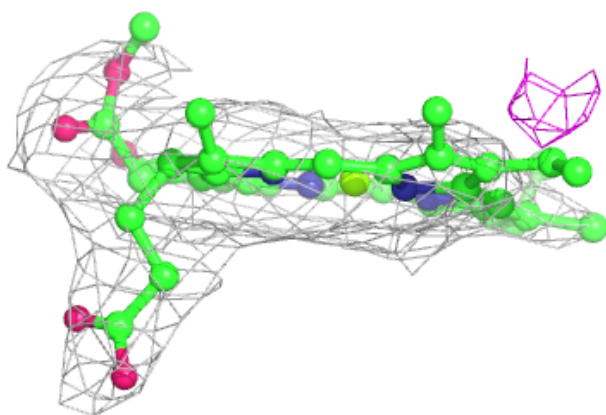
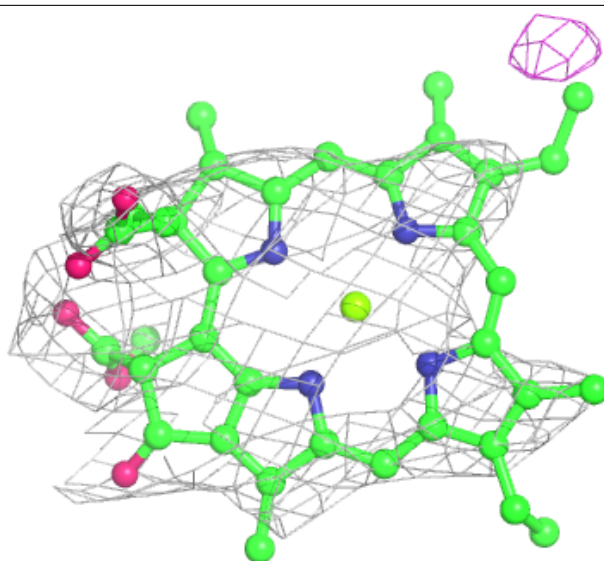
**Electron density around SQD L 5001:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



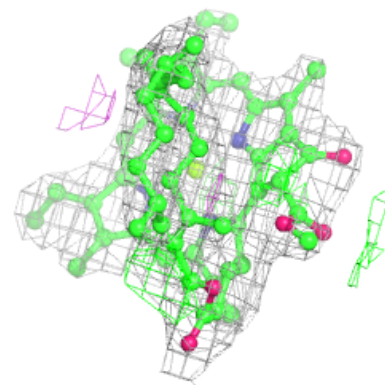
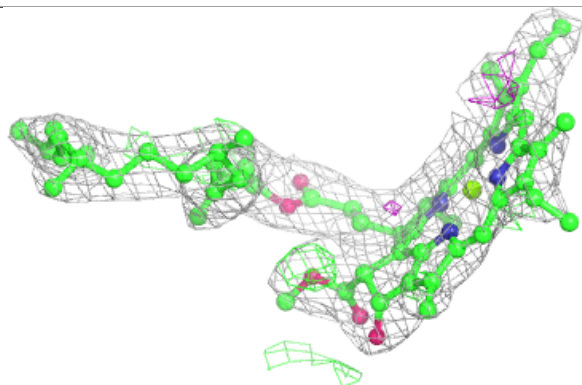
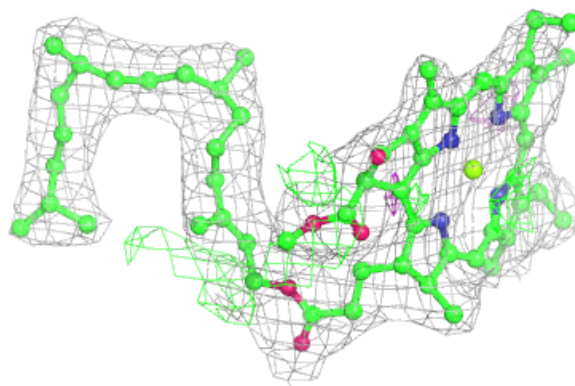
Electron density around CLA 2 1220:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

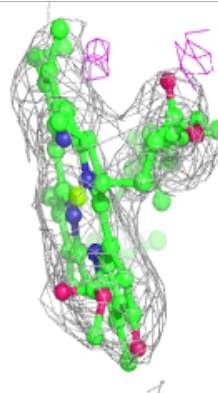
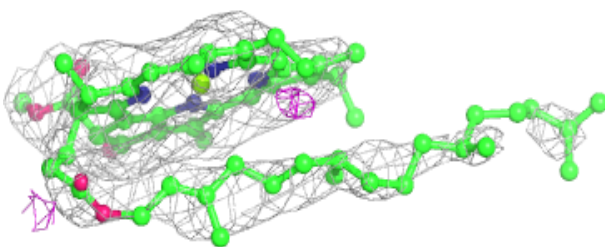
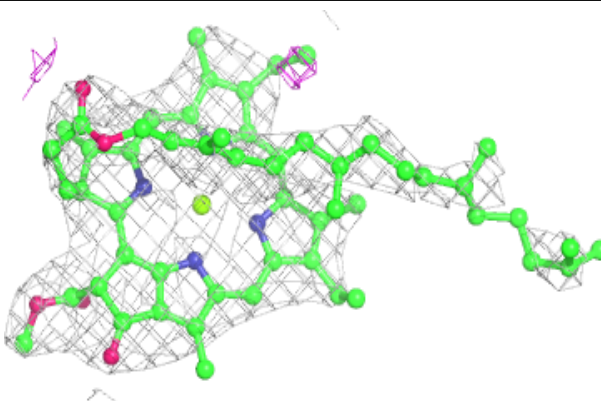


Electron density around CLA a 1011:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

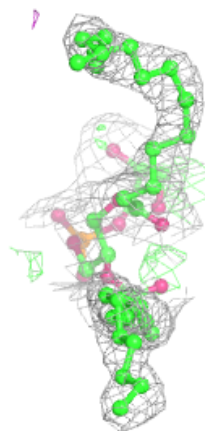
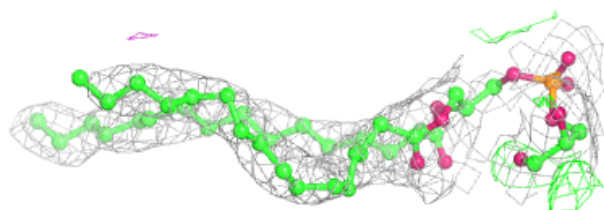
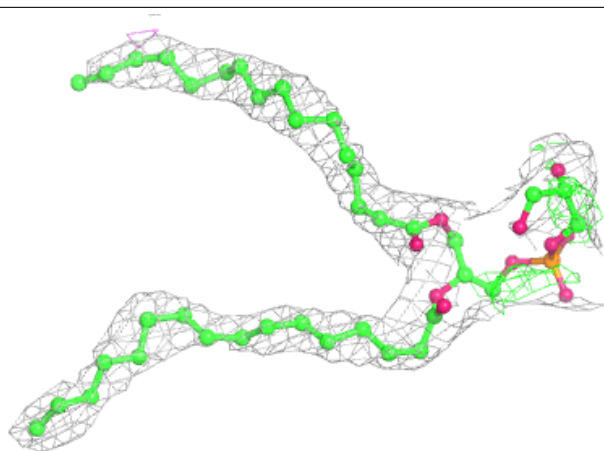
**Electron density around CLA 1 1116:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



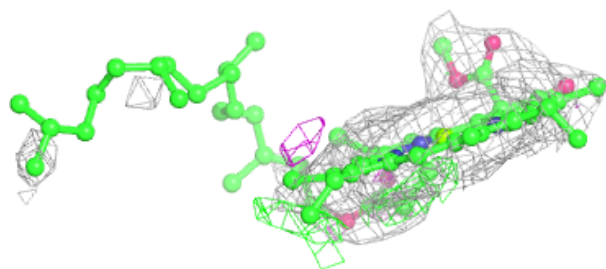
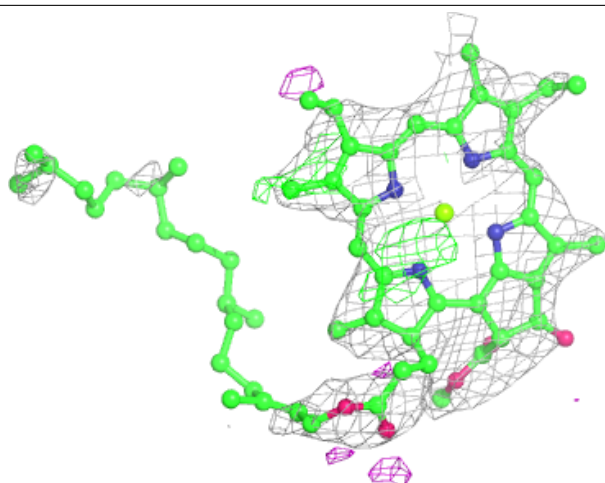
Electron density around LHG 0 5002:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



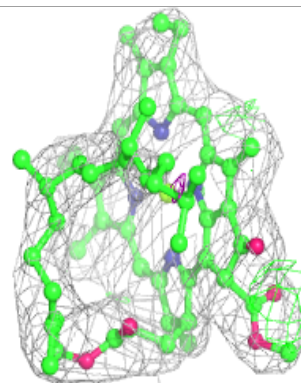
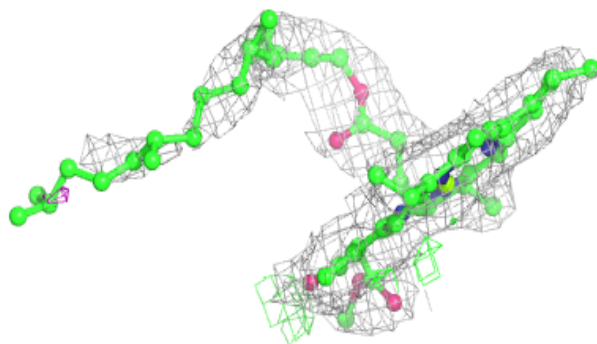
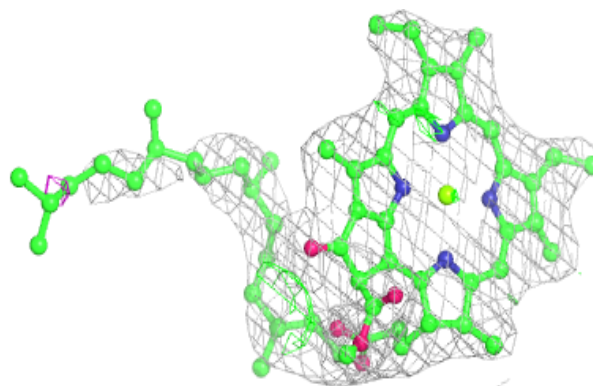
Electron density around CLA a 1111:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

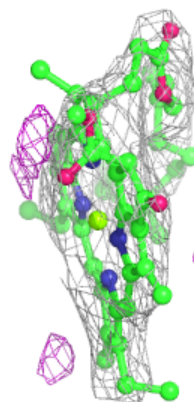
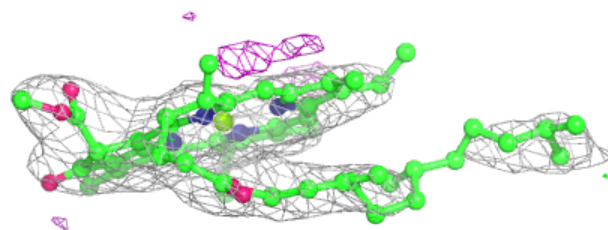
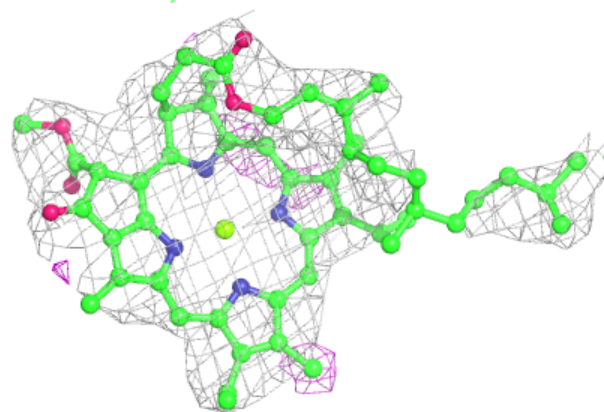


Electron density around CLA b 1231:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

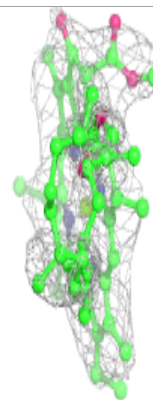
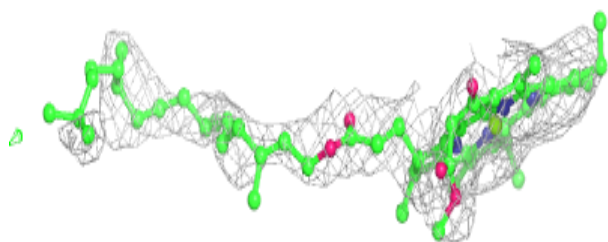
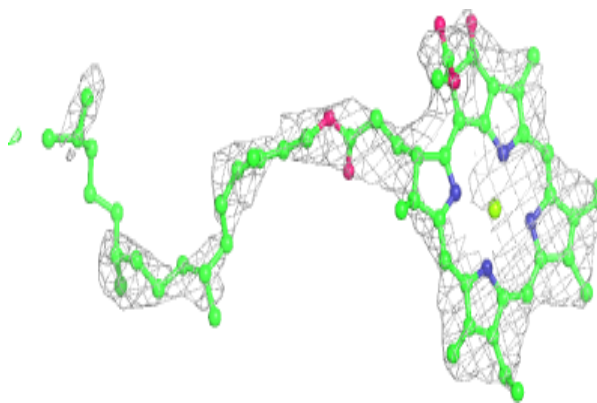
**Electron density around CLA 2 1215:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

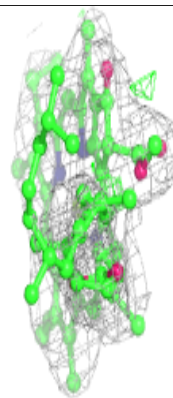
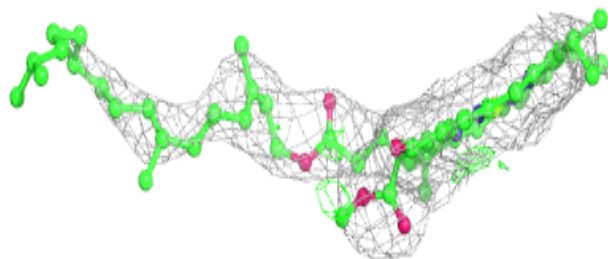
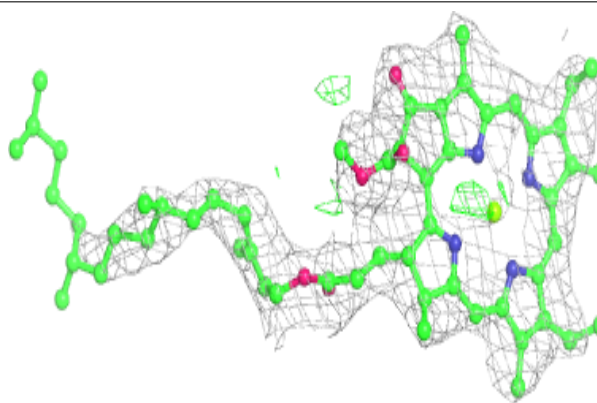


Electron density around CLA F 1302:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

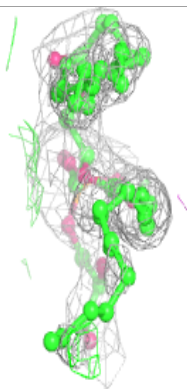
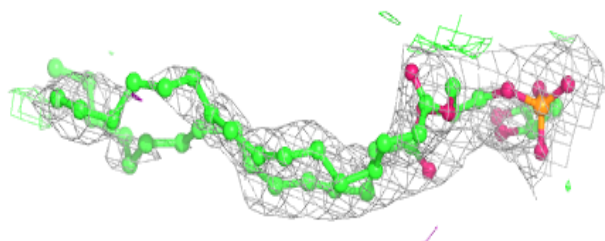
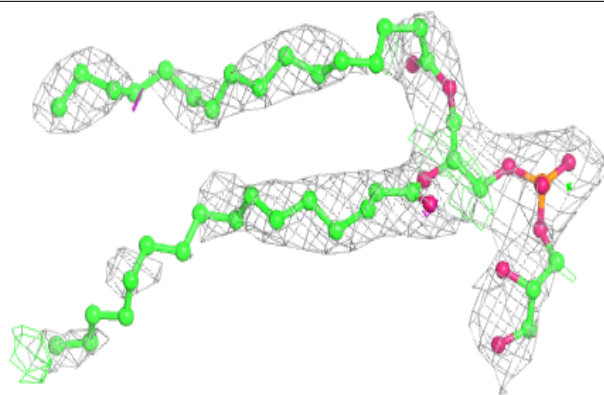
**Electron density around CLA a 1139:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

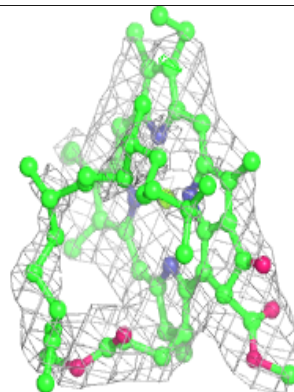
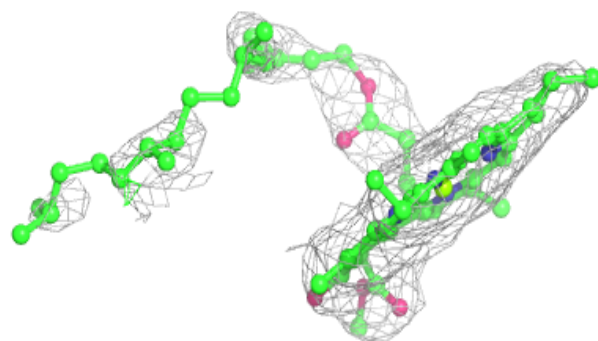
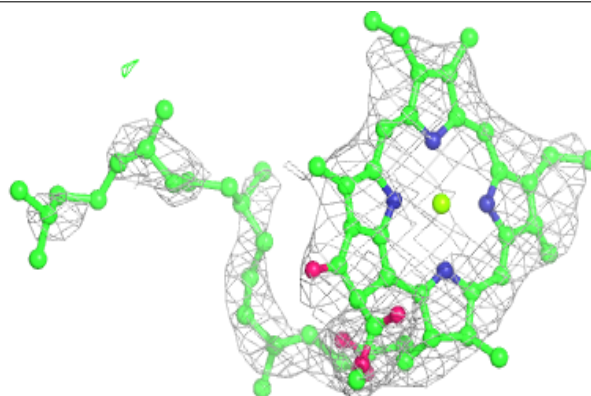


Electron density around LHG L 5005:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

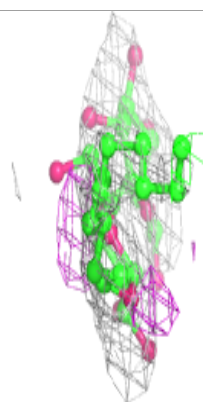
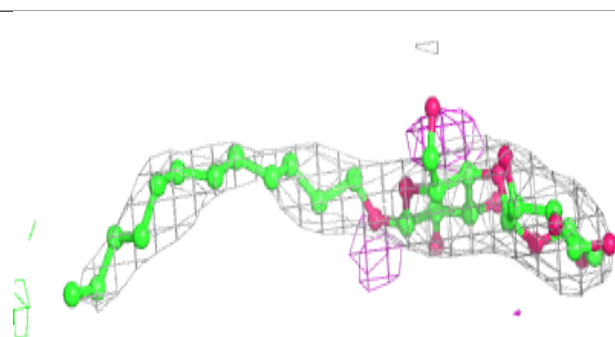
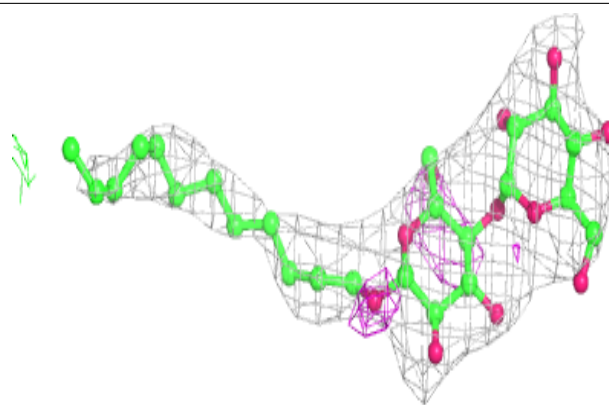
**Electron density around CLA B 1231:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



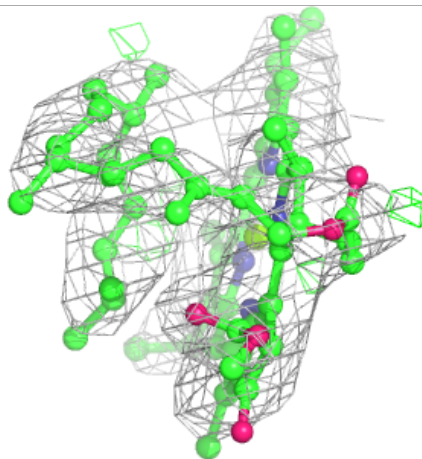
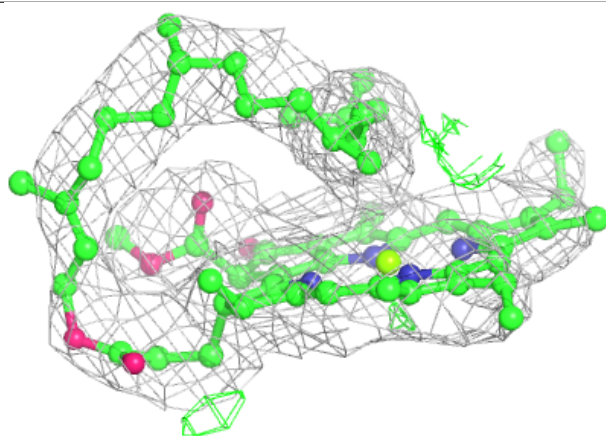
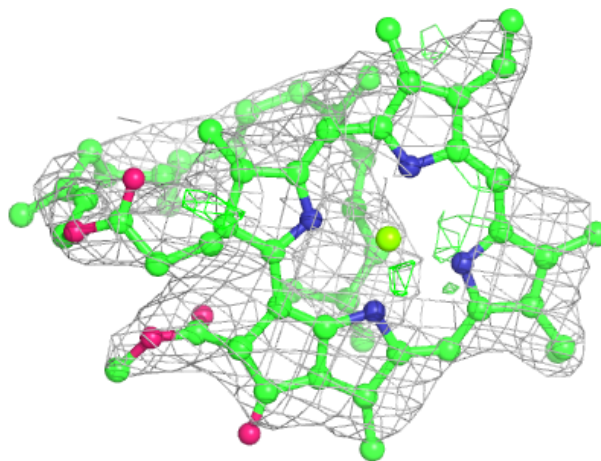
Electron density around LMT L 6001:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



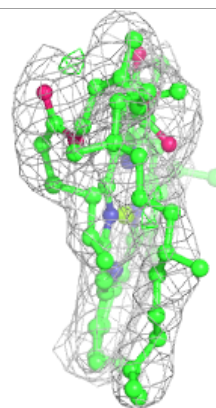
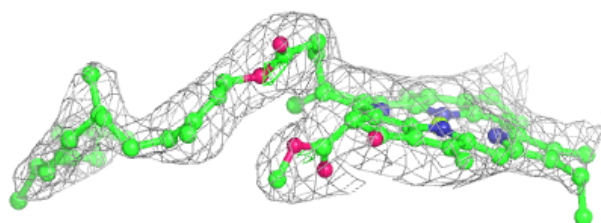
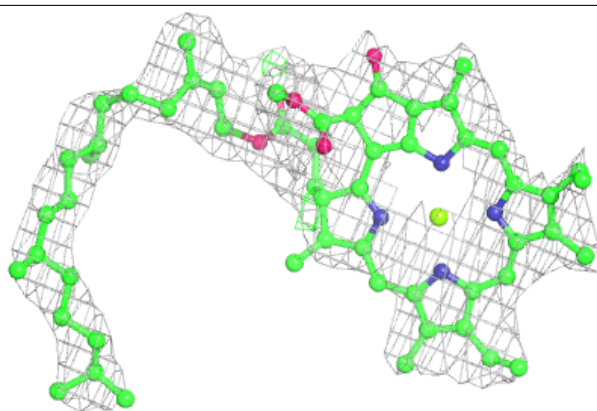
Electron density around CLA 1 1104:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

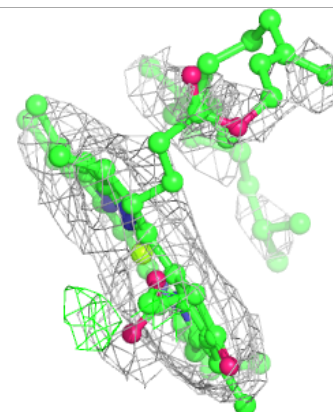
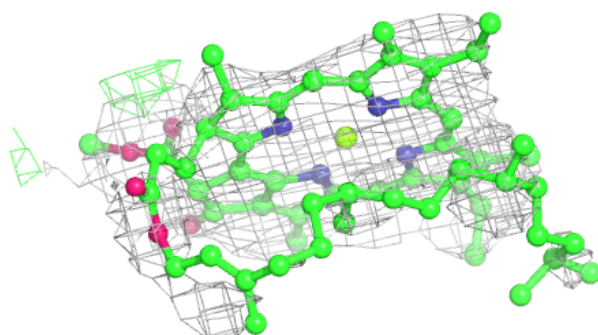
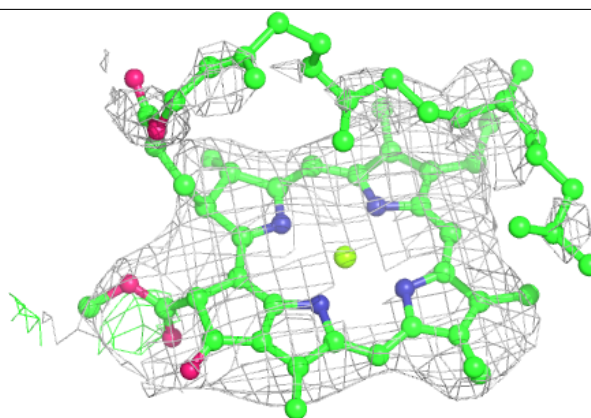


Electron density around CLA a 1101:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

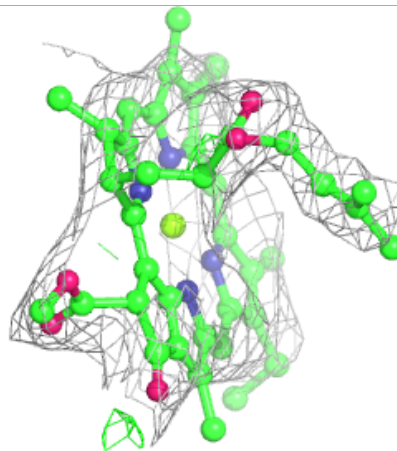
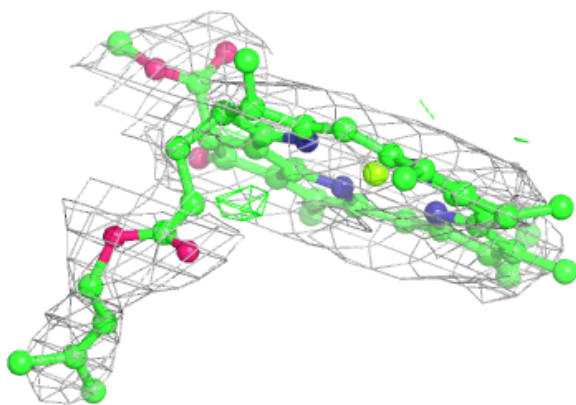
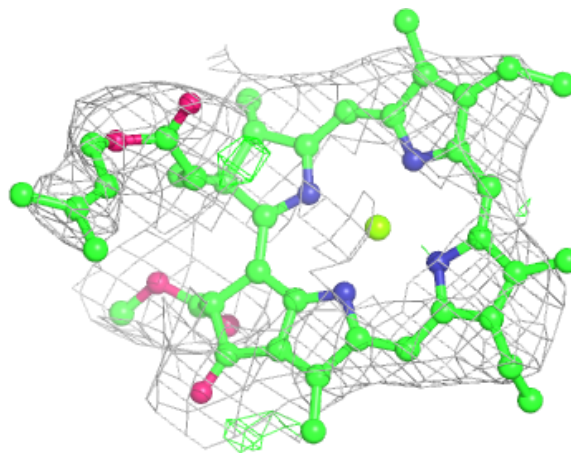
**Electron density around CLA 1 1118:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



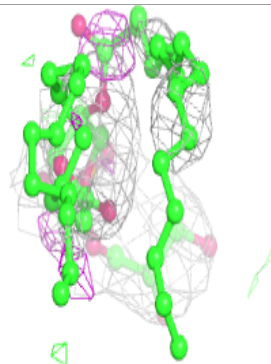
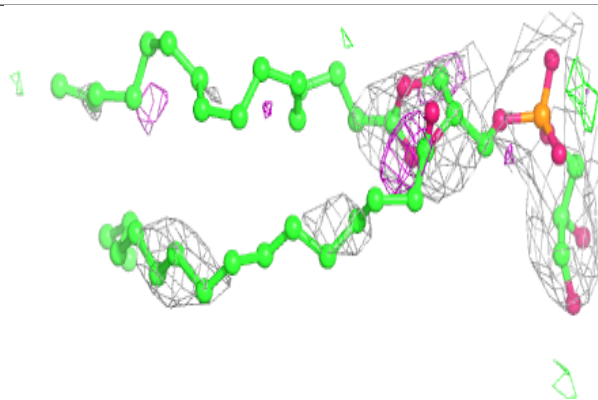
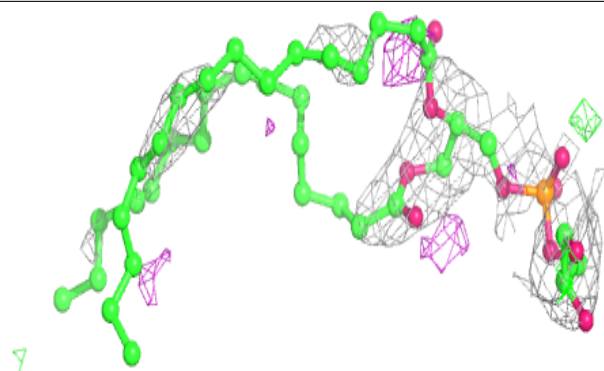
Electron density around CLA 2 1236:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

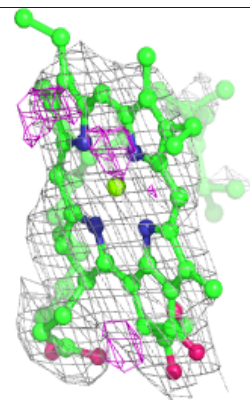
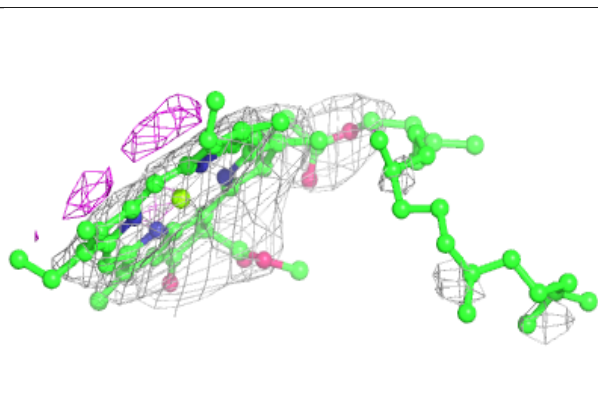
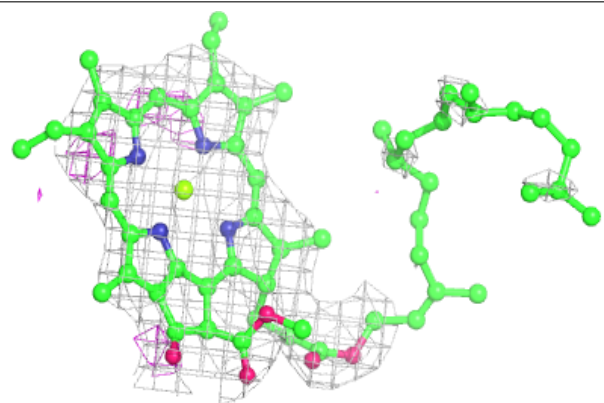


Electron density around LHG a 5003:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

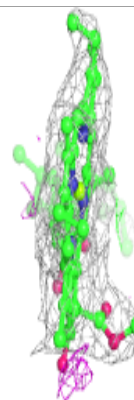
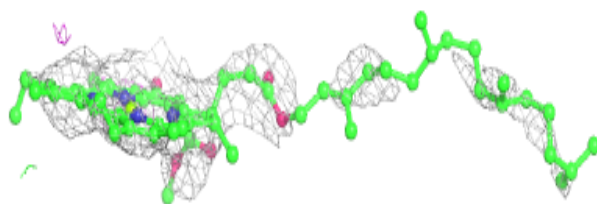
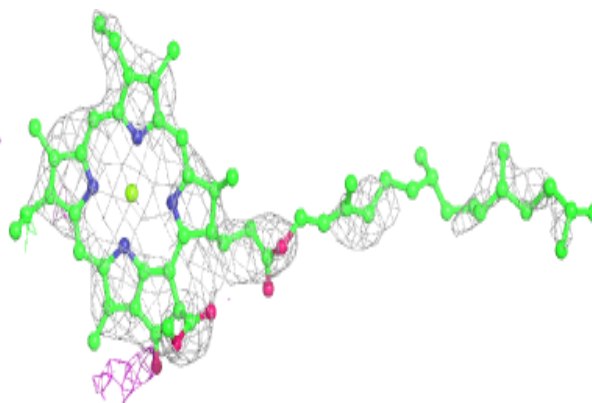
**Electron density around CLA 2 1221:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

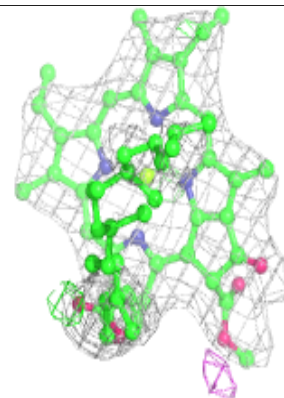
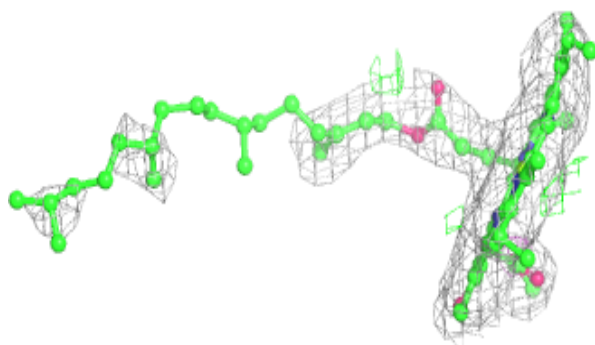
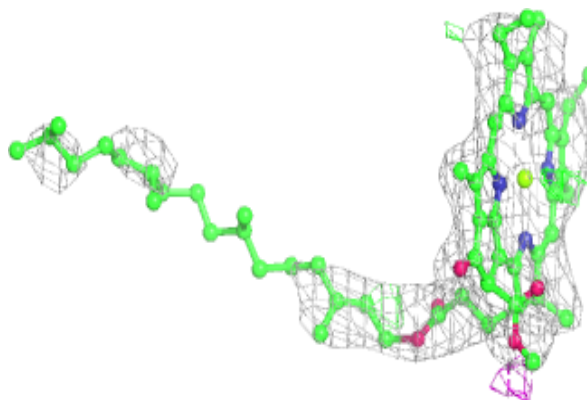


Electron density around CLA f 1302:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

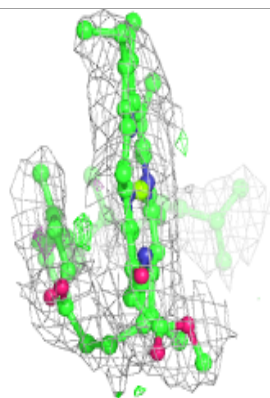
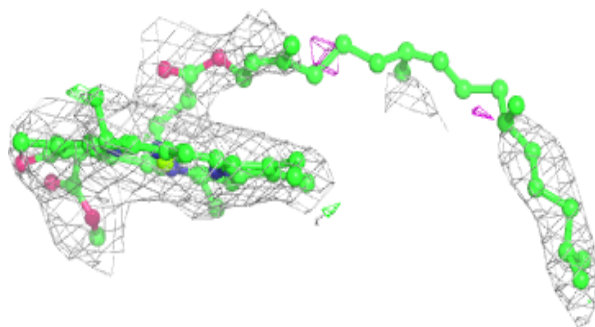
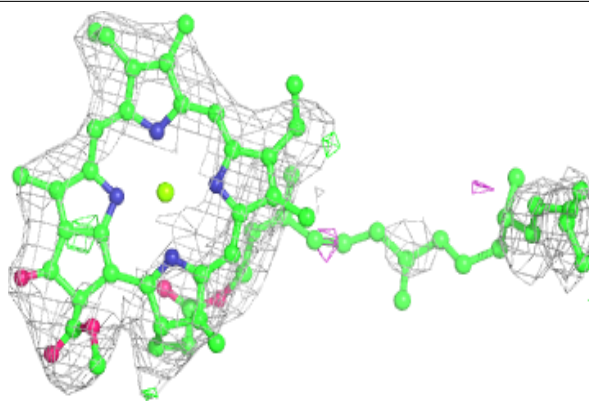
**Electron density around CLA b 1236:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

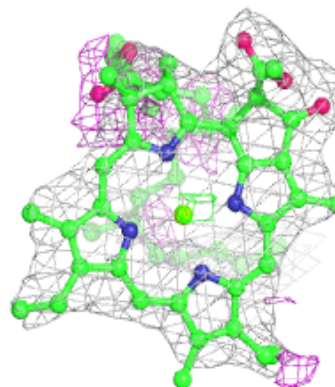
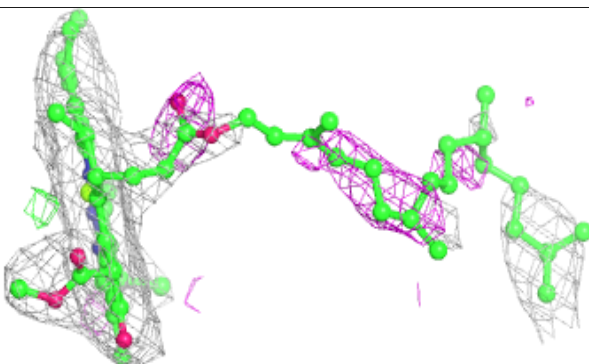
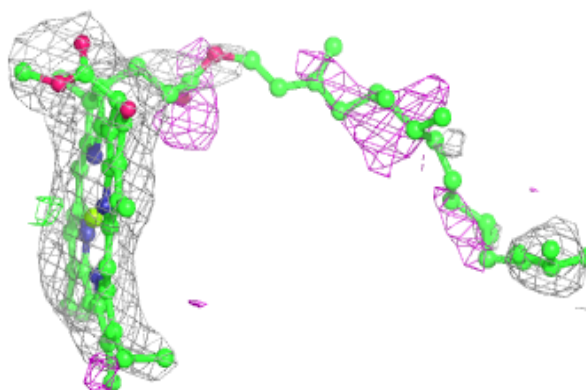


Electron density around CLA B 1209:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

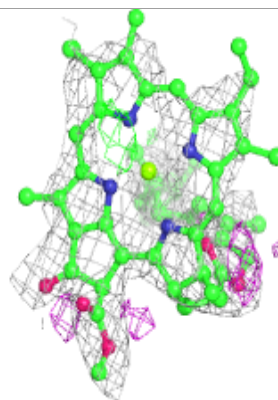
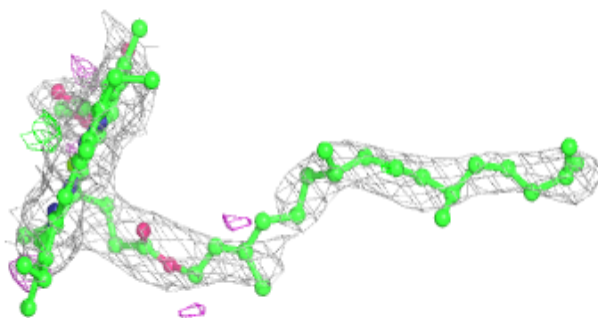
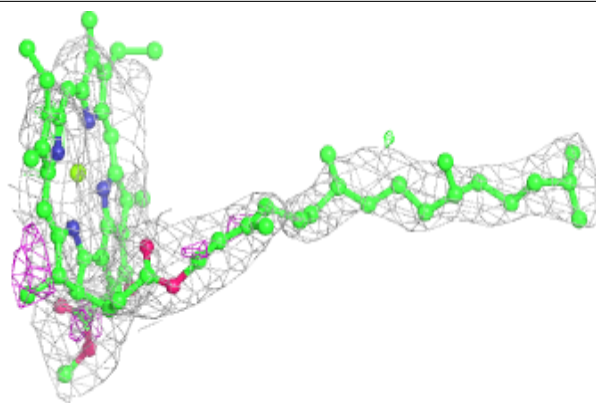
**Electron density around CLA A 1113:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



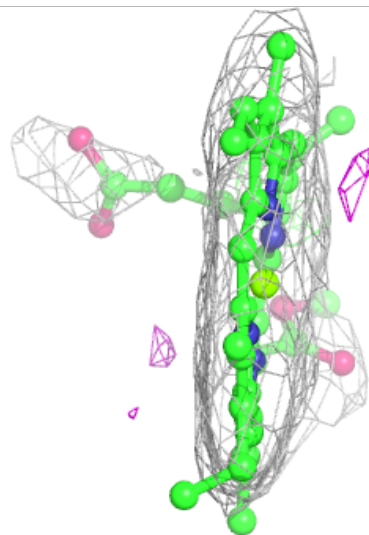
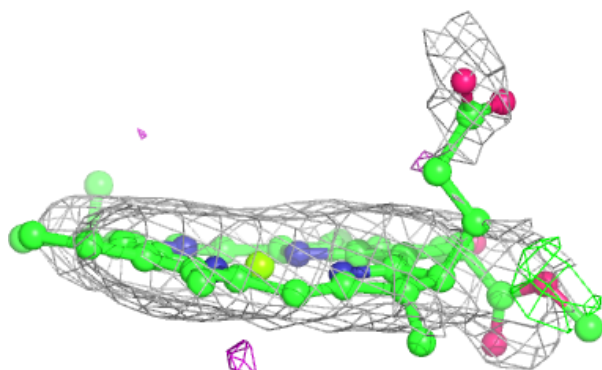
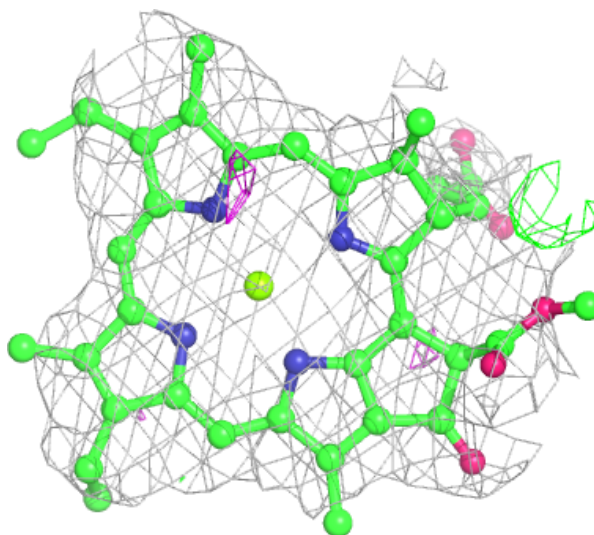
Electron density around CLA 2 1225:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



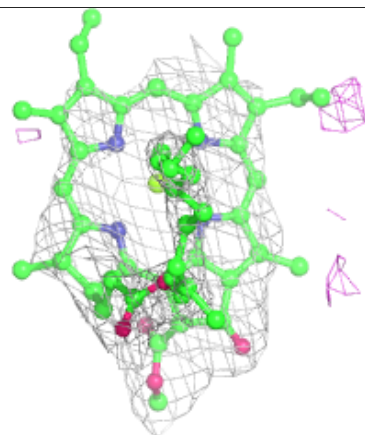
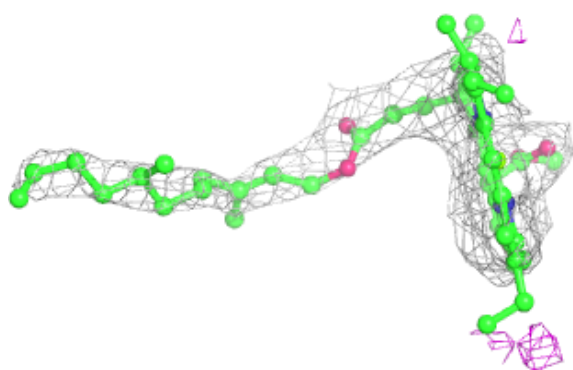
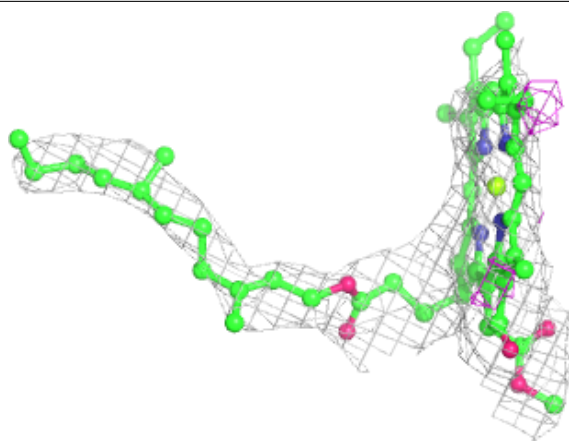
Electron density around CLA 2 1227:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

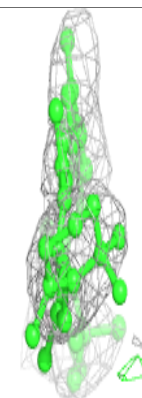
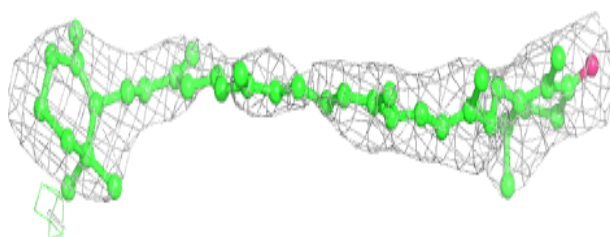
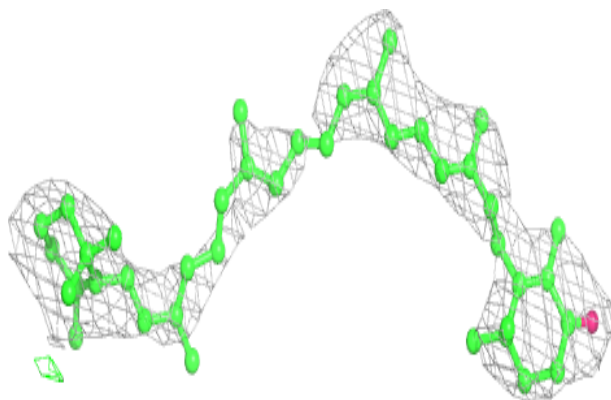


Electron density around CLA a 1105:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

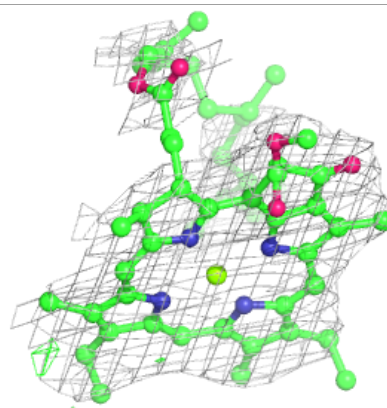
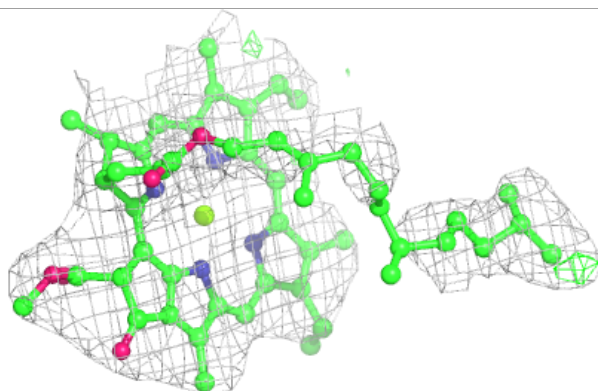
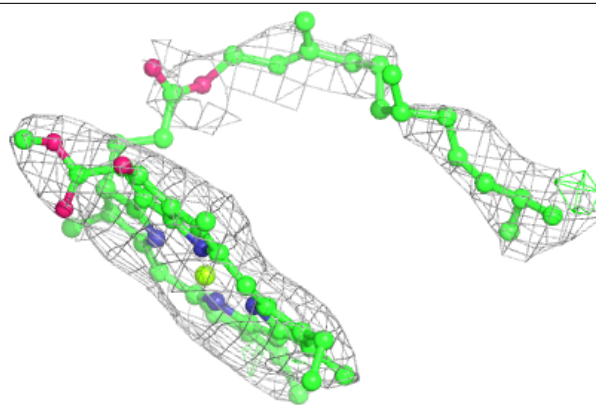
**Electron density around ECH b 4011:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

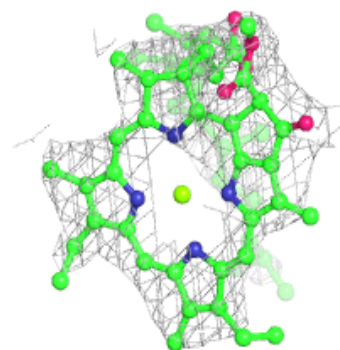
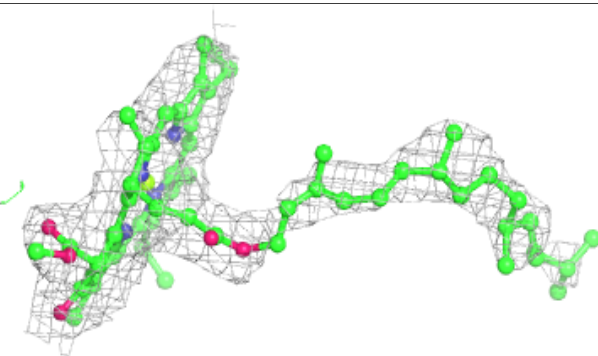
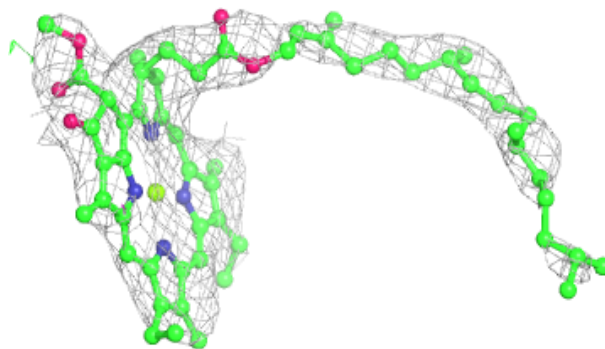


Electron density around CLA 2 1208:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

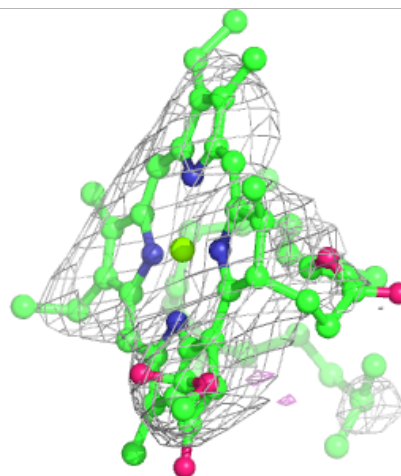
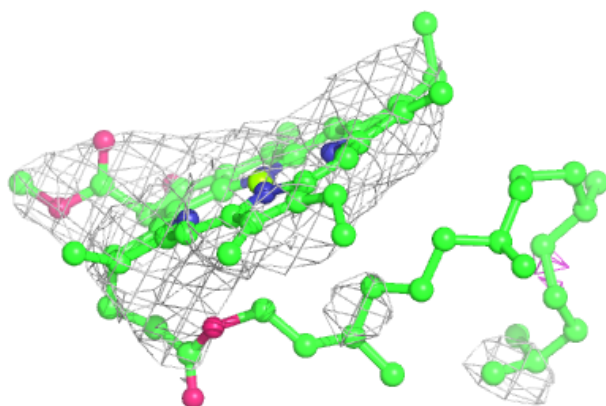
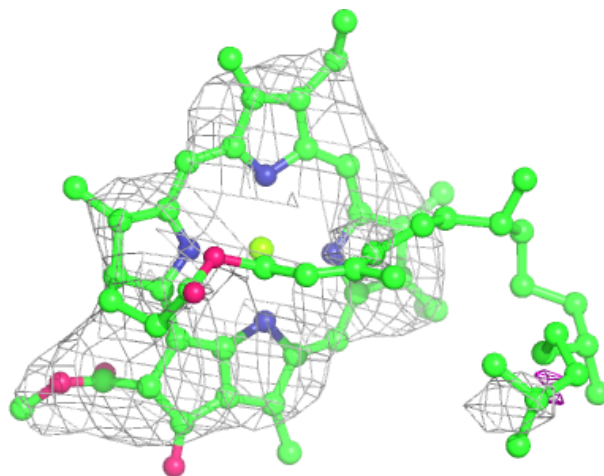
**Electron density around CLA 1 1133:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



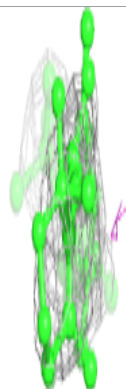
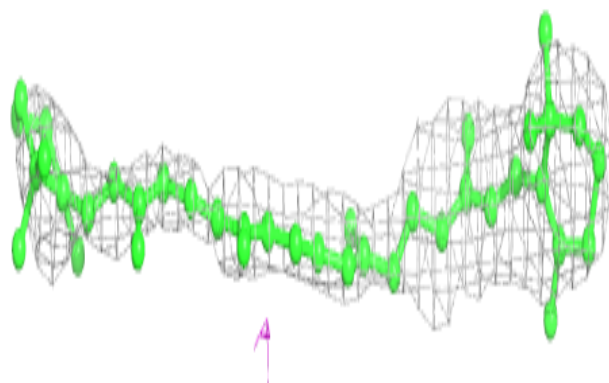
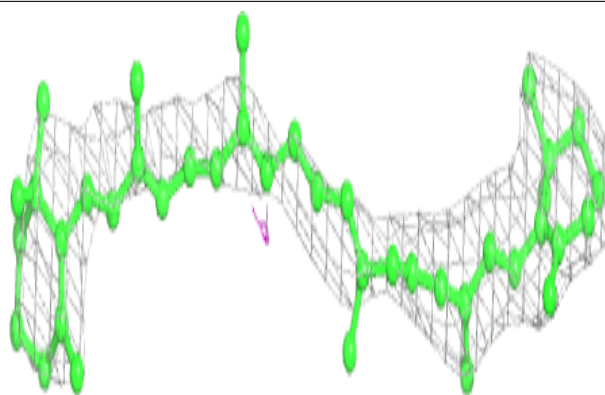
Electron density around CLA a 1121:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

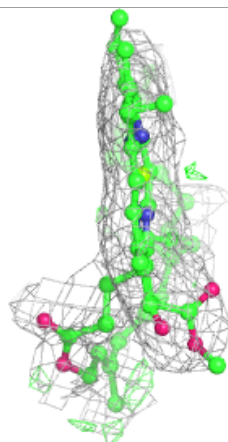
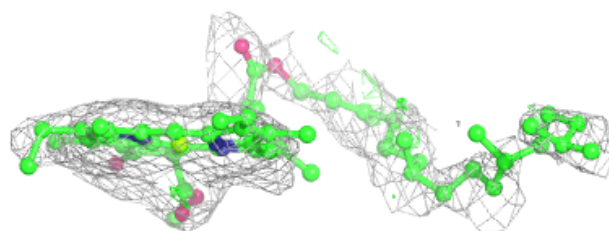
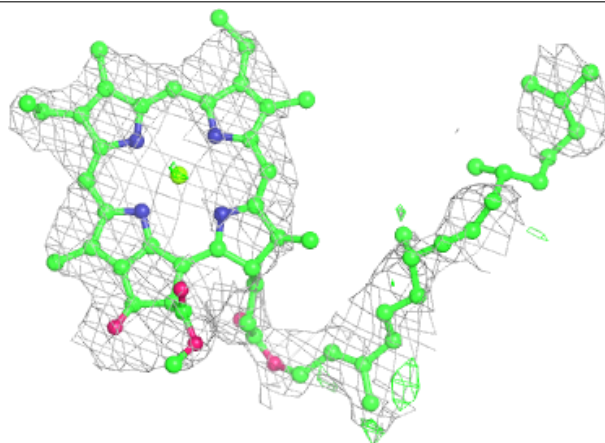


Electron density around BCR a 4012:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

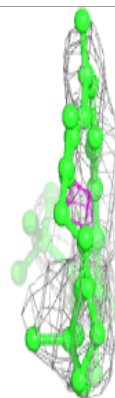
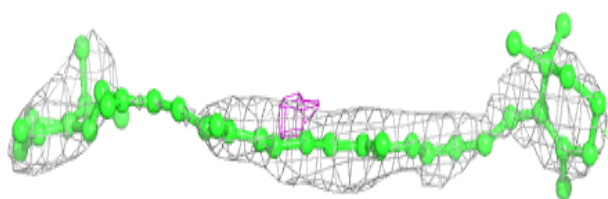
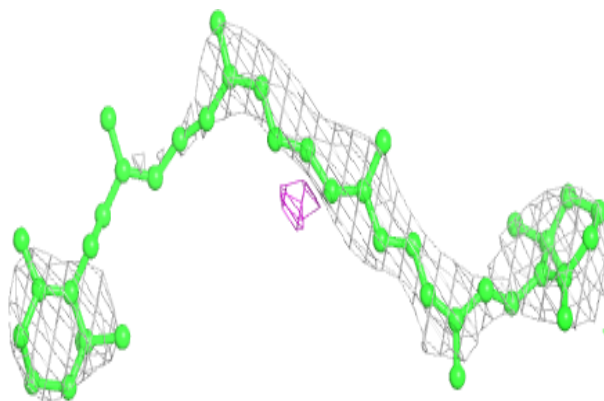
**Electron density around CLA B 1219:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

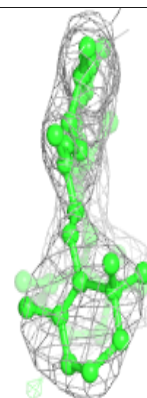
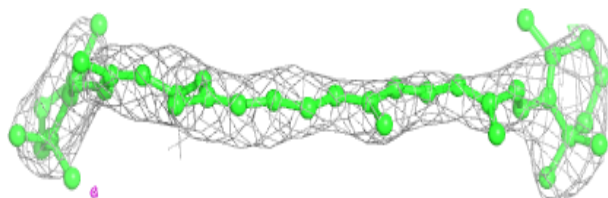
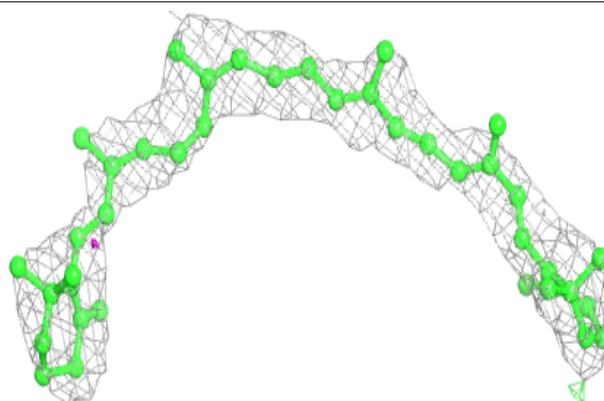


Electron density around BCR 2 4011:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

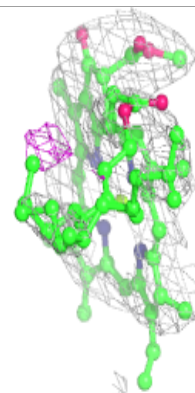
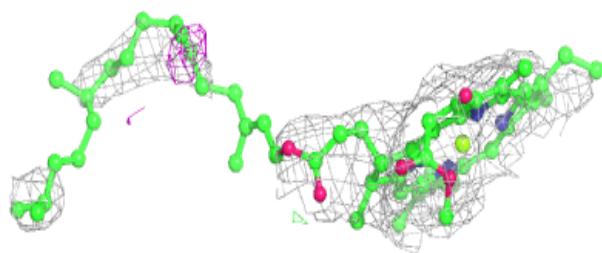
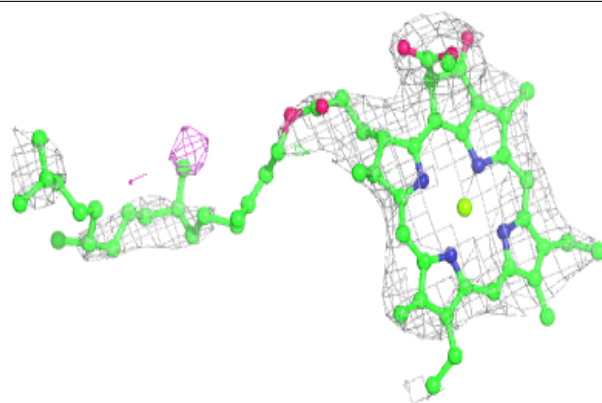
**Electron density around BCR f 4016:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

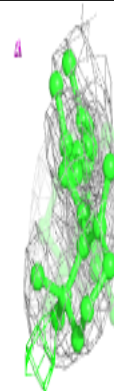
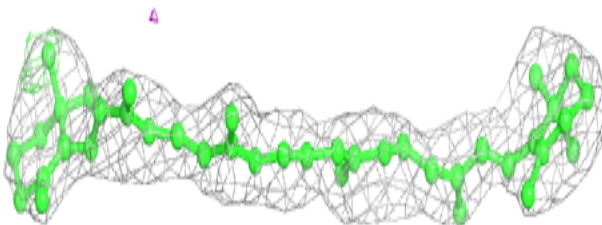
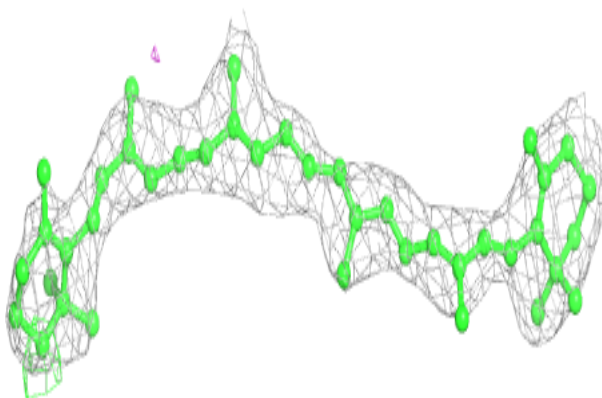


Electron density around CLA 2 1210:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

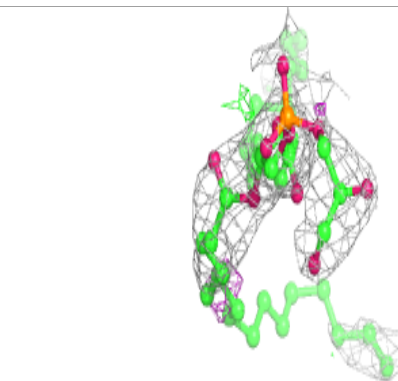
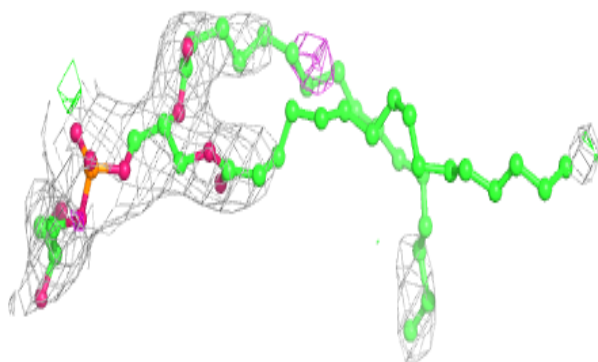
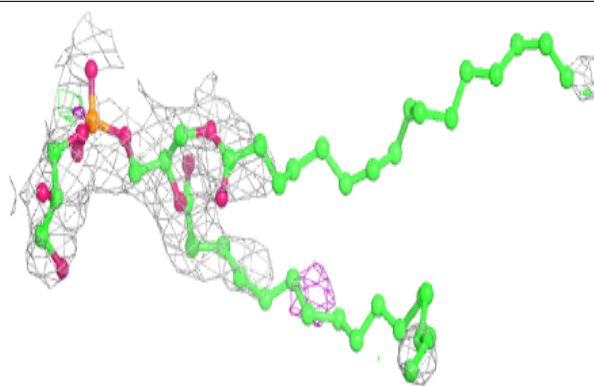
**Electron density around BCR B 4010:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

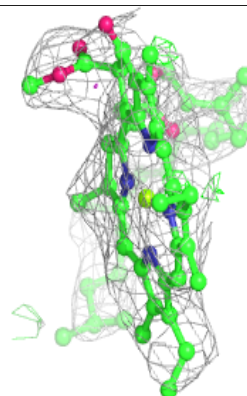
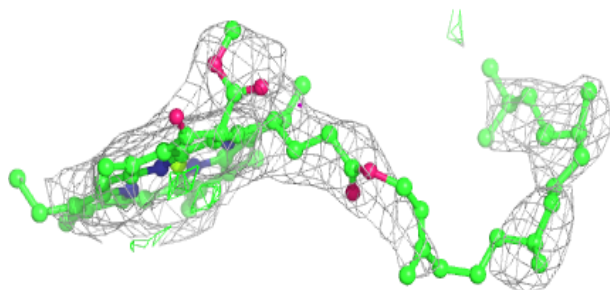
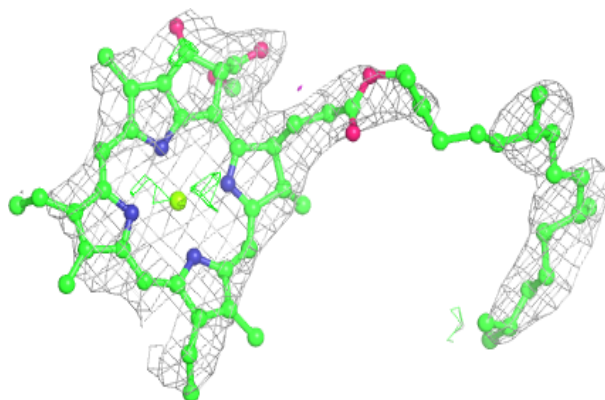


