



# wwPDB X-ray Structure Validation Summary Report ⓘ

May 13, 2020 – 08:09 am BST

PDB ID : 4L6V  
Title : Crystal structure of a virus like photosystem I from the cyanobacterium Synechocystis PCC 6803  
Authors : Mazor, Y.; Nataf, D.; Toporik, H.; Nelson, N.  
Deposited on : 2013-06-13  
Resolution : 3.80 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](mailto: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.

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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 : 2.11  
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) : 2.11

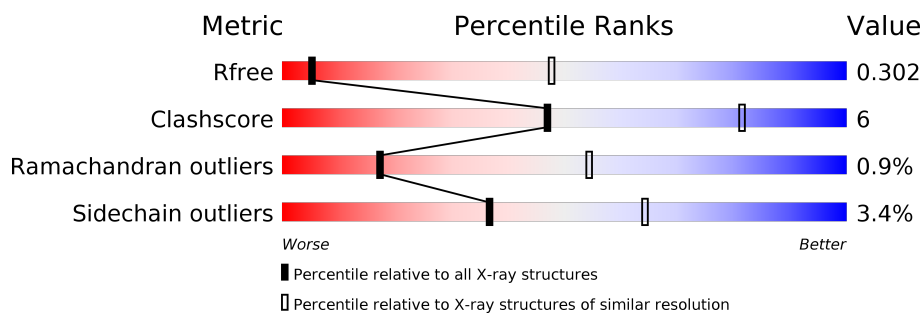
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.80 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	1212 (4.00-3.60)
Clashscore	141614	1288 (4.00-3.60)
Ramachandran outliers	138981	1243 (4.00-3.60)
Sidechain outliers	138945	1237 (4.00-3.60)


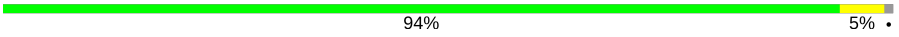


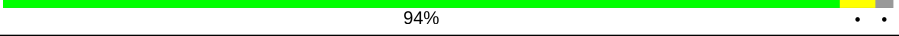



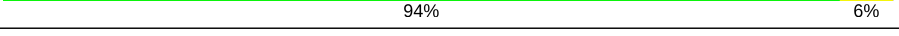

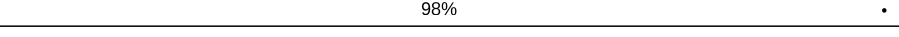
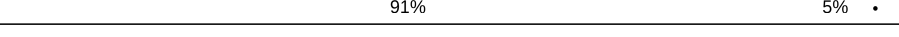

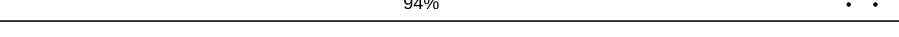


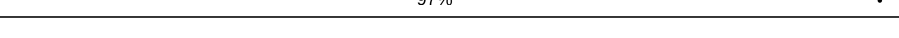

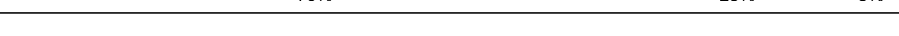
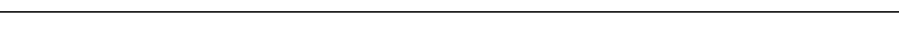

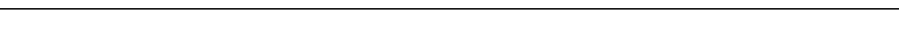
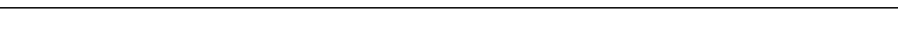
The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria 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  $\leq 5\%$ .

Mol	Chain	Length	Quality of chain
1	1	751	
1	A	751	
1	a	751	
2	2	731	
2	B	731	
2	b	731	
3	3	81	

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Mol	Chain	Length	Quality of chain
3	C	81	
3	c	81	
4	4	141	
4	D	141	
4	d	141	
5	5	74	
5	E	74	
5	e	74	
6	6	125	
6	F	125	
6	f	125	
7	8	157	
7	L	157	
7	l	157	
8	7	31	
8	M	31	
8	m	31	
9	9	40	
9	I	40	
9	i	40	
10	0	128	
10	K	128	
10	k	128	

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
11	CLA	0	1401	X	-	-	-
11	CLA	0	1402	X	-	-	-
11	CLA	1	1011	X	-	-	-
11	CLA	1	1012	X	-	-	-
11	CLA	1	1022	X	-	-	-
11	CLA	1	1101	X	-	-	-
11	CLA	1	1102	X	-	-	-
11	CLA	1	1103	X	-	-	-
11	CLA	1	1104	X	-	-	-
11	CLA	1	1105	X	-	-	-
11	CLA	1	1106	X	-	-	-
11	CLA	1	1107	X	-	-	-
11	CLA	1	1108	X	-	-	-
11	CLA	1	1109	X	-	-	-
11	CLA	1	1110	X	-	-	-
11	CLA	1	1111	X	-	-	-
11	CLA	1	1112	X	-	-	-
11	CLA	1	1113	X	-	-	-
11	CLA	1	1114	X	-	-	-
11	CLA	1	1115	X	-	-	-
11	CLA	1	1116	X	-	-	-
11	CLA	1	1117	X	-	-	-
11	CLA	1	1118	X	-	-	-
11	CLA	1	1119	X	-	-	-
11	CLA	1	1120	X	-	-	-
11	CLA	1	1121	X	-	-	-
11	CLA	1	1122	X	-	-	-
11	CLA	1	1123	X	-	-	-
11	CLA	1	1124	X	-	-	-
11	CLA	1	1125	X	-	-	-
11	CLA	1	1126	X	-	-	-
11	CLA	1	1127	X	-	-	-
11	CLA	1	1128	X	-	-	-
11	CLA	1	1129	X	-	-	-
11	CLA	1	1130	X	-	-	-
11	CLA	1	1131	X	-	-	-
11	CLA	1	1132	X	-	-	-
11	CLA	1	1133	X	-	-	-
11	CLA	1	1134	X	-	-	-
11	CLA	1	1135	X	-	-	-
11	CLA	1	1136	X	-	-	-
11	CLA	1	1137	X	-	-	-
11	CLA	1	1138	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
11	CLA	1	1139	X	-	-	-
11	CLA	1	1140	X	-	-	-
11	CLA	1	1237	X	-	-	-
11	CLA	1	1801	X	-	-	-
11	CLA	2	1013	X	-	-	-
11	CLA	2	1021	X	-	-	-
11	CLA	2	1023	X	-	-	-
11	CLA	2	1201	X	-	-	-
11	CLA	2	1202	X	-	-	-
11	CLA	2	1203	X	-	-	-
11	CLA	2	1204	X	-	-	-
11	CLA	2	1205	X	-	-	-
11	CLA	2	1206	X	-	-	-
11	CLA	2	1207	X	-	-	-
11	CLA	2	1208	X	-	-	-
11	CLA	2	1209	X	-	-	-
11	CLA	2	1210	X	-	-	-
11	CLA	2	1211	X	-	-	-
11	CLA	2	1212	X	-	-	-
11	CLA	2	1213	X	-	-	-
11	CLA	2	1214	X	-	-	-
11	CLA	2	1215	X	-	-	-
11	CLA	2	1216	X	-	-	-
11	CLA	2	1217	X	-	-	-
11	CLA	2	1218	X	-	-	-
11	CLA	2	1219	X	-	-	-
11	CLA	2	1220	X	-	-	-
11	CLA	2	1221	X	-	-	-
11	CLA	2	1222	X	-	-	-
11	CLA	2	1223	X	-	-	-
11	CLA	2	1224	X	-	-	-
11	CLA	2	1225	X	-	-	-
11	CLA	2	1226	X	-	-	-
11	CLA	2	1227	X	-	-	-
11	CLA	2	1228	X	-	-	-
11	CLA	2	1229	X	-	-	-
11	CLA	2	1230	X	-	-	-
11	CLA	2	1231	X	-	-	-
11	CLA	2	1232	X	-	-	-
11	CLA	2	1234	X	-	-	-
11	CLA	2	1235	X	-	-	-
11	CLA	2	1236	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
11	CLA	2	1238	X	-	-	-
11	CLA	2	1239	X	-	-	-
11	CLA	2	1240	X	-	-	-
11	CLA	8	1501	X	-	-	-
11	CLA	8	1502	X	-	-	-
11	CLA	8	1503	X	-	-	-
11	CLA	A	1011	X	-	-	-
11	CLA	A	1012	X	-	-	-
11	CLA	A	1022	X	-	-	-
11	CLA	A	1101	X	-	-	-
11	CLA	A	1102	X	-	-	-
11	CLA	A	1103	X	-	-	-
11	CLA	A	1104	X	-	-	-
11	CLA	A	1105	X	-	-	-
11	CLA	A	1106	X	-	-	-
11	CLA	A	1107	X	-	-	-
11	CLA	A	1108	X	-	-	-
11	CLA	A	1109	X	-	-	-
11	CLA	A	1110	X	-	-	-
11	CLA	A	1111	X	-	-	-
11	CLA	A	1112	X	-	-	-
11	CLA	A	1113	X	-	-	-
11	CLA	A	1114	X	-	-	-
11	CLA	A	1115	X	-	-	-
11	CLA	A	1116	X	-	-	-
11	CLA	A	1117	X	-	-	-
11	CLA	A	1118	X	-	-	-
11	CLA	A	1119	X	-	-	-
11	CLA	A	1120	X	-	-	-
11	CLA	A	1121	X	-	-	-
11	CLA	A	1122	X	-	-	-
11	CLA	A	1123	X	-	-	-
11	CLA	A	1124	X	-	-	-
11	CLA	A	1125	X	-	-	-
11	CLA	A	1126	X	-	-	-
11	CLA	A	1127	X	-	-	-
11	CLA	A	1128	X	-	-	-
11	CLA	A	1129	X	-	-	-
11	CLA	A	1130	X	-	-	-
11	CLA	A	1131	X	-	-	-
11	CLA	A	1132	X	-	-	-
11	CLA	A	1133	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
11	CLA	A	1134	X	-	-	-
11	CLA	A	1135	X	-	-	-
11	CLA	A	1136	X	-	-	-
11	CLA	A	1137	X	-	-	-
11	CLA	A	1138	X	-	-	-
11	CLA	A	1139	X	-	-	-
11	CLA	A	1140	X	-	-	-
11	CLA	A	1237	X	-	-	-
11	CLA	A	1801	X	-	-	-
11	CLA	B	1013	X	-	-	-
11	CLA	B	1021	X	-	-	-
11	CLA	B	1023	X	-	-	-
11	CLA	B	1201	X	-	-	-
11	CLA	B	1202	X	-	-	-
11	CLA	B	1203	X	-	-	-
11	CLA	B	1204	X	-	-	-
11	CLA	B	1205	X	-	-	-
11	CLA	B	1206	X	-	-	-
11	CLA	B	1207	X	-	-	-
11	CLA	B	1208	X	-	-	-
11	CLA	B	1209	X	-	-	-
11	CLA	B	1210	X	-	-	-
11	CLA	B	1211	X	-	-	-
11	CLA	B	1212	X	-	-	-
11	CLA	B	1213	X	-	-	-
11	CLA	B	1214	X	-	-	-
11	CLA	B	1215	X	-	-	-
11	CLA	B	1216	X	-	-	-
11	CLA	B	1217	X	-	-	-
11	CLA	B	1218	X	-	-	-
11	CLA	B	1219	X	-	-	-
11	CLA	B	1220	X	-	-	-
11	CLA	B	1221	X	-	-	-
11	CLA	B	1222	X	-	-	-
11	CLA	B	1223	X	-	-	-
11	CLA	B	1224	X	-	-	-
11	CLA	B	1225	X	-	-	-
11	CLA	B	1226	X	-	-	-
11	CLA	B	1227	X	-	-	-
11	CLA	B	1228	X	-	-	-
11	CLA	B	1229	X	-	-	-
11	CLA	B	1230	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
11	CLA	B	1231	X	-	-	-
11	CLA	B	1232	X	-	-	-
11	CLA	B	1234	X	-	-	-
11	CLA	B	1235	X	-	-	-
11	CLA	B	1236	X	-	-	-
11	CLA	B	1238	X	-	-	-
11	CLA	B	1239	X	-	-	-
11	CLA	B	1240	X	-	-	-
11	CLA	K	1401	X	-	-	-
11	CLA	K	1402	X	-	-	-
11	CLA	L	1501	X	-	-	-
11	CLA	L	1502	X	-	-	-
11	CLA	L	1503	X	-	-	-
11	CLA	a	1011	X	-	-	-
11	CLA	a	1012	X	-	-	-
11	CLA	a	1022	X	-	-	-
11	CLA	a	1101	X	-	-	-
11	CLA	a	1102	X	-	-	-
11	CLA	a	1103	X	-	-	-
11	CLA	a	1104	X	-	-	-
11	CLA	a	1105	X	-	-	-
11	CLA	a	1106	X	-	-	-
11	CLA	a	1107	X	-	-	-
11	CLA	a	1108	X	-	-	-
11	CLA	a	1109	X	-	-	-
11	CLA	a	1110	X	-	-	-
11	CLA	a	1111	X	-	-	-
11	CLA	a	1112	X	-	-	-
11	CLA	a	1113	X	-	-	-
11	CLA	a	1114	X	-	-	-
11	CLA	a	1115	X	-	-	-
11	CLA	a	1116	X	-	-	-
11	CLA	a	1117	X	-	-	-
11	CLA	a	1118	X	-	-	-
11	CLA	a	1119	X	-	-	-
11	CLA	a	1120	X	-	-	-
11	CLA	a	1121	X	-	-	-
11	CLA	a	1122	X	-	-	-
11	CLA	a	1123	X	-	-	-
11	CLA	a	1124	X	-	-	-
11	CLA	a	1125	X	-	-	-
11	CLA	a	1126	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
11	CLA	a	1127	X	-	-	-
11	CLA	a	1128	X	-	-	-
11	CLA	a	1129	X	-	-	-
11	CLA	a	1130	X	-	-	-
11	CLA	a	1131	X	-	-	-
11	CLA	a	1132	X	-	-	-
11	CLA	a	1133	X	-	-	-
11	CLA	a	1134	X	-	-	-
11	CLA	a	1135	X	-	-	-
11	CLA	a	1136	X	-	-	-
11	CLA	a	1137	X	-	-	-
11	CLA	a	1138	X	-	-	-
11	CLA	a	1139	X	-	-	-
11	CLA	a	1140	X	-	-	-
11	CLA	a	1237	X	-	-	-
11	CLA	a	1801	X	-	-	-
11	CLA	b	1013	X	-	-	-
11	CLA	b	1021	X	-	-	-
11	CLA	b	1023	X	-	-	-
11	CLA	b	1201	X	-	-	-
11	CLA	b	1202	X	-	-	-
11	CLA	b	1203	X	-	-	-
11	CLA	b	1204	X	-	-	-
11	CLA	b	1205	X	-	-	-
11	CLA	b	1206	X	-	-	-
11	CLA	b	1207	X	-	-	-
11	CLA	b	1208	X	-	-	-
11	CLA	b	1209	X	-	-	-
11	CLA	b	1210	X	-	-	-
11	CLA	b	1211	X	-	-	-
11	CLA	b	1212	X	-	-	-
11	CLA	b	1213	X	-	-	-
11	CLA	b	1214	X	-	-	-
11	CLA	b	1215	X	-	-	-
11	CLA	b	1216	X	-	-	-
11	CLA	b	1217	X	-	-	-
11	CLA	b	1218	X	-	-	-
11	CLA	b	1219	X	-	-	-
11	CLA	b	1220	X	-	-	-
11	CLA	b	1221	X	-	-	-
11	CLA	b	1222	X	-	-	-
11	CLA	b	1223	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
11	CLA	b	1224	X	-	-	-
11	CLA	b	1225	X	-	-	-
11	CLA	b	1226	X	-	-	-
11	CLA	b	1227	X	-	-	-
11	CLA	b	1228	X	-	-	-
11	CLA	b	1229	X	-	-	-
11	CLA	b	1230	X	-	-	-
11	CLA	b	1231	X	-	-	-
11	CLA	b	1232	X	-	-	-
11	CLA	b	1234	X	-	-	-
11	CLA	b	1235	X	-	-	-
11	CLA	b	1236	X	-	-	-
11	CLA	b	1238	X	-	-	-
11	CLA	b	1239	X	-	-	-
11	CLA	b	1240	X	-	-	-
11	CLA	k	1401	X	-	-	-
11	CLA	k	1402	X	-	-	-
11	CLA	l	1501	X	-	-	-
11	CLA	l	1502	X	-	-	-
11	CLA	l	1503	X	-	-	-
13	SF4	3	3002	-	-	X	-
13	SF4	3	3003	-	-	X	-
13	SF4	A	3001	-	-	X	-
13	SF4	C	3002	-	-	X	-
13	SF4	C	3003	-	-	X	-



## 2 Entry composition [i](#)

There are 16 unique types of molecules in this entry. The entry contains 68370 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	739	Total	C	N	O	S	0	0	0
			5772	3783	982	980	27			
1	a	739	Total	C	N	O	S	0	0	0
			5772	3783	982	980	27			
1	1	739	Total	C	N	O	S	0	0	0
			5772	3783	982	980	27			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	728	Total	C	N	O	S	0	0	0
			5765	3796	966	988	15			
2	b	728	Total	C	N	O	S	0	0	0
			5765	3796	966	988	15			
2	2	728	Total	C	N	O	S	0	0	0
			5765	3796	966	988	15			

- 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	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 subunit II.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	138	Total	C	N	O	S	0	0	0
			1079	683	187	206	3			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	d	138	Total	C	N	O	S	0	0	0
			1079	683	187	206	3			
4	4	138	Total	C	N	O	S	0	0	0
			1079	683	187	206	3			

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
5	E	68	Total	C	N	O	0	0	0
			529	332	93	104			
5	e	68	Total	C	N	O	0	0	0
			529	332	93	104			
5	5	68	Total	C	N	O	0	0	0
			529	332	93	104			

- Molecule 6 is a protein called Fusion protein of Photosystem I subunit III and subunit IX.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
6	F	125	Total	C	N	O	0	0	0
			676	420	126	130			
6	f	125	Total	C	N	O	0	0	0
			685	429	126	130			
6	6	125	Total	C	N	O	0	0	0
			685	429	126	130			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
F	41	CYS	-	LINKER	UNP L8AII8
F	42	SER	-	LINKER	UNP L8AII8
F	43	CYS	-	LINKER	UNP L8AII8
F	53	ILE	LEU	engineered mutation	UNP L8AII8
f	41	CYS	-	LINKER	UNP L8AII8
f	42	SER	-	LINKER	UNP L8AII8
f	43	CYS	-	LINKER	UNP L8AII8
f	53	ILE	LEU	engineered mutation	UNP L8AII8
6	41	CYS	-	LINKER	UNP L8AII8
6	42	SER	-	LINKER	UNP L8AII8
6	43	CYS	-	LINKER	UNP L8AII8
6	53	ILE	LEU	engineered mutation	UNP L8AII8

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	L	151	Total	C	N	O	S	0	0	0
			1133	741	183	207	2			
7	l	151	Total	C	N	O	S	0	0	0
			1133	741	183	207	2			
7	8	151	Total	C	N	O	S	0	0	0
			1133	741	183	207	2			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	M	31	Total	C	N	O		0	0	0
			235	157	36	42				
8	m	31	Total	C	N	O		0	0	0
			235	157	36	42				
8	7	31	Total	C	N	O		0	0	0
			235	157	36	42				

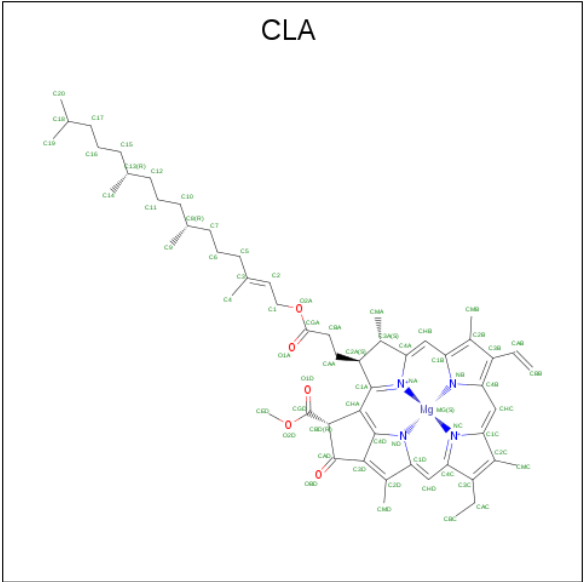
- Molecule 9 is a protein called Photosystem I subunit III.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	i	38	Total	C	N	O	S	0	0	0
			297	202	42	50	3			
9	9	38	Total	C	N	O	S	0	0	0
			297	202	42	50	3			
9	I	38	Total	C	N	O	S	0	0	0
			297	202	42	50	3			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	K	80	Total	C	N	O	S	0	0	0
			496	320	83	88	5			
10	k	80	Total	C	N	O	S	0	0	0
			496	320	83	88	5			
10	0	80	Total	C	N	O	S	0	0	0
			496	320	83	88	5			

- Molecule 11 is CHLOROPHYLL A (three-letter code: CLA) (formula: C<sub>55</sub>H<sub>72</sub>MgN<sub>4</sub>O<sub>5</sub>).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
11	A	1	Total	C	Mg	N	O	0	0
			52	42	1	4	5		
11	A	1	Total	C	Mg	N	O	0	0
			55	45	1	4	5		
11	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
11	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
11	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
11	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
11	A	1	Total	C	Mg	N	O	0	0
			48	38	1	4	5		
11	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
11	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
11	A	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
11	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
11	A	1	Total	C	Mg	N	O	0	0
			54	44	1	4	5		
11	A	1	Total	C	Mg	N	O	0	0
			60	50	1	4	5		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
11	A	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
11	A	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
11	A	1	Total	C	Mg	N	O	0	0
			46	36	1	4	5		
11	A	1	Total	C	Mg	N	O	0	0
			54	44	1	4	5		
11	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
11	A	1	Total	C	Mg	N	O	0	0
			61	51	1	4	5		
11	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
11	A	1	Total	C	Mg	N	O	0	0
			59	49	1	4	5		
11	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
11	A	1	Total	C	Mg	N	O	0	0
			55	45	1	4	5		
11	A	1	Total	C	Mg	N	O	0	0
			52	42	1	4	5		
11	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
11	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
11	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
11	A	1	Total	C	Mg	N	O	0	0
			46	36	1	4	5		
11	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
11	A	1	Total	C	Mg	N	O	0	0
			46	36	1	4	5		
11	A	1	Total	C	Mg	N	O	0	0
			50	40	1	4	5		
11	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
11	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
11	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
11	A	1	Total	C	Mg	N	O	0	0
			46	36	1	4	5		
11	A	1	Total	C	Mg	N	O	0	0
			46	36	1	4	5		
11	A	1	Total	C	Mg	N	O	0	0
			46	36	1	4	5		
11	A	1	Total	C	Mg	N	O	0	0
			46	36	1	4	5		
11	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
11	A	1	Total	C	Mg	N	O	0	0
			46	36	1	4	5		
11	A	1	Total	C	Mg	N	O	0	0
			51	41	1	4	5		
11	A	1	Total	C	Mg	N	O	0	0
			46	36	1	4	5		
11	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
11	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
11	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
11	B	1	Total	C	Mg	N	O	0	0
			54	44	1	4	5		
11	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
11	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
11	B	1	Total	C	Mg	N	O	0	0
			55	45	1	4	5		
11	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
11	B	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
11	B	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
11	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
11	B	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
11	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
11	B	1	Total	C	Mg	N	O	0	0
			59	49	1	4	5		
11	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
11	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
11	B	1	Total	C	Mg	N	O	0	0
			47	37	1	4	5		
11	B	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
11	B	1	Total	C	Mg	N	O	0	0
			55	45	1	4	5		
11	B	1	Total	C	Mg	N	O	0	0
			46	36	1	4	5		
11	B	1	Total	C	Mg	N	O	0	0
			54	44	1	4	5		
11	B	1	Total	C	Mg	N	O	0	0
			56	46	1	4	5		
11	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
11	B	1	Total	C	Mg	N	O	0	0
			55	45	1	4	5		
11	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
11	B	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
11	B	1	Total	C	Mg	N	O	0	0
			50	40	1	4	5		
11	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
11	B	1	Total	C	Mg	N	O	0	0
			58	48	1	4	5		
11	B	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
11	B	1	Total 45	C 35	Mg 1	N 4	O 5	0	0
11	B	1	Total 60	C 50	Mg 1	N 4	O 5	0	0
11	B	1	Total 60	C 50	Mg 1	N 4	O 5	0	0
11	B	1	Total 47	C 37	Mg 1	N 4	O 5	0	0
11	B	1	Total 45	C 35	Mg 1	N 4	O 5	0	0
11	B	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
11	B	1	Total 46	C 36	Mg 1	N 4	O 5	0	0
11	B	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
11	B	1	Total 46	C 36	Mg 1	N 4	O 5	0	0
11	L	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
11	L	1	Total 46	C 36	Mg 1	N 4	O 5	0	0
11	L	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
11	a	1	Total 52	C 42	Mg 1	N 4	O 5	0	0
11	a	1	Total 55	C 45	Mg 1	N 4	O 5	0	0
11	a	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
11	a	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
11	a	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
11	a	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
11	a	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
11	a	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
11	a	1	Total 48	C 38	Mg 1	N 4	O 5	0	0
11	a	1	Total 65	C 55	Mg 1	N 4	O 5	0	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
11	a	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
11	a	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
11	a	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
11	a	1	Total	C	Mg	N	O	0	0
			54	44	1	4	5		
11	a	1	Total	C	Mg	N	O	0	0
			60	50	1	4	5		
11	a	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
11	a	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
11	a	1	Total	C	Mg	N	O	0	0
			46	36	1	4	5		
11	a	1	Total	C	Mg	N	O	0	0
			54	44	1	4	5		
11	a	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
11	a	1	Total	C	Mg	N	O	0	0
			61	51	1	4	5		
11	a	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
11	a	1	Total	C	Mg	N	O	0	0
			59	49	1	4	5		
11	a	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
11	a	1	Total	C	Mg	N	O	0	0
			55	45	1	4	5		
11	a	1	Total	C	Mg	N	O	0	0
			52	42	1	4	5		
11	a	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
11	a	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
11	a	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
11	a	1	Total	C	Mg	N	O	0	0
			46	36	1	4	5		
11	a	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
11	a	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
11	a	1	Total	C	Mg	N	O	0	0
			46	36	1	4	5		
11	a	1	Total	C	Mg	N	O	0	0
			50	40	1	4	5		
11	a	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
11	a	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
11	a	1	Total	C	Mg	N	O	0	0
			46	36	1	4	5		
11	a	1	Total	C	Mg	N	O	0	0
			46	36	1	4	5		
11	a	1	Total	C	Mg	N	O	0	0
			46	36	1	4	5		
11	a	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
11	a	1	Total	C	Mg	N	O	0	0
			46	36	1	4	5		
11	a	1	Total	C	Mg	N	O	0	0
			51	41	1	4	5		
11	a	1	Total	C	Mg	N	O	0	0
			46	36	1	4	5		
11	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
11	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
11	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
11	b	1	Total	C	Mg	N	O	0	0
			54	44	1	4	5		
11	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
11	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
11	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
11	b	1	Total	C	Mg	N	O	0	0
			55	45	1	4	5		
11	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
11	b	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
11	b	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
11	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
11	b	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
11	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
11	b	1	Total	C	Mg	N	O	0	0
			59	49	1	4	5		
11	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
11	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
11	b	1	Total	C	Mg	N	O	0	0
			47	37	1	4	5		
11	b	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
11	b	1	Total	C	Mg	N	O	0	0
			55	45	1	4	5		
11	b	1	Total	C	Mg	N	O	0	0
			46	36	1	4	5		
11	b	1	Total	C	Mg	N	O	0	0
			54	44	1	4	5		
11	b	1	Total	C	Mg	N	O	0	0
			56	46	1	4	5		
11	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
11	b	1	Total	C	Mg	N	O	0	0
			55	45	1	4	5		
11	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
11	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
11	b	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
11	b	1	Total	C	Mg	N	O	0	0
			50	40	1	4	5		
11	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
11	b	1	Total	C	Mg	N	O	0	0
			58	48	1	4	5		
11	b	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
11	b	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
11	b	1	Total	C	Mg	N	O	0	0
			60	50	1	4	5		
11	b	1	Total	C	Mg	N	O	0	0
			60	50	1	4	5		
11	b	1	Total	C	Mg	N	O	0	0
			47	37	1	4	5		
11	b	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
11	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
11	b	1	Total	C	Mg	N	O	0	0
			46	36	1	4	5		
11	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
11	b	1	Total	C	Mg	N	O	0	0
			46	36	1	4	5		
11	l	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
11	l	1	Total	C	Mg	N	O	0	0
			46	36	1	4	5		
11	l	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
11	1	1	Total	C	Mg	N	O	0	0
			52	42	1	4	5		
11	1	1	Total	C	Mg	N	O	0	0
			55	45	1	4	5		
11	1	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
11	1	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
11	1	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
11	1	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
11	1	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
11	1	1	Total	C	Mg	N	O	0	0
			48	38	1	4	5		
11	1	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
11	1	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
11	1	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
11	1	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
11	1	1	Total	C	Mg	N	O	0	0
			54	44	1	4	5		
11	1	1	Total	C	Mg	N	O	0	0
			60	50	1	4	5		
11	1	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
11	1	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
11	1	1	Total	C	Mg	N	O	0	0
			46	36	1	4	5		
11	1	1	Total	C	Mg	N	O	0	0
			54	44	1	4	5		
11	1	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
11	1	1	Total	C	Mg	N	O	0	0
			61	51	1	4	5		
11	1	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
11	1	1	Total	C	Mg	N	O	0	0
			59	49	1	4	5		
11	1	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
11	1	1	Total	C	Mg	N	O	0	0
			55	45	1	4	5		
11	1	1	Total	C	Mg	N	O	0	0
			52	42	1	4	5		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
11	1	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
11	1	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
11	1	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
11	1	1	Total	C	Mg	N	O	0	0
			46	36	1	4	5		
11	1	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
11	1	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
11	1	1	Total	C	Mg	N	O	0	0
			46	36	1	4	5		
11	1	1	Total	C	Mg	N	O	0	0
			50	40	1	4	5		
11	1	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
11	1	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
11	1	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
11	1	1	Total	C	Mg	N	O	0	0
			46	36	1	4	5		
11	1	1	Total	C	Mg	N	O	0	0
			46	36	1	4	5		
11	1	1	Total	C	Mg	N	O	0	0
			46	36	1	4	5		
11	1	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
11	1	1	Total	C	Mg	N	O	0	0
			46	36	1	4	5		
11	1	1	Total	C	Mg	N	O	0	0
			46	36	1	4	5		
11	1	1	Total	C	Mg	N	O	0	0
			51	41	1	4	5		
11	1	1	Total	C	Mg	N	O	0	0
			46	36	1	4	5		
11	2	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
11	2	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
11	2	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
11	2	1	Total	C	Mg	N	O	0	0
			54	44	1	4	5		
11	2	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
11	2	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
11	2	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
11	2	1	Total	C	Mg	N	O	0	0
			55	45	1	4	5		
11	2	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
11	2	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
11	2	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
11	2	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
11	2	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
11	2	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
11	2	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
11	2	1	Total	C	Mg	N	O	0	0
			59	49	1	4	5		
11	2	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
11	2	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
11	2	1	Total	C	Mg	N	O	0	0
			47	37	1	4	5		
11	2	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
11	2	1	Total	C	Mg	N	O	0	0
			55	45	1	4	5		
11	2	1	Total	C	Mg	N	O	0	0
			46	36	1	4	5		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
11	2	1	Total	C	Mg	N	O	0	0
			54	44	1	4	5		
11	2	1	Total	C	Mg	N	O	0	0
			56	46	1	4	5		
11	2	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
11	2	1	Total	C	Mg	N	O	0	0
			55	45	1	4	5		
11	2	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
11	2	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
11	2	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
11	2	1	Total	C	Mg	N	O	0	0
			50	40	1	4	5		
11	2	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
11	2	1	Total	C	Mg	N	O	0	0
			58	48	1	4	5		
11	2	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
11	2	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
11	2	1	Total	C	Mg	N	O	0	0
			60	50	1	4	5		
11	2	1	Total	C	Mg	N	O	0	0
			60	50	1	4	5		
11	2	1	Total	C	Mg	N	O	0	0
			47	37	1	4	5		
11	2	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
11	2	1	Total	C	Mg	N	O	0	0
			46	36	1	4	5		
11	2	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
11	2	1	Total	C	Mg	N	O	0	0
			46	36	1	4	5		
11	8	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
11	8	1	Total	C	Mg	N	O	0	0
			46	36	1	4	5		

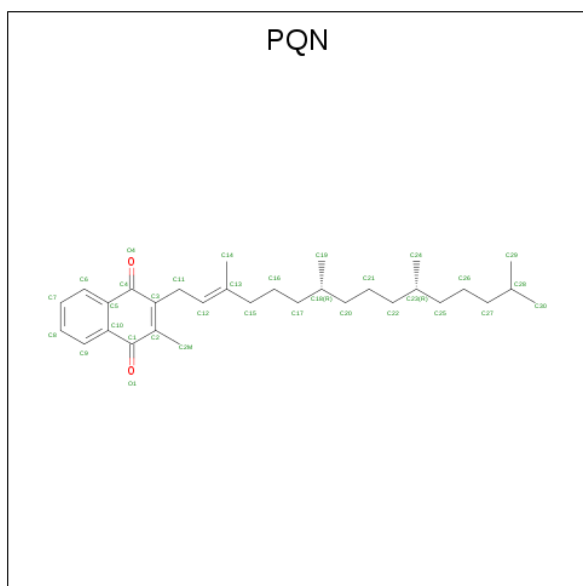
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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
11	8	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
11	K	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
11	K	1	Total	C	Mg	N	O	0	0
			50	40	1	4	5		
11	k	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
11	k	1	Total	C	Mg	N	O	0	0
			50	40	1	4	5		
11	0	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
11	0	1	Total	C	Mg	N	O	0	0
			50	40	1	4	5		

- Molecule 12 is PHYLLOQUINONE (three-letter code: PQN) (formula: C<sub>31</sub>H<sub>46</sub>O<sub>2</sub>).



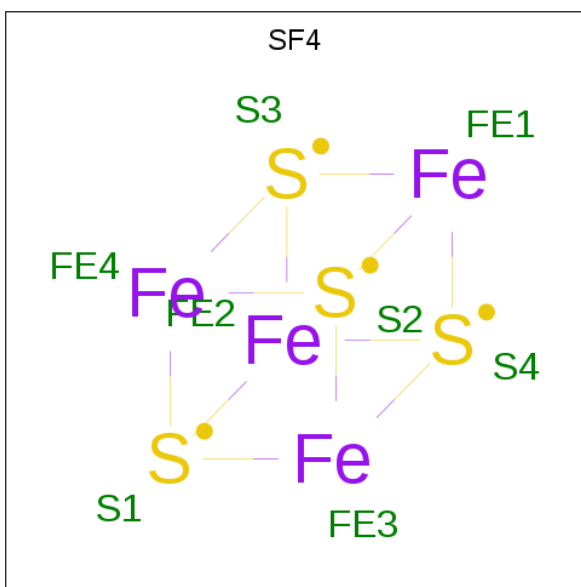
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
12	A	1	Total	C	O	0	0
			33	31	2		
12	B	1	Total	C	O	0	0
			33	31	2		
12	a	1	Total	C	O	0	0
			33	31	2		
12	b	1	Total	C	O	0	0
			33	31	2		

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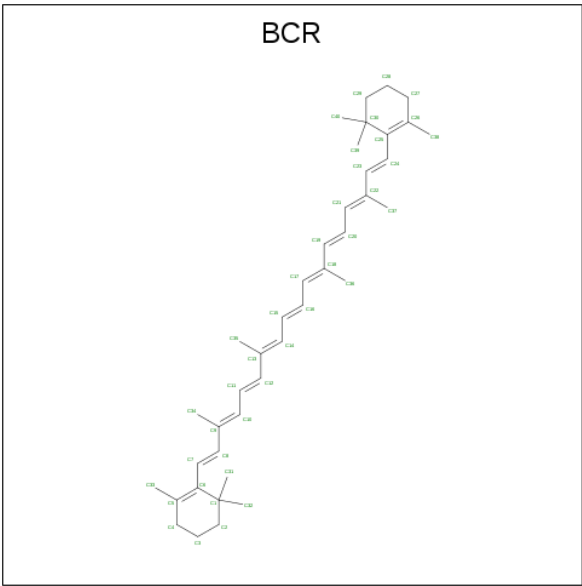
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
12	1	1	Total	C	O	0	0
			33	31	2		
12	2	1	Total	C	O	0	0
			33	31	2		

- Molecule 13 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe<sub>4</sub>S<sub>4</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
13	A	1	Total	Fe	S	0	0
			8	4	4		
13	C	1	Total	Fe	S	0	0
			8	4	4		
13	C	1	Total	Fe	S	0	0
			8	4	4		
13	a	1	Total	Fe	S	0	0
			8	4	4		
13	c	1	Total	Fe	S	0	0
			8	4	4		
13	c	1	Total	Fe	S	0	0
			8	4	4		
13	1	1	Total	Fe	S	0	0
			8	4	4		
13	3	1	Total	Fe	S	0	0
			8	4	4		
13	3	1	Total	Fe	S	0	0
			8	4	4		

- Molecule 14 is BETA-CAROTENE (three-letter code: BCR) (formula: C<sub>40</sub>H<sub>56</sub>).



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

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
14	F	1	Total C 40 40	0	0
14	F	1	Total C 40 40	0	0
14	F	1	Total C 40 40	0	0
14	L	1	Total C 40 40	0	0
14	L	1	Total C 40 40	0	0
14	M	1	Total C 40 40	0	0
14	a	1	Total C 40 40	0	0
14	a	1	Total C 40 40	0	0
14	a	1	Total C 40 40	0	0
14	a	1	Total C 40 40	0	0
14	a	1	Total C 40 40	0	0
14	b	1	Total C 40 40	0	0
14	b	1	Total C 40 40	0	0
14	b	1	Total C 40 40	0	0
14	b	1	Total C 40 40	0	0
14	b	1	Total C 40 40	0	0
14	b	1	Total C 40 40	0	0
14	b	1	Total C 40 40	0	0
14	b	1	Total C 40 40	0	0
14	f	1	Total C 40 40	0	0
14	f	1	Total C 40 40	0	0

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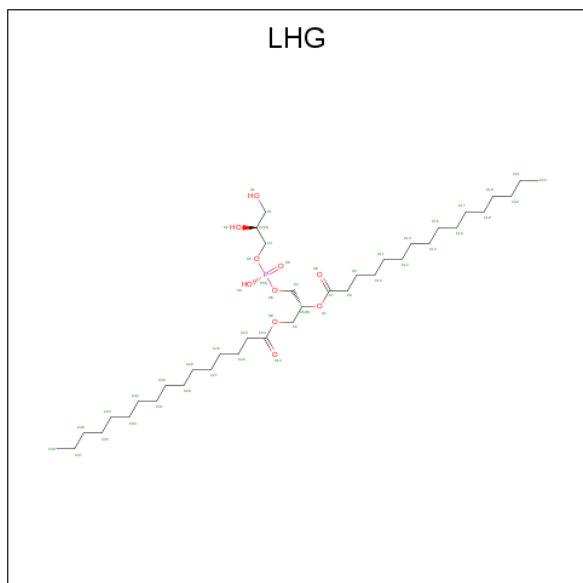
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
14	f	1	Total C 40 40	0	0
14	l	1	Total C 40 40	0	0
14	l	1	Total C 40 40	0	0
14	m	1	Total C 40 40	0	0
14	1	1	Total C 40 40	0	0
14	1	1	Total C 40 40	0	0
14	1	1	Total C 40 40	0	0
14	1	1	Total C 40 40	0	0
14	1	1	Total C 40 40	0	0
14	2	1	Total C 40 40	0	0
14	2	1	Total C 40 40	0	0
14	2	1	Total C 40 40	0	0
14	2	1	Total C 40 40	0	0
14	2	1	Total C 40 40	0	0
14	2	1	Total C 40 40	0	0
14	2	1	Total C 40 40	0	0
14	2	1	Total C 40 40	0	0
14	6	1	Total C 40 40	0	0
14	6	1	Total C 40 40	0	0
14	6	1	Total C 40 40	0	0
14	8	1	Total C 40 40	0	0

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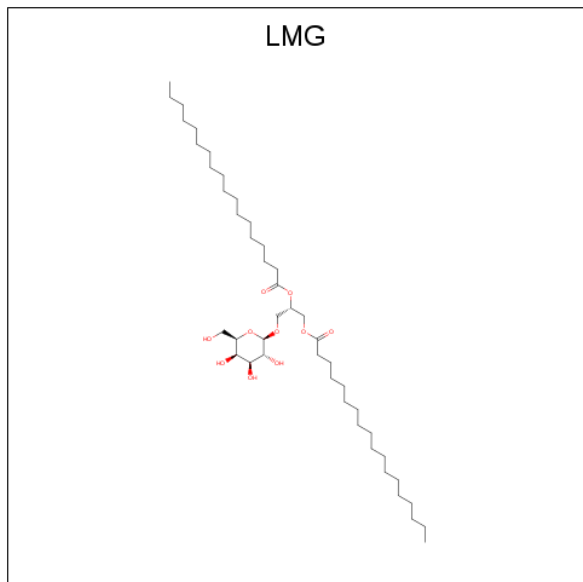
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
14	8	1	Total C 40 40	0	0
14	7	1	Total C 40 40	0	0

- Molecule 15 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (three-letter code: LHG) (formula:  $C_{38}H_{75}O_{10}P$ ).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
15	A	1	Total C O P 49 38 10 1	0	0
15	A	1	Total C O P 49 38 10 1	0	0
15	B	1	Total C O P 49 38 10 1	0	0
15	a	1	Total C O P 49 38 10 1	0	0
15	a	1	Total C O P 49 38 10 1	0	0
15	b	1	Total C O P 49 38 10 1	0	0
15	1	1	Total C O P 49 38 10 1	0	0
15	1	1	Total C O P 49 38 10 1	0	0
15	2	1	Total C O P 49 38 10 1	0	0

- Molecule 16 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (three-letter code: LMG) (formula: C<sub>45</sub>H<sub>86</sub>O<sub>10</sub>).

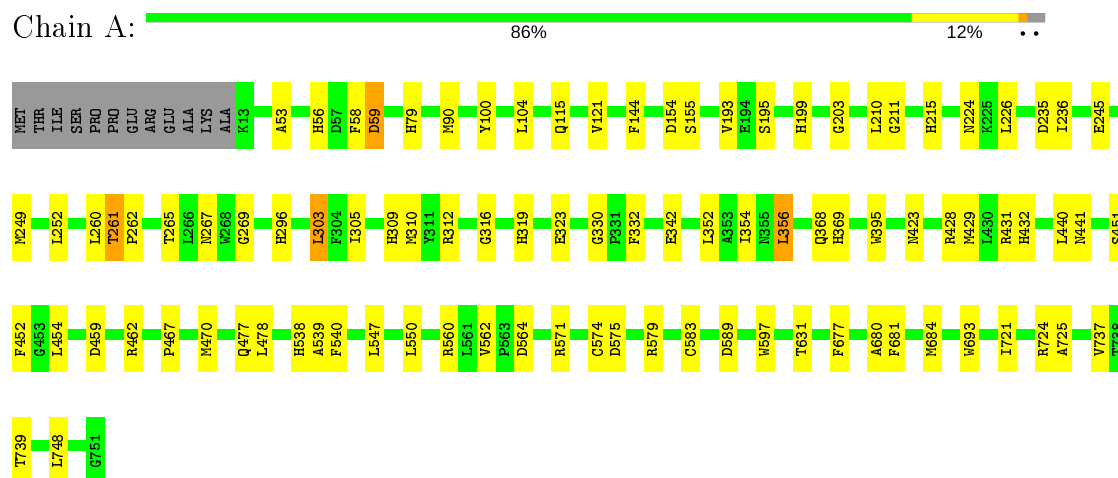


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
16	B	1	Total	C	O	0	0
			55	45	10		
16	b	1	Total	C	O	0	0
			55	45	10		
16	2	1	Total	C	O	0	0
			55	45	10		

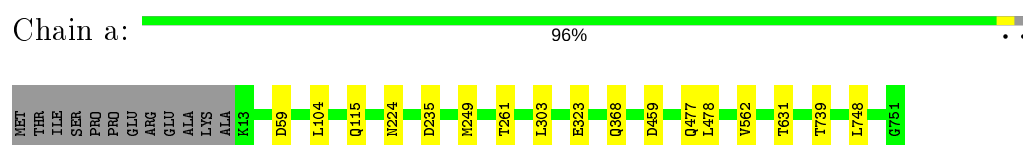
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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. 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. Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

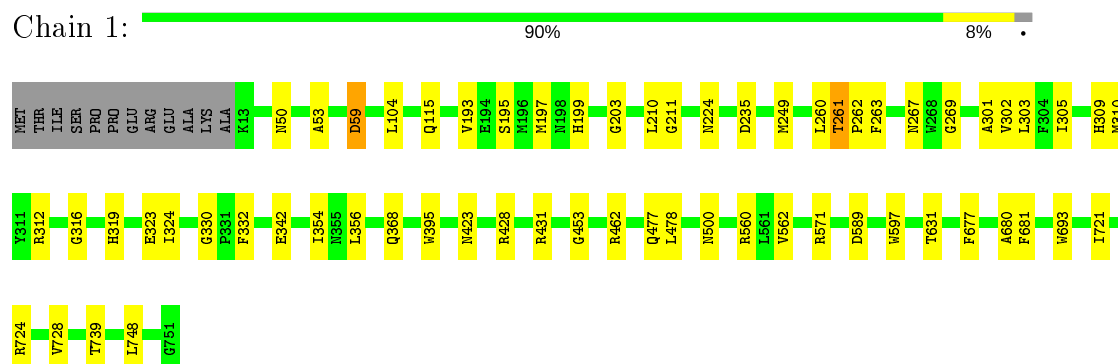
- Molecule 1: Photosystem I P700 chlorophyll a apoprotein A1



- Molecule 1: Photosystem I P700 chlorophyll a apoprotein A1




- Molecule 1: Photosystem I P700 chlorophyll a apoprotein A1



- Molecule 2: Photosystem I P700 chlorophyll a apoprotein A2



Chain B:  87% 11% .




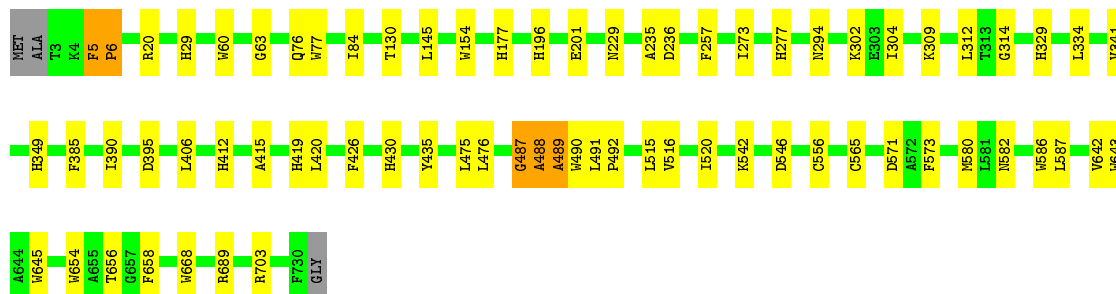
- Molecule 2: Photosystem I P700 chlorophyll a apoprotein A2

Chain b:  96% .




- Molecule 2: Photosystem I P700 chlorophyll a apoprotein A2

Chain 2:  90% 9% .



- Molecule 3: Photosystem I iron-sulfur center

Chain C:  84% 10% 5% .




- Molecule 3: Photosystem I iron-sulfur center

Chain c:  94% 5% .



- Molecule 3: Photosystem I iron-sulfur center

Chain 3:  88% 9% .



- Molecule 4: Photosystem I subunit II

Chain D: 88% 8% ..



- Molecule 4: Photosystem I subunit II

Chain d: 94% ..



- Molecule 4: Photosystem I subunit II

Chain 4: 91% ..



- Molecule 5: Photosystem I reaction center subunit IV

Chain E: 84% 7% 8% .



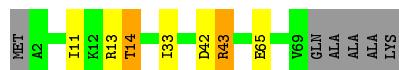
- Molecule 5: Photosystem I reaction center subunit IV

Chain e: 88% 8% .



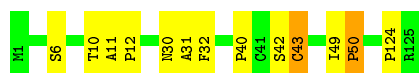
- Molecule 5: Photosystem I reaction center subunit IV

Chain 5: 82% 7% 8% .



- Molecule 6: Fusion protein of Photosystem I subunit III and subunit IX

Chain F: 90% 9% .



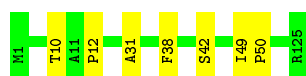
- Molecule 6: Fusion protein of Photosystem I subunit III and subunit IX

Chain f: 98% .



- Molecule 6: Fusion protein of Photosystem I subunit III and subunit IX

Chain 6: 94% 6%



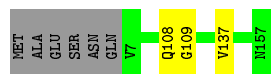
- Molecule 7: Photosystem I reaction center subunit XI

Chain L: 88% 8% . .



- Molecule 7: Photosystem I reaction center subunit XI

Chain l: 94% . .



- Molecule 7: Photosystem I reaction center subunit XI

Chain 8: 91% 5% .



- Molecule 8: Photosystem I reaction center subunit XII

Chain M: 84% 13% .

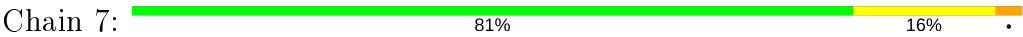


- Molecule 8: Photosystem I reaction center subunit XII

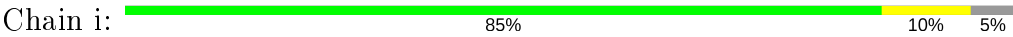
Chain m: 97% .



- Molecule 8: Photosystem I reaction center subunit XII



- Molecule 9: Photosystem I subunit III



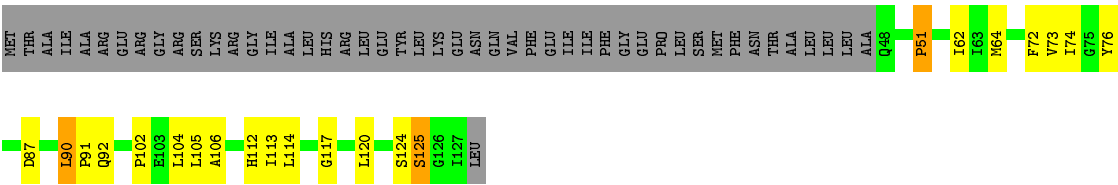
- Molecule 9: Photosystem I subunit III



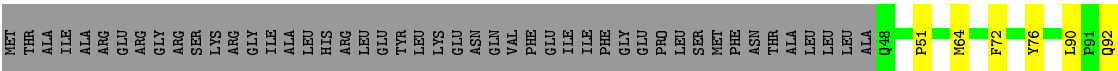
- Molecule 9: Photosystem I subunit III



- Molecule 10: Photosystem I reaction center subunit VIII

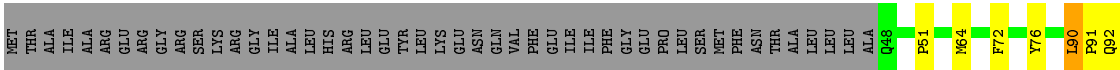


- Molecule 10: Photosystem I reaction center subunit VIII





● Molecule 10: Photosystem I reaction center subunit VIII



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	214.62Å 133.68Å 219.85Å 90.00° 111.14° 90.00°	Depositor
Resolution (Å)	30.00 – 3.80 39.96 – 3.40	Depositor EDS
% Data completeness (in resolution range)	95.4 (30.00-3.80) 71.5 (39.96-3.40)	Depositor EDS
$R_{merge}$	0.12	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	-0.02 (at 3.40Å)	Xtriage
Refinement program	PHENIX 1.8.2-1309, REFMAC 5.7.0032	Depositor
R, $R_{free}$	0.253 , 0.297 0.263 , 0.302	Depositor DCC
$R_{free}$ test set	7809 reflections (4.97%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	93.5	Xtriage
Anisotropy	0.250	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.25 , 77.1	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.45$ , $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	0.038 for l,-k,h	Xtriage
$F_o, F_c$ correlation	0.89	EDS
Total number of atoms	68370	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	173.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.75% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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 [i](#)

### 5.1 Standard geometry [i](#)

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

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	1	0.22	0/5970	0.37	0/8138
1	A	0.23	0/5970	0.38	0/8138
1	a	0.22	0/5970	0.37	0/8138
2	2	0.23	0/5976	0.39	0/8173
2	B	0.24	0/5976	0.39	0/8173
2	b	0.23	0/5976	0.38	0/8173
3	3	0.28	0/610	0.44	0/826
3	C	0.24	0/610	0.46	0/826
3	c	0.25	0/610	0.43	0/826
4	4	0.23	0/1103	0.40	0/1487
4	D	0.23	0/1103	0.40	0/1487
4	d	0.23	0/1103	0.39	0/1487
5	5	0.23	0/538	0.45	0/729
5	E	0.24	0/538	0.43	0/729
5	e	0.23	0/538	0.42	0/729
6	6	0.23	0/700	0.43	0/976
6	F	0.24	0/690	0.47	0/963
6	f	0.23	0/700	0.43	0/976
7	8	0.23	0/1163	0.38	0/1580
7	L	0.23	0/1163	0.38	0/1580
7	l	0.23	0/1163	0.38	0/1580
8	7	0.26	0/238	0.38	0/323
8	M	0.26	0/238	0.39	0/323
8	m	0.25	0/238	0.38	0/323
9	9	0.25	0/308	0.42	0/421
9	I	0.24	0/308	0.41	0/421
9	i	0.25	0/308	0.43	0/421
10	0	0.22	0/504	0.48	0/688
10	K	0.24	0/504	0.45	0/688
10	k	0.23	0/504	0.45	0/688
All	All	0.23	0/51320	0.39	0/70010

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
2	2	0	1
2	B	0	1
2	b	0	1
4	4	0	1
4	D	0	1
4	d	0	1
6	F	0	1
10	k	0	1
All	All	0	8

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

5 of 8 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	5	PHE	Peptide
4	D	98	HIS	Peptide
6	F	40	PRO	Mainchain
2	b	5	PHE	Peptide
4	d	98	HIS	Peptide

## 5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	1	5772	0	5621	48	0
1	A	5772	0	5621	94	0
1	a	5772	0	5621	0	0
2	2	5765	0	5546	48	0
2	B	5765	0	5546	64	0
2	b	5765	0	5545	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	3	600	0	588	22	0
3	C	600	0	586	25	0
3	c	600	0	587	0	0
4	4	1079	0	1073	5	0
4	D	1079	0	1073	9	0
4	d	1079	0	1073	0	0
5	5	529	0	506	4	0
5	E	529	0	506	2	0
5	e	529	0	506	0	0
6	6	685	0	411	3	0
6	F	676	0	395	11	0
6	f	685	0	411	0	0
7	8	1133	0	1108	5	0
7	L	1133	0	1108	9	0
7	l	1133	0	1108	0	0
8	7	235	0	253	7	0
8	M	235	0	253	7	0
8	m	235	0	253	0	0
9	9	297	0	295	10	0
9	I	297	0	295	7	0
9	i	297	0	295	0	0
10	0	496	0	439	4	0
10	K	496	0	439	12	0
10	k	496	0	439	0	0
11	0	115	0	111	4	0
11	1	2546	0	2430	89	0
11	2	2313	0	2213	84	0
11	8	176	0	177	8	0
11	A	2546	0	2435	159	0
11	B	2313	0	2213	127	0
11	K	115	0	111	8	0
11	L	176	0	177	8	0
11	a	2546	0	2434	0	0
11	b	2313	0	2213	0	0
11	k	115	0	111	0	0
11	l	176	0	177	0	0
12	1	33	0	45	1	0
12	2	33	0	45	3	0
12	A	33	0	45	5	0
12	B	33	0	45	4	0
12	a	33	0	46	0	0
12	b	33	0	45	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
13	1	8	0	0	1	0
13	3	16	0	0	21	0
13	A	8	0	0	4	0
13	C	16	0	0	22	0
13	a	8	0	0	0	0
13	c	16	0	0	0	0
14	1	200	0	242	23	0
14	2	320	0	391	40	0
14	6	120	0	147	20	0
14	7	40	0	49	6	0
14	8	80	0	97	15	0
14	A	200	0	244	35	0
14	B	320	0	390	62	0
14	F	120	0	146	23	0
14	L	80	0	97	22	0
14	M	40	0	49	7	0
14	a	200	0	243	0	0
14	b	320	0	389	0	0
14	f	120	0	147	0	0
14	l	80	0	97	0	0
14	m	40	0	49	0	0
15	1	98	0	148	16	0
15	2	49	0	74	7	0
15	A	98	0	148	15	0
15	B	49	0	74	8	0
15	a	98	0	148	0	0
15	b	49	0	74	0	0
16	2	55	0	86	1	0
16	B	55	0	86	1	0
16	b	55	0	86	0	0
All	All	68370	0	66274	831	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 6.

The worst 5 of 831 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:48:CYS:SG	13:C:3002:SF4:FE4	0.75	1.74
3:3:48:CYS:SG	13:3:3002:SF4:FE4	0.87	1.64
1:A:56:HIS:CG	11:A:1103:CLA:HBB2	3.55	1.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:3:11:CYS:SG	13:3:3003:SF4:FE3	0.88	1.61
3:C:58:CYS:SG	13:C:3003:SF4:FE1	1.08	1.57

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all 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	1	737/751 (98%)	697 (95%)	38 (5%)	2 (0%)	41	74
1	A	737/751 (98%)	693 (94%)	42 (6%)	2 (0%)	41	74
1	a	737/751 (98%)	698 (95%)	37 (5%)	2 (0%)	41	74
2	2	726/731 (99%)	691 (95%)	28 (4%)	7 (1%)	15	52
2	B	726/731 (99%)	690 (95%)	30 (4%)	6 (1%)	19	57
2	b	726/731 (99%)	692 (95%)	28 (4%)	6 (1%)	19	57
3	3	78/81 (96%)	75 (96%)	3 (4%)	0	100	100
3	C	78/81 (96%)	74 (95%)	4 (5%)	0	100	100
3	c	78/81 (96%)	74 (95%)	4 (5%)	0	100	100
4	4	136/141 (96%)	121 (89%)	14 (10%)	1 (1%)	22	60
4	D	136/141 (96%)	122 (90%)	13 (10%)	1 (1%)	22	60
4	d	136/141 (96%)	122 (90%)	13 (10%)	1 (1%)	22	60
5	5	66/74 (89%)	58 (88%)	7 (11%)	1 (2%)	10	46
5	E	66/74 (89%)	57 (86%)	8 (12%)	1 (2%)	10	46
5	e	66/74 (89%)	58 (88%)	7 (11%)	1 (2%)	10	46
6	6	123/125 (98%)	115 (94%)	6 (5%)	2 (2%)	9	44
6	F	123/125 (98%)	114 (93%)	6 (5%)	3 (2%)	6	37
6	f	123/125 (98%)	115 (94%)	6 (5%)	2 (2%)	9	44

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
7	8	149/157 (95%)	135 (91%)	12 (8%)	2 (1%)	12	48
7	L	149/157 (95%)	135 (91%)	11 (7%)	3 (2%)	7	41
7	l	149/157 (95%)	135 (91%)	12 (8%)	2 (1%)	12	48
8	7	29/31 (94%)	29 (100%)	0	0	100	100
8	M	29/31 (94%)	28 (97%)	1 (3%)	0	100	100
8	m	29/31 (94%)	29 (100%)	0	0	100	100
9	9	36/40 (90%)	34 (94%)	2 (6%)	0	100	100
9	I	36/40 (90%)	34 (94%)	2 (6%)	0	100	100
9	i	36/40 (90%)	34 (94%)	2 (6%)	0	100	100
10	0	78/128 (61%)	65 (83%)	9 (12%)	4 (5%)	2	23
10	K	78/128 (61%)	66 (85%)	7 (9%)	5 (6%)	1	20
10	k	78/128 (61%)	66 (85%)	9 (12%)	3 (4%)	3	29
All	All	6474/6777 (96%)	6056 (94%)	361 (6%)	57 (1%)	17	54

5 of 57 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	261	THR
2	B	6	PRO
4	D	99	PRO
6	F	43	CYS
1	a	261	THR

### 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	1	588/603 (98%)	573 (97%)	15 (3%)	46	69
1	A	588/603 (98%)	570 (97%)	18 (3%)	40	65
1	a	588/603 (98%)	573 (97%)	15 (3%)	46	69
2	2	582/583 (100%)	565 (97%)	17 (3%)	42	67

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	B	582/583 (100%)	562 (97%)	20 (3%)	37	64
2	b	582/583 (100%)	566 (97%)	16 (3%)	44	69
3	3	68/69 (99%)	65 (96%)	3 (4%)	28	57
3	C	68/69 (99%)	61 (90%)	7 (10%)	7	31
3	c	68/69 (99%)	64 (94%)	4 (6%)	19	51
4	4	113/116 (97%)	109 (96%)	4 (4%)	36	64
4	D	113/116 (97%)	111 (98%)	2 (2%)	59	77
4	d	113/116 (97%)	110 (97%)	3 (3%)	44	69
5	5	56/60 (93%)	54 (96%)	2 (4%)	35	63
5	E	56/60 (93%)	54 (96%)	2 (4%)	35	63
5	e	56/60 (93%)	54 (96%)	2 (4%)	35	63
6	6	21/106 (20%)	20 (95%)	1 (5%)	25	56
6	F	19/106 (18%)	19 (100%)	0	100	100
6	f	21/106 (20%)	20 (95%)	1 (5%)	25	56
7	8	113/118 (96%)	113 (100%)	0	100	100
7	L	113/118 (96%)	112 (99%)	1 (1%)	78	88
7	l	113/118 (96%)	112 (99%)	1 (1%)	78	88
8	7	24/25 (96%)	23 (96%)	1 (4%)	30	58
8	M	24/25 (96%)	23 (96%)	1 (4%)	30	58
8	m	24/25 (96%)	23 (96%)	1 (4%)	30	58
9	9	31/32 (97%)	28 (90%)	3 (10%)	8	33
9	I	31/32 (97%)	27 (87%)	4 (13%)	4	23
9	i	31/32 (97%)	27 (87%)	4 (13%)	4	23
10	0	37/100 (37%)	30 (81%)	7 (19%)	1	10
10	K	37/100 (37%)	30 (81%)	7 (19%)	1	10
10	k	37/100 (37%)	31 (84%)	6 (16%)	2	15
All	All	4897/5436 (90%)	4729 (97%)	168 (3%)	37	64

5 of 168 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	b	334	LEU
9	i	21	LEU

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Mol	Chain	Res	Type
10	k	64	MET
2	b	516	VAL
3	c	69	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 24 such sidechains are listed below:

Mol	Chain	Res	Type
2	b	34	HIS
1	1	76	HIS
2	2	437	HIS
2	b	437	HIS
2	b	582	ASN

### 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 carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

357 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
11	CLA	2	1218	-	36,53,73	2.83	14 (38%)	39,89,113	2.36	11 (28%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
11	CLA	a	1122	-	53,67,73	2.49	15 (28%)	59,105,113	2.37	16 (27%)
11	CLA	A	1101	-	59,73,73	2.32	15 (25%)	67,113,113	2.07	17 (25%)
11	CLA	b	1218	-	36,53,73	2.87	15 (41%)	39,89,113	2.30	9 (23%)
11	CLA	1	1801	15	46,60,73	2.67	15 (32%)	51,97,113	2.49	18 (35%)
11	CLA	A	1125	-	46,60,73	2.66	15 (32%)	51,97,113	2.60	19 (37%)
14	BCR	1	4008	-	41,41,41	2.72	6 (14%)	56,56,56	6.79	28 (50%)
11	CLA	b	1222	-	50,64,73	2.53	16 (32%)	56,102,113	2.49	18 (32%)
14	BCR	b	4010	-	41,41,41	2.79	6 (14%)	56,56,56	6.71	24 (42%)
11	CLA	2	1224	-	49,63,73	2.53	16 (32%)	55,101,113	2.46	17 (30%)
14	BCR	6	4020	-	41,41,41	2.86	7 (17%)	56,56,56	6.54	24 (42%)
11	CLA	K	1401	-	59,73,73	2.33	15 (25%)	67,113,113	2.22	18 (26%)
11	CLA	a	1124	-	49,63,73	2.56	16 (32%)	55,101,113	2.38	17 (30%)
11	CLA	1	1133	-	40,54,73	2.91	15 (37%)	44,90,113	2.36	13 (29%)
11	CLA	1	1139	-	44,58,73	2.72	16 (36%)	49,95,113	2.45	16 (32%)
15	LHG	1	5001	-	48,48,48	0.95	2 (4%)	51,54,54	1.08	4 (7%)
11	CLA	2	1208	-	36,53,73	2.86	14 (38%)	39,89,113	2.28	9 (23%)
11	CLA	1	1111	-	54,68,73	2.40	14 (25%)	61,107,113	2.32	20 (32%)
11	CLA	a	1114	-	40,54,73	2.91	15 (37%)	44,90,113	2.34	12 (27%)
14	BCR	a	4008	-	41,41,41	2.74	7 (17%)	56,56,56	6.57	29 (51%)
11	CLA	b	1213	-	59,73,73	2.35	16 (27%)	67,113,113	2.16	15 (22%)
15	LHG	a	5003	11	48,48,48	0.94	2 (4%)	51,54,54	1.03	3 (5%)
11	CLA	B	1210	-	59,73,73	2.35	15 (25%)	67,113,113	2.20	18 (26%)
14	BCR	b	4011	-	41,41,41	2.75	6 (14%)	56,56,56	6.79	25 (44%)
11	CLA	b	1240	-	36,53,73	2.89	15 (41%)	39,89,113	2.25	10 (25%)
11	CLA	a	1022	-	59,73,73	2.35	16 (27%)	67,113,113	2.16	16 (23%)
11	CLA	A	1120	-	40,54,73	2.91	16 (40%)	44,90,113	2.37	13 (29%)
11	CLA	8	1501	-	59,73,73	2.32	15 (25%)	67,113,113	2.25	18 (26%)
11	CLA	B	1216	-	59,73,73	2.34	15 (25%)	67,113,113	2.06	15 (22%)
11	CLA	B	1213	-	59,73,73	2.35	15 (25%)	67,113,113	2.15	16 (23%)
15	LHG	B	5004	11	48,48,48	0.95	2 (4%)	51,54,54	1.12	4 (7%)
11	CLA	1	1120	-	40,54,73	2.92	16 (40%)	44,90,113	2.39	13 (29%)
11	CLA	2	1217	-	41,55,73	2.77	15 (36%)	45,91,113	2.54	16 (35%)
13	SF4	3	3002	3	0,12,12	0.00	-	-	-	-
14	BCR	2	4014	-	41,41,41	2.80	6 (14%)	56,56,56	6.44	23 (41%)
11	CLA	a	1237	-	49,63,73	2.55	15 (30%)	55,101,113	2.37	15 (27%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
14	BCR	b	4004	-	41,41,41	2.73	6 (14%)	56,56,56	6.57	26 (46%)
11	CLA	1	1108	-	36,53,73	2.88	15 (41%)	39,89,113	2.31	9 (23%)
14	BCR	l	4022	-	41,41,41	2.74	6 (14%)	56,56,56	6.41	26 (46%)
11	CLA	2	1204	-	59,73,73	2.34	15 (25%)	67,113,113	2.04	15 (22%)
11	CLA	B	1215	-	59,73,73	2.33	15 (25%)	67,113,113	2.31	17 (25%)
11	CLA	A	1133	-	40,54,73	2.87	15 (37%)	44,90,113	2.46	14 (31%)
14	BCR	7	4021	-	41,41,41	2.78	6 (14%)	56,56,56	6.61	21 (37%)
11	CLA	1	1138	-	40,54,73	2.88	15 (37%)	44,90,113	2.30	12 (27%)
14	BCR	F	4020	-	41,41,41	2.79	6 (14%)	56,56,56	6.41	23 (41%)
11	CLA	b	1220	-	40,54,73	2.94	16 (40%)	44,90,113	2.35	13 (29%)
11	CLA	b	1216	-	59,73,73	2.36	16 (27%)	67,113,113	2.17	21 (31%)
11	CLA	b	1234	-	54,68,73	2.45	15 (27%)	61,107,113	2.28	16 (26%)
11	CLA	B	1207	-	59,73,73	2.31	14 (23%)	67,113,113	2.24	16 (23%)
14	BCR	B	4010	-	41,41,41	2.72	6 (14%)	56,56,56	6.41	26 (46%)
11	CLA	a	1103	-	59,73,73	2.36	16 (27%)	67,113,113	2.11	16 (23%)
11	CLA	1	1129	-	40,54,73	2.90	16 (40%)	44,90,113	2.40	12 (27%)
11	CLA	b	1239	-	40,54,73	2.90	15 (37%)	44,90,113	2.42	14 (31%)
11	CLA	1	1109	-	59,73,73	2.34	15 (25%)	67,113,113	2.17	16 (23%)
11	CLA	1	1132	-	59,73,73	2.32	15 (25%)	67,113,113	2.04	14 (20%)
11	CLA	A	1126	-	59,73,73	2.34	15 (25%)	67,113,113	2.21	17 (25%)
11	CLA	1	1103	-	59,73,73	2.32	15 (25%)	67,113,113	2.24	19 (28%)
14	BCR	a	4003	-	41,41,41	2.75	6 (14%)	56,56,56	6.20	26 (46%)
11	CLA	A	1109	11	59,73,73	2.36	15 (25%)	67,113,113	2.15	15 (22%)
11	CLA	B	1202	-	59,73,73	2.37	16 (27%)	67,113,113	2.15	15 (22%)
11	CLA	k	1402	-	44,58,73	2.73	15 (34%)	49,95,113	2.39	16 (32%)
11	CLA	B	1203	-	59,73,73	2.32	14 (23%)	67,113,113	2.07	14 (20%)
16	LMG	b	5002	-	55,55,55	0.88	2 (3%)	63,63,63	1.04	5 (7%)
11	CLA	8	1502	-	40,54,73	2.88	15 (37%)	44,90,113	2.44	14 (31%)
11	CLA	A	1119	-	59,73,73	2.31	15 (25%)	67,113,113	2.07	19 (28%)
11	CLA	A	1113	-	36,53,73	2.85	15 (41%)	39,89,113	2.36	12 (30%)
14	BCR	B	4011	-	41,41,41	2.81	7 (17%)	56,56,56	6.71	27 (48%)
11	CLA	L	1502	-	40,54,73	2.88	14 (35%)	44,90,113	2.40	12 (27%)
11	CLA	A	1131	-	59,73,73	2.35	15 (25%)	67,113,113	2.13	18 (26%)
11	CLA	1	1022	-	59,73,73	2.35	16 (27%)	67,113,113	2.15	17 (25%)
11	CLA	a	1112	-	36,53,73	2.86	15 (41%)	39,89,113	2.27	11 (28%)



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
11	CLA	1	1123	-	59,73,73	2.35	16 (27%)	67,113,113	2.18	16 (23%)
11	CLA	a	1115	-	40,54,73	2.91	15 (37%)	44,90,113	2.26	13 (29%)
11	CLA	0	1401	-	59,73,73	2.33	15 (25%)	67,113,113	2.23	17 (25%)
11	CLA	b	1225	-	59,73,73	2.36	16 (27%)	67,113,113	2.12	15 (22%)
11	CLA	a	1012	-	59,73,73	2.37	16 (27%)	67,113,113	2.29	16 (23%)
11	CLA	1	1106	1	59,73,73	2.34	15 (25%)	67,113,113	2.08	17 (25%)
14	BCR	A	4001	-	41,41,41	2.78	6 (14%)	56,56,56	6.39	27 (48%)
11	CLA	A	1127	-	59,73,73	2.32	16 (27%)	67,113,113	2.18	18 (26%)
12	PQN	A	2001	-	34,34,34	1.65	2 (5%)	42,45,45	1.12	6 (14%)
11	CLA	A	1114	-	40,54,73	2.91	15 (37%)	44,90,113	2.27	12 (27%)
11	CLA	2	1221	-	48,62,73	2.59	16 (33%)	53,99,113	2.45	16 (30%)
11	CLA	B	1223	-	59,73,73	2.35	16 (27%)	67,113,113	2.24	19 (28%)
14	BCR	2	4011	-	41,41,41	2.80	6 (14%)	56,56,56	6.77	26 (46%)
11	CLA	a	1140	-	59,73,73	2.34	15 (25%)	67,113,113	2.16	16 (23%)
11	CLA	A	1134	1	40,54,73	2.89	15 (37%)	44,90,113	2.39	14 (31%)
11	CLA	1	1114	-	40,54,73	2.91	15 (37%)	44,90,113	2.34	12 (27%)
11	CLA	b	1235	-	54,68,73	2.47	16 (29%)	61,107,113	2.32	19 (31%)
11	CLA	a	1116	-	48,62,73	2.61	15 (31%)	53,99,113	2.32	16 (30%)
13	SF4	3	3003	-	0,12,12	0.00	-	-	-	-
11	CLA	A	1117	-	59,73,73	2.40	15 (25%)	67,113,113	2.10	16 (23%)
11	CLA	a	1119	-	59,73,73	2.32	15 (25%)	67,113,113	2.17	18 (26%)
11	CLA	B	1231	-	36,53,73	2.86	14 (38%)	39,89,113	2.52	14 (35%)
14	BCR	b	4014	-	41,41,41	2.74	6 (14%)	56,56,56	6.49	24 (42%)
13	SF4	a	3001	1,2	0,12,12	0.00	-	-	-	-
15	LHG	A	5003	11	48,48,48	0.95	2 (4%)	51,54,54	1.13	4 (7%)
11	CLA	2	1231	-	36,53,73	2.86	14 (38%)	39,89,113	2.48	15 (38%)
11	CLA	A	1128	-	59,73,73	2.31	14 (23%)	67,113,113	2.12	15 (22%)
11	CLA	B	1224	-	49,63,73	2.55	15 (30%)	55,101,113	2.44	16 (29%)
11	CLA	1	1137	-	59,73,73	2.35	15 (25%)	67,113,113	2.32	19 (28%)
14	BCR	f	4020	-	41,41,41	2.79	6 (14%)	56,56,56	6.58	22 (39%)
11	CLA	1	1130	-	40,54,73	2.92	16 (40%)	44,90,113	2.24	11 (25%)
11	CLA	B	1206	2	59,73,73	2.30	15 (25%)	67,113,113	2.20	17 (25%)
14	BCR	b	4009	-	41,41,41	2.65	6 (14%)	56,56,56	6.93	25 (44%)
11	CLA	a	1102	11	59,73,73	2.34	16 (27%)	67,113,113	2.12	14 (20%)
15	LHG	A	5001	-	48,48,48	0.93	2 (4%)	51,54,54	1.13	4 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
11	CLA	b	1219	-	49,63,73	2.60	15 (30%)	55,101,113	2.38	16 (29%)
11	CLA	a	1120	-	40,54,73	2.90	16 (40%)	44,90,113	2.47	13 (29%)
11	CLA	b	1230	-	52,66,73	2.53	16 (30%)	58,104,113	2.41	18 (31%)
11	CLA	0	1402	-	44,58,73	2.75	16 (36%)	49,95,113	2.35	12 (24%)
11	CLA	1	1124	-	49,63,73	2.56	16 (32%)	55,101,113	2.34	15 (27%)
14	BCR	A	4003	-	41,41,41	2.85	6 (14%)	56,56,56	6.29	24 (42%)
11	CLA	L	1503	-	59,73,73	2.30	14 (23%)	67,113,113	2.14	14 (20%)
11	CLA	B	1234	-	54,68,73	2.42	15 (27%)	61,107,113	2.32	19 (31%)
11	CLA	a	1106	1	59,73,73	2.34	16 (27%)	67,113,113	2.19	17 (25%)
11	CLA	2	1229	-	59,73,73	2.33	16 (27%)	67,113,113	2.11	16 (23%)
11	CLA	a	1801	15	46,60,73	2.68	15 (32%)	51,97,113	2.45	16 (31%)
11	CLA	B	1205	-	49,63,73	2.50	14 (28%)	55,101,113	2.56	15 (27%)
11	CLA	2	1201	-	48,62,73	2.60	15 (31%)	53,99,113	2.37	15 (28%)
11	CLA	a	1136	-	40,54,73	2.88	15 (37%)	44,90,113	2.35	11 (25%)
14	BCR	a	4001	-	41,41,41	2.74	6 (14%)	56,56,56	6.52	27 (48%)
11	CLA	2	1236	-	41,55,73	2.76	16 (39%)	45,91,113	2.52	13 (28%)
11	CLA	2	1219	-	49,63,73	2.61	16 (32%)	55,101,113	2.39	16 (29%)
11	CLA	1	1237	-	49,63,73	2.52	15 (30%)	55,101,113	2.33	18 (32%)
11	CLA	2	1212	-	36,53,73	2.87	14 (38%)	39,89,113	2.35	12 (30%)
11	CLA	1	1135	-	45,59,73	2.68	16 (35%)	50,96,113	2.50	16 (32%)
11	CLA	1	1116	-	48,62,73	2.60	16 (33%)	53,99,113	2.36	17 (32%)
11	CLA	2	1232	-	36,53,73	2.87	15 (41%)	39,89,113	2.23	10 (25%)
14	BCR	L	4019	-	41,41,41	2.69	6 (14%)	56,56,56	6.58	25 (44%)
11	CLA	a	1117	-	59,73,73	2.36	15 (25%)	67,113,113	2.11	16 (23%)
11	CLA	b	1228	-	44,58,73	2.72	15 (34%)	49,95,113	2.43	14 (28%)
11	CLA	2	1227	-	36,53,73	2.84	14 (38%)	39,89,113	2.41	10 (25%)
11	CLA	A	1011	-	59,73,73	2.30	14 (23%)	67,113,113	2.24	18 (26%)
14	BCR	B	4004	-	41,41,41	2.80	6 (14%)	56,56,56	6.56	27 (48%)
11	CLA	b	1227	-	36,53,73	2.87	15 (41%)	39,89,113	2.45	12 (30%)
11	CLA	l	1501	7	59,73,73	2.35	16 (27%)	67,113,113	2.20	17 (25%)
11	CLA	a	1105	-	42,56,73	2.80	15 (35%)	46,92,113	2.49	14 (30%)
11	CLA	b	1201	-	48,62,73	2.60	15 (31%)	53,99,113	2.45	17 (32%)
11	CLA	B	1239	-	40,54,73	2.89	16 (40%)	44,90,113	2.38	11 (25%)
11	CLA	A	1237	-	49,63,73	2.55	15 (30%)	55,101,113	2.37	15 (27%)
11	CLA	B	1209	-	36,53,73	2.87	14 (38%)	39,89,113	2.38	12 (30%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
11	CLA	a	1118	-	55,69,73	2.39	14 (25%)	62,108,113	2.28	15 (24%)
11	CLA	A	1116	-	48,62,73	2.61	16 (33%)	53,99,113	2.34	17 (32%)
11	CLA	2	1209	-	36,53,73	2.87	14 (38%)	39,89,113	2.37	12 (30%)
11	CLA	k	1401	-	59,73,73	2.34	15 (25%)	67,113,113	2.23	18 (26%)
11	CLA	A	1022	-	59,73,73	2.32	15 (25%)	67,113,113	2.18	17 (25%)
14	BCR	M	4021	-	41,41,41	2.79	6 (14%)	56,56,56	6.58	21 (37%)
15	LHG	2	5004	11	48,48,48	0.95	2 (4%)	51,54,54	1.05	3 (5%)
11	CLA	2	1023	-	59,73,73	2.32	15 (25%)	67,113,113	2.34	20 (29%)
15	LHG	1	5003	11	48,48,48	0.96	2 (4%)	51,54,54	1.03	3 (5%)
11	CLA	b	1212	-	36,53,73	2.85	15 (41%)	39,89,113	2.43	9 (23%)
11	CLA	A	1106	1	59,73,73	2.33	15 (25%)	67,113,113	2.12	14 (20%)
14	BCR	a	4007	-	41,41,41	2.72	6 (14%)	56,56,56	6.74	25 (44%)
11	CLA	2	1238	-	59,73,73	2.35	16 (27%)	67,113,113	2.05	15 (22%)
11	CLA	a	1125	-	46,60,73	2.61	16 (34%)	51,97,113	2.34	16 (31%)
11	CLA	A	1801	15	46,60,73	2.70	15 (32%)	51,97,113	2.47	16 (31%)
11	CLA	b	1224	-	49,63,73	2.58	16 (32%)	55,101,113	2.41	16 (29%)
11	CLA	2	1214	-	53,67,73	2.46	15 (28%)	59,105,113	2.20	17 (28%)
11	CLA	B	1217	-	41,55,73	2.75	15 (36%)	45,91,113	2.45	13 (28%)
12	PQN	B	2002	-	34,34,34	1.64	2 (5%)	42,45,45	1.13	5 (11%)
14	BCR	2	4009	-	41,41,41	2.72	6 (14%)	56,56,56	6.76	25 (44%)
11	CLA	8	1503	-	59,73,73	2.37	16 (27%)	67,113,113	2.09	13 (19%)
13	SF4	c	3003	3	0,12,12	0.00	-	-	-	-
11	CLA	a	1133	-	40,54,73	2.89	15 (37%)	44,90,113	2.40	12 (27%)
11	CLA	a	1139	-	44,58,73	2.72	16 (36%)	49,95,113	2.49	15 (30%)
15	LHG	a	5001	-	48,48,48	0.96	2 (4%)	51,54,54	1.06	4 (7%)
11	CLA	a	1134	-	40,54,73	2.90	15 (37%)	44,90,113	2.38	15 (34%)
11	CLA	1	1127	-	59,73,73	2.36	15 (25%)	67,113,113	2.05	16 (23%)
11	CLA	1	1126	-	59,73,73	2.35	16 (27%)	67,113,113	2.17	19 (28%)
11	CLA	a	1107	1	59,73,73	2.32	15 (25%)	67,113,113	2.33	20 (29%)
14	BCR	A	4002	-	41,41,41	2.74	6 (14%)	56,56,56	6.31	24 (42%)
11	CLA	A	1129	-	40,54,73	2.88	15 (37%)	44,90,113	2.26	12 (27%)
11	CLA	K	1402	-	44,58,73	2.71	15 (34%)	49,95,113	2.37	14 (28%)
11	CLA	A	1115	-	40,54,73	2.91	16 (40%)	44,90,113	2.32	12 (27%)
14	BCR	B	4009	-	41,41,41	2.75	6 (14%)	56,56,56	6.71	22 (39%)
11	CLA	a	1113	-	36,53,73	2.87	15 (41%)	39,89,113	2.32	11 (28%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
11	CLA	a	1128	-	59,73,73	2.35	15 (25%)	67,113,113	2.15	17 (25%)
11	CLA	1	1122	-	53,67,73	2.48	16 (30%)	59,105,113	2.27	16 (27%)
11	CLA	a	1110	-	48,62,73	2.61	16 (33%)	53,99,113	2.36	17 (32%)
11	CLA	B	1212	-	36,53,73	2.87	15 (41%)	39,89,113	2.27	9 (23%)
11	CLA	L	1501	7	59,73,73	2.34	16 (27%)	67,113,113	2.11	15 (22%)
11	CLA	1	1140	-	59,73,73	2.36	16 (27%)	67,113,113	2.28	18 (26%)
14	BCR	b	4005	-	41,41,41	2.76	6 (14%)	56,56,56	6.58	25 (44%)
11	CLA	b	1215	-	59,73,73	2.36	15 (25%)	67,113,113	2.31	20 (29%)
14	BCR	6	4018	-	41,41,41	2.87	7 (17%)	56,56,56	6.30	26 (46%)
11	CLA	A	1123	-	59,73,73	2.31	15 (25%)	67,113,113	2.24	17 (25%)
11	CLA	b	1226	-	59,73,73	2.32	16 (27%)	67,113,113	2.15	17 (25%)
11	CLA	a	1108	-	36,53,73	2.87	14 (38%)	39,89,113	2.35	11 (28%)
11	CLA	2	1234	-	54,68,73	2.41	15 (27%)	61,107,113	2.23	16 (26%)
11	CLA	2	1213	-	59,73,73	2.40	16 (27%)	67,113,113	2.25	17 (25%)
13	SF4	1	3001	1,2	0,12,12	0.00	-	-	-	-
14	BCR	b	4017	-	41,41,41	2.81	7 (17%)	56,56,56	6.66	28 (50%)
11	CLA	A	1130	-	40,54,73	2.90	16 (40%)	44,90,113	2.27	11 (25%)
11	CLA	B	1232	-	36,53,73	2.85	14 (38%)	39,89,113	2.37	10 (25%)
11	CLA	A	1012	-	59,73,73	2.34	16 (27%)	67,113,113	2.49	20 (29%)
11	CLA	A	1103	-	59,73,73	2.32	14 (23%)	67,113,113	2.11	17 (25%)
11	CLA	b	1238	-	59,73,73	2.34	15 (25%)	67,113,113	2.04	13 (19%)
11	CLA	a	1011	-	59,73,73	2.36	16 (27%)	67,113,113	2.26	17 (25%)
11	CLA	b	1204	-	59,73,73	2.32	15 (25%)	67,113,113	2.05	14 (20%)
11	CLA	b	1223	-	59,73,73	2.37	15 (25%)	67,113,113	2.10	17 (25%)
14	BCR	2	4005	-	41,41,41	2.73	6 (14%)	56,56,56	6.39	21 (37%)
11	CLA	b	1229	-	59,73,73	2.34	16 (27%)	67,113,113	2.07	17 (25%)
11	CLA	b	1023	-	59,73,73	2.31	15 (25%)	67,113,113	2.18	19 (28%)
11	CLA	a	1104	-	59,73,73	2.31	15 (25%)	67,113,113	2.12	18 (26%)
13	SF4	C	3003	3	0,12,12	0.00	-	-	-	-
14	BCR	f	4013	-	41,41,41	2.76	6 (14%)	56,56,56	6.62	23 (41%)
14	BCR	2	4006	-	41,41,41	2.72	6 (14%)	56,56,56	6.83	28 (50%)
11	CLA	B	1222	-	50,64,73	2.58	15 (30%)	56,102,113	2.55	19 (33%)
14	BCR	A	4007	-	41,41,41	2.76	6 (14%)	56,56,56	6.80	22 (39%)
11	CLA	b	1232	-	36,53,73	2.88	15 (41%)	39,89,113	2.30	10 (25%)
11	CLA	A	1132	-	59,73,73	2.34	15 (25%)	67,113,113	2.24	14 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
11	CLA	b	1231	-	36,53,73	2.85	15 (41%)	39,89,113	2.31	11 (28%)
13	SF4	C	3002	3	0,12,12	0.00	-	-		
14	BCR	A	4008	-	41,41,41	2.72	7 (17%)	56,56,56	6.70	30 (53%)
11	CLA	B	1236	-	41,55,73	2.71	15 (36%)	45,91,113	2.49	14 (31%)
11	CLA	l	1502	-	40,54,73	2.89	15 (37%)	44,90,113	2.43	13 (29%)
11	CLA	a	1126	-	59,73,73	2.36	15 (25%)	67,113,113	2.20	16 (23%)
11	CLA	B	1235	-	54,68,73	2.47	16 (29%)	61,107,113	2.24	13 (21%)
11	CLA	A	1104	-	59,73,73	2.27	14 (23%)	67,113,113	2.31	20 (29%)
11	CLA	2	1230	-	52,66,73	2.52	15 (28%)	58,104,113	2.38	18 (31%)
12	PQN	1	2001	-	34,34,34	1.66	2 (5%)	42,45,45	1.09	3 (7%)
11	CLA	2	1203	-	59,73,73	2.30	15 (25%)	67,113,113	2.15	18 (26%)
11	CLA	A	1137	-	59,73,73	2.36	16 (27%)	67,113,113	2.34	18 (26%)
11	CLA	1	1125	-	46,60,73	2.63	15 (32%)	51,97,113	2.41	18 (35%)
11	CLA	B	1021	-	59,73,73	2.28	15 (25%)	67,113,113	2.37	20 (29%)
11	CLA	A	1122	-	53,67,73	2.44	14 (26%)	59,105,113	2.38	17 (28%)
13	SF4	A	3001	1,2	0,12,12	0.00	-	-		
11	CLA	B	1221	-	48,62,73	2.58	16 (33%)	53,99,113	2.47	16 (30%)
14	BCR	1	4002	-	41,41,41	2.72	6 (14%)	56,56,56	6.93	23 (41%)
11	CLA	1	1101	-	59,73,73	2.32	15 (25%)	67,113,113	2.13	19 (28%)
12	PQN	a	2001	-	34,34,34	1.63	2 (5%)	42,45,45	1.04	4 (9%)
11	CLA	A	1138	-	40,54,73	2.86	15 (37%)	44,90,113	2.46	14 (31%)
11	CLA	b	1021	-	59,73,73	2.35	15 (25%)	67,113,113	2.32	23 (34%)
14	BCR	L	4022	-	41,41,41	2.69	6 (14%)	56,56,56	6.11	25 (44%)
11	CLA	2	1215	-	59,73,73	2.35	15 (25%)	67,113,113	2.33	19 (28%)
11	CLA	b	1207	-	59,73,73	2.32	15 (25%)	67,113,113	2.26	16 (23%)
14	BCR	1	4001	-	41,41,41	2.73	6 (14%)	56,56,56	6.55	27 (48%)
11	CLA	b	1214	-	53,67,73	2.46	16 (30%)	59,105,113	2.23	19 (32%)
11	CLA	1	1115	-	40,54,73	2.89	15 (37%)	44,90,113	2.41	12 (27%)
11	CLA	b	1013	-	59,73,73	2.35	15 (25%)	67,113,113	2.14	17 (25%)
11	CLA	1	1121	-	40,54,73	2.90	15 (37%)	44,90,113	2.37	13 (29%)
11	CLA	b	1217	-	41,55,73	2.78	16 (39%)	45,91,113	2.43	12 (26%)
14	BCR	8	4019	-	41,41,41	2.75	6 (14%)	56,56,56	6.65	24 (42%)
11	CLA	b	1205	-	49,63,73	2.53	15 (30%)	55,101,113	2.41	15 (27%)
11	CLA	A	1140	-	59,73,73	2.33	15 (25%)	67,113,113	2.24	16 (23%)
11	CLA	2	1225	-	59,73,73	2.34	15 (25%)	67,113,113	2.09	16 (23%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
11	CLA	a	1123	-	59,73,73	2.35	16 (27%)	67,113,113	2.15	17 (25%)
11	CLA	B	1023	-	59,73,73	2.29	15 (25%)	67,113,113	2.23	20 (29%)
14	BCR	B	4006	-	41,41,41	2.74	6 (14%)	56,56,56	6.81	27 (48%)
11	CLA	b	1202	-	59,73,73	2.34	15 (25%)	67,113,113	2.13	15 (22%)
11	CLA	2	1226	-	59,73,73	2.32	14 (23%)	67,113,113	2.22	16 (23%)
11	CLA	B	1238	-	59,73,73	2.32	14 (23%)	67,113,113	2.05	14 (20%)
11	CLA	A	1111	-	54,68,73	2.41	15 (27%)	61,107,113	2.22	16 (26%)
11	CLA	B	1204	-	59,73,73	2.30	14 (23%)	67,113,113	2.11	16 (23%)
11	CLA	1	1131	-	59,73,73	2.33	15 (25%)	67,113,113	2.15	18 (26%)
11	CLA	a	1135	-	45,59,73	2.67	15 (33%)	50,96,113	2.48	14 (28%)
11	CLA	1	1119	-	59,73,73	2.34	15 (25%)	67,113,113	2.13	17 (25%)
14	BCR	B	4017	-	41,41,41	2.77	6 (14%)	56,56,56	6.60	31 (55%)
11	CLA	B	1226	-	59,73,73	2.30	14 (23%)	67,113,113	2.23	17 (25%)
11	CLA	A	1112	-	36,53,73	2.86	15 (41%)	39,89,113	2.41	11 (28%)
11	CLA	1	1118	-	55,69,73	2.39	15 (27%)	62,108,113	2.20	18 (29%)
11	CLA	2	1235	-	54,68,73	2.45	16 (29%)	61,107,113	2.22	20 (32%)
11	CLA	A	1124	-	49,63,73	2.56	15 (30%)	55,101,113	2.33	17 (30%)
11	CLA	1	1136	-	40,54,73	2.89	15 (37%)	44,90,113	2.32	11 (25%)
14	BCR	l	4019	-	41,41,41	2.75	6 (14%)	56,56,56	6.70	23 (41%)
11	CLA	2	1211	-	40,54,73	2.87	14 (35%)	44,90,113	2.38	12 (27%)
11	CLA	B	1214	-	53,67,73	2.45	16 (30%)	59,105,113	2.45	20 (33%)
11	CLA	B	1220	-	40,54,73	2.89	15 (37%)	44,90,113	2.24	11 (25%)
11	CLA	A	1136	-	40,54,73	2.88	15 (37%)	44,90,113	2.38	11 (25%)
11	CLA	a	1127	-	59,73,73	2.34	15 (25%)	67,113,113	2.28	20 (29%)
11	CLA	1	1110	-	48,62,73	2.60	15 (31%)	53,99,113	2.44	16 (30%)
14	BCR	F	4013	-	41,41,41	2.78	6 (14%)	56,56,56	6.78	21 (37%)
11	CLA	l	1503	-	59,73,73	2.33	16 (27%)	67,113,113	2.08	13 (19%)
11	CLA	A	1118	-	55,69,73	2.36	14 (25%)	62,108,113	2.31	15 (24%)
11	CLA	B	1218	-	36,53,73	2.86	14 (38%)	39,89,113	2.33	10 (25%)
14	BCR	8	4022	-	41,41,41	2.79	6 (14%)	56,56,56	6.49	31 (55%)
11	CLA	a	1132	-	59,73,73	2.35	16 (27%)	67,113,113	2.10	15 (22%)
11	CLA	1	1112	-	36,53,73	2.87	14 (38%)	39,89,113	2.35	13 (33%)
11	CLA	A	1139	-	44,58,73	2.71	16 (36%)	49,95,113	2.42	15 (30%)
11	CLA	2	1202	-	59,73,73	2.34	15 (25%)	67,113,113	2.14	17 (25%)
11	CLA	B	1208	-	36,53,73	2.87	14 (38%)	39,89,113	2.29	10 (25%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
11	CLA	B	1227	-	36,53,73	2.83	14 (38%)	39,89,113	2.53	12 (30%)
13	SF4	c	3002	3	0,12,12	0.00	-	-		
11	CLA	1	1011	-	59,73,73	2.31	16 (27%)	67,113,113	2.52	18 (26%)
11	CLA	B	1228	-	44,58,73	2.73	15 (34%)	49,95,113	2.40	14 (28%)
11	CLA	B	1240	15	36,53,73	2.91	15 (41%)	39,89,113	2.32	11 (28%)
11	CLA	A	1135	-	45,59,73	2.66	15 (33%)	50,96,113	2.48	17 (34%)
11	CLA	1	1134	-	40,54,73	2.91	15 (37%)	44,90,113	2.35	13 (29%)
11	CLA	B	1219	-	49,63,73	2.57	16 (32%)	55,101,113	2.27	17 (30%)
11	CLA	1	1012	-	59,73,73	2.36	15 (25%)	67,113,113	2.39	20 (29%)
11	CLA	1	1104	-	59,73,73	2.32	15 (25%)	67,113,113	2.18	16 (23%)
11	CLA	2	1206	2	59,73,73	2.32	15 (25%)	67,113,113	2.16	16 (23%)
11	CLA	2	1240	15	36,53,73	2.88	14 (38%)	39,89,113	2.29	11 (28%)
11	CLA	2	1220	-	40,54,73	2.90	15 (37%)	44,90,113	2.35	12 (27%)
11	CLA	2	1239	-	40,54,73	2.93	15 (37%)	44,90,113	2.41	14 (31%)
11	CLA	A	1105	-	42,56,73	2.75	16 (38%)	46,92,113	2.39	14 (30%)
11	CLA	A	1121	-	40,54,73	2.91	16 (40%)	44,90,113	2.29	12 (27%)
11	CLA	A	1107	1	59,73,73	2.31	14 (23%)	67,113,113	2.21	18 (26%)
11	CLA	b	1208	-	36,53,73	2.88	14 (38%)	39,89,113	2.42	12 (30%)
11	CLA	a	1101	-	59,73,73	2.35	15 (25%)	67,113,113	2.13	17 (25%)
16	LMG	B	5002	-	55,55,55	0.89	2 (3%)	63,63,63	1.07	4 (6%)
11	CLA	B	1013	-	59,73,73	2.32	15 (25%)	67,113,113	2.25	20 (29%)
11	CLA	B	1225	-	59,73,73	2.33	15 (25%)	67,113,113	2.11	17 (25%)
14	BCR	2	4010	-	41,41,41	2.84	6 (14%)	56,56,56	6.40	26 (46%)
14	BCR	1	4003	-	41,41,41	2.78	6 (14%)	56,56,56	6.39	27 (48%)
11	CLA	a	1111	-	54,68,73	2.40	16 (29%)	61,107,113	2.31	18 (29%)
11	CLA	2	1021	-	59,73,73	2.32	15 (25%)	67,113,113	2.32	20 (29%)
11	CLA	2	1223	-	59,73,73	2.35	16 (27%)	67,113,113	2.15	18 (26%)
11	CLA	B	1201	-	48,62,73	2.57	15 (31%)	53,99,113	2.49	18 (33%)
11	CLA	B	1211	-	40,54,73	2.86	15 (37%)	44,90,113	2.40	12 (27%)
14	BCR	a	4002	-	41,41,41	2.76	6 (14%)	56,56,56	6.59	26 (46%)
12	PQN	b	2002	-	34,34,34	1.64	2 (5%)	42,45,45	1.11	4 (9%)
12	PQN	2	2002	-	34,34,34	1.64	2 (5%)	42,45,45	1.08	6 (14%)
11	CLA	B	1230	-	52,66,73	2.50	15 (28%)	58,104,113	2.42	18 (31%)
11	CLA	b	1221	-	48,62,73	2.60	16 (33%)	53,99,113	2.51	17 (32%)
16	LMG	2	5002	-	55,55,55	0.91	2 (3%)	63,63,63	1.06	4 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
11	CLA	b	1209	-	36,53,73	2.88	14 (38%)	39,89,113	2.38	11 (28%)
11	CLA	b	1203	-	59,73,73	2.34	16 (27%)	67,113,113	2.12	15 (22%)
11	CLA	2	1205	-	49,63,73	2.50	15 (30%)	55,101,113	2.46	14 (25%)
14	BCR	2	4004	-	41,41,41	2.71	6 (14%)	56,56,56	6.47	29 (51%)
14	BCR	b	4006	-	41,41,41	2.76	6 (14%)	56,56,56	6.93	27 (48%)
11	CLA	A	1108	-	36,53,73	2.85	14 (38%)	39,89,113	2.29	12 (30%)
14	BCR	1	4007	-	41,41,41	2.71	6 (14%)	56,56,56	6.67	26 (46%)
14	BCR	m	4021	-	41,41,41	2.84	6 (14%)	56,56,56	6.50	24 (42%)
14	BCR	F	4018	-	41,41,41	2.91	7 (17%)	56,56,56	6.56	24 (42%)
11	CLA	1	1113	-	36,53,73	2.86	14 (38%)	39,89,113	2.34	10 (25%)
11	CLA	2	1210	-	59,73,73	2.31	15 (25%)	67,113,113	2.19	20 (29%)
11	CLA	a	1131	-	59,73,73	2.35	15 (25%)	67,113,113	2.13	18 (26%)
11	CLA	1	1107	-	59,73,73	2.35	15 (25%)	67,113,113	2.21	15 (22%)
14	BCR	6	4013	-	41,41,41	2.69	6 (14%)	56,56,56	6.63	24 (42%)
11	CLA	a	1109	11	59,73,73	2.36	16 (27%)	67,113,113	2.16	16 (23%)
11	CLA	b	1236	-	41,55,73	2.76	16 (39%)	45,91,113	2.43	12 (26%)
14	BCR	B	4014	-	41,41,41	2.77	7 (17%)	56,56,56	6.29	25 (44%)
15	LHG	b	5004	-	48,48,48	0.94	2 (4%)	51,54,54	1.05	3 (5%)
14	BCR	2	4017	-	41,41,41	2.78	7 (17%)	56,56,56	6.54	29 (51%)
14	BCR	B	4005	-	41,41,41	2.79	7 (17%)	56,56,56	6.53	25 (44%)
11	CLA	a	1137	-	59,73,73	2.35	15 (25%)	67,113,113	2.24	18 (26%)
11	CLA	1	1105	-	42,56,73	2.77	15 (35%)	46,92,113	2.43	14 (30%)
11	CLA	2	1216	-	59,73,73	2.35	16 (27%)	67,113,113	2.20	16 (23%)
11	CLA	1	1102	-	59,73,73	2.36	16 (27%)	67,113,113	2.03	12 (17%)
11	CLA	b	1206	2	59,73,73	2.32	15 (25%)	67,113,113	2.18	18 (26%)
11	CLA	1	1117	-	59,73,73	2.35	15 (25%)	67,113,113	2.13	17 (25%)
11	CLA	A	1102	11	59,73,73	2.35	16 (27%)	67,113,113	2.17	18 (26%)
11	CLA	a	1129	-	40,54,73	2.89	15 (37%)	44,90,113	2.41	12 (27%)
11	CLA	2	1013	-	59,73,73	2.34	15 (25%)	67,113,113	2.20	18 (26%)
11	CLA	2	1207	-	59,73,73	2.31	15 (25%)	67,113,113	2.26	18 (26%)
11	CLA	b	1211	-	40,54,73	2.90	16 (40%)	44,90,113	2.37	13 (29%)
11	CLA	2	1228	-	44,58,73	2.71	16 (36%)	49,95,113	2.46	15 (30%)
11	CLA	a	1130	-	40,54,73	2.92	15 (37%)	44,90,113	2.28	13 (29%)
11	CLA	B	1229	-	59,73,73	2.33	15 (25%)	67,113,113	2.15	17 (25%)
14	BCR	f	4018	-	41,41,41	2.85	7 (17%)	56,56,56	6.36	24 (42%)



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
11	CLA	a	1138	-	40,54,73	2.89	15 (37%)	44,90,113	2.44	16 (36%)
11	CLA	b	1210	-	59,73,73	2.36	16 (27%)	67,113,113	2.13	20 (29%)
11	CLA	2	1222	-	50,64,73	2.54	16 (32%)	56,102,113	2.38	17 (30%)
11	CLA	A	1110	-	48,62,73	2.61	15 (31%)	53,99,113	2.46	16 (30%)
11	CLA	1	1128	-	59,73,73	2.33	15 (25%)	67,113,113	2.09	16 (23%)
11	CLA	a	1121	-	40,54,73	2.91	16 (40%)	44,90,113	2.38	13 (29%)

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
11	CLA	2	1218	-	3/3/16/25	4/11/111/135	-
11	CLA	a	1122	-	3/3/18/25	14/30/128/135	-
11	CLA	A	1101	-	2/2/20/25	19/37/135/135	-
11	CLA	b	1218	-	3/3/16/25	3/11/111/135	-
11	CLA	1	1801	15	3/3/17/25	13/22/120/135	-
11	CLA	A	1125	-	2/2/17/25	9/22/120/135	-
14	BCR	1	4008	-	-	11/29/63/63	0/2/2/2
11	CLA	b	1222	-	3/3/18/25	12/27/125/135	-
14	BCR	b	4010	-	-	11/29/63/63	0/2/2/2
11	CLA	2	1224	-	3/3/18/25	8/25/123/135	-
11	CLA	K	1401	-	3/3/20/25	19/37/135/135	-
11	CLA	a	1124	-	3/3/18/25	8/25/123/135	-
11	CLA	1	1133	-	3/3/16/25	8/15/113/135	-
11	CLA	1	1139	-	3/3/17/25	10/19/117/135	-
15	LHG	1	5001	-	-	26/53/53/53	-
11	CLA	2	1208	-	3/3/16/25	3/11/111/135	-
11	CLA	1	1111	-	3/3/19/25	18/31/129/135	-
11	CLA	a	1114	-	2/2/16/25	6/15/113/135	-
14	BCR	a	4008	-	-	11/29/63/63	0/2/2/2
11	CLA	b	1213	-	3/3/20/25	13/37/135/135	-
15	LHG	a	5003	11	-	25/53/53/53	-
11	CLA	B	1210	-	3/3/20/25	27/37/135/135	-
14	BCR	b	4011	-	-	15/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
11	CLA	b	1240	-	3/3/16/25	7/11/111/135	-
11	CLA	a	1022	-	2/2/20/25	12/37/135/135	-
11	CLA	A	1120	-	3/3/16/25	6/15/113/135	-
11	CLA	8	1501	-	3/3/20/25	18/37/135/135	-
11	CLA	B	1216	-	3/3/20/25	8/37/135/135	-
11	CLA	B	1213	-	3/3/20/25	18/37/135/135	-
15	LHG	B	5004	11	-	25/53/53/53	-
11	CLA	1	1120	-	3/3/16/25	9/15/113/135	-
11	CLA	2	1217	-	3/3/16/25	14/16/114/135	-
13	SF4	3	3002	3	-	-	0/6/5/5
14	BCR	2	4014	-	-	14/29/63/63	0/2/2/2
11	CLA	a	1237	-	3/3/18/25	10/25/123/135	-
14	BCR	b	4004	-	-	11/29/63/63	0/2/2/2
11	CLA	1	1108	-	3/3/16/25	3/11/111/135	-
14	BCR	l	4022	-	-	11/29/63/63	0/2/2/2
11	CLA	2	1204	-	2/2/20/25	11/37/135/135	-
11	CLA	B	1215	-	2/2/20/25	16/37/135/135	-
11	CLA	A	1133	-	3/3/16/25	4/15/113/135	-
14	BCR	7	4021	-	-	13/29/63/63	0/2/2/2
11	CLA	1	1138	-	3/3/16/25	6/15/113/135	-
14	BCR	F	4020	-	-	12/29/63/63	0/2/2/2
11	CLA	b	1220	-	3/3/16/25	8/15/113/135	-
11	CLA	b	1216	-	3/3/20/25	15/37/135/135	-
11	CLA	1	1136	-	3/3/16/25	10/15/113/135	-
11	CLA	b	1234	-	3/3/19/25	16/31/129/135	-
11	CLA	B	1207	-	2/2/20/25	12/37/135/135	-
14	BCR	B	4010	-	-	13/29/63/63	0/2/2/2
11	CLA	a	1103	-	3/3/20/25	19/37/135/135	-
11	CLA	1	1129	-	3/3/16/25	6/15/113/135	-
11	CLA	b	1239	-	3/3/16/25	7/15/113/135	-
11	CLA	1	1109	-	2/2/20/25	15/37/135/135	-
11	CLA	1	1132	-	3/3/20/25	11/37/135/135	-
11	CLA	A	1126	-	3/3/20/25	12/37/135/135	-
11	CLA	1	1103	-	3/3/20/25	21/37/135/135	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
14	BCR	a	4003	-	-	14/29/63/63	0/2/2/2
11	CLA	A	1109	11	2/2/20/25	13/37/135/135	-
11	CLA	B	1202	-	3/3/20/25	19/37/135/135	-
11	CLA	k	1402	-	3/3/17/25	7/19/117/135	-
11	CLA	B	1203	-	1/1/20/25	15/37/135/135	-
16	LMG	b	5002	-	-	27/50/70/70	0/1/1/1
11	CLA	8	1502	-	3/3/16/25	4/15/113/135	-
11	CLA	A	1119	-	3/3/20/25	17/37/135/135	-
11	CLA	A	1113	-	3/3/16/25	5/11/111/135	-
14	BCR	B	4011	-	-	13/29/63/63	0/2/2/2
11	CLA	L	1502	-	3/3/16/25	5/15/113/135	-
11	CLA	A	1131	-	2/2/20/25	15/37/135/135	-
11	CLA	1	1022	-	3/3/20/25	17/37/135/135	-
11	CLA	a	1112	-	3/3/16/25	3/11/111/135	-
11	CLA	1	1123	-	2/2/20/25	14/37/135/135	-
11	CLA	a	1115	-	2/2/16/25	6/15/113/135	-
11	CLA	0	1401	-	3/3/20/25	19/37/135/135	-
11	CLA	b	1225	-	3/3/20/25	14/37/135/135	-
11	CLA	a	1012	-	2/2/20/25	20/37/135/135	-
11	CLA	1	1106	1	2/2/20/25	23/37/135/135	-
14	BCR	A	4001	-	-	10/29/63/63	0/2/2/2
11	CLA	A	1127	-	3/3/20/25	13/37/135/135	-
12	PQN	A	2001	-	-	10/23/43/43	0/2/2/2
11	CLA	A	1114	-	3/3/16/25	7/15/113/135	-
11	CLA	2	1221	-	3/3/17/25	6/24/122/135	-
11	CLA	B	1223	-	2/2/20/25	9/37/135/135	-
14	BCR	2	4011	-	-	13/29/63/63	0/2/2/2
11	CLA	a	1140	-	3/3/20/25	14/37/135/135	-
11	CLA	A	1134	1	3/3/16/25	9/15/113/135	-
11	CLA	1	1114	-	3/3/16/25	10/15/113/135	-
11	CLA	b	1235	-	3/3/19/25	16/31/129/135	-
11	CLA	a	1116	-	3/3/17/25	9/24/122/135	-
13	SF4	3	3003	-	-	-	0/6/5/5
11	CLA	A	1117	-	3/3/20/25	13/37/135/135	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
11	CLA	a	1119	-	3/3/20/25	16/37/135/135	-
11	CLA	B	1231	-	3/3/16/25	7/11/111/135	-
14	BCR	b	4014	-	-	13/29/63/63	0/2/2/2
13	SF4	a	3001	1,2	-	-	0/6/5/5
15	LHG	A	5003	11	-	31/53/53/53	-
11	CLA	2	1231	-	3/3/16/25	5/11/111/135	-
11	CLA	A	1128	-	3/3/20/25	12/37/135/135	-
11	CLA	B	1224	-	3/3/18/25	11/25/123/135	-
11	CLA	1	1137	-	3/3/20/25	18/37/135/135	-
14	BCR	f	4020	-	-	15/29/63/63	0/2/2/2
11	CLA	1	1130	-	1/1/16/25	5/15/113/135	-
11	CLA	B	1206	2	2/2/20/25	13/37/135/135	-
14	BCR	b	4009	-	-	14/29/63/63	0/2/2/2
11	CLA	a	1102	11	3/3/20/25	13/37/135/135	-
15	LHG	A	5001	-	-	31/53/53/53	-
11	CLA	b	1219	-	3/3/18/25	8/25/123/135	-
11	CLA	a	1120	-	3/3/16/25	8/15/113/135	-
11	CLA	b	1230	-	3/3/18/25	12/29/127/135	-
11	CLA	0	1402	-	3/3/17/25	5/19/117/135	-
11	CLA	1	1124	-	3/3/18/25	12/25/123/135	-
14	BCR	A	4003	-	-	13/29/63/63	0/2/2/2
11	CLA	L	1503	-	2/2/20/25	13/37/135/135	-
11	CLA	B	1234	-	3/3/19/25	14/31/129/135	-
11	CLA	a	1106	1	3/3/20/25	19/37/135/135	-
11	CLA	2	1229	-	3/3/20/25	17/37/135/135	-
11	CLA	a	1801	15	3/3/17/25	11/22/120/135	-
11	CLA	B	1205	-	3/3/18/25	9/25/123/135	-
11	CLA	2	1201	-	3/3/17/25	8/24/122/135	-
11	CLA	a	1136	-	3/3/16/25	6/15/113/135	-
14	BCR	a	4001	-	-	10/29/63/63	0/2/2/2
11	CLA	2	1236	-	3/3/16/25	8/16/114/135	-
11	CLA	2	1219	-	3/3/18/25	12/25/123/135	-
11	CLA	1	1237	-	3/3/18/25	9/25/123/135	-
11	CLA	2	1212	-	3/3/16/25	3/11/111/135	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
11	CLA	A	1012	-	3/3/20/25	15/37/135/135	-
11	CLA	1	1116	-	3/3/17/25	9/24/122/135	-
11	CLA	2	1232	-	2/2/16/25	3/11/111/135	-
14	BCR	L	4019	-	-	13/29/63/63	0/2/2/2
11	CLA	a	1117	-	3/3/20/25	18/37/135/135	-
11	CLA	b	1228	-	3/3/17/25	6/19/117/135	-
11	CLA	2	1227	-	2/2/16/25	6/11/111/135	-
14	BCR	B	4004	-	-	10/29/63/63	0/2/2/2
11	CLA	b	1227	-	2/2/16/25	5/11/111/135	-
11	CLA	l	1501	7	2/2/20/25	16/37/135/135	-
11	CLA	a	1105	-	3/3/16/25	8/17/115/135	-
11	CLA	2	1235	-	3/3/19/25	17/31/129/135	-
11	CLA	b	1201	-	3/3/17/25	9/24/122/135	-
11	CLA	B	1239	-	3/3/16/25	10/15/113/135	-
11	CLA	A	1237	-	3/3/18/25	12/25/123/135	-
11	CLA	a	1134	-	3/3/16/25	8/15/113/135	-
11	CLA	a	1118	-	3/3/19/25	10/33/131/135	-
11	CLA	A	1116	-	3/3/17/25	8/24/122/135	-
11	CLA	2	1209	-	3/3/16/25	2/11/111/135	-
11	CLA	k	1401	-	3/3/20/25	19/37/135/135	-
11	CLA	A	1022	-	2/2/20/25	13/37/135/135	-
14	BCR	M	4021	-	-	8/29/63/63	0/2/2/2
15	LHG	2	5004	11	-	28/53/53/53	-
11	CLA	2	1023	-	3/3/20/25	15/37/135/135	-
15	LHG	1	5003	11	-	32/53/53/53	-
11	CLA	b	1212	-	3/3/16/25	5/11/111/135	-
11	CLA	A	1106	1	3/3/20/25	16/37/135/135	-
14	BCR	a	4007	-	-	11/29/63/63	0/2/2/2
11	CLA	2	1238	-	3/3/20/25	12/37/135/135	-
11	CLA	a	1125	-	2/2/17/25	8/22/120/135	-
11	CLA	A	1801	15	3/3/17/25	14/22/120/135	-
11	CLA	b	1224	-	3/3/18/25	12/25/123/135	-
11	CLA	2	1214	-	3/3/18/25	11/30/128/135	-
11	CLA	B	1217	-	3/3/16/25	12/16/114/135	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
12	PQN	B	2002	-	-	8/23/43/43	0/2/2/2
14	BCR	2	4009	-	-	15/29/63/63	0/2/2/2
11	CLA	8	1503	-	3/3/20/25	12/37/135/135	-
13	SF4	c	3003	3	-	-	0/6/5/5
14	BCR	6	4020	-	-	15/29/63/63	0/2/2/2
14	BCR	l	4019	-	-	17/29/63/63	0/2/2/2
15	LHG	a	5001	-	-	30/53/53/53	-
11	CLA	B	1209	-	3/3/16/25	4/11/111/135	-
11	CLA	1	1127	-	3/3/20/25	15/37/135/135	-
11	CLA	1	1126	-	3/3/20/25	20/37/135/135	-
11	CLA	a	1107	1	3/3/20/25	9/37/135/135	-
14	BCR	A	4002	-	-	13/29/63/63	0/2/2/2
11	CLA	A	1129	-	3/3/16/25	6/15/113/135	-
11	CLA	K	1402	-	3/3/17/25	8/19/117/135	-
11	CLA	A	1115	-	3/3/16/25	7/15/113/135	-
14	BCR	B	4009	-	-	13/29/63/63	0/2/2/2
11	CLA	a	1113	-	3/3/16/25	4/11/111/135	-
11	CLA	a	1128	-	3/3/20/25	11/37/135/135	-
11	CLA	1	1122	-	3/3/18/25	18/30/128/135	-
11	CLA	a	1110	-	2/2/17/25	11/24/122/135	-
11	CLA	B	1212	-	3/3/16/25	5/11/111/135	-
11	CLA	L	1501	7	3/3/20/25	13/37/135/135	-
11	CLA	1	1140	-	3/3/20/25	15/37/135/135	-
14	BCR	b	4005	-	-	13/29/63/63	0/2/2/2
11	CLA	b	1215	-	2/2/20/25	14/37/135/135	-
14	BCR	6	4018	-	-	10/29/63/63	0/2/2/2
11	CLA	A	1123	-	2/2/20/25	17/37/135/135	-
11	CLA	b	1226	-	3/3/20/25	13/37/135/135	-
11	CLA	a	1108	-	3/3/16/25	2/11/111/135	-
11	CLA	2	1234	-	2/2/19/25	18/31/129/135	-
11	CLA	2	1213	-	3/3/20/25	18/37/135/135	-
13	SF4	1	3001	1,2	-	-	0/6/5/5
14	BCR	b	4017	-	-	6/29/63/63	0/2/2/2
11	CLA	A	1130	-	2/2/16/25	5/15/113/135	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
11	CLA	B	1232	-	3/3/16/25	3/11/111/135	-
11	CLA	1	1135	-	2/2/17/25	9/21/119/135	-
11	CLA	A	1103	-	3/3/20/25	17/37/135/135	-
11	CLA	b	1238	-	3/3/20/25	12/37/135/135	-
11	CLA	a	1011	-	1/1/20/25	11/37/135/135	-
11	CLA	b	1204	-	2/2/20/25	16/37/135/135	-
11	CLA	b	1223	-	3/3/20/25	19/37/135/135	-
14	BCR	2	4005	-	-	9/29/63/63	0/2/2/2
11	CLA	b	1229	-	3/3/20/25	24/37/135/135	-
11	CLA	b	1023	-	3/3/20/25	17/37/135/135	-
11	CLA	a	1104	-	3/3/20/25	15/37/135/135	-
13	SF4	C	3003	3	-	-	0/6/5/5
14	BCR	f	4013	-	-	17/29/63/63	0/2/2/2
14	BCR	2	4006	-	-	13/29/63/63	0/2/2/2
11	CLA	B	1222	-	3/3/18/25	15/27/125/135	-
14	BCR	A	4007	-	-	13/29/63/63	0/2/2/2
11	CLA	b	1232	-	3/3/16/25	4/11/111/135	-
11	CLA	A	1132	-	3/3/20/25	16/37/135/135	-
11	CLA	b	1231	-	3/3/16/25	6/11/111/135	-
13	SF4	C	3002	3	-	-	0/6/5/5
14	BCR	A	4008	-	-	11/29/63/63	0/2/2/2
11	CLA	B	1236	-	3/3/16/25	6/16/114/135	-
11	CLA	l	1502	-	3/3/16/25	3/15/113/135	-
11	CLA	a	1126	-	3/3/20/25	18/37/135/135	-
11	CLA	B	1235	-	3/3/19/25	14/31/129/135	-
11	CLA	A	1104	-	3/3/20/25	21/37/135/135	-
11	CLA	2	1230	-	2/2/18/25	7/29/127/135	-
12	PQN	1	2001	-	-	7/23/43/43	0/2/2/2
11	CLA	2	1203	-	3/3/20/25	17/37/135/135	-
11	CLA	A	1137	-	3/3/20/25	14/37/135/135	-
11	CLA	1	1125	-	2/2/17/25	9/22/120/135	-
11	CLA	B	1021	-	3/3/20/25	23/37/135/135	-
11	CLA	A	1122	-	3/3/18/25	8/30/128/135	-
13	SF4	A	3001	1,2	-	-	0/6/5/5
11	CLA	B	1221	-	3/3/17/25	9/24/122/135	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
14	BCR	1	4002	-	-	13/29/63/63	0/2/2/2
11	CLA	1	1101	-	2/2/20/25	19/37/135/135	-
12	PQN	a	2001	-	-	6/23/43/43	0/2/2/2
11	CLA	A	1138	-	3/3/16/25	2/15/113/135	-
11	CLA	b	1021	-	3/3/20/25	25/37/135/135	-
14	BCR	L	4022	-	-	12/29/63/63	0/2/2/2
11	CLA	2	1215	-	3/3/20/25	16/37/135/135	-
11	CLA	b	1207	-	2/2/20/25	16/37/135/135	-
14	BCR	1	4001	-	-	11/29/63/63	0/2/2/2
11	CLA	b	1214	-	3/3/18/25	10/30/128/135	-
11	CLA	1	1115	-	2/2/16/25	4/15/113/135	-
11	CLA	b	1013	-	1/1/20/25	10/37/135/135	-
11	CLA	1	1121	-	2/2/16/25	6/15/113/135	-
11	CLA	b	1217	-	3/3/16/25	7/16/114/135	-
14	BCR	8	4019	-	-	15/29/63/63	0/2/2/2
11	CLA	b	1205	-	3/3/18/25	8/25/123/135	-
11	CLA	A	1140	-	2/2/20/25	18/37/135/135	-
11	CLA	2	1225	-	3/3/20/25	10/37/135/135	-
11	CLA	a	1123	-	2/2/20/25	15/37/135/135	-
11	CLA	B	1023	-	3/3/20/25	15/37/135/135	-
14	BCR	B	4006	-	-	15/29/63/63	0/2/2/2
11	CLA	b	1202	-	3/3/20/25	18/37/135/135	-
11	CLA	2	1226	-	3/3/20/25	12/37/135/135	-
11	CLA	B	1238	-	3/3/20/25	13/37/135/135	-
11	CLA	A	1111	-	3/3/19/25	16/31/129/135	-
11	CLA	B	1204	-	2/2/20/25	14/37/135/135	-
11	CLA	1	1131	-	2/2/20/25	20/37/135/135	-
11	CLA	a	1135	-	2/2/17/25	7/21/119/135	-
11	CLA	1	1119	-	3/3/20/25	18/37/135/135	-
14	BCR	B	4017	-	-	6/29/63/63	0/2/2/2
11	CLA	B	1226	-	3/3/20/25	13/37/135/135	-
11	CLA	A	1112	-	3/3/16/25	6/11/111/135	-
11	CLA	1	1118	-	3/3/19/25	17/33/131/135	-
11	CLA	a	1133	-	3/3/16/25	4/15/113/135	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
11	CLA	A	1124	-	3/3/18/25	12/25/123/135	-
11	CLA	A	1011	-	2/2/20/25	17/37/135/135	-
11	CLA	a	1139	-	3/3/17/25	7/19/117/135	-
11	CLA	2	1211	-	3/3/16/25	9/15/113/135	-
11	CLA	B	1214	-	3/3/18/25	13/30/128/135	-
11	CLA	B	1220	-	1/1/16/25	8/15/113/135	-
11	CLA	A	1136	-	3/3/16/25	6/15/113/135	-
11	CLA	a	1127	-	3/3/20/25	14/37/135/135	-
11	CLA	1	1110	-	2/2/17/25	14/24/122/135	-
14	BCR	F	4013	-	-	15/29/63/63	0/2/2/2
11	CLA	l	1503	-	2/2/20/25	16/37/135/135	-
11	CLA	A	1118	-	3/3/19/25	17/33/131/135	-
11	CLA	B	1218	-	3/3/16/25	3/11/111/135	-
14	BCR	8	4022	-	-	6/29/63/63	0/2/2/2
11	CLA	a	1132	-	3/3/20/25	15/37/135/135	-
11	CLA	1	1112	-	3/3/16/25	3/11/111/135	-
11	CLA	A	1139	-	3/3/17/25	7/19/117/135	-
11	CLA	2	1202	-	3/3/20/25	15/37/135/135	-
11	CLA	B	1208	-	2/2/16/25	5/11/111/135	-
11	CLA	B	1227	-	3/3/16/25	4/11/111/135	-
13	SF4	c	3002	3	-	-	0/6/5/5
11	CLA	1	1011	-	1/1/20/25	15/37/135/135	-
11	CLA	2	1013	-	1/1/20/25	14/37/135/135	-
11	CLA	B	1240	15	3/3/16/25	6/11/111/135	-
11	CLA	A	1135	-	3/3/17/25	8/21/119/135	-
11	CLA	1	1134	-	3/3/16/25	7/15/113/135	-
11	CLA	B	1219	-	3/3/18/25	10/25/123/135	-
11	CLA	1	1012	-	2/2/20/25	18/37/135/135	-
11	CLA	1	1104	-	2/2/20/25	14/37/135/135	-
11	CLA	2	1206	2	3/3/20/25	19/37/135/135	-
11	CLA	2	1240	15	3/3/16/25	3/11/111/135	-
11	CLA	2	1220	-	2/2/16/25	7/15/113/135	-
11	CLA	2	1239	-	3/3/16/25	12/15/113/135	-
11	CLA	A	1105	-	3/3/16/25	5/17/115/135	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
11	CLA	A	1121	-	3/3/16/25	5/15/113/135	-
11	CLA	A	1107	1	3/3/20/25	13/37/135/135	-
11	CLA	b	1208	-	3/3/16/25	2/11/111/135	-
11	CLA	a	1101	-	2/2/20/25	17/37/135/135	-
16	LMG	B	5002	-	-	27/50/70/70	0/1/1/1
11	CLA	2	1228	-	3/3/17/25	3/19/117/135	-
11	CLA	B	1225	-	3/3/20/25	11/37/135/135	-
14	BCR	2	4010	-	-	11/29/63/63	0/2/2/2
14	BCR	1	4003	-	-	12/29/63/63	0/2/2/2
11	CLA	a	1111	-	3/3/19/25	18/31/129/135	-
11	CLA	2	1021	-	3/3/20/25	21/37/135/135	-
11	CLA	2	1223	-	3/3/20/25	16/37/135/135	-
11	CLA	B	1201	-	3/3/17/25	8/24/122/135	-
11	CLA	B	1211	-	3/3/16/25	6/15/113/135	-
14	BCR	a	4002	-	-	15/29/63/63	0/2/2/2
12	PQN	b	2002	-	-	8/23/43/43	0/2/2/2
12	PQN	2	2002	-	-	8/23/43/43	0/2/2/2
11	CLA	B	1230	-	2/2/18/25	8/29/127/135	-
11	CLA	b	1221	-	3/3/17/25	7/24/122/135	-
16	LMG	2	5002	-	-	30/50/70/70	0/1/1/1
11	CLA	b	1209	-	3/3/16/25	5/11/111/135	-
11	CLA	b	1203	-	3/3/20/25	12/37/135/135	-
11	CLA	2	1205	-	3/3/18/25	7/25/123/135	-
14	BCR	2	4004	-	-	10/29/63/63	0/2/2/2
14	BCR	b	4006	-	-	15/29/63/63	0/2/2/2
11	CLA	A	1108	-	3/3/16/25	3/11/111/135	-
14	BCR	1	4007	-	-	12/29/63/63	0/2/2/2
14	BCR	m	4021	-	-	11/29/63/63	0/2/2/2
14	BCR	F	4018	-	-	5/29/63/63	0/2/2/2
11	CLA	1	1113	-	3/3/16/25	3/11/111/135	-
11	CLA	2	1210	-	3/3/20/25	15/37/135/135	-
11	CLA	a	1131	-	3/3/20/25	16/37/135/135	-
11	CLA	1	1107	-	3/3/20/25	14/37/135/135	-
14	BCR	6	4013	-	-	16/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
11	CLA	a	1109	11	2/2/20/25	19/37/135/135	-
11	CLA	b	1236	-	3/3/16/25	7/16/114/135	-
14	BCR	B	4014	-	-	11/29/63/63	0/2/2/2
15	LHG	b	5004	-	-	26/53/53/53	-
14	BCR	2	4017	-	-	6/29/63/63	0/2/2/2
14	BCR	B	4005	-	-	8/29/63/63	0/2/2/2
11	CLA	a	1137	-	3/3/20/25	12/37/135/135	-
11	CLA	1	1105	-	3/3/16/25	5/17/115/135	-
11	CLA	2	1216	-	3/3/20/25	17/37/135/135	-
11	CLA	1	1102	-	3/3/20/25	15/37/135/135	-
11	CLA	b	1206	2	3/3/20/25	16/37/135/135	-
11	CLA	1	1117	-	3/3/20/25	16/37/135/135	-
11	CLA	A	1102	11	2/2/20/25	19/37/135/135	-
11	CLA	a	1129	-	3/3/16/25	7/15/113/135	-
11	CLA	B	1228	-	3/3/17/25	7/19/117/135	-
11	CLA	2	1207	-	1/1/20/25	13/37/135/135	-
11	CLA	b	1211	-	3/3/16/25	4/15/113/135	-
11	CLA	B	1013	-	2/2/20/25	18/37/135/135	-
11	CLA	a	1130	-	2/2/16/25	7/15/113/135	-
11	CLA	B	1229	-	2/2/20/25	24/37/135/135	-
14	BCR	f	4018	-	-	6/29/63/63	0/2/2/2
11	CLA	a	1138	-	3/3/16/25	8/15/113/135	-
11	CLA	b	1210	-	3/3/20/25	20/37/135/135	-
11	CLA	2	1222	-	3/3/18/25	11/27/125/135	-
11	CLA	A	1110	-	3/3/17/25	11/24/122/135	-
11	CLA	1	1128	-	3/3/20/25	13/37/135/135	-
11	CLA	a	1121	-	3/3/16/25	5/15/113/135	-

The worst 5 of 4528 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	A	1125	CLA	MG-NA	9.70	2.29	2.06
11	a	1103	CLA	MG-NA	9.70	2.29	2.06
11	B	1223	CLA	MG-NA	9.65	2.29	2.06
11	b	1223	CLA	MG-NA	9.64	2.29	2.06
11	a	1139	CLA	MG-NA	9.64	2.29	2.06

The worst 5 of 5701 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	1	4002	BCR	C16-C17-C18	28.55	168.05	127.31
14	b	4009	BCR	C16-C17-C18	27.86	167.07	127.31
14	6	4013	BCR	C20-C21-C22	26.01	164.43	127.31
14	F	4013	BCR	C20-C21-C22	25.73	164.03	127.31
14	f	4013	BCR	C20-C21-C22	25.36	163.51	127.31

5 of 748 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
11	2	1218	CLA	NC
11	2	1218	CLA	ND
11	2	1218	CLA	NA
11	a	1122	CLA	NC
11	a	1122	CLA	ND

5 of 4167 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
11	a	1122	CLA	C2-C1-O2A-CGA
11	a	1122	CLA	CHA-CBD-CGD-O1D
11	a	1122	CLA	CHA-CBD-CGD-O2D
11	A	1101	CLA	C3A-C2A-CAA-CBA
11	A	1101	CLA	C2-C1-O2A-CGA

There are no ring outliers.

208 monomers are involved in 696 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
11	A	1101	CLA	4	0
11	1	1801	CLA	5	0
11	A	1125	CLA	7	0
14	1	4008	BCR	4	0
14	6	4020	BCR	4	0
11	K	1401	CLA	4	0
11	1	1133	CLA	2	0
15	1	5001	LHG	10	0
11	2	1208	CLA	1	0
11	1	1111	CLA	1	0
11	B	1210	CLA	3	0
11	8	1501	CLA	6	0
15	B	5004	LHG	8	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
13	3	3002	SF4	9	0
14	2	4014	BCR	7	0
11	2	1204	CLA	3	0
11	B	1215	CLA	1	0
11	A	1133	CLA	4	0
14	7	4021	BCR	6	0
14	F	4020	BCR	7	0
11	B	1207	CLA	3	0
14	B	4010	BCR	15	0
11	1	1129	CLA	2	0
11	1	1109	CLA	2	0
11	1	1132	CLA	3	0
11	A	1126	CLA	9	0
11	1	1103	CLA	2	0
11	A	1109	CLA	1	0
11	B	1202	CLA	1	0
11	B	1203	CLA	2	0
11	A	1119	CLA	11	0
11	A	1113	CLA	2	0
14	B	4011	BCR	10	0
11	A	1131	CLA	4	0
11	1	1022	CLA	5	0
11	1	1123	CLA	5	0
11	0	1401	CLA	3	0
11	1	1106	CLA	8	0
14	A	4001	BCR	6	0
11	A	1127	CLA	3	0
12	A	2001	PQN	5	0
11	A	1114	CLA	2	0
11	B	1223	CLA	20	0
14	2	4011	BCR	7	0
11	A	1134	CLA	1	0
13	3	3003	SF4	12	0
11	A	1117	CLA	2	0
11	B	1231	CLA	3	0
15	A	5003	LHG	10	0
11	2	1231	CLA	8	0
11	A	1128	CLA	6	0
11	B	1224	CLA	1	0
11	1	1137	CLA	4	0
11	1	1130	CLA	2	0
11	B	1206	CLA	5	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
15	A	5001	LHG	5	0
11	0	1402	CLA	1	0
11	1	1124	CLA	2	0
14	A	4003	BCR	9	0
11	L	1503	CLA	3	0
11	B	1234	CLA	2	0
11	2	1229	CLA	5	0
11	B	1205	CLA	5	0
11	2	1201	CLA	2	0
11	1	1237	CLA	3	0
11	2	1212	CLA	4	0
11	2	1232	CLA	3	0
14	L	4019	BCR	13	0
11	2	1227	CLA	3	0
11	A	1011	CLA	3	0
14	B	4004	BCR	4	0
11	A	1237	CLA	4	0
11	B	1209	CLA	6	0
11	A	1116	CLA	2	0
11	2	1209	CLA	1	0
11	A	1022	CLA	6	0
14	M	4021	BCR	7	0
15	2	5004	LHG	7	0
11	2	1023	CLA	3	0
15	1	5003	LHG	6	0
11	A	1106	CLA	6	0
11	2	1238	CLA	5	0
11	A	1801	CLA	8	0
11	2	1214	CLA	2	0
11	B	1217	CLA	2	0
12	B	2002	PQN	4	0
14	2	4009	BCR	5	0
11	8	1503	CLA	3	0
11	1	1127	CLA	4	0
11	1	1126	CLA	4	0
14	A	4002	BCR	9	0
11	A	1129	CLA	4	0
11	K	1402	CLA	4	0
11	A	1115	CLA	2	0
14	B	4009	BCR	7	0
11	1	1122	CLA	1	0
11	B	1212	CLA	5	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
11	L	1501	CLA	8	0
11	1	1140	CLA	2	0
14	6	4018	BCR	9	0
11	A	1123	CLA	6	0
11	2	1234	CLA	4	0
13	1	3001	SF4	1	0
11	A	1012	CLA	5	0
11	A	1103	CLA	20	0
14	2	4005	BCR	3	0
13	C	3003	SF4	11	0
14	2	4006	BCR	1	0
11	B	1222	CLA	7	0
14	A	4007	BCR	9	0
11	A	1132	CLA	4	0
13	C	3002	SF4	11	0
14	A	4008	BCR	5	0
11	B	1235	CLA	3	0
11	A	1104	CLA	8	0
11	2	1230	CLA	3	0
12	1	2001	PQN	1	0
11	2	1203	CLA	1	0
11	A	1137	CLA	5	0
11	1	1125	CLA	2	0
11	B	1021	CLA	7	0
11	A	1122	CLA	2	0
13	A	3001	SF4	4	0
11	B	1221	CLA	4	0
14	1	4002	BCR	5	0
11	1	1101	CLA	3	0
11	A	1138	CLA	6	0
14	L	4022	BCR	9	0
14	1	4001	BCR	8	0
11	1	1115	CLA	4	0
11	1	1121	CLA	1	0
14	8	4019	BCR	7	0
11	A	1140	CLA	1	0
11	2	1225	CLA	1	0
11	B	1023	CLA	8	0
14	B	4006	BCR	3	0
11	B	1238	CLA	7	0
11	A	1111	CLA	4	0
11	B	1204	CLA	3	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
11	1	1131	CLA	2	0
11	1	1119	CLA	4	0
14	B	4017	BCR	10	0
11	B	1226	CLA	1	0
11	A	1112	CLA	7	0
11	1	1118	CLA	2	0
11	2	1235	CLA	2	0
11	A	1124	CLA	3	0
11	2	1211	CLA	2	0
11	B	1214	CLA	2	0
11	B	1220	CLA	3	0
11	A	1136	CLA	4	0
11	1	1110	CLA	2	0
14	F	4013	BCR	6	0
11	A	1118	CLA	5	0
14	8	4022	BCR	8	0
11	1	1112	CLA	3	0
11	2	1202	CLA	3	0
11	B	1208	CLA	3	0
11	B	1227	CLA	4	0
11	1	1011	CLA	1	0
11	B	1228	CLA	2	0
11	B	1240	CLA	1	0
11	A	1135	CLA	1	0
11	1	1134	CLA	3	0
11	B	1219	CLA	2	0
11	1	1012	CLA	5	0
11	1	1104	CLA	1	0
11	2	1206	CLA	6	0
11	2	1240	CLA	2	0
11	2	1220	CLA	1	0
11	2	1239	CLA	4	0
11	A	1105	CLA	1	0
11	A	1121	CLA	4	0
11	A	1107	CLA	5	0
16	B	5002	LMG	1	0
11	B	1013	CLA	9	0
11	B	1225	CLA	3	0
14	2	4010	BCR	6	0
14	1	4003	BCR	2	0
11	2	1021	CLA	6	0
11	2	1223	CLA	2	0

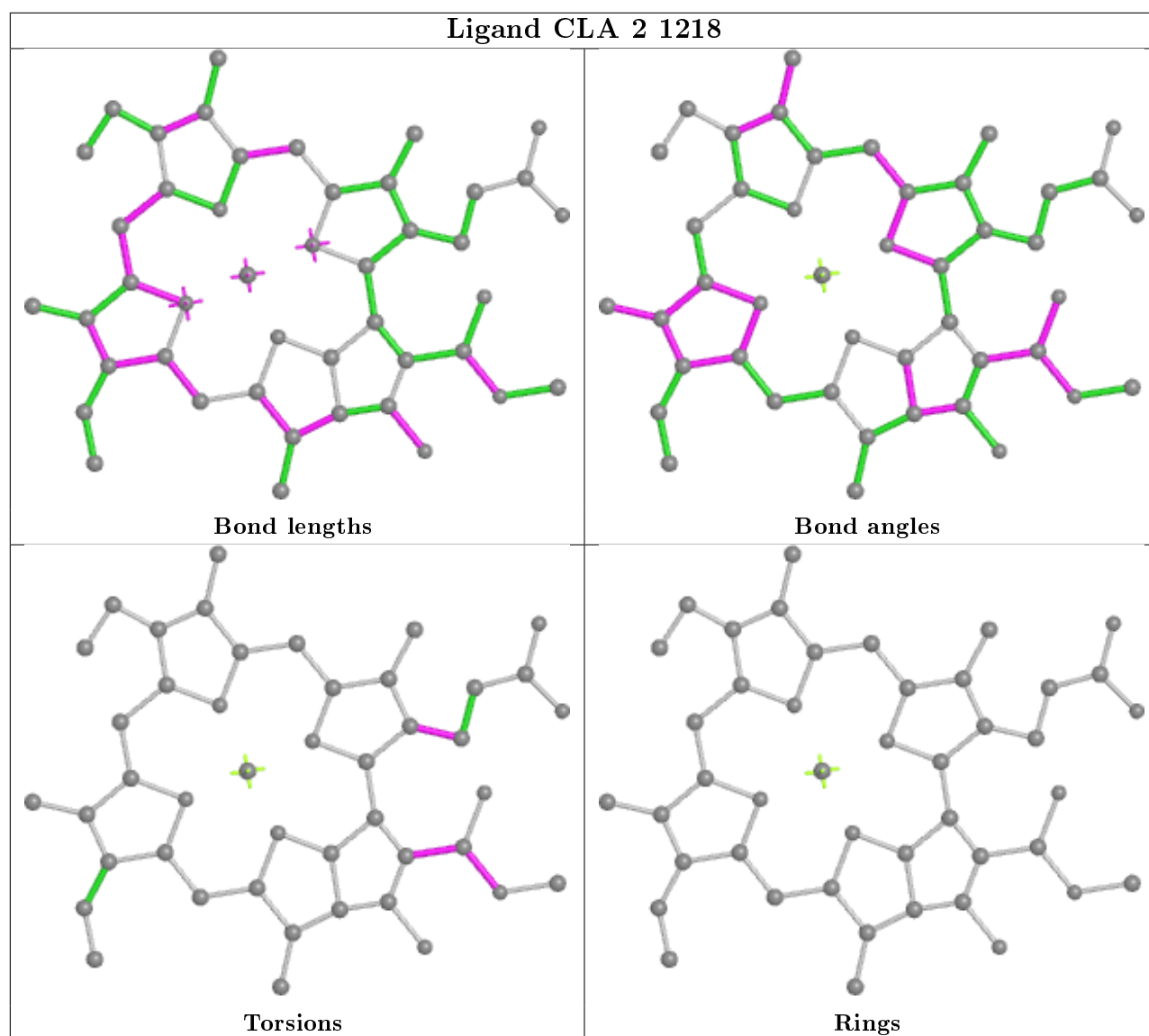
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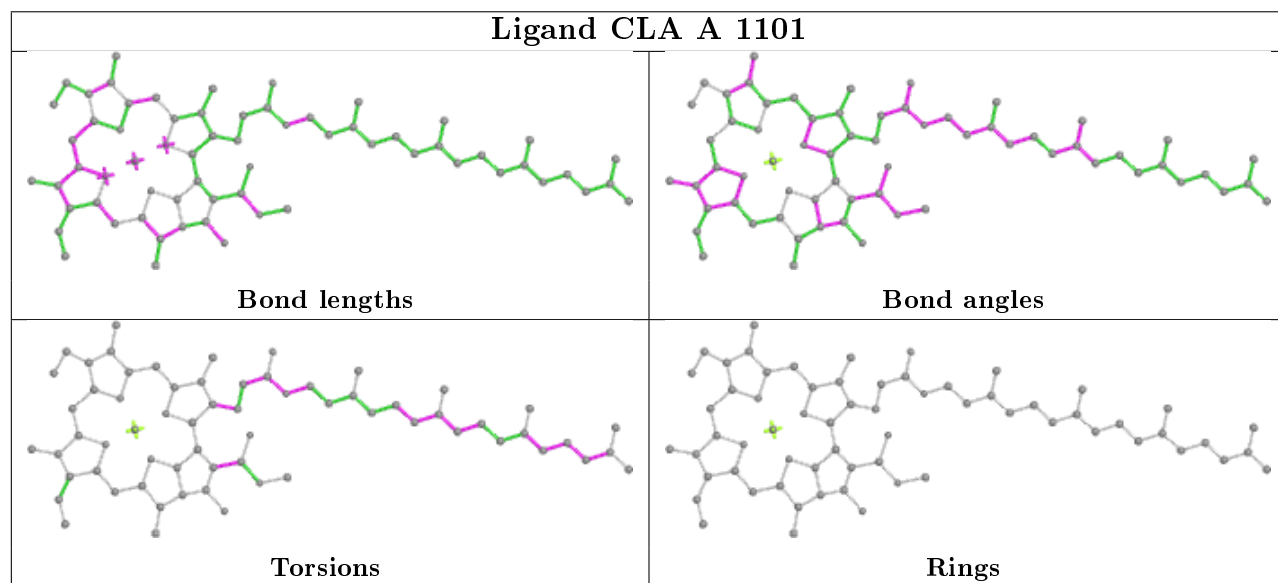
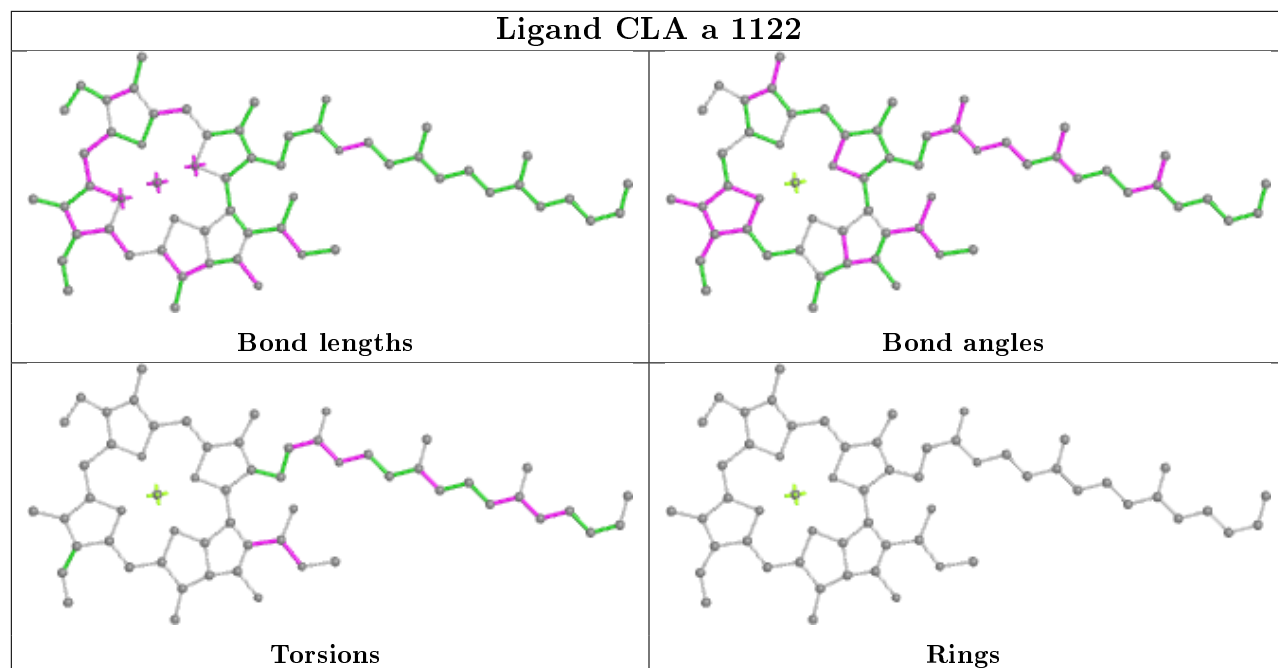


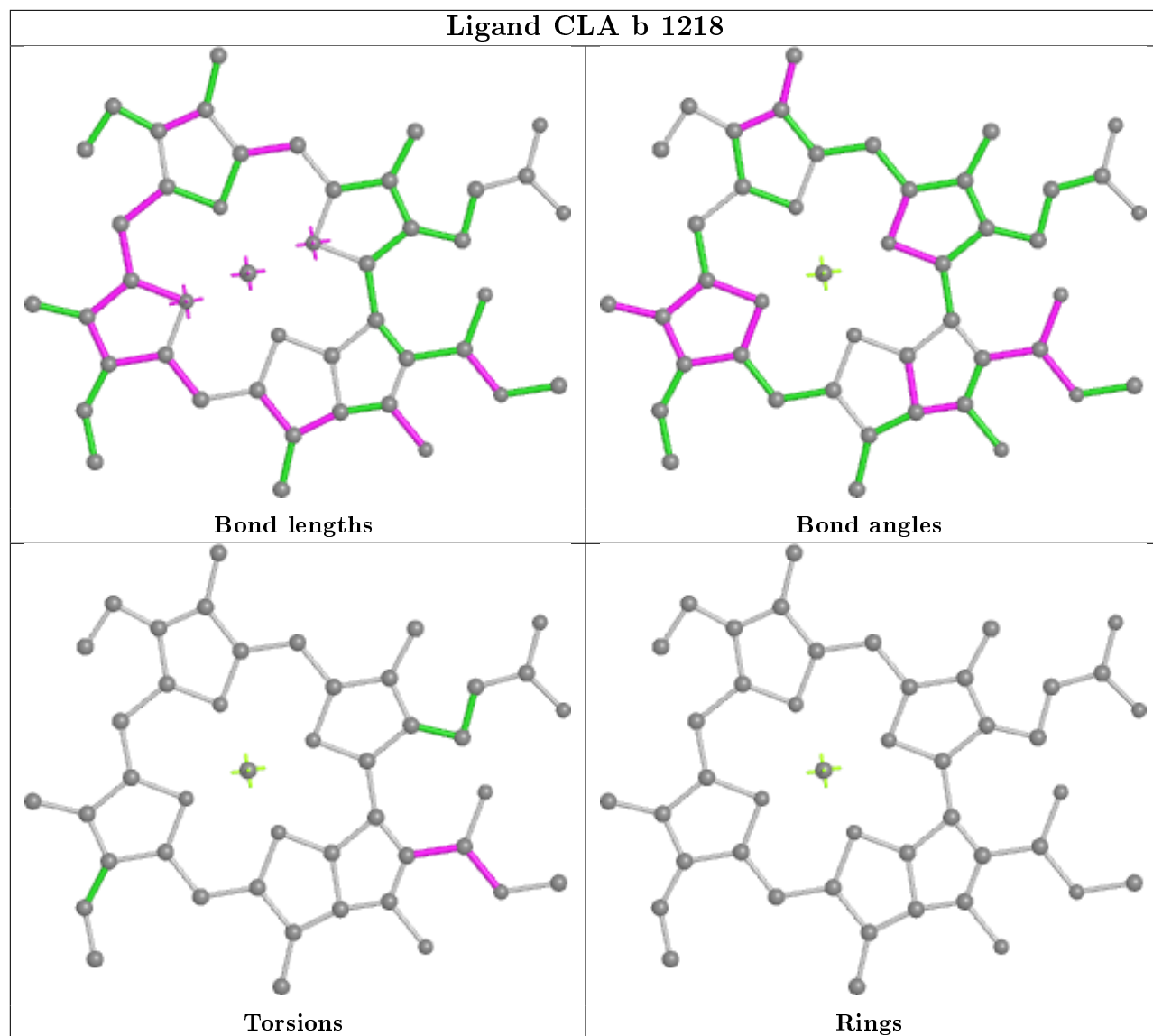
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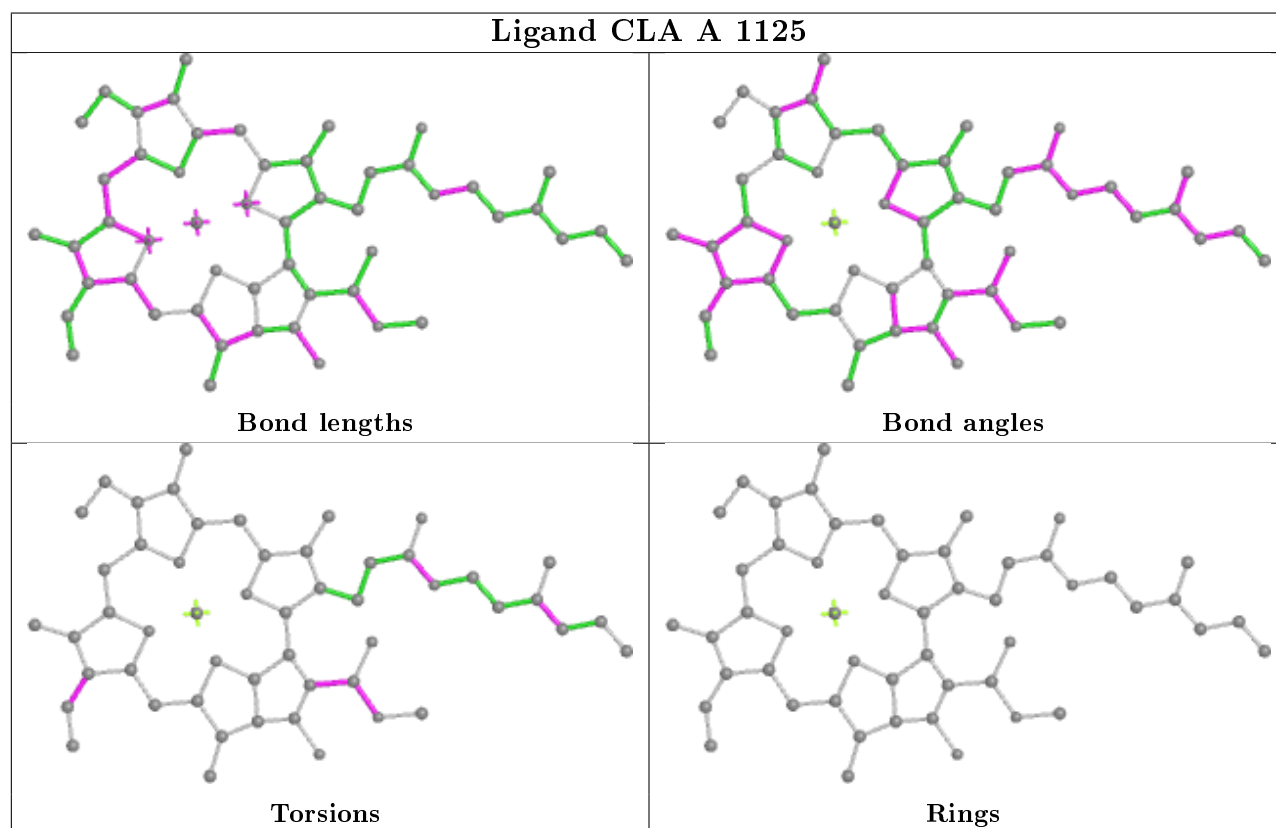
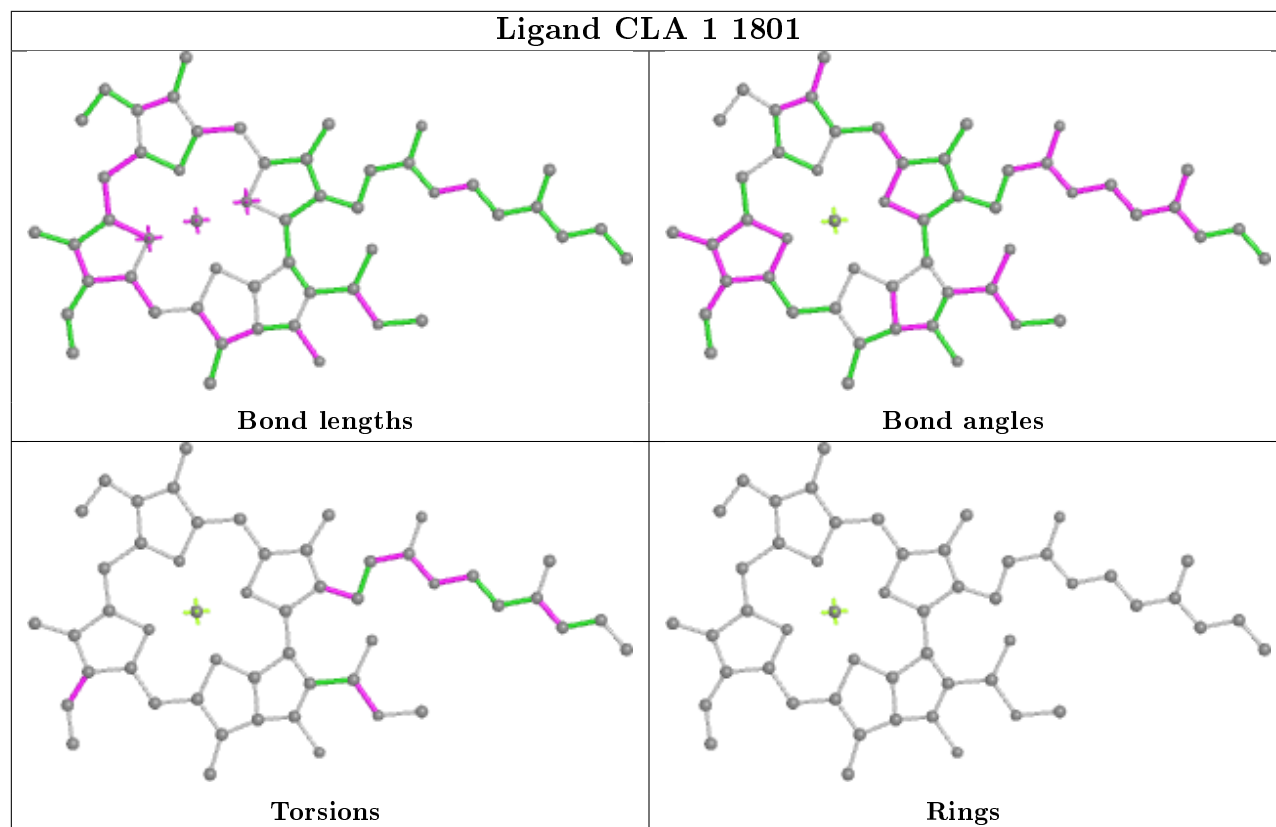
Mol	Chain	Res	Type	Clashes	Symm-Clashes
11	B	1201	CLA	4	0
11	B	1211	CLA	5	0
12	2	2002	PQN	3	0
11	B	1230	CLA	5	0
16	2	5002	LMG	1	0
11	2	1205	CLA	4	0
14	2	4004	BCR	2	0
11	A	1108	CLA	2	0
14	1	4007	BCR	7	0
14	F	4018	BCR	11	0
11	1	1113	CLA	3	0
11	2	1210	CLA	2	0
11	1	1107	CLA	3	0
14	6	4013	BCR	7	0
14	B	4014	BCR	6	0
14	2	4017	BCR	9	0
14	B	4005	BCR	7	0
11	1	1105	CLA	1	0
11	1	1102	CLA	1	0
11	1	1117	CLA	2	0
11	A	1102	CLA	4	0
11	2	1013	CLA	5	0
11	2	1207	CLA	4	0
11	B	1229	CLA	6	0
11	2	1222	CLA	3	0
11	A	1110	CLA	2	0
11	1	1128	CLA	9	0

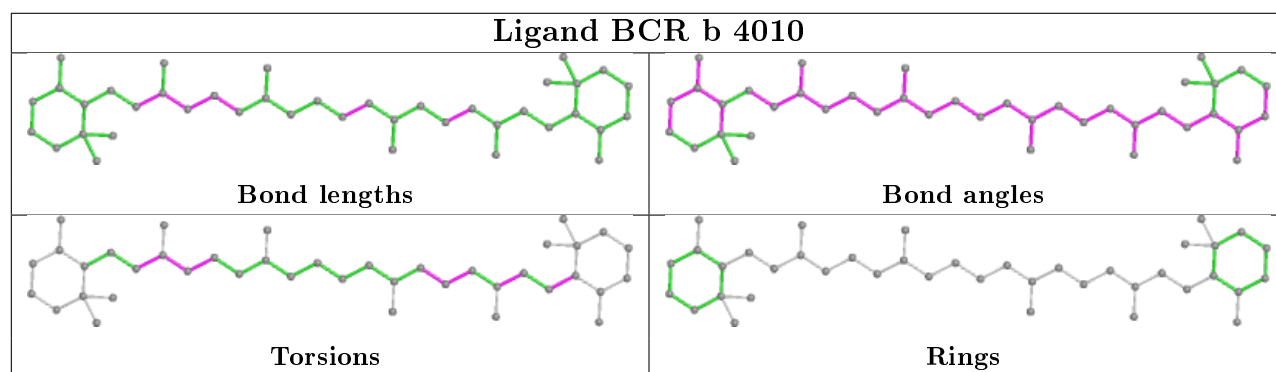
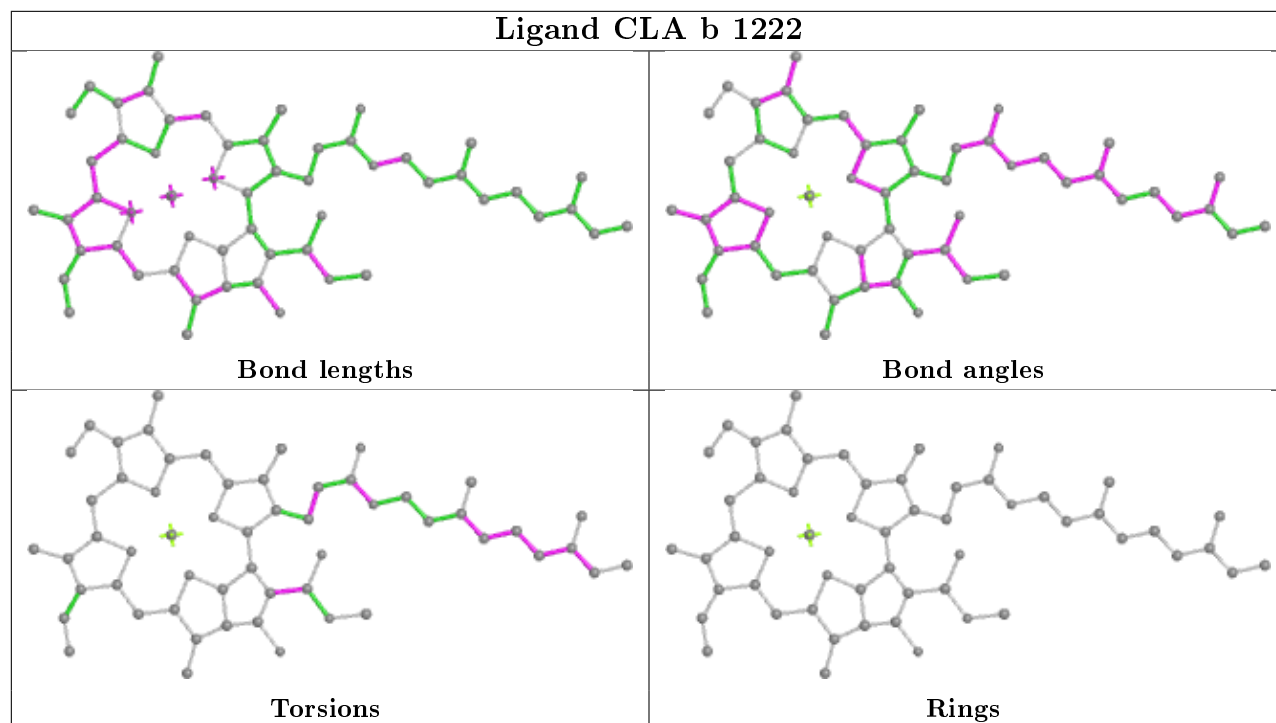
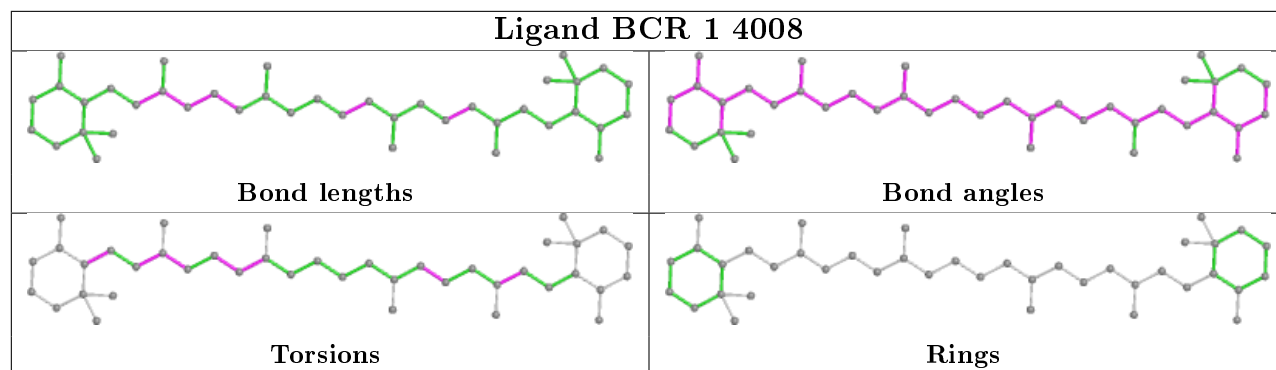
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

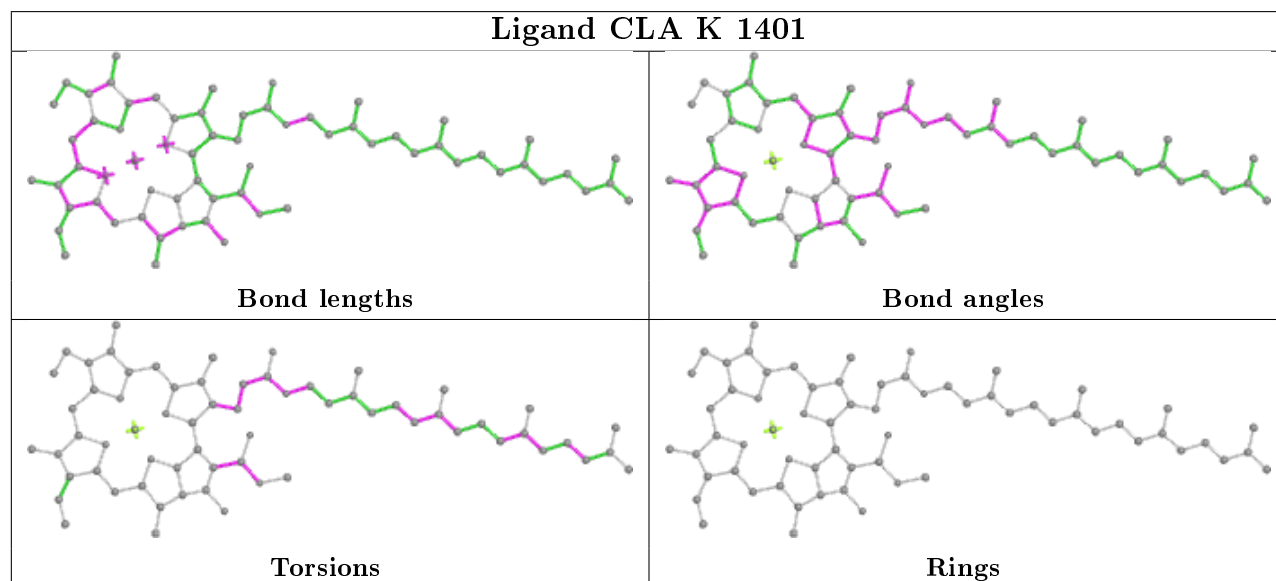
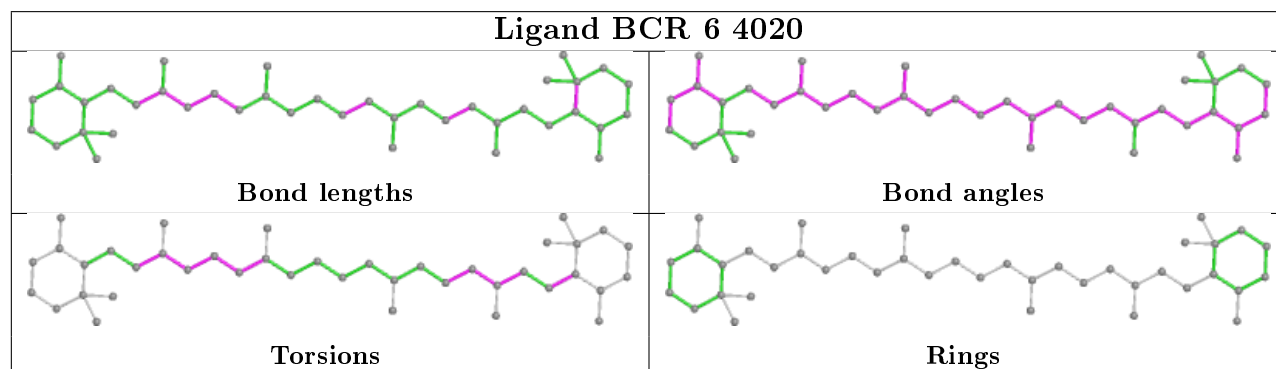
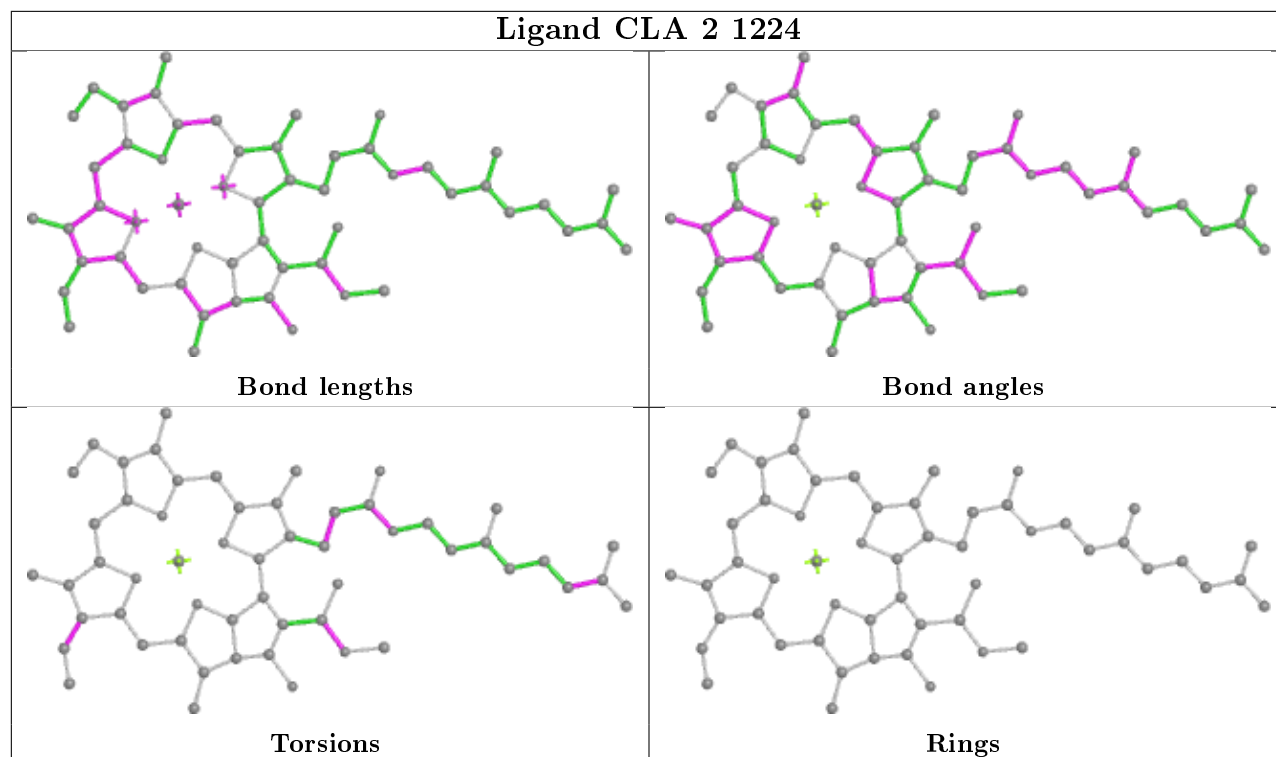


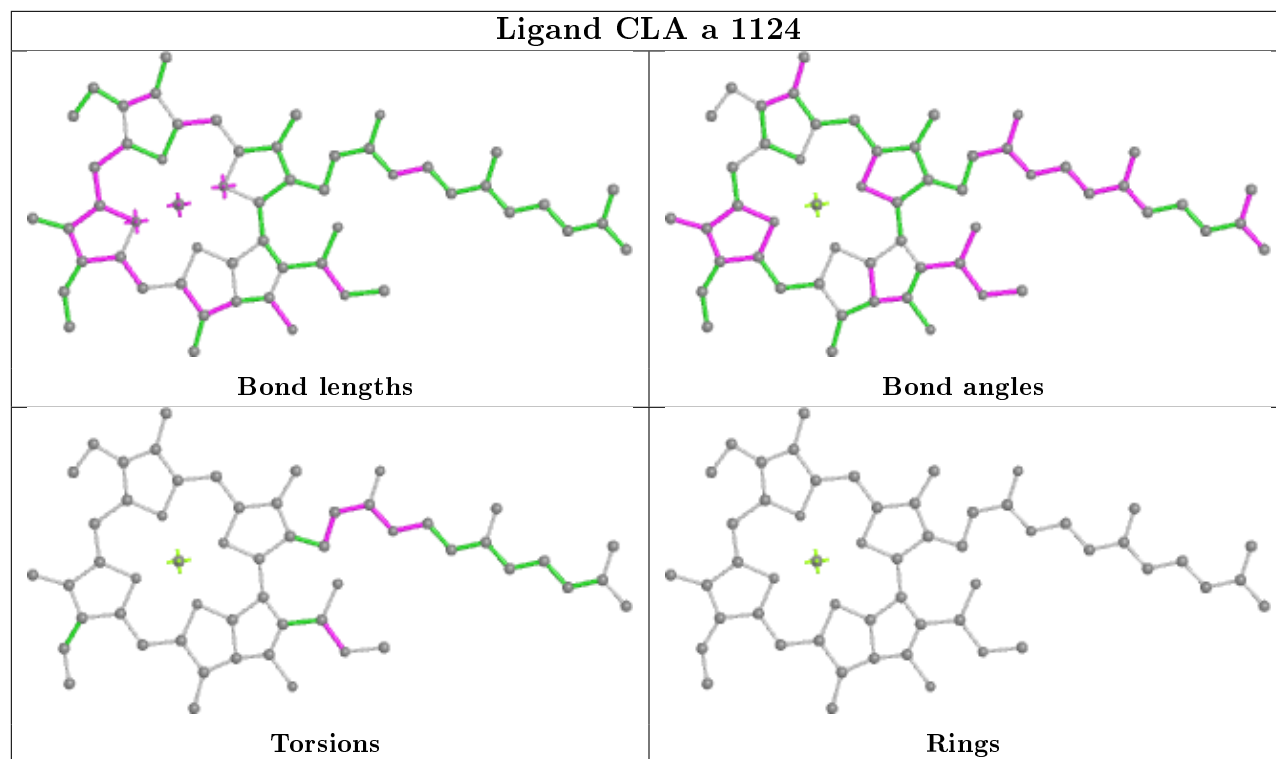




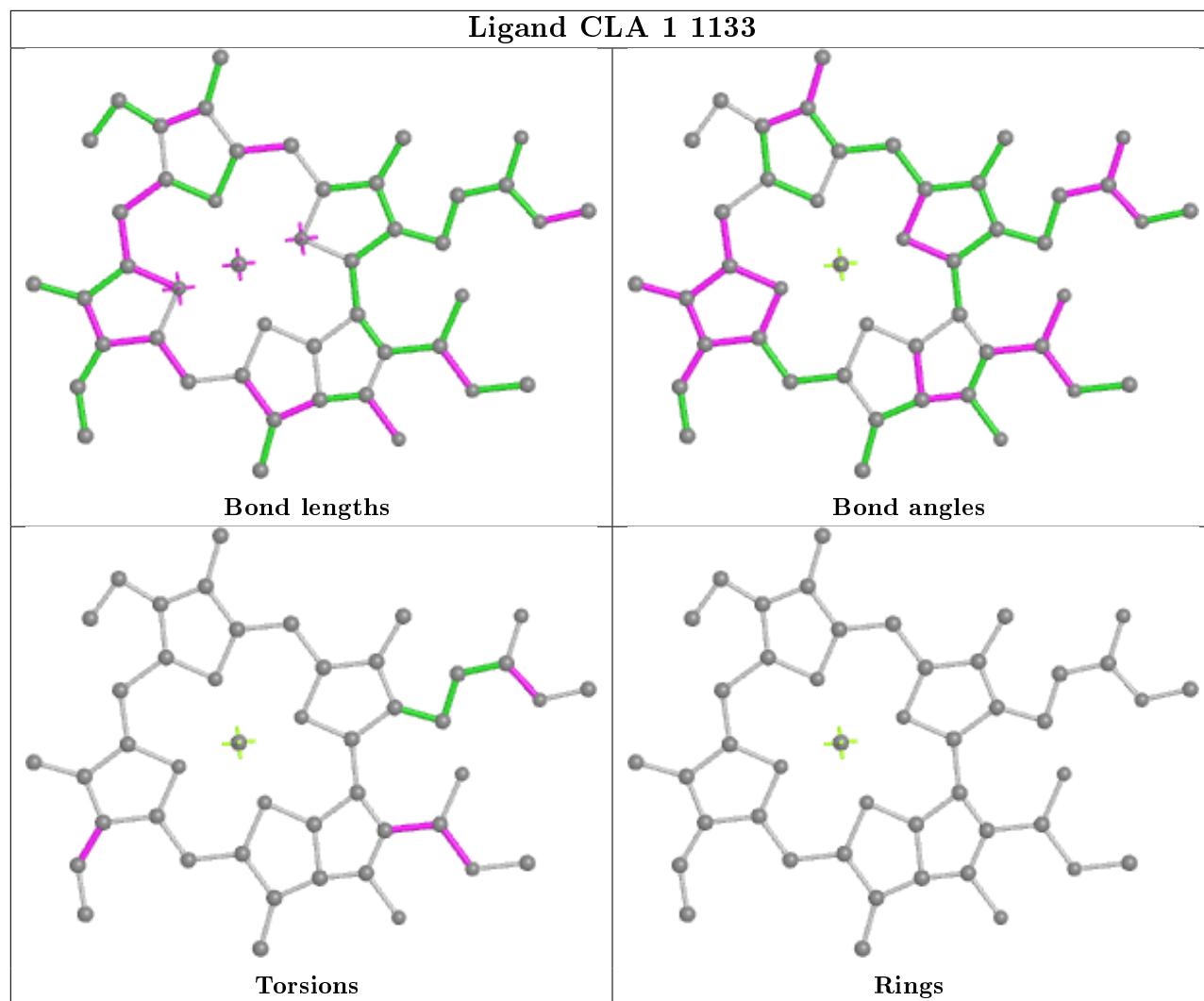


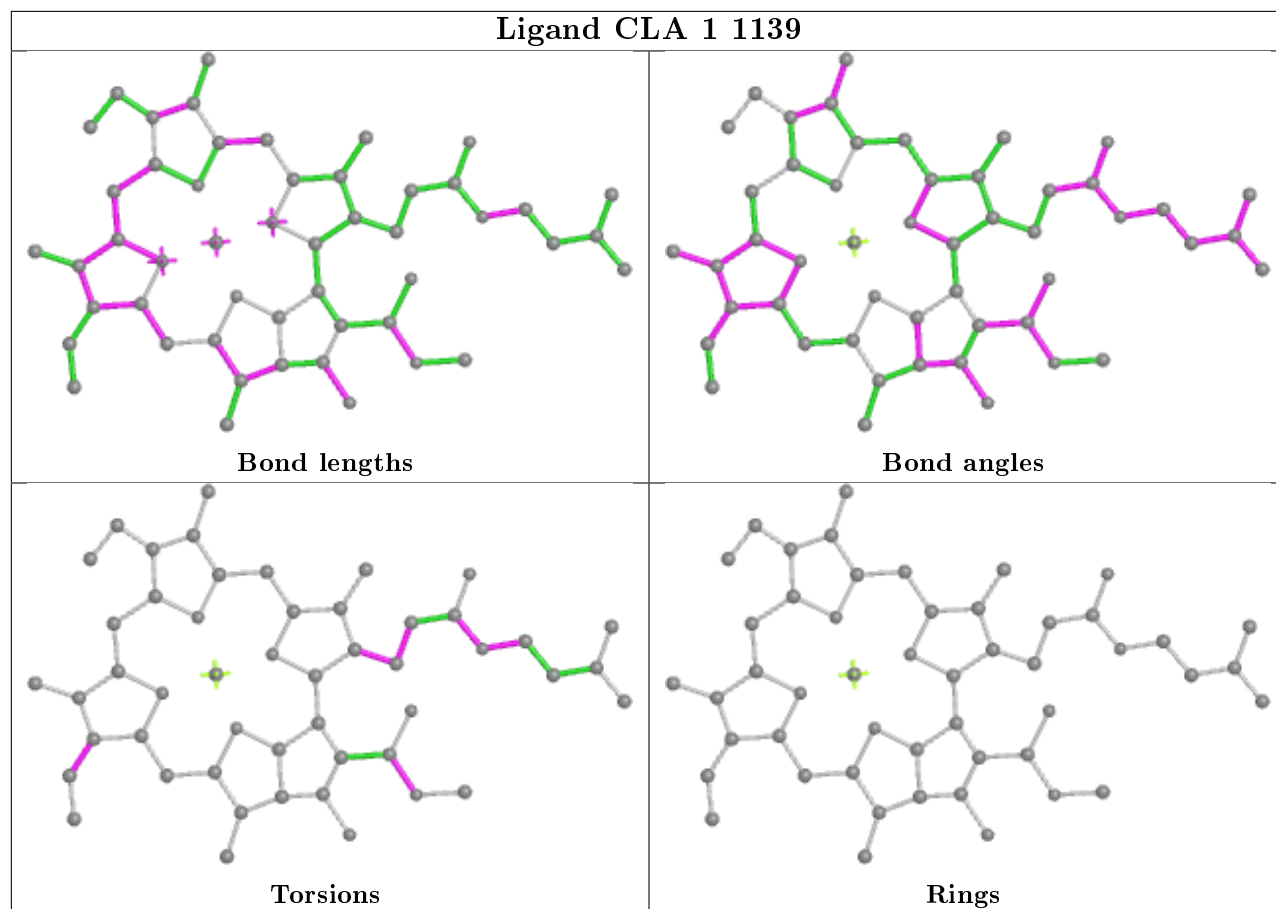


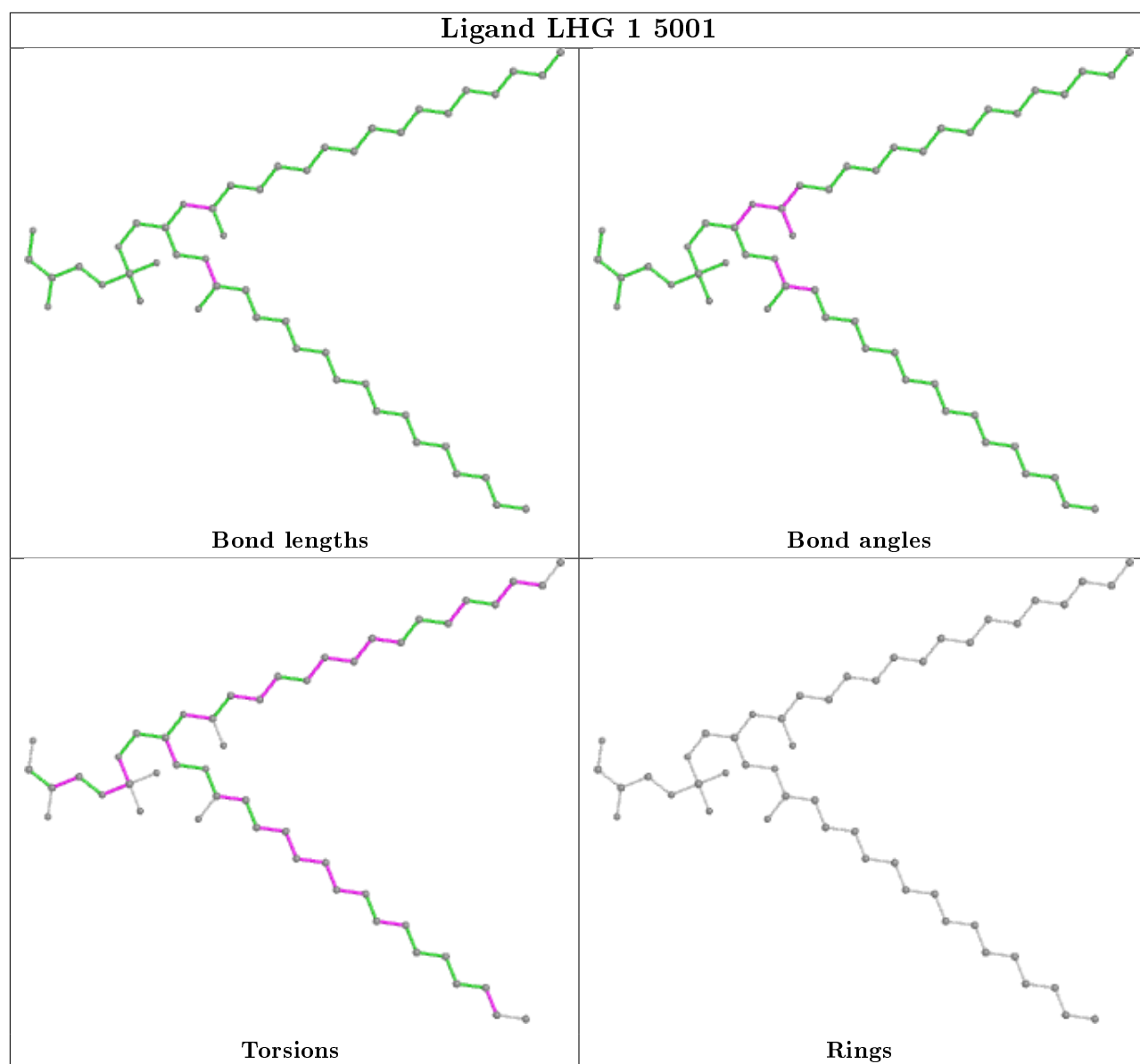


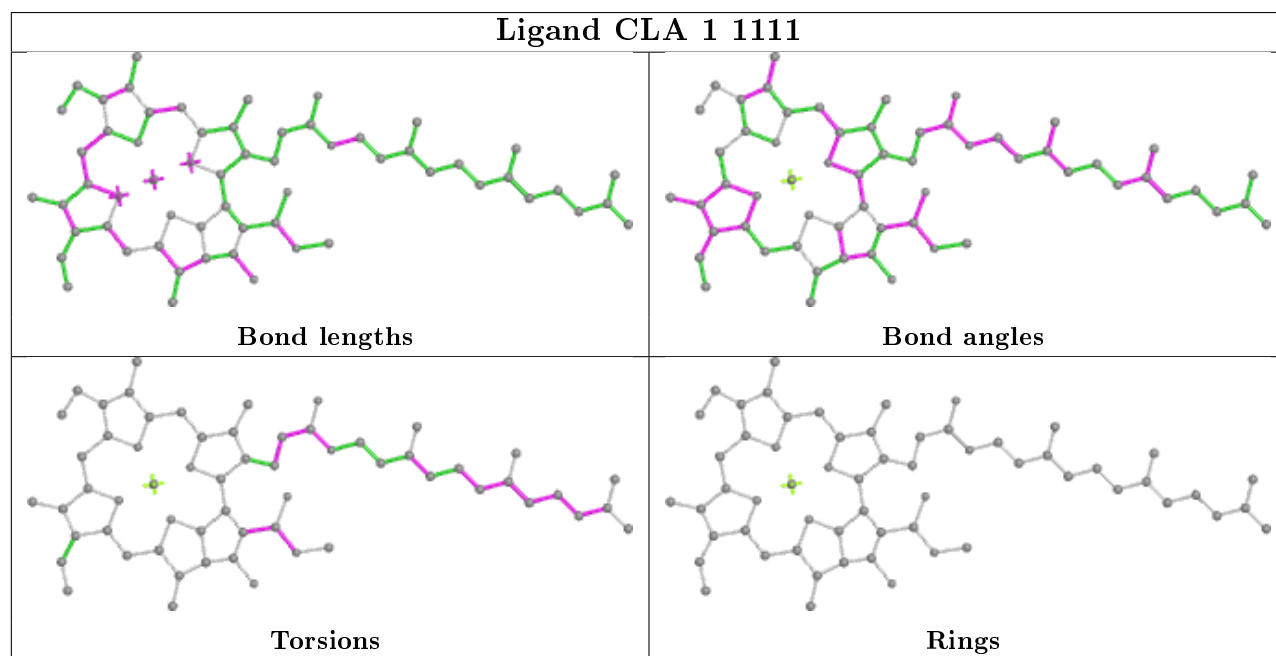
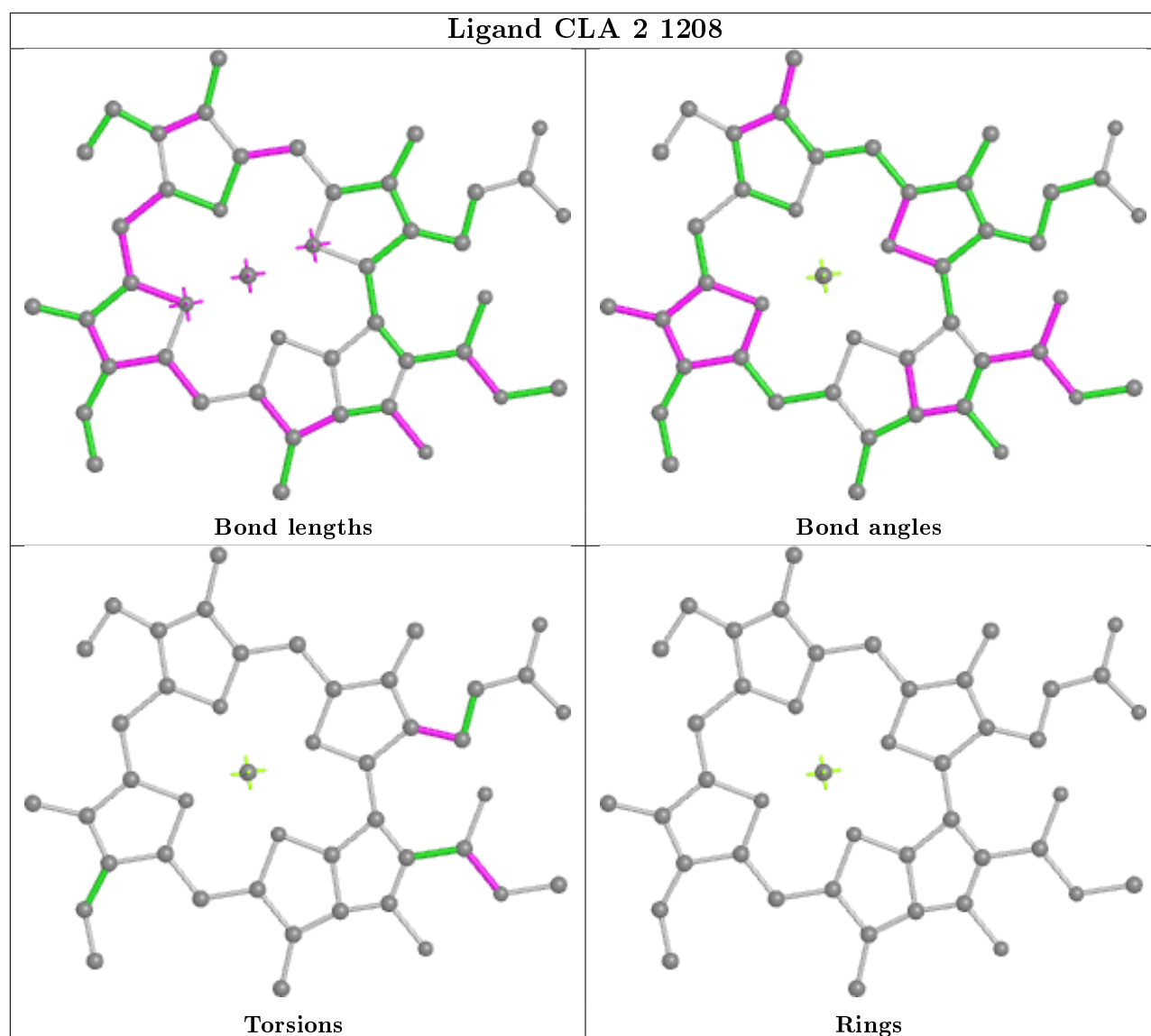


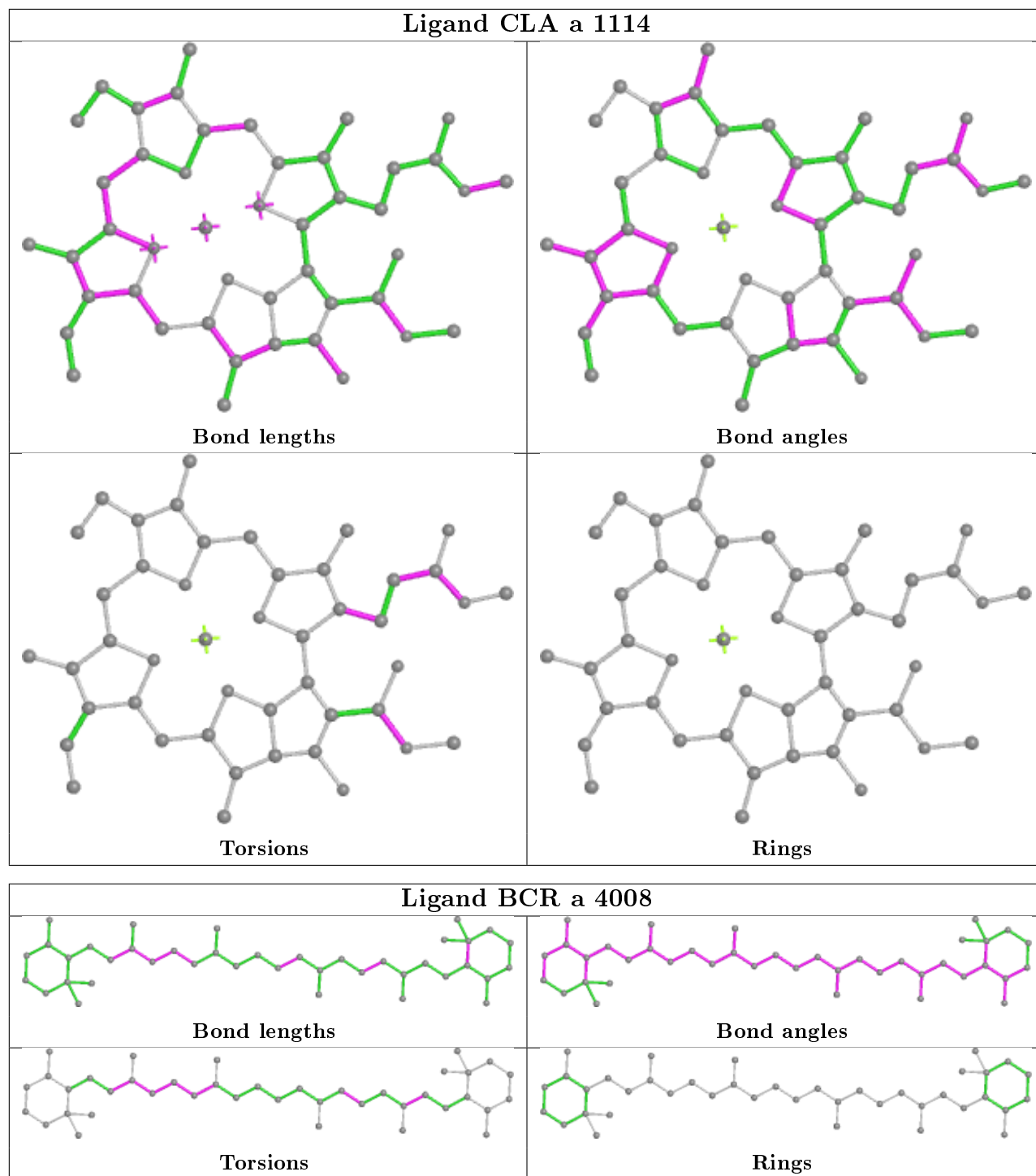


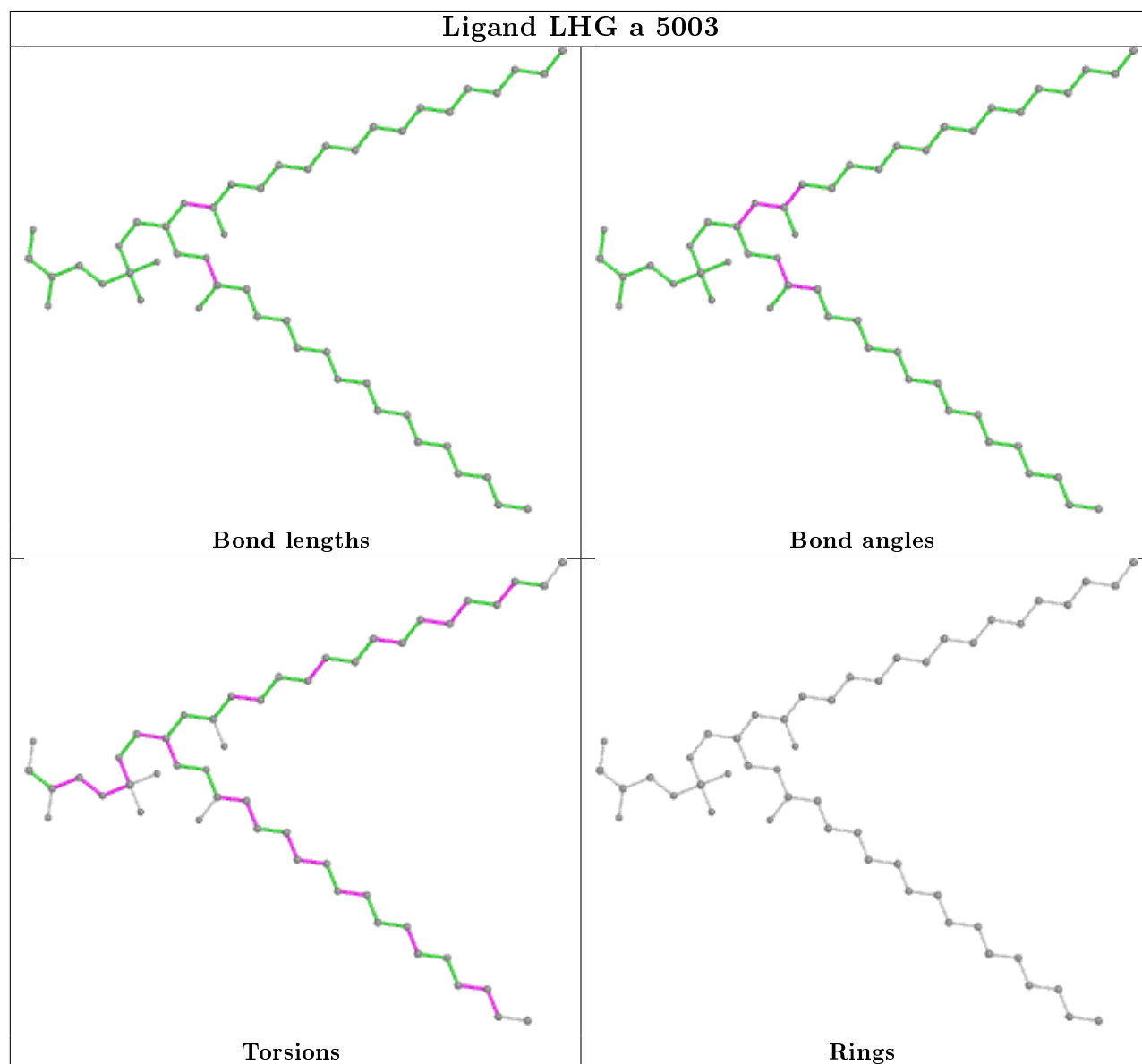
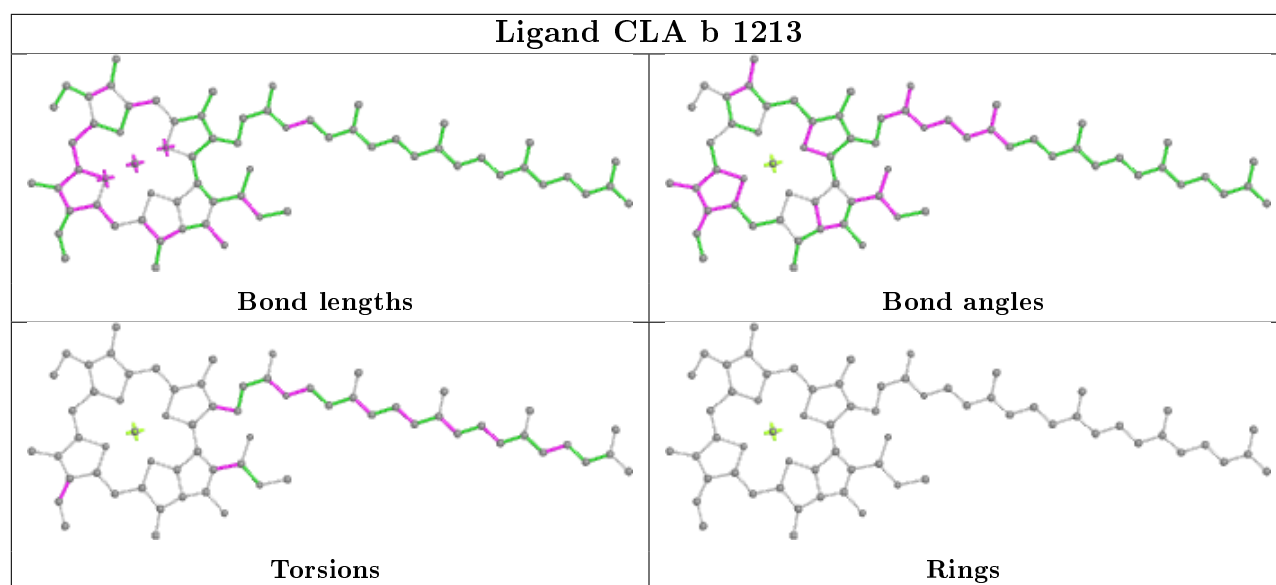


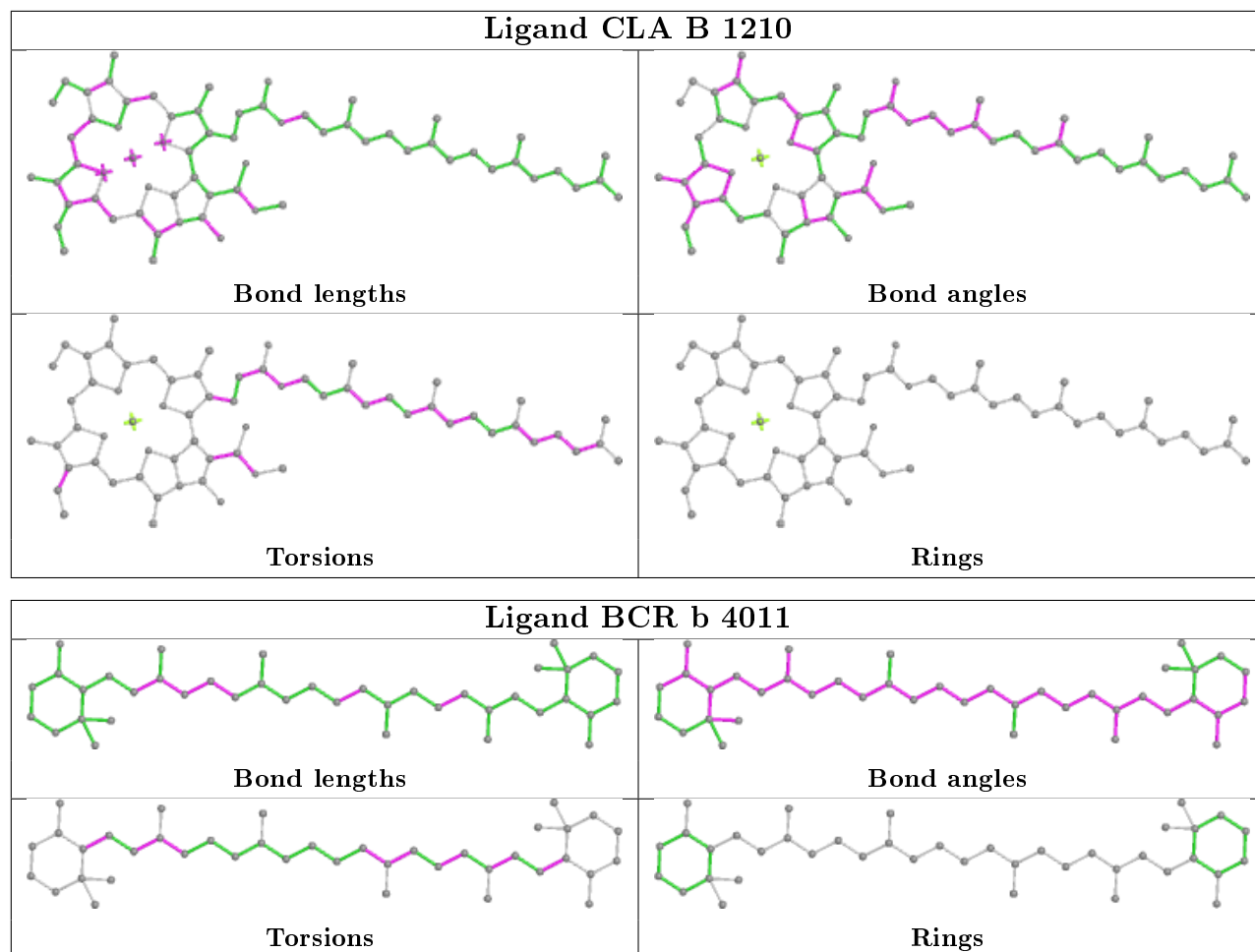


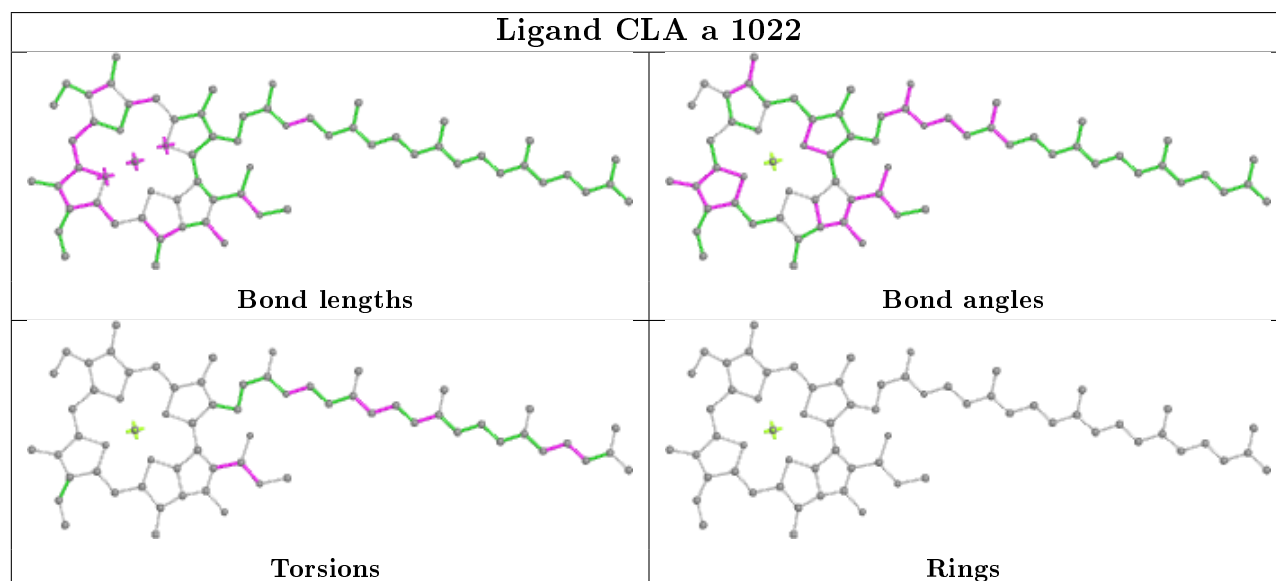
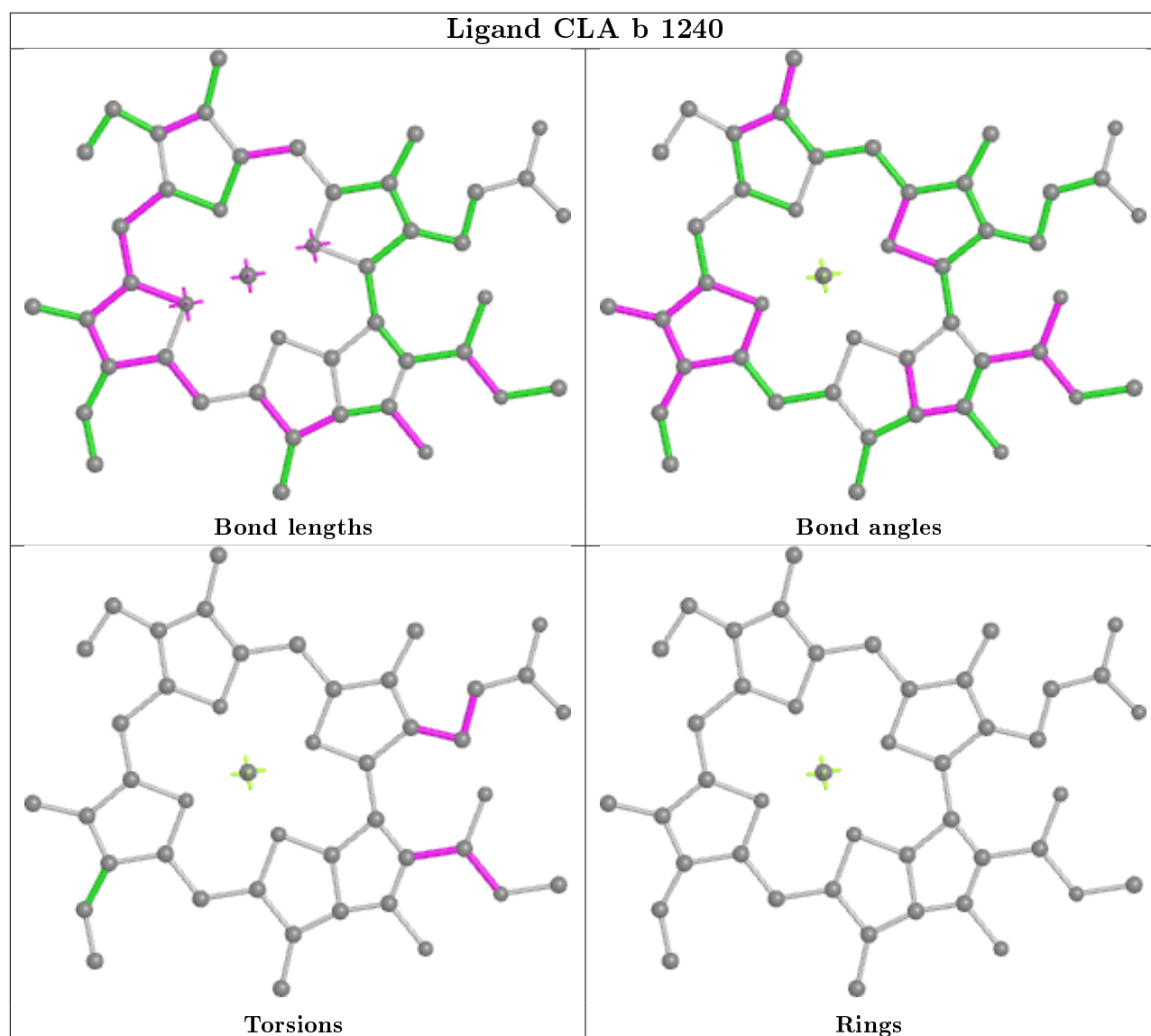






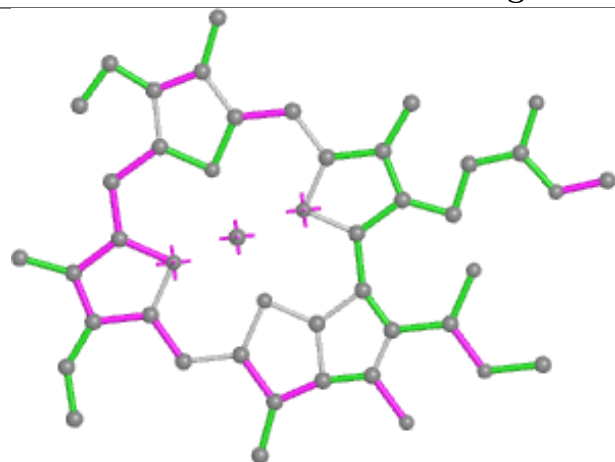




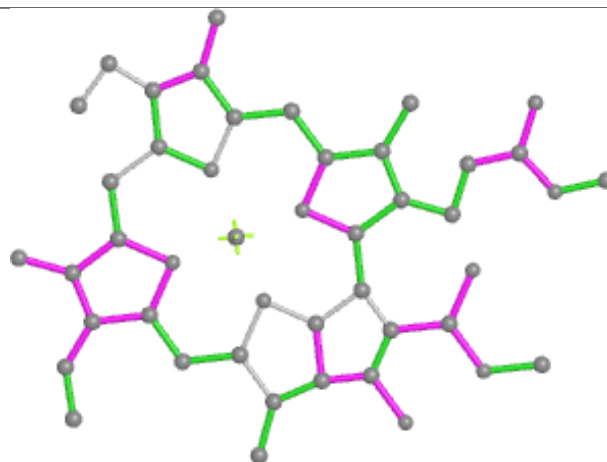




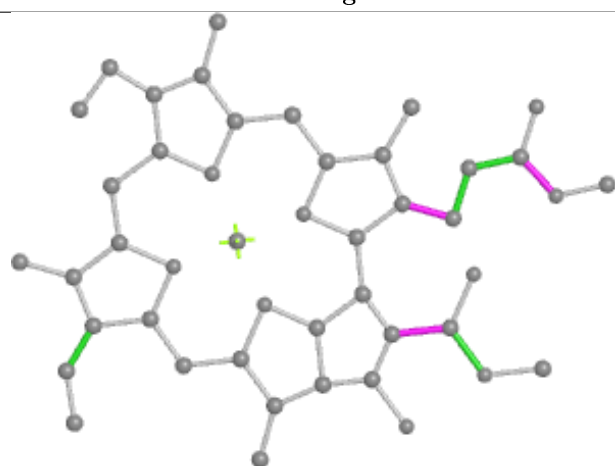
## Ligand CLA A 1120



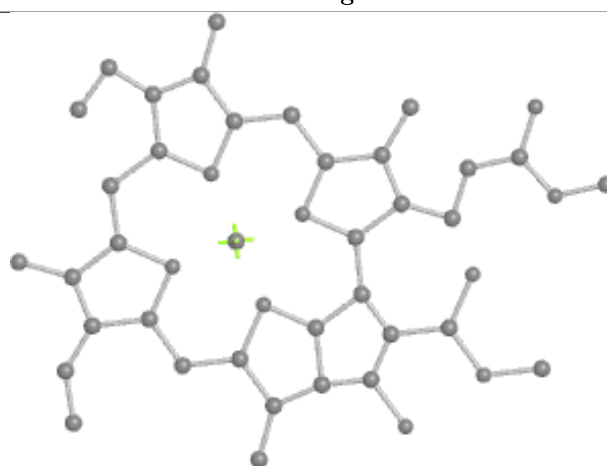
Bond lengths



Bond angles

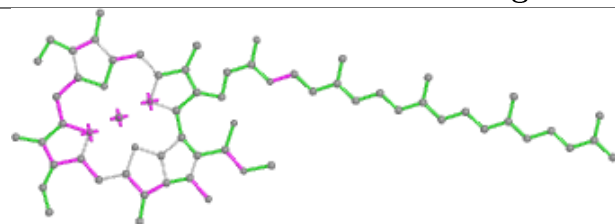


Torsions

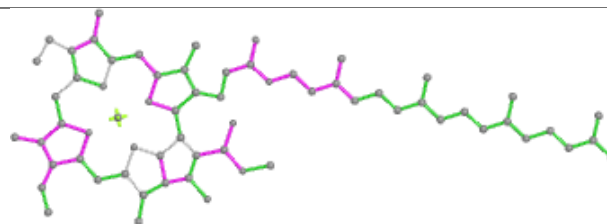


Rings

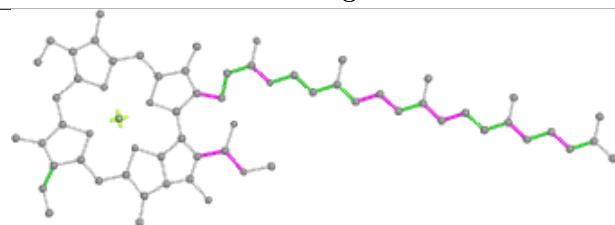
## Ligand CLA 8 1501



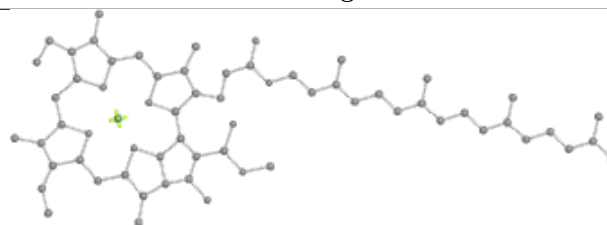
Bond lengths



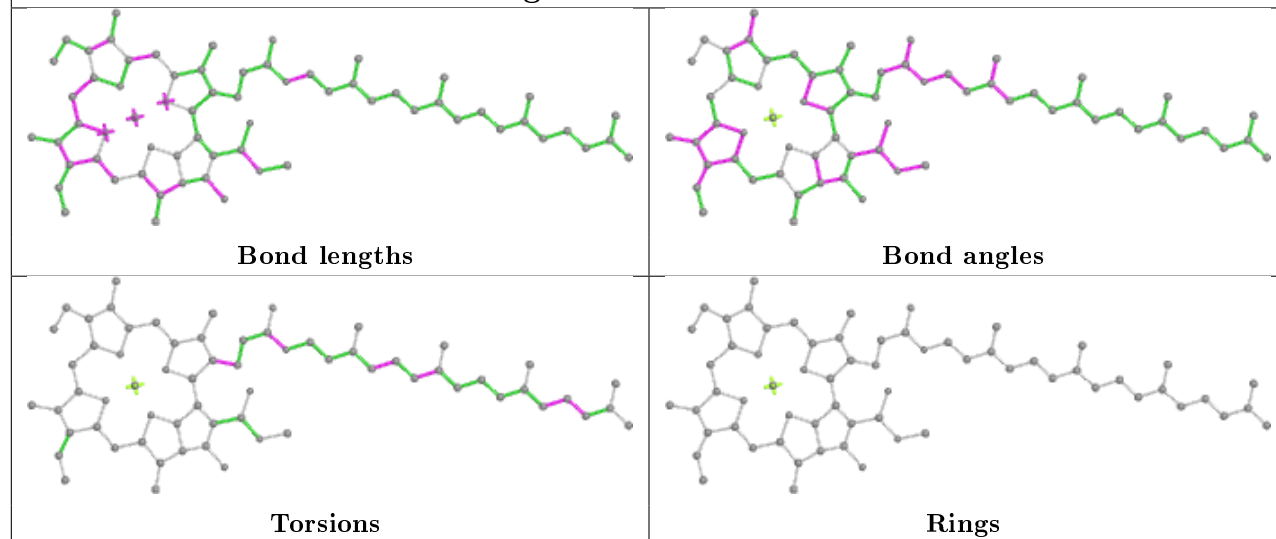
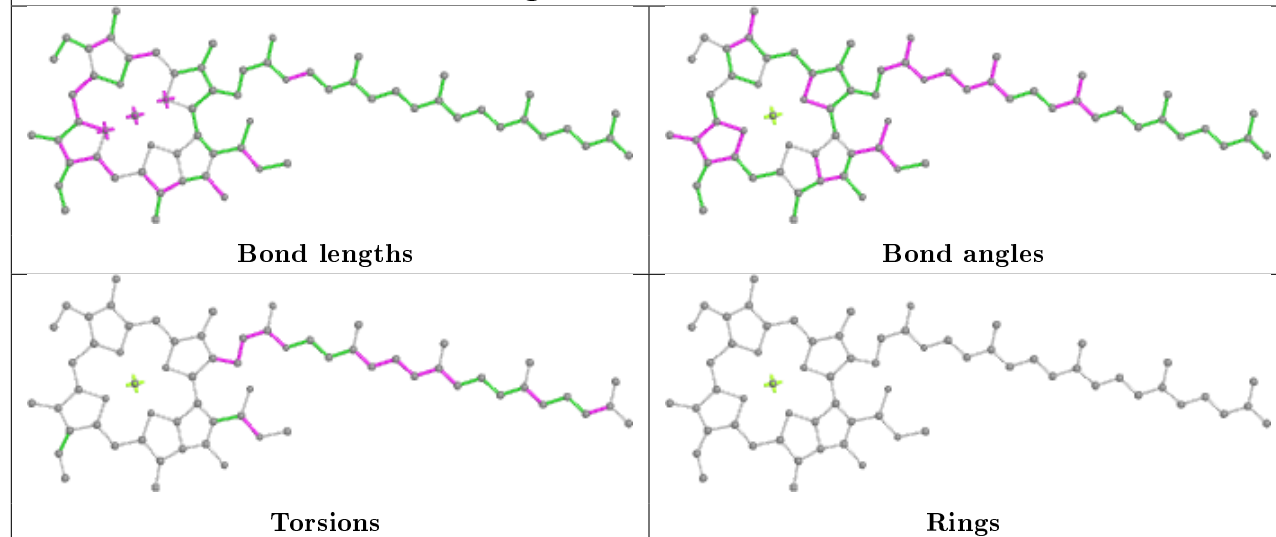
Bond angles

