



wwPDB X-ray Structure Validation Summary Report ⓘ

Sep 11, 2023 – 06:03 PM EDT

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) 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 : 2.35.1
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.35.1

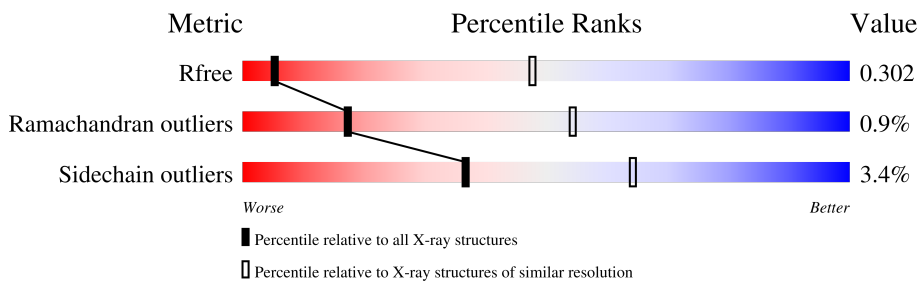
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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.



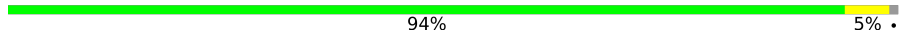
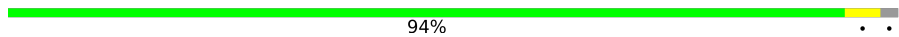
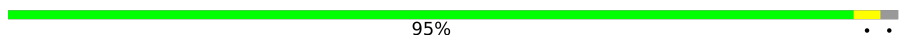
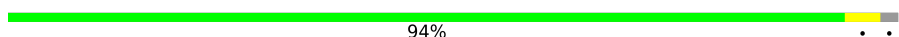






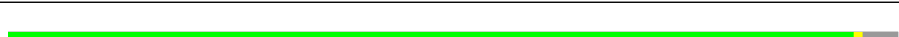


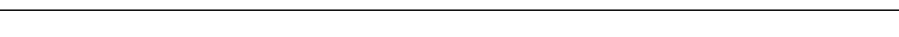
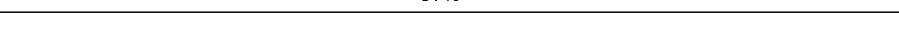
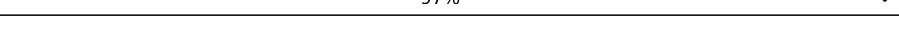
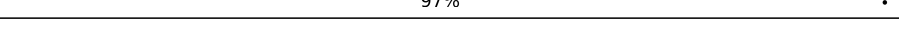





Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1212 (4.00-3.60)
Ramachandran outliers	138981	1243 (4.00-3.60)
Sidechain outliers	138945	1237 (4.00-3.60)

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 of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$.

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	
3	C	81	

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Mol	Chain	Length	Quality of chain
3	c	81	 94% 5%
4	4	141	 94%
4	D	141	 95%
4	d	141	 94%
5	5	74	 88% 8%
5	E	74	 88% 8%
5	e	74	 88% 8%
6	6	125	 98%
6	F	125	 97%
6	f	125	 98%
7	8	157	 95%
7	L	157	 94%
7	l	157	 94%
8	7	31	 97%
8	M	31	 97%
8	m	31	 97%
9	9	40	 88% 8% 5%
9	I	40	 85% 10% 5%
9	i	40	 85% 10% 5%
10	0	128	 54% 9% 38%
10	K	128	 53% 9% 38%
10	k	128	 55% 8% 38%

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	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	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	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	-	-	-
11	CLA	1	1139	X	-	-	-
11	CLA	1	1140	X	-	-	-
11	CLA	1	1237	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
11	CLA	1	1801	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	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	1228	X	-	-	-
11	CLA	2	1229	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	-	-	-
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	1012	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
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	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	-	-	-
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	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
11	CLA	B	1021	X	-	-	-
11	CLA	B	1023	X	-	-	-
11	CLA	B	1201	X	-	-	-
11	CLA	B	1202	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	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	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	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
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	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	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	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	1021	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
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	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	1502	X	-	-	-
11	CLA	l	1503	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
			Total	C	N	O	S			
1	A	739	5772	3783	982	980	27	0	0	0
1	a	739	5772	3783	982	980	27	0	0	0
1	1	739	5772	3783	982	980	27	0	0	0

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

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

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

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

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

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

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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			

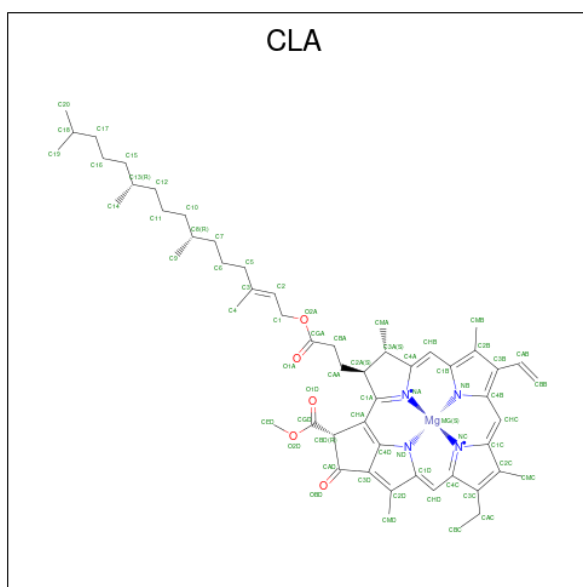
- Molecule 9 is a protein called Photosystem I subunit III.

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: C₅₅H₇₂MgN₄O₅).



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

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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
			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	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
			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		

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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
			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
			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	l	1	Total	C	Mg	N	O	0	0
			52	42	1	4	5		
11	l	1	Total	C	Mg	N	O	0	0
			55	45	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
			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
			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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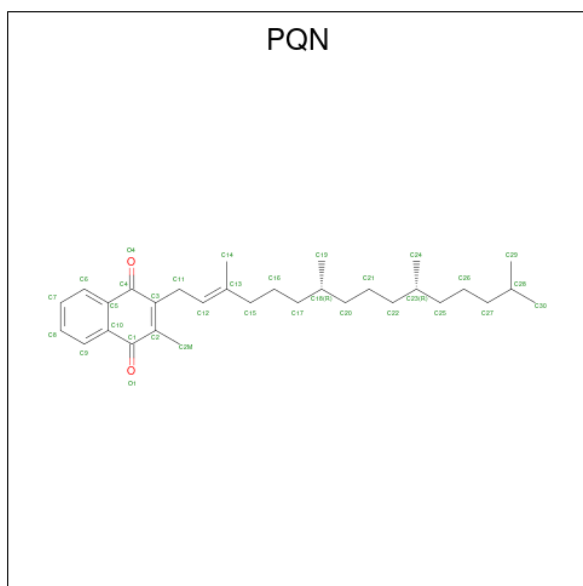
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
11	2	1	Total	C	Mg	N	O	0	0
			54	44	1	4	5		
11	2	1	Total	C	Mg	N	O	0	0
			56	46	1	4	5		
11	2	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
11	2	1	Total	C	Mg	N	O	0	0
			55	45	1	4	5		
11	2	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
11	2	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
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: $C_{31}H_{46}O_2$).



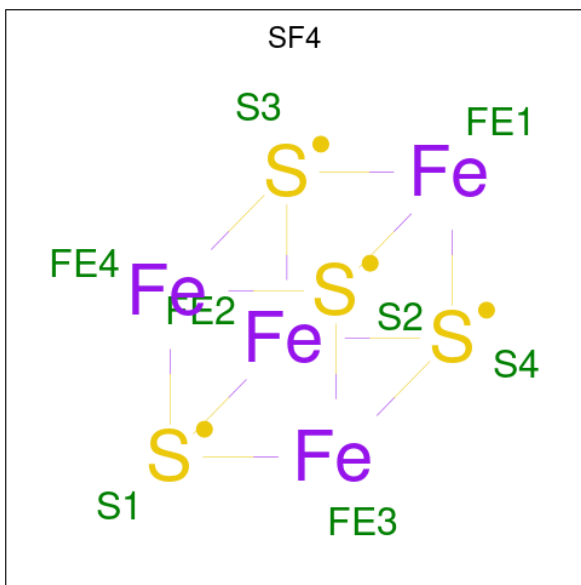
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
12	A	1	Total	C	O	0	0
			33	31	2		
12	B	1	Total	C	O	0	0
			33	31	2		
12	a	1	Total	C	O	0	0
			33	31	2		
12	b	1	Total	C	O	0	0
			33	31	2		

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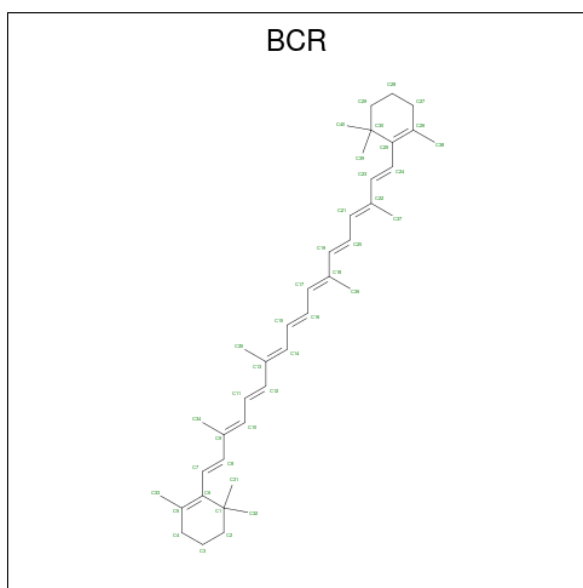
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
12	1	1	Total	C	O	0	0
			33	31	2		
12	2	1	Total	C	O	0	0
			33	31	2		

- Molecule 13 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe₄S₄).



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: C₄₀H₅₆).



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	f	1	Total C 40 40	0	0
14	f	1	Total C 40 40	0	0

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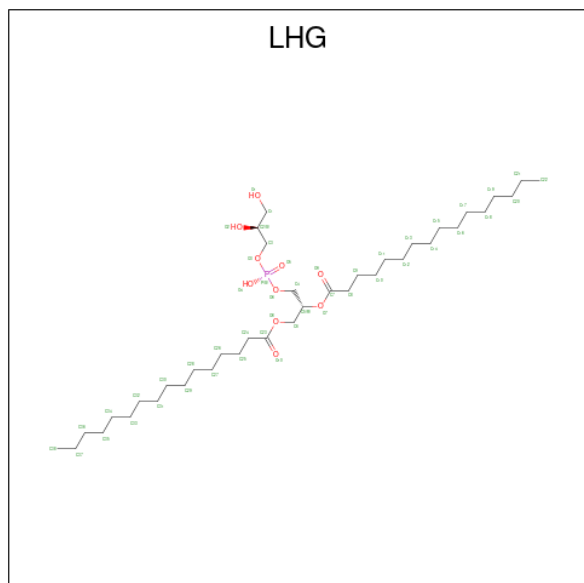
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
14	f	1	Total C 40 40	0	0
14	l	1	Total C 40 40	0	0
14	l	1	Total C 40 40	0	0
14	m	1	Total C 40 40	0	0
14	1	1	Total C 40 40	0	0
14	1	1	Total C 40 40	0	0
14	1	1	Total C 40 40	0	0
14	1	1	Total C 40 40	0	0
14	1	1	Total C 40 40	0	0
14	2	1	Total C 40 40	0	0
14	2	1	Total 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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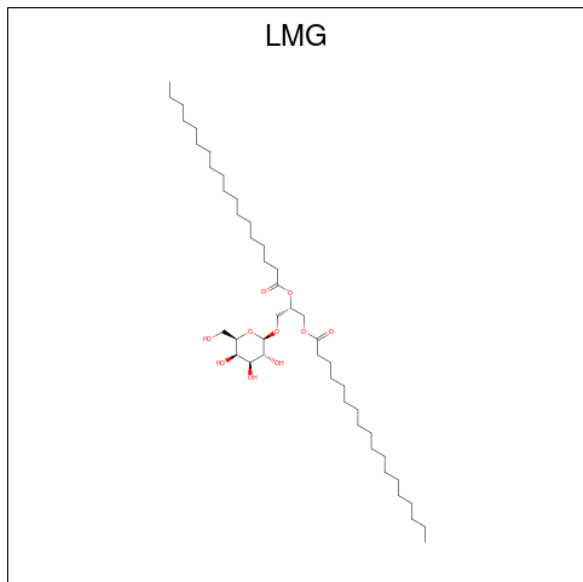
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
14	8	1	Total C 40 40	0	0
14	7	1	Total C 40 40	0	0

- 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: $C_{45}H_{86}O_{10}$).



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

3 Residue-property plots [i](#)

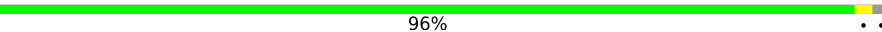
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded 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

Chain A:  96%



- Molecule 1: Photosystem I P700 chlorophyll a apoprotein A1

Chain a:  96%



- Molecule 1: Photosystem I P700 chlorophyll a apoprotein A1

Chain 1:  96%



- Molecule 2: Photosystem I P700 chlorophyll a apoprotein A2

Chain B:  96%



- Molecule 2: Photosystem I P700 chlorophyll a apoprotein A2

Chain b:  96%

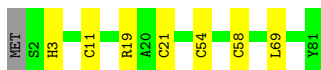
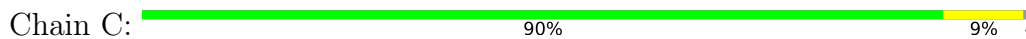


- Molecule 2: Photosystem I P700 chlorophyll a apoprotein A2

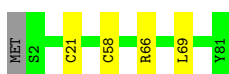
Chain 2:  96%



- Molecule 3: Photosystem I iron-sulfur center



- Molecule 3: Photosystem I iron-sulfur center



- Molecule 3: Photosystem I iron-sulfur center



- Molecule 4: Photosystem I subunit II



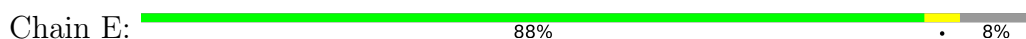
- Molecule 4: Photosystem I subunit II



- Molecule 4: Photosystem I subunit II

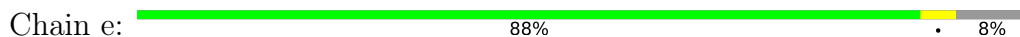


- Molecule 5: Photosystem I reaction center subunit IV

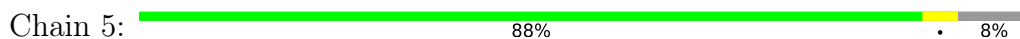




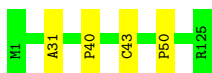
- Molecule 5: Photosystem I reaction center subunit IV



- Molecule 5: Photosystem I reaction center subunit IV



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



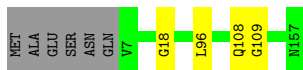
- Molecule 6: Fusion protein of Photosystem I subunit III and subunit IX



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

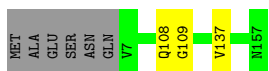


- Molecule 7: Photosystem I reaction center subunit XI

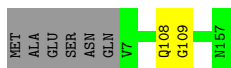


- Molecule 7: Photosystem I reaction center subunit XI





- Molecule 7: Photosystem I reaction center subunit XI



- Molecule 8: Photosystem I reaction center subunit XII



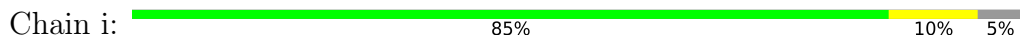
- Molecule 8: Photosystem I reaction center subunit XII



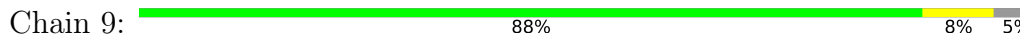
- Molecule 8: Photosystem I reaction center subunit XII



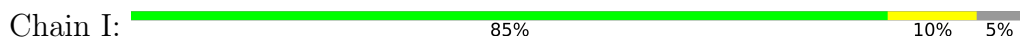
- Molecule 9: Photosystem I subunit III



- Molecule 9: Photosystem I subunit III

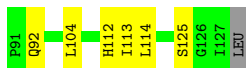
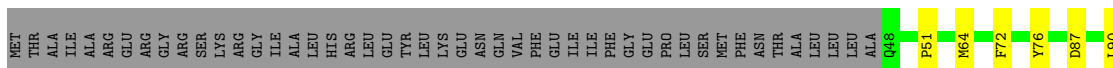


- Molecule 9: Photosystem I subunit III

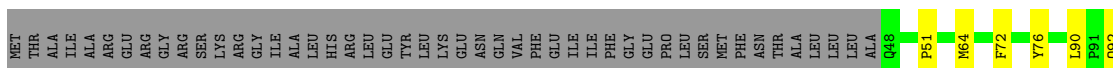




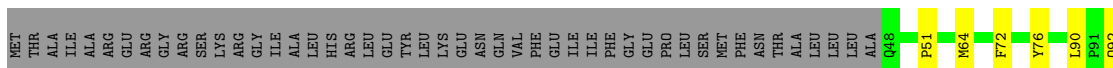
- Molecule 10: Photosystem I reaction center subunit VIII



- 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, α , β , γ	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
$\langle I/\sigma(I) \rangle$ ¹	-0.02 (at 3.40Å)	Xtrriage
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 ²)	93.5	Xtrriage
Anisotropy	0.250	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.25 , 77.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.28$	Xtrriage
Estimated twinning fraction	0.038 for l,-k,h	Xtrriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	68370	wwPDB-VP
Average B, all atoms (Å ²)	173.0	wwPDB-VP

Xtrriage'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.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

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](#)

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

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
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 [i](#)

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
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

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
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	2	196	HIS
8	7	5	ASP
2	2	302	LYS
3	3	58	CYS
10	K	114	LEU

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

Mol	Chain	Res	Type
1	1	224	ASN
1	1	488	HIS
1	1	432	HIS
1	1	608	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 monosaccharides 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	L	1503	-	65,73,73	2.33	18 (27%)	76,113,113	2.61	21 (27%)
11	CLA	b	1223	-	65,73,73	2.39	19 (29%)	76,113,113	2.54	24 (31%)
11	CLA	a	1125	-	52,60,73	2.62	20 (38%)	60,97,113	2.86	22 (36%)
11	CLA	2	1023	-	65,73,73	2.35	19 (29%)	76,113,113	2.67	27 (35%)
11	CLA	1	1125	-	52,60,73	2.64	19 (36%)	60,97,113	2.90	25 (41%)
11	CLA	B	1214	-	59,67,73	2.47	20 (33%)	68,105,113	2.83	26 (38%)
11	CLA	b	1240	-	45,53,73	2.76	19 (42%)	52,89,113	2.89	19 (36%)
11	CLA	1	1139	-	50,58,73	2.72	20 (40%)	58,95,113	2.86	22 (37%)
11	CLA	L	1501	7	65,73,73	2.37	20 (30%)	76,113,113	2.56	22 (28%)
11	CLA	A	1119	-	65,73,73	2.36	19 (29%)	76,113,113	2.52	25 (32%)
11	CLA	2	1240	15	45,53,73	2.75	18 (40%)	52,89,113	2.86	19 (36%)
11	CLA	2	1217	-	47,55,73	2.77	19 (40%)	54,91,113	2.92	23 (42%)
11	CLA	1	1108	-	45,53,73	2.75	19 (42%)	52,89,113	2.91	18 (34%)
11	CLA	b	1225	-	65,73,73	2.39	20 (30%)	76,113,113	2.47	22 (28%)
11	CLA	A	1113	-	45,53,73	2.72	19 (42%)	52,89,113	2.93	20 (38%)
11	CLA	1	1801	15	52,60,73	2.67	19 (36%)	60,97,113	2.92	25 (41%)
11	CLA	A	1138	-	46,54,73	2.83	19 (41%)	53,90,113	2.98	20 (37%)
11	CLA	K	1401	-	65,73,73	2.37	19 (29%)	76,113,113	2.65	25 (32%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
14	BCR	b	4005	-	41,41,41	2.76	6 (14%)	56,56,56	6.58	25 (44%)
14	BCR	f	4018	-	41,41,41	2.85	7 (17%)	56,56,56	6.36	24 (42%)
11	CLA	a	1101	-	65,73,73	2.38	19 (29%)	76,113,113	2.58	24 (31%)
11	CLA	2	1219	-	55,63,73	2.62	20 (36%)	64,101,113	2.82	23 (35%)
11	CLA	2	1231	-	45,53,73	2.76	18 (40%)	52,89,113	2.97	23 (44%)
11	CLA	B	1230	-	58,66,73	2.51	18 (31%)	67,104,113	2.76	25 (37%)
11	CLA	b	1218	-	45,53,73	2.75	19 (42%)	52,89,113	2.91	18 (34%)
14	BCR	M	4021	-	41,41,41	2.79	6 (14%)	56,56,56	6.58	21 (37%)
11	CLA	2	1210	-	65,73,73	2.33	19 (29%)	76,113,113	2.64	27 (35%)
11	CLA	2	1227	-	45,53,73	2.72	18 (40%)	52,89,113	2.98	19 (36%)
11	CLA	l	1501	7	65,73,73	2.38	20 (30%)	76,113,113	2.61	23 (30%)
11	CLA	2	1235	-	60,68,73	2.47	20 (33%)	70,107,113	2.69	27 (38%)
11	CLA	a	1124	-	55,63,73	2.57	20 (36%)	64,101,113	2.82	24 (37%)
11	CLA	b	1201	-	54,62,73	2.61	19 (35%)	62,99,113	2.86	24 (38%)
11	CLA	a	1118	-	61,69,73	2.42	18 (29%)	71,108,113	2.66	22 (30%)
11	CLA	A	1122	-	59,67,73	2.46	18 (30%)	68,105,113	2.83	24 (35%)
11	CLA	B	1240	15	45,53,73	2.78	19 (42%)	52,89,113	2.90	20 (38%)
11	CLA	a	1109	11	65,73,73	2.39	20 (30%)	76,113,113	2.62	23 (30%)
14	BCR	A	4008	-	41,41,41	2.72	7 (17%)	56,56,56	6.70	30 (53%)
11	CLA	A	1114	-	46,54,73	2.88	19 (41%)	53,90,113	2.80	19 (35%)
11	CLA	1	1022	-	65,73,73	2.38	20 (30%)	76,113,113	2.46	22 (28%)
11	CLA	2	1230	-	58,66,73	2.53	19 (32%)	67,104,113	2.76	25 (37%)
11	CLA	A	1123	-	65,73,73	2.34	19 (29%)	76,113,113	2.64	22 (28%)
11	CLA	A	1101	-	65,73,73	2.34	19 (29%)	76,113,113	2.56	24 (31%)
11	CLA	B	1218	-	45,53,73	2.73	18 (40%)	52,89,113	2.93	19 (36%)
11	CLA	A	1126	-	65,73,73	2.38	19 (29%)	76,113,113	2.66	24 (31%)
14	BCR	6	4020	-	41,41,41	2.86	7 (17%)	56,56,56	6.54	24 (42%)
11	CLA	1	1118	-	61,69,73	2.42	19 (31%)	71,108,113	2.59	25 (35%)
11	CLA	1	1011	-	65,73,73	2.34	20 (30%)	76,113,113	2.81	24 (31%)
11	CLA	b	1235	-	60,68,73	2.50	20 (33%)	70,107,113	2.74	26 (37%)
11	CLA	2	1208	-	45,53,73	2.73	18 (40%)	52,89,113	2.88	17 (32%)
11	CLA	1	1140	-	65,73,73	2.38	20 (30%)	76,113,113	2.67	25 (32%)
14	BCR	b	4010	-	41,41,41	2.79	6 (14%)	56,56,56	6.71	24 (42%)
11	CLA	b	1232	-	45,53,73	2.76	19 (42%)	52,89,113	2.86	19 (36%)
11	CLA	B	1021	-	65,73,73	2.33	20 (30%)	76,113,113	2.68	27 (35%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
11	CLA	1	1124	-	55,63,73	2.57	20 (36%)	64,101,113	2.80	22 (34%)
11	CLA	2	1232	-	45,53,73	2.75	19 (42%)	52,89,113	2.85	19 (36%)
11	CLA	B	1211	-	46,54,73	2.85	19 (41%)	53,90,113	2.84	18 (33%)
11	CLA	1	1121	-	46,54,73	2.87	19 (41%)	53,90,113	2.89	20 (37%)
15	LHG	b	5004	-	48,48,48	0.94	2 (4%)	51,54,54	1.05	3 (5%)
11	CLA	b	1213	-	65,73,73	2.38	20 (30%)	76,113,113	2.60	22 (28%)
15	LHG	2	5004	11	48,48,48	0.95	2 (4%)	51,54,54	1.05	3 (5%)
11	CLA	b	1215	-	65,73,73	2.39	19 (29%)	76,113,113	2.65	26 (34%)
11	CLA	B	1220	-	46,54,73	2.86	19 (41%)	53,90,113	2.79	18 (33%)
11	CLA	B	1226	-	65,73,73	2.34	18 (27%)	76,113,113	2.63	24 (31%)
11	CLA	B	1228	-	50,58,73	2.72	19 (38%)	58,95,113	2.87	21 (36%)
11	CLA	2	1229	-	65,73,73	2.36	20 (30%)	76,113,113	2.55	23 (30%)
14	BCR	B	4011	-	41,41,41	2.81	7 (17%)	56,56,56	6.71	27 (48%)
11	CLA	B	1208	-	45,53,73	2.74	18 (40%)	52,89,113	2.94	19 (36%)
11	CLA	A	1120	-	46,54,73	2.89	20 (43%)	53,90,113	2.87	20 (37%)
14	BCR	f	4020	-	41,41,41	2.79	6 (14%)	56,56,56	6.58	22 (39%)
14	BCR	1	4002	-	41,41,41	2.72	6 (14%)	56,56,56	6.93	23 (41%)
12	PQN	2	2002	-	34,34,34	1.64	2 (5%)	42,45,45	1.08	6 (14%)
14	BCR	2	4017	-	41,41,41	2.78	7 (17%)	56,56,56	6.54	29 (51%)
14	BCR	7	4021	-	41,41,41	2.78	6 (14%)	56,56,56	6.61	21 (37%)
11	CLA	B	1204	-	65,73,73	2.33	18 (27%)	76,113,113	2.56	23 (30%)
11	CLA	B	1225	-	65,73,73	2.37	19 (29%)	76,113,113	2.45	23 (30%)
11	CLA	0	1401	-	65,73,73	2.37	19 (29%)	76,113,113	2.66	24 (31%)
11	CLA	1	1136	-	46,54,73	2.85	19 (41%)	53,90,113	2.90	18 (33%)
14	BCR	B	4005	-	41,41,41	2.79	7 (17%)	56,56,56	6.53	25 (44%)
11	CLA	B	1217	-	47,55,73	2.74	19 (40%)	54,91,113	2.93	20 (37%)
11	CLA	A	1130	-	46,54,73	2.86	20 (43%)	53,90,113	2.83	18 (33%)
11	CLA	2	1221	-	54,62,73	2.59	20 (37%)	62,99,113	2.87	23 (37%)
11	CLA	A	1111	-	60,68,73	2.43	19 (31%)	70,107,113	2.67	23 (32%)
11	CLA	b	1202	-	65,73,73	2.36	19 (29%)	76,113,113	2.60	22 (28%)
11	CLA	B	1219	-	55,63,73	2.58	20 (36%)	64,101,113	2.71	24 (37%)
15	LHG	A	5001	-	48,48,48	0.93	2 (4%)	51,54,54	1.13	4 (7%)
11	CLA	8	1503	-	65,73,73	2.40	20 (30%)	76,113,113	2.53	20 (26%)
11	CLA	B	1210	-	65,73,73	2.37	19 (29%)	76,113,113	2.59	25 (32%)
12	PQN	a	2001	-	34,34,34	1.63	2 (5%)	42,45,45	1.04	4 (9%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
11	CLA	A	1139	-	50,58,73	2.71	20 (40%)	58,95,113	2.86	21 (36%)
11	CLA	a	1108	-	45,53,73	2.75	18 (40%)	52,89,113	2.92	20 (38%)
11	CLA	a	1801	15	52,60,73	2.68	19 (36%)	60,97,113	2.85	22 (36%)
14	BCR	L	4019	-	41,41,41	2.69	6 (14%)	56,56,56	6.58	25 (44%)
11	CLA	b	1211	-	46,54,73	2.87	20 (43%)	53,90,113	2.86	20 (37%)
11	CLA	1	1128	-	65,73,73	2.36	19 (29%)	76,113,113	2.49	23 (30%)
11	CLA	a	1138	-	46,54,73	2.87	19 (41%)	53,90,113	2.92	22 (41%)
14	BCR	m	4021	-	41,41,41	2.84	6 (14%)	56,56,56	6.50	24 (42%)
11	CLA	A	1011	-	65,73,73	2.34	18 (27%)	76,113,113	2.59	25 (32%)
14	BCR	1	4008	-	41,41,41	2.72	6 (14%)	56,56,56	6.79	28 (50%)
14	BCR	A	4003	-	41,41,41	2.85	6 (14%)	56,56,56	6.29	24 (42%)
11	CLA	b	1205	-	55,63,73	2.55	19 (34%)	64,101,113	2.76	21 (32%)
11	CLA	B	1229	-	65,73,73	2.36	19 (29%)	76,113,113	2.56	24 (31%)
11	CLA	b	1234	-	60,68,73	2.47	19 (31%)	70,107,113	2.67	23 (32%)
13	SF4	3	3002	3	0,12,12	-	-	-	-	-
11	CLA	a	1103	-	65,73,73	2.40	20 (30%)	76,113,113	2.54	23 (30%)
11	CLA	b	1013	-	65,73,73	2.38	19 (29%)	76,113,113	2.56	24 (31%)
11	CLA	1	1126	-	65,73,73	2.38	20 (30%)	76,113,113	2.60	26 (34%)
16	LMG	b	5002	-	55,55,55	0.88	2 (3%)	63,63,63	1.04	5 (7%)
11	CLA	1	1110	-	54,62,73	2.61	19 (35%)	62,99,113	2.83	23 (37%)
16	LMG	2	5002	-	55,55,55	0.91	2 (3%)	63,63,63	1.06	4 (6%)
11	CLA	b	1222	-	56,64,73	2.55	20 (35%)	65,102,113	2.88	25 (38%)
14	BCR	6	4013	-	41,41,41	2.69	6 (14%)	56,56,56	6.63	24 (42%)
11	CLA	A	1125	-	52,60,73	2.68	19 (36%)	60,97,113	2.95	27 (45%)
11	CLA	1	1106	1	65,73,73	2.38	19 (29%)	76,113,113	2.54	24 (31%)
11	CLA	a	1114	-	46,54,73	2.87	19 (41%)	53,90,113	2.83	19 (35%)
15	LHG	a	5003	11	48,48,48	0.94	2 (4%)	51,54,54	1.03	3 (5%)
11	CLA	A	1116	-	54,62,73	2.61	20 (37%)	62,99,113	2.79	24 (38%)
14	BCR	B	4010	-	41,41,41	2.72	6 (14%)	56,56,56	6.41	26 (46%)
11	CLA	B	1227	-	45,53,73	2.72	18 (40%)	52,89,113	3.04	21 (40%)
11	CLA	a	1127	-	65,73,73	2.38	19 (29%)	76,113,113	2.56	27 (35%)
11	CLA	1	1120	-	46,54,73	2.89	20 (43%)	53,90,113	2.88	20 (37%)
11	CLA	b	1217	-	47,55,73	2.76	20 (42%)	54,91,113	2.93	19 (35%)
11	CLA	1	1127	-	65,73,73	2.38	19 (29%)	76,113,113	2.50	23 (30%)
11	CLA	a	1022	-	65,73,73	2.37	20 (30%)	76,113,113	2.45	20 (26%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
11	CLA	1	1237	-	55,63,73	2.54	19 (34%)	64,101,113	2.82	25 (39%)
15	LHG	B	5004	11	48,48,48	0.95	2 (4%)	51,54,54	1.12	4 (7%)
11	CLA	k	1402	-	50,58,73	2.72	19 (38%)	58,95,113	2.89	23 (39%)
11	CLA	1	1115	-	46,54,73	2.86	19 (41%)	53,90,113	2.88	19 (35%)
11	CLA	l	1502	-	46,54,73	2.85	19 (41%)	53,90,113	2.93	19 (35%)
11	CLA	b	1216	-	65,73,73	2.39	20 (30%)	76,113,113	2.56	28 (36%)
11	CLA	B	1234	-	60,68,73	2.44	19 (31%)	70,107,113	2.71	25 (35%)
11	CLA	a	1129	-	46,54,73	2.85	19 (41%)	53,90,113	2.93	19 (35%)
11	CLA	A	1109	11	65,73,73	2.39	19 (29%)	76,113,113	2.63	22 (28%)
11	CLA	2	1234	-	60,68,73	2.44	19 (31%)	70,107,113	2.66	23 (32%)
11	CLA	1	1107	-	65,73,73	2.38	19 (29%)	76,113,113	2.62	22 (28%)
15	LHG	1	5003	11	48,48,48	0.96	2 (4%)	51,54,54	1.03	3 (5%)
11	CLA	2	1209	-	45,53,73	2.75	18 (40%)	52,89,113	2.90	20 (38%)
11	CLA	A	1012	-	65,73,73	2.36	20 (30%)	76,113,113	2.65	25 (32%)
11	CLA	B	1201	-	54,62,73	2.59	19 (35%)	62,99,113	2.86	25 (40%)
14	BCR	A	4007	-	41,41,41	2.76	6 (14%)	56,56,56	6.80	22 (39%)
14	BCR	F	4013	-	41,41,41	2.78	6 (14%)	56,56,56	6.78	21 (37%)
11	CLA	2	1218	-	45,53,73	2.72	18 (40%)	52,89,113	2.94	20 (38%)
11	CLA	1	1103	-	65,73,73	2.37	20 (30%)	76,113,113	2.64	27 (35%)
11	CLA	b	1224	-	55,63,73	2.59	20 (36%)	64,101,113	2.85	23 (35%)
11	CLA	1	1111	-	60,68,73	2.41	18 (30%)	70,107,113	2.80	27 (38%)
11	CLA	2	1224	-	55,63,73	2.54	20 (36%)	64,101,113	2.96	24 (37%)
11	CLA	A	1128	-	65,73,73	2.34	18 (27%)	76,113,113	2.52	22 (28%)
12	PQN	b	2002	-	34,34,34	1.64	2 (5%)	42,45,45	1.11	4 (9%)
11	CLA	a	1139	-	50,58,73	2.73	20 (40%)	58,95,113	2.84	22 (37%)
14	BCR	F	4018	-	41,41,41	2.91	7 (17%)	56,56,56	6.56	24 (42%)
11	CLA	2	1214	-	59,67,73	2.49	19 (32%)	68,105,113	2.65	24 (35%)
11	CLA	B	1213	-	65,73,73	2.37	19 (29%)	76,113,113	2.59	23 (30%)
11	CLA	2	1212	-	45,53,73	2.74	18 (40%)	52,89,113	2.86	20 (38%)
11	CLA	a	1237	-	55,63,73	2.55	19 (34%)	64,101,113	2.79	22 (34%)
11	CLA	A	1121	-	46,54,73	2.88	20 (43%)	53,90,113	2.86	18 (33%)
14	BCR	B	4014	-	41,41,41	2.77	7 (17%)	56,56,56	6.29	25 (44%)
14	BCR	1	4001	-	41,41,41	2.73	6 (14%)	56,56,56	6.55	27 (48%)
11	CLA	B	1232	-	45,53,73	2.74	18 (40%)	52,89,113	2.89	19 (36%)
11	CLA	A	1136	-	46,54,73	2.85	19 (41%)	53,90,113	2.92	18 (33%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
11	CLA	b	1203	-	65,73,73	2.36	20 (30%)	76,113,113	2.56	22 (28%)
11	CLA	1	1105	-	48,56,73	2.75	19 (39%)	55,92,113	2.90	20 (36%)
11	CLA	1	1133	-	46,54,73	2.88	19 (41%)	53,90,113	2.84	20 (37%)
12	PQN	1	2001	-	34,34,34	1.66	2 (5%)	42,45,45	1.09	3 (7%)
11	CLA	a	1132	-	65,73,73	2.38	20 (30%)	76,113,113	2.54	22 (28%)
11	CLA	B	1221	-	54,62,73	2.58	19 (35%)	62,99,113	2.86	23 (37%)
11	CLA	2	1206	2	65,73,73	2.36	19 (29%)	76,113,113	2.51	23 (30%)
11	CLA	B	1224	-	55,63,73	2.54	19 (34%)	64,101,113	2.98	23 (35%)
11	CLA	2	1021	-	65,73,73	2.37	20 (30%)	76,113,113	2.62	27 (35%)
13	SF4	C	3002	3	0,12,12	-	-	-	-	-
11	CLA	1	1129	-	46,54,73	2.87	20 (43%)	53,90,113	2.91	19 (35%)
11	CLA	2	1239	-	46,54,73	2.90	19 (41%)	53,90,113	2.87	20 (37%)
14	BCR	2	4004	-	41,41,41	2.71	6 (14%)	56,56,56	6.47	29 (51%)
14	BCR	2	4009	-	41,41,41	2.72	6 (14%)	56,56,56	6.76	25 (44%)
14	BCR	a	4002	-	41,41,41	2.76	6 (14%)	56,56,56	6.59	26 (46%)
14	BCR	L	4022	-	41,41,41	2.69	6 (14%)	56,56,56	6.11	25 (44%)
11	CLA	2	1204	-	65,73,73	2.38	19 (29%)	76,113,113	2.50	22 (28%)
11	CLA	1	1114	-	46,54,73	2.88	19 (41%)	53,90,113	2.84	19 (35%)
11	CLA	A	1108	-	45,53,73	2.72	18 (40%)	52,89,113	2.92	21 (40%)
11	CLA	A	1127	-	65,73,73	2.35	20 (30%)	76,113,113	2.56	24 (31%)
13	SF4	c	3002	3	0,12,12	-	-	-	-	-
11	CLA	B	1236	-	47,55,73	2.70	19 (40%)	54,91,113	3.05	21 (38%)
11	CLA	1	1104	-	65,73,73	2.34	19 (29%)	76,113,113	2.64	23 (30%)
11	CLA	a	1115	-	46,54,73	2.87	19 (41%)	53,90,113	2.84	20 (37%)
11	CLA	B	1013	-	65,73,73	2.36	19 (29%)	76,113,113	2.58	25 (32%)
11	CLA	B	1223	-	65,73,73	2.38	20 (30%)	76,113,113	2.61	25 (32%)
11	CLA	a	1107	1	65,73,73	2.35	19 (29%)	76,113,113	2.72	27 (35%)
11	CLA	b	1206	2	65,73,73	2.36	19 (29%)	76,113,113	2.54	24 (31%)
11	CLA	A	1132	-	65,73,73	2.37	19 (29%)	76,113,113	2.62	21 (27%)
11	CLA	1	1137	-	65,73,73	2.37	19 (29%)	76,113,113	2.71	24 (31%)
11	CLA	a	1130	-	46,54,73	2.90	19 (41%)	53,90,113	2.82	20 (37%)
11	CLA	b	1236	-	47,55,73	2.75	20 (42%)	54,91,113	3.04	19 (35%)
11	CLA	a	1121	-	46,54,73	2.89	20 (43%)	53,90,113	2.89	19 (35%)
11	CLA	8	1502	-	46,54,73	2.84	19 (41%)	53,90,113	2.95	20 (37%)
11	CLA	2	1202	-	65,73,73	2.38	19 (29%)	76,113,113	2.62	23 (30%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
11	CLA	b	1226	-	65,73,73	2.35	20 (30%)	76,113,113	2.56	24 (31%)
11	CLA	B	1216	-	65,73,73	2.38	19 (29%)	76,113,113	2.53	22 (28%)
11	CLA	1	1132	-	65,73,73	2.35	19 (29%)	76,113,113	2.48	21 (27%)
11	CLA	b	1023	-	65,73,73	2.34	19 (29%)	76,113,113	2.60	26 (34%)
11	CLA	b	1231	-	45,53,73	2.73	19 (42%)	52,89,113	2.91	20 (38%)
11	CLA	A	1117	-	65,73,73	2.43	19 (29%)	76,113,113	2.52	23 (30%)
11	CLA	1	1102	-	65,73,73	2.39	20 (30%)	76,113,113	2.49	19 (25%)
16	LMG	B	5002	-	55,55,55	0.89	2 (3%)	63,63,63	1.07	4 (6%)
15	LHG	A	5003	11	48,48,48	0.95	2 (4%)	51,54,54	1.13	4 (7%)
11	CLA	a	1140	-	65,73,73	2.37	19 (29%)	76,113,113	2.58	23 (30%)
11	CLA	b	1238	-	65,73,73	2.36	19 (29%)	76,113,113	2.51	20 (26%)
11	CLA	A	1124	-	55,63,73	2.58	19 (34%)	64,101,113	2.77	24 (37%)
14	BCR	2	4006	-	41,41,41	2.72	6 (14%)	56,56,56	6.83	28 (50%)
13	SF4	1	3001	2,1	0,12,12	-	-	-	-	-
11	CLA	1	1112	-	45,53,73	2.74	18 (40%)	52,89,113	2.95	22 (42%)
11	CLA	1	1123	-	65,73,73	2.39	20 (30%)	76,113,113	2.58	23 (30%)
11	CLA	b	1220	-	46,54,73	2.91	20 (43%)	53,90,113	2.80	20 (37%)
11	CLA	A	1135	-	51,59,73	2.66	19 (37%)	59,96,113	2.88	24 (40%)
11	CLA	A	1115	-	46,54,73	2.89	20 (43%)	53,90,113	2.90	19 (35%)
11	CLA	1	1135	-	51,59,73	2.68	20 (39%)	59,96,113	2.94	23 (38%)
11	CLA	b	1208	-	45,53,73	2.76	18 (40%)	52,89,113	2.92	19 (36%)
11	CLA	a	1131	-	65,73,73	2.38	19 (29%)	76,113,113	2.53	25 (32%)
11	CLA	A	1103	-	65,73,73	2.36	18 (27%)	76,113,113	2.61	24 (31%)
11	CLA	B	1235	-	60,68,73	2.48	20 (33%)	70,107,113	2.69	20 (28%)
14	BCR	2	4010	-	41,41,41	2.84	6 (14%)	56,56,56	6.40	26 (46%)
11	CLA	a	1122	-	59,67,73	2.50	19 (32%)	68,105,113	2.76	23 (33%)
14	BCR	F	4020	-	41,41,41	2.79	6 (14%)	56,56,56	6.41	23 (41%)
11	CLA	A	1110	-	54,62,73	2.61	19 (35%)	62,99,113	2.84	23 (37%)
11	CLA	1	1109	-	65,73,73	2.37	19 (29%)	76,113,113	2.60	23 (30%)
11	CLA	2	1222	-	56,64,73	2.56	20 (35%)	65,102,113	2.79	24 (36%)
11	CLA	L	1502	-	46,54,73	2.84	18 (39%)	53,90,113	2.94	19 (35%)
11	CLA	A	1118	-	61,69,73	2.40	18 (29%)	71,108,113	2.68	21 (29%)
11	CLA	2	1225	-	65,73,73	2.38	19 (29%)	76,113,113	2.53	22 (28%)
11	CLA	8	1501	-	65,73,73	2.36	19 (29%)	76,113,113	2.64	25 (32%)
14	BCR	2	4014	-	41,41,41	2.80	6 (14%)	56,56,56	6.44	23 (41%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
11	CLA	1	1138	-	46,54,73	2.85	19 (41%)	53,90,113	2.86	19 (35%)
11	CLA	b	1207	-	65,73,73	2.35	19 (29%)	76,113,113	2.64	23 (30%)
11	CLA	a	1112	-	45,53,73	2.74	19 (42%)	52,89,113	2.89	20 (38%)
11	CLA	1	1117	-	65,73,73	2.38	19 (29%)	76,113,113	2.55	24 (31%)
14	BCR	6	4018	-	41,41,41	2.87	7 (17%)	56,56,56	6.30	26 (46%)
11	CLA	b	1212	-	45,53,73	2.72	19 (42%)	52,89,113	2.96	17 (32%)
14	BCR	1	4003	-	41,41,41	2.78	6 (14%)	56,56,56	6.39	27 (48%)
11	CLA	a	1134	-	46,54,73	2.87	19 (41%)	53,90,113	2.91	21 (39%)
11	CLA	B	1212	-	45,53,73	2.74	19 (42%)	52,89,113	2.88	18 (34%)
11	CLA	a	1133	-	46,54,73	2.86	19 (41%)	53,90,113	2.90	19 (35%)
11	CLA	2	1223	-	65,73,73	2.38	20 (30%)	76,113,113	2.58	25 (32%)
14	BCR	a	4001	-	41,41,41	2.74	6 (14%)	56,56,56	6.52	27 (48%)
11	CLA	A	1237	-	55,63,73	2.56	19 (34%)	64,101,113	2.79	22 (34%)
11	CLA	b	1219	-	55,63,73	2.61	19 (34%)	64,101,113	2.76	23 (35%)
11	CLA	1	1131	-	65,73,73	2.36	19 (29%)	76,113,113	2.57	24 (31%)
11	CLA	a	1011	-	65,73,73	2.40	20 (30%)	76,113,113	2.59	23 (30%)
11	CLA	B	1206	2	65,73,73	2.34	19 (29%)	76,113,113	2.51	23 (30%)
11	CLA	1	1119	-	65,73,73	2.36	19 (29%)	76,113,113	2.60	24 (31%)
11	CLA	2	1238	-	65,73,73	2.38	20 (30%)	76,113,113	2.51	22 (28%)
11	CLA	1	1130	-	46,54,73	2.89	20 (43%)	53,90,113	2.80	18 (33%)
11	CLA	b	1229	-	65,73,73	2.37	20 (30%)	76,113,113	2.56	24 (31%)
14	BCR	f	4013	-	41,41,41	2.76	6 (14%)	56,56,56	6.62	23 (41%)
11	CLA	b	1210	-	65,73,73	2.38	20 (30%)	76,113,113	2.58	27 (35%)
11	CLA	a	1137	-	65,73,73	2.38	19 (29%)	76,113,113	2.70	25 (32%)
11	CLA	a	1102	11	65,73,73	2.37	20 (30%)	76,113,113	2.55	21 (27%)
11	CLA	a	1106	1	65,73,73	2.38	20 (30%)	76,113,113	2.54	23 (30%)
11	CLA	b	1227	-	45,53,73	2.74	19 (42%)	52,89,113	3.00	20 (38%)
11	CLA	A	1102	11	65,73,73	2.39	20 (30%)	76,113,113	2.56	25 (32%)
11	CLA	b	1214	-	59,67,73	2.47	20 (33%)	68,105,113	2.72	26 (38%)
11	CLA	a	1105	-	48,56,73	2.78	19 (39%)	55,92,113	2.94	21 (38%)
14	BCR	8	4019	-	41,41,41	2.75	6 (14%)	56,56,56	6.65	24 (42%)
14	BCR	b	4017	-	41,41,41	2.81	7 (17%)	56,56,56	6.66	28 (50%)
11	CLA	b	1230	-	58,66,73	2.55	20 (34%)	67,104,113	2.77	25 (37%)
11	CLA	b	1239	-	46,54,73	2.87	19 (41%)	53,90,113	2.91	21 (39%)
14	BCR	A	4002	-	41,41,41	2.74	6 (14%)	56,56,56	6.31	24 (42%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
11	CLA	1	1134	-	46,54,73	2.88	19 (41%)	53,90,113	2.91	20 (37%)
11	CLA	B	1239	-	46,54,73	2.86	20 (43%)	53,90,113	2.89	18 (33%)
11	CLA	2	1203	-	65,73,73	2.34	19 (29%)	76,113,113	2.60	25 (32%)
13	SF4	C	3003	3	0,12,12	-	-	-	-	-
11	CLA	2	1205	-	55,63,73	2.52	18 (32%)	64,101,113	2.79	20 (31%)
11	CLA	B	1215	-	65,73,73	2.36	19 (29%)	76,113,113	2.69	24 (31%)
11	CLA	b	1228	-	50,58,73	2.71	19 (38%)	58,95,113	2.88	21 (36%)
11	CLA	A	1133	-	46,54,73	2.85	19 (41%)	53,90,113	2.89	21 (39%)
11	CLA	2	1216	-	65,73,73	2.39	20 (30%)	76,113,113	2.54	23 (30%)
11	CLA	B	1231	-	45,53,73	2.75	18 (40%)	52,89,113	2.92	22 (42%)
14	BCR	a	4007	-	41,41,41	2.72	6 (14%)	56,56,56	6.74	25 (44%)
11	CLA	2	1201	-	54,62,73	2.62	19 (35%)	62,99,113	2.77	22 (35%)
11	CLA	2	1207	-	65,73,73	2.34	19 (29%)	76,113,113	2.64	25 (32%)
11	CLA	a	1135	-	51,59,73	2.68	19 (37%)	59,96,113	2.89	21 (35%)
13	SF4	c	3003	3	0,12,12	-	-	-	-	-
11	CLA	l	1503	-	65,73,73	2.36	20 (30%)	76,113,113	2.53	20 (26%)
12	PQN	B	2002	-	34,34,34	1.64	2 (5%)	42,45,45	1.13	5 (11%)
11	CLA	B	1023	-	65,73,73	2.32	19 (29%)	76,113,113	2.61	26 (34%)
11	CLA	A	1801	15	52,60,73	2.70	19 (36%)	60,97,113	2.86	23 (38%)
11	CLA	a	1136	-	46,54,73	2.85	19 (41%)	53,90,113	2.93	18 (33%)
14	BCR	l	4019	-	41,41,41	2.75	6 (14%)	56,56,56	6.70	23 (41%)
11	CLA	A	1107	1	65,73,73	2.33	18 (27%)	76,113,113	2.65	25 (32%)
11	CLA	B	1238	-	65,73,73	2.34	18 (27%)	76,113,113	2.54	21 (27%)
11	CLA	B	1209	-	45,53,73	2.75	18 (40%)	52,89,113	2.91	21 (40%)
11	CLA	k	1401	-	65,73,73	2.37	19 (29%)	76,113,113	2.65	25 (32%)
11	CLA	B	1205	-	55,63,73	2.51	17 (30%)	64,101,113	2.89	21 (32%)
11	CLA	2	1013	-	65,73,73	2.37	19 (29%)	76,113,113	2.60	25 (32%)
11	CLA	a	1117	-	65,73,73	2.38	19 (29%)	76,113,113	2.56	23 (30%)
11	CLA	A	1104	-	65,73,73	2.31	18 (27%)	76,113,113	2.74	27 (35%)
11	CLA	2	1215	-	65,73,73	2.38	19 (29%)	76,113,113	2.70	26 (34%)
11	CLA	a	1012	-	65,73,73	2.38	20 (30%)	76,113,113	2.55	21 (27%)
11	CLA	1	1116	-	54,62,73	2.61	20 (37%)	62,99,113	2.81	24 (38%)
11	CLA	a	1123	-	65,73,73	2.38	20 (30%)	76,113,113	2.56	24 (31%)
11	CLA	1	1122	-	59,67,73	2.50	20 (33%)	68,105,113	2.72	23 (33%)
11	CLA	1	1012	-	65,73,73	2.38	18 (27%)	76,113,113	2.65	25 (32%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
11	CLA	A	1112	-	45,53,73	2.74	20 (44%)	52,89,113	2.99	20 (38%)
11	CLA	B	1202	-	65,73,73	2.40	20 (30%)	76,113,113	2.60	22 (28%)
11	CLA	a	1113	-	45,53,73	2.74	19 (42%)	52,89,113	2.89	20 (38%)
11	CLA	a	1128	-	65,73,73	2.38	19 (29%)	76,113,113	2.55	24 (31%)
11	CLA	b	1209	-	45,53,73	2.76	18 (40%)	52,89,113	2.91	20 (38%)
11	CLA	A	1131	-	65,73,73	2.39	19 (29%)	76,113,113	2.53	25 (32%)
11	CLA	0	1402	-	50,58,73	2.73	20 (40%)	58,95,113	2.90	19 (32%)
13	SF4	a	3001	2,1	0,12,12	-	-	-	-	-
14	BCR	a	4008	-	41,41,41	2.74	7 (17%)	56,56,56	6.57	29 (51%)
11	CLA	2	1220	-	46,54,73	2.87	19 (41%)	53,90,113	2.88	19 (35%)
11	CLA	A	1022	-	65,73,73	2.35	19 (29%)	76,113,113	2.50	22 (28%)
14	BCR	l	4022	-	41,41,41	2.74	6 (14%)	56,56,56	6.41	26 (46%)
14	BCR	B	4004	-	41,41,41	2.80	6 (14%)	56,56,56	6.56	27 (48%)
13	SF4	A	3001	2,1	0,12,12	-	-	-	-	-
15	LHG	a	5001	-	48,48,48	0.96	2 (4%)	51,54,54	1.06	4 (7%)
11	CLA	2	1228	-	50,58,73	2.71	20 (40%)	58,95,113	2.88	22 (37%)
14	BCR	1	4007	-	41,41,41	2.71	6 (14%)	56,56,56	6.67	26 (46%)
11	CLA	a	1120	-	46,54,73	2.88	20 (43%)	53,90,113	2.96	20 (37%)
15	LHG	1	5001	-	48,48,48	0.95	2 (4%)	51,54,54	1.08	4 (7%)
11	CLA	2	1236	-	47,55,73	2.75	20 (42%)	54,91,113	2.99	19 (35%)
11	CLA	a	1126	-	65,73,73	2.38	19 (29%)	76,113,113	2.60	23 (30%)
11	CLA	1	1113	-	45,53,73	2.73	18 (40%)	52,89,113	2.91	19 (36%)
11	CLA	K	1402	-	50,58,73	2.69	19 (38%)	58,95,113	2.85	20 (34%)
11	CLA	a	1104	-	65,73,73	2.34	19 (29%)	76,113,113	2.60	25 (32%)
11	CLA	a	1110	-	54,62,73	2.61	20 (37%)	62,99,113	2.78	23 (37%)
13	SF4	3	3003	-	0,12,12	-	-	-	-	-
14	BCR	B	4006	-	41,41,41	2.74	6 (14%)	56,56,56	6.81	27 (48%)
11	CLA	A	1105	-	48,56,73	2.74	20 (41%)	55,92,113	2.89	21 (38%)
14	BCR	8	4022	-	41,41,41	2.79	6 (14%)	56,56,56	6.49	31 (55%)
11	CLA	A	1134	1	46,54,73	2.87	19 (41%)	53,90,113	2.90	21 (39%)
11	CLA	a	1116	-	54,62,73	2.62	19 (35%)	62,99,113	2.79	23 (37%)
11	CLA	b	1221	-	54,62,73	2.60	20 (37%)	62,99,113	2.95	24 (38%)
14	BCR	A	4001	-	41,41,41	2.78	6 (14%)	56,56,56	6.39	27 (48%)
11	CLA	B	1222	-	56,64,73	2.59	19 (33%)	65,102,113	2.91	26 (40%)
11	CLA	a	1119	-	65,73,73	2.36	19 (29%)	76,113,113	2.58	25 (32%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
11	CLA	B	1207	-	65,73,73	2.34	18 (27%)	76,113,113	2.68	22 (28%)
11	CLA	2	1211	-	46,54,73	2.84	18 (39%)	53,90,113	2.92	19 (35%)
11	CLA	A	1140	-	65,73,73	2.36	19 (29%)	76,113,113	2.61	22 (28%)
12	PQN	A	2001	-	34,34,34	1.65	2 (5%)	42,45,45	1.12	6 (14%)
11	CLA	b	1021	-	65,73,73	2.39	20 (30%)	76,113,113	2.65	30 (39%)
14	BCR	B	4017	-	41,41,41	2.77	6 (14%)	56,56,56	6.60	31 (55%)
11	CLA	1	1101	-	65,73,73	2.36	19 (29%)	76,113,113	2.56	26 (34%)
11	CLA	2	1213	-	65,73,73	2.42	20 (30%)	76,113,113	2.69	24 (31%)
14	BCR	2	4005	-	41,41,41	2.73	6 (14%)	56,56,56	6.39	21 (37%)
11	CLA	A	1106	1	65,73,73	2.37	19 (29%)	76,113,113	2.52	21 (27%)
11	CLA	A	1137	-	65,73,73	2.38	20 (30%)	76,113,113	2.76	25 (32%)
11	CLA	a	1111	-	60,68,73	2.41	20 (33%)	70,107,113	2.75	25 (35%)
14	BCR	b	4004	-	41,41,41	2.73	6 (14%)	56,56,56	6.57	26 (46%)
14	BCR	a	4003	-	41,41,41	2.75	6 (14%)	56,56,56	6.20	26 (46%)
14	BCR	b	4009	-	41,41,41	2.65	6 (14%)	56,56,56	6.93	25 (44%)
14	BCR	B	4009	-	41,41,41	2.75	6 (14%)	56,56,56	6.71	22 (39%)
14	BCR	b	4006	-	41,41,41	2.76	6 (14%)	56,56,56	6.93	27 (48%)
14	BCR	b	4014	-	41,41,41	2.74	6 (14%)	56,56,56	6.49	24 (42%)
14	BCR	b	4011	-	41,41,41	2.75	6 (14%)	56,56,56	6.79	25 (44%)
11	CLA	b	1204	-	65,73,73	2.36	19 (29%)	76,113,113	2.50	20 (26%)
11	CLA	B	1203	-	65,73,73	2.35	18 (27%)	76,113,113	2.59	21 (27%)
14	BCR	2	4011	-	41,41,41	2.80	6 (14%)	56,56,56	6.77	26 (46%)
11	CLA	A	1129	-	46,54,73	2.85	19 (41%)	53,90,113	2.84	19 (35%)
11	CLA	2	1226	-	65,73,73	2.36	18 (27%)	76,113,113	2.64	23 (30%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
11	CLA	L	1503	-	1/1/15/20	13/37/115/115	-
11	CLA	b	1223	-	1/1/15/20	19/37/115/115	-
11	CLA	a	1125	-	1/1/12/20	8/22/100/115	-
11	CLA	2	1023	-	1/1/15/20	15/37/115/115	-
11	CLA	1	1125	-	1/1/12/20	9/22/100/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
11	CLA	B	1214	-	1/1/13/20	13/30/108/115	-
11	CLA	b	1240	-	1/1/11/20	9/13/91/115	-
11	CLA	1	1139	-	1/1/12/20	10/19/97/115	-
11	CLA	L	1501	7	1/1/15/20	13/37/115/115	-
11	CLA	A	1119	-	1/1/15/20	17/37/115/115	-
11	CLA	2	1240	15	1/1/11/20	5/13/91/115	-
11	CLA	2	1217	-	1/1/11/20	14/16/94/115	-
11	CLA	1	1108	-	1/1/11/20	5/13/91/115	-
11	CLA	b	1225	-	1/1/15/20	14/37/115/115	-
11	CLA	A	1113	-	1/1/11/20	7/13/91/115	-
11	CLA	1	1801	15	1/1/12/20	13/22/100/115	-
11	CLA	A	1138	-	1/1/11/20	2/15/93/115	-
11	CLA	K	1401	-	1/1/15/20	19/37/115/115	-
14	BCR	b	4005	-	-	13/29/63/63	0/2/2/2
14	BCR	f	4018	-	-	6/29/63/63	0/2/2/2
11	CLA	a	1101	-	1/1/15/20	17/37/115/115	-
11	CLA	2	1219	-	1/1/13/20	12/25/103/115	-
11	CLA	2	1231	-	1/1/11/20	5/13/91/115	-
11	CLA	B	1230	-	-	8/29/107/115	-
11	CLA	b	1218	-	1/1/11/20	5/13/91/115	-
14	BCR	M	4021	-	-	8/29/63/63	0/2/2/2
11	CLA	2	1210	-	1/1/15/20	15/37/115/115	-
11	CLA	2	1227	-	-	8/13/91/115	-
11	CLA	l	1501	7	-	16/37/115/115	-
11	CLA	2	1235	-	1/1/14/20	17/31/109/115	-
11	CLA	a	1124	-	1/1/13/20	8/25/103/115	-
11	CLA	b	1201	-	1/1/12/20	9/24/102/115	-
11	CLA	a	1118	-	1/1/14/20	10/33/111/115	-
11	CLA	A	1122	-	1/1/13/20	8/30/108/115	-
11	CLA	B	1240	15	1/1/11/20	8/13/91/115	-
11	CLA	a	1109	11	-	19/37/115/115	-
14	BCR	A	4008	-	-	11/29/63/63	0/2/2/2
11	CLA	A	1114	-	1/1/11/20	7/15/93/115	-
11	CLA	1	1022	-	1/1/15/20	17/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
11	CLA	2	1230	-	-	7/29/107/115	-
11	CLA	A	1123	-	1/1/15/20	17/37/115/115	-
11	CLA	A	1101	-	1/1/15/20	19/37/115/115	-
11	CLA	B	1218	-	1/1/11/20	5/13/91/115	-
11	CLA	A	1126	-	1/1/15/20	12/37/115/115	-
14	BCR	6	4020	-	-	15/29/63/63	0/2/2/2
11	CLA	1	1118	-	1/1/14/20	17/33/111/115	-
11	CLA	1	1011	-	-	15/37/115/115	-
11	CLA	b	1235	-	1/1/14/20	16/31/109/115	-
11	CLA	2	1208	-	1/1/11/20	3/13/91/115	-
11	CLA	1	1140	-	1/1/15/20	15/37/115/115	-
14	BCR	b	4010	-	-	11/29/63/63	0/2/2/2
11	CLA	b	1232	-	1/1/11/20	4/13/91/115	-
11	CLA	B	1021	-	1/1/15/20	23/37/115/115	-
11	CLA	1	1124	-	1/1/13/20	12/25/103/115	-
11	CLA	2	1232	-	1/1/11/20	5/13/91/115	-
11	CLA	B	1211	-	1/1/11/20	6/15/93/115	-
11	CLA	1	1121	-	1/1/11/20	6/15/93/115	-
15	LHG	b	5004	-	-	26/53/53/53	-
11	CLA	b	1213	-	1/1/15/20	13/37/115/115	-
15	LHG	2	5004	11	-	28/53/53/53	-
11	CLA	b	1215	-	1/1/15/20	14/37/115/115	-
11	CLA	B	1220	-	-	8/15/93/115	-
11	CLA	B	1226	-	1/1/15/20	13/37/115/115	-
11	CLA	B	1228	-	1/1/12/20	7/19/97/115	-
11	CLA	2	1229	-	1/1/15/20	17/37/115/115	-
14	BCR	B	4011	-	-	13/29/63/63	0/2/2/2
11	CLA	B	1208	-	1/1/11/20	5/13/91/115	-
11	CLA	A	1120	-	1/1/11/20	6/15/93/115	-
14	BCR	f	4020	-	-	15/29/63/63	0/2/2/2
14	BCR	1	4002	-	-	13/29/63/63	0/2/2/2
12	PQN	2	2002	-	-	8/23/43/43	0/2/2/2
14	BCR	2	4017	-	-	6/29/63/63	0/2/2/2
14	BCR	7	4021	-	-	13/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
11	CLA	B	1204	-	1/1/15/20	14/37/115/115	-
11	CLA	B	1225	-	1/1/15/20	11/37/115/115	-
11	CLA	0	1401	-	1/1/15/20	19/37/115/115	-
11	CLA	1	1136	-	1/1/11/20	10/15/93/115	-
14	BCR	B	4005	-	-	8/29/63/63	0/2/2/2
11	CLA	B	1217	-	1/1/11/20	12/16/94/115	-
11	CLA	A	1130	-	1/1/11/20	5/15/93/115	-
11	CLA	2	1221	-	1/1/12/20	6/24/102/115	-
11	CLA	A	1111	-	1/1/14/20	16/31/109/115	-
11	CLA	b	1202	-	1/1/15/20	18/37/115/115	-
11	CLA	B	1219	-	1/1/13/20	10/25/103/115	-
15	LHG	A	5001	-	-	31/53/53/53	-
11	CLA	8	1503	-	1/1/15/20	12/37/115/115	-
11	CLA	B	1210	-	1/1/15/20	27/37/115/115	-
12	PQN	a	2001	-	-	6/23/43/43	0/2/2/2
11	CLA	A	1139	-	1/1/12/20	7/19/97/115	-
11	CLA	a	1108	-	1/1/11/20	4/13/91/115	-
11	CLA	a	1801	15	1/1/12/20	11/22/100/115	-
14	BCR	L	4019	-	-	13/29/63/63	0/2/2/2
11	CLA	b	1211	-	1/1/11/20	4/15/93/115	-
11	CLA	1	1128	-	1/1/15/20	13/37/115/115	-
11	CLA	a	1138	-	1/1/11/20	8/15/93/115	-
14	BCR	m	4021	-	-	11/29/63/63	0/2/2/2
11	CLA	A	1011	-	-	17/37/115/115	-
14	BCR	1	4008	-	-	11/29/63/63	0/2/2/2
14	BCR	A	4003	-	-	13/29/63/63	0/2/2/2
11	CLA	b	1205	-	1/1/13/20	8/25/103/115	-
11	CLA	B	1229	-	1/1/15/20	24/37/115/115	-
11	CLA	b	1234	-	1/1/14/20	16/31/109/115	-
13	SF4	3	3002	3	-	-	0/6/5/5
11	CLA	a	1103	-	1/1/15/20	19/37/115/115	-
11	CLA	b	1013	-	-	10/37/115/115	-
11	CLA	1	1126	-	1/1/15/20	20/37/115/115	-
16	LMG	b	5002	-	-	27/50/70/70	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
11	CLA	1	1110	-	1/1/12/20	14/24/102/115	-
16	LMG	2	5002	-	-	30/50/70/70	0/1/1/1
11	CLA	b	1222	-	1/1/13/20	12/27/105/115	-
14	BCR	6	4013	-	-	16/29/63/63	0/2/2/2
11	CLA	A	1125	-	1/1/12/20	9/22/100/115	-
11	CLA	1	1106	1	1/1/15/20	23/37/115/115	-
11	CLA	a	1114	-	1/1/11/20	6/15/93/115	-
15	LHG	a	5003	11	-	25/53/53/53	-
11	CLA	A	1116	-	1/1/12/20	8/24/102/115	-
14	BCR	B	4010	-	-	13/29/63/63	0/2/2/2
11	CLA	B	1227	-	1/1/11/20	4/13/91/115	-
11	CLA	a	1127	-	1/1/15/20	14/37/115/115	-
11	CLA	1	1120	-	1/1/11/20	9/15/93/115	-
11	CLA	b	1217	-	1/1/11/20	7/16/94/115	-
11	CLA	1	1127	-	1/1/15/20	15/37/115/115	-
11	CLA	a	1022	-	1/1/15/20	12/37/115/115	-
11	CLA	1	1237	-	1/1/13/20	9/25/103/115	-
15	LHG	B	5004	11	-	25/53/53/53	-
11	CLA	k	1402	-	1/1/12/20	7/19/97/115	-
11	CLA	1	1115	-	1/1/11/20	4/15/93/115	-
11	CLA	l	1502	-	1/1/11/20	3/15/93/115	-
11	CLA	b	1216	-	1/1/15/20	15/37/115/115	-
11	CLA	B	1234	-	1/1/14/20	14/31/109/115	-
11	CLA	a	1129	-	1/1/11/20	7/15/93/115	-
11	CLA	A	1109	11	-	13/37/115/115	-
11	CLA	2	1234	-	1/1/14/20	18/31/109/115	-
11	CLA	1	1107	-	1/1/15/20	14/37/115/115	-
15	LHG	1	5003	11	-	32/53/53/53	-
11	CLA	2	1209	-	1/1/11/20	4/13/91/115	-
11	CLA	A	1012	-	1/1/15/20	15/37/115/115	-
11	CLA	B	1201	-	1/1/12/20	8/24/102/115	-
14	BCR	A	4007	-	-	13/29/63/63	0/2/2/2
14	BCR	F	4013	-	-	15/29/63/63	0/2/2/2
11	CLA	2	1218	-	1/1/11/20	4/13/91/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
11	CLA	1	1103	-	1/1/15/20	21/37/115/115	-
11	CLA	b	1224	-	1/1/13/20	12/25/103/115	-
11	CLA	1	1111	-	1/1/14/20	18/31/109/115	-
11	CLA	2	1224	-	1/1/13/20	8/25/103/115	-
11	CLA	A	1128	-	1/1/15/20	12/37/115/115	-
12	PQN	b	2002	-	-	8/23/43/43	0/2/2/2
11	CLA	a	1139	-	1/1/12/20	7/19/97/115	-
14	BCR	F	4018	-	-	5/29/63/63	0/2/2/2
11	CLA	2	1214	-	1/1/13/20	11/30/108/115	-
11	CLA	B	1213	-	1/1/15/20	18/37/115/115	-
11	CLA	2	1212	-	1/1/11/20	3/13/91/115	-
11	CLA	a	1237	-	1/1/13/20	10/25/103/115	-
11	CLA	A	1121	-	1/1/11/20	5/15/93/115	-
14	BCR	B	4014	-	-	11/29/63/63	0/2/2/2
14	BCR	1	4001	-	-	11/29/63/63	0/2/2/2
11	CLA	B	1232	-	1/1/11/20	5/13/91/115	-
11	CLA	A	1136	-	1/1/11/20	6/15/93/115	-
11	CLA	b	1203	-	1/1/15/20	12/37/115/115	-
11	CLA	1	1105	-	1/1/11/20	5/17/95/115	-
11	CLA	1	1133	-	1/1/11/20	8/15/93/115	-
12	PQN	1	2001	-	-	7/23/43/43	0/2/2/2
11	CLA	a	1132	-	1/1/15/20	15/37/115/115	-
11	CLA	B	1221	-	1/1/12/20	9/24/102/115	-
11	CLA	2	1206	2	1/1/15/20	19/37/115/115	-
11	CLA	B	1224	-	1/1/13/20	11/25/103/115	-
11	CLA	2	1021	-	1/1/15/20	21/37/115/115	-
13	SF4	C	3002	3	-	-	0/6/5/5
11	CLA	1	1129	-	1/1/11/20	6/15/93/115	-
11	CLA	2	1239	-	1/1/11/20	12/15/93/115	-
14	BCR	2	4004	-	-	10/29/63/63	0/2/2/2
14	BCR	2	4009	-	-	15/29/63/63	0/2/2/2
14	BCR	a	4002	-	-	15/29/63/63	0/2/2/2
14	BCR	L	4022	-	-	12/29/63/63	0/2/2/2
11	CLA	2	1204	-	1/1/15/20	11/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
11	CLA	1	1114	-	1/1/11/20	10/15/93/115	-
11	CLA	A	1108	-	1/1/11/20	3/13/91/115	-
11	CLA	A	1127	-	1/1/15/20	13/37/115/115	-
13	SF4	c	3002	3	-	-	0/6/5/5
11	CLA	B	1236	-	1/1/11/20	6/16/94/115	-
11	CLA	1	1104	-	1/1/15/20	14/37/115/115	-
11	CLA	a	1115	-	-	6/15/93/115	-
11	CLA	B	1013	-	-	18/37/115/115	-
11	CLA	B	1223	-	1/1/15/20	9/37/115/115	-
11	CLA	a	1107	1	1/1/15/20	9/37/115/115	-
11	CLA	b	1206	2	1/1/15/20	16/37/115/115	-
11	CLA	A	1132	-	1/1/15/20	16/37/115/115	-
11	CLA	1	1137	-	1/1/15/20	18/37/115/115	-
11	CLA	a	1130	-	-	7/15/93/115	-
11	CLA	b	1236	-	1/1/11/20	7/16/94/115	-
11	CLA	a	1121	-	1/1/11/20	5/15/93/115	-
11	CLA	8	1502	-	1/1/11/20	4/15/93/115	-
11	CLA	2	1202	-	1/1/15/20	15/37/115/115	-
11	CLA	b	1226	-	1/1/15/20	13/37/115/115	-
11	CLA	B	1216	-	1/1/15/20	8/37/115/115	-
11	CLA	1	1132	-	1/1/15/20	11/37/115/115	-
11	CLA	b	1023	-	1/1/15/20	17/37/115/115	-
11	CLA	b	1231	-	1/1/11/20	6/13/91/115	-
11	CLA	A	1117	-	1/1/15/20	13/37/115/115	-
11	CLA	1	1102	-	1/1/15/20	15/37/115/115	-
16	LMG	B	5002	-	-	27/50/70/70	0/1/1/1
15	LHG	A	5003	11	-	31/53/53/53	-
11	CLA	a	1140	-	1/1/15/20	14/37/115/115	-
11	CLA	b	1238	-	1/1/15/20	12/37/115/115	-
11	CLA	A	1124	-	1/1/13/20	12/25/103/115	-
14	BCR	2	4006	-	-	13/29/63/63	0/2/2/2
13	SF4	1	3001	2,1	-	-	0/6/5/5
11	CLA	1	1112	-	1/1/11/20	3/13/91/115	-
11	CLA	1	1123	-	1/1/15/20	14/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
11	CLA	b	1220	-	1/1/11/20	8/15/93/115	-
11	CLA	A	1135	-	1/1/12/20	8/21/99/115	-
11	CLA	A	1115	-	1/1/11/20	7/15/93/115	-
11	CLA	1	1135	-	1/1/12/20	9/21/99/115	-
11	CLA	b	1208	-	1/1/11/20	4/13/91/115	-
11	CLA	a	1131	-	1/1/15/20	16/37/115/115	-
11	CLA	A	1103	-	1/1/15/20	17/37/115/115	-
11	CLA	B	1235	-	1/1/14/20	14/31/109/115	-
14	BCR	2	4010	-	-	11/29/63/63	0/2/2/2
11	CLA	a	1122	-	1/1/13/20	14/30/108/115	-
14	BCR	F	4020	-	-	12/29/63/63	0/2/2/2
11	CLA	A	1110	-	1/1/12/20	11/24/102/115	-
11	CLA	1	1109	-	-	15/37/115/115	-
11	CLA	2	1222	-	1/1/13/20	11/27/105/115	-
11	CLA	L	1502	-	1/1/11/20	5/15/93/115	-
11	CLA	A	1118	-	1/1/14/20	17/33/111/115	-
11	CLA	2	1225	-	1/1/15/20	10/37/115/115	-
11	CLA	8	1501	-	1/1/15/20	18/37/115/115	-
14	BCR	2	4014	-	-	14/29/63/63	0/2/2/2
11	CLA	1	1138	-	1/1/11/20	6/15/93/115	-
11	CLA	b	1207	-	1/1/15/20	16/37/115/115	-
11	CLA	a	1112	-	1/1/11/20	3/13/91/115	-
11	CLA	1	1117	-	1/1/15/20	16/37/115/115	-
14	BCR	6	4018	-	-	10/29/63/63	0/2/2/2
11	CLA	b	1212	-	1/1/11/20	5/13/91/115	-
14	BCR	1	4003	-	-	12/29/63/63	0/2/2/2
11	CLA	a	1134	-	1/1/11/20	8/15/93/115	-
11	CLA	B	1212	-	1/1/11/20	7/13/91/115	-
11	CLA	a	1133	-	1/1/11/20	4/15/93/115	-
11	CLA	2	1223	-	1/1/15/20	16/37/115/115	-
14	BCR	a	4001	-	-	10/29/63/63	0/2/2/2
11	CLA	A	1237	-	1/1/13/20	12/25/103/115	-
11	CLA	b	1219	-	1/1/13/20	8/25/103/115	-
11	CLA	1	1131	-	1/1/15/20	20/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
11	CLA	1	1119	-	1/1/15/20	18/37/115/115	-
11	CLA	B	1206	2	1/1/15/20	13/37/115/115	-
11	CLA	a	1011	-	-	11/37/115/115	-
11	CLA	2	1238	-	1/1/15/20	12/37/115/115	-
11	CLA	1	1130	-	-	5/15/93/115	-
11	CLA	b	1229	-	1/1/15/20	24/37/115/115	-
14	BCR	f	4013	-	-	17/29/63/63	0/2/2/2
11	CLA	b	1210	-	1/1/15/20	20/37/115/115	-
11	CLA	a	1137	-	1/1/15/20	12/37/115/115	-
11	CLA	a	1102	11	1/1/15/20	13/37/115/115	-
11	CLA	a	1106	1	1/1/15/20	19/37/115/115	-
11	CLA	b	1227	-	-	7/13/91/115	-
11	CLA	A	1102	11	1/1/15/20	19/37/115/115	-
11	CLA	b	1214	-	1/1/13/20	10/30/108/115	-
11	CLA	a	1105	-	1/1/11/20	8/17/95/115	-
14	BCR	8	4019	-	-	15/29/63/63	0/2/2/2
14	BCR	b	4017	-	-	6/29/63/63	0/2/2/2
11	CLA	b	1230	-	1/1/13/20	12/29/107/115	-
11	CLA	b	1239	-	1/1/11/20	7/15/93/115	-
14	BCR	A	4002	-	-	13/29/63/63	0/2/2/2
11	CLA	1	1134	-	1/1/11/20	7/15/93/115	-
11	CLA	B	1239	-	1/1/11/20	10/15/93/115	-
11	CLA	2	1203	-	1/1/15/20	17/37/115/115	-
13	SF4	C	3003	3	-	-	0/6/5/5
11	CLA	2	1205	-	1/1/13/20	7/25/103/115	-
11	CLA	B	1215	-	1/1/15/20	16/37/115/115	-
11	CLA	b	1228	-	1/1/12/20	6/19/97/115	-
11	CLA	A	1133	-	1/1/11/20	4/15/93/115	-
11	CLA	2	1216	-	1/1/15/20	17/37/115/115	-
11	CLA	B	1231	-	1/1/11/20	9/13/91/115	-
14	BCR	a	4007	-	-	11/29/63/63	0/2/2/2
11	CLA	2	1201	-	1/1/12/20	8/24/102/115	-
11	CLA	2	1207	-	-	13/37/115/115	-
11	CLA	a	1135	-	1/1/12/20	7/21/99/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
13	SF4	c	3003	3	-	-	0/6/5/5
11	CLA	l	1503	-	1/1/15/20	16/37/115/115	-
12	PQN	B	2002	-	-	8/23/43/43	0/2/2/2
11	CLA	B	1023	-	1/1/15/20	15/37/115/115	-
11	CLA	A	1801	15	1/1/12/20	14/22/100/115	-
11	CLA	a	1136	-	1/1/11/20	6/15/93/115	-
14	BCR	l	4019	-	-	17/29/63/63	0/2/2/2
11	CLA	A	1107	1	1/1/15/20	13/37/115/115	-
11	CLA	B	1238	-	1/1/15/20	13/37/115/115	-
11	CLA	B	1209	-	1/1/11/20	6/13/91/115	-
11	CLA	k	1401	-	1/1/15/20	19/37/115/115	-
11	CLA	B	1205	-	1/1/13/20	9/25/103/115	-
11	CLA	2	1013	-	-	14/37/115/115	-
11	CLA	a	1117	-	1/1/15/20	18/37/115/115	-
11	CLA	A	1104	-	1/1/15/20	21/37/115/115	-
11	CLA	2	1215	-	1/1/15/20	16/37/115/115	-
11	CLA	a	1012	-	1/1/15/20	20/37/115/115	-
11	CLA	l	1116	-	1/1/12/20	9/24/102/115	-
11	CLA	a	1123	-	1/1/15/20	15/37/115/115	-
11	CLA	l	1122	-	1/1/13/20	18/30/108/115	-
11	CLA	l	1012	-	1/1/15/20	18/37/115/115	-
11	CLA	A	1112	-	1/1/11/20	8/13/91/115	-
11	CLA	B	1202	-	1/1/15/20	19/37/115/115	-
11	CLA	a	1113	-	1/1/11/20	6/13/91/115	-
11	CLA	a	1128	-	1/1/15/20	11/37/115/115	-
11	CLA	b	1209	-	1/1/11/20	7/13/91/115	-
11	CLA	A	1131	-	1/1/15/20	15/37/115/115	-
11	CLA	0	1402	-	1/1/12/20	5/19/97/115	-
13	SF4	a	3001	2,1	-	-	0/6/5/5
14	BCR	a	4008	-	-	11/29/63/63	0/2/2/2
11	CLA	2	1220	-	1/1/11/20	7/15/93/115	-
11	CLA	A	1022	-	1/1/15/20	13/37/115/115	-
14	BCR	l	4022	-	-	11/29/63/63	0/2/2/2
14	BCR	B	4004	-	-	10/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
15	LHG	a	5001	-	-	30/53/53/53	-
13	SF4	A	3001	2,1	-	-	0/6/5/5
11	CLA	2	1228	-	1/1/12/20	3/19/97/115	-
14	BCR	1	4007	-	-	12/29/63/63	0/2/2/2
11	CLA	a	1120	-	1/1/11/20	8/15/93/115	-
15	LHG	1	5001	-	-	26/53/53/53	-
11	CLA	2	1236	-	1/1/11/20	8/16/94/115	-
11	CLA	a	1126	-	1/1/15/20	18/37/115/115	-
11	CLA	1	1113	-	1/1/11/20	5/13/91/115	-
11	CLA	K	1402	-	1/1/12/20	8/19/97/115	-
11	CLA	a	1104	-	1/1/15/20	15/37/115/115	-
11	CLA	a	1110	-	1/1/12/20	11/24/102/115	-
14	BCR	B	4006	-	-	15/29/63/63	0/2/2/2
13	SF4	3	3003	-	-	-	0/6/5/5
11	CLA	A	1105	-	1/1/11/20	5/17/95/115	-
14	BCR	8	4022	-	-	6/29/63/63	0/2/2/2
11	CLA	A	1134	1	1/1/11/20	9/15/93/115	-
11	CLA	a	1116	-	1/1/12/20	9/24/102/115	-
11	CLA	b	1221	-	1/1/12/20	7/24/102/115	-
14	BCR	A	4001	-	-	10/29/63/63	0/2/2/2
11	CLA	B	1222	-	1/1/13/20	15/27/105/115	-
11	CLA	a	1119	-	1/1/15/20	16/37/115/115	-
11	CLA	B	1207	-	1/1/15/20	12/37/115/115	-
11	CLA	2	1211	-	1/1/11/20	9/15/93/115	-
11	CLA	A	1140	-	1/1/15/20	18/37/115/115	-
12	PQN	A	2001	-	-	10/23/43/43	0/2/2/2
11	CLA	b	1021	-	1/1/15/20	25/37/115/115	-
14	BCR	B	4017	-	-	6/29/63/63	0/2/2/2
11	CLA	1	1101	-	1/1/15/20	19/37/115/115	-
11	CLA	2	1213	-	1/1/15/20	18/37/115/115	-
14	BCR	2	4005	-	-	9/29/63/63	0/2/2/2
11	CLA	A	1106	1	1/1/15/20	16/37/115/115	-
11	CLA	A	1137	-	1/1/15/20	14/37/115/115	-
11	CLA	a	1111	-	1/1/14/20	18/31/109/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
14	BCR	b	4009	-	-	14/29/63/63	0/2/2/2
14	BCR	a	4003	-	-	14/29/63/63	0/2/2/2
14	BCR	b	4004	-	-	11/29/63/63	0/2/2/2
14	BCR	B	4009	-	-	13/29/63/63	0/2/2/2
14	BCR	b	4006	-	-	15/29/63/63	0/2/2/2
14	BCR	b	4014	-	-	13/29/63/63	0/2/2/2
14	BCR	b	4011	-	-	15/29/63/63	0/2/2/2
11	CLA	b	1204	-	1/1/15/20	16/37/115/115	-
11	CLA	B	1203	-	-	15/37/115/115	-
14	BCR	2	4011	-	-	13/29/63/63	0/2/2/2
11	CLA	A	1129	-	1/1/11/20	6/15/93/115	-
11	CLA	2	1226	-	1/1/15/20	12/37/115/115	-

The worst 5 of 5620 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 7609 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 253 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
11	A	1801	CLA	ND
11	A	1237	CLA	ND
11	A	1022	CLA	ND
11	A	1101	CLA	ND
11	A	1102	CLA	ND

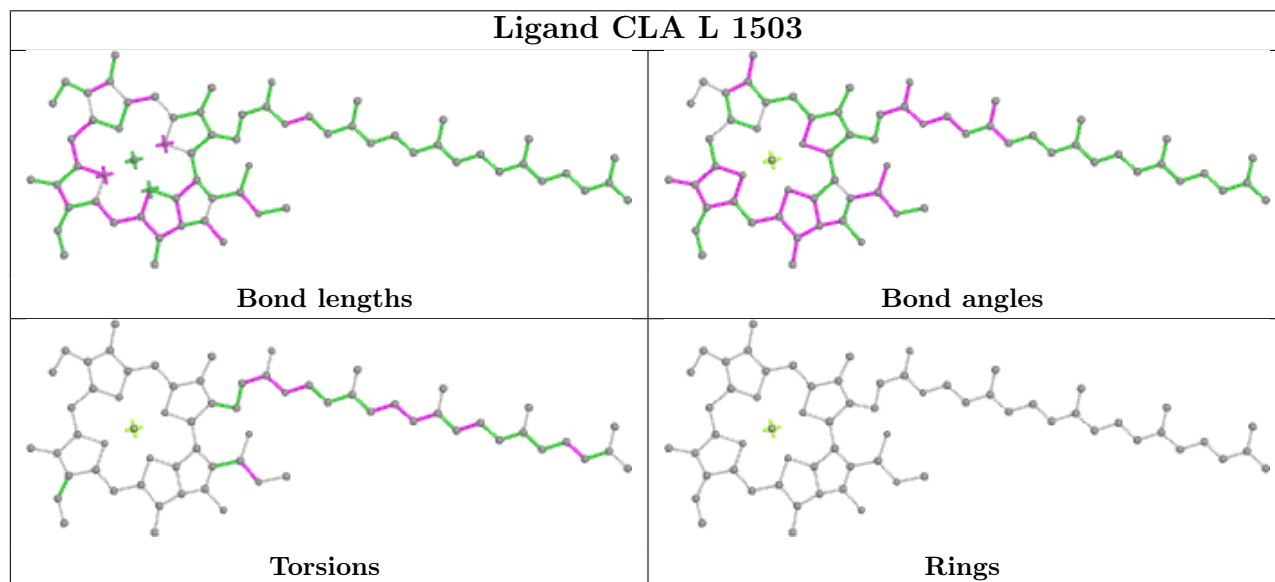
5 of 4209 torsion outliers are listed below:

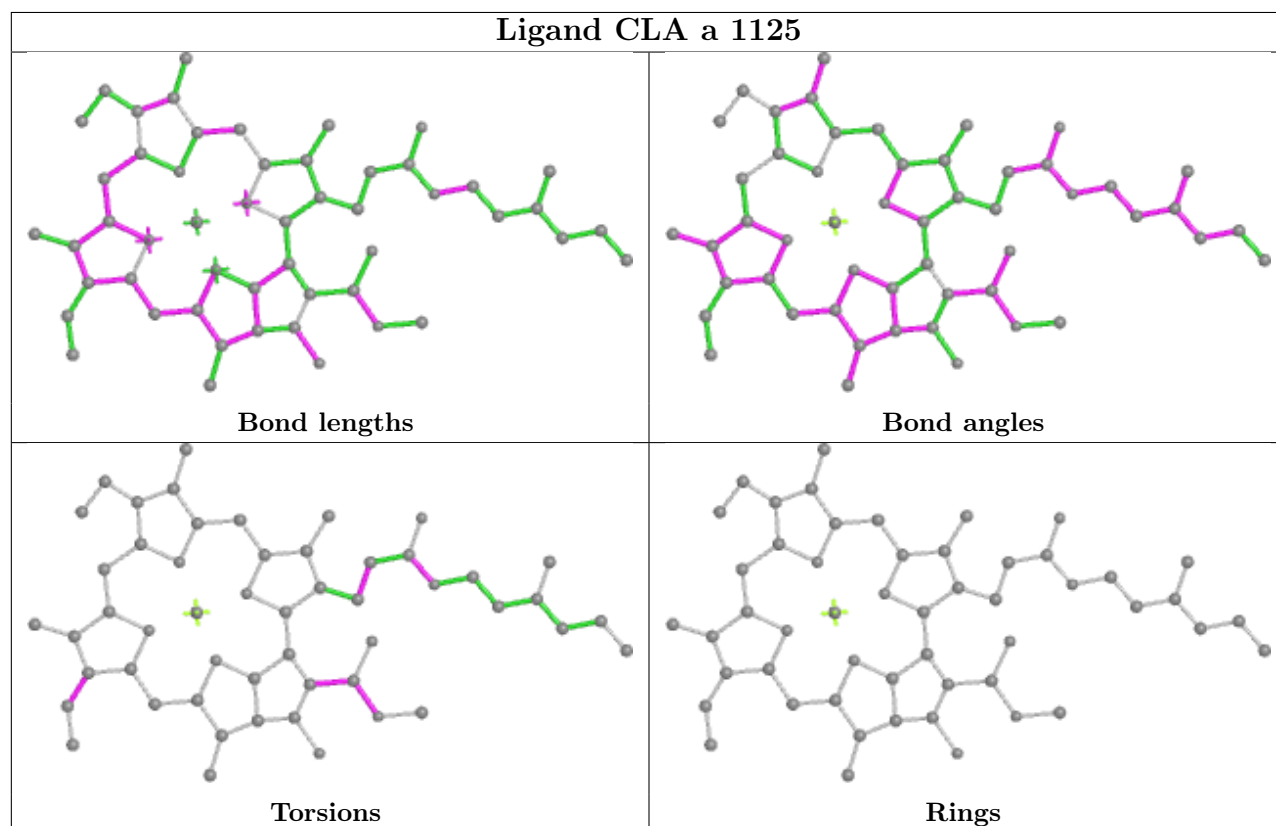
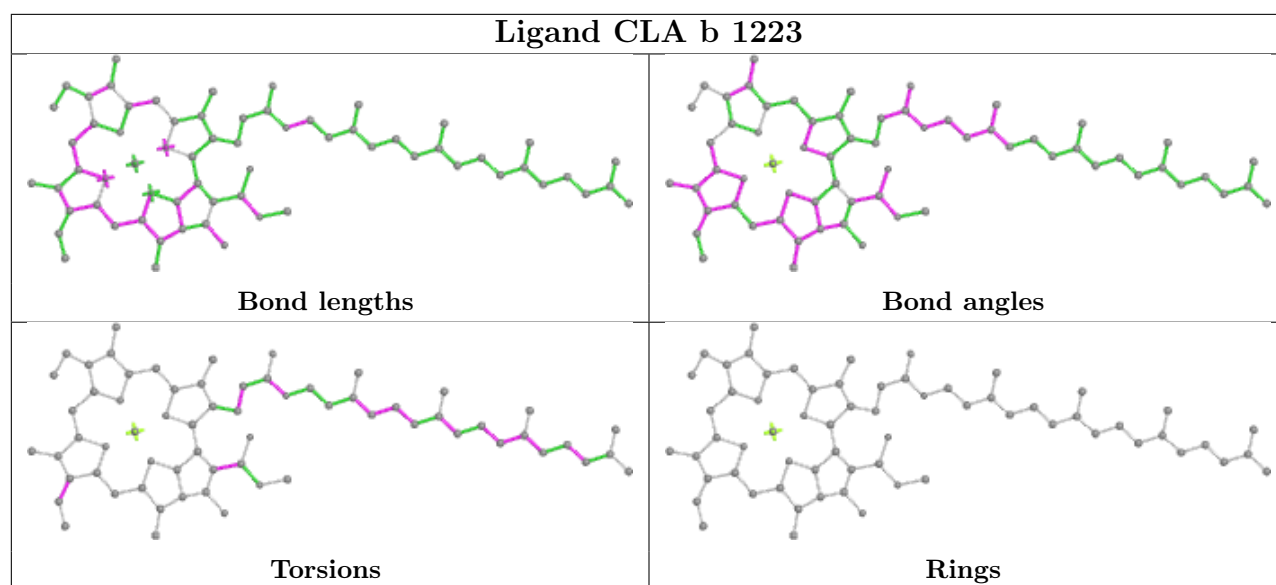
Mol	Chain	Res	Type	Atoms
11	A	1237	CLA	C1A-C2A-CAA-CBA
11	A	1237	CLA	CHA-CBD-CGD-O1D
11	A	1237	CLA	CHA-CBD-CGD-O2D
11	A	1237	CLA	O2A-C1-C2-C3
11	A	1022	CLA	C2-C1-O2A-CGA

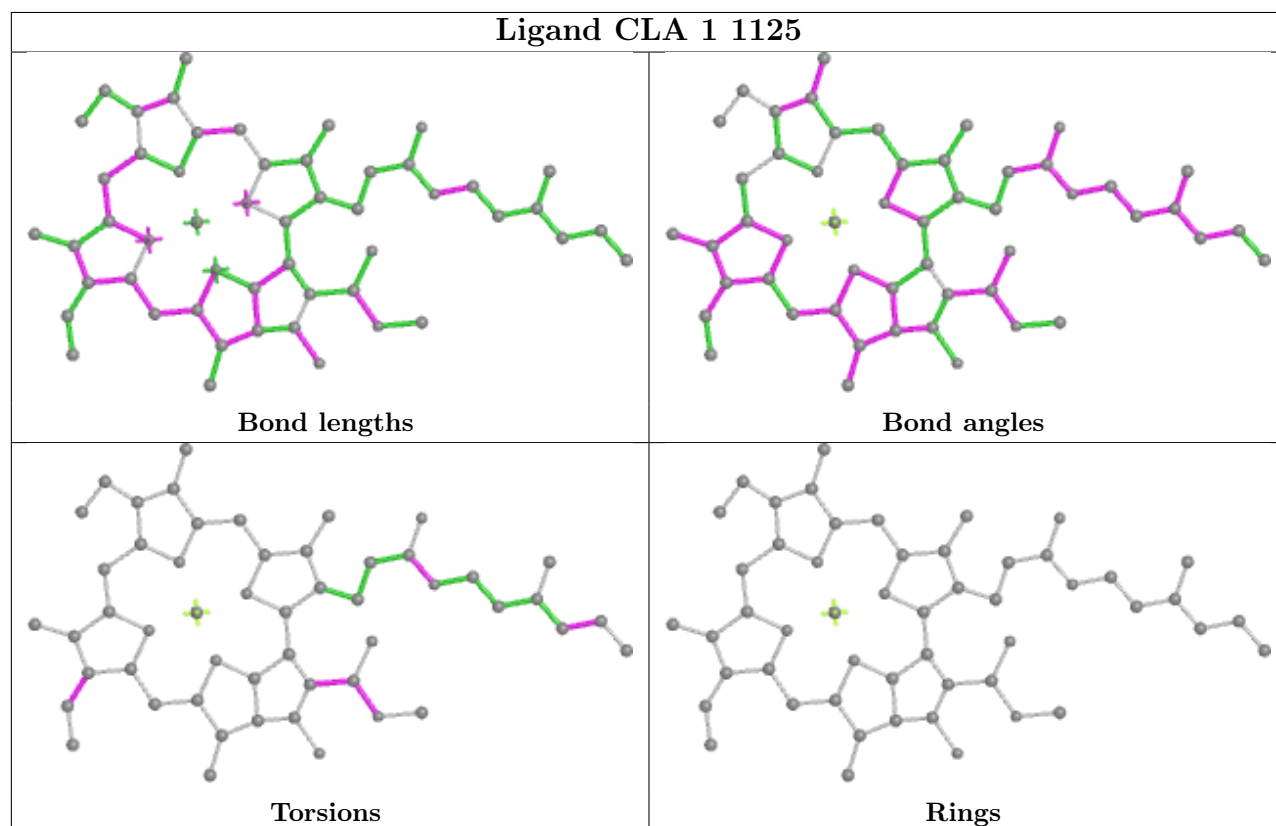
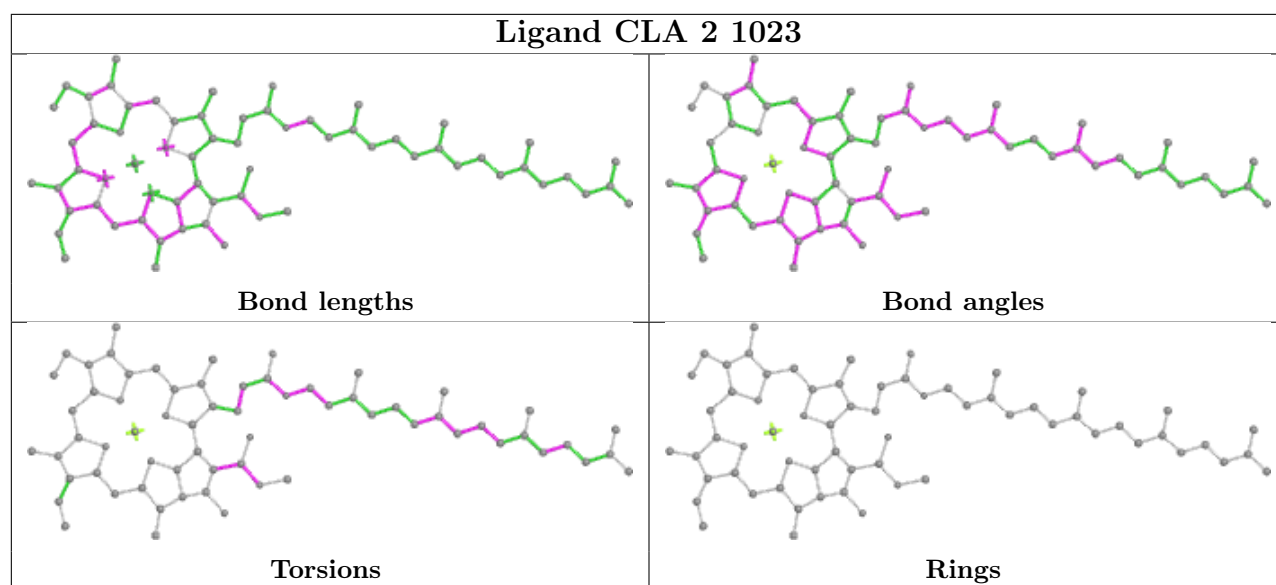
There are no ring outliers.

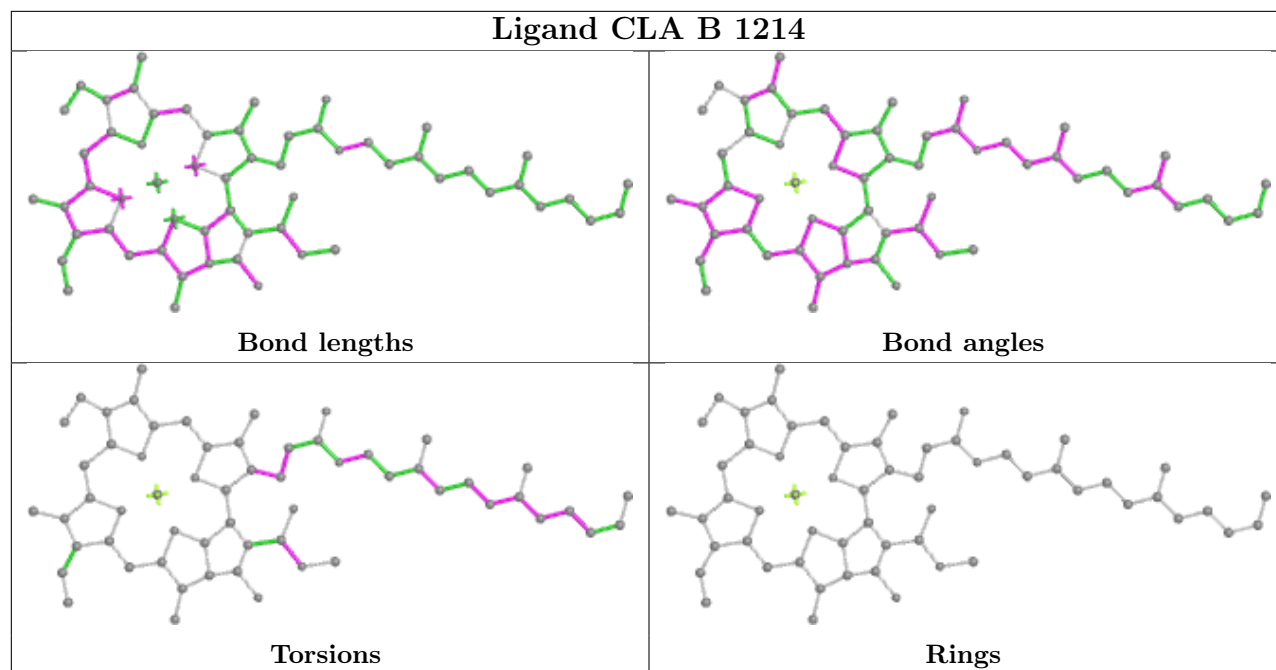
No monomer is involved in short contacts.

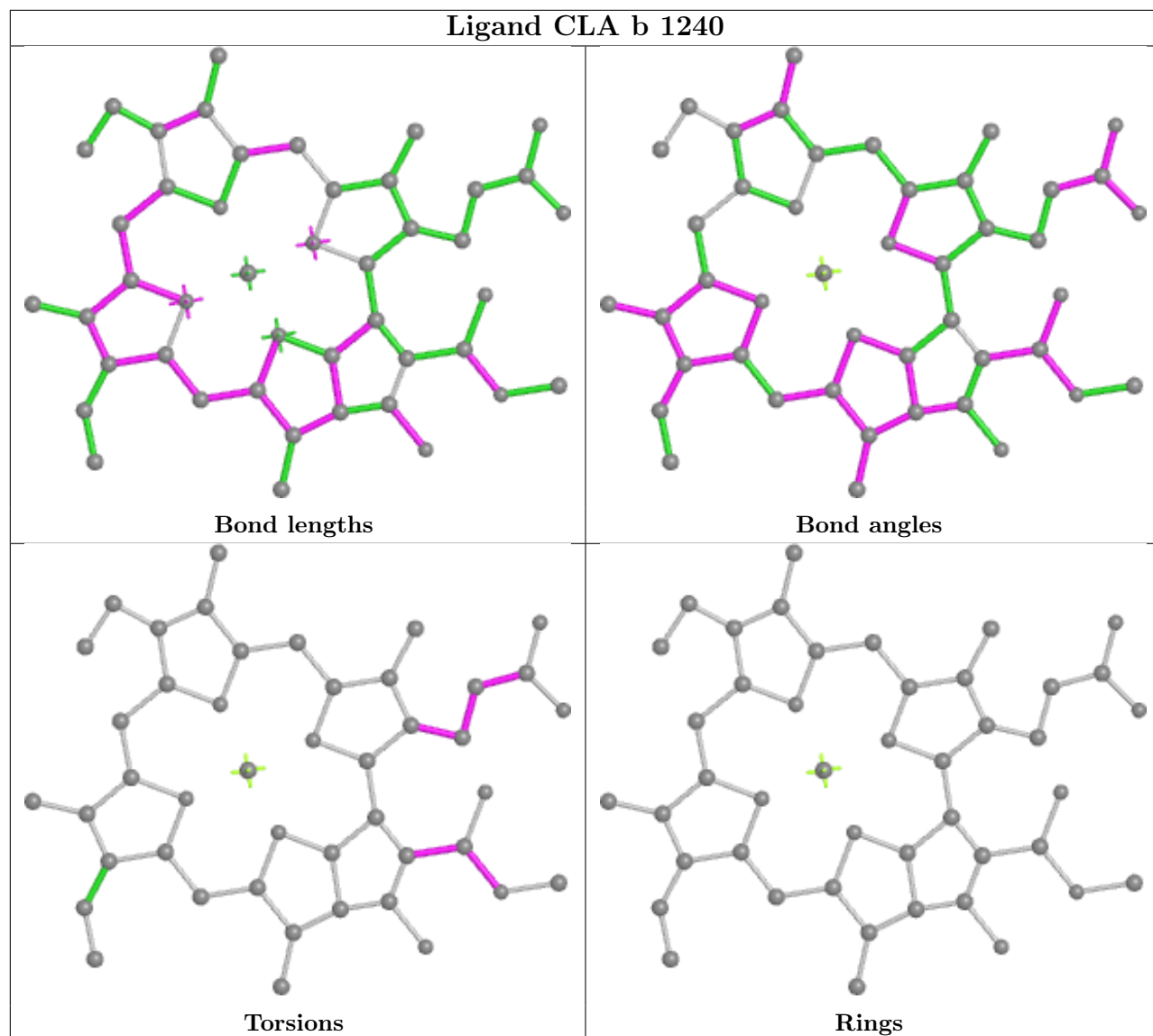
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

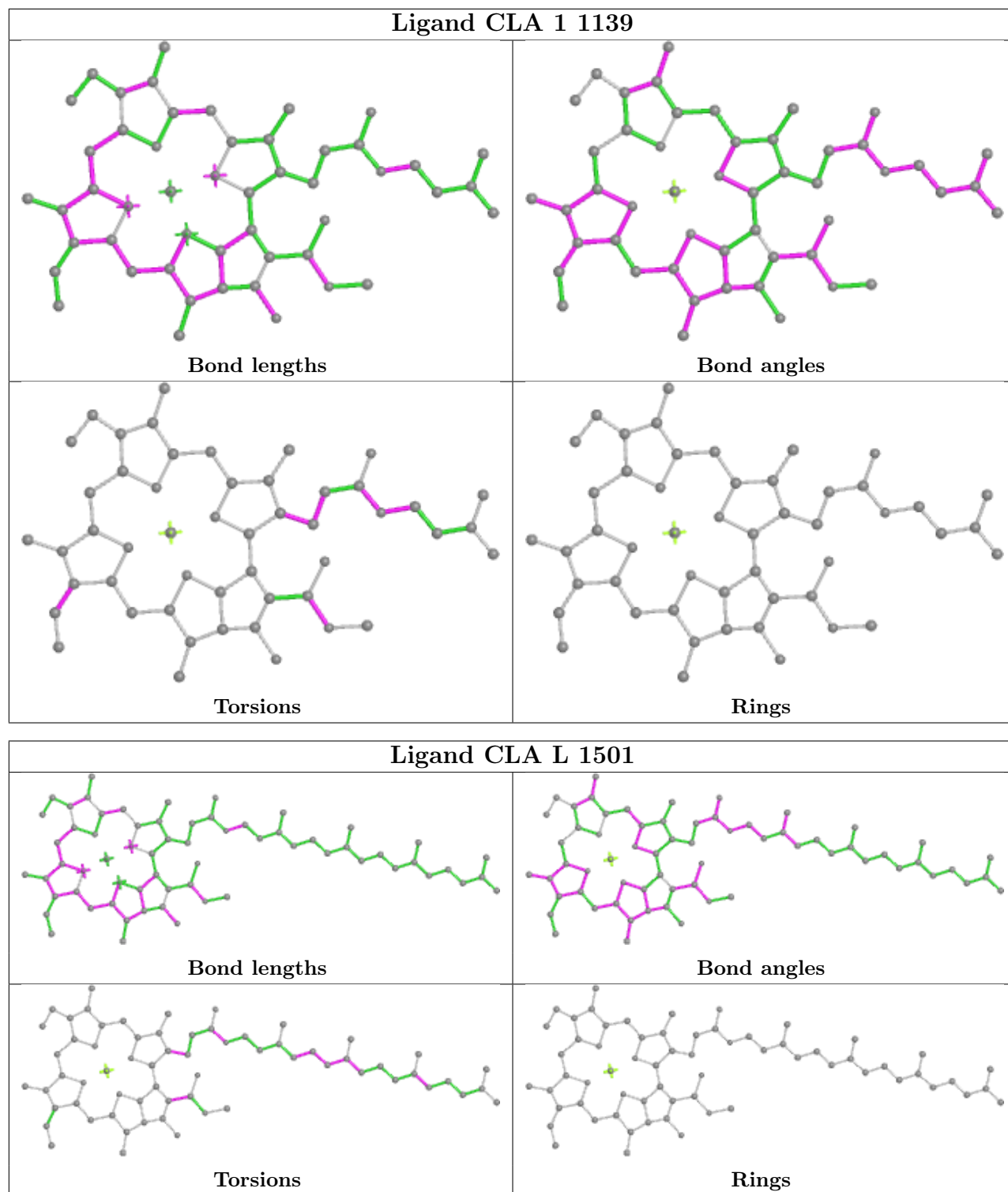


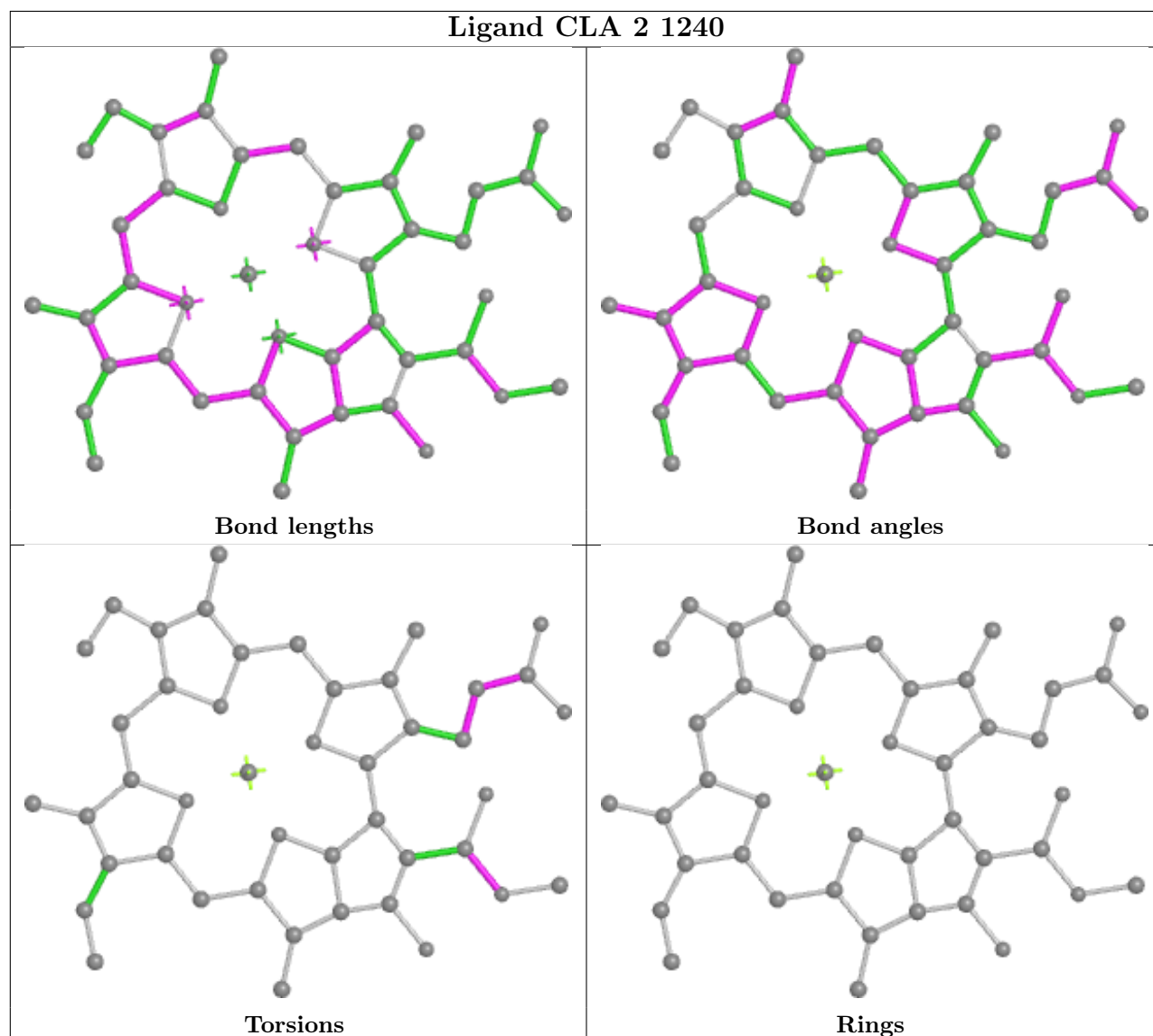
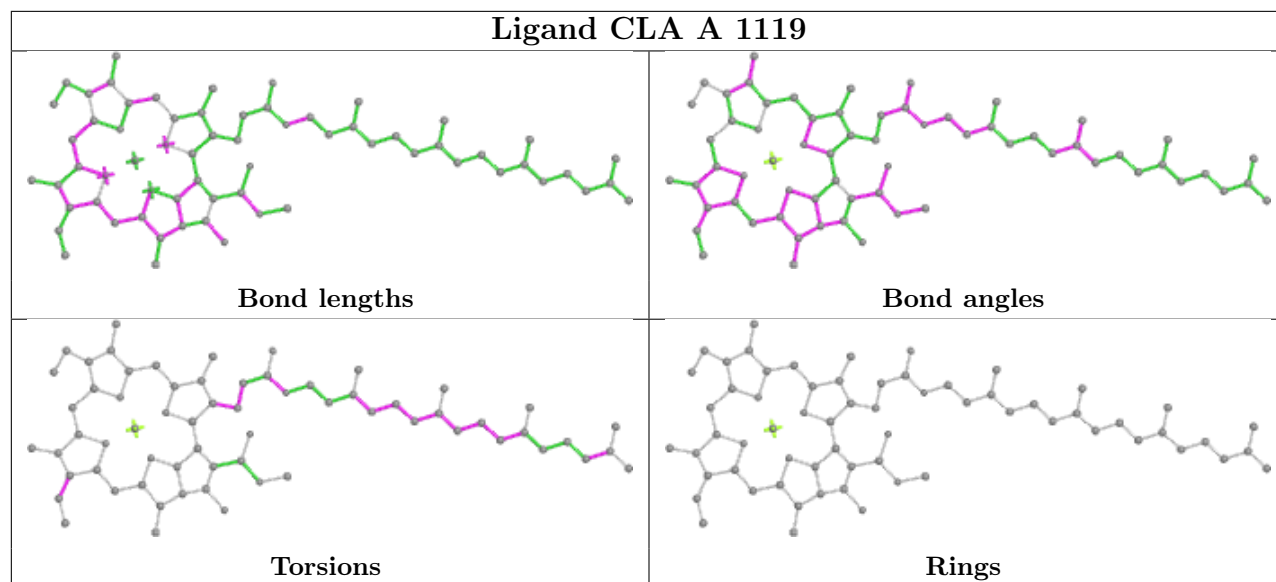


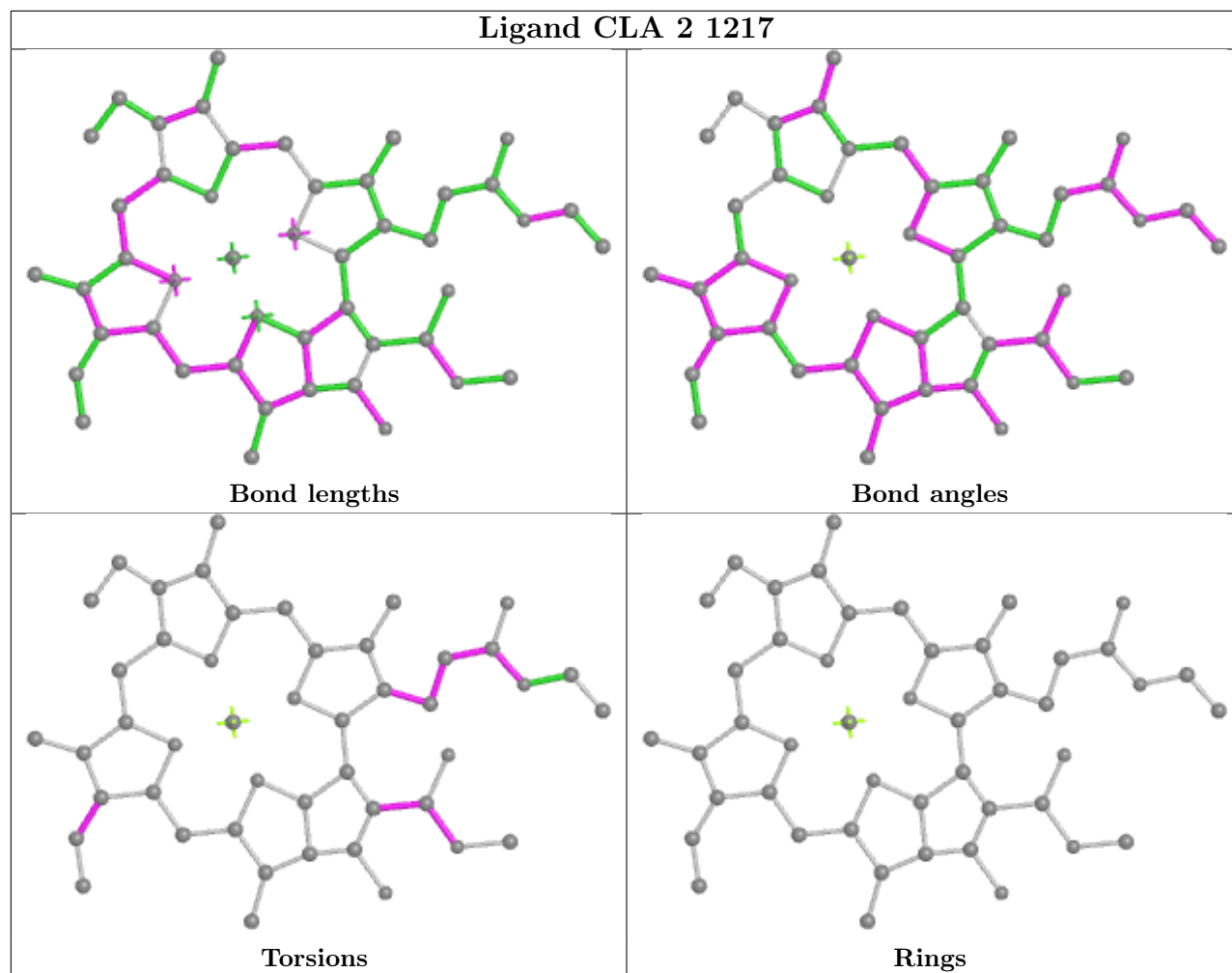


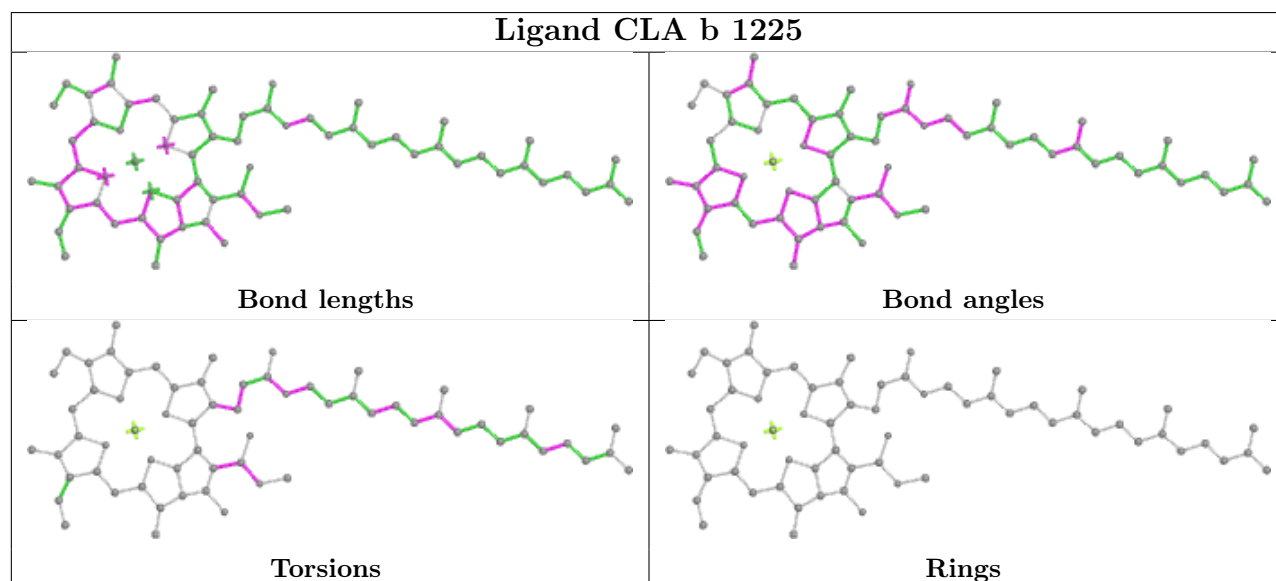
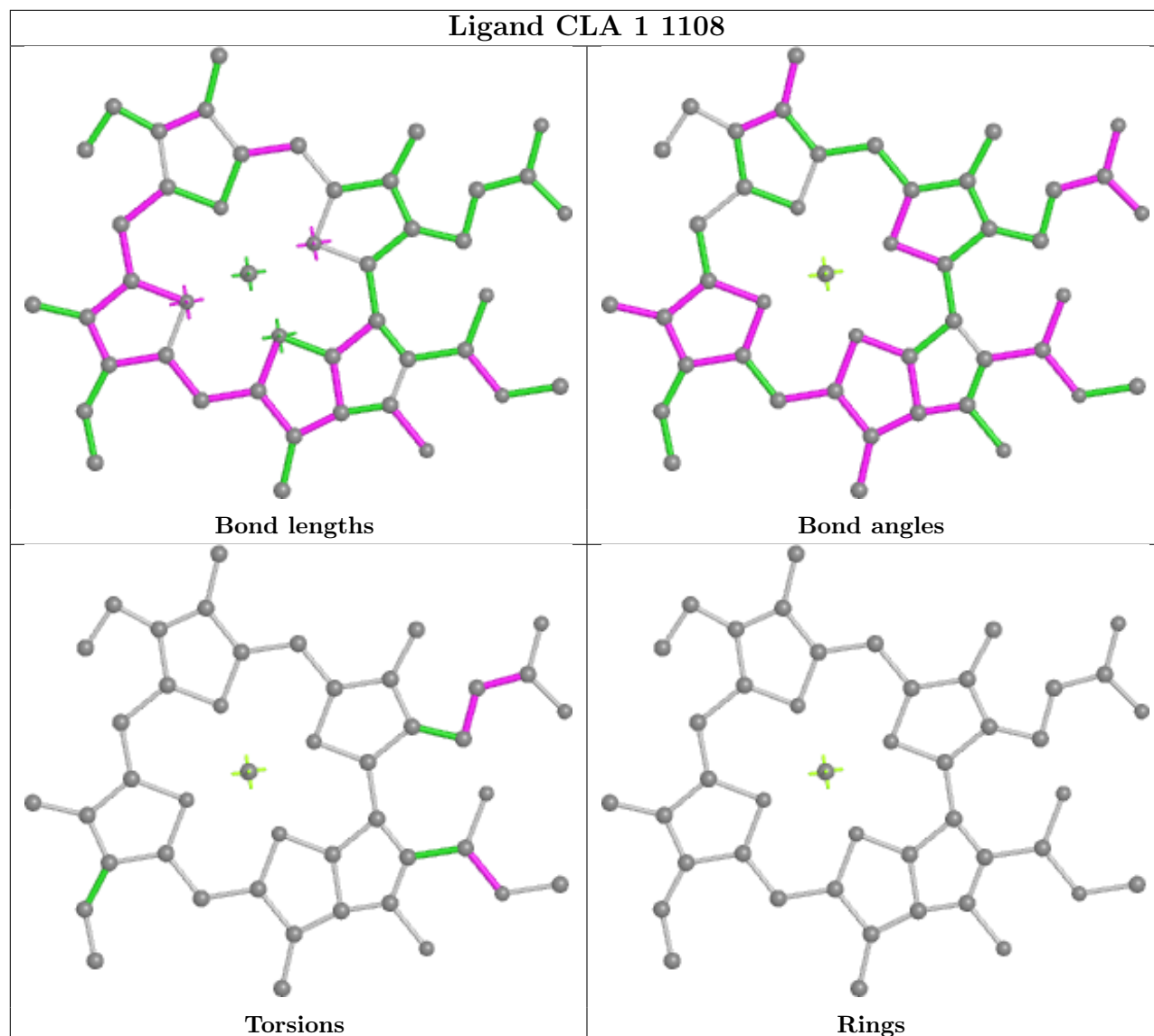


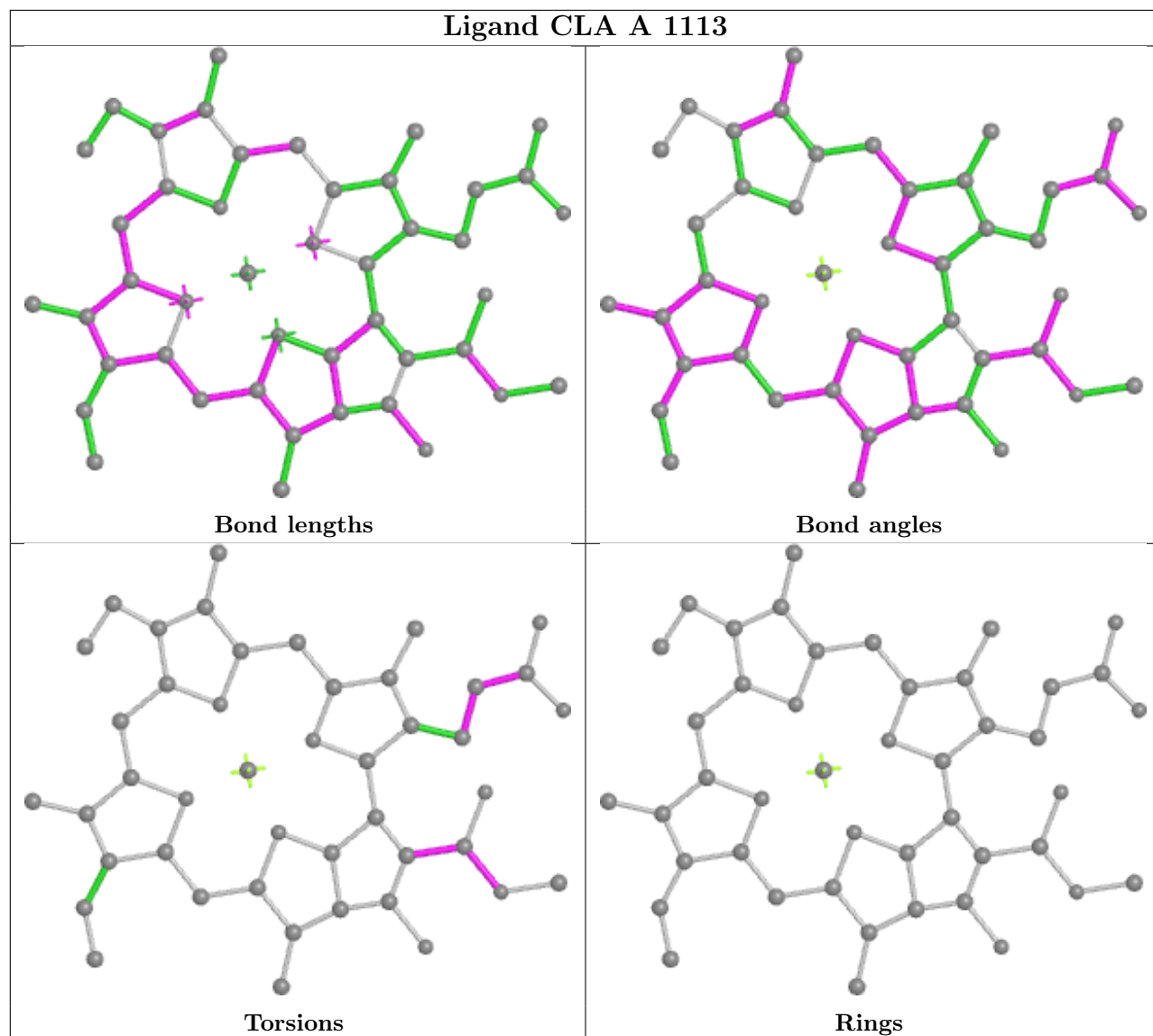


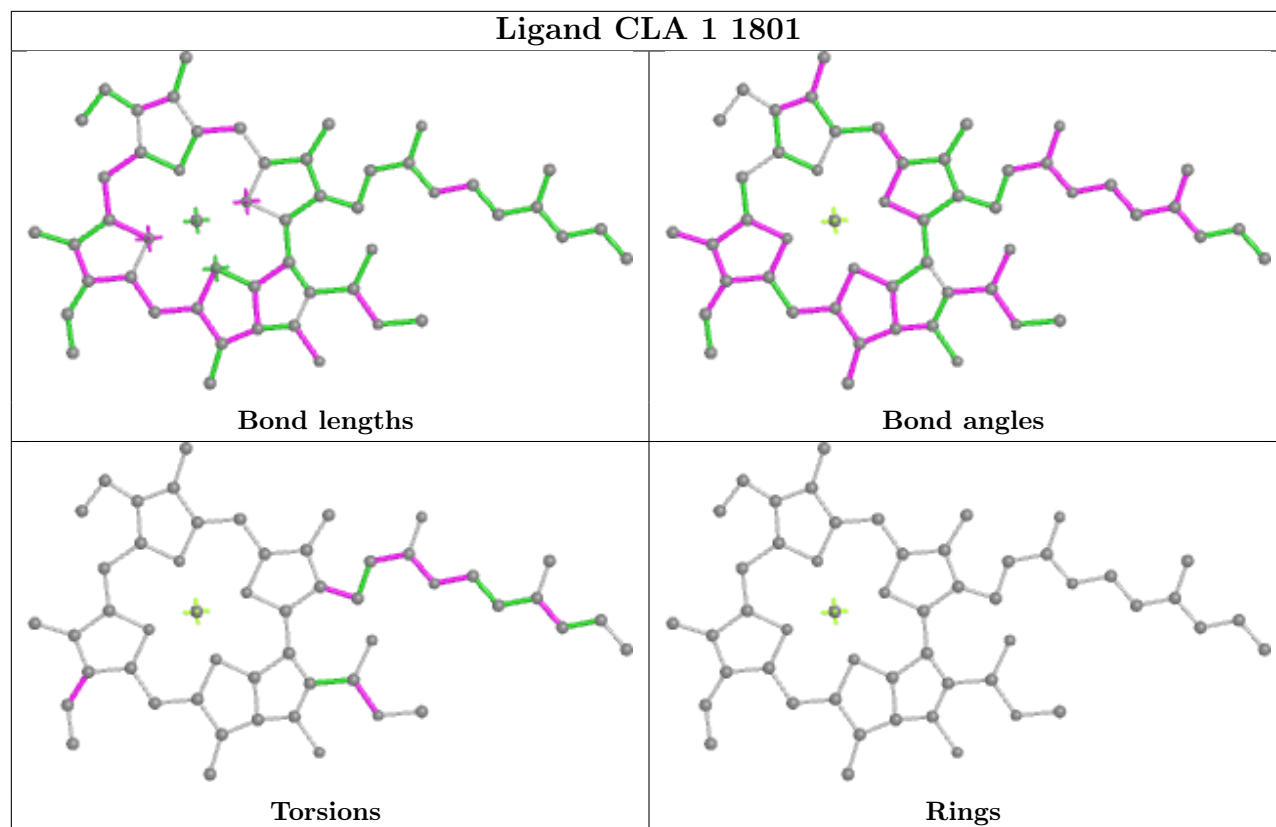


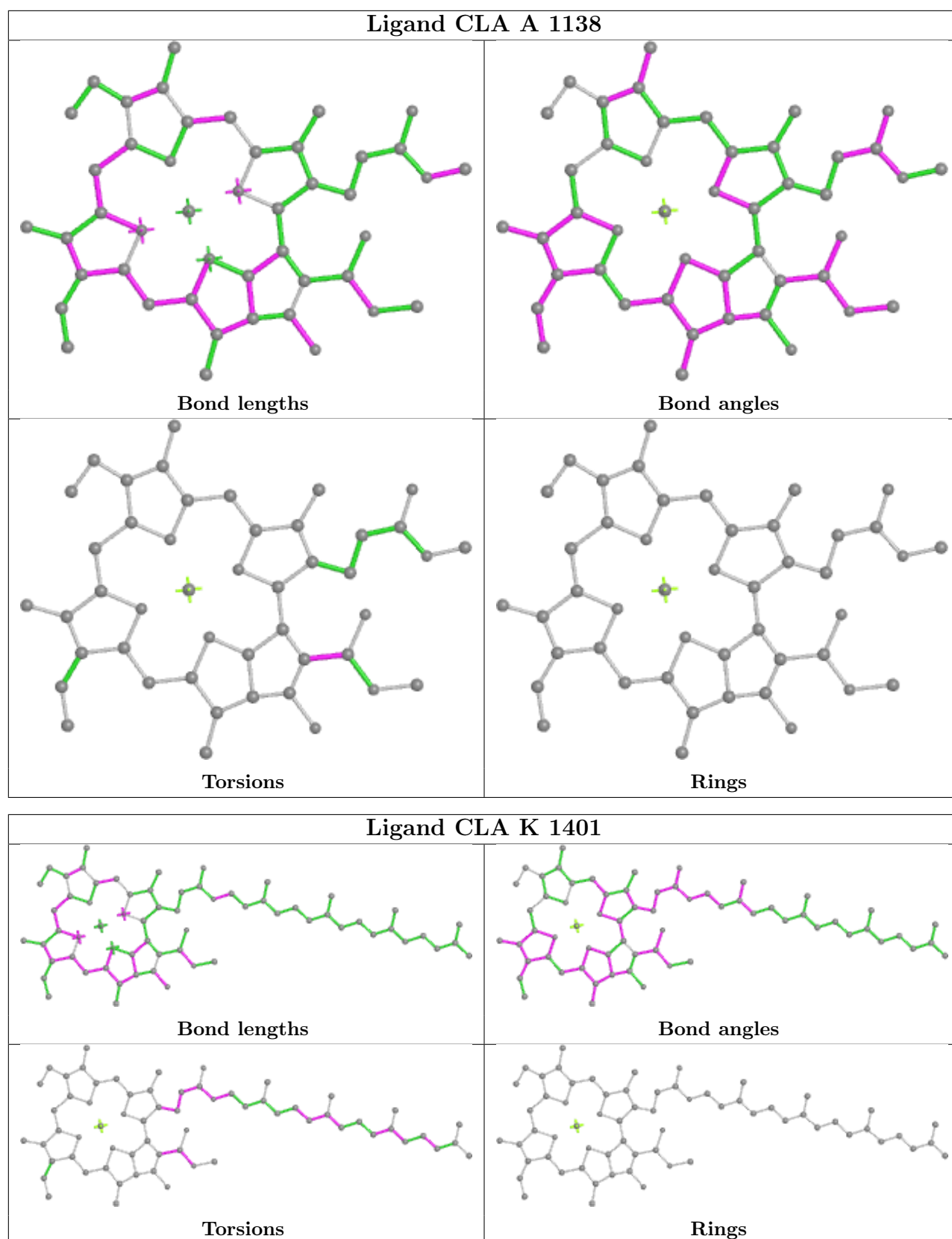


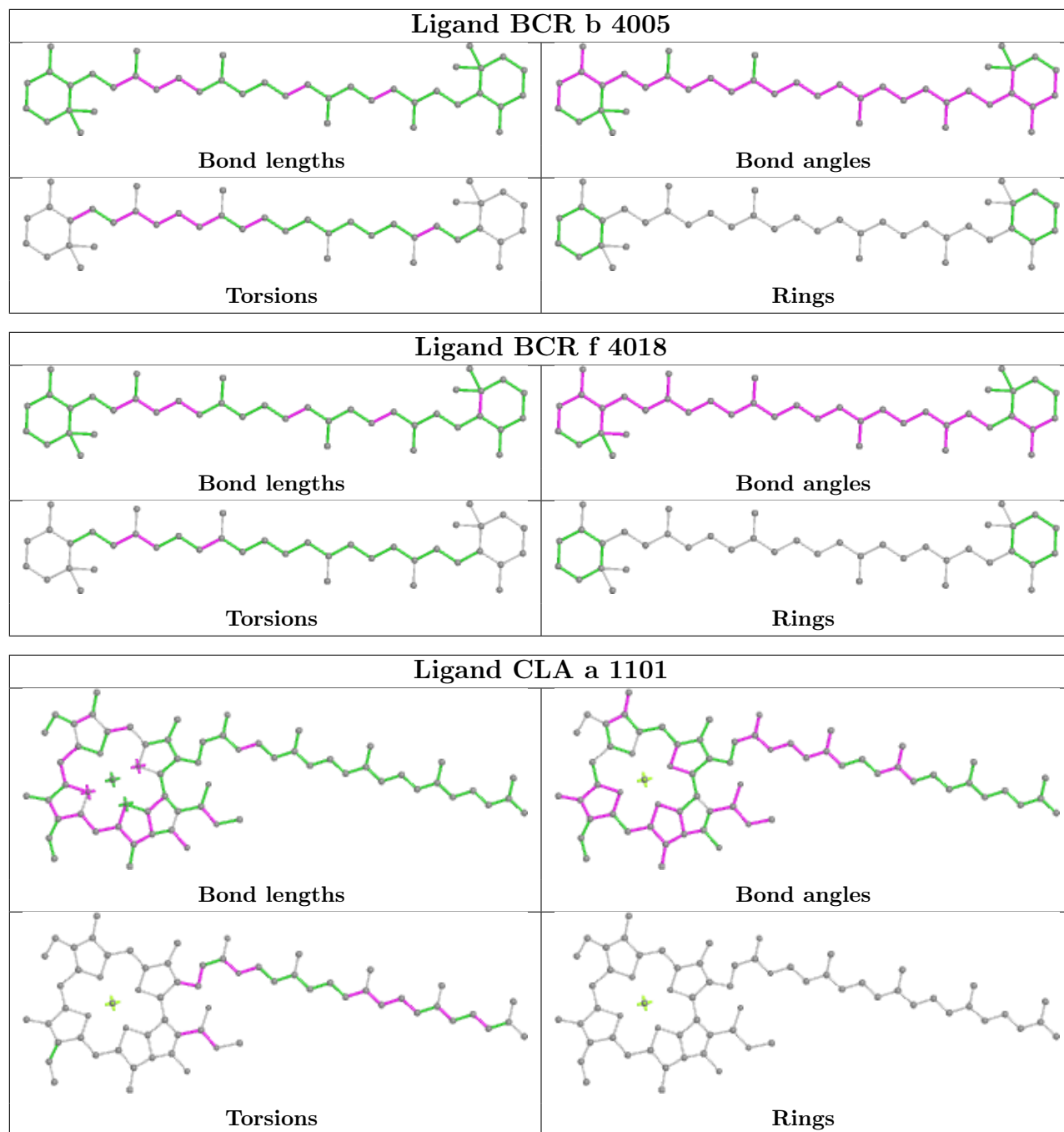


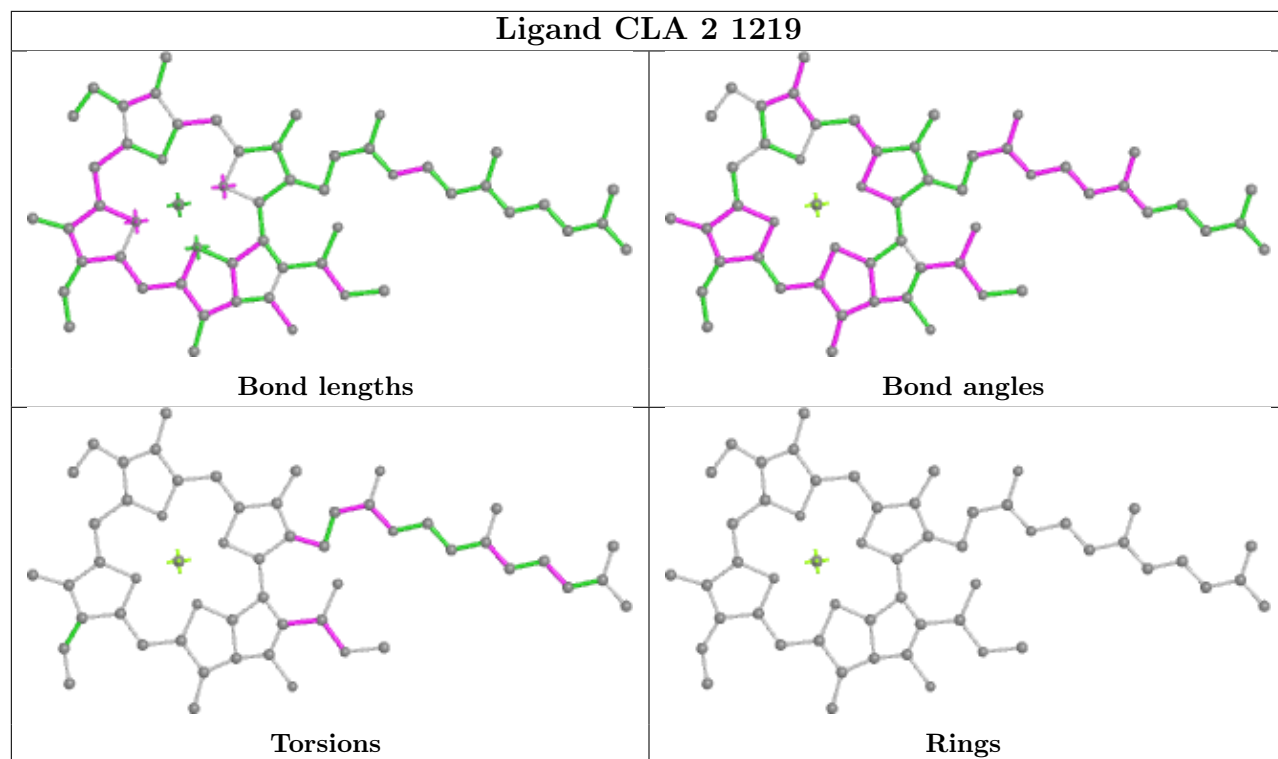


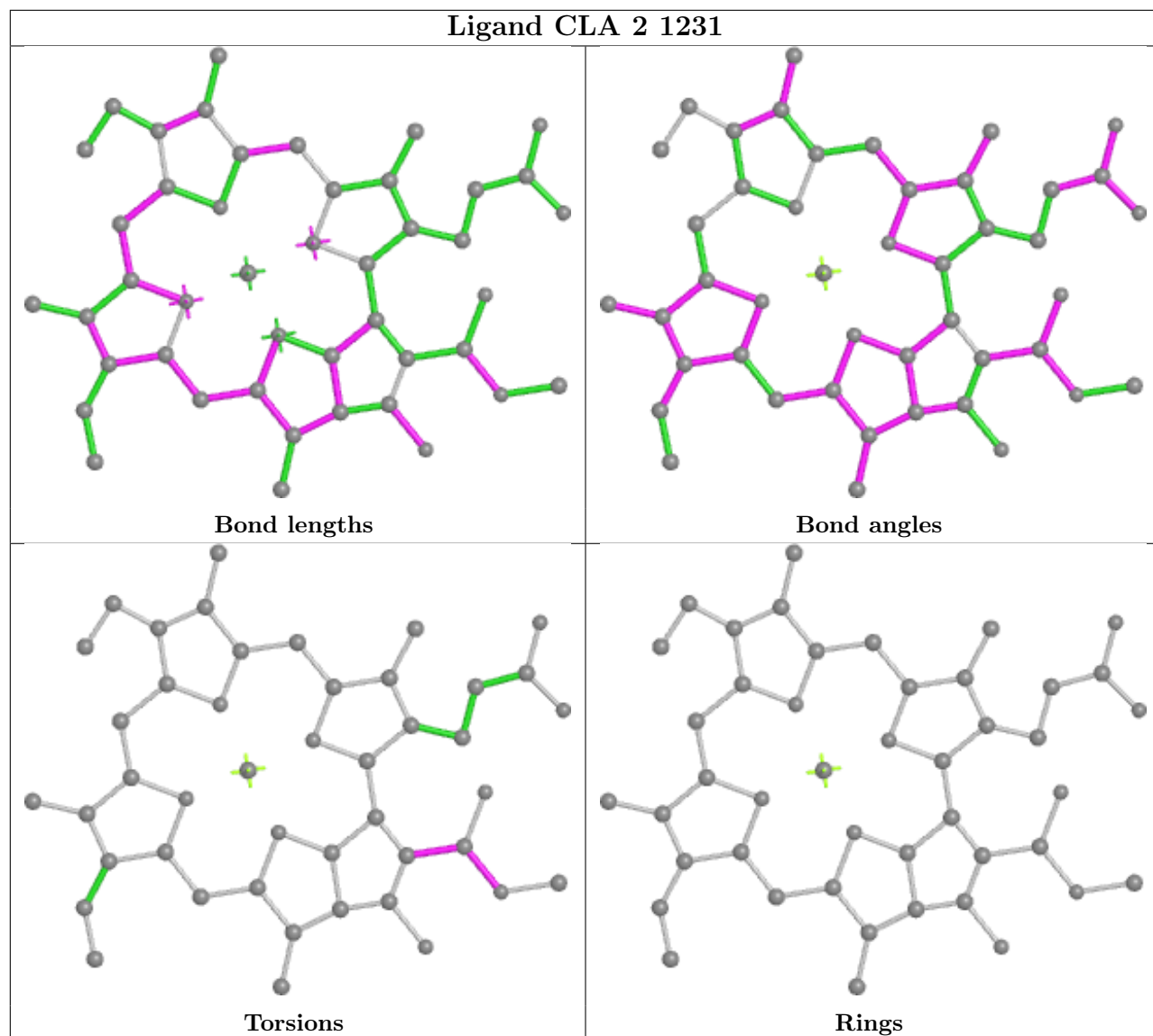


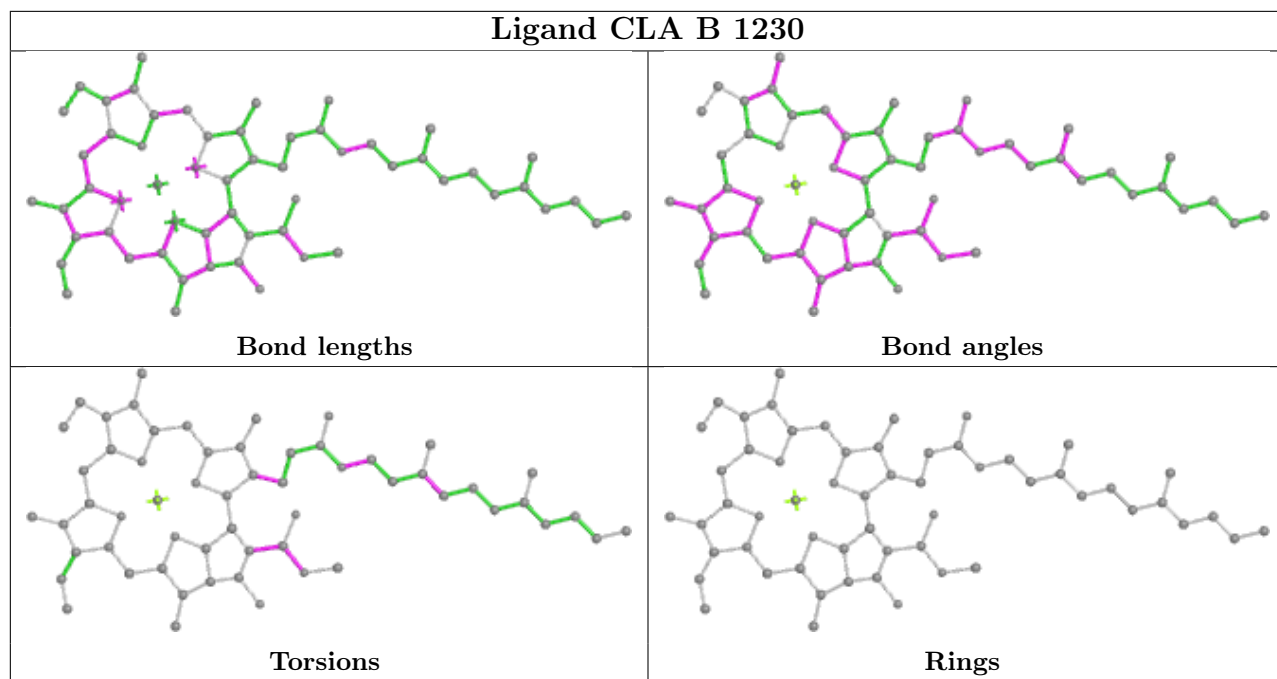


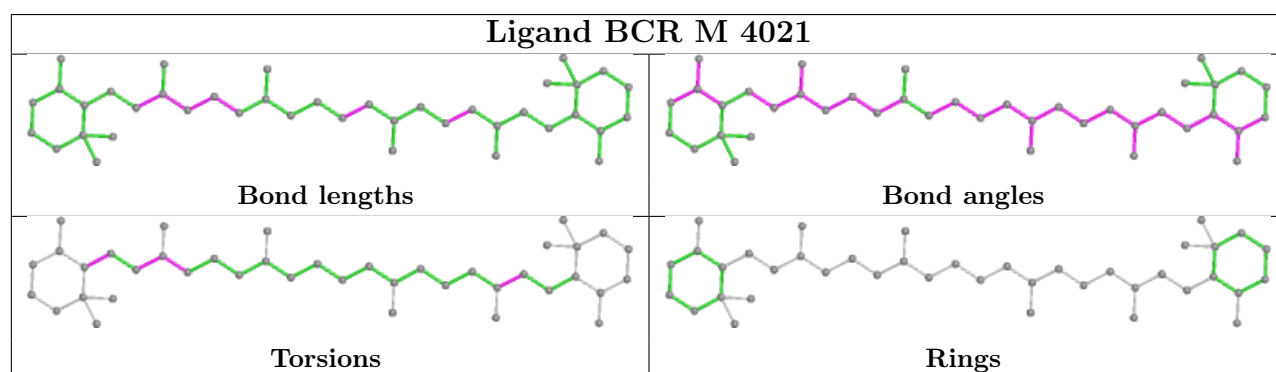
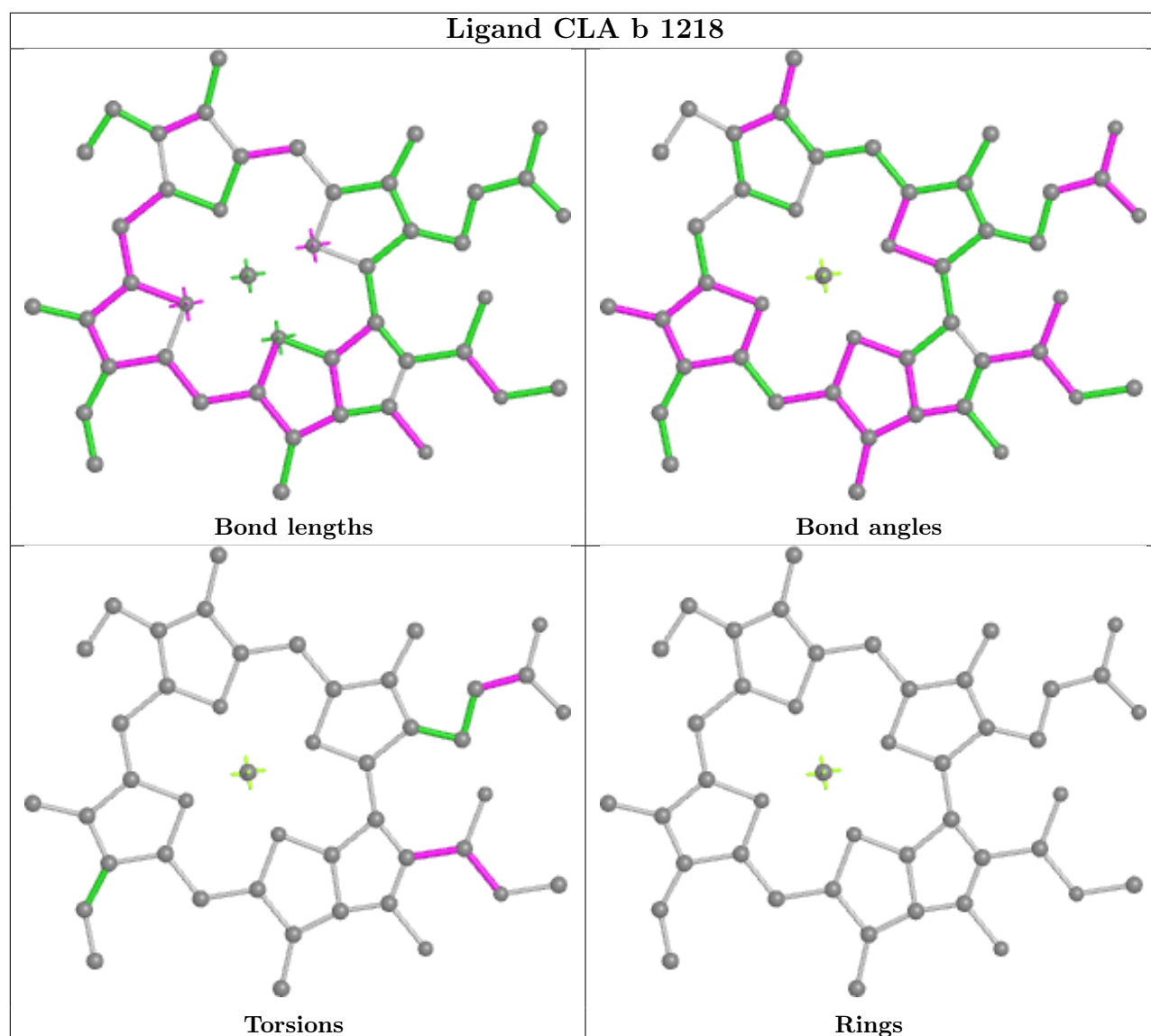