Electron density around LHG 1 5003:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

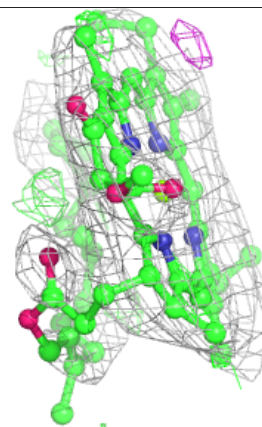
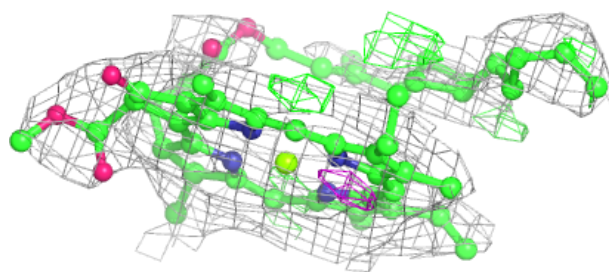
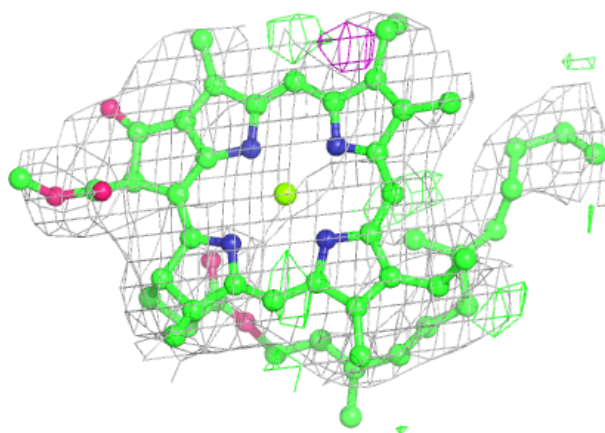
**Electron density around CLA a 1125:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



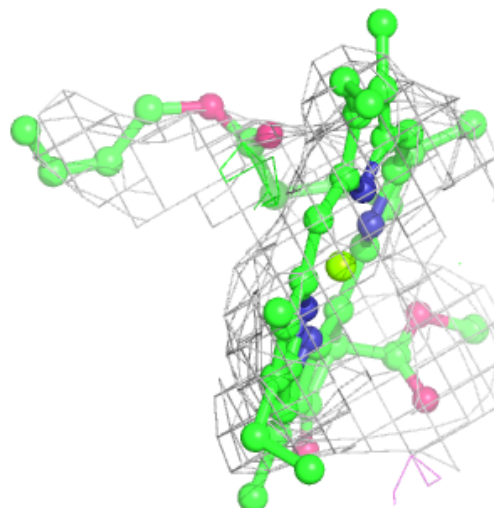
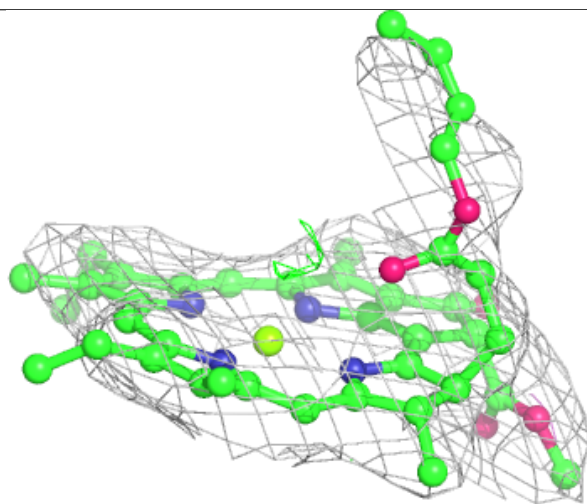
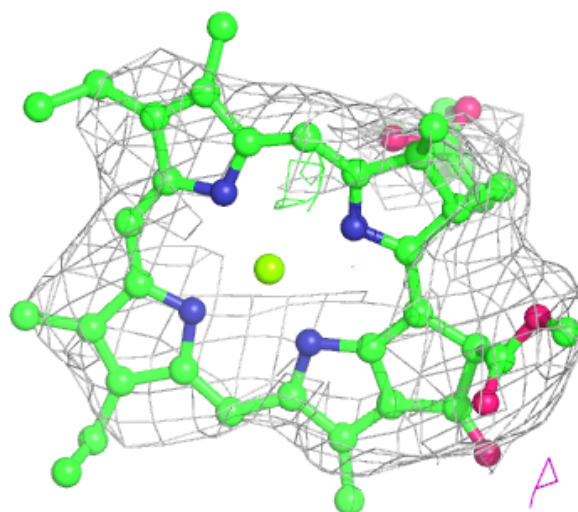
Electron density around CLA a 1110:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



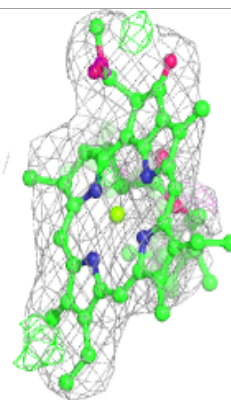
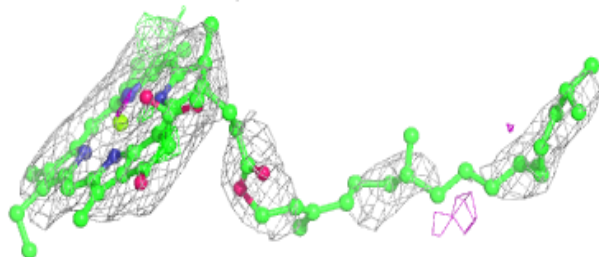
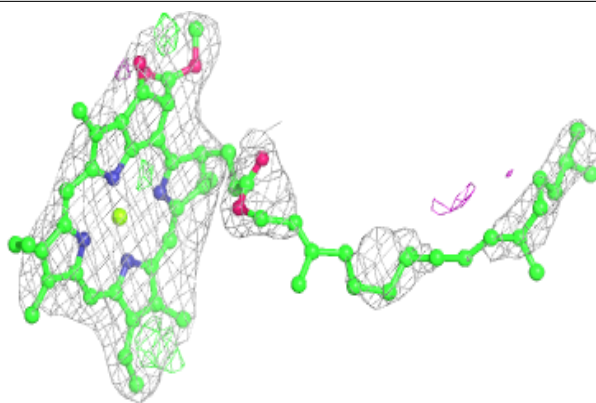
Electron density around CLA a 1134:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

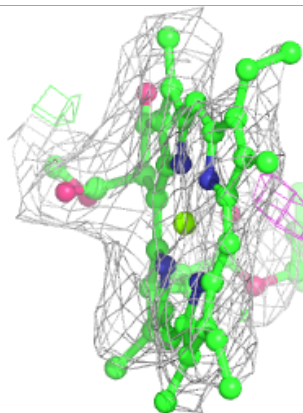
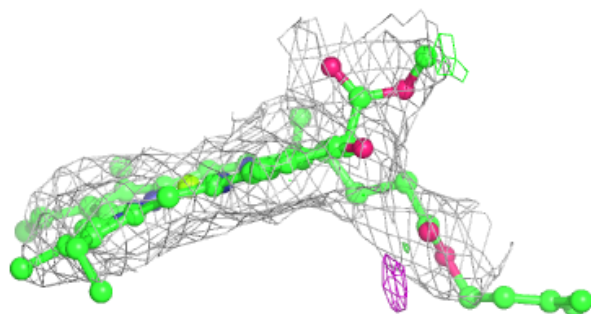
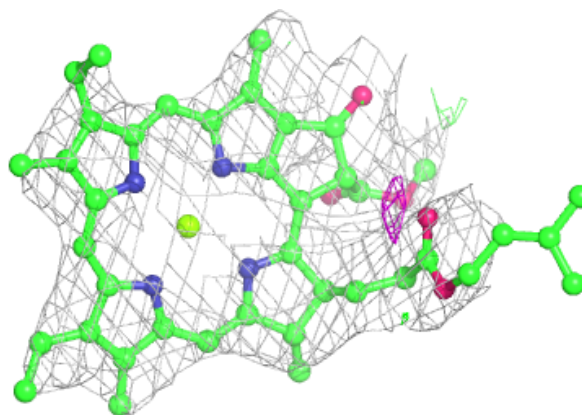


Electron density around CLA a 1119:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

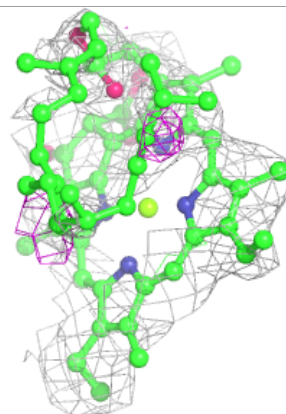
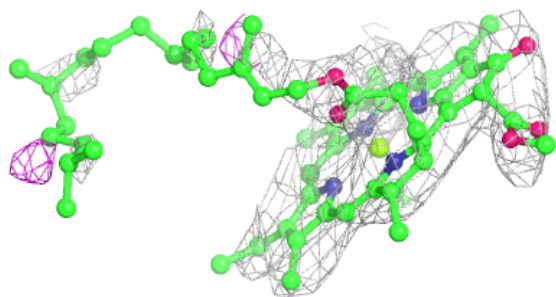
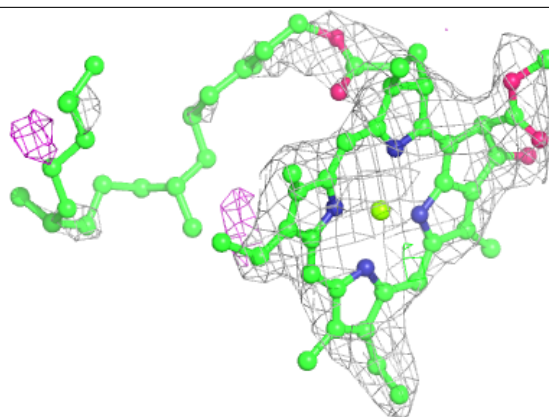
**Electron density around CLA a 1107:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

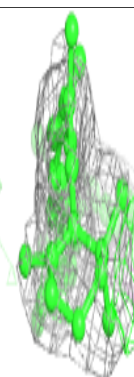
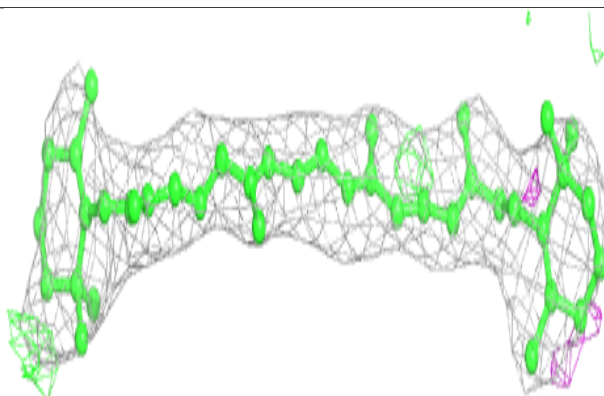
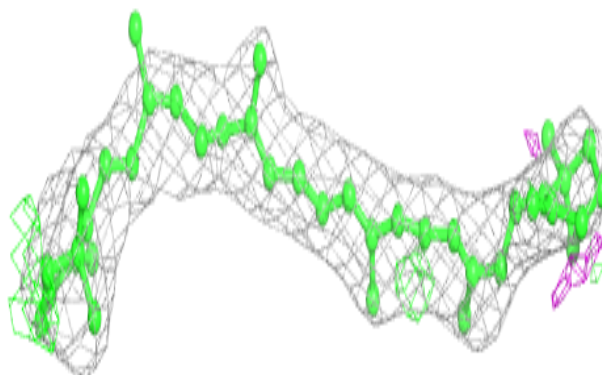


Electron density around CLA a 1122:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

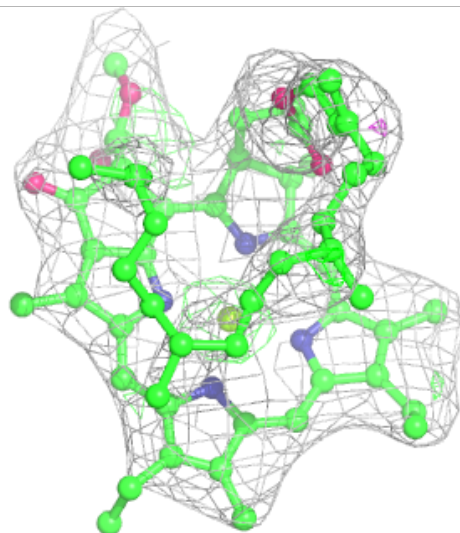
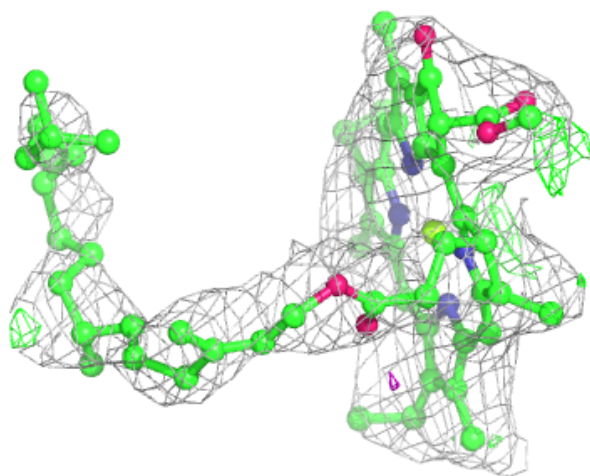
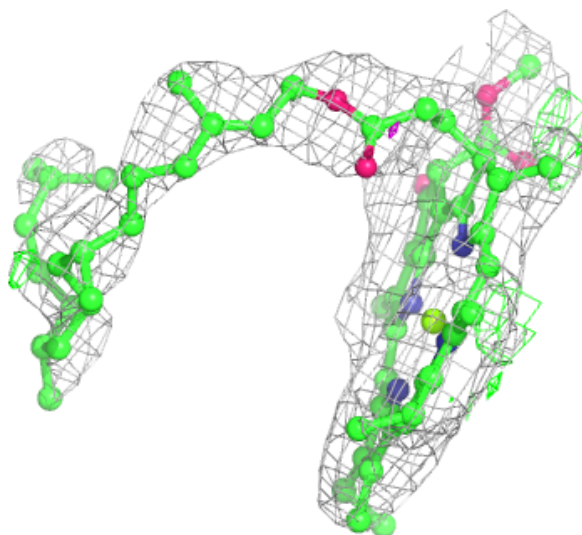
**Electron density around BCR 0 4022:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



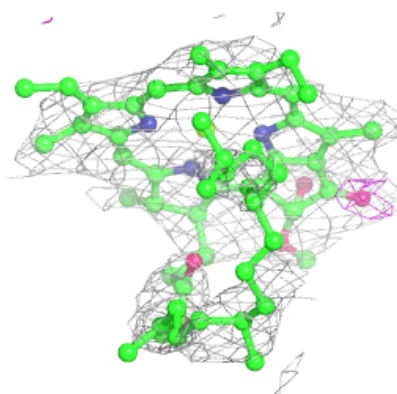
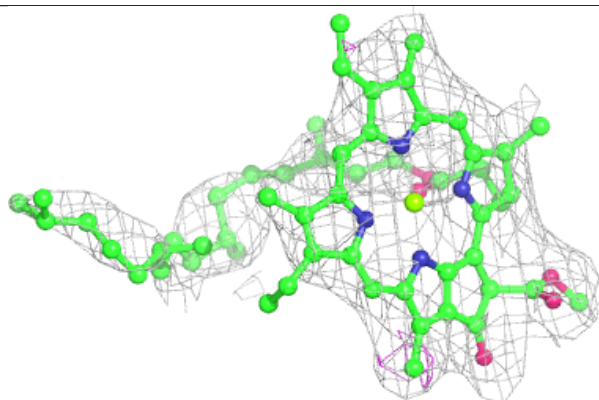
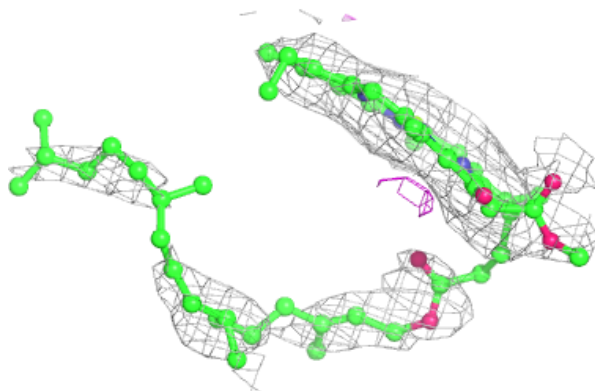
Electron density around CLA B 1216:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

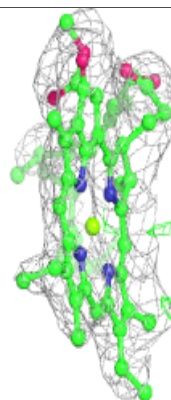
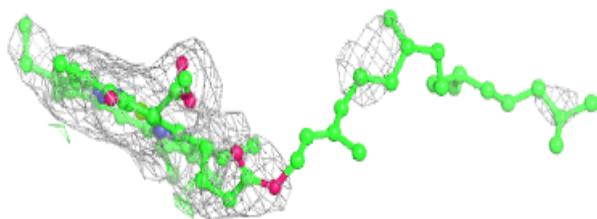
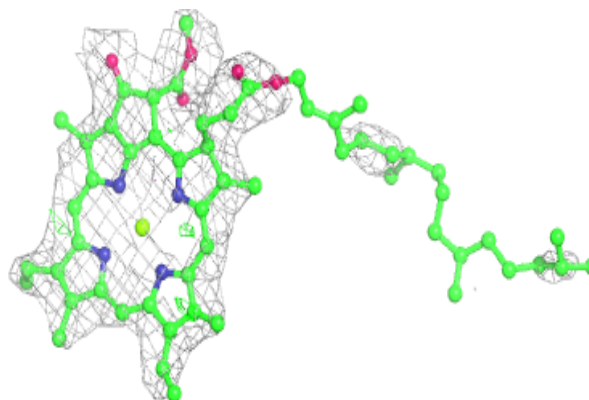


Electron density around CLA a 1109:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

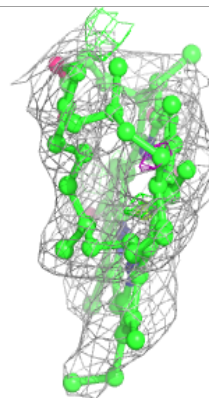
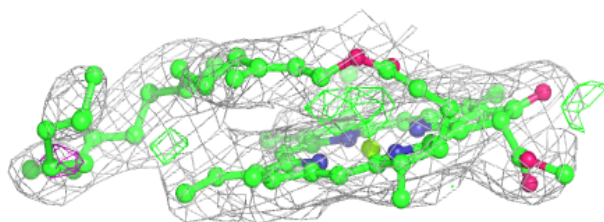
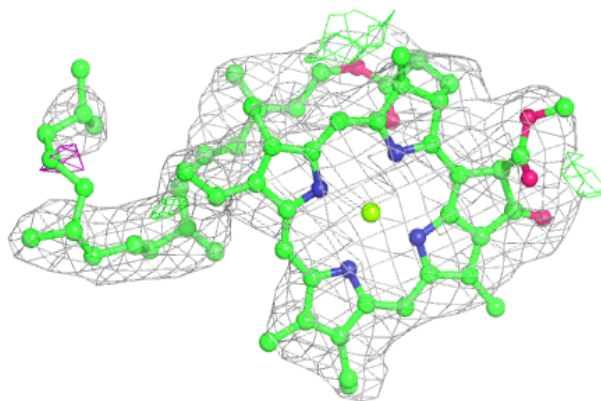
**Electron density around CLA F 1301:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

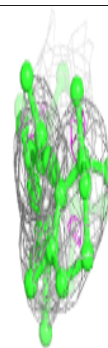
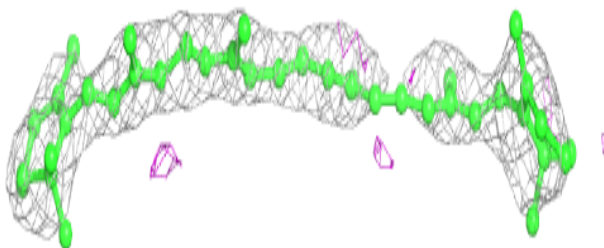
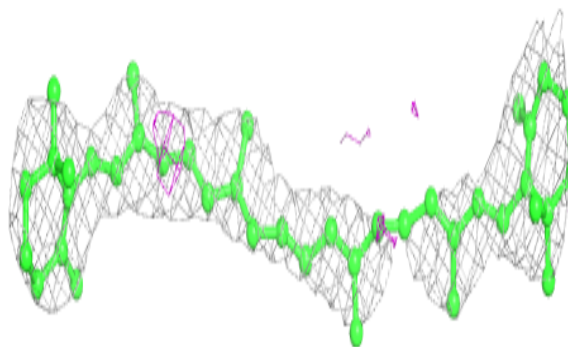


Electron density around CLA a 1117:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

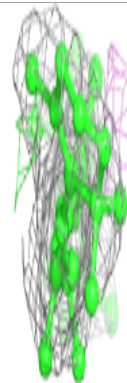
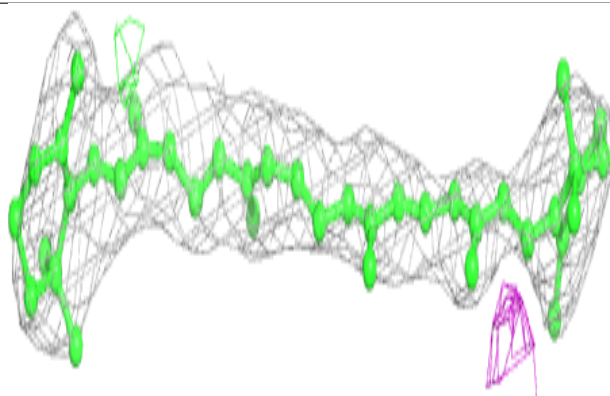
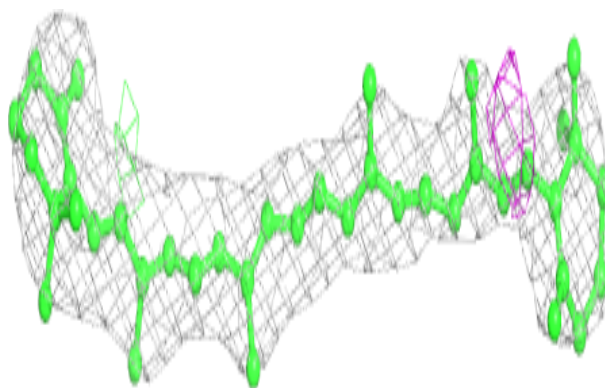
**Electron density around BCR 1 4008:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



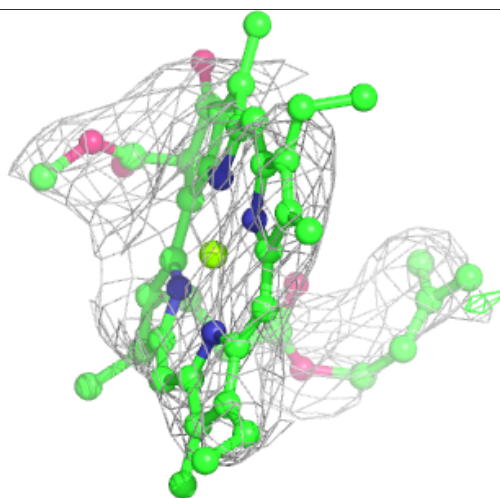
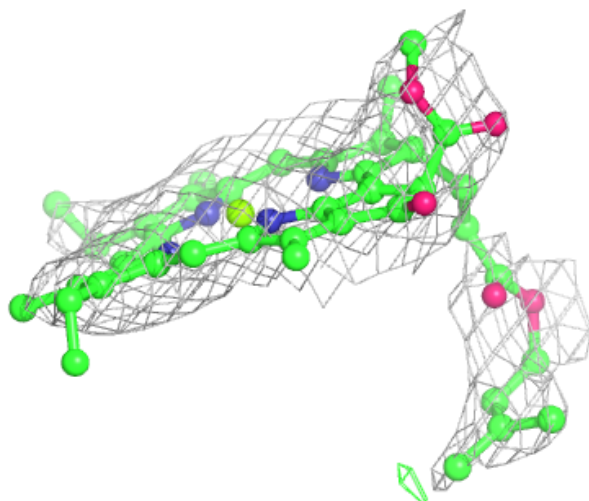
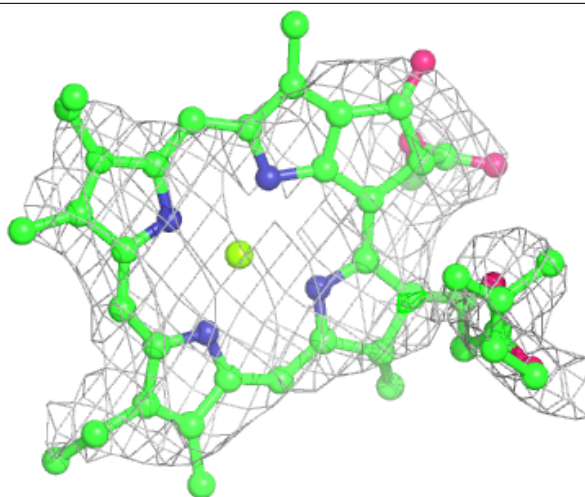
Electron density around BCR A 4002:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



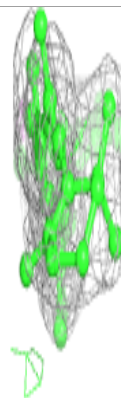
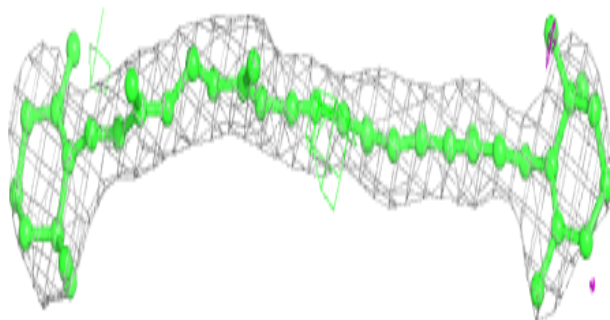
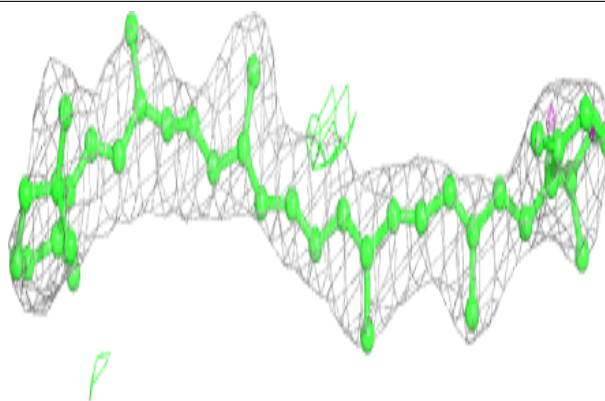
Electron density around CLA 1 1112:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

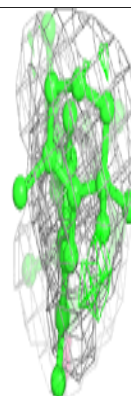
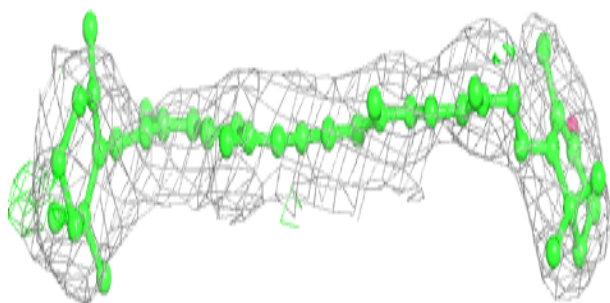
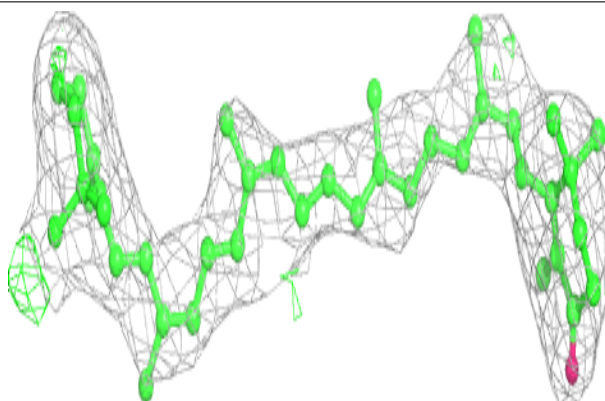


Electron density around BCR L 4022:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

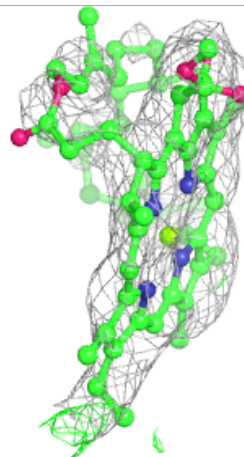
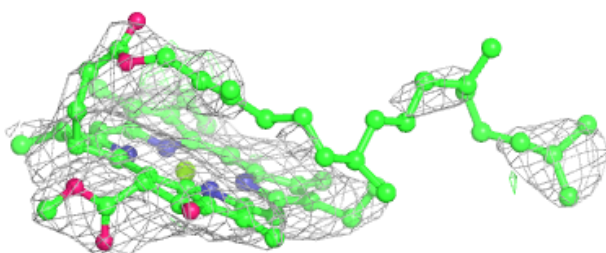
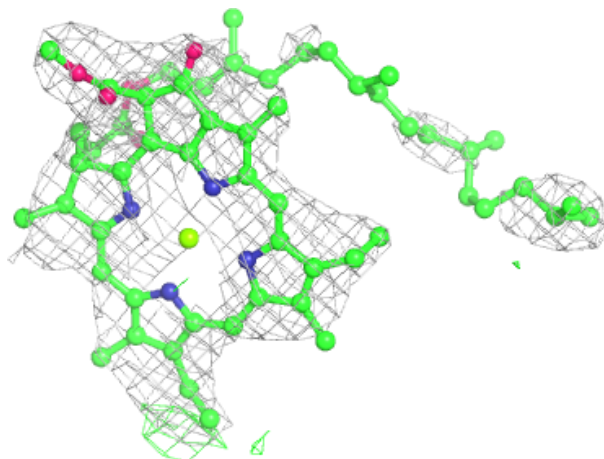
**Electron density around ECH B 4006:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



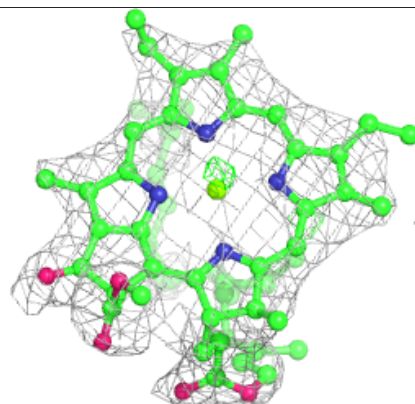
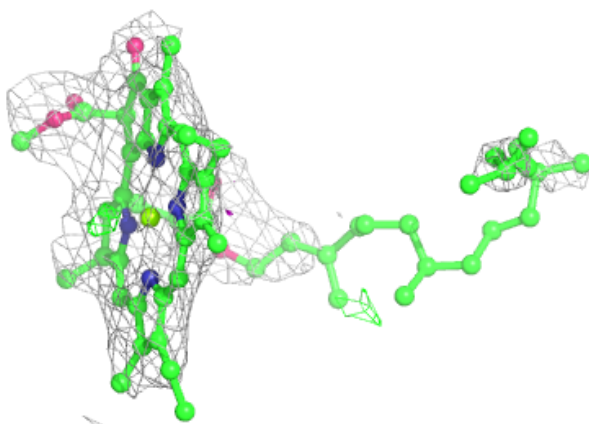
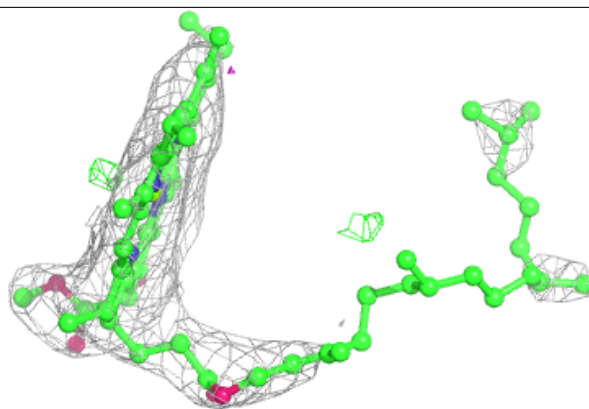
Electron density around CLA 1 1127:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

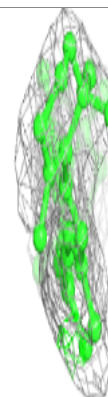
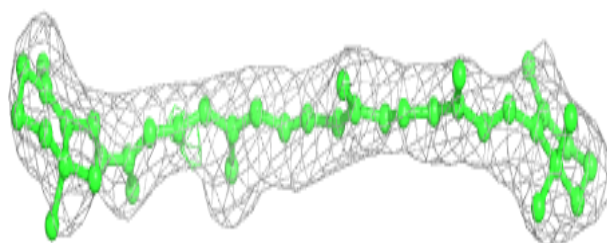
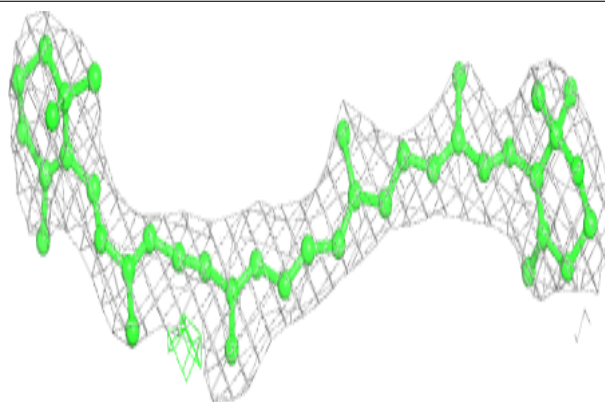


Electron density around CLA b 1227:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

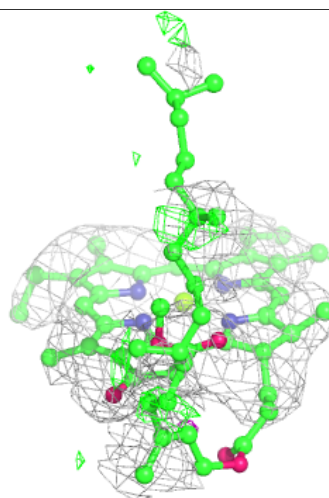
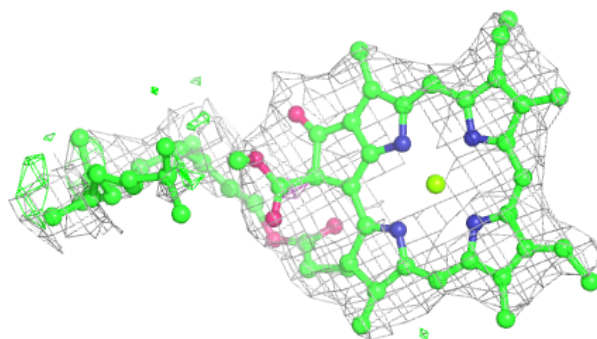
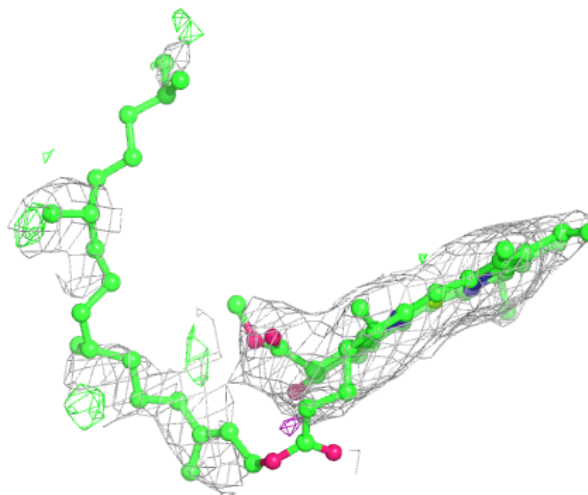
**Electron density around BCR b 4010:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



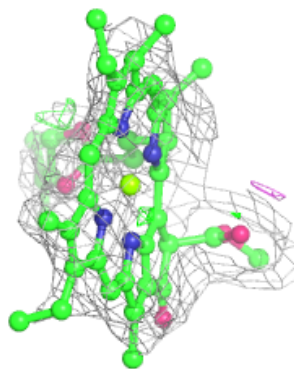
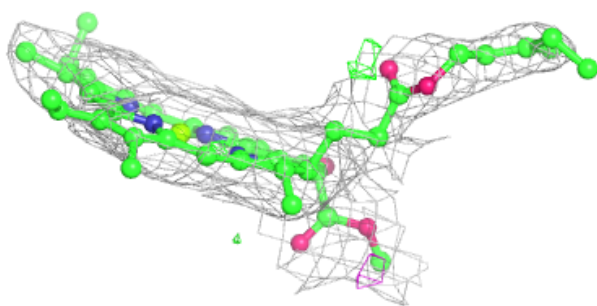
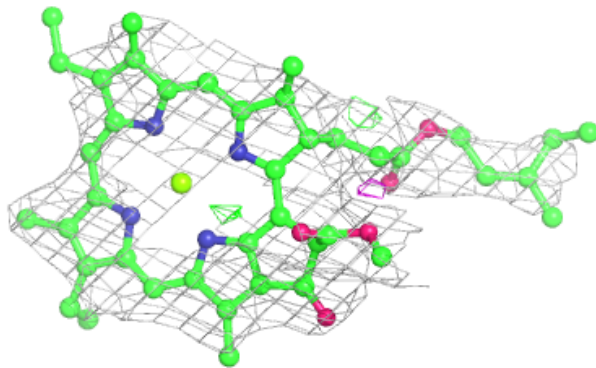
Electron density around CLA b 1240:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



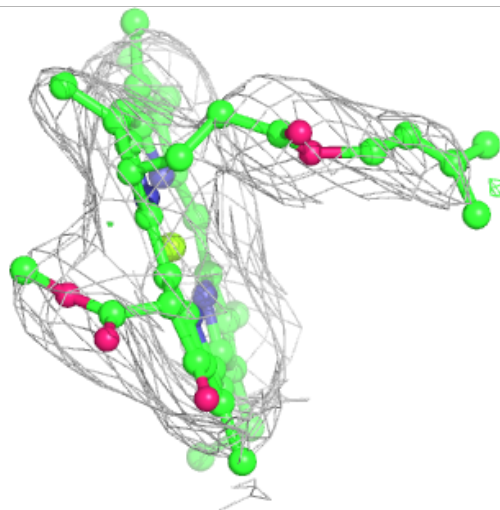
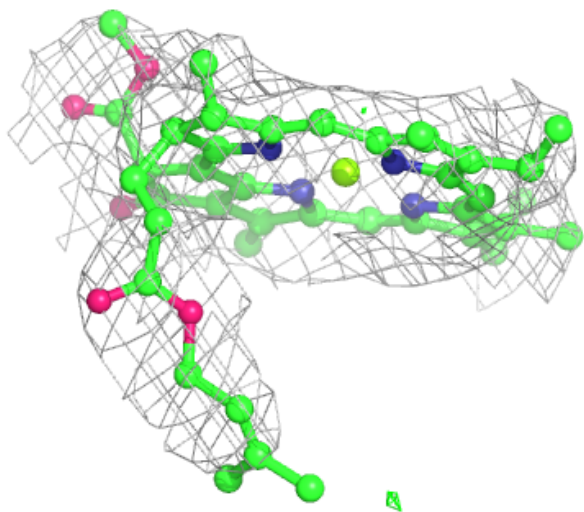
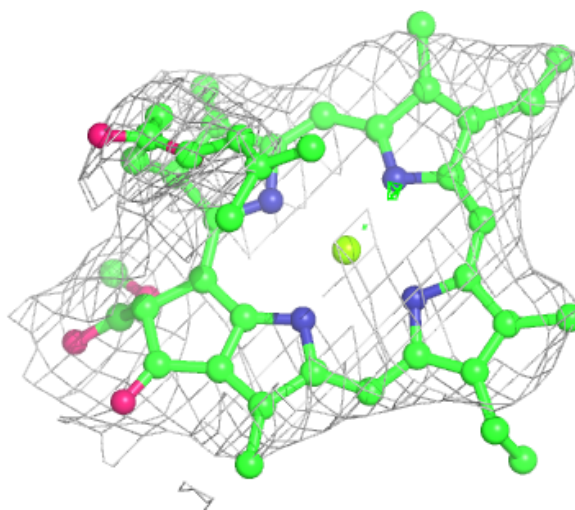
Electron density around CLA 1 1107:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



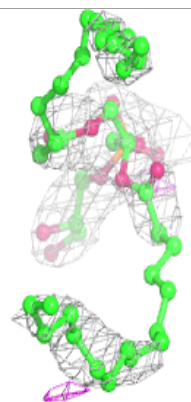
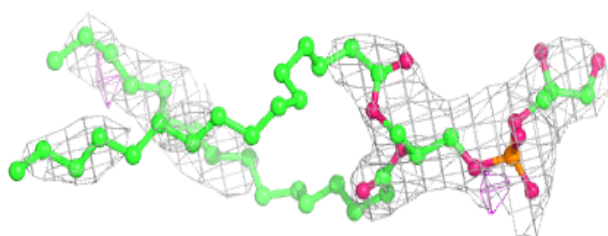
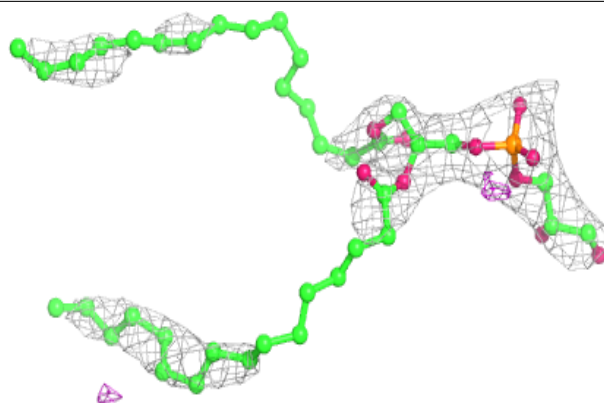
Electron density around CLA 2 1211:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

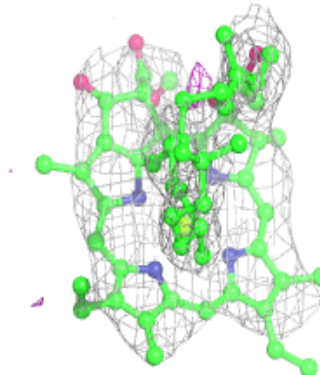
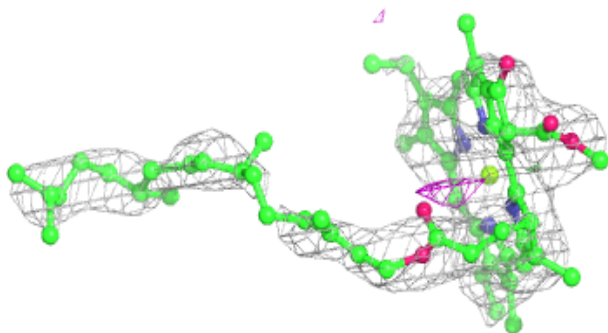
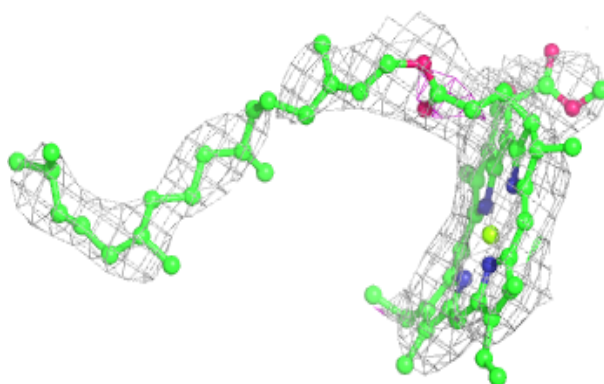


Electron density around LHG 1 5001:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

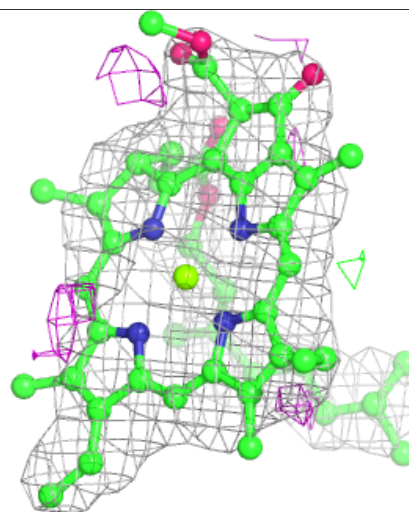
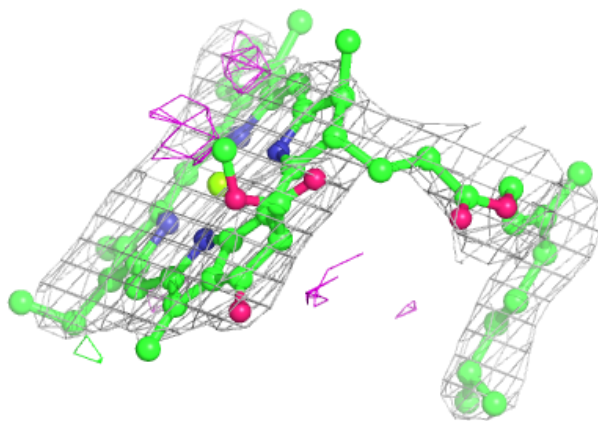
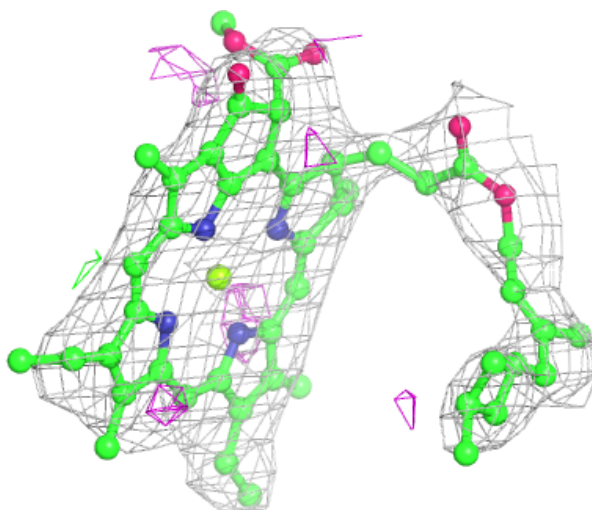
**Electron density around CLA a 1128:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



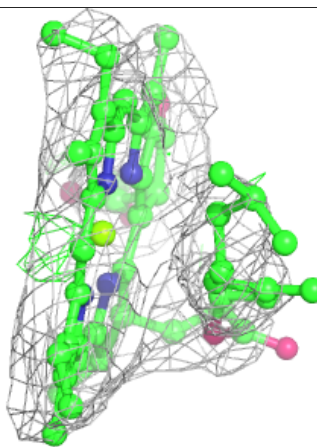
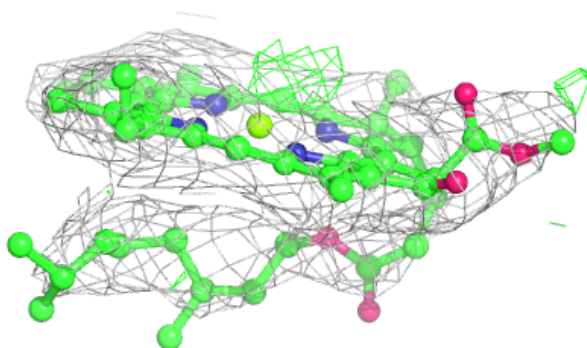
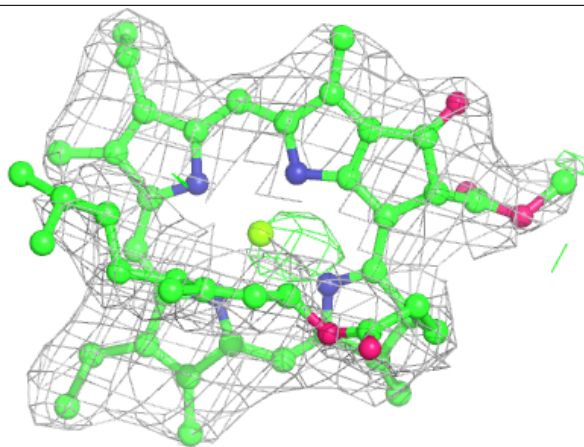
Electron density around CLA 1 1102:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

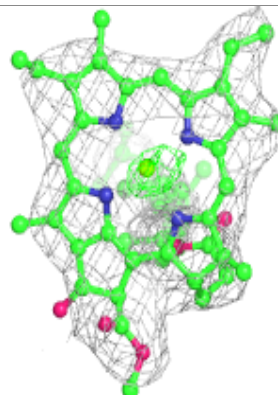
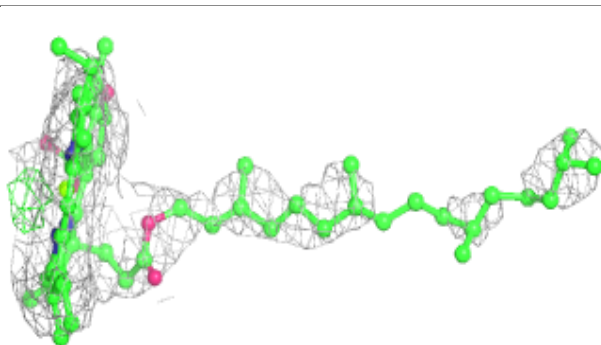
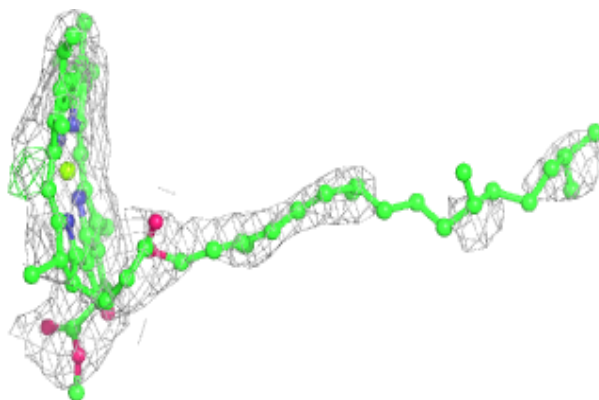


Electron density around CLA 1 1121:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

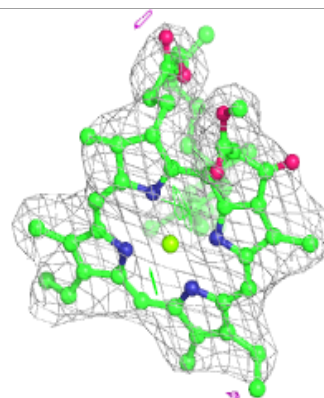
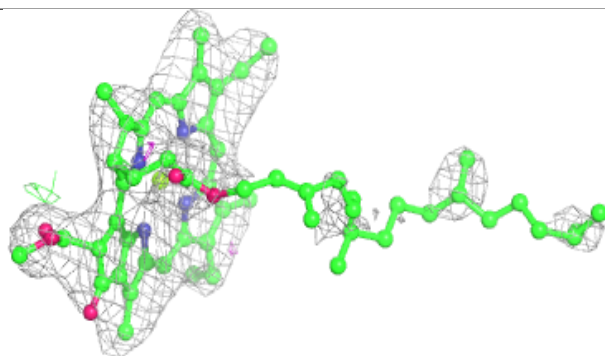
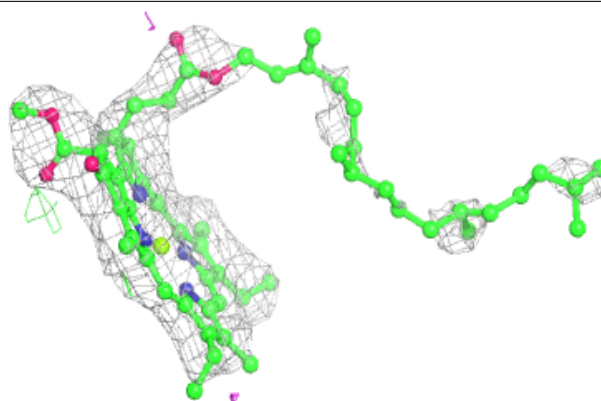
**Electron density around CLA 1 1126:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

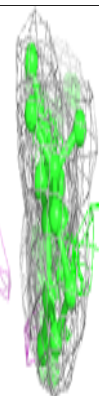
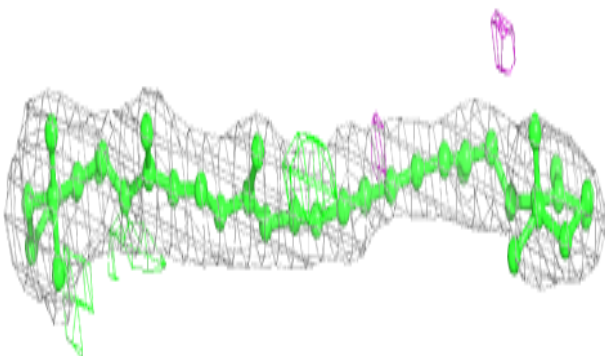
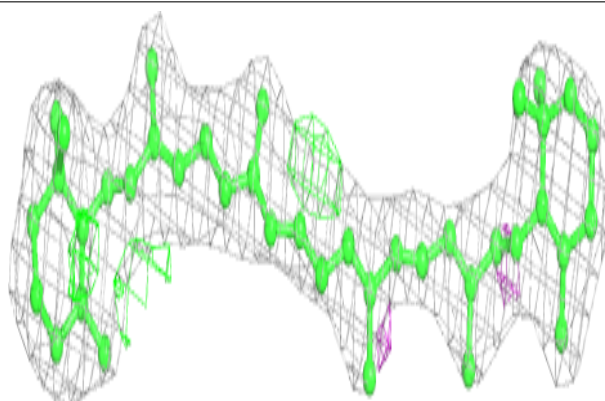


Electron density around CLA b 1232:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

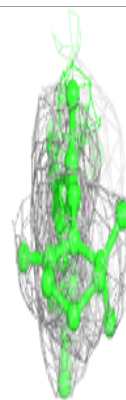
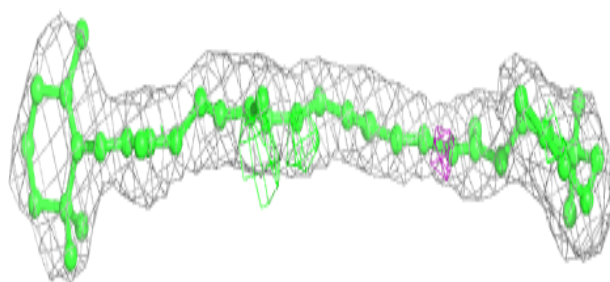
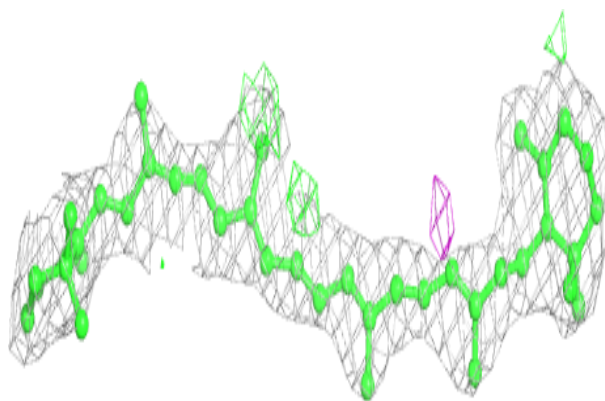
**Electron density around BCR 1 4019:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

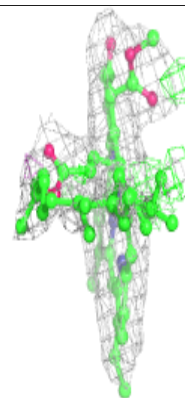
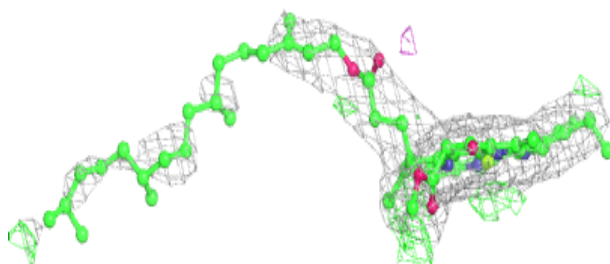
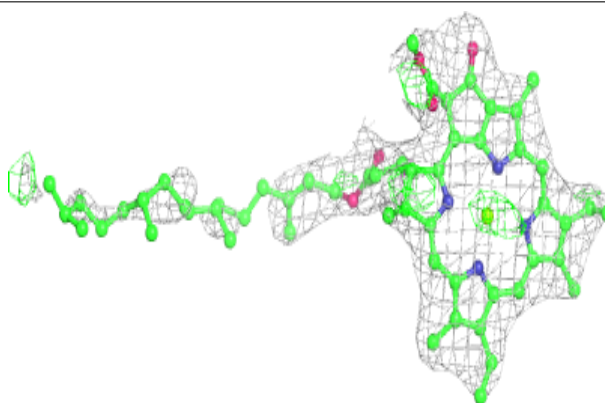


Electron density around BCR b 4005:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

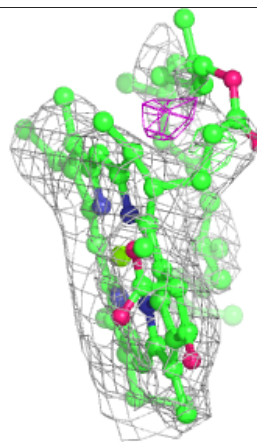
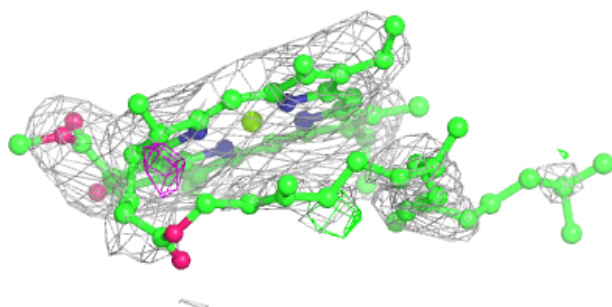
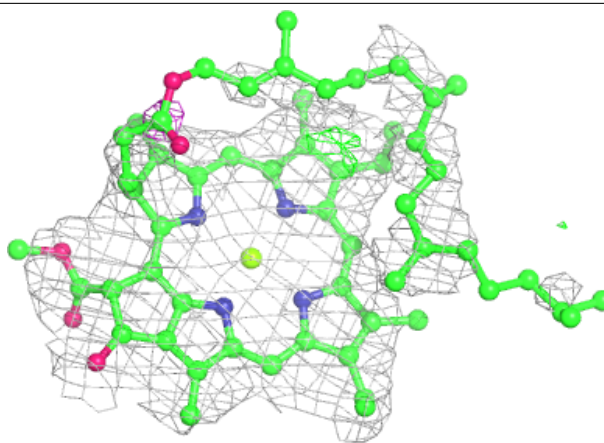
**Electron density around CLA b 1222:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

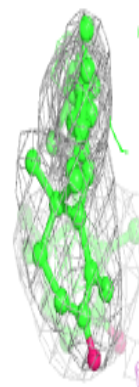
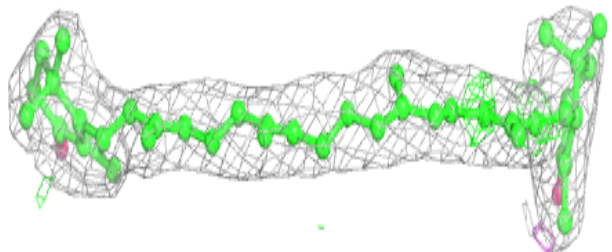
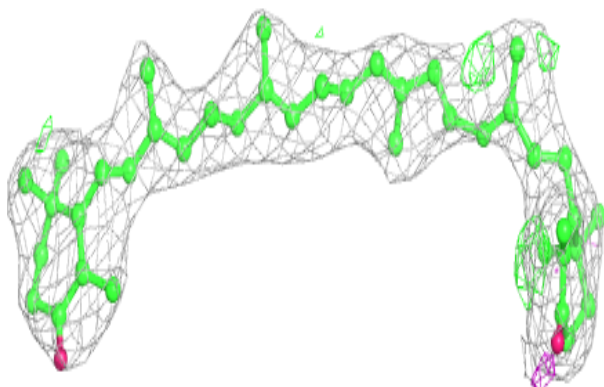


Electron density around CLA B 1218:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

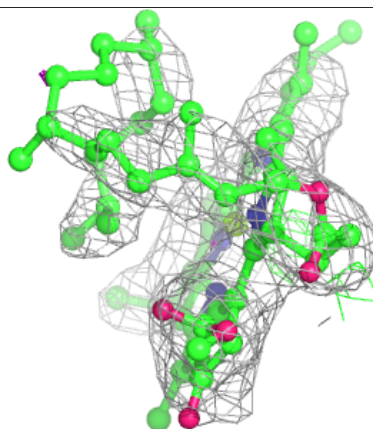
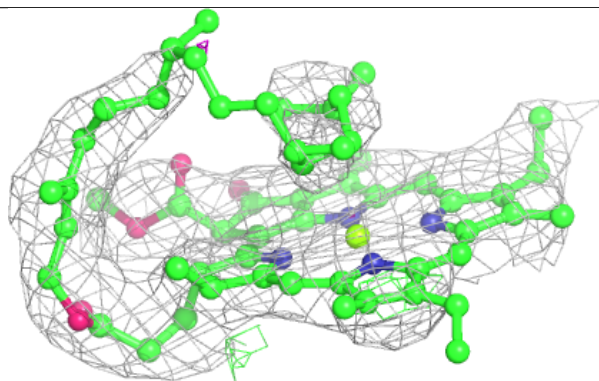
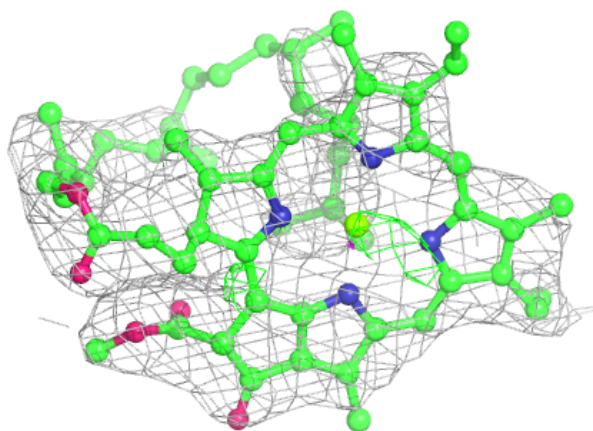
**Electron density around 45D h 4020:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

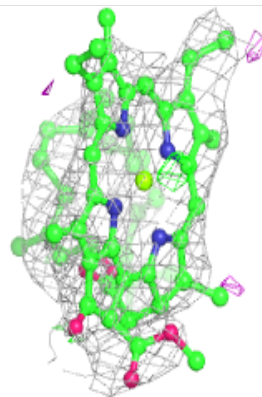
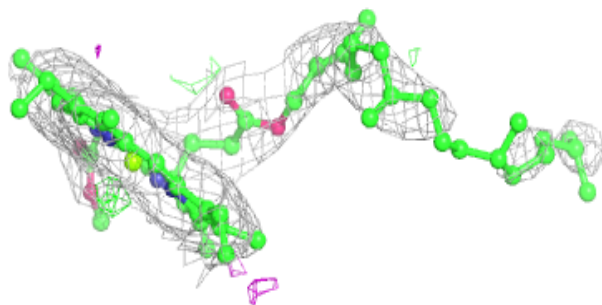
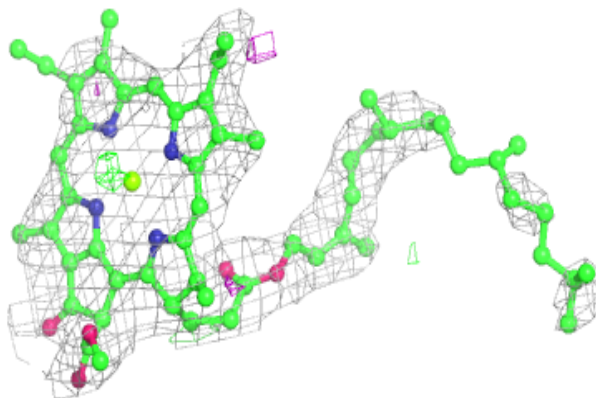


Electron density around CLA 2 1203:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

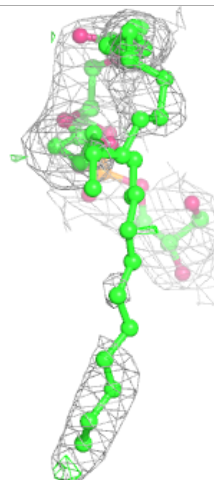
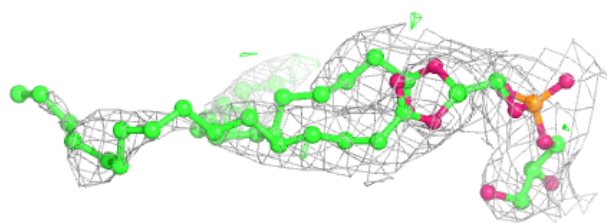
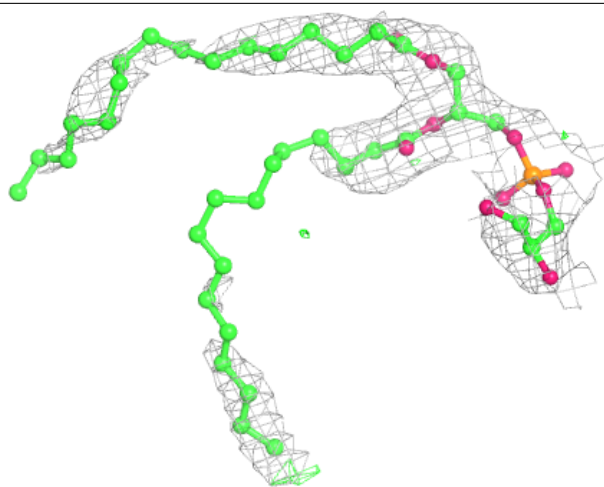
**Electron density around CLA a 1106:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