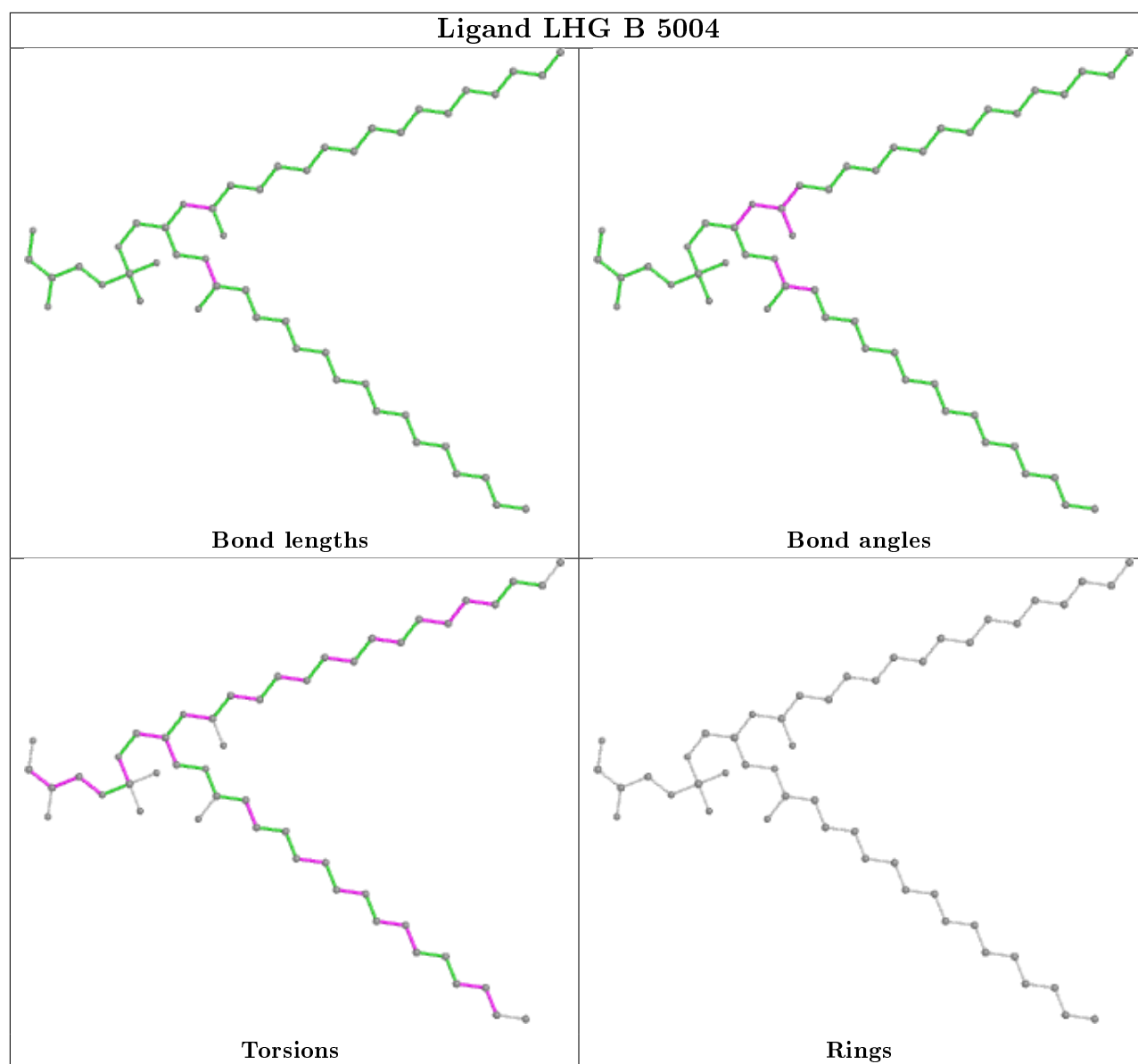


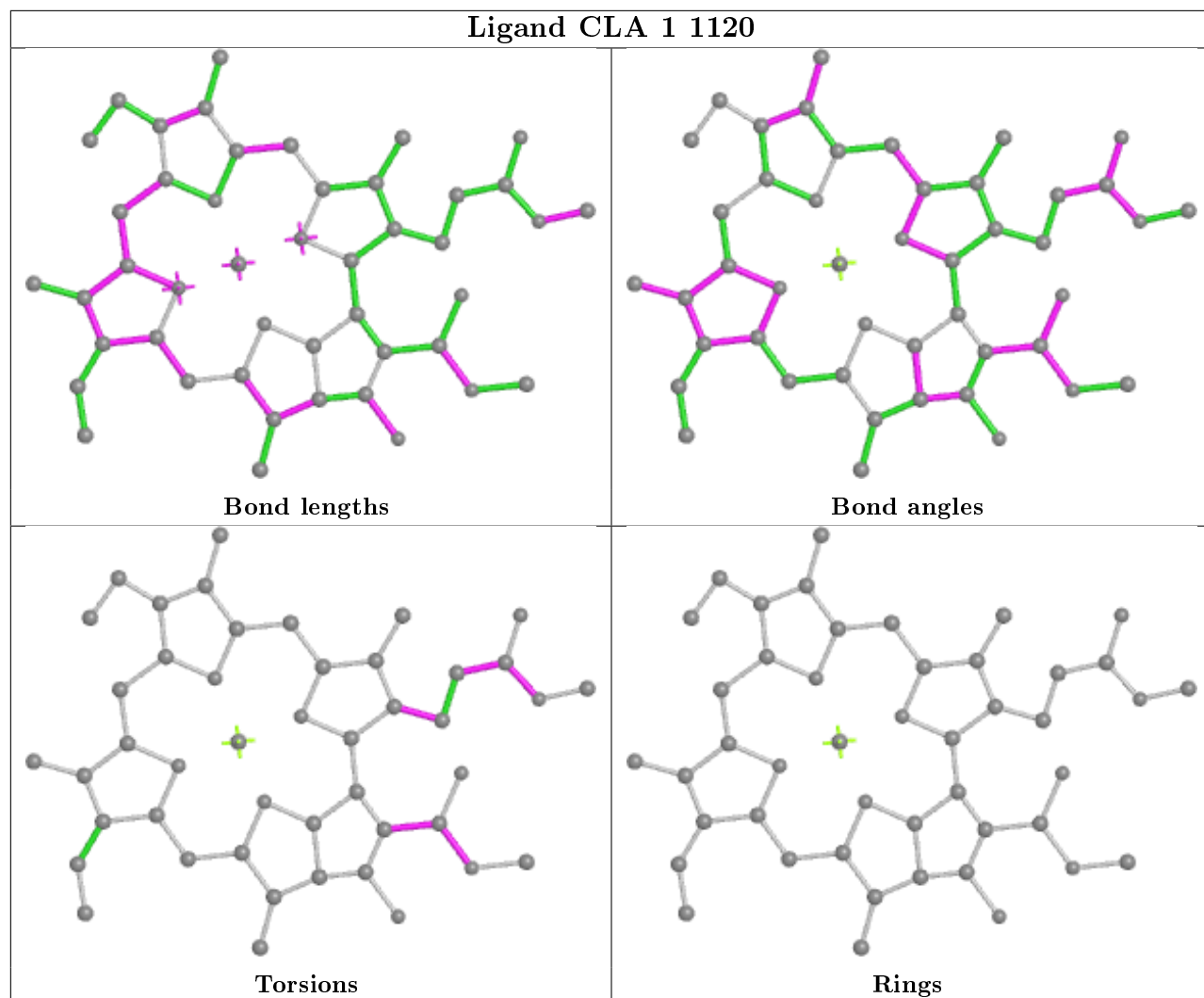
Torsions

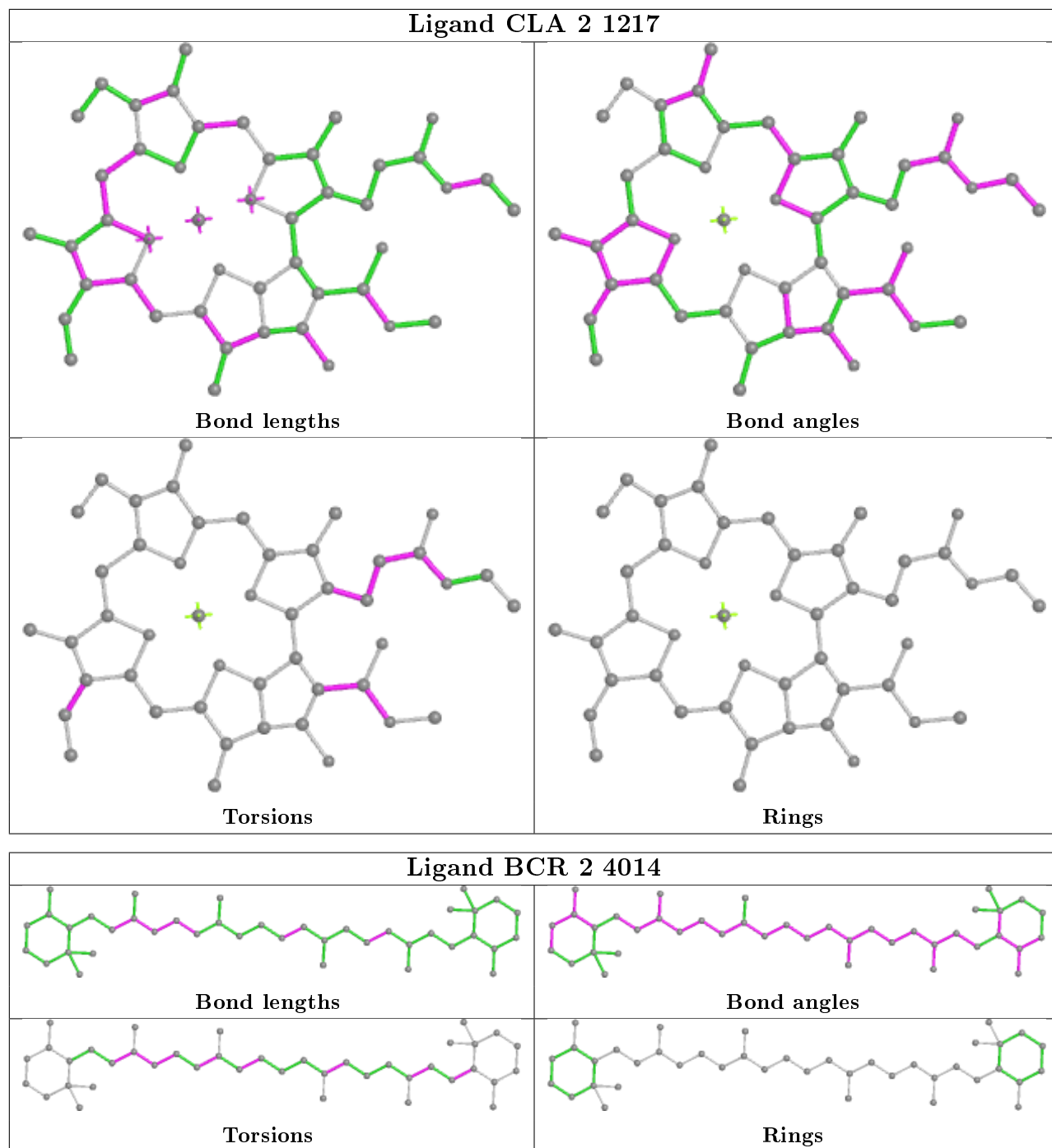


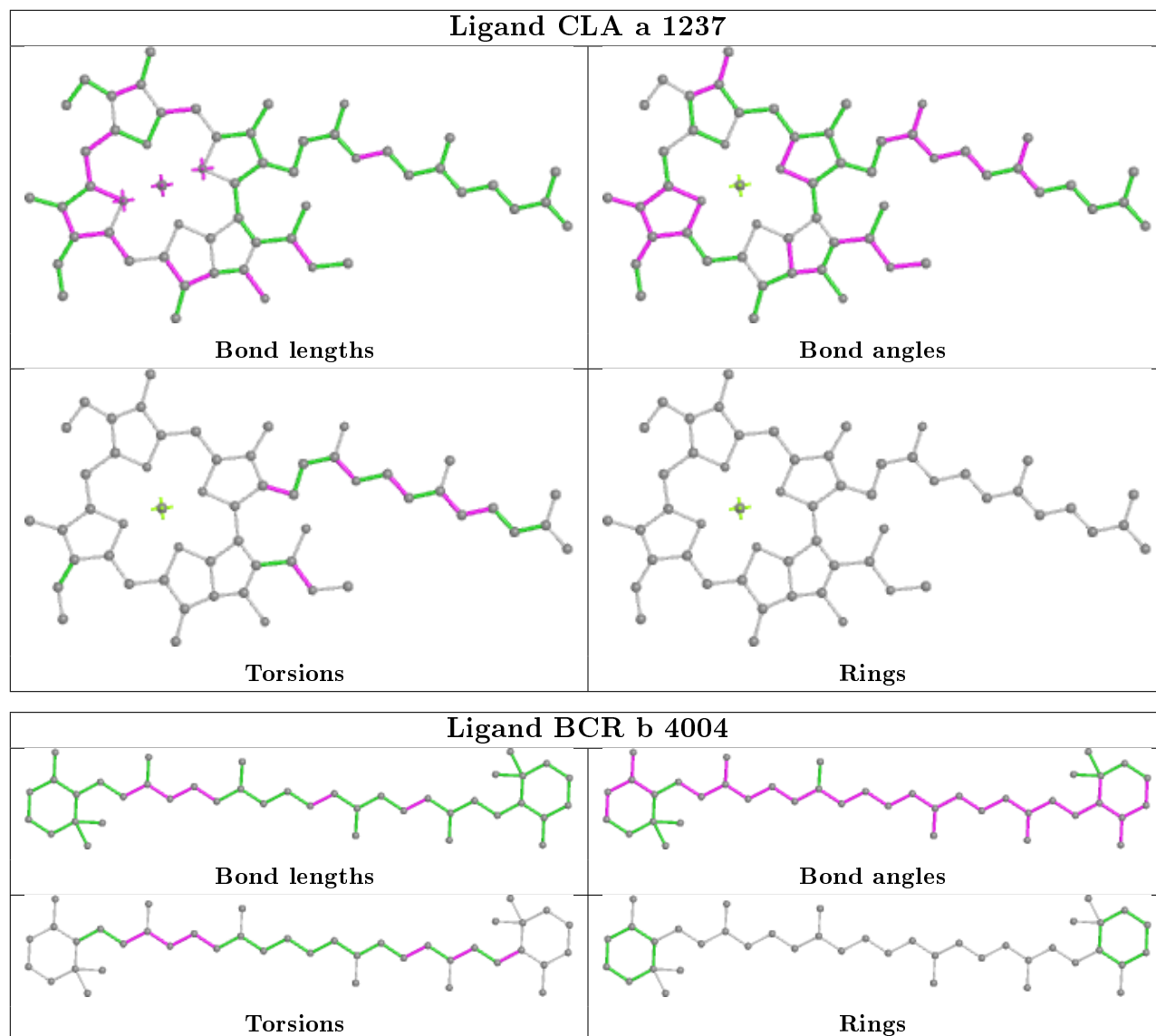
Rings

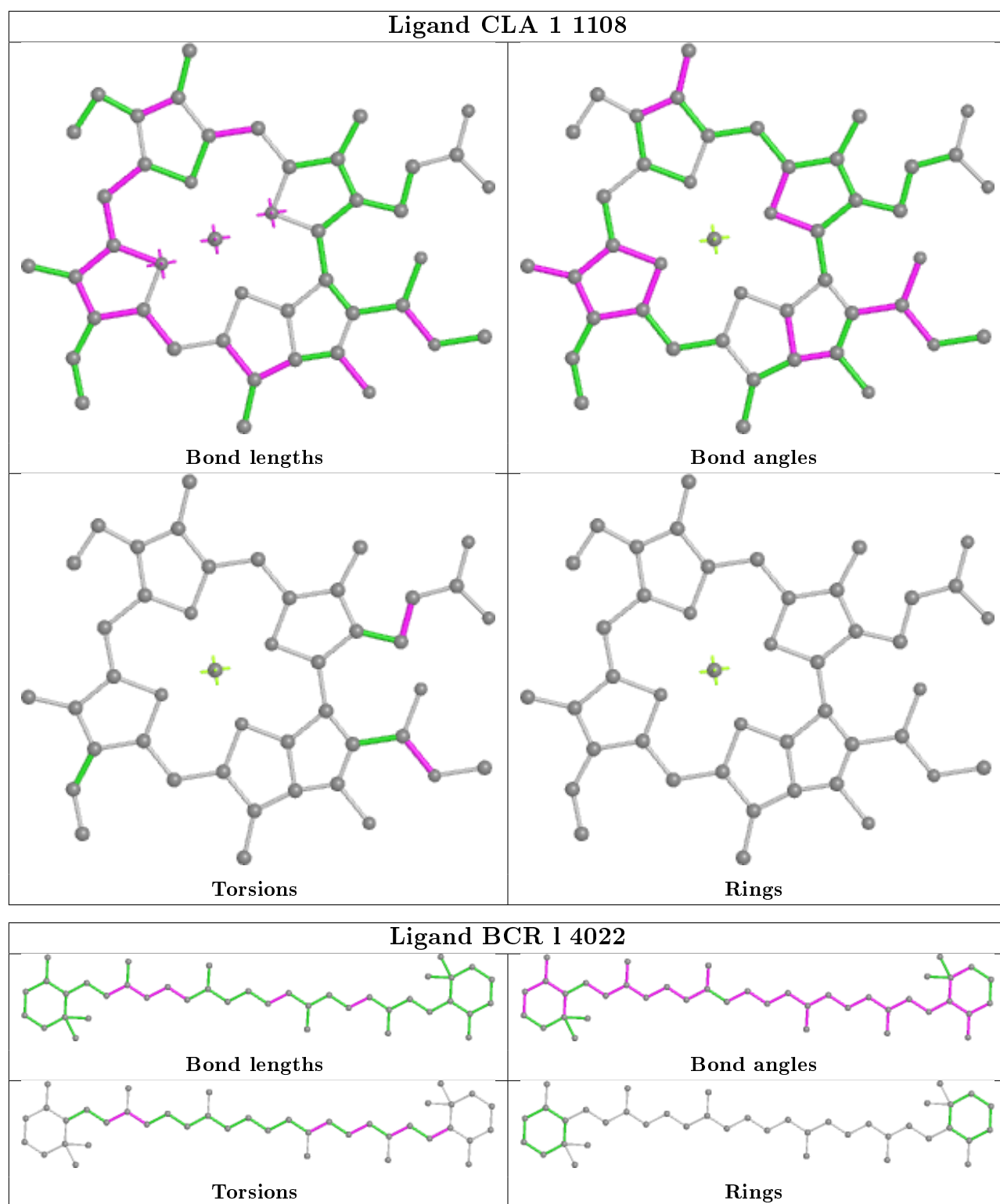
**Ligand CLA B 1216****Ligand CLA B 1213**

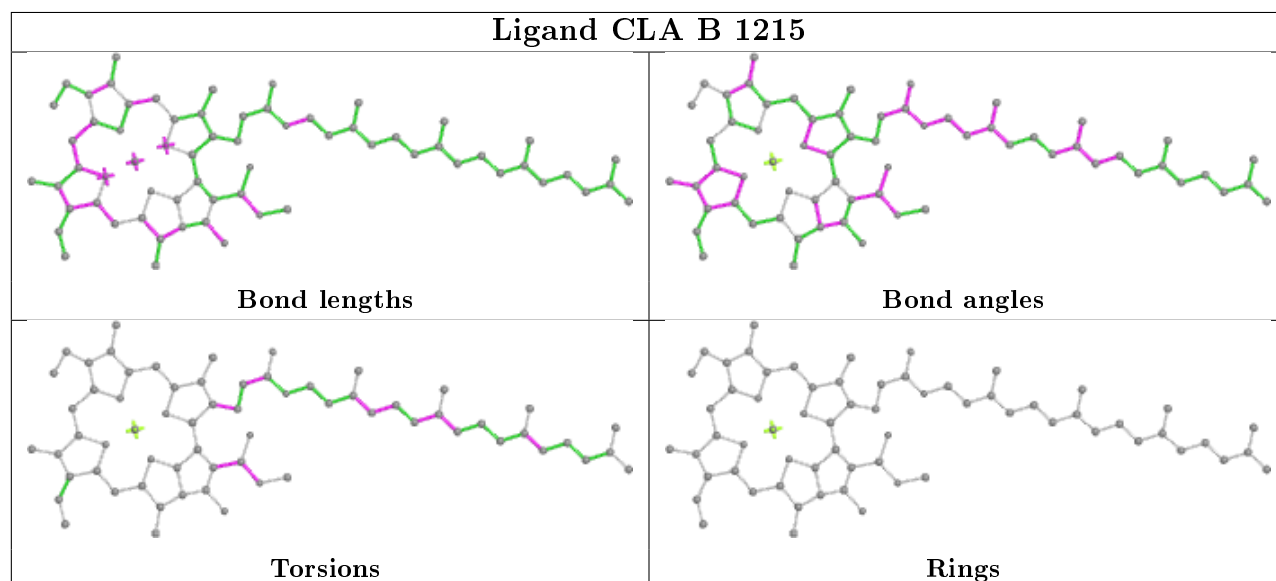
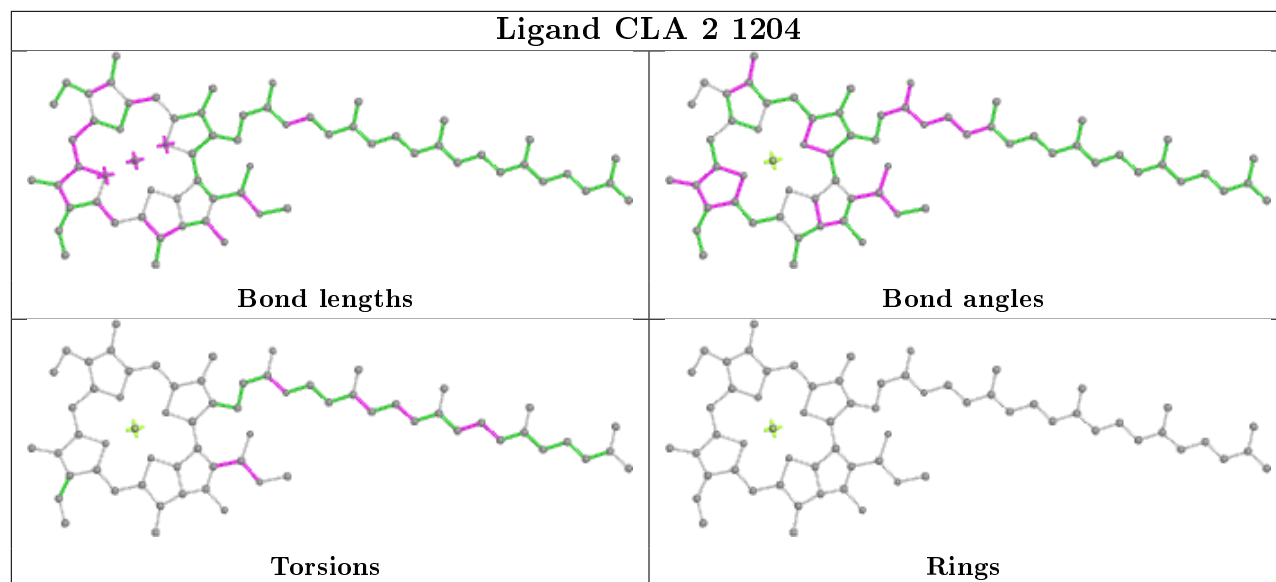






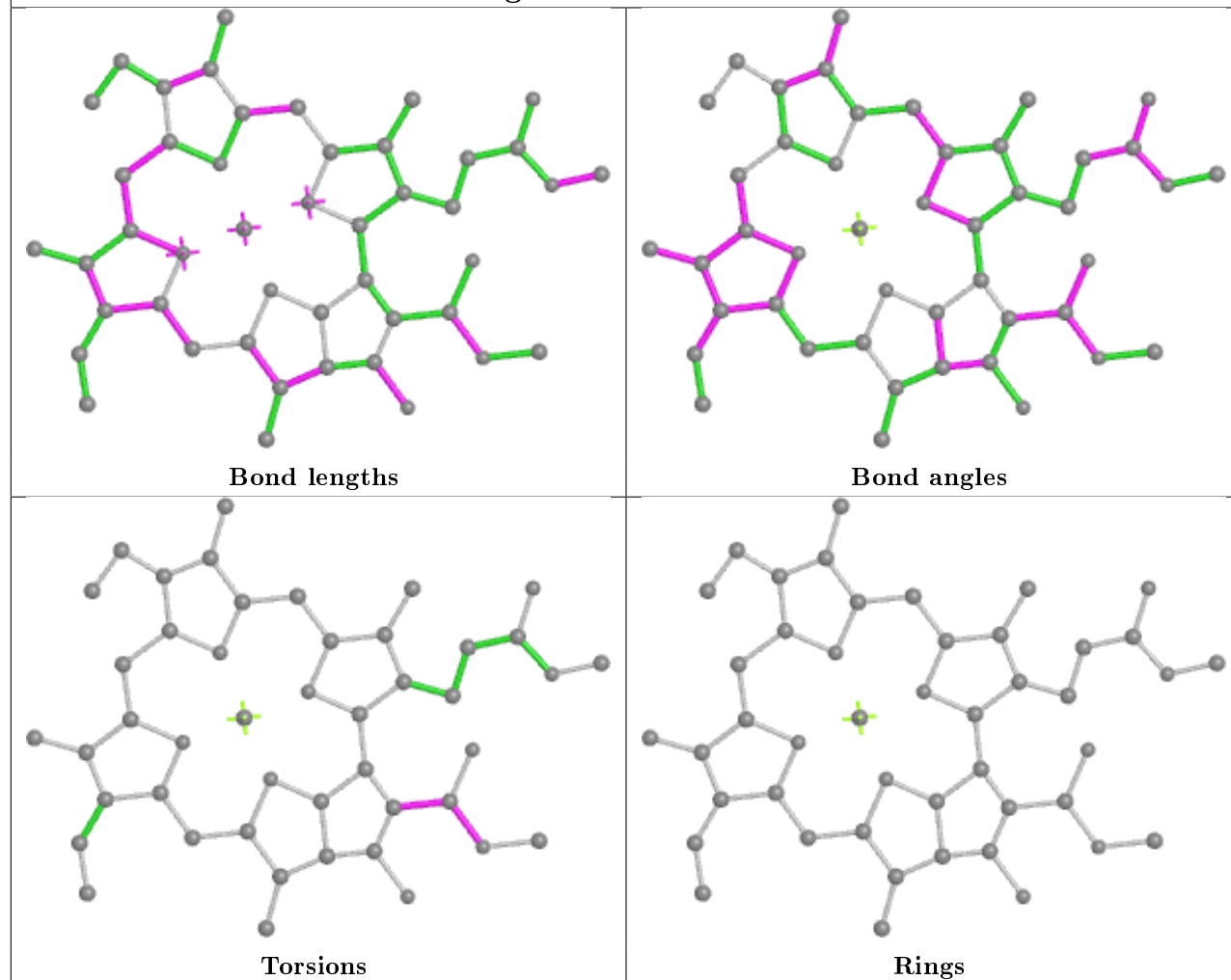




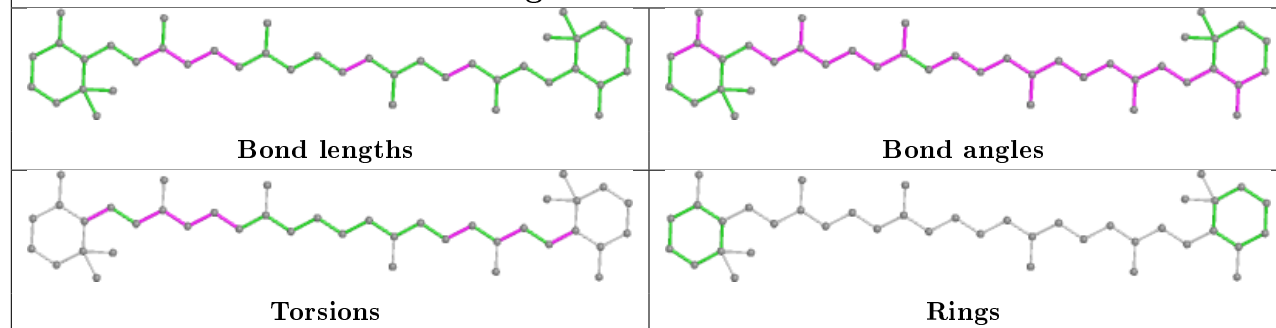




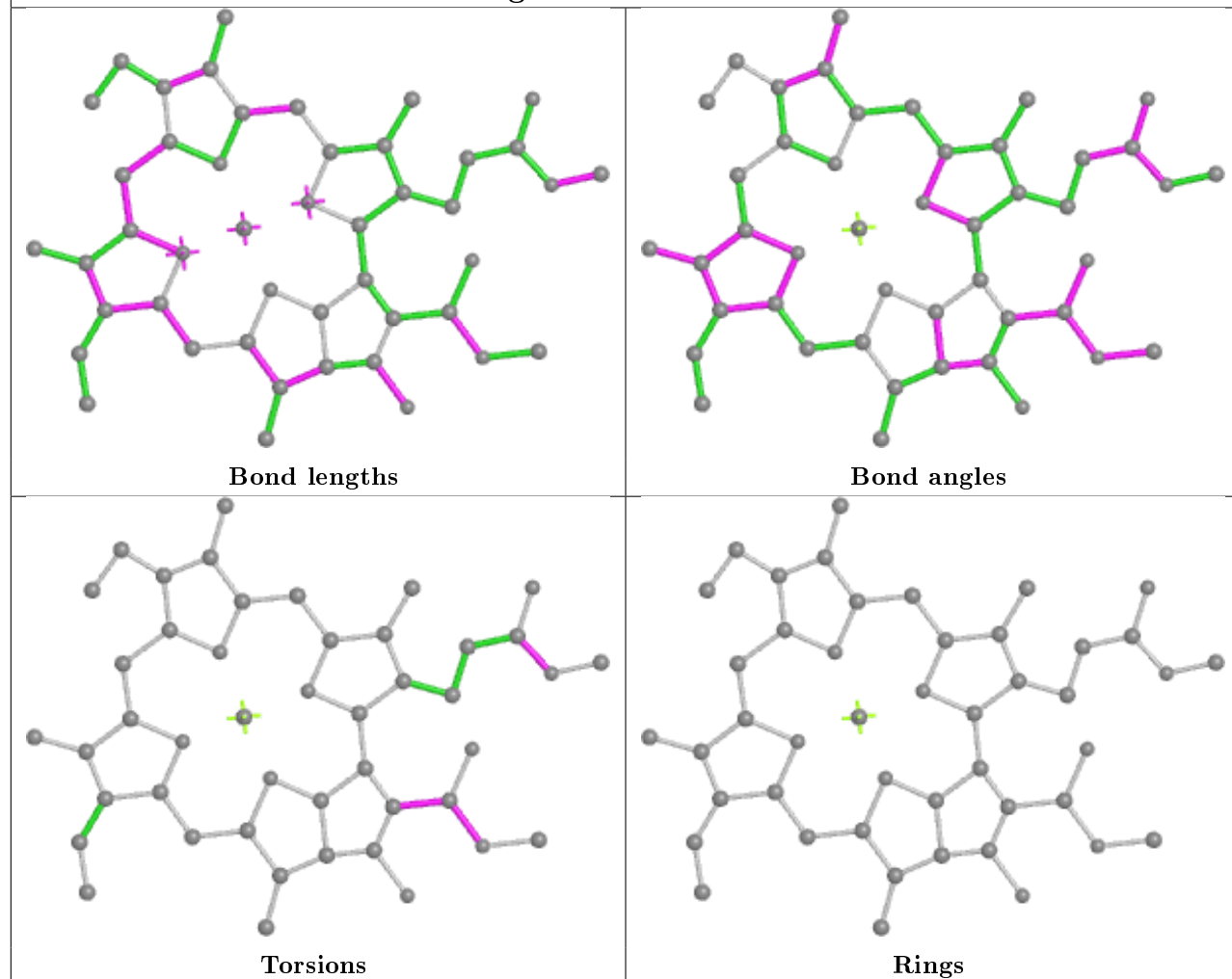
## Ligand CLA A 1133



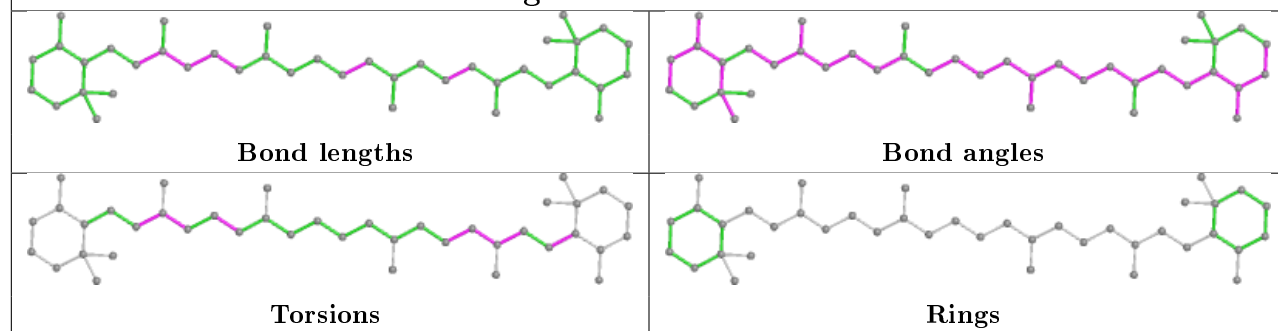
## Ligand BCR 7 4021



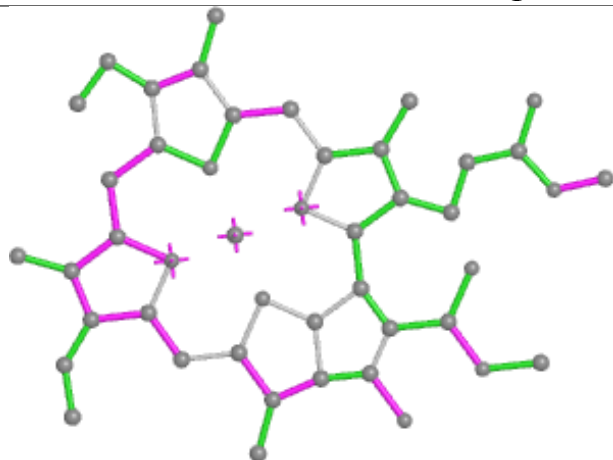
## Ligand CLA 1 1138



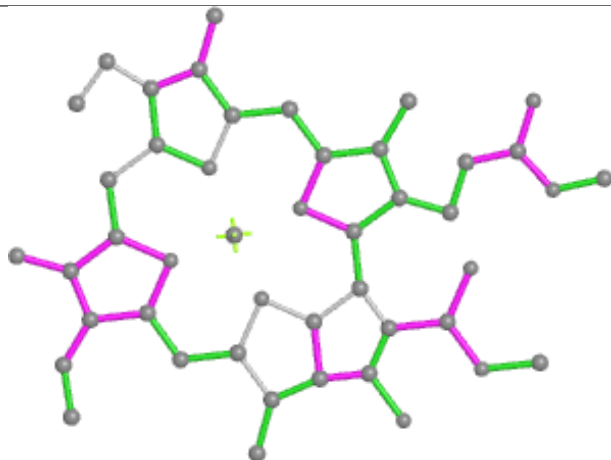
## Ligand BCR F 4020



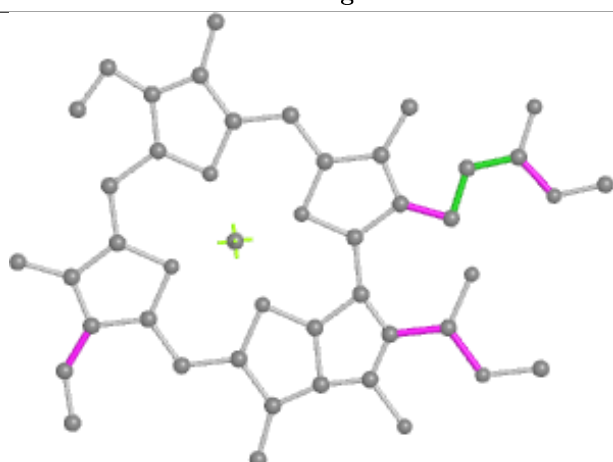
## Ligand CLA b 1220



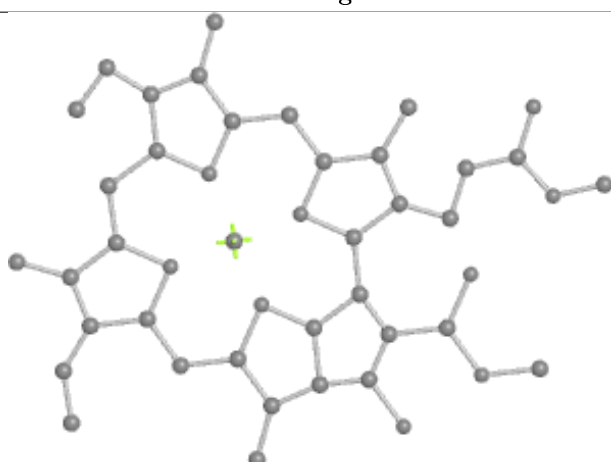
Bond lengths



Bond angles

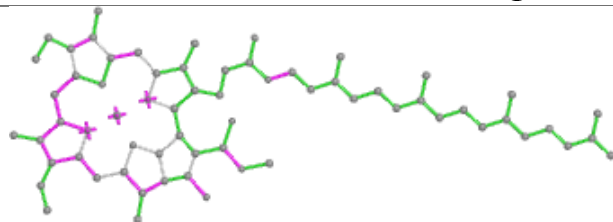


Torsions

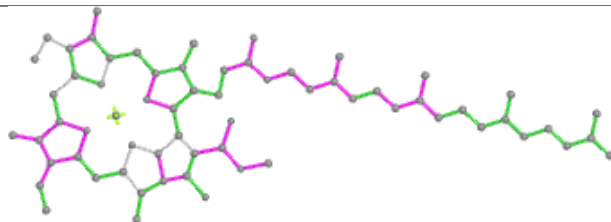


Rings

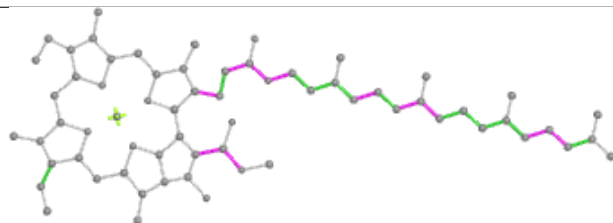
## Ligand CLA b 1216



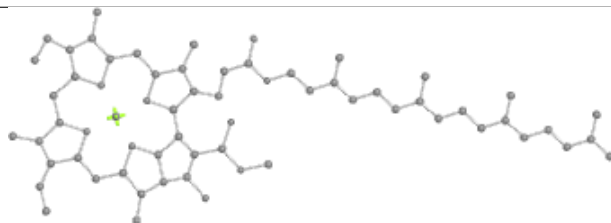
Bond lengths



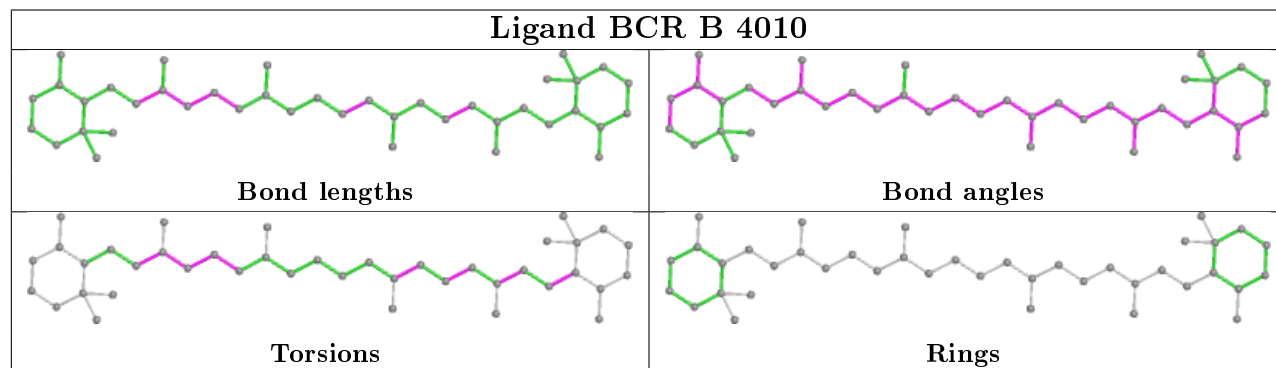
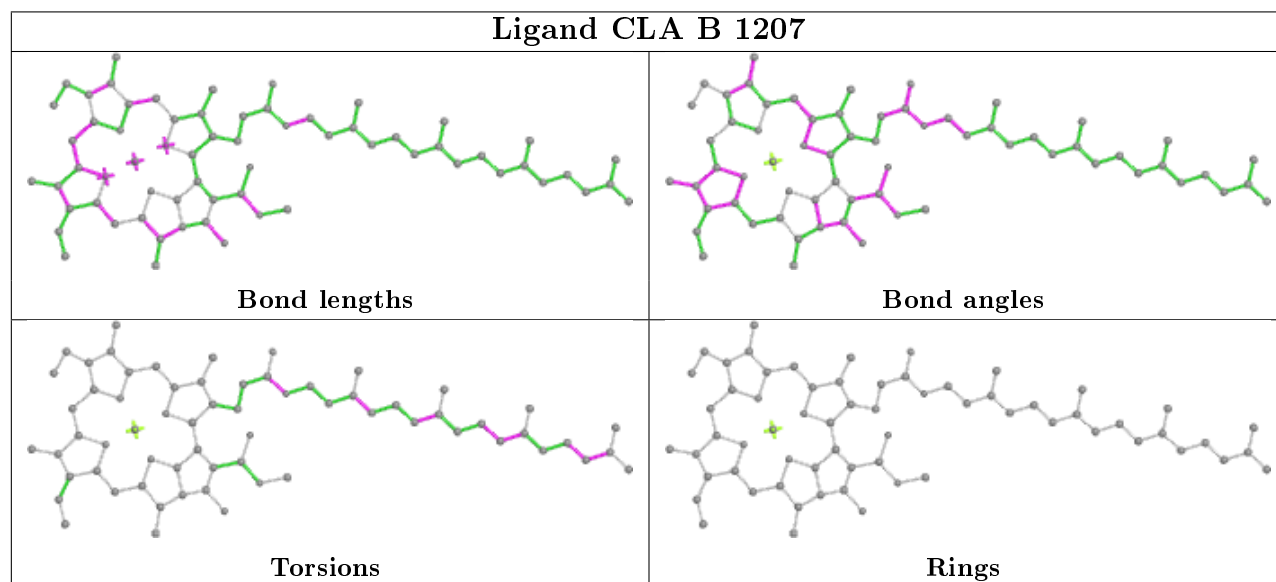
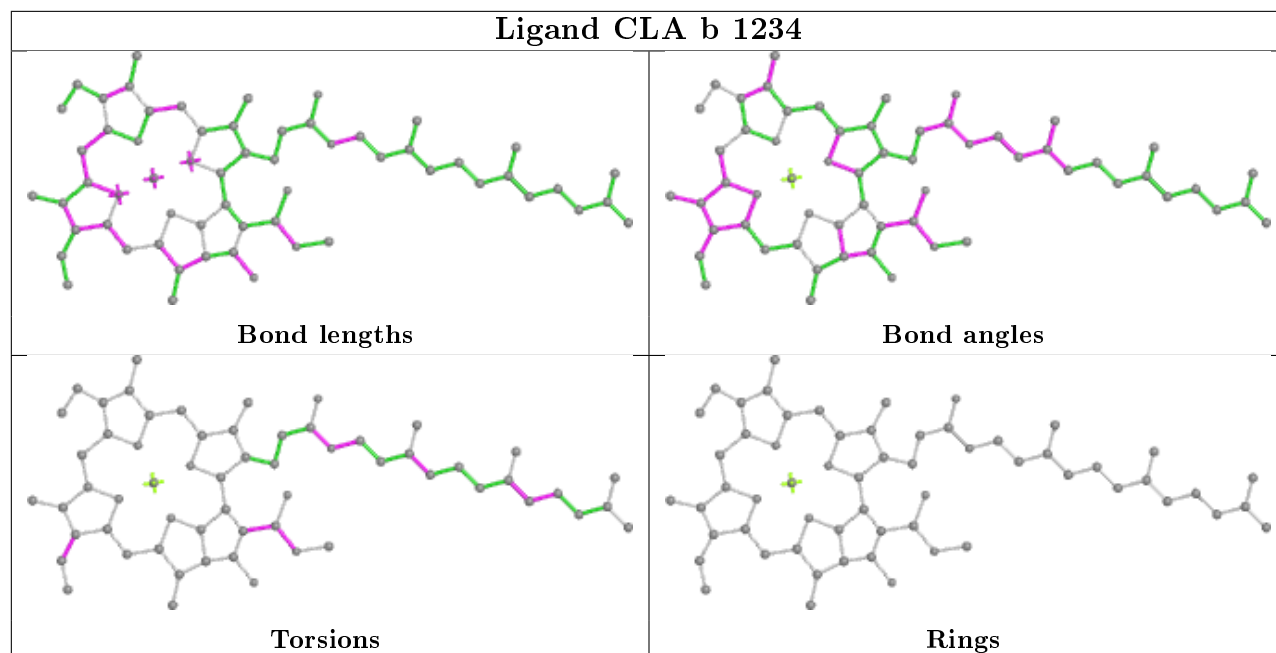
Bond angles

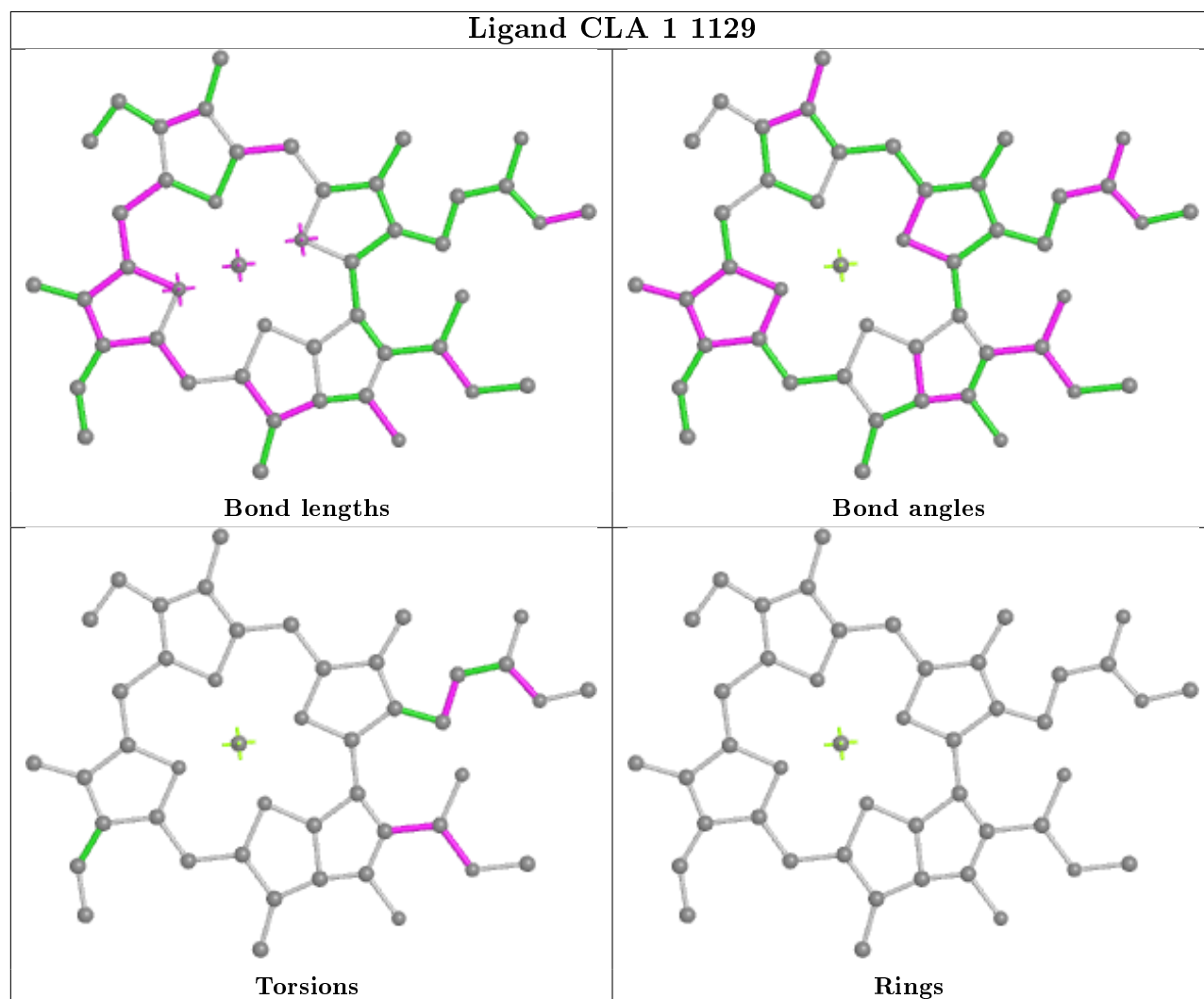
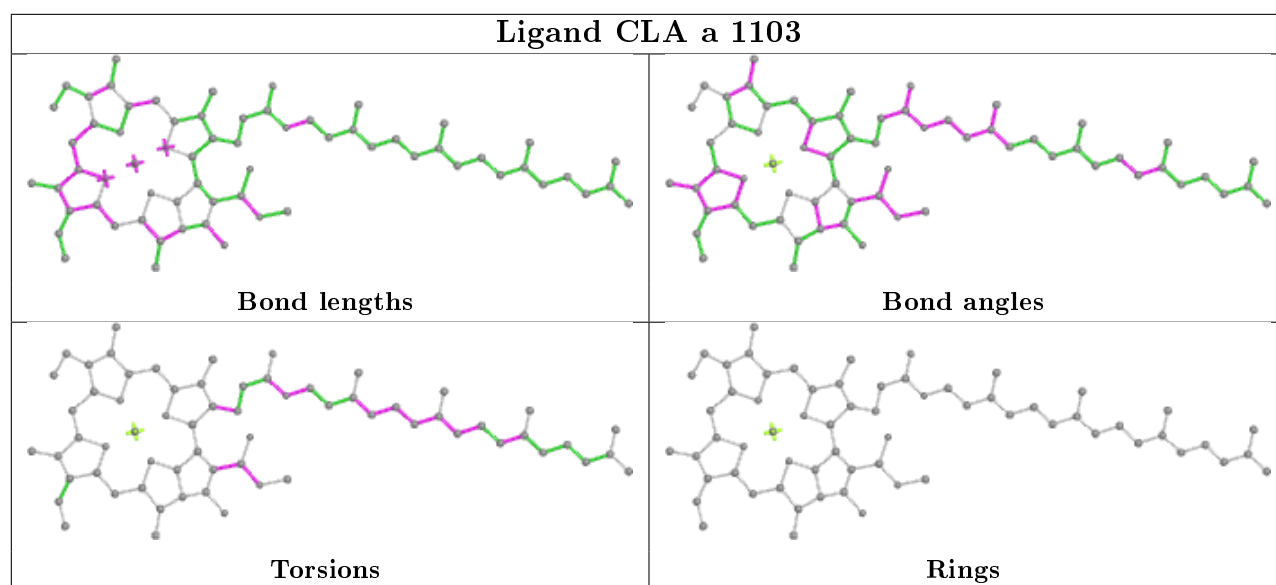


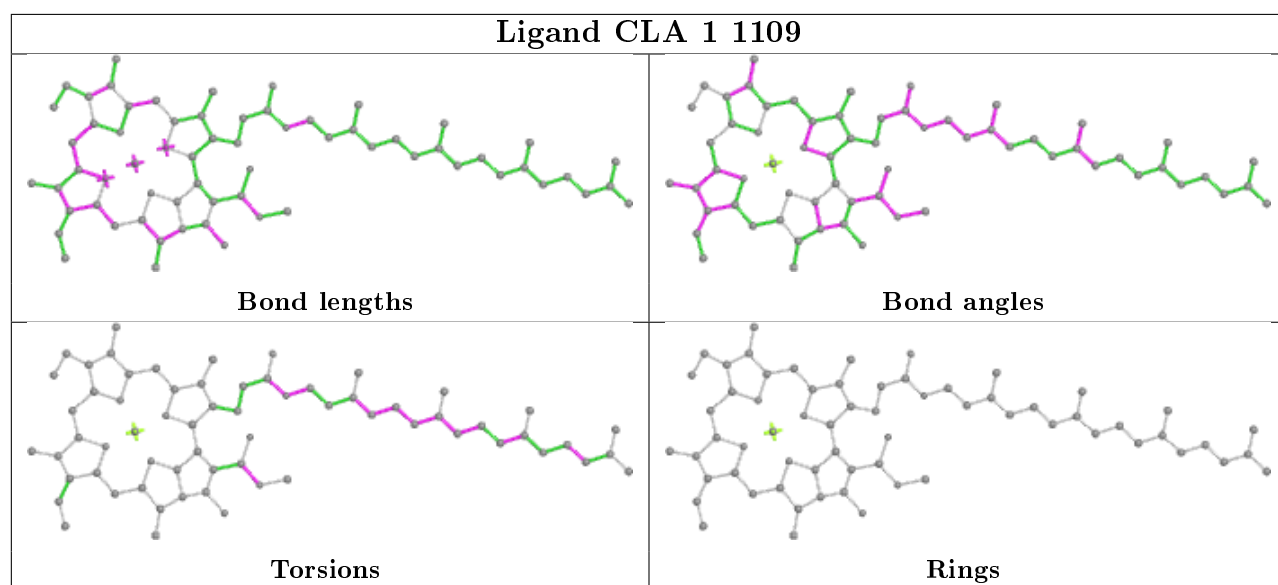
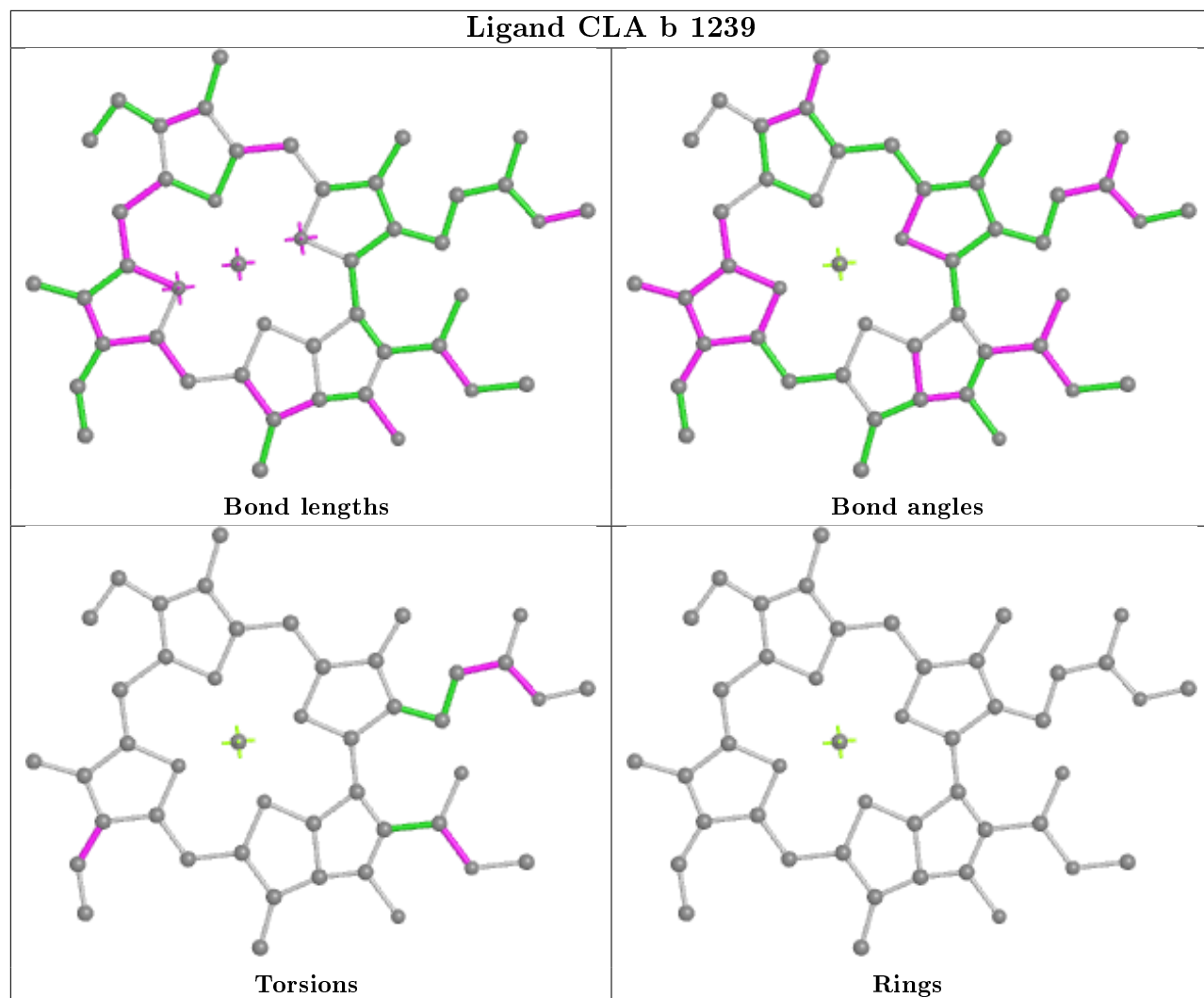
Torsions

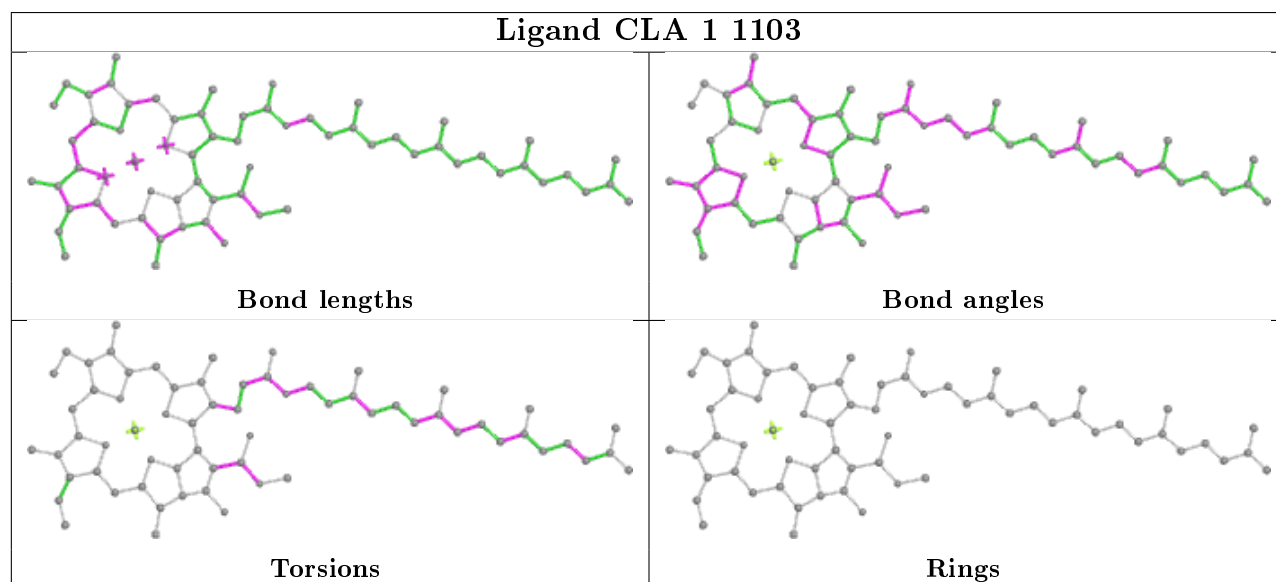
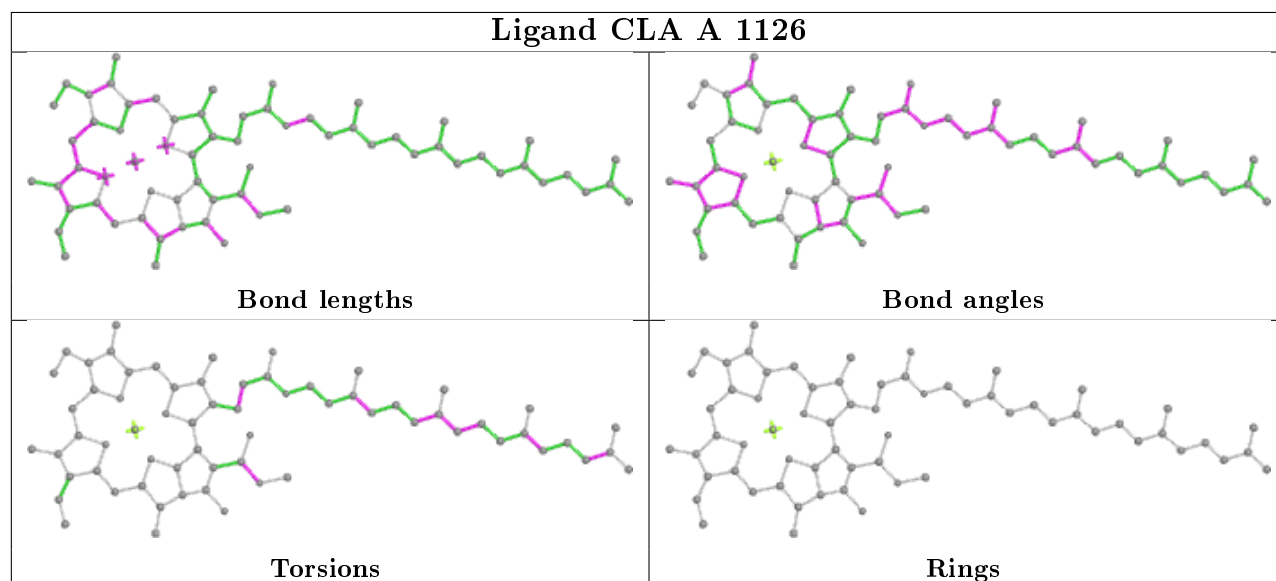
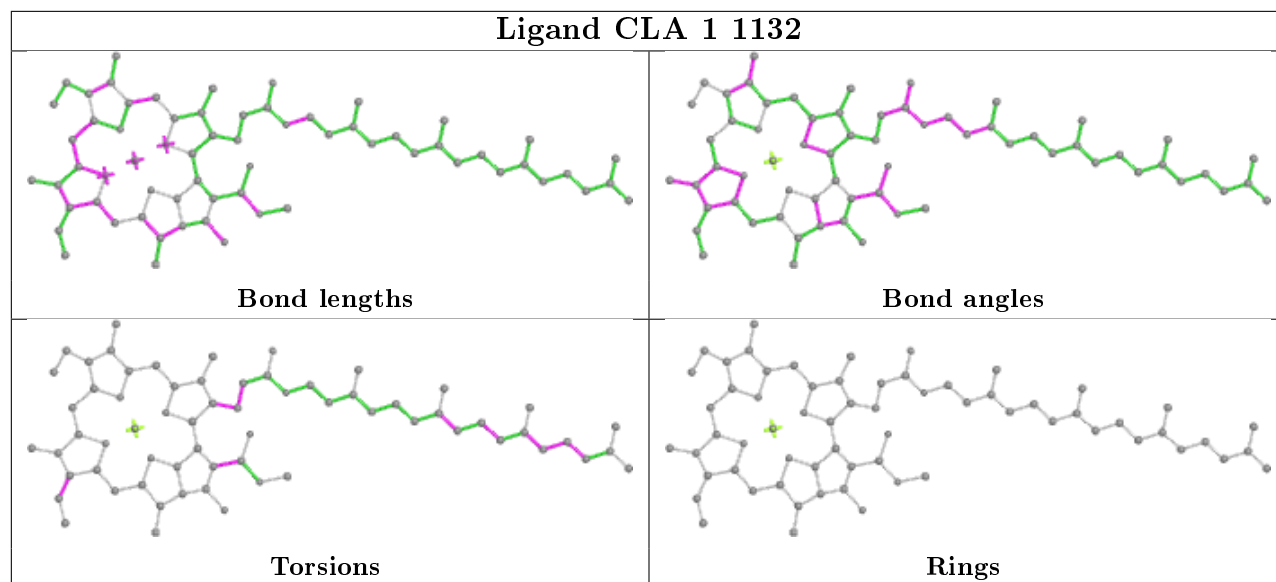


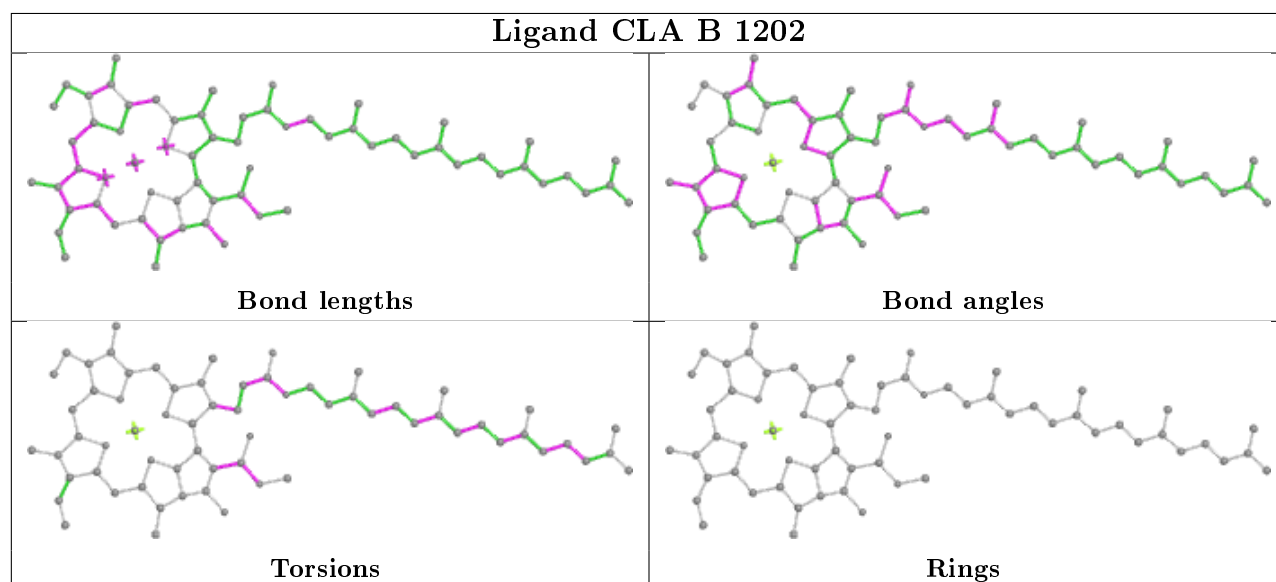
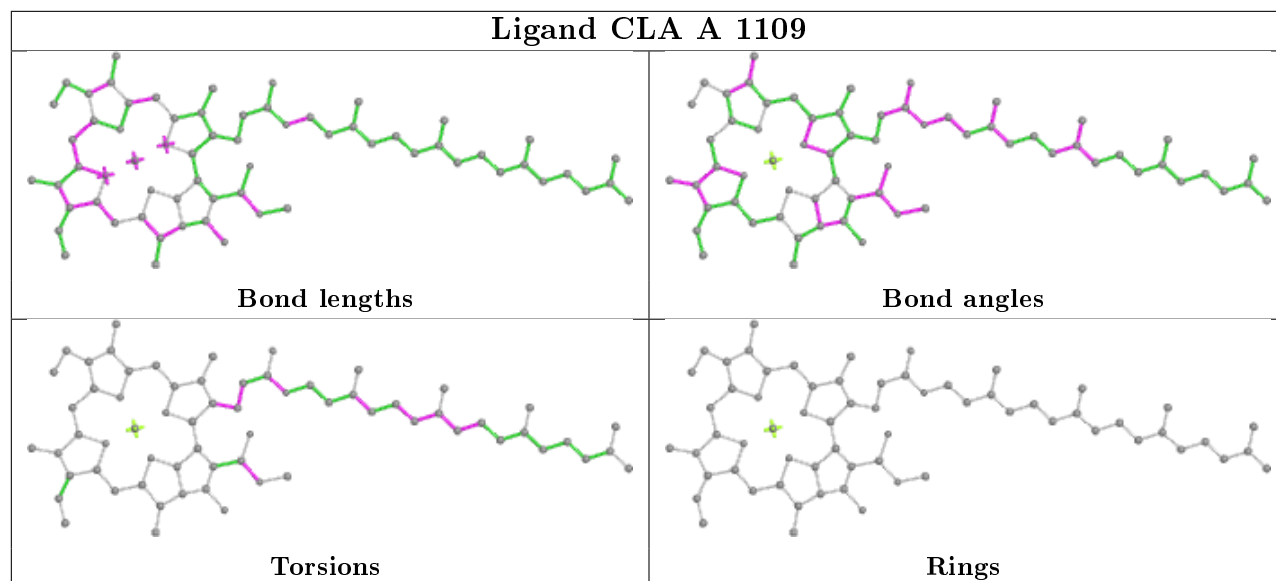
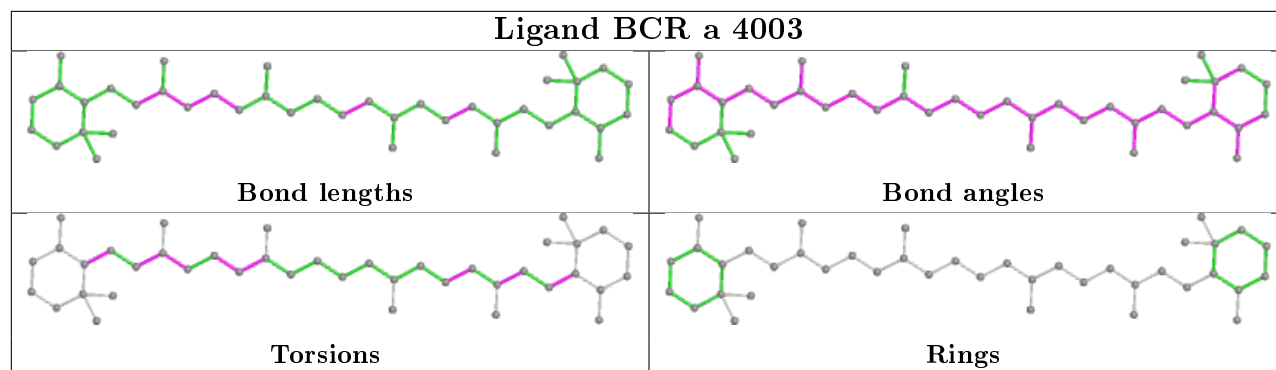
Rings



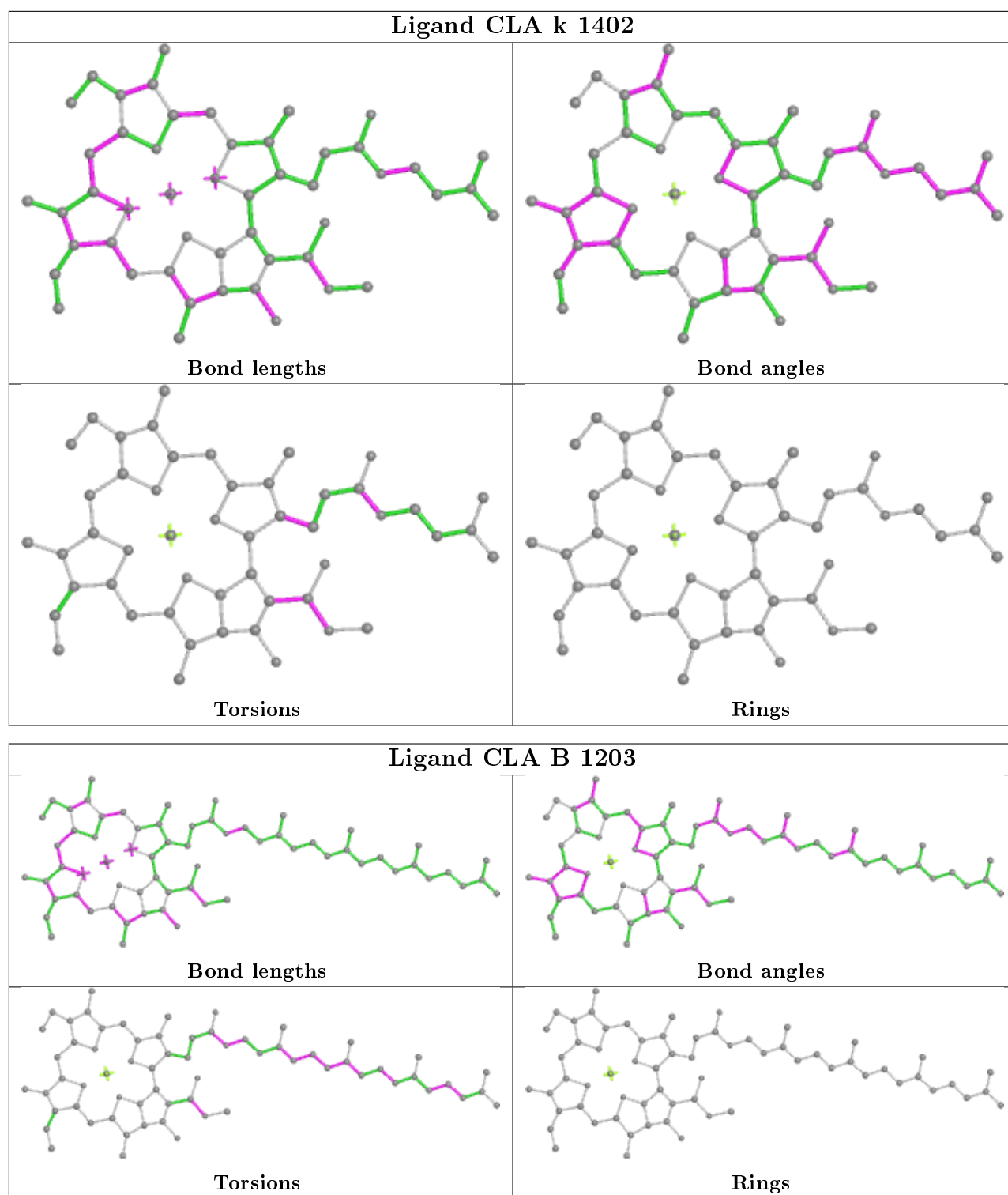


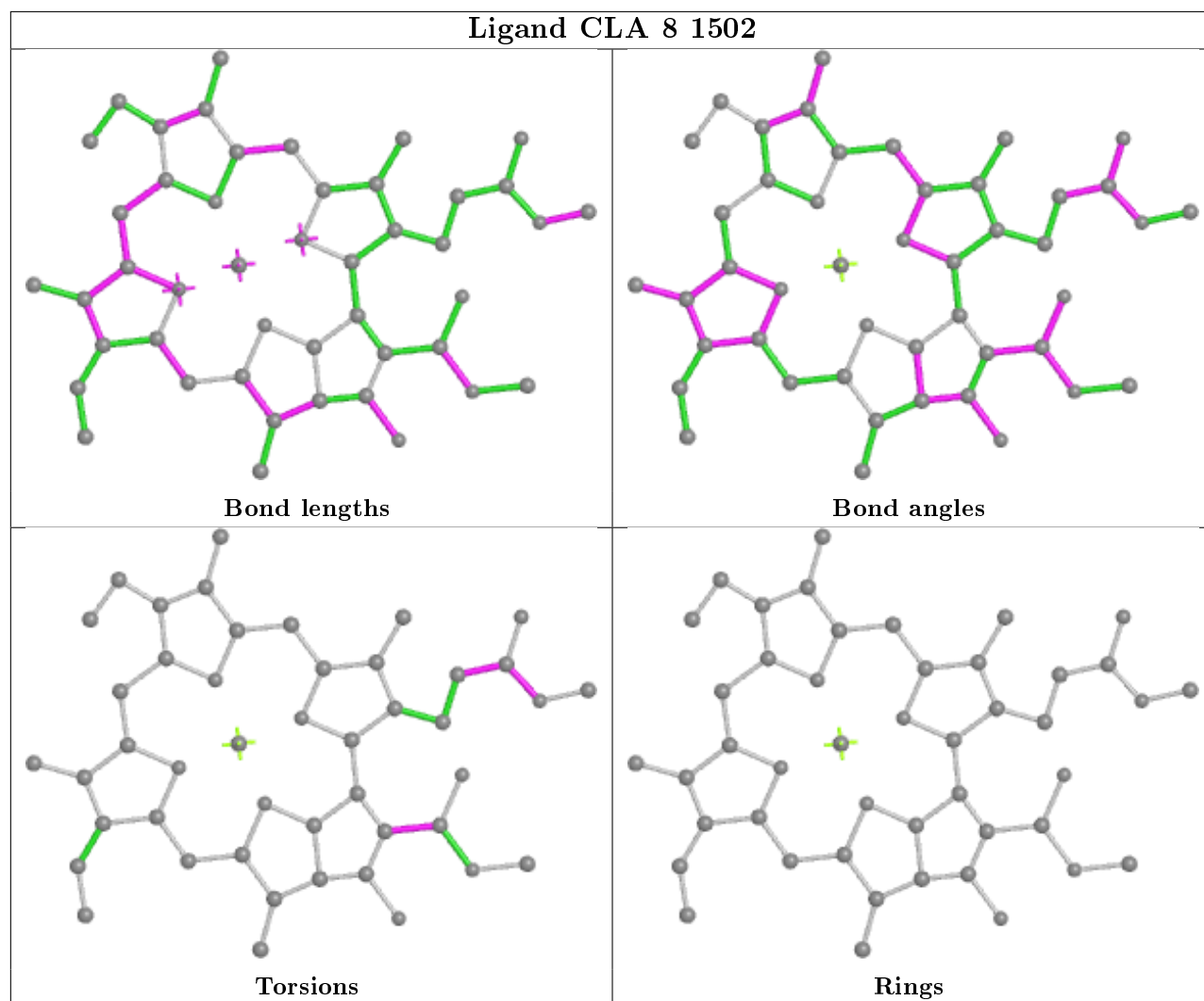
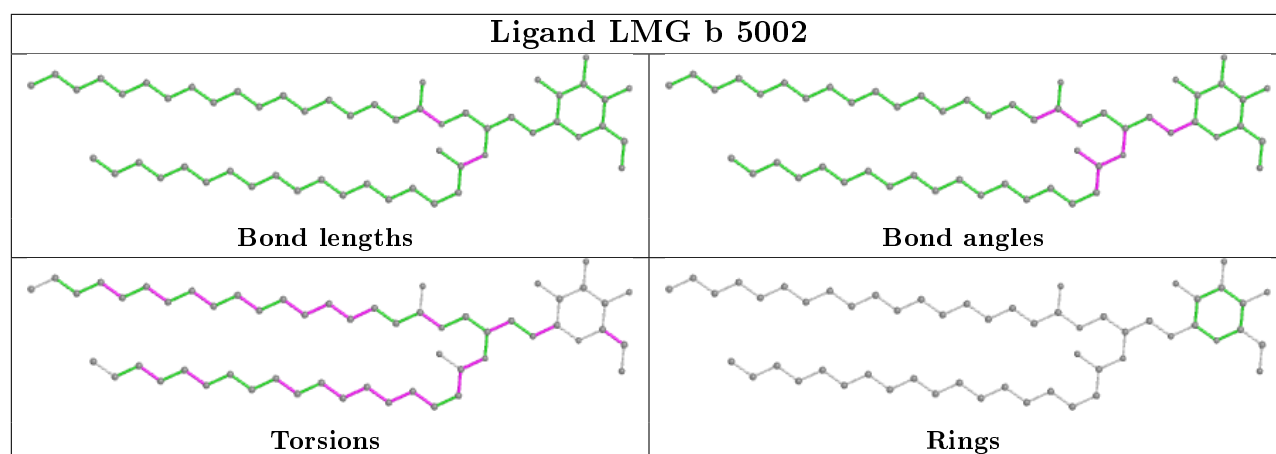




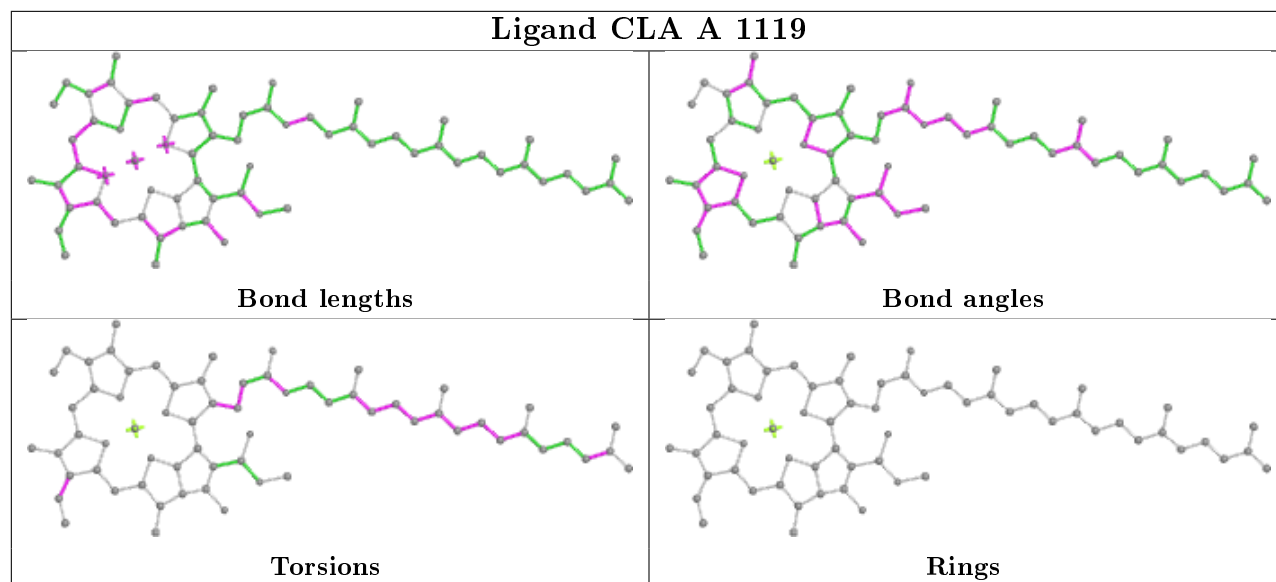




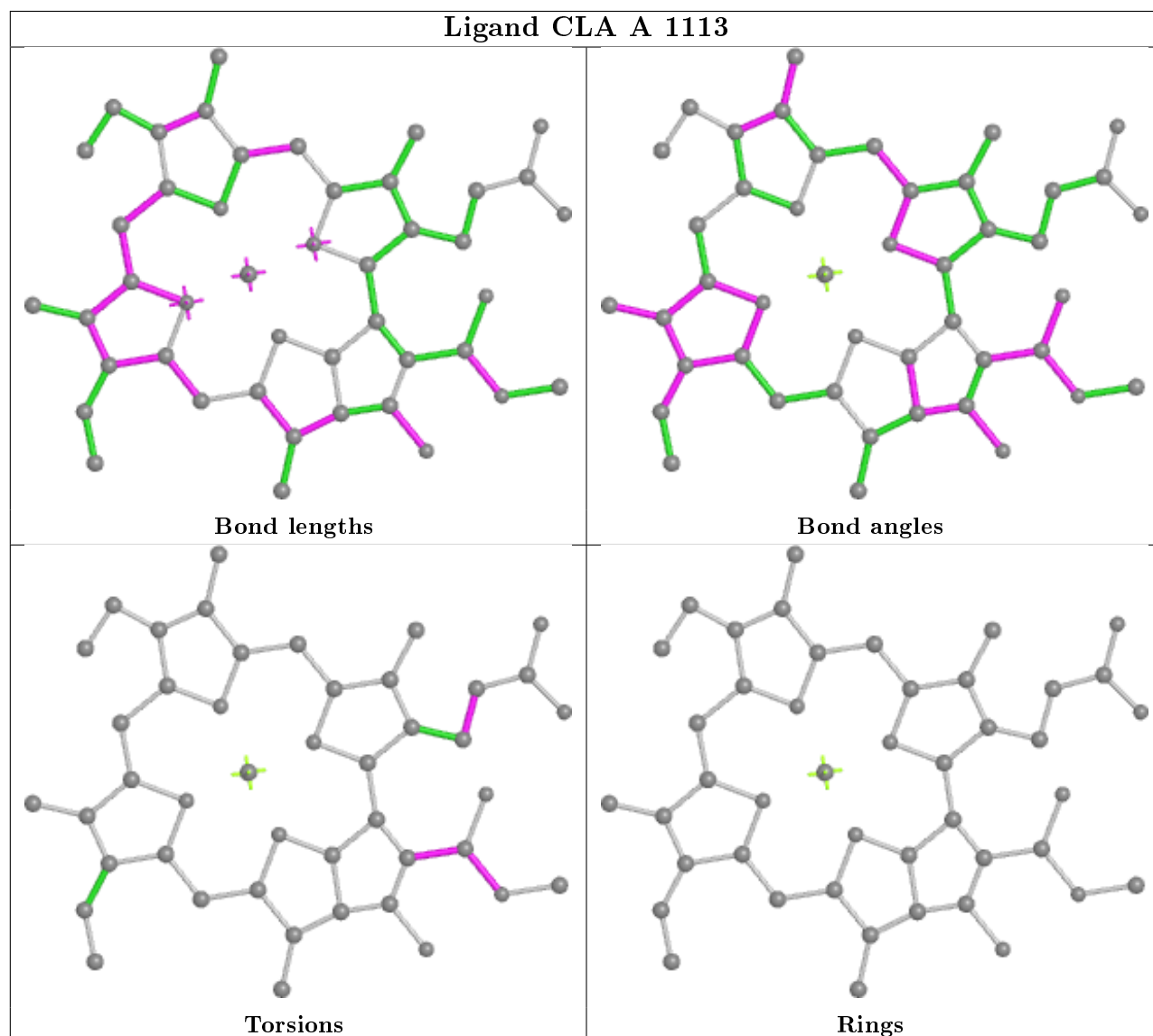


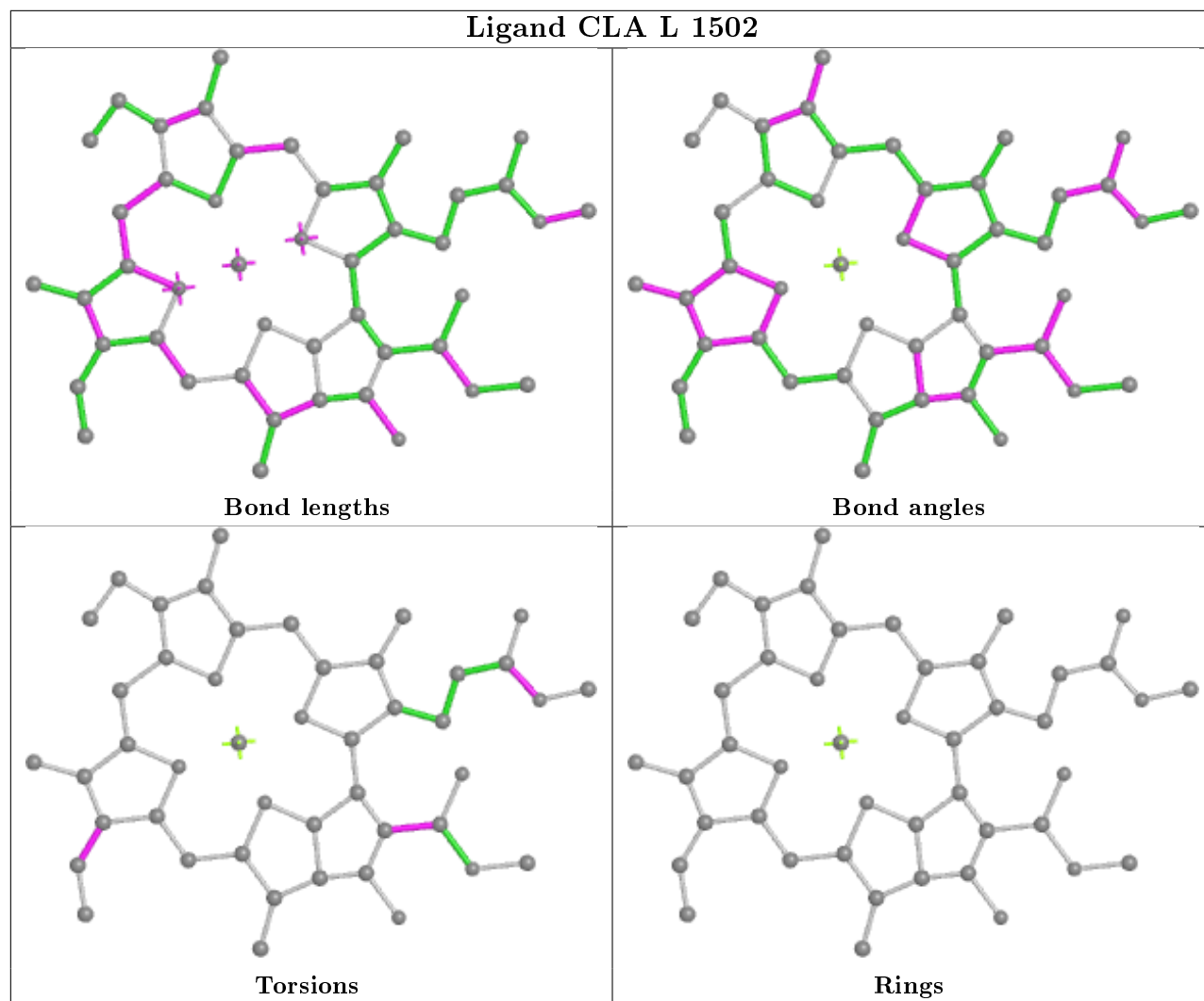
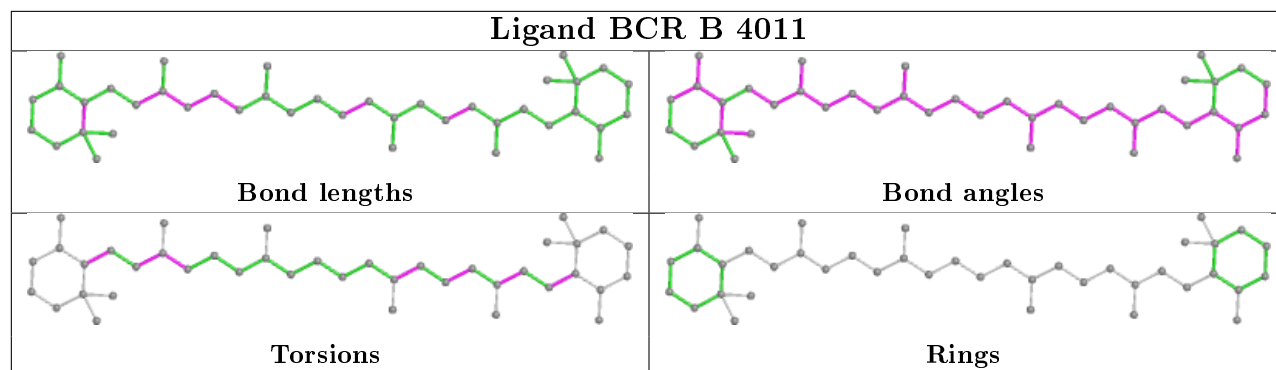


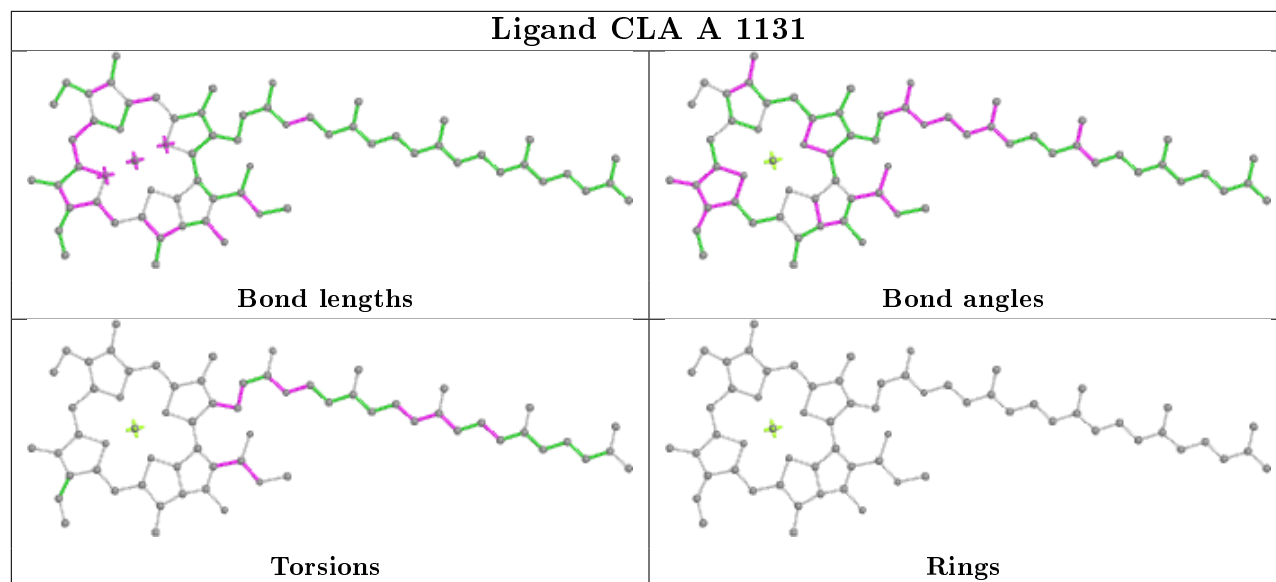
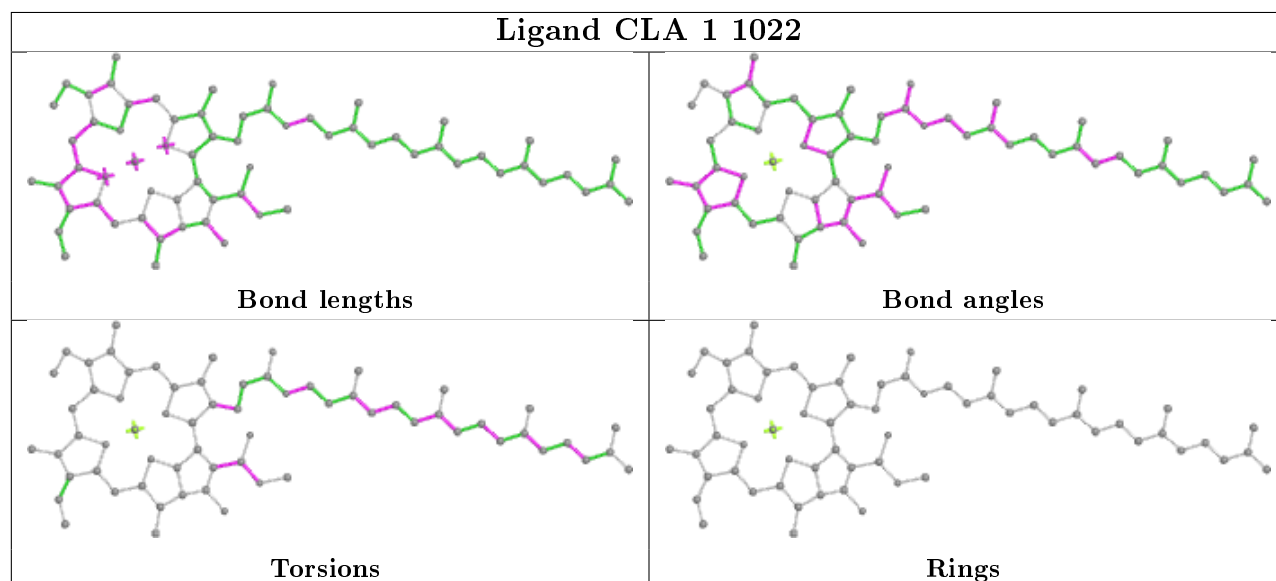
## Ligand CLA A 1119

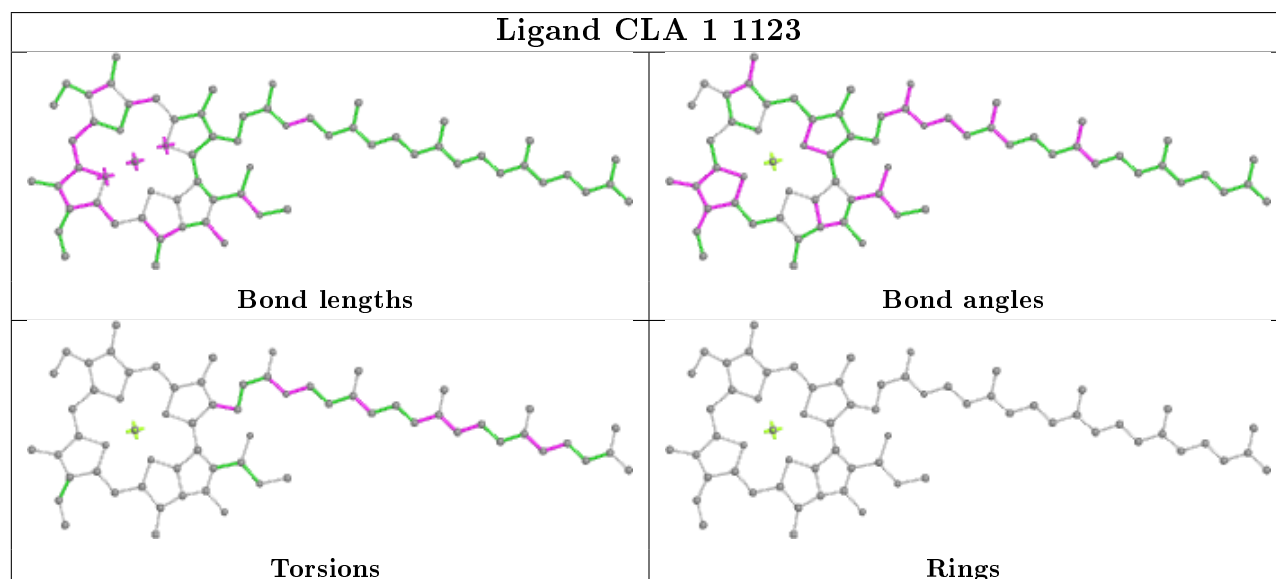
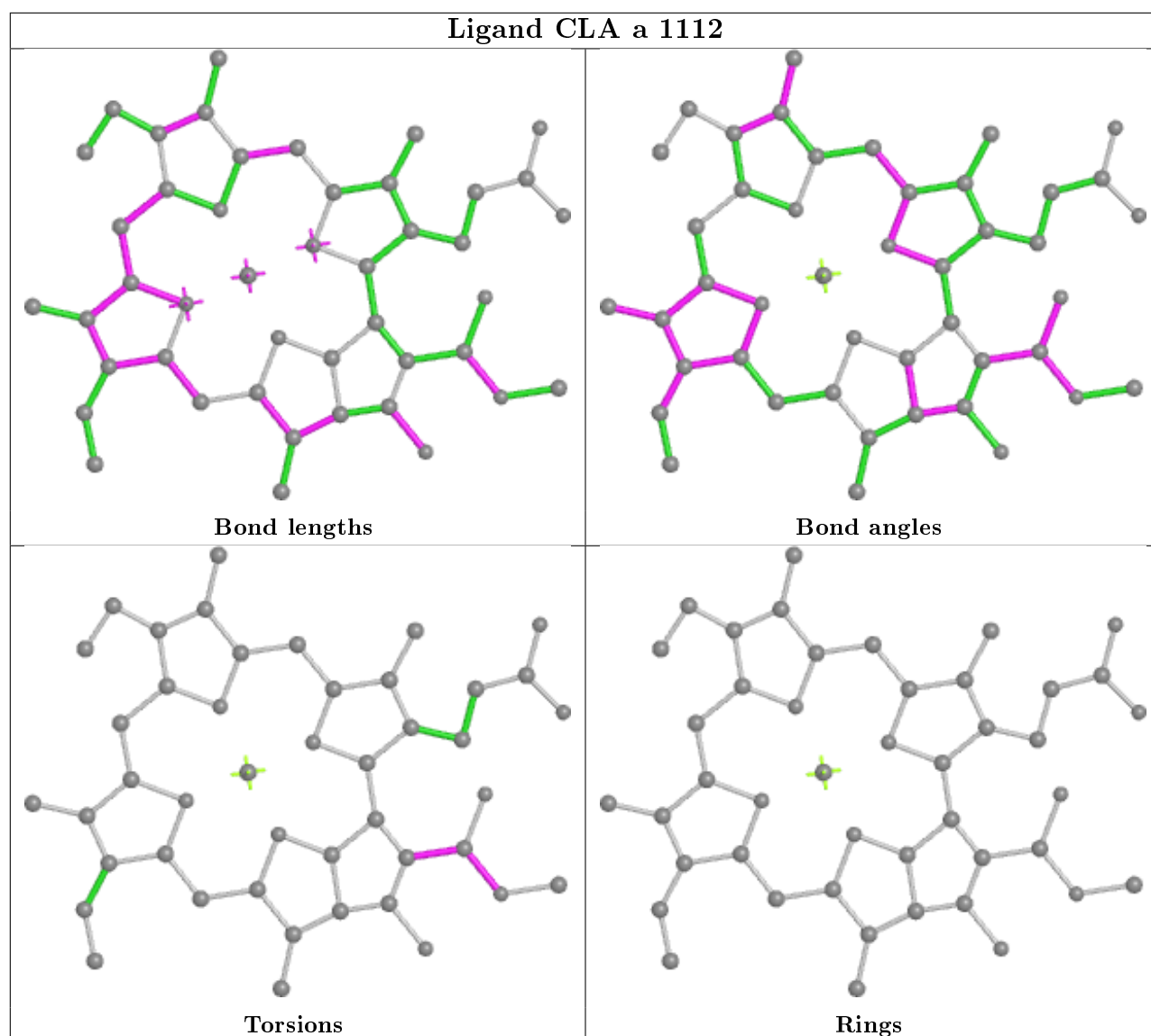


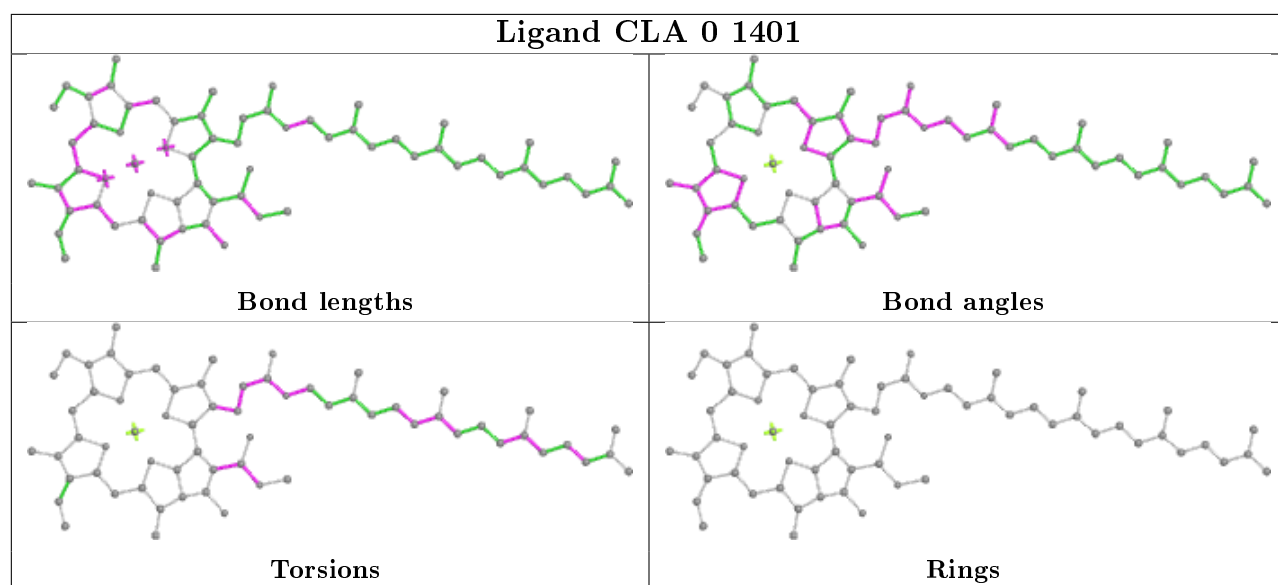
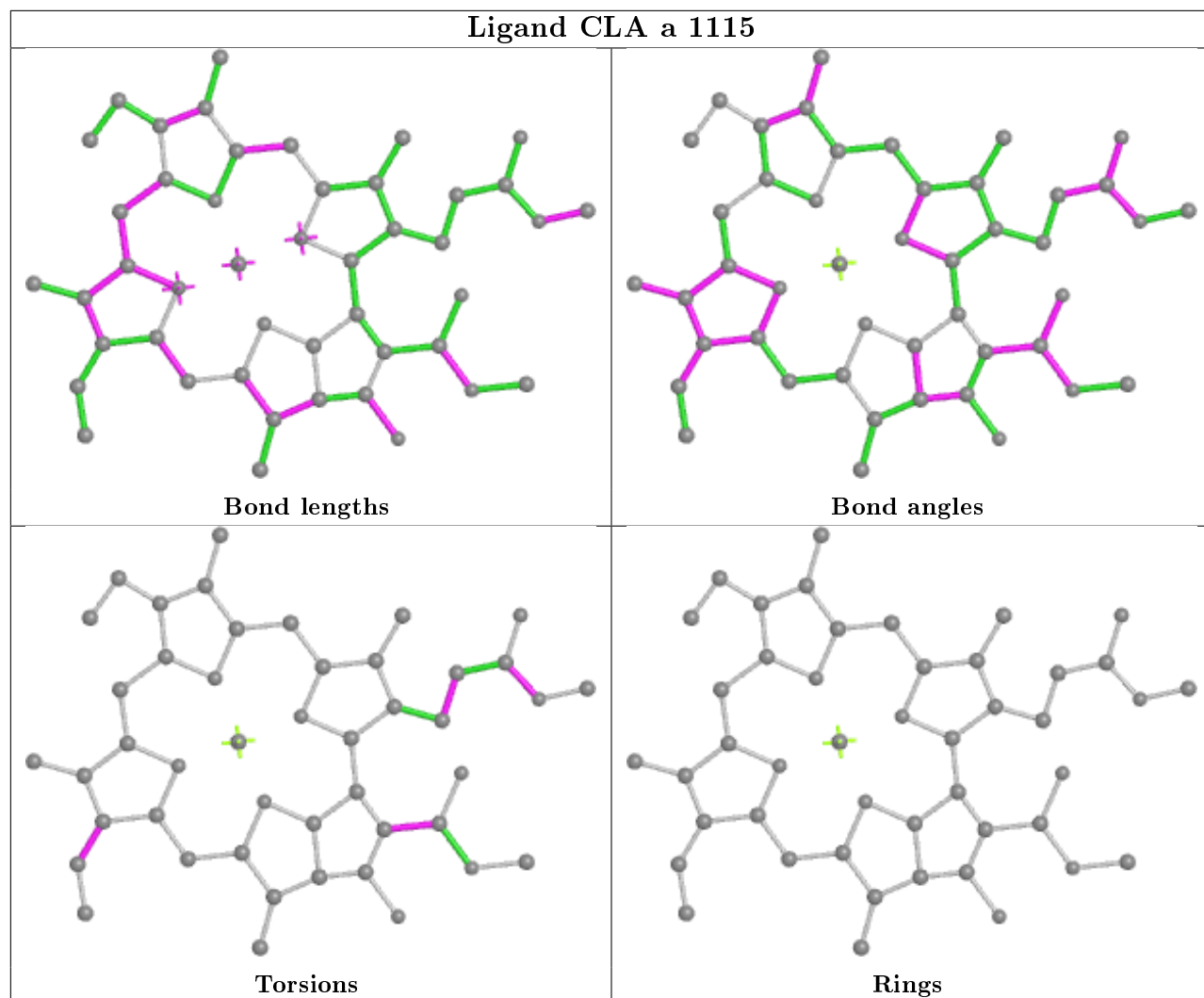
## Ligand CLA A 1113

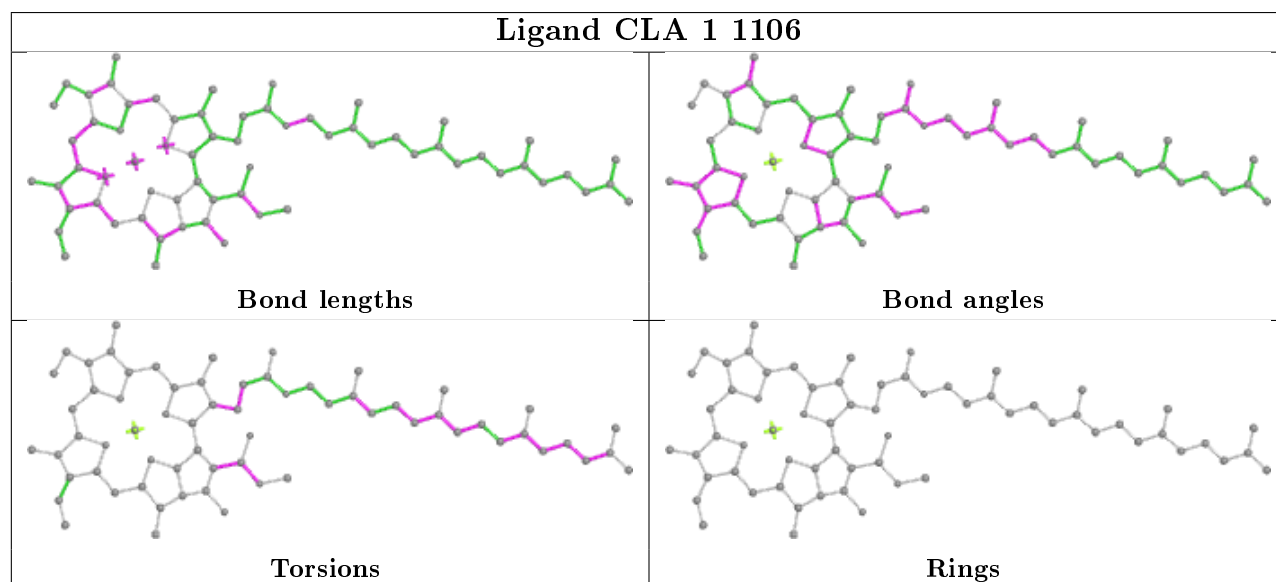
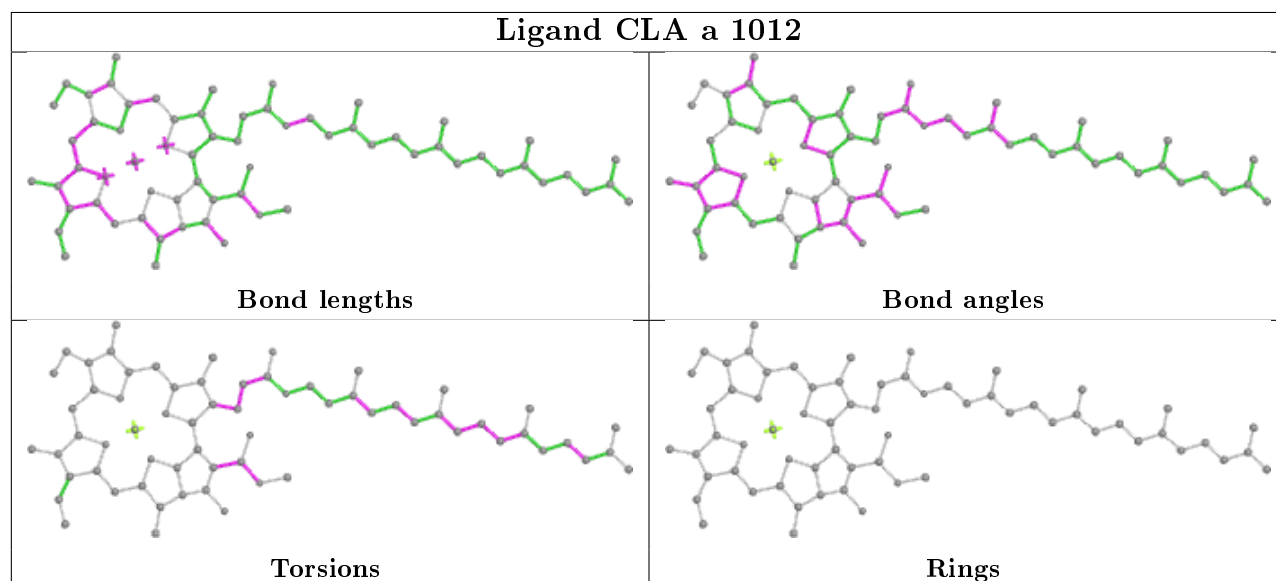
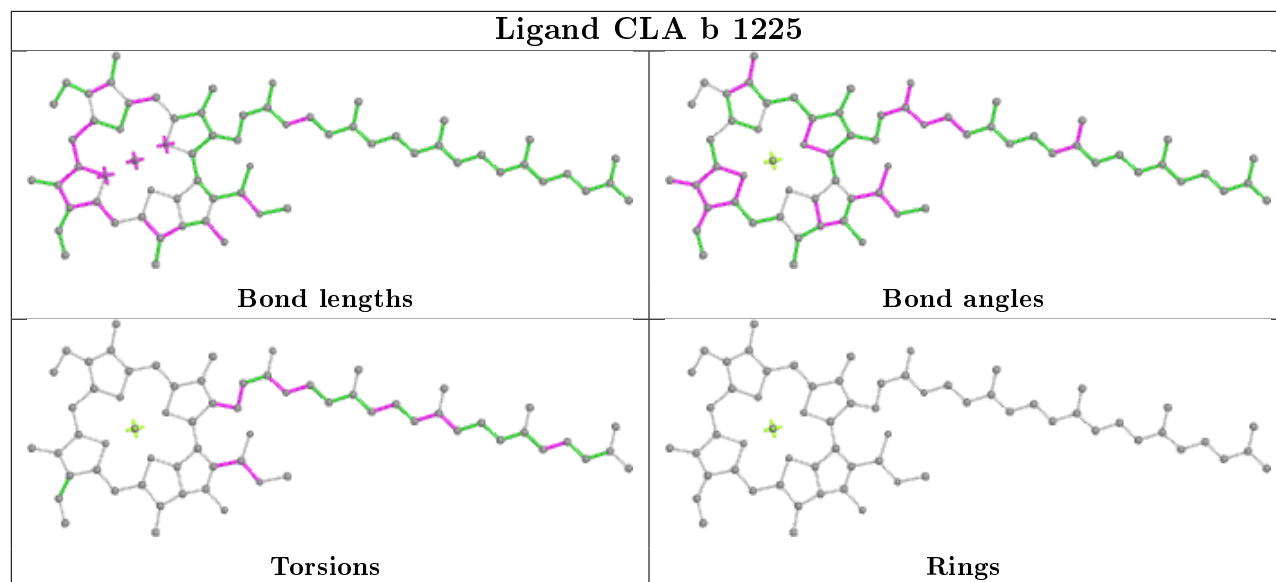




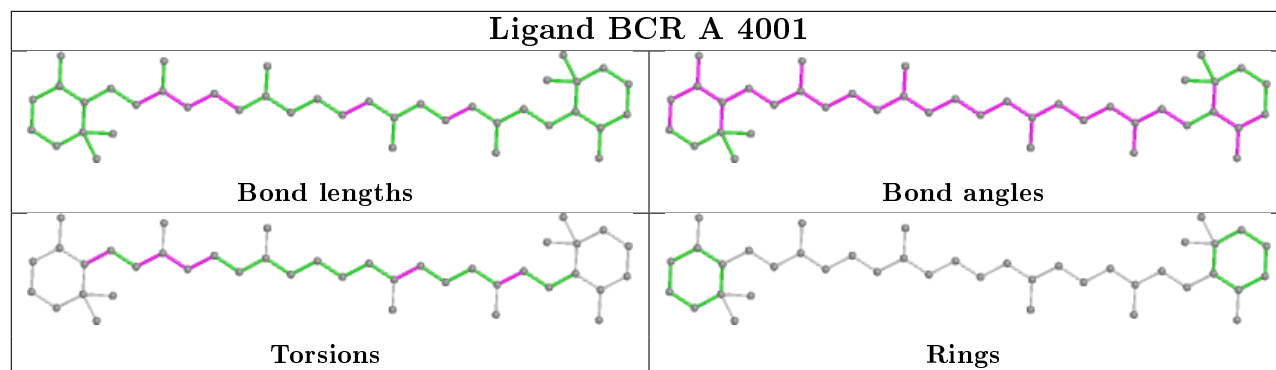
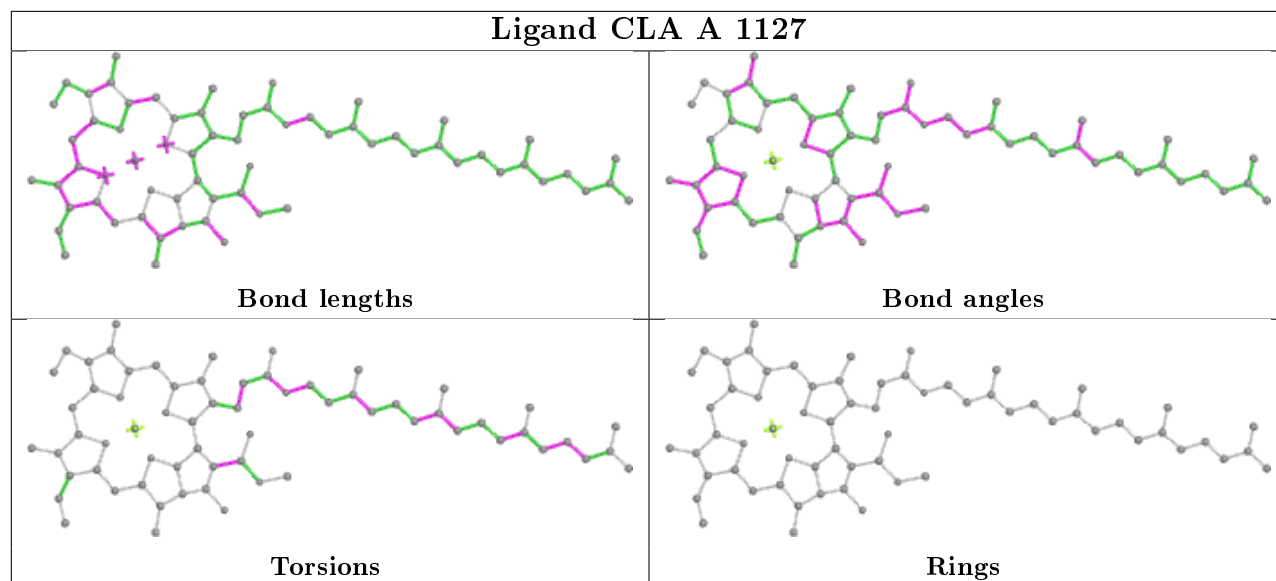
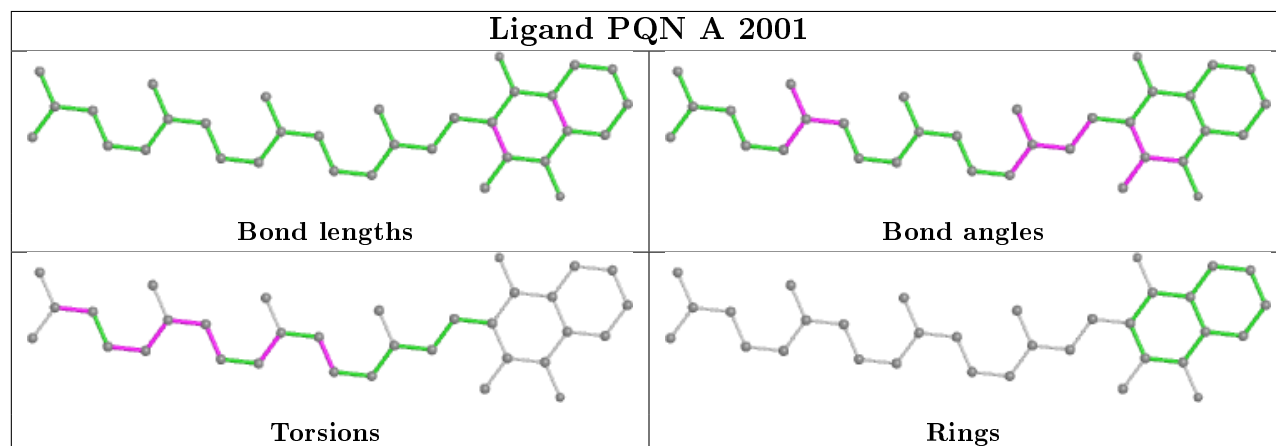
**Ligand CLA A 1131****Ligand CLA 1 1022**



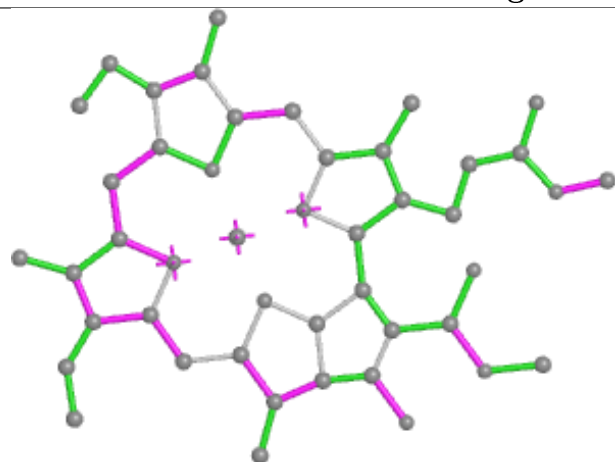




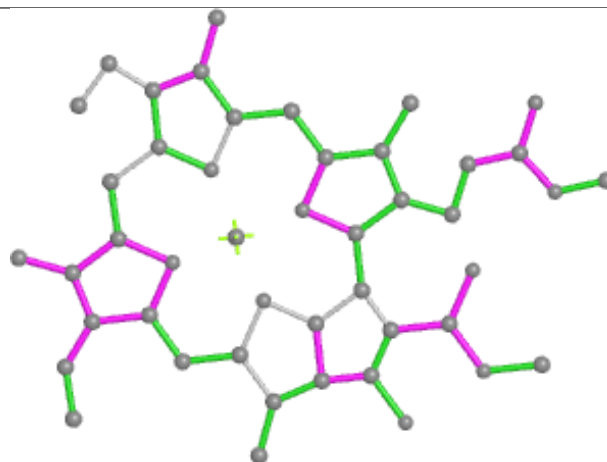


**Ligand BCR A 4001****Ligand CLA A 1127****Ligand PQN A 2001**

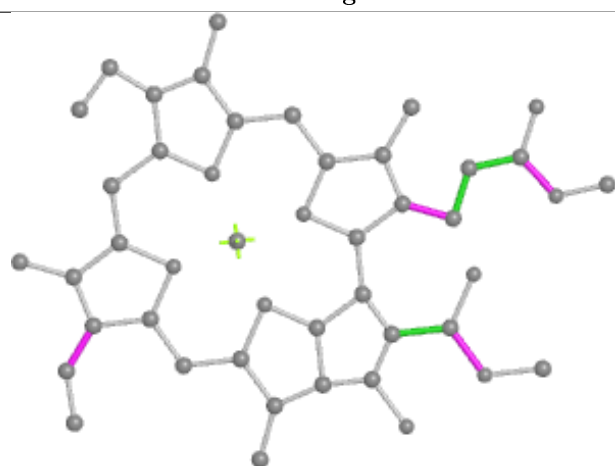
## Ligand CLA A 1114



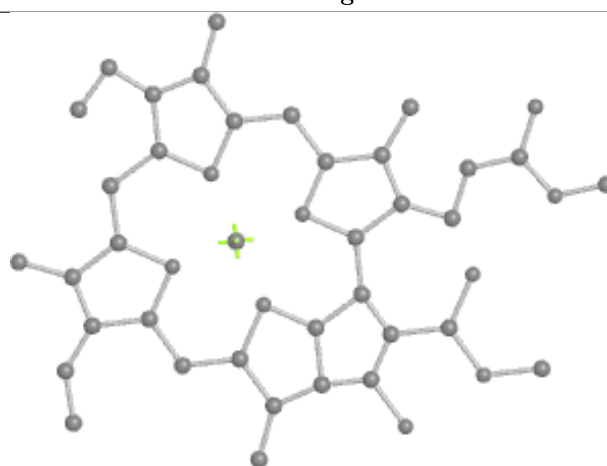
Bond lengths



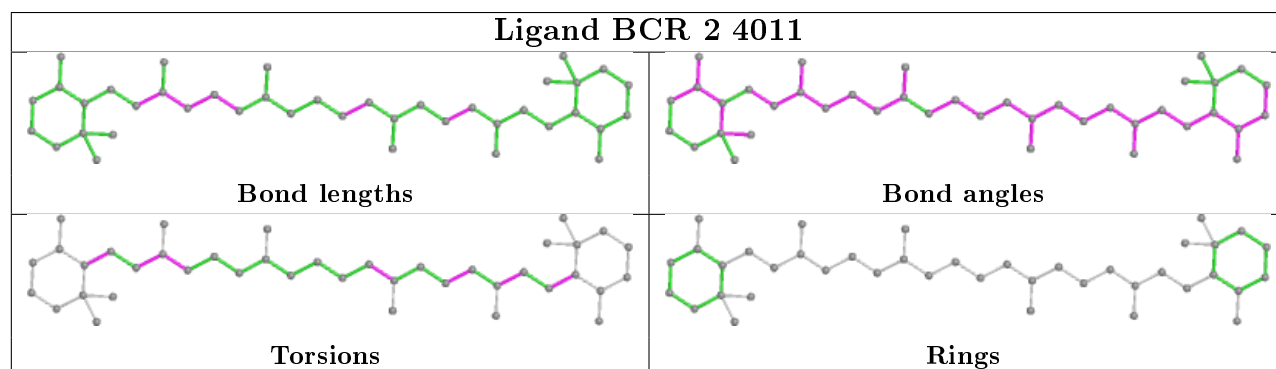
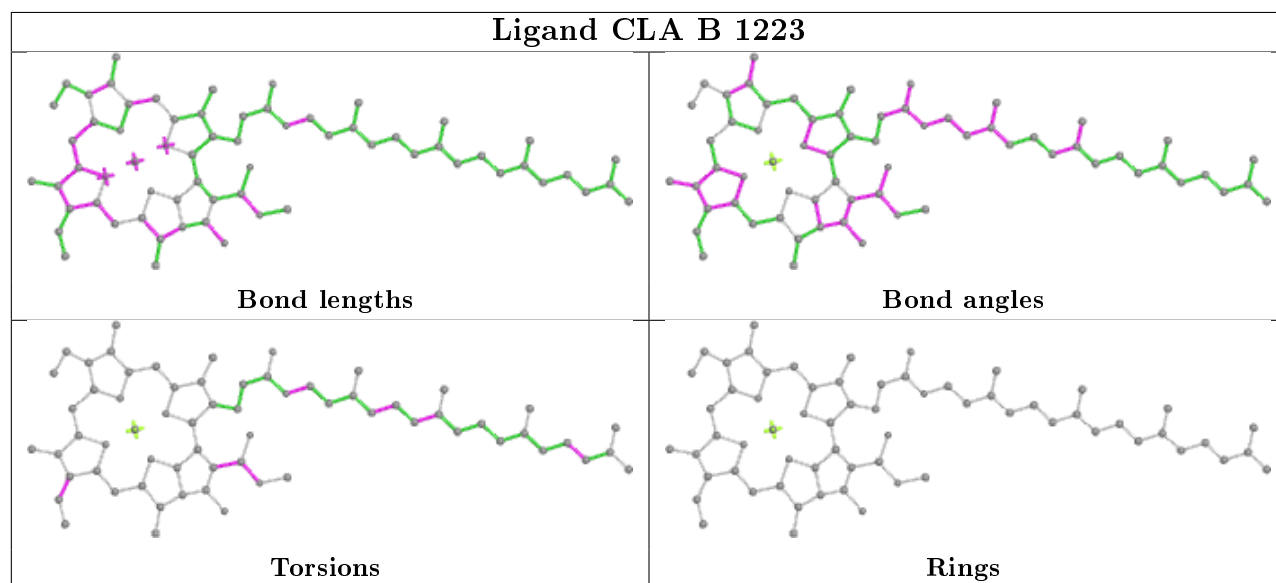
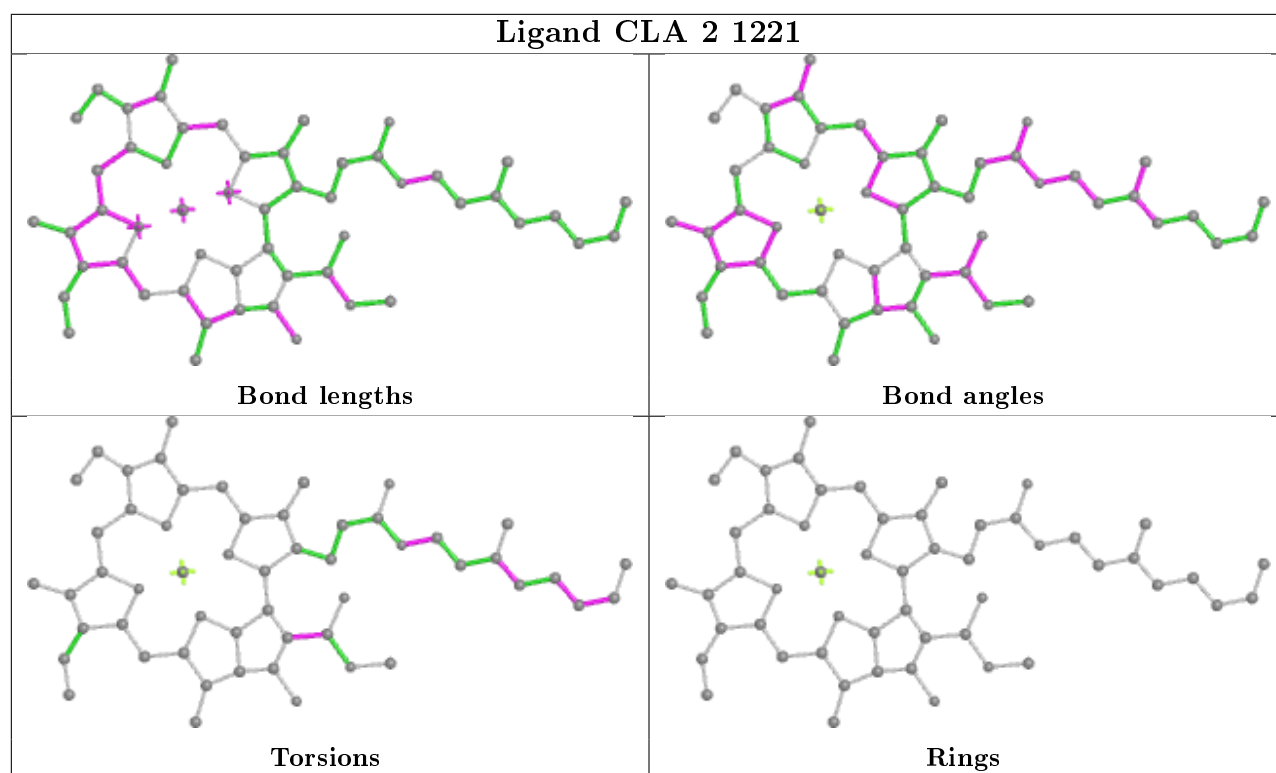
Bond angles

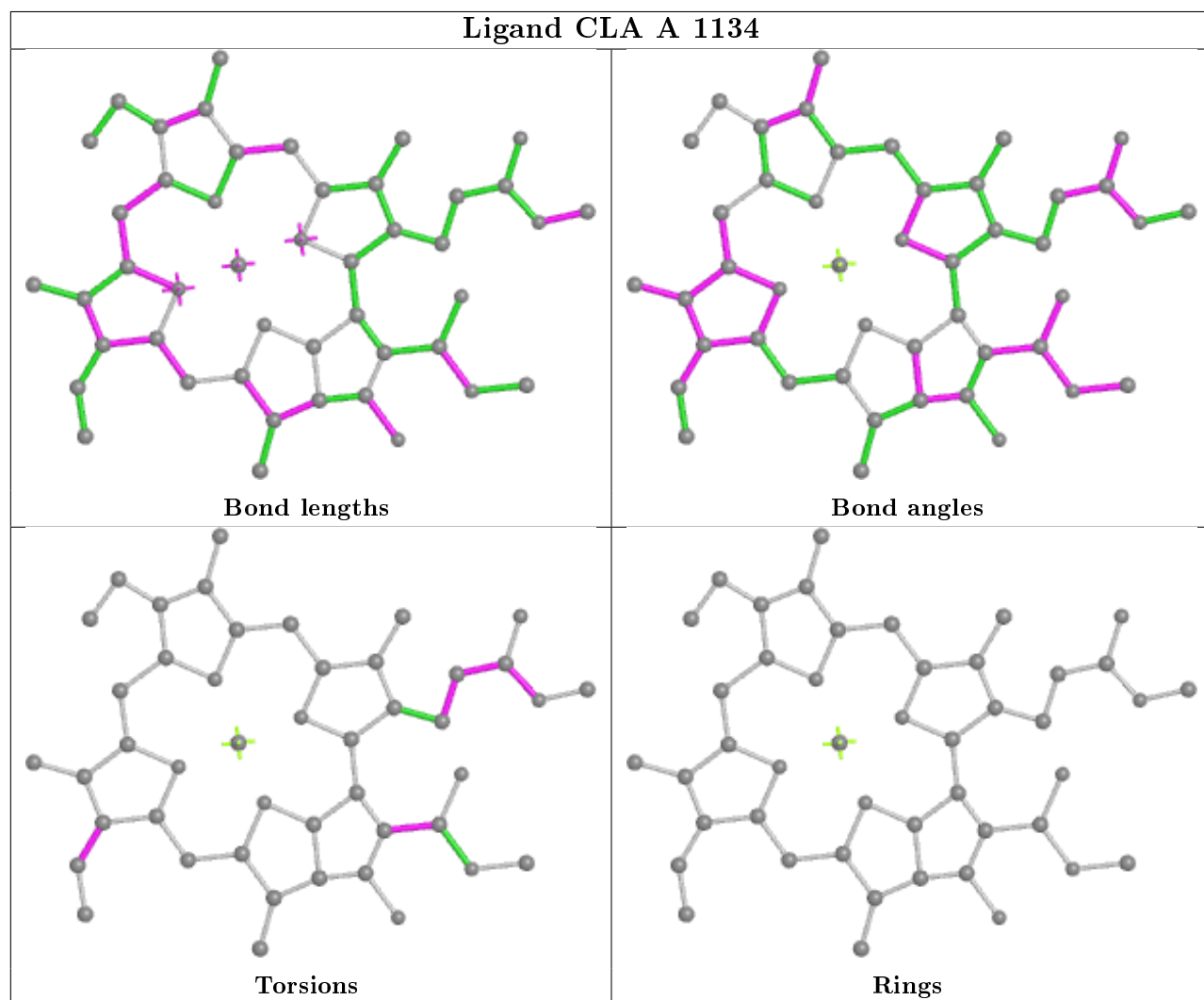
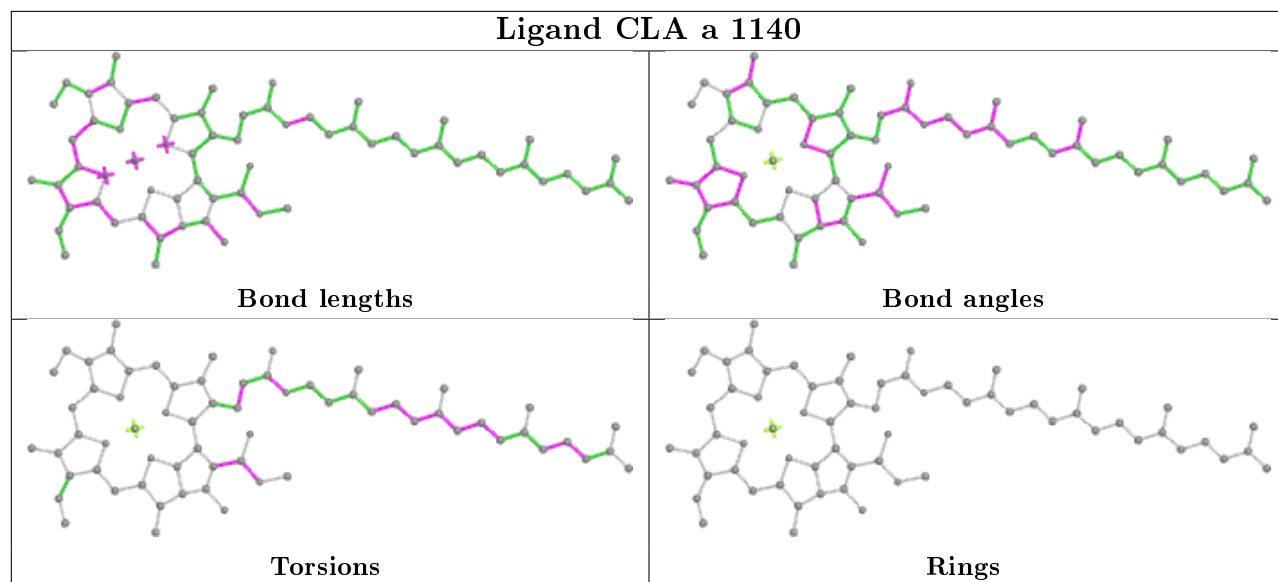


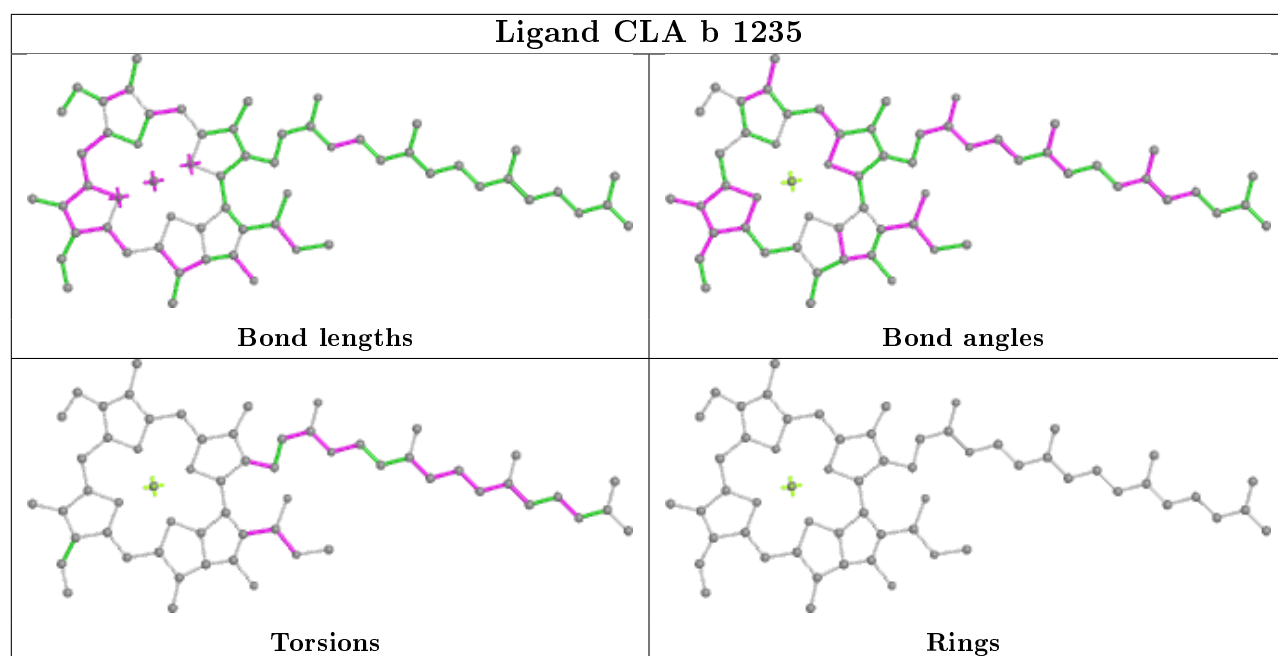
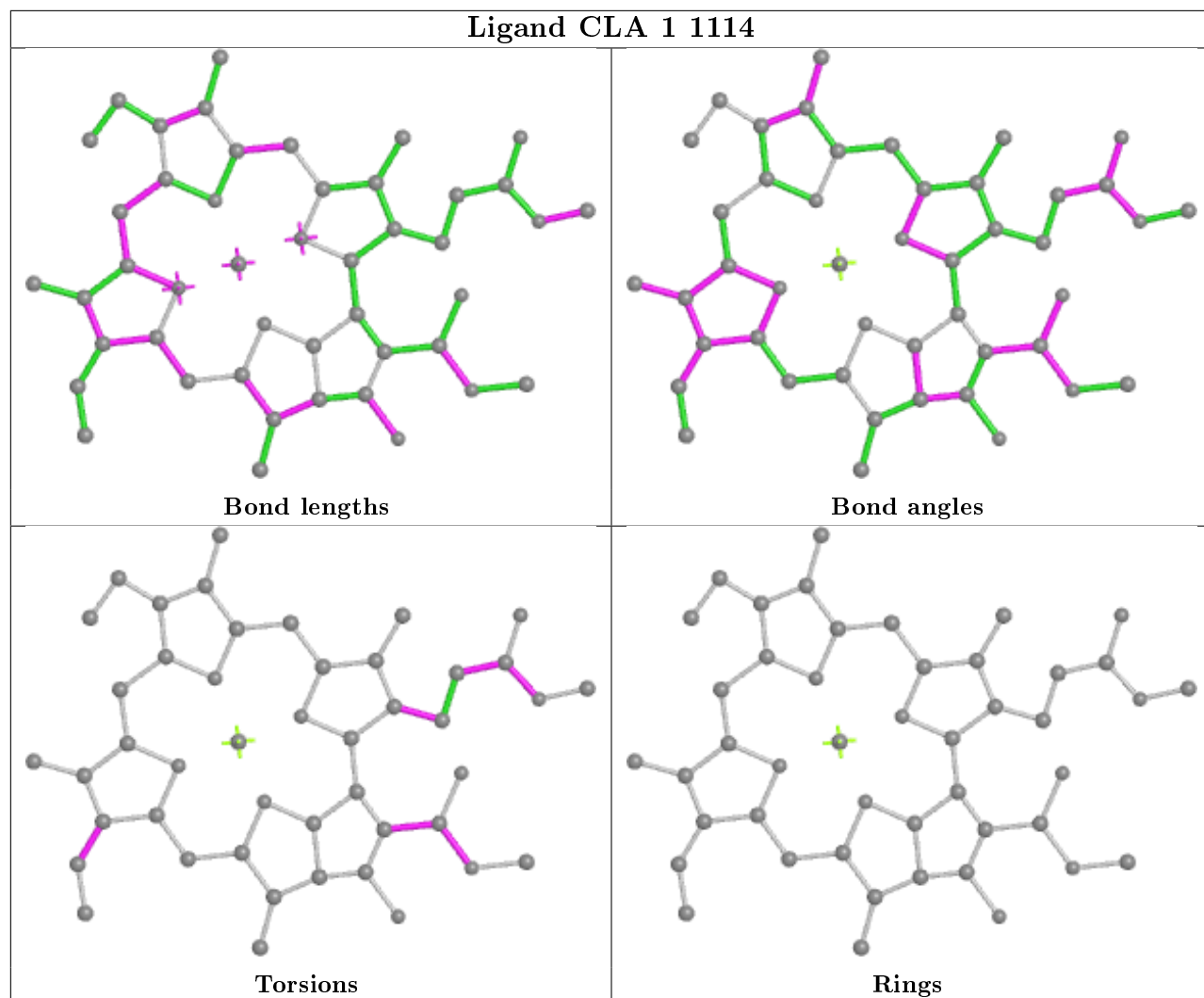
Torsions

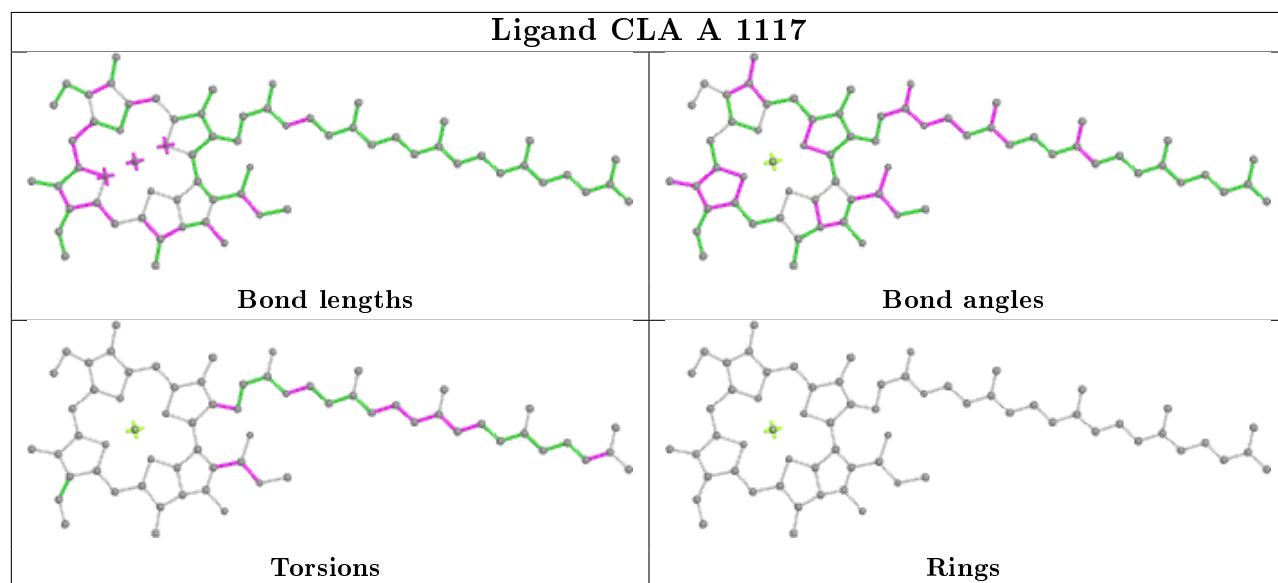
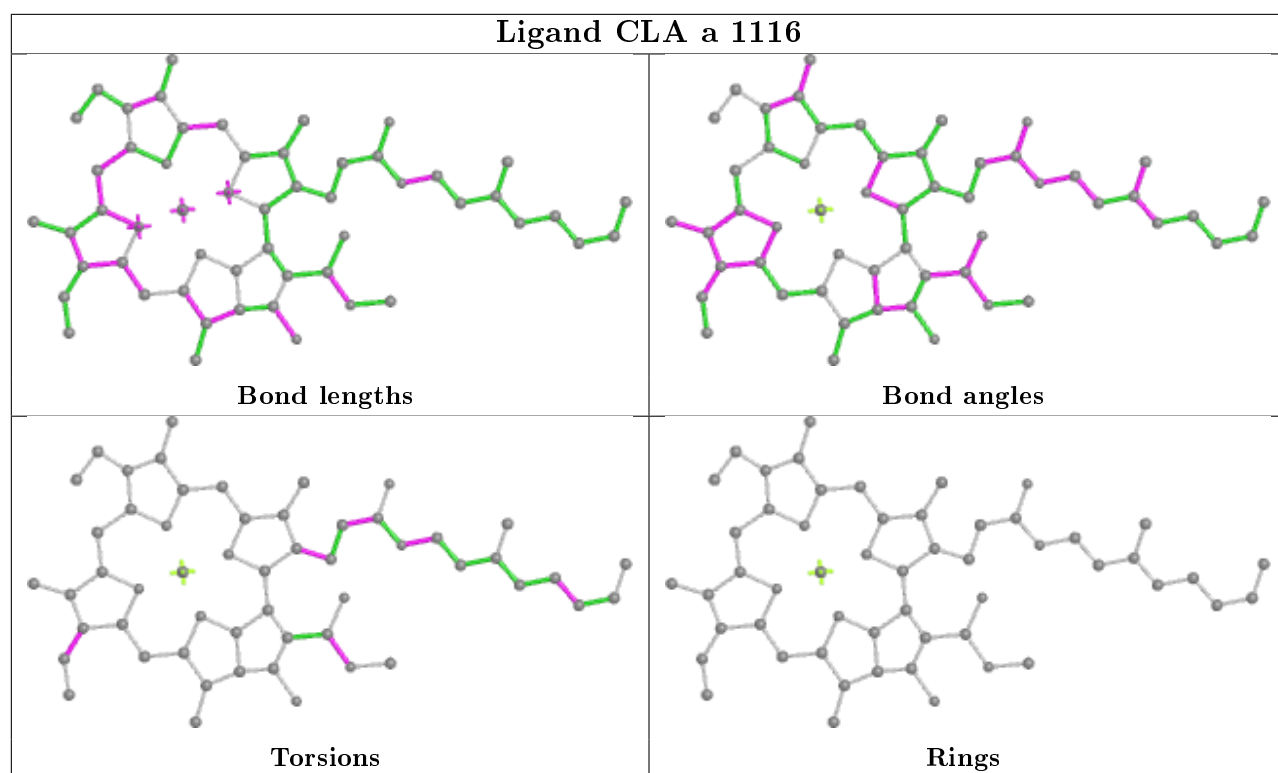


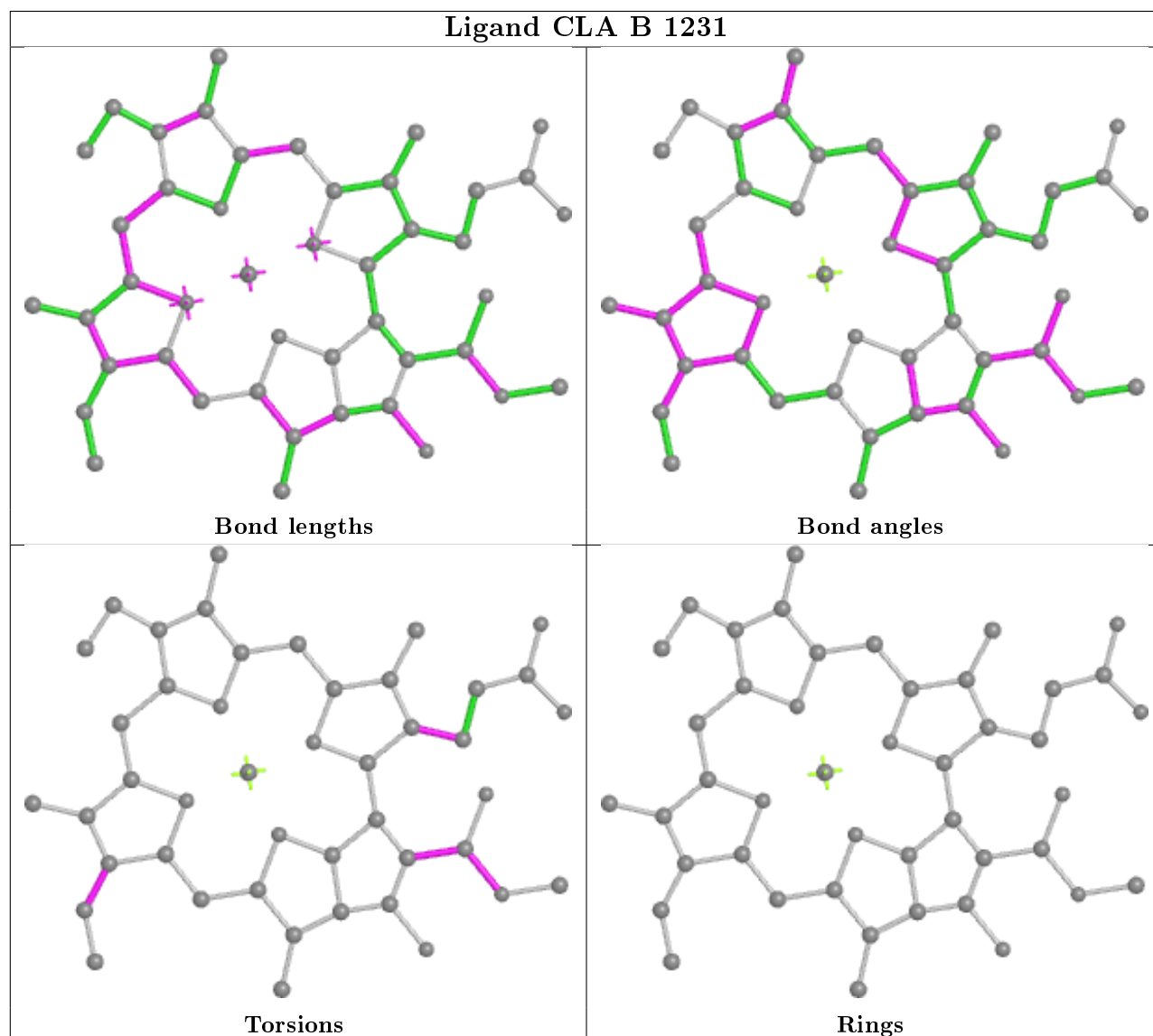
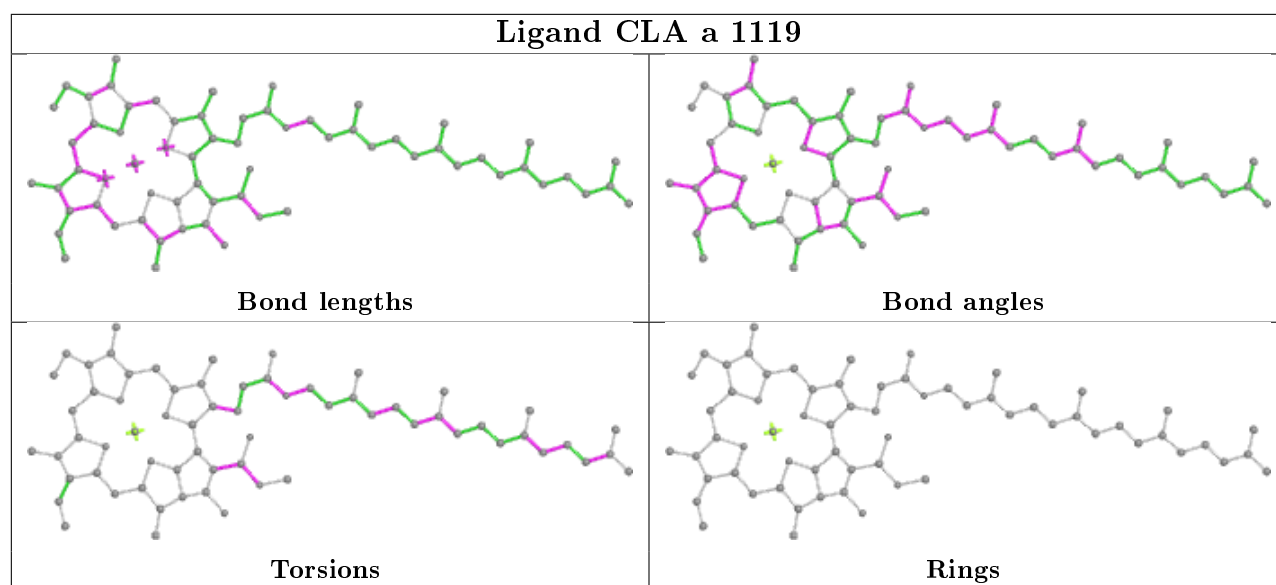
Rings

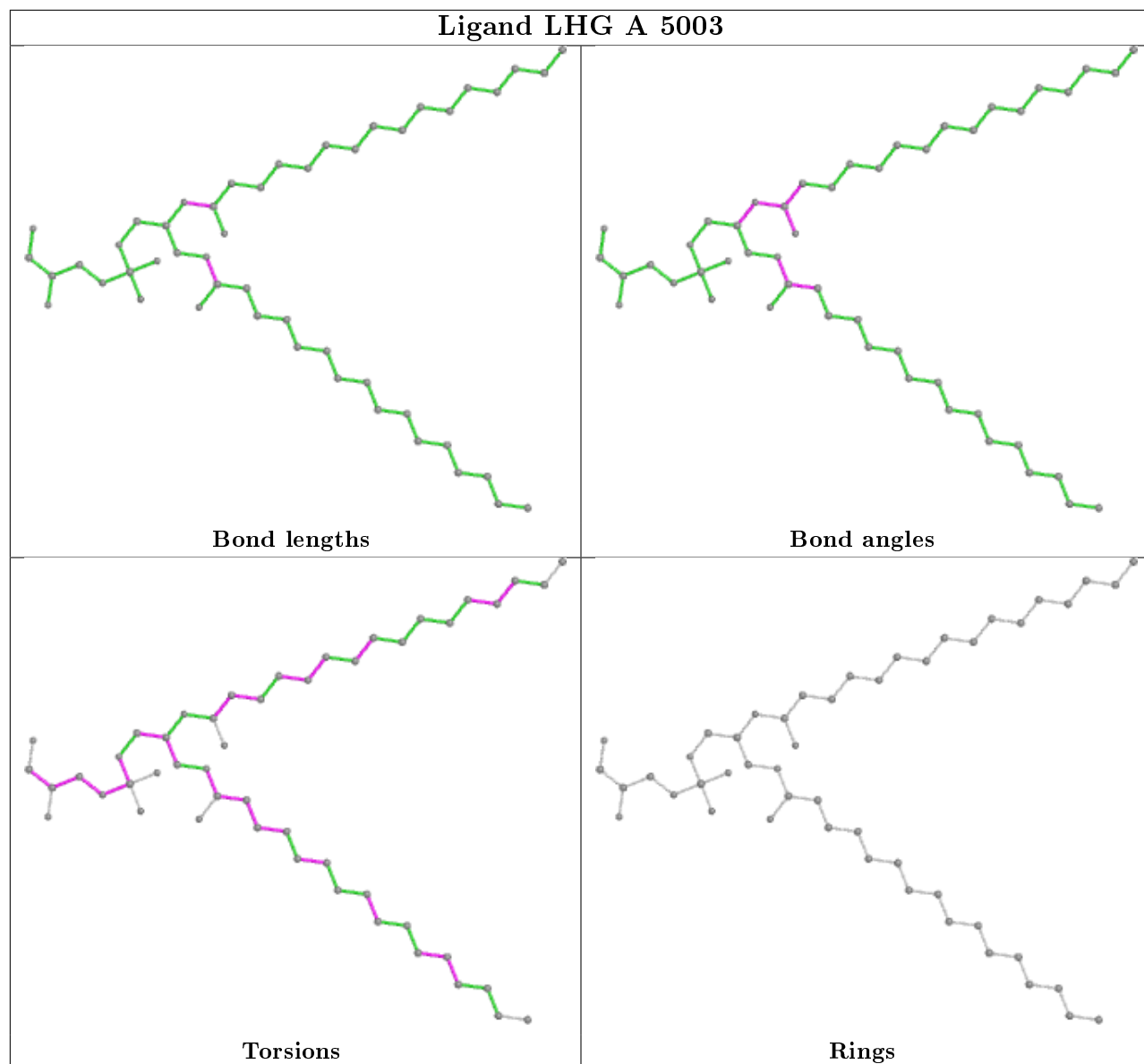
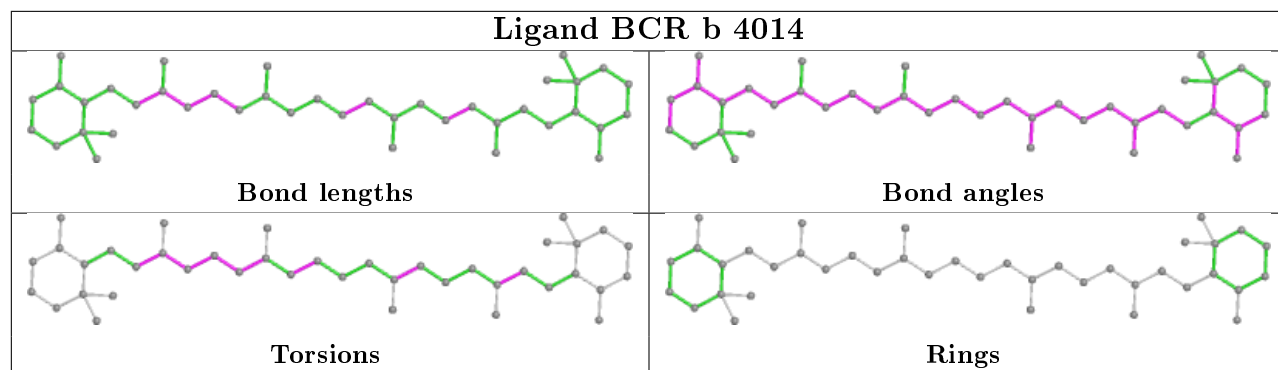




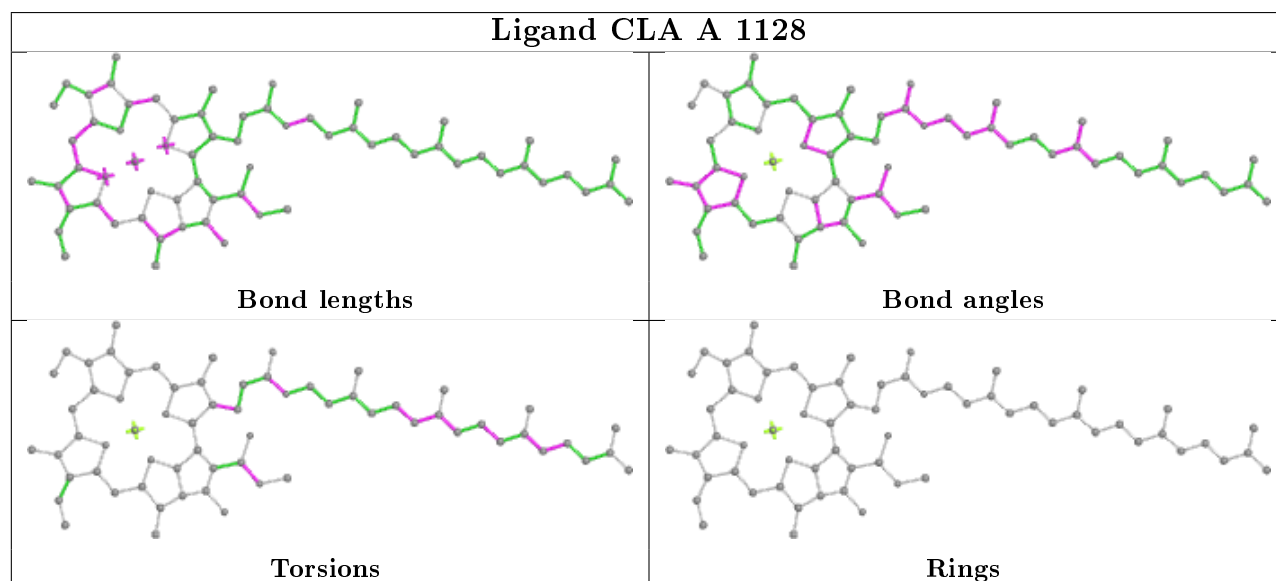
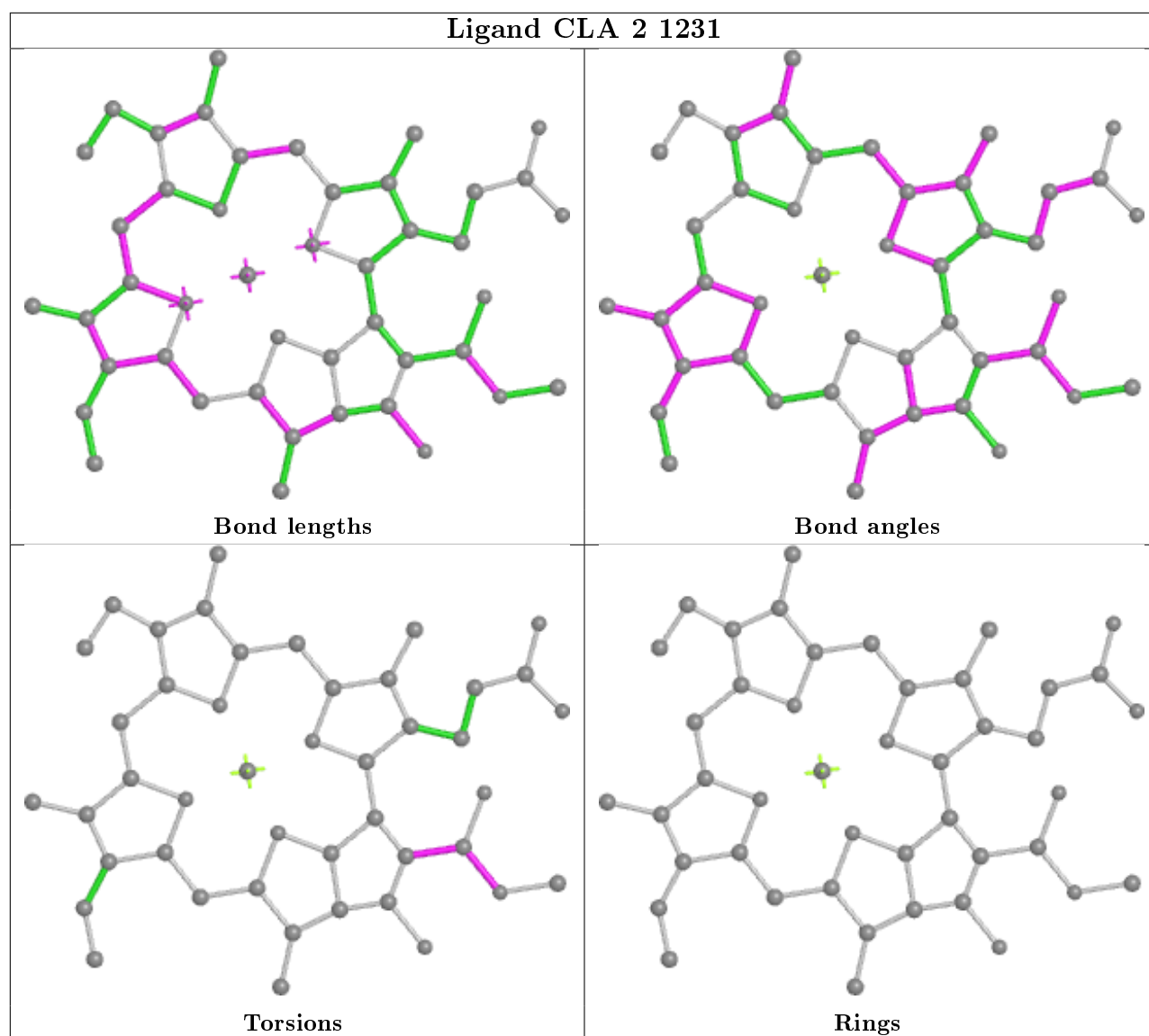




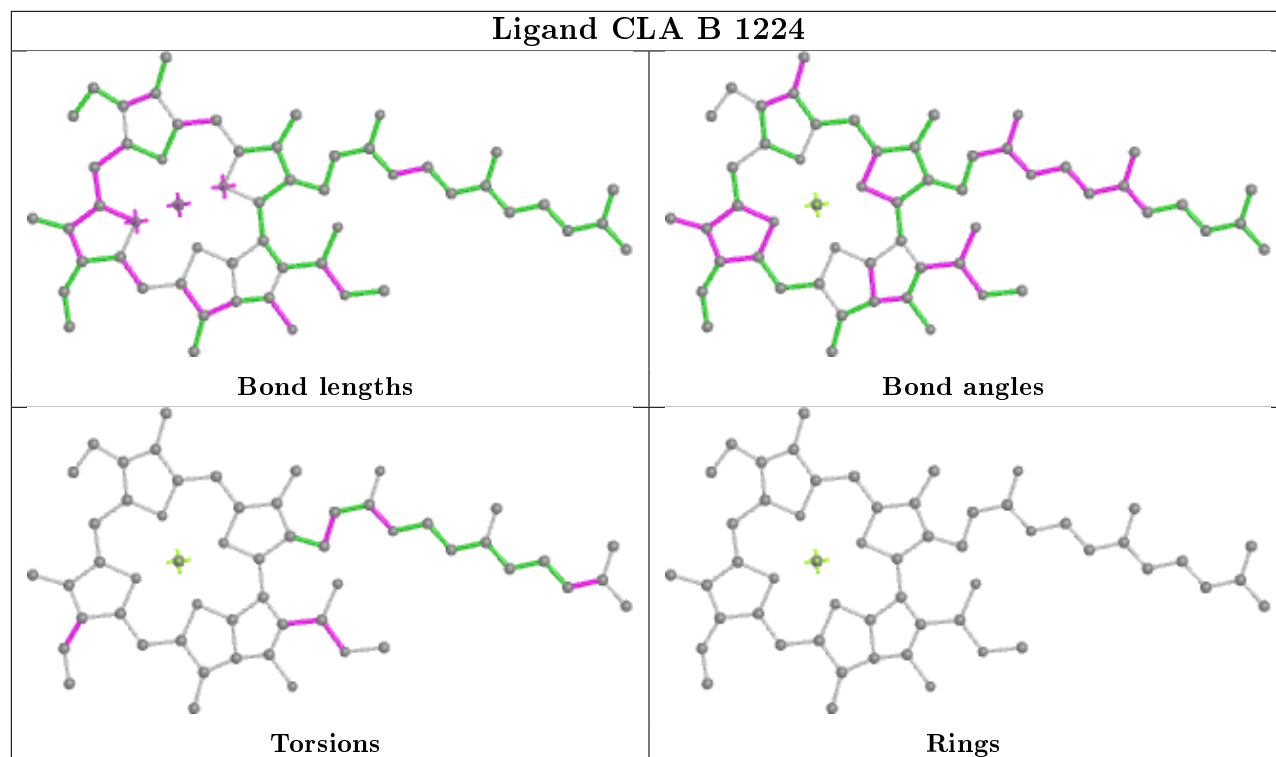




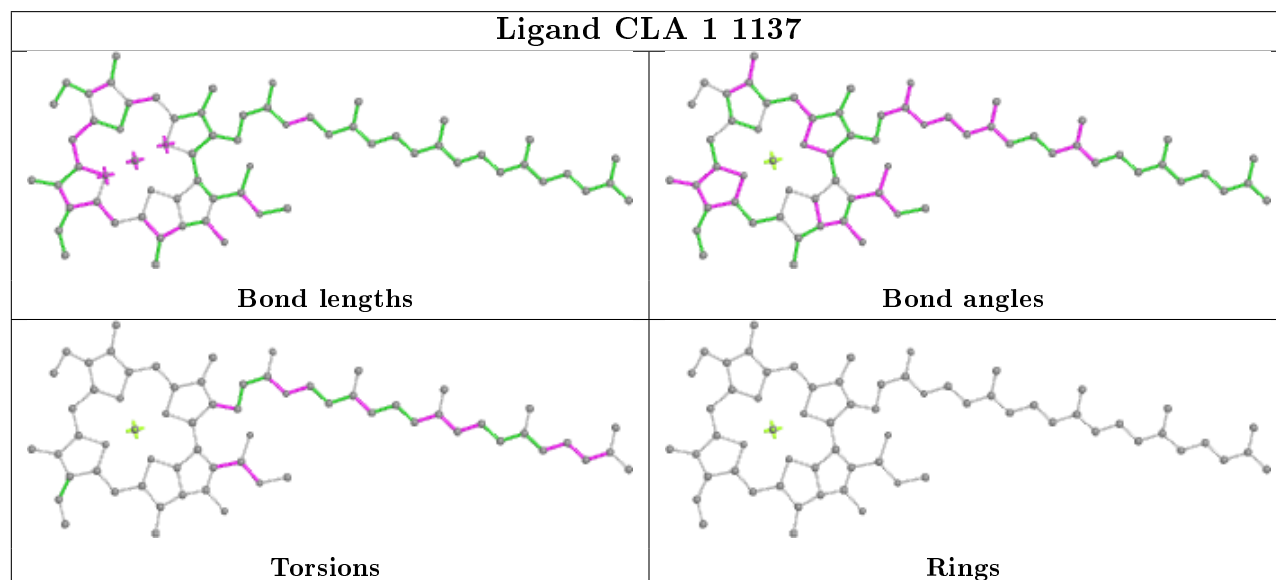




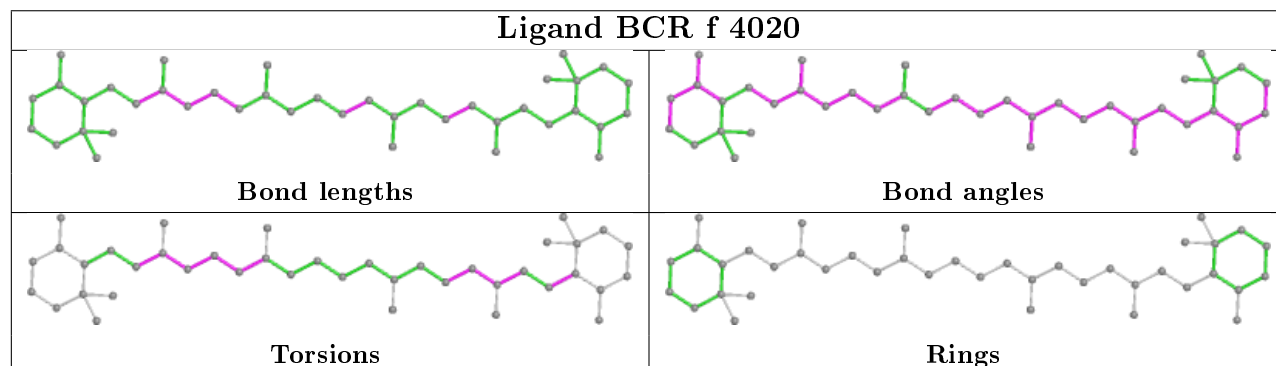
## Ligand CLA B 1224



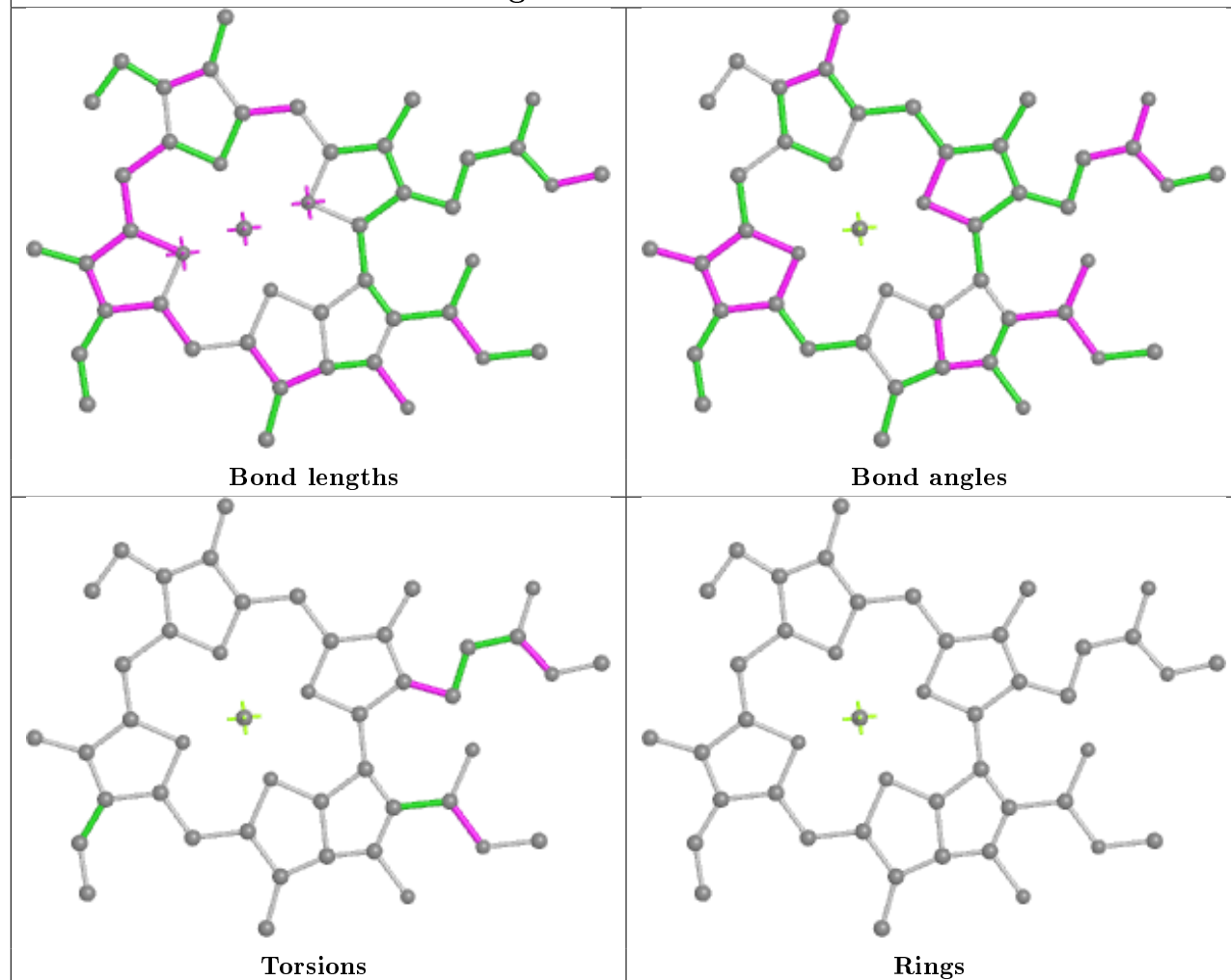
## Ligand CLA 1 1137



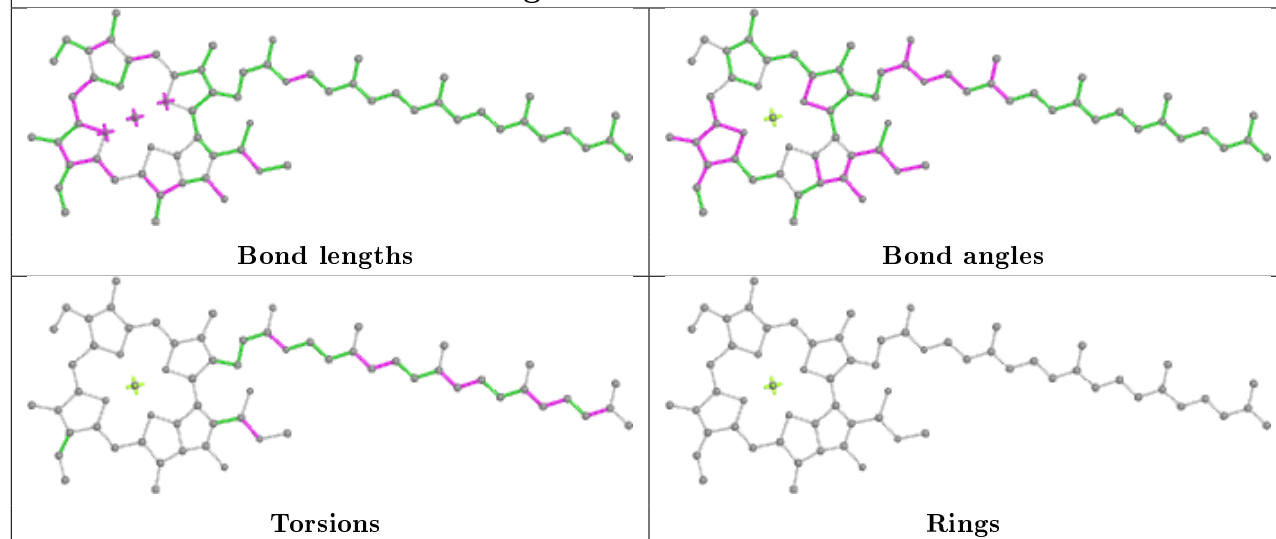
## Ligand BCR f 4020

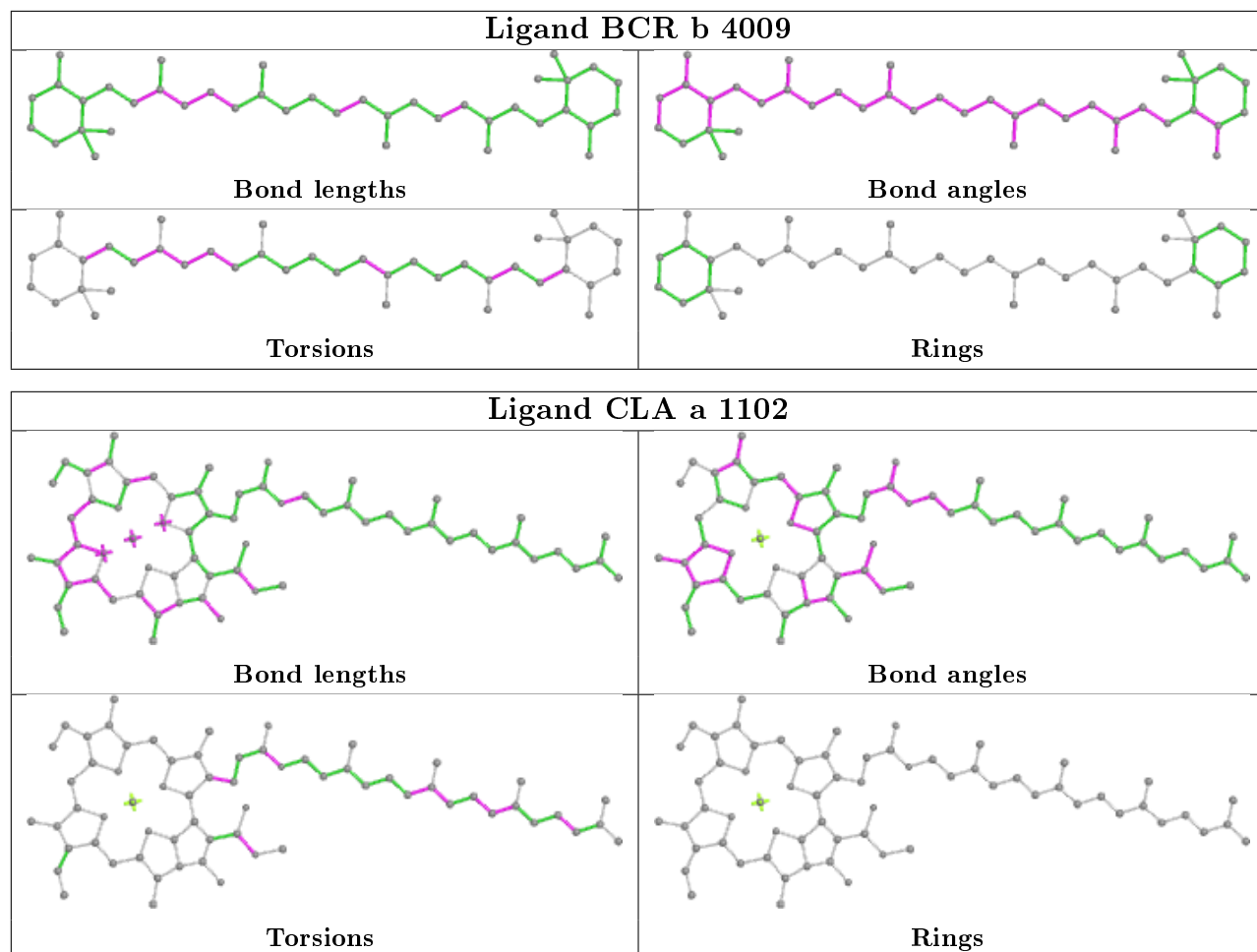


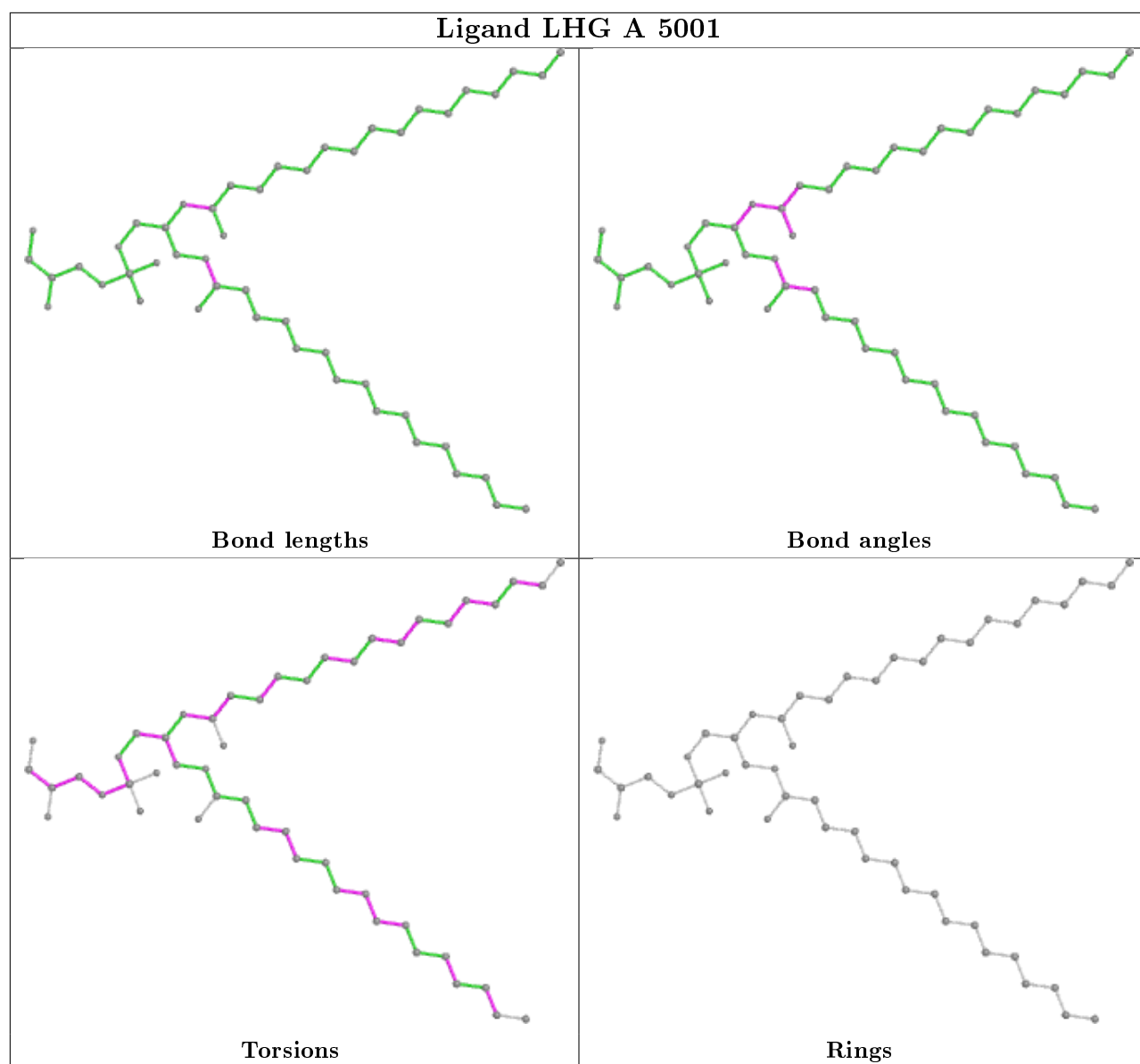
## Ligand CLA 1 1130

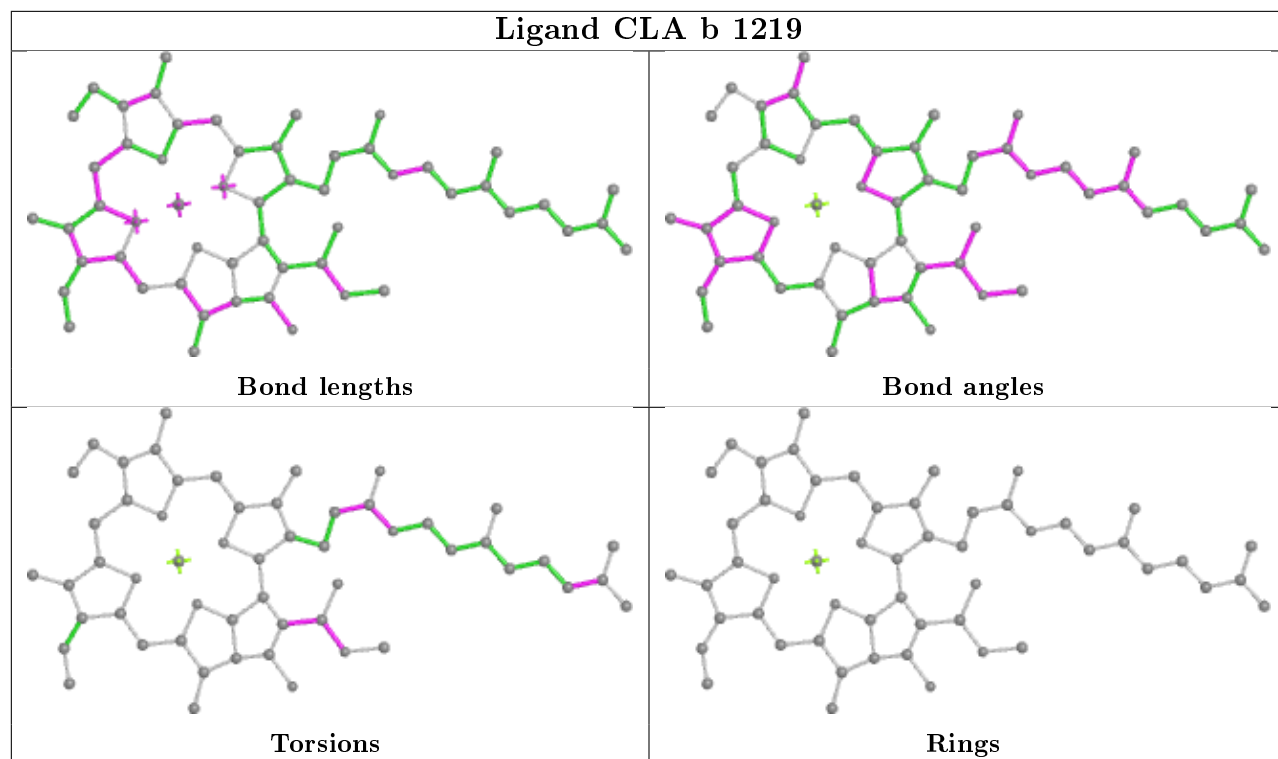


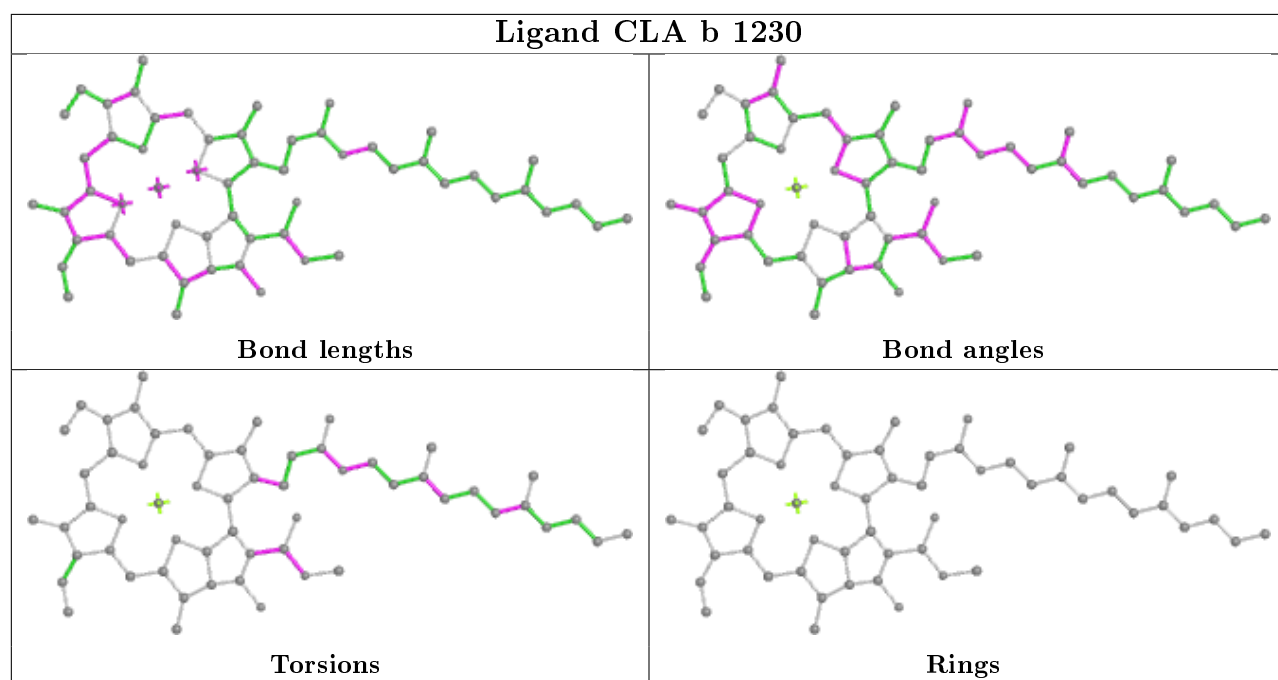
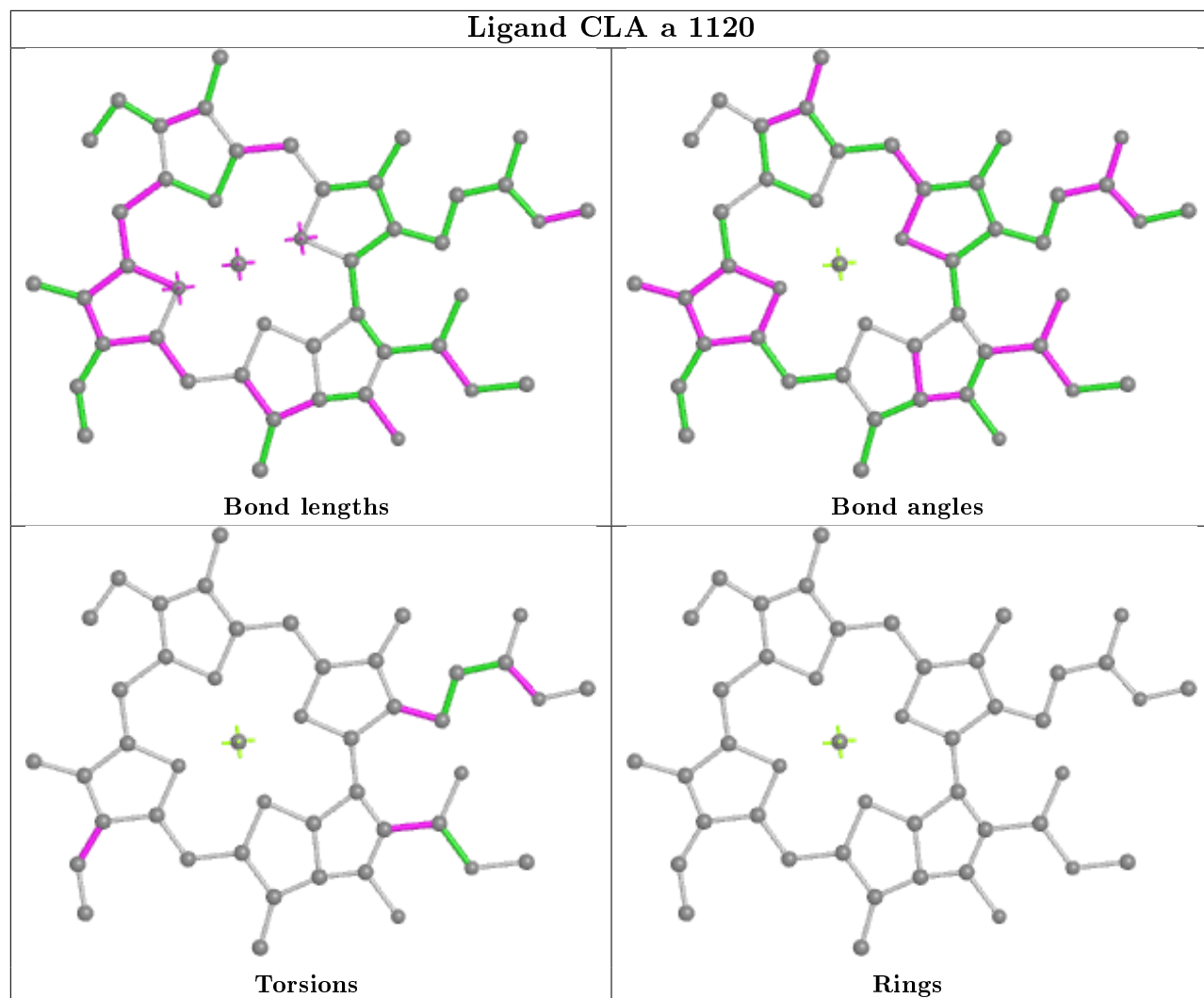
## Ligand CLA B 1206

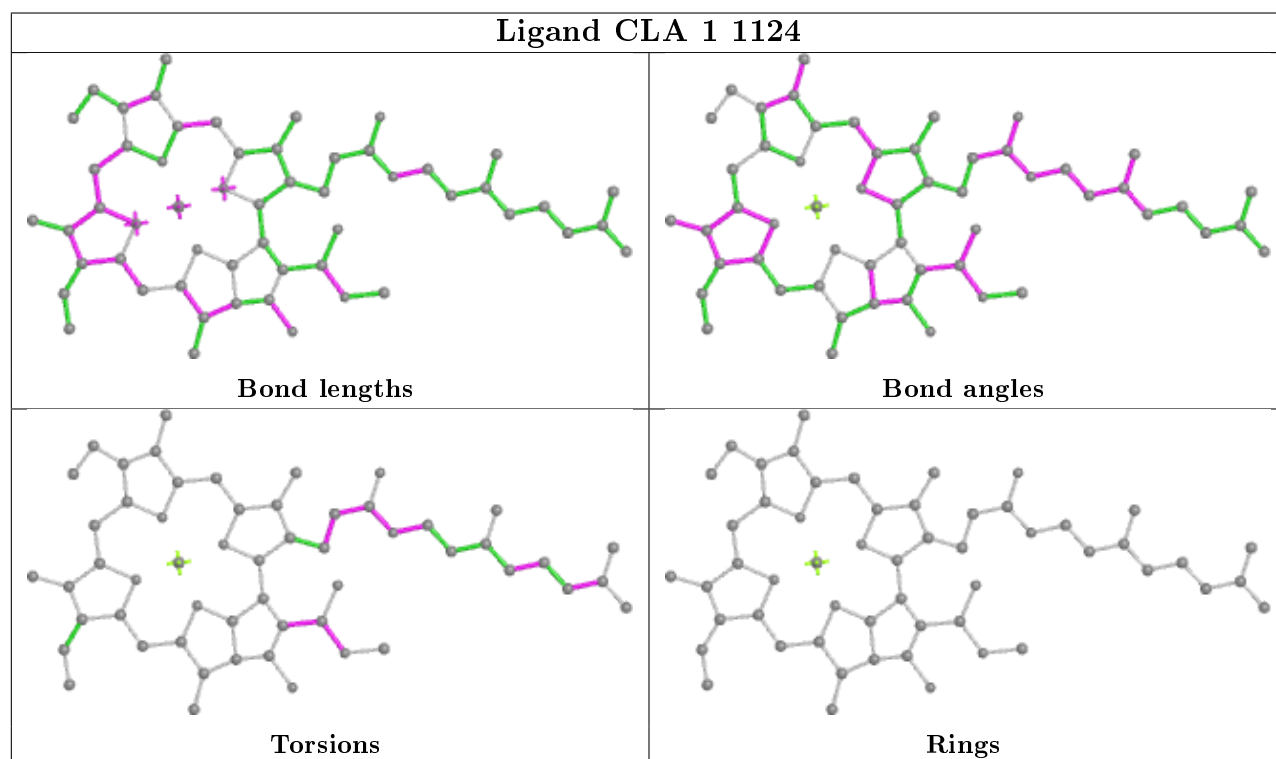
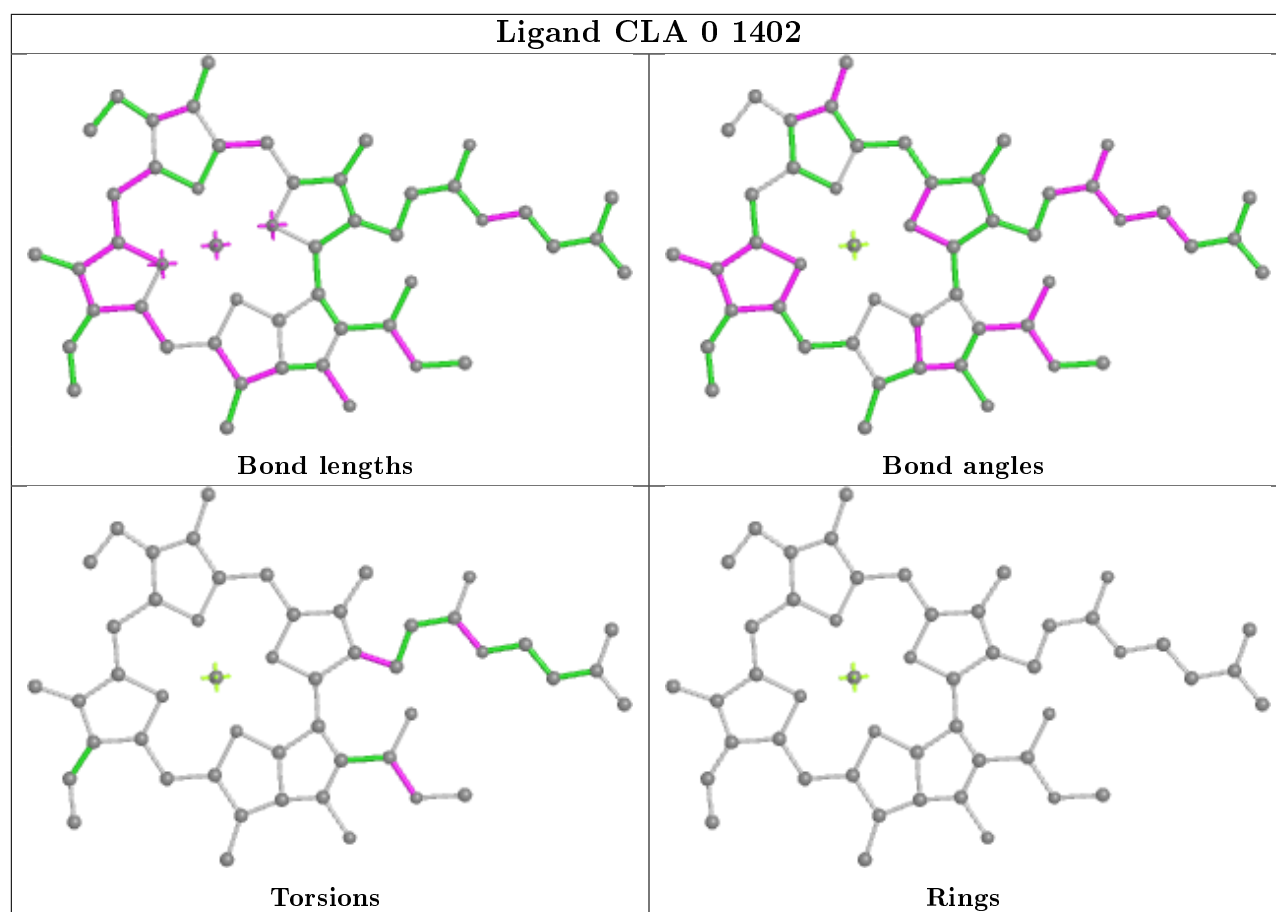




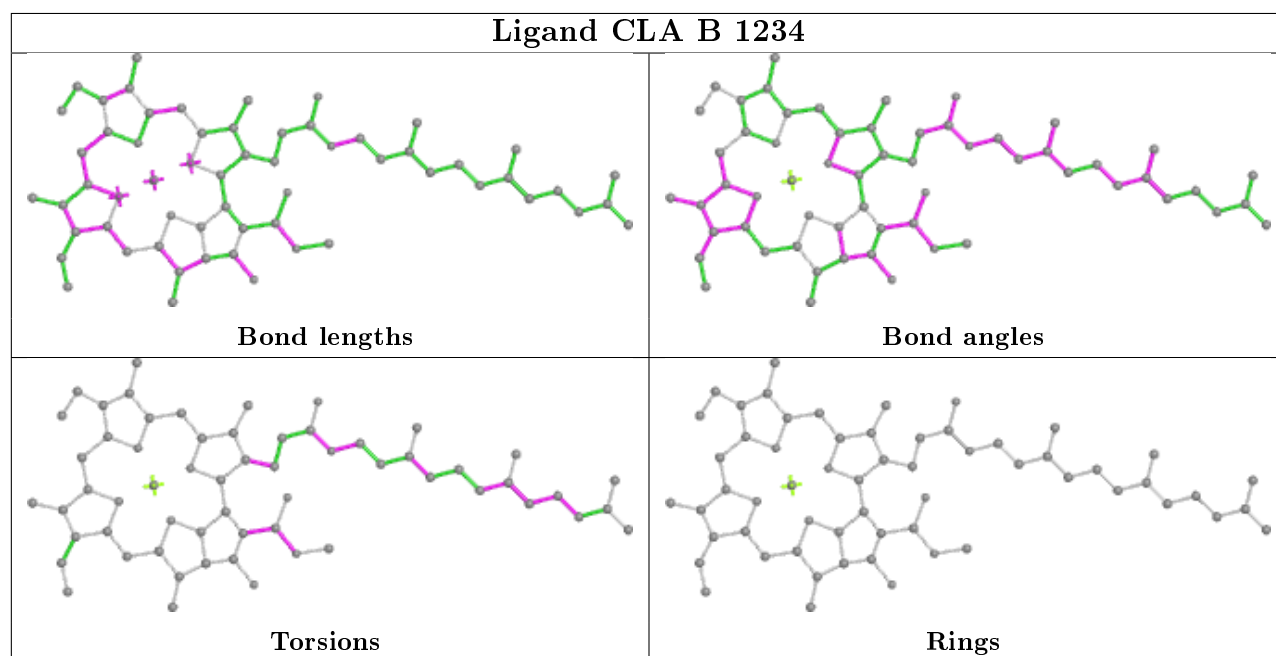
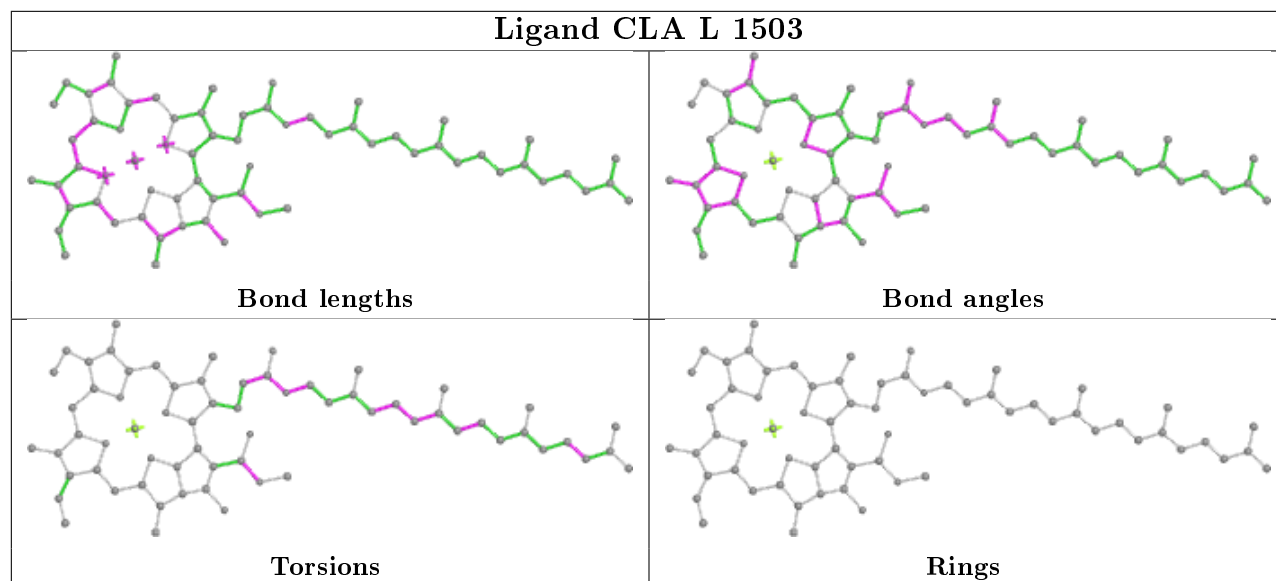
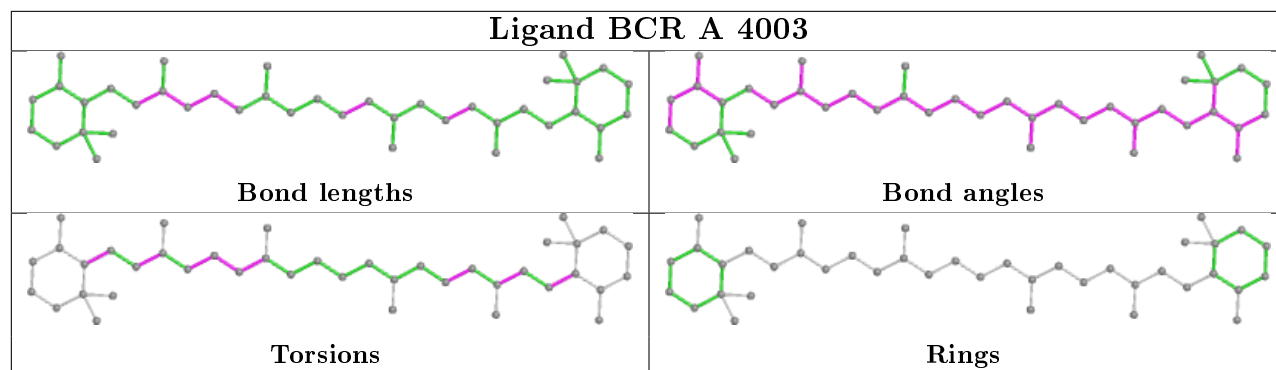


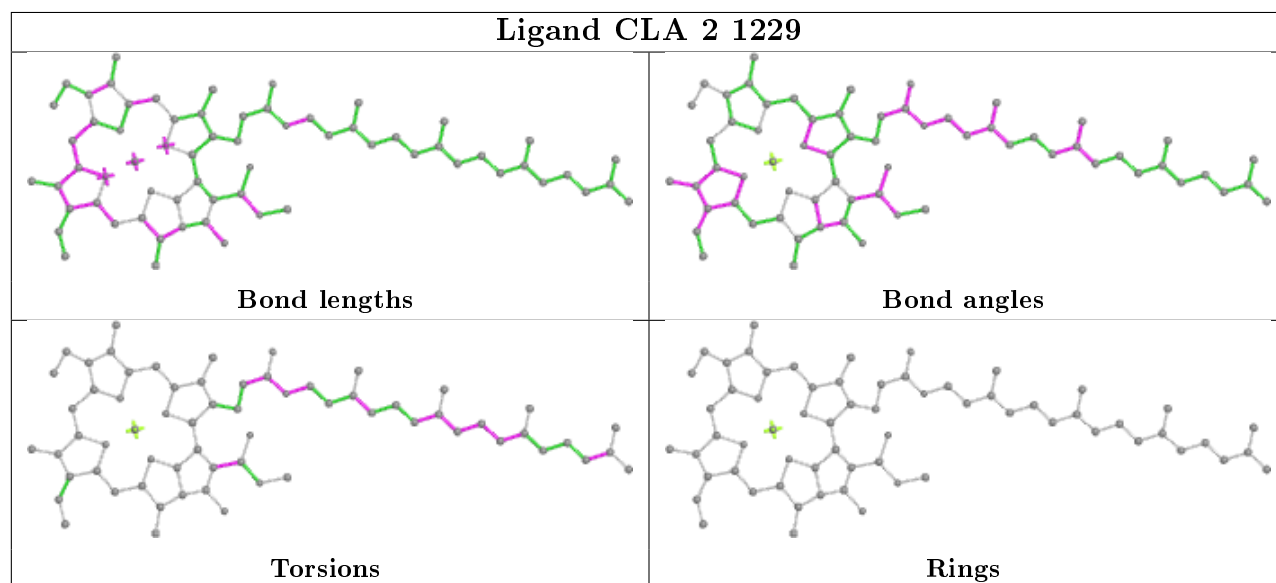
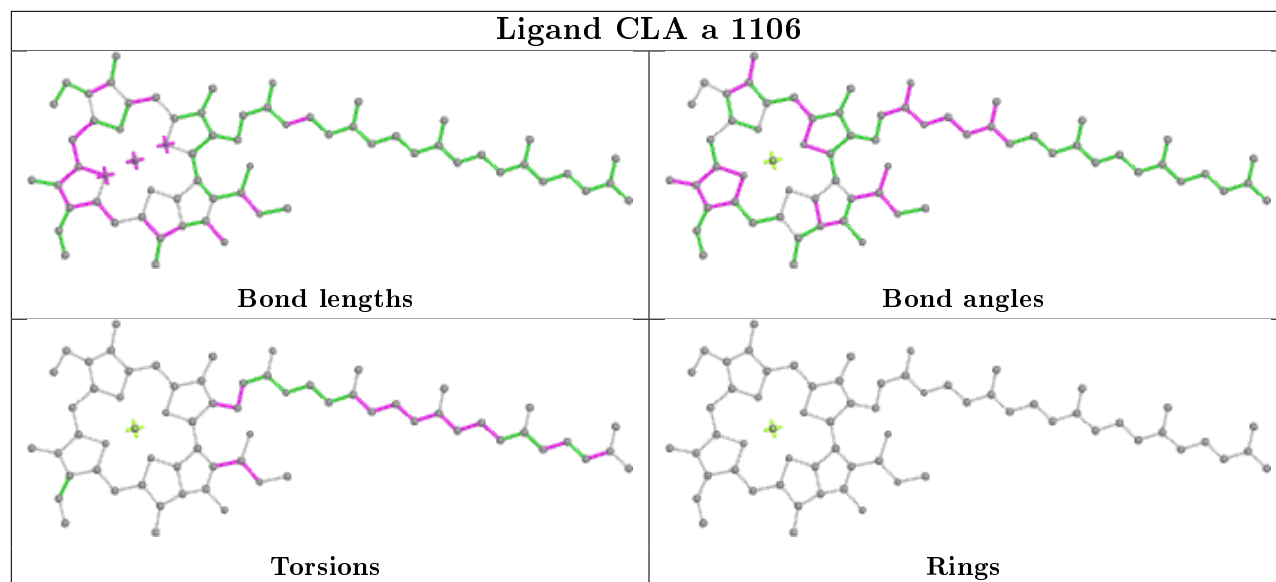