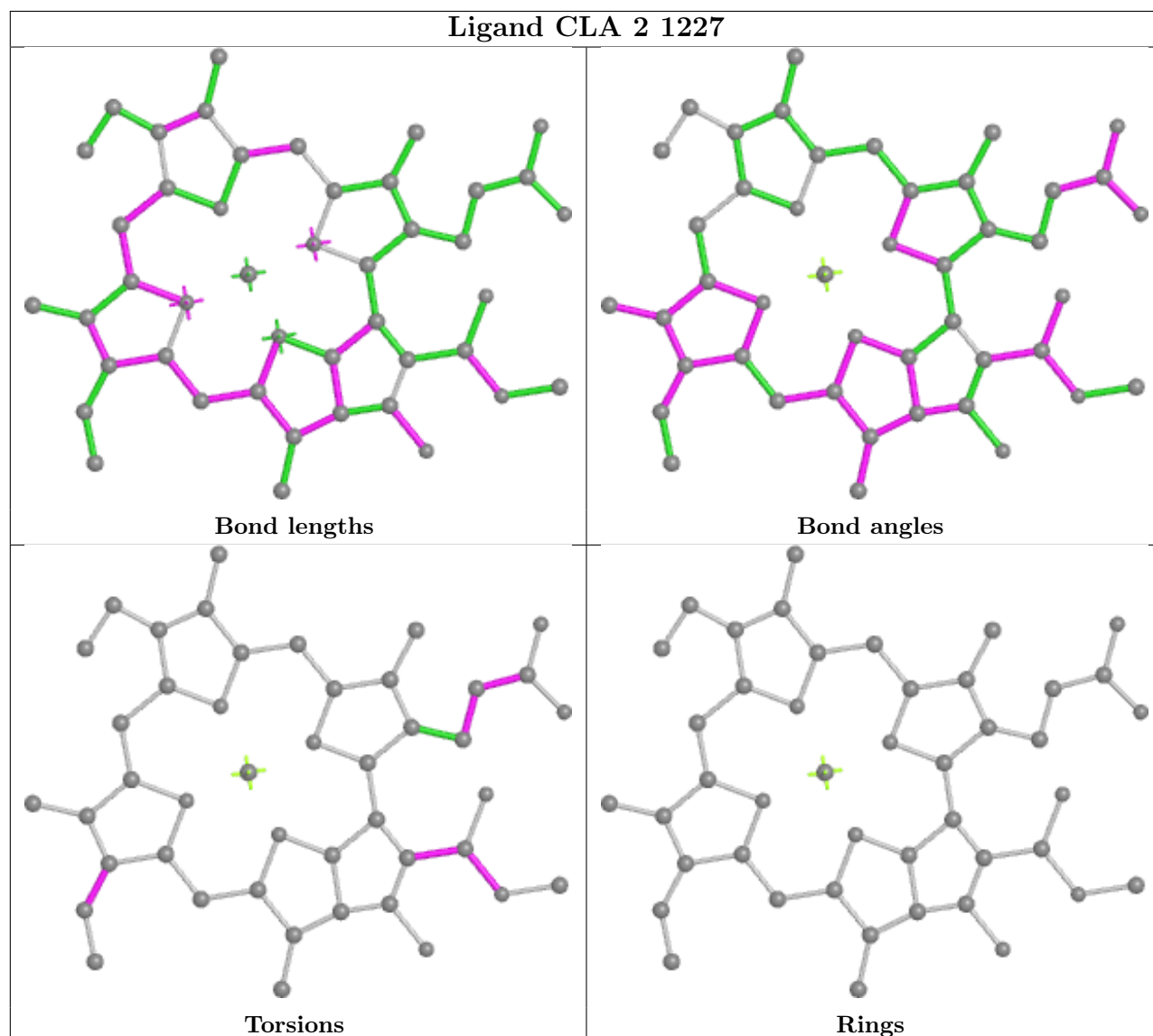
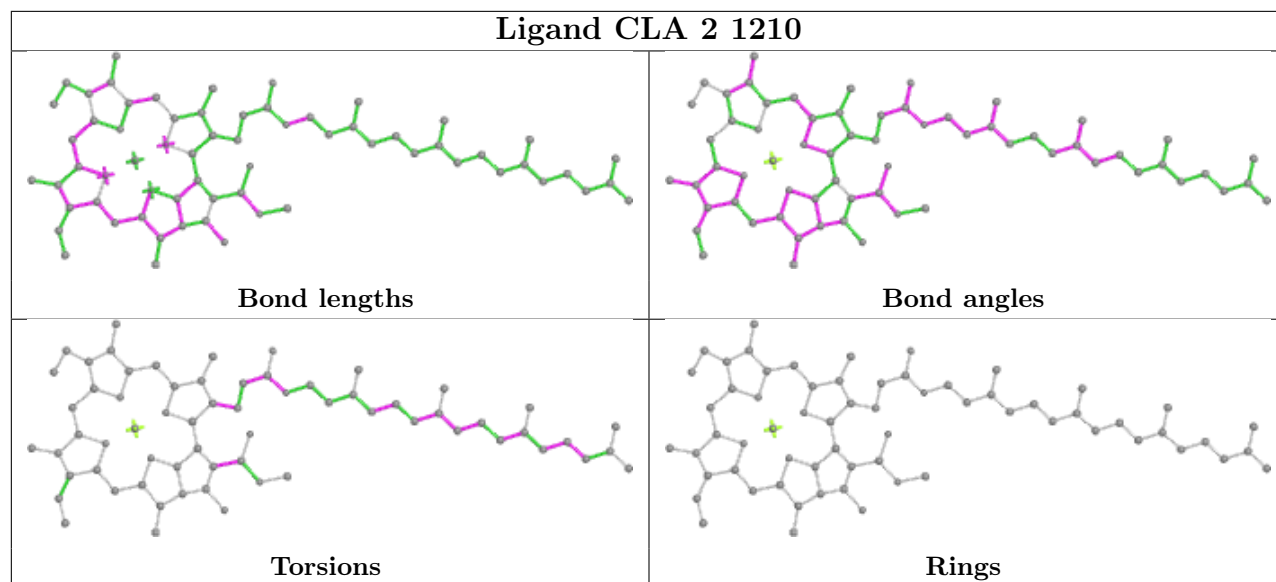


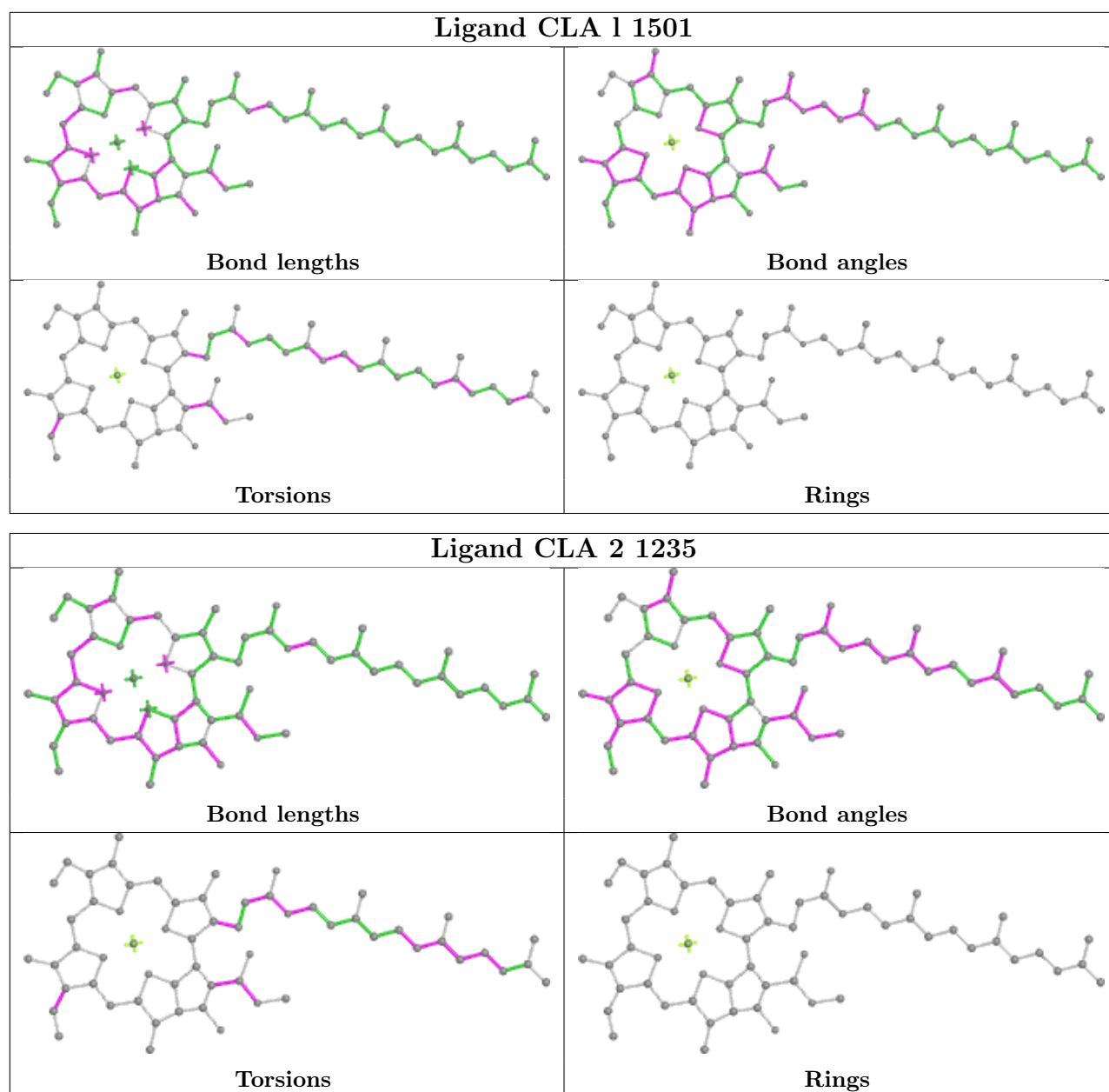


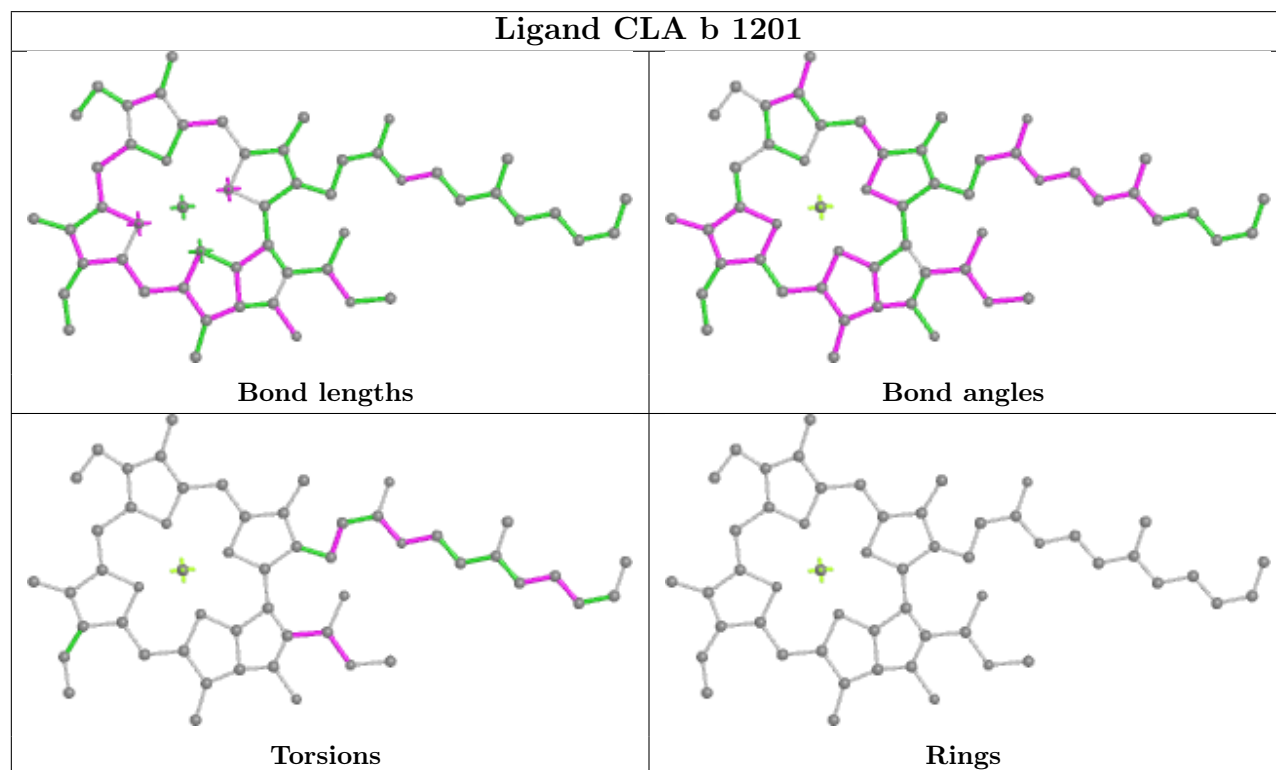
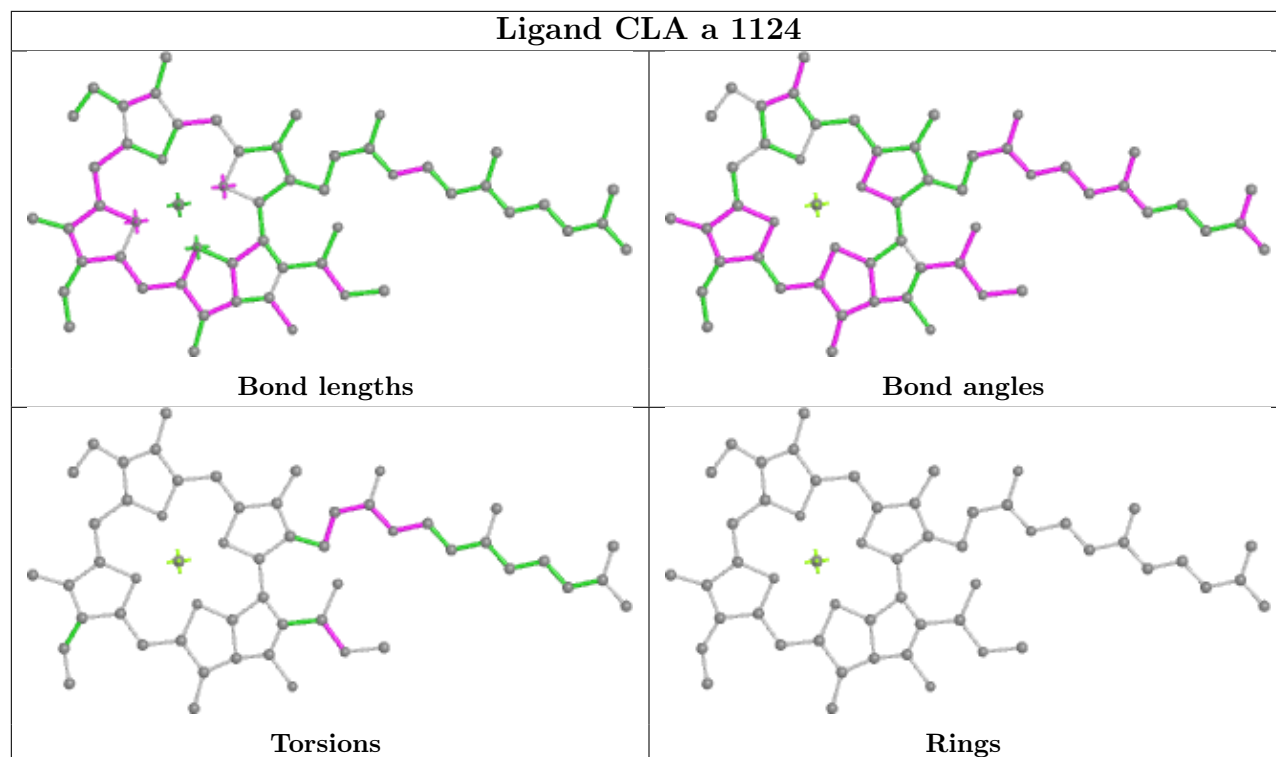


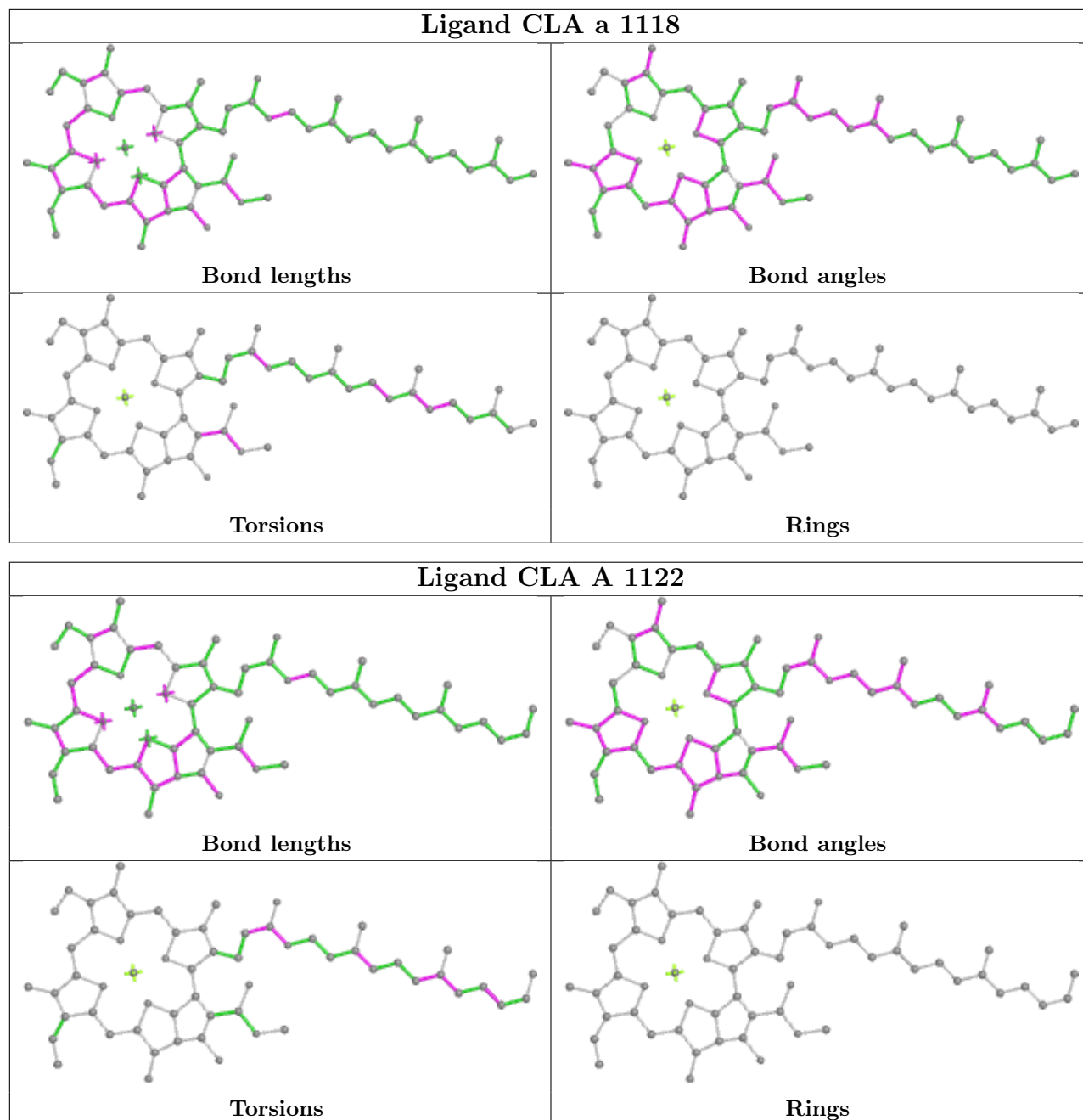


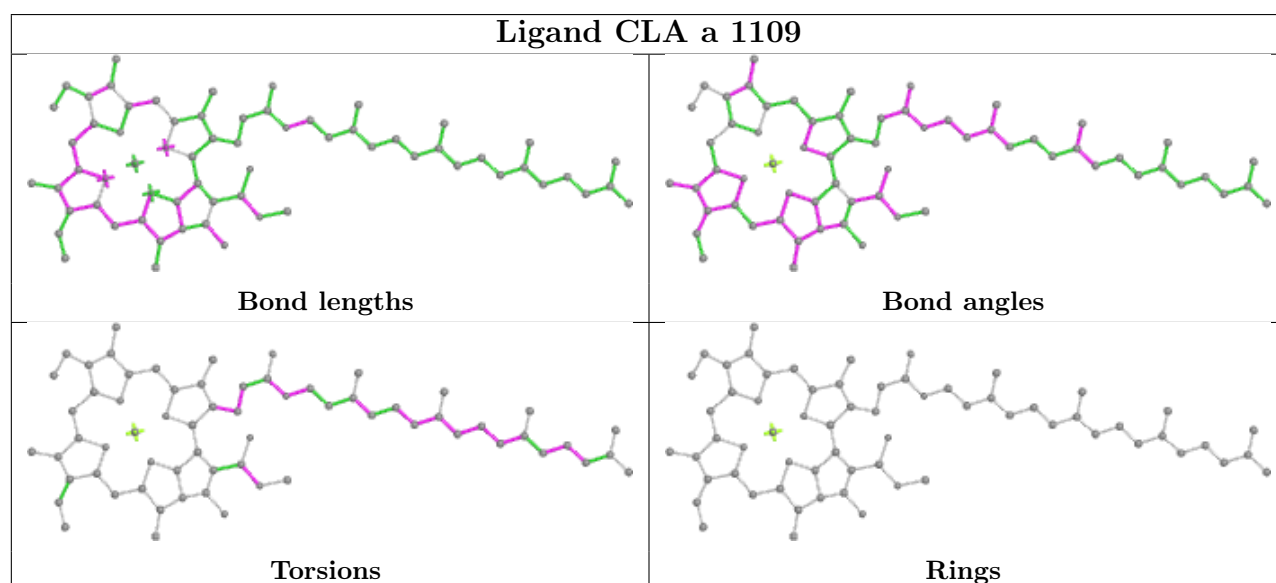
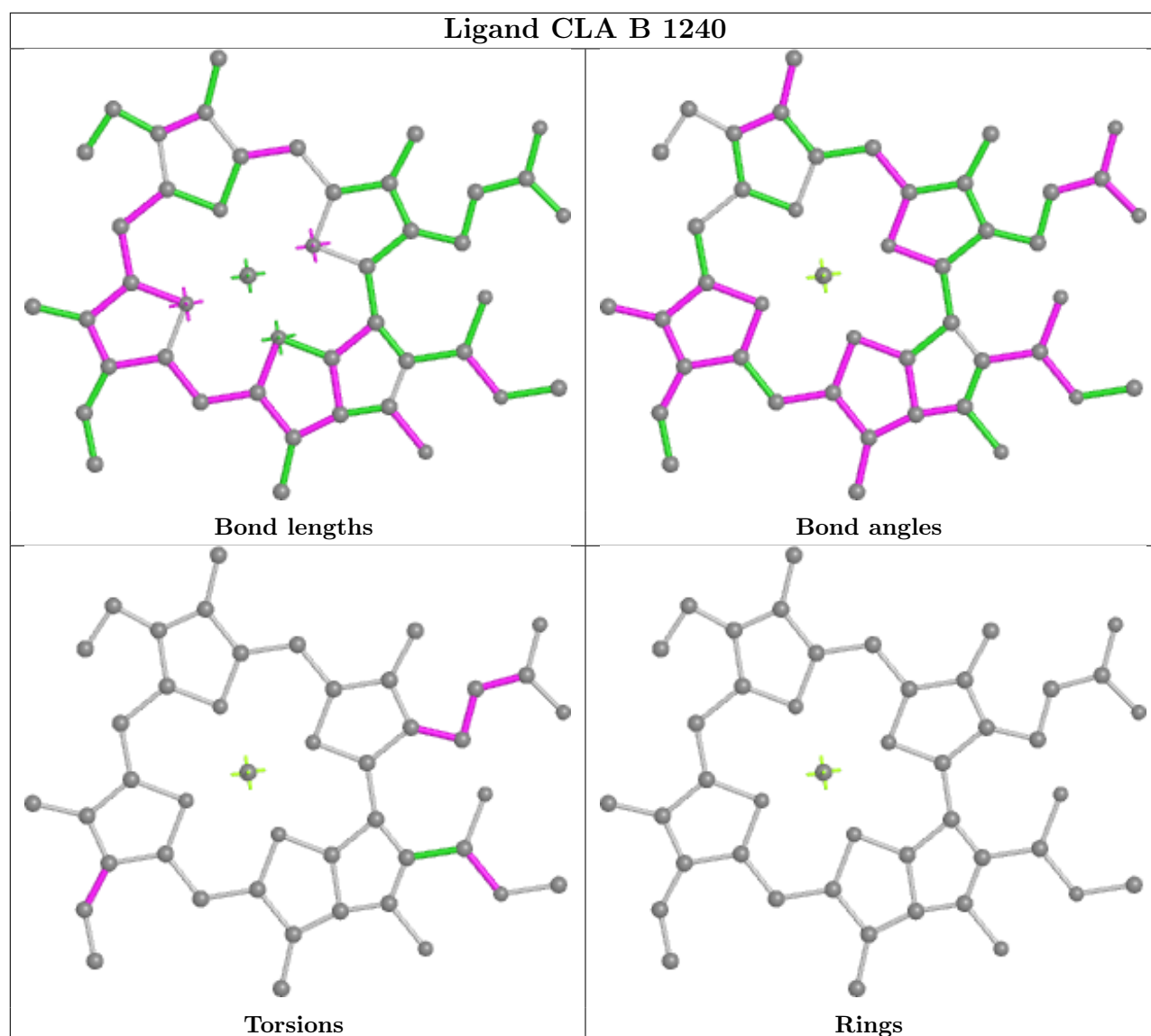


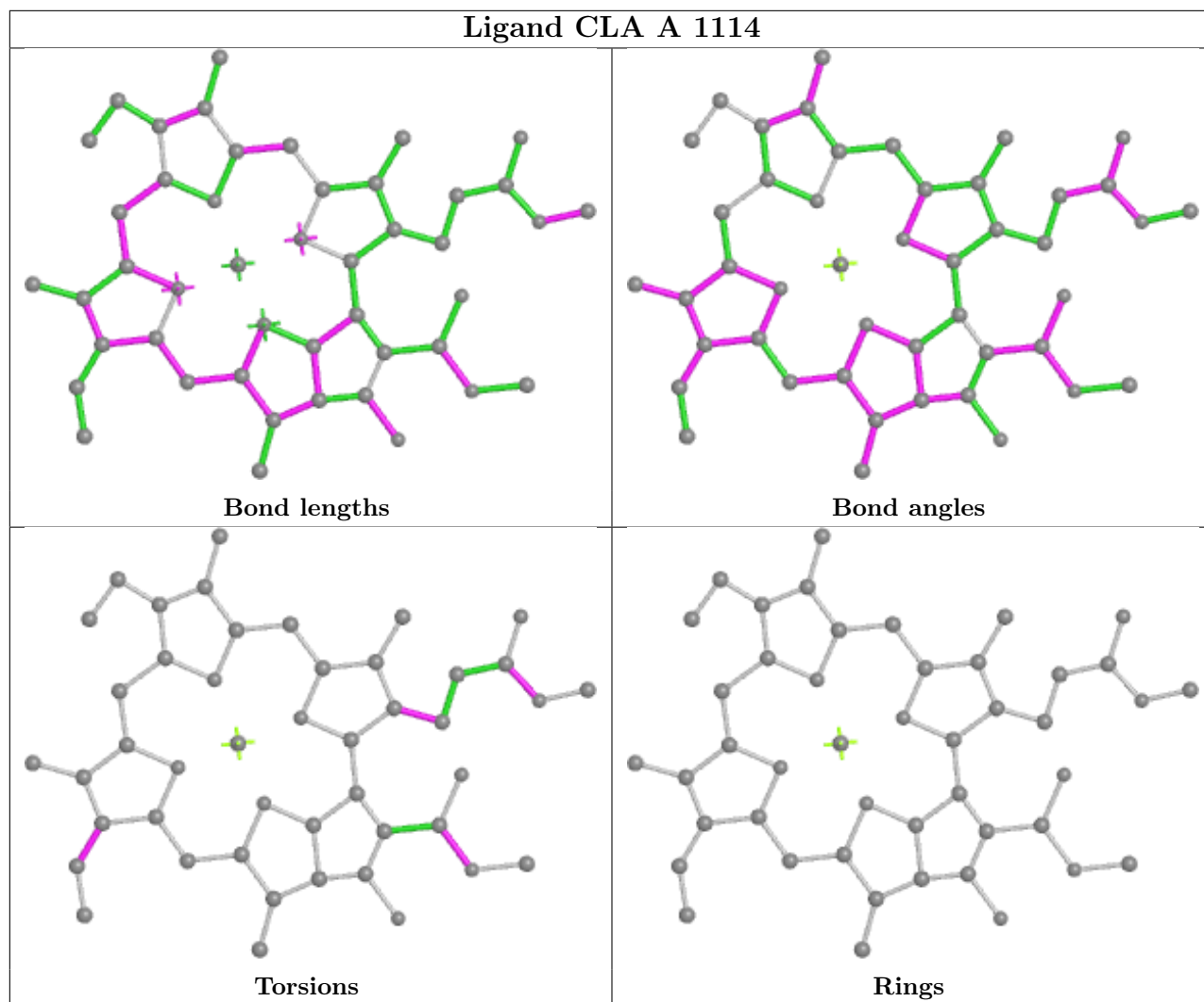
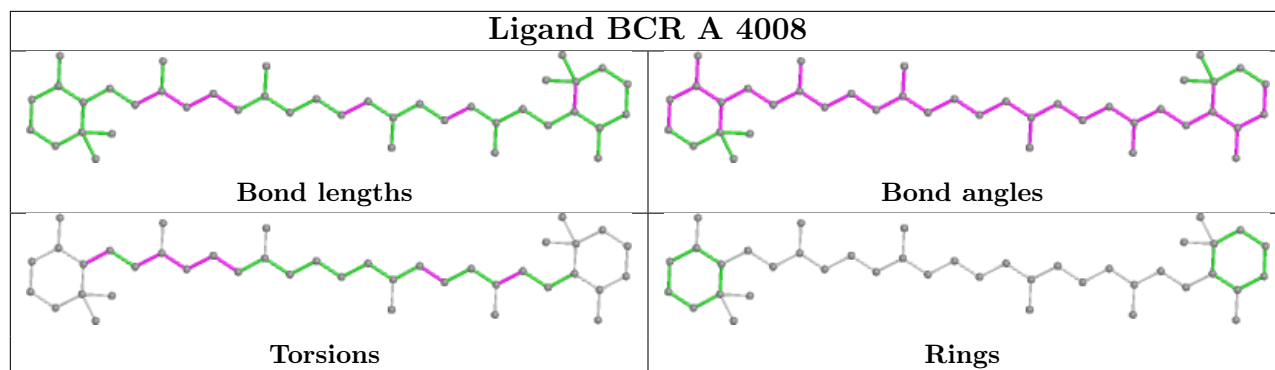


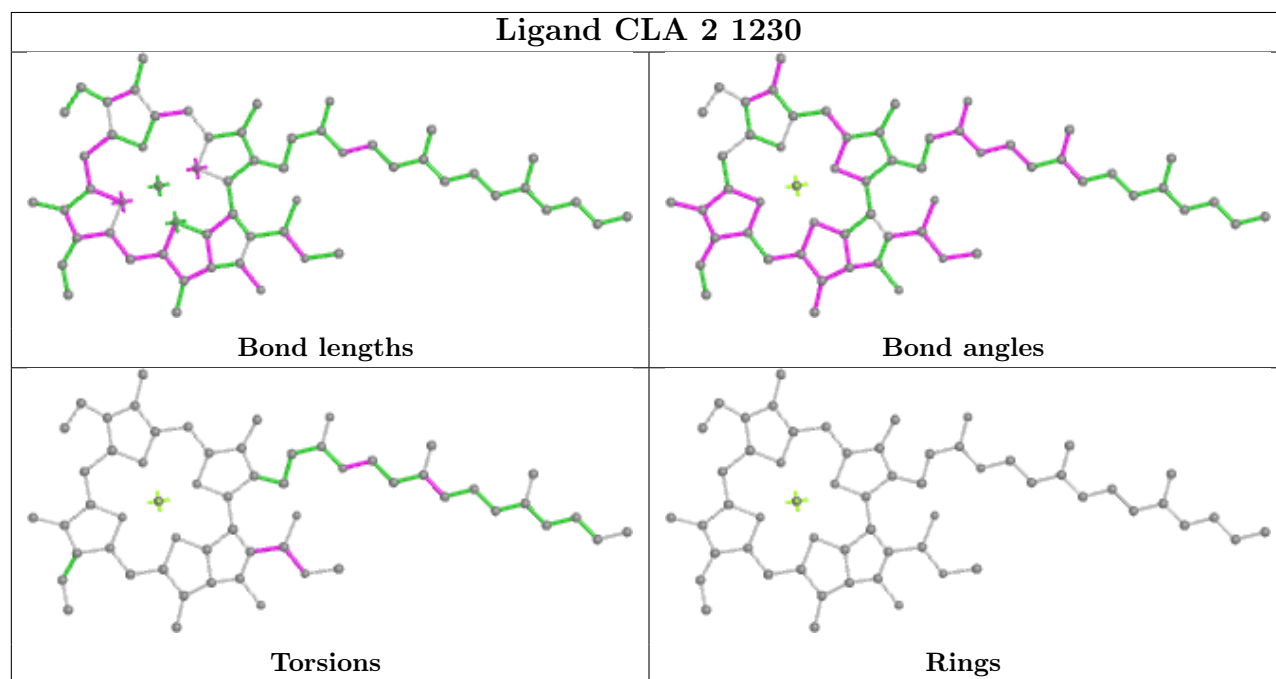
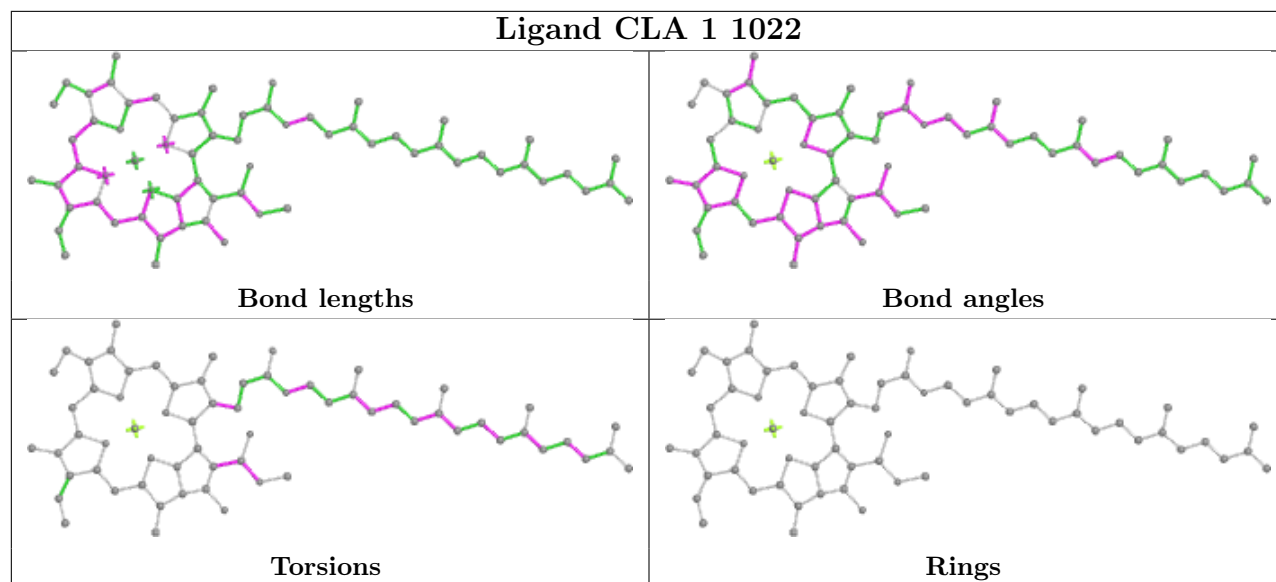


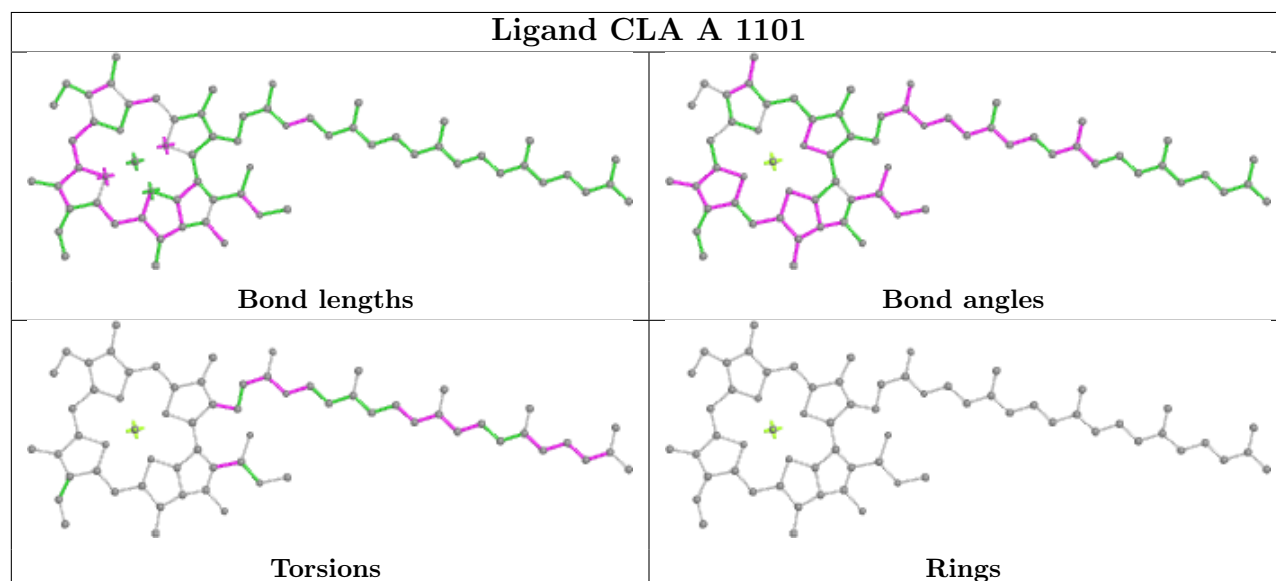
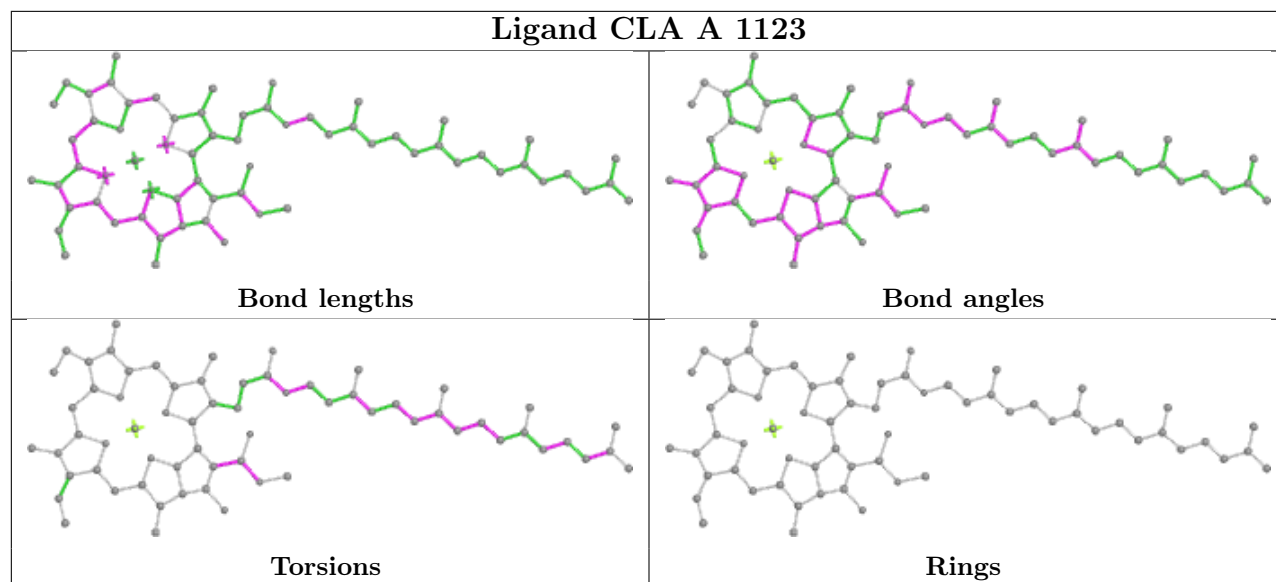


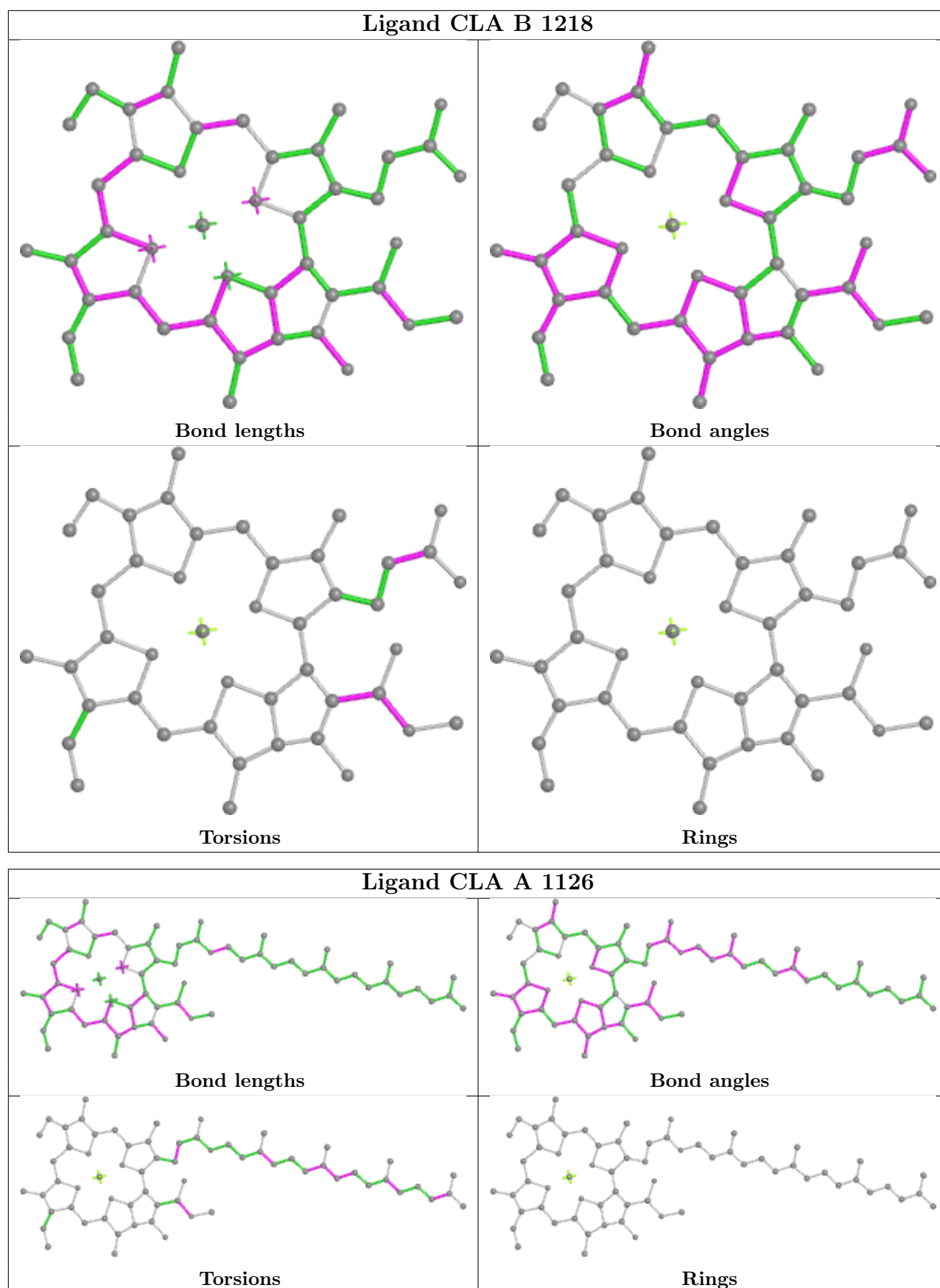


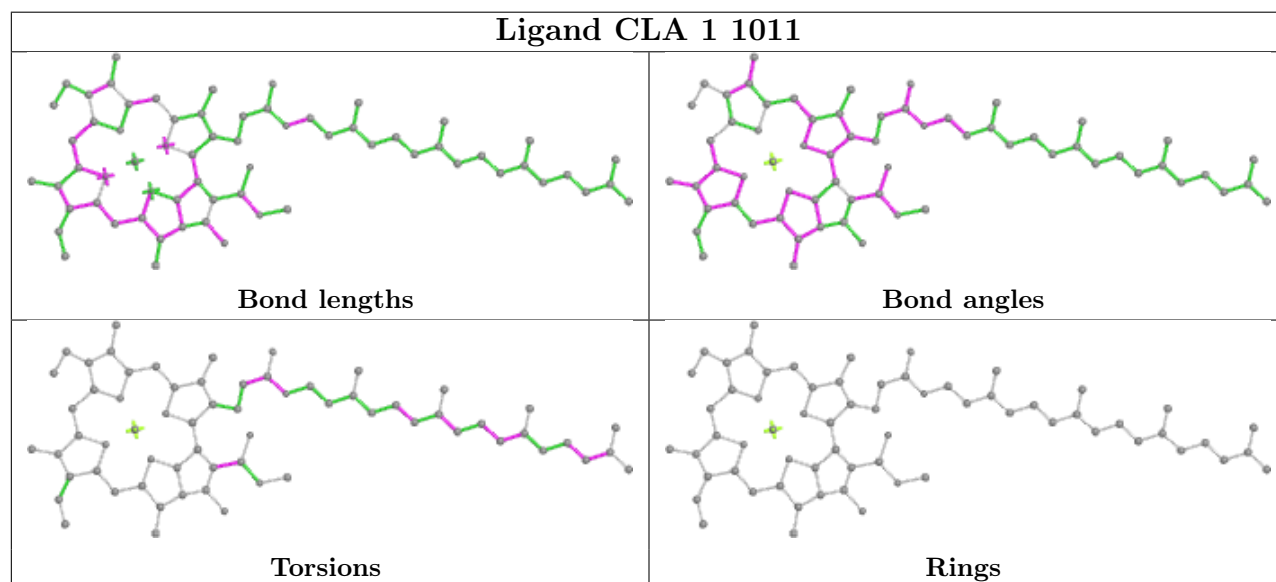
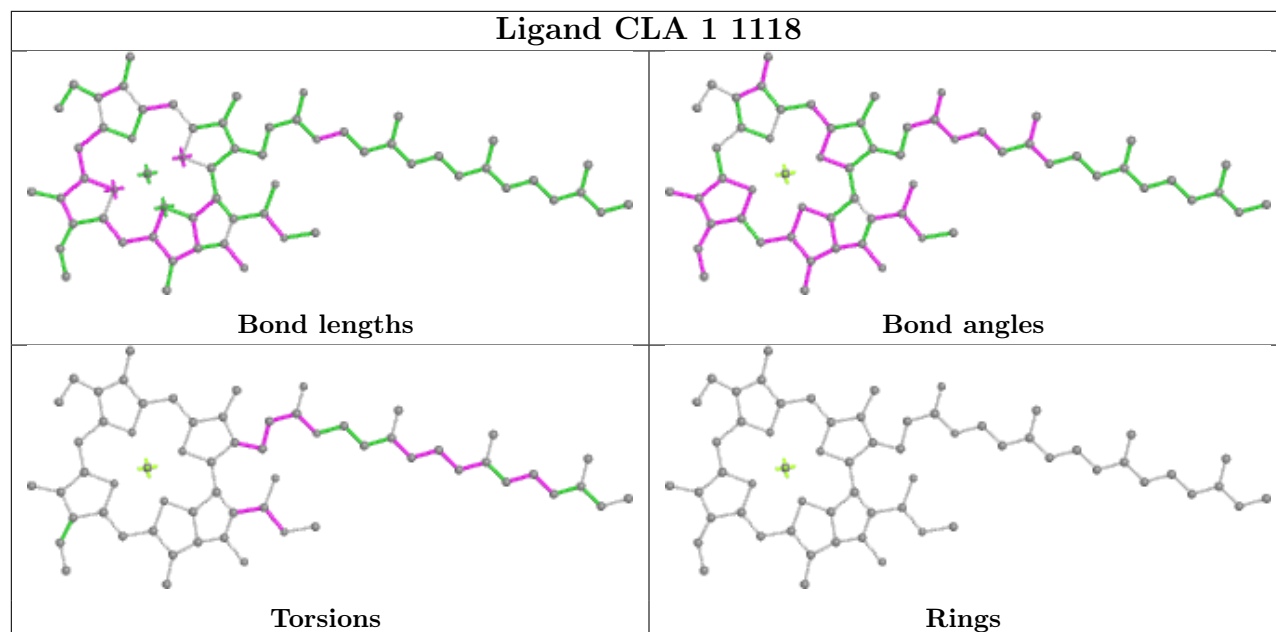
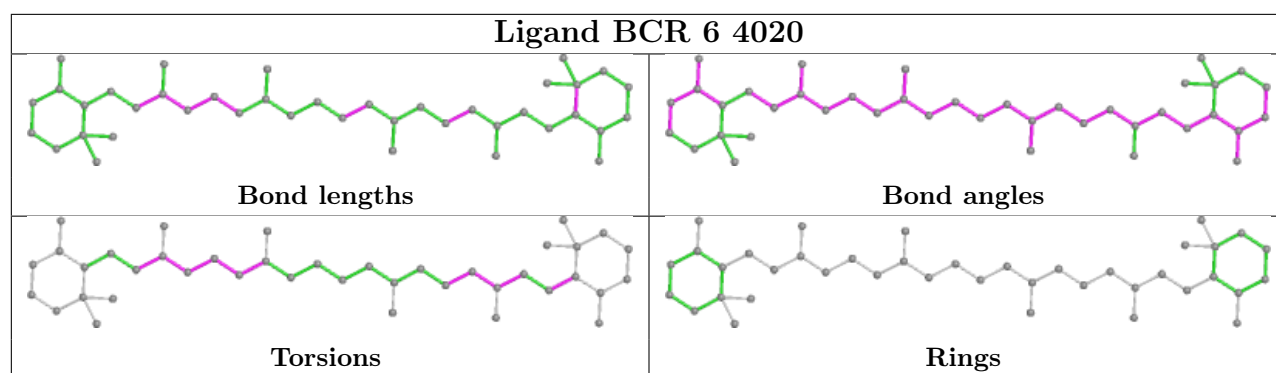


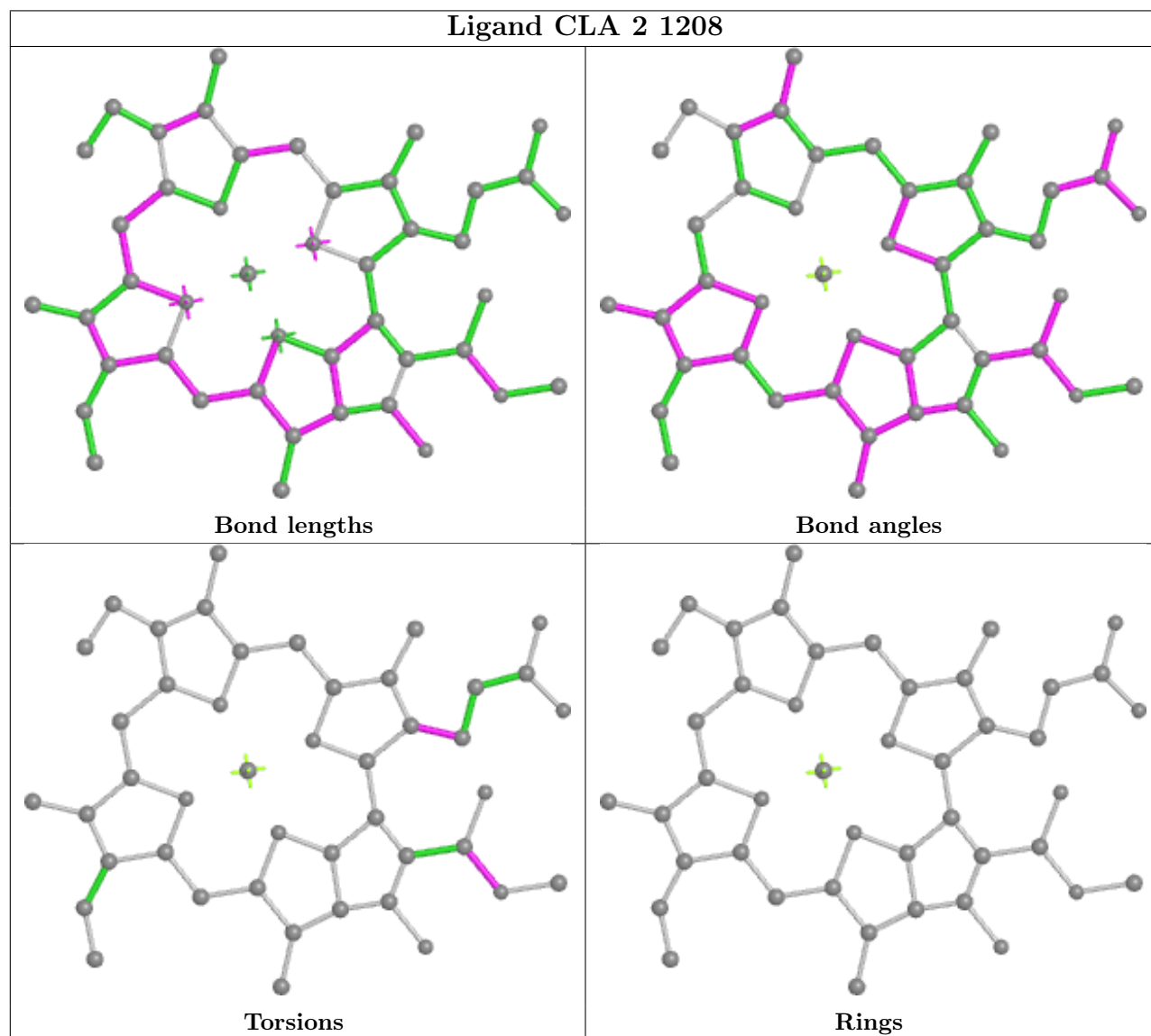
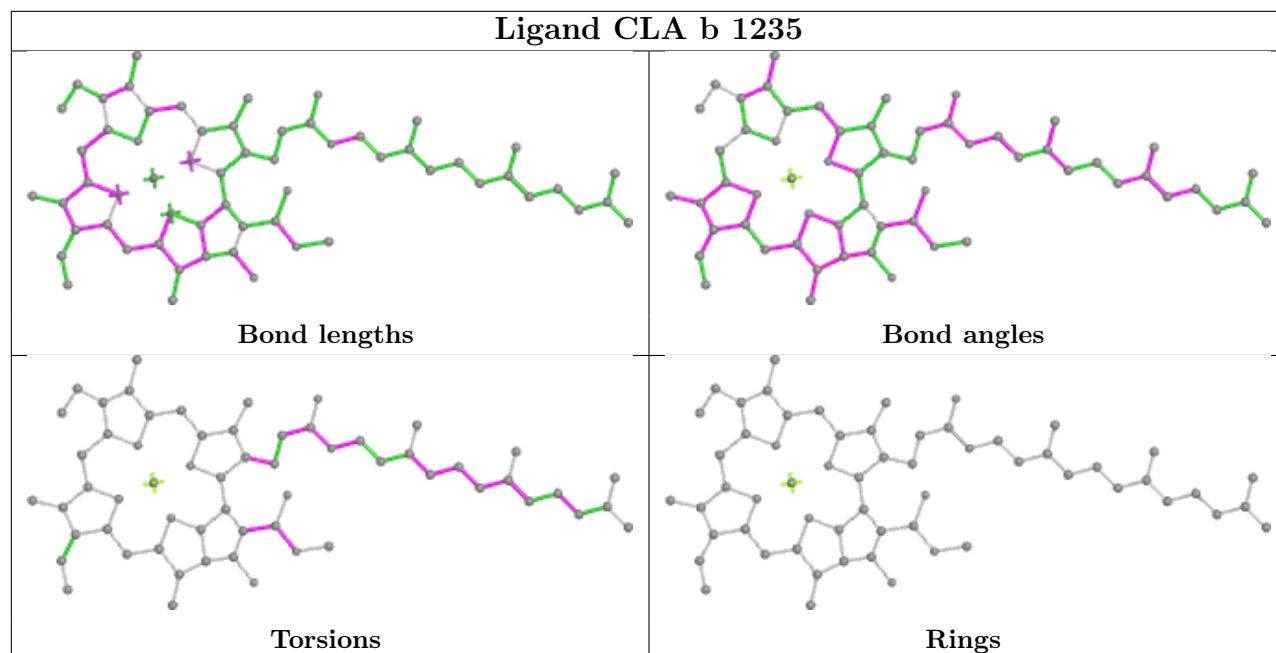


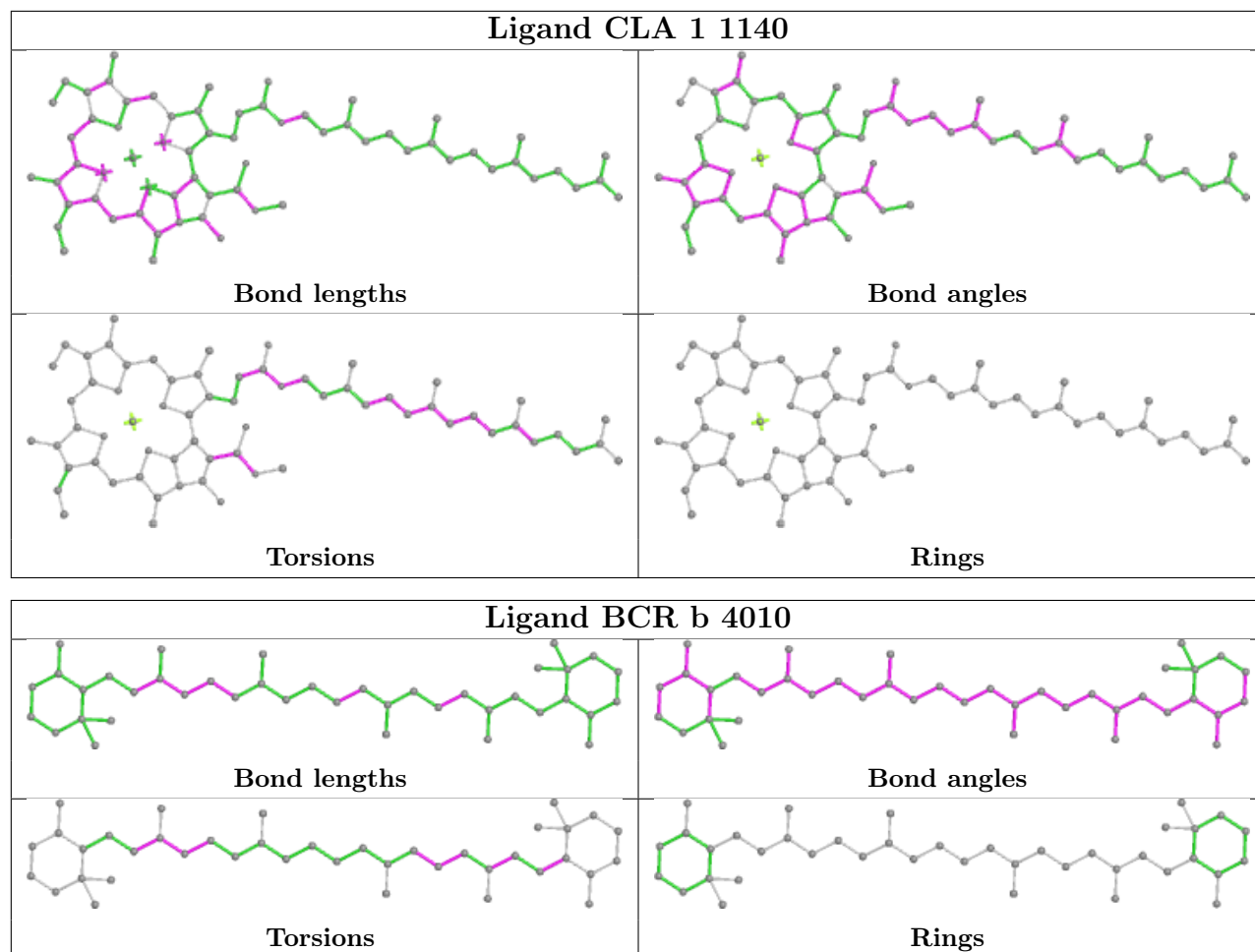


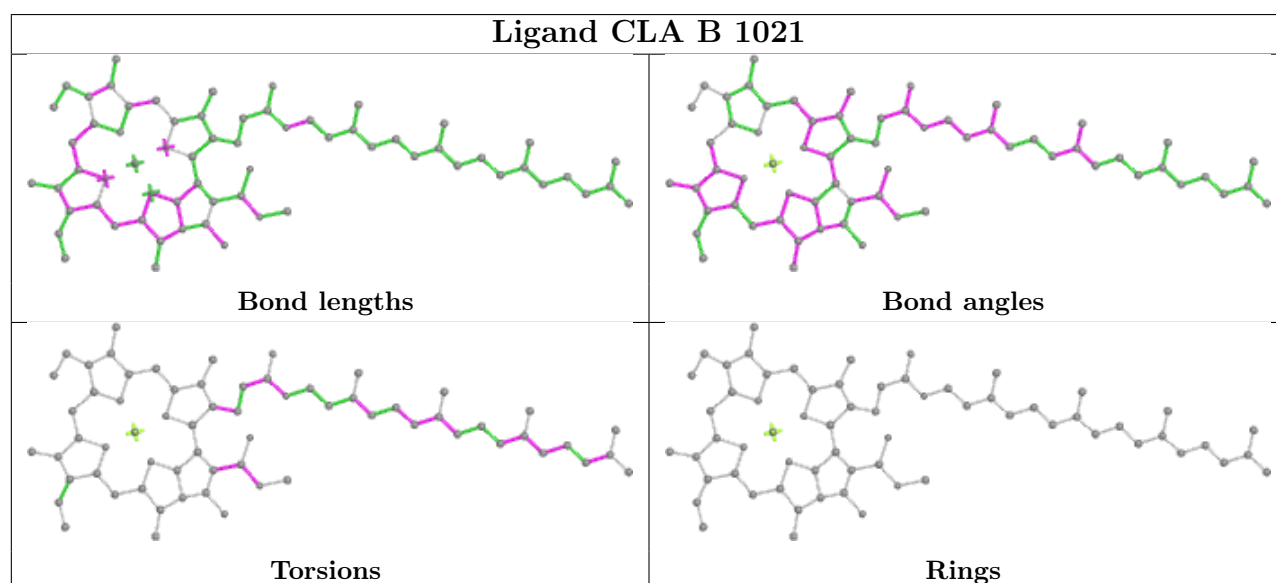
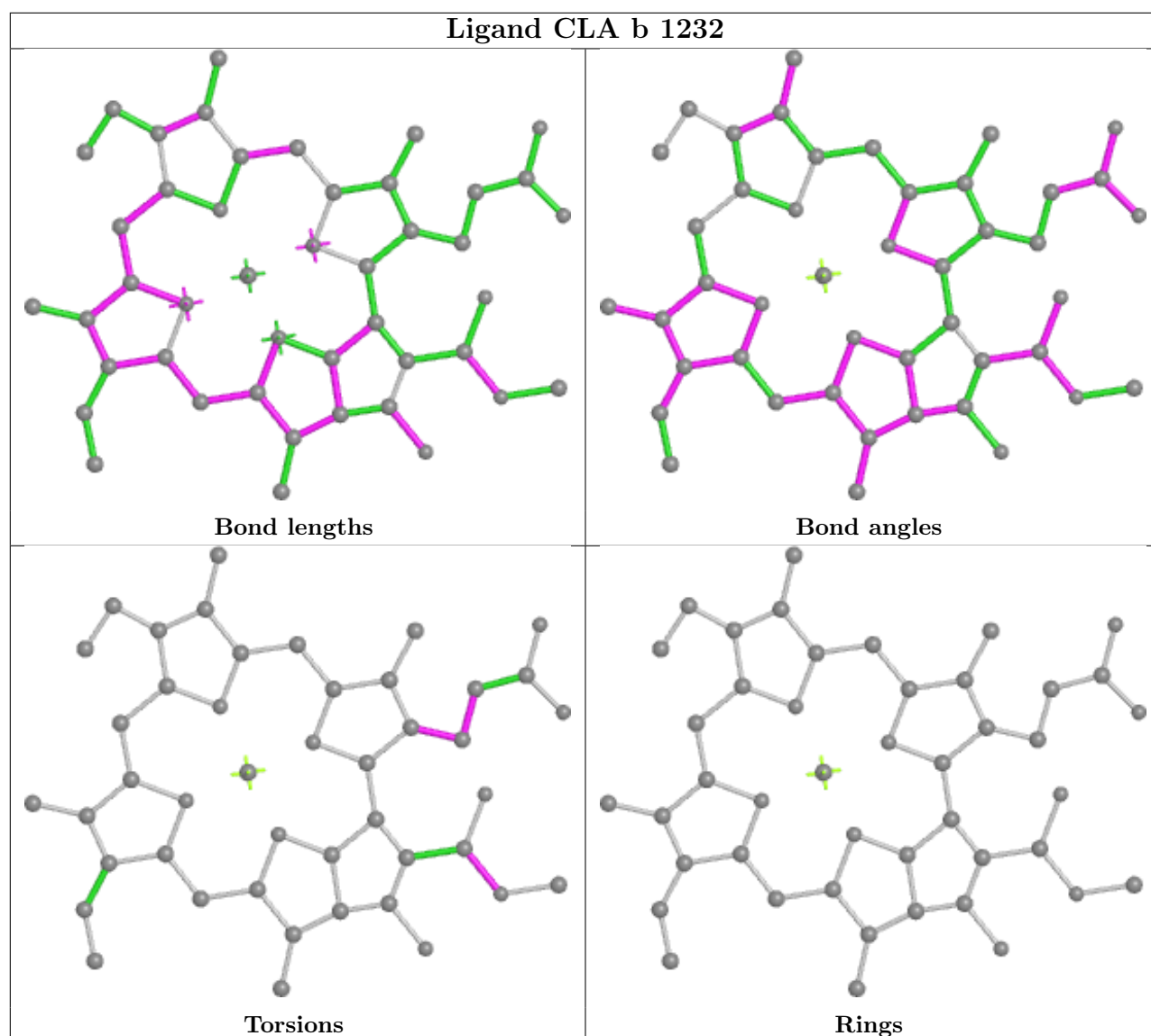


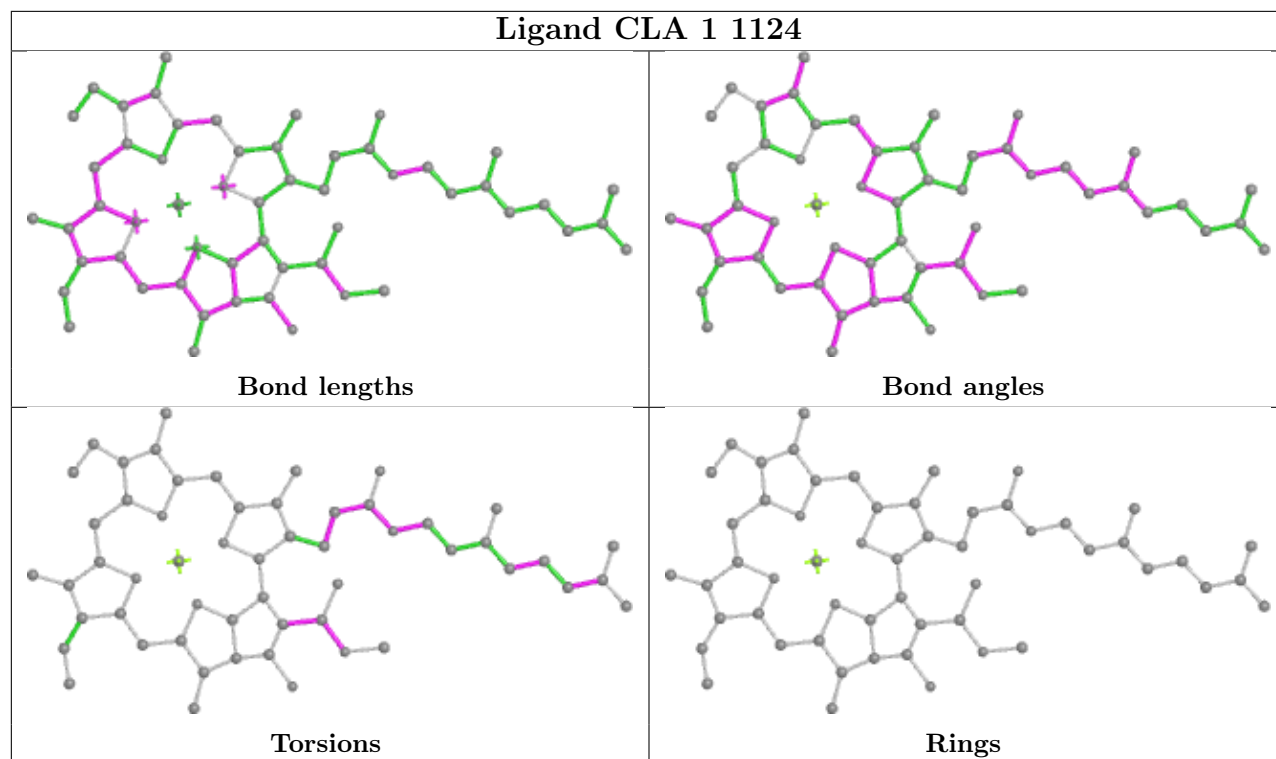


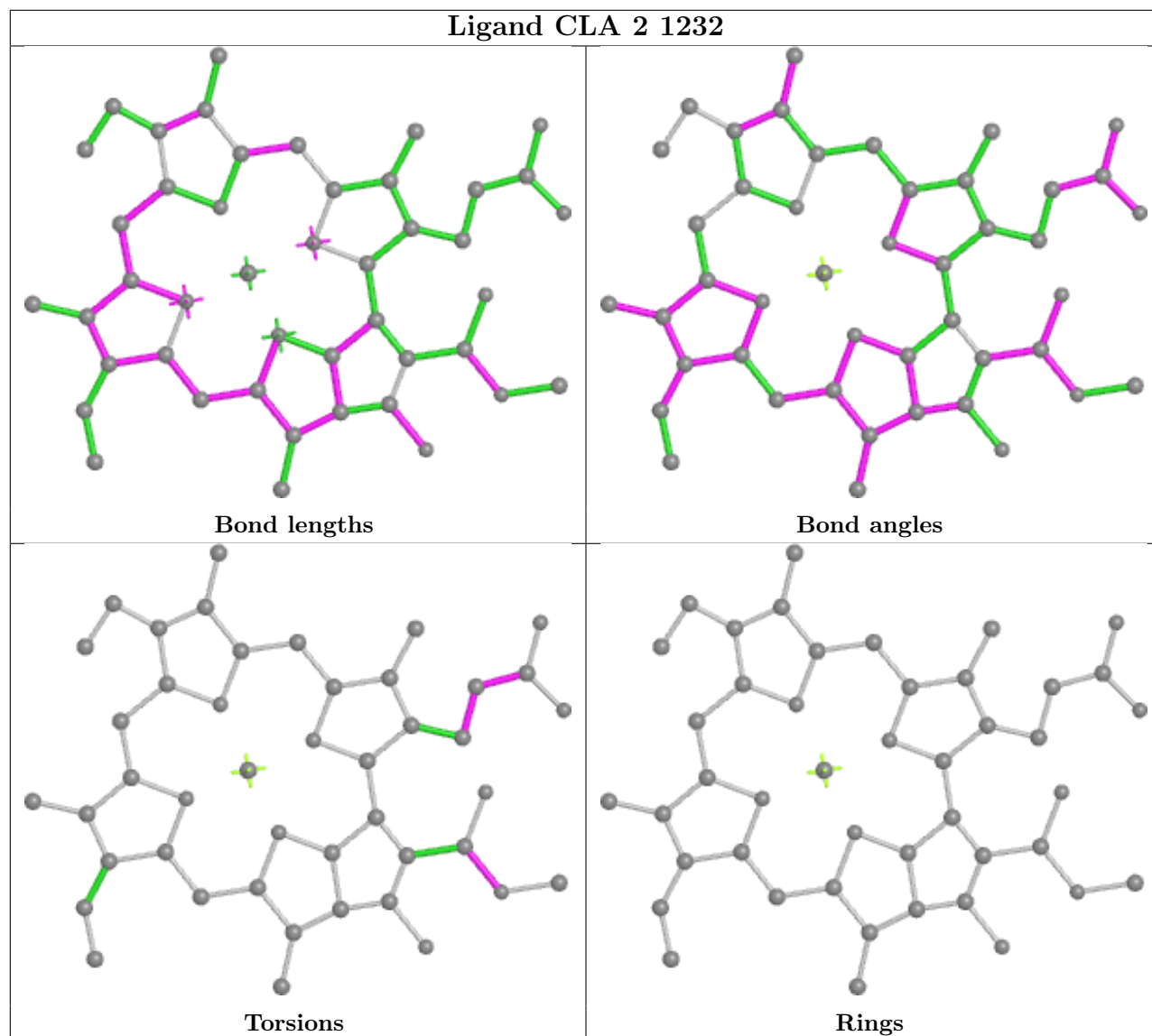


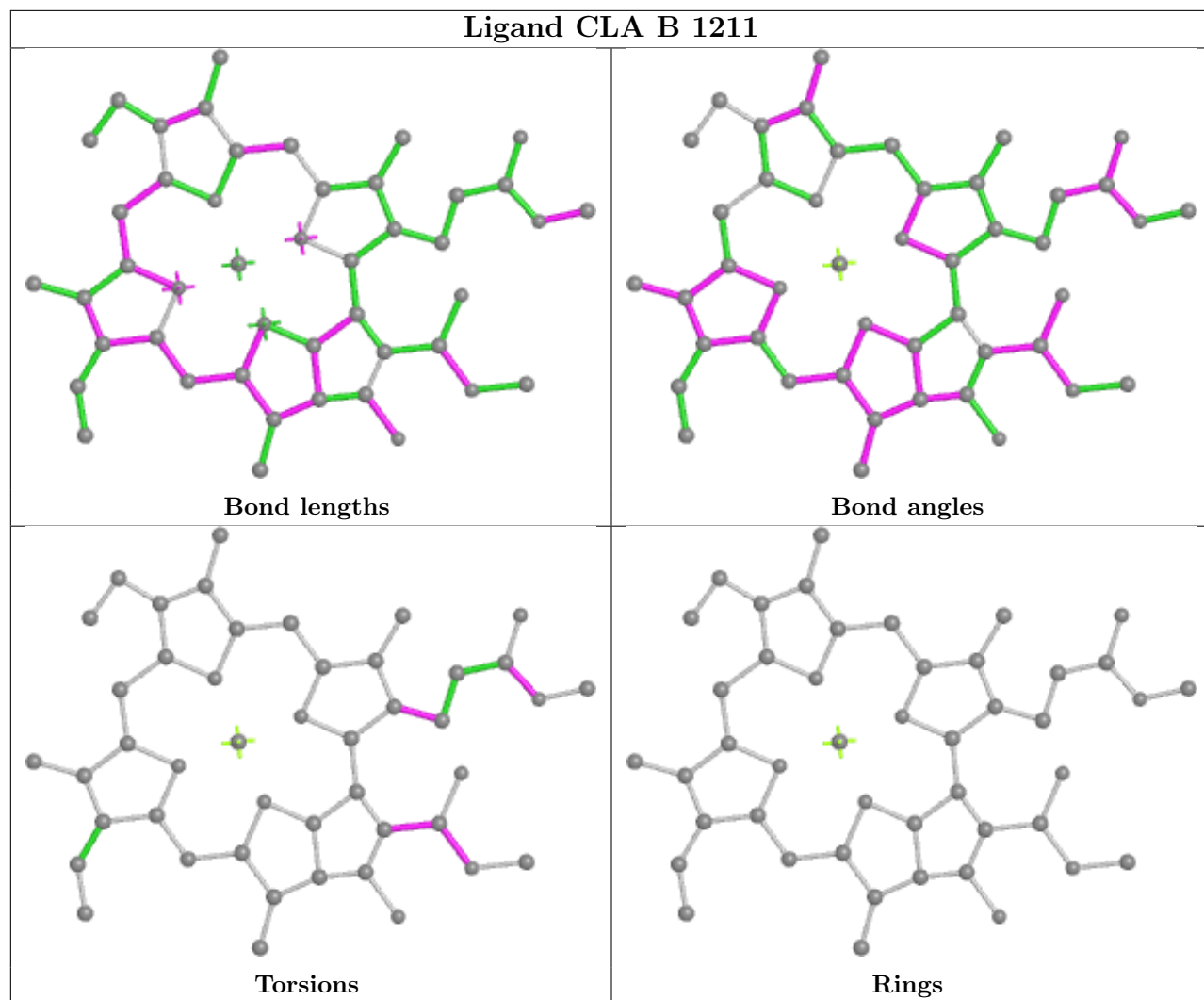


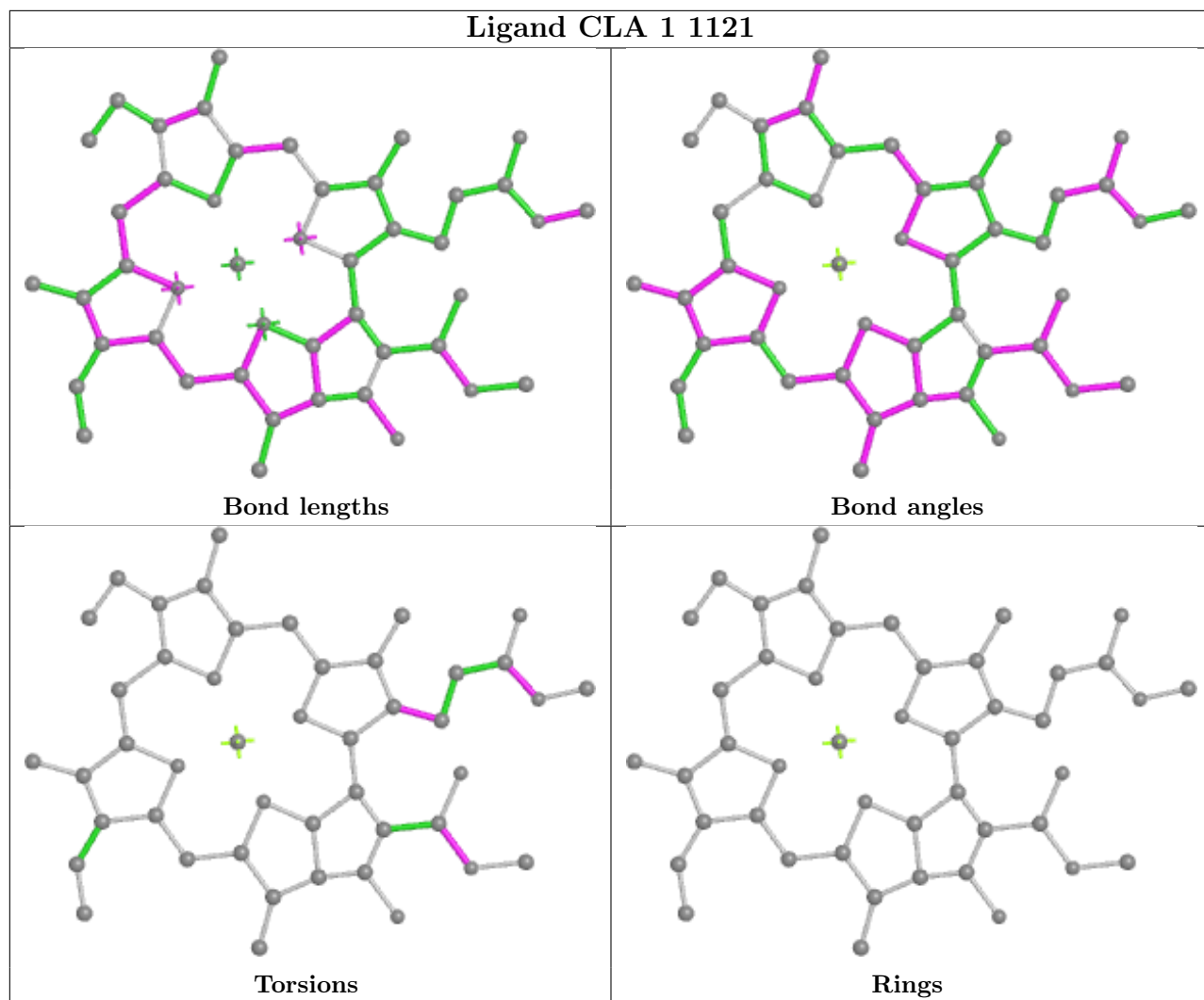


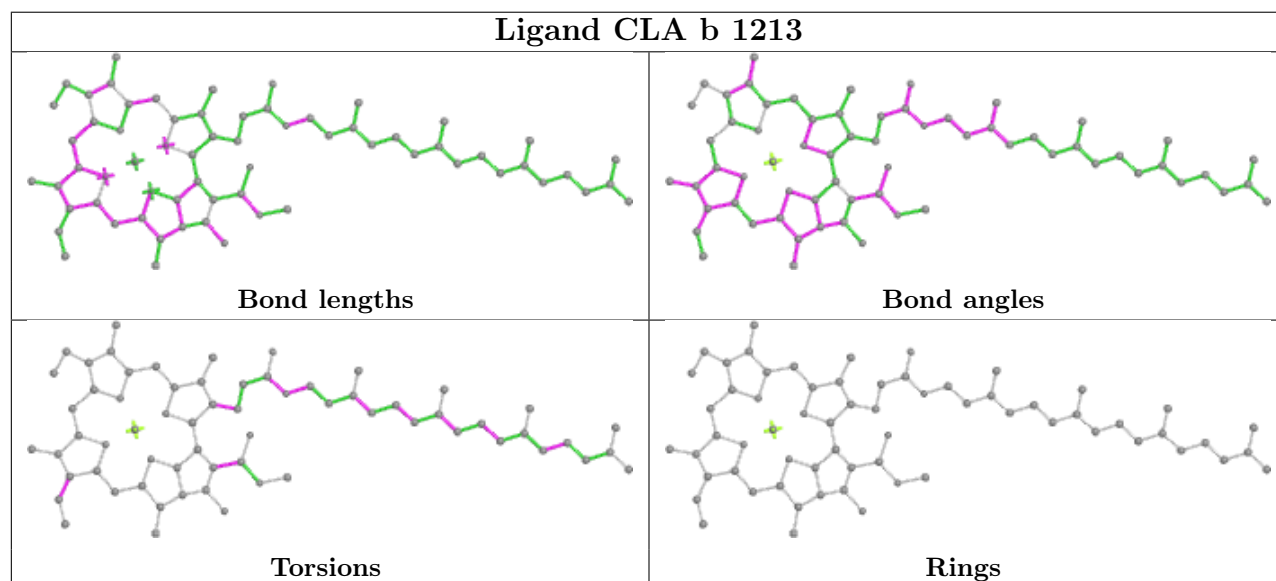
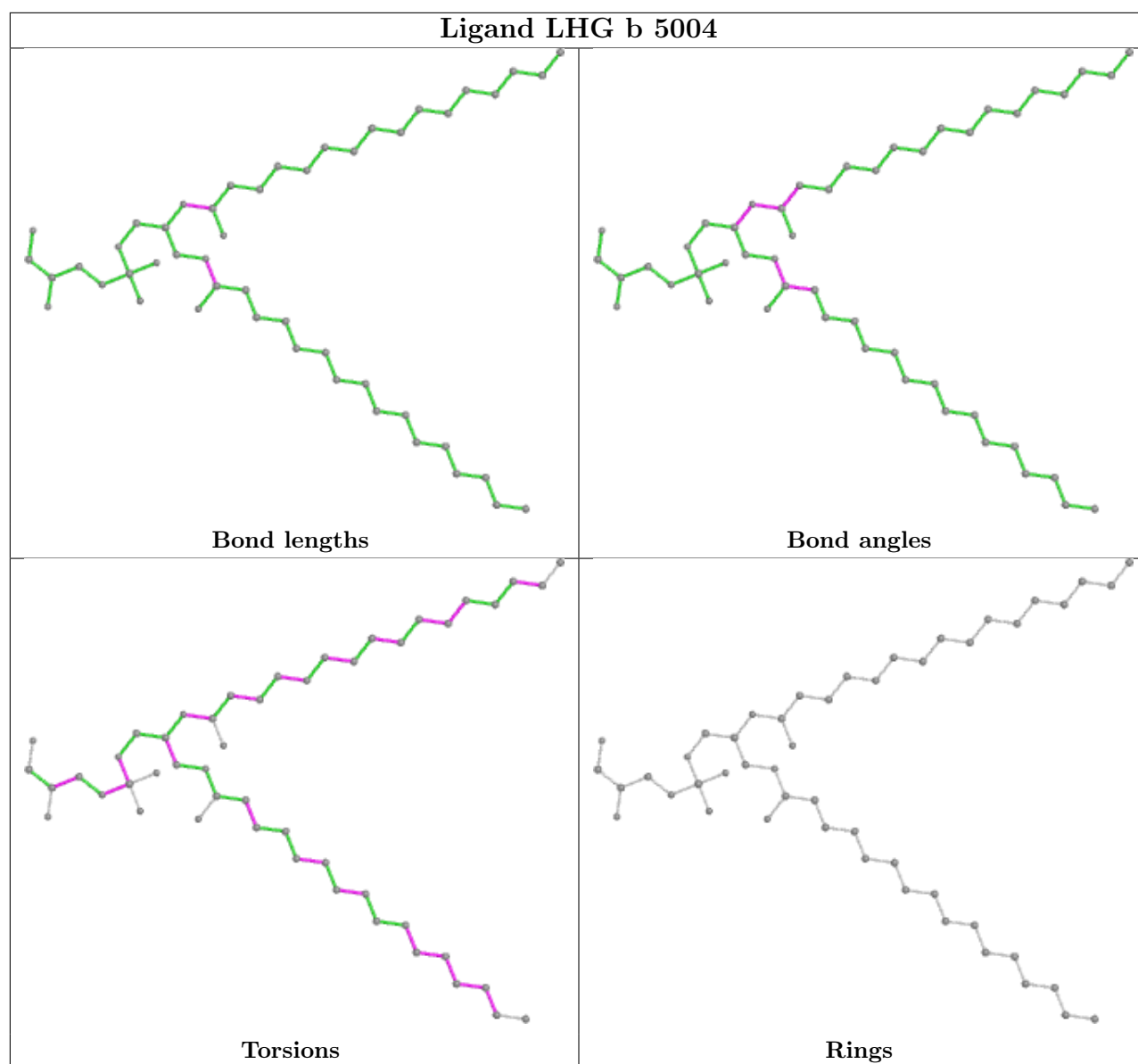


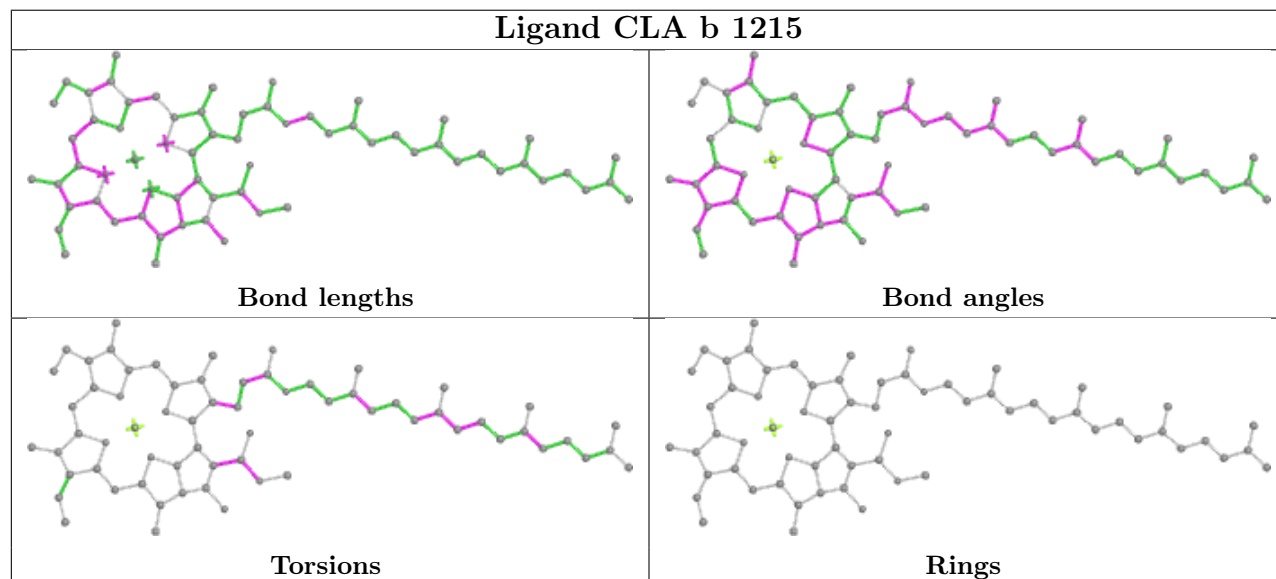
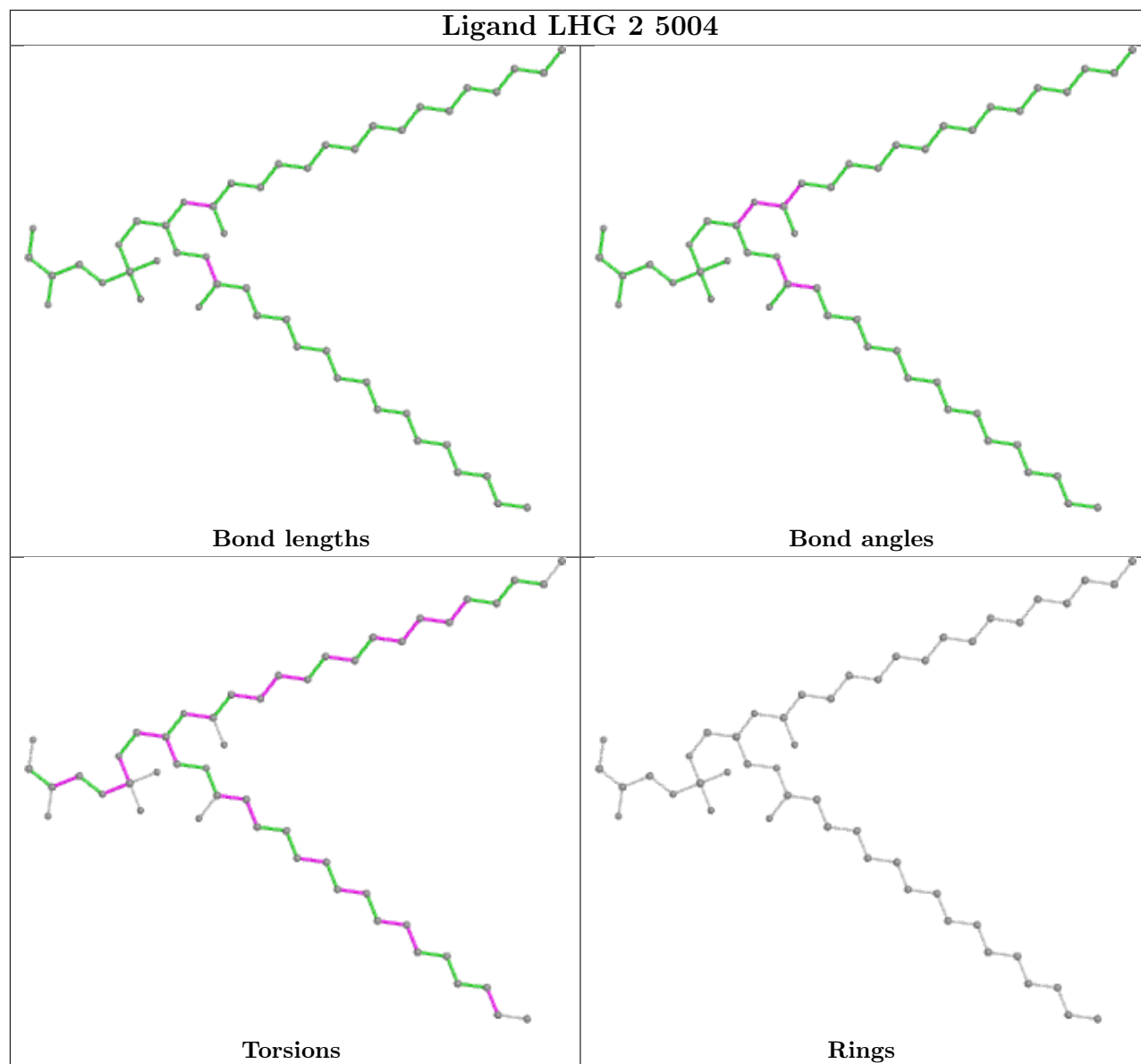


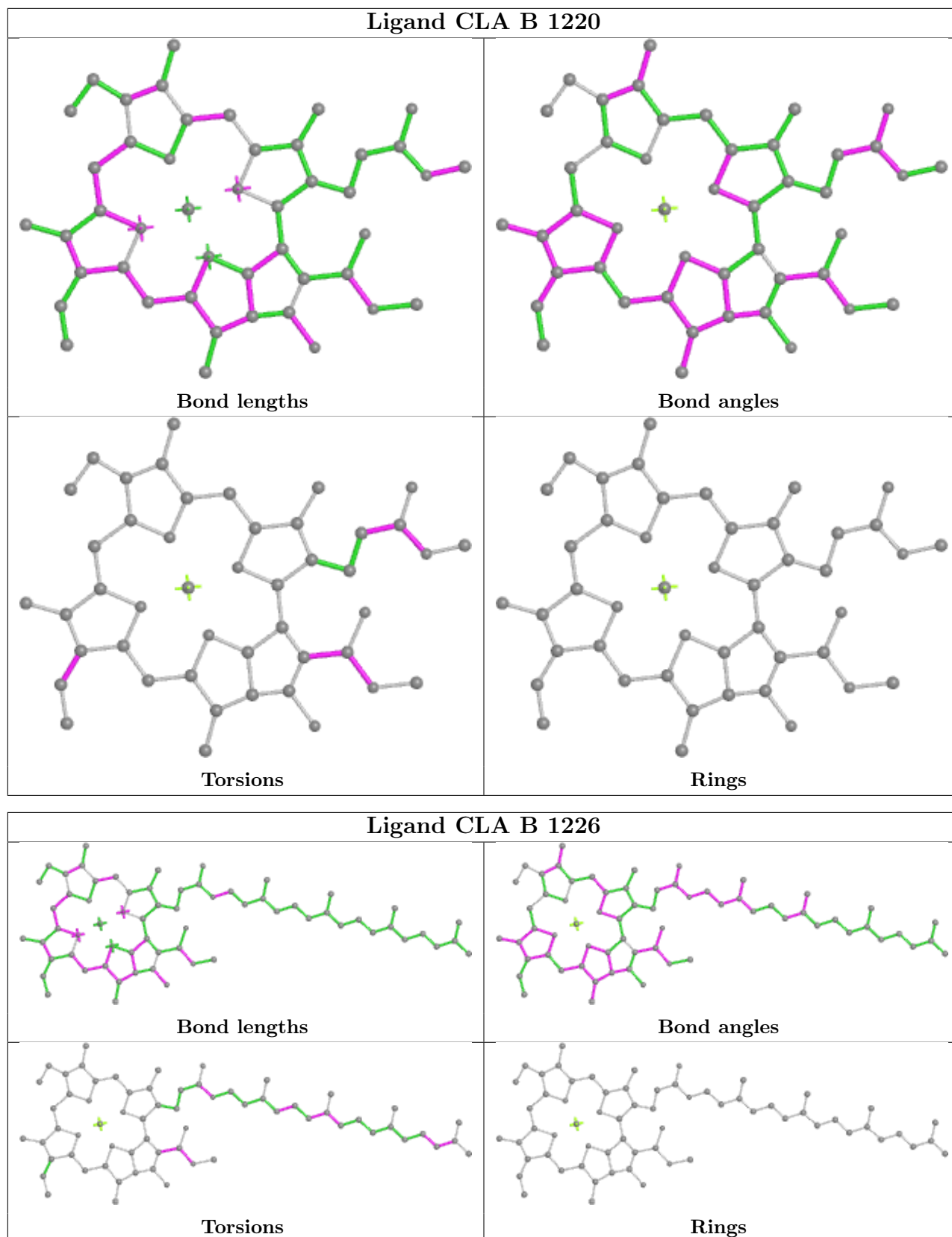


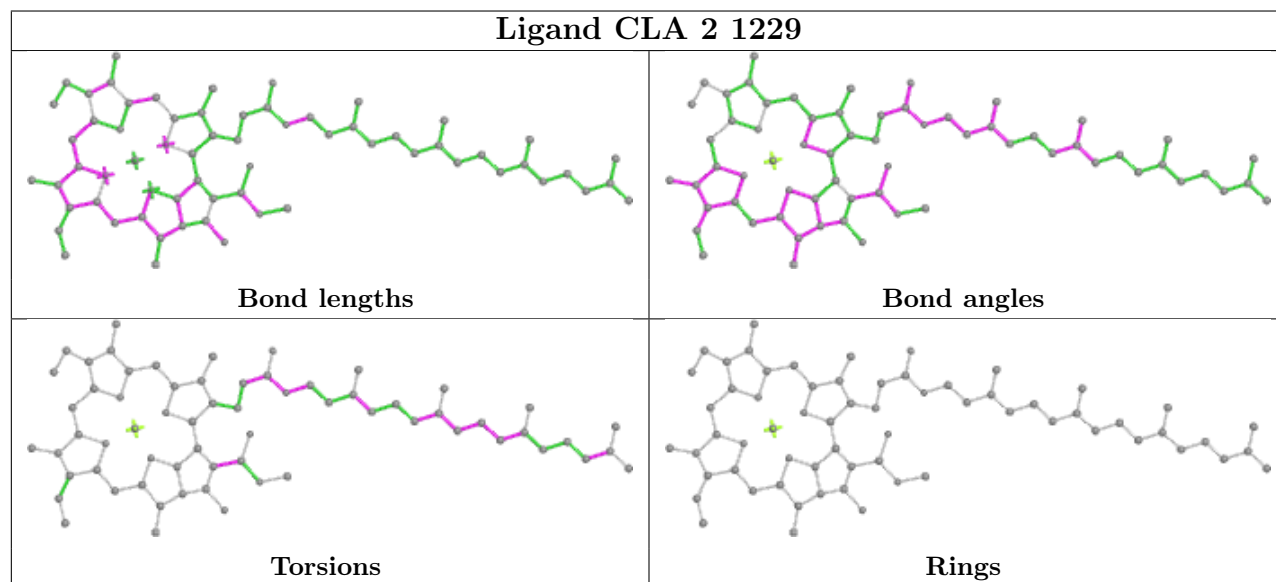
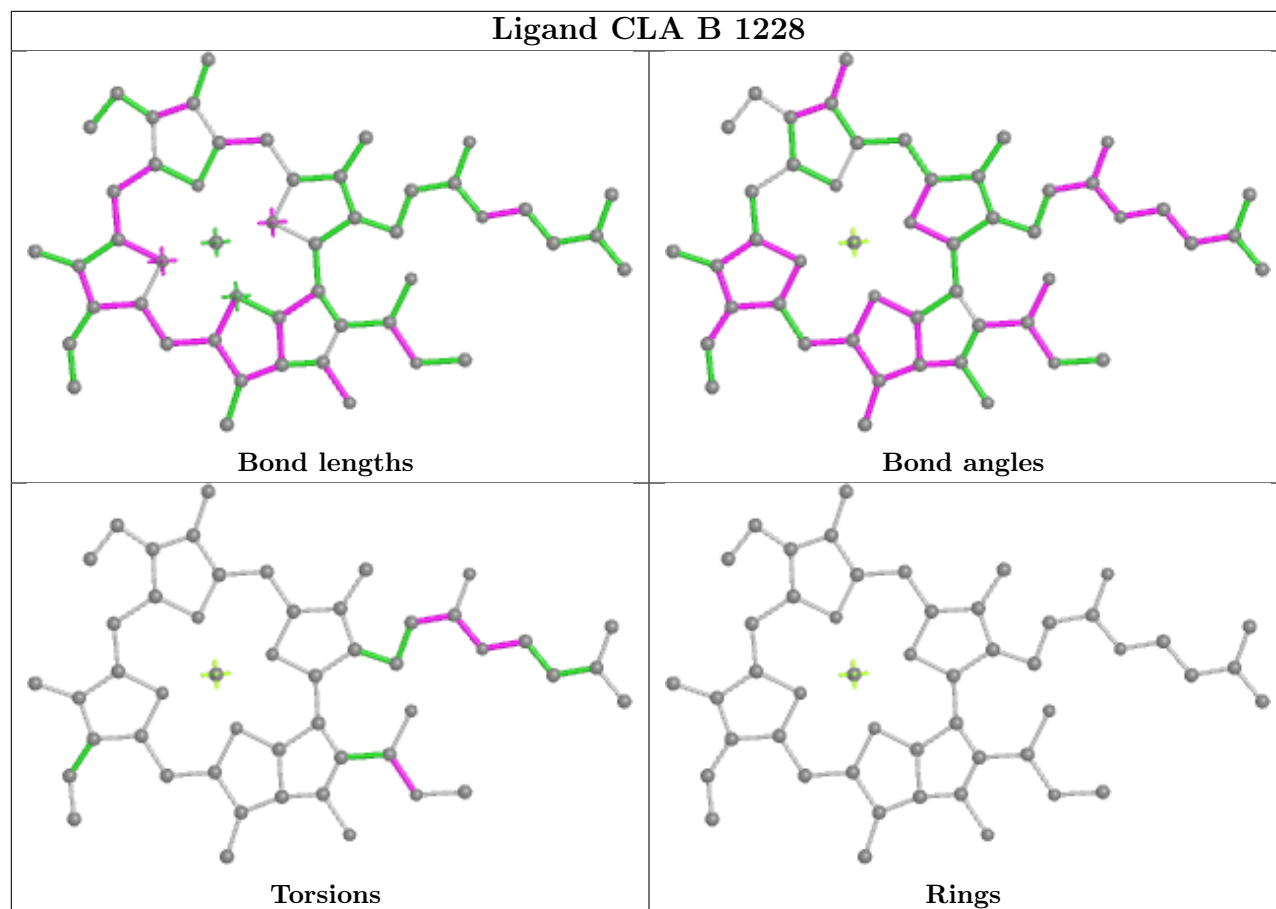


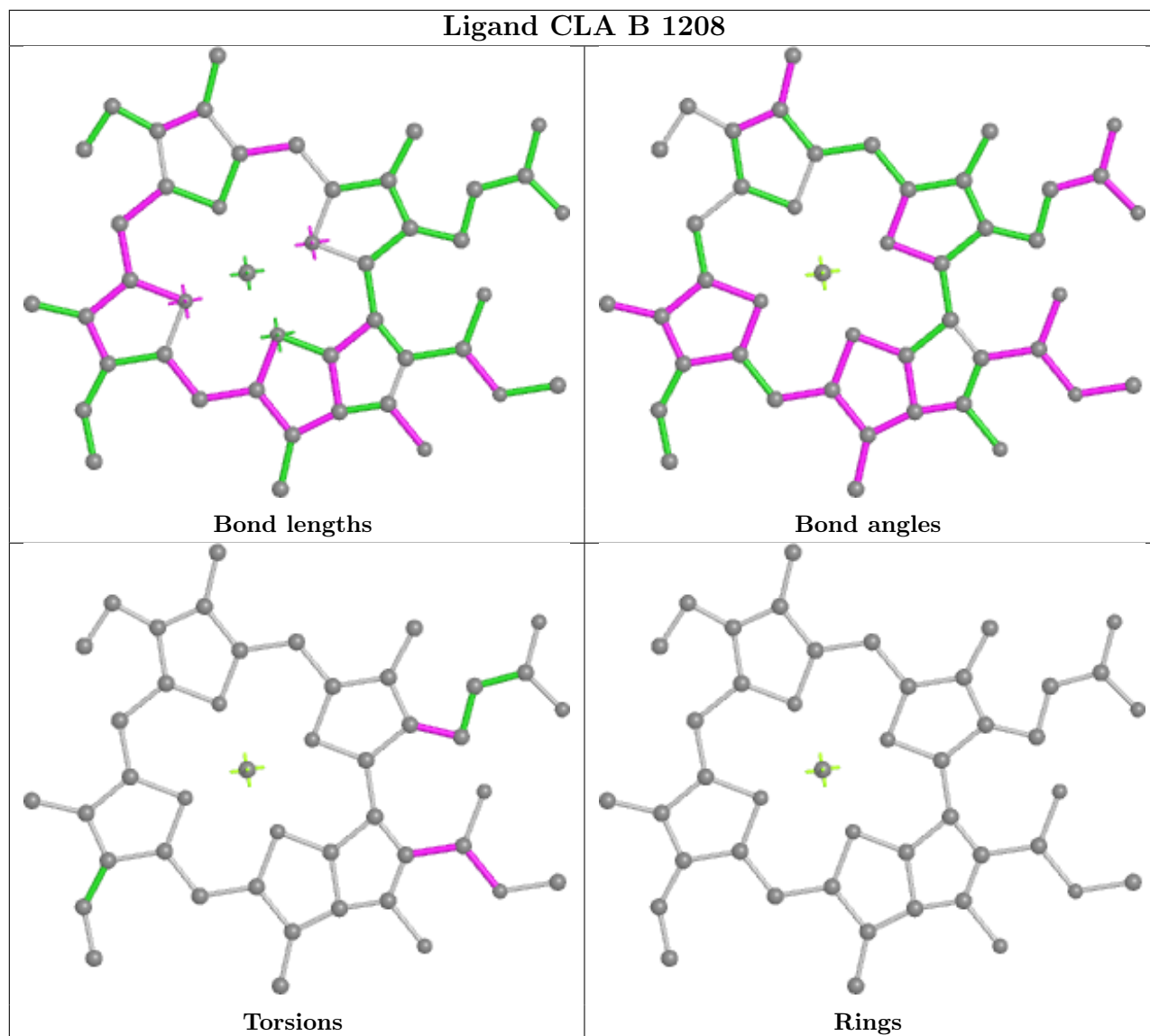
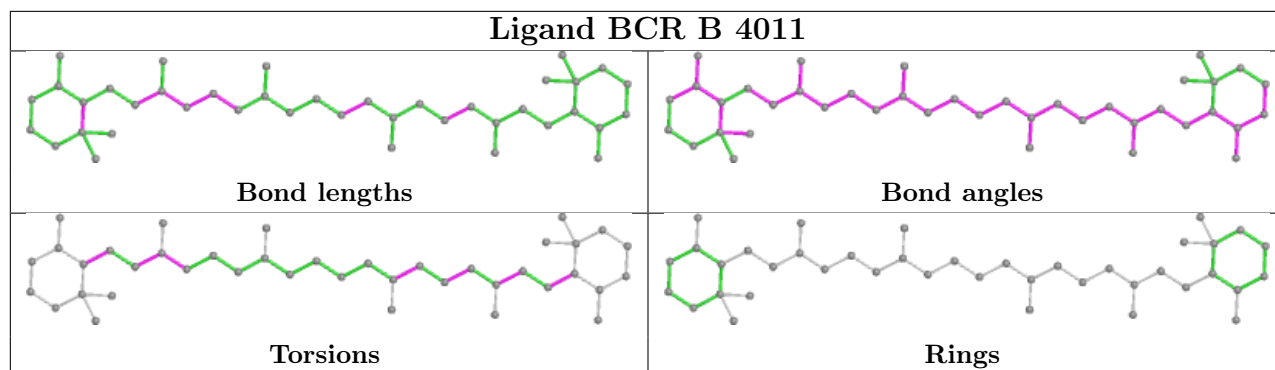


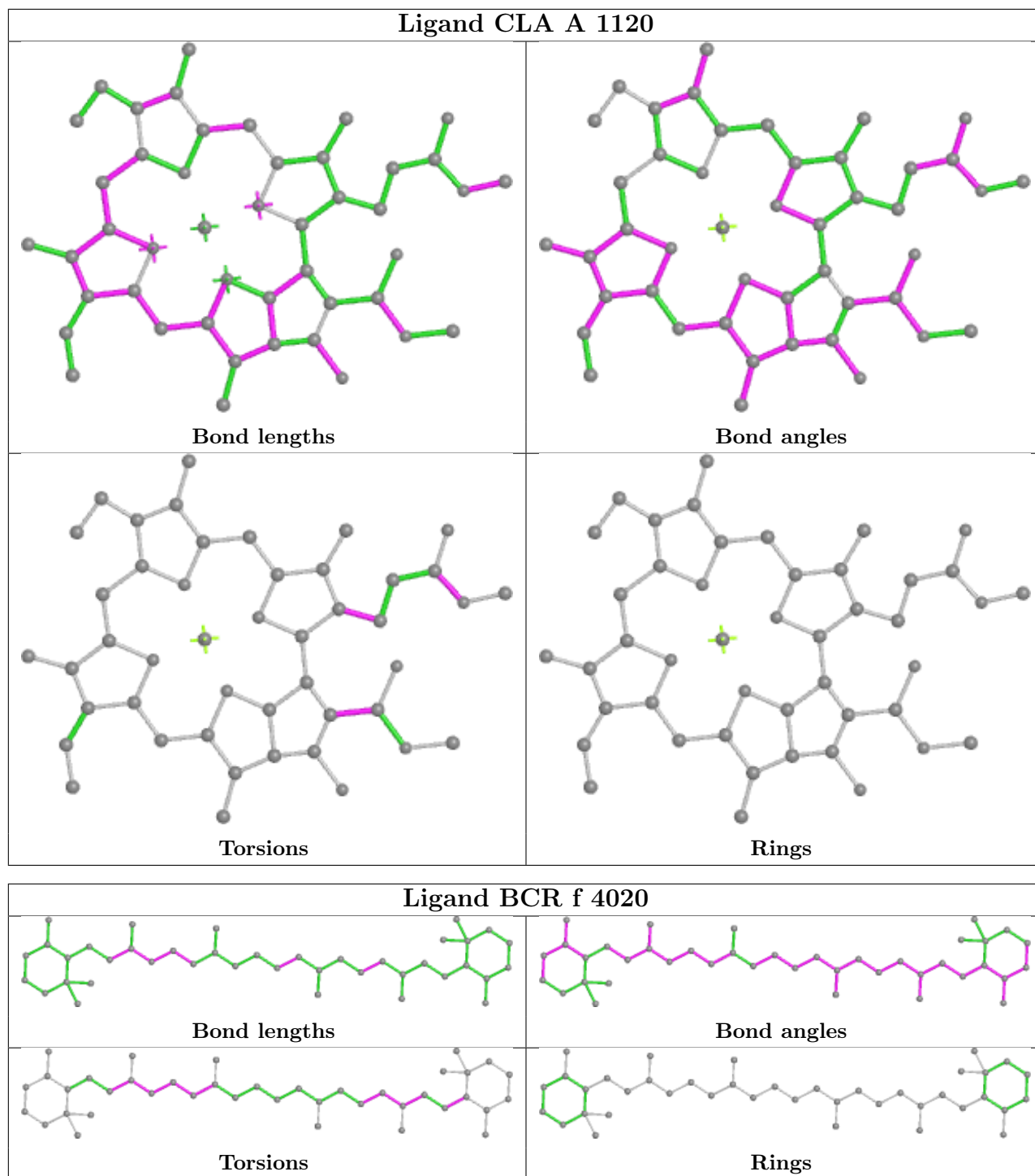


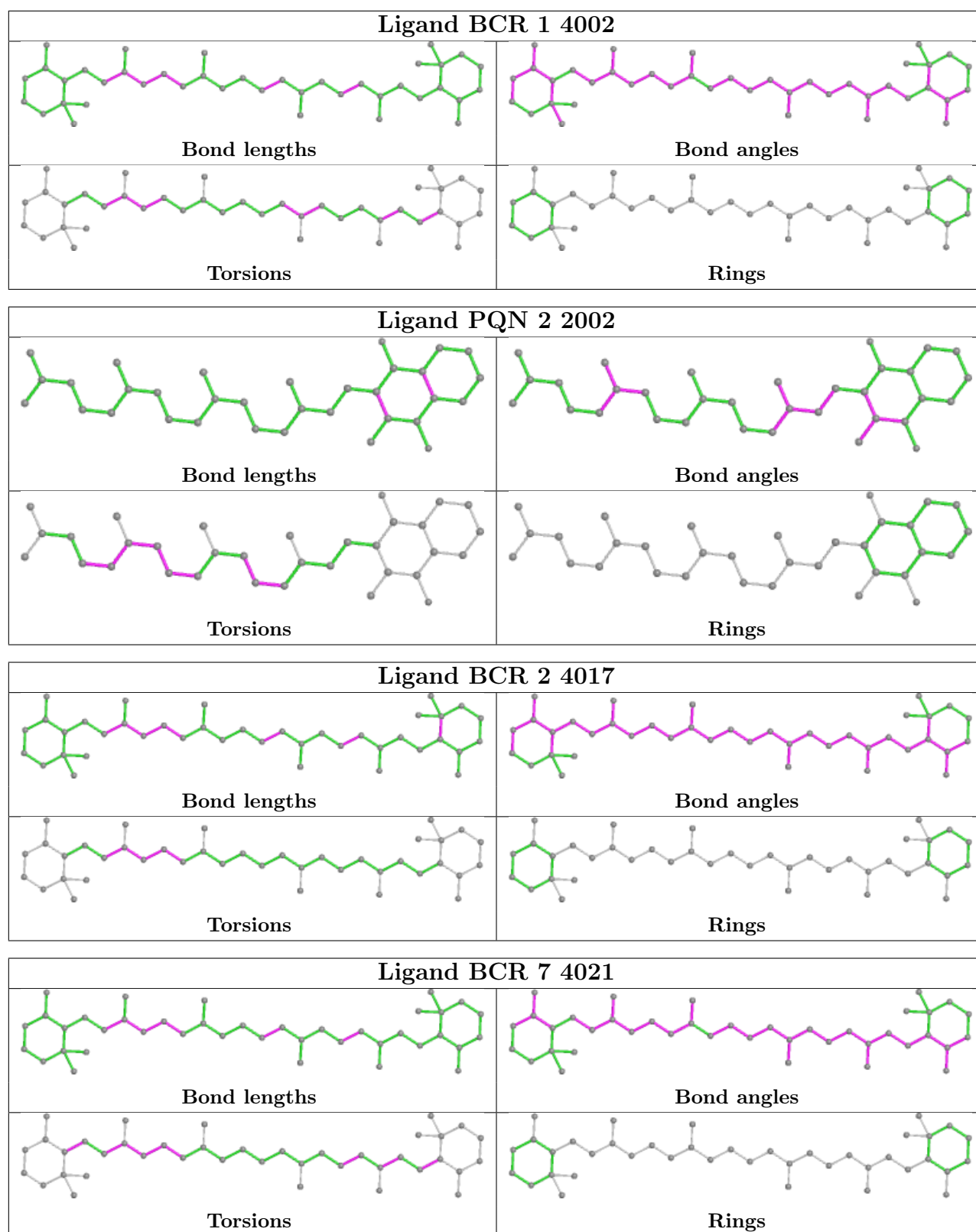


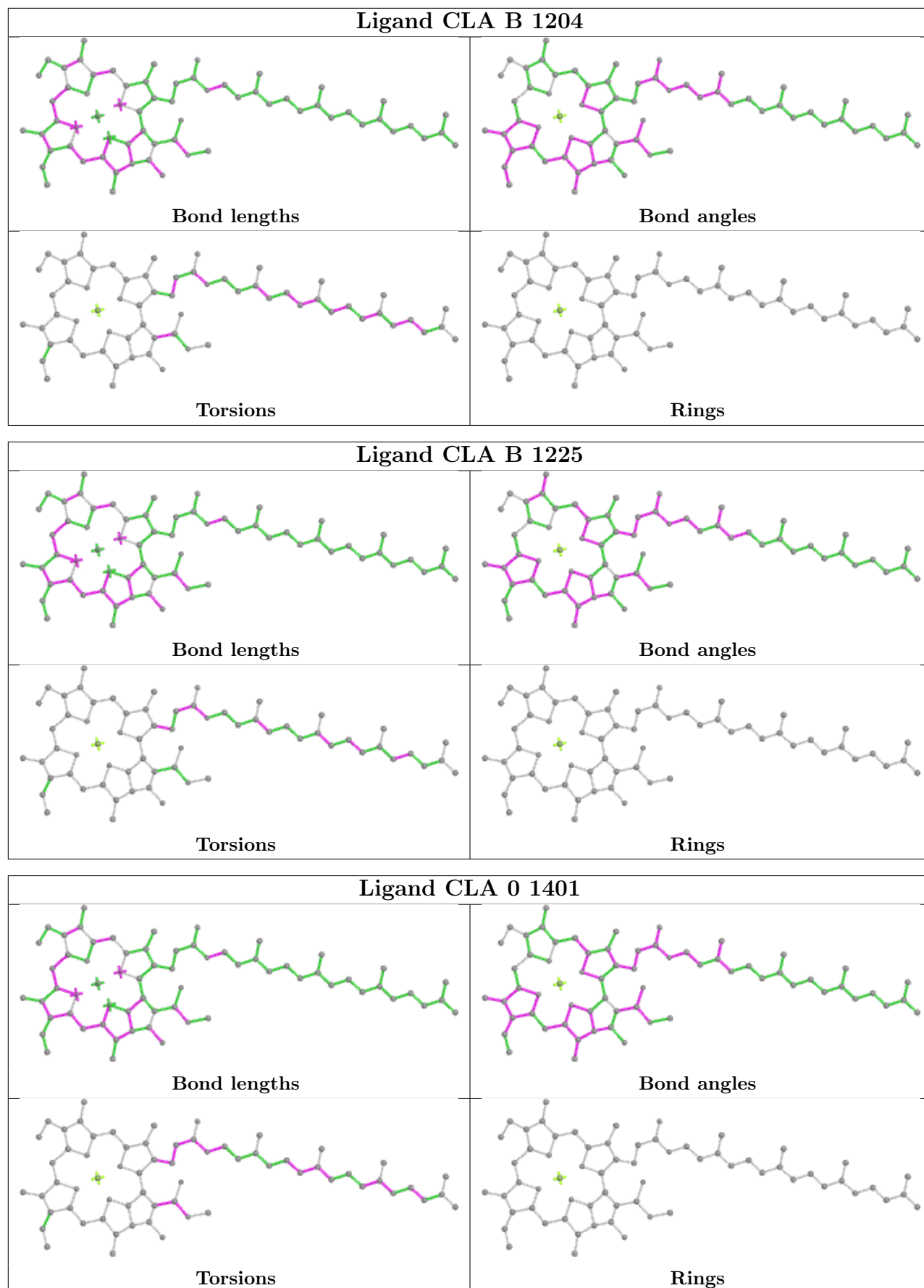


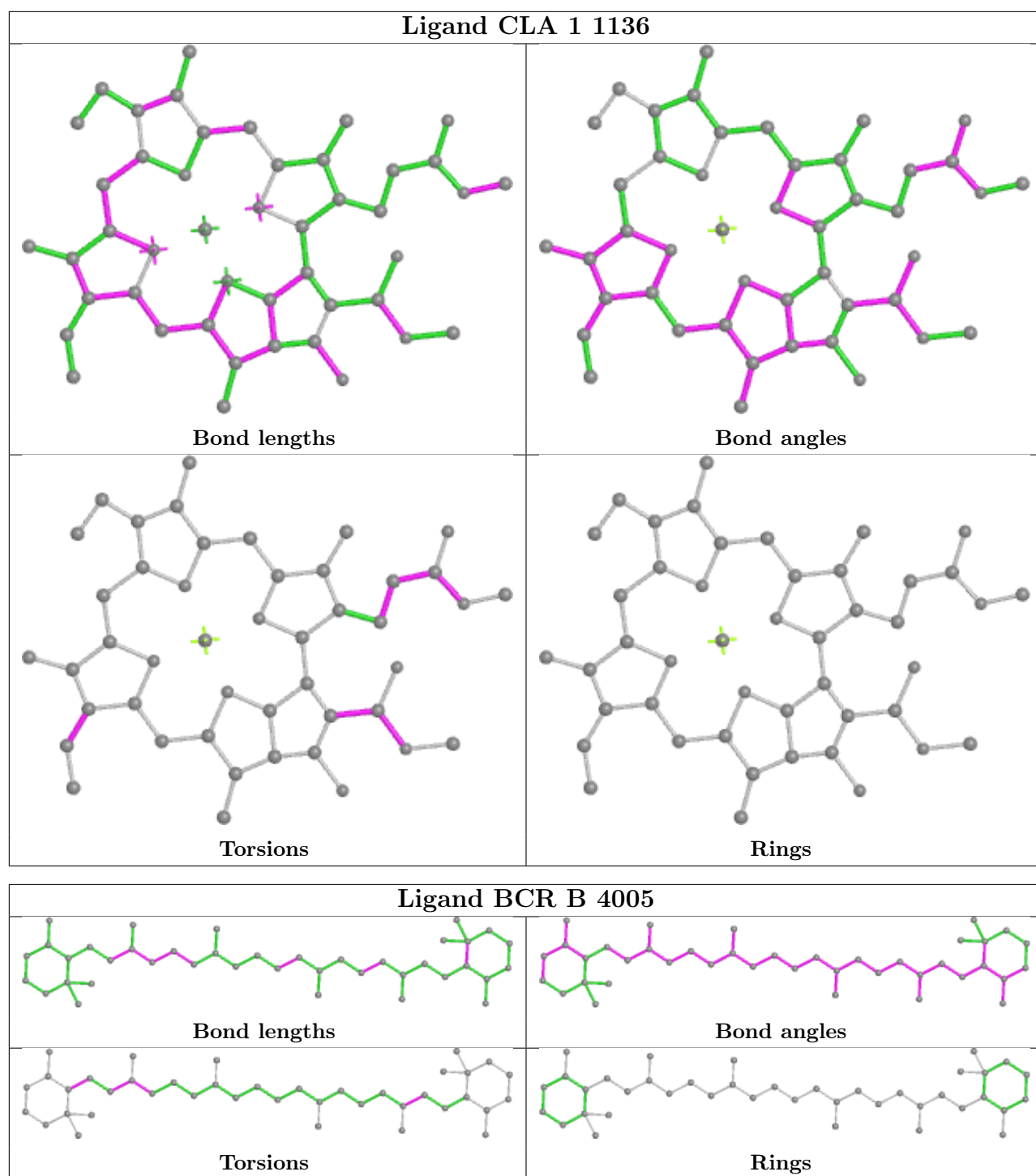


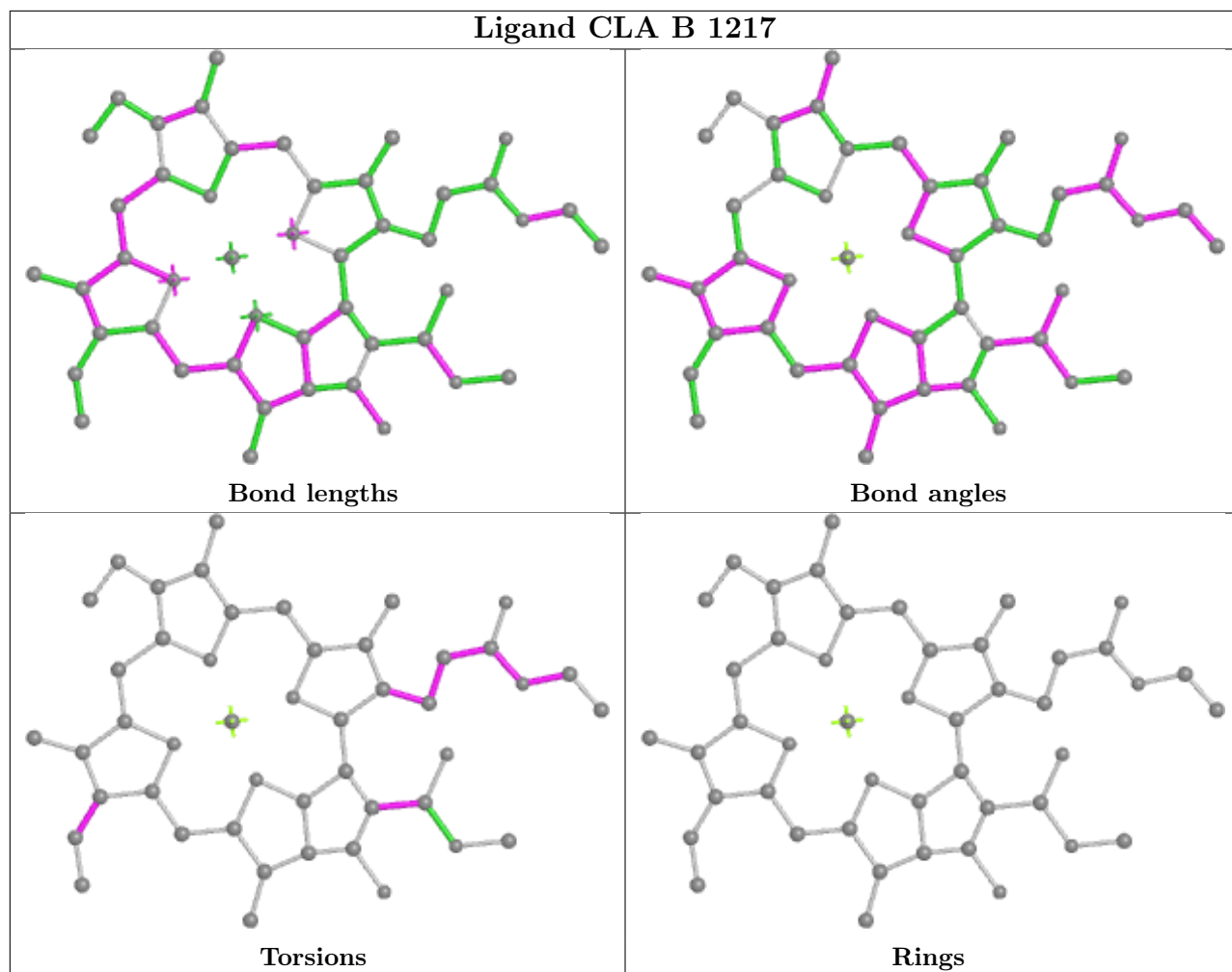


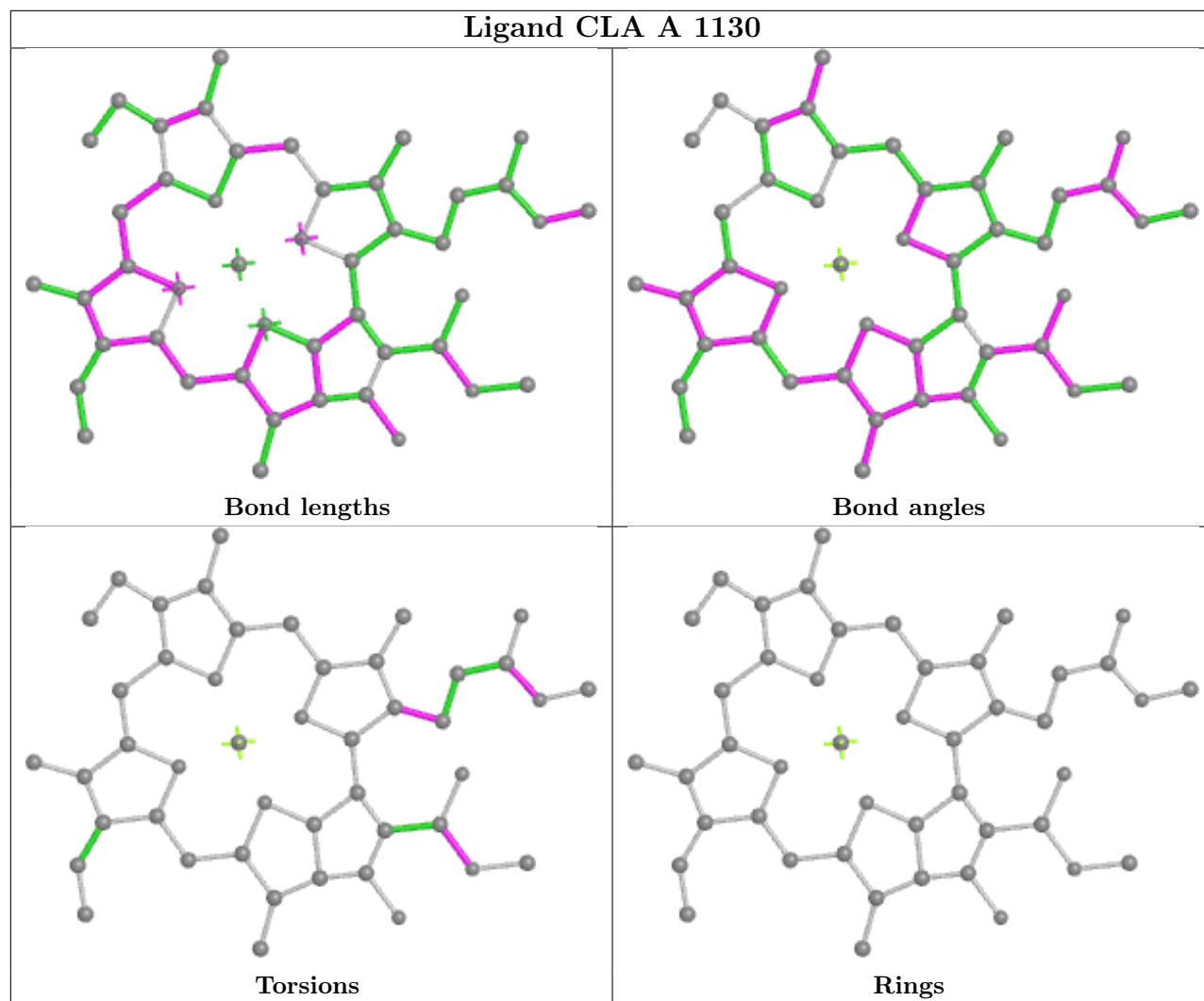


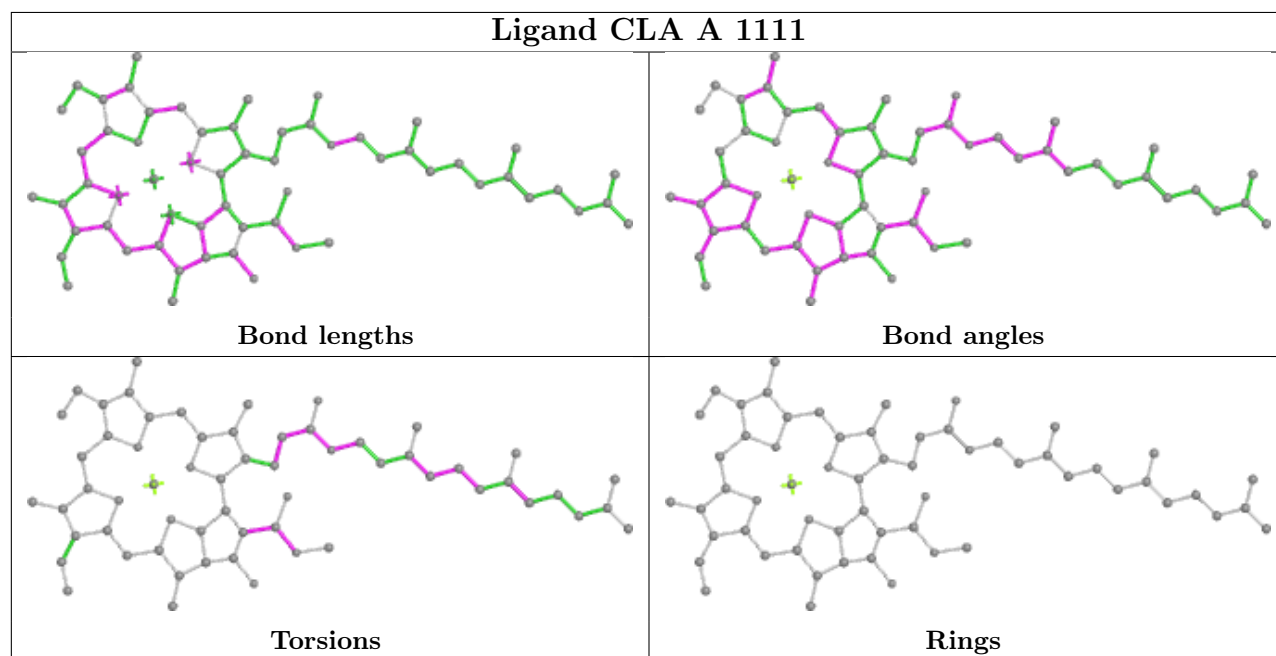
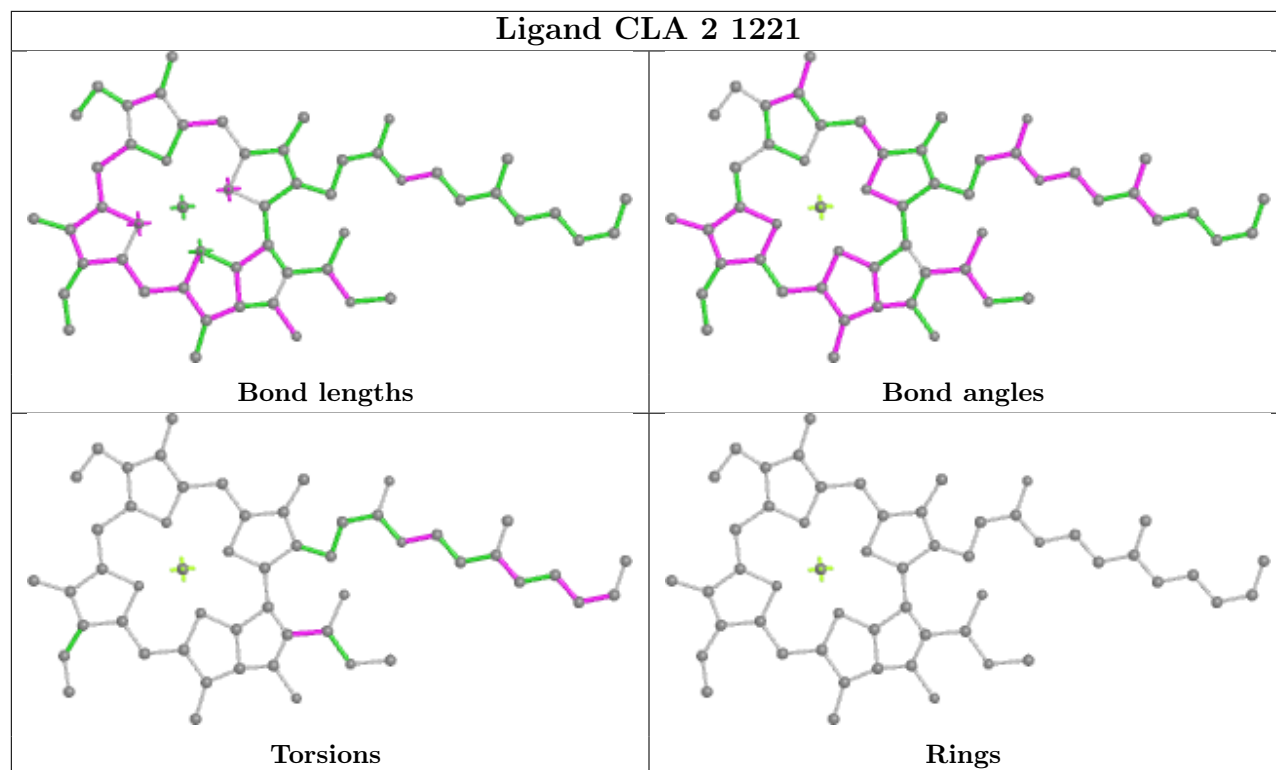


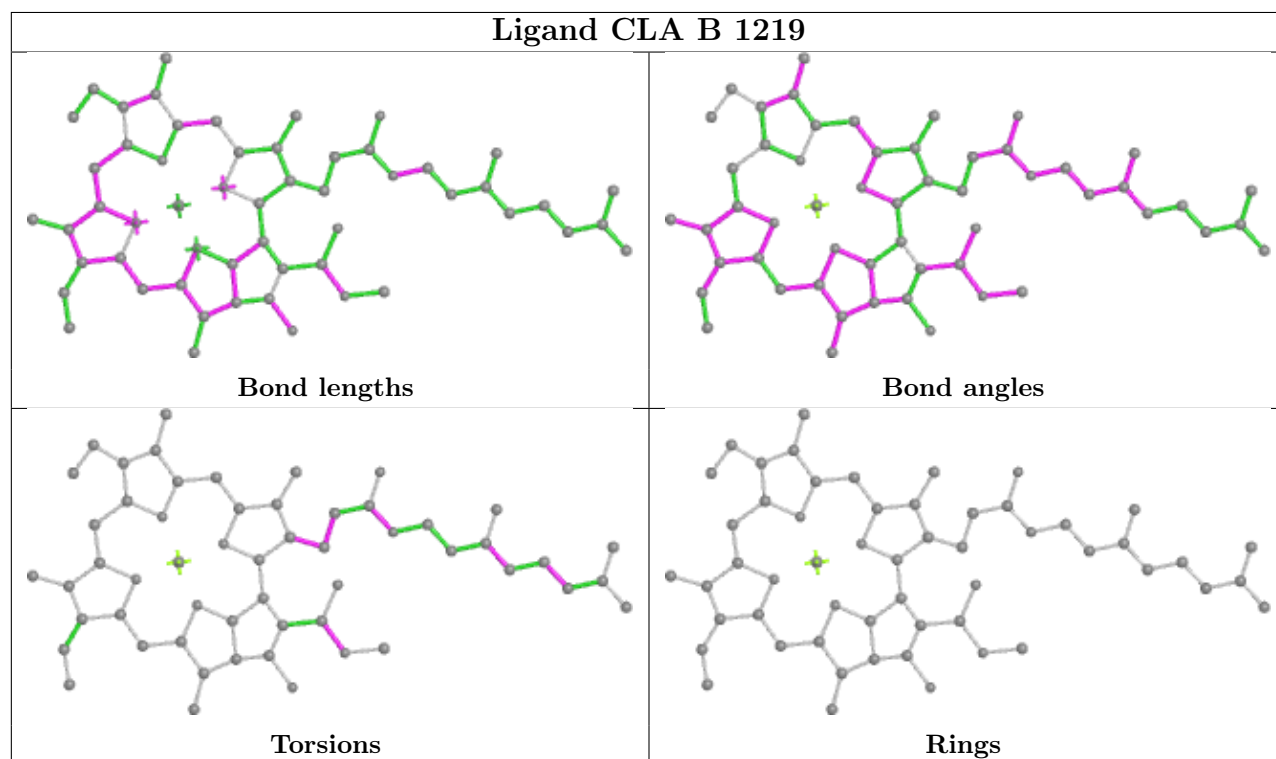
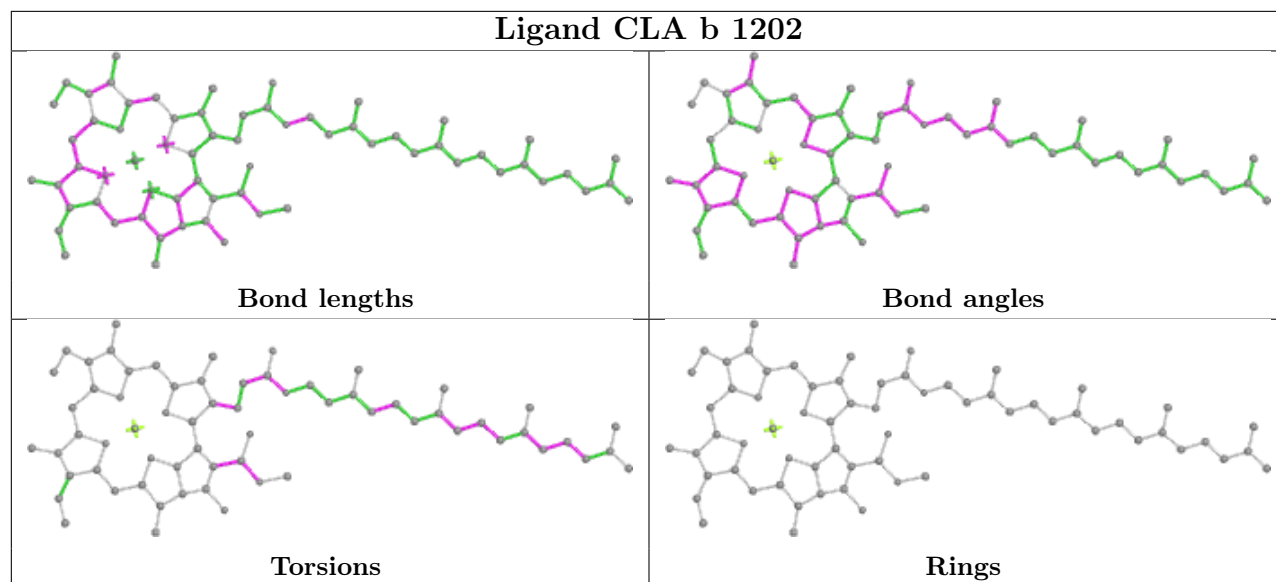


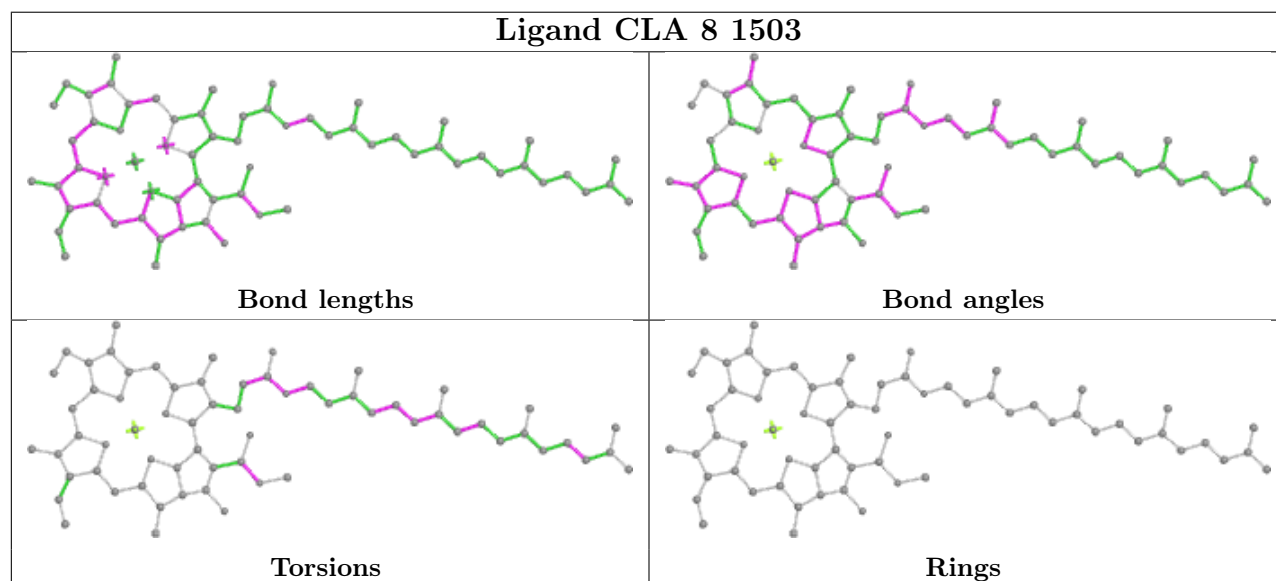
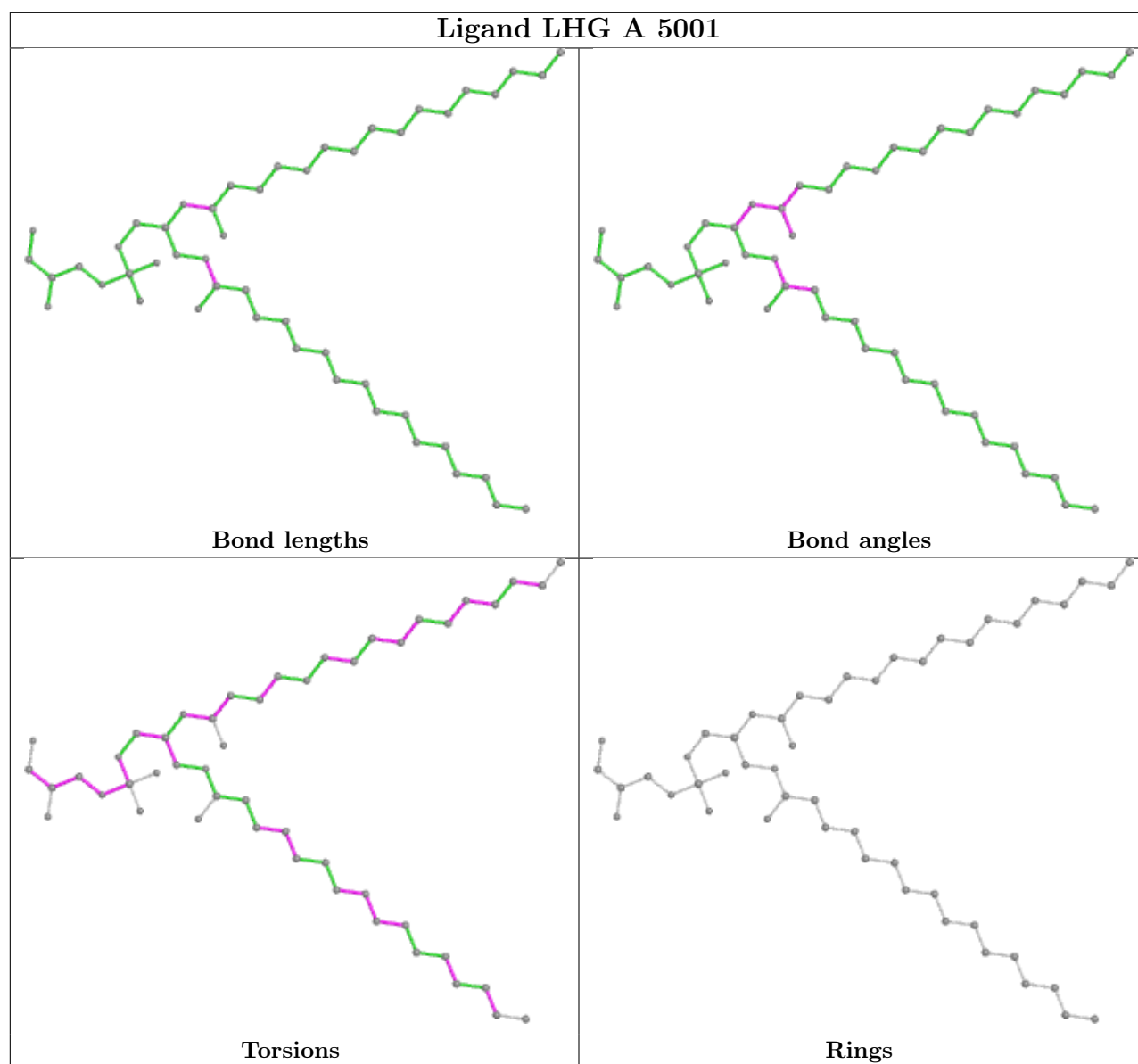