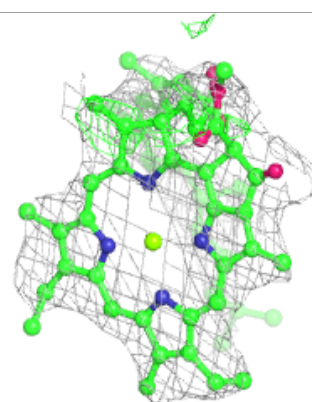
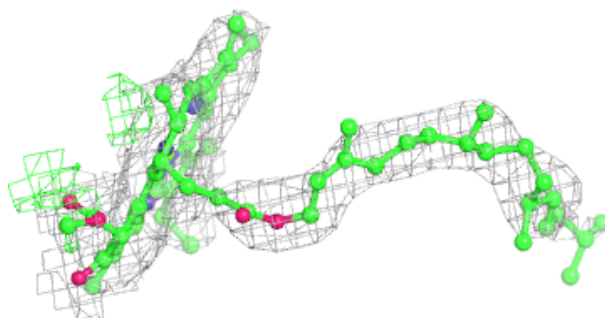
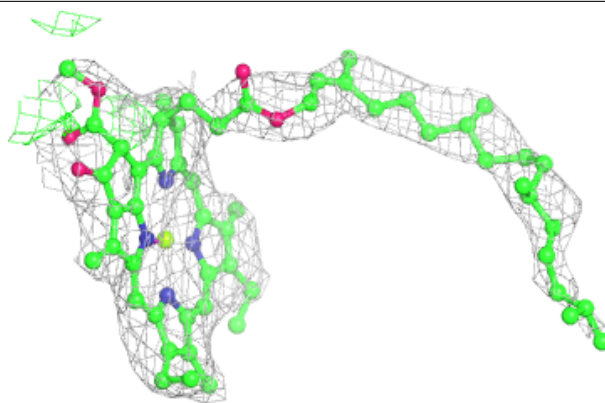
Electron density around LHG b 5004:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

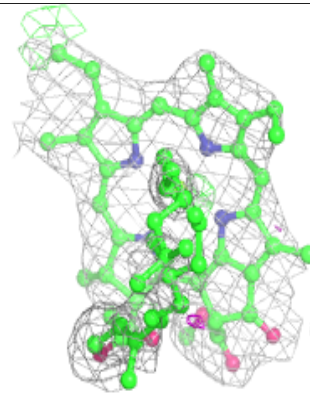
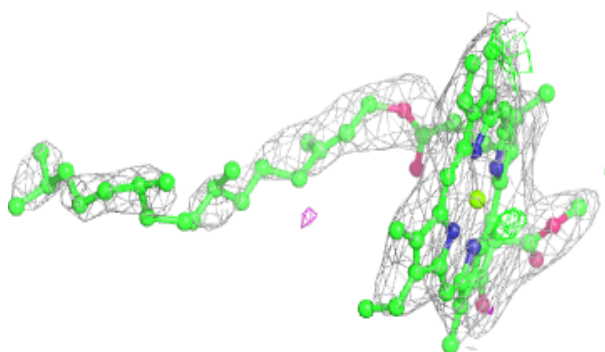
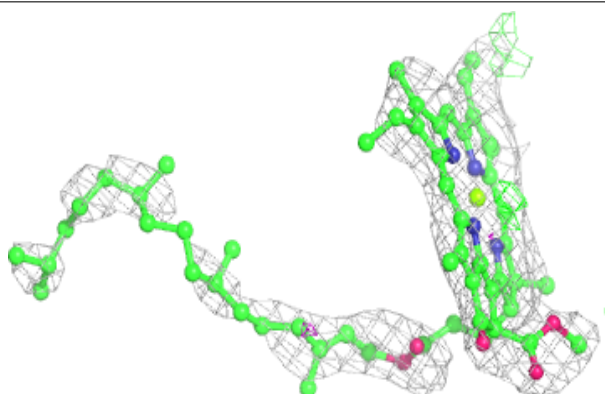


Electron density around CLA a 1133:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

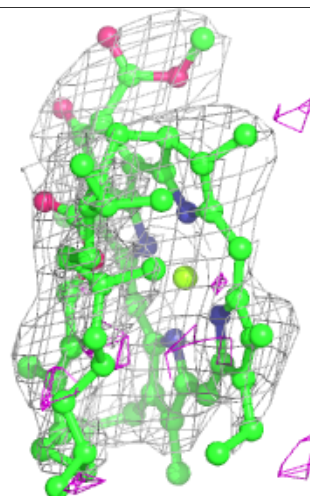
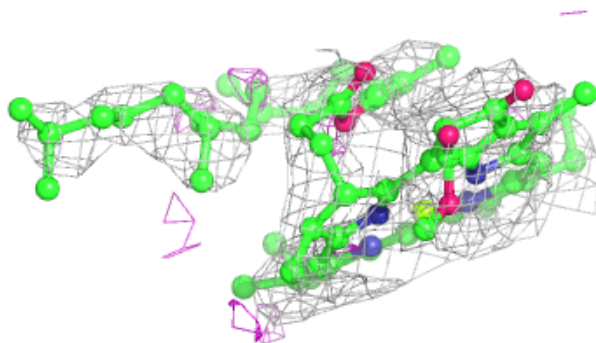
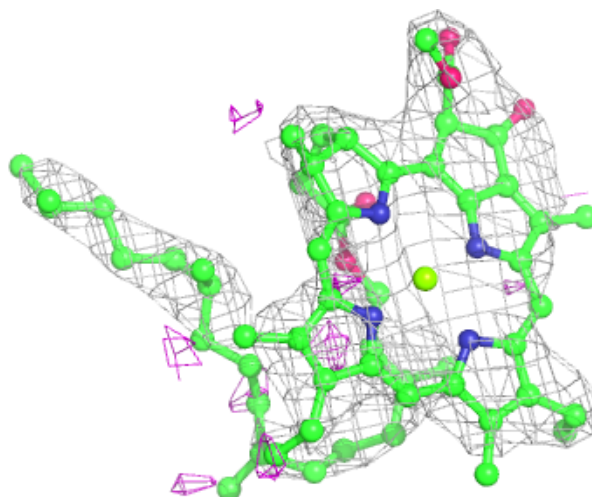
**Electron density around CLA 1 1128:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



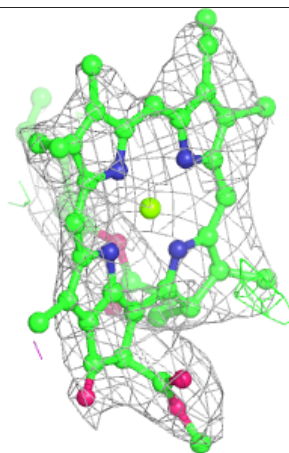
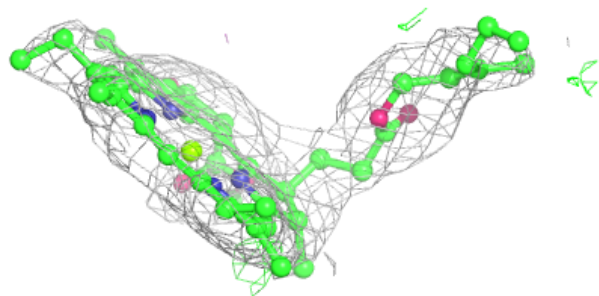
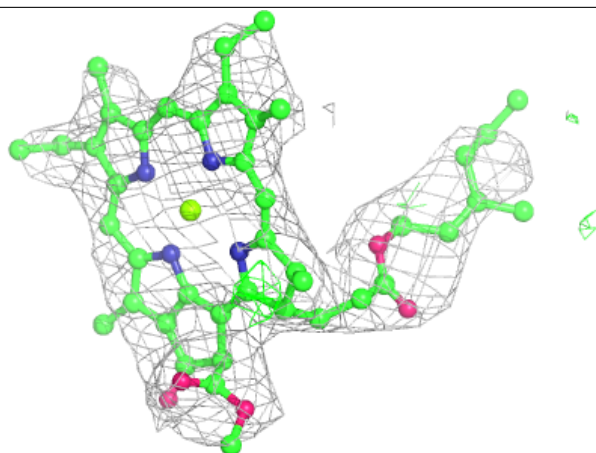
Electron density around CLA 2 1205:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

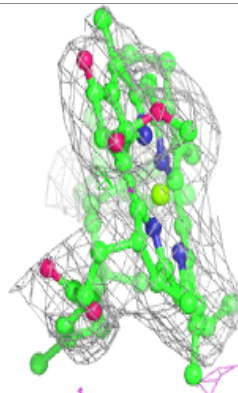
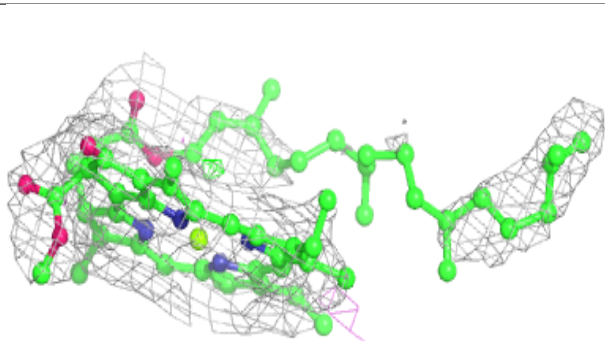
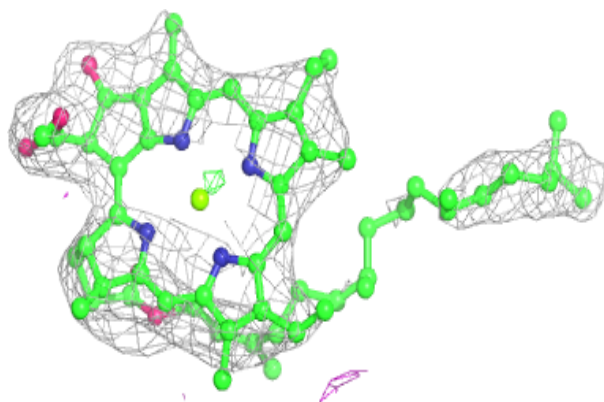


Electron density around CLA a 1129:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

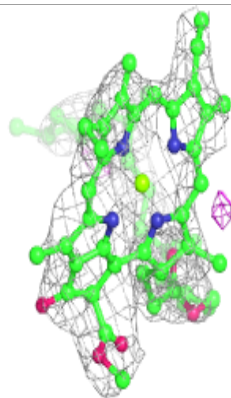
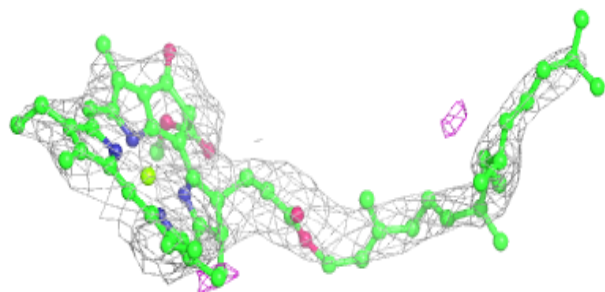
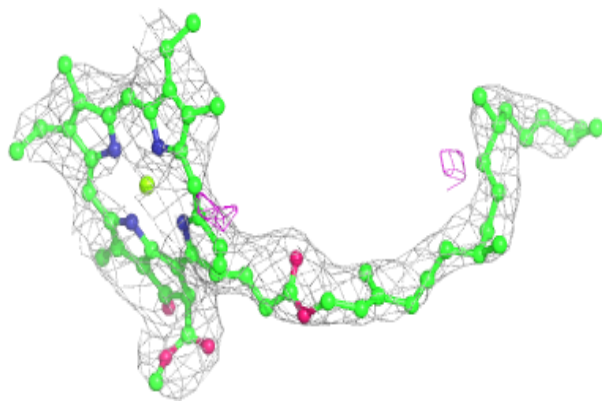
**Electron density around CLA B 1217:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

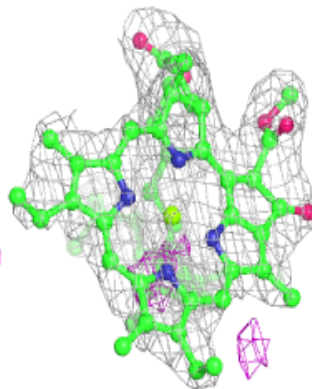
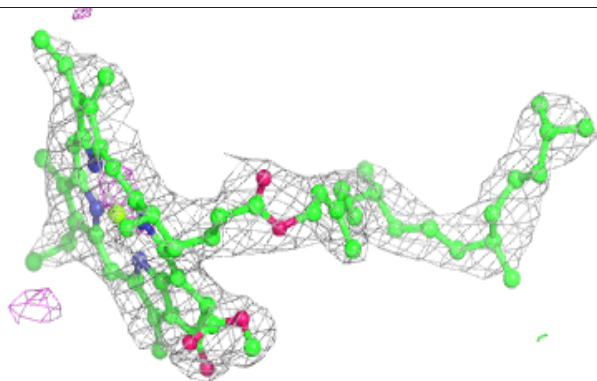
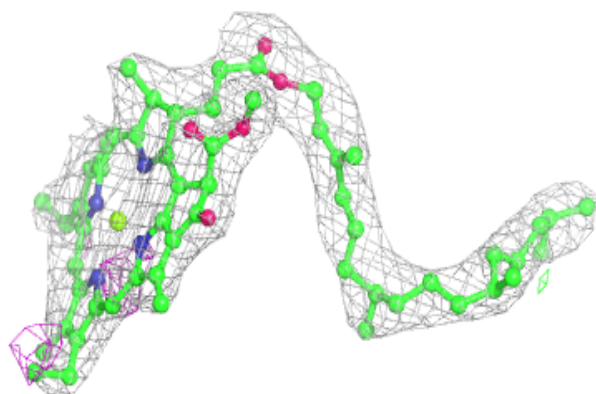


Electron density around CLA 1 1012:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

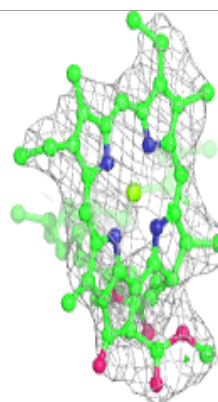
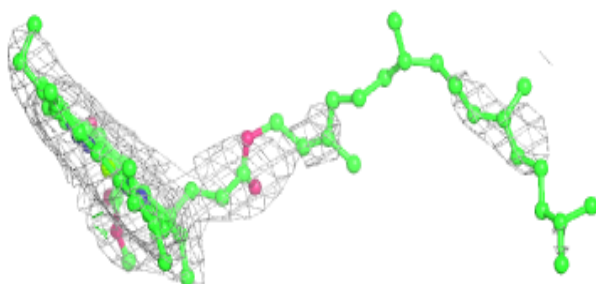
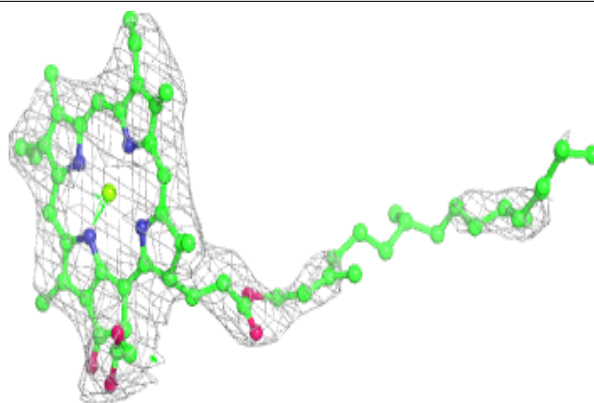
**Electron density around CLA b 1021:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

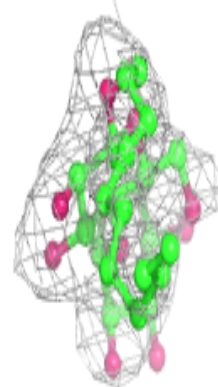
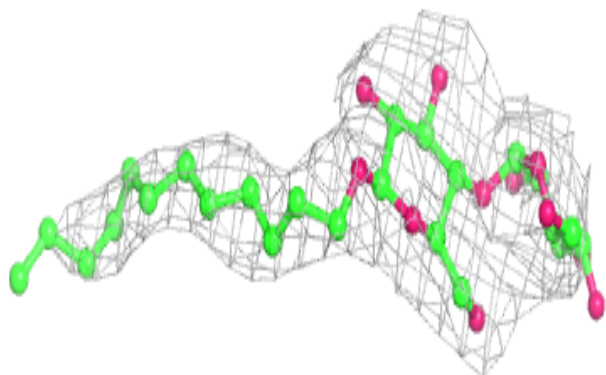
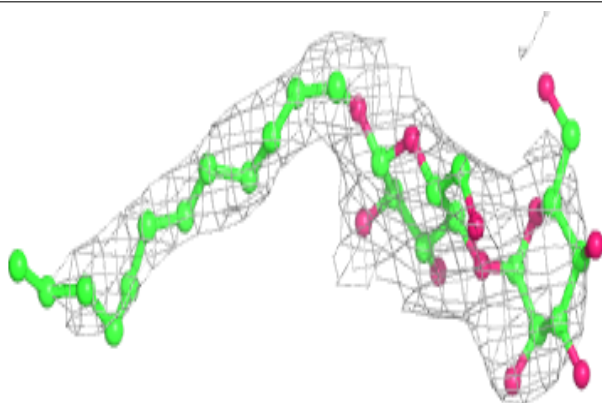


Electron density around CLA b 1230:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

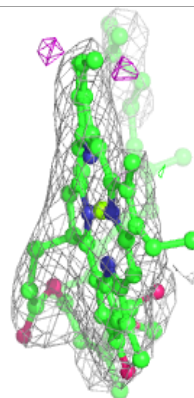
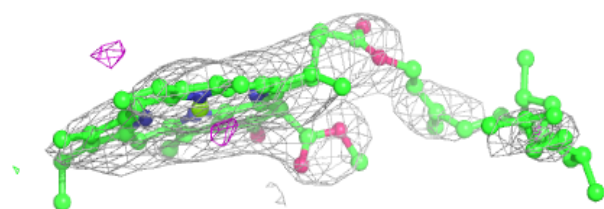
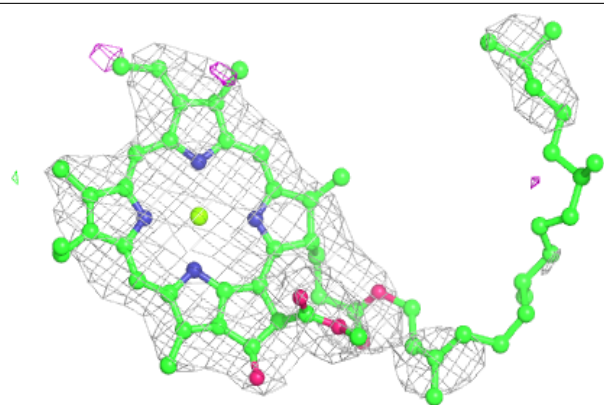
**Electron density around LMT F 6001:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

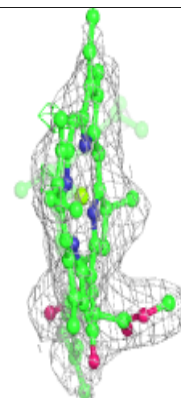
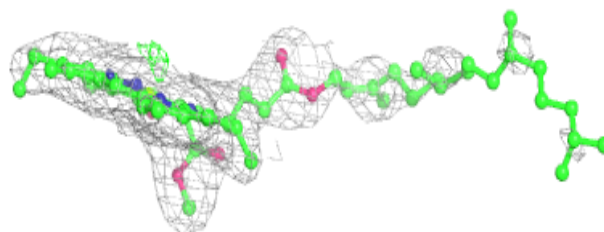
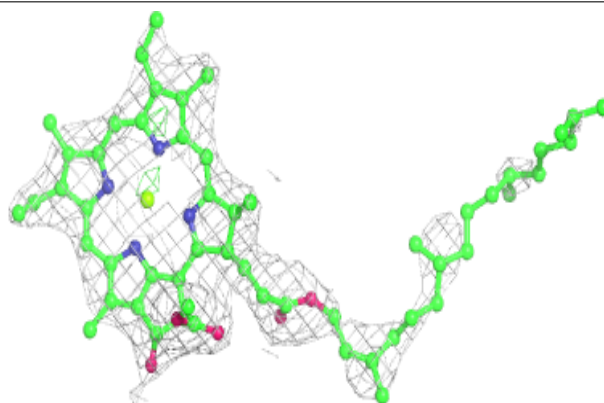


Electron density around CLA 1 1101:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

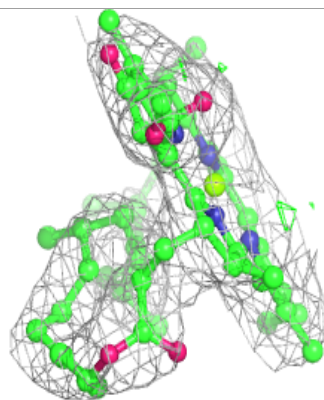
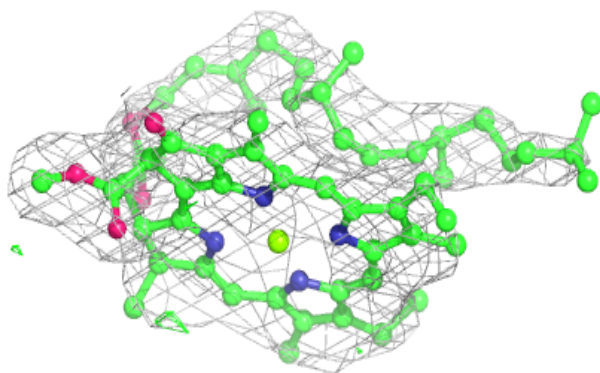
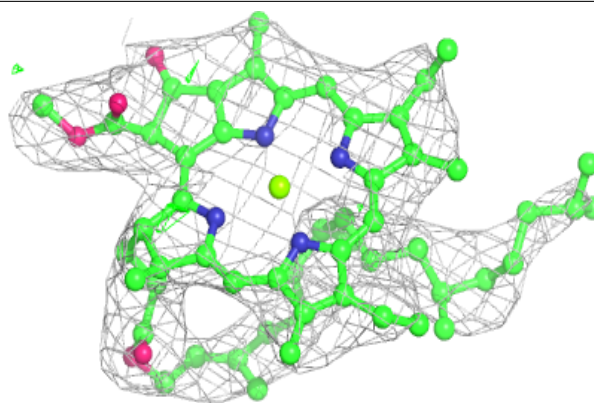
**Electron density around CLA B 1234:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

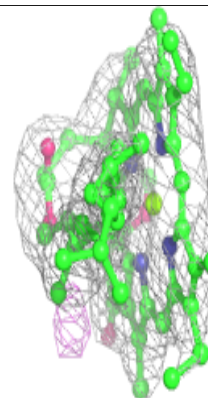
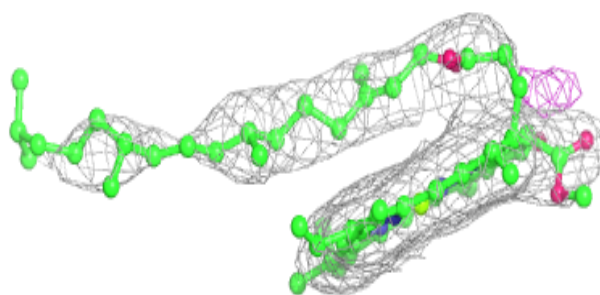
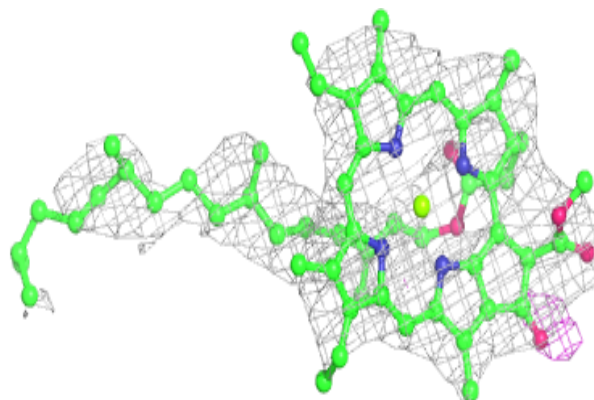


Electron density around CLA B 1214:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

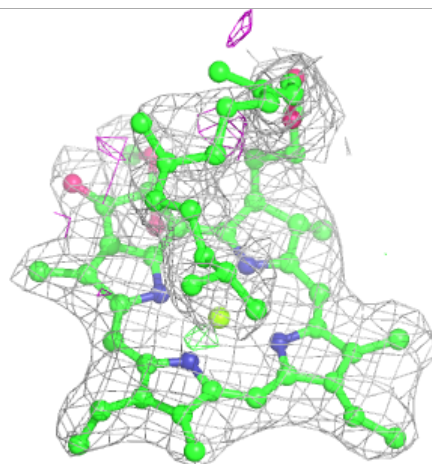
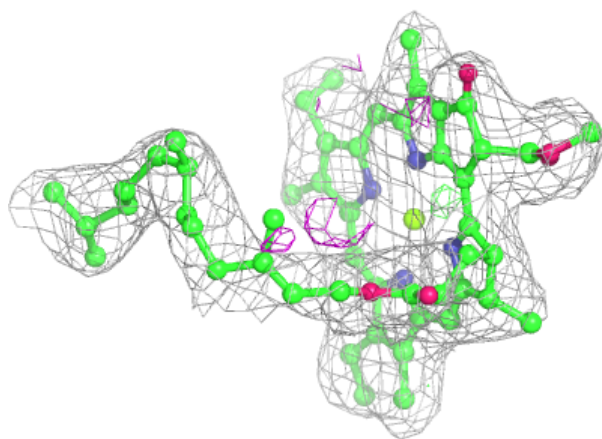
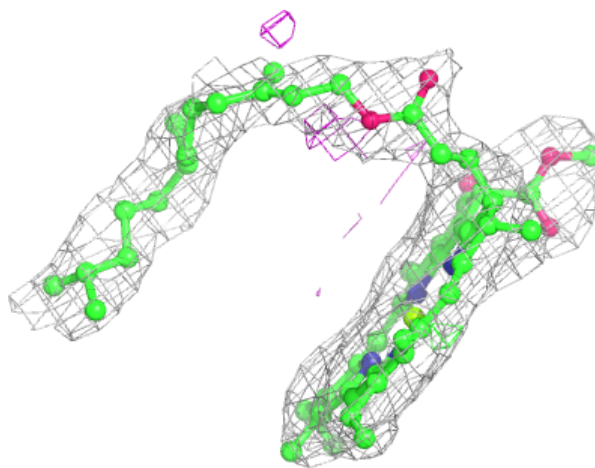
**Electron density around CLA B 1213:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



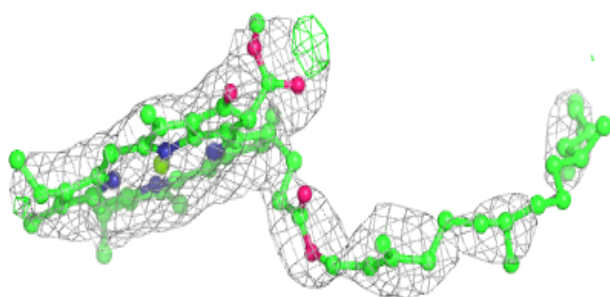
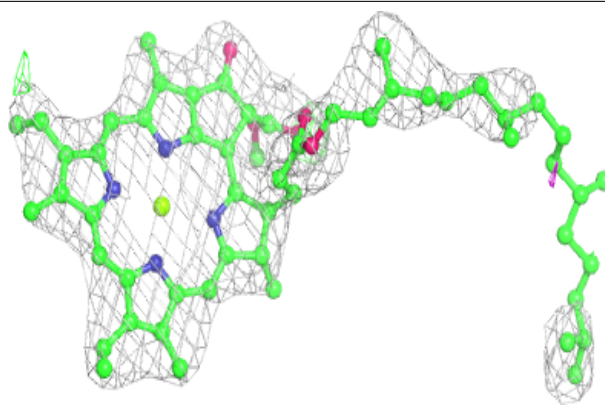
Electron density around CLA b 1208:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



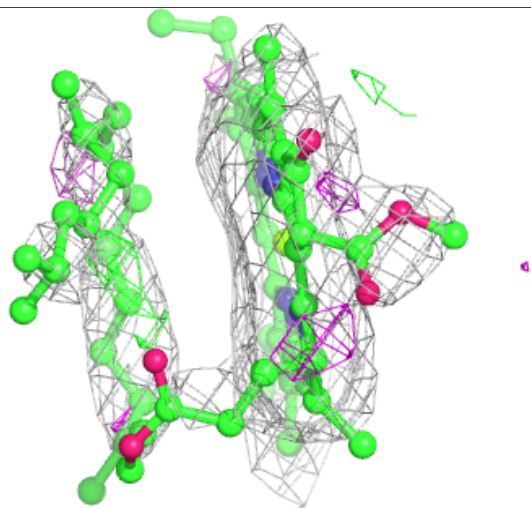
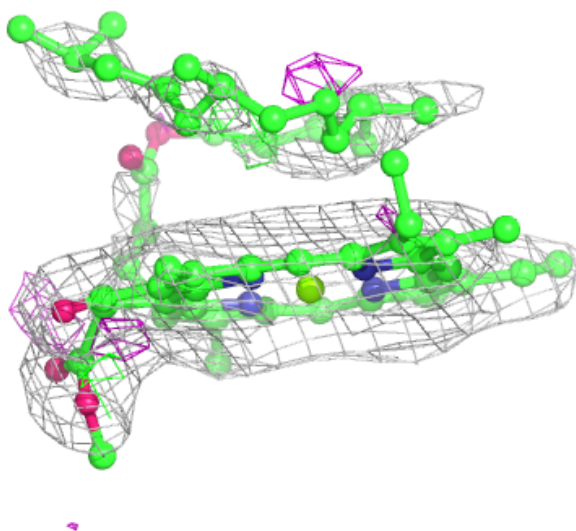
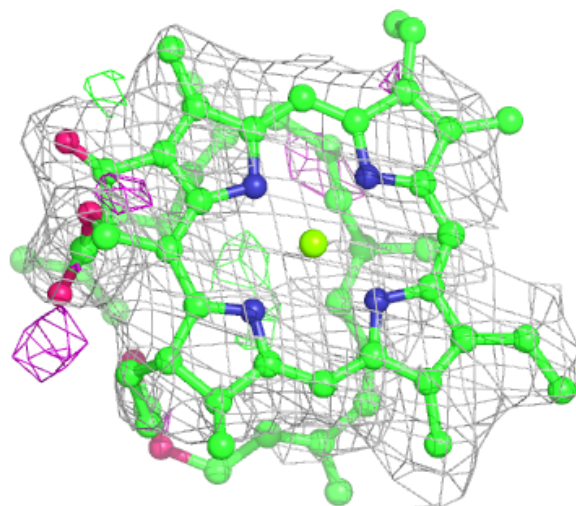
Electron density around CLA b 1220:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



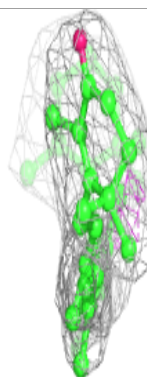
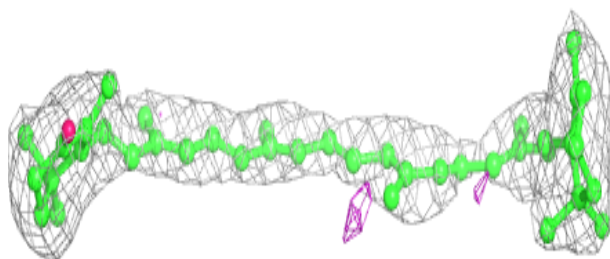
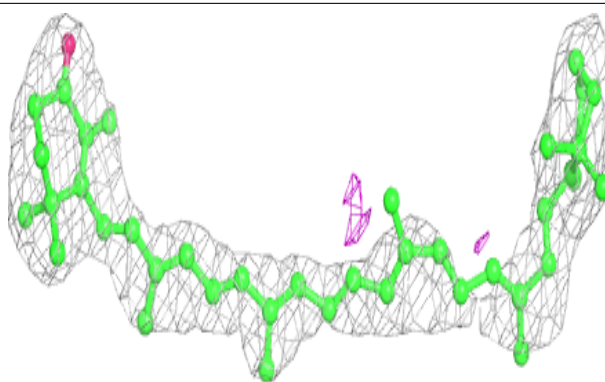
Electron density around CLA 11501:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

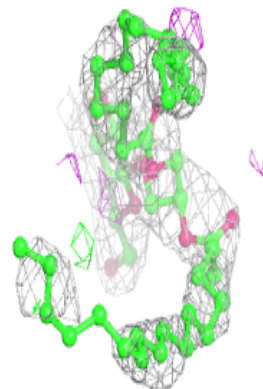
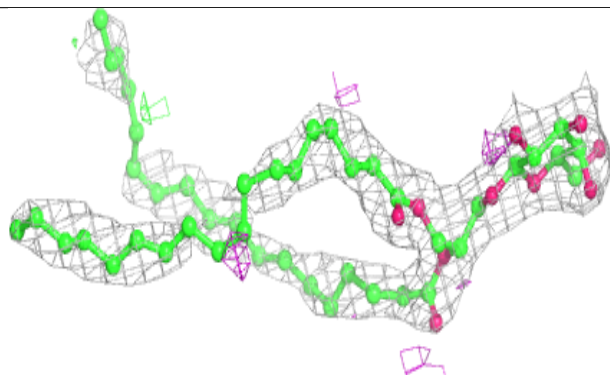
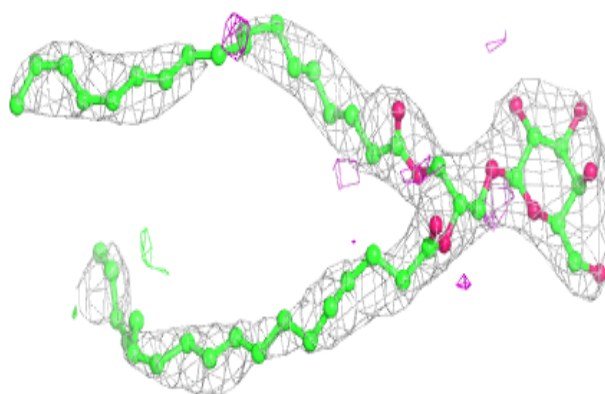


Electron density around ECH i 4020:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

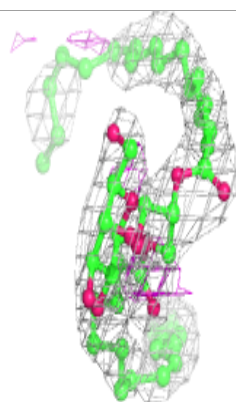
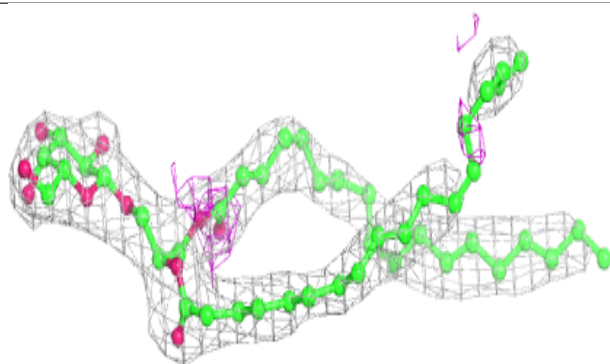
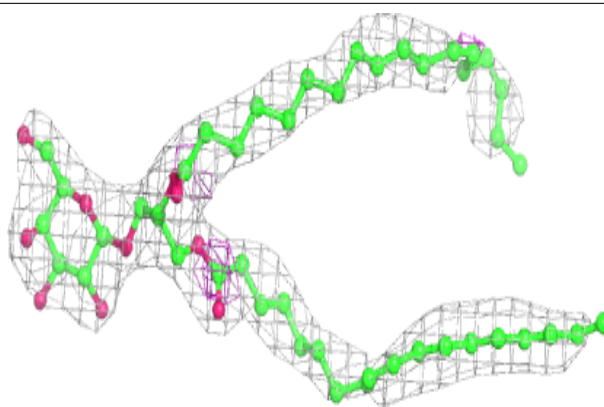
**Electron density around LMG b 5002:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

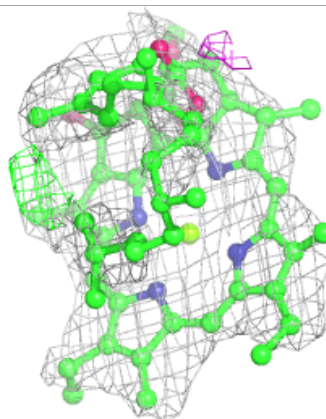
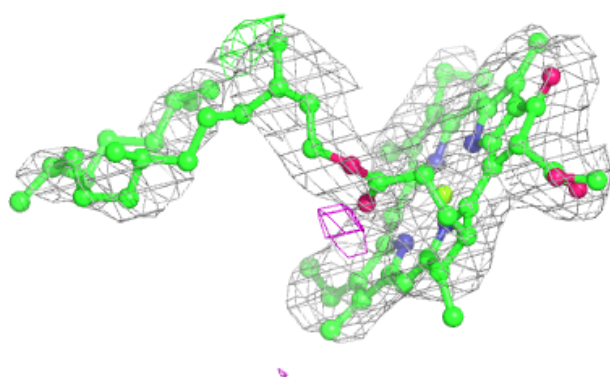
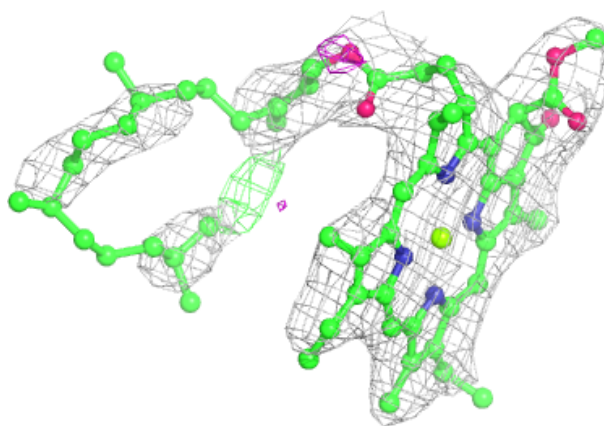


Electron density around LMG B 5002:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

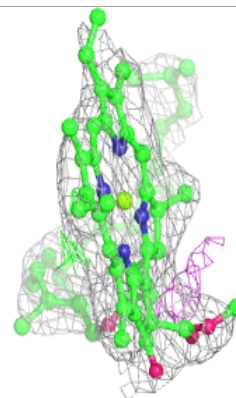
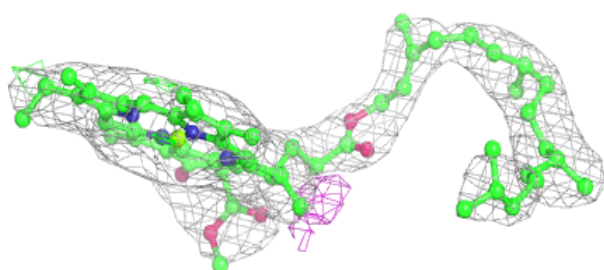
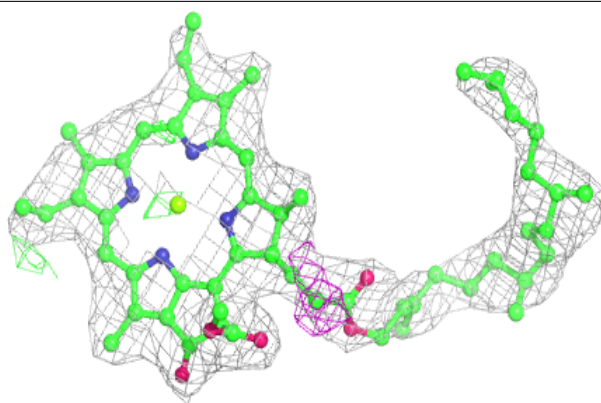
**Electron density around CLA b 1228:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

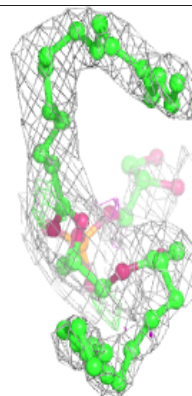
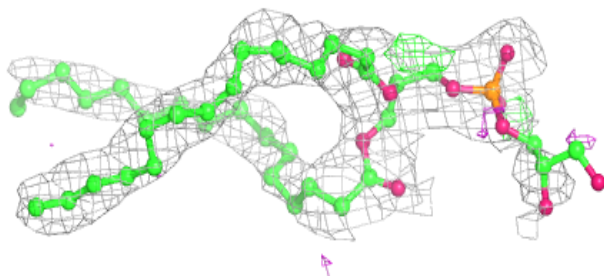
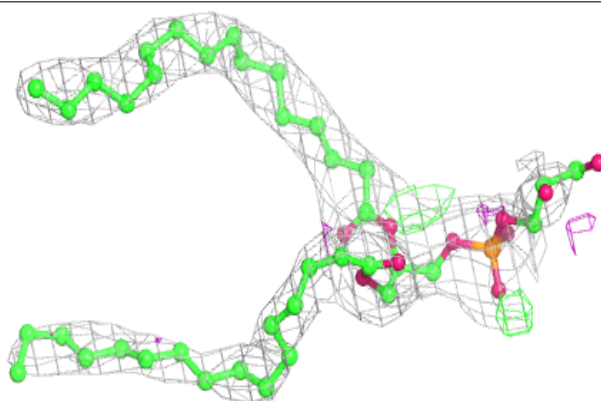


Electron density around CLA 1 1125:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

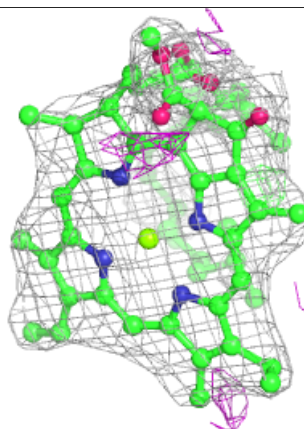
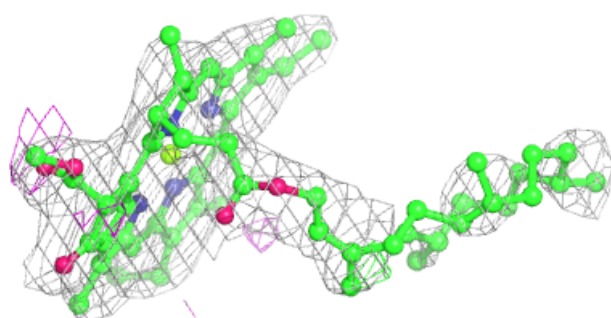
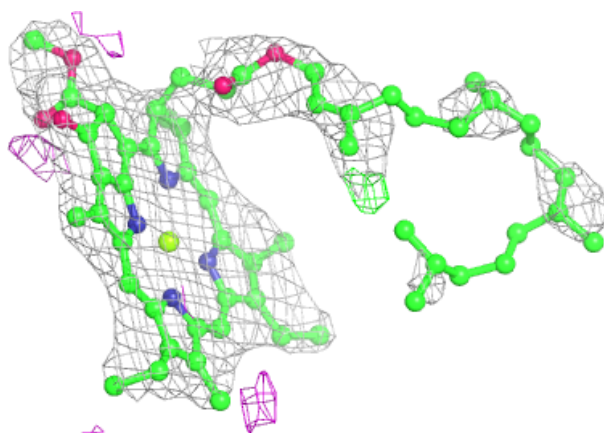
**Electron density around LHG a 5001:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

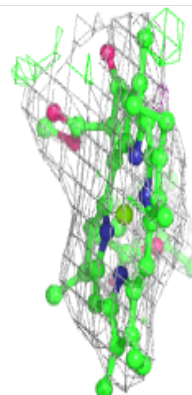
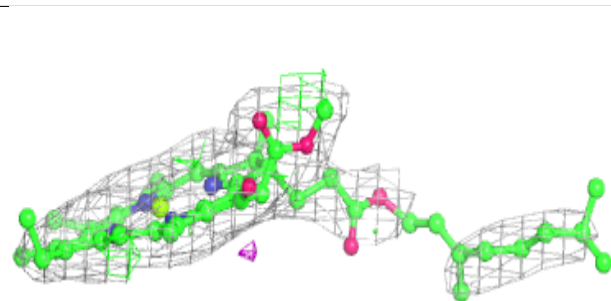
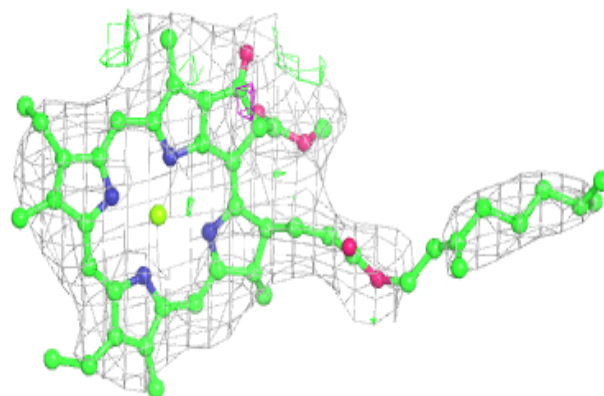


Electron density around CLA B 1228:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

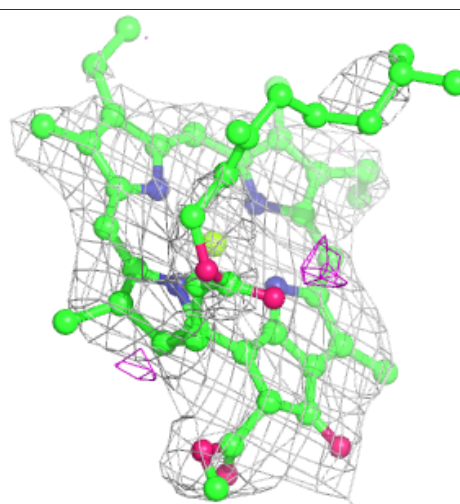
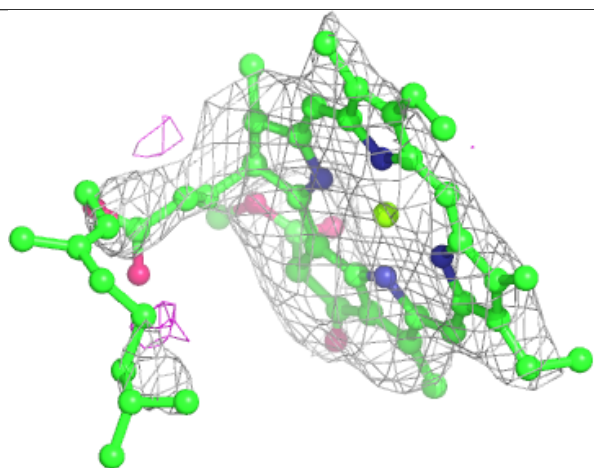
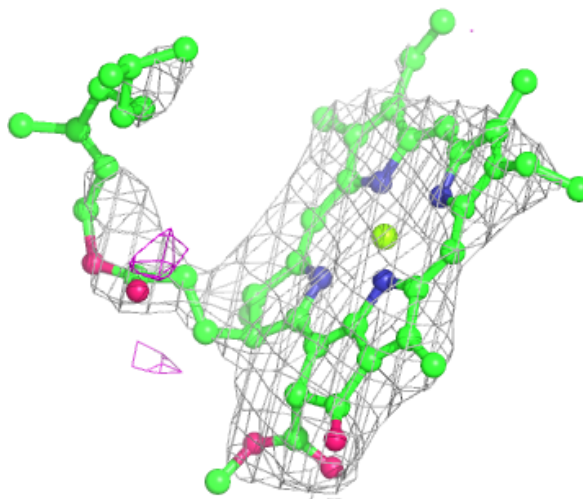
**Electron density around CLA 2 1223:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



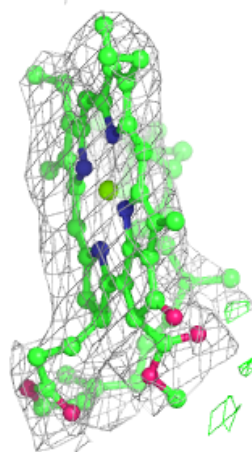
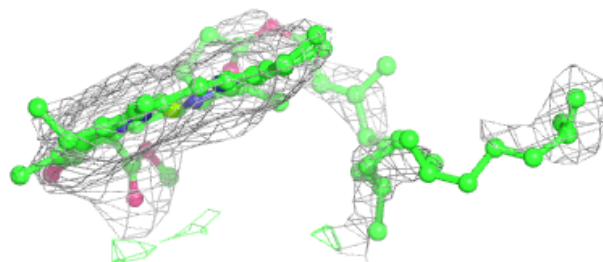
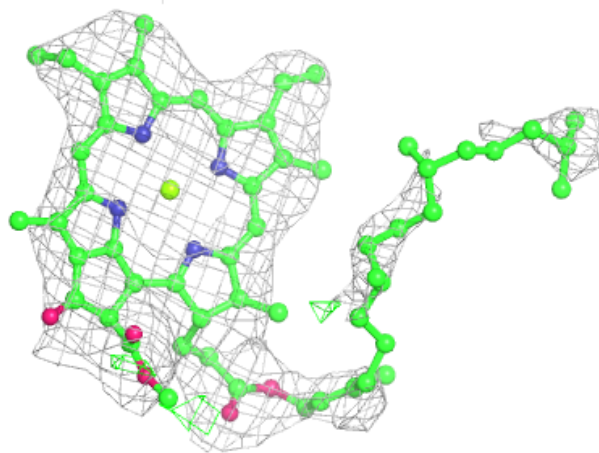
Electron density around CLA B 1227:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



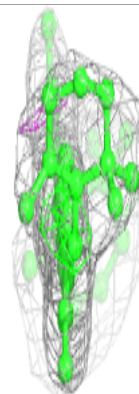
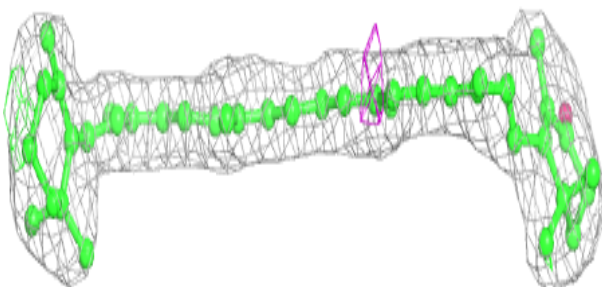
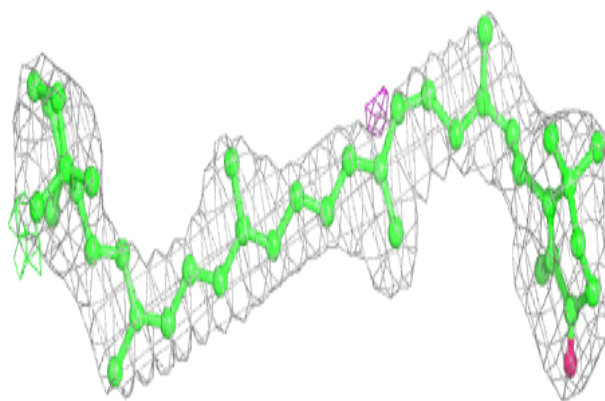
Electron density around CLA 1 1111:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



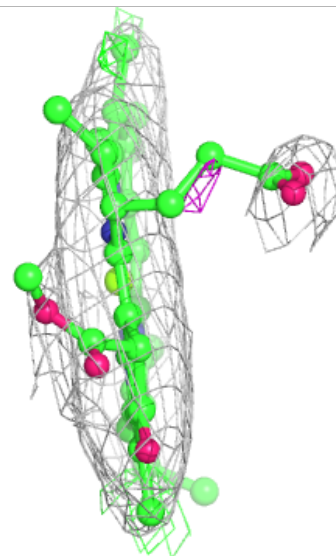
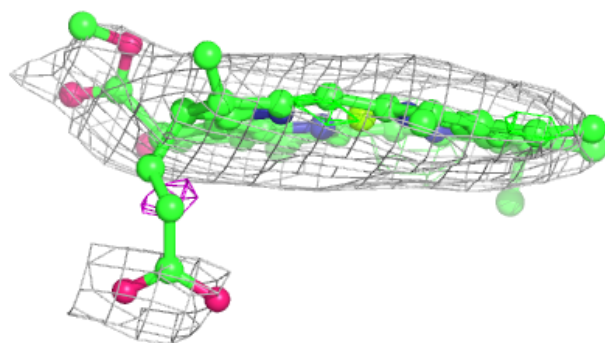
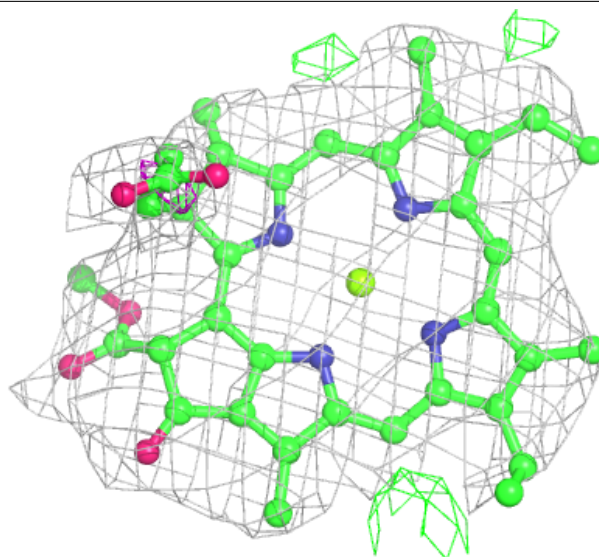
Electron density around ECH b 4006:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



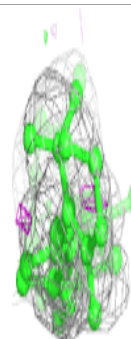
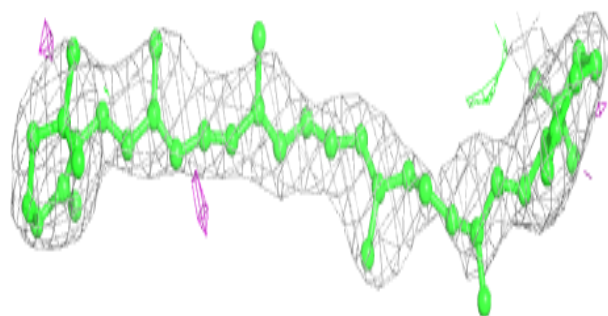
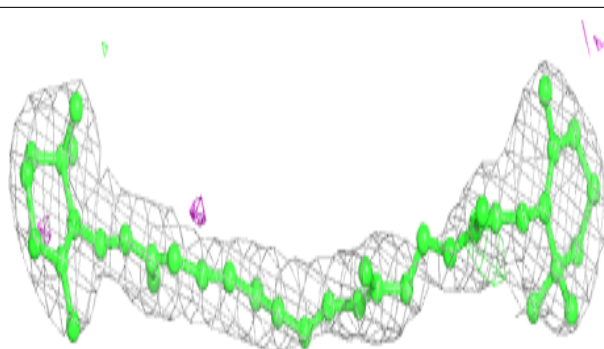
Electron density around CLA 2 1228:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

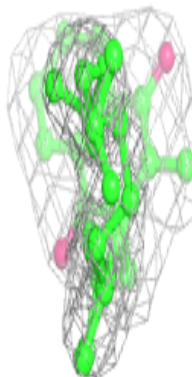
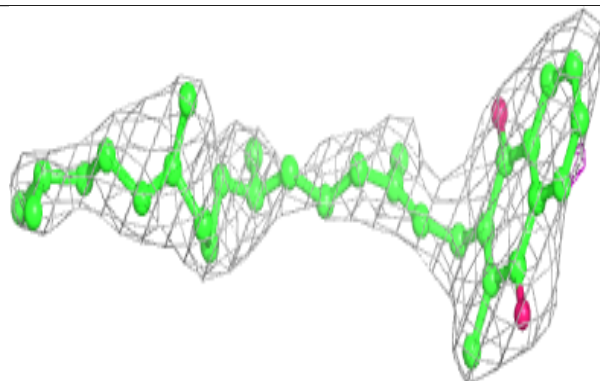
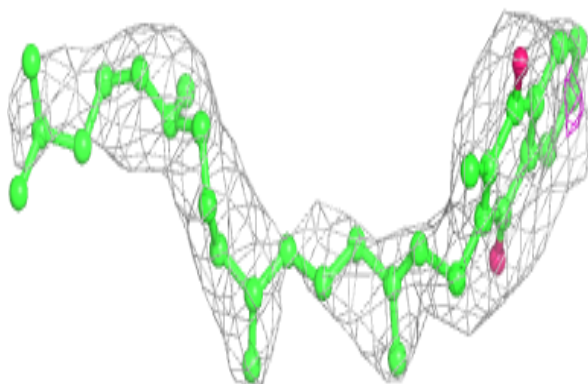


Electron density around BCR J 4013:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

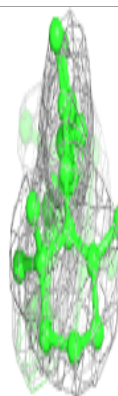
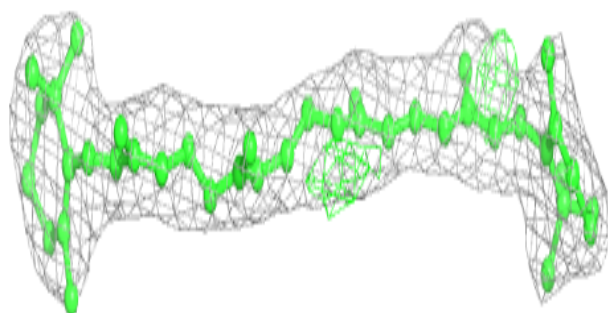
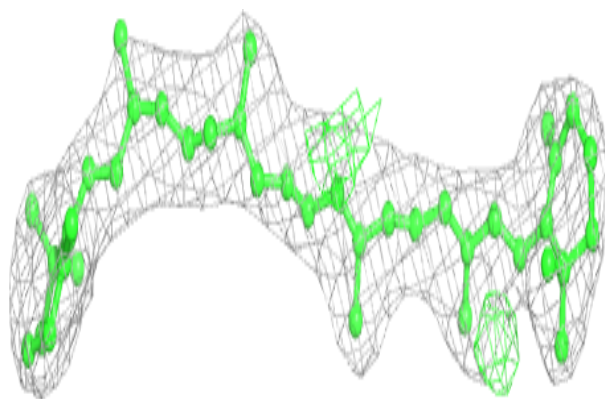
**Electron density around PQN a 2001:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

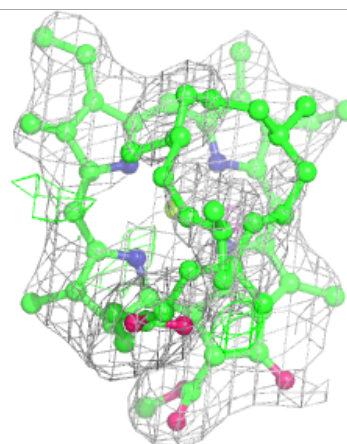
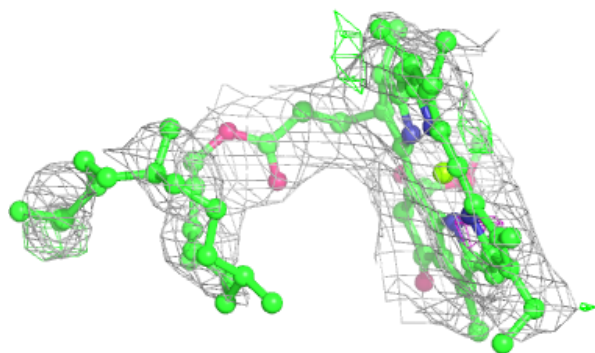
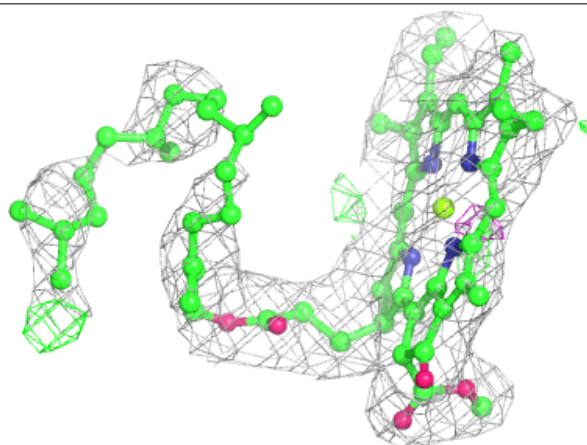


Electron density around BCR B 4017:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

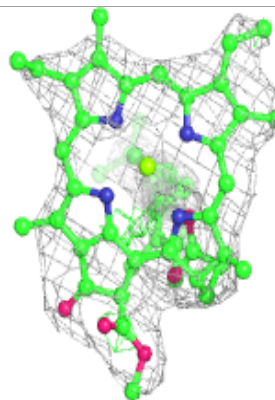
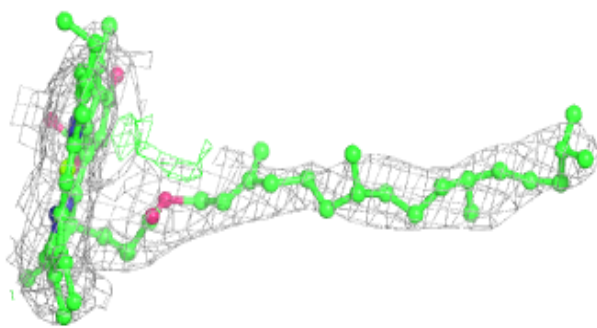
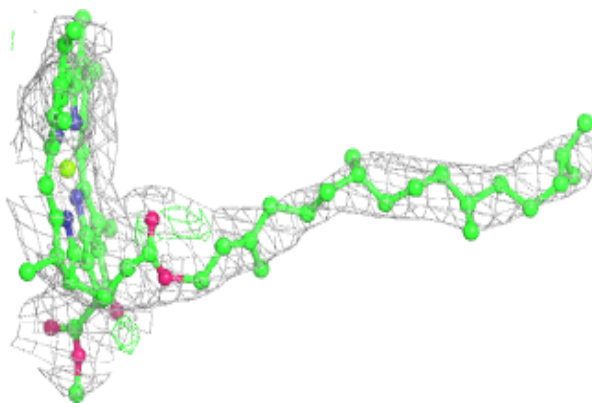
**Electron density around CLA A 1112:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



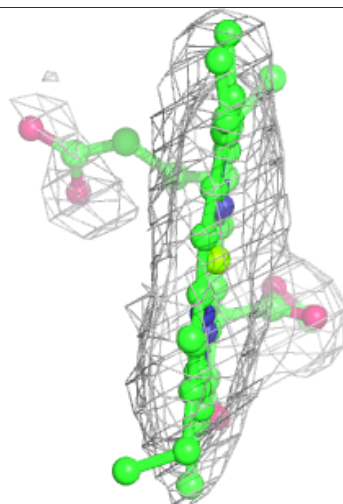
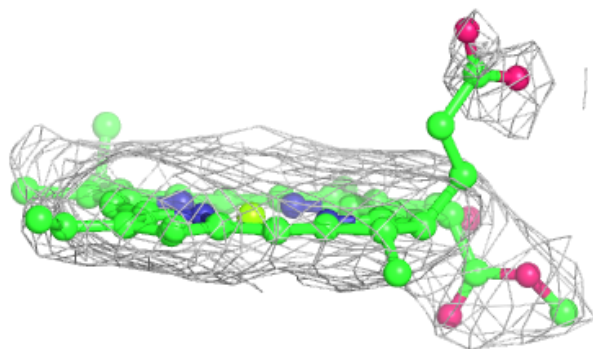
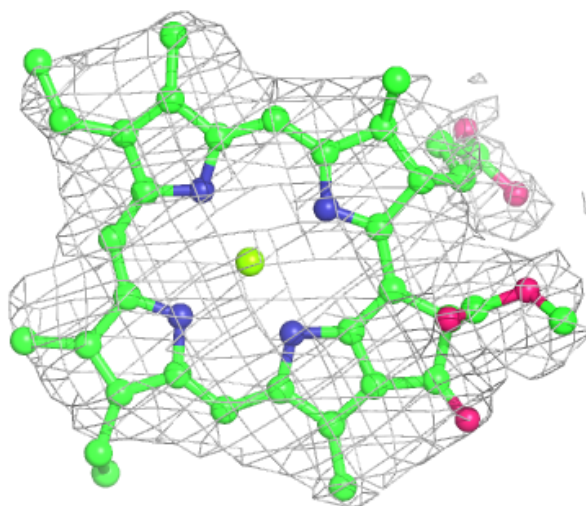
Electron density around CLA a 1126:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



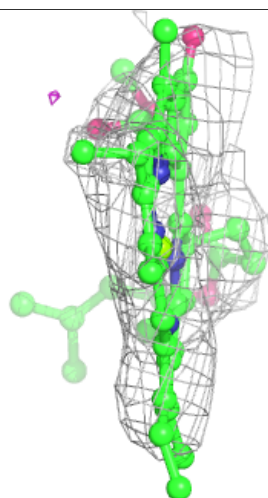
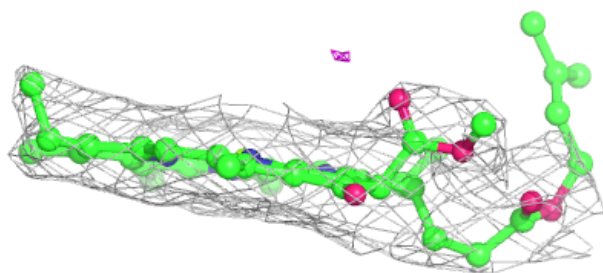
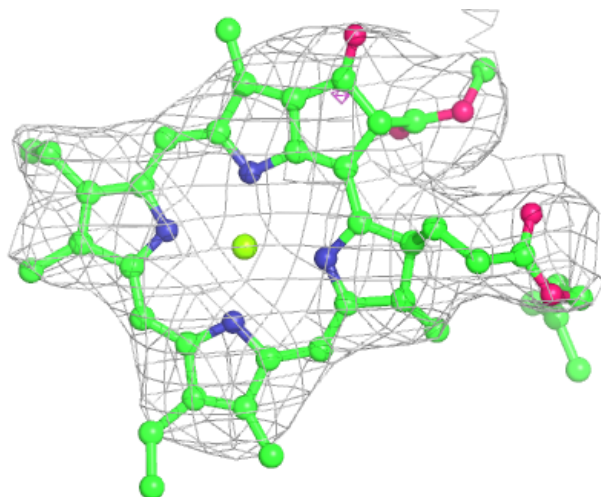
Electron density around CLA 8 1401:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