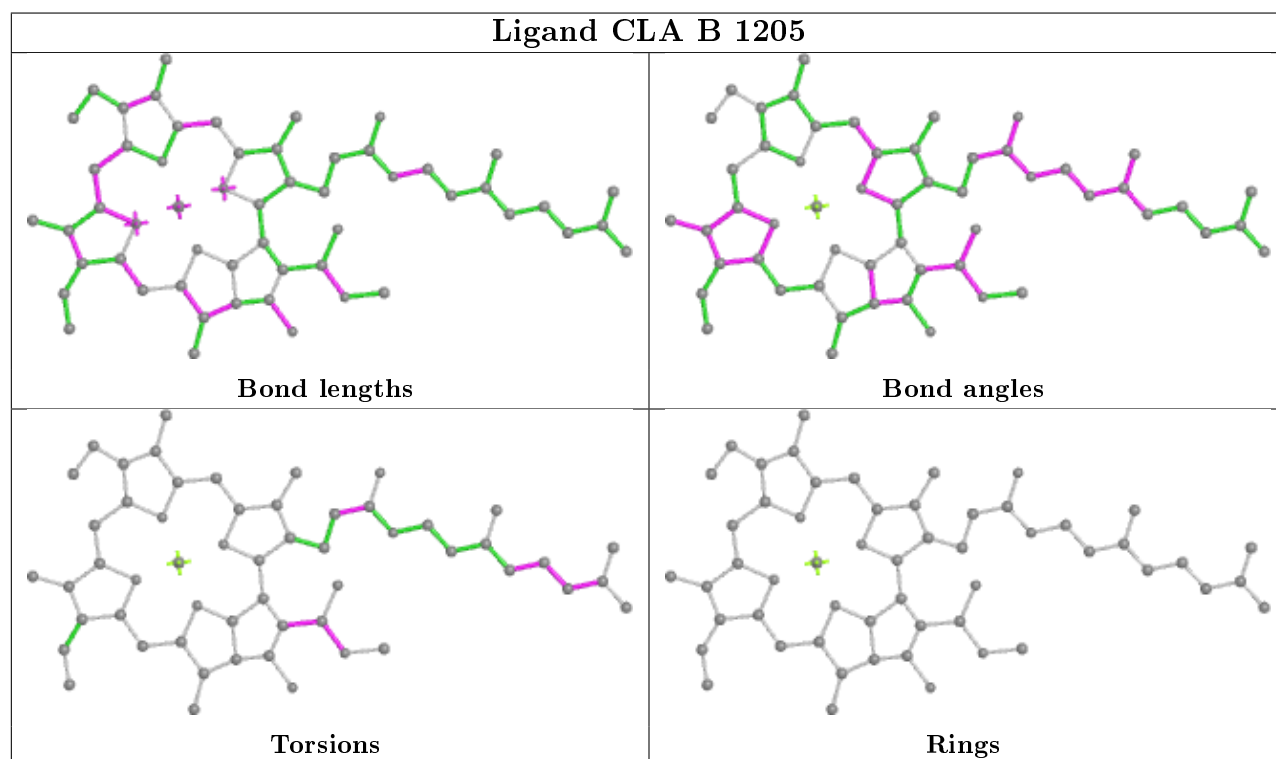
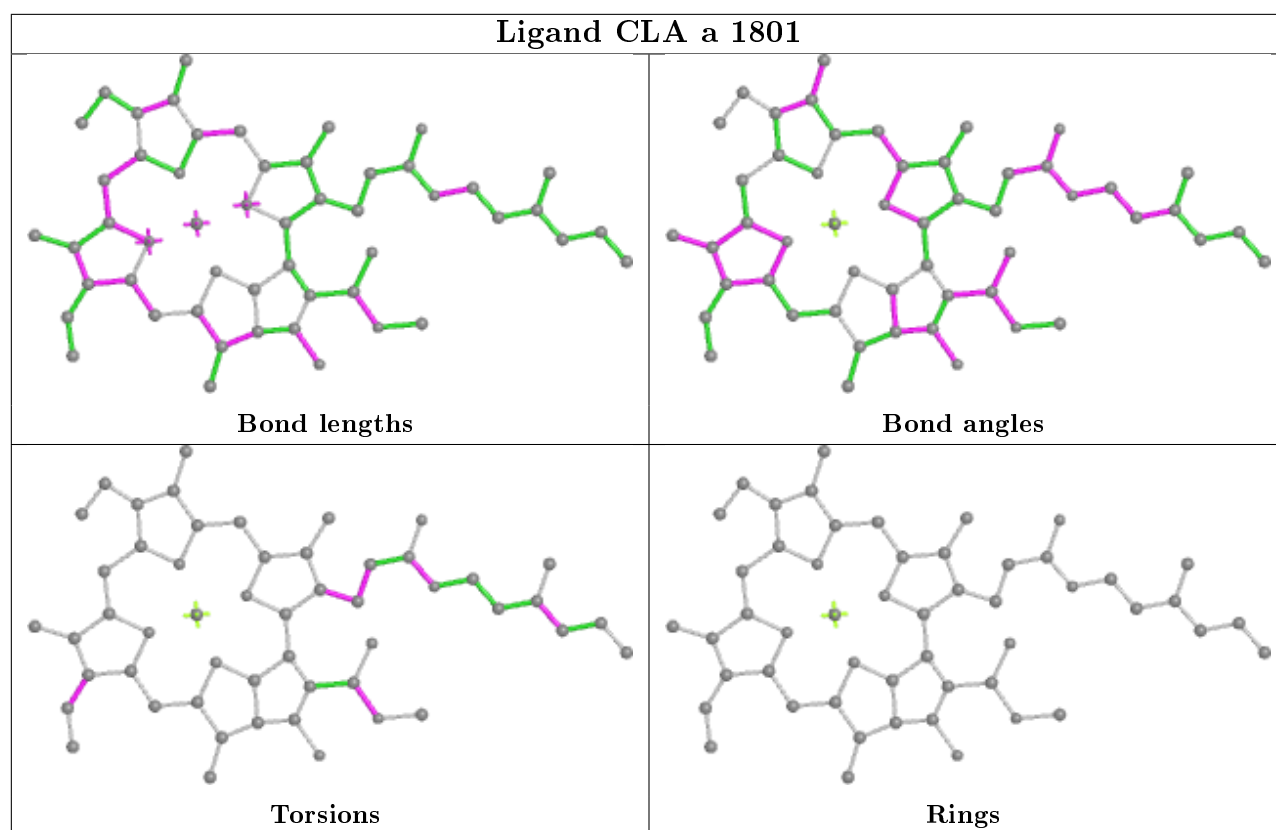


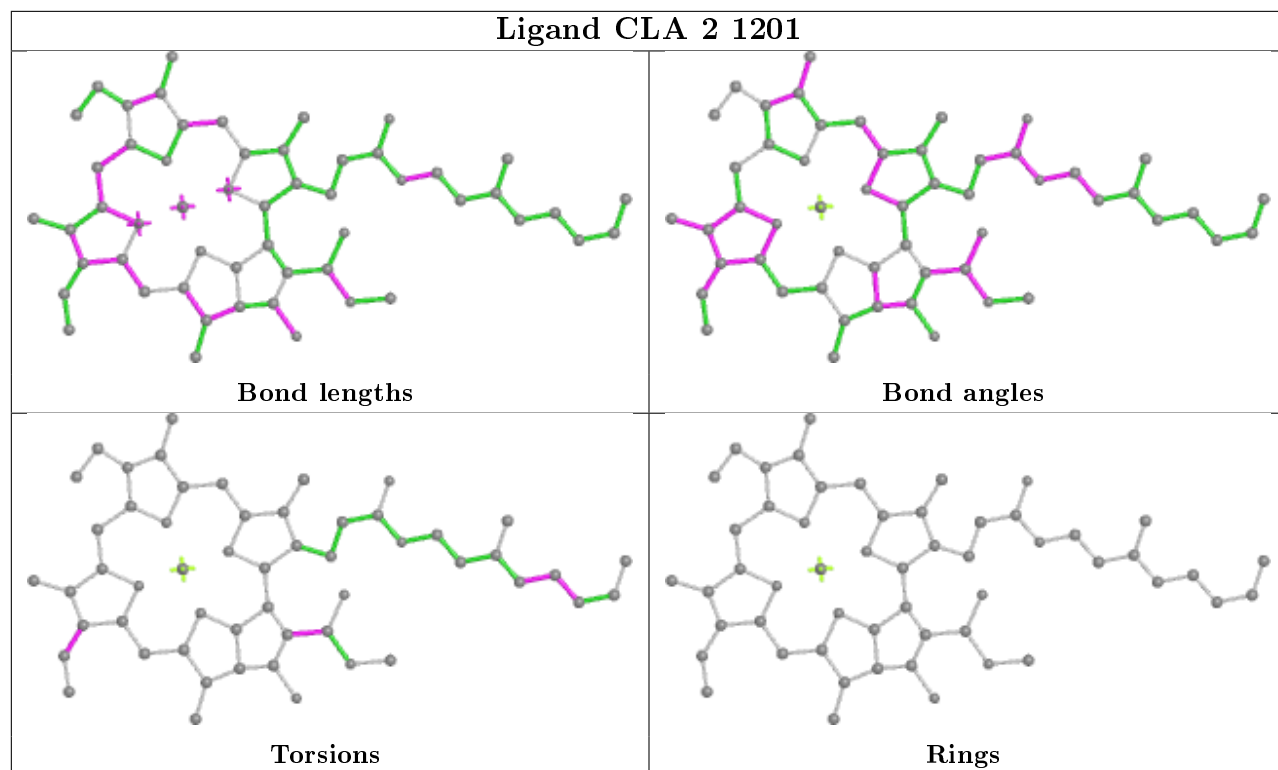


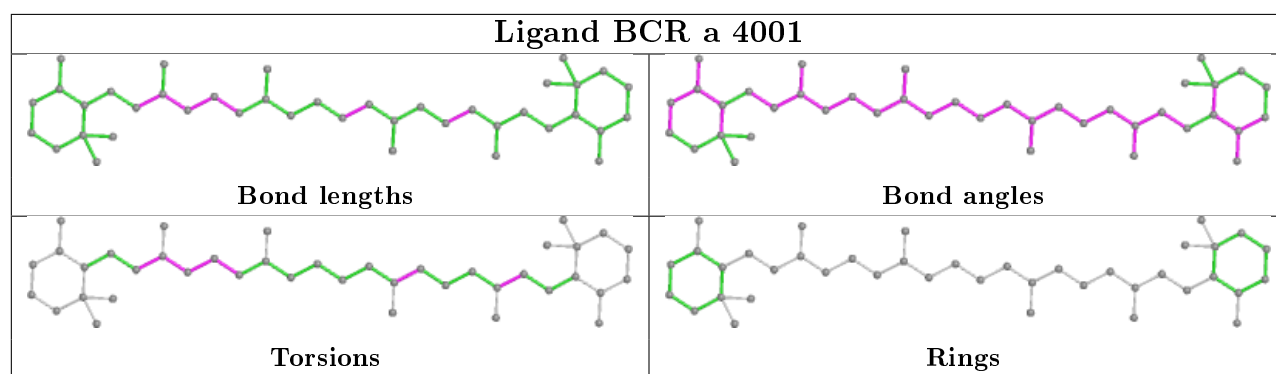
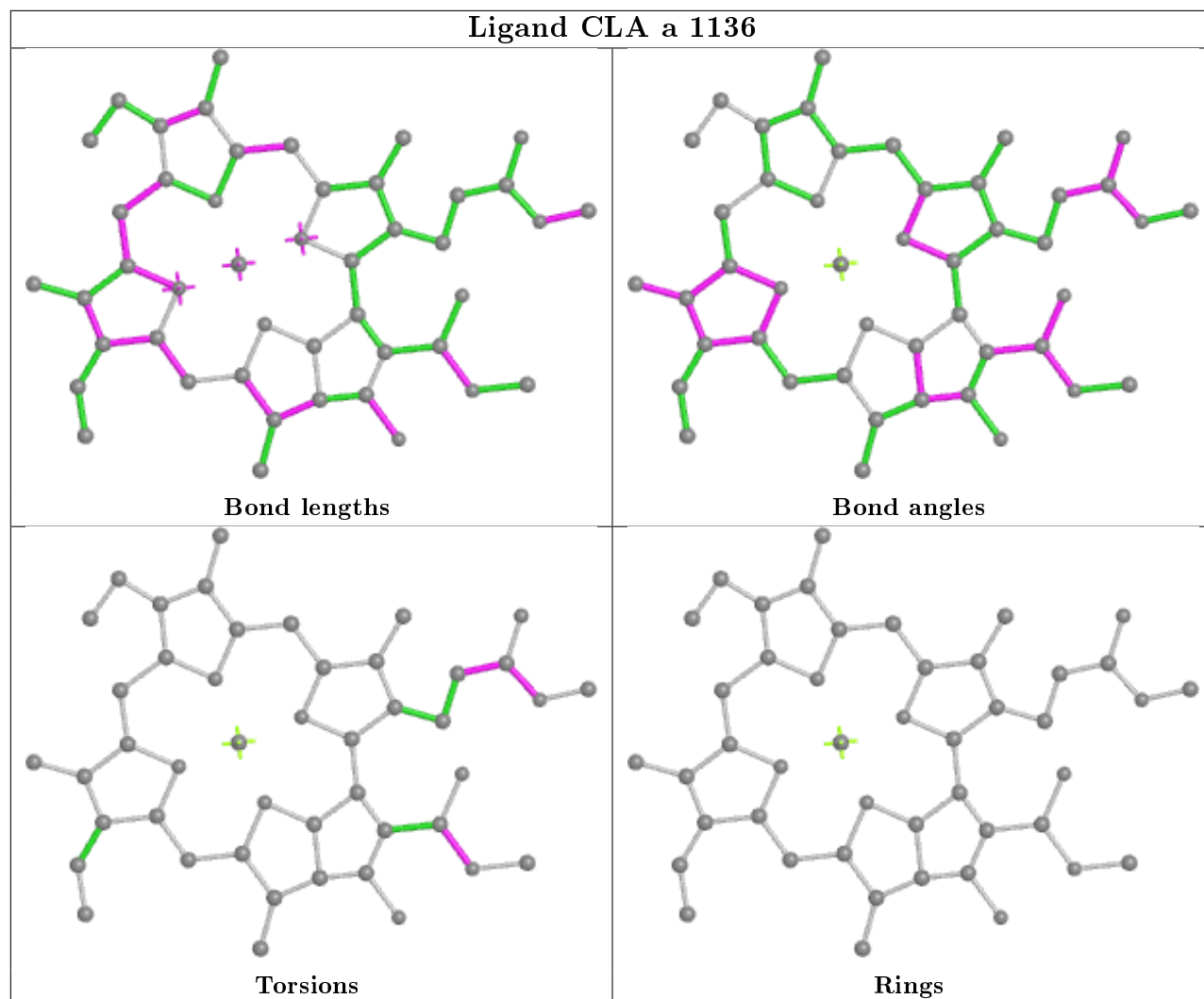




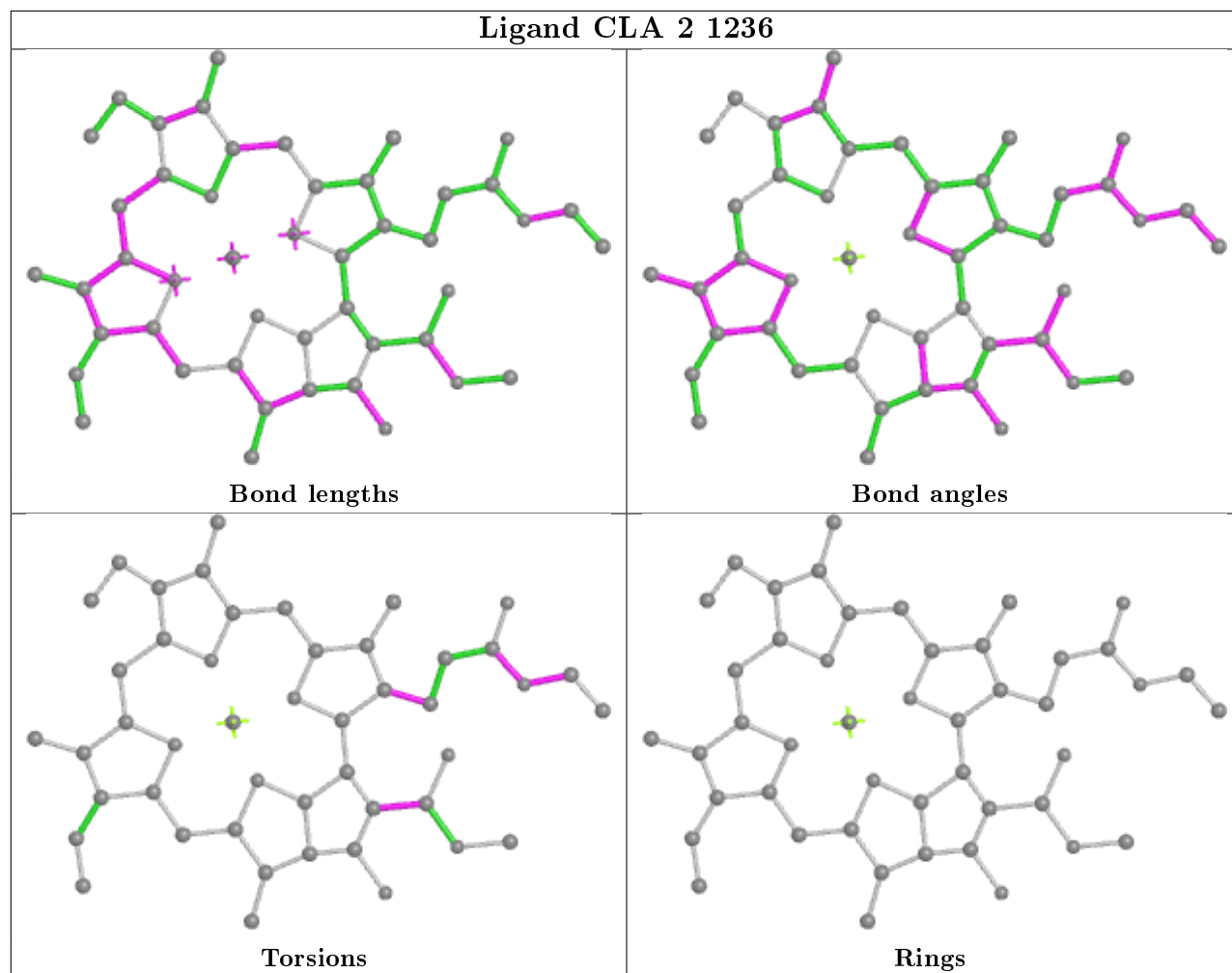




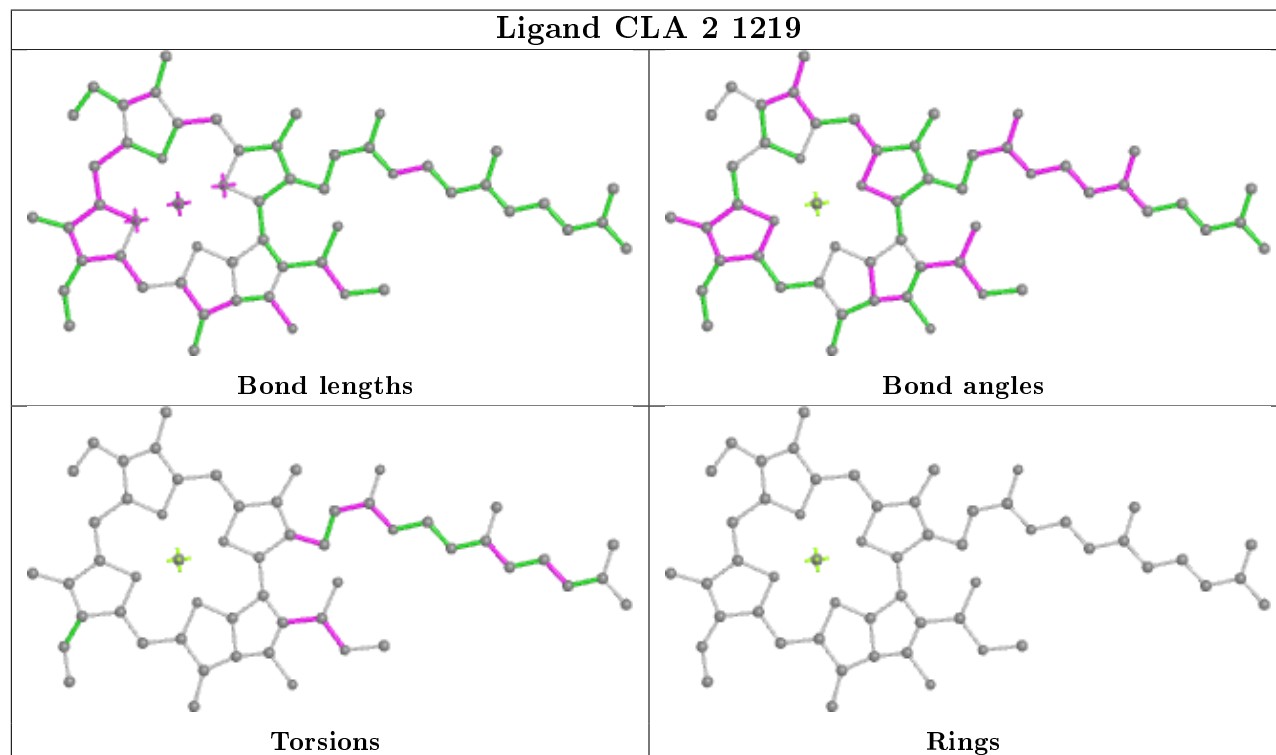


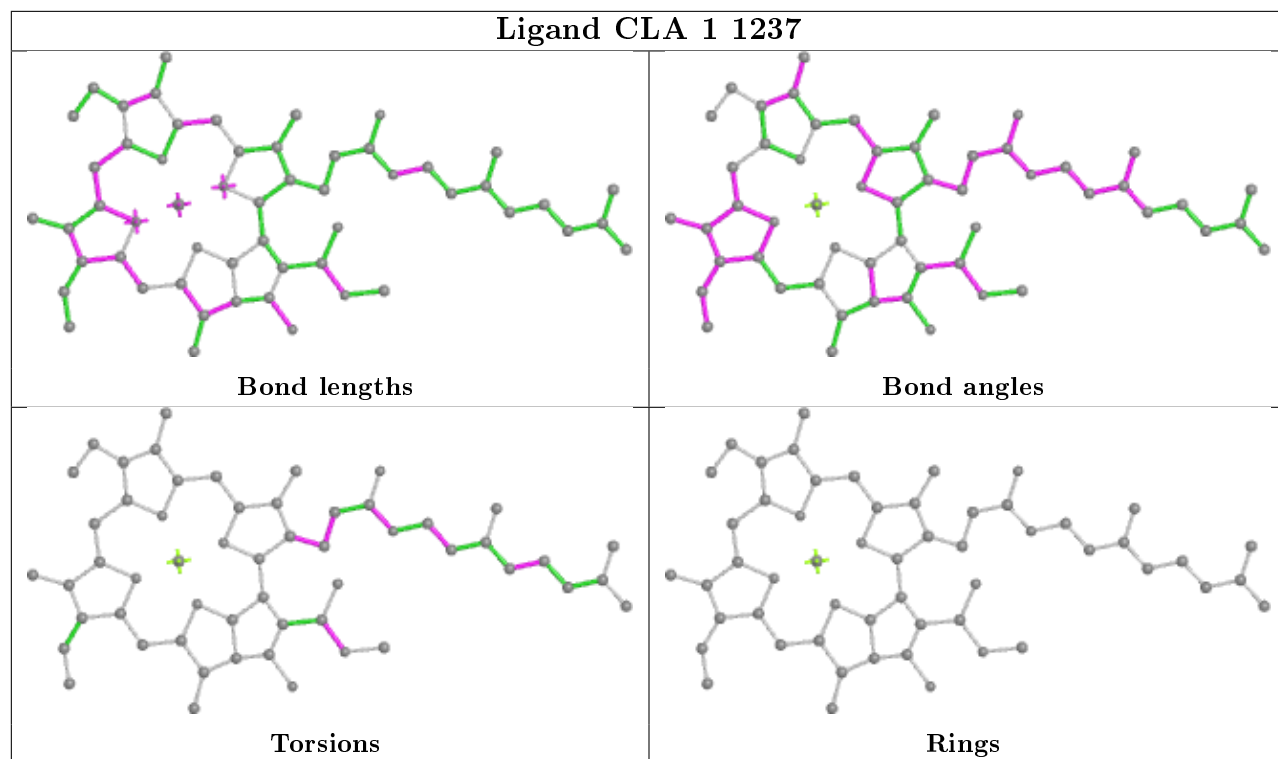


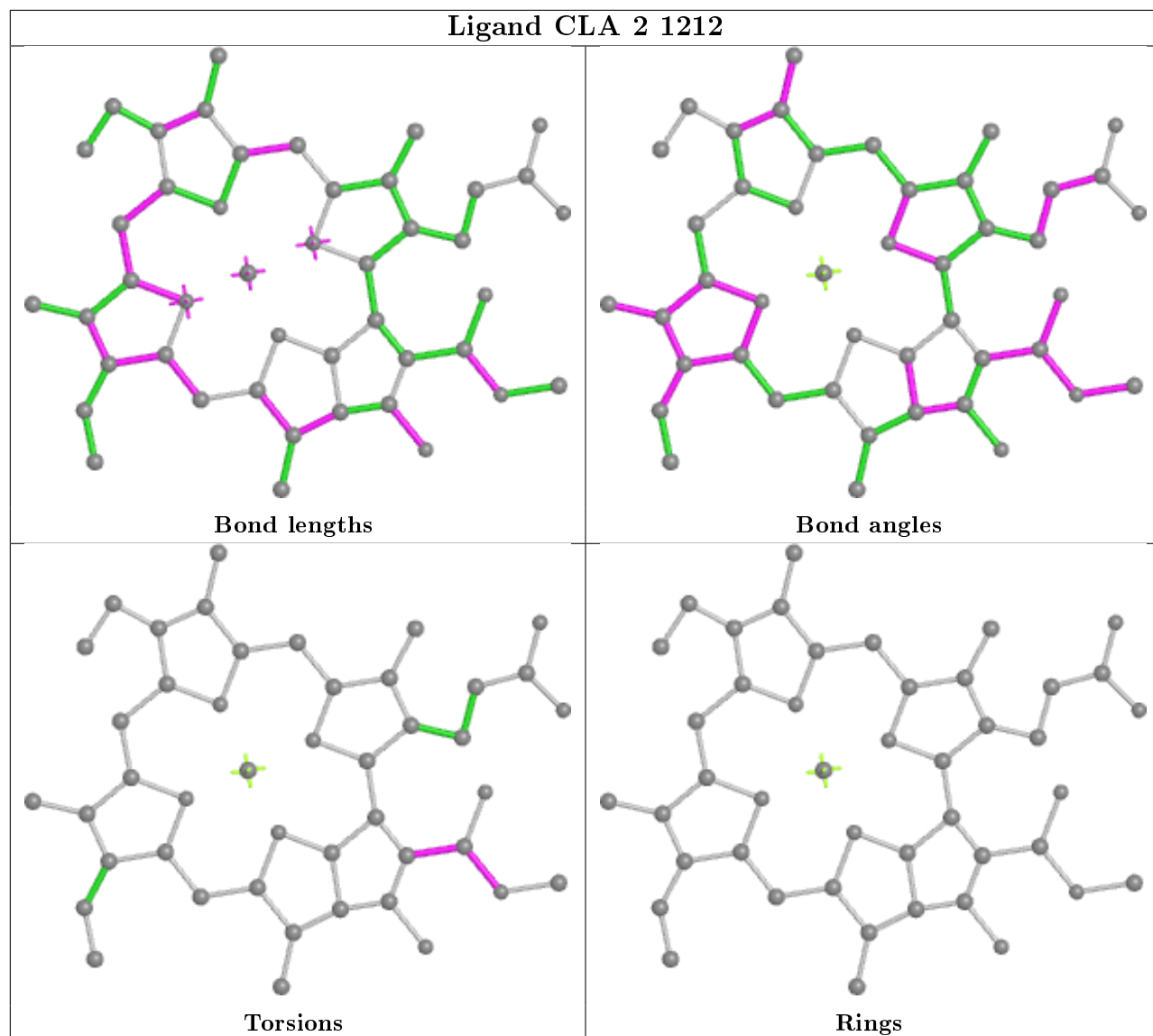
## Ligand CLA 2 1236



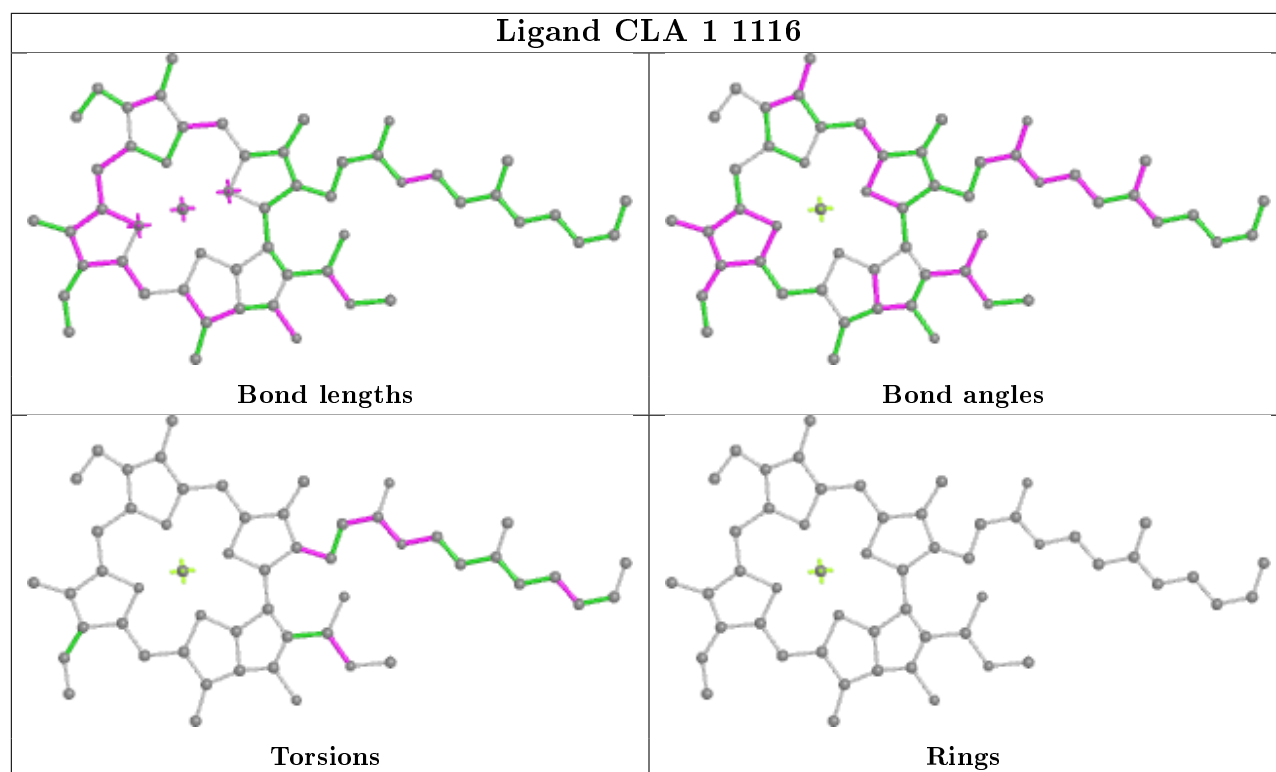
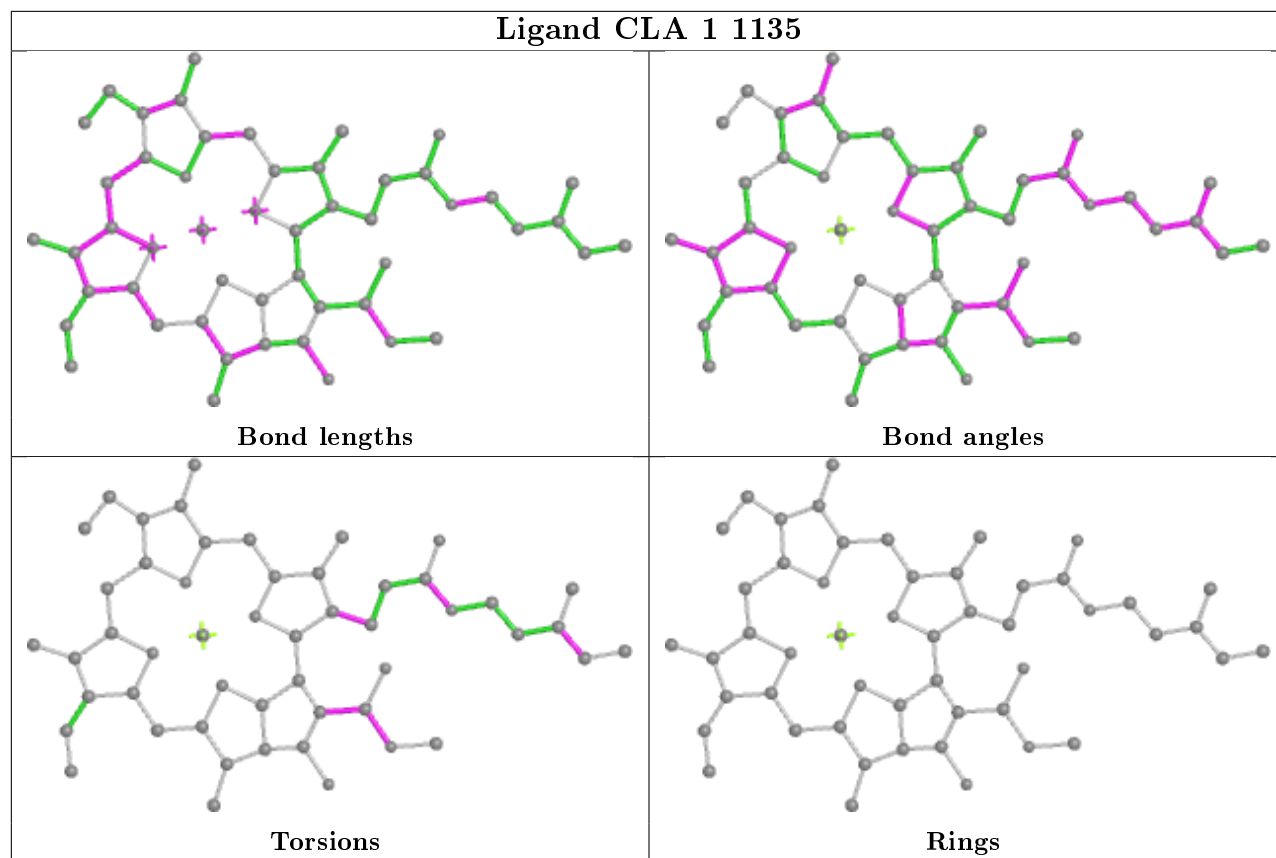
## Ligand CLA 2 1219

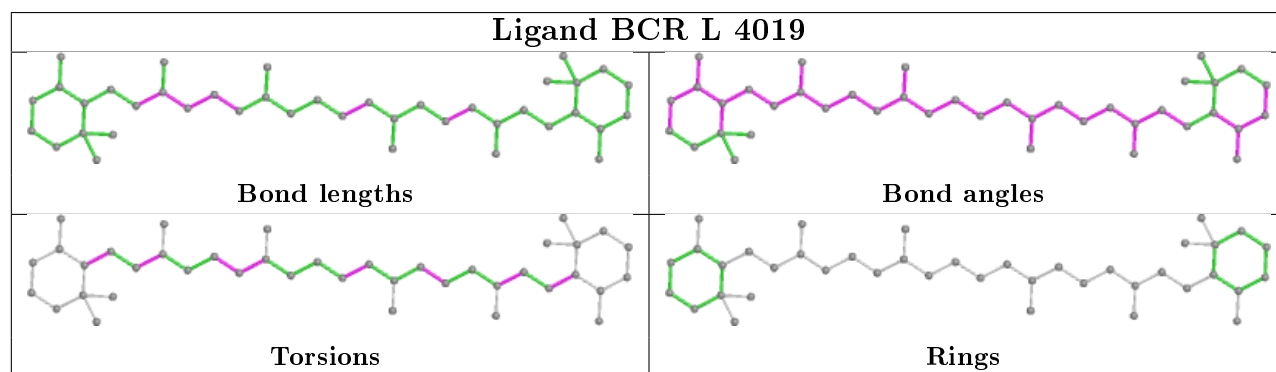
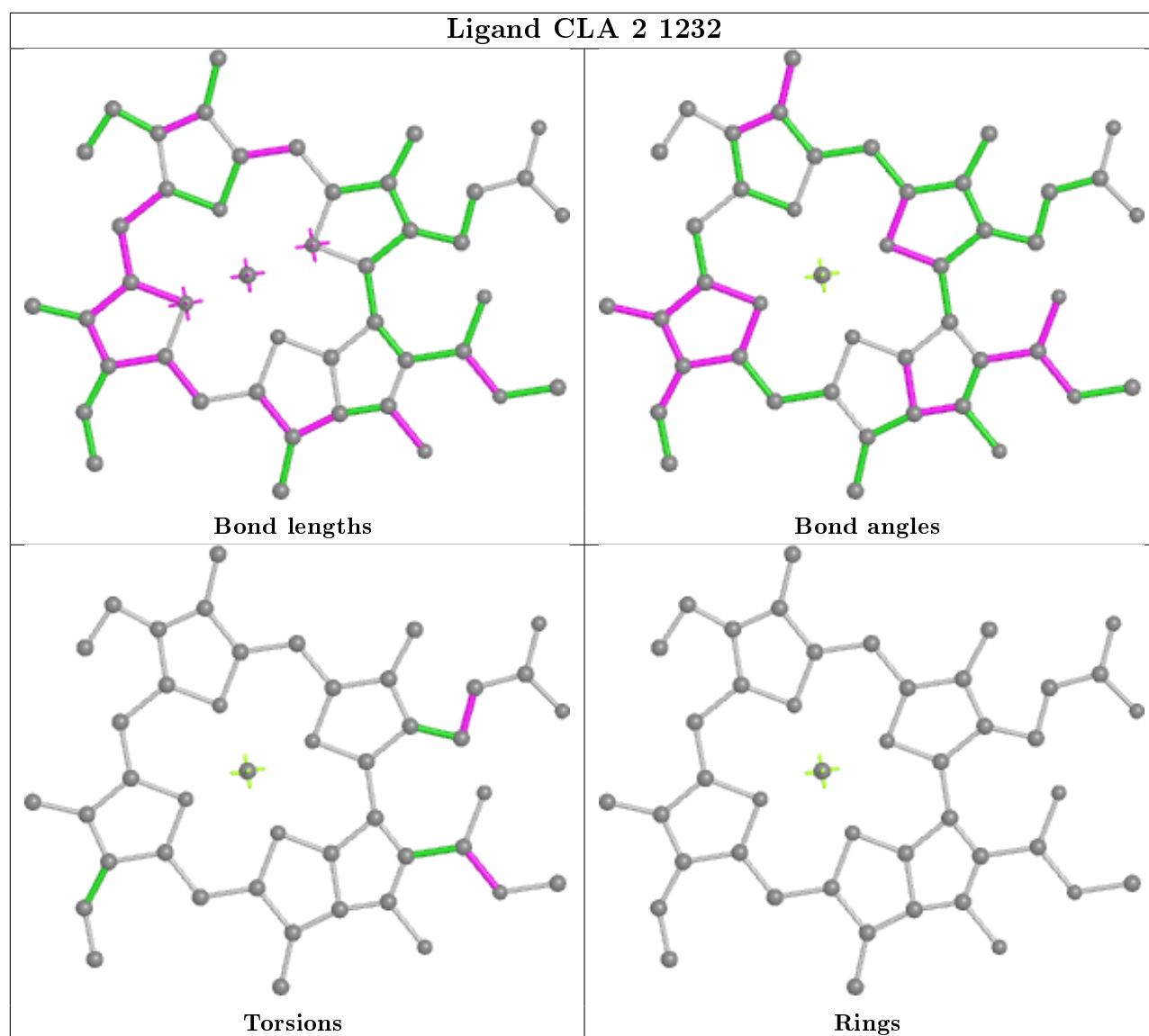


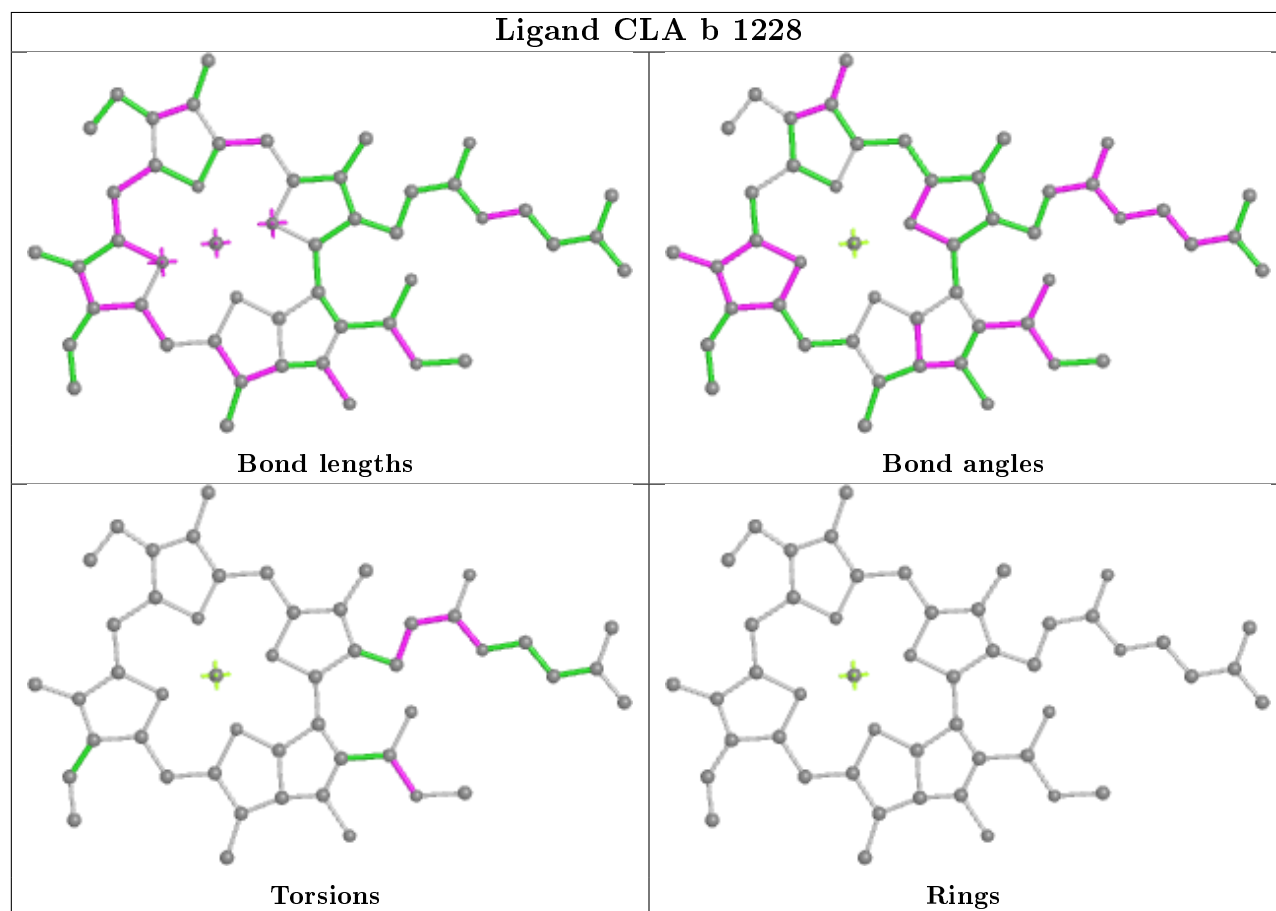
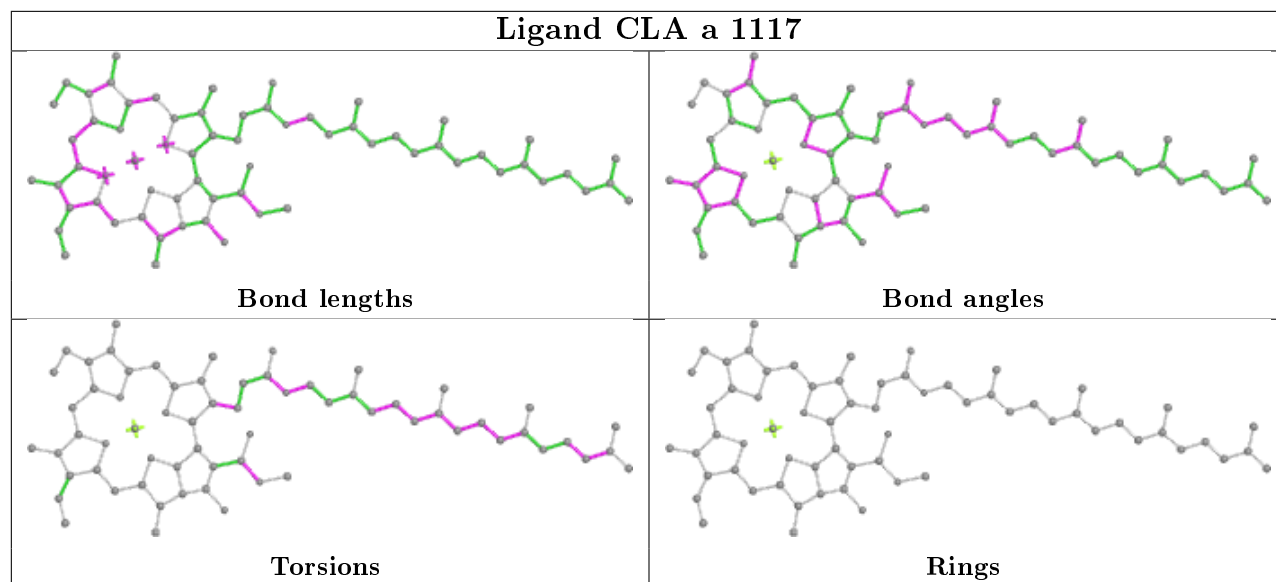


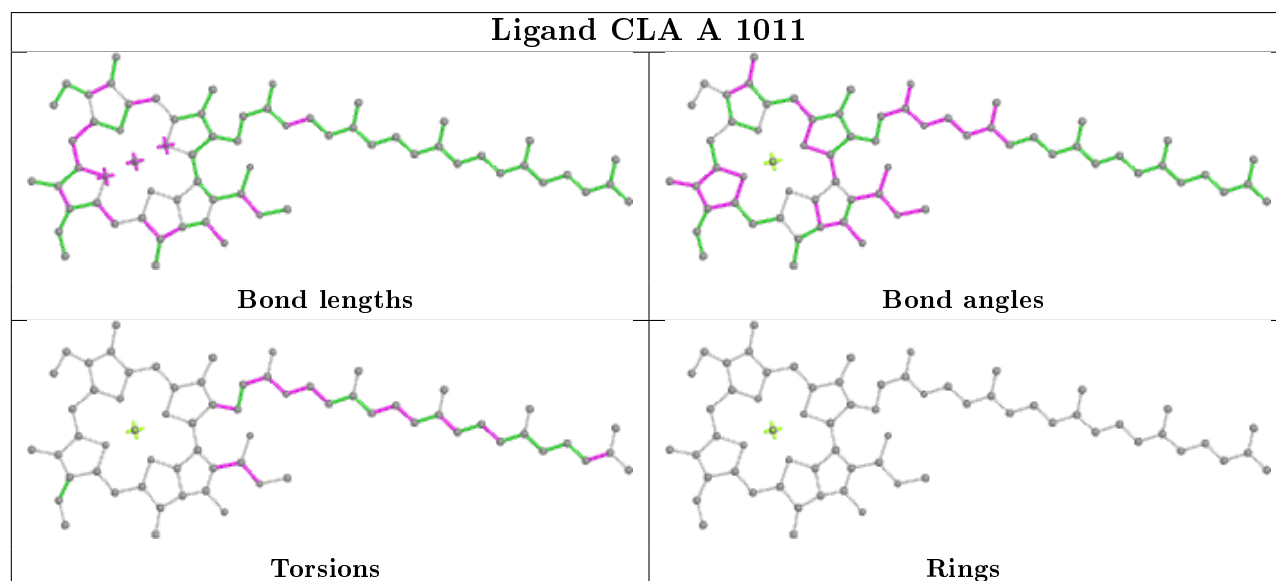
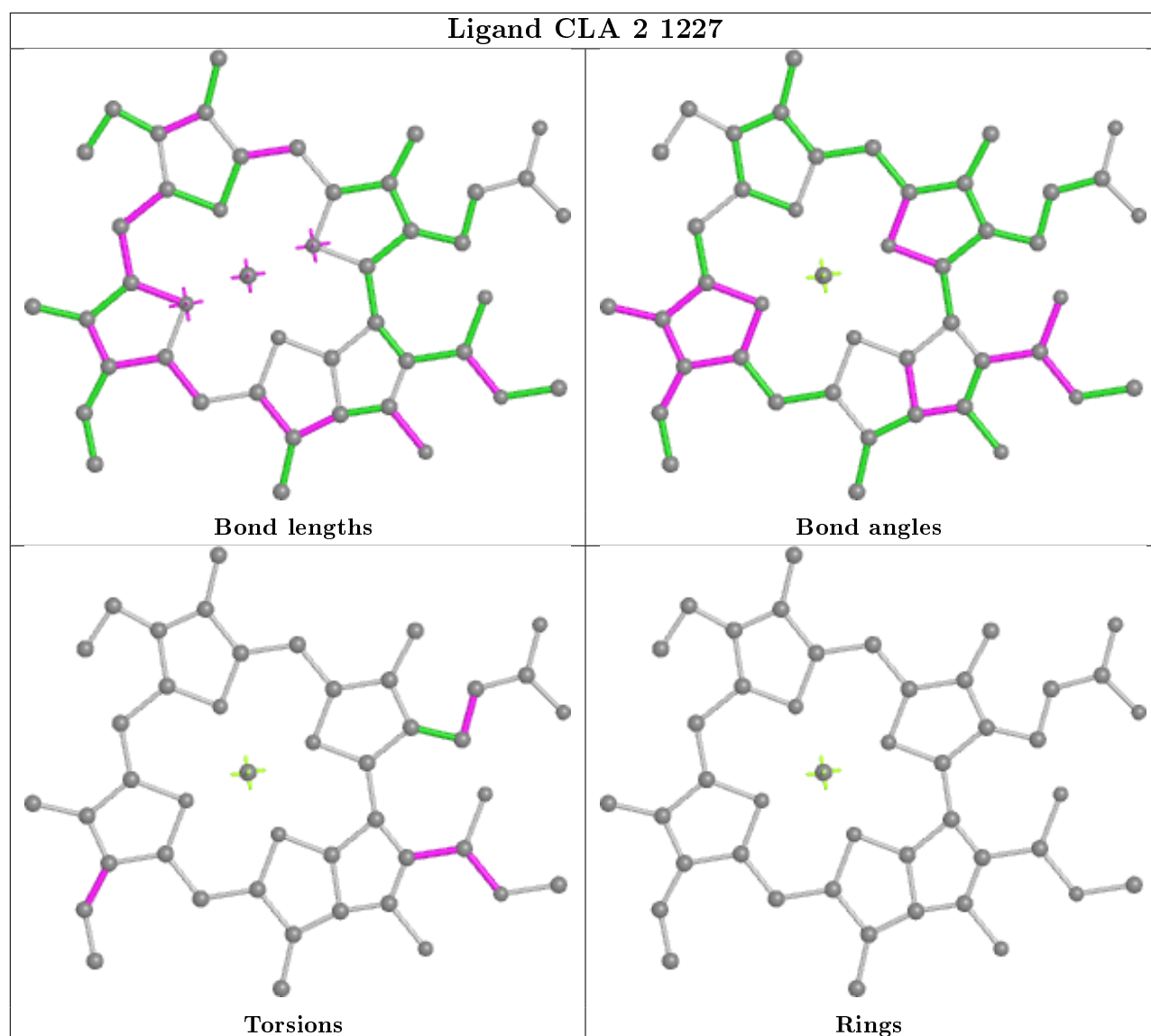


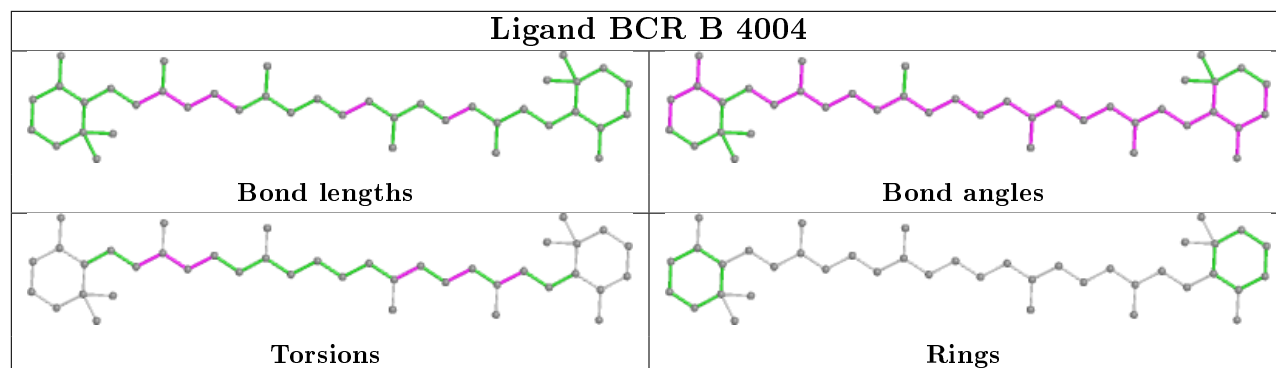
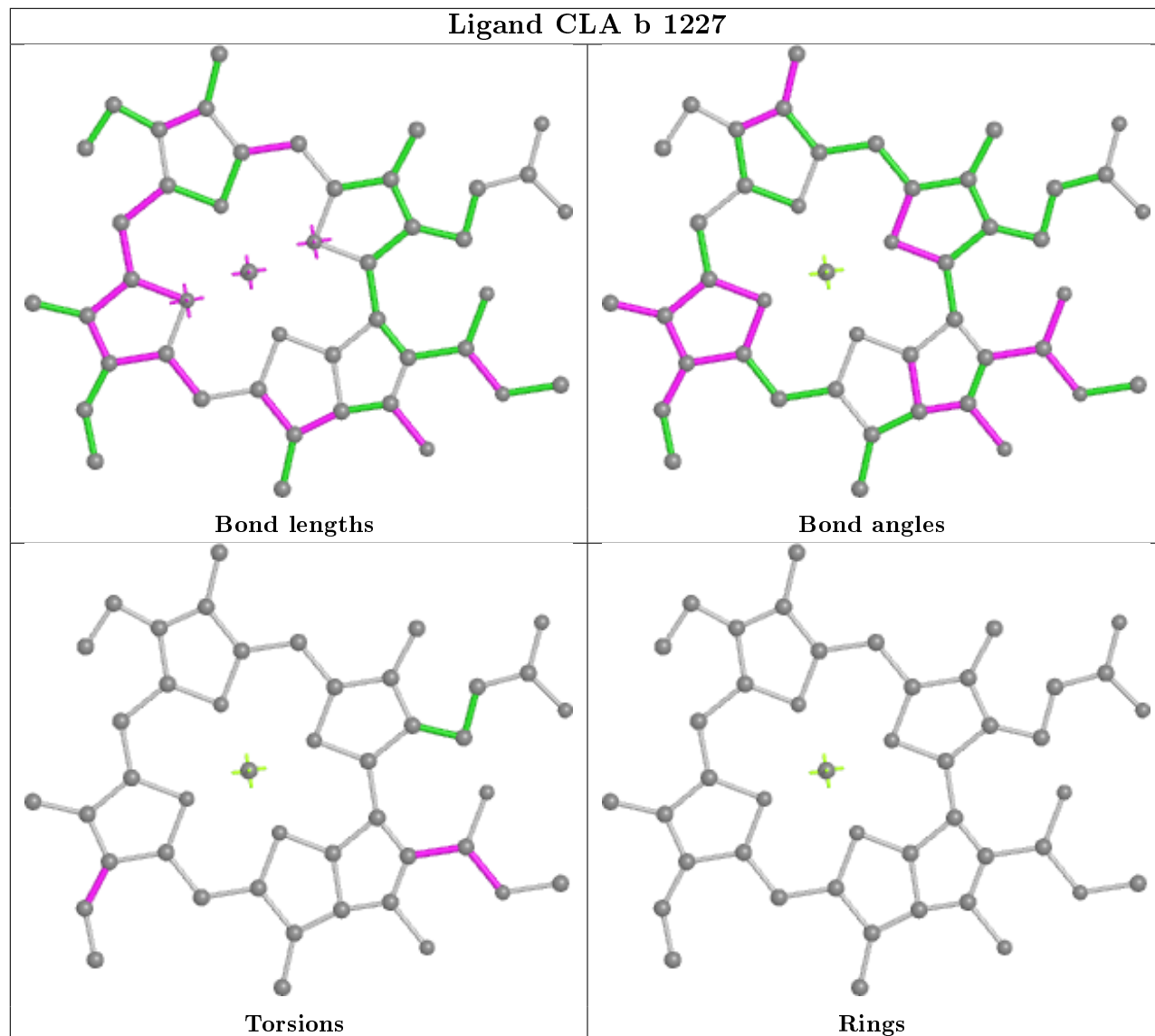




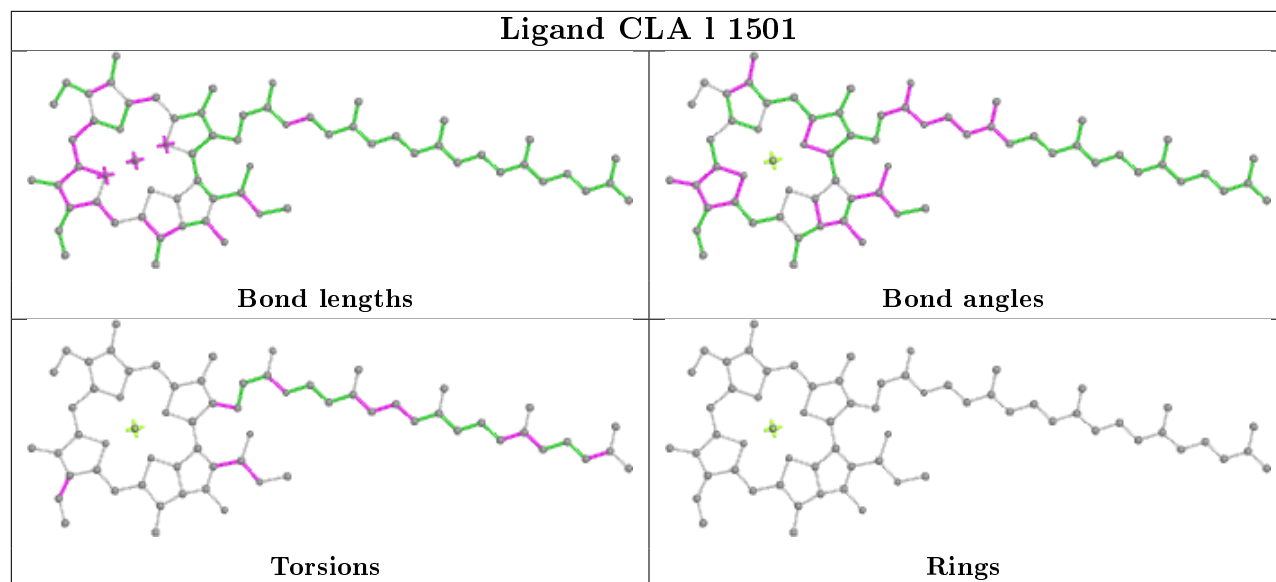




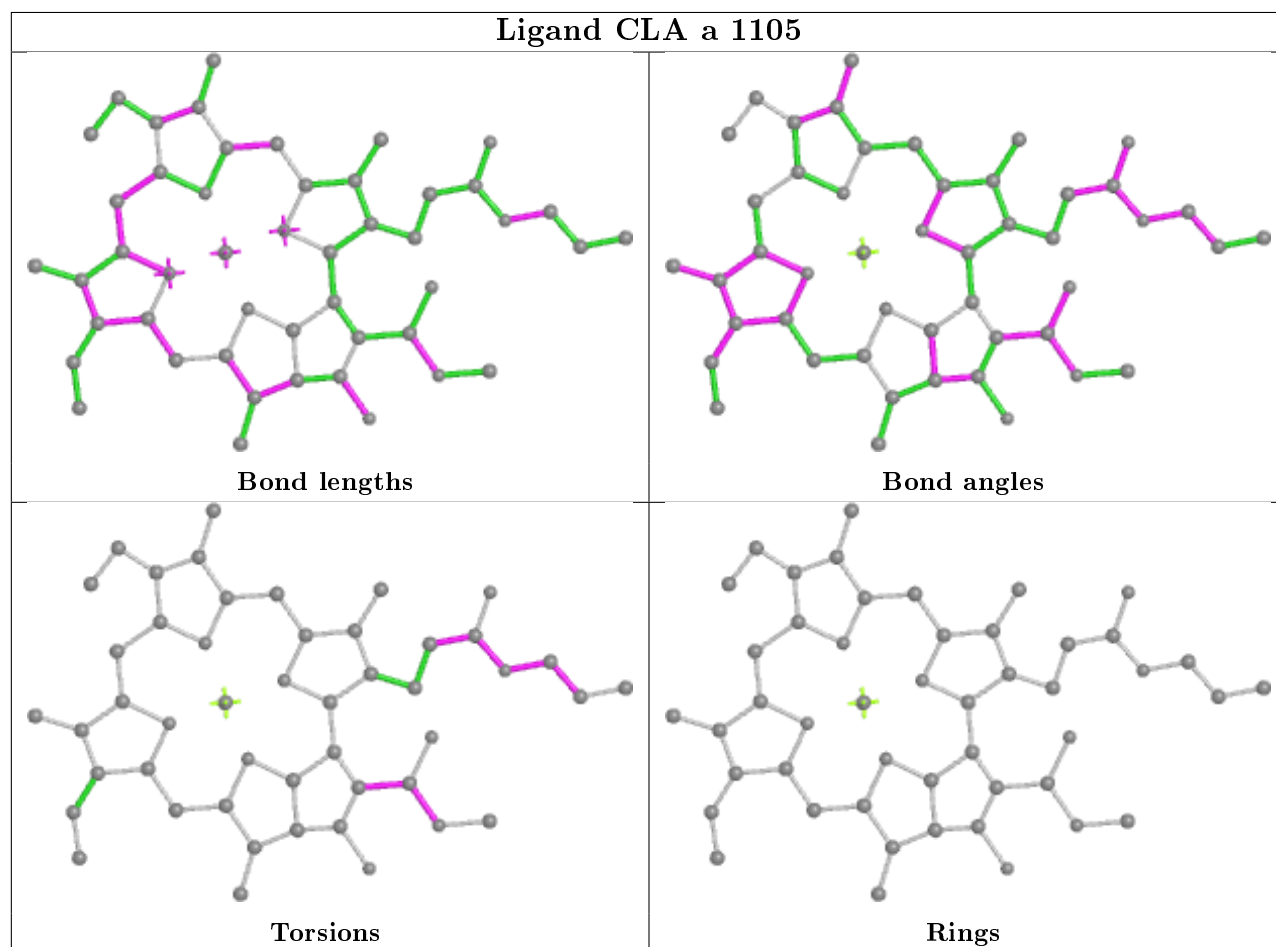


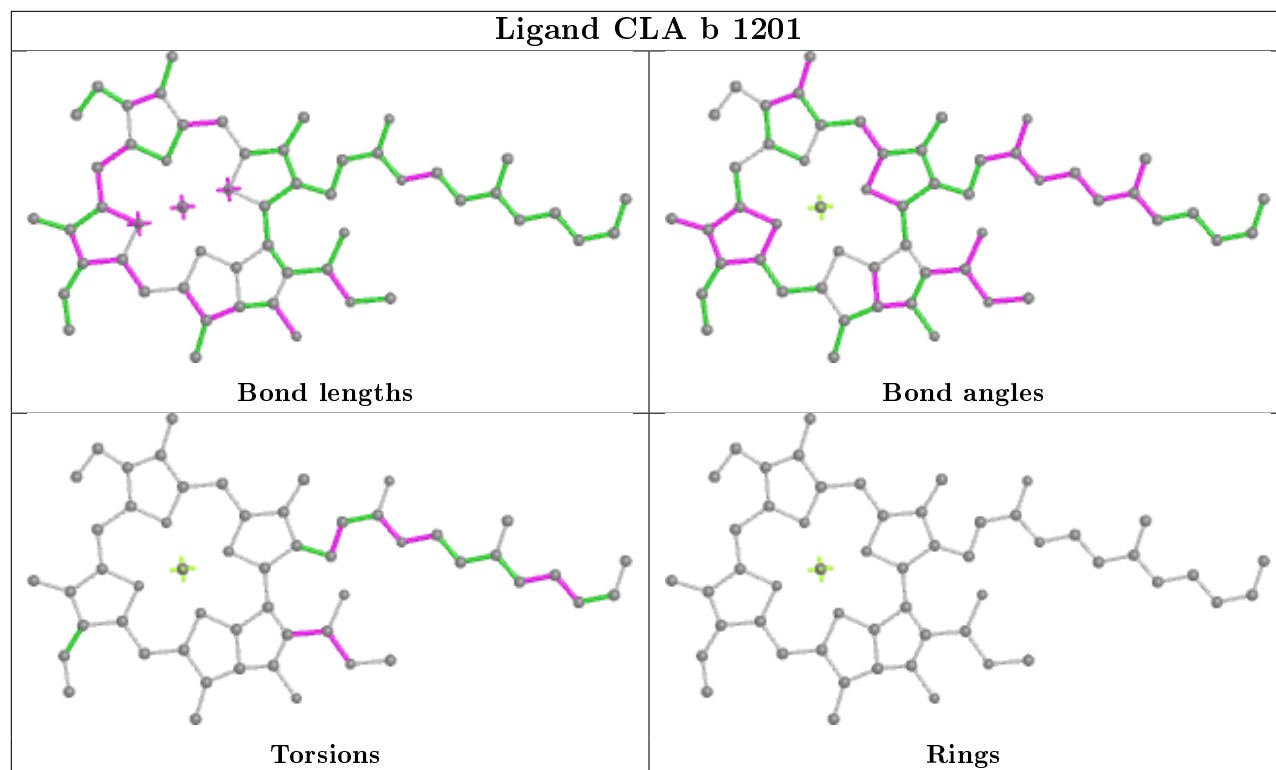
**Ligand BCR B 4004****Ligand CLA b 1227**

## Ligand CLA 1 1501

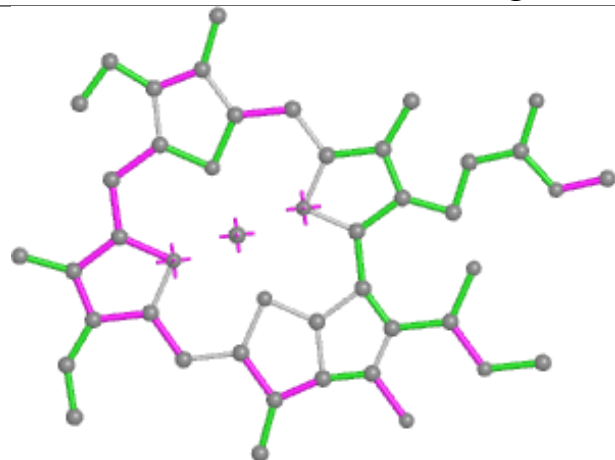


## Ligand CLA a 1105

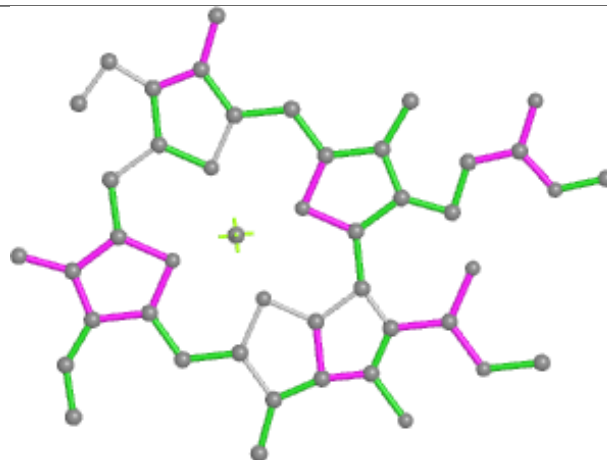




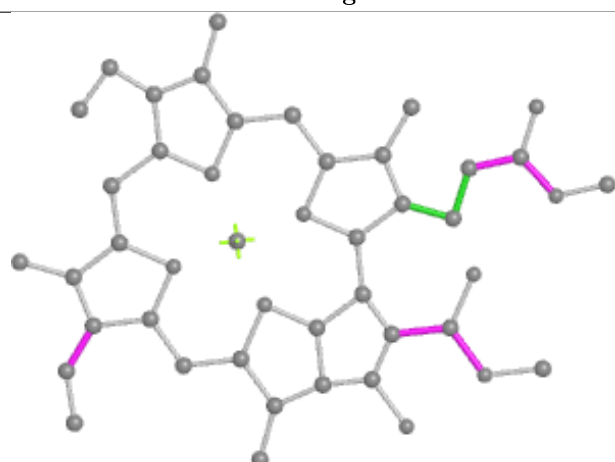
## Ligand CLA B 1239



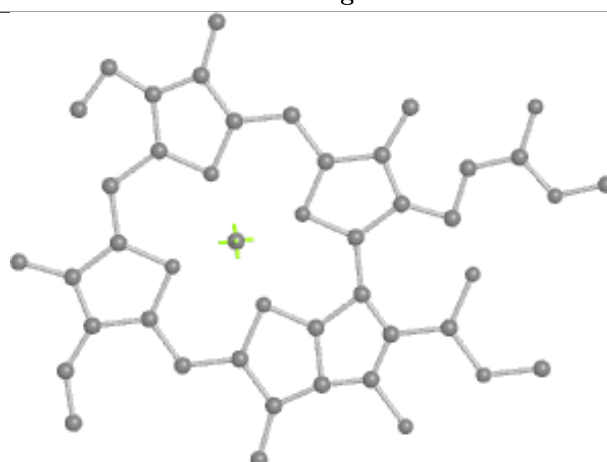
Bond lengths



Bond angles

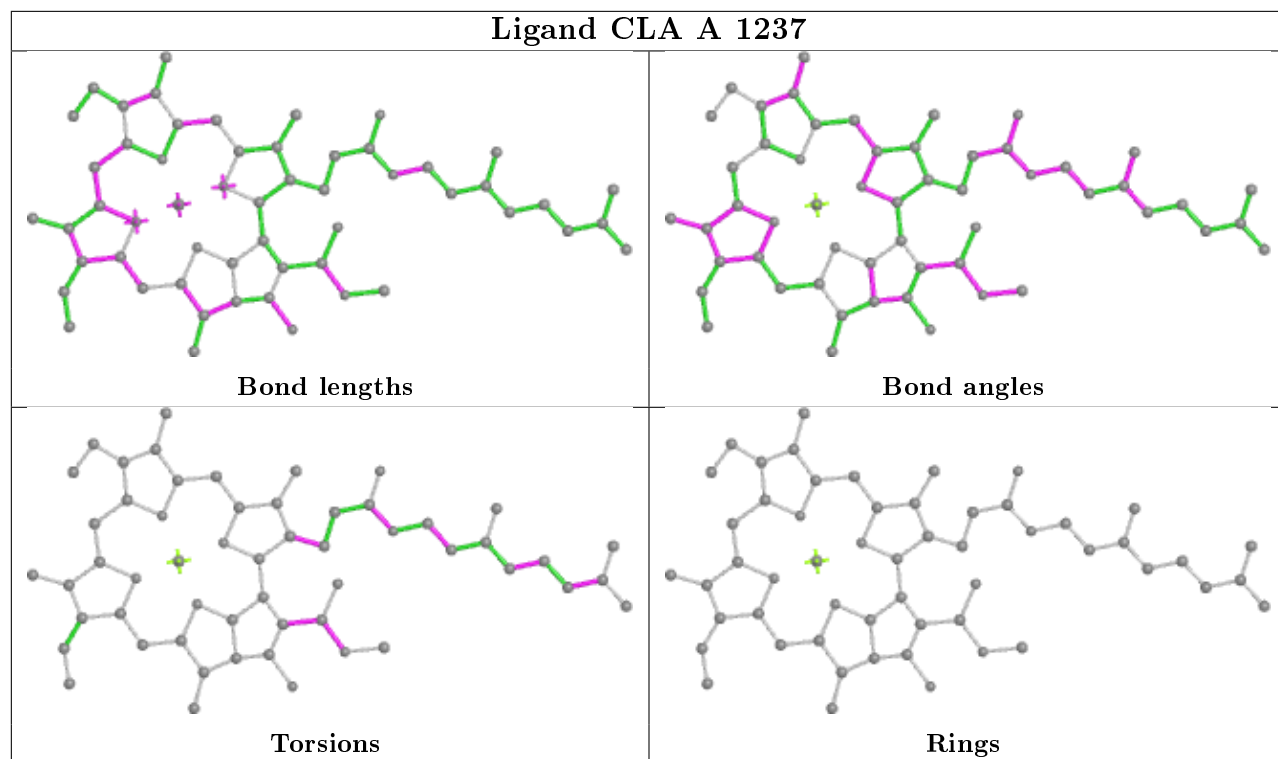


Torsions

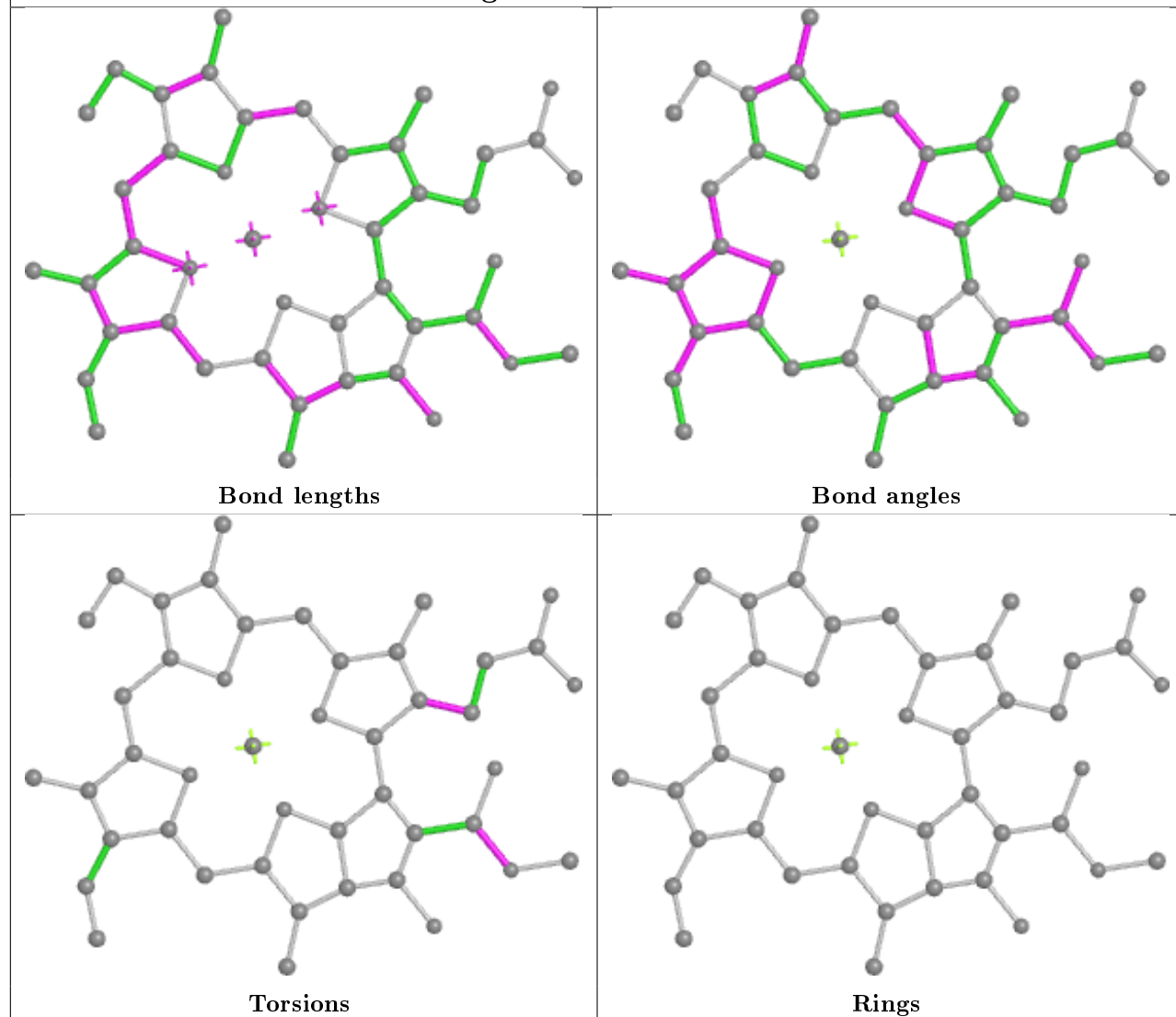


Rings

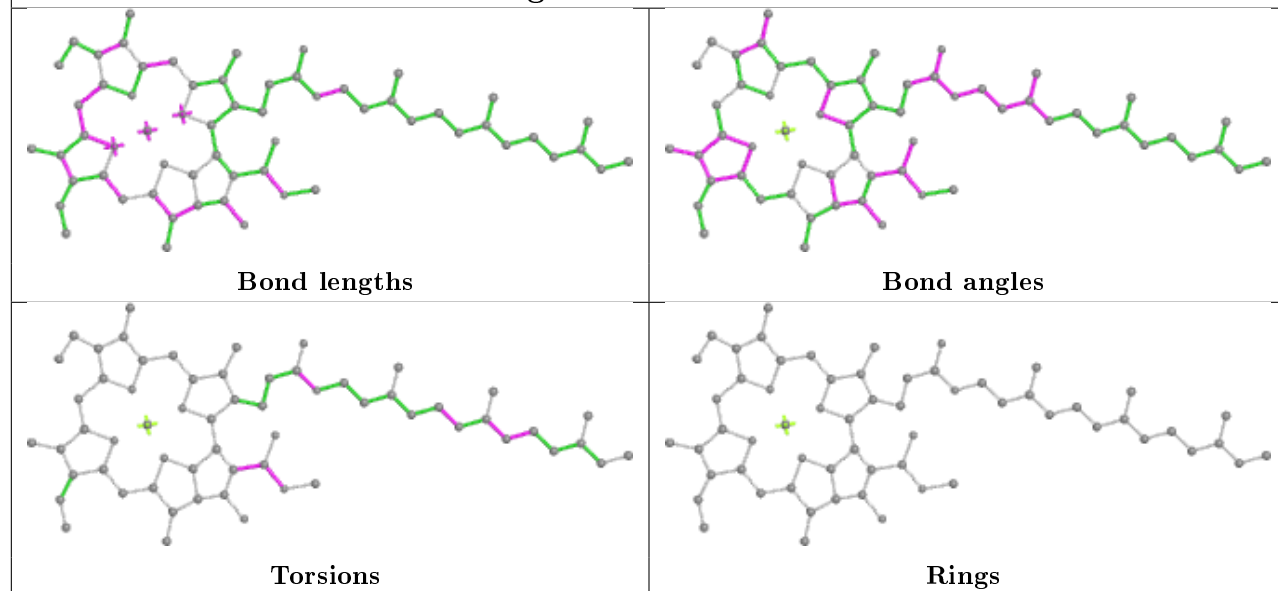


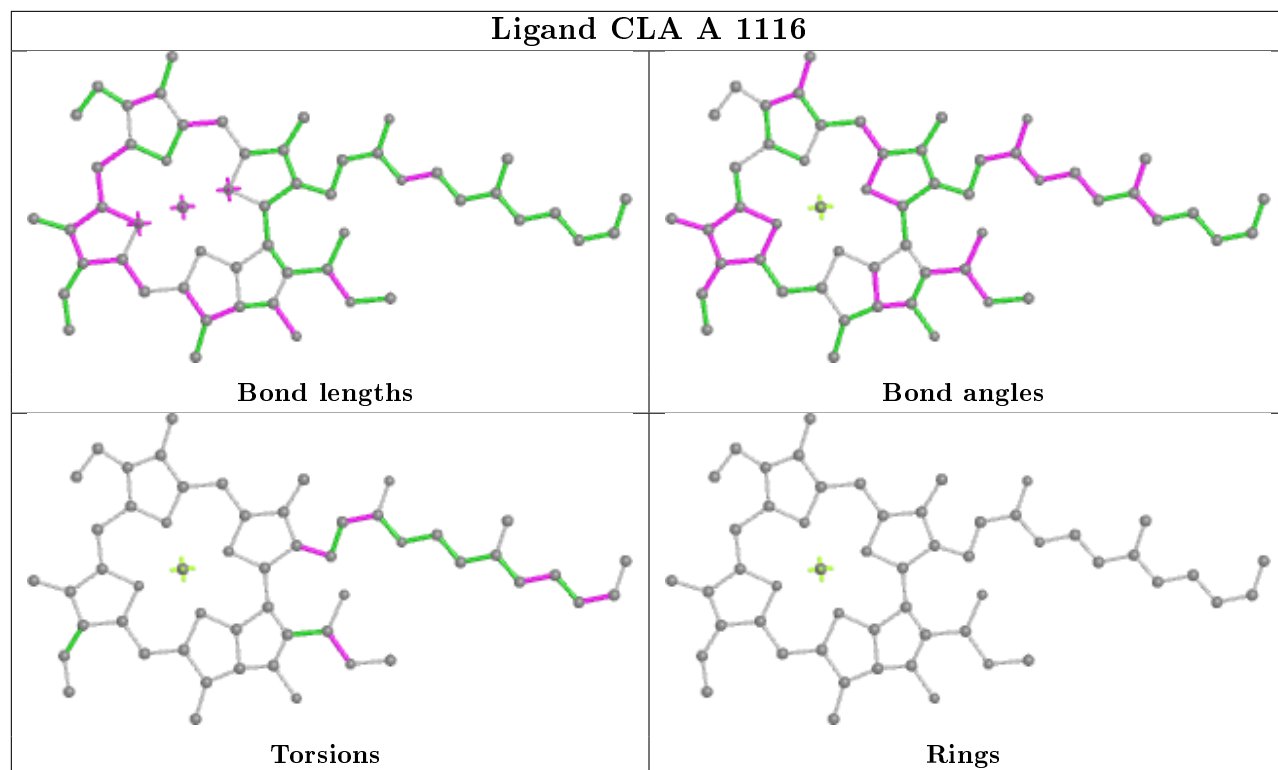


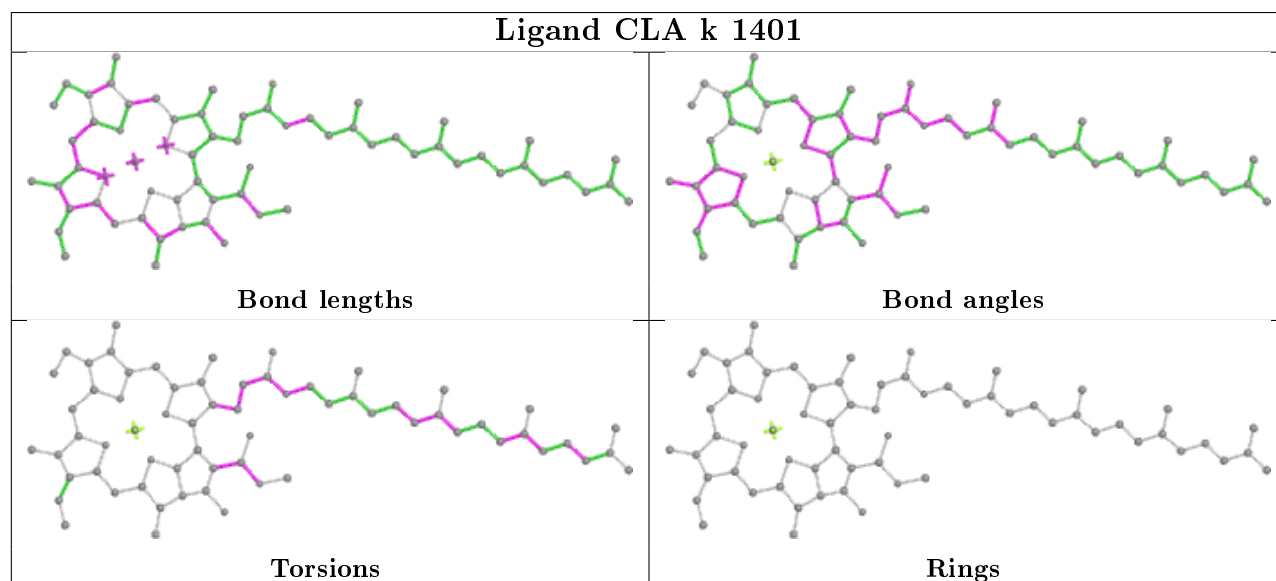
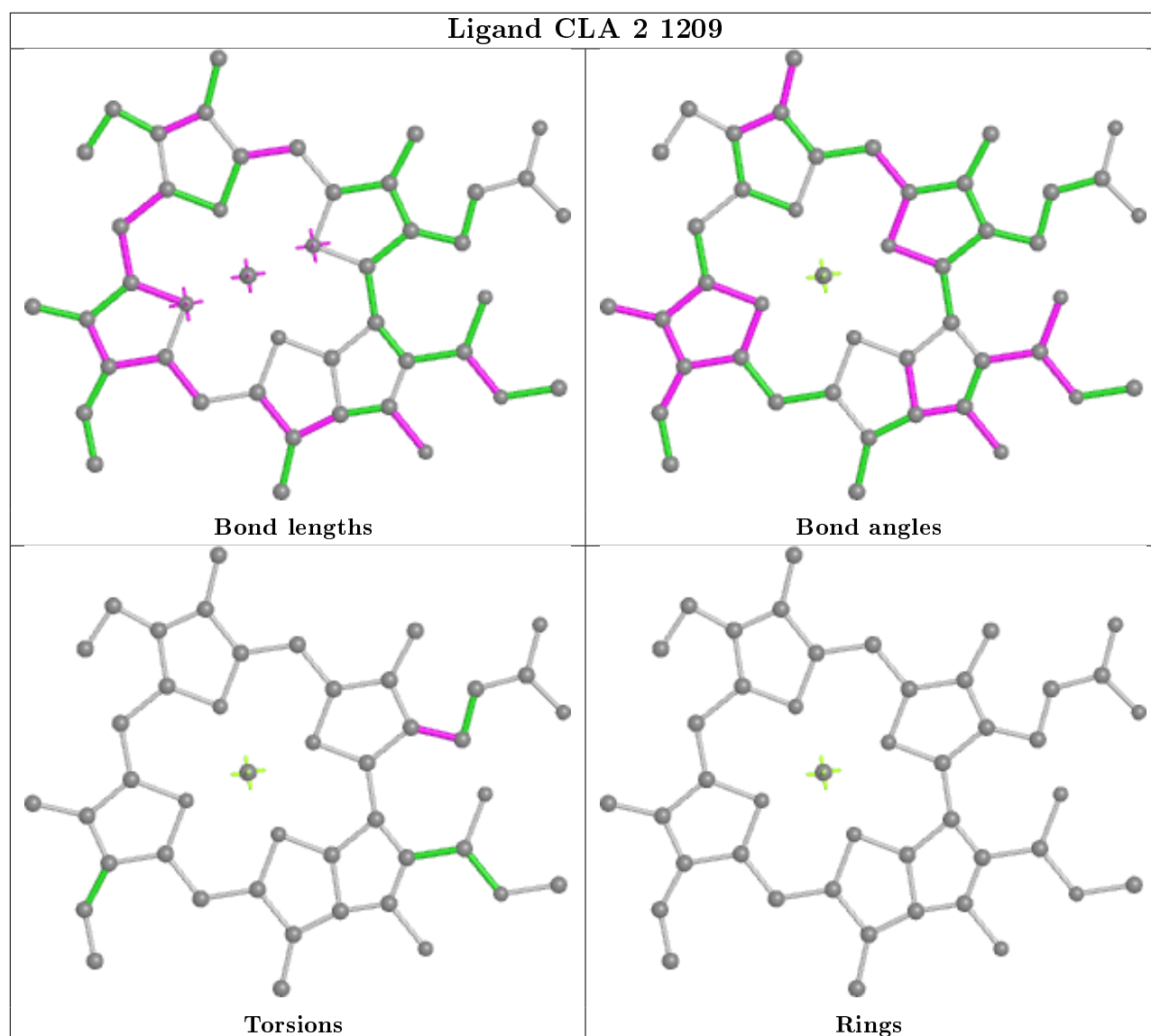
## Ligand CLA B 1209

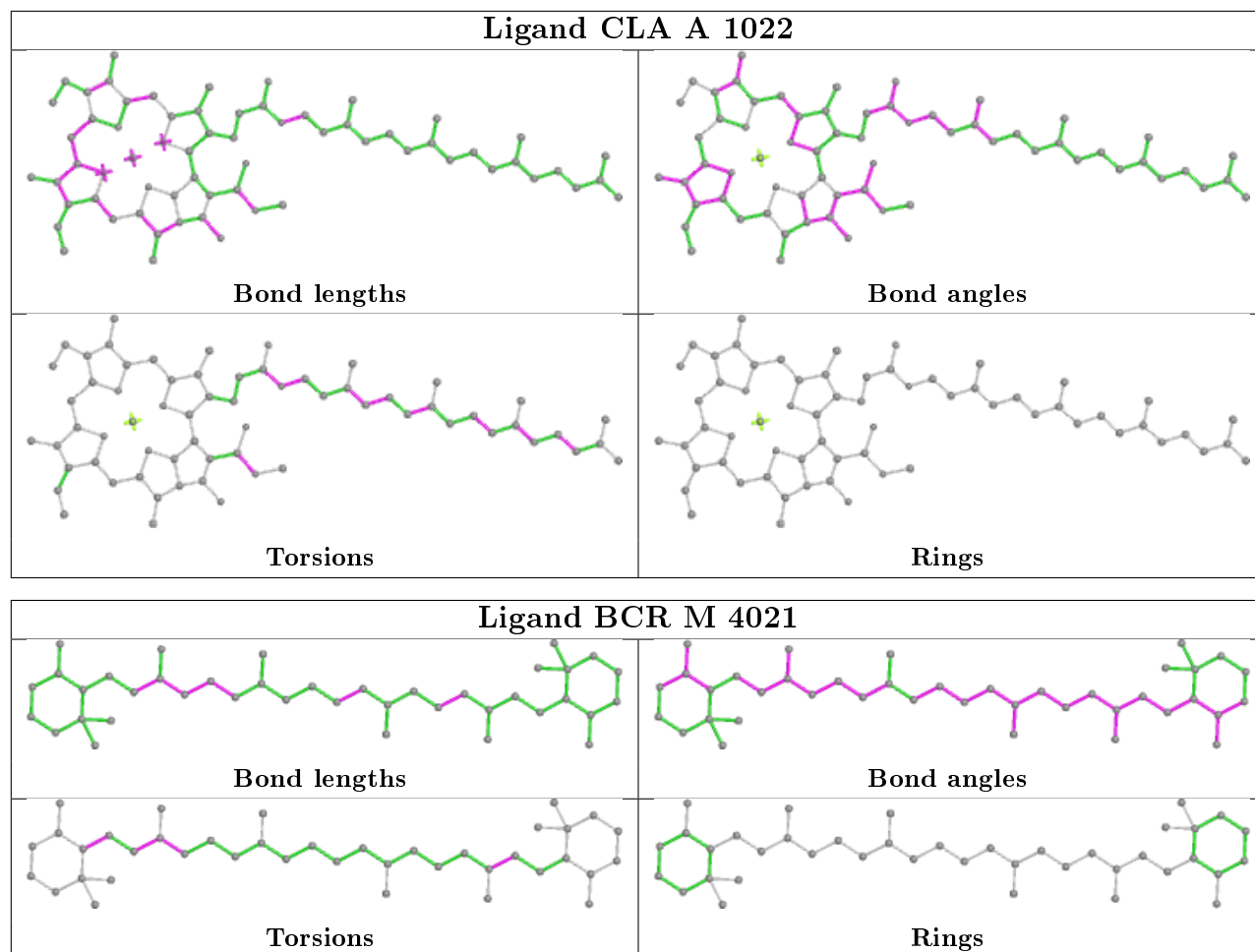


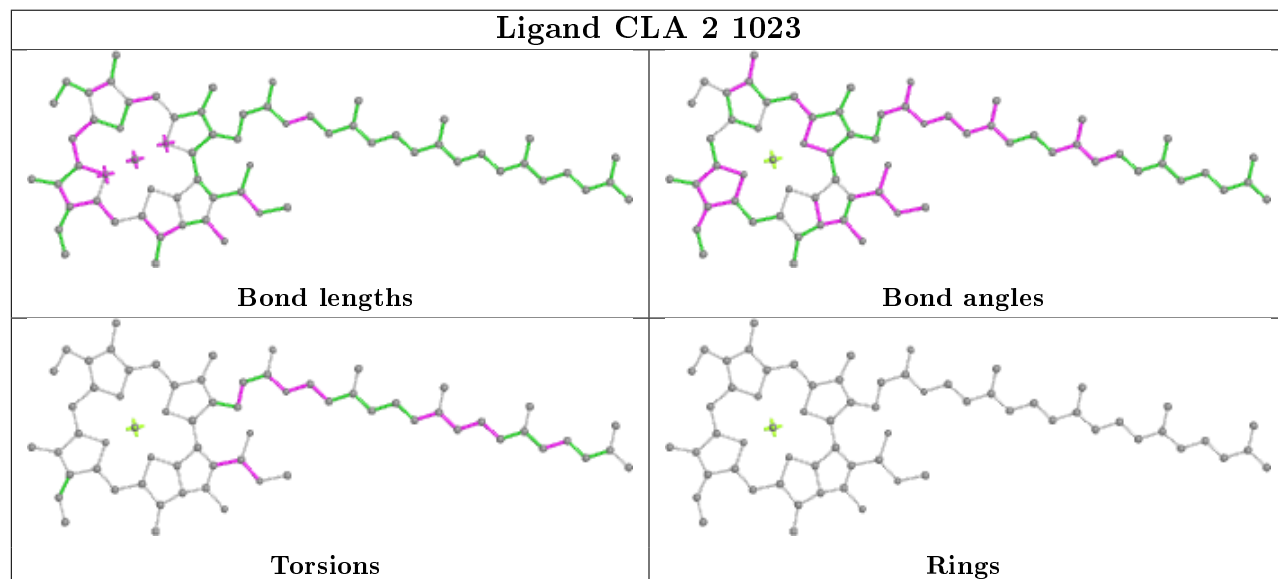
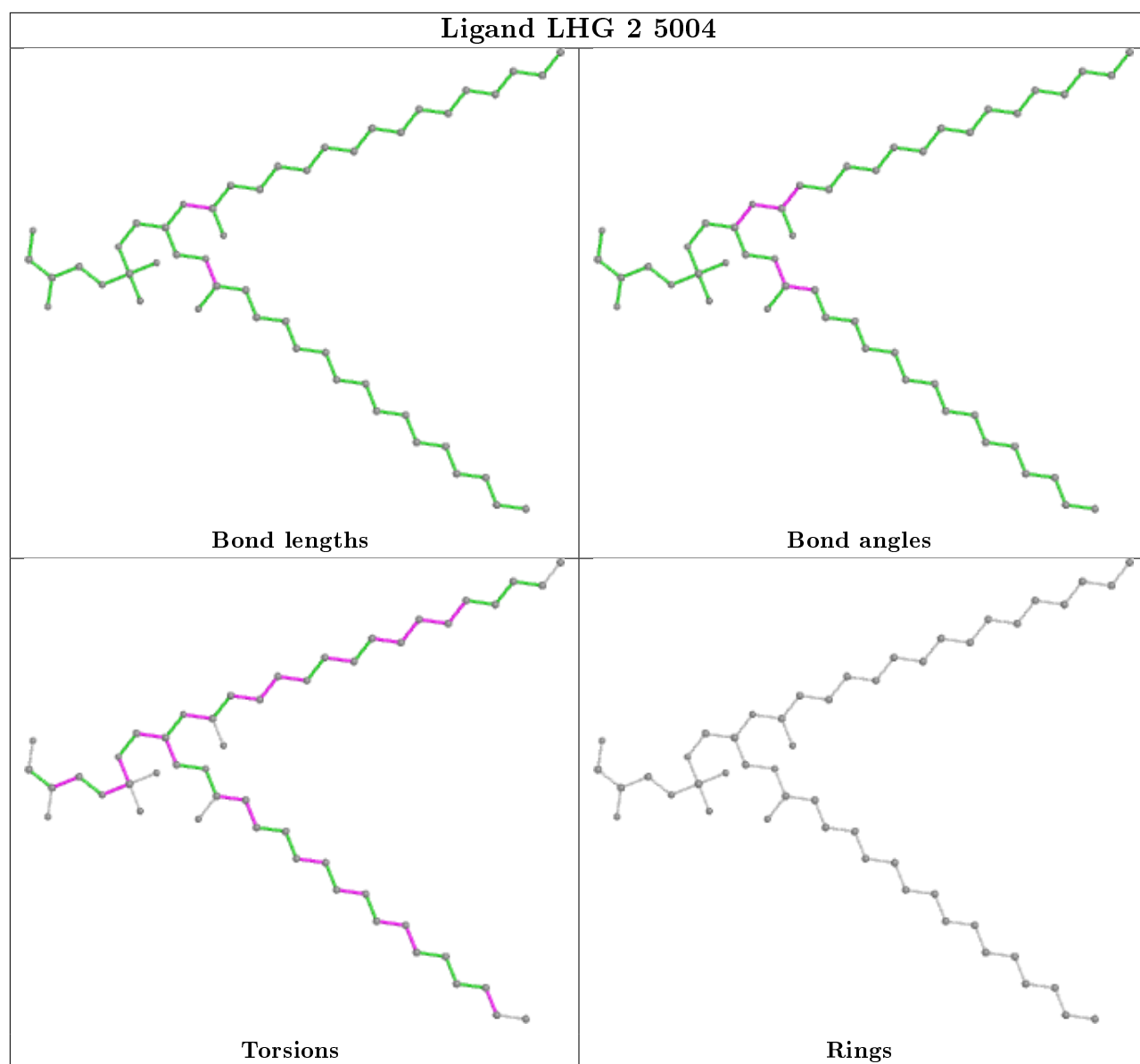
## Ligand CLA a 1118

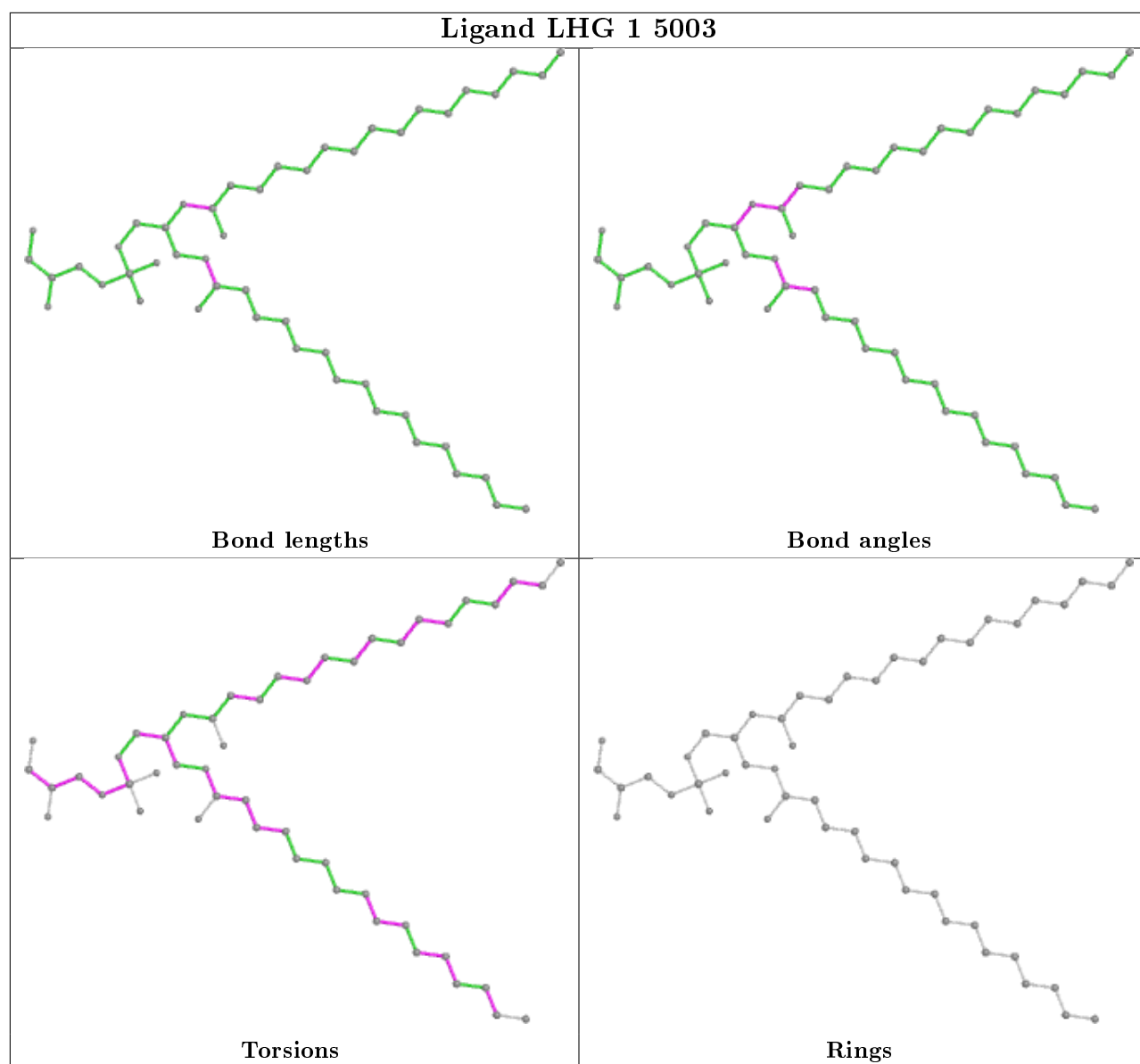


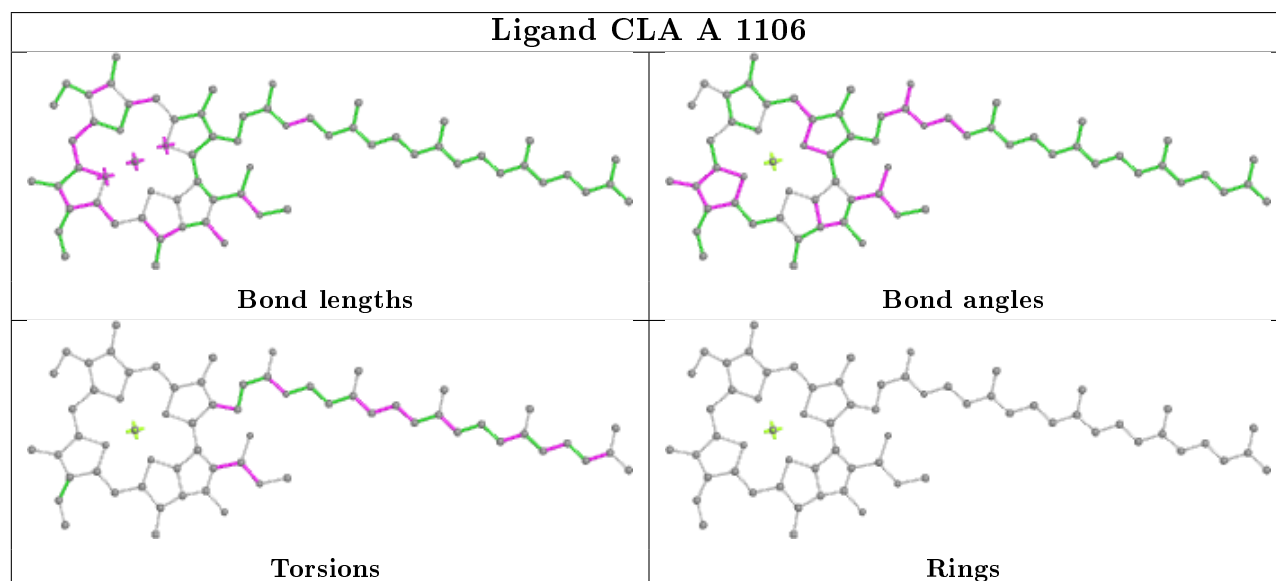
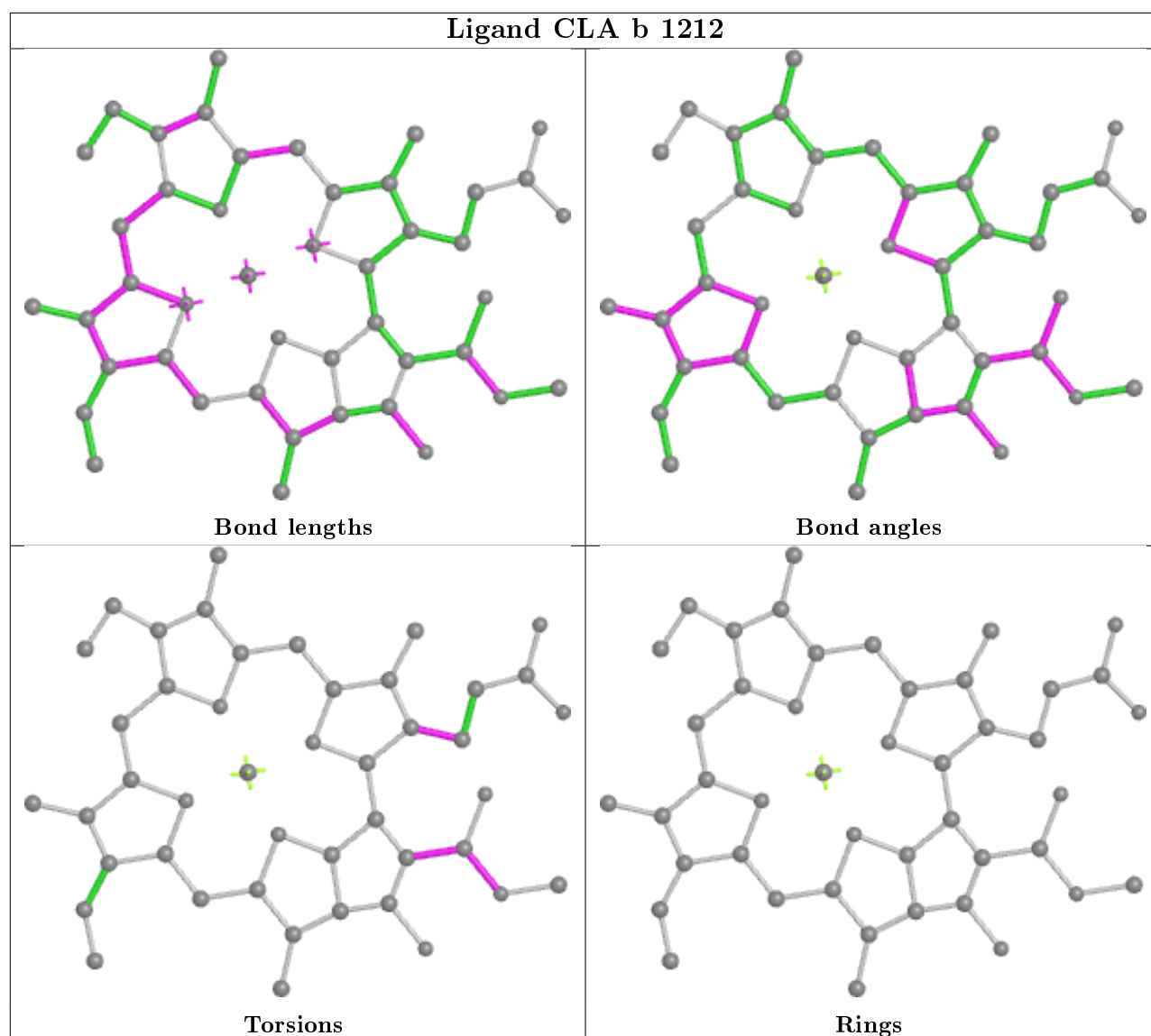




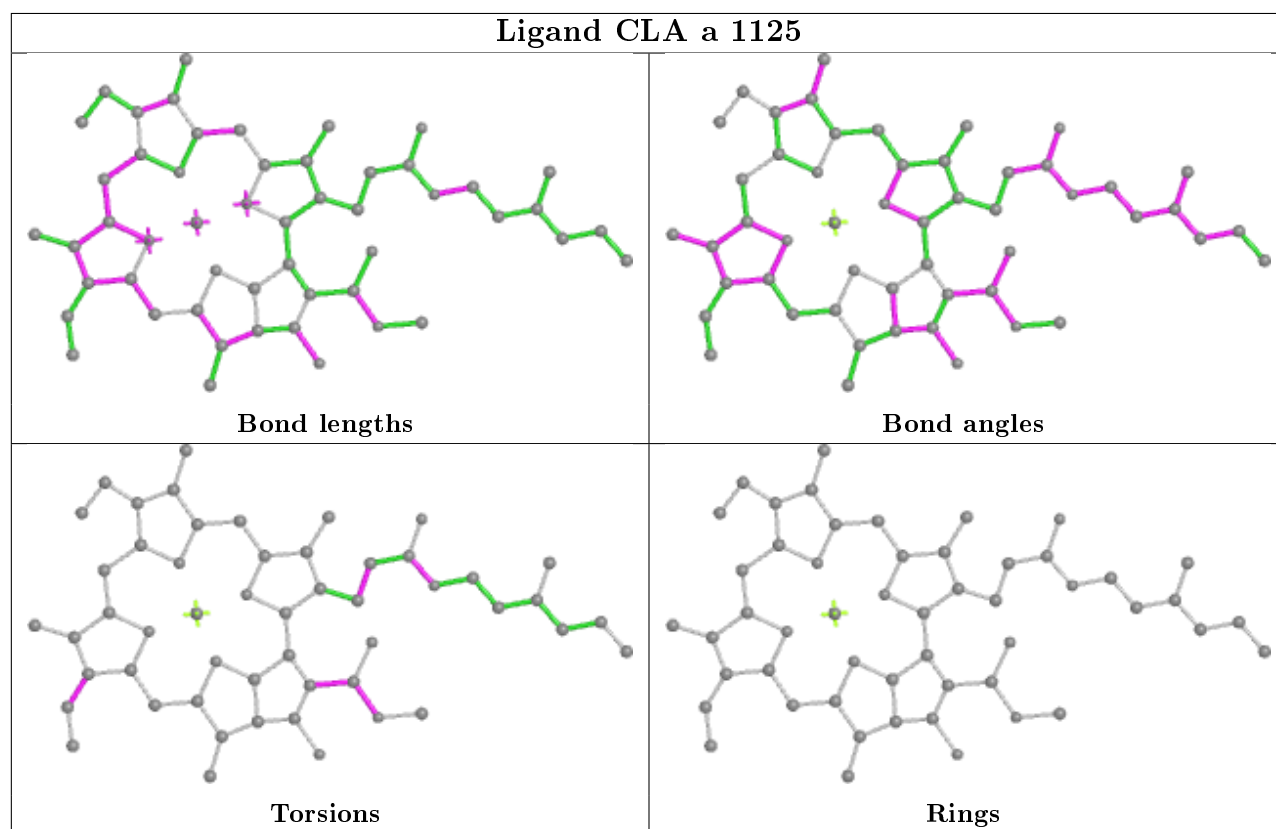
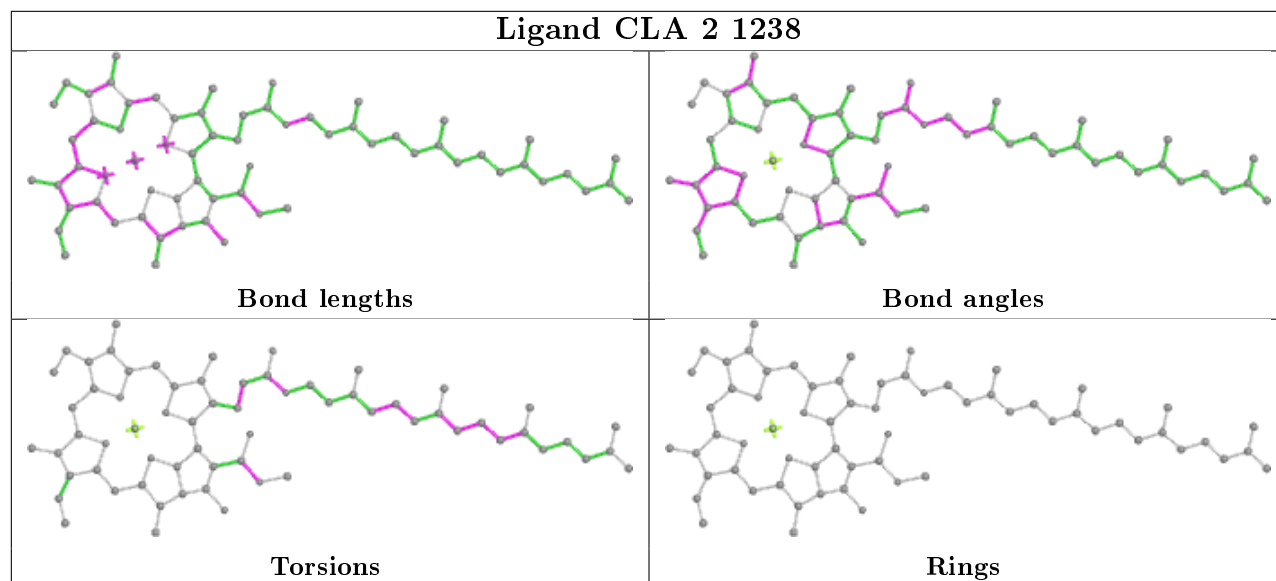
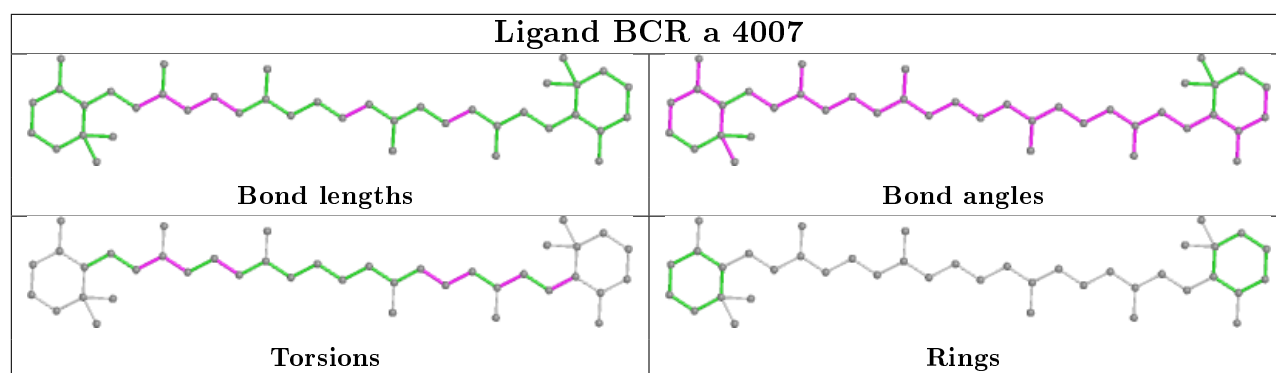




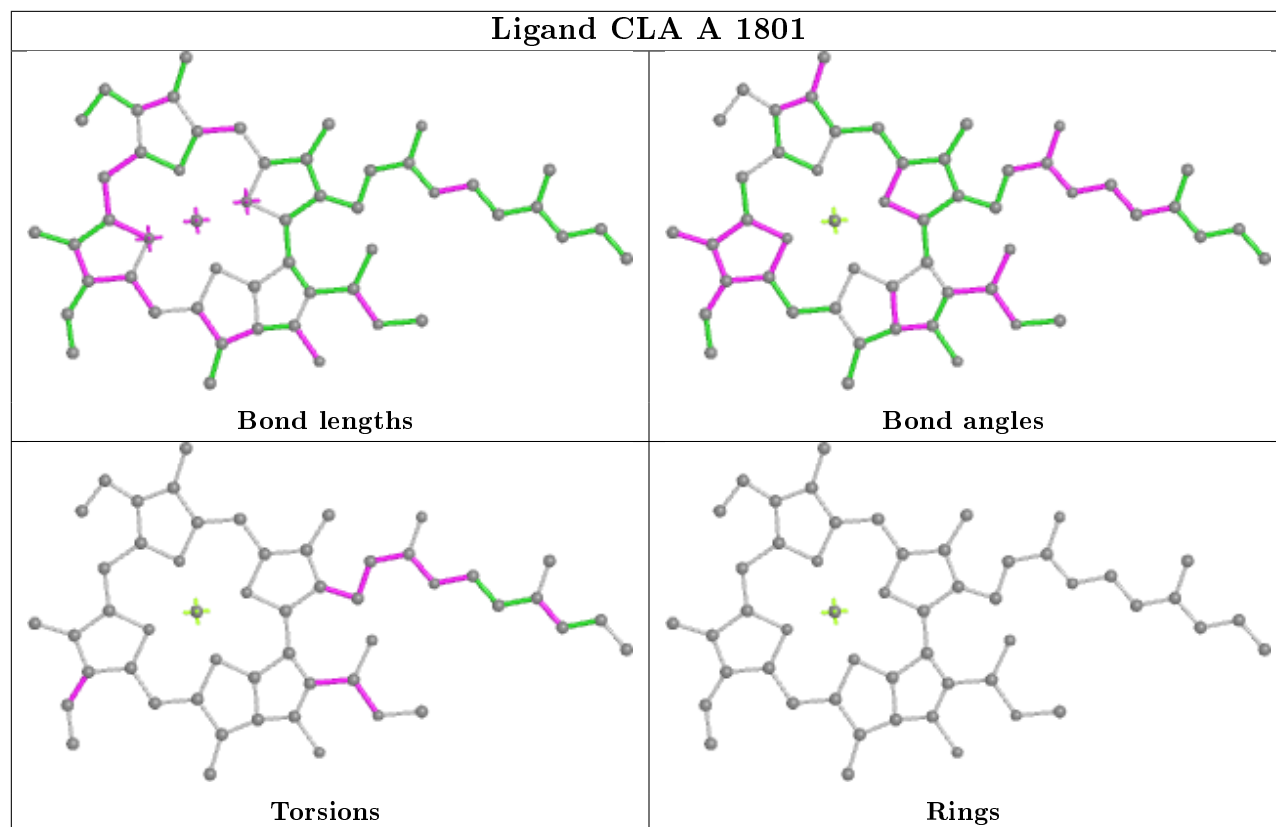




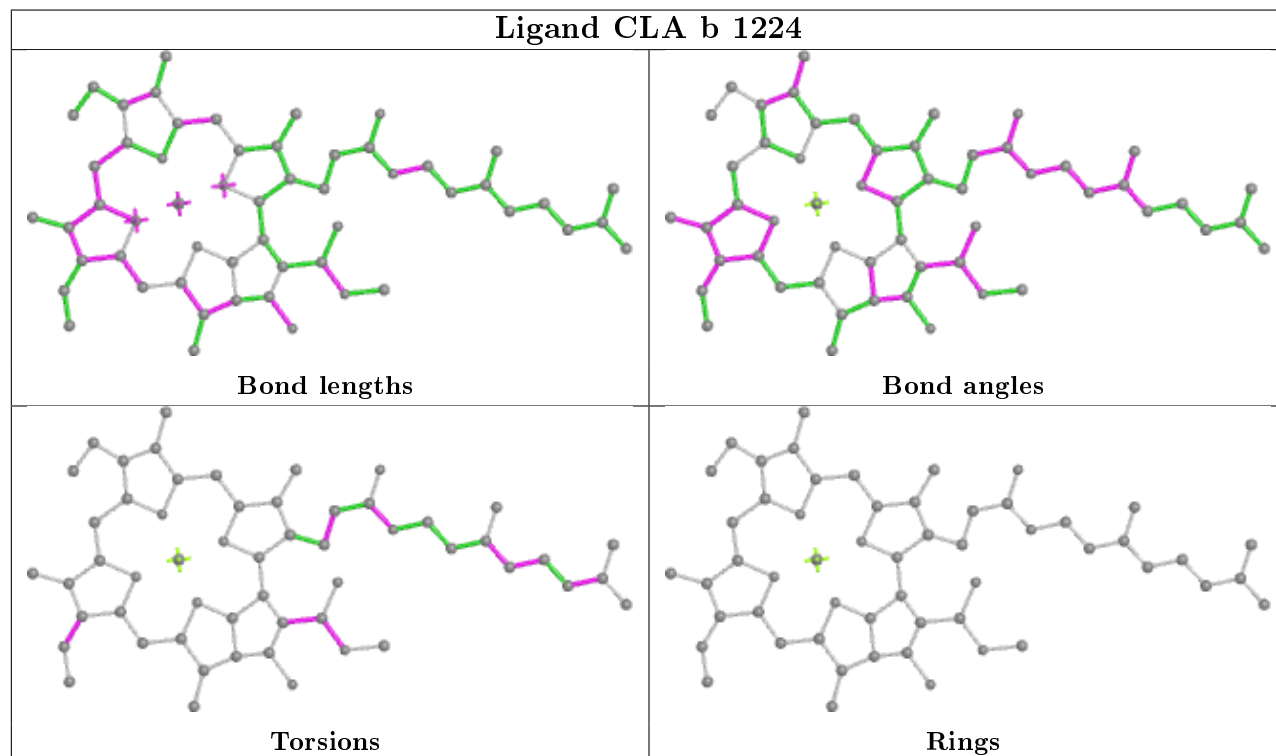


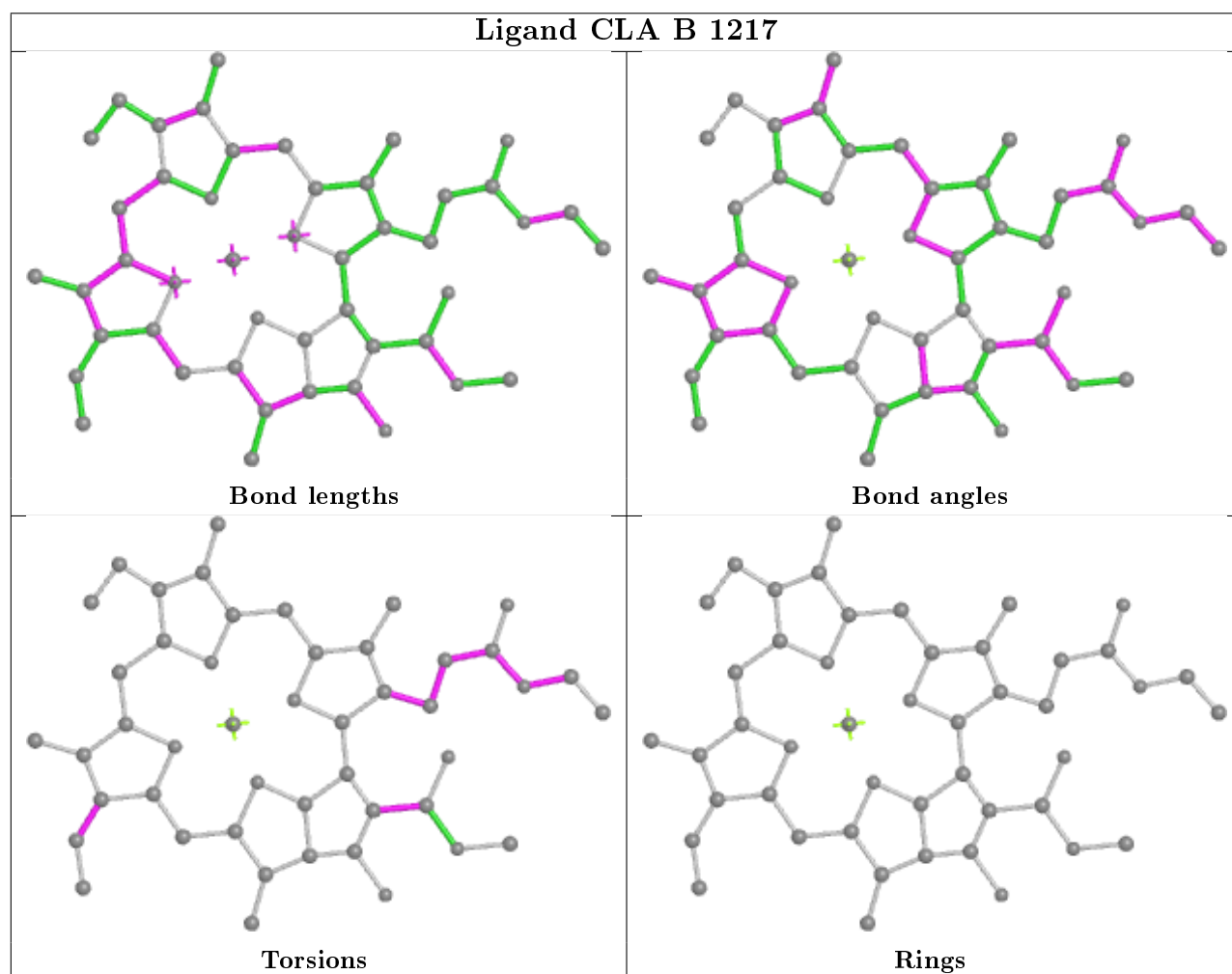
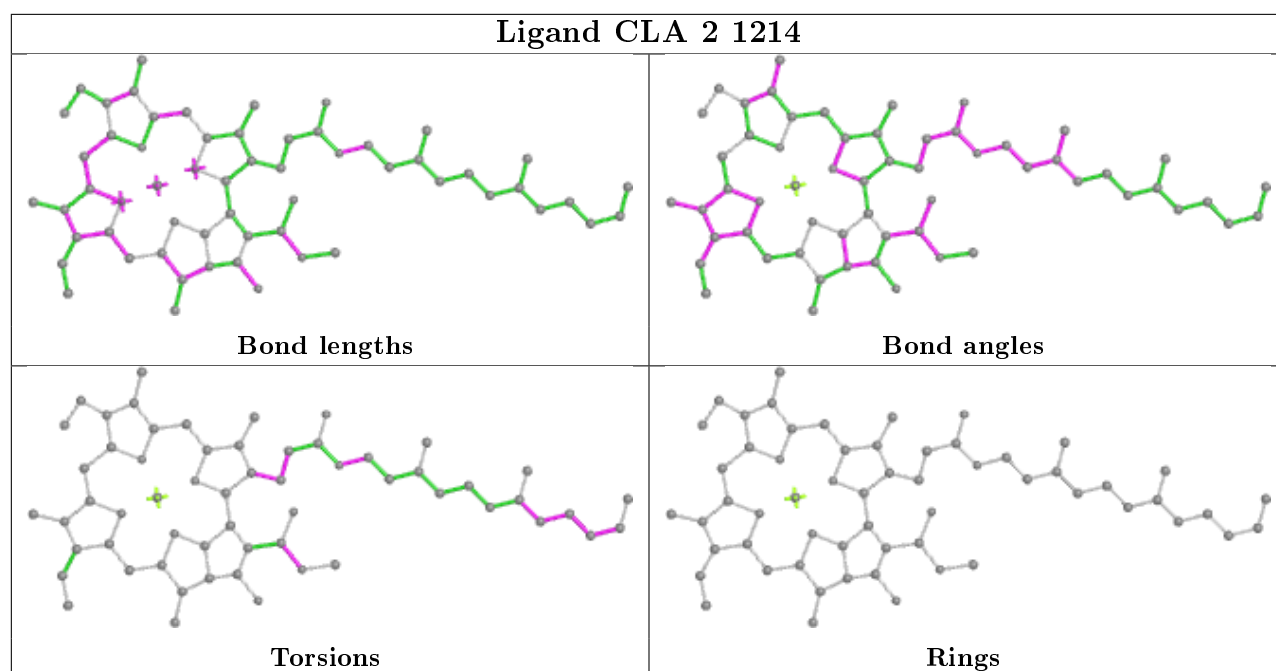


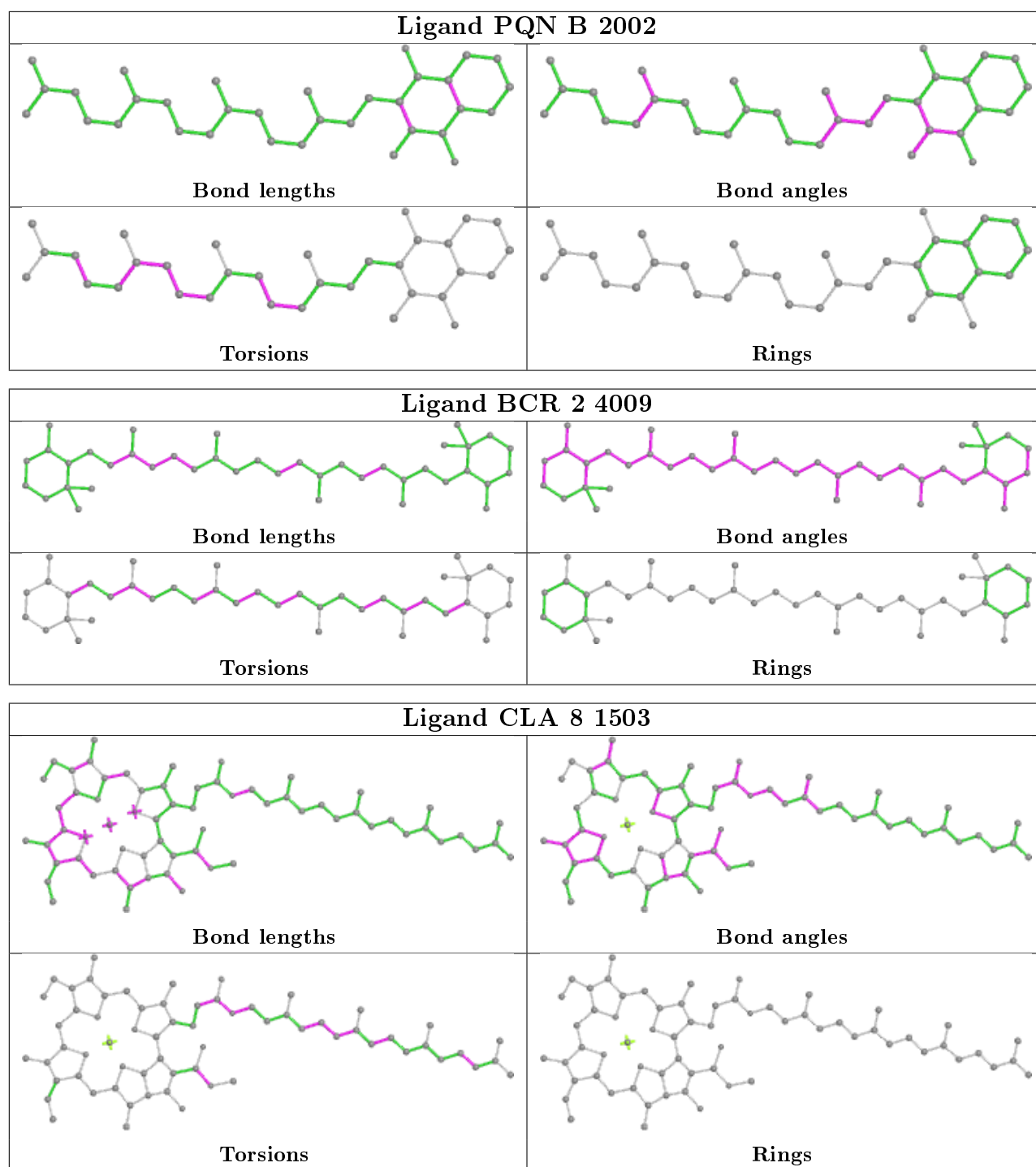
## Ligand CLA A 1801

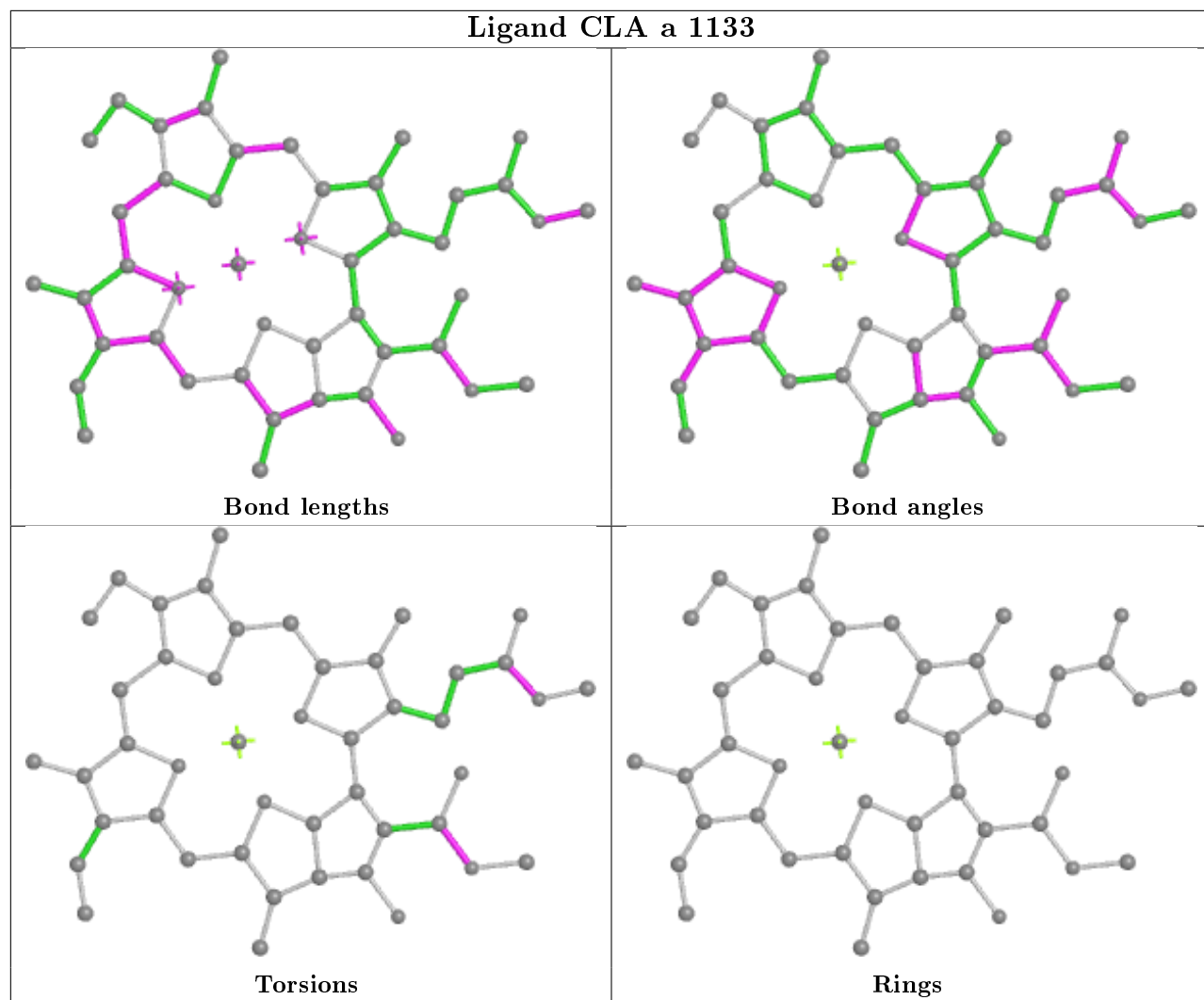


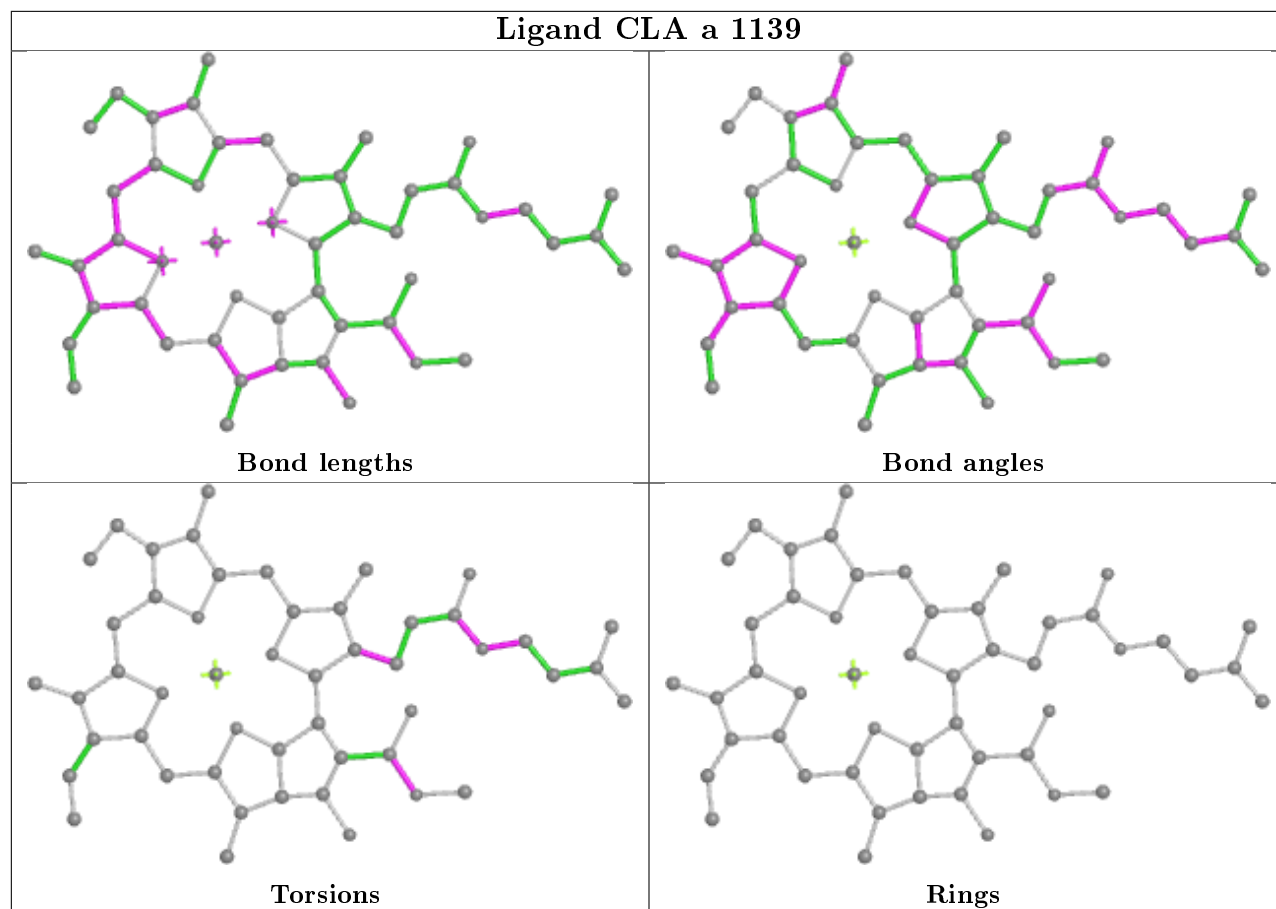
## Ligand CLA b 1224

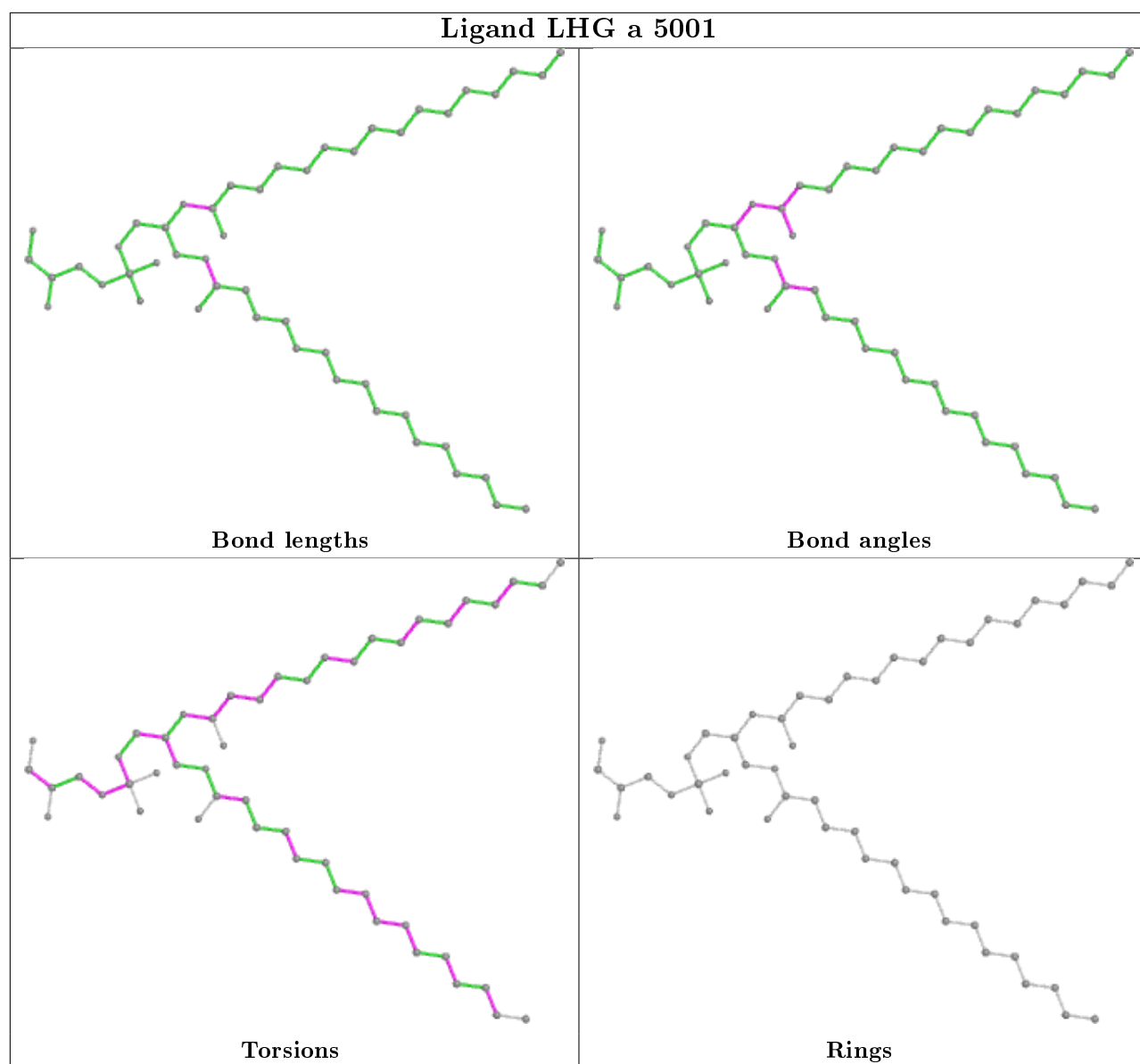


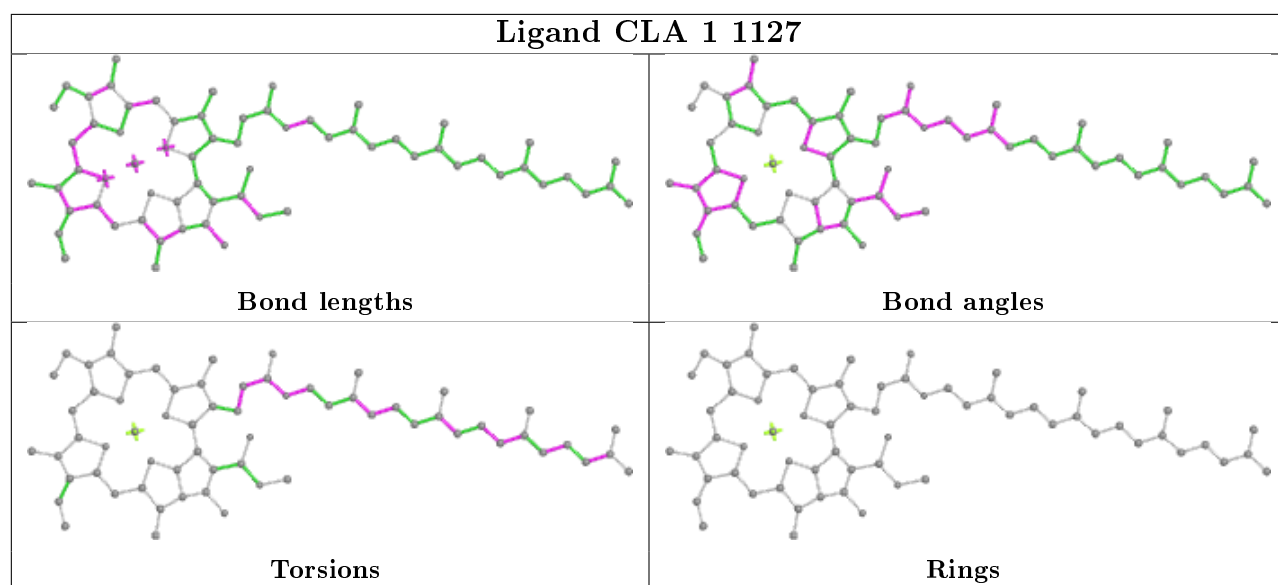
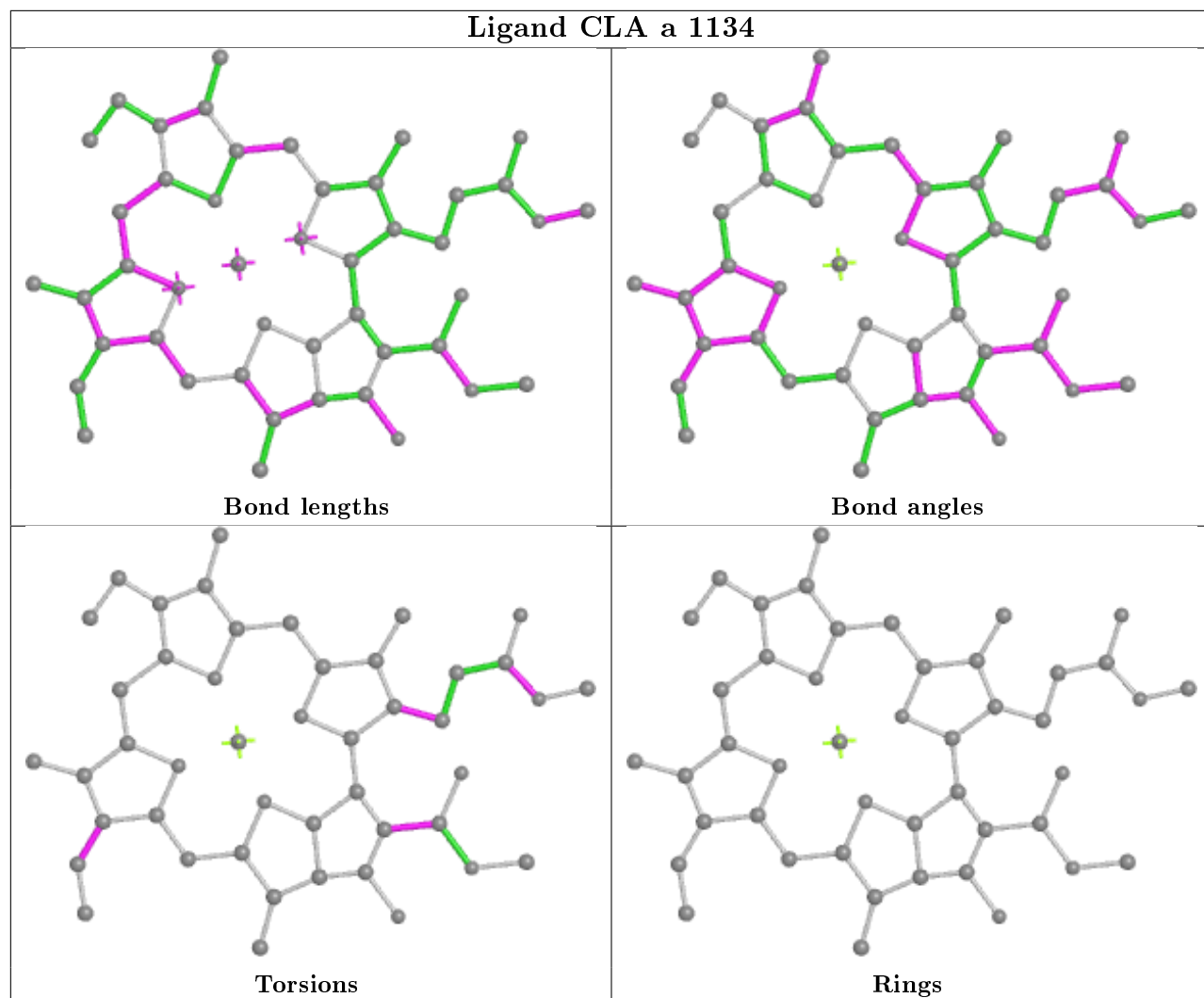




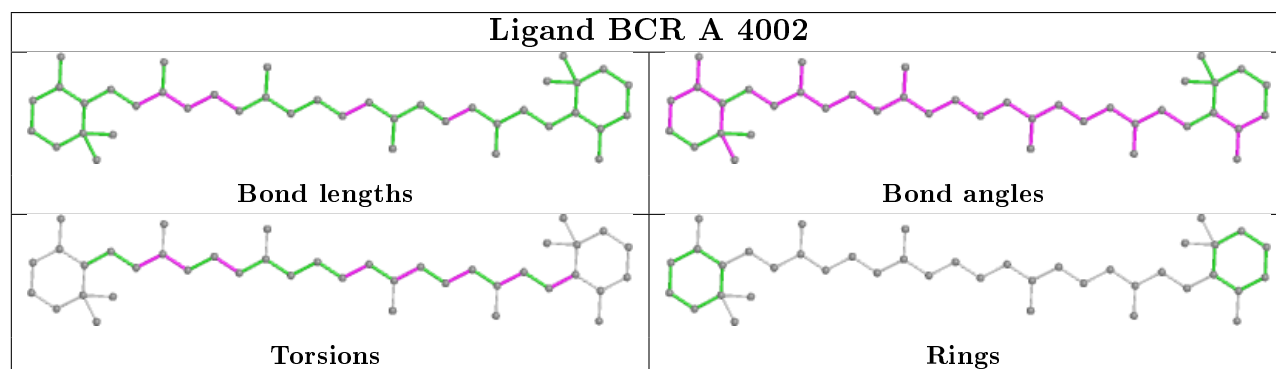
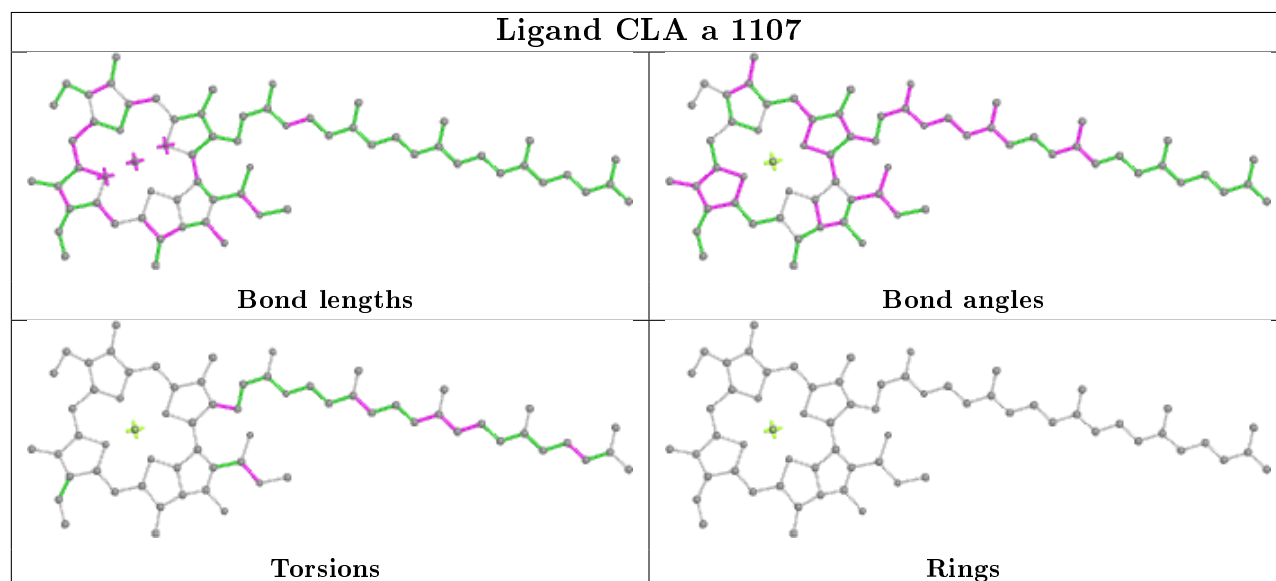
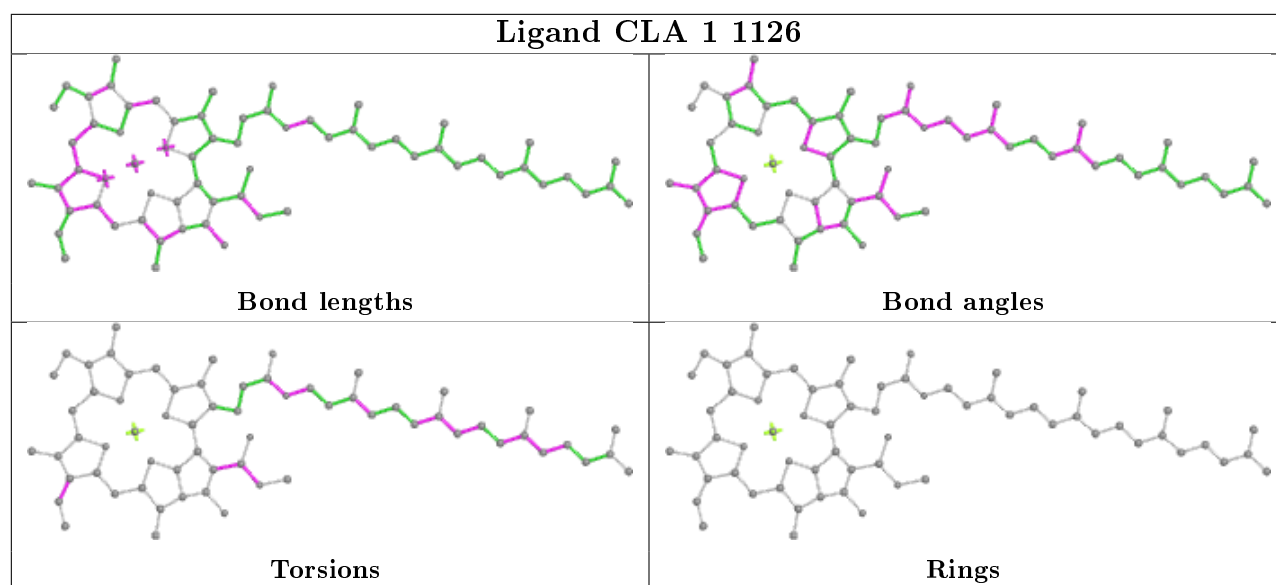




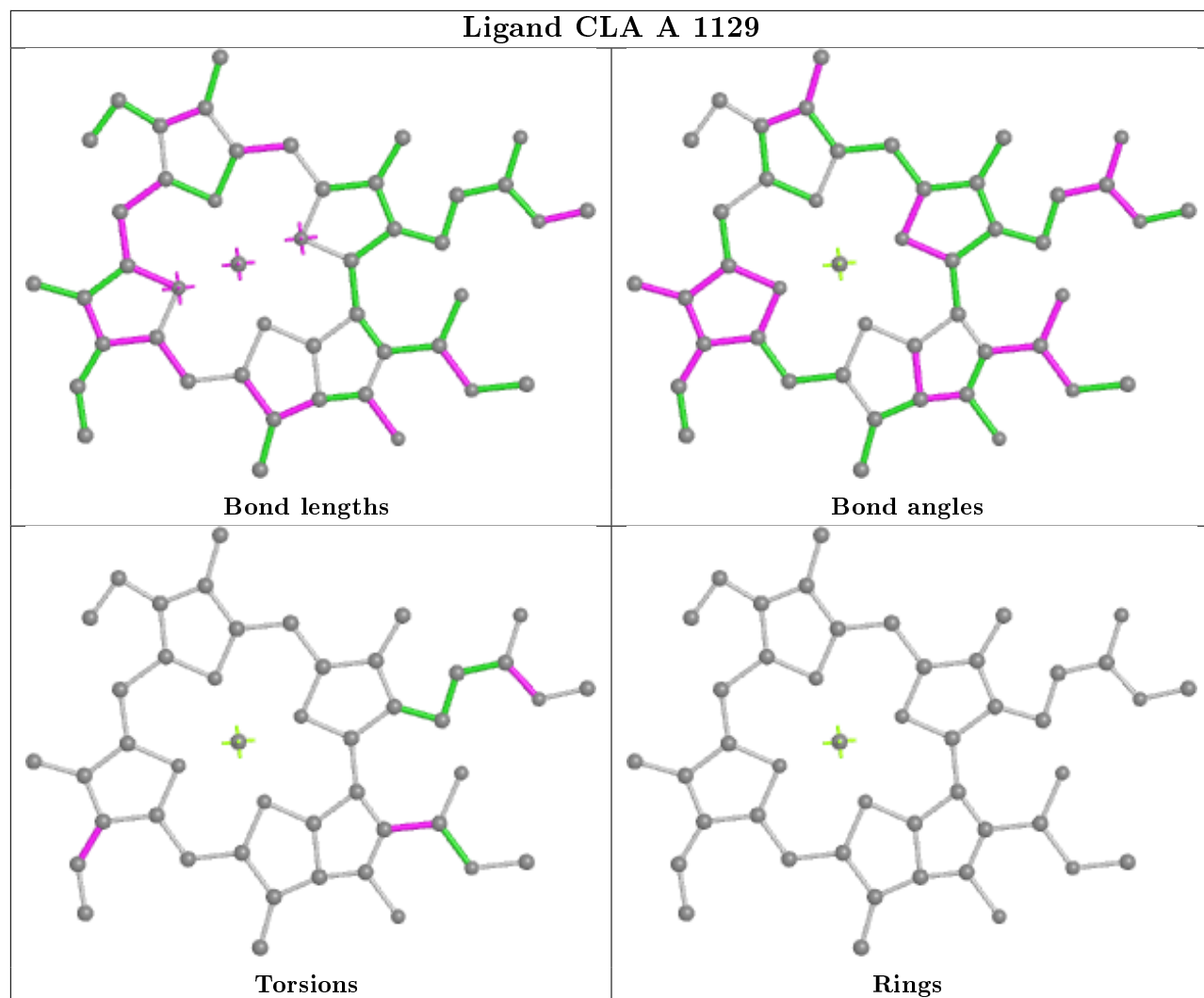


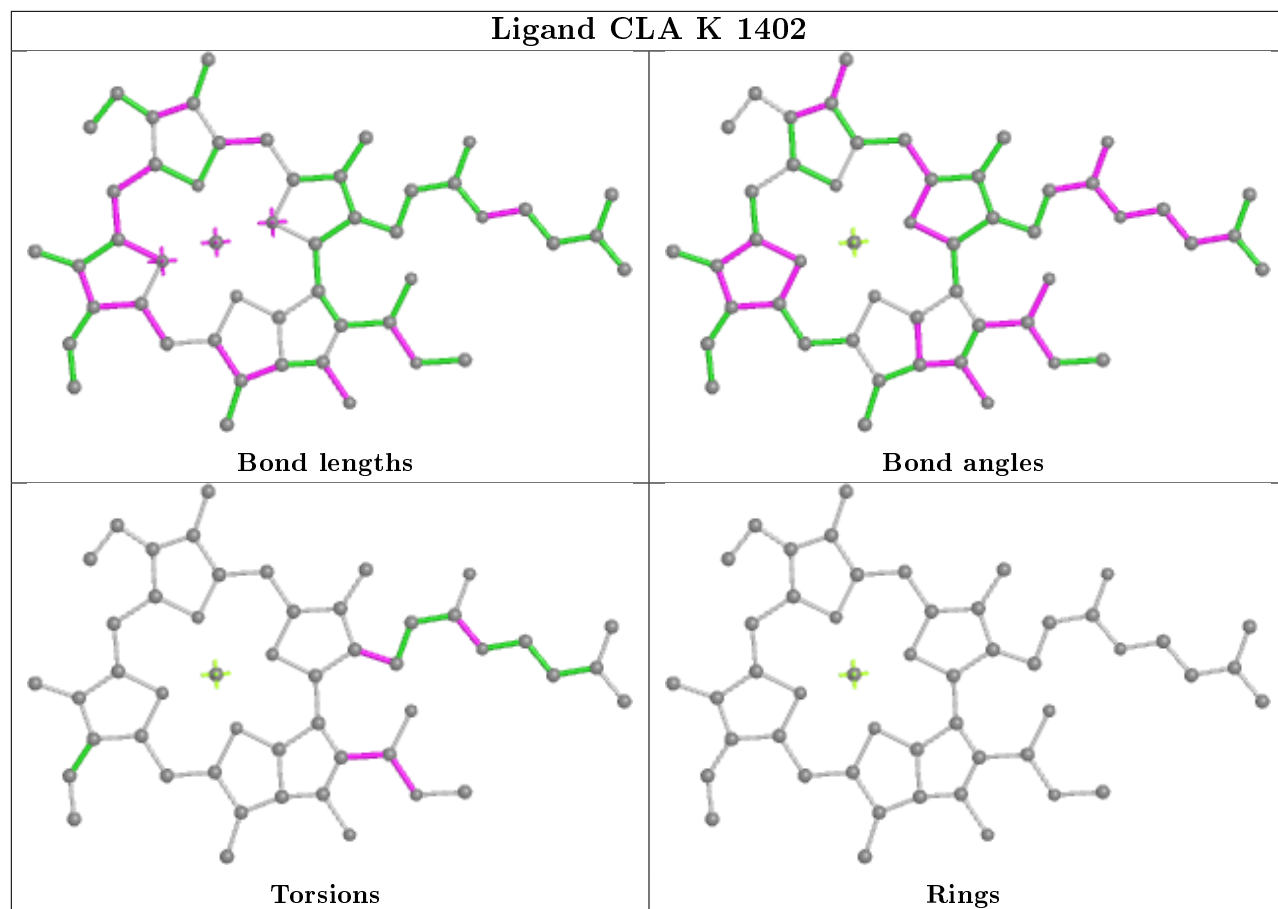




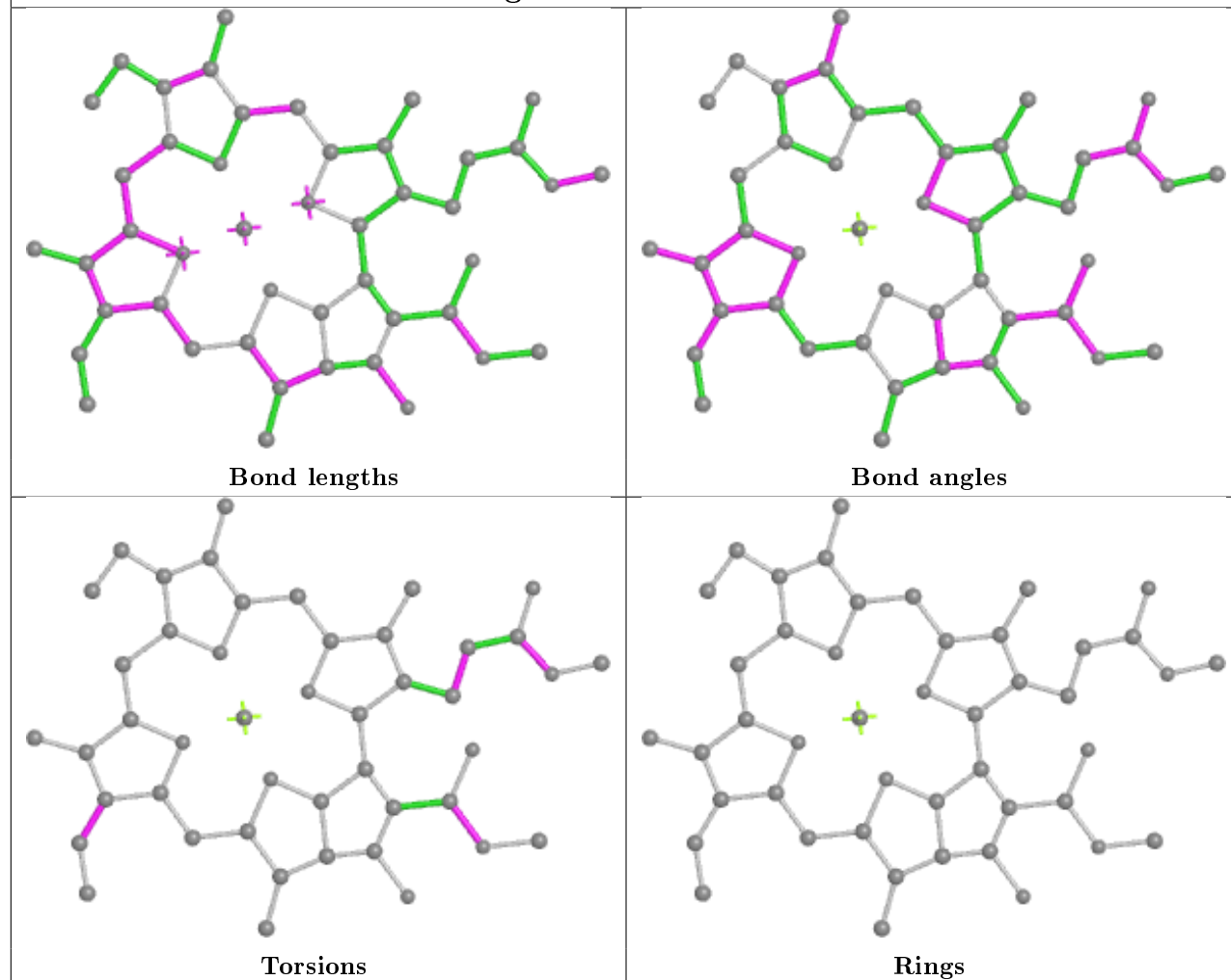


## Ligand CLA A 1129

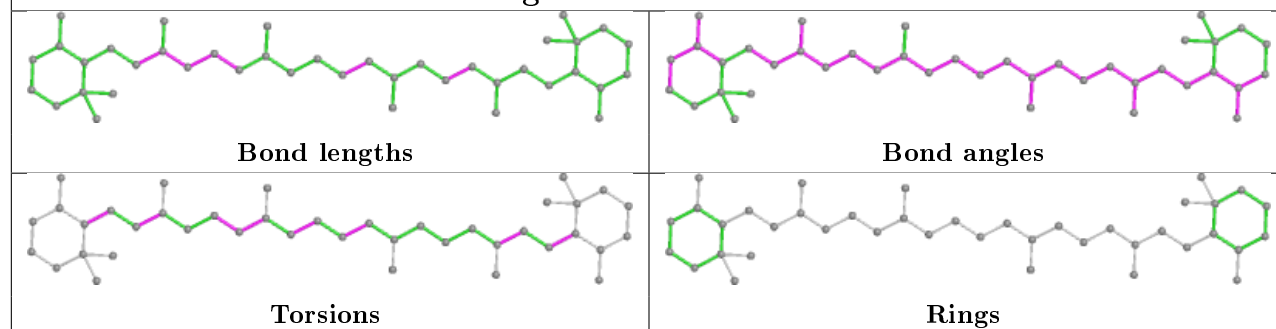


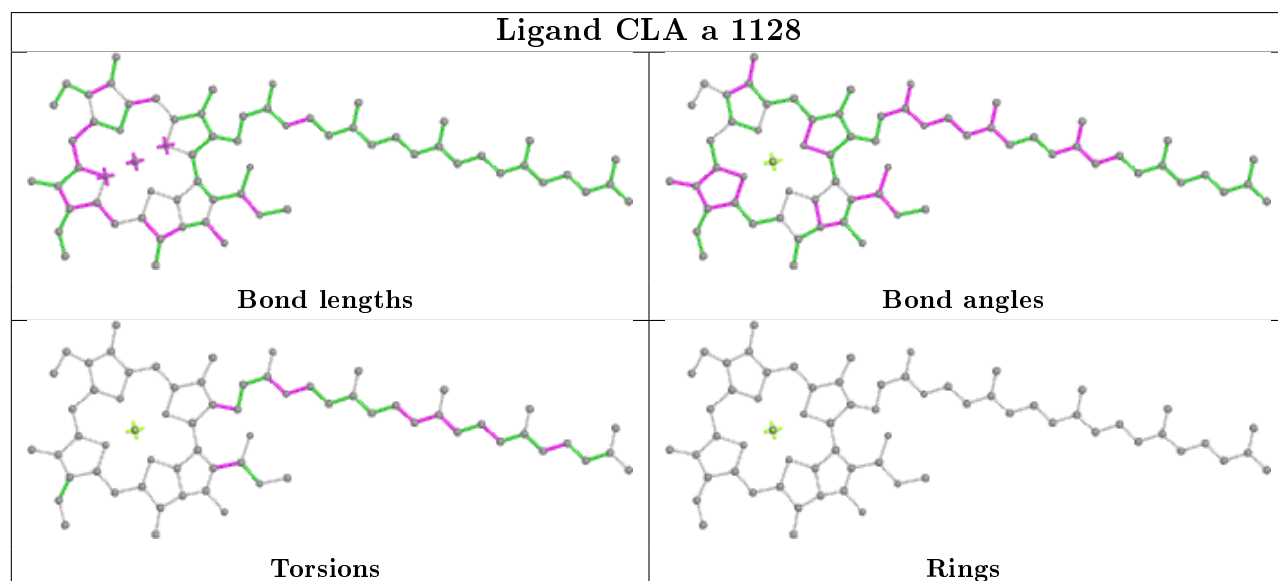
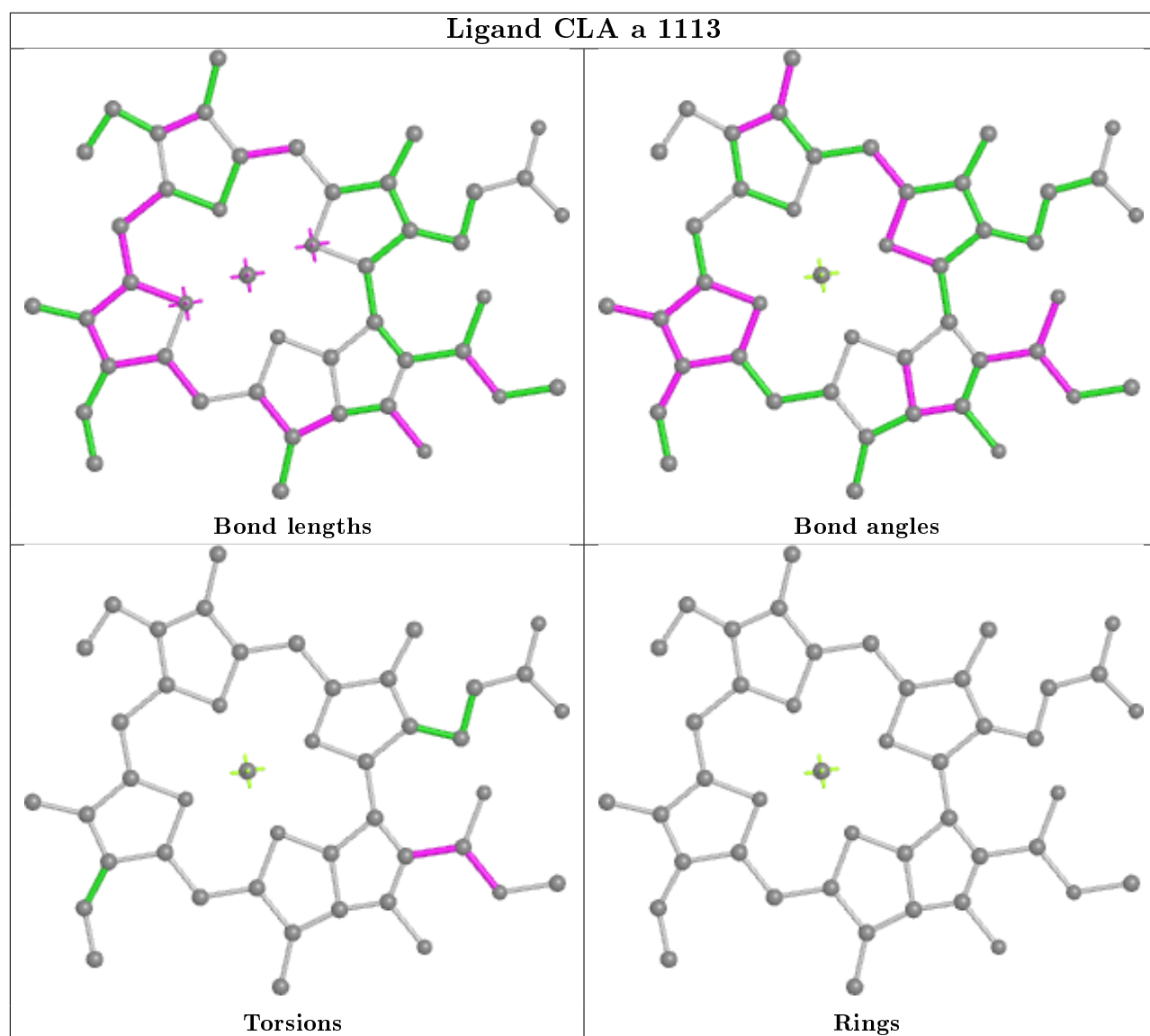


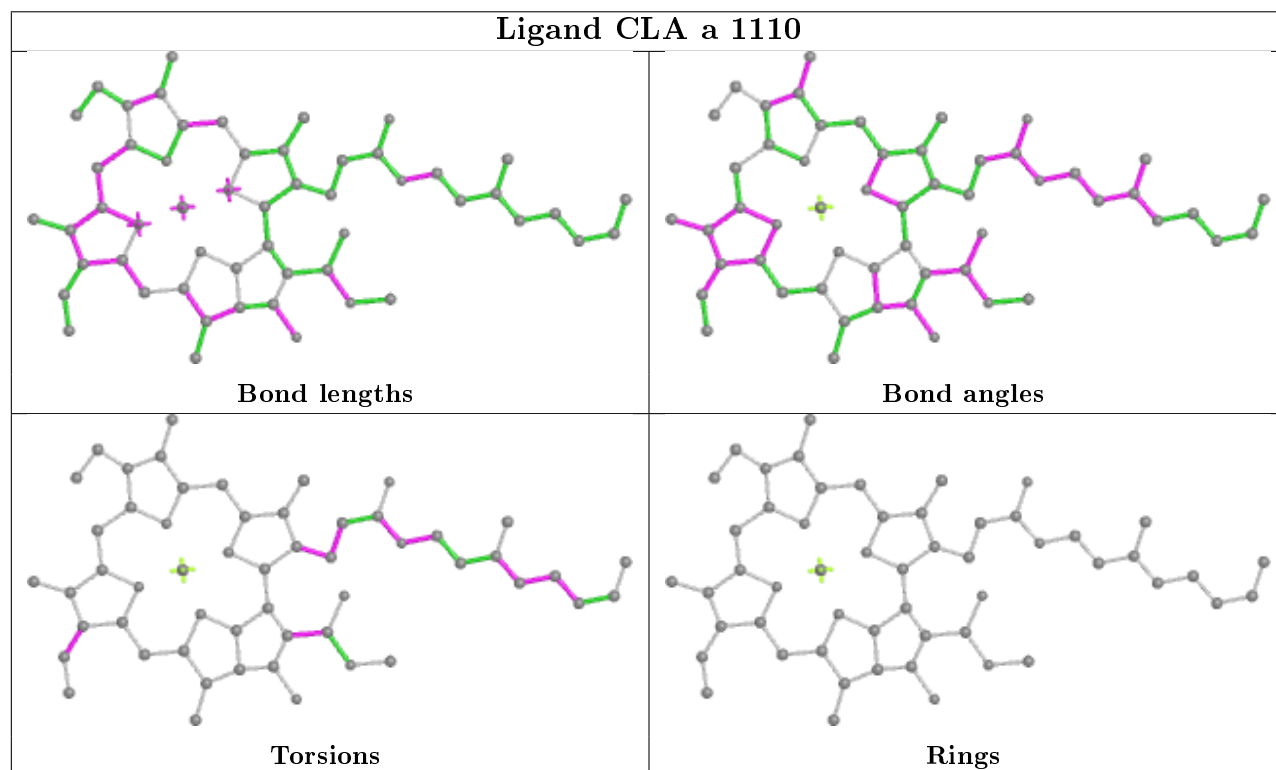
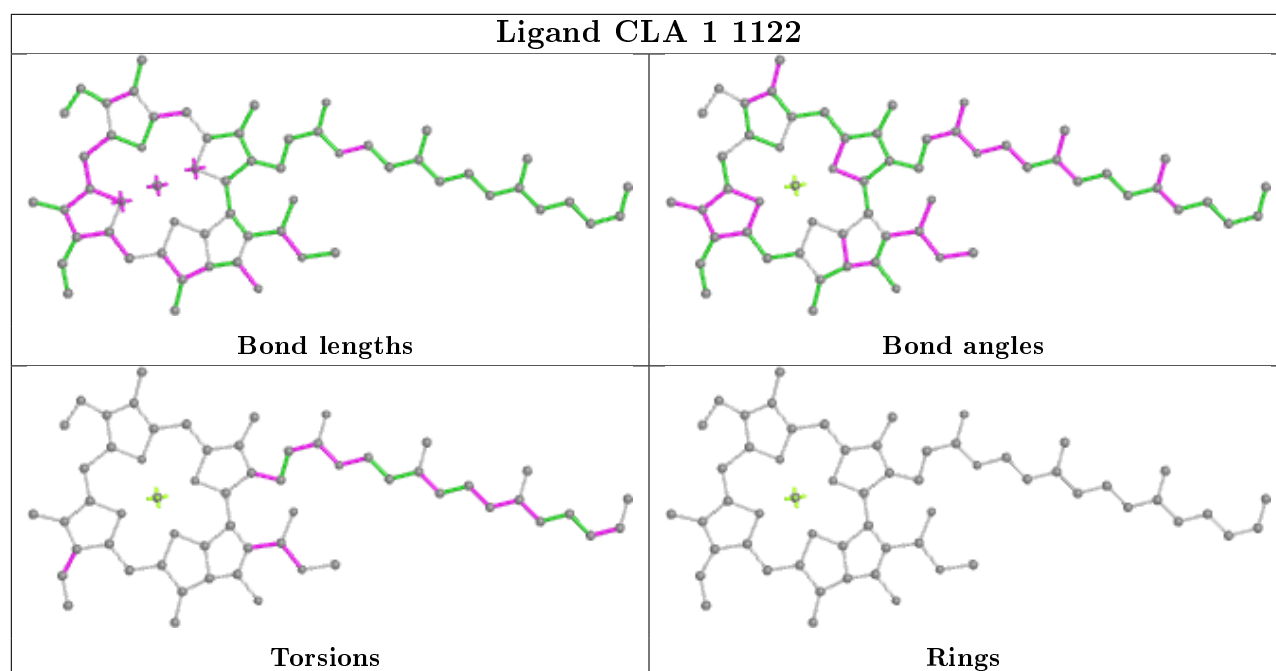
## Ligand CLA A 1115



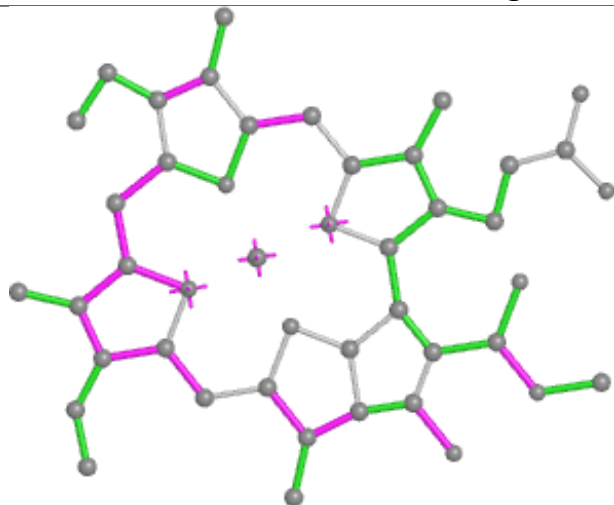
## Ligand BCR B 4009



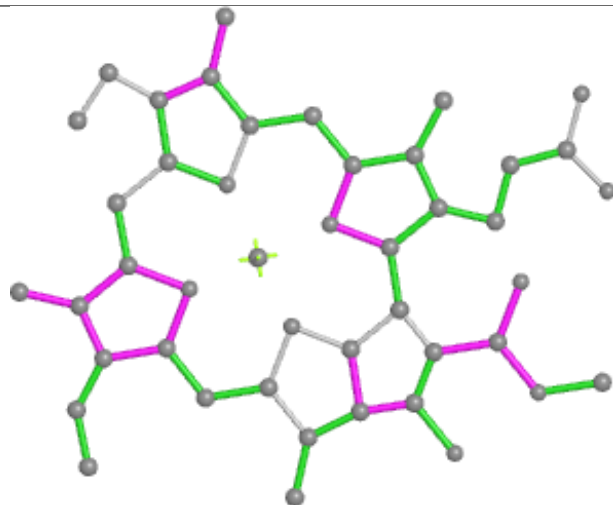




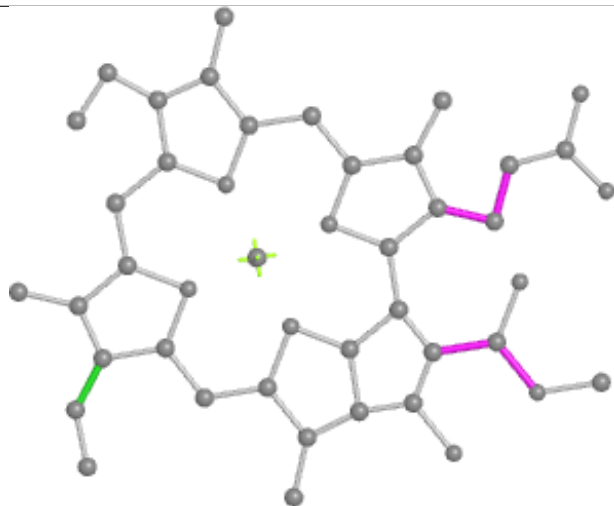
## Ligand CLA B 1212



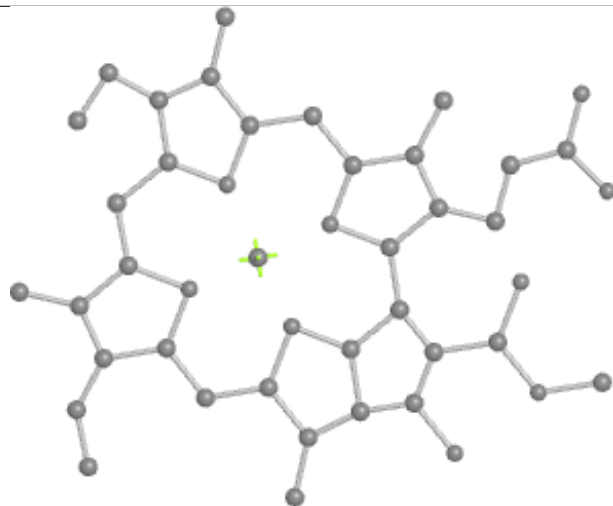
Bond lengths



Bond angles

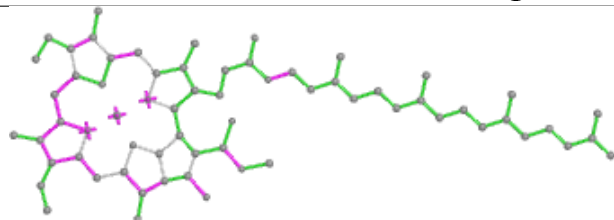


Torsions

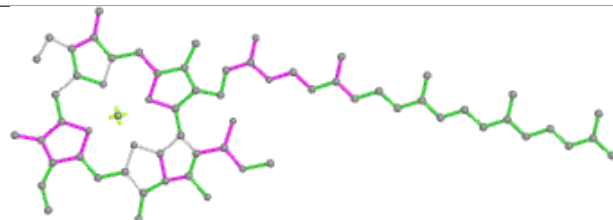


Rings

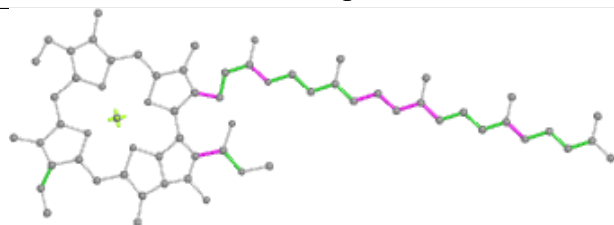
## Ligand CLA L 1501



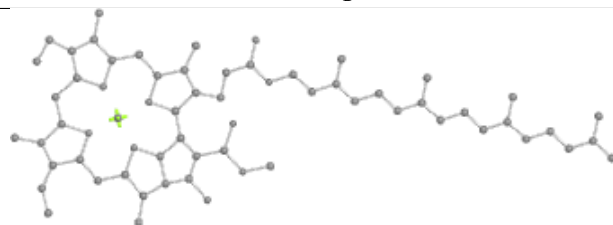
Bond lengths



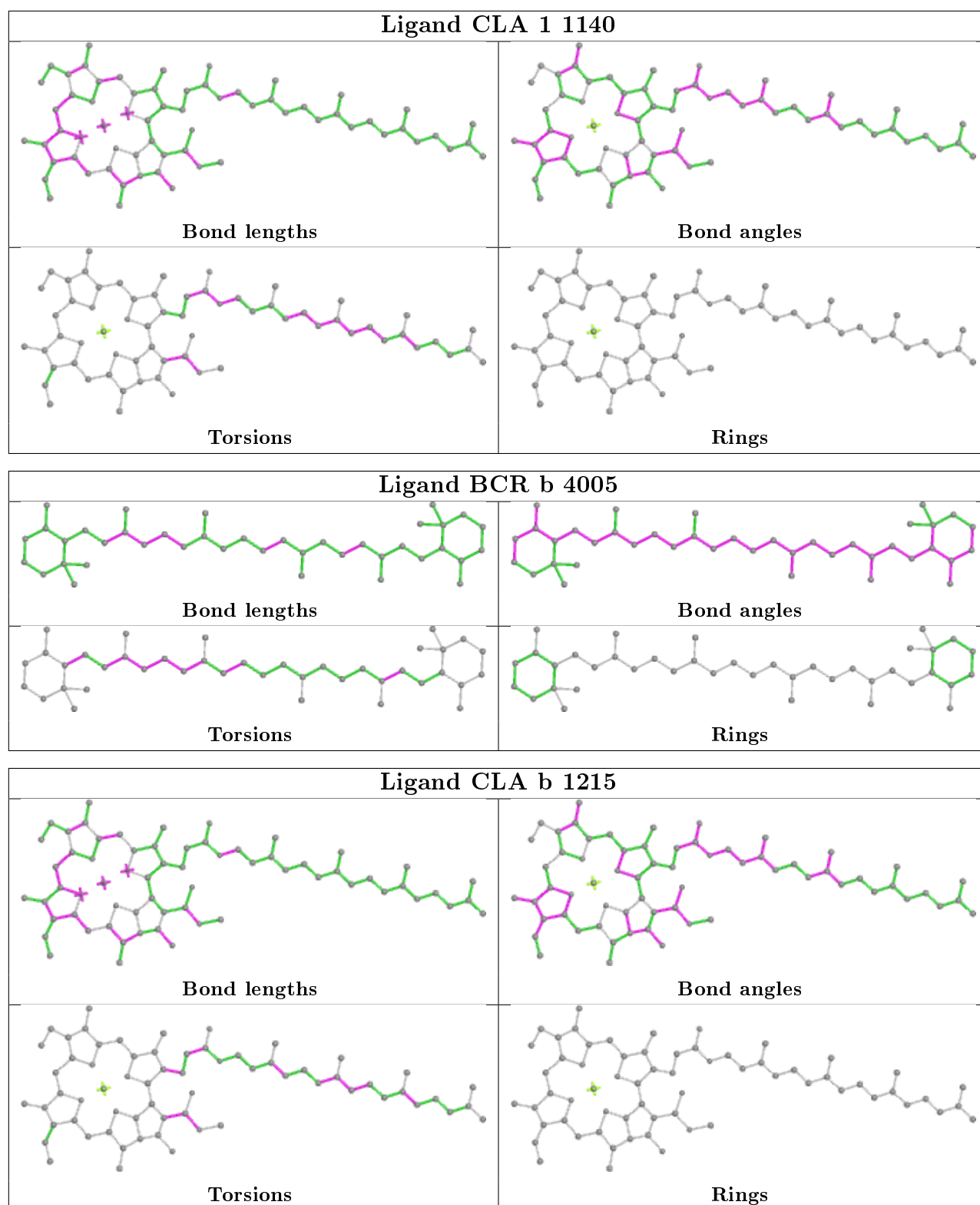
Bond angles



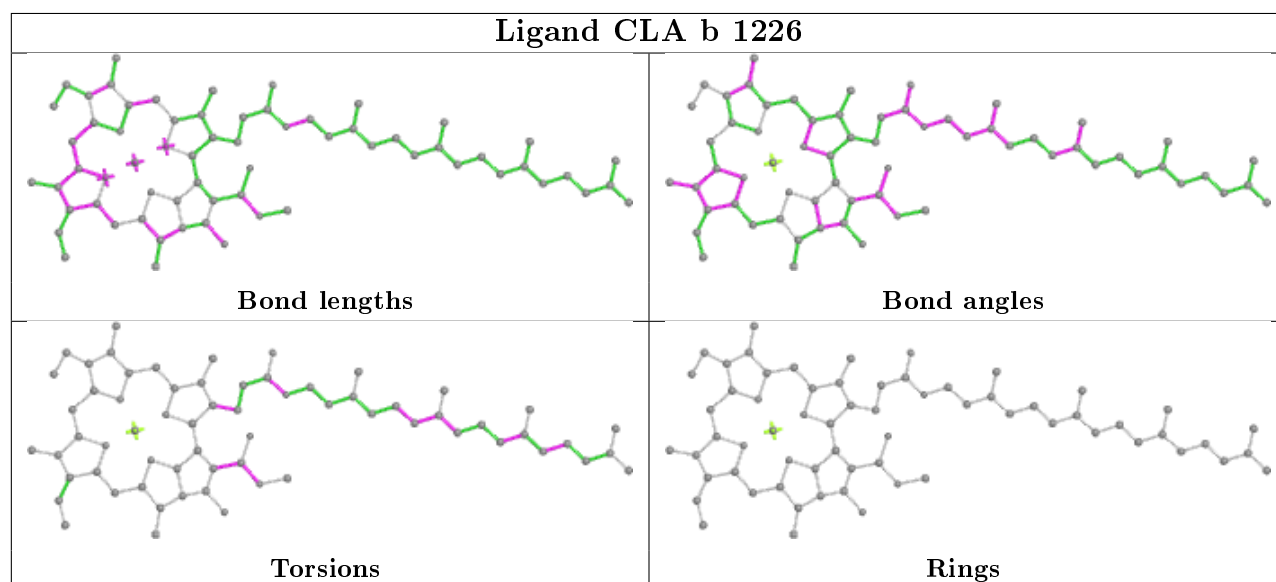
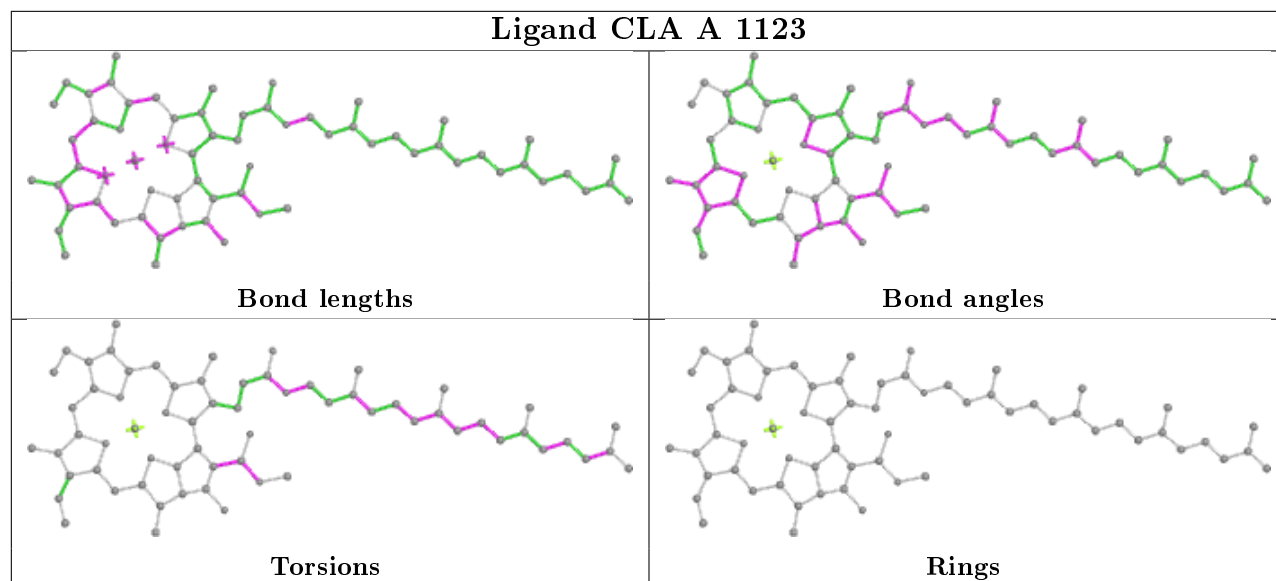
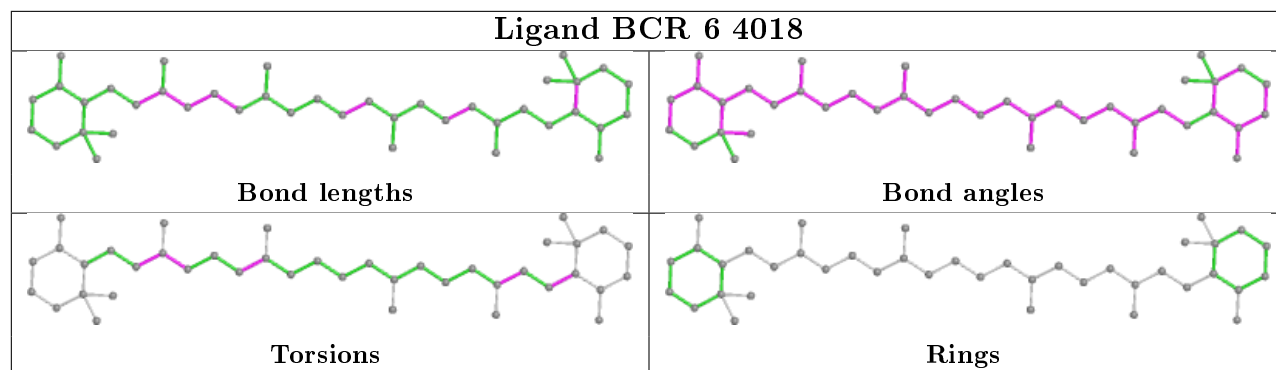
Torsions

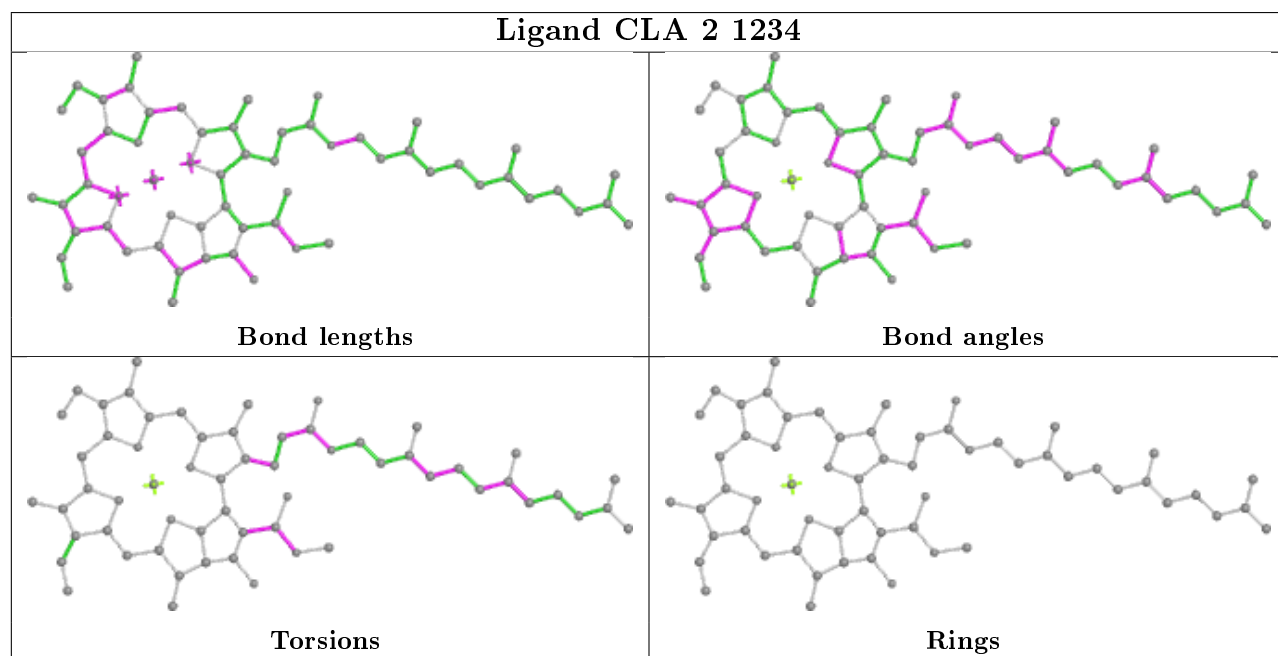
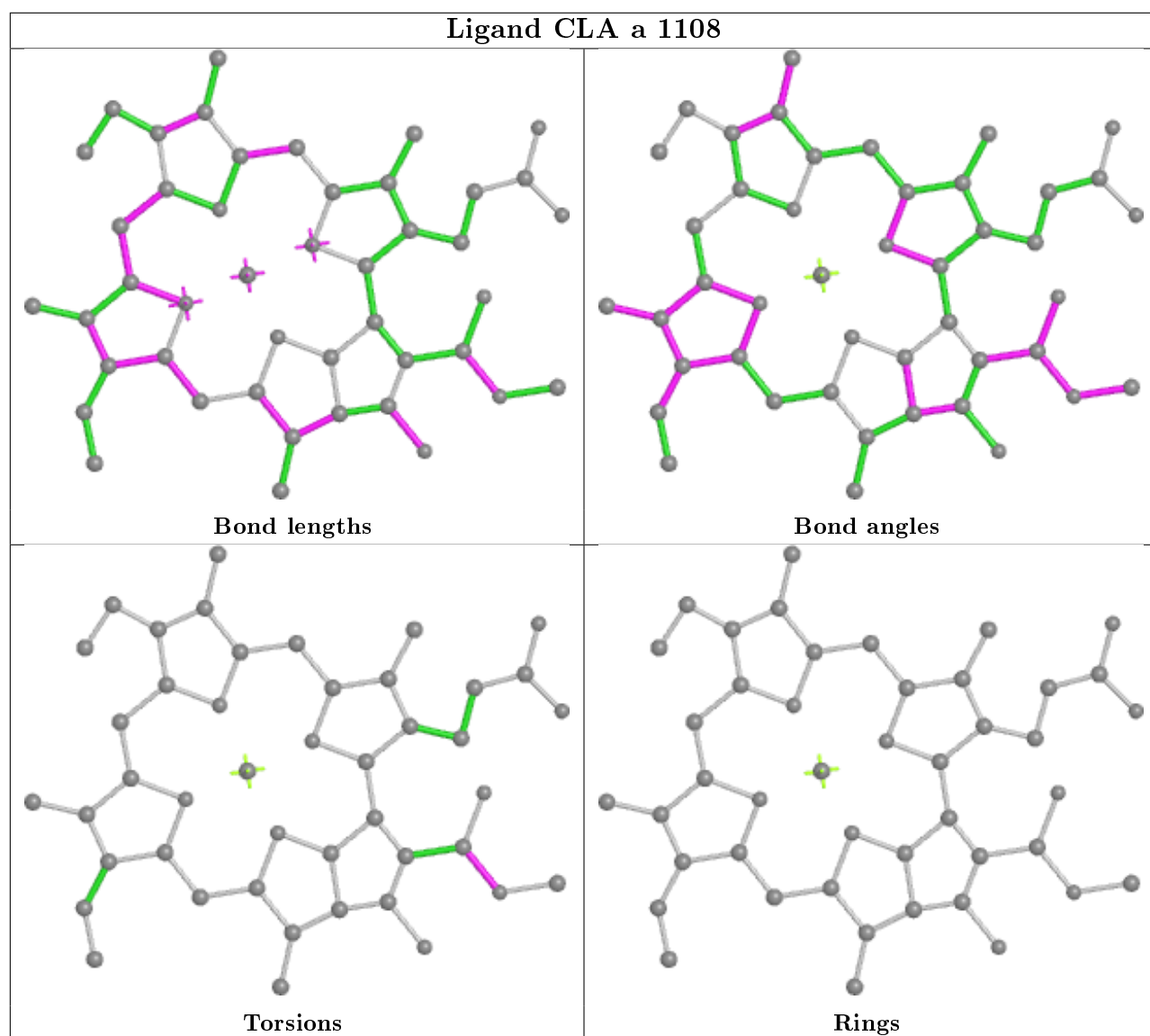


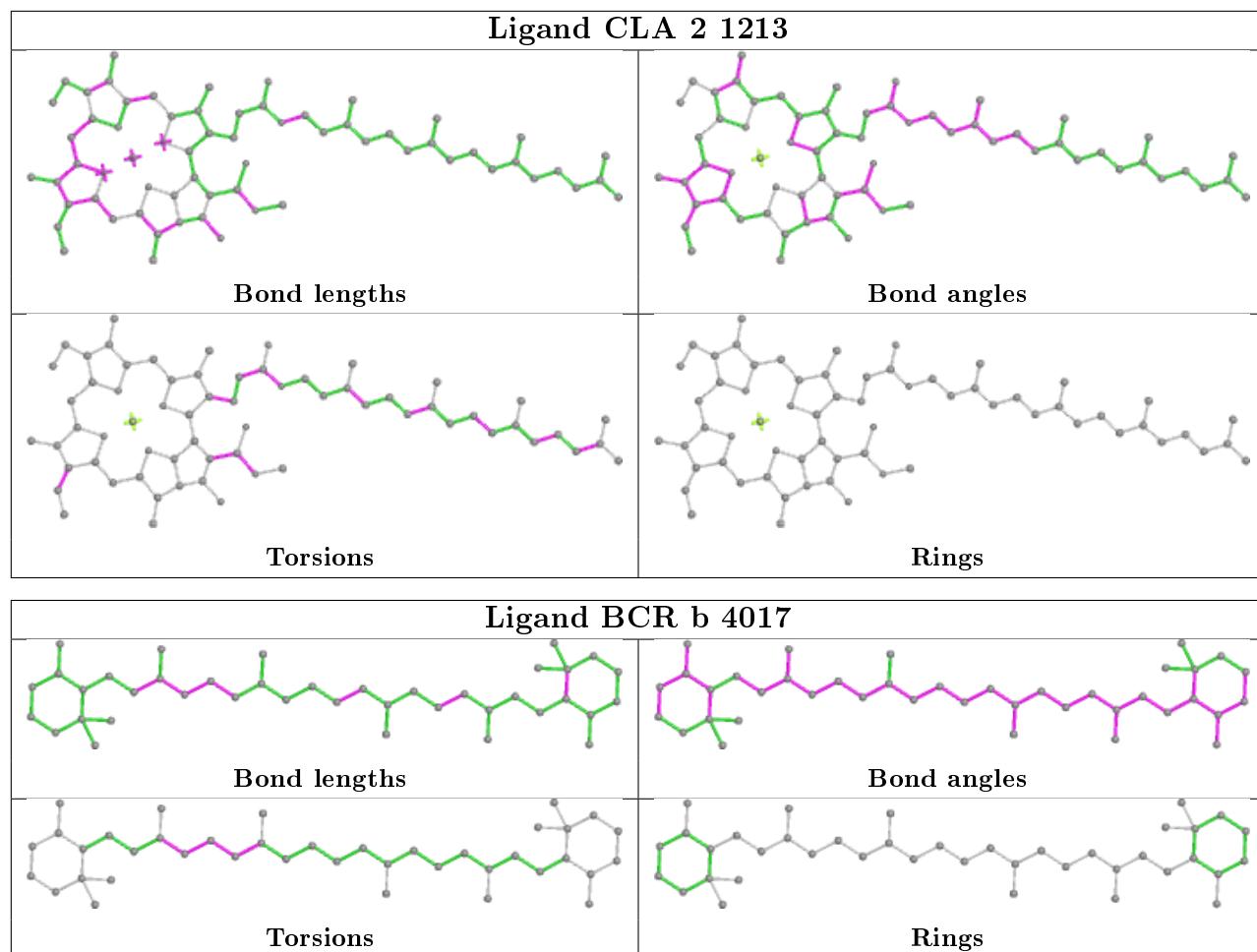
Rings



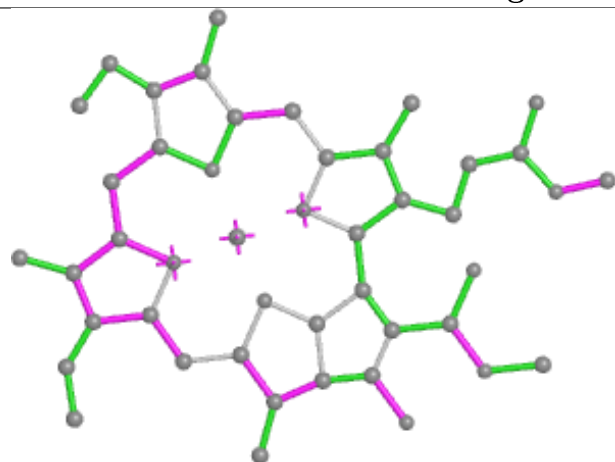




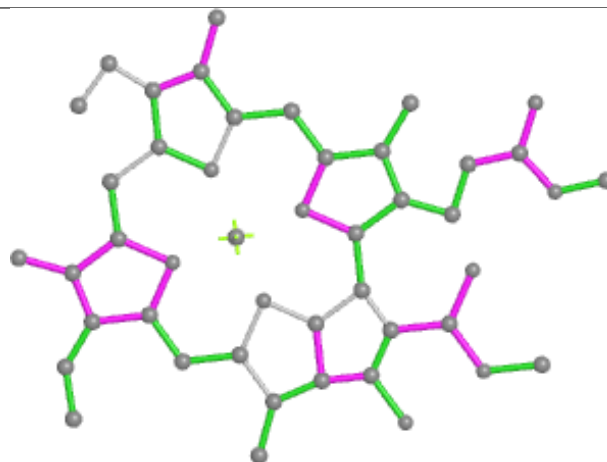




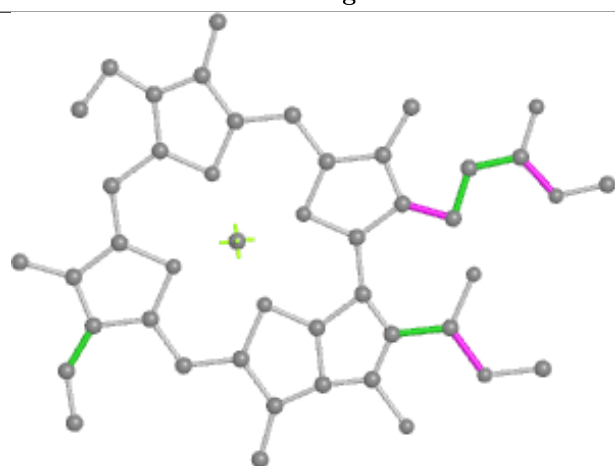
## Ligand CLA A 1130



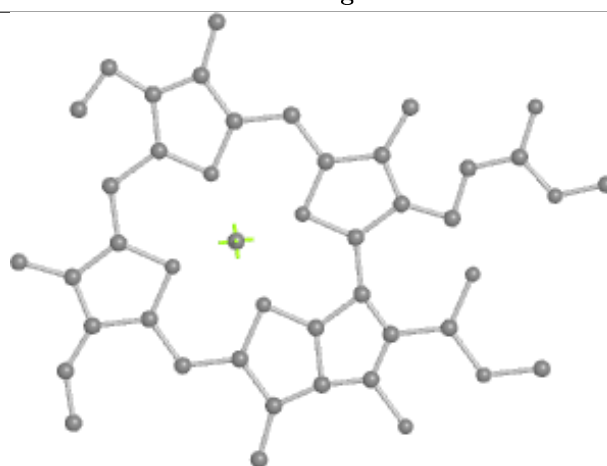
Bond lengths



Bond angles

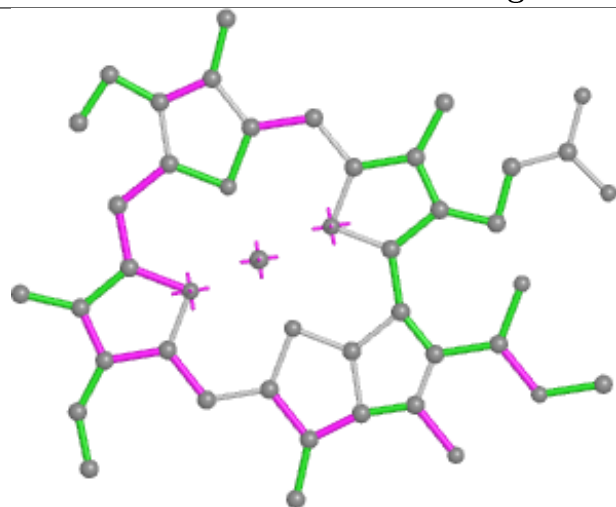


Torsions

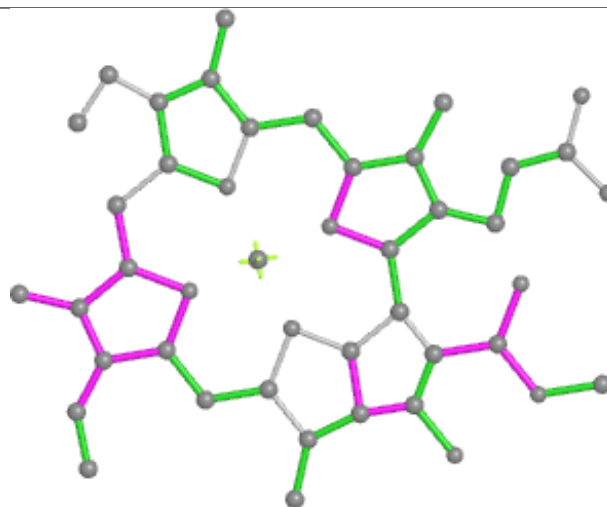


Rings

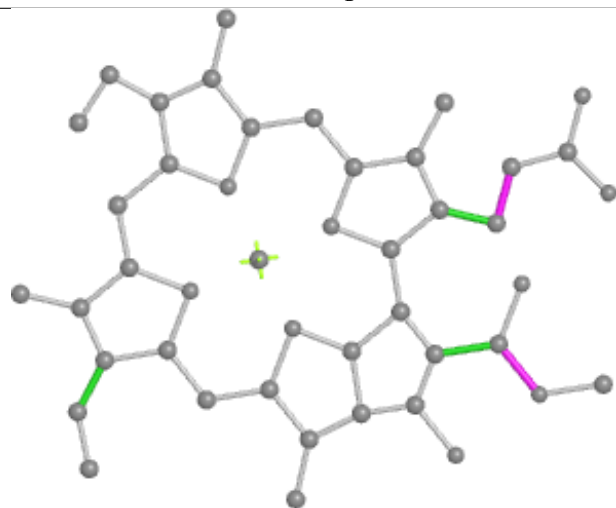
## Ligand CLA B 1232



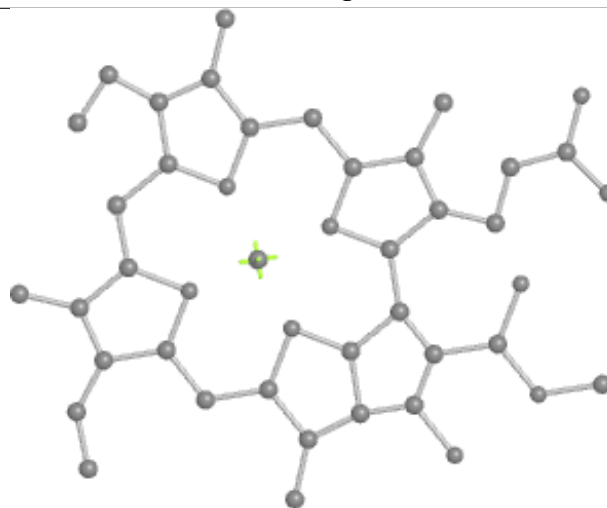
Bond lengths



Bond angles

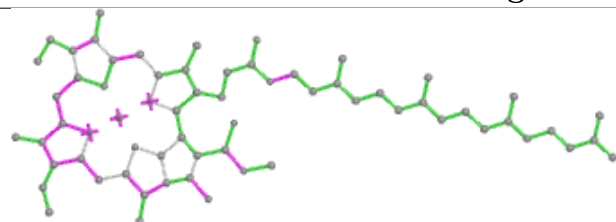


Torsions

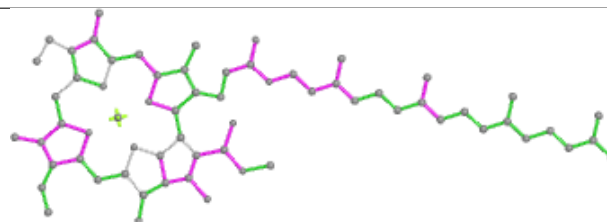


Rings

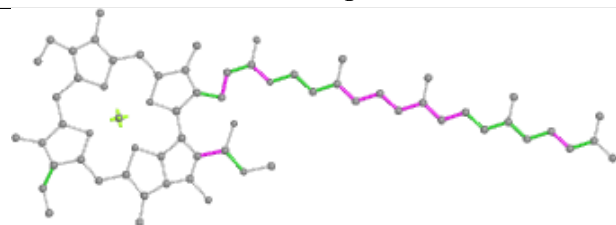
## Ligand CLA A 1012



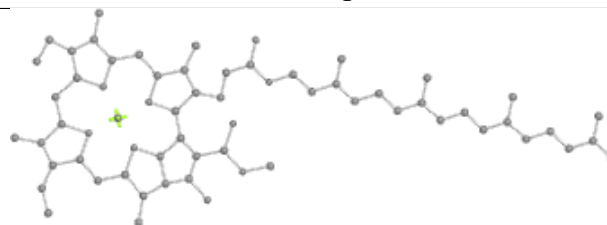
Bond lengths



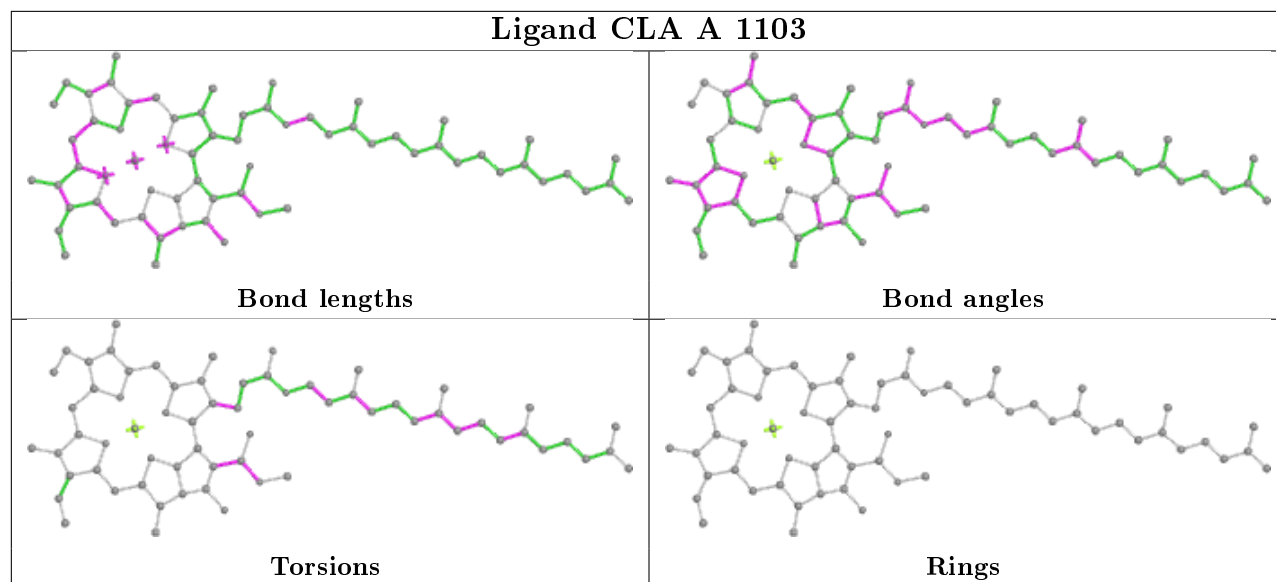
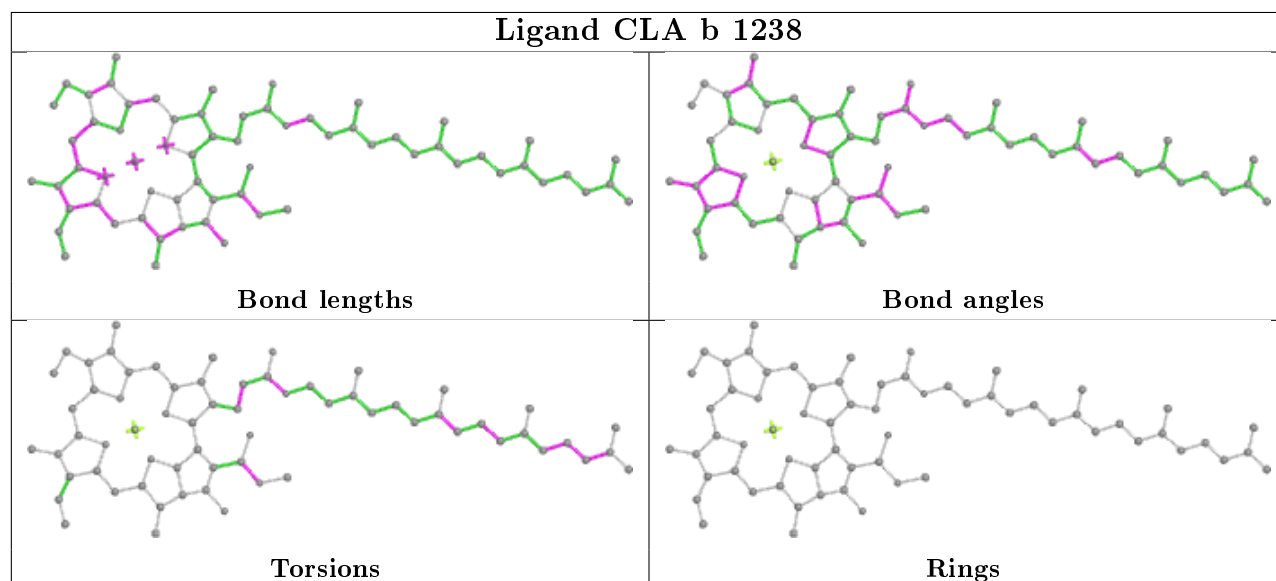
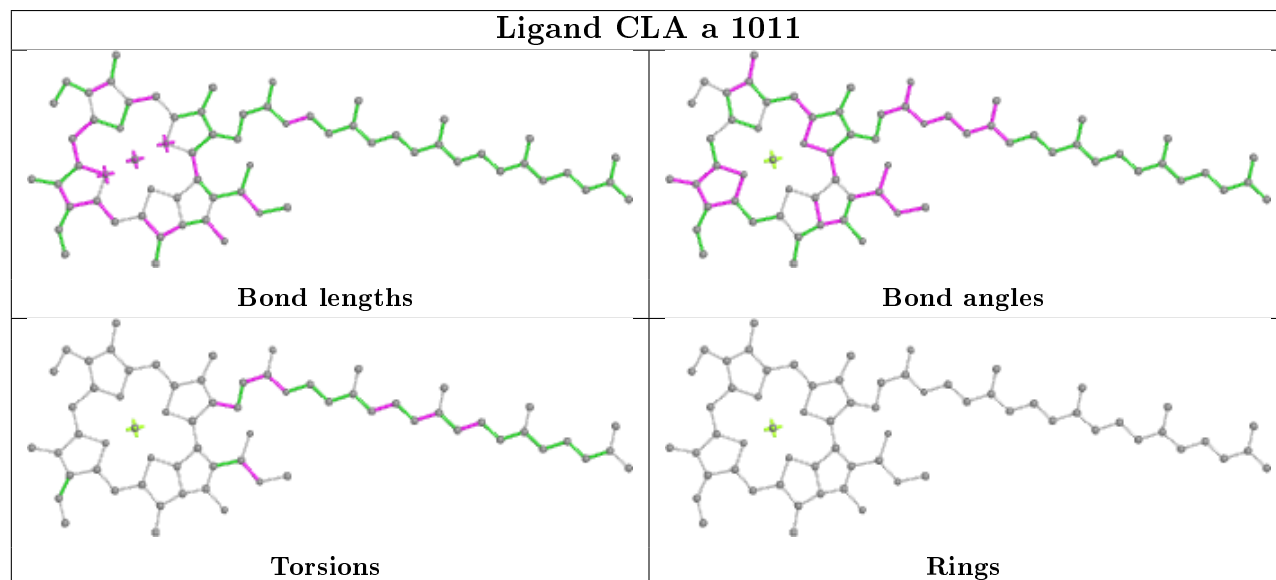
Bond angles