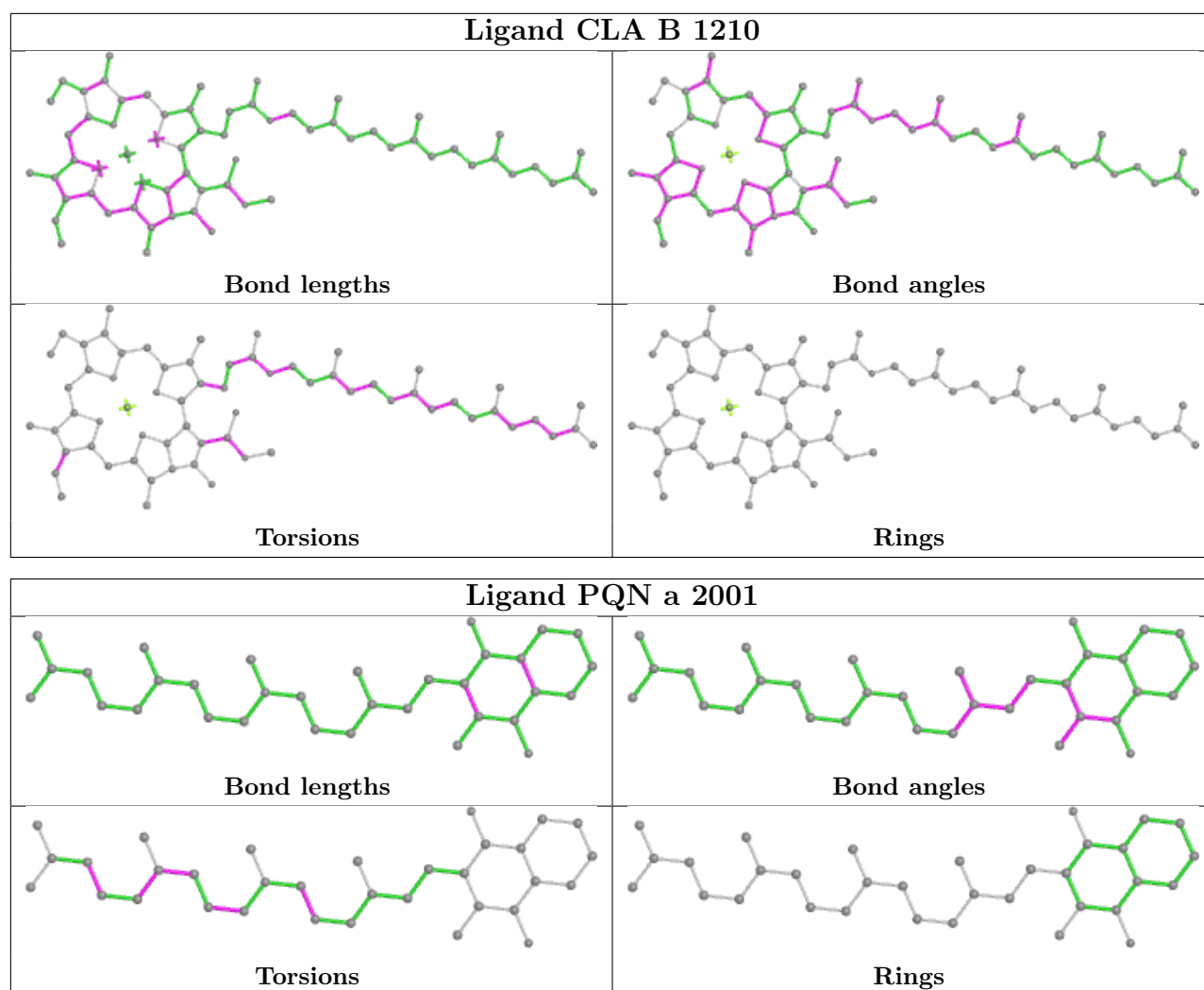


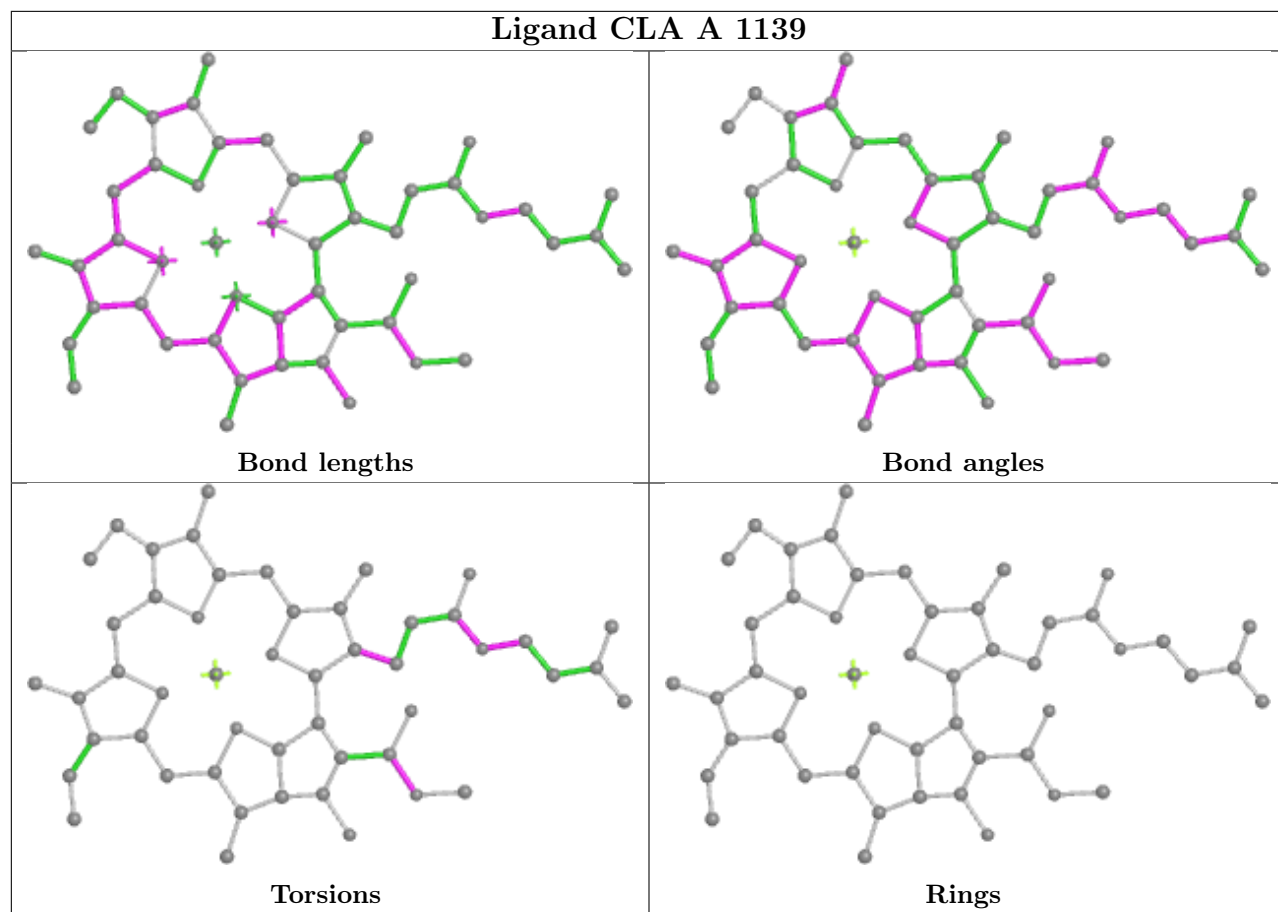


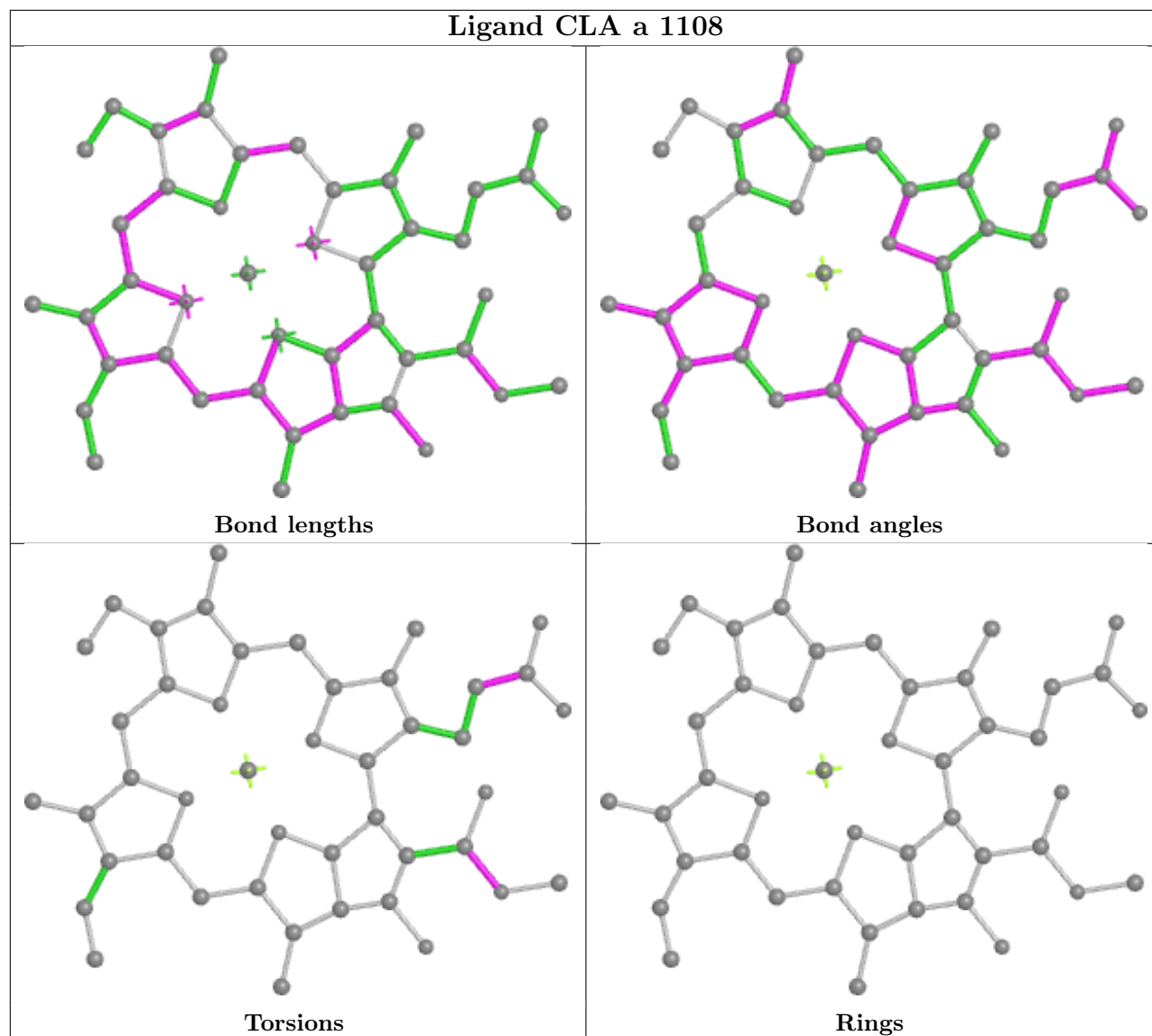


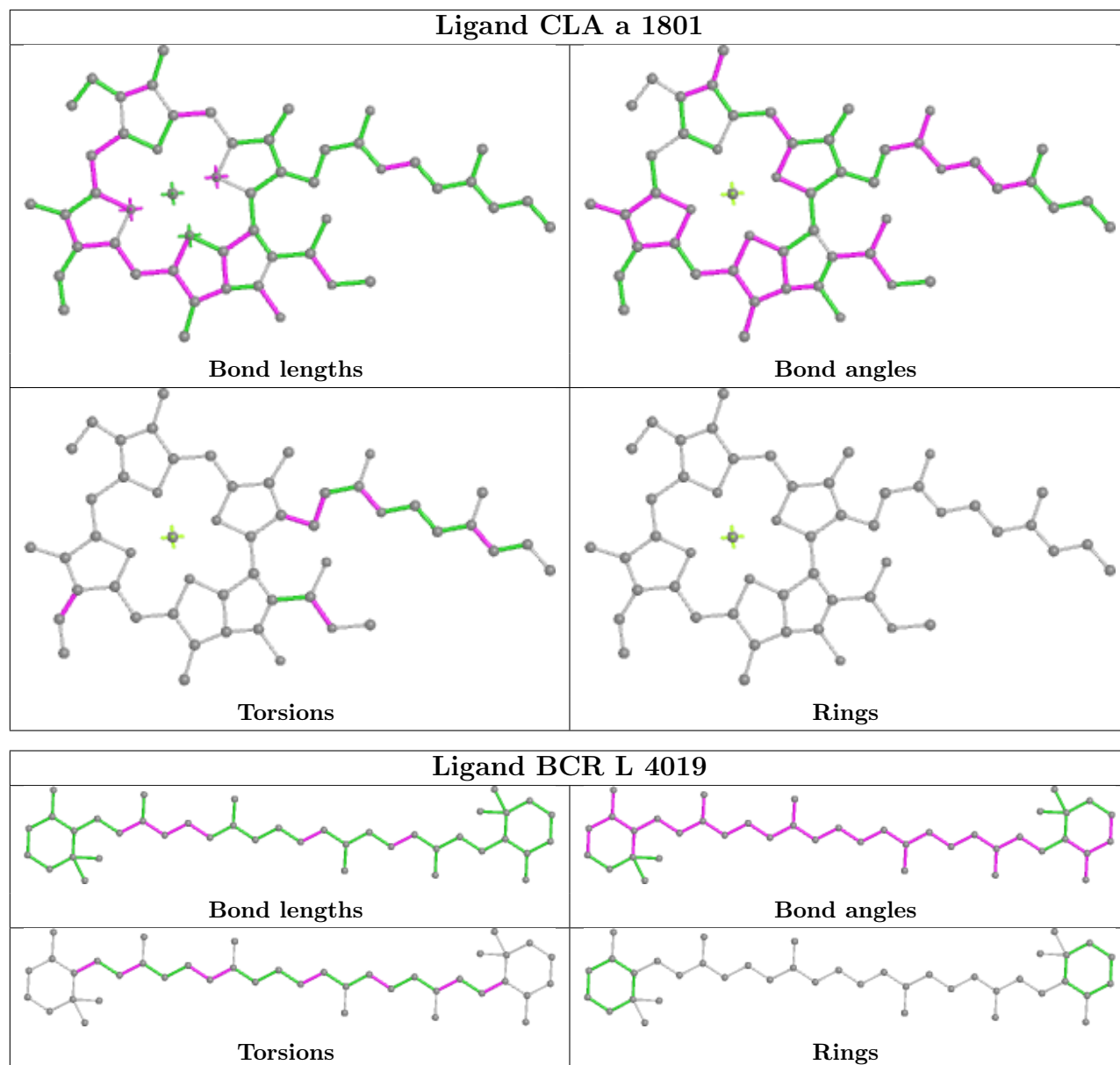


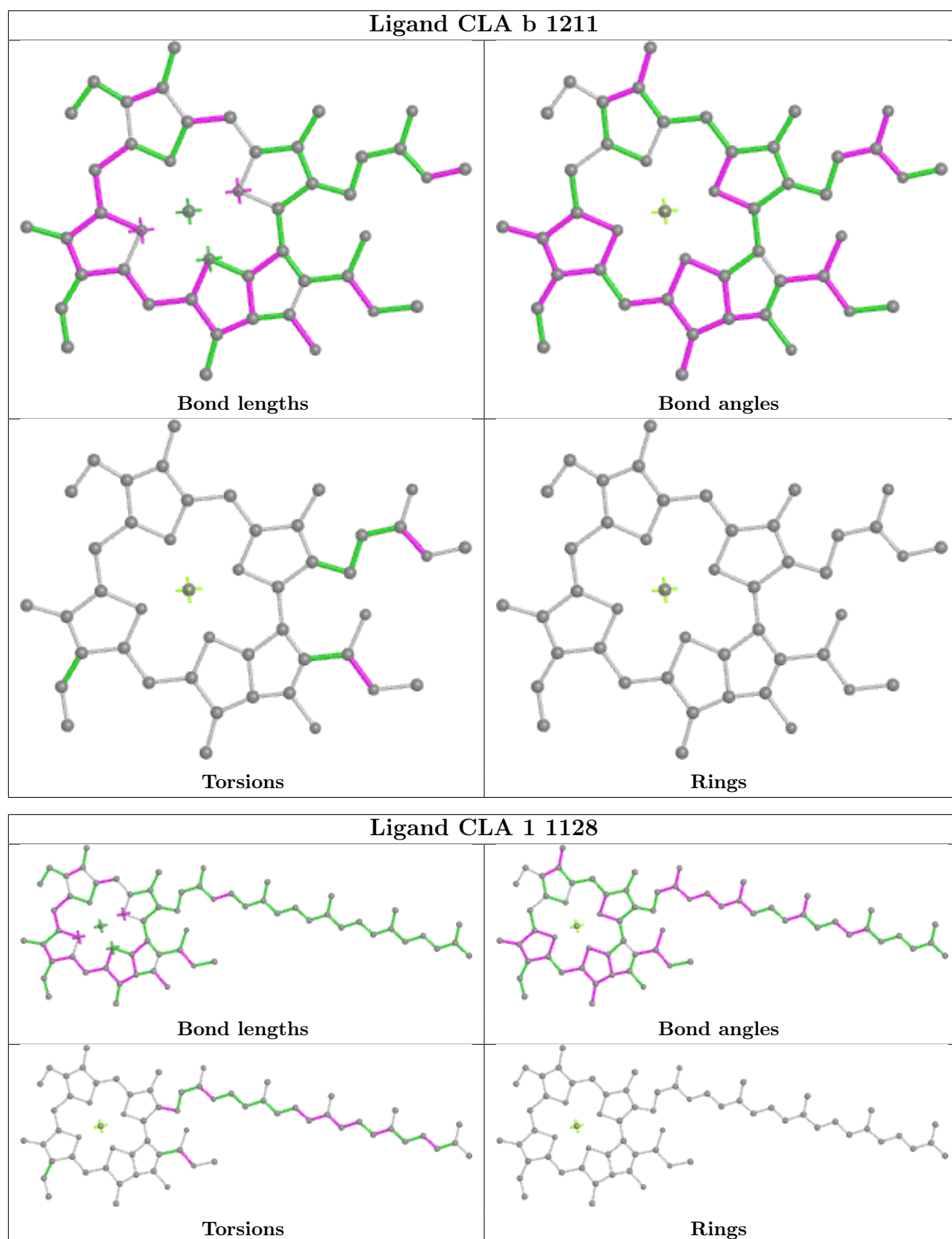


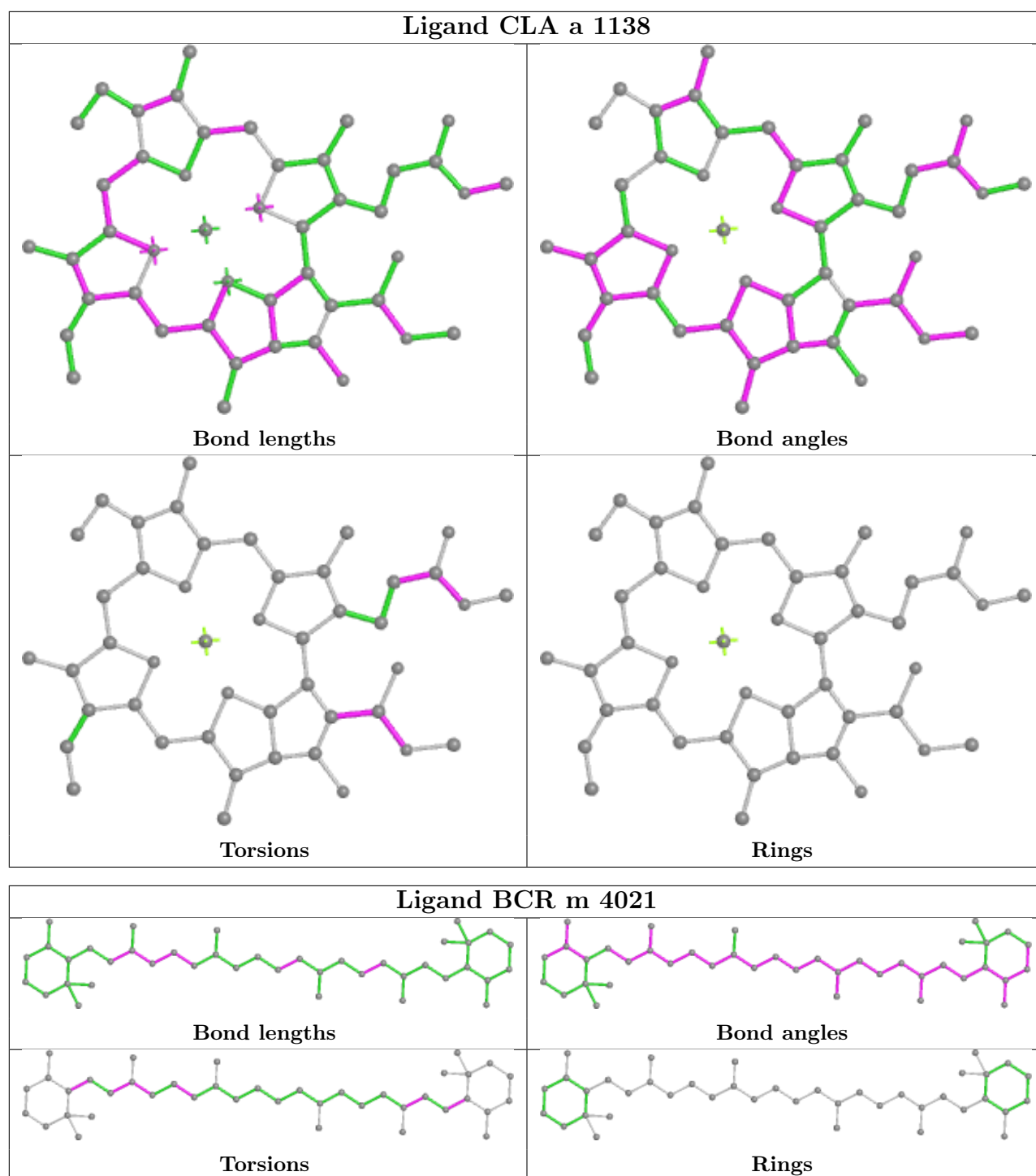


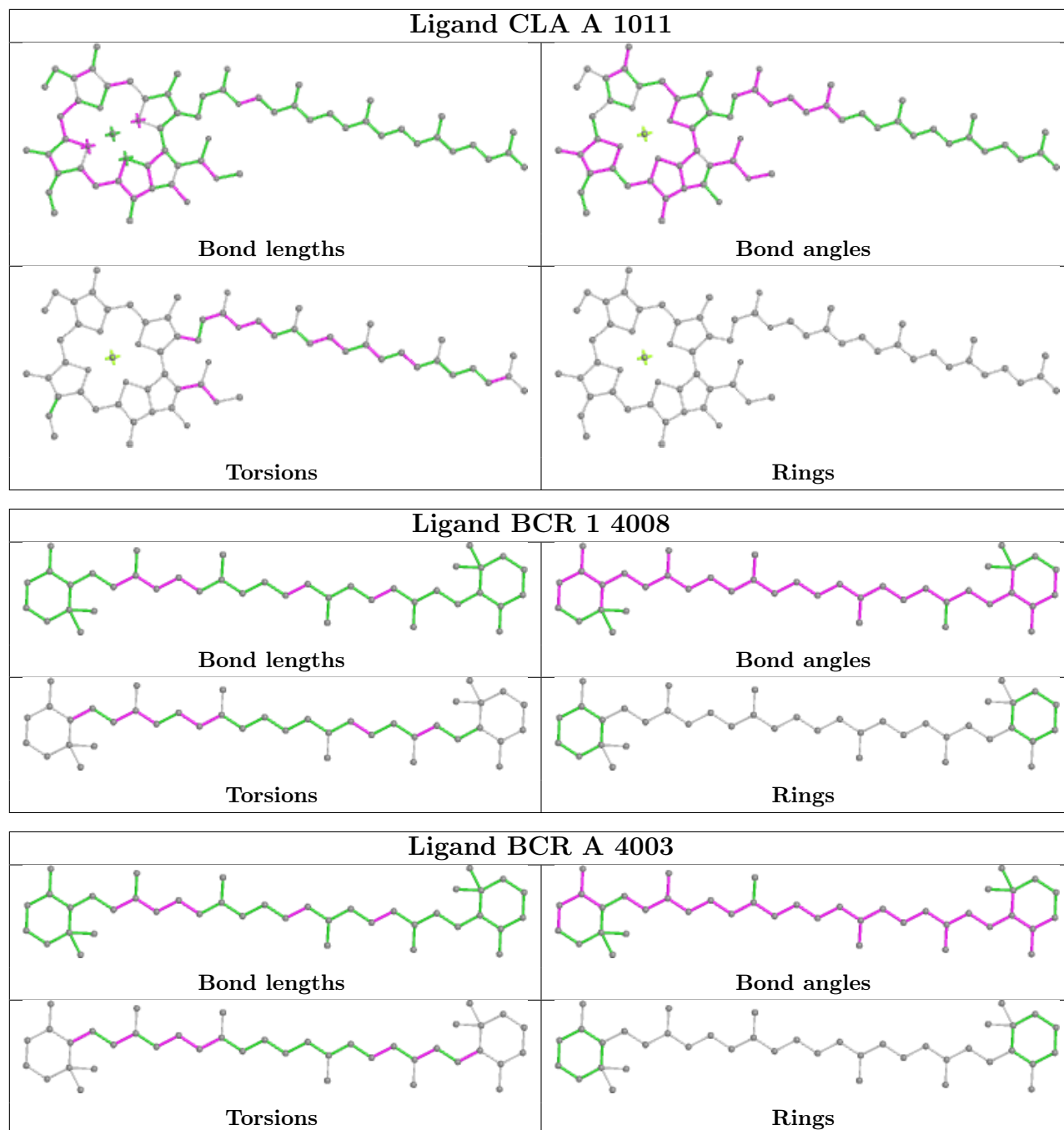


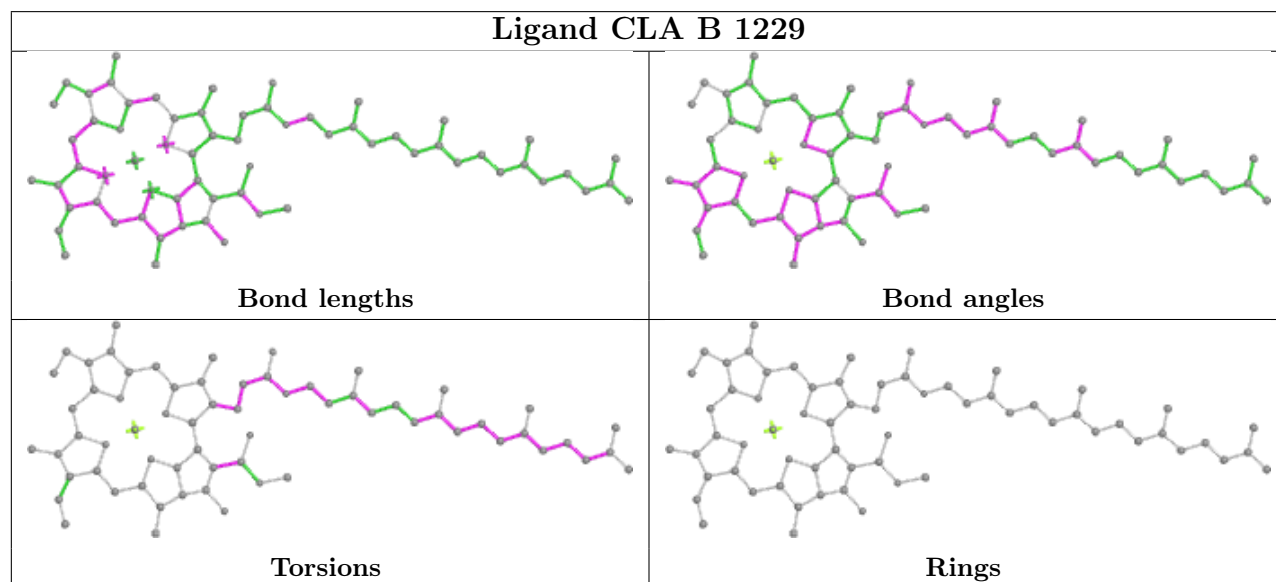
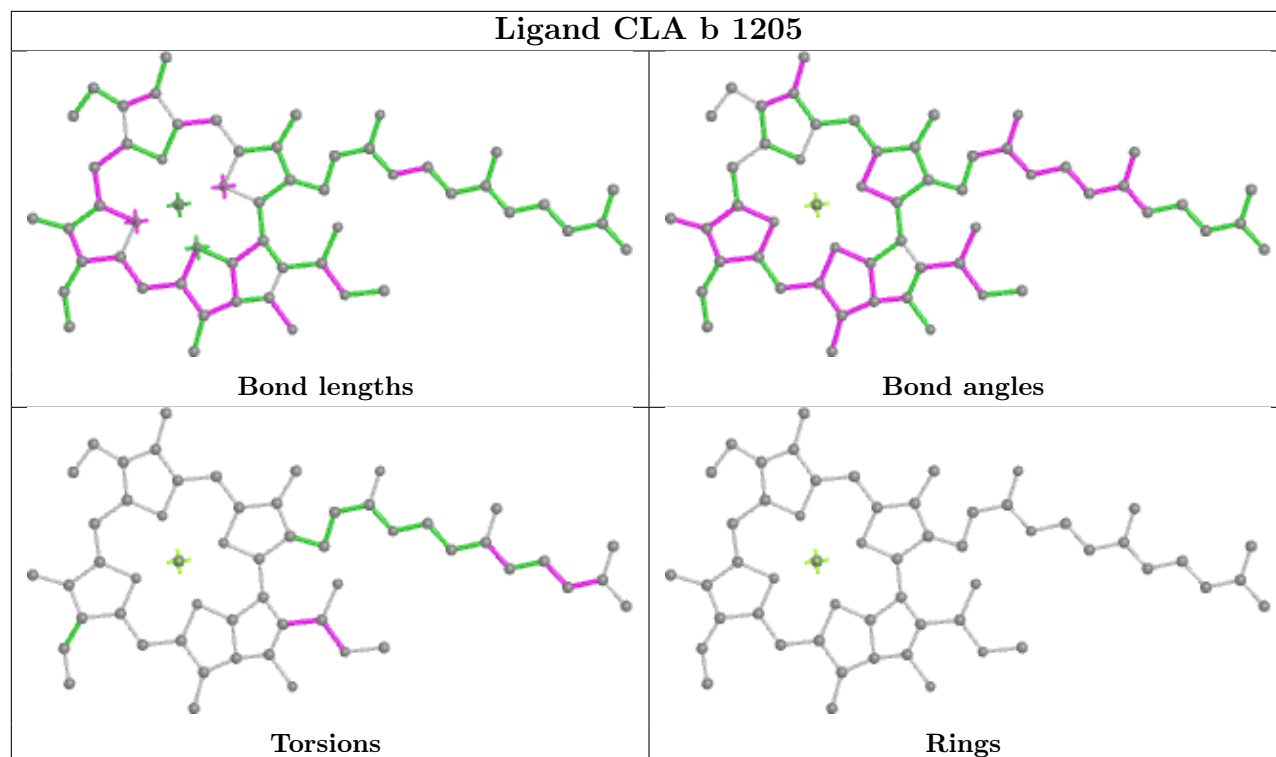


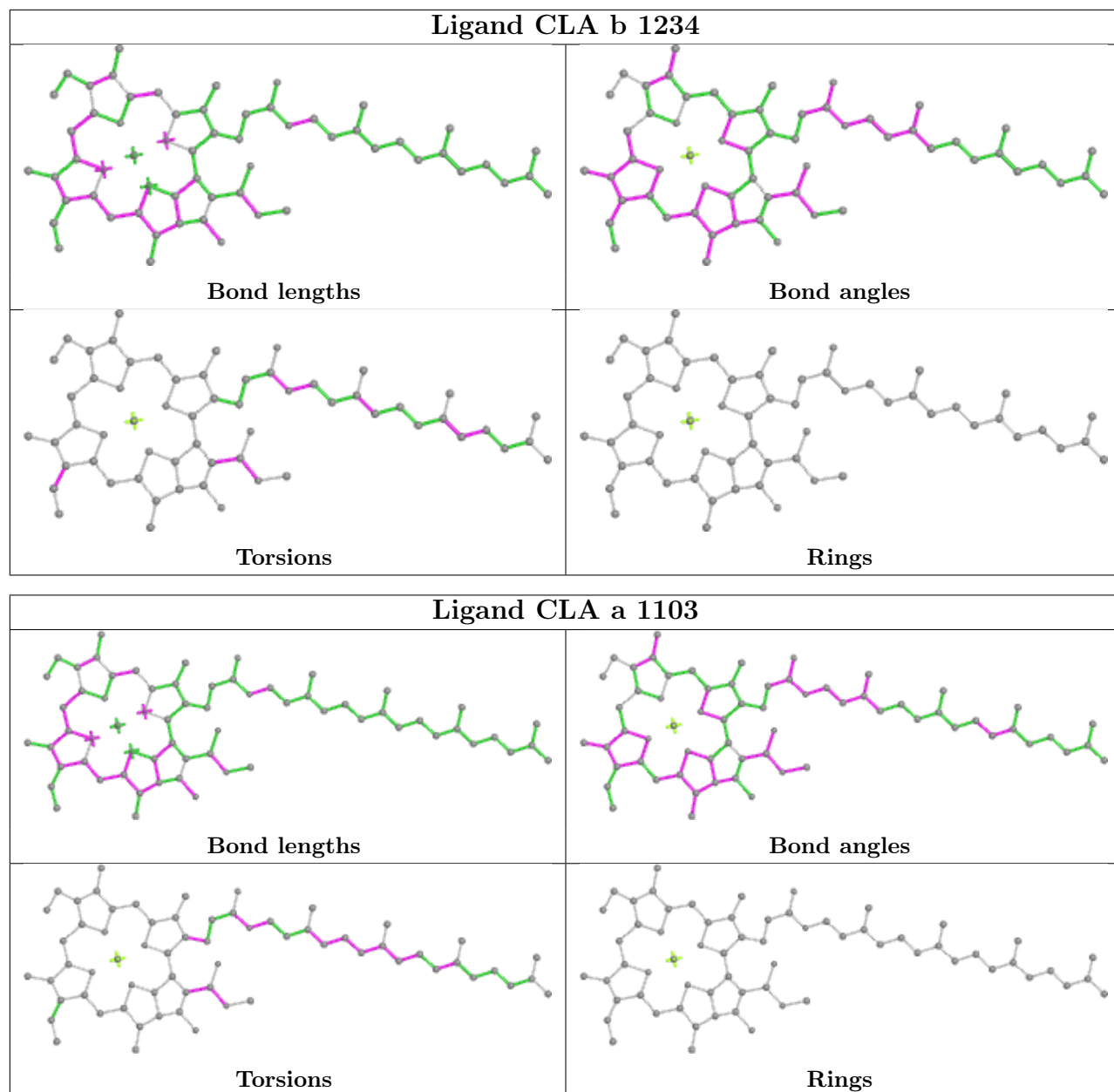


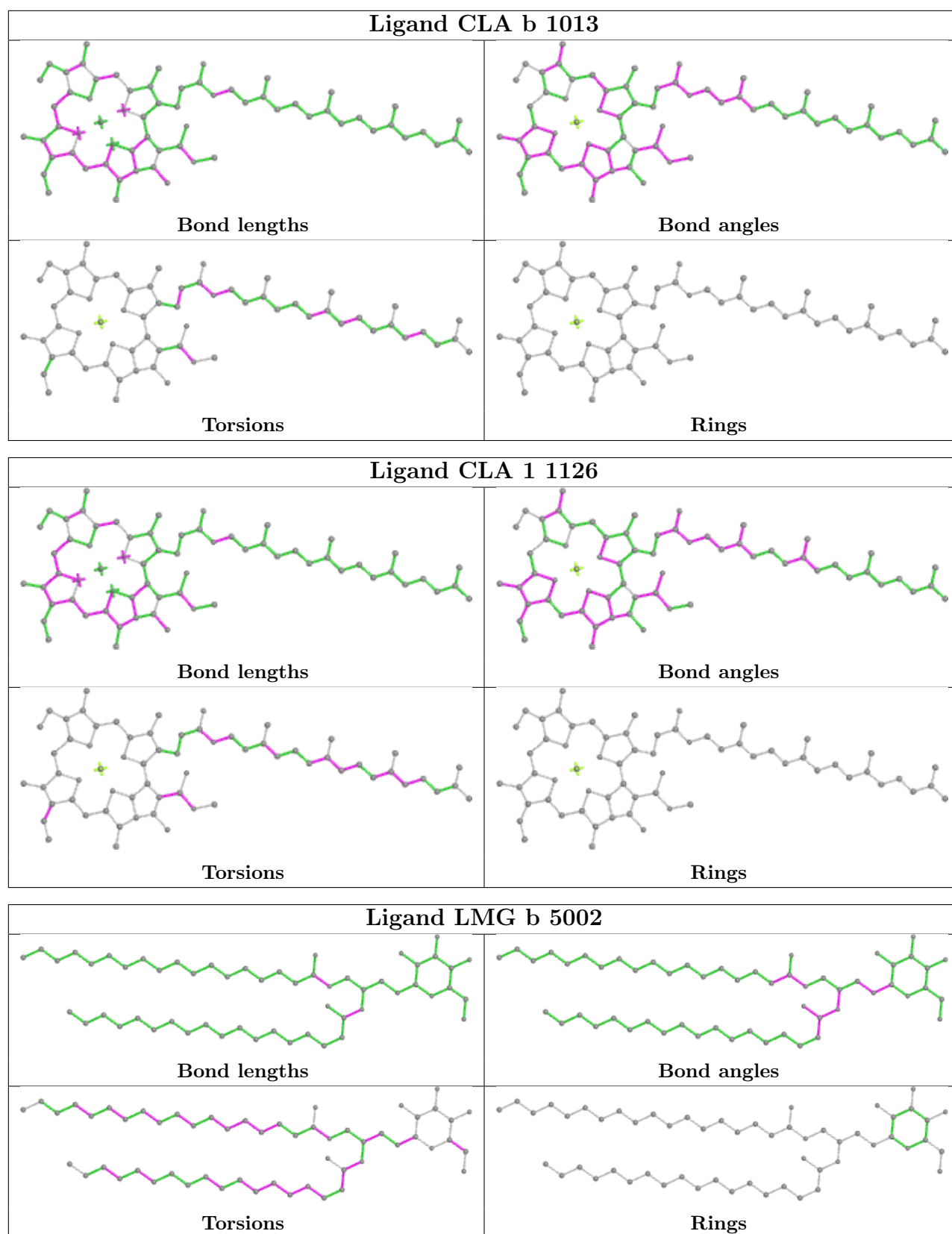


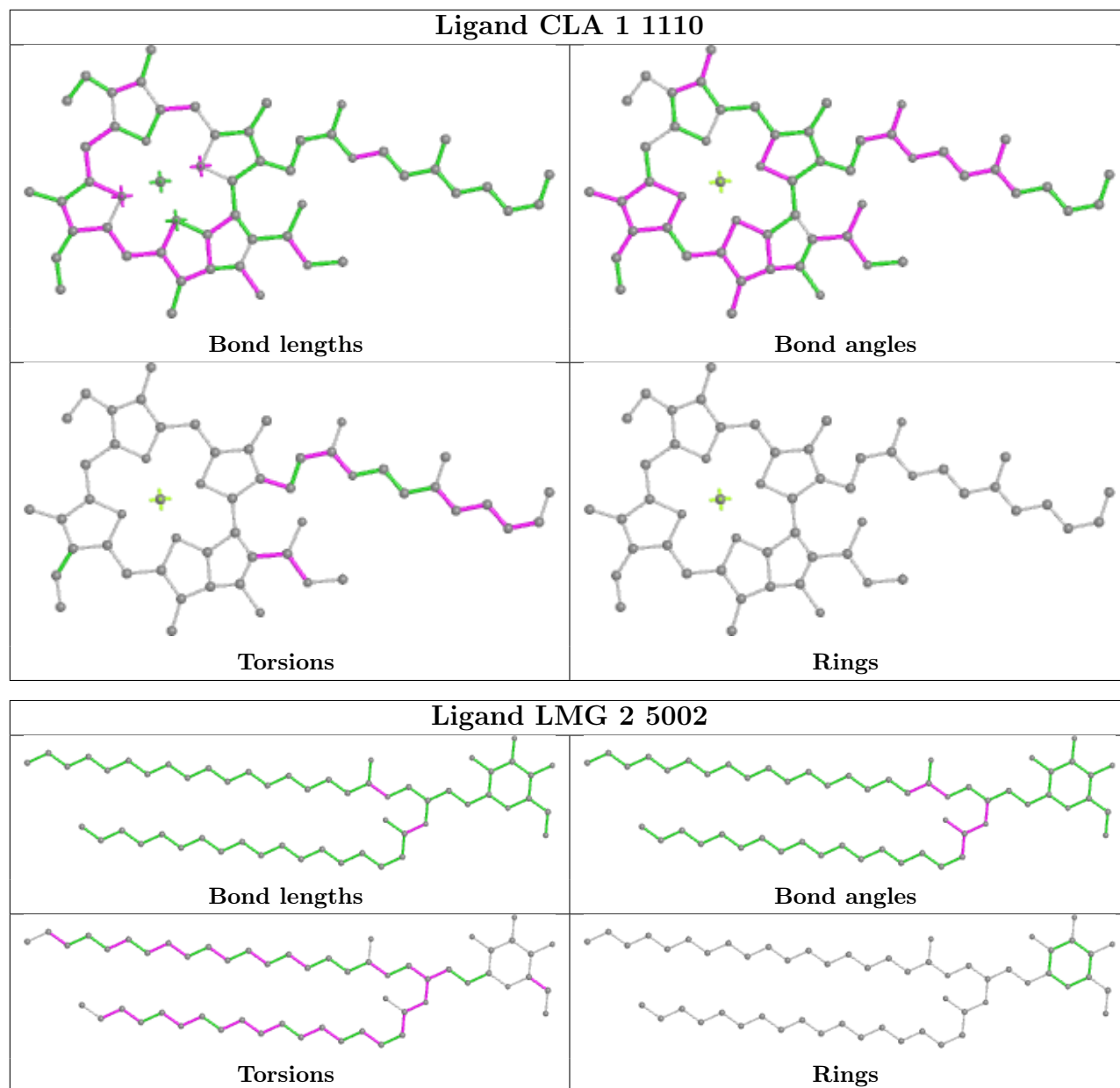


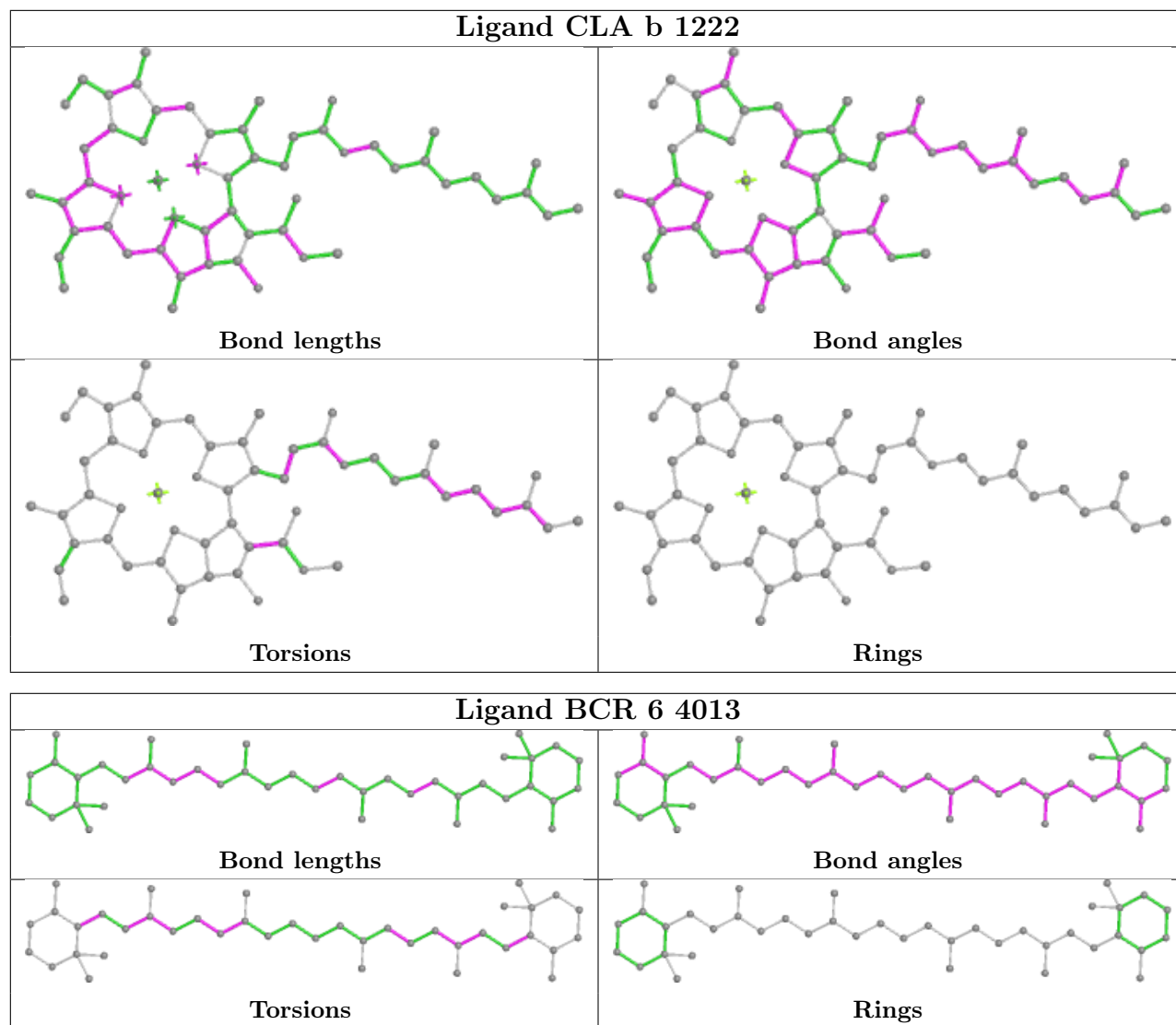


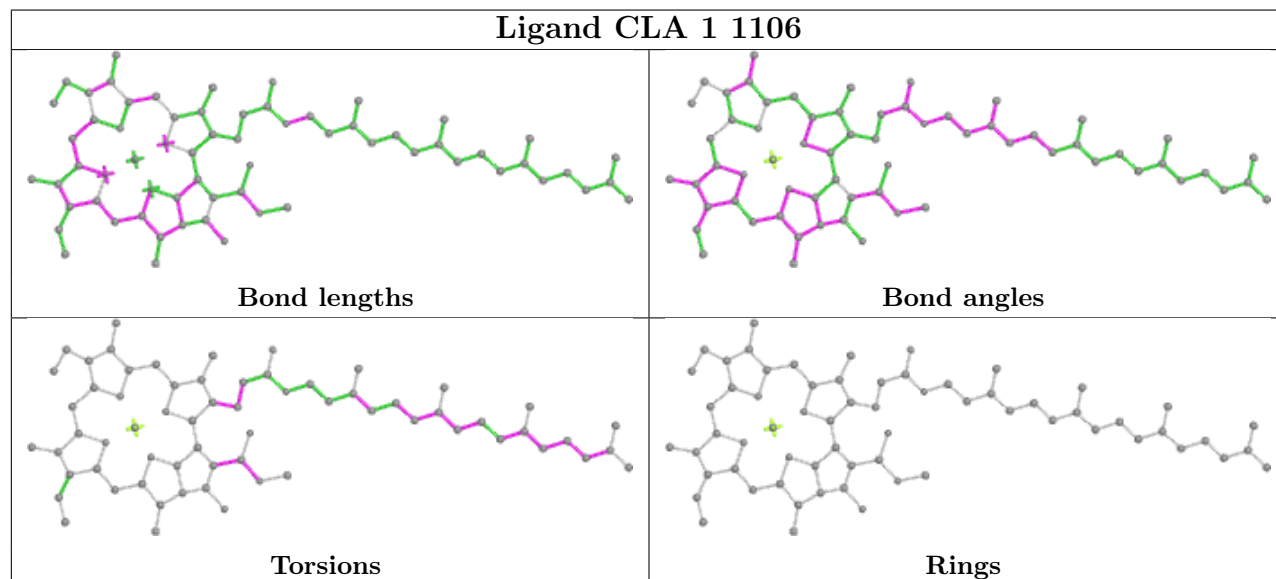
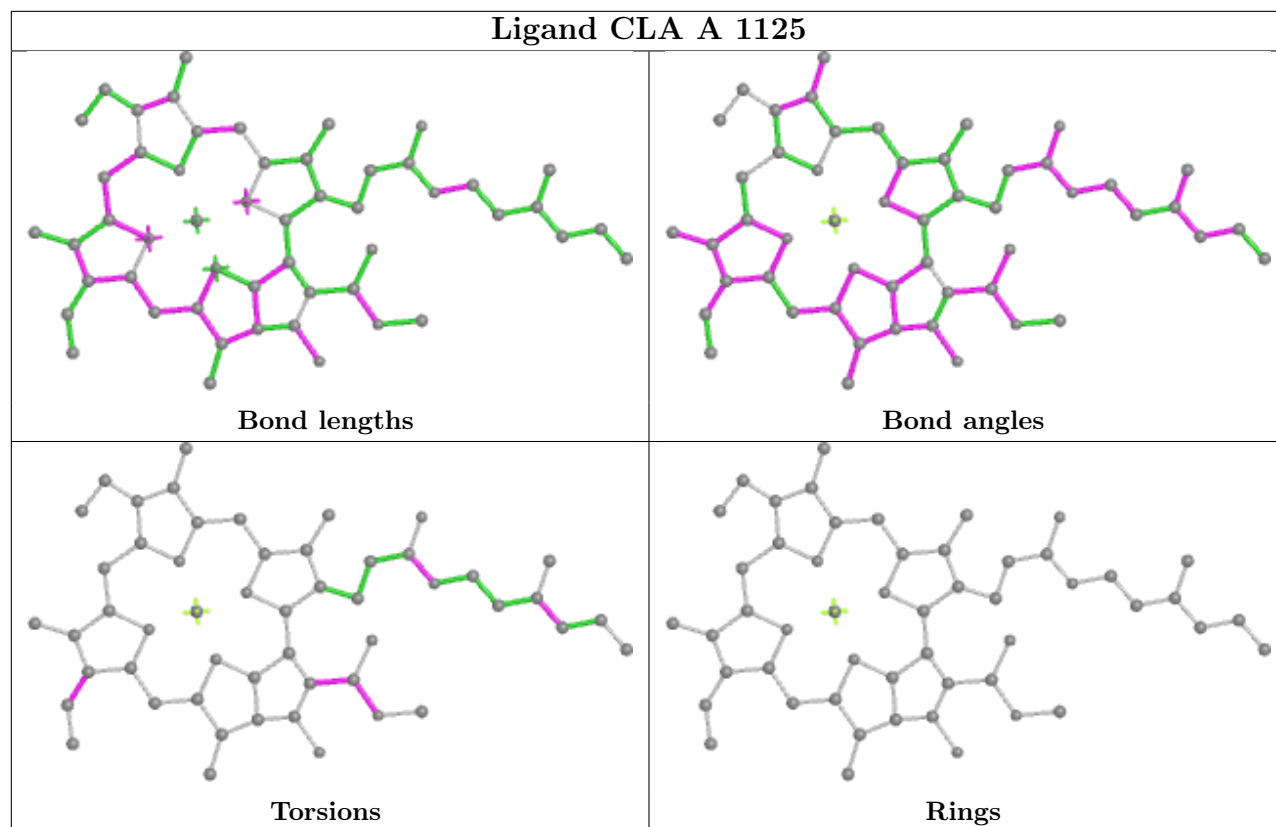


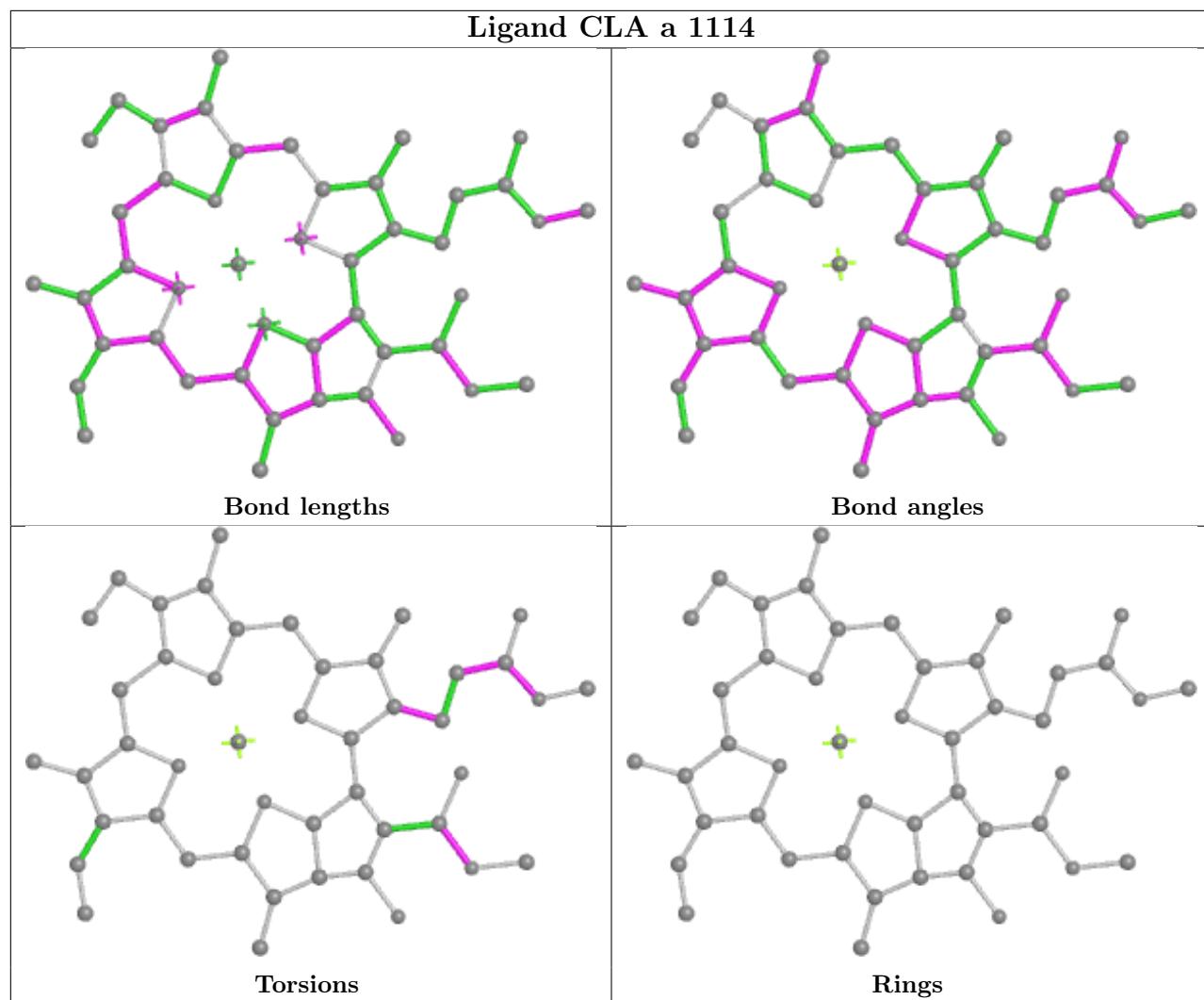


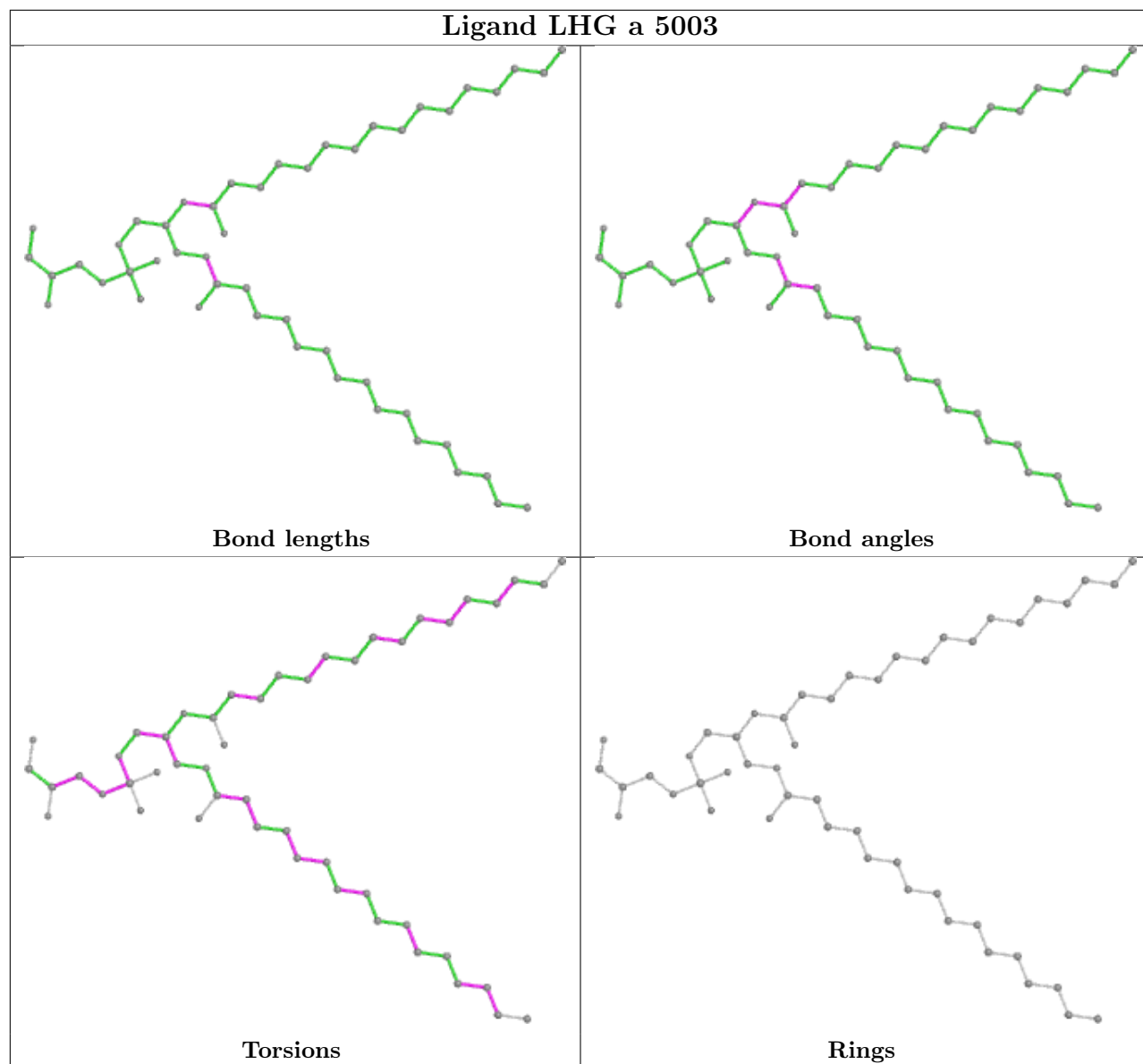


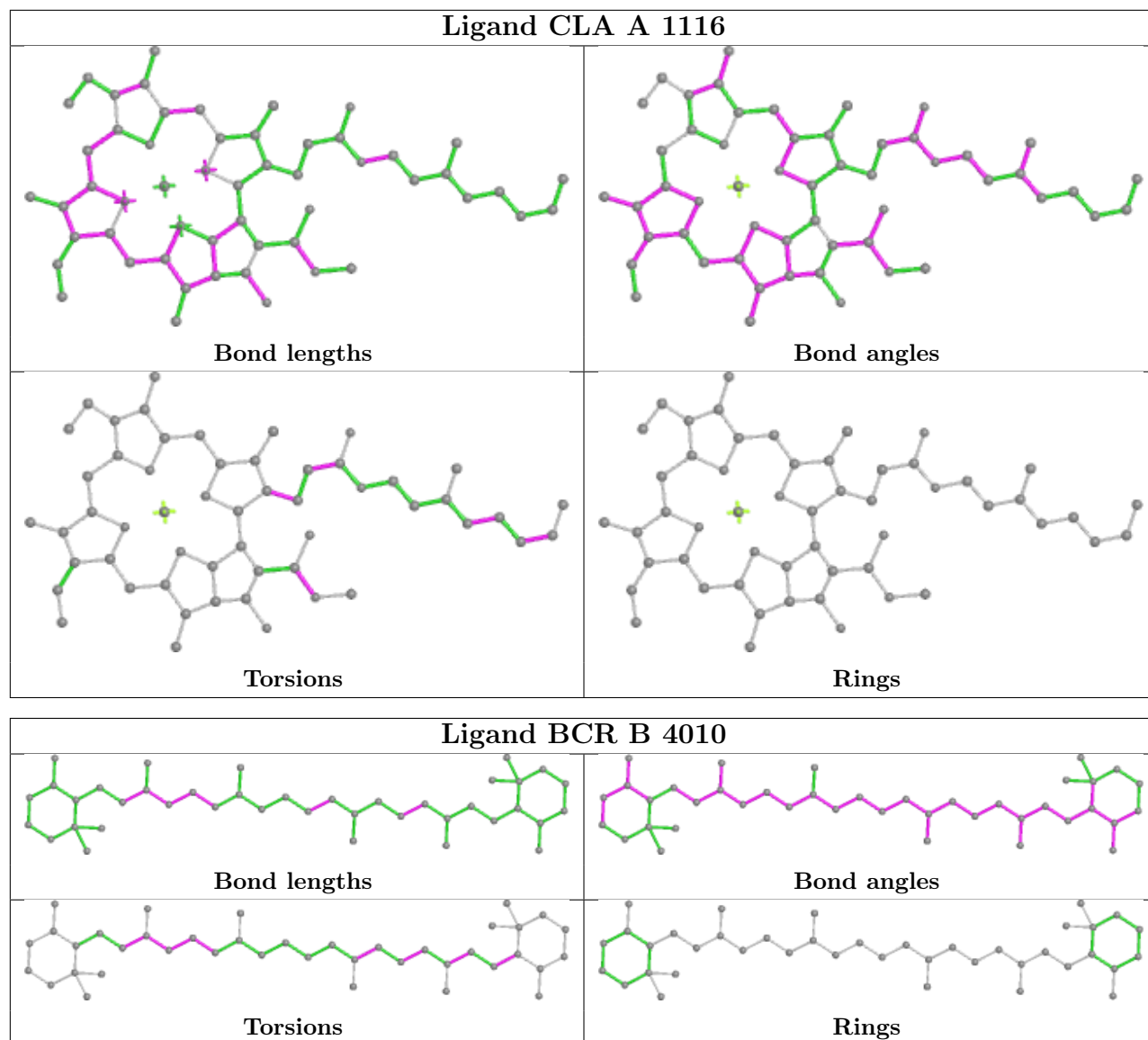


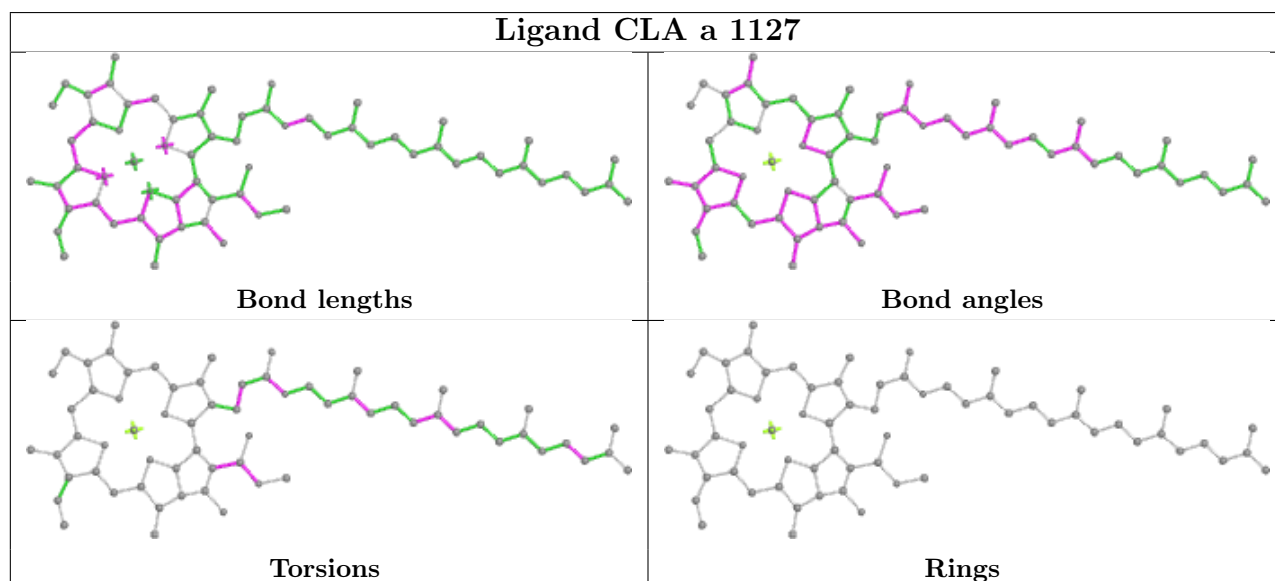
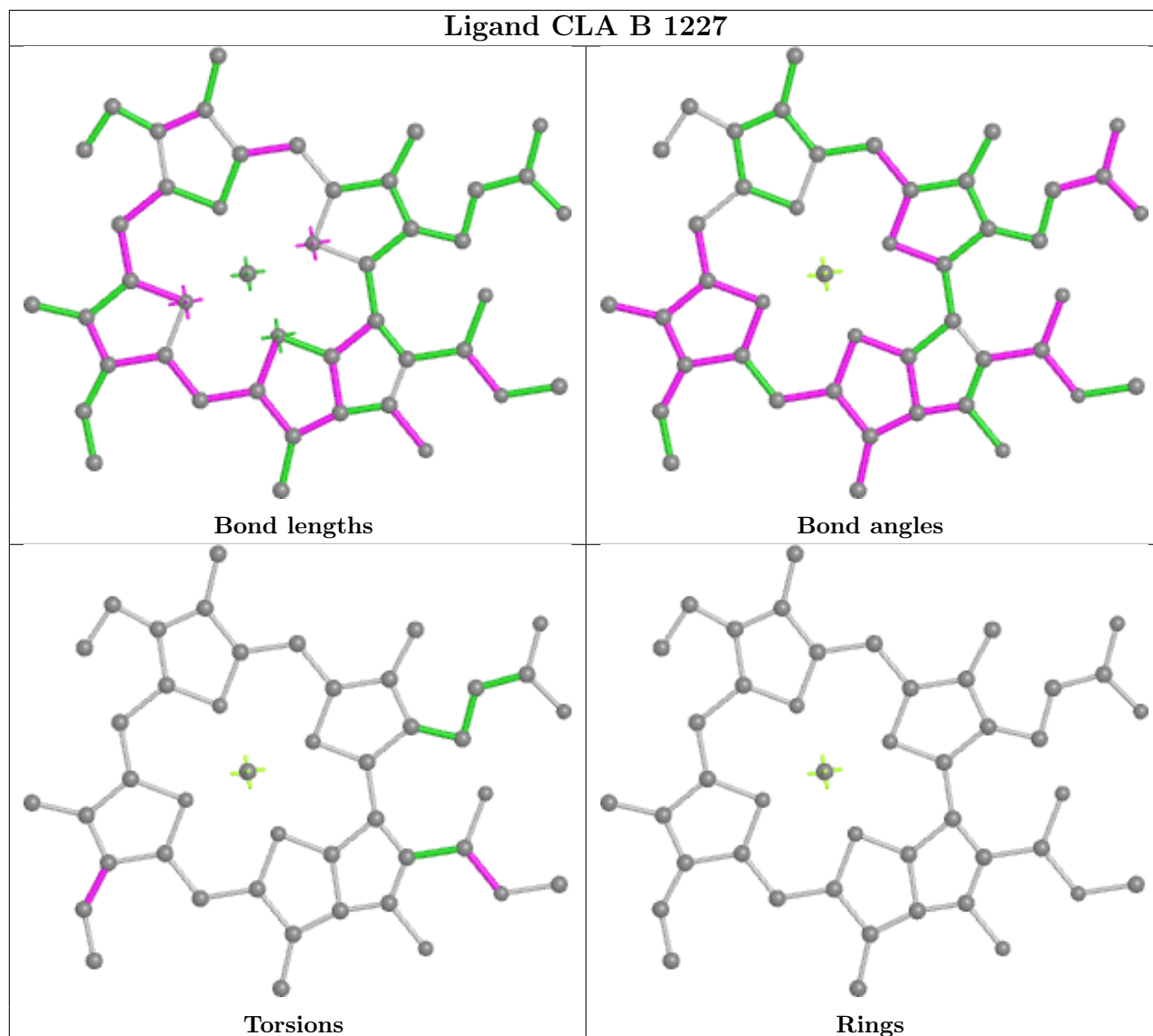


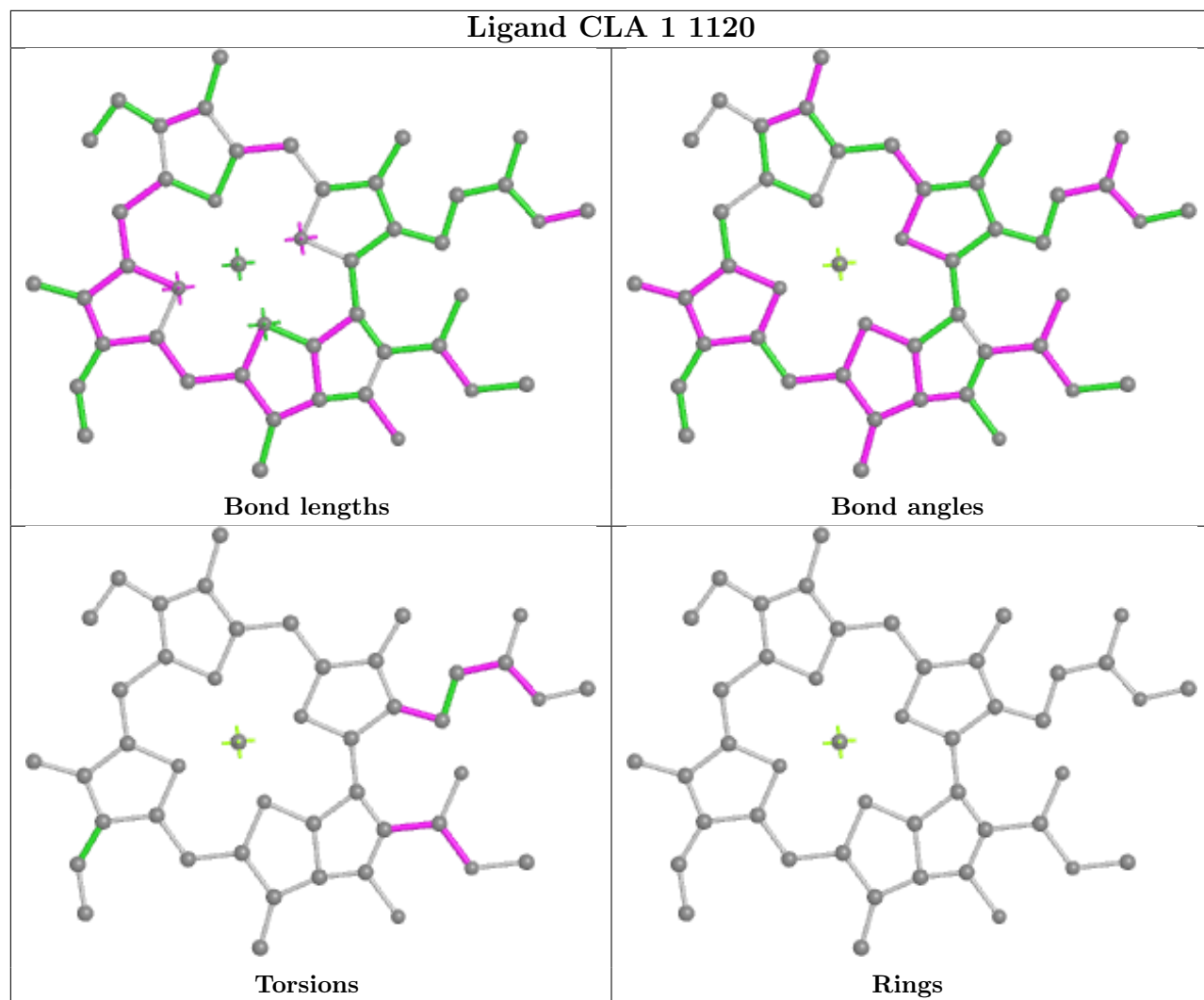


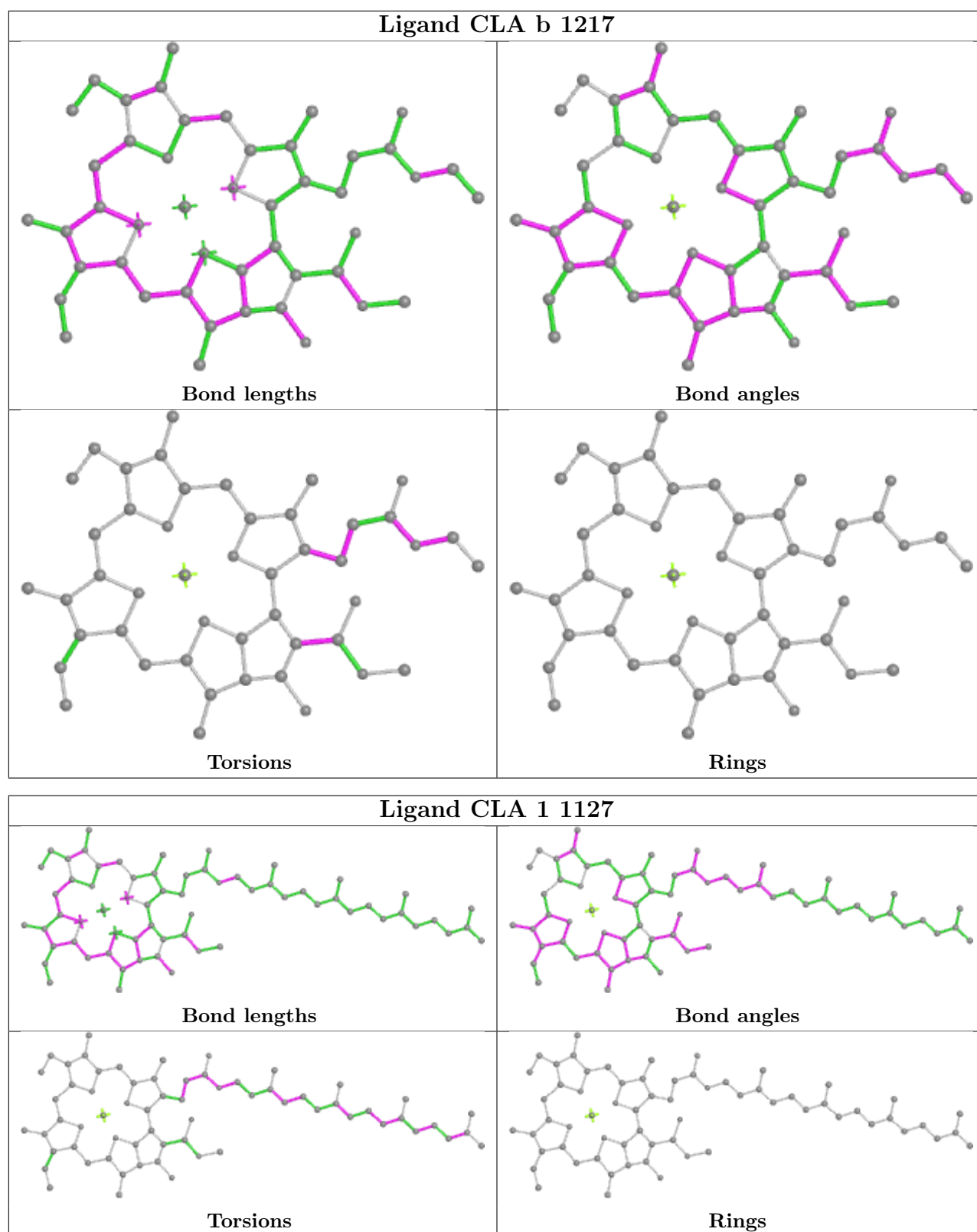


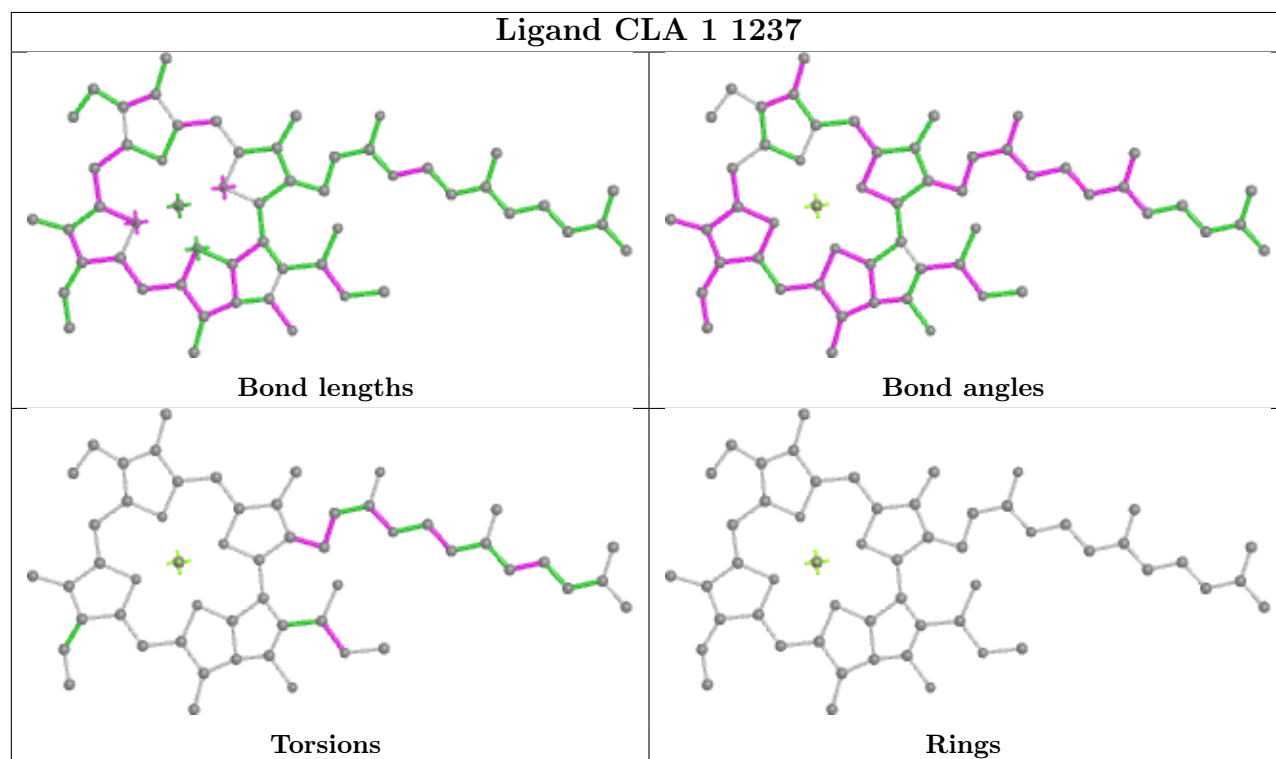
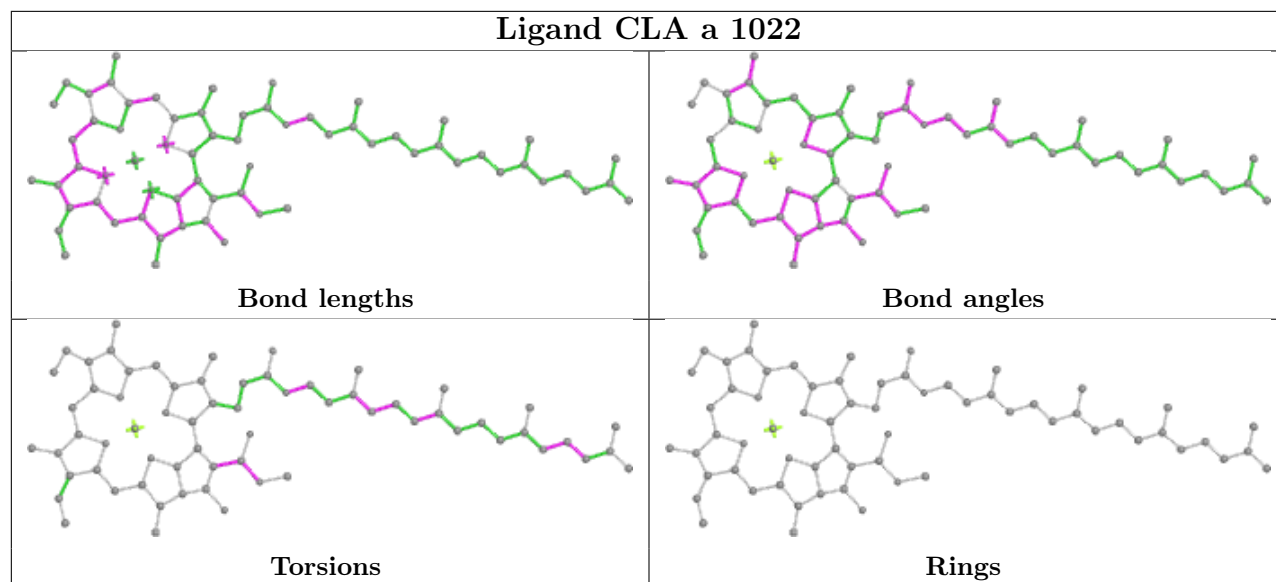


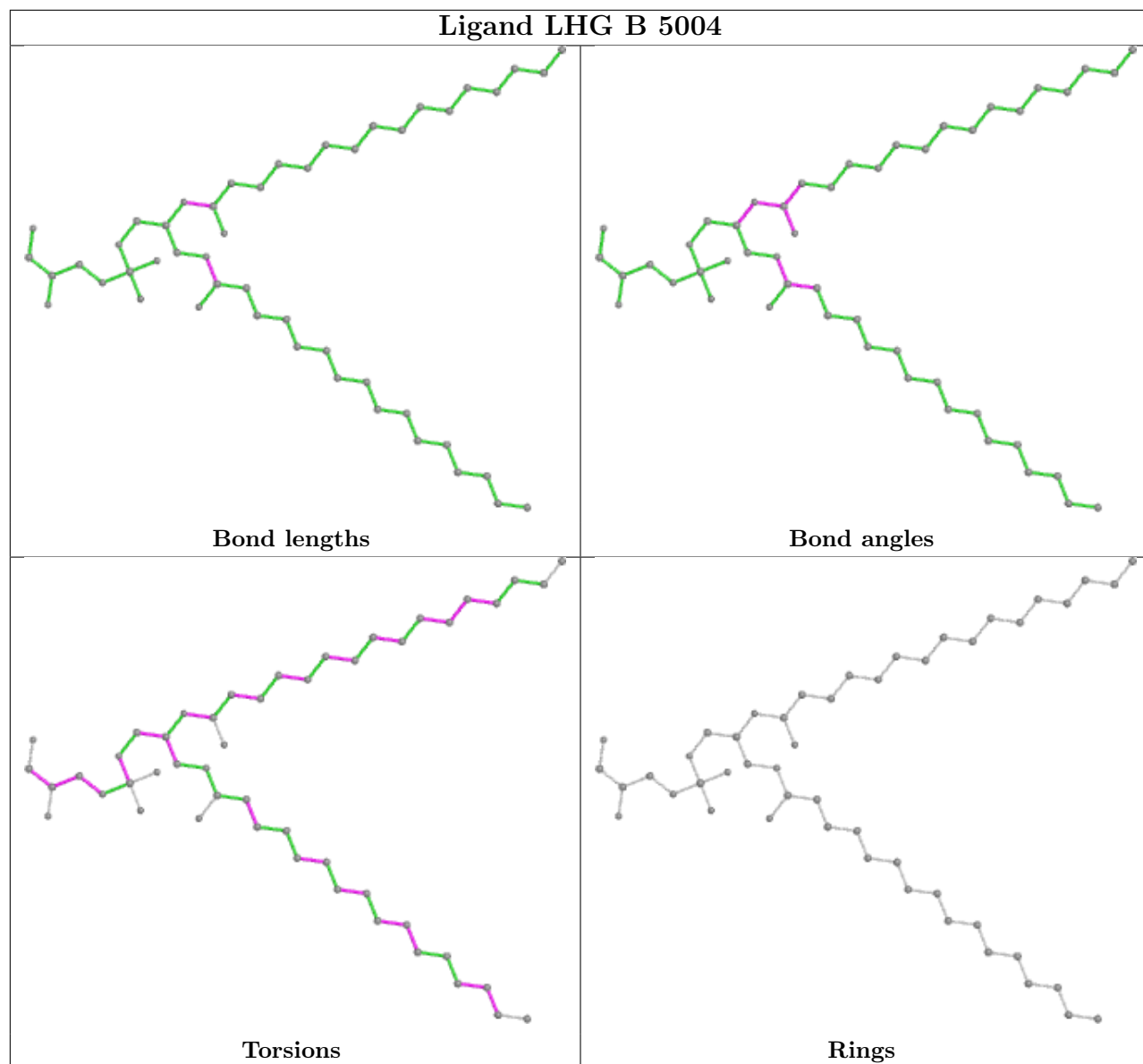


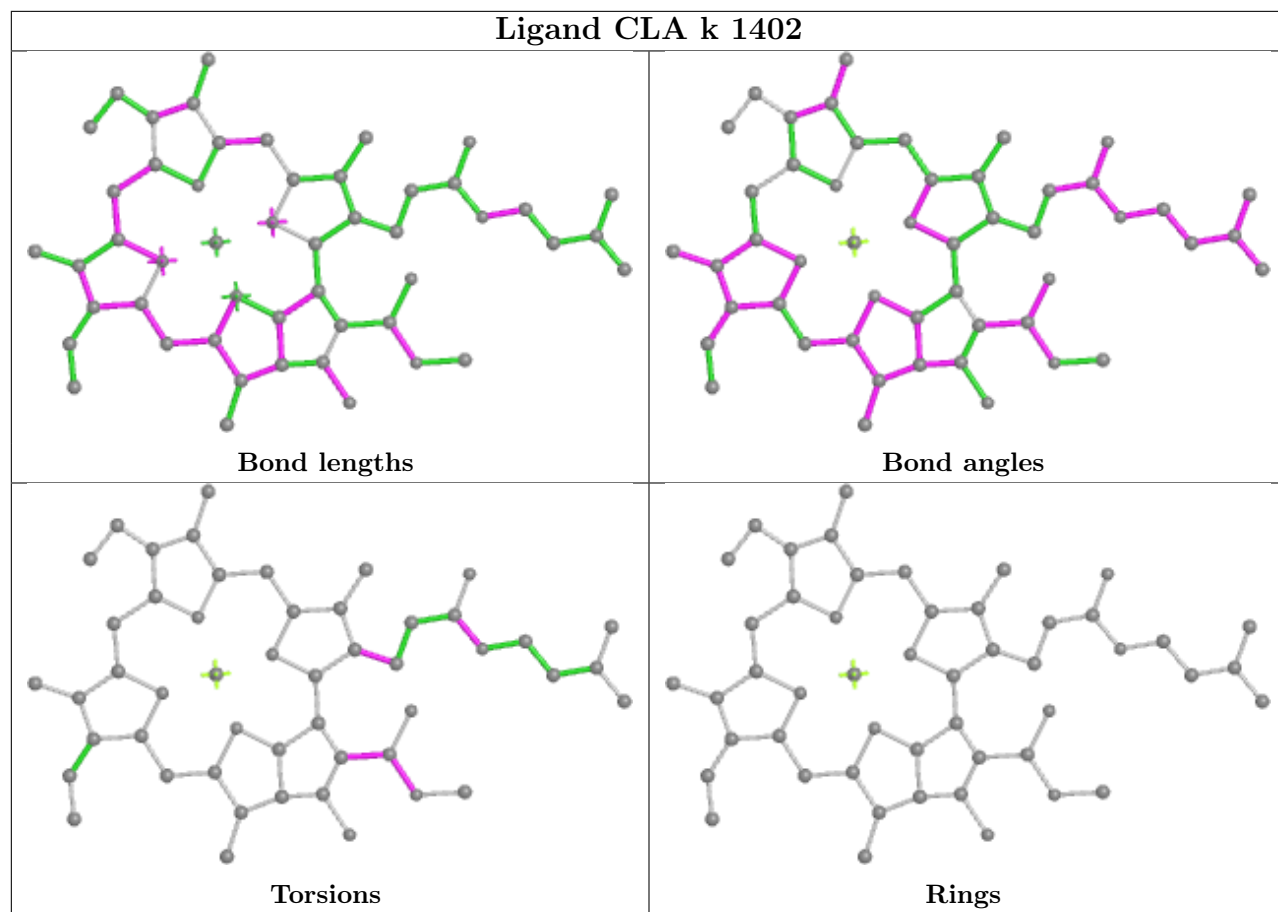


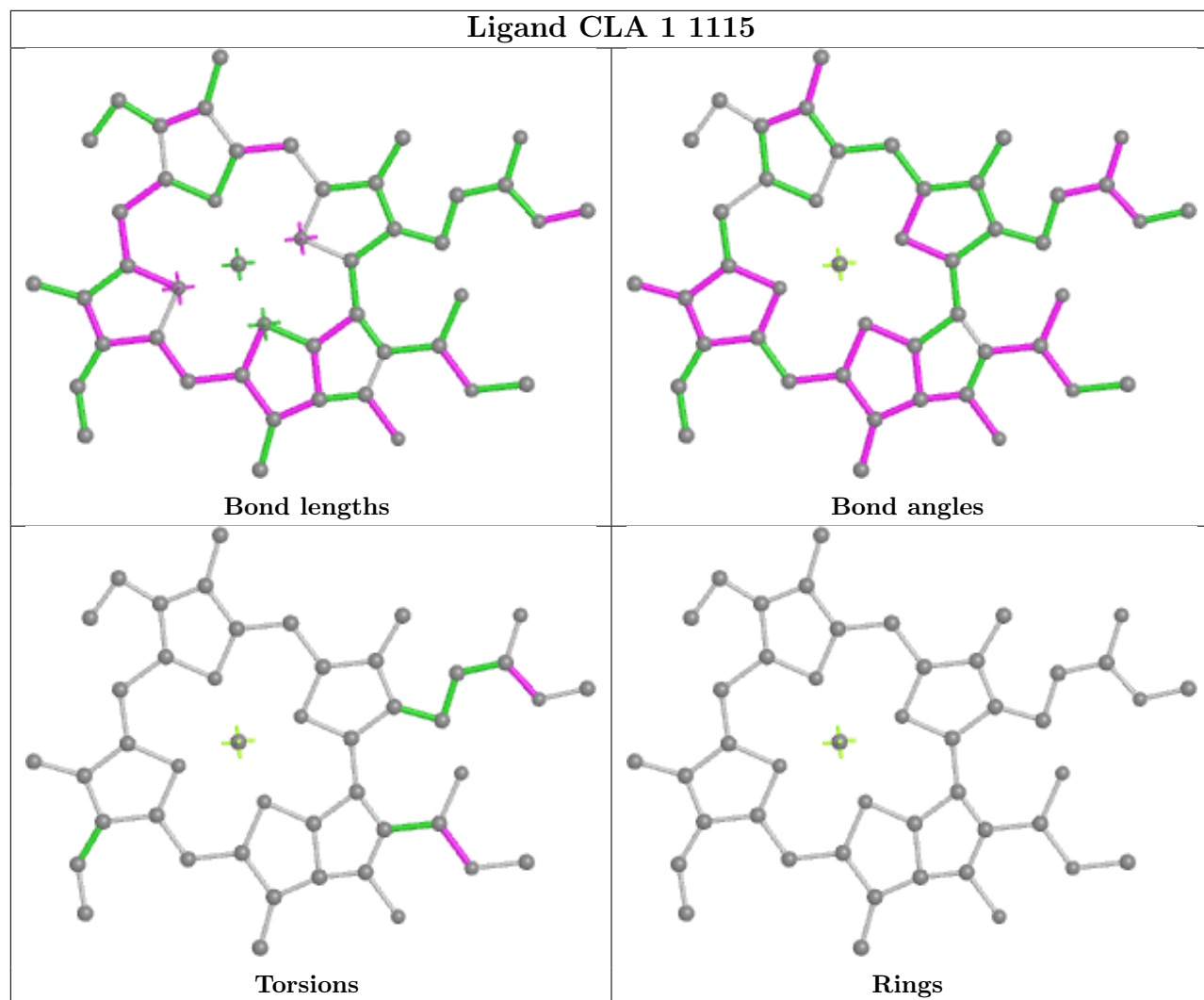


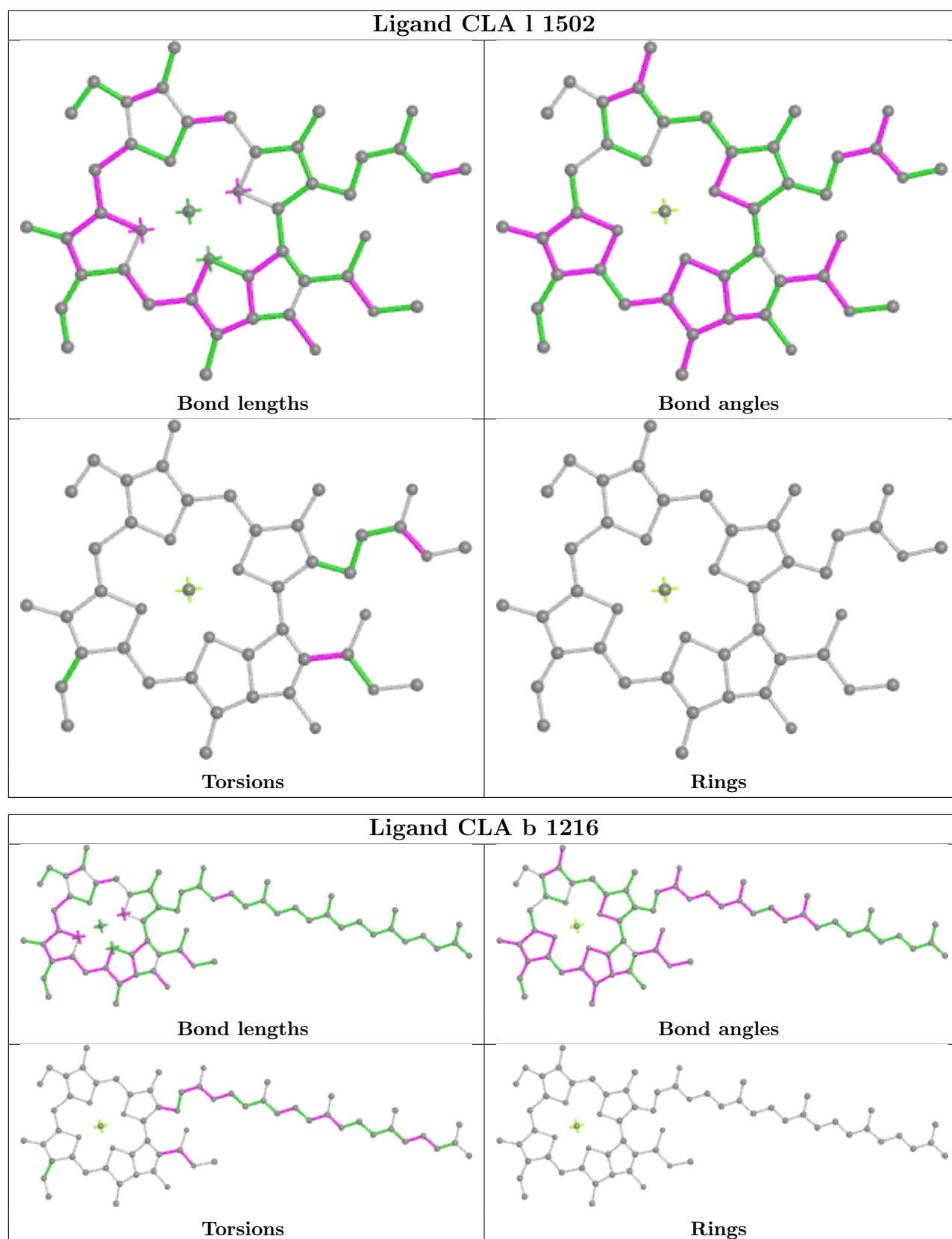


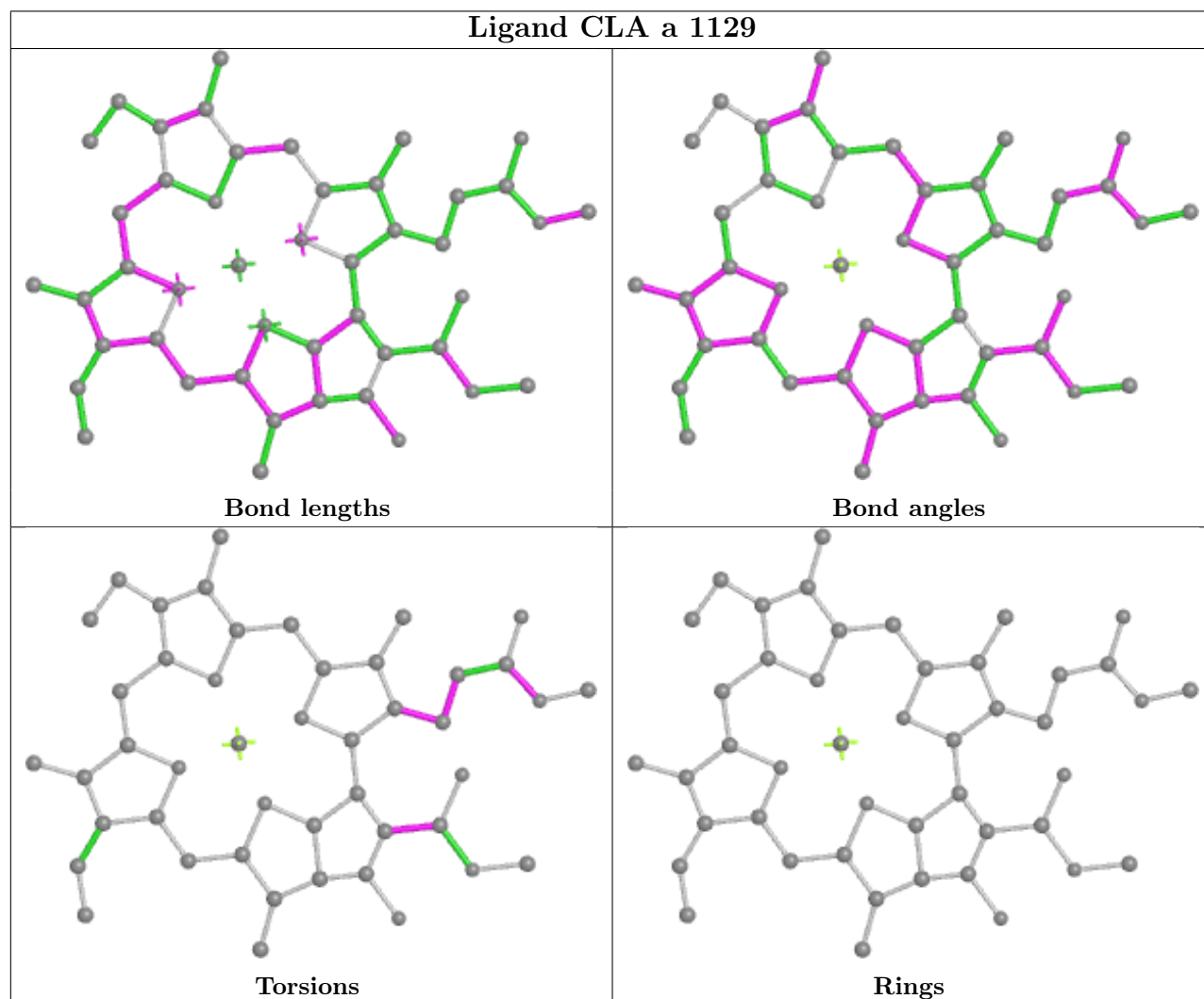
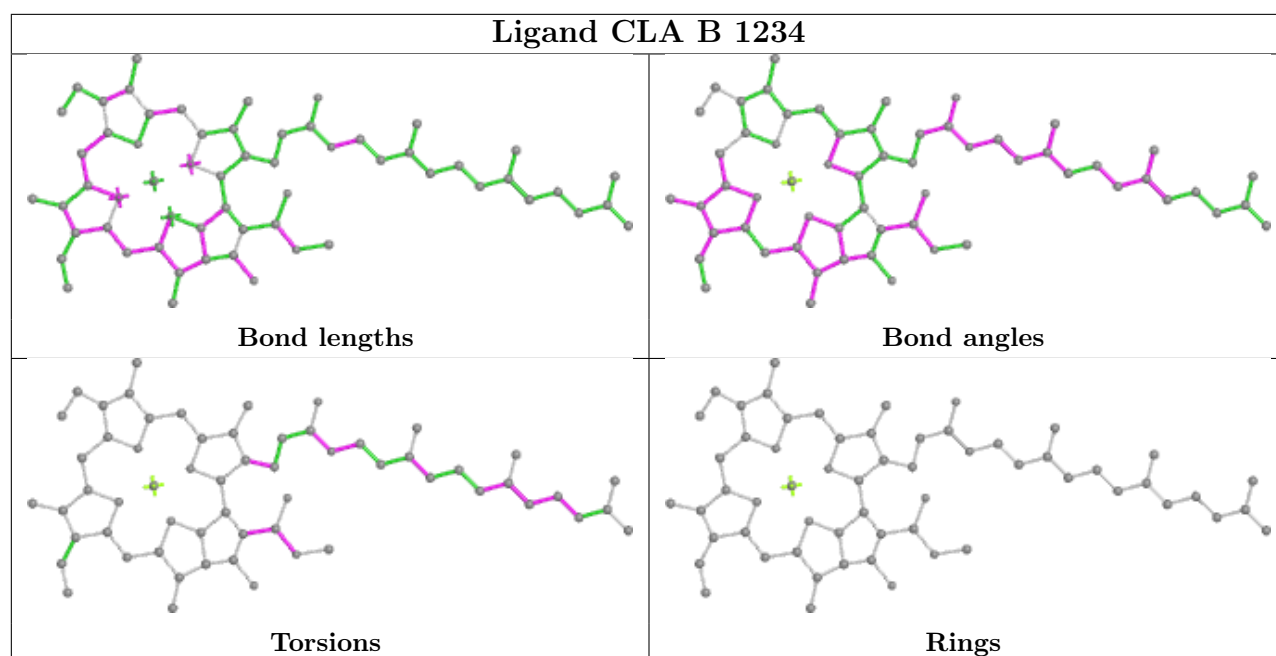


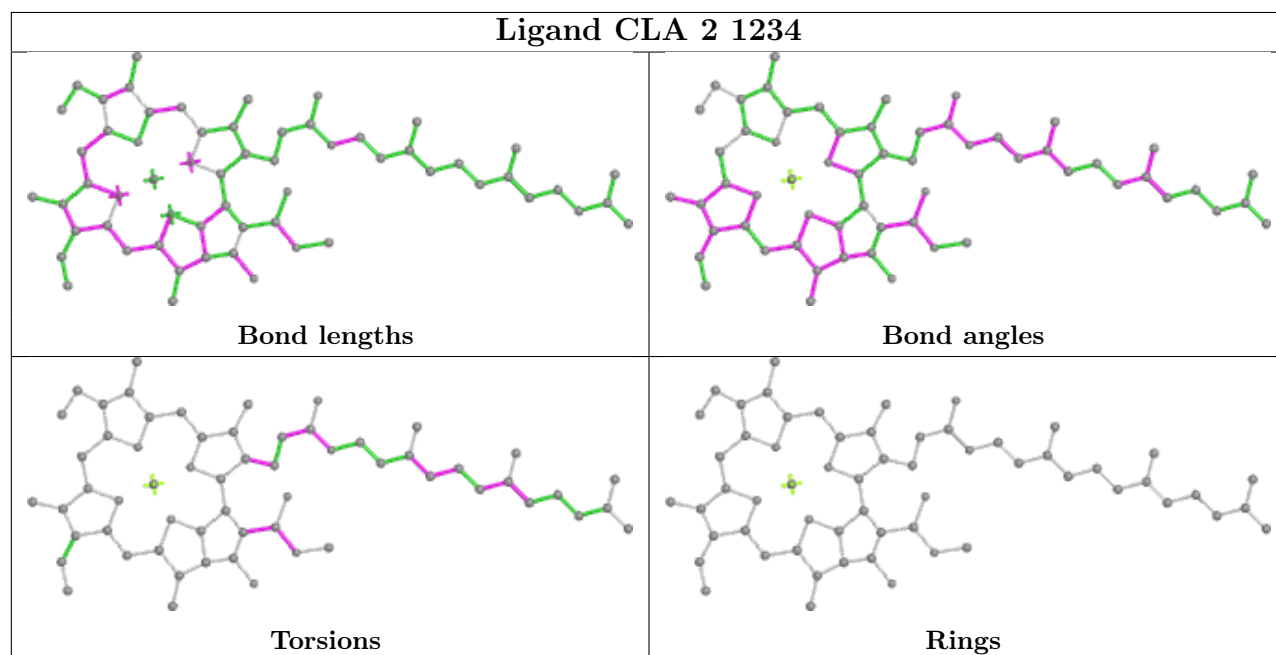
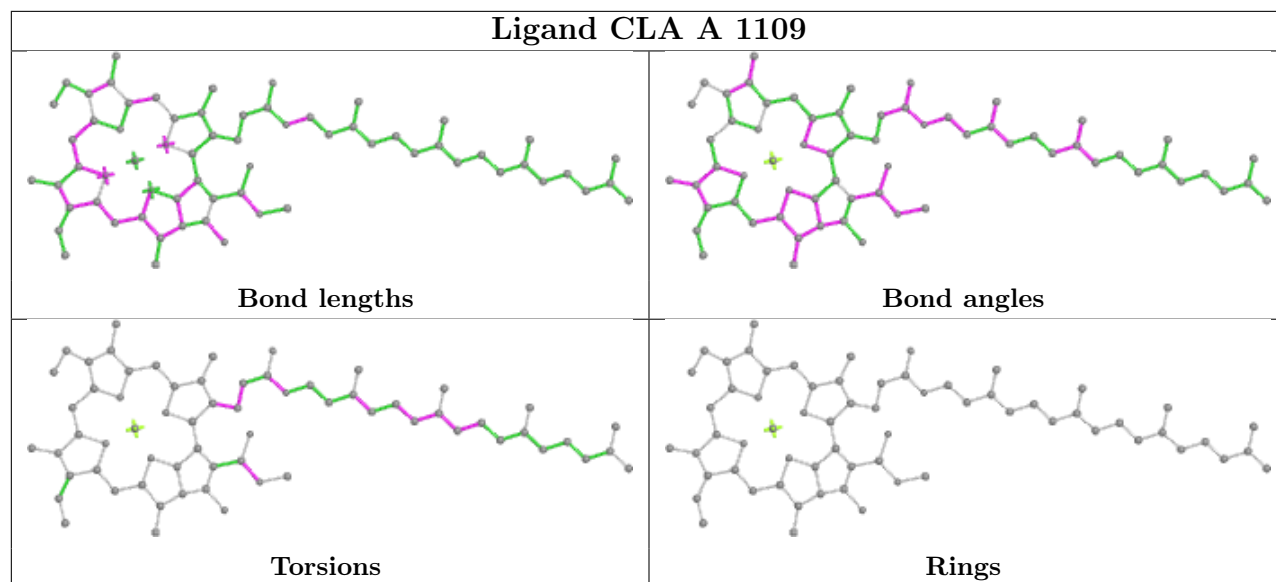


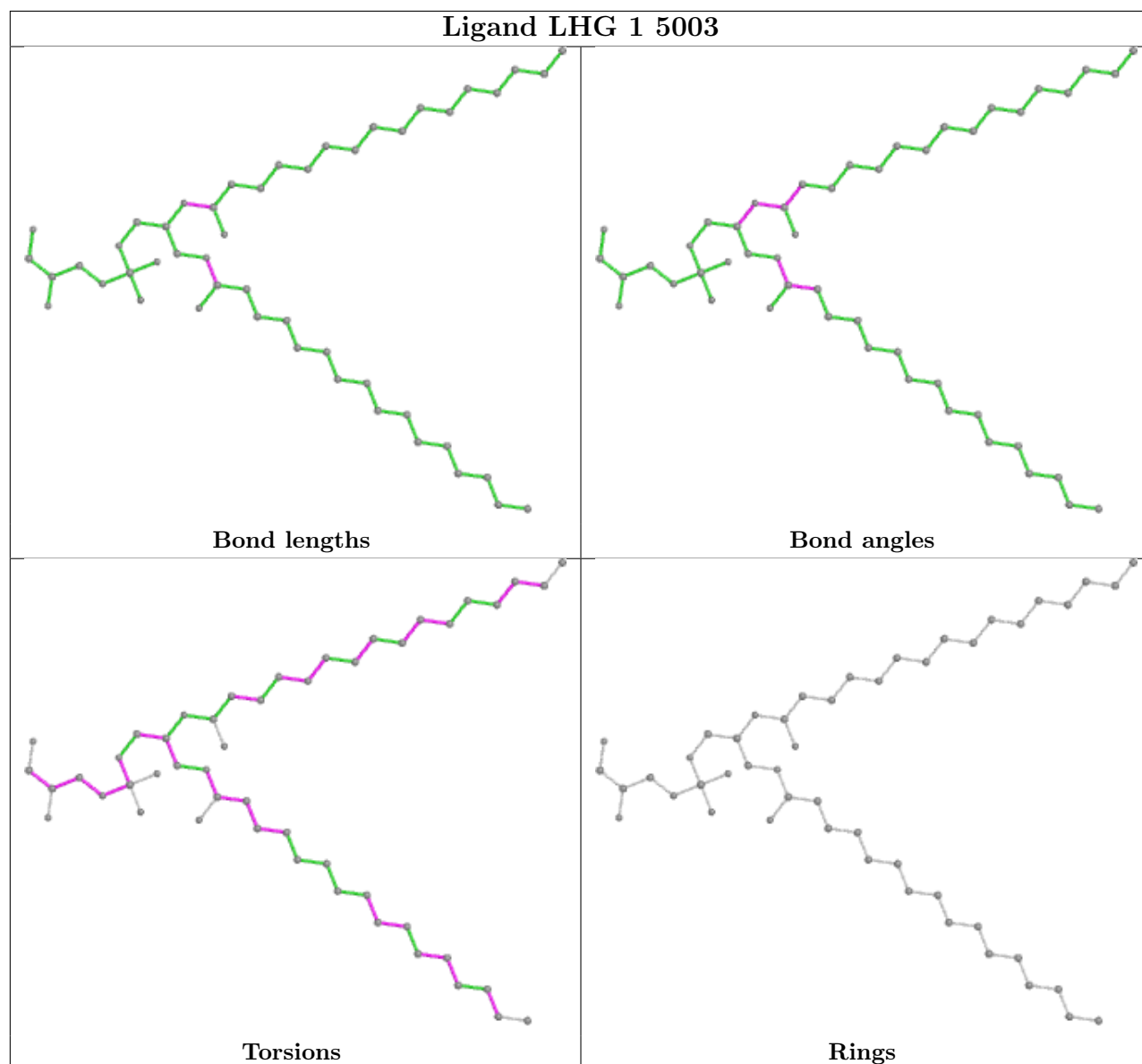
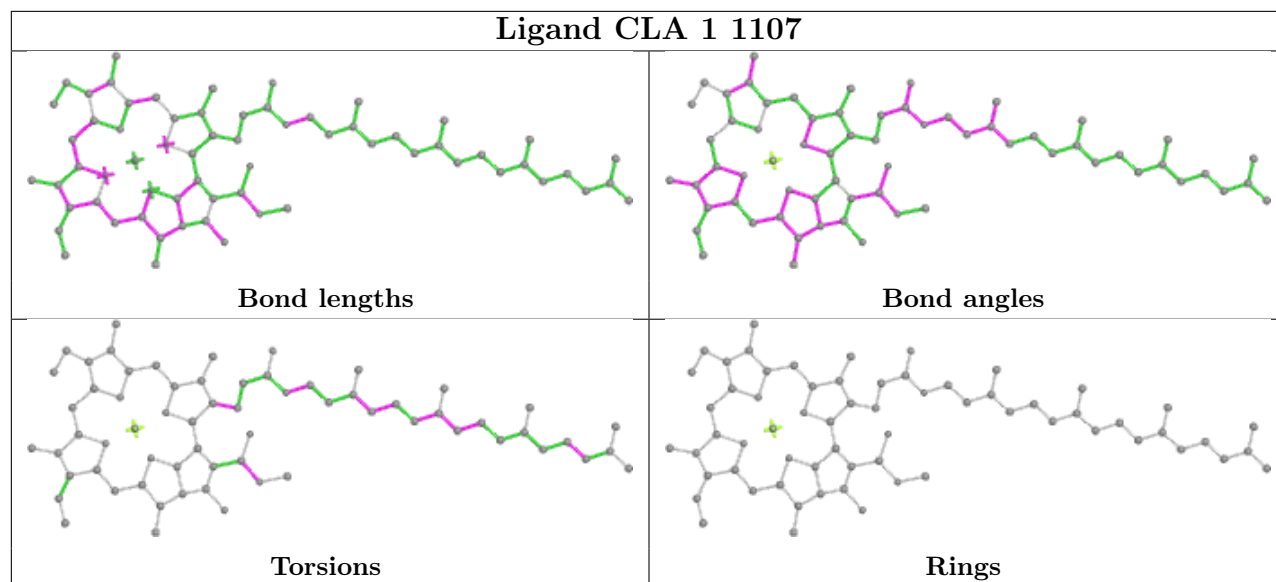


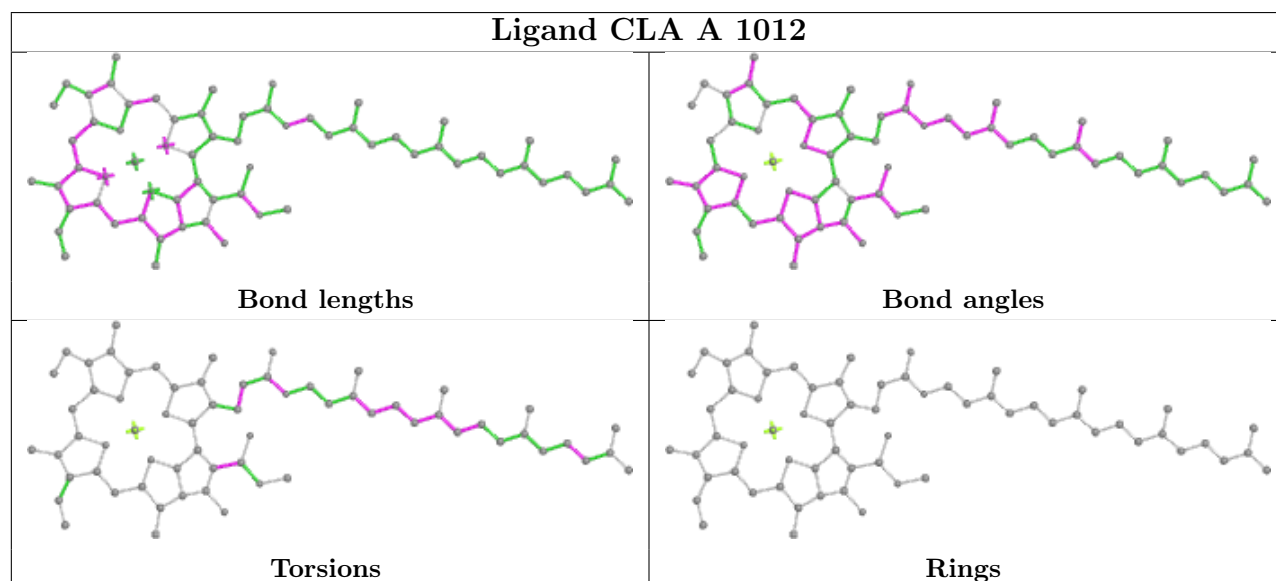
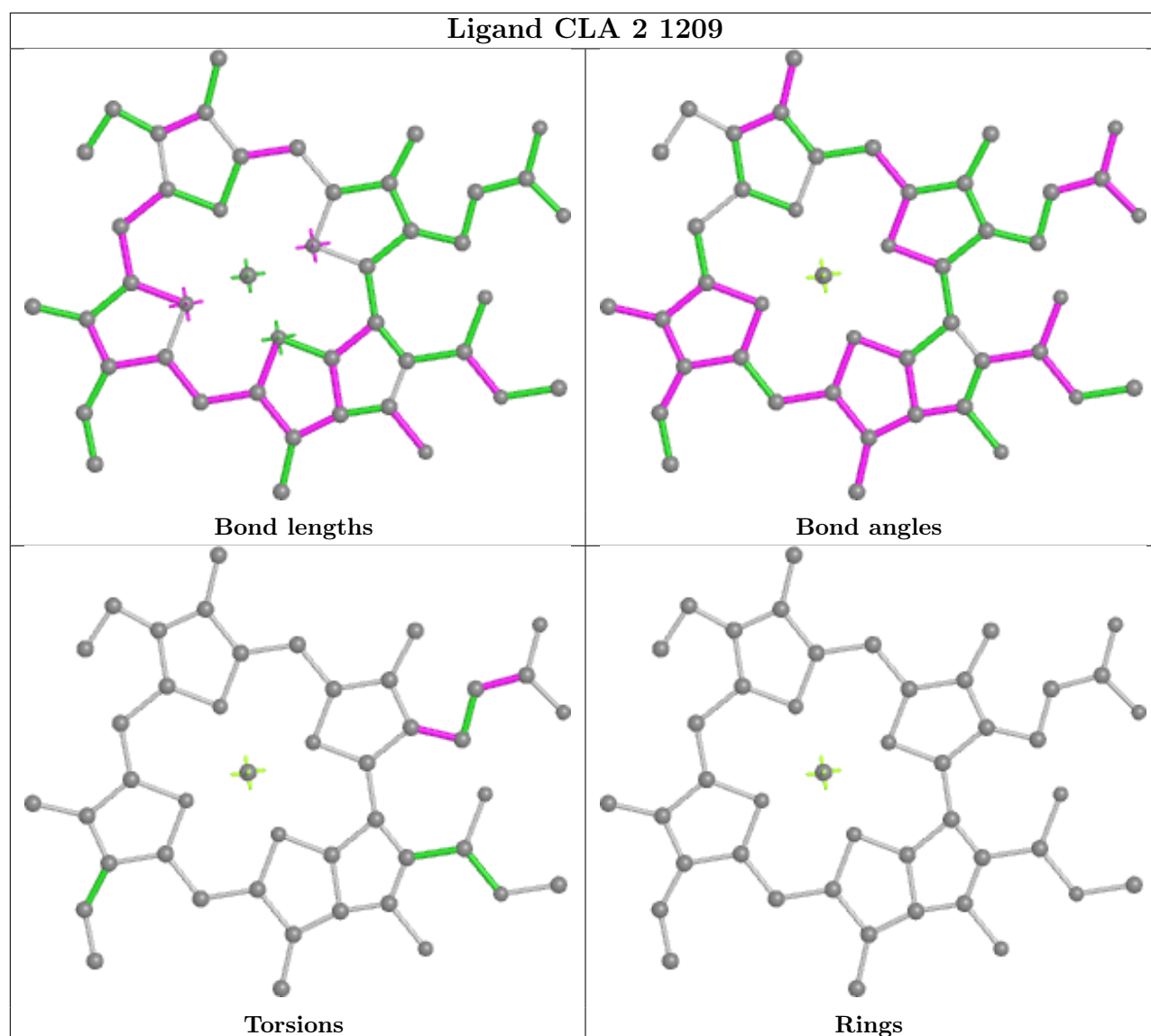


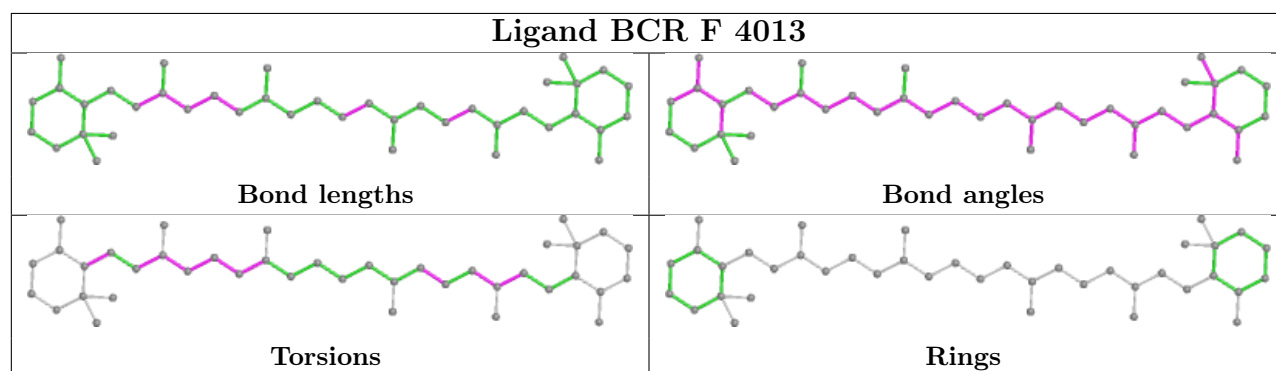
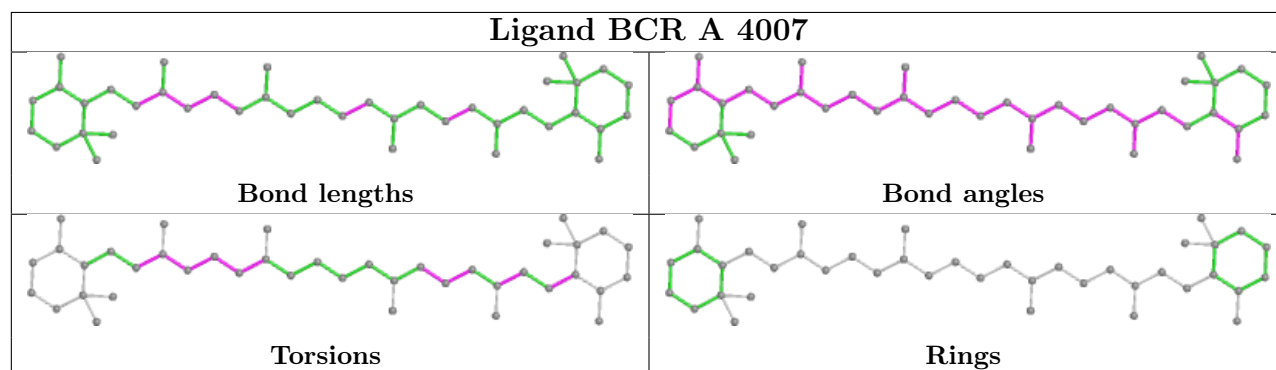
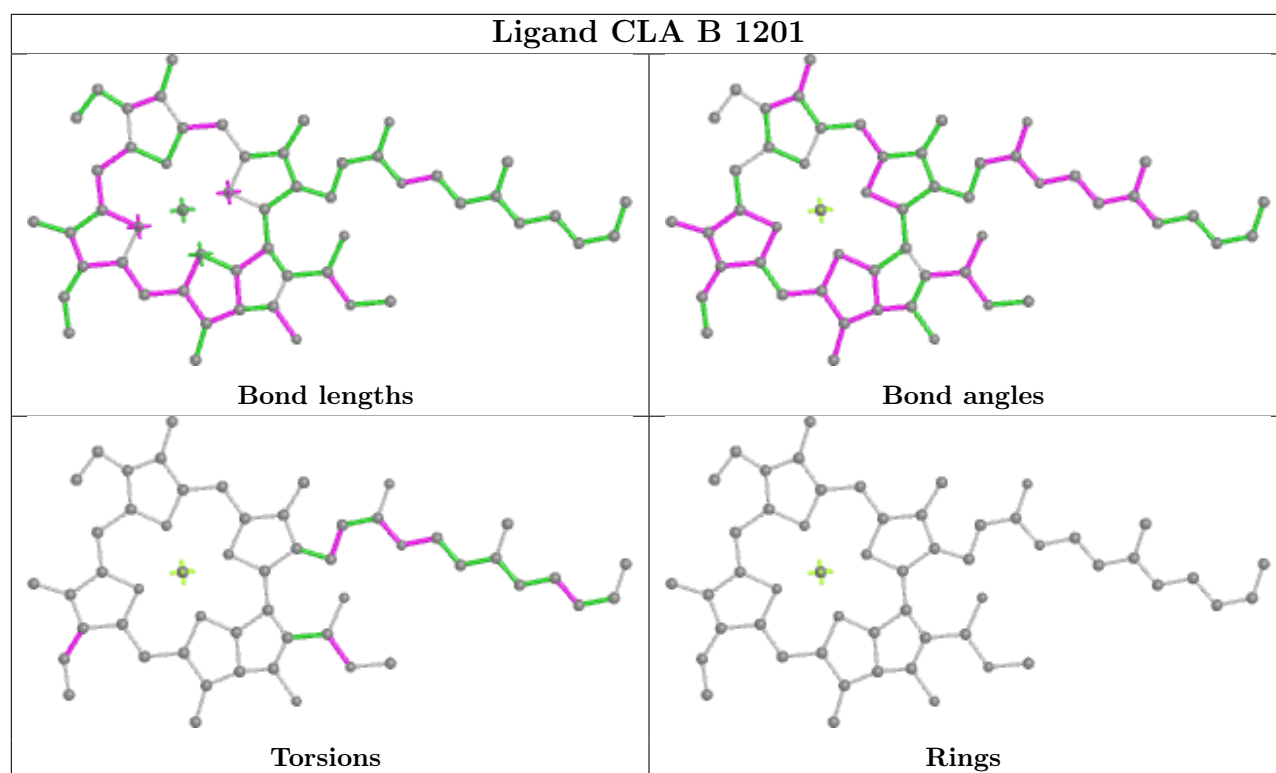


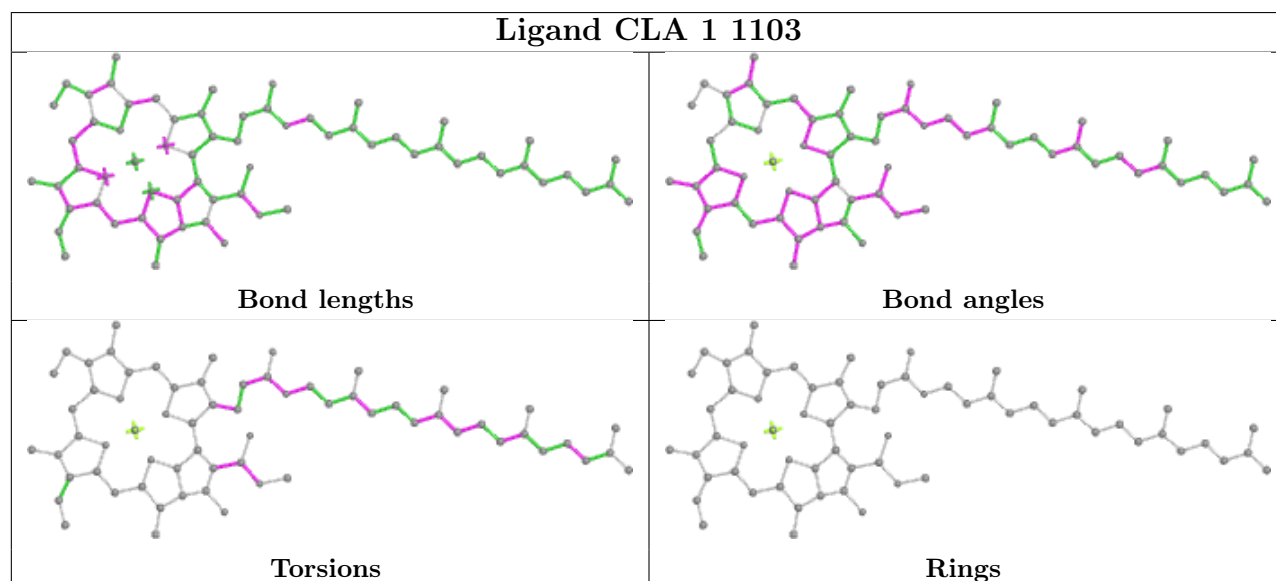
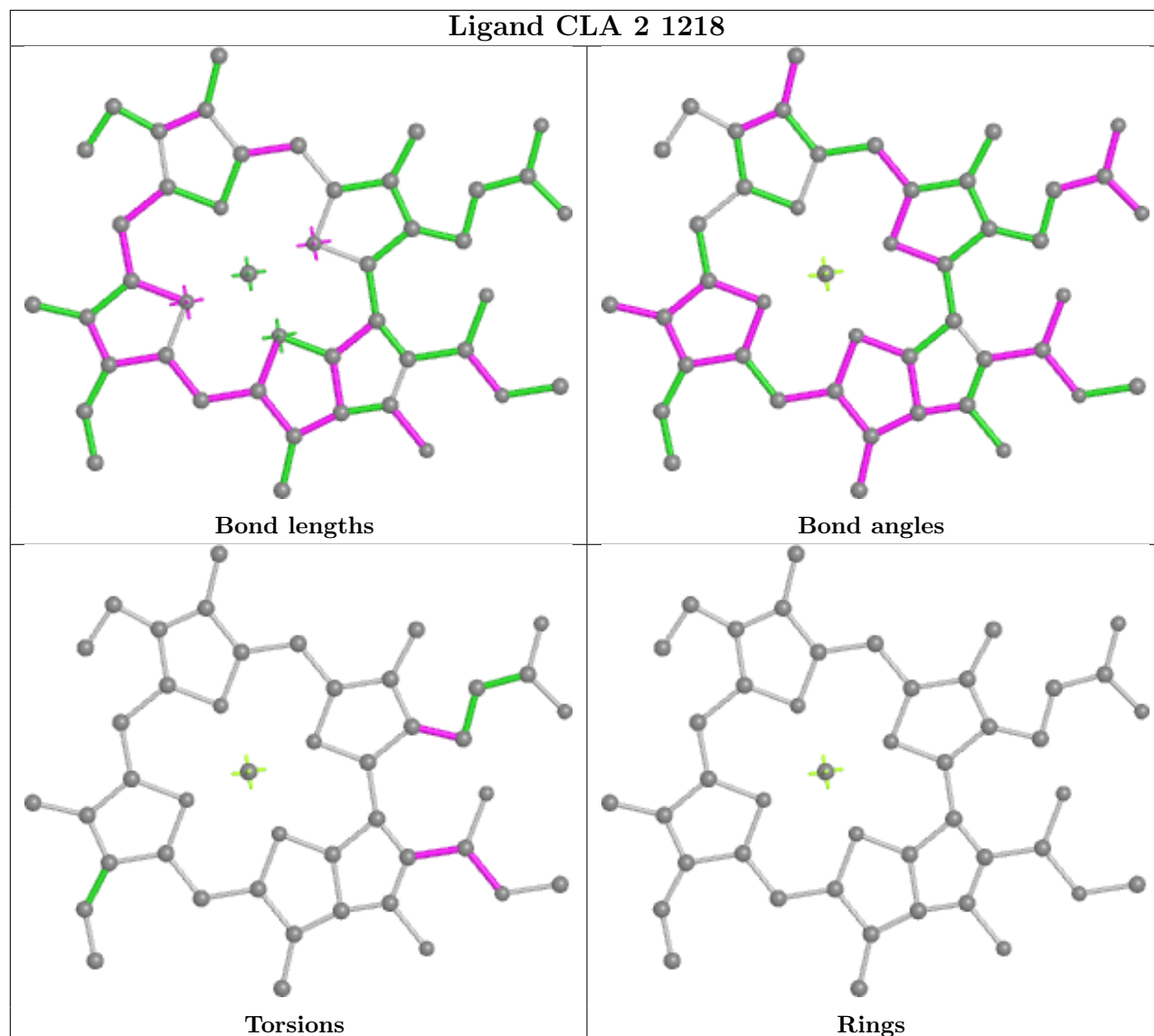


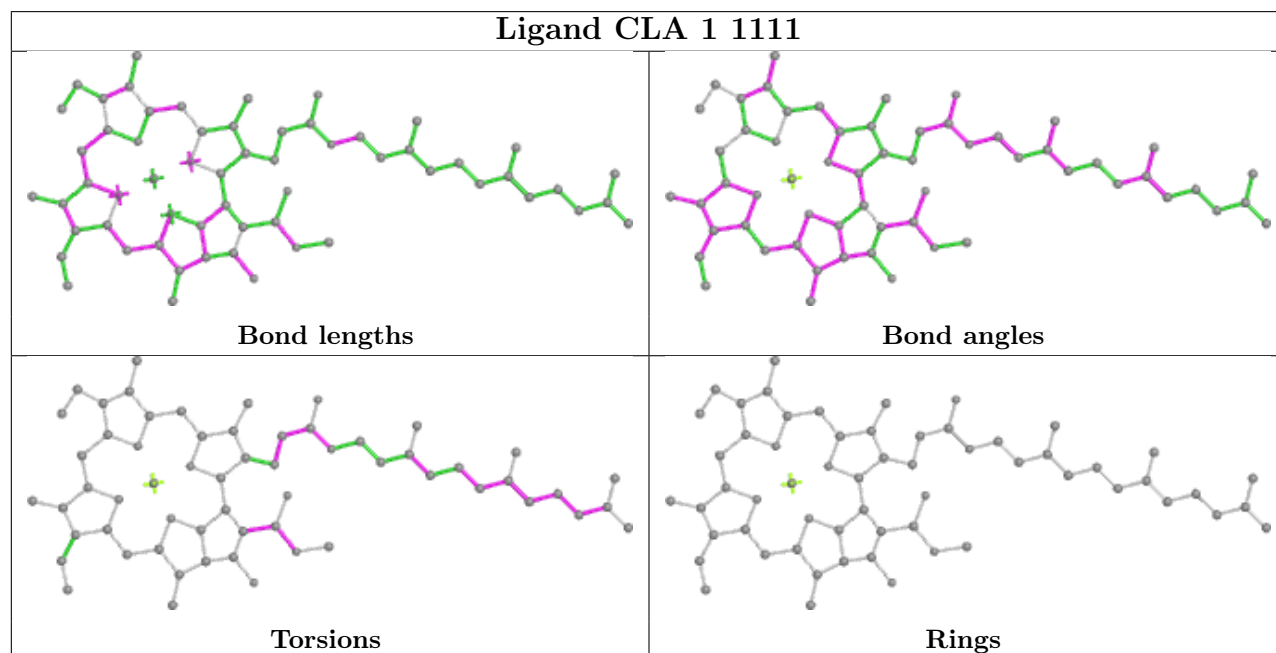
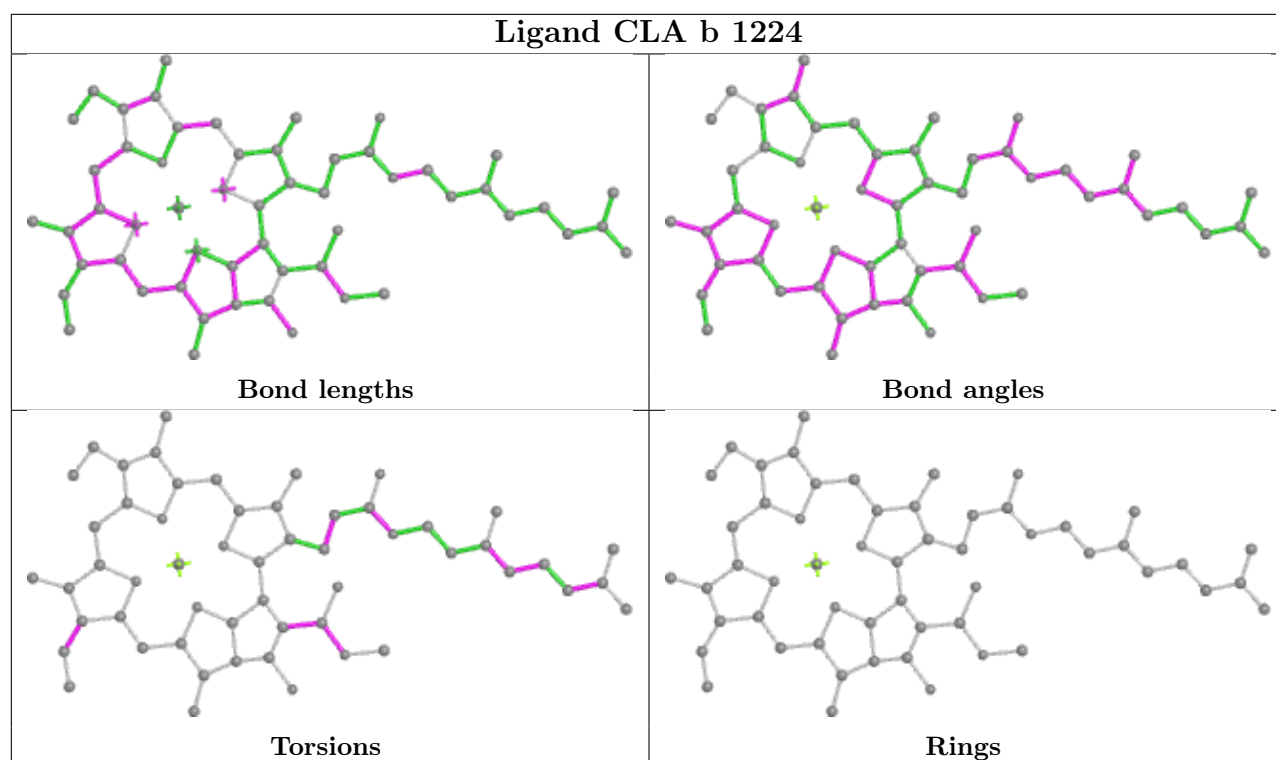


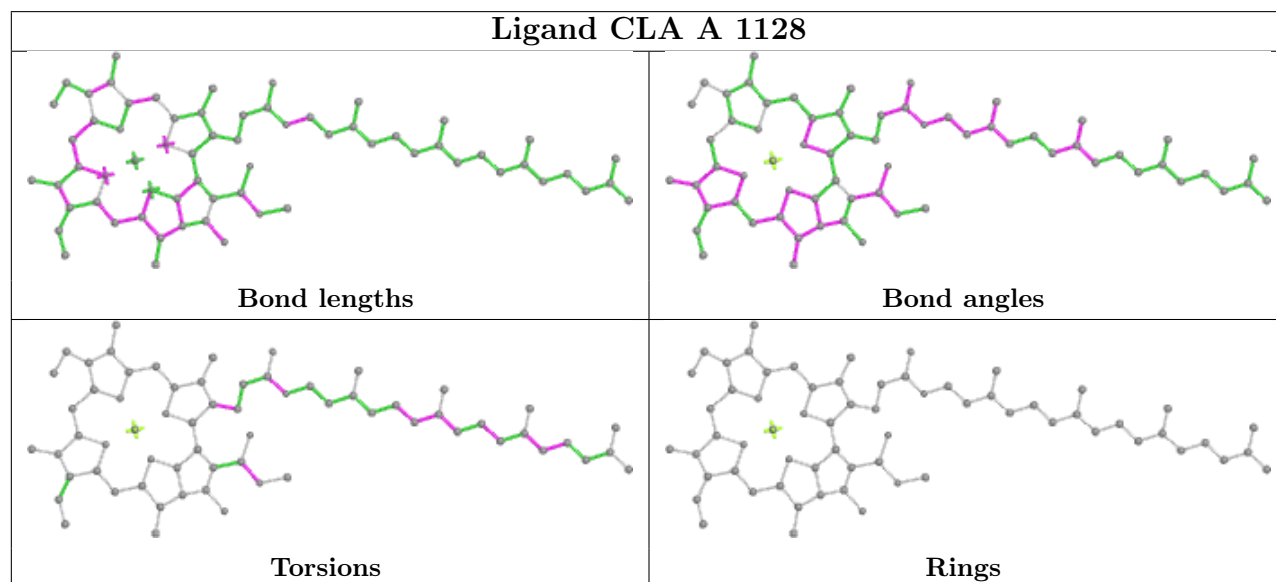
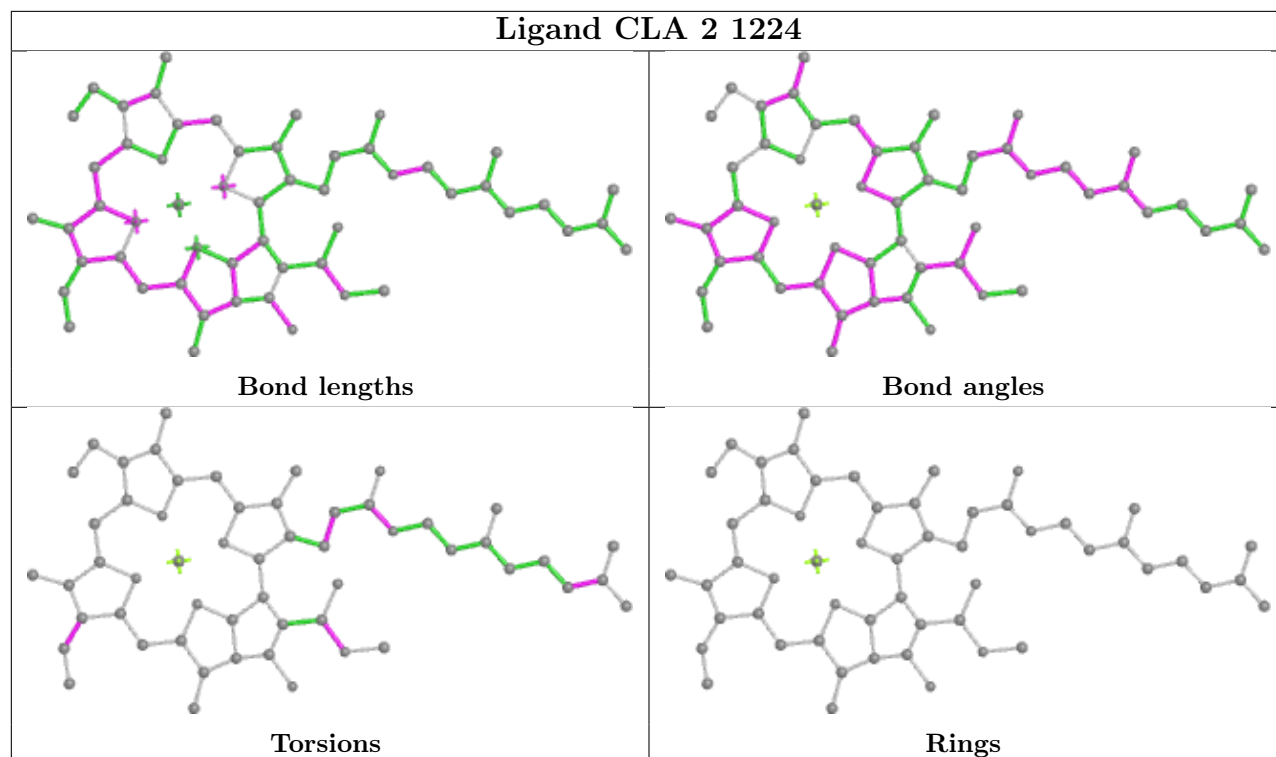


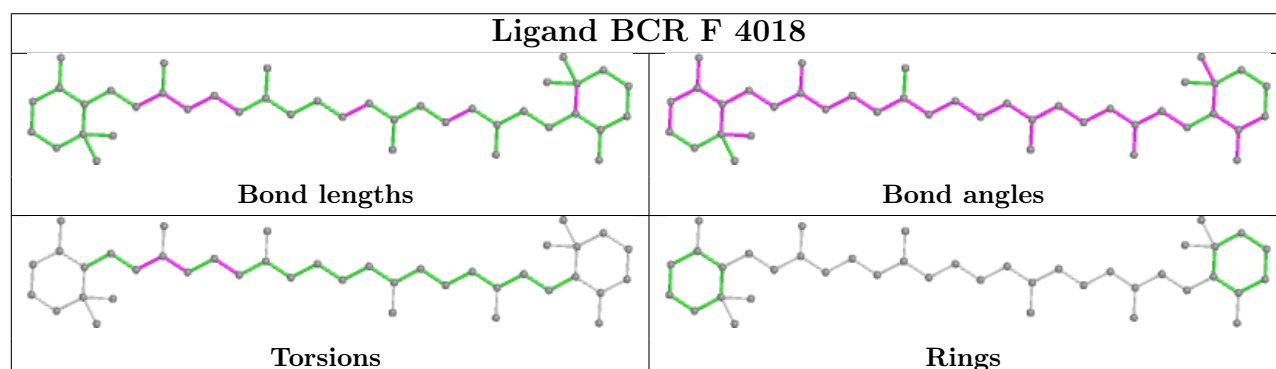
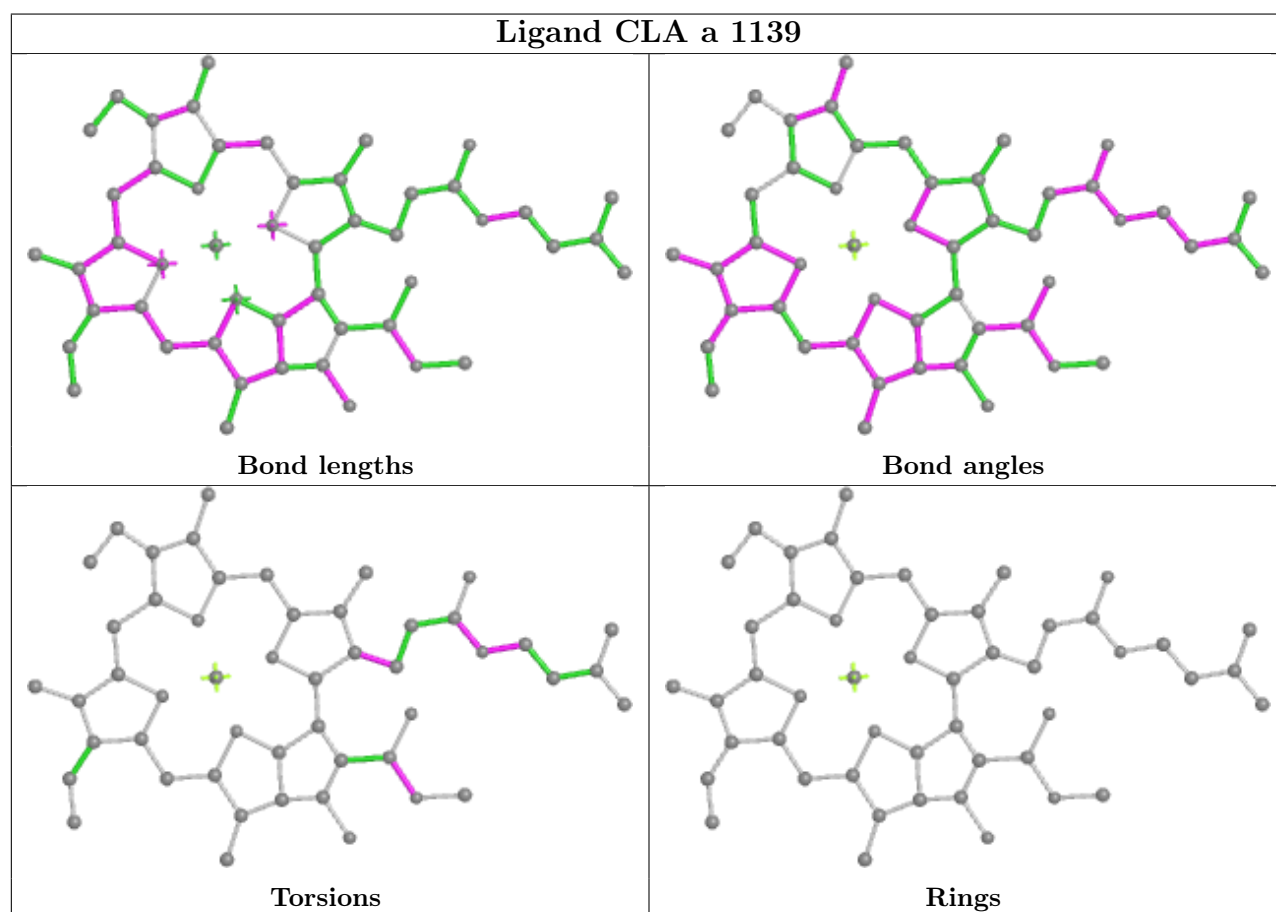
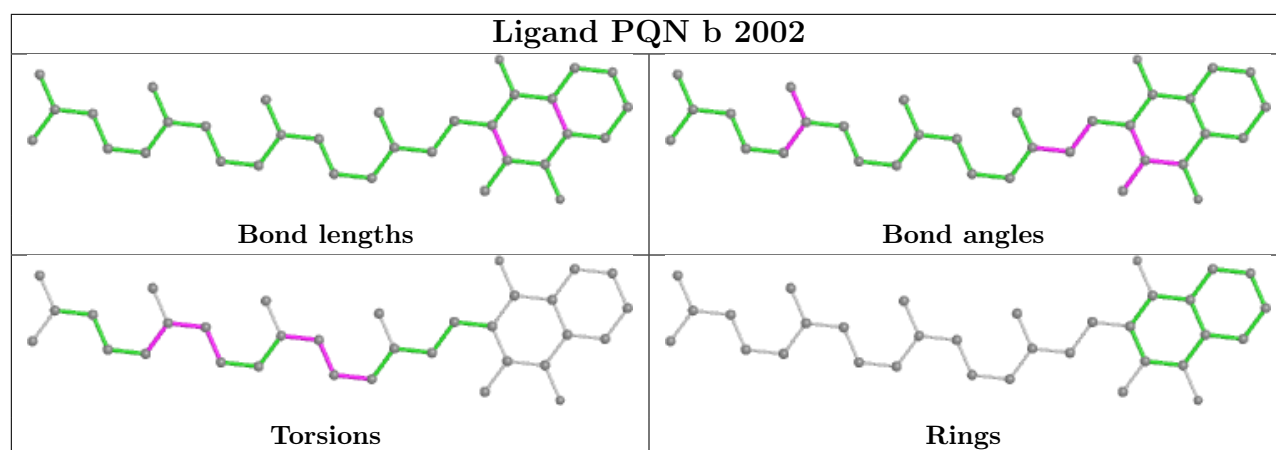