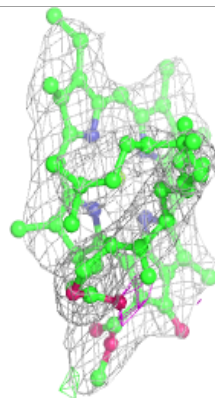
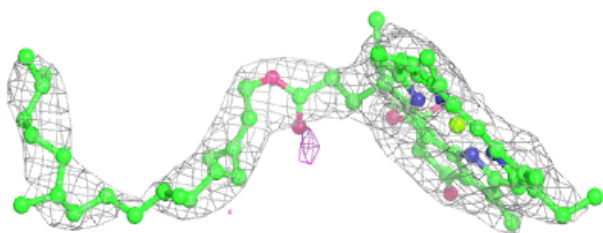
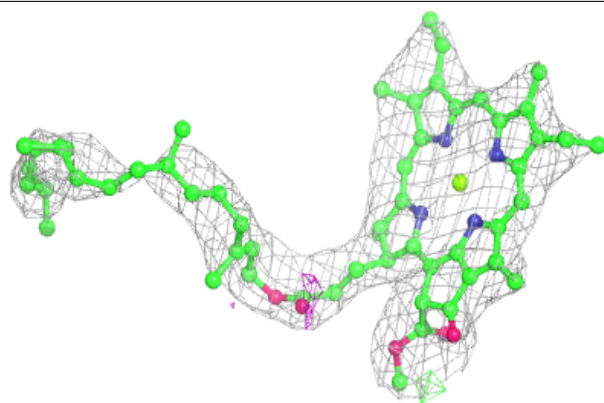
Electron density around CLA f 1301:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

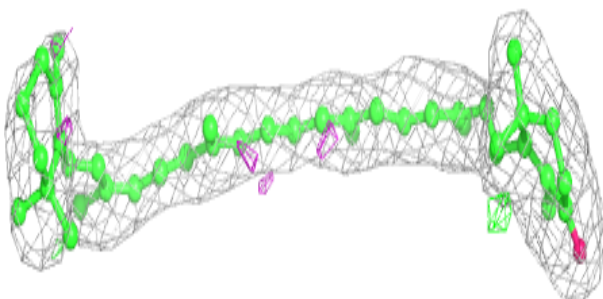
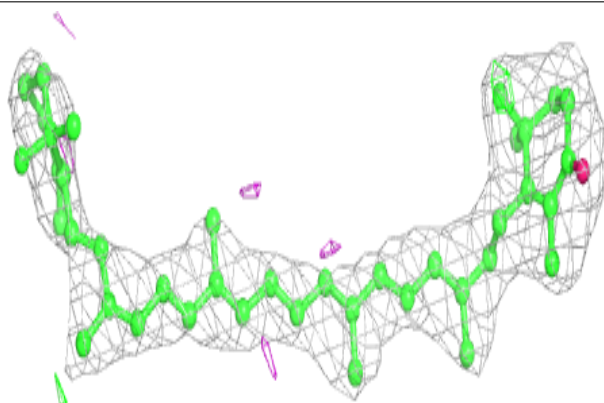


Electron density around CLA 2 1206:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

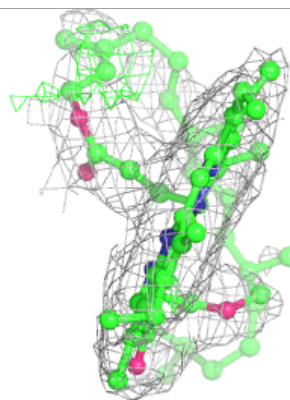
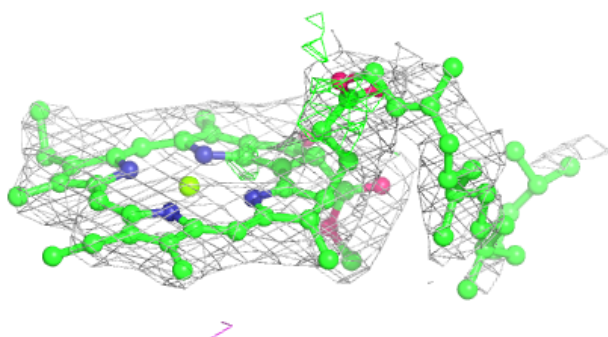
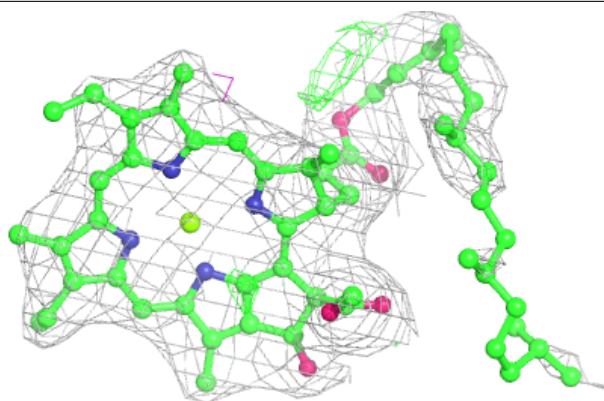
**Electron density around ECH m 4021:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

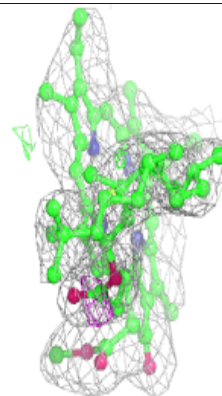
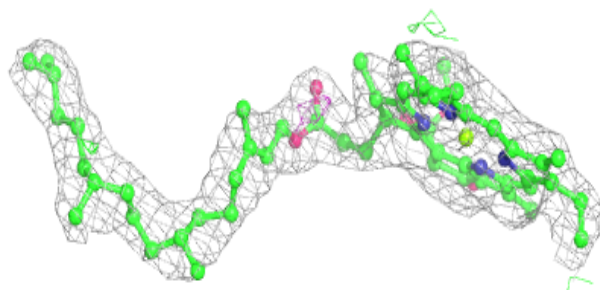
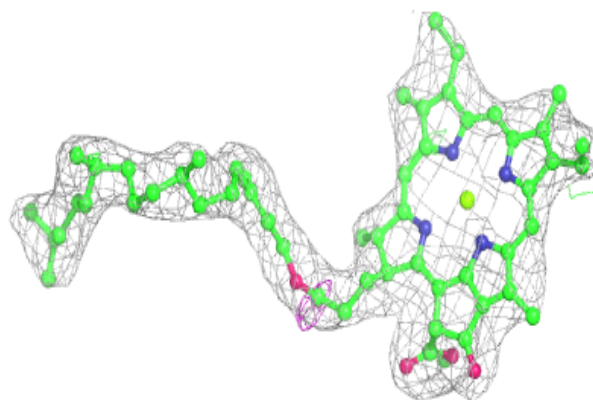


Electron density around CLA K 1402:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

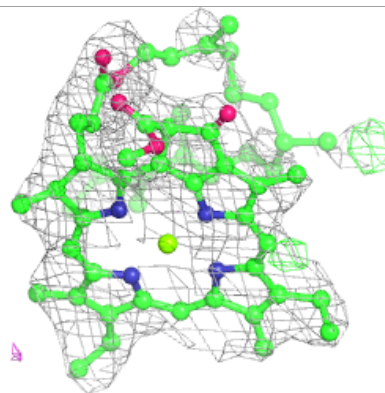
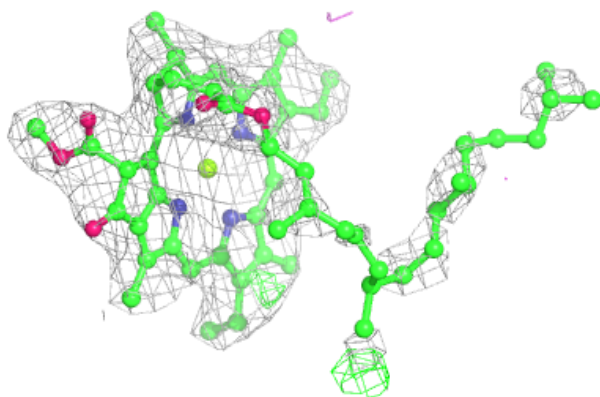
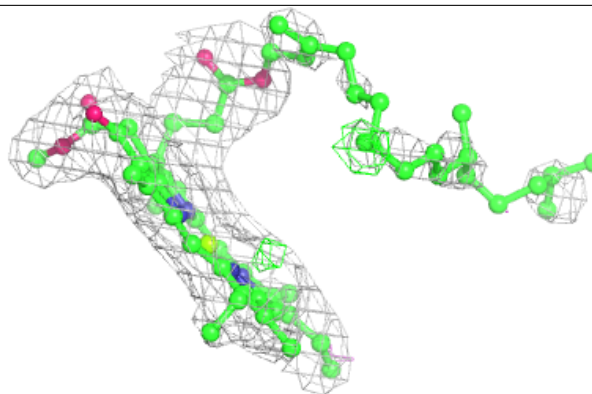
**Electron density around CLA B 1210:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



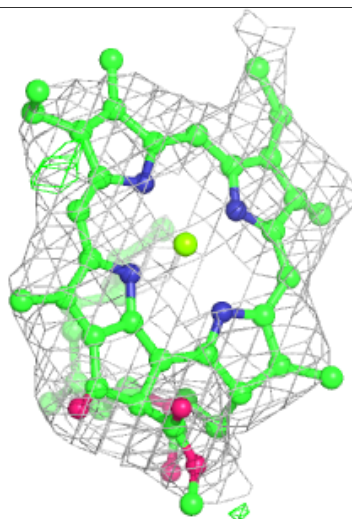
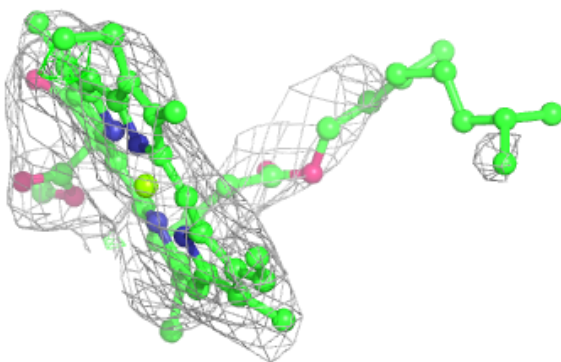
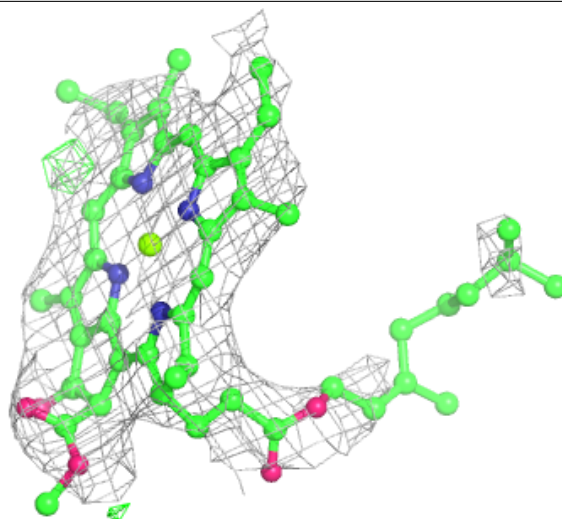
Electron density around CLA B 1211:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



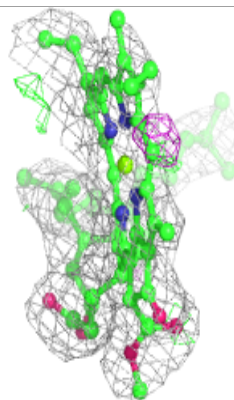
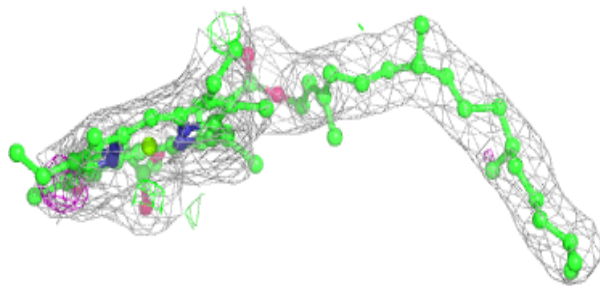
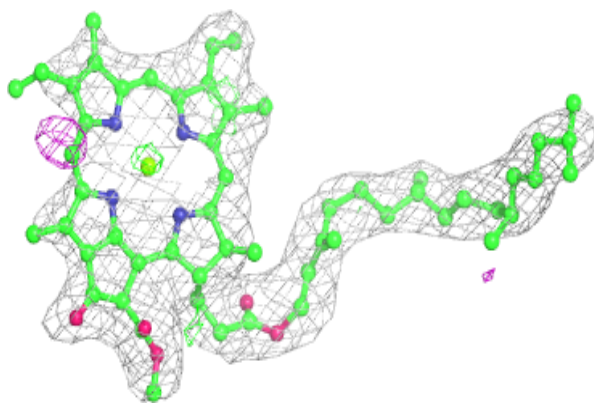
Electron density around CLA B 1212:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



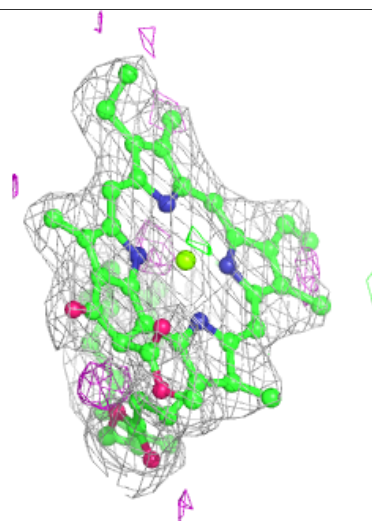
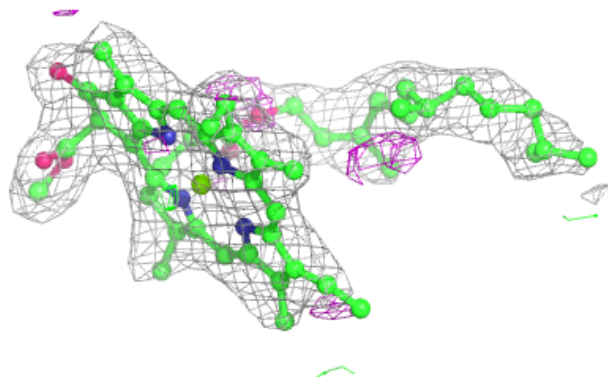
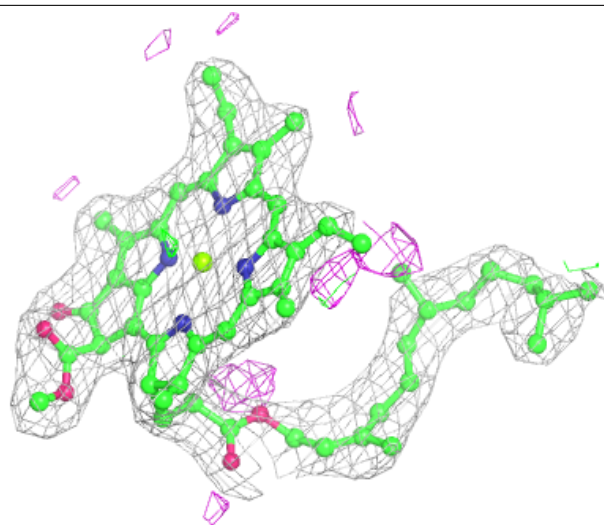
Electron density around CLA 2 1023:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



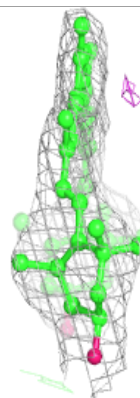
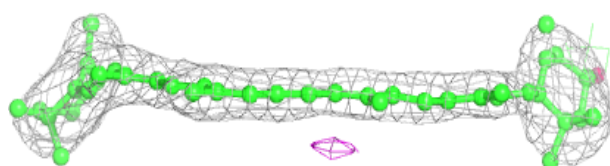
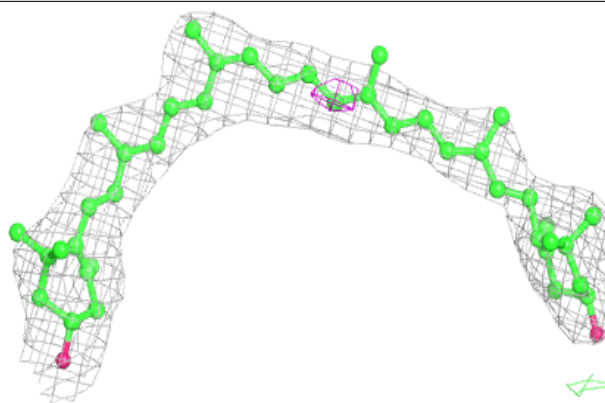
Electron density around CLA A 1122:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

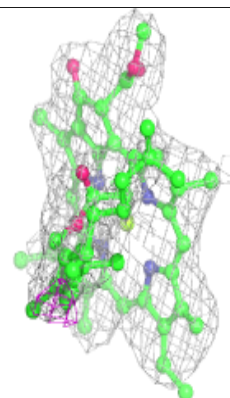
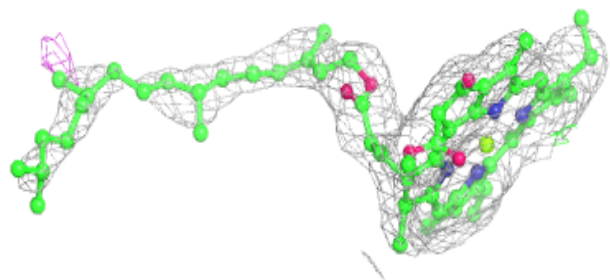
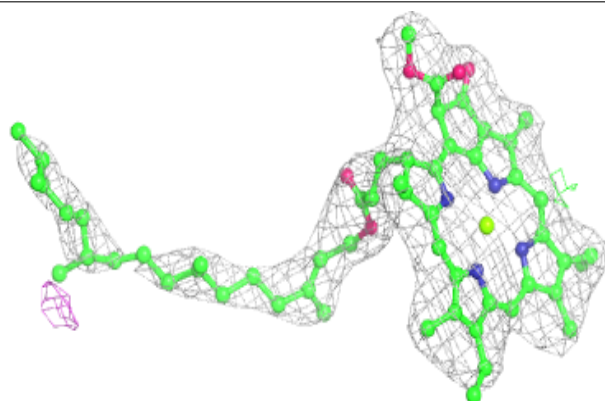


Electron density around ZEX F 4016:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

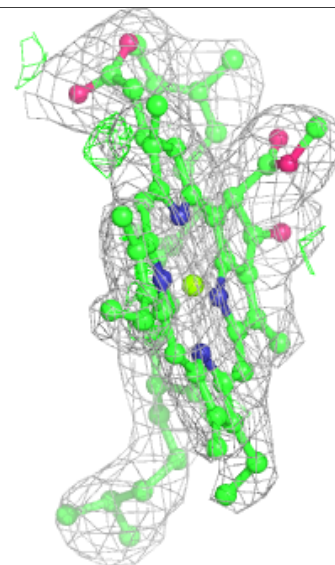
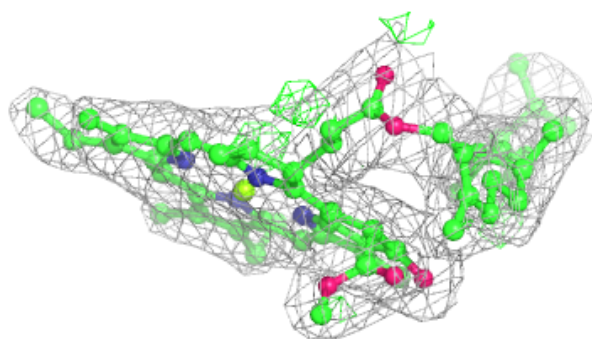
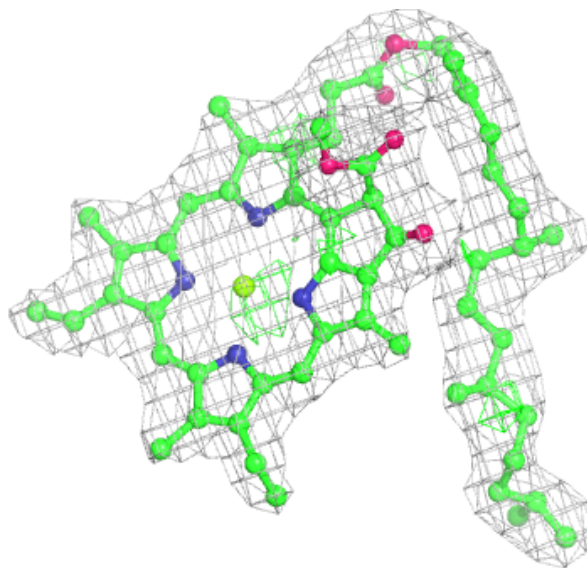
**Electron density around CLA 1 1119:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



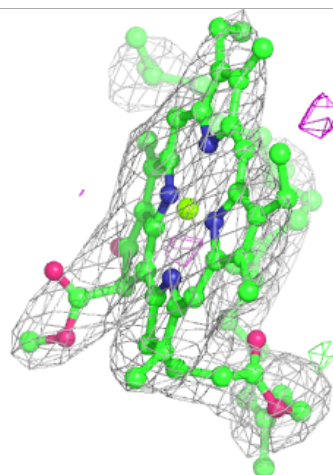
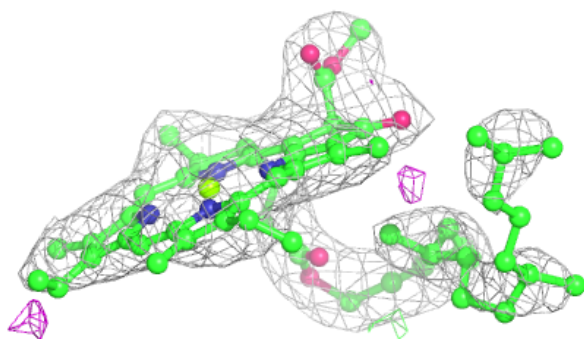
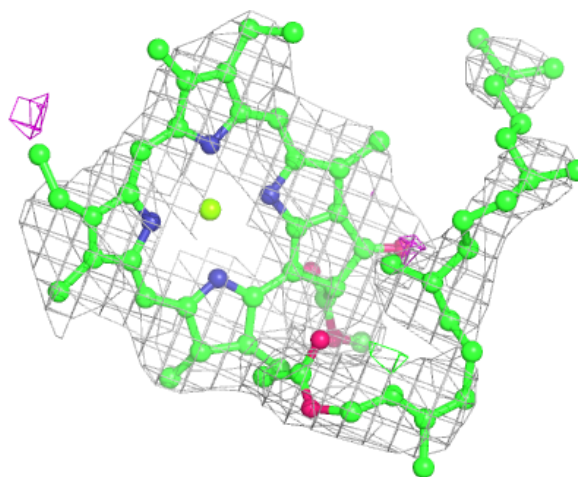
Electron density around CLA A 1123:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



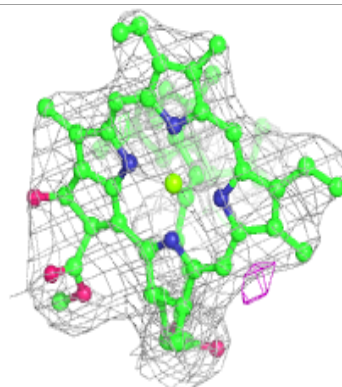
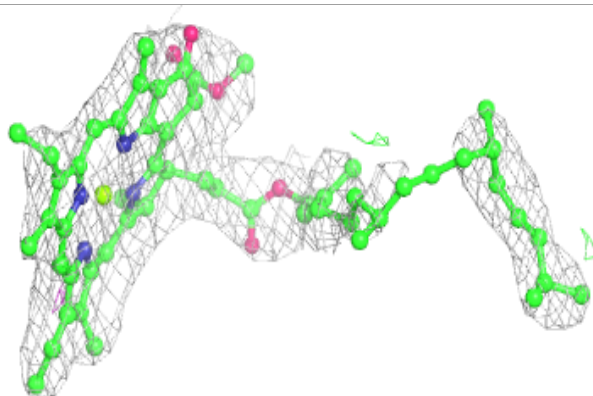
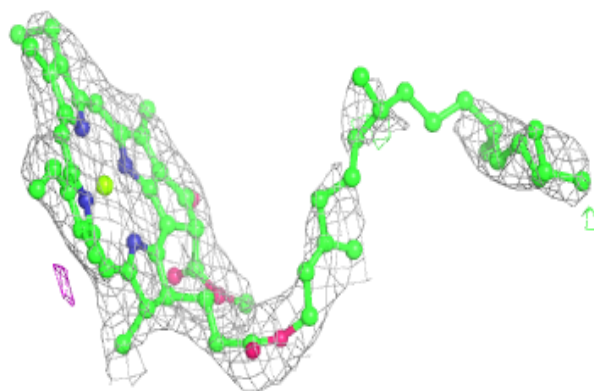
Electron density around CLA b 1229:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

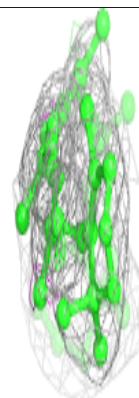
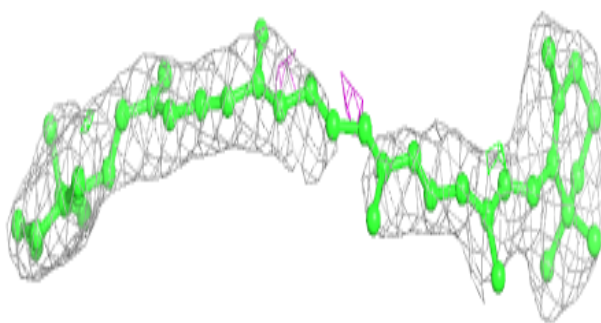
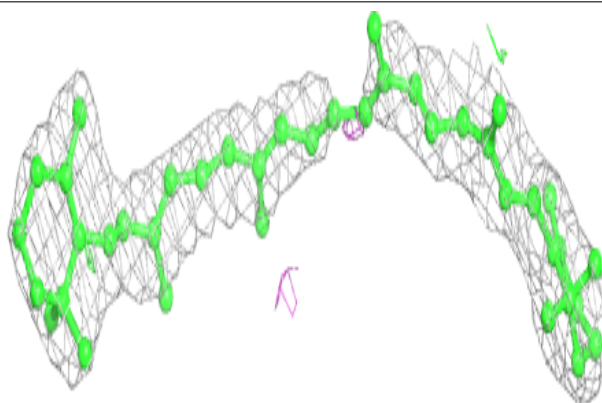


Electron density around CLA 2 1021:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

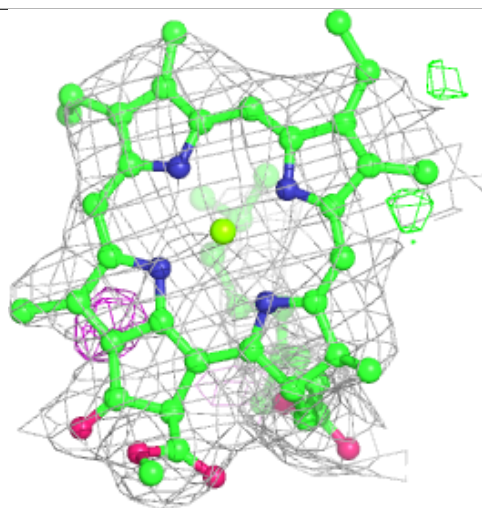
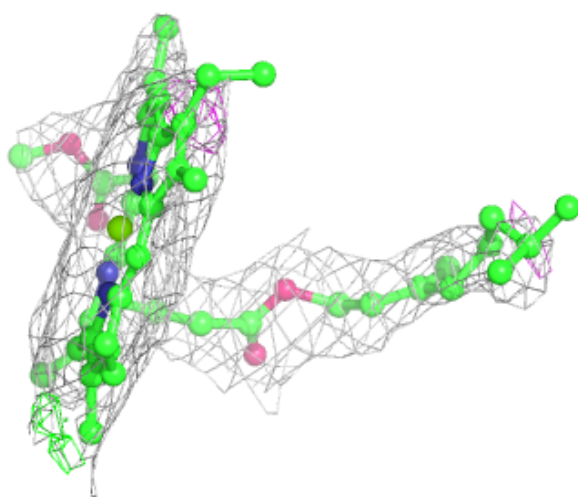
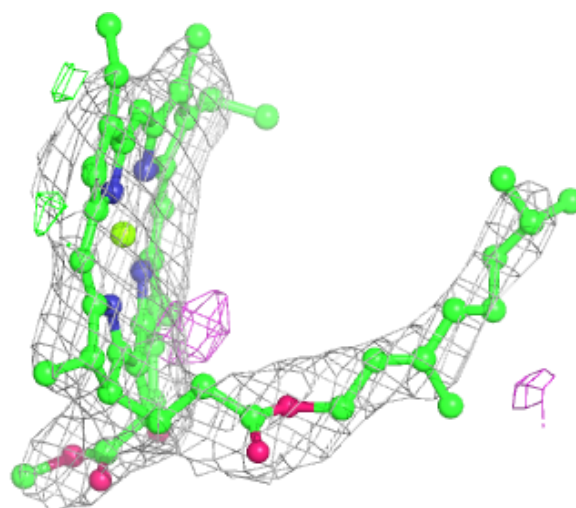
**Electron density around BCR B 4014:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



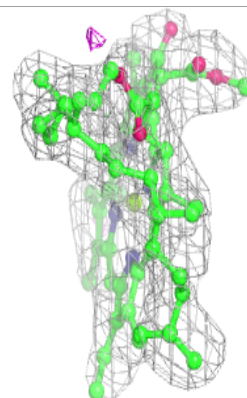
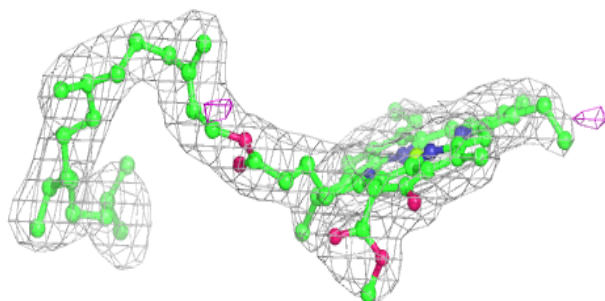
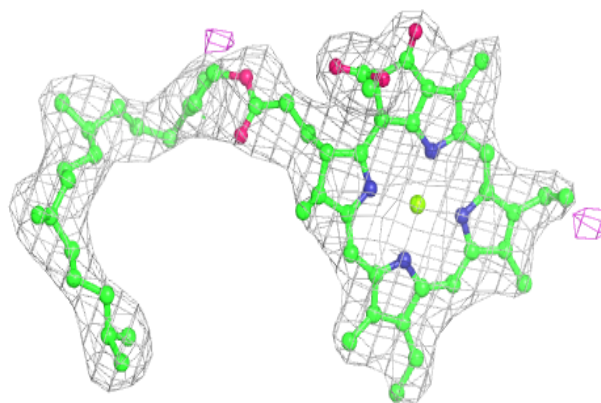
Electron density around CLA 2 1226:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

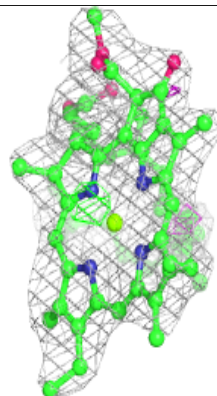
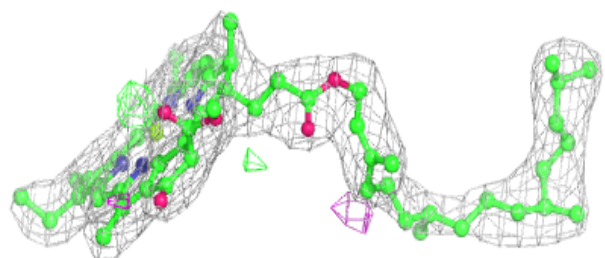
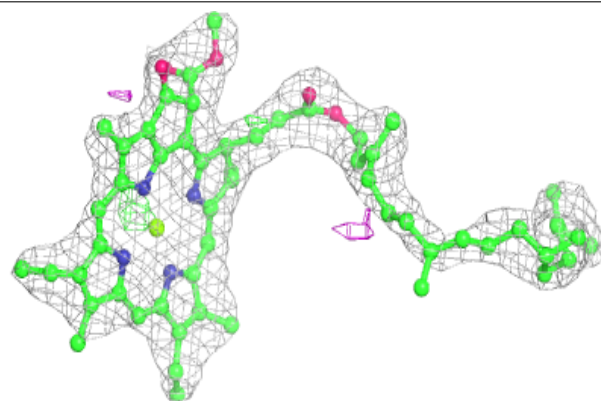


Electron density around CLA A 1125:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

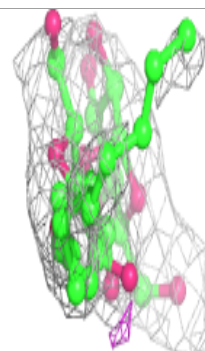
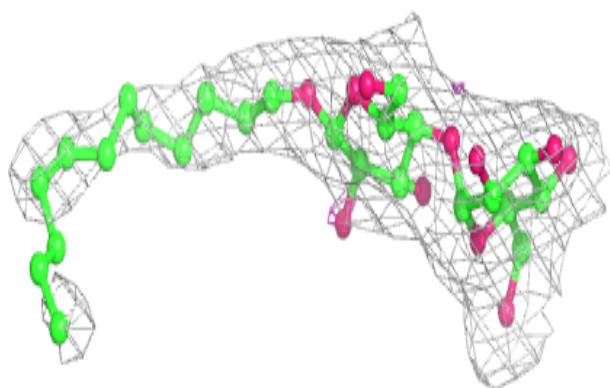
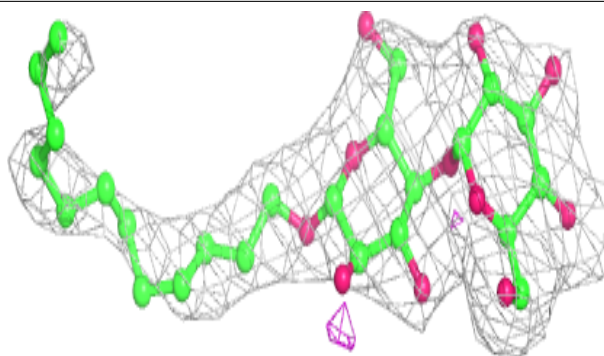
**Electron density around CLA b 1206:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

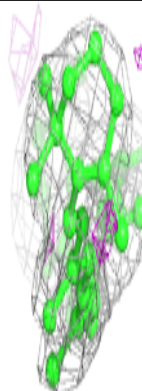
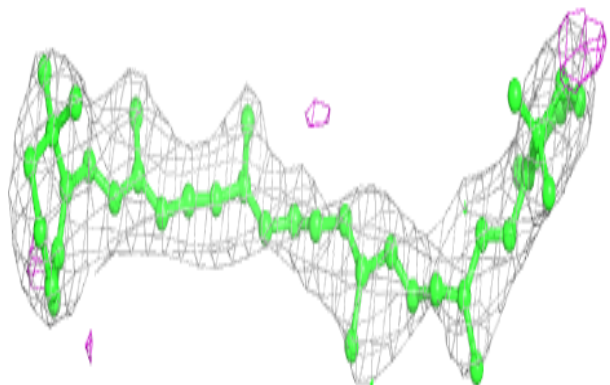
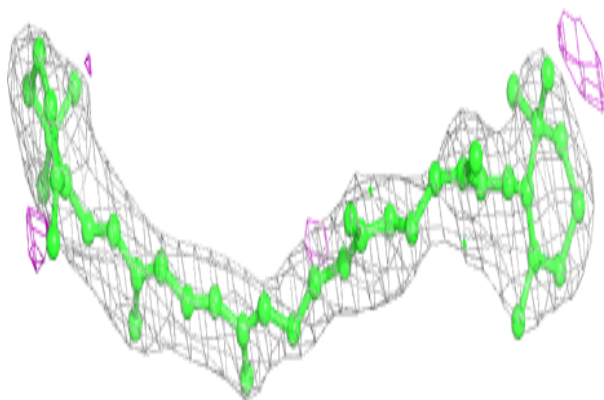


Electron density around LMT 0 6001:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

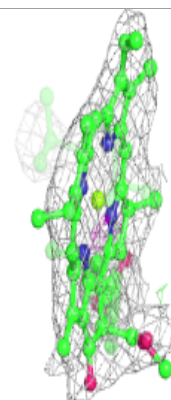
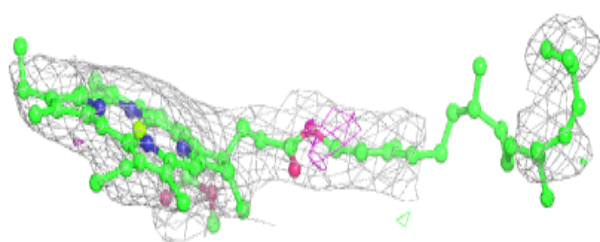
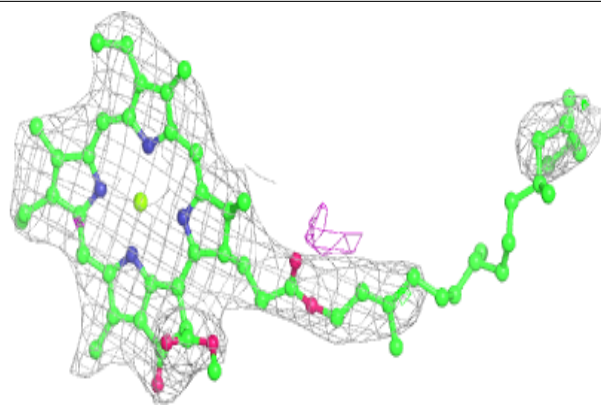
**Electron density around BCR h 4018:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

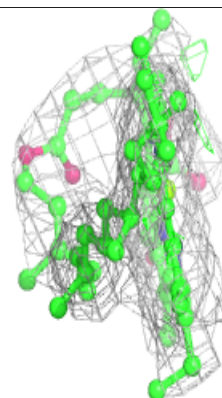
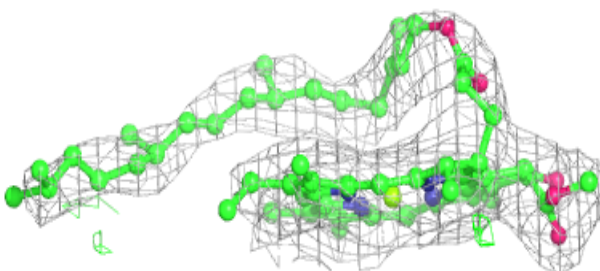
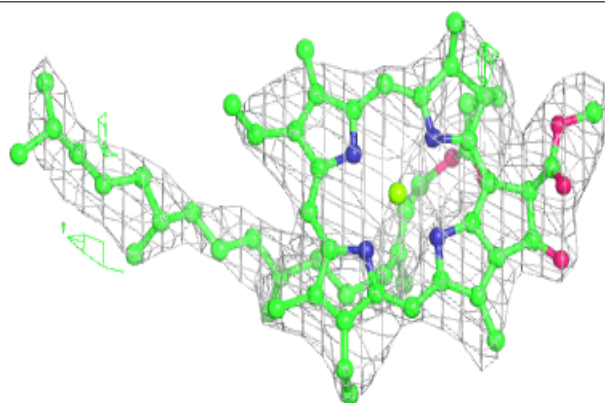


Electron density around CLA a 1135:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

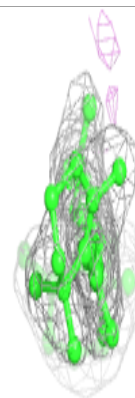
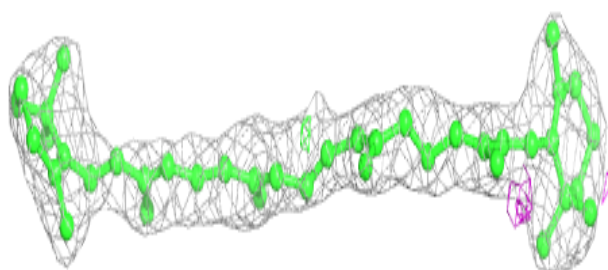
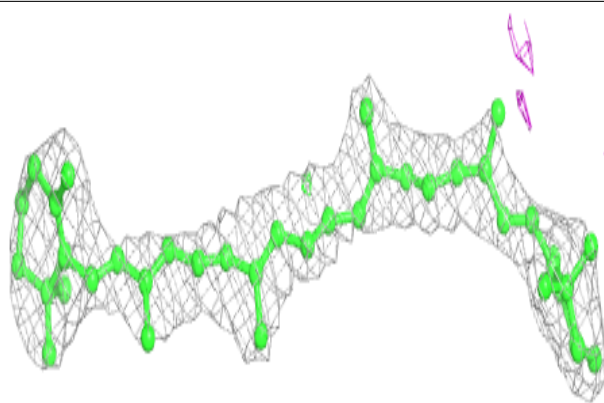
**Electron density around CLA a 1138:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

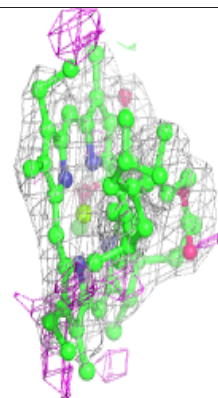
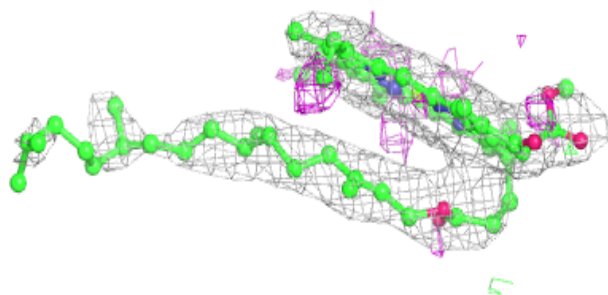
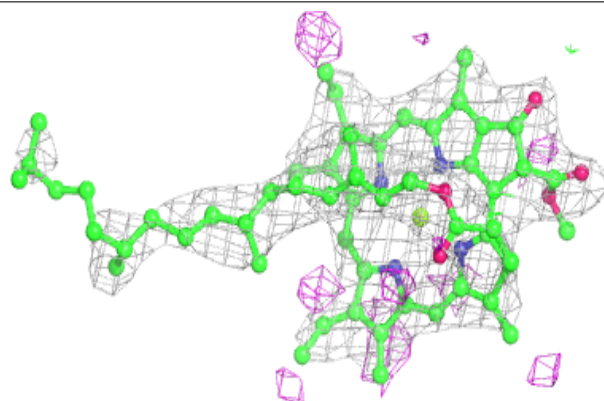


Electron density around BCR b 4017:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

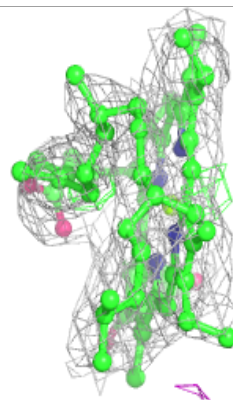
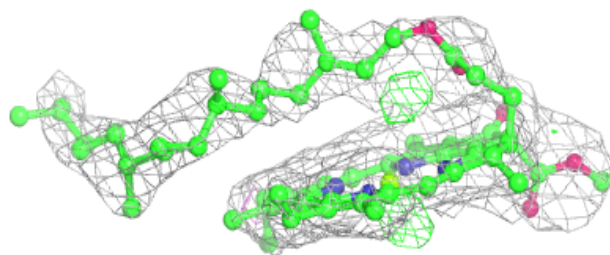
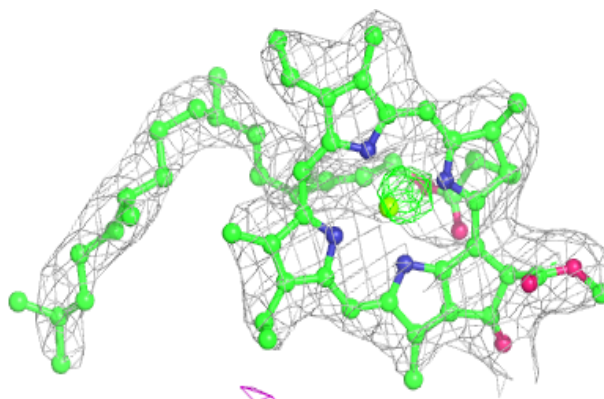
**Electron density around CLA b 1213:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

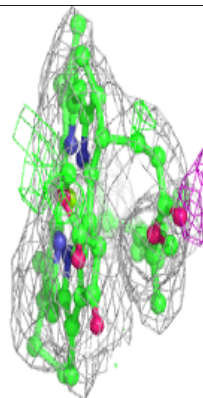
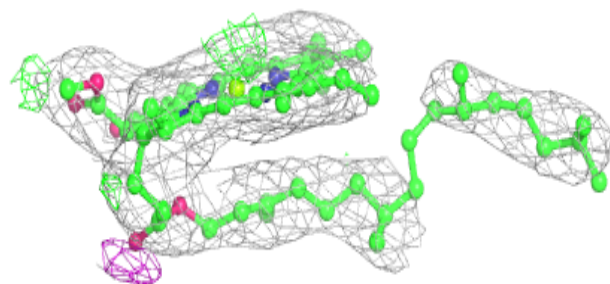
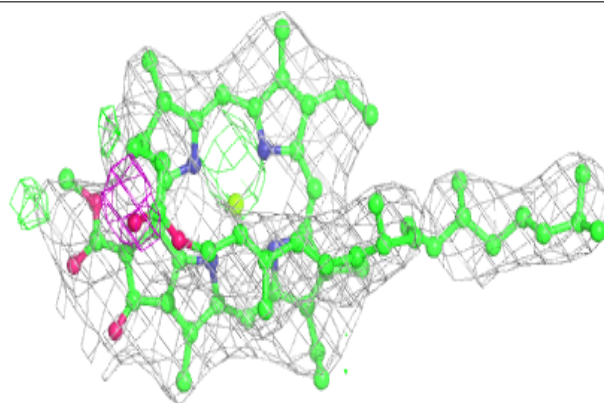


Electron density around CLA b 1235:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

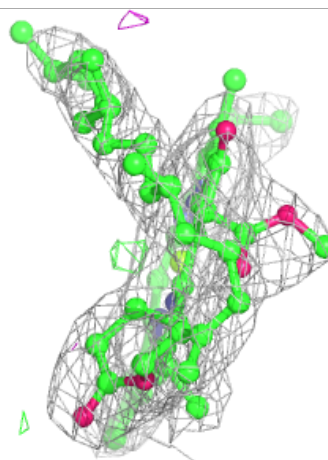
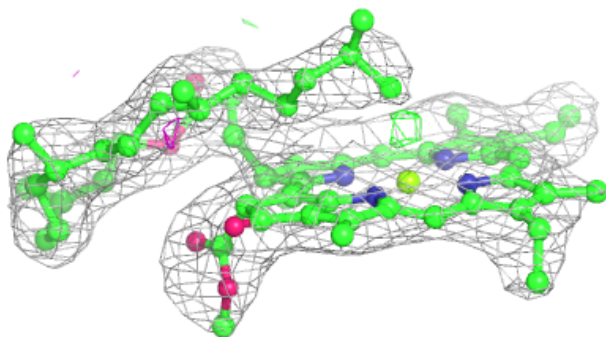
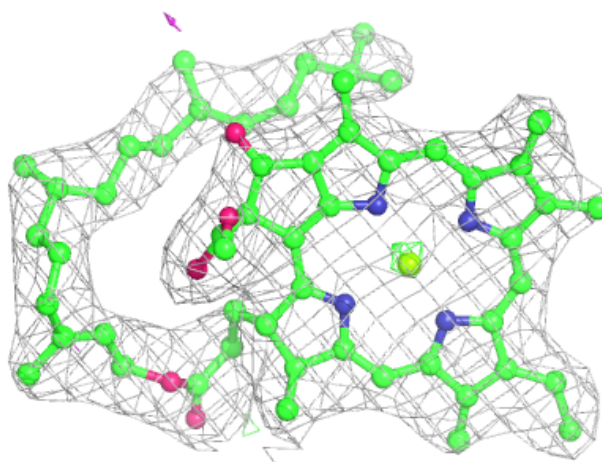
**Electron density around CLA a 1136:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



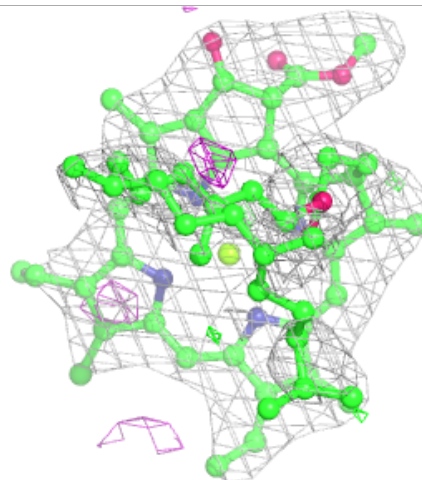
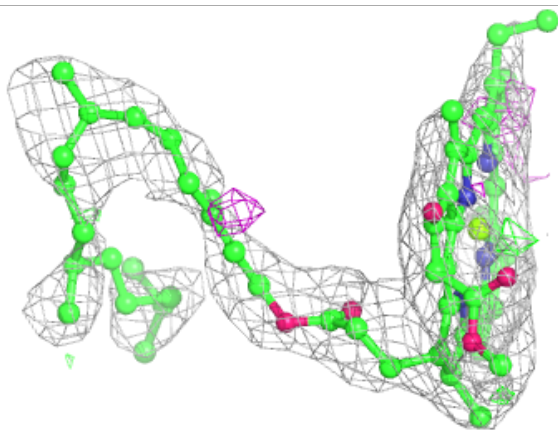
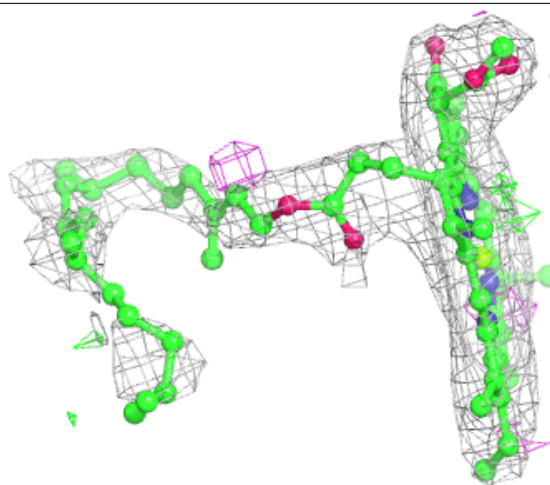
Electron density around CLA B 1202:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



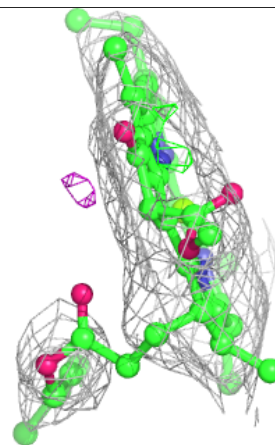
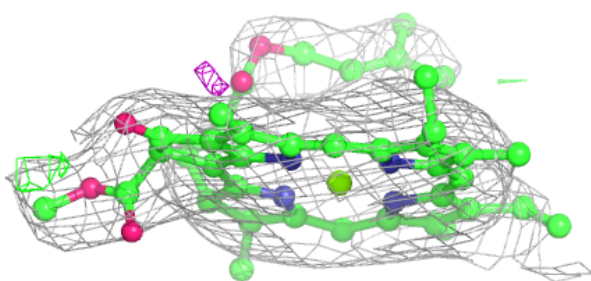
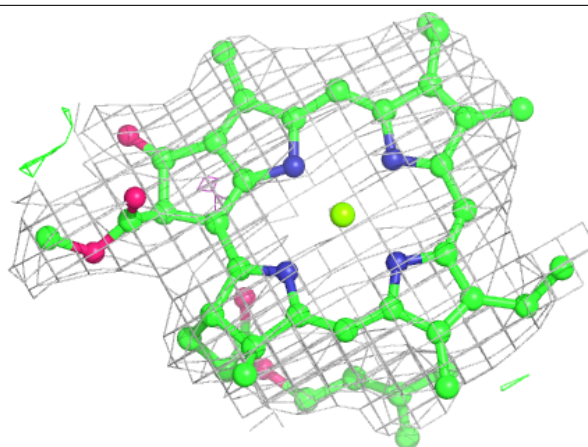
Electron density around CLA A 1134:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

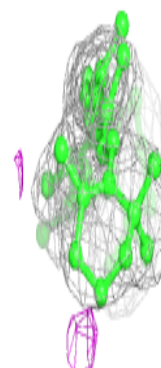
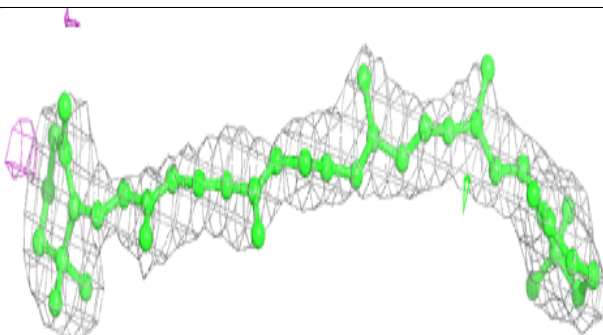
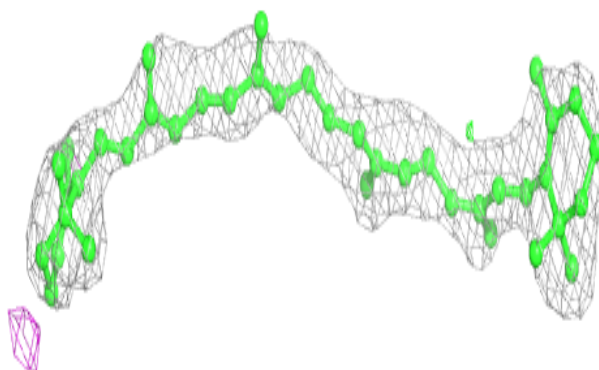


Electron density around CLA 1 1110:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

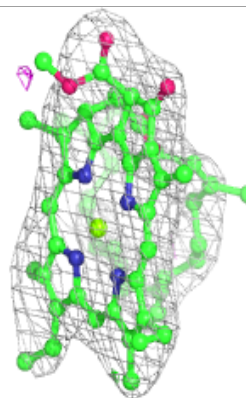
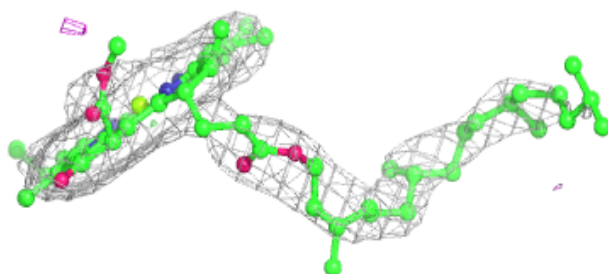
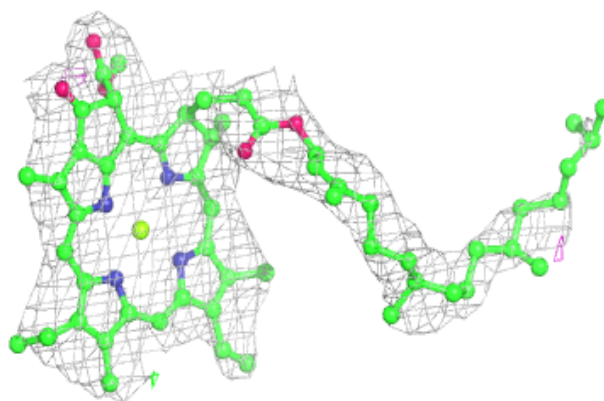
**Electron density around BCR i 4018:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

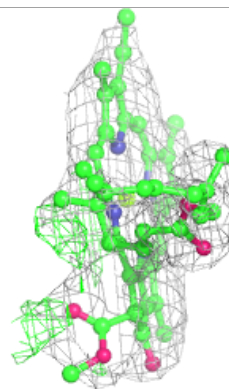
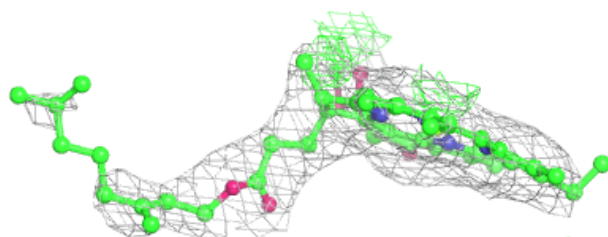
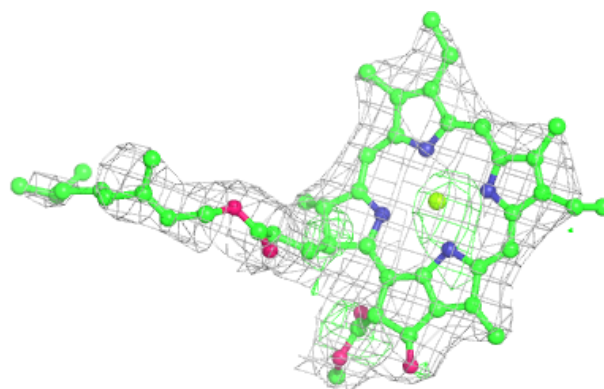


Electron density around CLA 1 1106:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

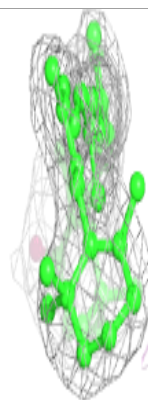
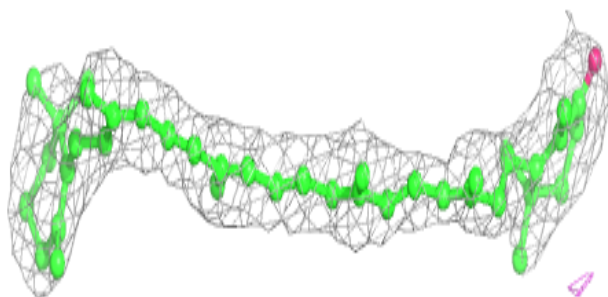
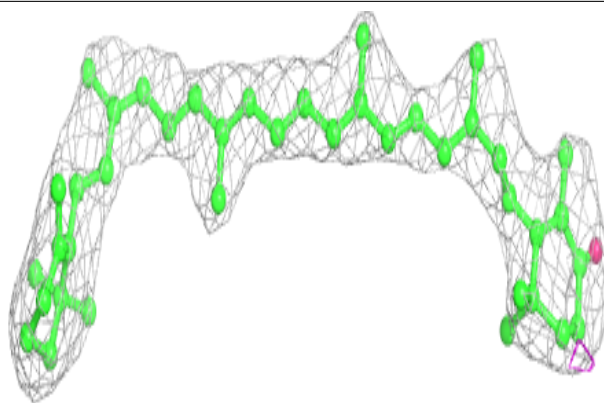
**Electron density around CLA B 1222:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

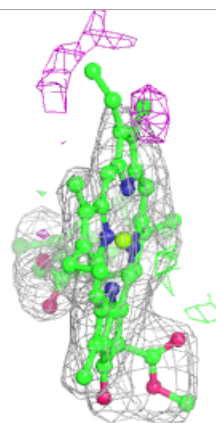
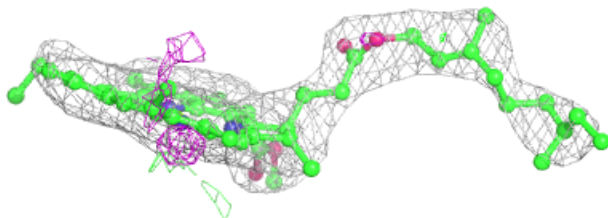
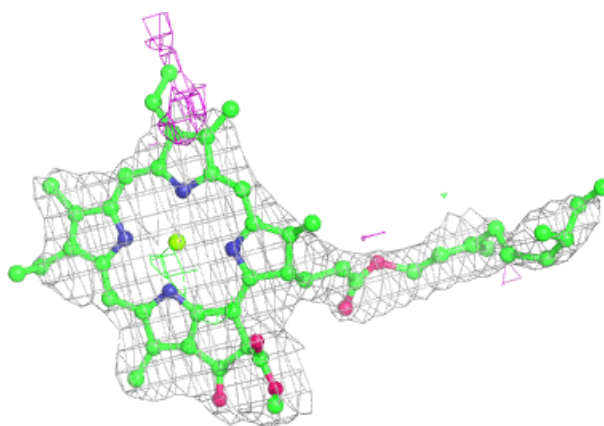


Electron density around ECH M 4021:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

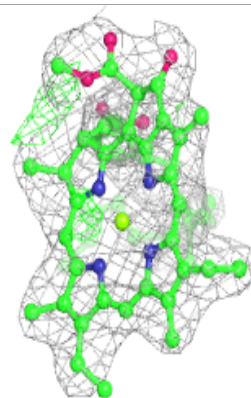
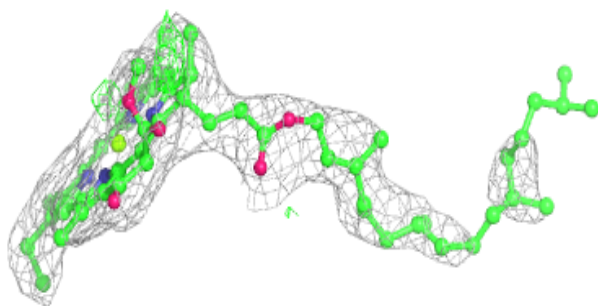
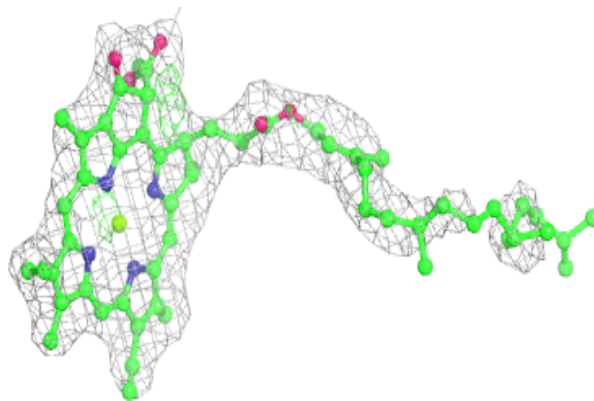
**Electron density around CLA 1 1124:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

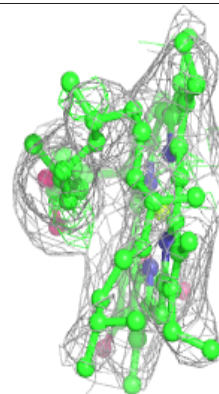
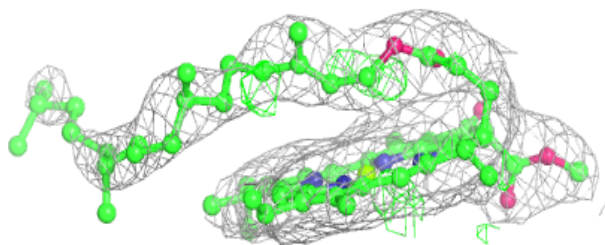
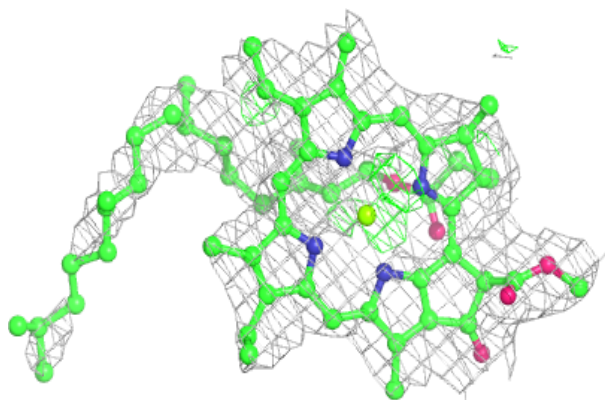


Electron density around CLA B 1230:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

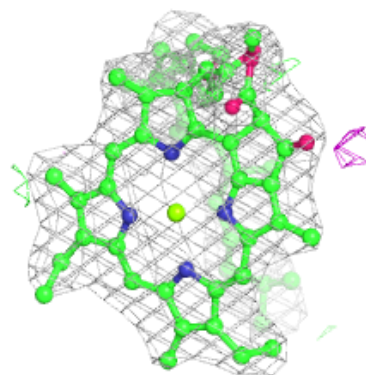
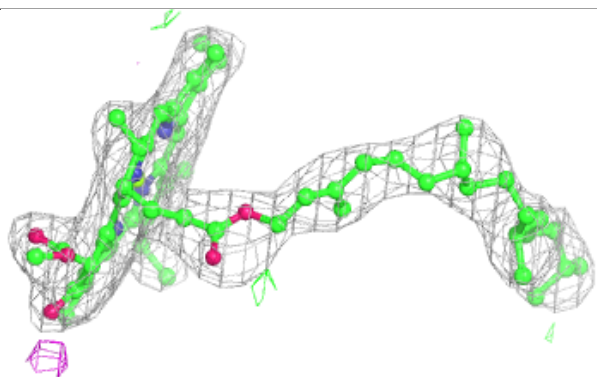
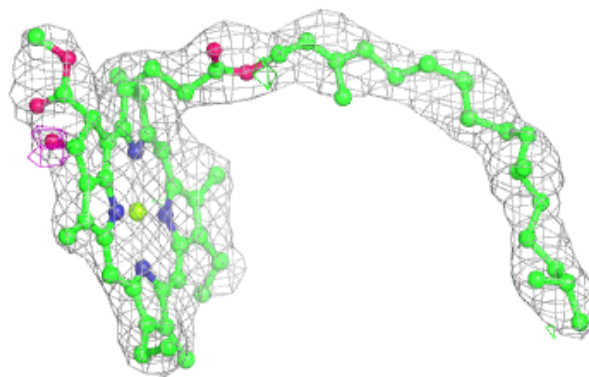
**Electron density around CLA B 1235:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

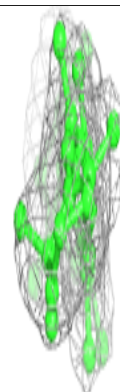
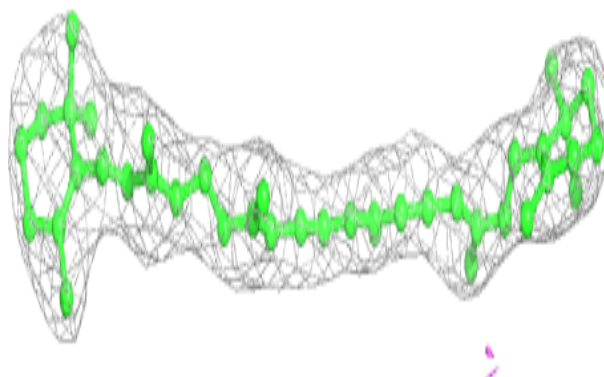
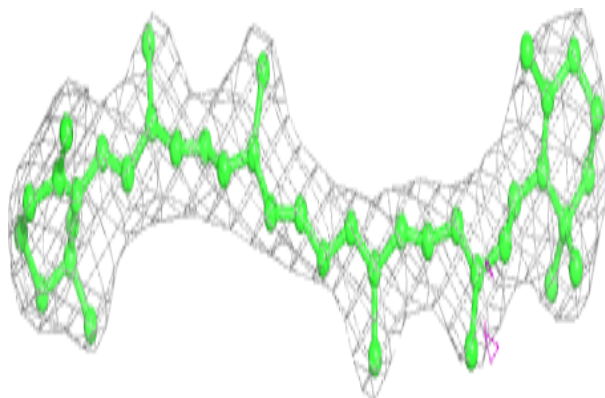