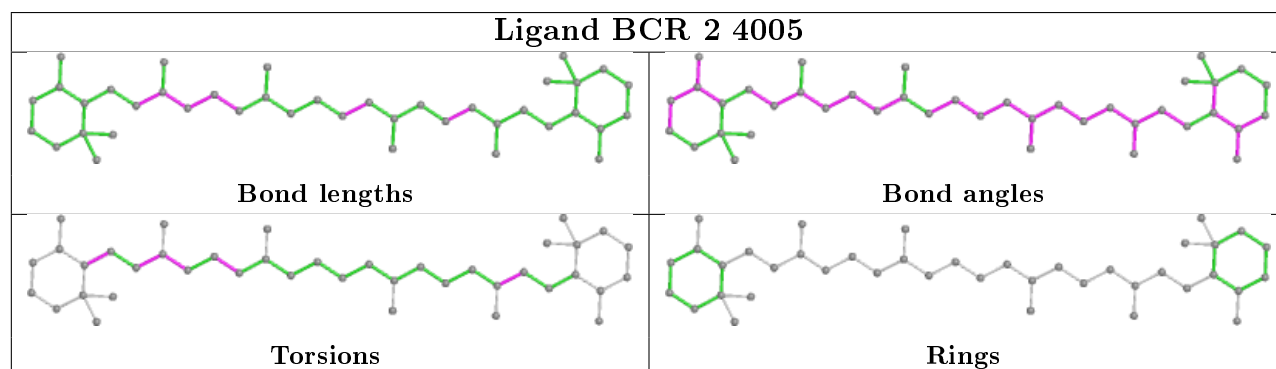
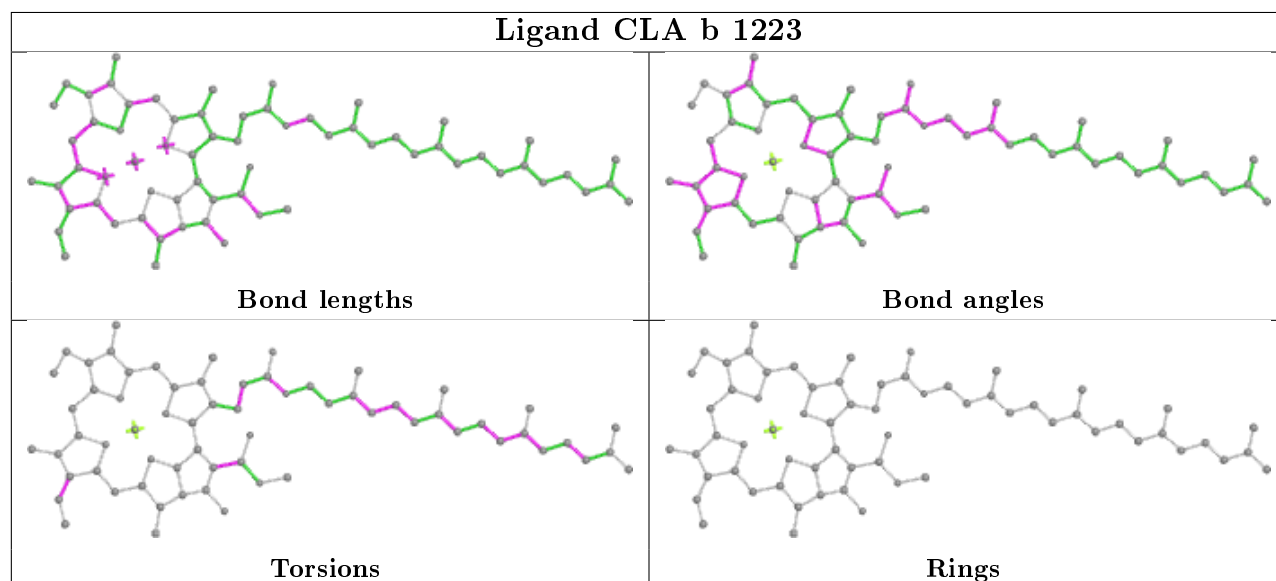
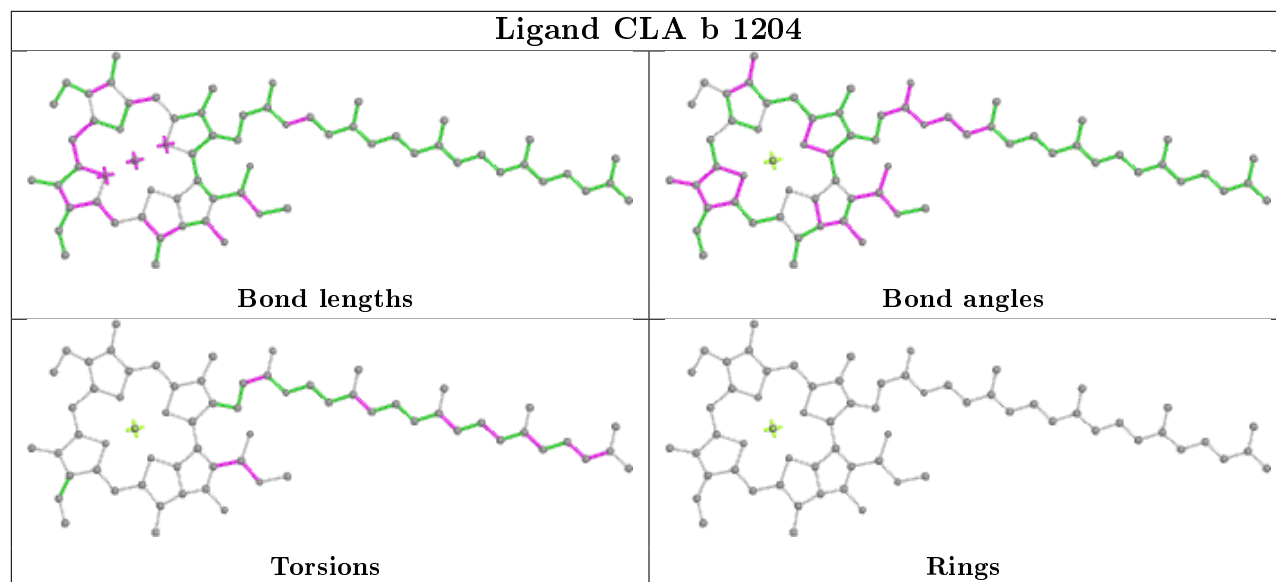


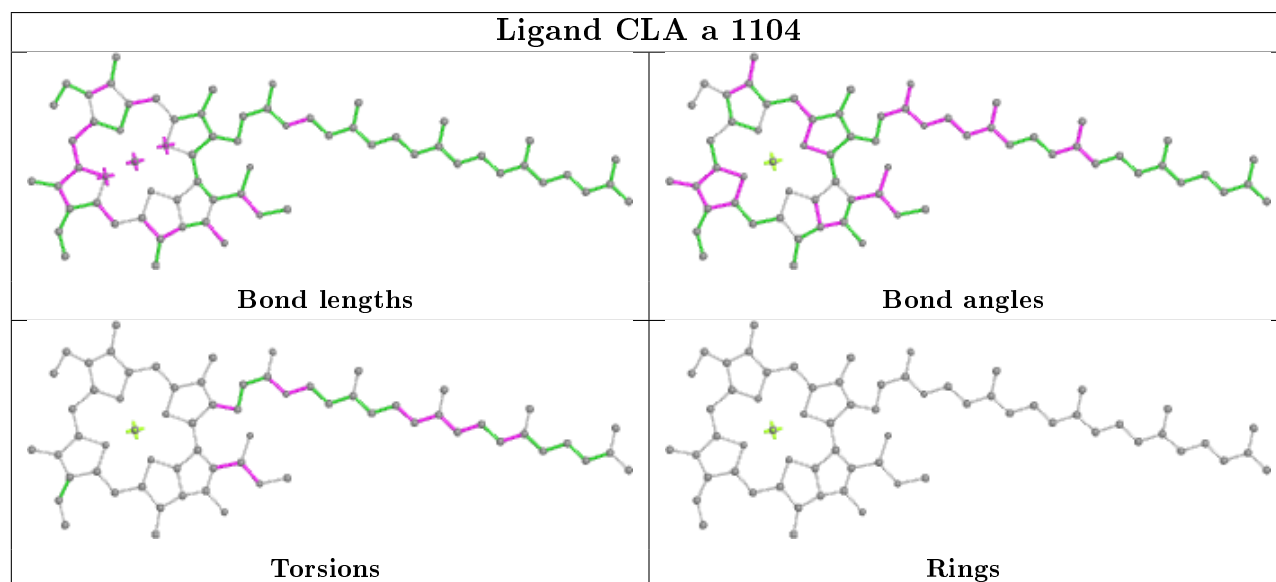
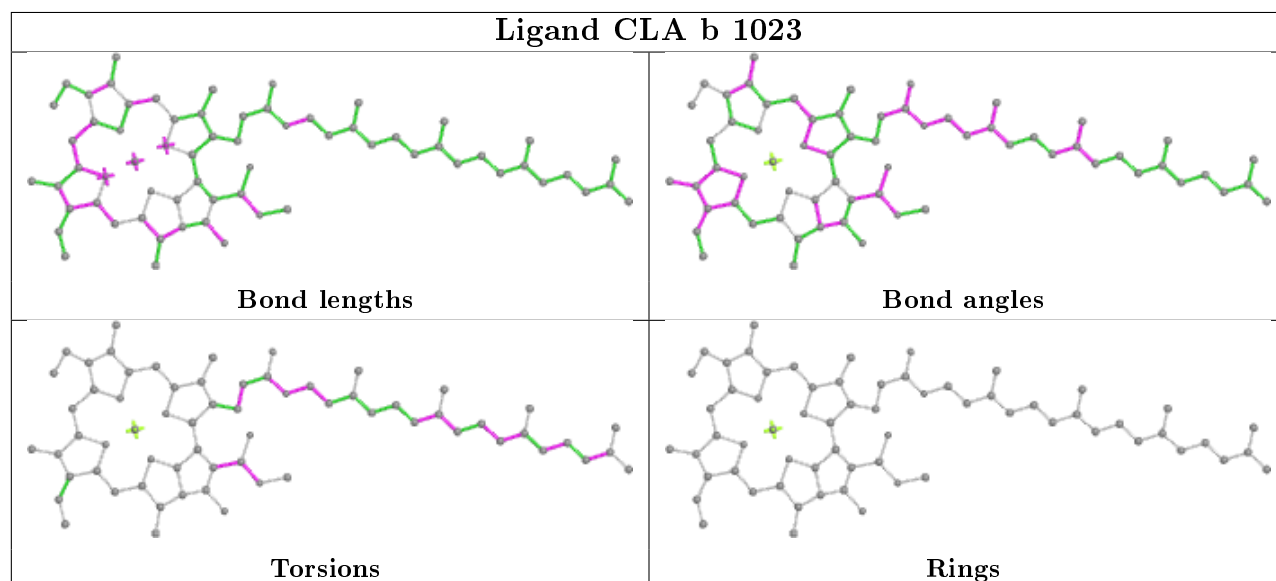
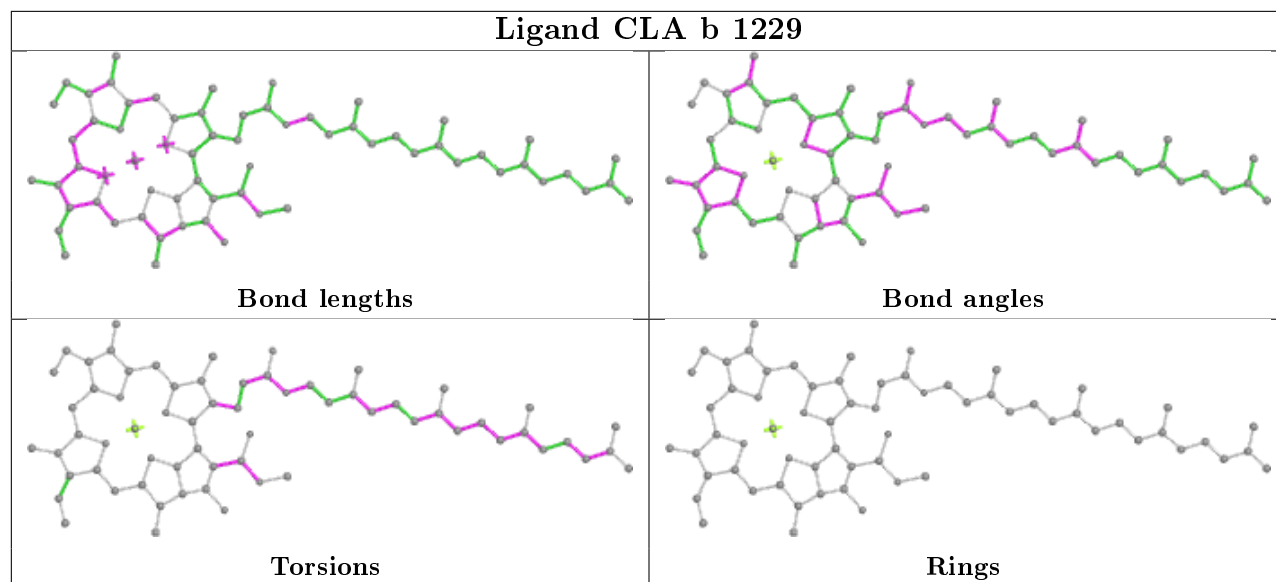
Torsions



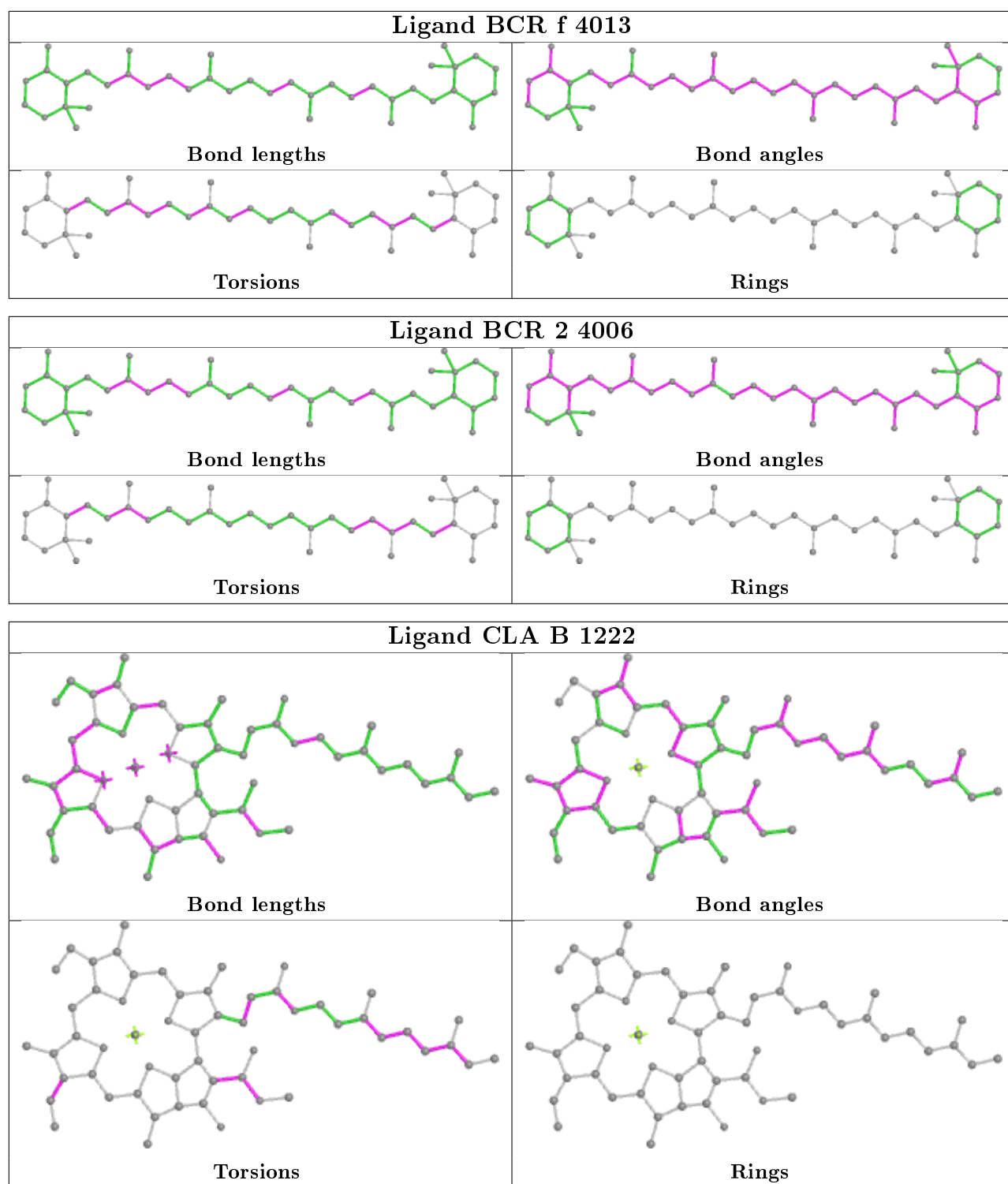
Rings

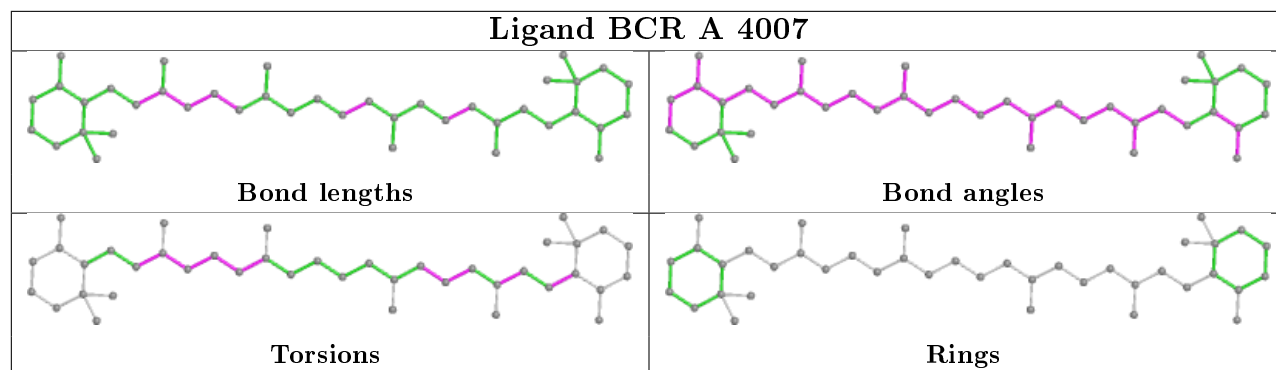
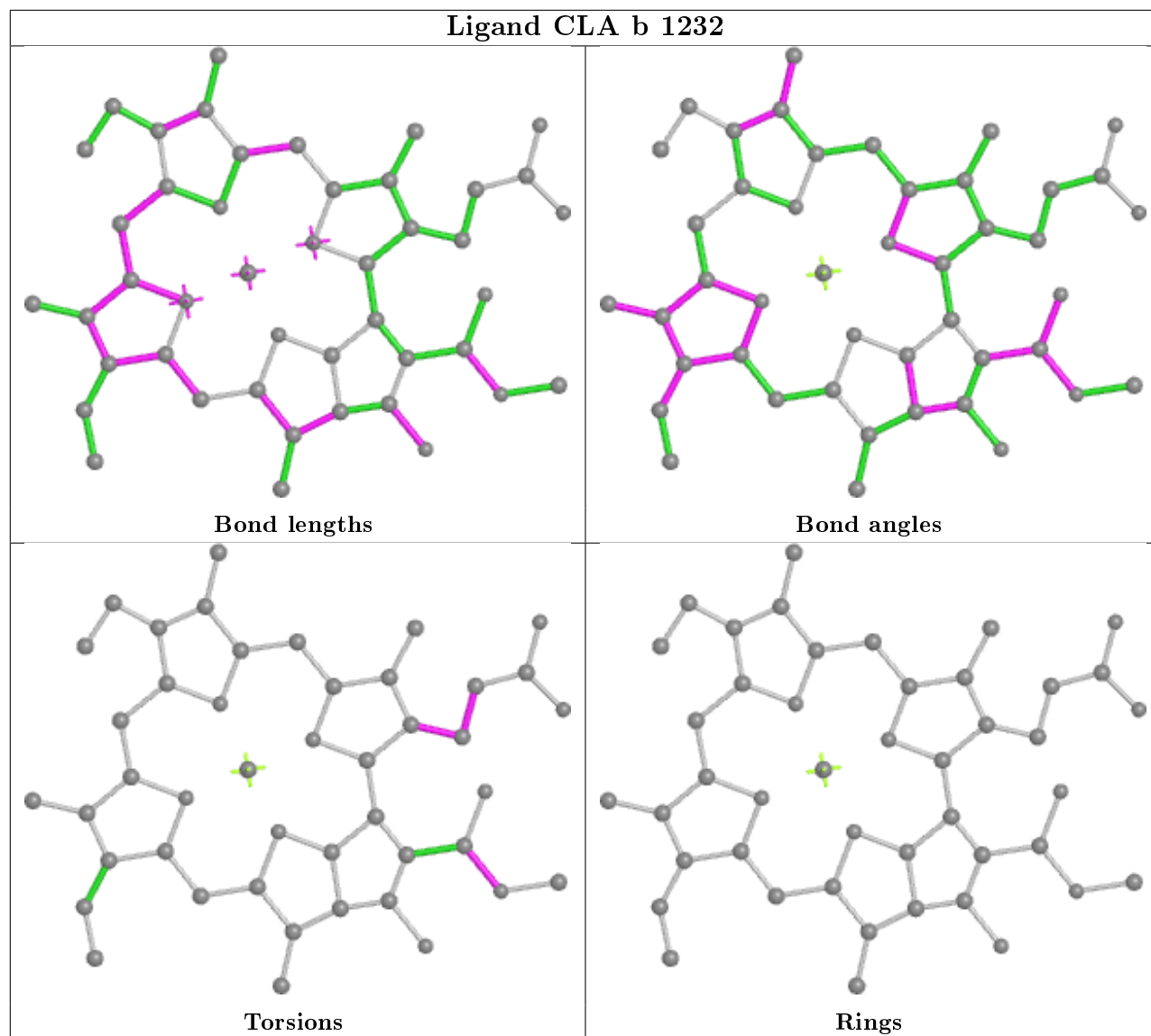
**Ligand CLA A 1103****Ligand CLA b 1238****Ligand CLA a 1011**



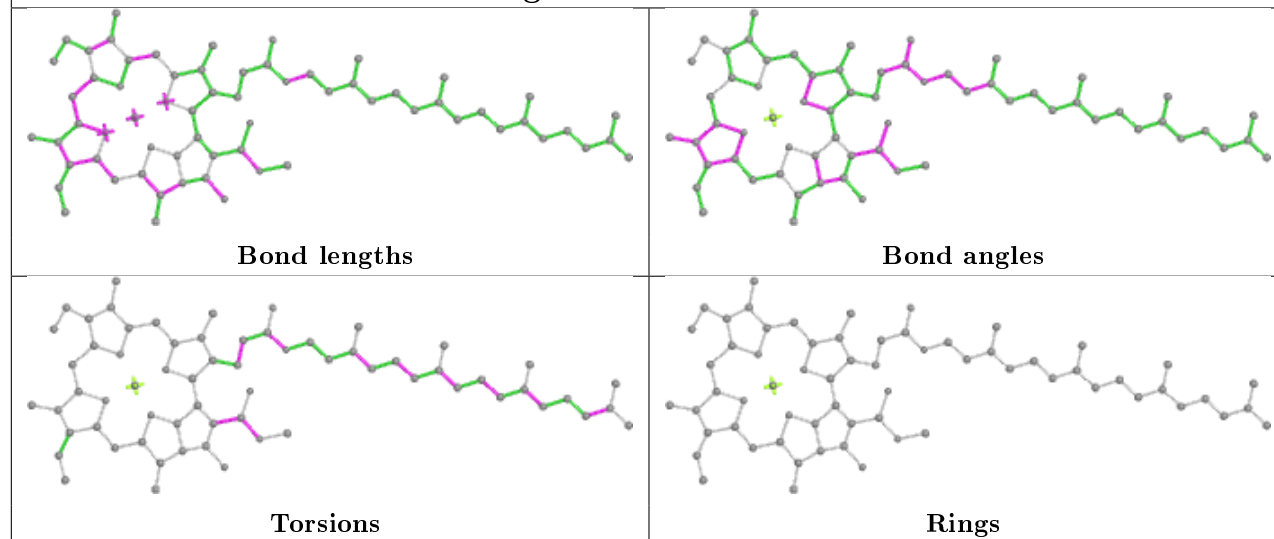




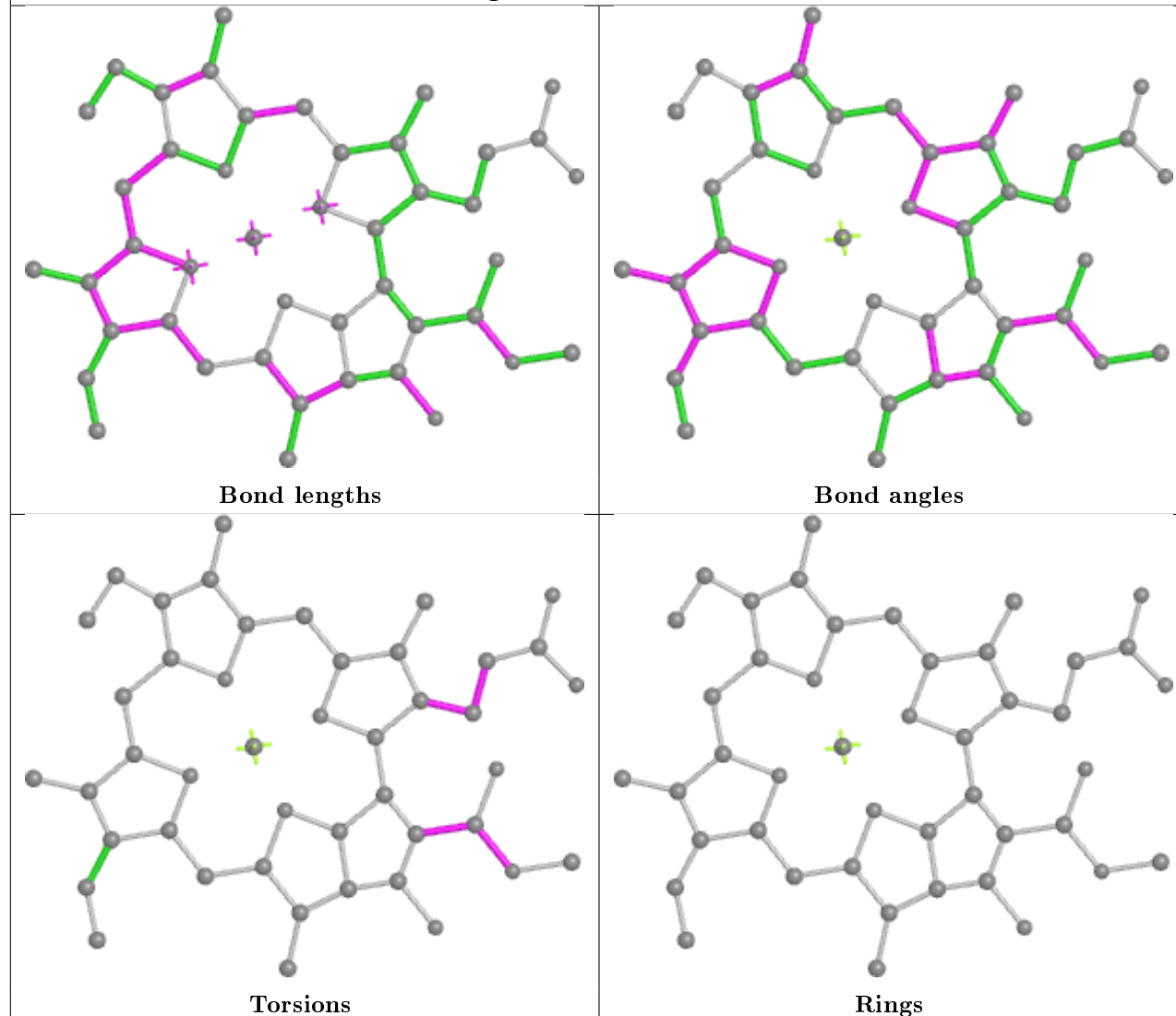


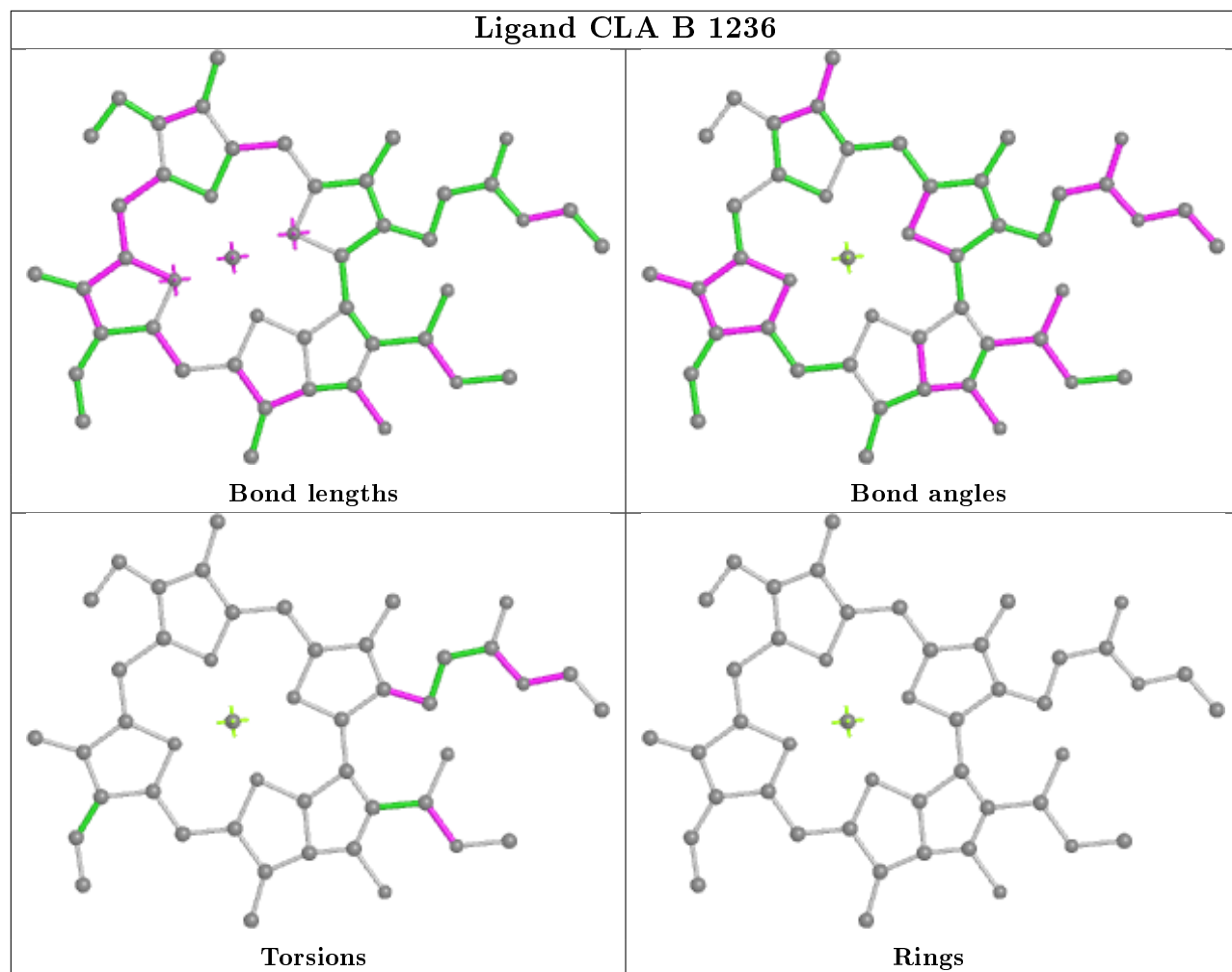
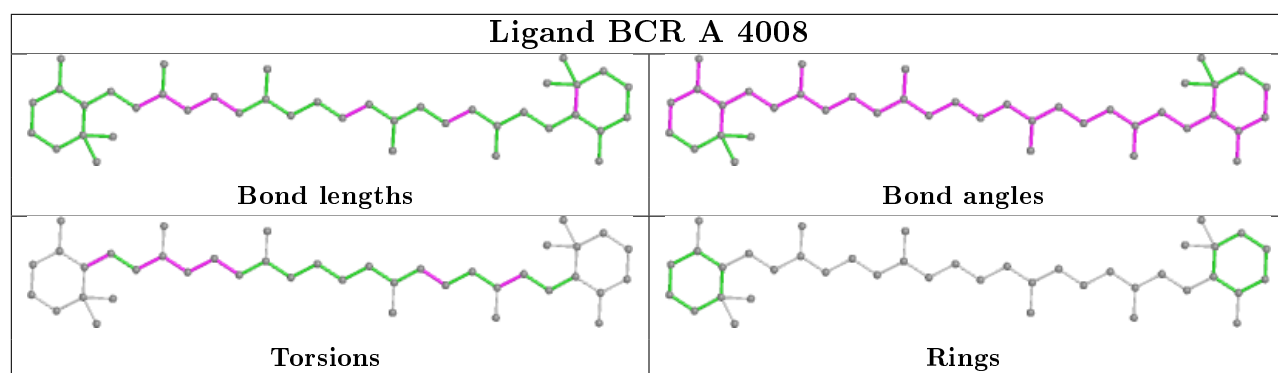
**Ligand BCR A 4007****Ligand CLA b 1232**

## Ligand CLA A 1132

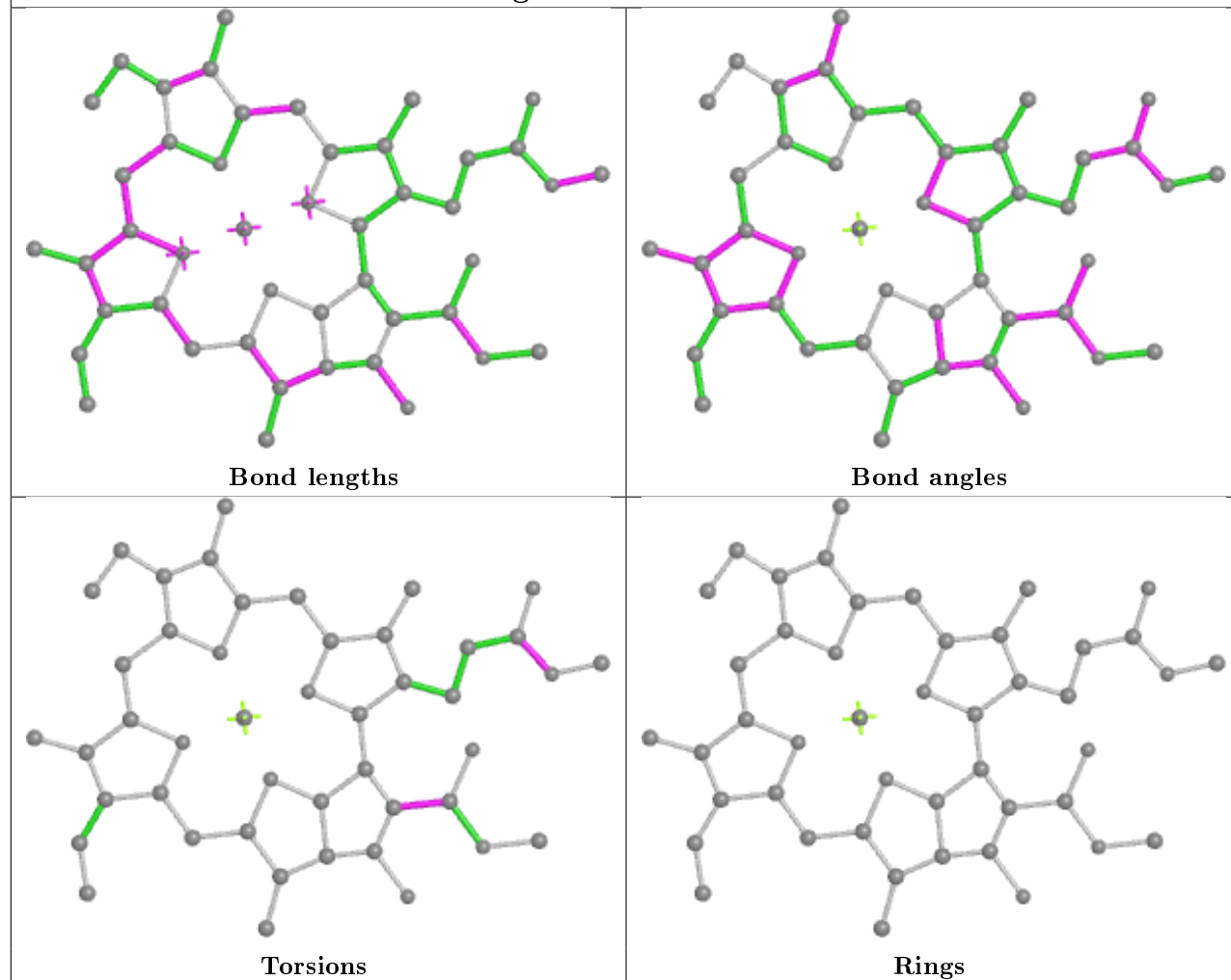


## Ligand CLA b 1231

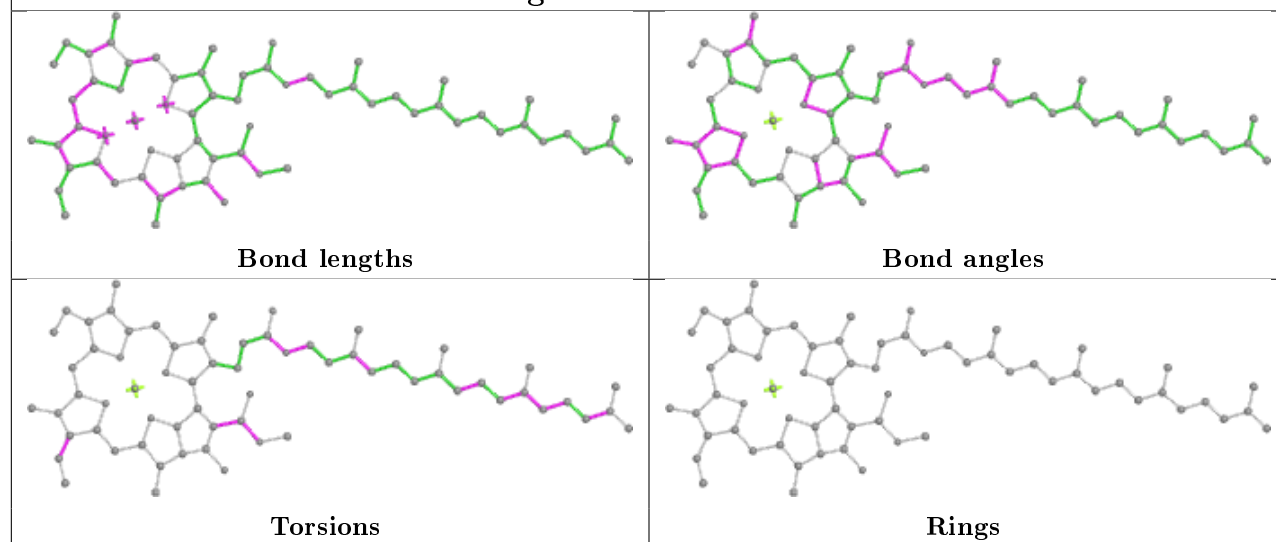


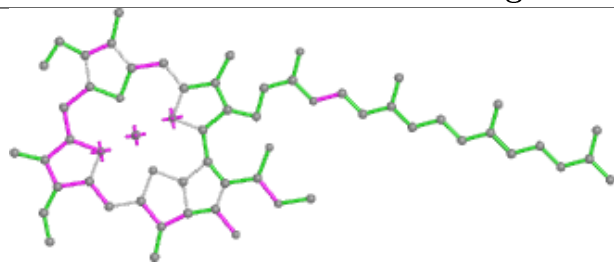
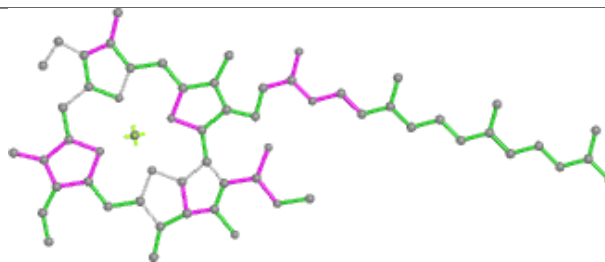
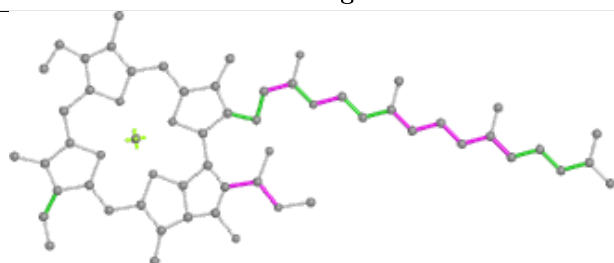
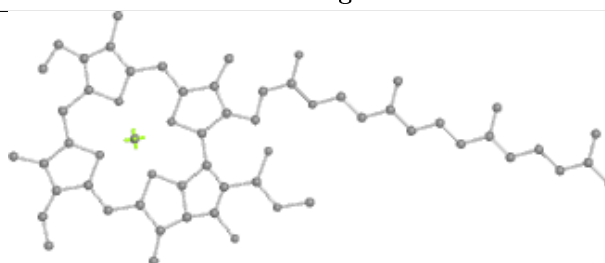
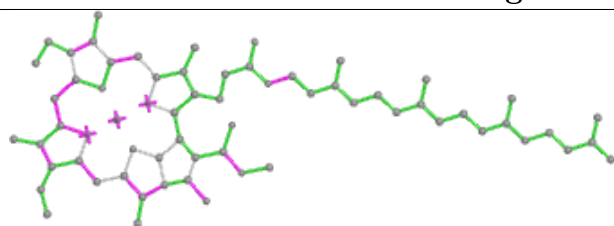
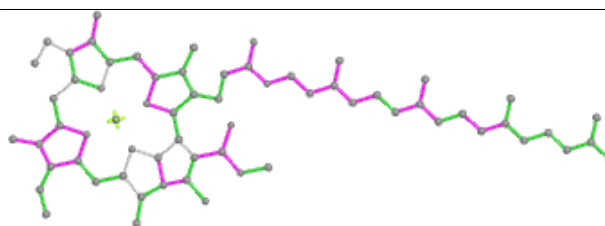
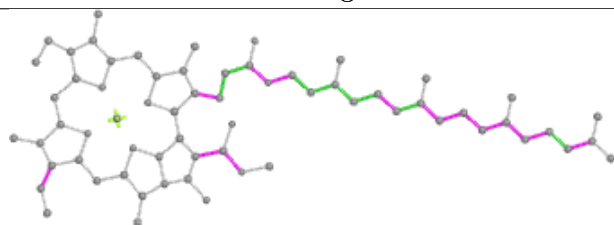
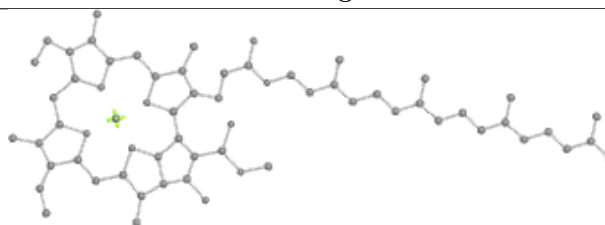


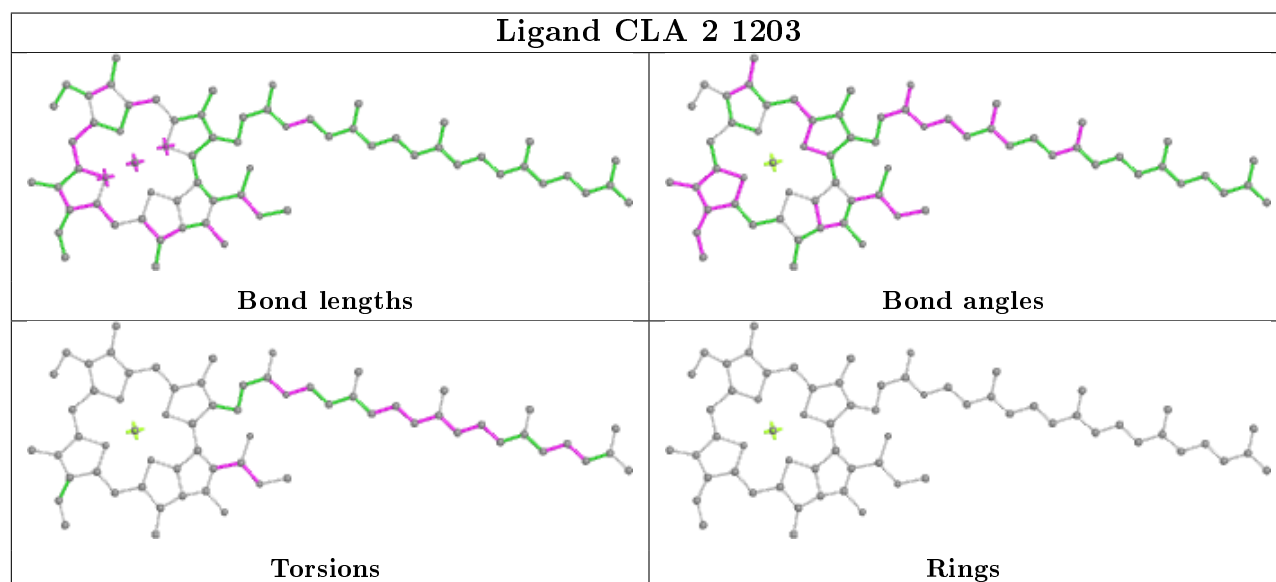
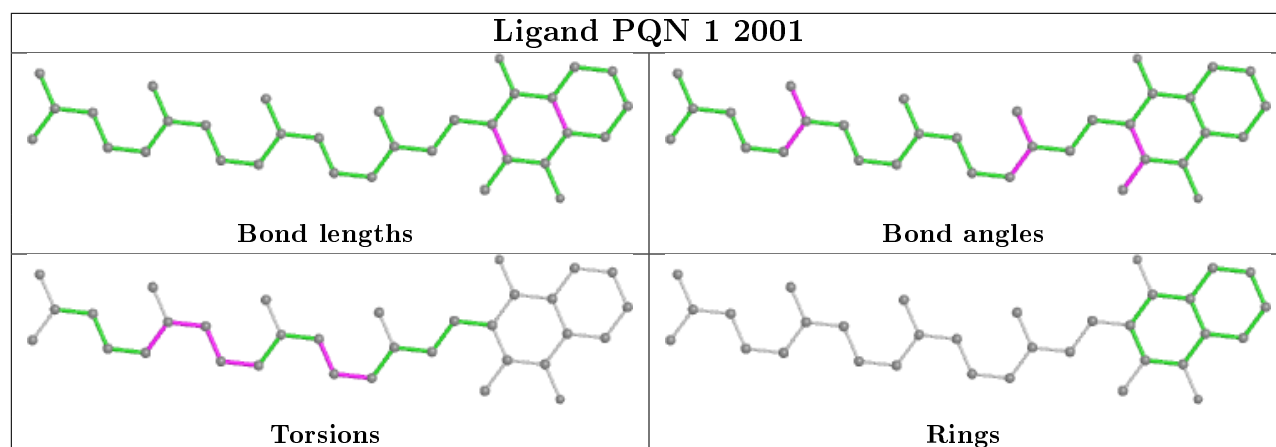
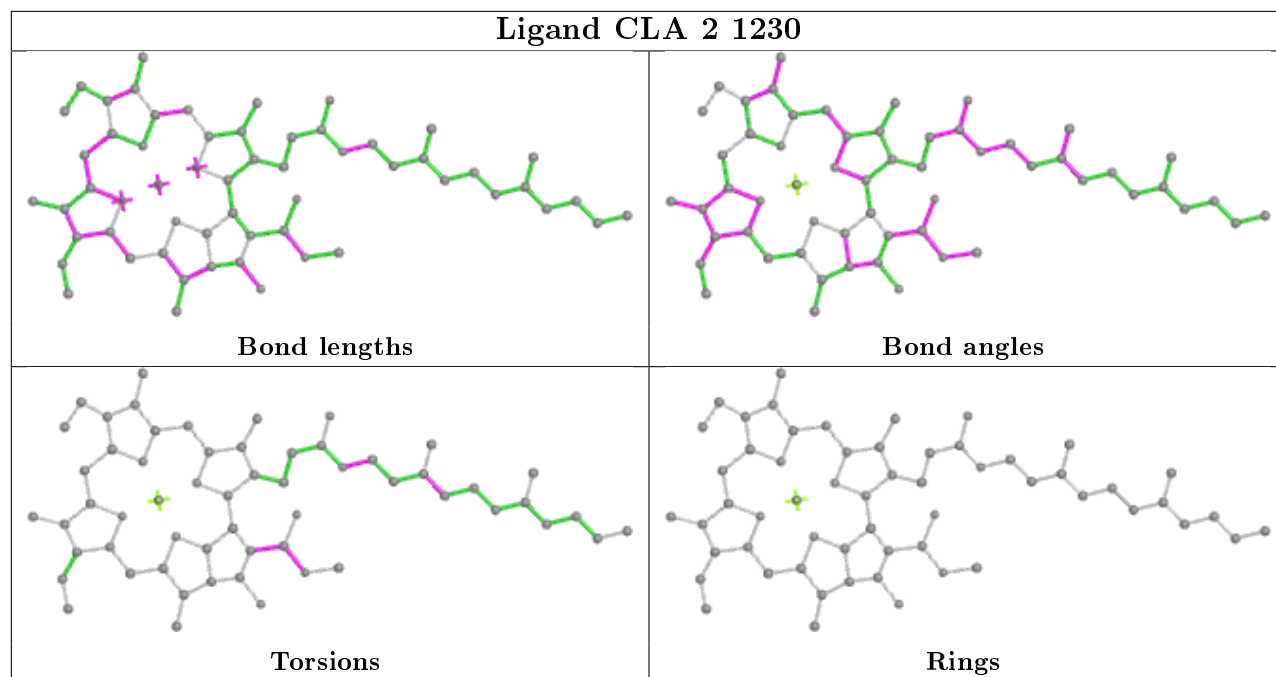
## Ligand CLA 1 1502



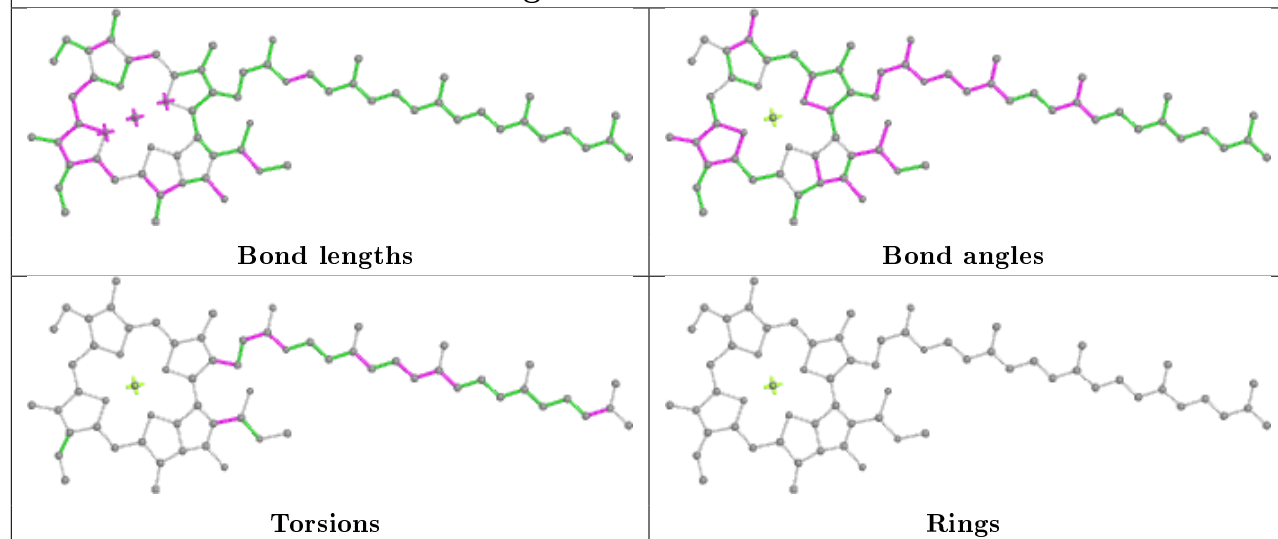
## Ligand CLA a 1126



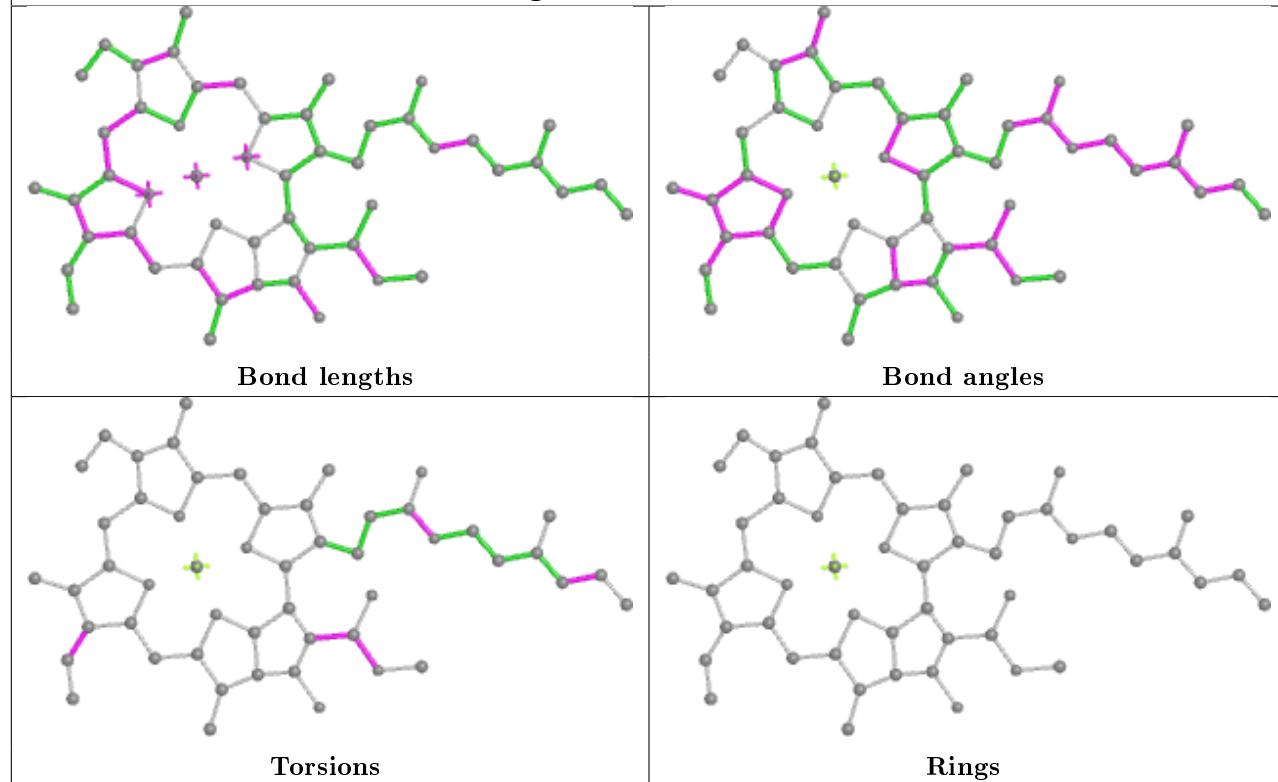
**Ligand CLA B 1235****Bond lengths****Bond angles****Torsions****Rings****Ligand CLA A 1104****Bond lengths****Bond angles****Torsions****Rings**



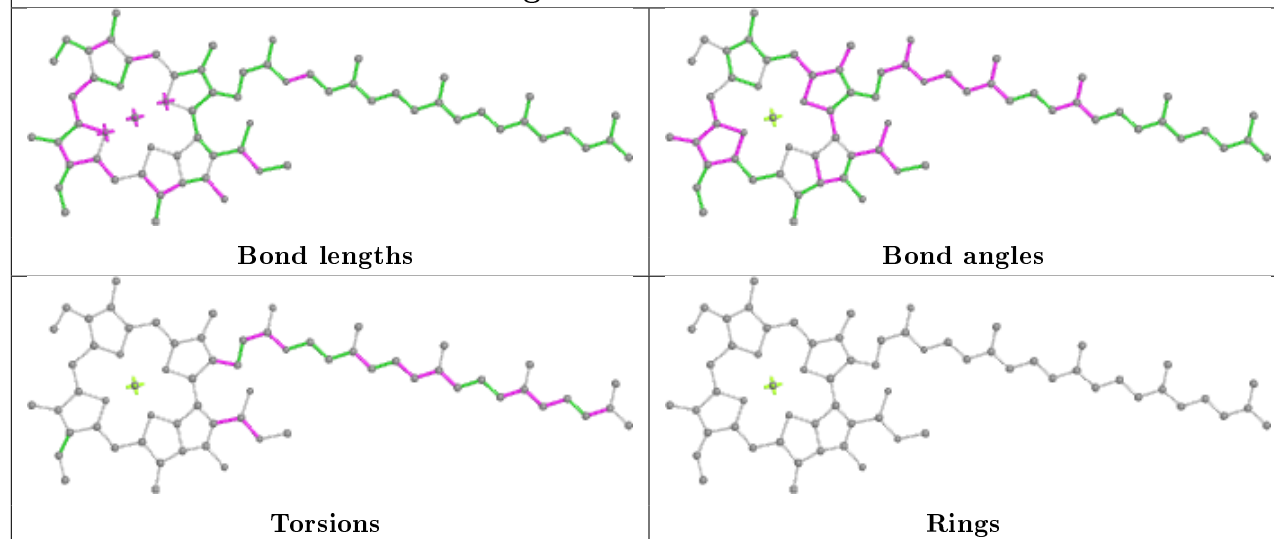
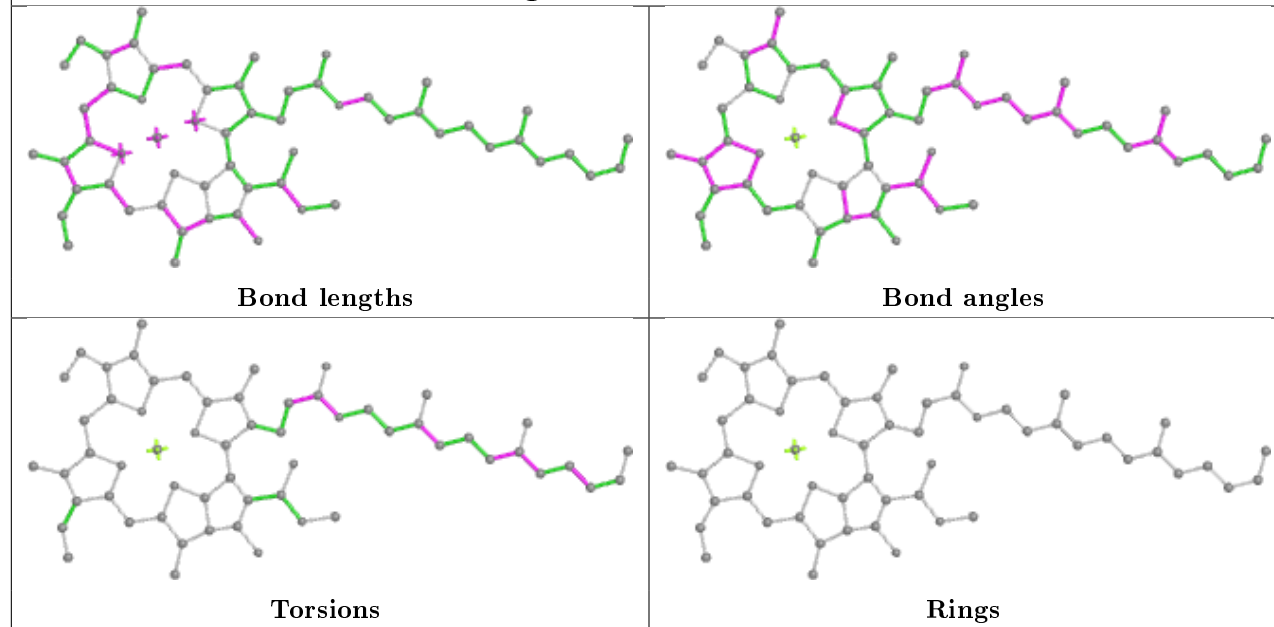
## Ligand CLA A 1137

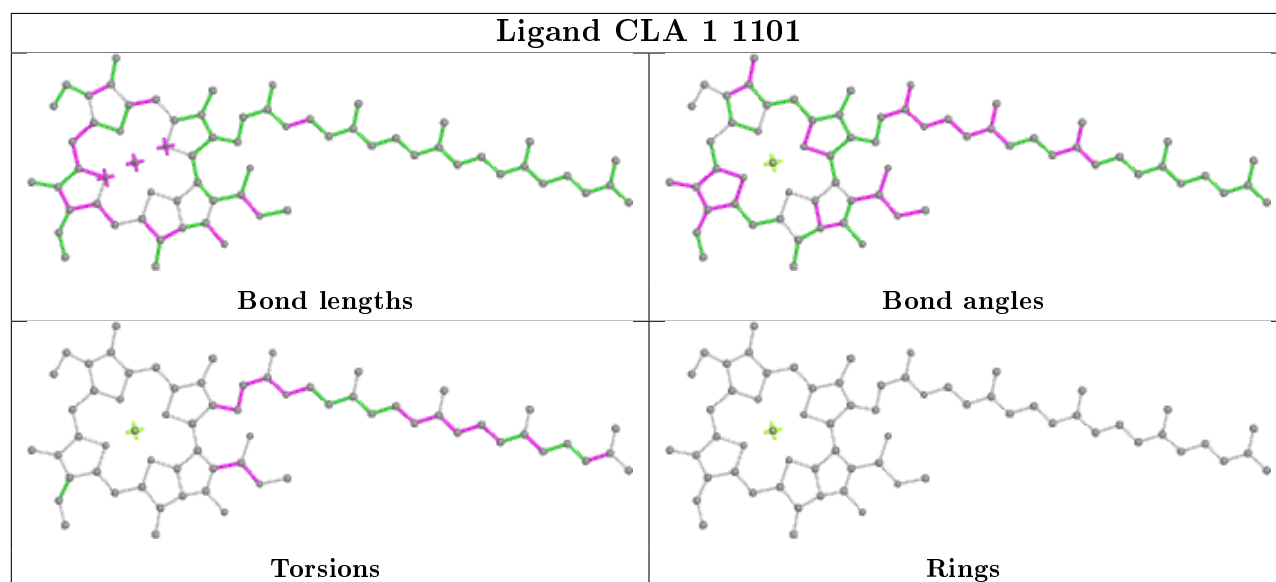
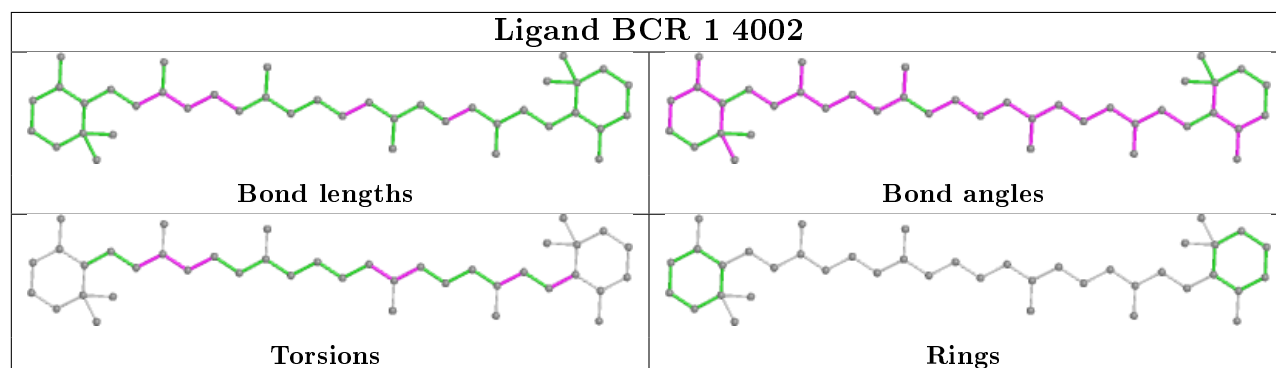
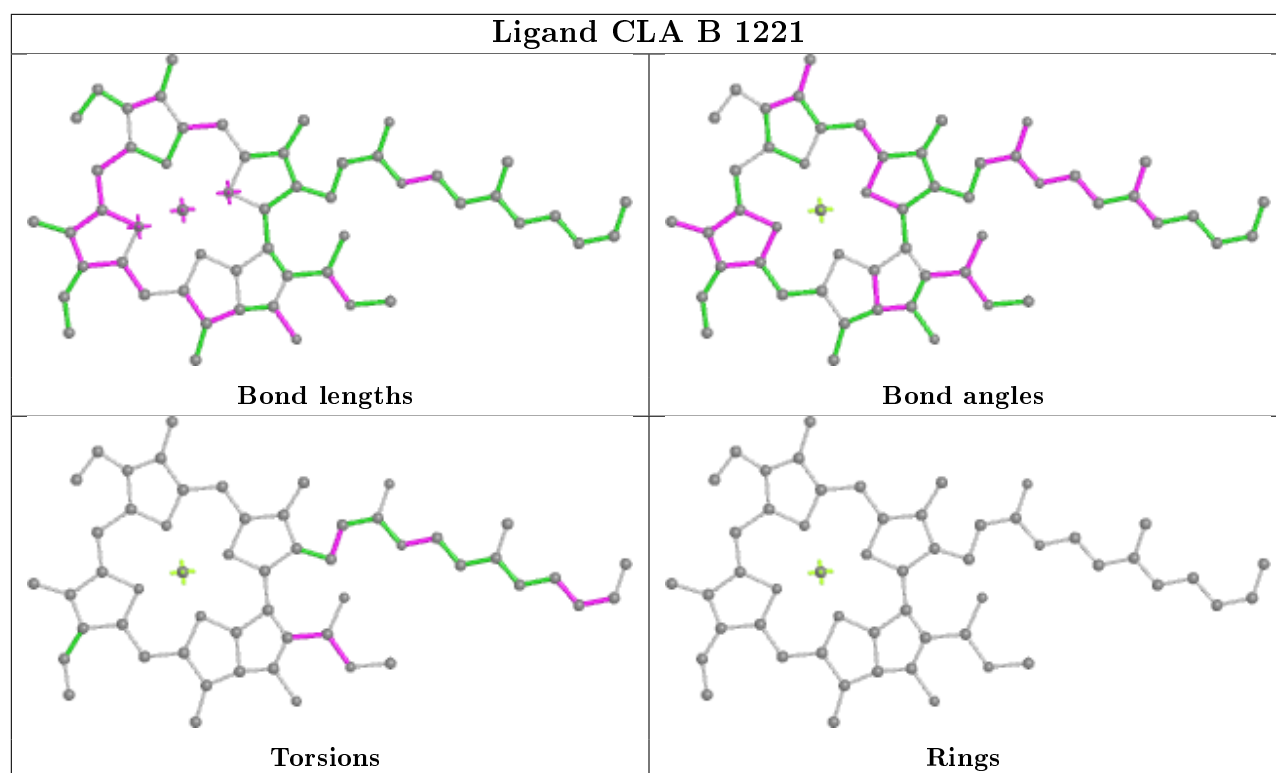


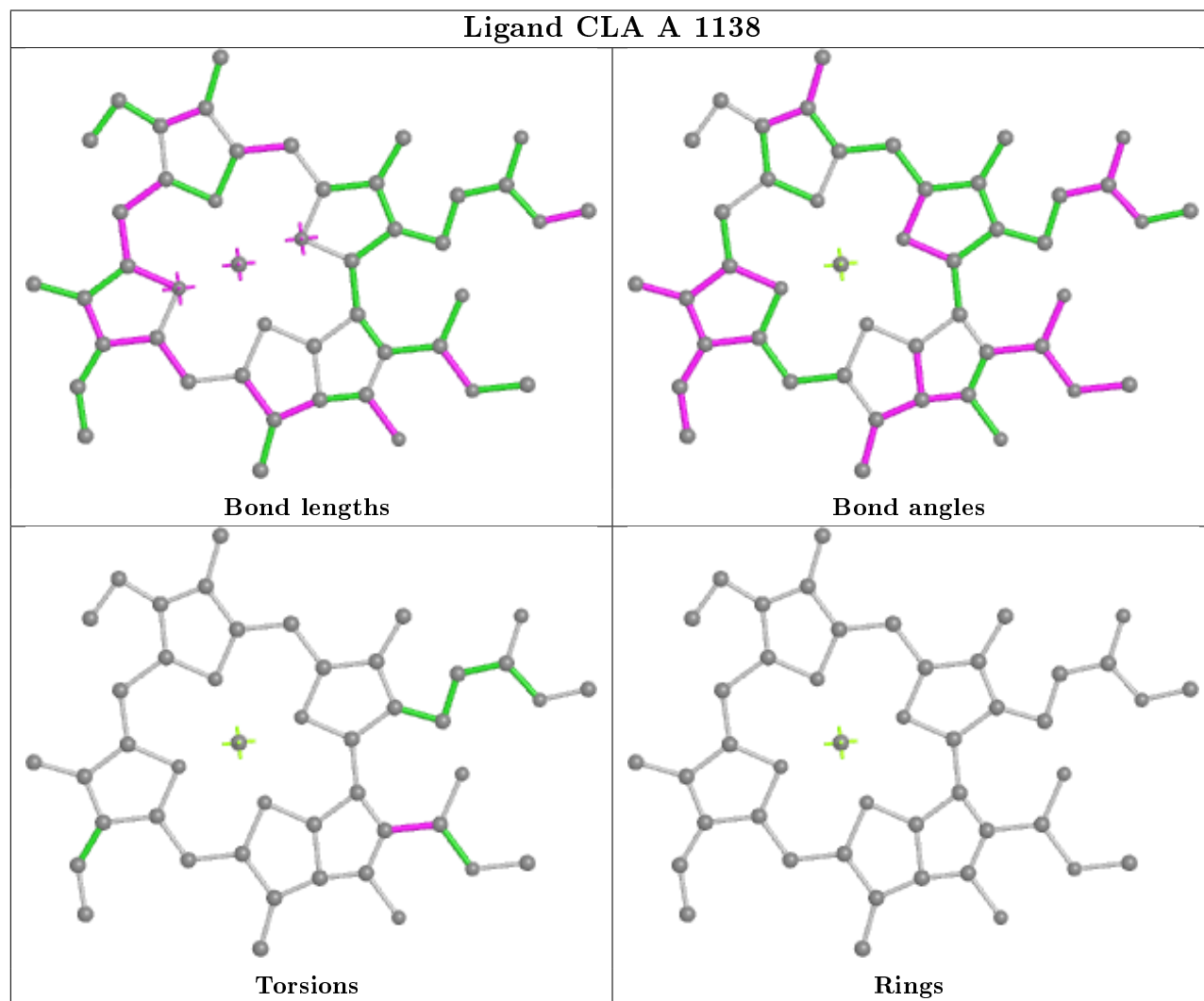
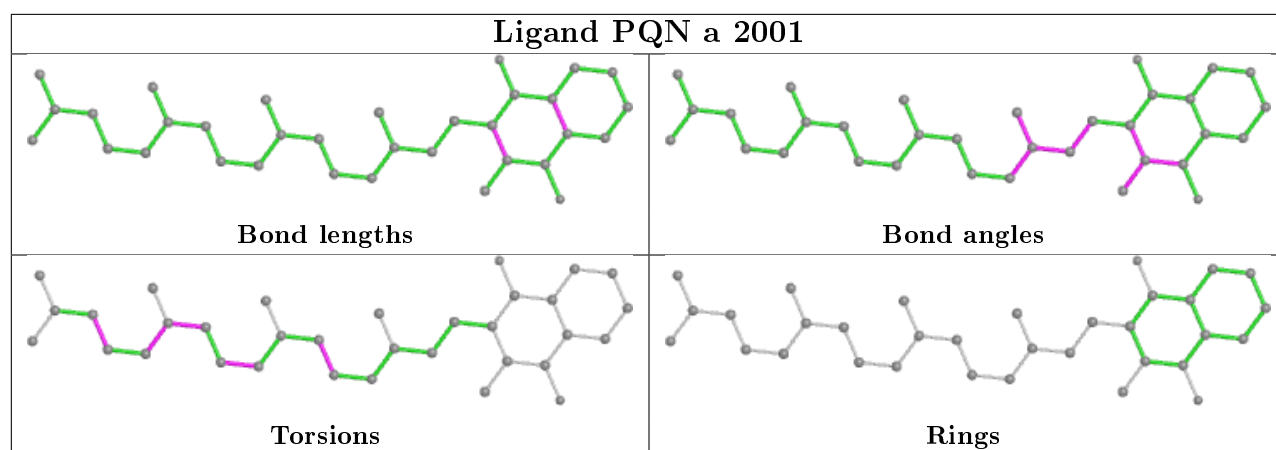
## Ligand CLA 1 1125

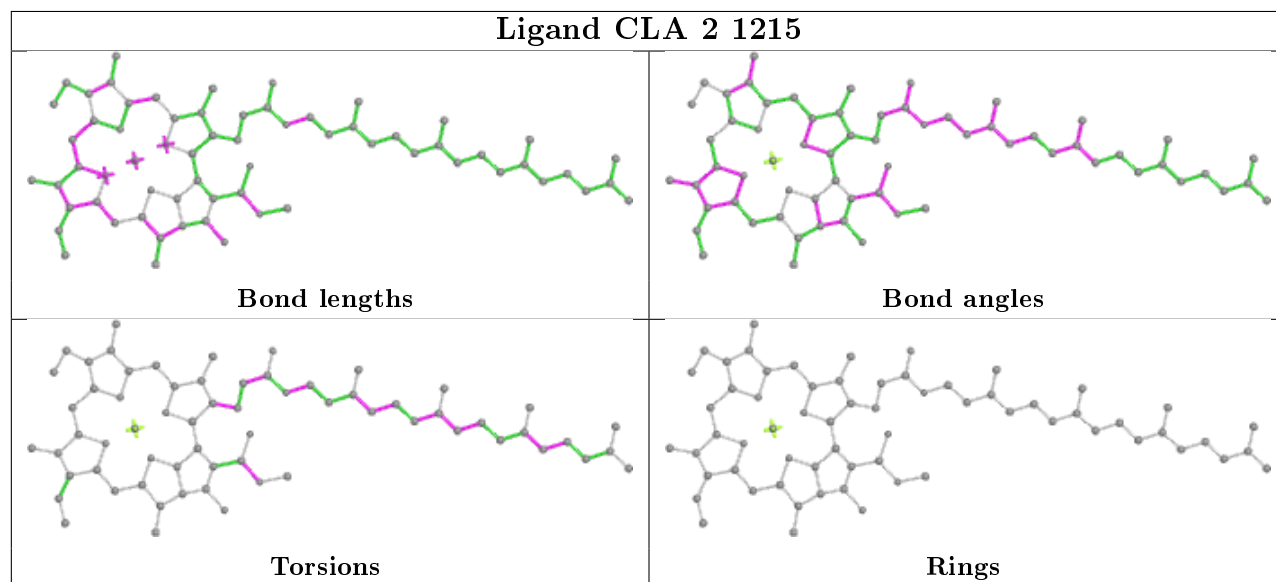
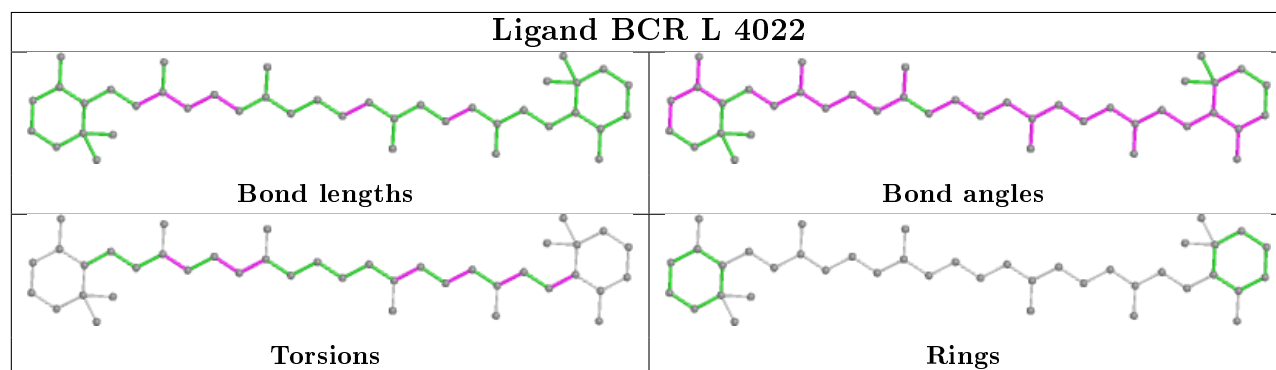
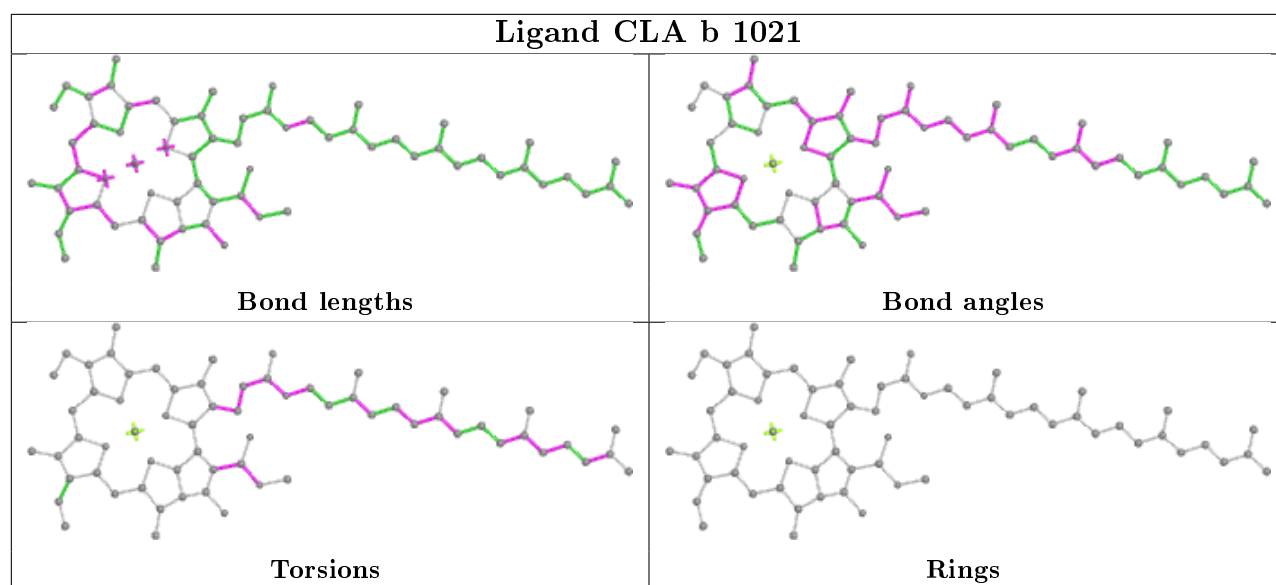


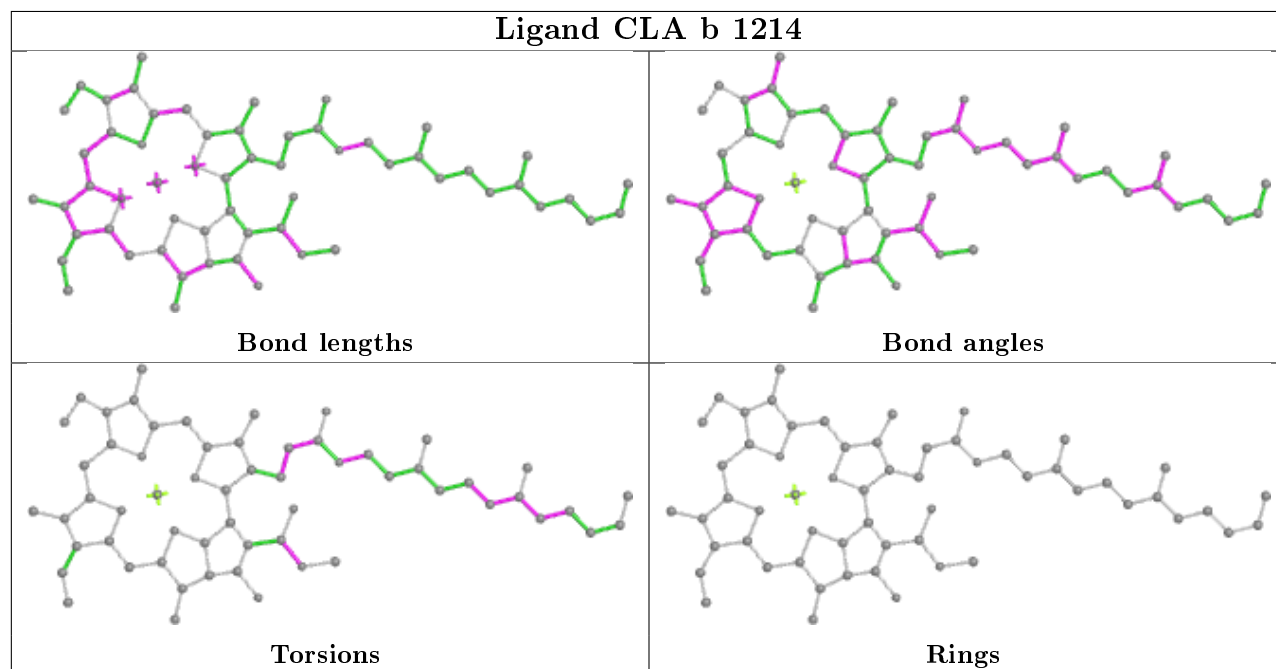
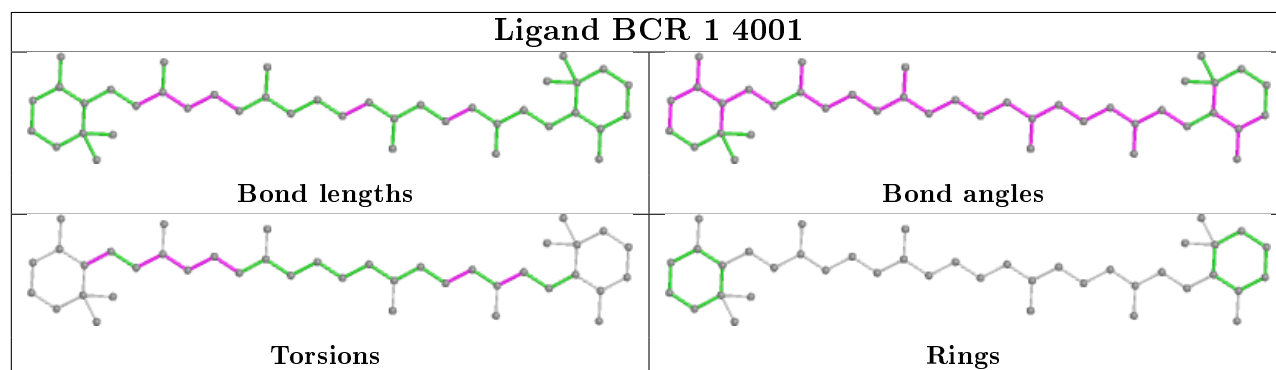
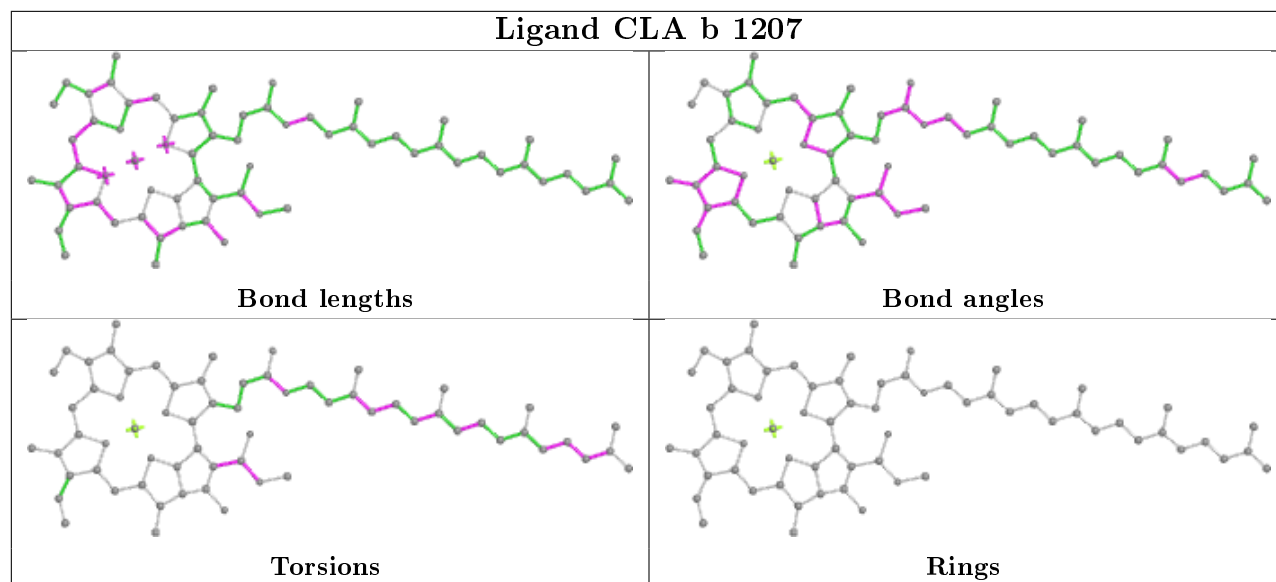


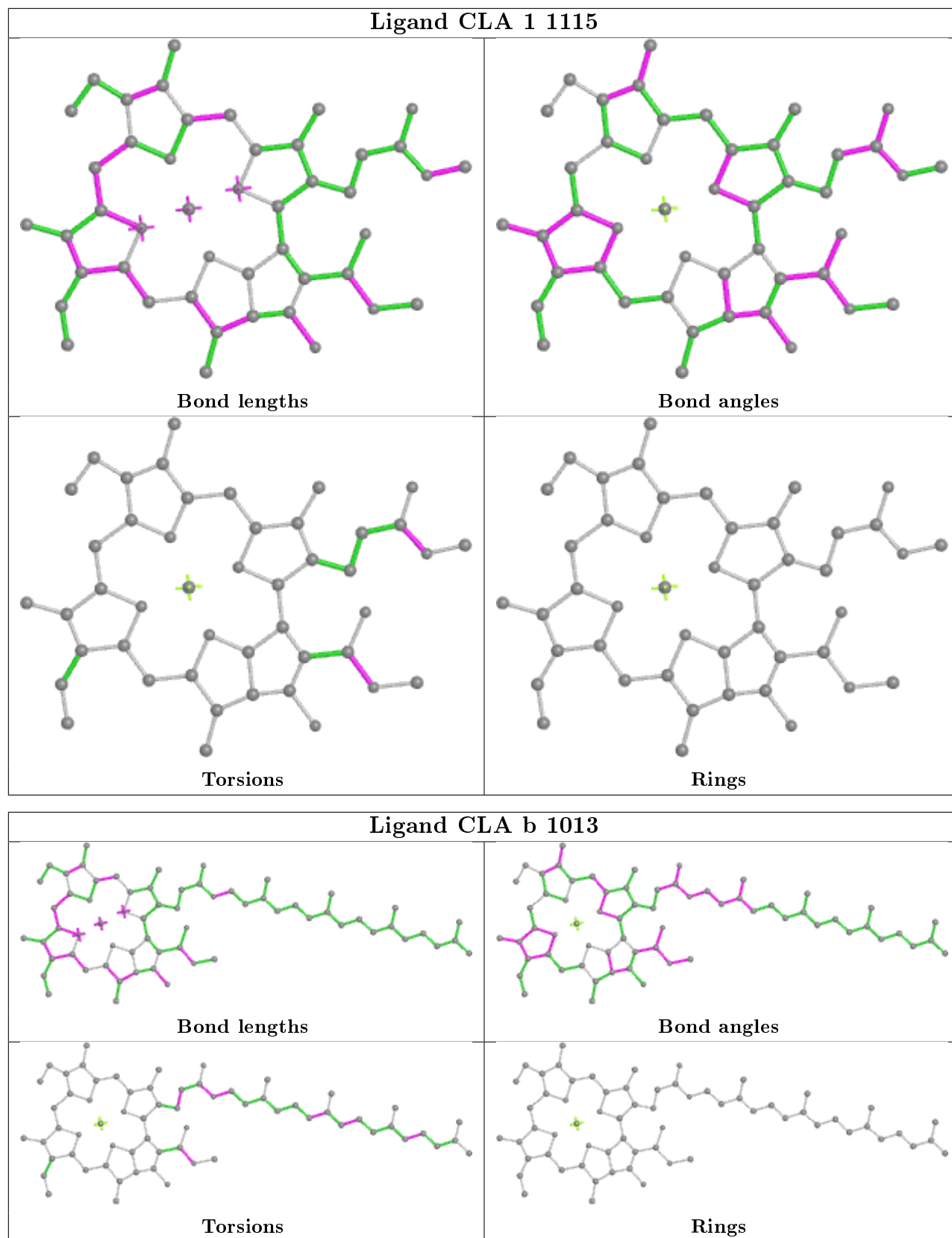
**Ligand CLA B 1021****Ligand CLA A 1122**

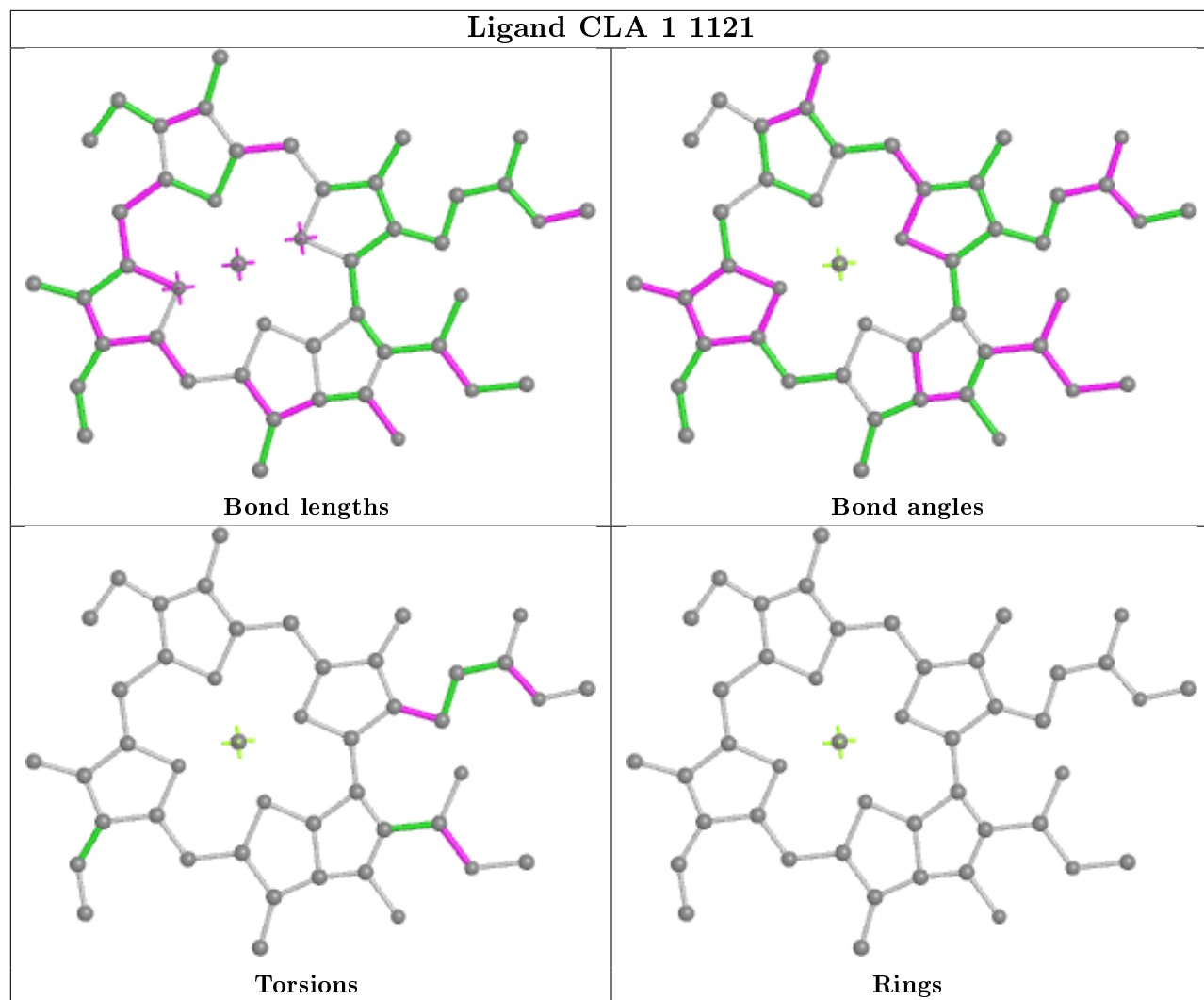


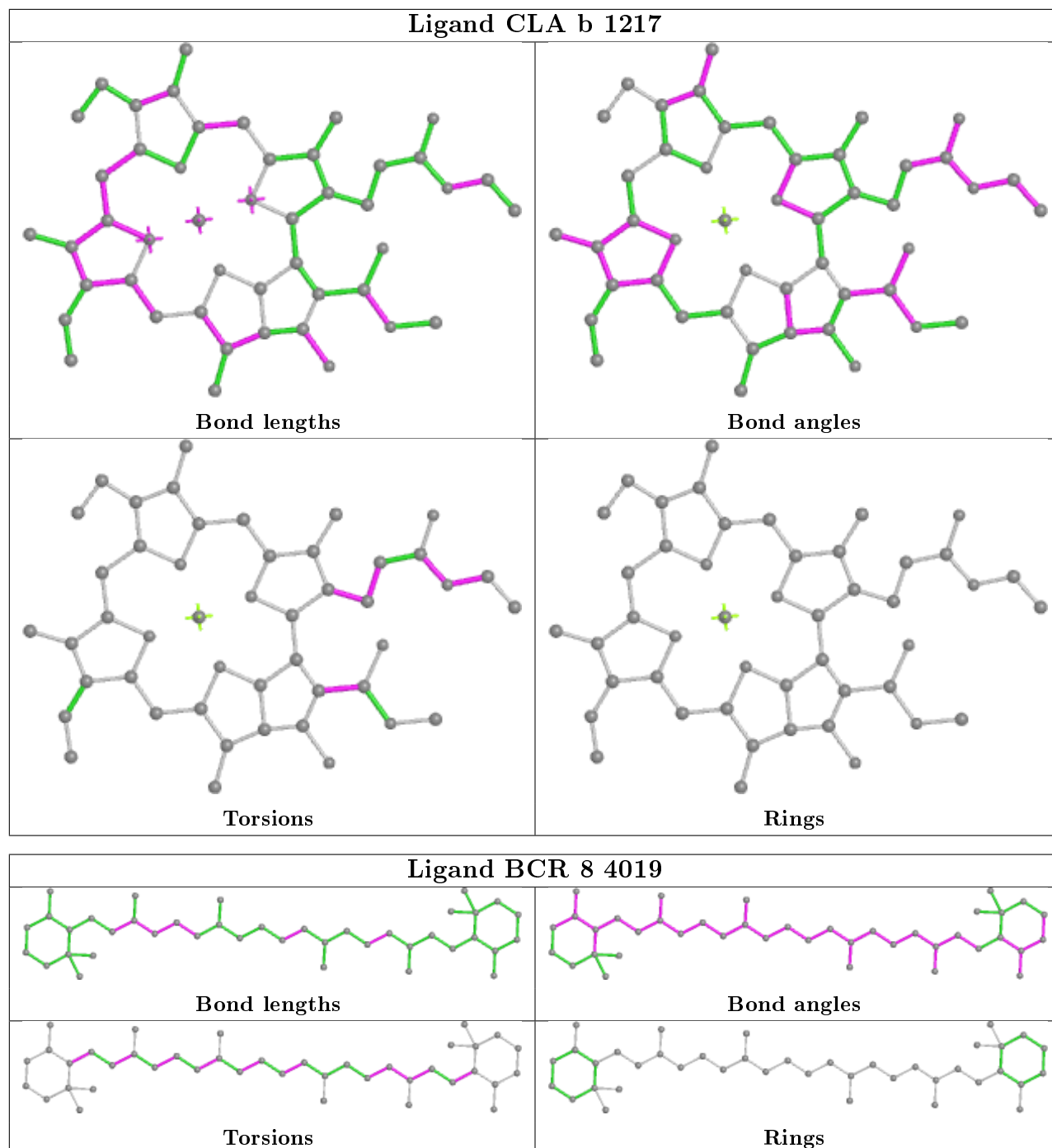




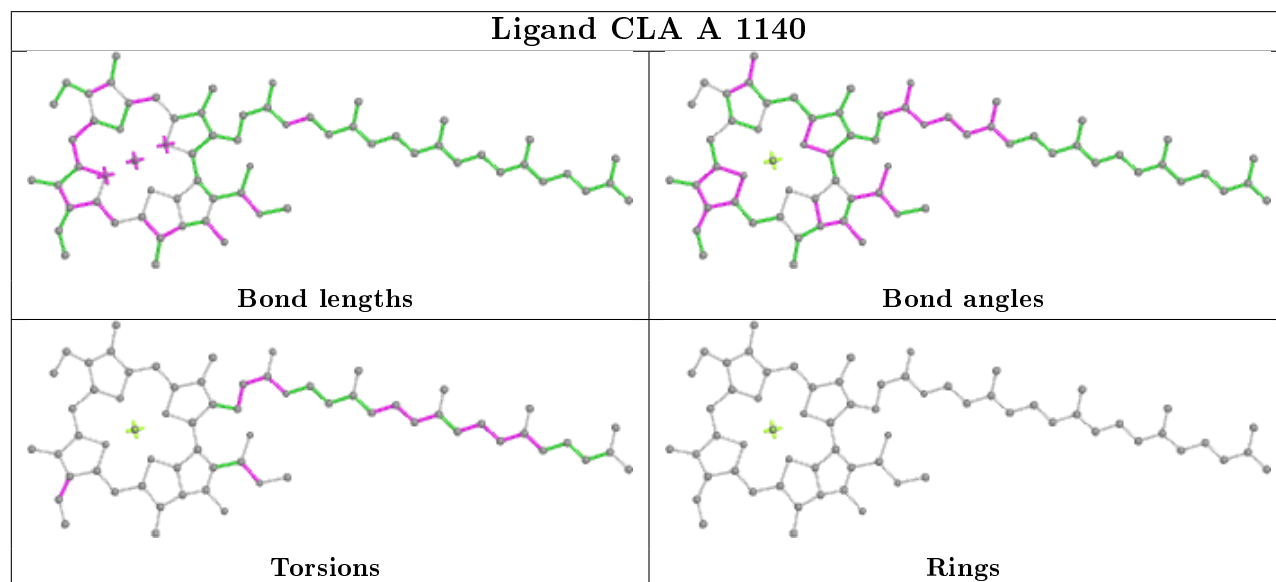
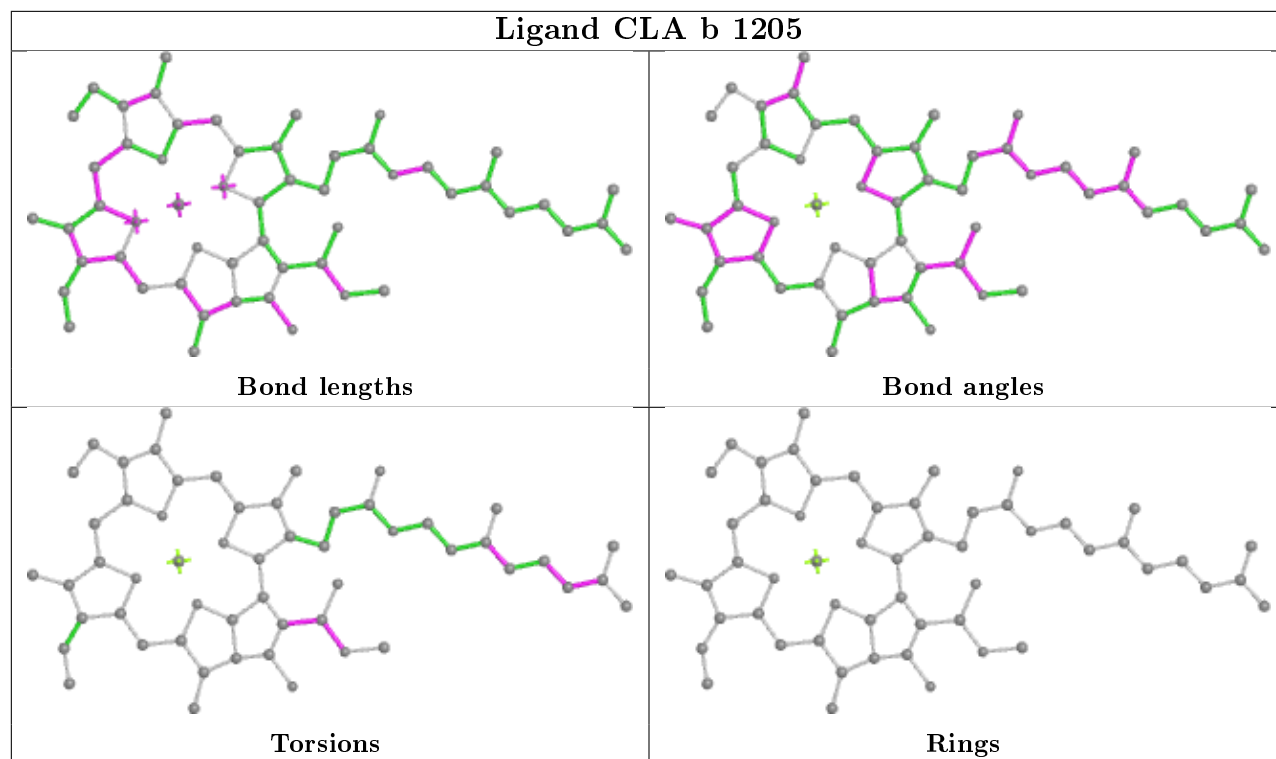


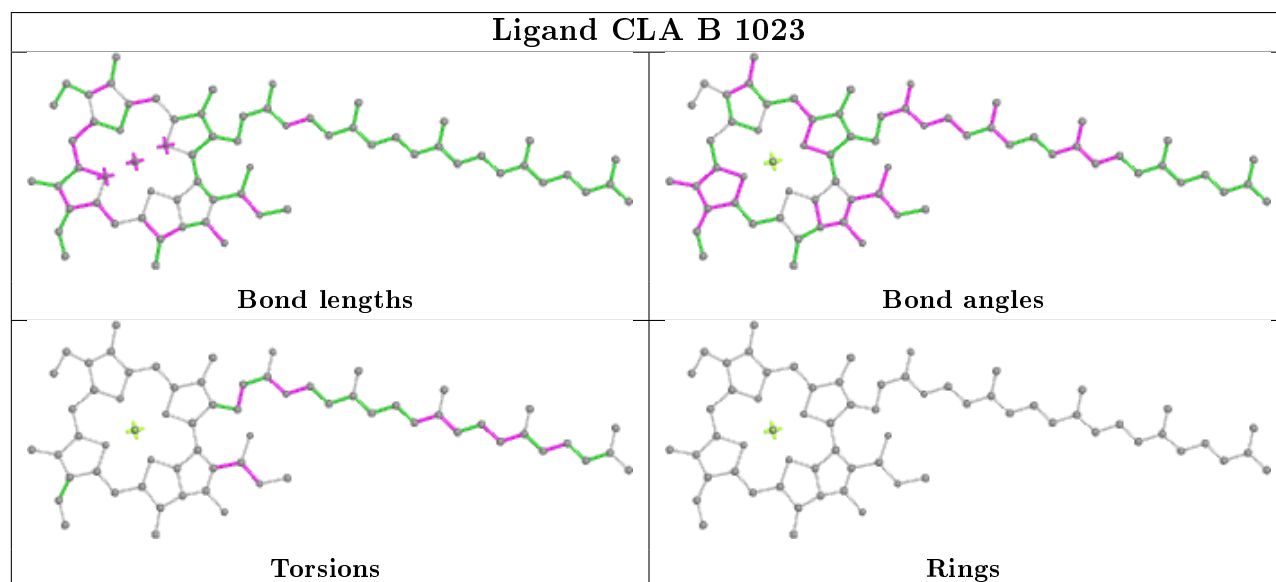
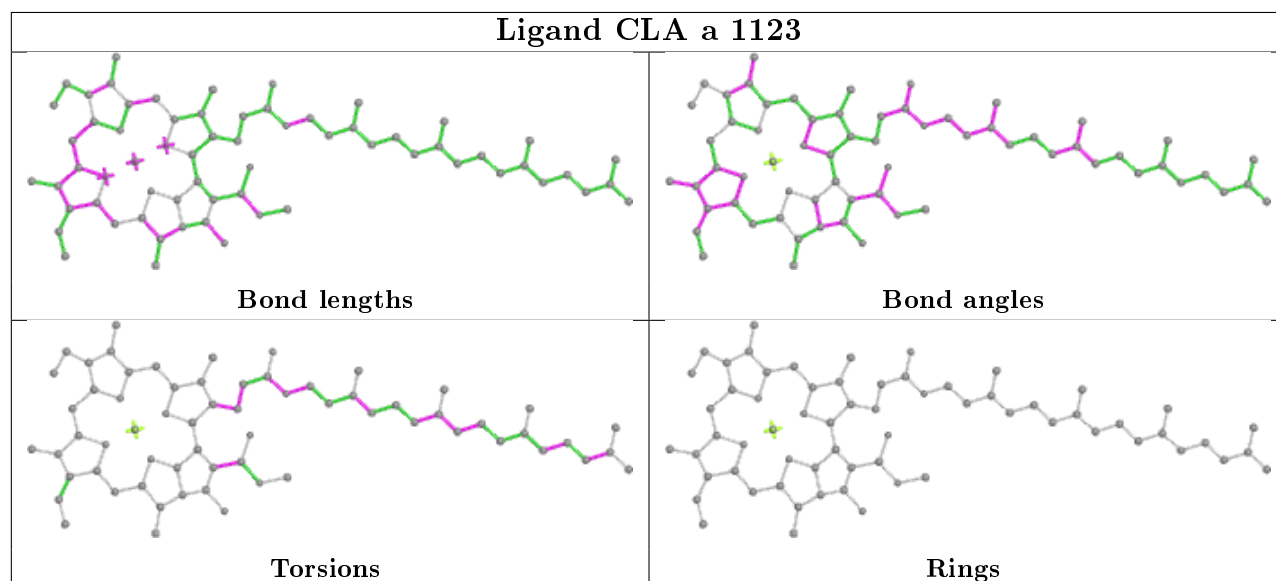
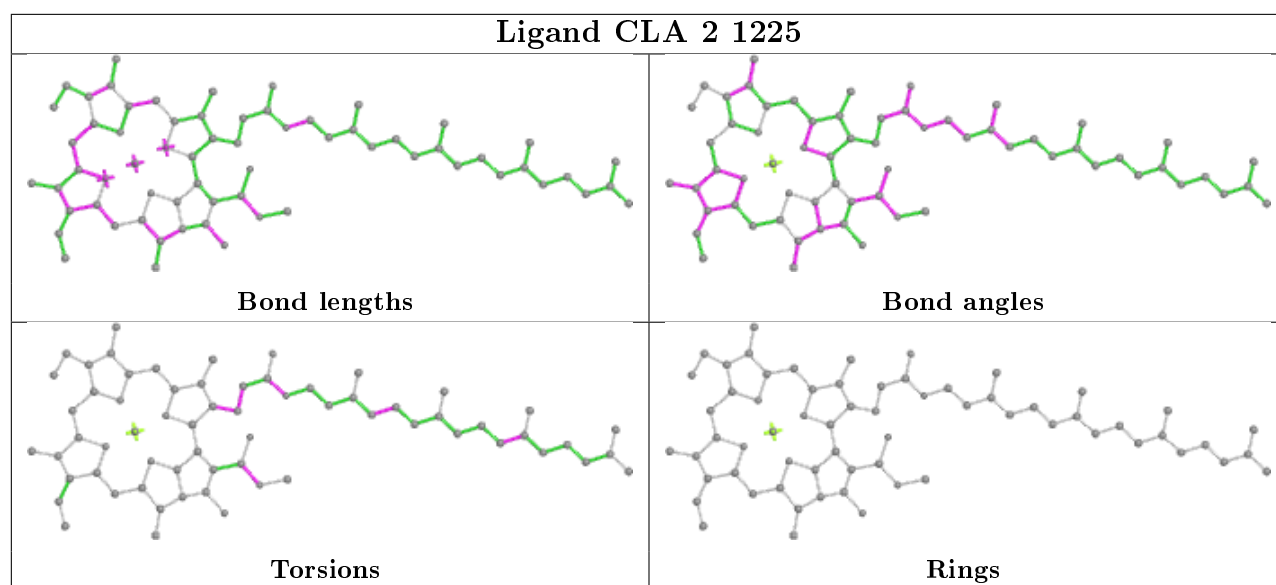


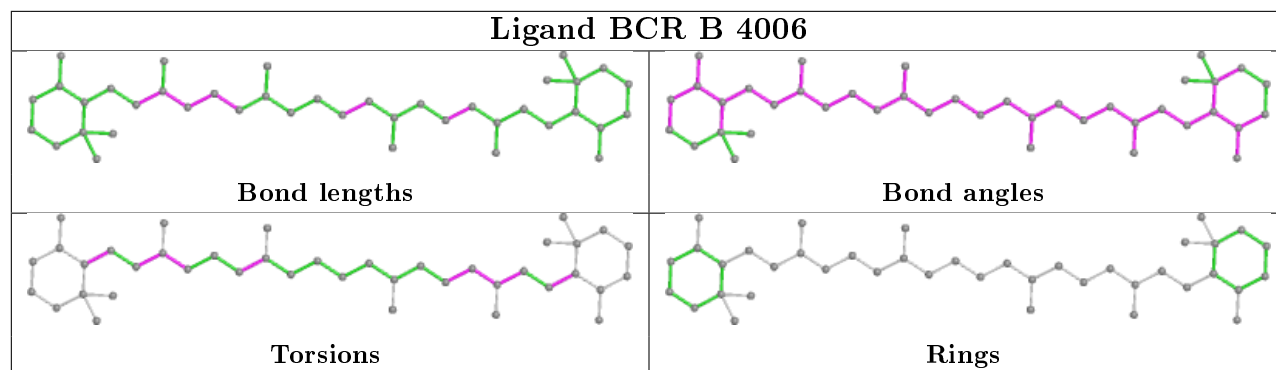
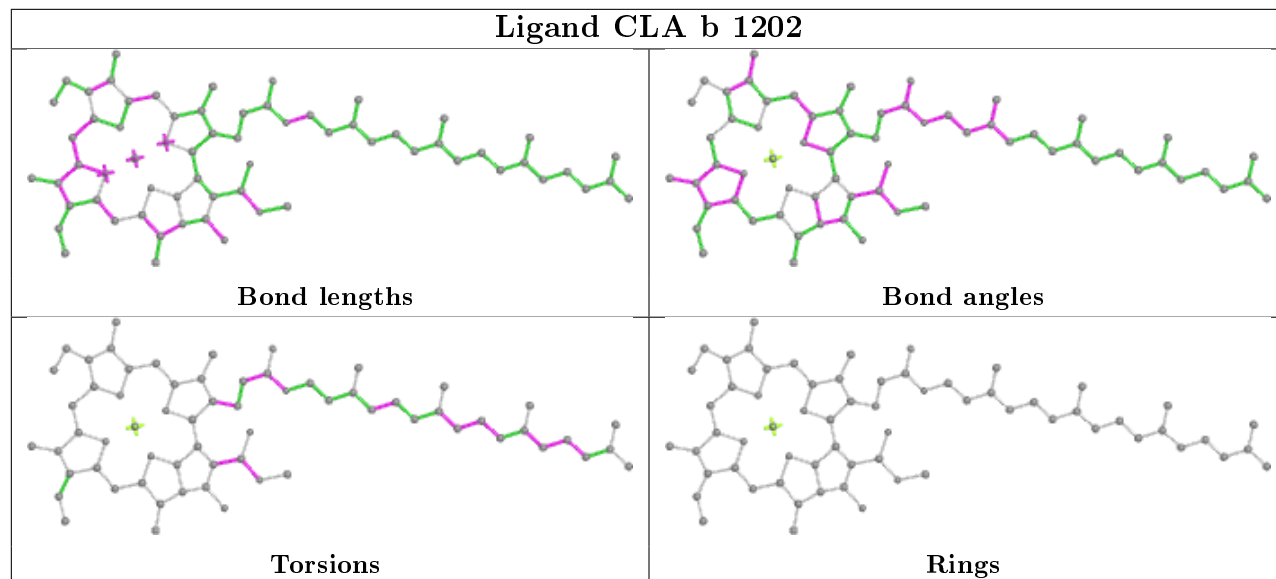
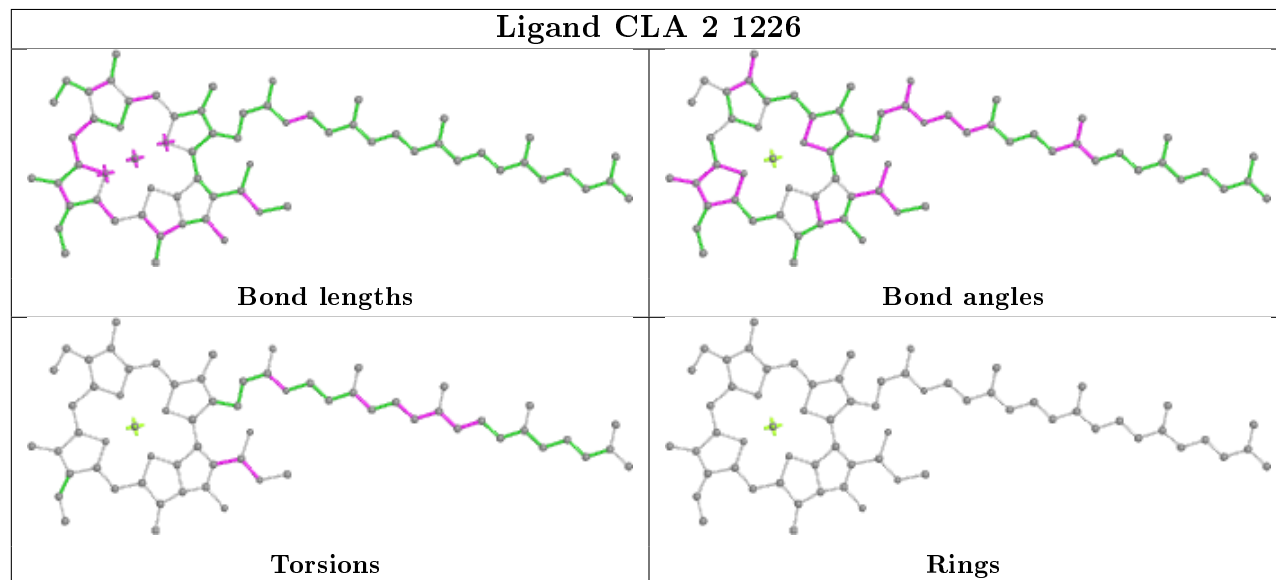


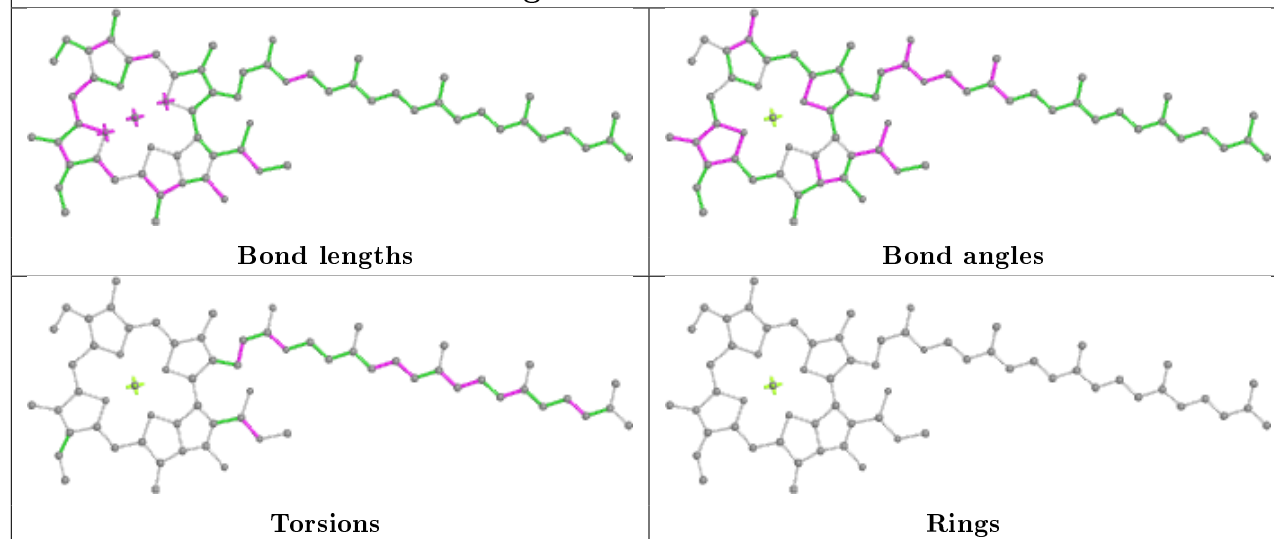
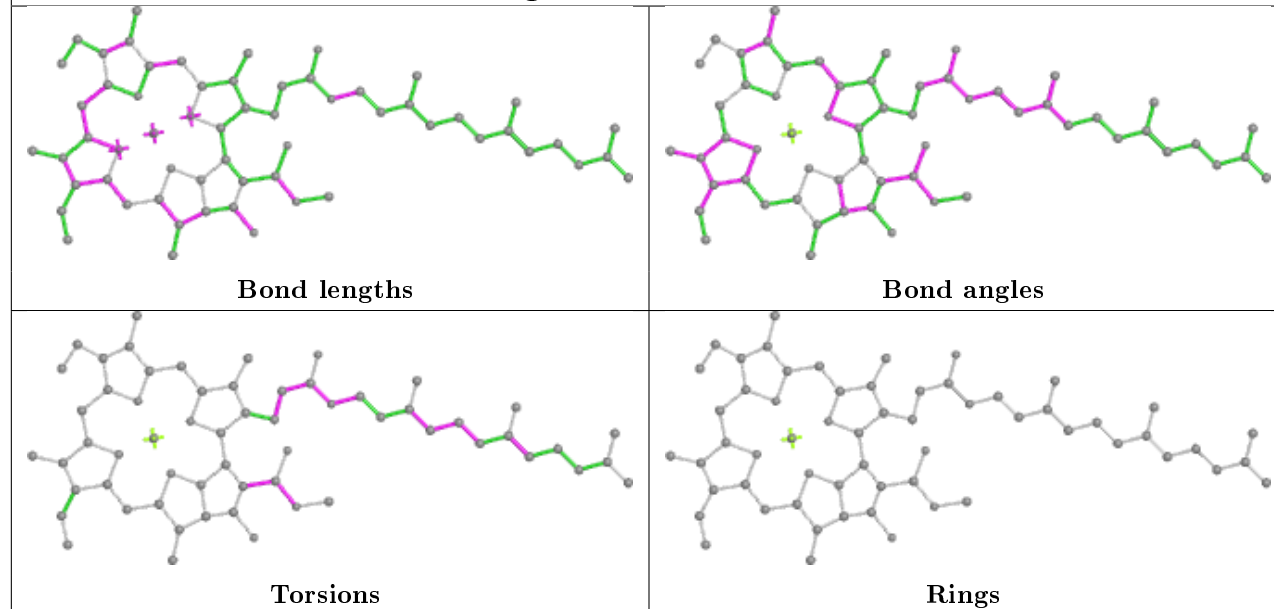


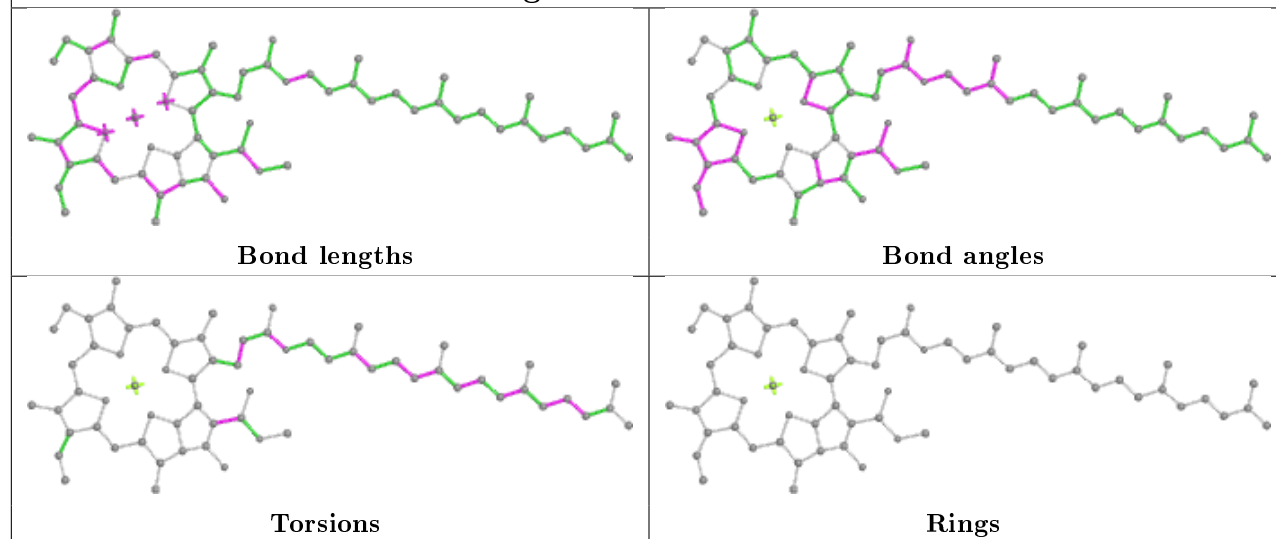
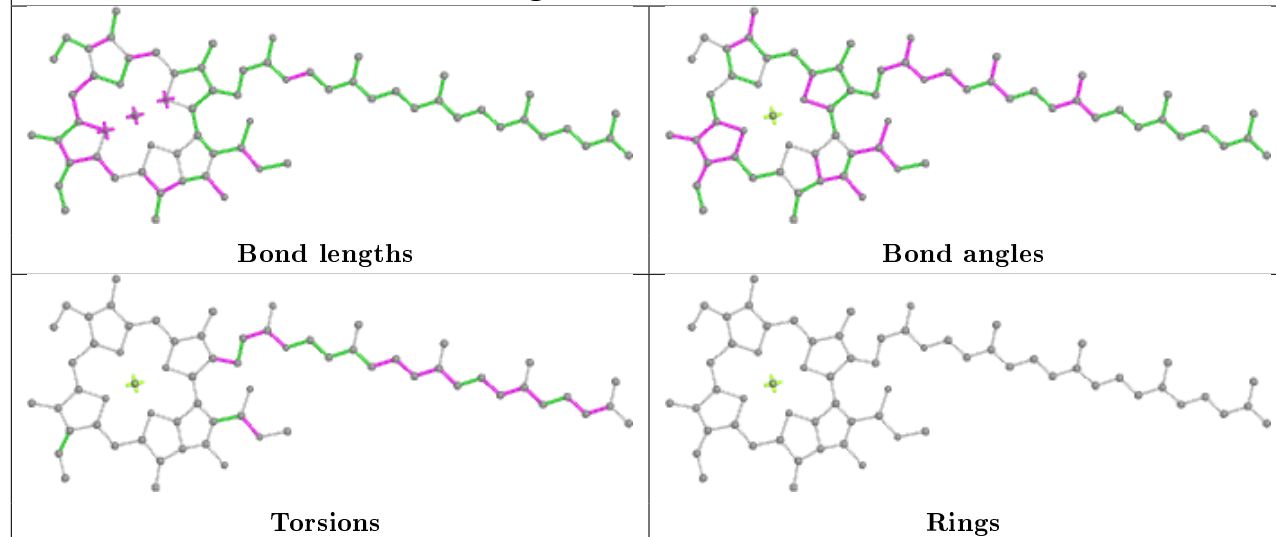


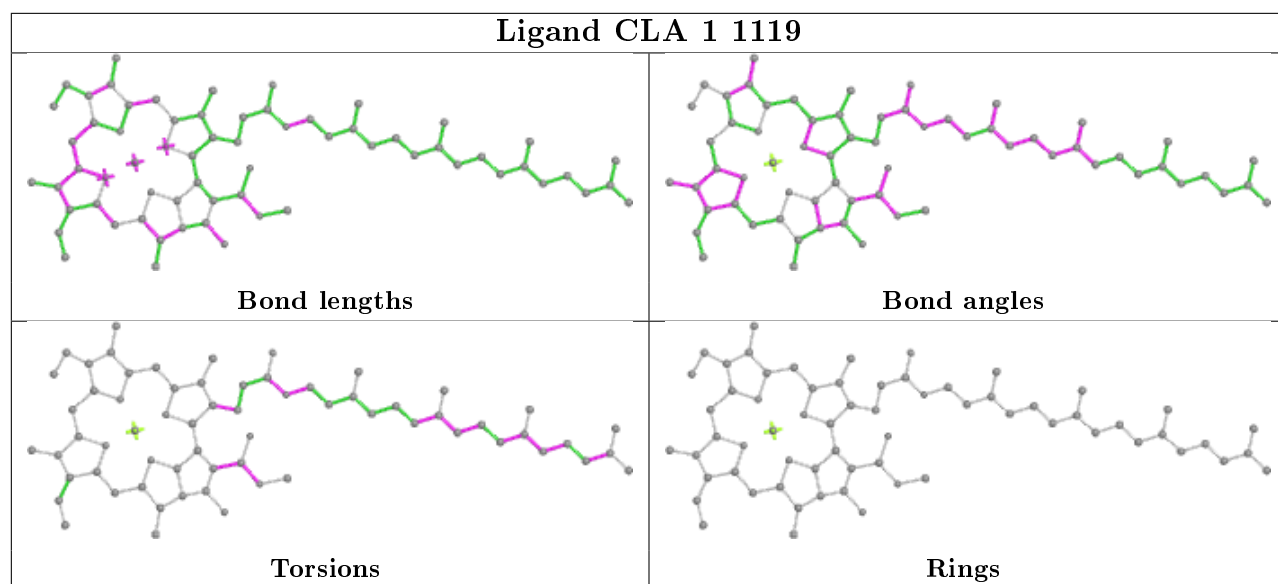
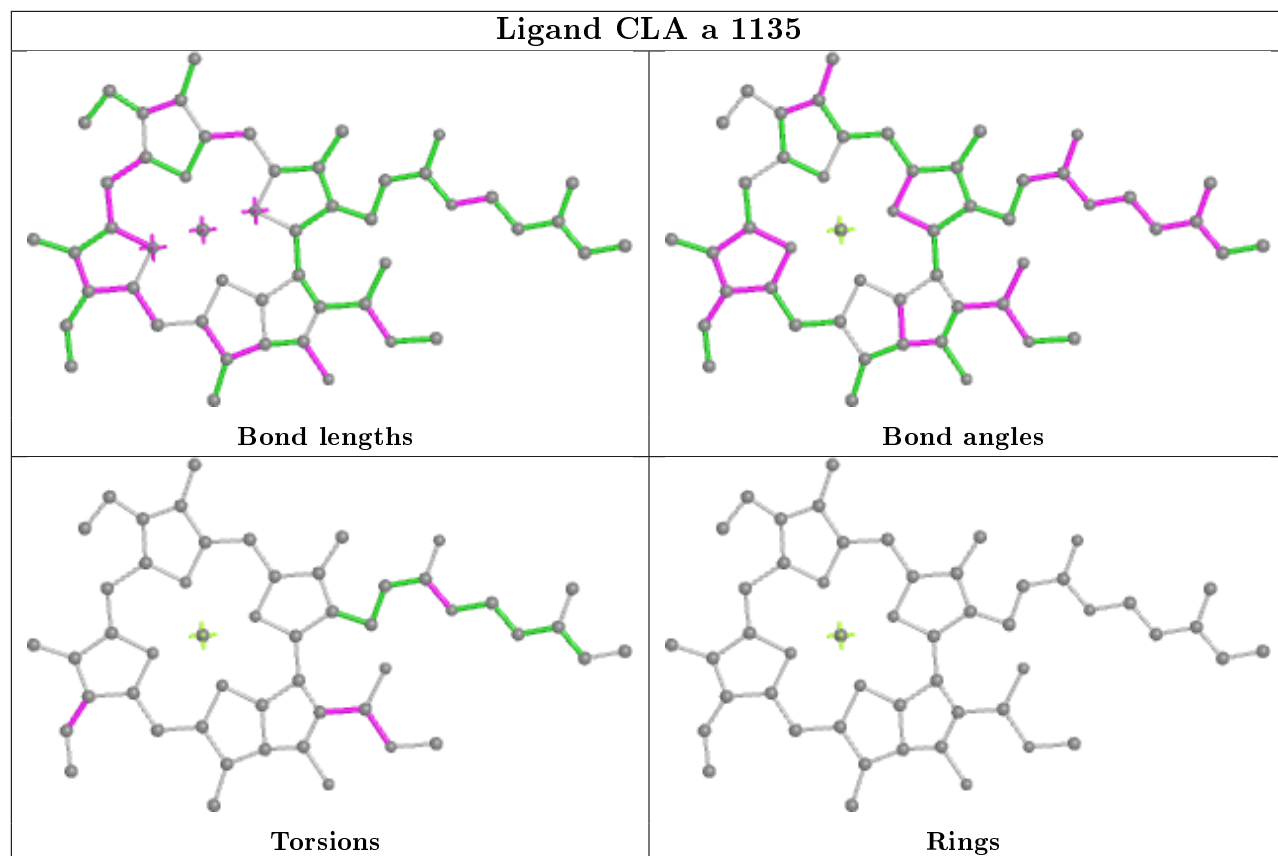


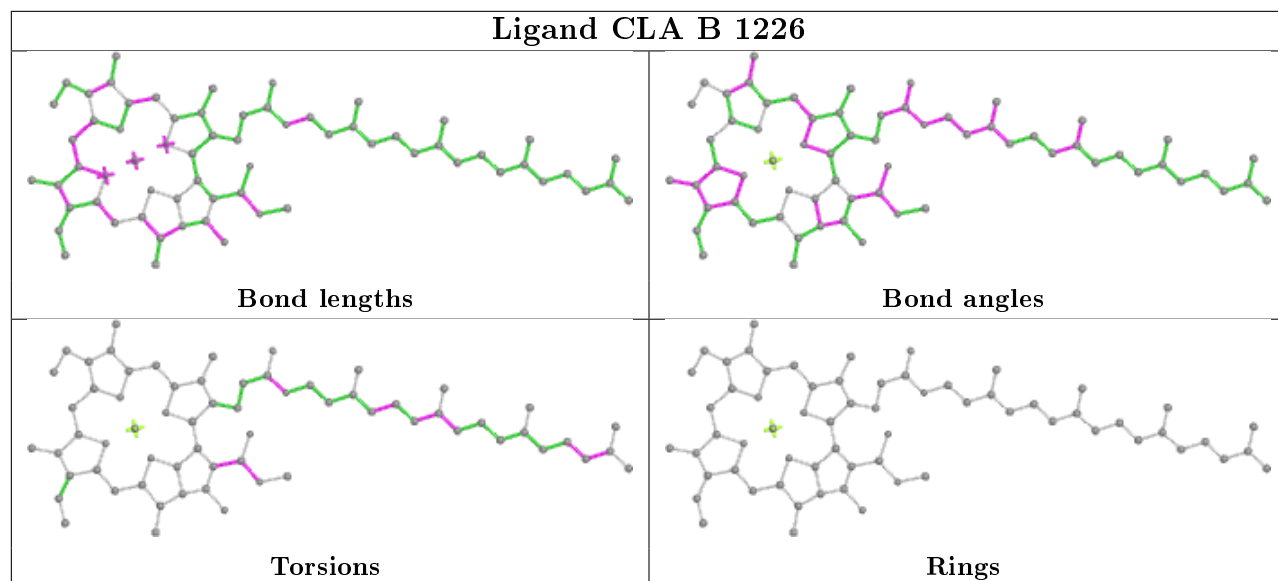
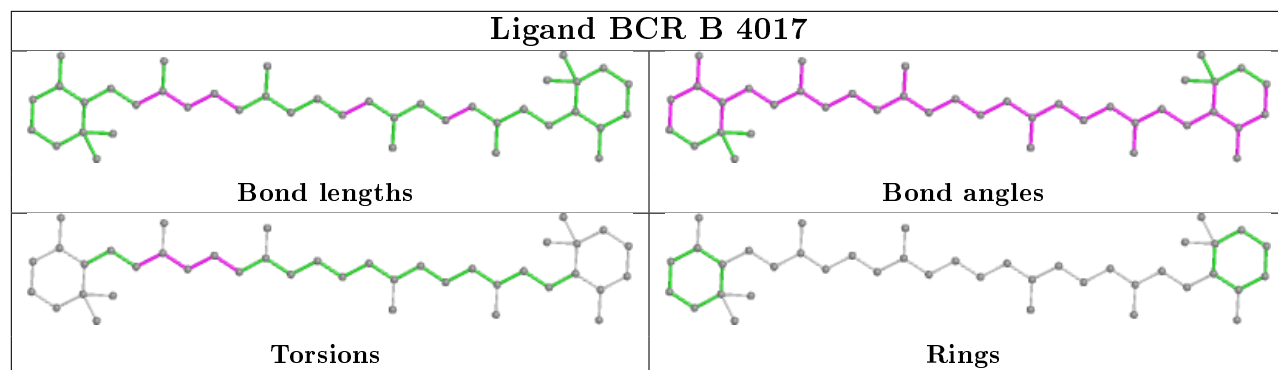


**Ligand BCR B 4006****Ligand CLA b 1202****Ligand CLA 2 1226**

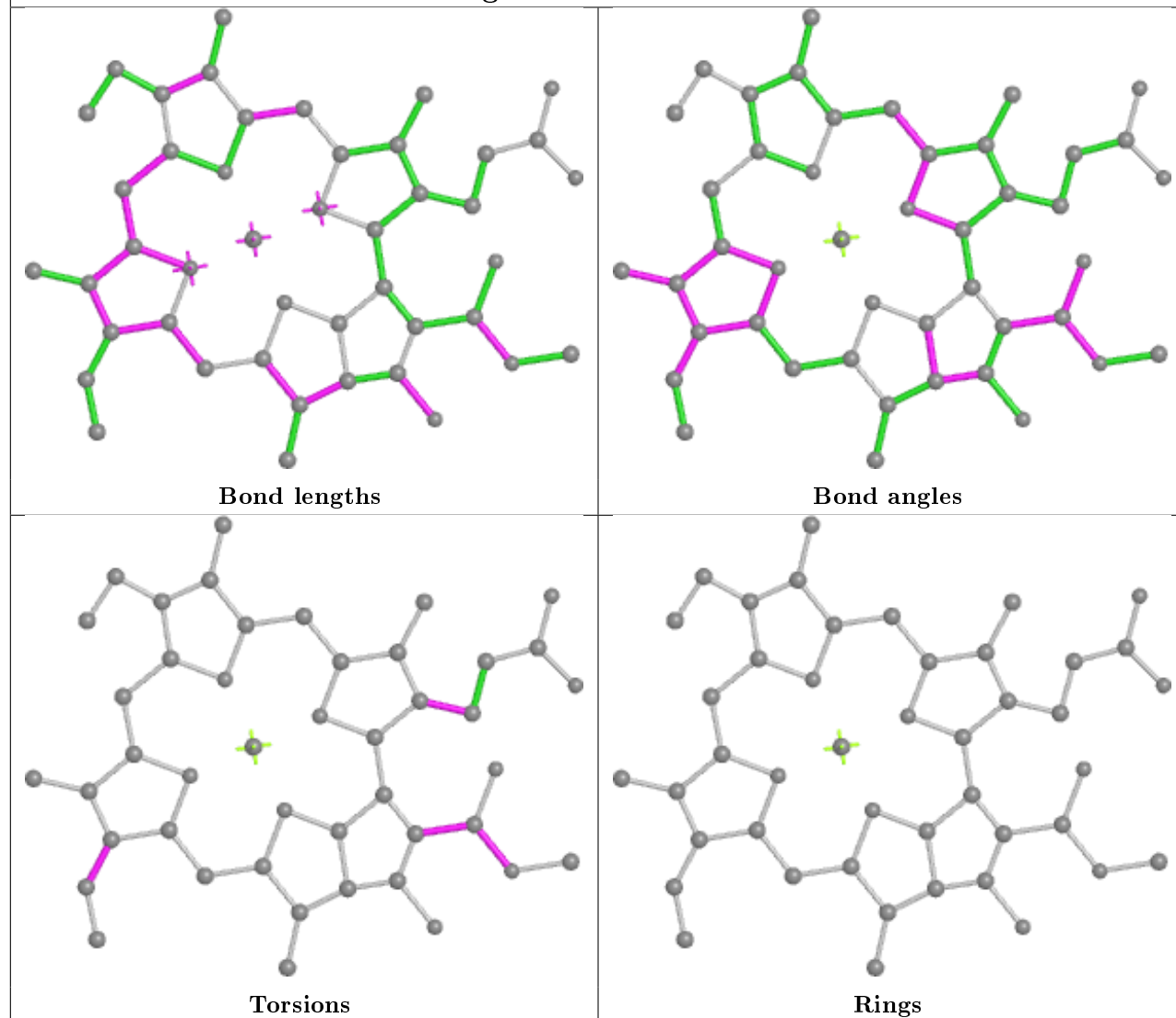
**Ligand CLA B 1238****Ligand CLA A 1111**

**Ligand CLA B 1204****Ligand CLA 1 1131**

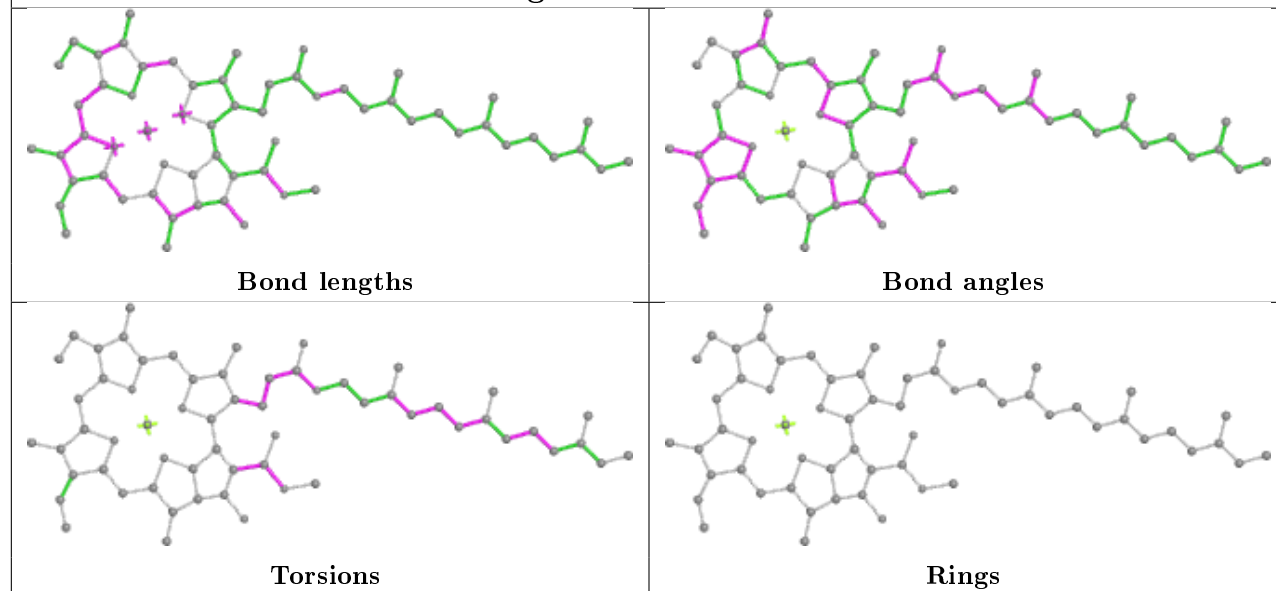




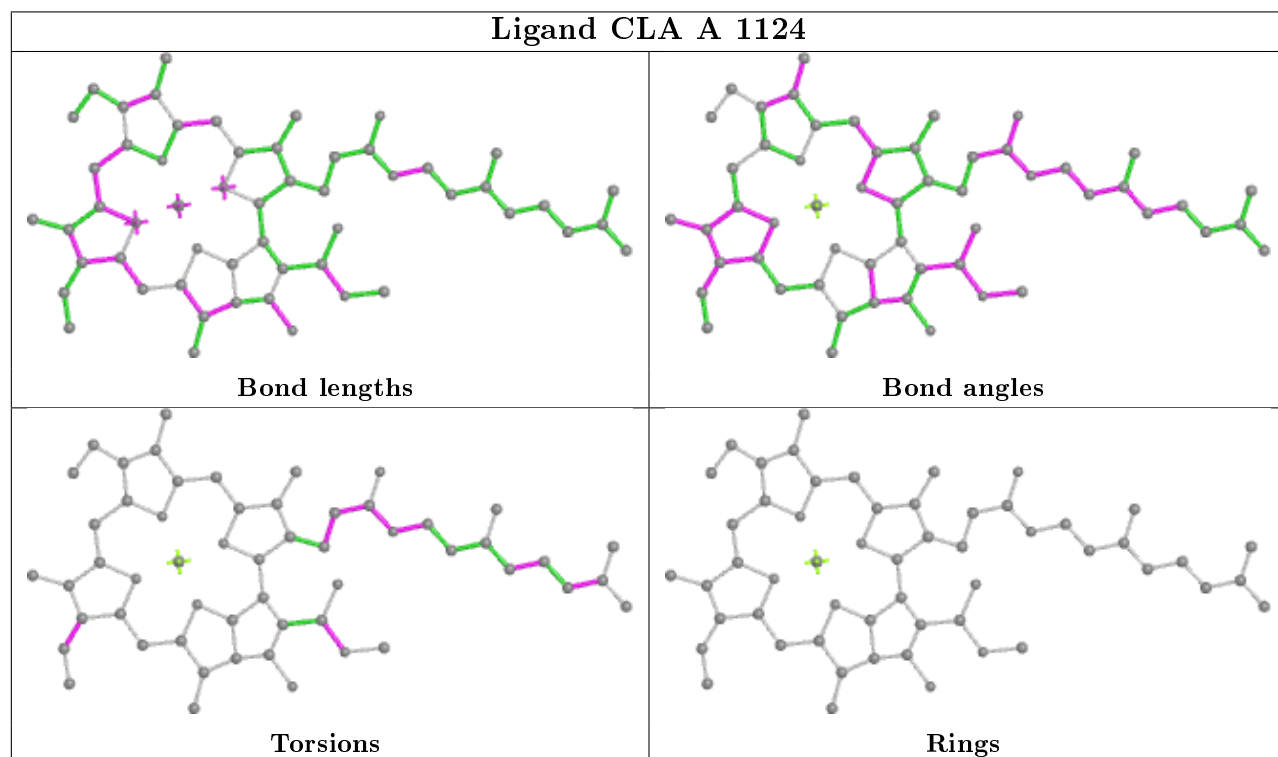
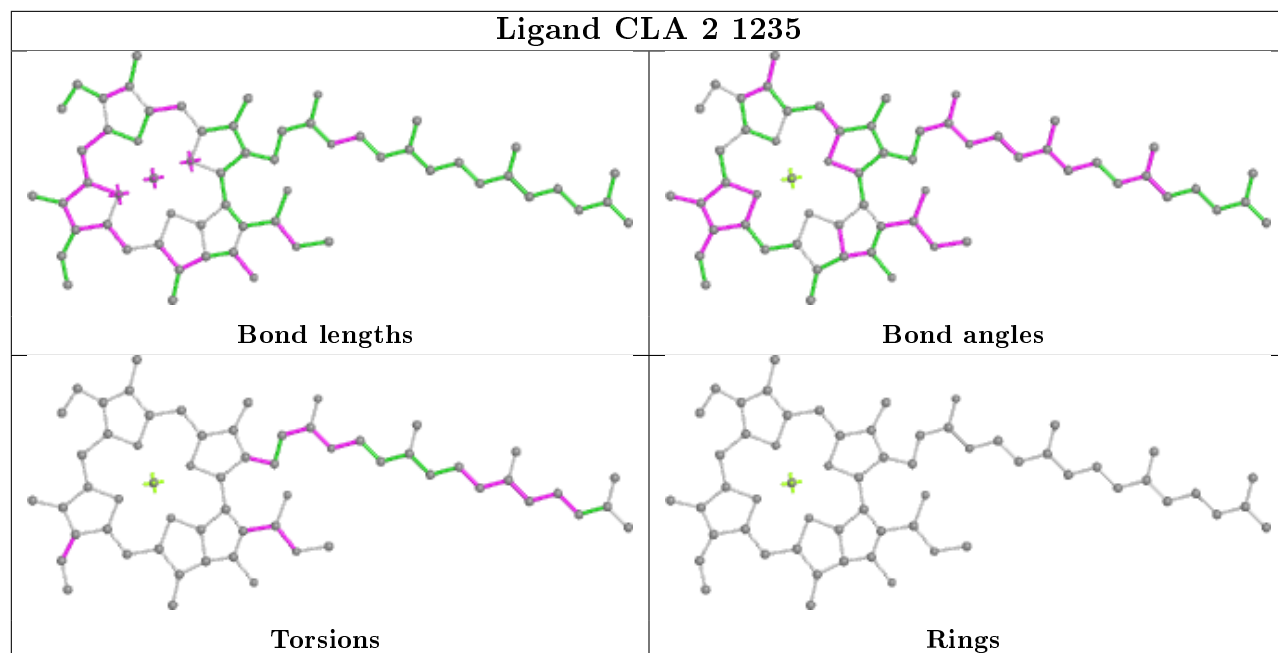
## Ligand CLA A 1112

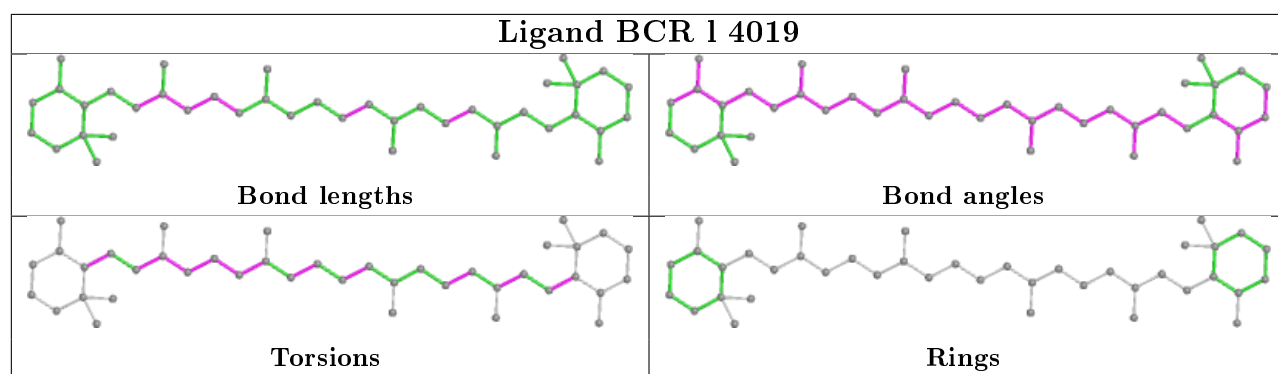
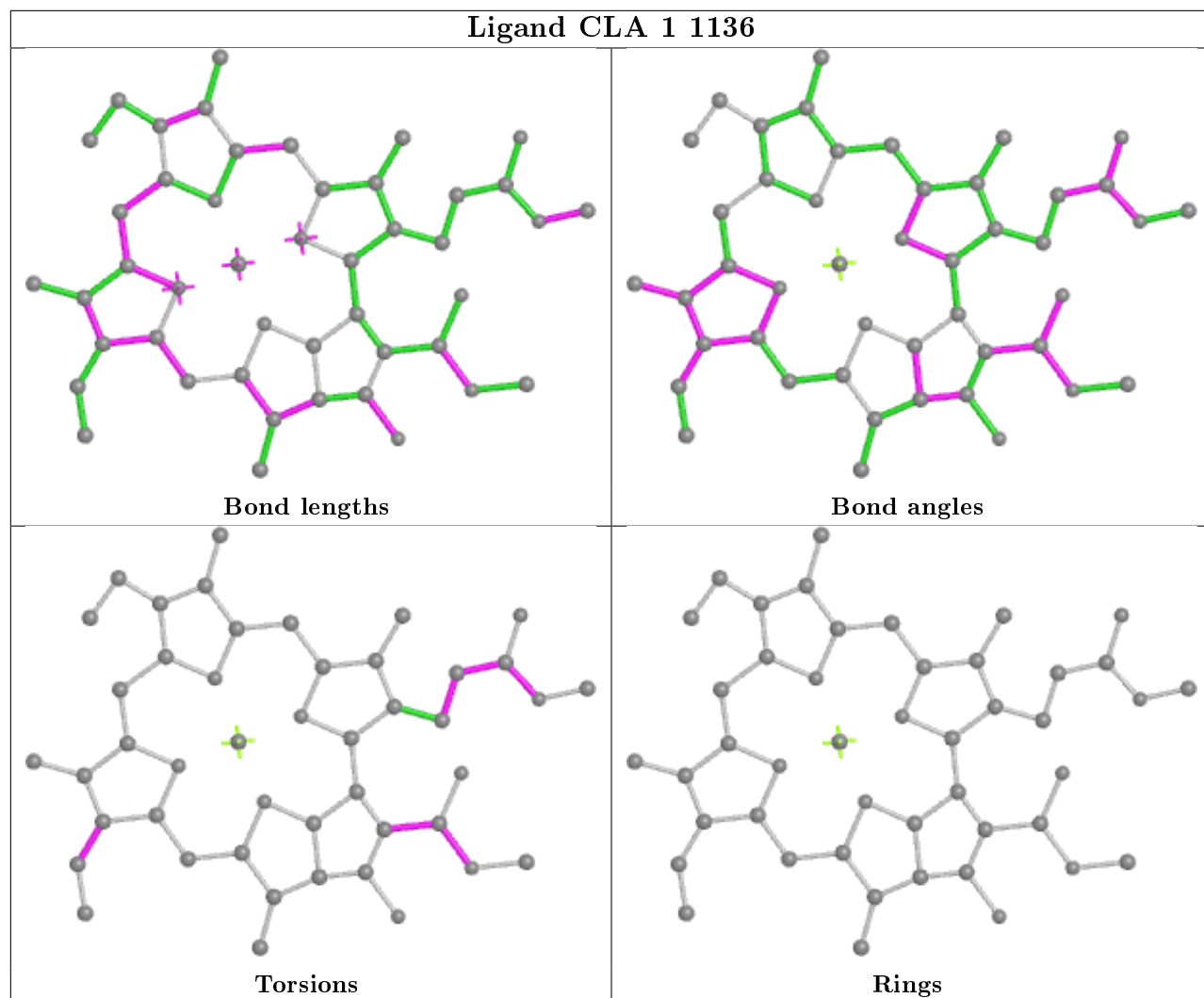


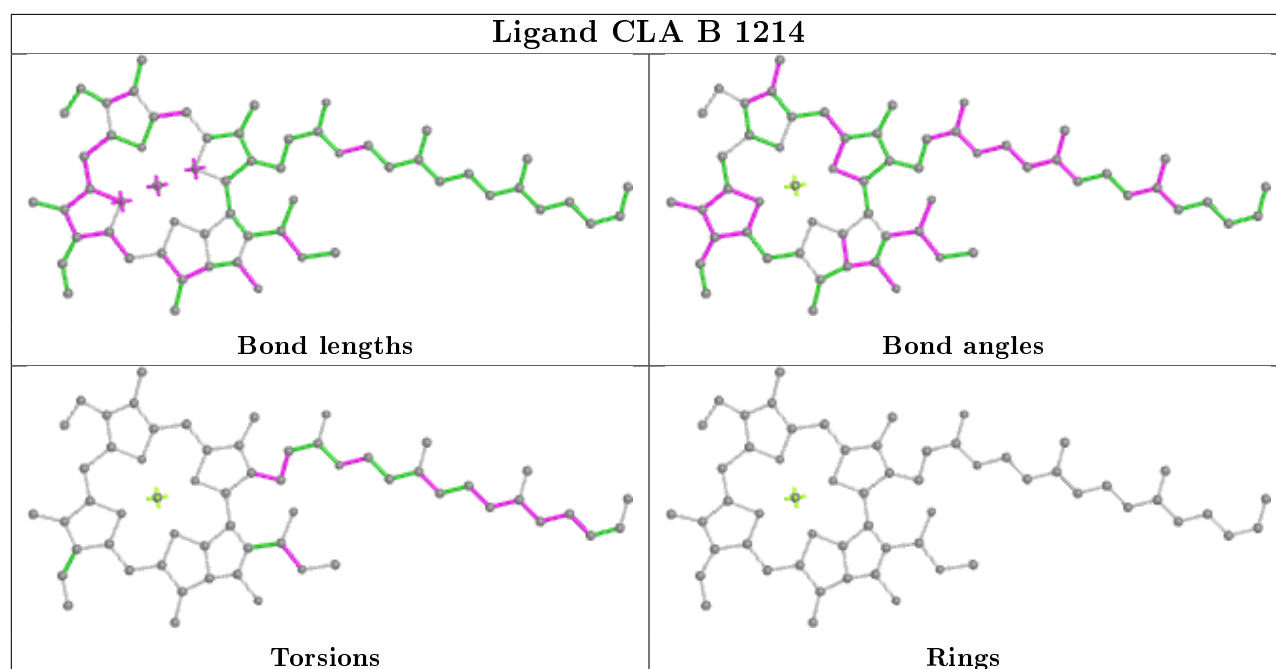
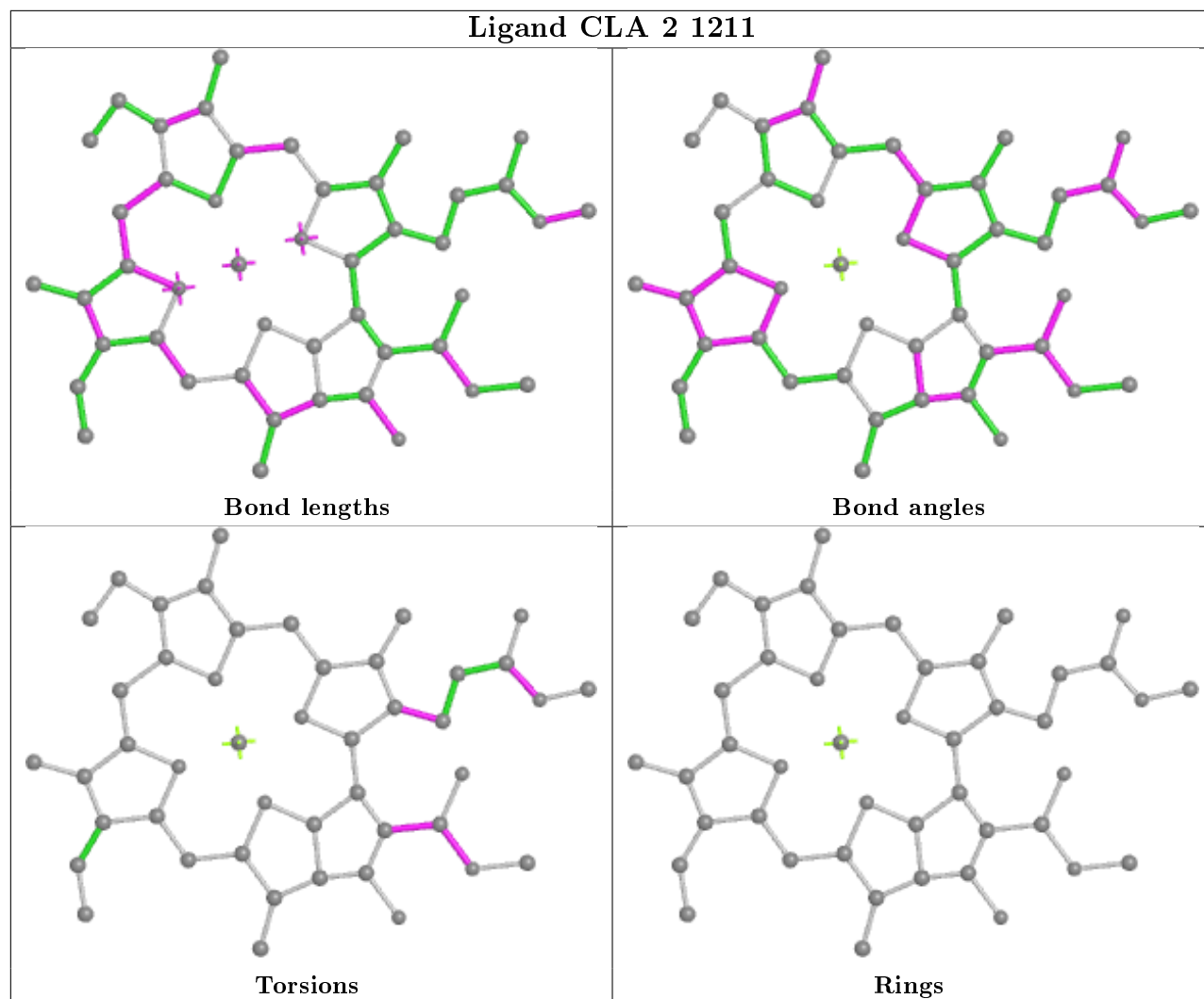
## Ligand CLA 1 1118



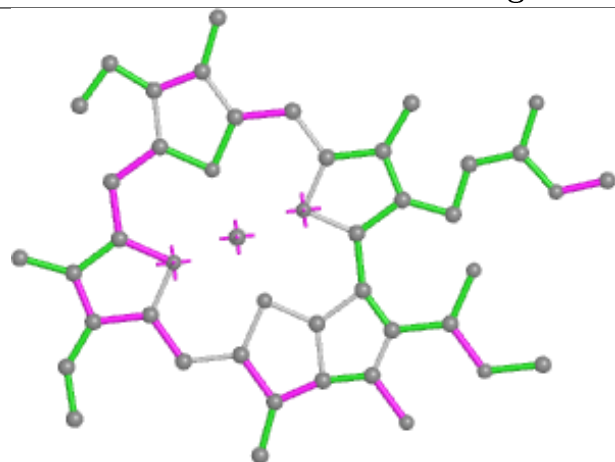




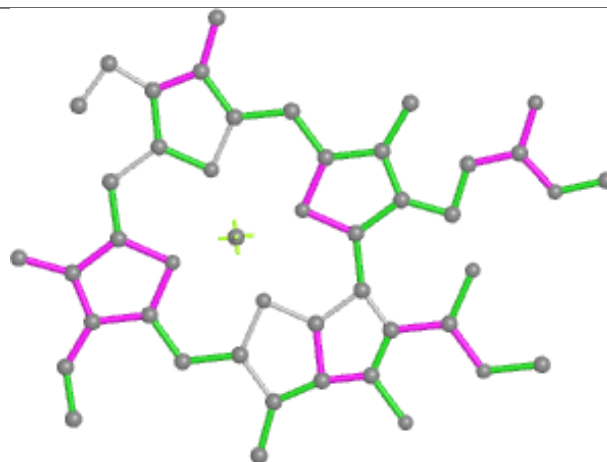




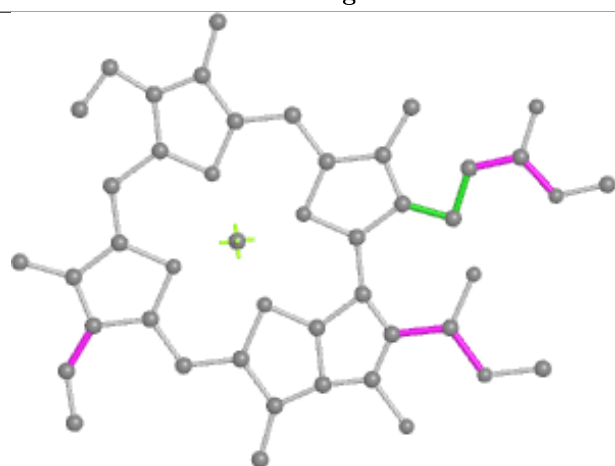
## Ligand CLA B 1220



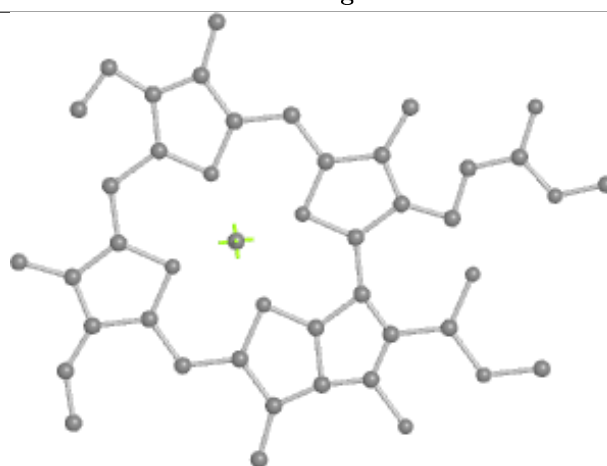
Bond lengths



Bond angles

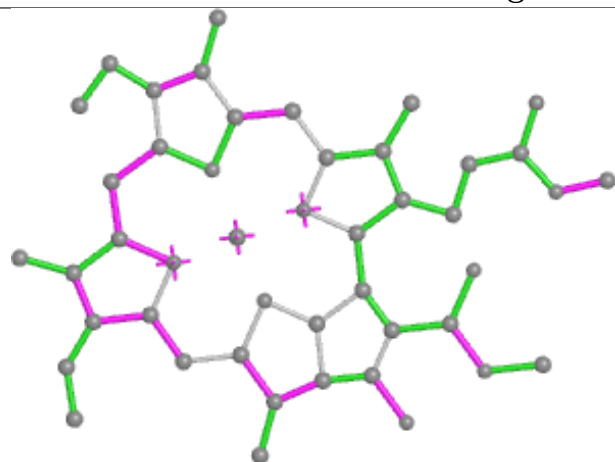


Torsions

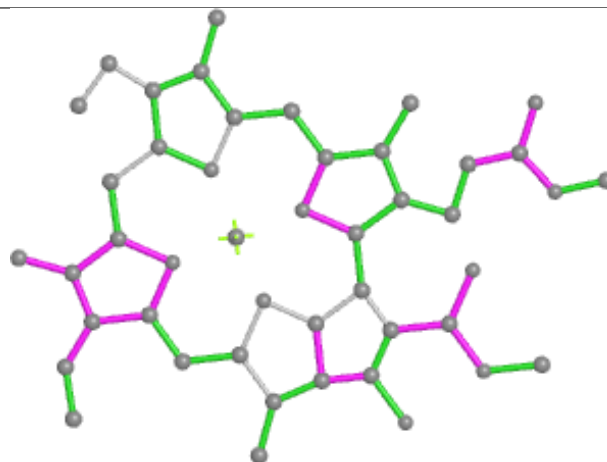


Rings

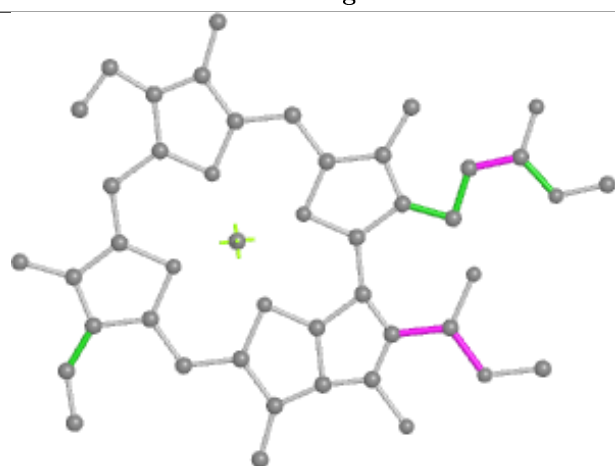
## Ligand CLA A 1136



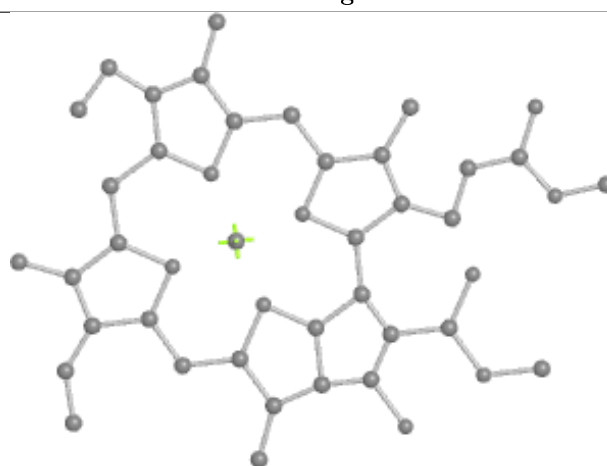
Bond lengths



Bond angles

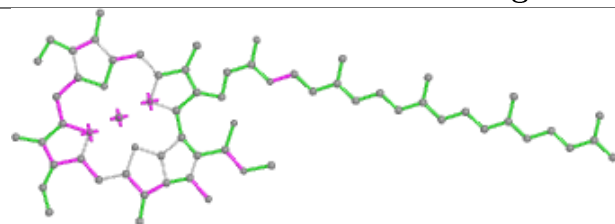


Torsions

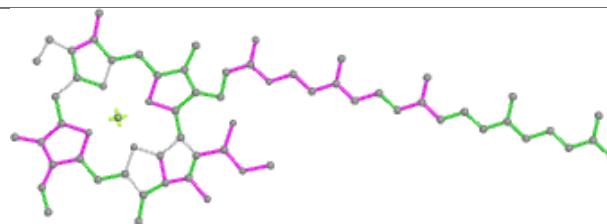


Rings

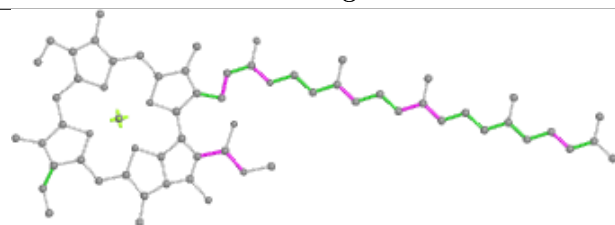
## Ligand CLA a 1127



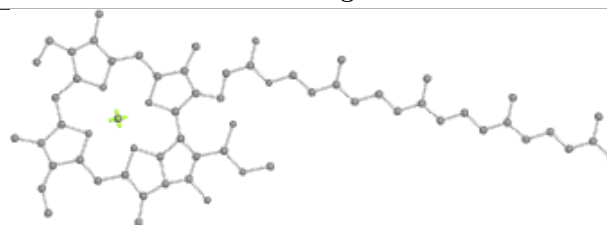
Bond lengths



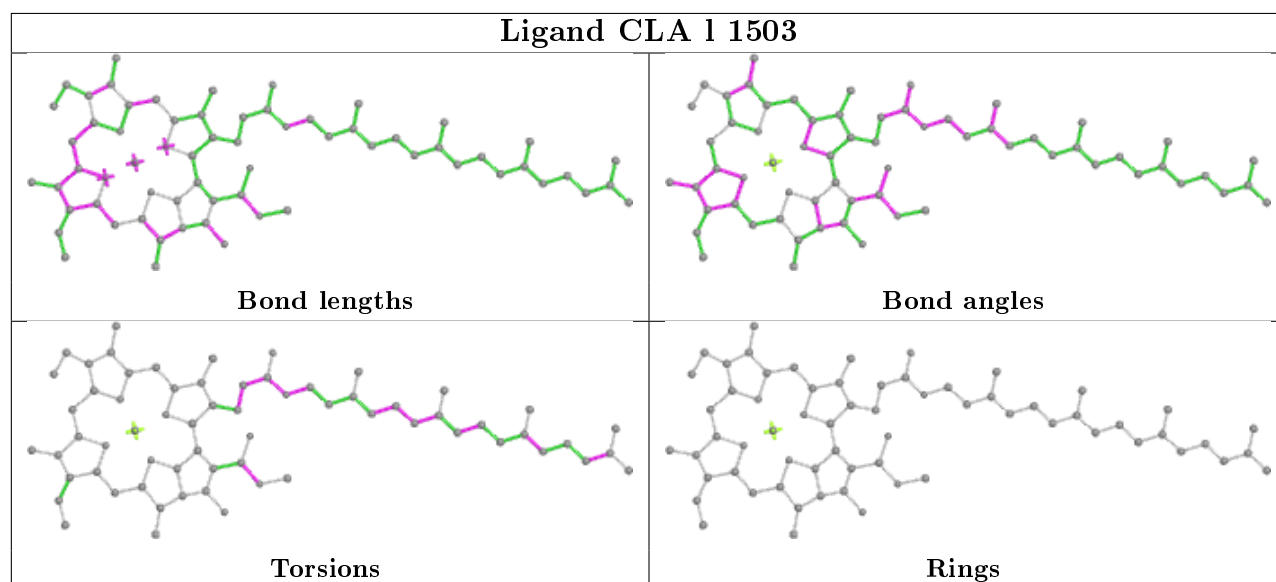
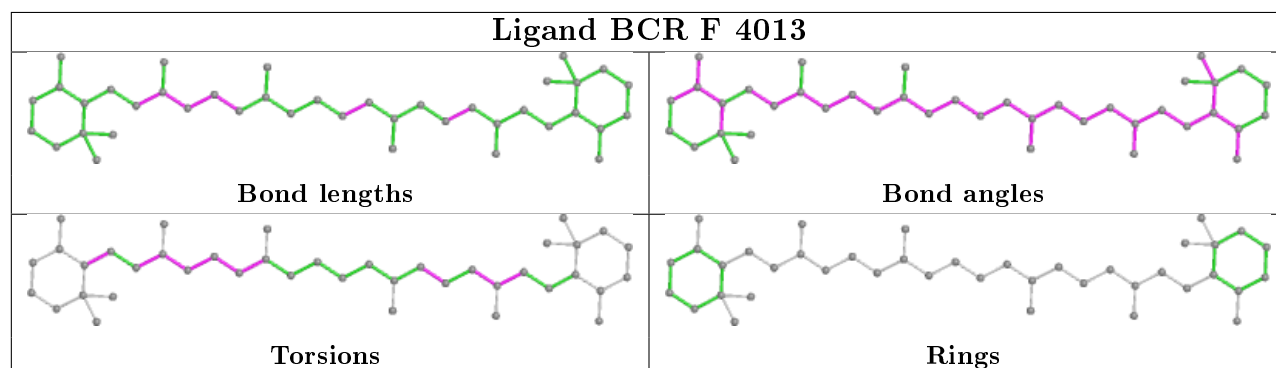
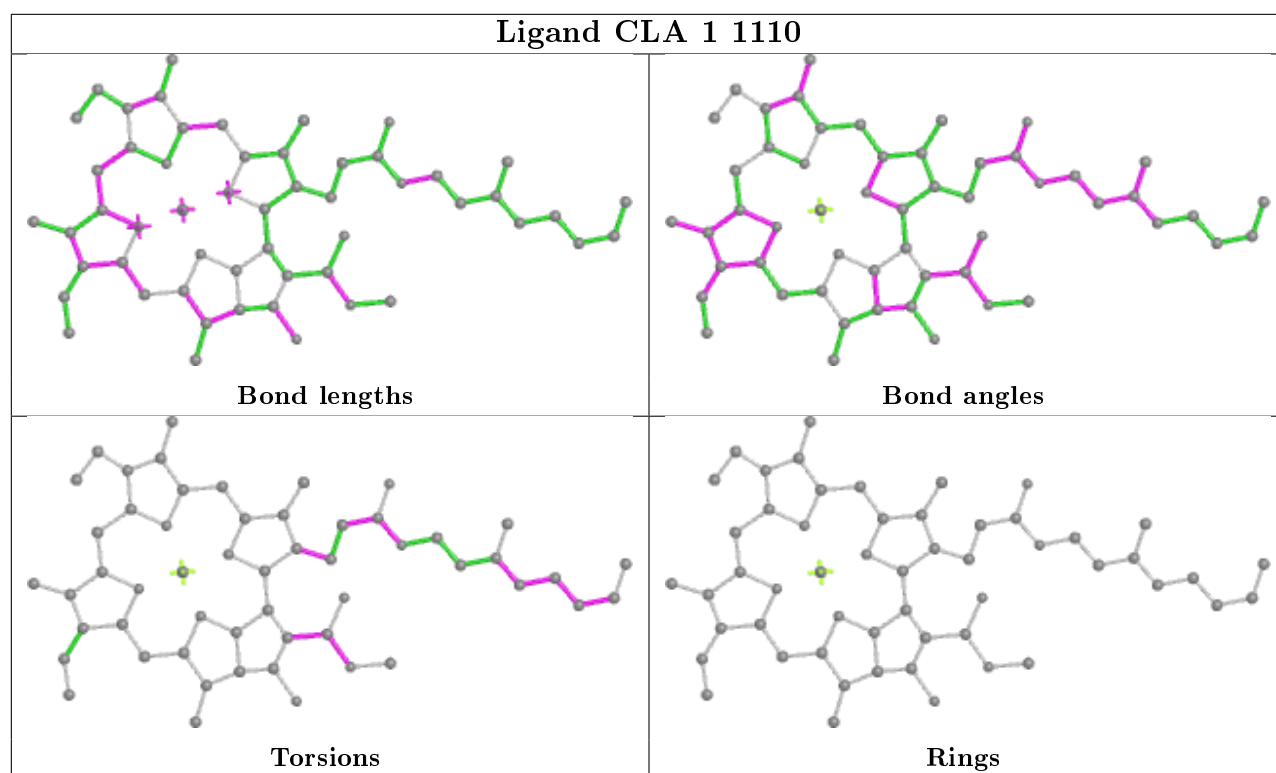
Bond angles



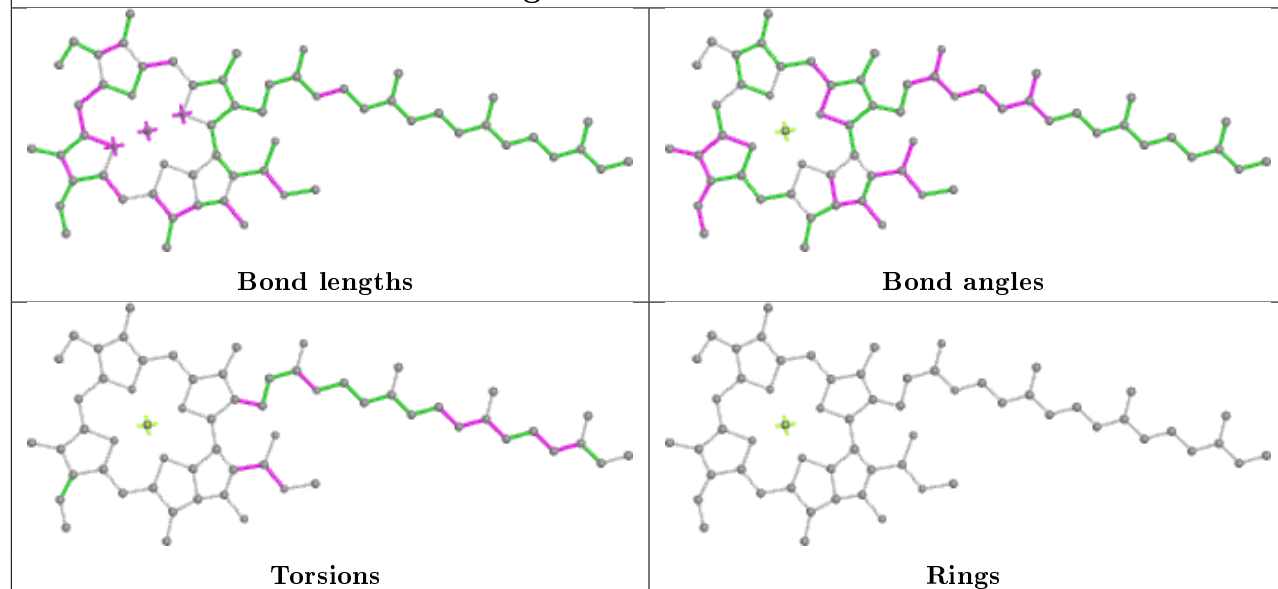
Torsions



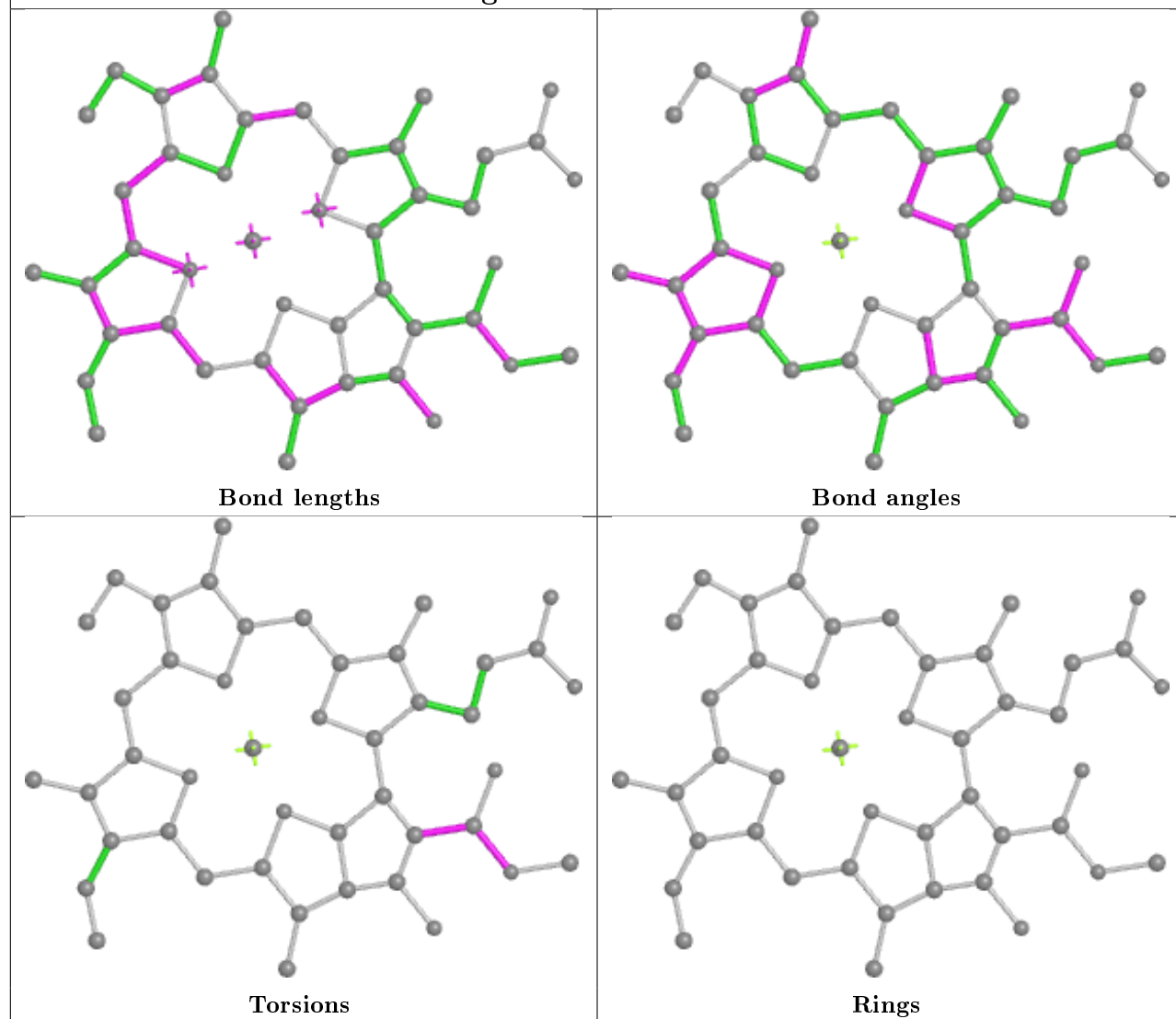
Rings

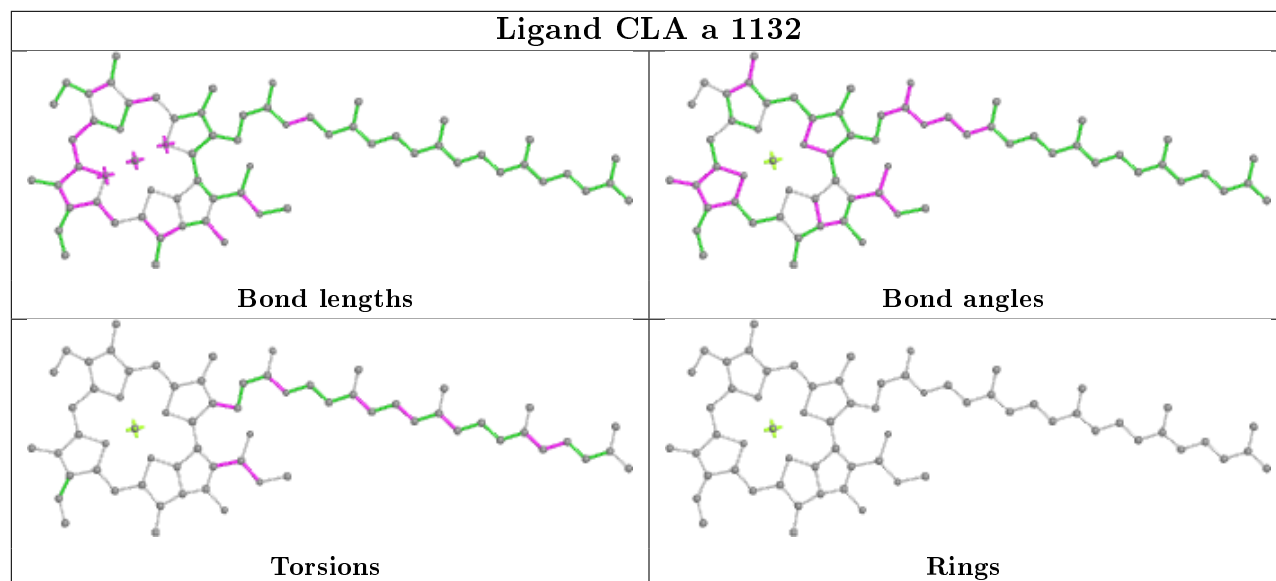
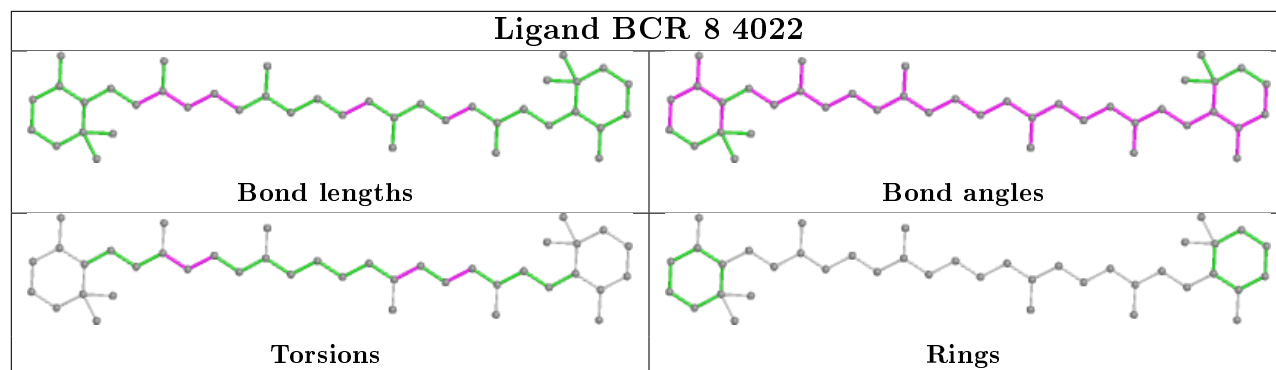


## Ligand CLA A 1118

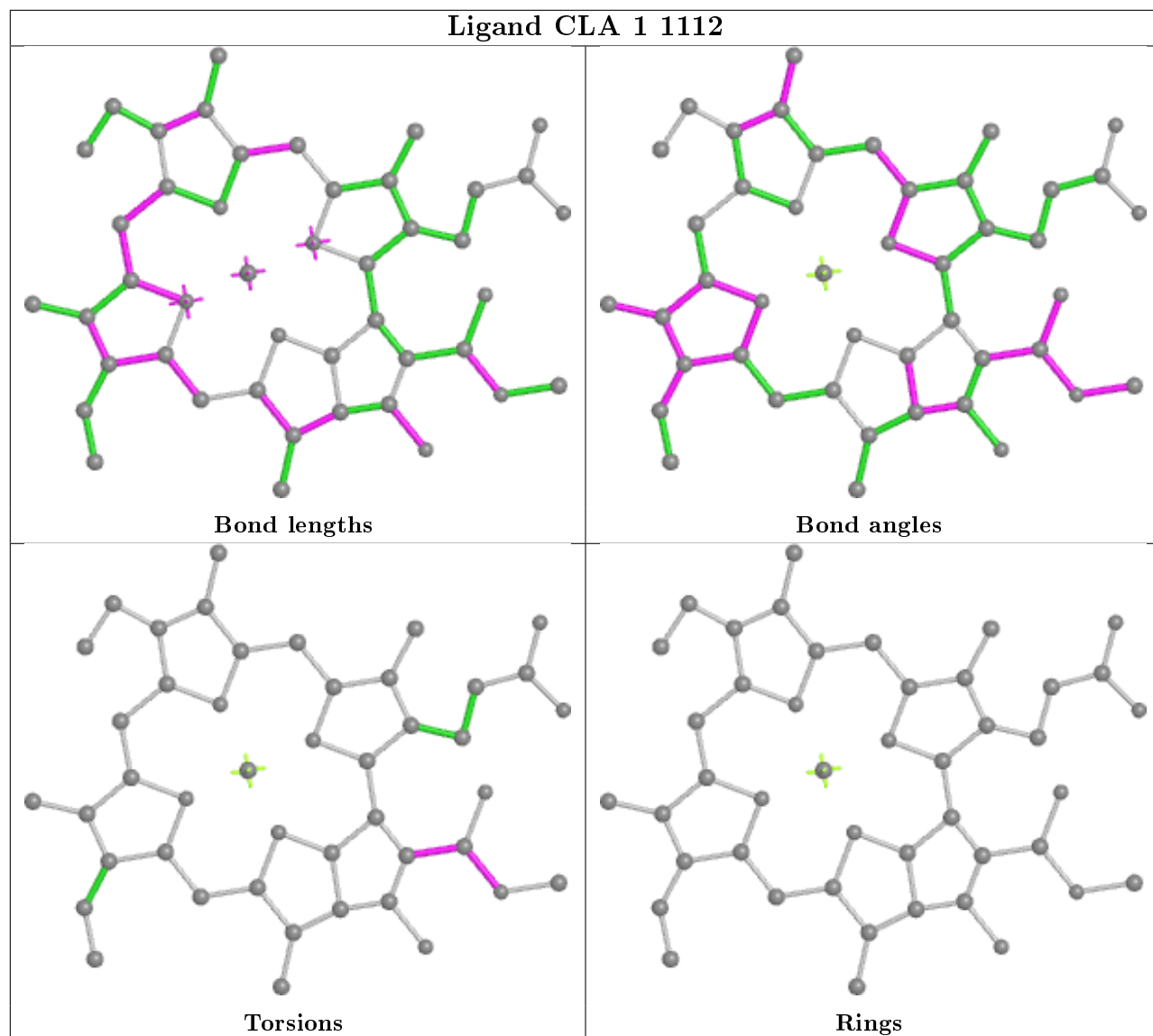


## Ligand CLA B 1218

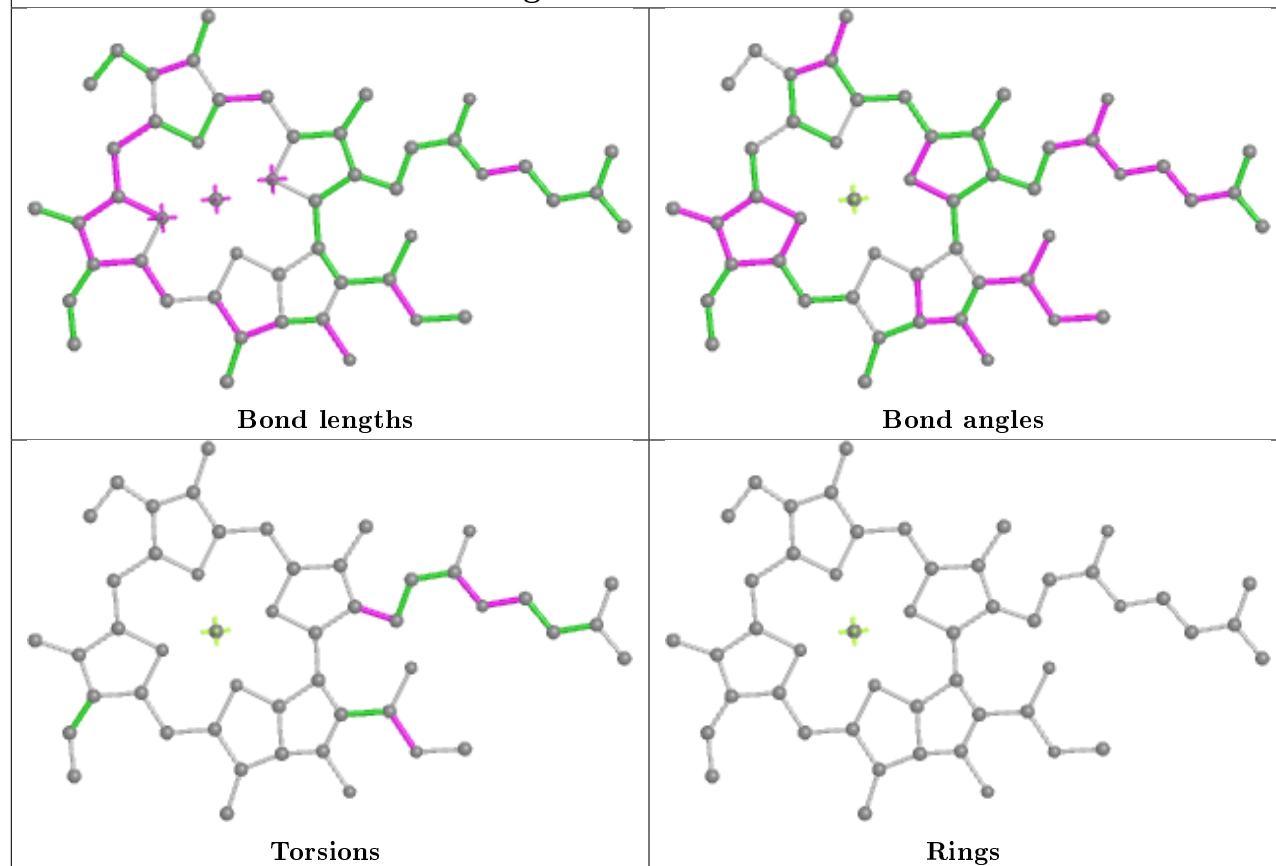




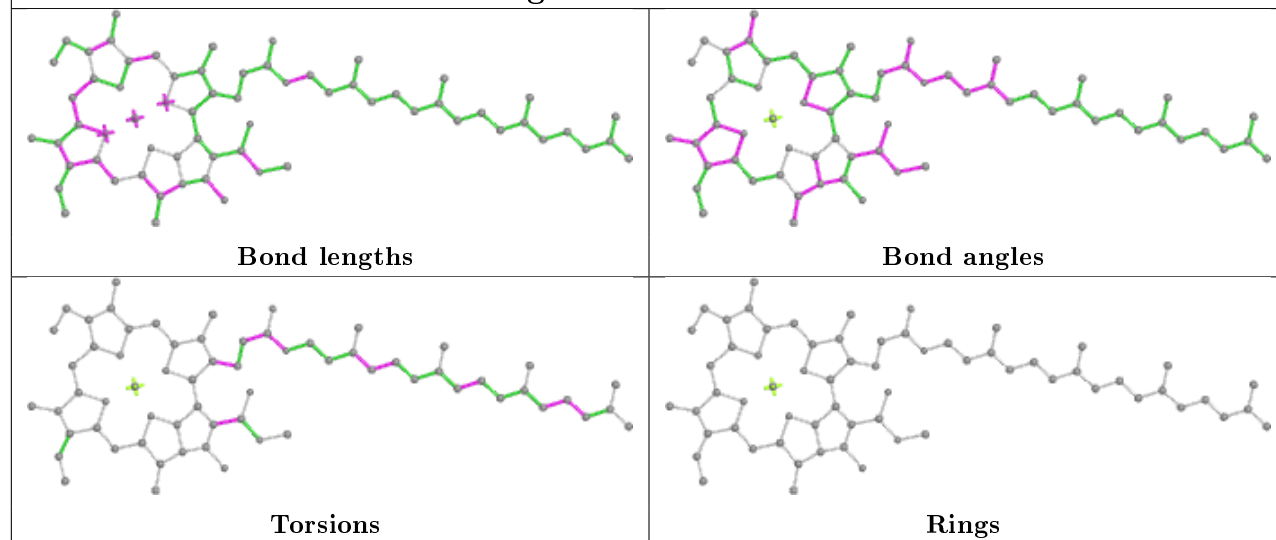




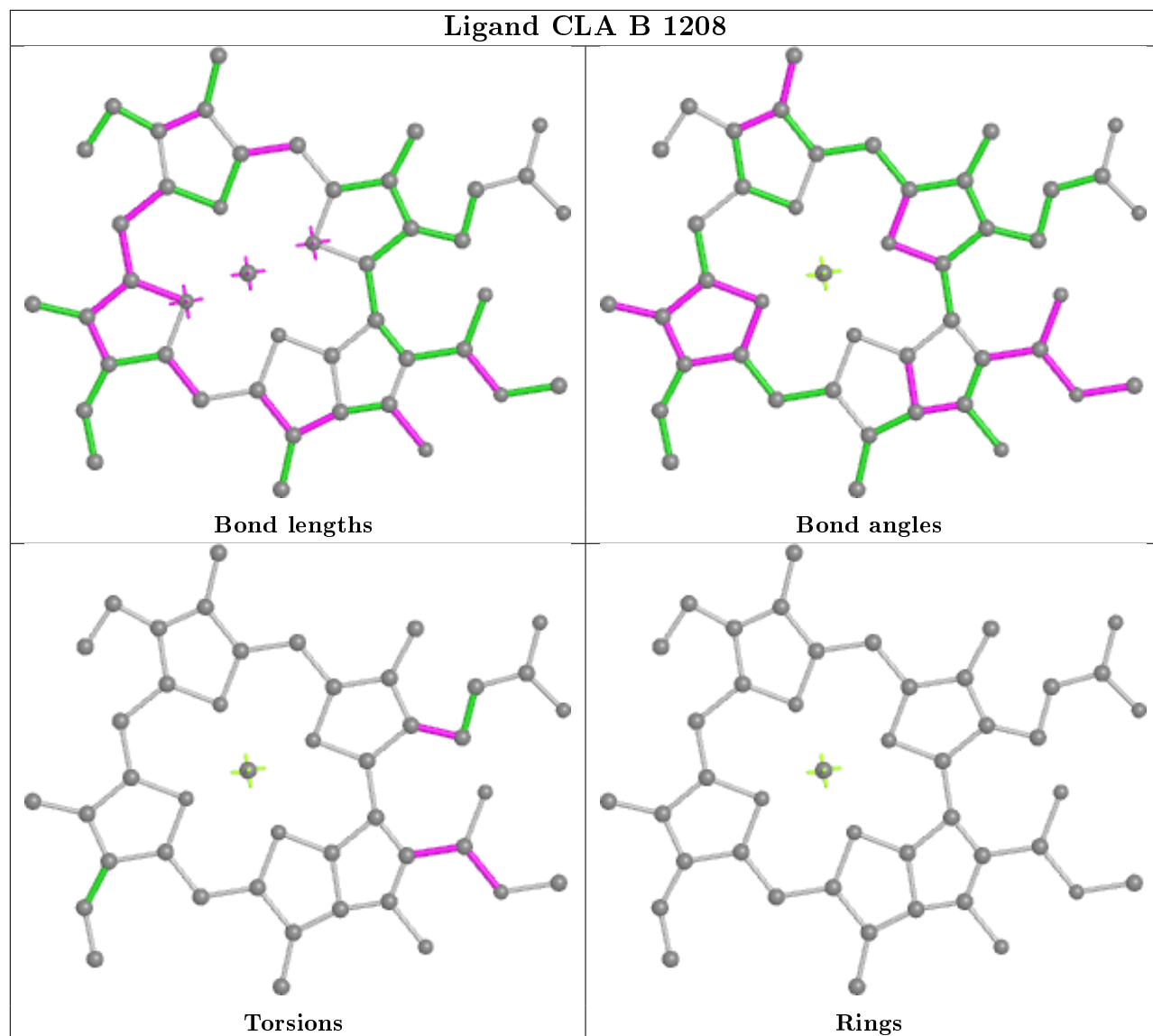
## Ligand CLA A 1139



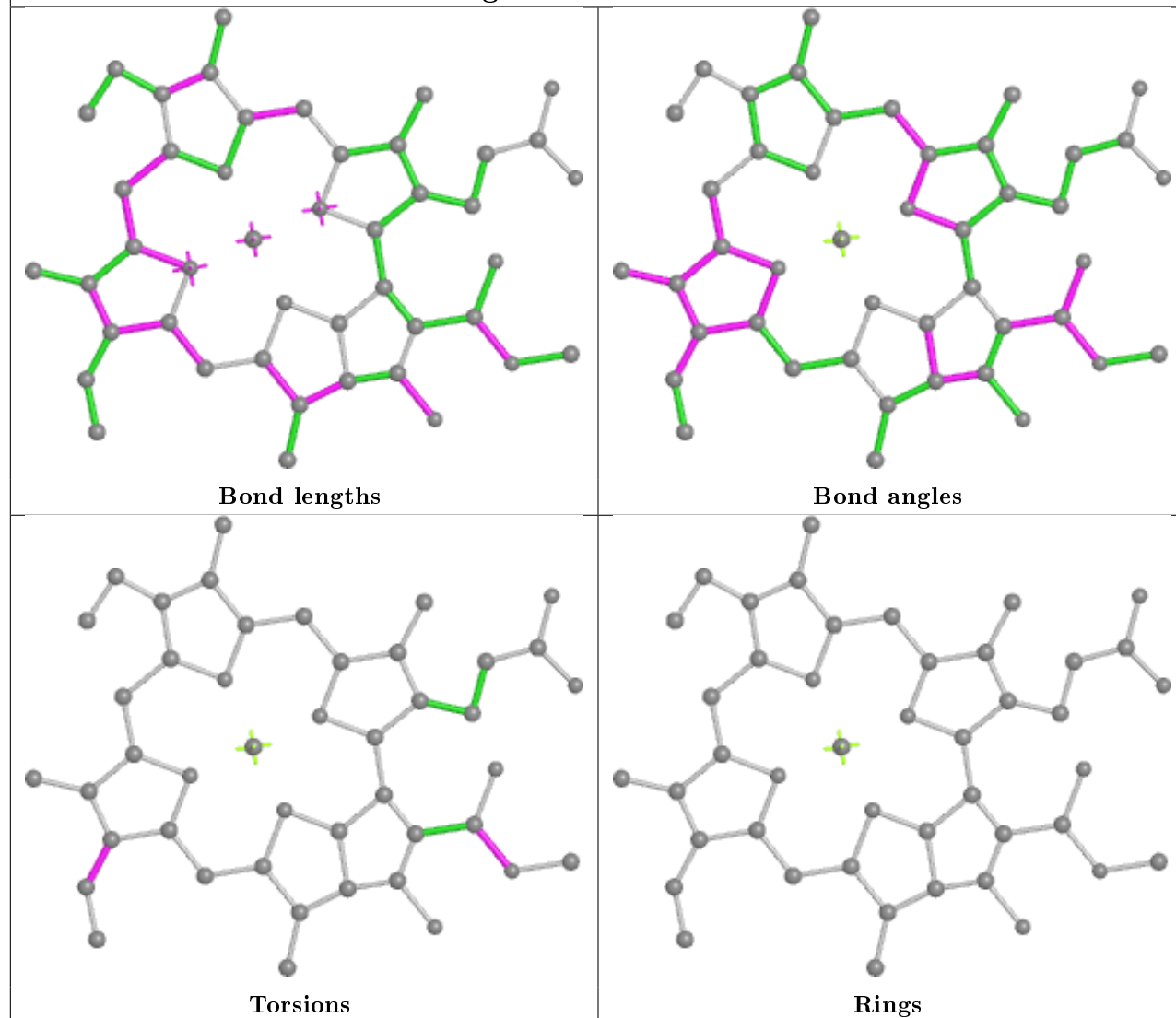
## Ligand CLA 2 1202



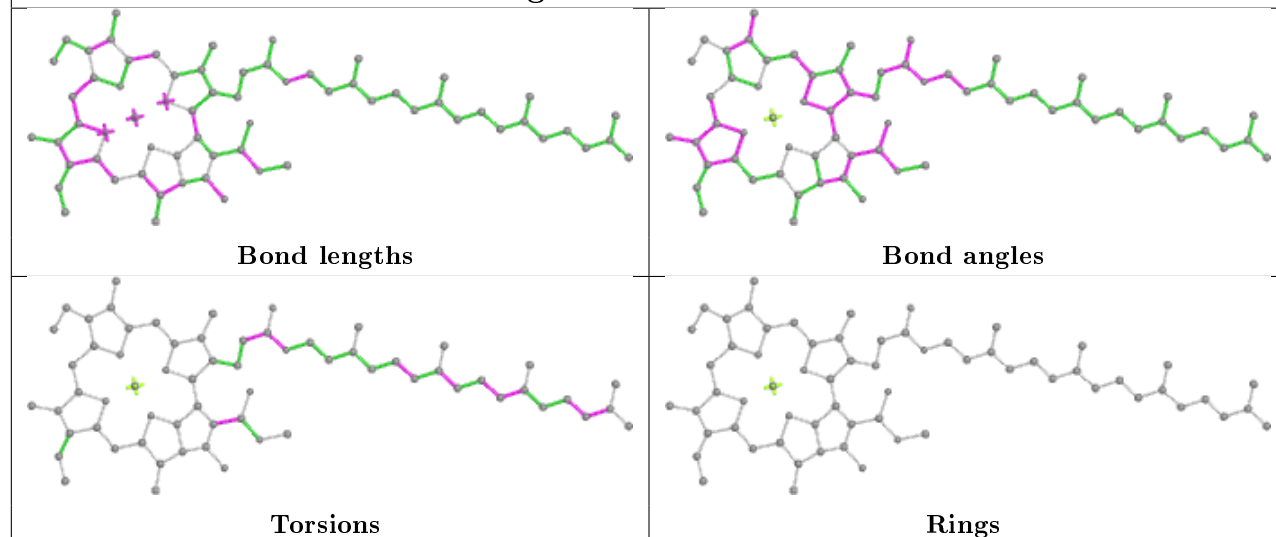
## Ligand CLA B 1208

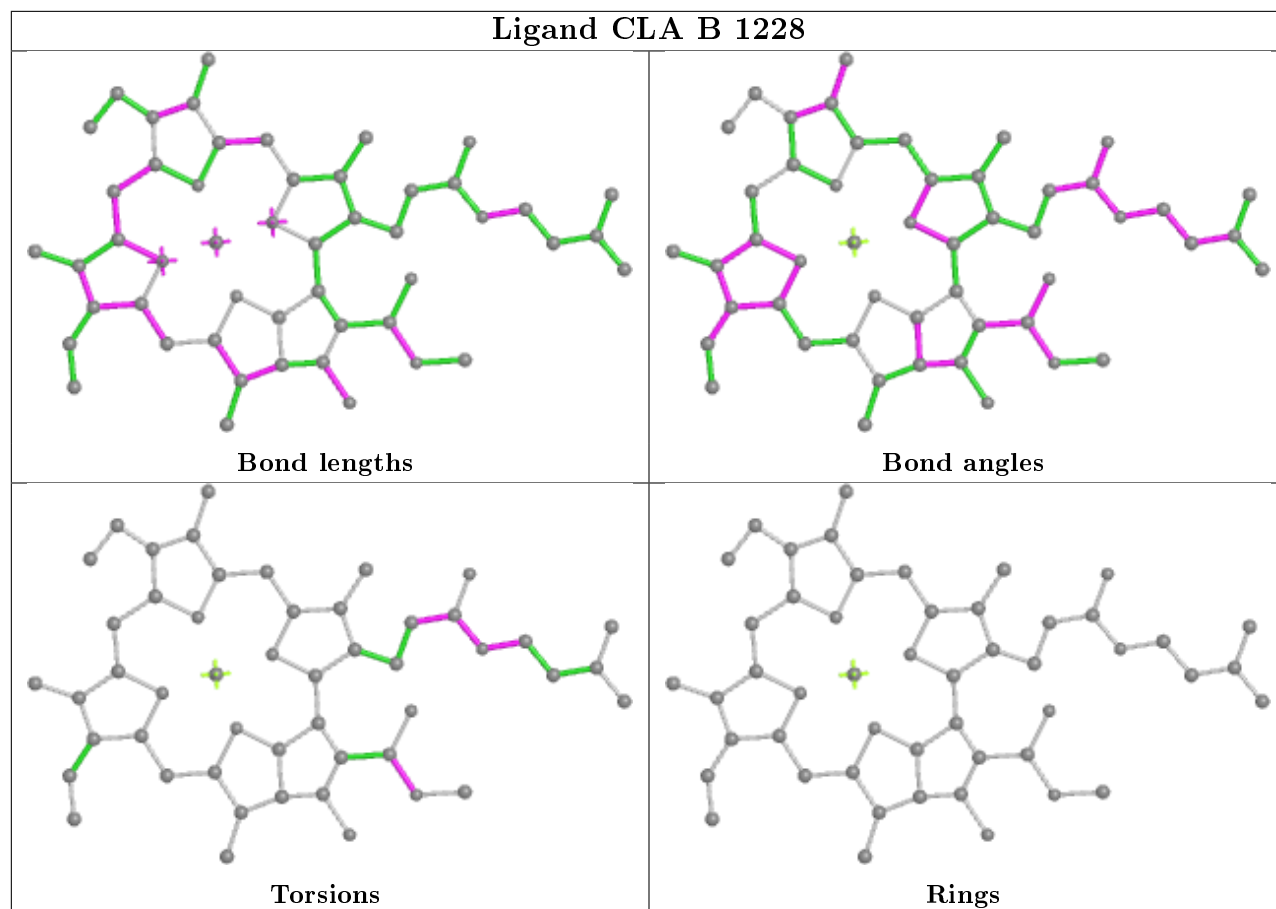


## Ligand CLA B 1227

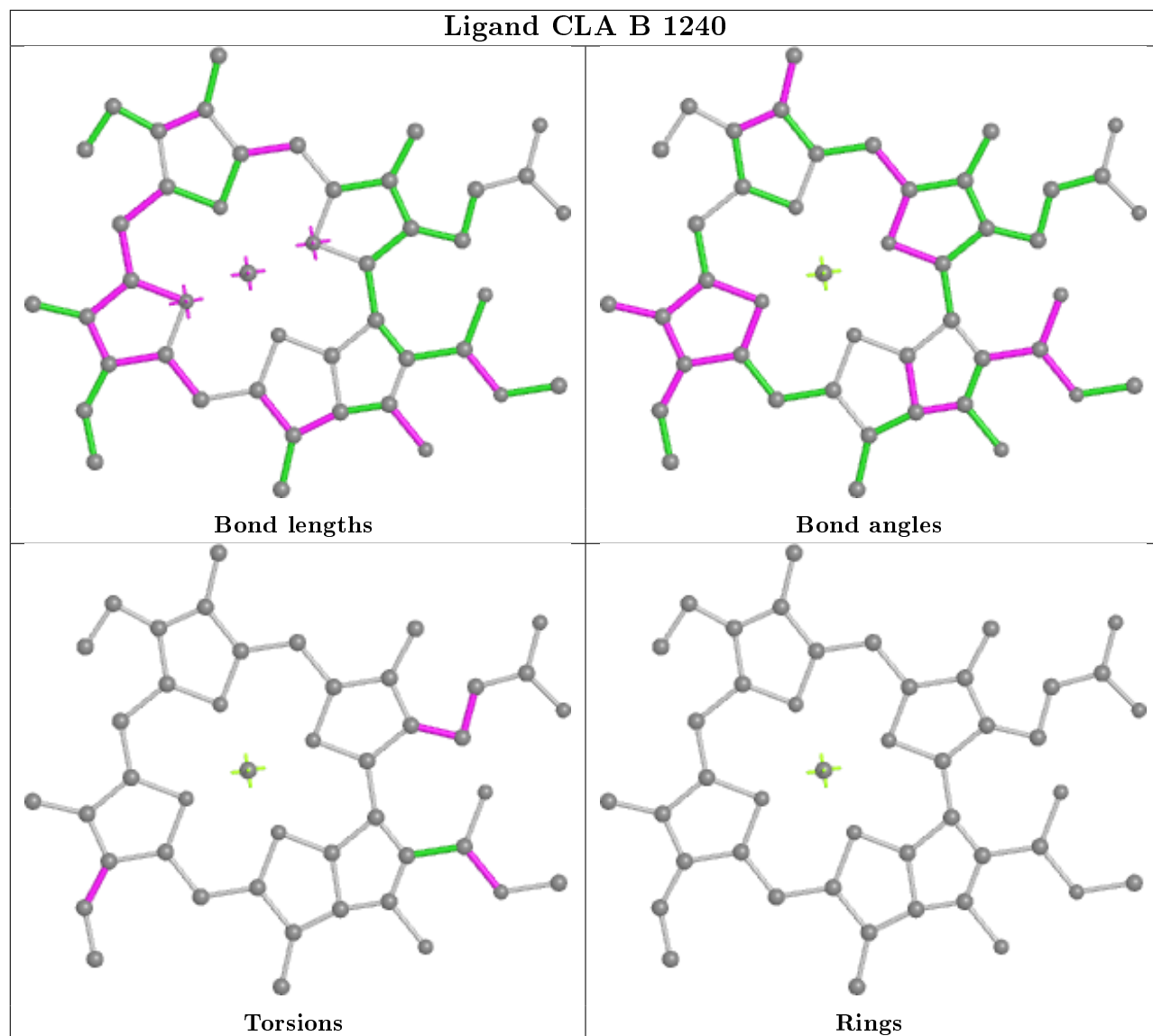


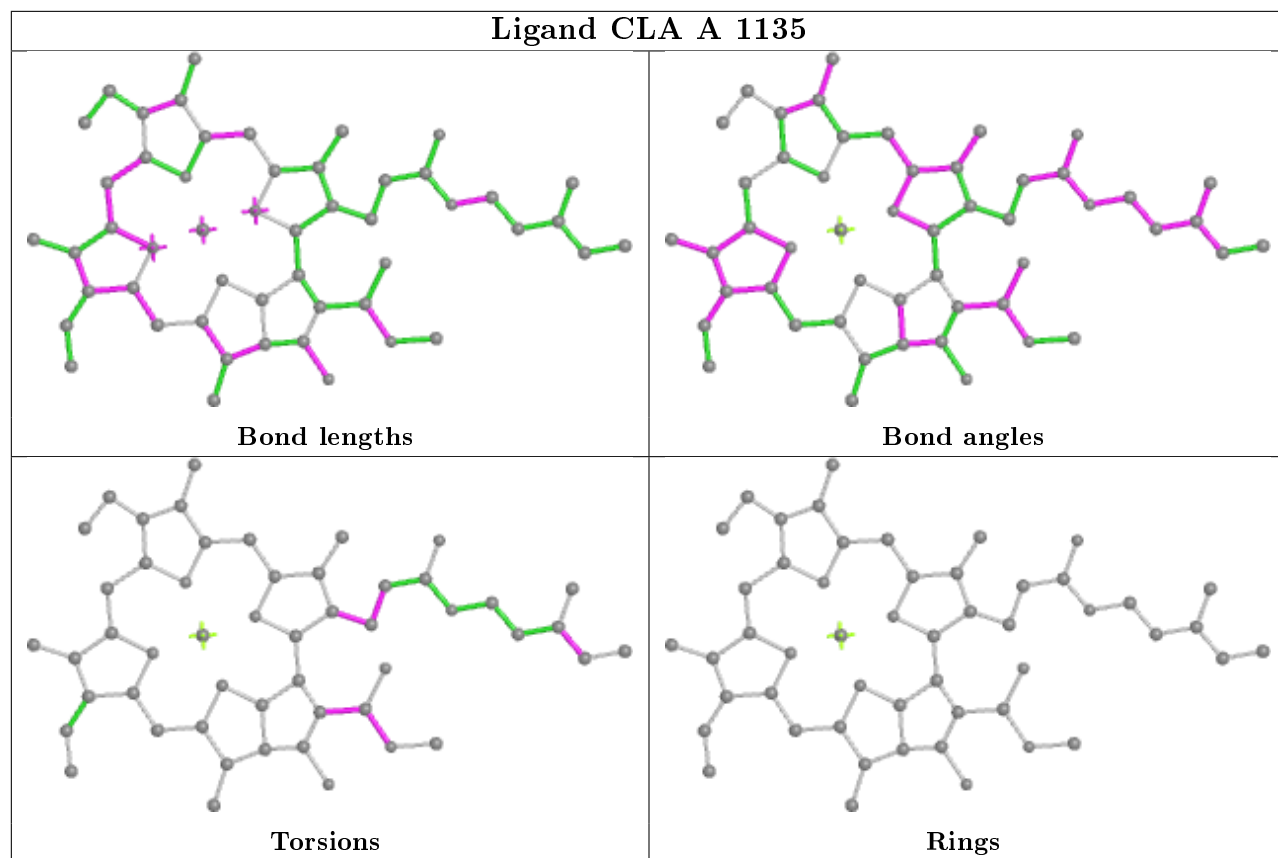
## Ligand CLA 1 1011

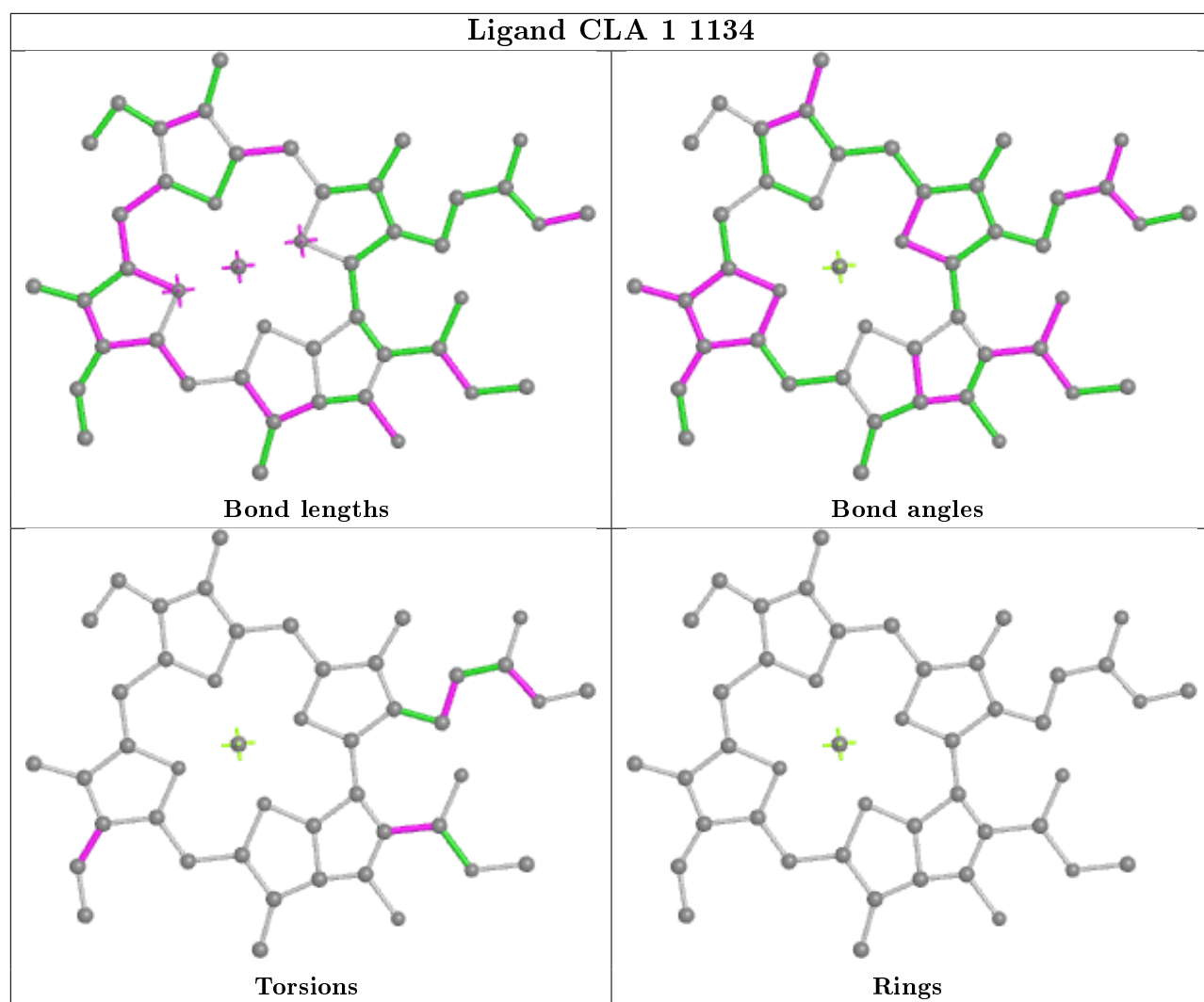




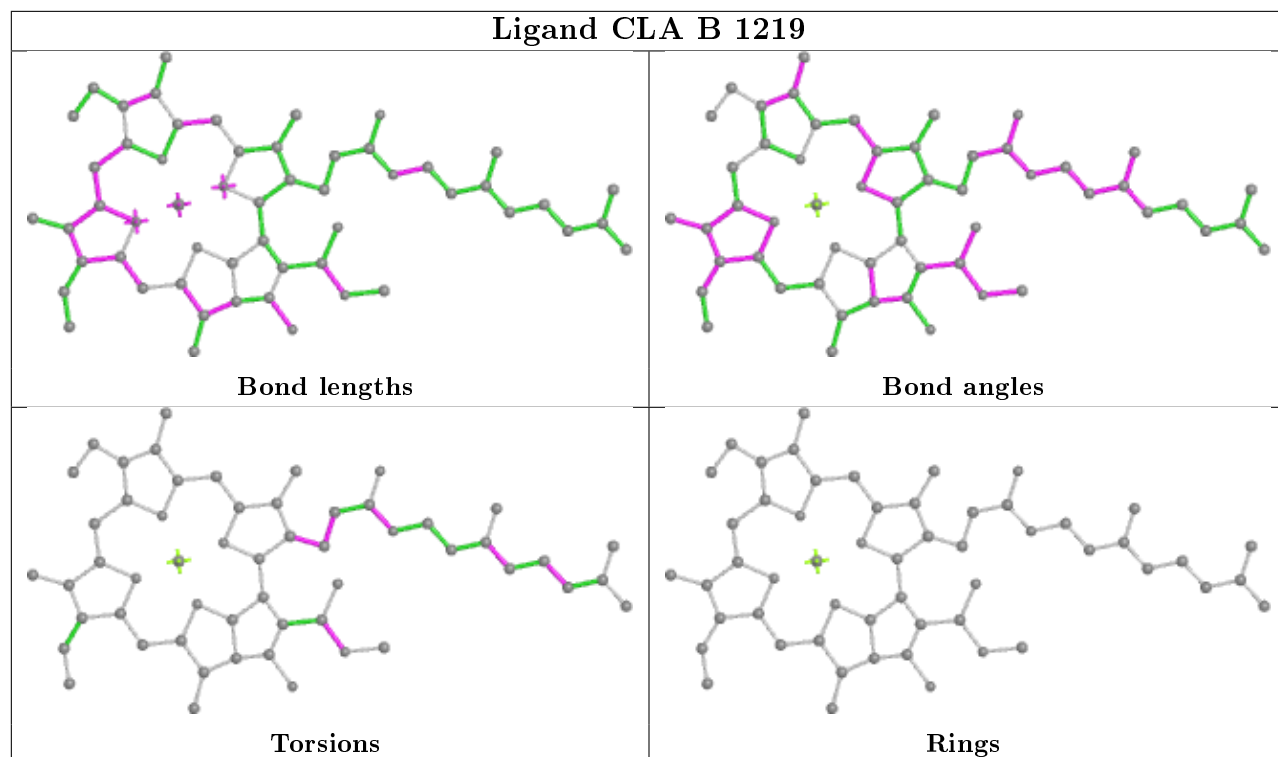
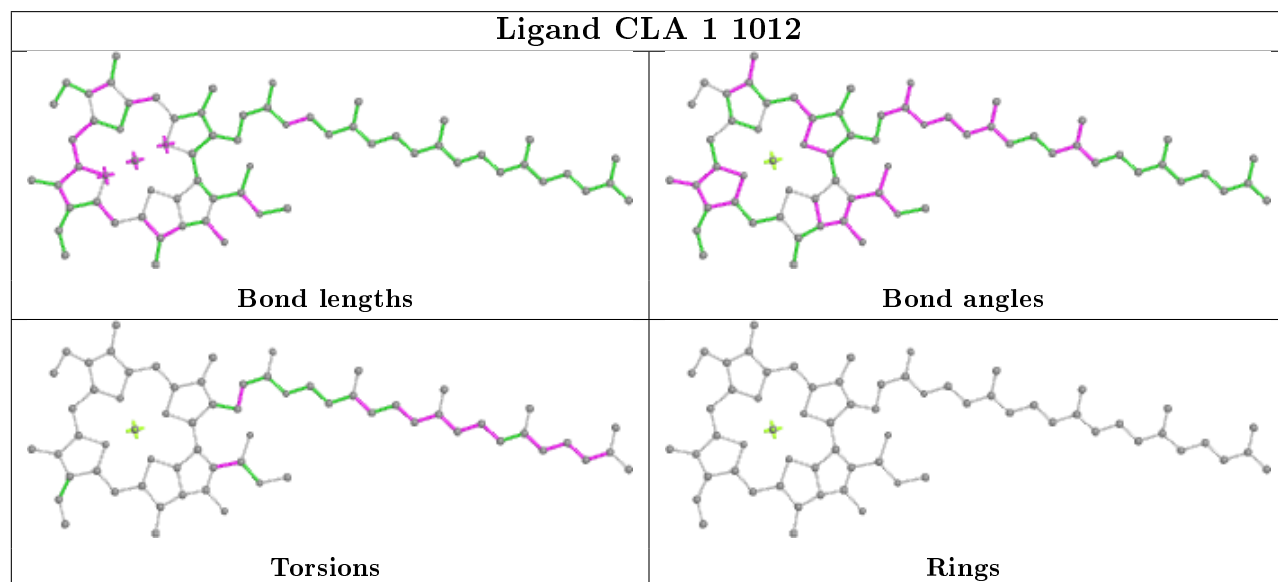
## Ligand CLA B 1240