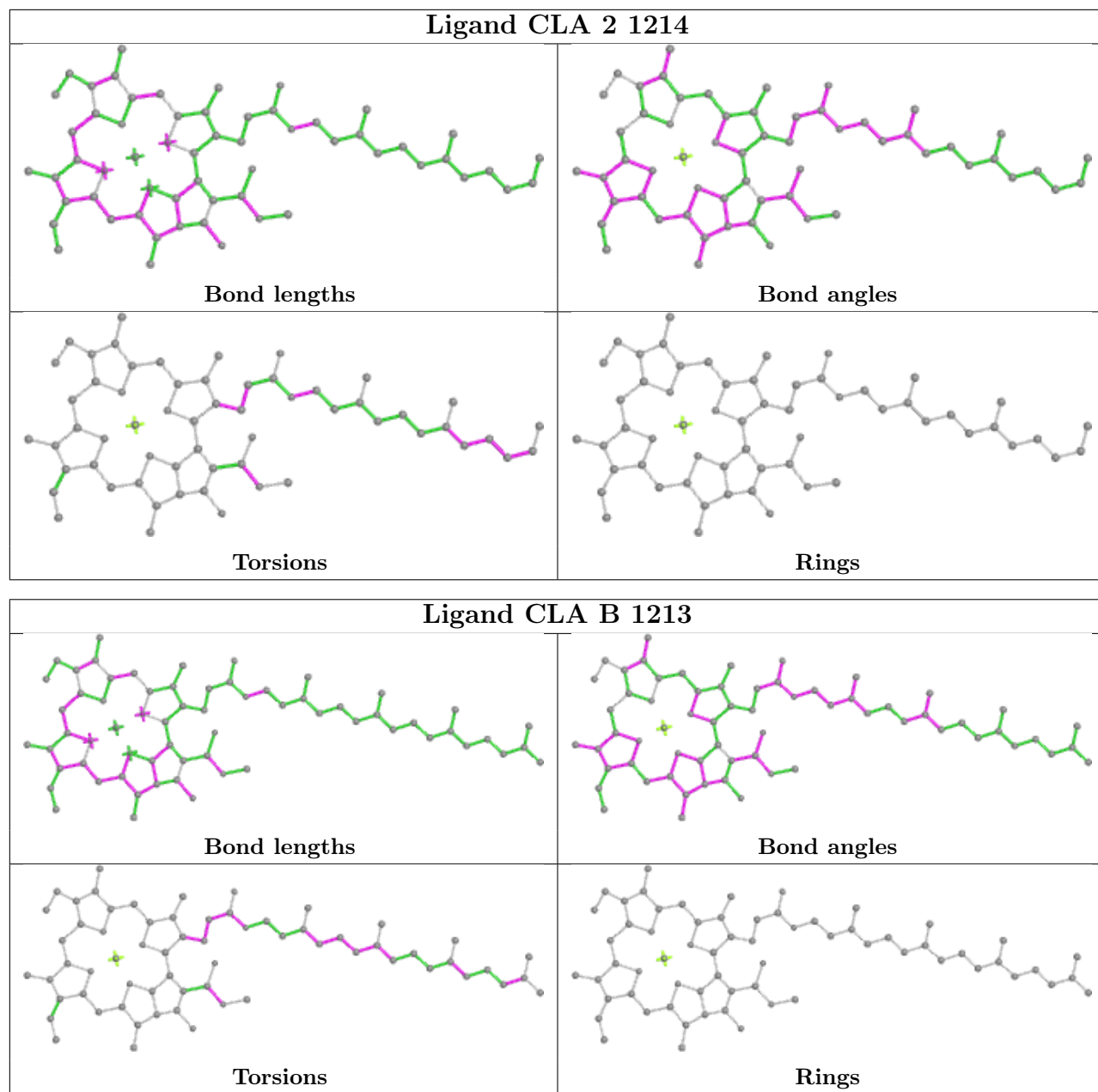


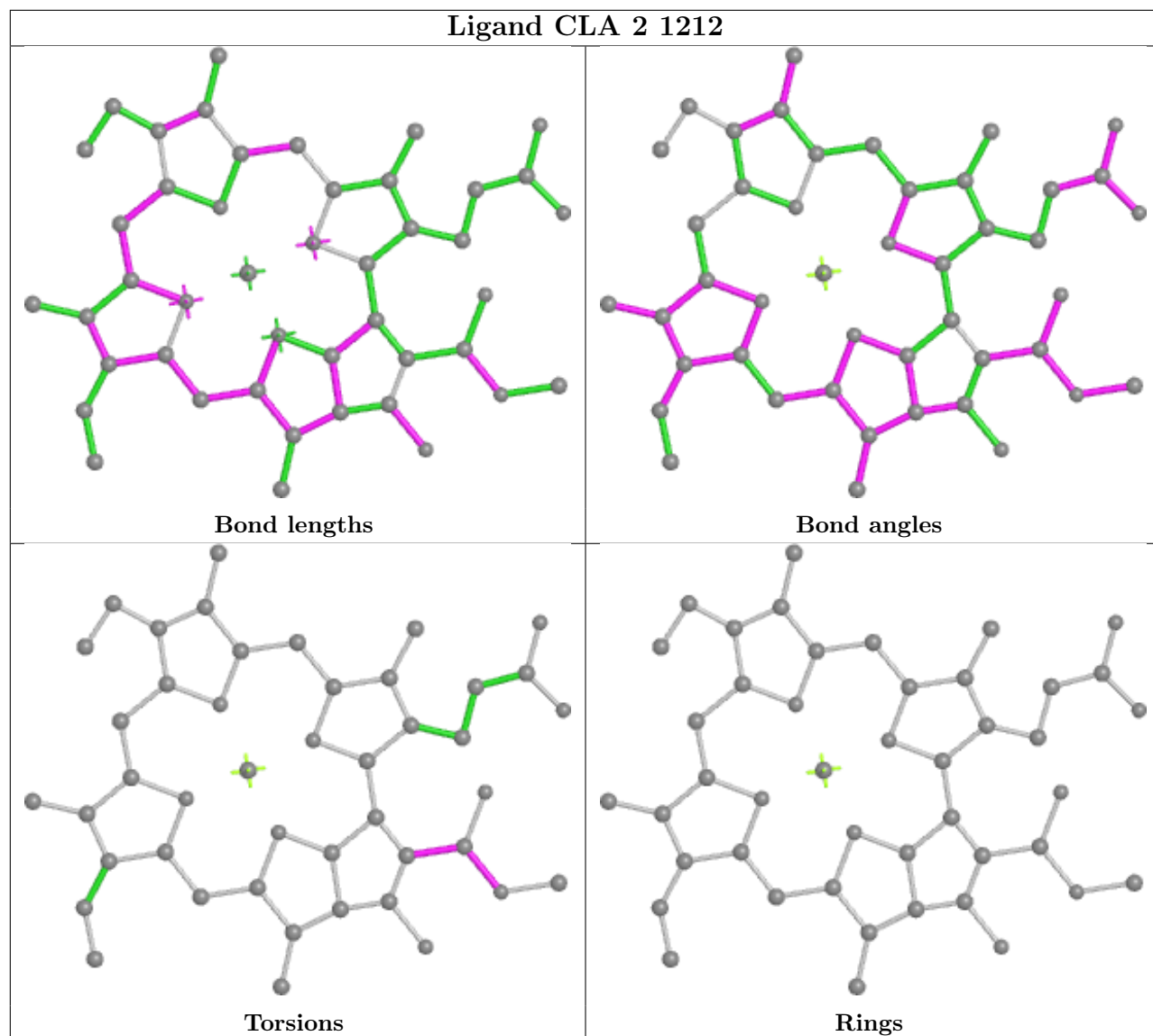


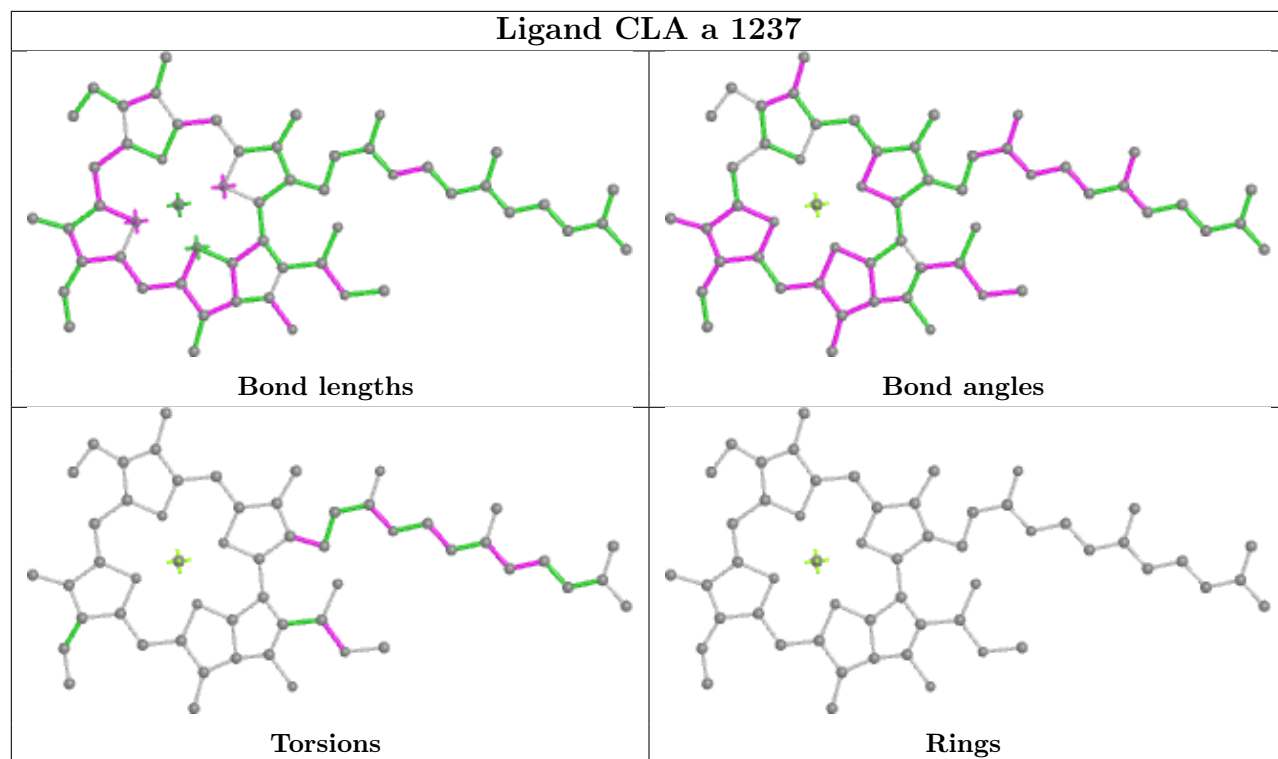


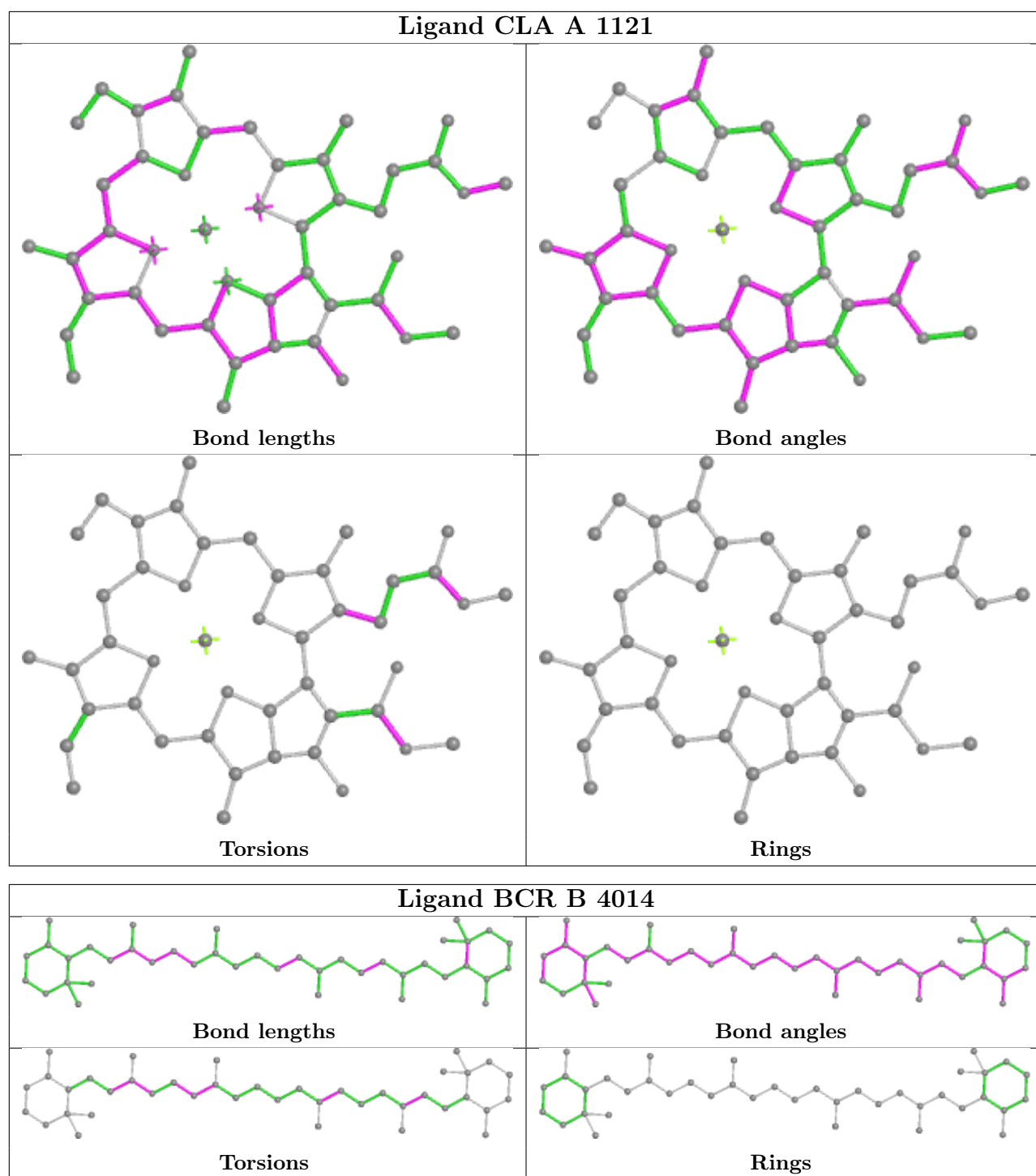


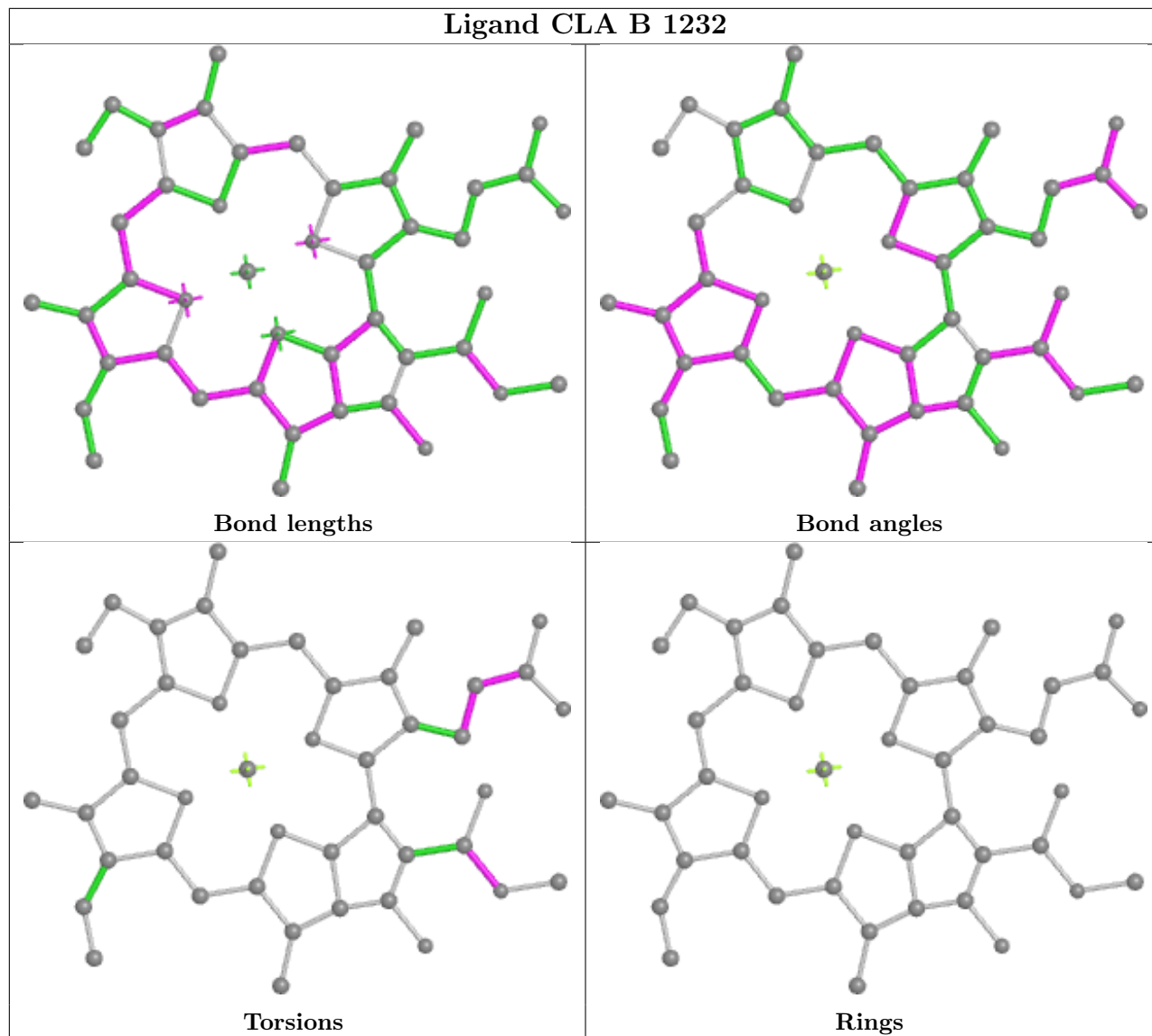
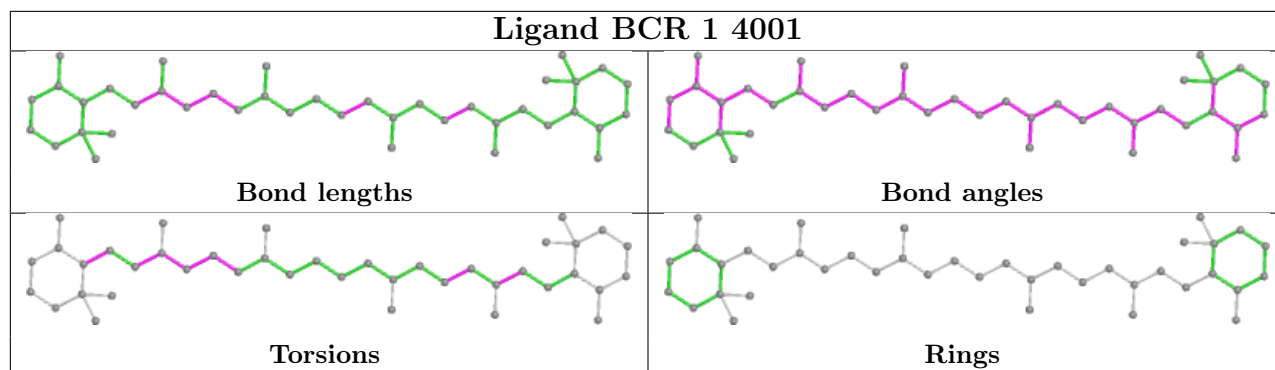


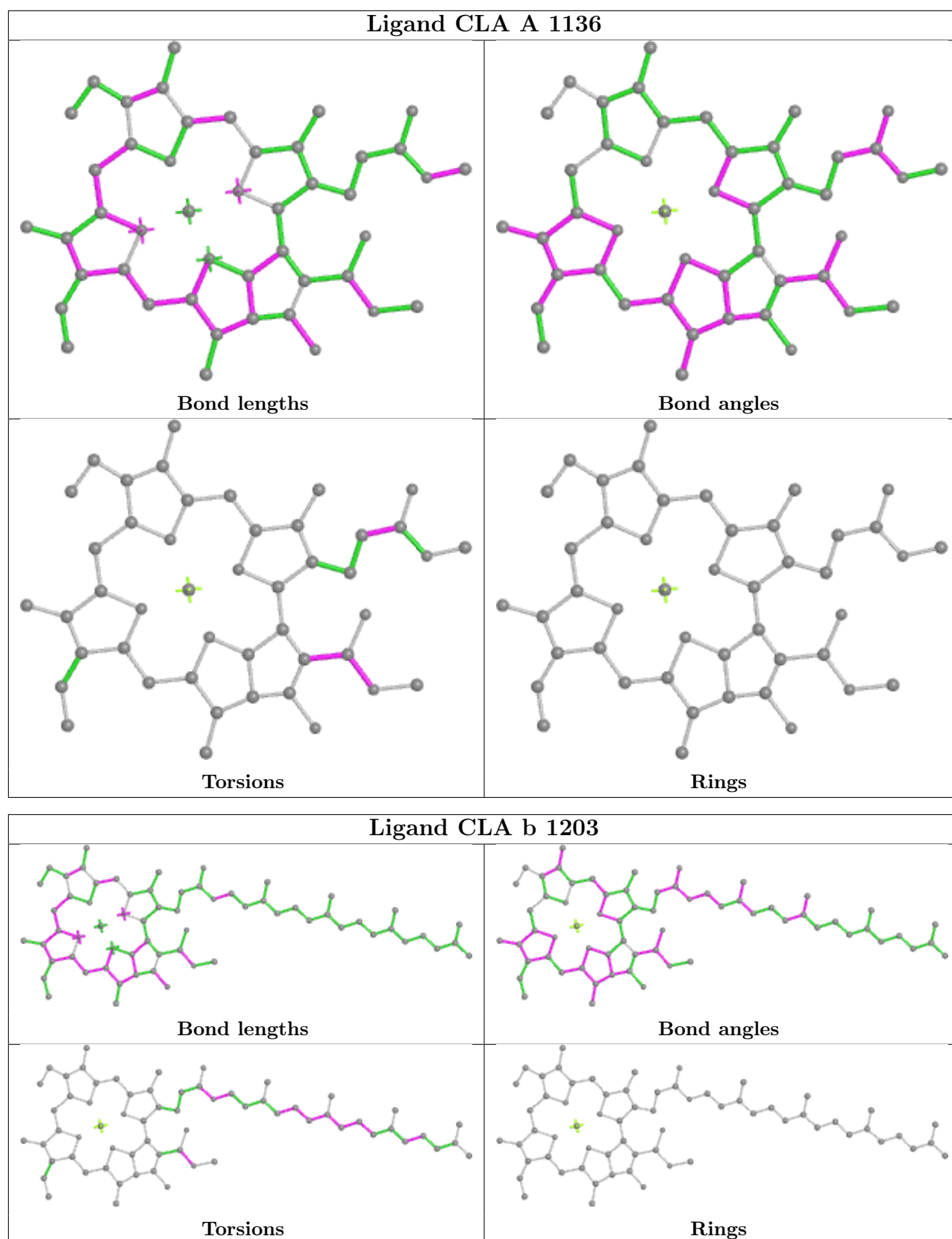


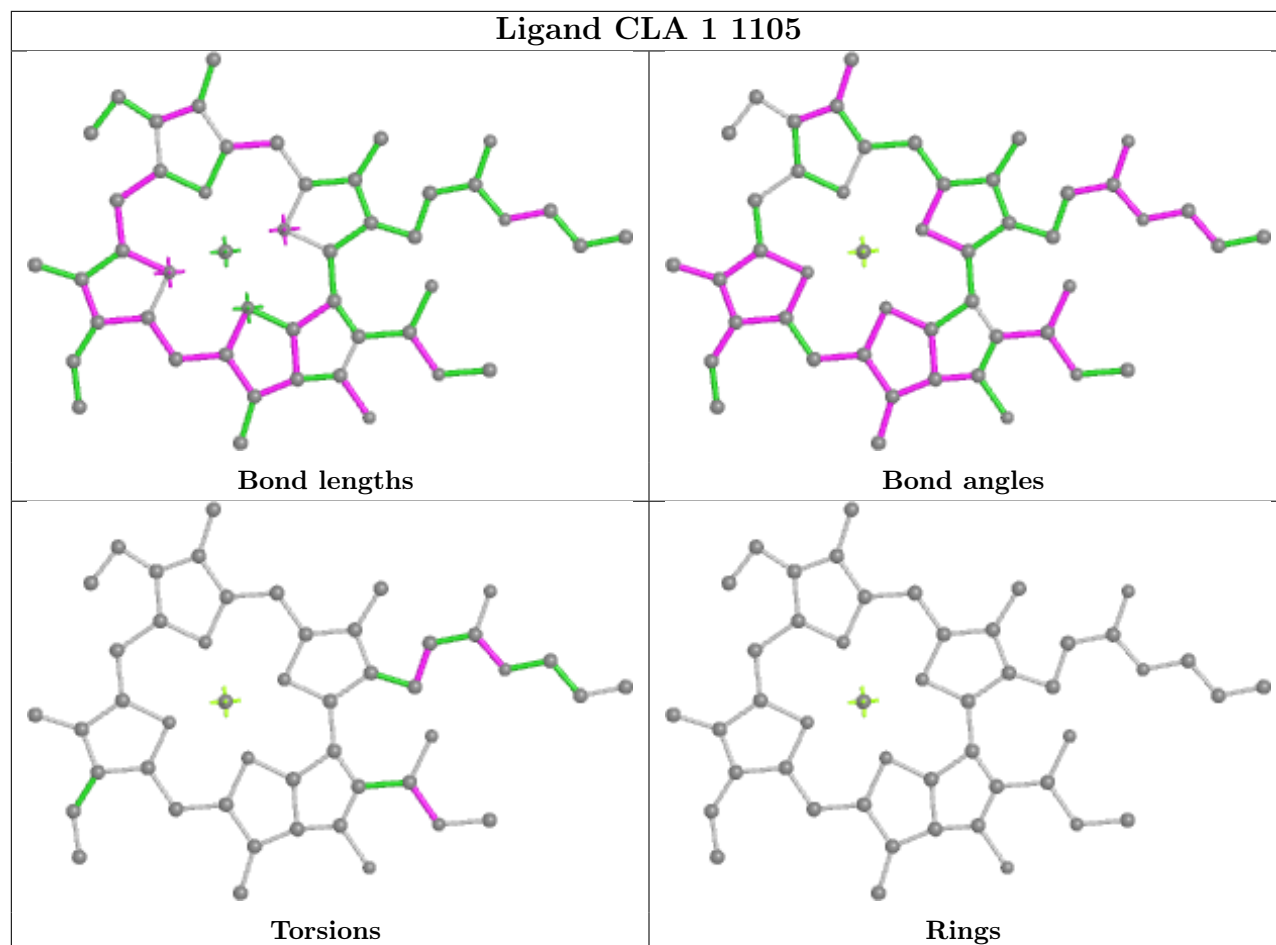


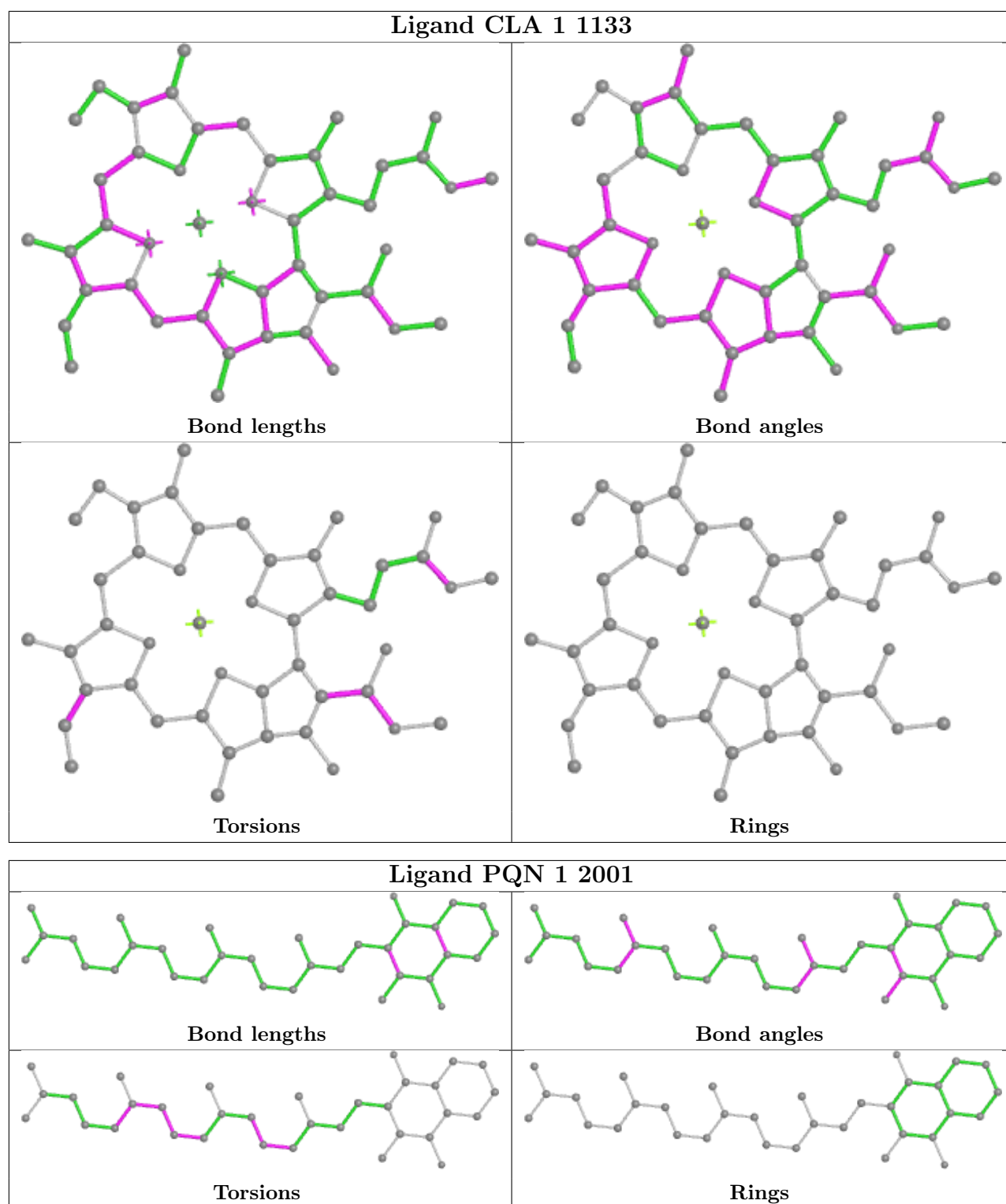


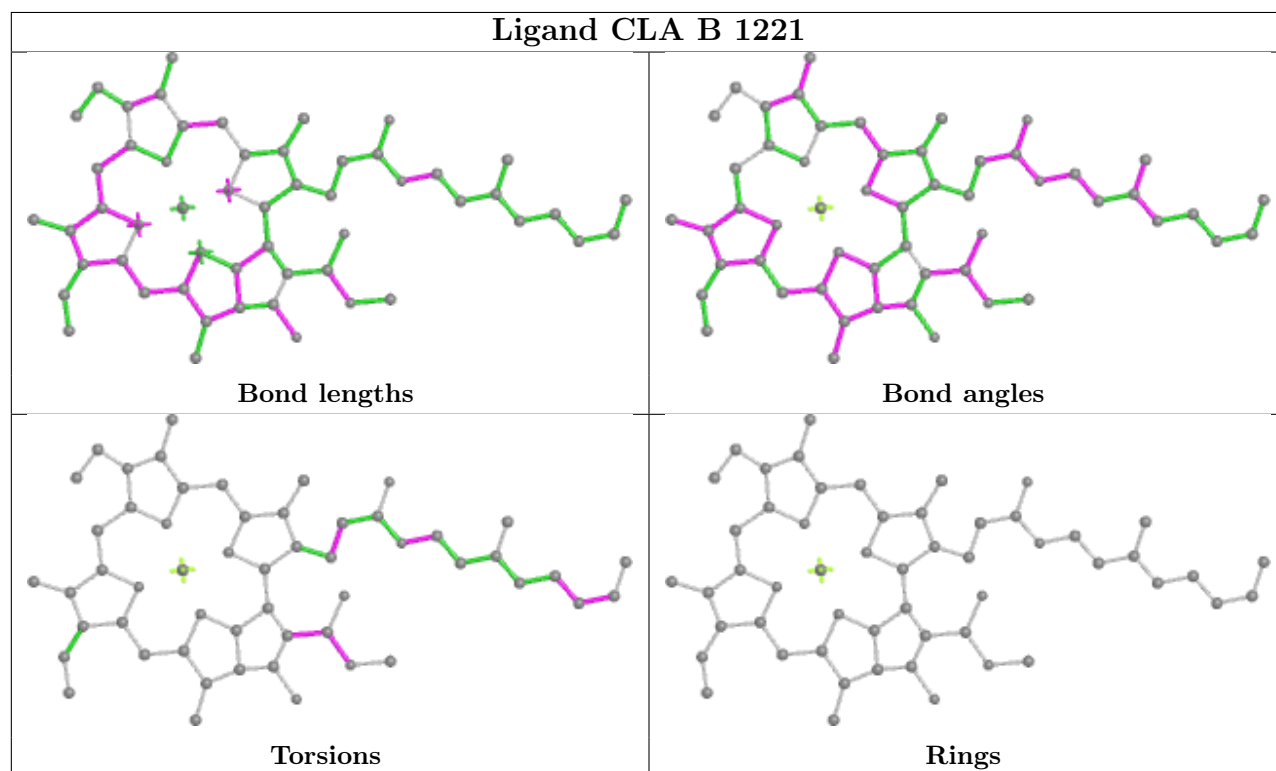
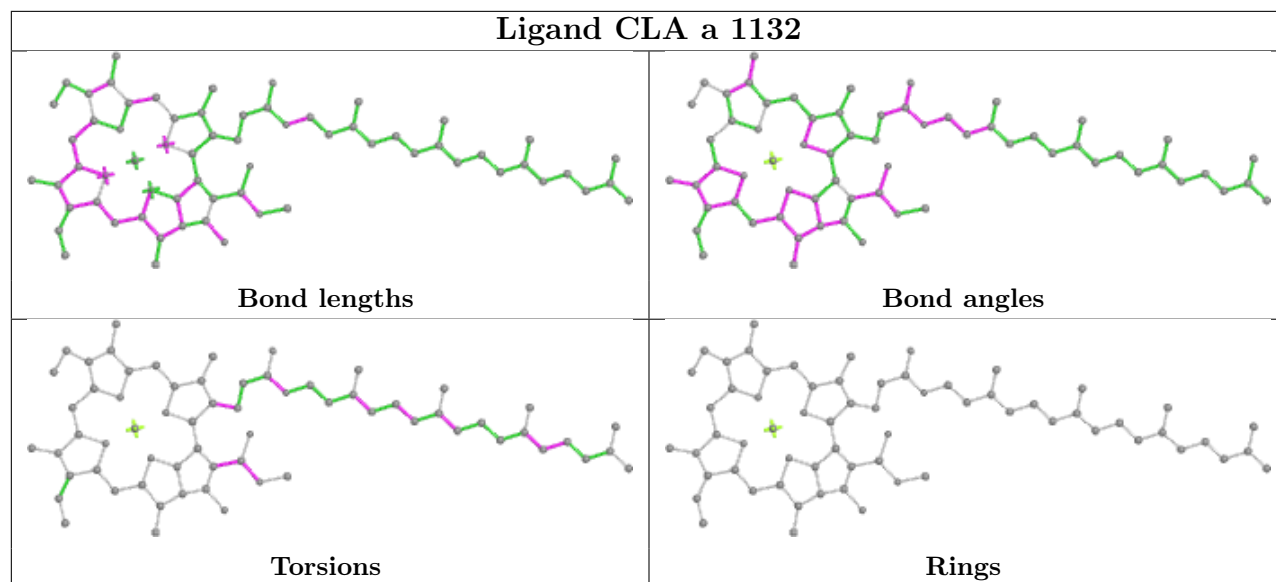


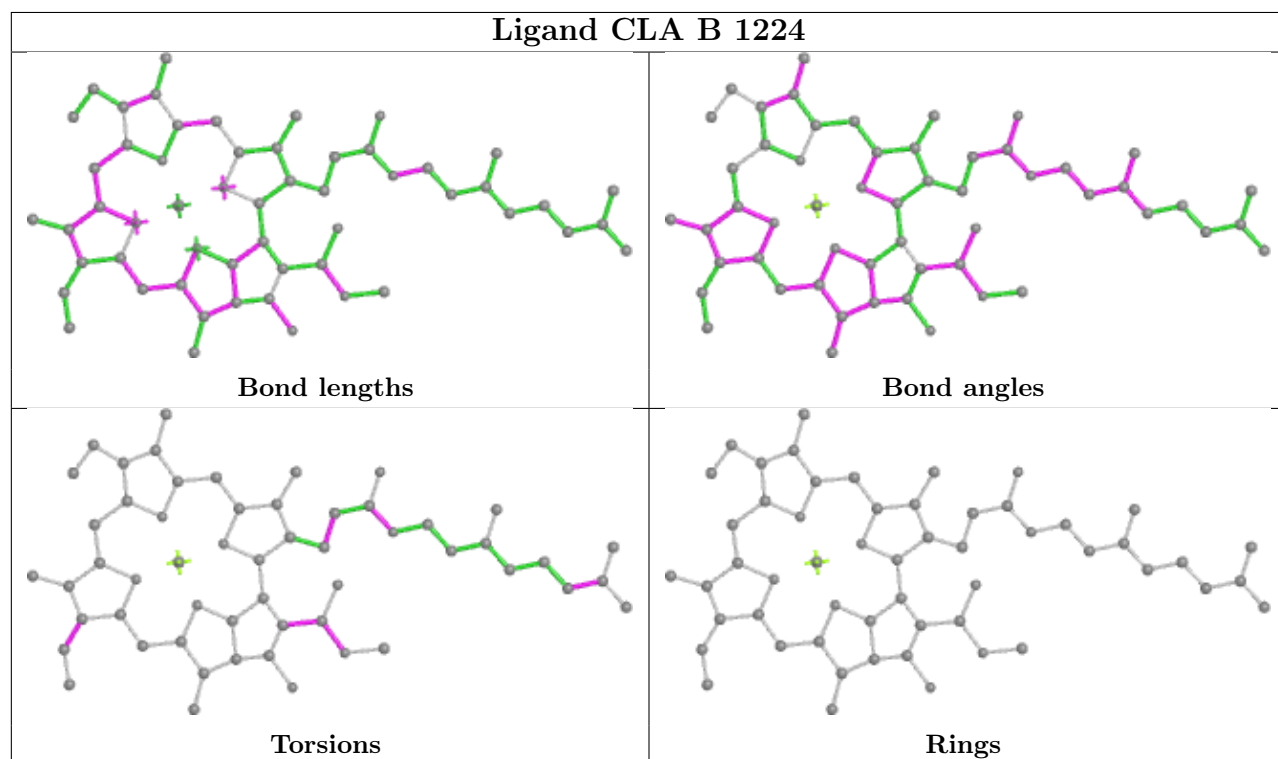
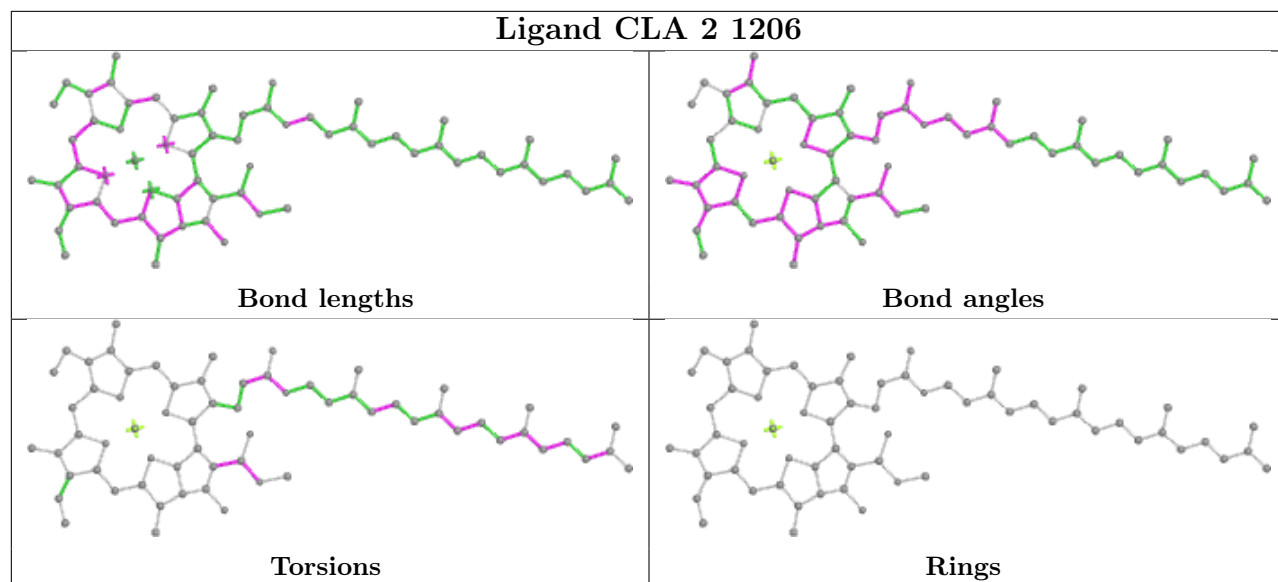


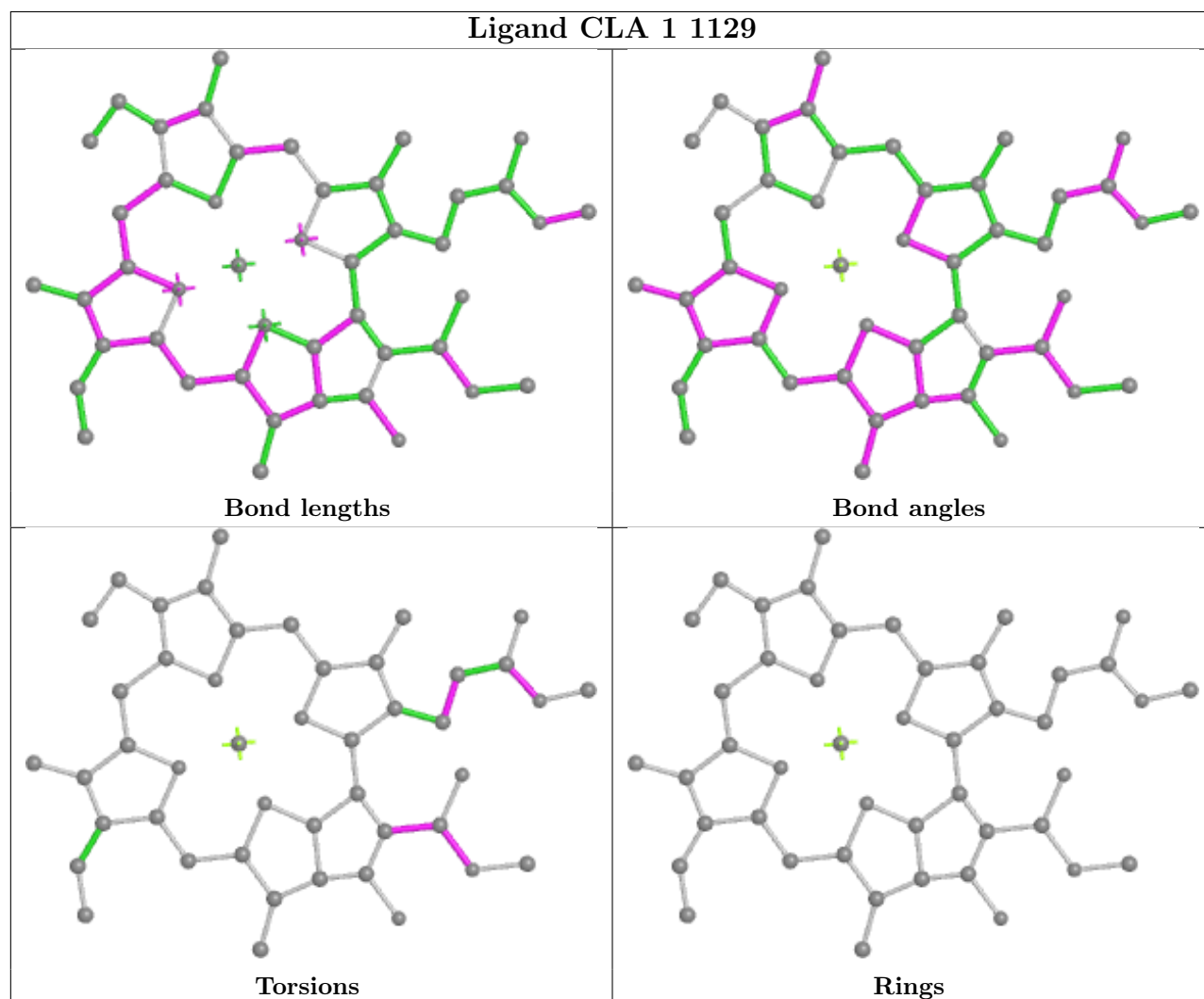
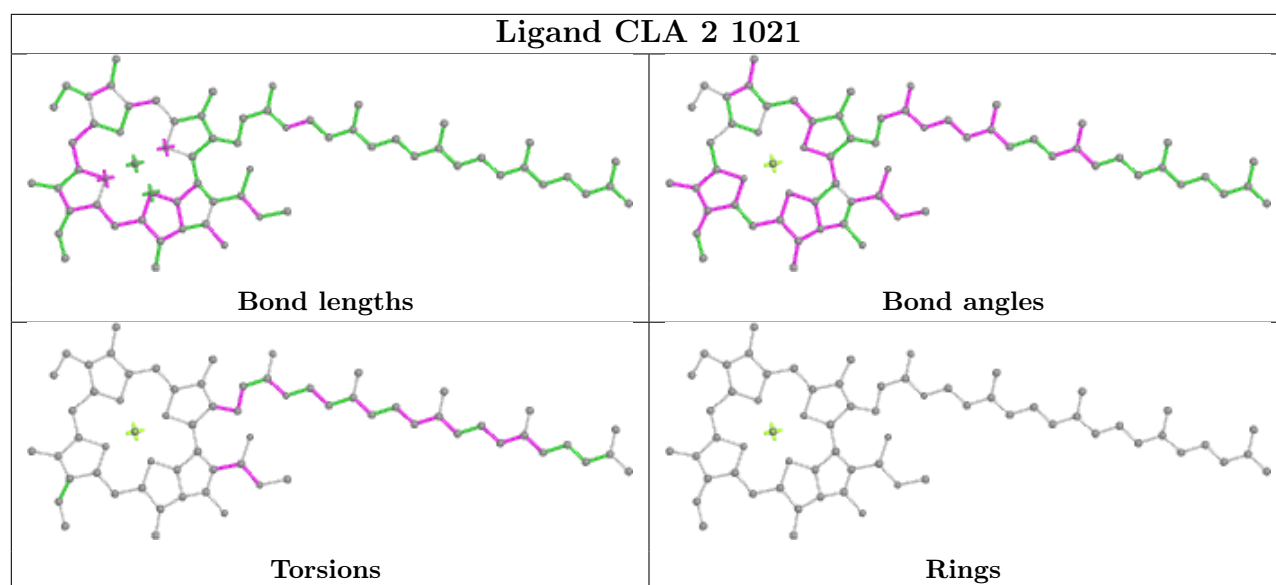


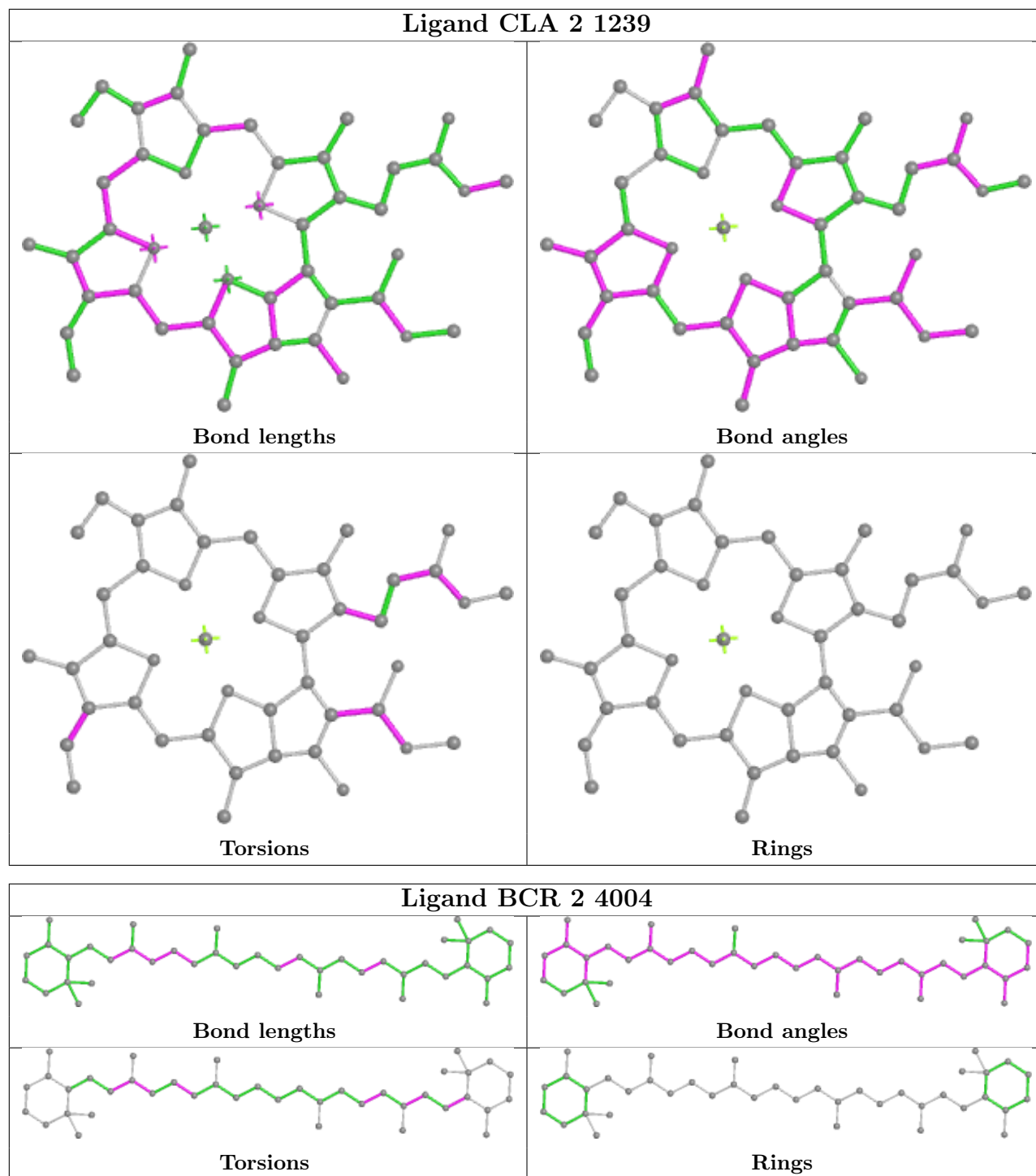


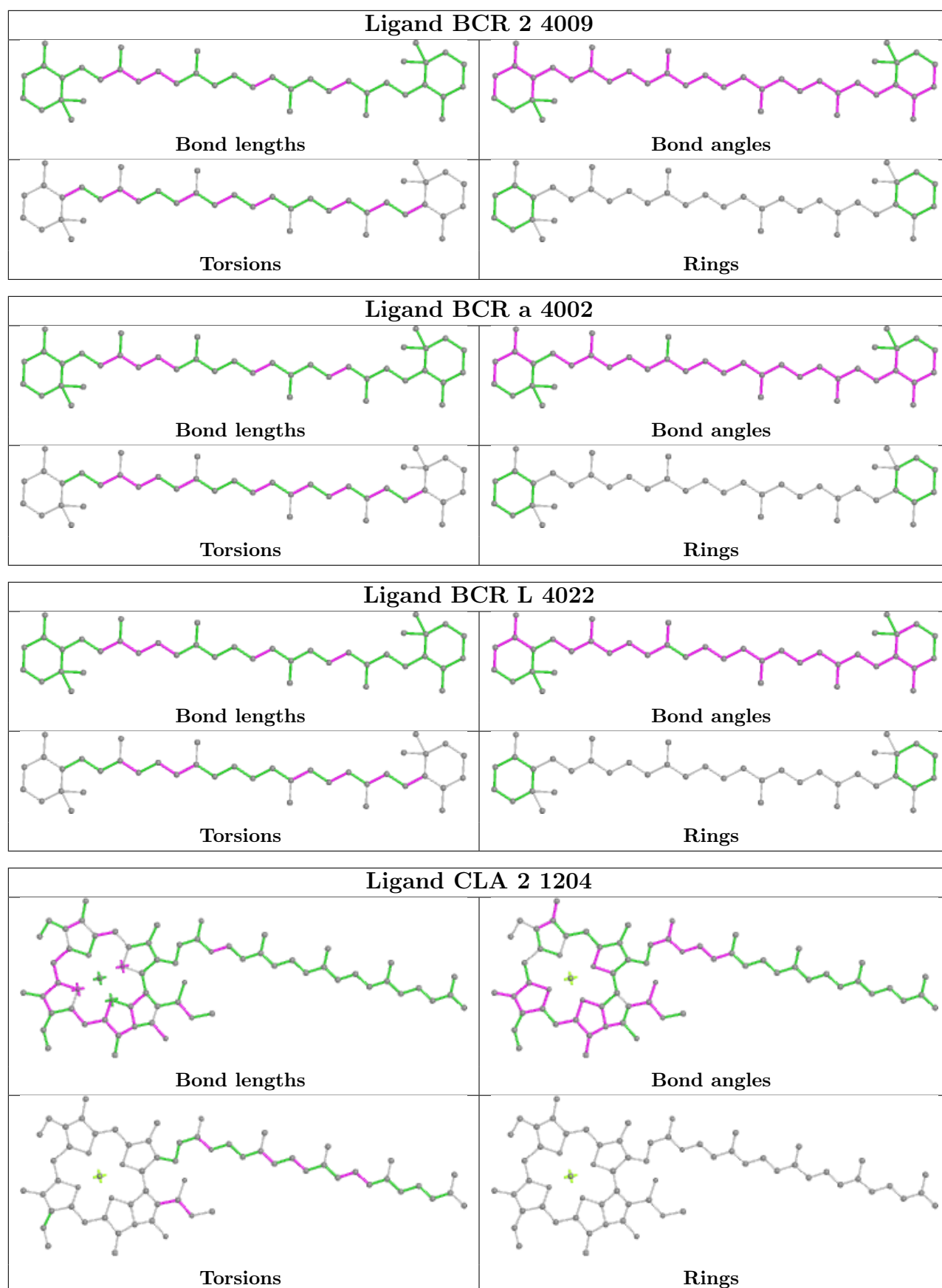


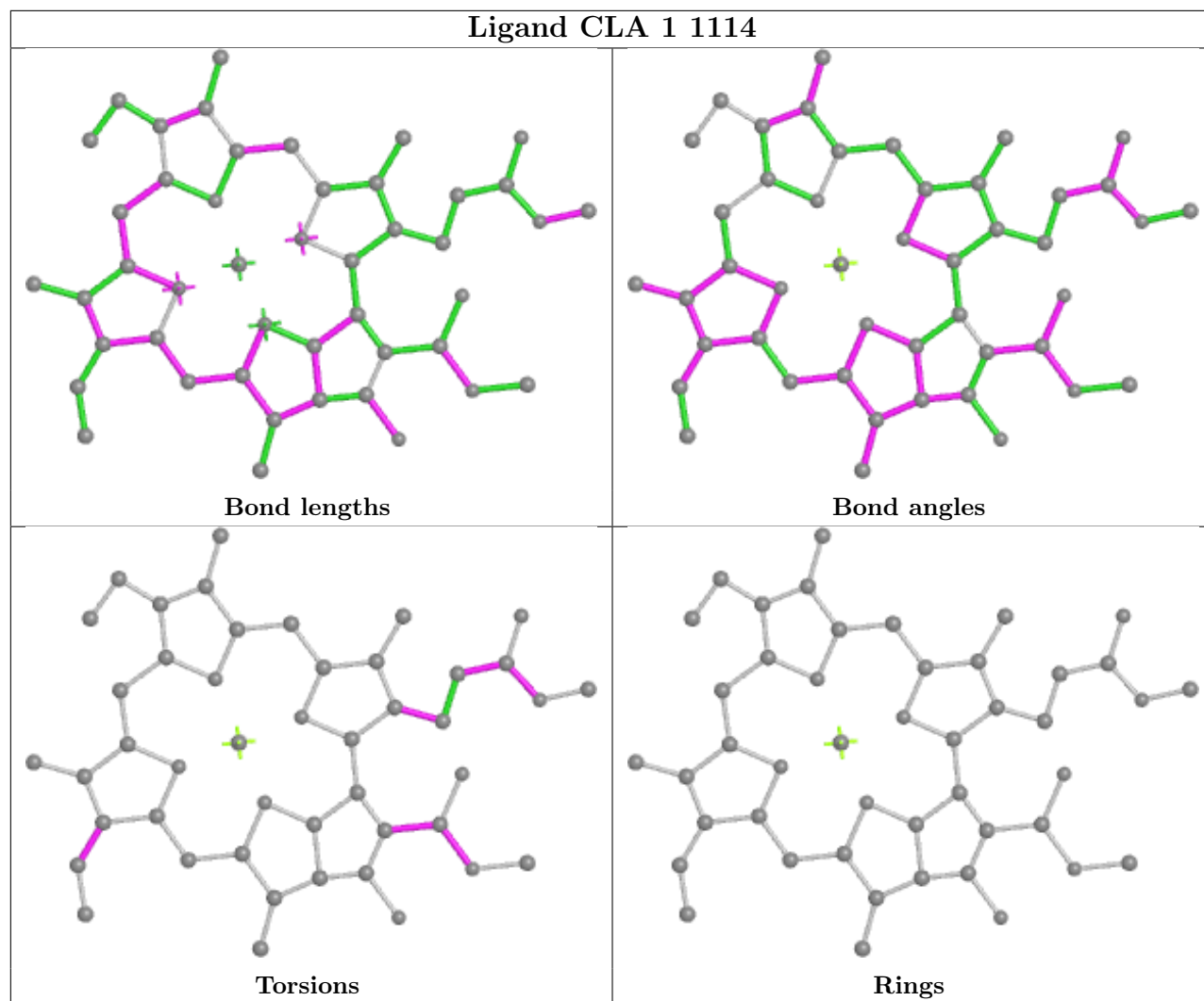




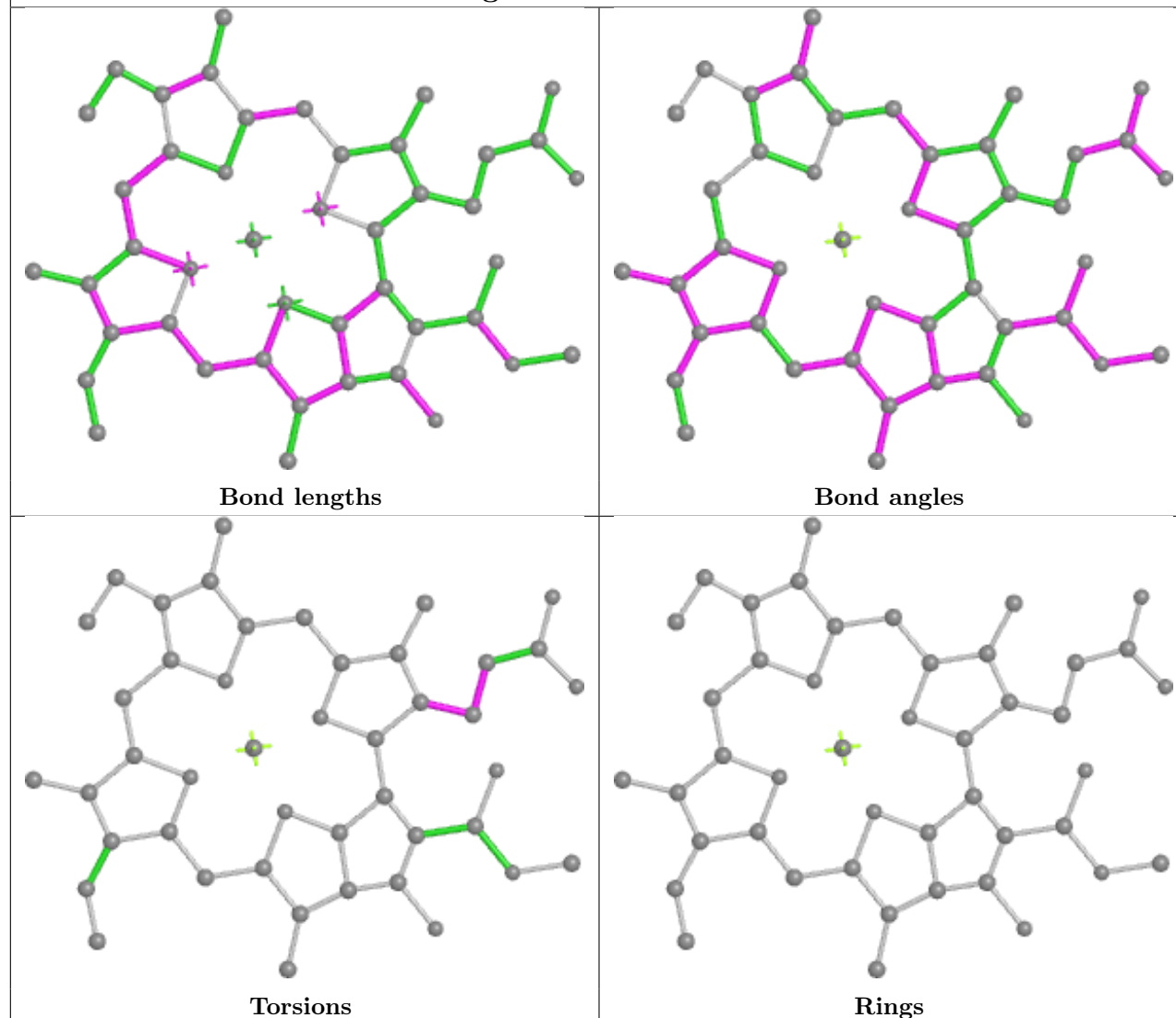




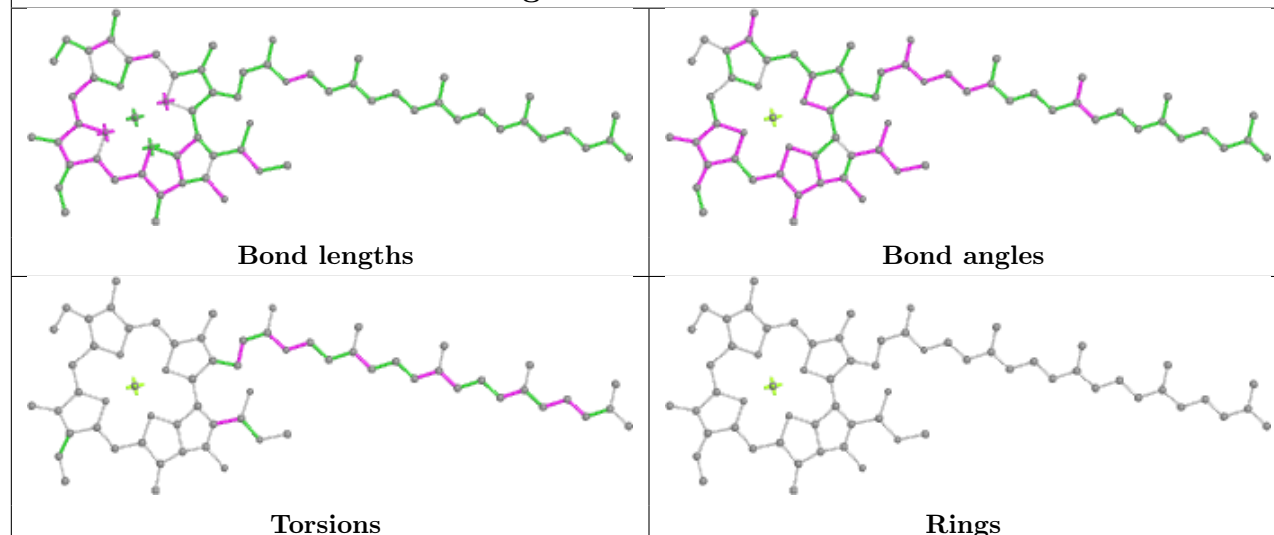


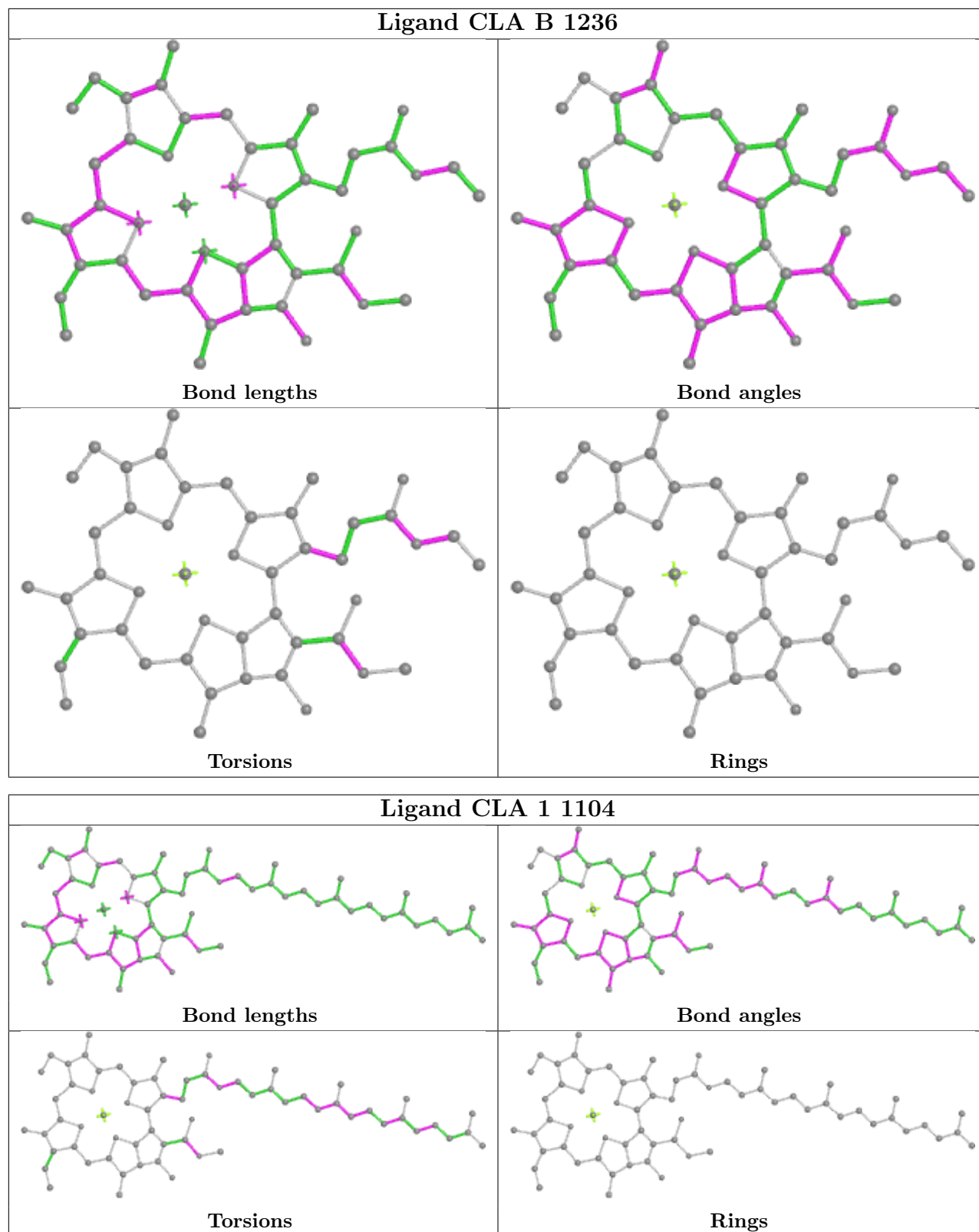


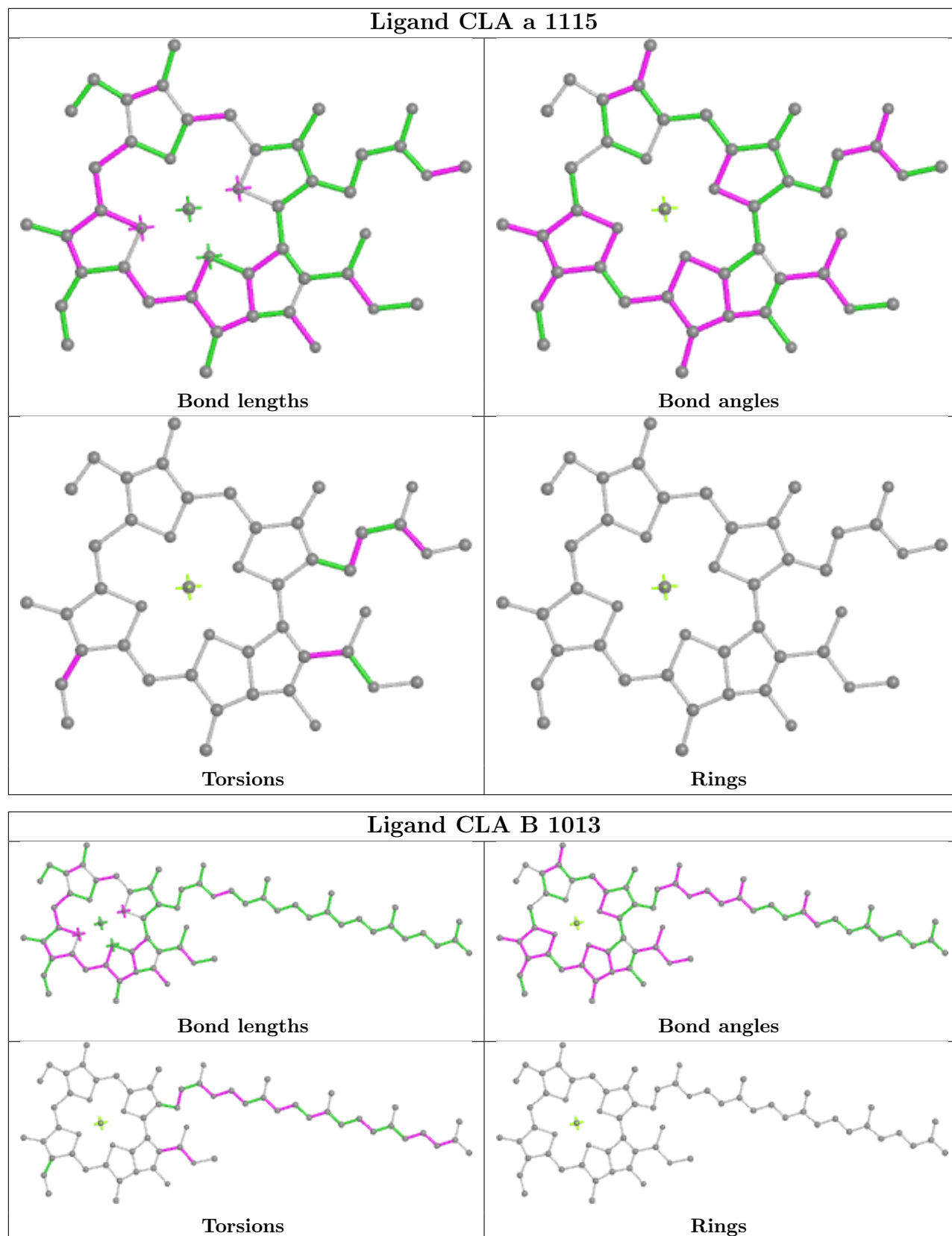
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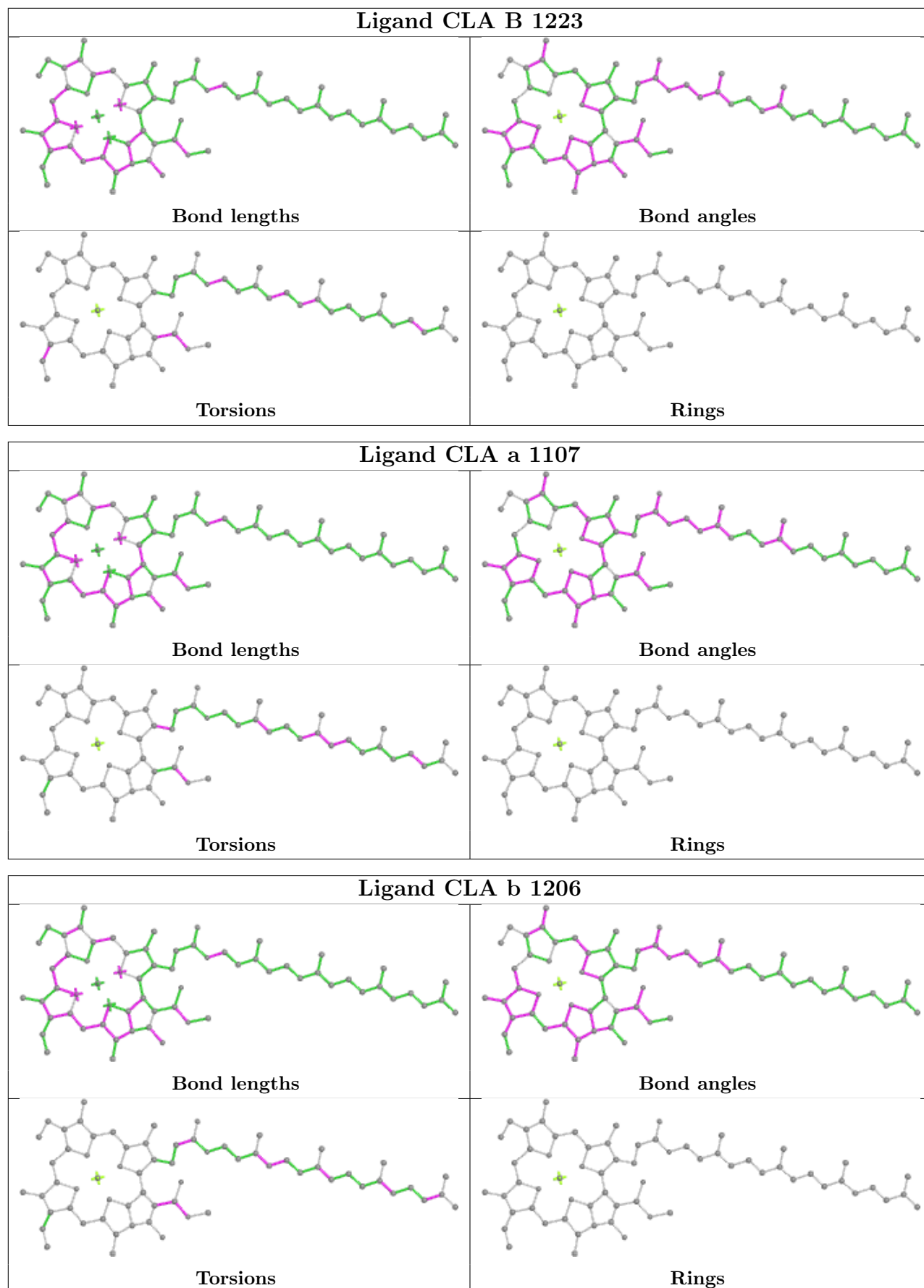


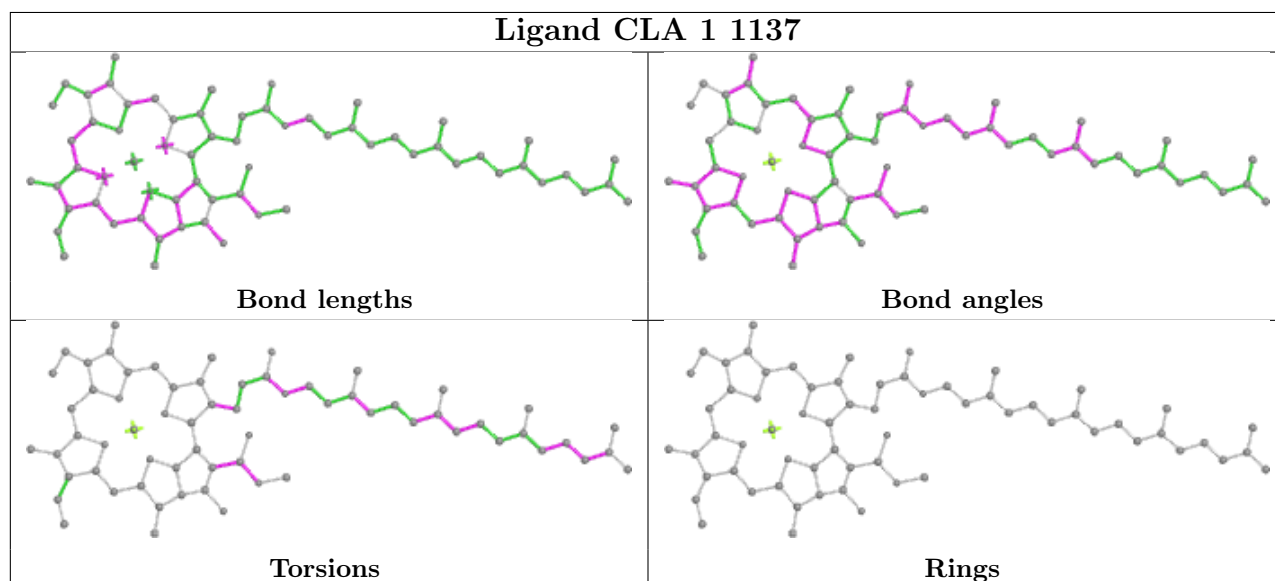
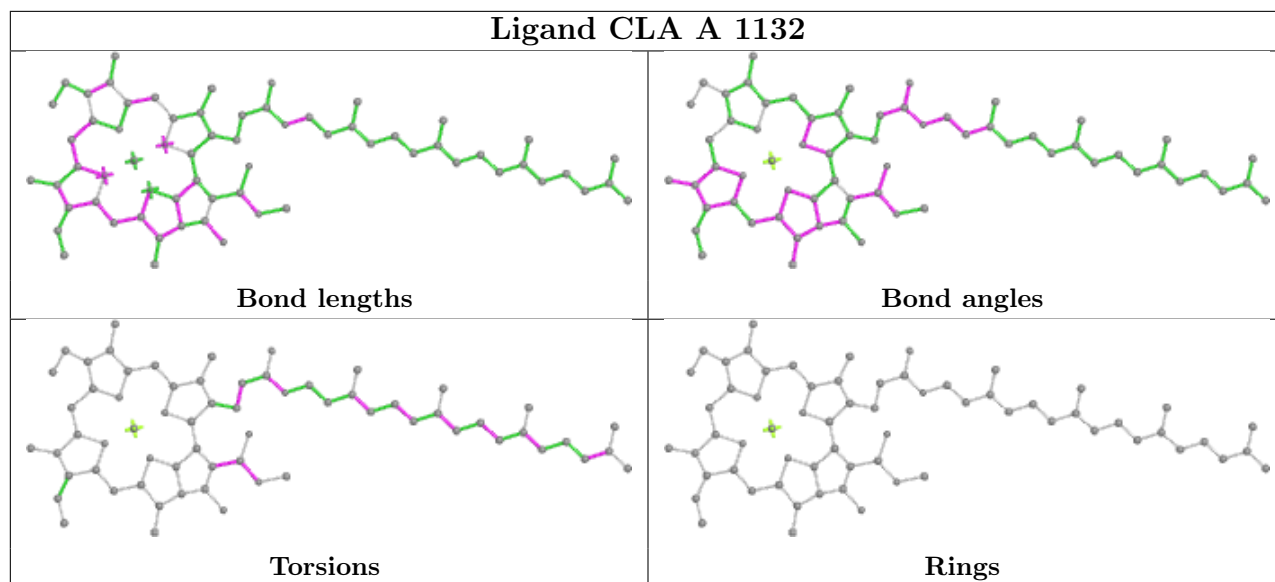
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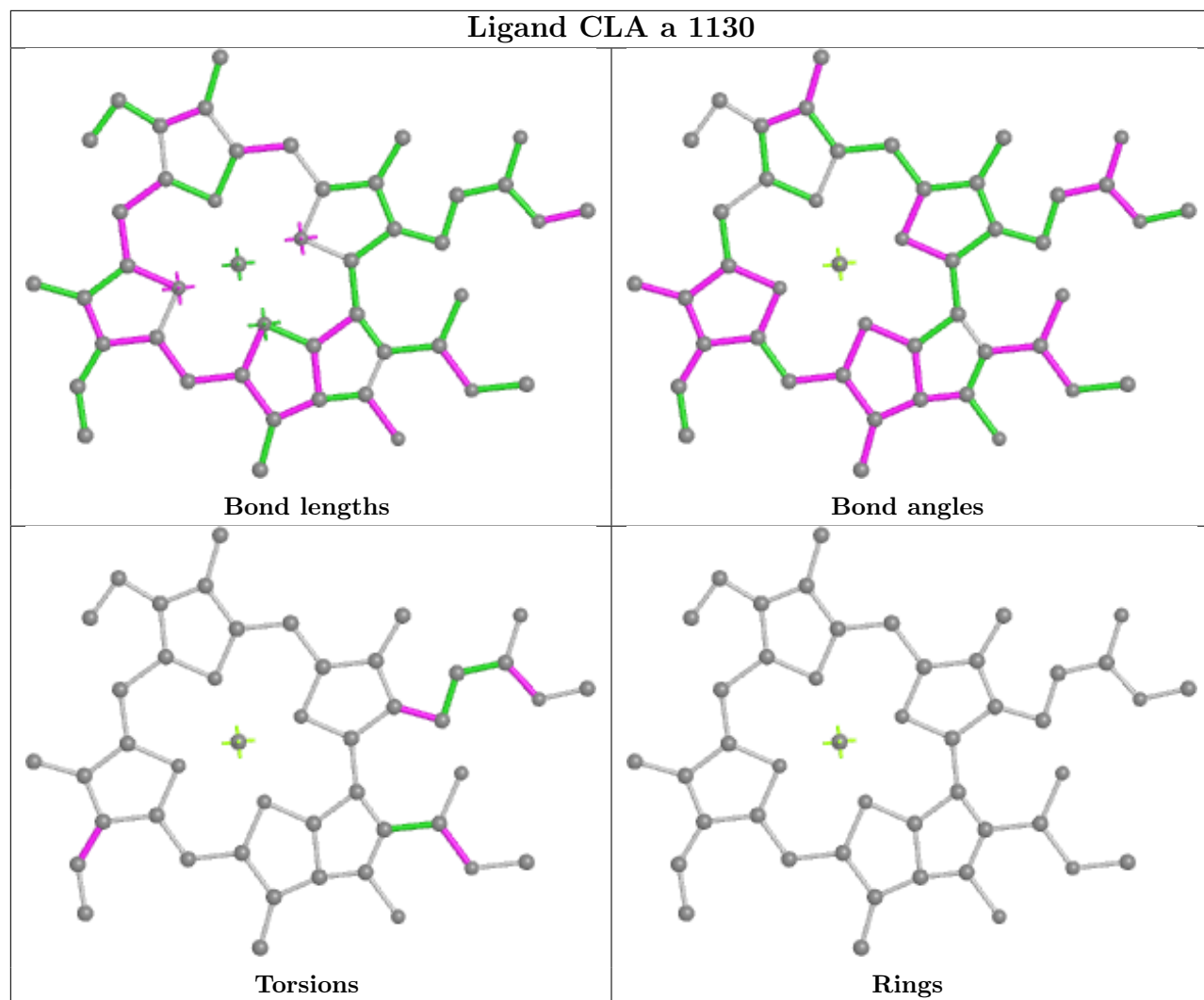


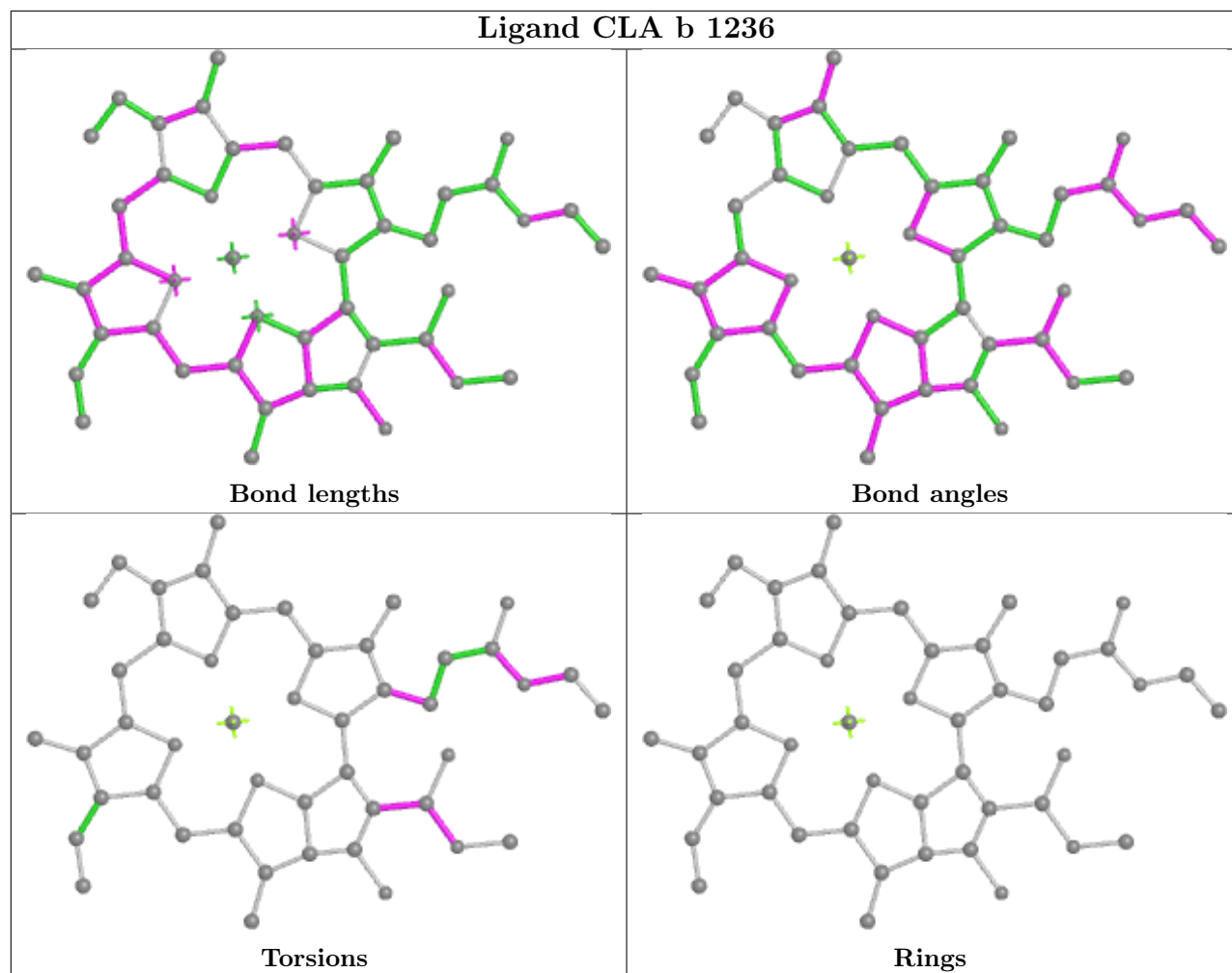


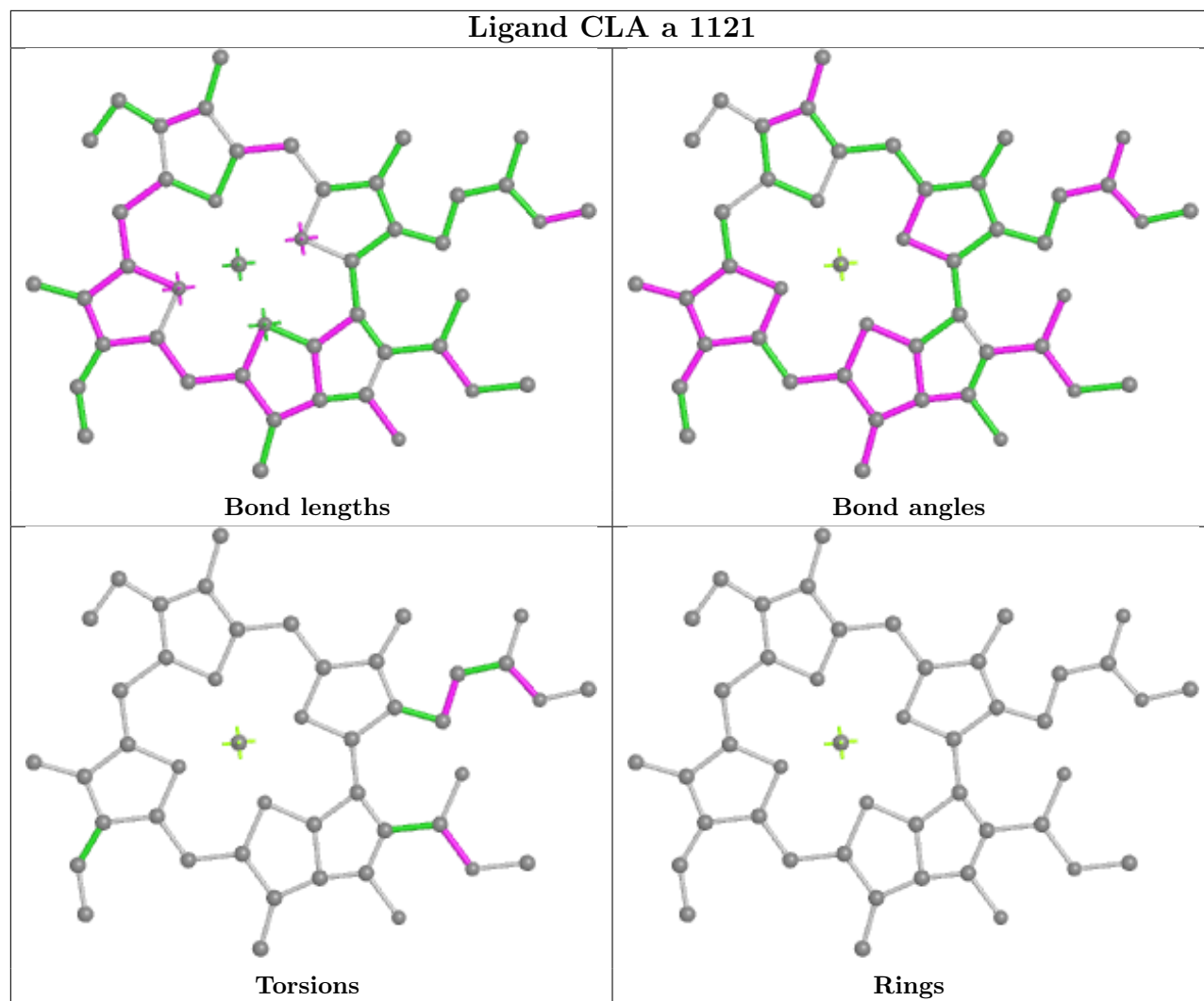


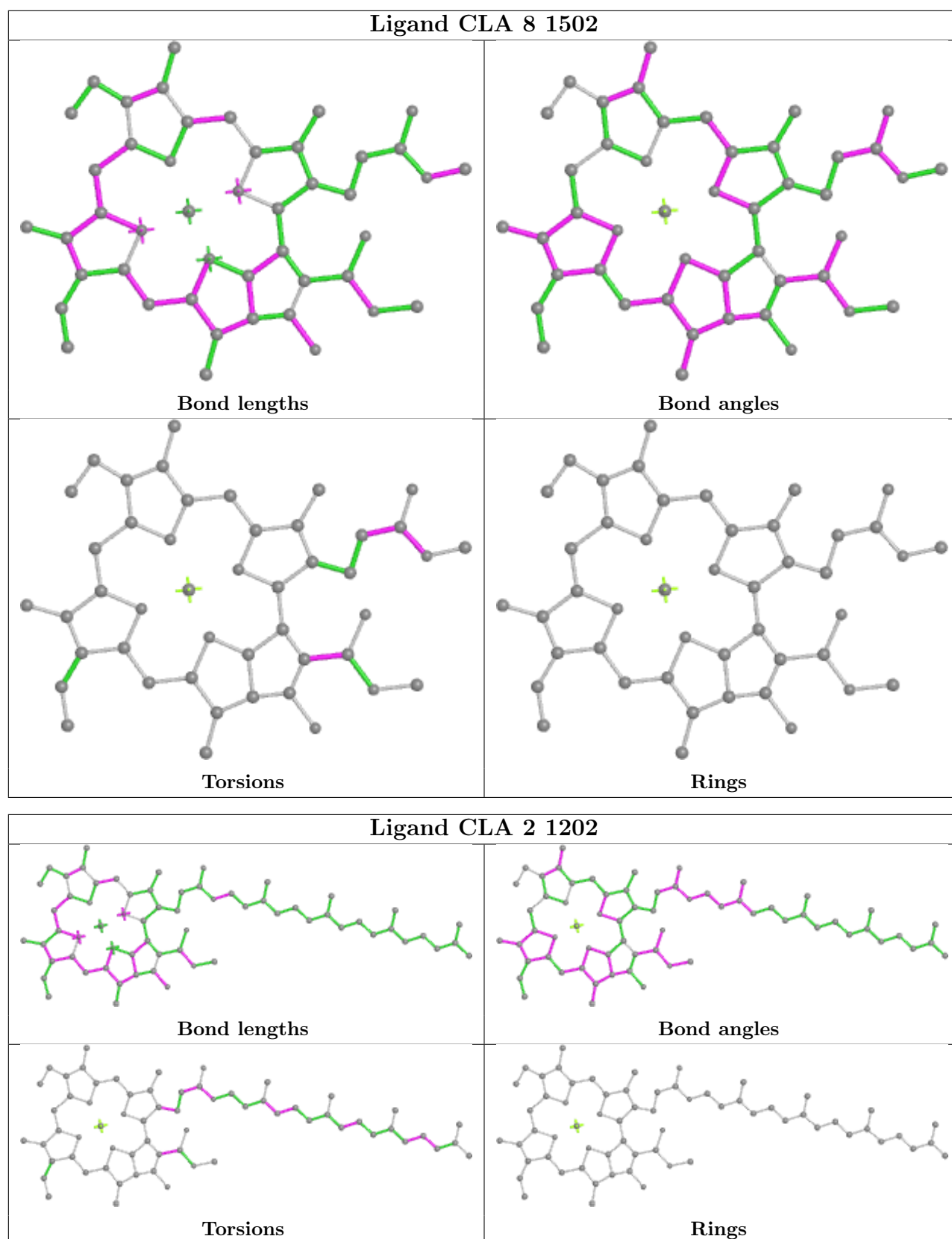


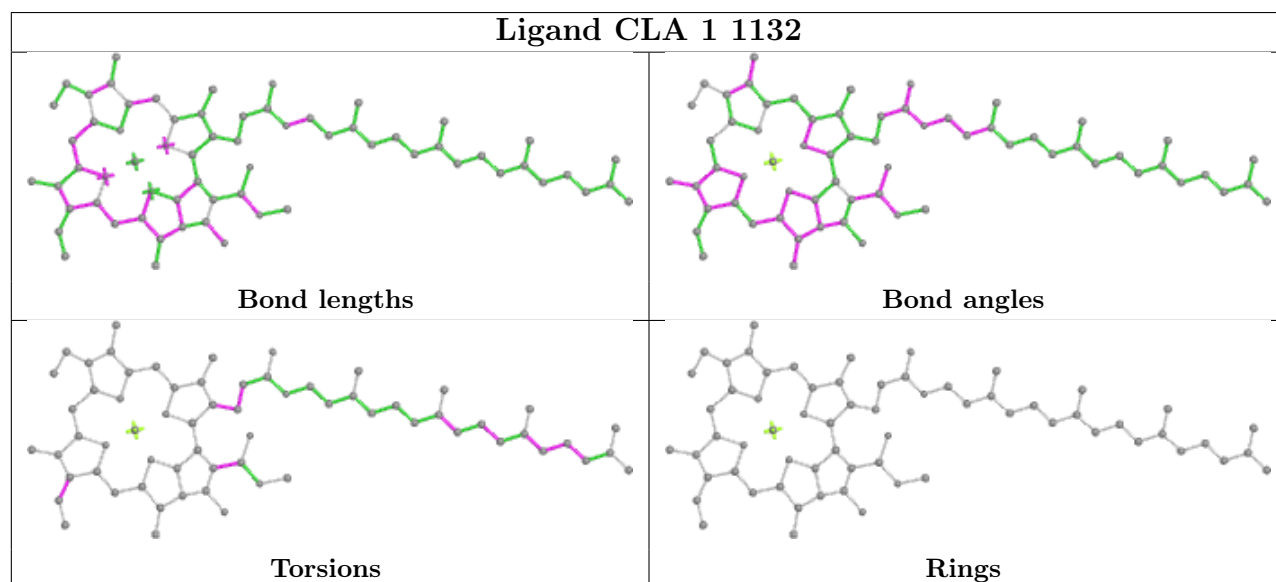
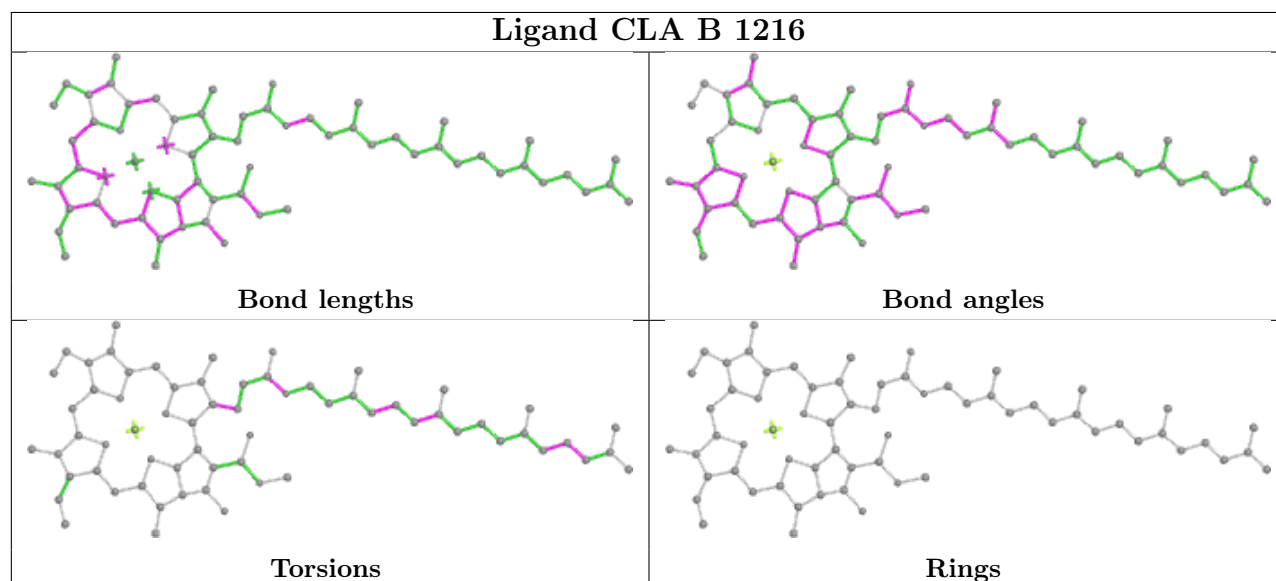
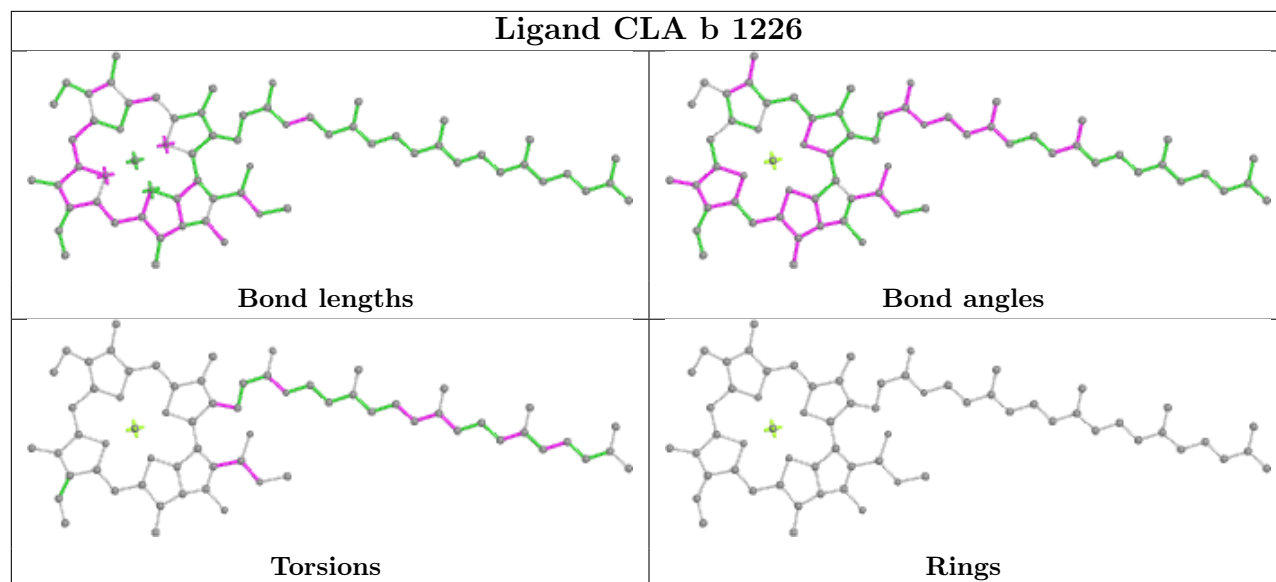


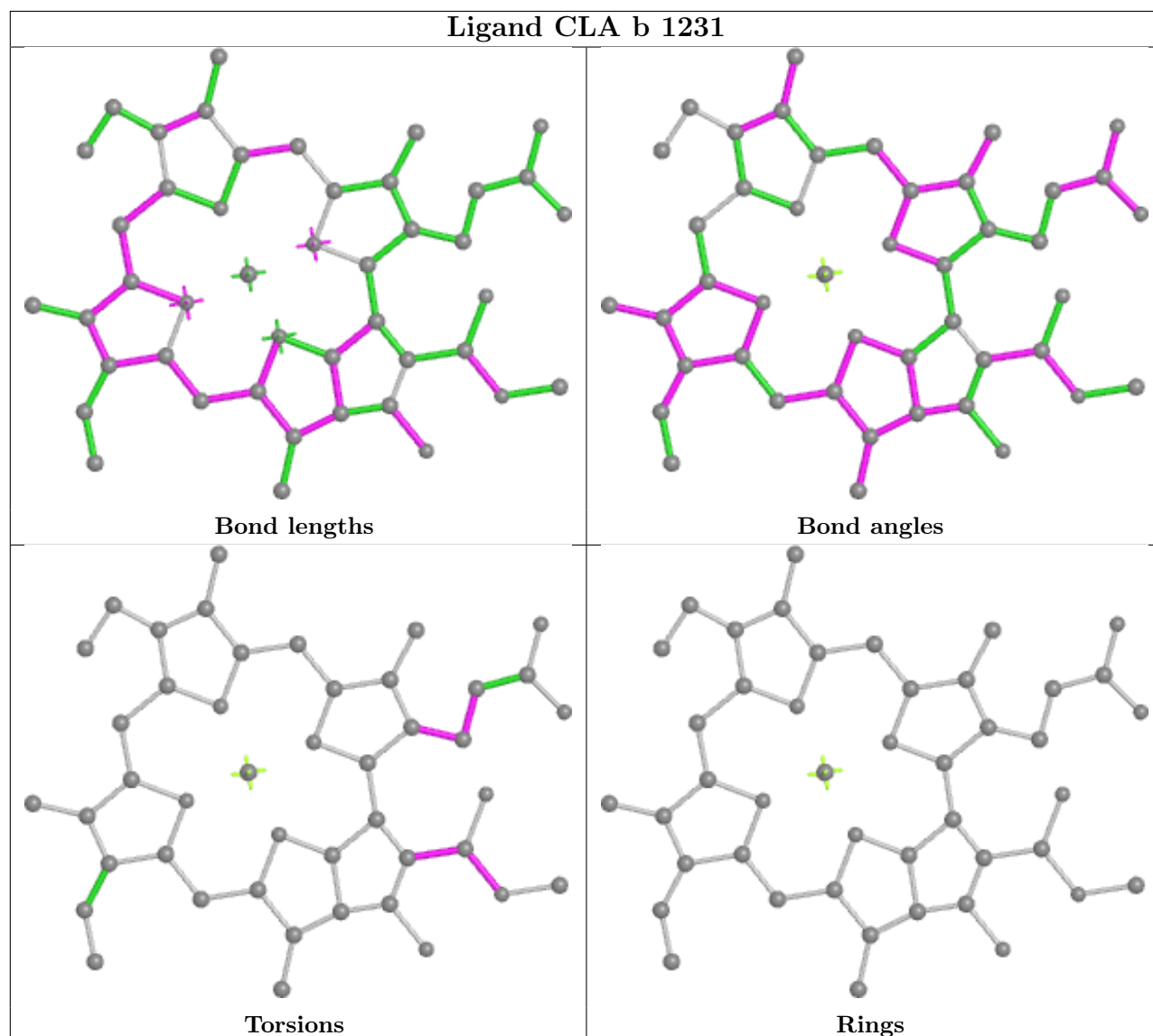
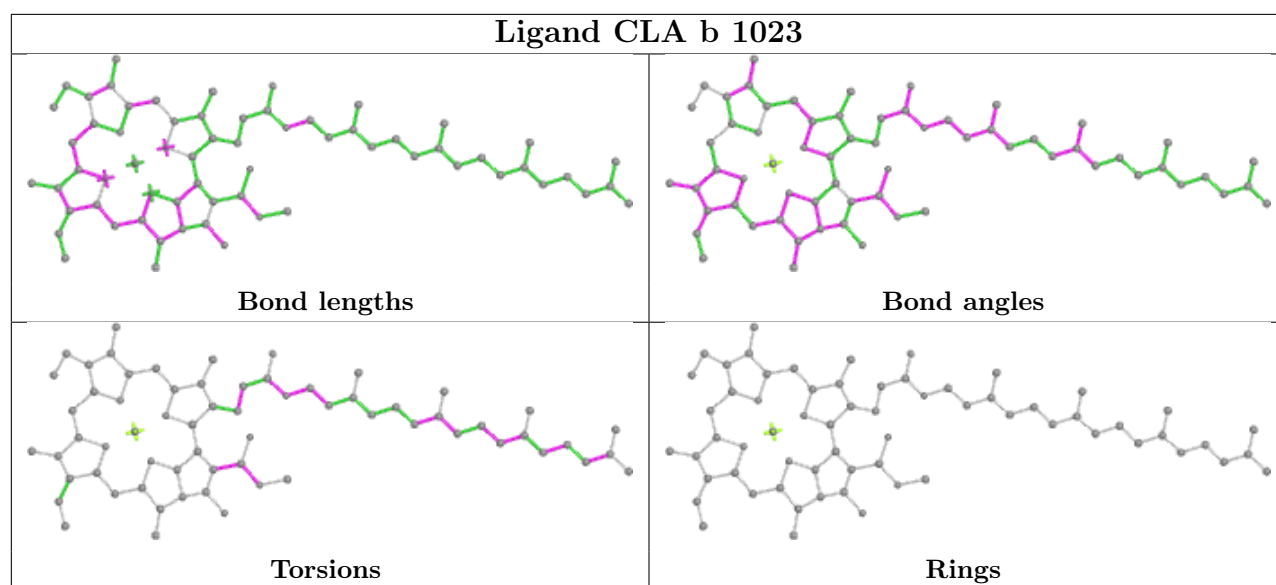


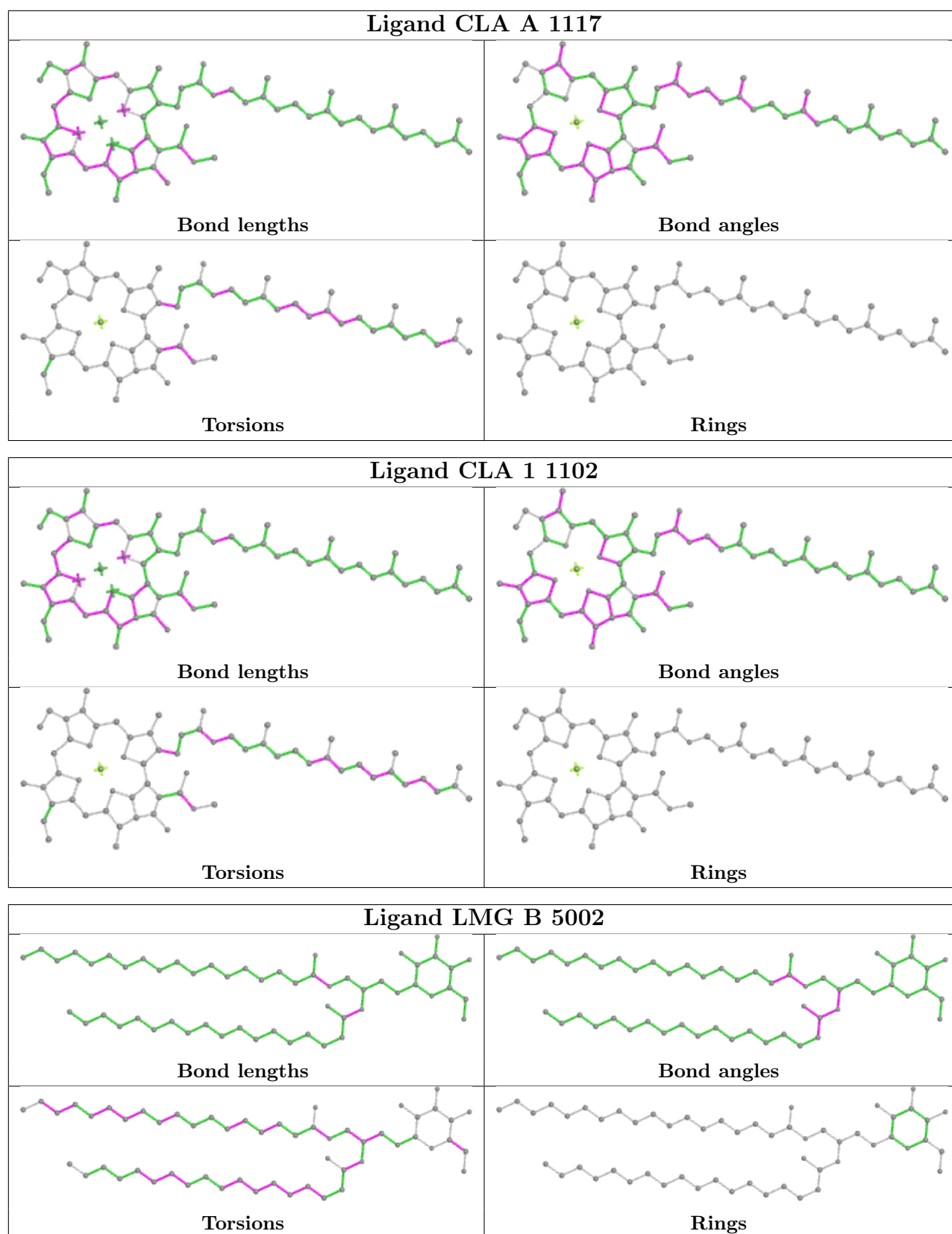


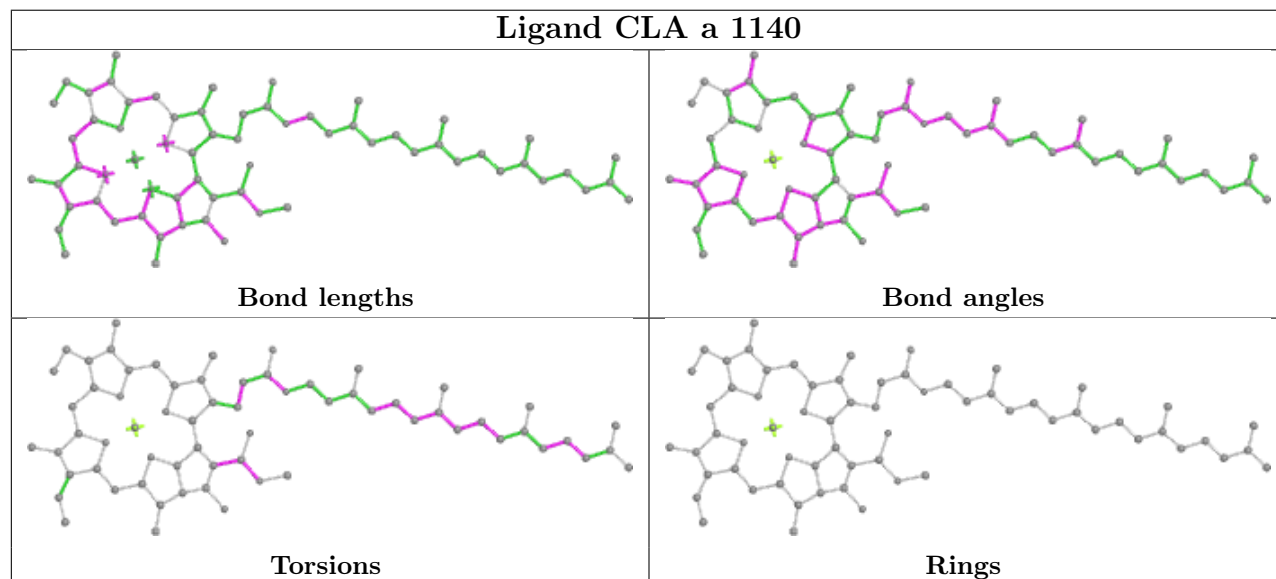
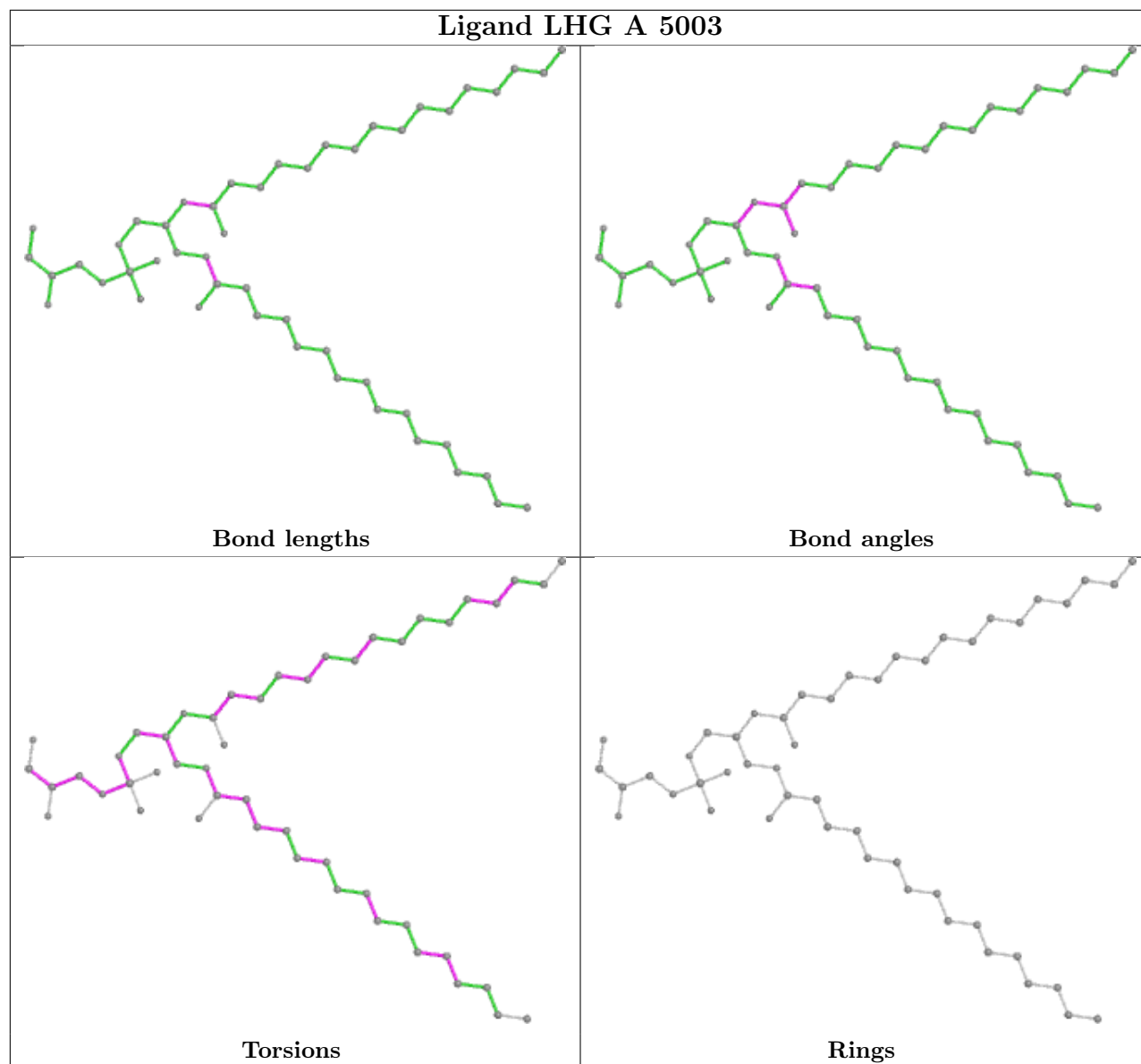


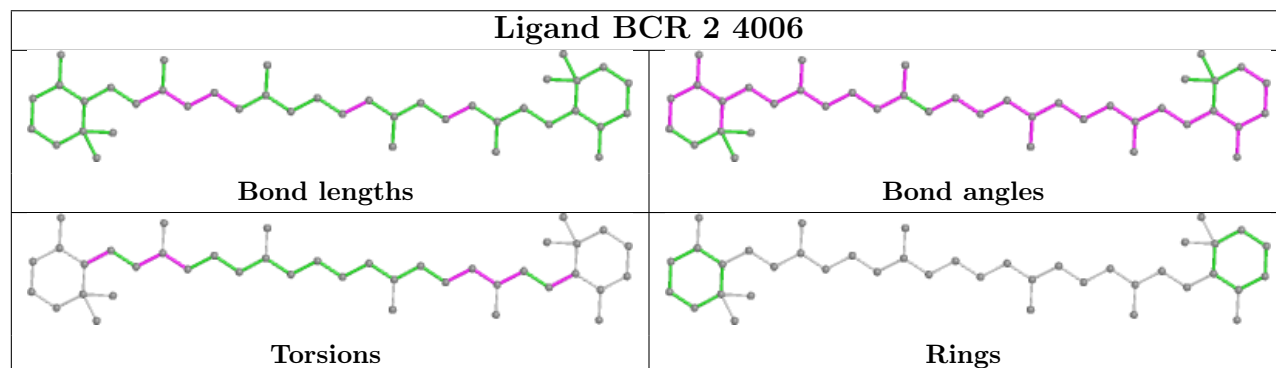
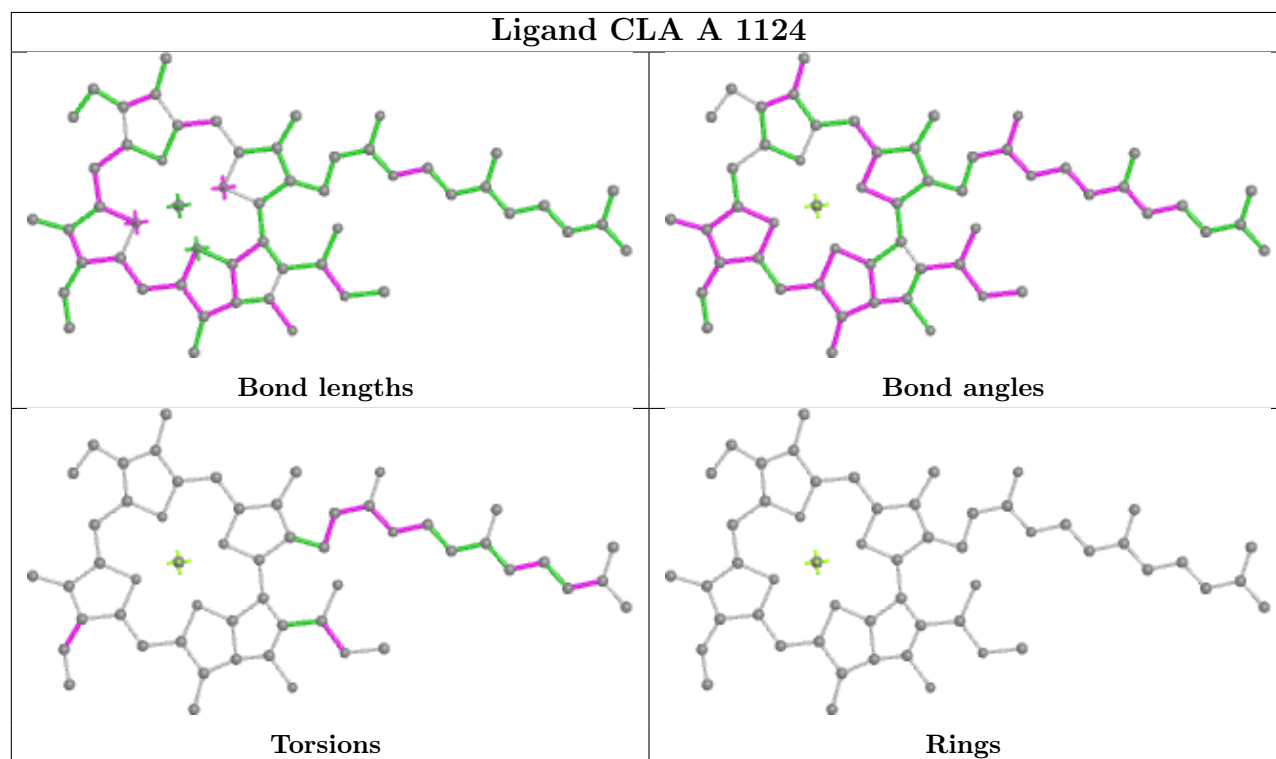
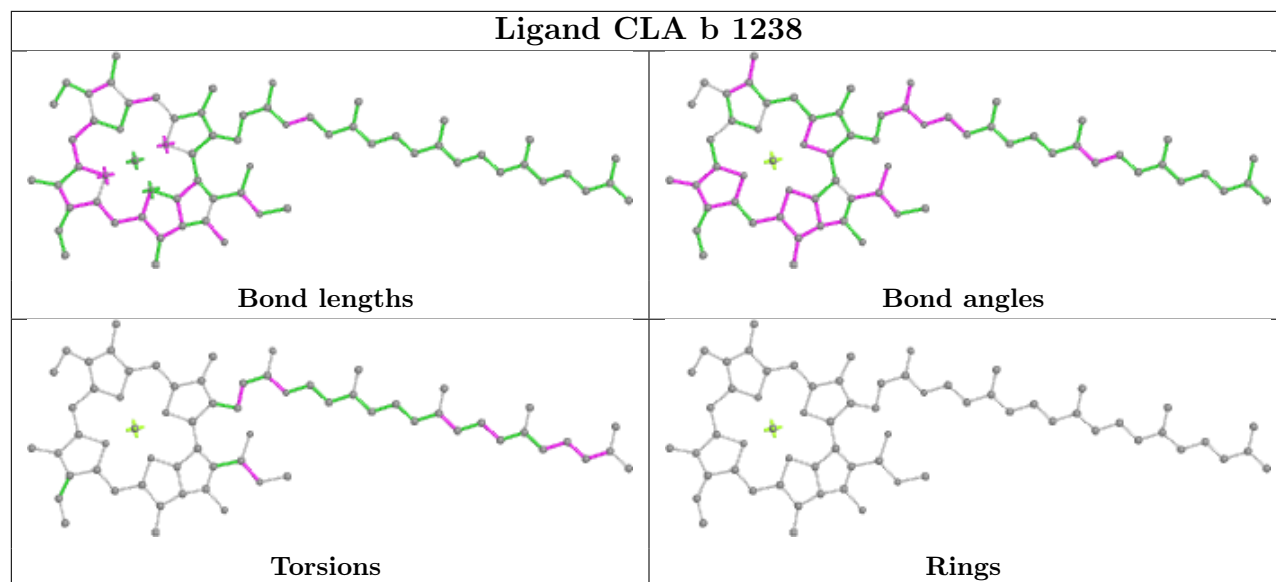


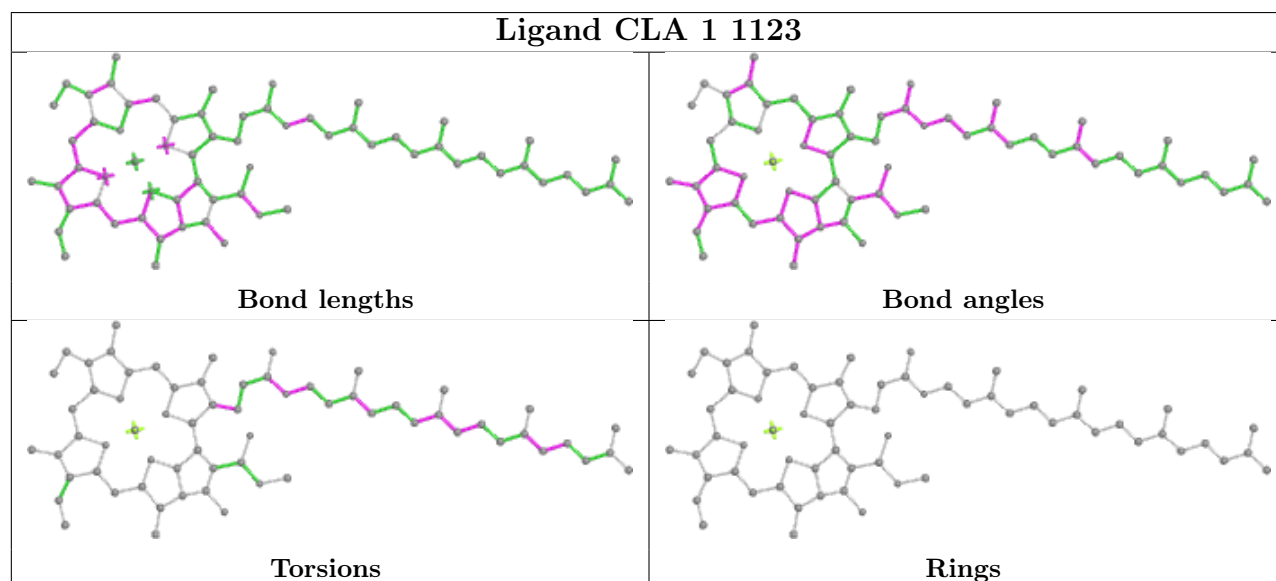
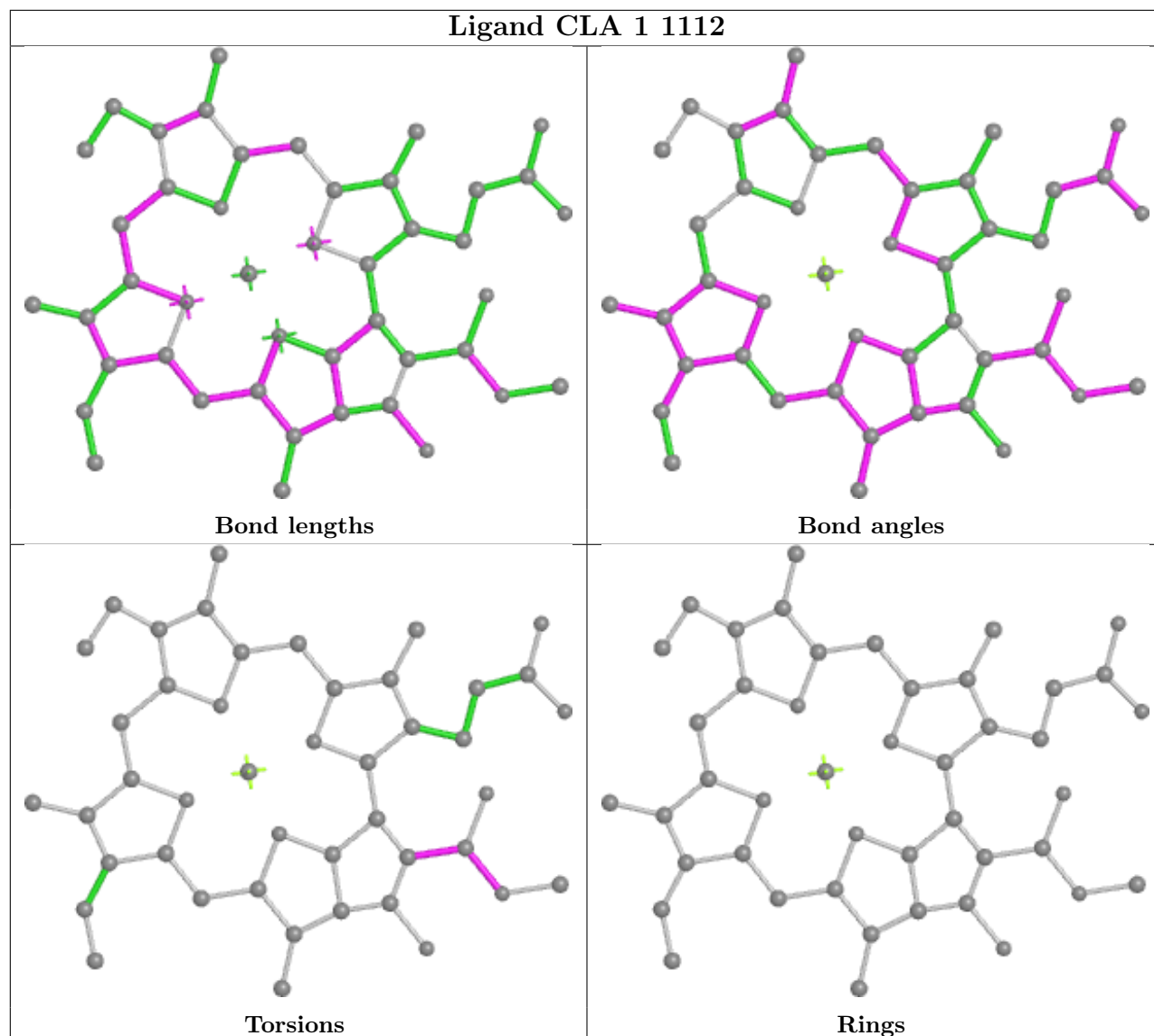


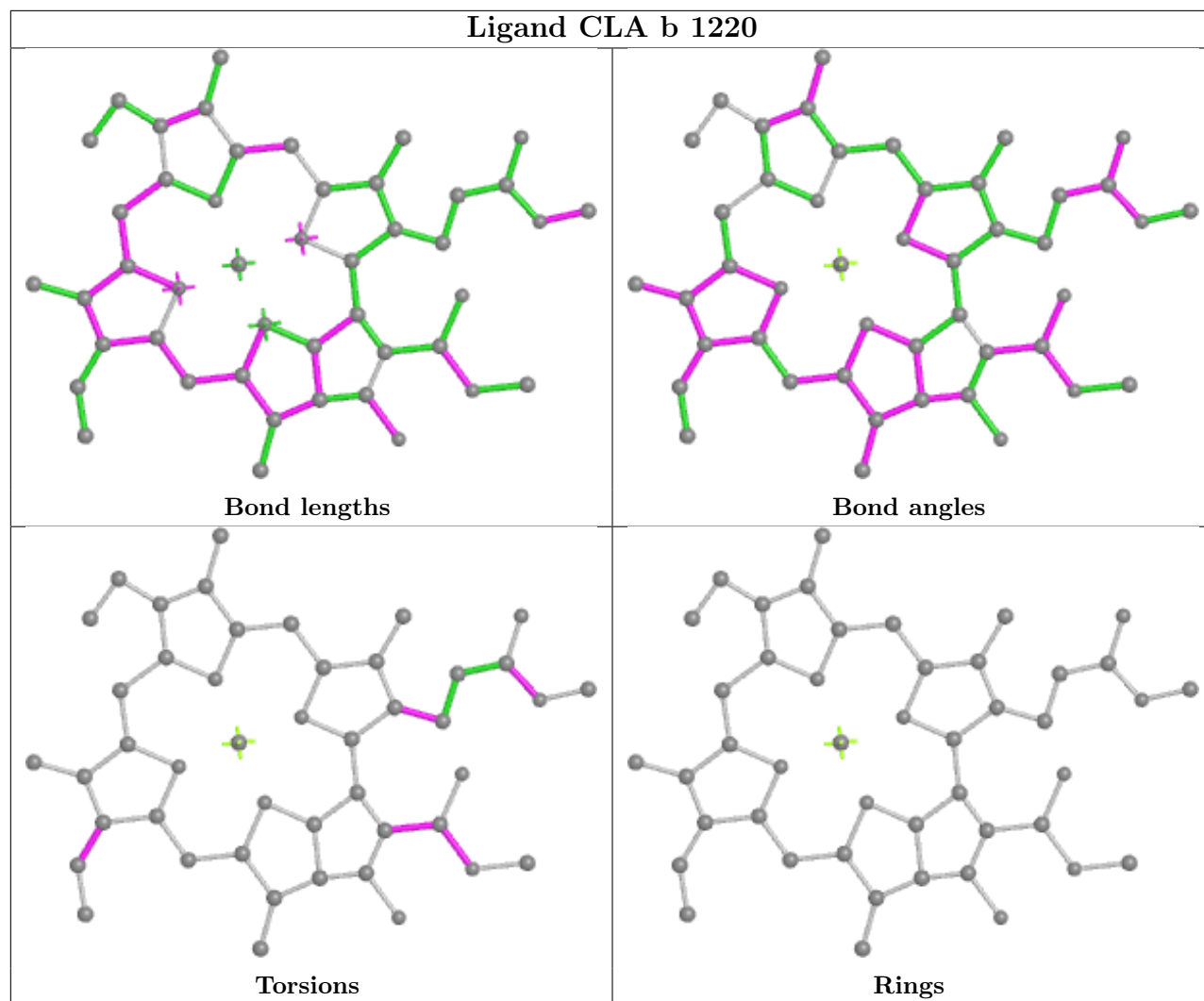


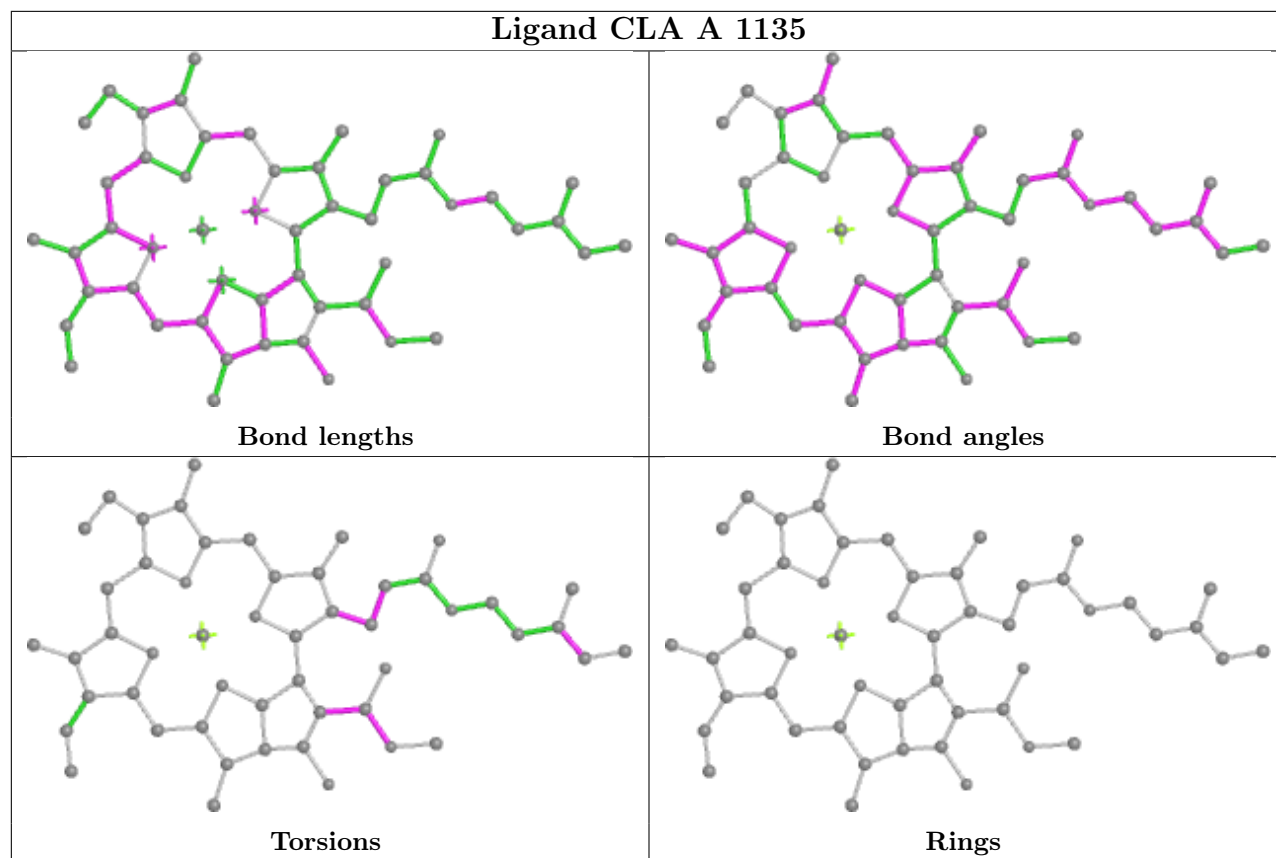


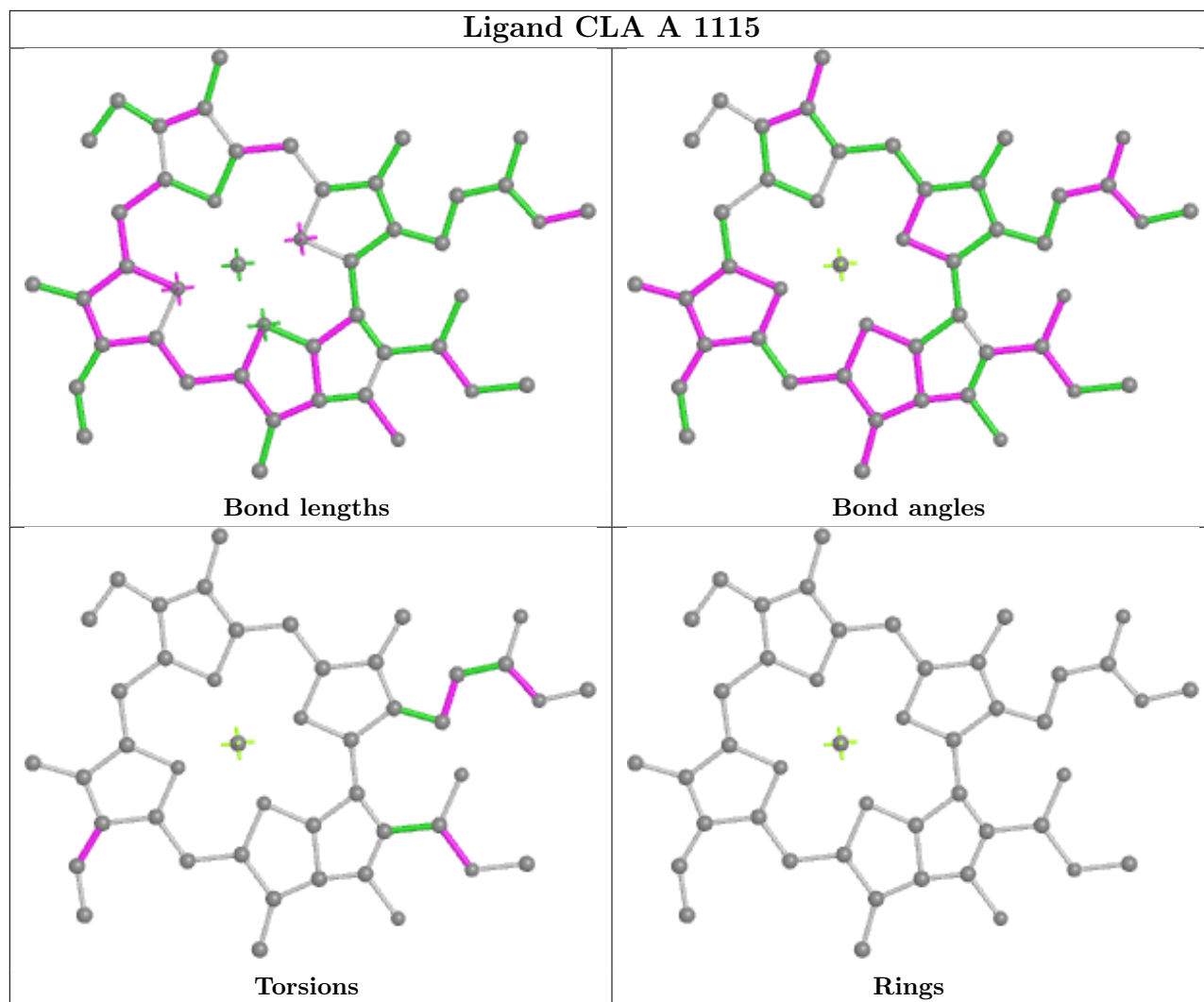


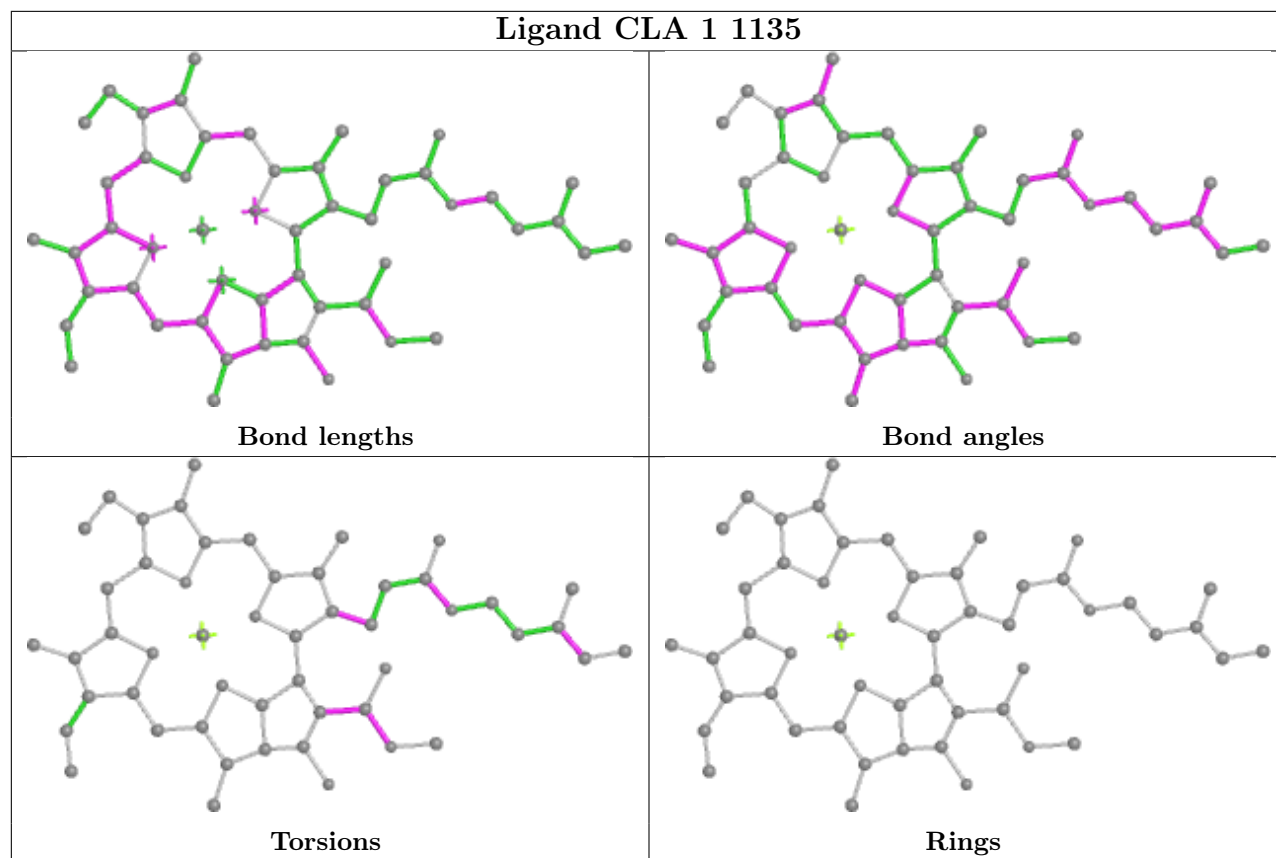


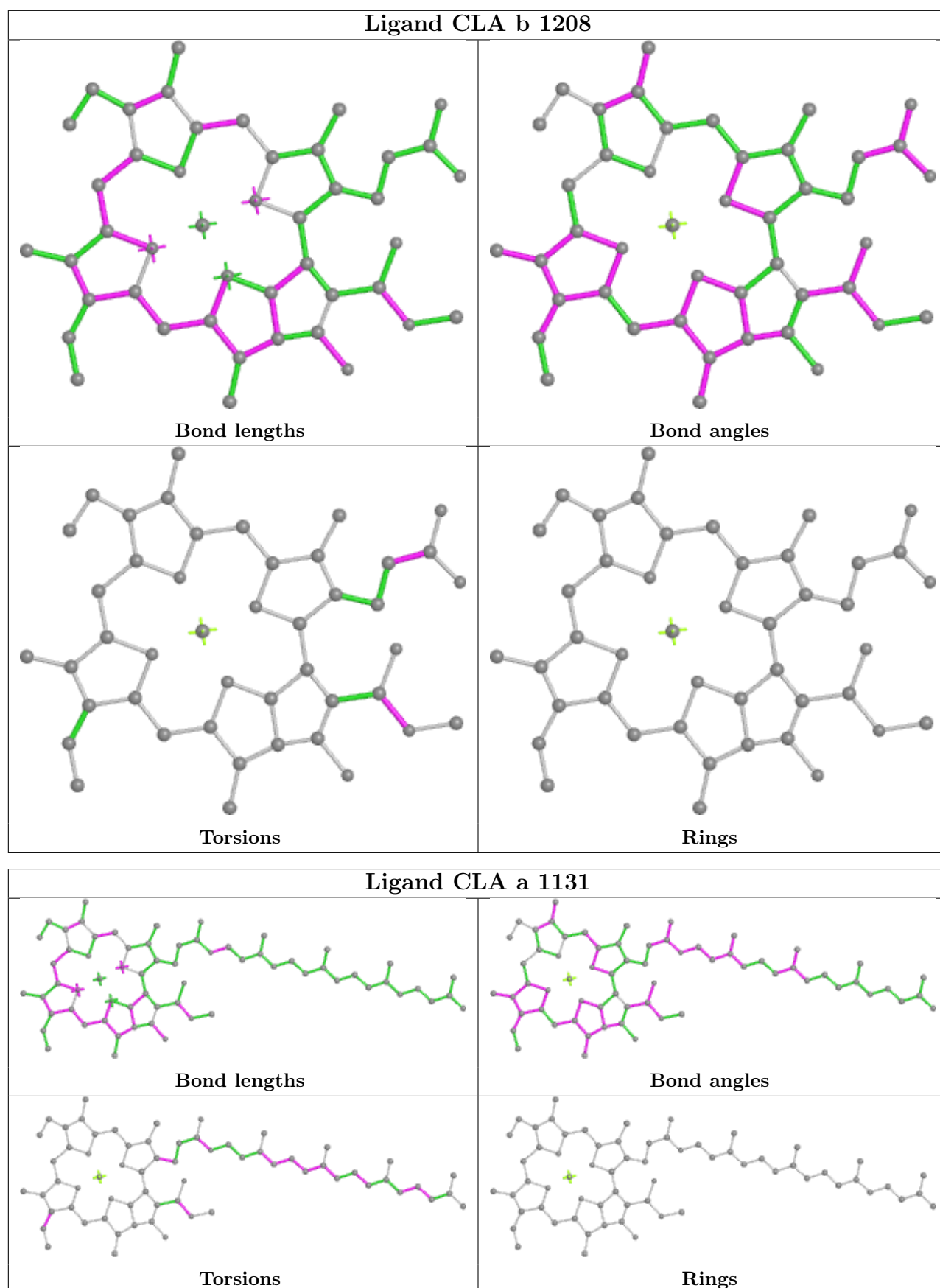


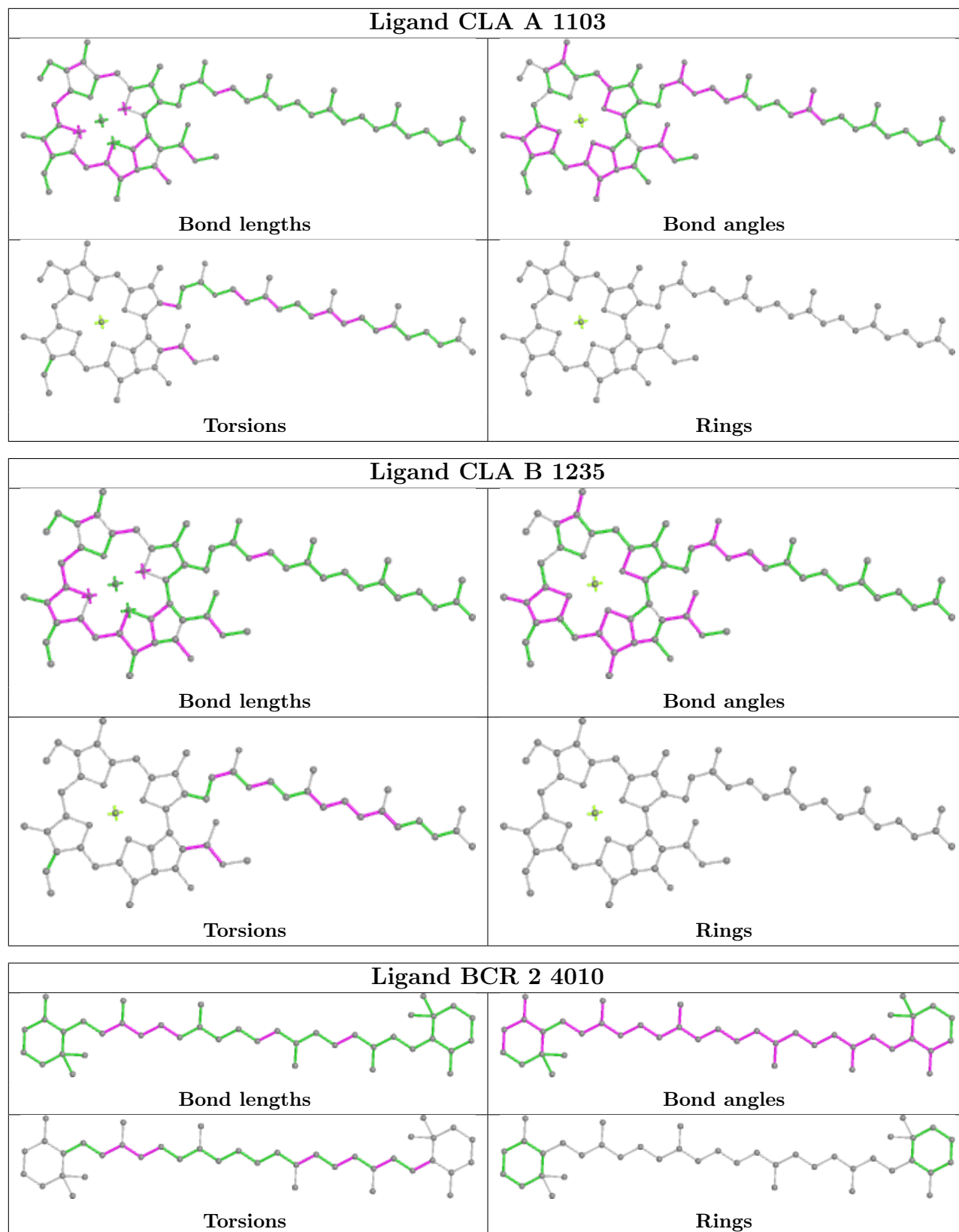


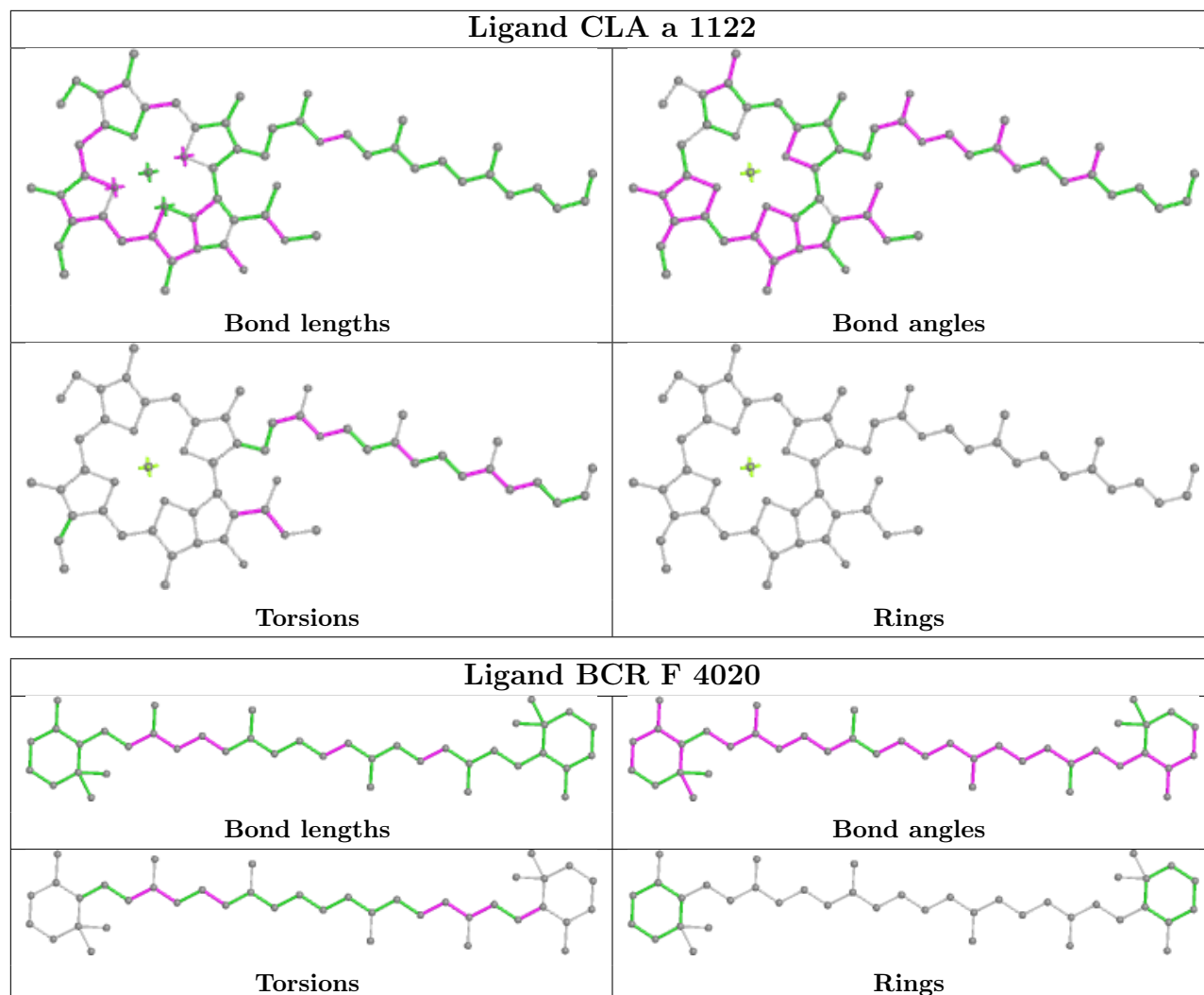


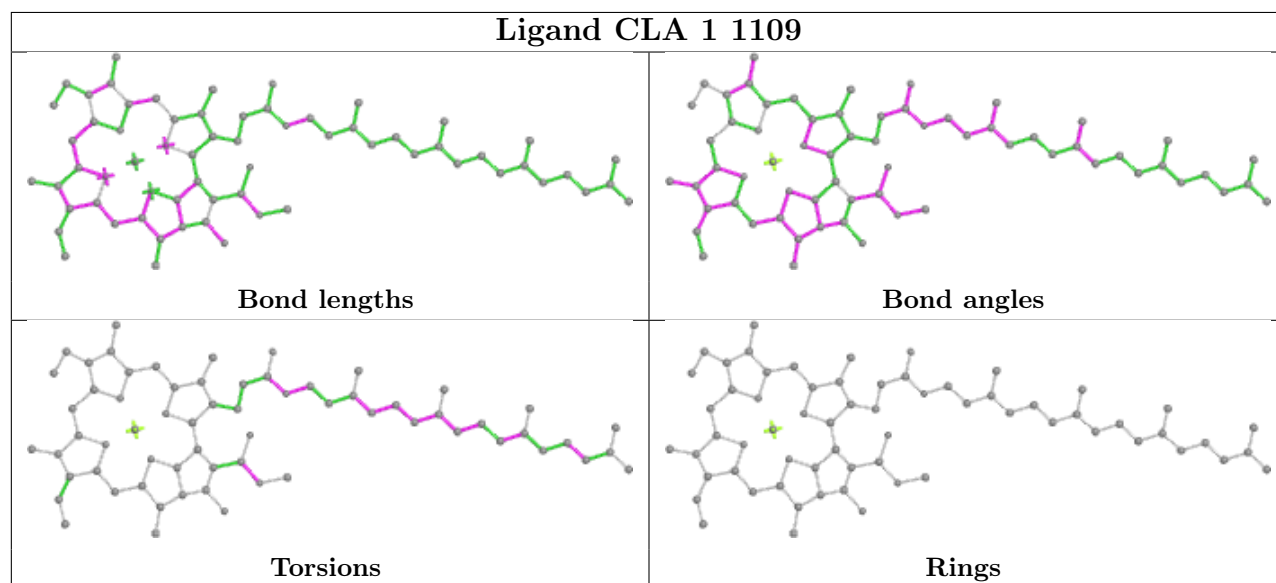
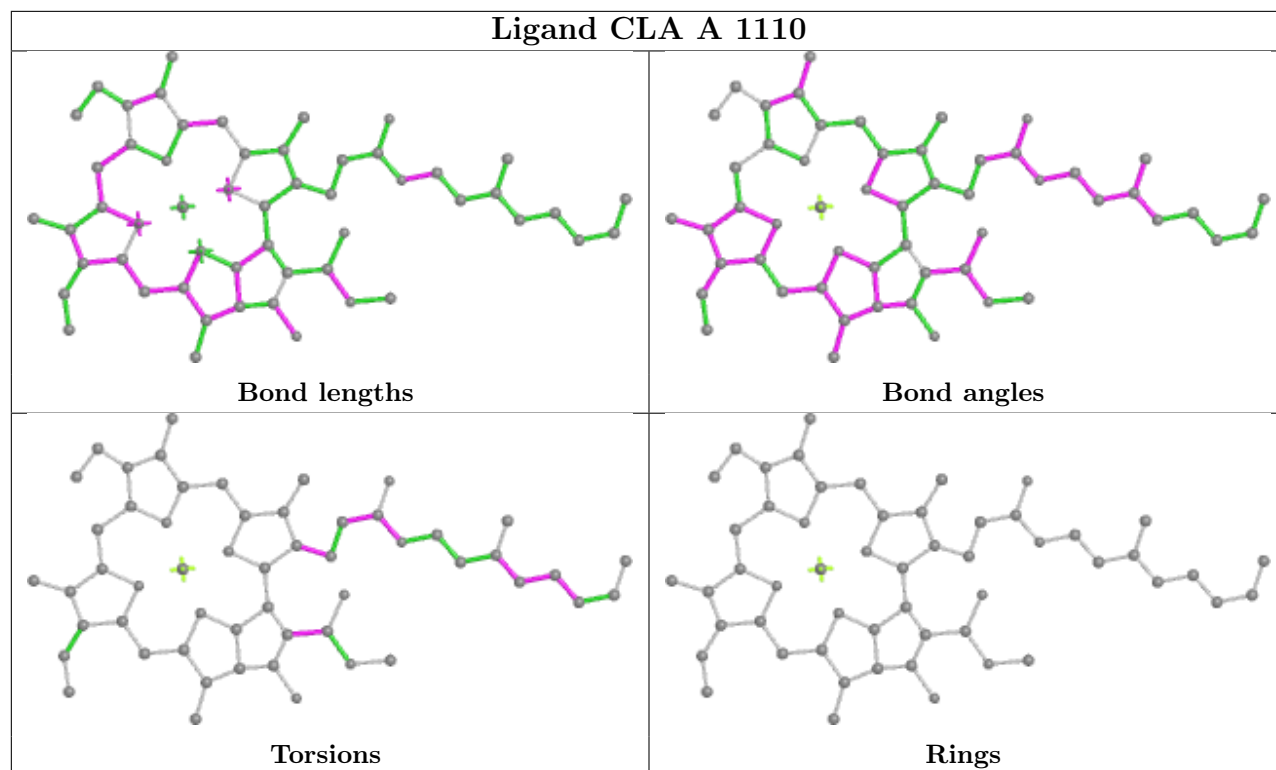