Electron density around CLA A 1133:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

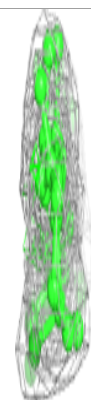
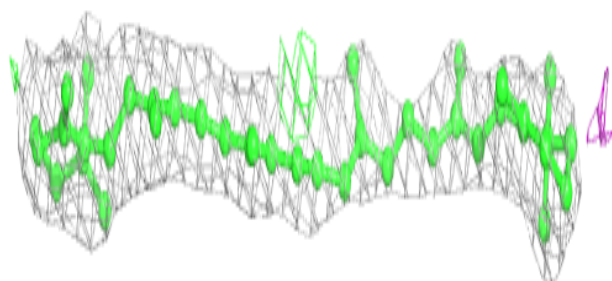
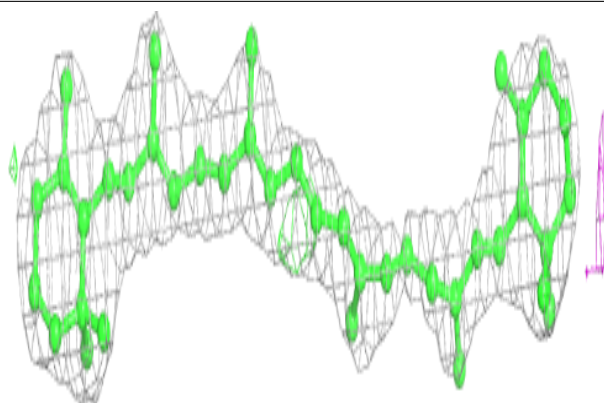
**Electron density around BCR A 4012:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

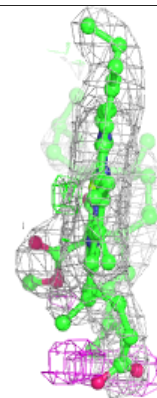
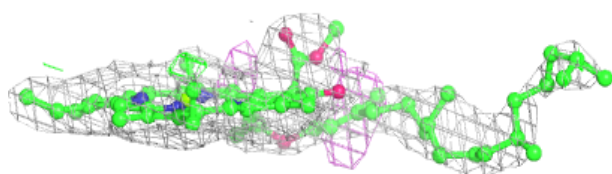
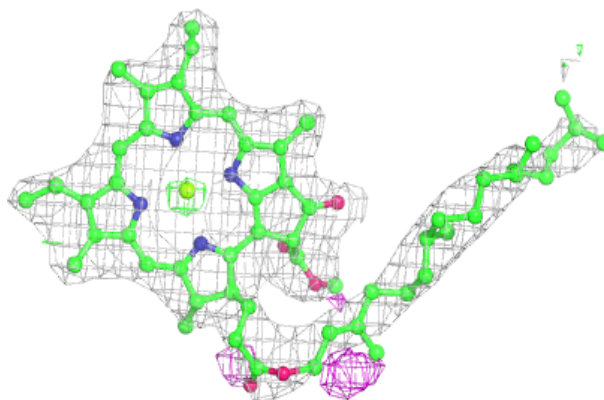


Electron density around BCR 0 4019:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

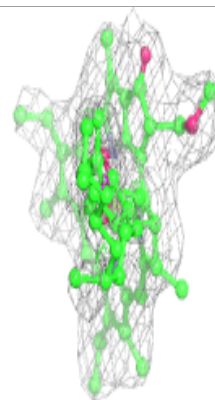
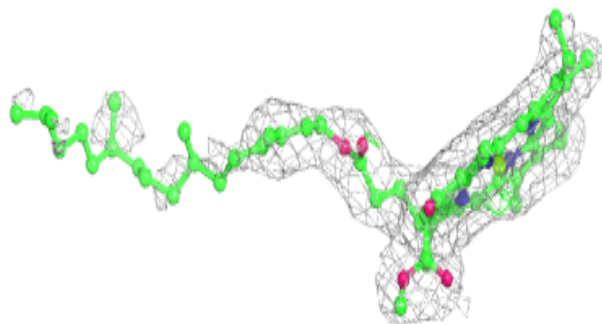
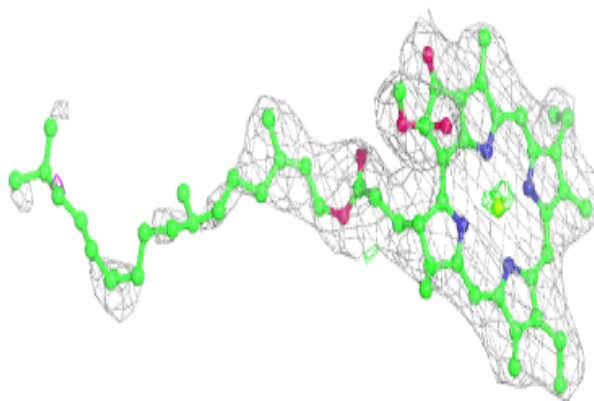
**Electron density around CLA L 1503:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

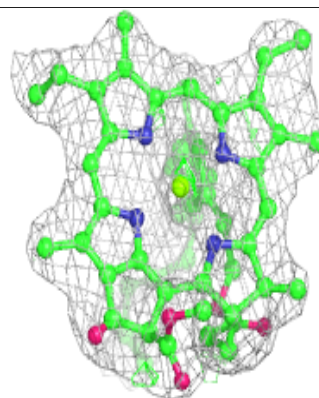
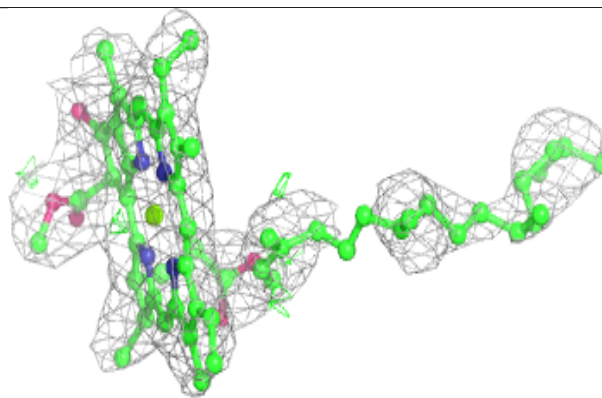
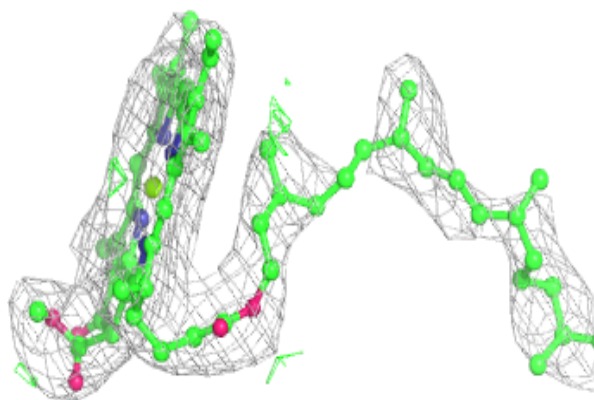


Electron density around CLA A 1107:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

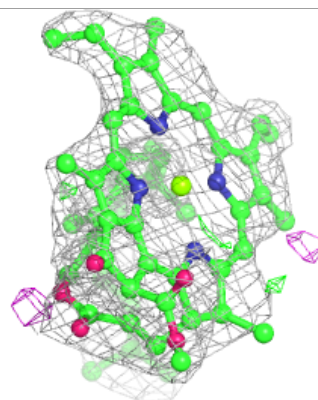
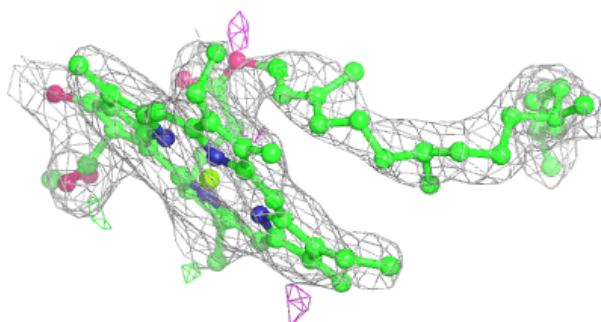
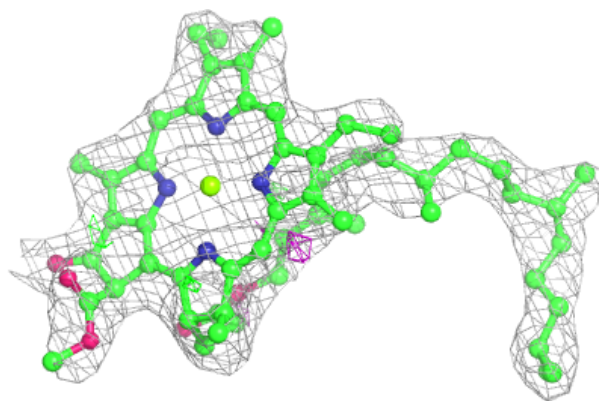
**Electron density around CLA A 1120:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

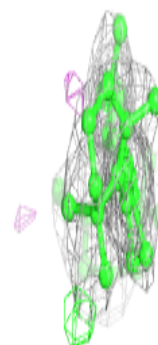
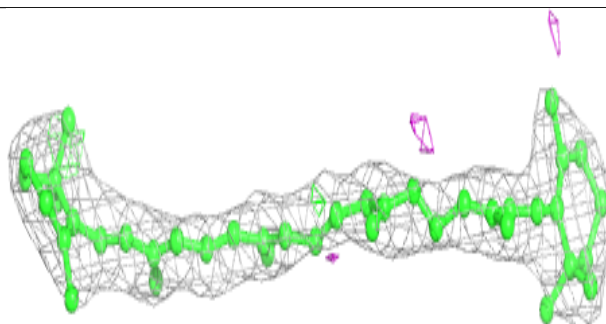
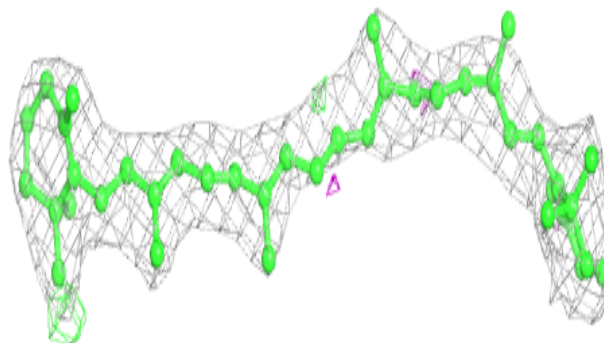


Electron density around CLA b 1237:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

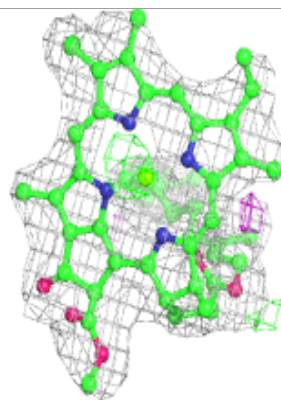
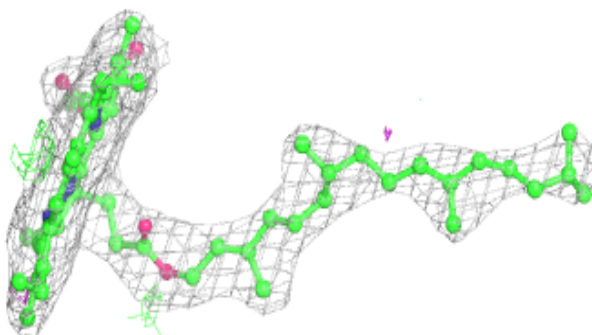
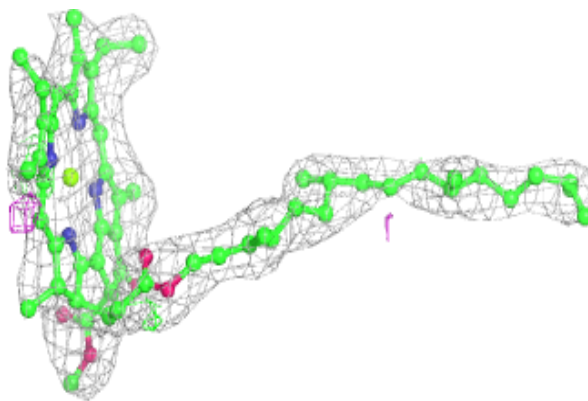
**Electron density around BCR 2 4017:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



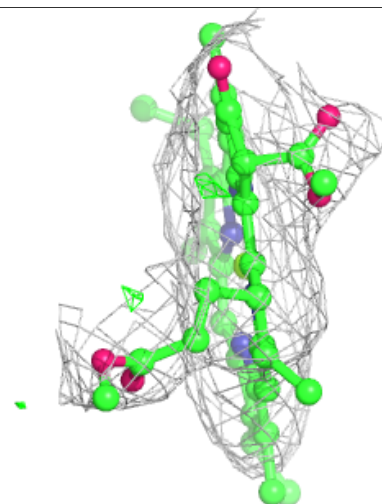
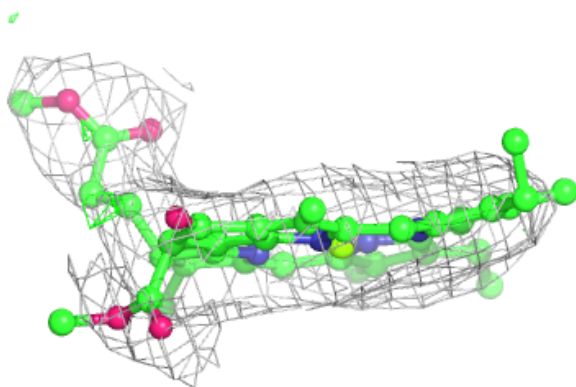
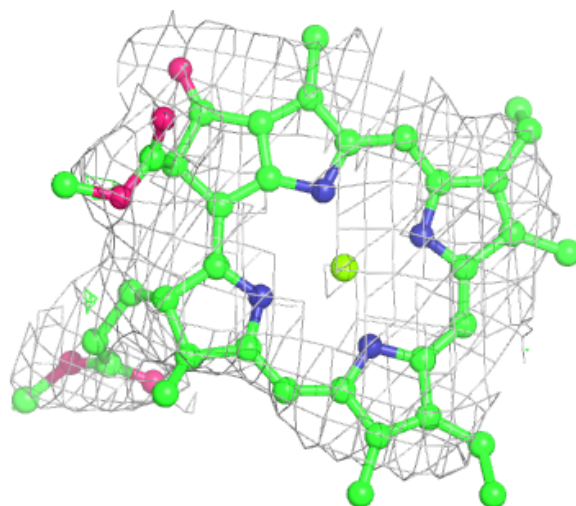
Electron density around CLA B 1225:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



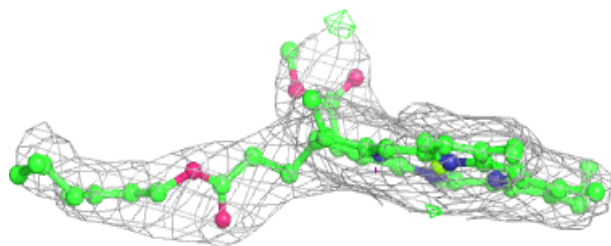
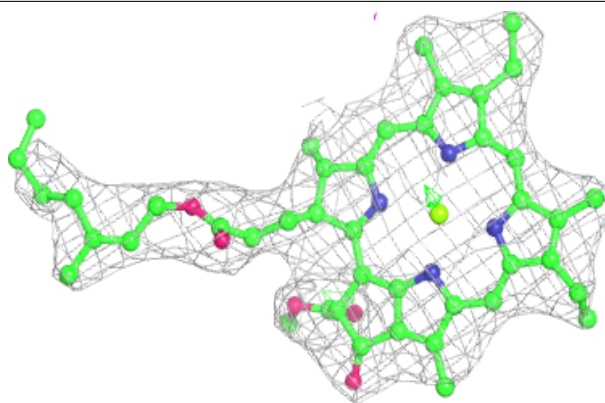
Electron density around CLA 8 1402:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

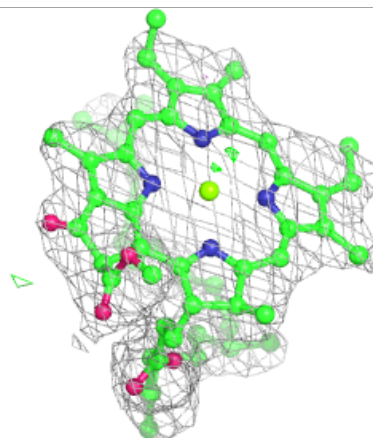
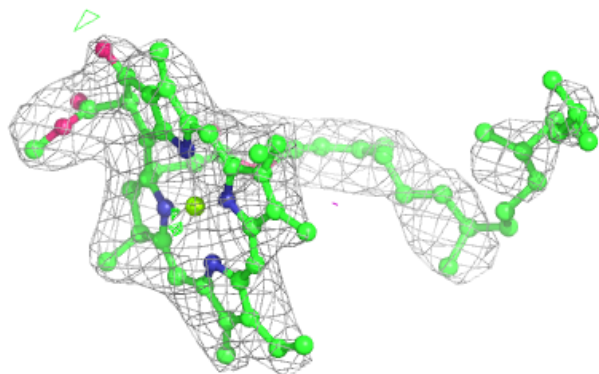
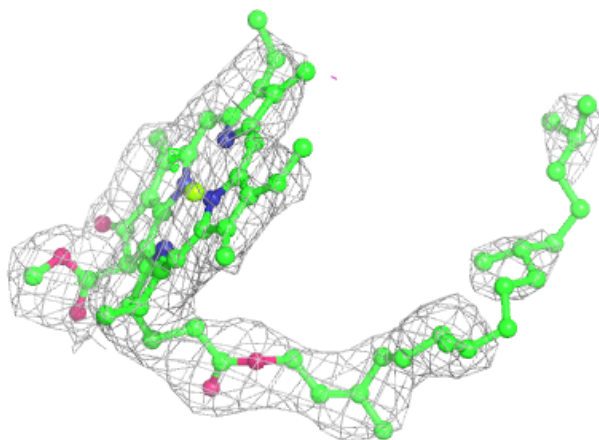


Electron density around CLA b 1234:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

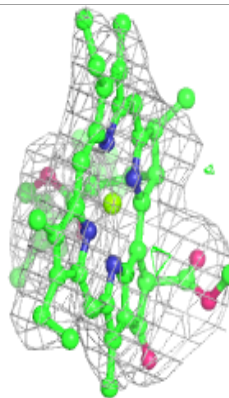
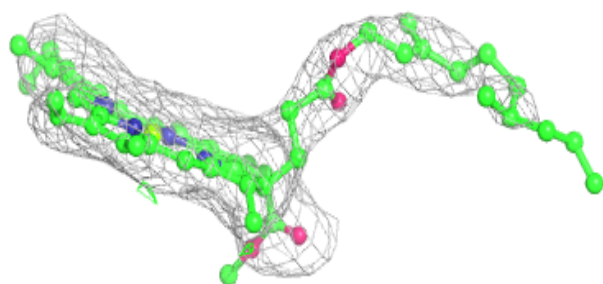
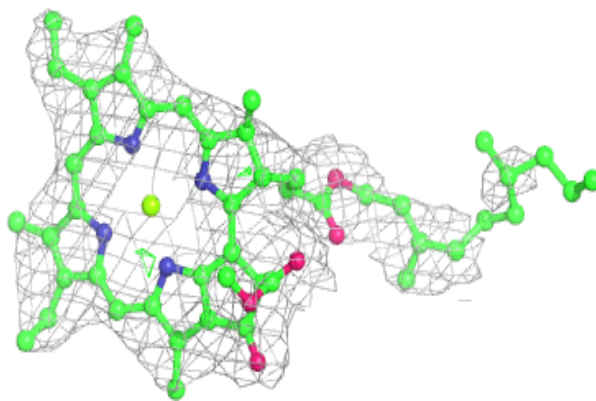
**Electron density around CLA b 1212:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

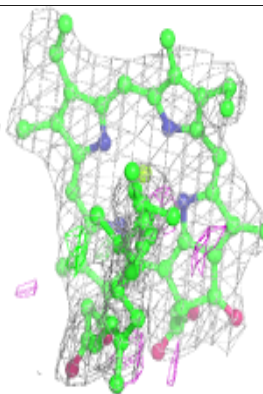
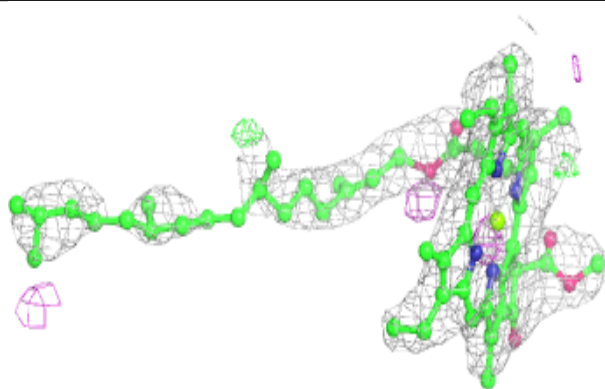
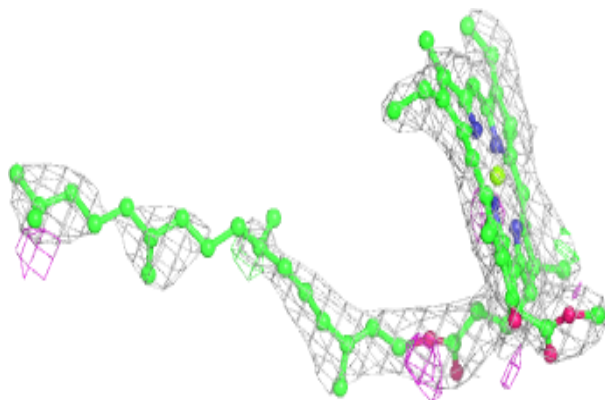


Electron density around CLA B 1220:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

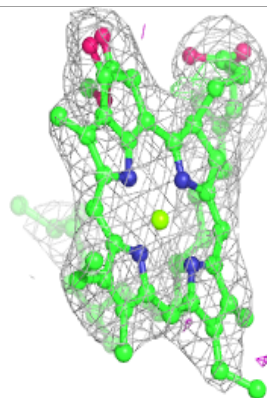
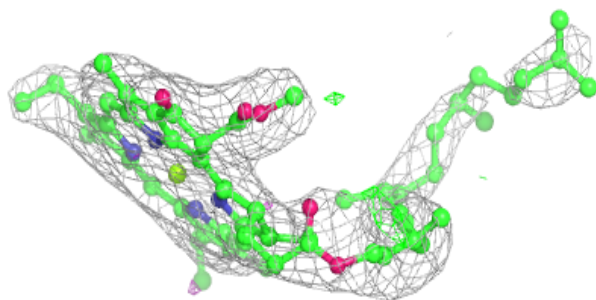
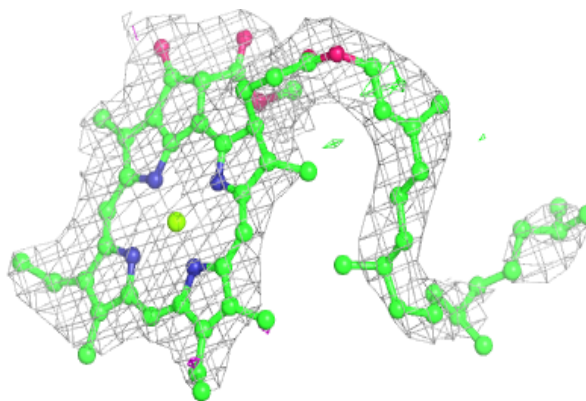
**Electron density around CLA b 1226:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

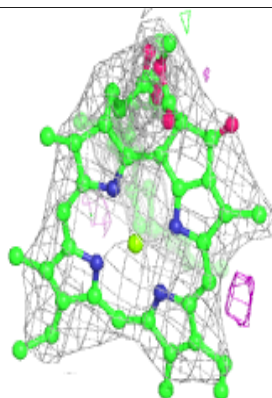
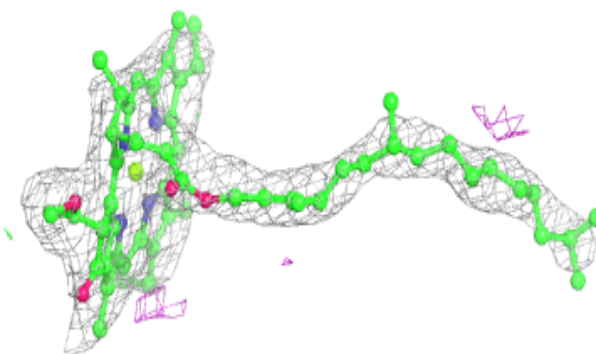
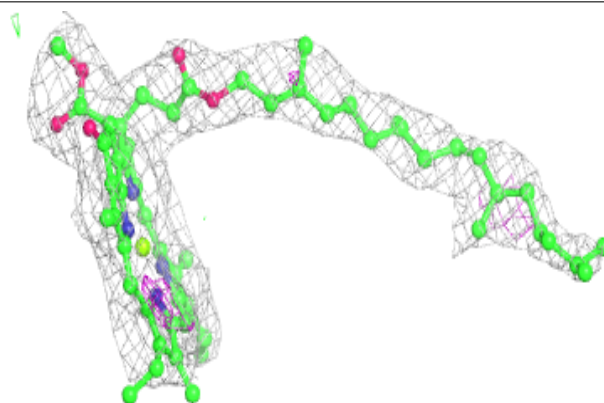


Electron density around CLA B 1221:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

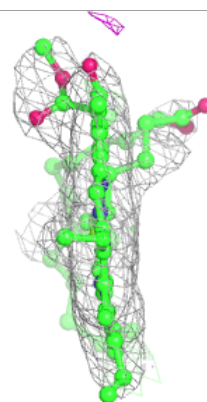
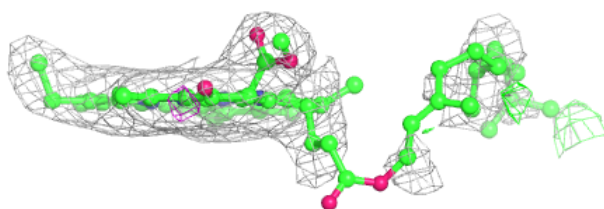
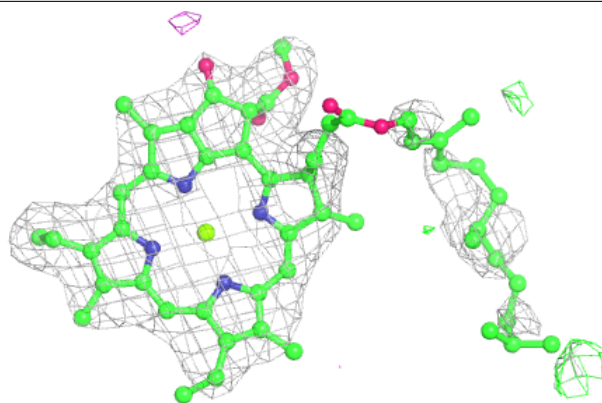
**Electron density around CLA 2 1201:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

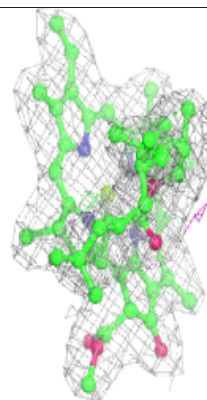
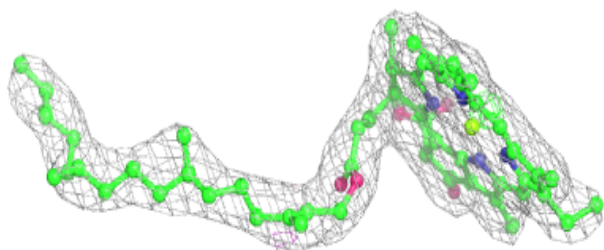
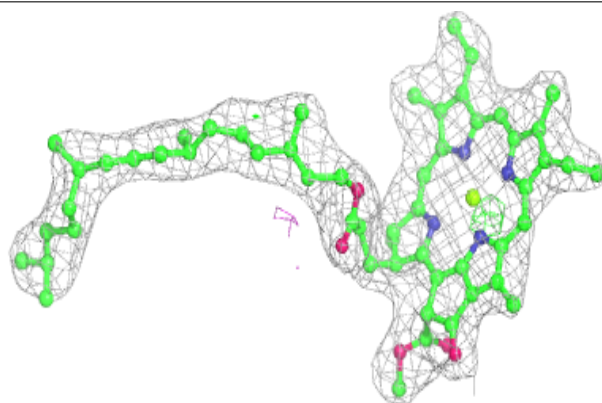


Electron density around CLA b 1219:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

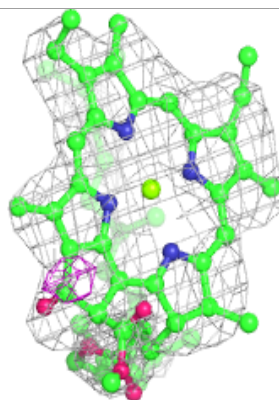
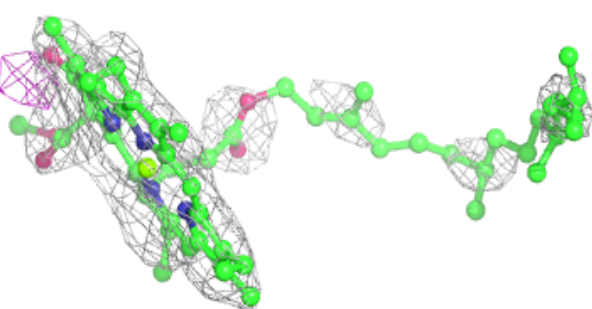
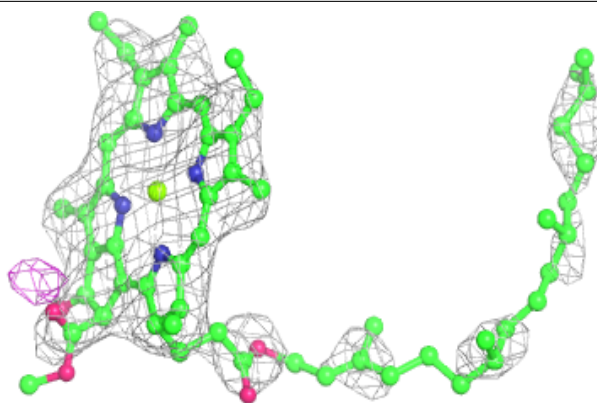
**Electron density around CLA A 1119:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

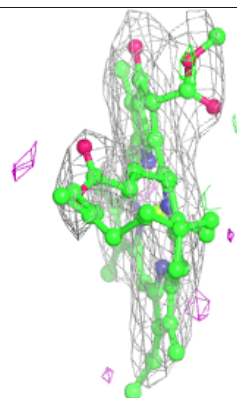
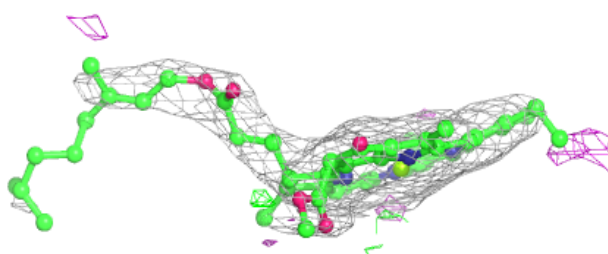
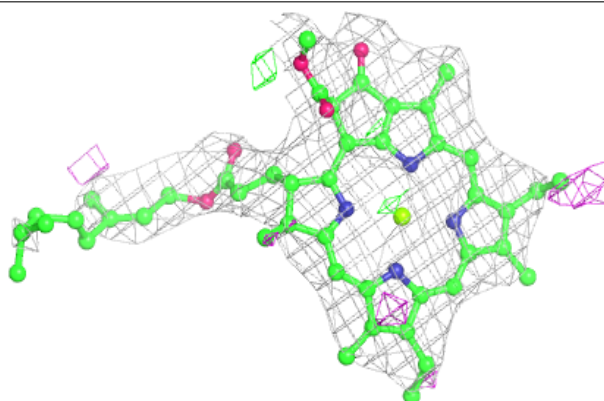


Electron density around CLA 1 1140:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

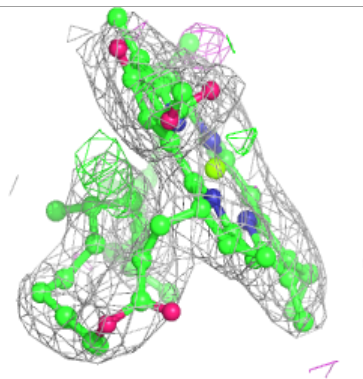
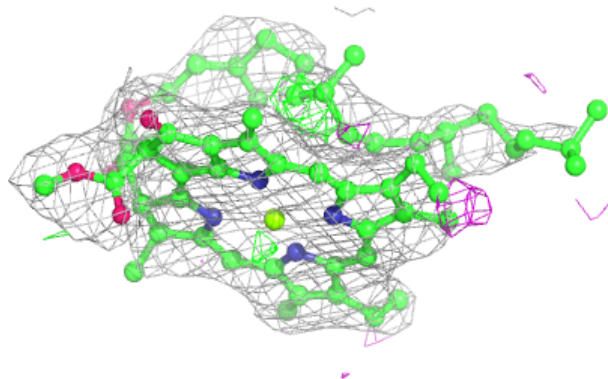
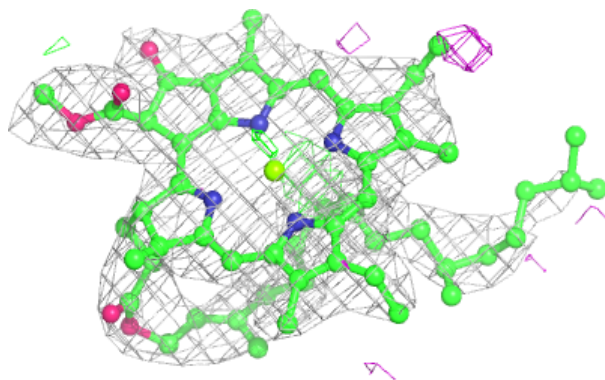
**Electron density around CLA a 1124:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



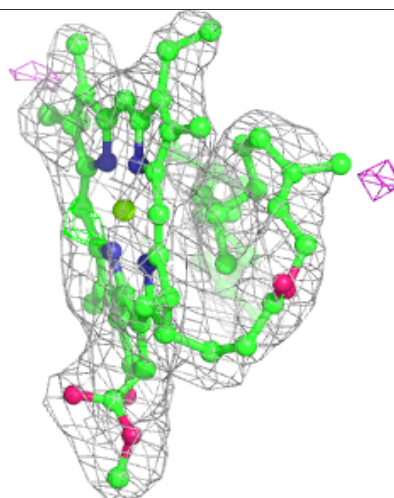
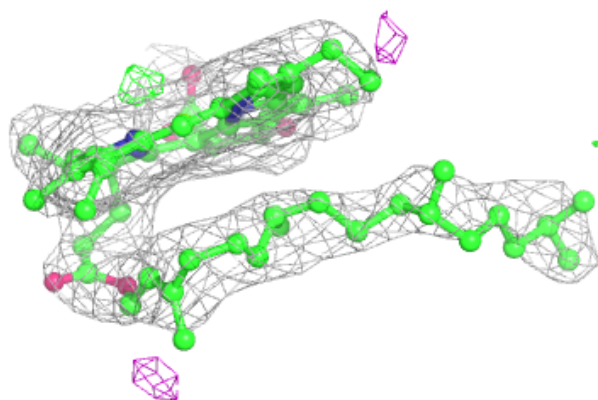
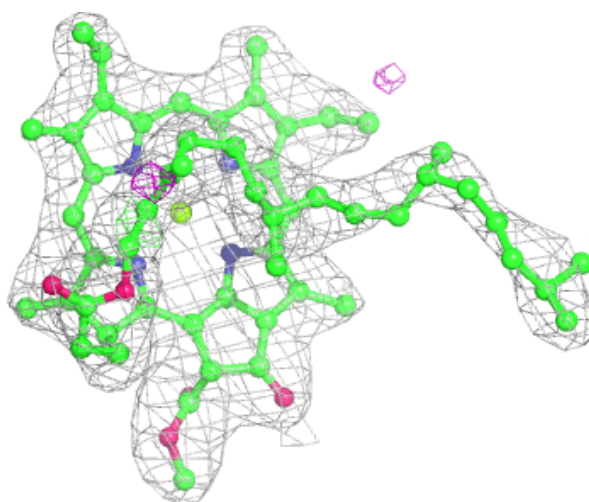
Electron density around CLA b 1214:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



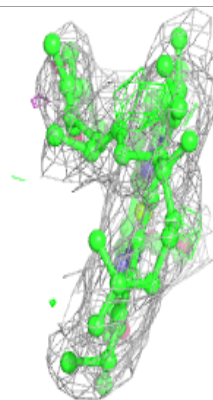
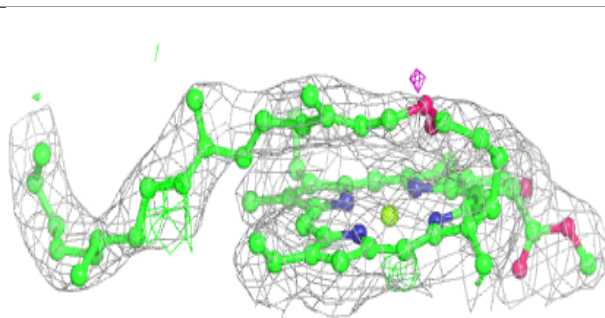
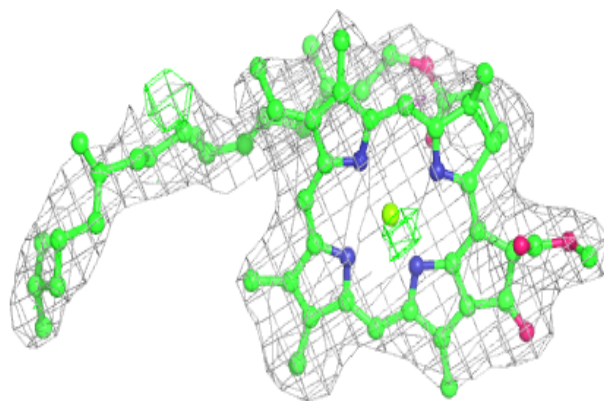
Electron density around CLA b 1224:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



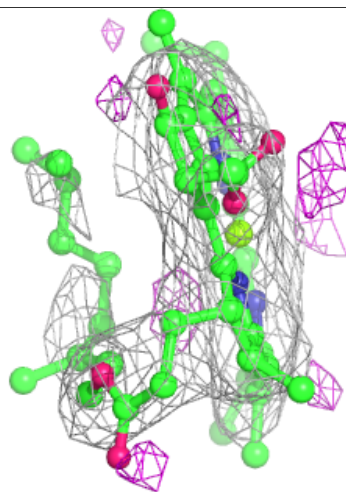
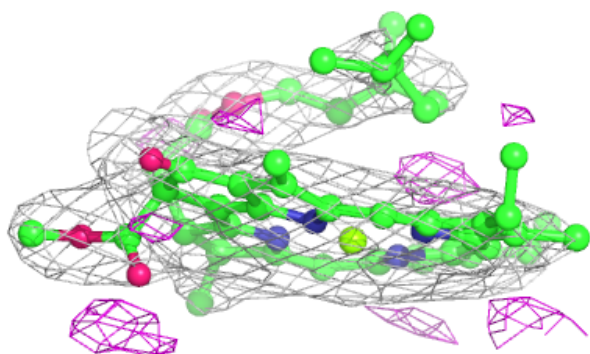
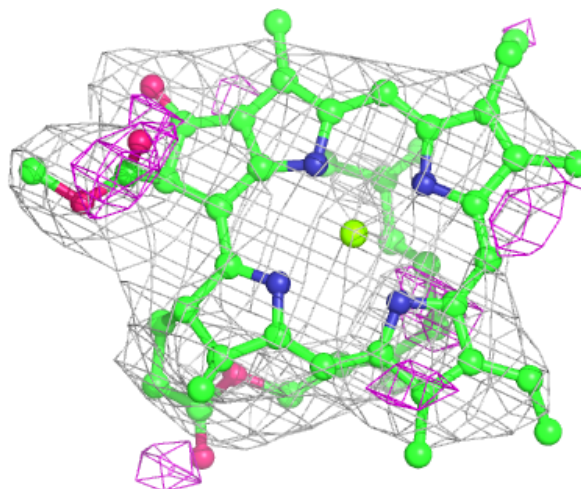
Electron density around CLA b 1209:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



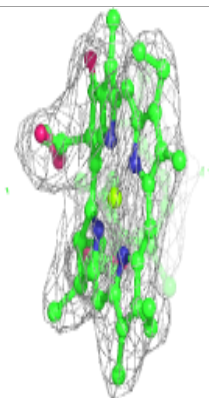
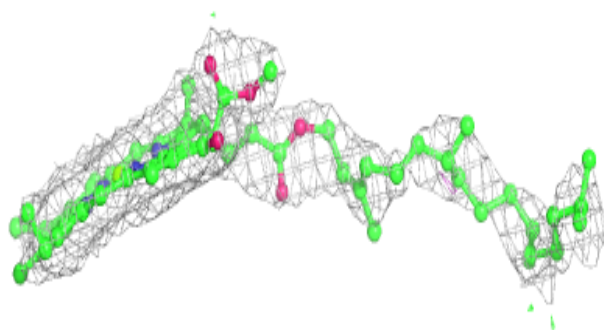
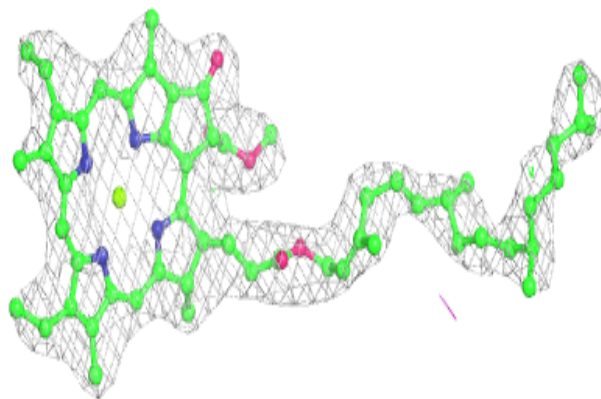
Electron density around CLA 2 1224:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

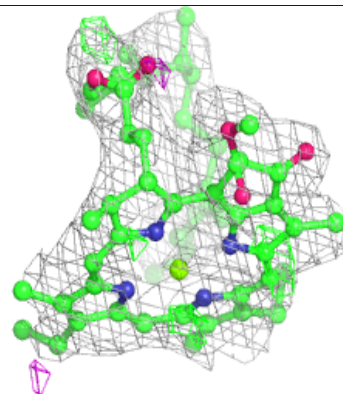
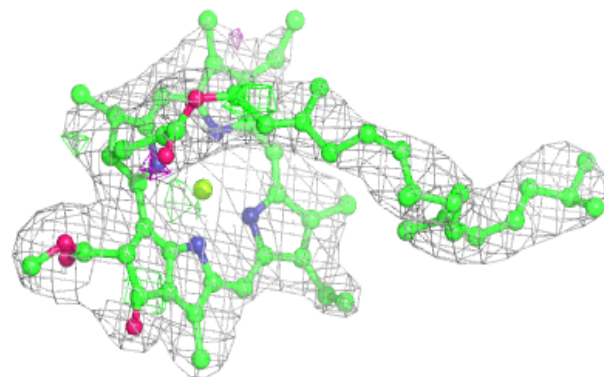
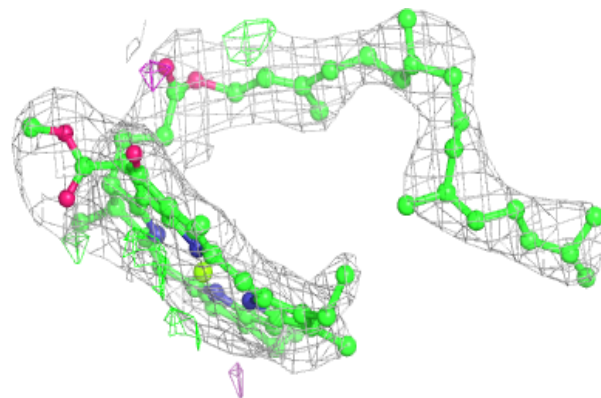


Electron density around CLA A 1139:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

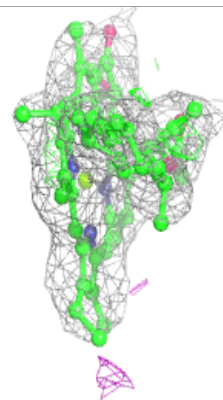
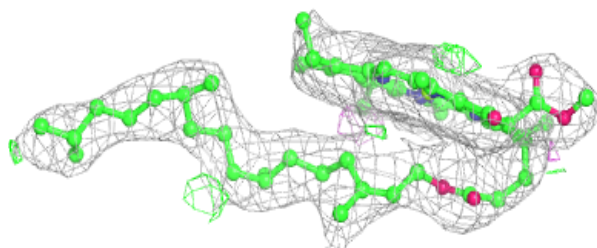
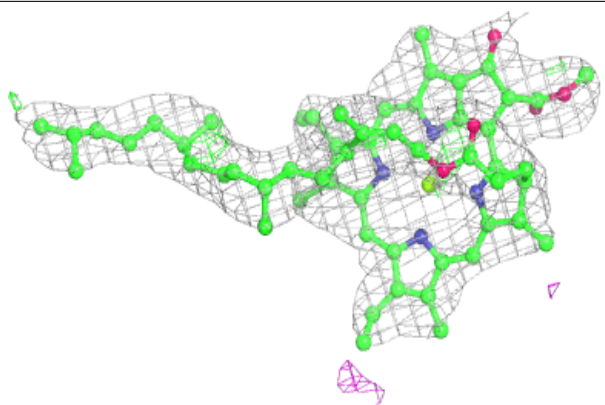
**Electron density around CLA A 1109:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



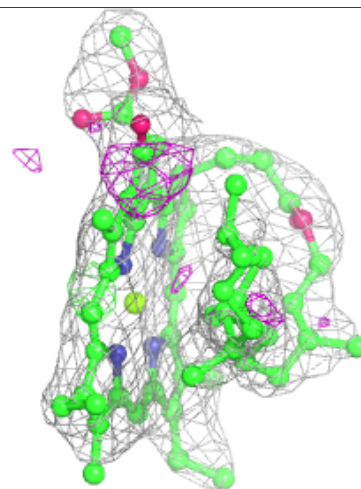
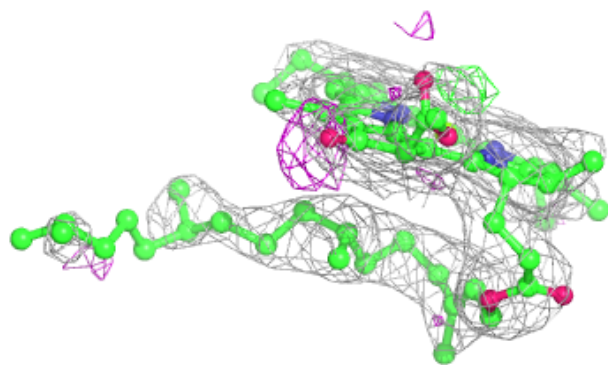
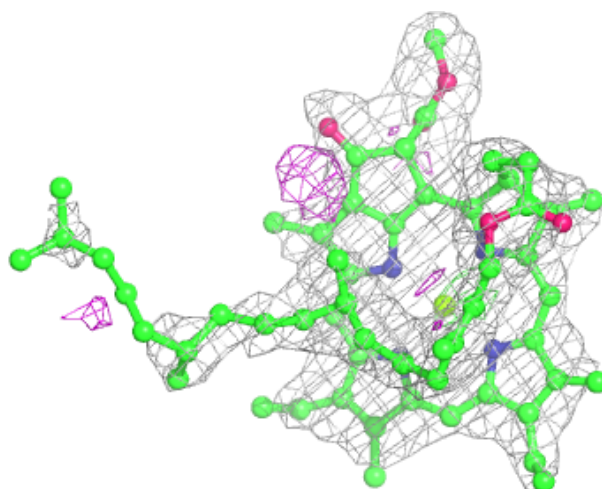
Electron density around CLA A 1115:

$2mF_o - DF_c$ (at 0.7 rmsd) in gray
 $mF_o - DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)



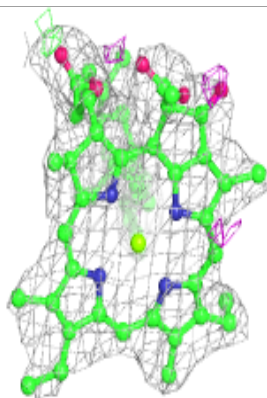
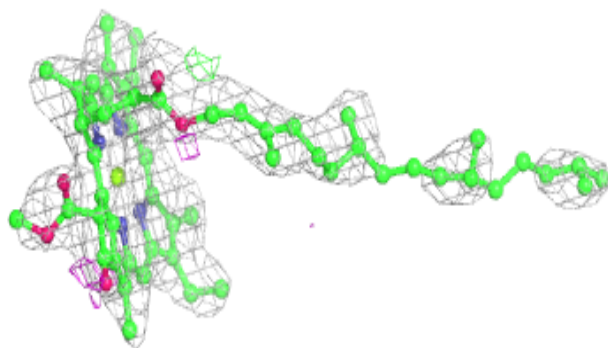
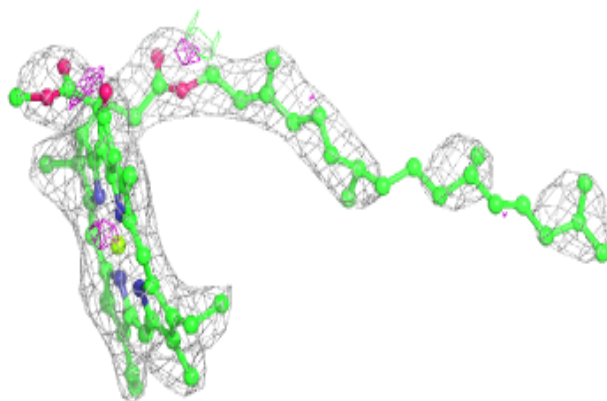
Electron density around CLA B 1224:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

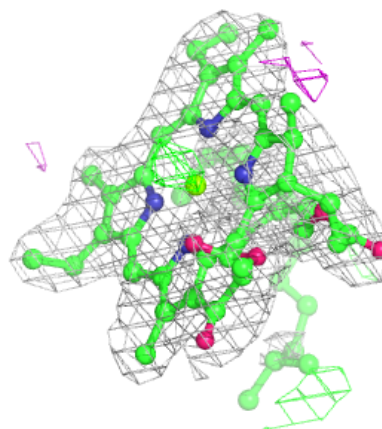
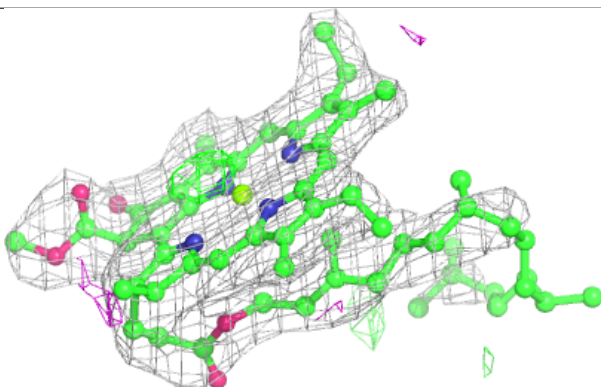
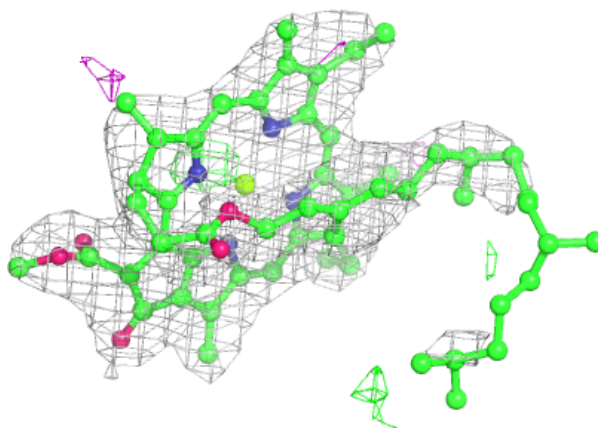


Electron density around CLA B 1226:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

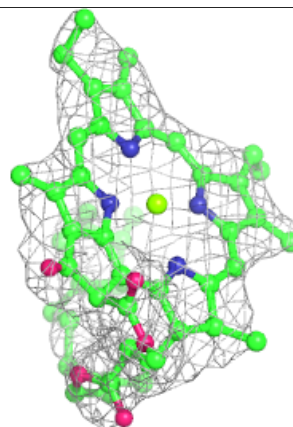
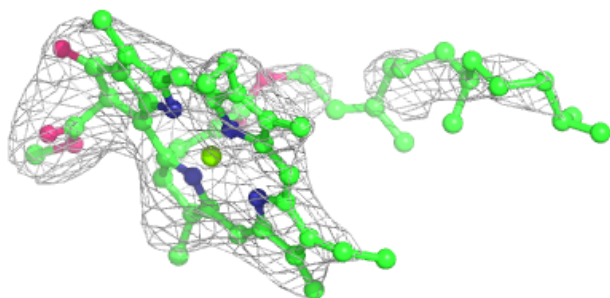
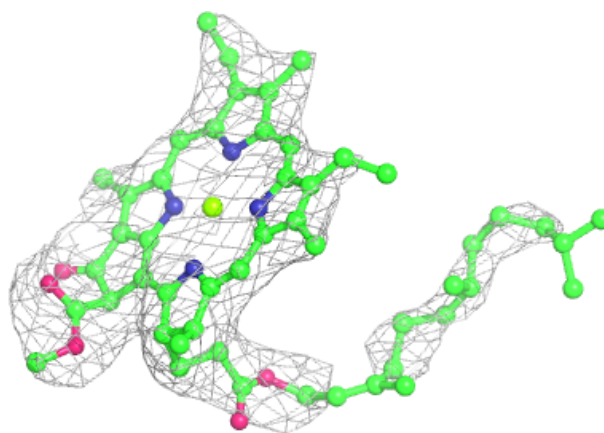
**Electron density around CLA A 1121:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

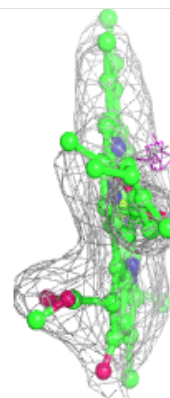
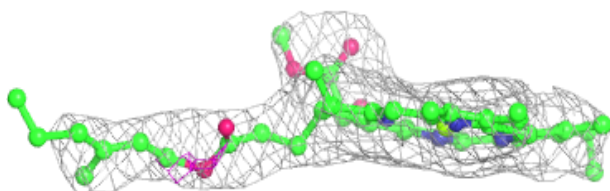
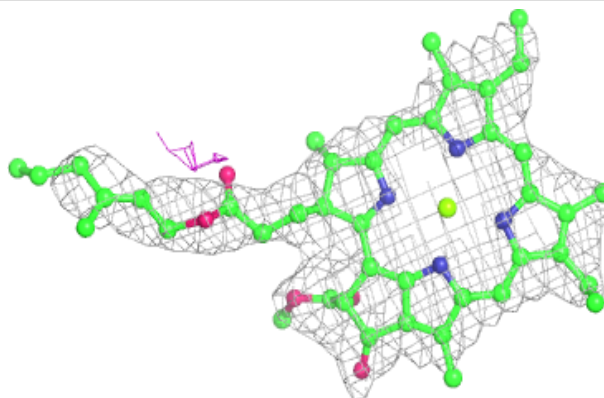


Electron density around CLA 1 1122:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

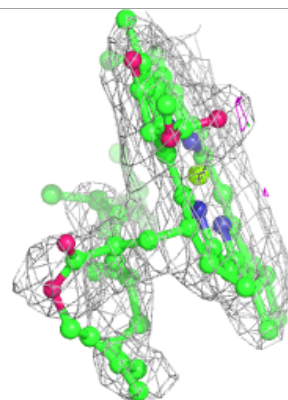
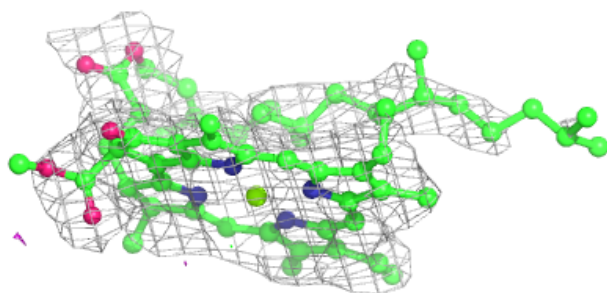
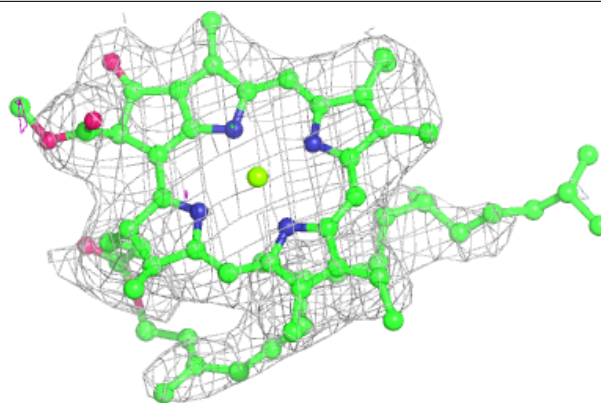
**Electron density around CLA 1 1135:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

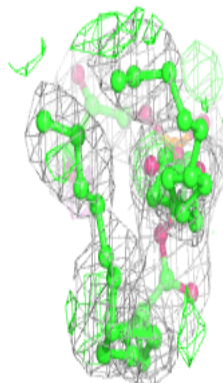
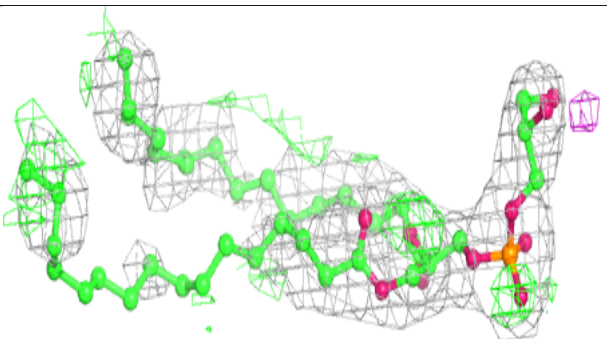
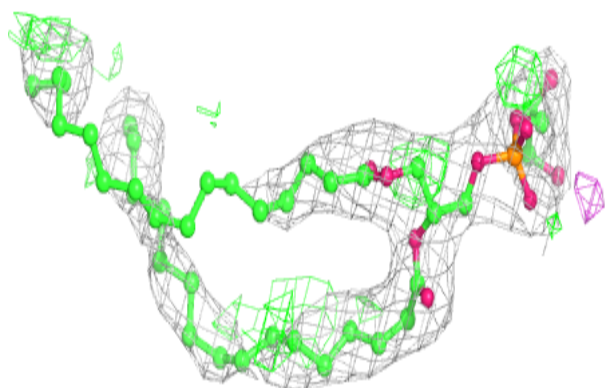


Electron density around CLA b 1218:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

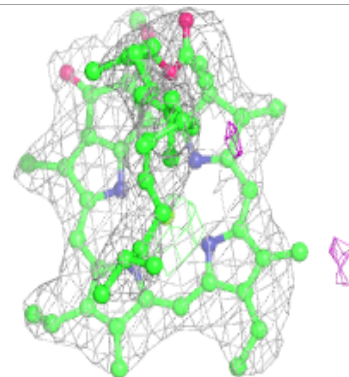
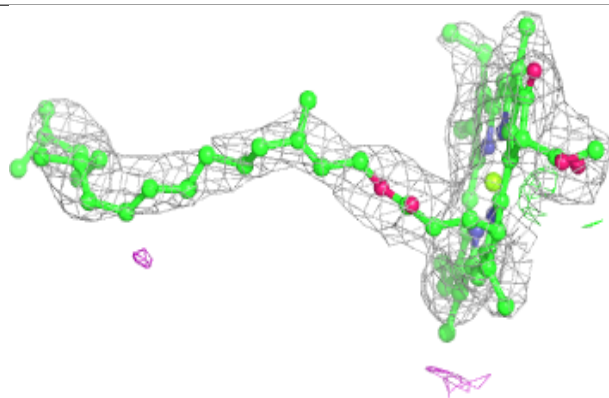
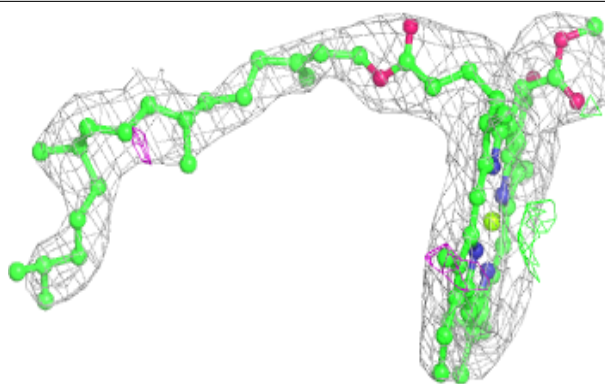
**Electron density around LHG A 5003:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



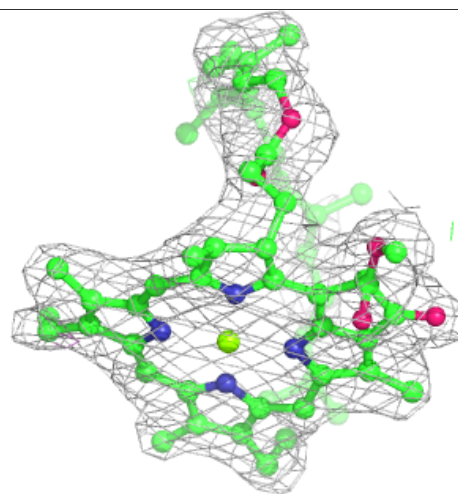
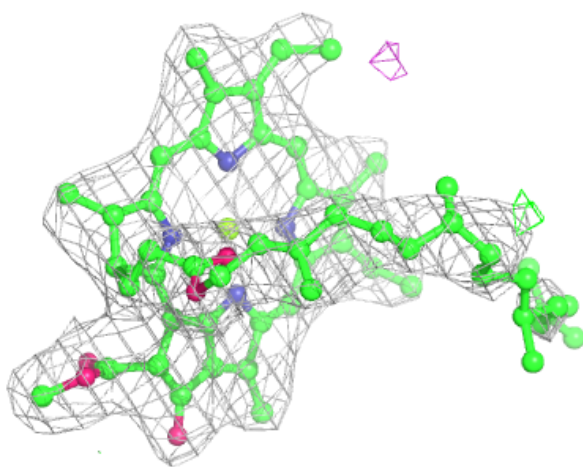
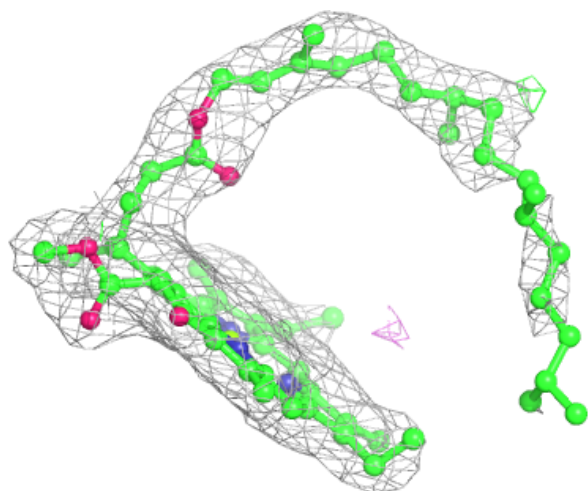
Electron density around CLA A 1105:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



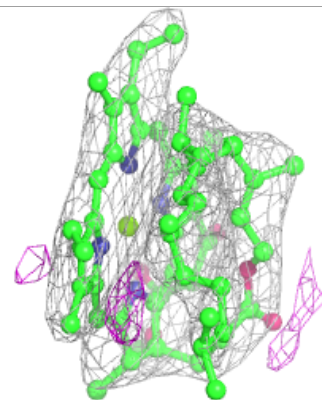
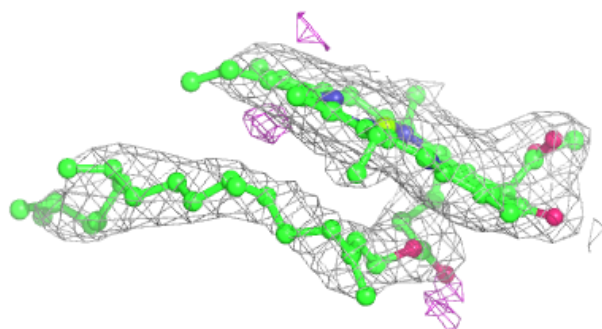
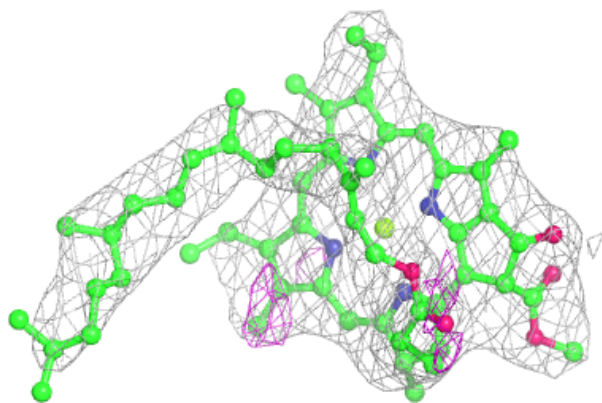
Electron density around CLA b 1216:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