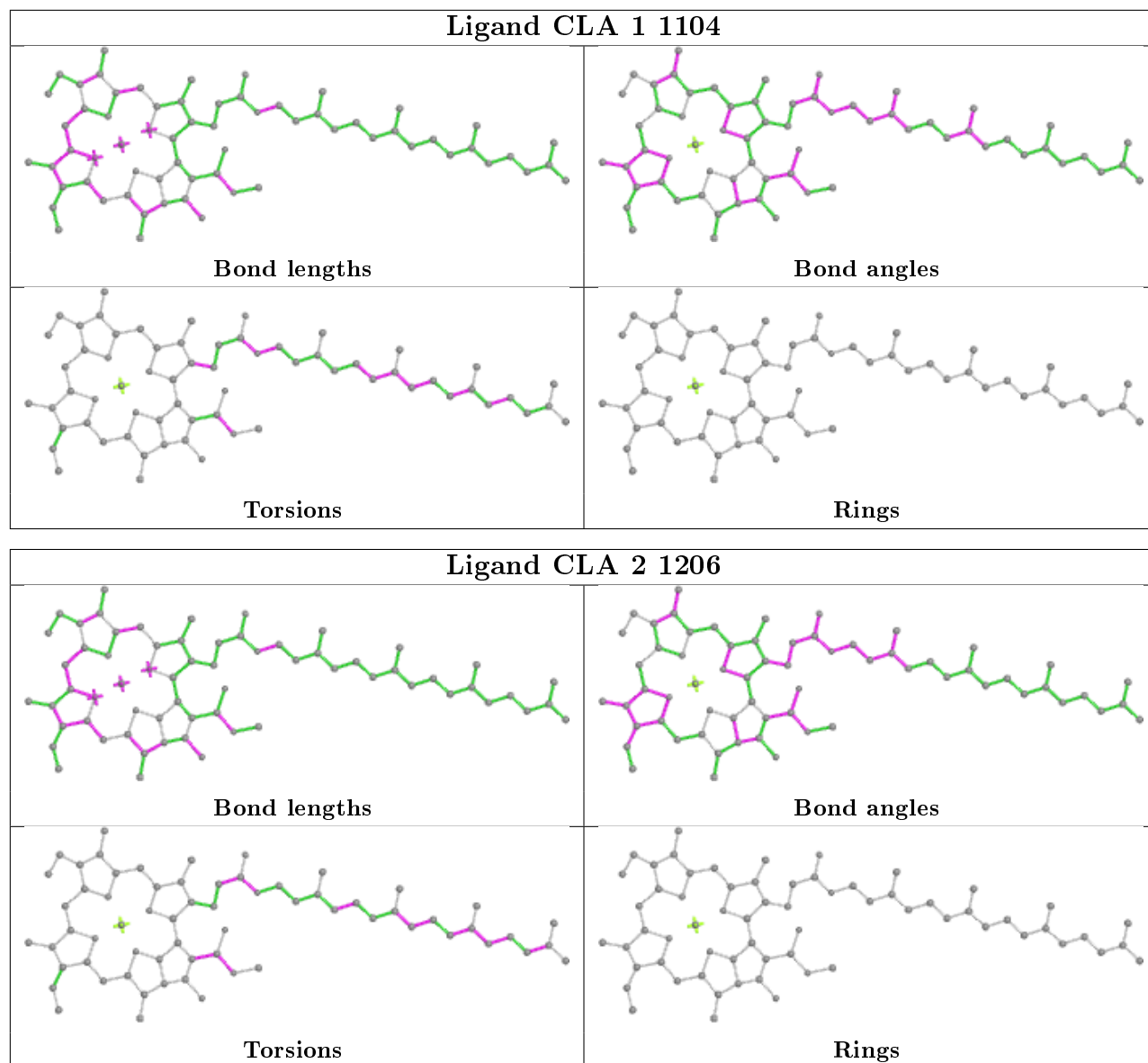


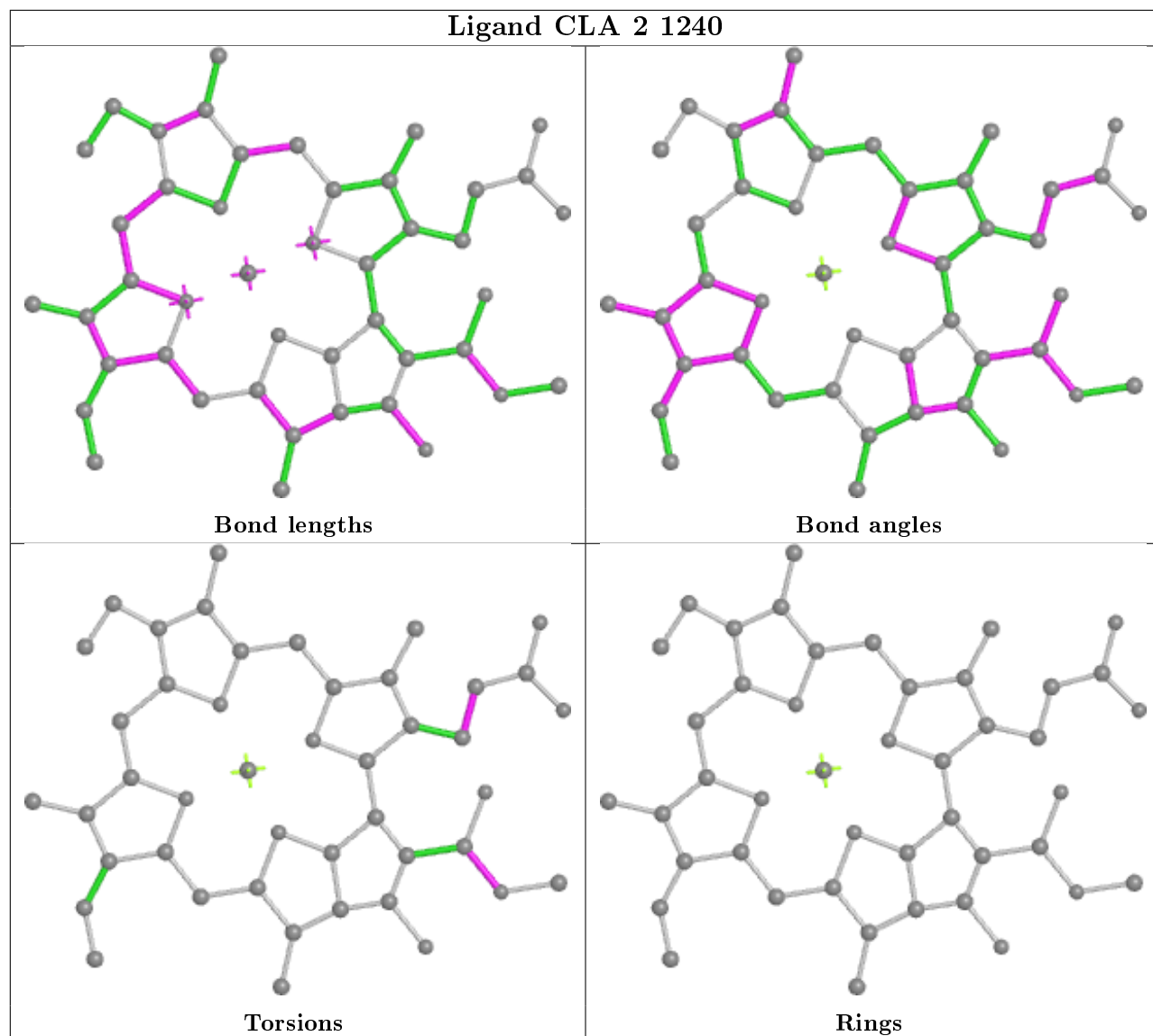


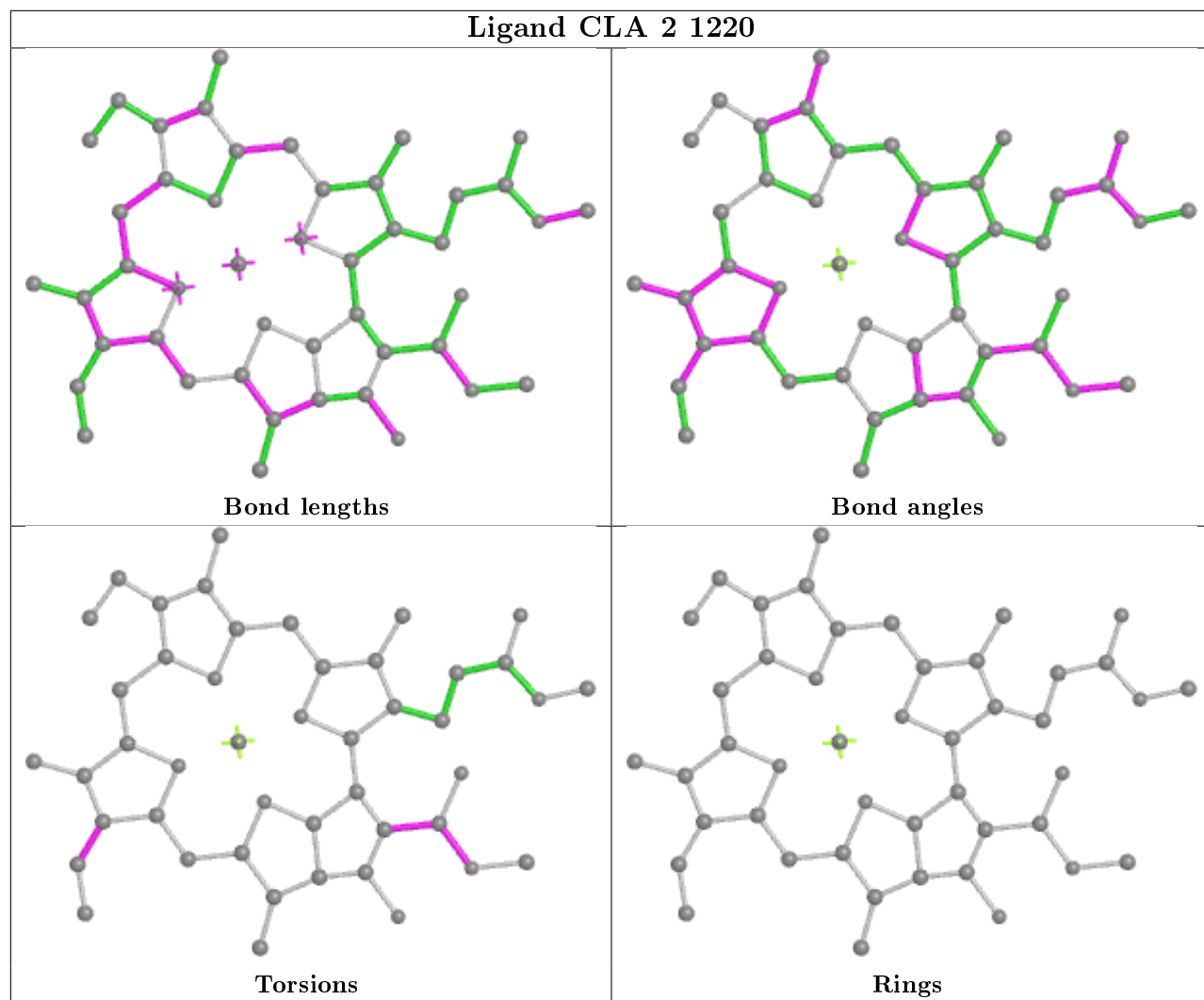


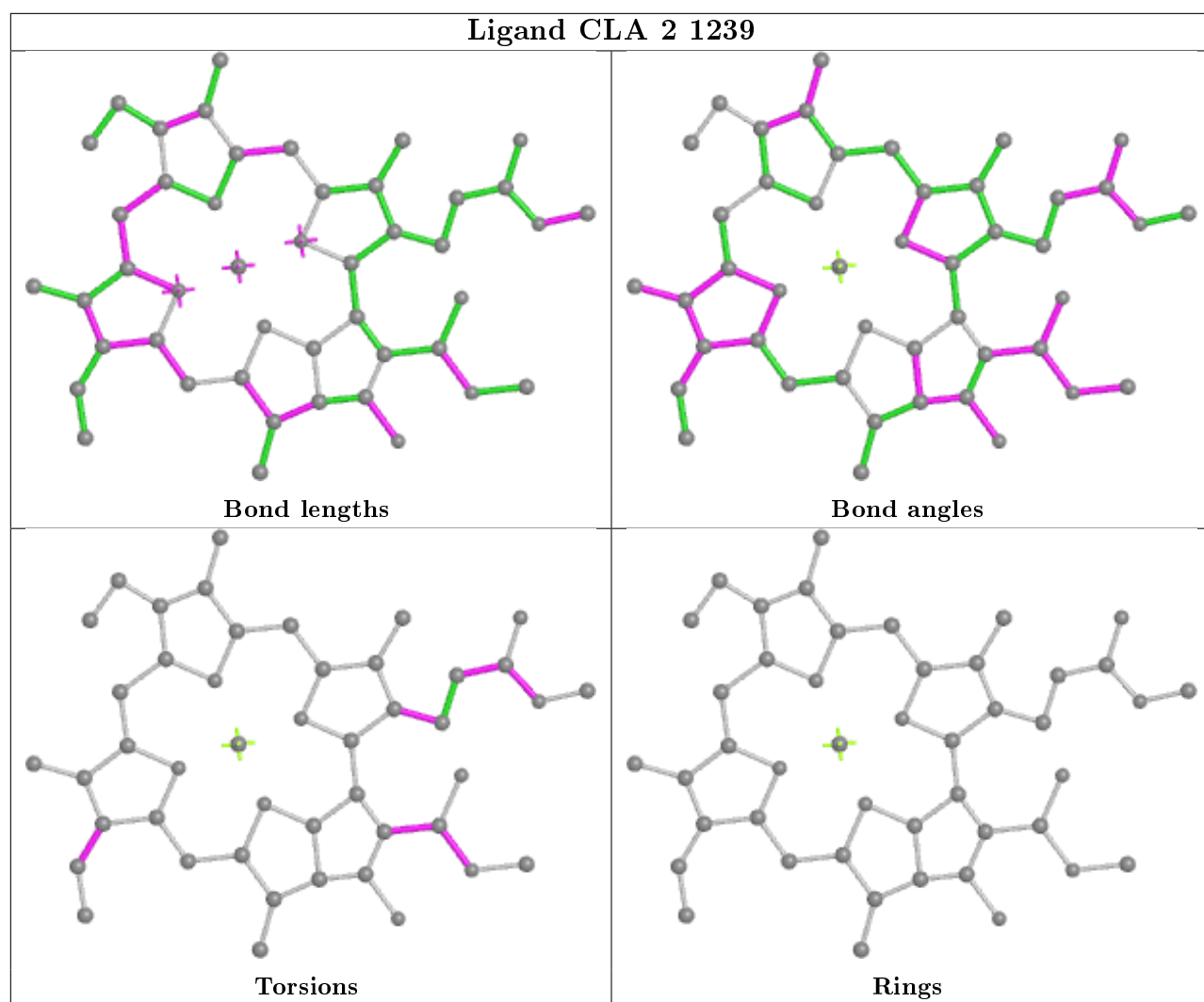


**Ligand CLA B 1219****Ligand CLA 1 1012**

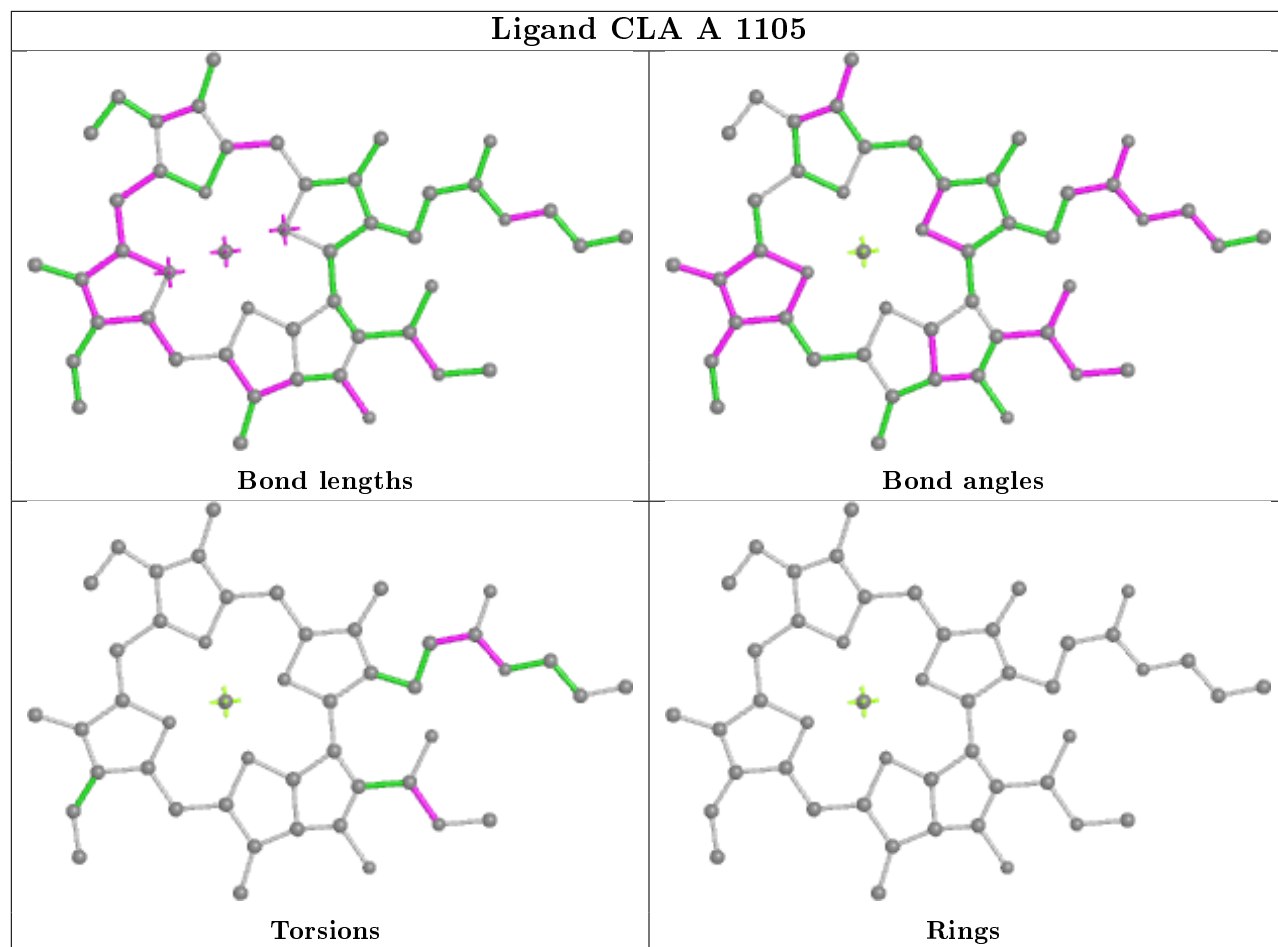




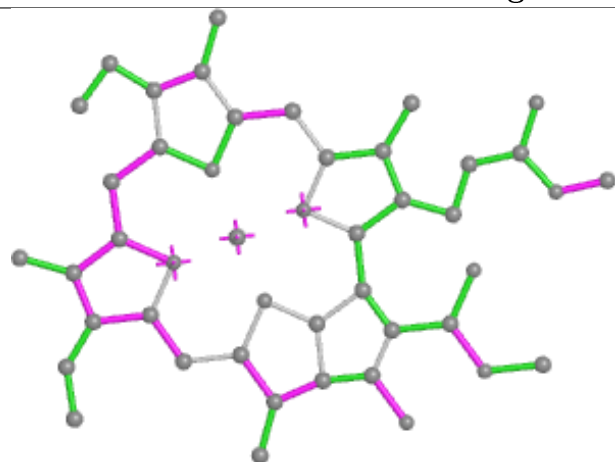




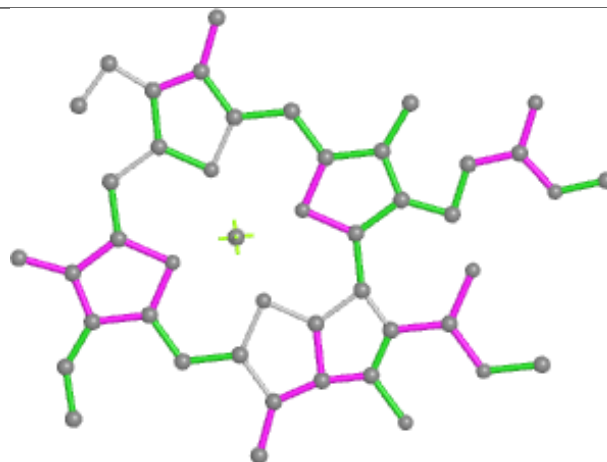
## Ligand CLA A 1105



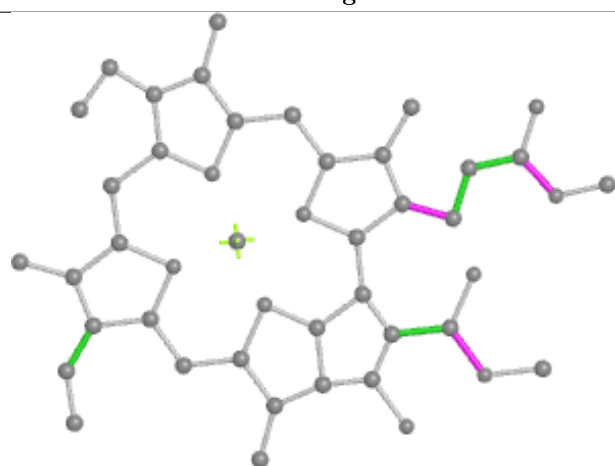
## Ligand CLA A 1121



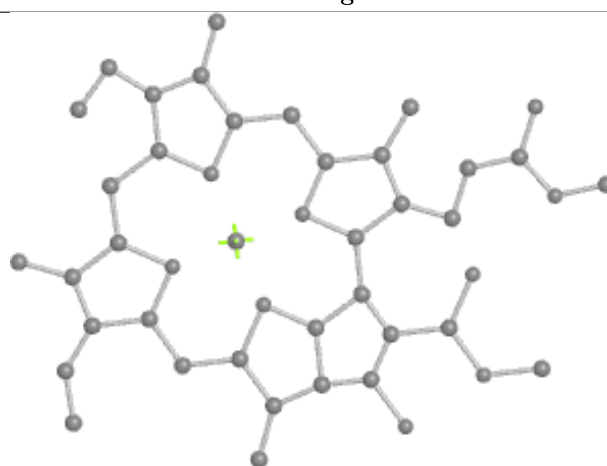
Bond lengths



Bond angles

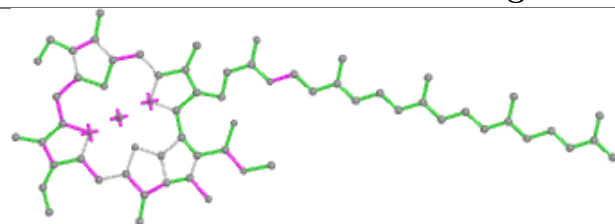


Torsions

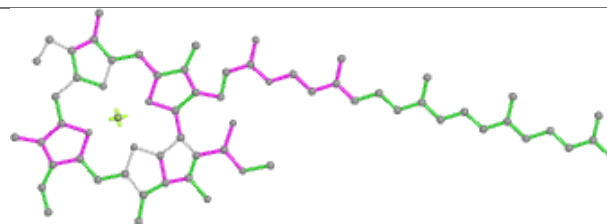


Rings

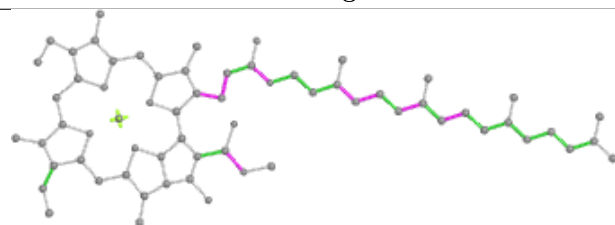
## Ligand CLA A 1107



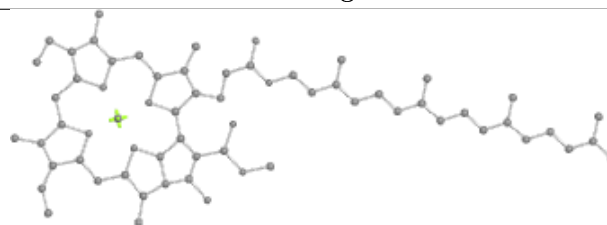
Bond lengths



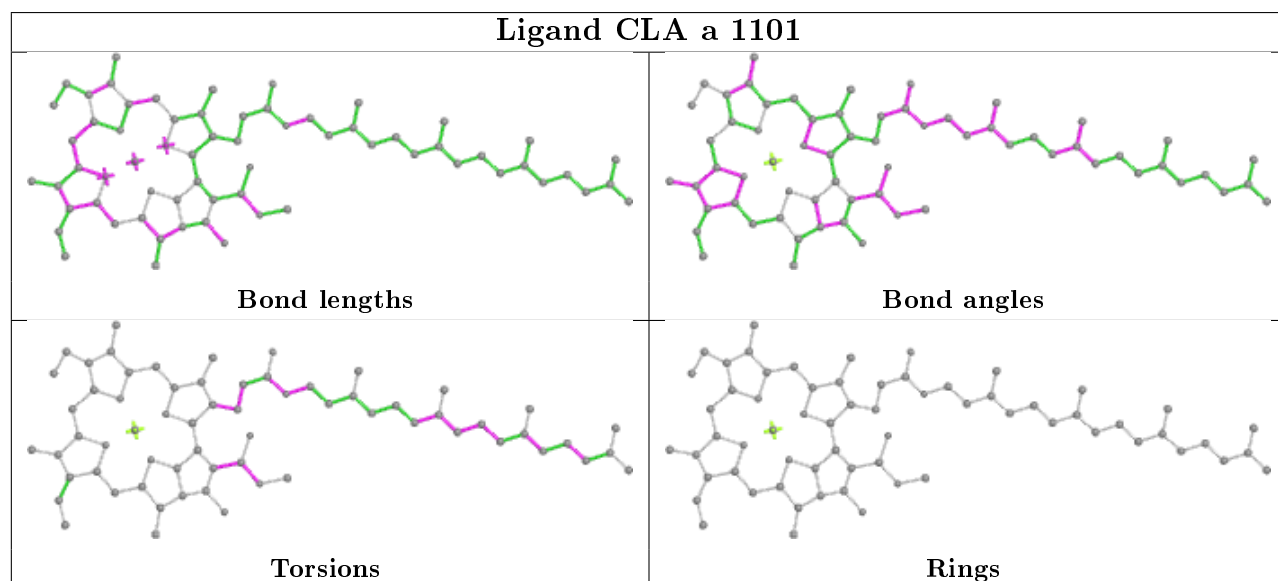
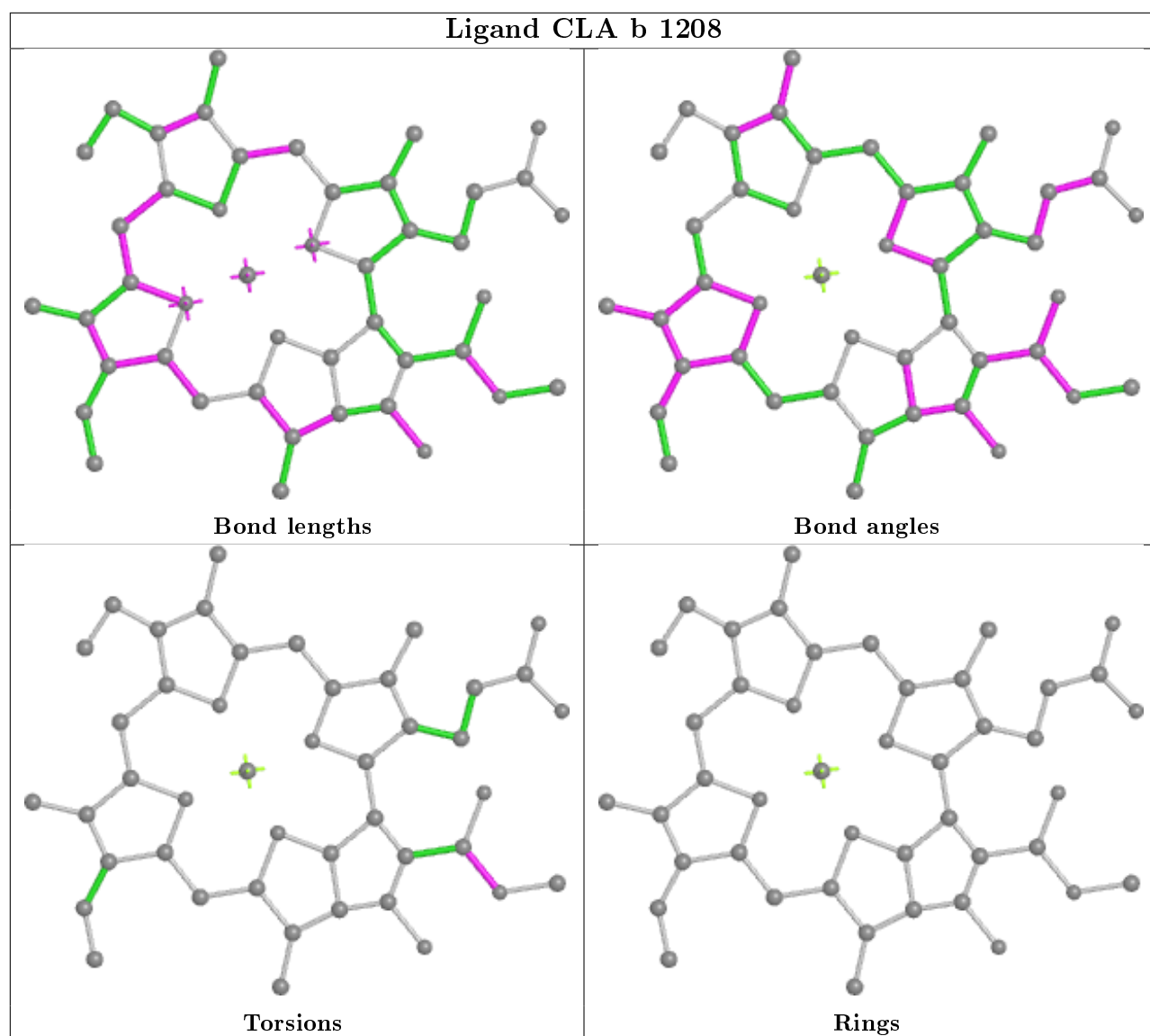
Bond angles



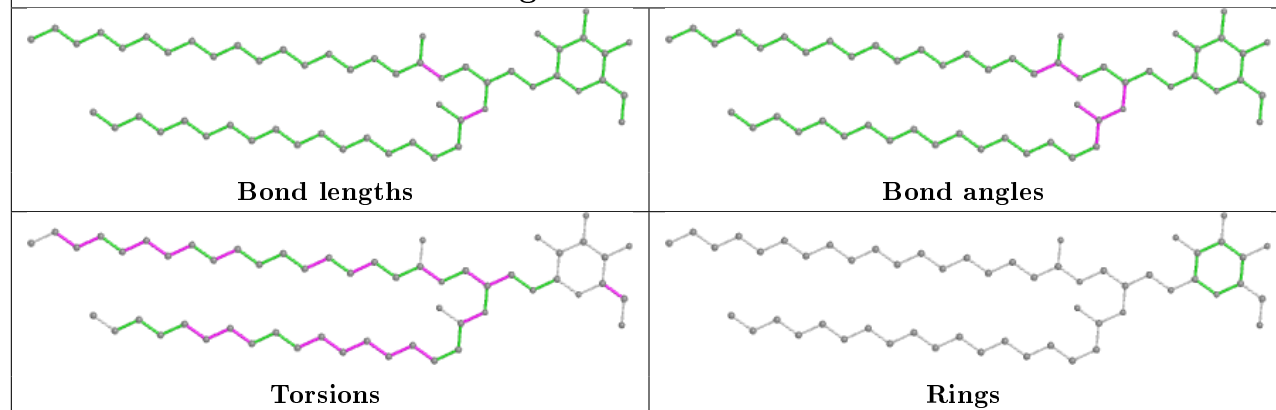
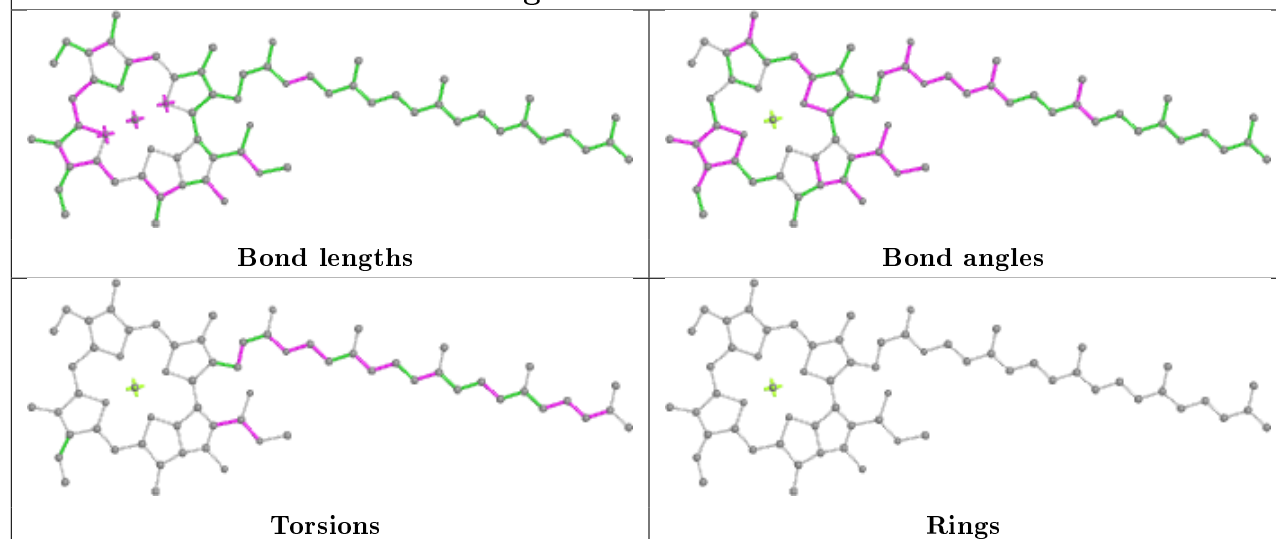
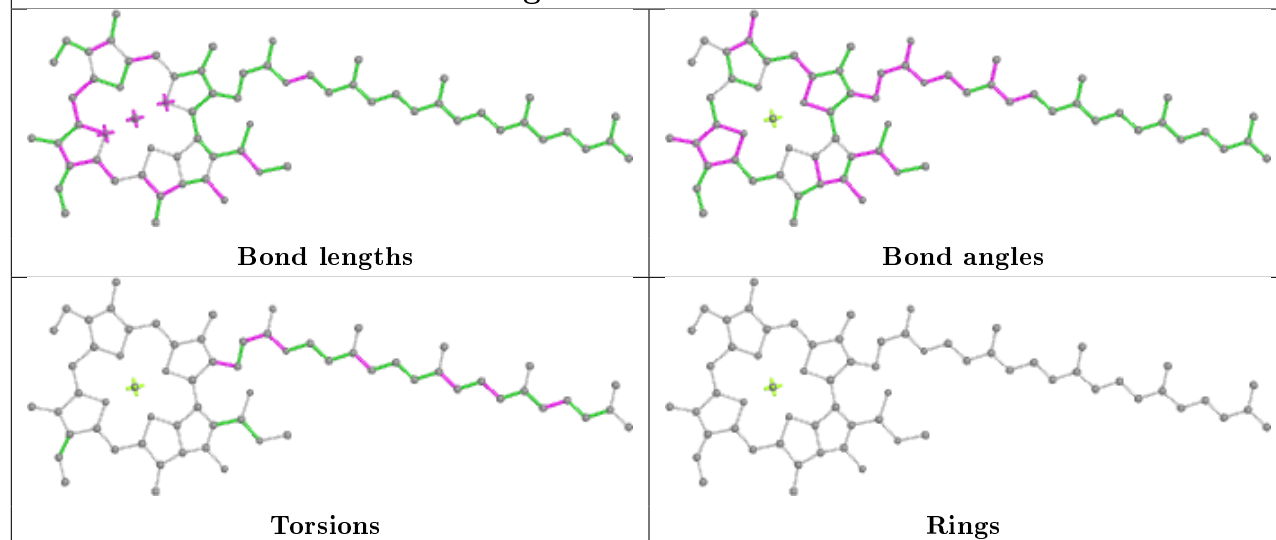
Torsions

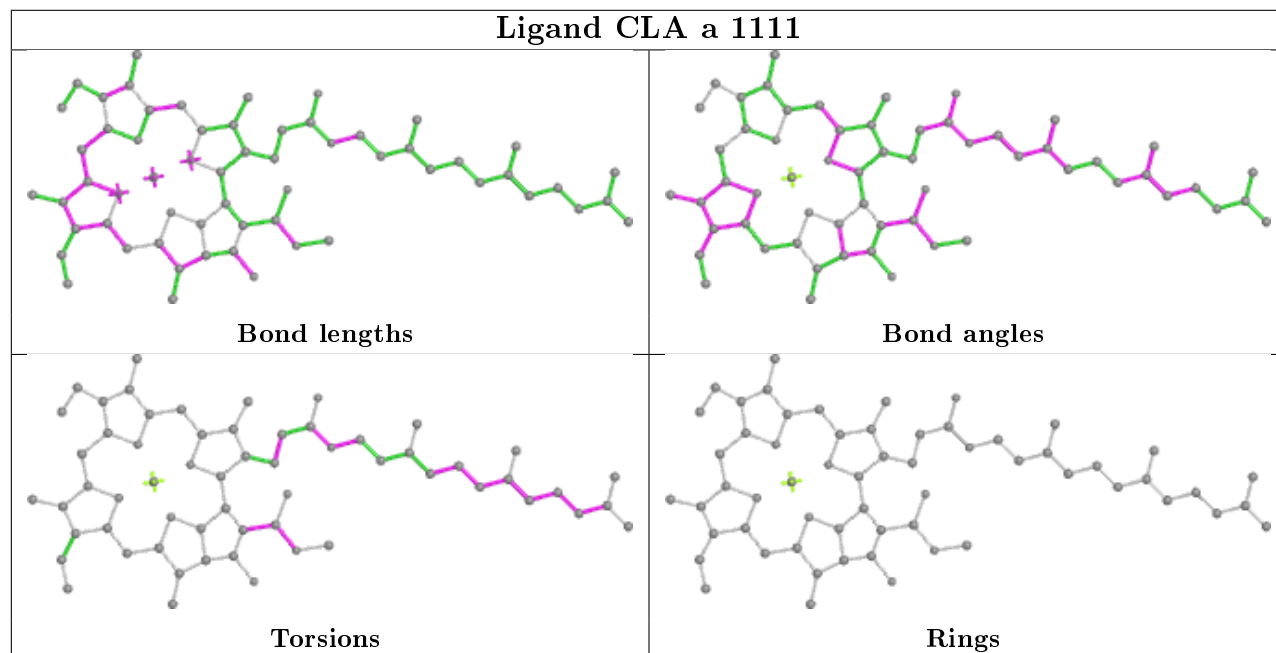
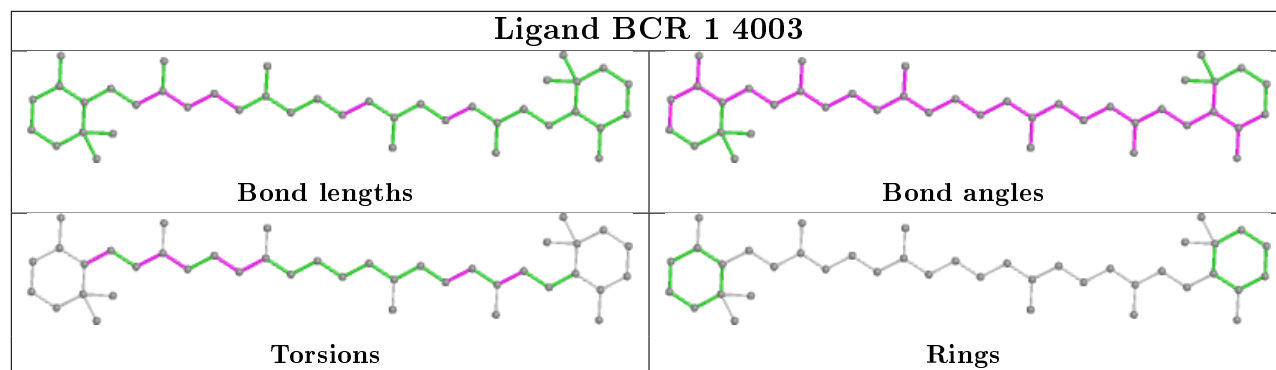
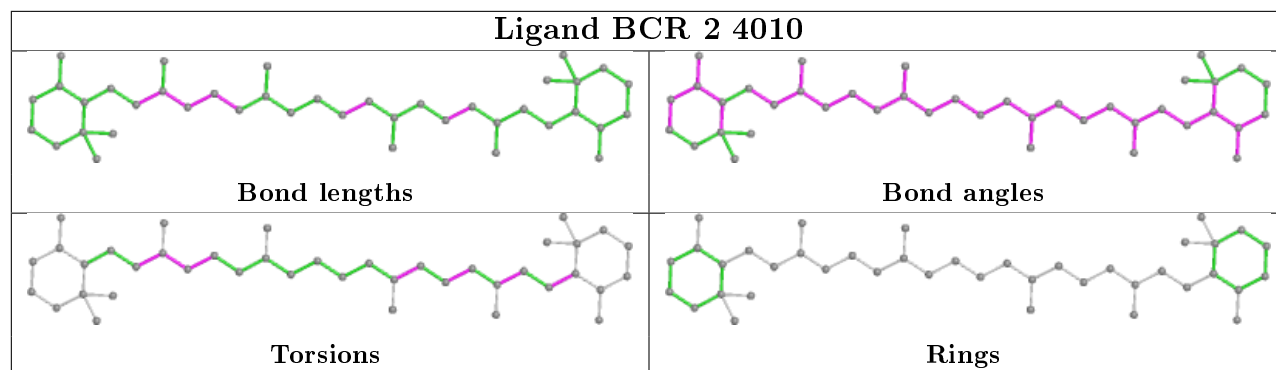


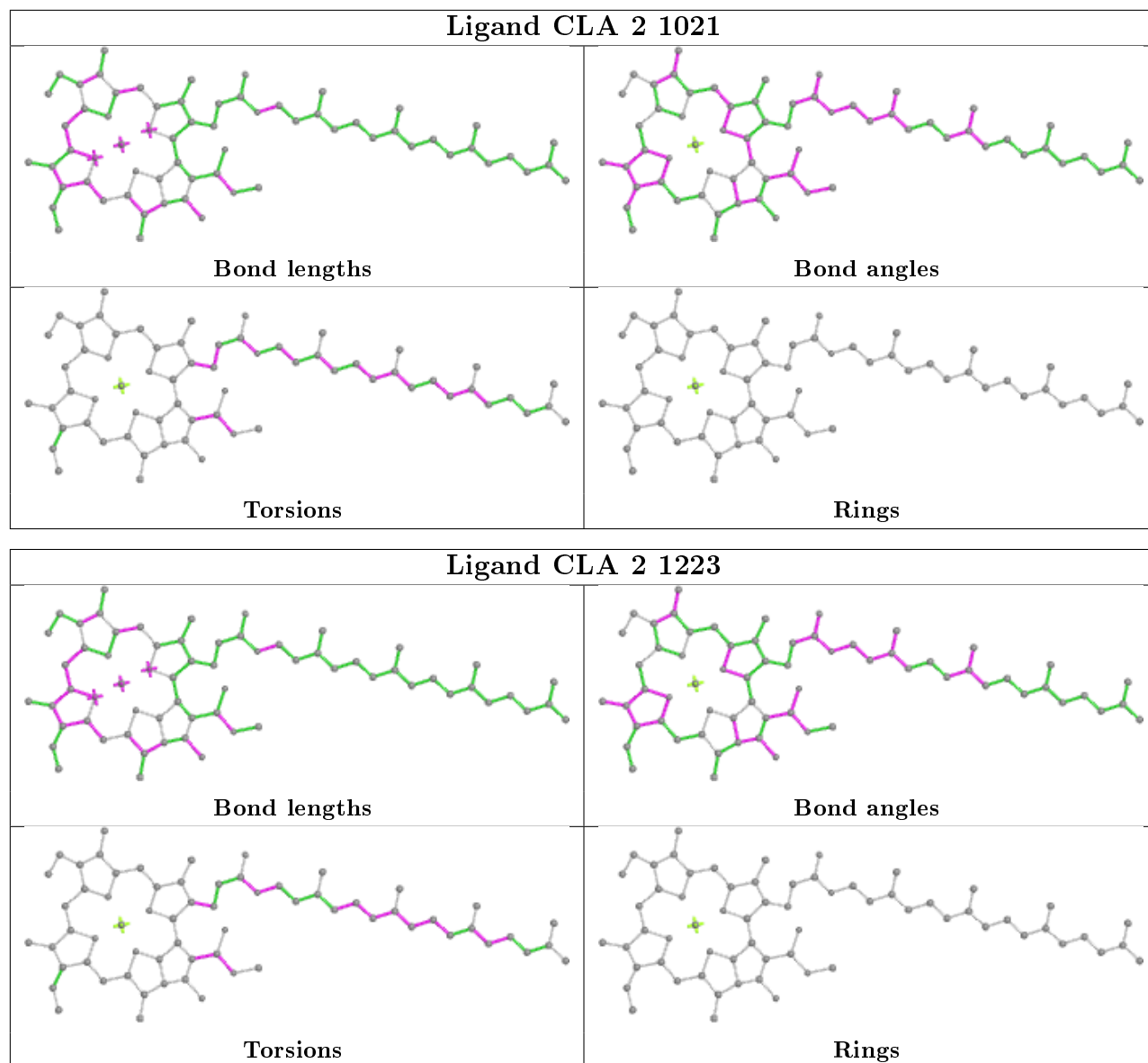
Rings

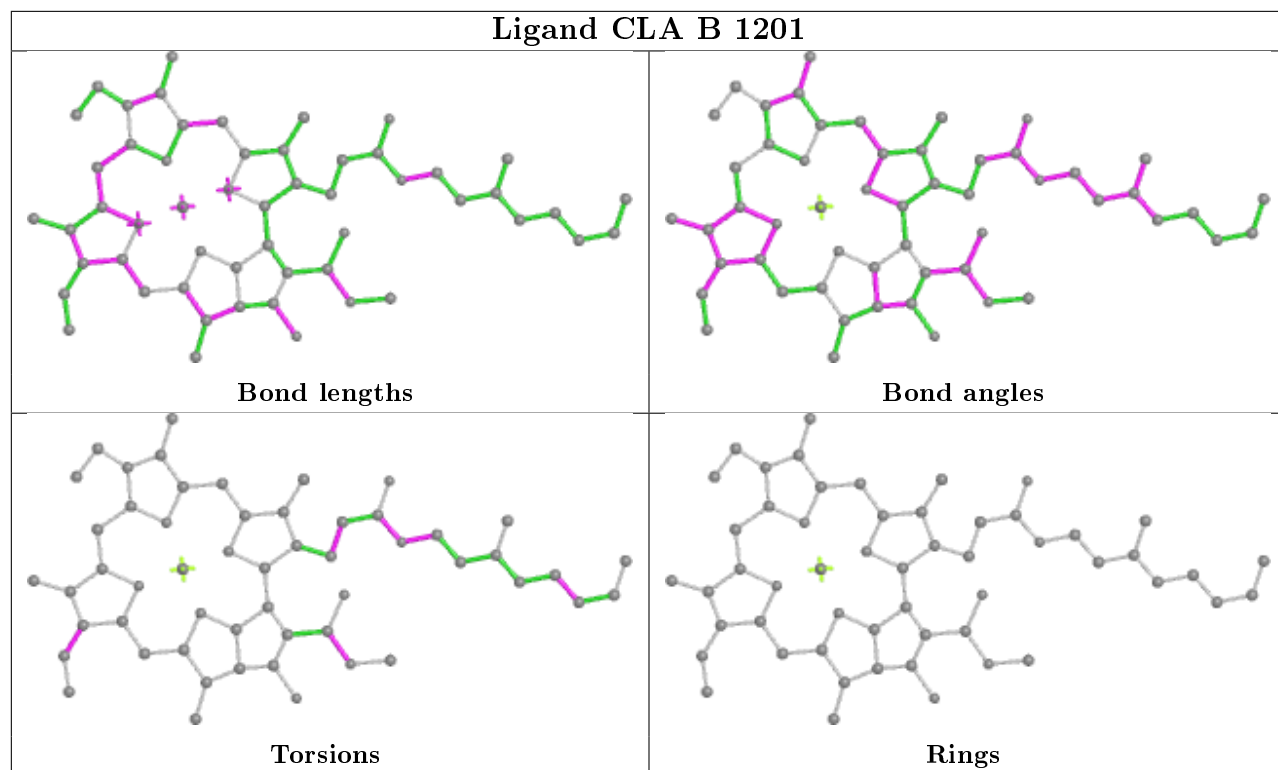




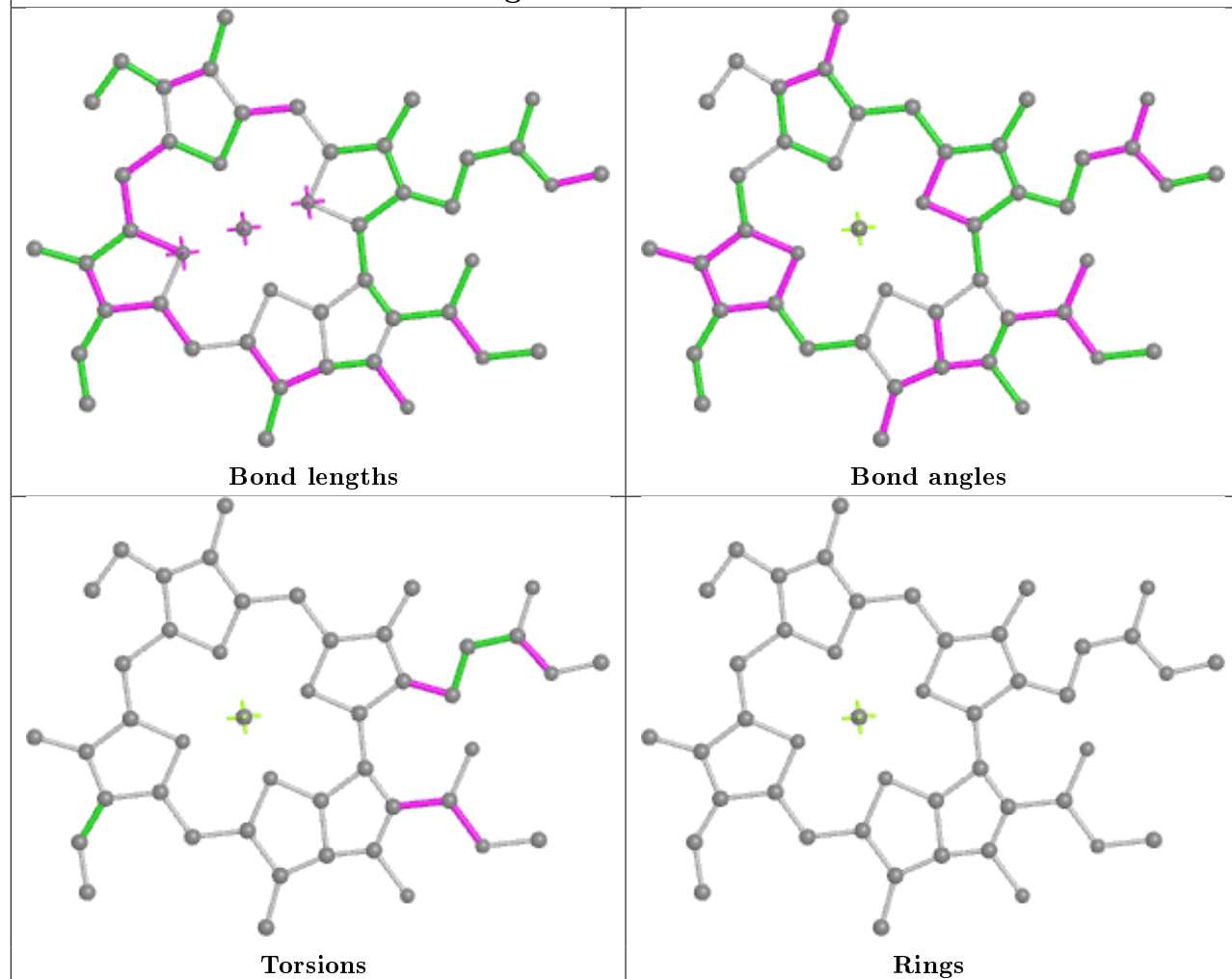
**Ligand LMG B 5002****Ligand CLA B 1013****Ligand CLA B 1225**



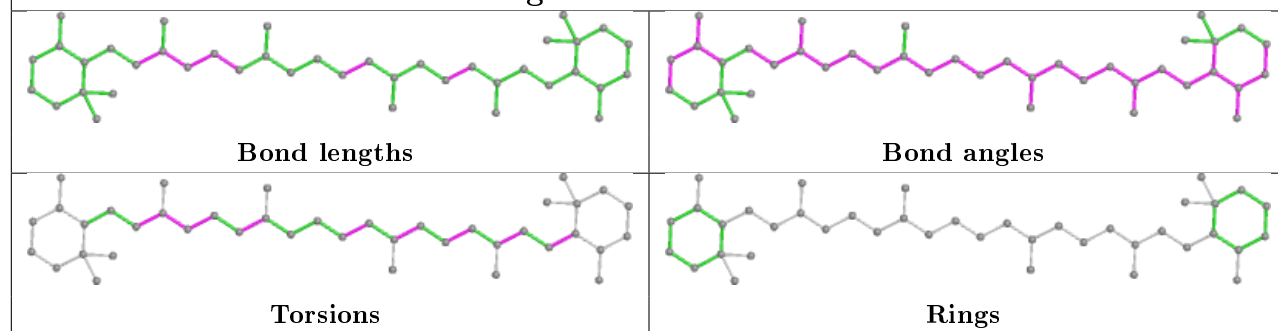


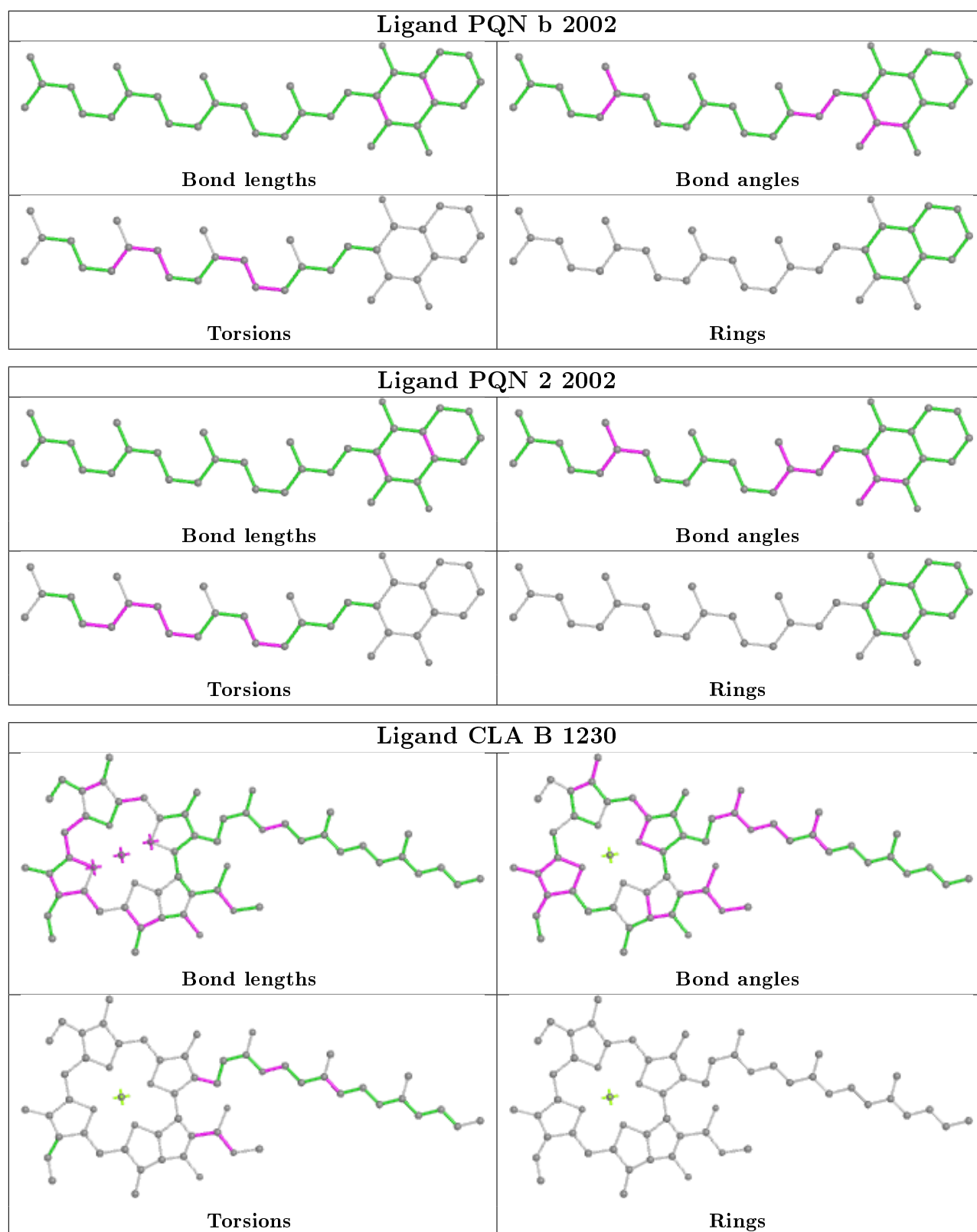


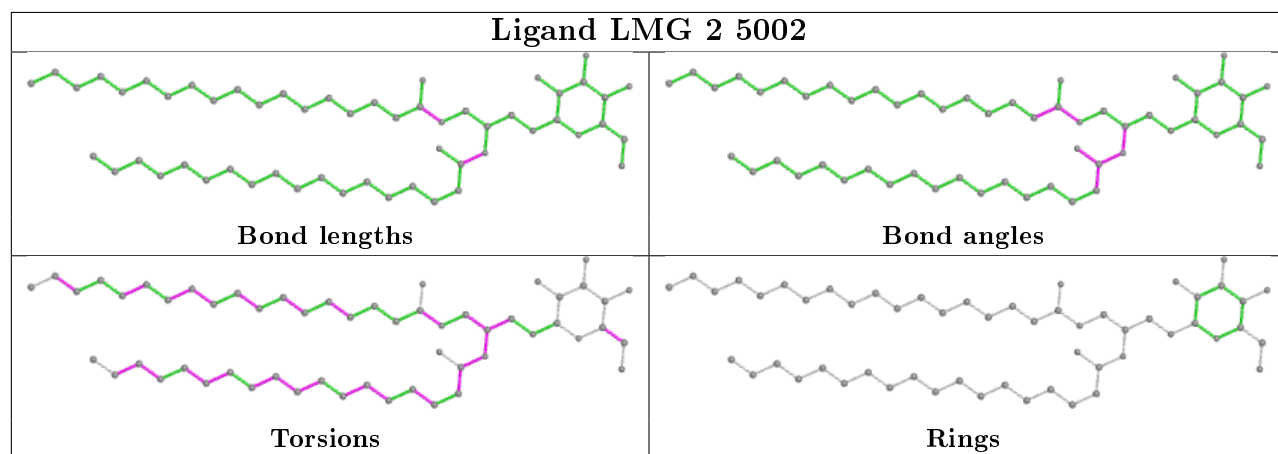
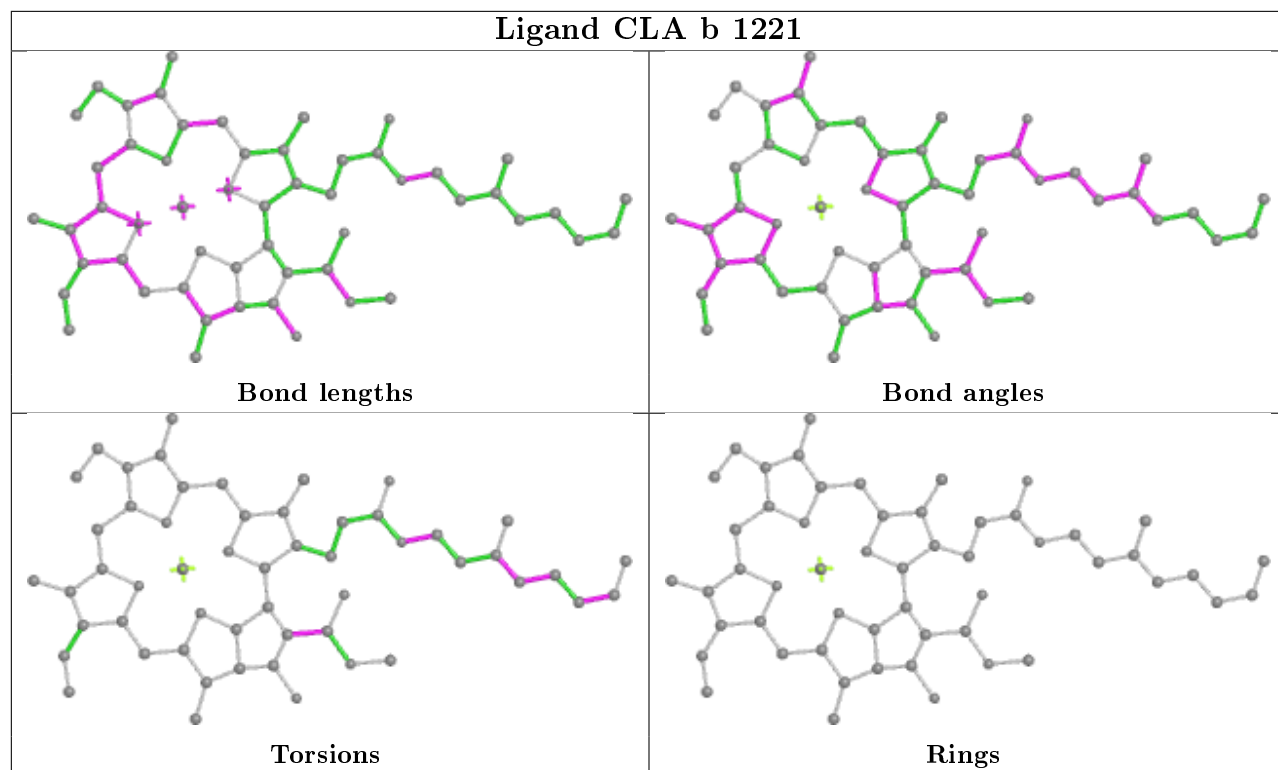
## Ligand CLA B 1211

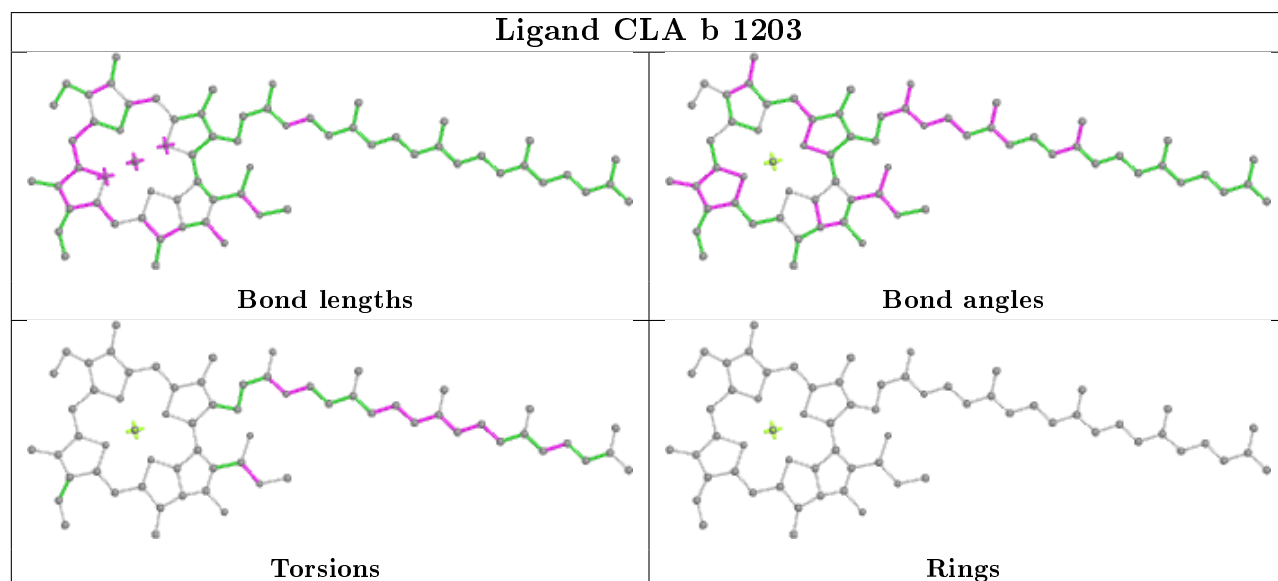
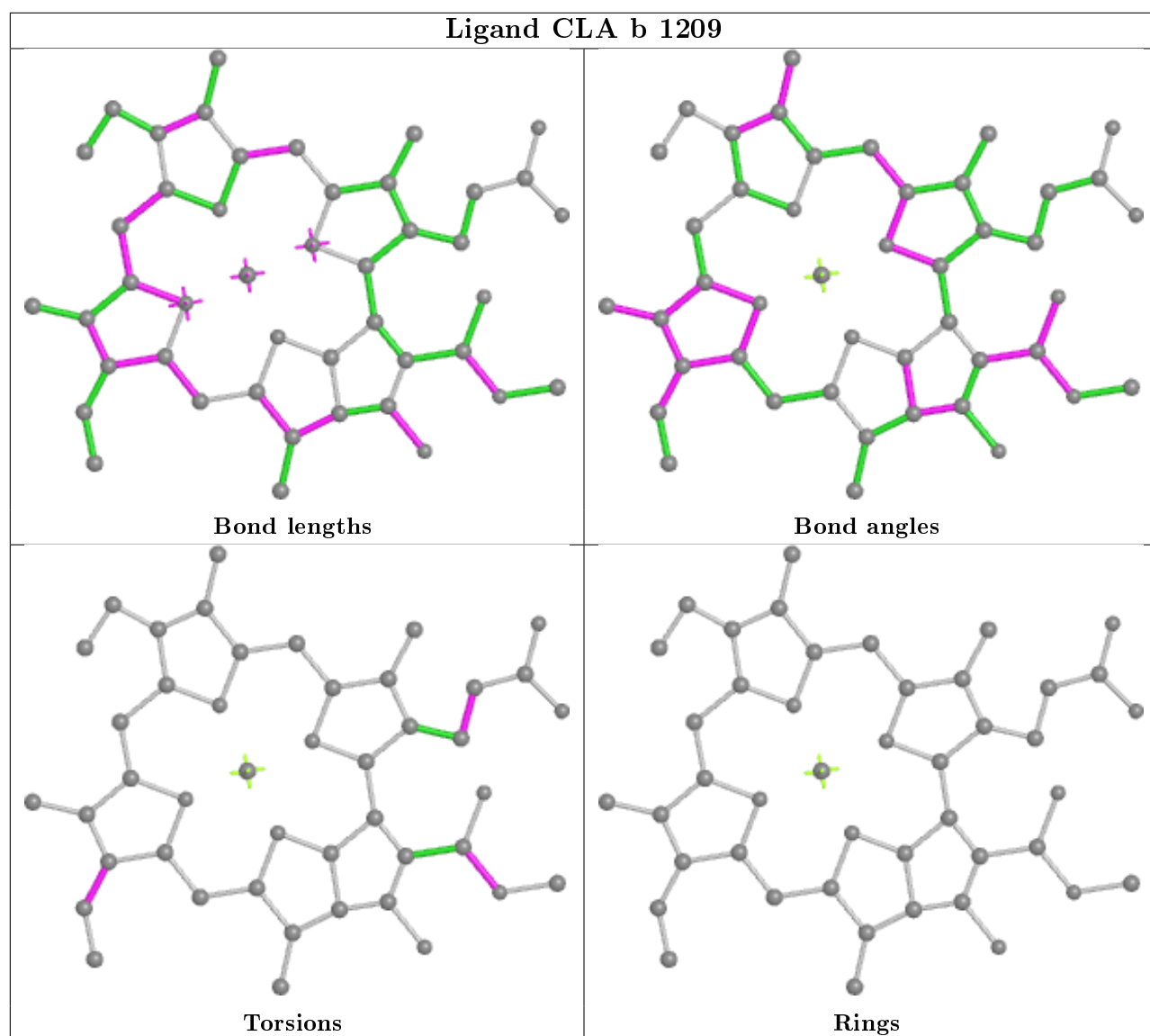


## Ligand BCR a 4002

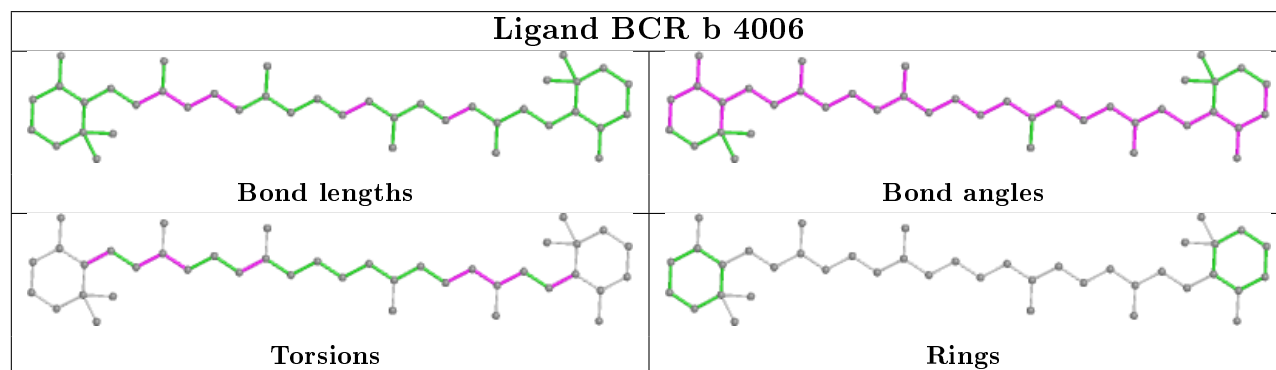
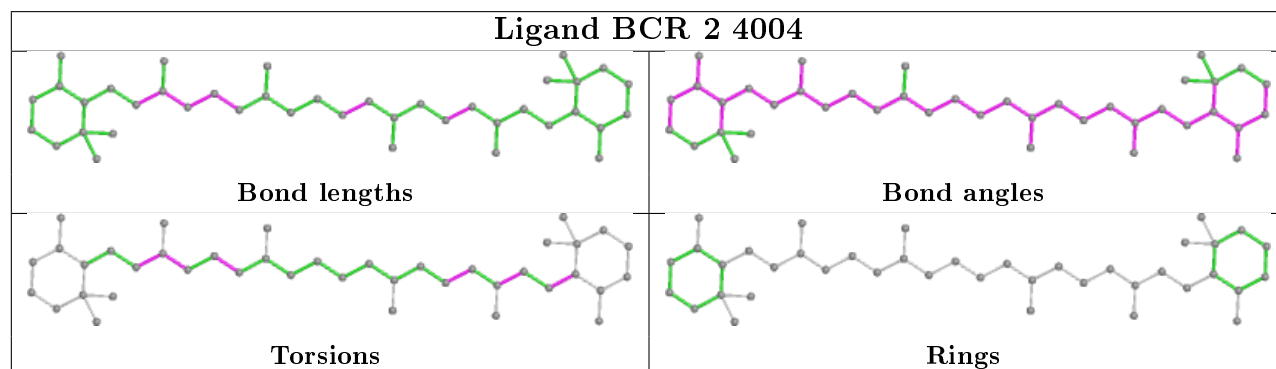
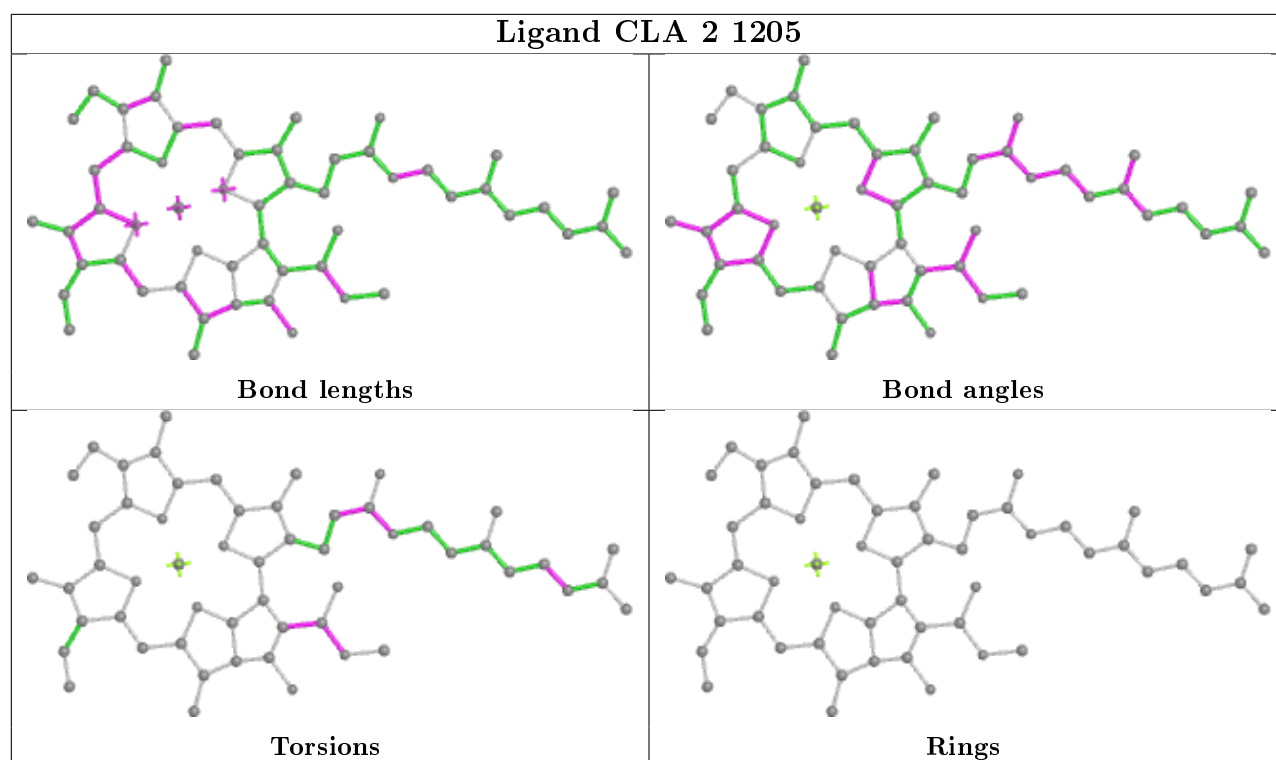




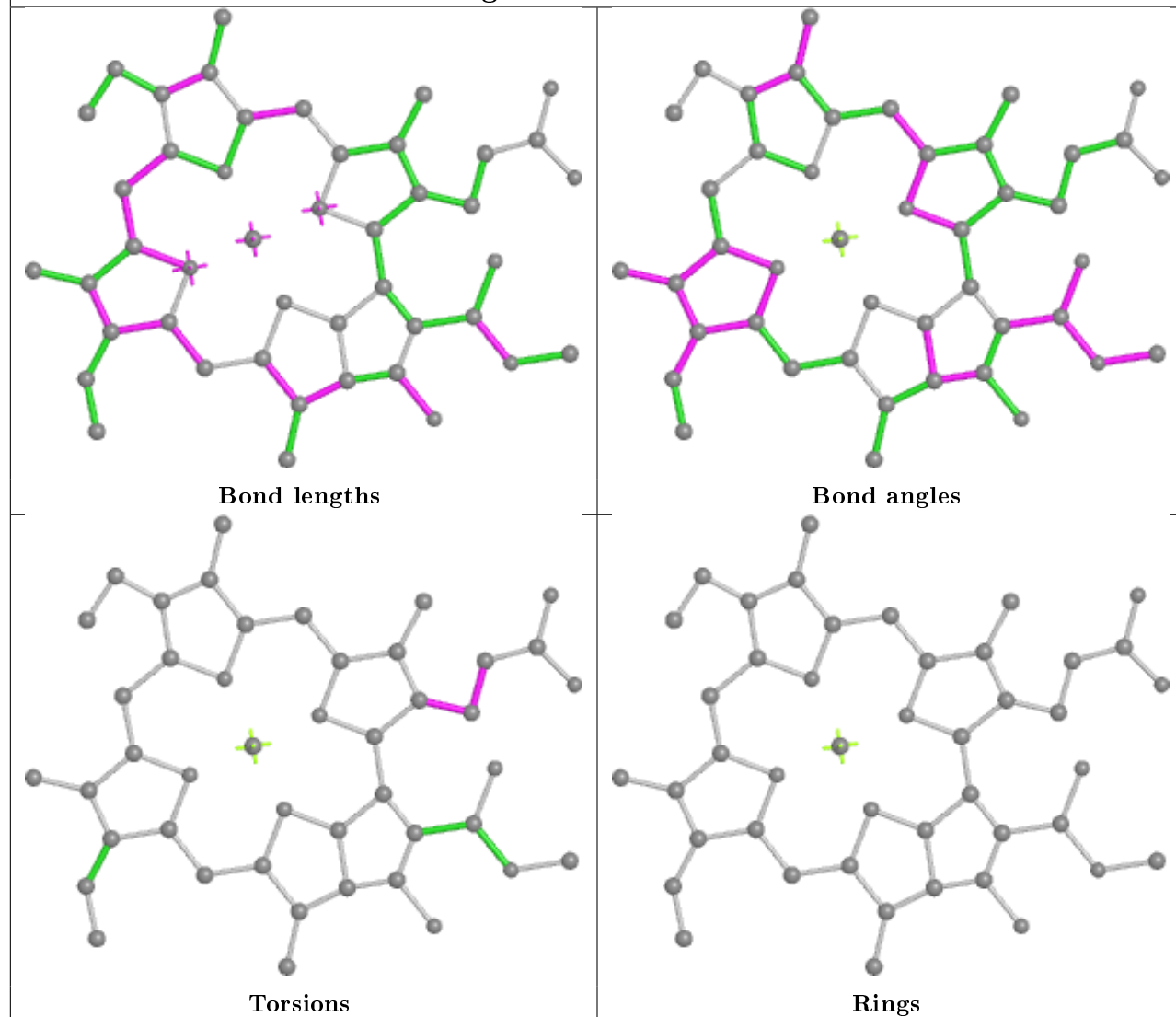




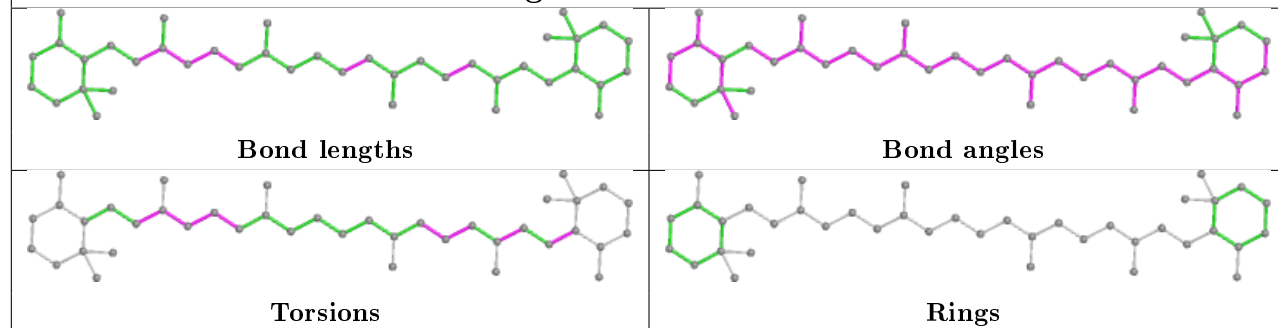


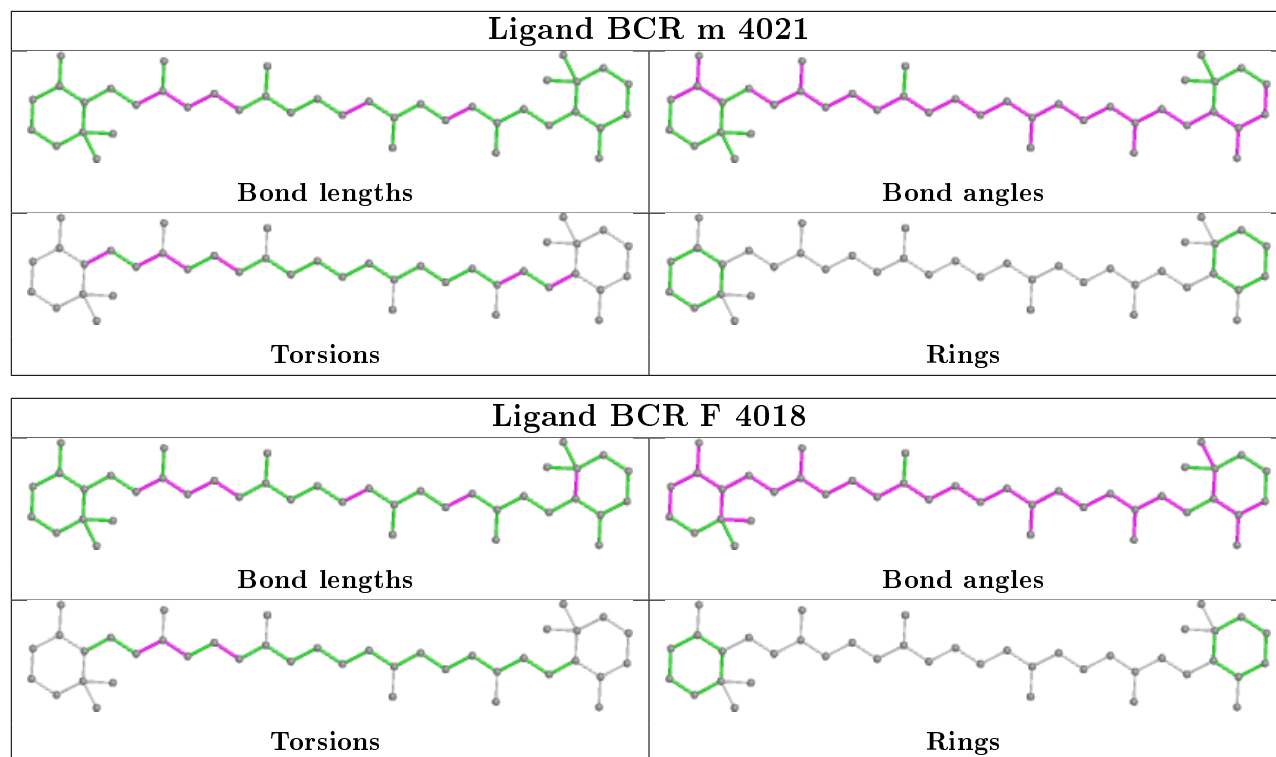


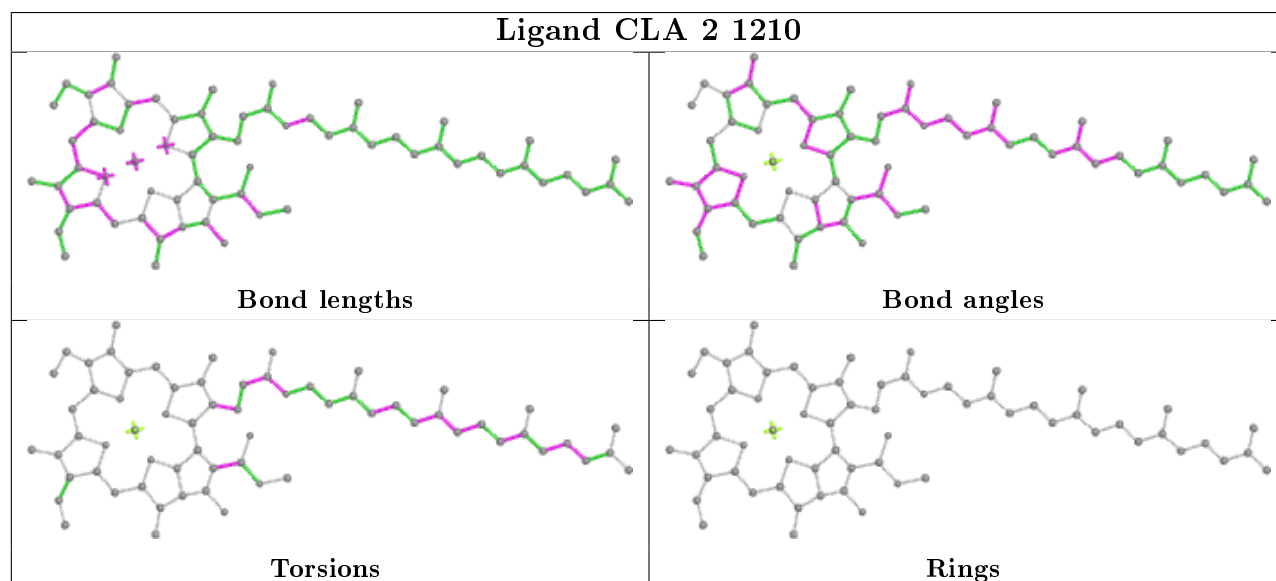
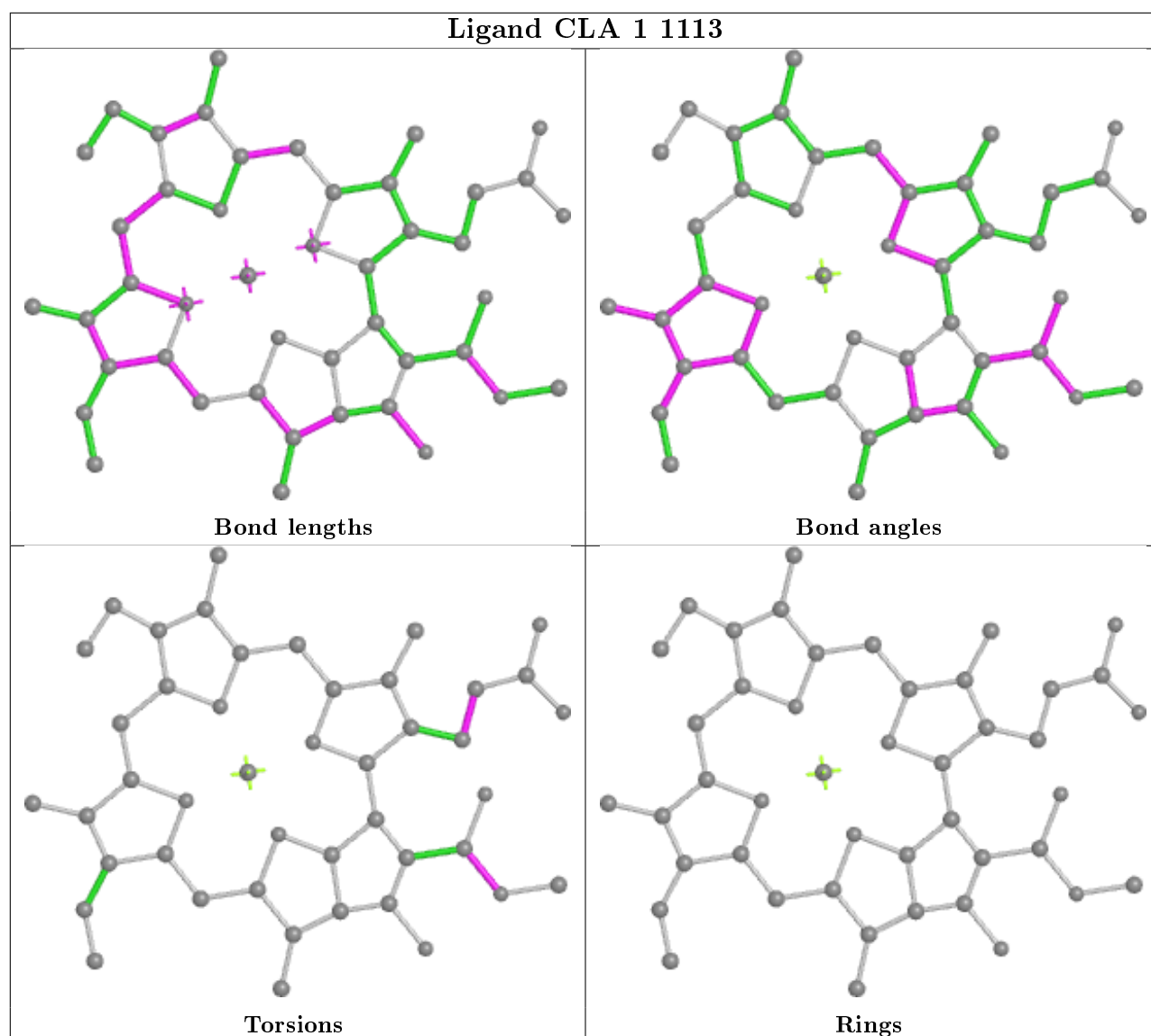
## Ligand CLA A 1108

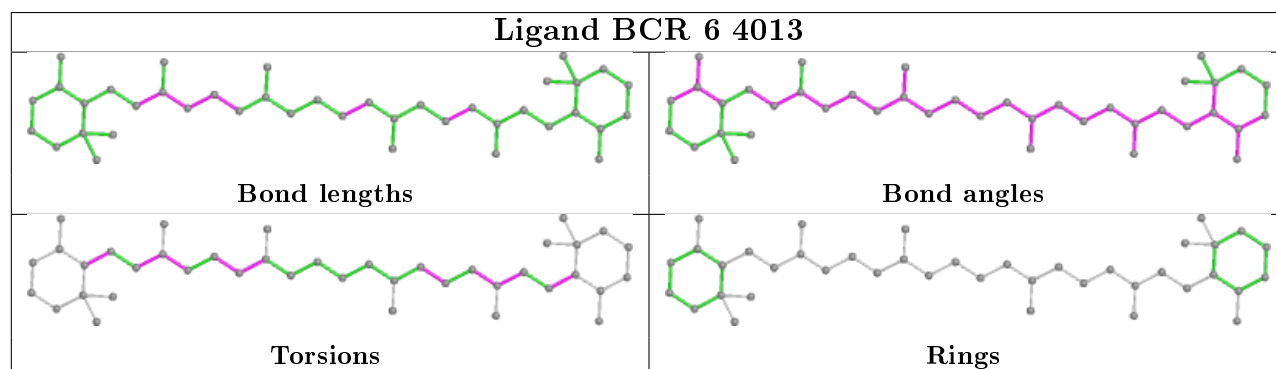
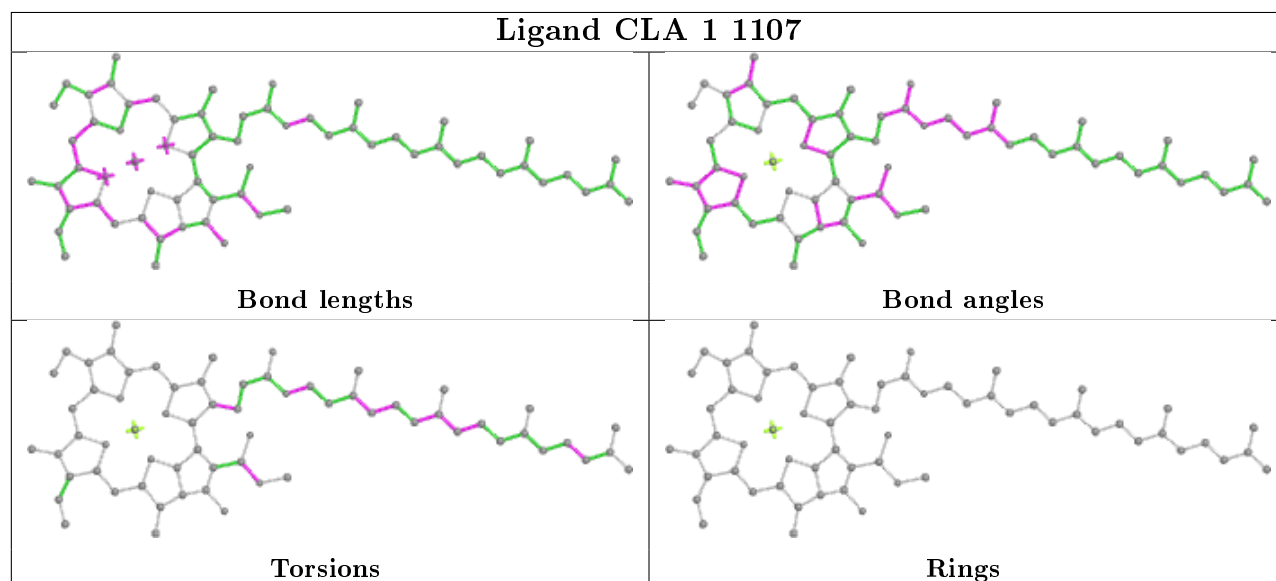
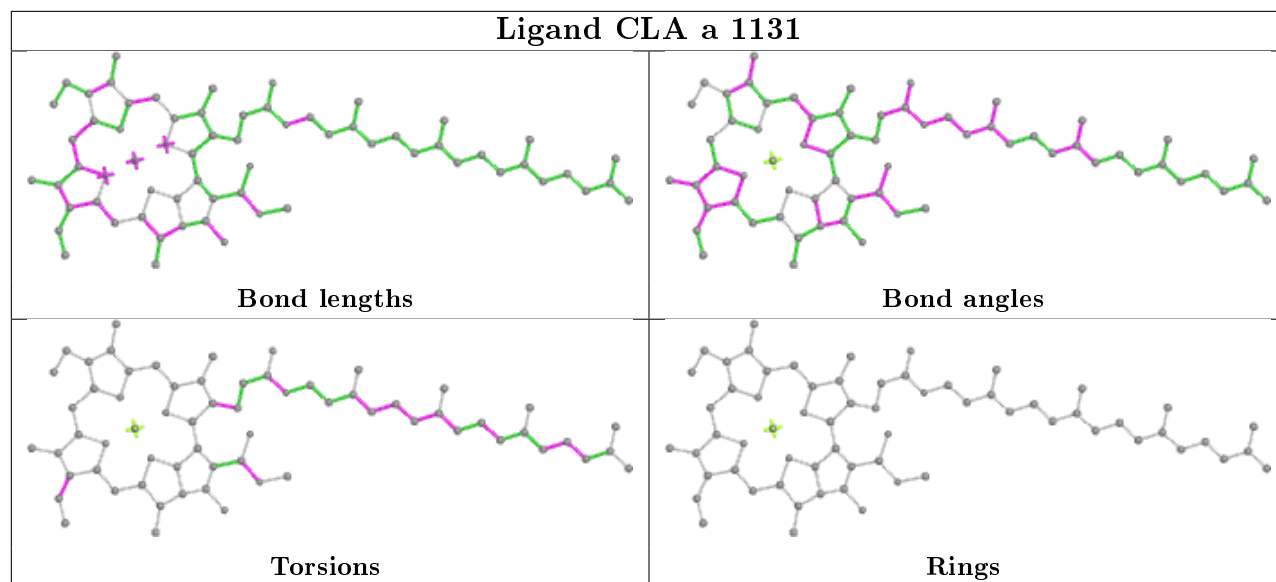


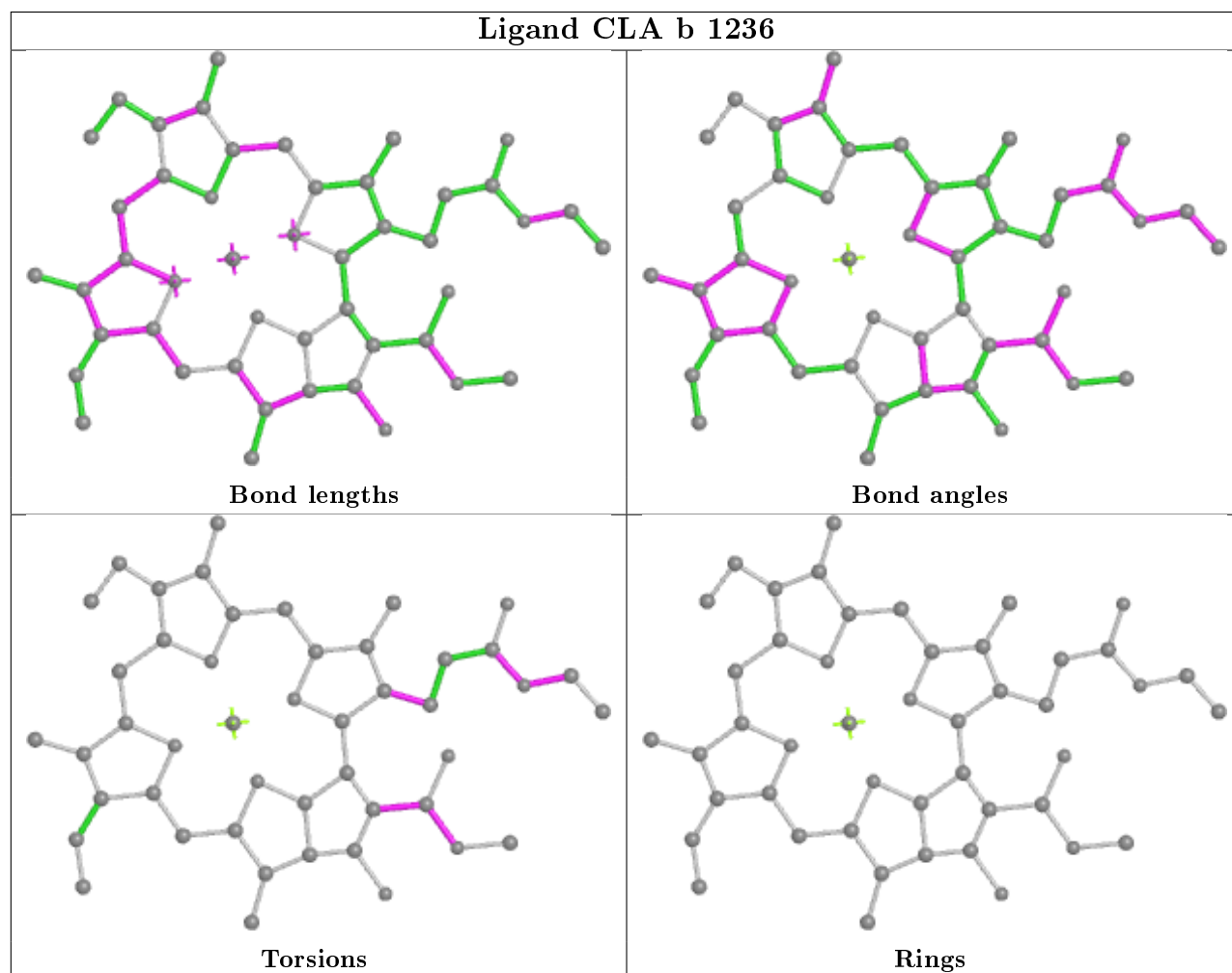
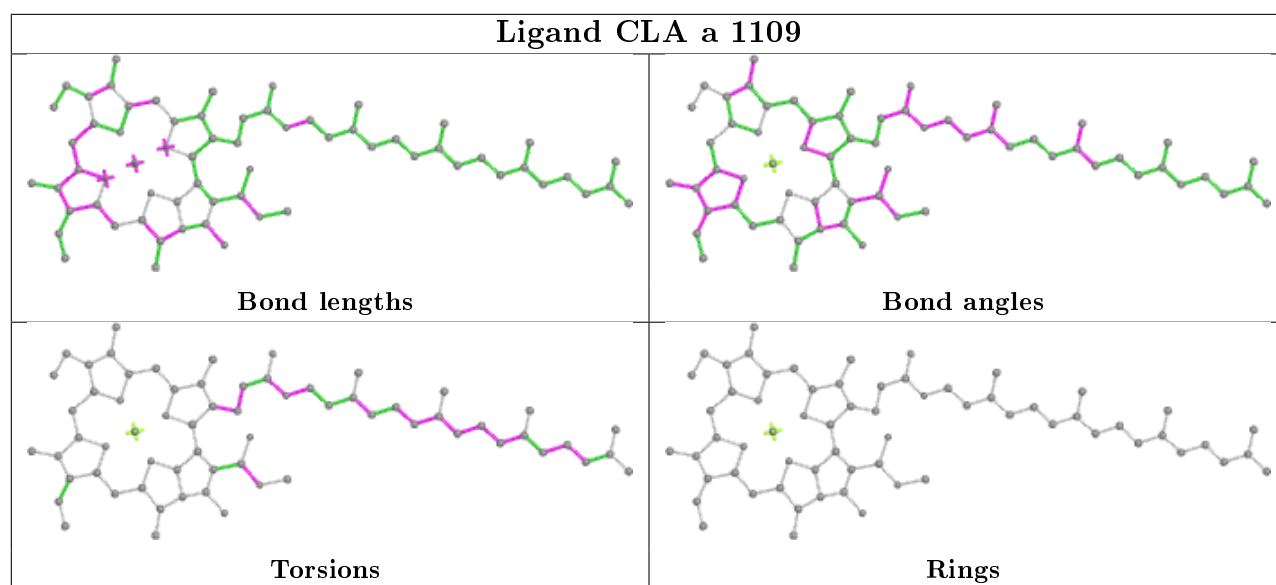
## Ligand BCR 1 4007

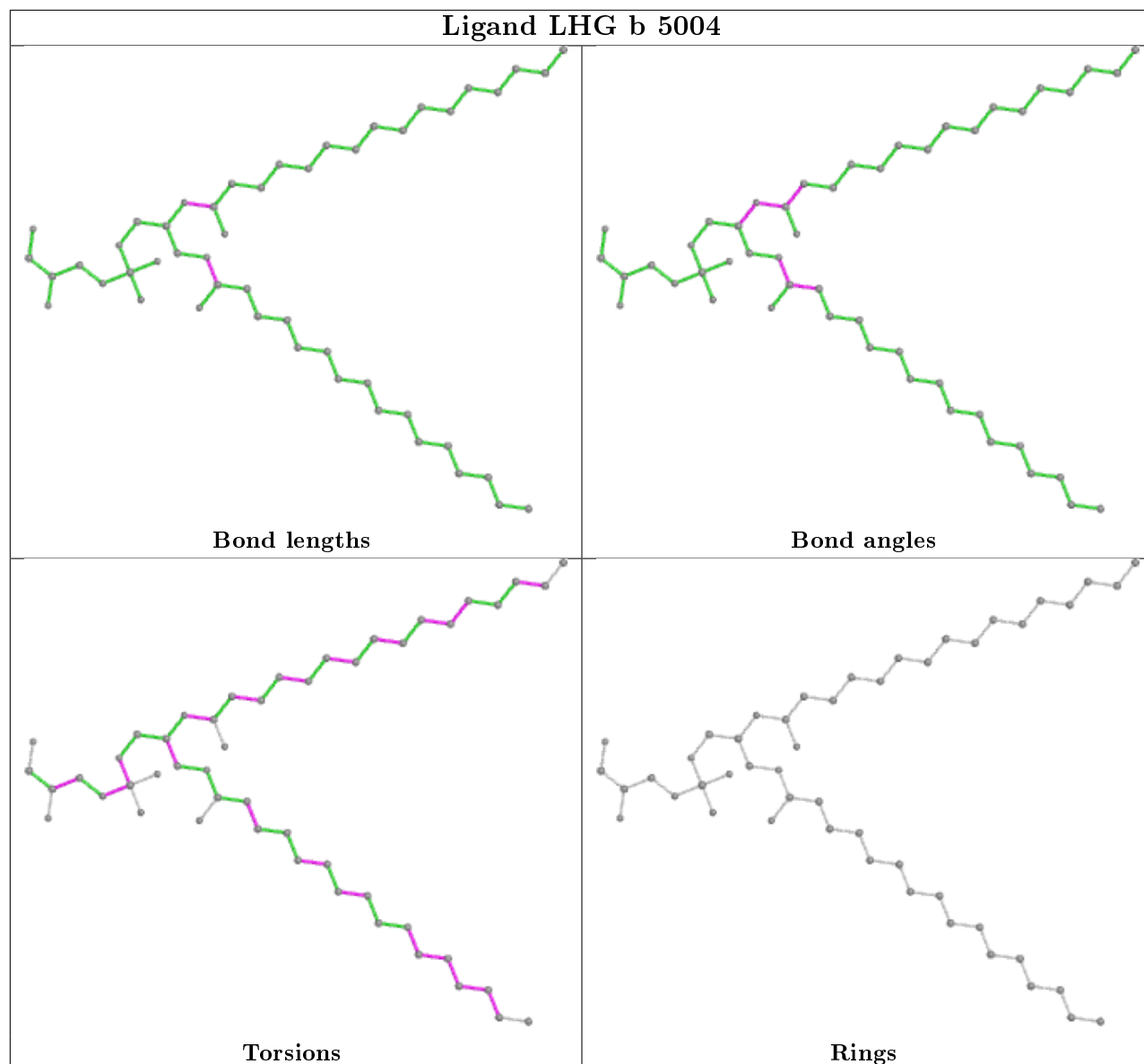
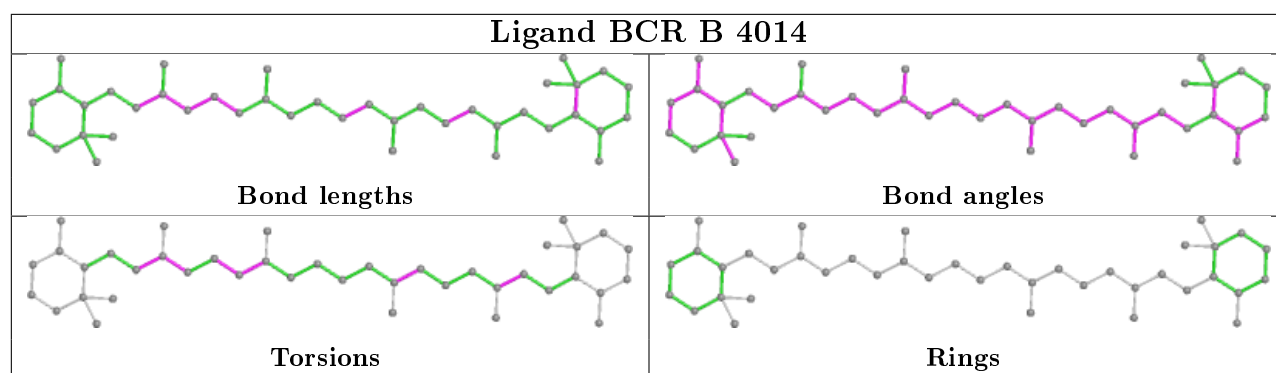


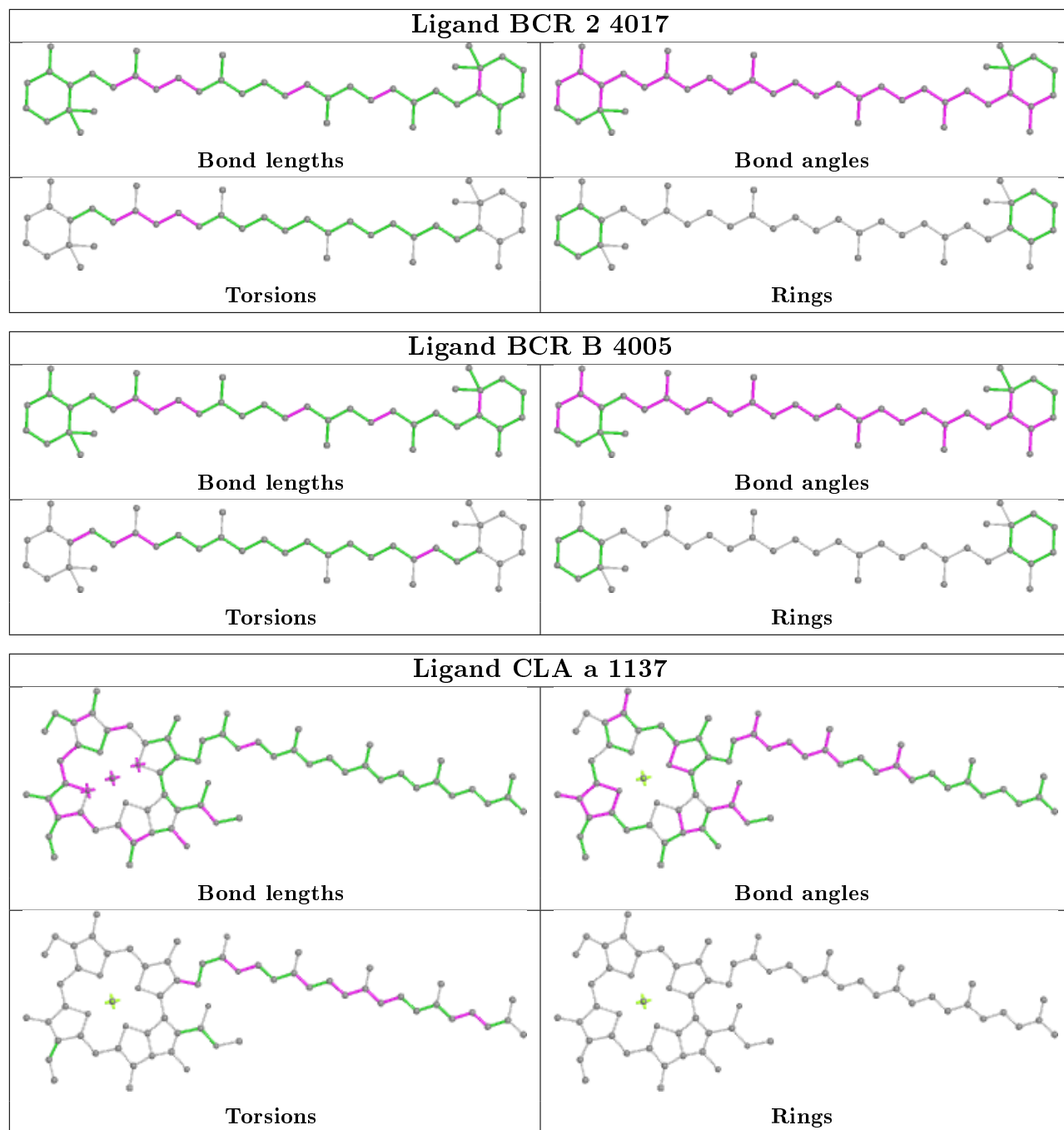




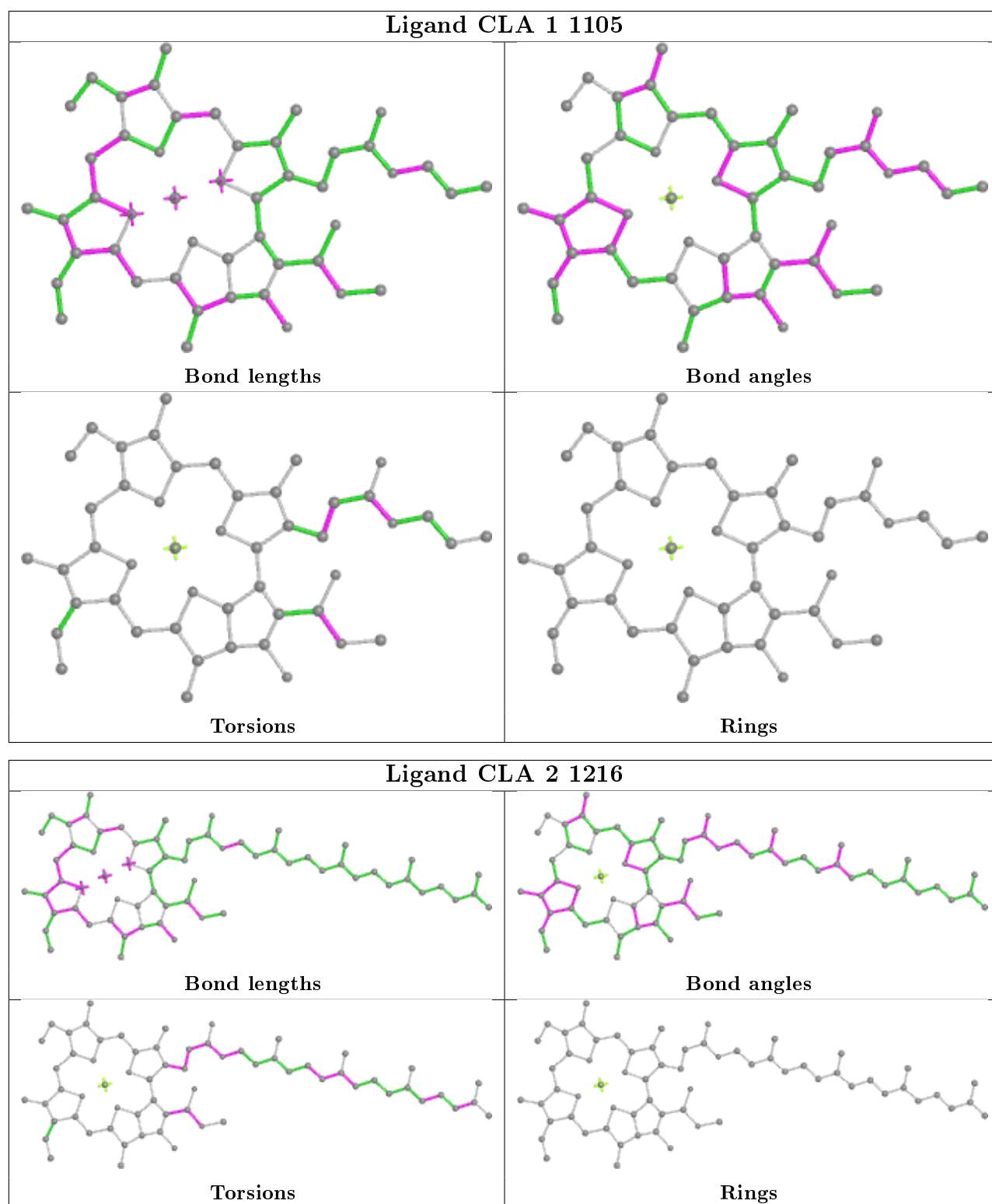


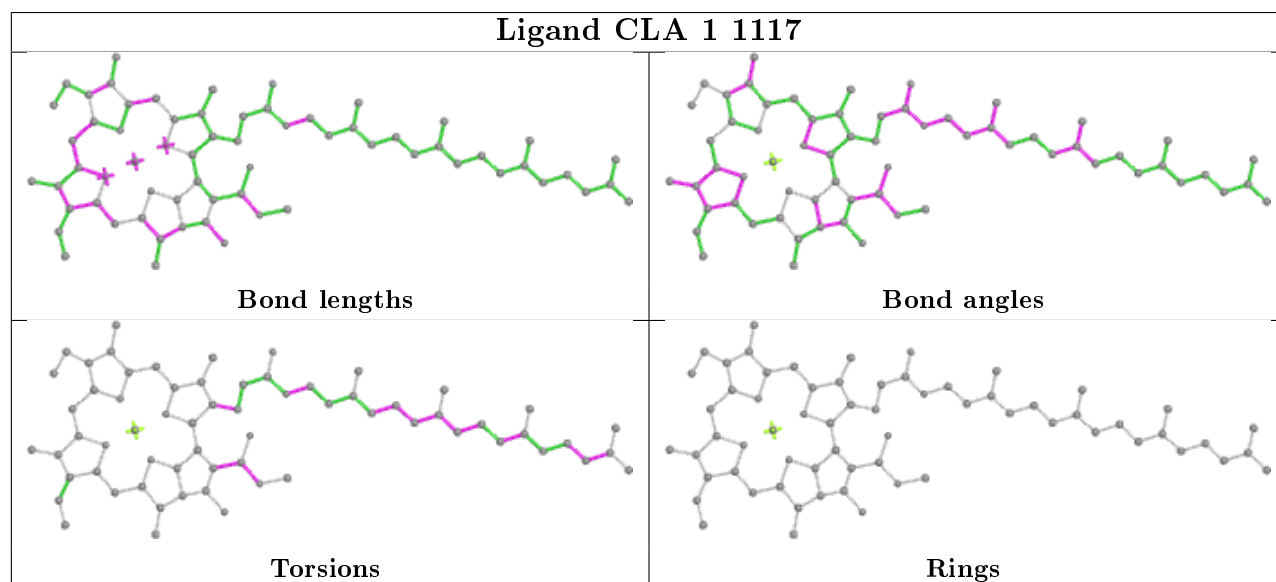
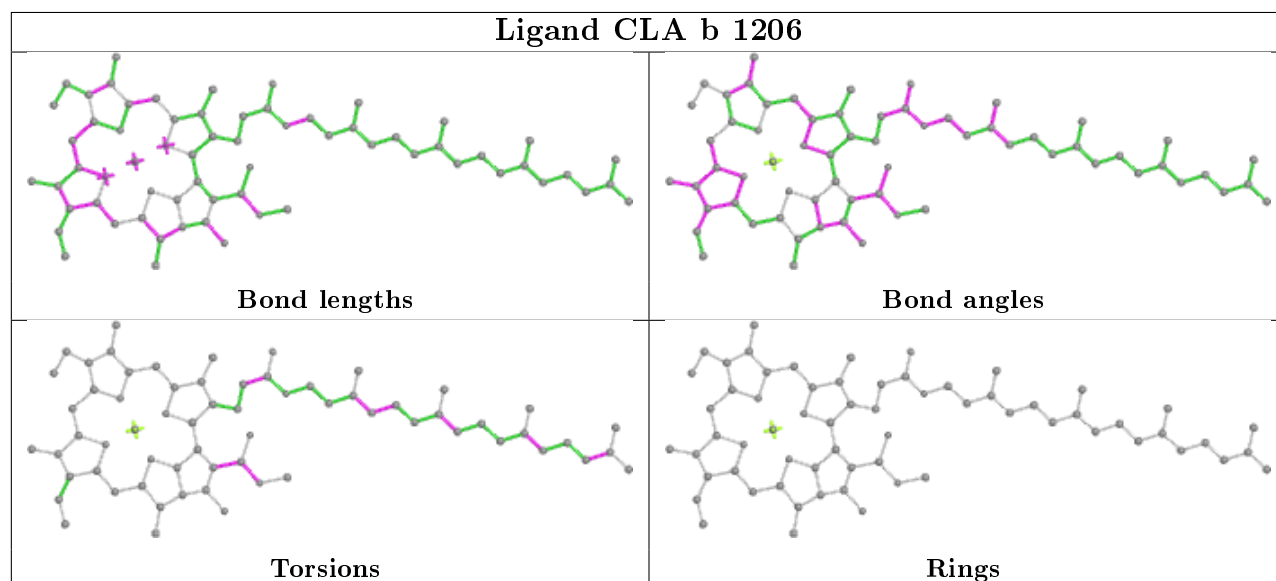
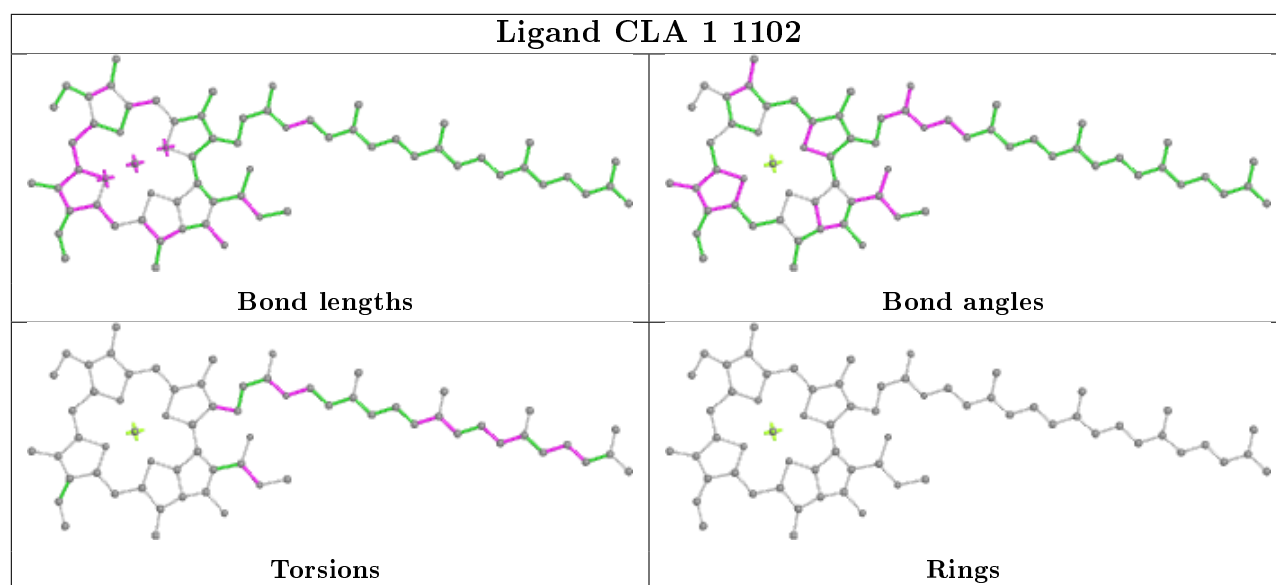




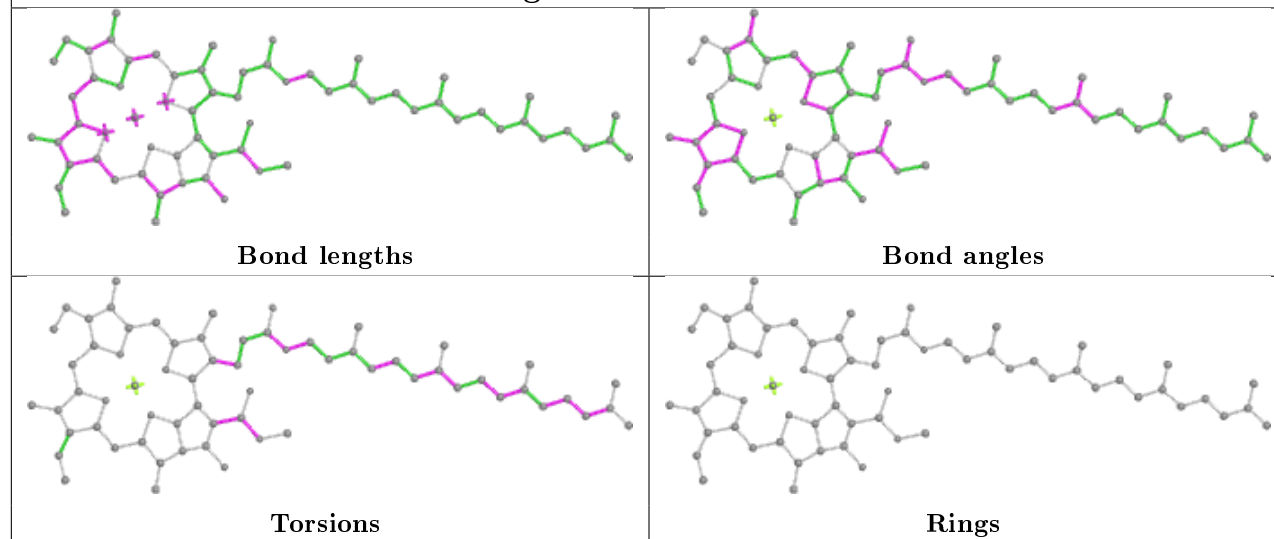




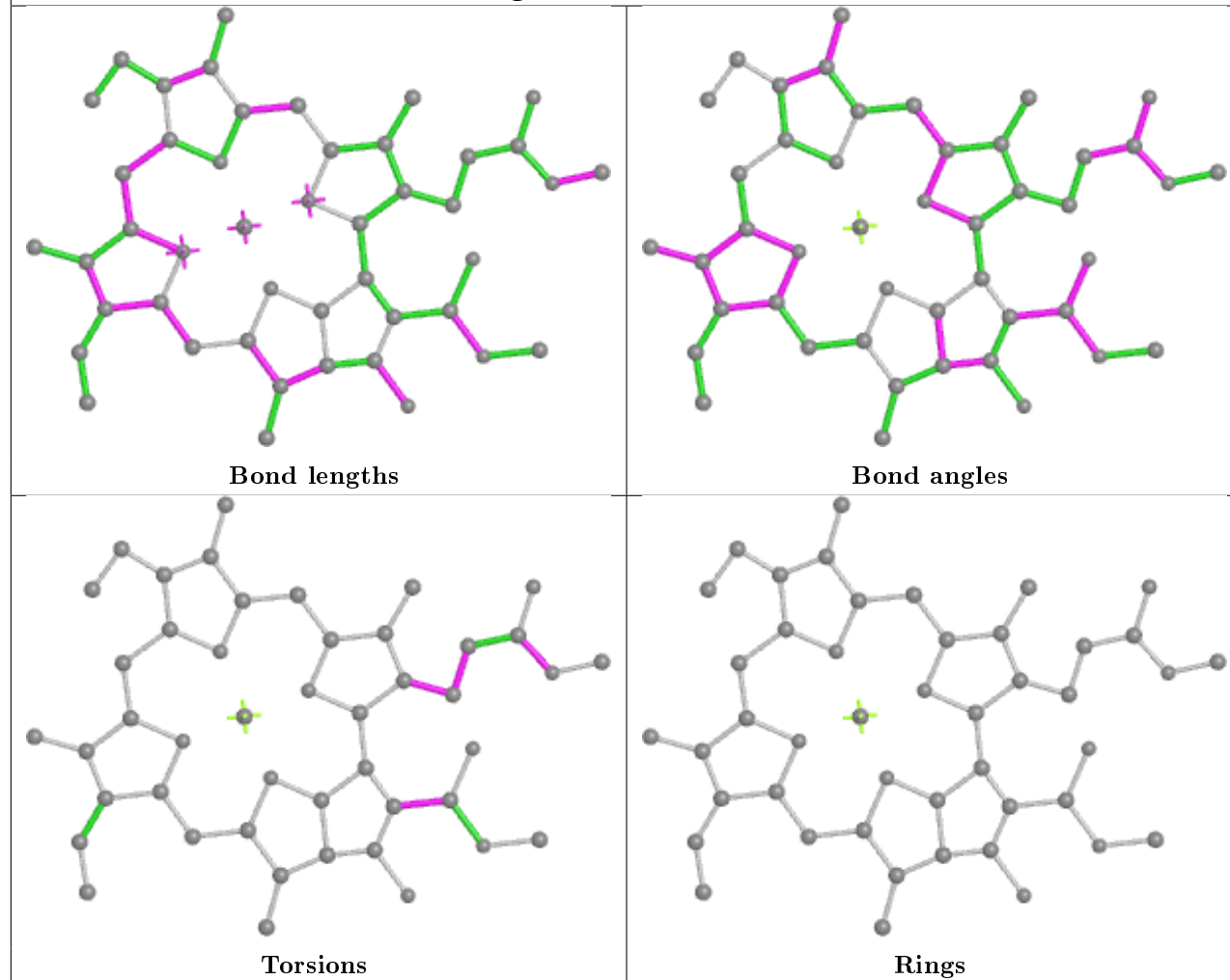


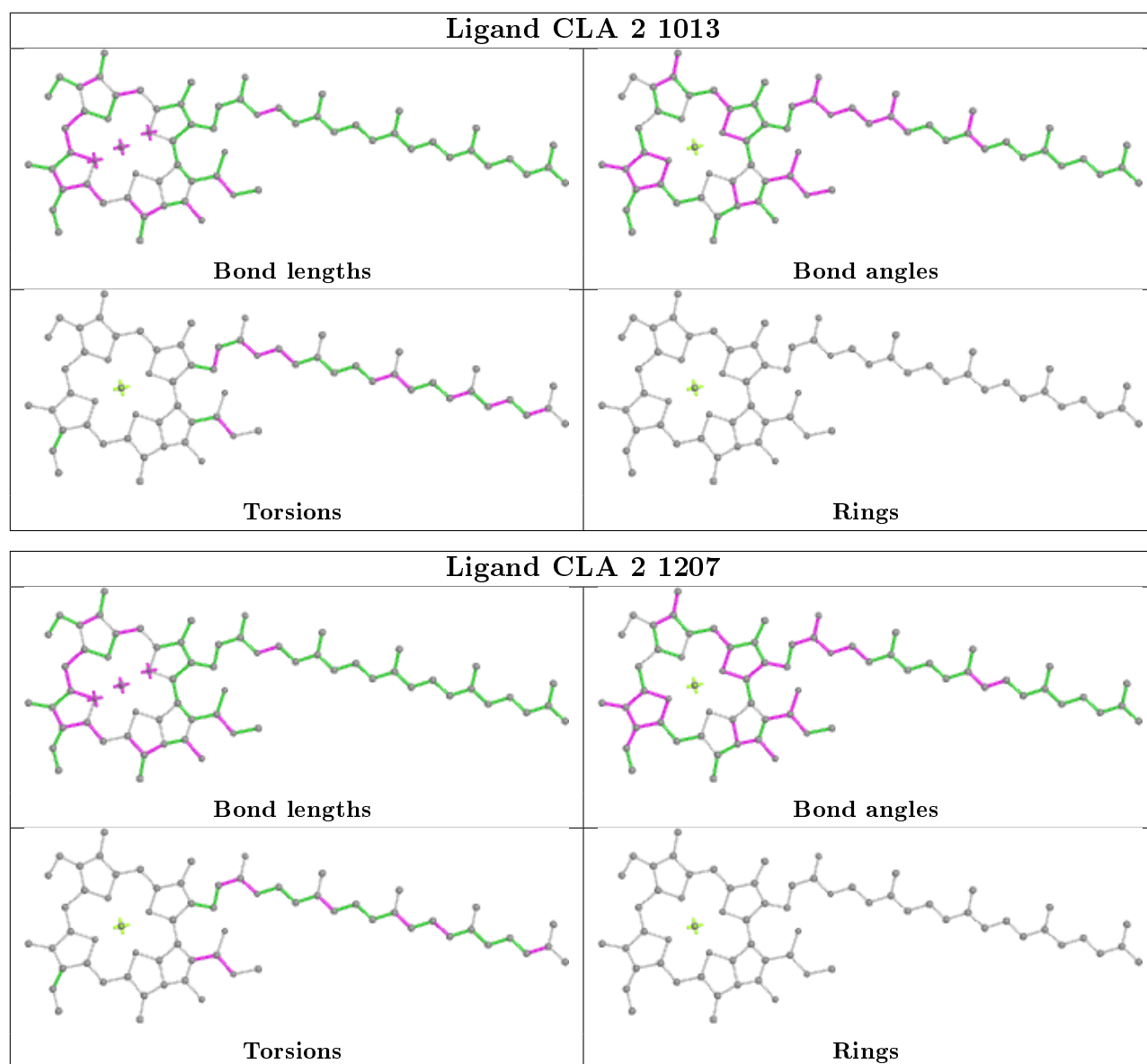


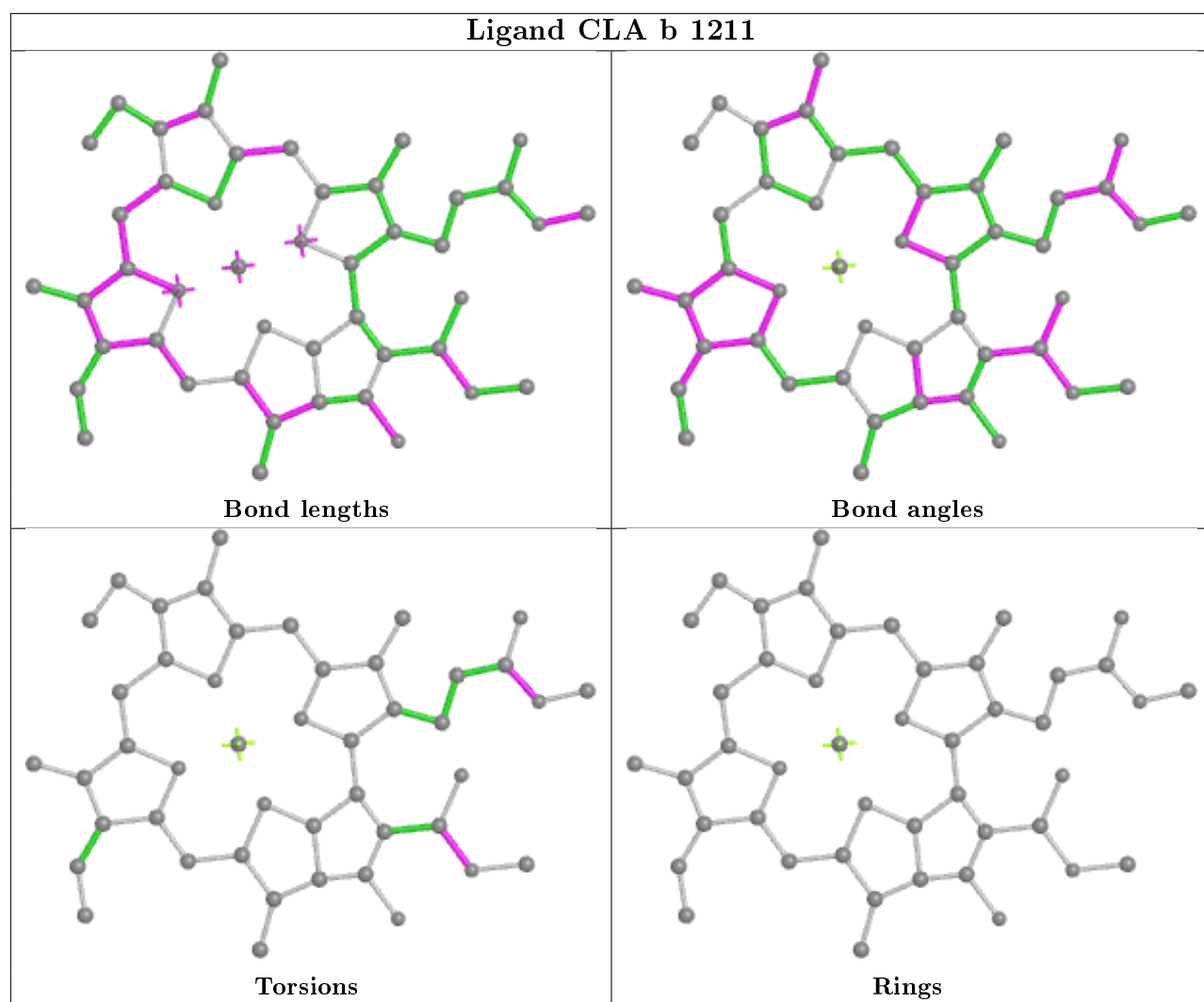
## Ligand CLA A 1102

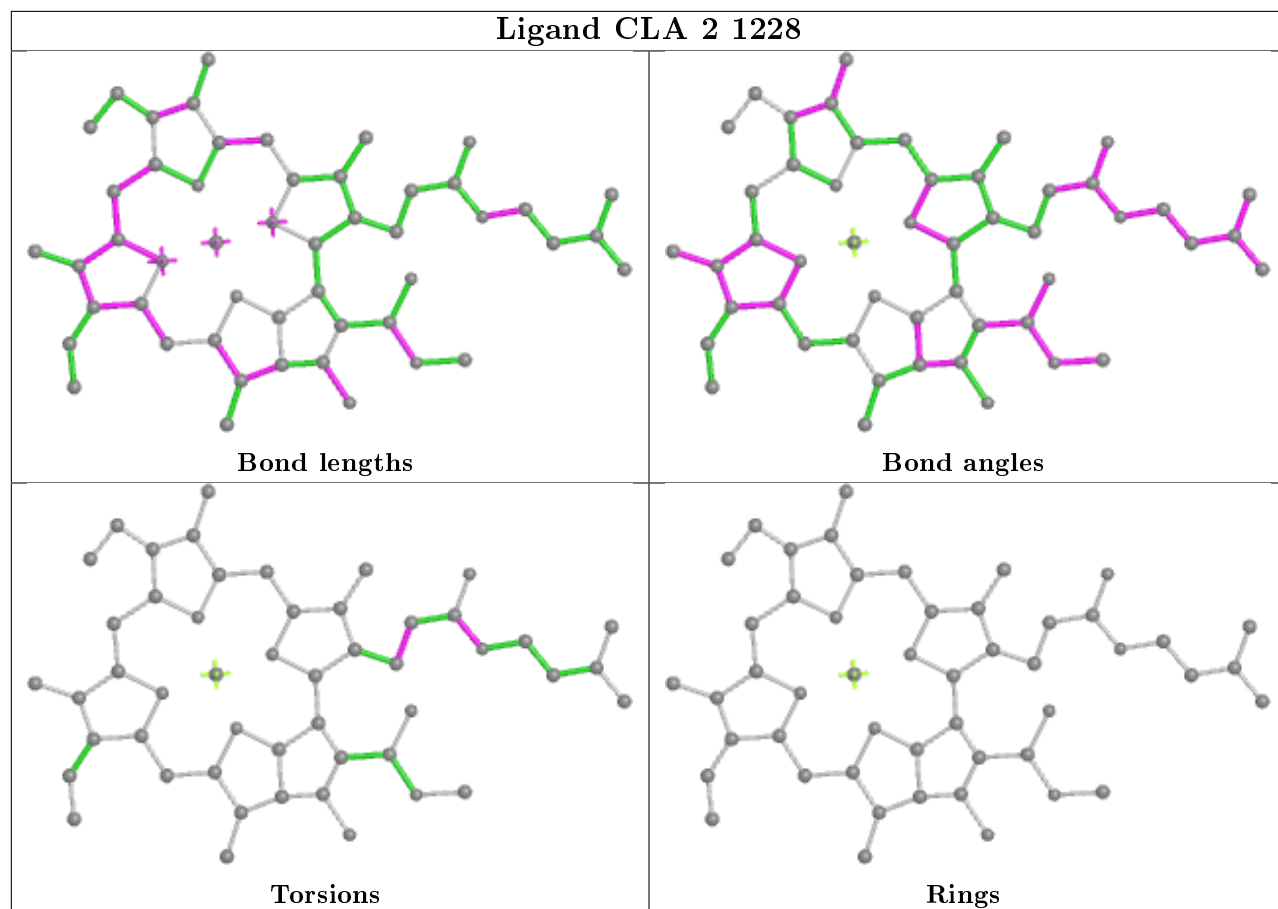


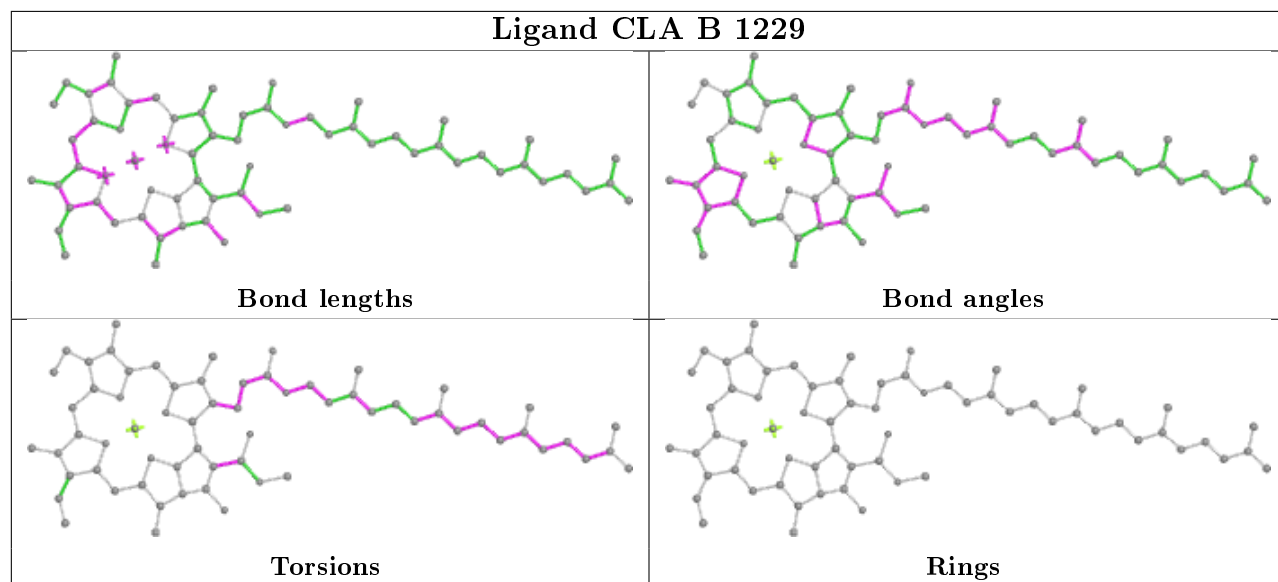
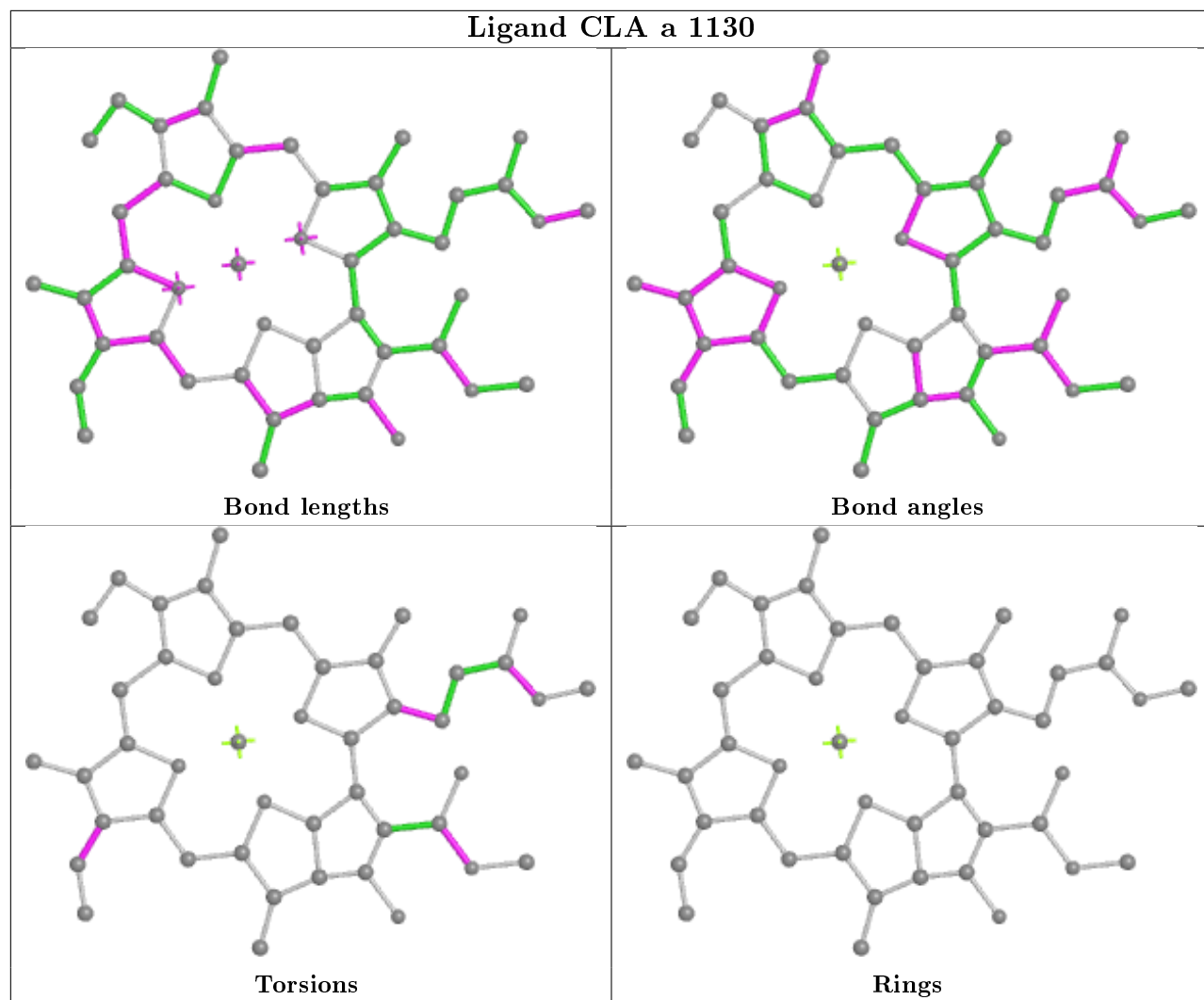
## Ligand CLA a 1129

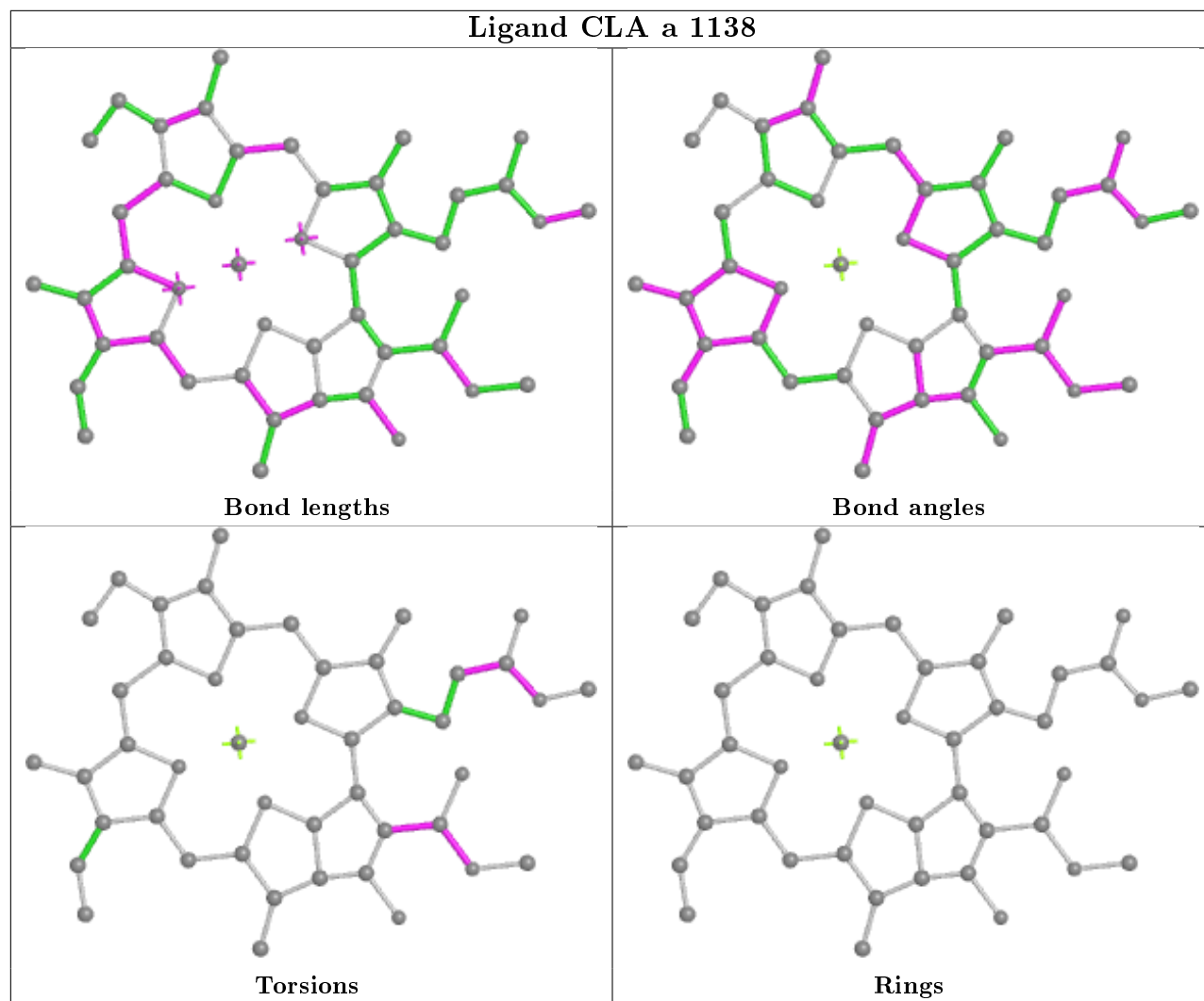
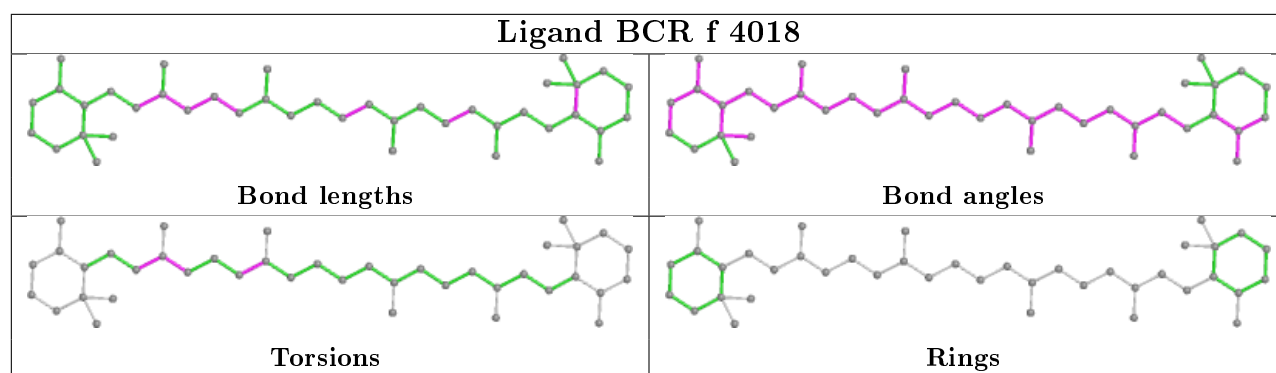




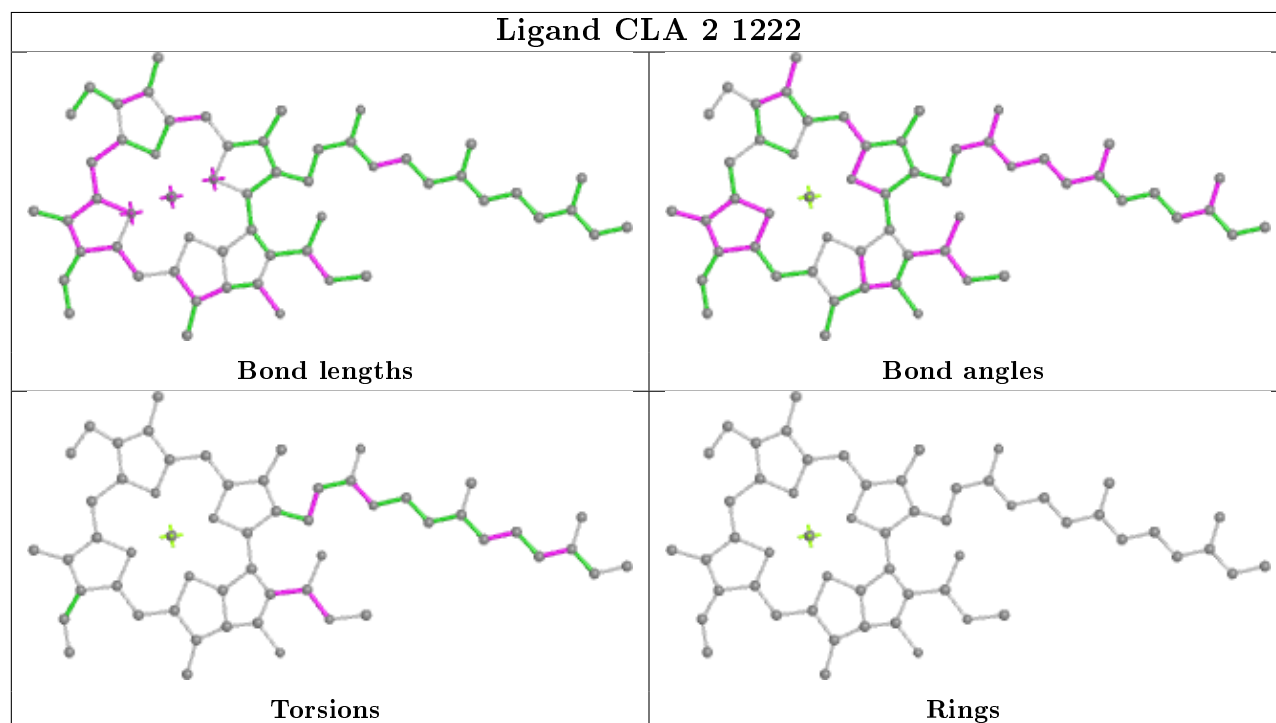
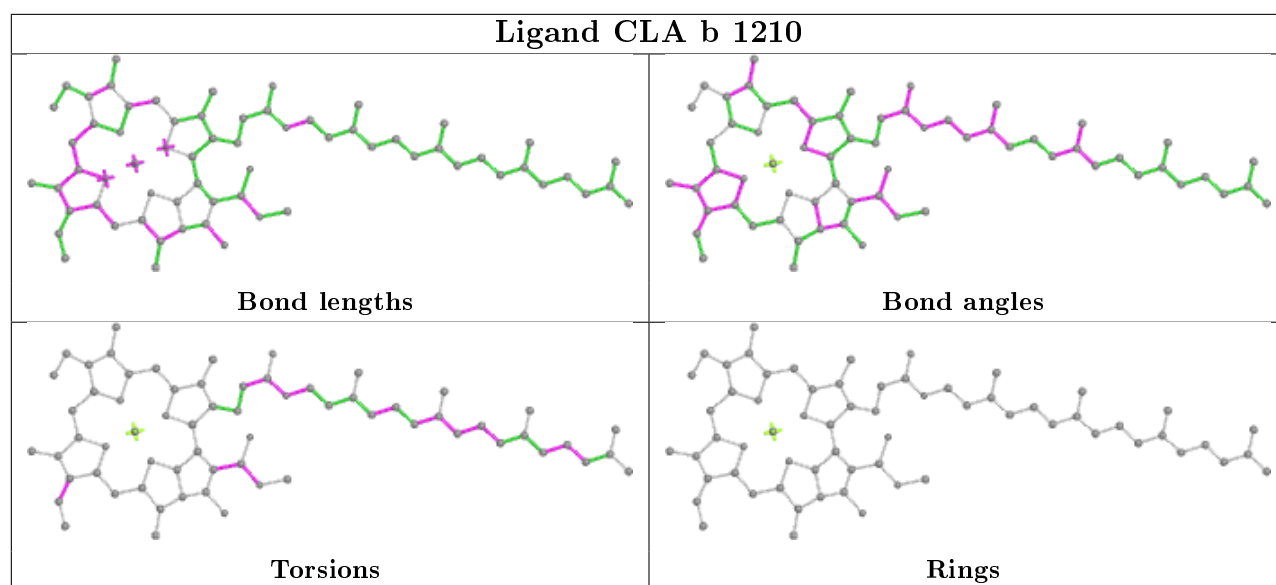




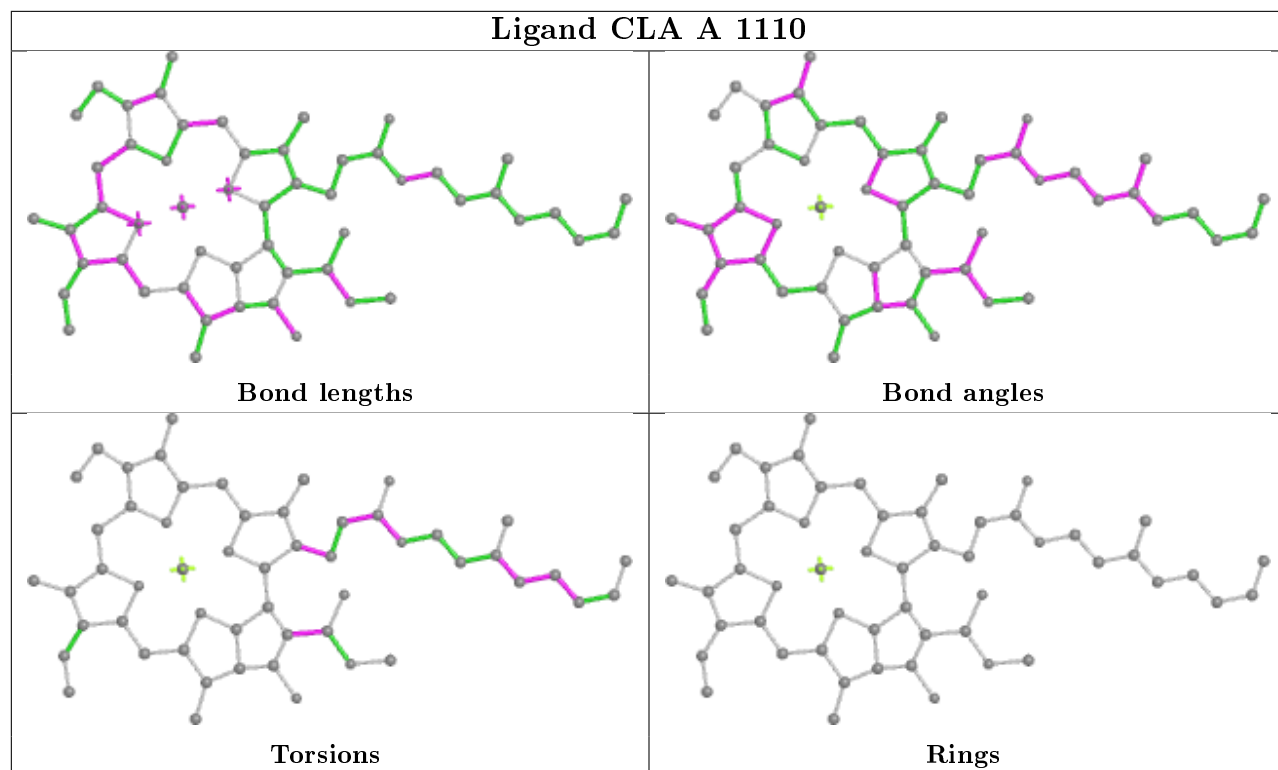




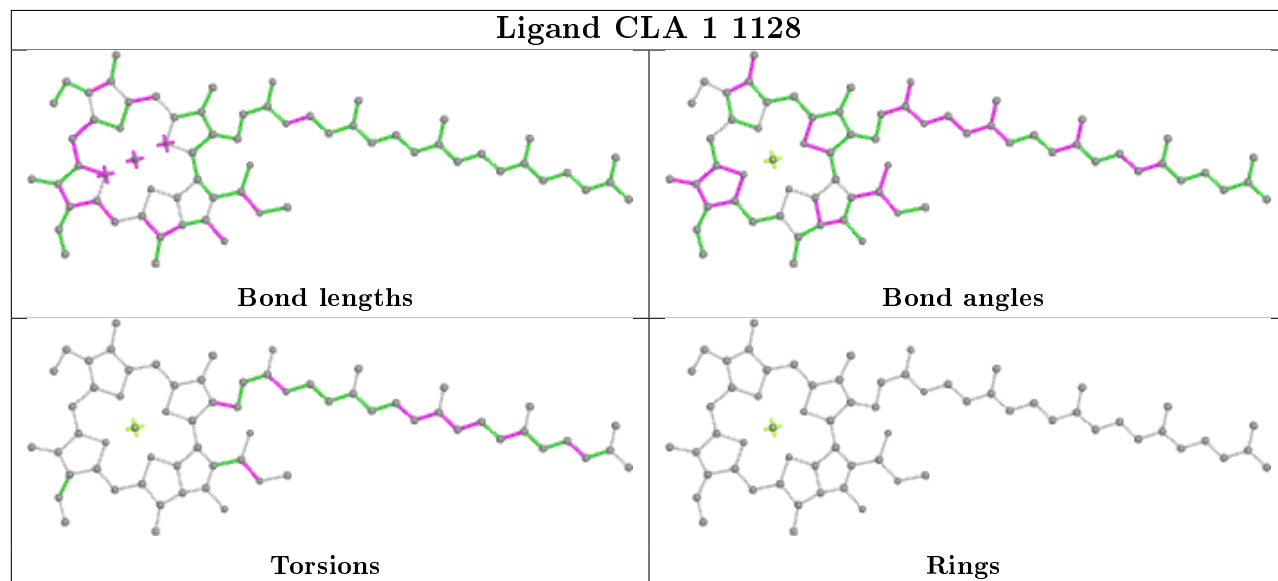


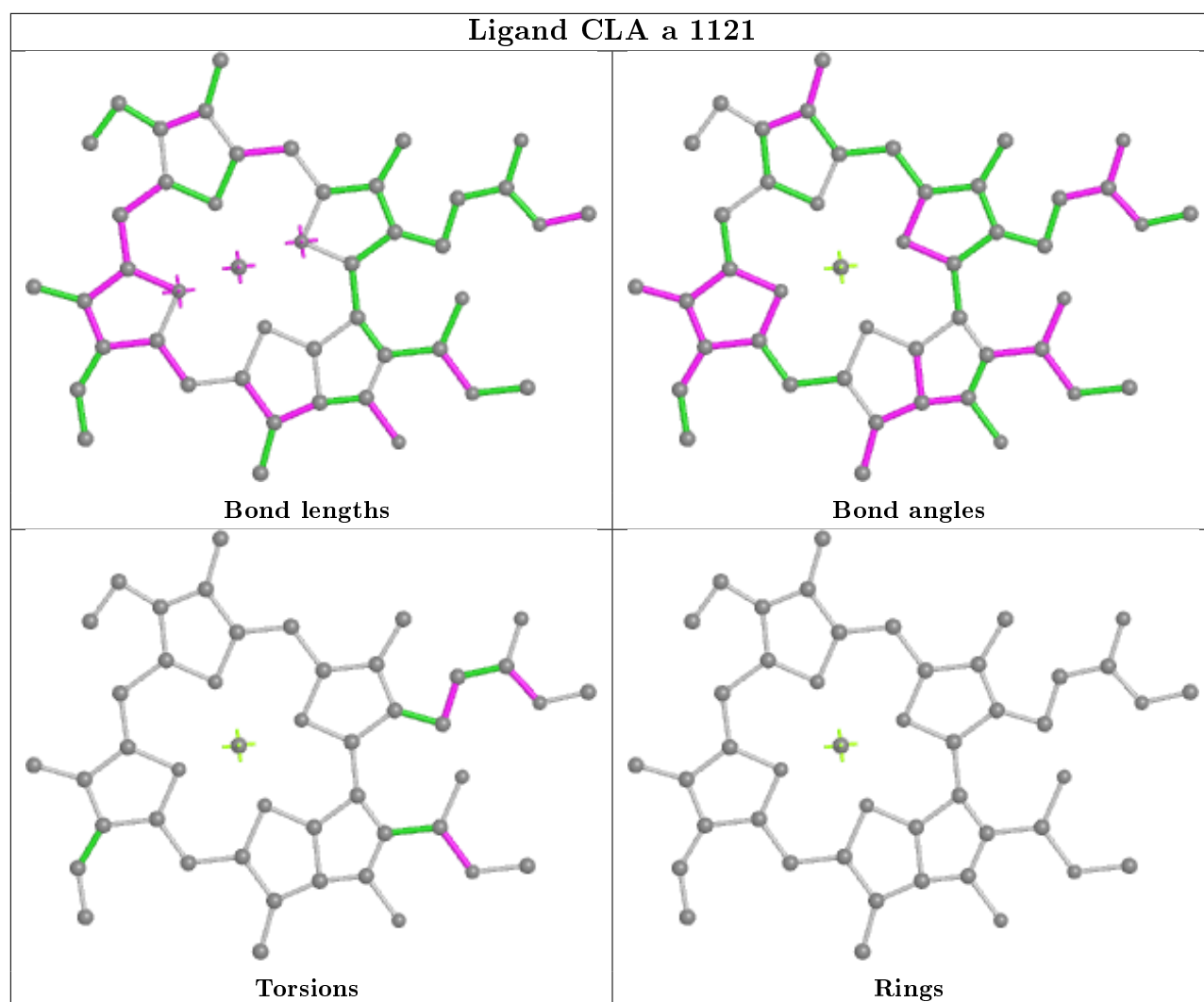


## Ligand CLA A 1110



## Ligand CLA 1 1128





## 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

Unable to reproduce the depositors R factor - this section is therefore empty.

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

Unable to reproduce the depositors R factor - this section is therefore empty.

### 6.3 Carbohydrates

Unable to reproduce the depositors R factor - this section is therefore empty.

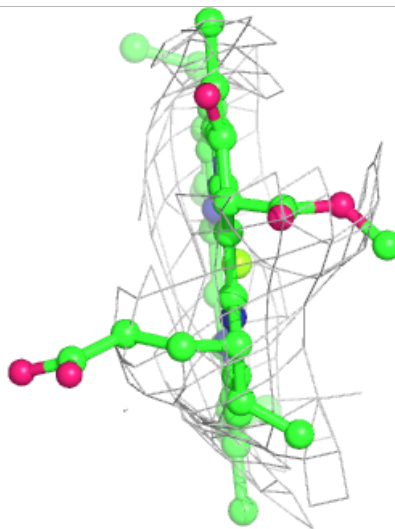
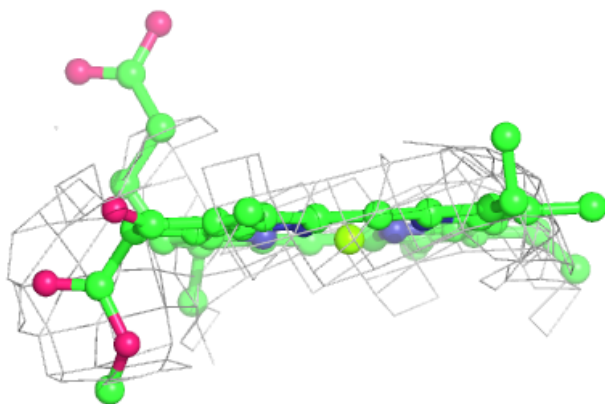
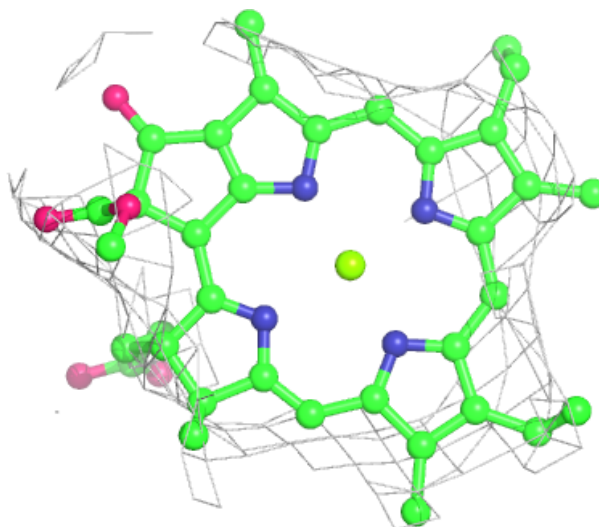
### 6.4 Ligands

Unable to reproduce the depositors R factor - this section is therefore empty.

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.

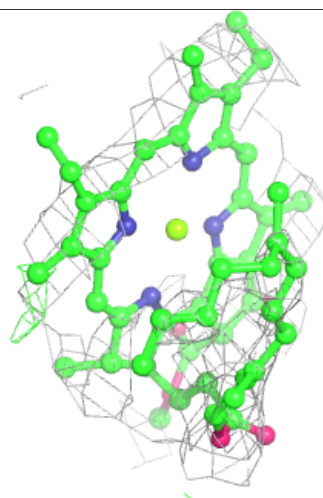
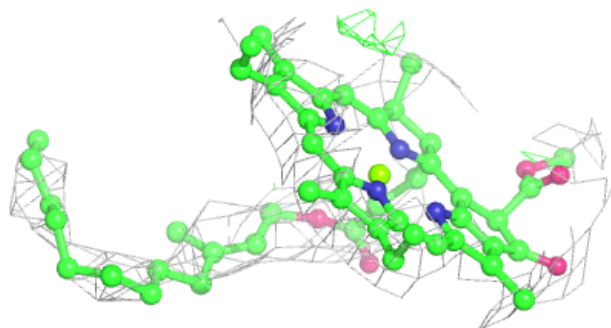
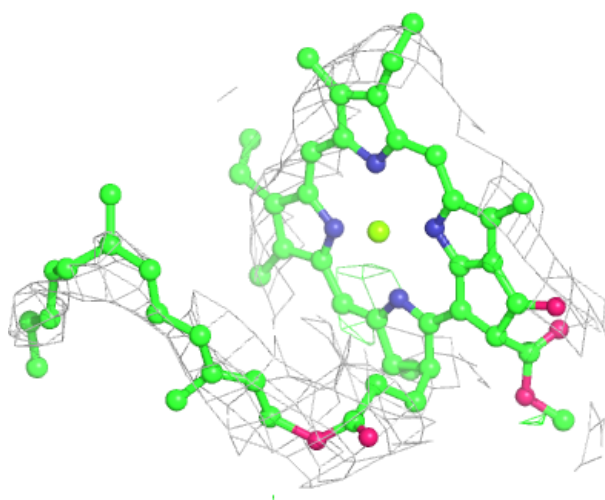
**Electron density around CLA 2 1218:**

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



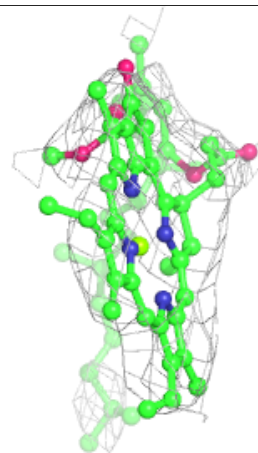
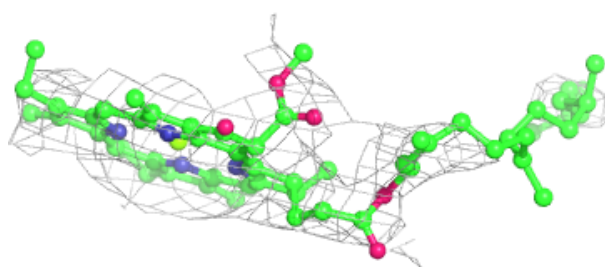
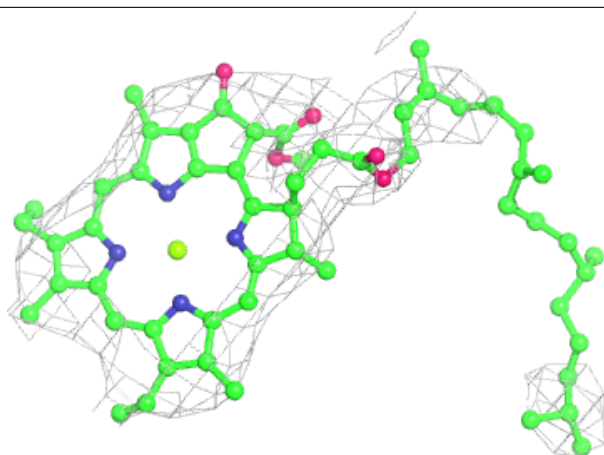
**Electron density around CLA a 1122:**

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



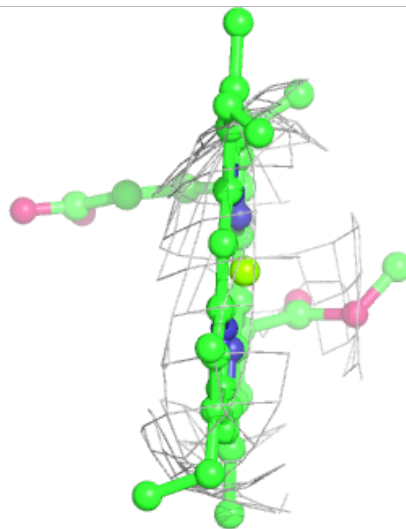
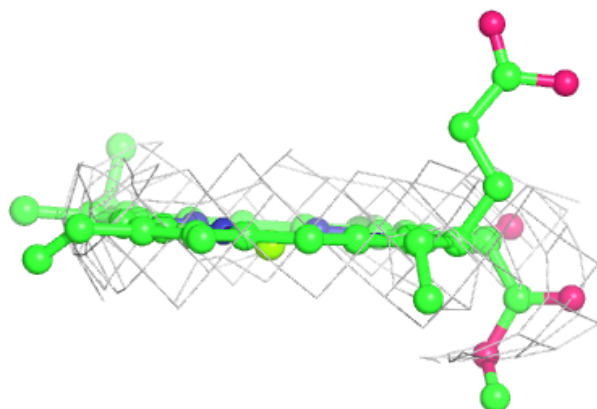
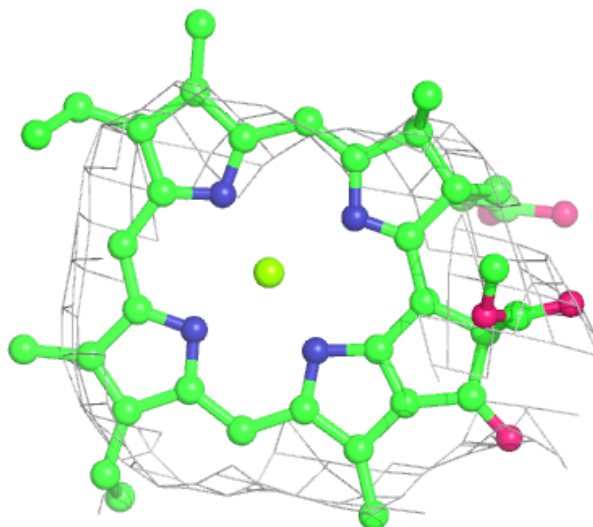
**Electron density around CLA A 1101:**

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



**Electron density around CLA b 1218:**

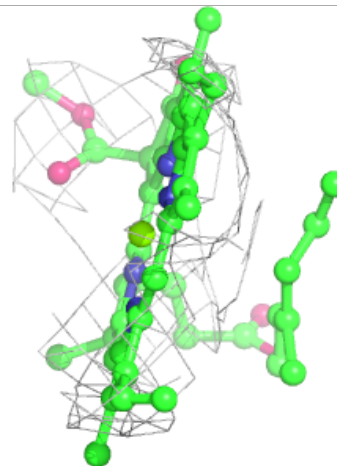
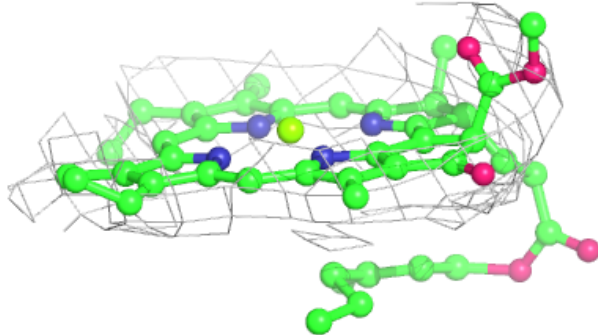
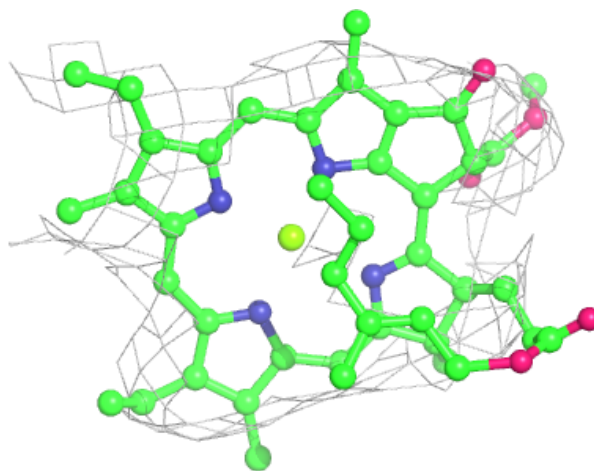
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





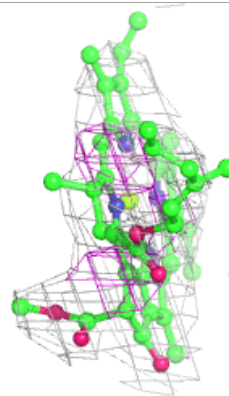
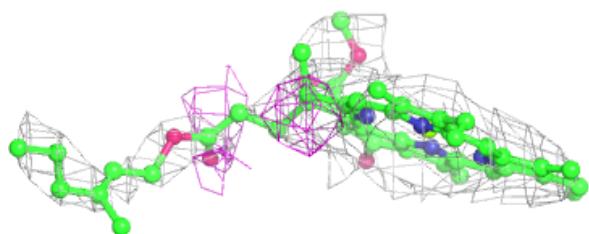
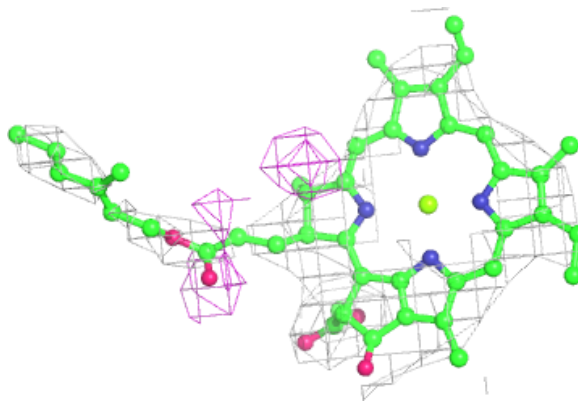
**Electron density around CLA 1 1801:**

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

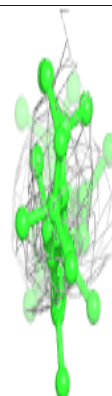
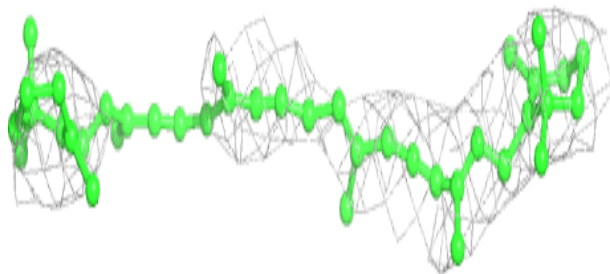
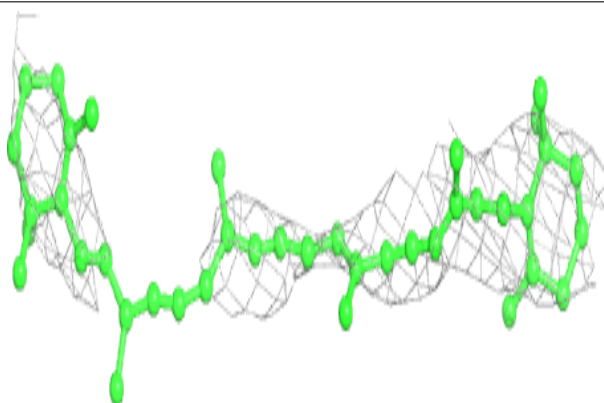


**Electron density around CLA A 1125:**

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

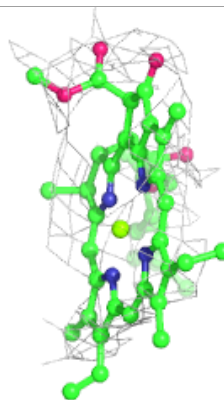
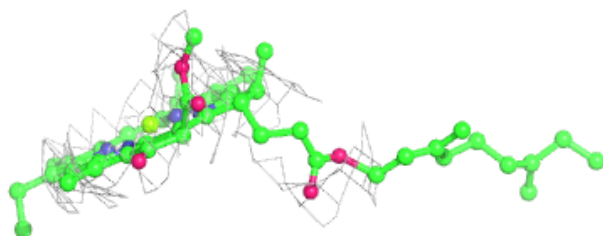
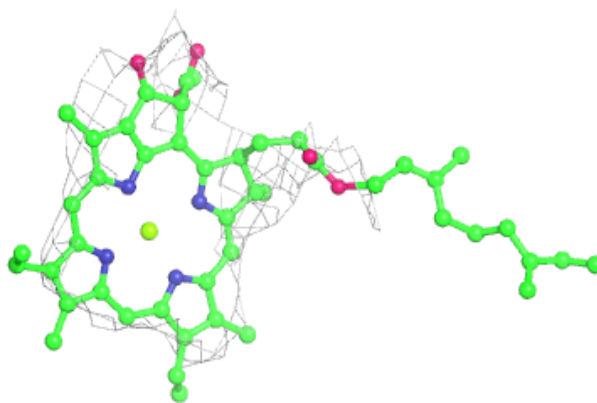
**Electron density around BCR 1 4008:**

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

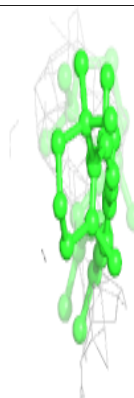
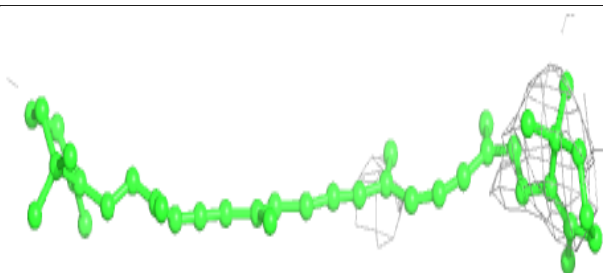
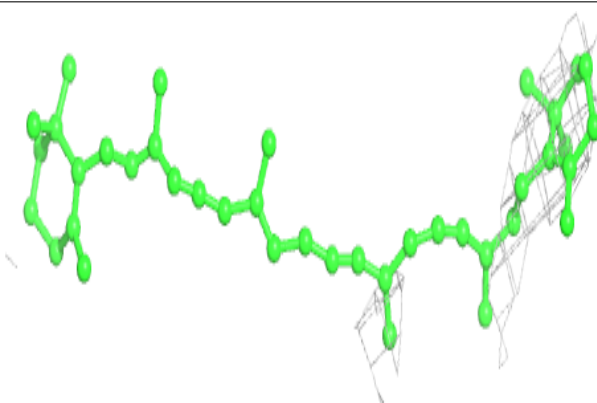


**Electron density around CLA b 1222:**

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

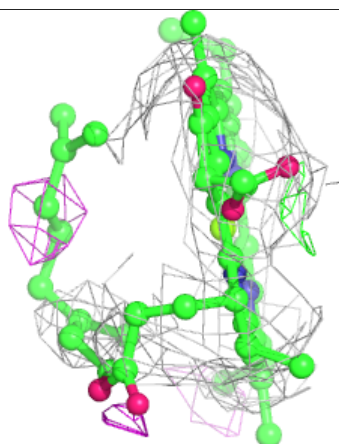
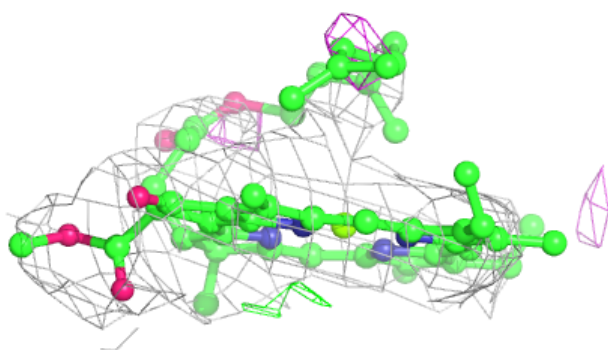
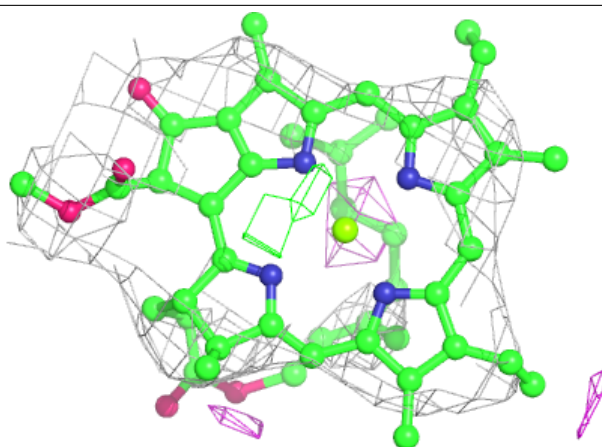
**Electron density around BCR b 4010:**

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



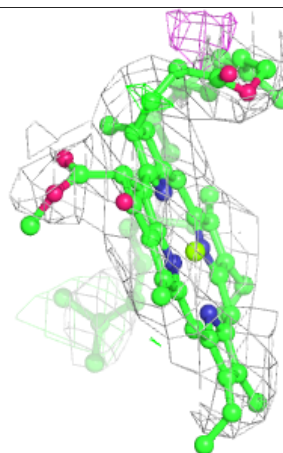
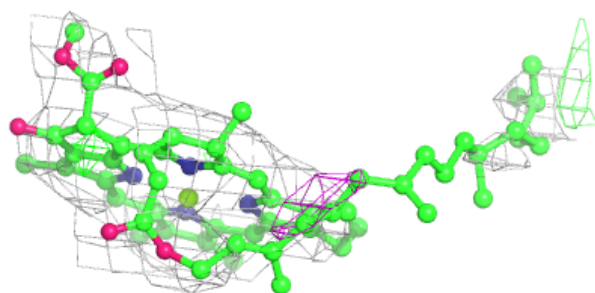
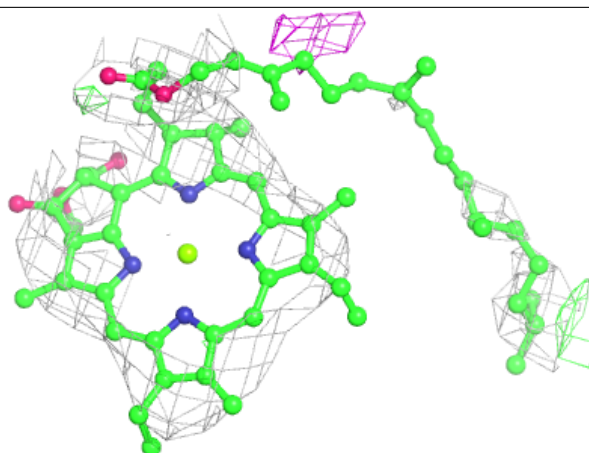
**Electron density around CLA 2 1224:**

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

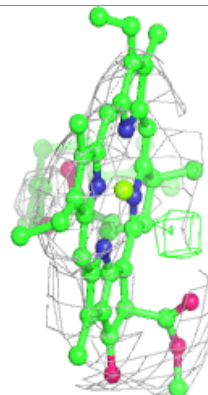
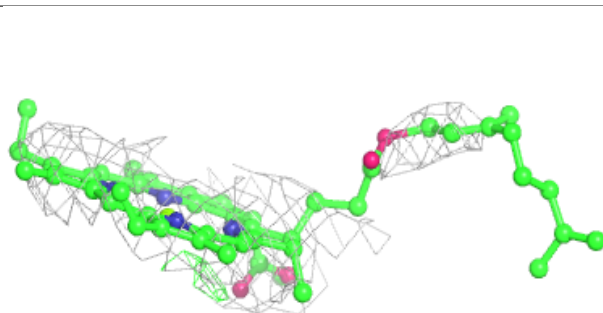
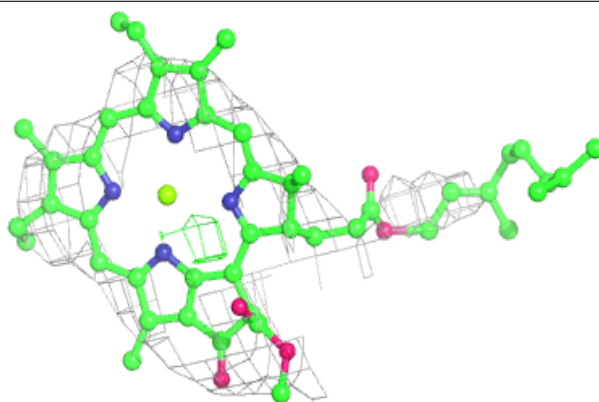


**Electron density around CLA K 1401:**

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

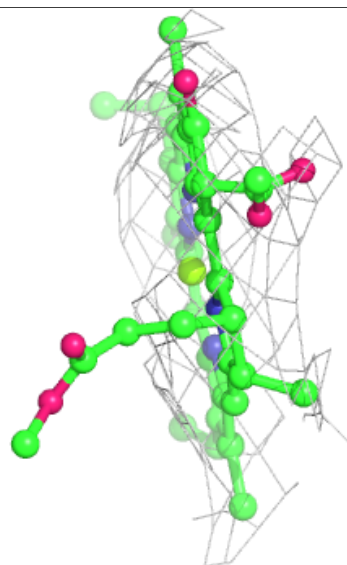
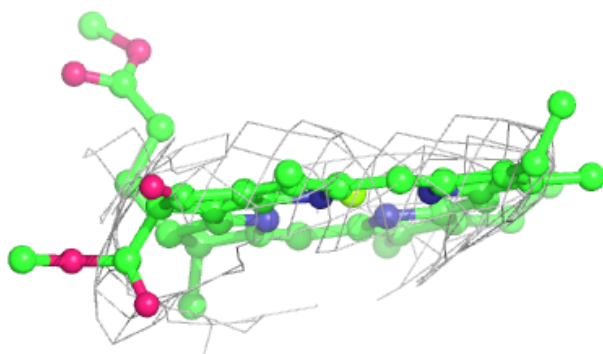
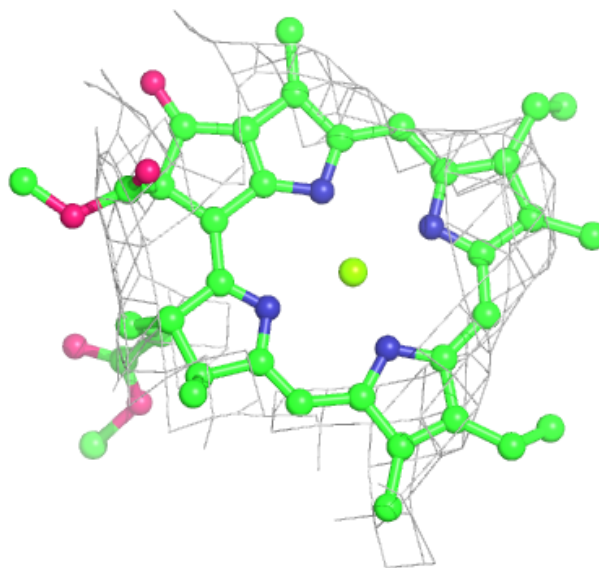
**Electron density around CLA a 1124:**

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



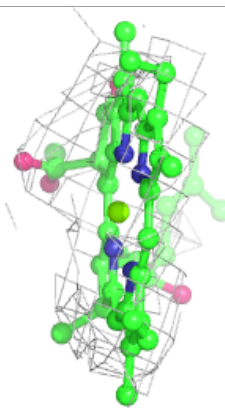
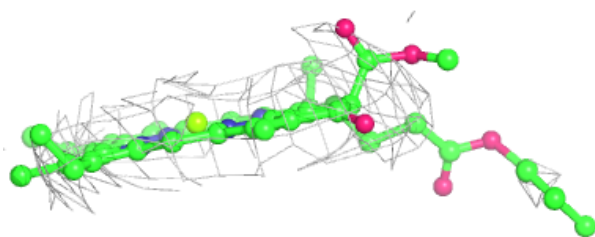
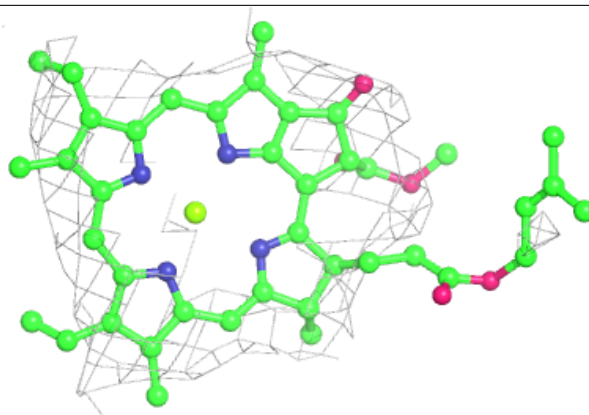
**Electron density around CLA 1 1133:**

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

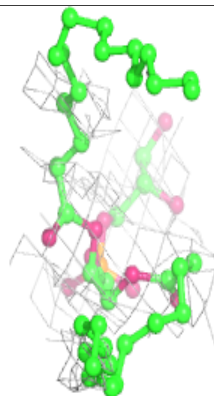
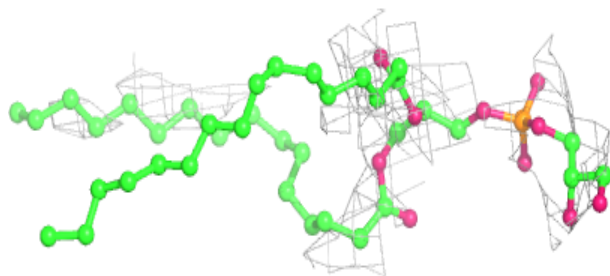
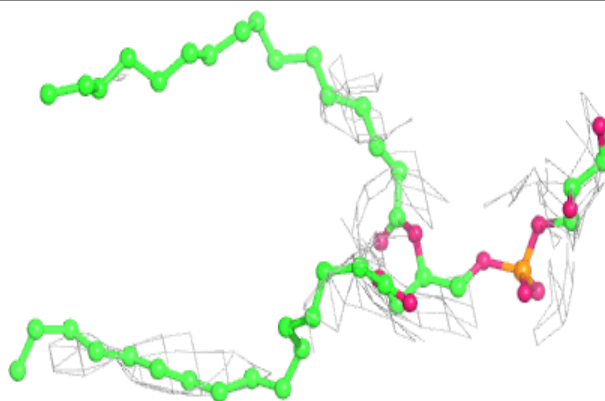


**Electron density around CLA 1 1139:**

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

**Electron density around LHG 1 5001:**

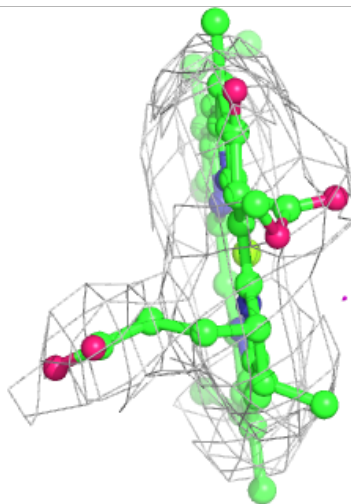
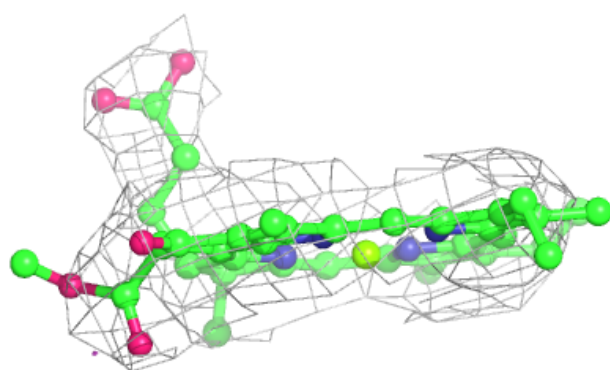
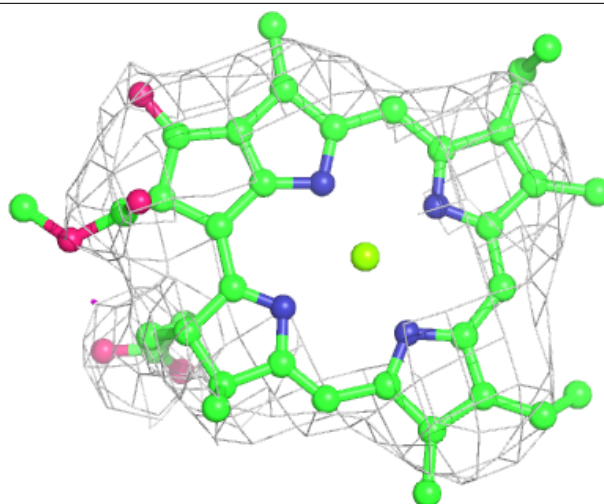
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





**Electron density around CLA 2 1208:**

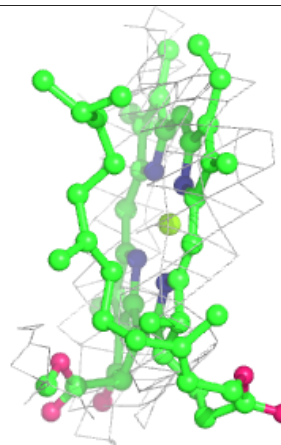
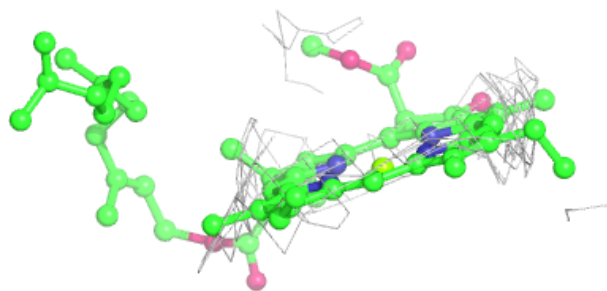
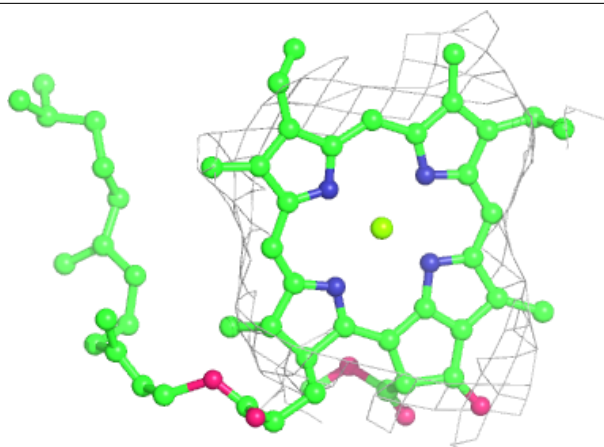
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





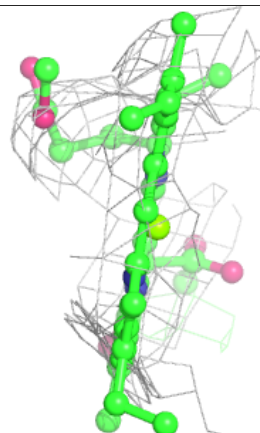
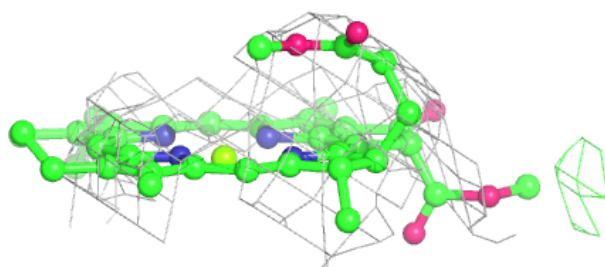
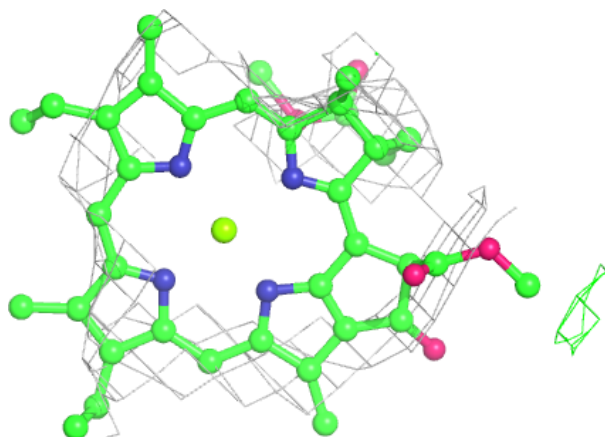
**Electron density around CLA 1 1111:**

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

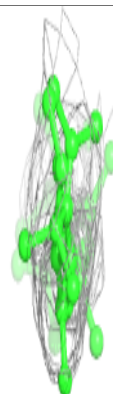
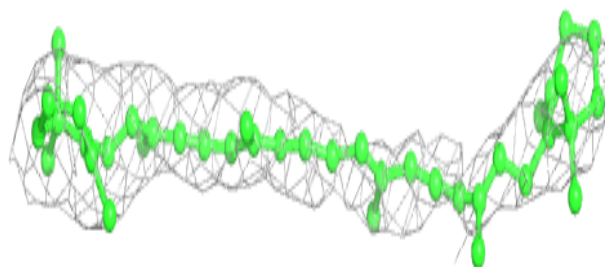
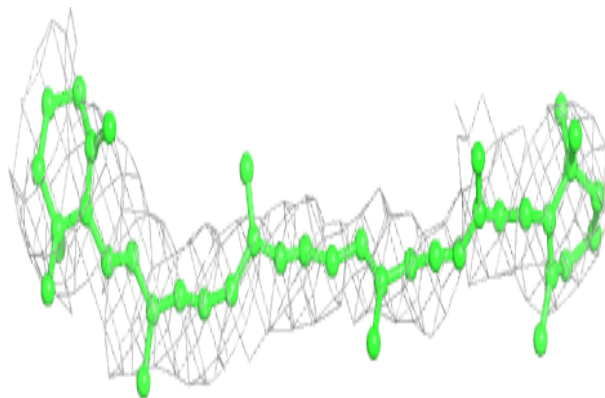


**Electron density around CLA a 1114:**

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

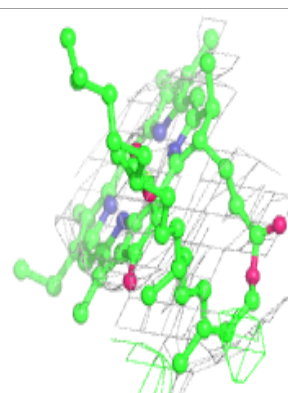
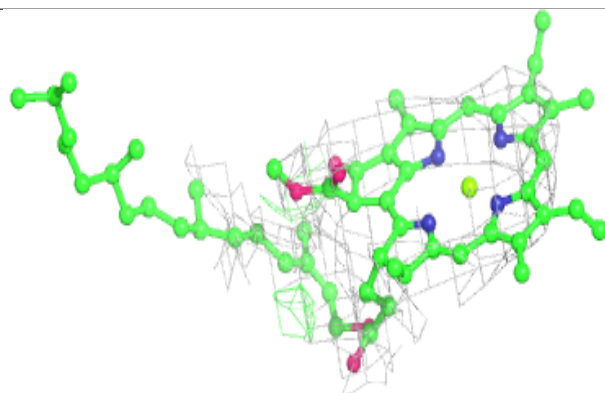
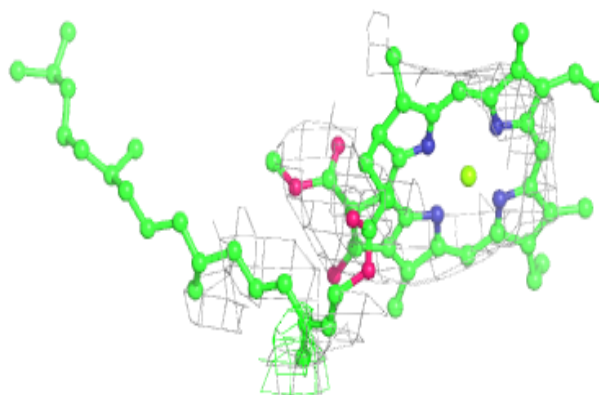
**Electron density around BCR a 4008:**