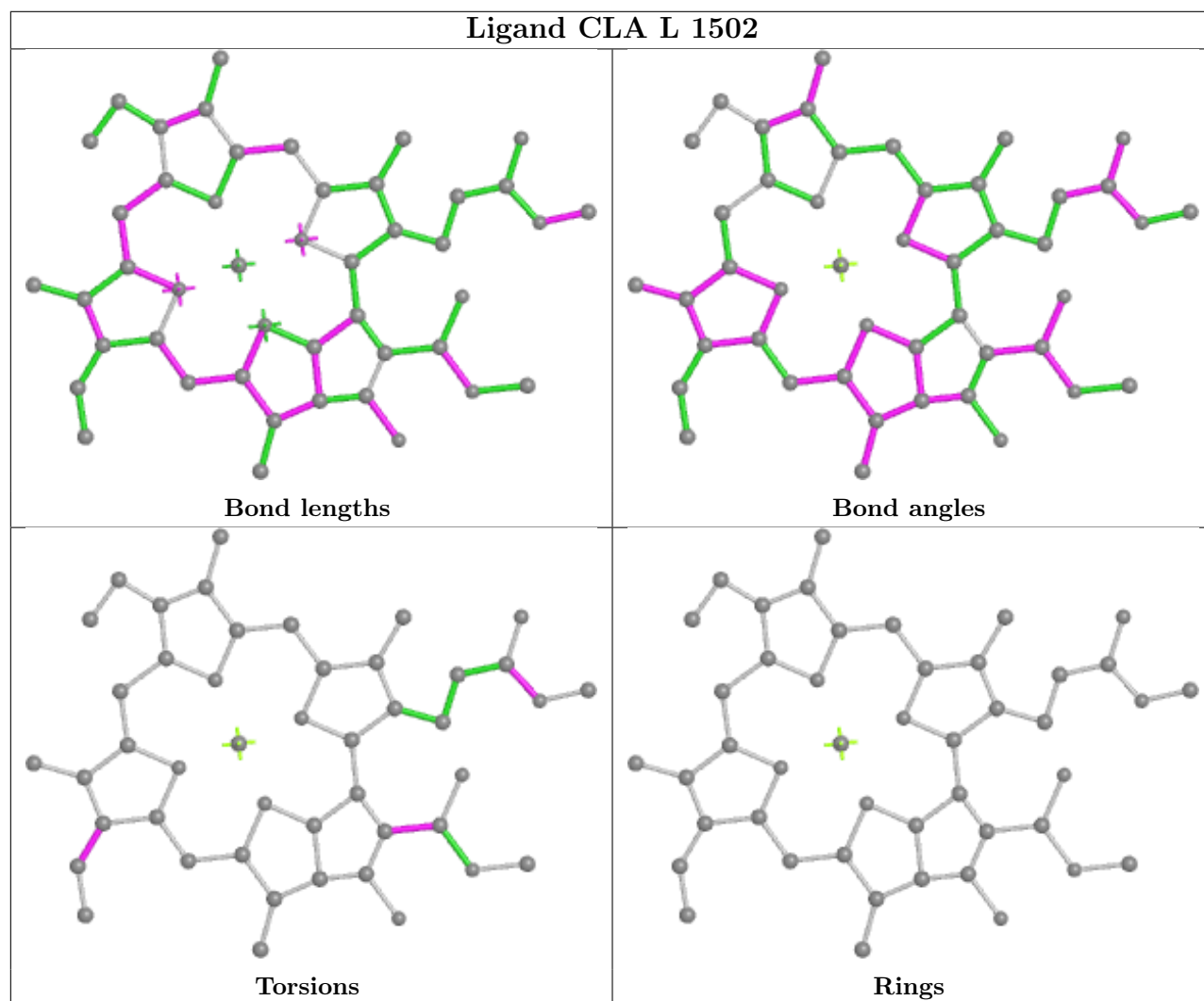
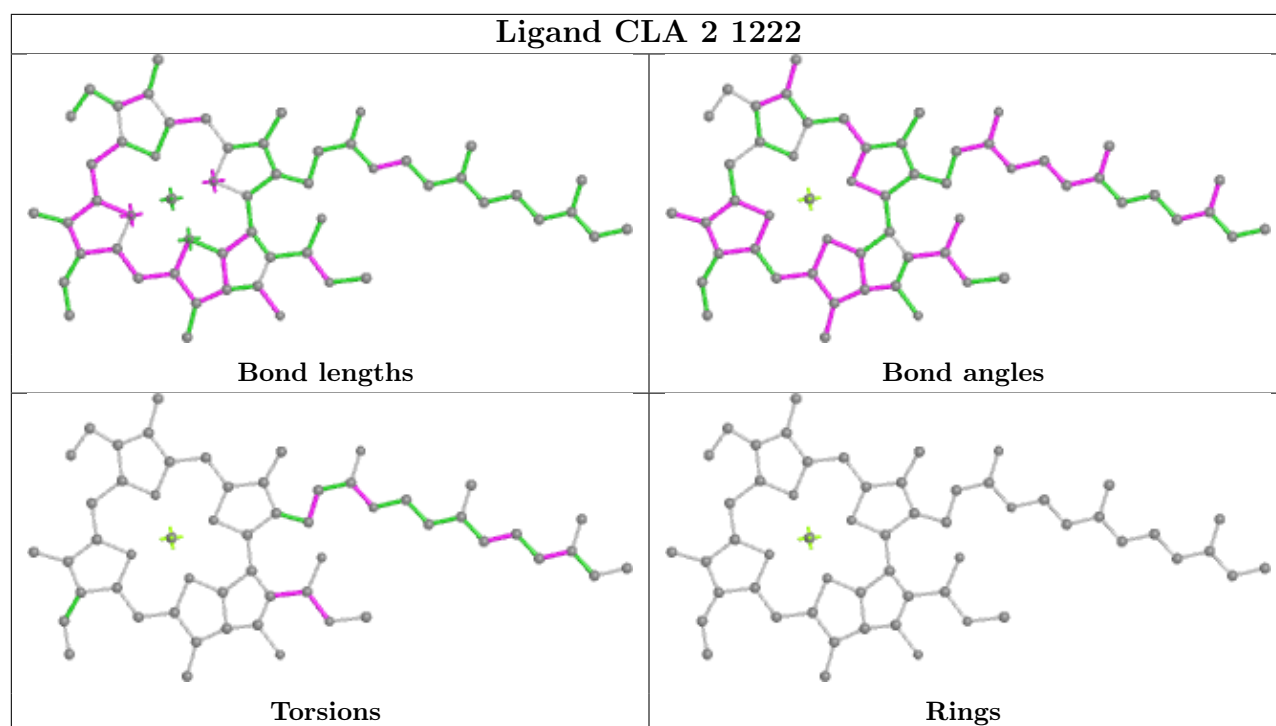


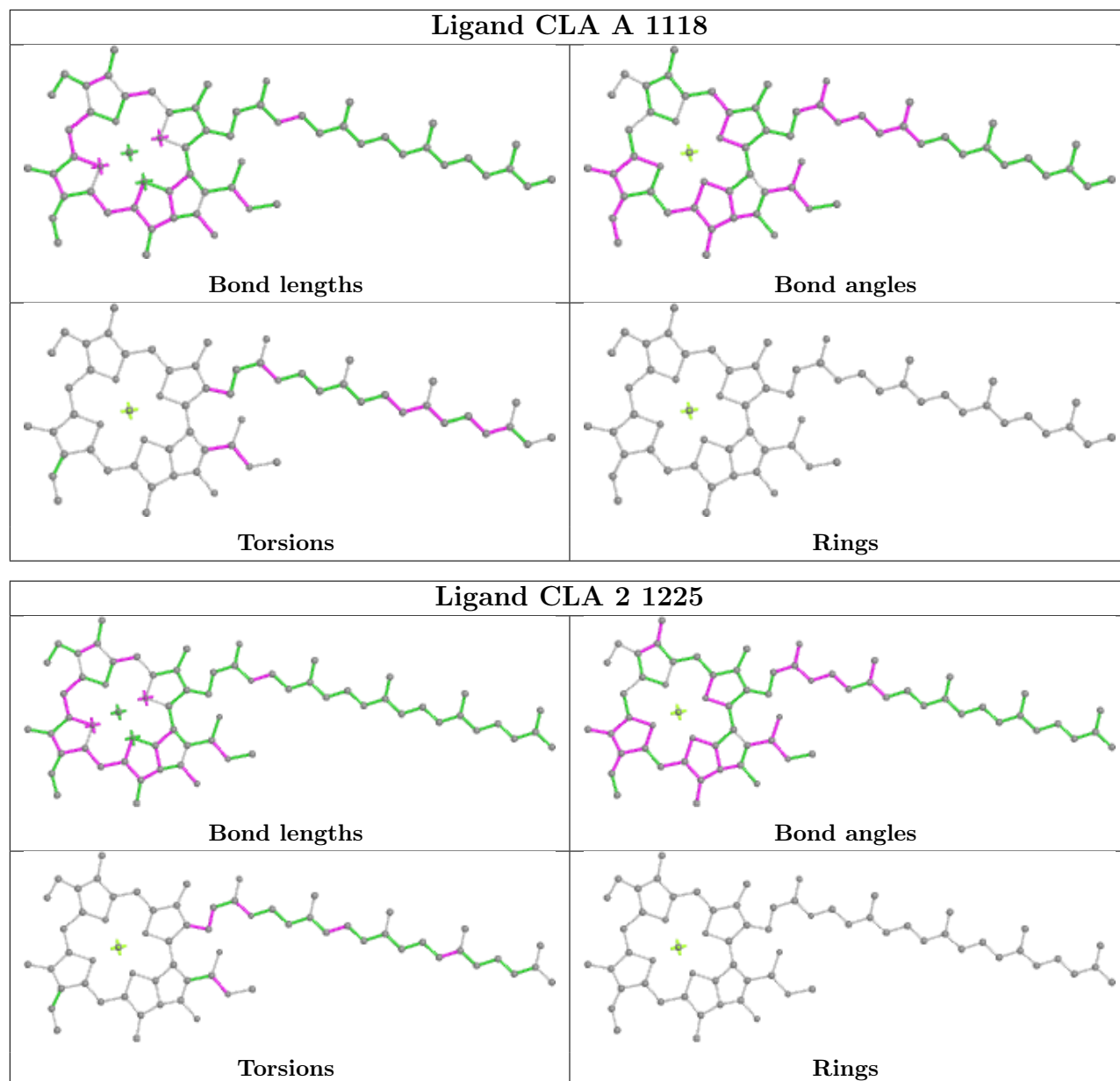


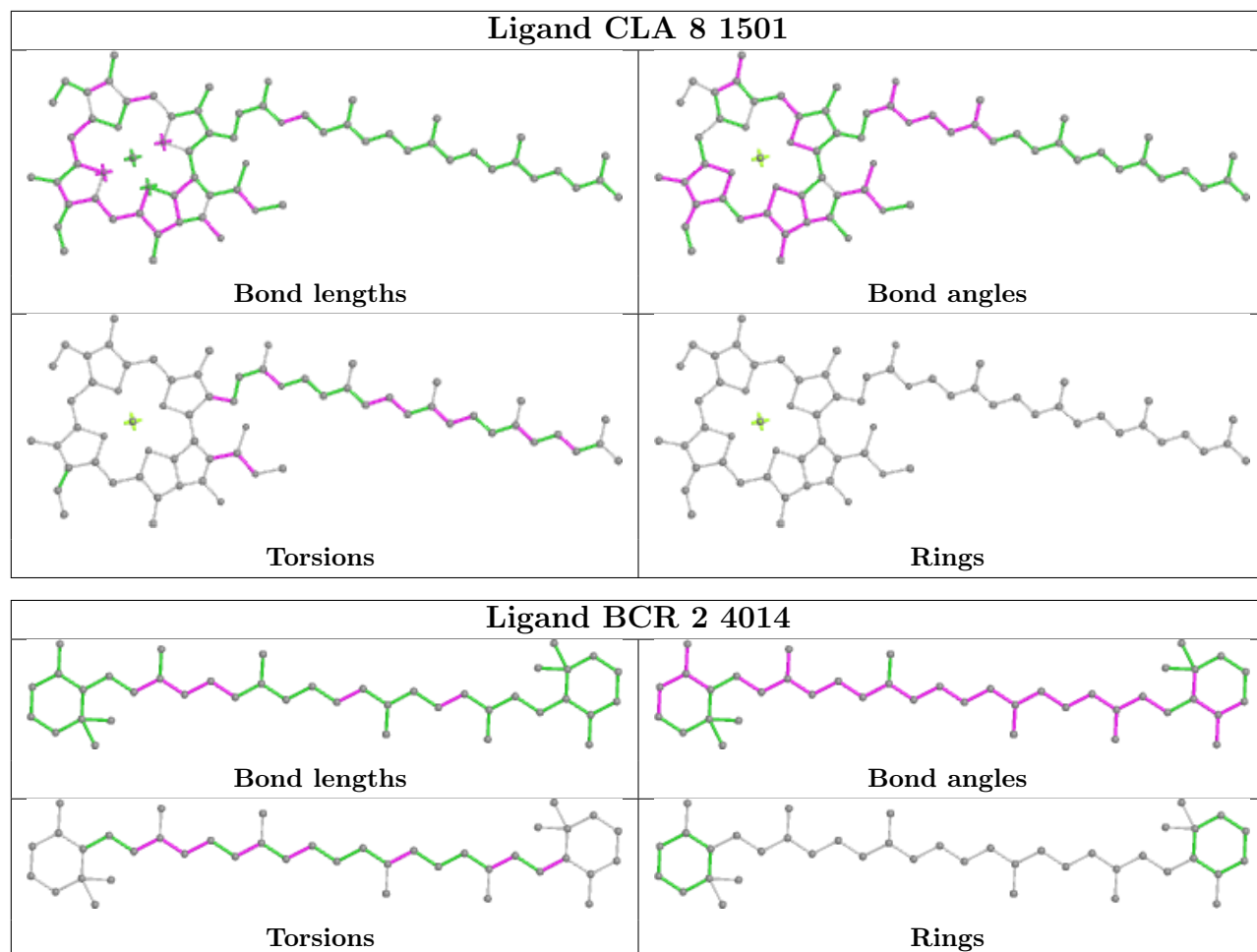


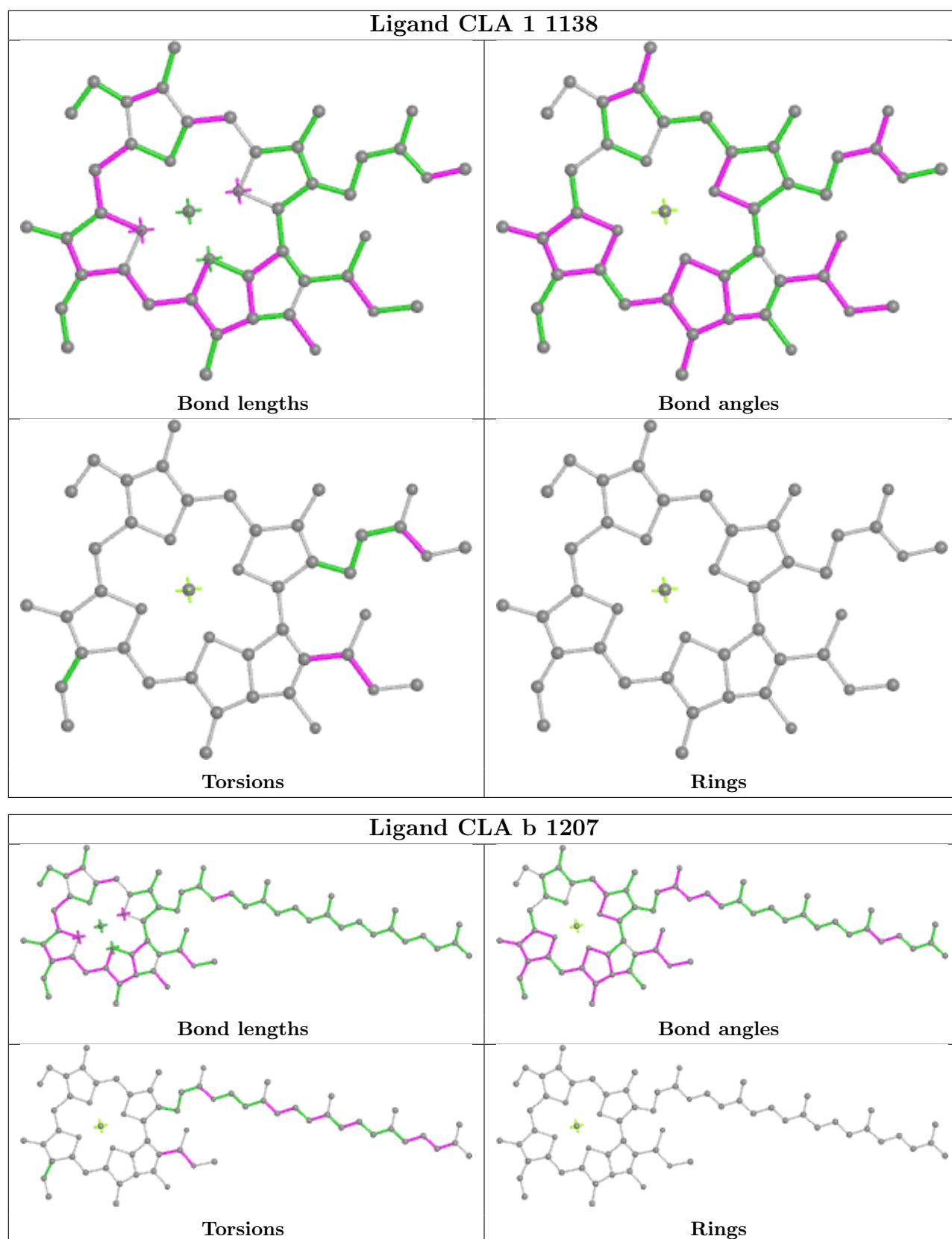


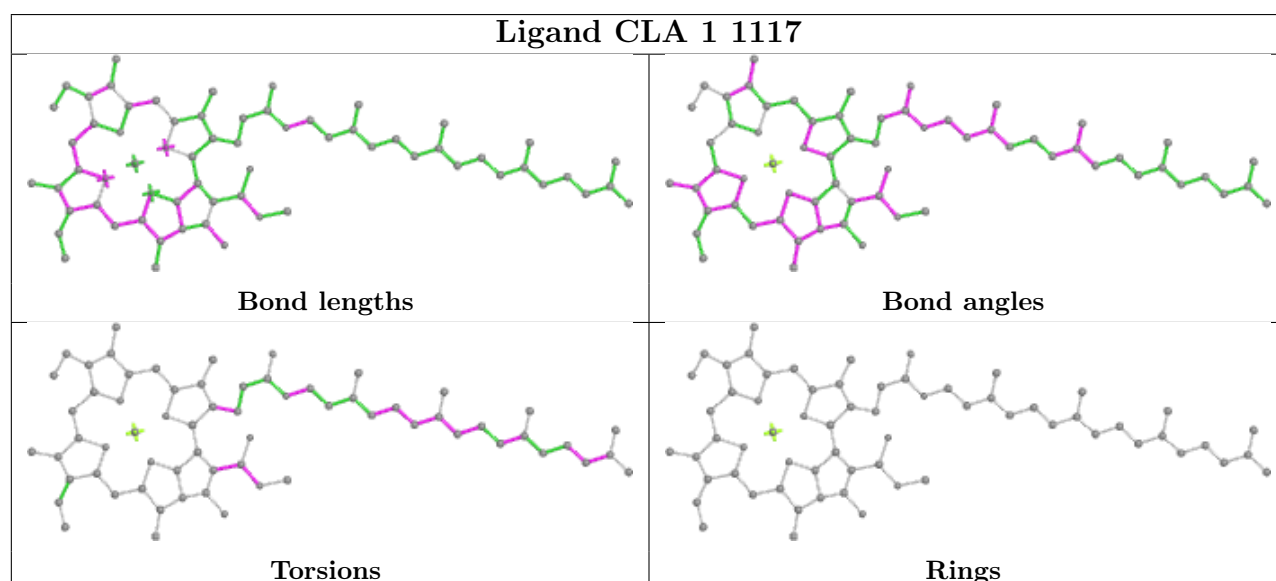
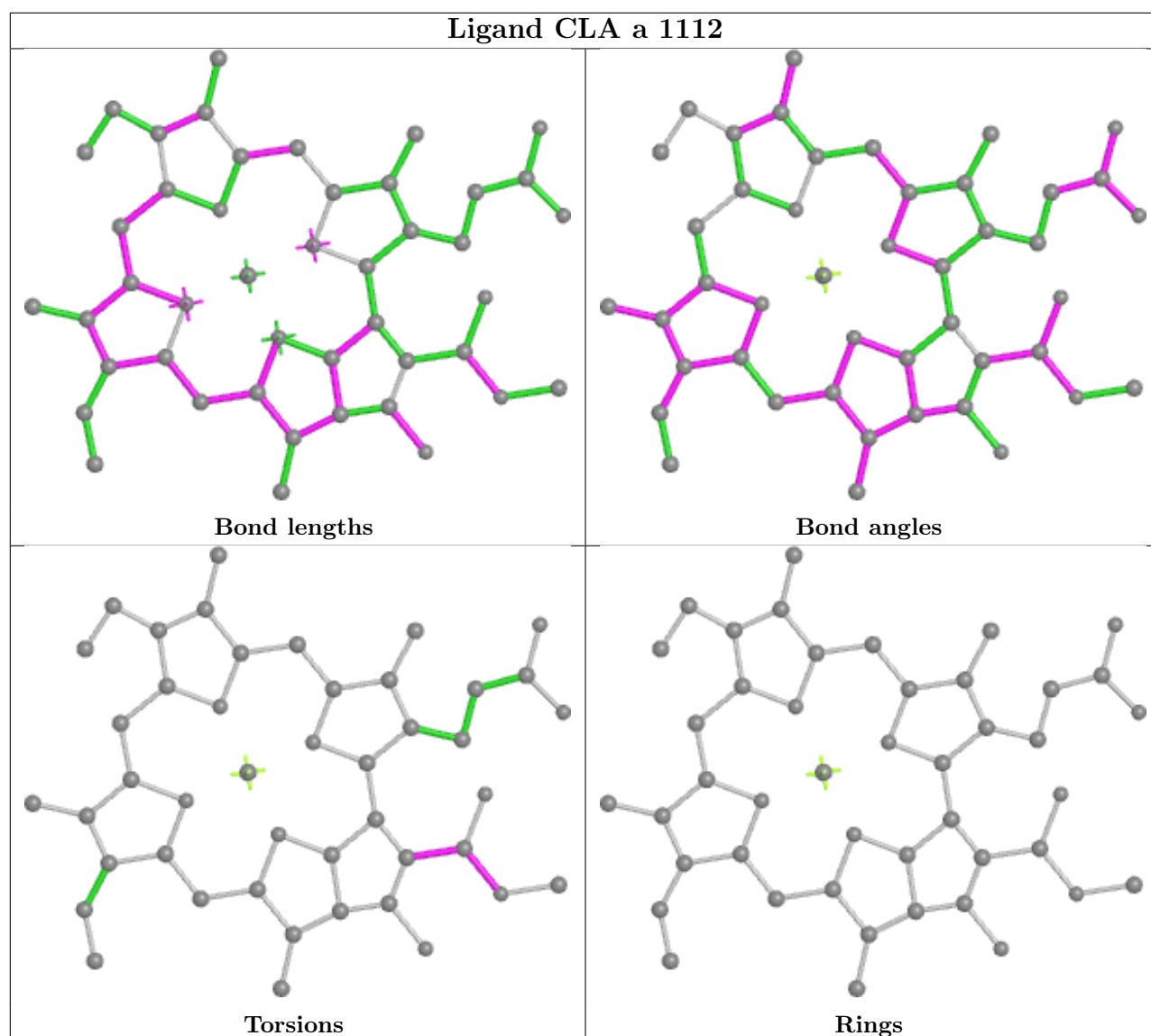


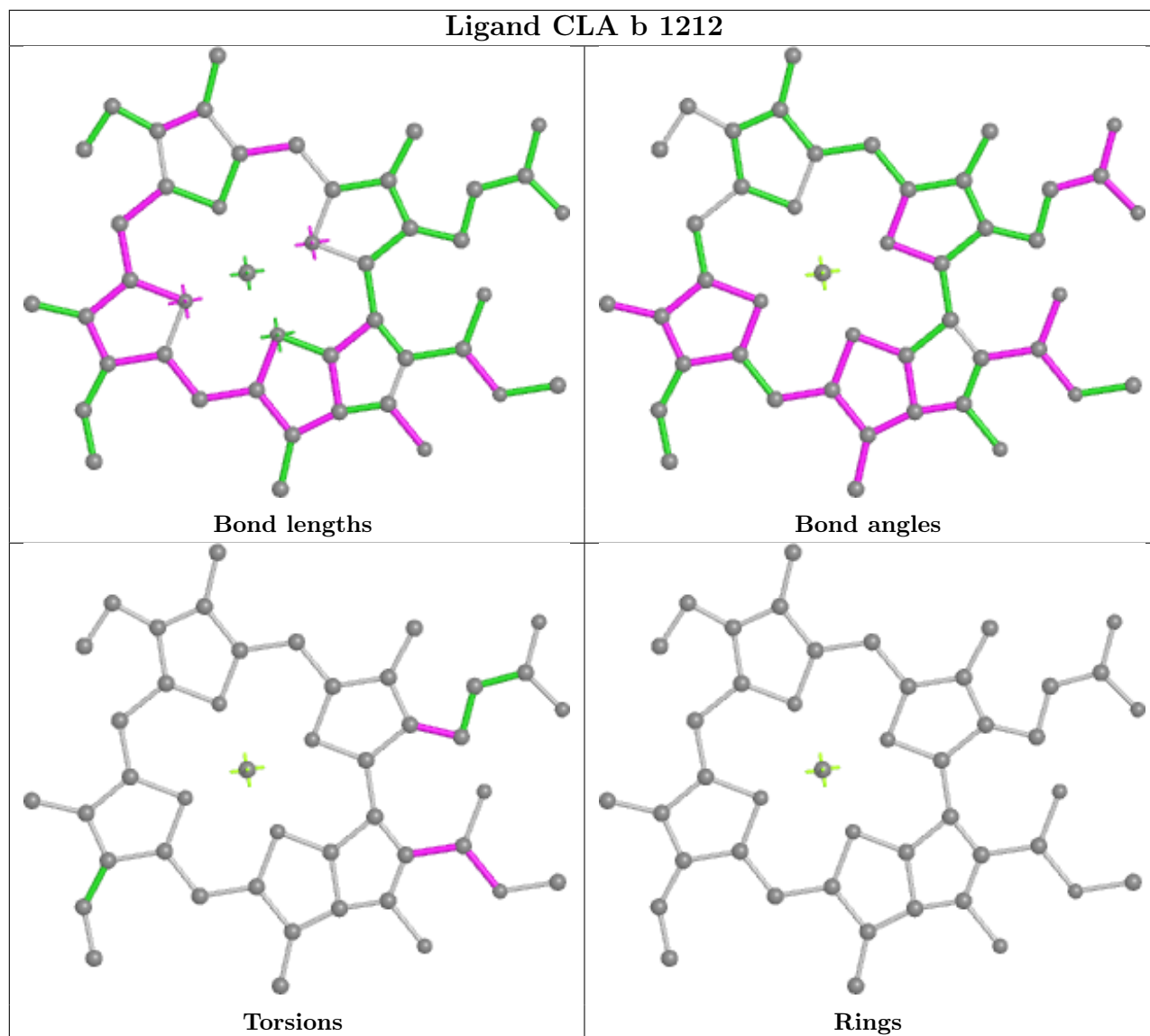
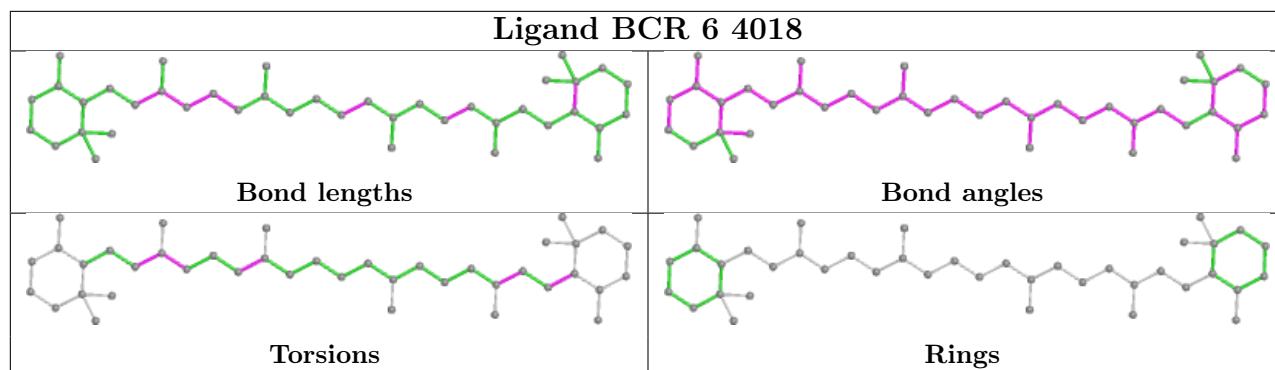


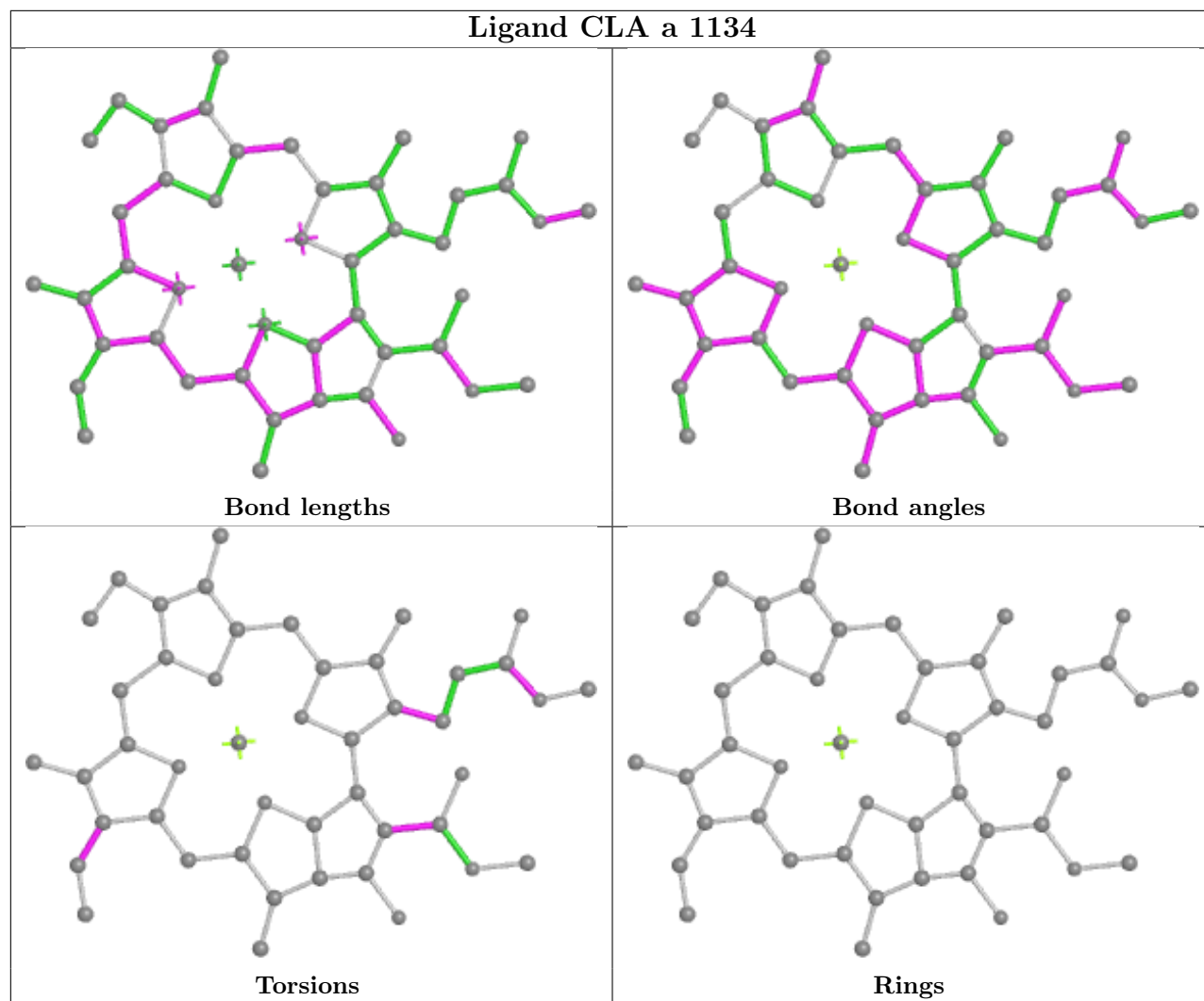
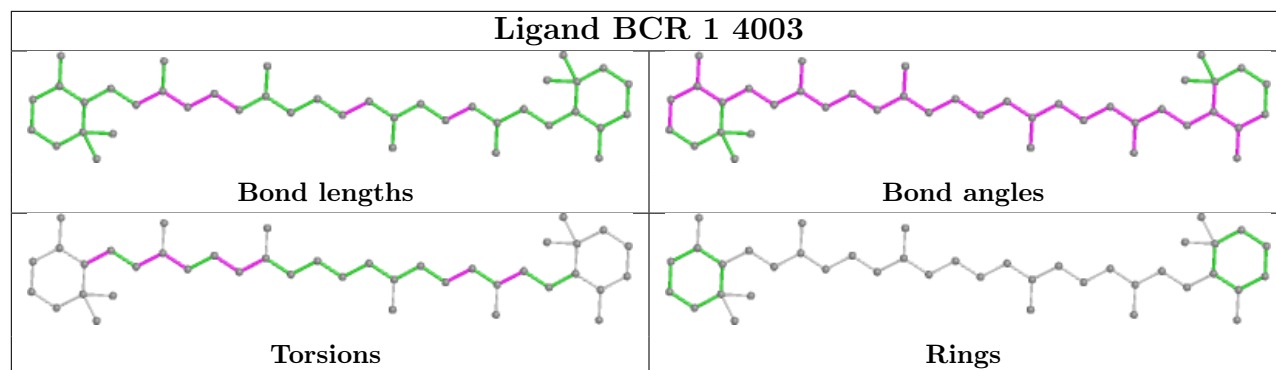


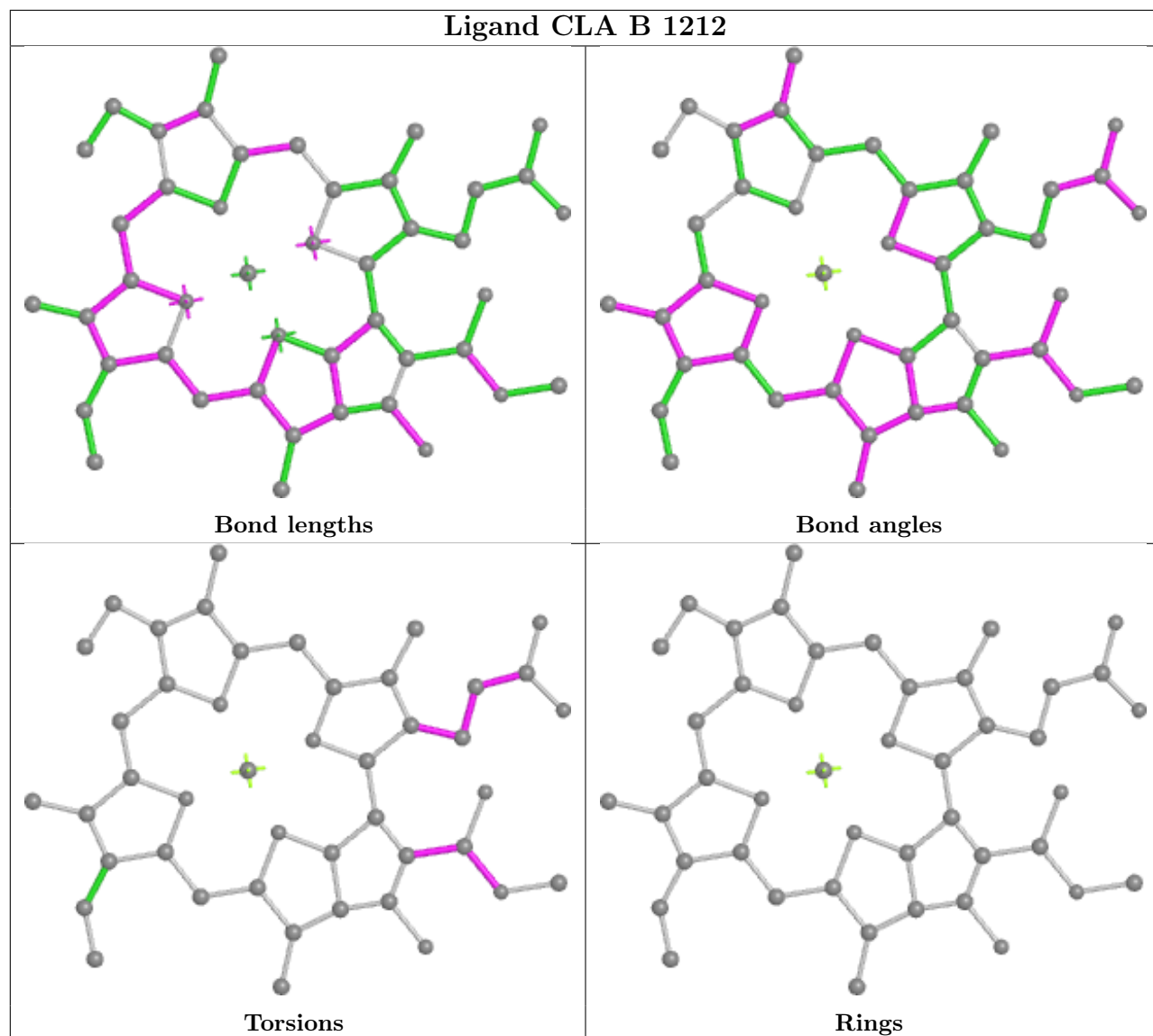


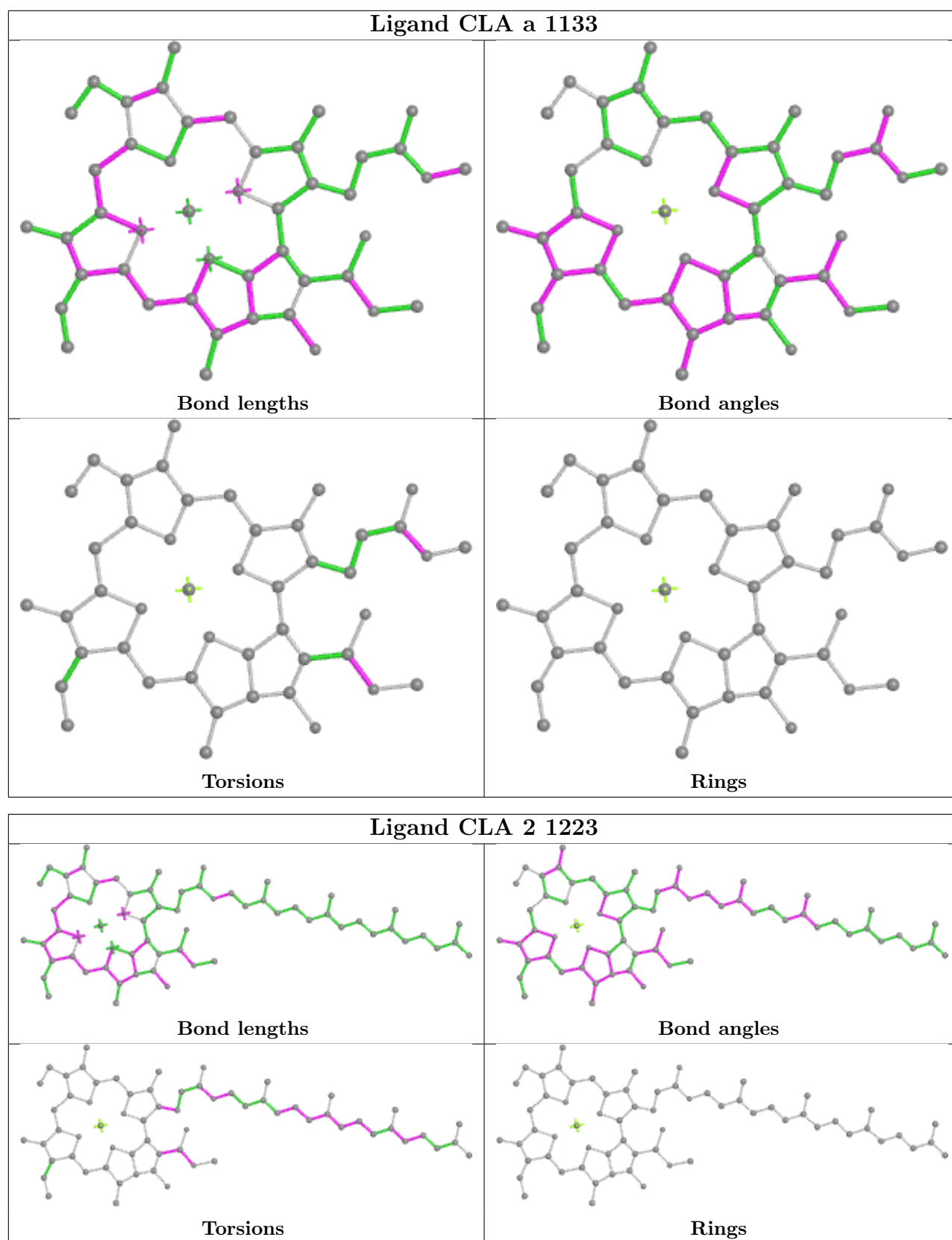


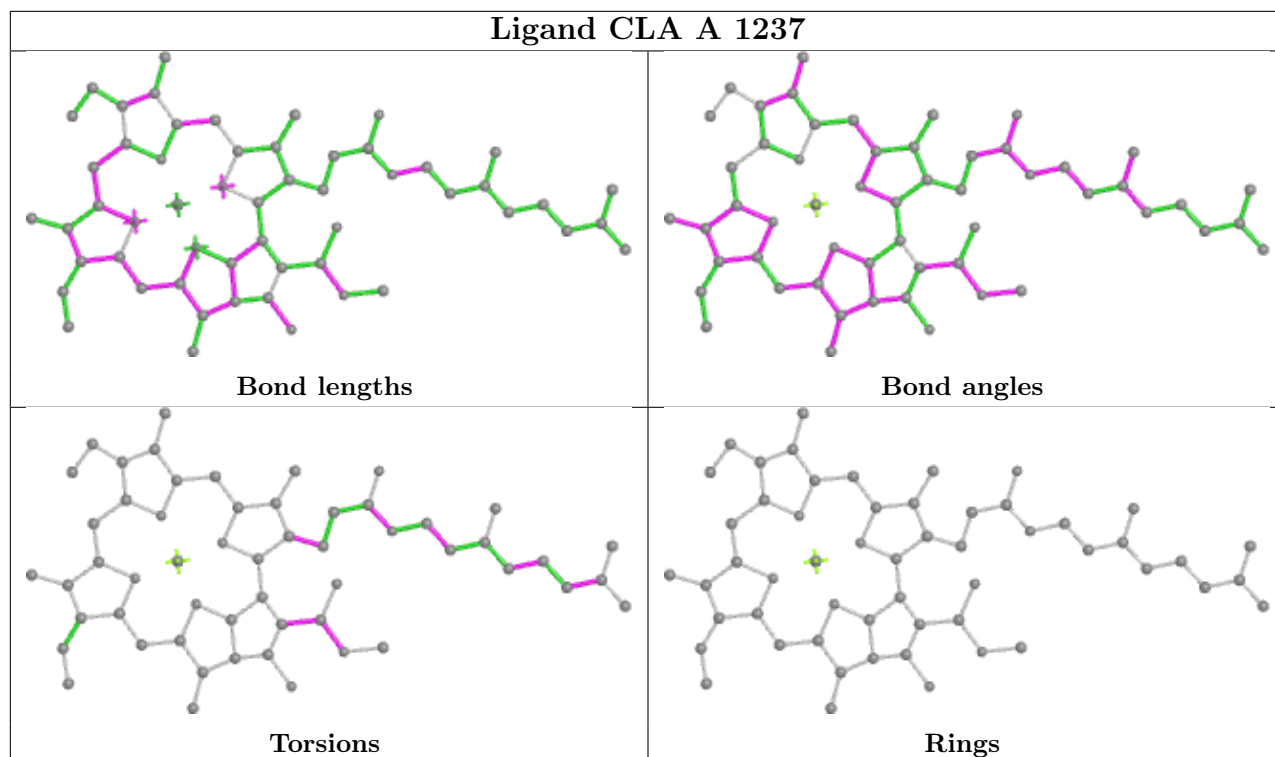
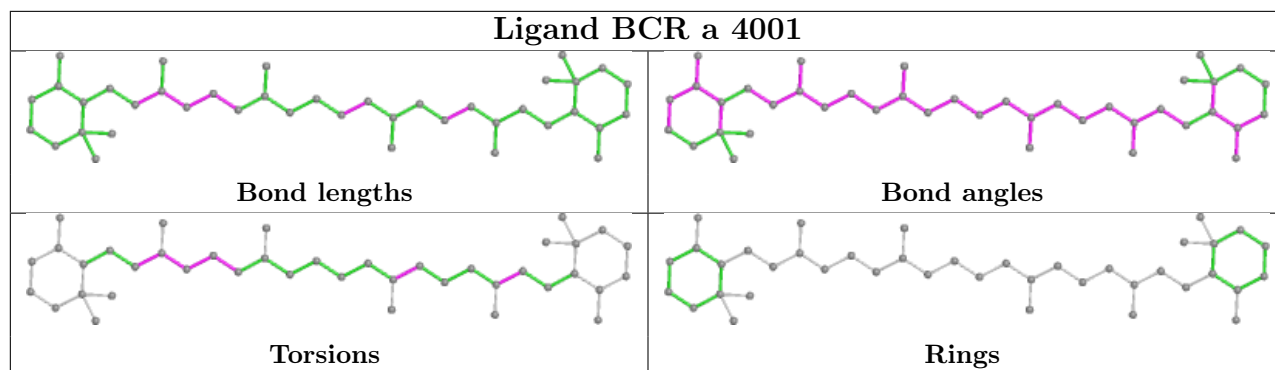


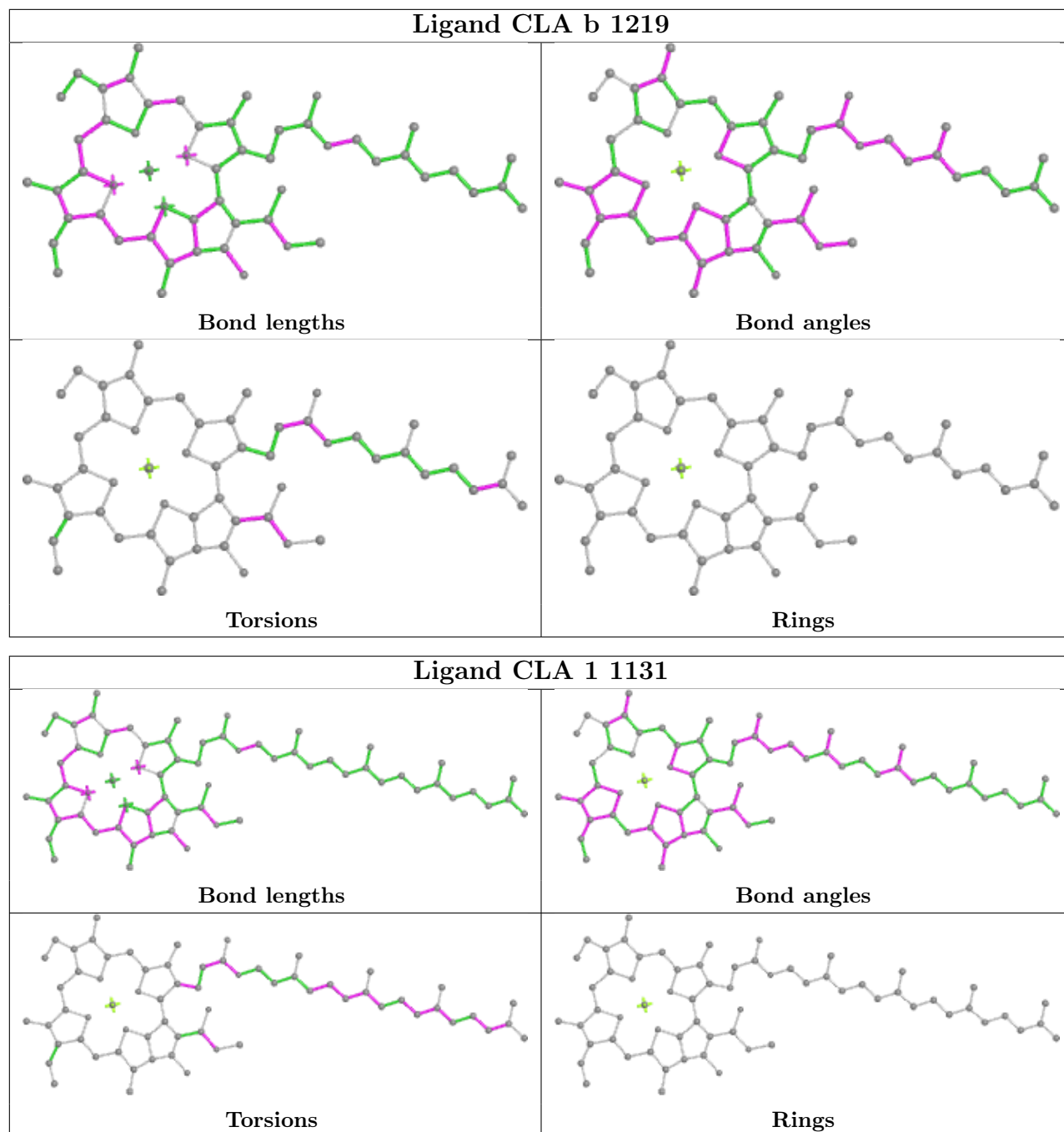


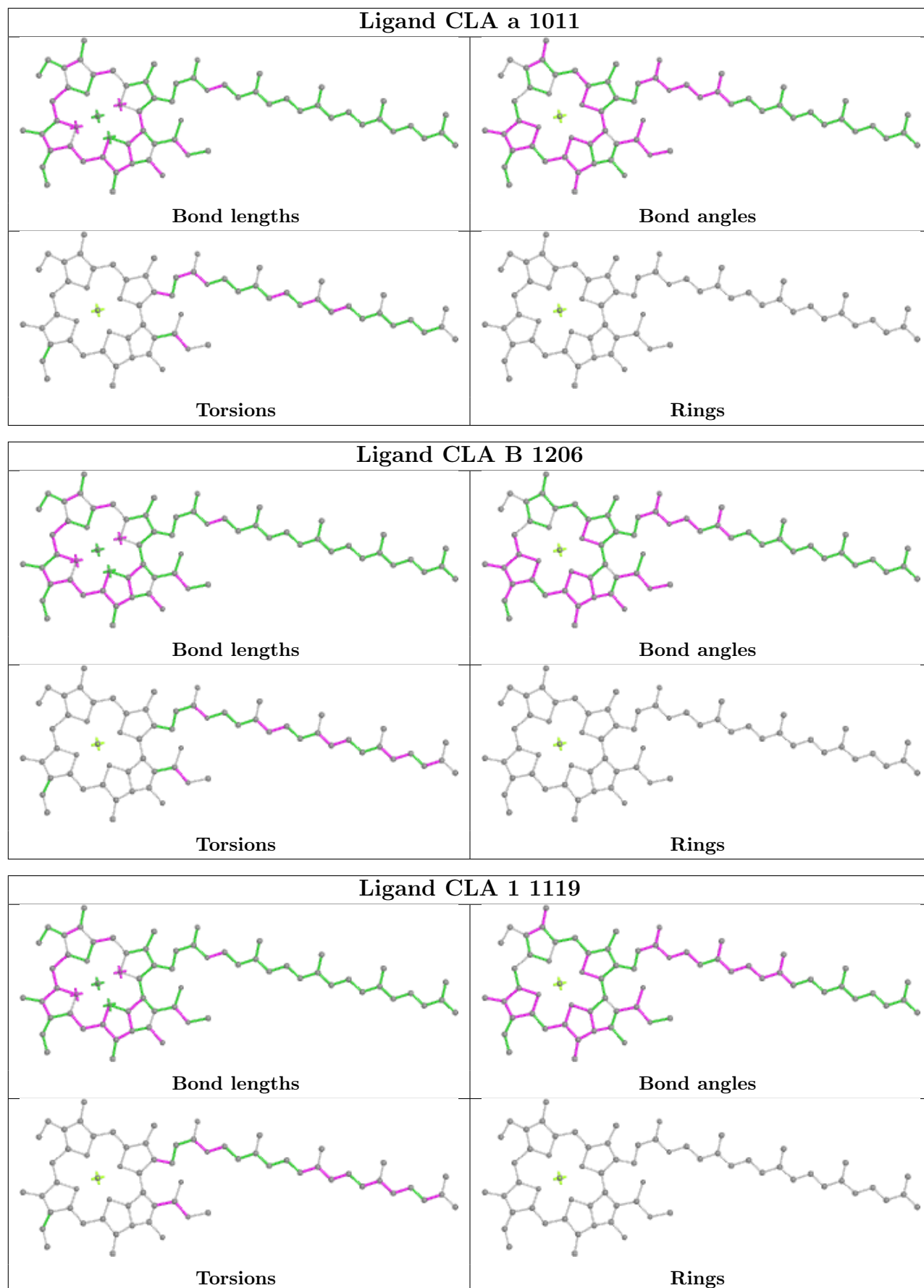


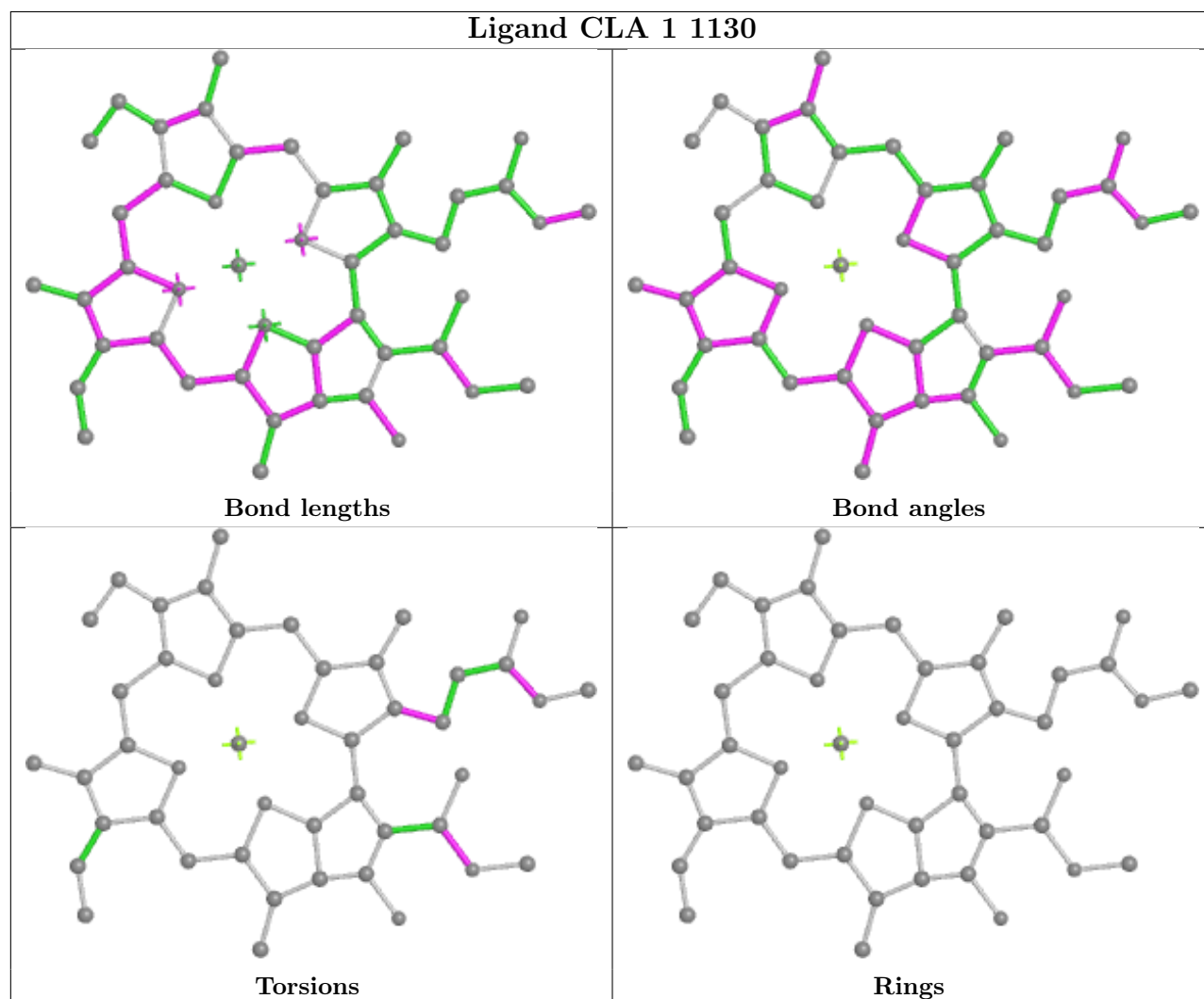
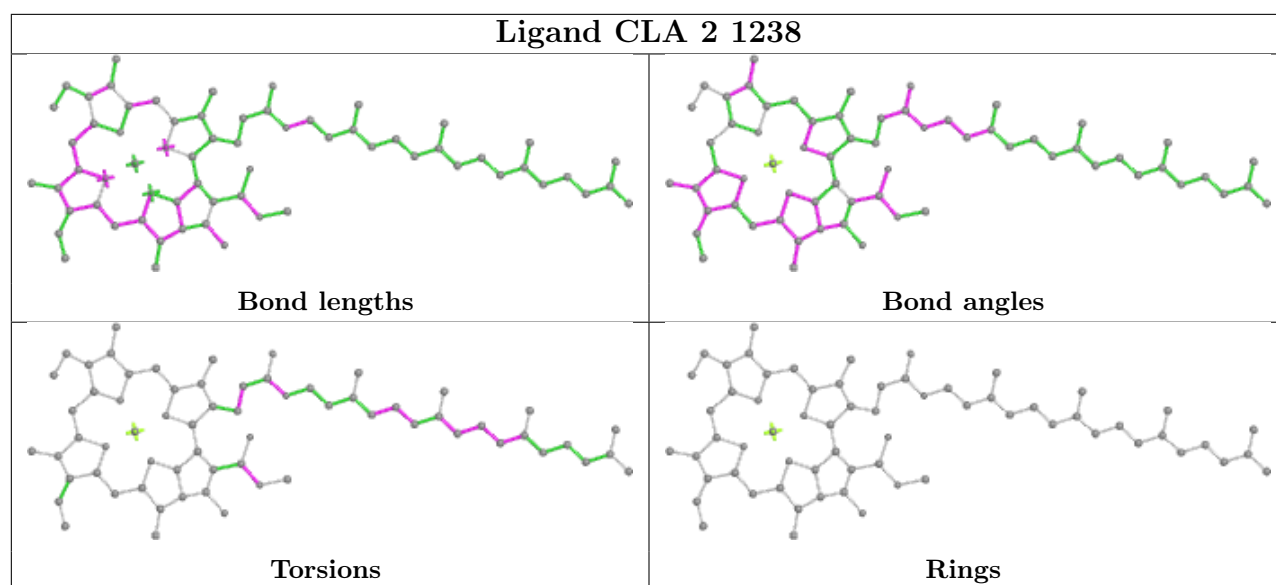


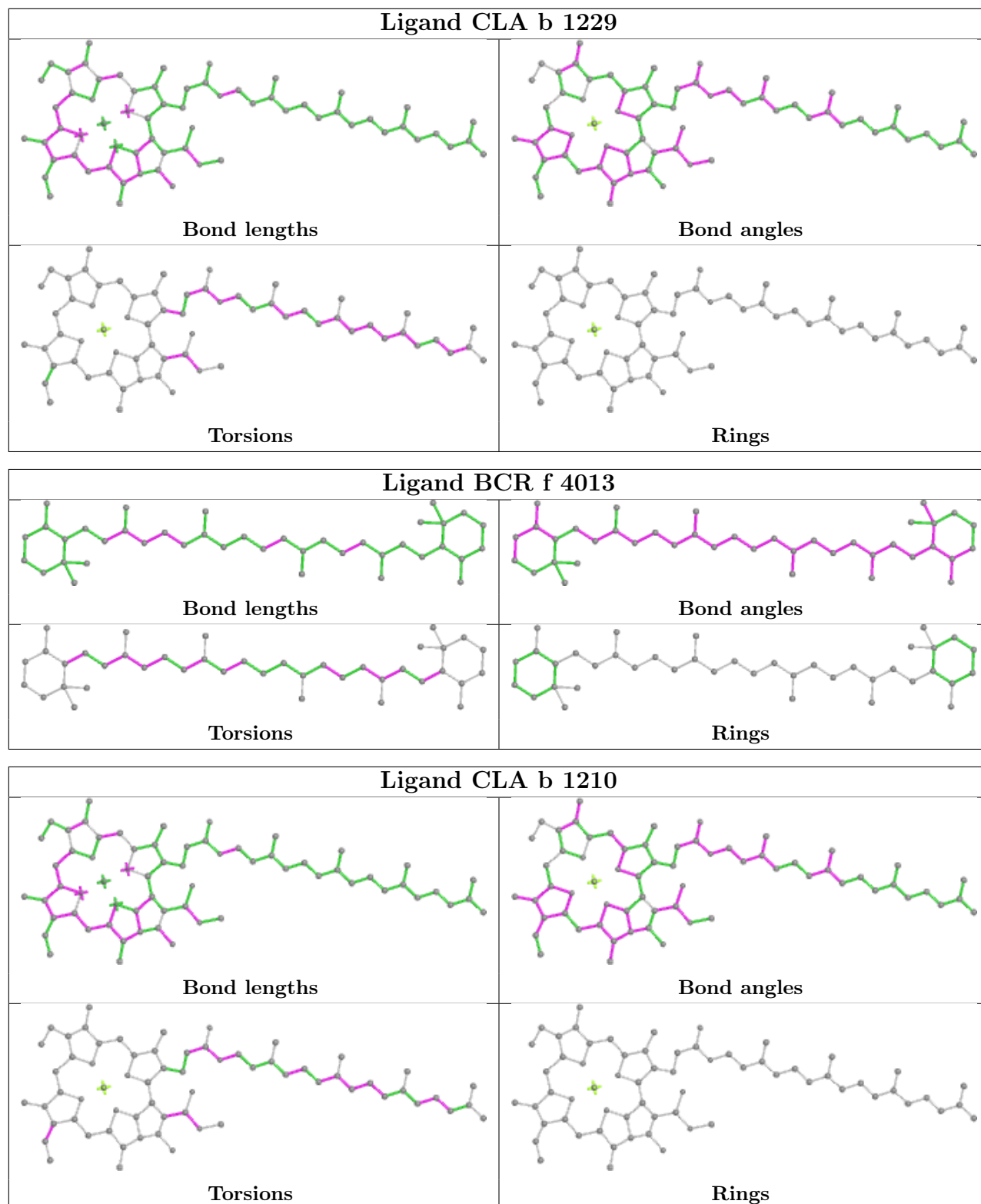


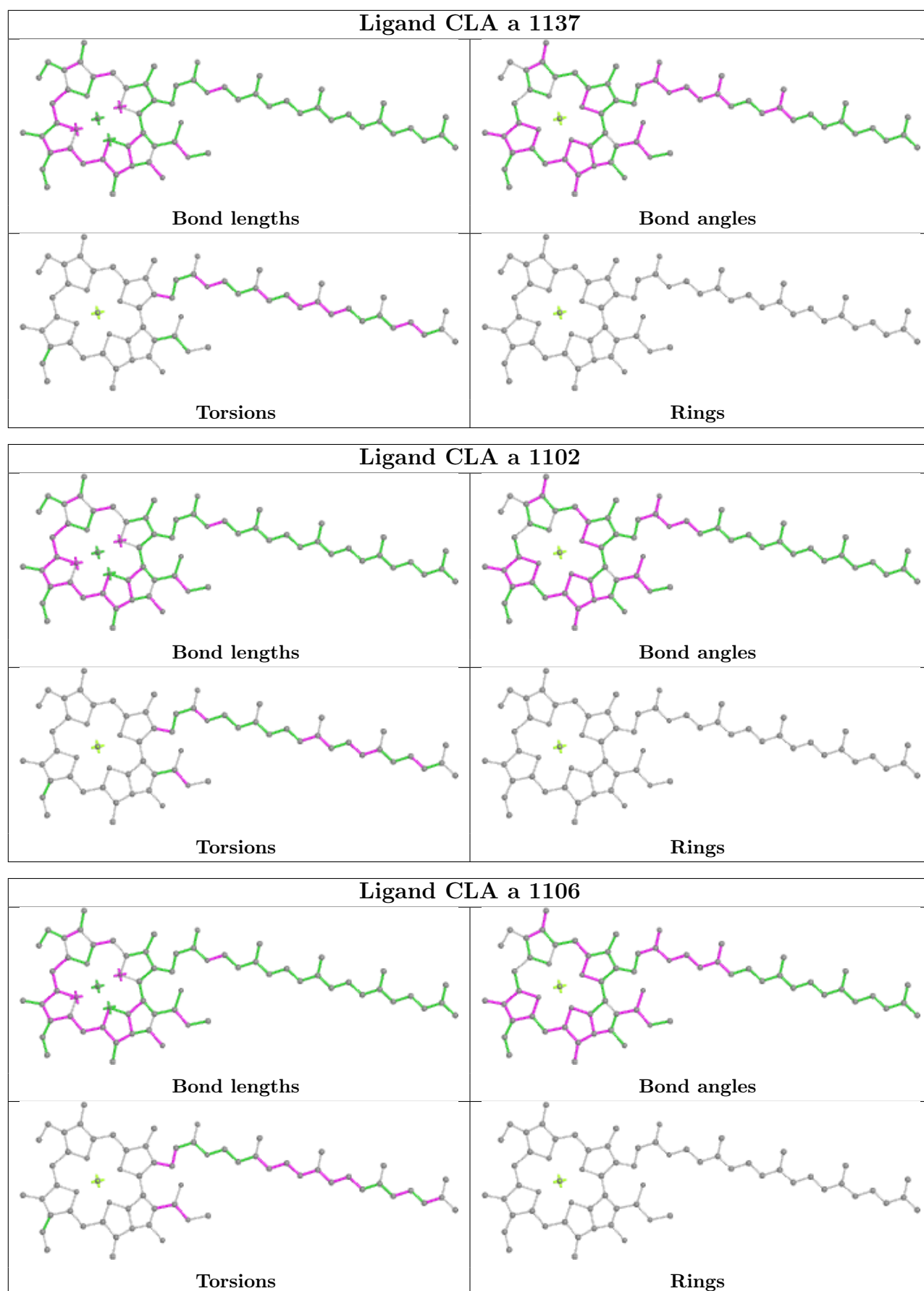


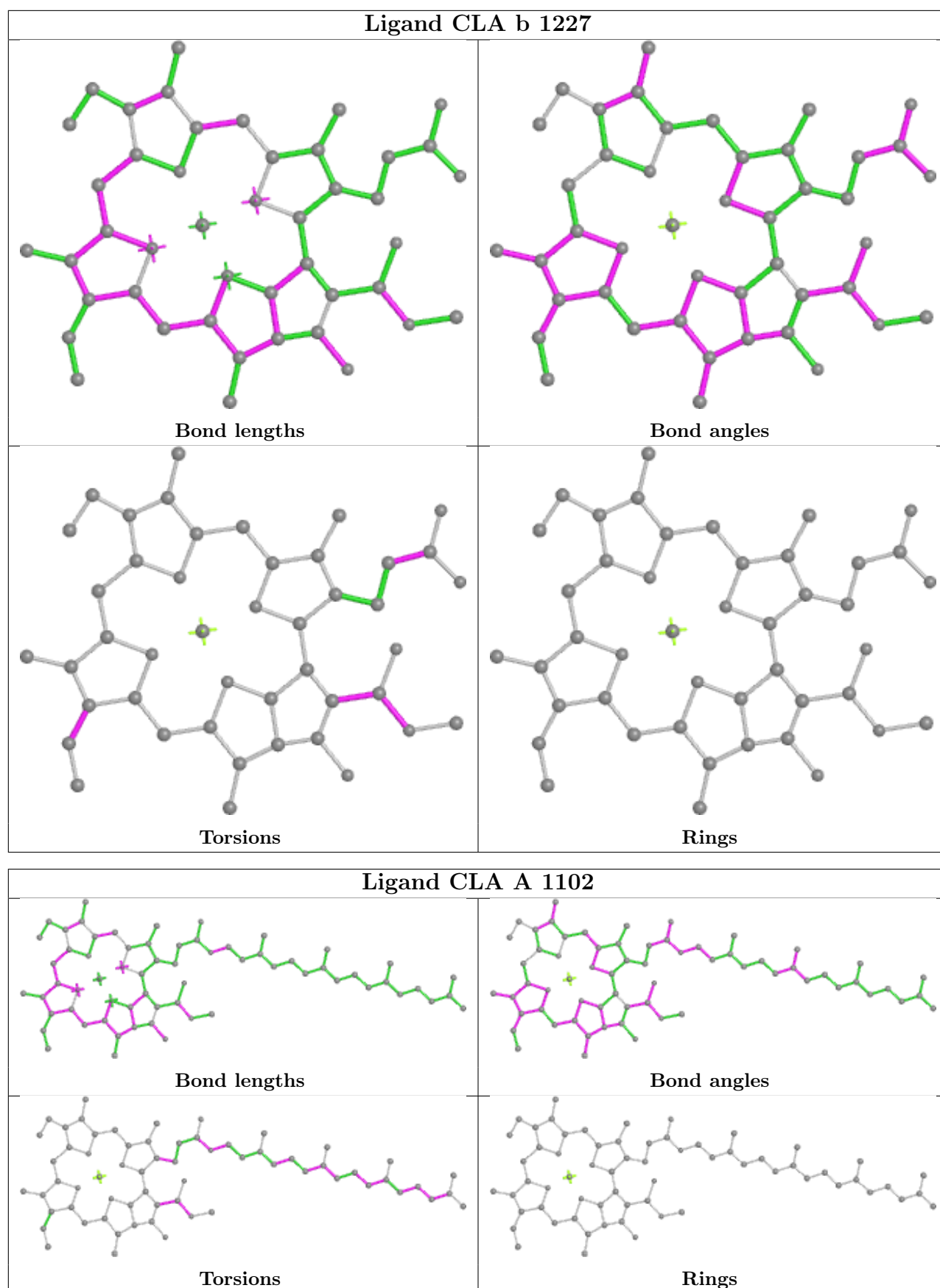


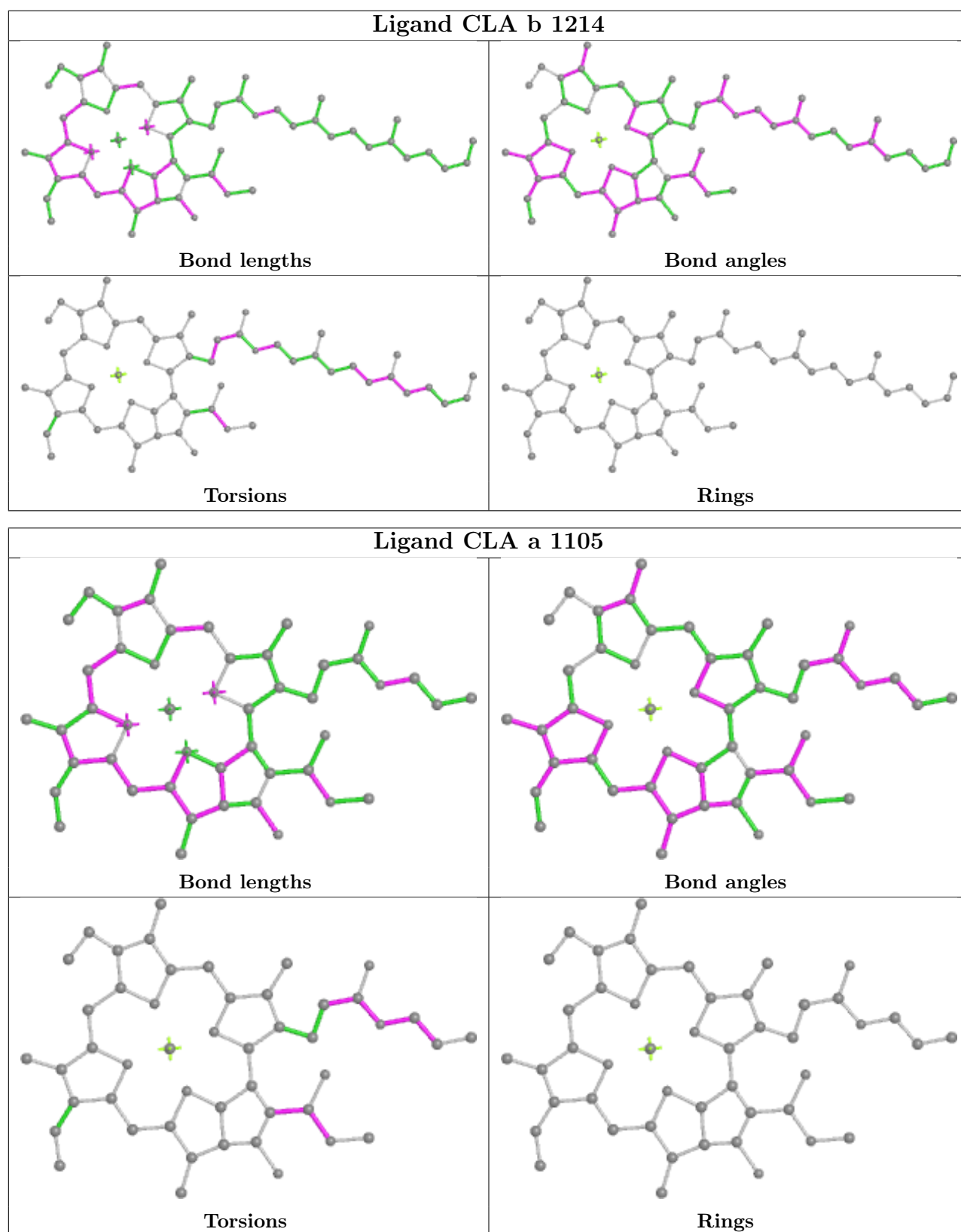


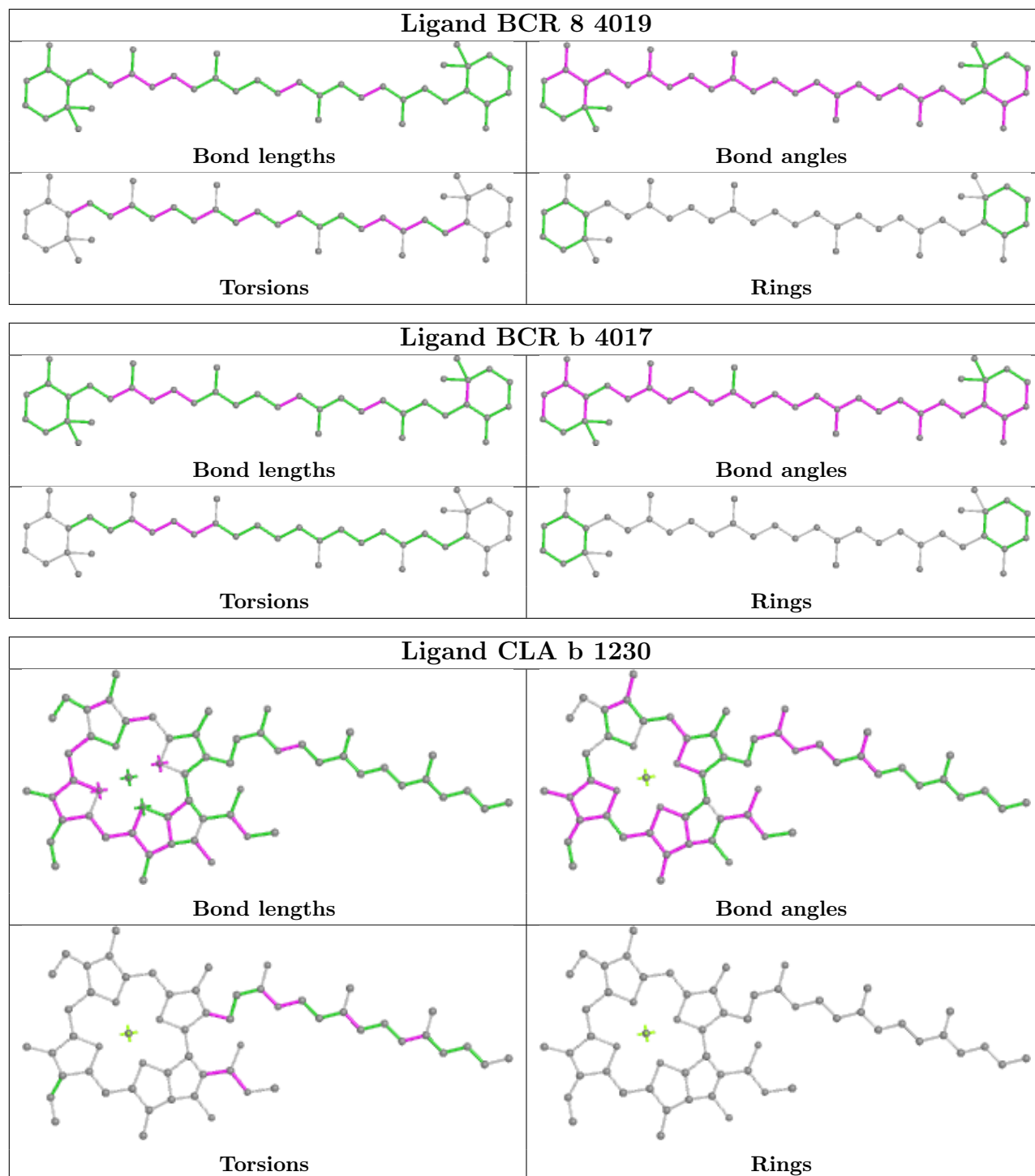


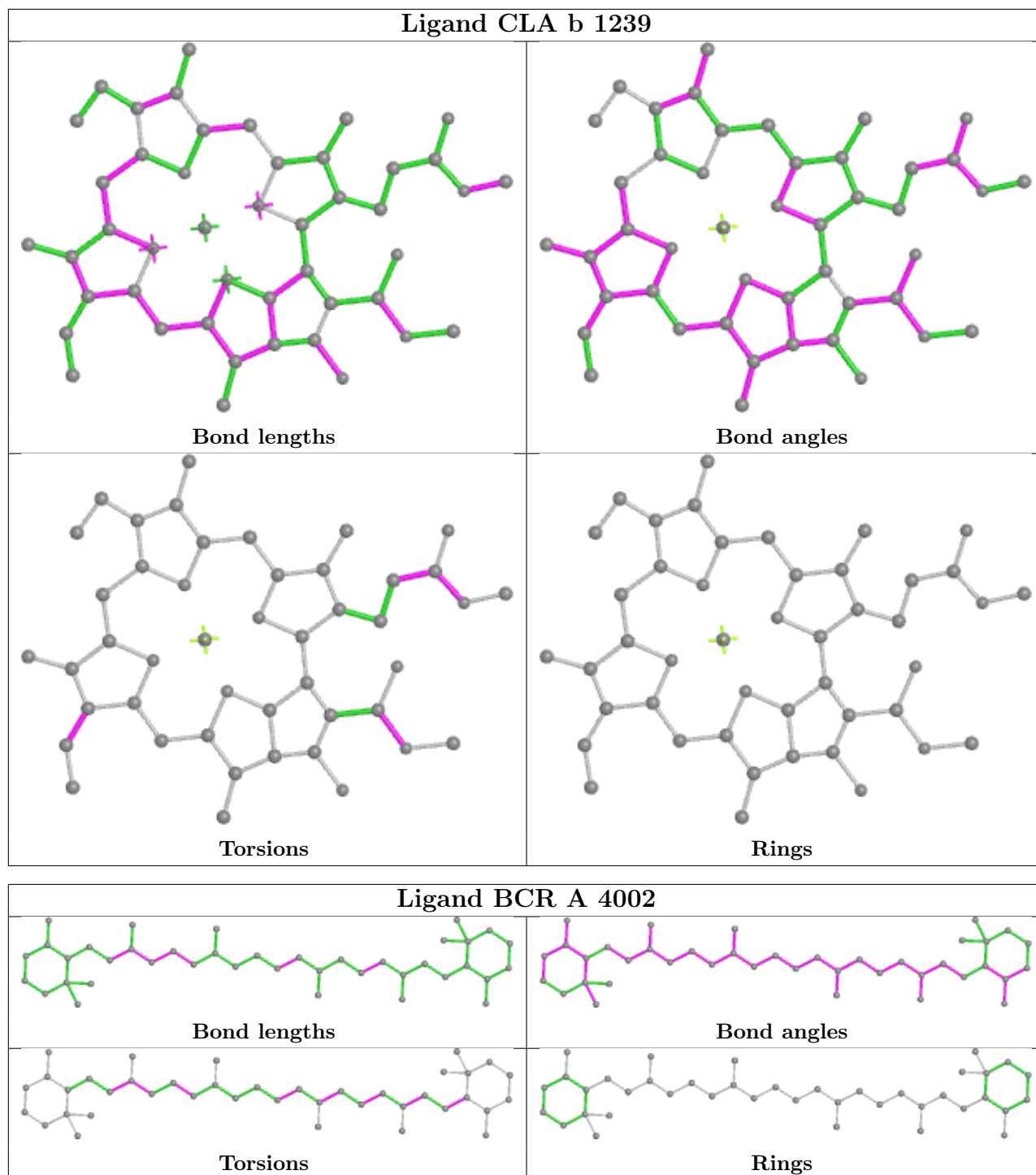


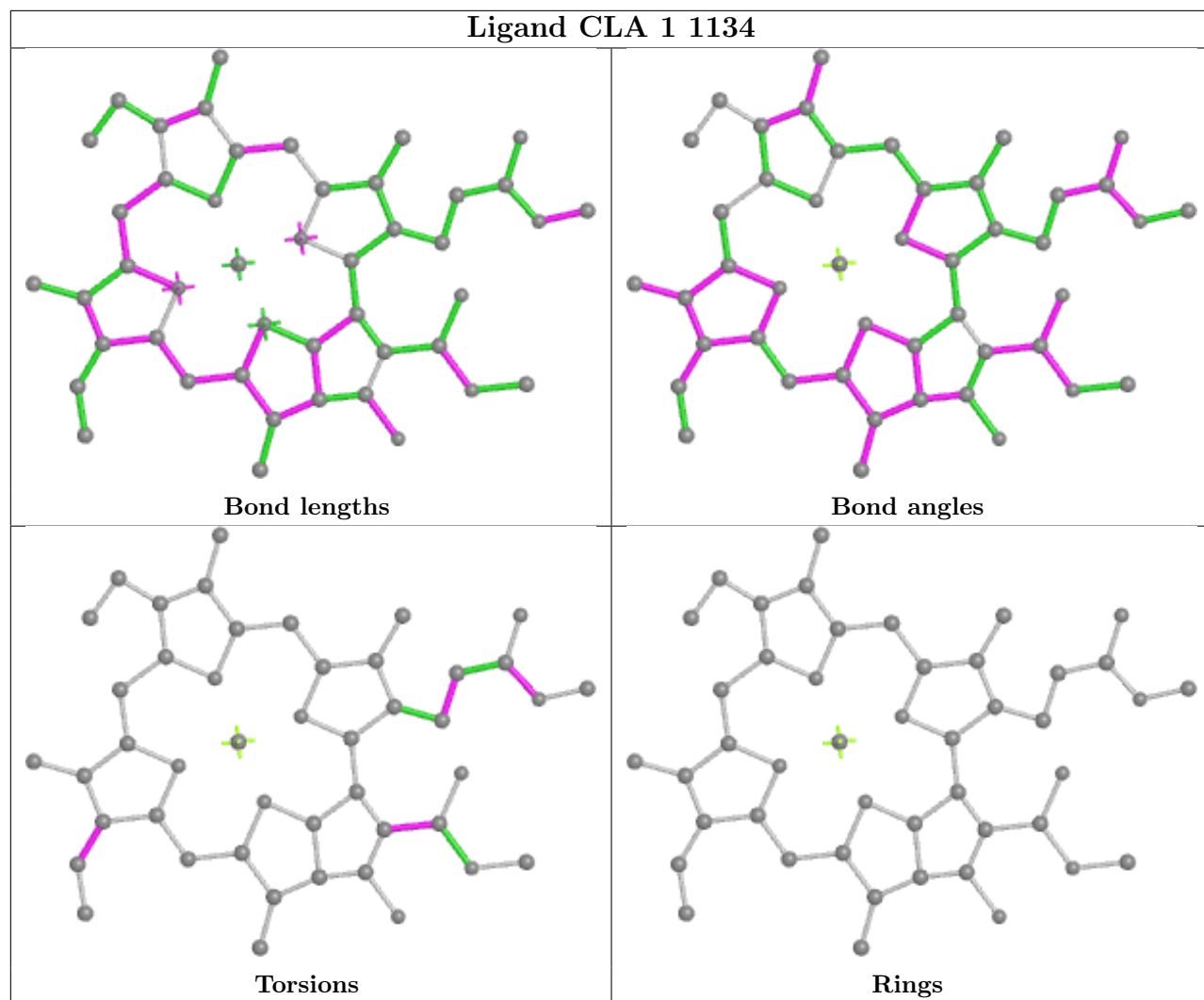


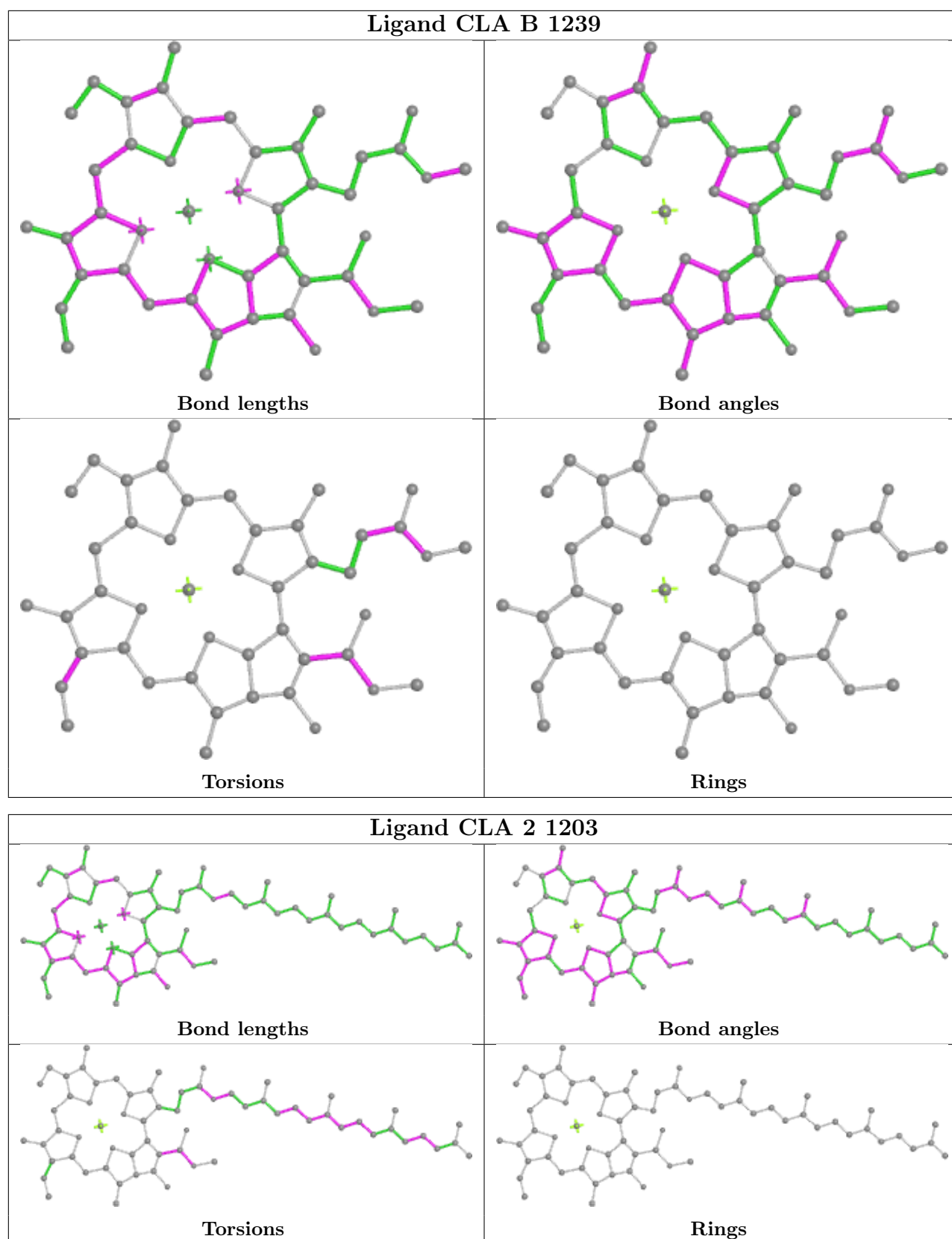


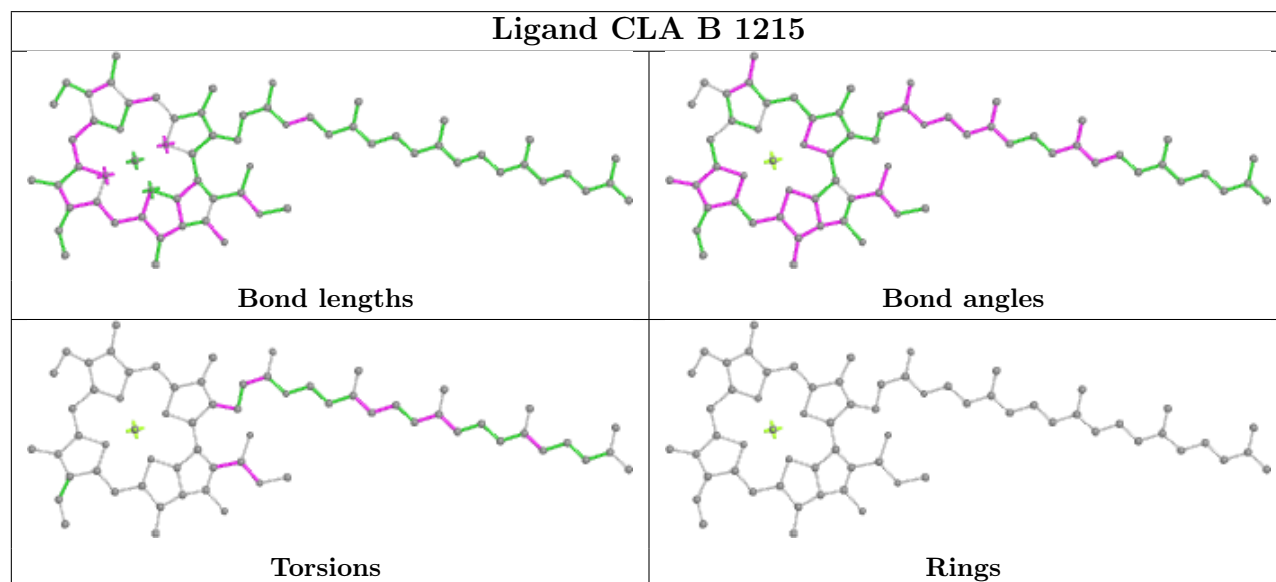
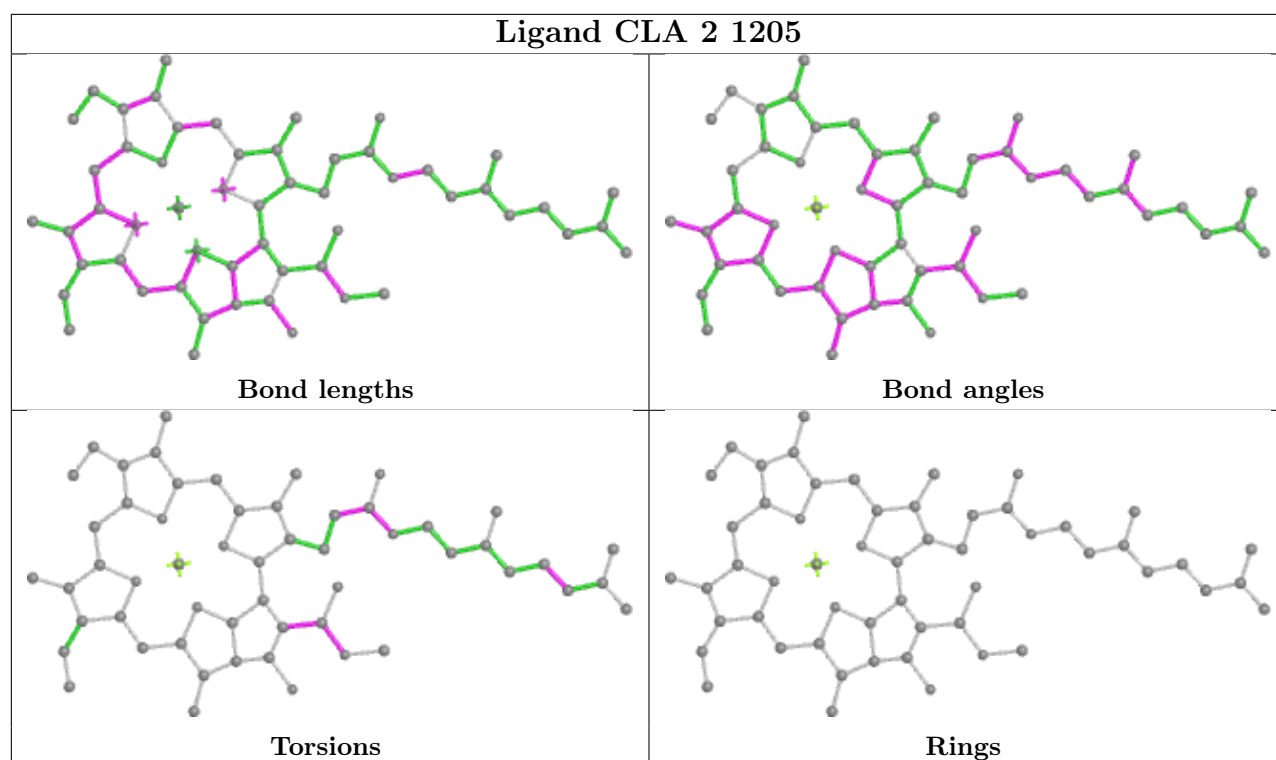


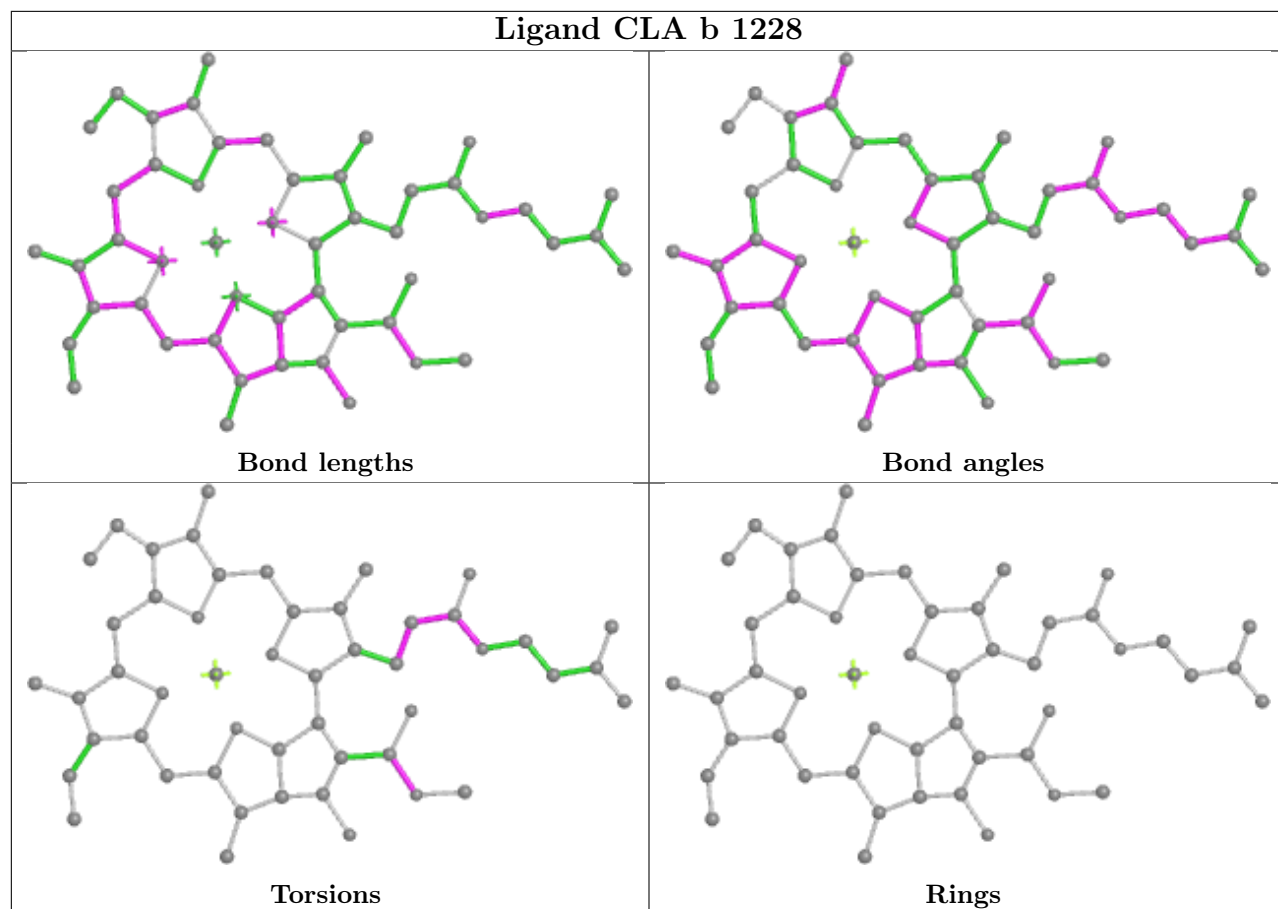


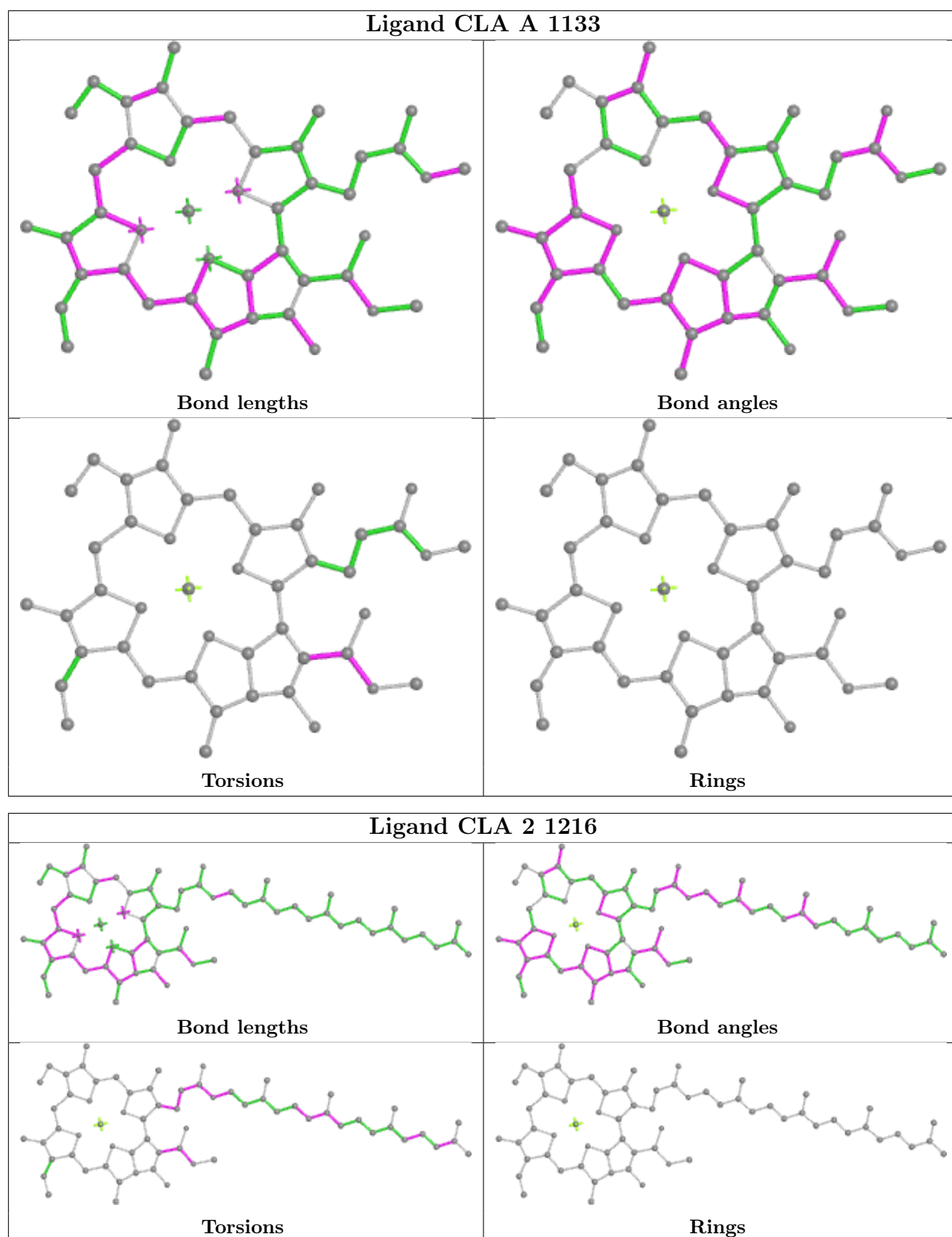


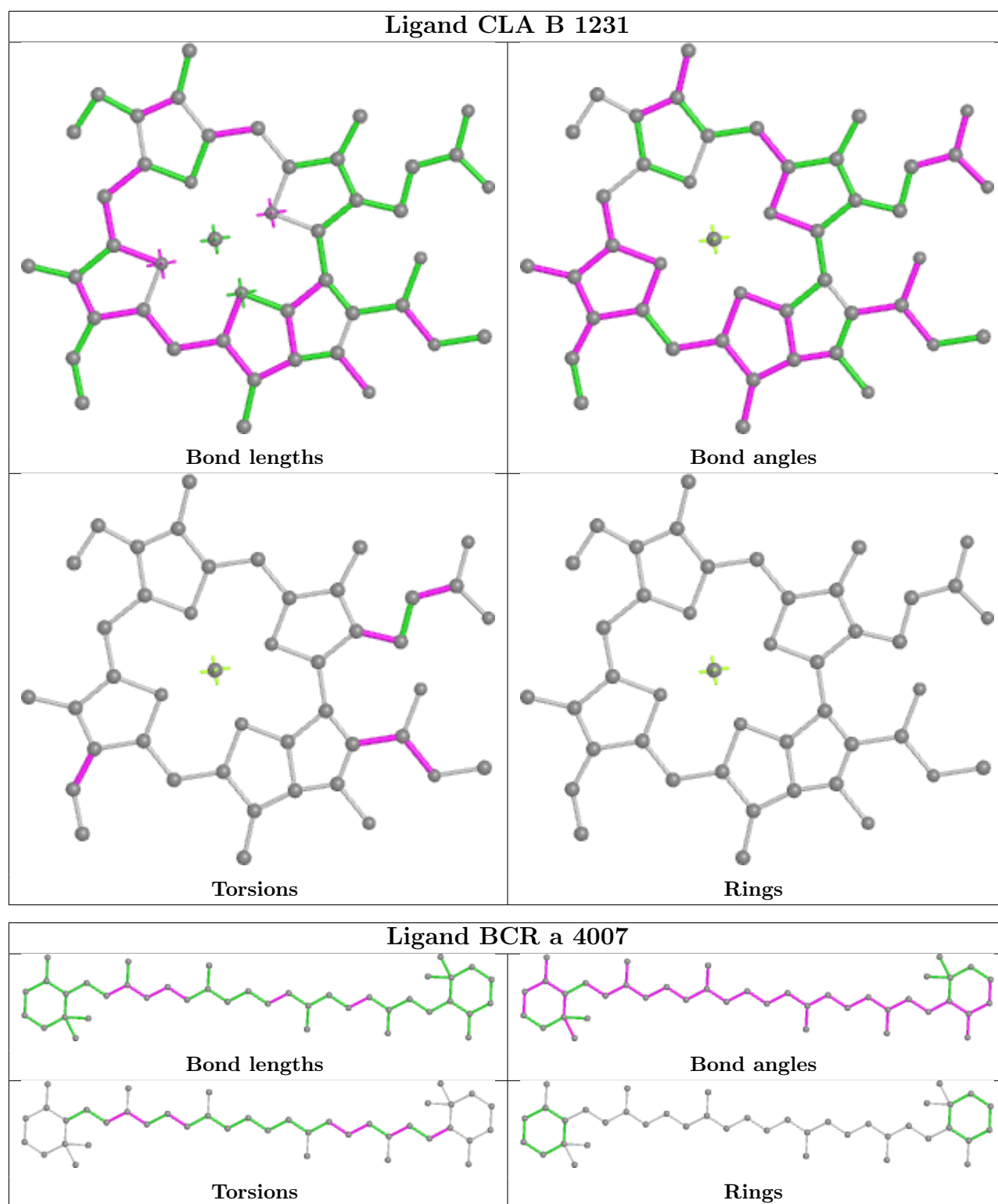


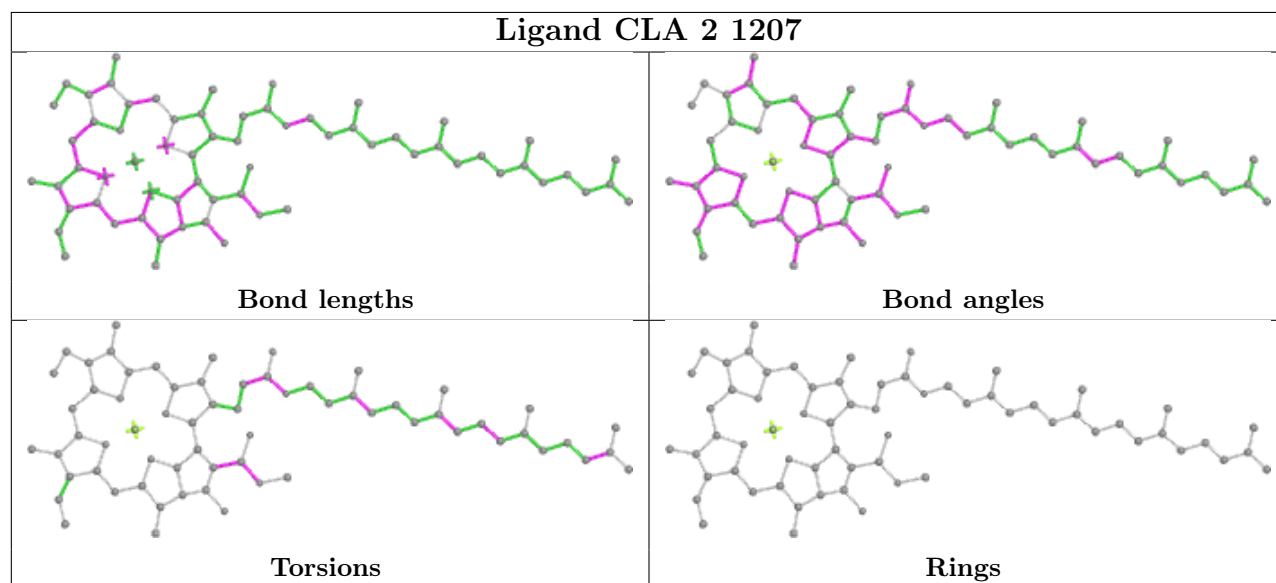
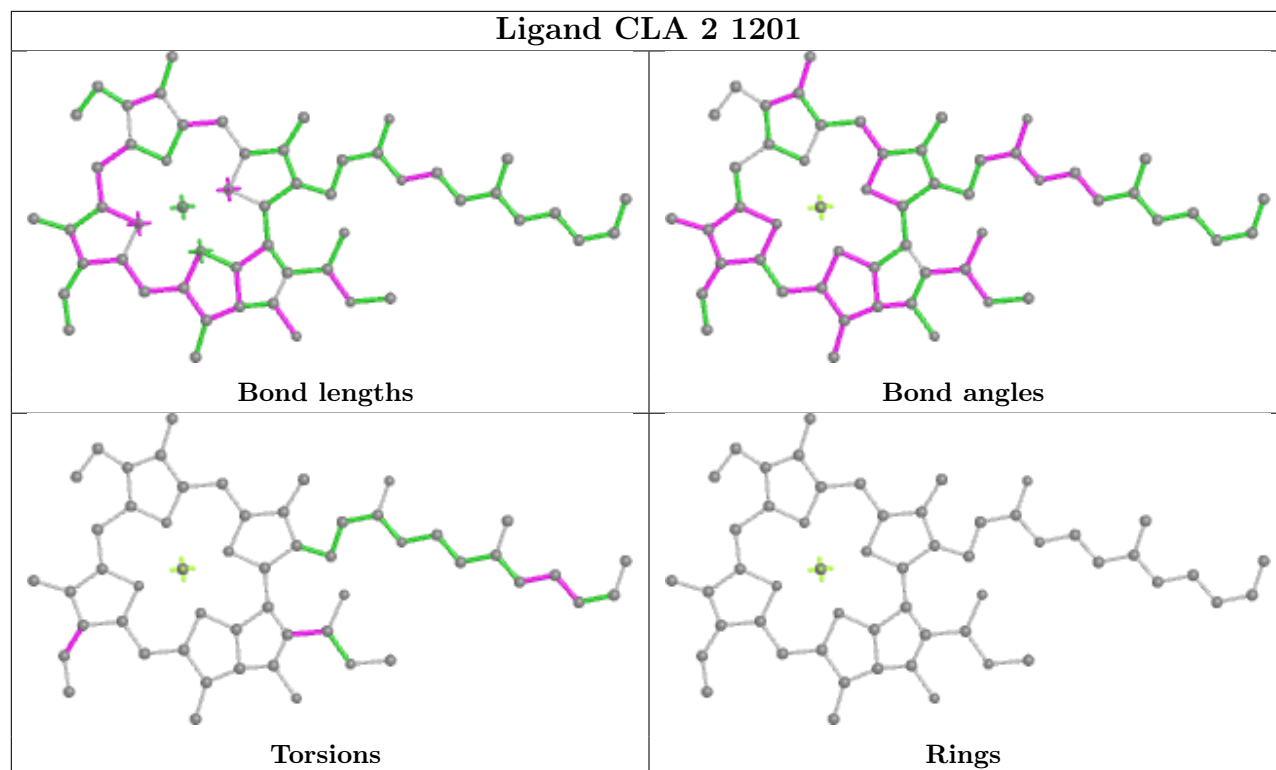


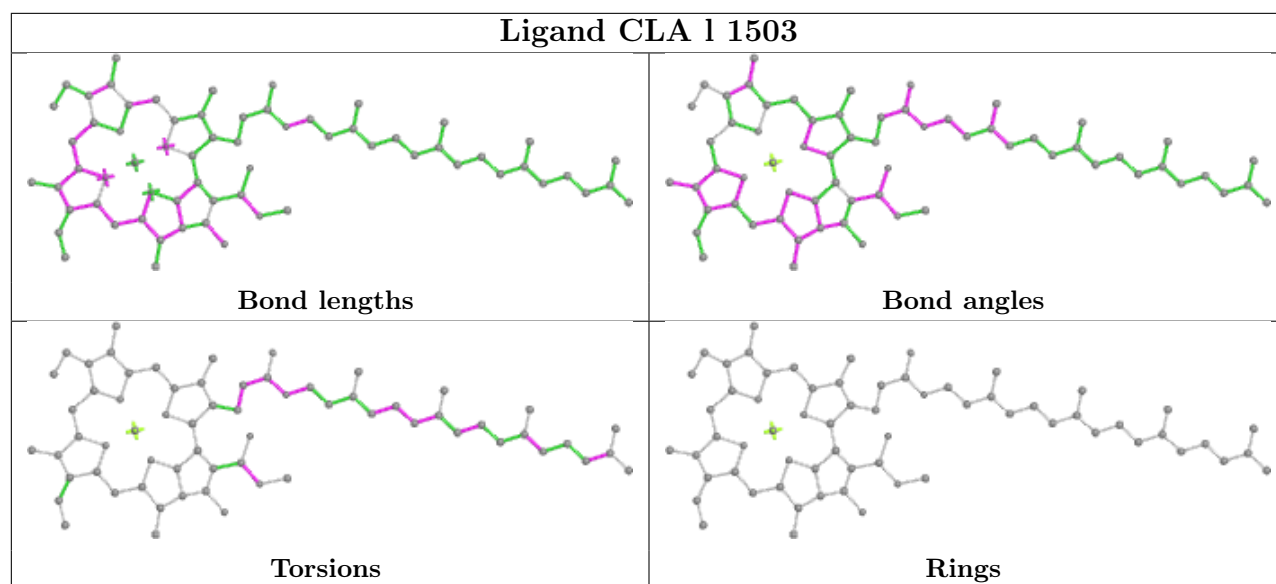
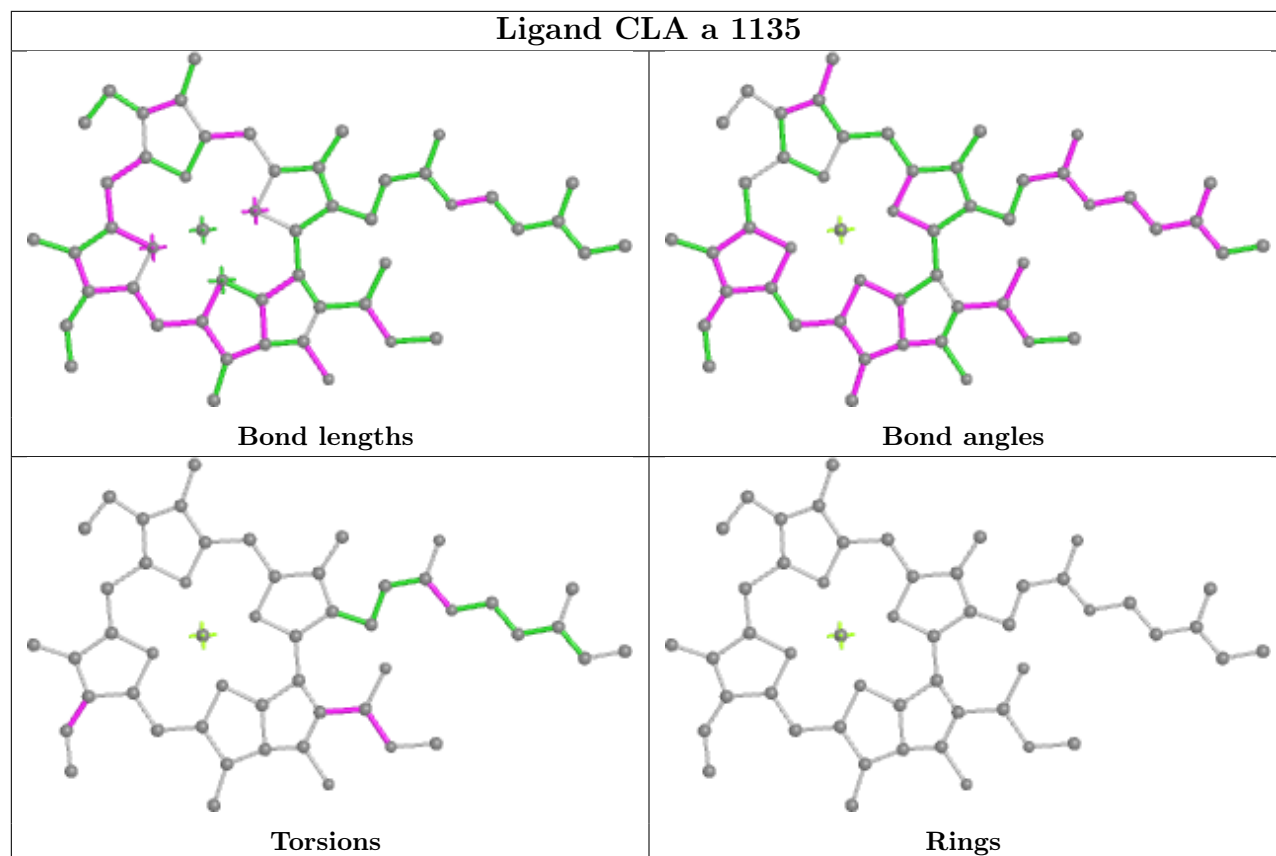


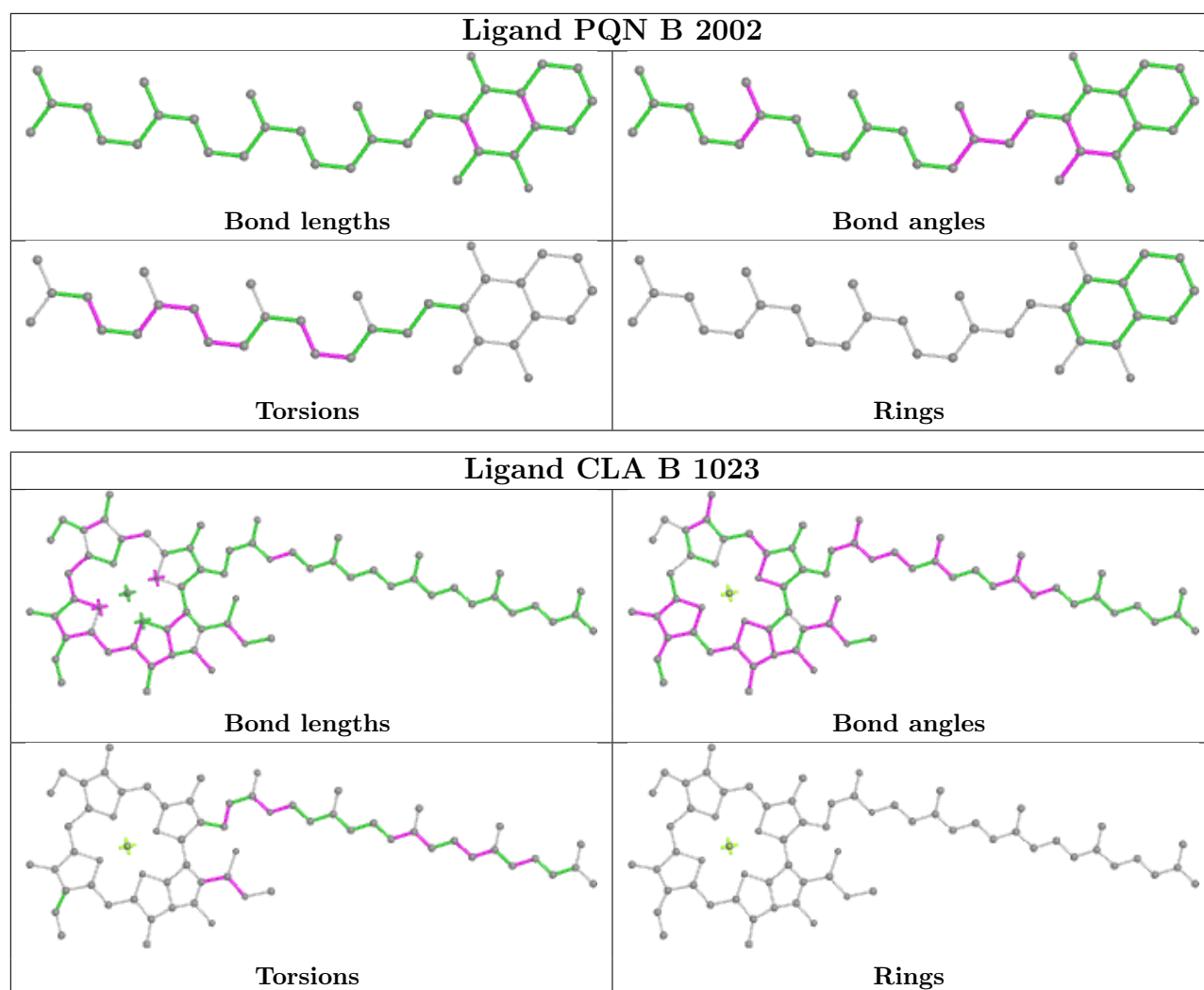


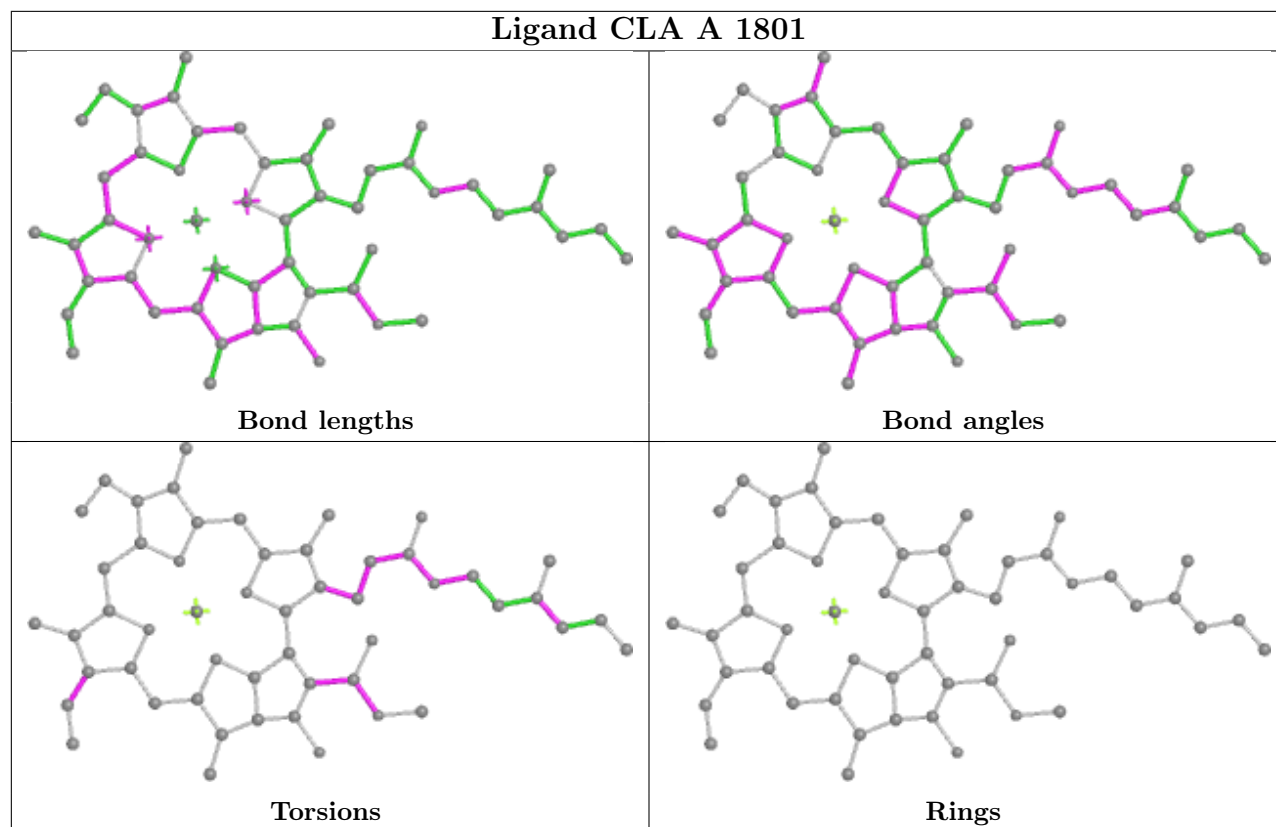


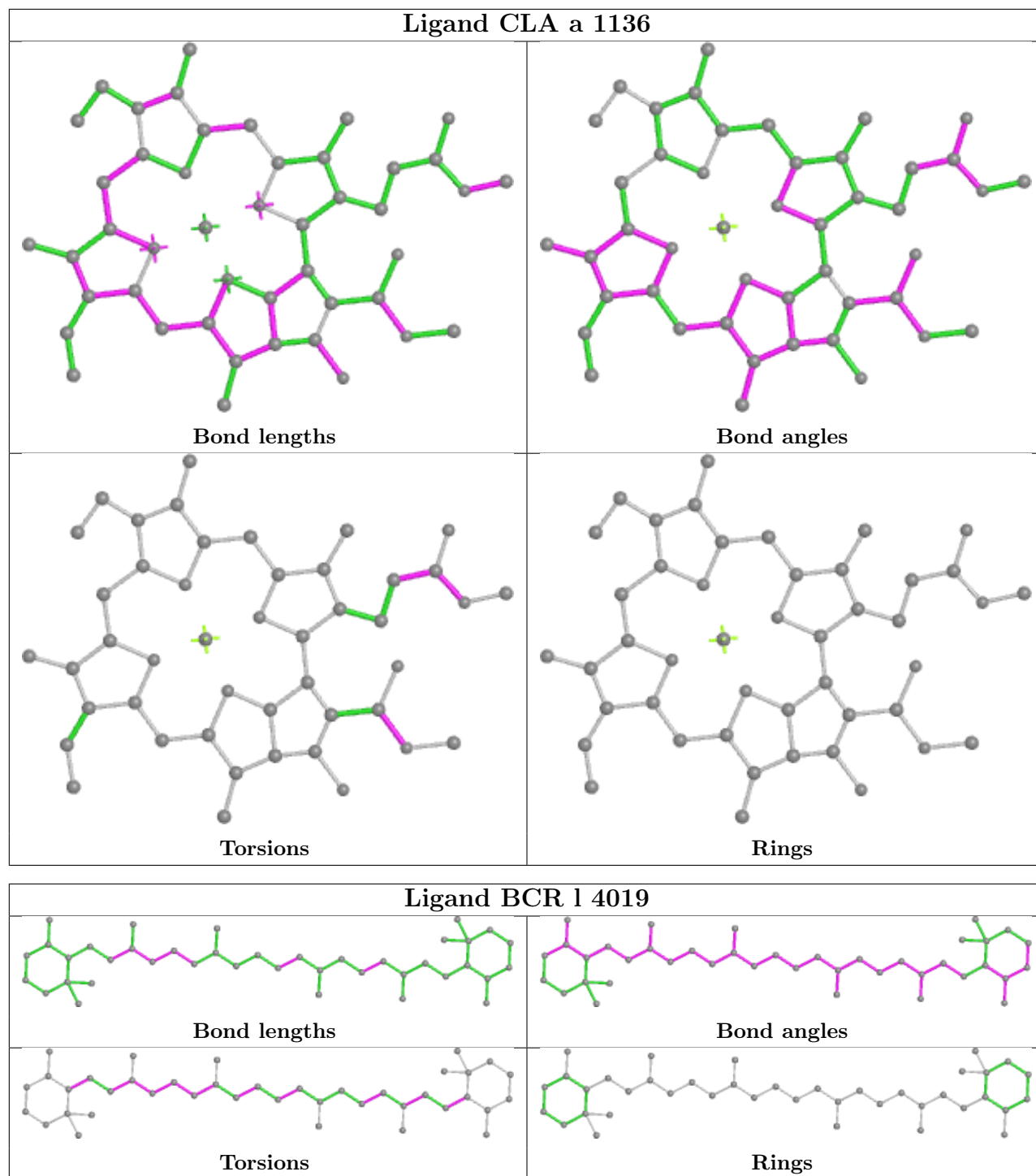


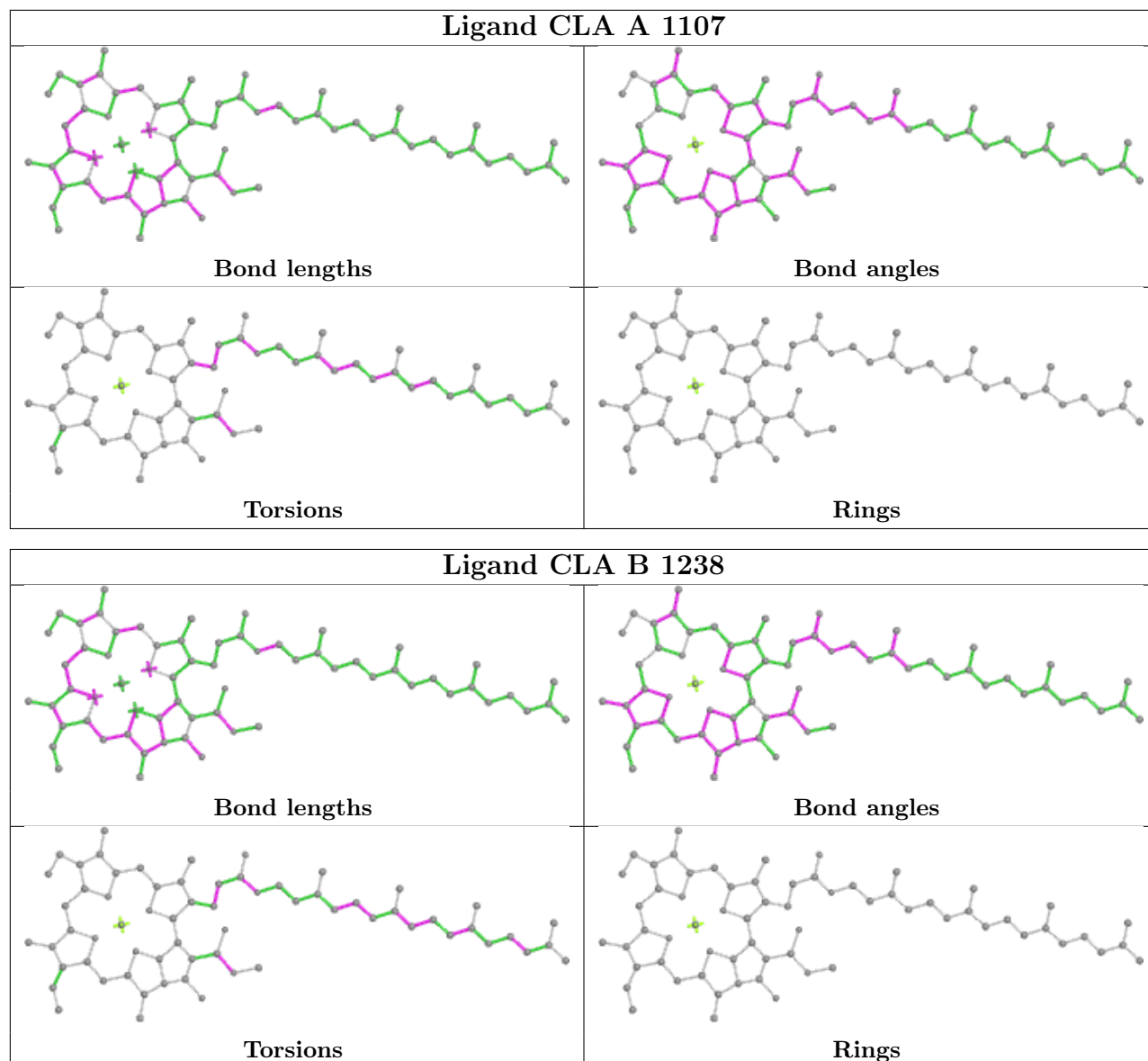


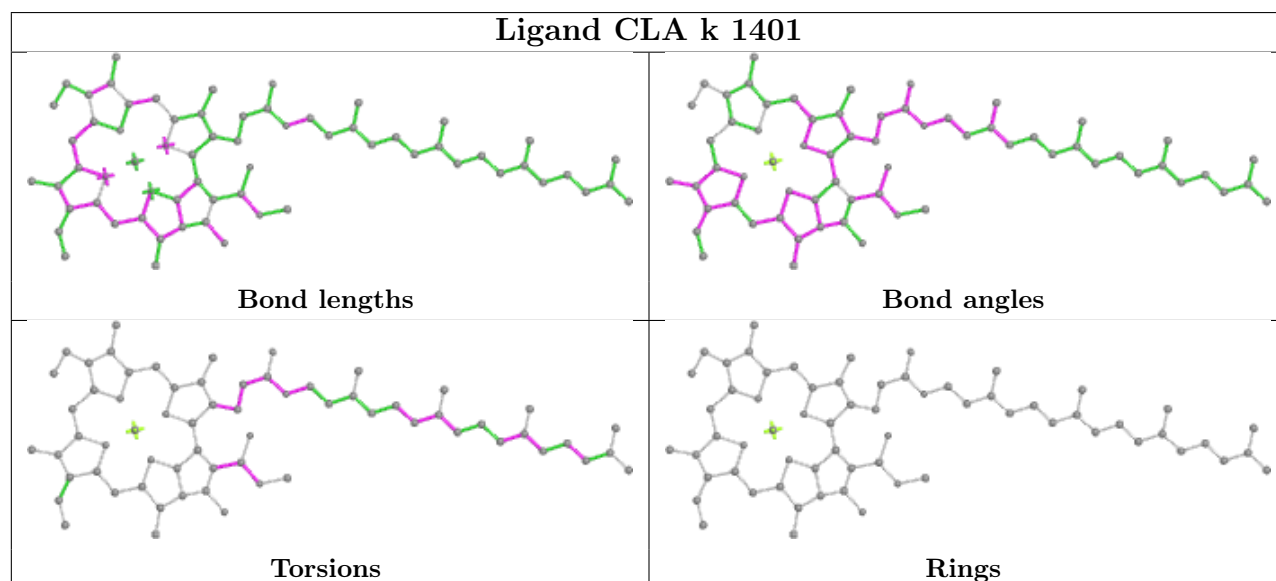
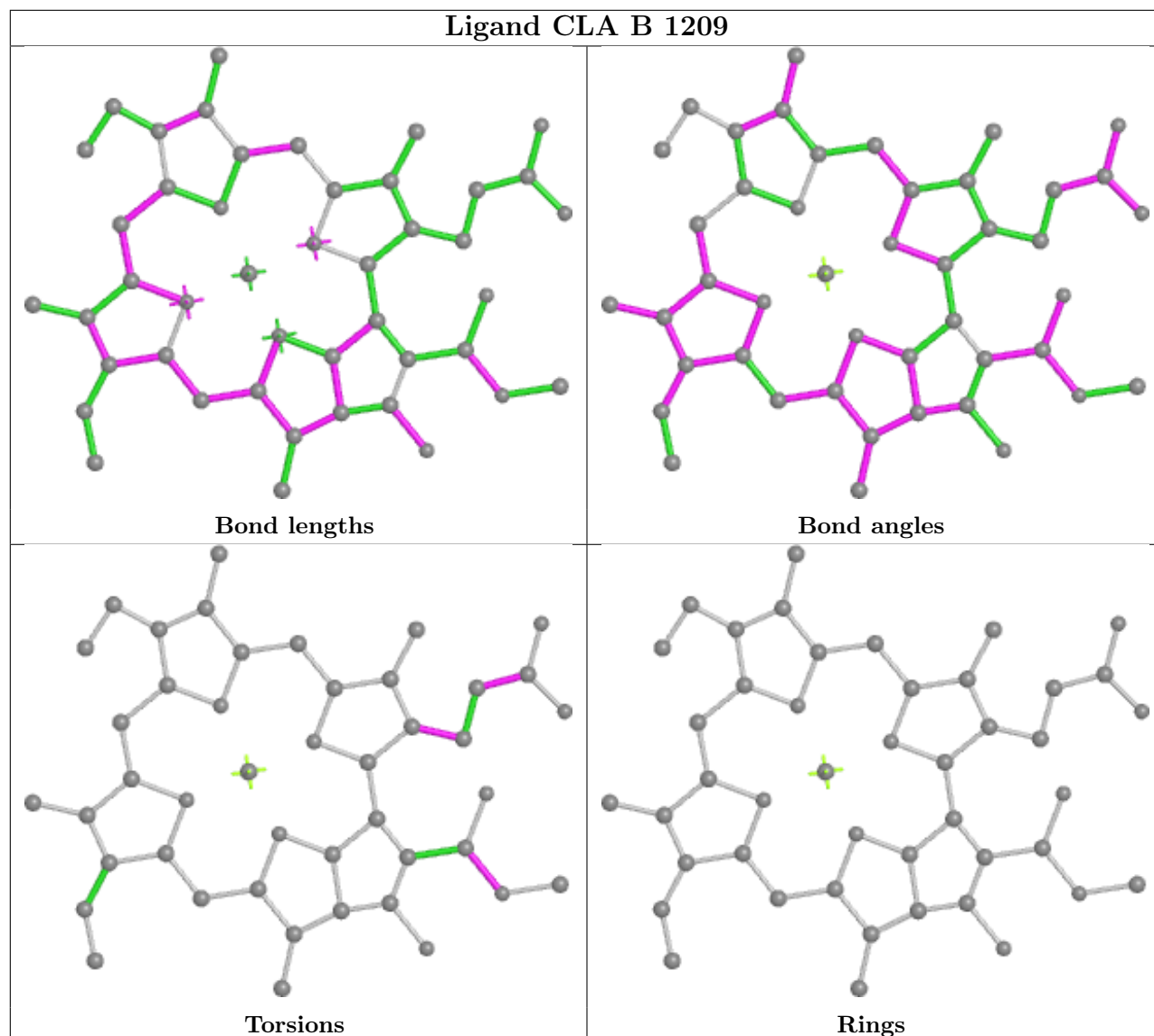


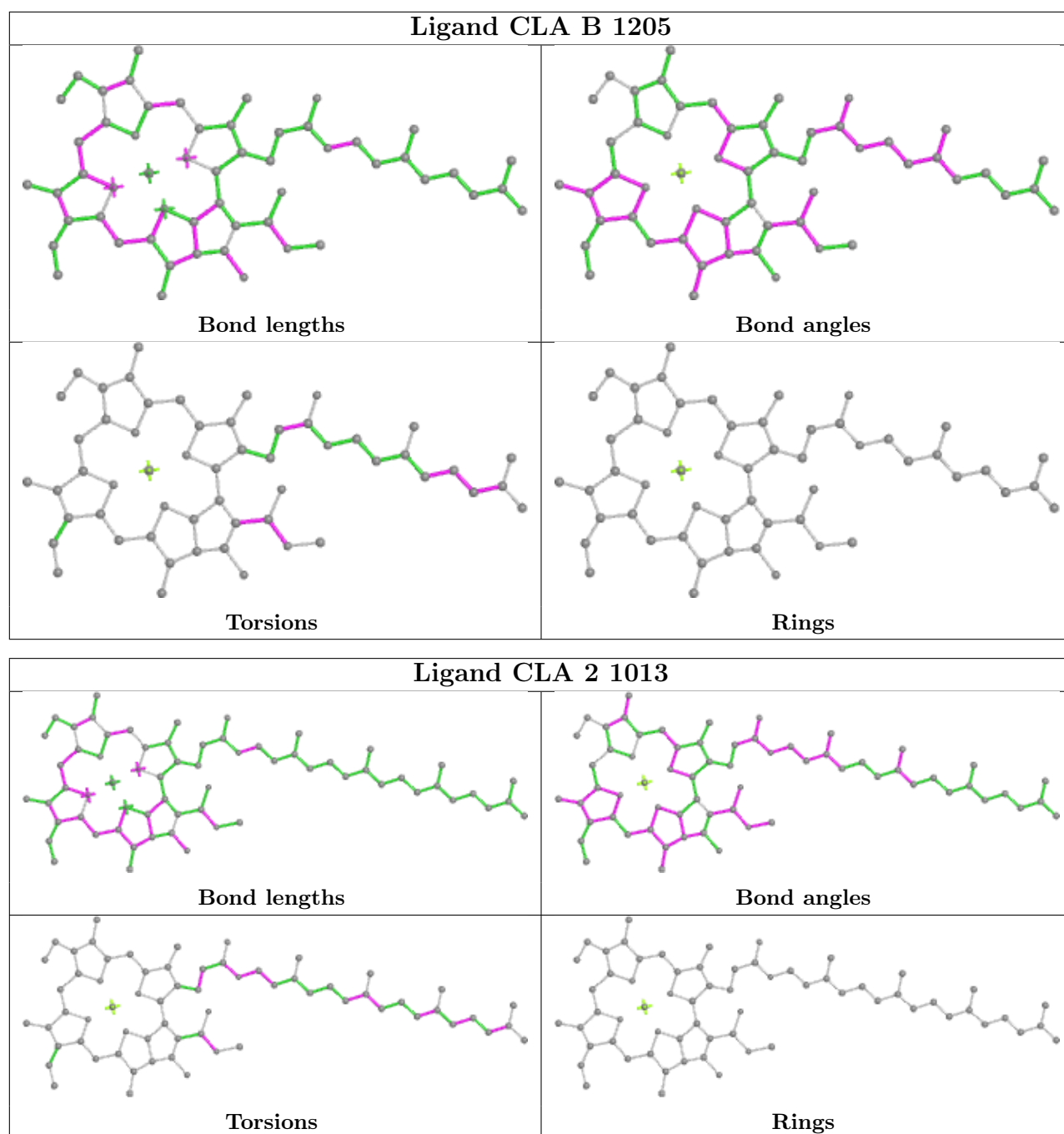


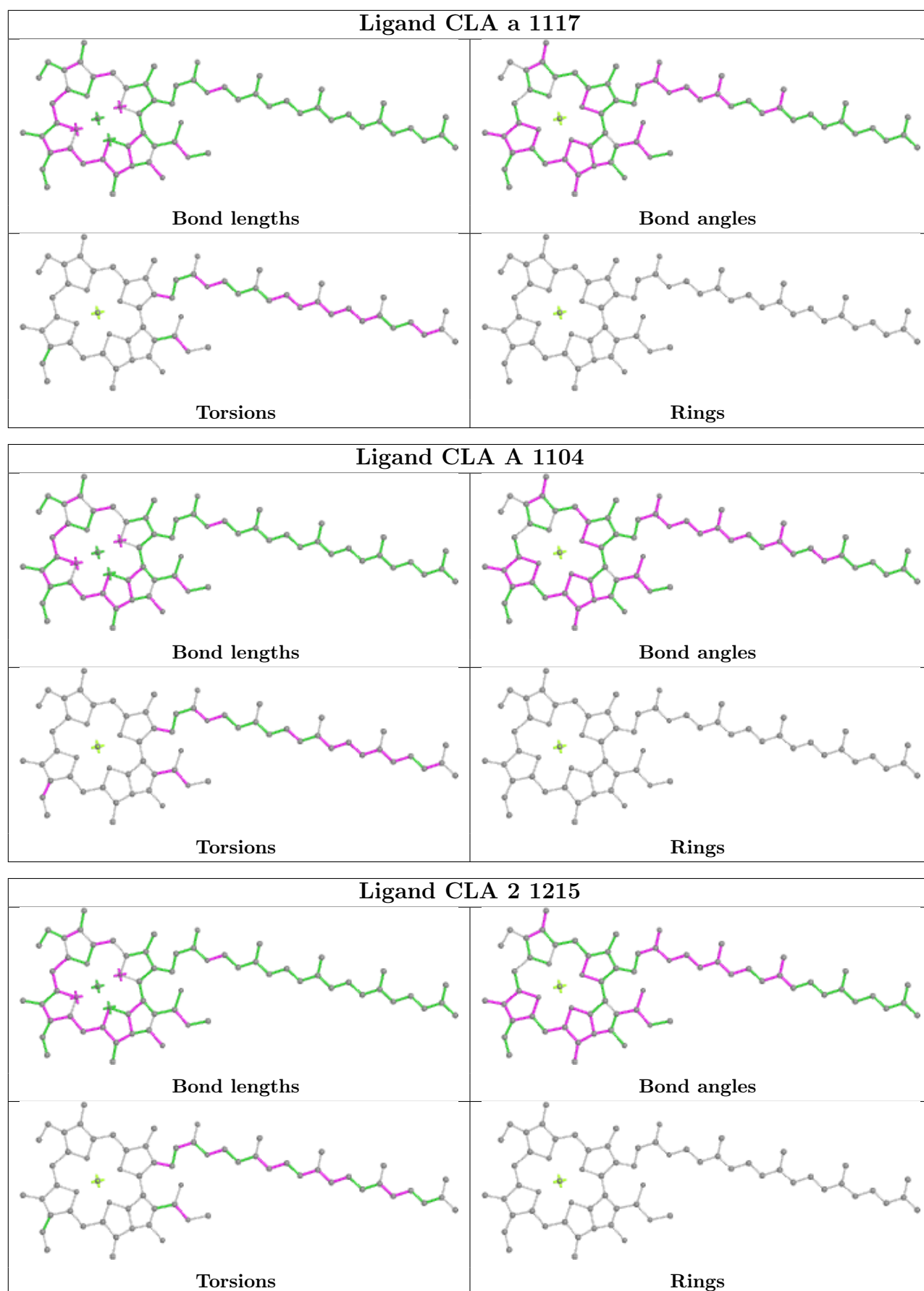


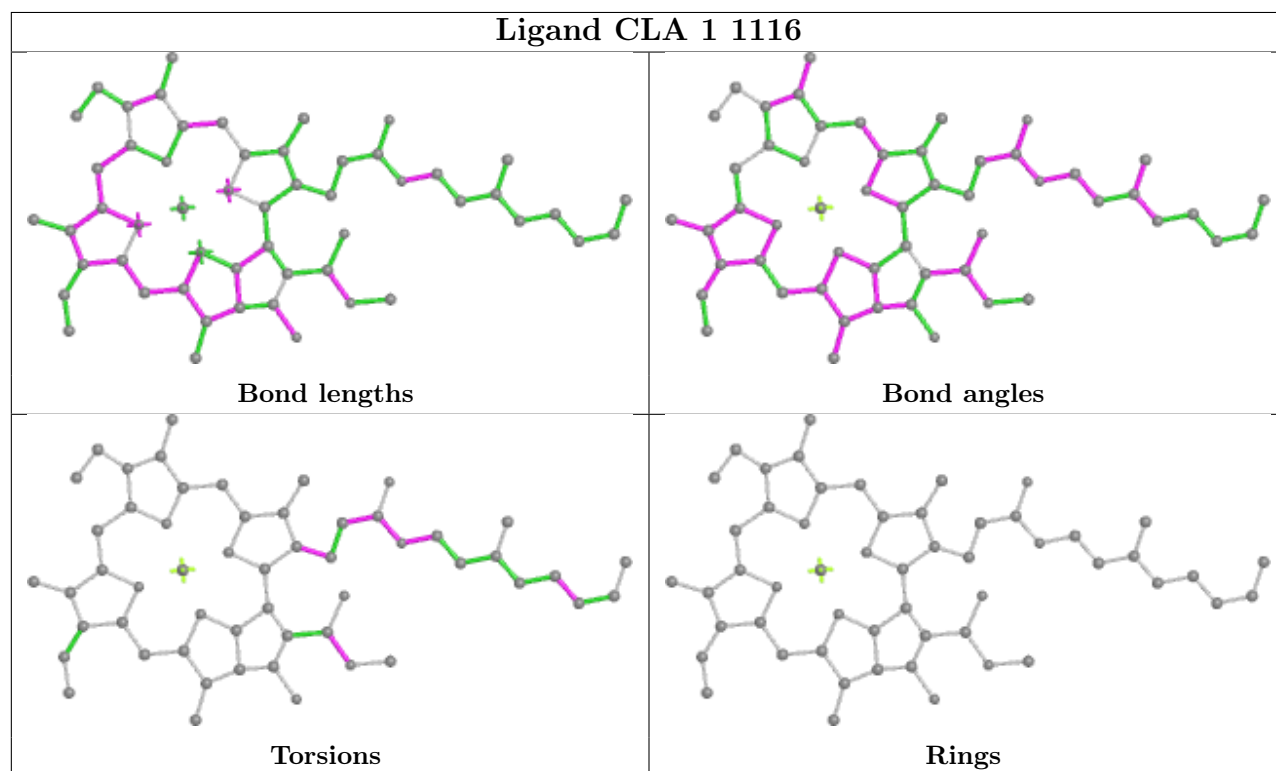
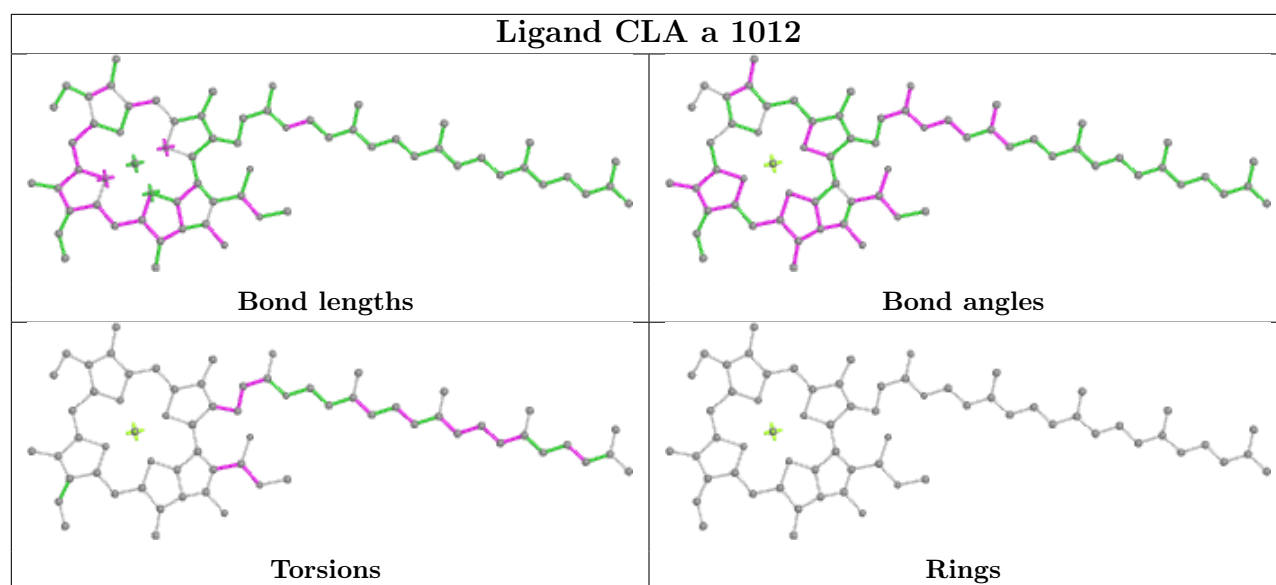