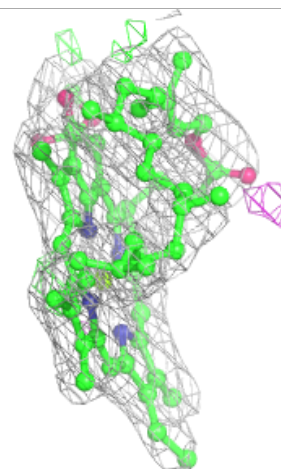
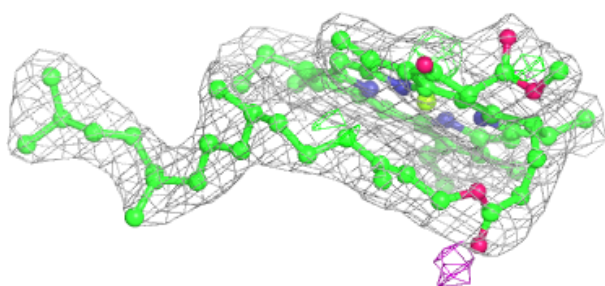
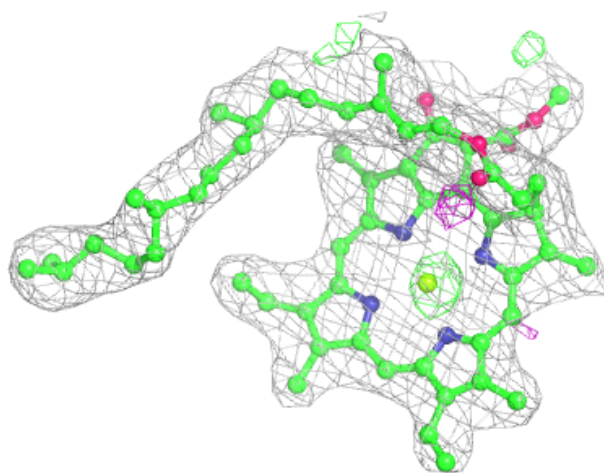
Electron density around CLA 2 1204:

$2mF_o - DF_c$ (at 0.7 rmsd) in gray
 $mF_o - DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)



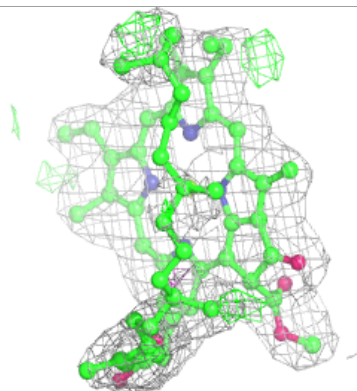
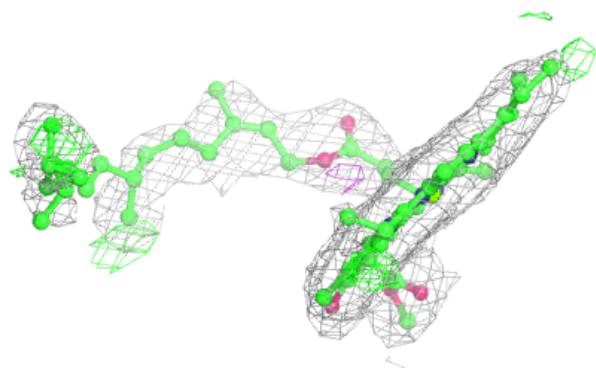
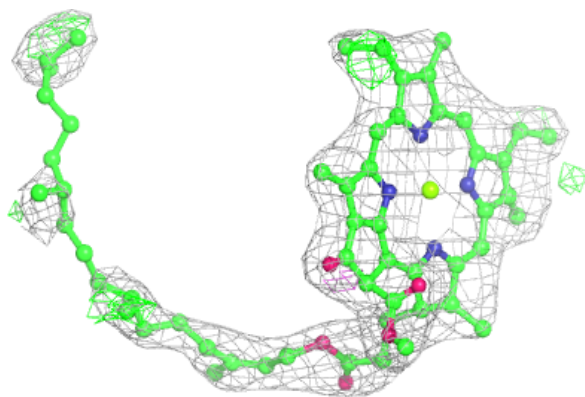
Electron density around CLA A 1127:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



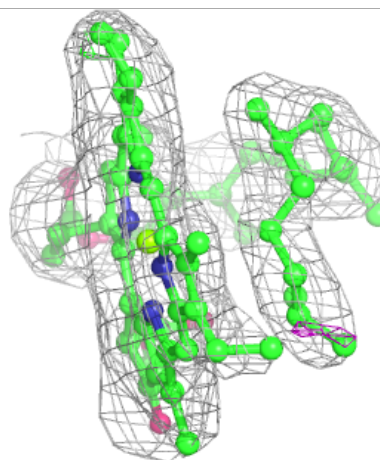
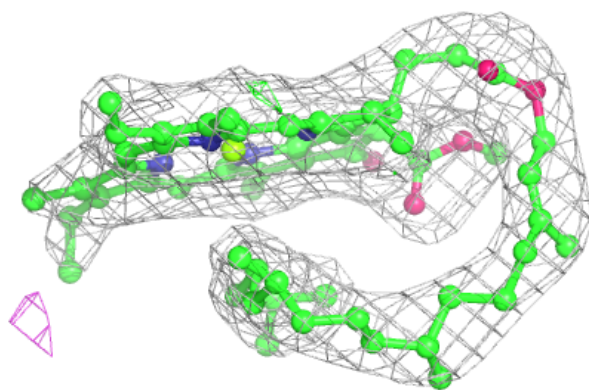
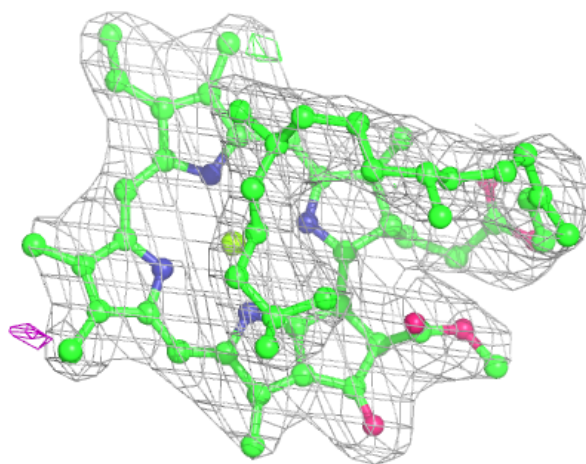
Electron density around CLA K 1401:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



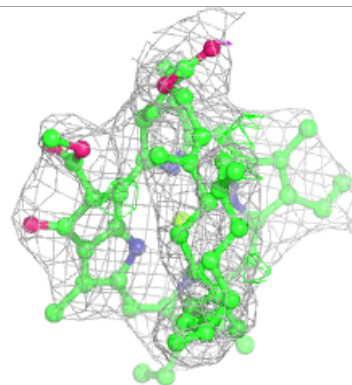
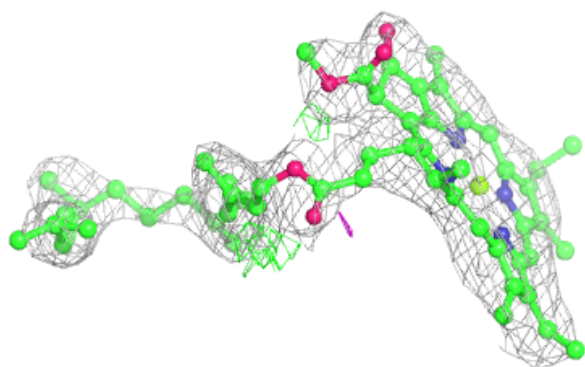
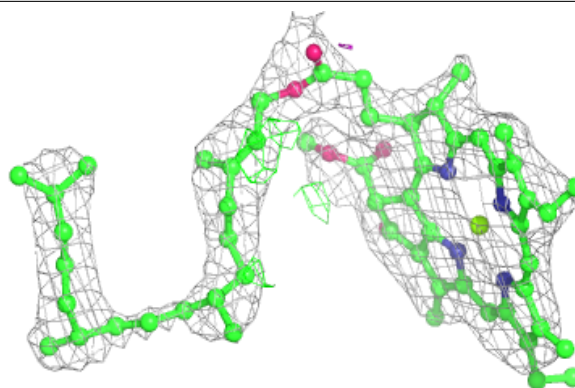
Electron density around CLA A 1104:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

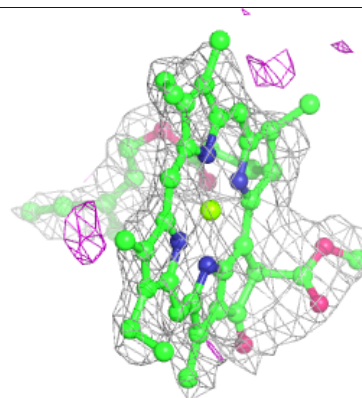
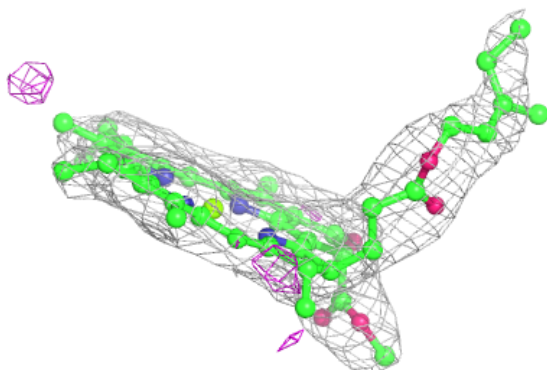
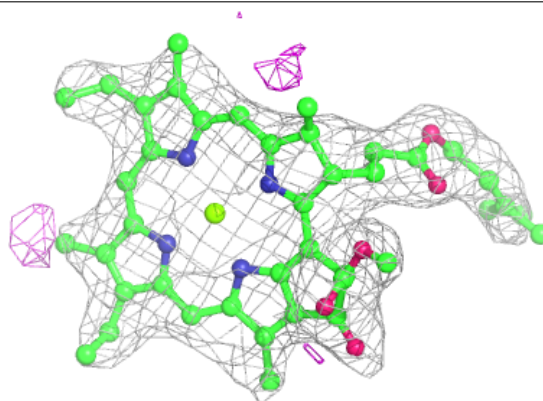


Electron density around CLA 1 1011:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

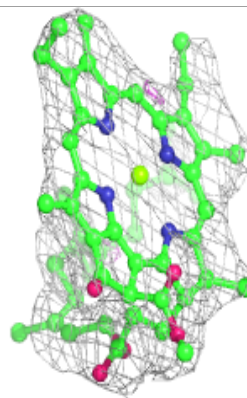
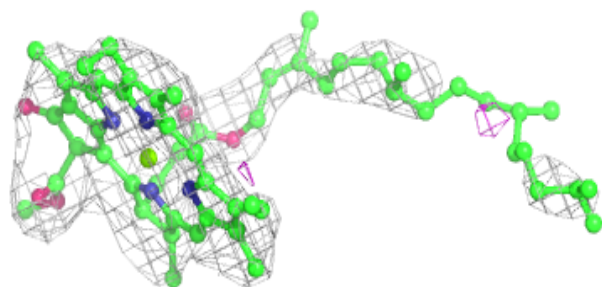
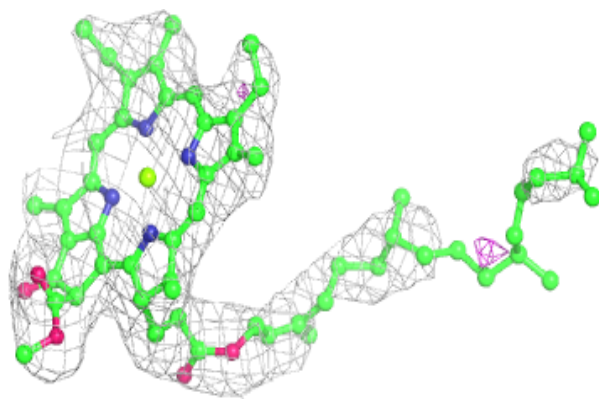
**Electron density around CLA 1 1137:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



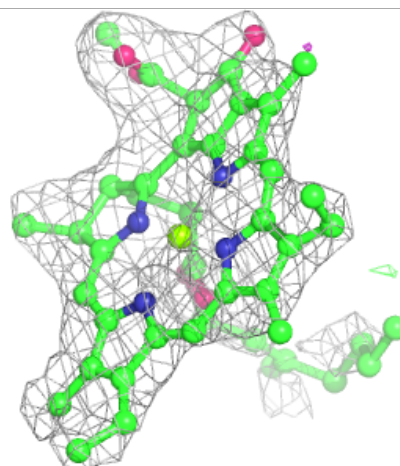
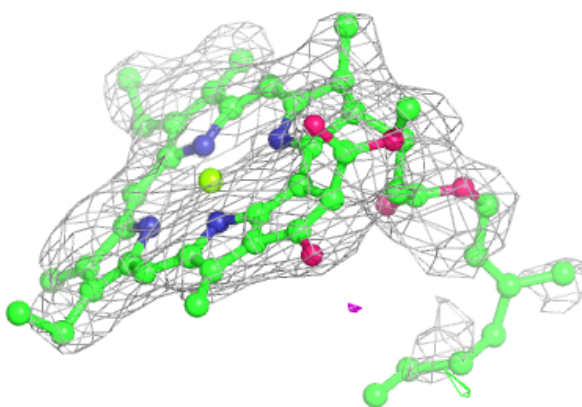
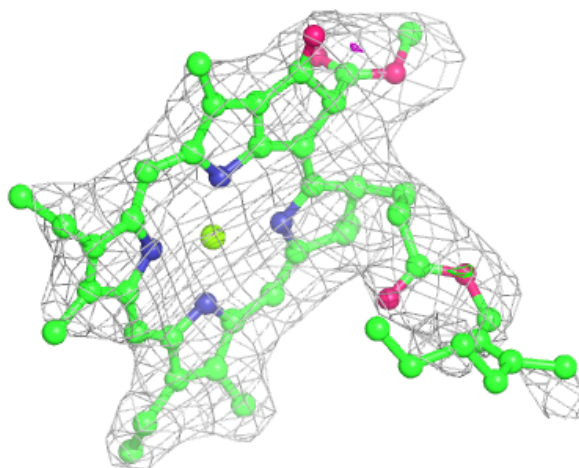
Electron density around CLA A 1114:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



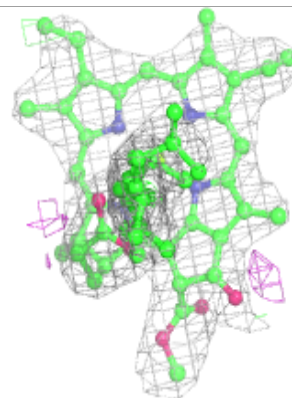
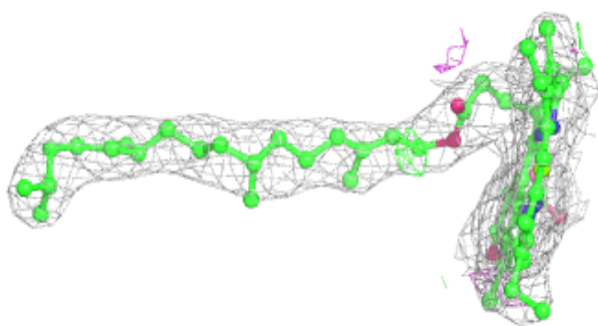
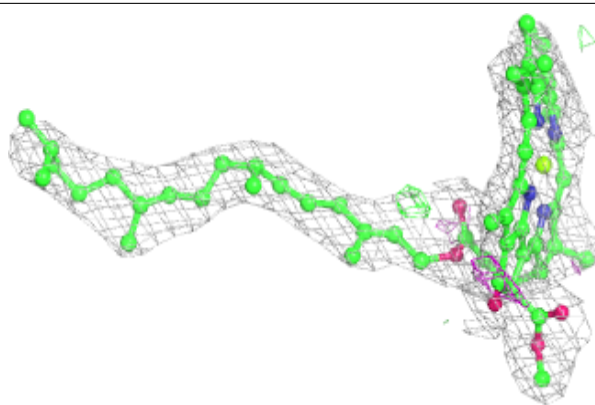
Electron density around CLA A 1108:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

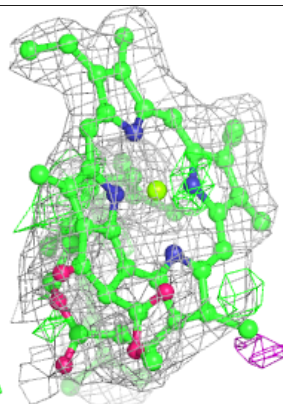
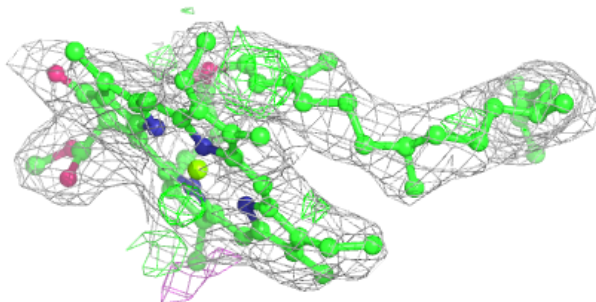
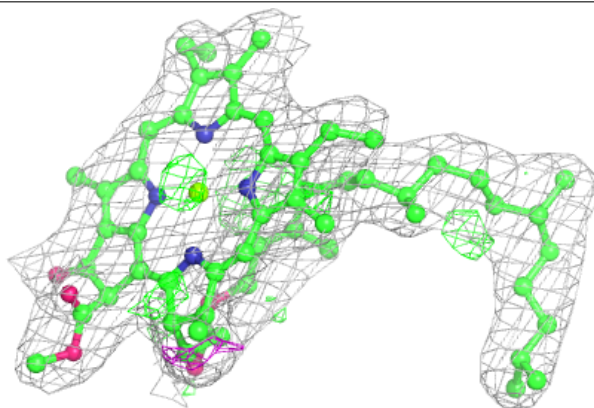


Electron density around CLA A 1126:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

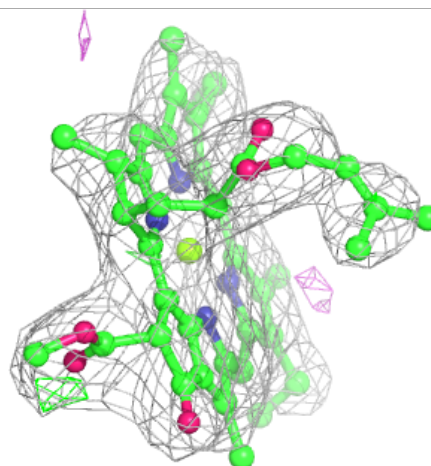
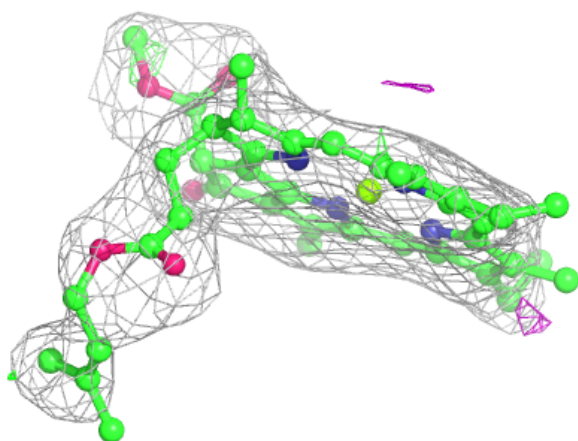
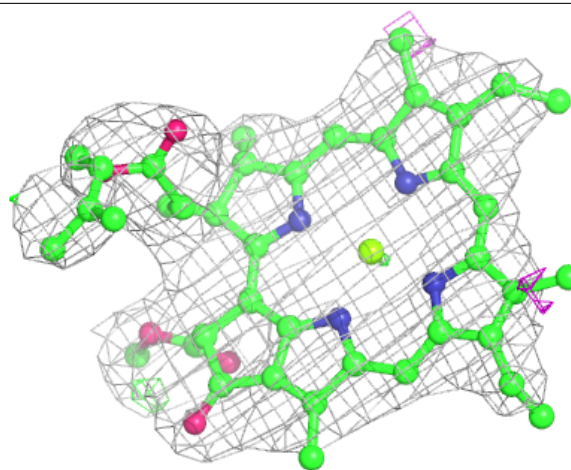
**Electron density around CLA 2 1237:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



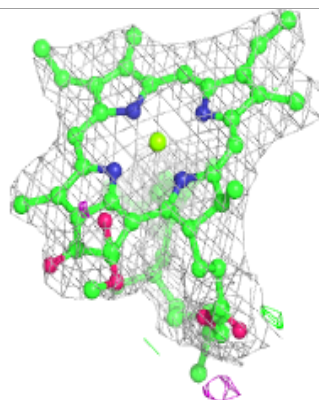
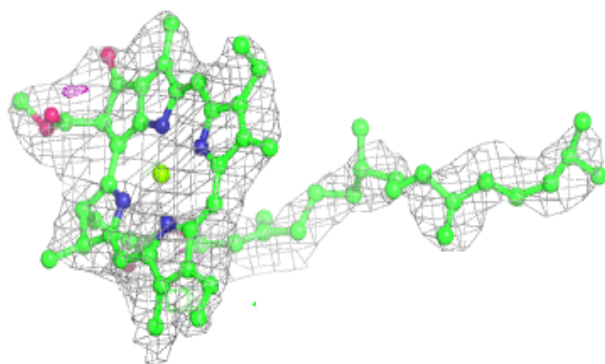
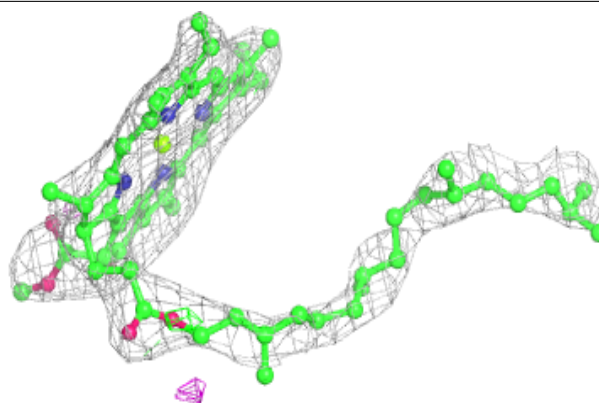
Electron density around CLA B 1236:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

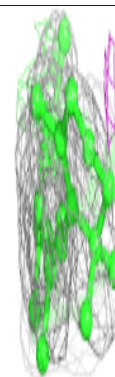
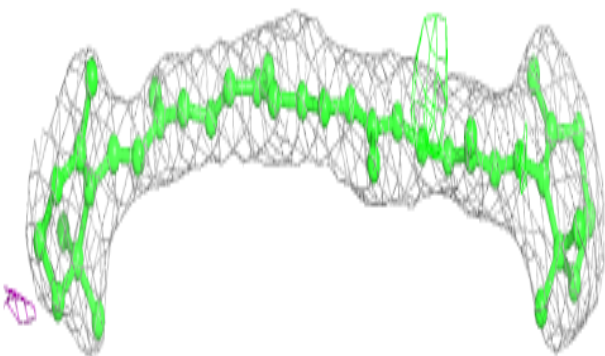
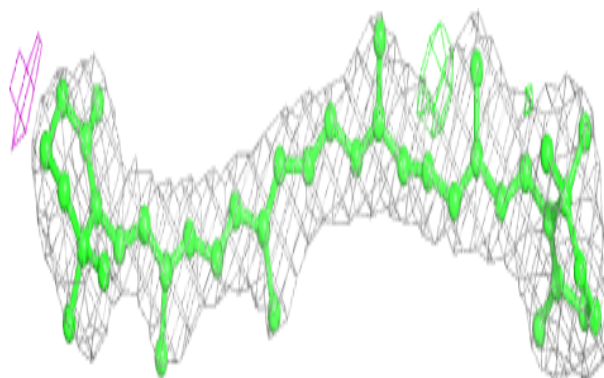


Electron density around CLA B 1208:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

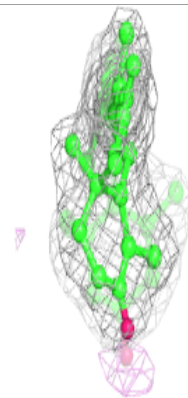
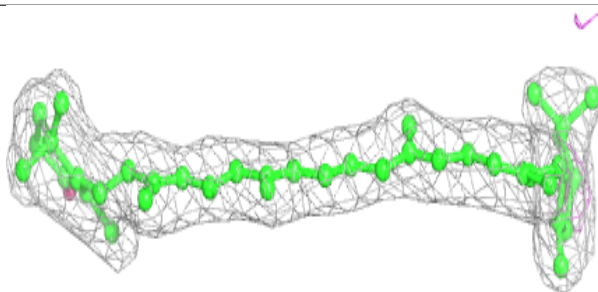
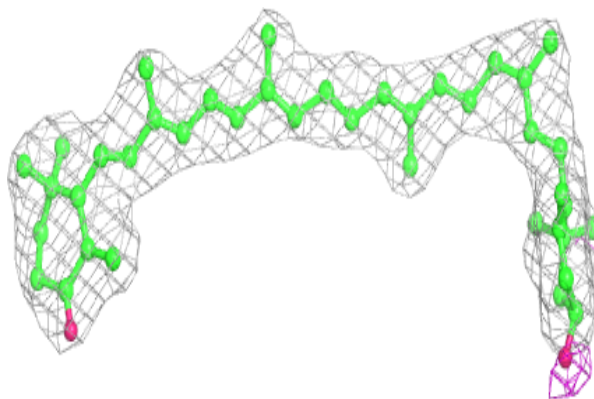
**Electron density around BCR A 4001:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

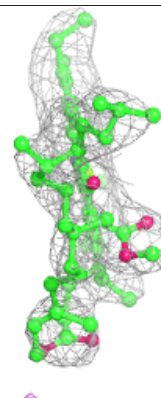
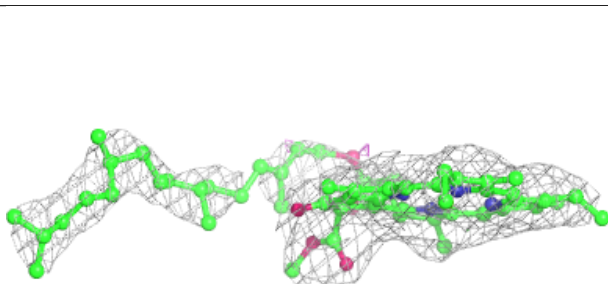
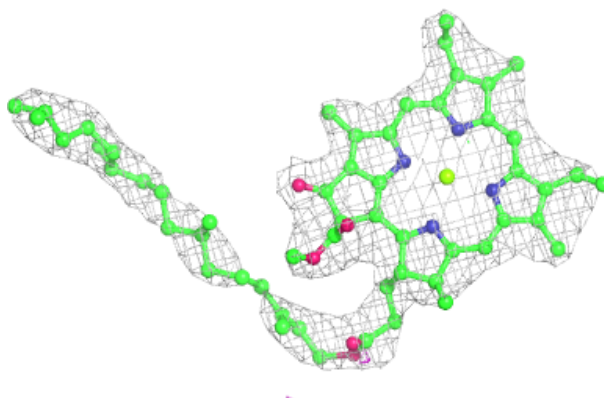


Electron density around EQ3 I 4020:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

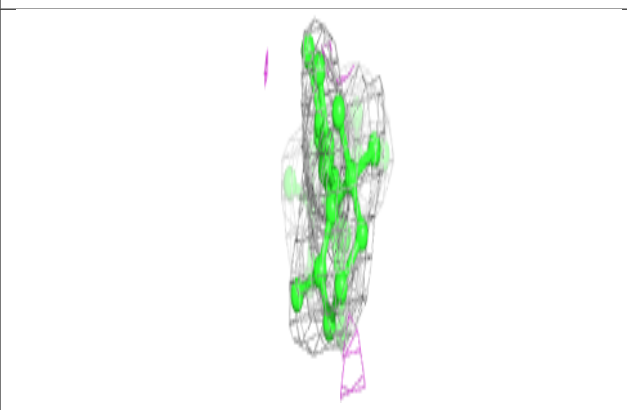
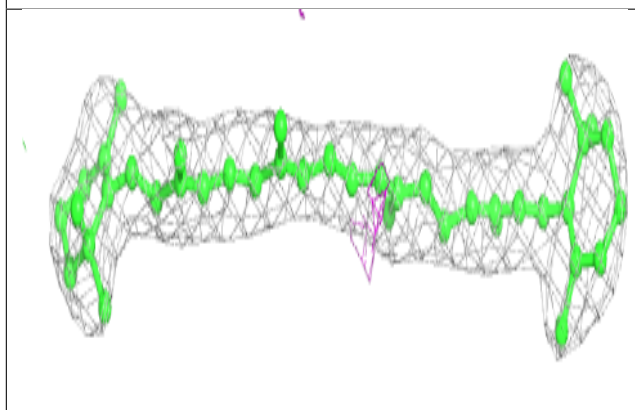
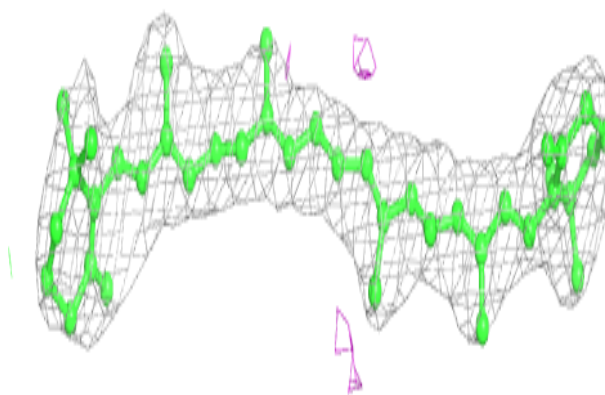
**Electron density around CLA 0 1503:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



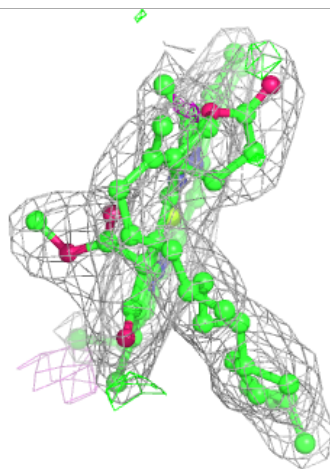
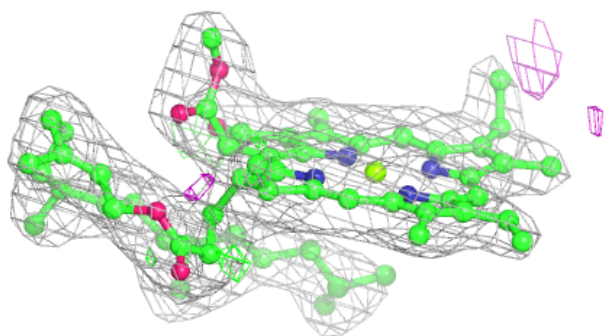
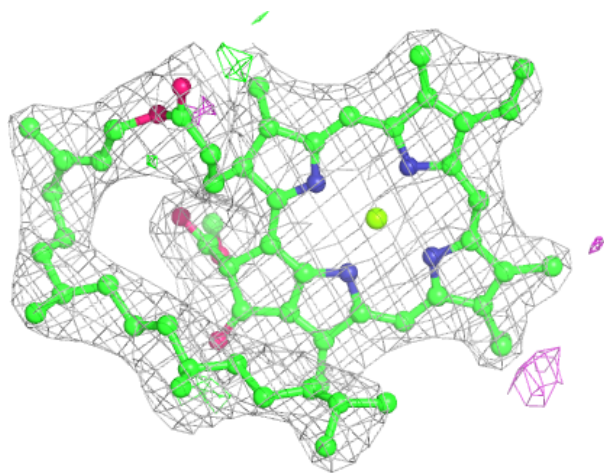
Electron density around BCR A 4007:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



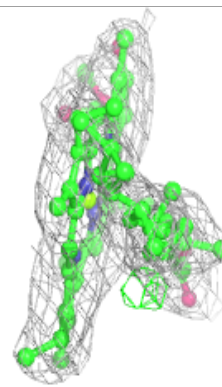
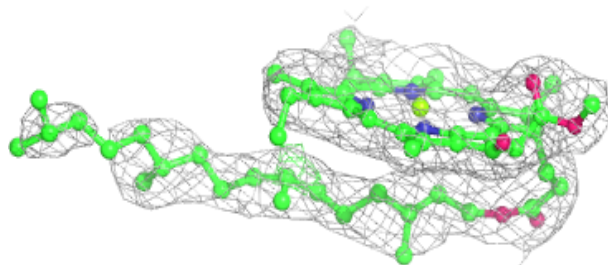
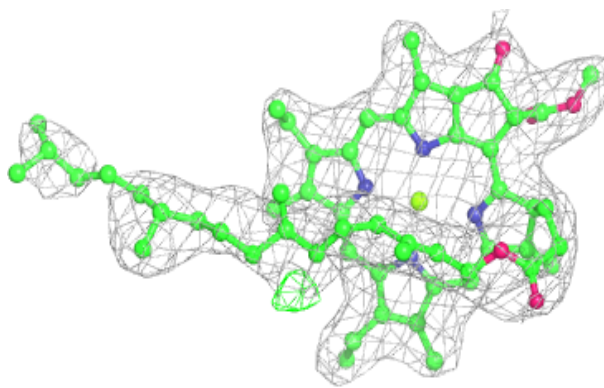
Electron density around CLA b 1202:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

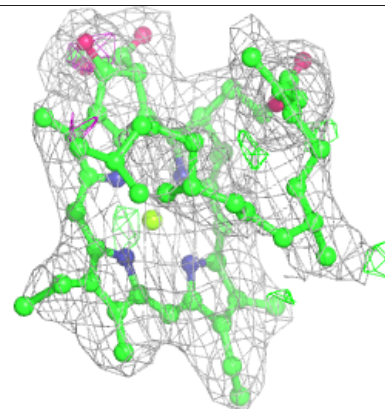
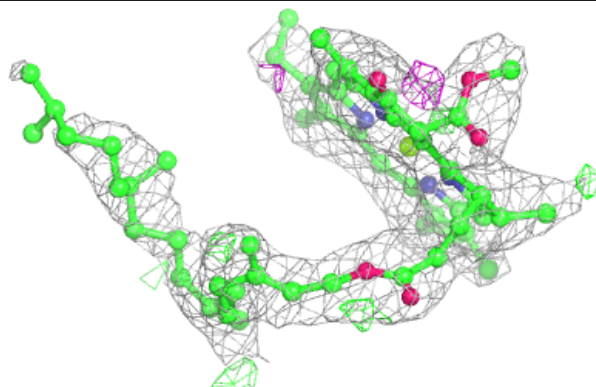
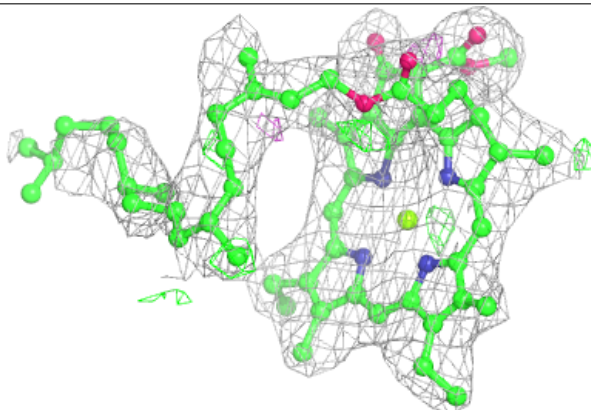


Electron density around CLA A 1116:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

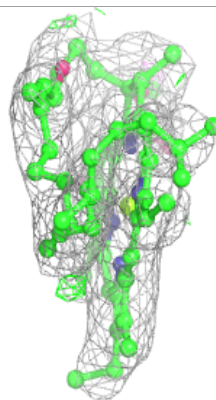
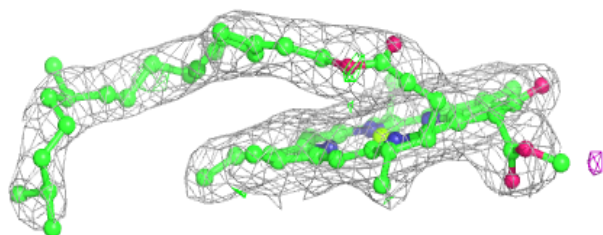
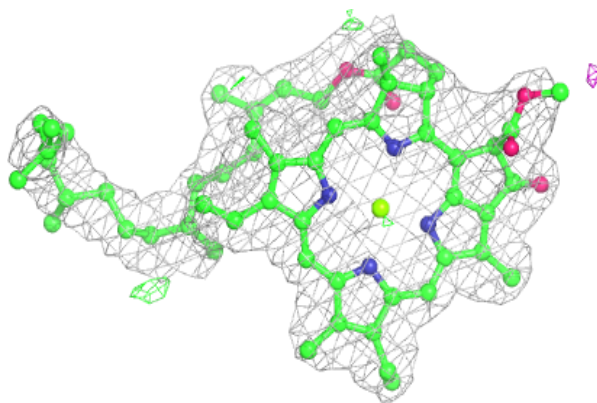
**Electron density around CLA b 1211:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

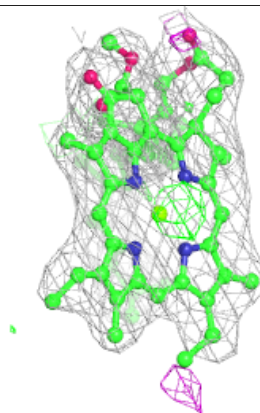
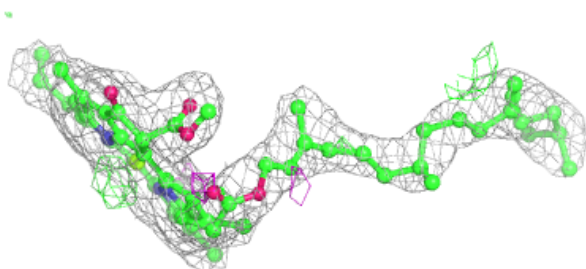
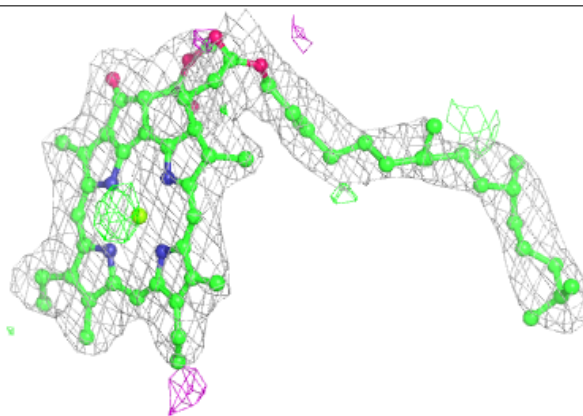


Electron density around CLA B 1215:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

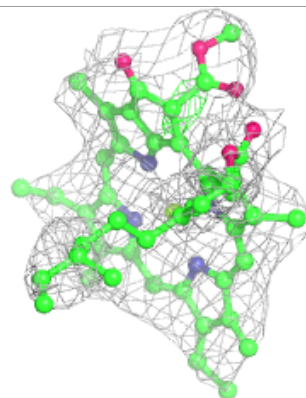
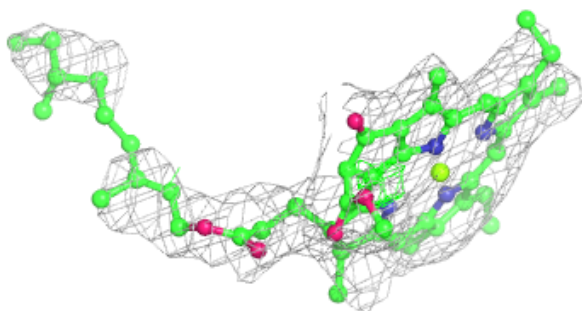
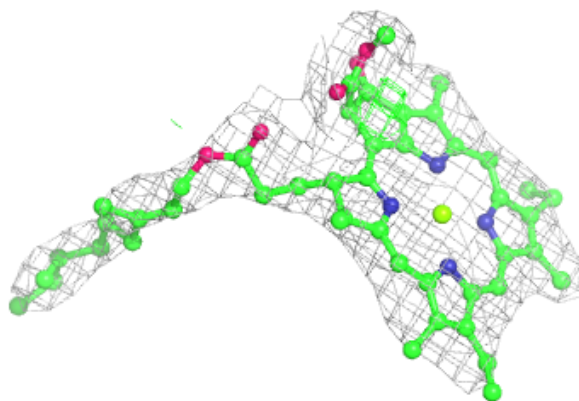
**Electron density around CLA B 1207:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

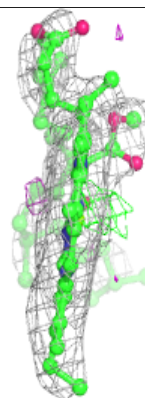
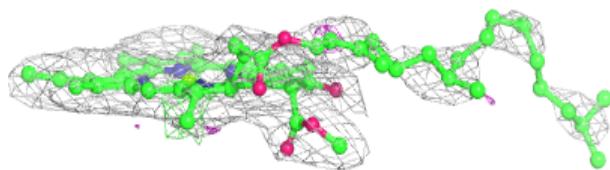
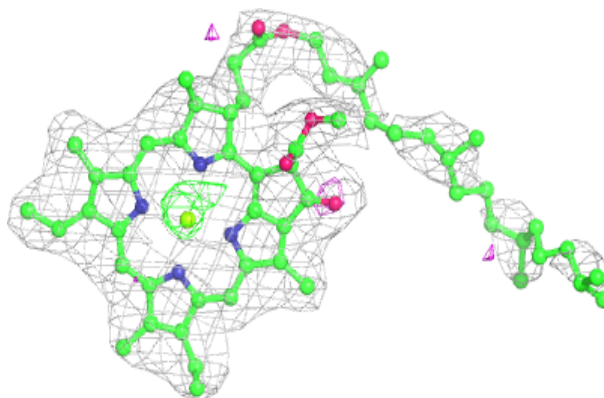


Electron density around CLA 1 1801:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

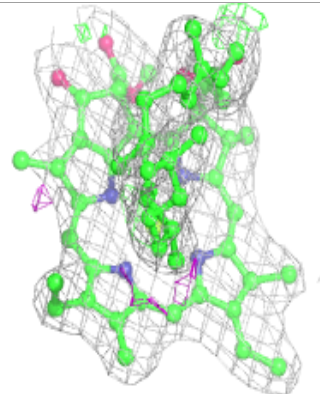
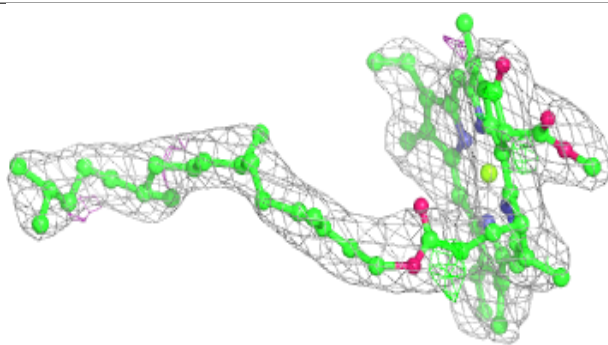
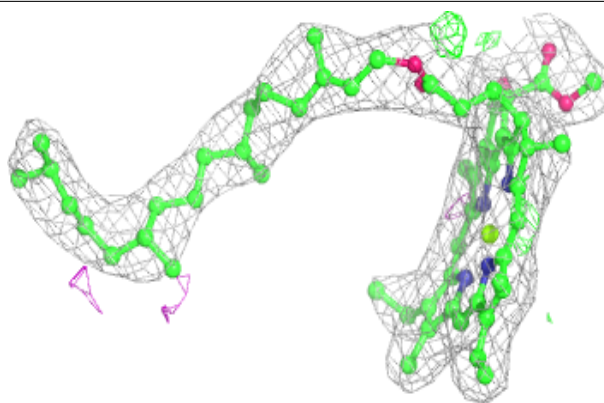
**Electron density around CLA 1 1503:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

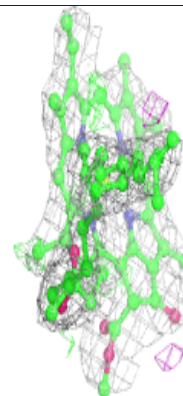
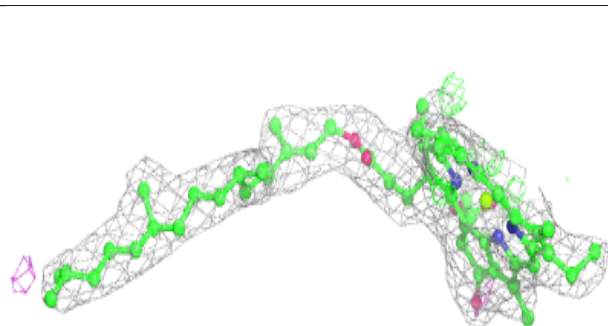
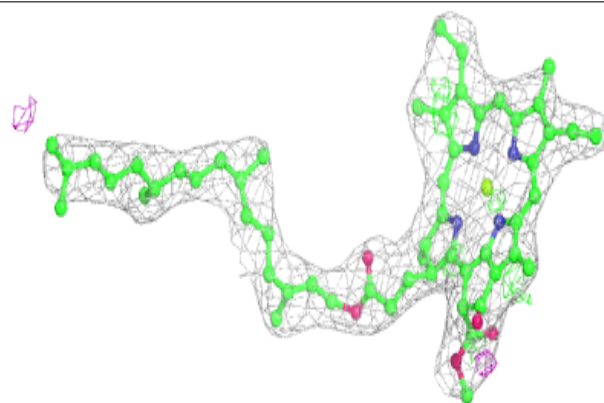


Electron density around CLA A 1128:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

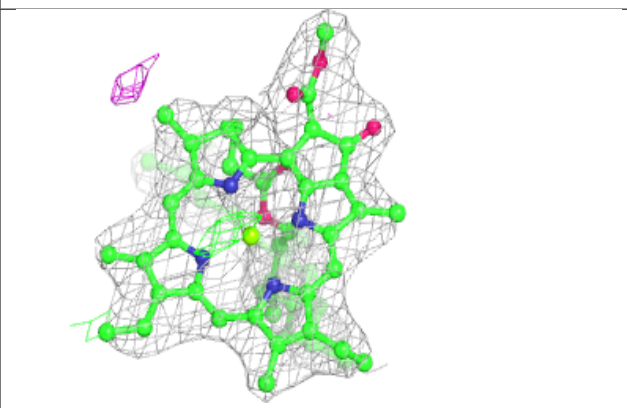
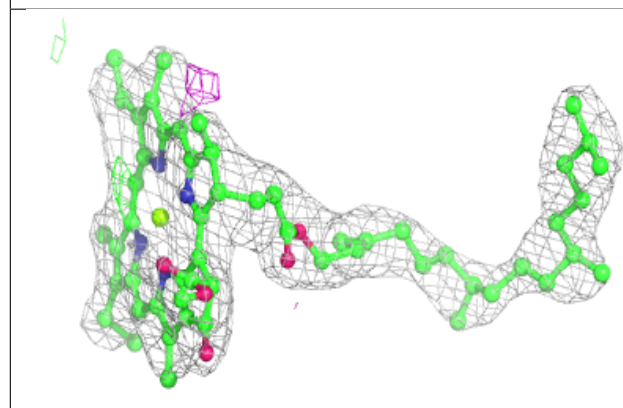
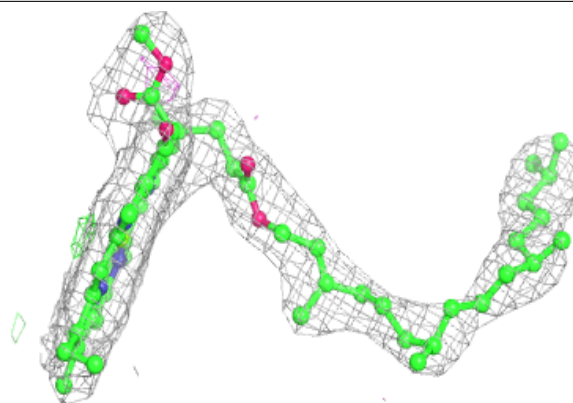
**Electron density around CLA 2 1022:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

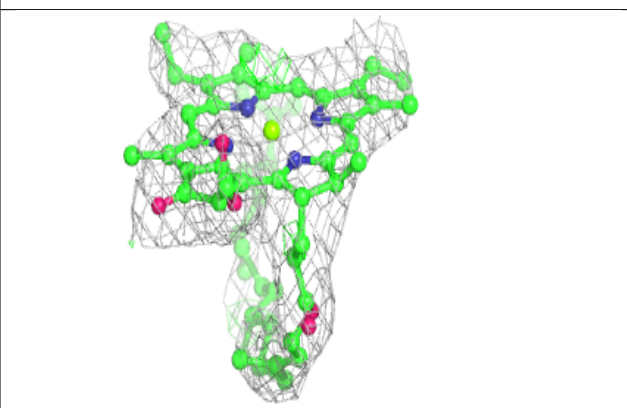
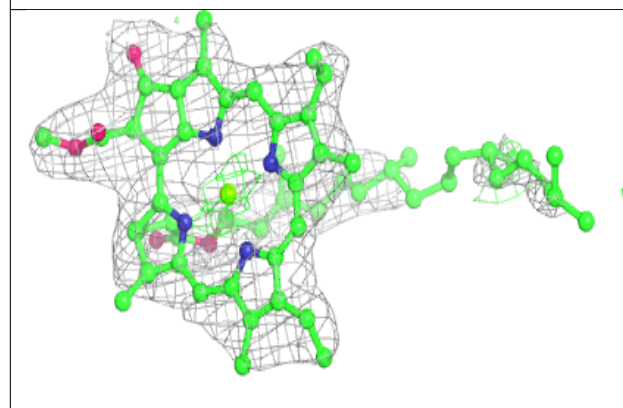
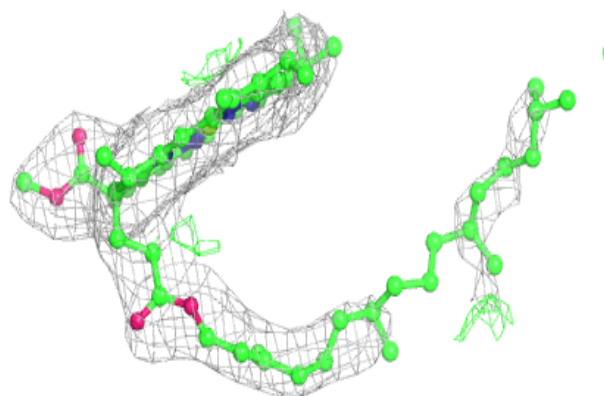


Electron density around CLA b 1238:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

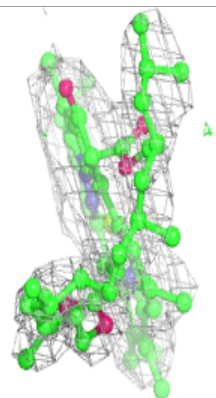
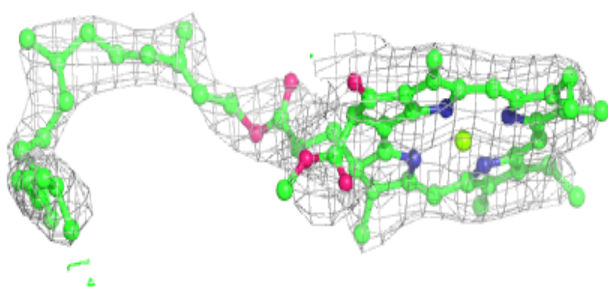
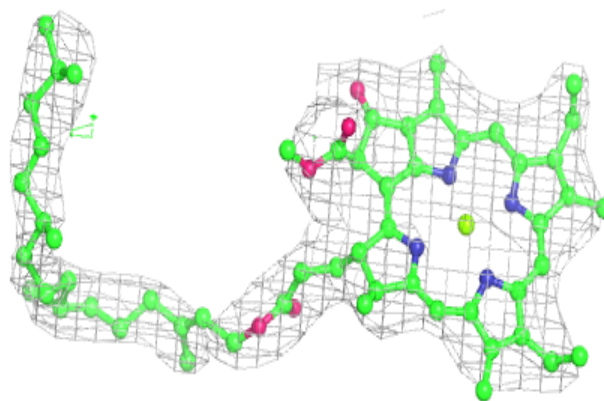
**Electron density around CLA a 1130:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

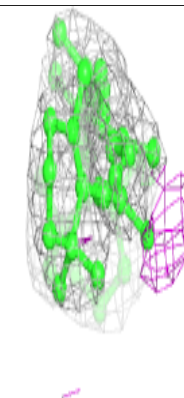
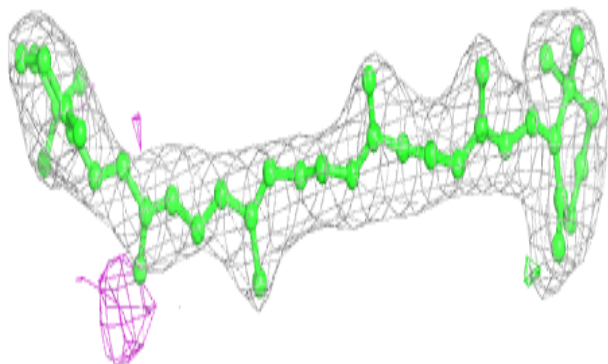
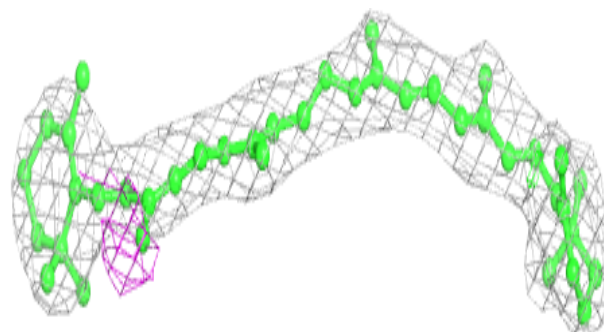


Electron density around CLA B 1223:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

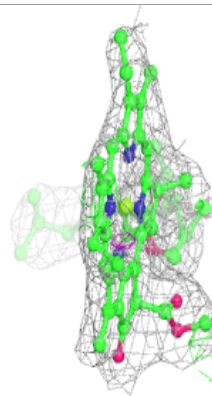
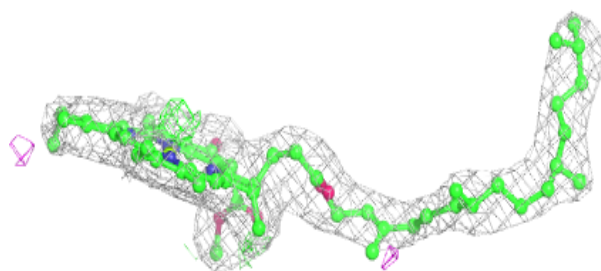
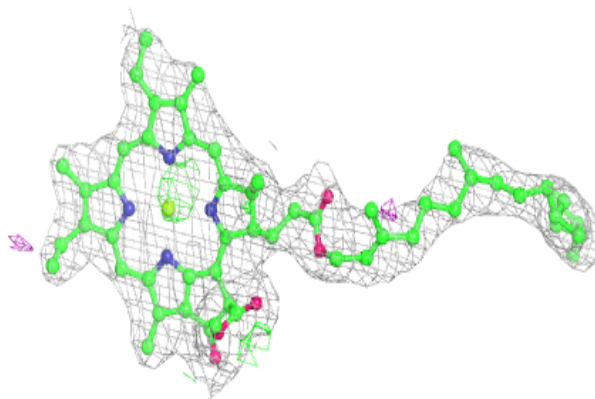
**Electron density around BCR I 4018:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

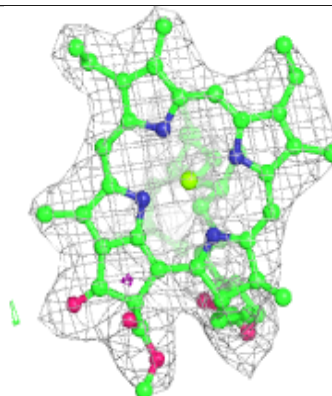
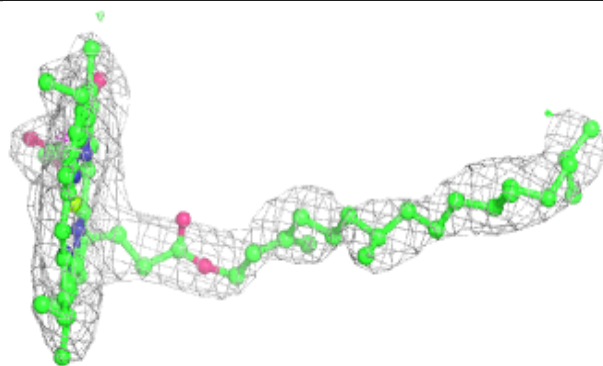
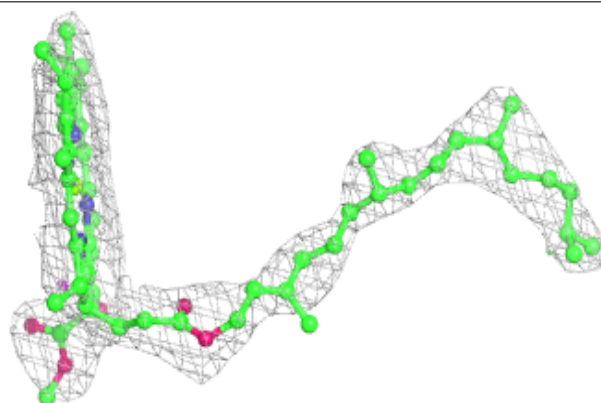


Electron density around CLA A 1103:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

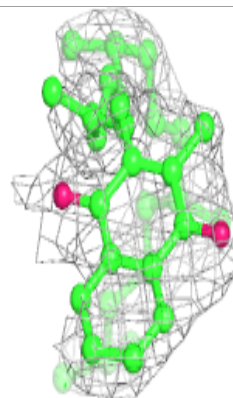
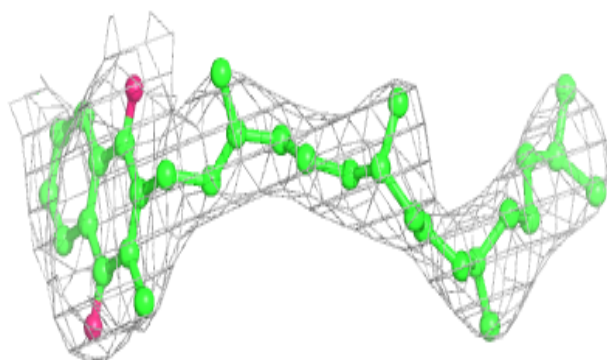
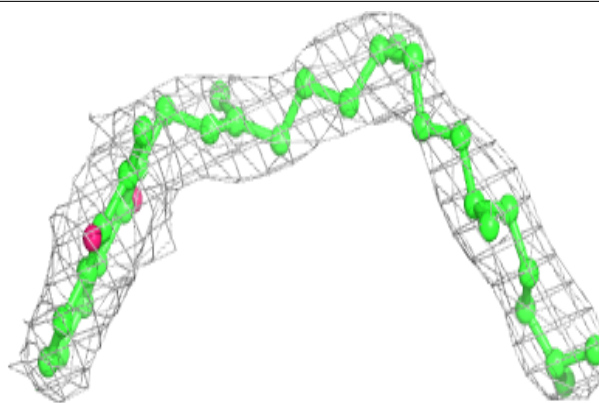
**Electron density around CLA 2 1239:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

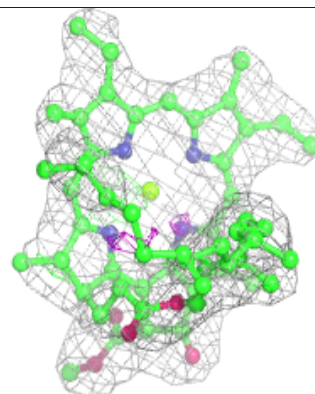
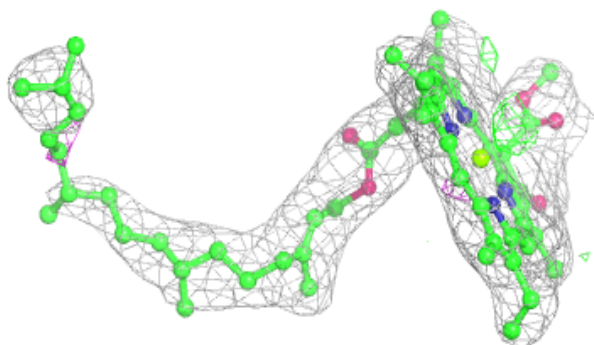
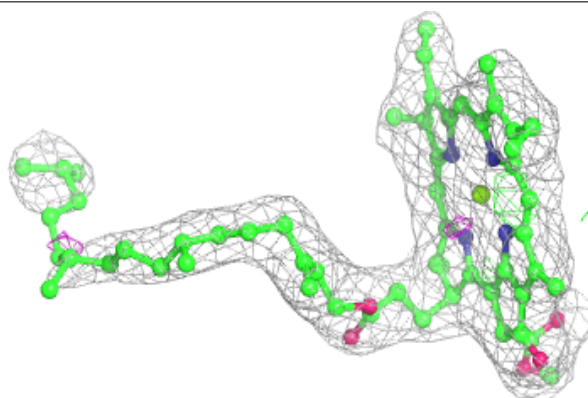


Electron density around PQN 2 2002:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

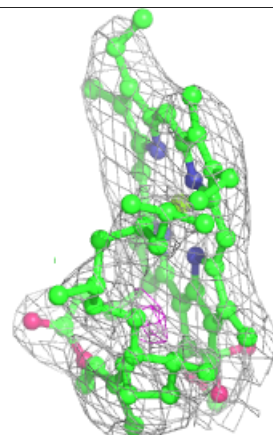
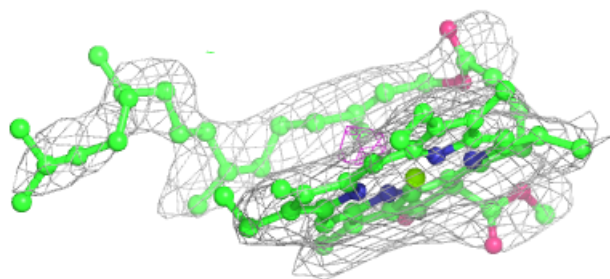
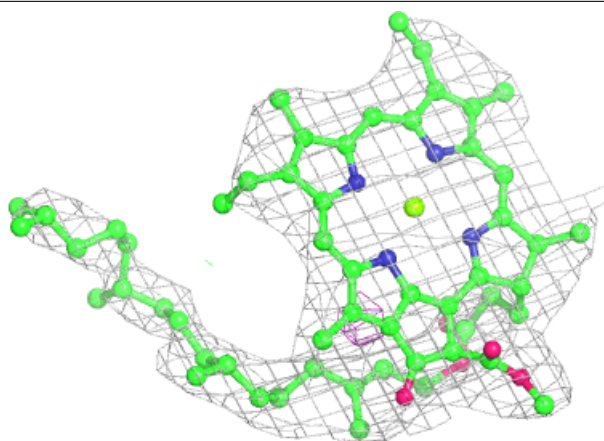
**Electron density around CLA 0 1502:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

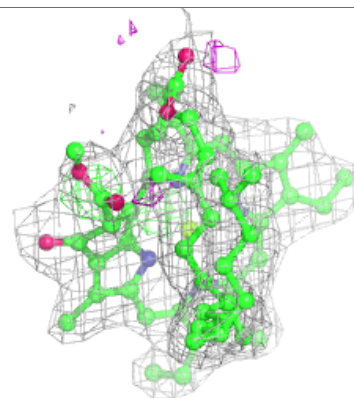
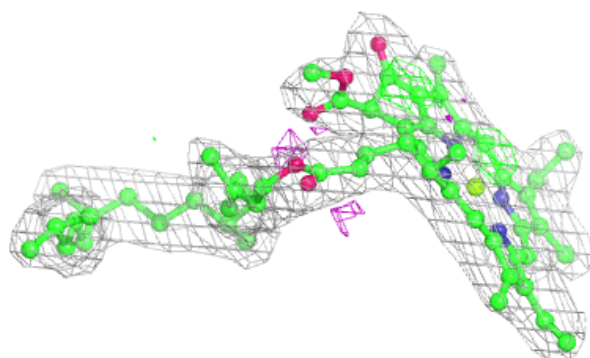
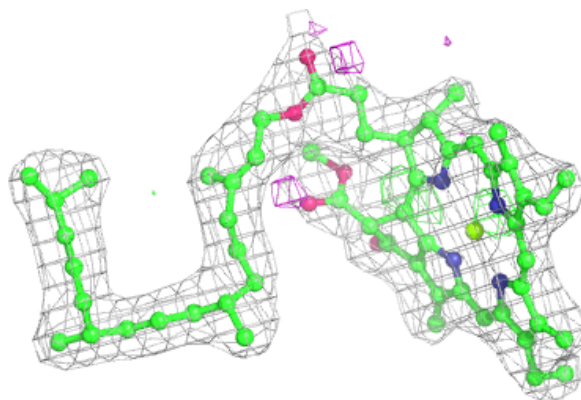


Electron density around CLA a 1127:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

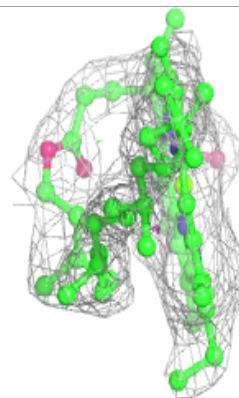
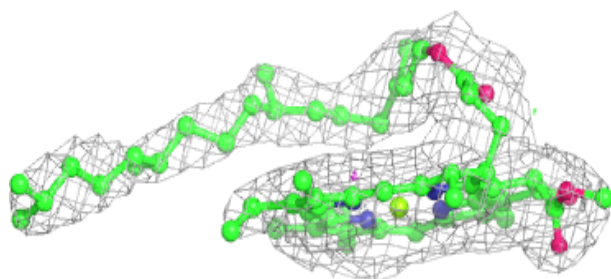
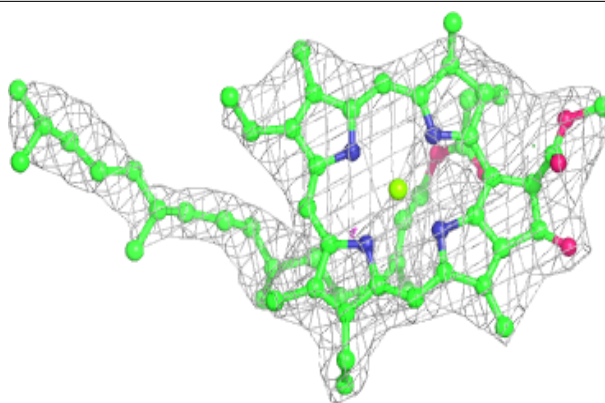
**Electron density around CLA A 1011:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