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

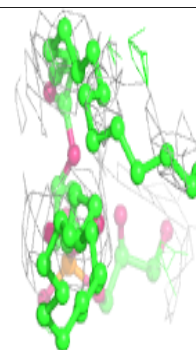
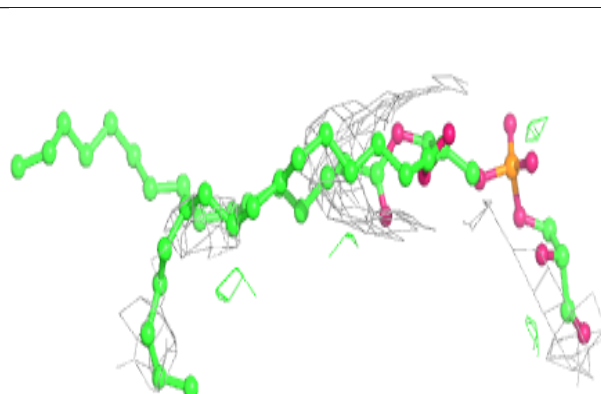
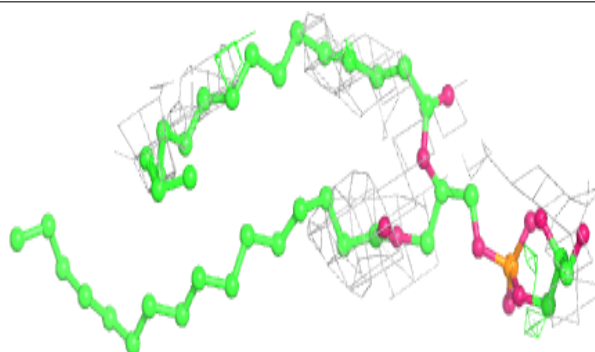


**Electron density around CLA b 1213:**

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

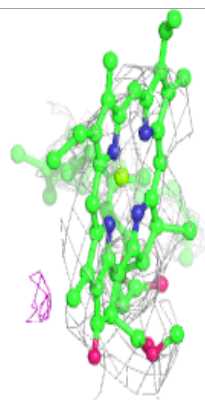
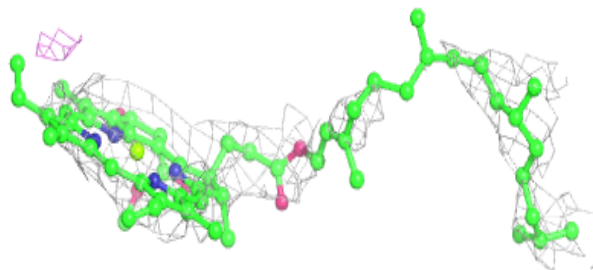
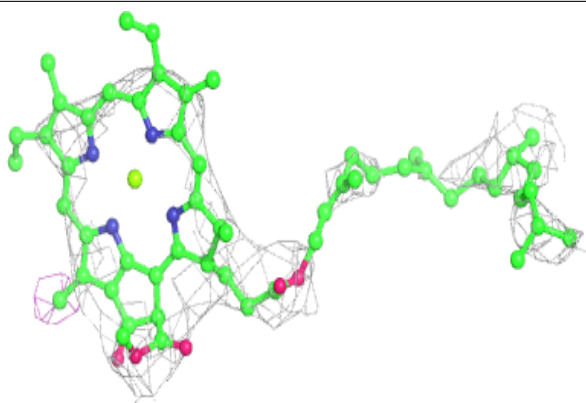
**Electron density around LHG a 5003:**

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

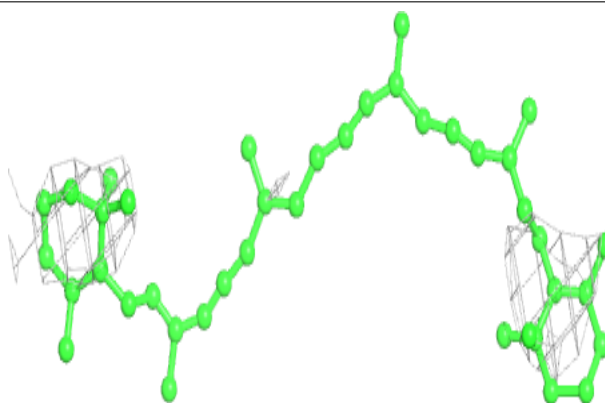


**Electron density around CLA B 1210:**

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

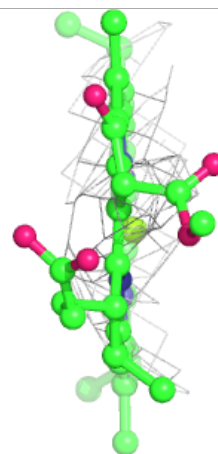
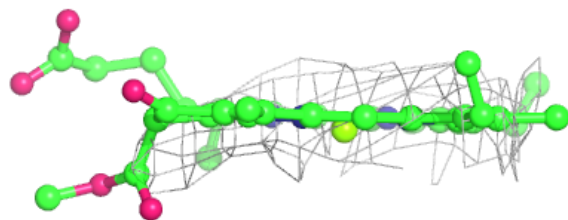
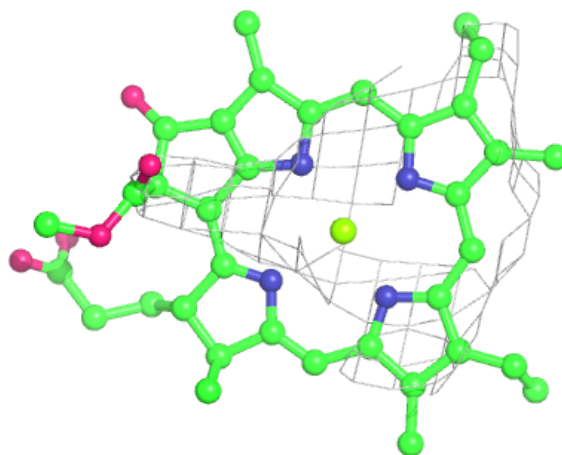
**Electron density around BCR b 4011:**

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



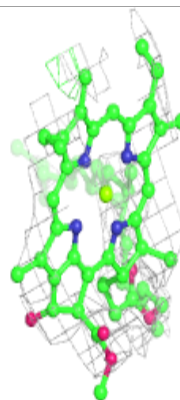
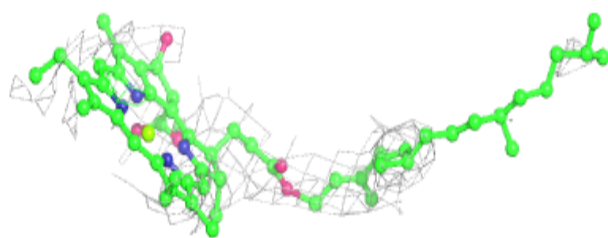
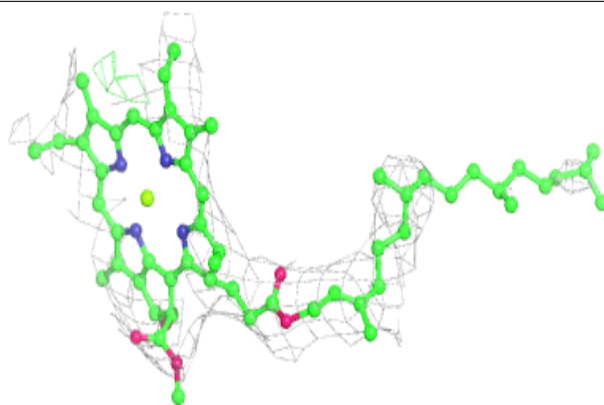
**Electron density around CLA b 1240:**

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



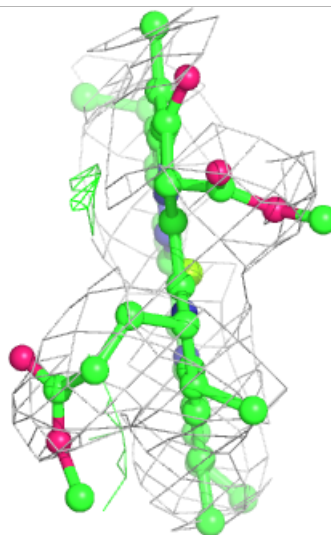
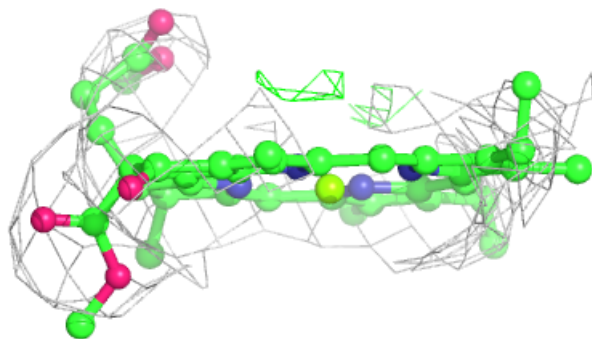
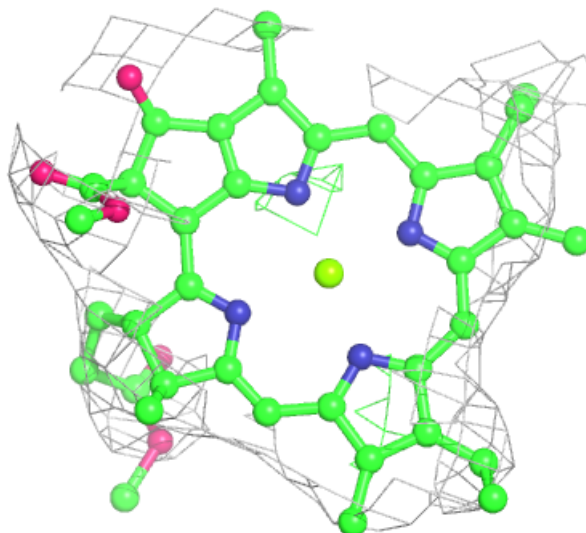
**Electron density around CLA a 1022:**

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



**Electron density around CLA A 1120:**

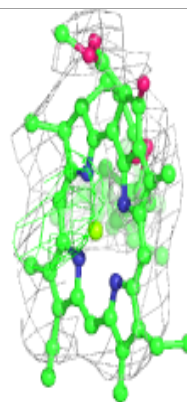
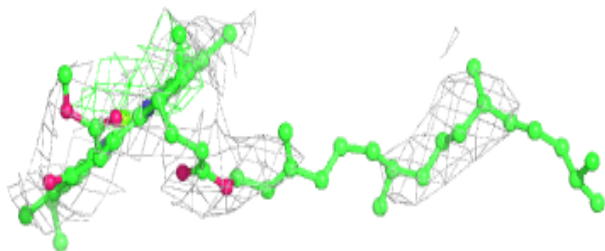
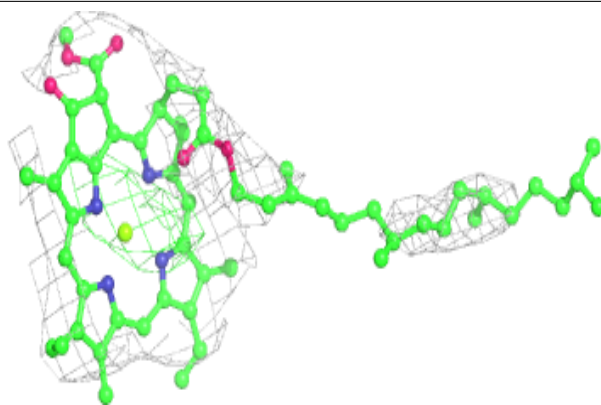
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



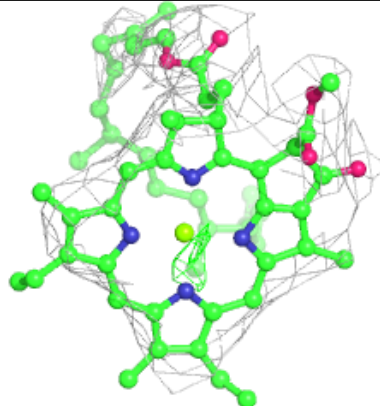
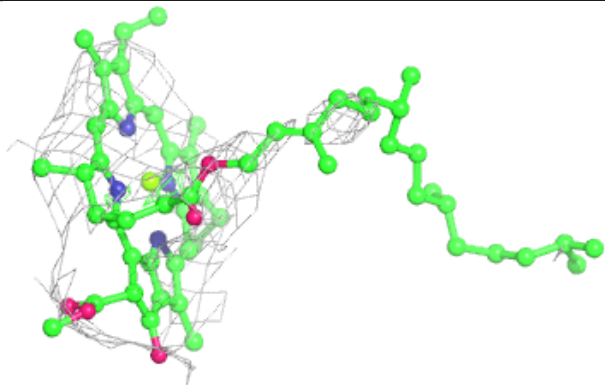
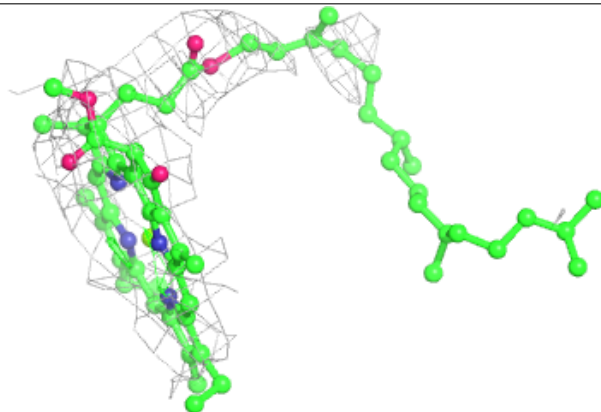


**Electron density around CLA 8 1501:**

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

**Electron density around CLA B 1216:**

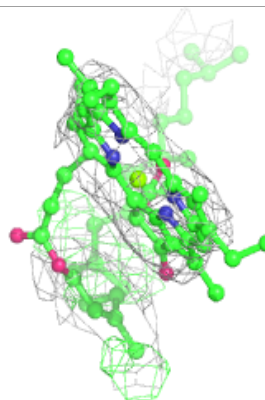
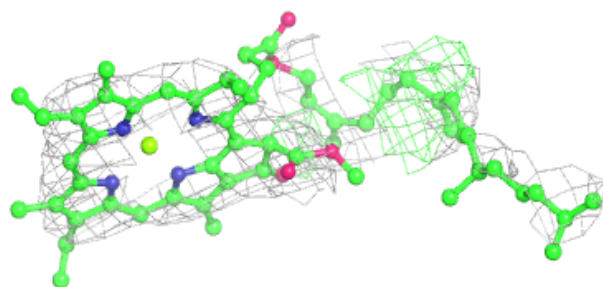
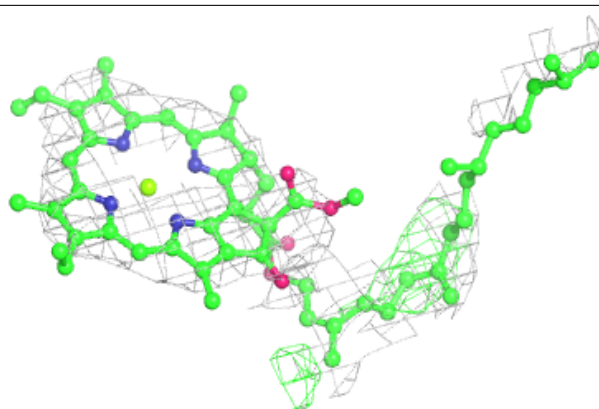
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





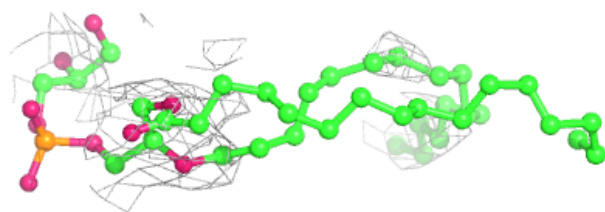
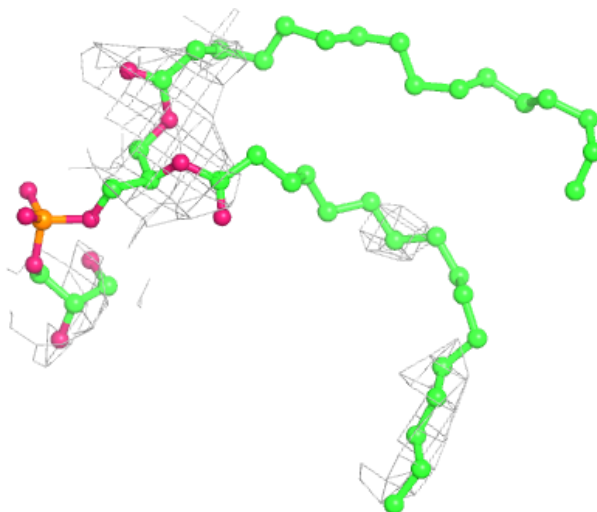
**Electron density around CLA B 1213:**

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



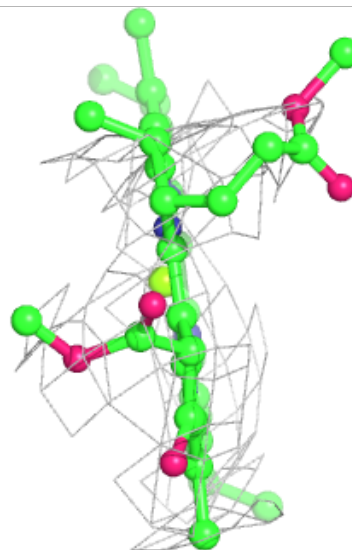
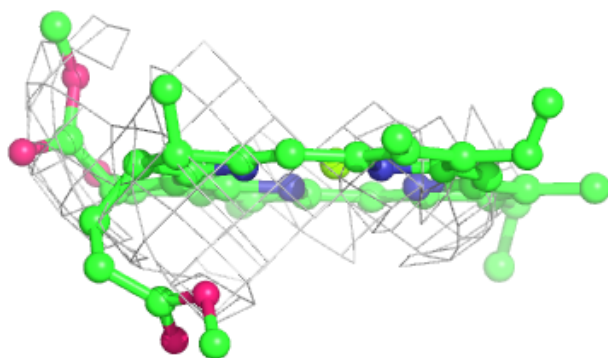
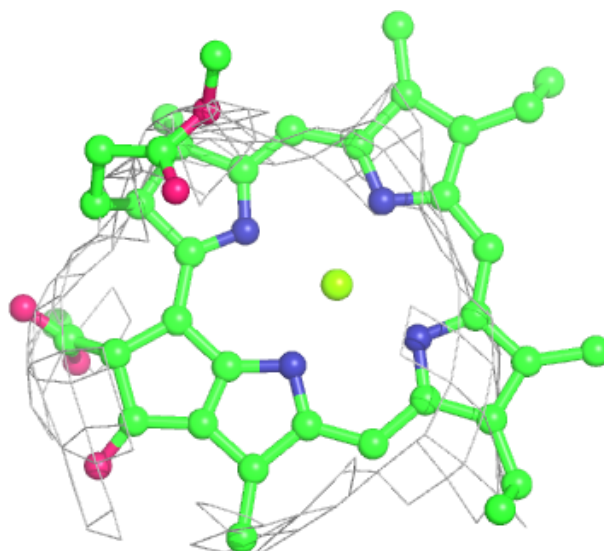
**Electron density around LHG B 5004:**

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



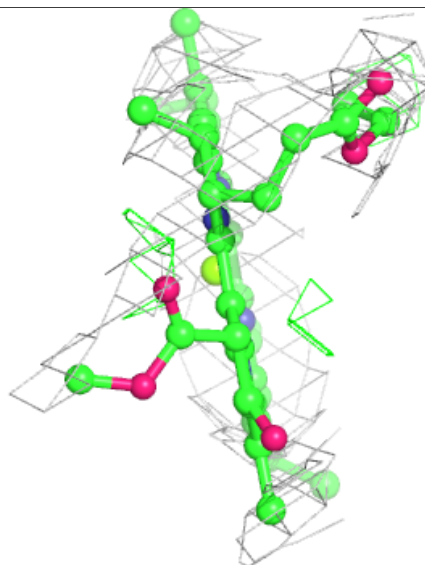
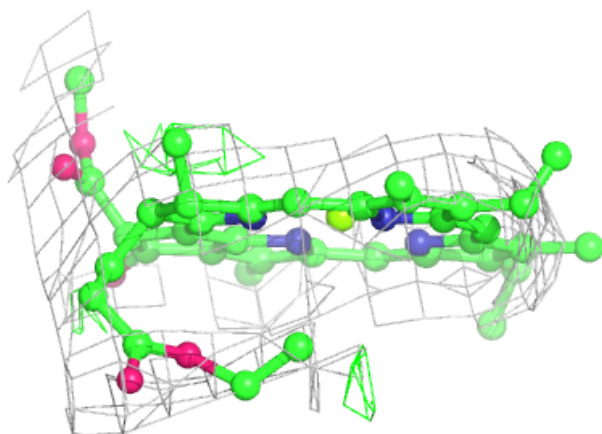
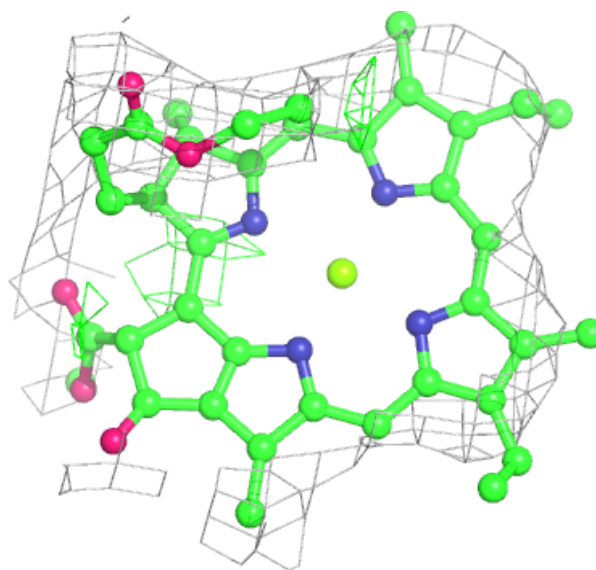
**Electron density around CLA 1 1120:**

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



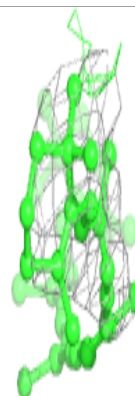
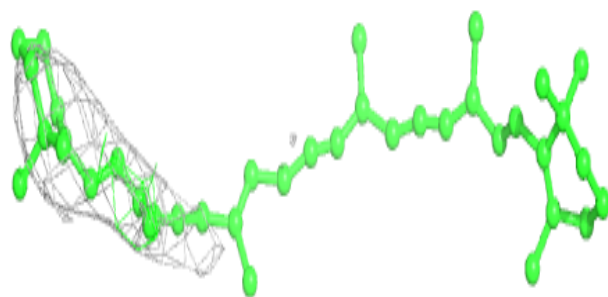
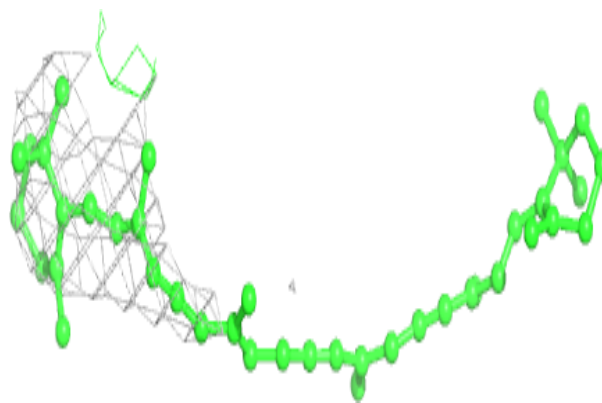
**Electron density around CLA 2 1217:**

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



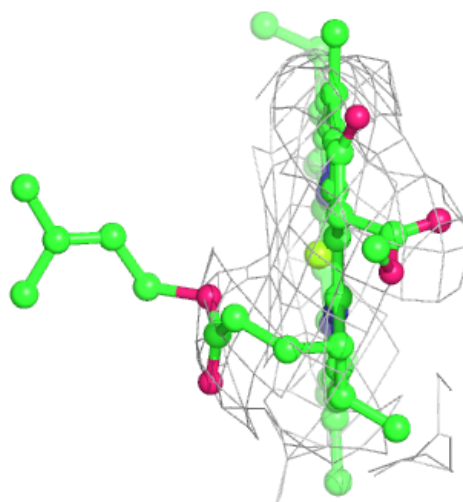
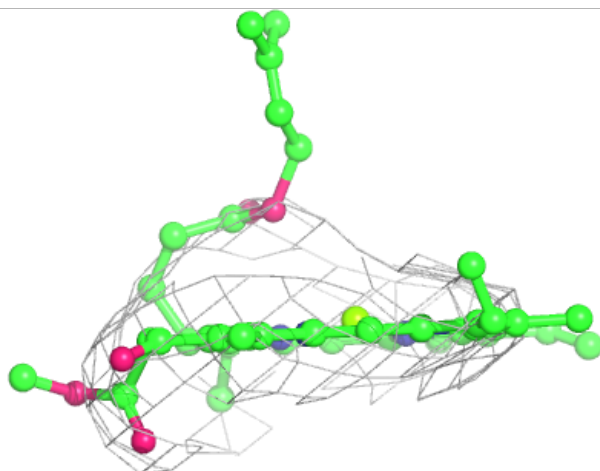
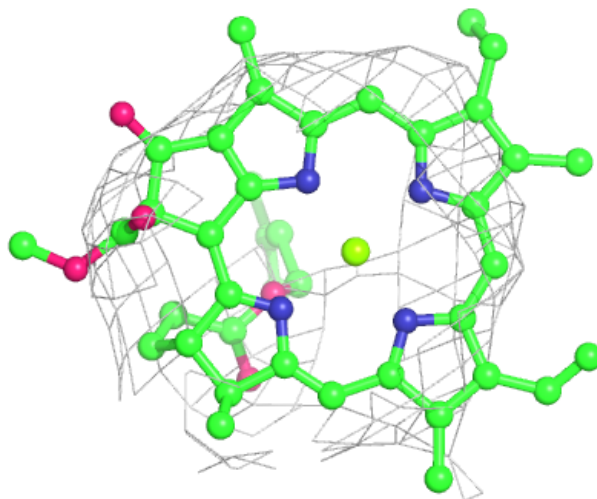
**Electron density around BCR 2 4014:**

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



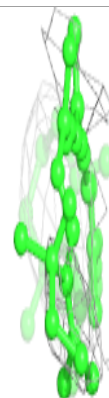
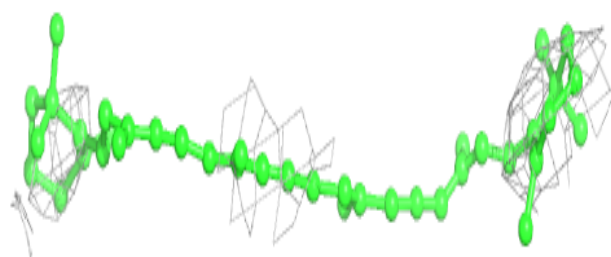
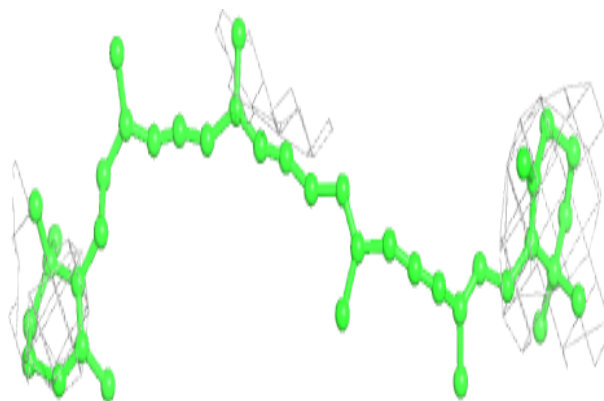
**Electron density around CLA K 1402:**

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



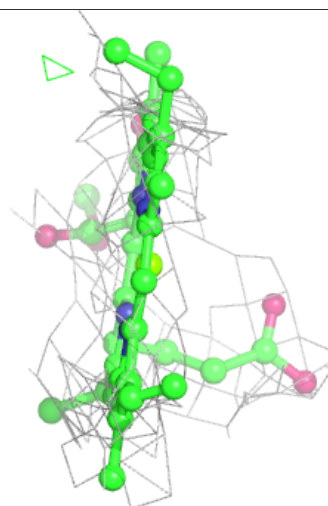
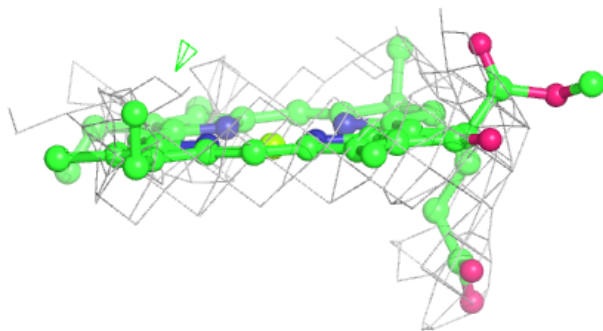
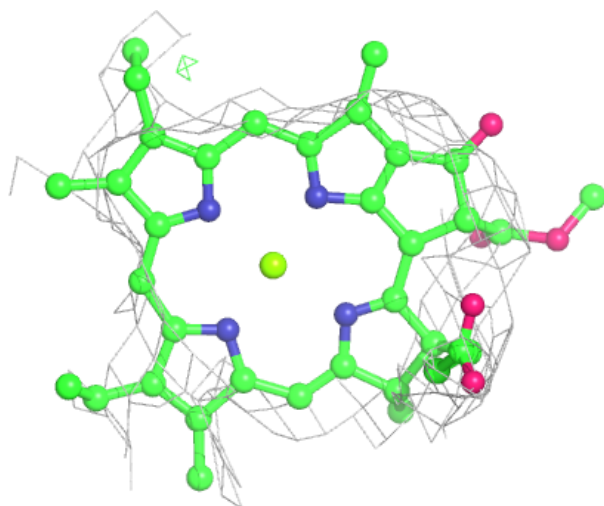
**Electron density around BCR b 4004:**

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



**Electron density around CLA 1 1108:**

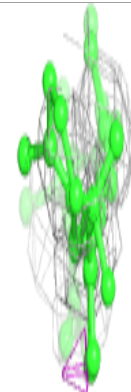
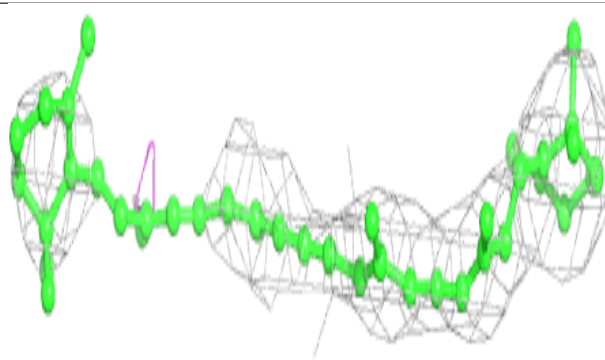
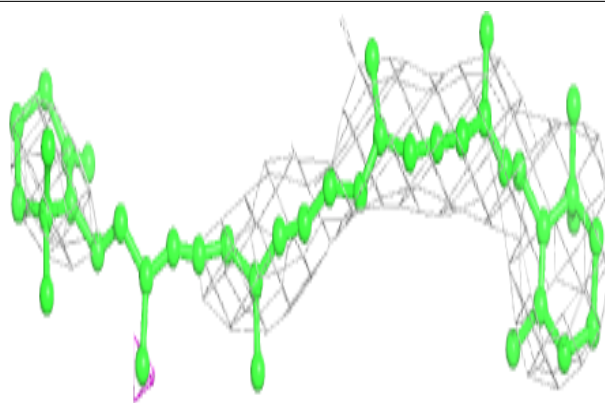
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



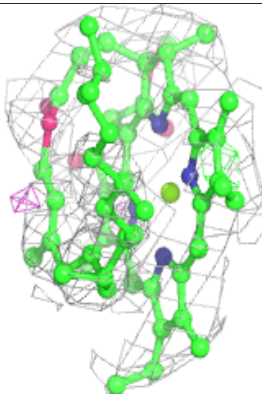
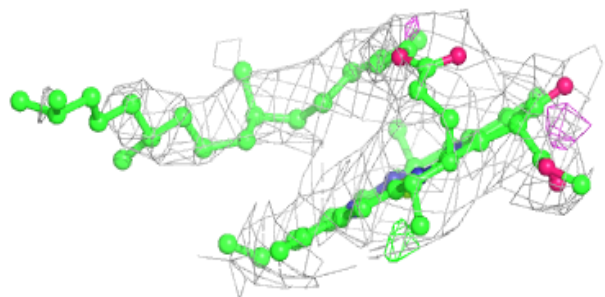
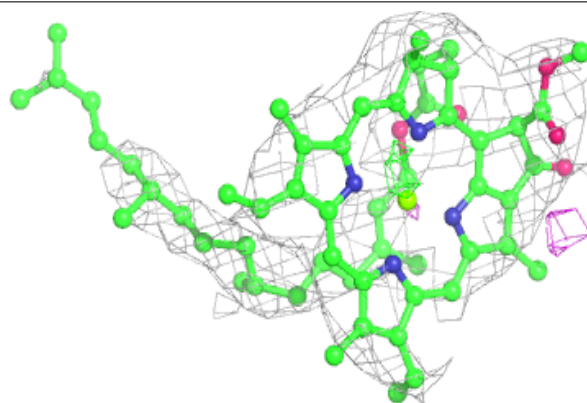


**Electron density around BCR 1 4022:**

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

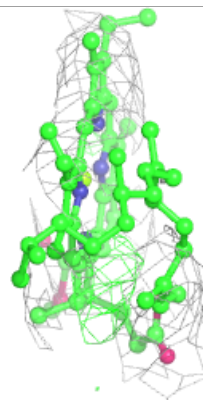
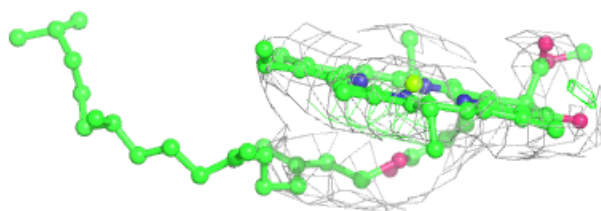
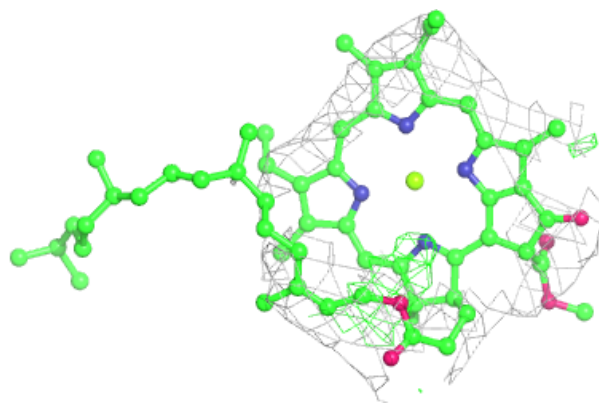
**Electron density around CLA 2 1204:**

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



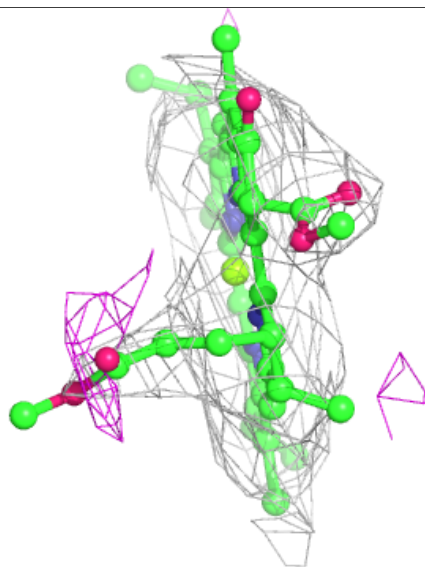
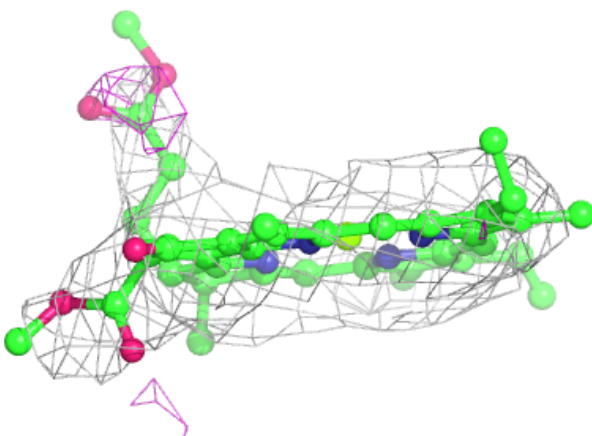
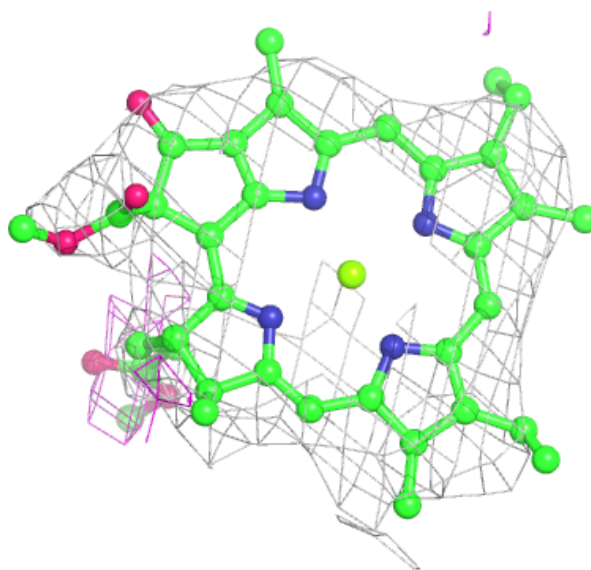
**Electron density around CLA B 1215:**

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



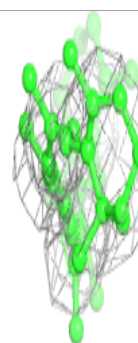
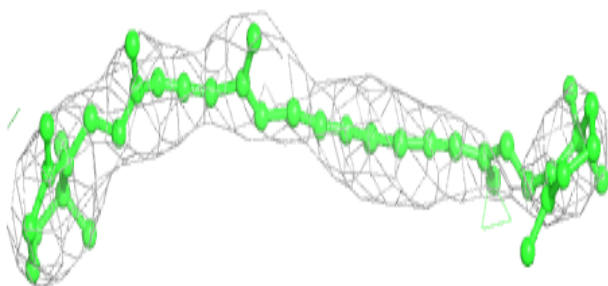
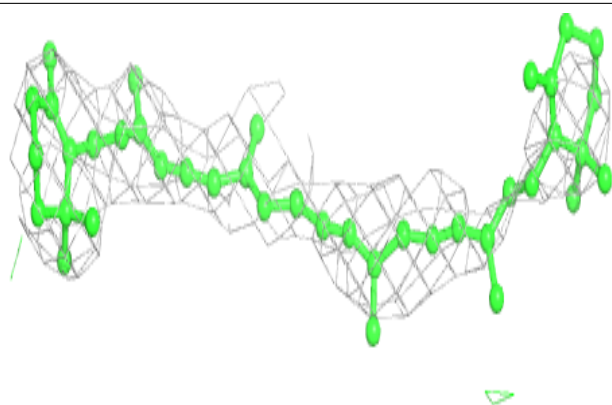
**Electron density around CLA A 1133:**

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

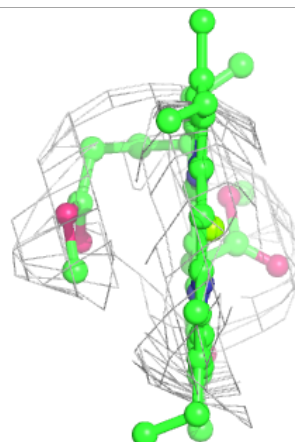
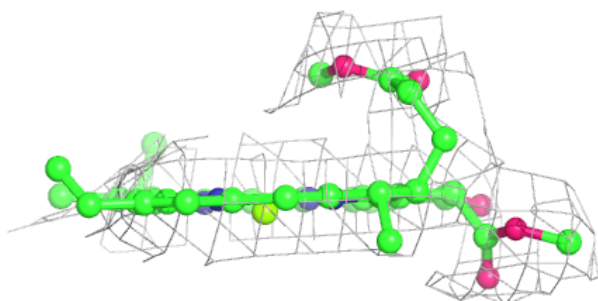
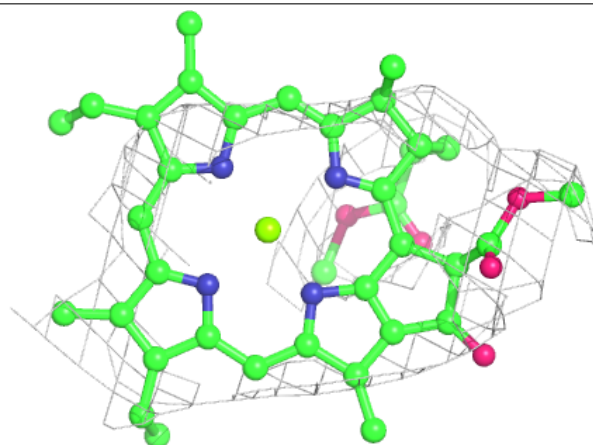


**Electron density around BCR 7 4021:**

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

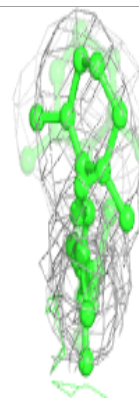
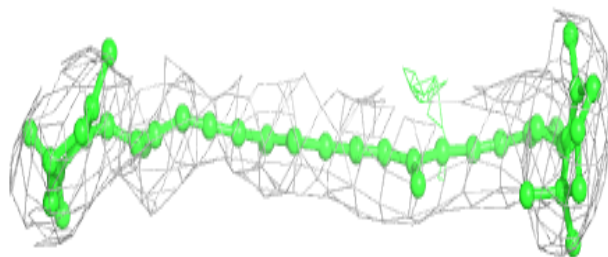
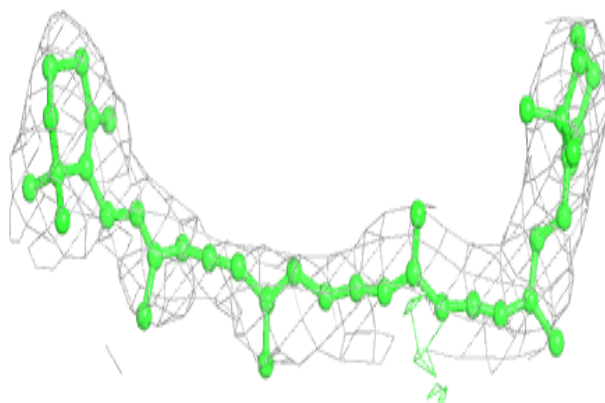
**Electron density around CLA 1 1138:**

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



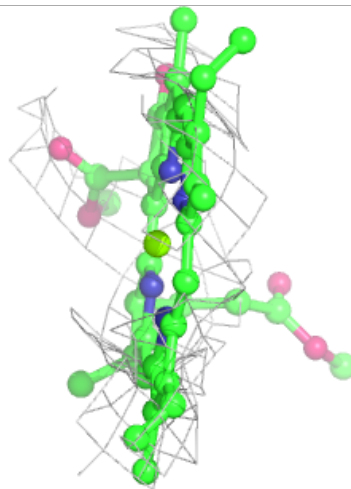
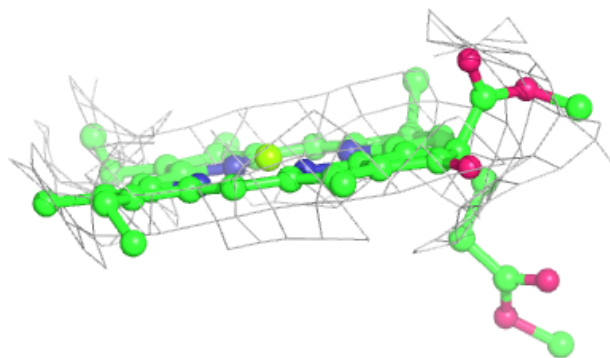
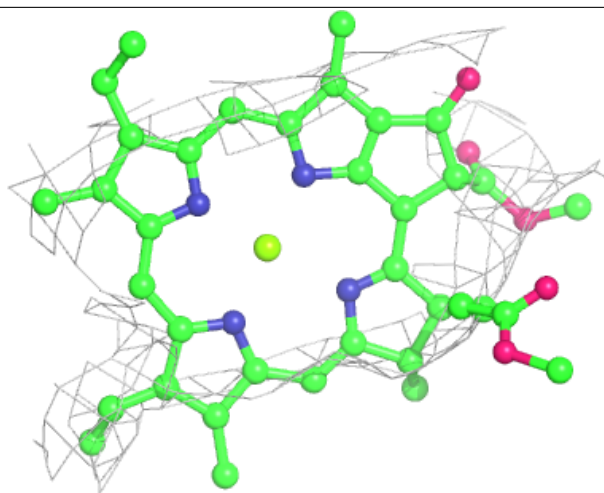
**Electron density around BCR F 4020:**

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



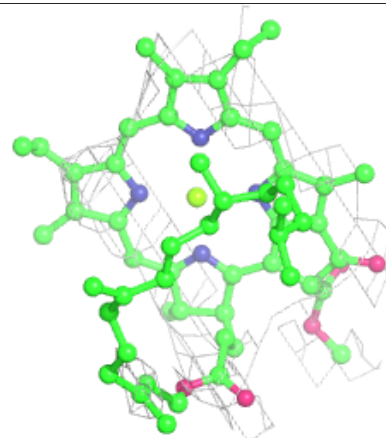
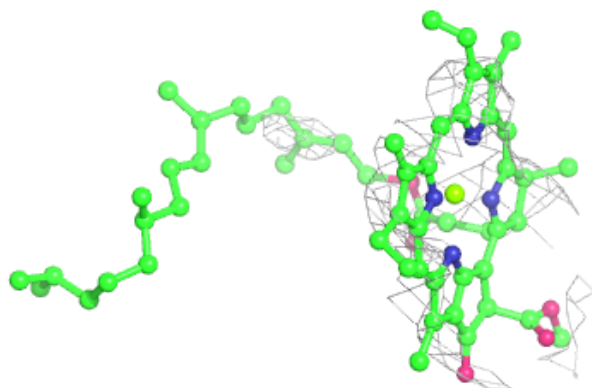
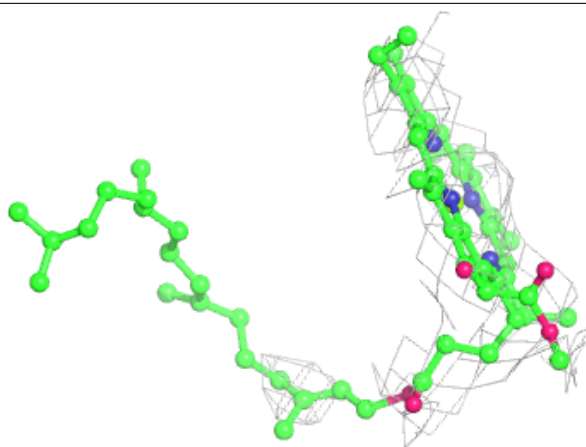
**Electron density around CLA b 1220:**

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

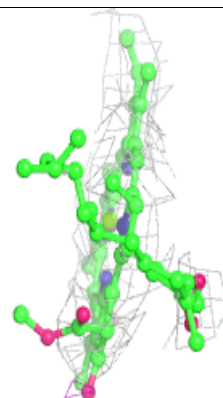
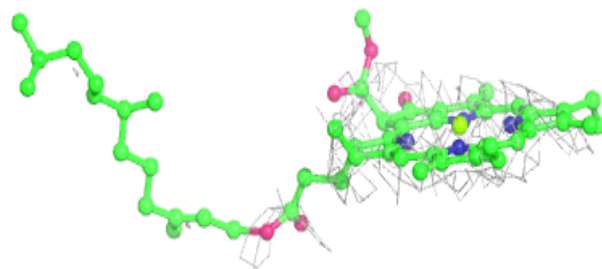
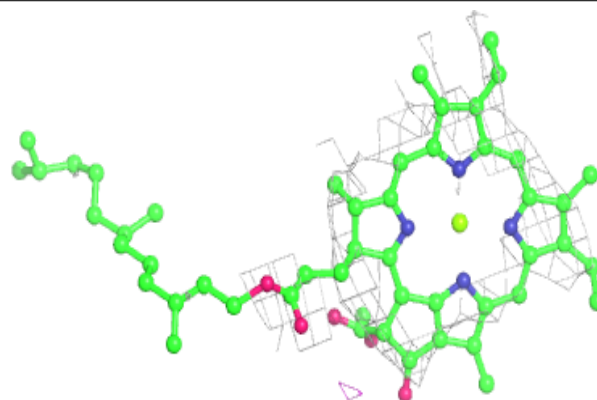


**Electron density around CLA b 1216:**

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

**Electron density around CLA b 1234:**

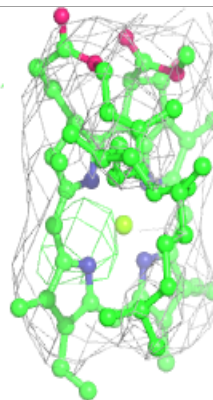
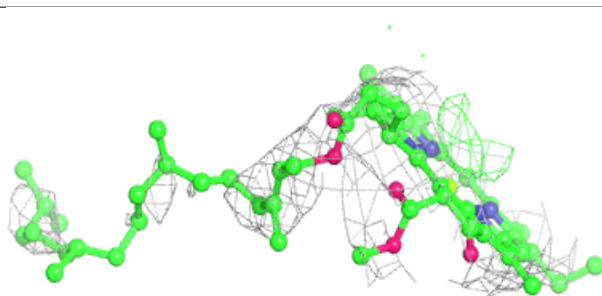
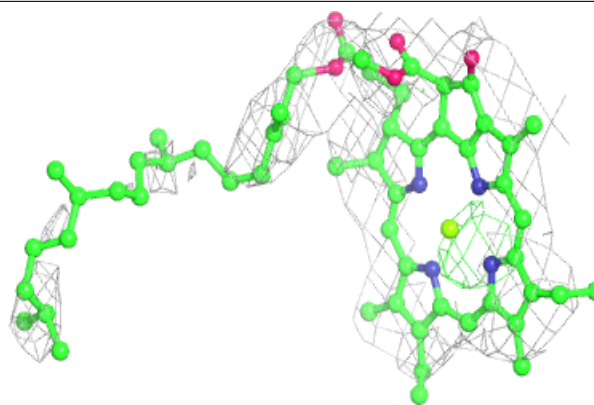
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



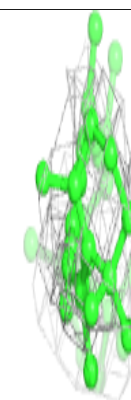
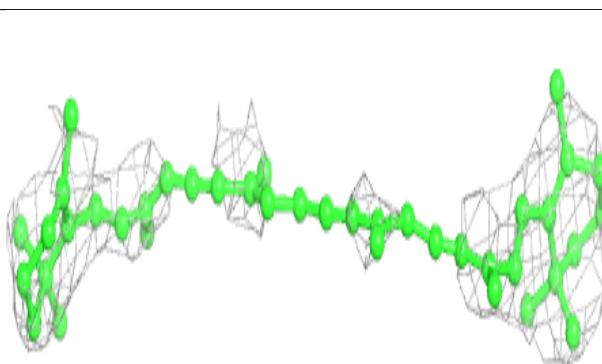
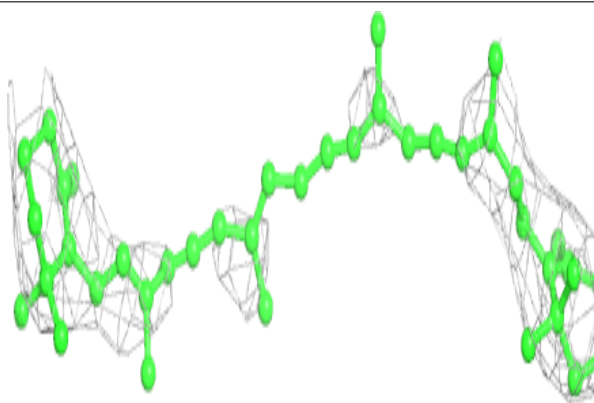


**Electron density around CLA B 1207:**

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

**Electron density around BCR B 4010:**

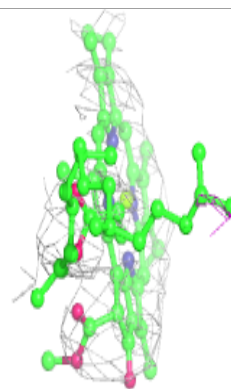
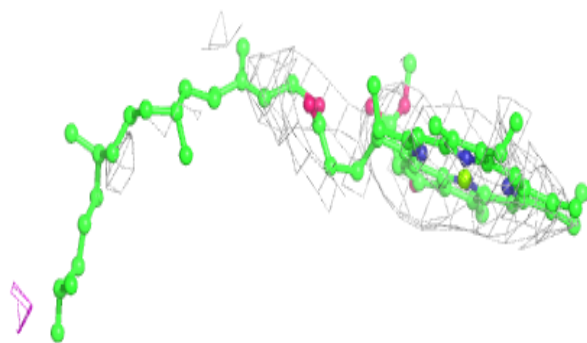
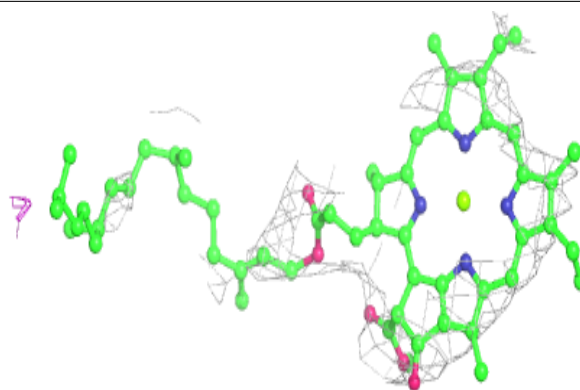
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





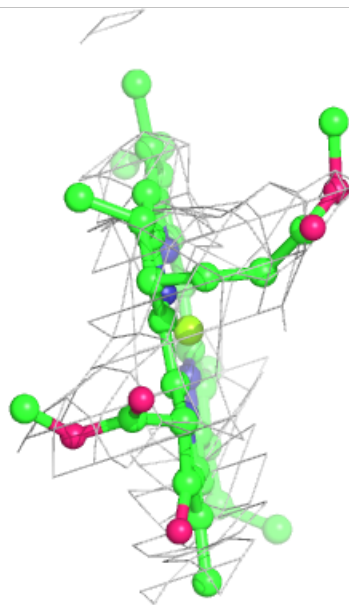
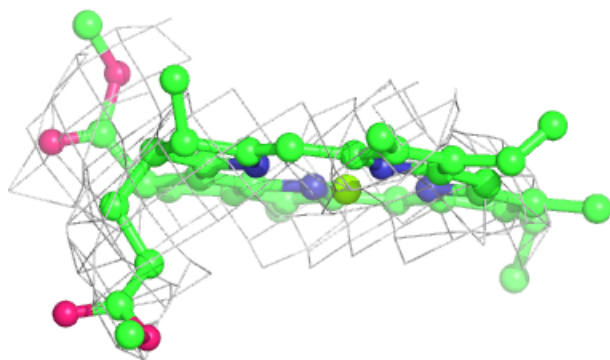
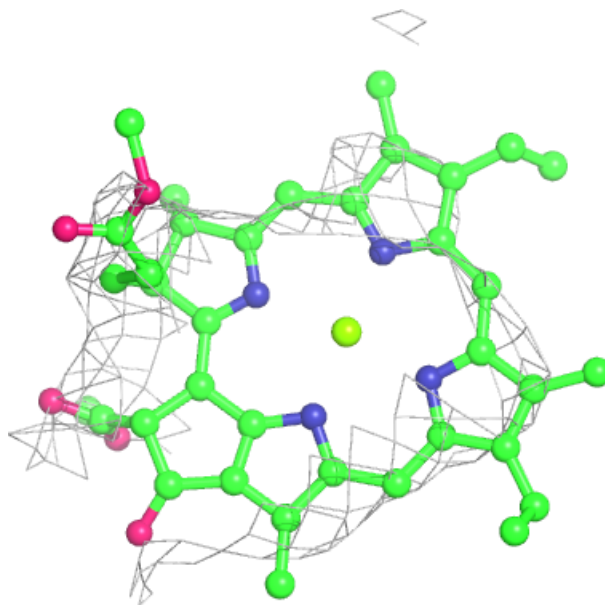
**Electron density around CLA a 1103:**

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



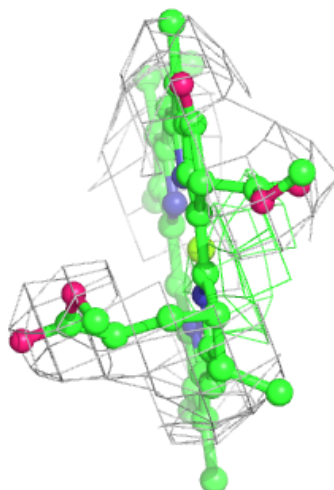
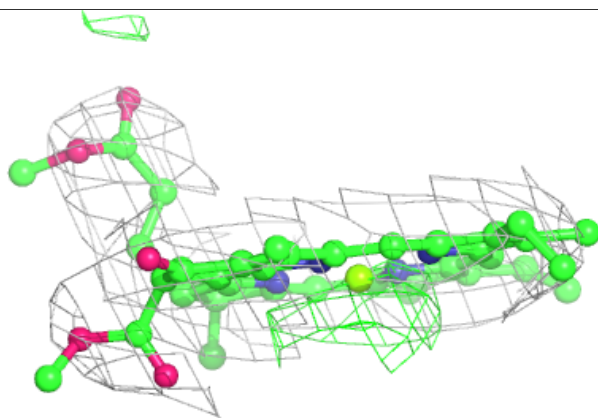
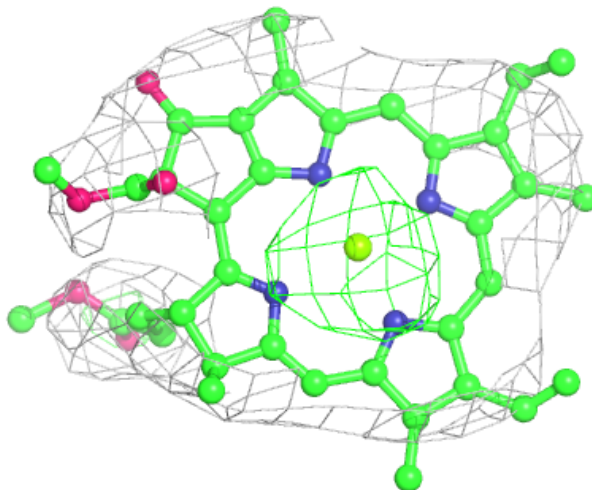
**Electron density around CLA 1 1129:**

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



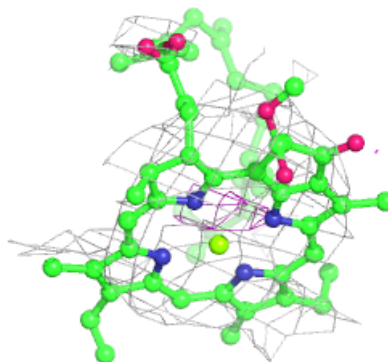
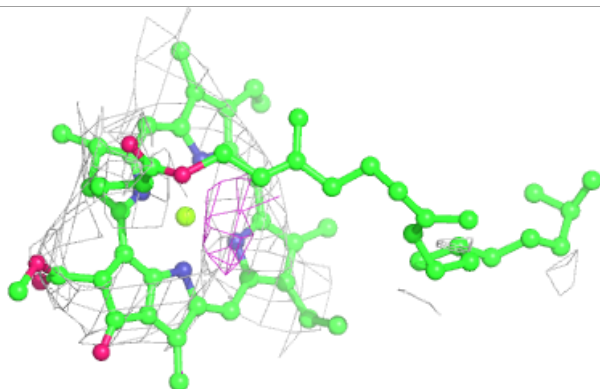
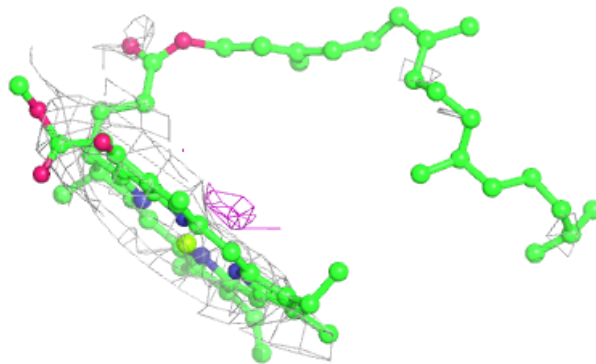
**Electron density around CLA b 1239:**

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

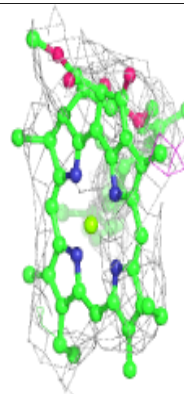
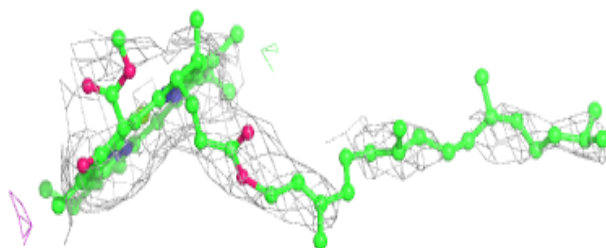
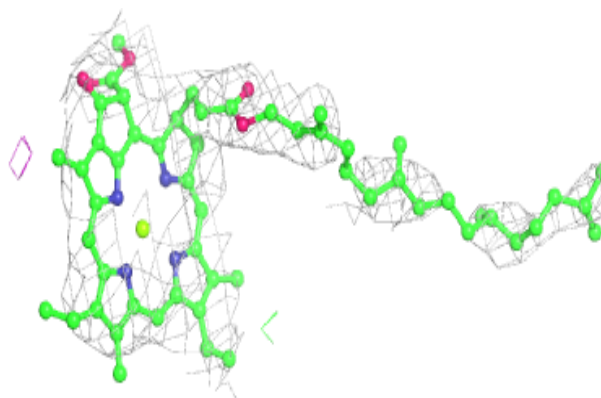


**Electron density around CLA 1 1109:**

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

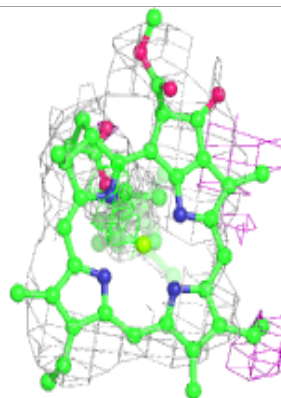
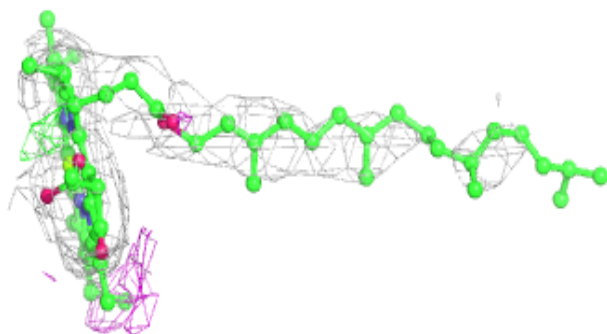
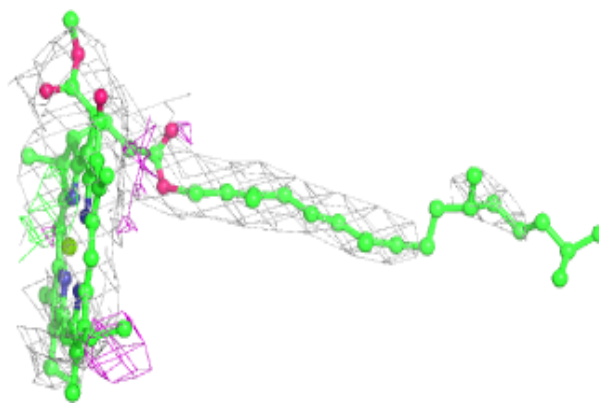
**Electron density around CLA 1 1132:**

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

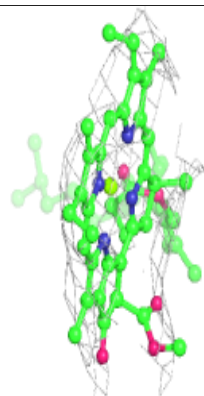
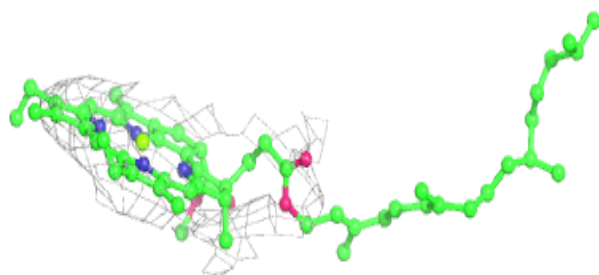
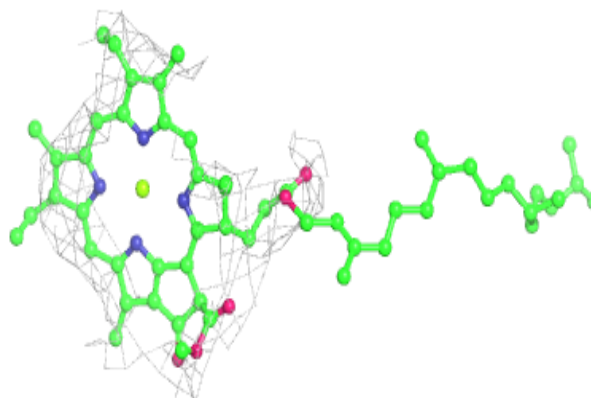


**Electron density around CLA A 1126:**

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

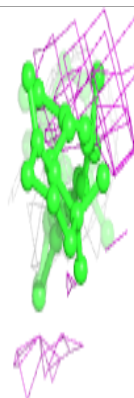
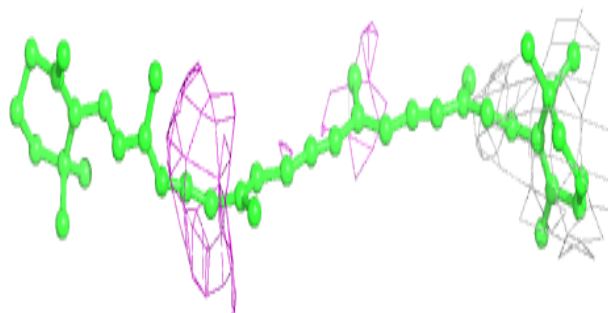
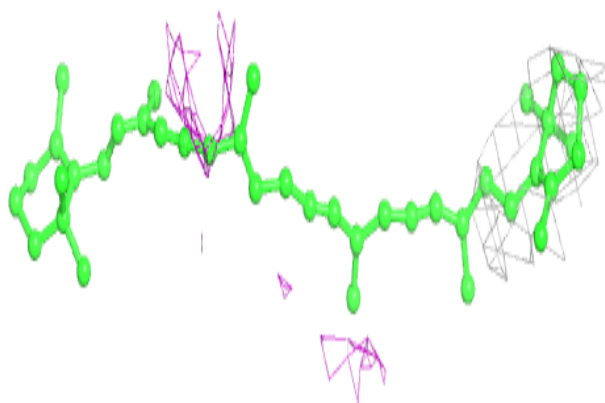
**Electron density around CLA 1 1103:**

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

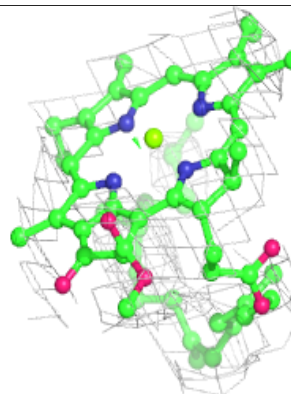
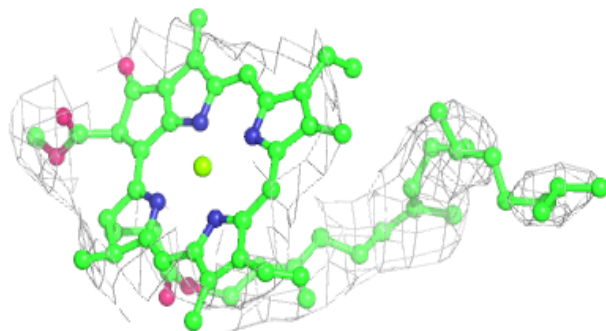
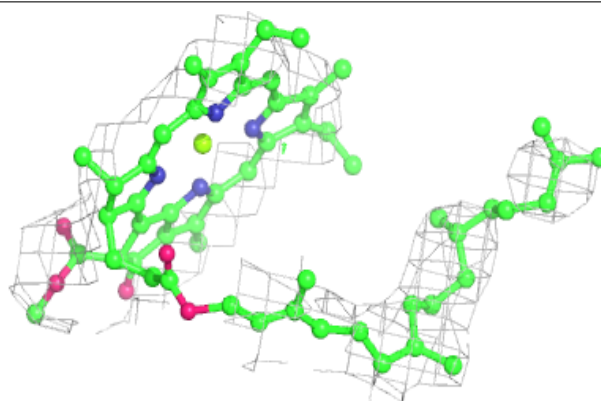


**Electron density around BCR a 4003:**

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

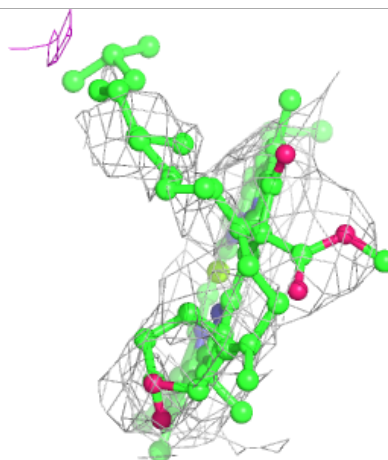
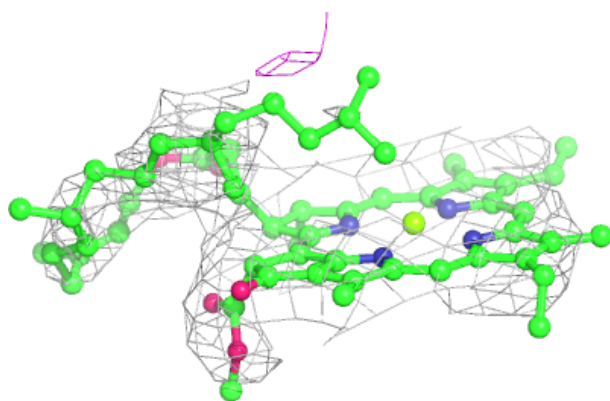
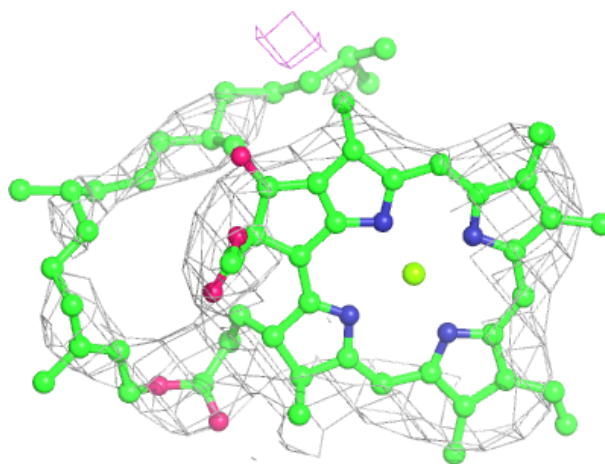
**Electron density around CLA A 1109:**

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



**Electron density around CLA B 1202:**

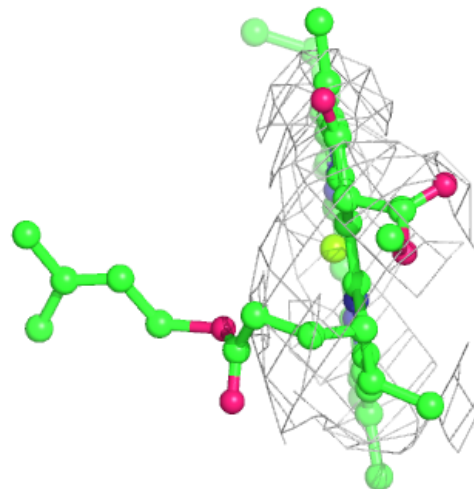
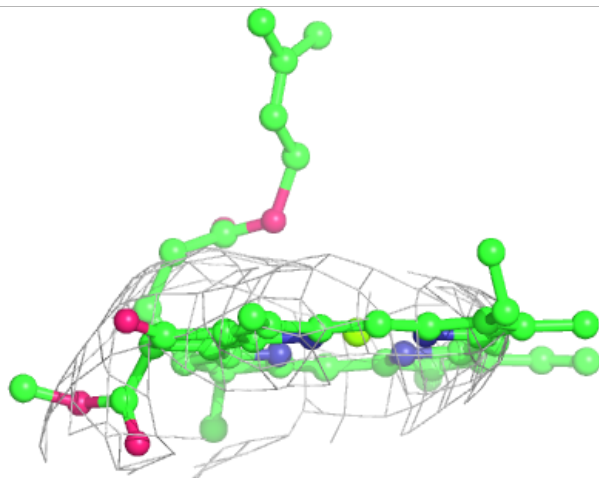
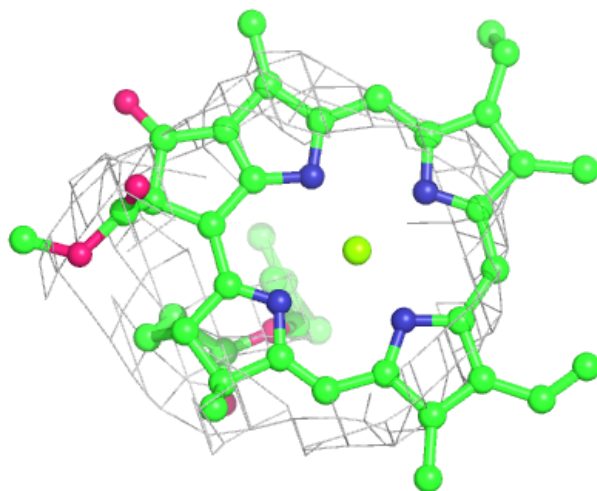
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





**Electron density around CLA k 1402:**

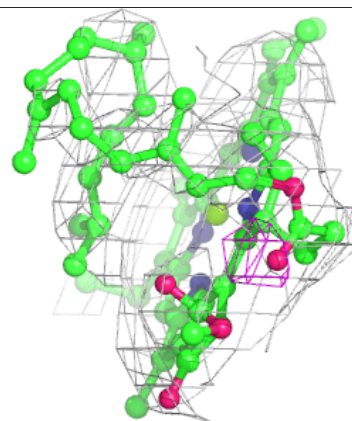
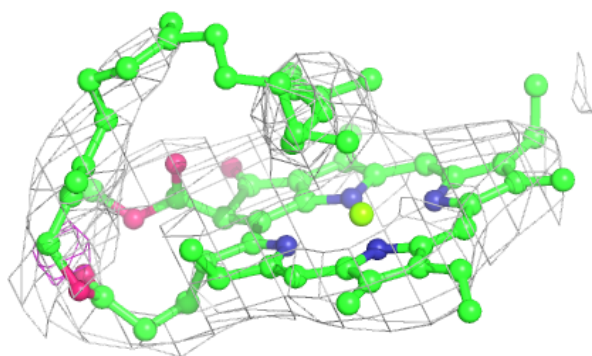
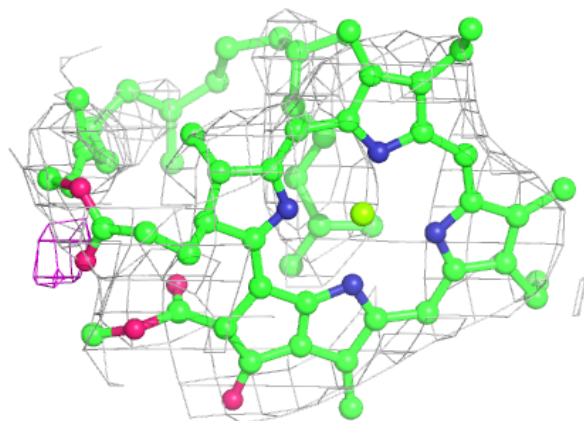
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



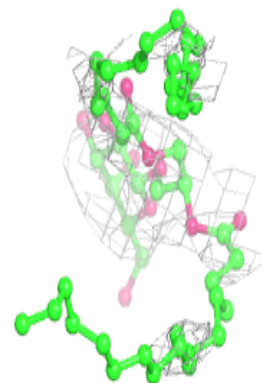
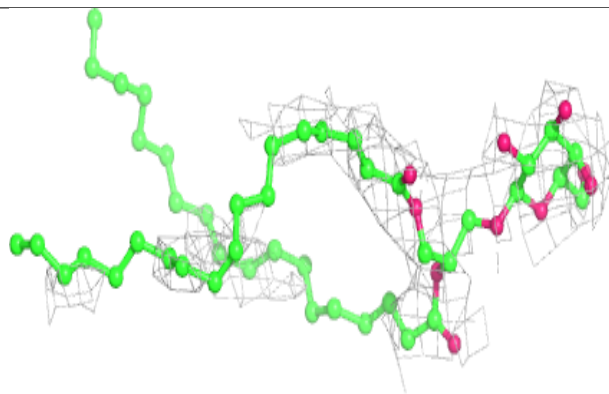
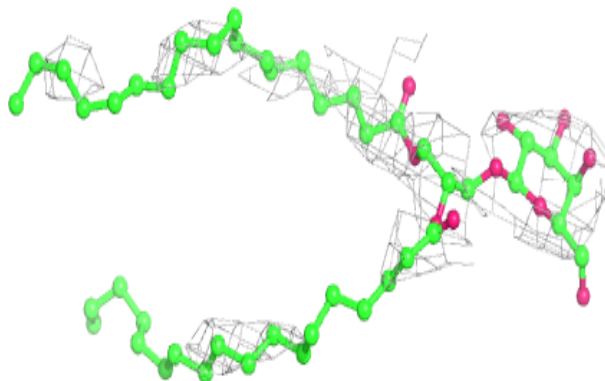


**Electron density around CLA B 1203:**

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

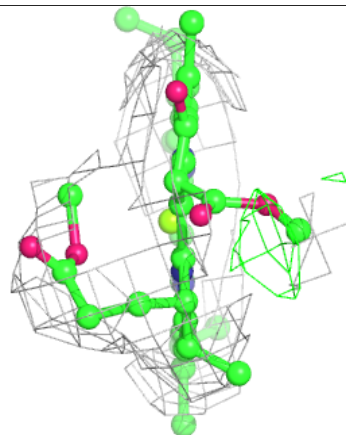
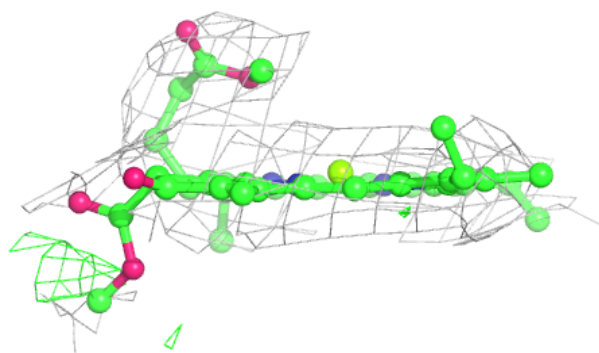
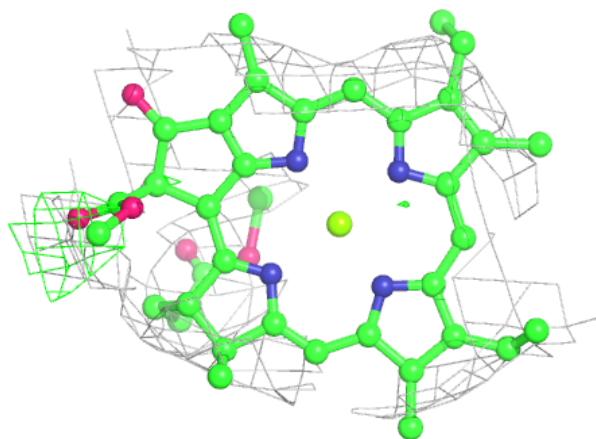
**Electron density around LMG b 5002:**

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

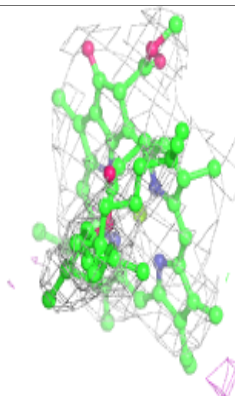
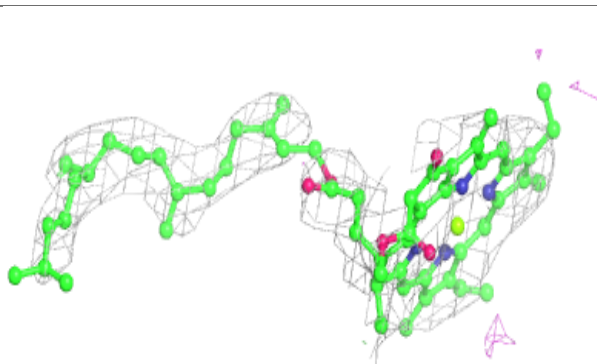
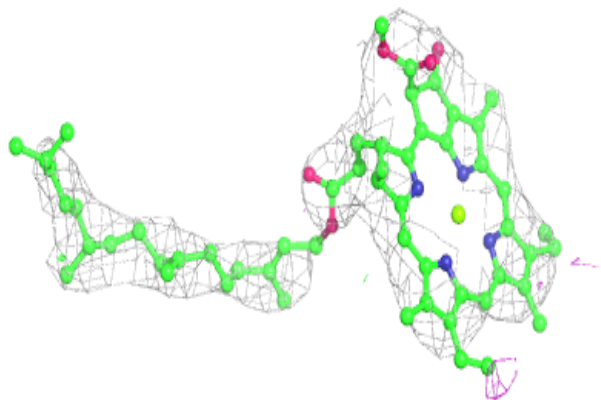


**Electron density around CLA 8 1502:**

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

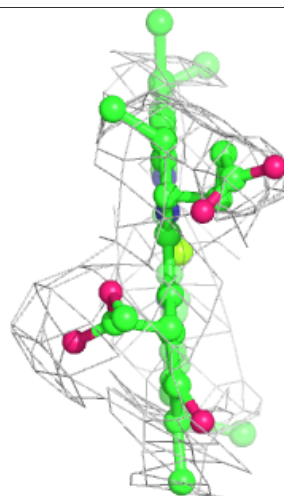
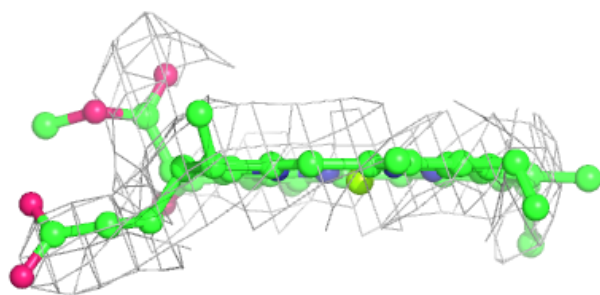
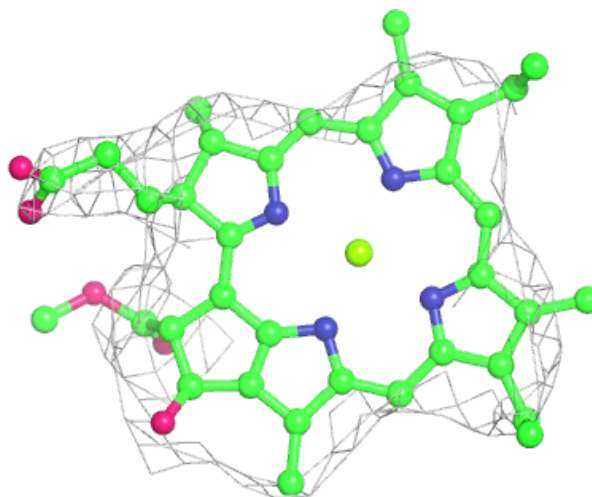
**Electron density around CLA A 1119:**

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



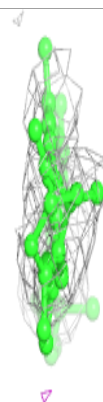
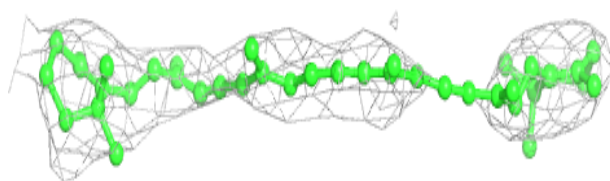
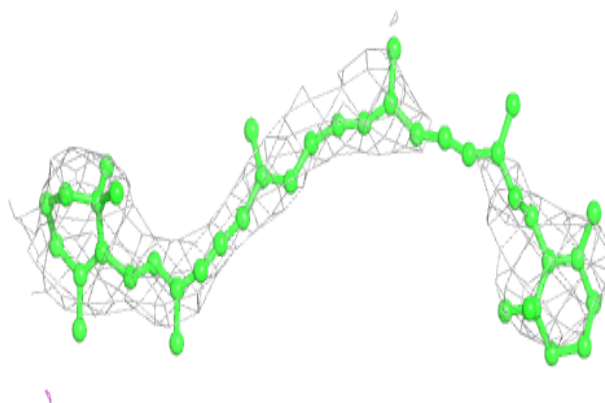
**Electron density around CLA A 1113:**

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



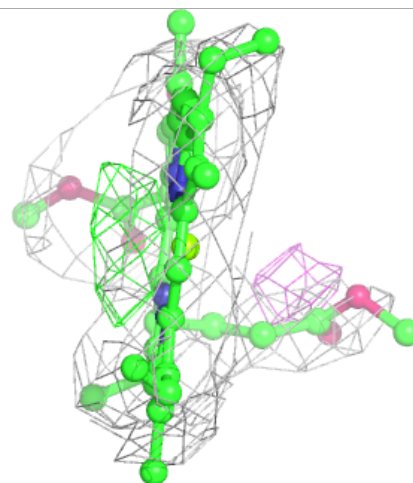
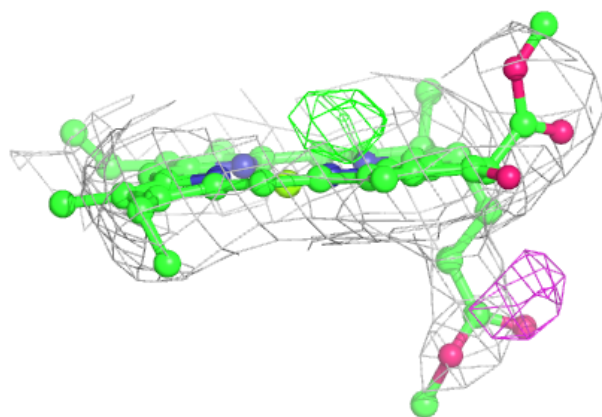
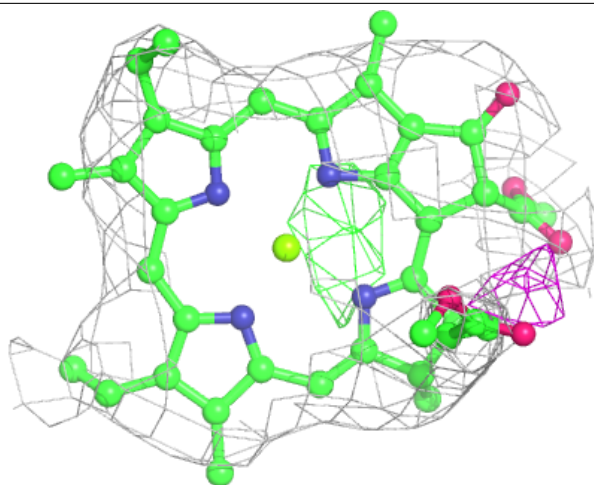
**Electron density around BCR B 4011:**

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



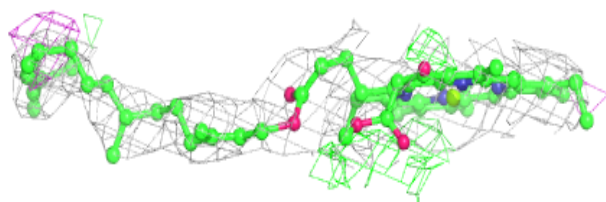
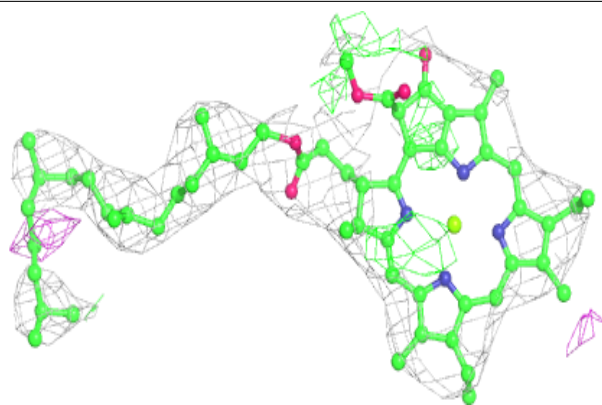
**Electron density around CLA L 1502:**

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

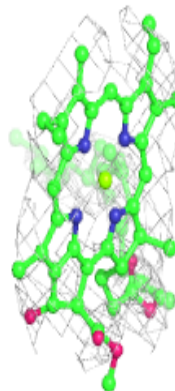
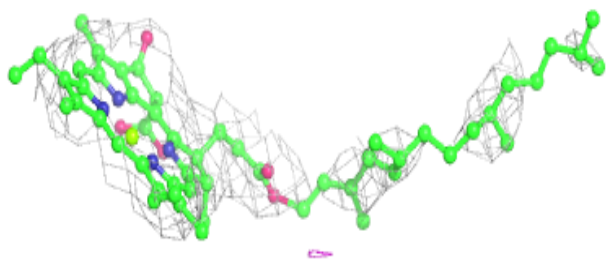
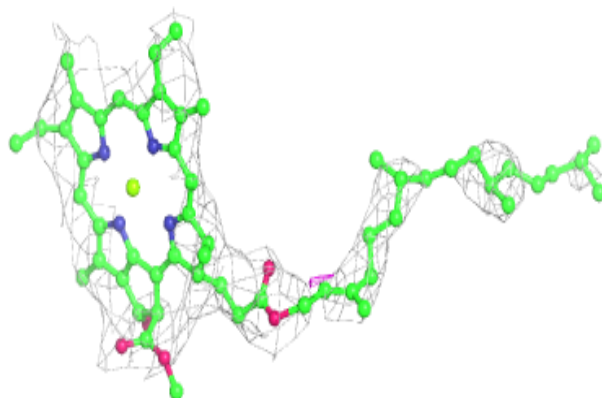


**Electron density around CLA A 1131:**

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

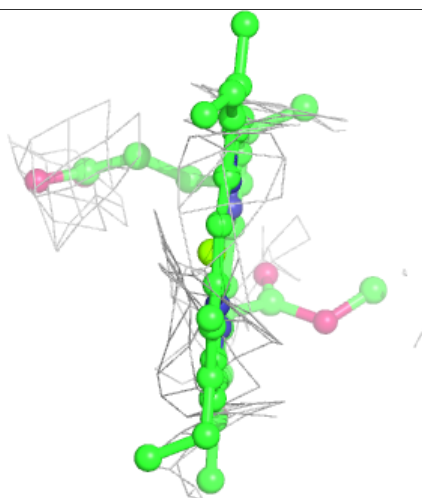
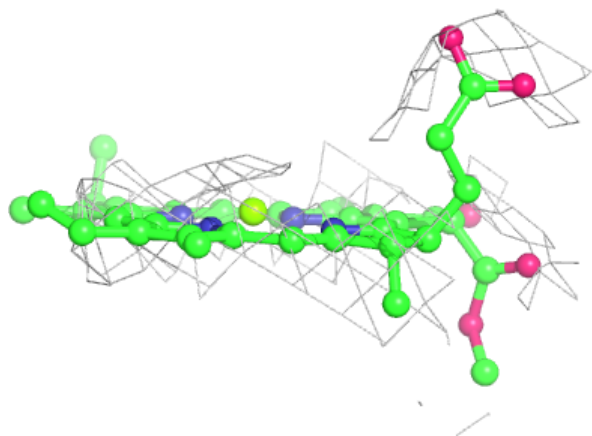
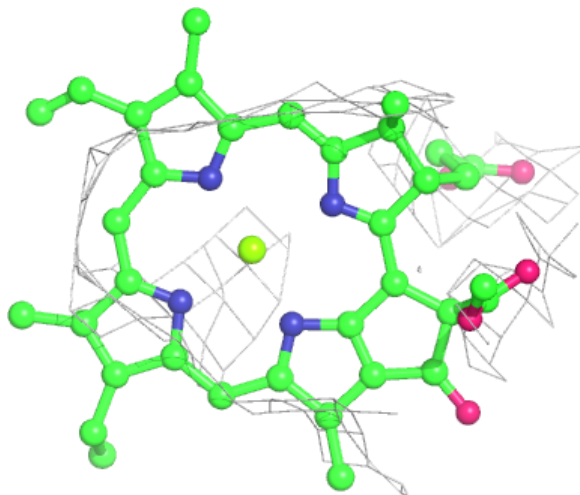
**Electron density around CLA 1 1022:**

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



**Electron density around CLA a 1112:**

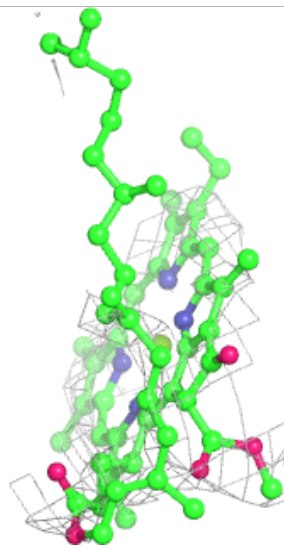
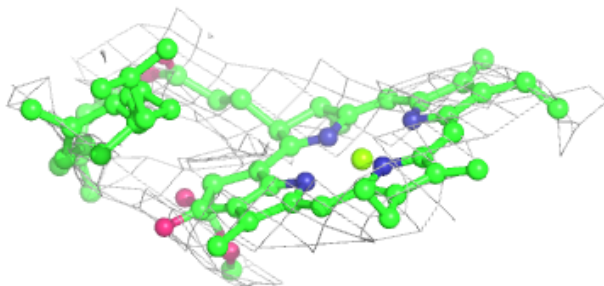
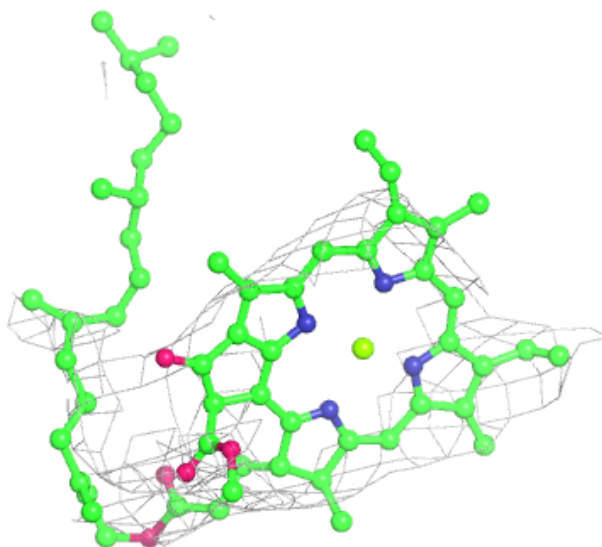
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





**Electron density around CLA 1 1123:**

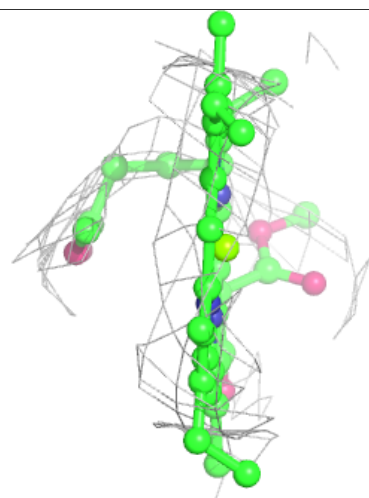
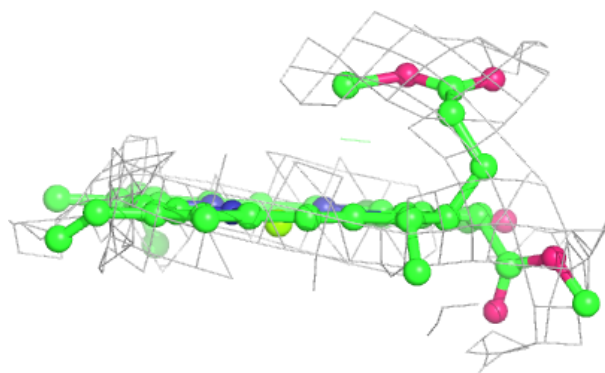
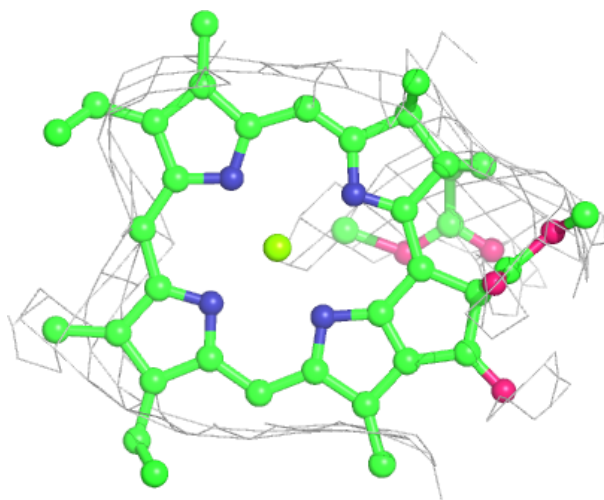
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





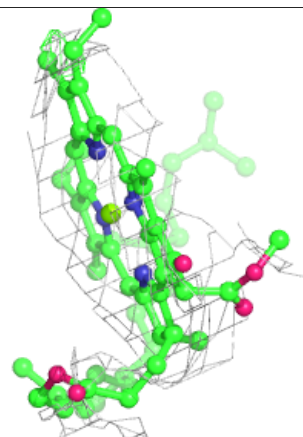
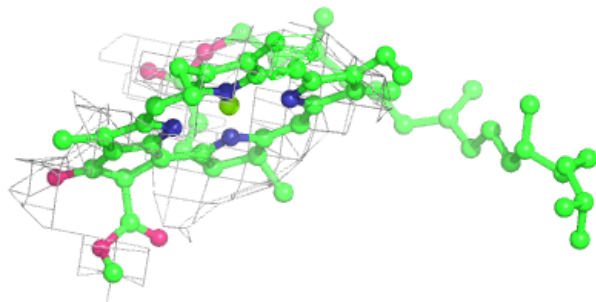
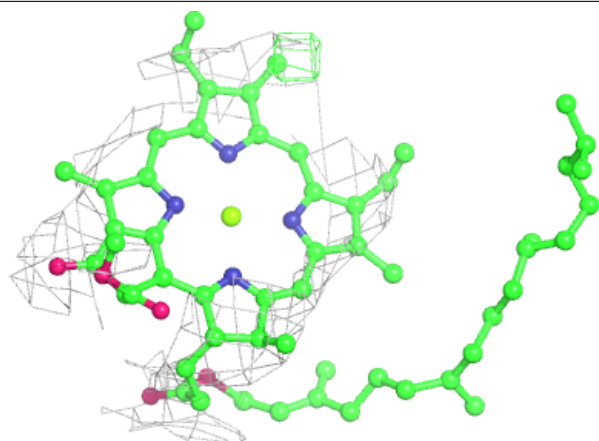
**Electron density around CLA a 1115:**

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

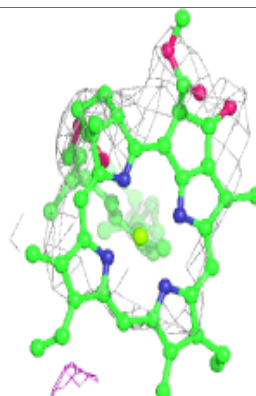
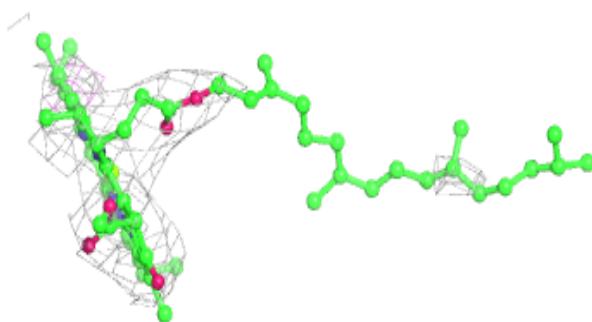
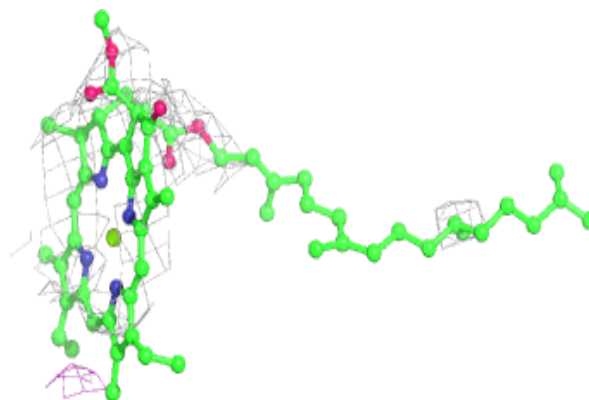


**Electron density around CLA 0 1401:**

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

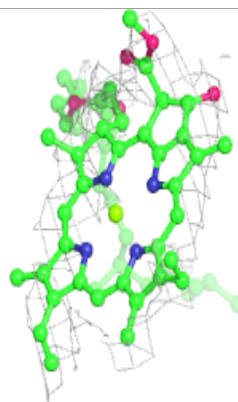
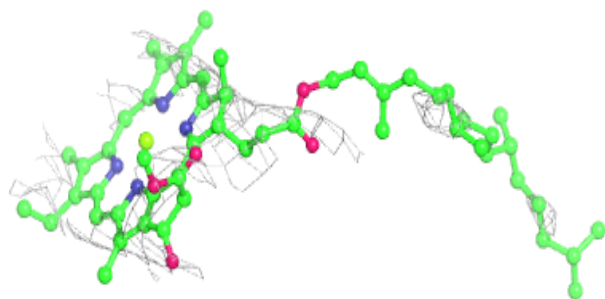
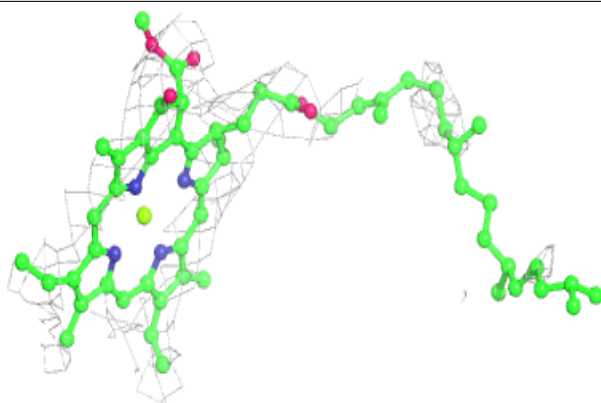
**Electron density around CLA b 1225:**

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

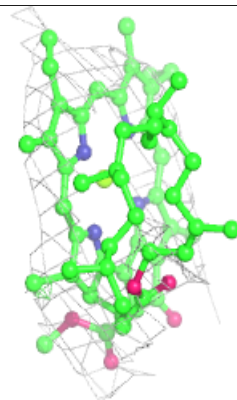
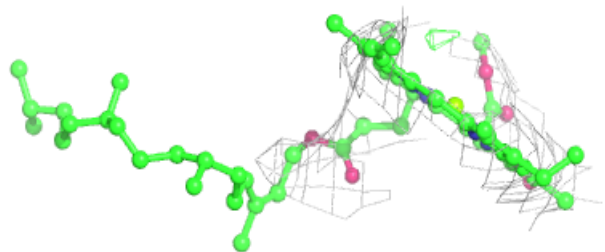
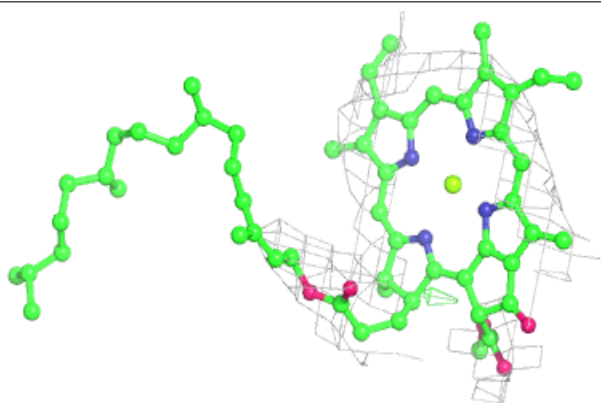


**Electron density around CLA a 1012:**

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

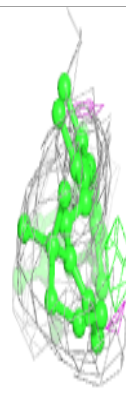
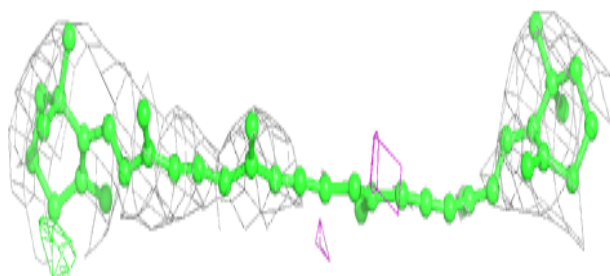
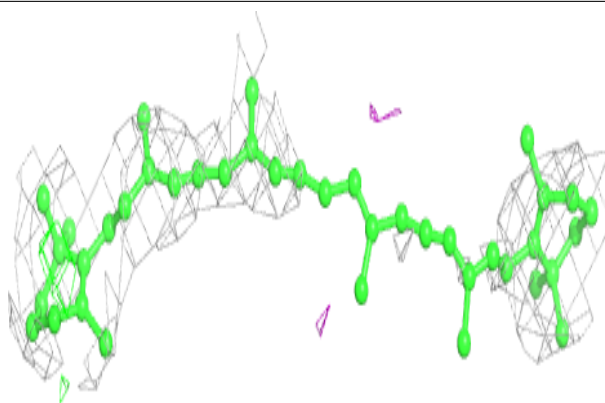
**Electron density around CLA 1 1106:**

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



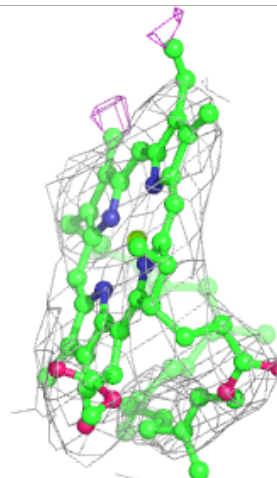
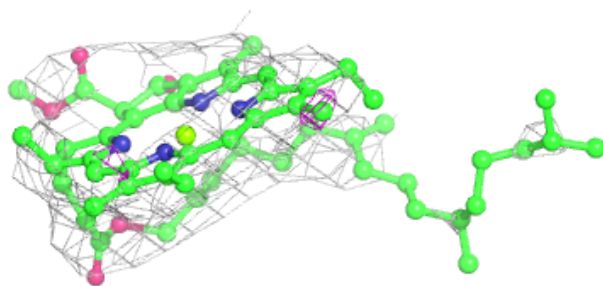
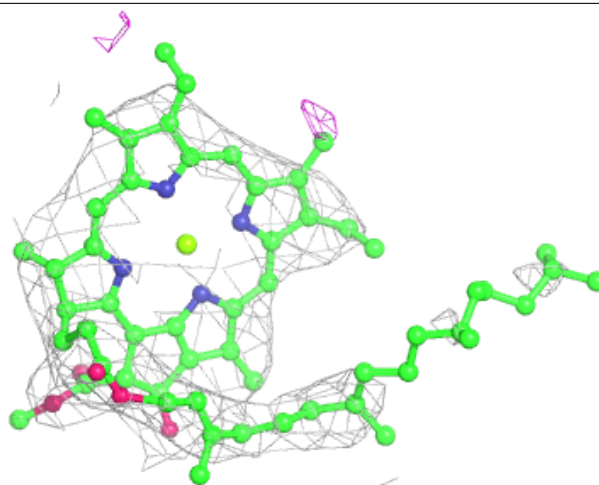
**Electron density around BCR A 4001:**

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



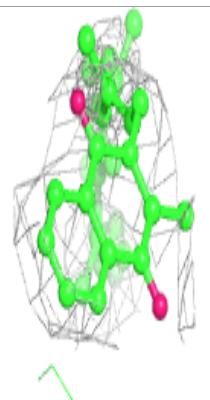
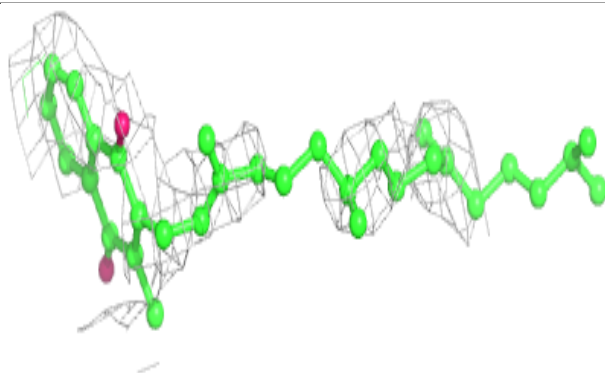
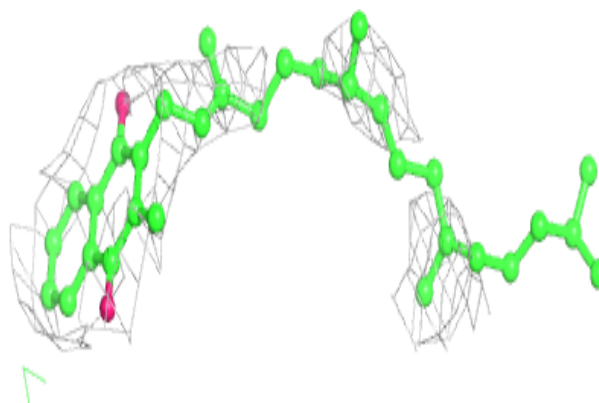
**Electron density around CLA A 1127:**

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



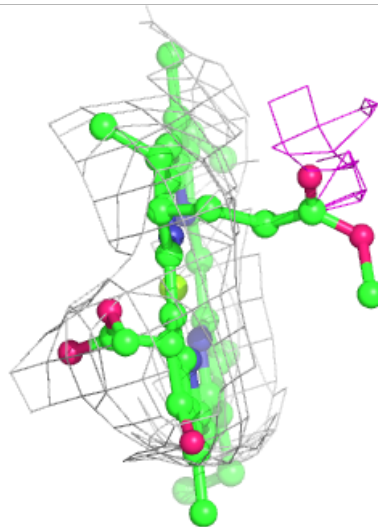
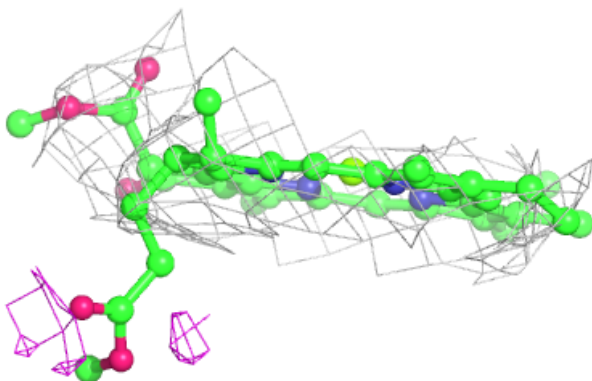
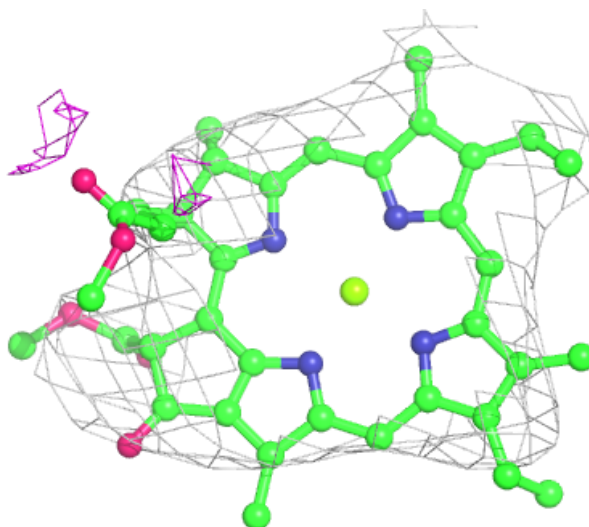
**Electron density around PQN A 2001:**

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



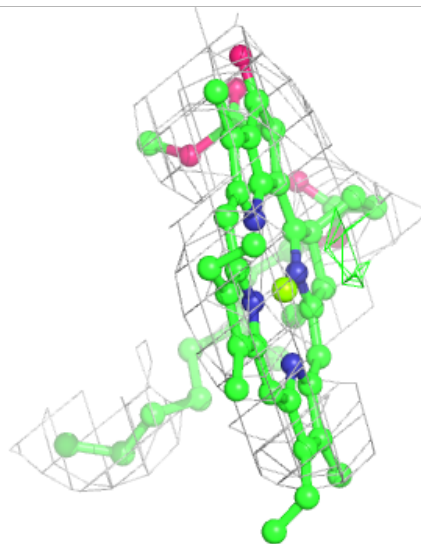
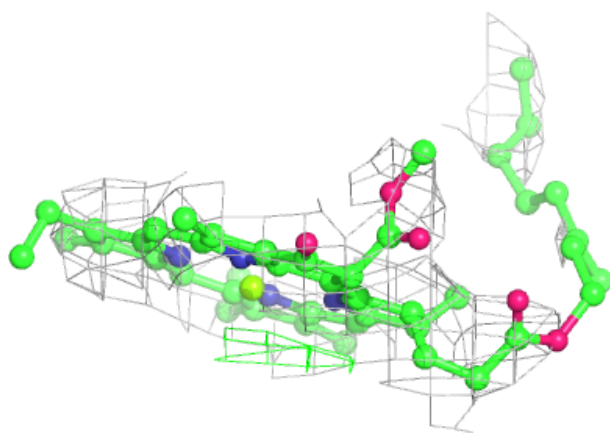
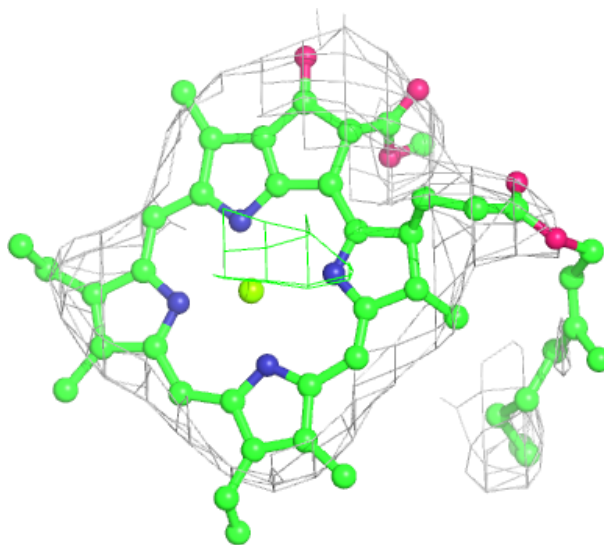
**Electron density around CLA A 1114:**

2mF<sub>o</sub>-DF<sub>c</sub> (at 0.7 rmsd) in gray  
mF<sub>o</sub>-DF<sub>c</sub> (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around CLA 2 1221:**

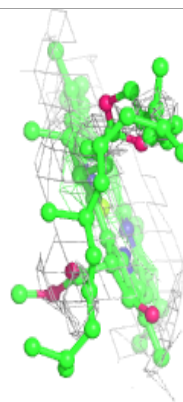
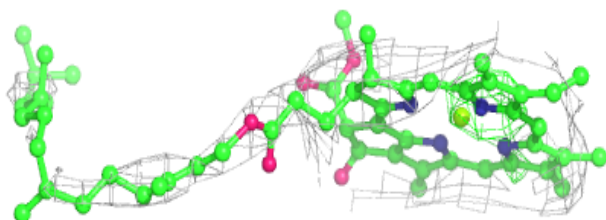
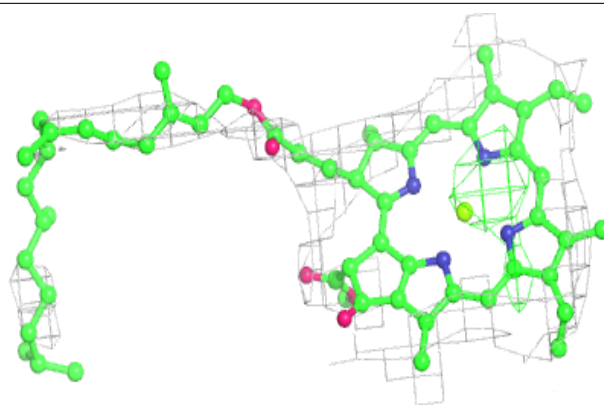
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



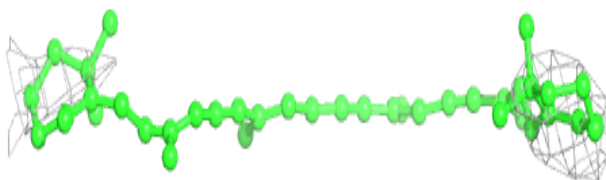
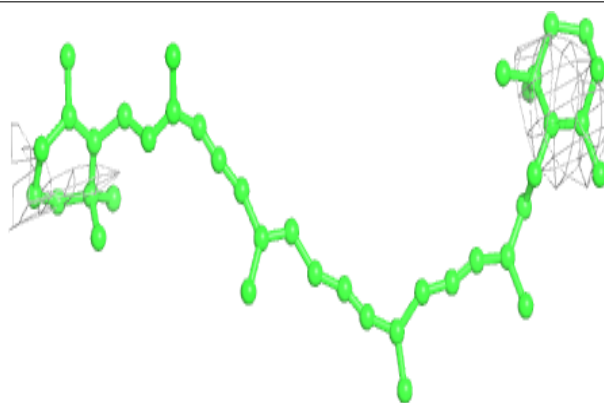


**Electron density around CLA B 1223:**

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

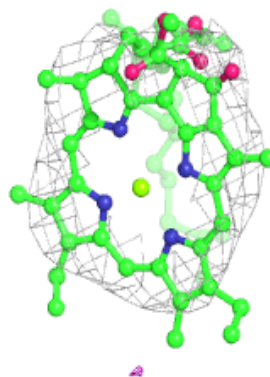
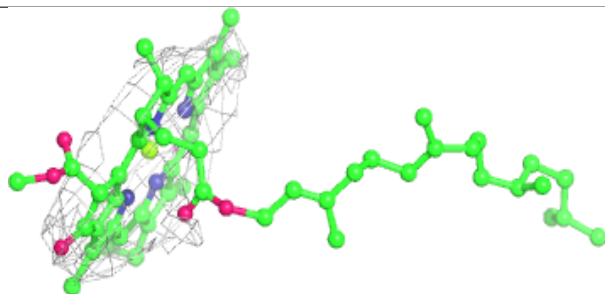
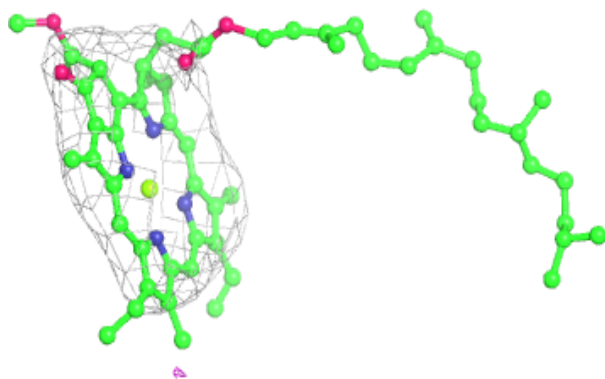
**Electron density around BCR 2 4011:**

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



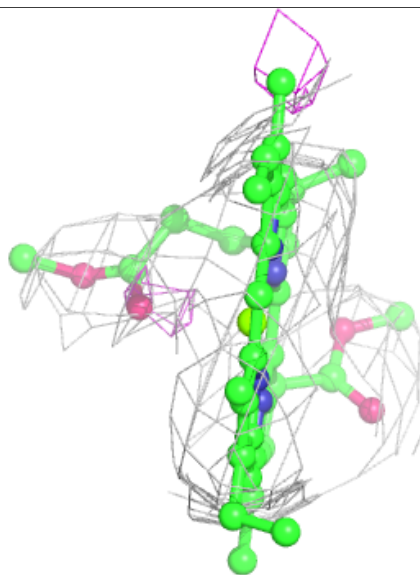
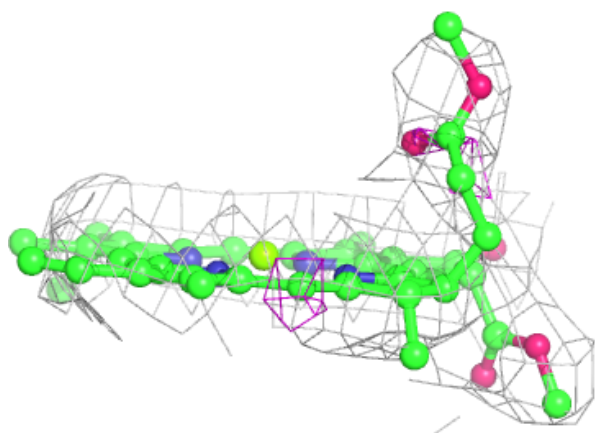
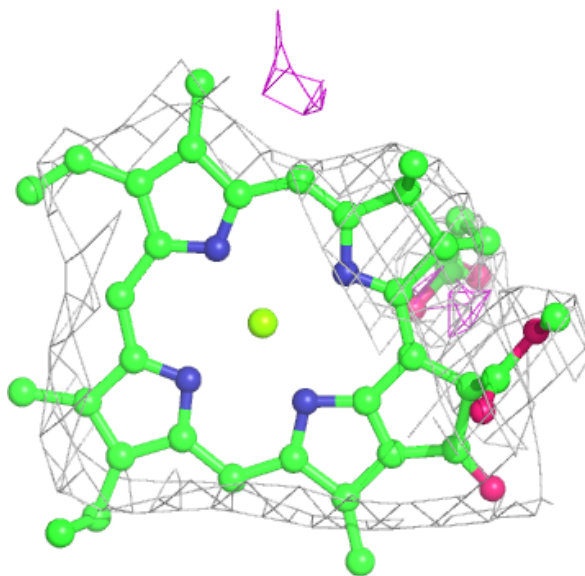
**Electron density around CLA a 1140:**

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



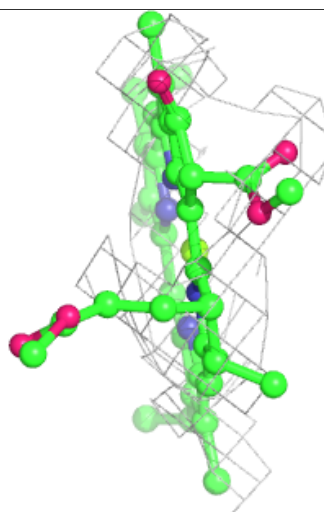
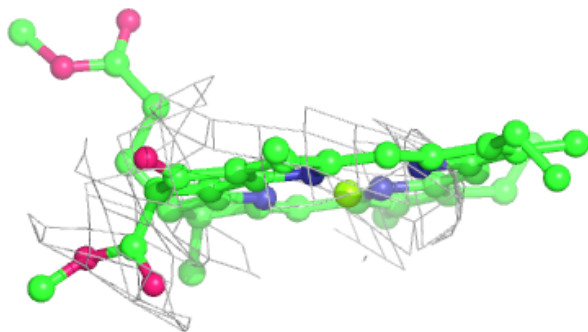
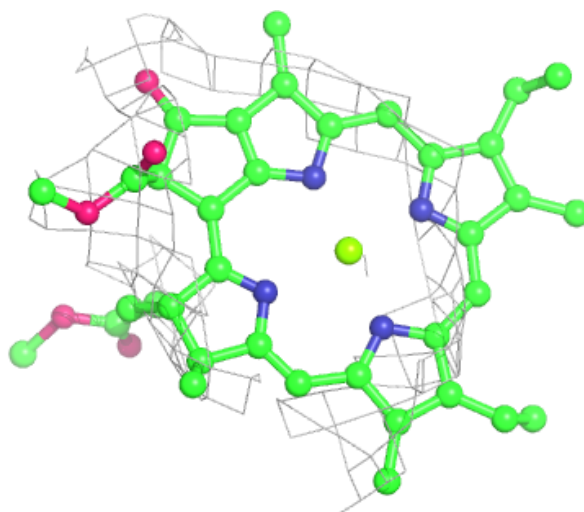
**Electron density around CLA A 1134:**

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



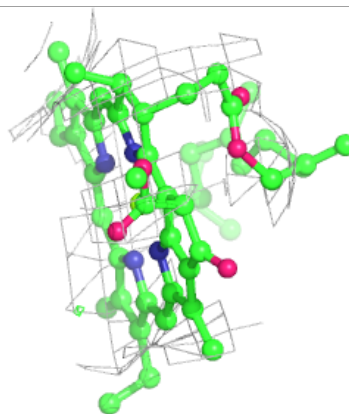
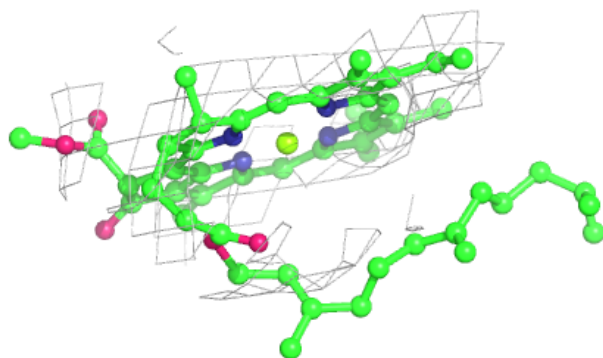
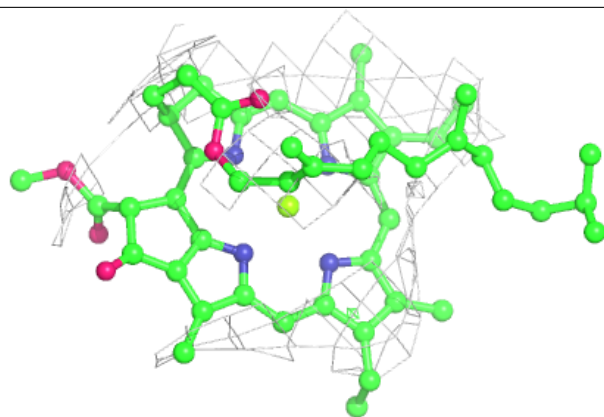
**Electron density around CLA 1 1114:**

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



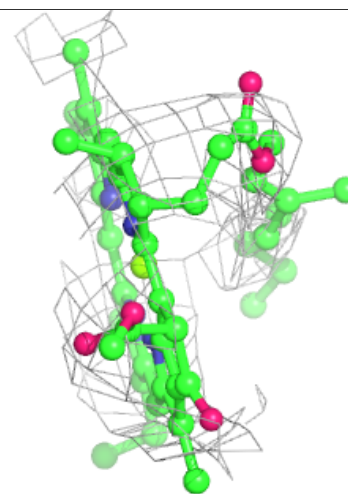
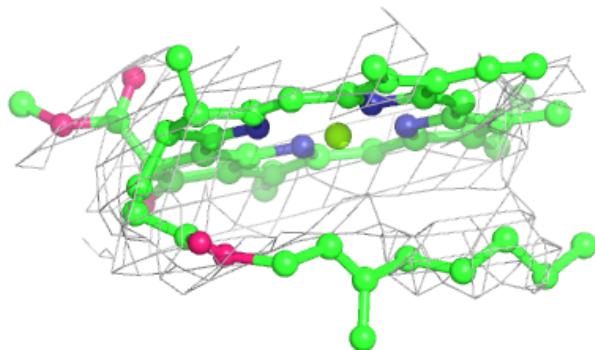
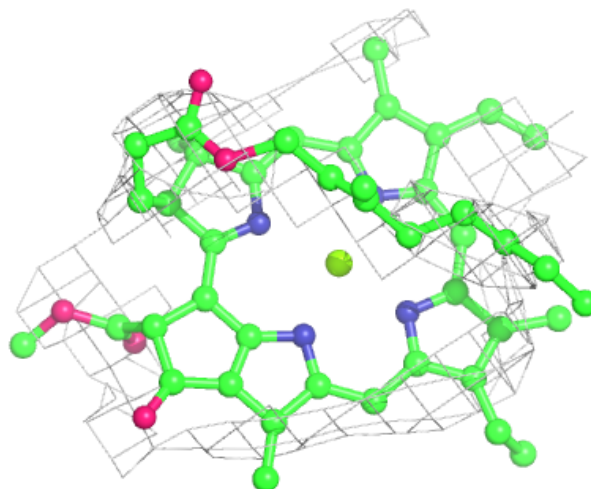
**Electron density around CLA b 1235:**

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



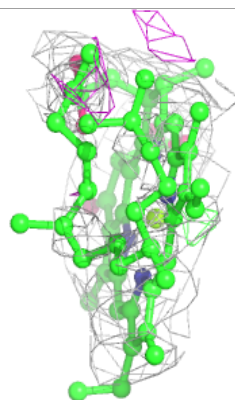
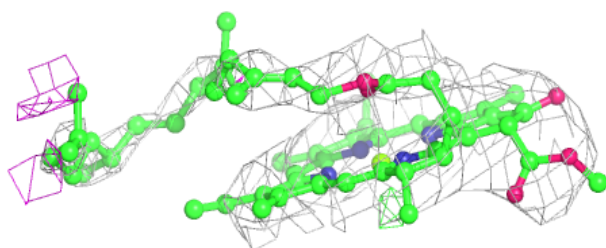
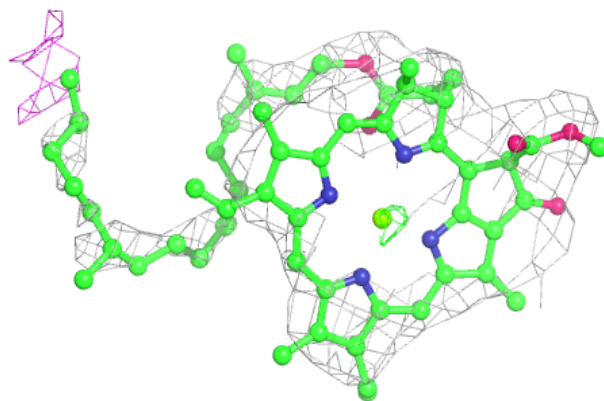
**Electron density around CLA a 1116:**

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

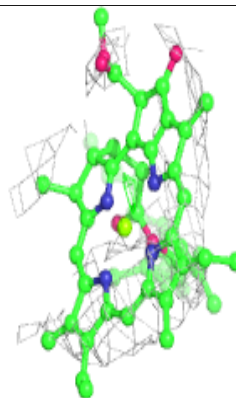
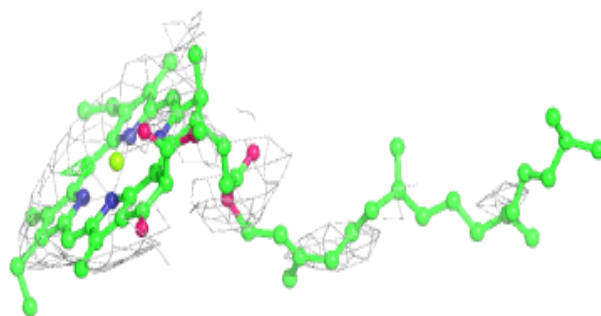
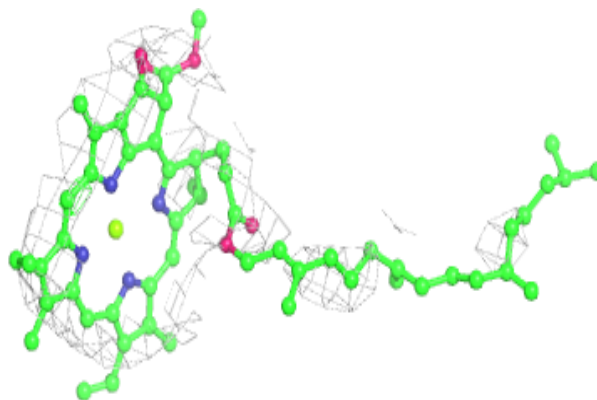


**Electron density around CLA A 1117:**

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

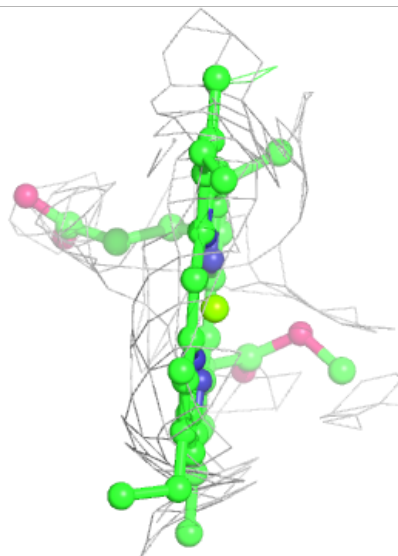
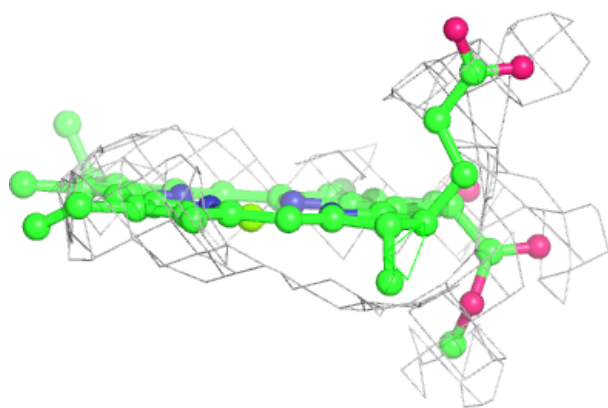
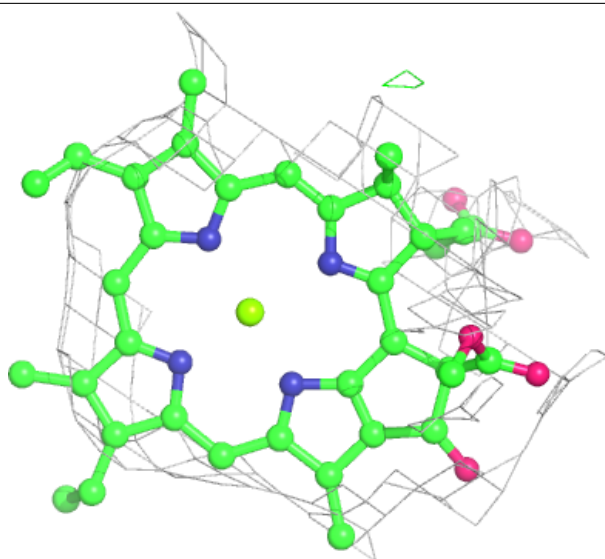
**Electron density around CLA a 1119:**

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



**Electron density around CLA B 1231:**

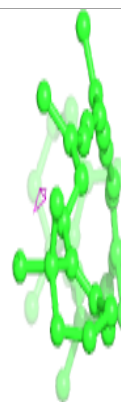
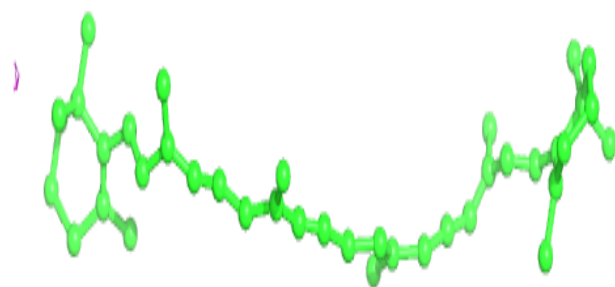
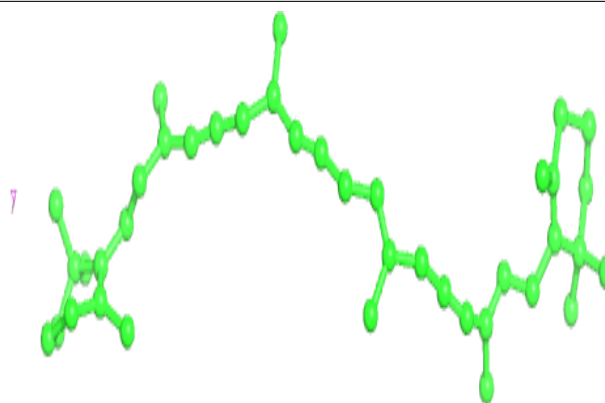
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



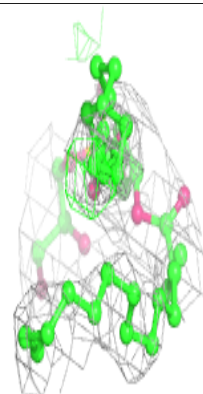
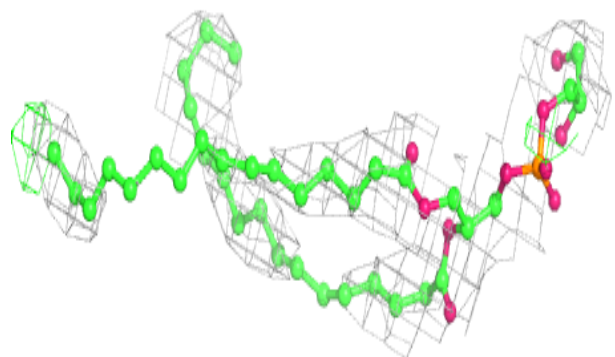
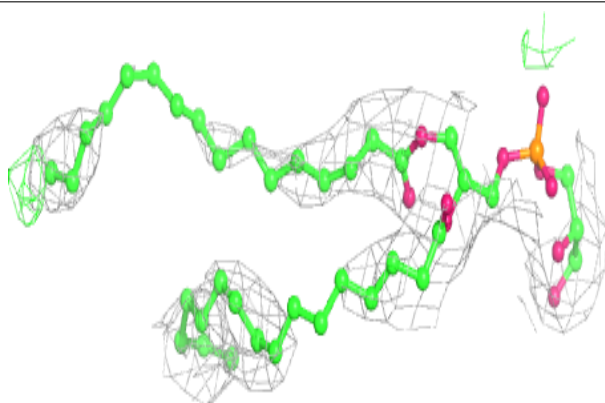


**Electron density around BCR b 4014:**

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

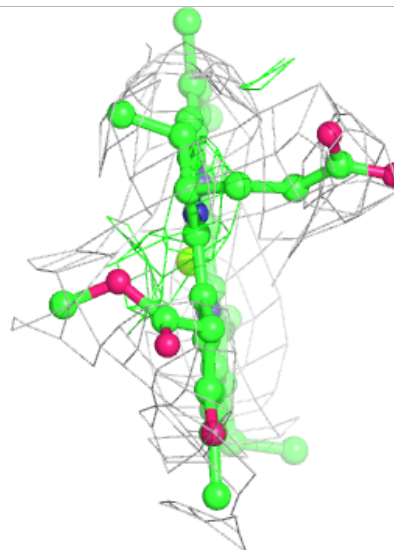
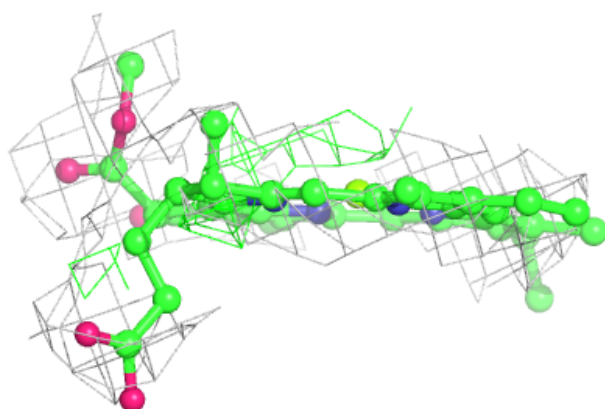
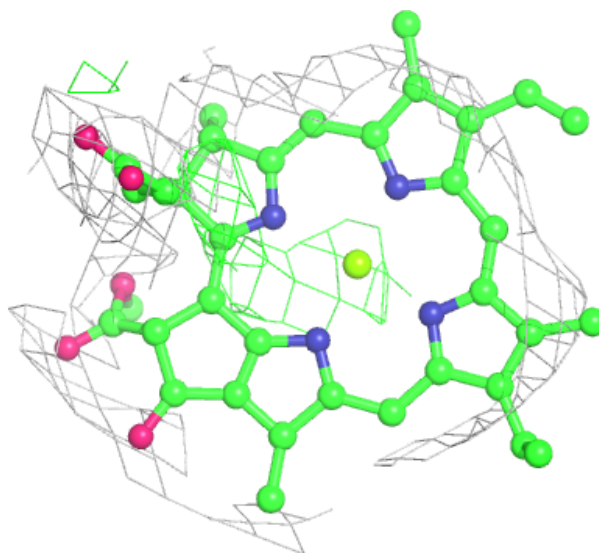
**Electron density around LHG A 5003:**

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



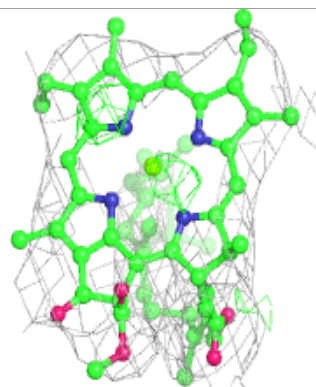
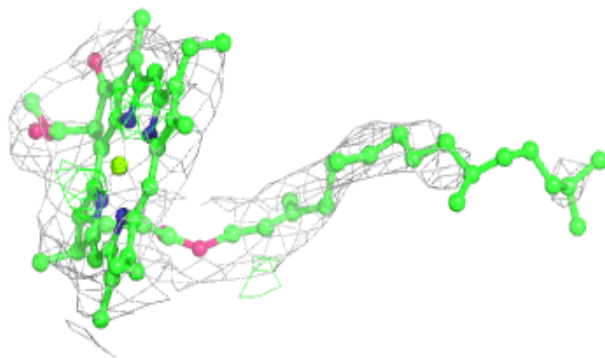
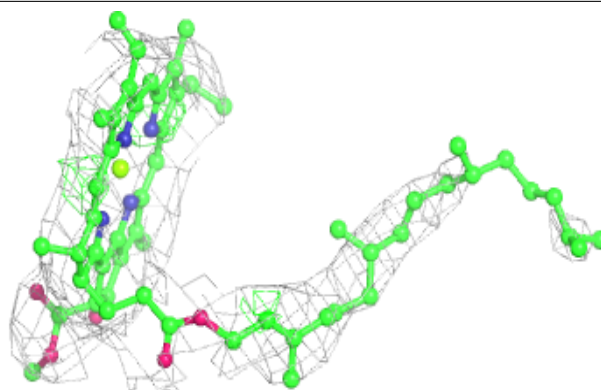
**Electron density around CLA 2 1231:**

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



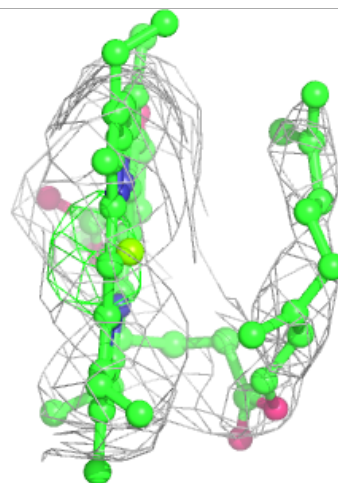
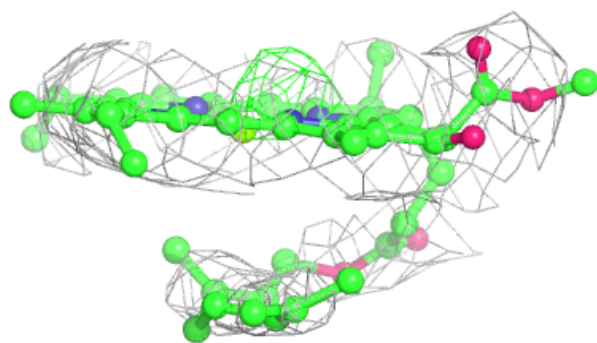
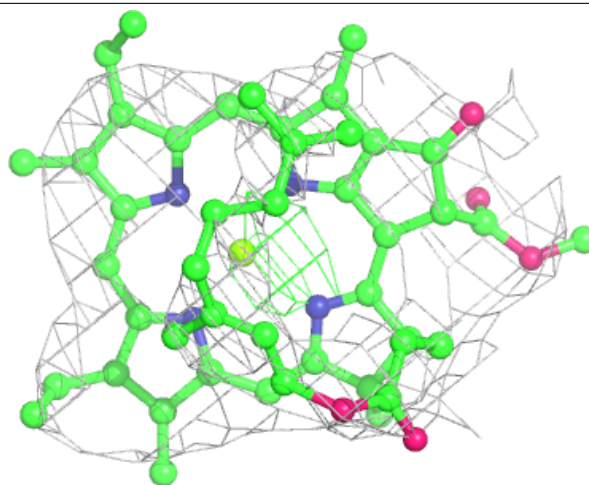
**Electron density around CLA A 1128:**

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



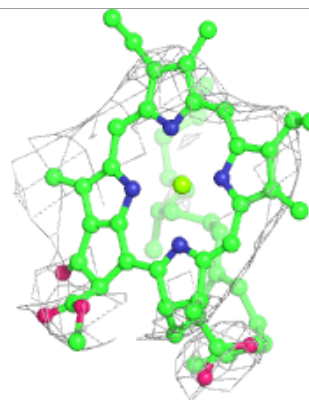
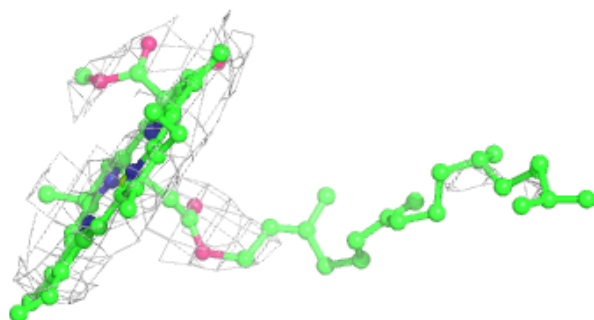
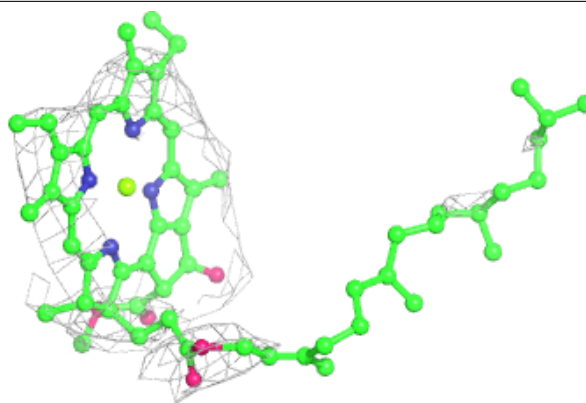
**Electron density around CLA B 1224:**

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

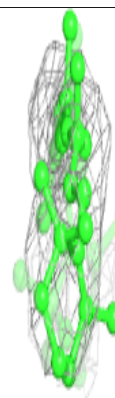
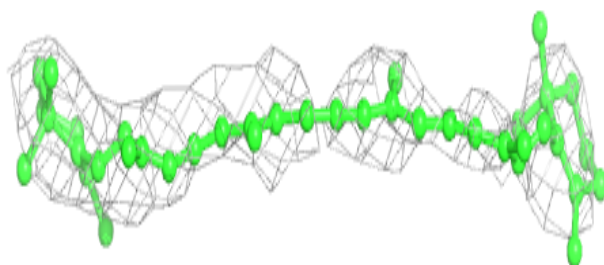
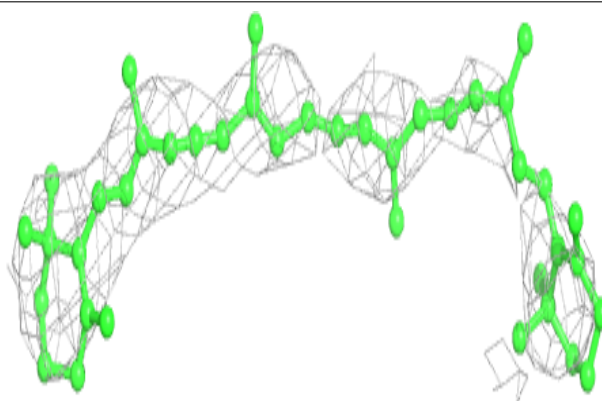


**Electron density around CLA 1 1137:**

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

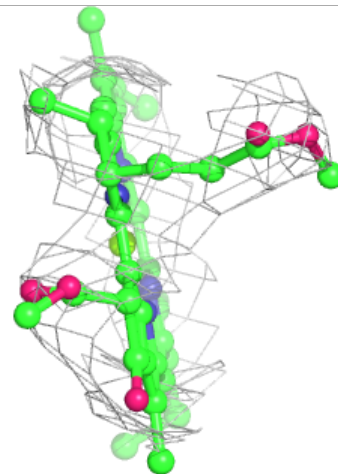
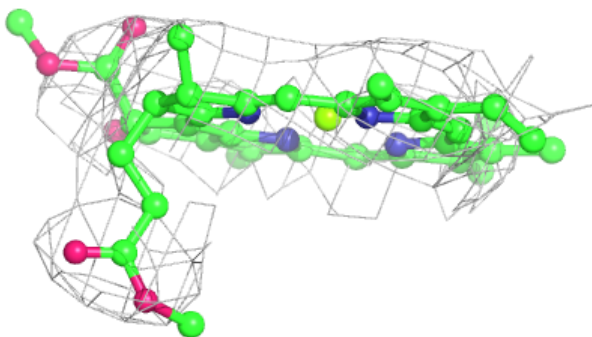
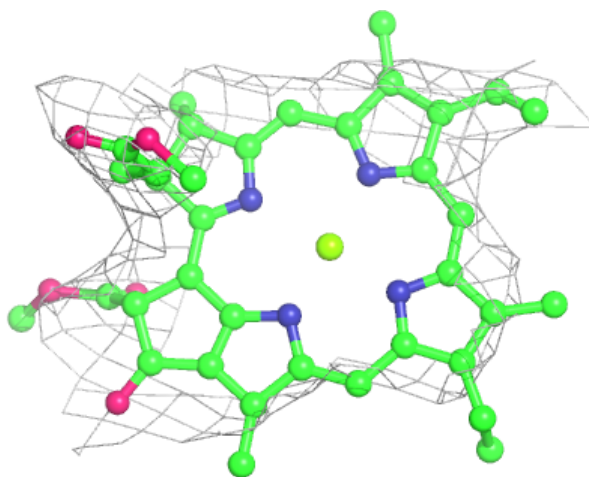
**Electron density around BCR f 4020:**

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



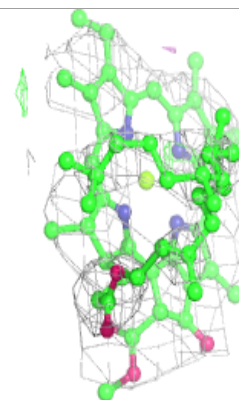
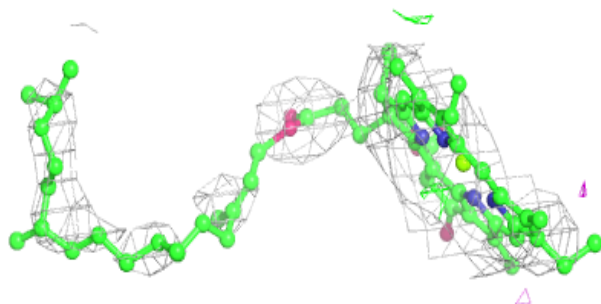
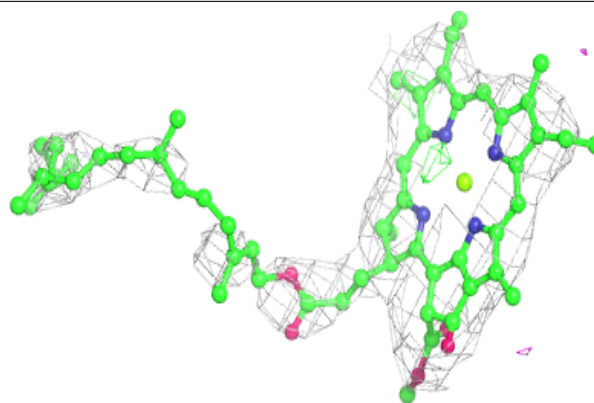
**Electron density around CLA 1 1130:**

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

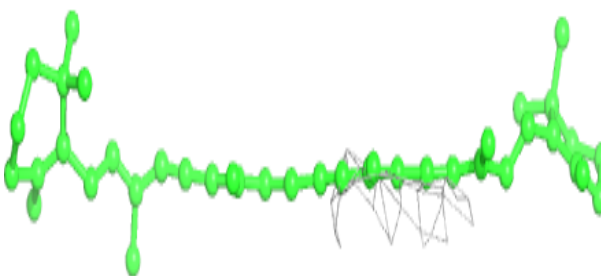
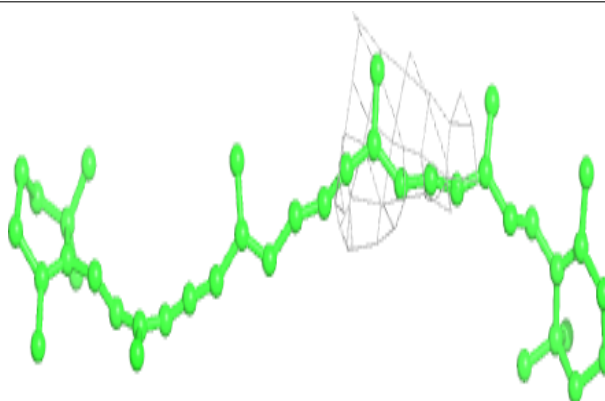


**Electron density around CLA B 1206:**

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

**Electron density around BCR b 4009:**

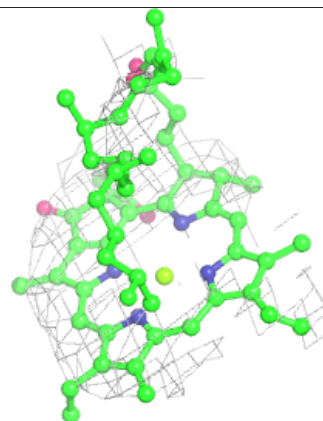
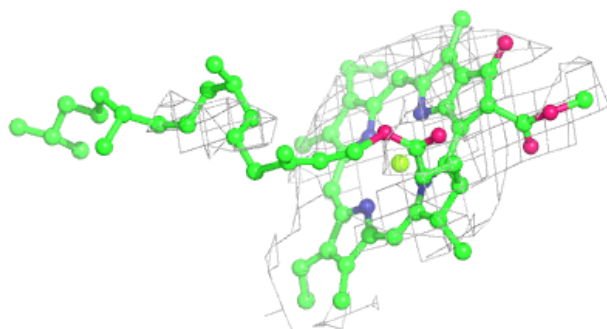
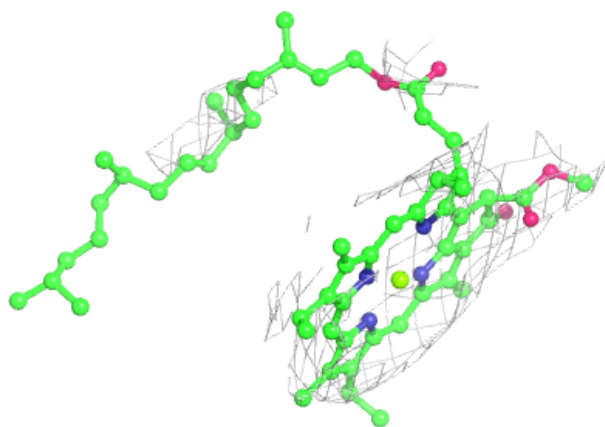
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



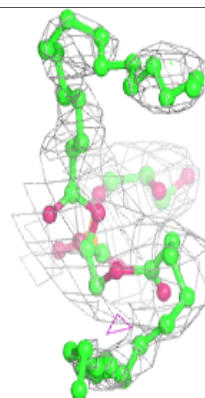
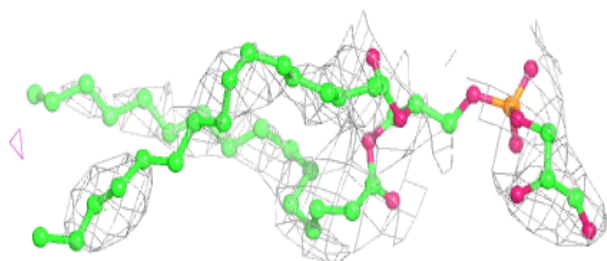
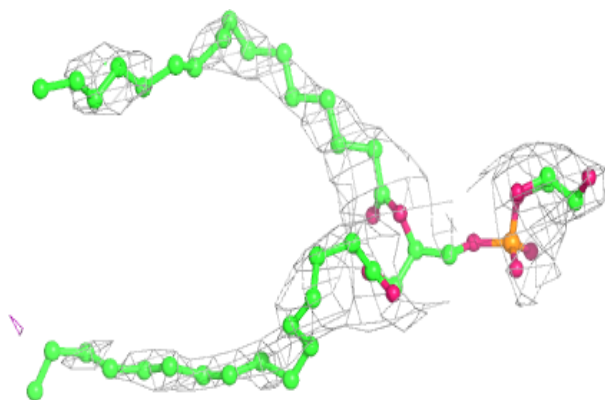


**Electron density around CLA a 1102:**

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

**Electron density around LHG A 5001:**

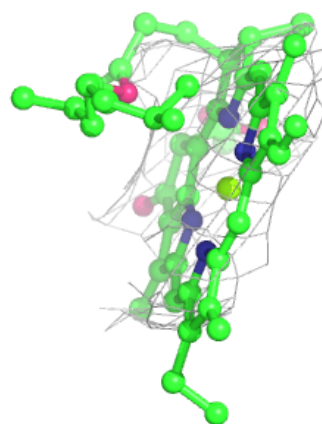
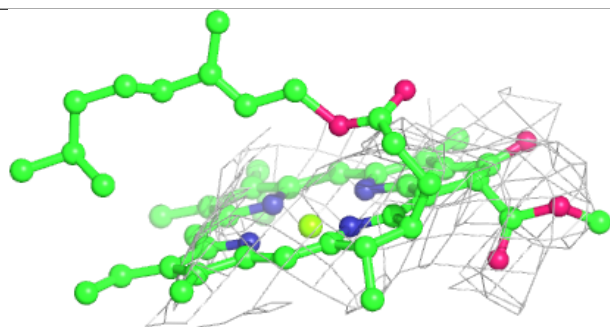
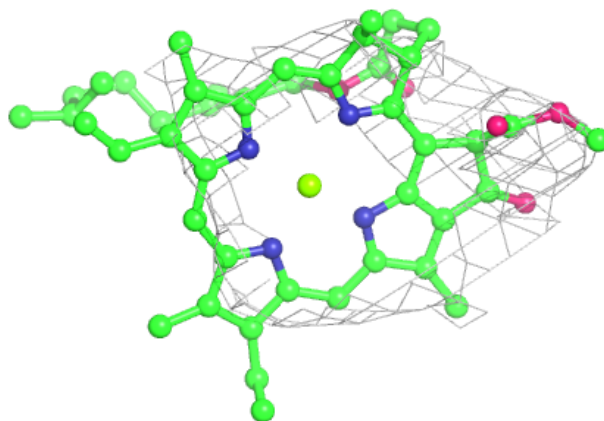
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





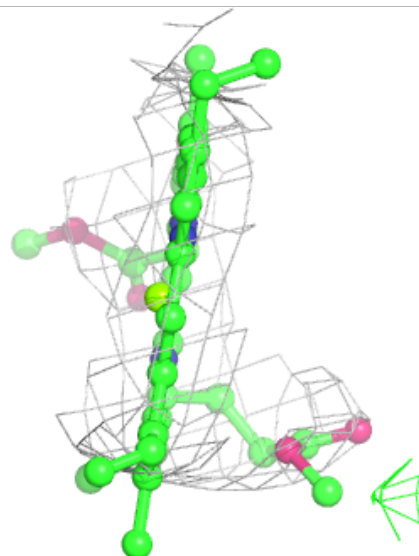
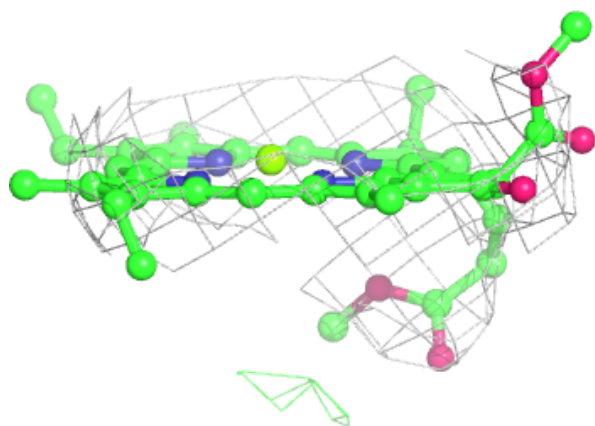
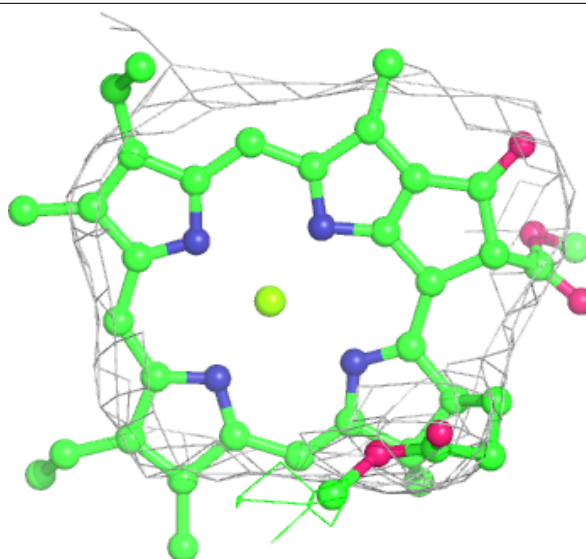
**Electron density around CLA b 1219:**

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



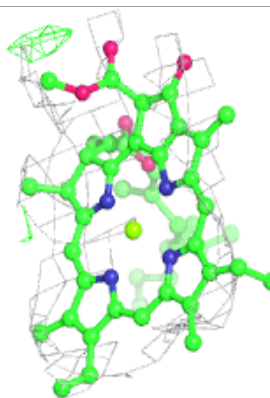
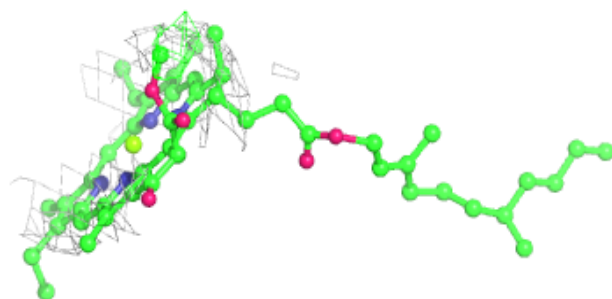
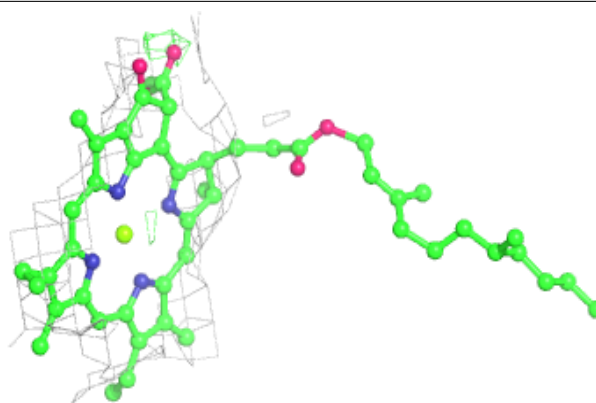
**Electron density around CLA a 1120:**

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



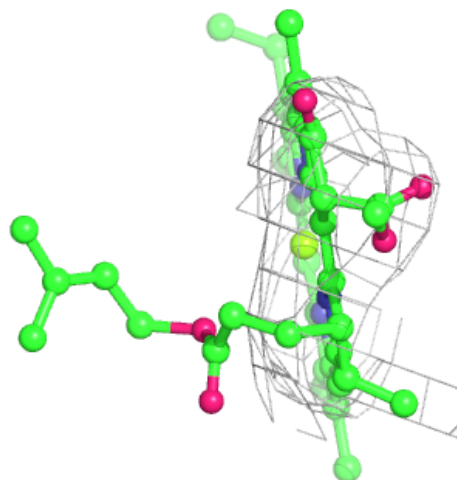
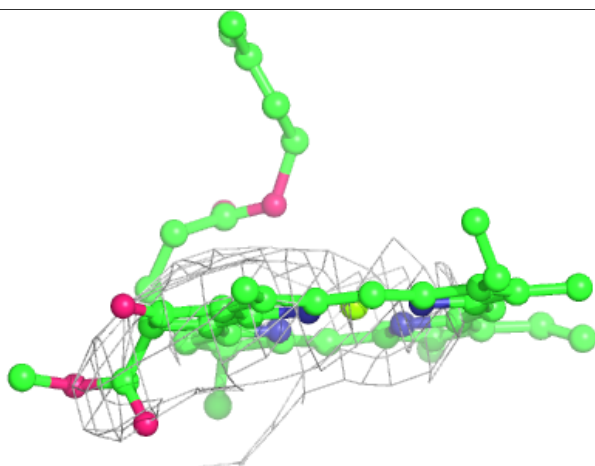
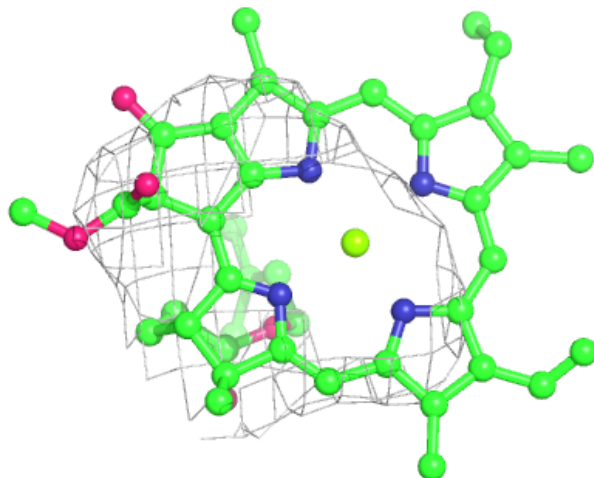
**Electron density around CLA b 1230:**

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



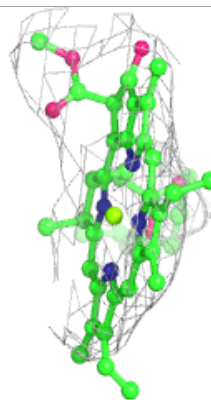
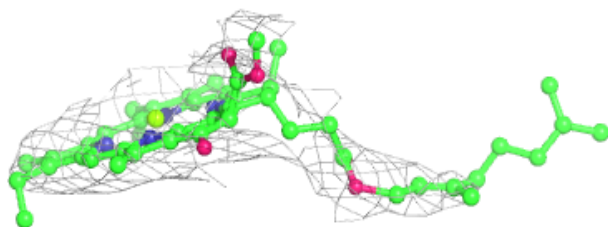
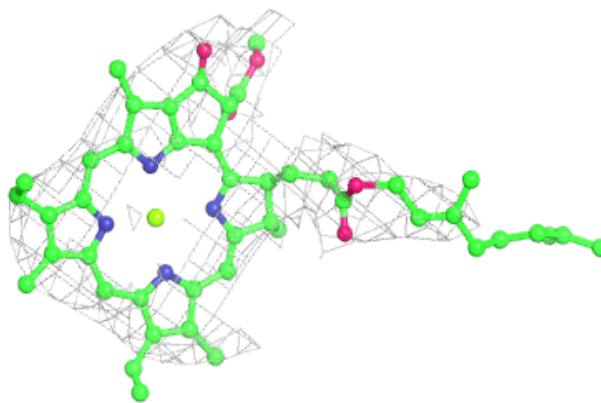
**Electron density around CLA 0 1402:**

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

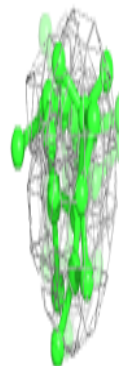
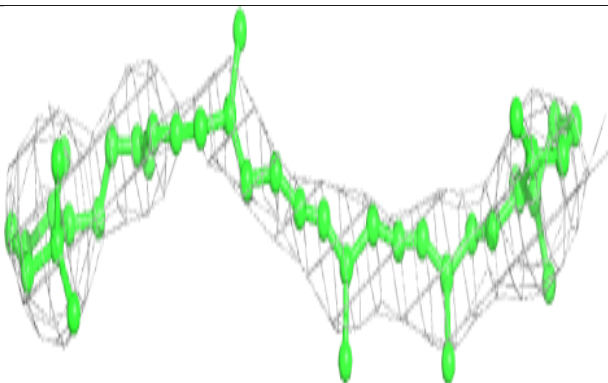
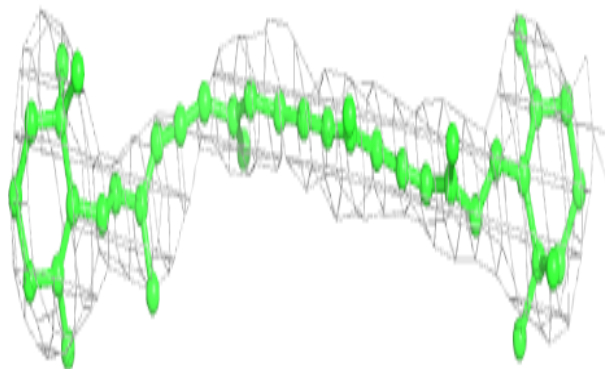


**Electron density around CLA 1 1124:**

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

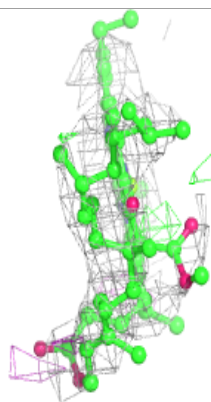
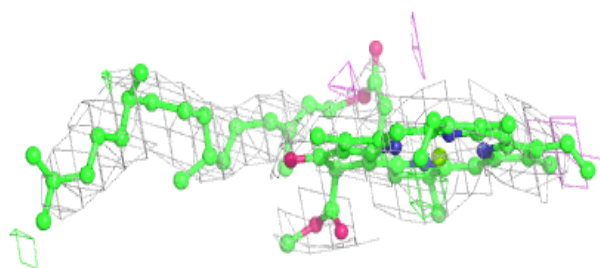
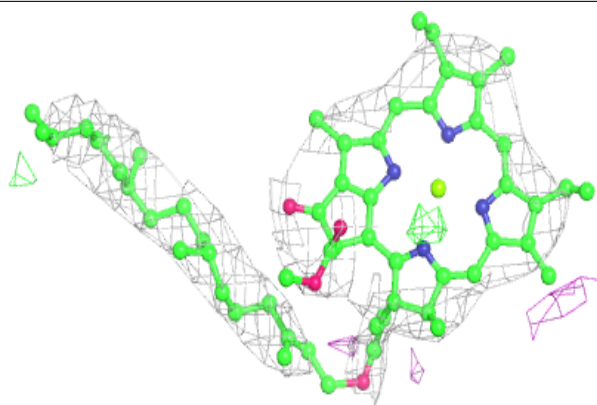
**Electron density around BCR A 4003:**

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

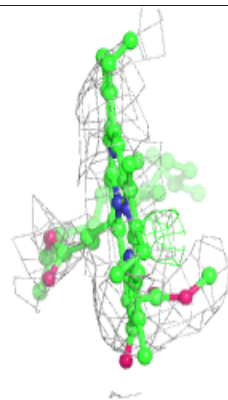
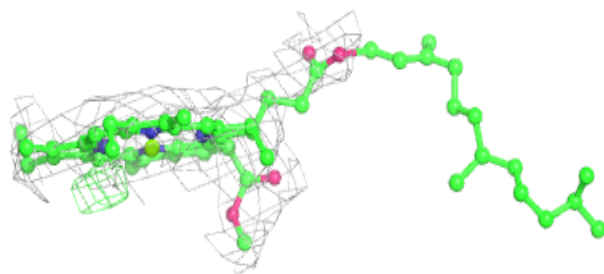
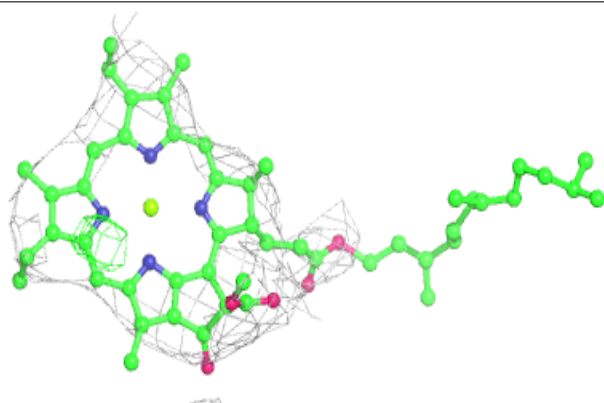


**Electron density around CLA L 1503:**

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

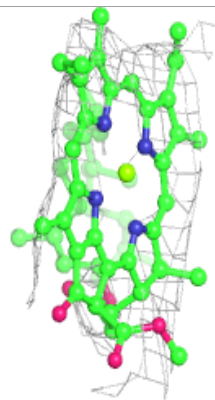
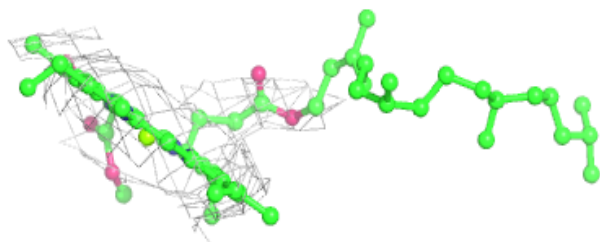
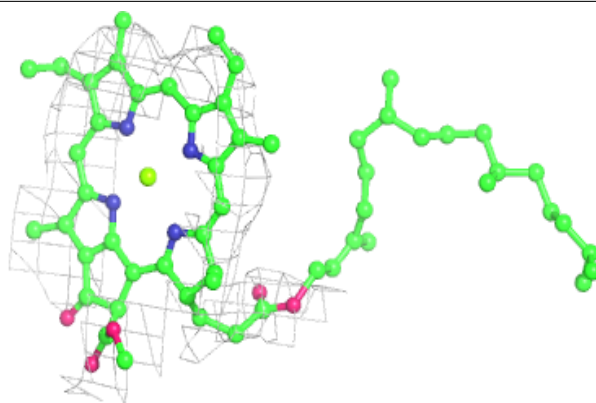
**Electron density around CLA B 1234:**

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



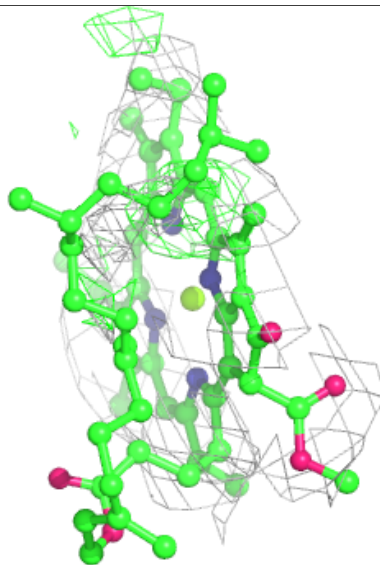
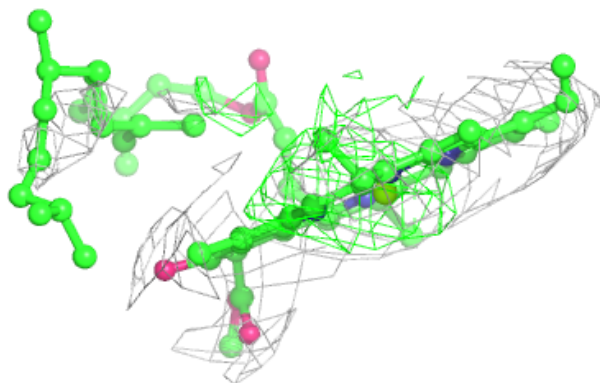
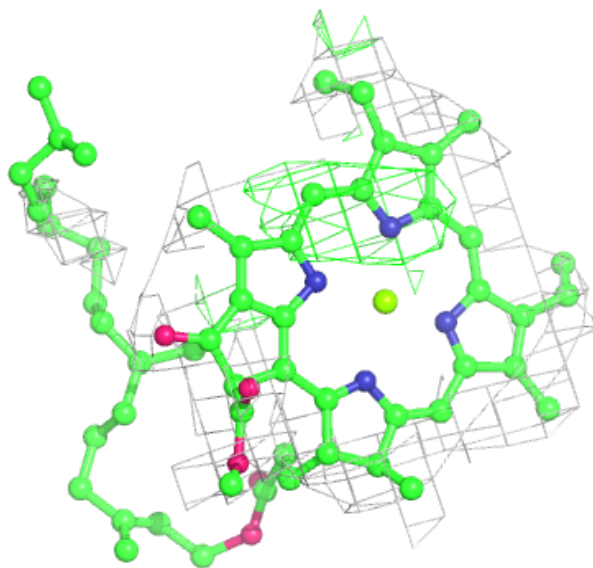
**Electron density around CLA a 1106:**

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



**Electron density around CLA 2 1229:**

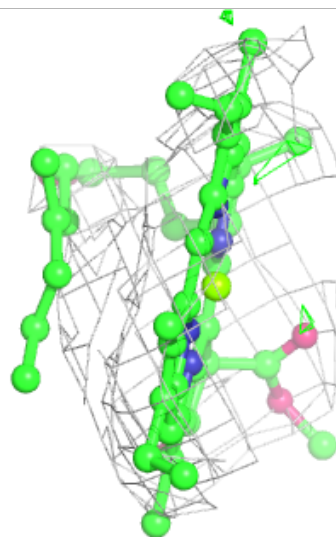
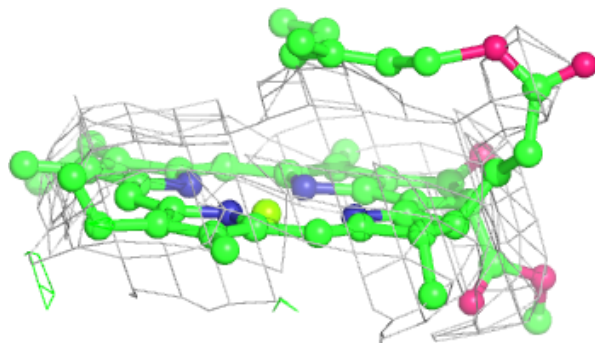
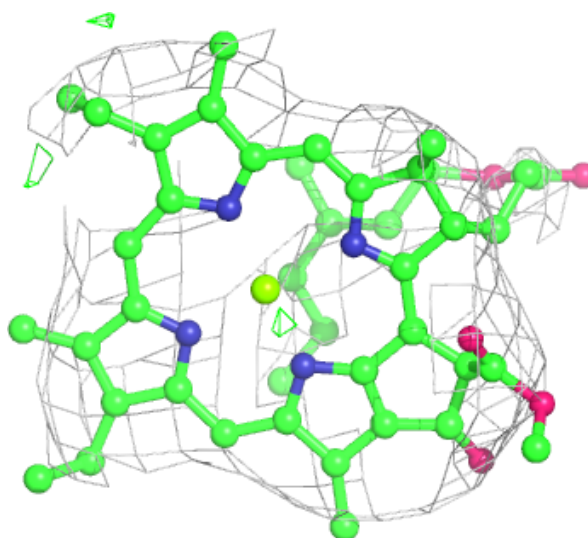
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





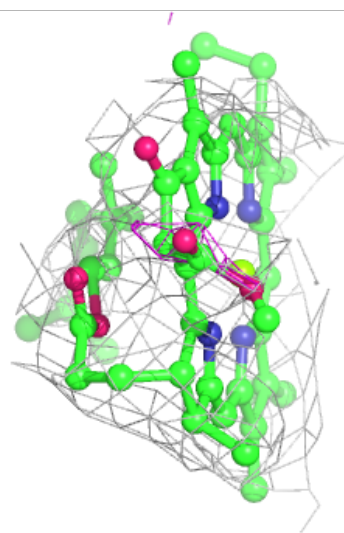
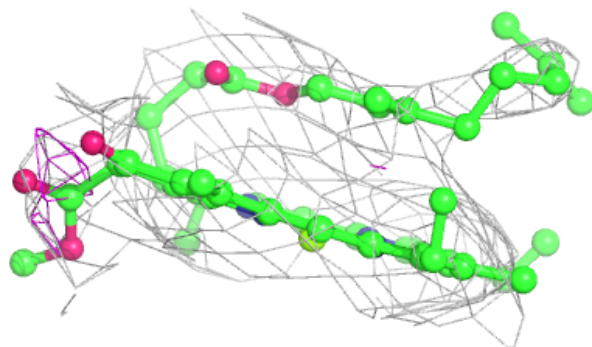
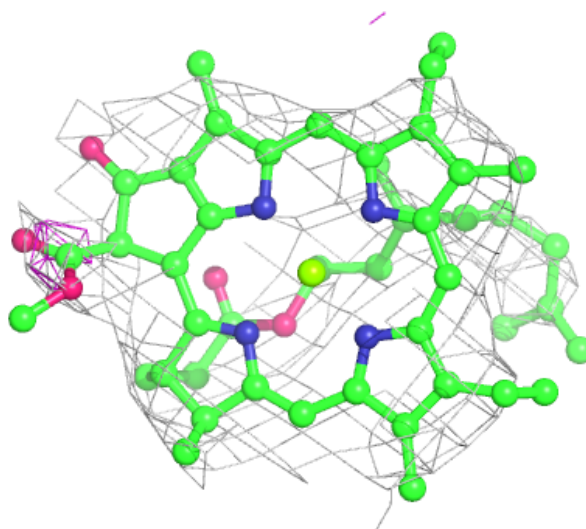
**Electron density around CLA a 1801:**

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



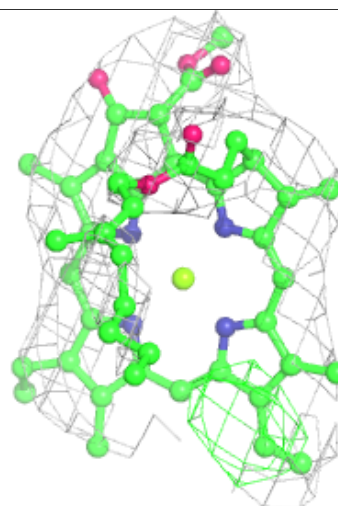
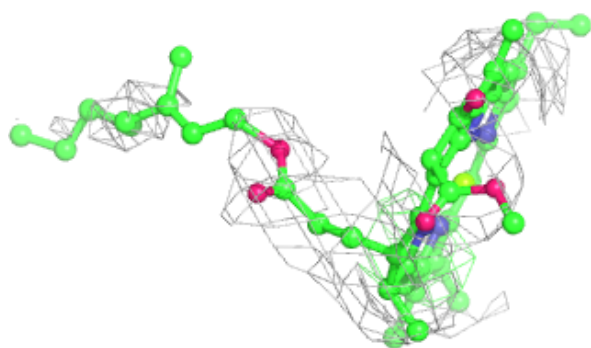
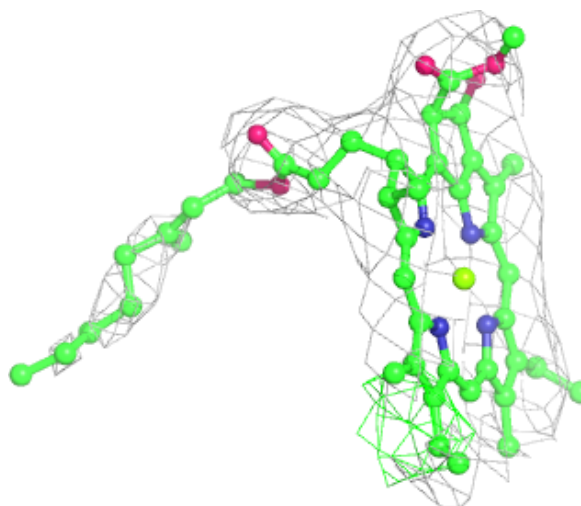
**Electron density around CLA B 1205:**

2mF<sub>o</sub>-DF<sub>c</sub> (at 0.7 rmsd) in gray  
mF<sub>o</sub>-DF<sub>c</sub> (at 3 rmsd) in purple (negative)  
and green (positive)



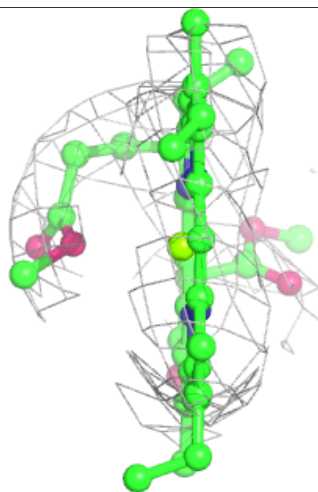
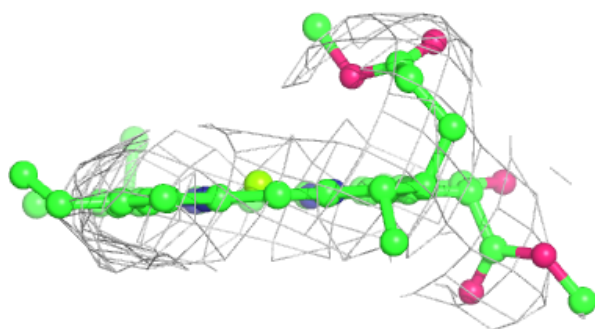
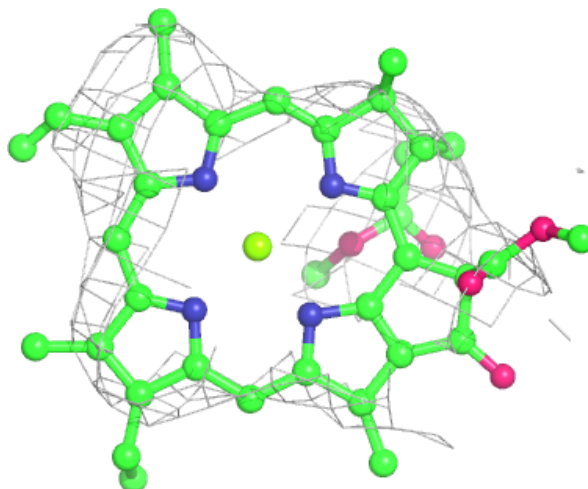
**Electron density around CLA 2 1201:**

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



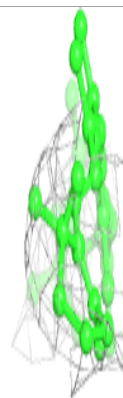
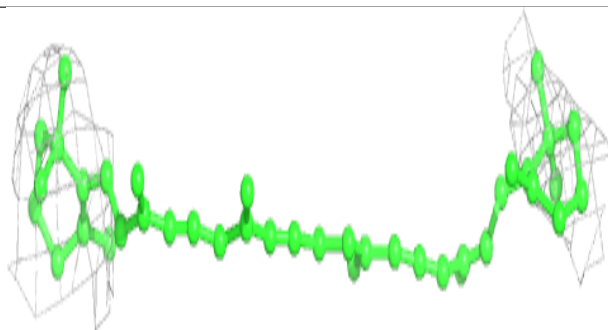
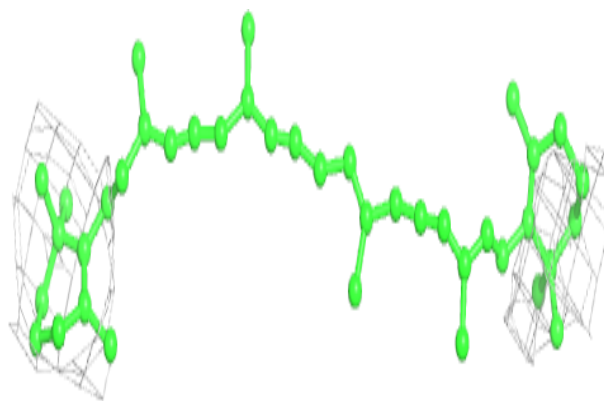
**Electron density around CLA a 1136:**

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



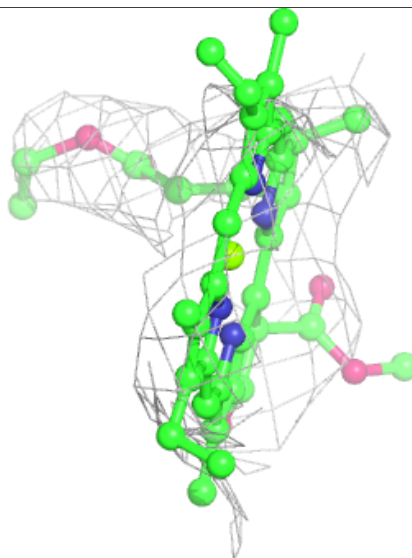
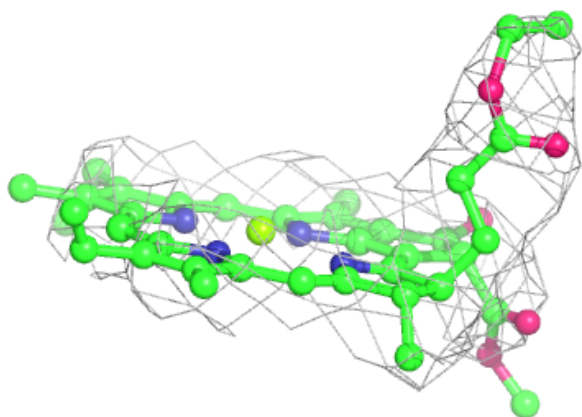
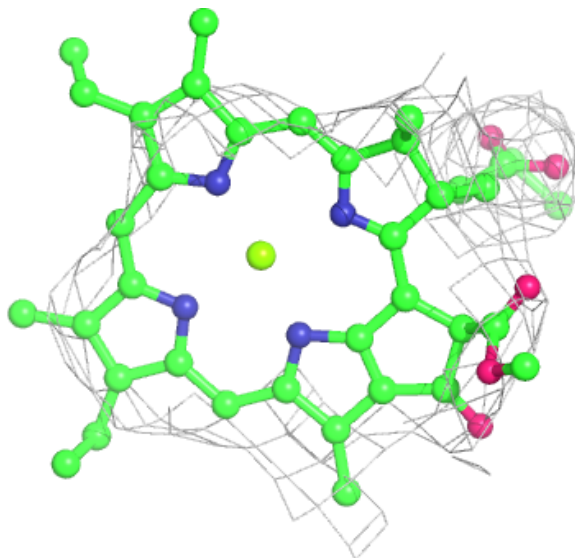
**Electron density around BCR a 4001:**

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



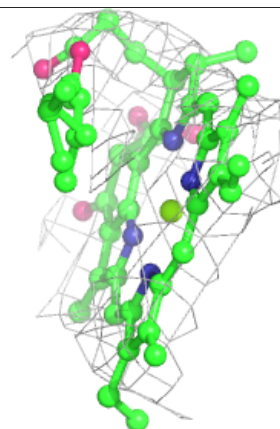
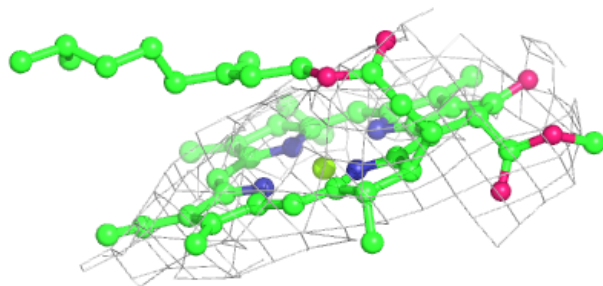
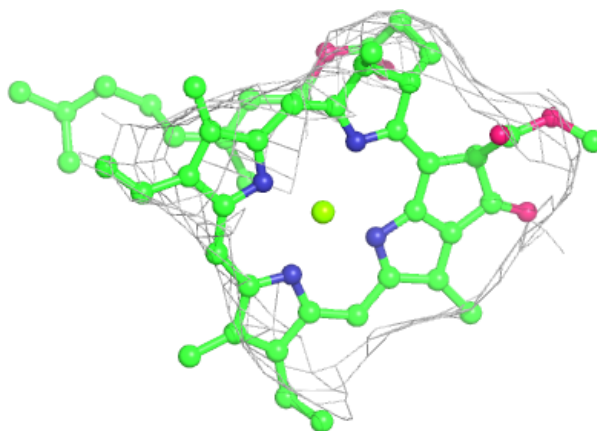
**Electron density around CLA 2 1236:**

2mF<sub>o</sub>-DF<sub>c</sub> (at 0.7 rmsd) in gray  
mF<sub>o</sub>-DF<sub>c</sub> (at 3 rmsd) in purple (negative)  
and green (positive)



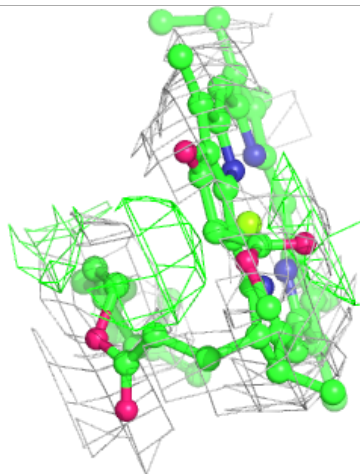
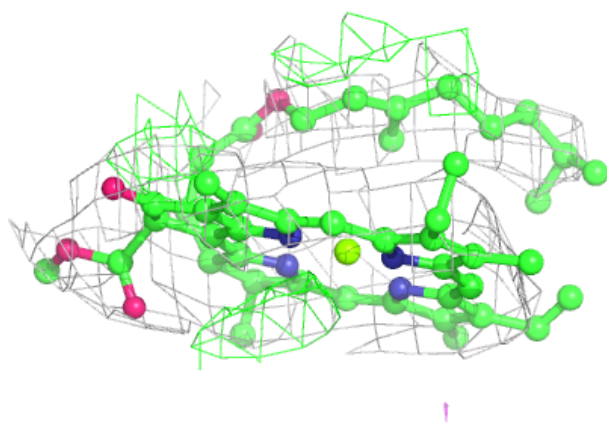
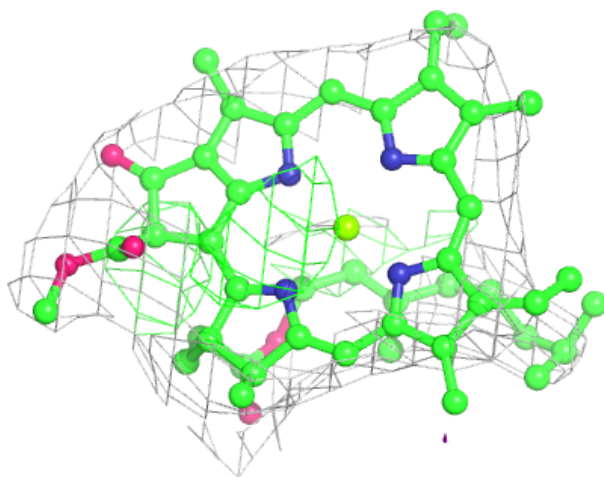
**Electron density around CLA 2 1219:**

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



**Electron density around CLA 1 1237:**

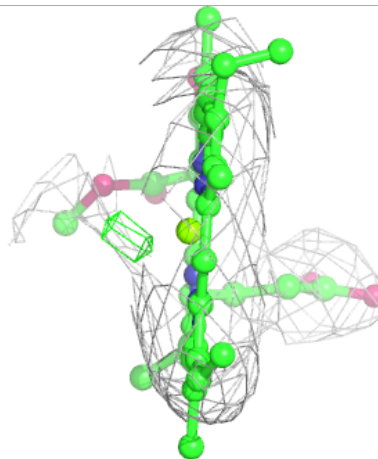
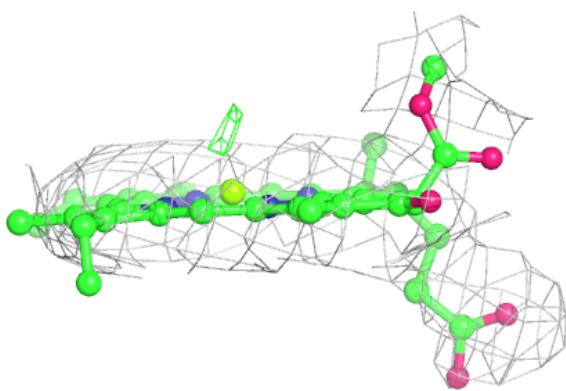
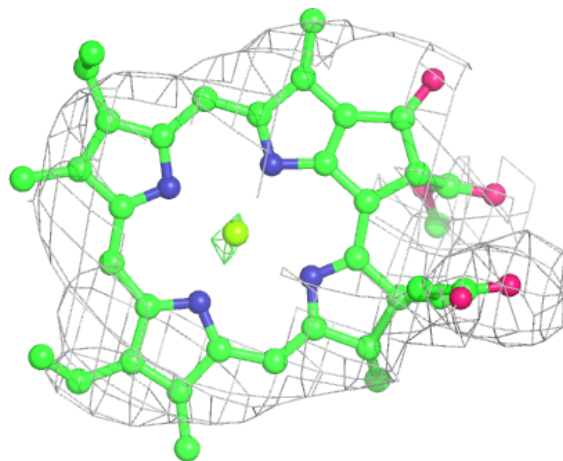
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





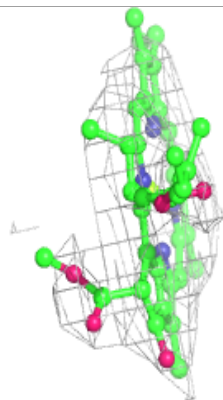
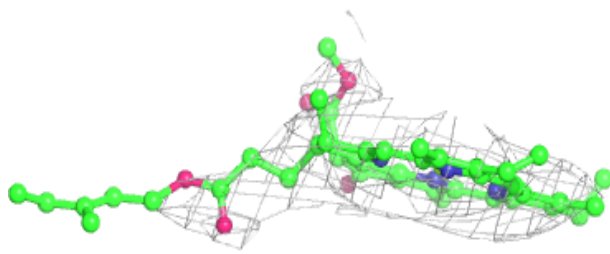
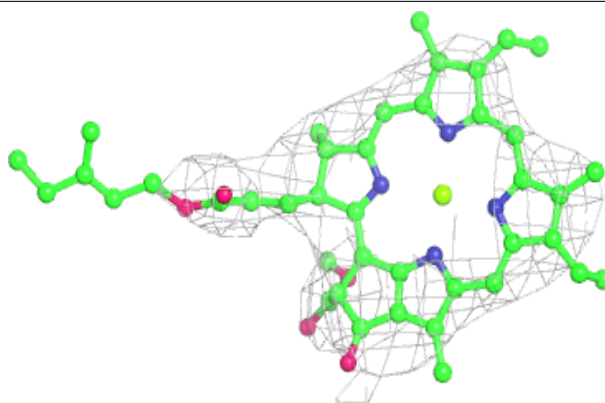
**Electron density around CLA 2 1212:**

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



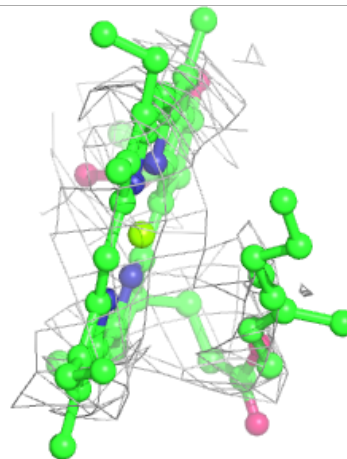
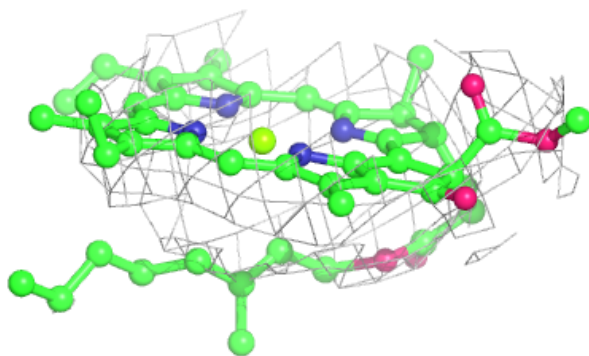
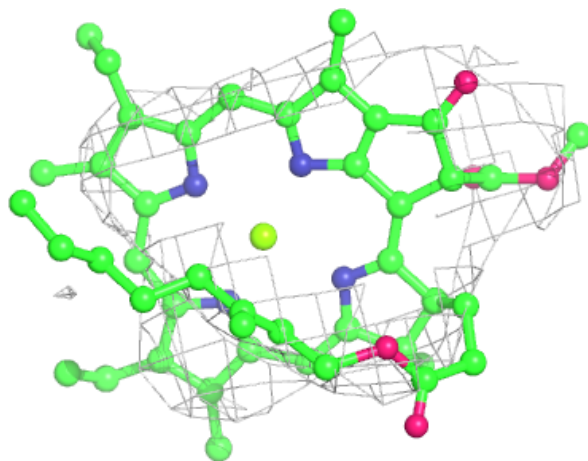
**Electron density around CLA 1 1135:**

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



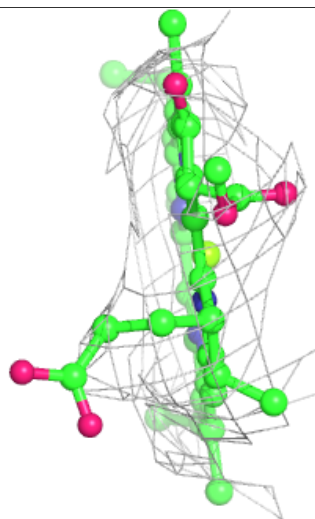
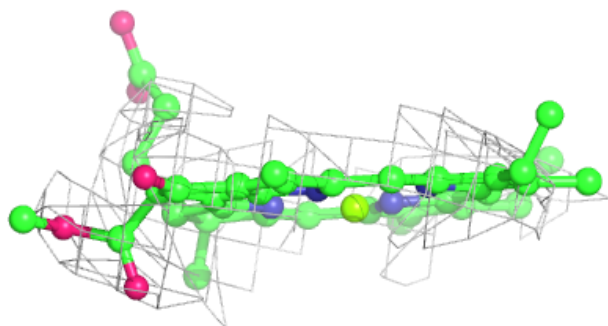
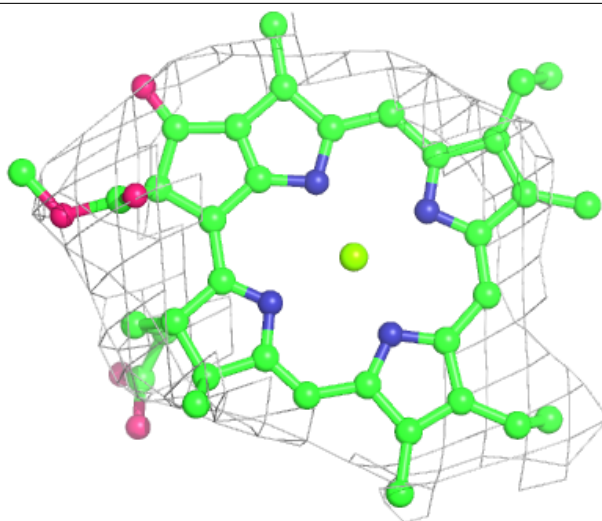
**Electron density around CLA 1 1116:**

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



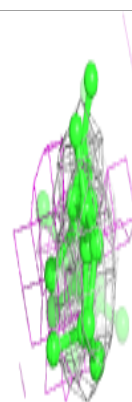
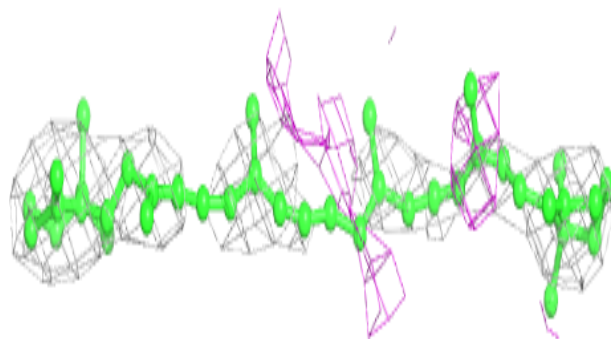
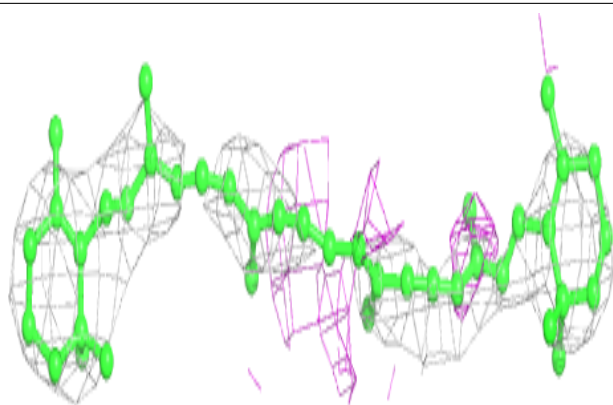
**Electron density around CLA 2 1232:**

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

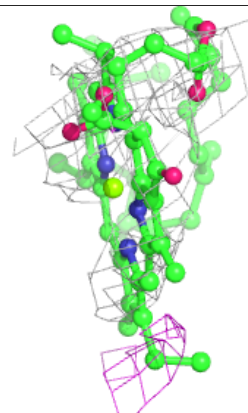
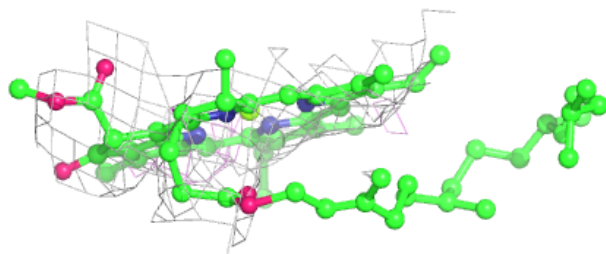
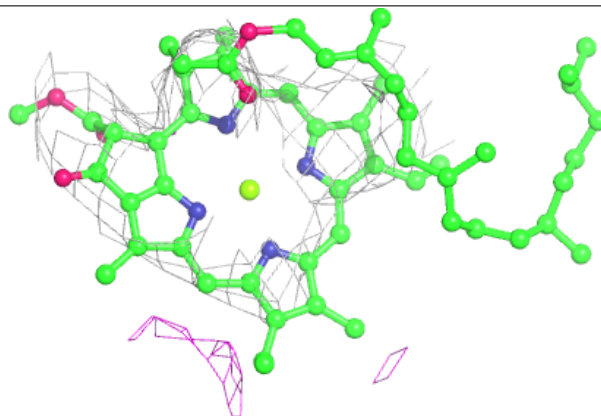


**Electron density around BCR L 4019:**

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

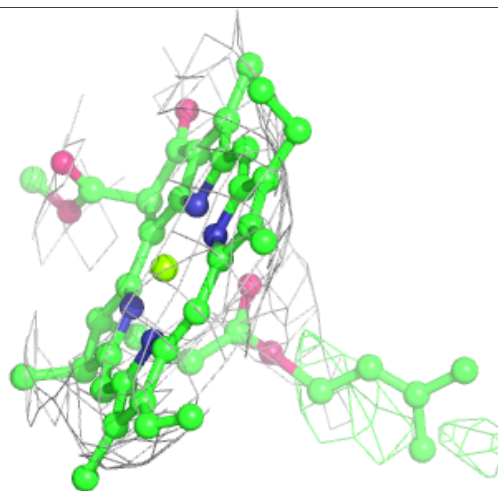
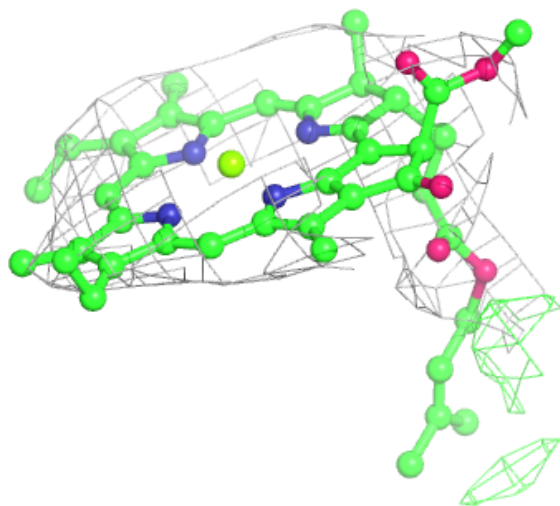
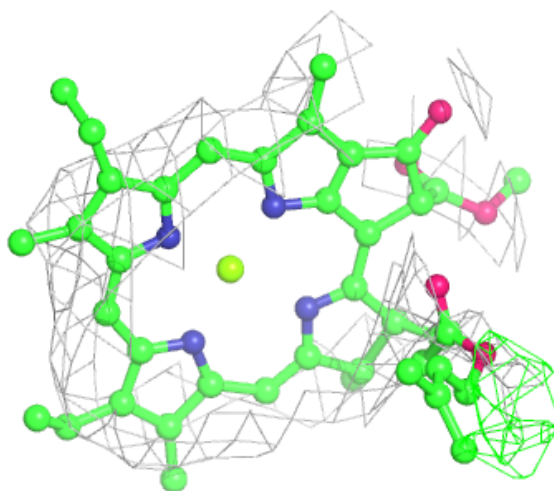
**Electron density around CLA a 1117:**

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



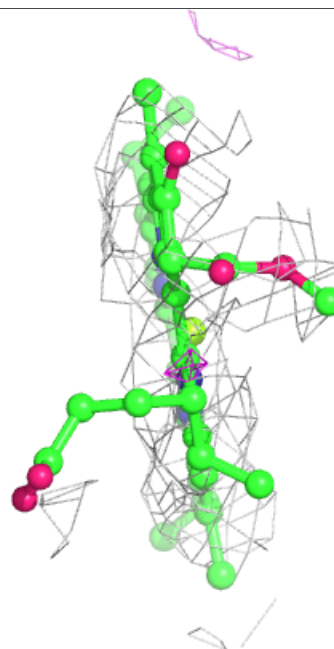
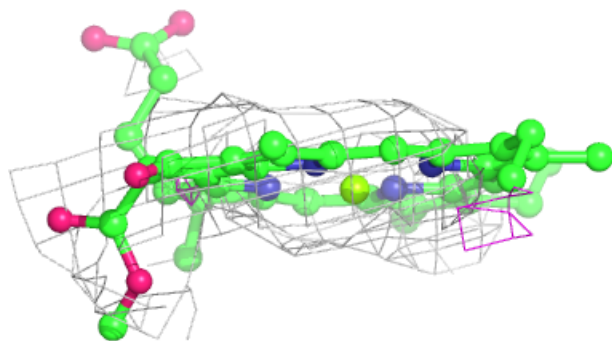
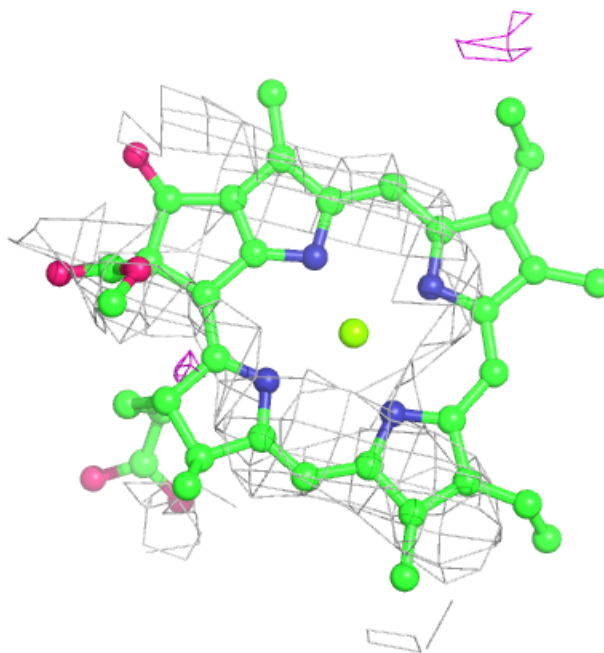
**Electron density around CLA b 1228:**

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



**Electron density around CLA 2 1227:**

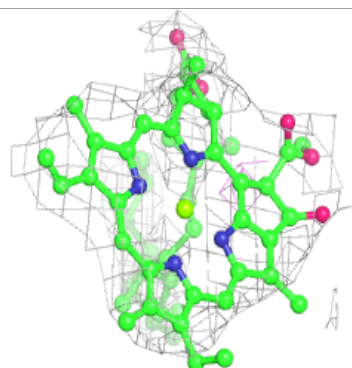
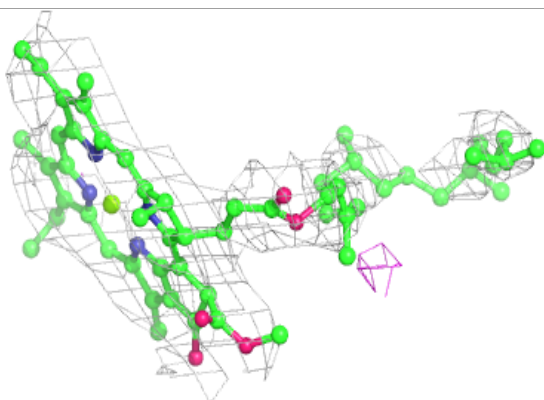
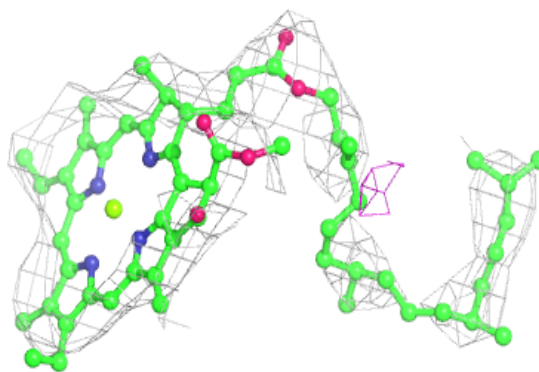
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