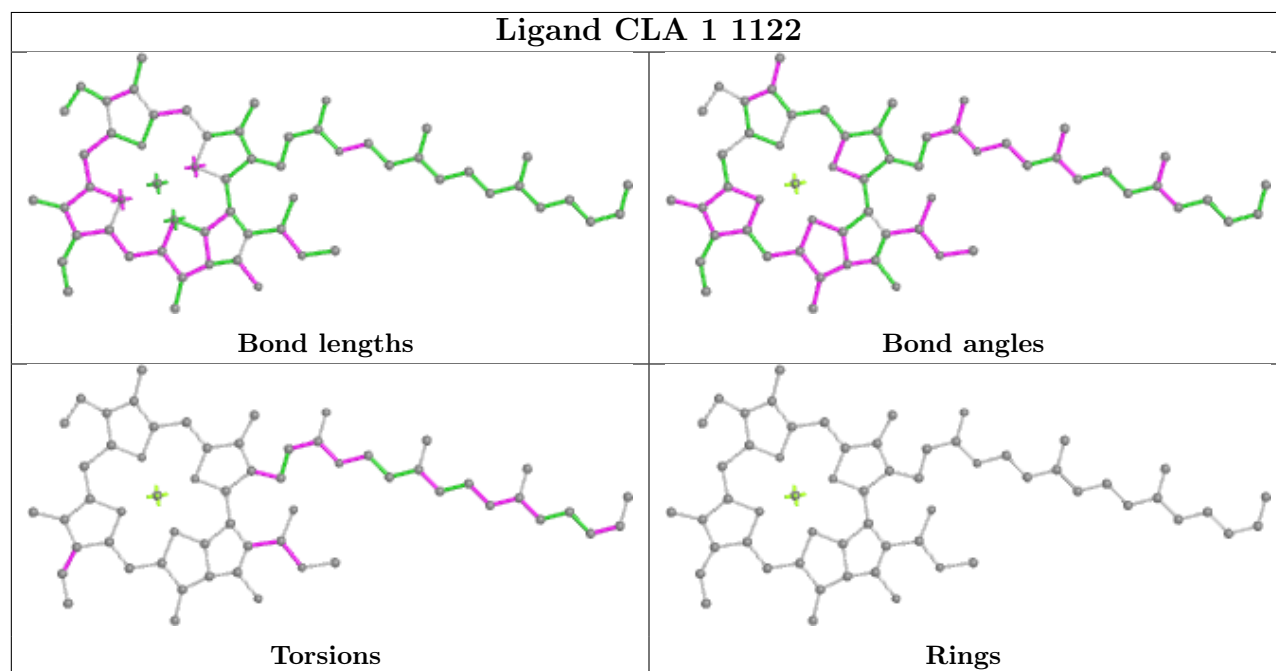
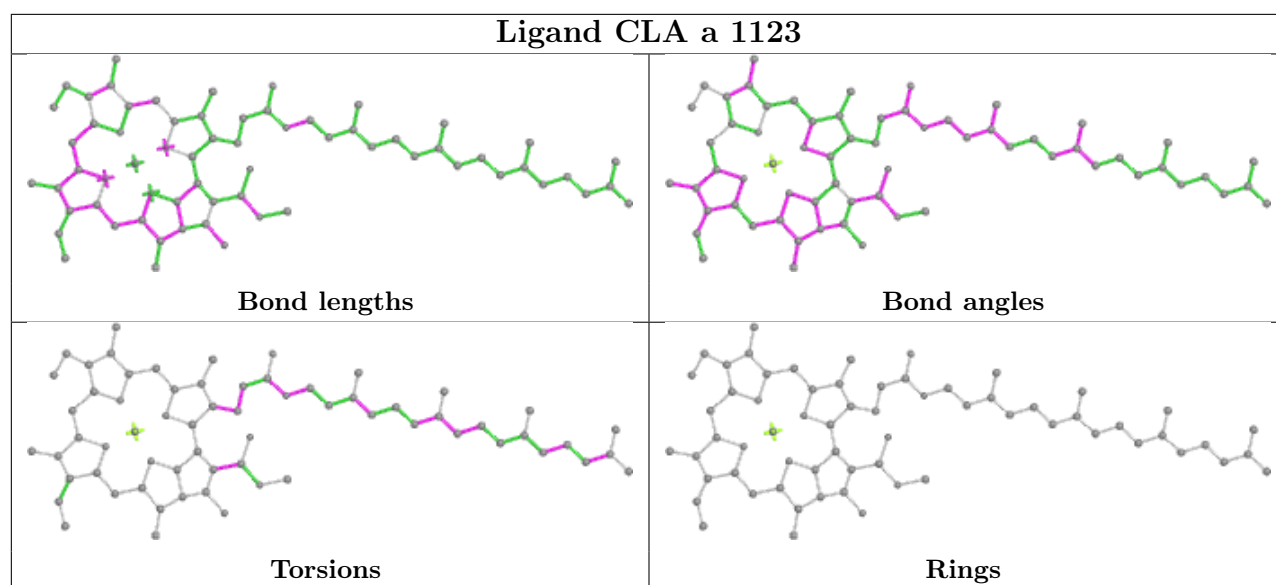


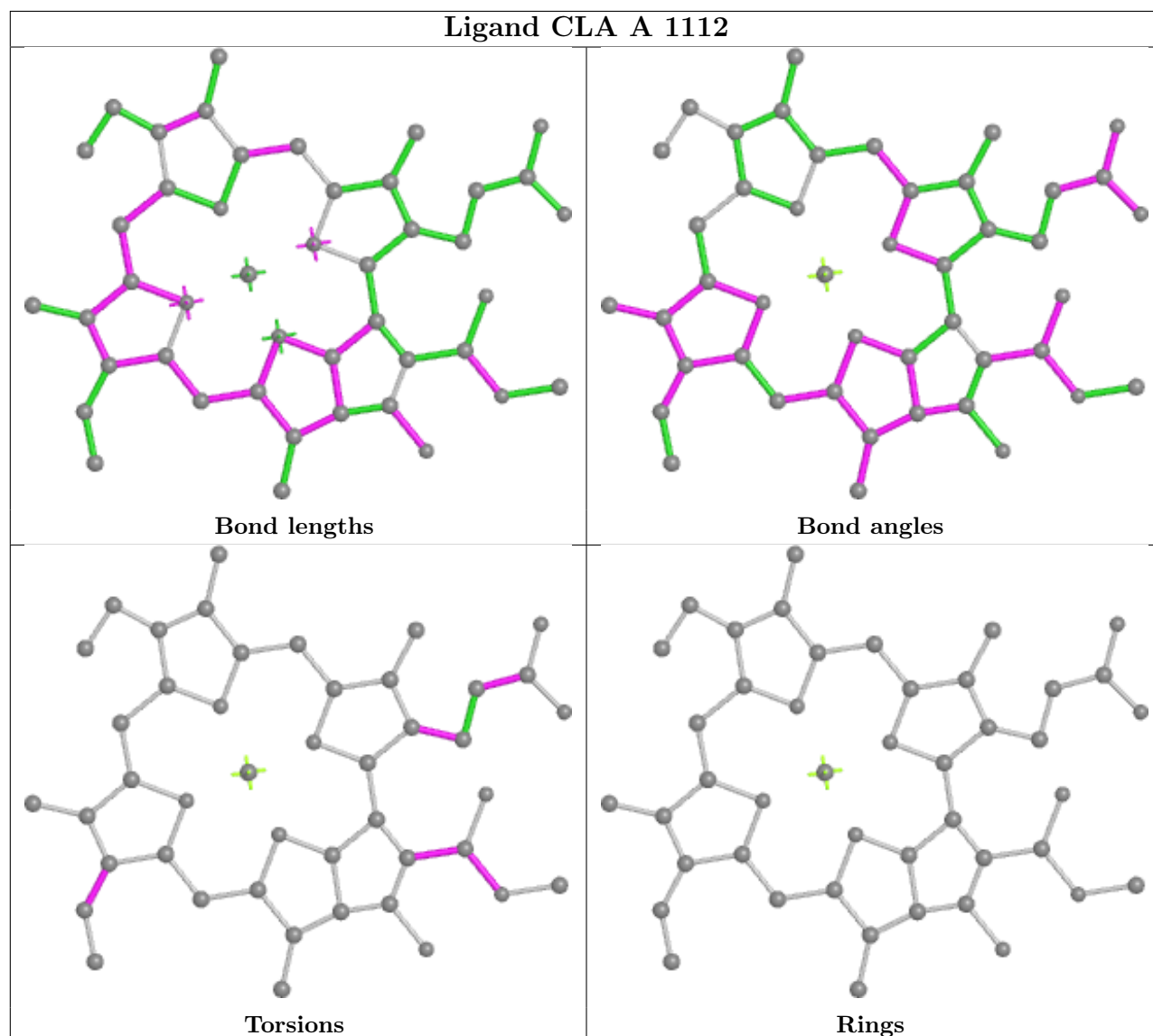
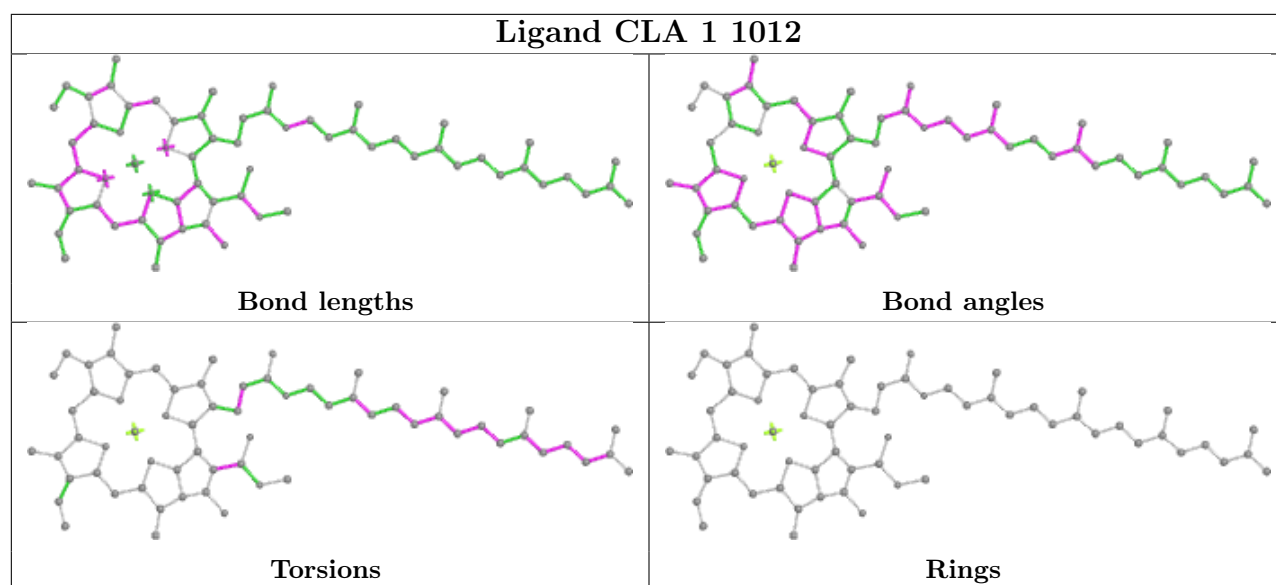


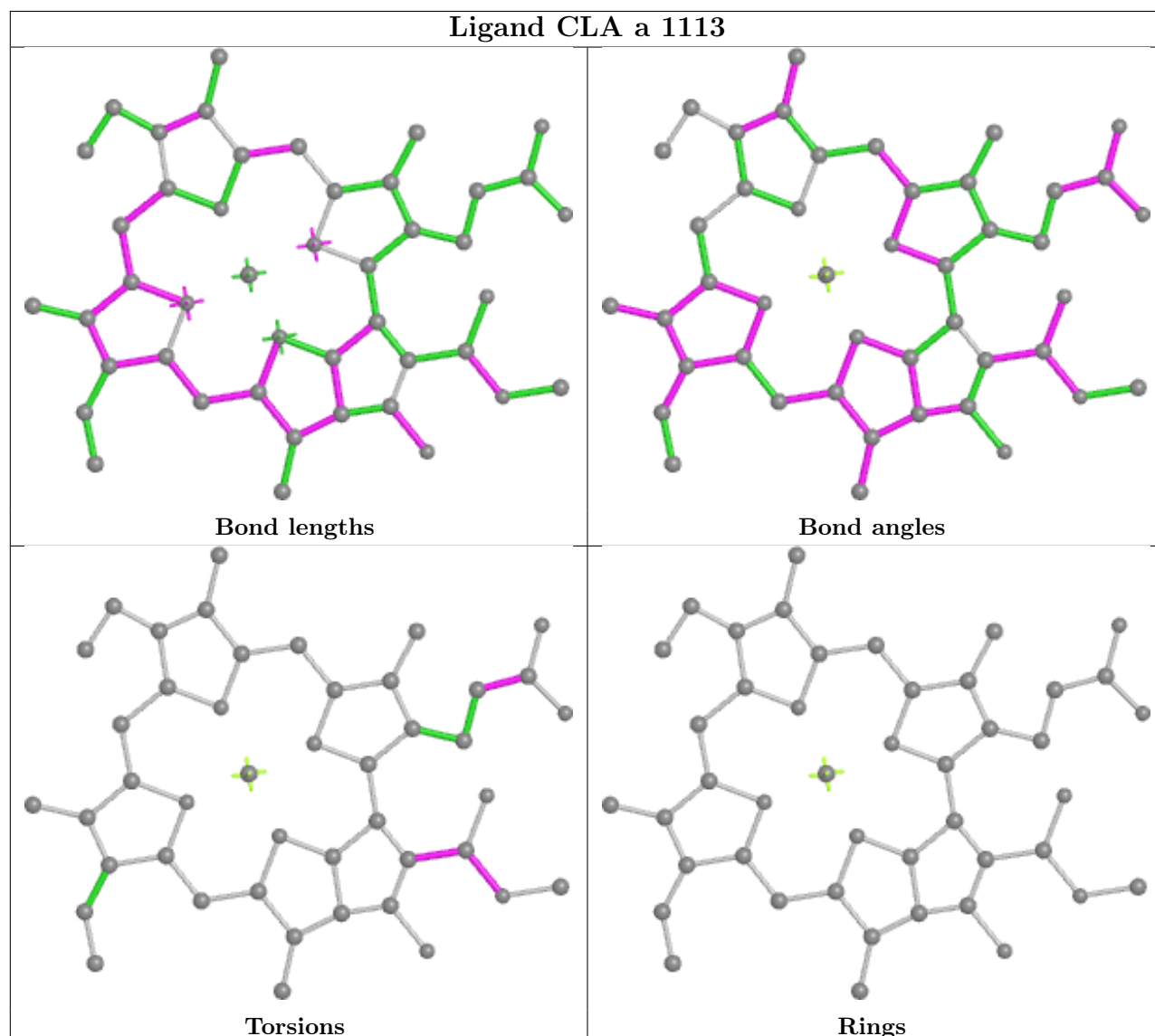
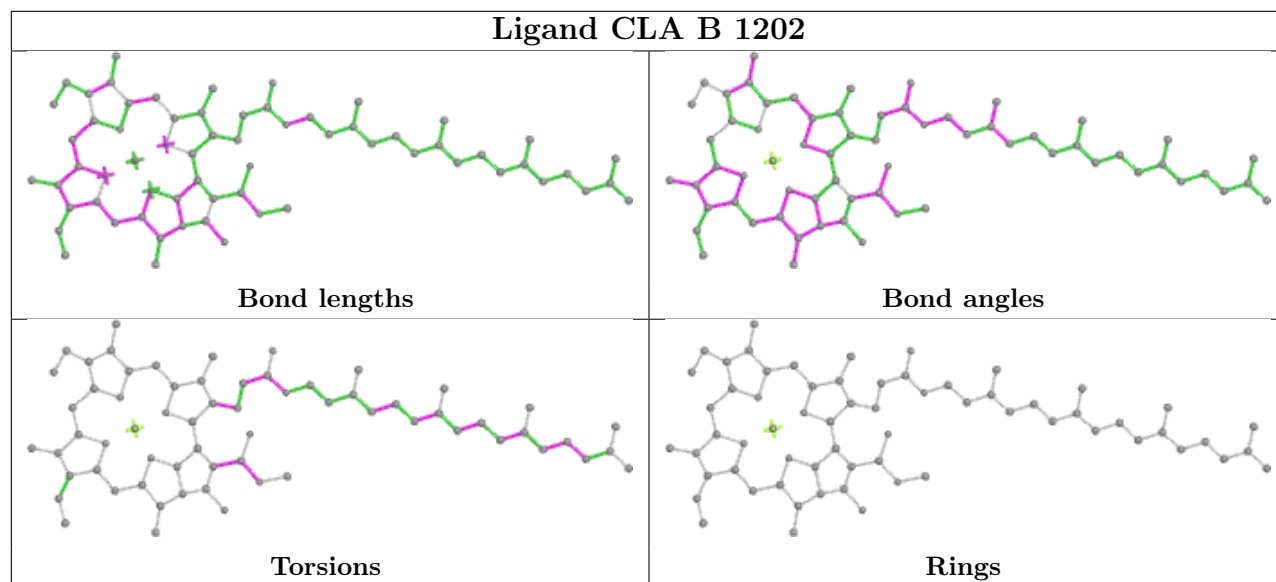


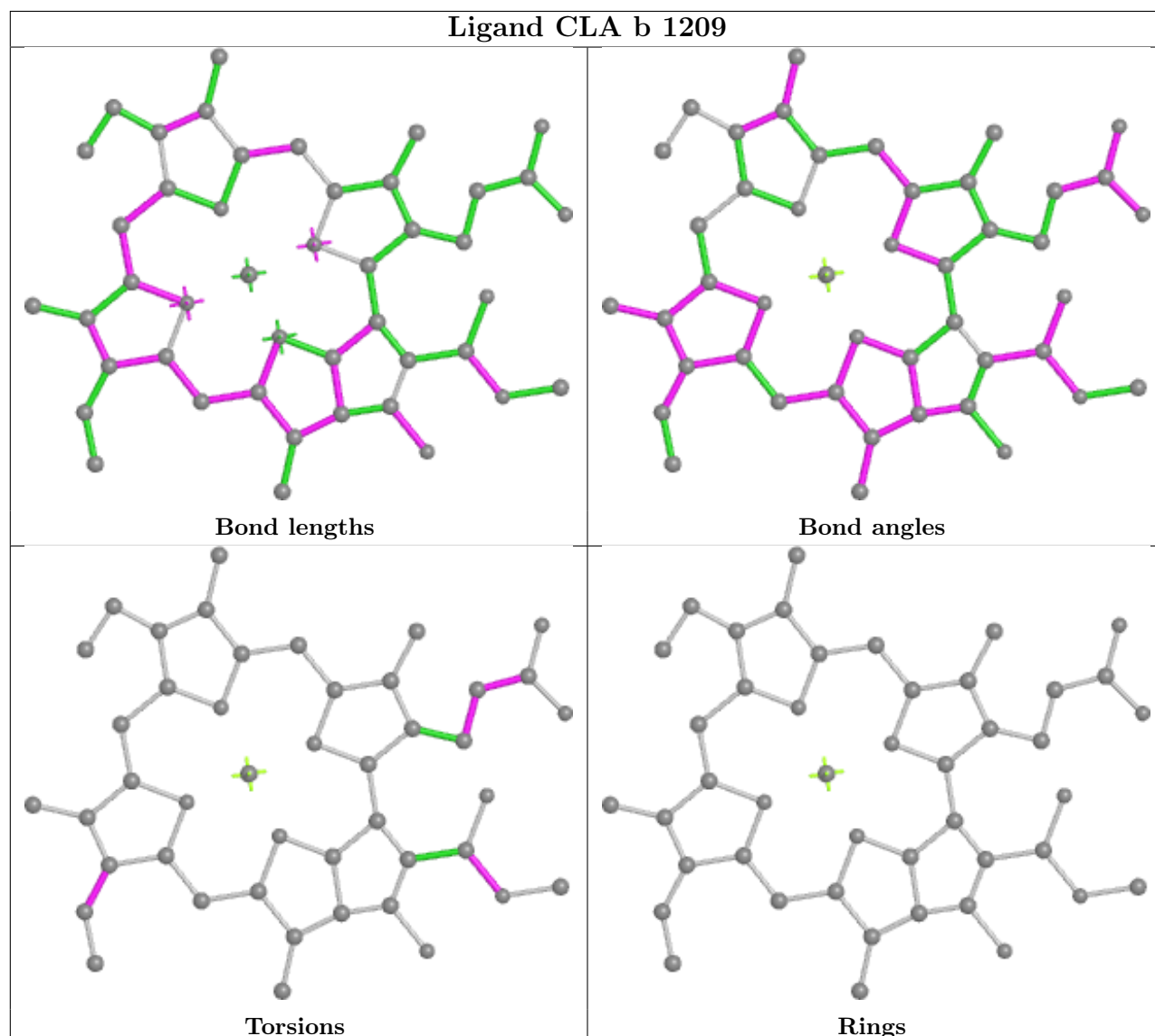
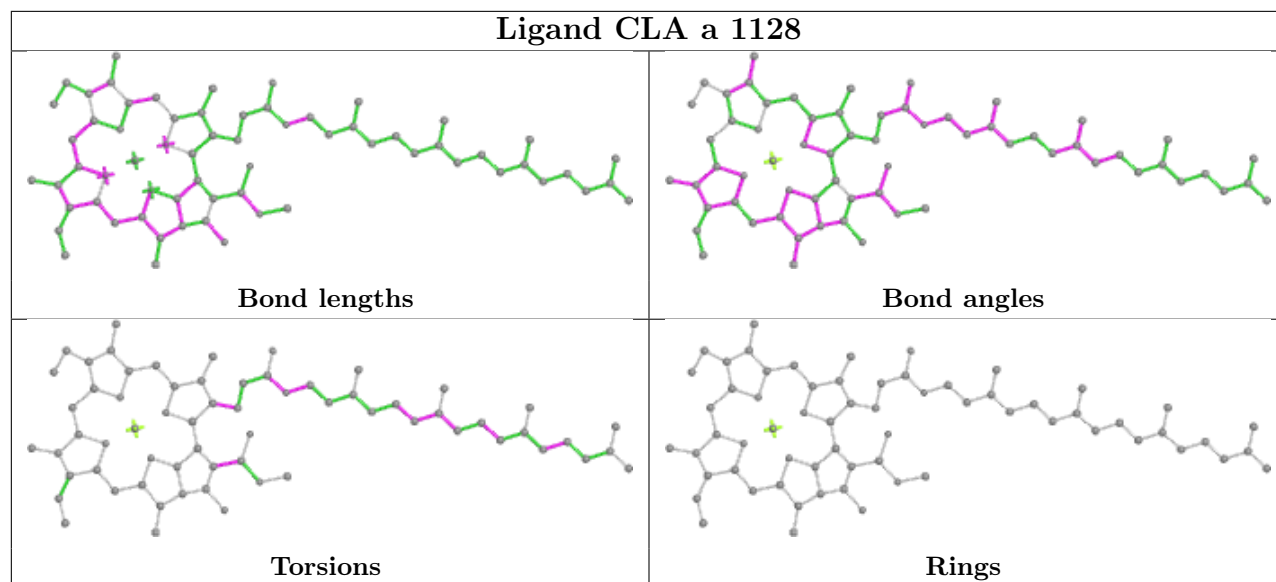


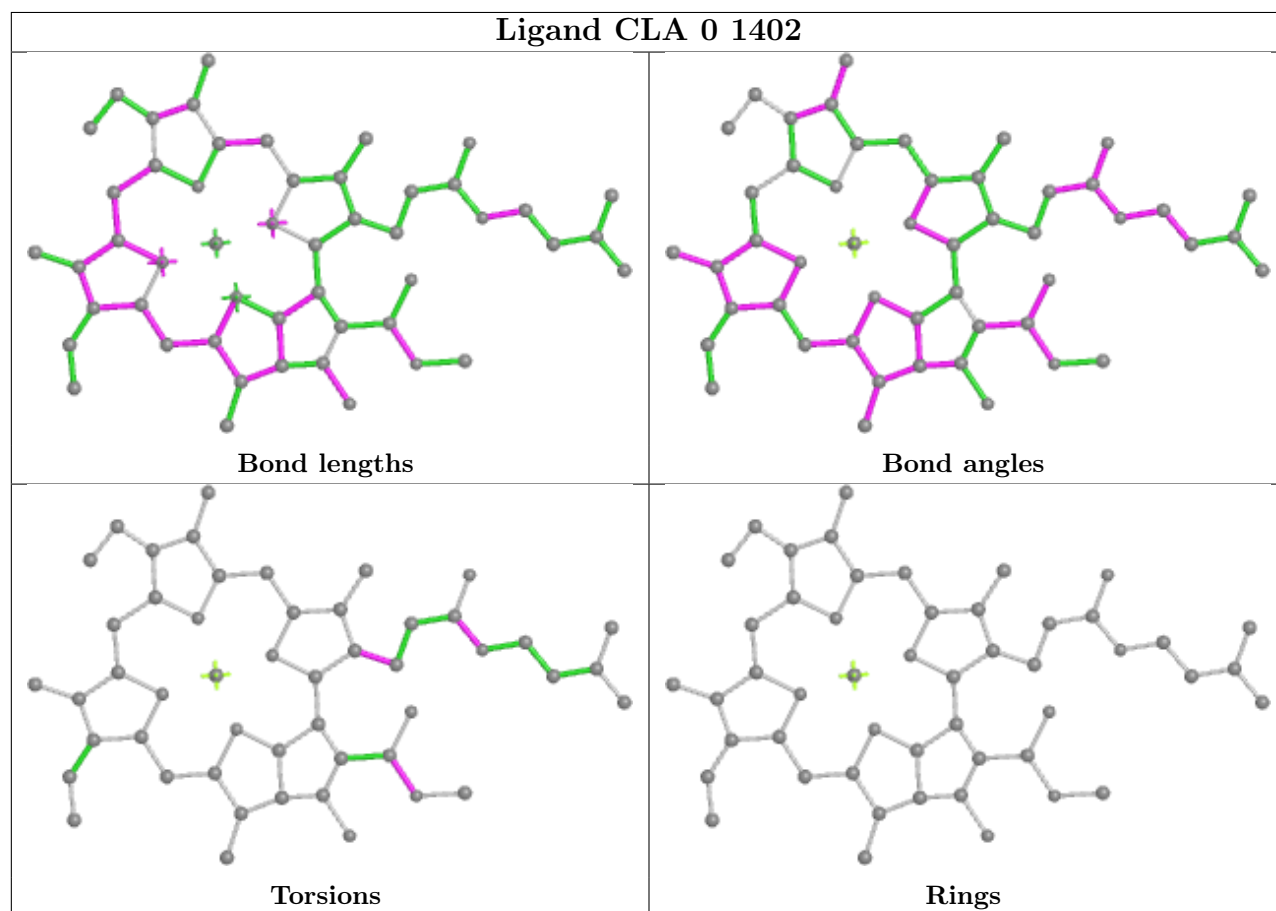
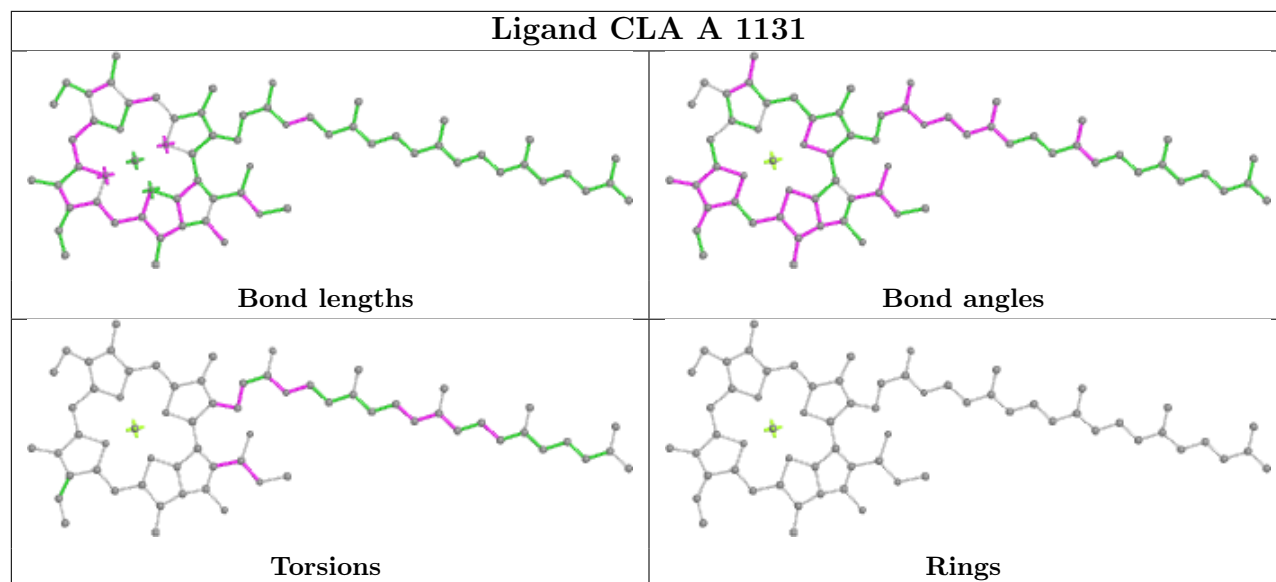


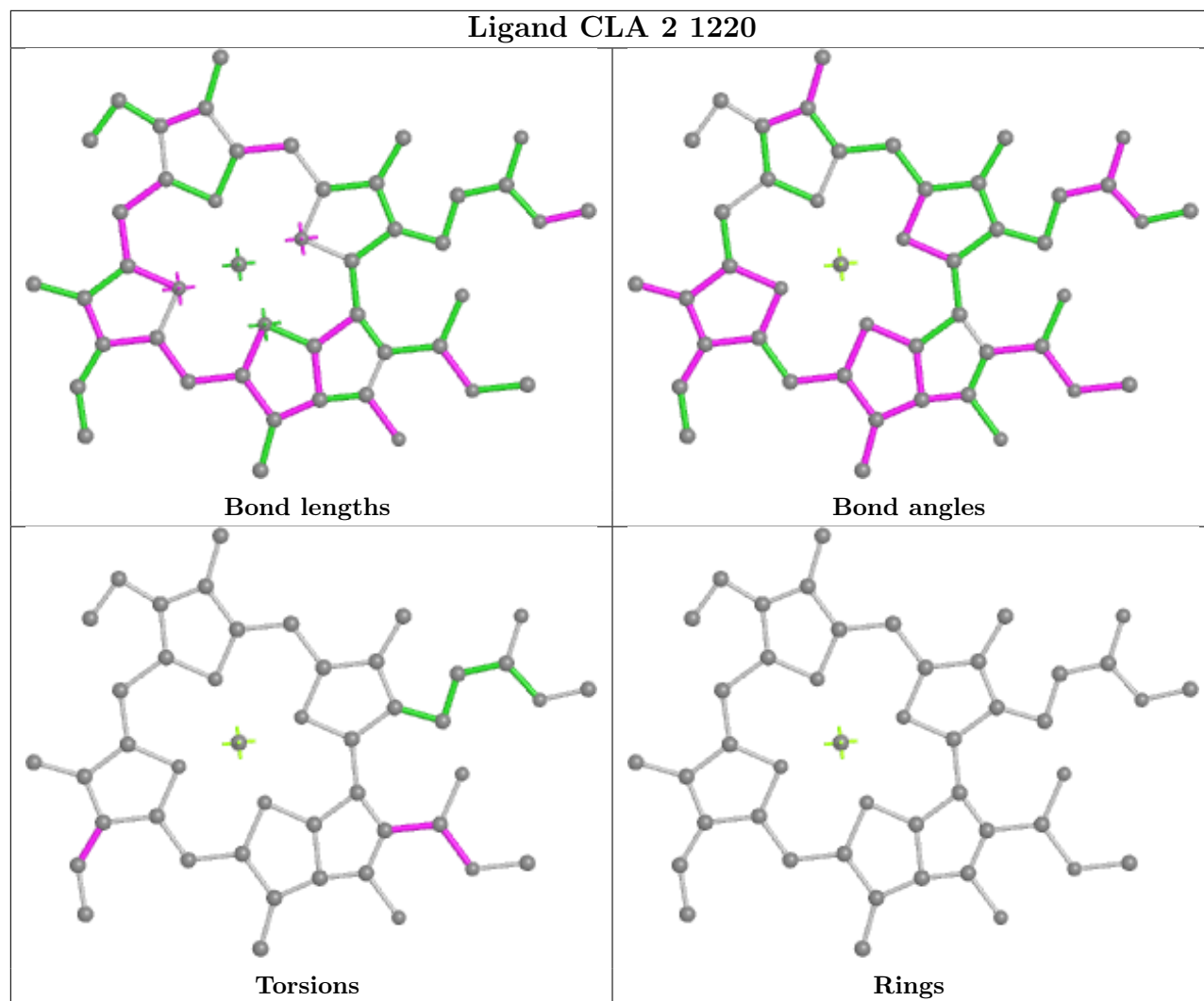
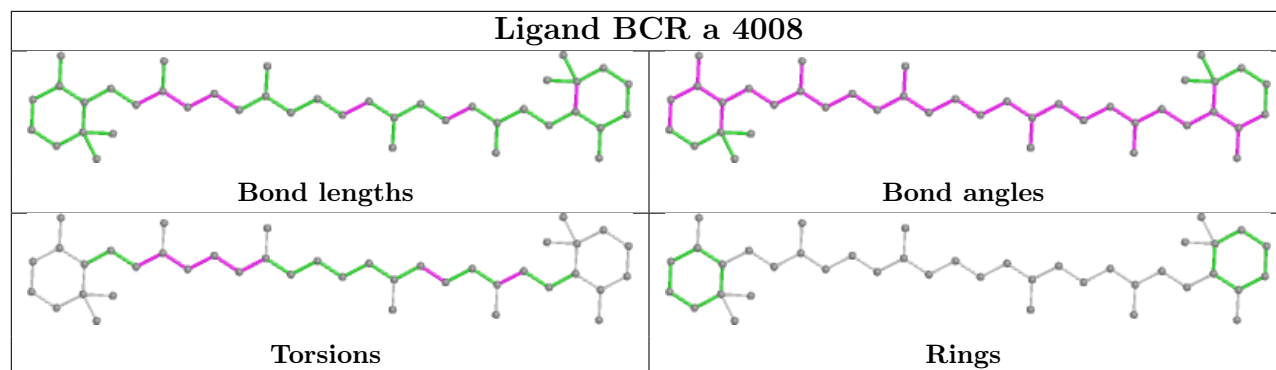


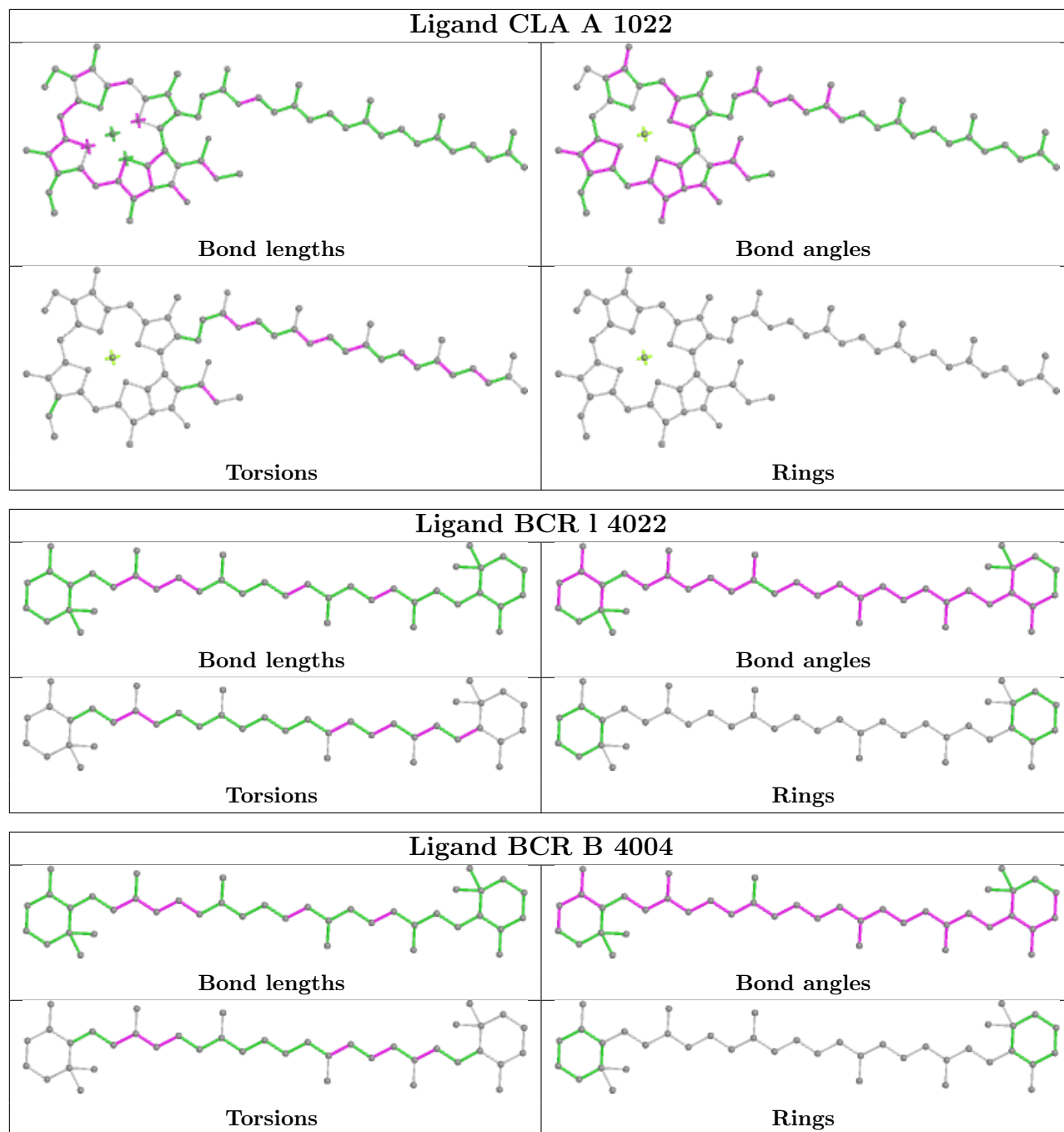


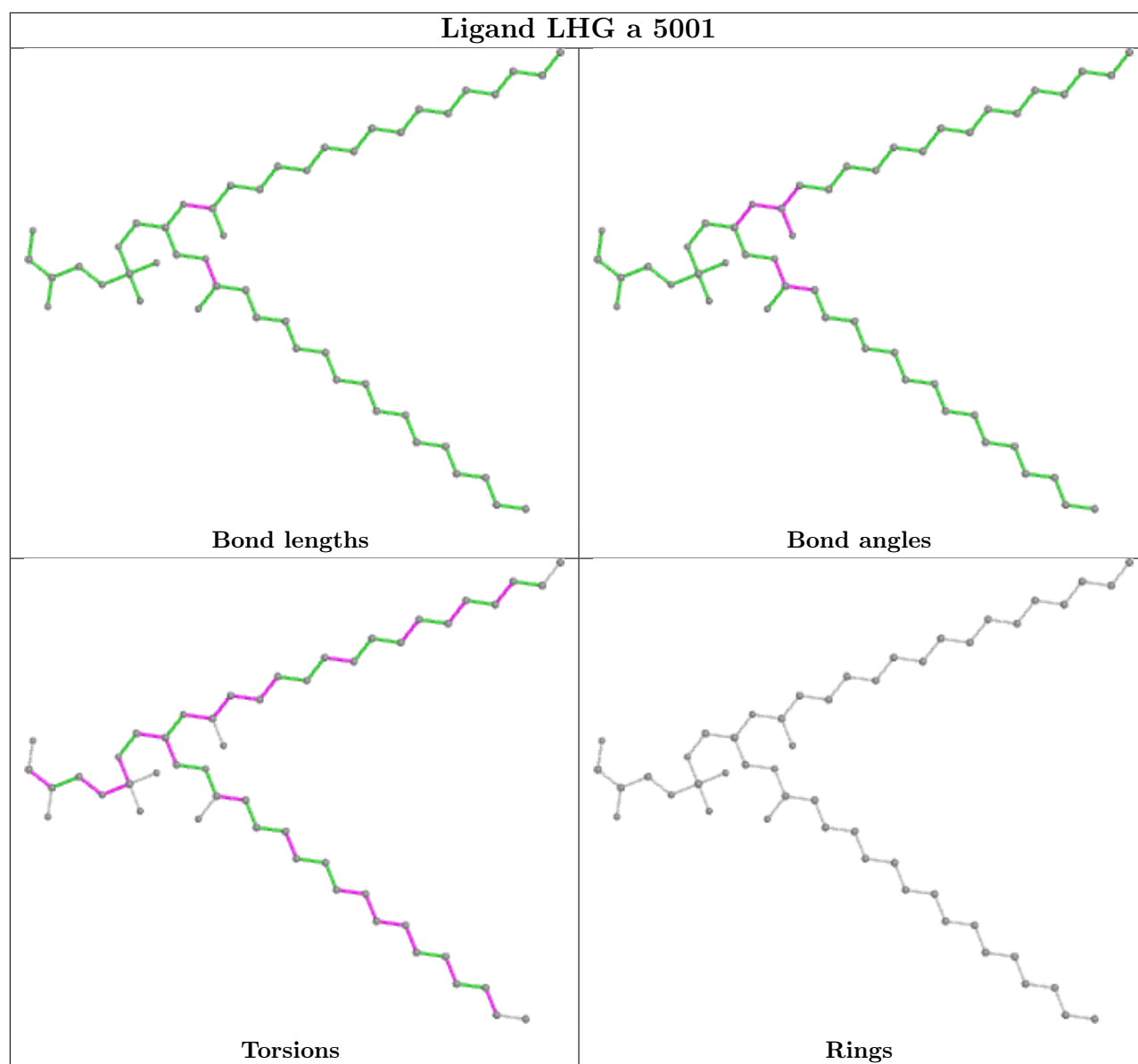


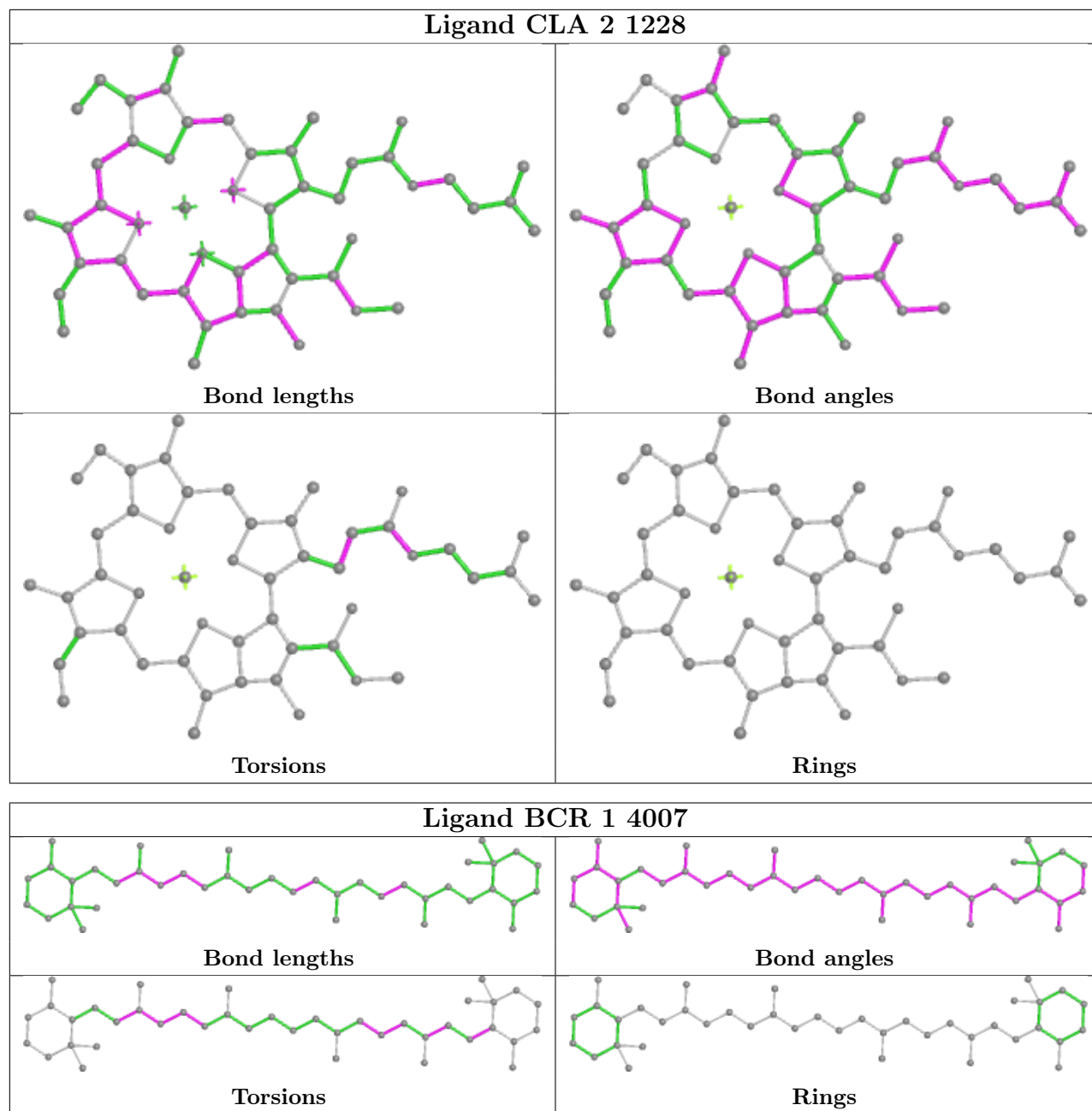


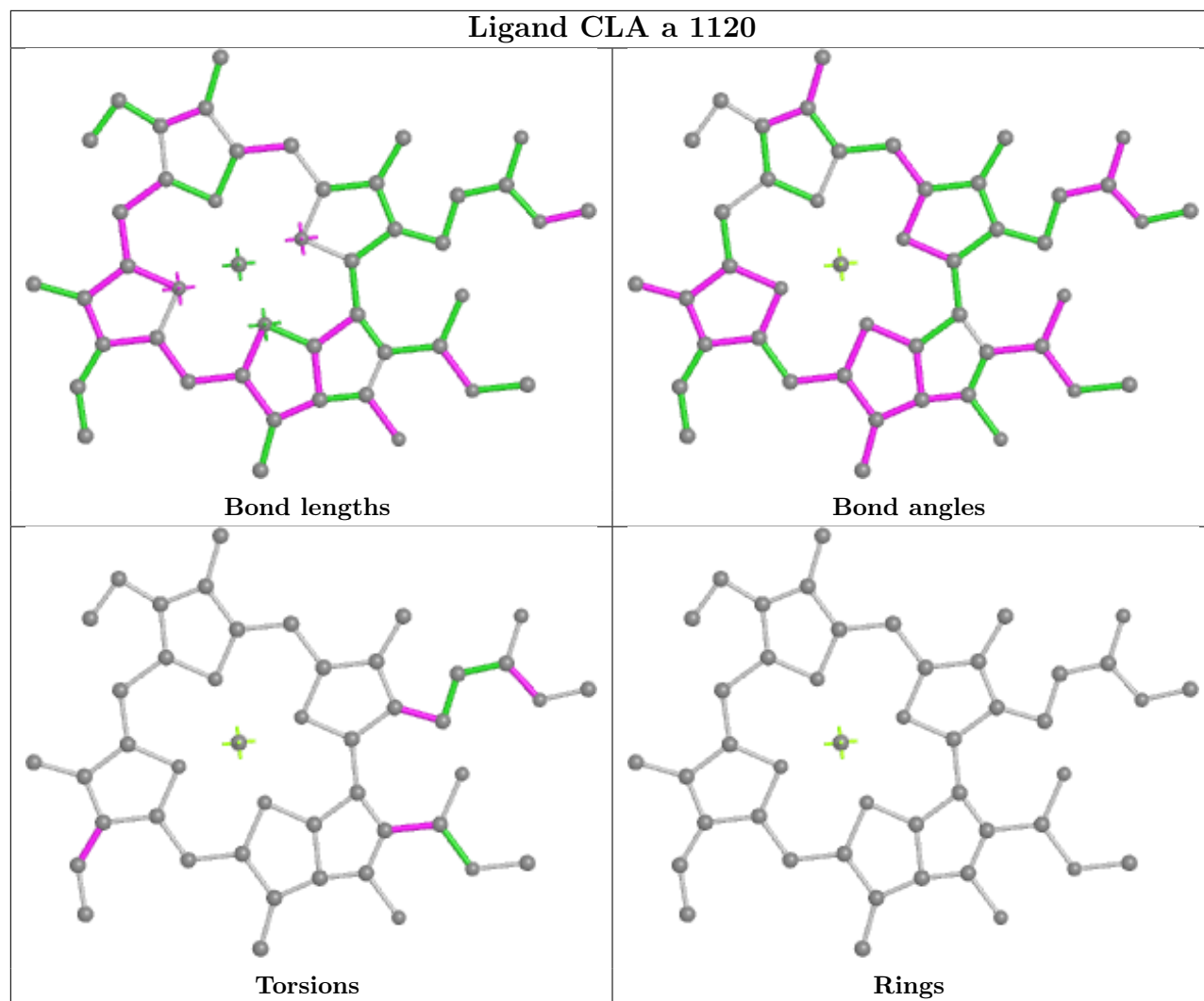


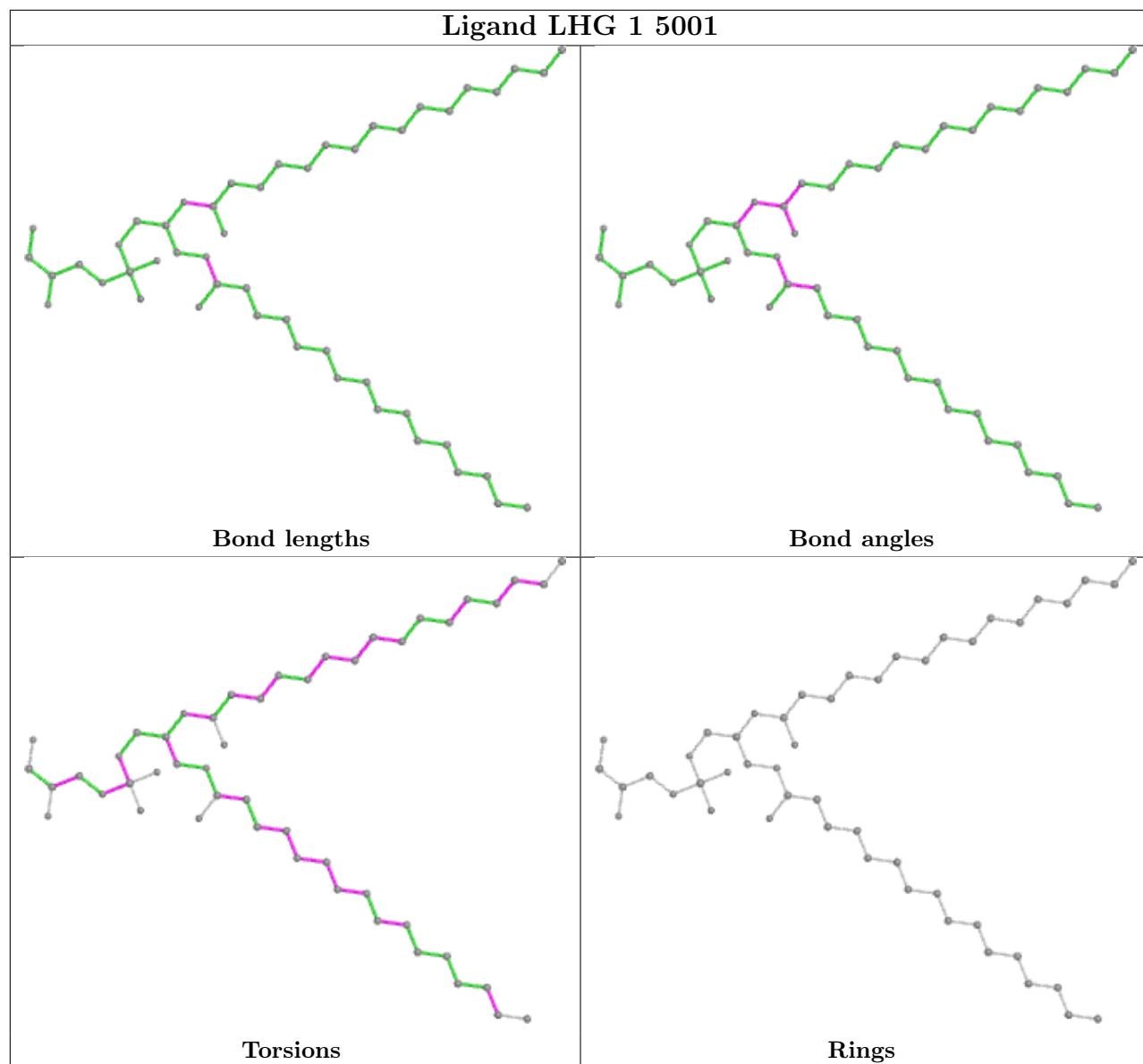


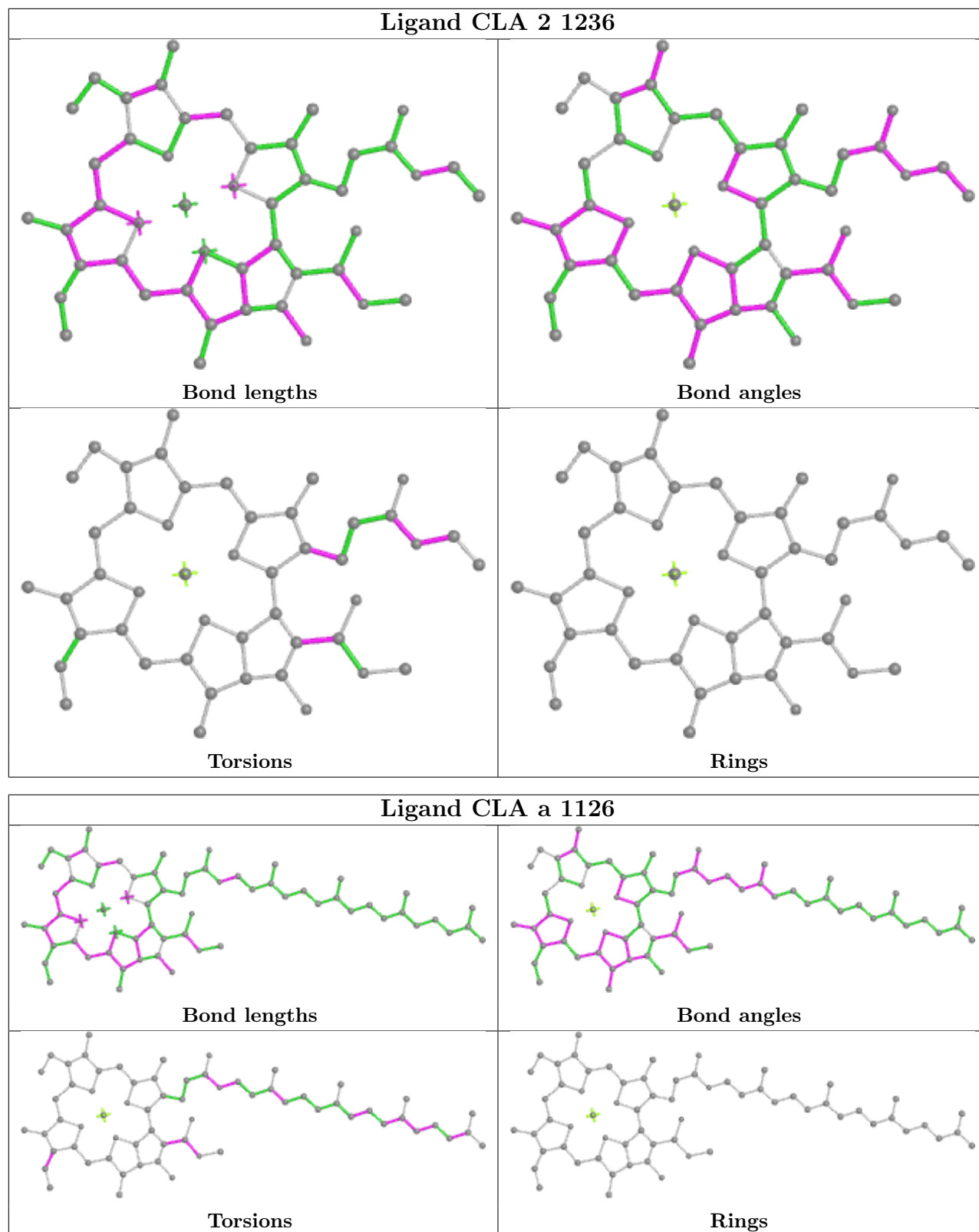


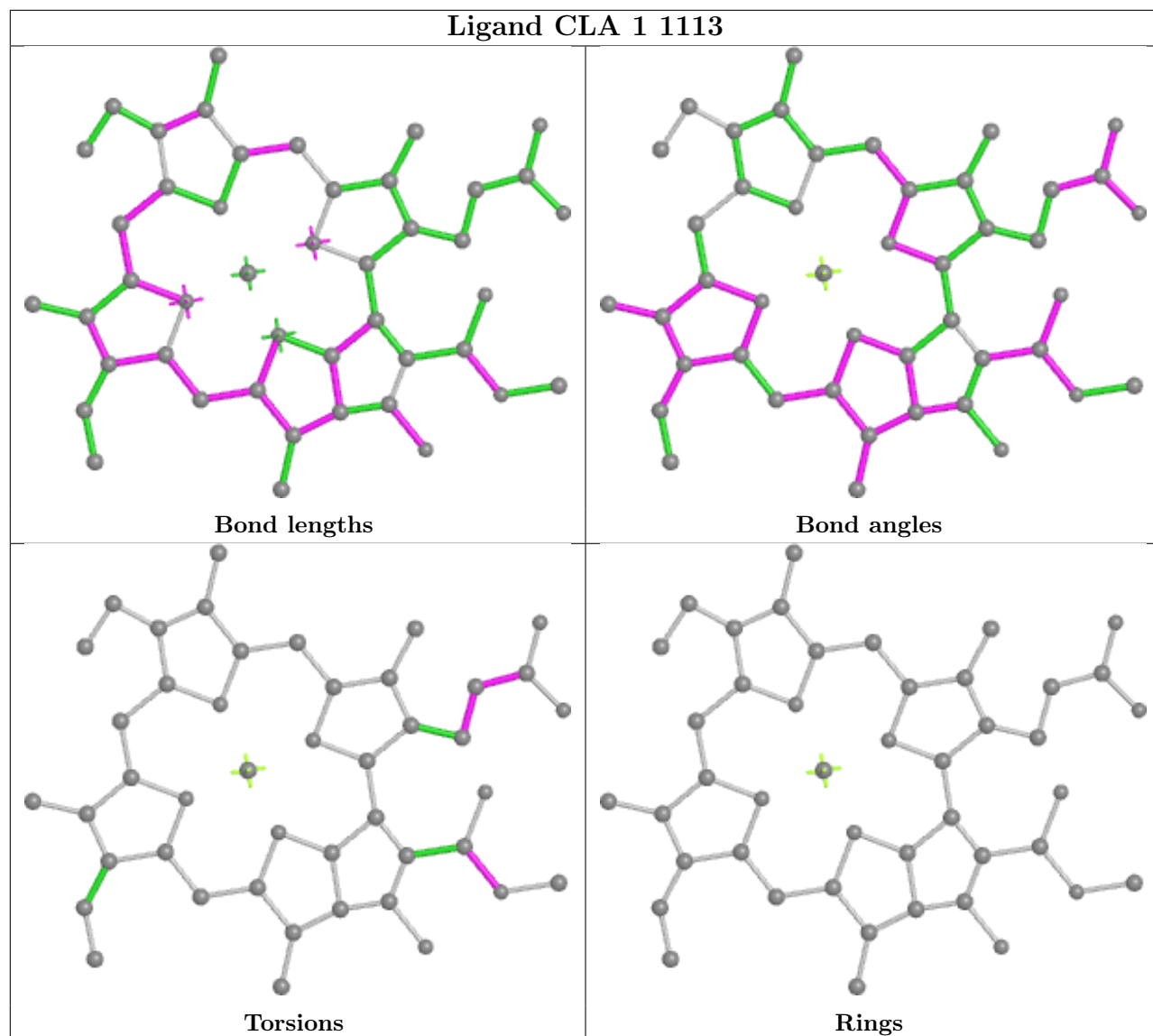


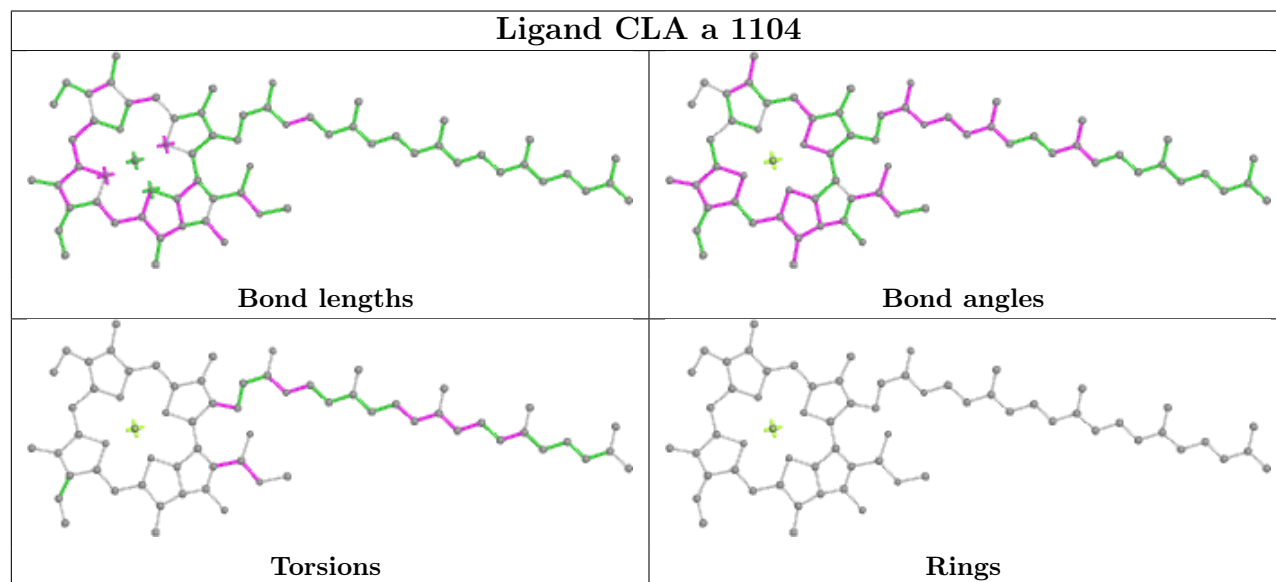
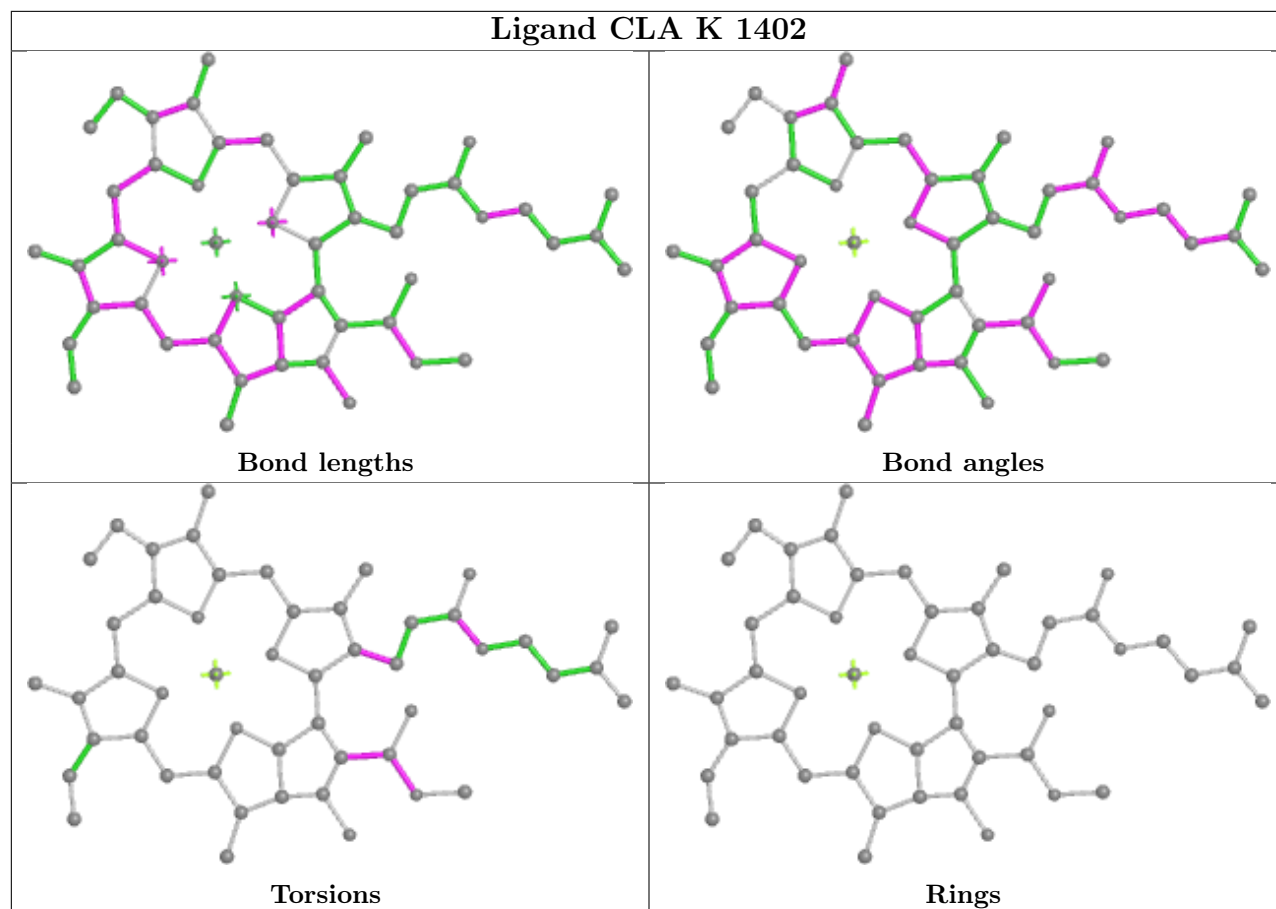


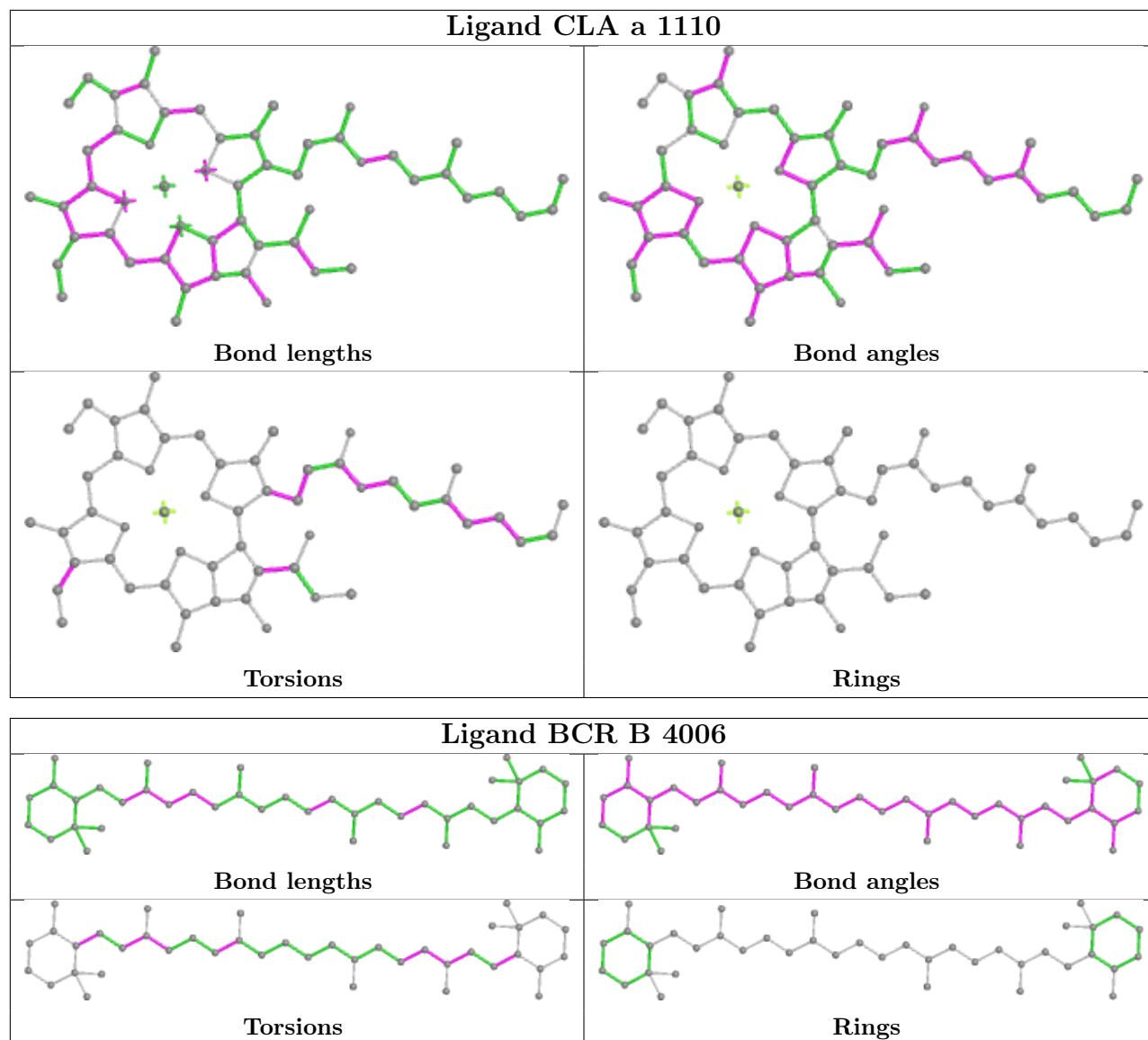


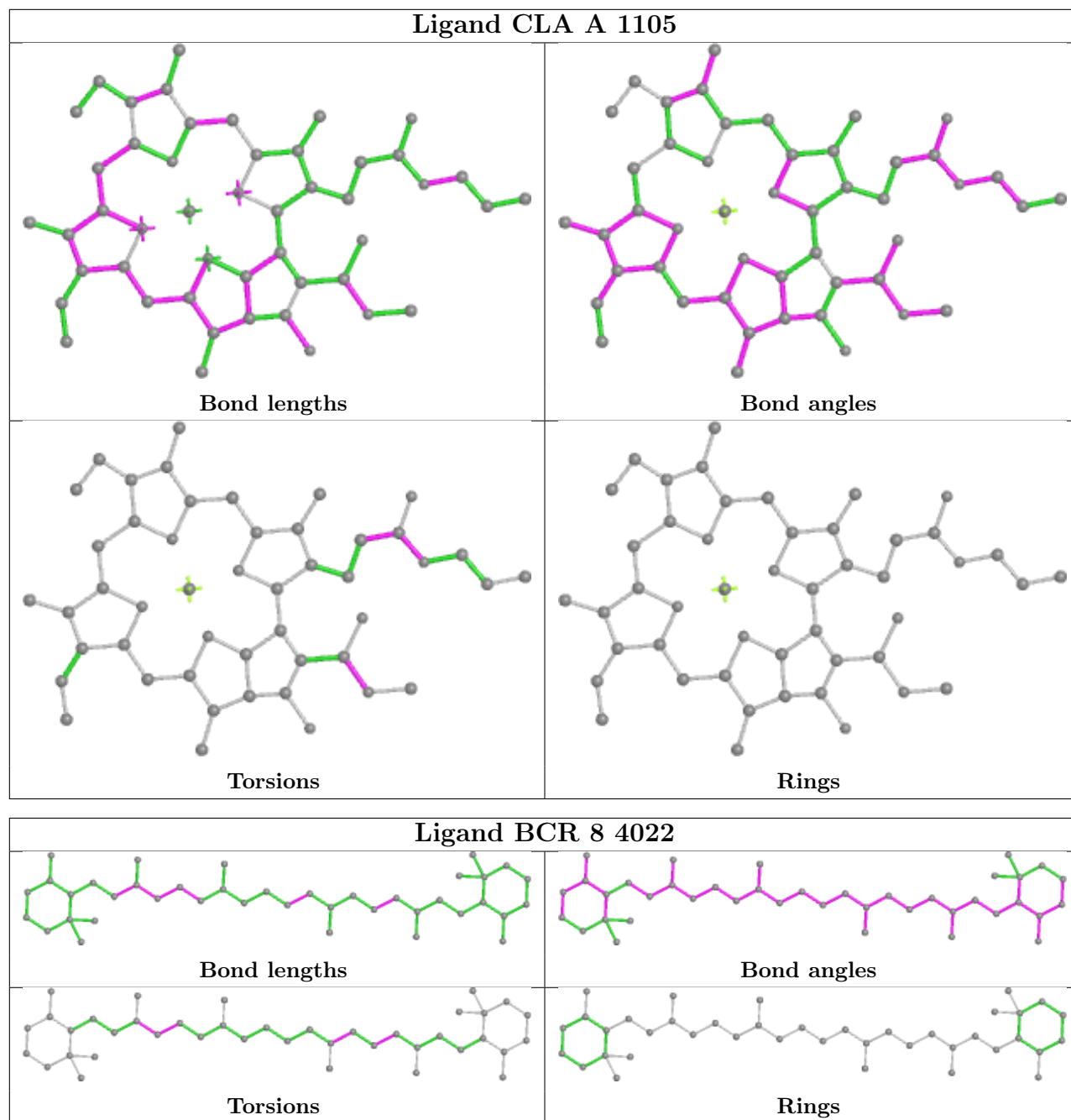


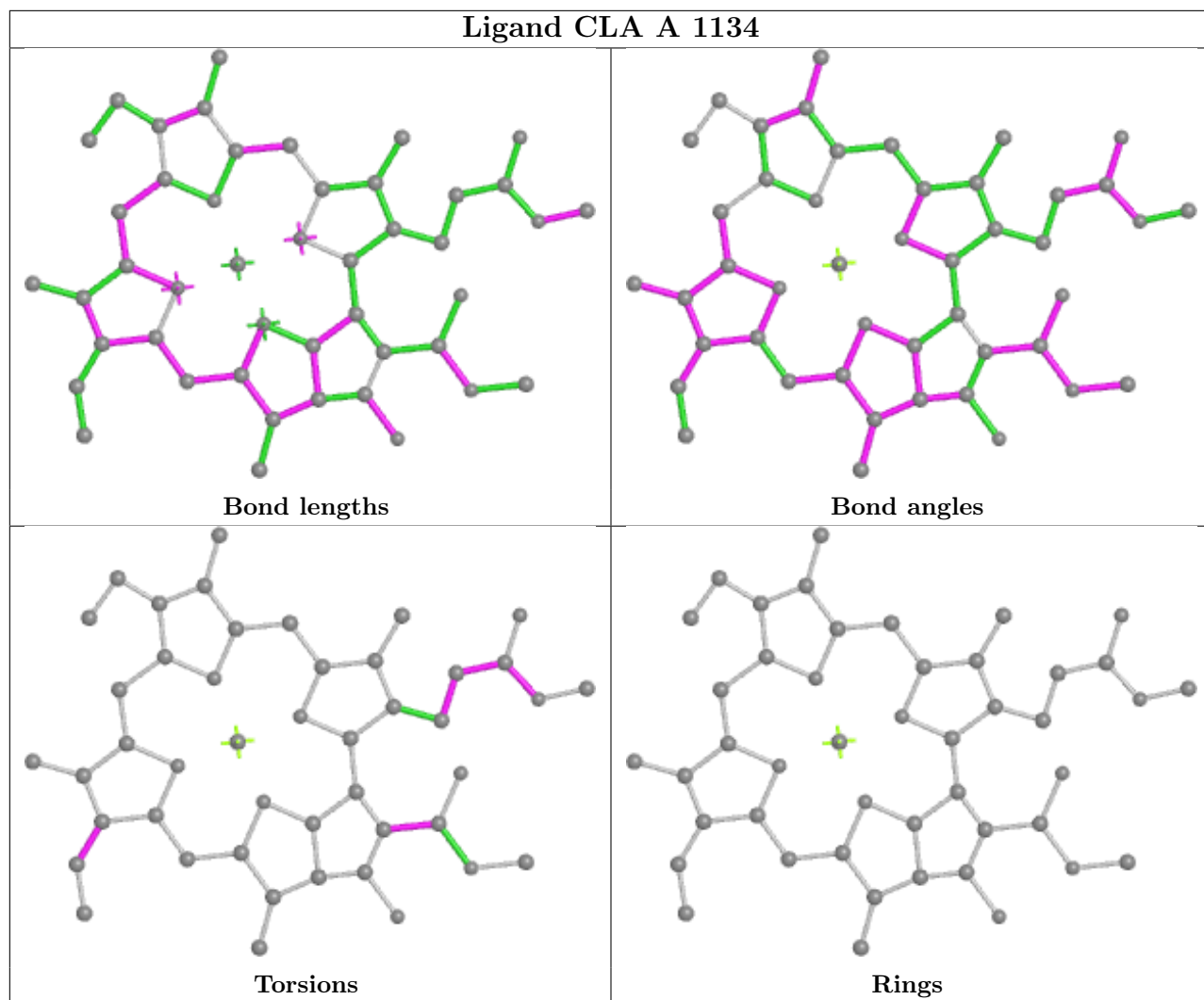


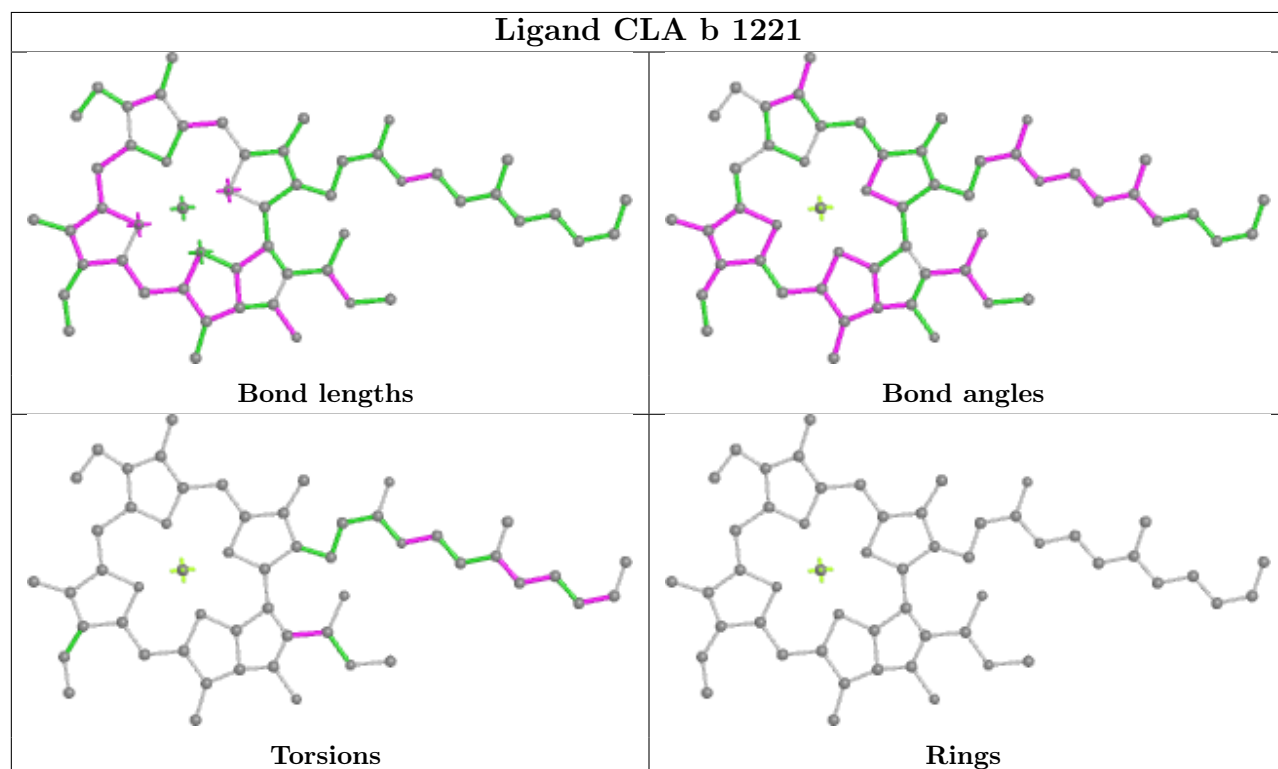
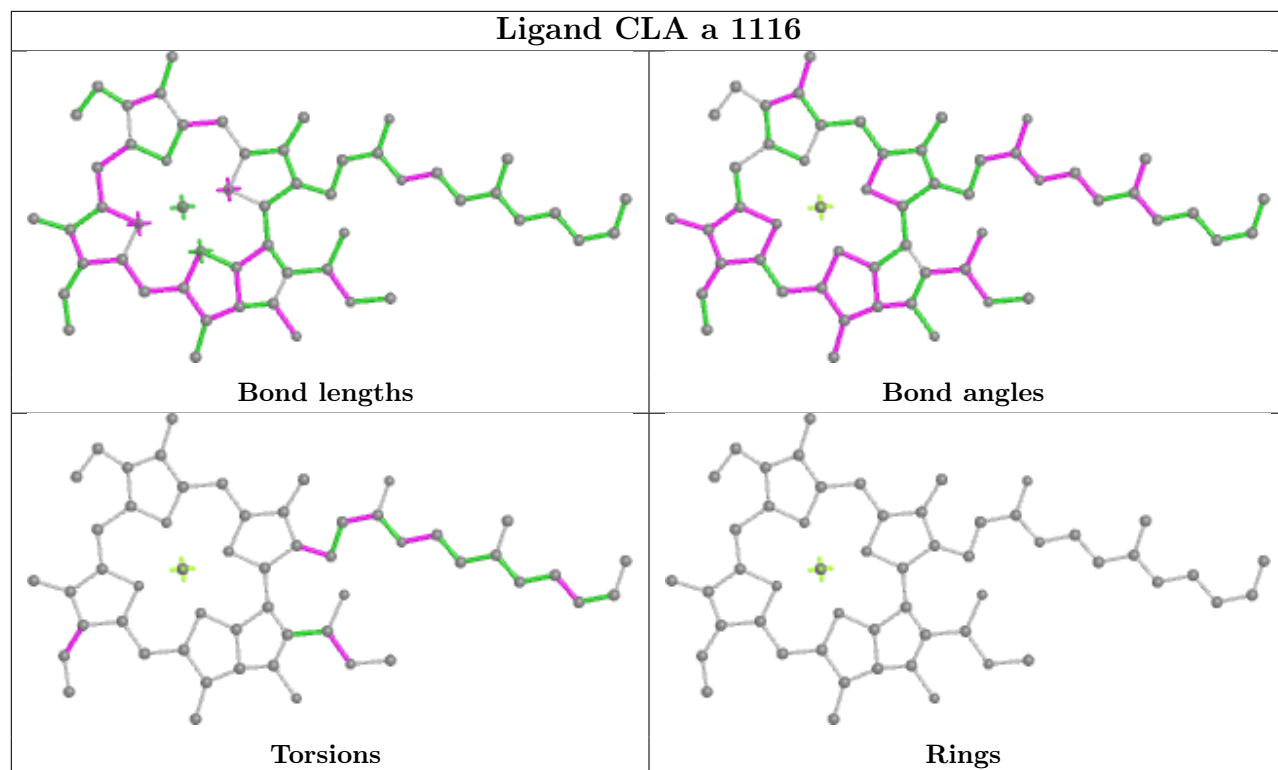


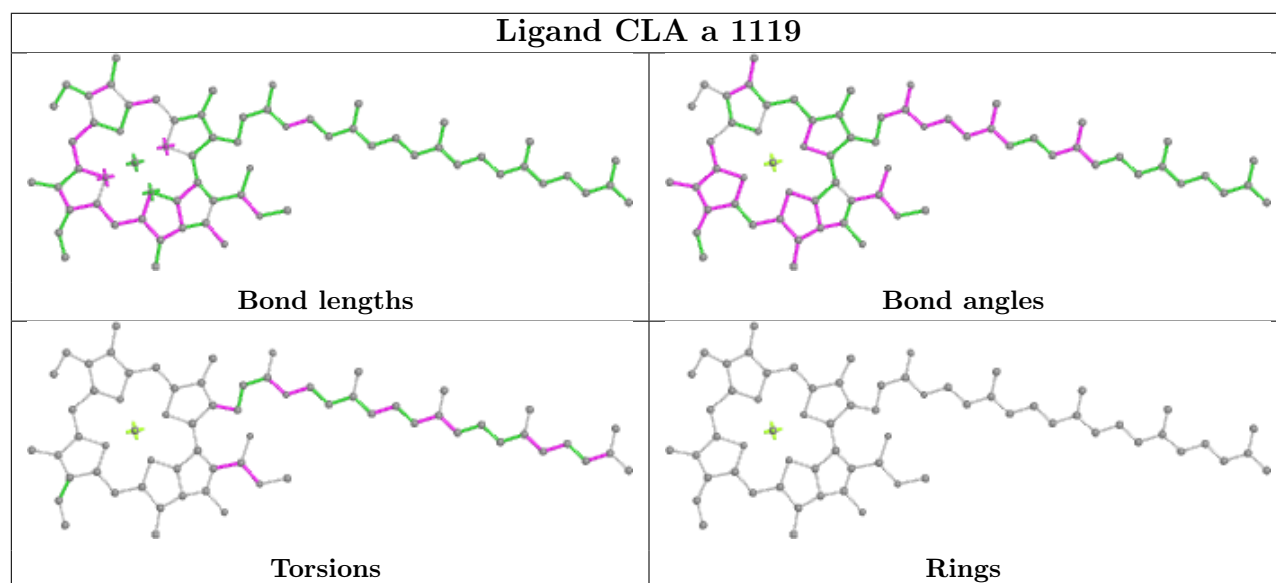
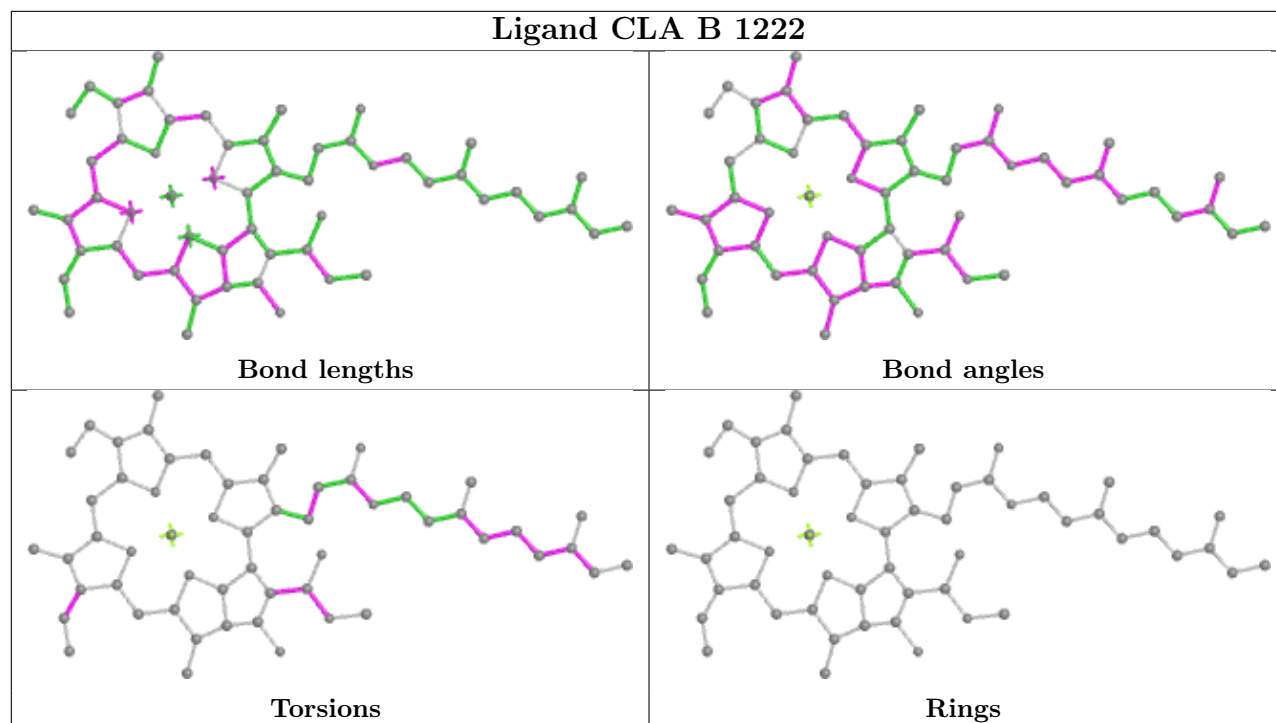
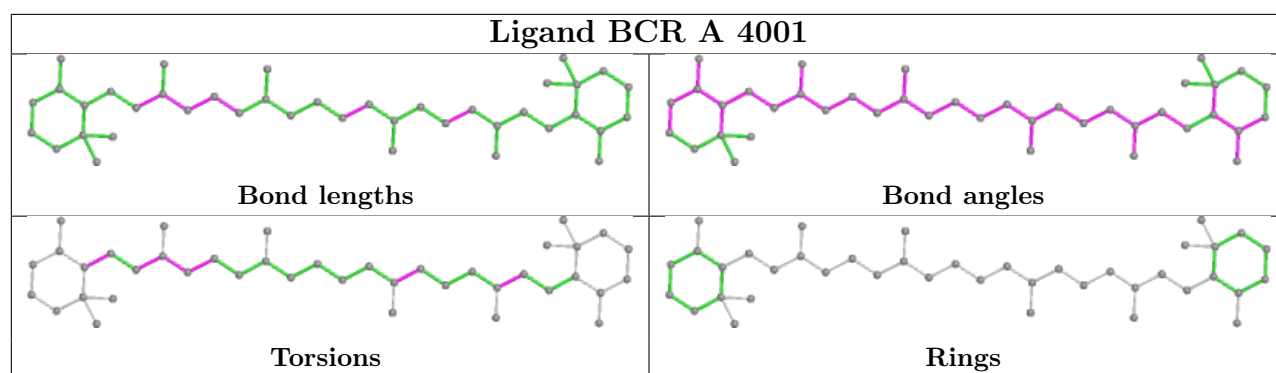


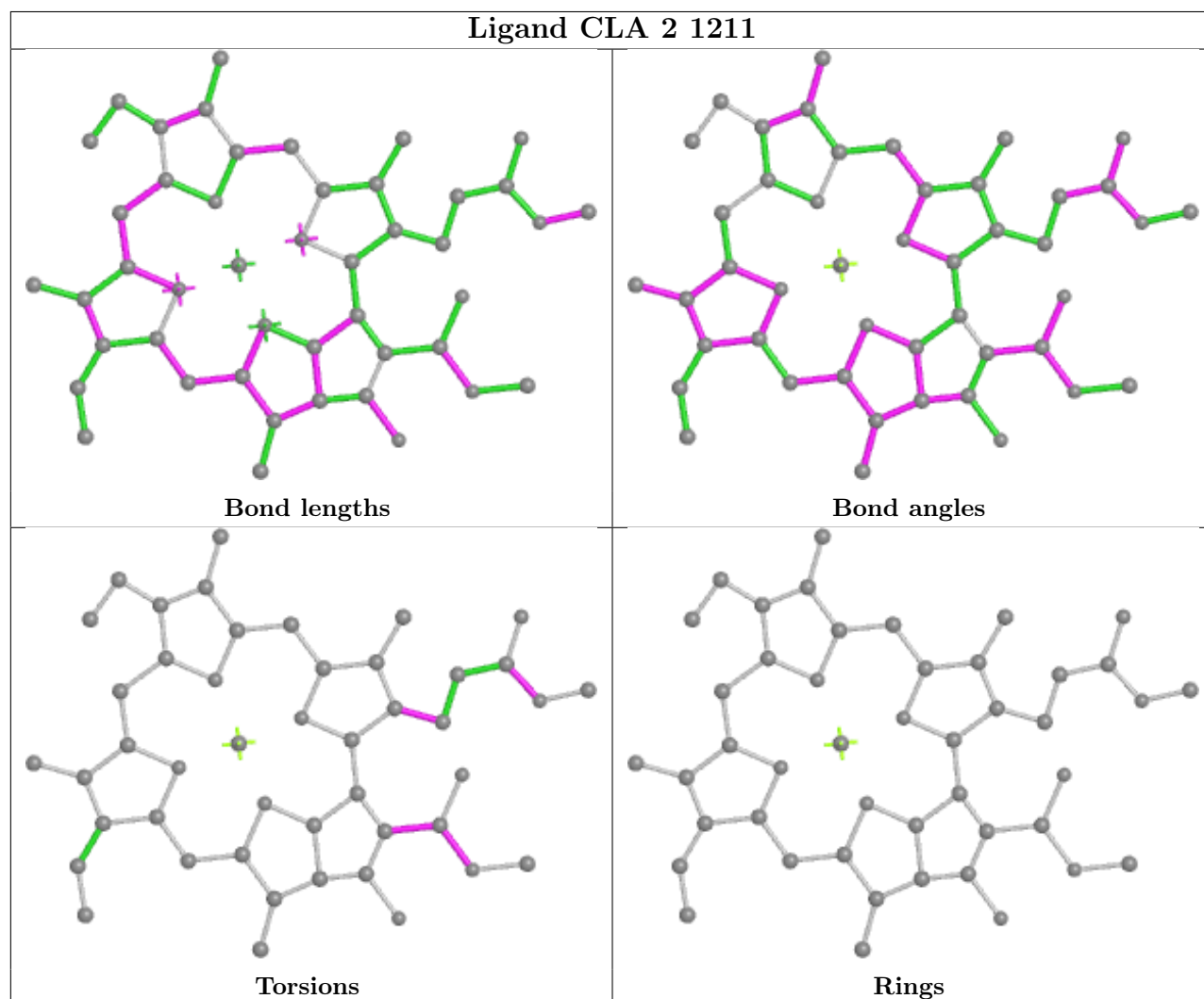
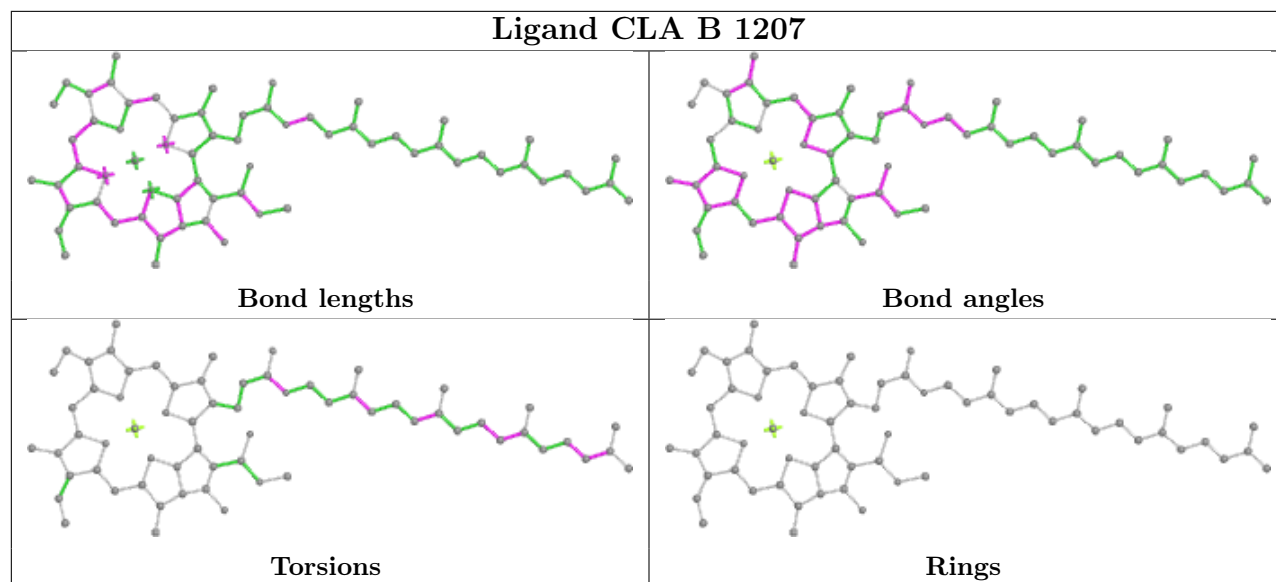


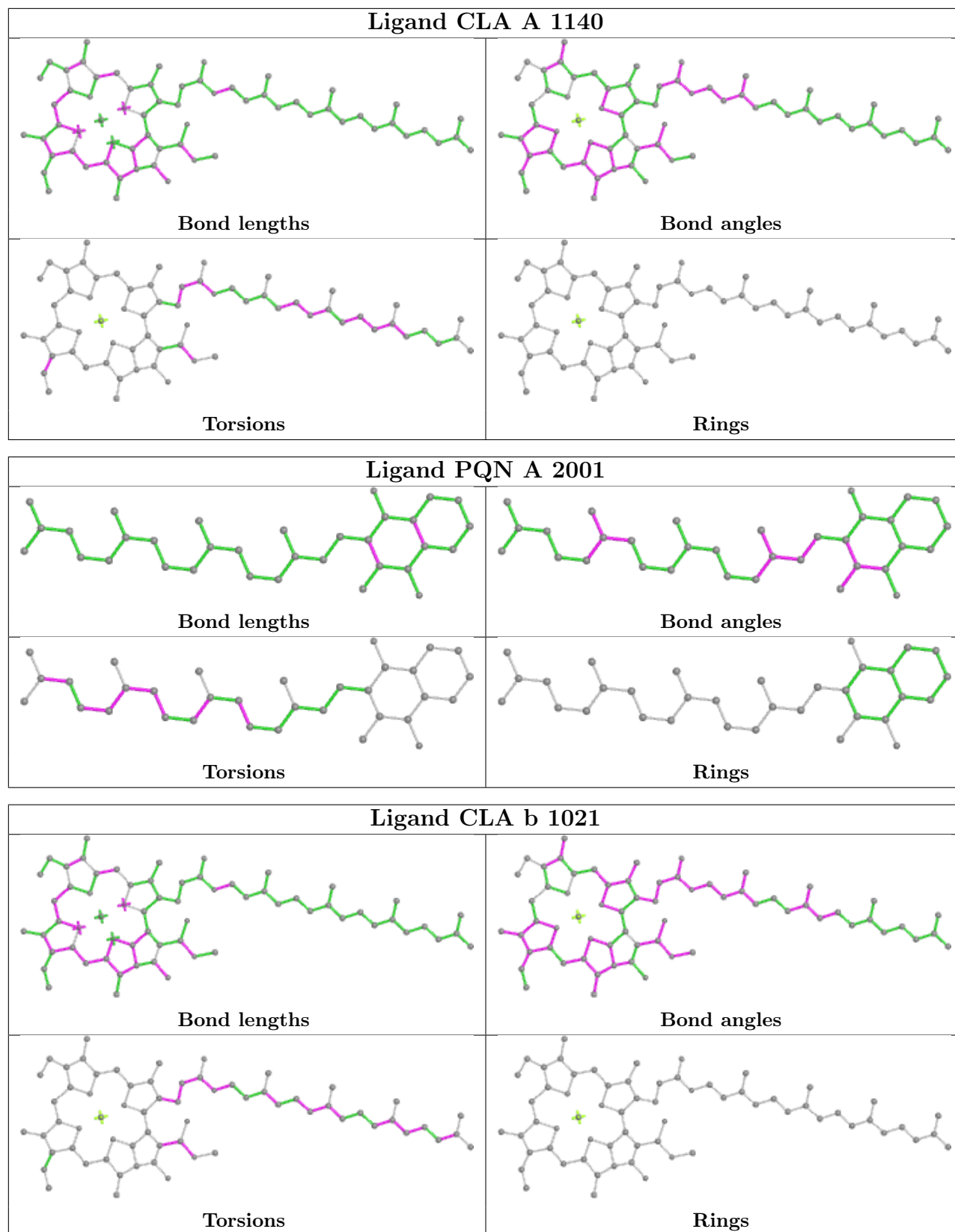


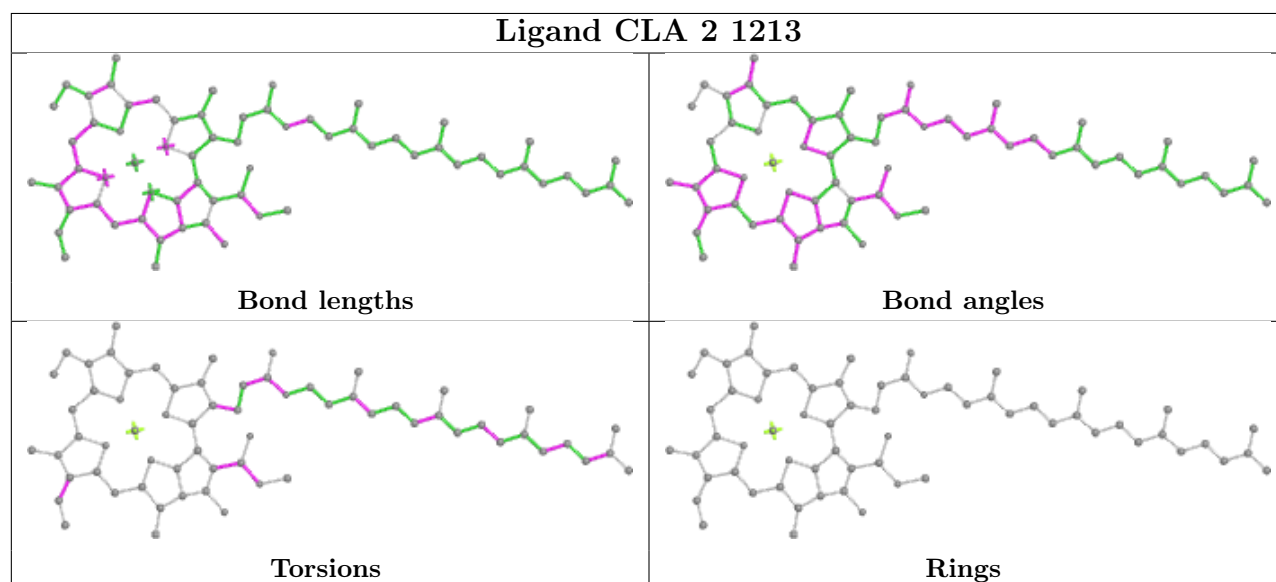
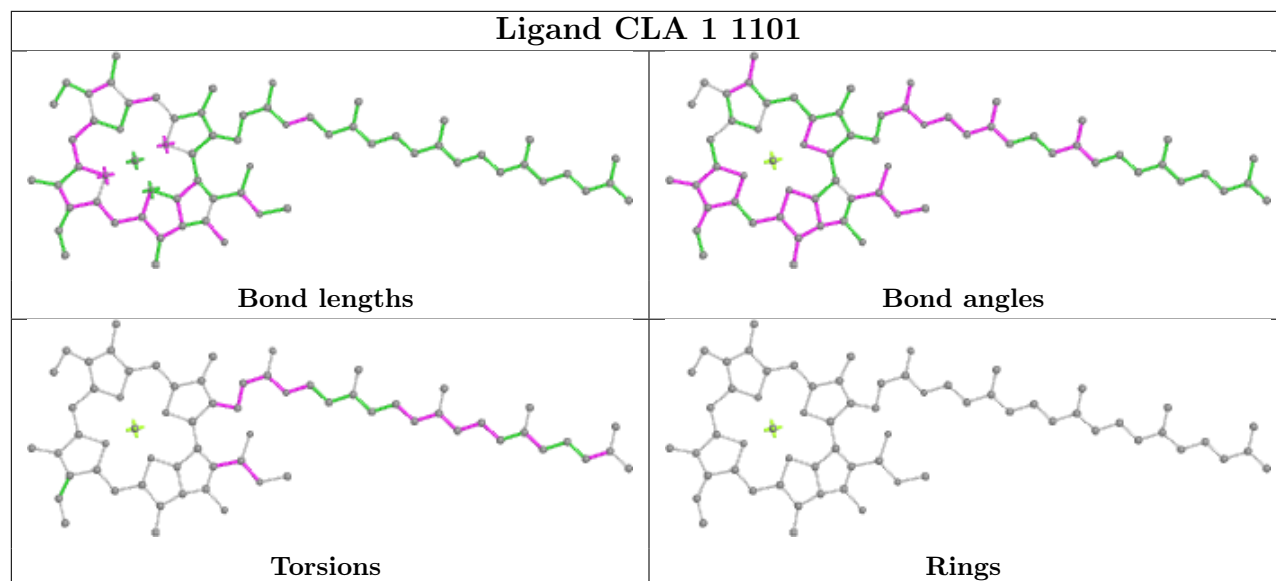
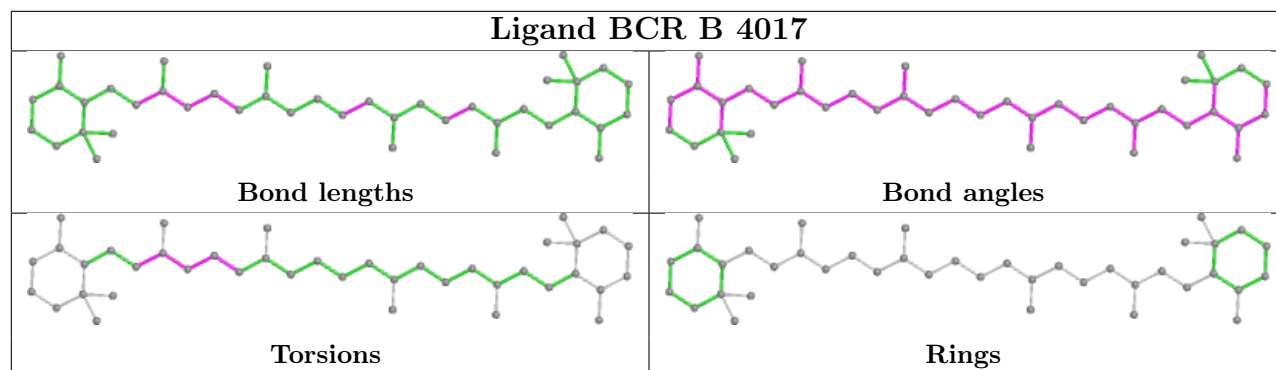


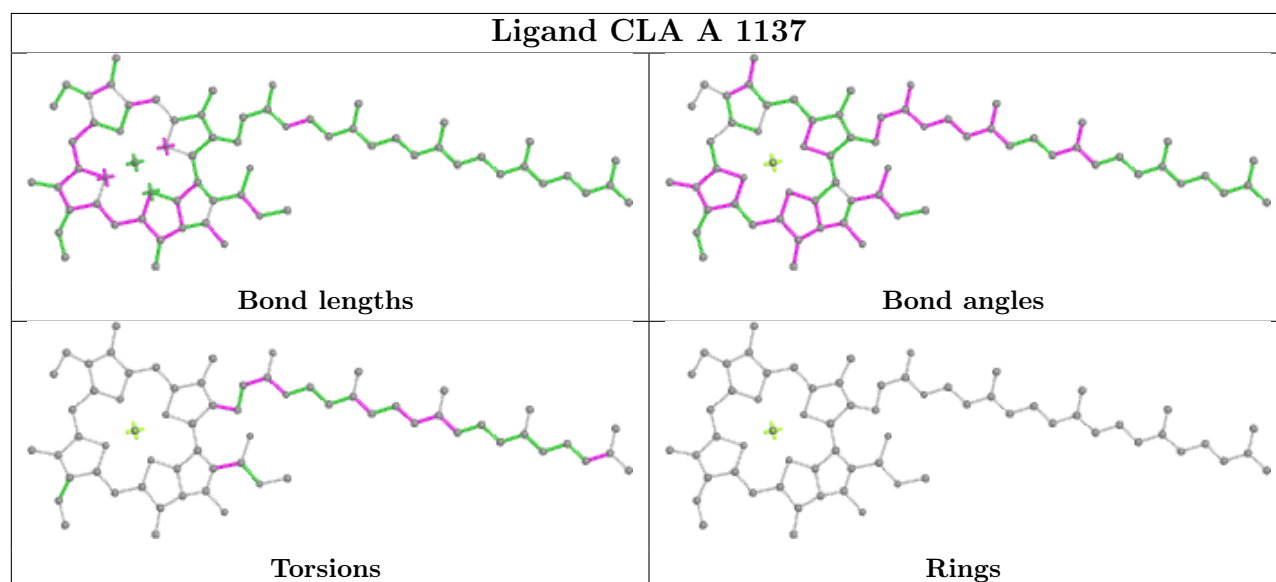
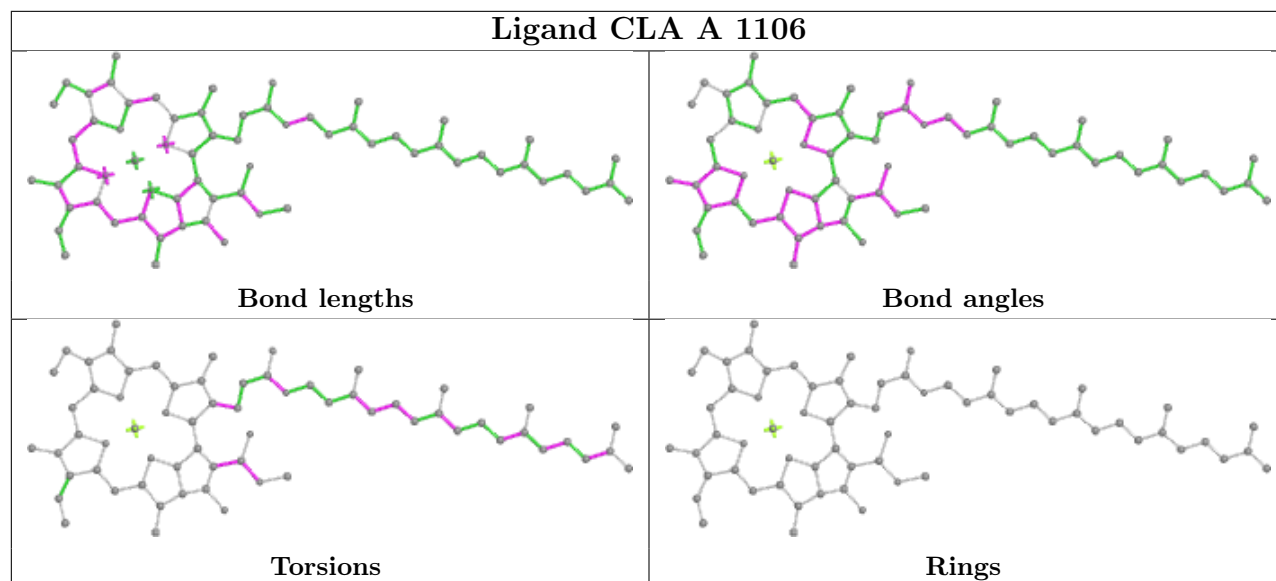
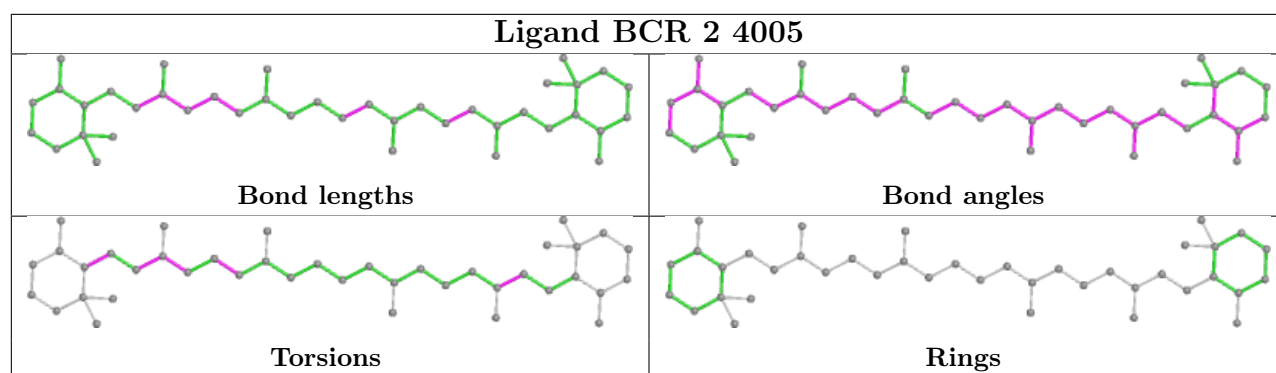


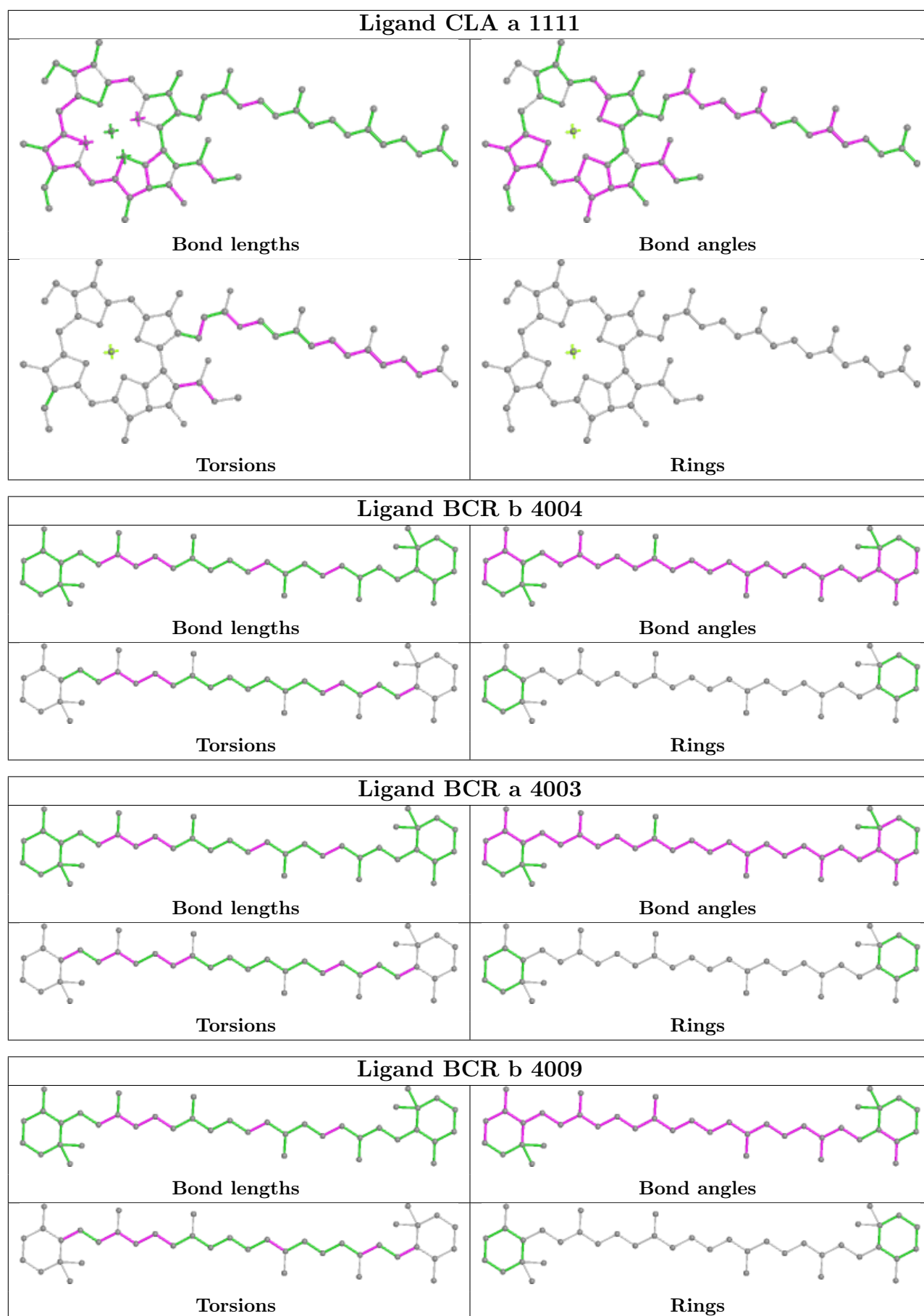


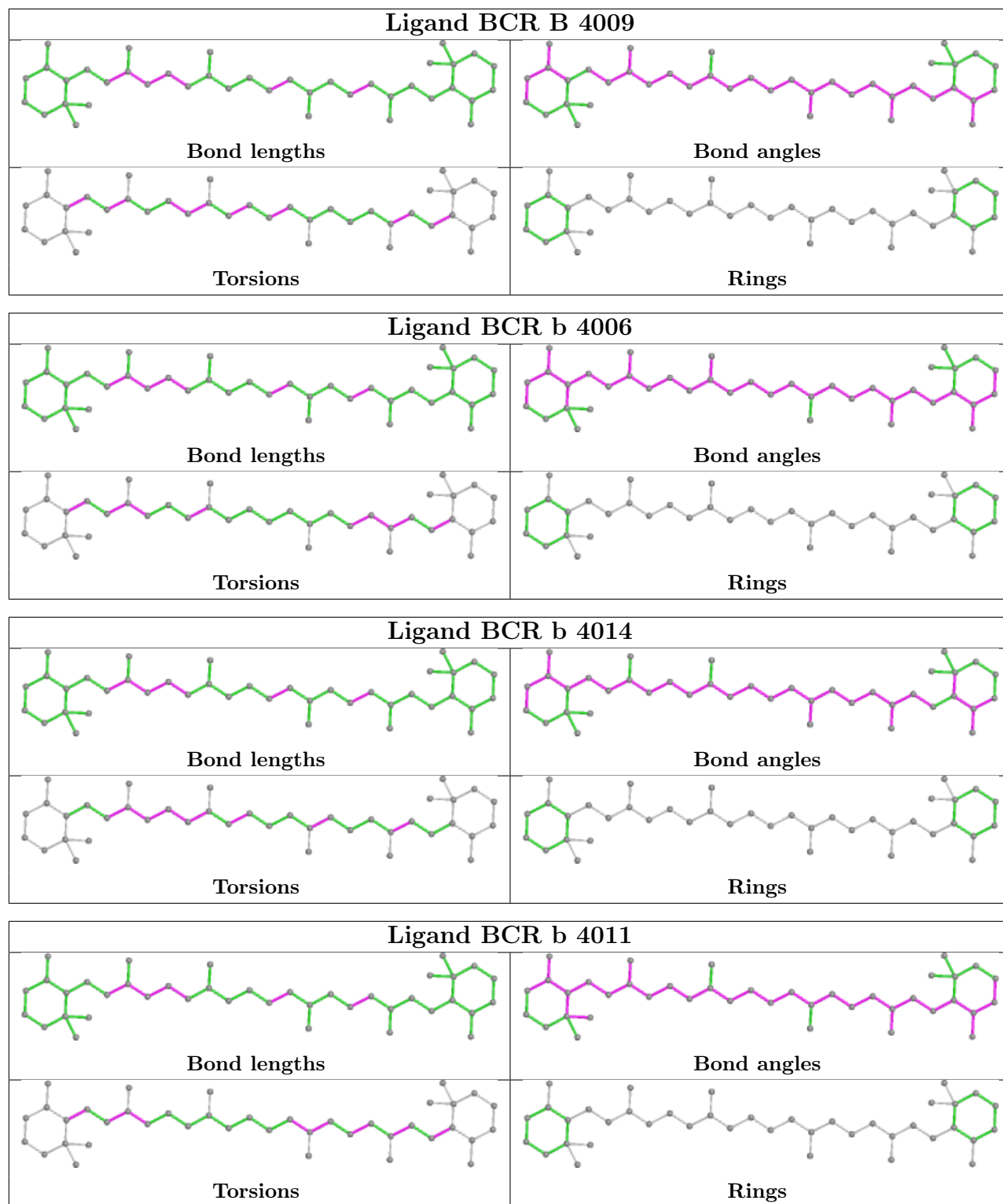


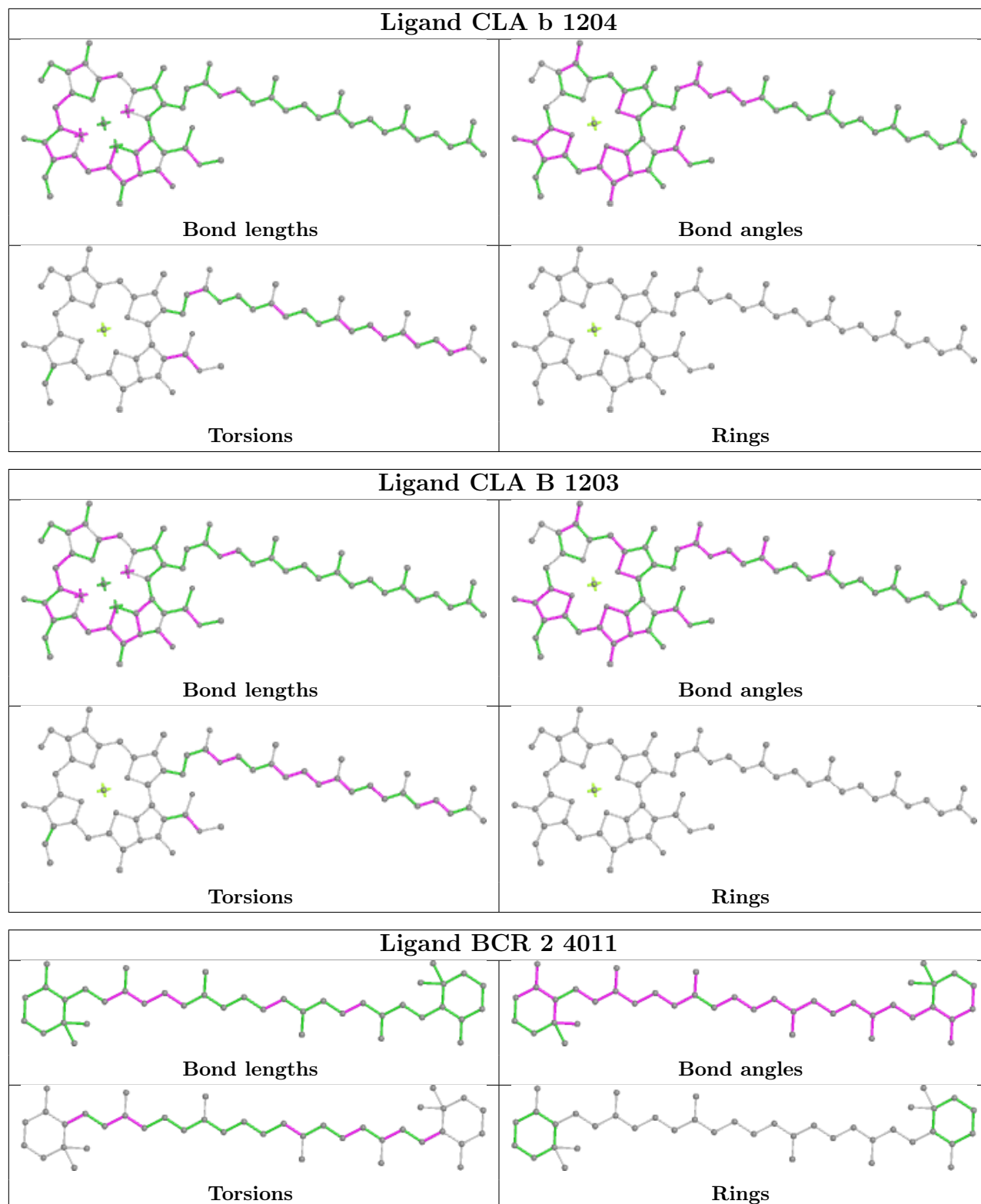


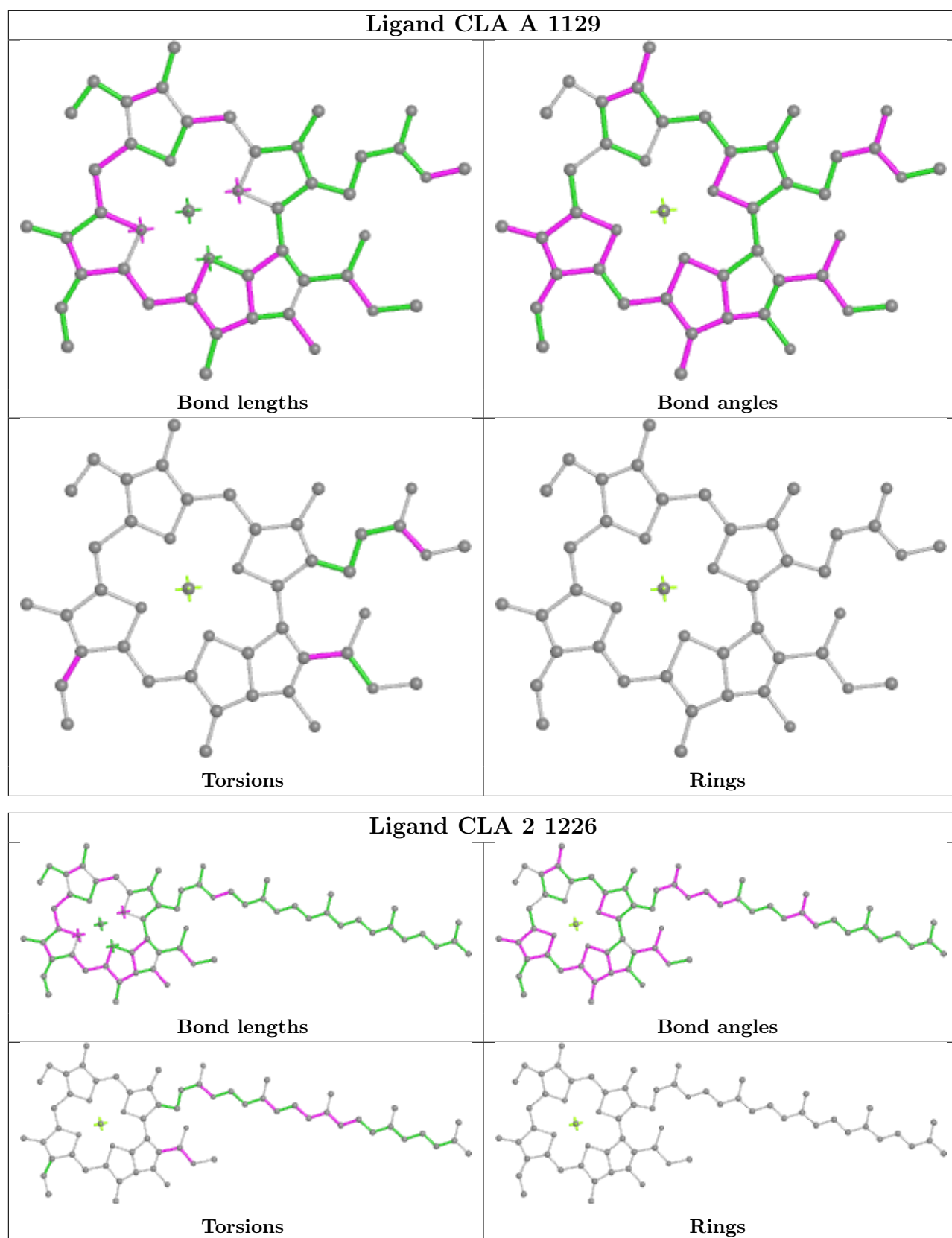












5.7 Other polymers [i](#)

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.

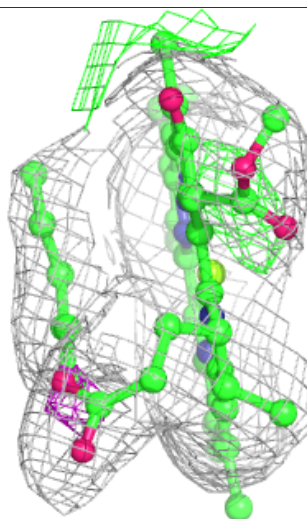
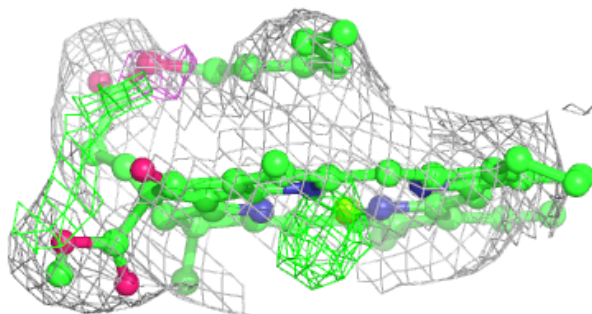
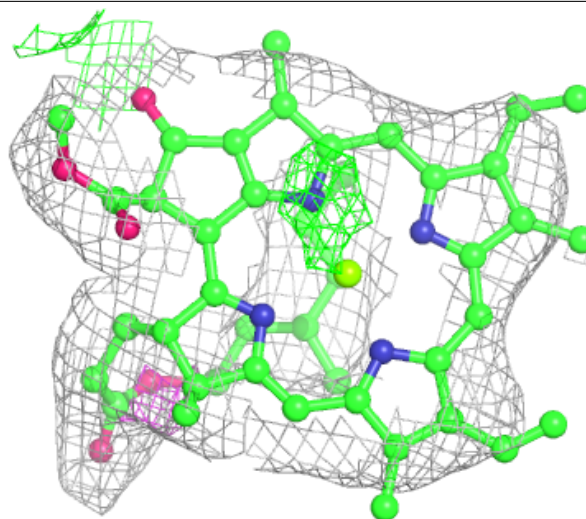
6.4 Ligands

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.