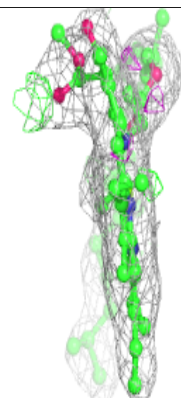
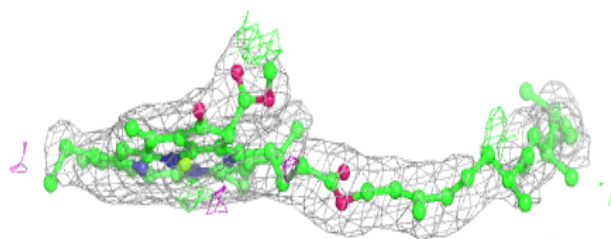
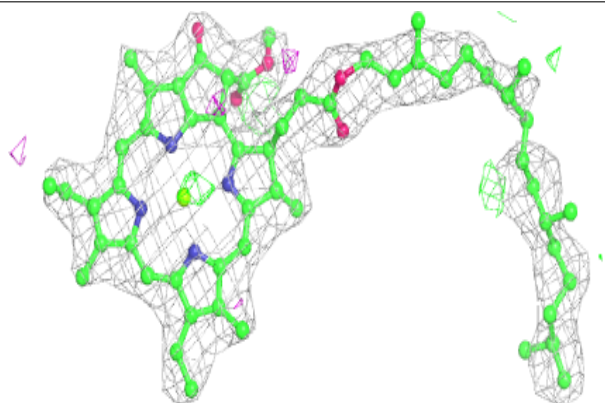


Electron density around CLA A 1138:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

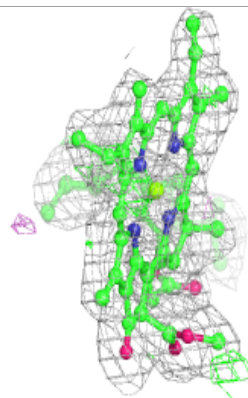
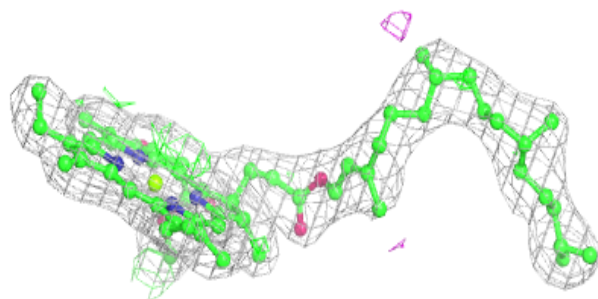
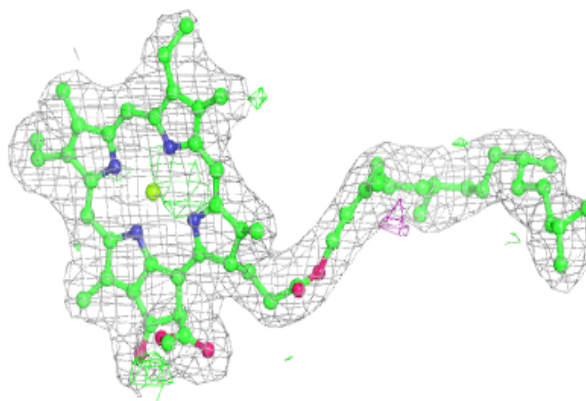
**Electron density around CLA A 1135:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



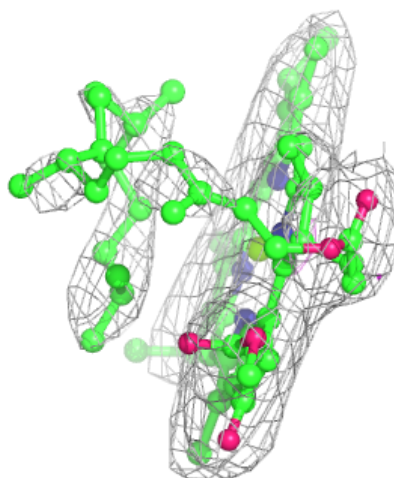
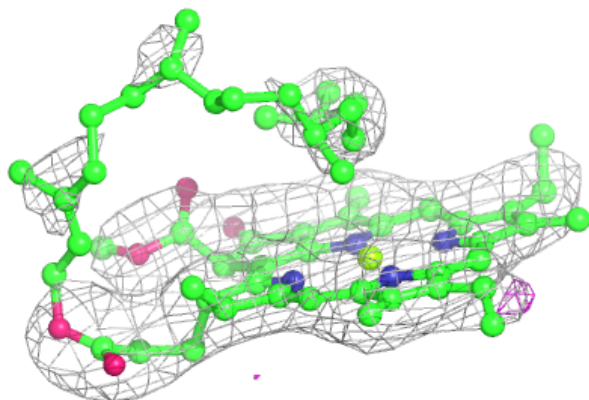
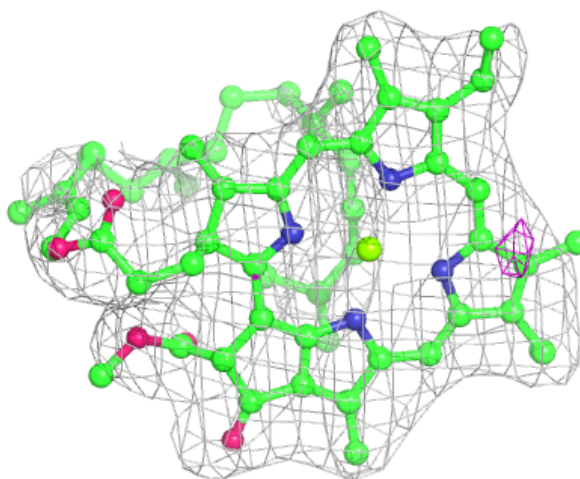
Electron density around CLA b 1210:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



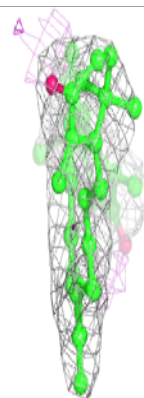
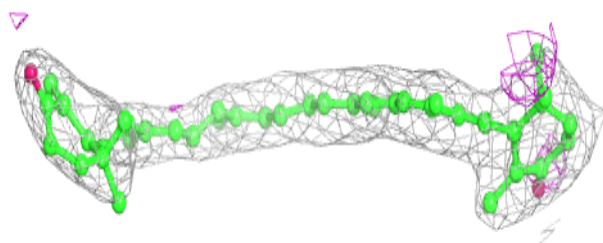
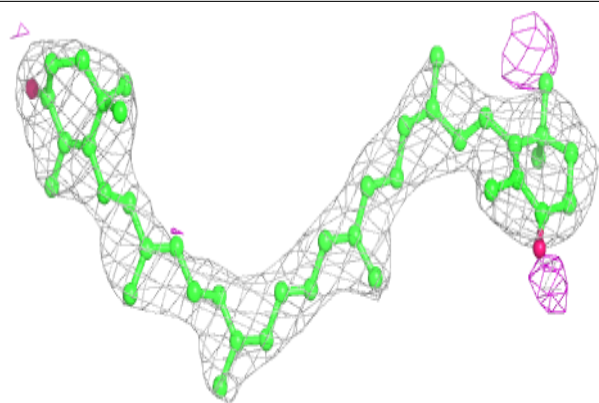
Electron density around CLA a 1104:

2mF_o-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

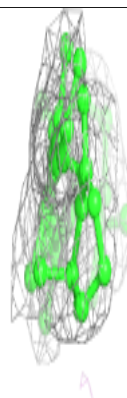
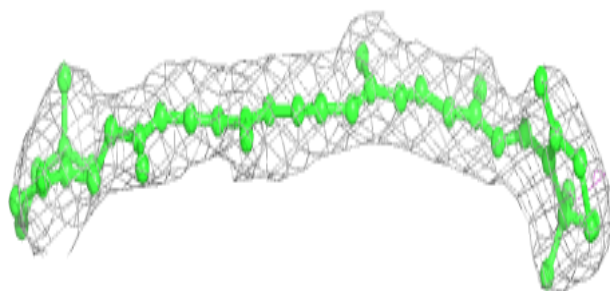
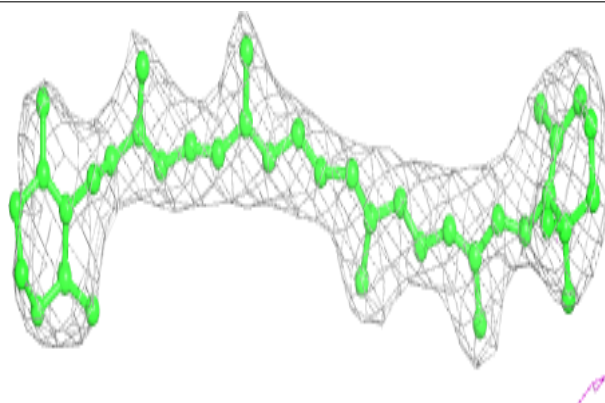


Electron density around 45D B 4011:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

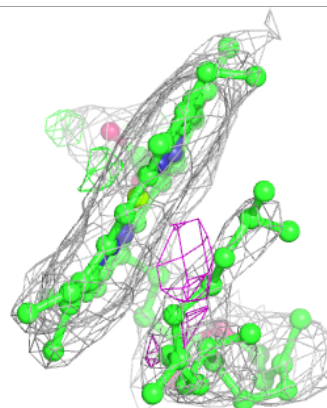
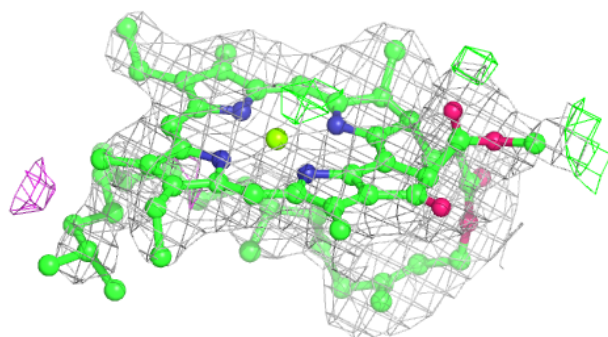
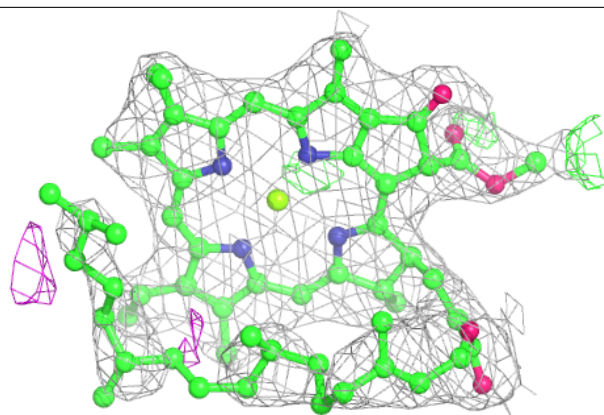
**Electron density around BCR A 4008:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

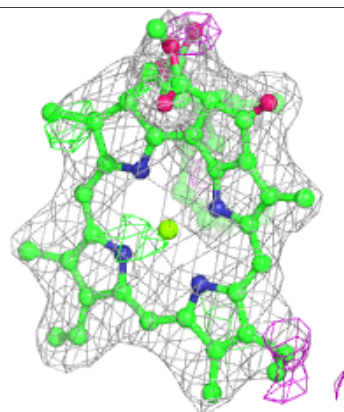
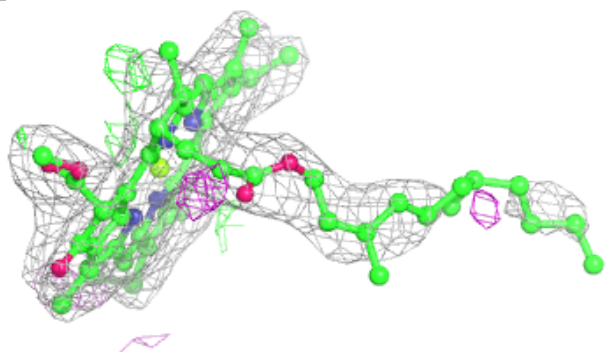
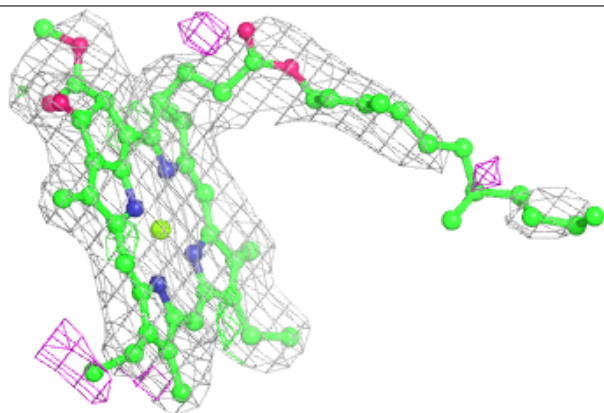


Electron density around CLA A 1118:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

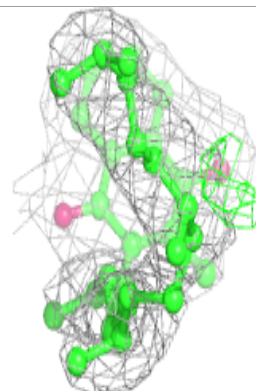
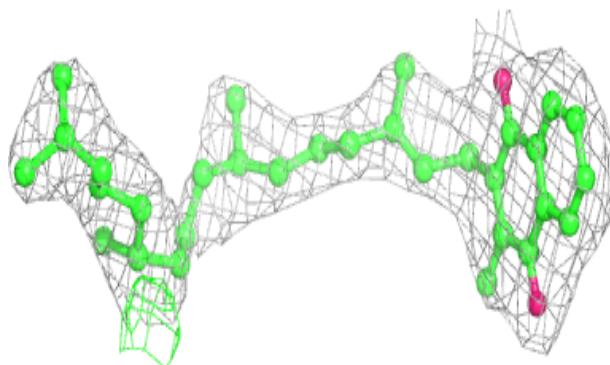
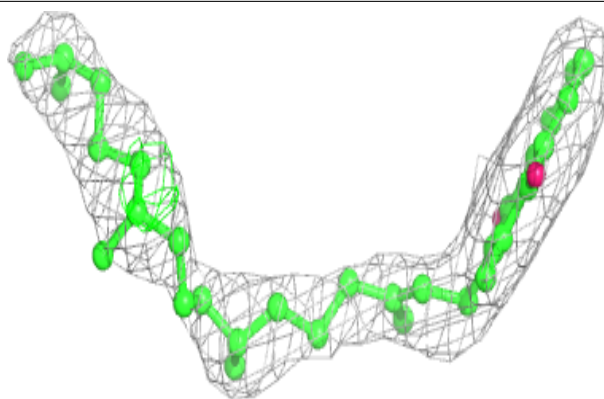
**Electron density around CLA A 1129:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

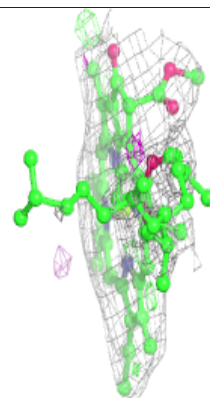
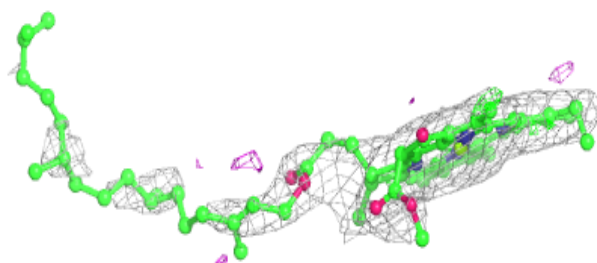
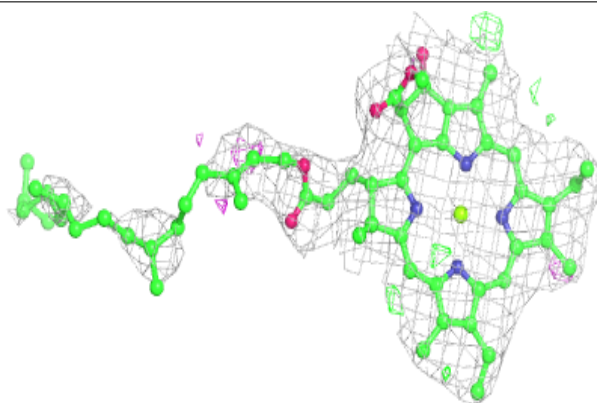


Electron density around PQN b 2002:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

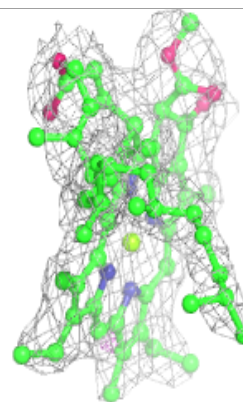
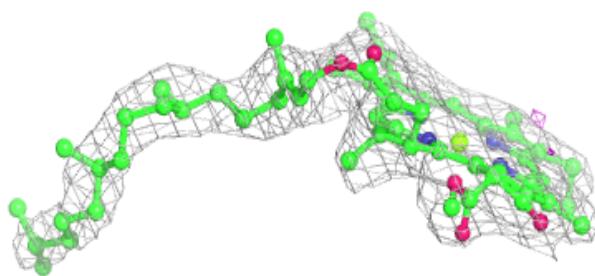
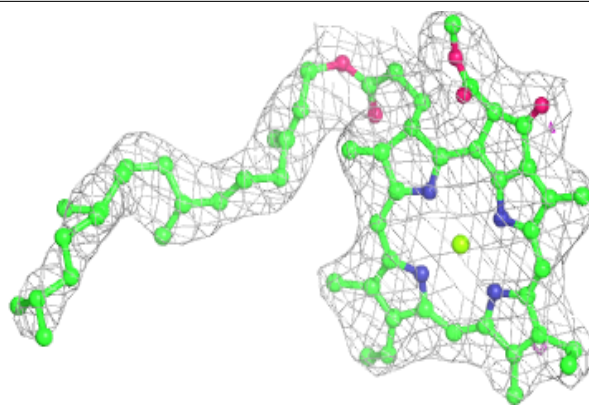
**Electron density around CLA a 1103:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

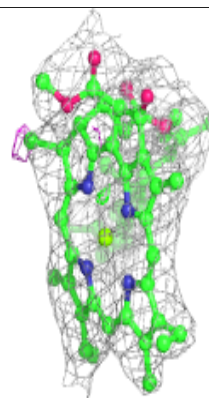
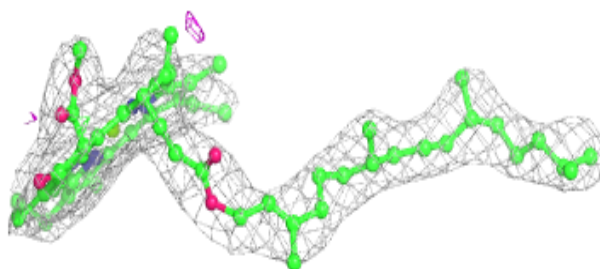
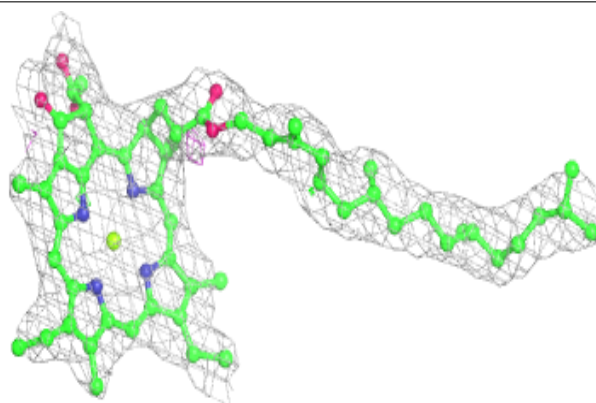


Electron density around CLA a 1013:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

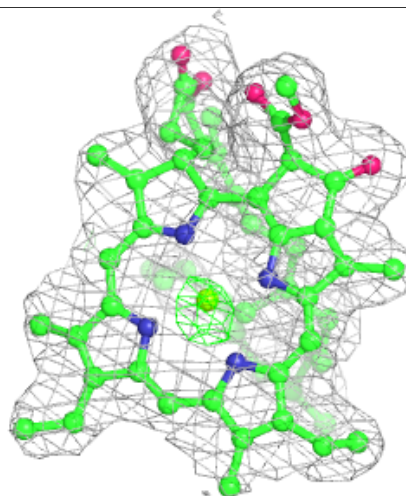
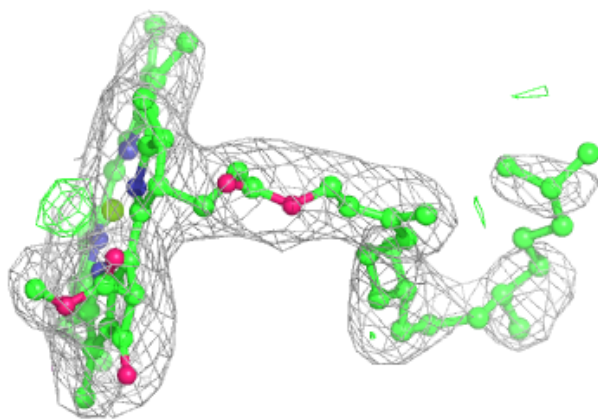
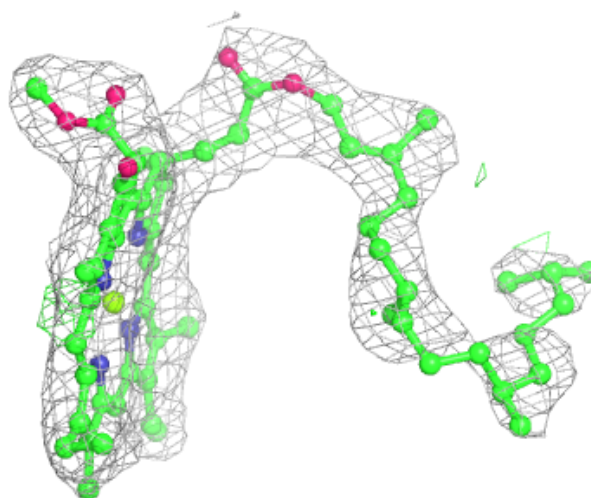
**Electron density around CLA 1 1132:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



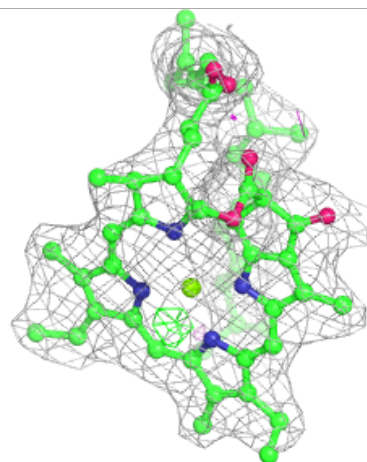
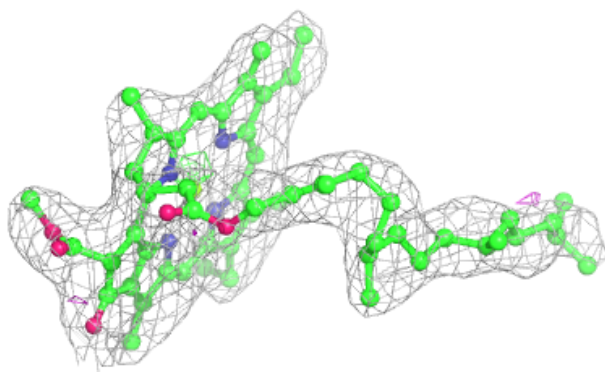
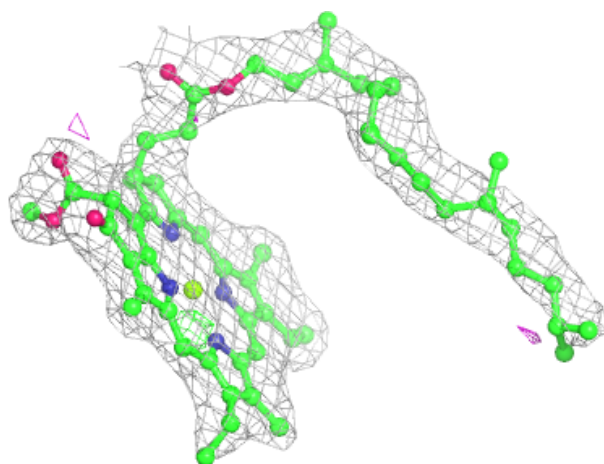
Electron density around CLA A 1801:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



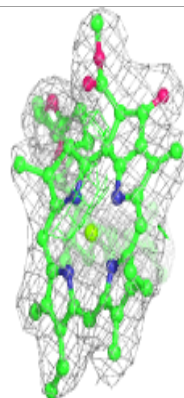
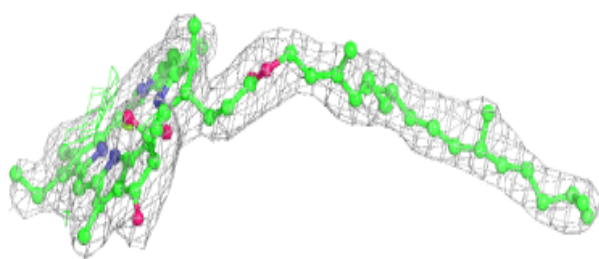
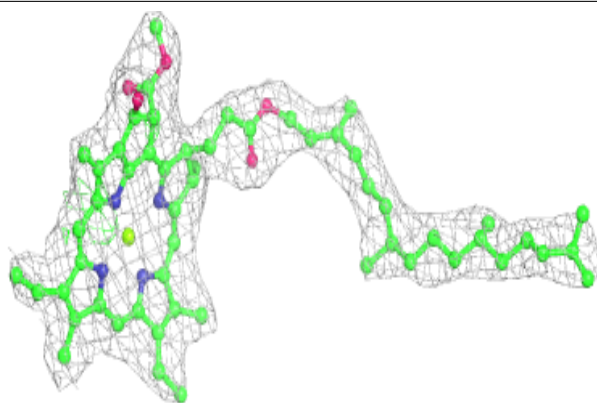
Electron density around CLA A 1102:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

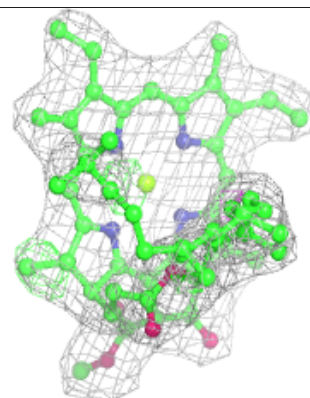
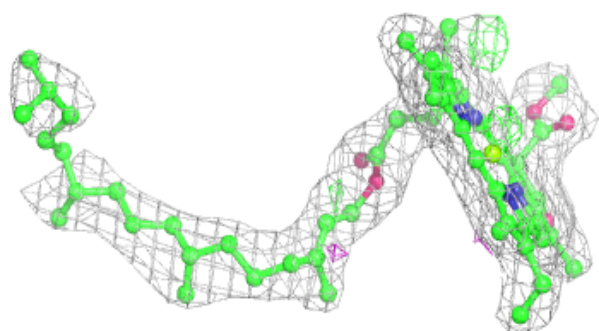
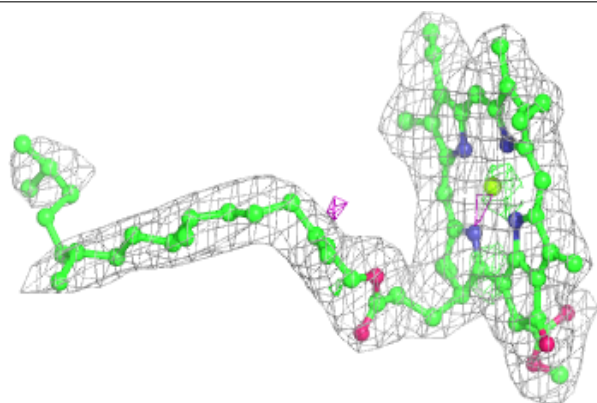


Electron density around CLA b 1022:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

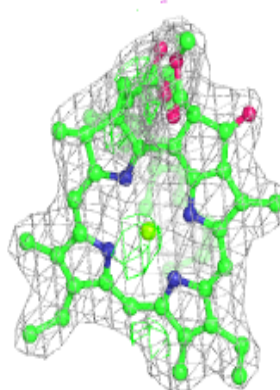
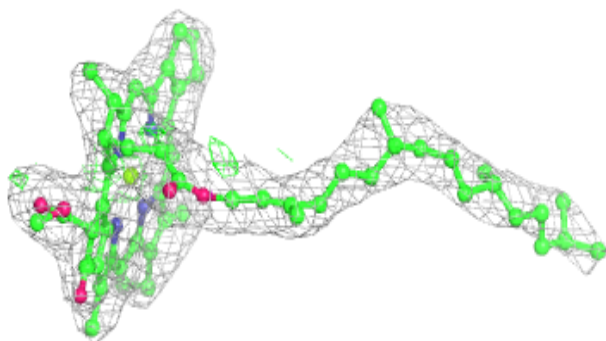
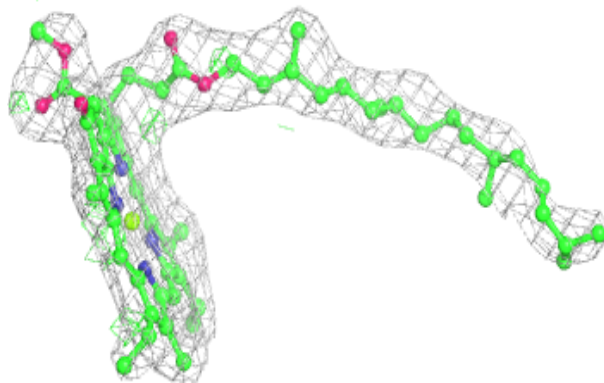
**Electron density around CLA L 1502:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

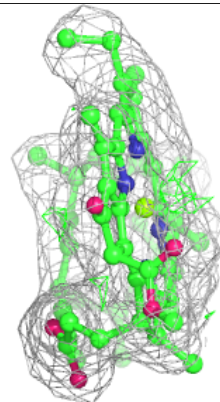
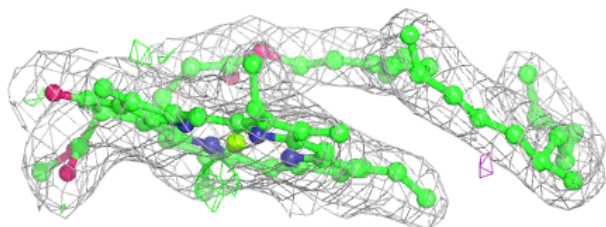
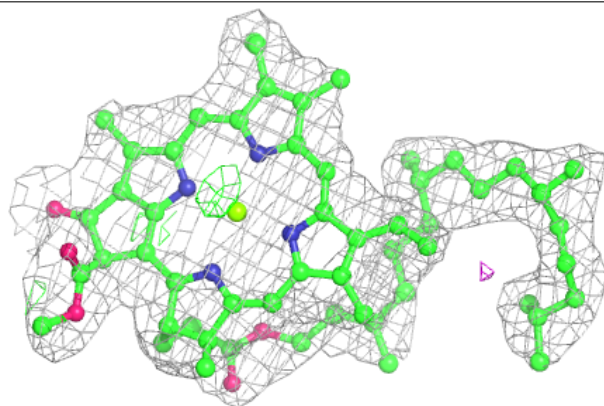


Electron density around CLA b 1201:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

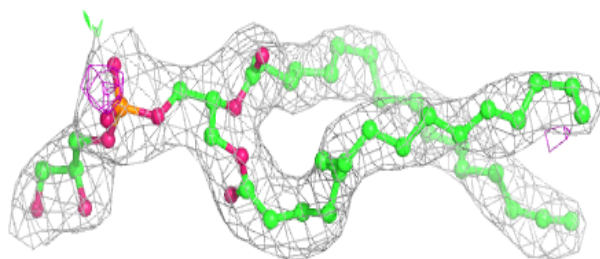
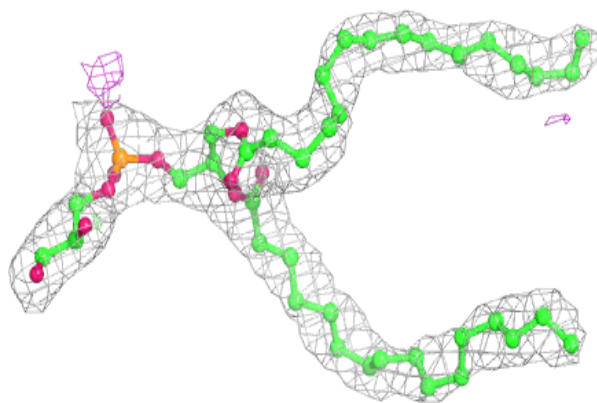
**Electron density around CLA A 1117:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



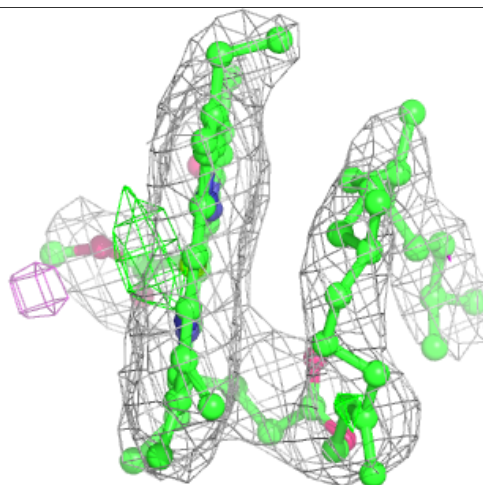
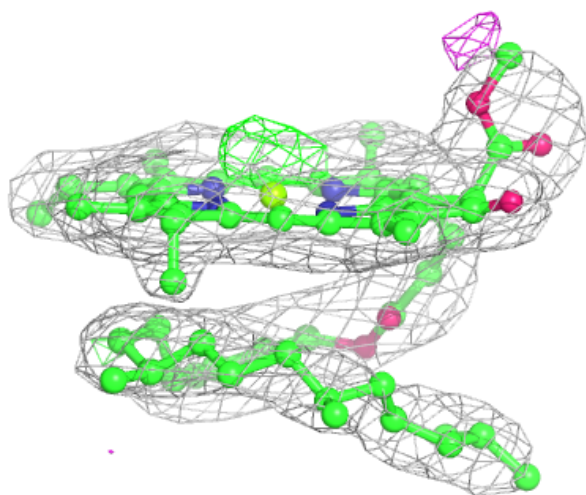
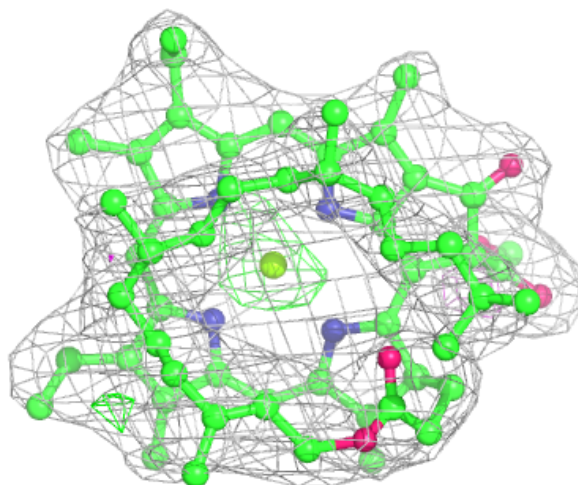
Electron density around LHG A 5001:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



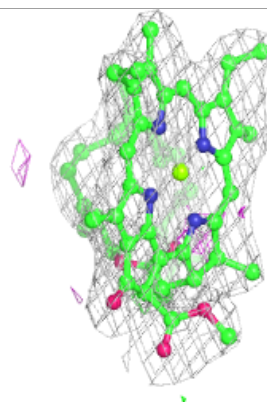
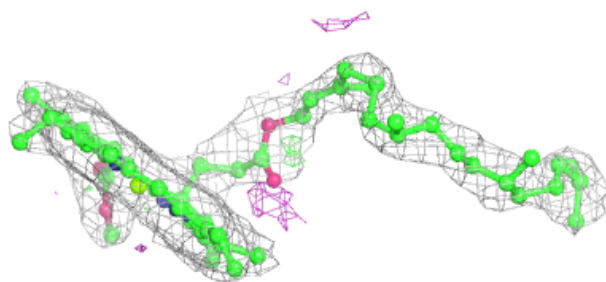
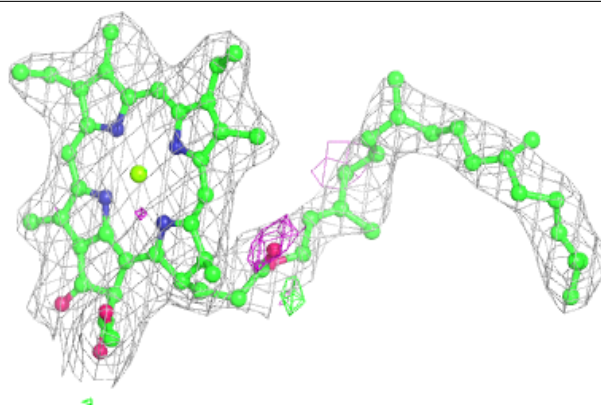
Electron density around CLA 0 1501:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

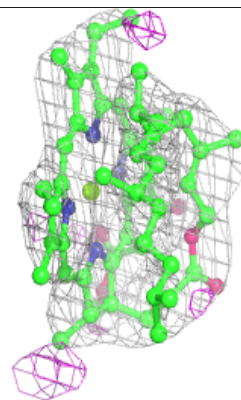
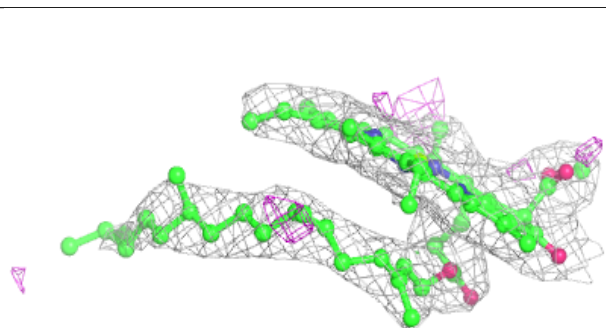
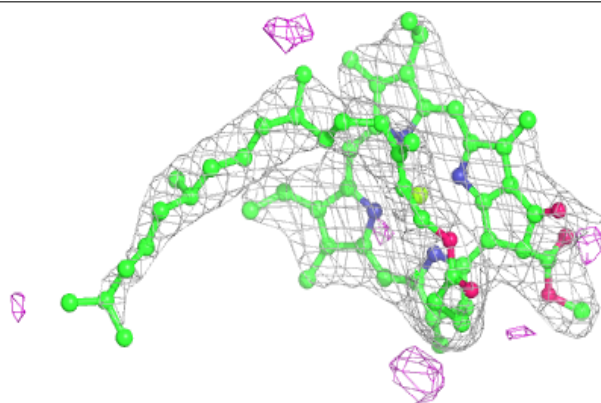


Electron density around CLA A 1106:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

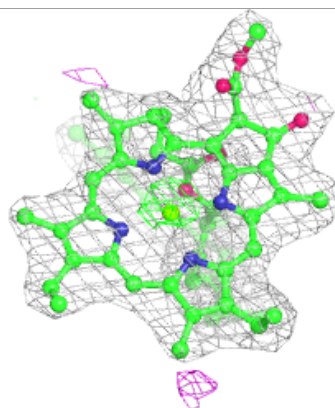
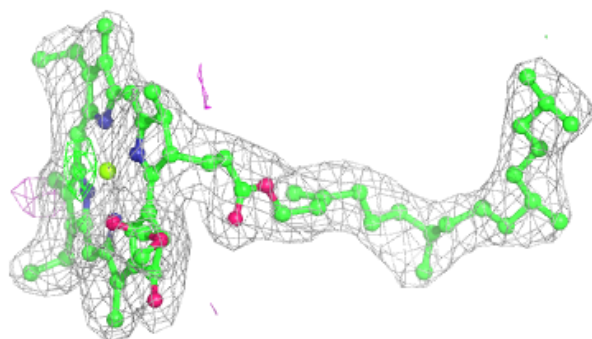
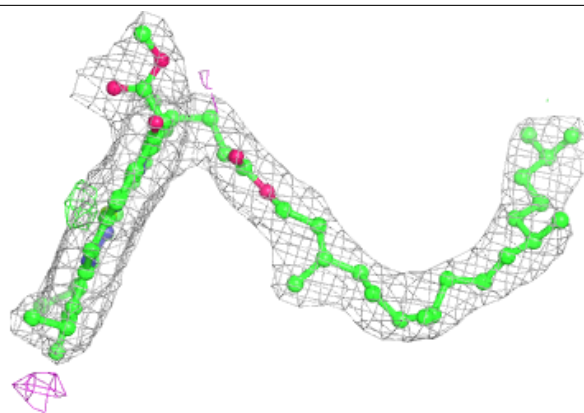
**Electron density around CLA B 1204:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

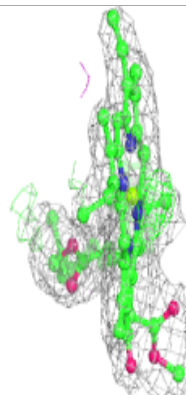
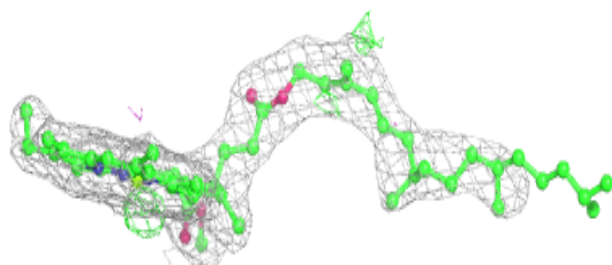
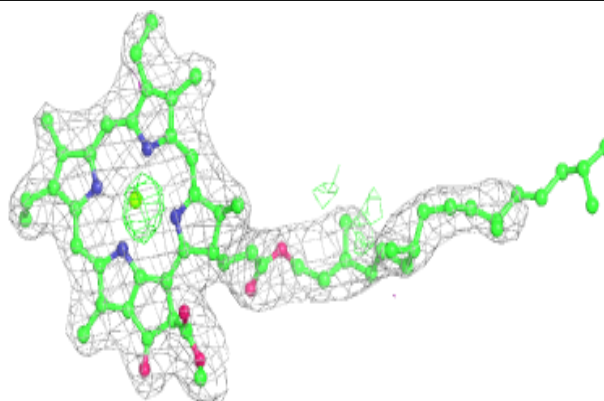


Electron density around CLA B 1238:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

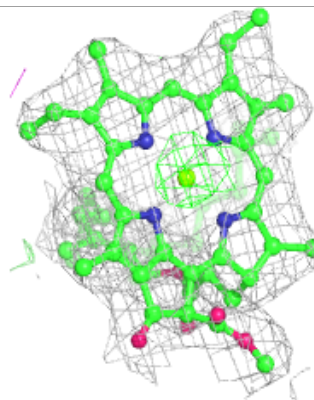
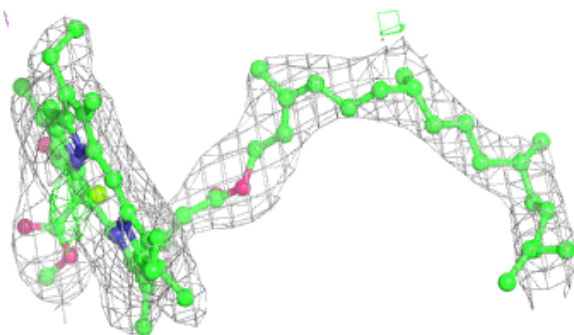
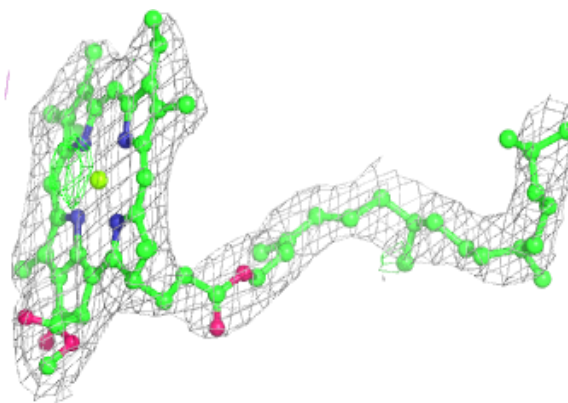
**Electron density around CLA A 1124:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

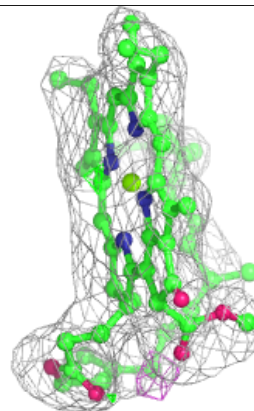
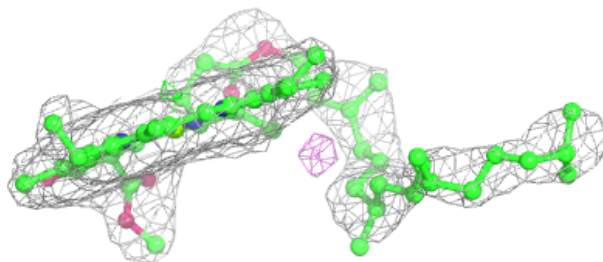
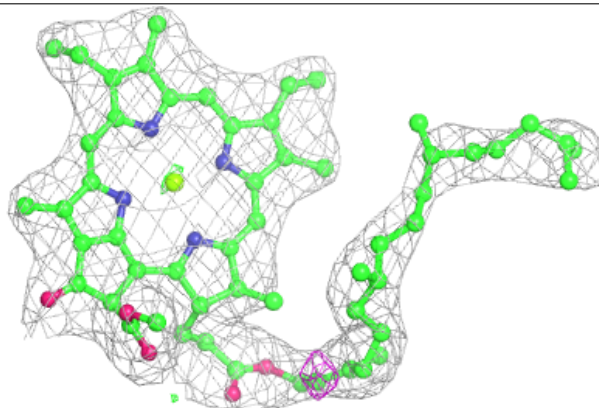


Electron density around CLA 1 1502:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

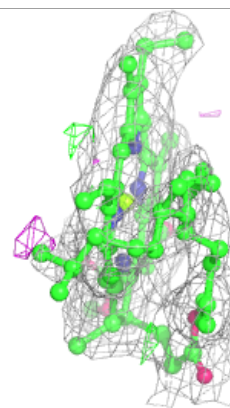
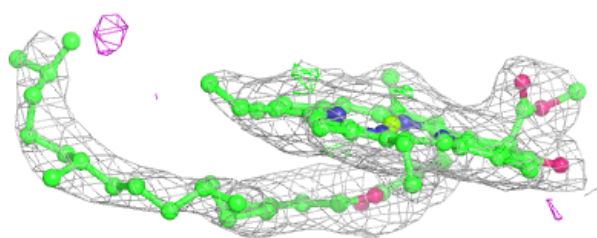
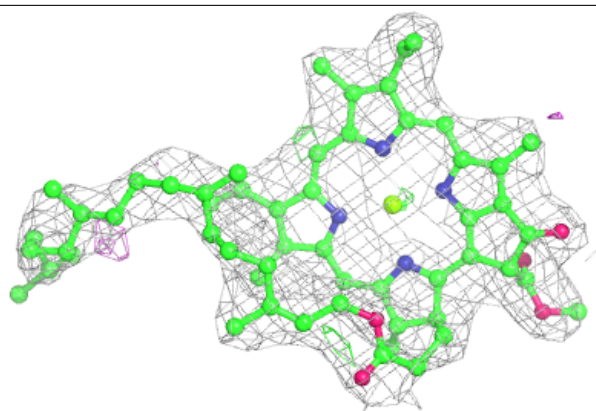
**Electron density around CLA A 1111:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

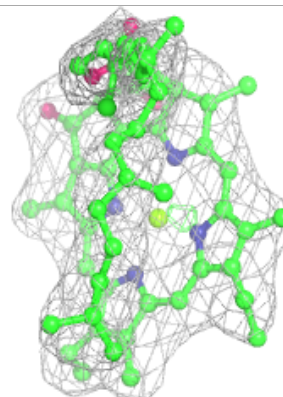
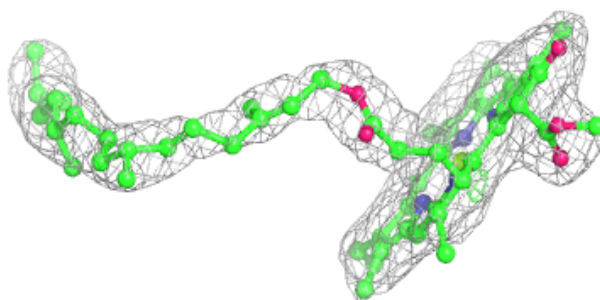
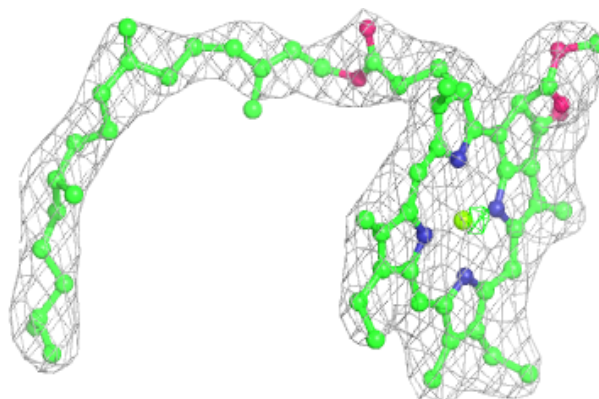


Electron density around CLA b 1215:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

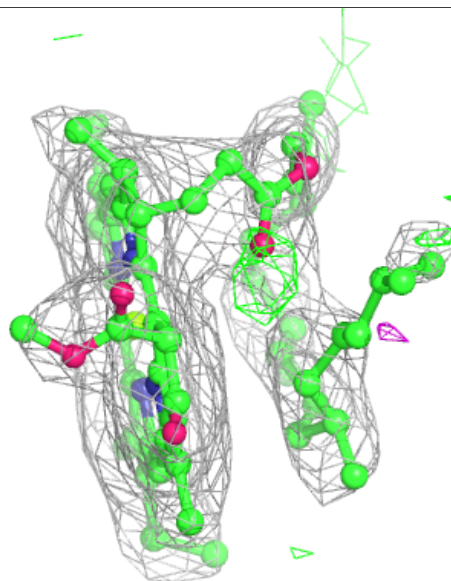
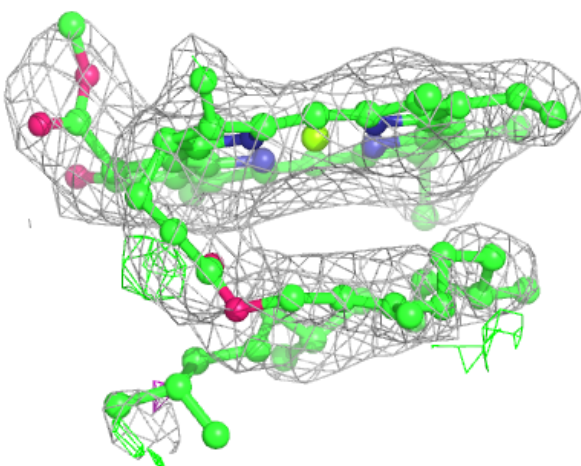
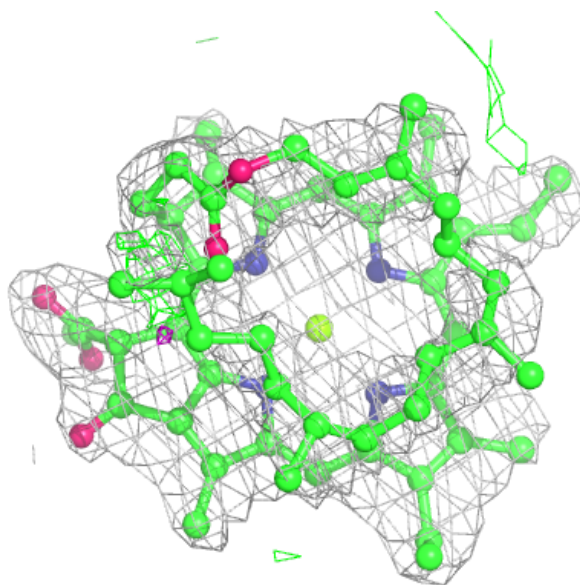
**Electron density around CLA A 1140:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



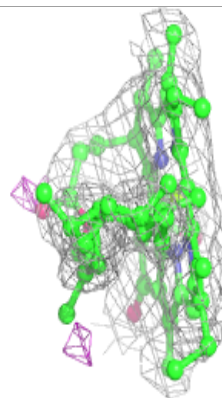
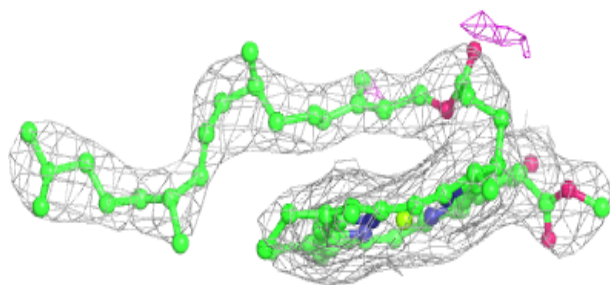
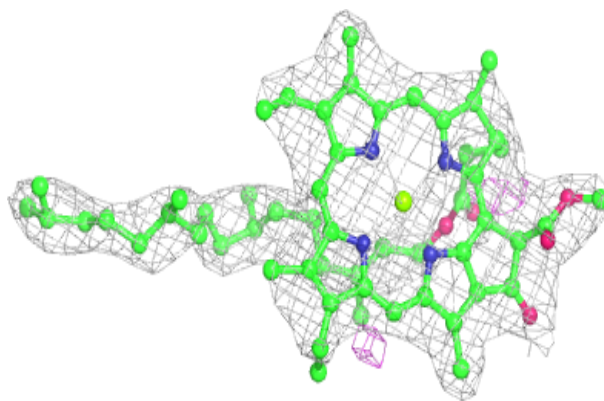
Electron density around CLA L 1501:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

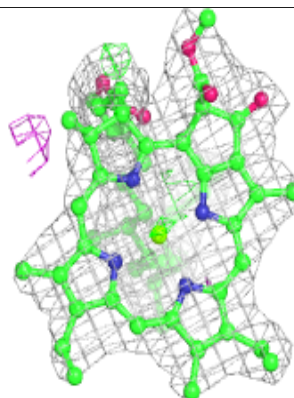
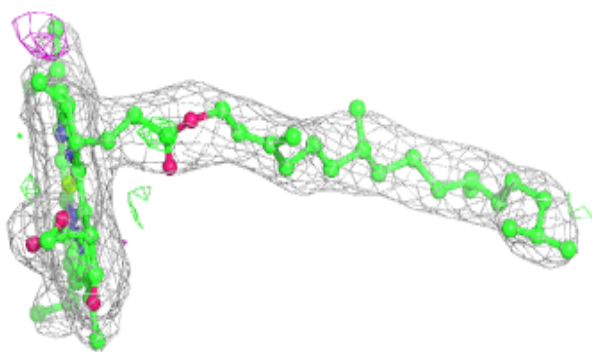
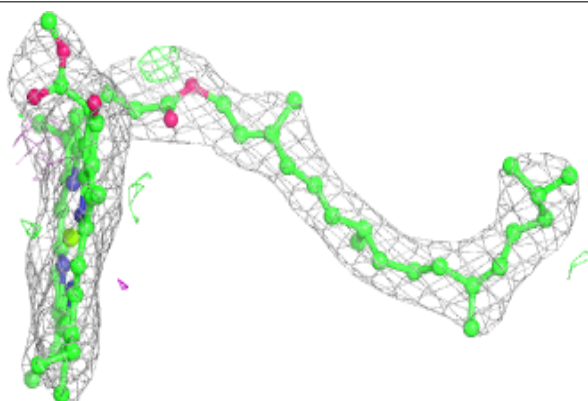


Electron density around CLA 1 1136:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

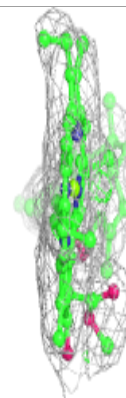
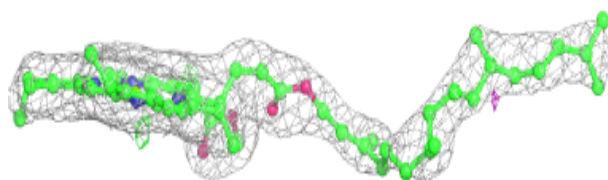
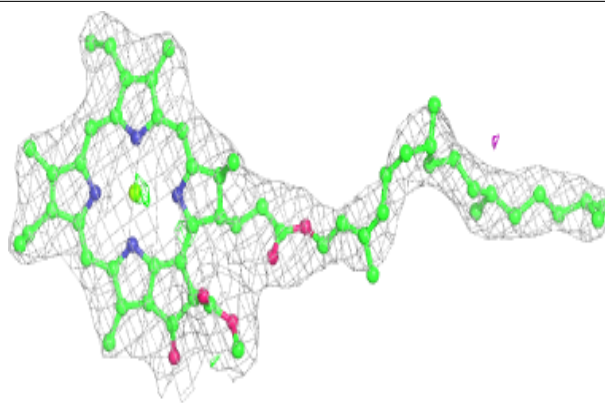
**Electron density around CLA b 1239:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

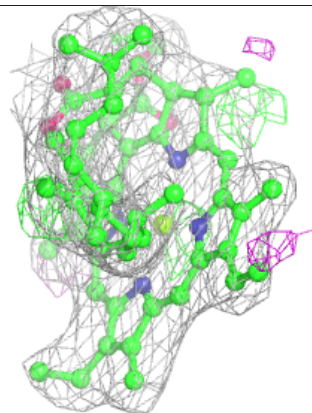
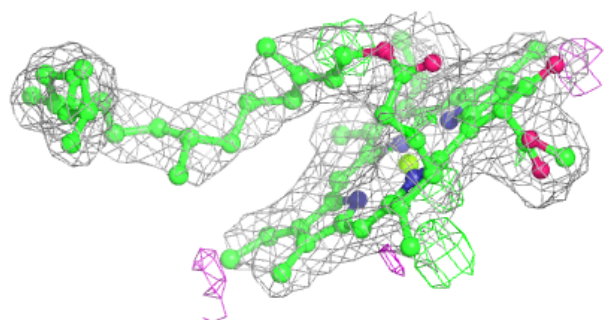
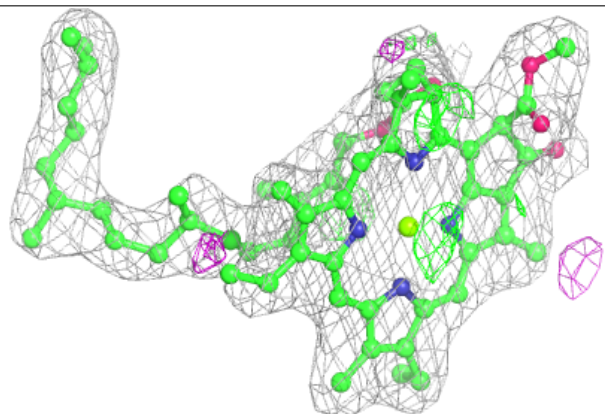


Electron density around CLA 1 1131:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

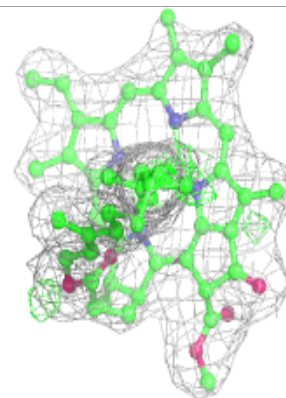
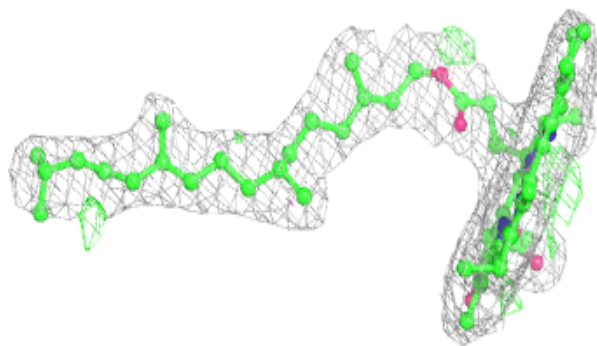
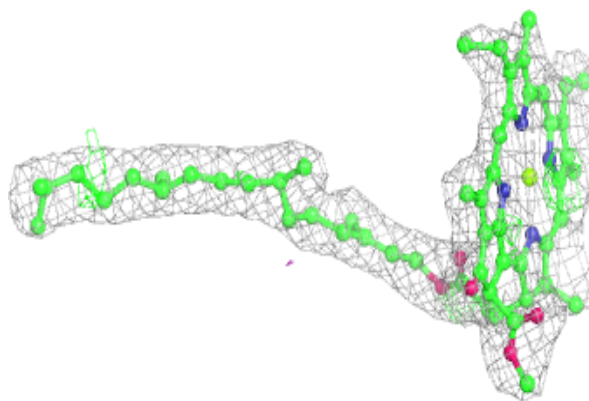
**Electron density around CLA B 1237:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

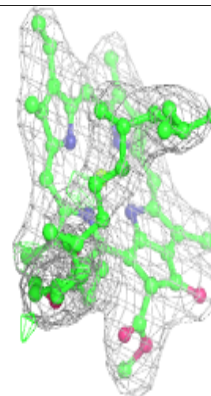
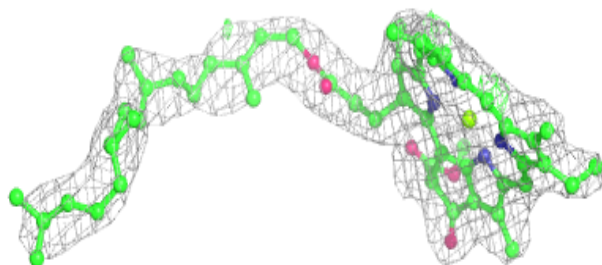
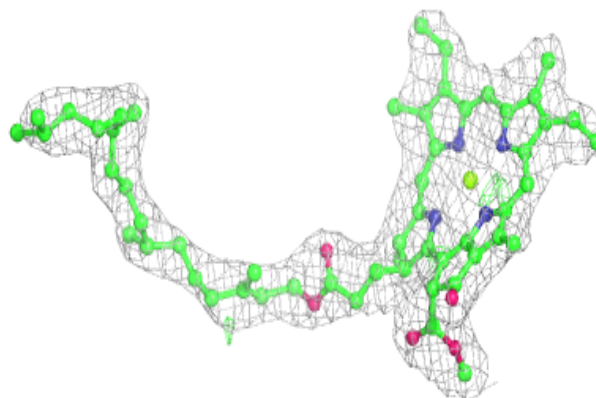


Electron density around CLA b 1225:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

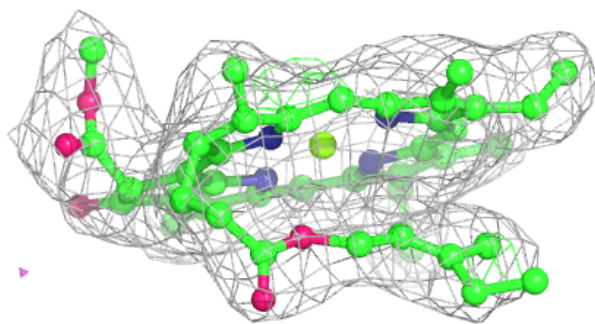
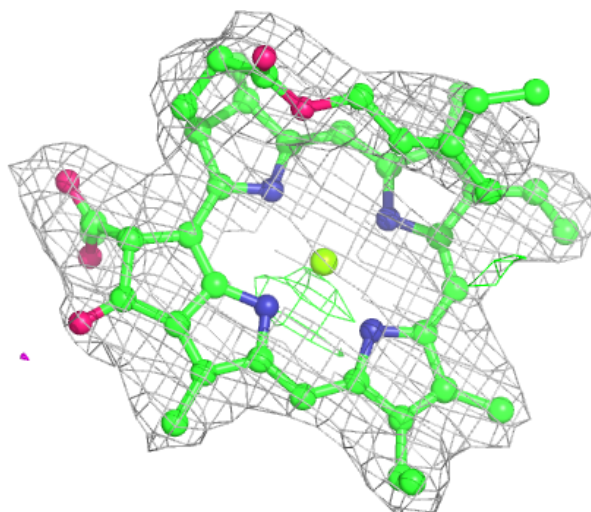
**Electron density around CLA A 1012:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



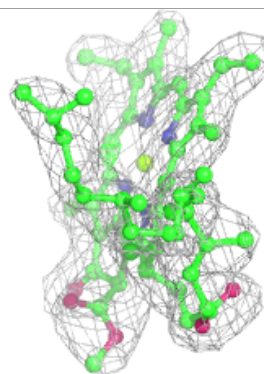
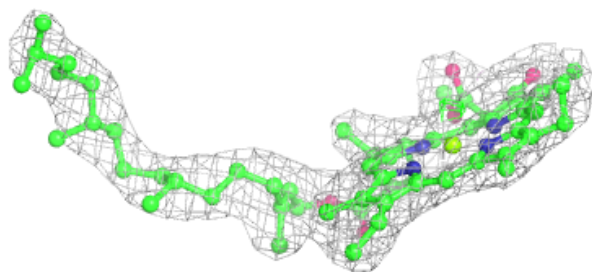
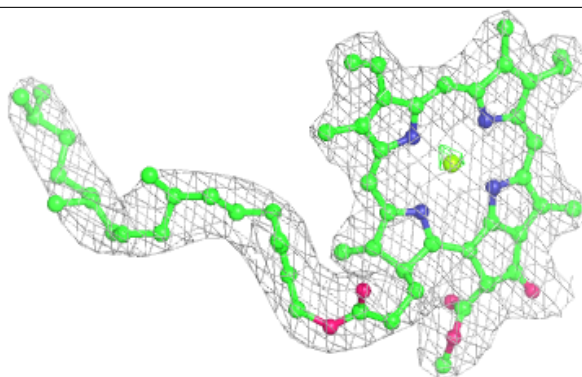
Electron density around CLA b 1217:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

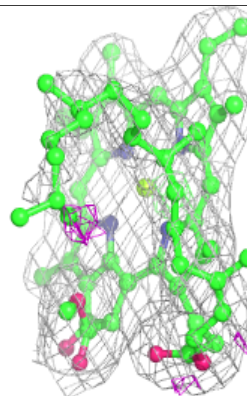
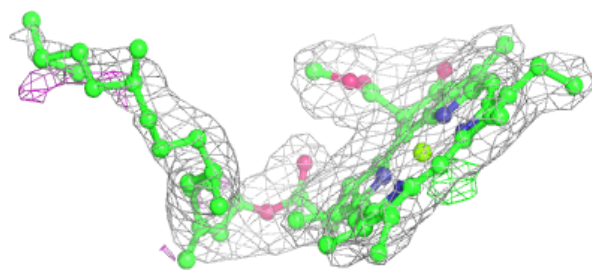
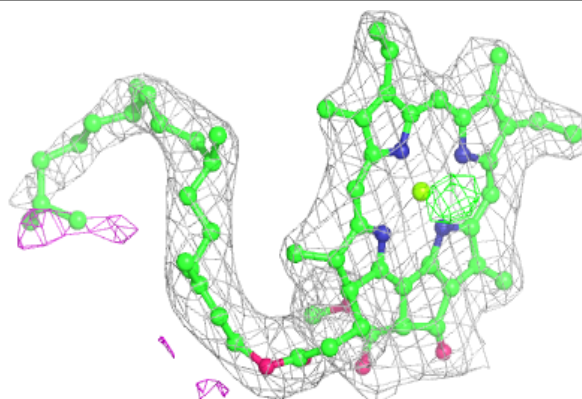