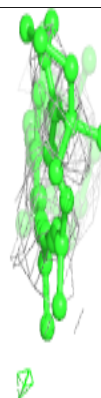
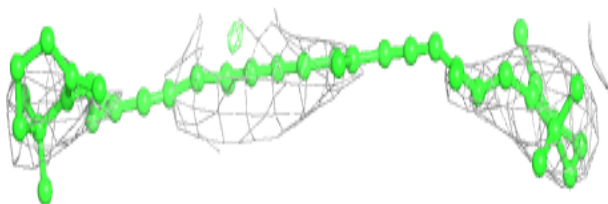
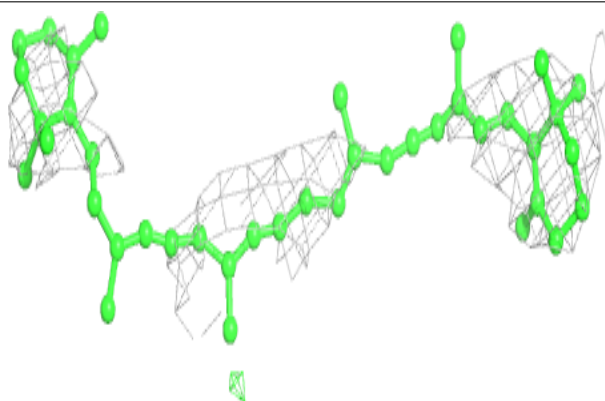


**Electron density around CLA A 1011:**

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

**Electron density around BCR B 4004:**

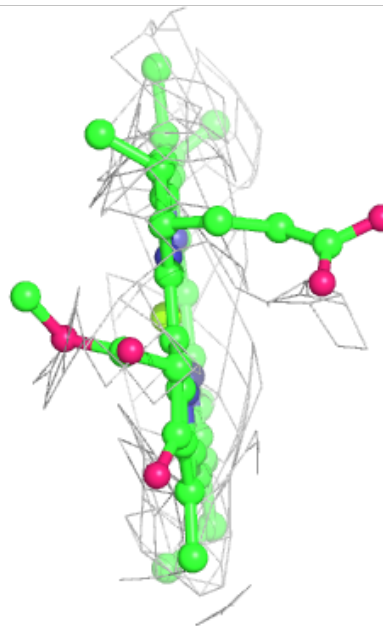
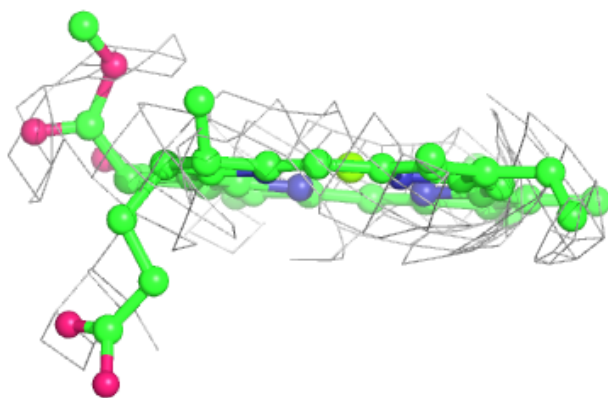
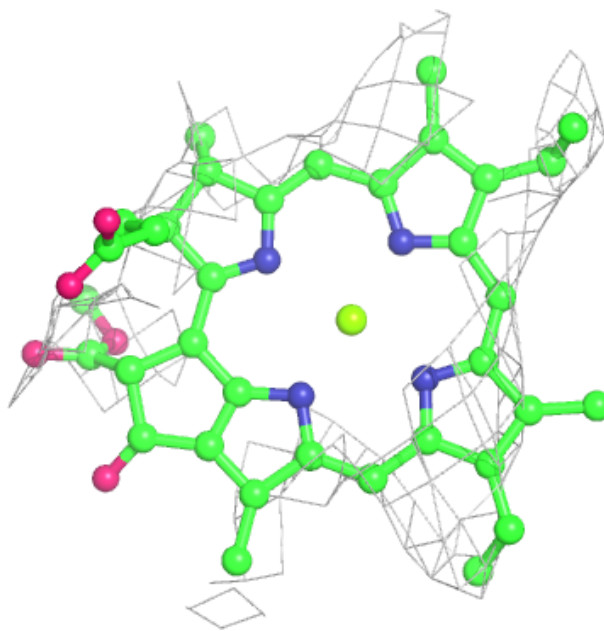
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





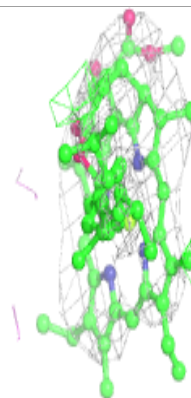
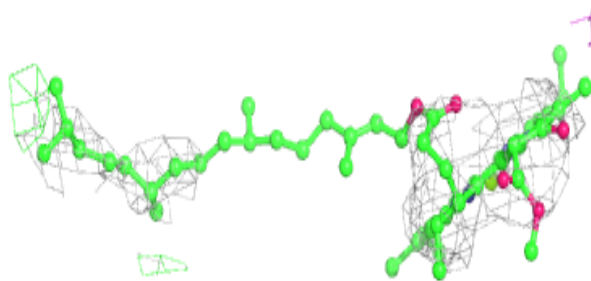
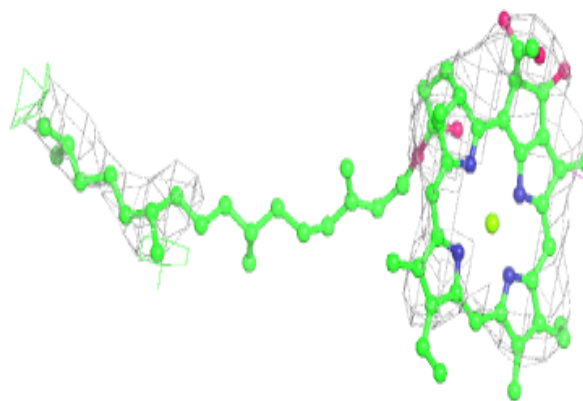
**Electron density around CLA b 1227:**

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



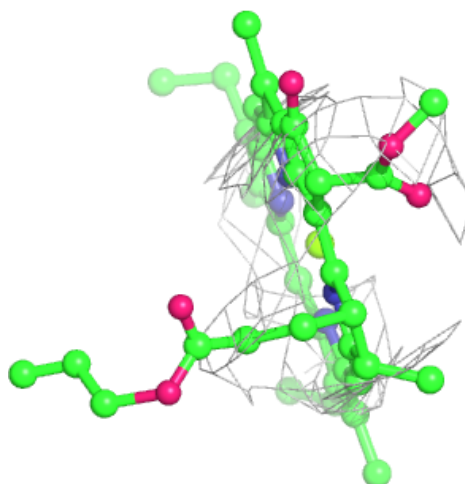
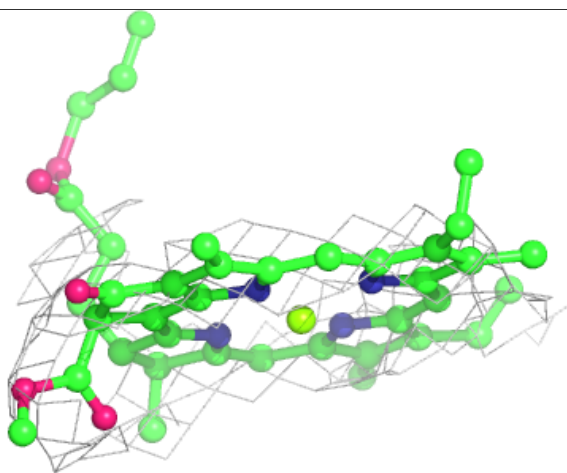
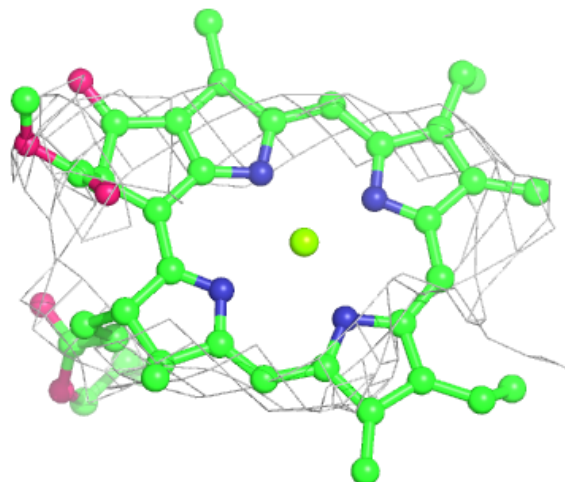
**Electron density around CLA 1 1501:**

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



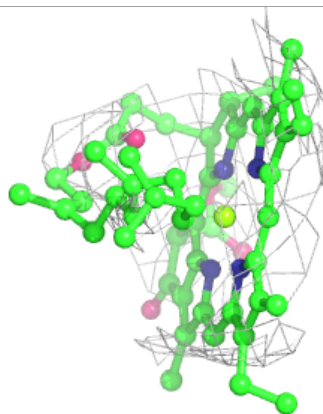
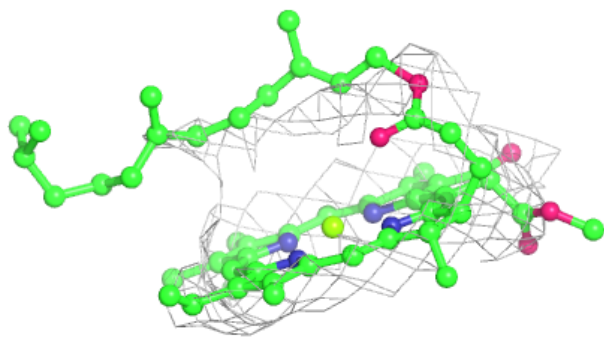
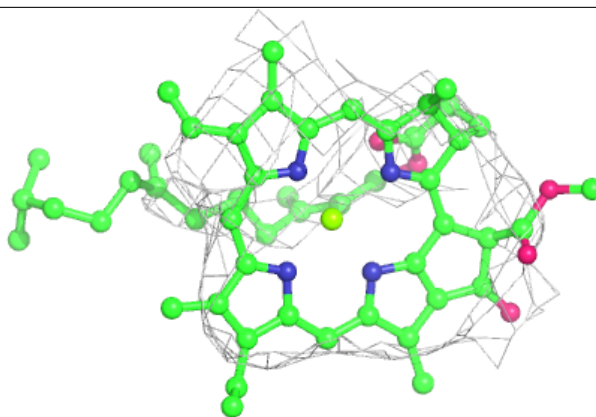
**Electron density around CLA a 1105:**

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



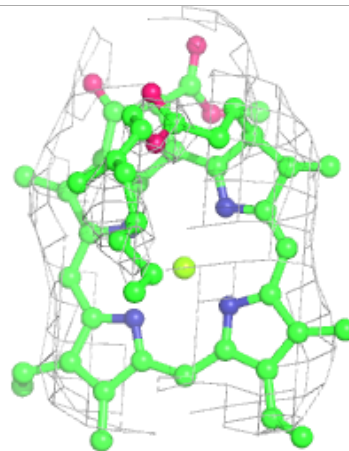
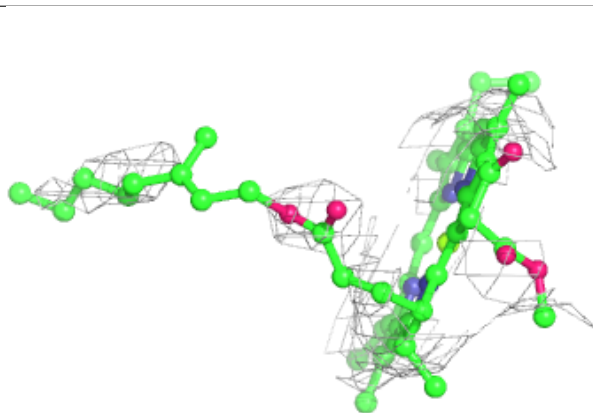
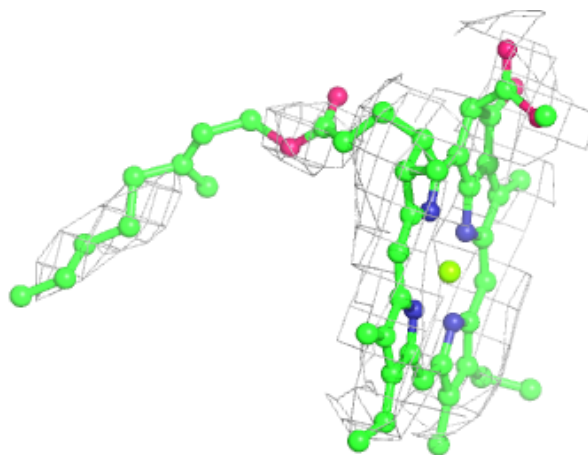
**Electron density around CLA 2 1235:**

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



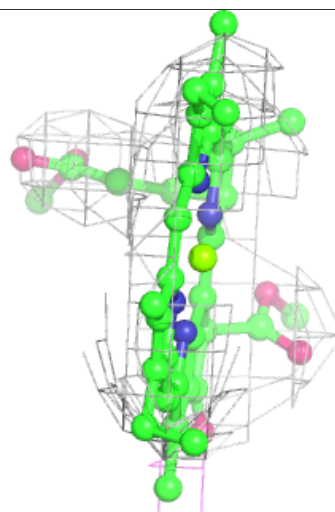
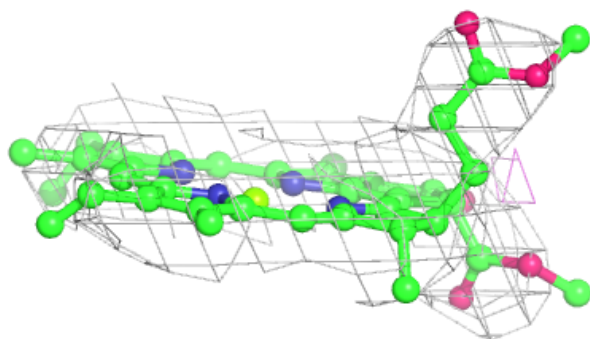
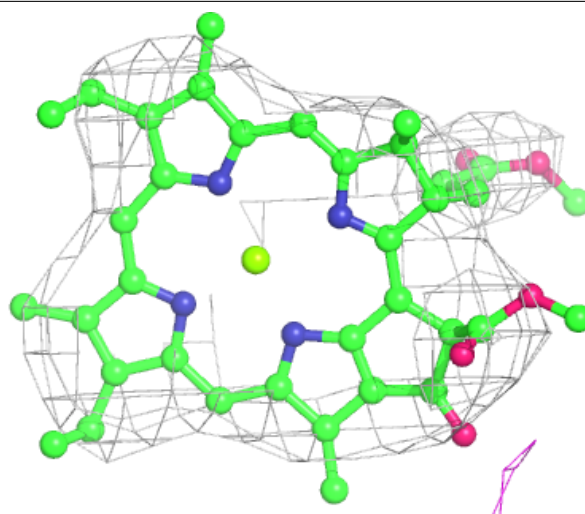
**Electron density around CLA b 1201:**

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



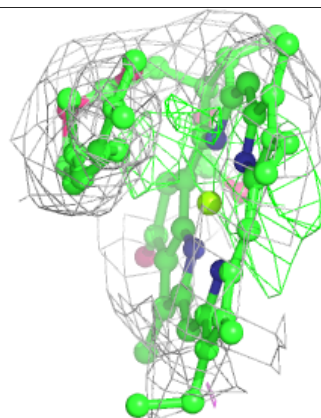
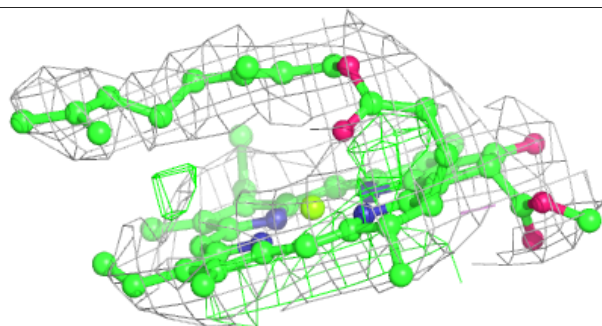
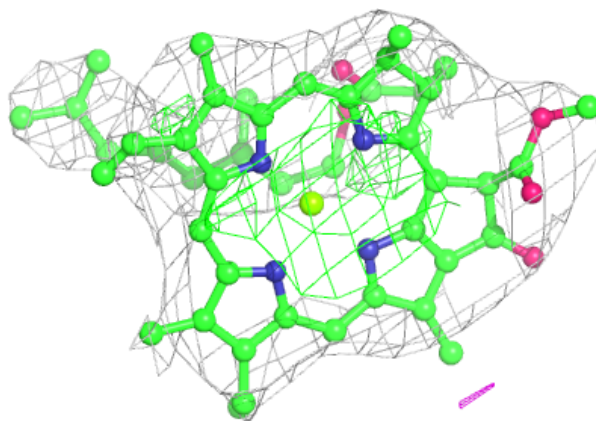
**Electron density around CLA B 1239:**

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



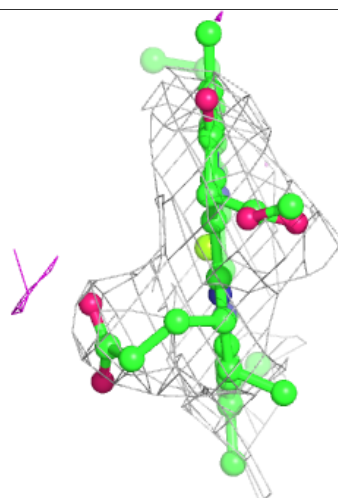
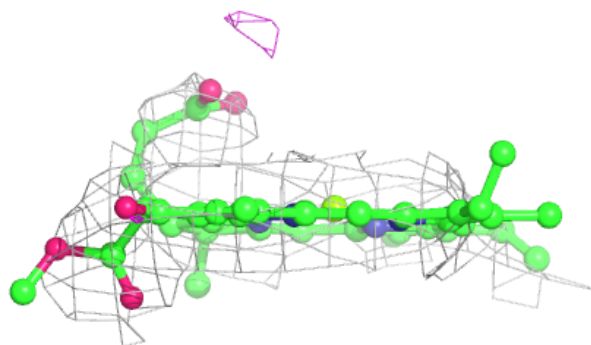
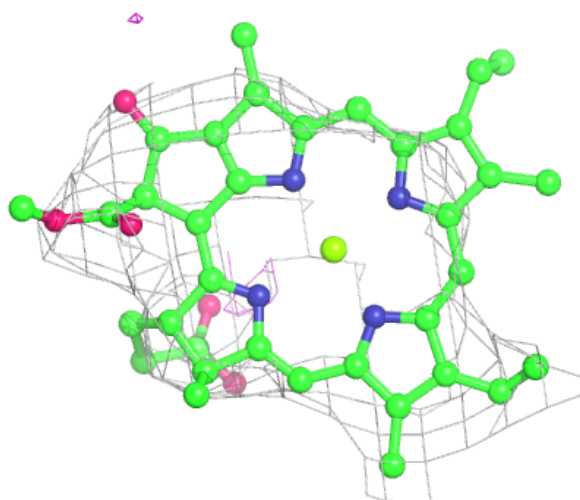
**Electron density around CLA A 1237:**

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



**Electron density around CLA B 1209:**

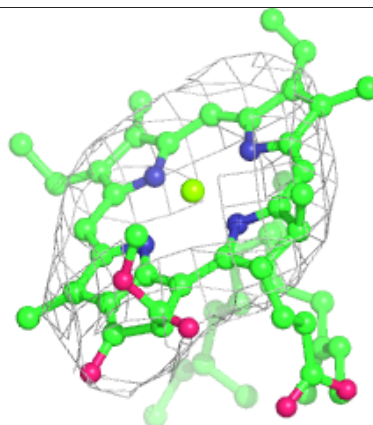
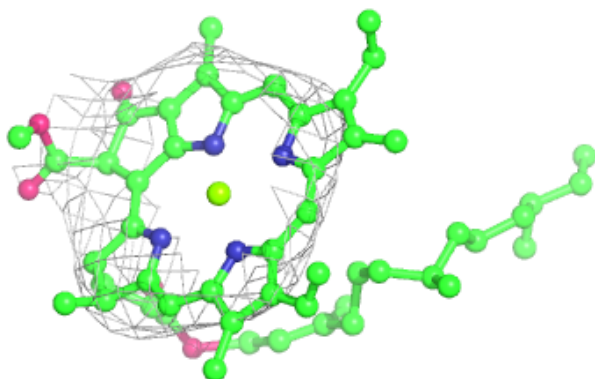
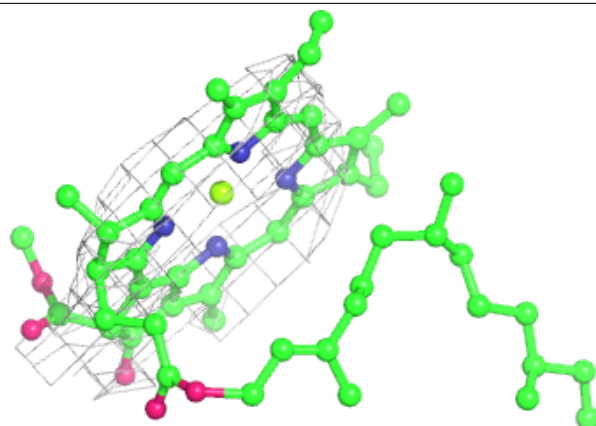
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





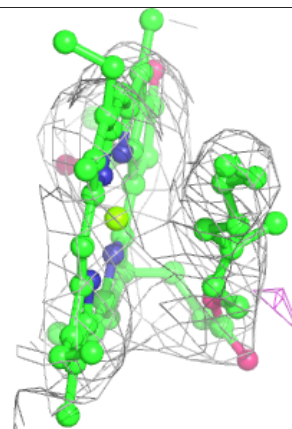
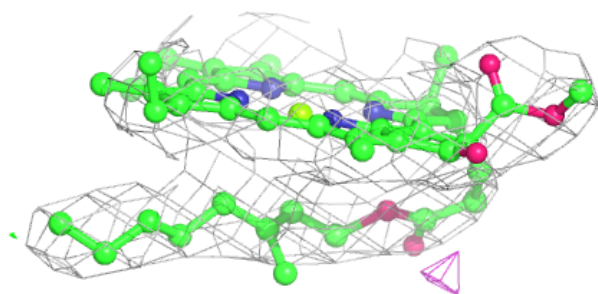
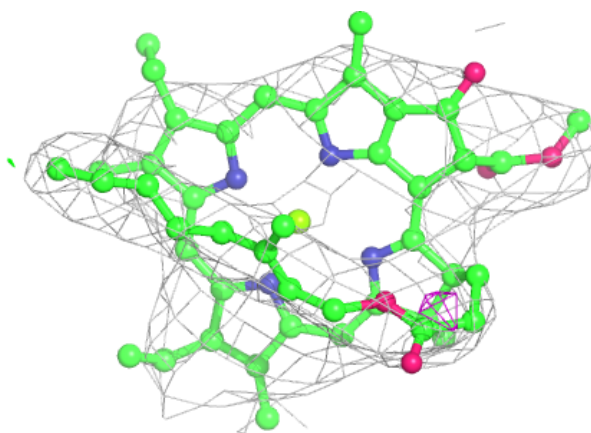
**Electron density around CLA a 1118:**

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



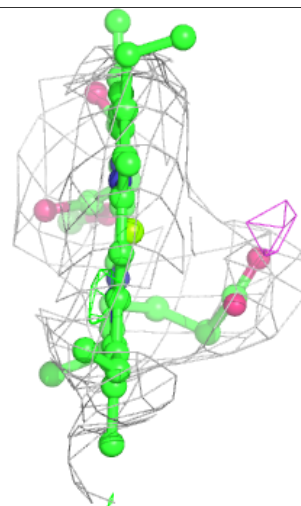
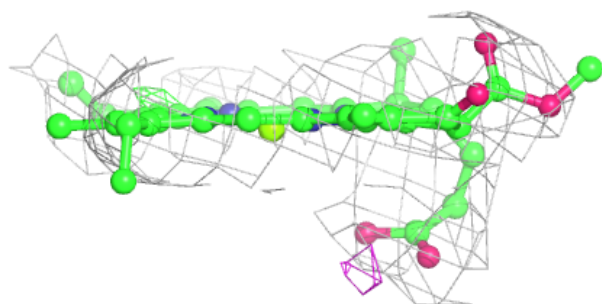
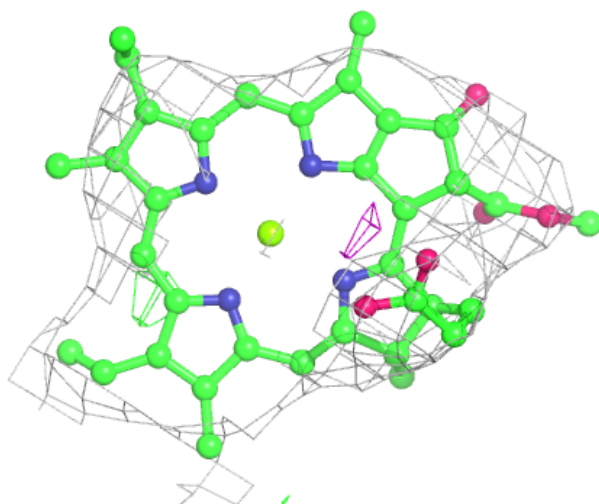
**Electron density around CLA A 1116:**

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



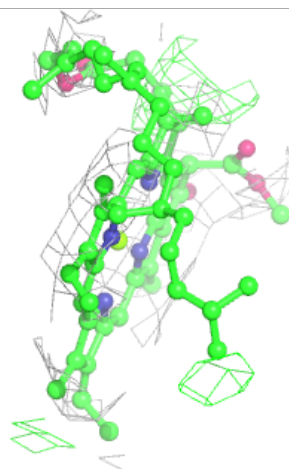
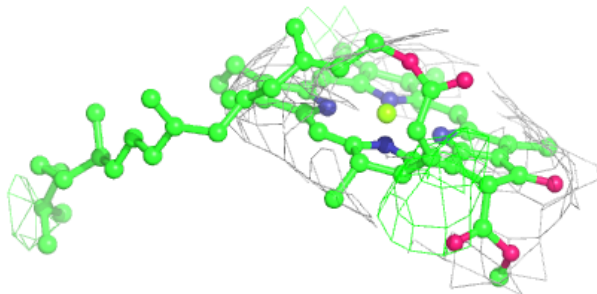
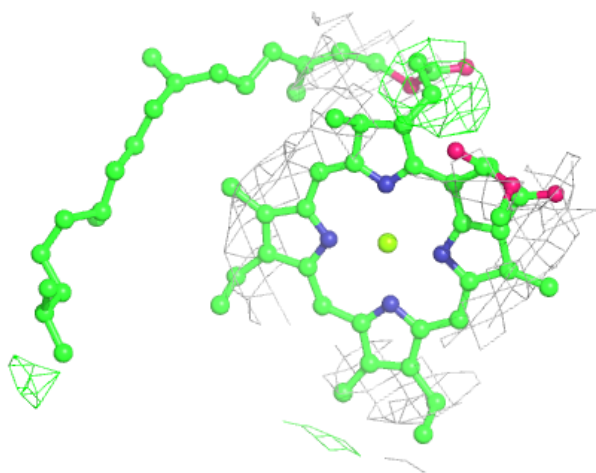
**Electron density around CLA 2 1209:**

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



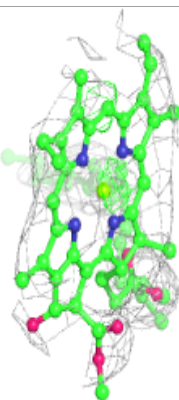
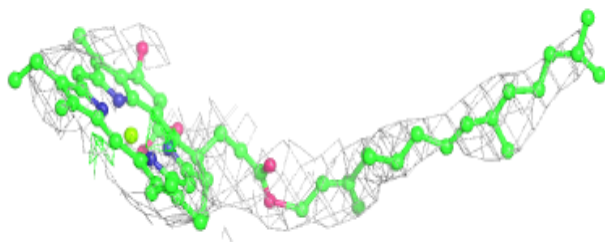
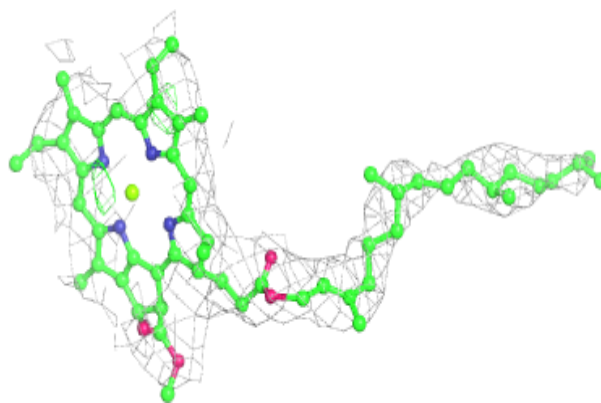
**Electron density around CLA k 1401:**

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

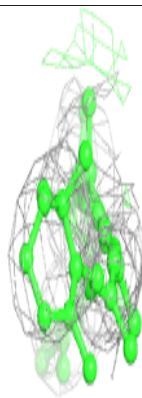
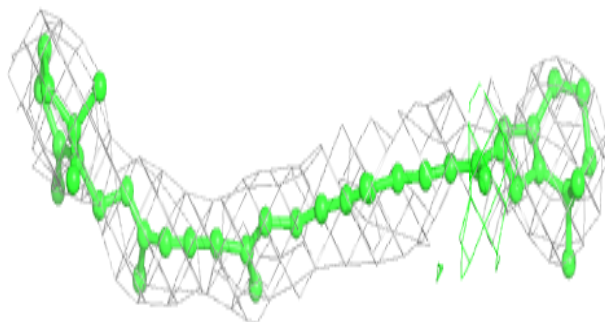
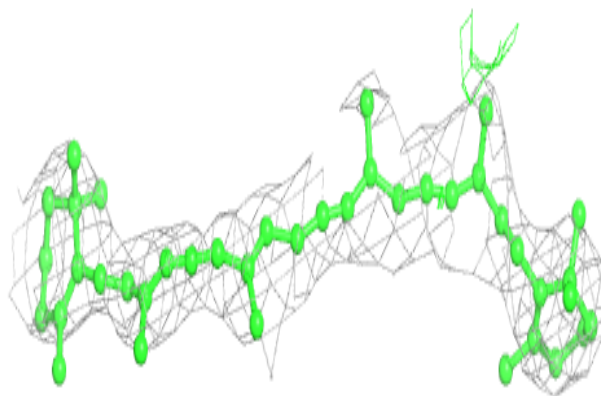


**Electron density around CLA A 1022:**

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

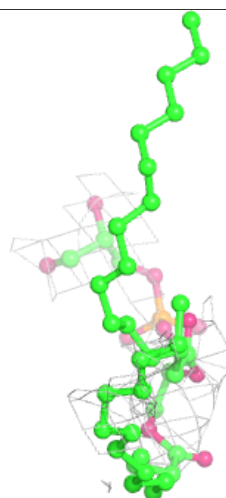
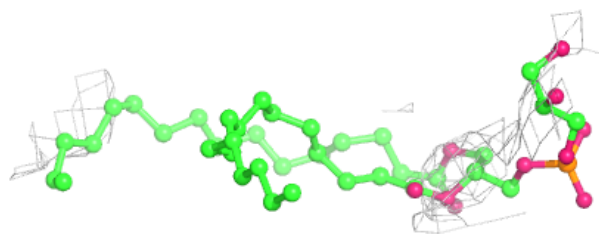
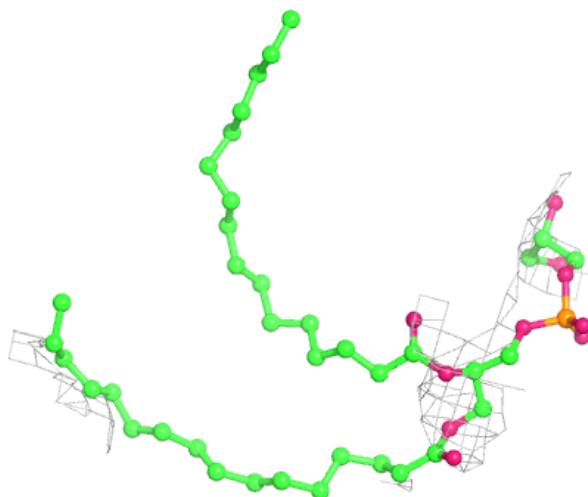
**Electron density around BCR M 4021:**

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



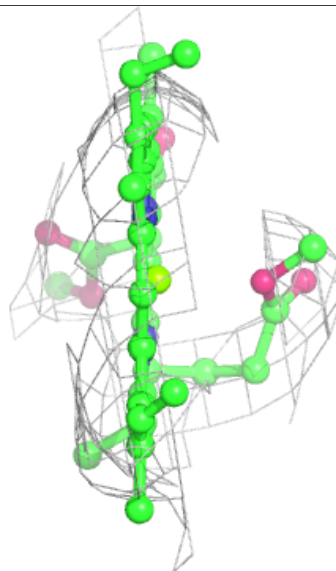
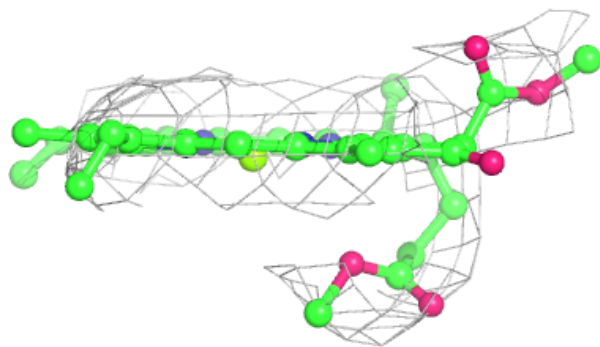
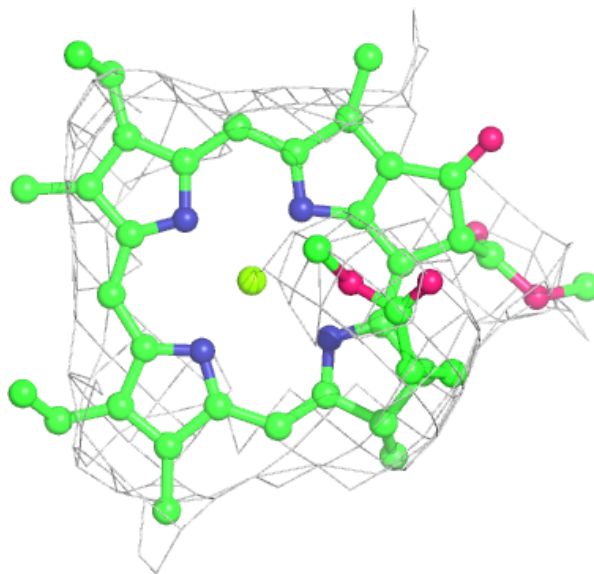
**Electron density around LHG 2 5004:**

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



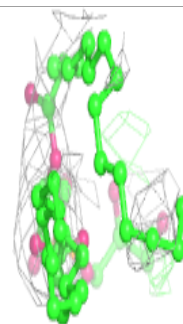
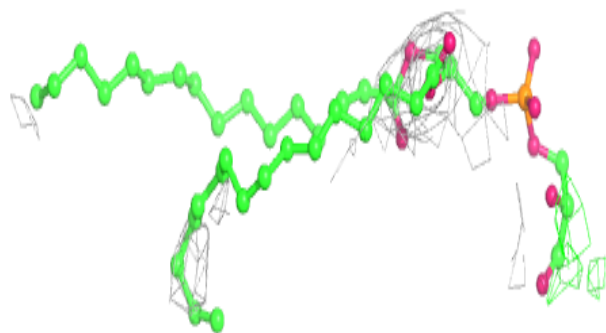
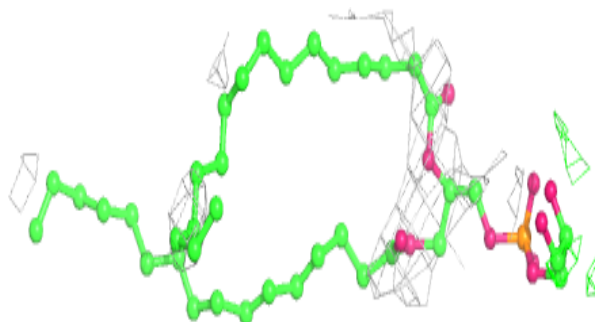
**Electron density around CLA 1 1136:**

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



**Electron density around LHG 1 5003:**

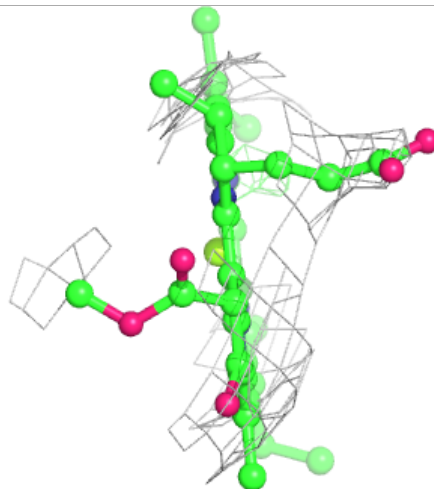
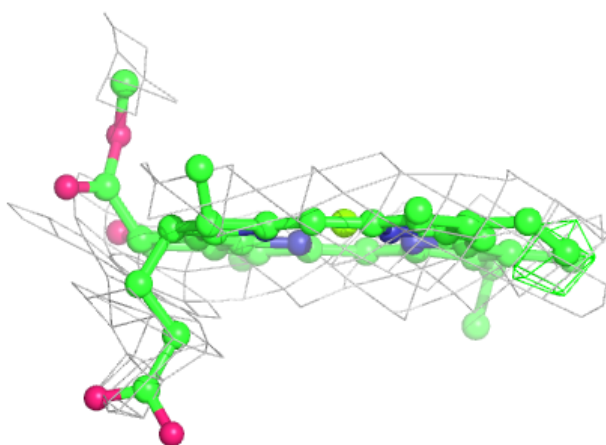
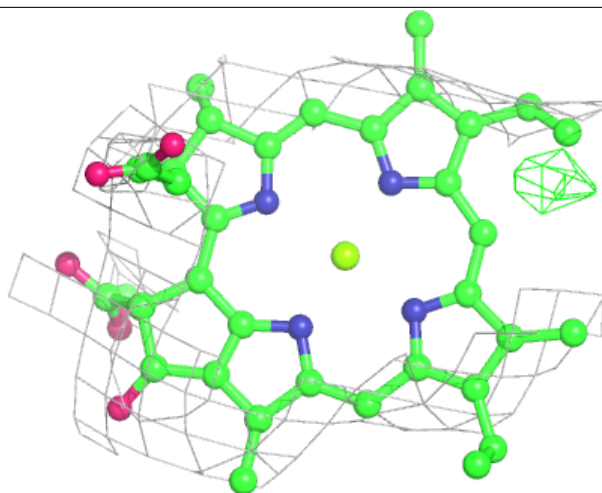
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





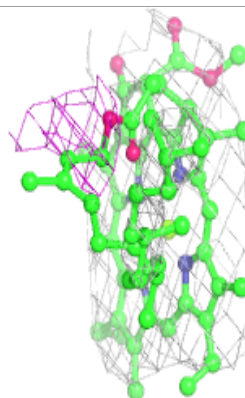
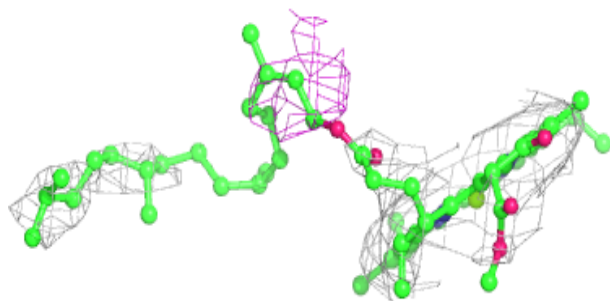
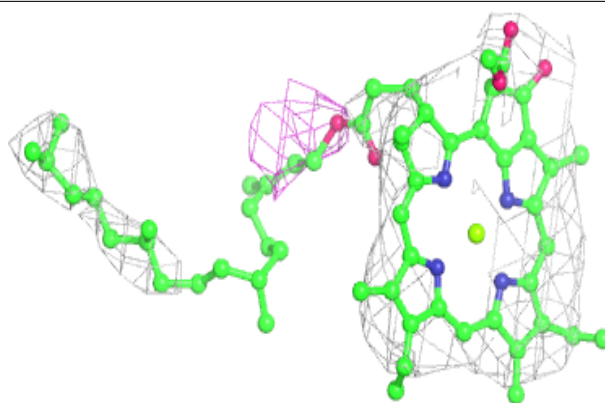
**Electron density around CLA b 1212:**

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

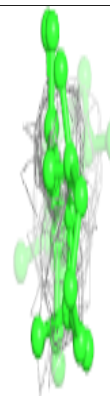
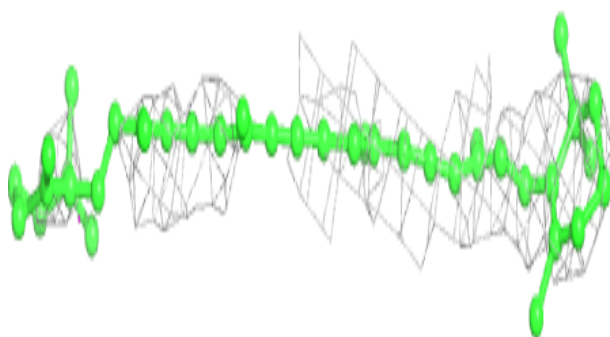
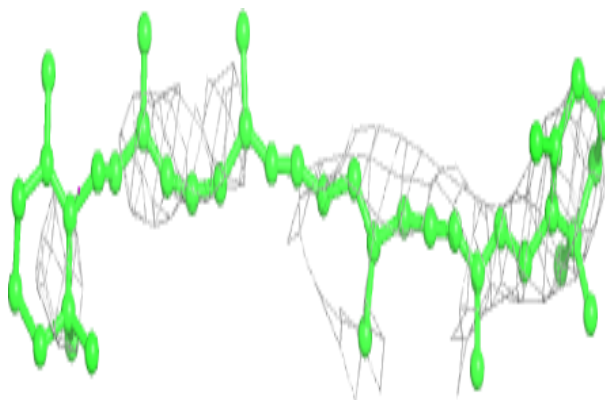


**Electron density around CLA A 1106:**

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

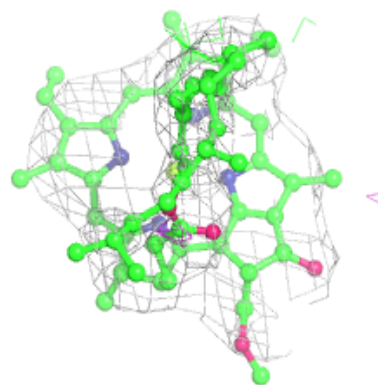
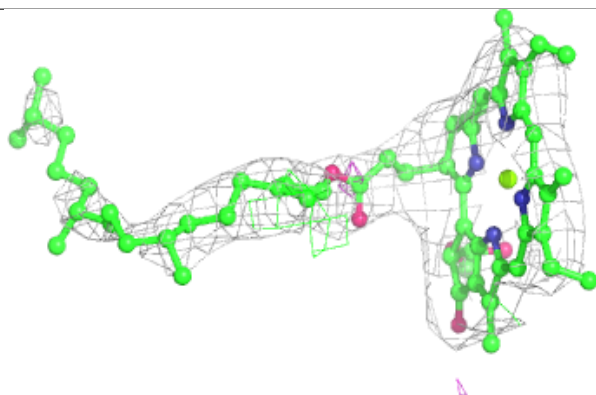
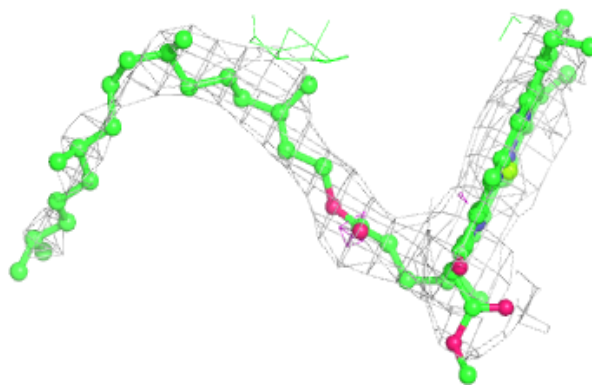
**Electron density around BCR a 4007:**

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

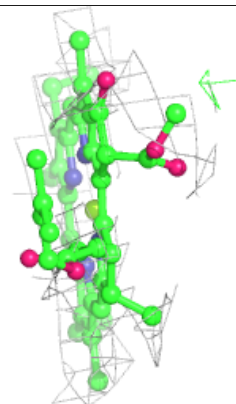
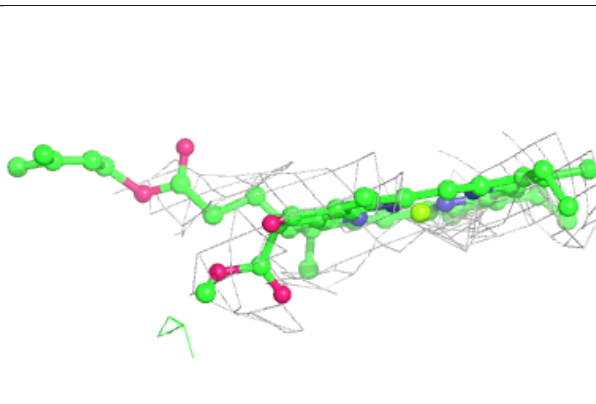
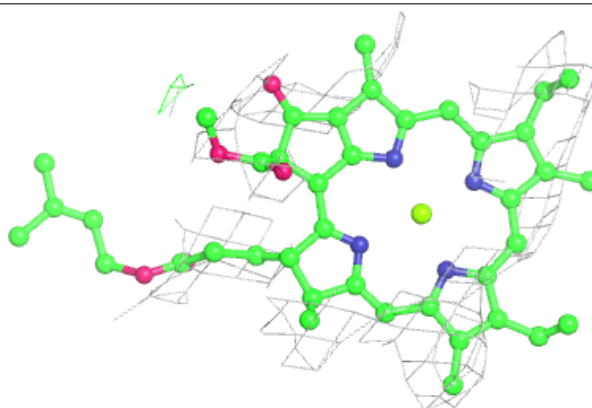


**Electron density around CLA 2 1238:**

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

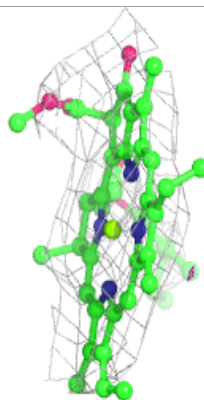
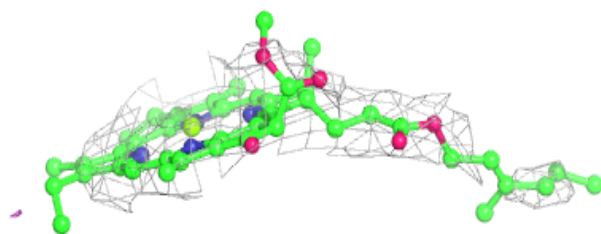
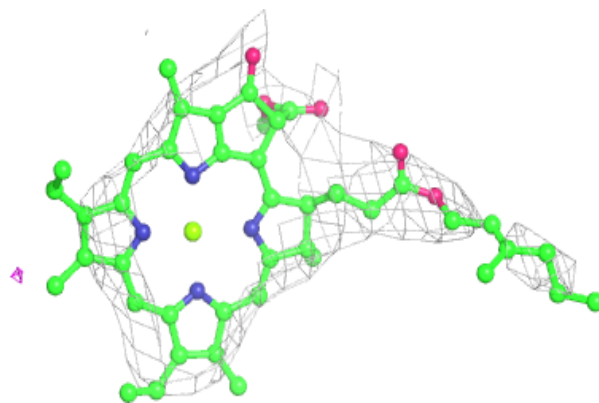
**Electron density around CLA a 1139:**

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



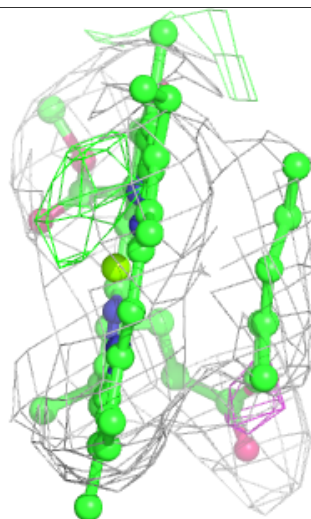
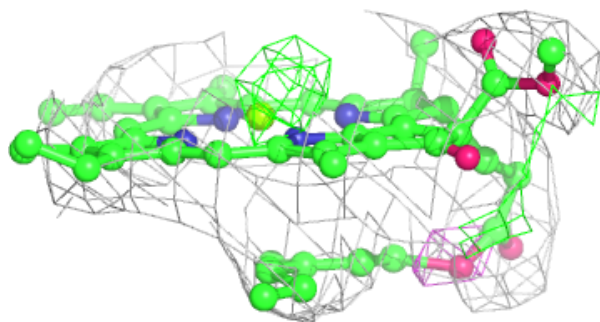
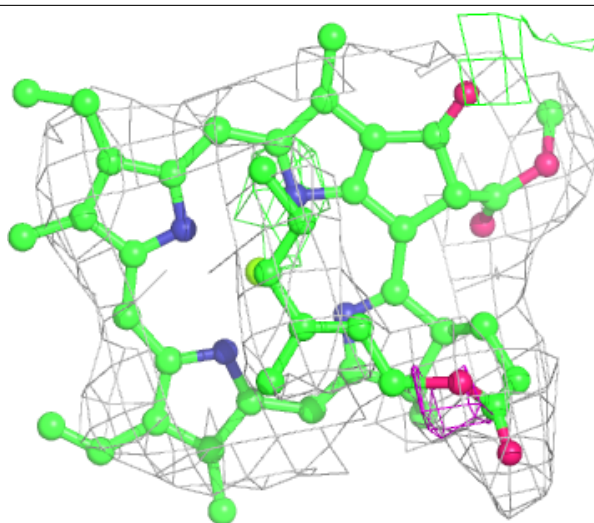
**Electron density around CLA a 1125:**

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



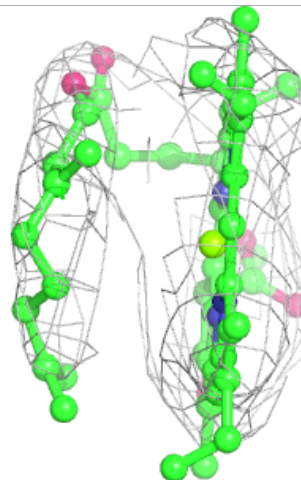
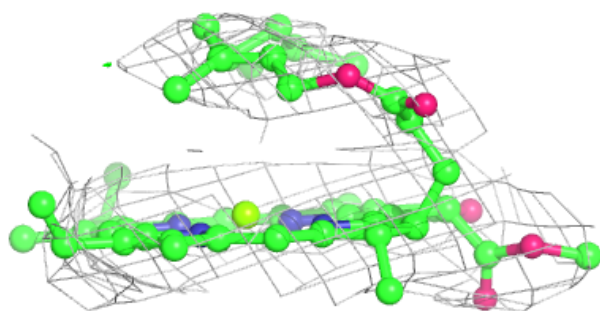
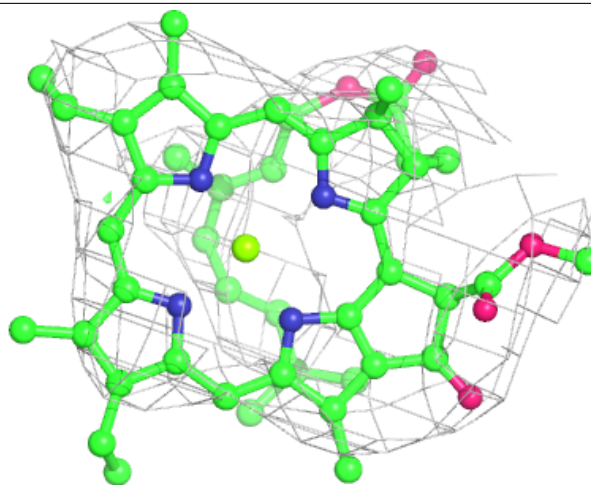
**Electron density around CLA A 1801:**

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



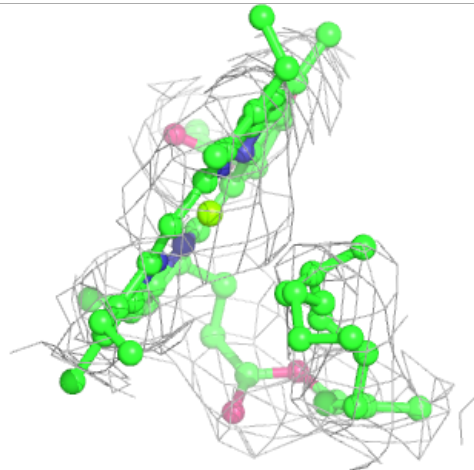
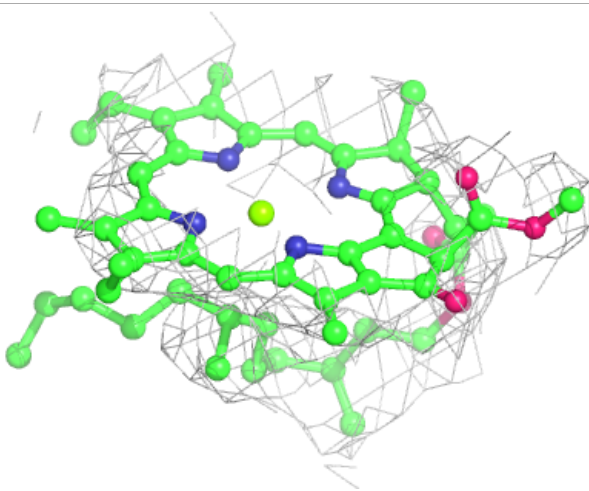
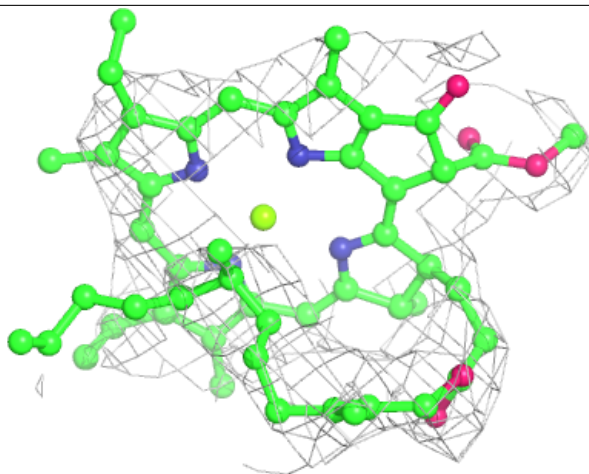
**Electron density around CLA b 1224:**

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



**Electron density around CLA 2 1214:**

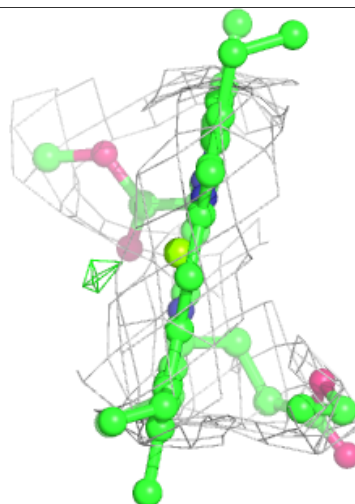
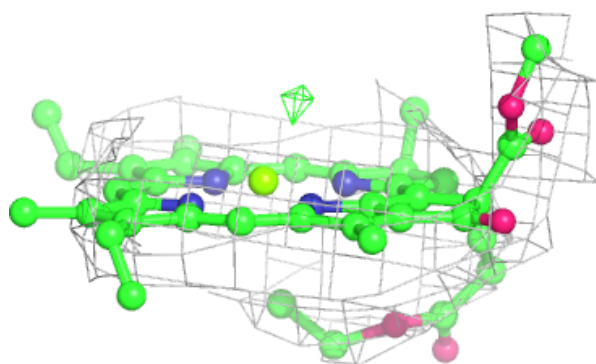
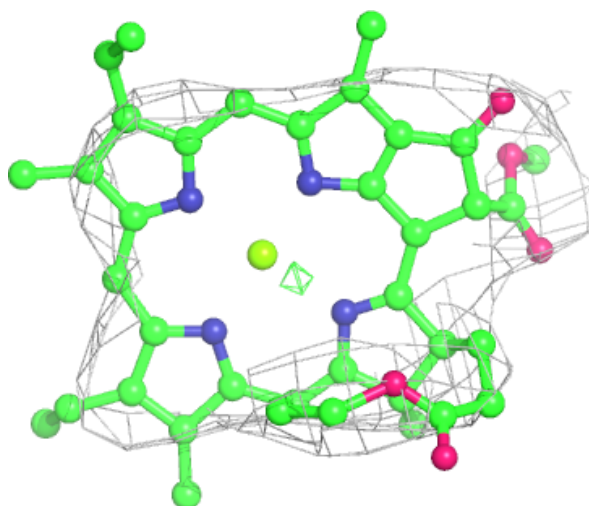
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





**Electron density around CLA B 1217:**

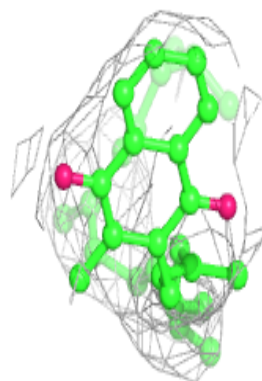
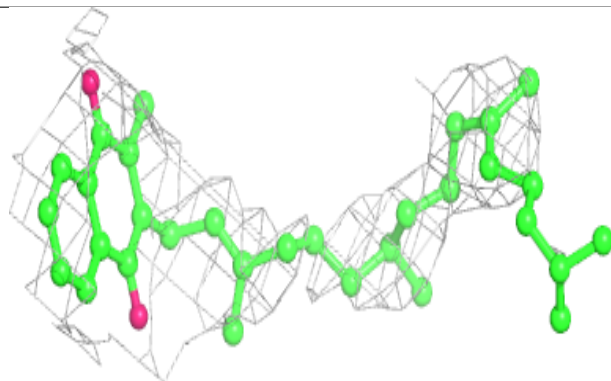
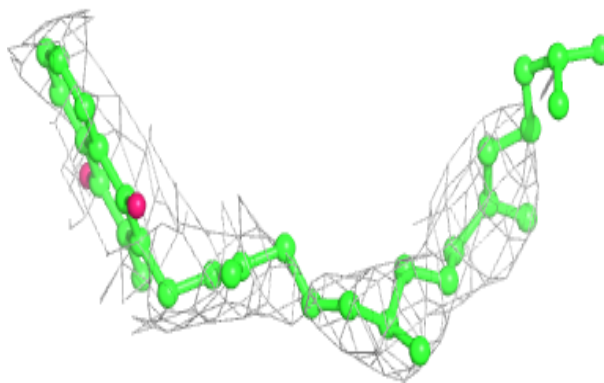
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



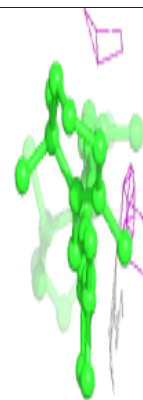
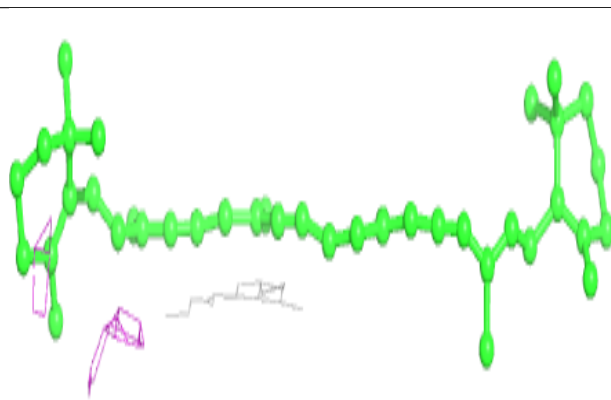
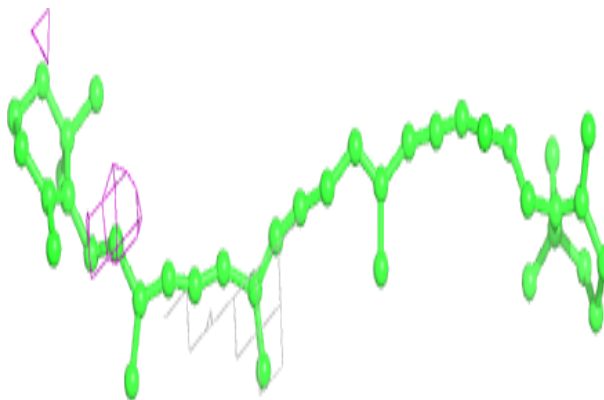


**Electron density around PQN B 2002:**

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

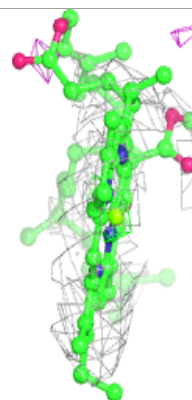
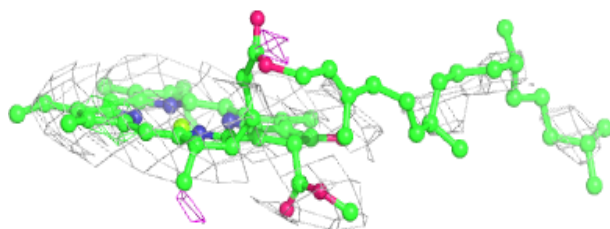
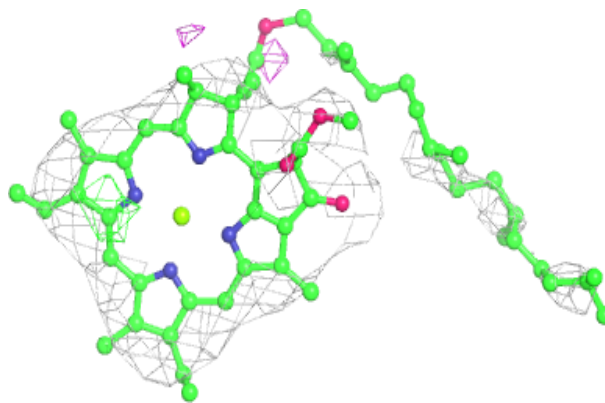
**Electron density around BCR 2 4009:**

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

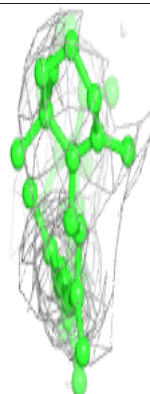
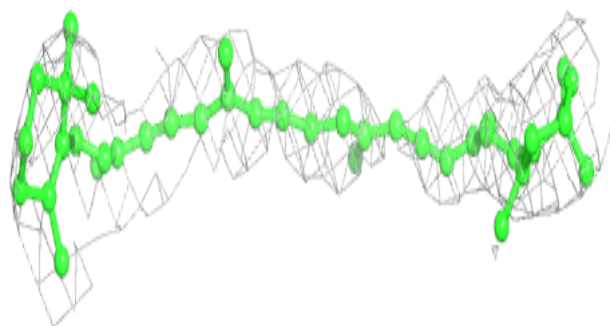
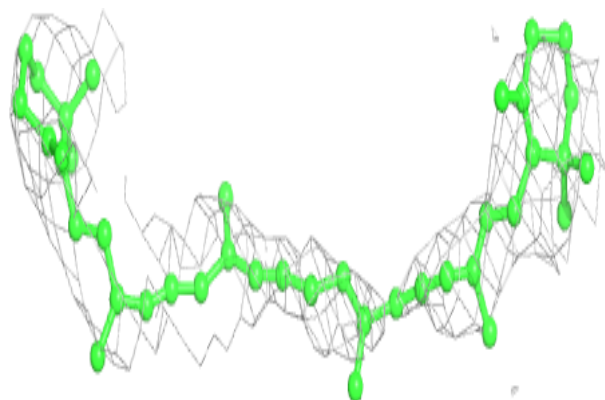


**Electron density around CLA 8 1503:**

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

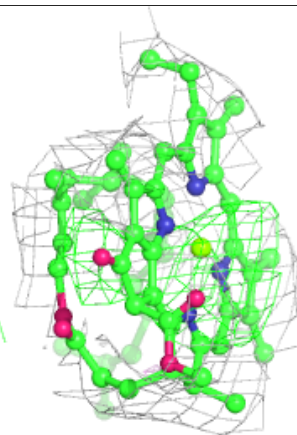
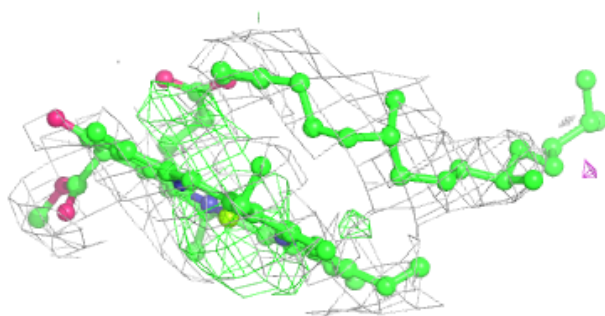
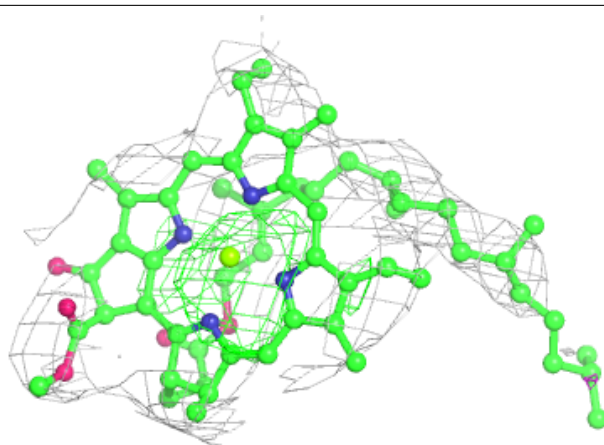
**Electron density around BCR 6 4020:**

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

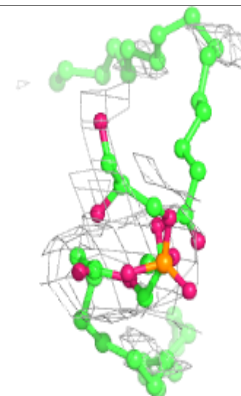
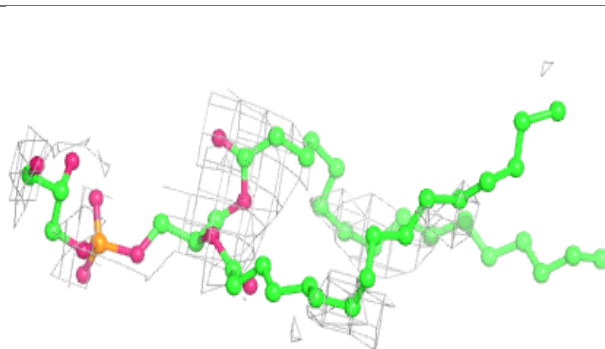
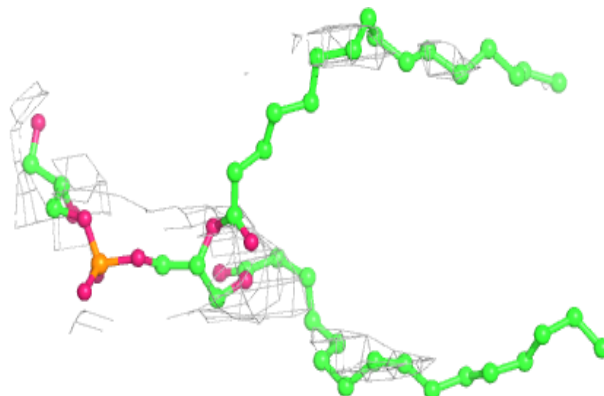


**Electron density around CLA B 1204:**

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

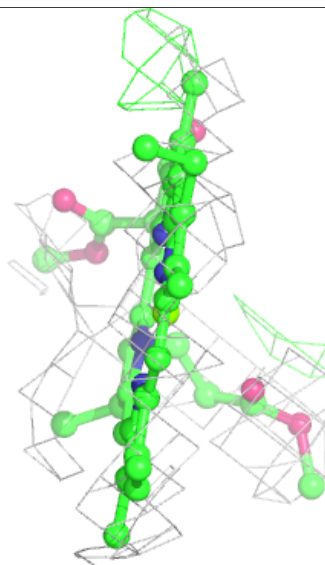
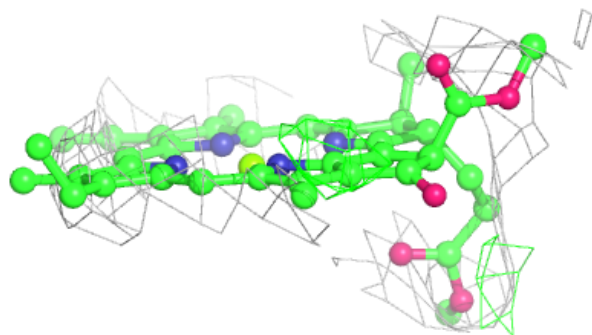
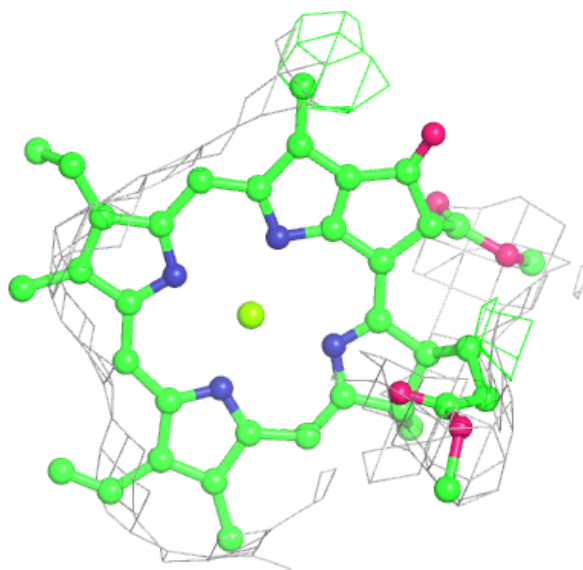
**Electron density around LHG a 5001:**

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



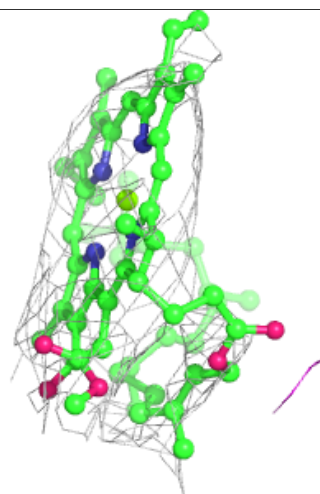
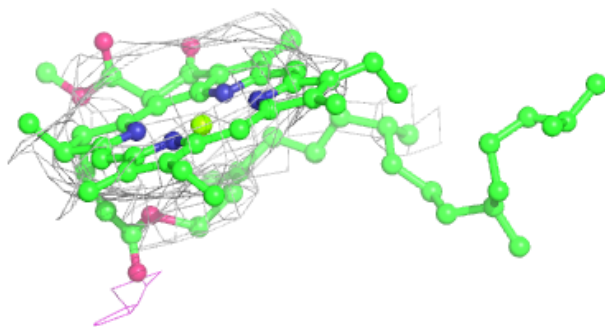
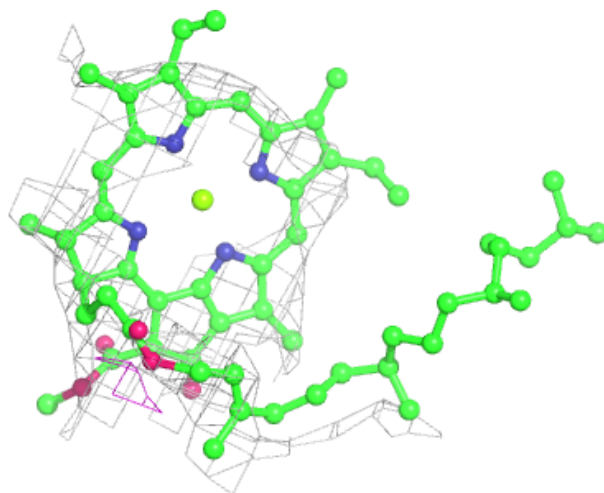
**Electron density around CLA a 1134:**

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



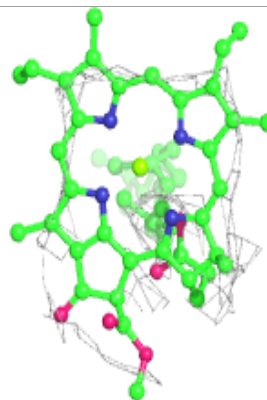
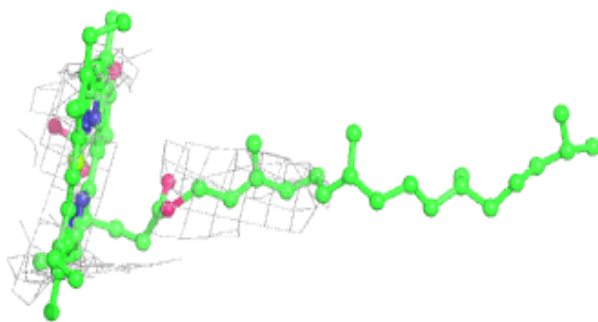
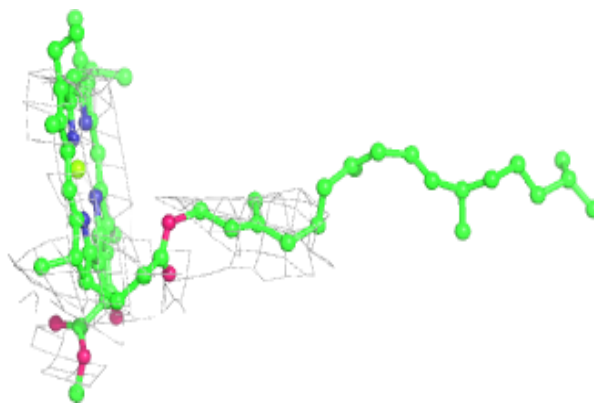
**Electron density around CLA 1 1127:**

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

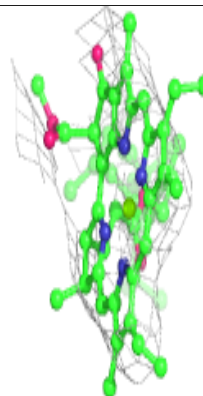
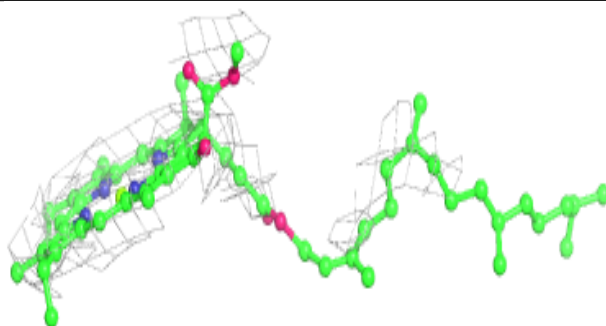
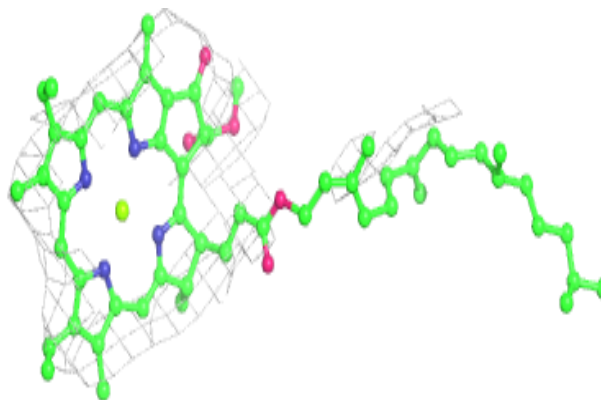


**Electron density around CLA 1 1126:**

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

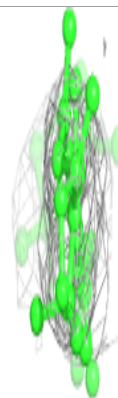
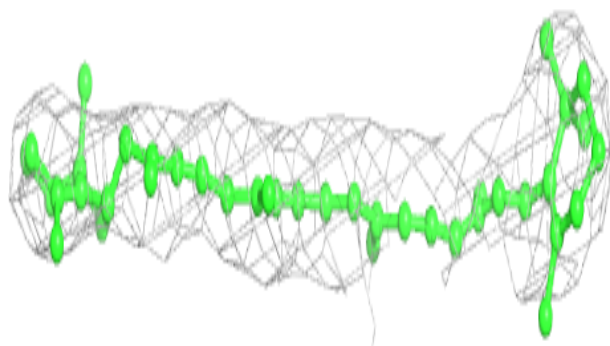
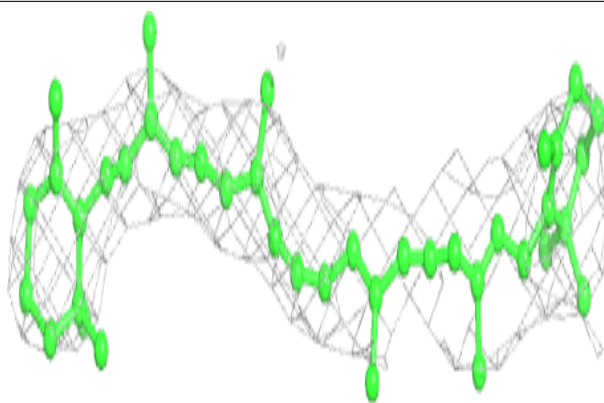
**Electron density around CLA a 1107:**

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



**Electron density around BCR A 4002:**

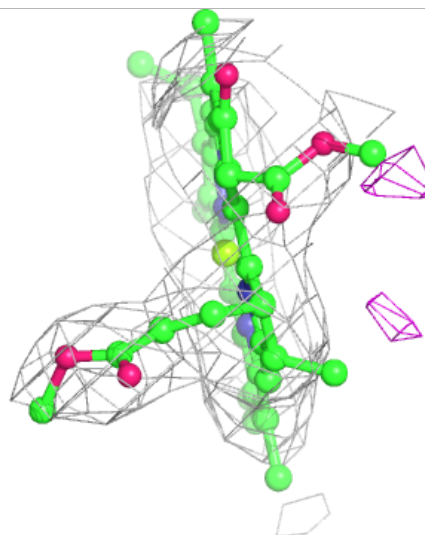
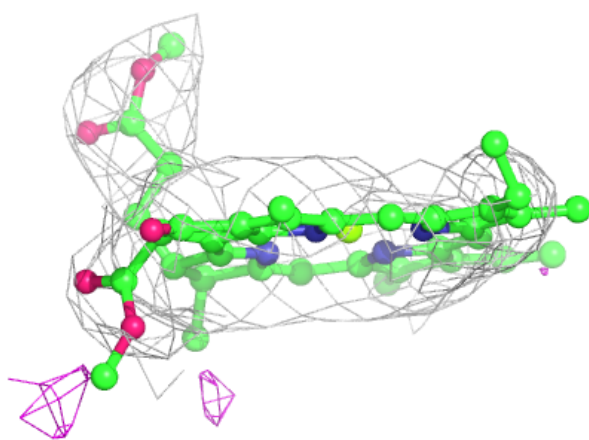
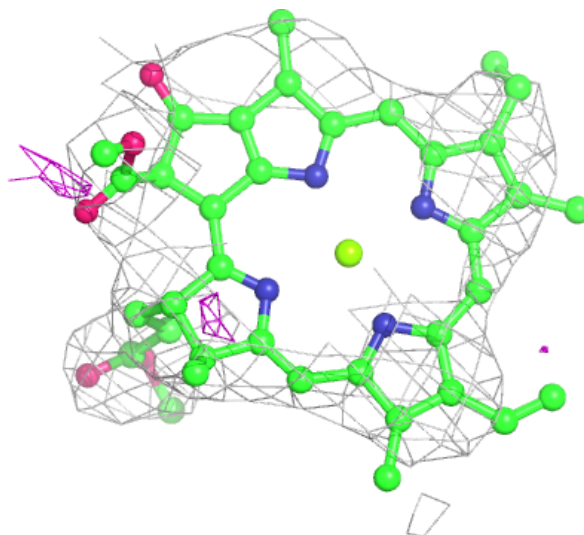
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





**Electron density around CLA A 1129:**

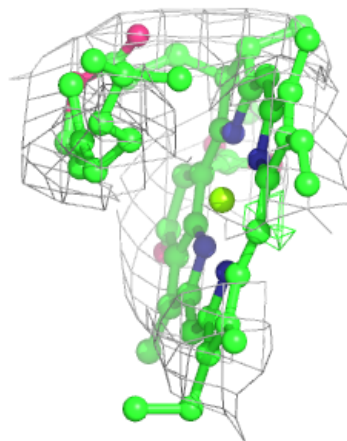
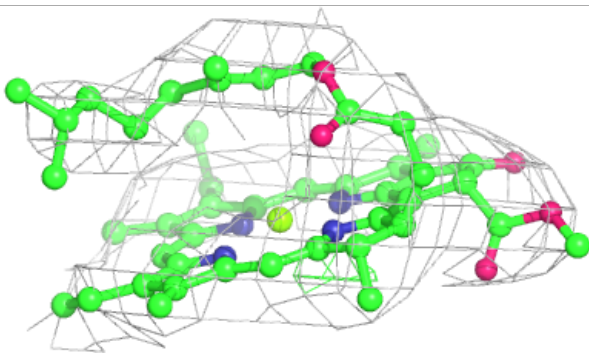
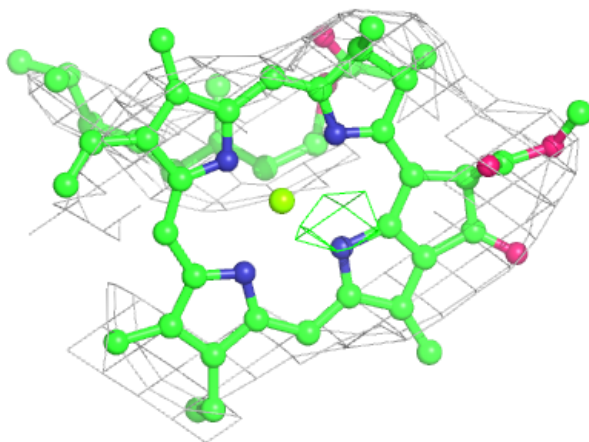
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





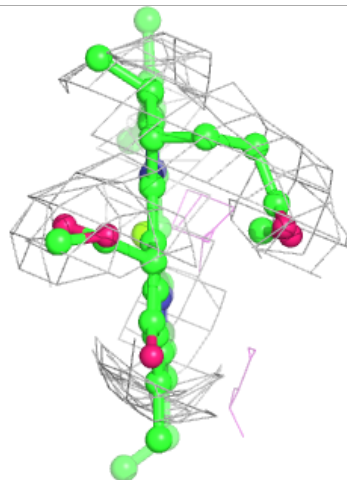
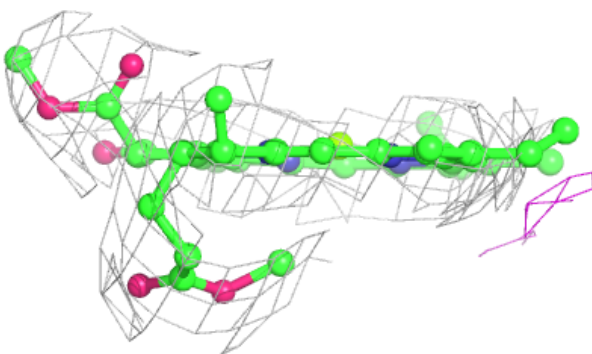
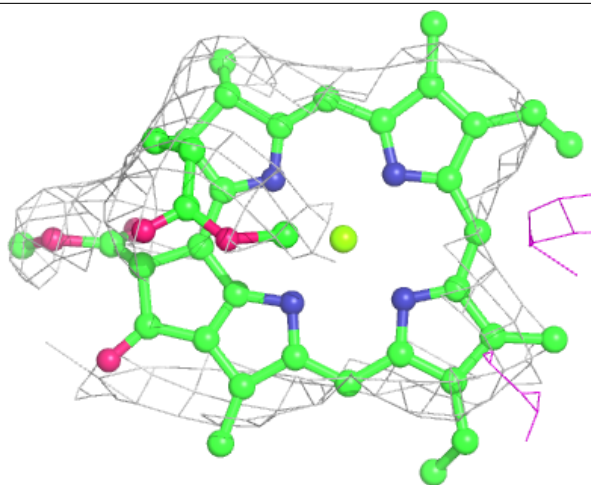
**Electron density around CLA a 1237:**

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



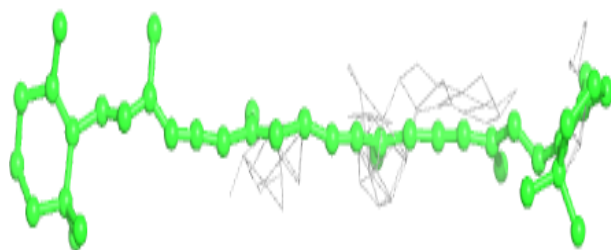
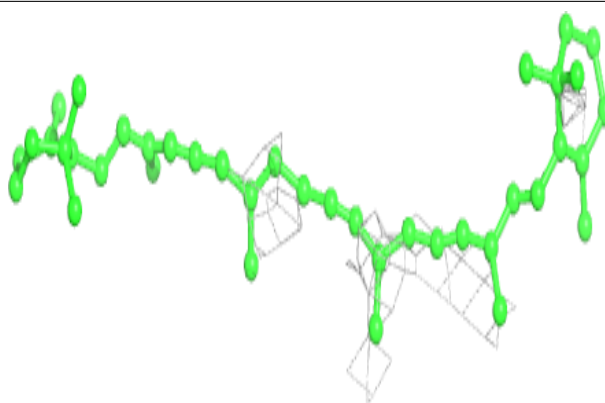
**Electron density around CLA A 1115:**

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



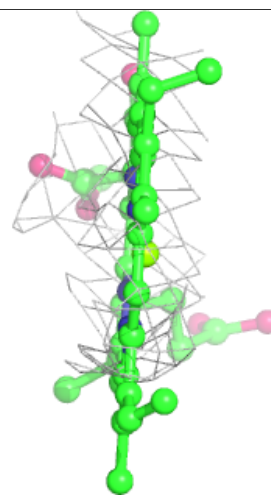
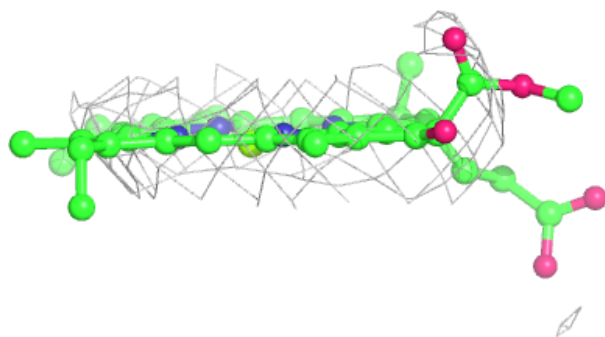
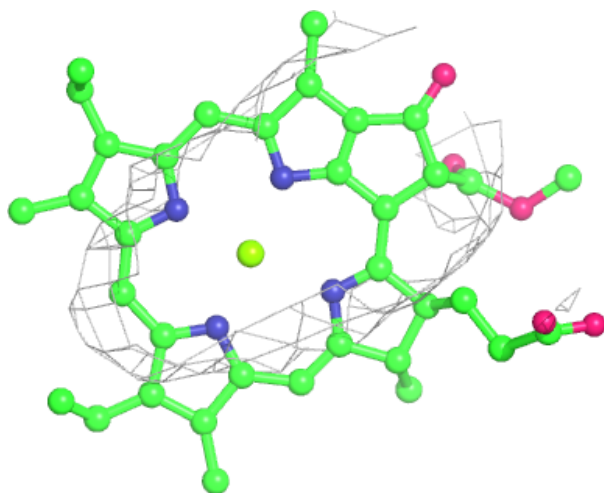
**Electron density around BCR B 4009:**

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



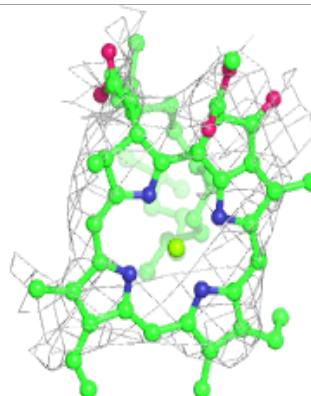
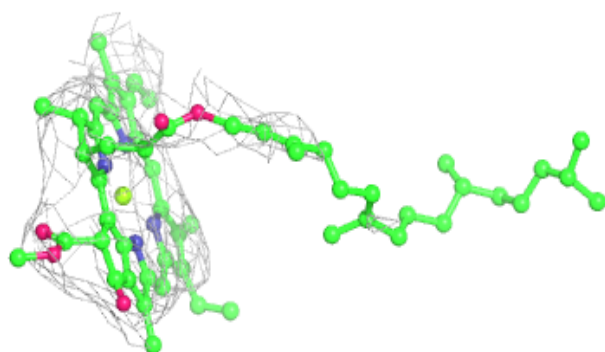
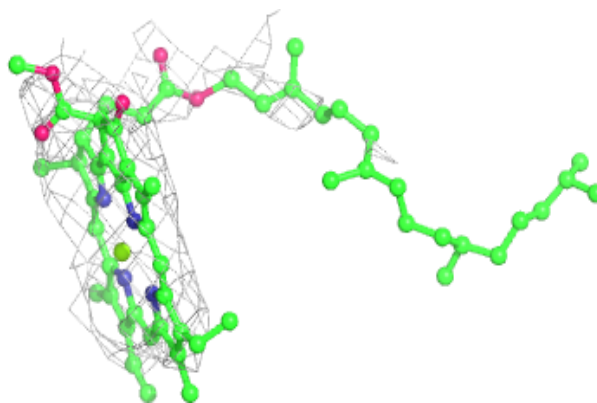
**Electron density around CLA a 1113:**

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



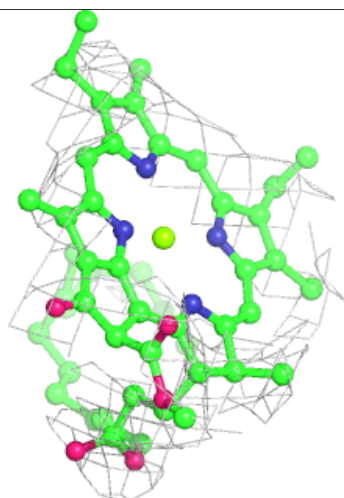
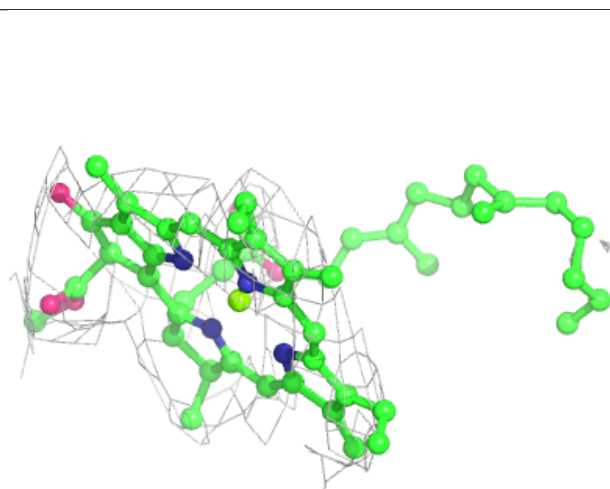
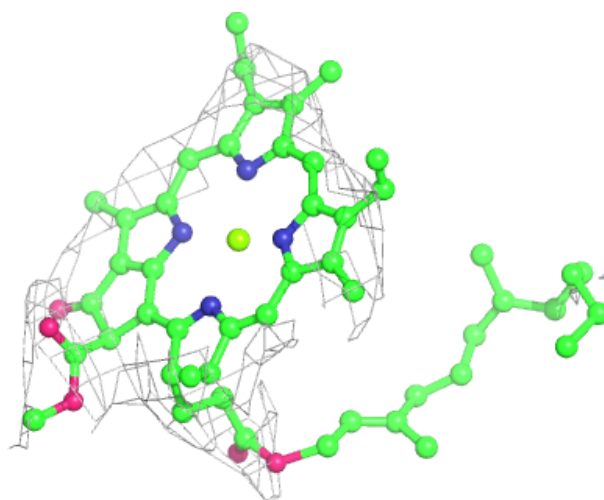
**Electron density around CLA a 1128:**

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



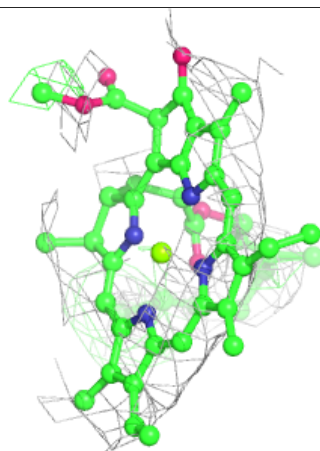
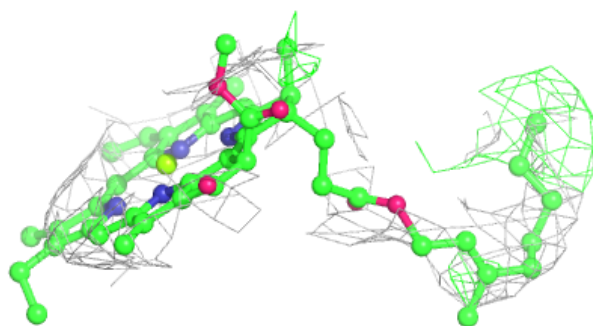
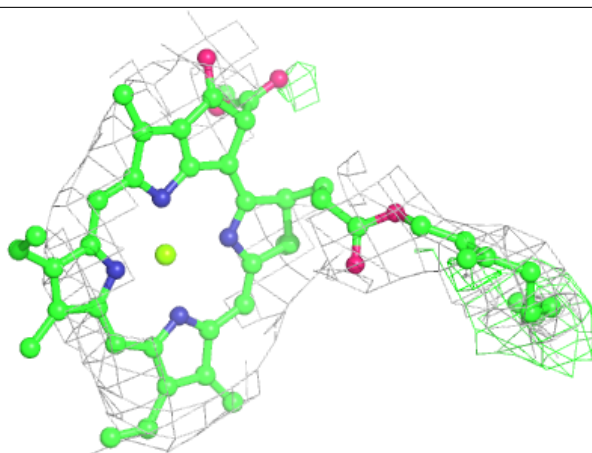
**Electron density around CLA 1 1122:**

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



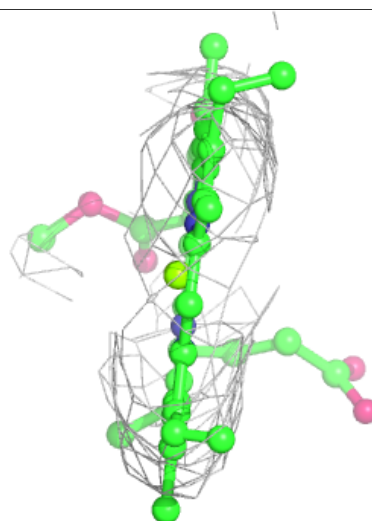
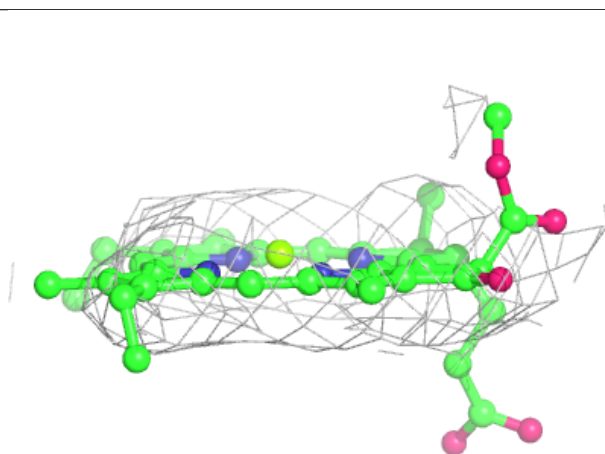
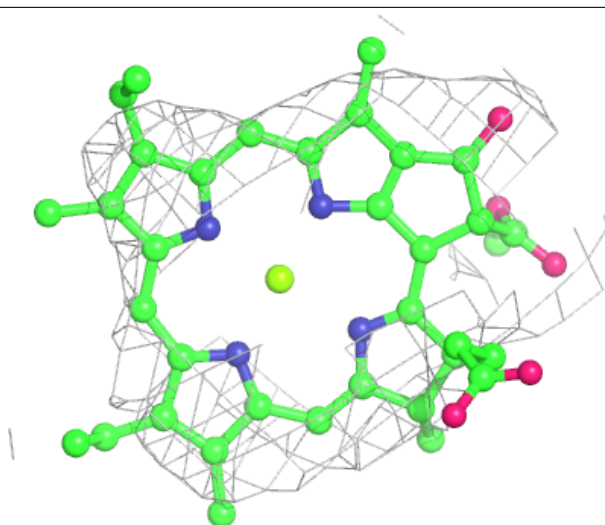
**Electron density around CLA a 1110:**

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



**Electron density around CLA B 1212:**

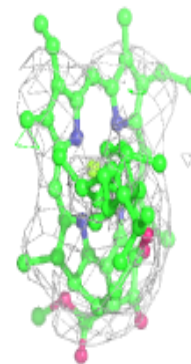
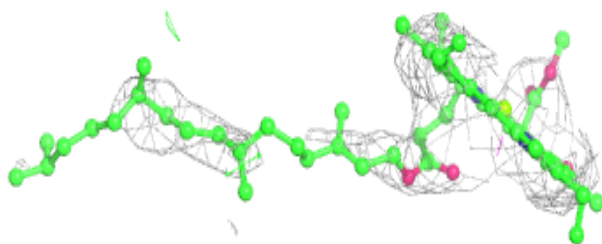
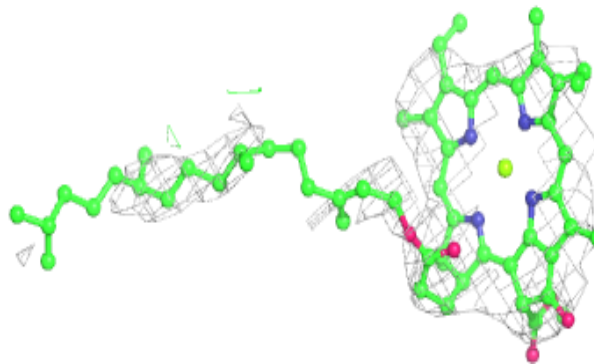
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



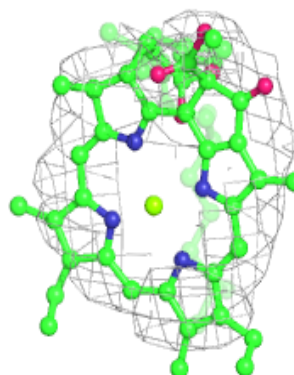
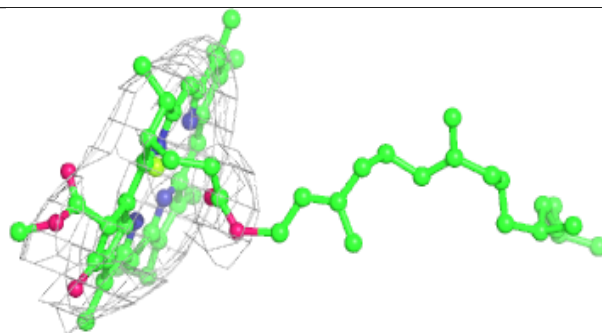
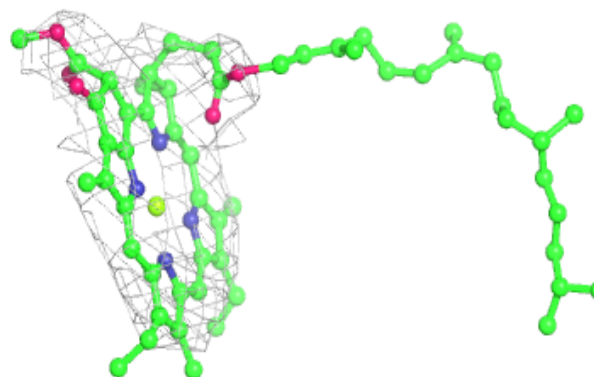


**Electron density around CLA L 1501:**

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

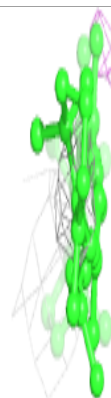
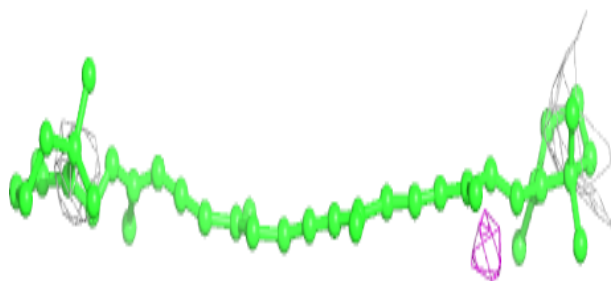
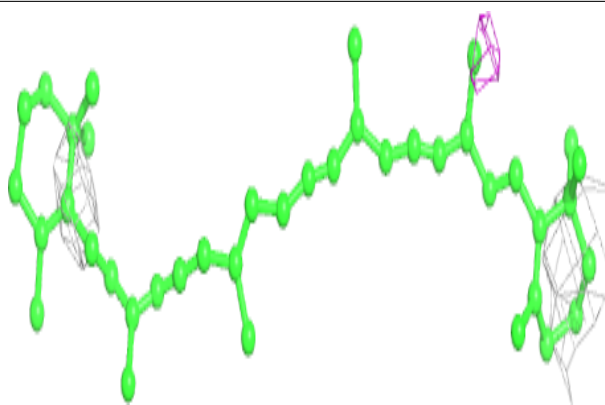
**Electron density around CLA 1 1140:**

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

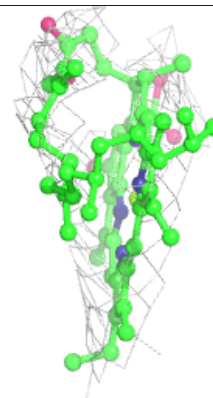
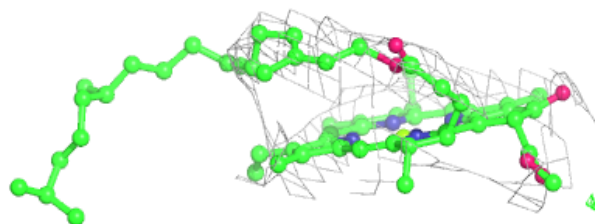
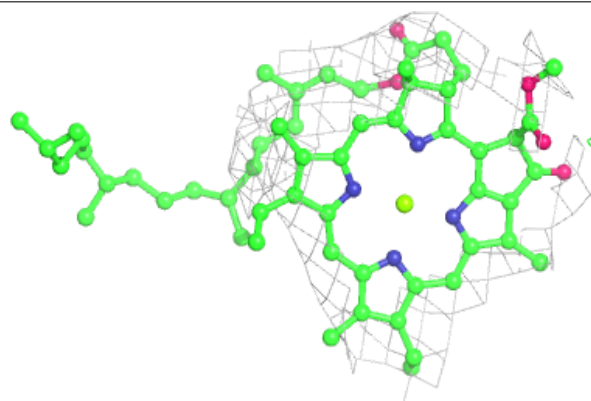


**Electron density around BCR b 4005:**

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

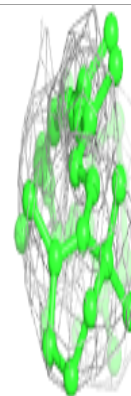
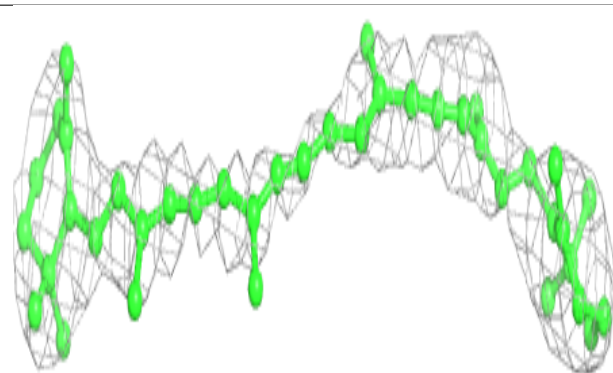
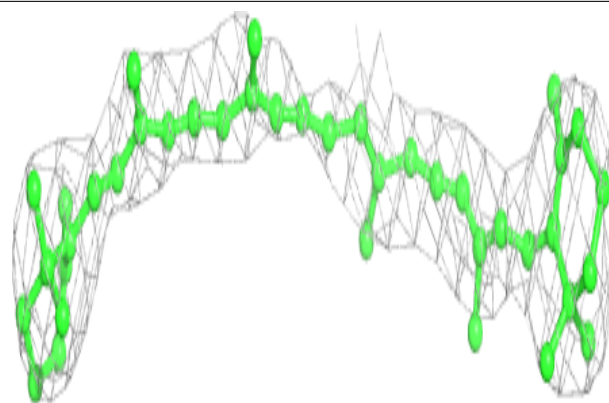
**Electron density around CLA b 1215:**

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



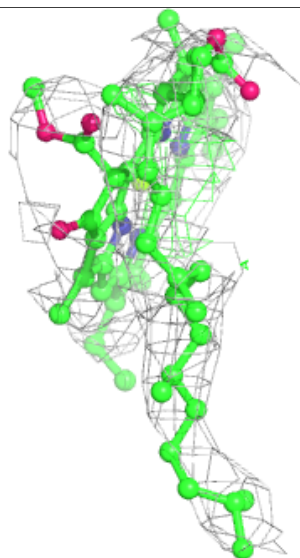
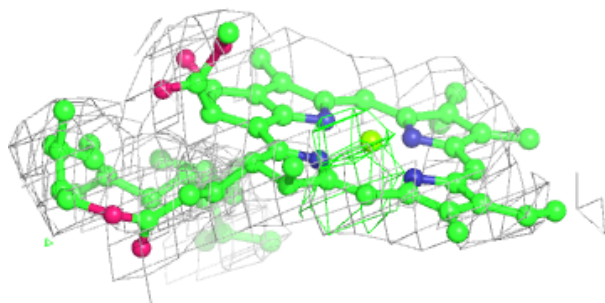
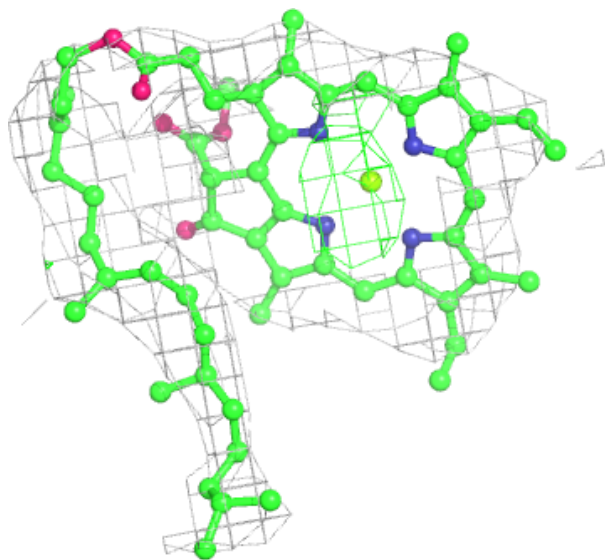
**Electron density around BCR 6 4018:**

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



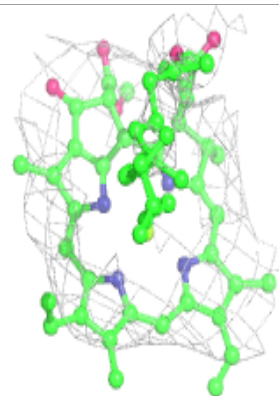
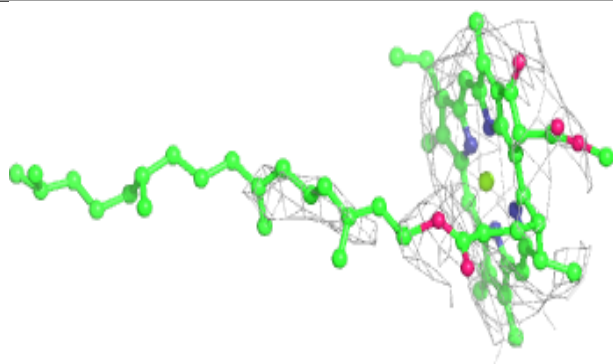
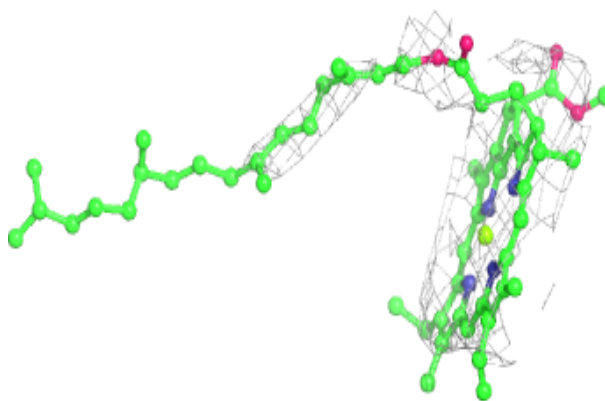
**Electron density around CLA A 1123:**

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

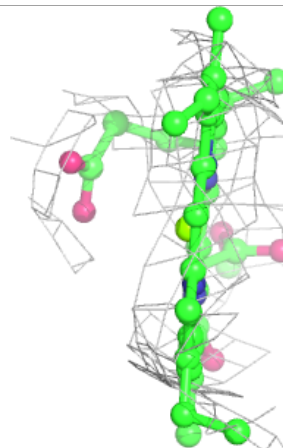
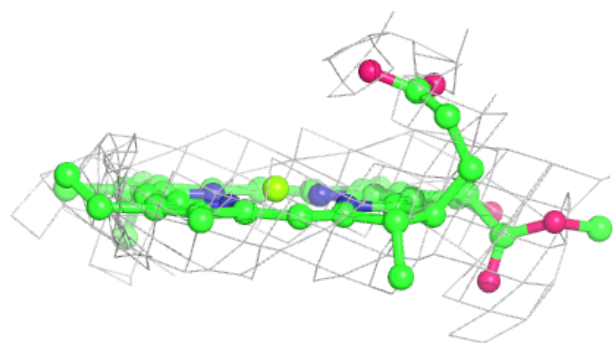
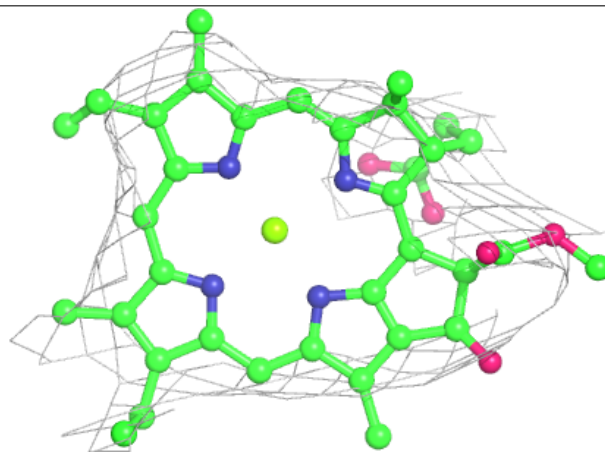


**Electron density around CLA b 1226:**

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

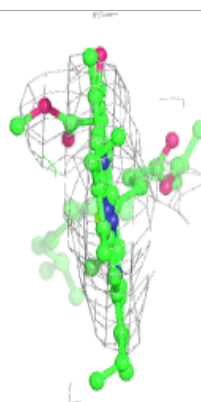
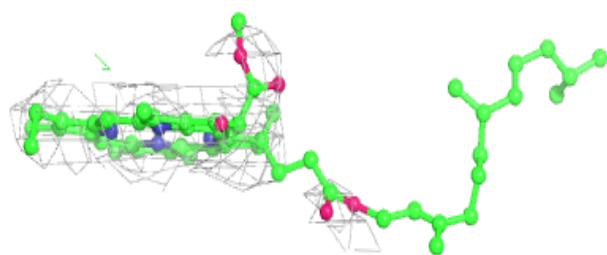
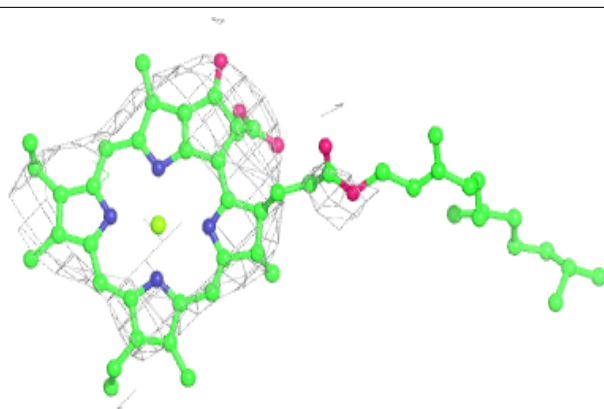
**Electron density around CLA a 1108:**

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

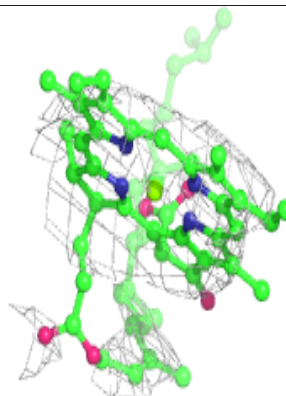
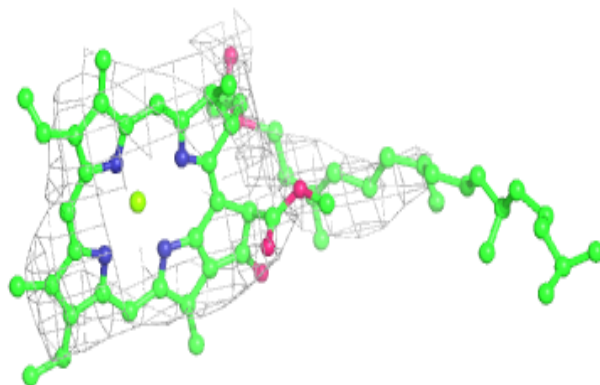
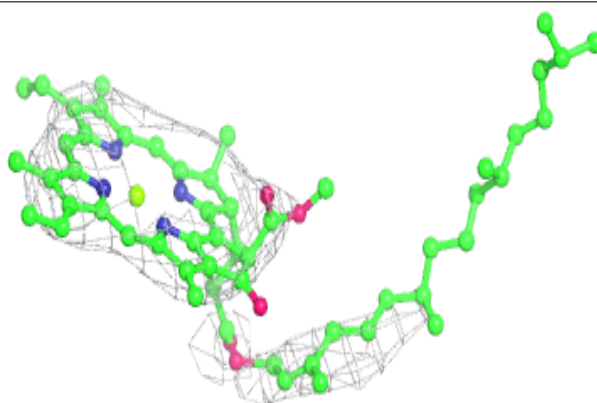


**Electron density around CLA 2 1234:**

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

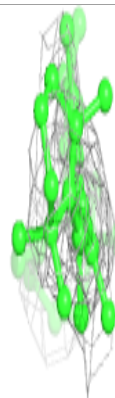
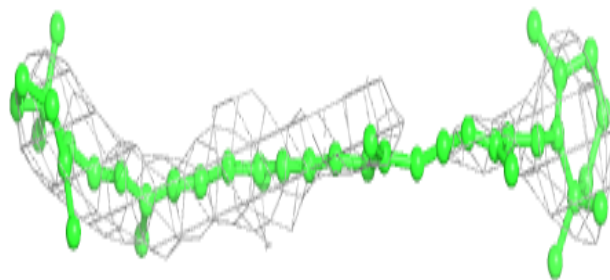
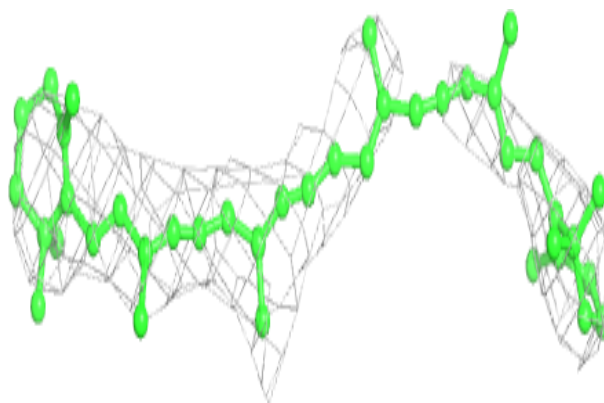
**Electron density around CLA 2 1213:**

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



**Electron density around BCR b 4017:**

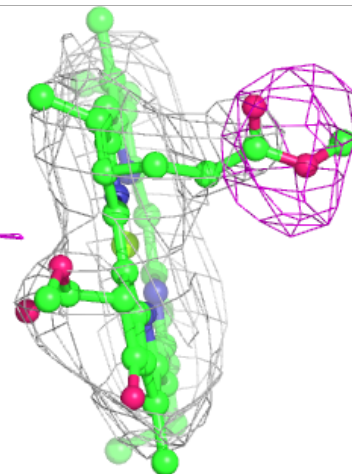
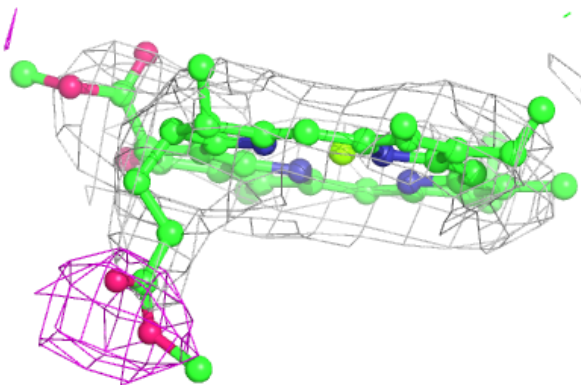
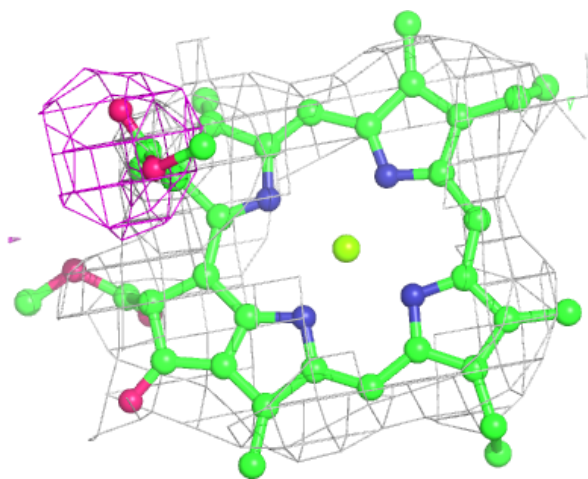
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





**Electron density around CLA A 1130:**

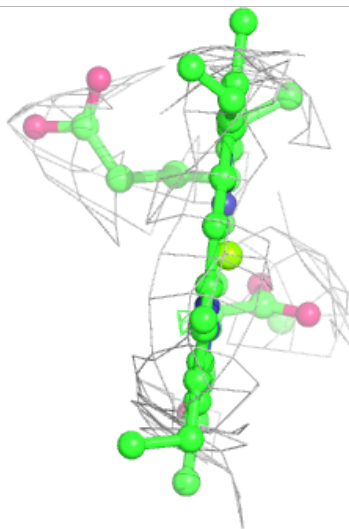
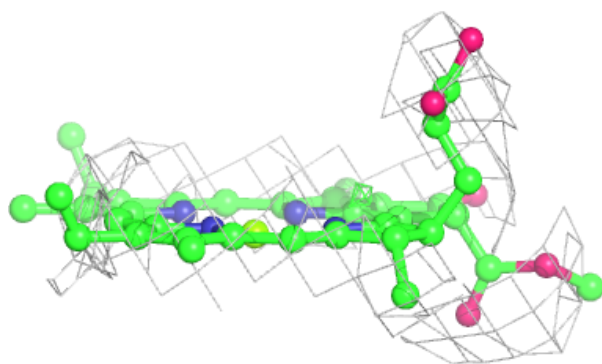
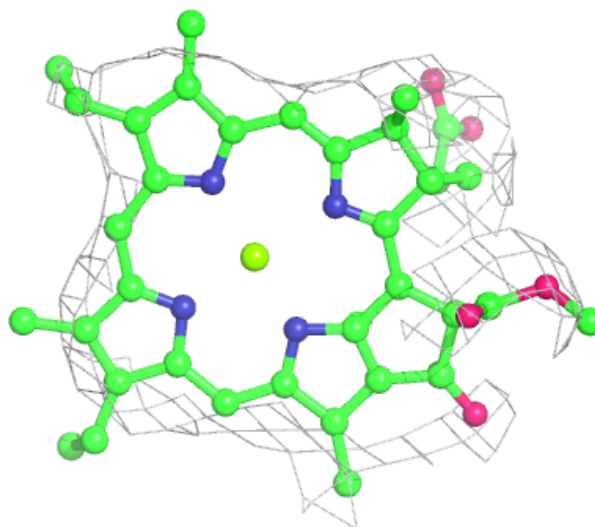
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





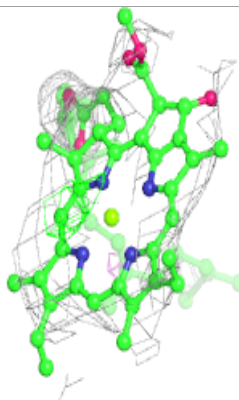
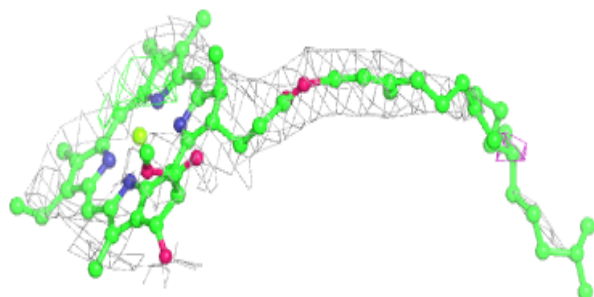
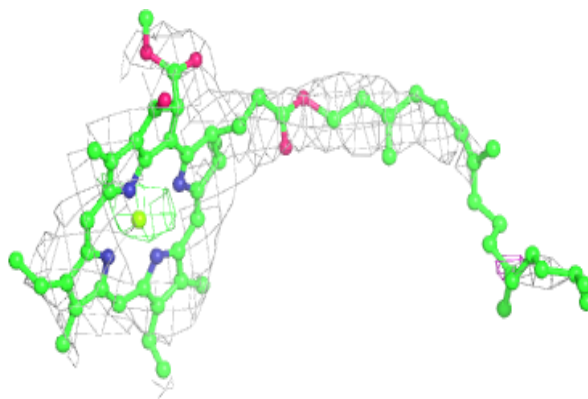
**Electron density around CLA B 1232:**

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

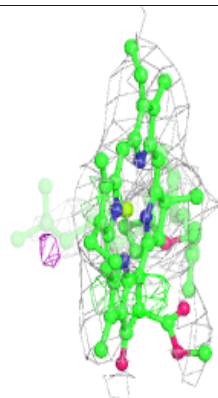
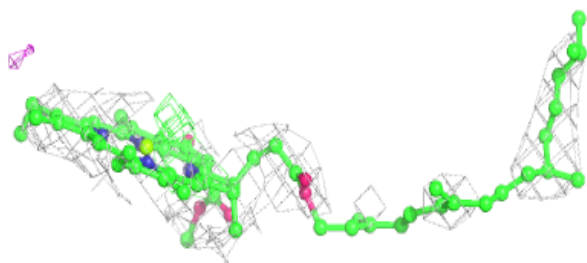
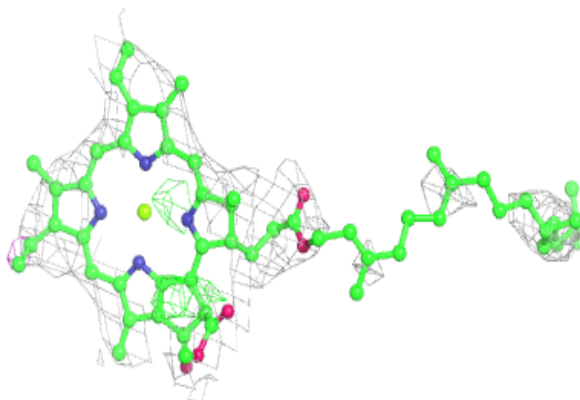


**Electron density around CLA A 1012:**

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

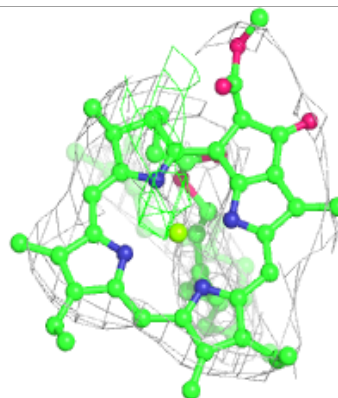
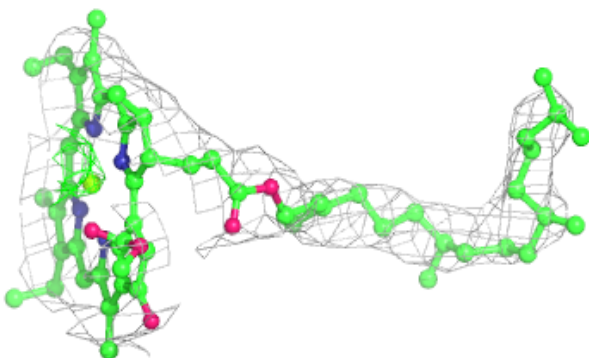
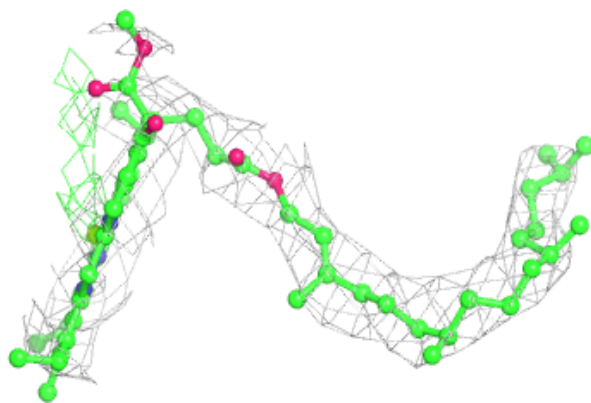
**Electron density around CLA A 1103:**

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

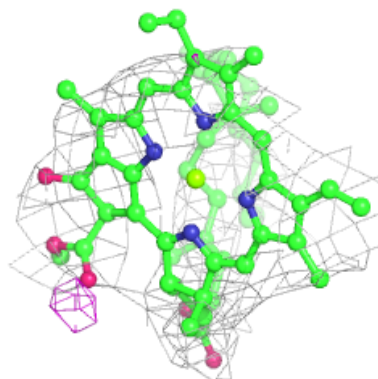
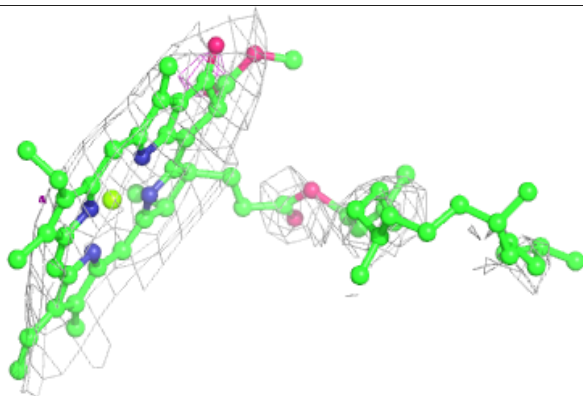
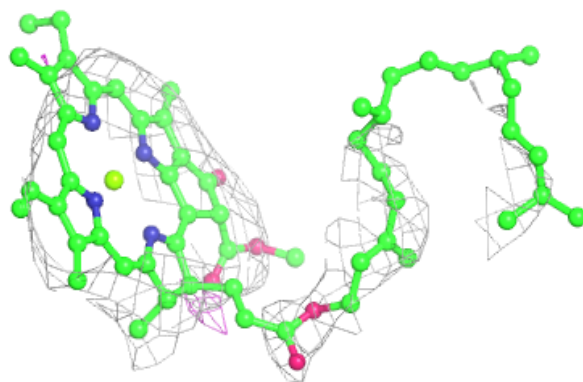


**Electron density around CLA b 1238:**

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

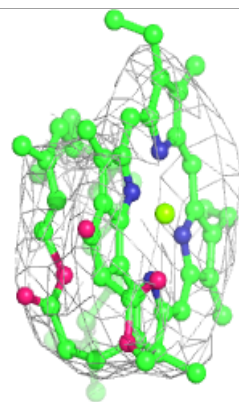
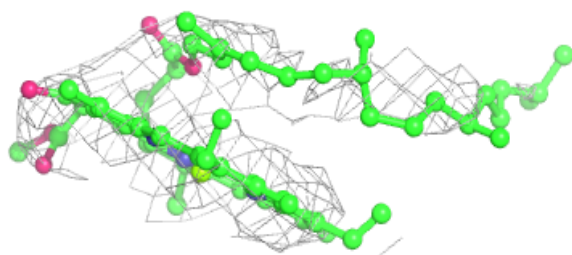
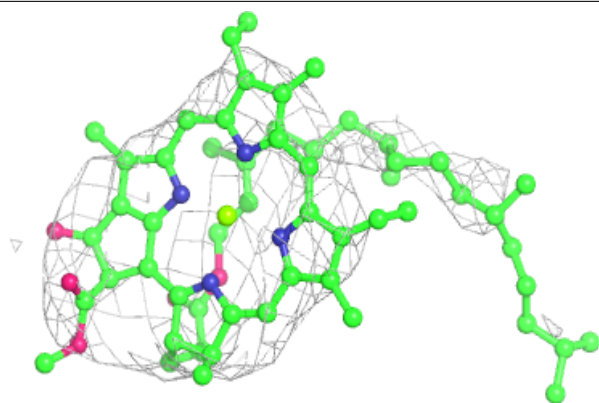
**Electron density around CLA a 1011:**

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

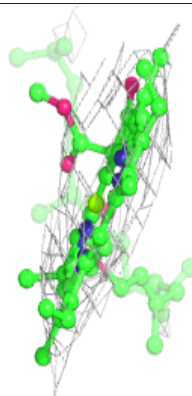
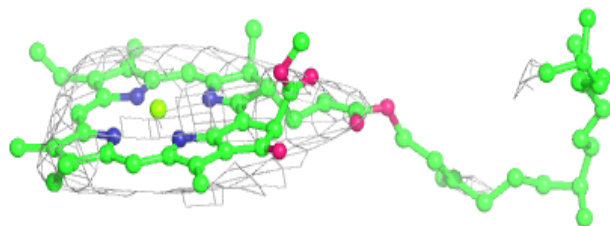
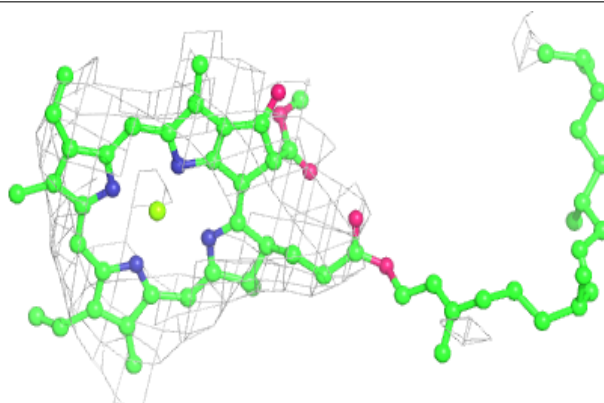


**Electron density around CLA b 1204:**

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

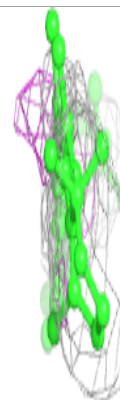
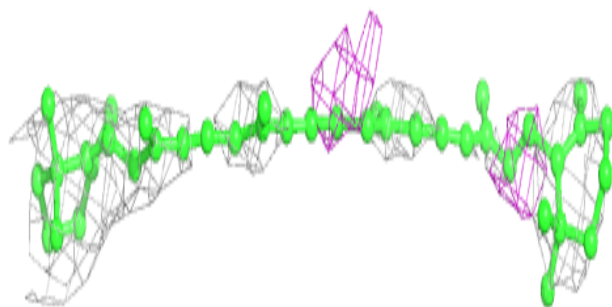
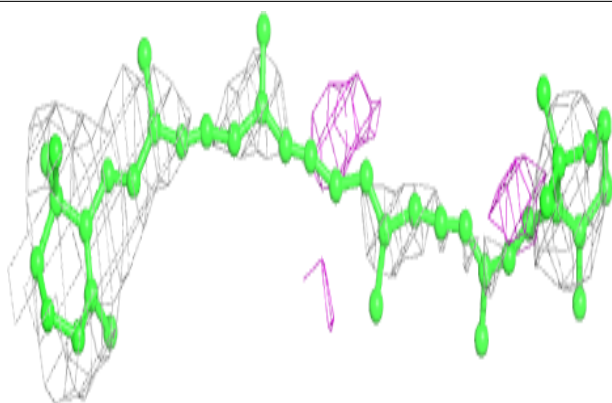
**Electron density around CLA b 1223:**

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



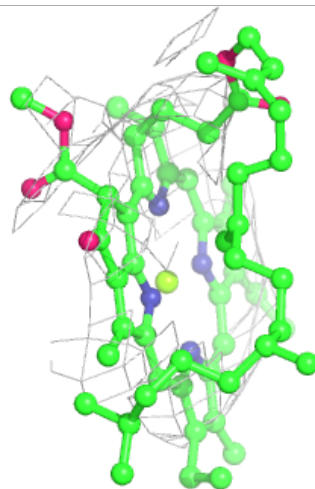
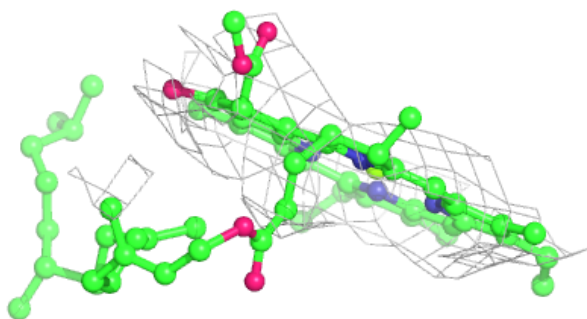
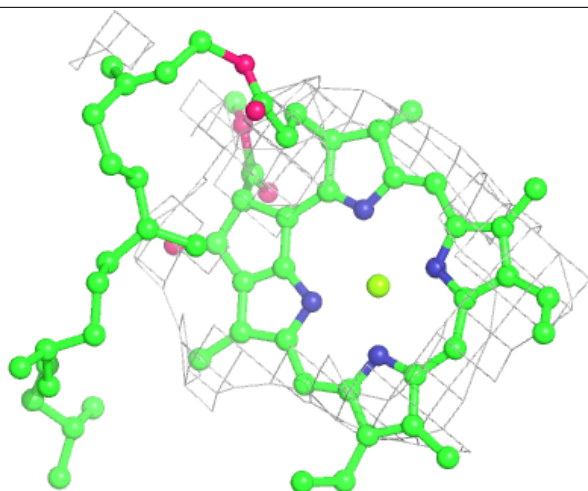
**Electron density around BCR 2 4005:**

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



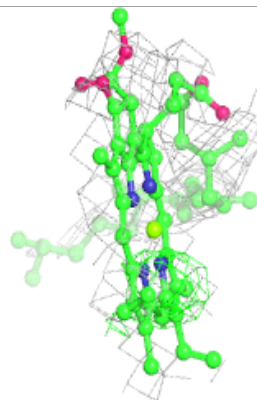
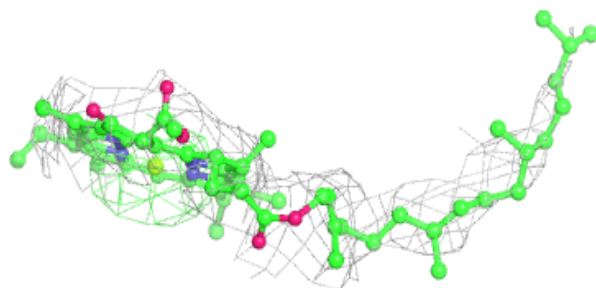
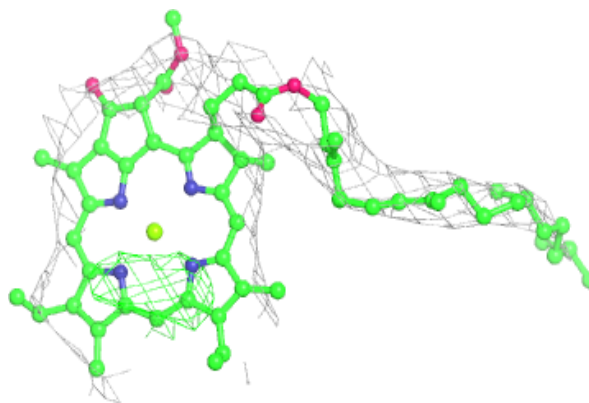
**Electron density around CLA b 1229:**

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



**Electron density around CLA b 1023:**

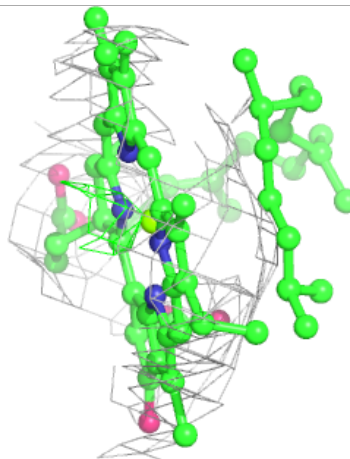
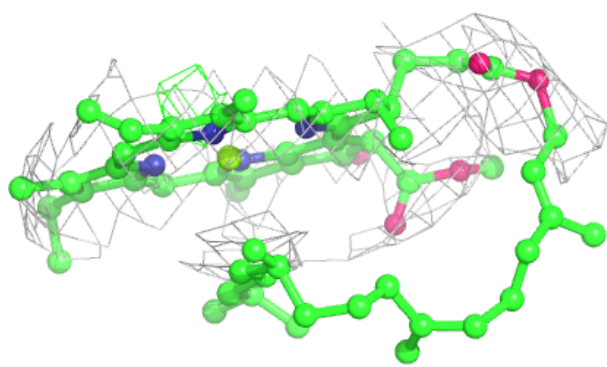
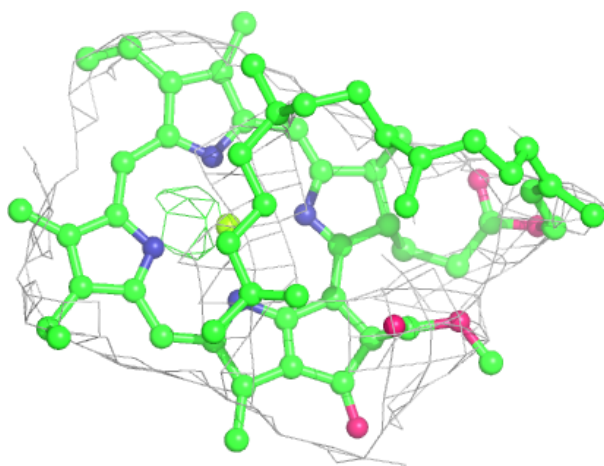
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





**Electron density around CLA a 1104:**

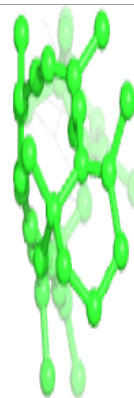
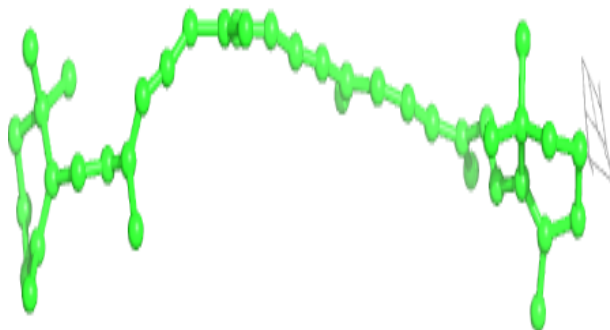
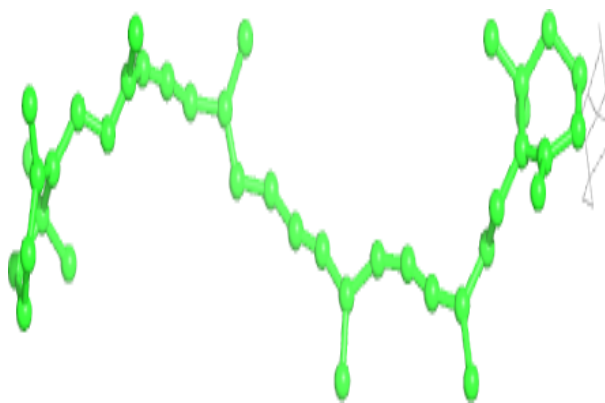
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



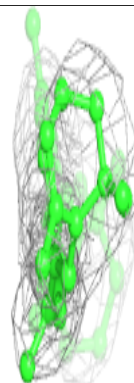
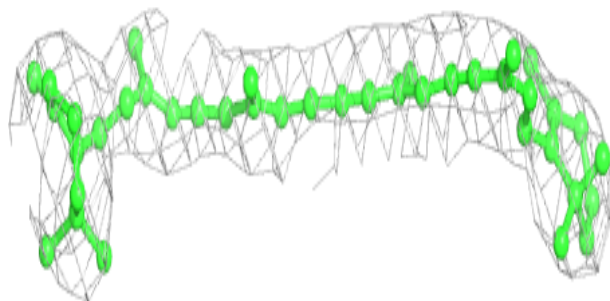
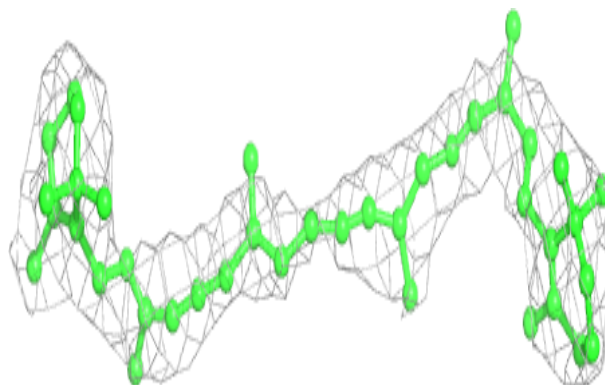


**Electron density around BCR f 4013:**

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

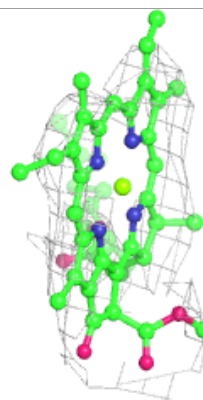
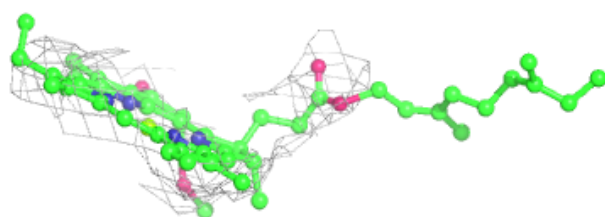
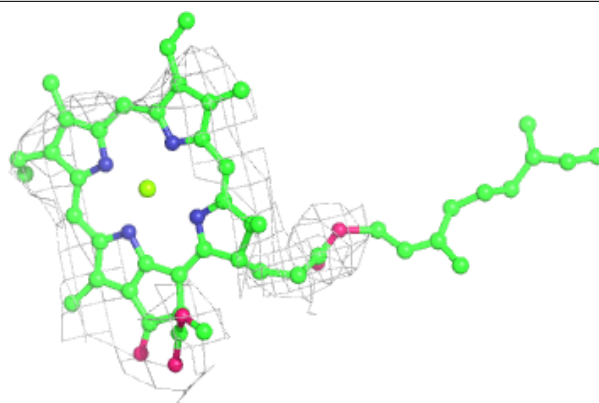
**Electron density around BCR 2 4006:**

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

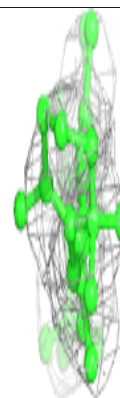
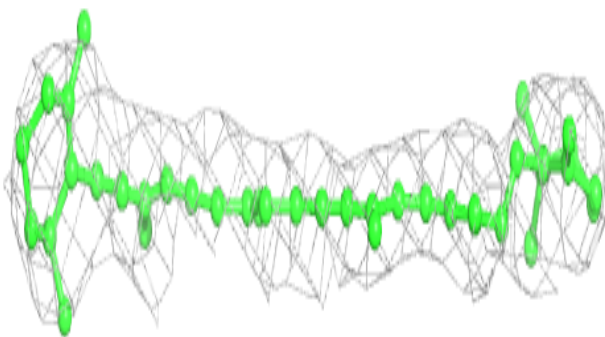
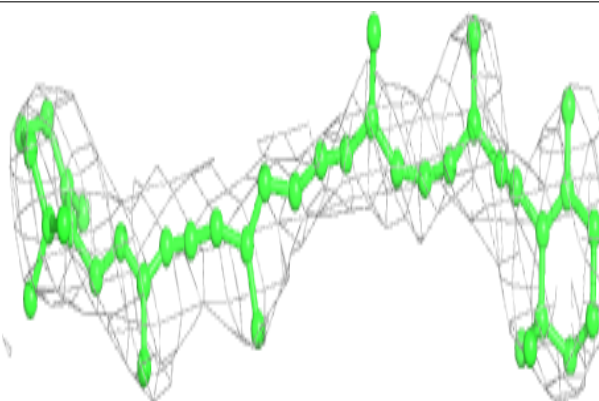


**Electron density around CLA B 1222:**

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

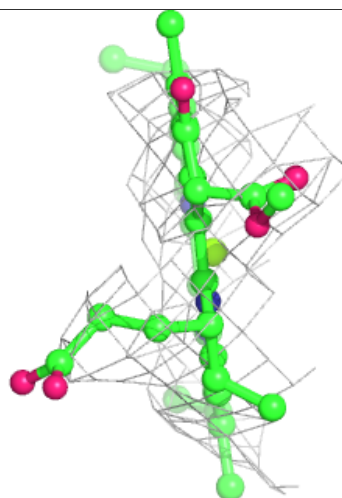
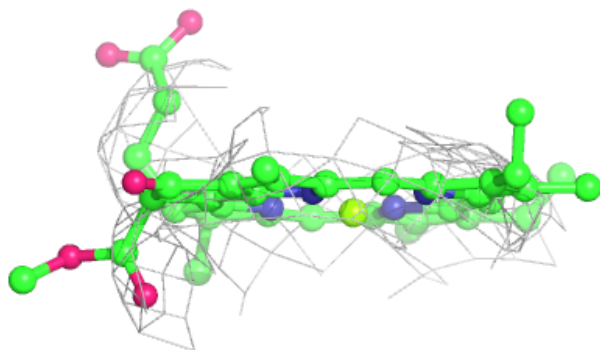
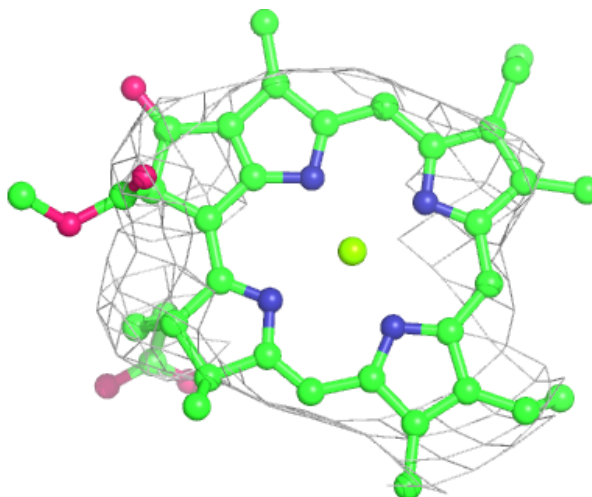
**Electron density around BCR A 4007:**

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



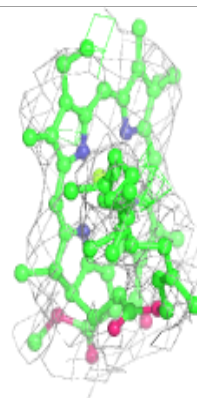
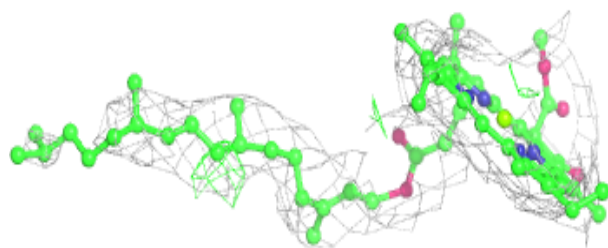
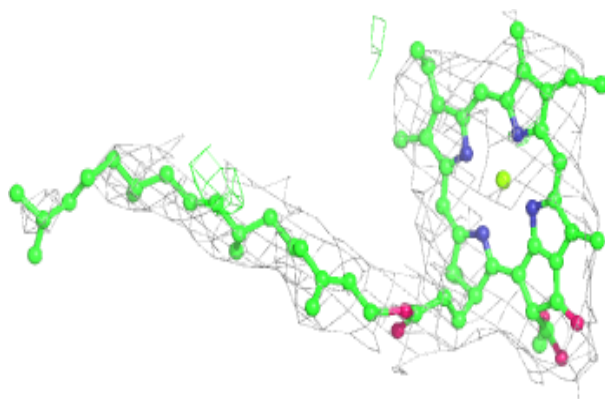
**Electron density around CLA b 1232:**

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



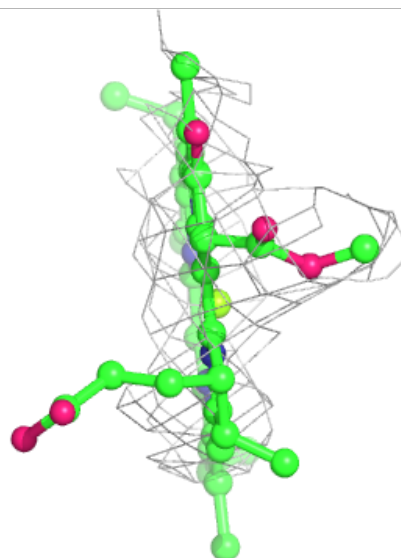
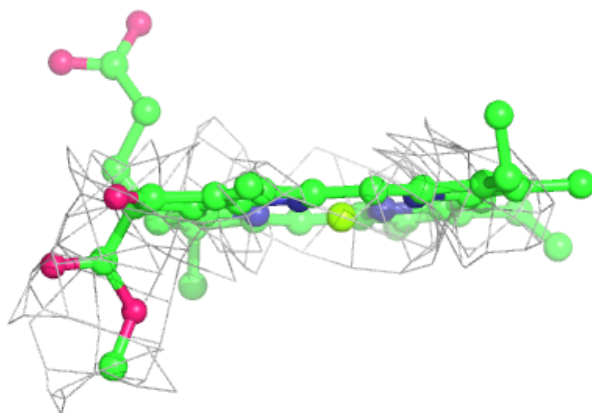
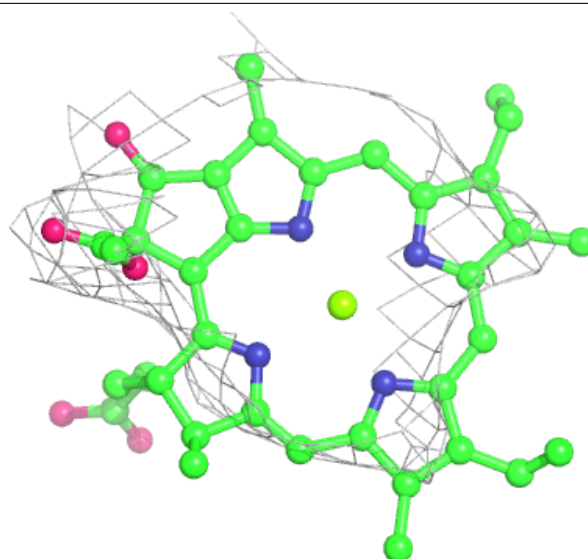
**Electron density around CLA A 1132:**

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



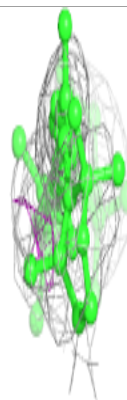
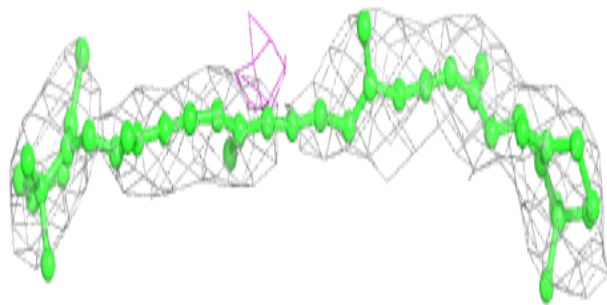
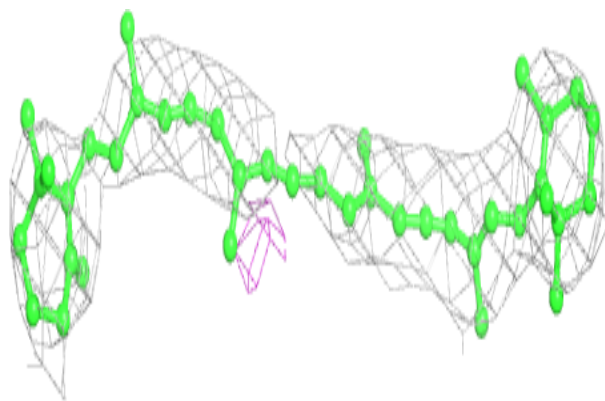
**Electron density around CLA b 1231:**

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



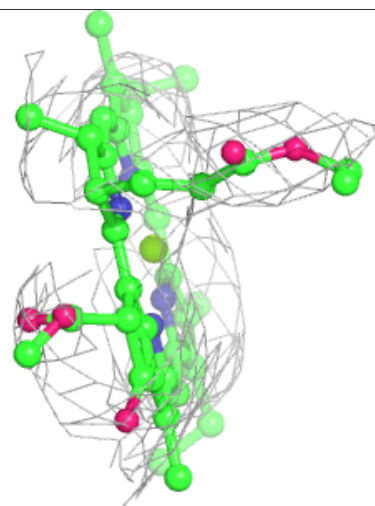
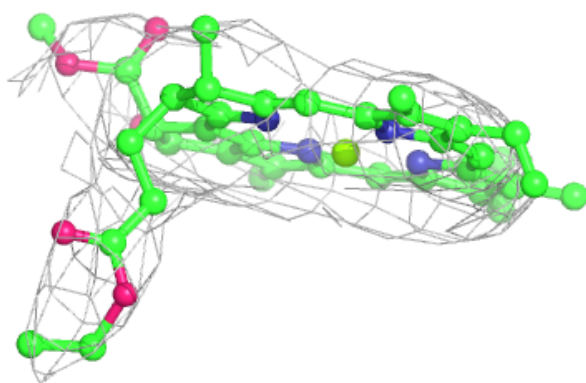
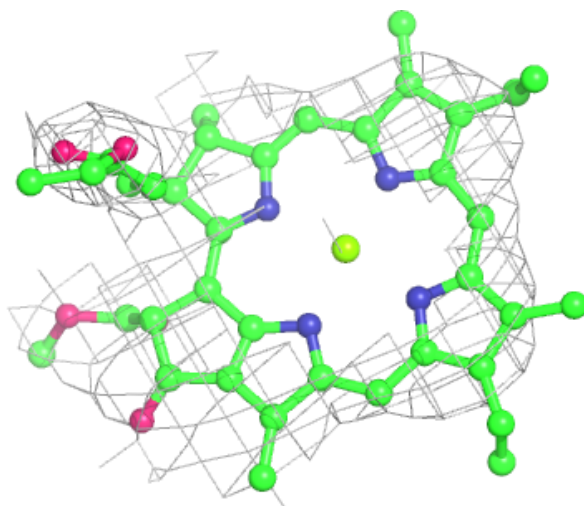
**Electron density around BCR A 4008:**

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



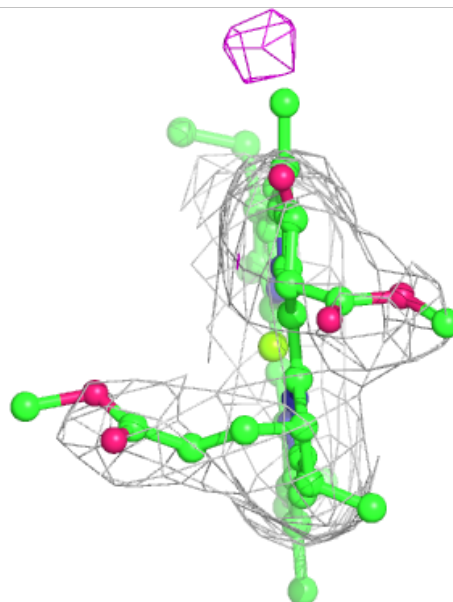
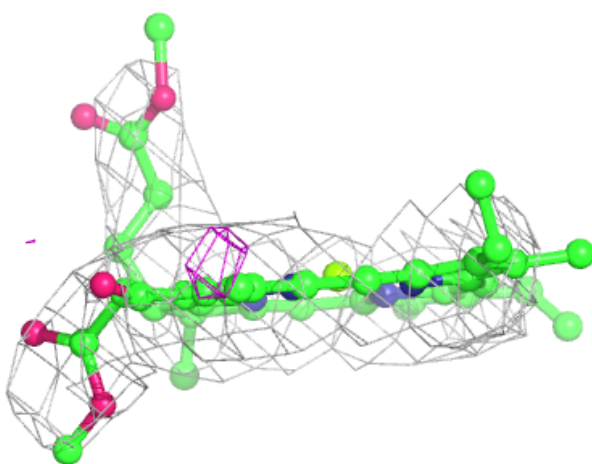
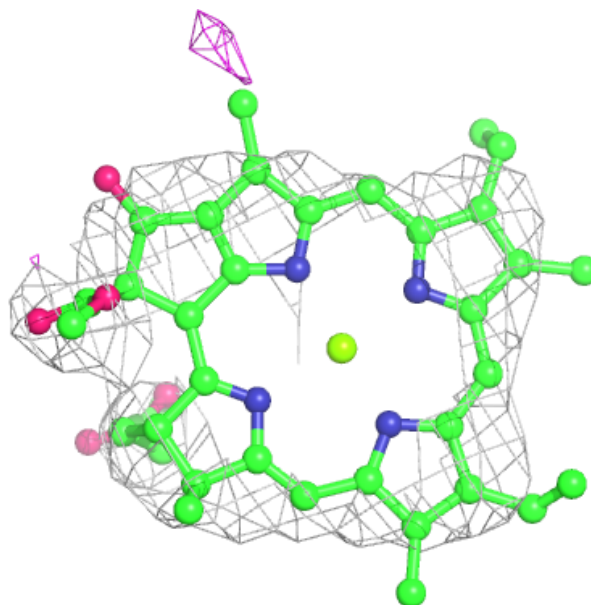
**Electron density around CLA B 1236:**

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



**Electron density around CLA 1 1502:**

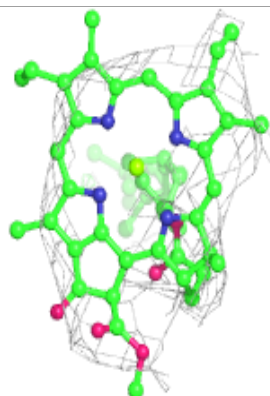
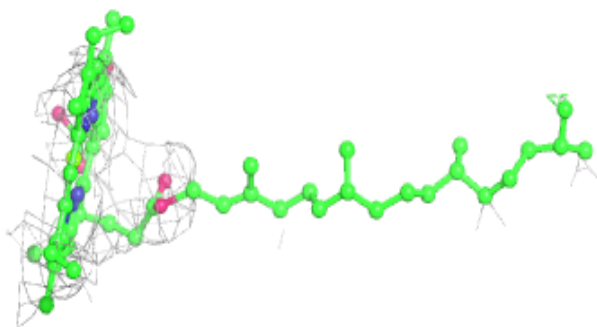
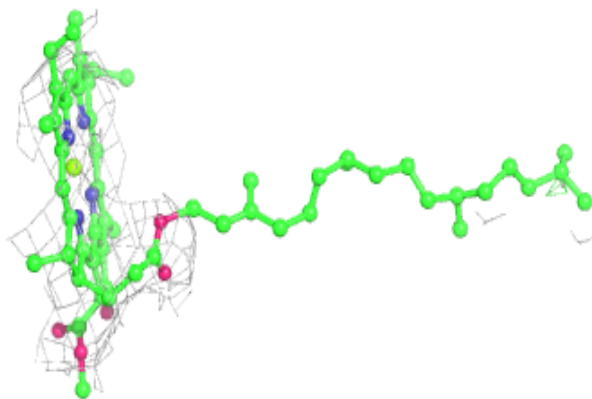
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



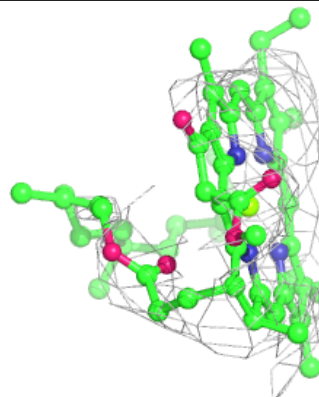
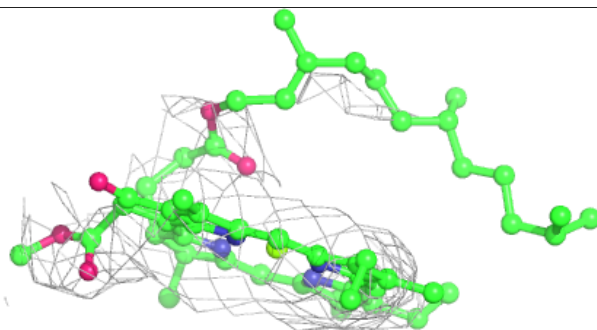
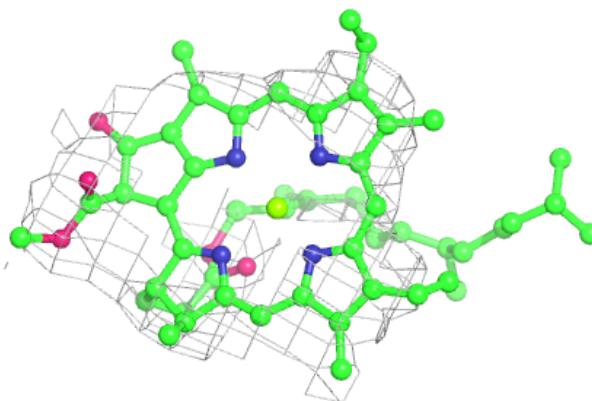


**Electron density around CLA a 1126:**

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

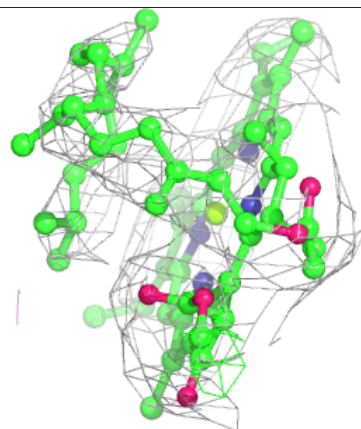
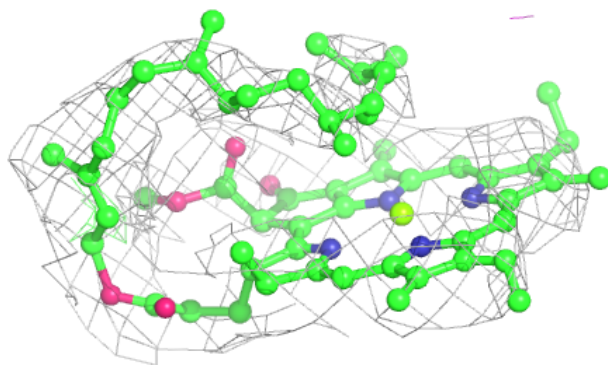
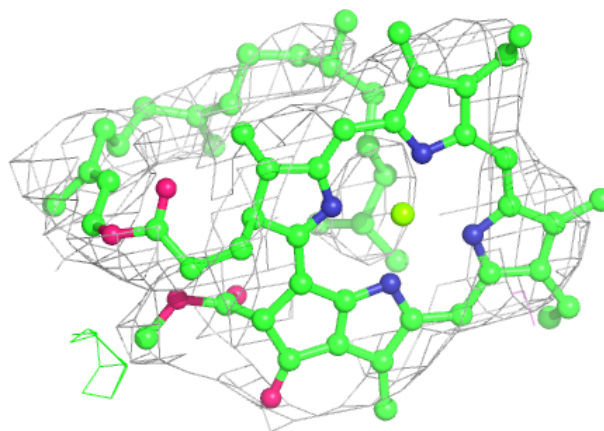
**Electron density around CLA B 1235:**

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

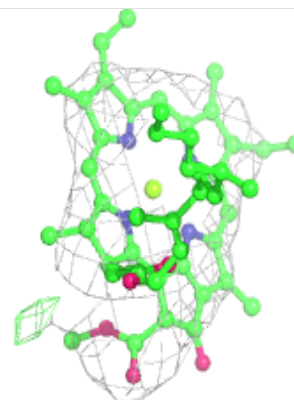
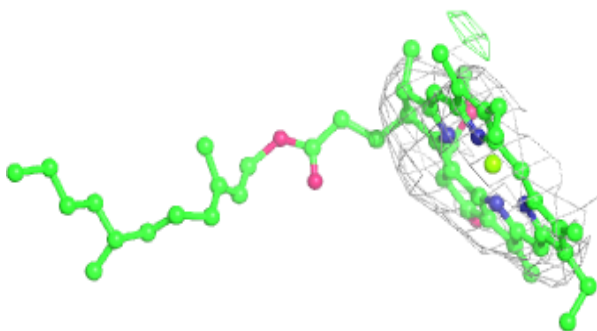
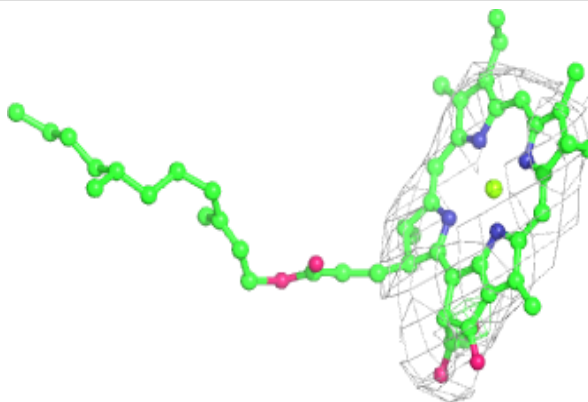


**Electron density around CLA A 1104:**

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

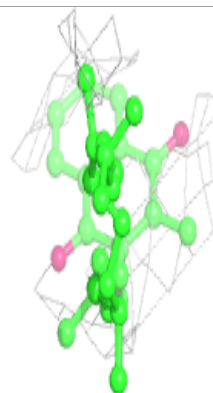
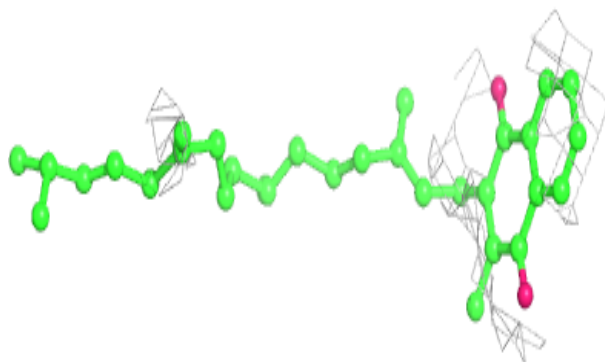
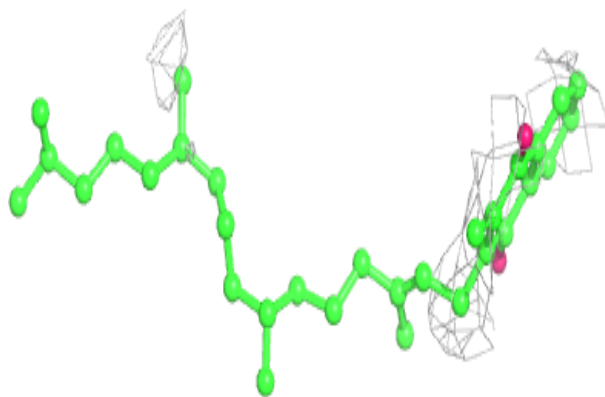
**Electron density around CLA 2 1230:**

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

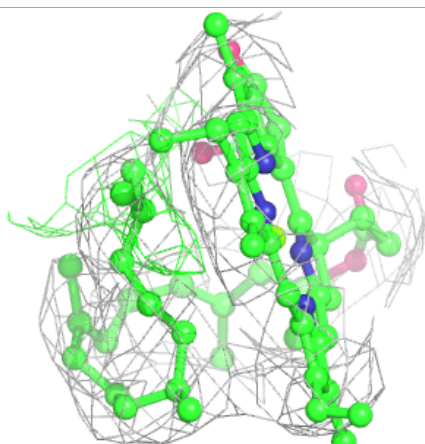
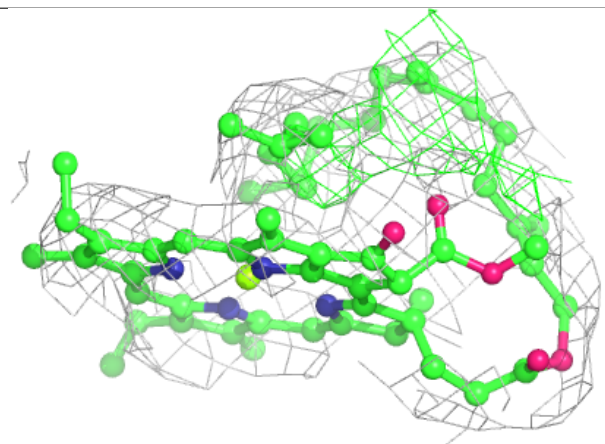
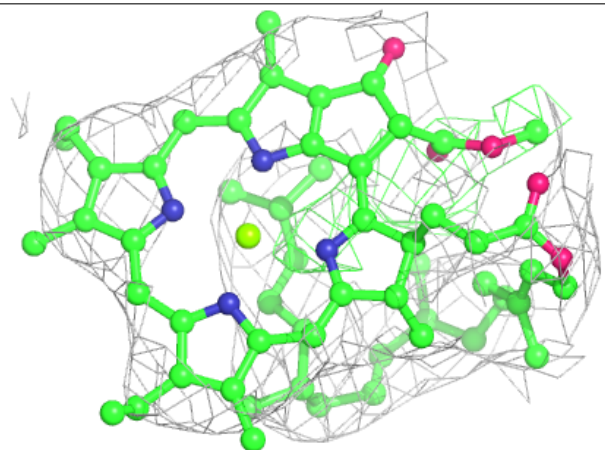


**Electron density around PQN 1 2001:**

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

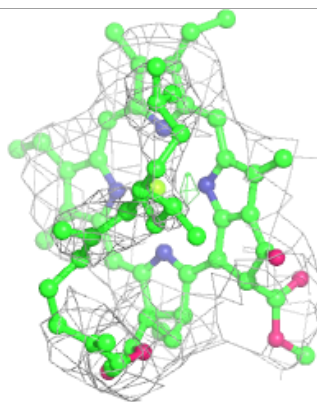
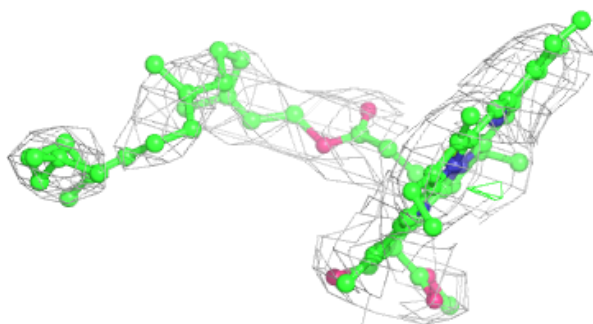
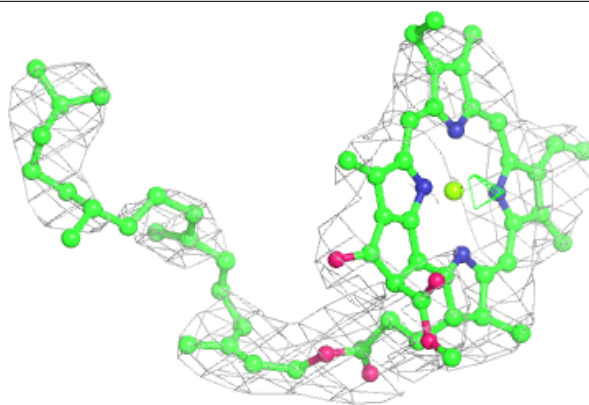
**Electron density around CLA 2 1203:**

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

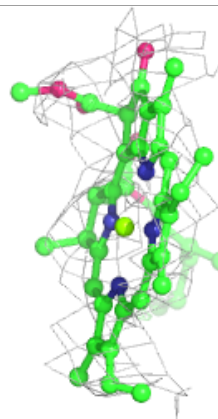
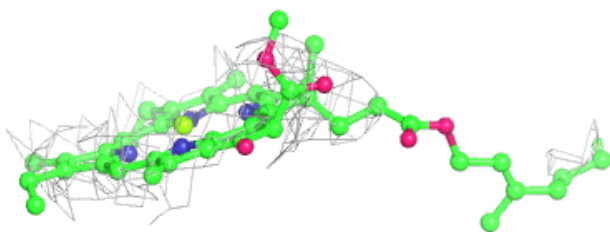
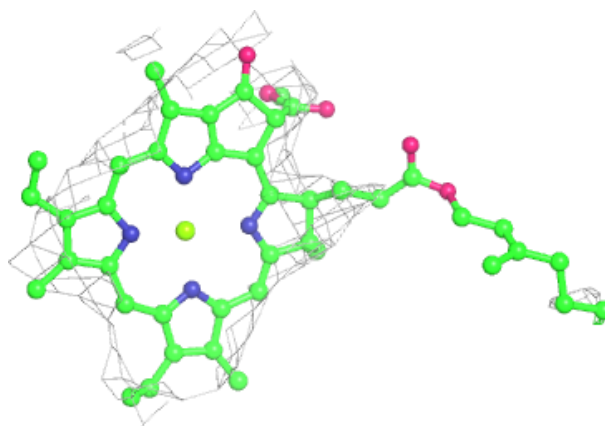


**Electron density around CLA A 1137:**

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

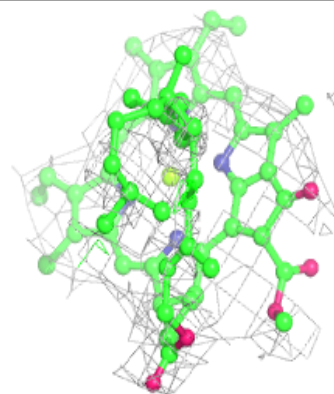
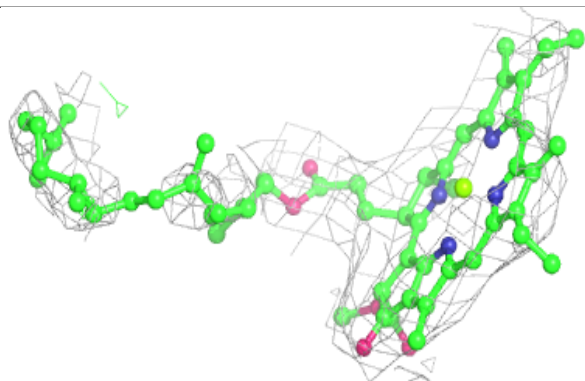
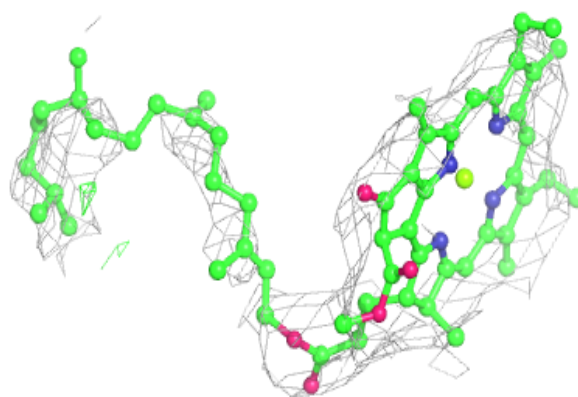
**Electron density around CLA 1 1125:**

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



**Electron density around CLA B 1021:**

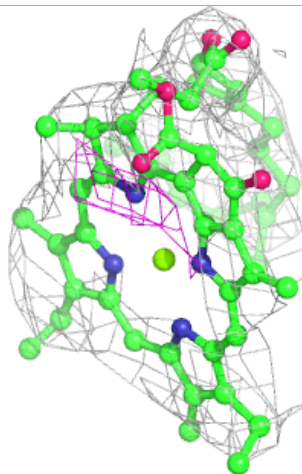
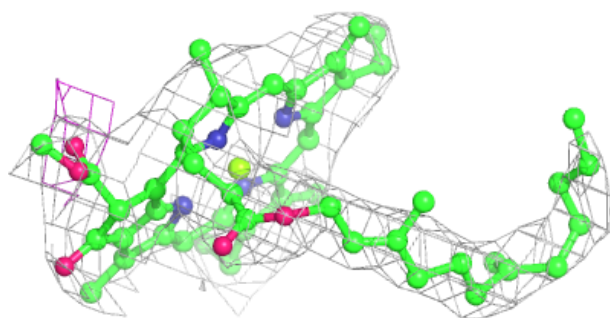
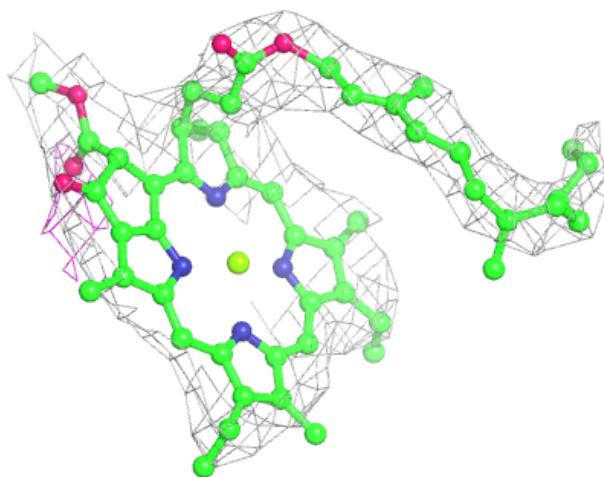
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





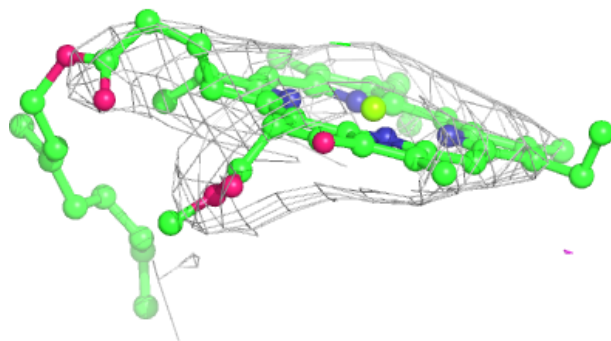
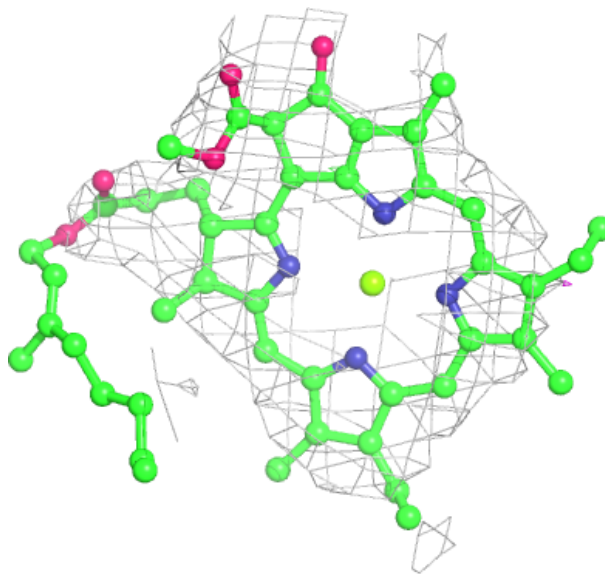
**Electron density around CLA A 1122:**

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



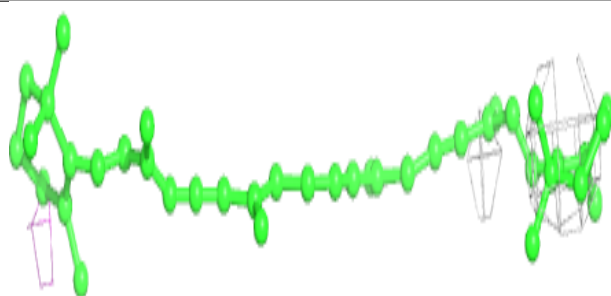
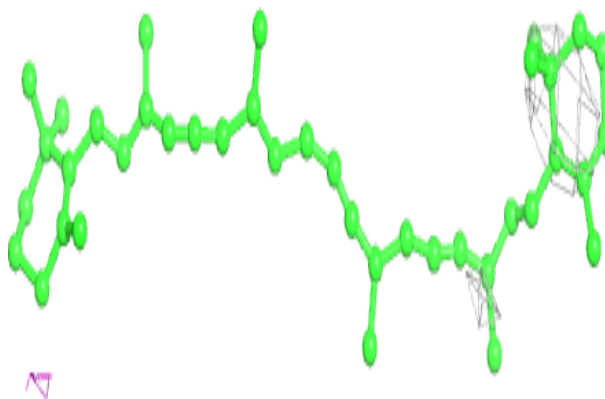
**Electron density around CLA B 1221:**

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

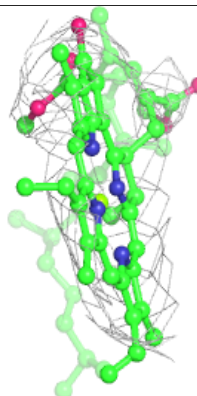
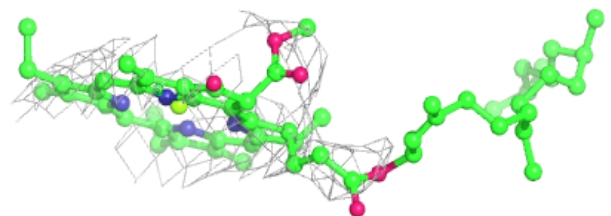
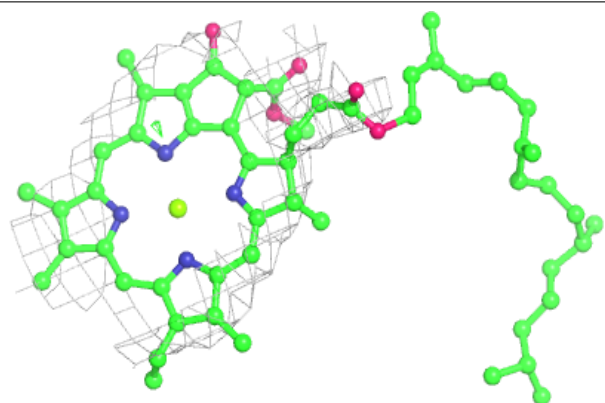


**Electron density around BCR 1 4002:**

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

**Electron density around CLA 1 1101:**

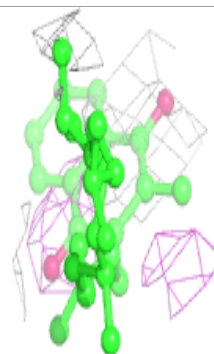
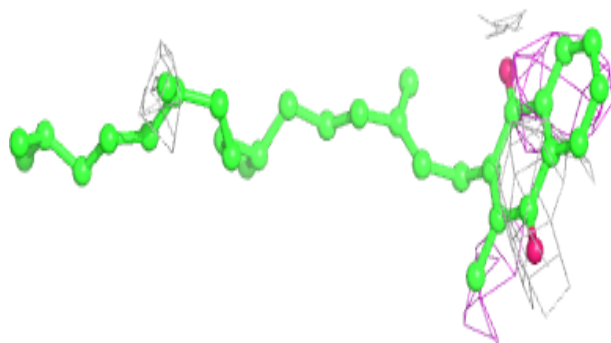
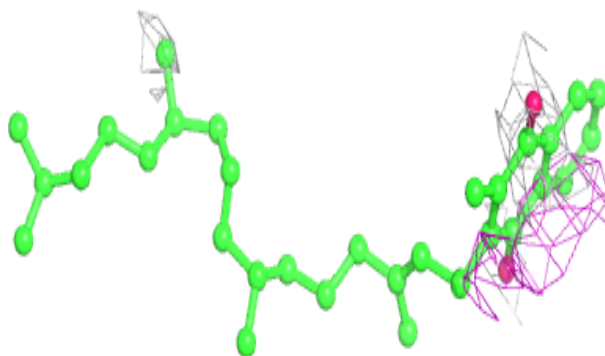
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





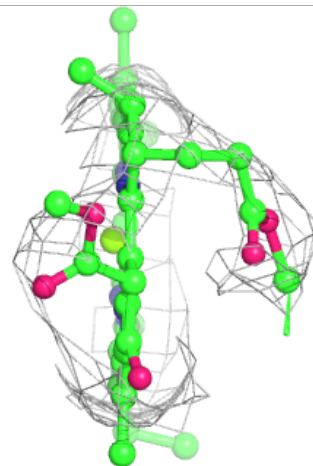
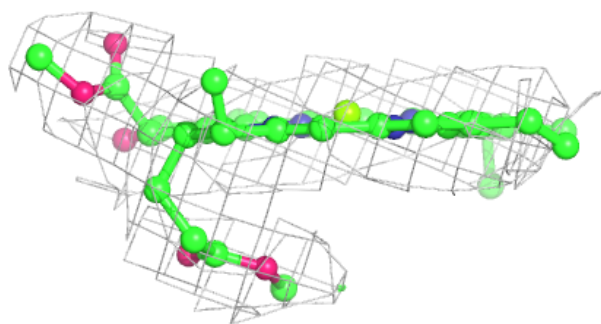
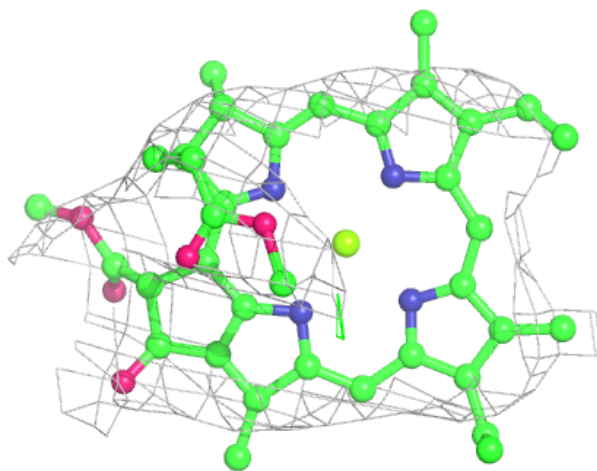
**Electron density around PQN a 2001:**

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



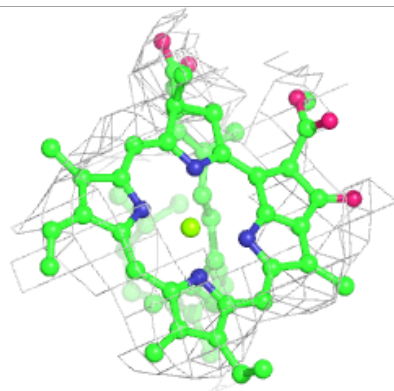
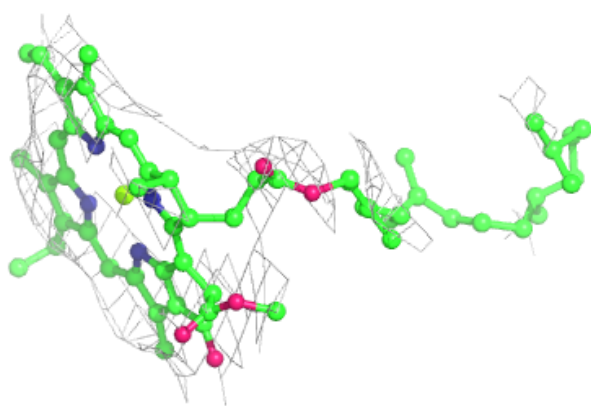
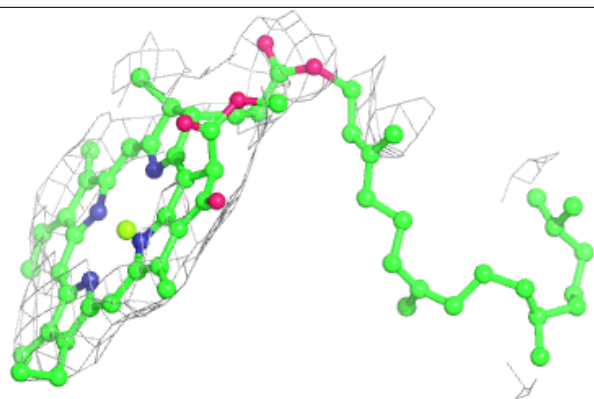
**Electron density around CLA A 1138:**

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

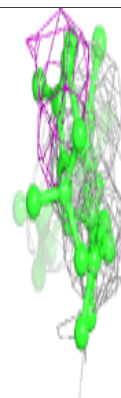
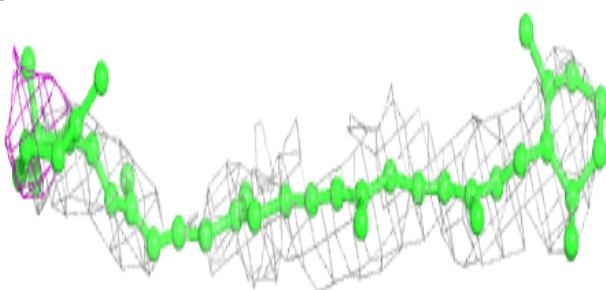
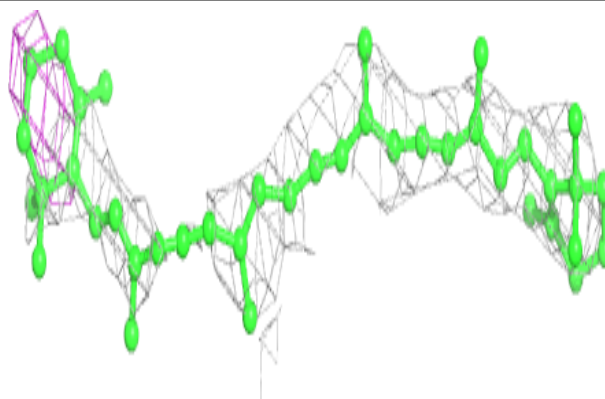


**Electron density around CLA b 1021:**

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

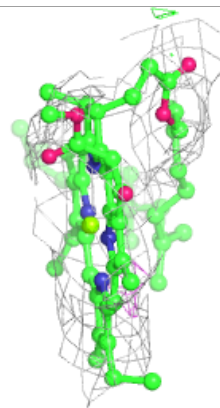
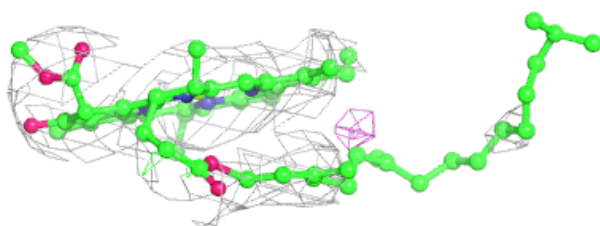
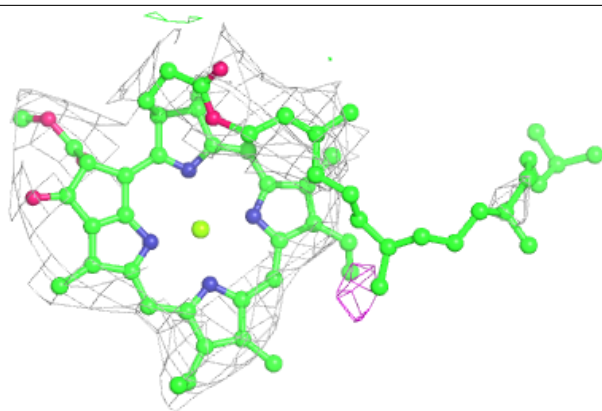
**Electron density around BCR L 4022:**

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

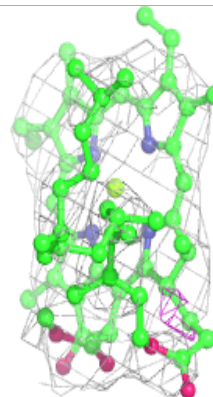
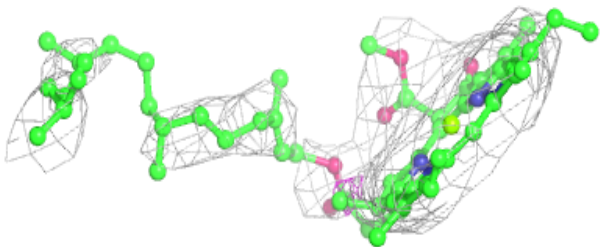
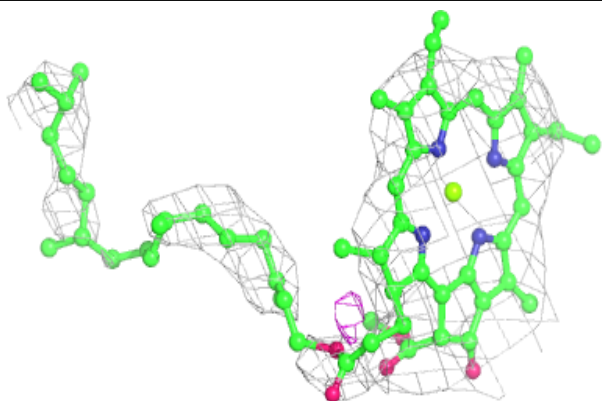


**Electron density around CLA 2 1215:**

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

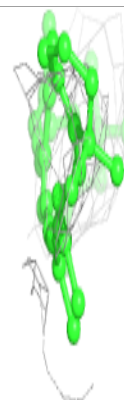
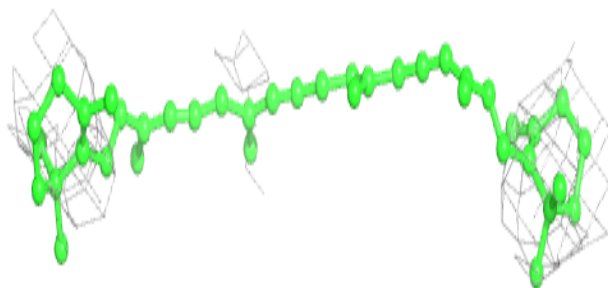
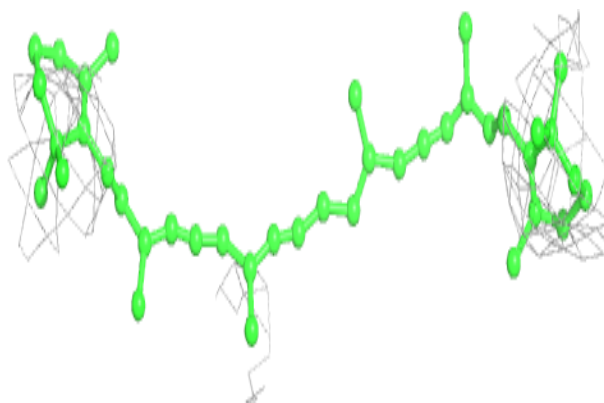
**Electron density around CLA b 1207:**

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

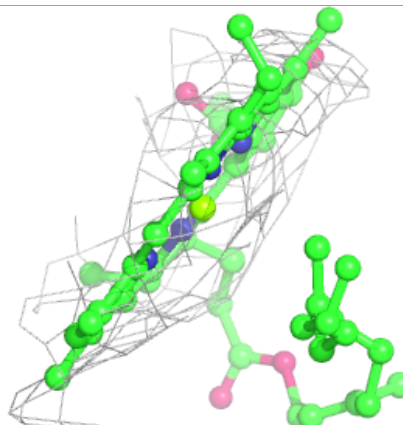
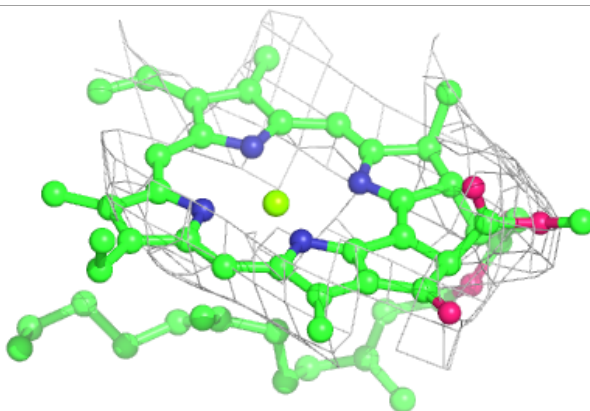
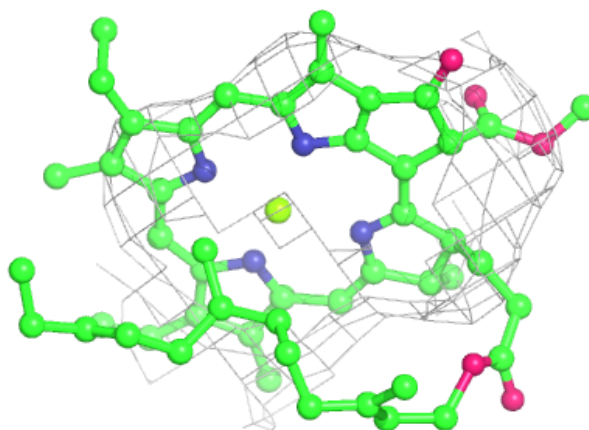


**Electron density around BCR 1 4001:**

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

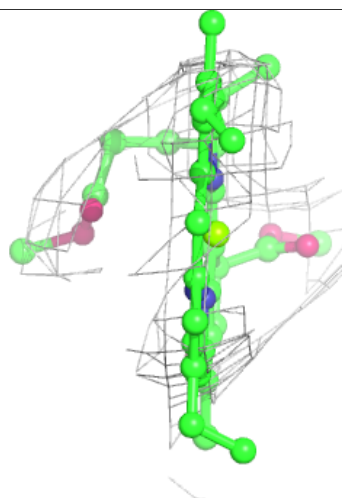
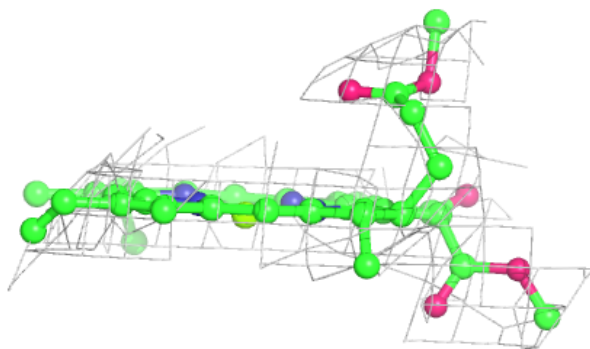
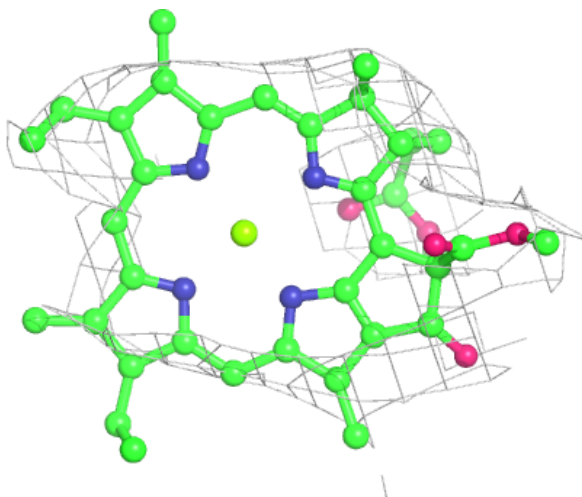
**Electron density around CLA b 1214:**

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



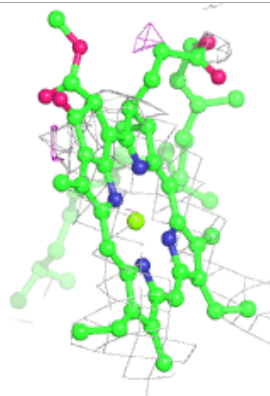
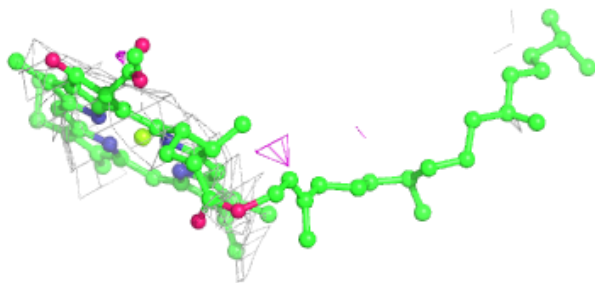
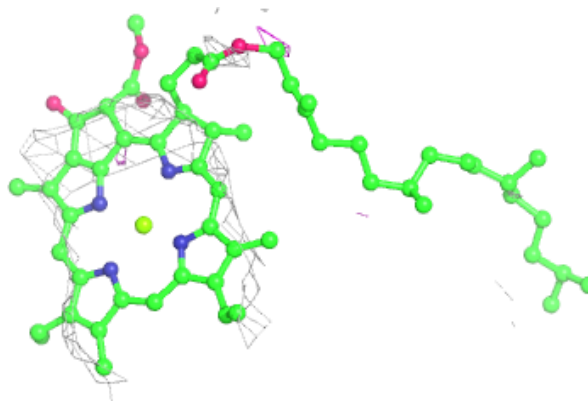
**Electron density around CLA 1 1115:**

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



**Electron density around CLA b 1013:**

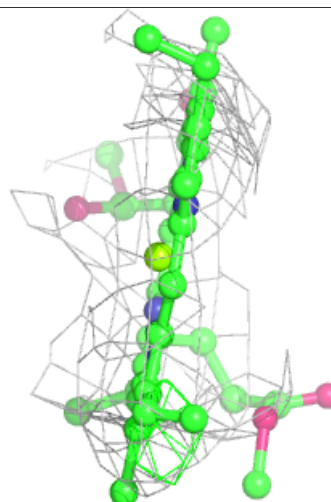
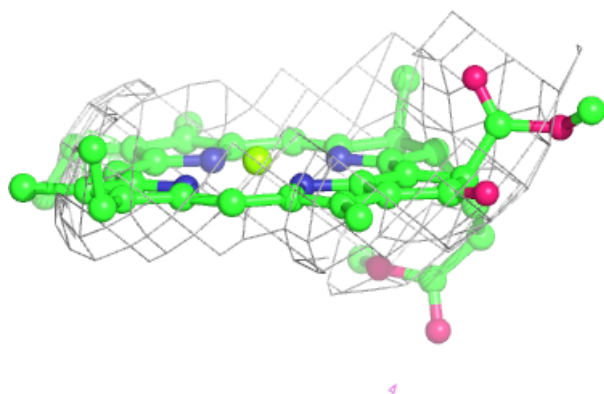
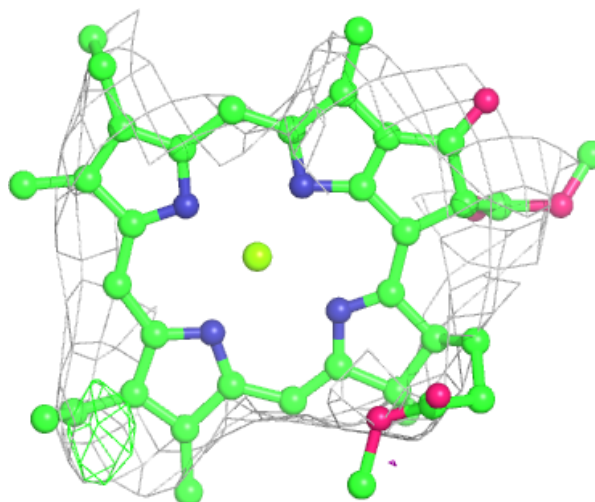
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





**Electron density around CLA 1 1121:**

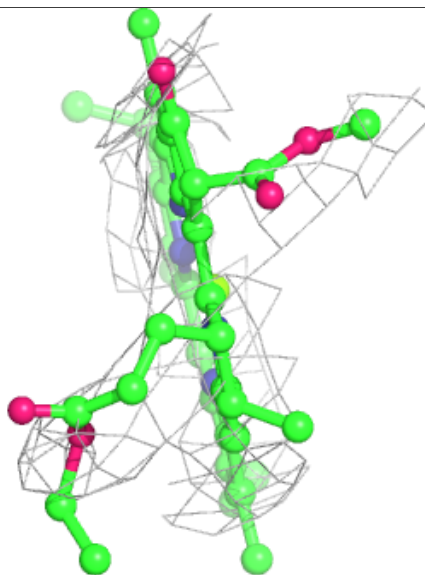
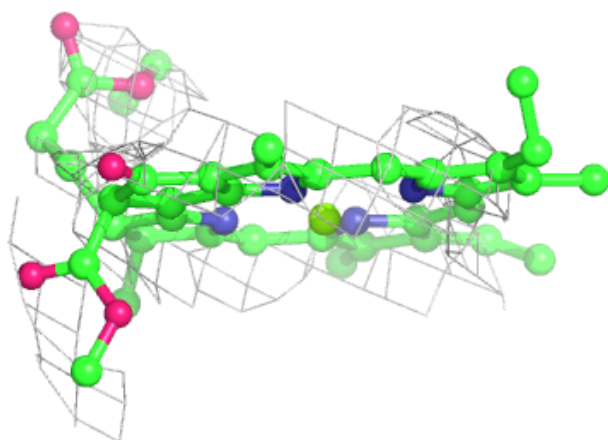
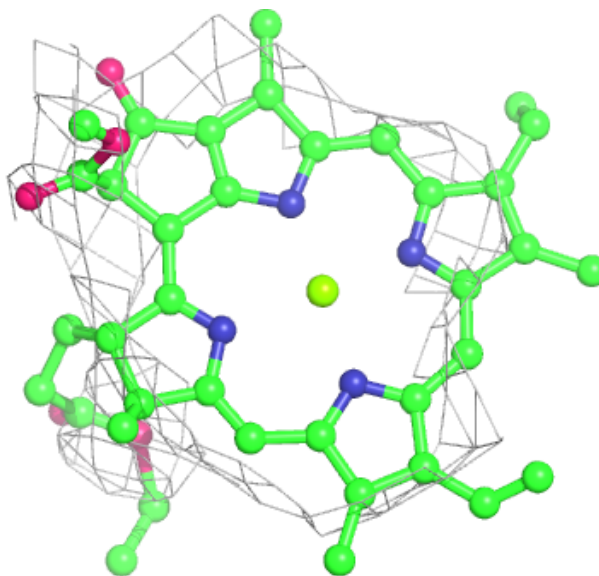
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





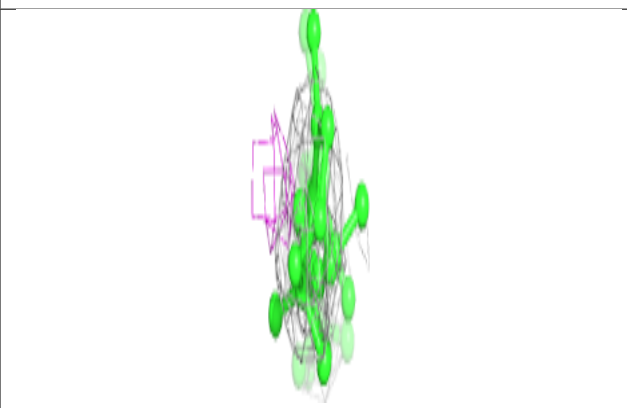
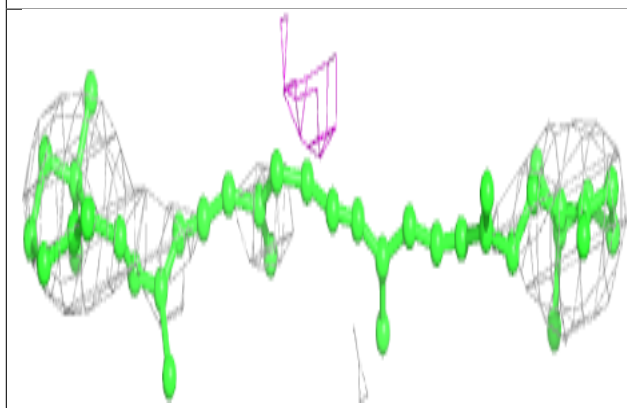
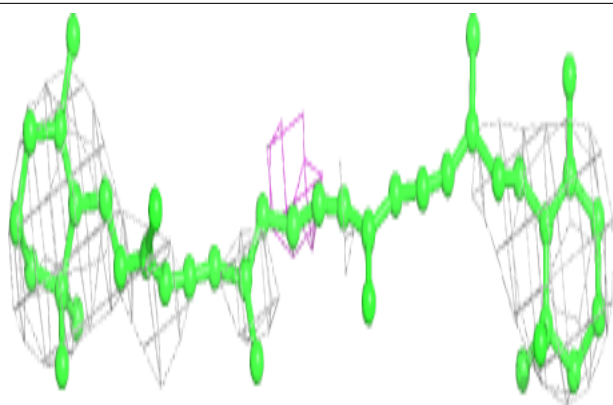
**Electron density around CLA b 1217:**

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



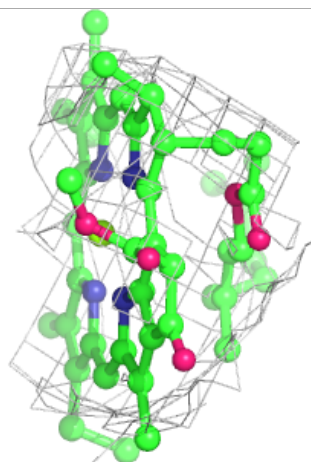
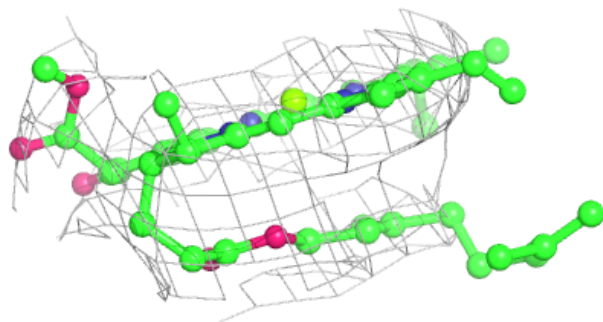
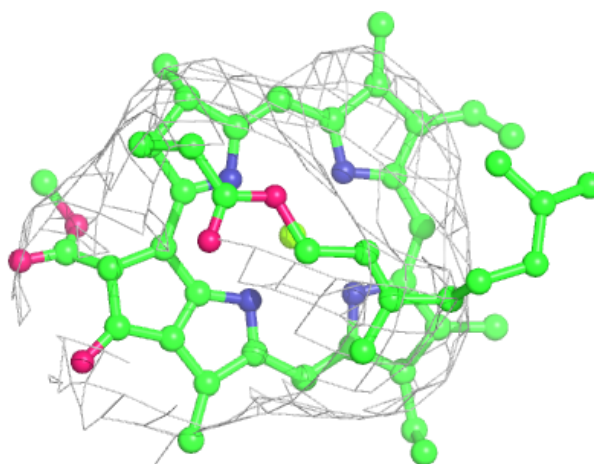
**Electron density around BCR 8 4019:**

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



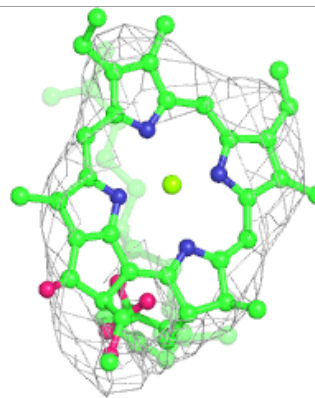
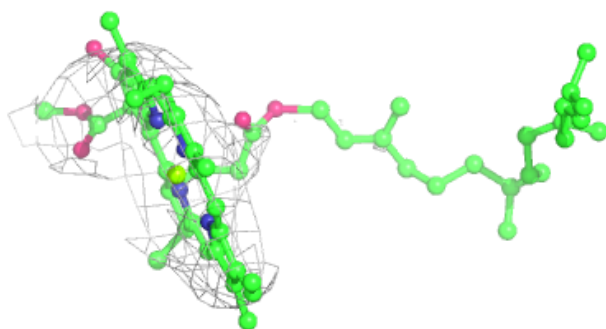
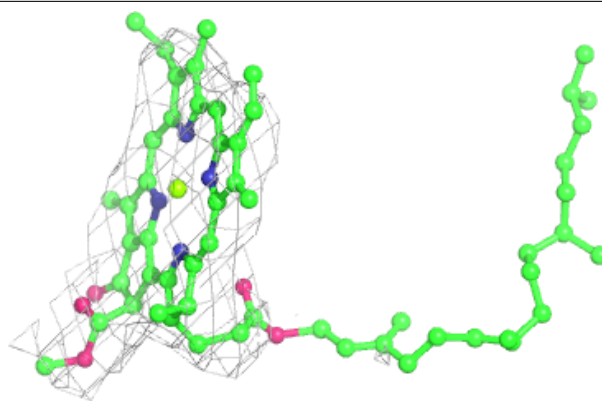
**Electron density around CLA b 1205:**

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

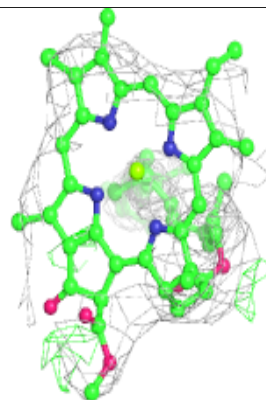
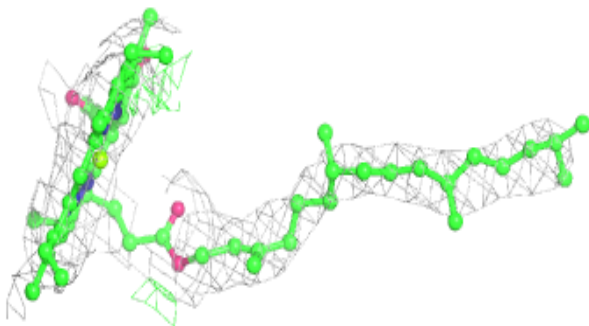
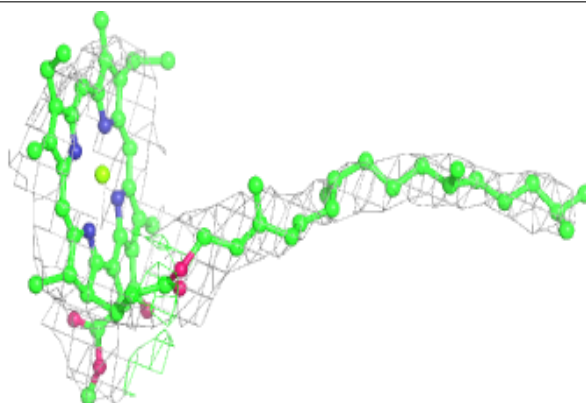