Electron density around CLA A 1013:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

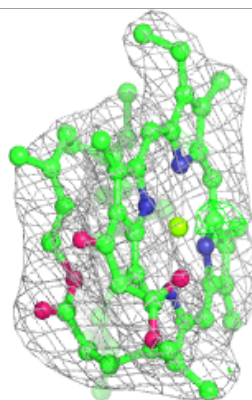
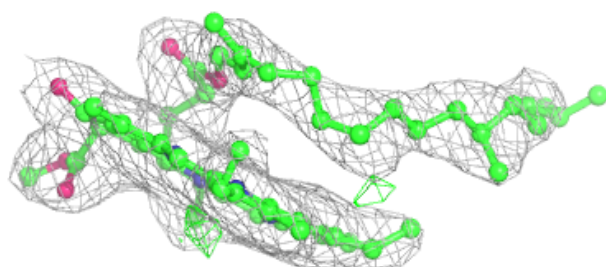
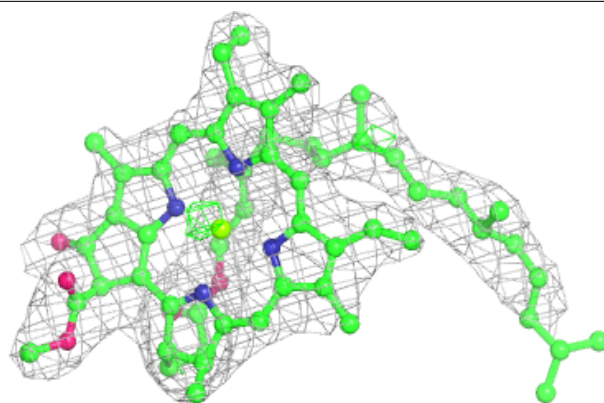
**Electron density around CLA b 1221:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

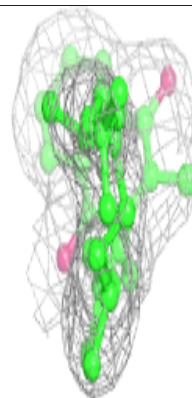
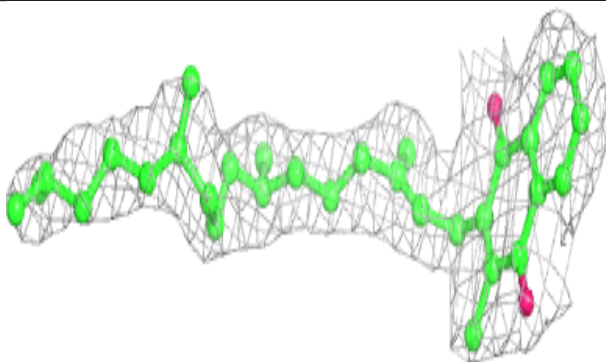
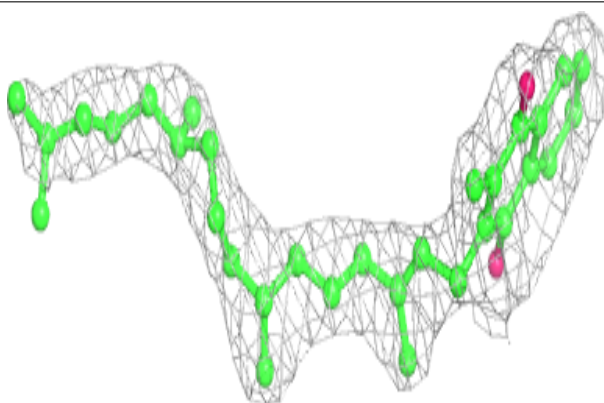


Electron density around CLA b 1204:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

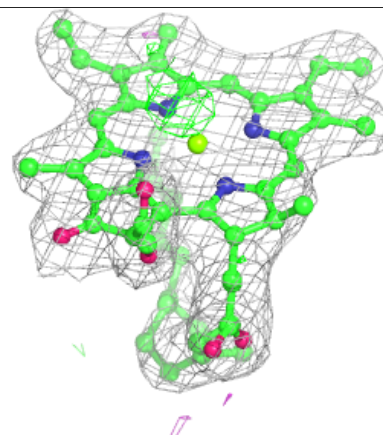
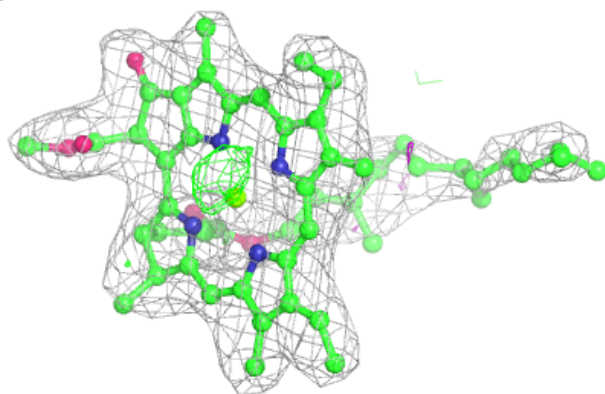
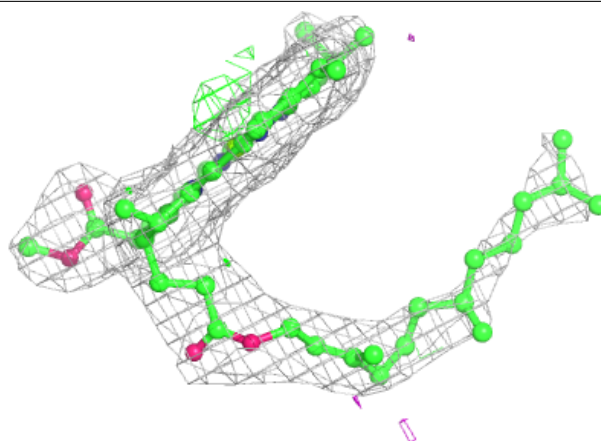
**Electron density around PQN A 2001:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

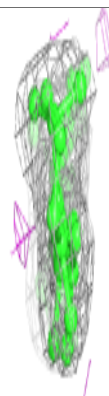
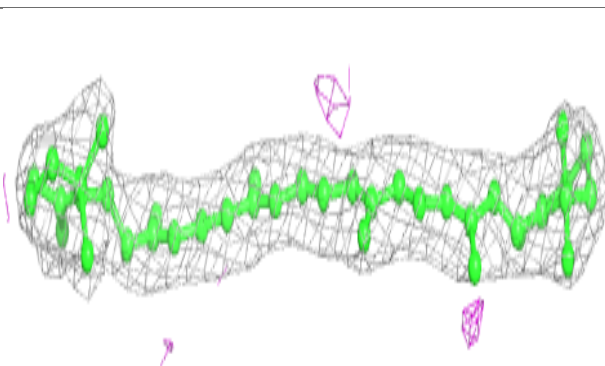
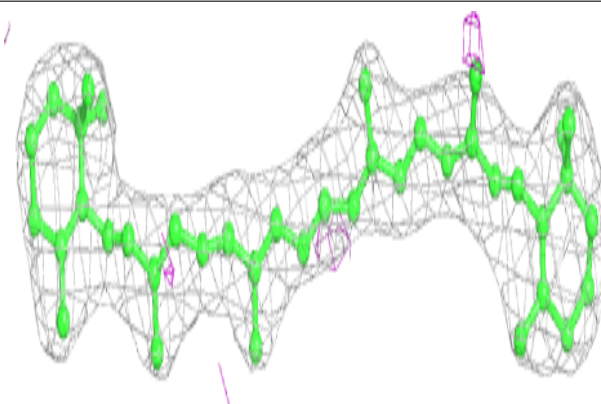


Electron density around CLA A 1130:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

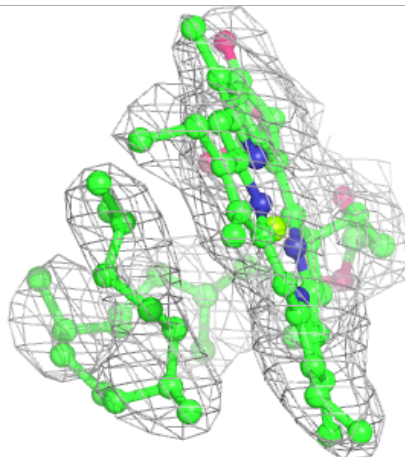
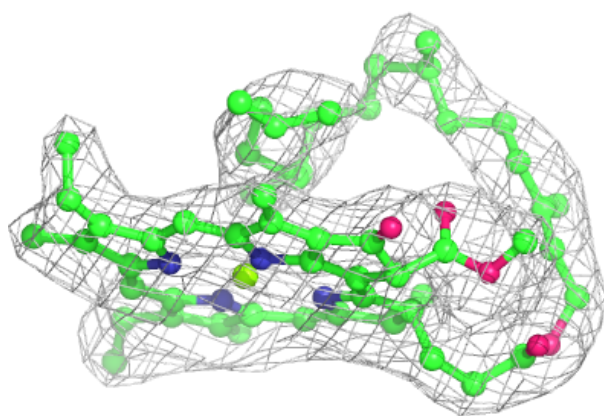
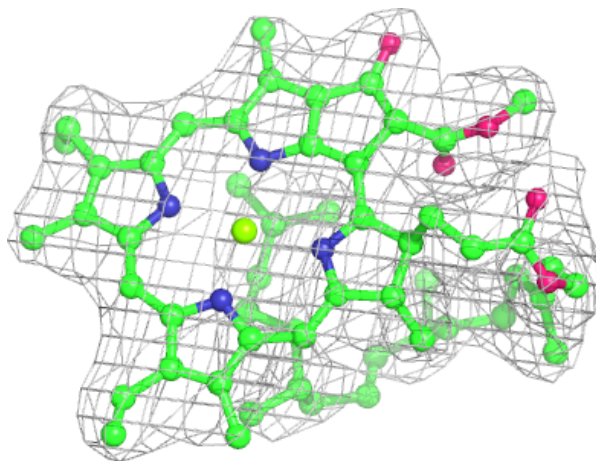
**Electron density around BCR L 4019:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



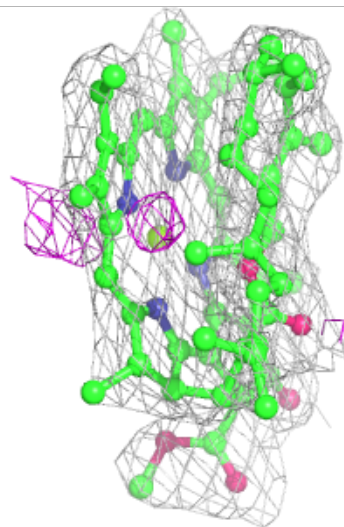
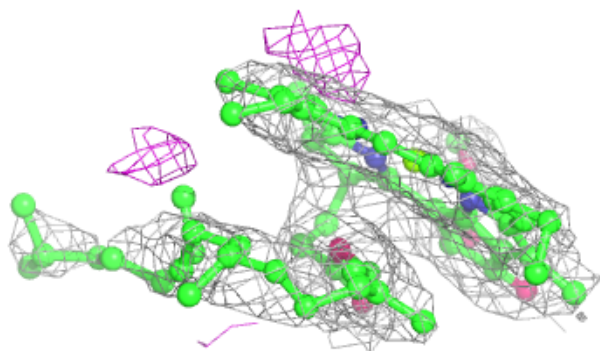
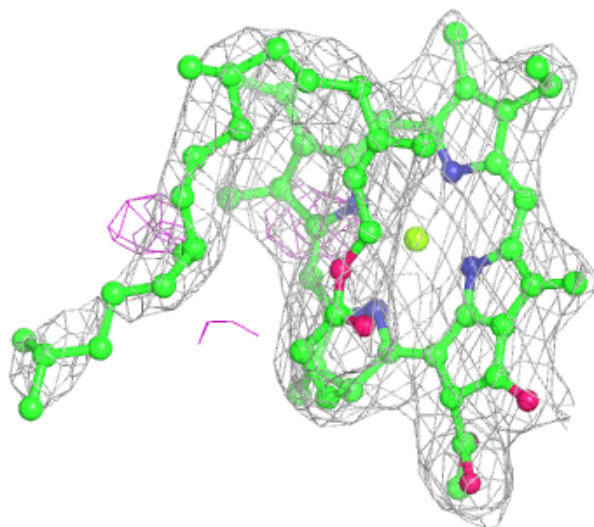
Electron density around CLA B 1203:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



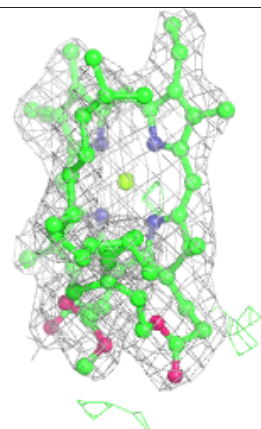
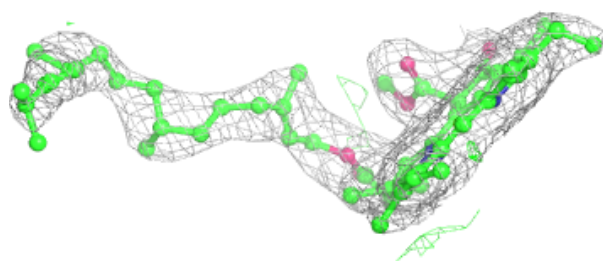
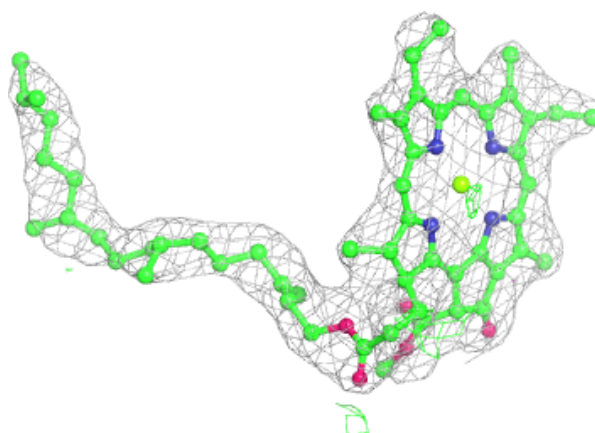
Electron density around CLA B 1205:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

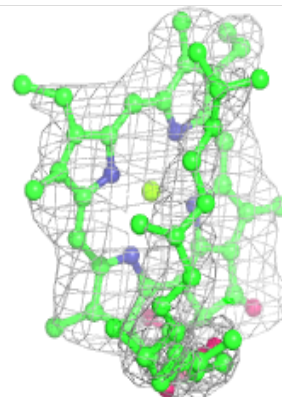
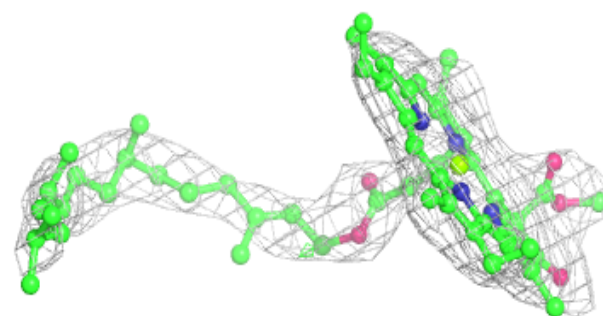
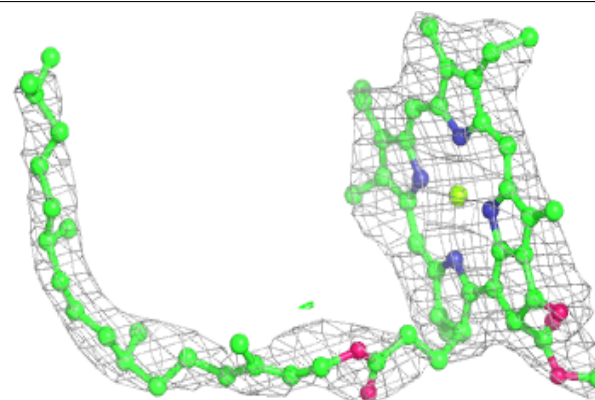


Electron density around CLA b 1207:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

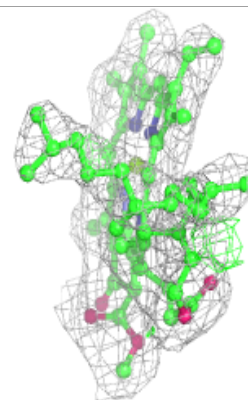
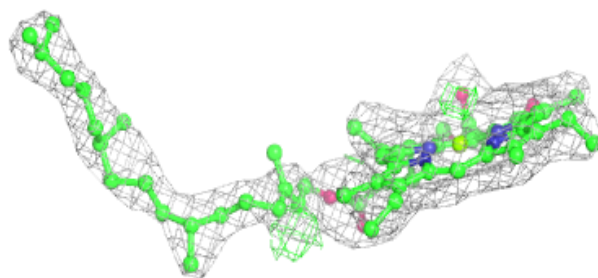
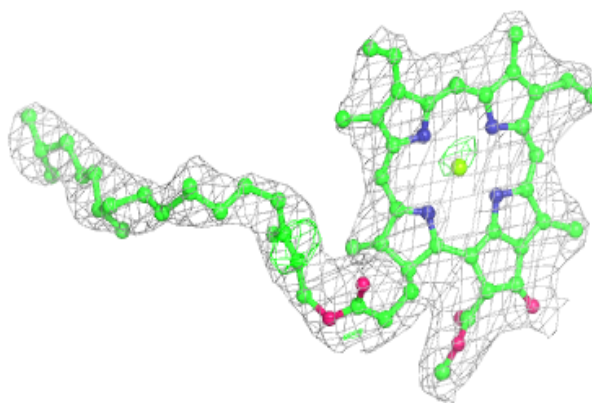
**Electron density around CLA a 1140:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



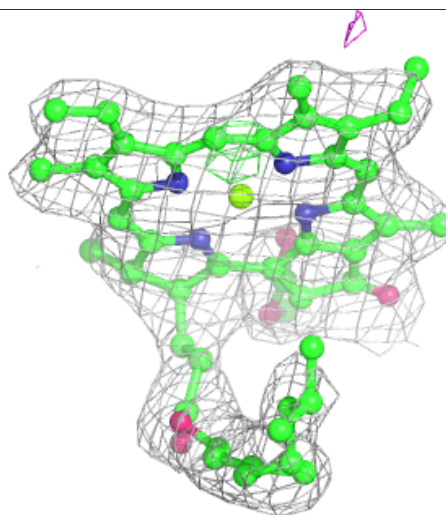
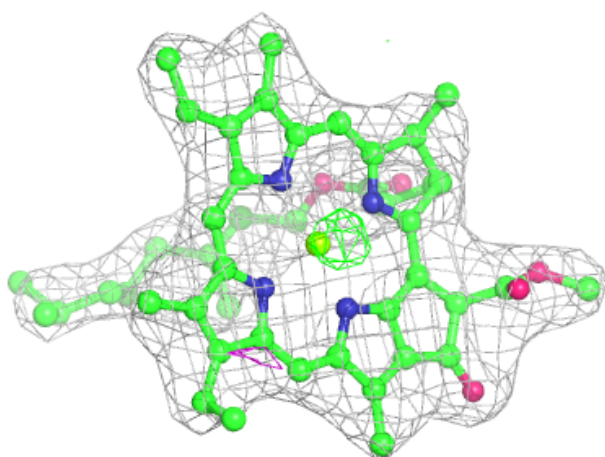
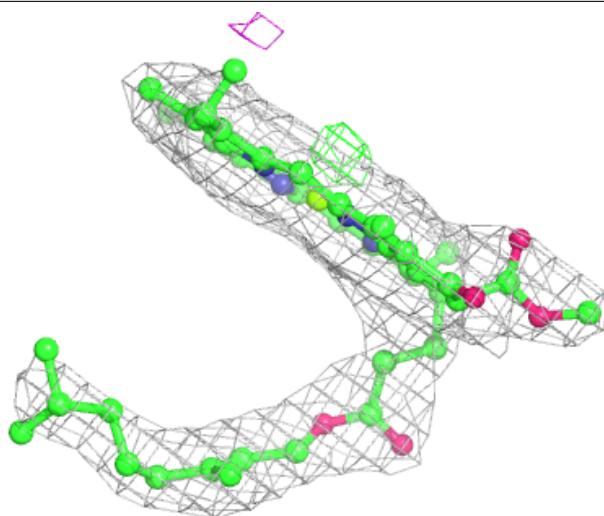
Electron density around CLA b 1023:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



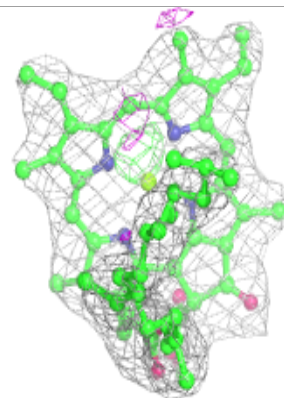
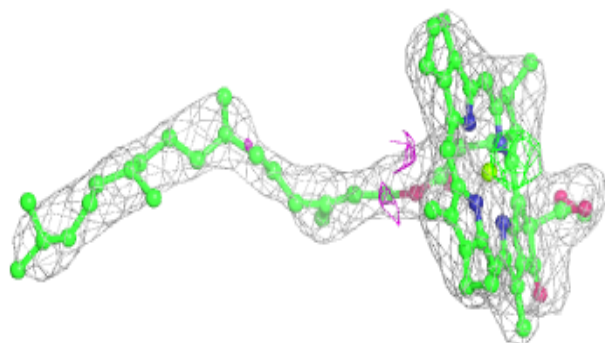
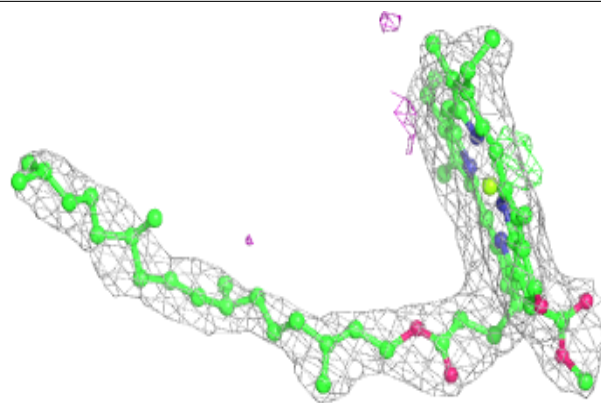
Electron density around CLA 1 1130:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

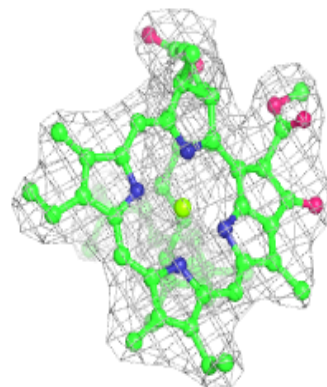
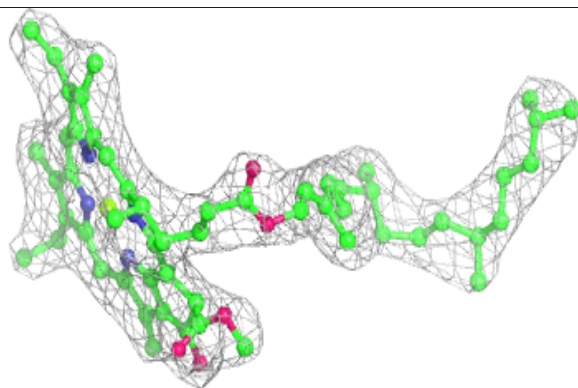
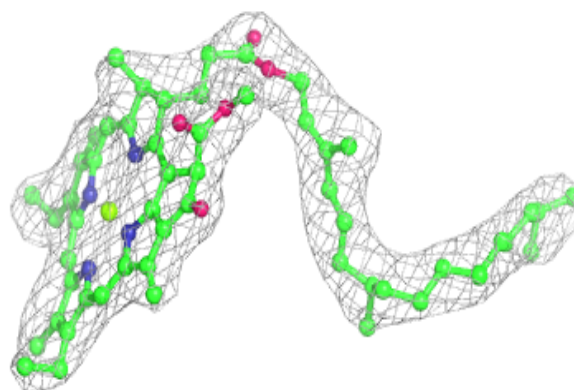


Electron density around CLA B 1201:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

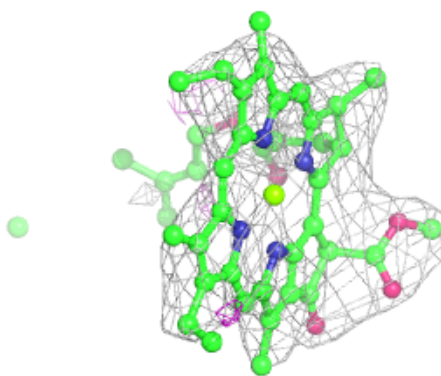
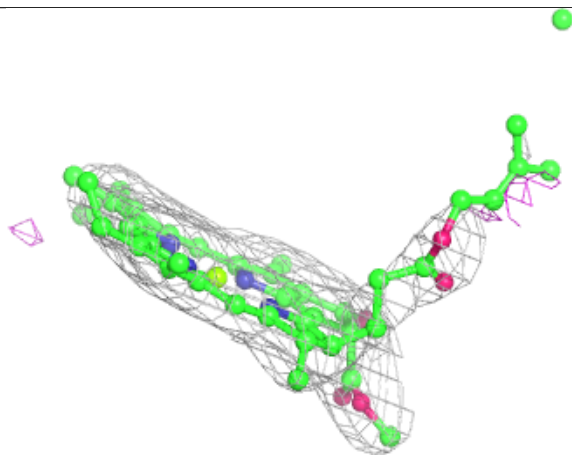
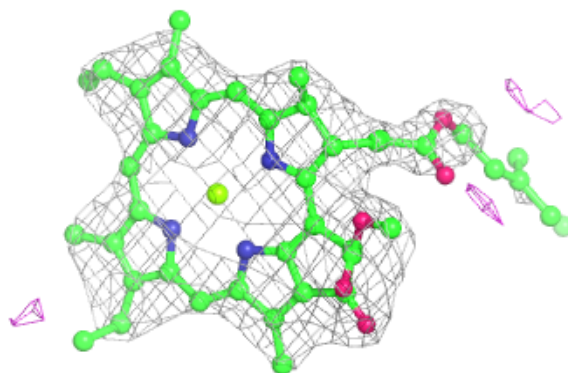
**Electron density around CLA B 1021:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



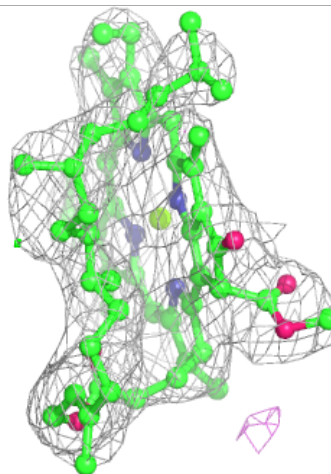
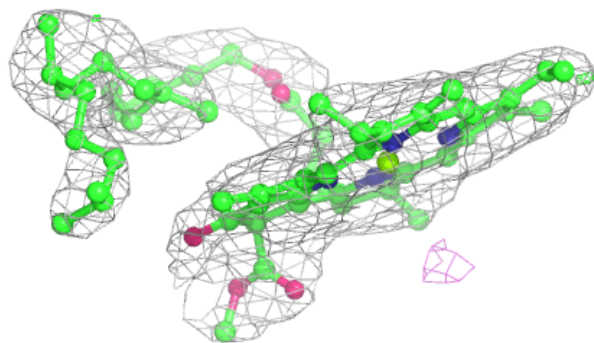
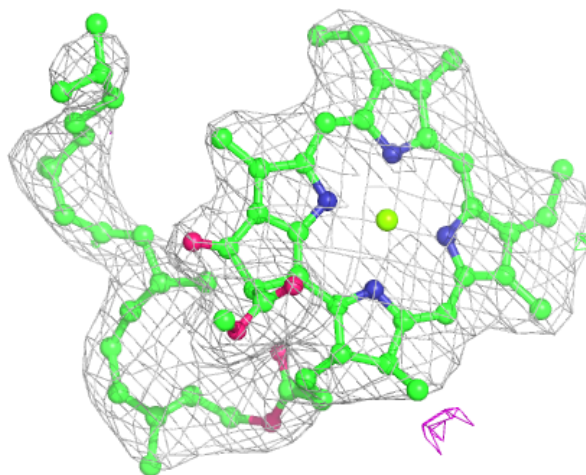
Electron density around CLA a 1137:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



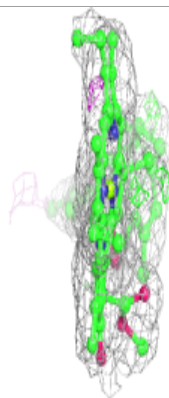
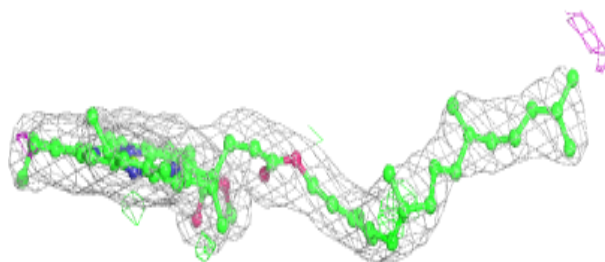
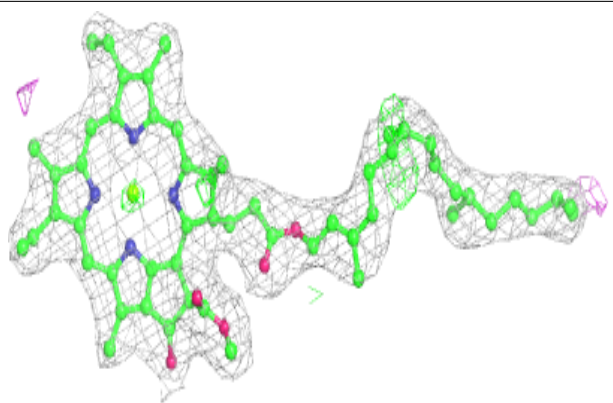
Electron density around CLA B 1229:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

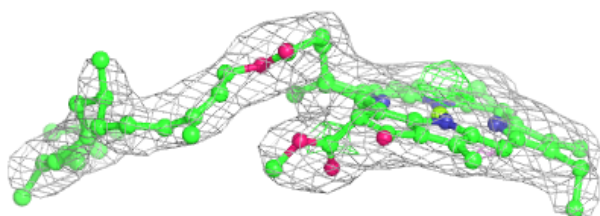
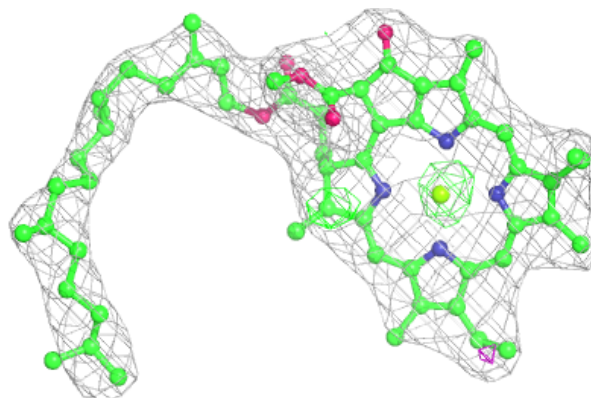


Electron density around CLA A 1131:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

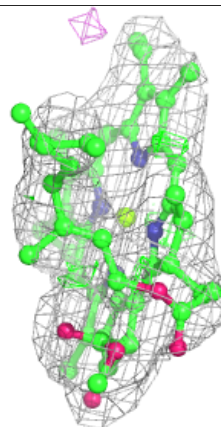
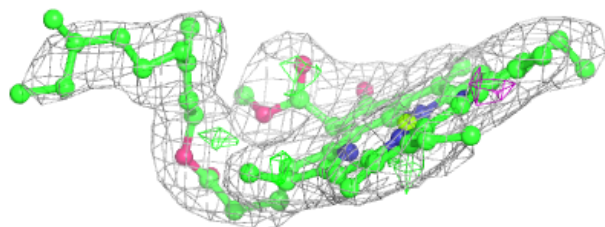
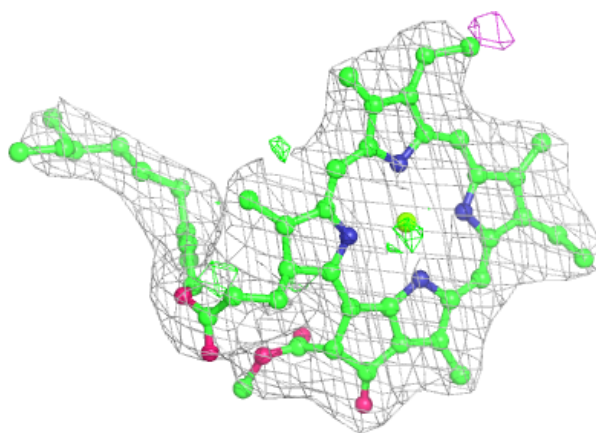
**Electron density around CLA A 1101:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

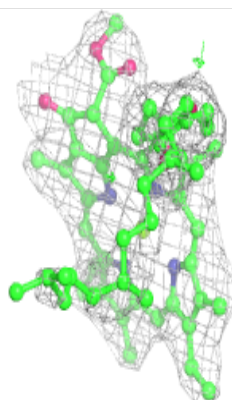
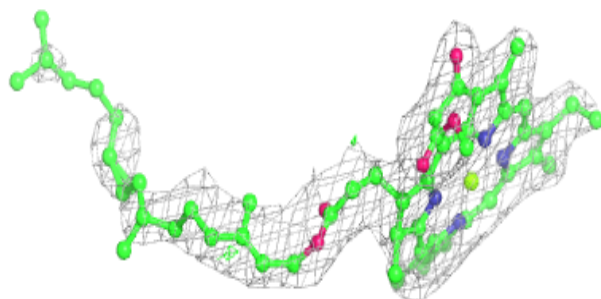
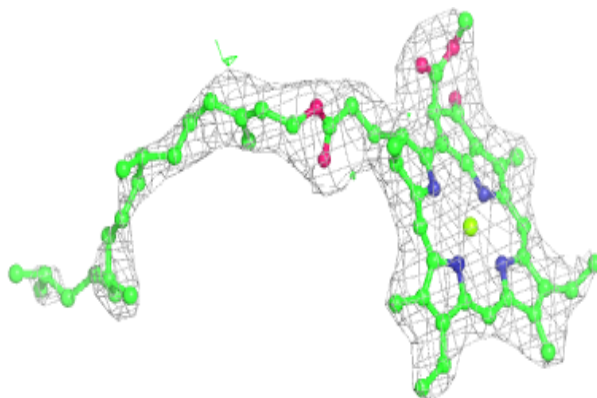


Electron density around CLA 2 1207:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

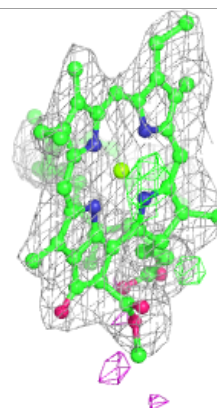
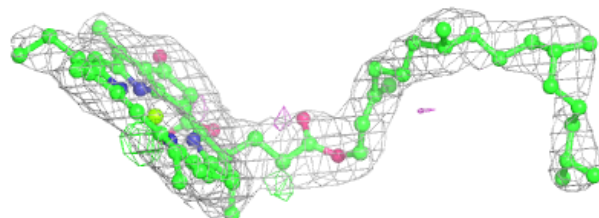
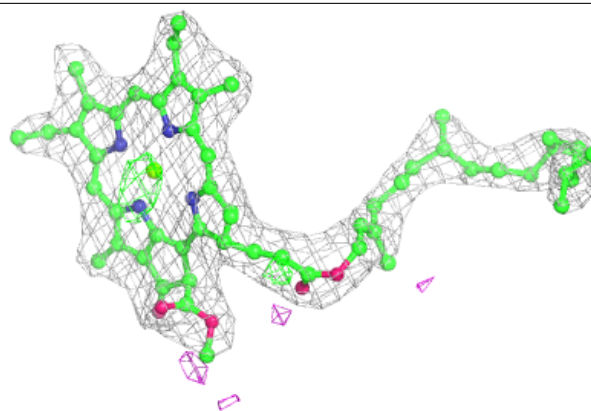
**Electron density around CLA a 1012:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

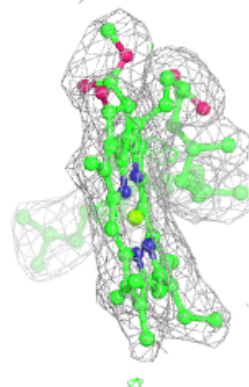
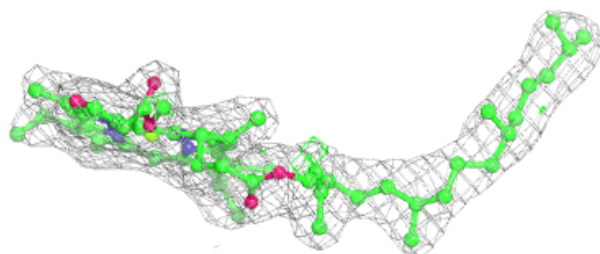
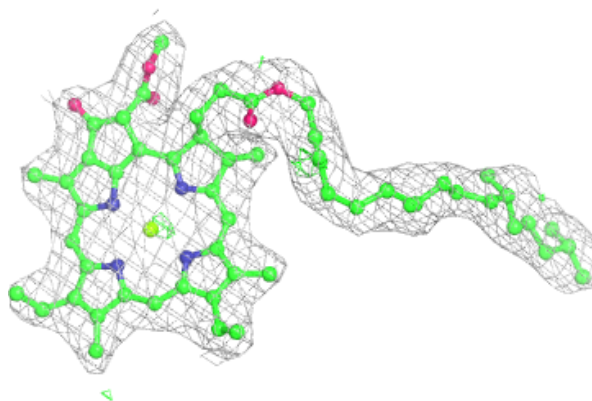


Electron density around CLA B 1206:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

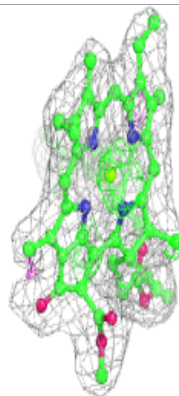
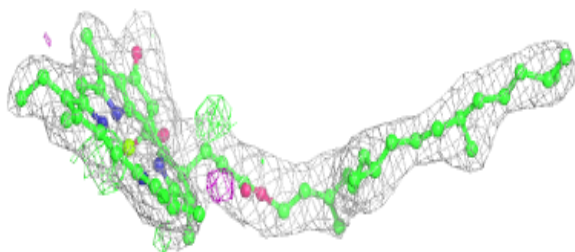
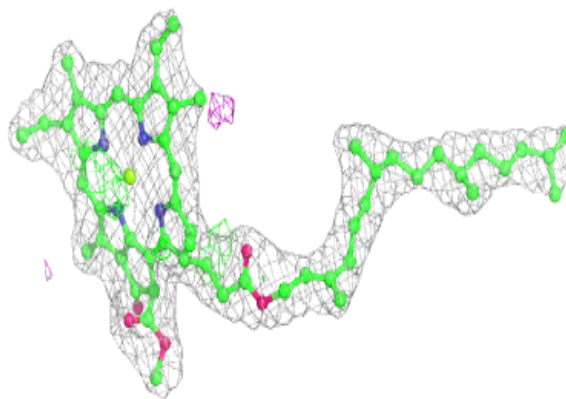
**Electron density around CLA B 1023:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

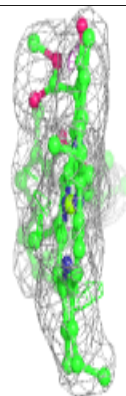
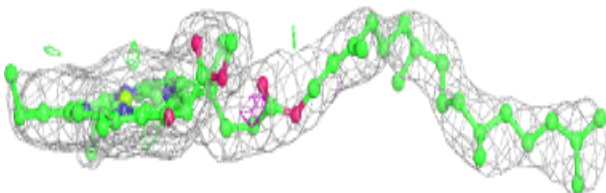
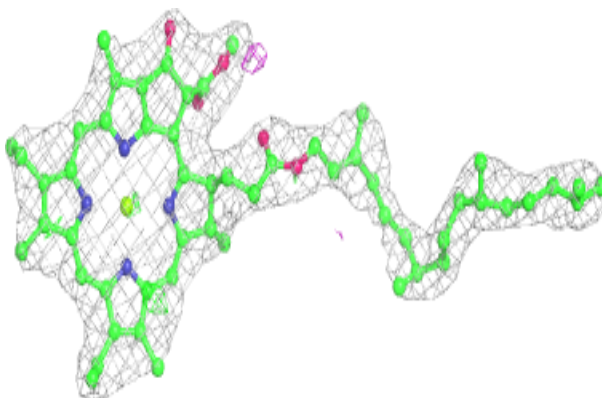


Electron density around CLA B 1022:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

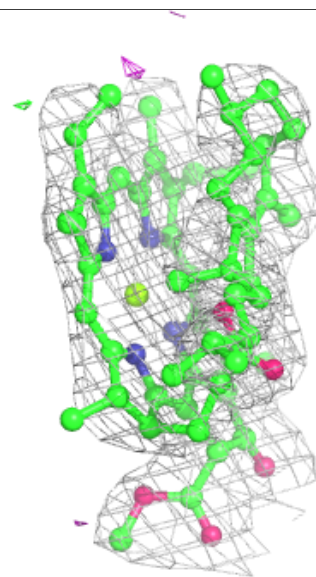
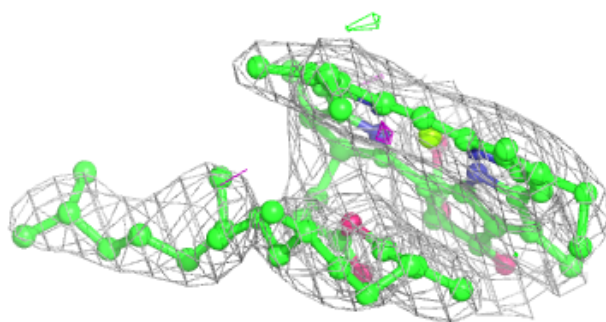
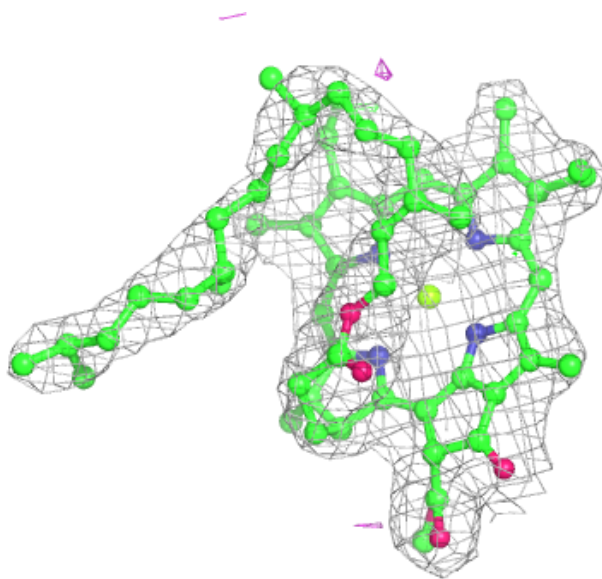
**Electron density around CLA a 1131:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



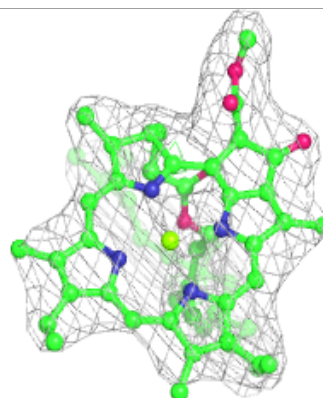
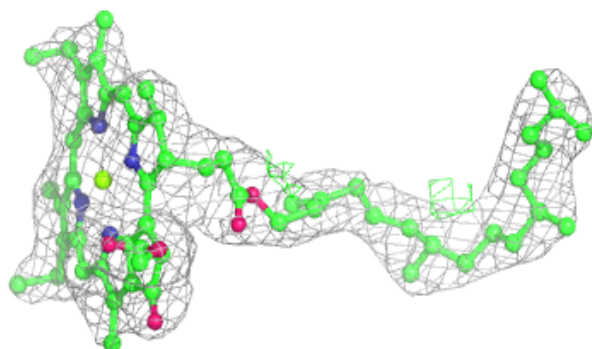
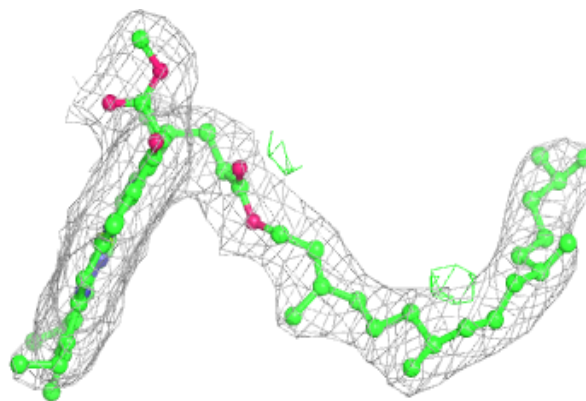
Electron density around CLA b 1205:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

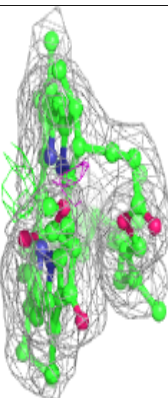
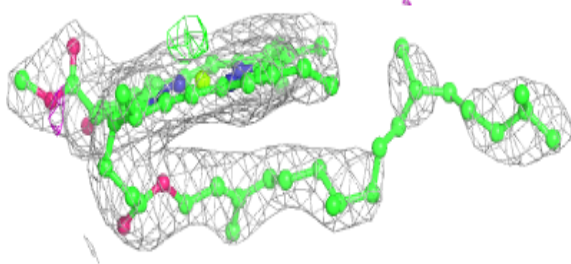
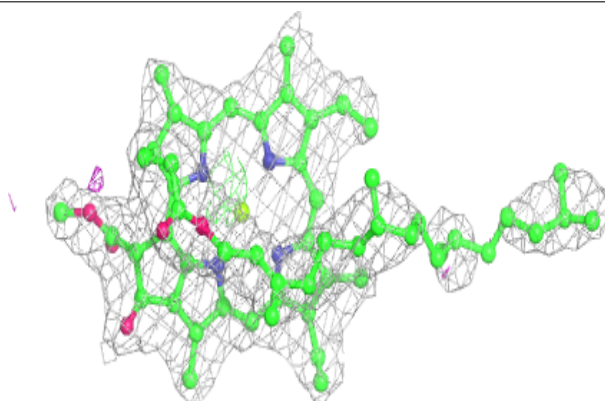


Electron density around CLA 2 1238:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

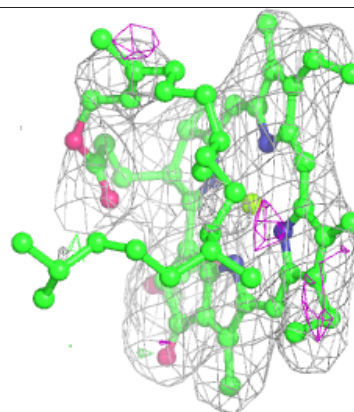
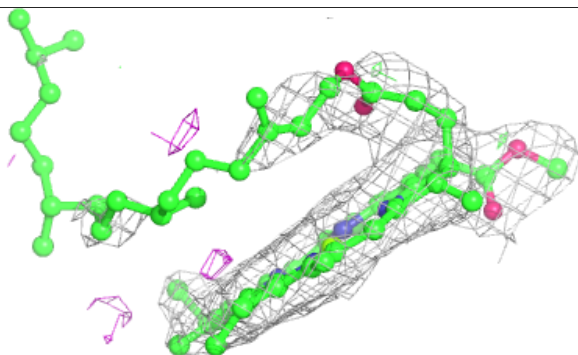
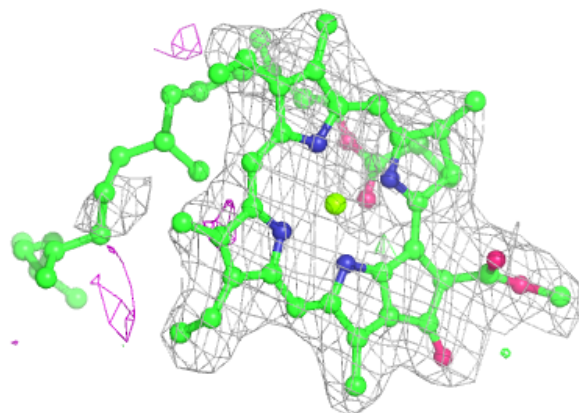
**Electron density around CLA A 1136:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



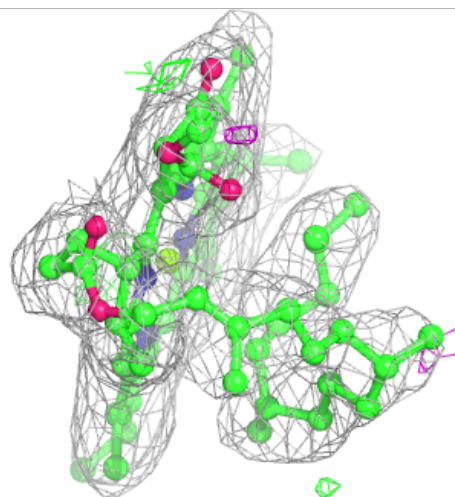
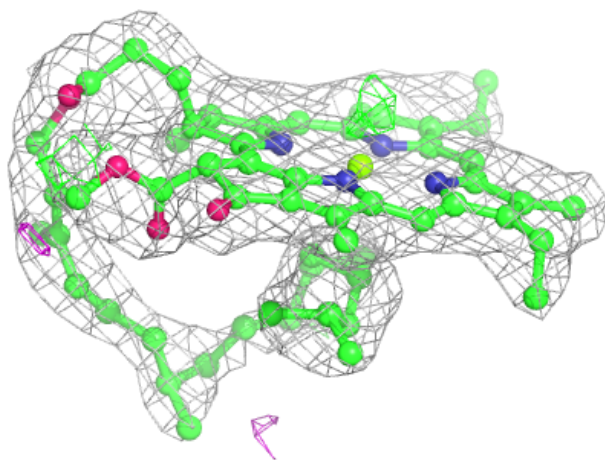
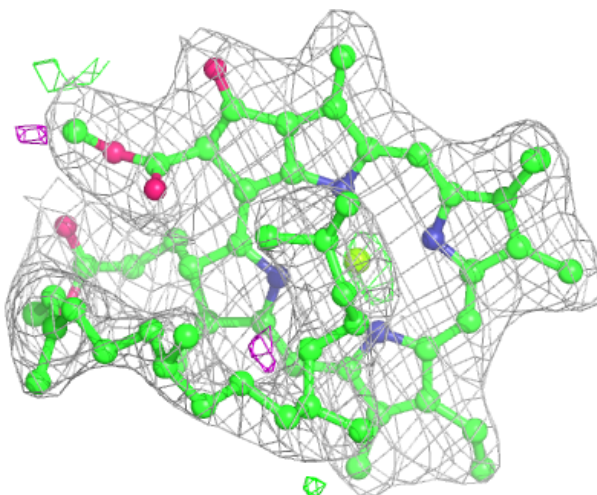
Electron density around CLA A 1110:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



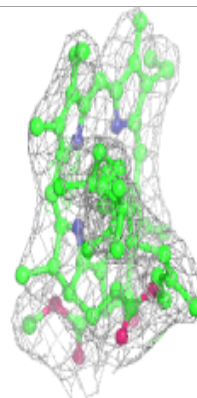
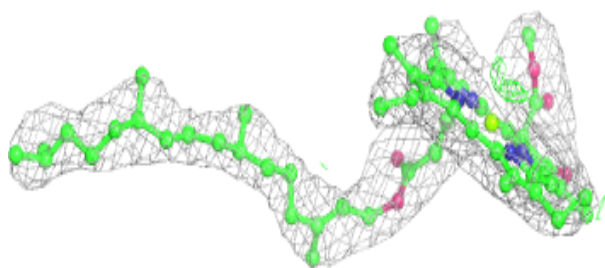
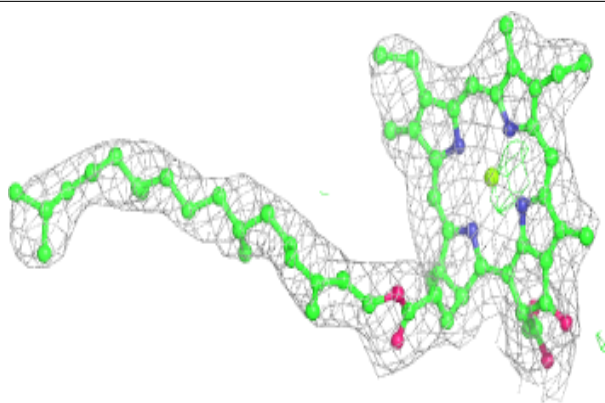
Electron density around CLA b 1203:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

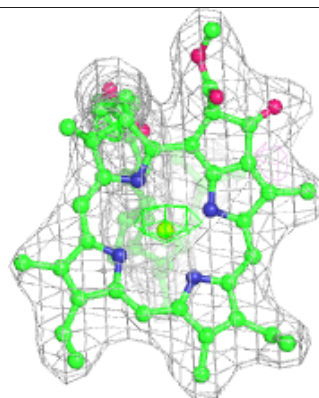
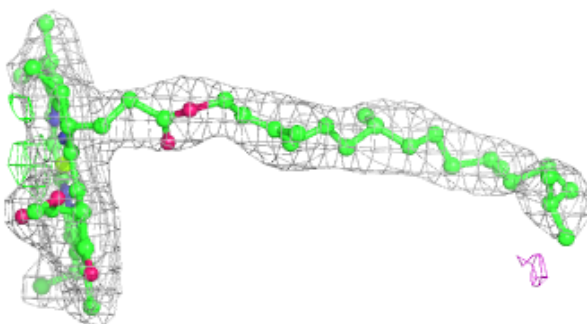
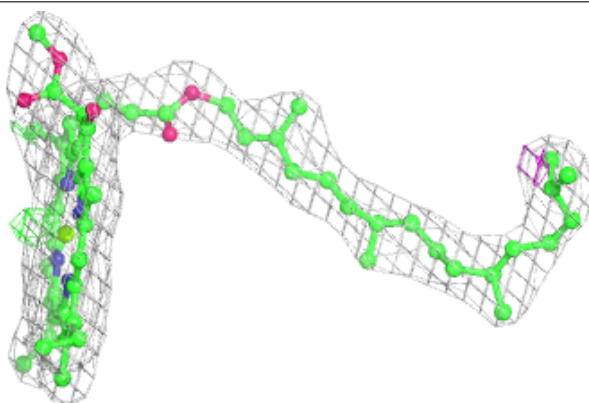


Electron density around CLA a 1132:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

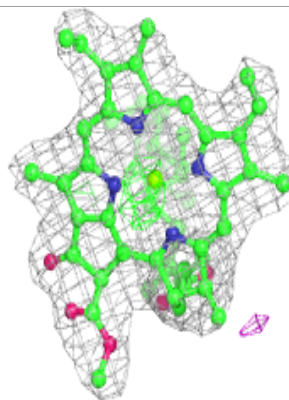
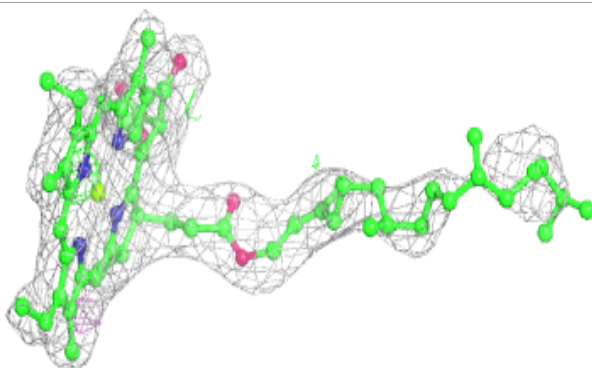
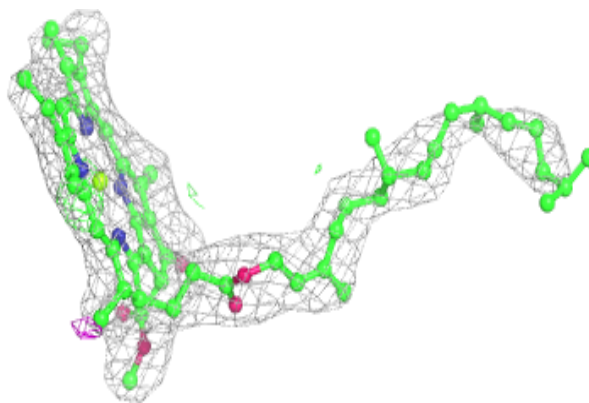
**Electron density around CLA B 1239:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



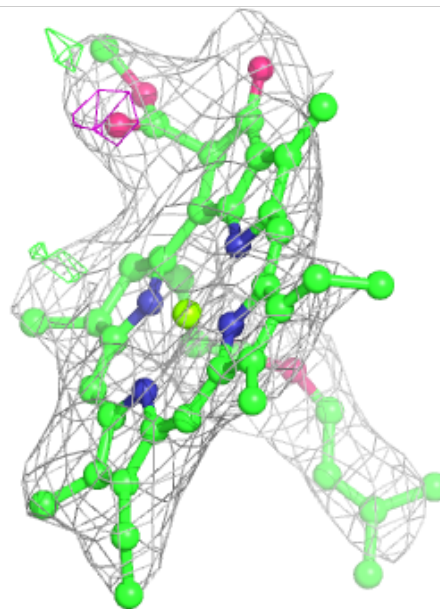
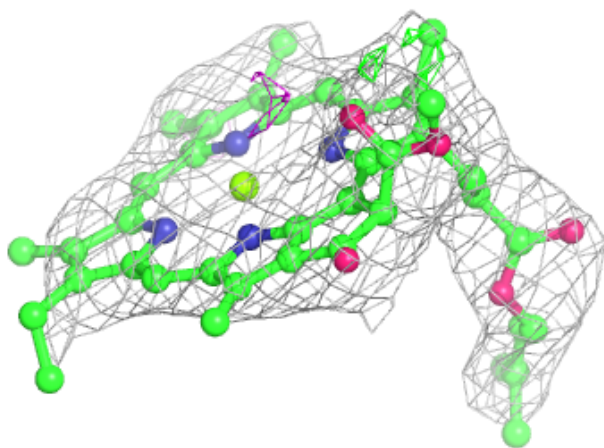
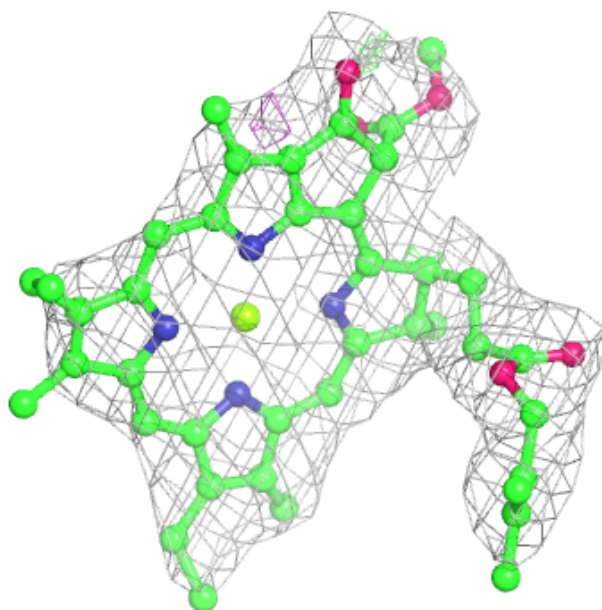
Electron density around CLA A 1137:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



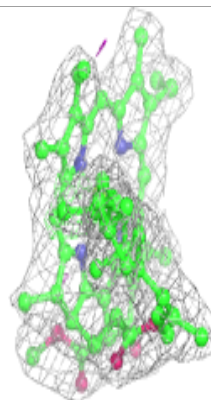
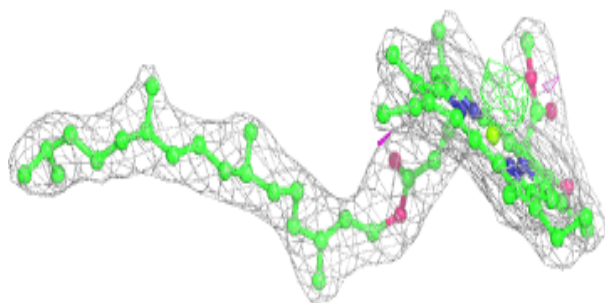
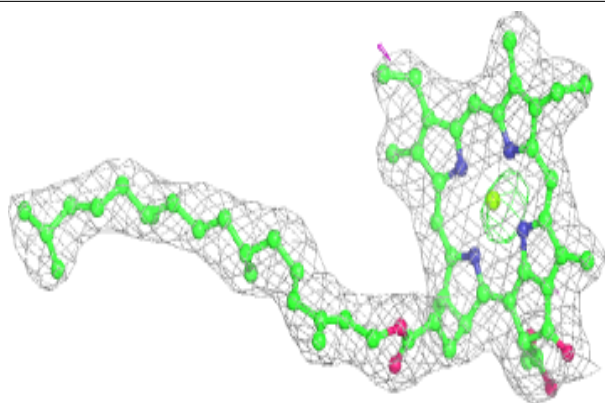
Electron density around CLA 1 1129:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

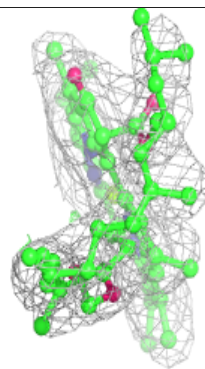
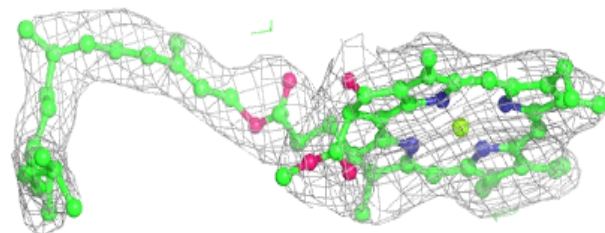
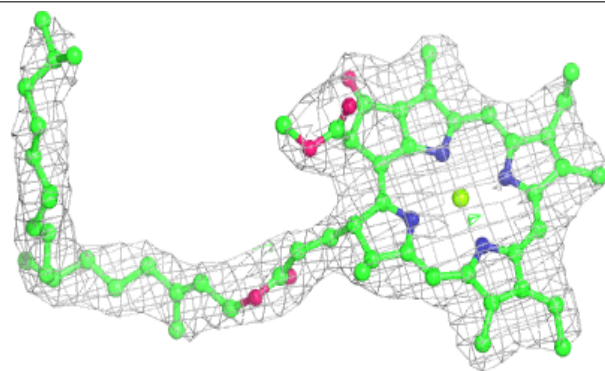


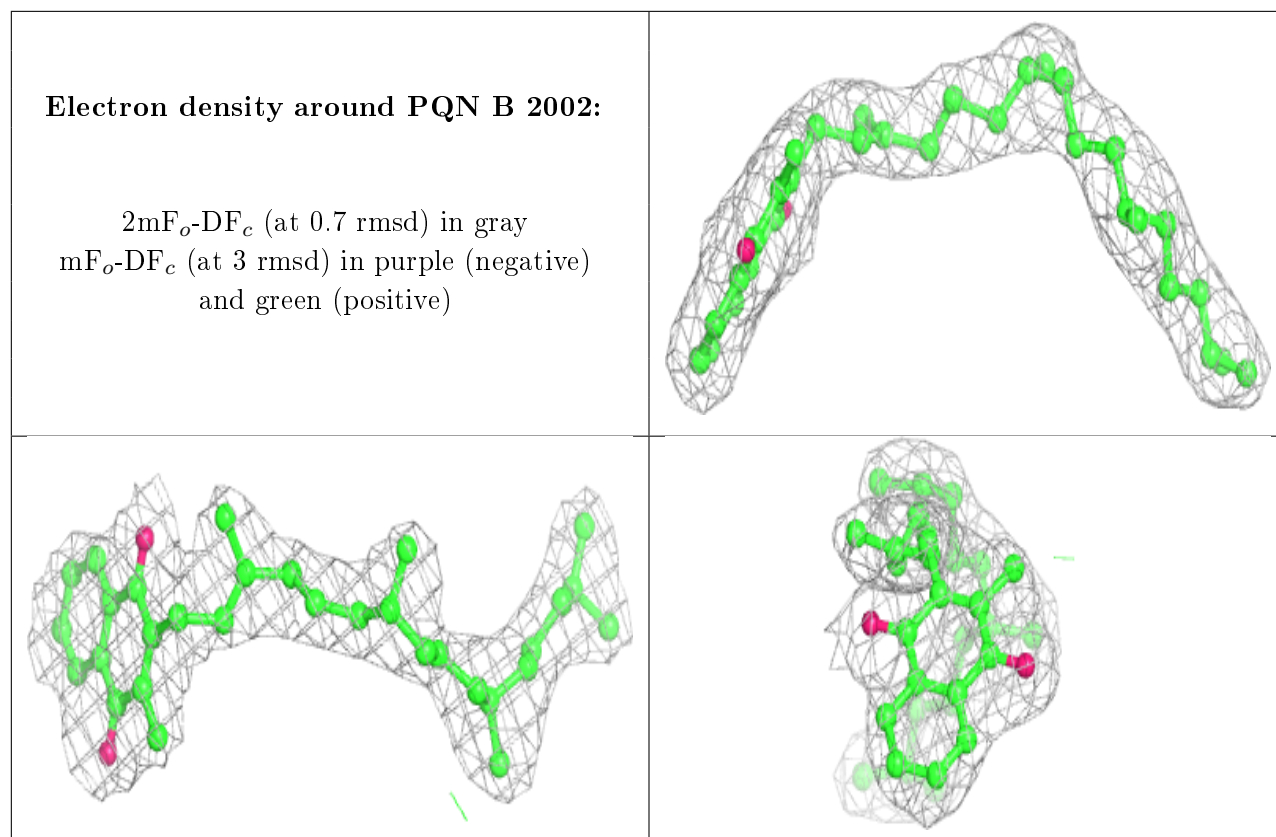
Electron density around CLA A 1132:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

**Electron density around CLA b 1223:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





6.5 Other polymers [i](#)

There are no such residues in this entry.