**Electron density around CLA A 1140:**

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

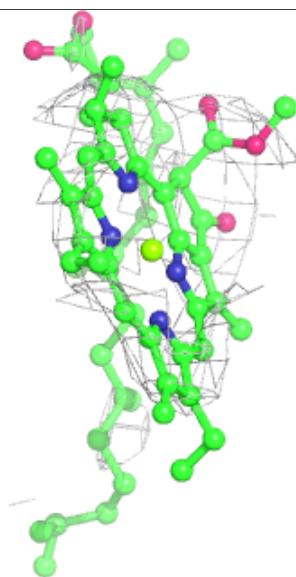
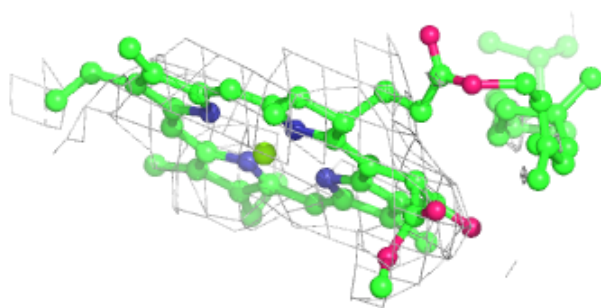
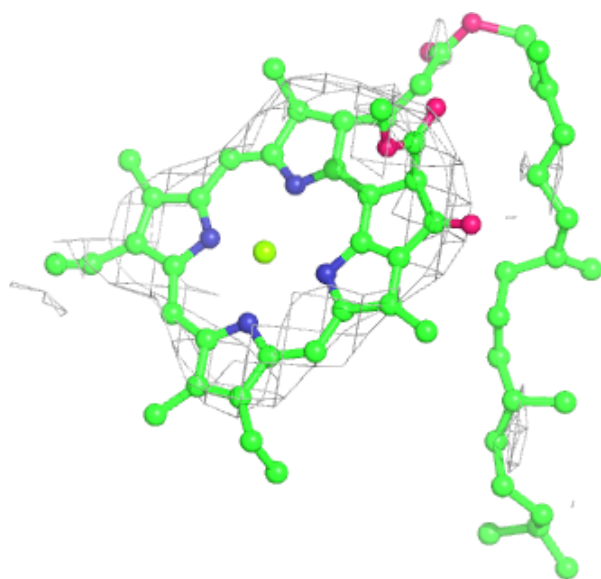
**Electron density around CLA 2 1225:**

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



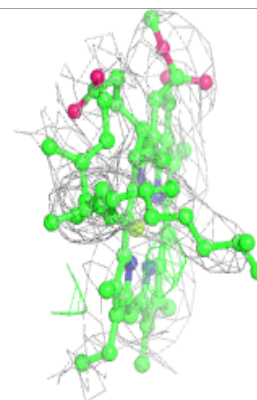
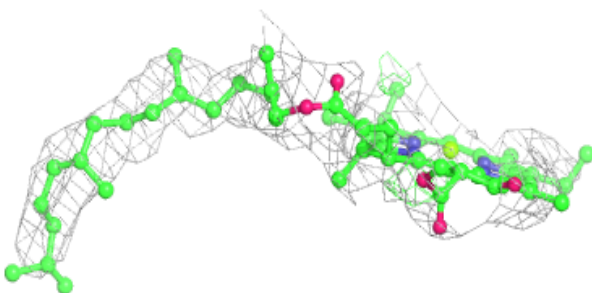
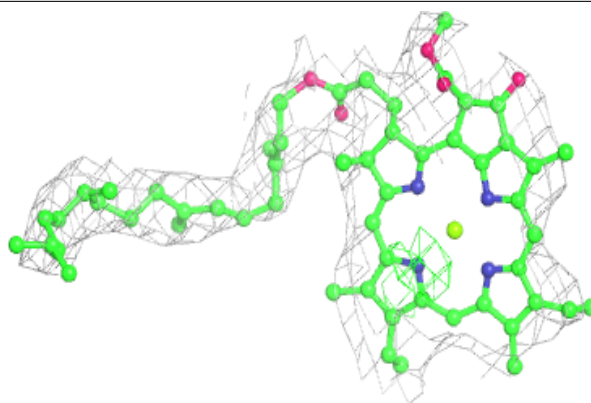
**Electron density around CLA a 1123:**

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

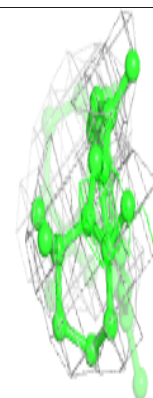
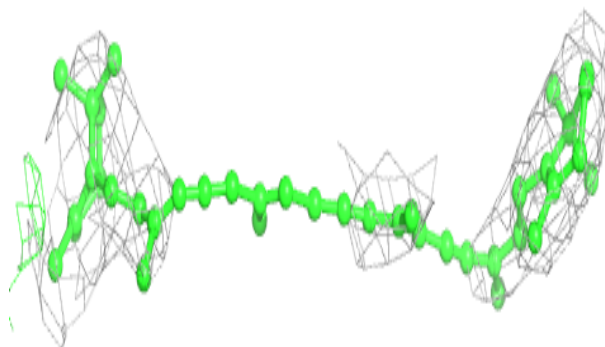
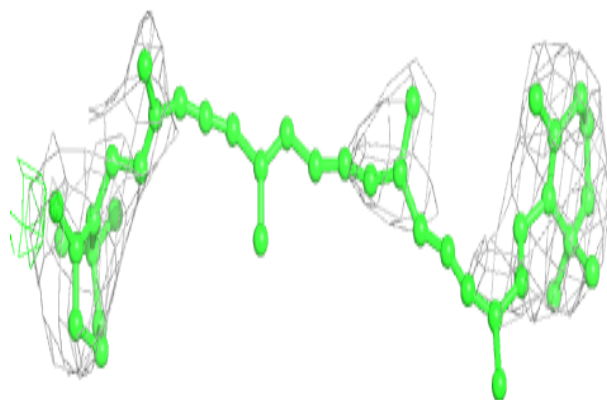


**Electron density around CLA B 1023:**

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

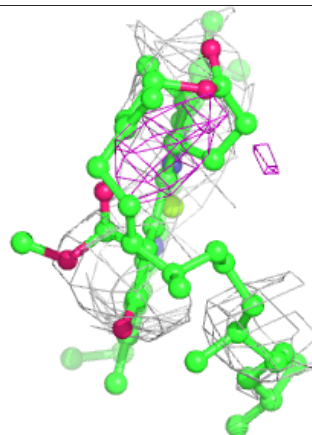
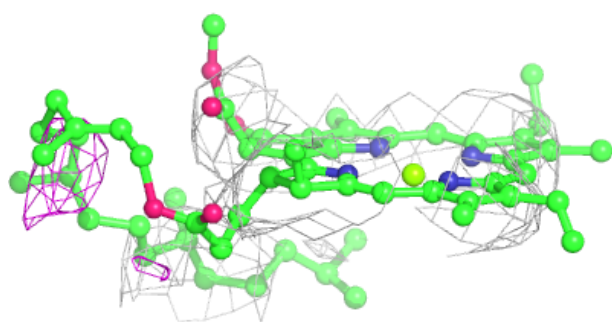
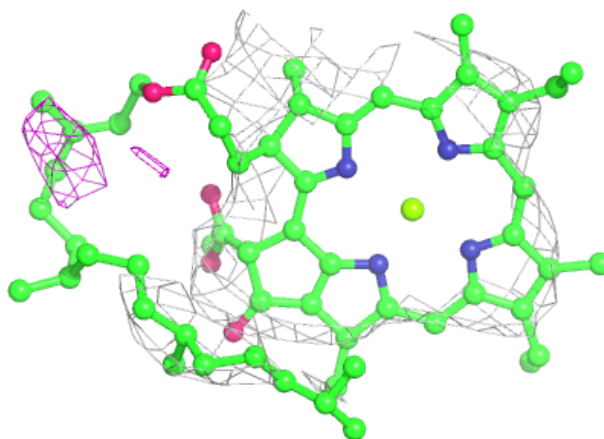
**Electron density around BCR B 4006:**

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

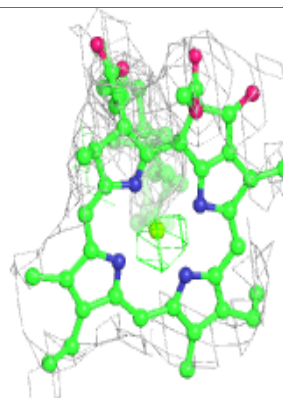
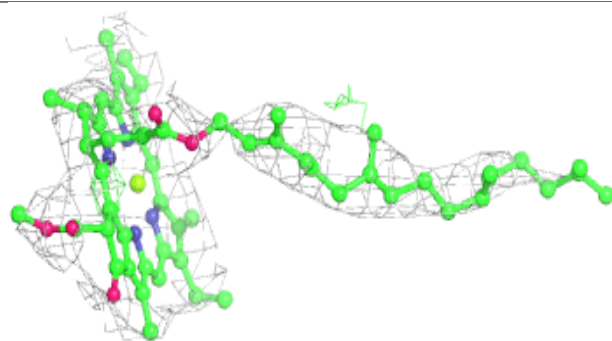
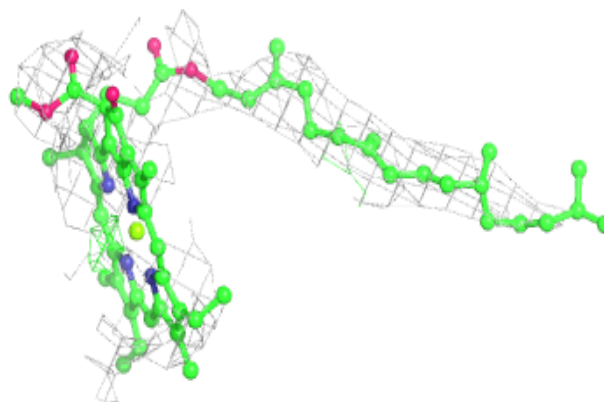


**Electron density around CLA b 1202:**

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

**Electron density around CLA 2 1226:**

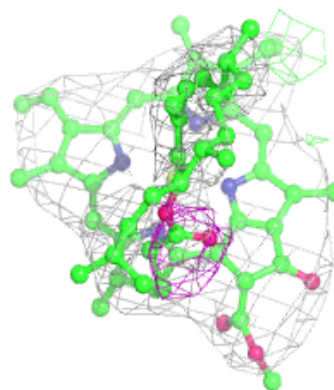
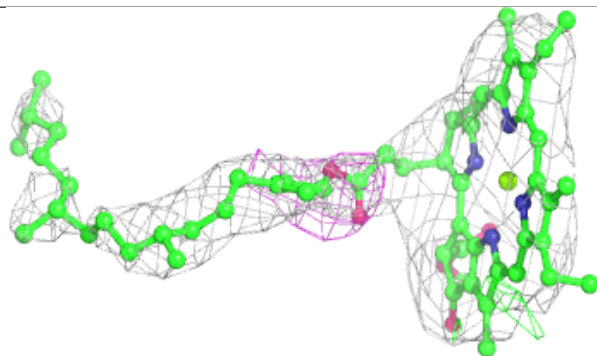
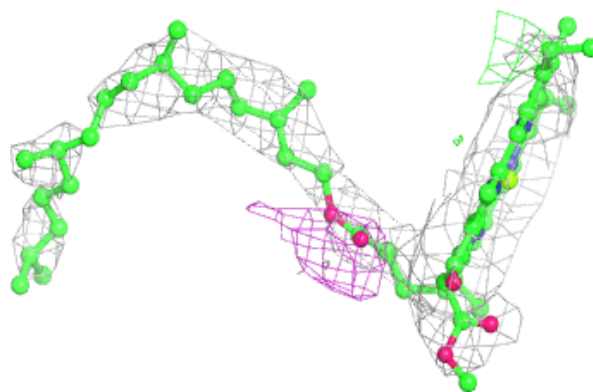
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





**Electron density around CLA B 1238:**

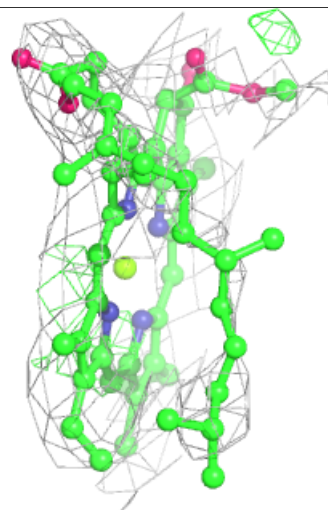
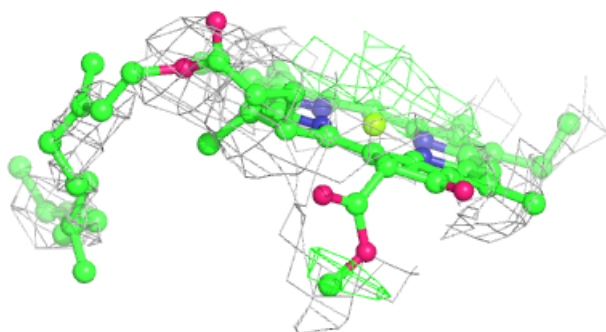
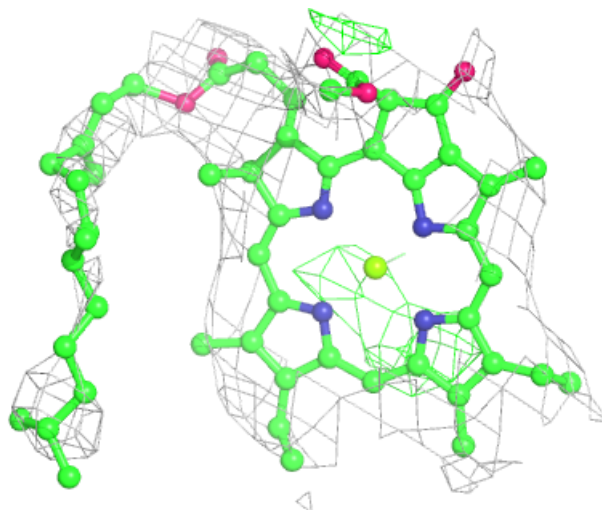
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





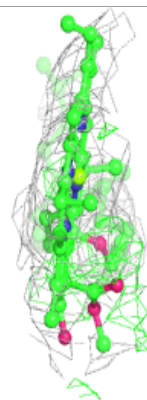
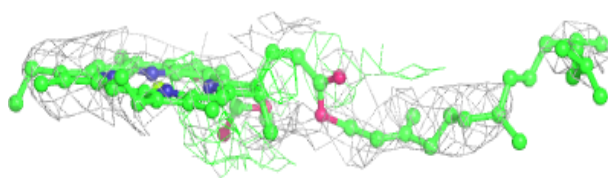
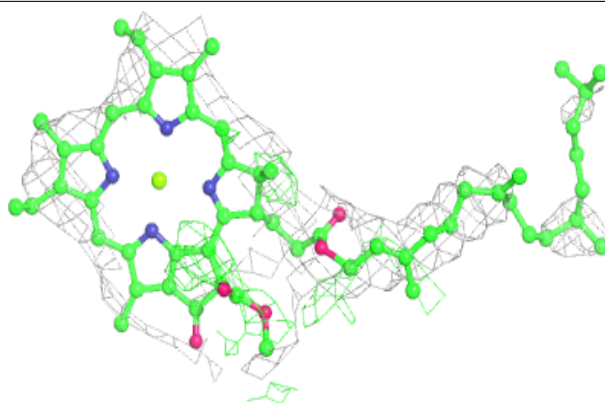
**Electron density around CLA A 1111:**

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

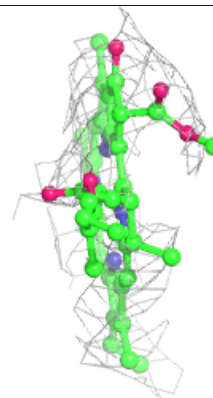
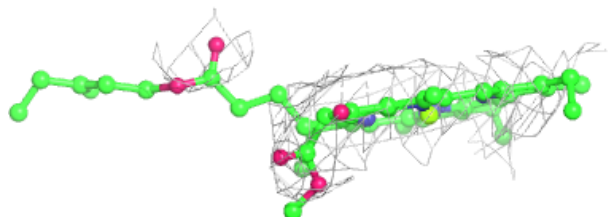
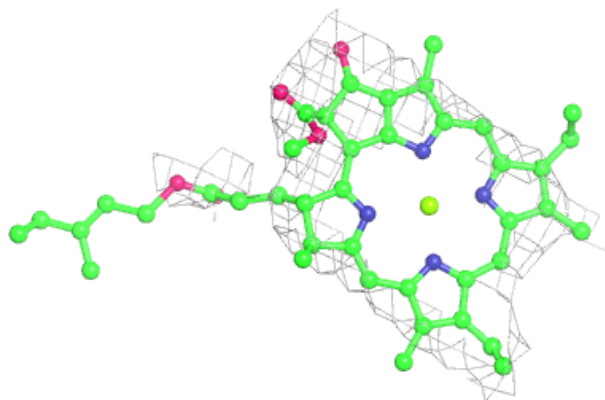


**Electron density around CLA 1 1131:**

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

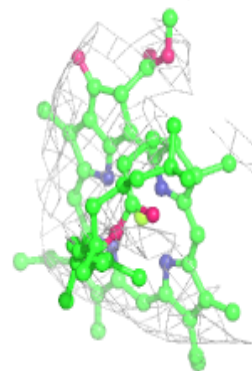
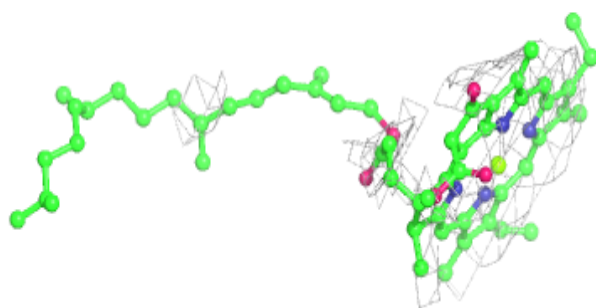
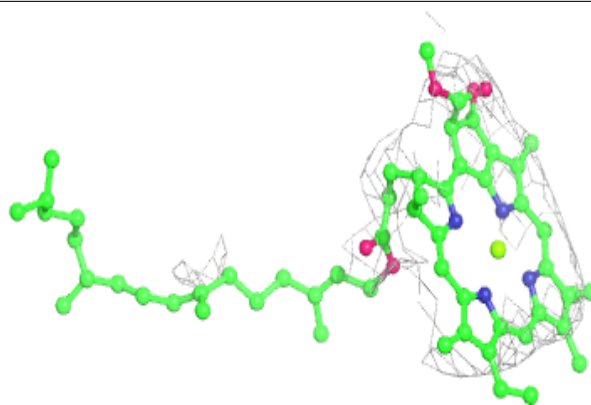
**Electron density around CLA a 1135:**

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

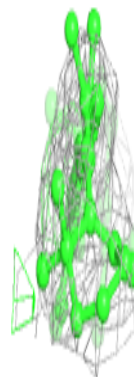
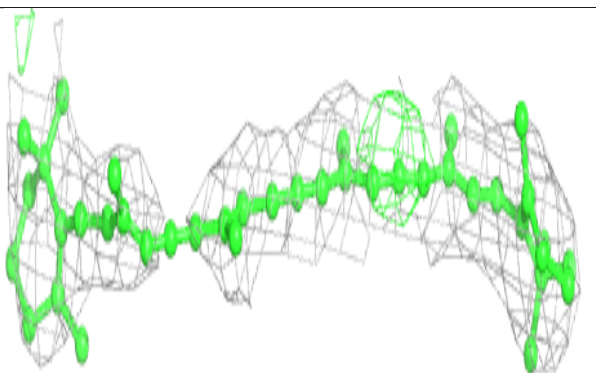
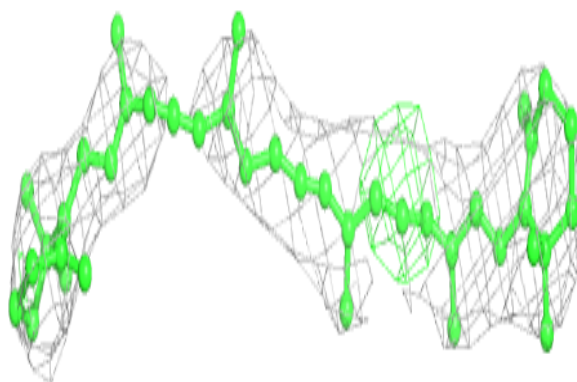


**Electron density around CLA 1 1119:**

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

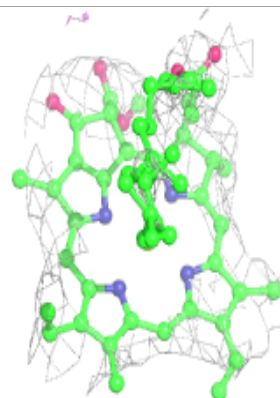
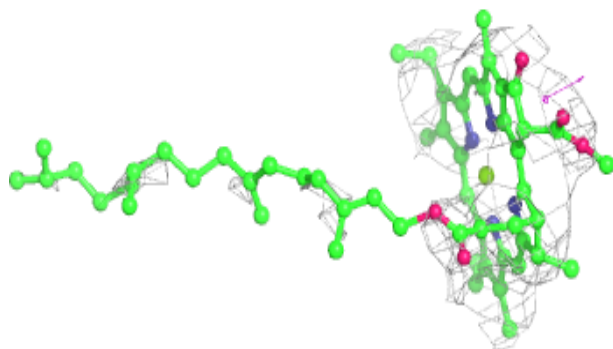
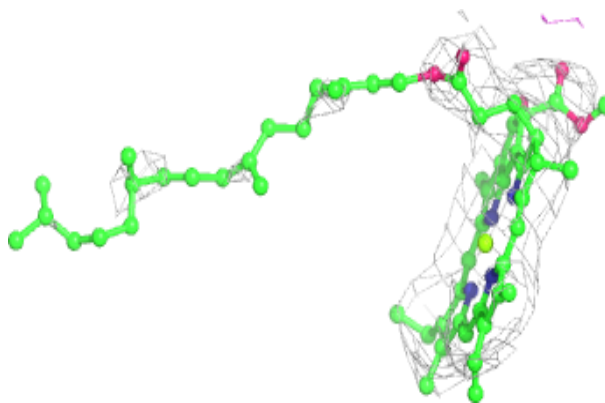
**Electron density around BCR B 4017:**

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



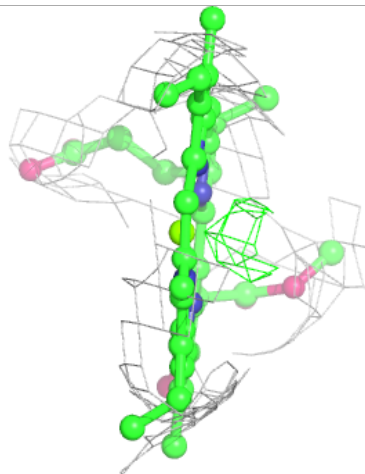
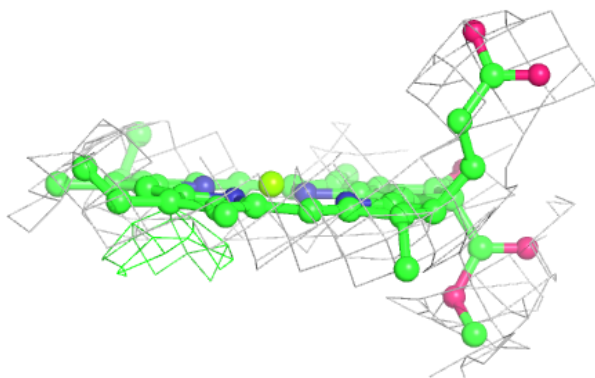
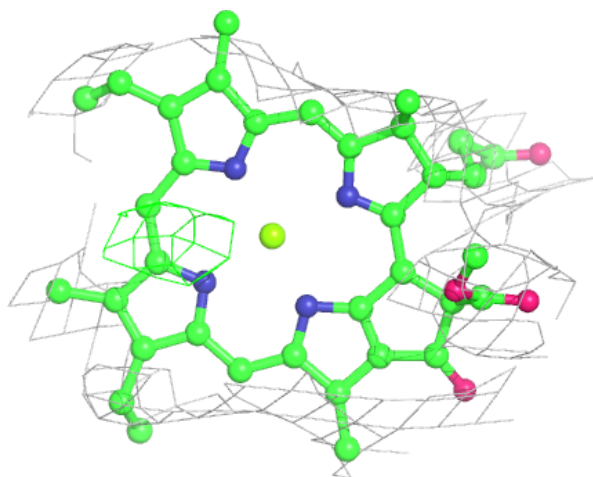
**Electron density around CLA B 1226:**

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



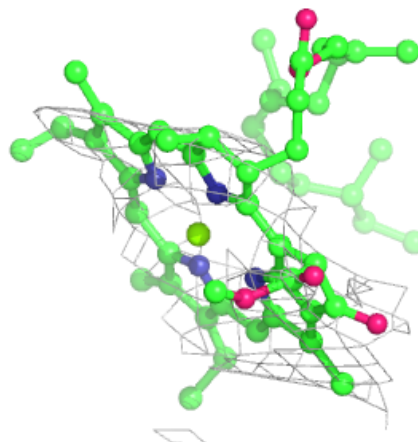
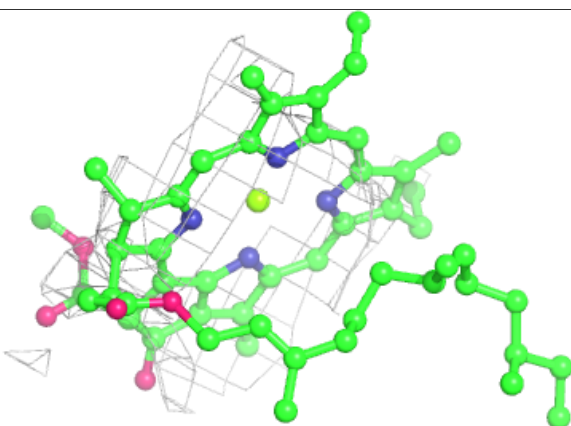
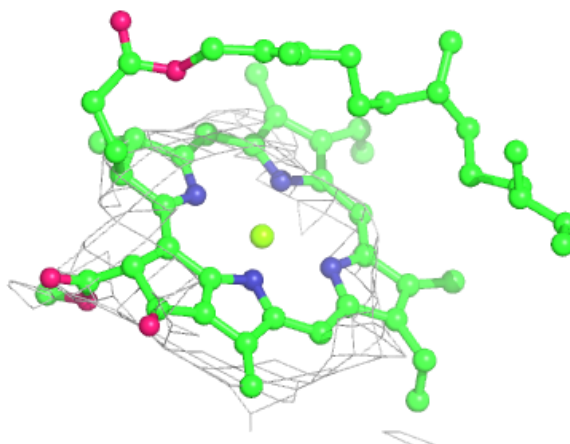
**Electron density around CLA A 1112:**

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



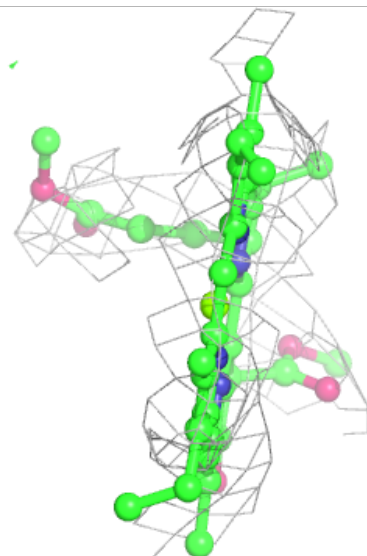
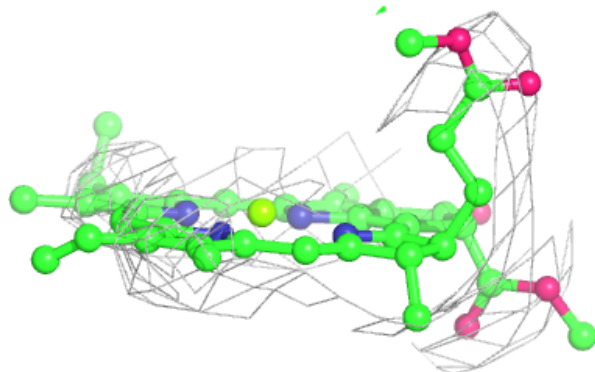
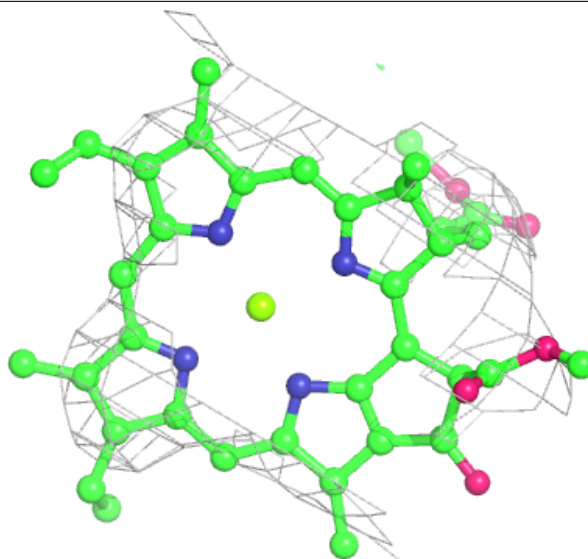
**Electron density around CLA 1 1118:**

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



**Electron density around CLA a 1133:**

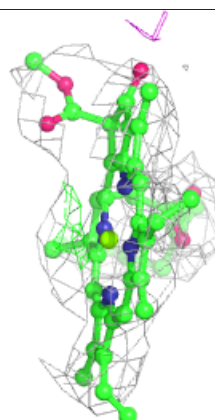
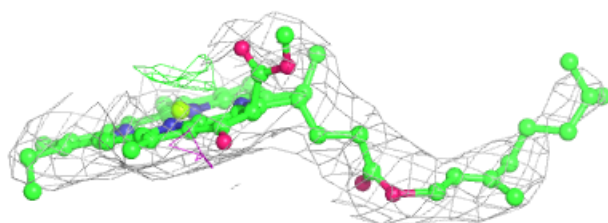
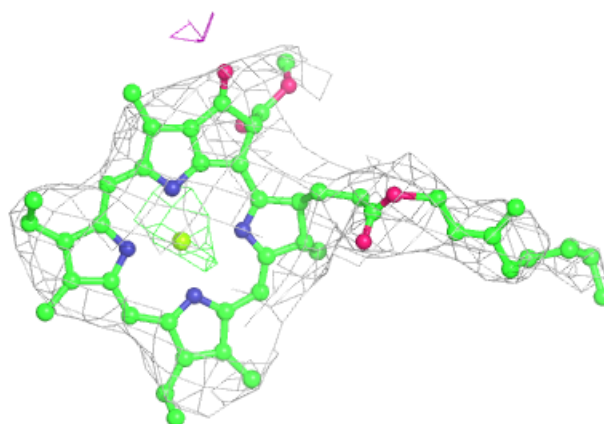
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



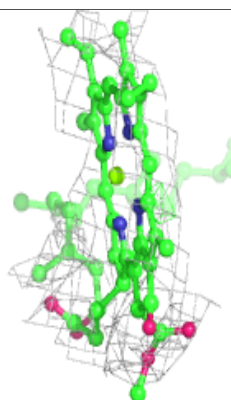
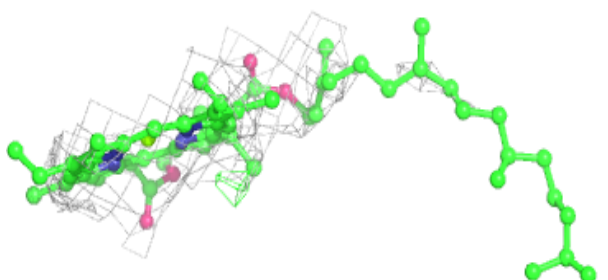
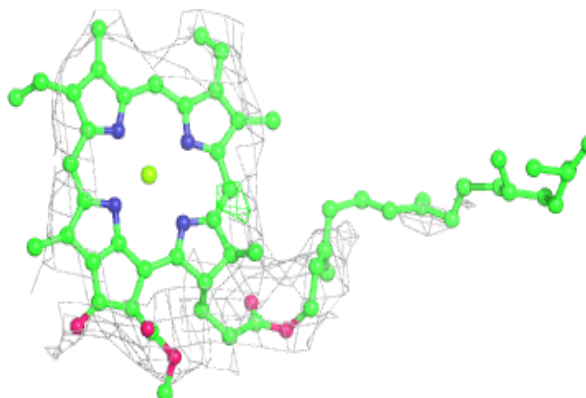


**Electron density around CLA A 1124:**

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

**Electron density around CLA 2 1023:**

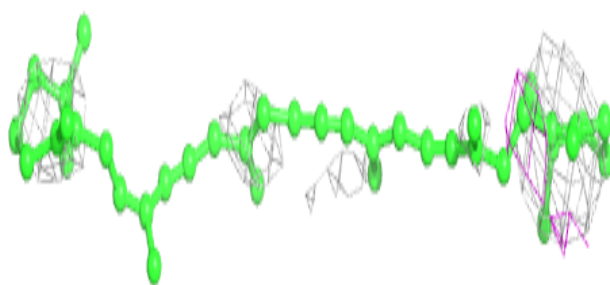
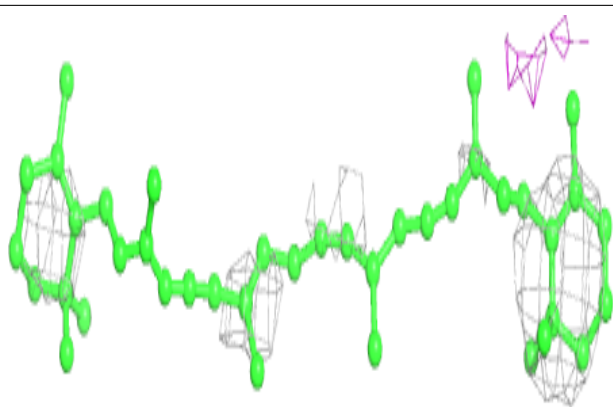
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





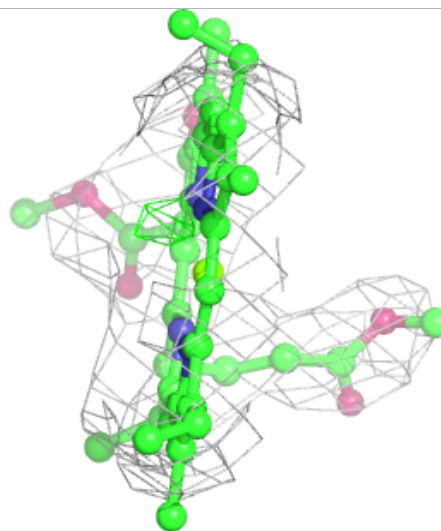
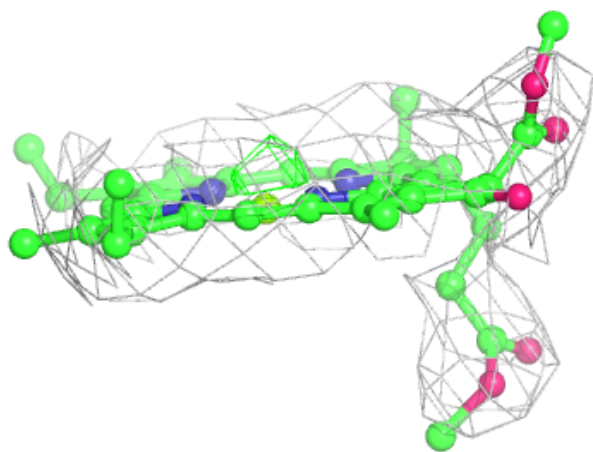
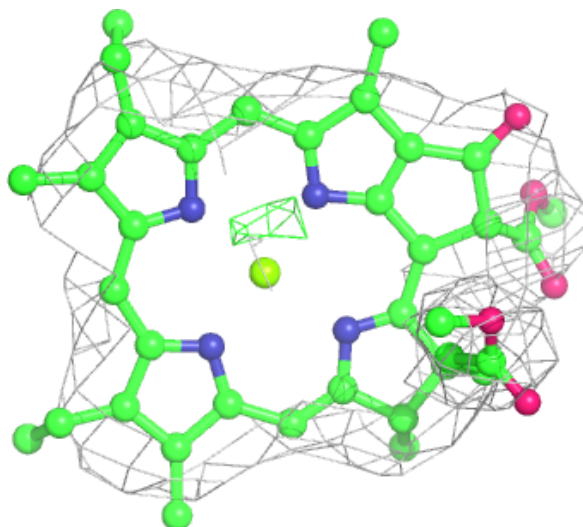
**Electron density around BCR 1 4019:**

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



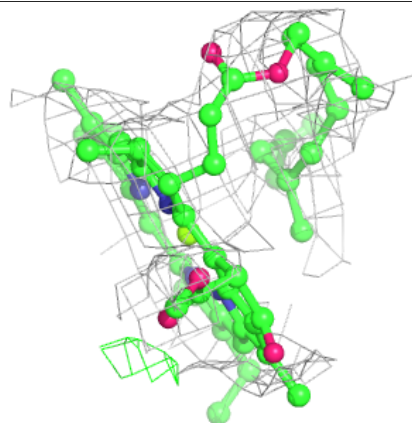
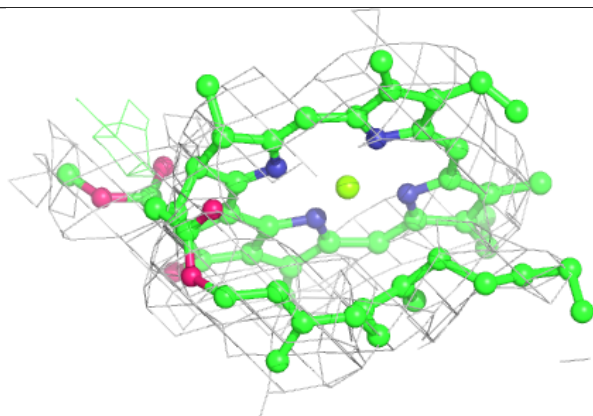
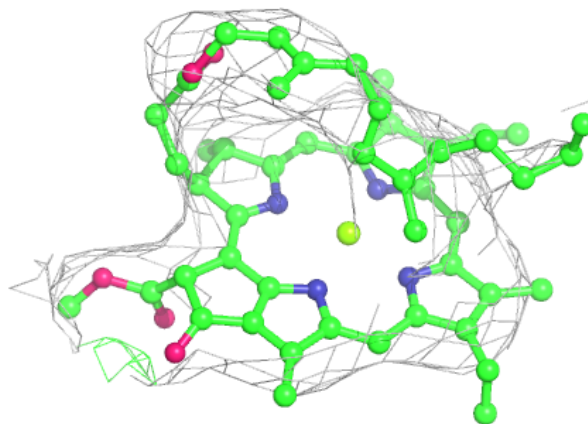
**Electron density around CLA 2 1211:**

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



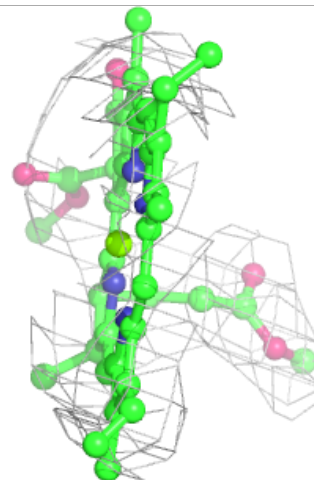
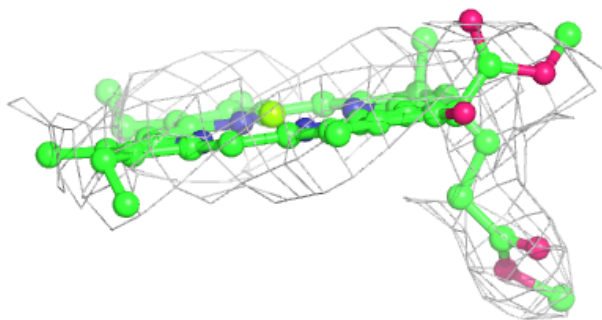
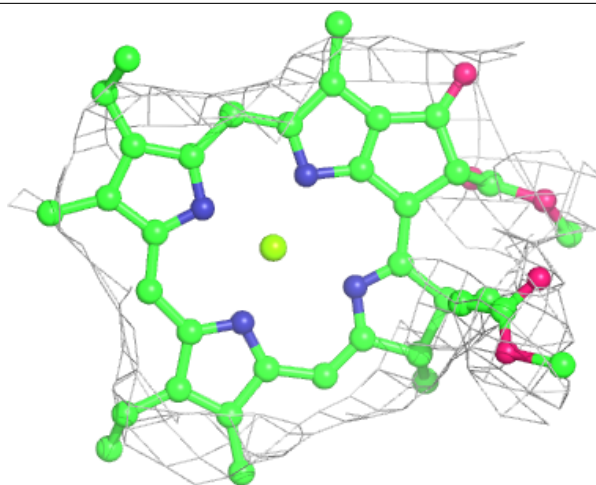
**Electron density around CLA B 1214:**

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



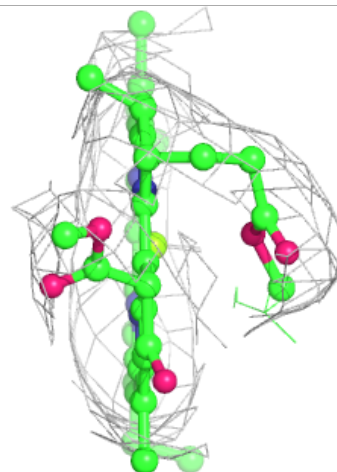
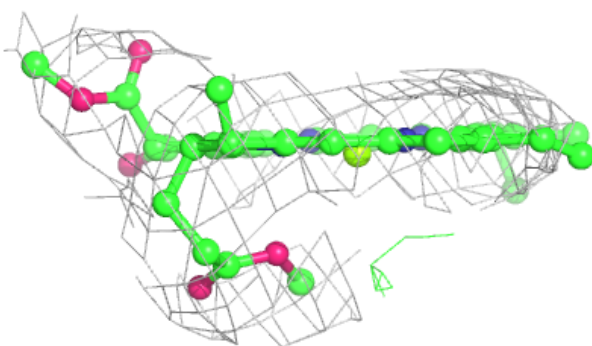
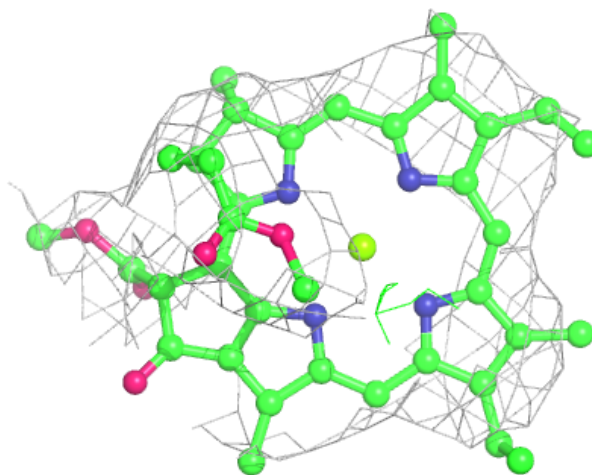
**Electron density around CLA B 1220:**

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



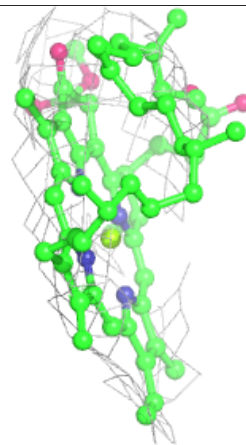
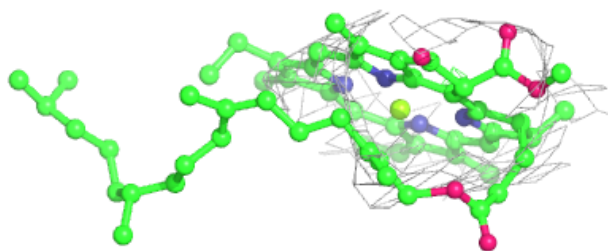
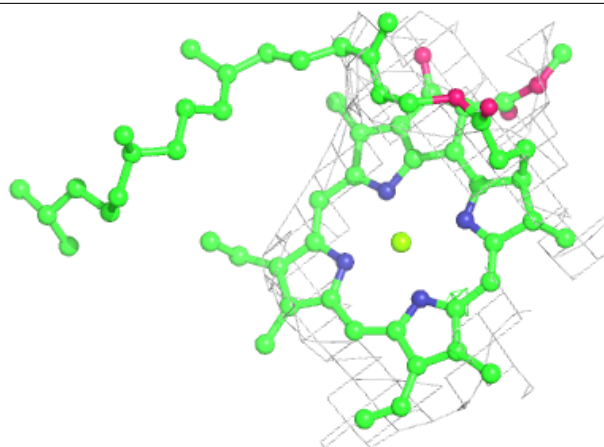
**Electron density around CLA A 1136:**

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



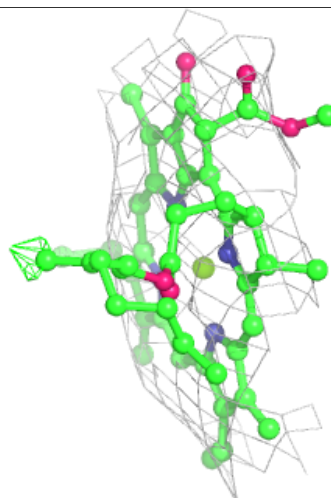
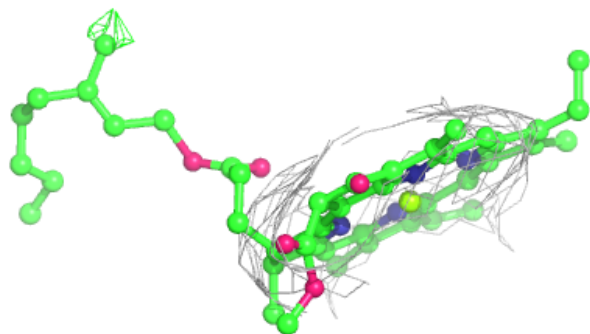
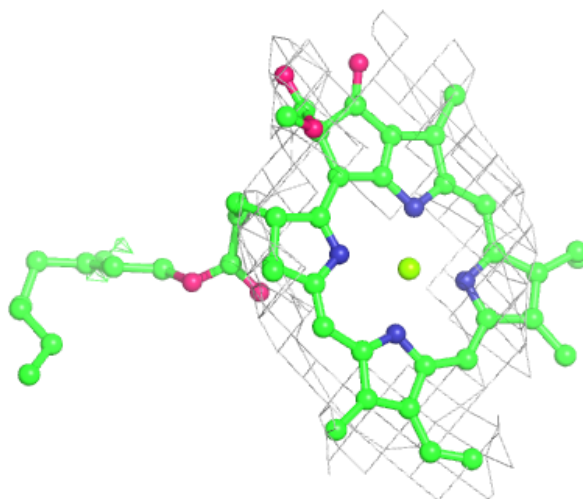
**Electron density around CLA a 1127:**

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



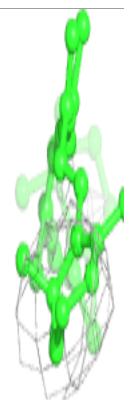
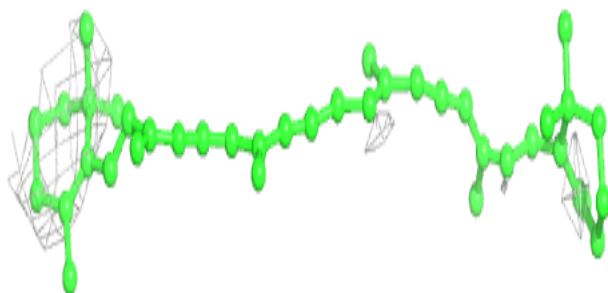
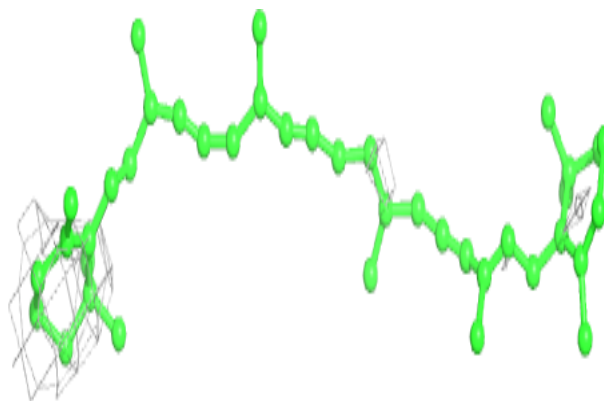
**Electron density around CLA 1 1110:**

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

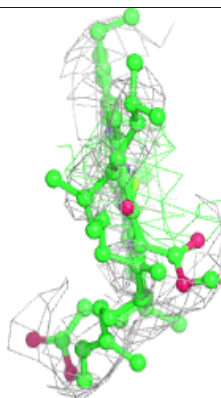
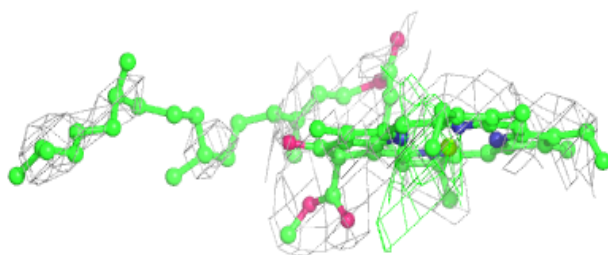
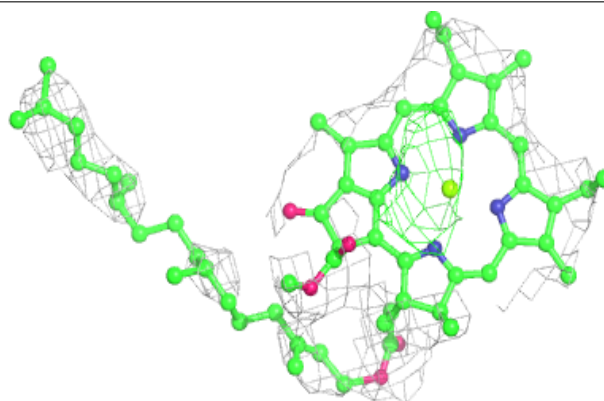


**Electron density around BCR F 4013:**

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

**Electron density around CLA 1 1503:**

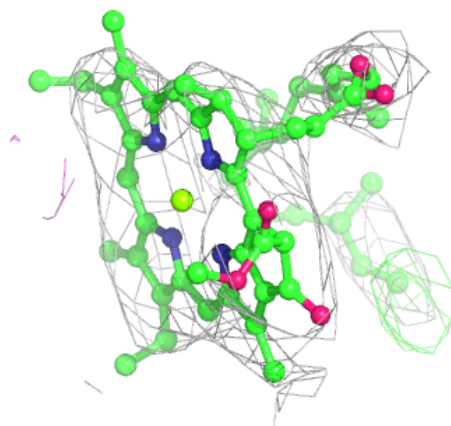
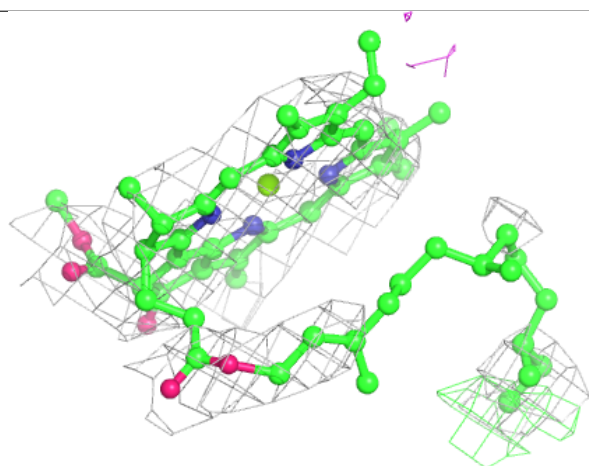
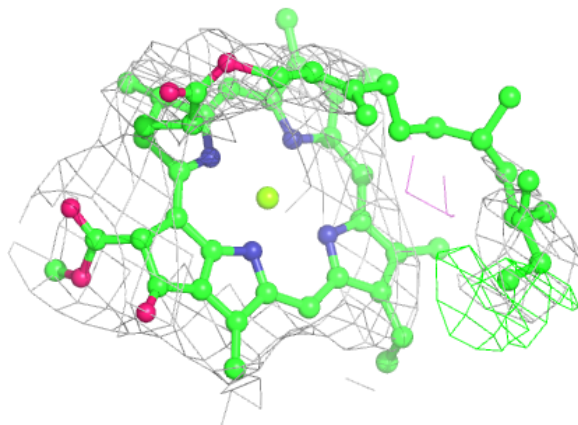
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





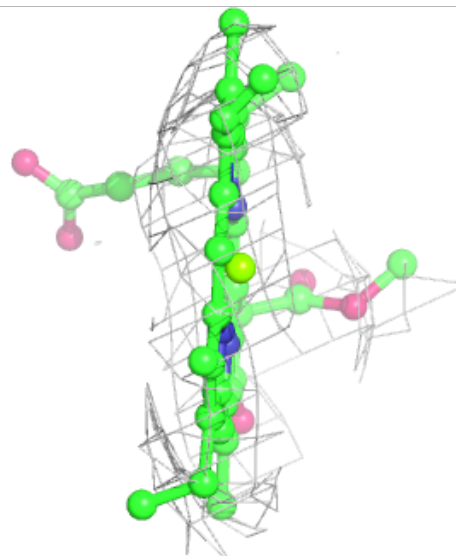
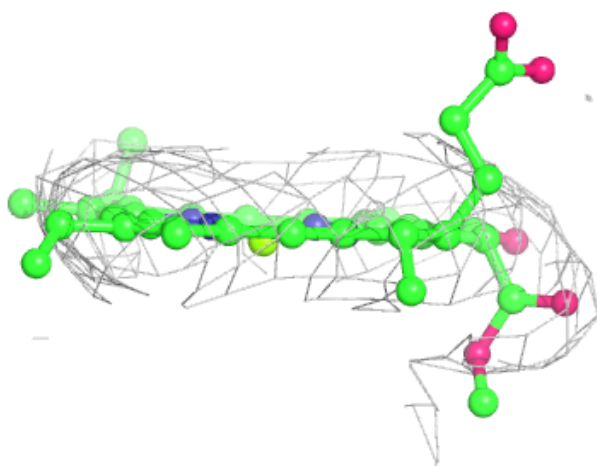
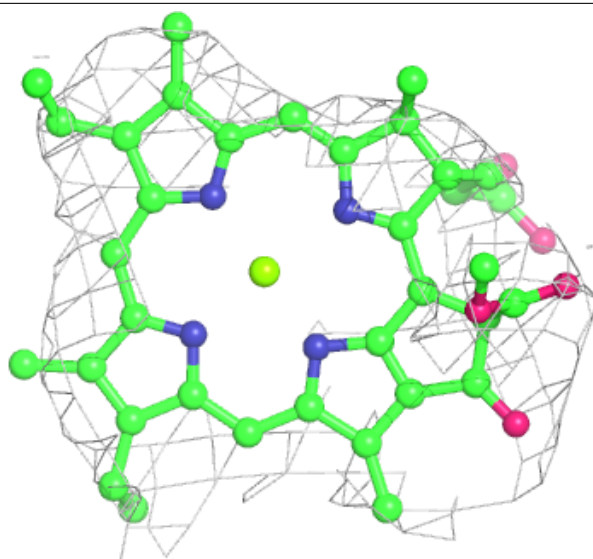
**Electron density around CLA A 1118:**

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



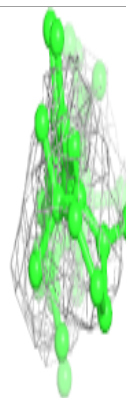
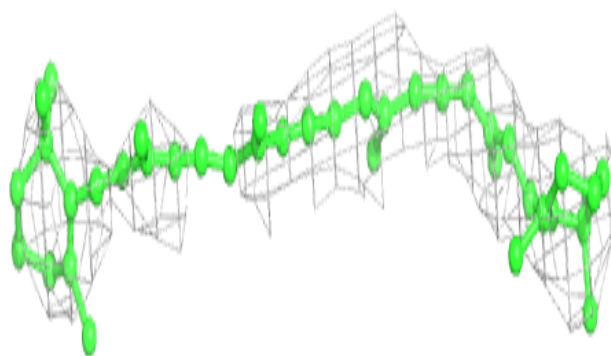
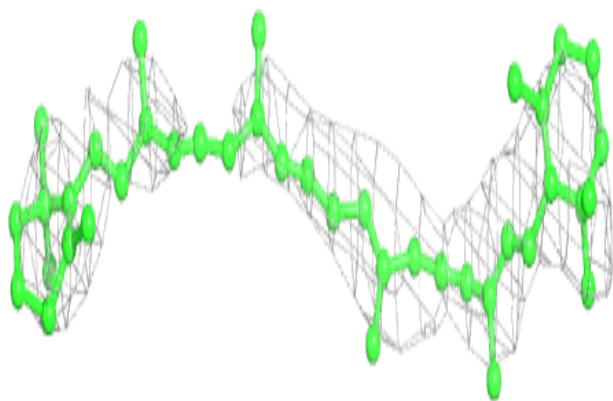
**Electron density around CLA B 1218:**

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

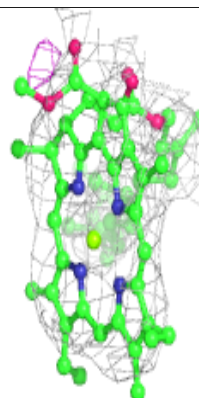
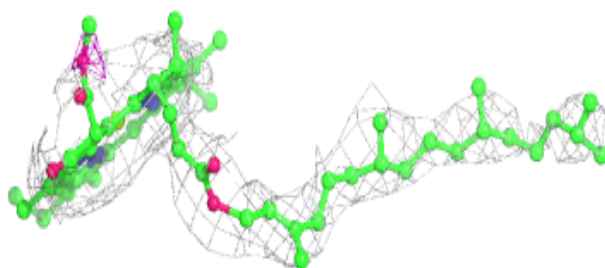
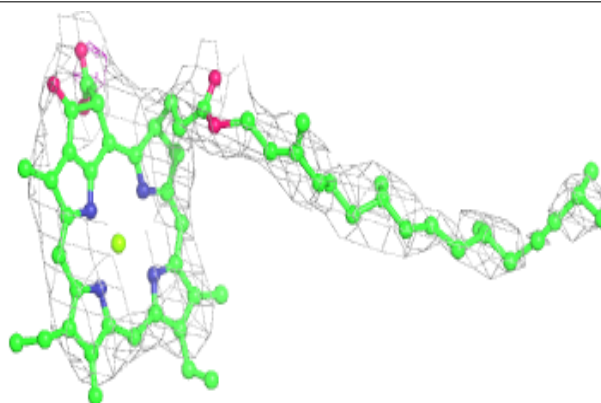


**Electron density around BCR 8 4022:**

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

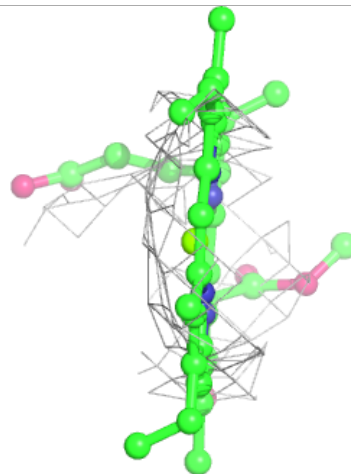
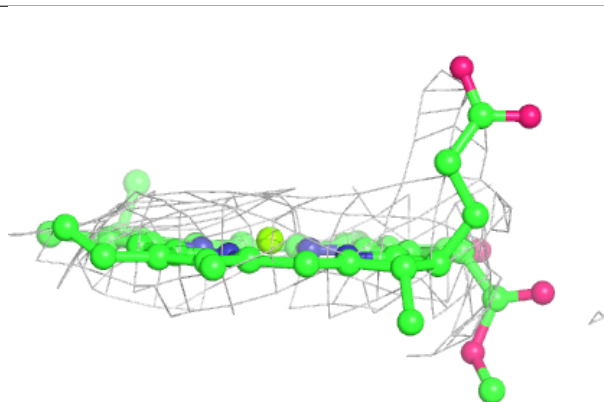
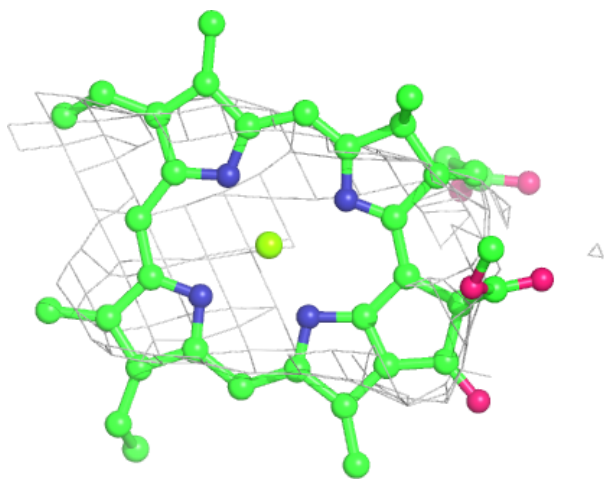
**Electron density around CLA a 1132:**

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



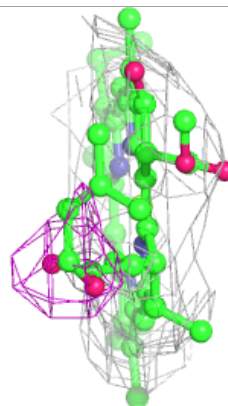
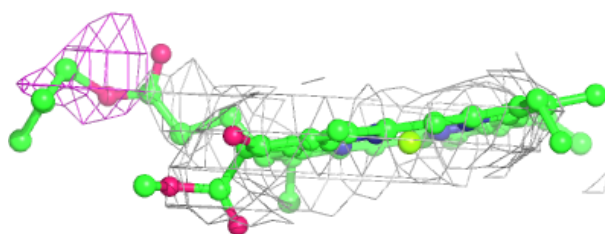
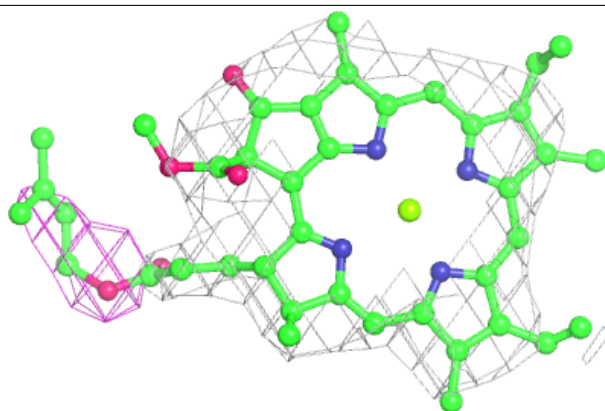
**Electron density around CLA 1 1112:**

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

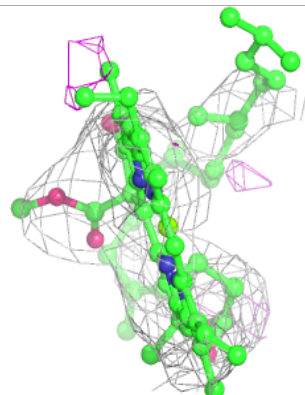
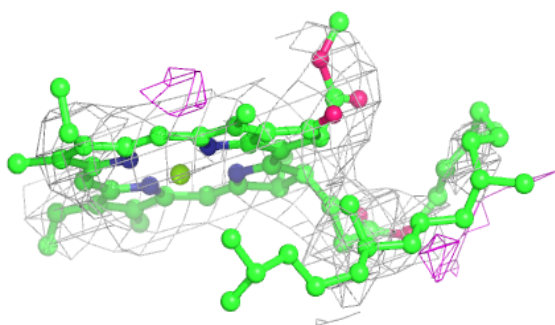
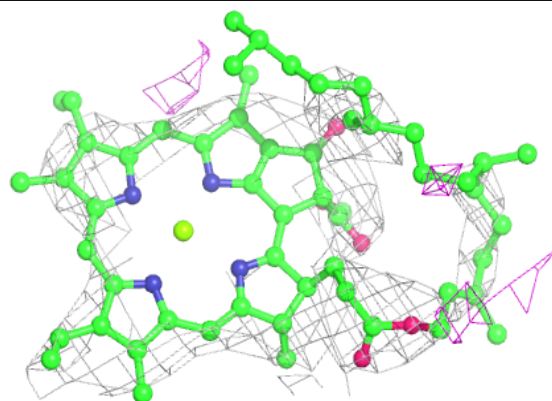


**Electron density around CLA A 1139:**

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

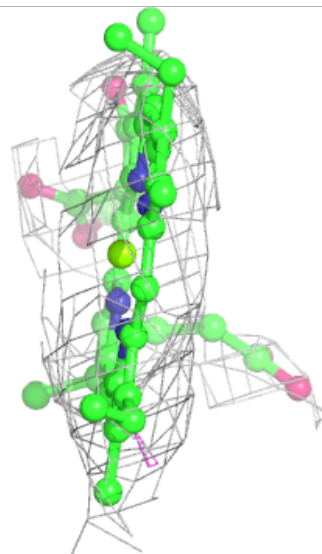
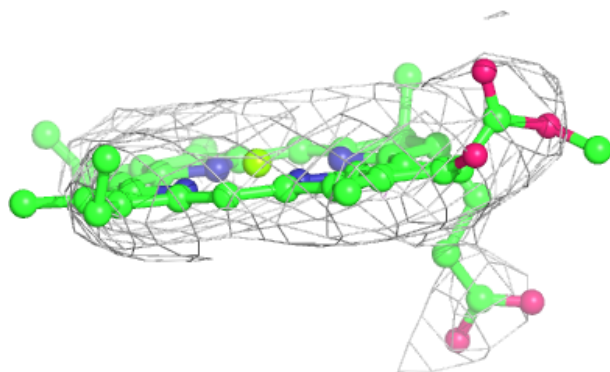
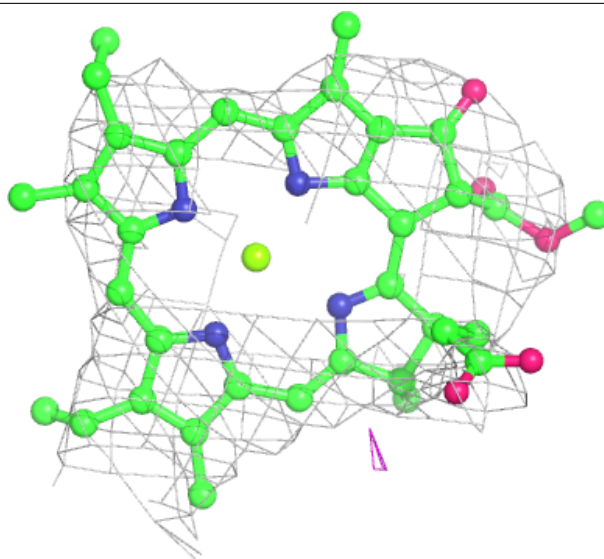
**Electron density around CLA 2 1202:**

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



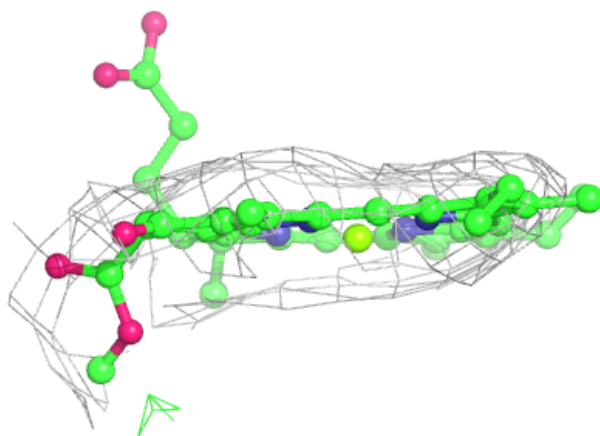
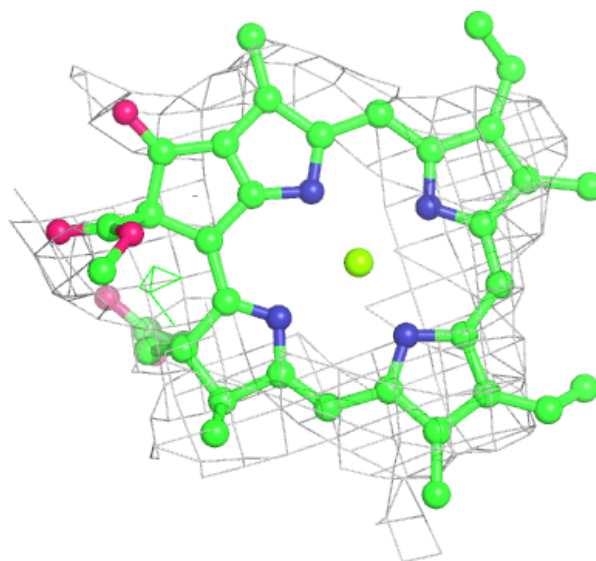
**Electron density around CLA B 1208:**

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



**Electron density around CLA B 1227:**

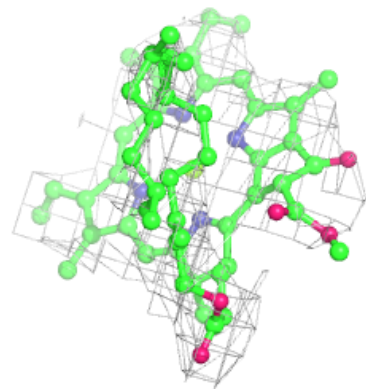
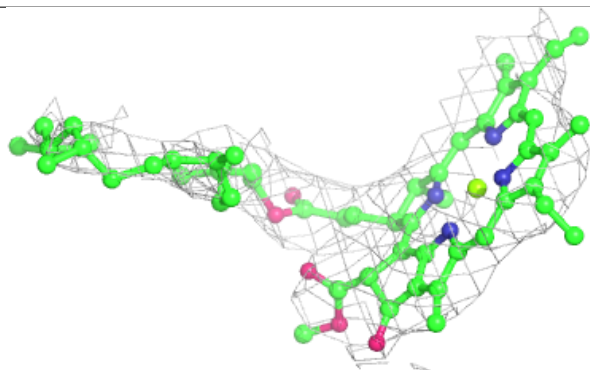
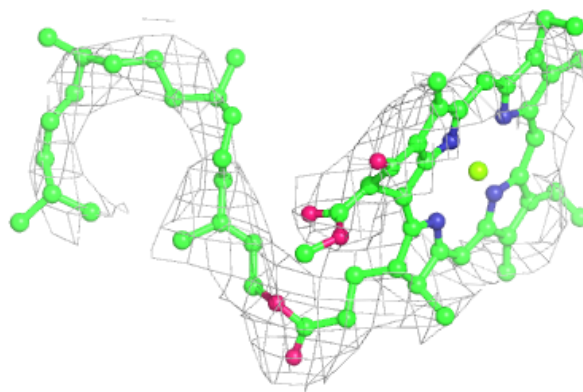
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





**Electron density around CLA 1 1011:**

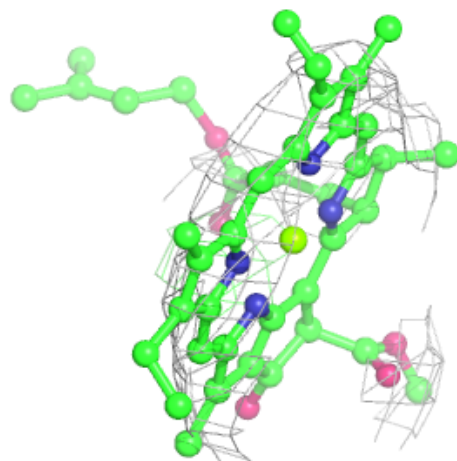
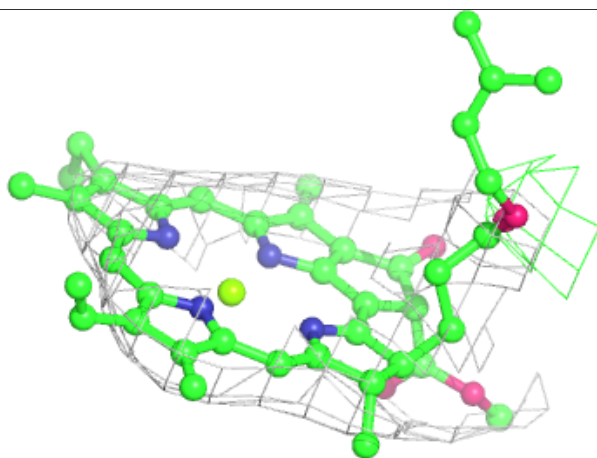
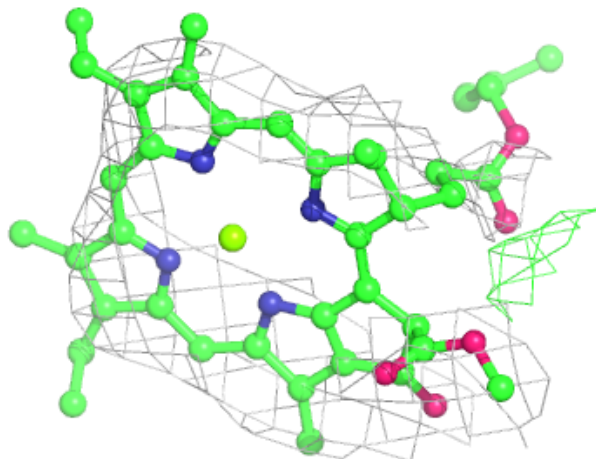
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





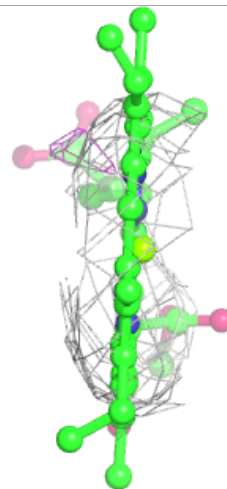
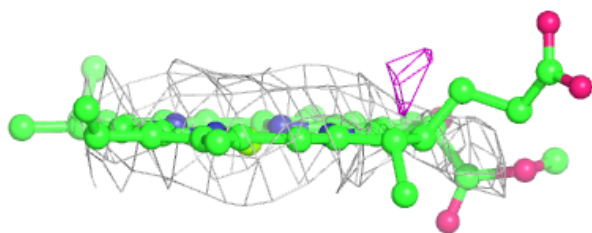
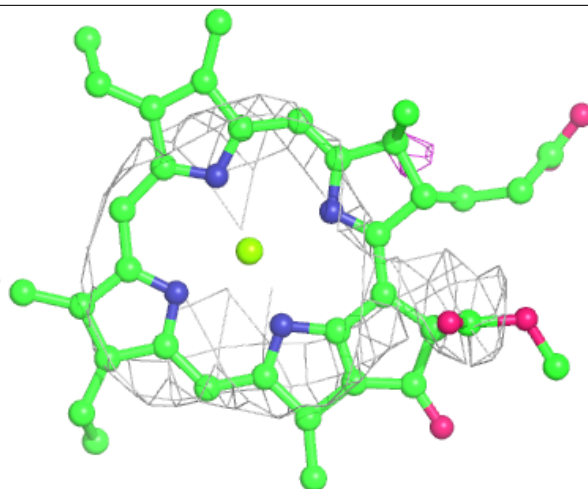
**Electron density around CLA B 1228:**

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



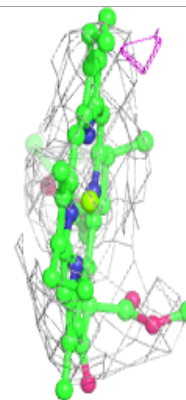
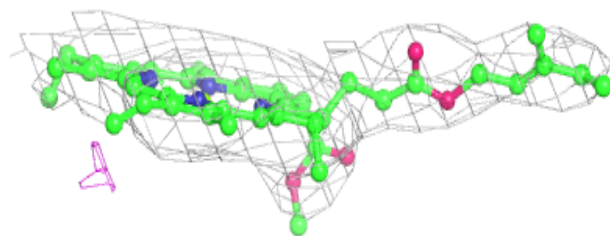
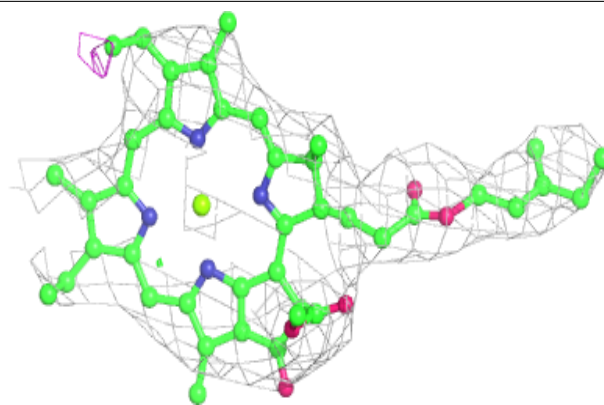
**Electron density around CLA B 1240:**

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



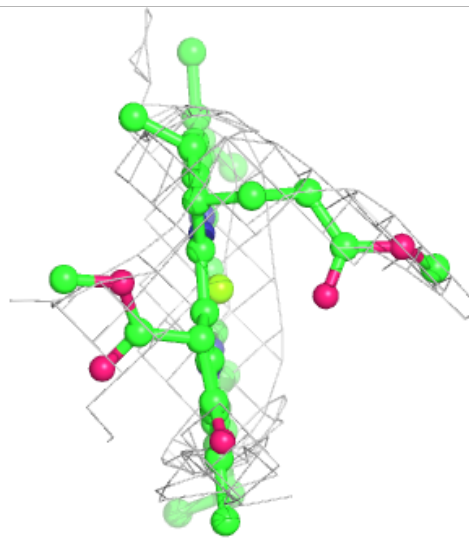
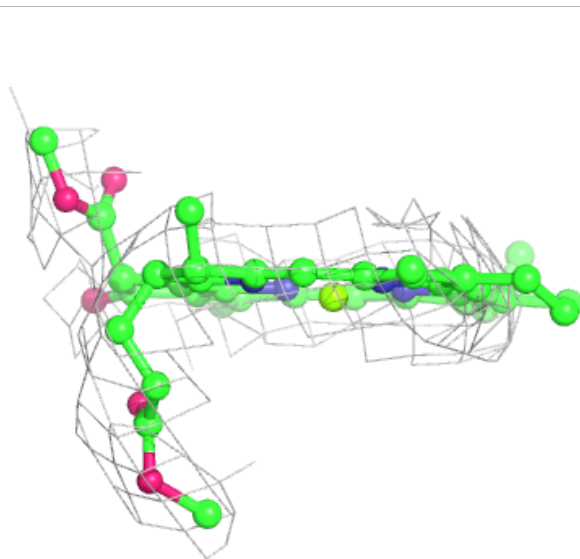
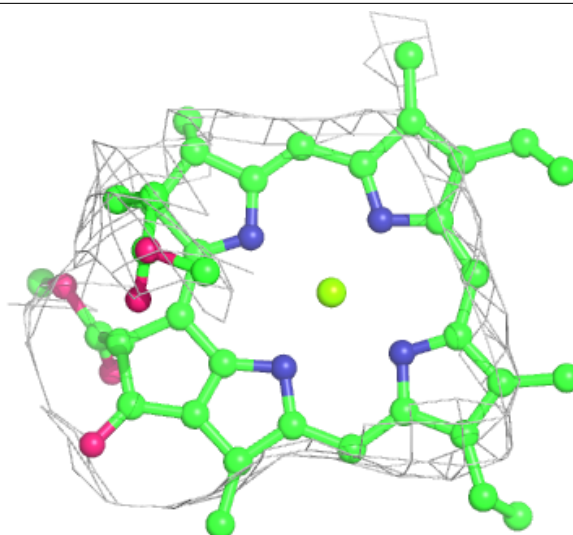
**Electron density around CLA A 1135:**

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



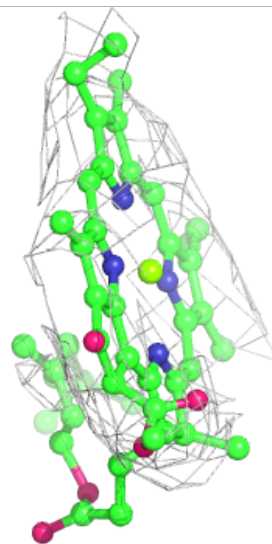
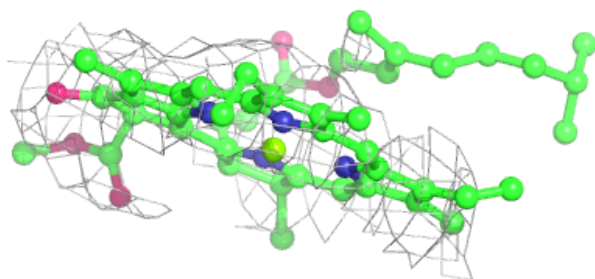
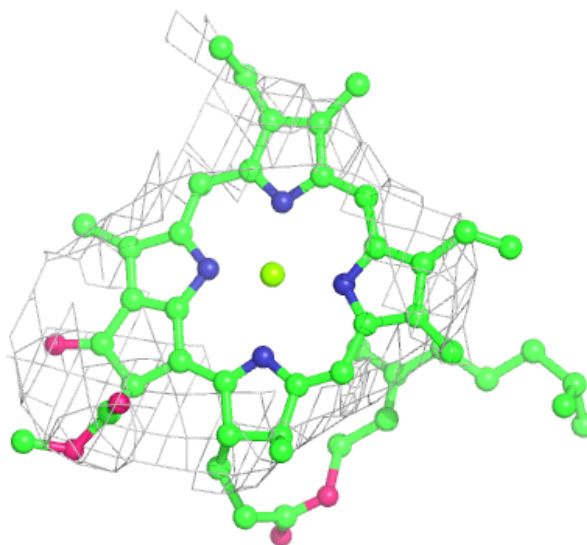
**Electron density around CLA 1 1134:**

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



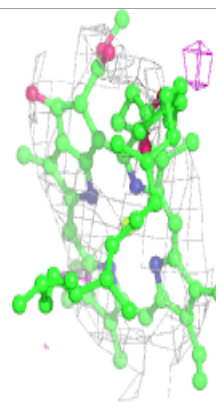
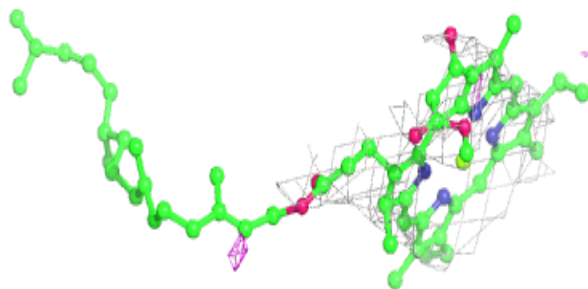
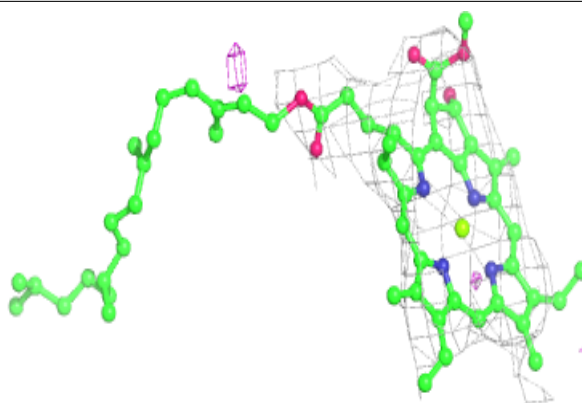
**Electron density around CLA B 1219:**

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

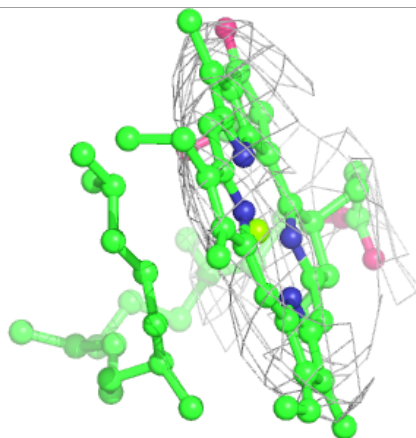
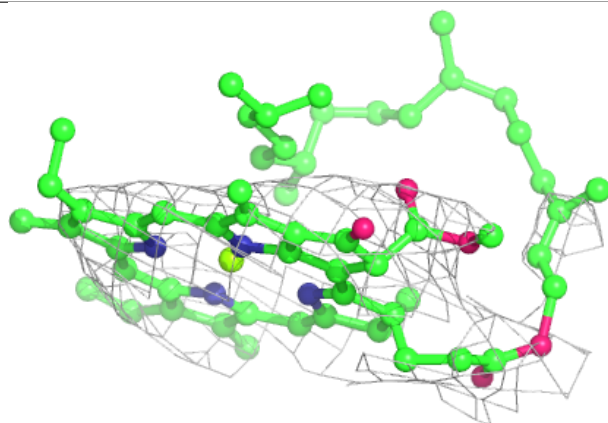
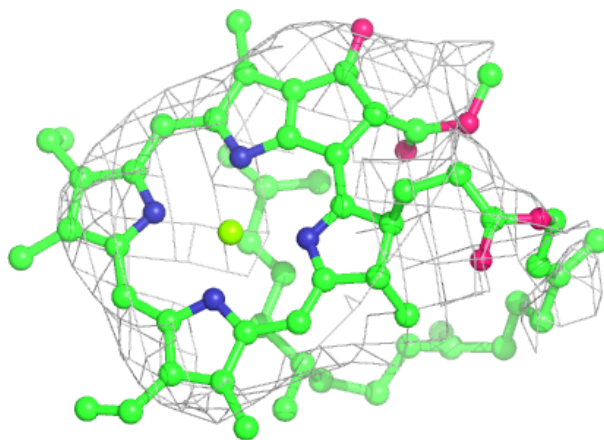


**Electron density around CLA 1 1012:**

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

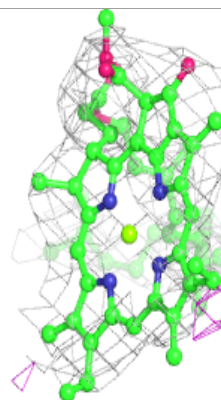
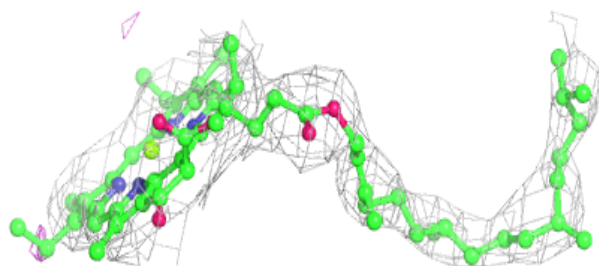
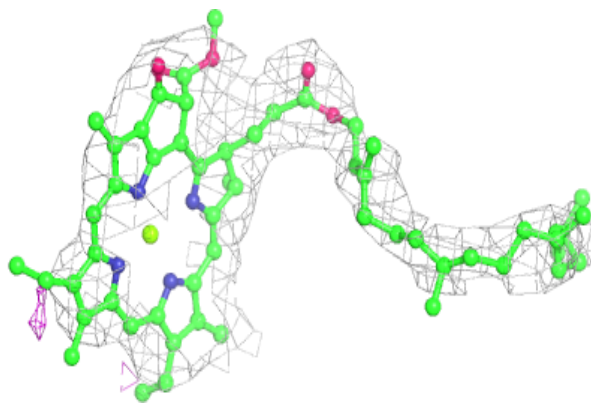
**Electron density around CLA 1 1104:**

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



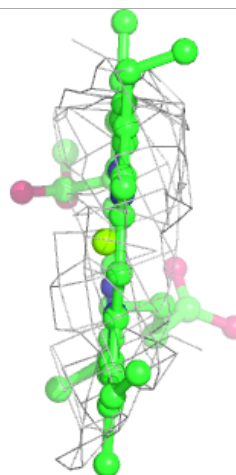
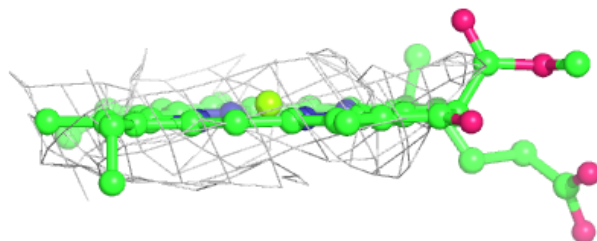
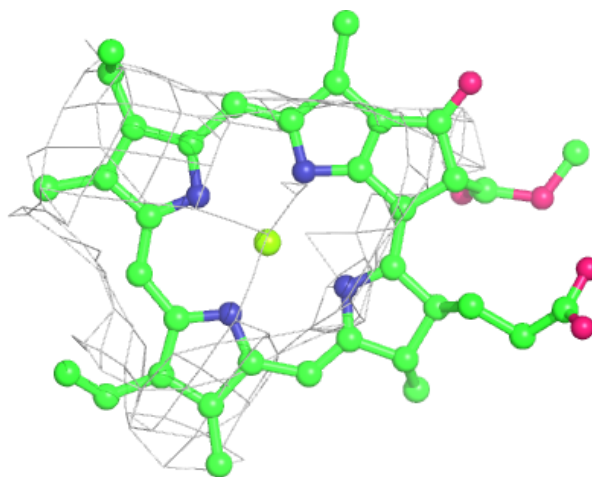
**Electron density around CLA 2 1206:**

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



**Electron density around CLA 2 1240:**

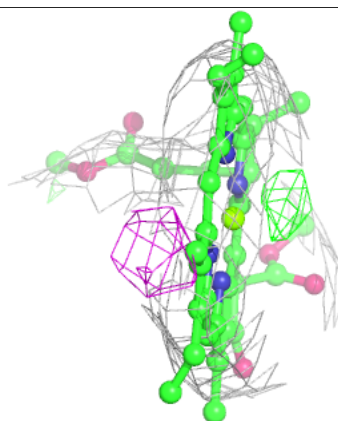
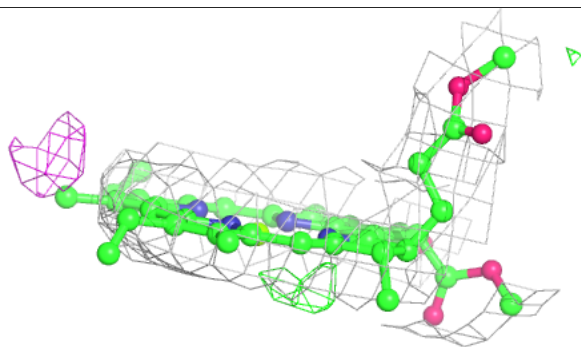
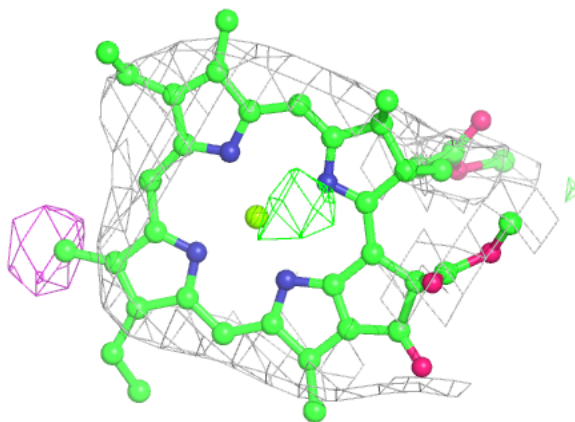
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





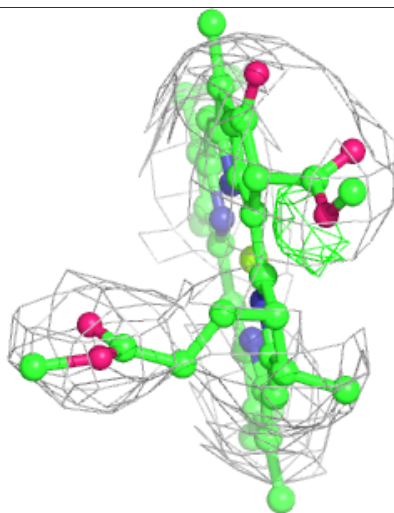
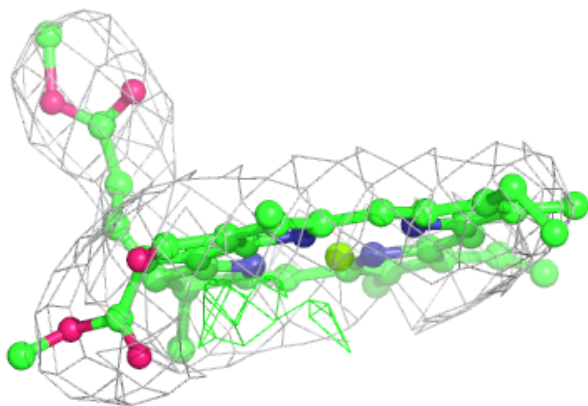
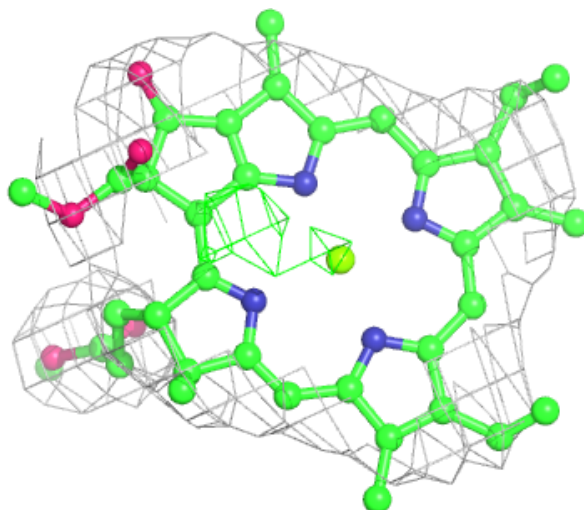
**Electron density around CLA 2 1220:**

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



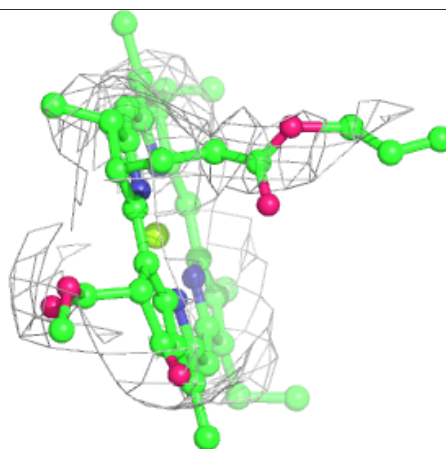
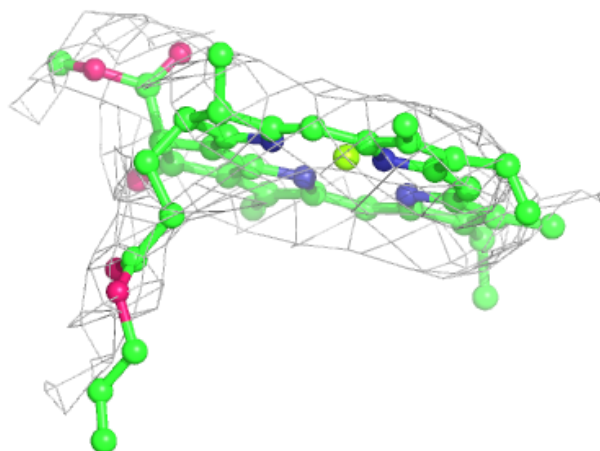
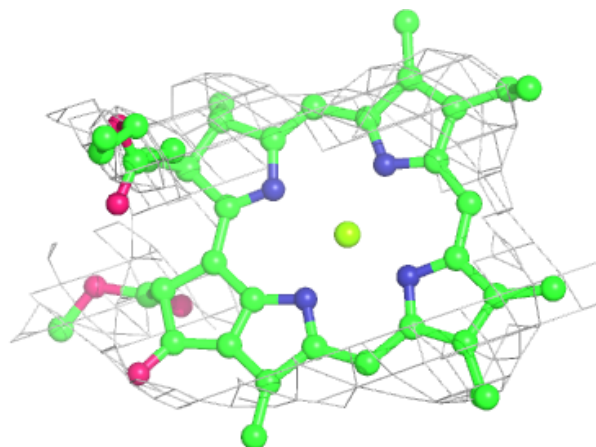
**Electron density around CLA 2 1239:**

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



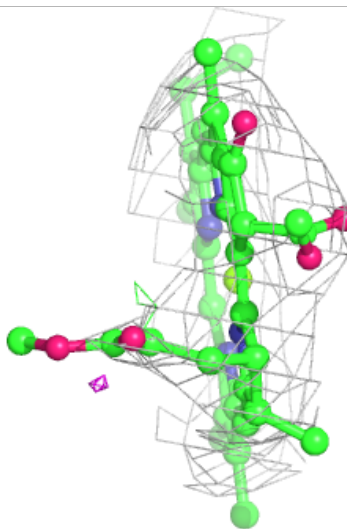
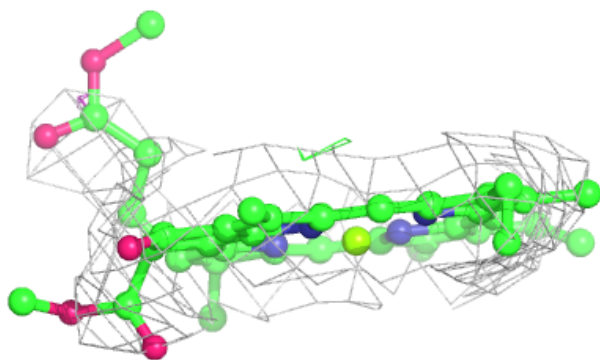
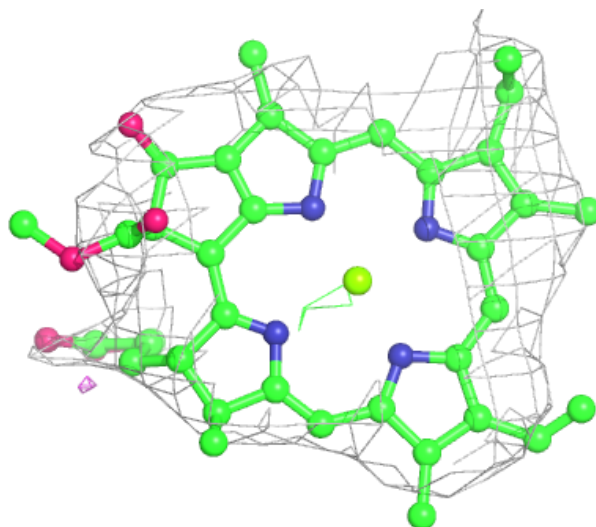
**Electron density around CLA A 1105:**

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



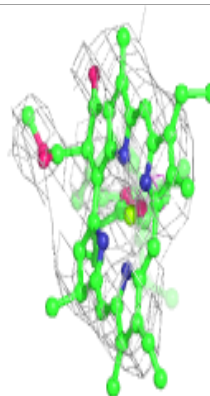
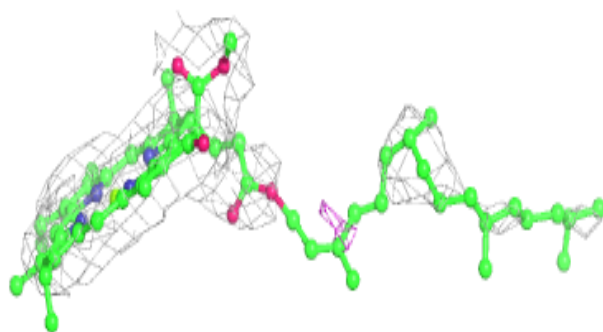
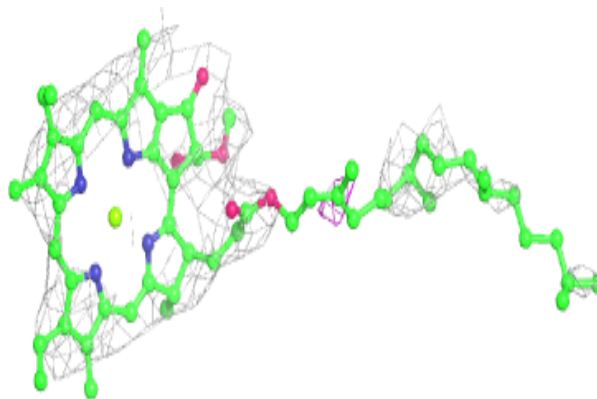
**Electron density around CLA A 1121:**

2mF<sub>o</sub>-DF<sub>c</sub> (at 0.7 rmsd) in gray  
mF<sub>o</sub>-DF<sub>c</sub> (at 3 rmsd) in purple (negative)  
and green (positive)

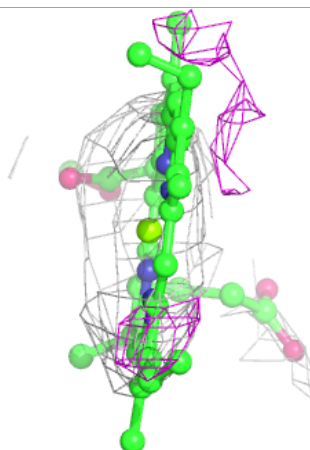
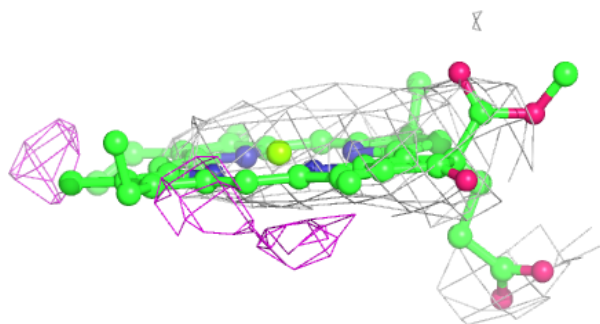
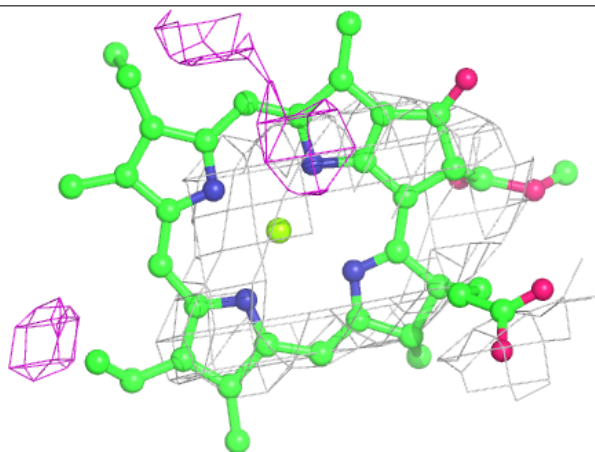


**Electron density around CLA A 1107:**

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

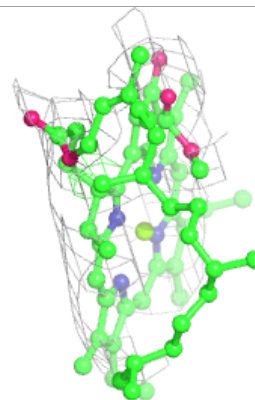
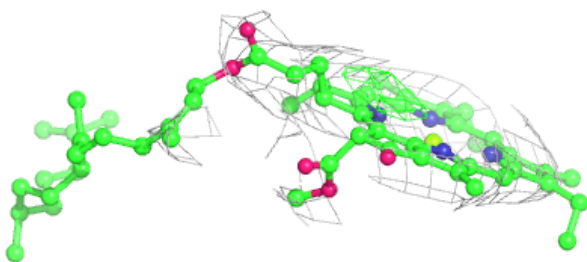
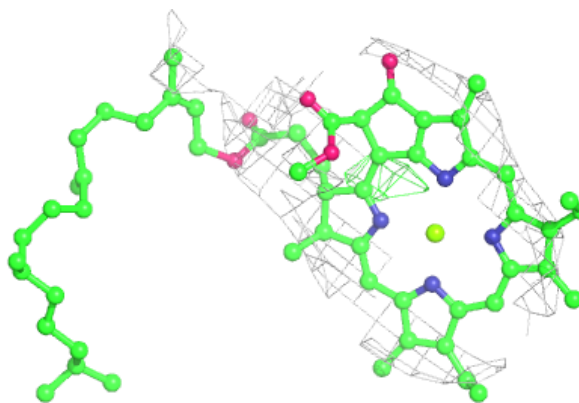
**Electron density around CLA b 1208:**

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

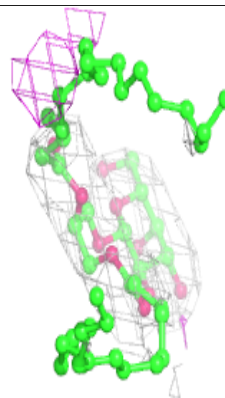
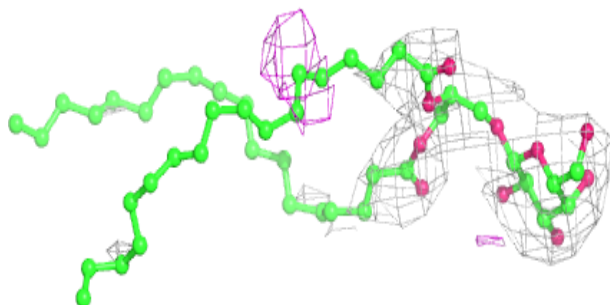
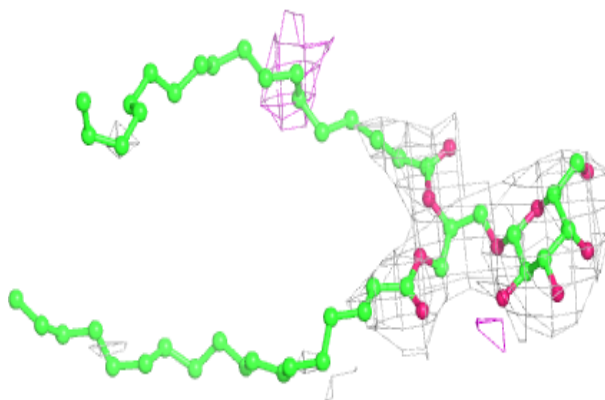


**Electron density around CLA a 1101:**

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

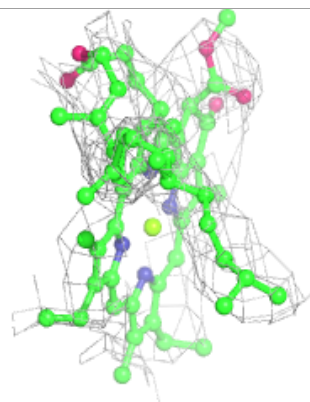
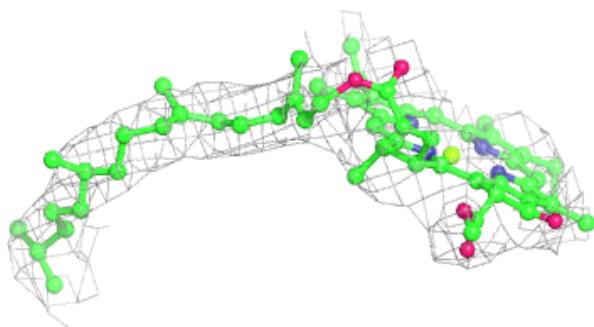
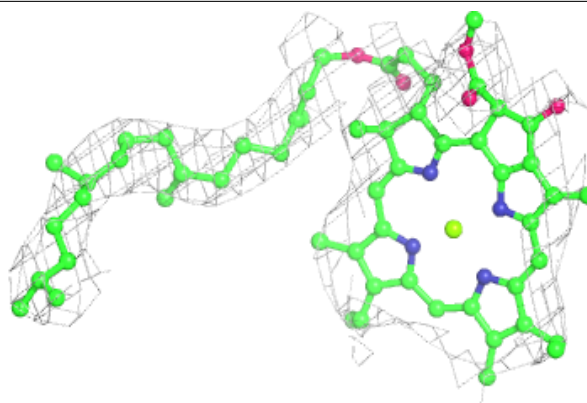
**Electron density around LMG B 5002:**

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

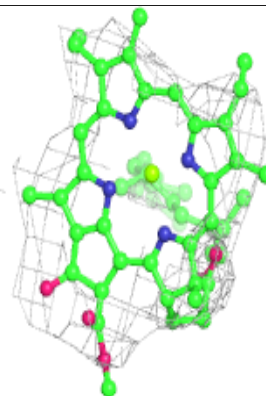
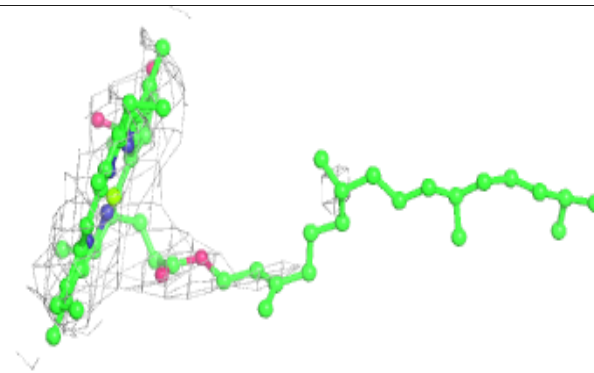
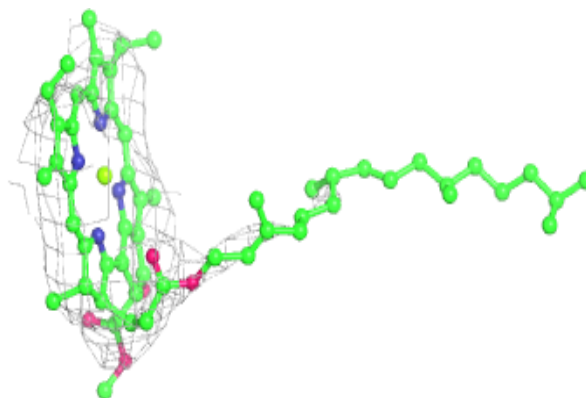


**Electron density around CLA B 1013:**

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

**Electron density around CLA B 1225:**

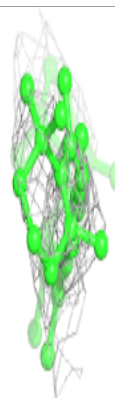
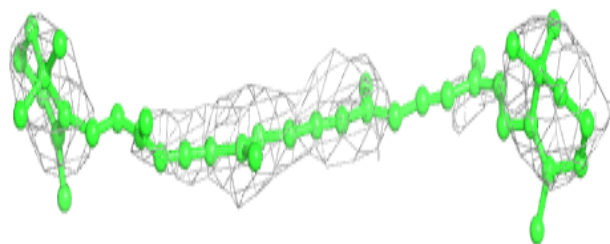
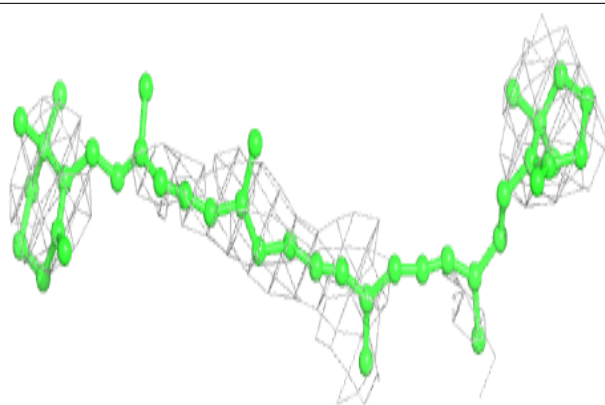
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



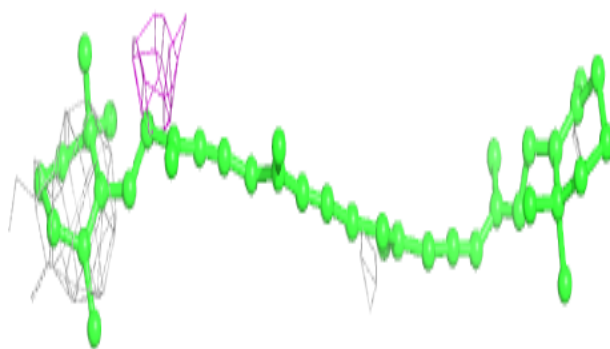
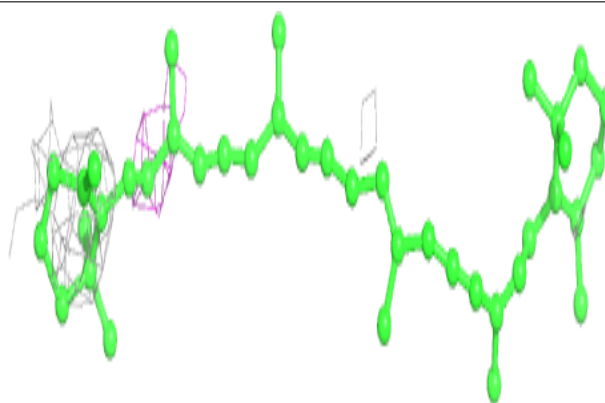


**Electron density around BCR 2 4010:**

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

**Electron density around BCR 1 4003:**

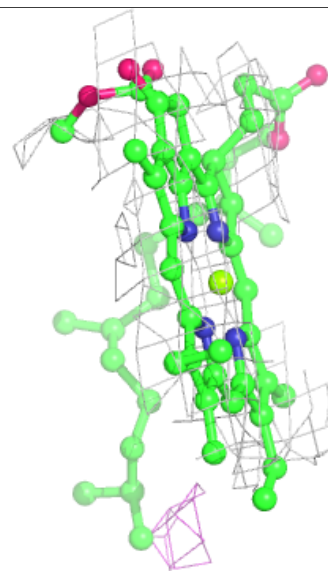
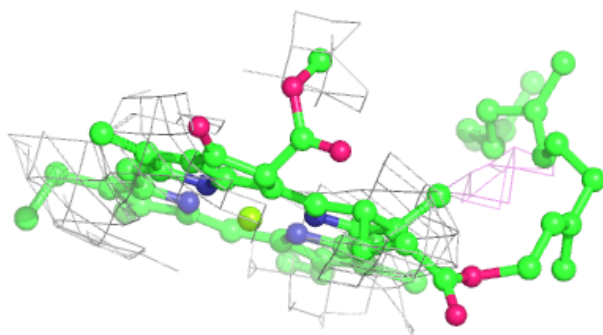
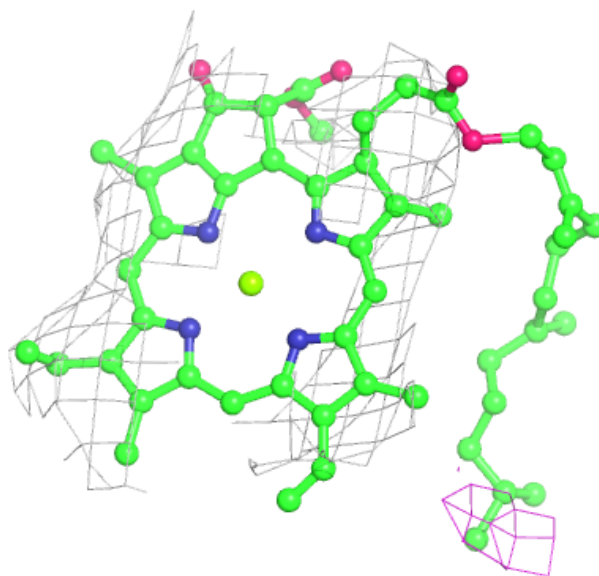
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





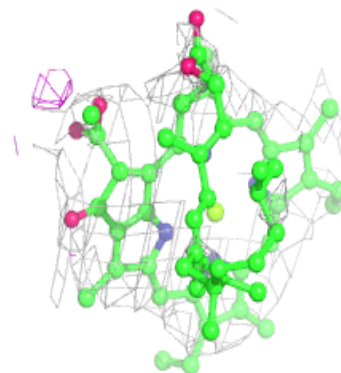
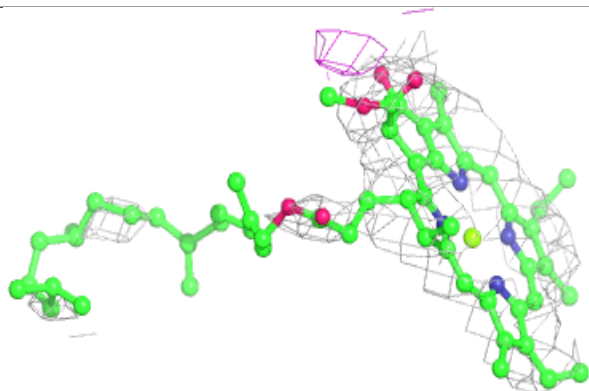
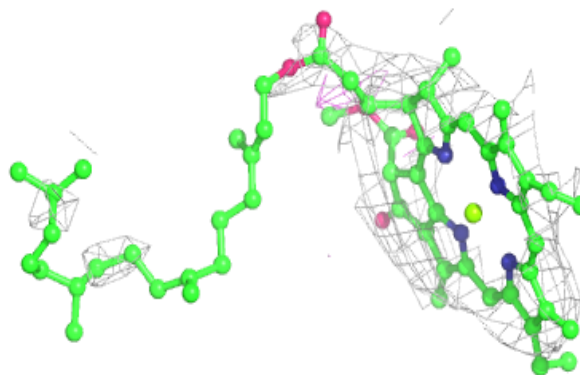
**Electron density around CLA a 1111:**

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

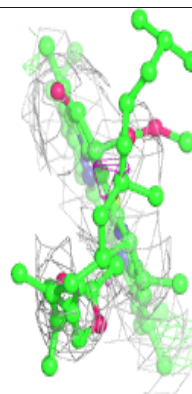
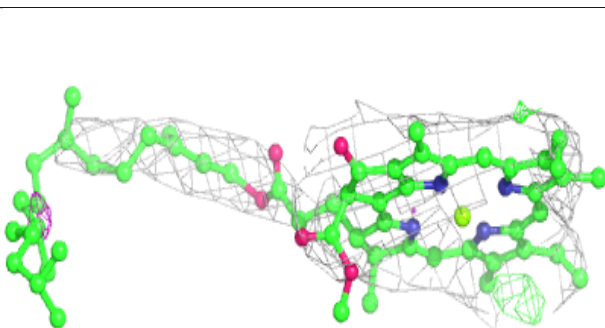
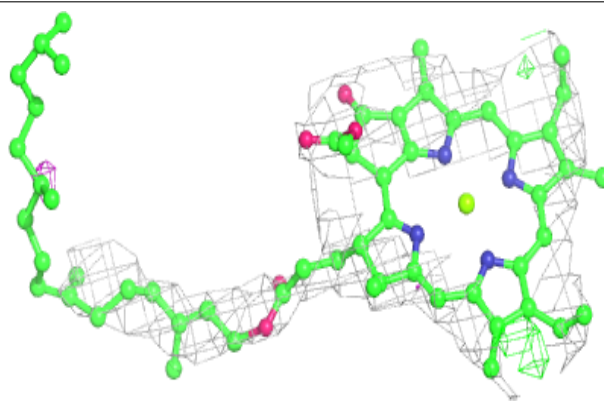


**Electron density around CLA 2 1021:**

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

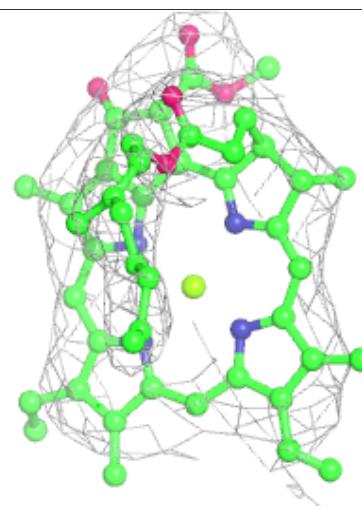
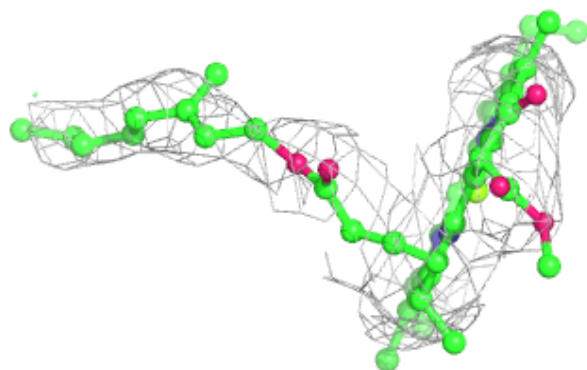
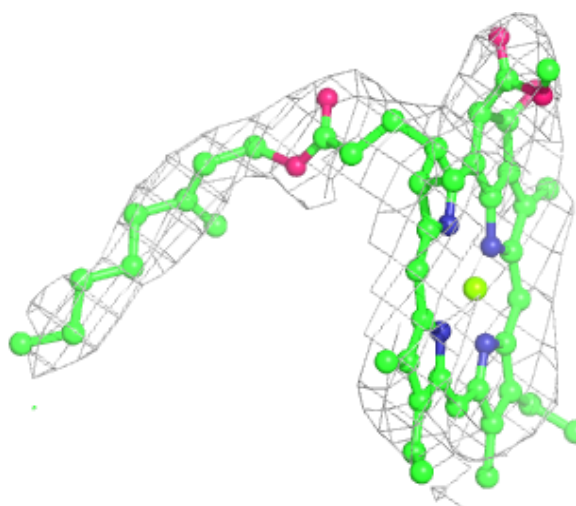
**Electron density around CLA 2 1223:**

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



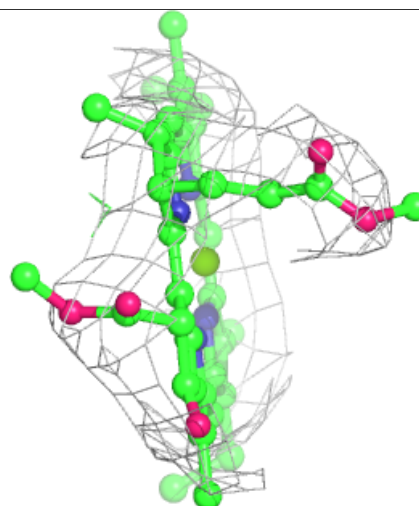
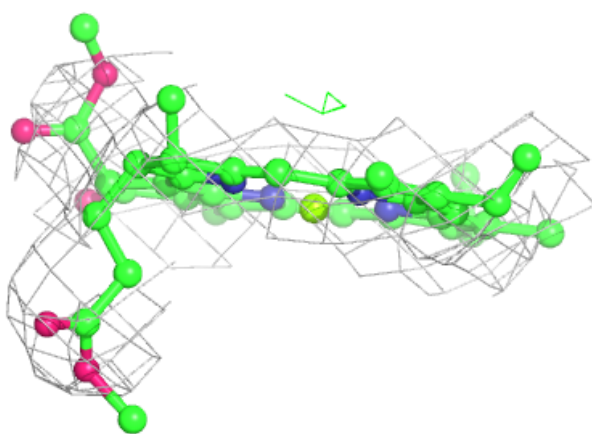
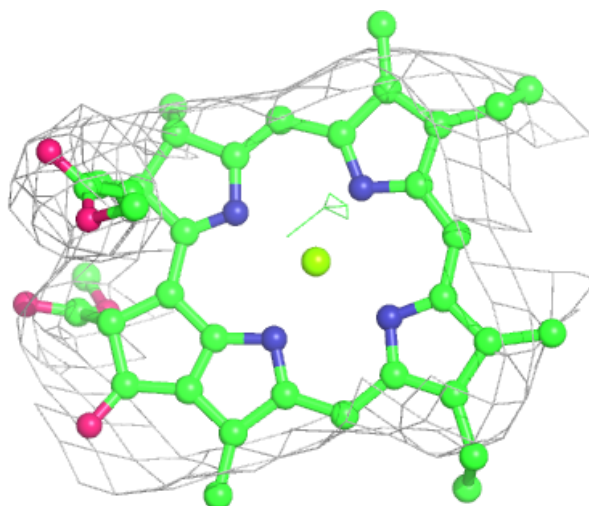
**Electron density around CLA B 1201:**

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



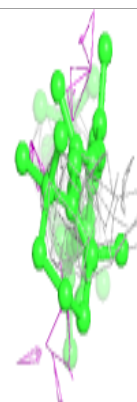
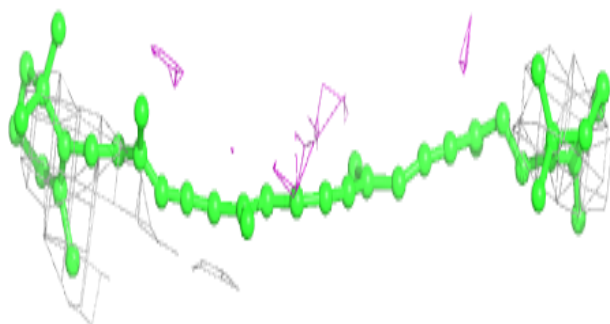
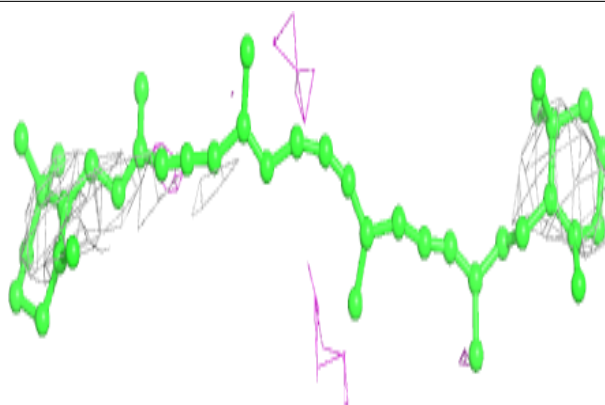
**Electron density around CLA B 1211:**

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

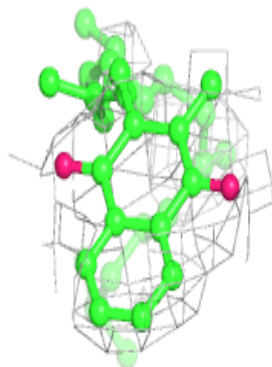
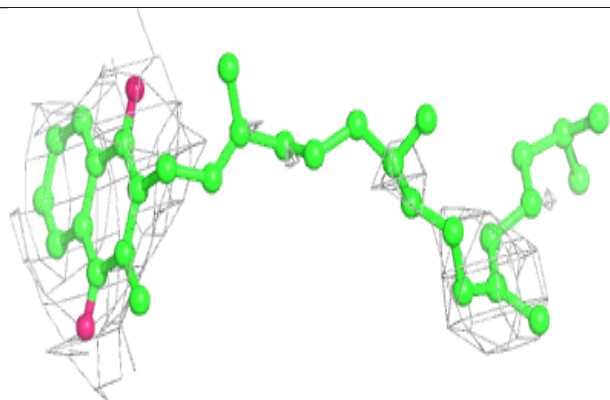
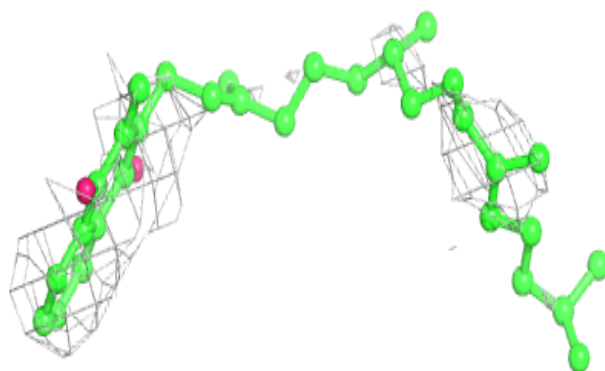


**Electron density around BCR a 4002:**

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

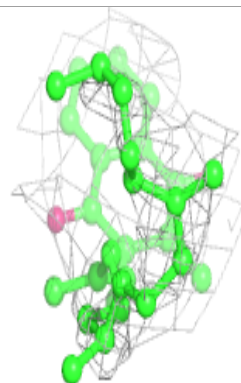
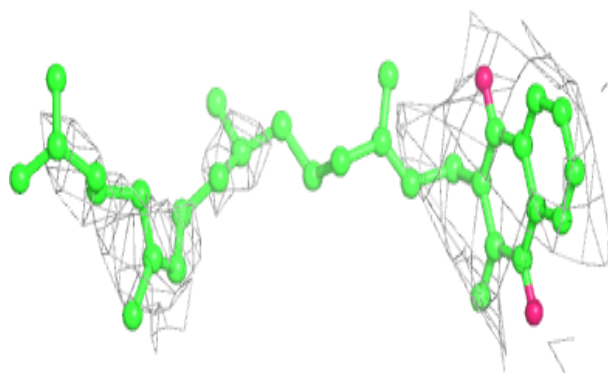
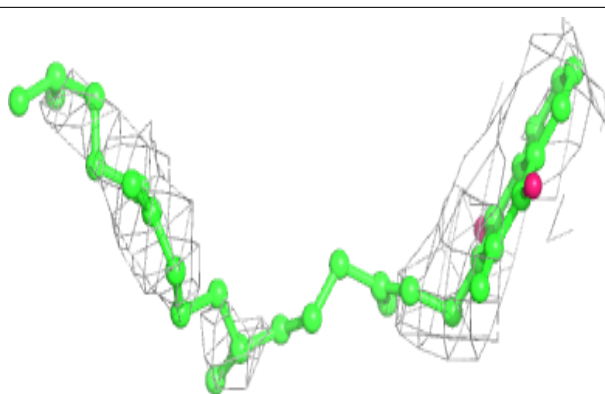
**Electron density around PQN b 2002:**

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

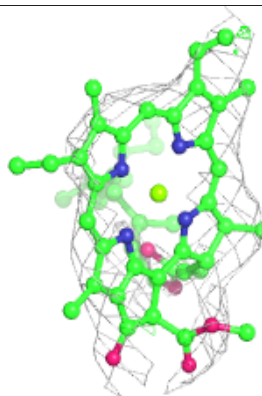
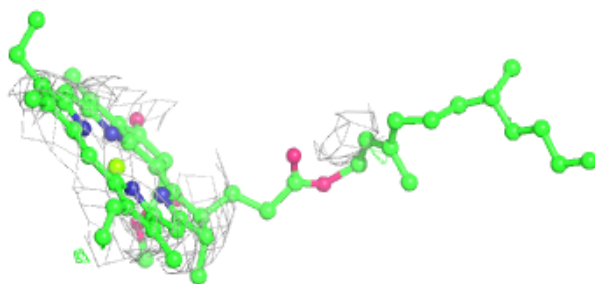
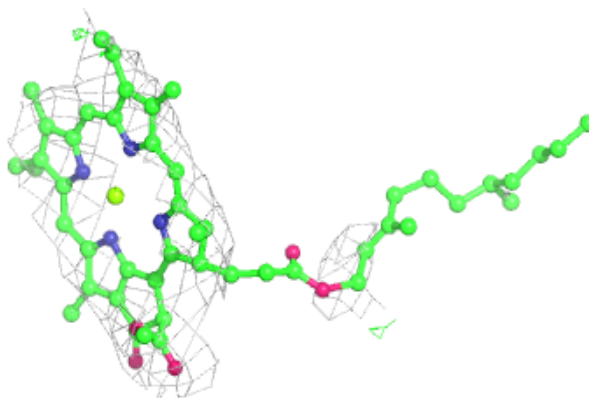


**Electron density around PQN 2 2002:**

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

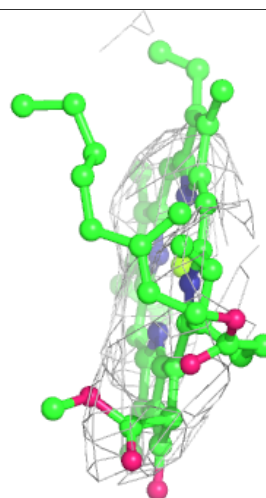
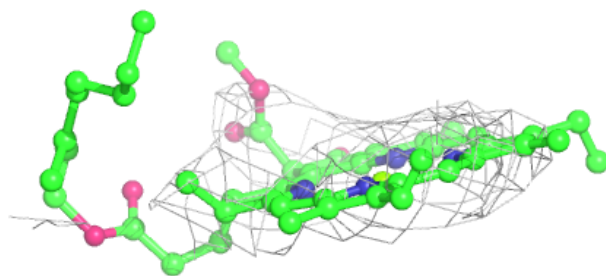
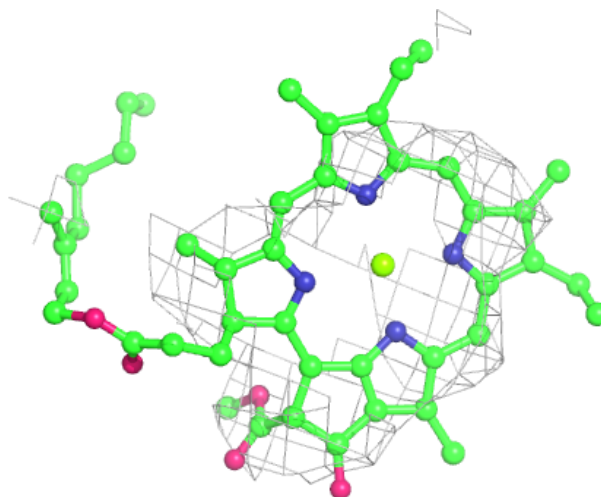
**Electron density around CLA B 1230:**

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



**Electron density around CLA b 1221:**

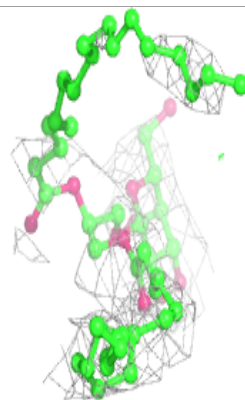
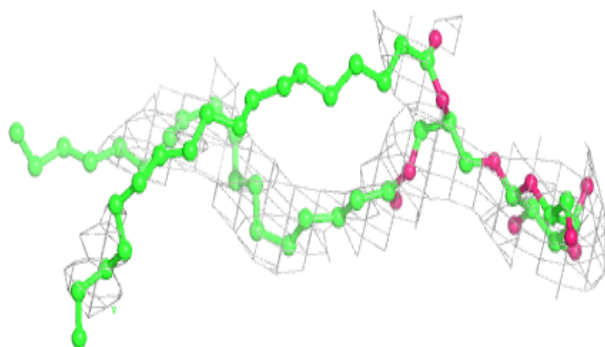
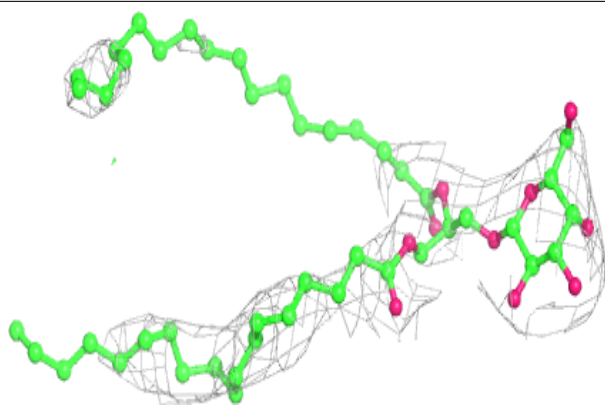
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





**Electron density around LMG 2 5002:**

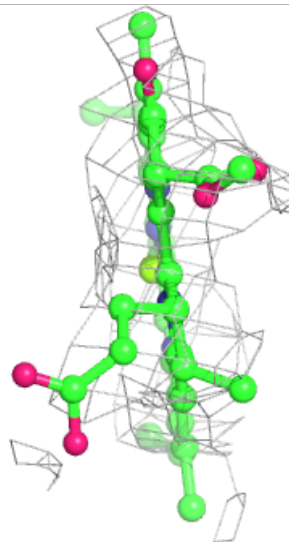
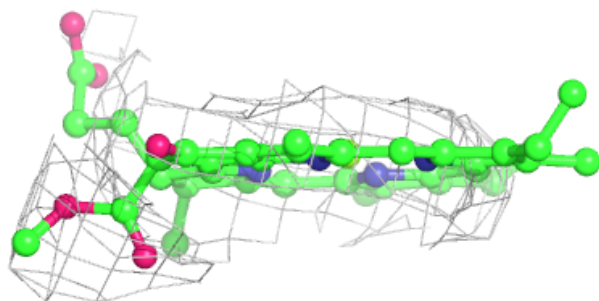
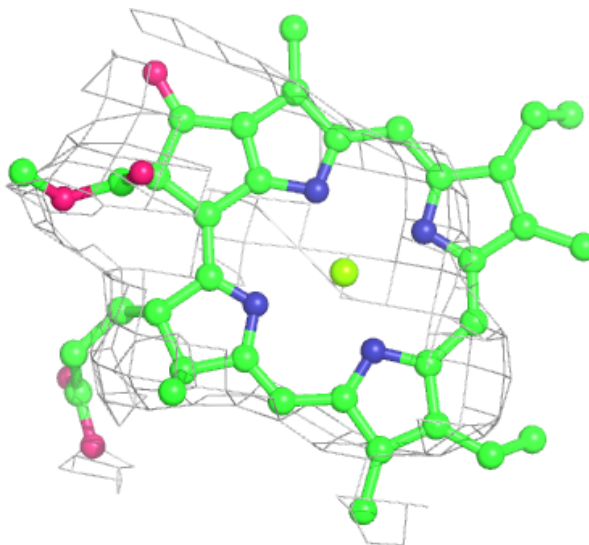
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





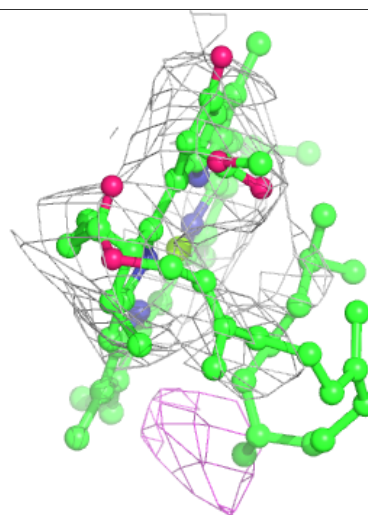
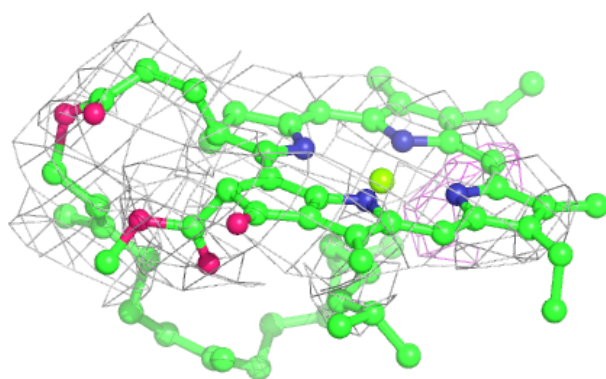
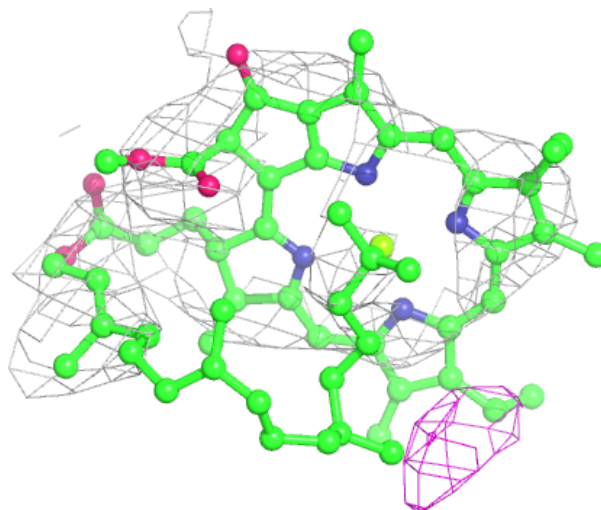
**Electron density around CLA b 1209:**

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



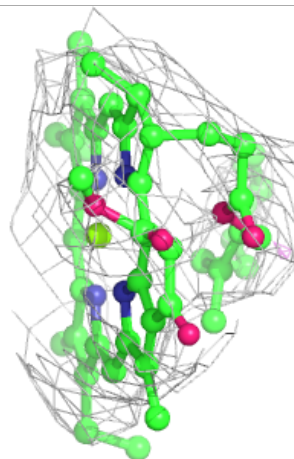
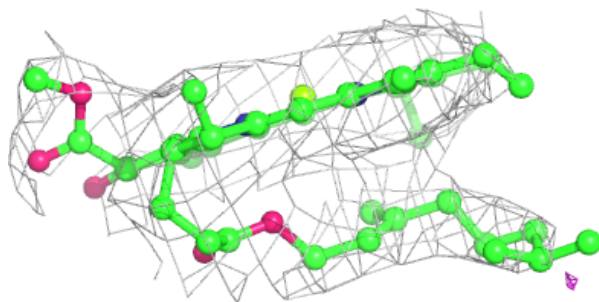
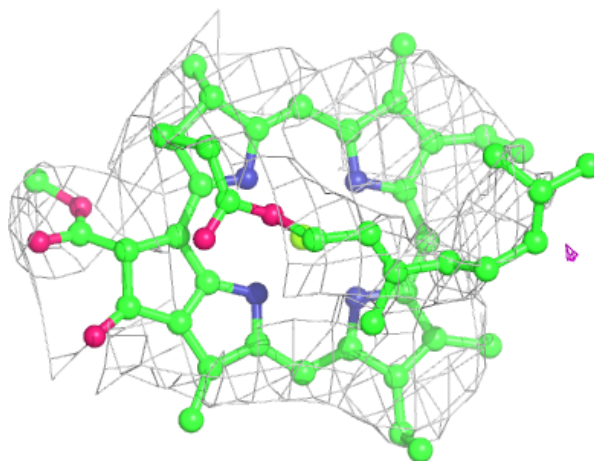
**Electron density around CLA b 1203:**

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



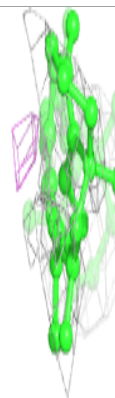
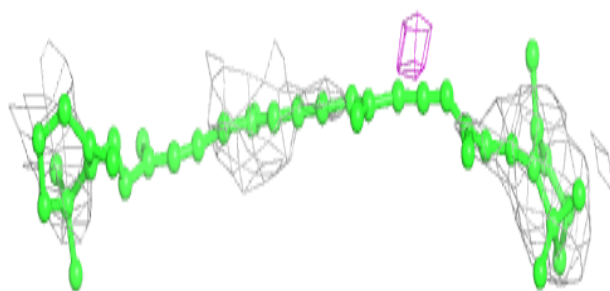
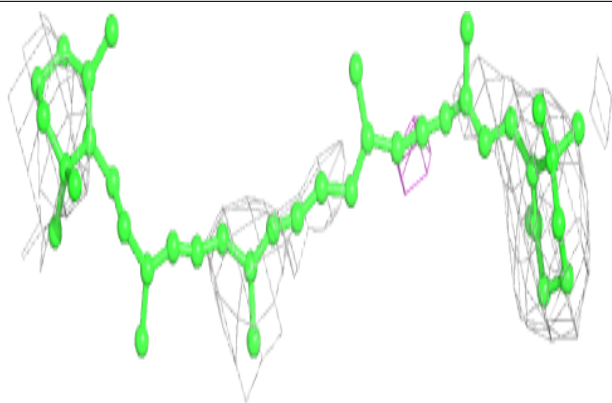
**Electron density around CLA 2 1205:**

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

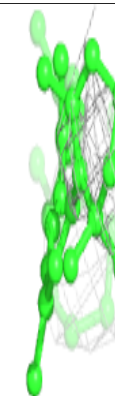
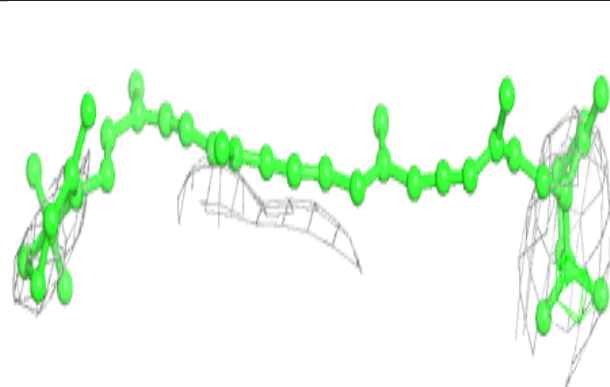
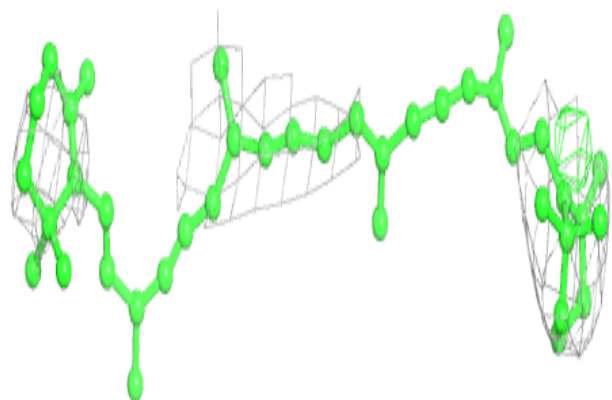


**Electron density around BCR 2 4004:**

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

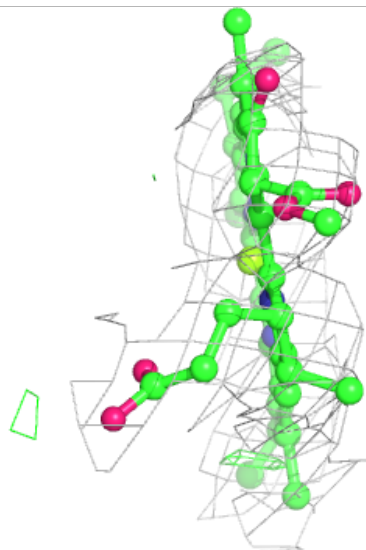
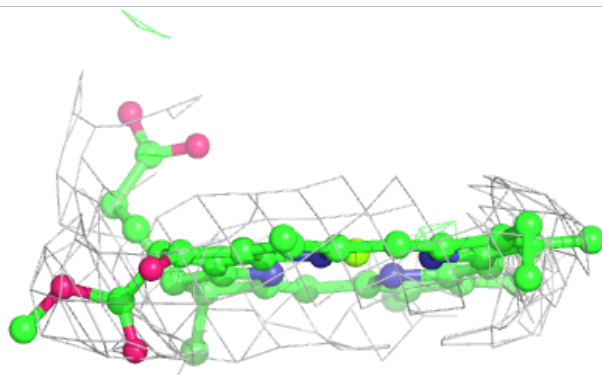
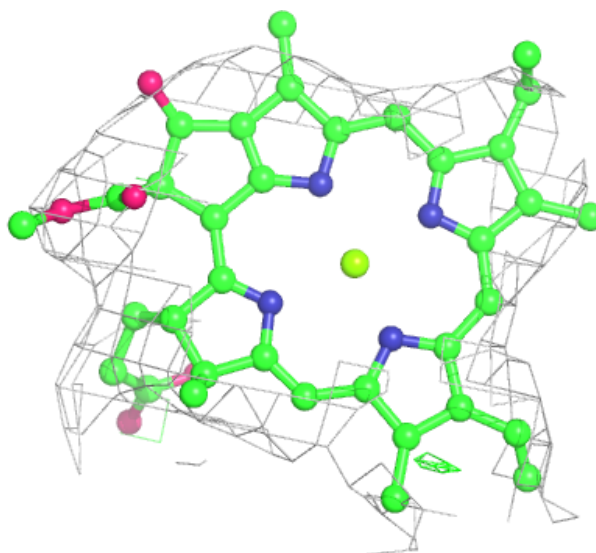
**Electron density around BCR b 4006:**

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



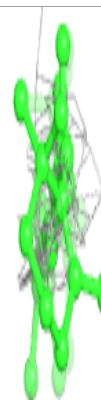
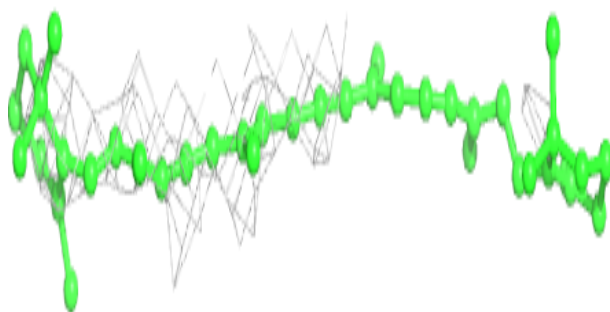
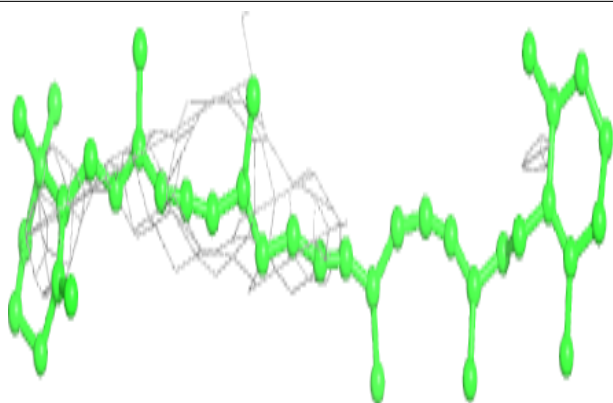
**Electron density around CLA A 1108:**

2mF<sub>o</sub>-DF<sub>c</sub> (at 0.7 rmsd) in gray  
mF<sub>o</sub>-DF<sub>c</sub> (at 3 rmsd) in purple (negative)  
and green (positive)

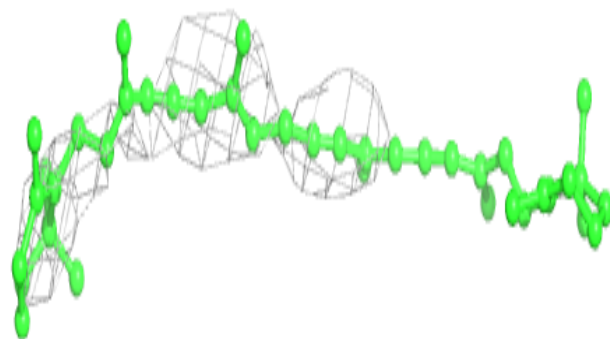
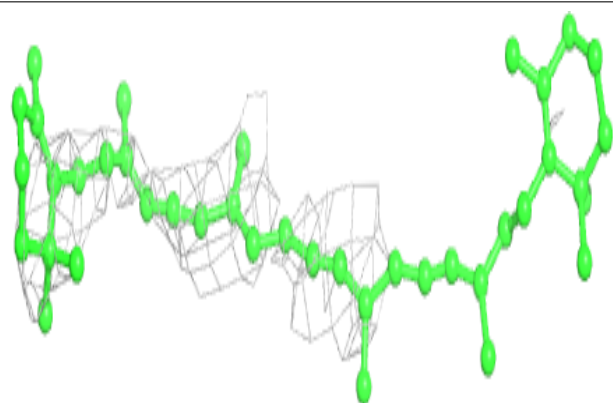


**Electron density around BCR 1 4007:**

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

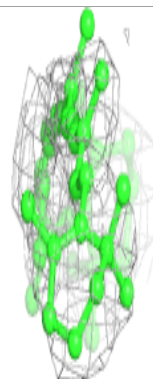
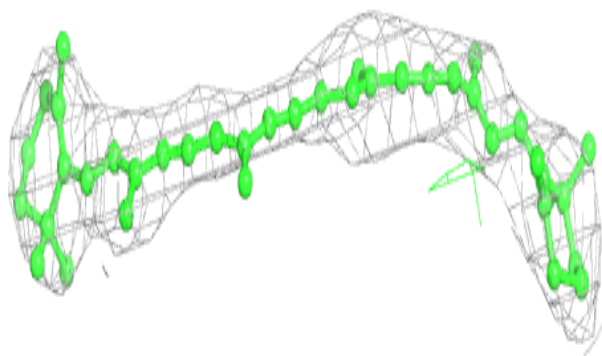
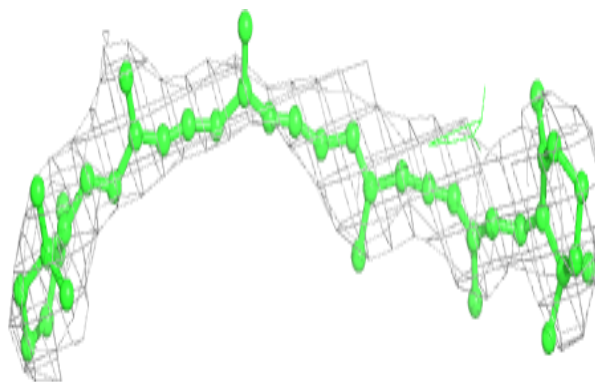
**Electron density around BCR m 4021:**

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



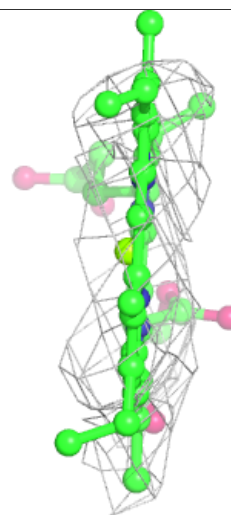
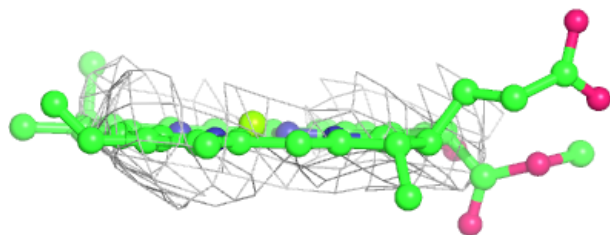
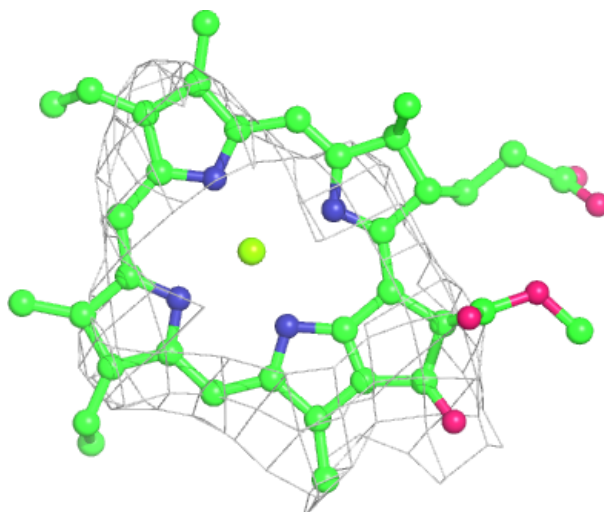
**Electron density around BCR F 4018:**

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



**Electron density around CLA 1 1113:**

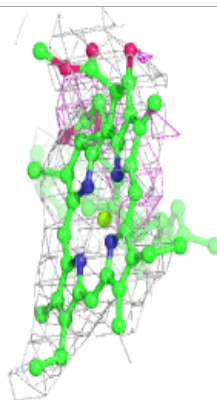
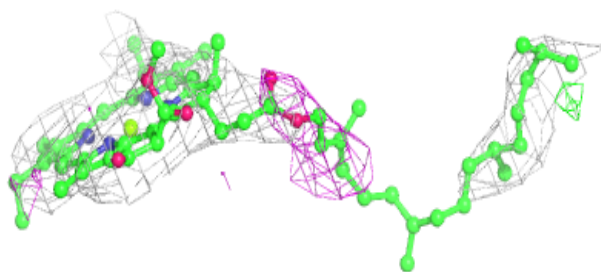
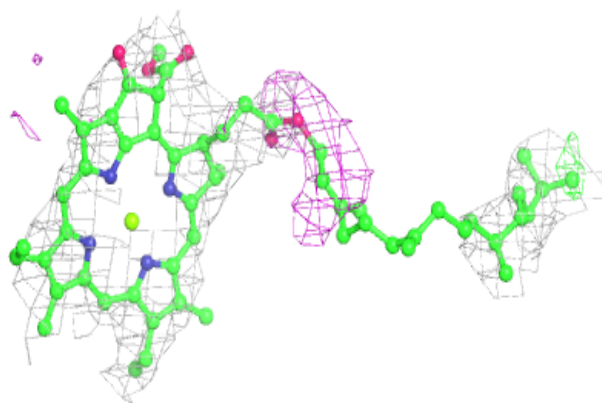
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



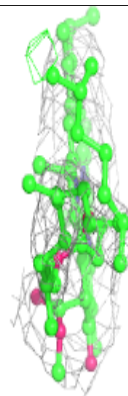
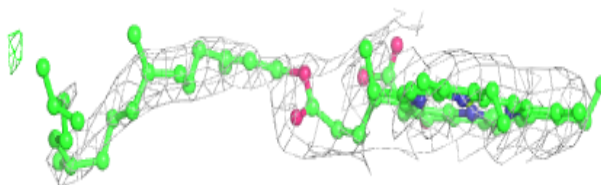
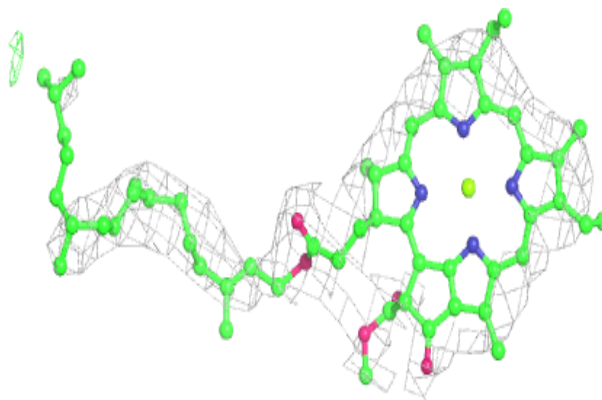


**Electron density around CLA 2 1210:**

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

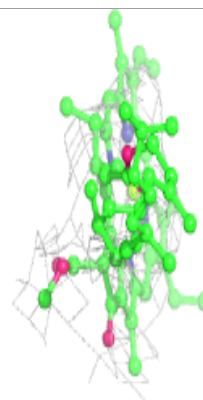
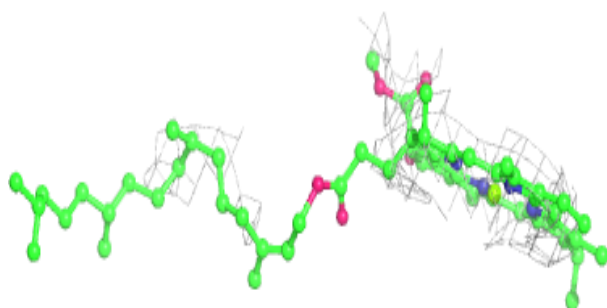
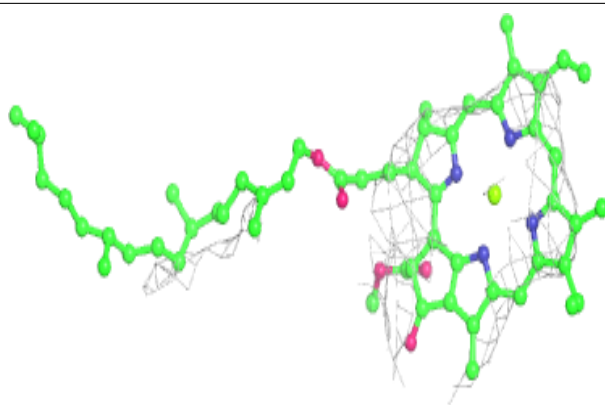
**Electron density around CLA a 1131:**

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

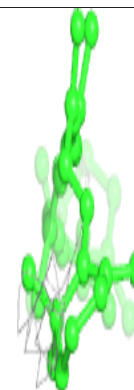
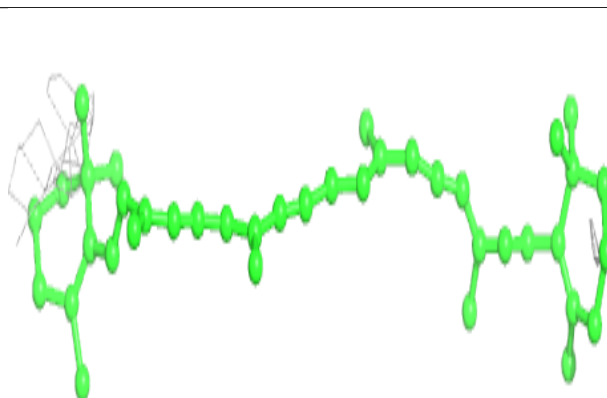
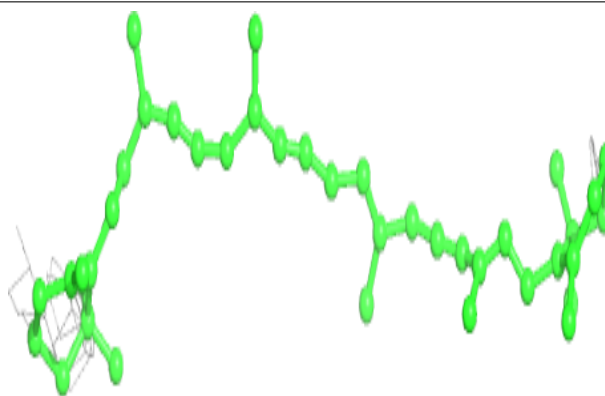


**Electron density around CLA 1 1107:**

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

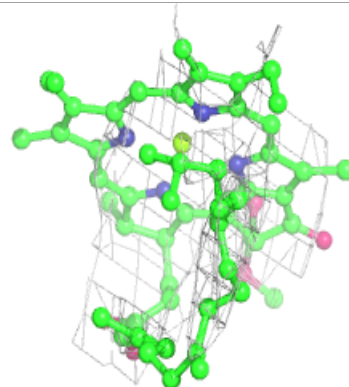
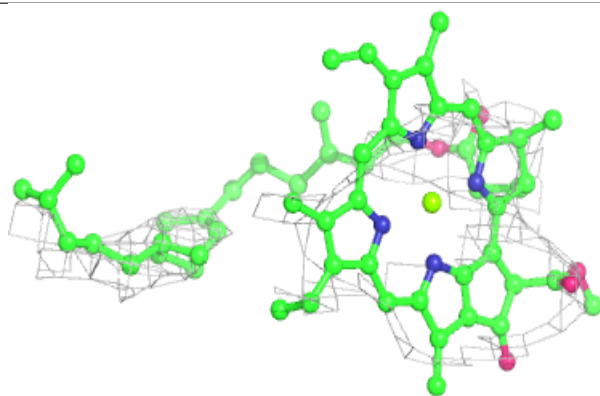
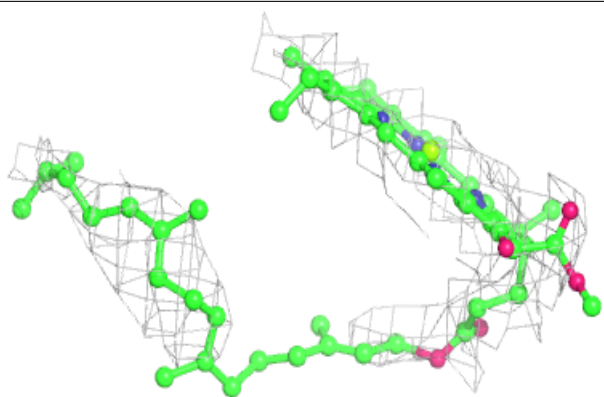
**Electron density around BCR 6 4013:**

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



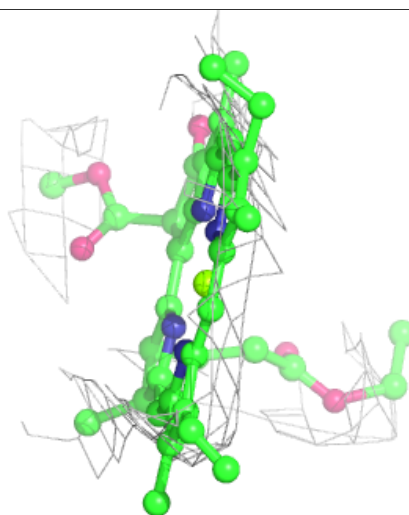
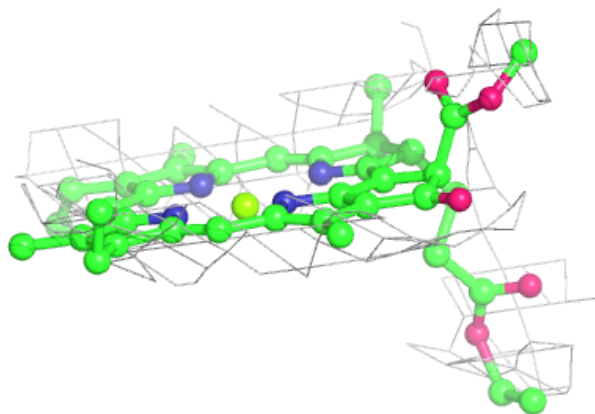
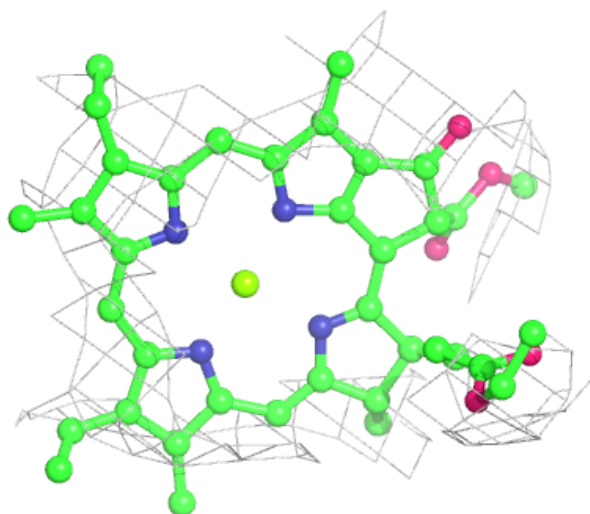
**Electron density around CLA a 1109:**

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



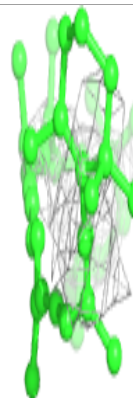
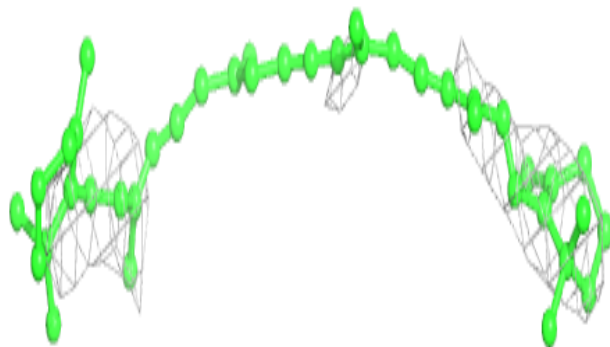
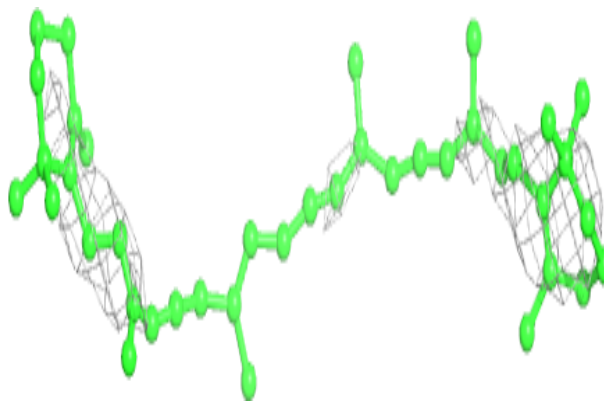
**Electron density around CLA b 1236:**

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



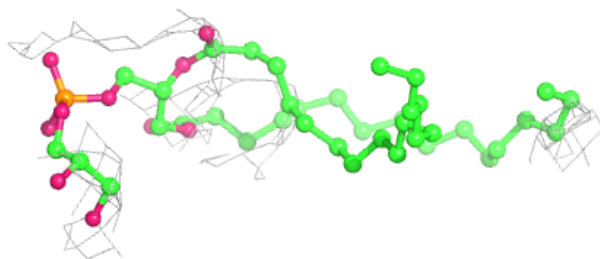
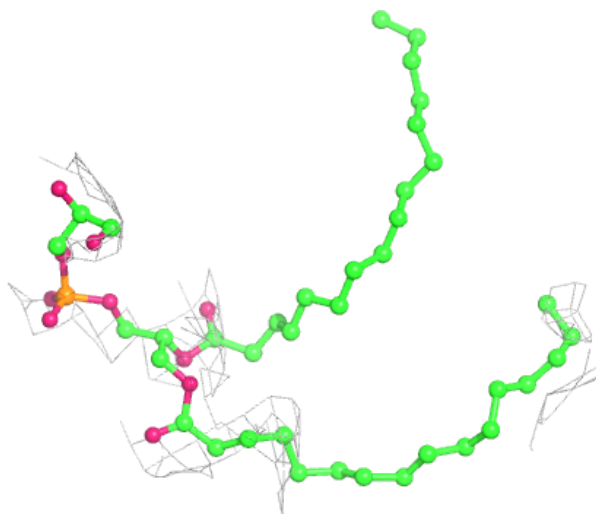
**Electron density around BCR B 4014:**

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



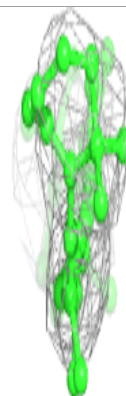
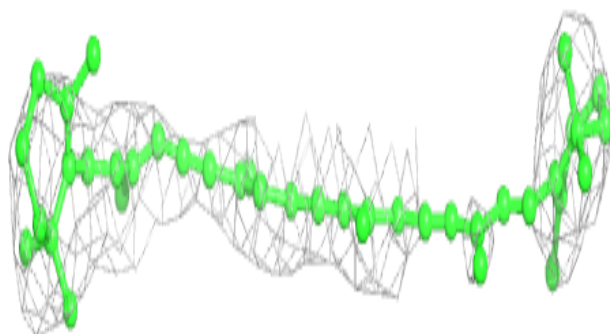
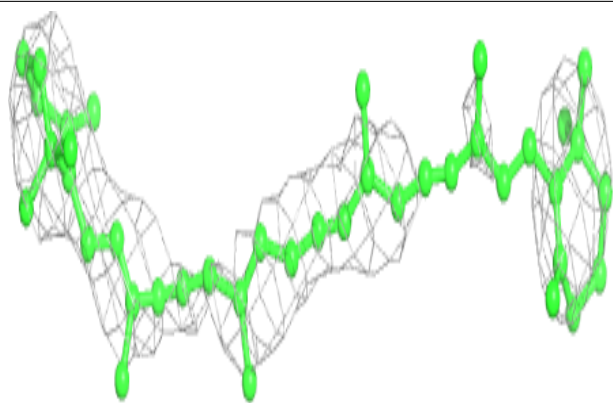
**Electron density around LHG b 5004:**

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

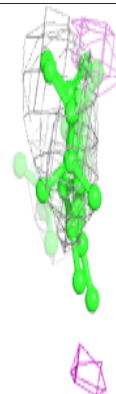
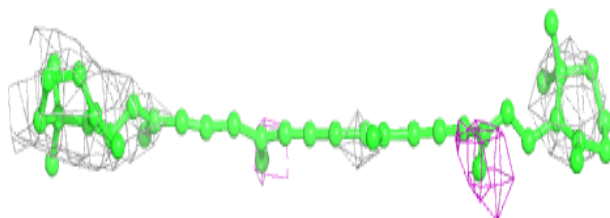
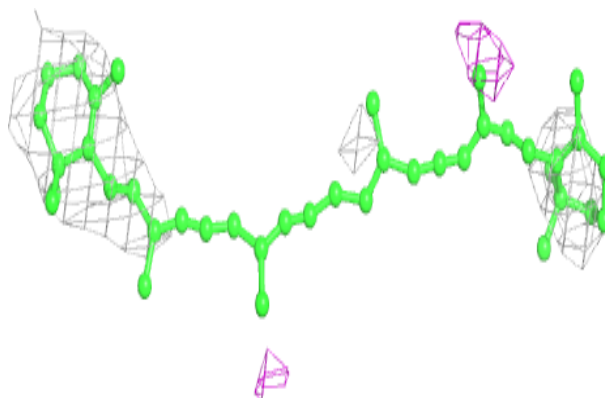


**Electron density around BCR 2 4017:**

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

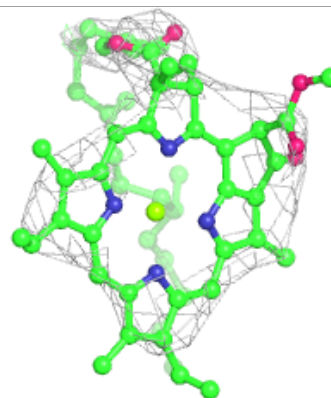
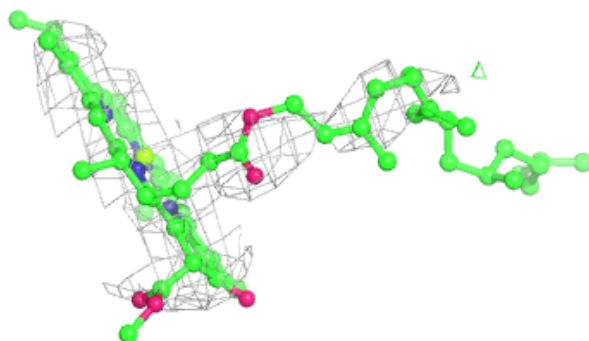
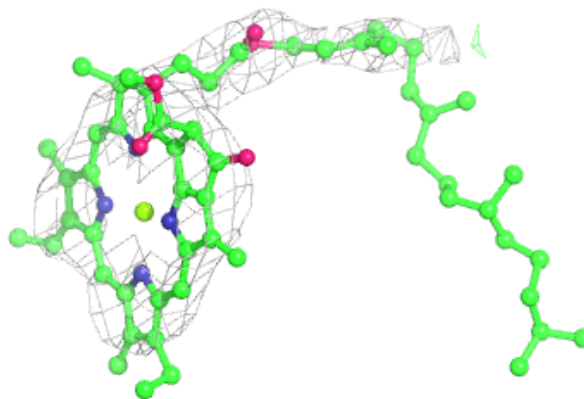
**Electron density around BCR B 4005:**

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



**Electron density around CLA a 1137:**

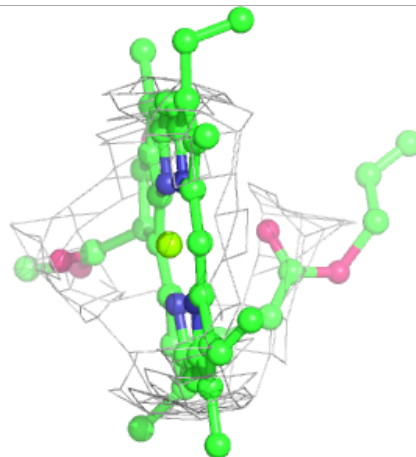
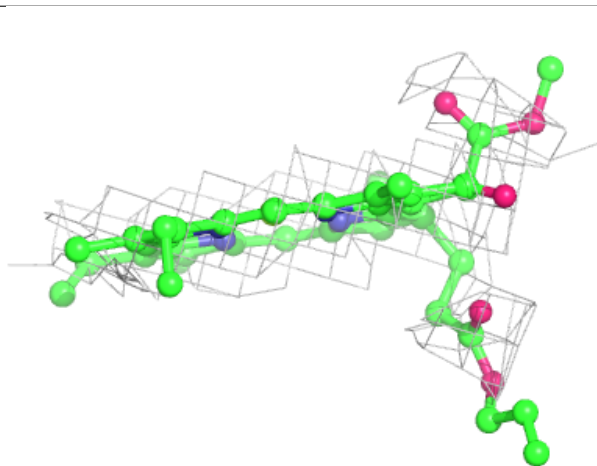
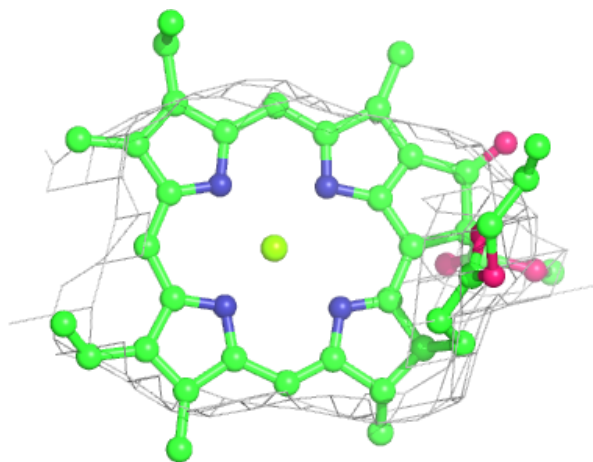
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





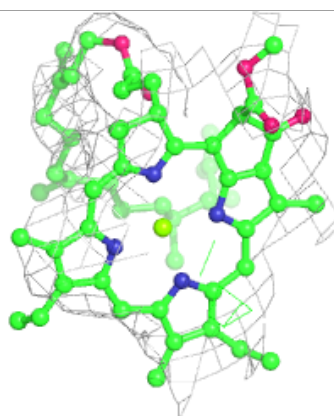
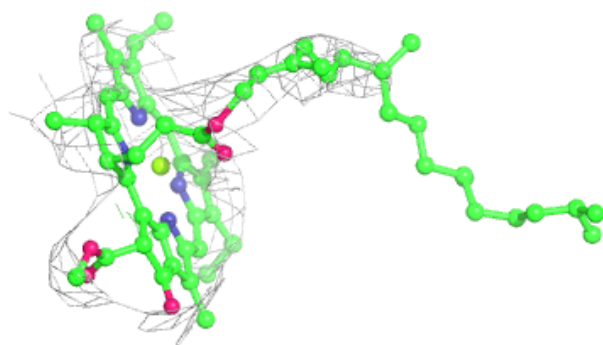
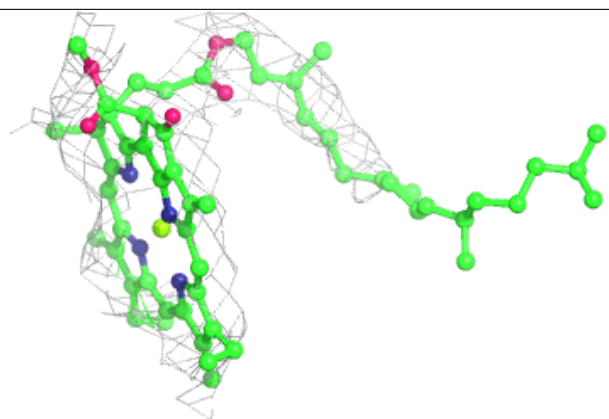
**Electron density around CLA 1 1105:**

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

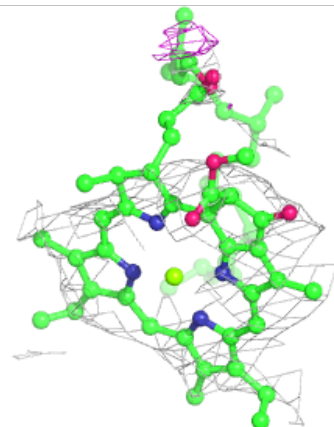
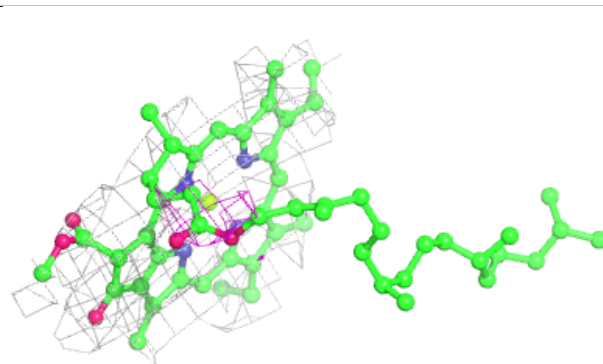
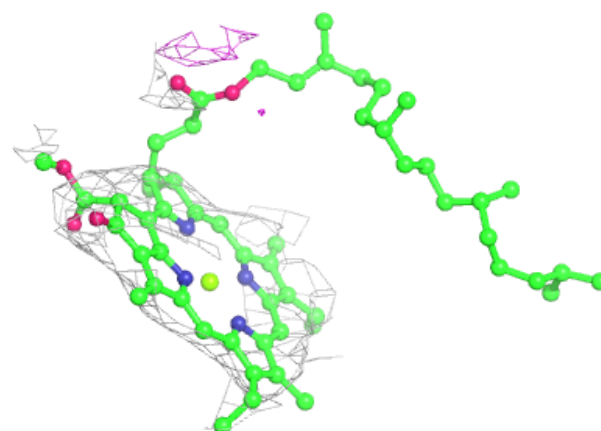


**Electron density around CLA 2 1216:**

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

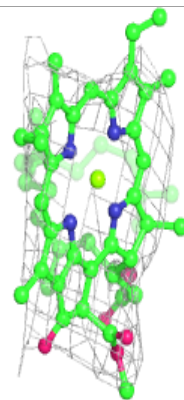
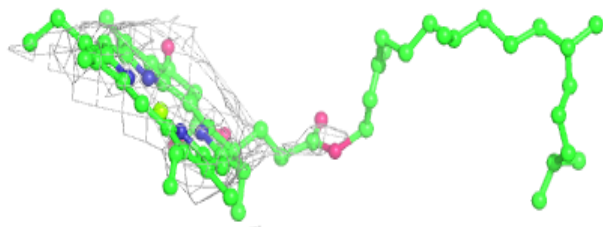
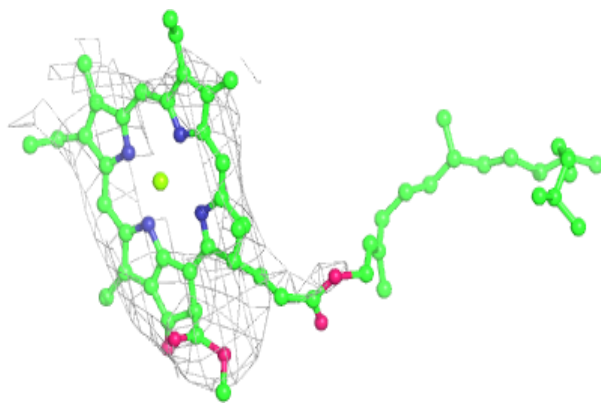
**Electron density around CLA 1 1102:**

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

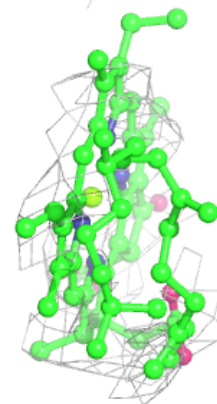
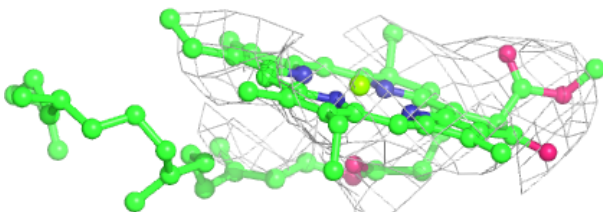
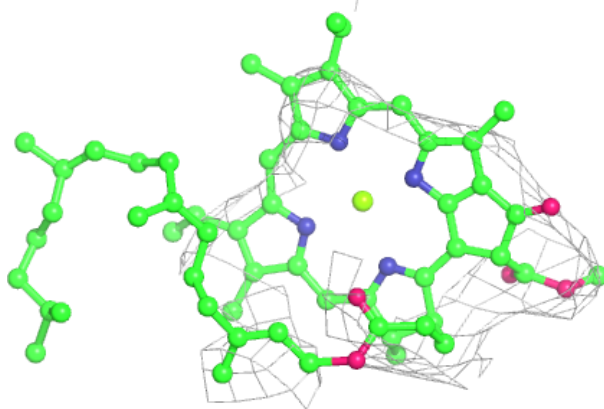


**Electron density around CLA b 1206:**

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

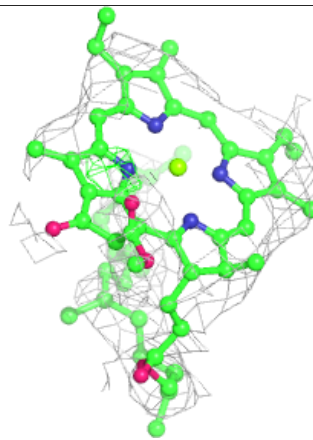
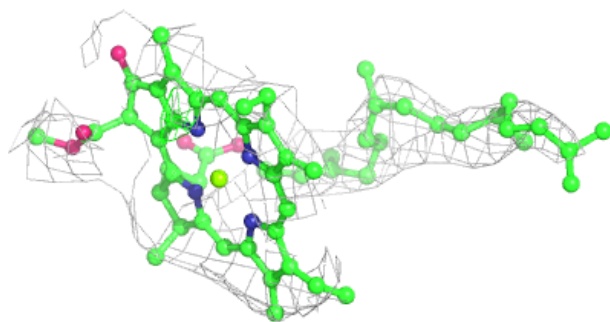
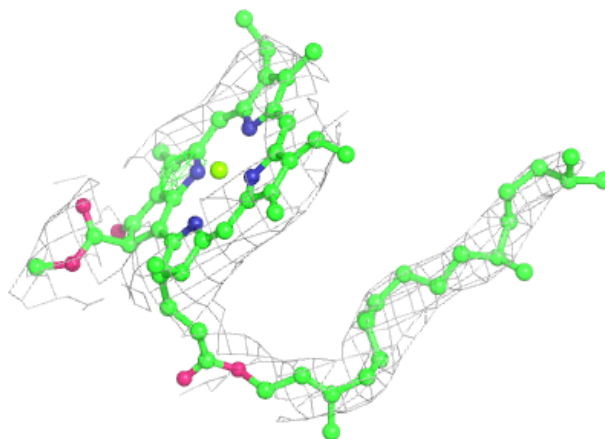
**Electron density around CLA 1 1117:**

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



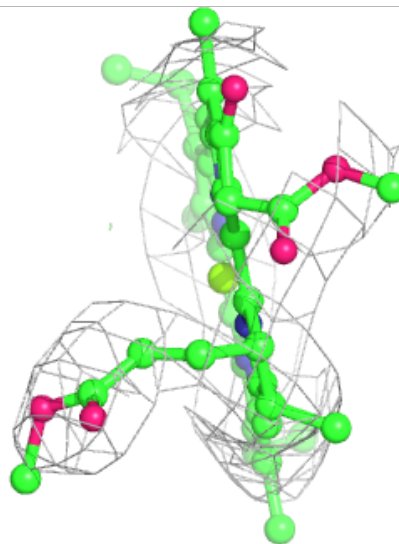
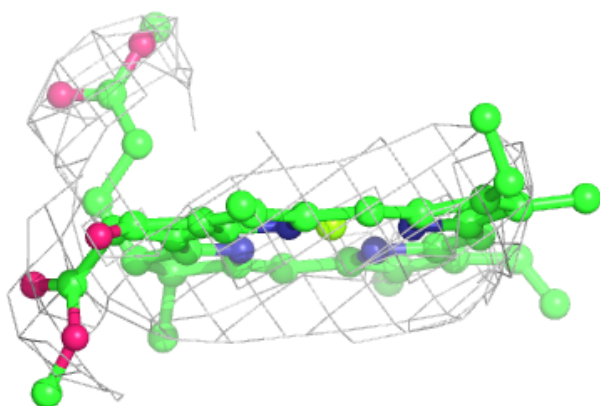
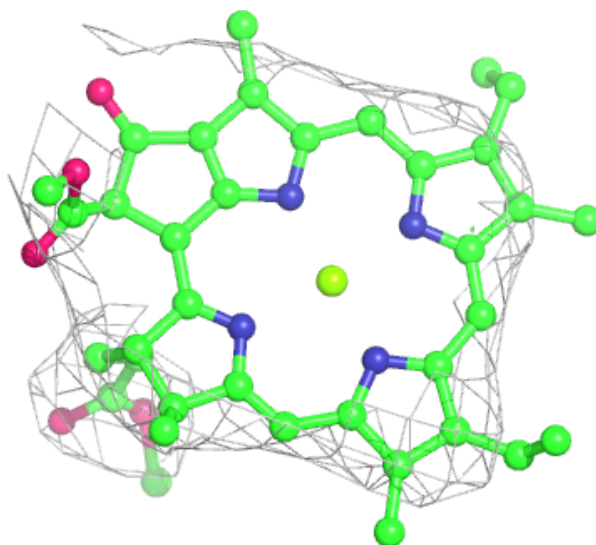
**Electron density around CLA A 1102:**

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



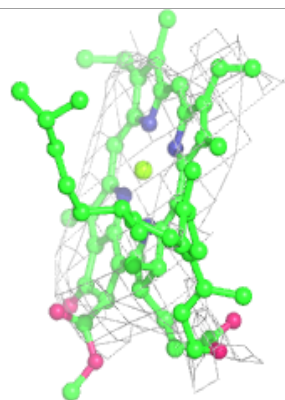
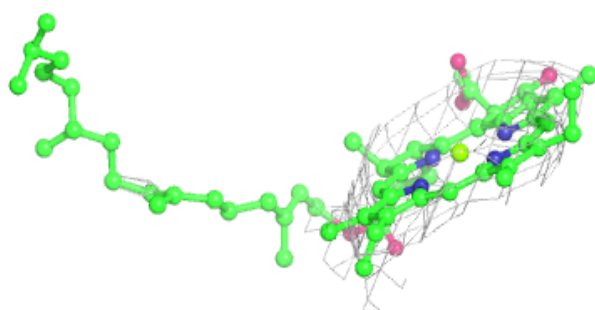
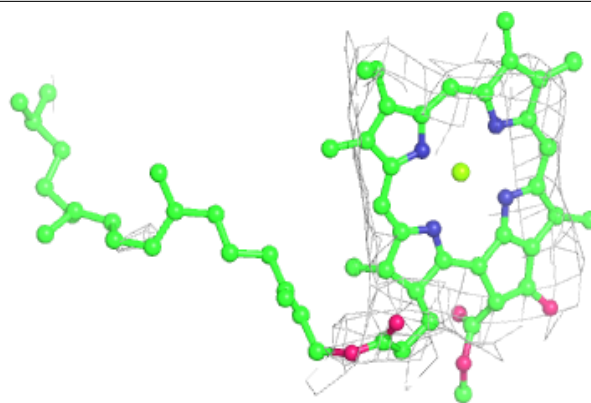
**Electron density around CLA a 1129:**

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

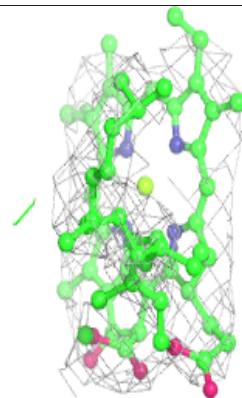
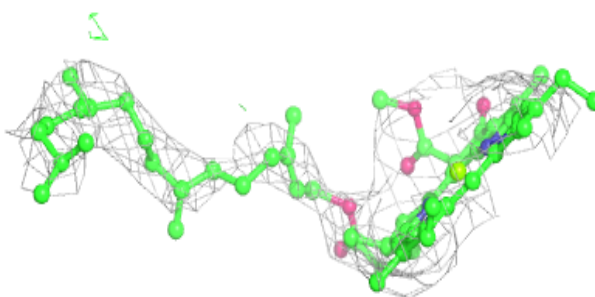
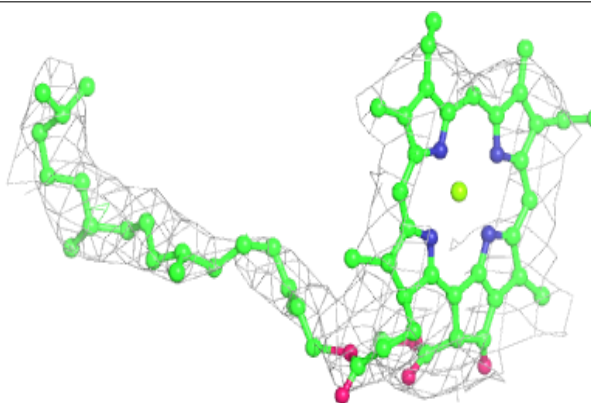


**Electron density around CLA 2 1013:**

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

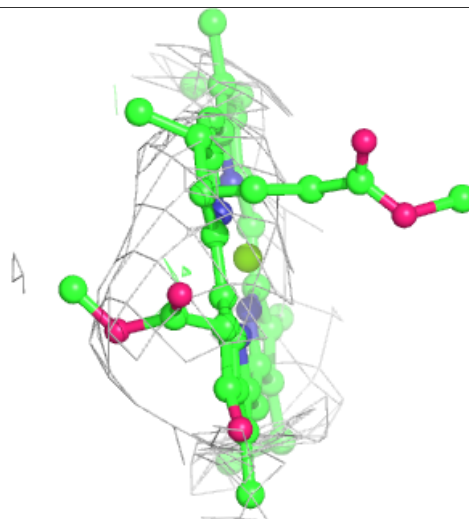
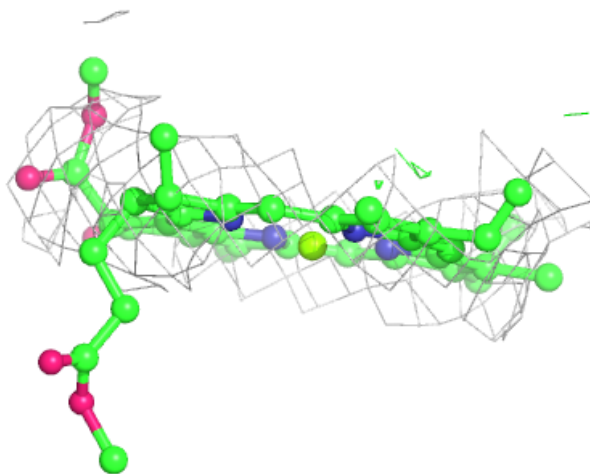
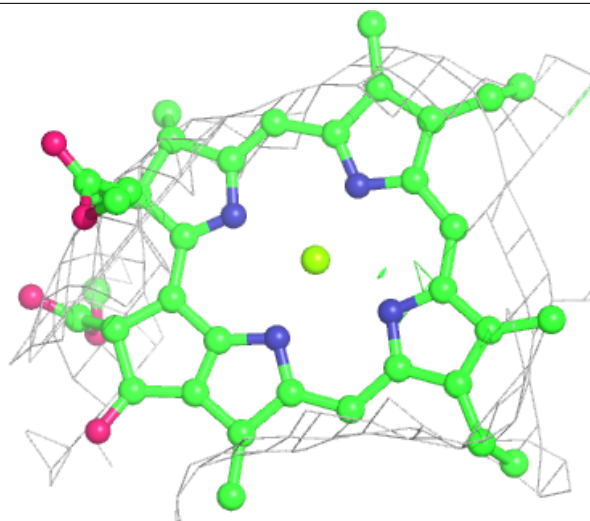
**Electron density around CLA 2 1207:**

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



**Electron density around CLA b 1211:**

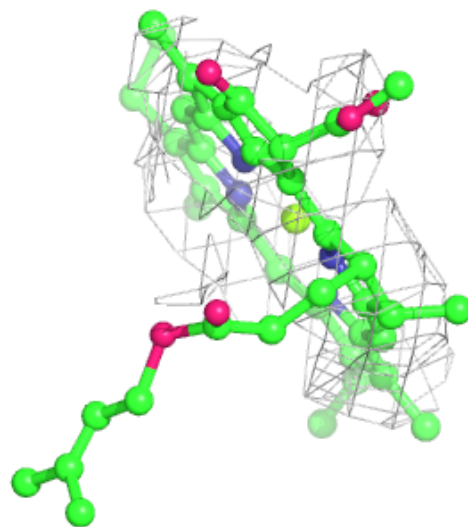
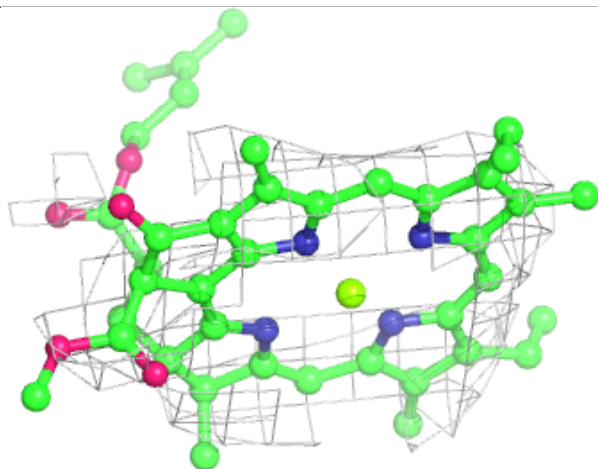
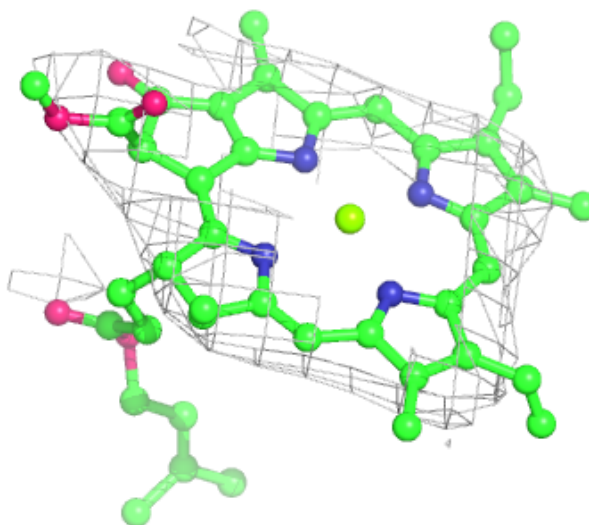
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





**Electron density around CLA 2 1228:**

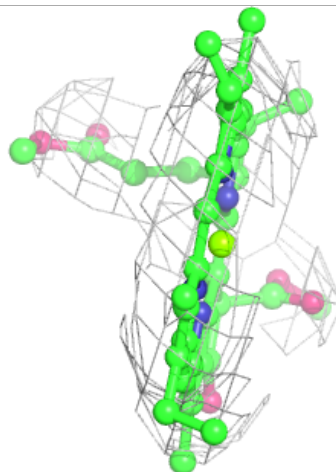
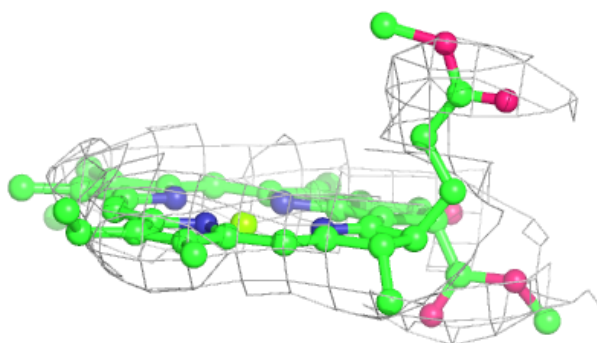
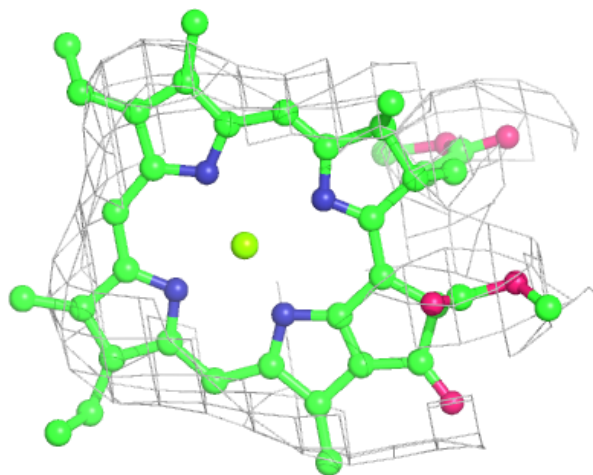
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





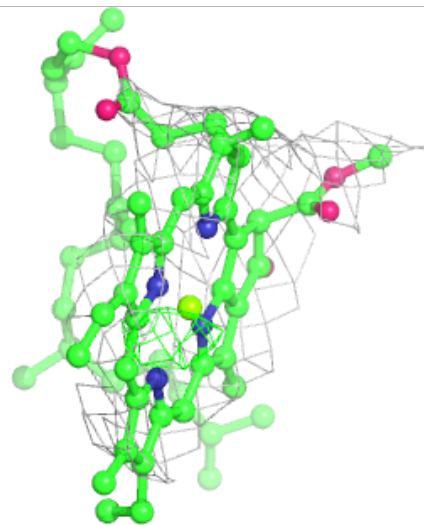
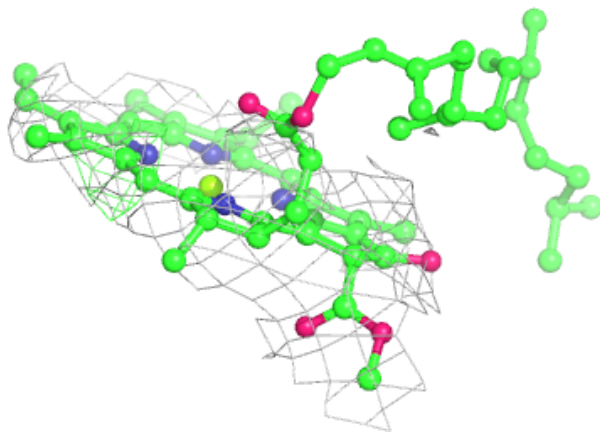
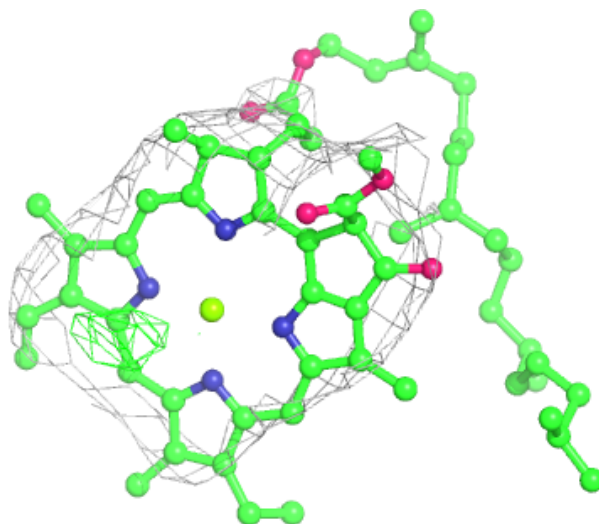
**Electron density around CLA a 1130:**

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



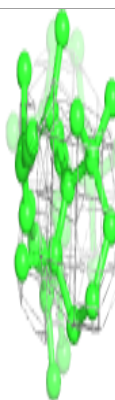
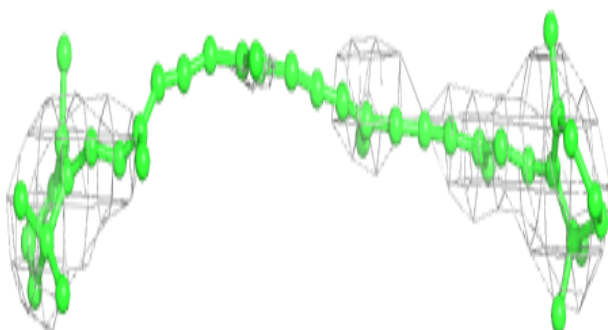
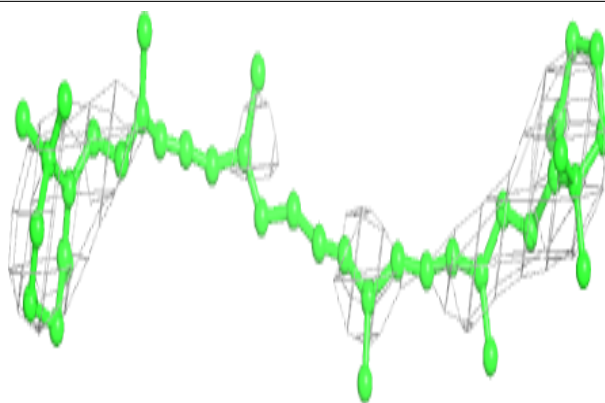
**Electron density around CLA B 1229:**

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

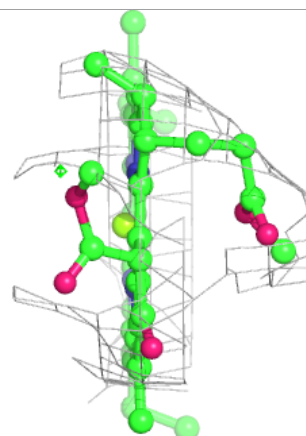
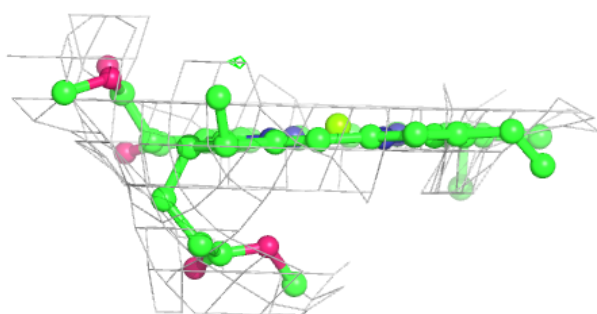
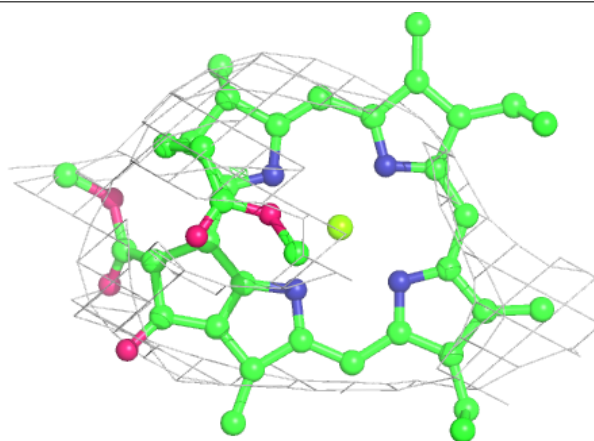


**Electron density around BCR f 4018:**

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

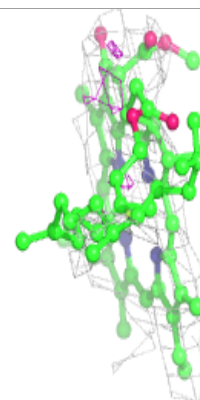
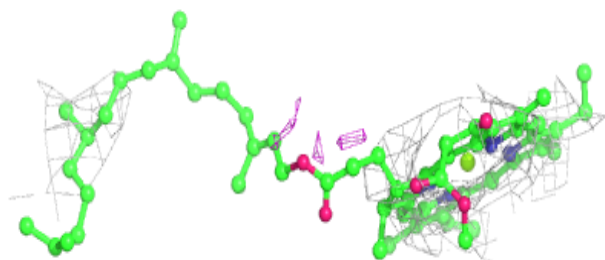
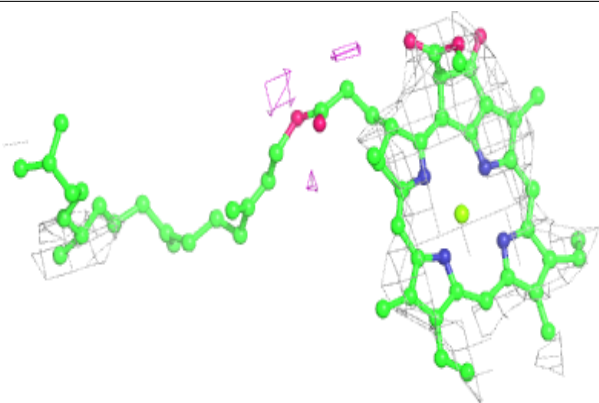
**Electron density around CLA a 1138:**

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

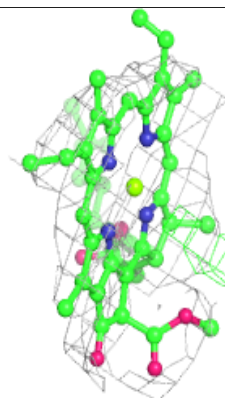
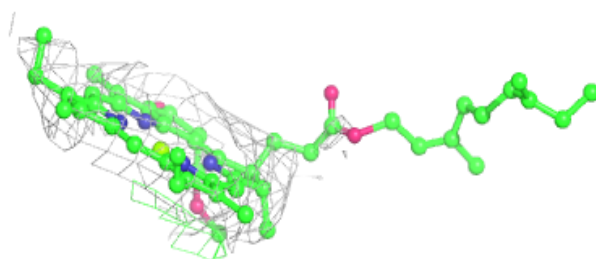
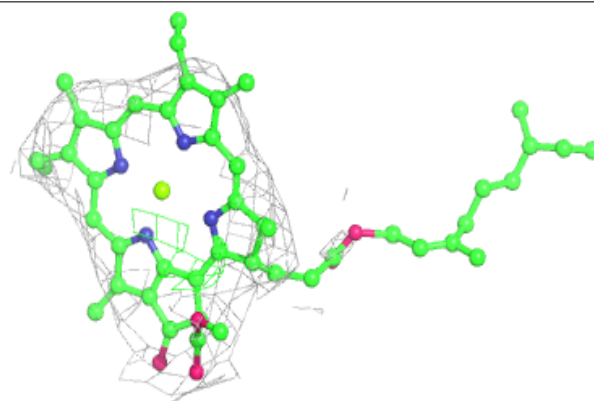


**Electron density around CLA b 1210:**

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

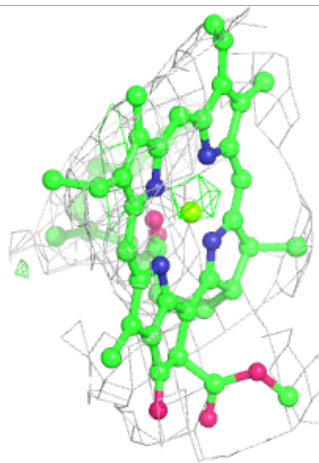
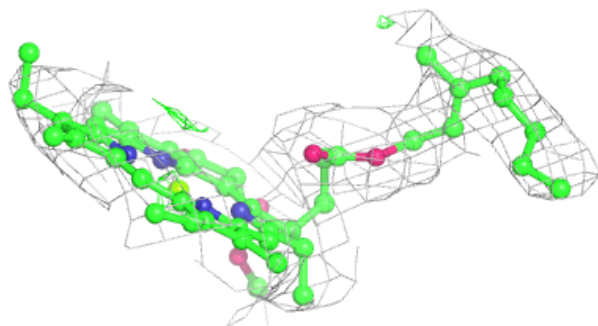
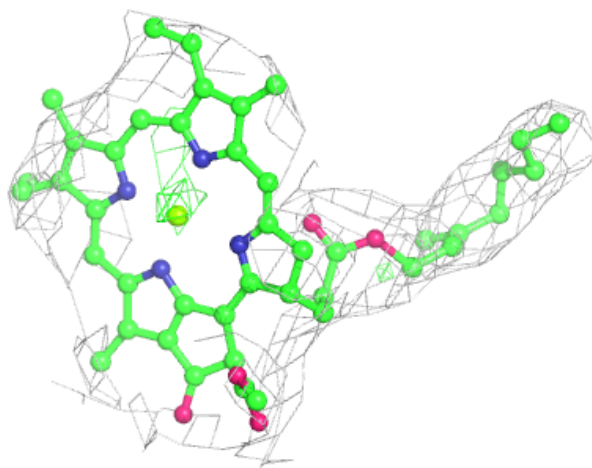
**Electron density around CLA 2 1222:**

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



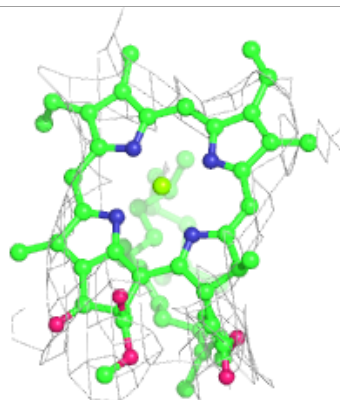
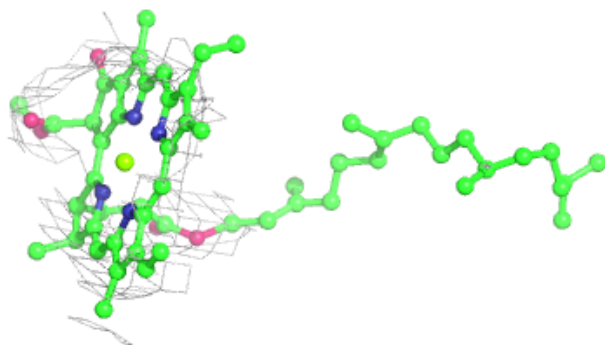
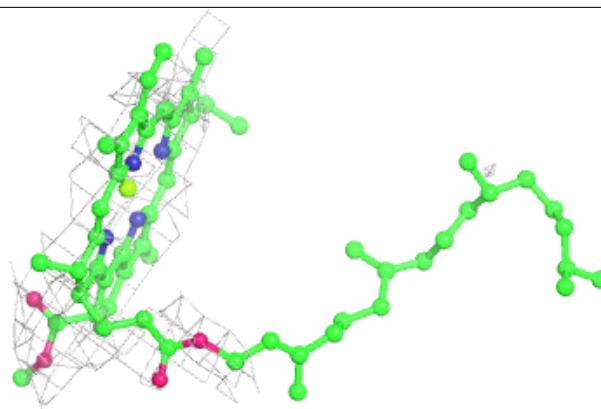
**Electron density around CLA A 1110:**

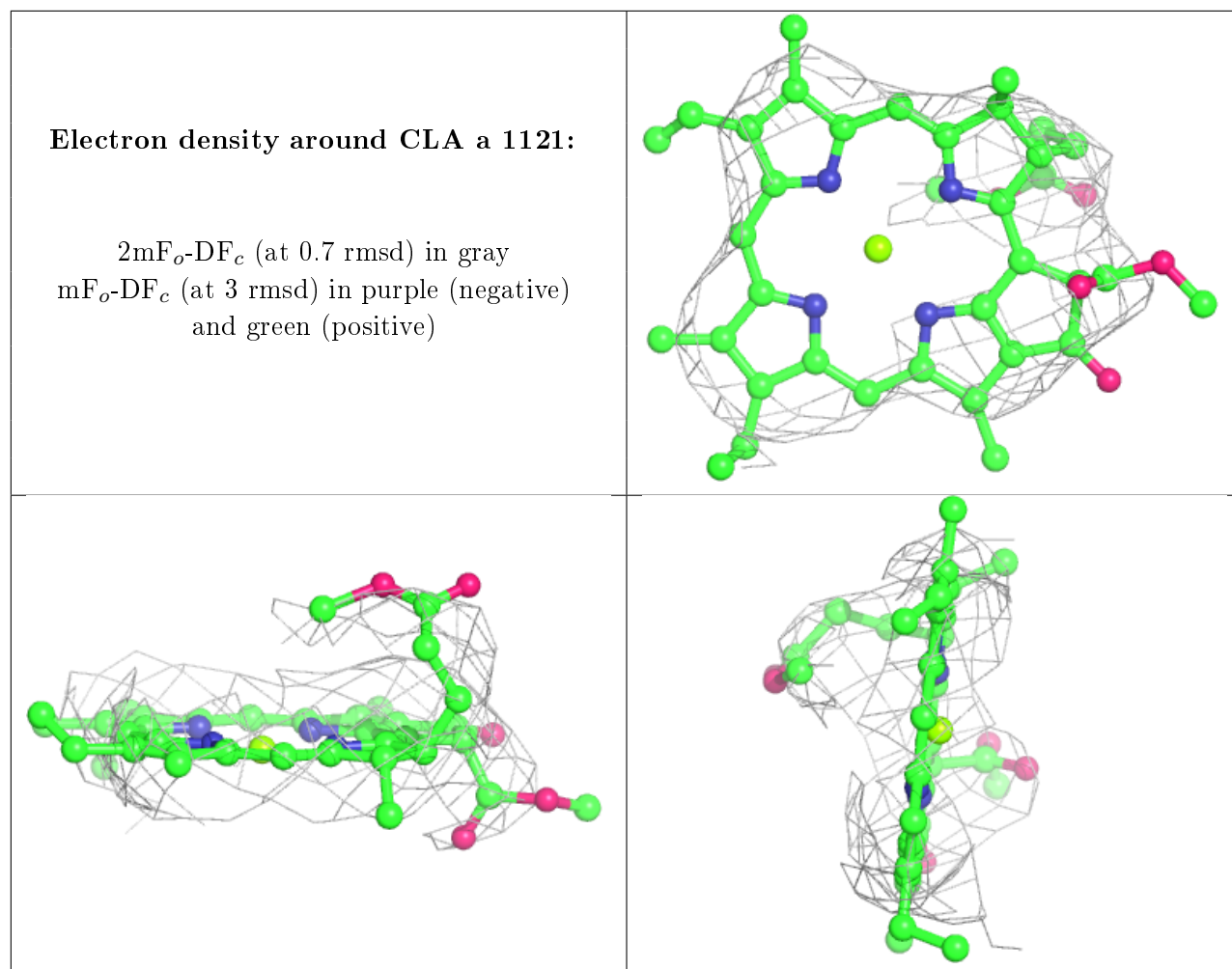
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around CLA 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)





## 6.5 Other polymers [i](#)

Unable to reproduce the depositors R factor - this section is therefore empty.