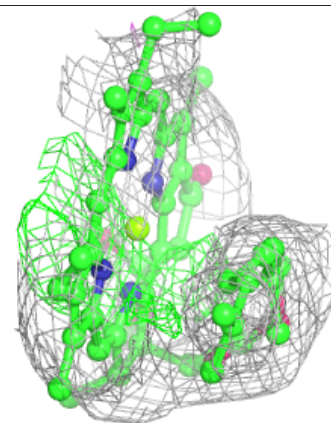
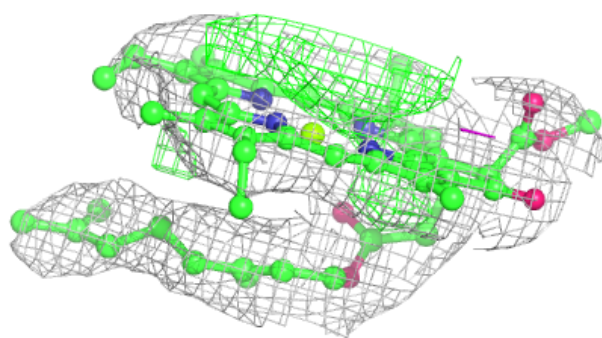
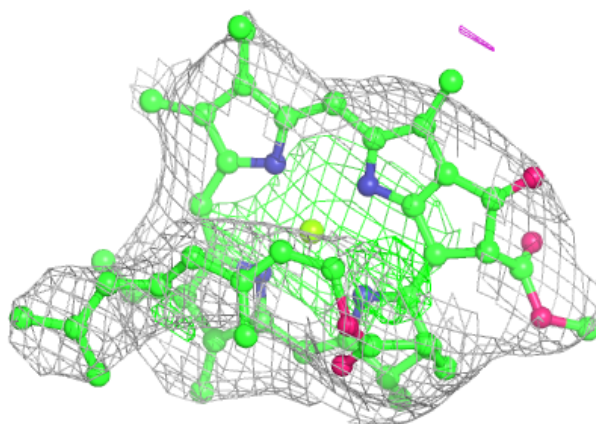
Electron density around CLA A 1801:

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

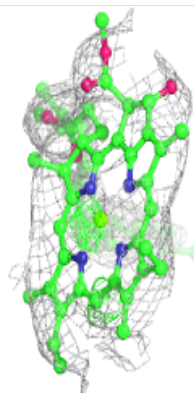
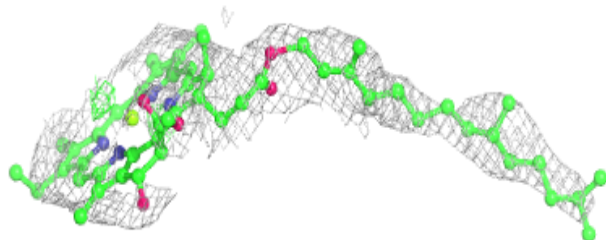
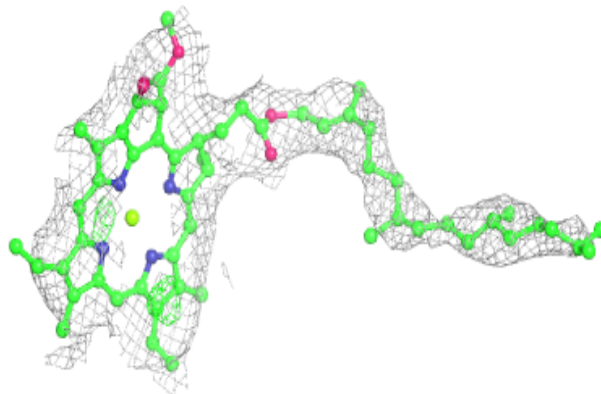


Electron density around CLA A 1237:

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

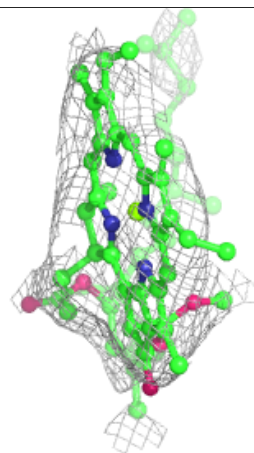
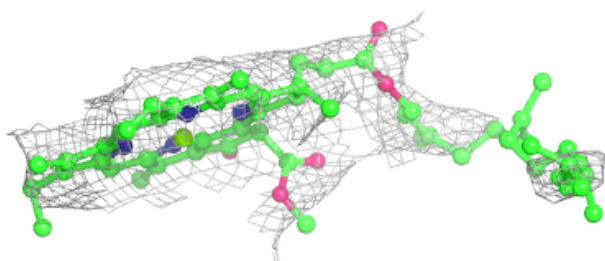
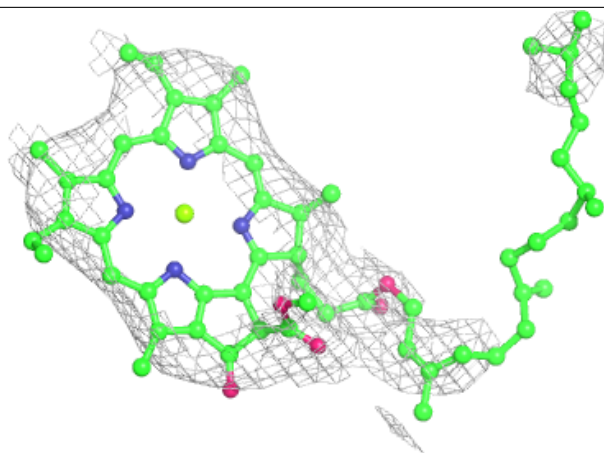
**Electron density around CLA A 1022:**

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



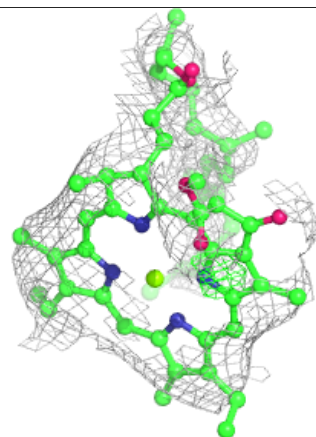
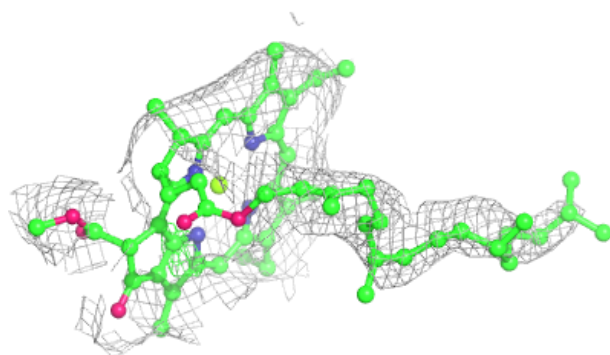
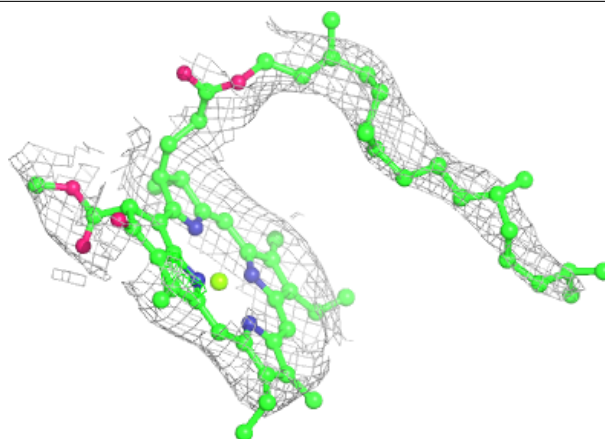
Electron density around CLA A 1101:

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

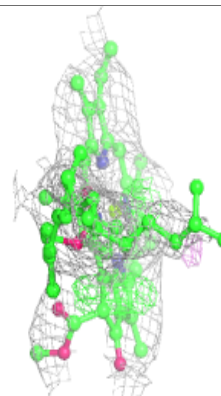
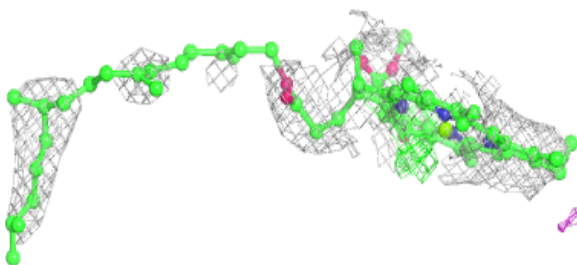
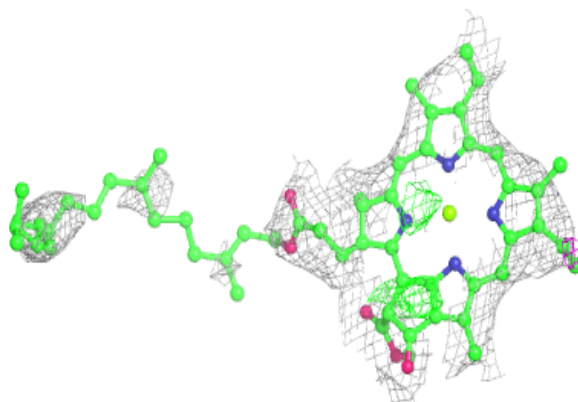


Electron density around CLA A 1102:

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

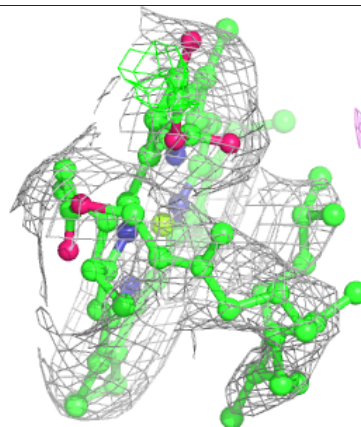
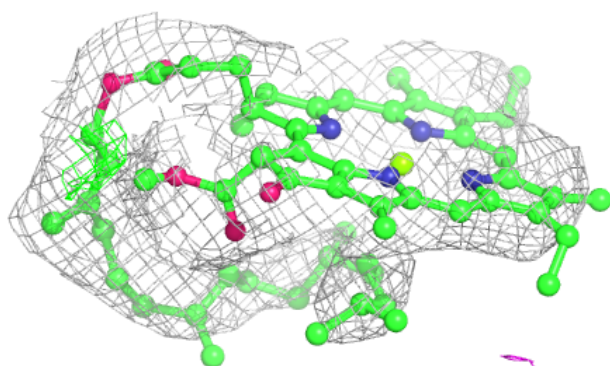
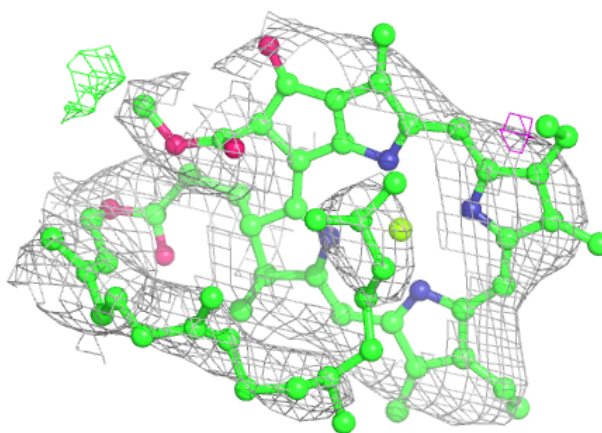
**Electron density around CLA A 1103:**

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



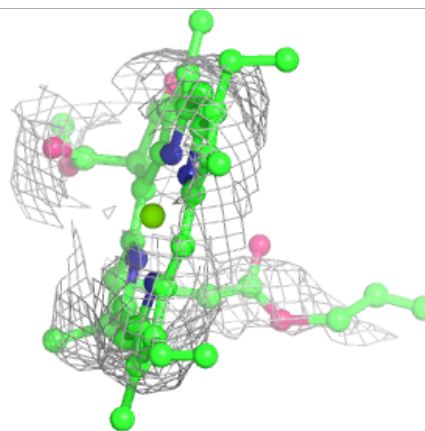
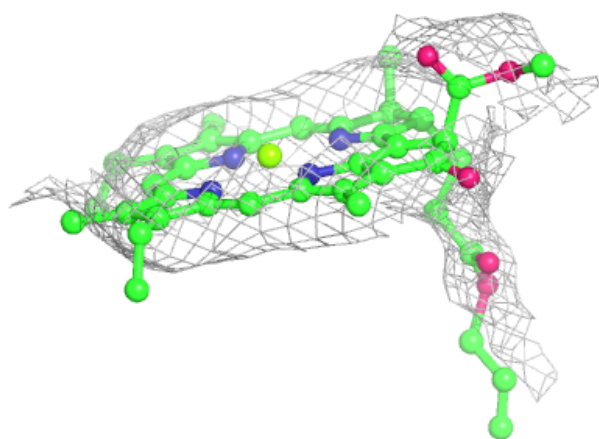
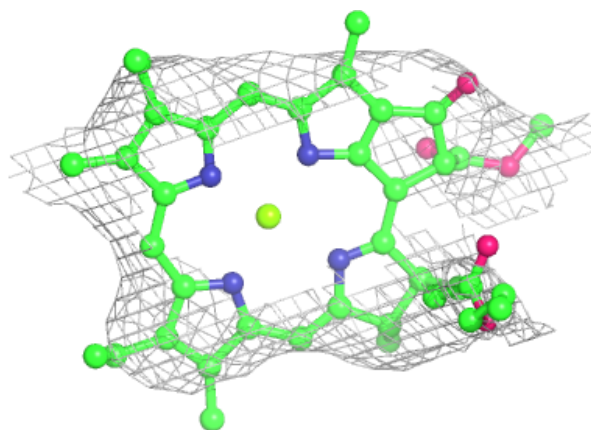
Electron density around CLA A 1104:

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



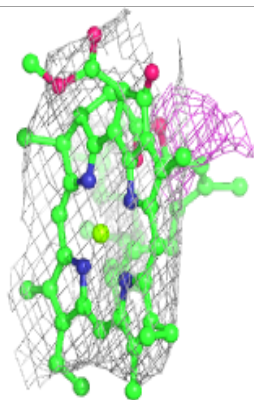
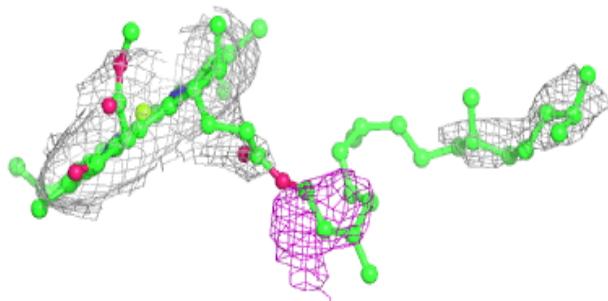
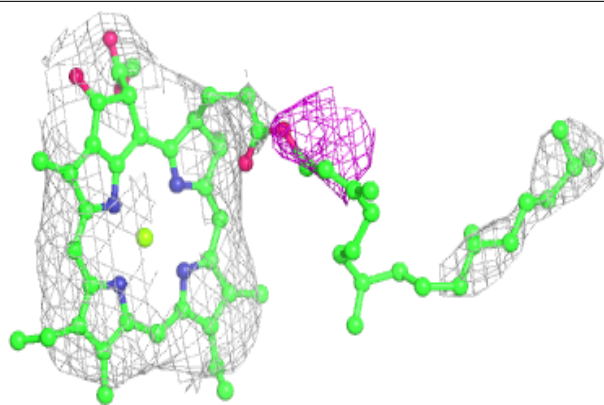
Electron density around CLA A 1105:

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

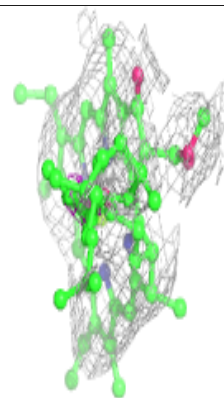
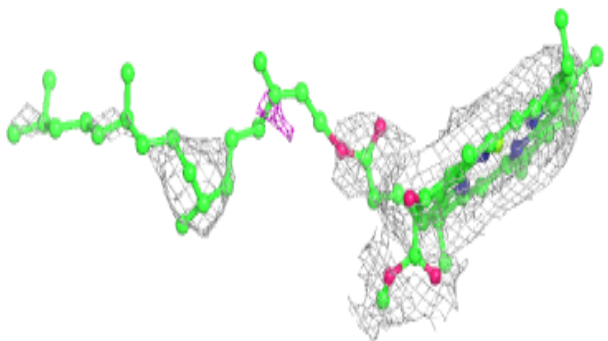
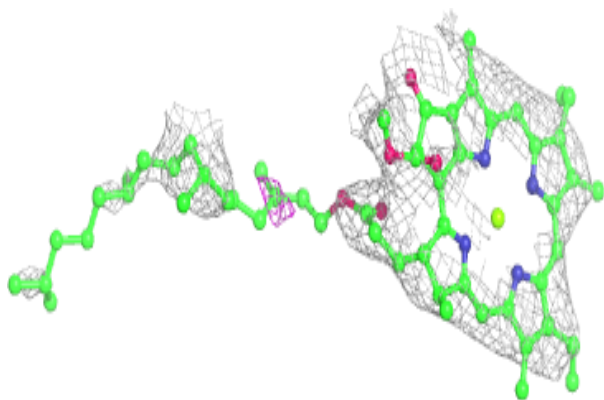


Electron density around CLA A 1106:

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

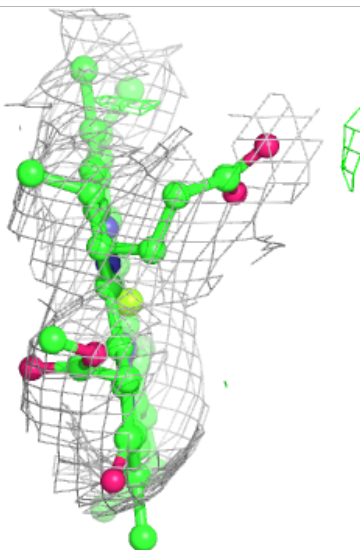
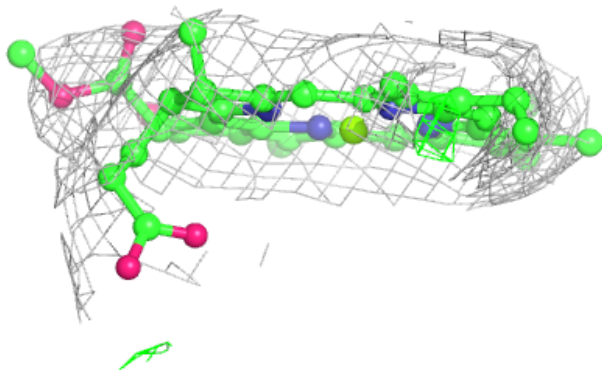
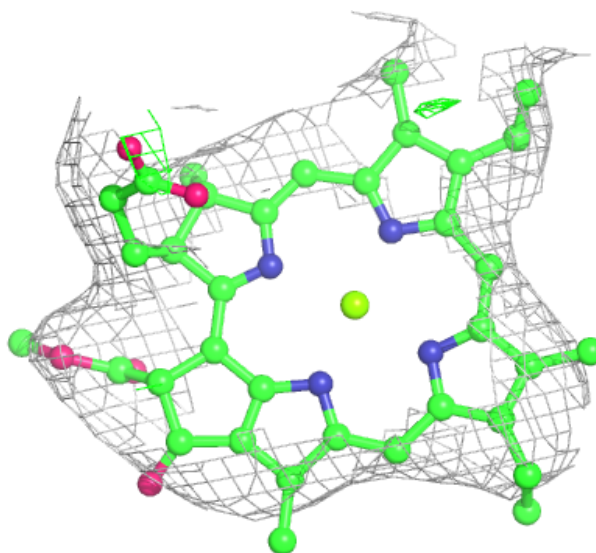
**Electron density around CLA A 1107:**

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



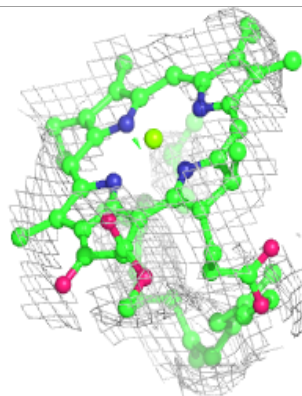
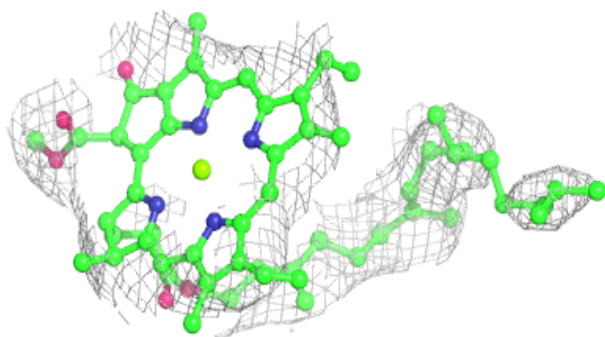
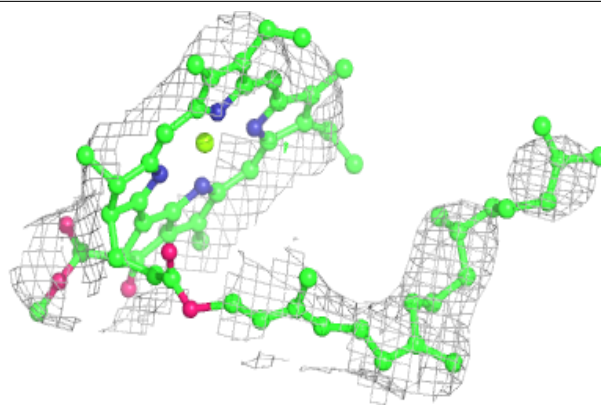
Electron density around CLA A 1108:

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



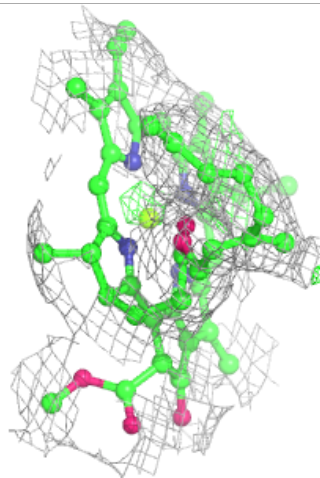
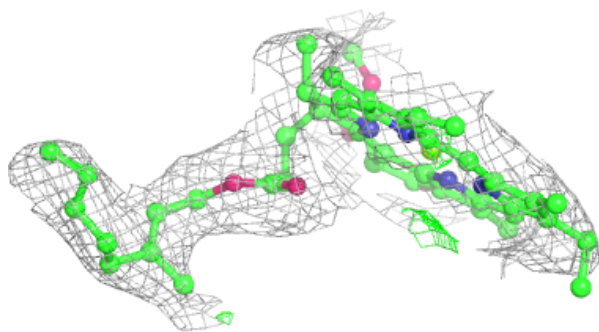
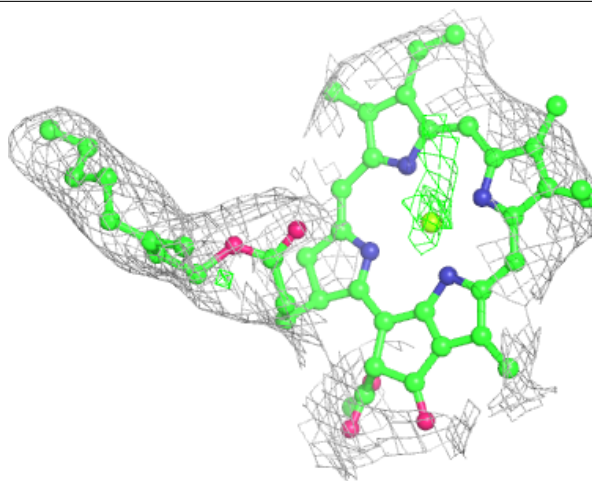
Electron density around CLA A 1109:

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



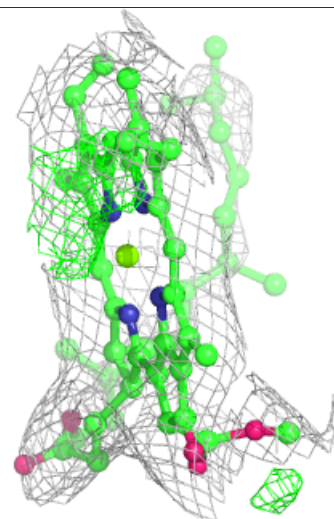
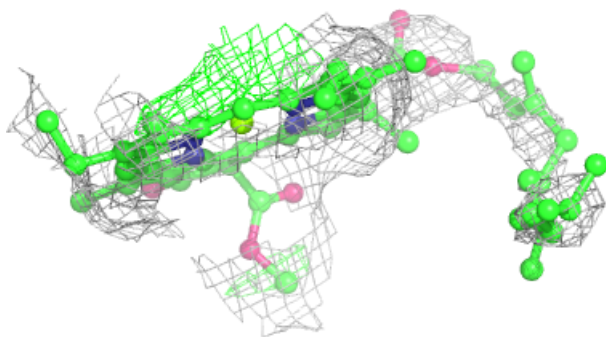
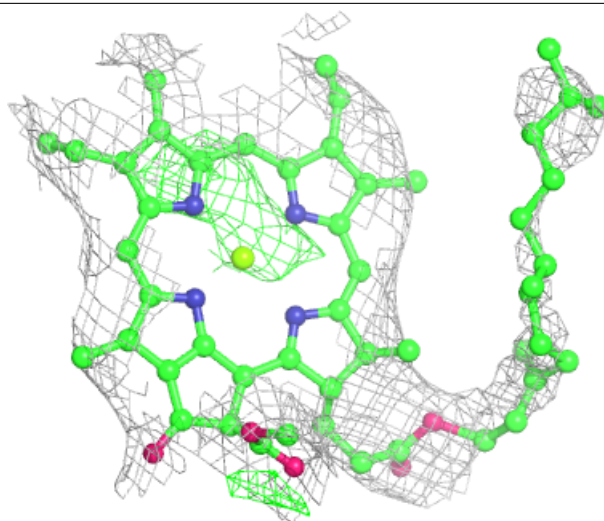
Electron density around CLA A 1110:

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



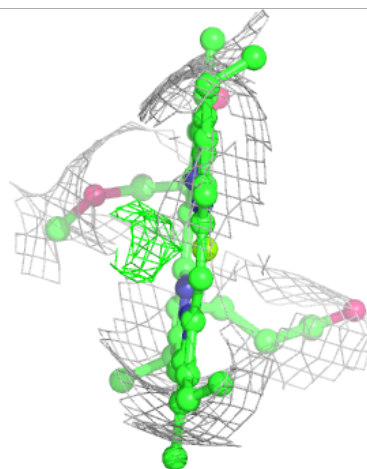
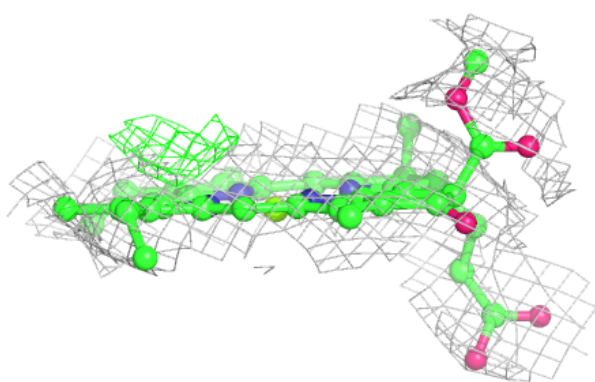
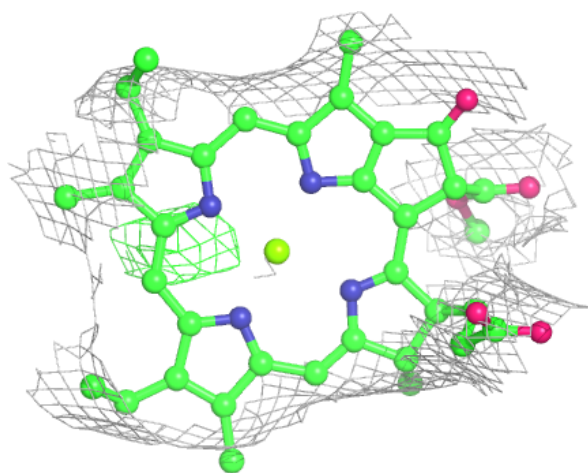
Electron density around CLA A 1111:

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



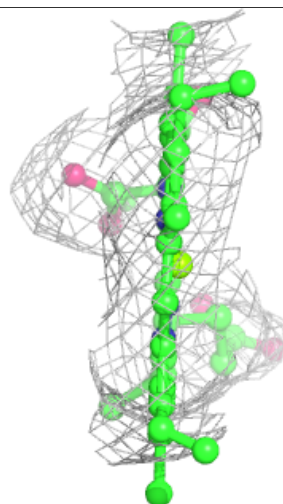
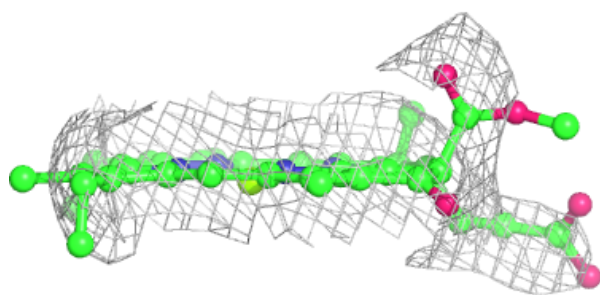
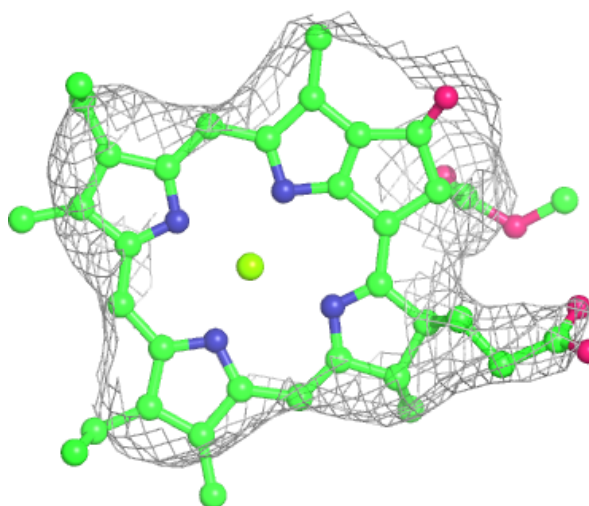
Electron density around CLA A 1112:

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



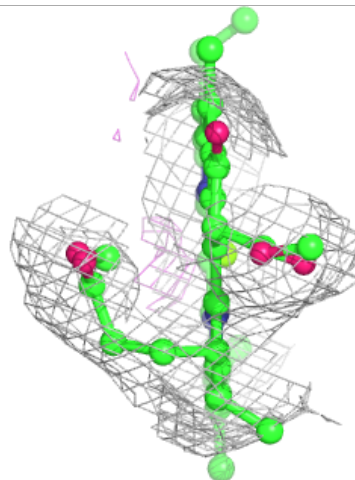
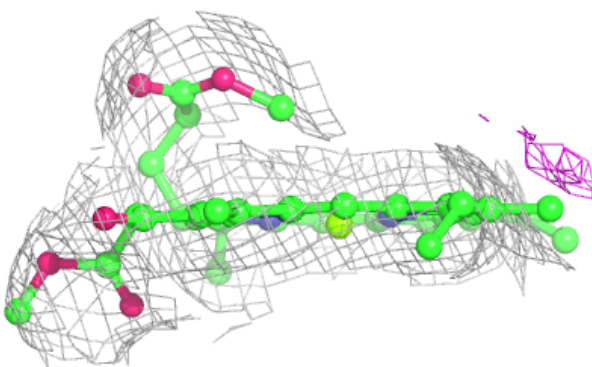
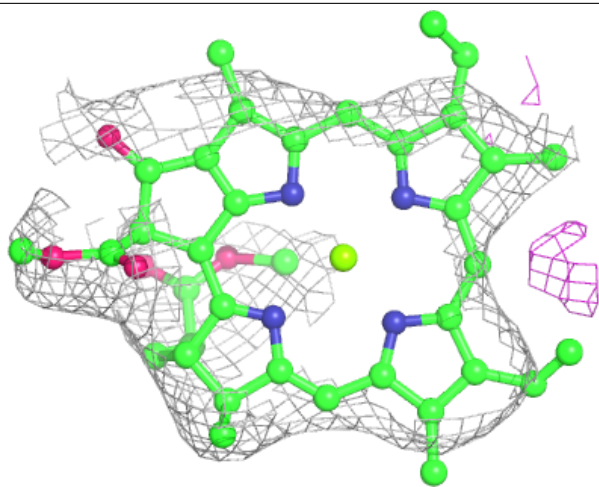
Electron density around CLA A 1113:

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



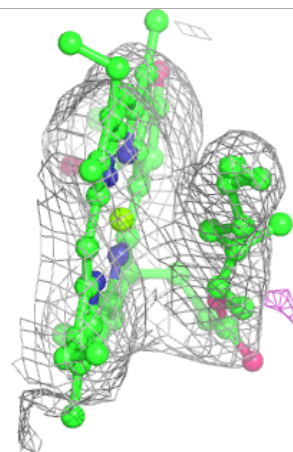
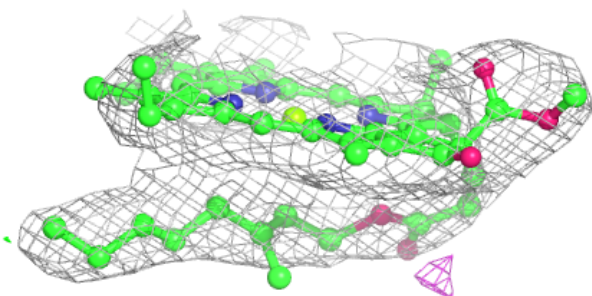
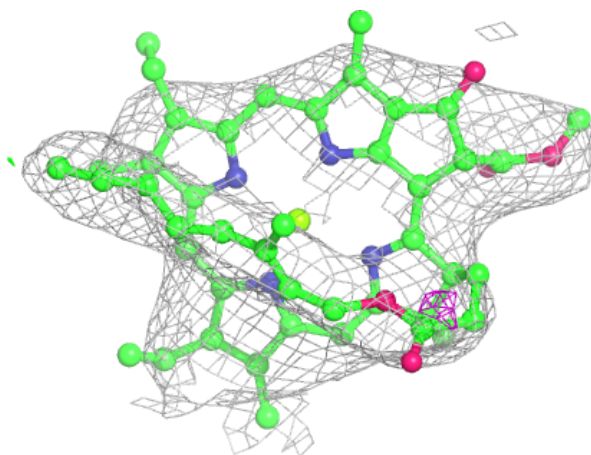
Electron density around CLA A 1115:

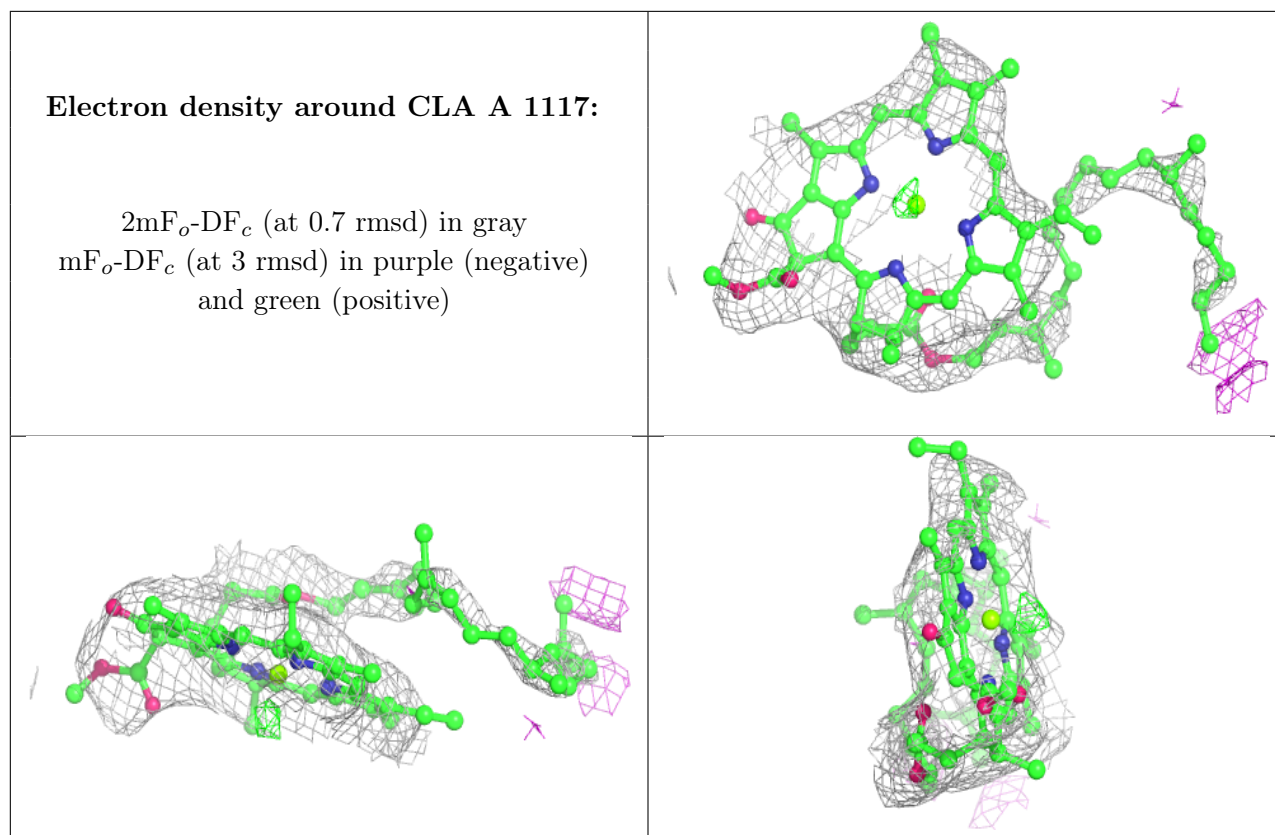
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around CLA A 1116:

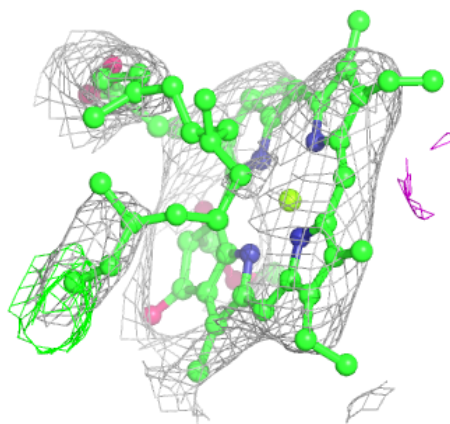
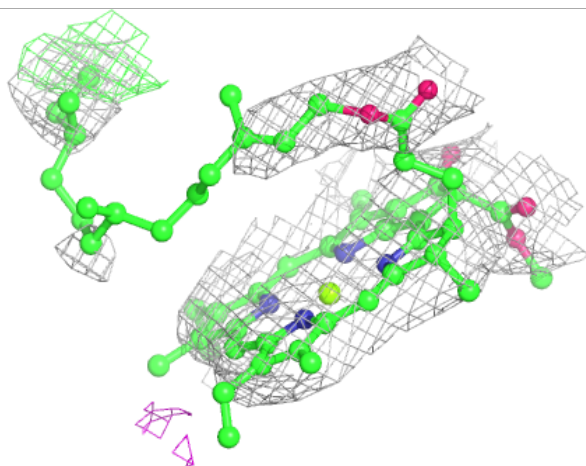
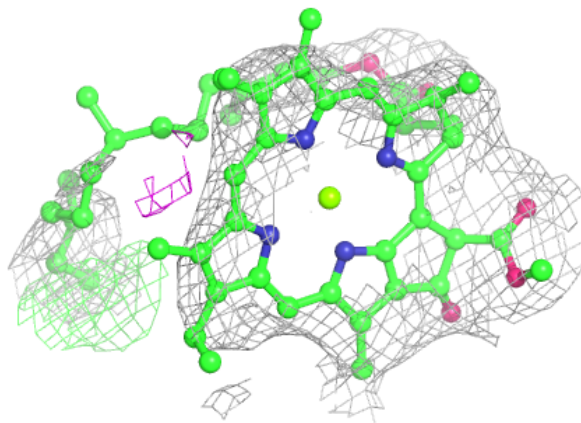
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

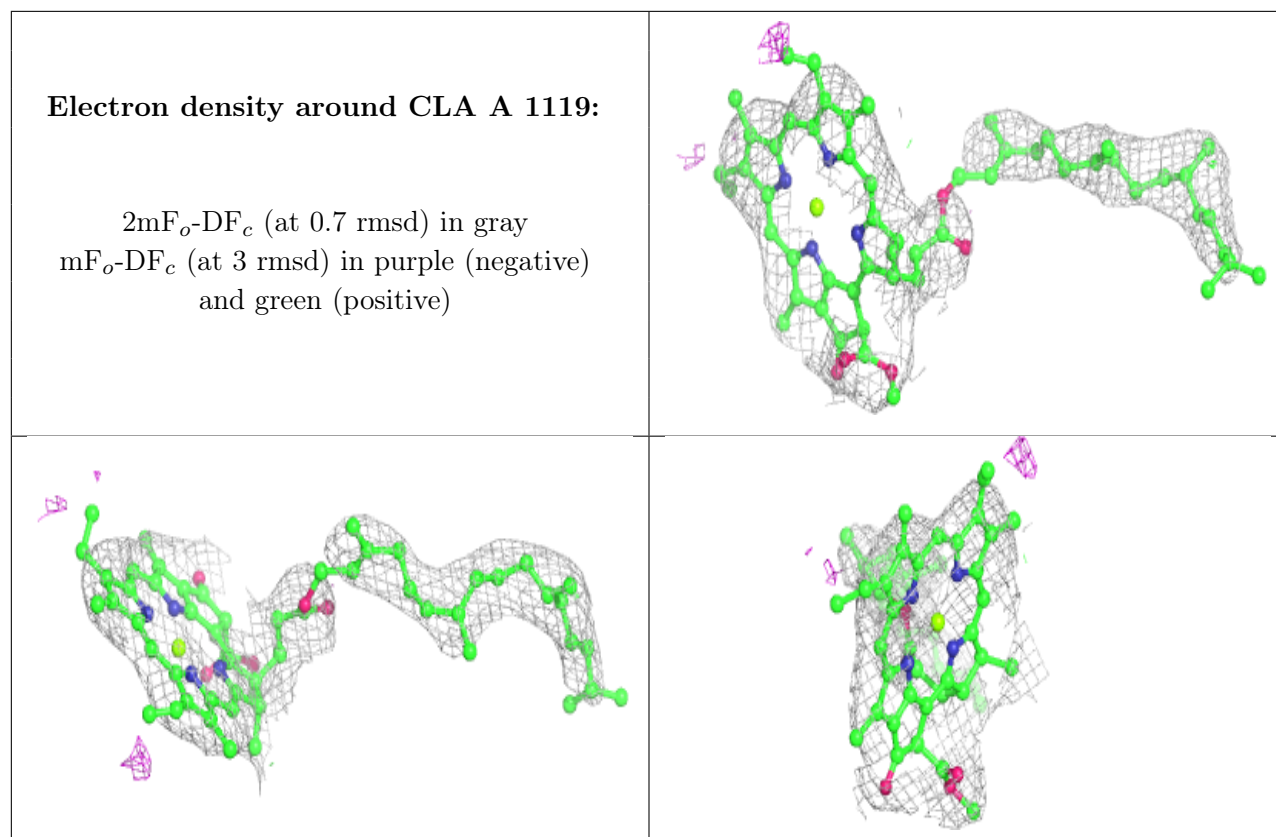




Electron density around CLA A 1118:

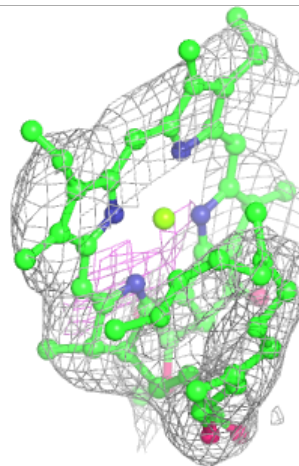
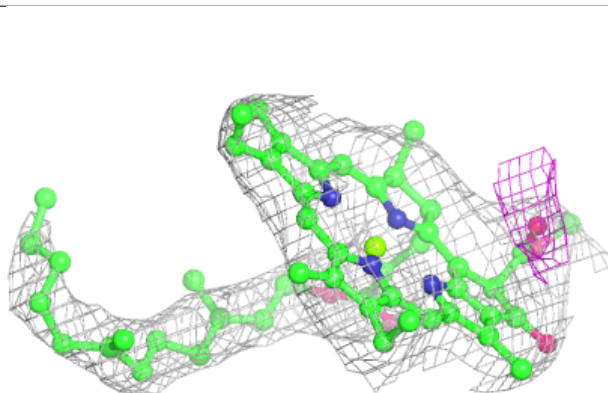
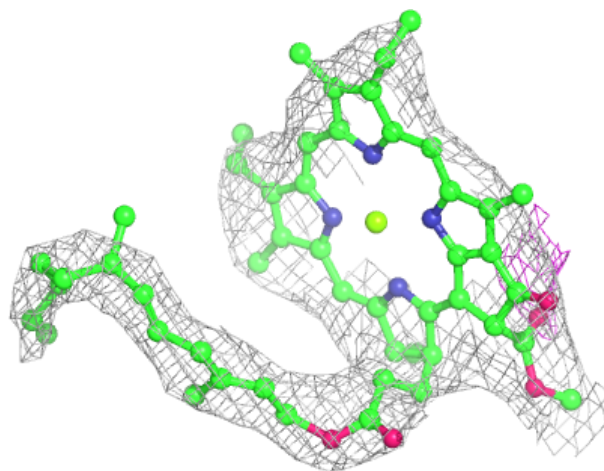
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





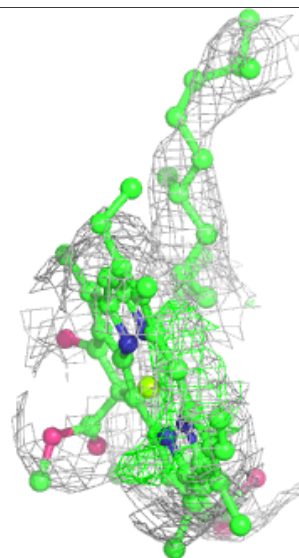
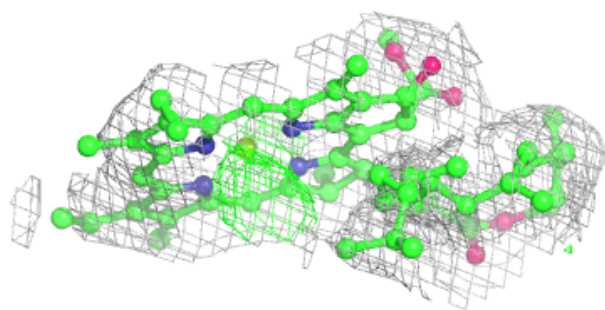
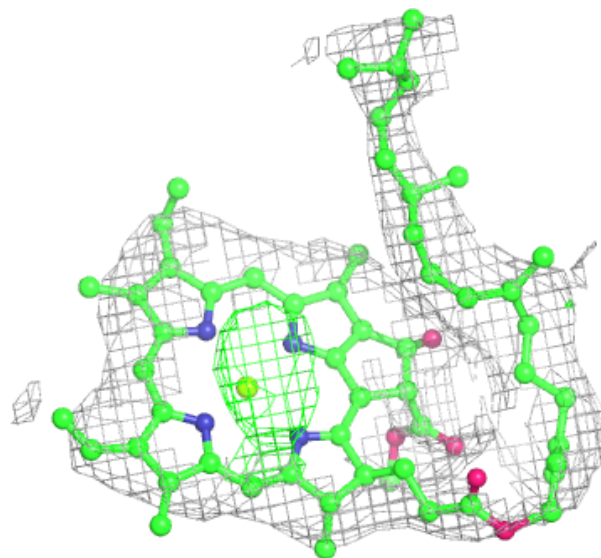
Electron density around CLA A 1122:

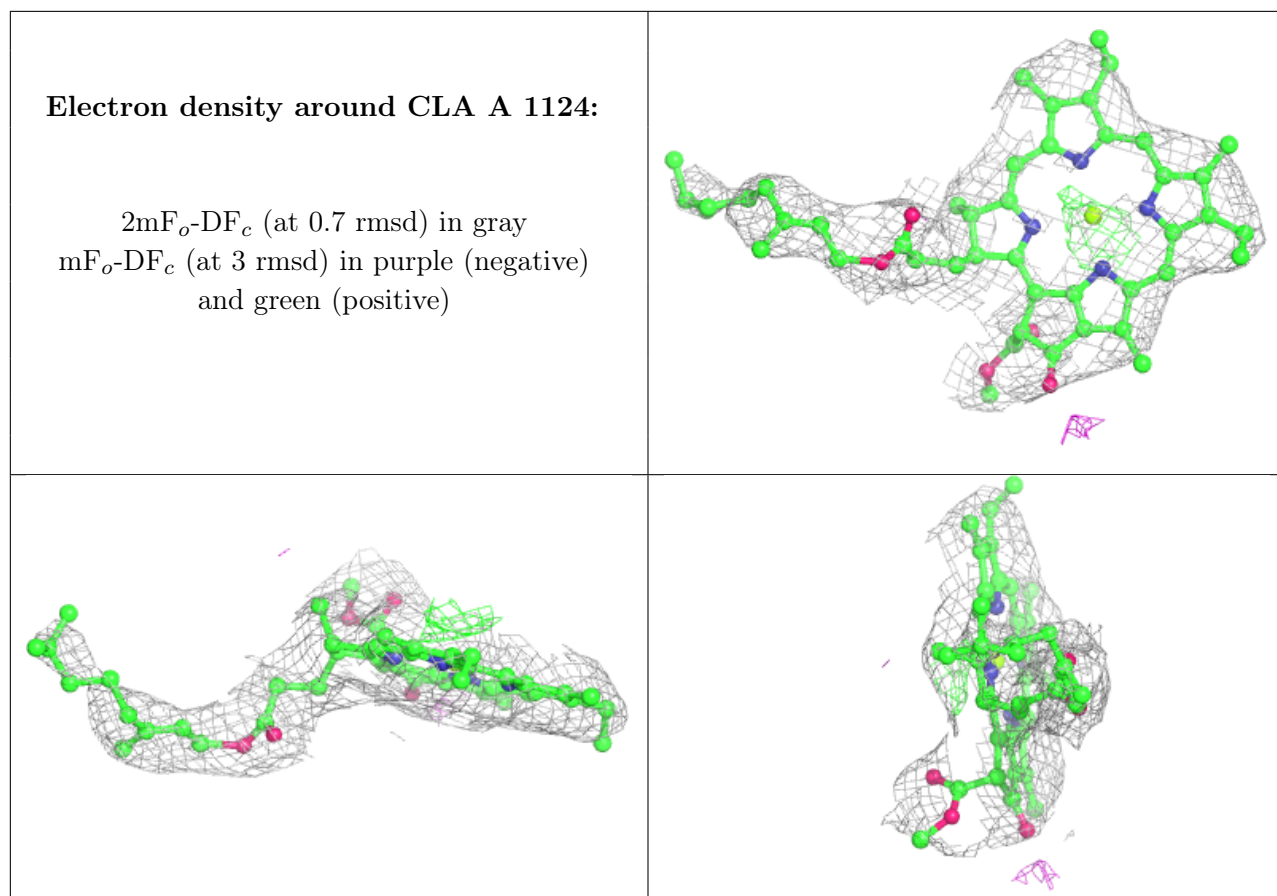
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around CLA A 1123:

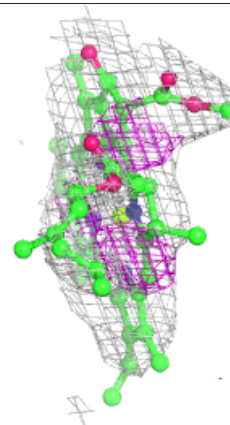
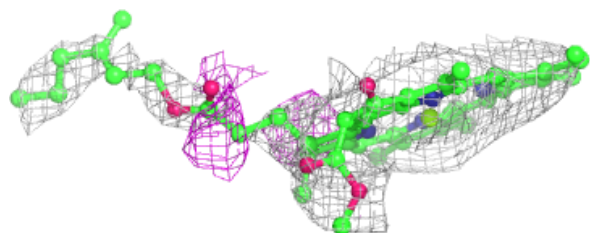
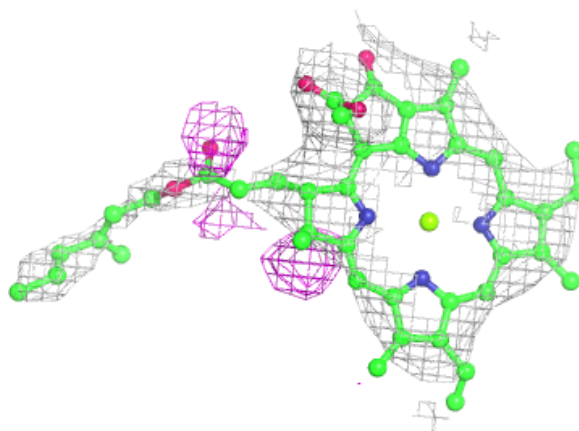
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



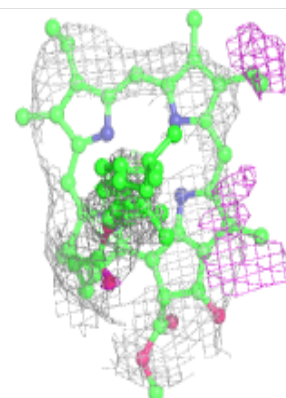
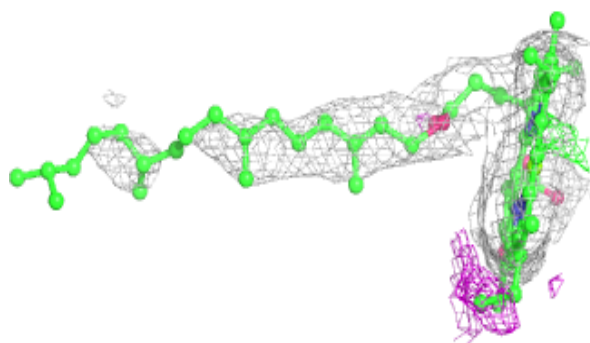
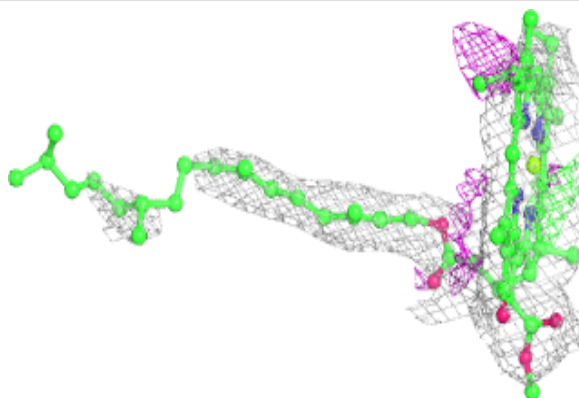


Electron density around CLA A 1125:

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

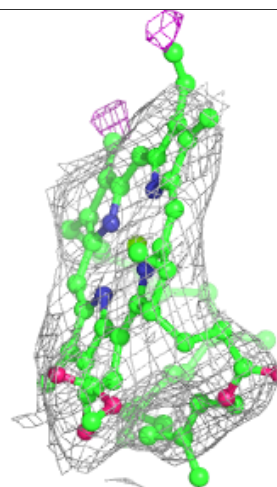
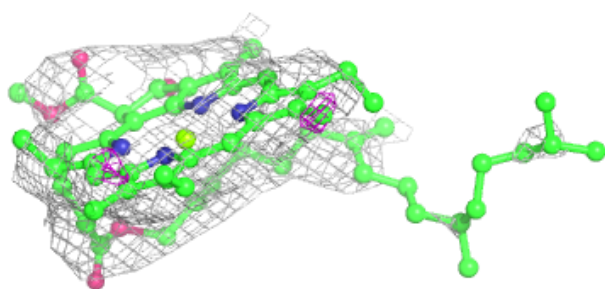
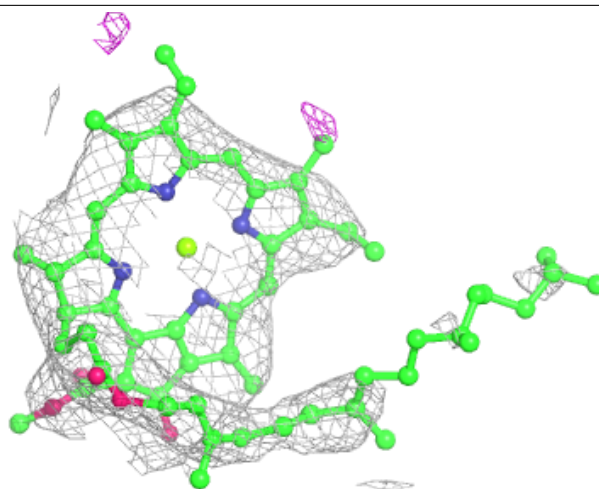
**Electron density around CLA A 1126:**

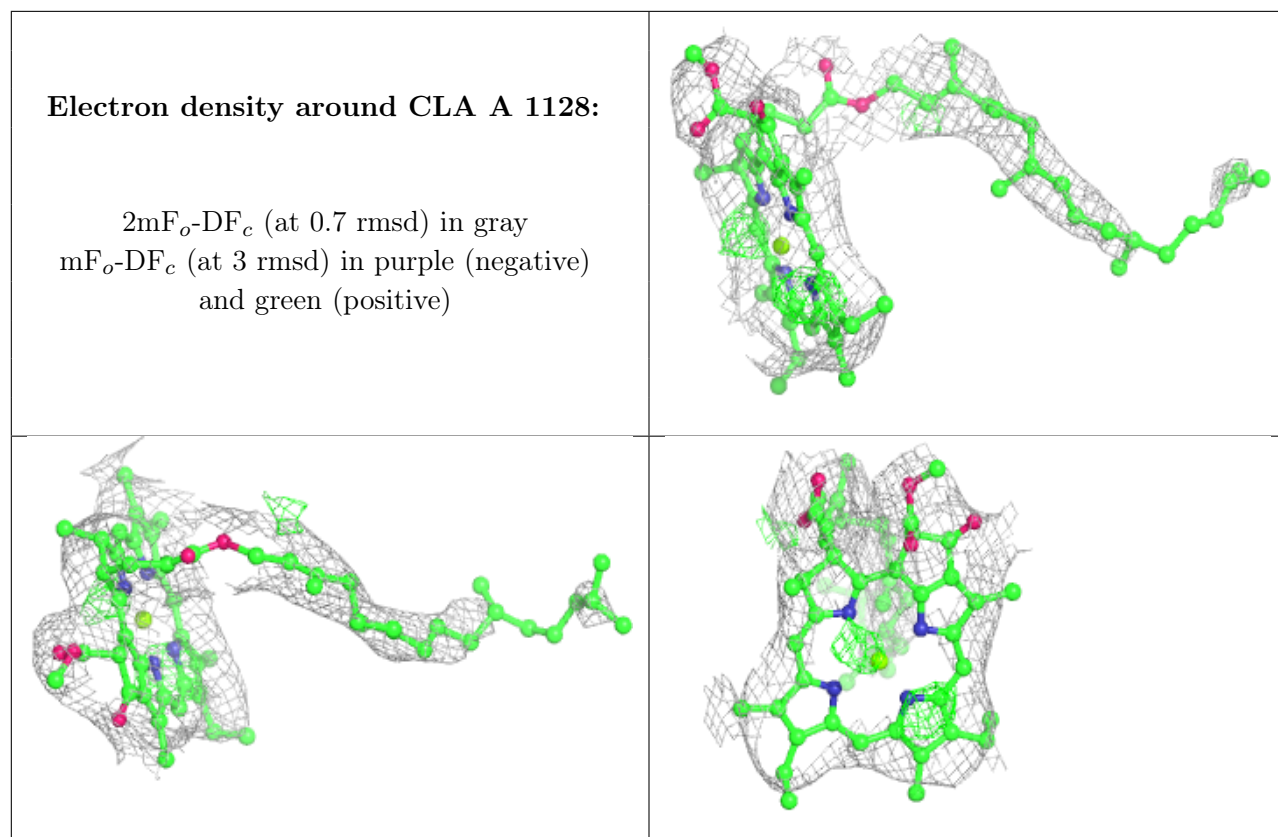
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around CLA A 1127:

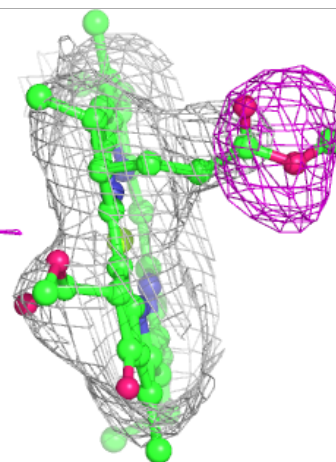
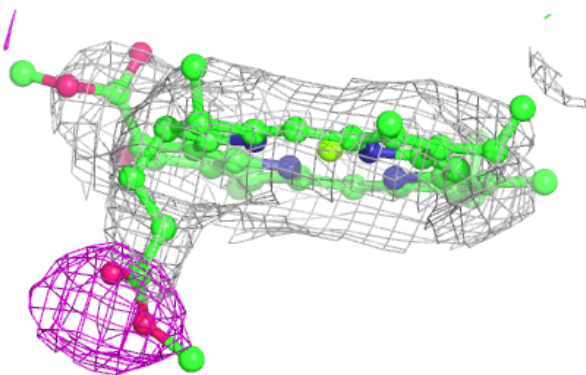
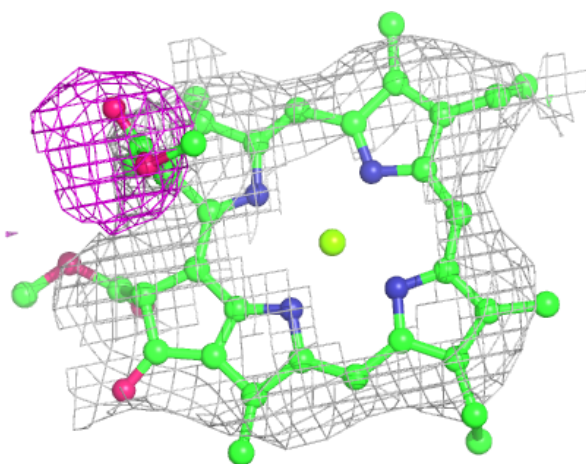
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





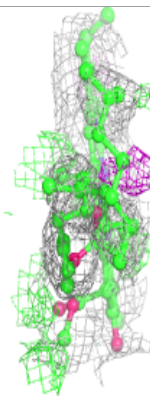
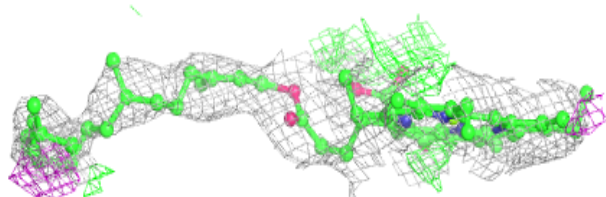
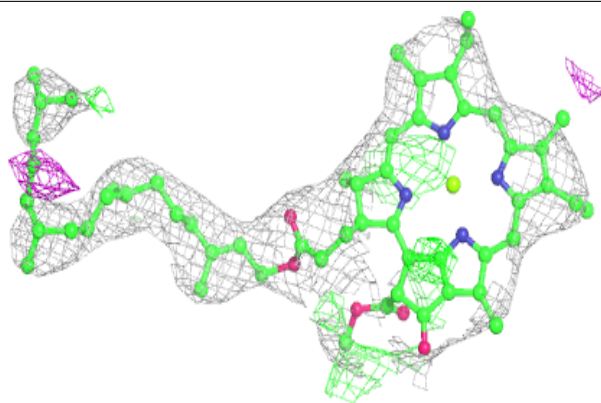
Electron density around CLA A 1130:

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

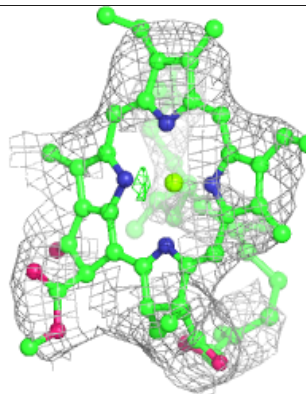
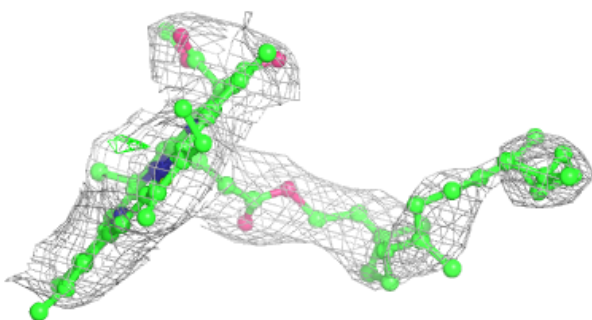
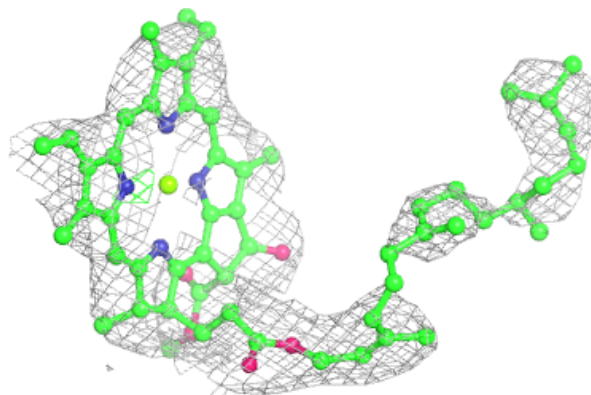


Electron density around CLA A 1131:

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

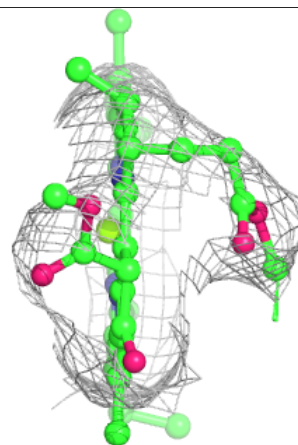
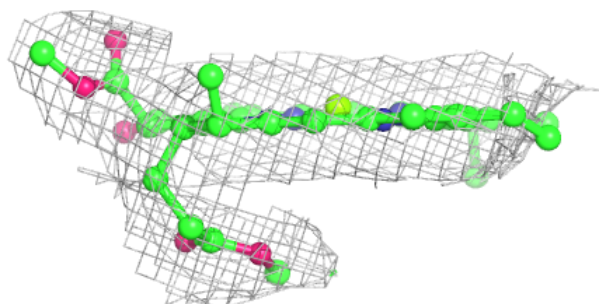
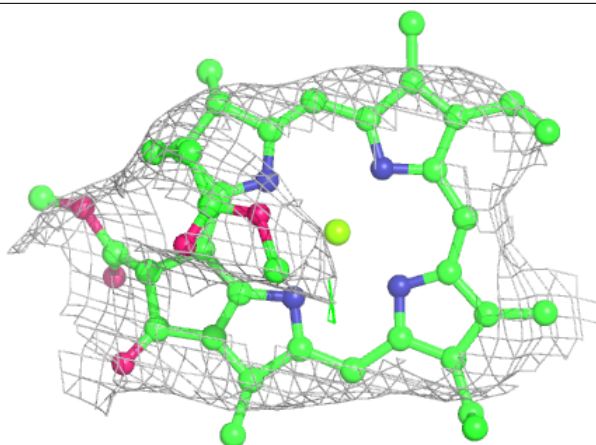
**Electron density around CLA A 1137:**

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

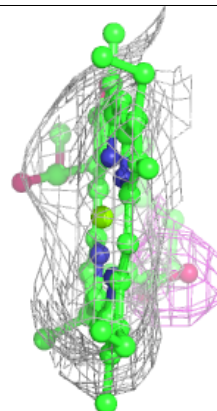
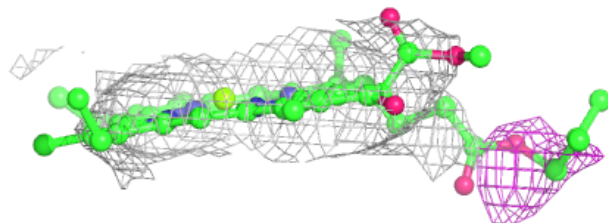
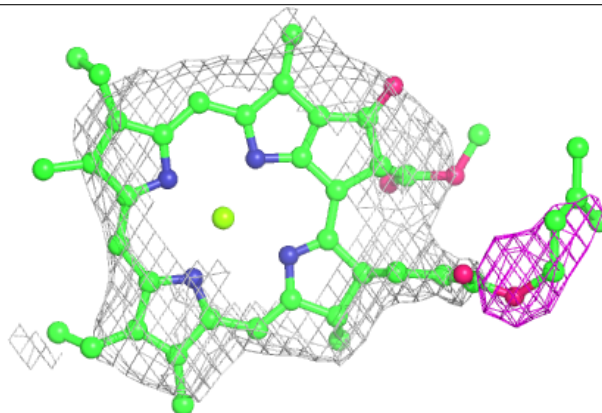


Electron density around CLA A 1138:

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

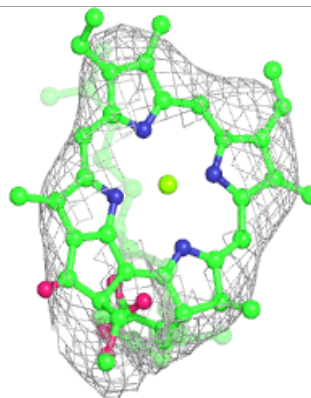
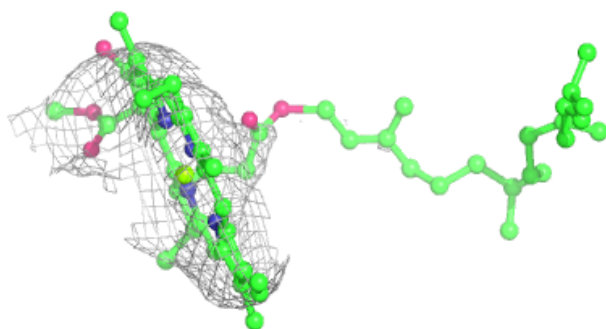
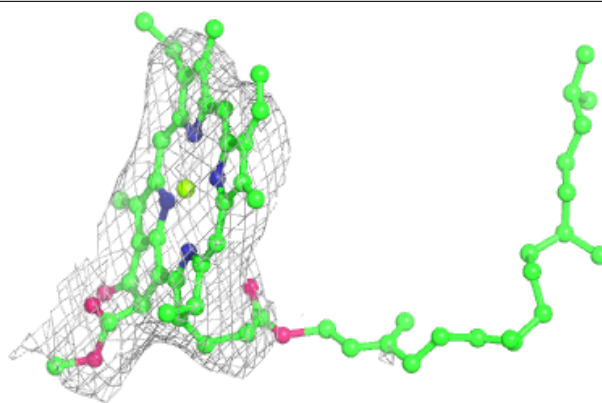
**Electron density around CLA A 1139:**

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

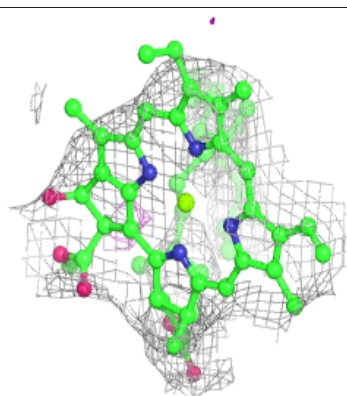
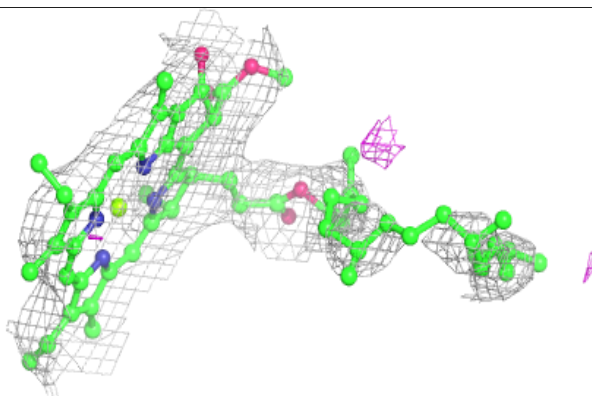
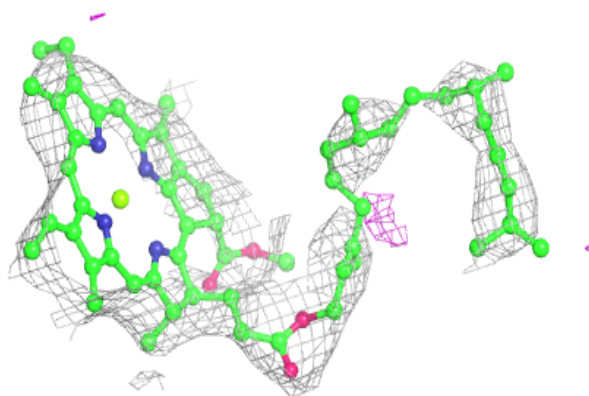


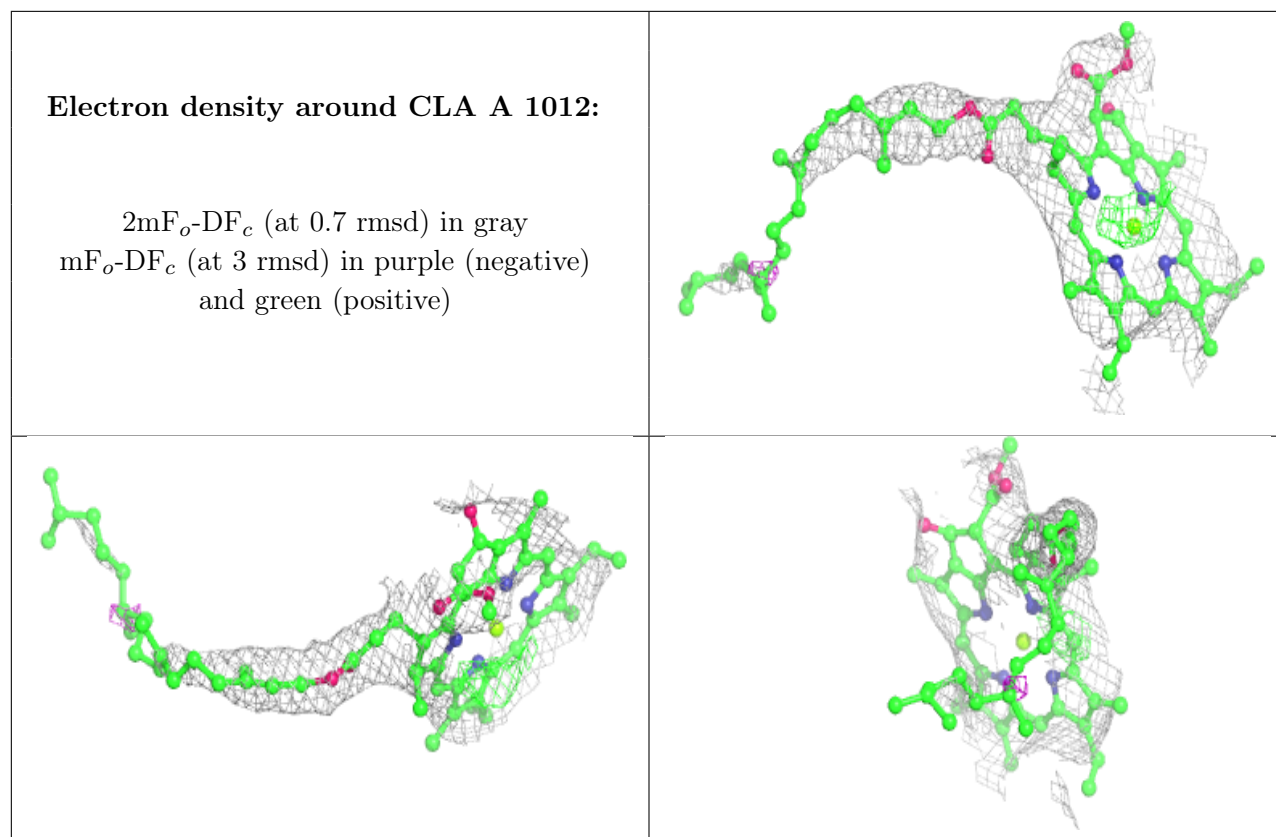
Electron density around CLA A 1140:

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

**Electron density around CLA A 1011:**

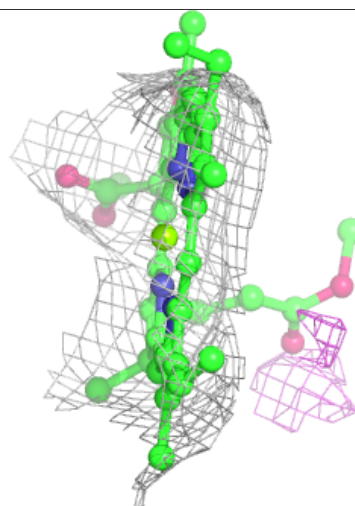
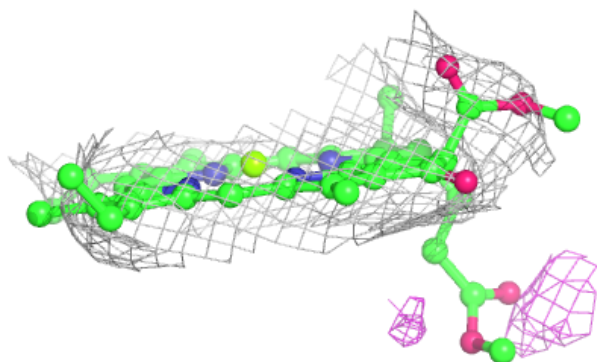
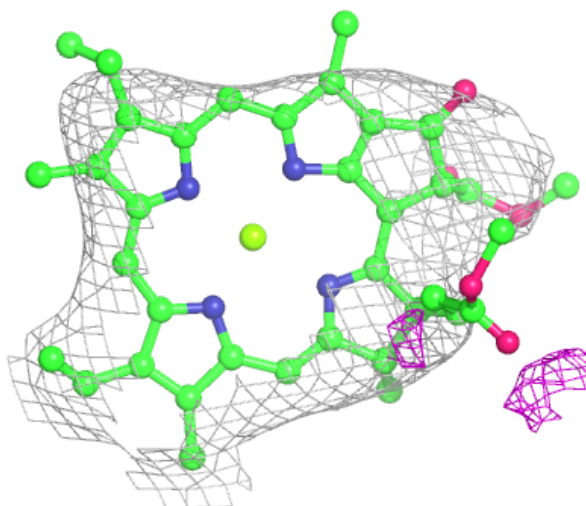
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





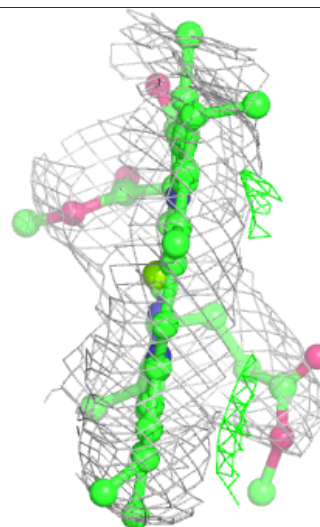
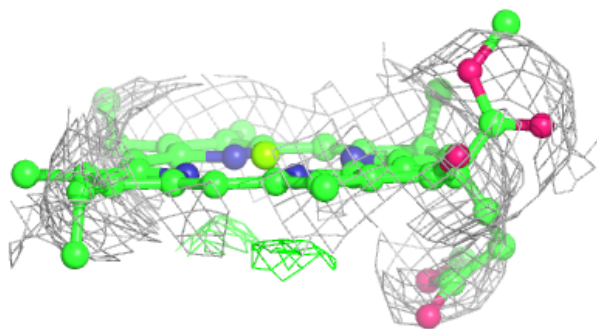
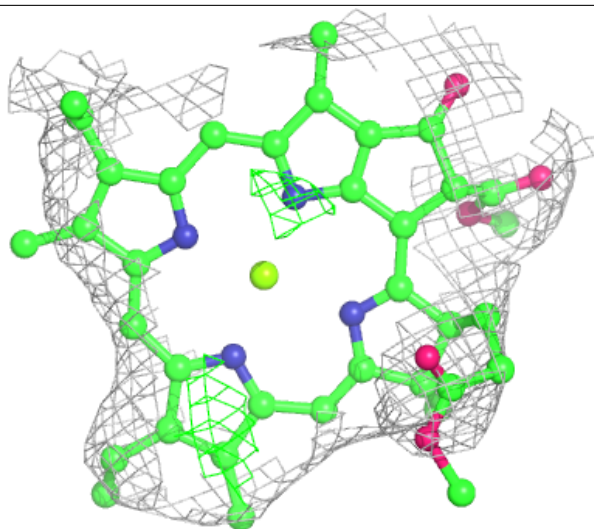
Electron density around CLA A 1114:

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



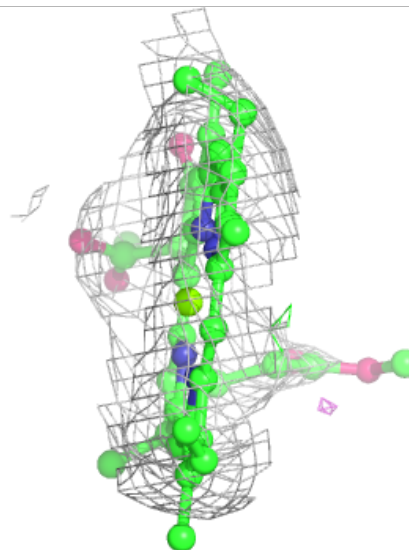
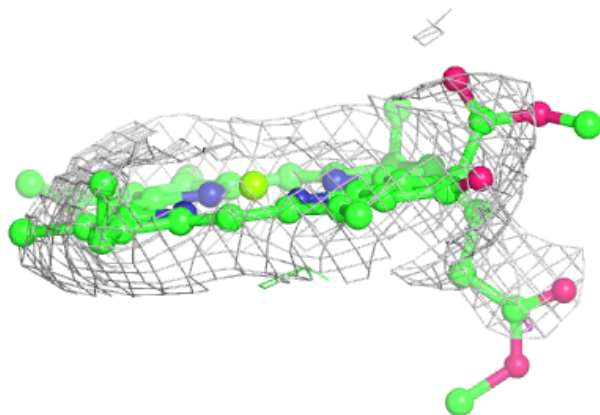
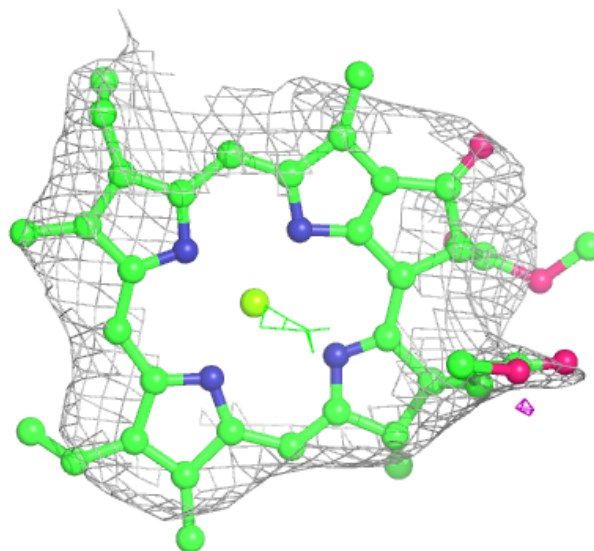
Electron density around CLA A 1120:

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



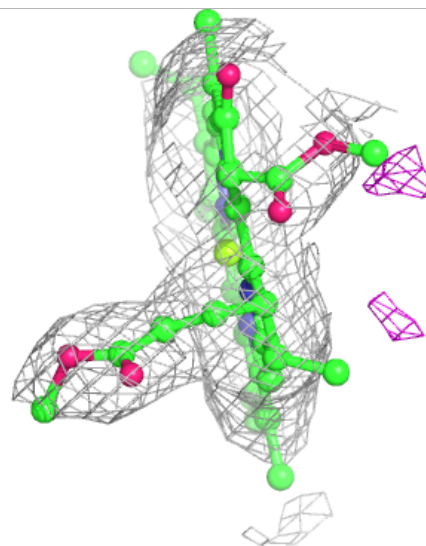
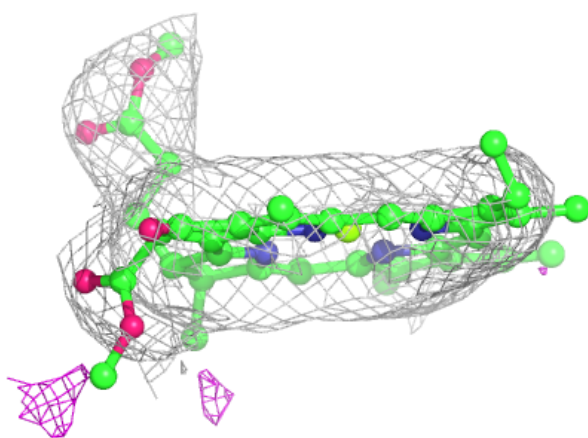
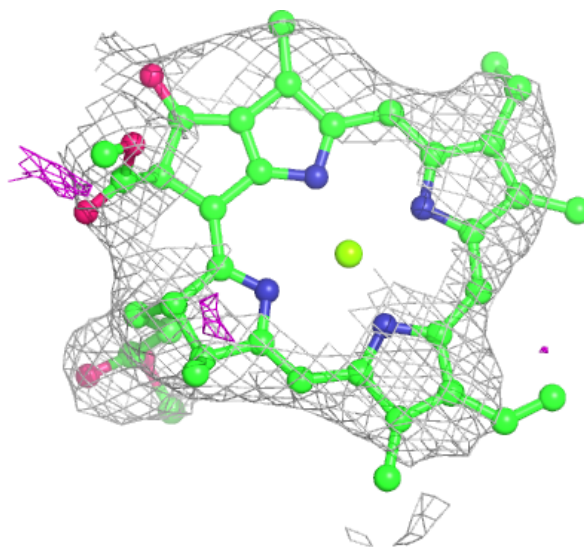
Electron density around CLA A 1121:

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



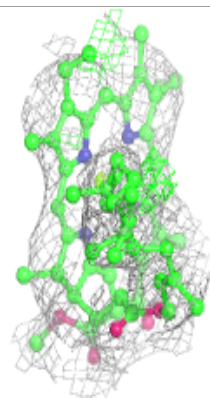
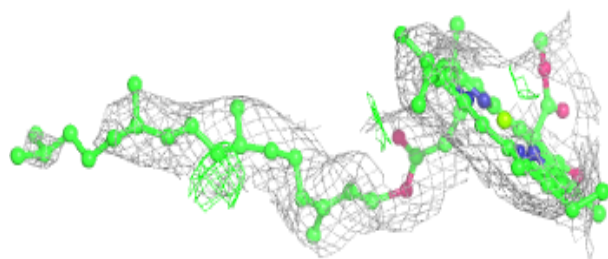
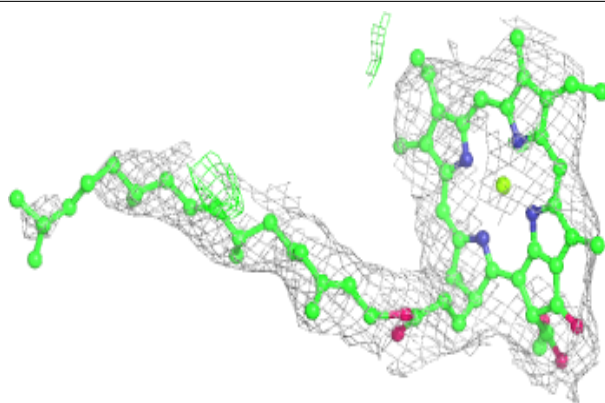
Electron density around CLA A 1129:

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



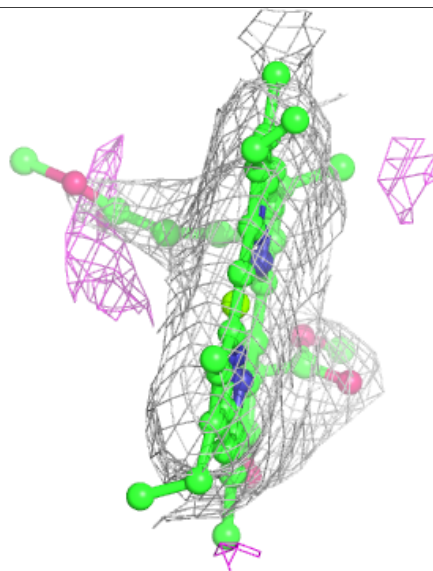
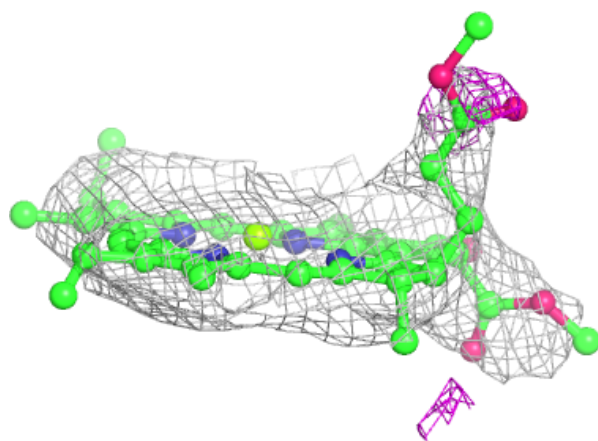
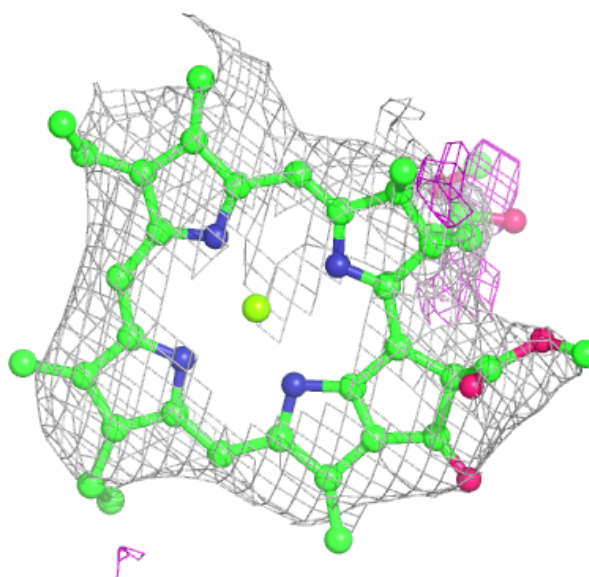
Electron density around CLA A 1132:

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



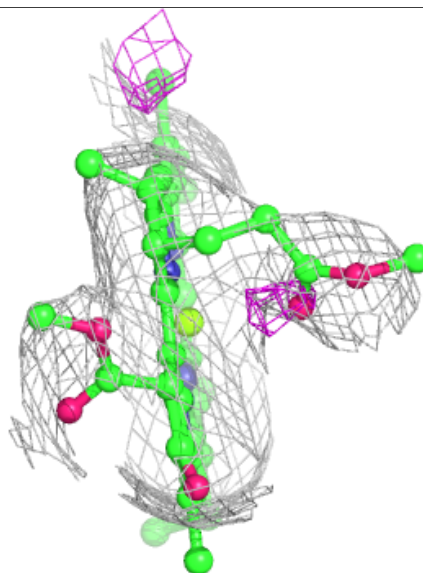
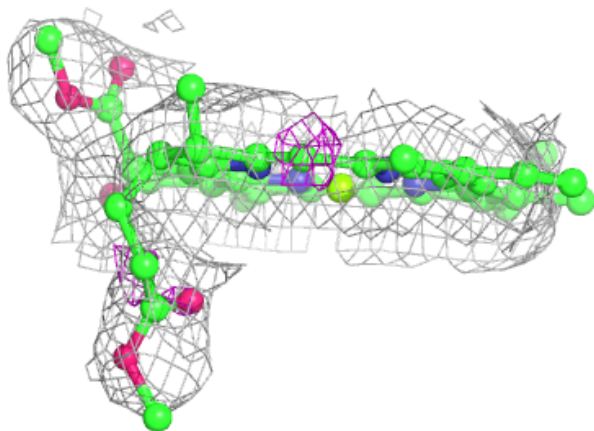
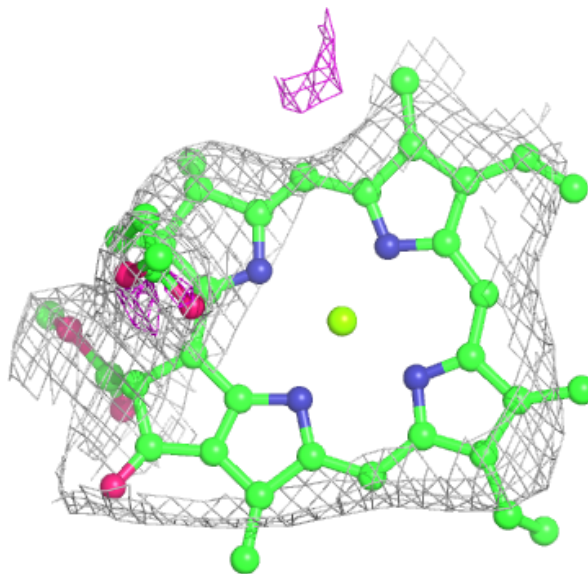
Electron density around CLA A 1133:

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



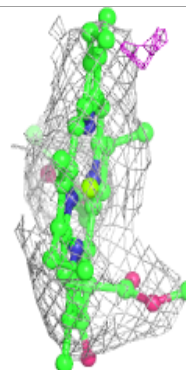
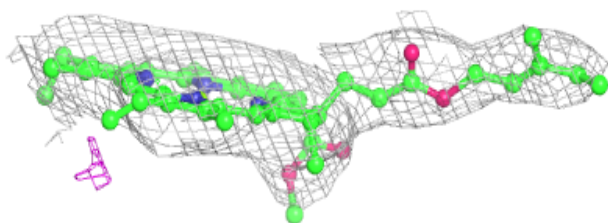
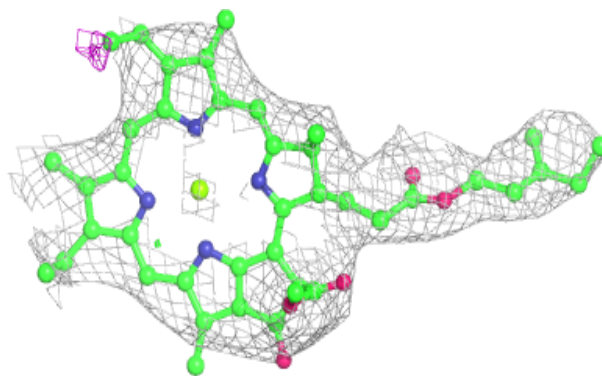
Electron density around CLA A 1134:

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

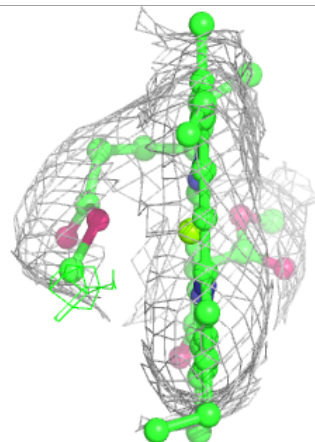
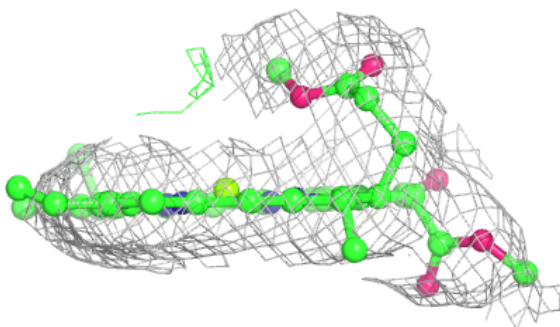
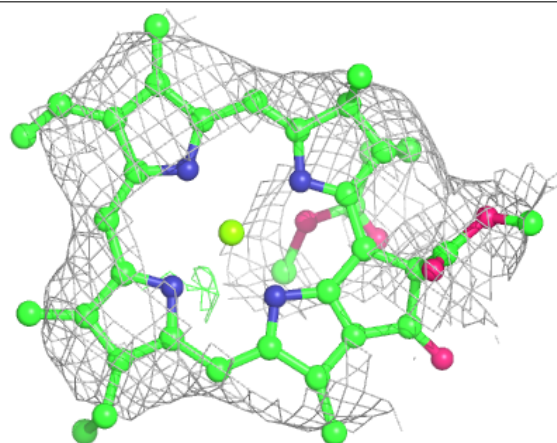


Electron density around CLA A 1135:

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

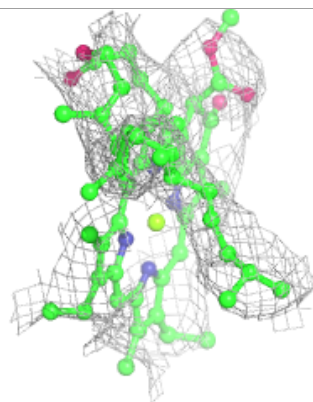
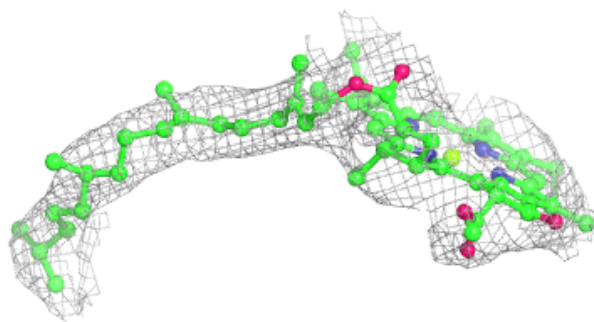
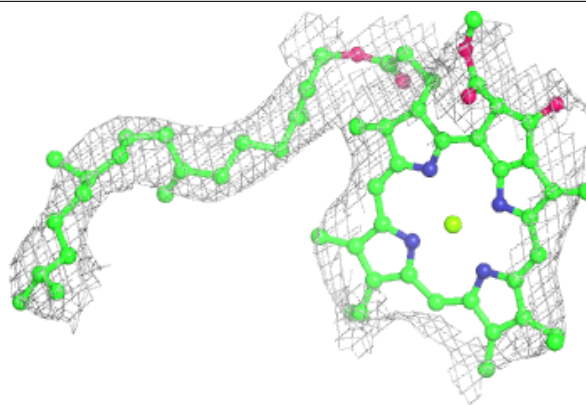
**Electron density around CLA A 1136:**

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

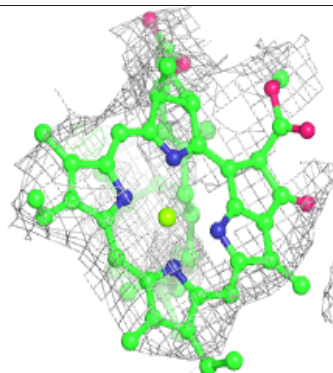
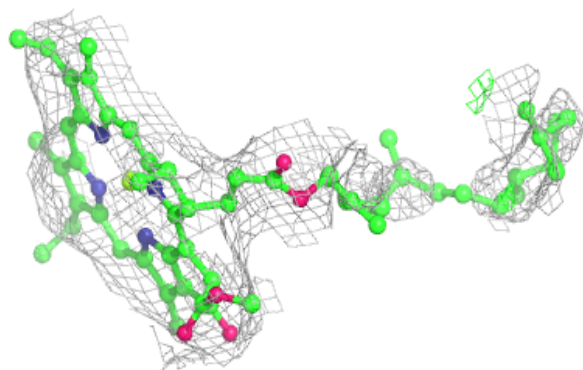
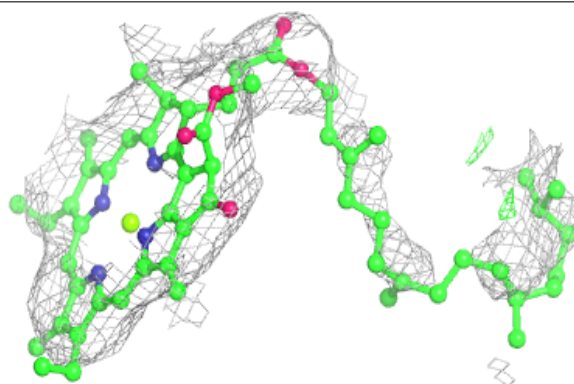


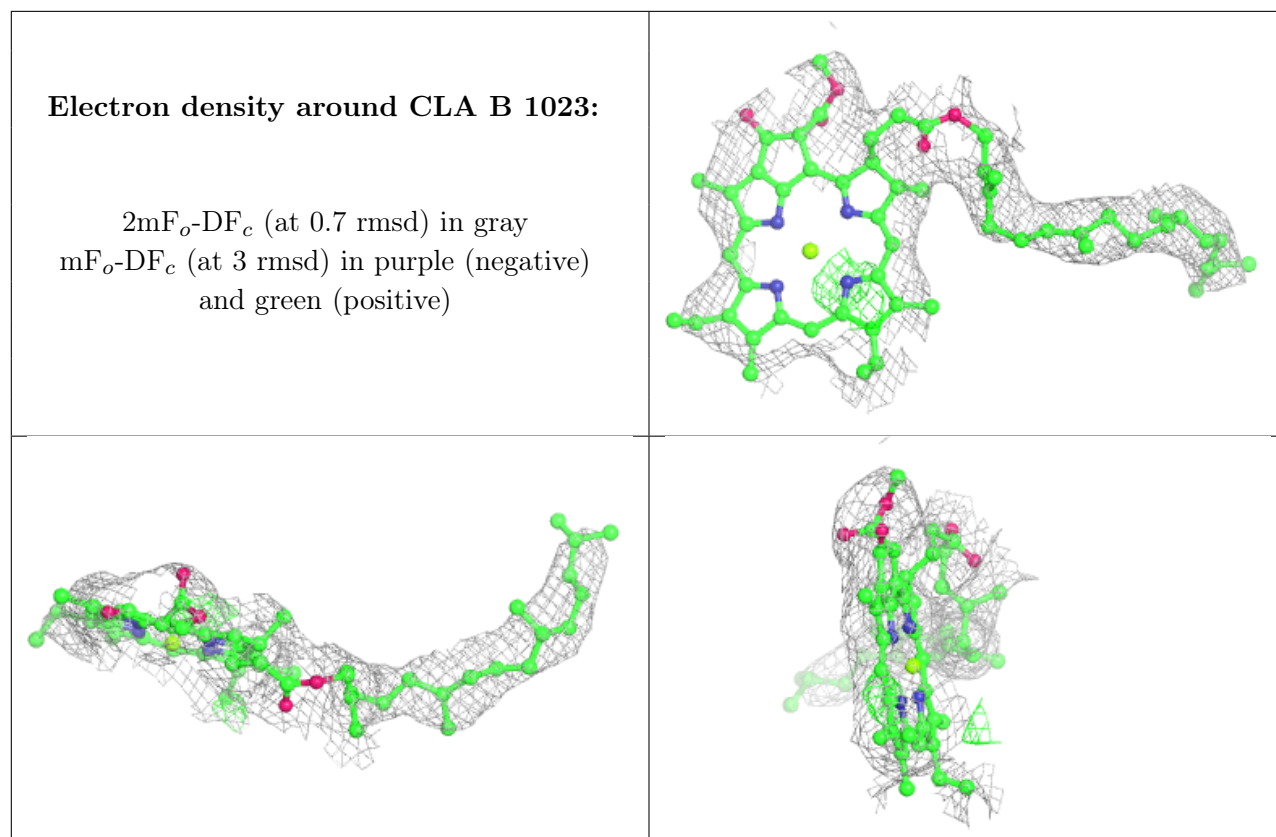
Electron density around CLA B 1013:

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

**Electron density around CLA B 1021:**

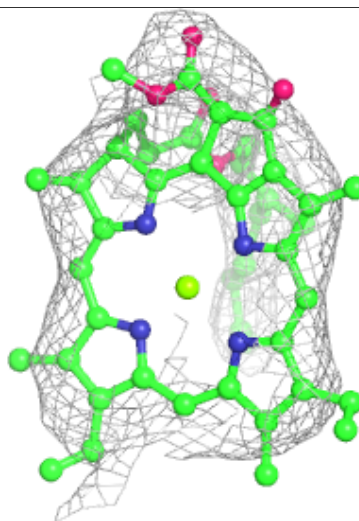
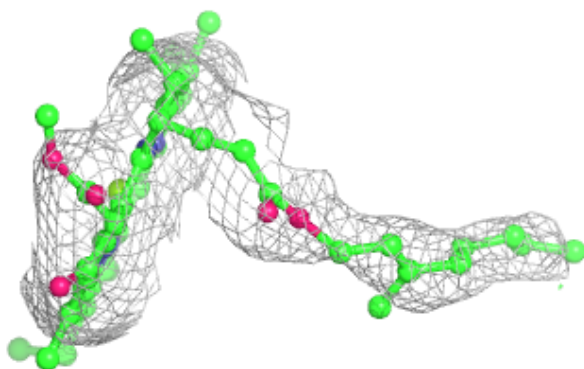
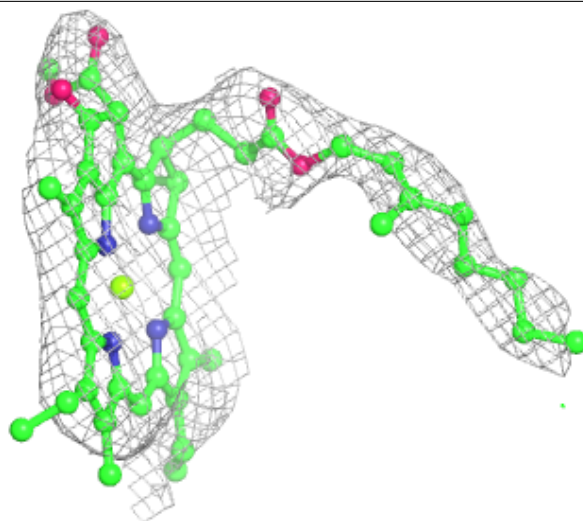
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





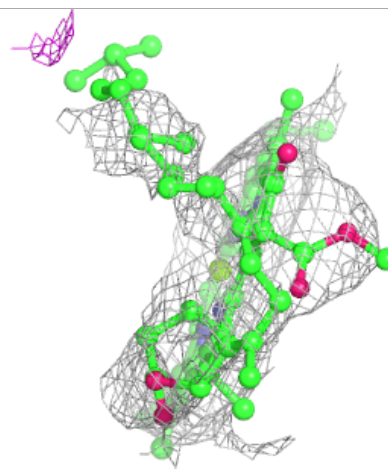
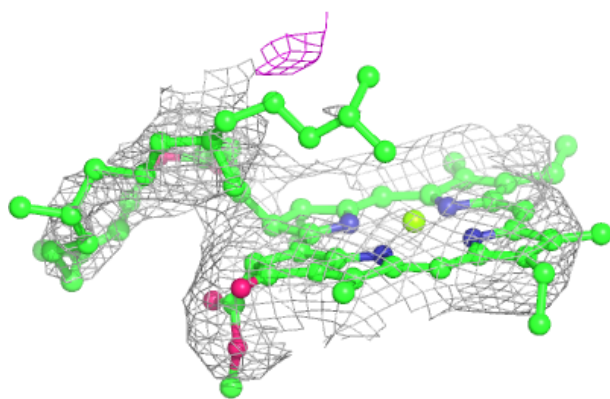
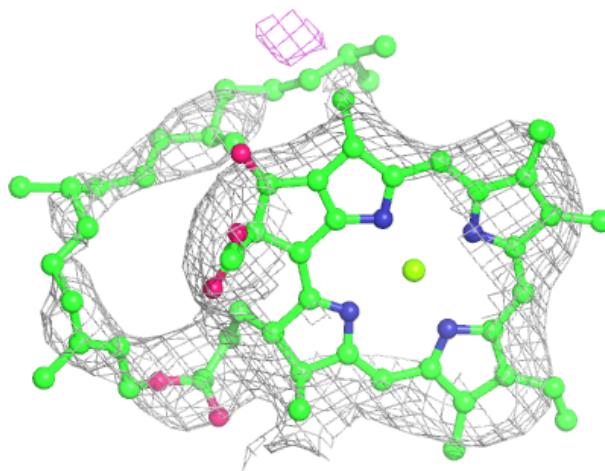
Electron density around CLA B 1201:

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



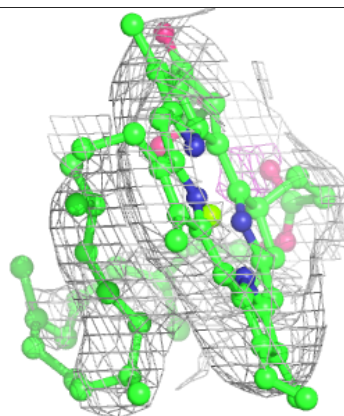
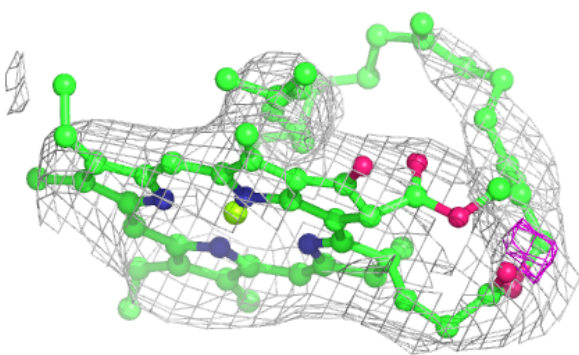
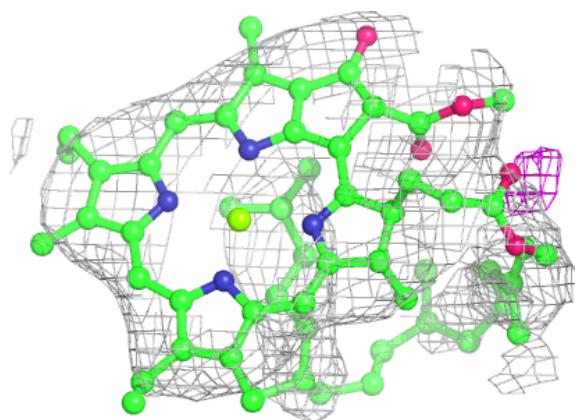
Electron density around CLA B 1202:

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



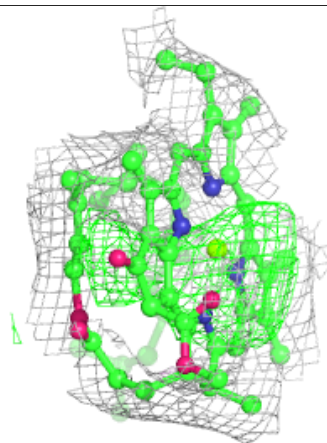
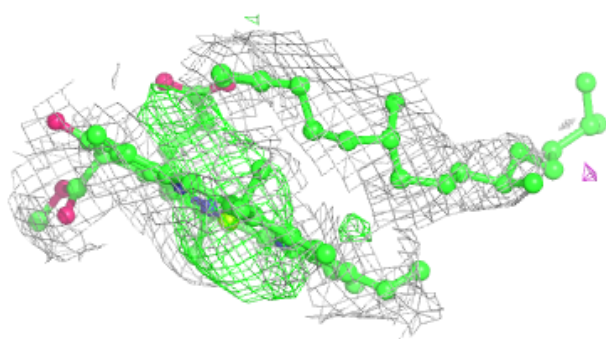
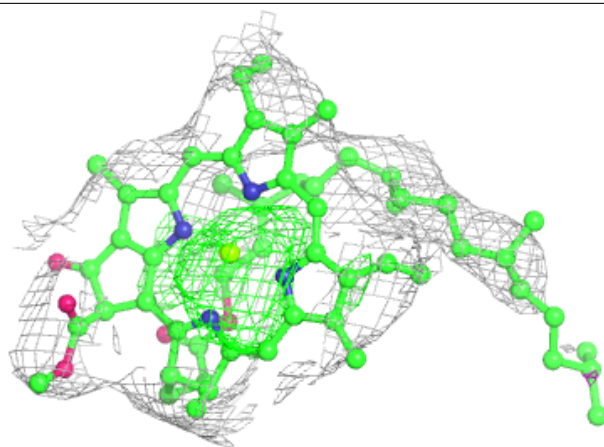
Electron density around CLA B 1203:

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



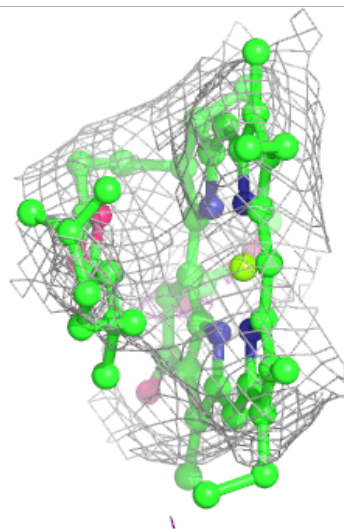
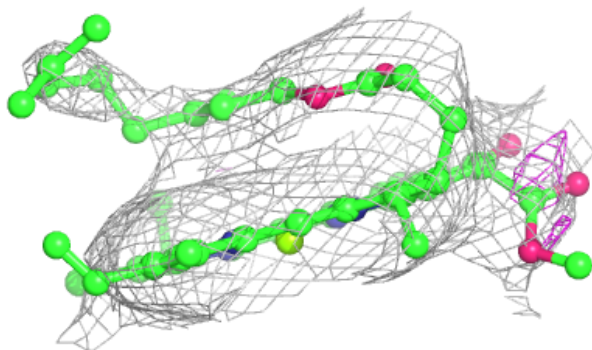
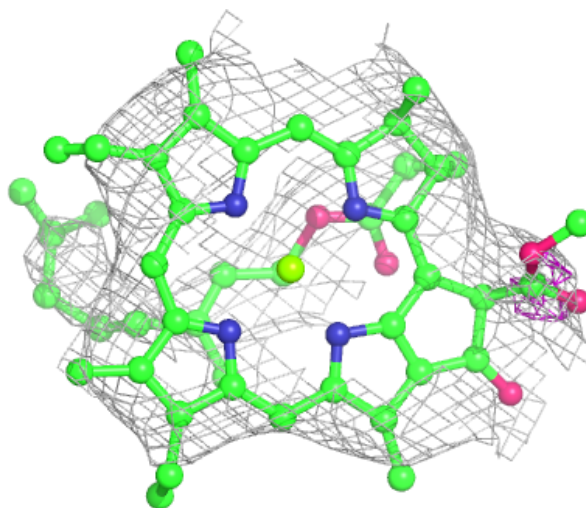
Electron density around CLA B 1204:

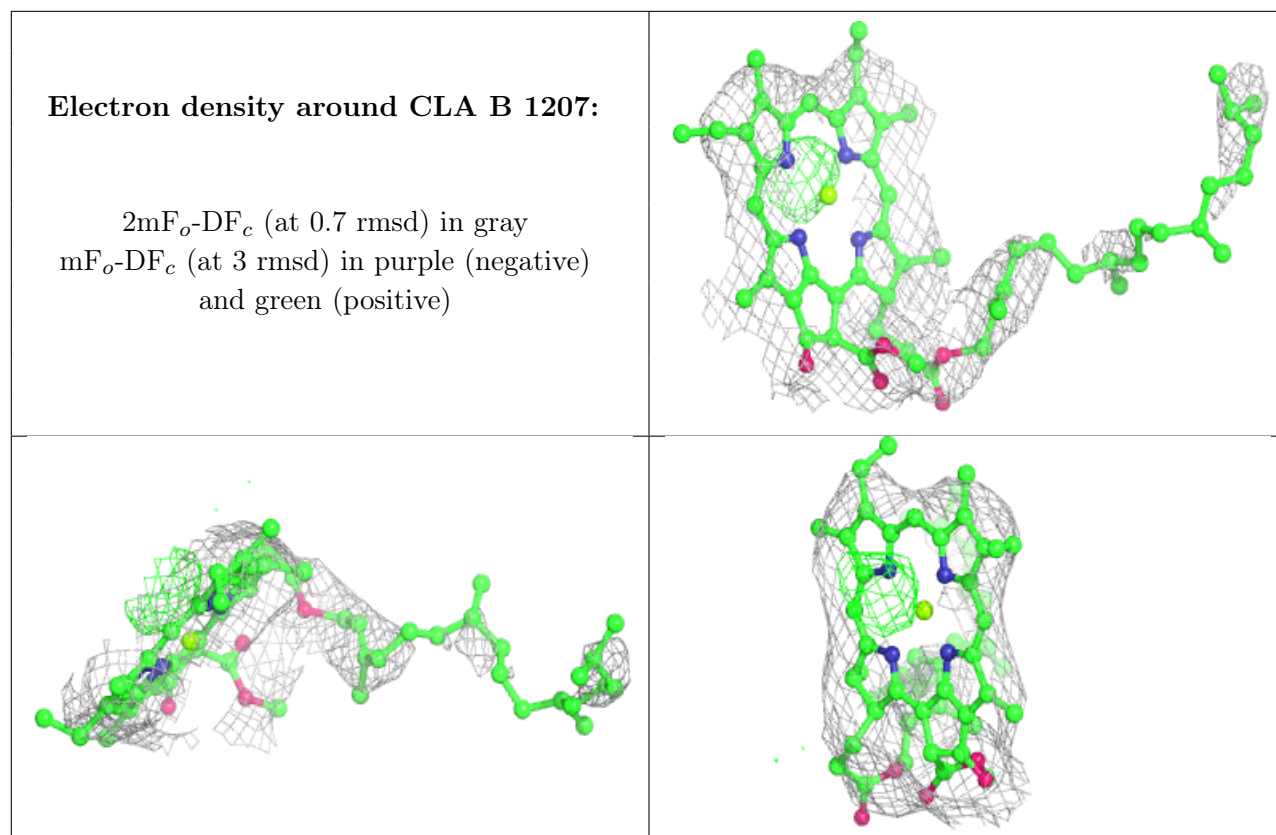
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around CLA B 1205:

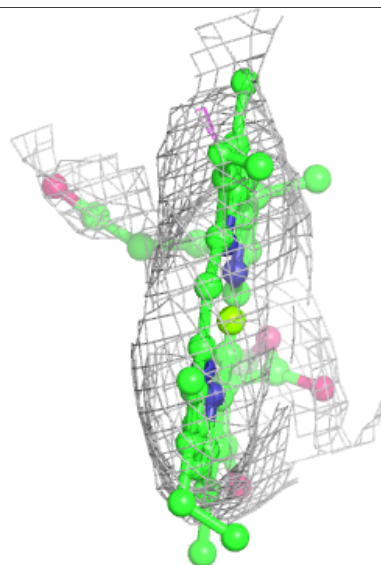
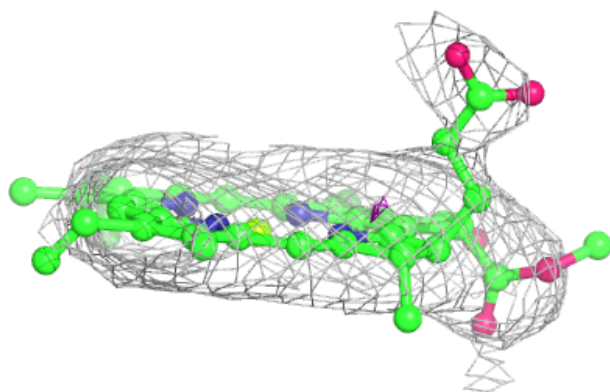
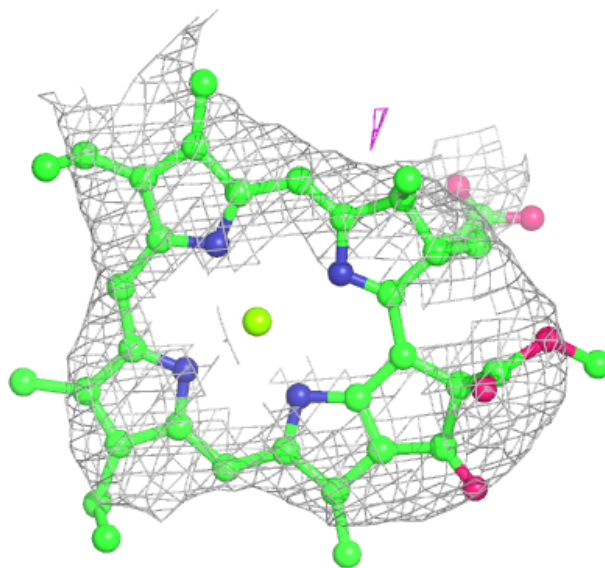
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





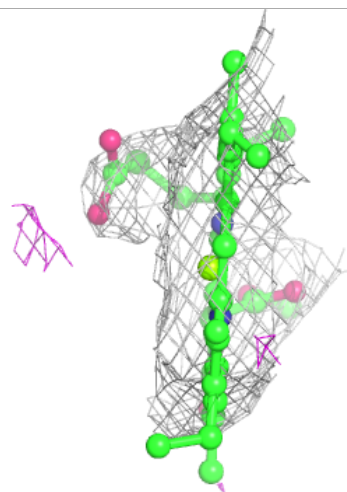
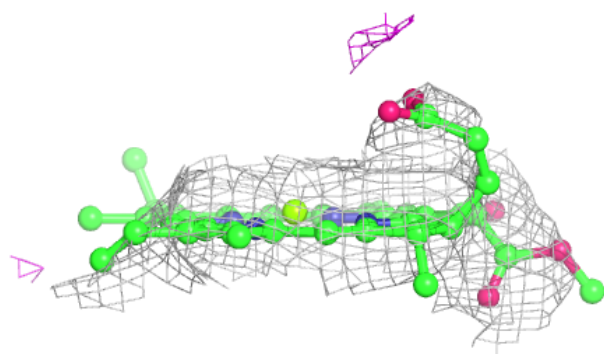
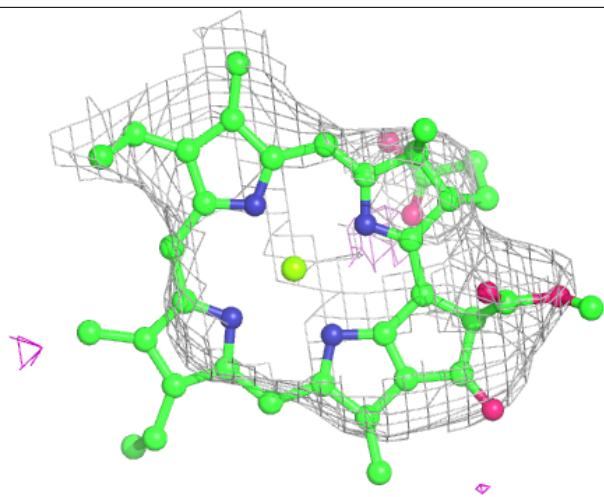
Electron density around CLA B 1208:

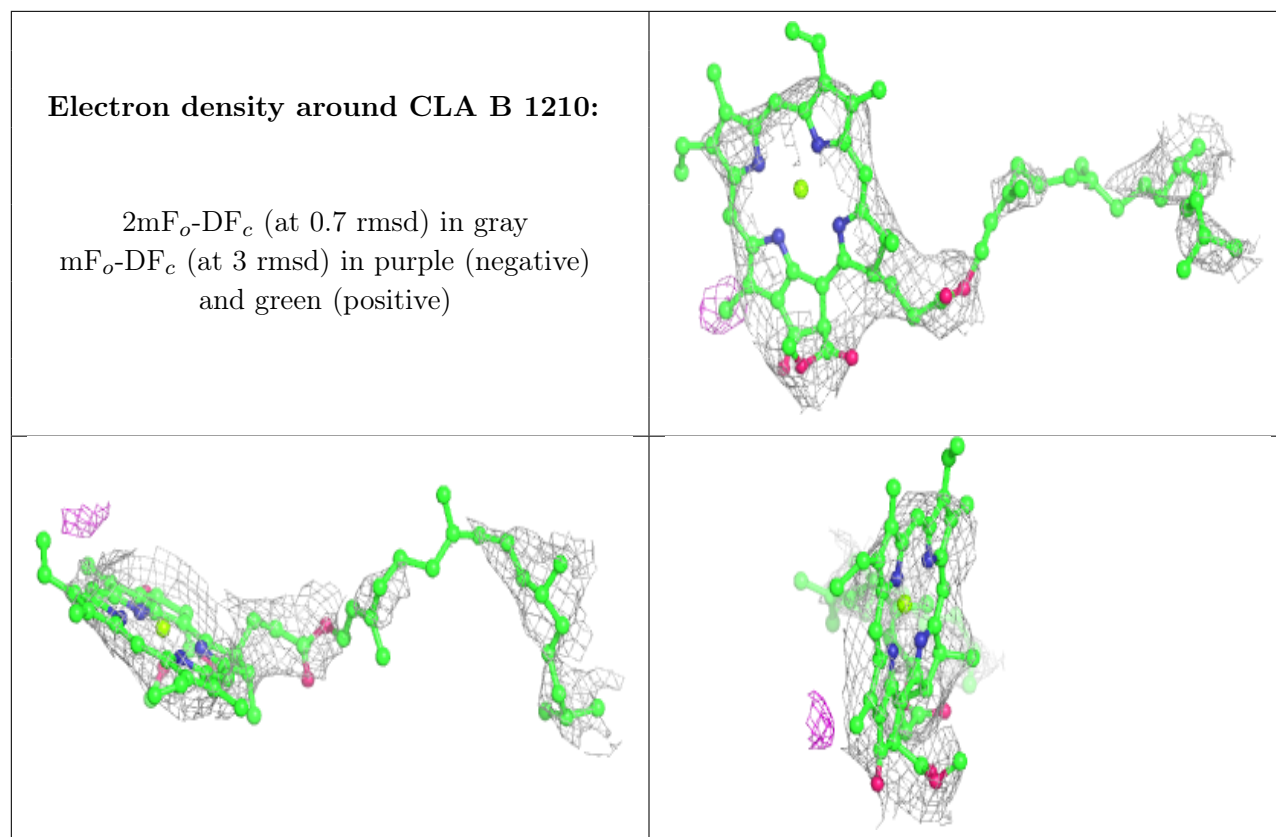
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around CLA B 1209:

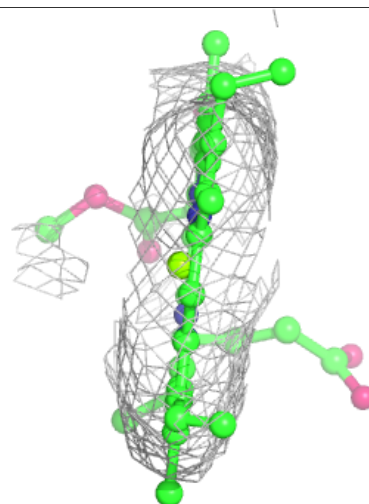
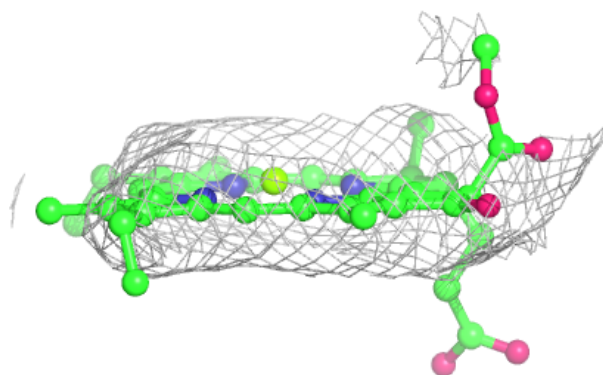
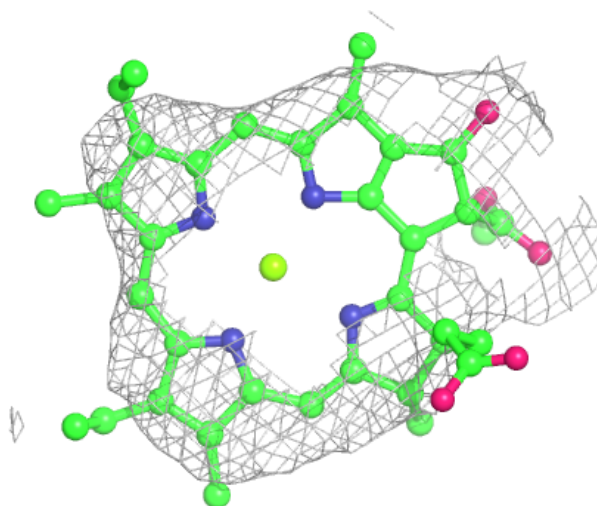
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





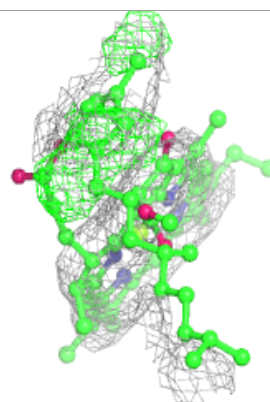
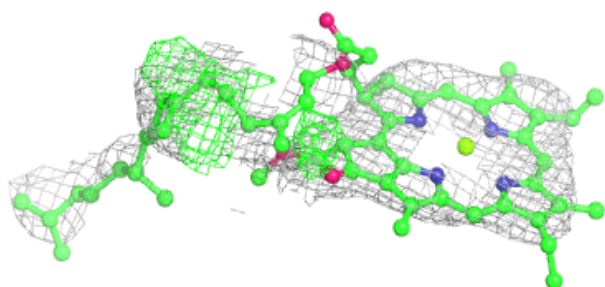
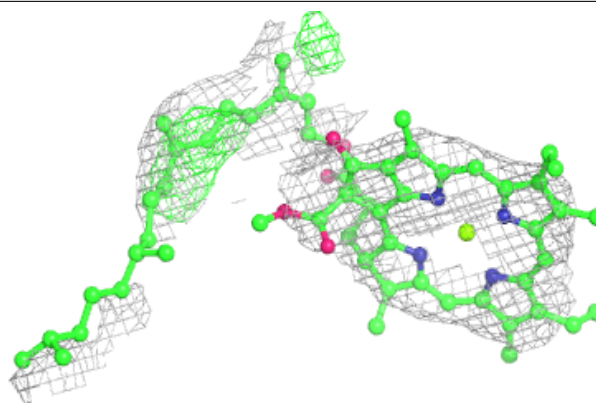
Electron density around CLA B 1212:

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

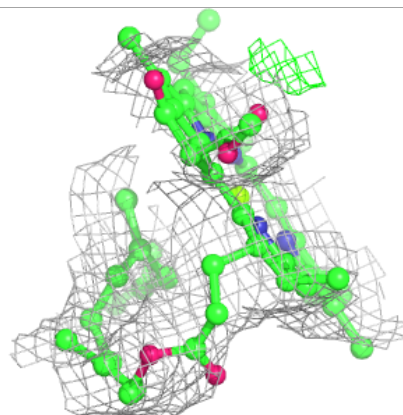
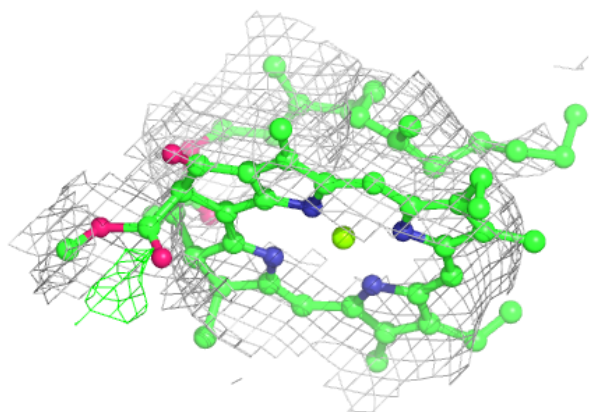
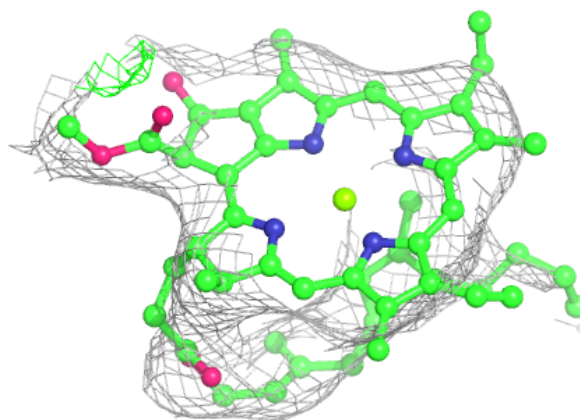


Electron density around CLA B 1213:

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

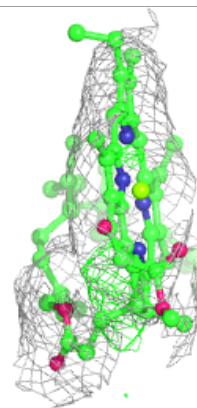
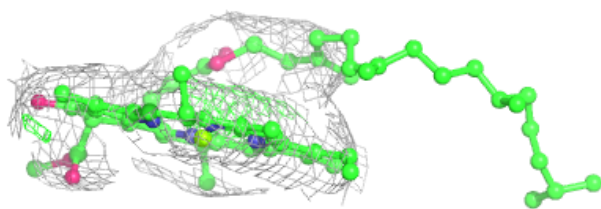
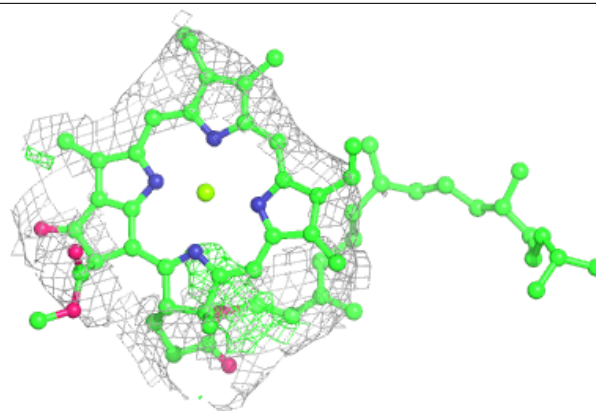
**Electron density around CLA B 1214:**

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

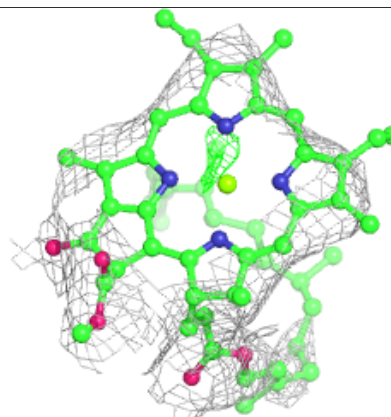
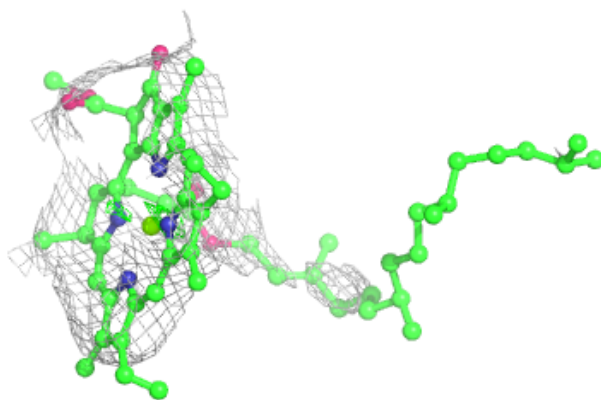
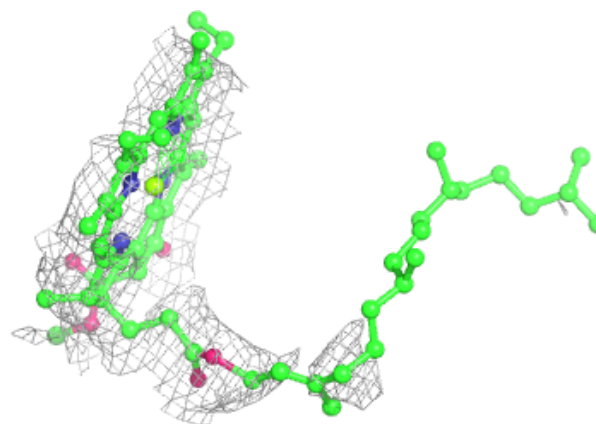


Electron density around CLA B 1215:

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

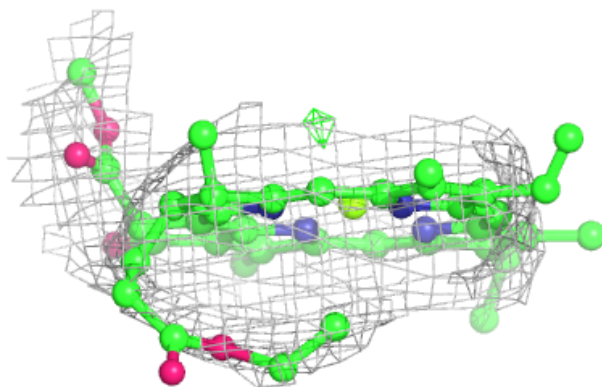
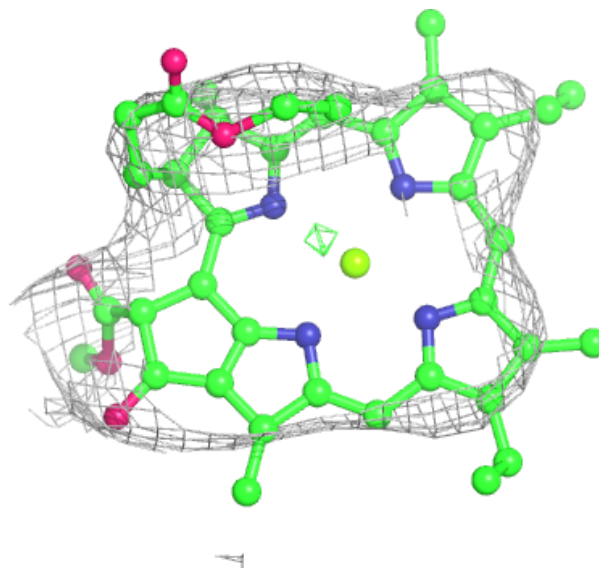
**Electron density around CLA B 1216:**

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



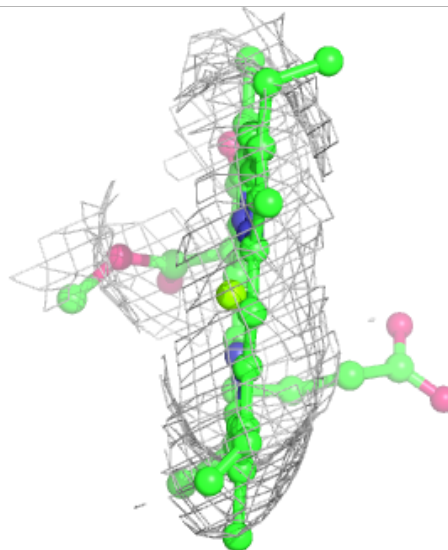
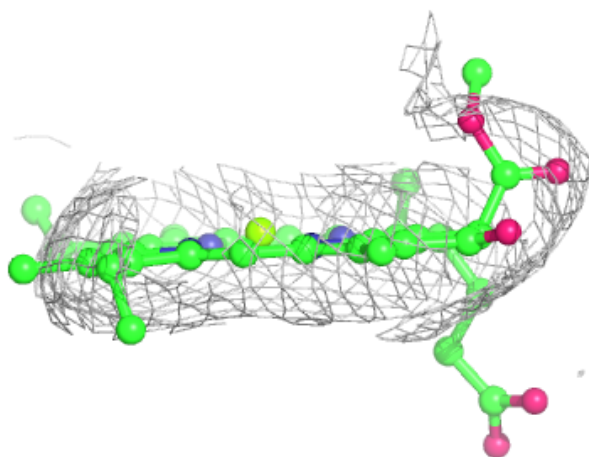
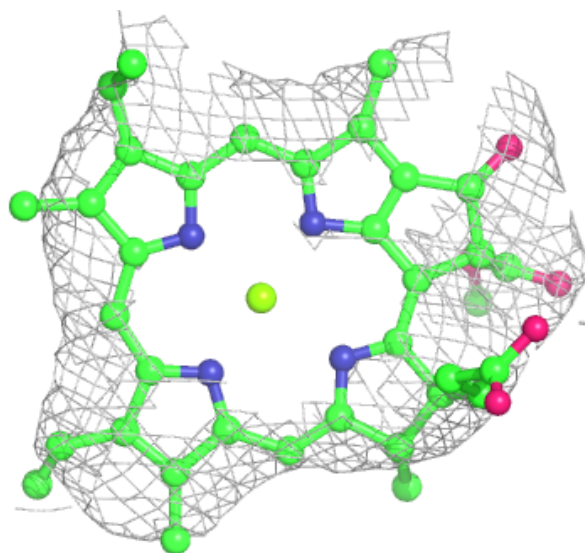
Electron density around CLA B 1217:

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



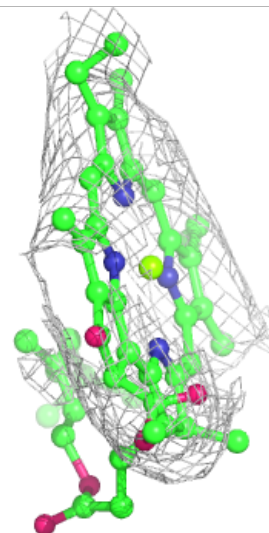
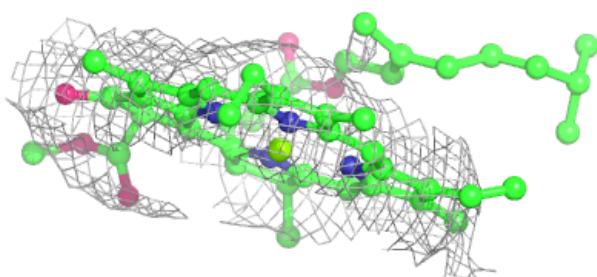
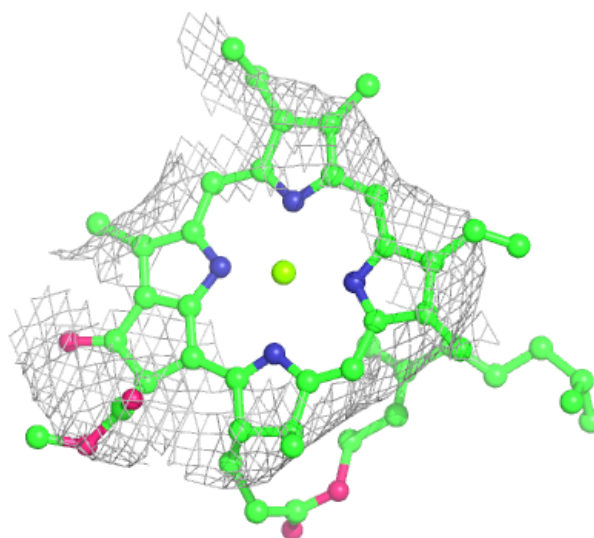
Electron density around CLA B 1218:

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



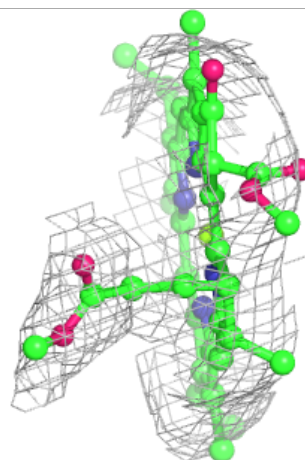
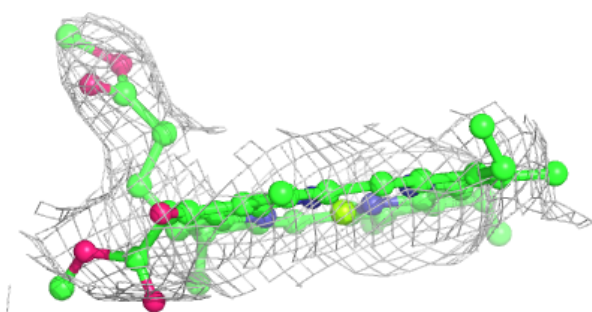
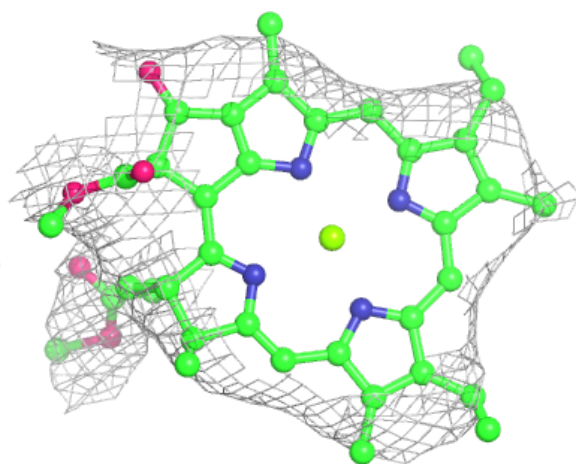
Electron density around CLA B 1219:

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



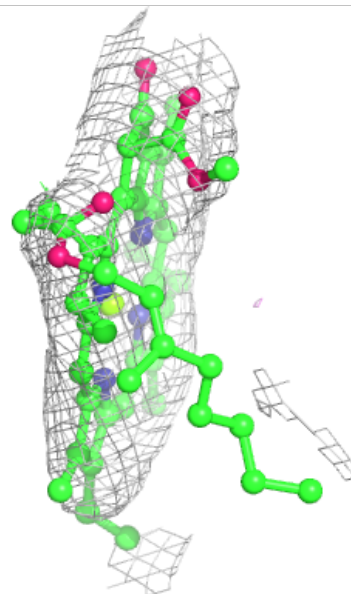
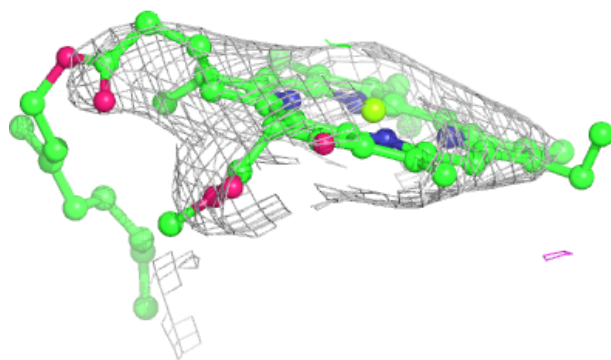
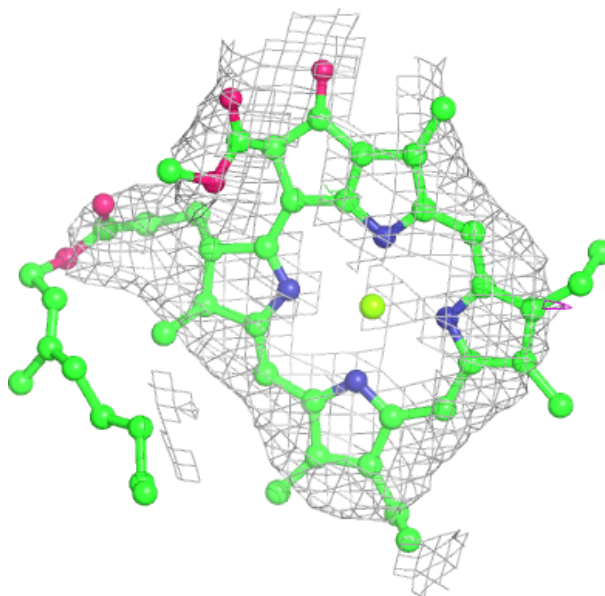
Electron density around CLA B 1220:

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



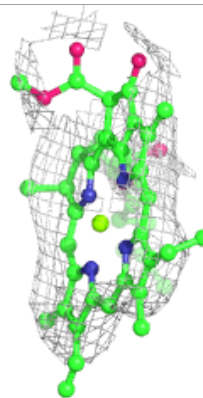
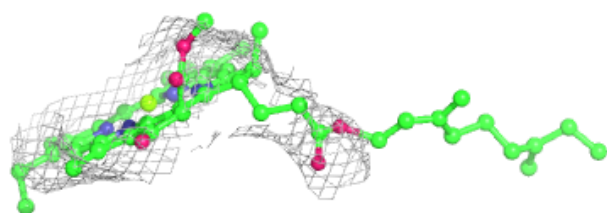
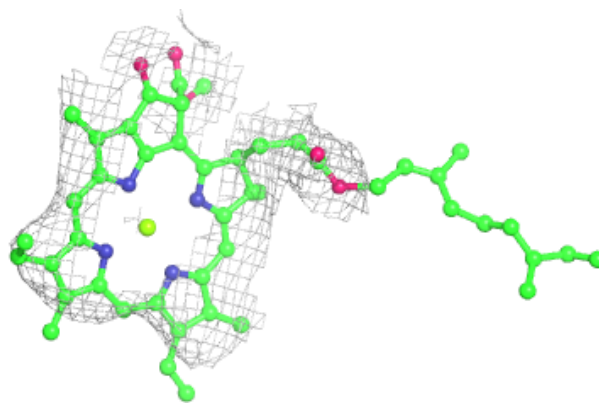
Electron density around CLA B 1221:

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

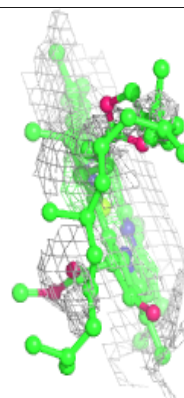
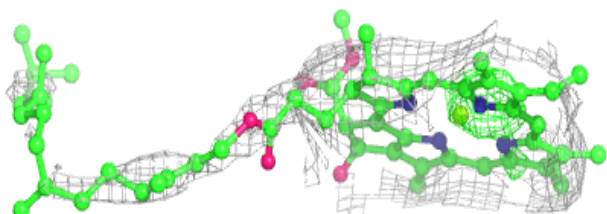
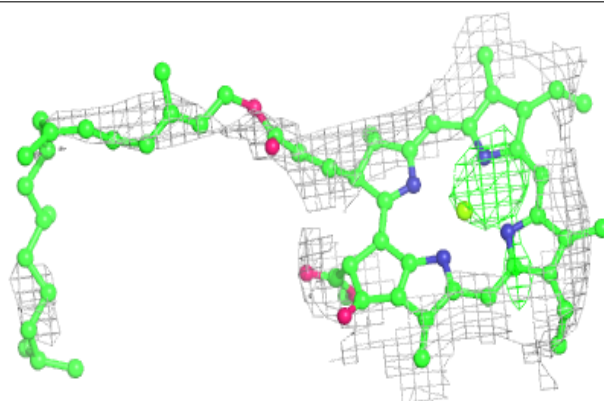


Electron density around CLA B 1222:

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

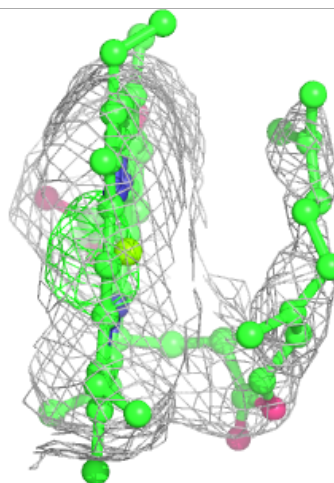
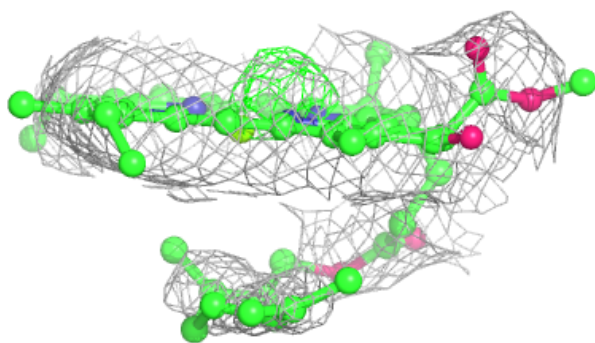
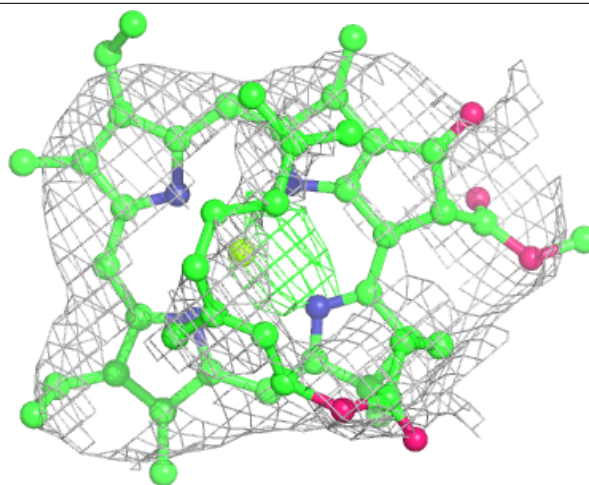
**Electron density around CLA B 1223:**

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



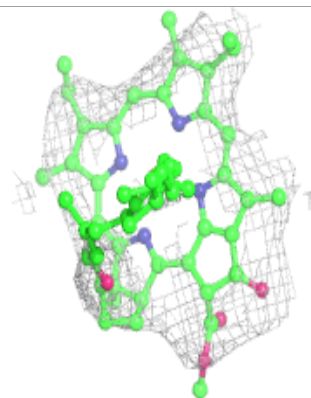
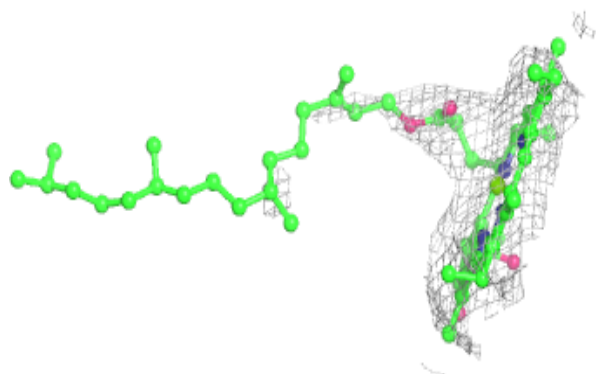
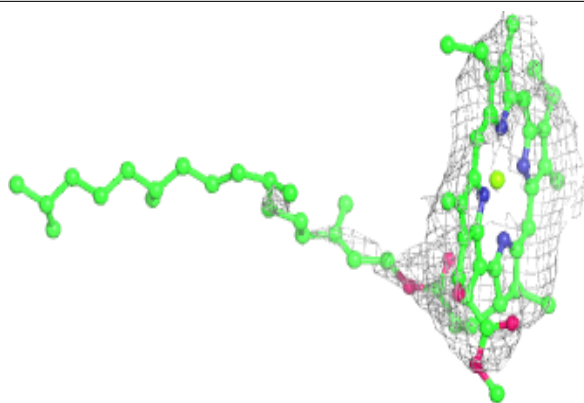
Electron density around CLA B 1224:

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

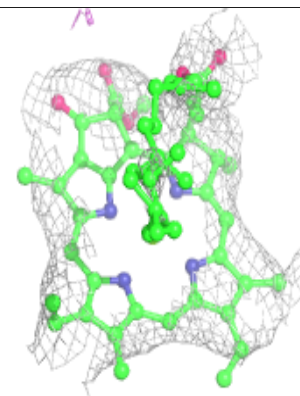
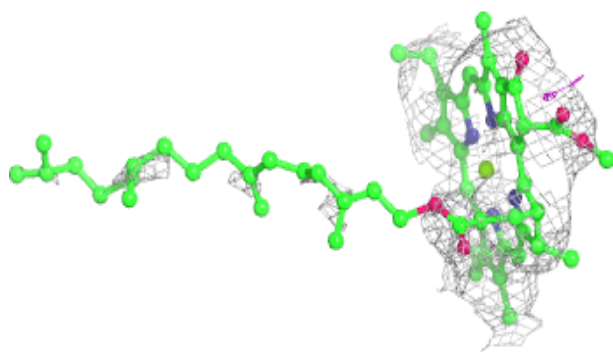
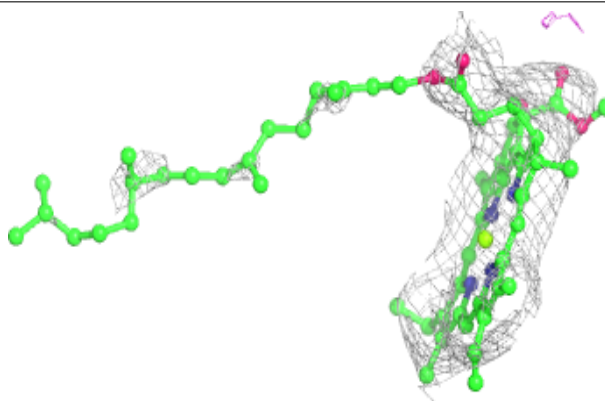


Electron density around CLA B 1225:

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

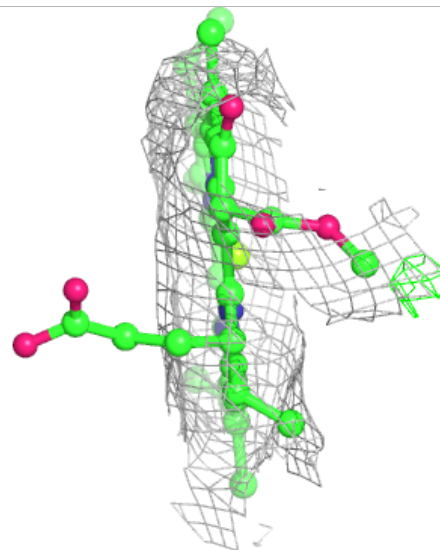
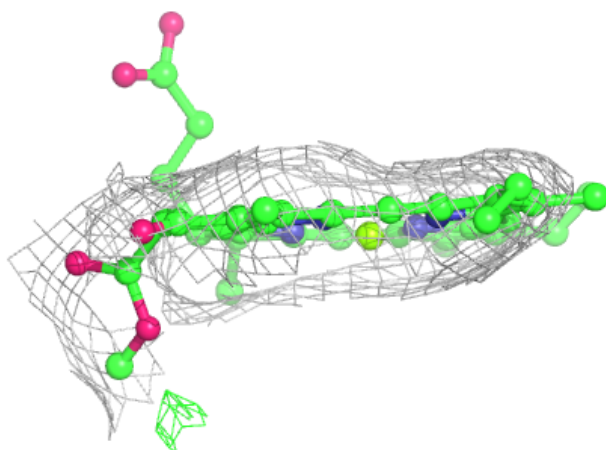
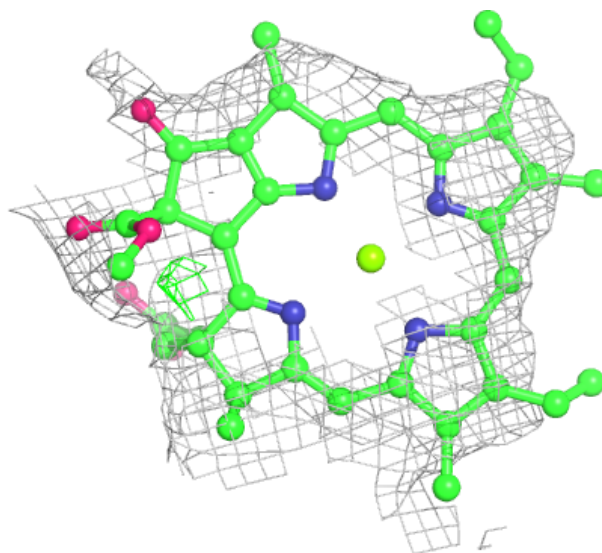
**Electron density around CLA B 1226:**

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



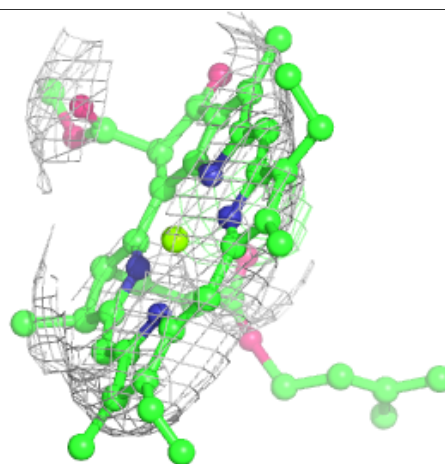
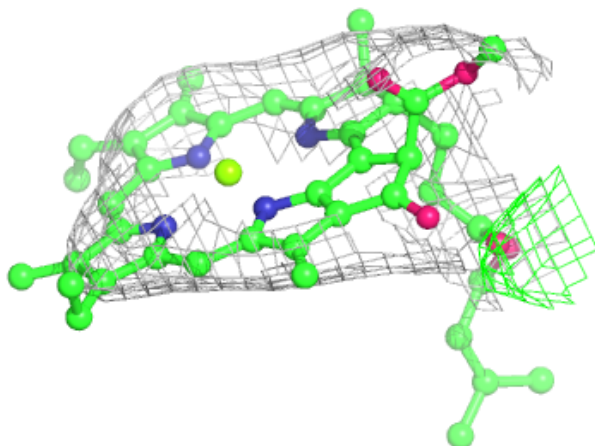
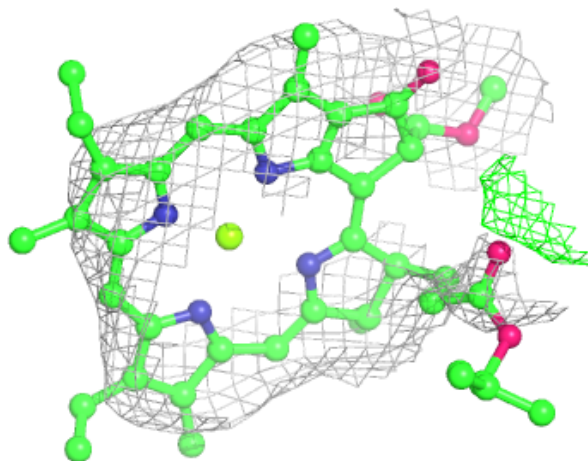
Electron density around CLA B 1227:

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



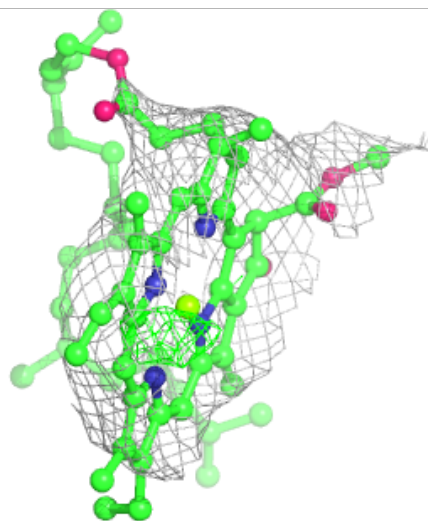
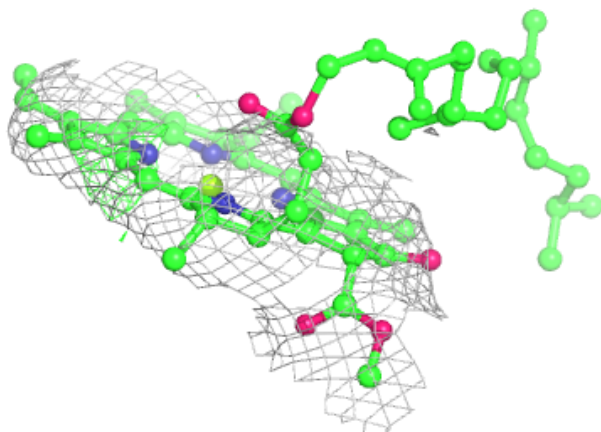
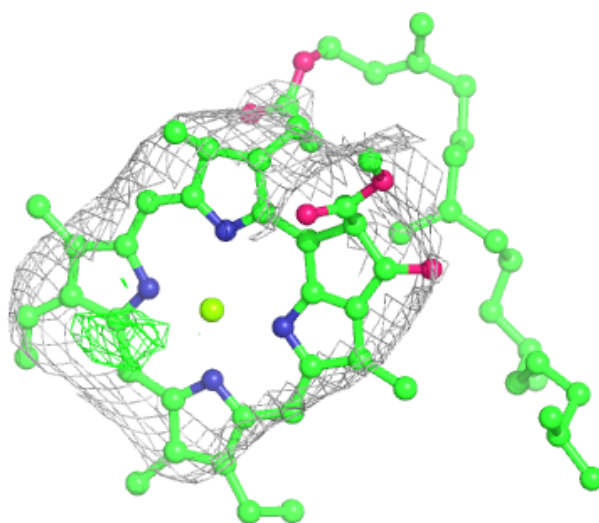
Electron density around CLA B 1228:

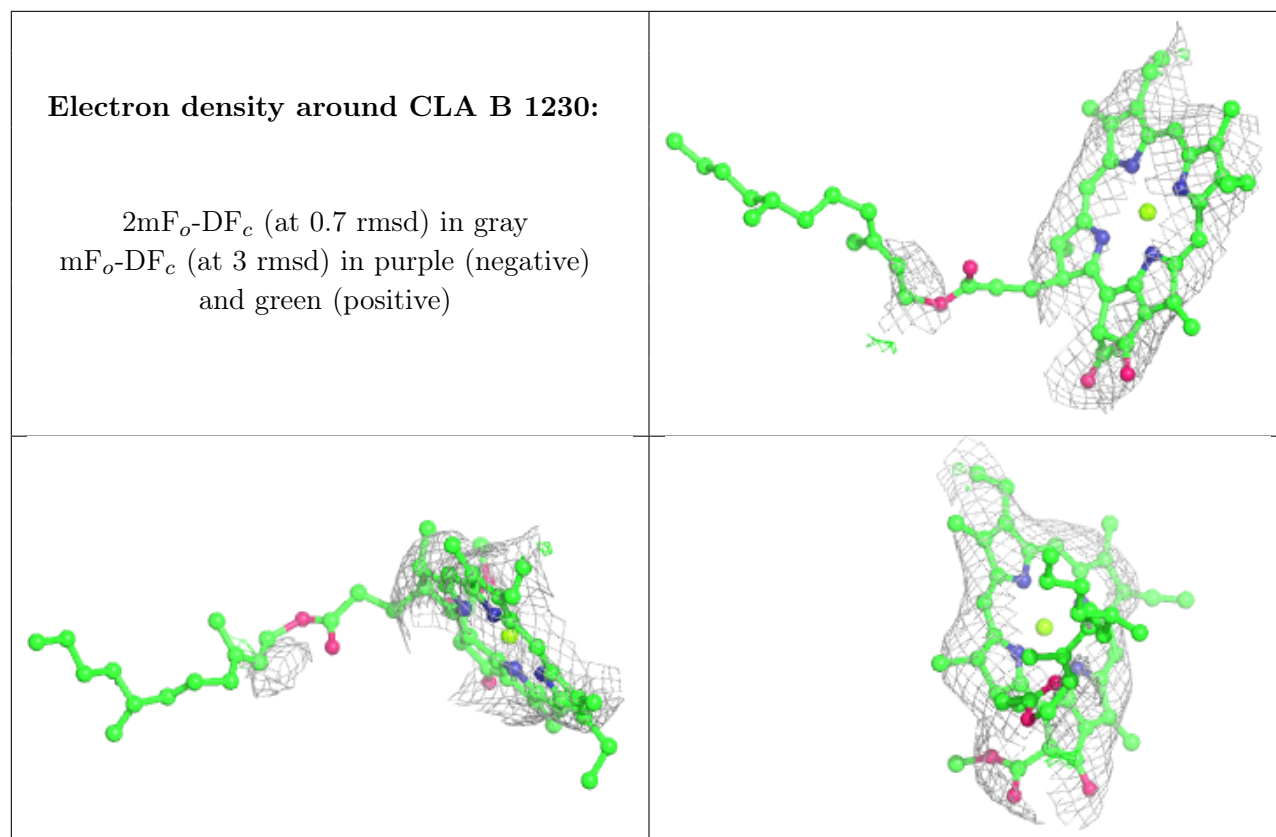
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around CLA B 1229:

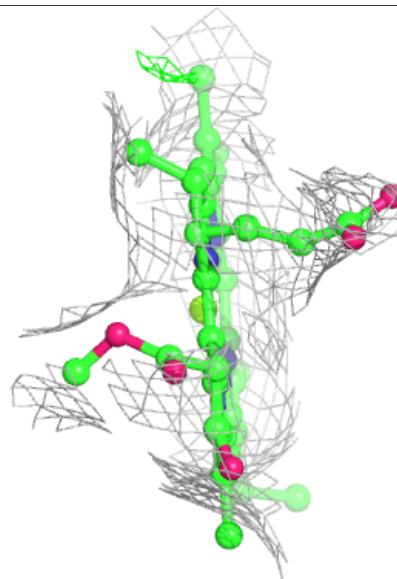
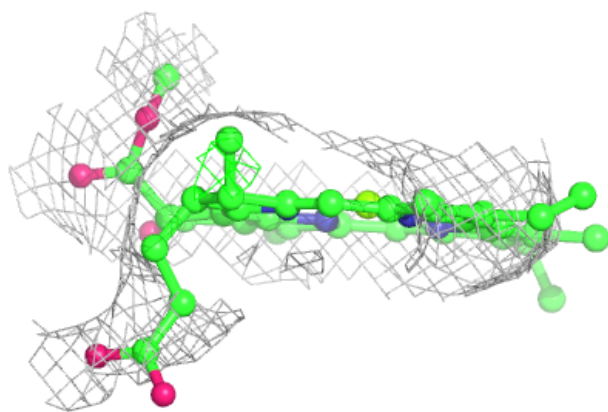
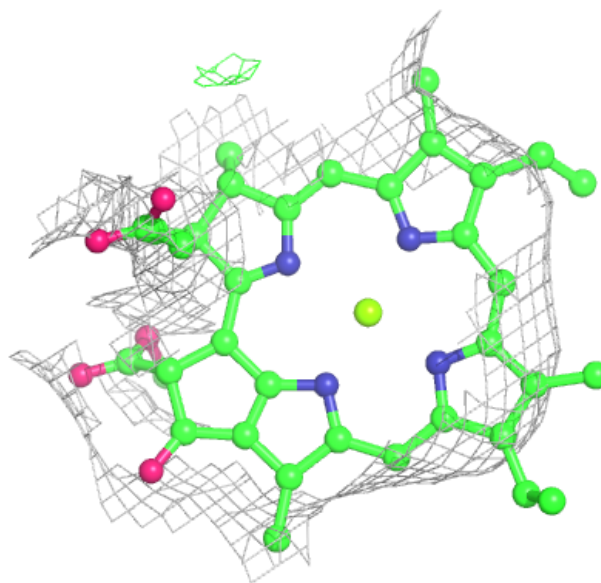
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





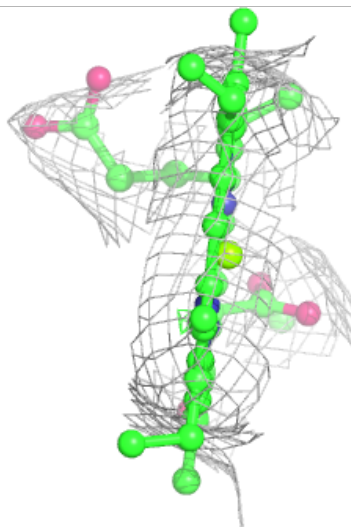
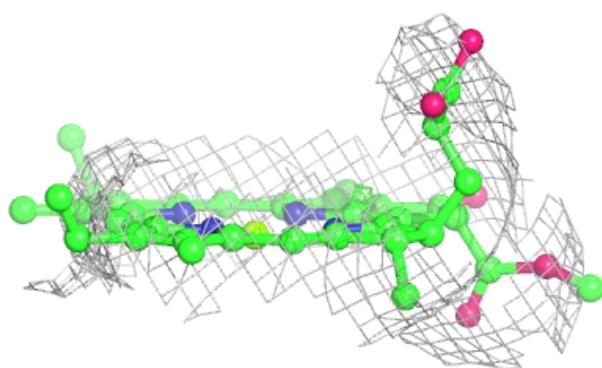
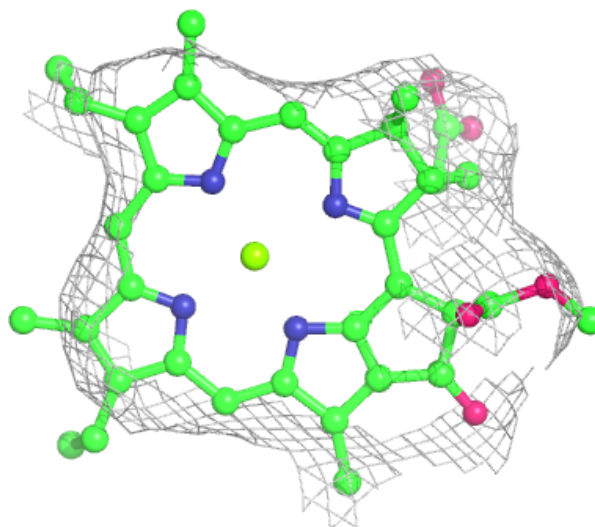
Electron density around CLA B 1231:

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



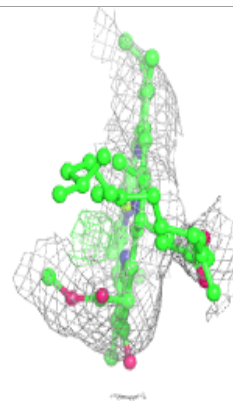
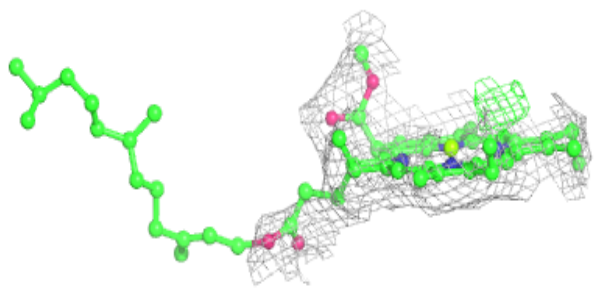
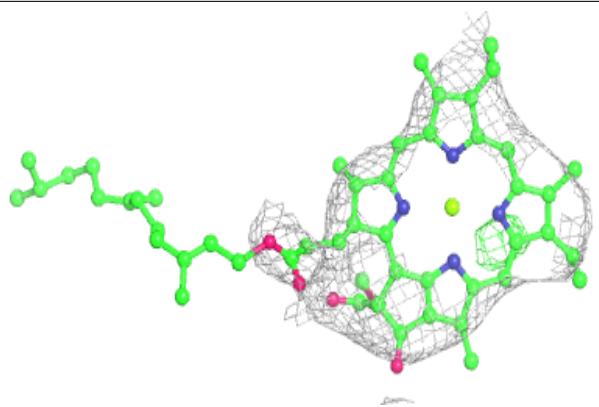
Electron density around CLA B 1232:

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

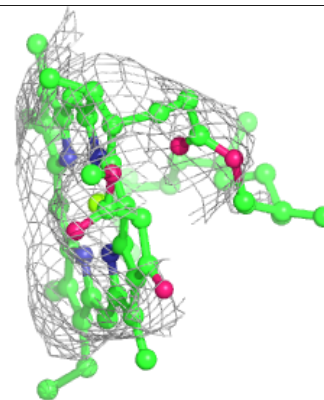
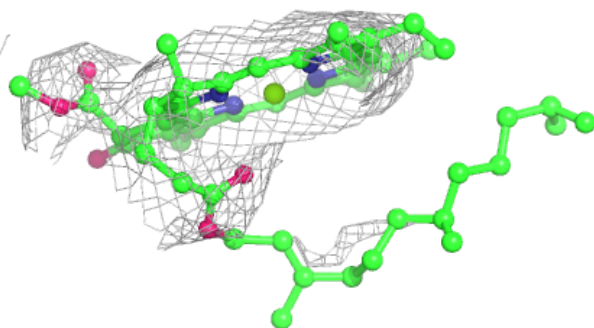
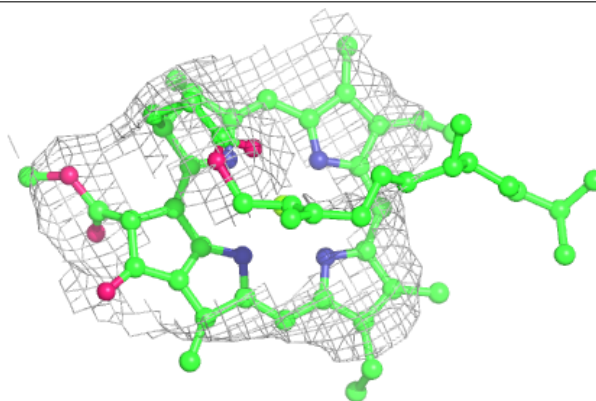


Electron density around CLA B 1234:

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

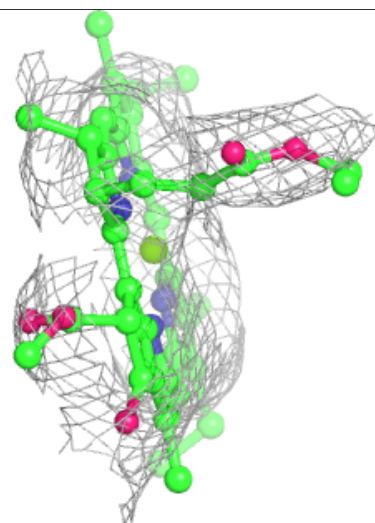
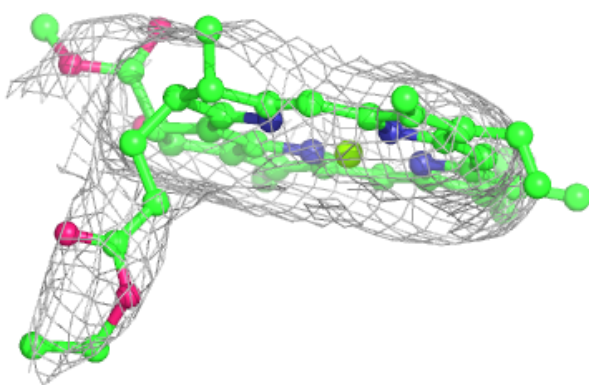
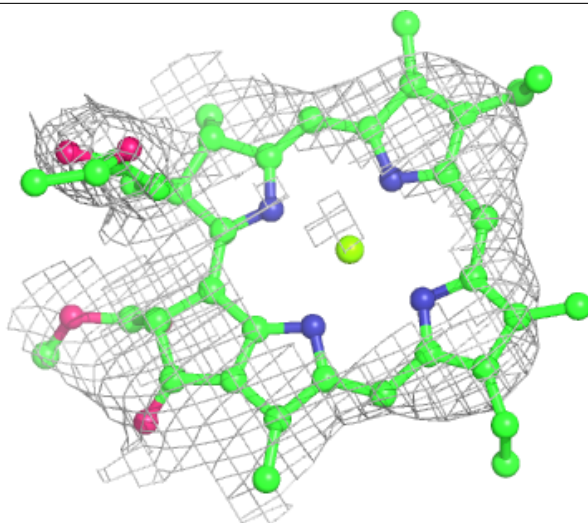
**Electron density around CLA B 1235:**

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



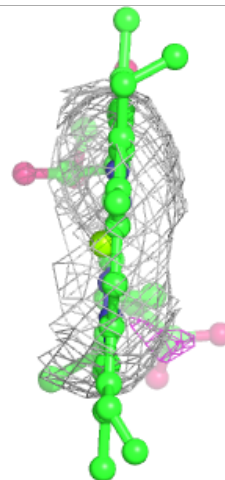
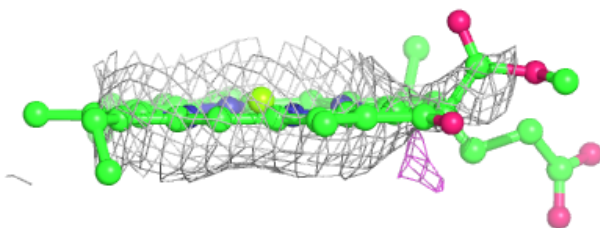
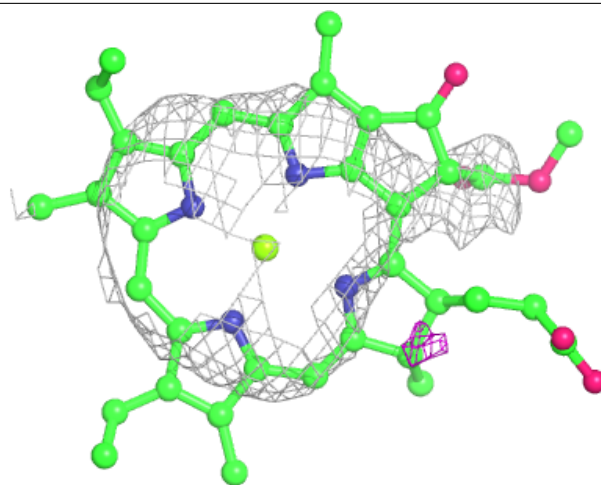
Electron density around CLA B 1236:

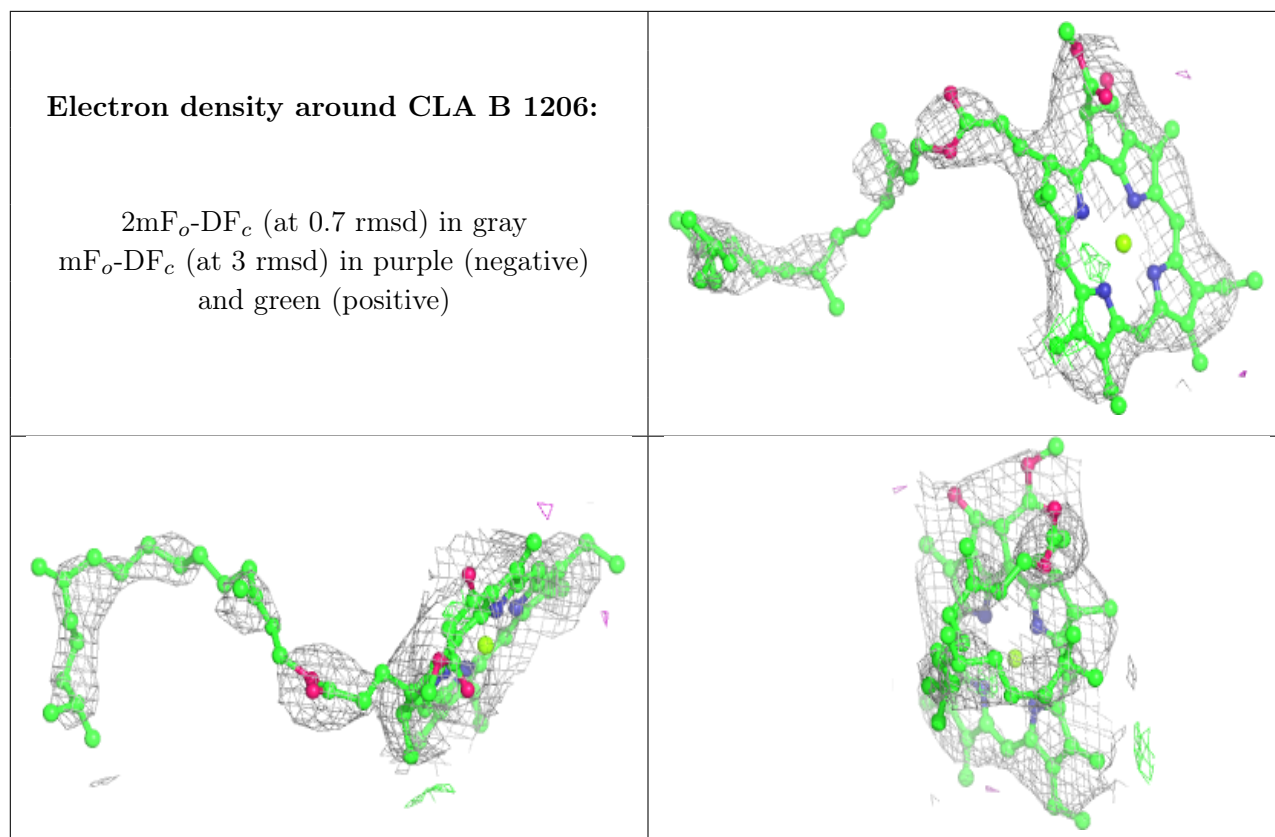
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around CLA B 1240:

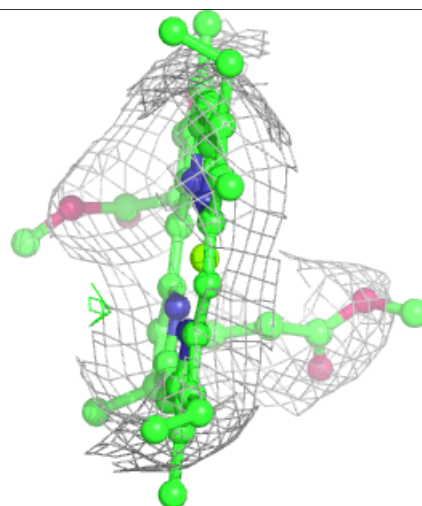
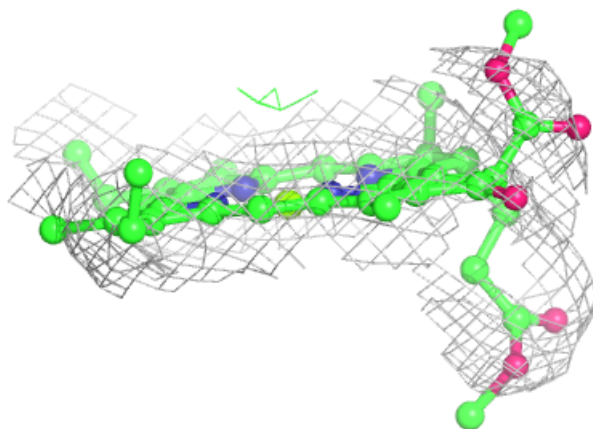
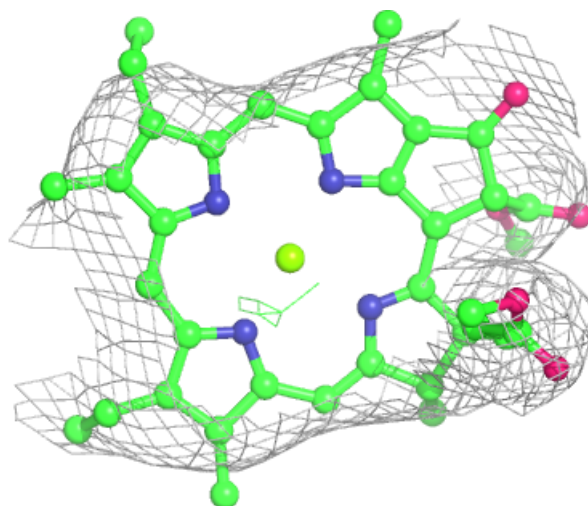
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

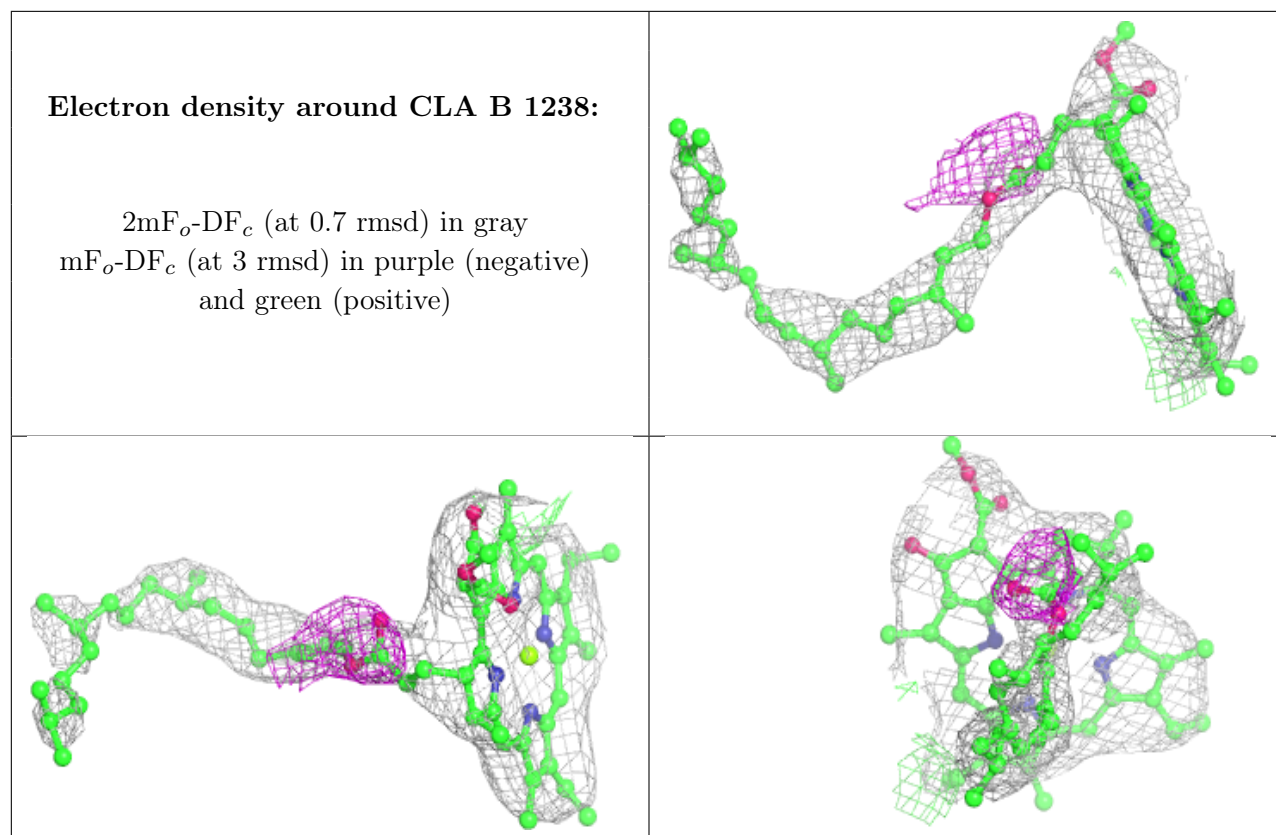




Electron density around CLA B 1211:

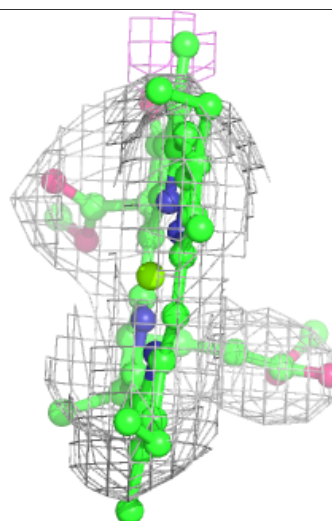
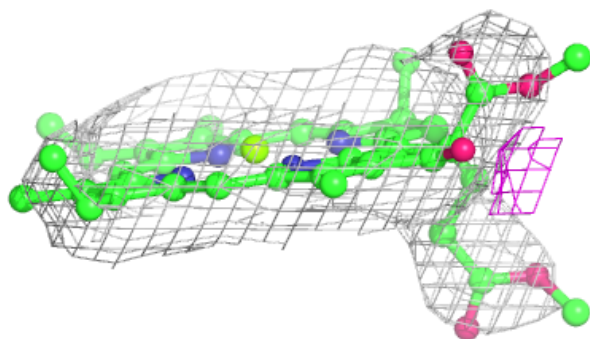
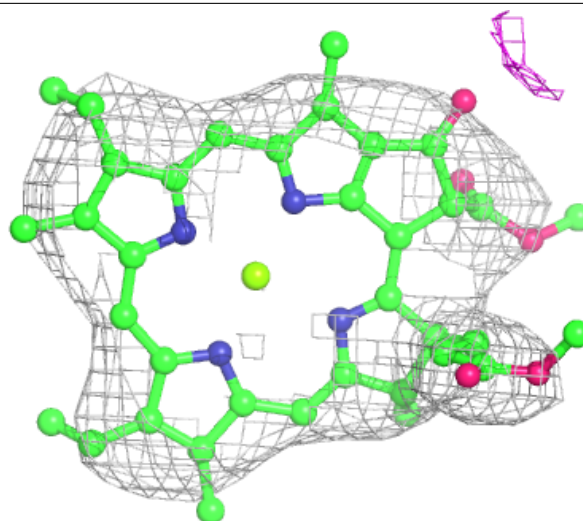
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

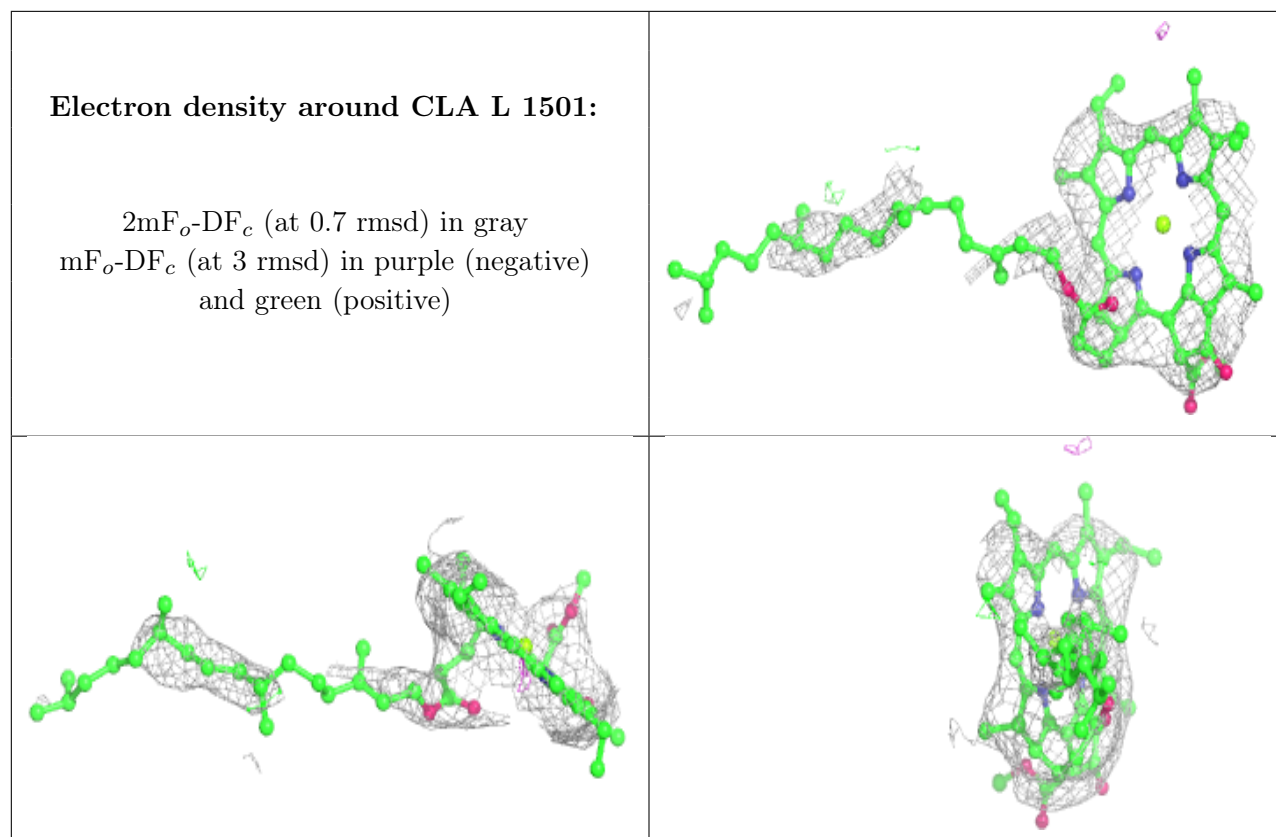




Electron density around CLA B 1239:

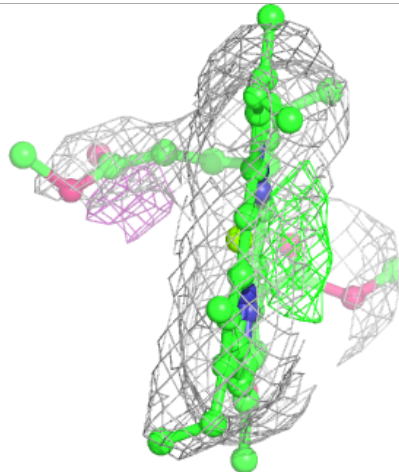
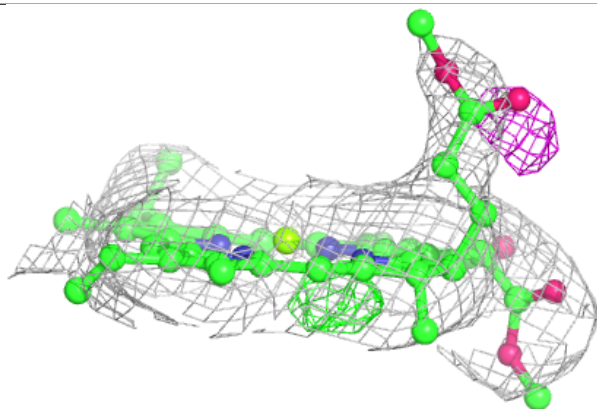
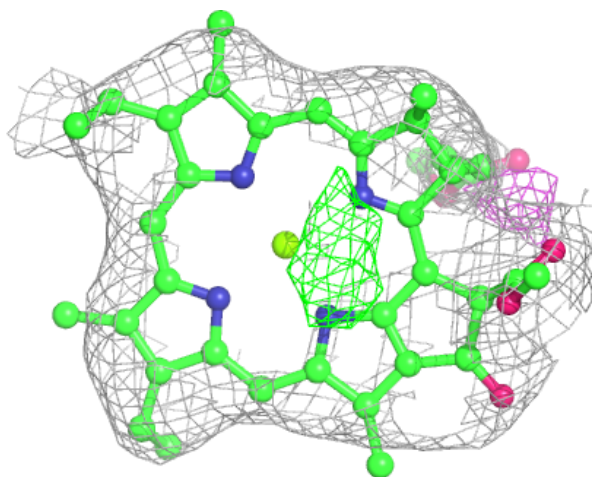
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

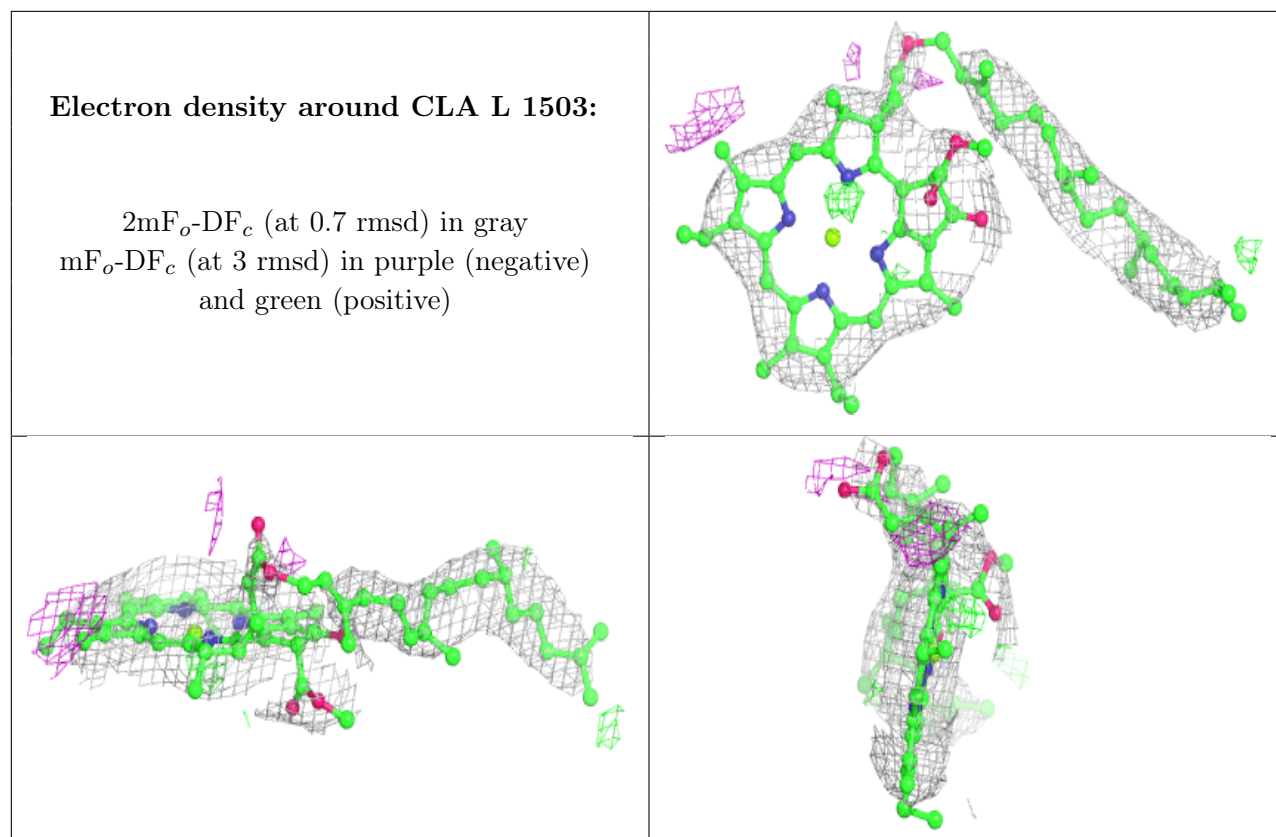




Electron density around CLA L 1502:

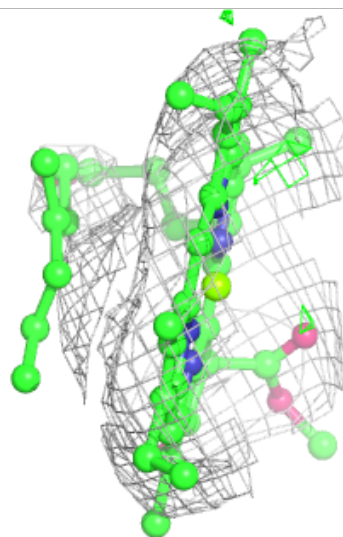
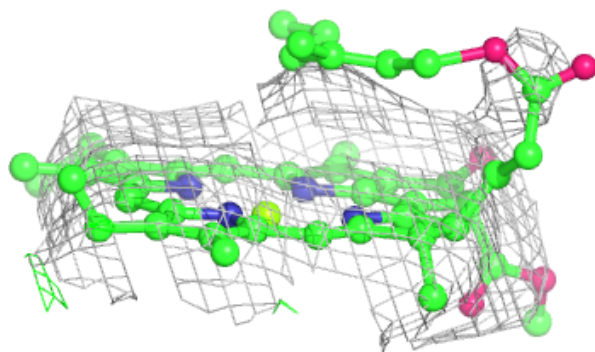
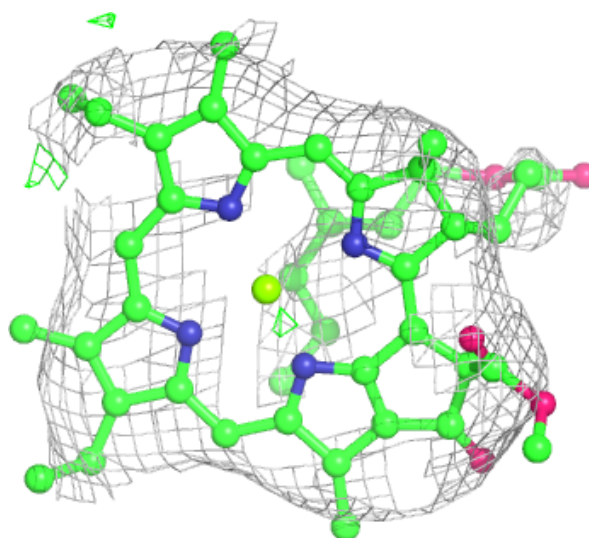
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





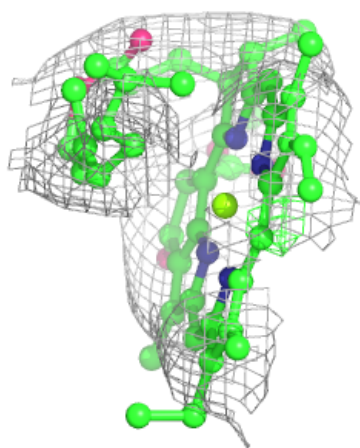
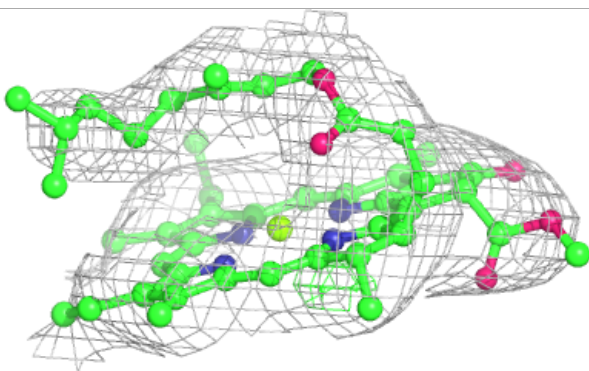
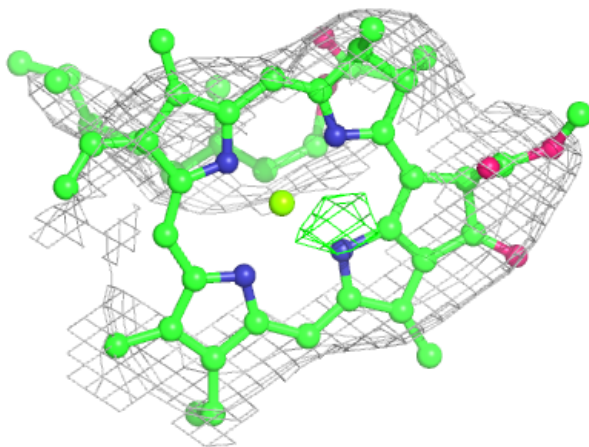
Electron density around CLA a 1801:

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



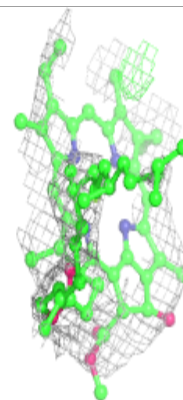
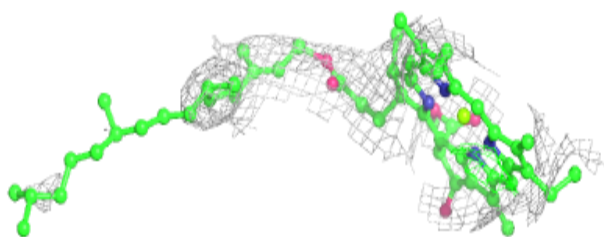
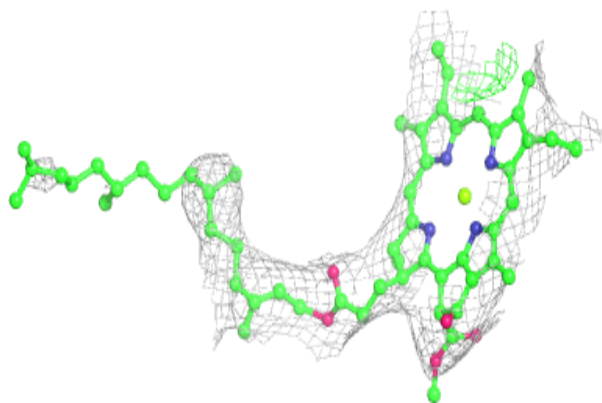
Electron density around CLA a 1237:

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

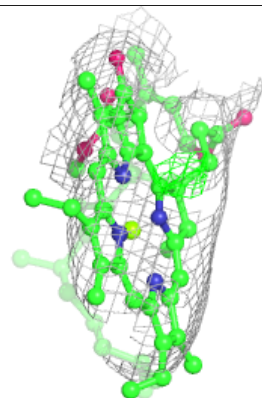
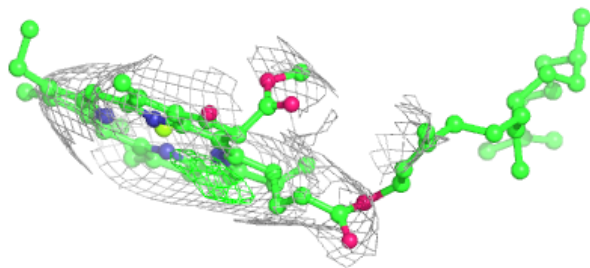
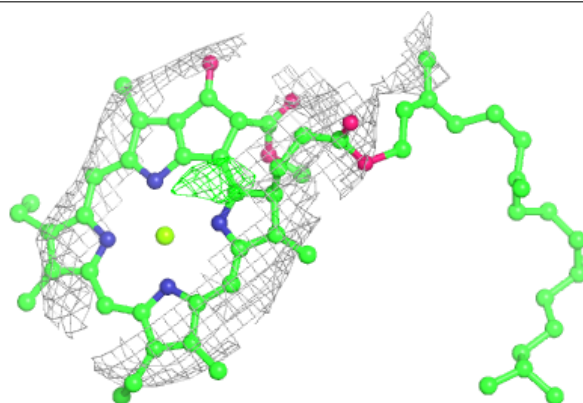


Electron density around CLA a 1022:

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

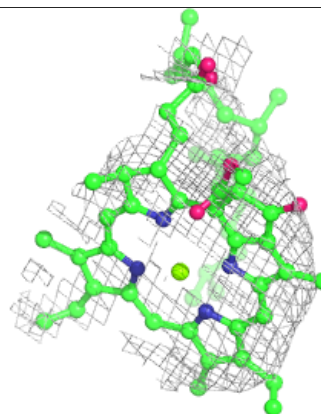
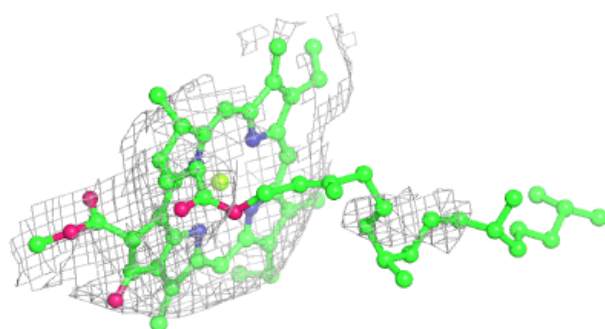
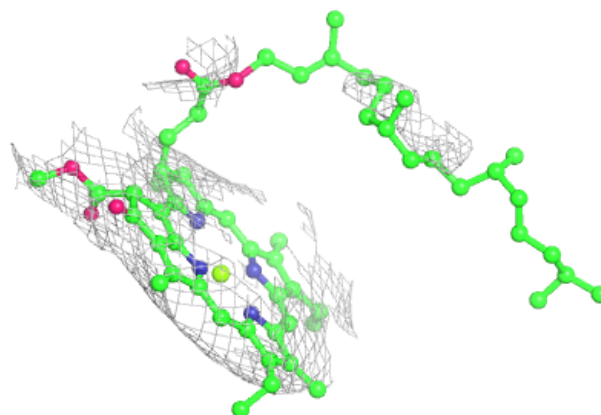
**Electron density around CLA a 1101:**

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

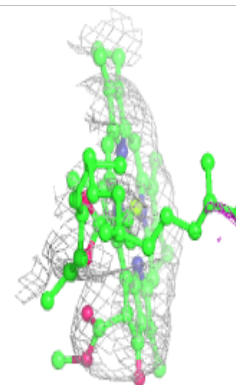
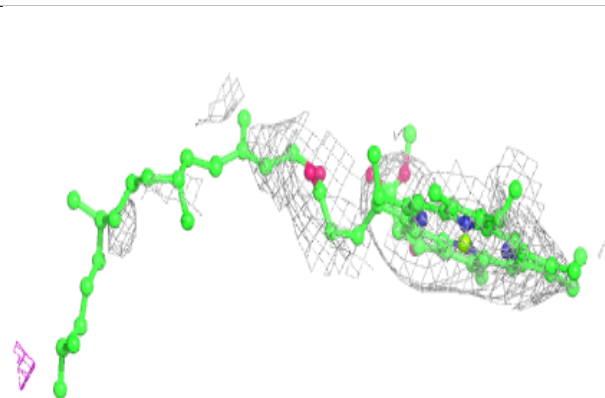
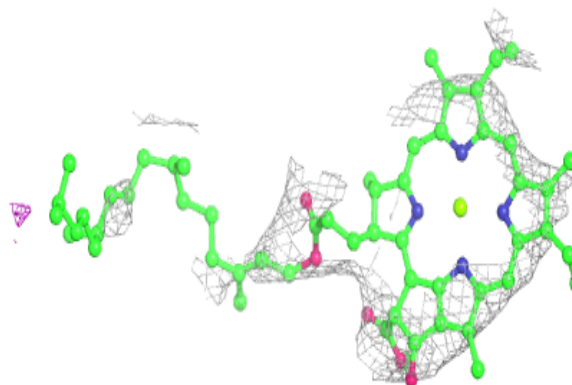


Electron density around CLA a 1102:

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

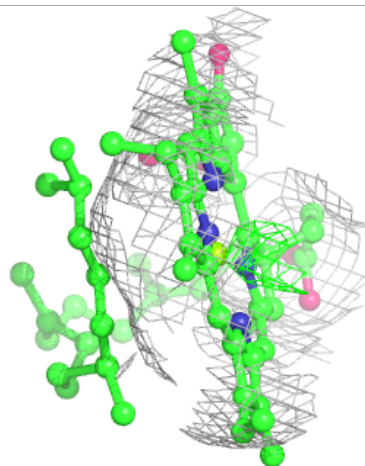
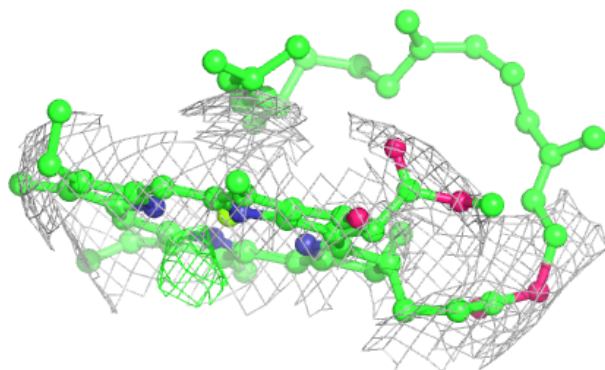
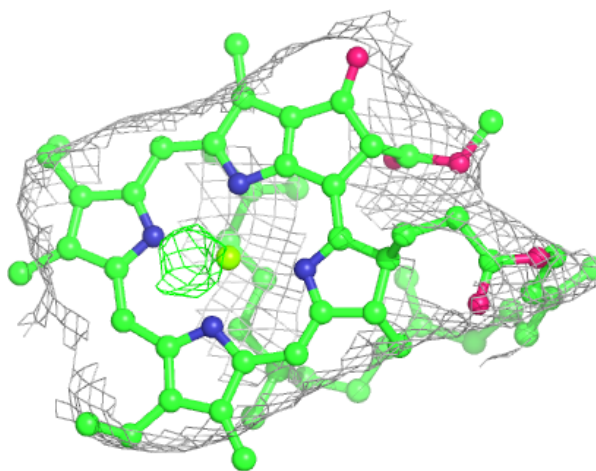
**Electron density around CLA a 1103:**

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



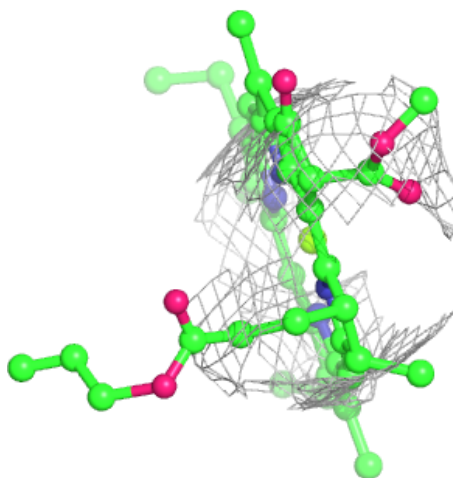
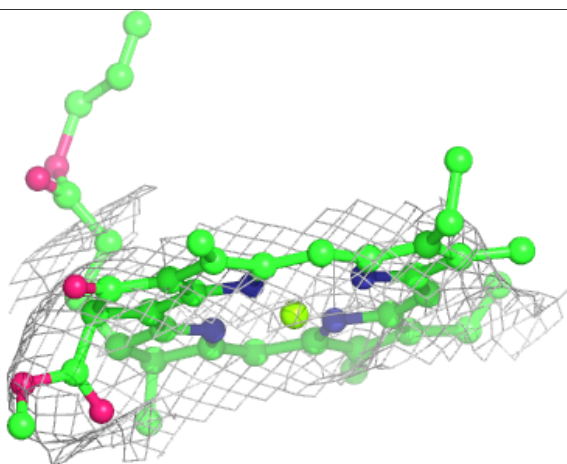
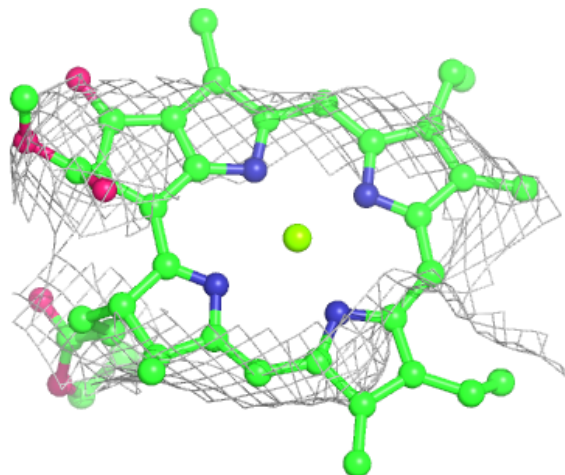
Electron density around CLA a 1104:

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



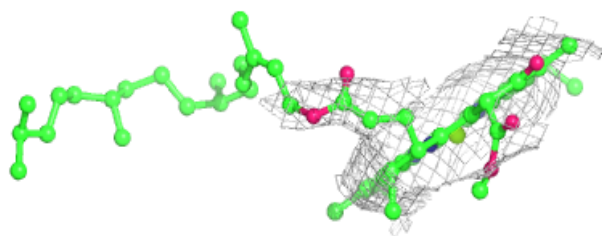
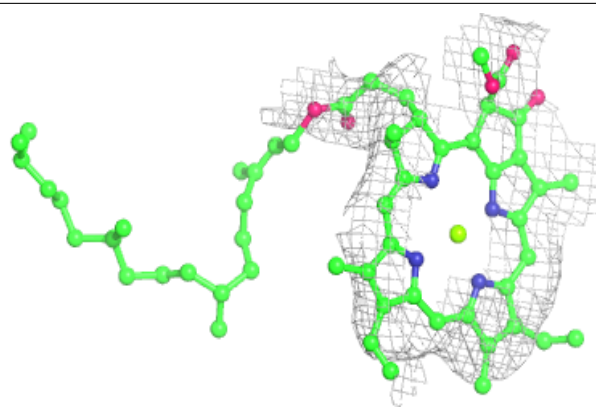
Electron density around CLA a 1105:

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

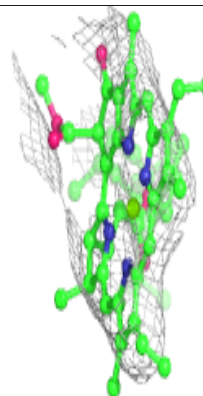
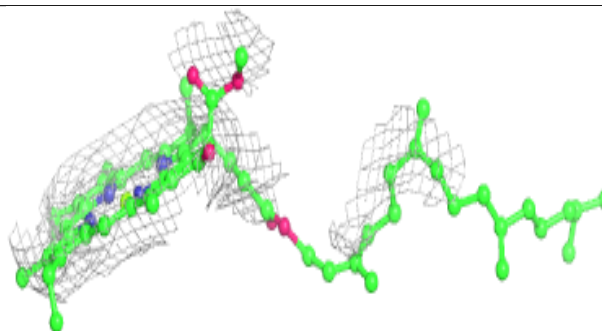
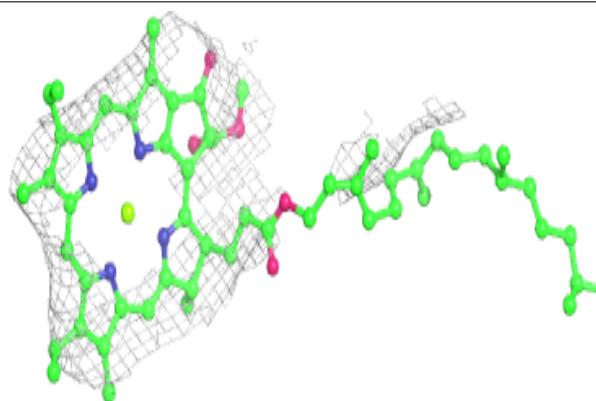


Electron density around CLA a 1106:

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

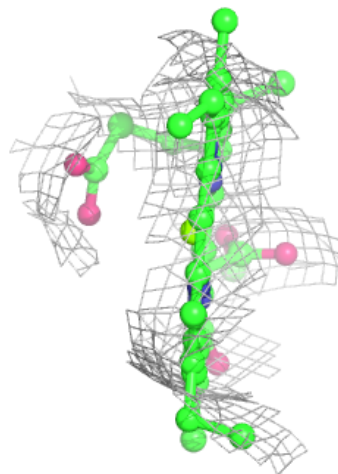
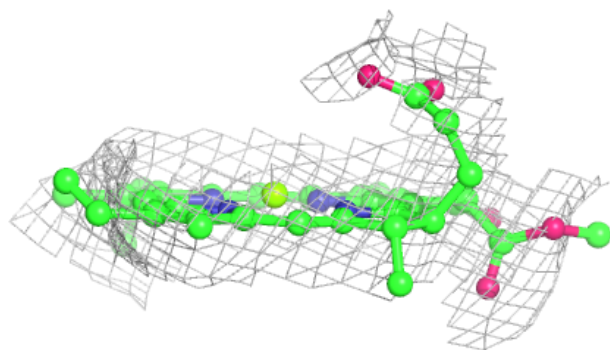
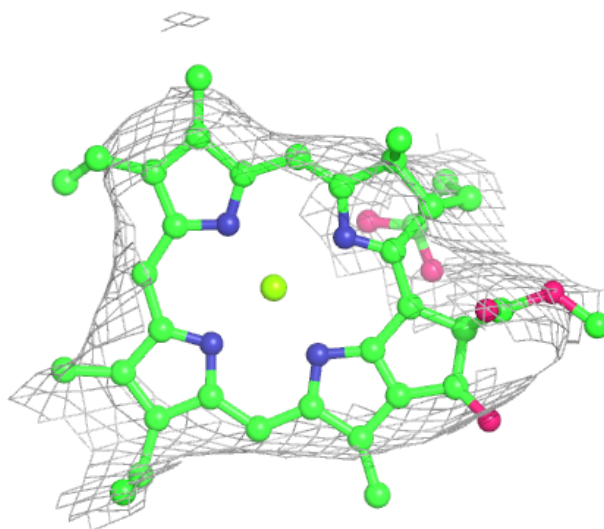
**Electron density around CLA a 1107:**

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



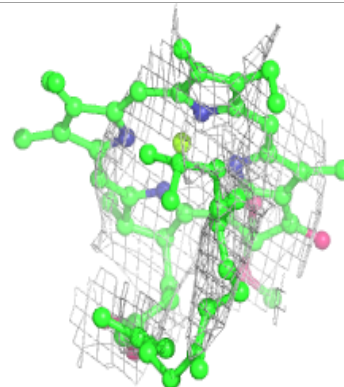
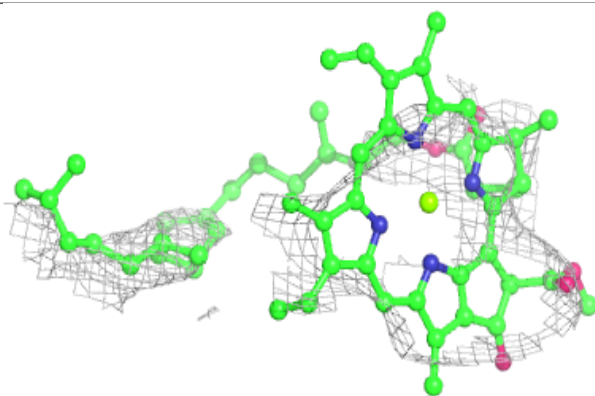
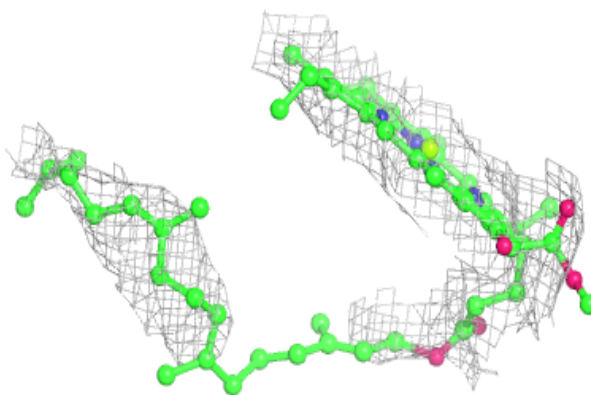
Electron density around CLA a 1108:

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



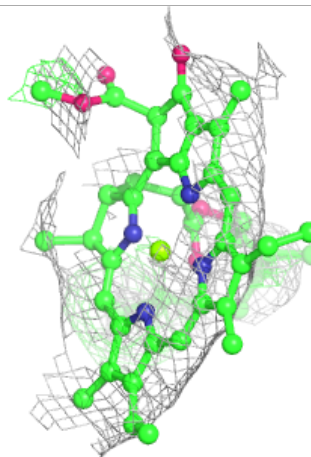
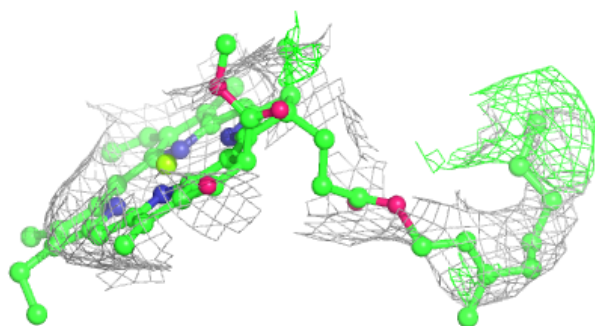
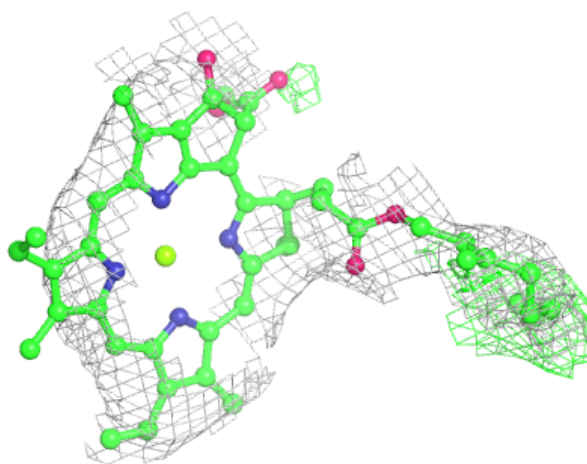
Electron density around CLA a 1109:

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



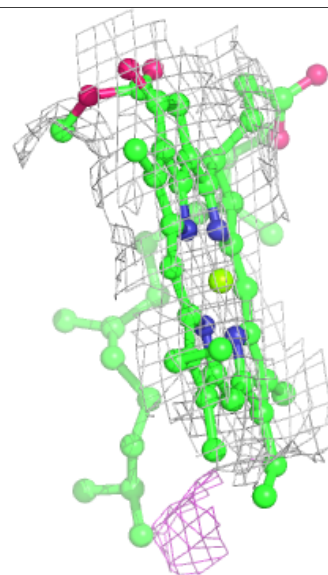
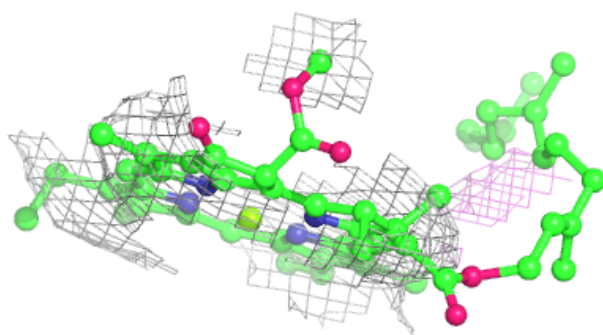
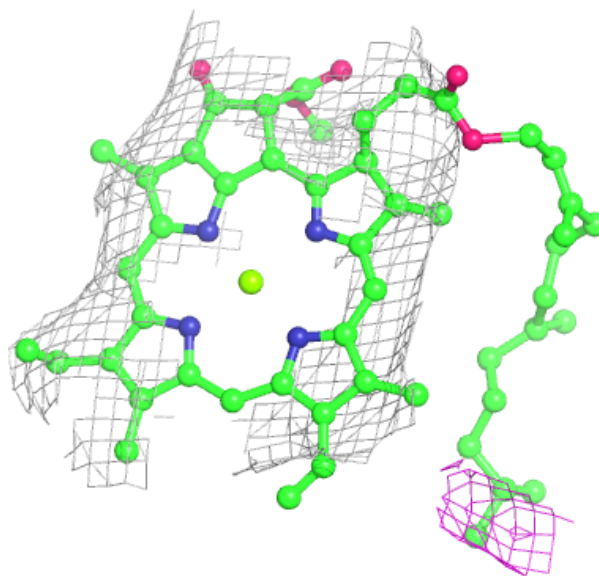
Electron density around CLA a 1110:

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



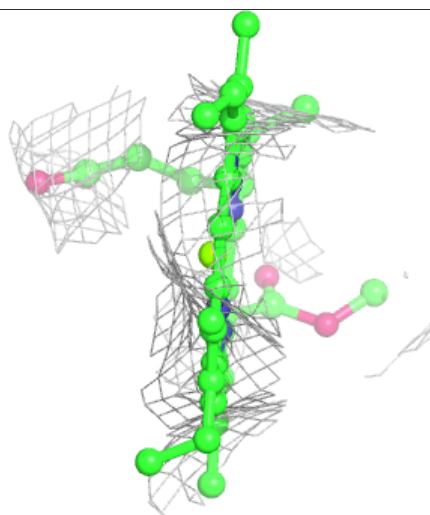
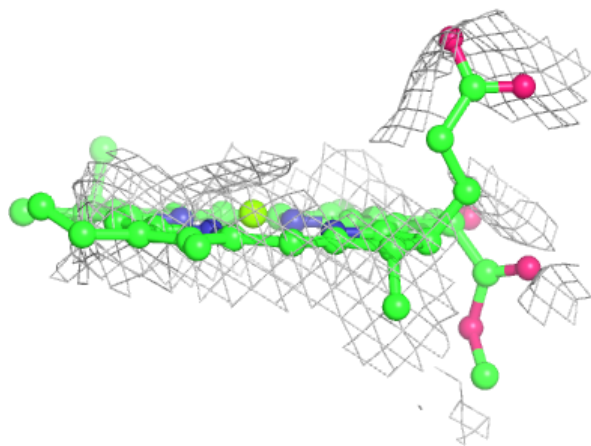
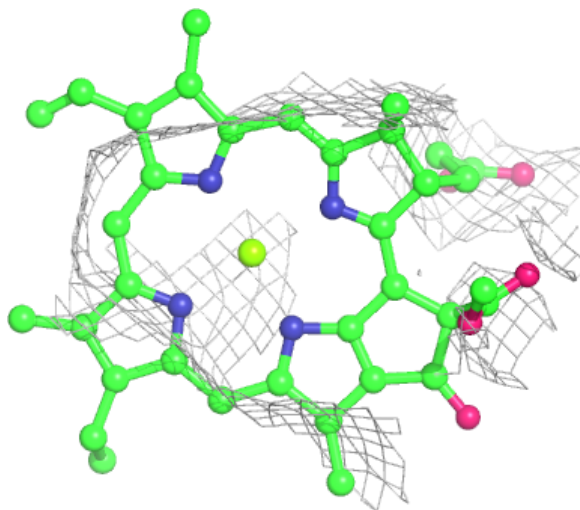
Electron density around CLA a 1111:

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



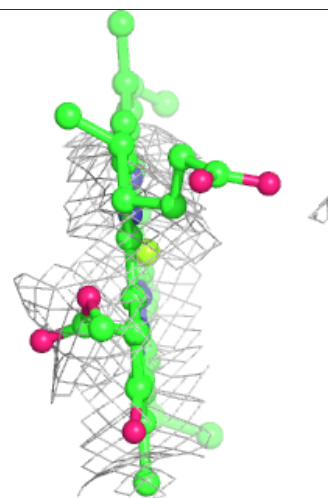
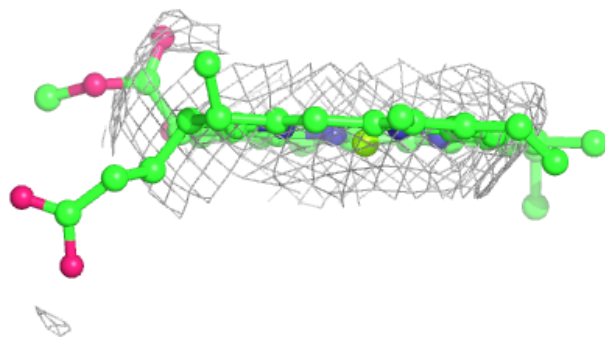
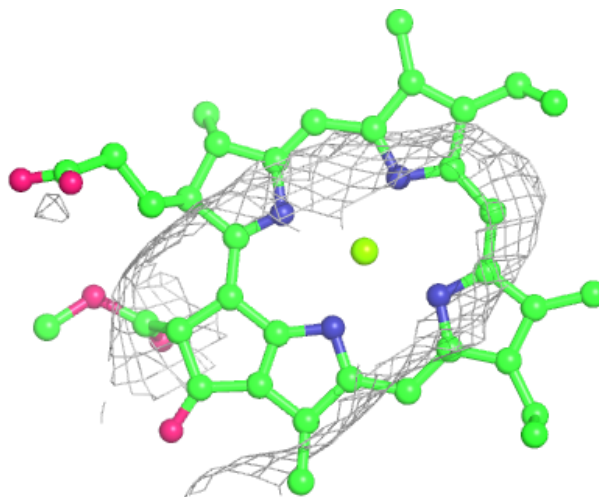
Electron density around CLA a 1112:

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



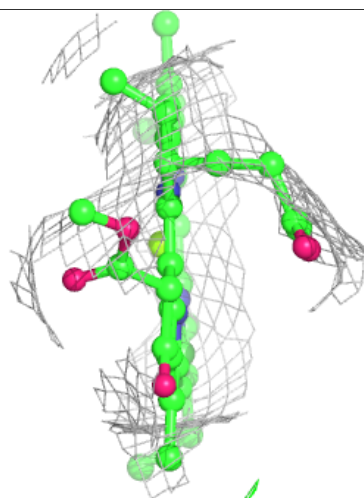
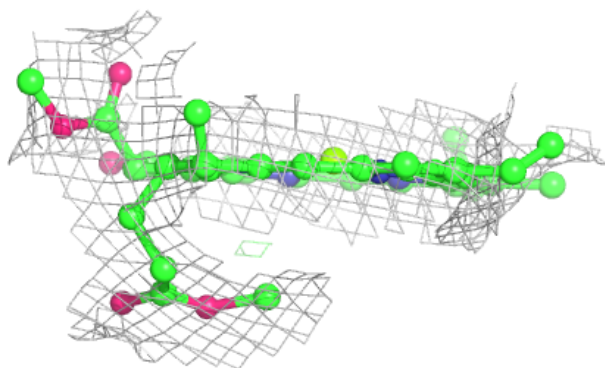
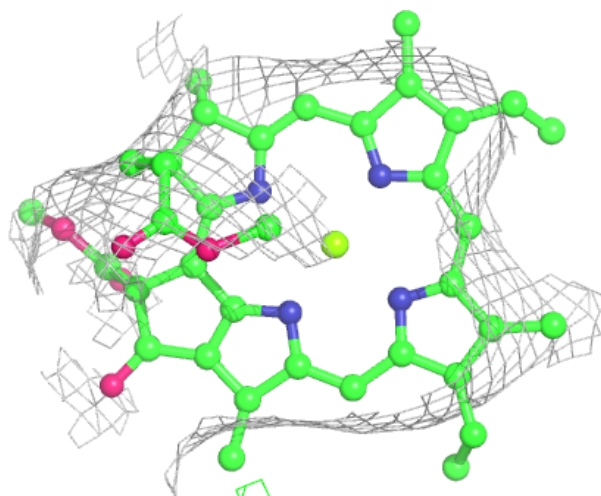
Electron density around CLA a 1113:

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



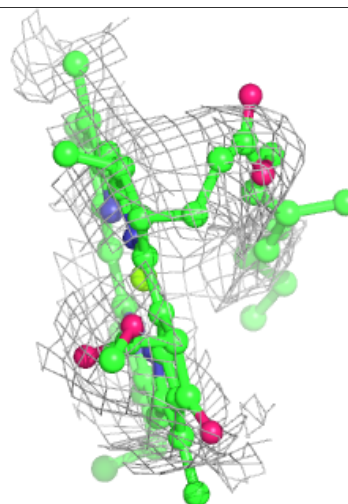
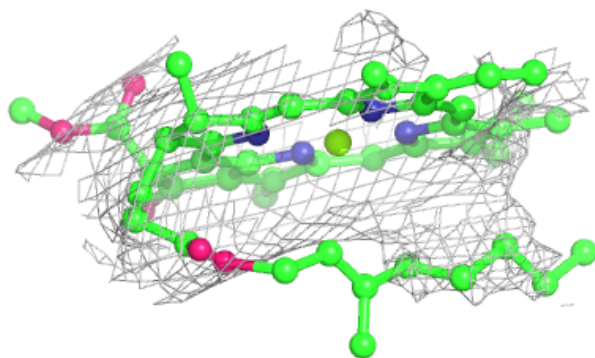
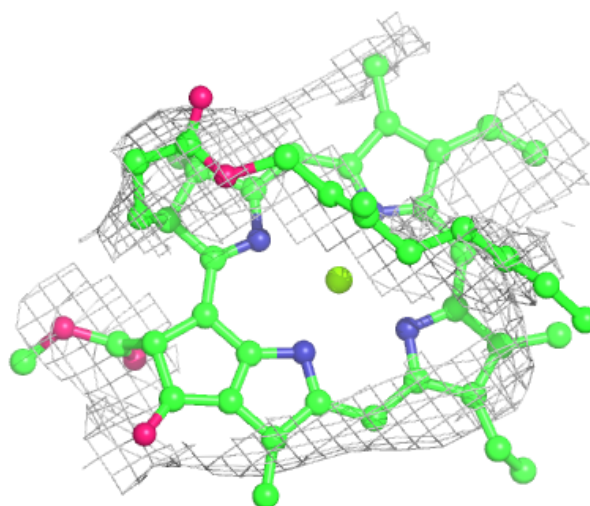
Electron density around CLA a 1115:

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



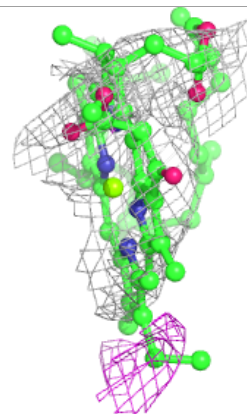
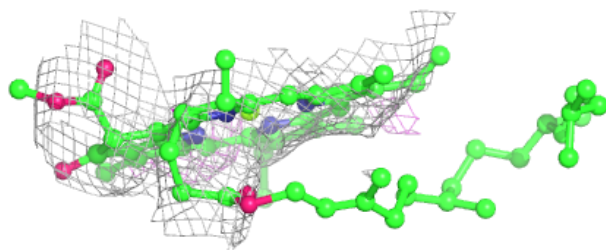
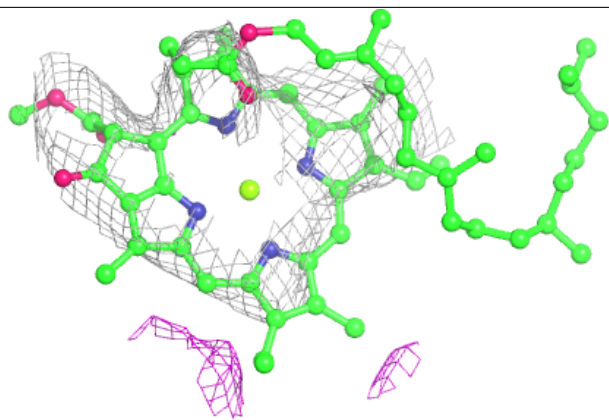
Electron density around CLA a 1116:

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

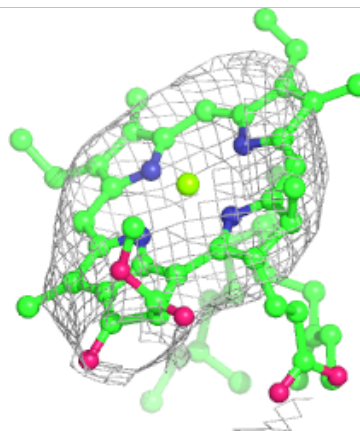
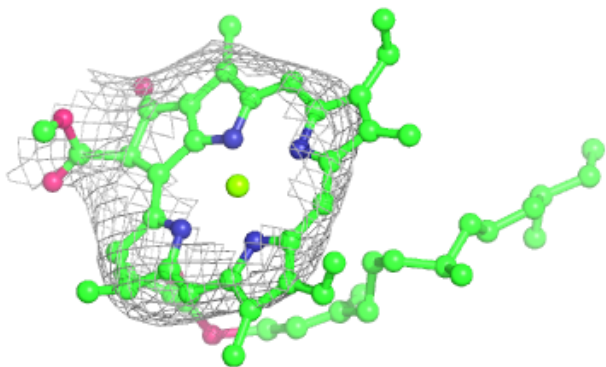
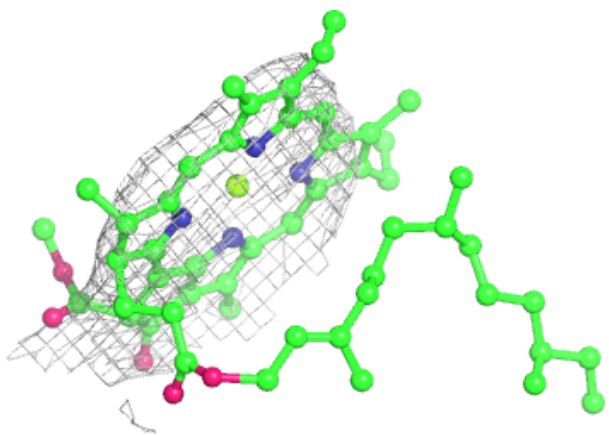


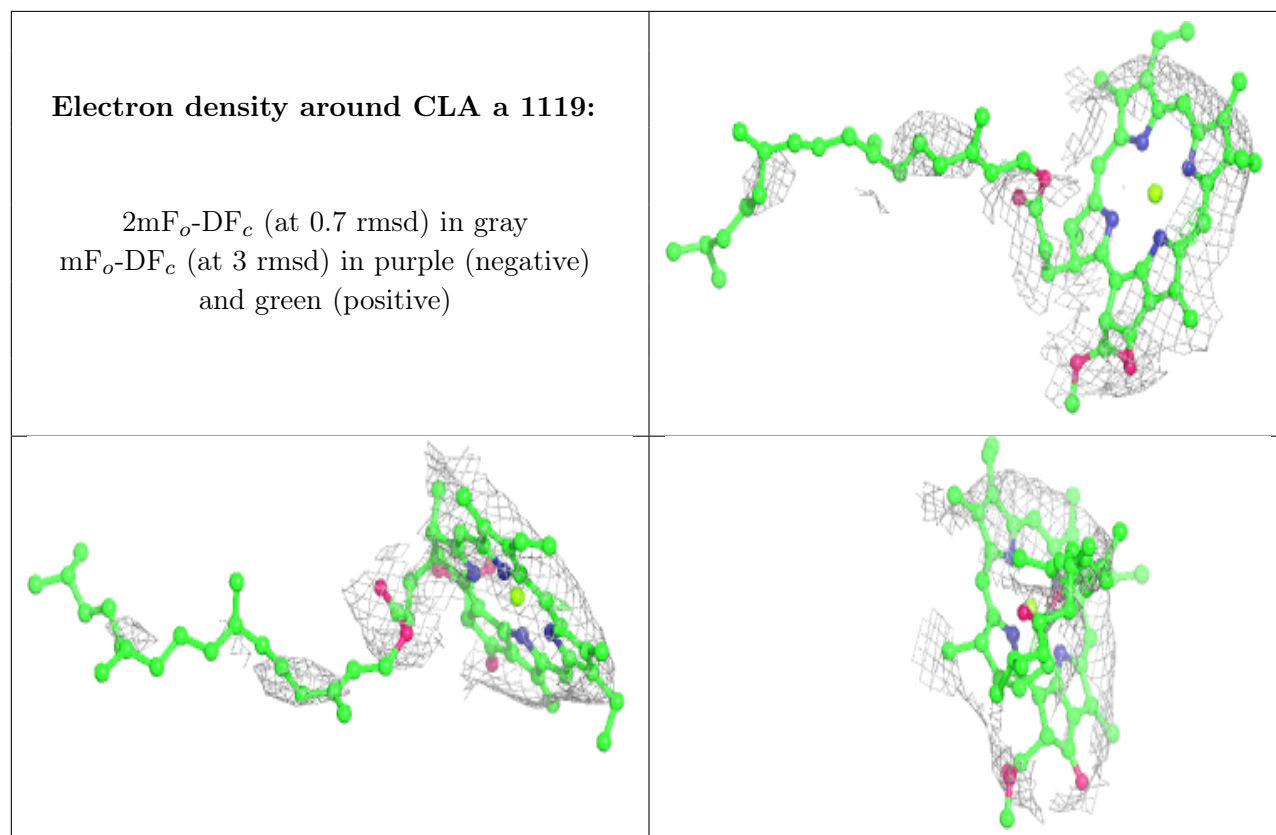
Electron density around CLA a 1117:

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

**Electron density around CLA a 1118:**

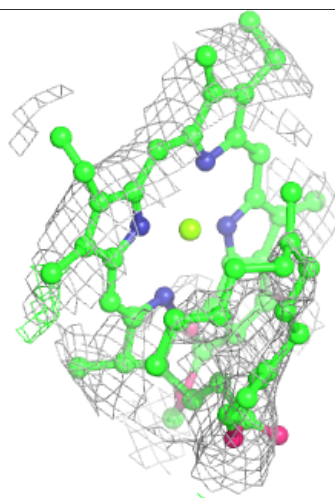
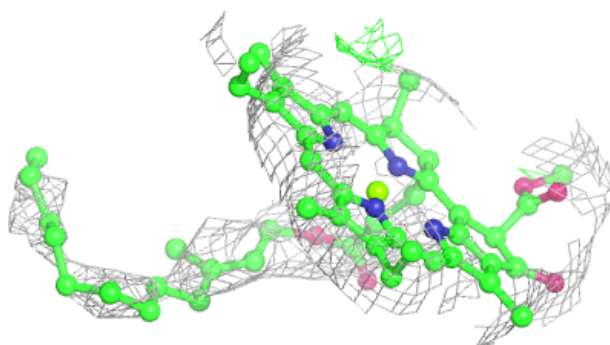
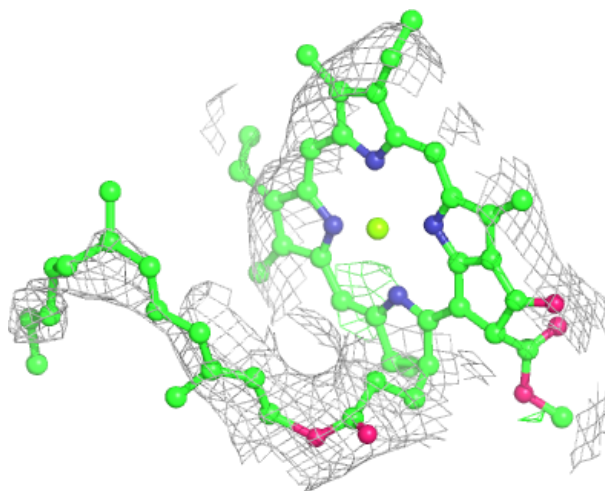
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





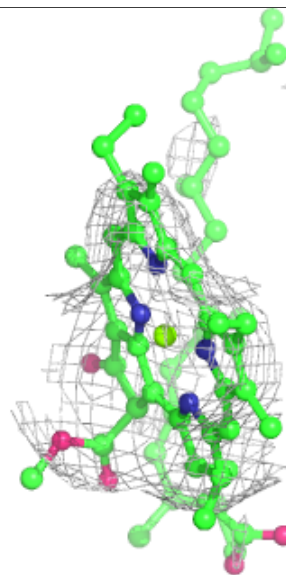
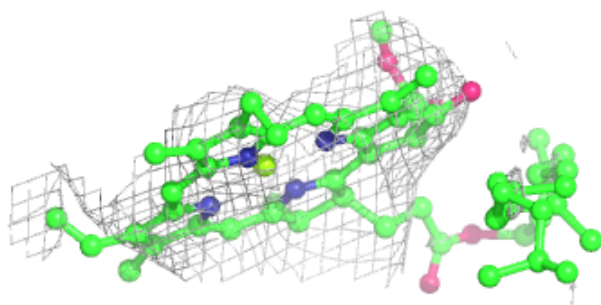
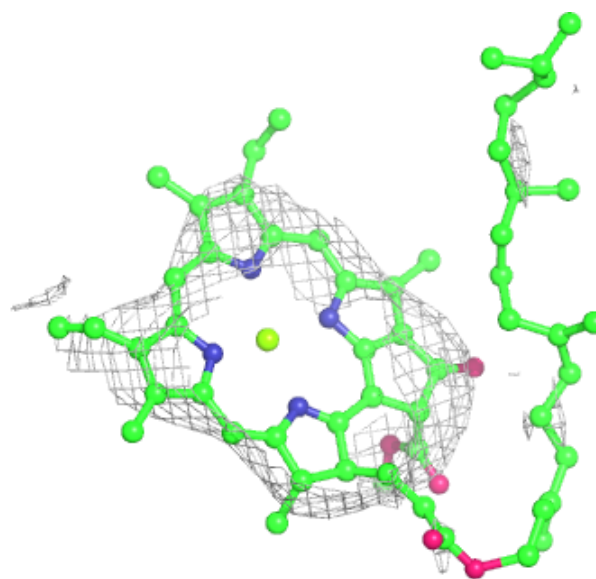
Electron density around CLA a 1122:

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



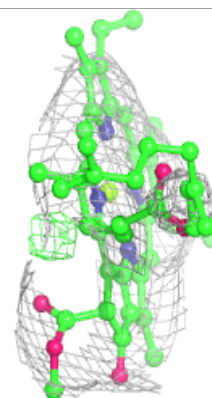
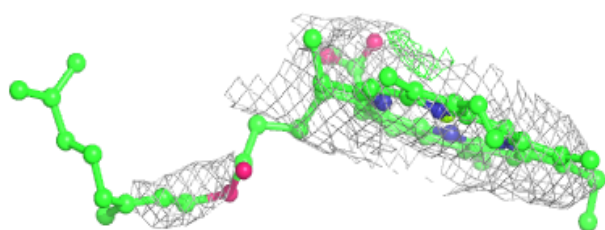
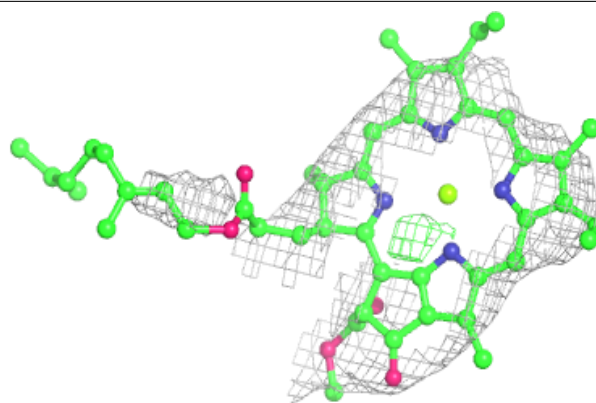
Electron density around CLA a 1123:

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

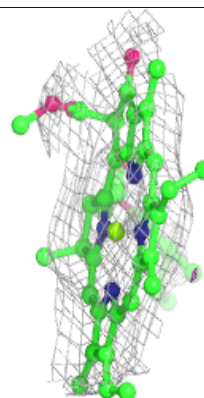
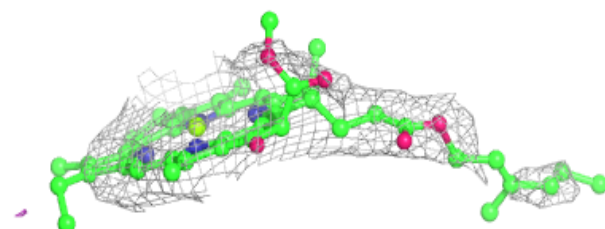
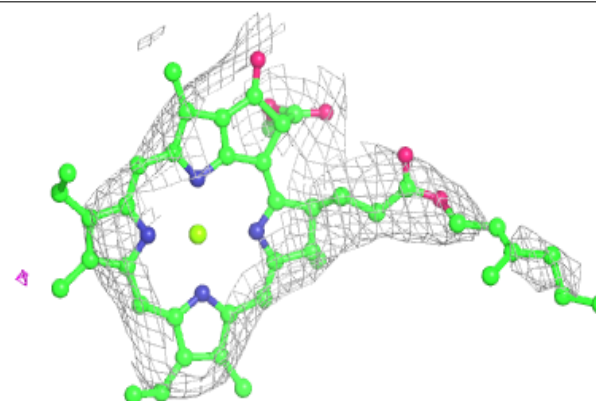


Electron density around CLA a 1124:

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

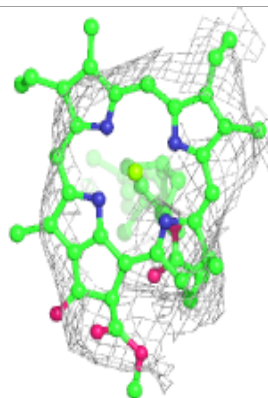
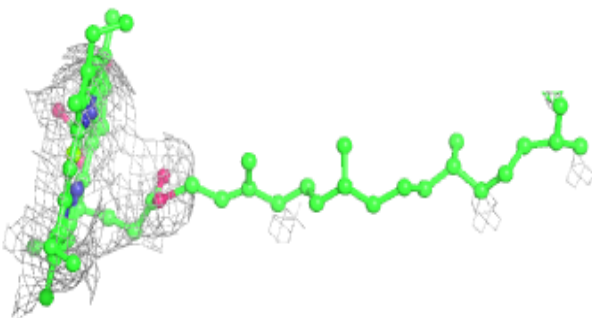
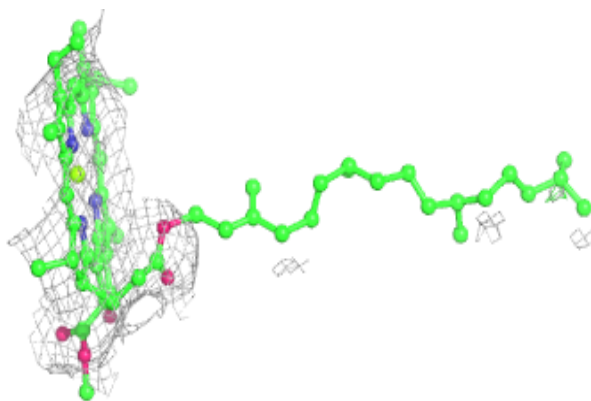
**Electron density around CLA a 1125:**

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



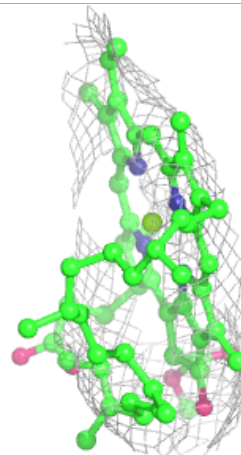
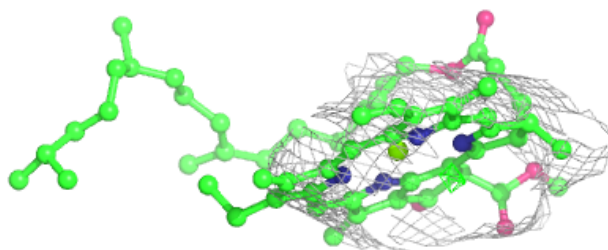
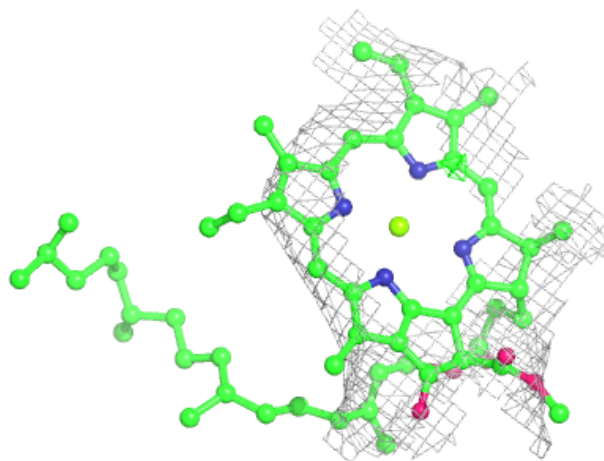
Electron density around CLA a 1126:

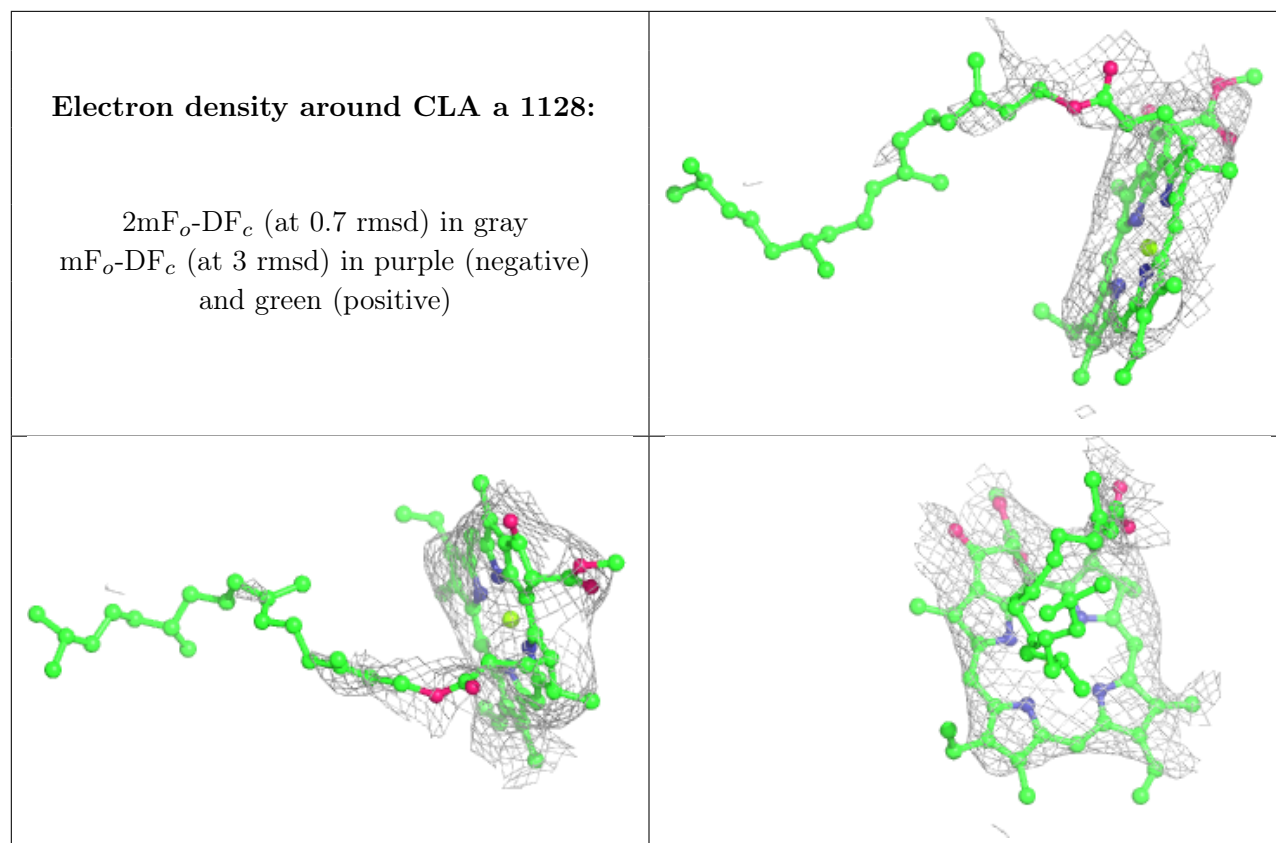
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around CLA a 1127:

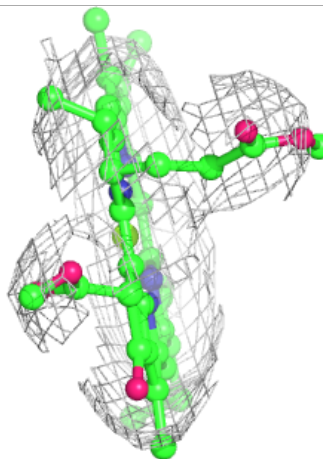
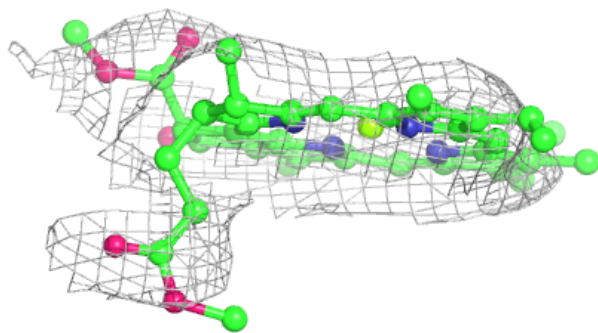
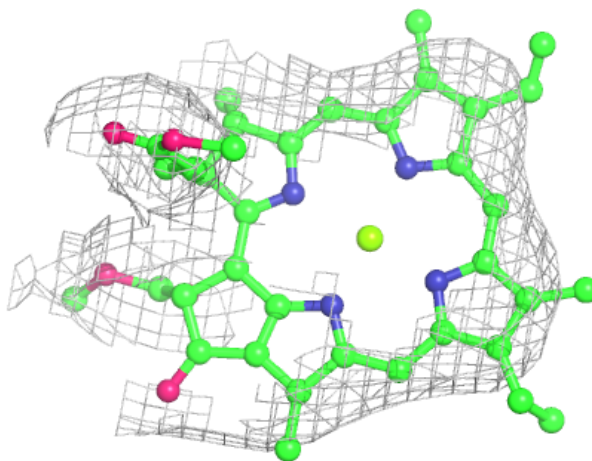
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





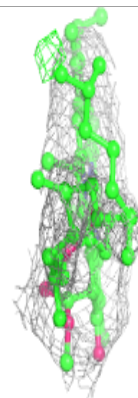
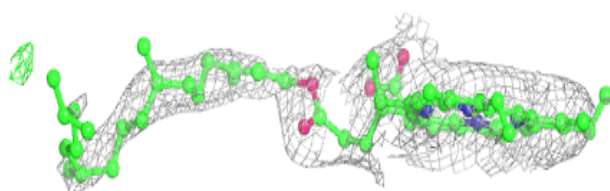
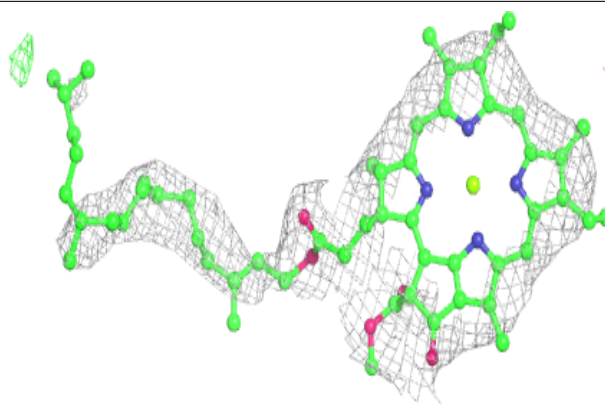
Electron density around CLA a 1130:

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

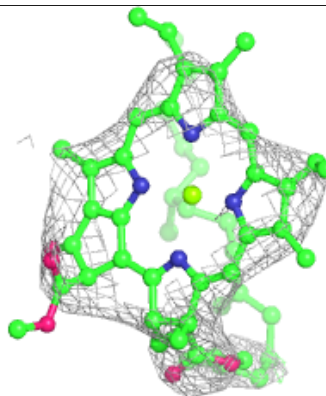
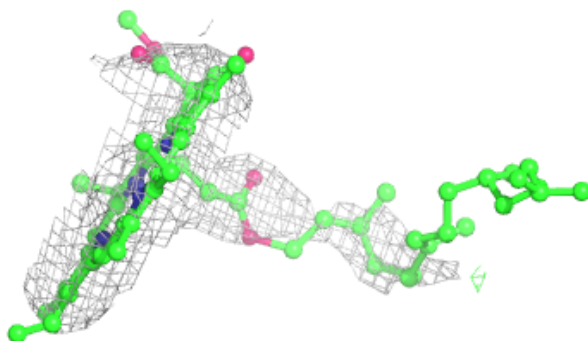
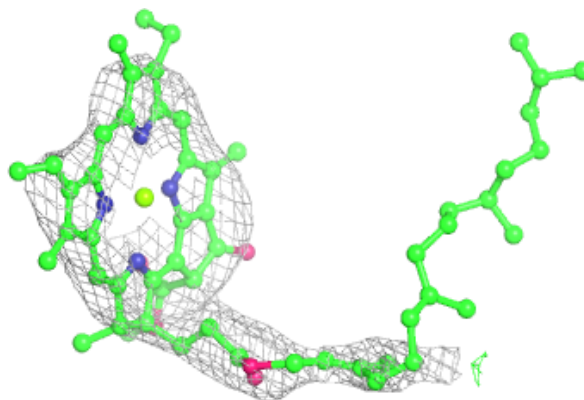


Electron density around CLA a 1131:

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

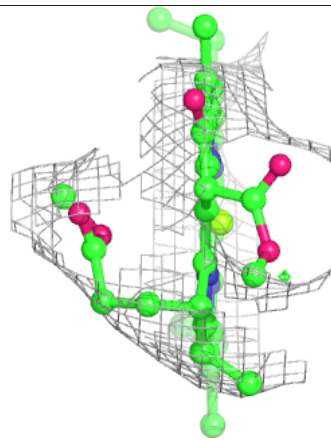
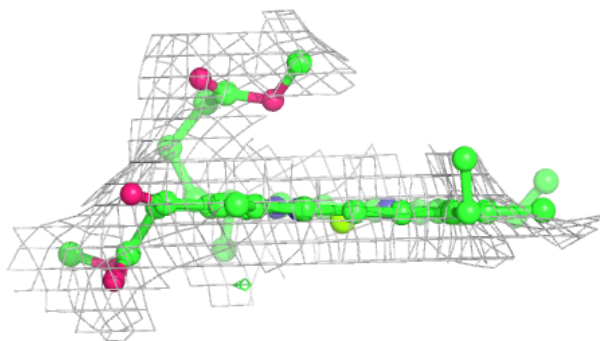
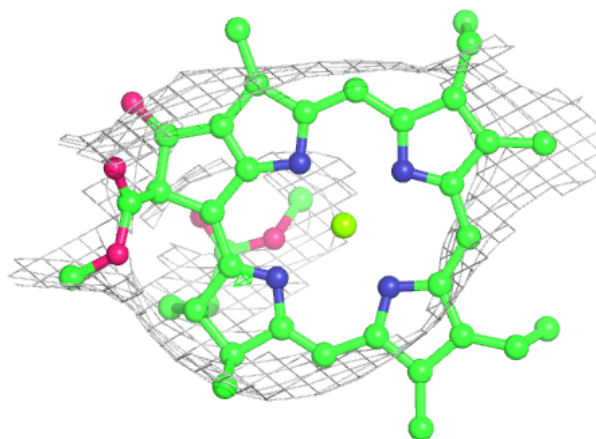
**Electron density around CLA a 1137:**

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



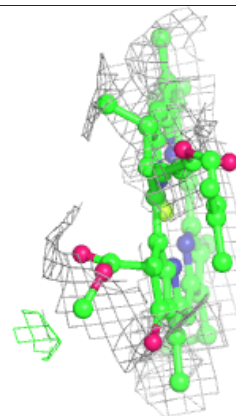
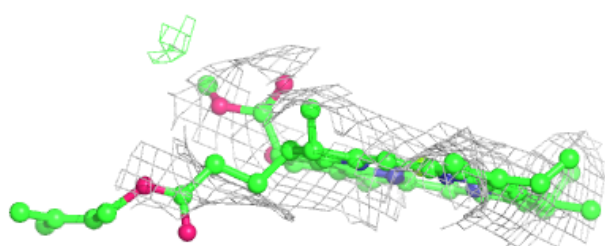
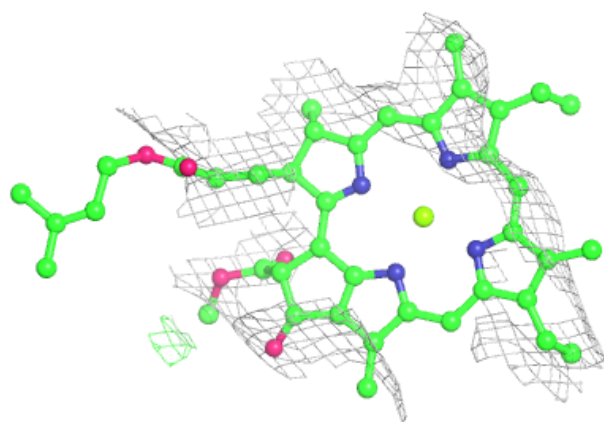
Electron density around CLA a 1138:

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

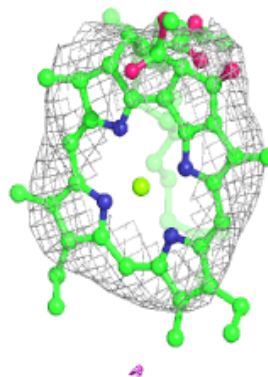
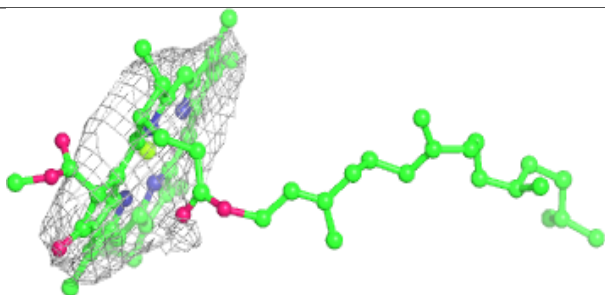
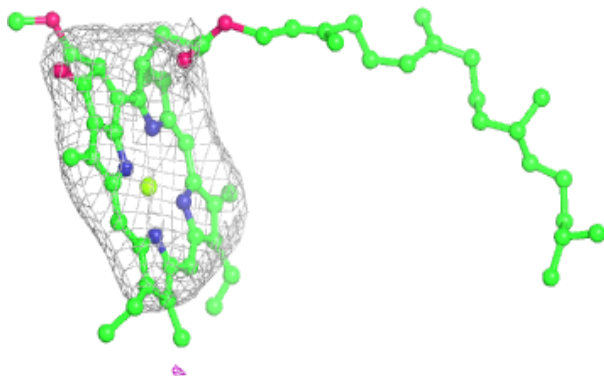


Electron density around CLA a 1139:

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

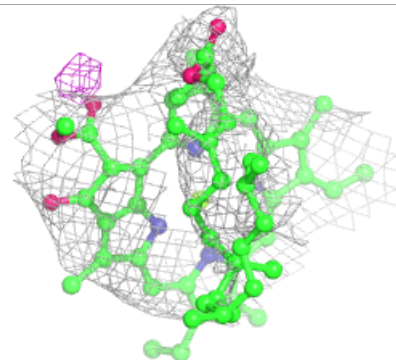
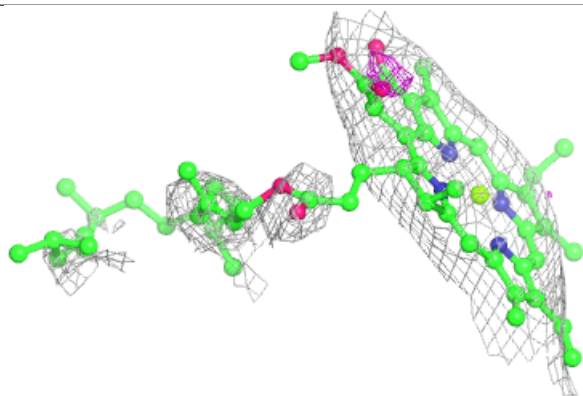
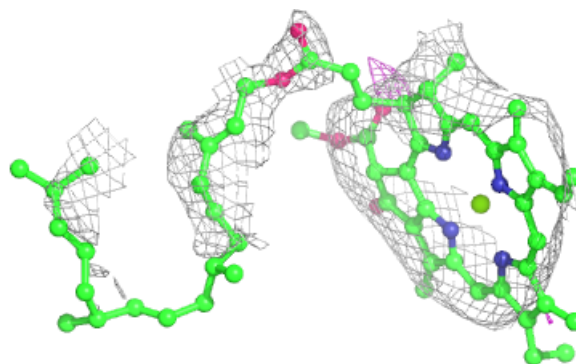
**Electron density around CLA a 1140:**

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

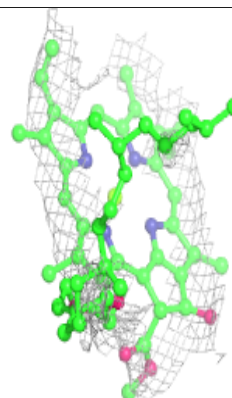
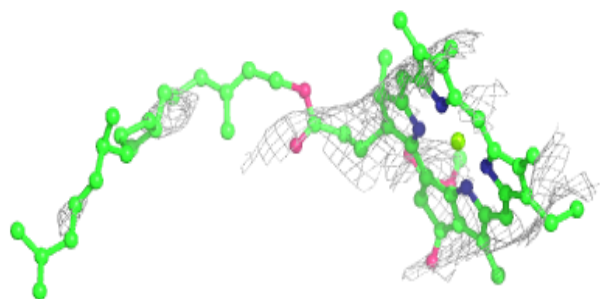
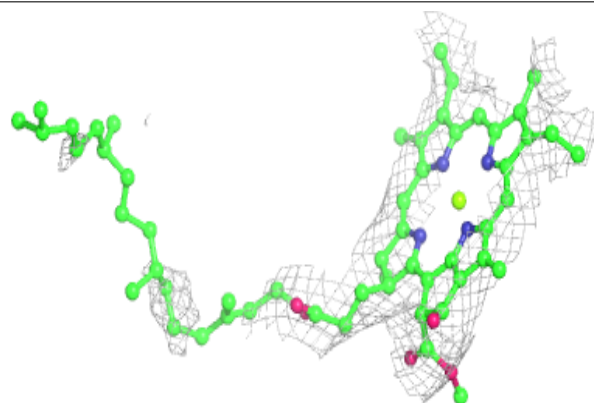


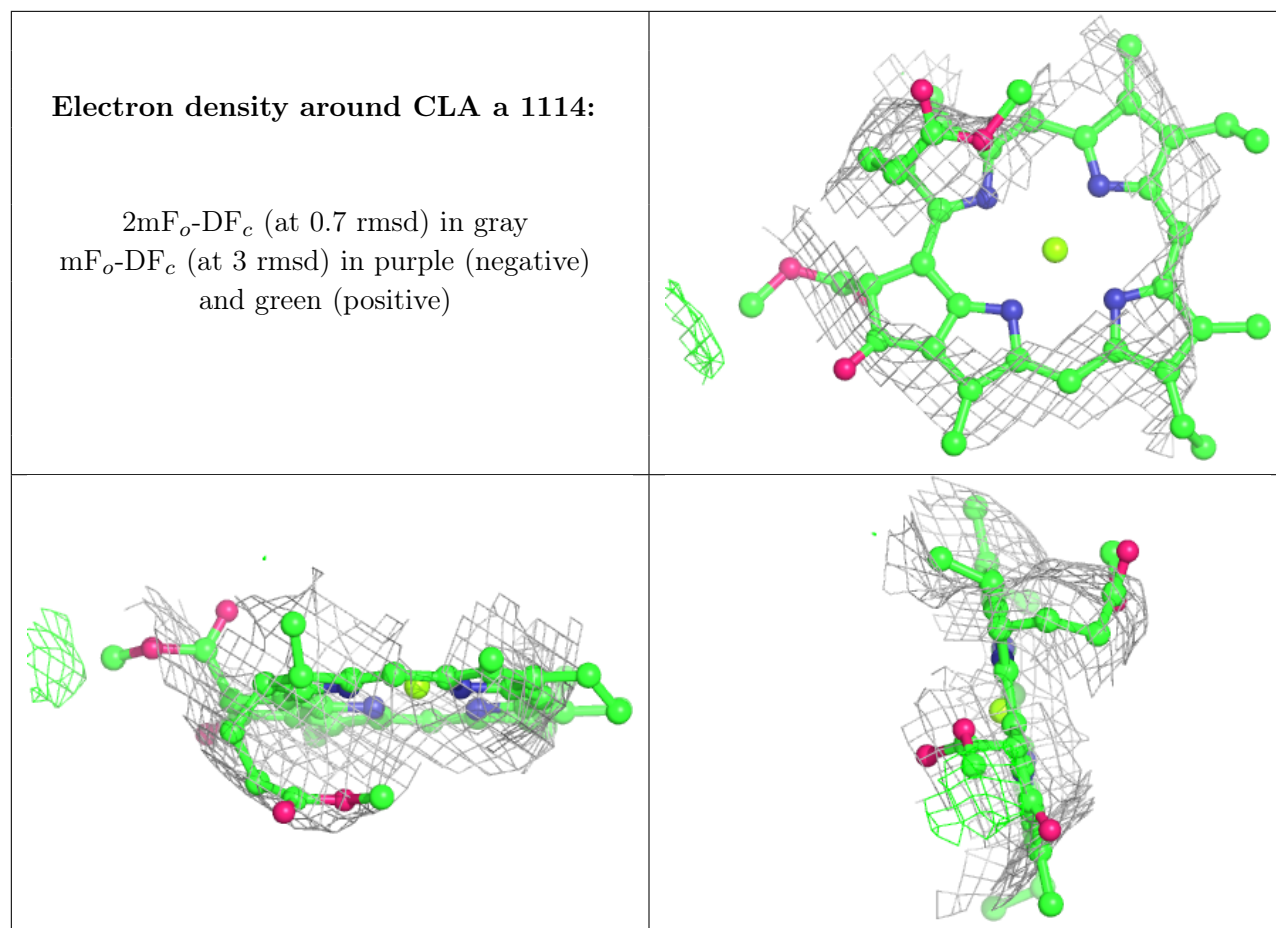
Electron density around CLA a 1011:

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

**Electron density around CLA a 1012:**

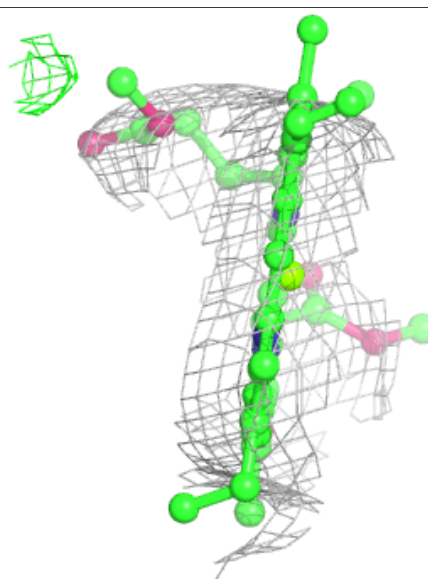
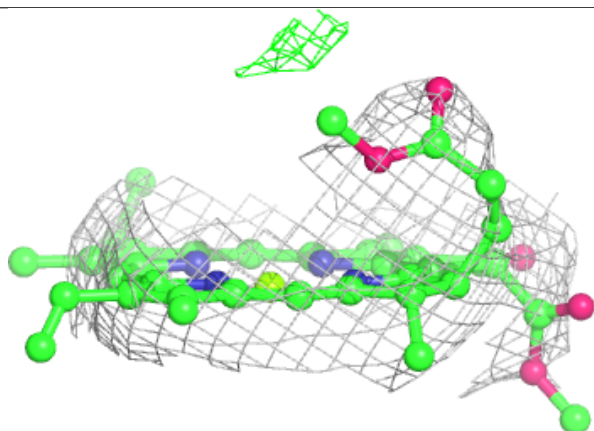
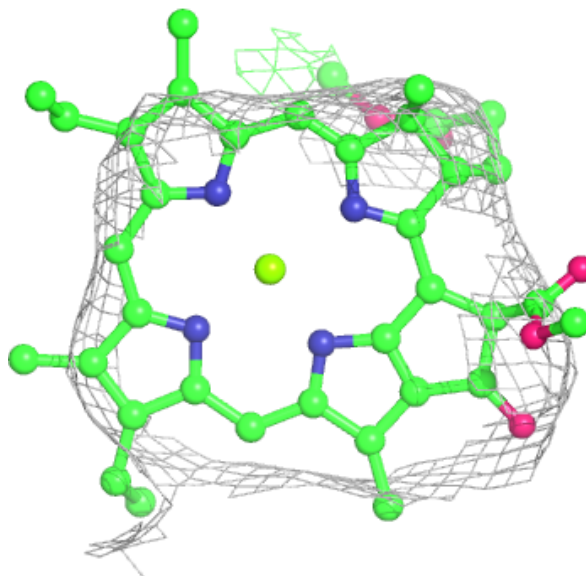
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





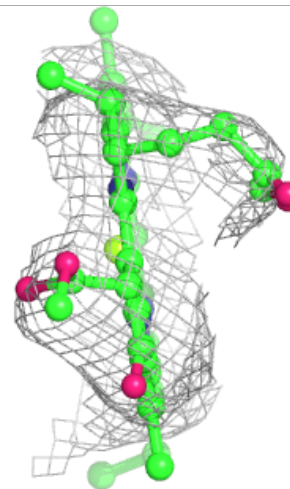
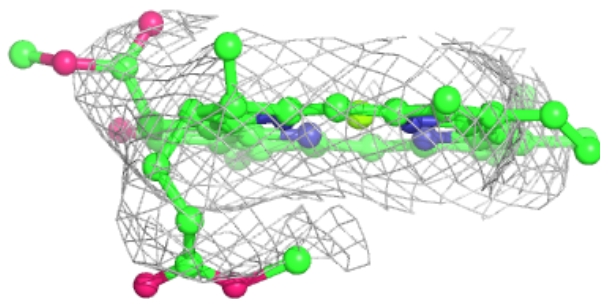
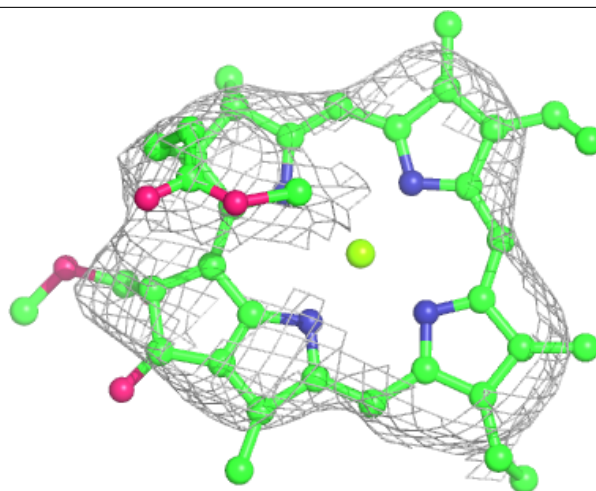
Electron density around CLA a 1120:

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



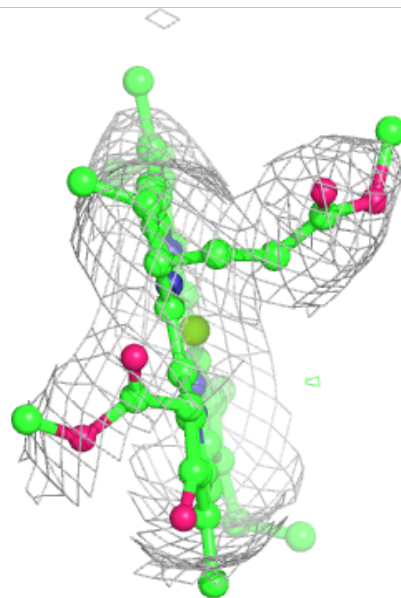
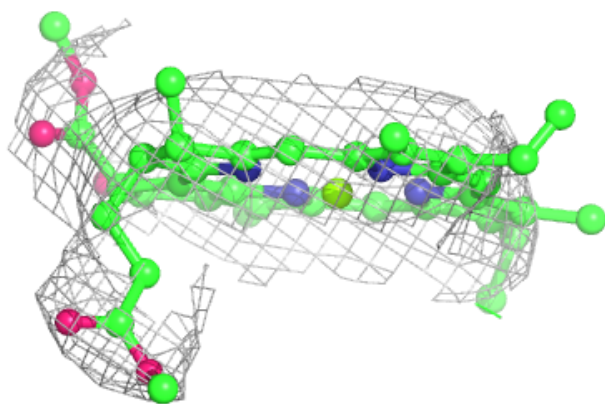
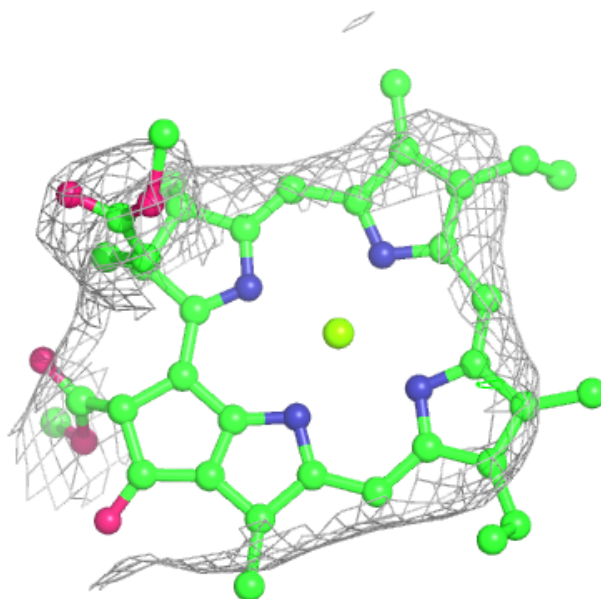
Electron density around CLA a 1121:

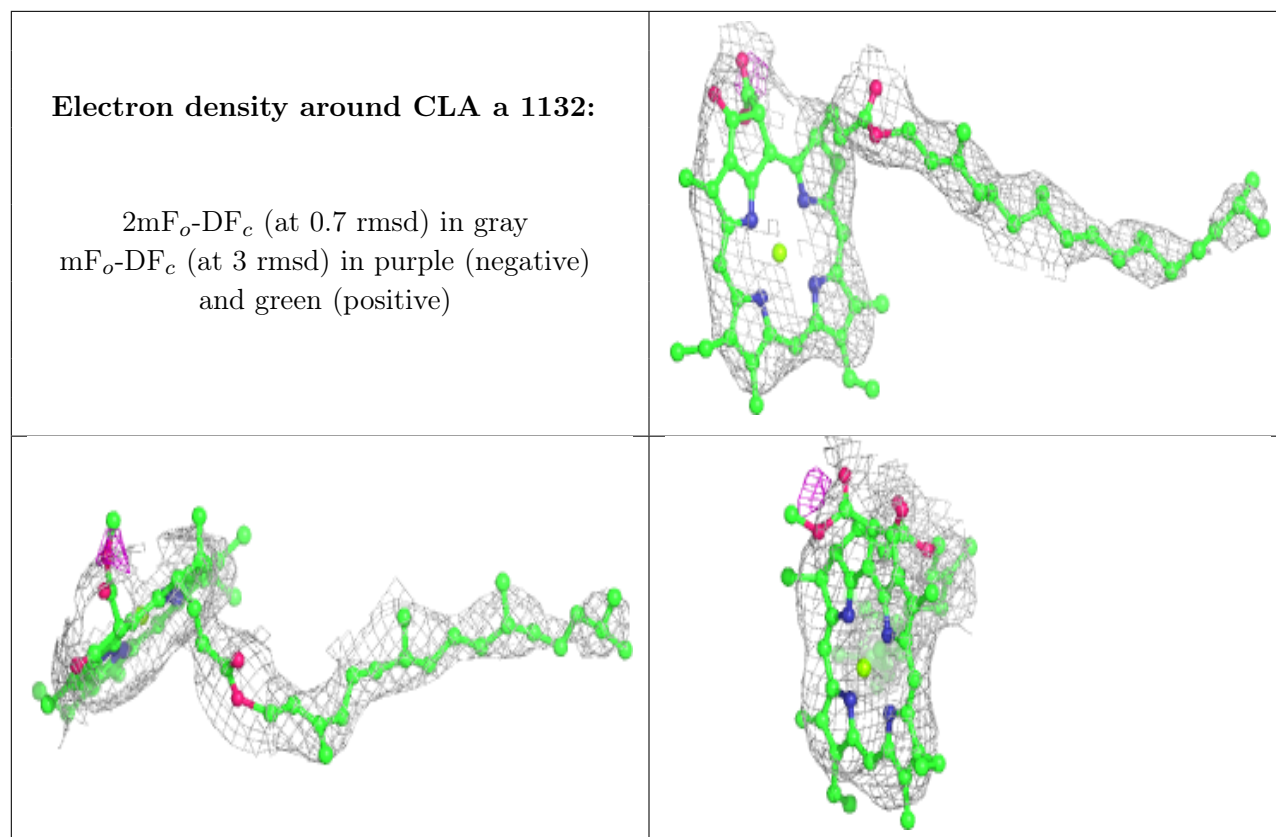
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around CLA a 1129:

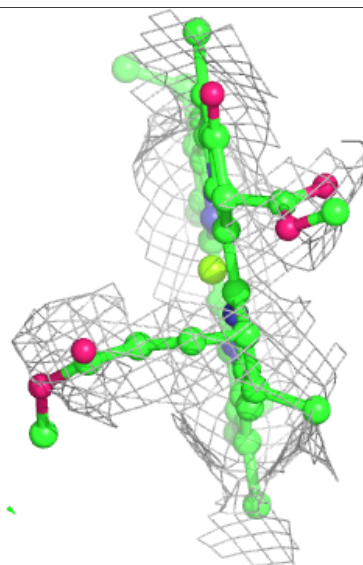
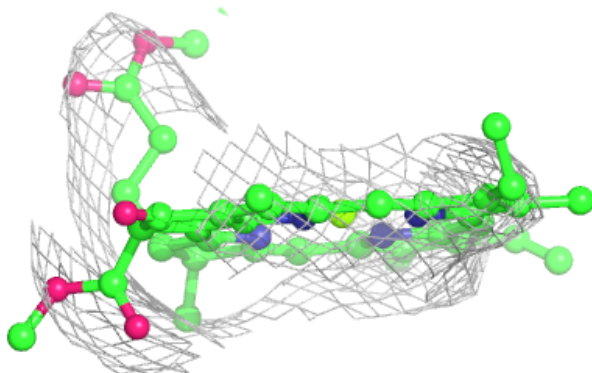
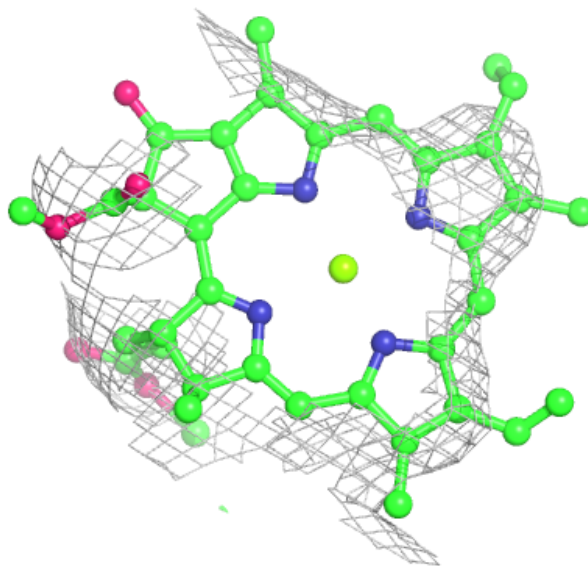
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





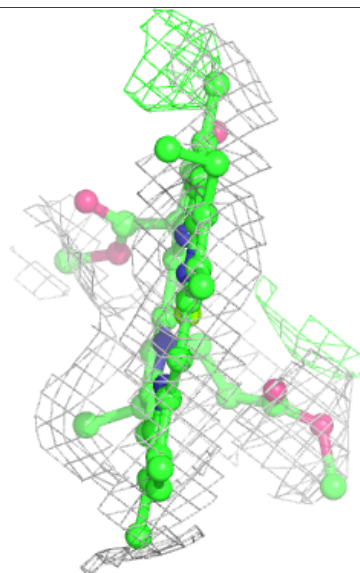
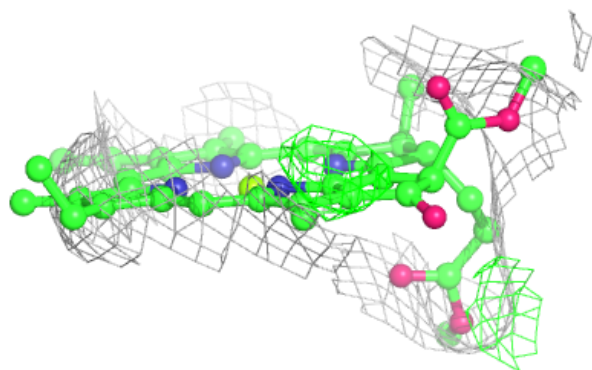
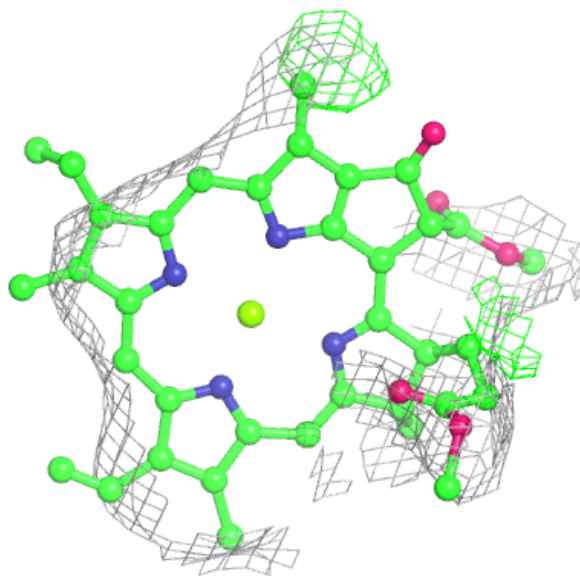
Electron density around CLA a 1133:

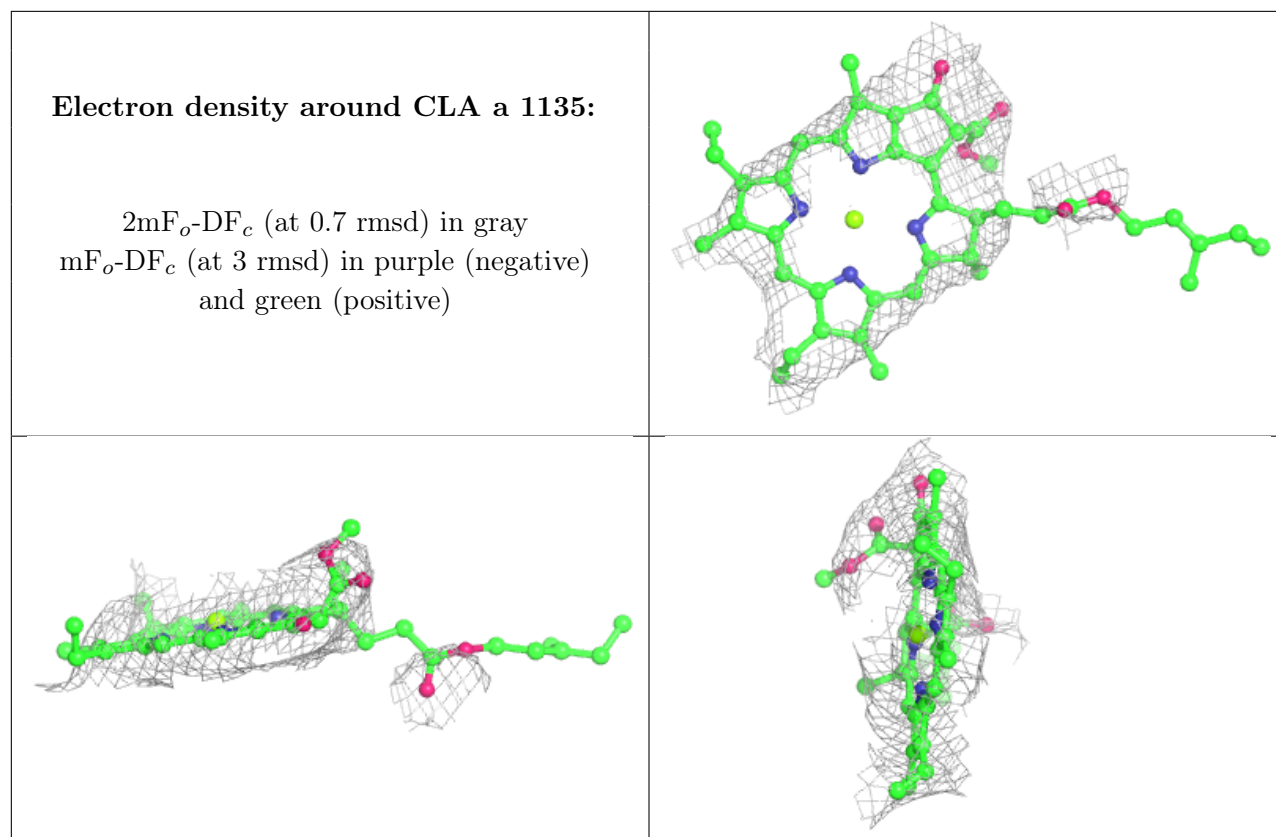
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around CLA a 1134:

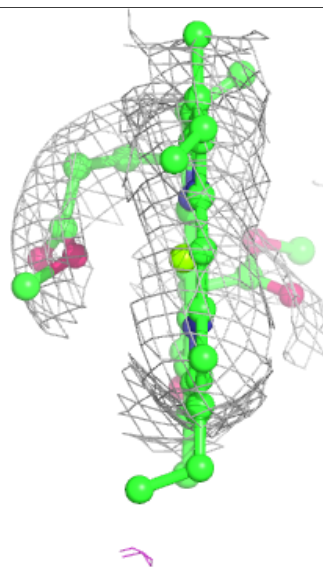
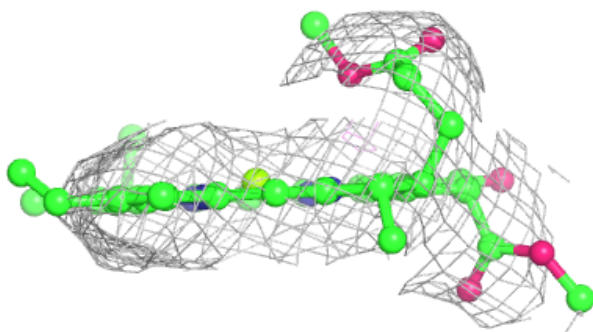
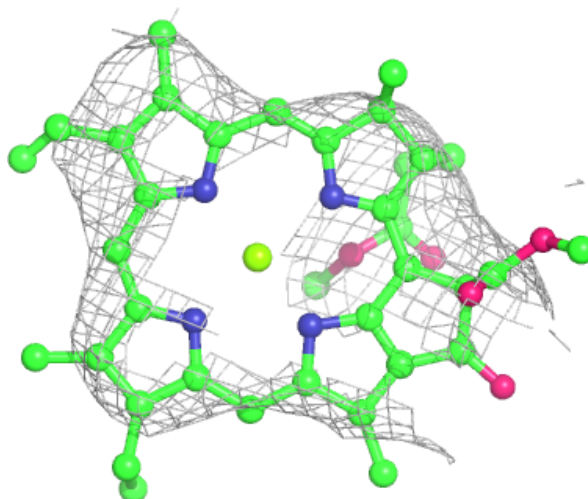
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





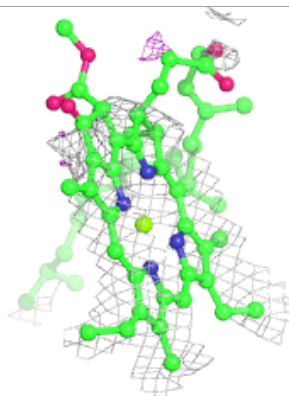
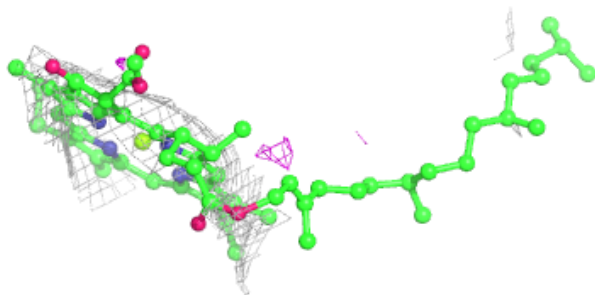
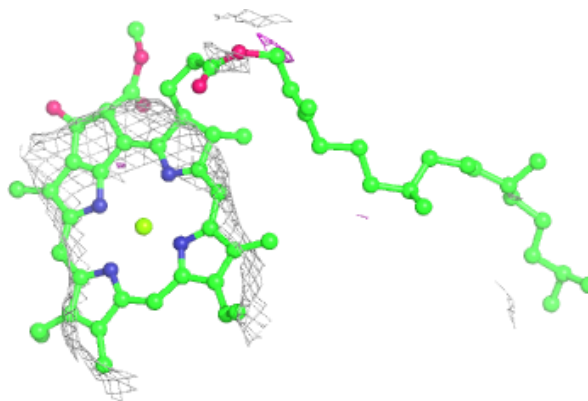
Electron density around CLA a 1136:

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

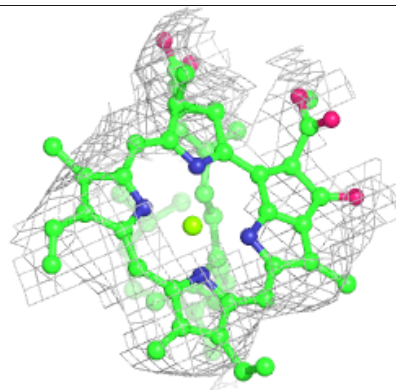
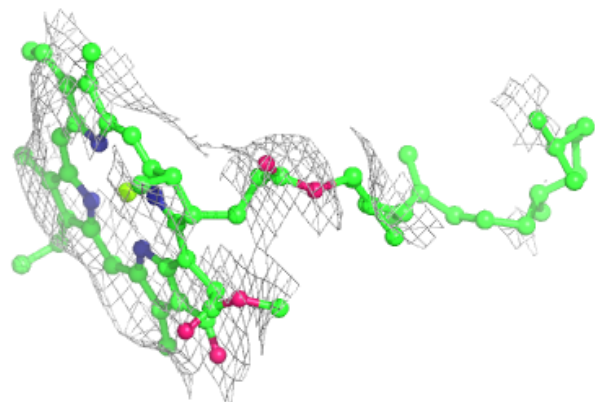
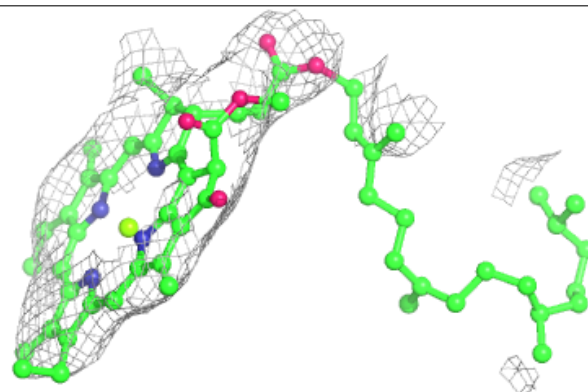


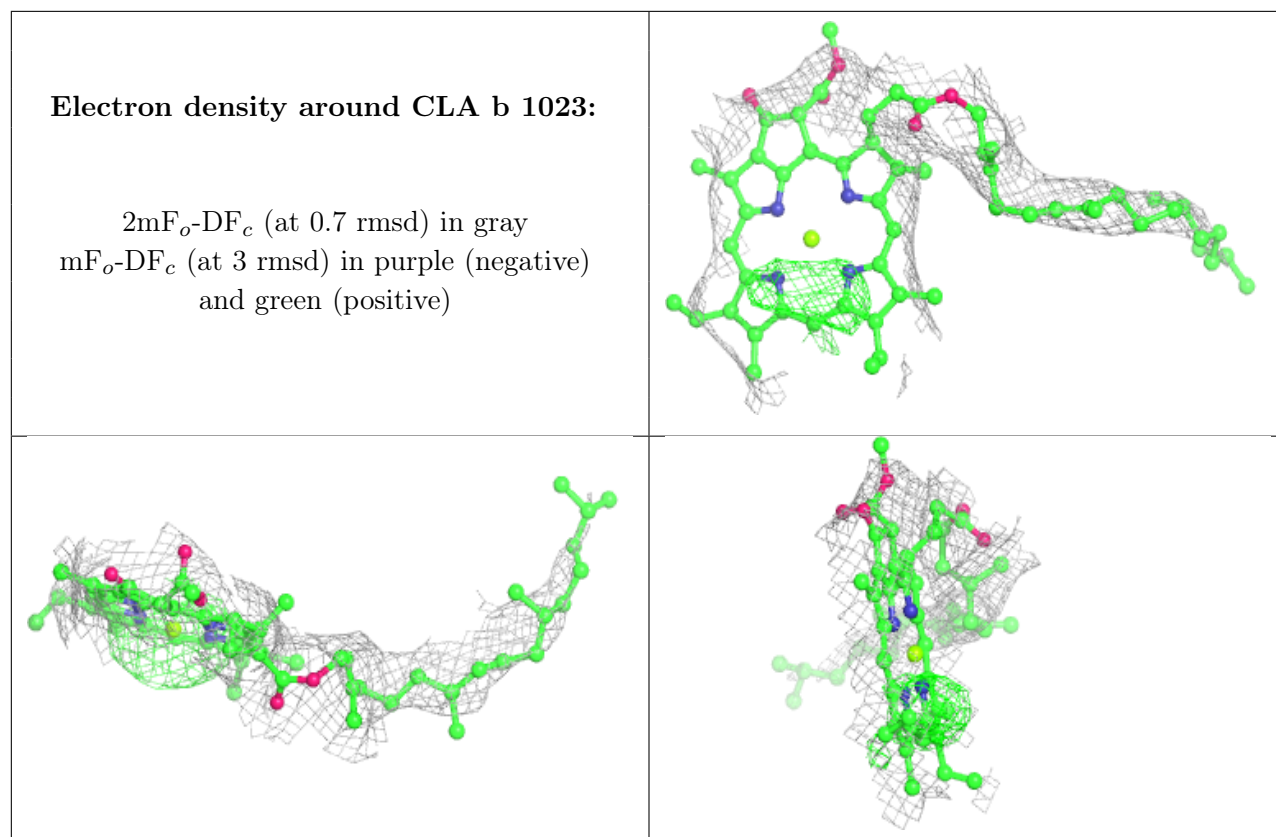
Electron density around CLA b 1013:

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

**Electron density around CLA b 1021:**

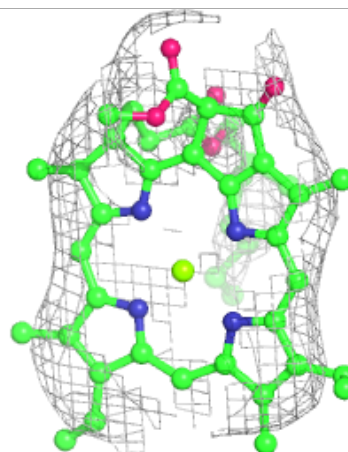
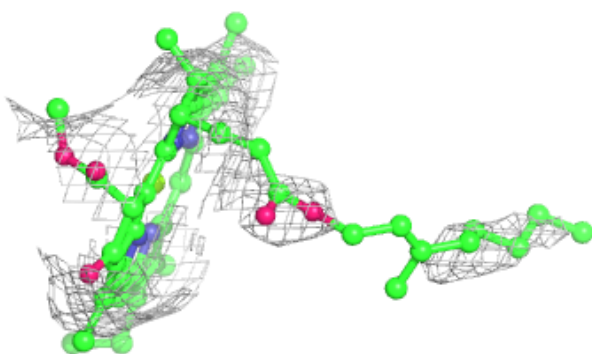
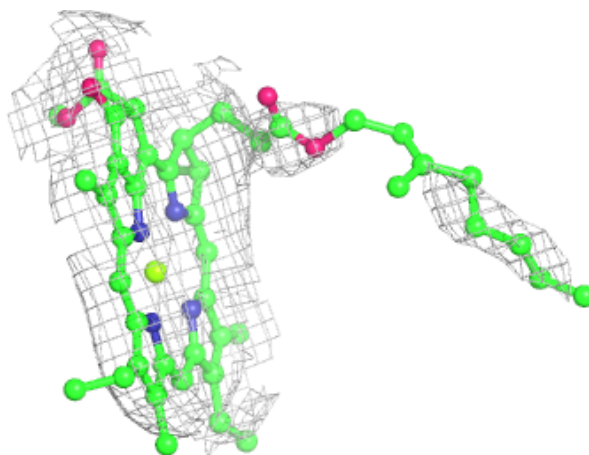
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

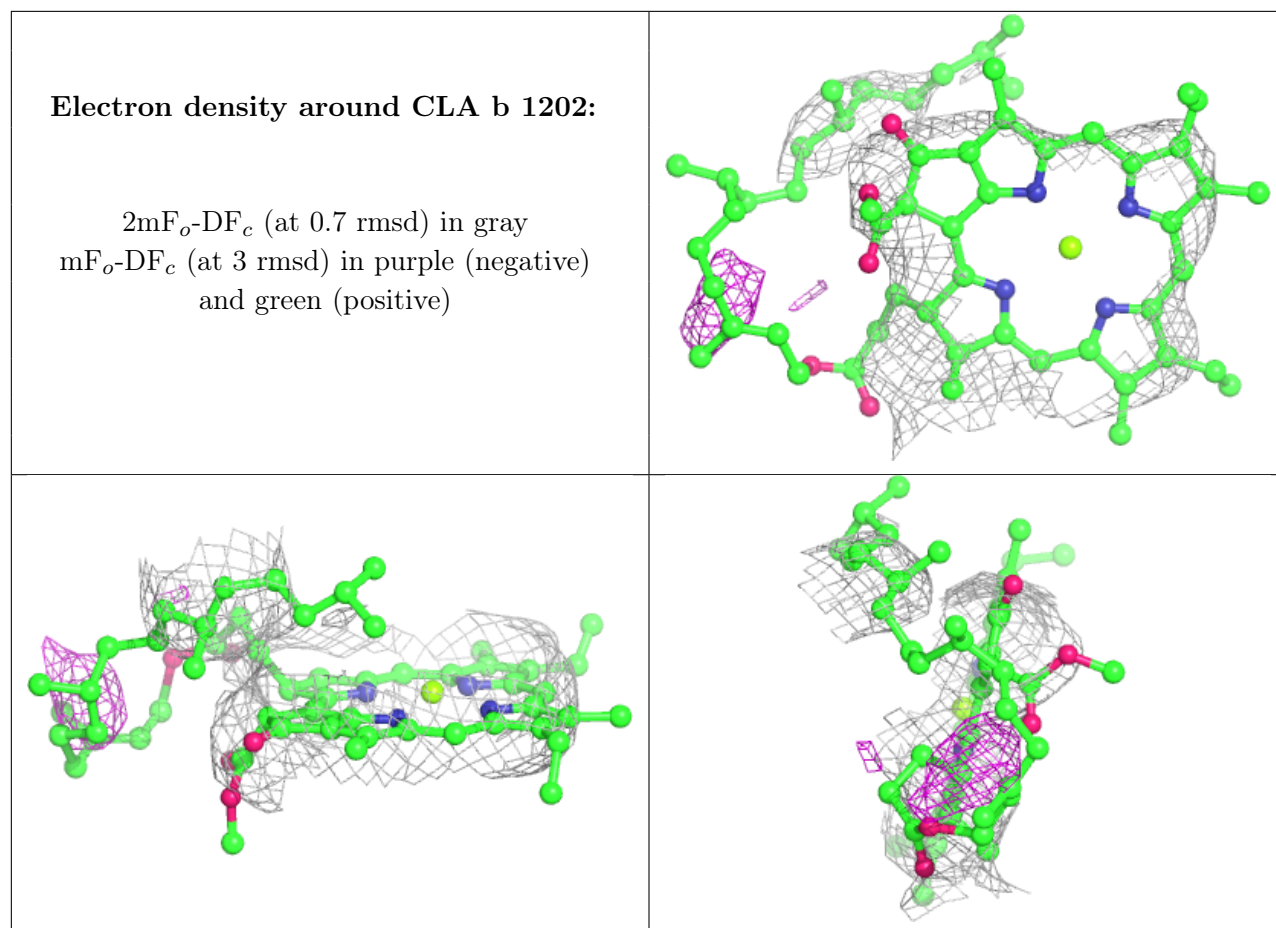




Electron density around CLA b 1201:

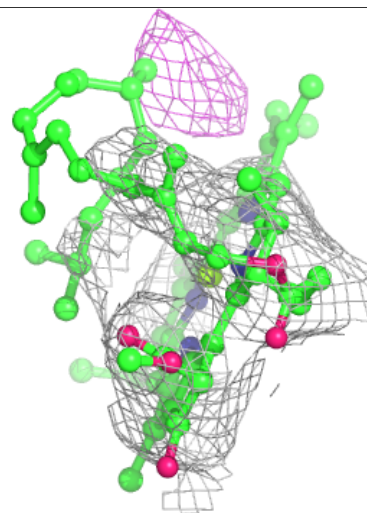
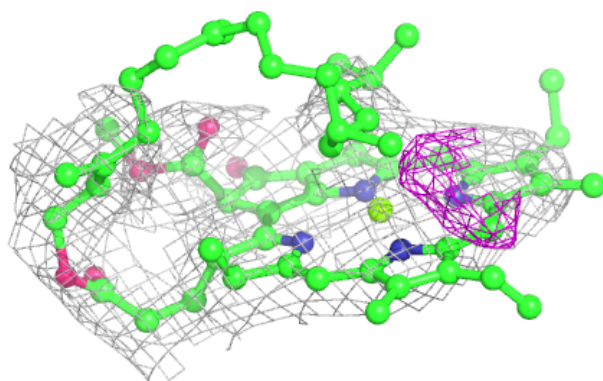
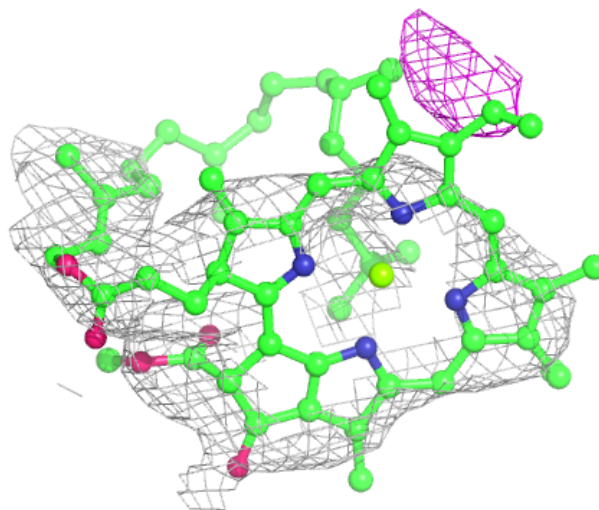
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





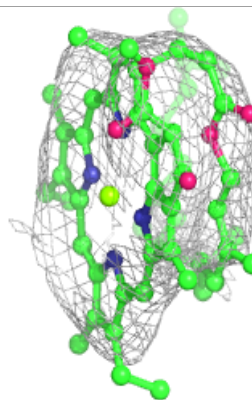
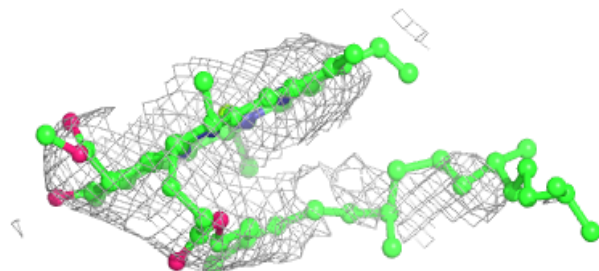
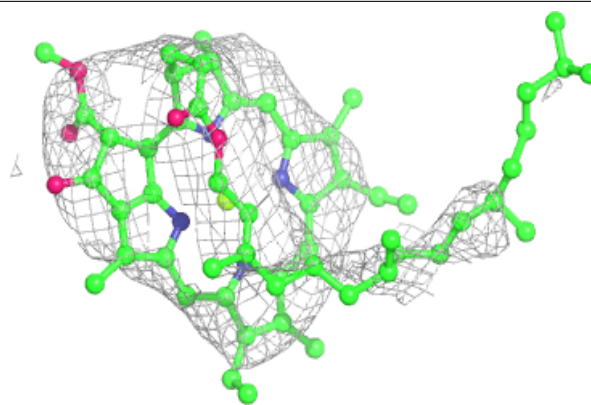
Electron density around CLA b 1203:

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



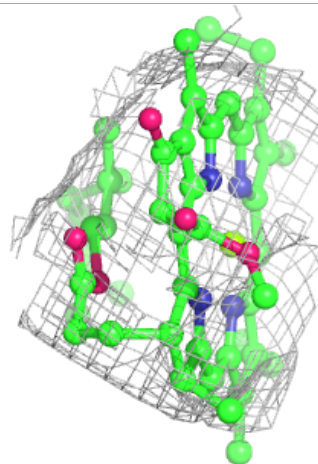
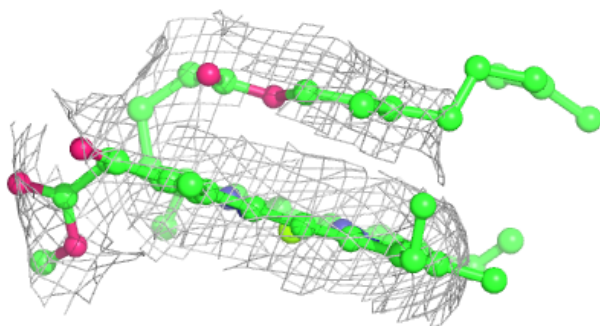
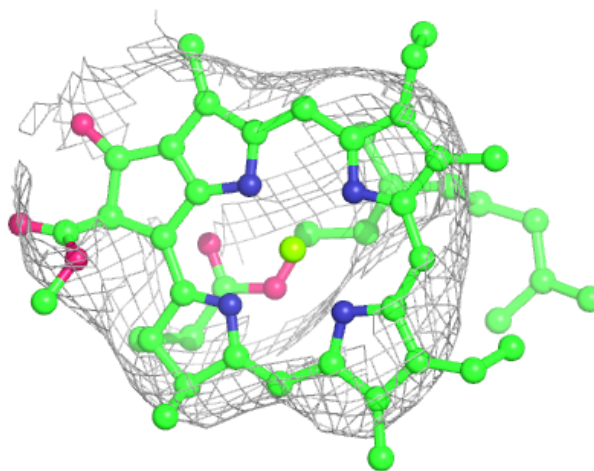
Electron density around CLA b 1204:

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



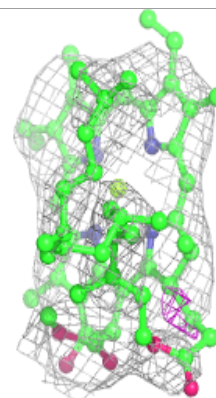
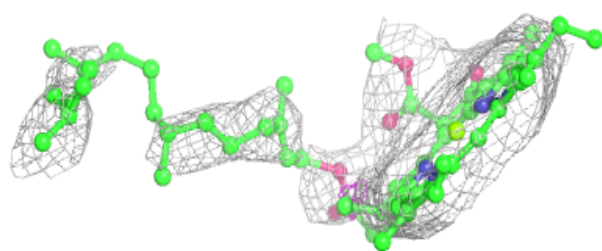
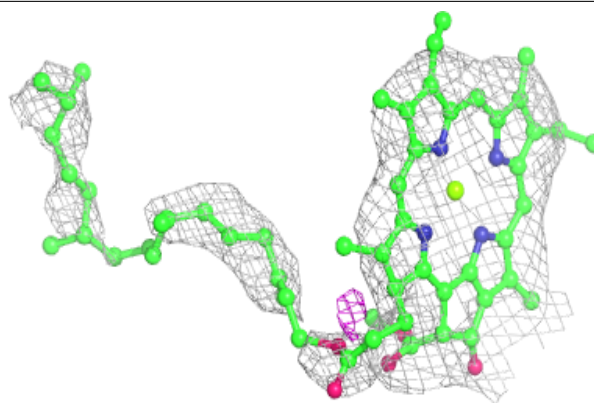
Electron density around CLA b 1205:

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

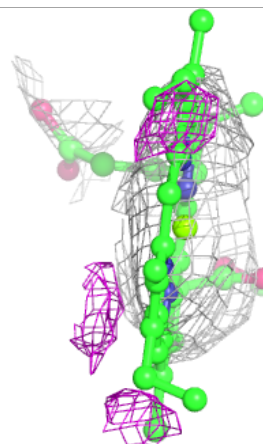
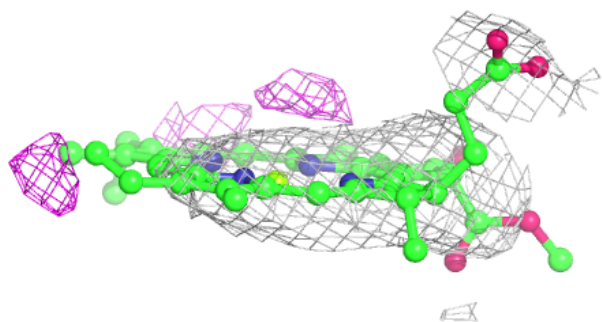
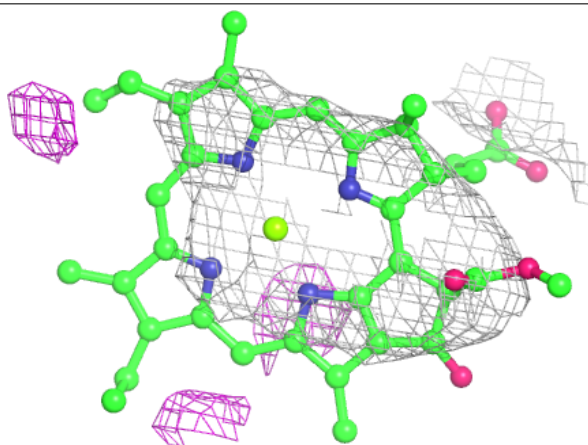


Electron density around CLA b 1207:

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

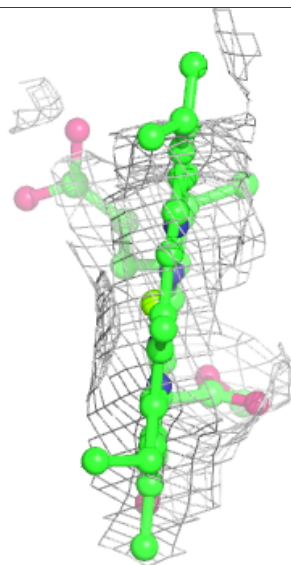
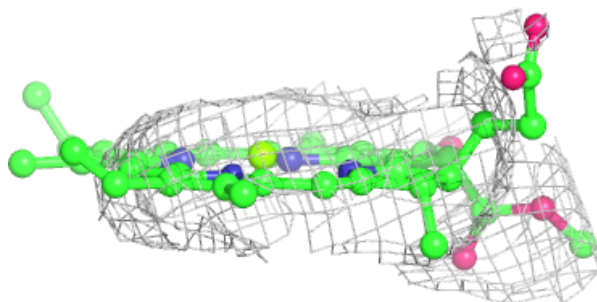
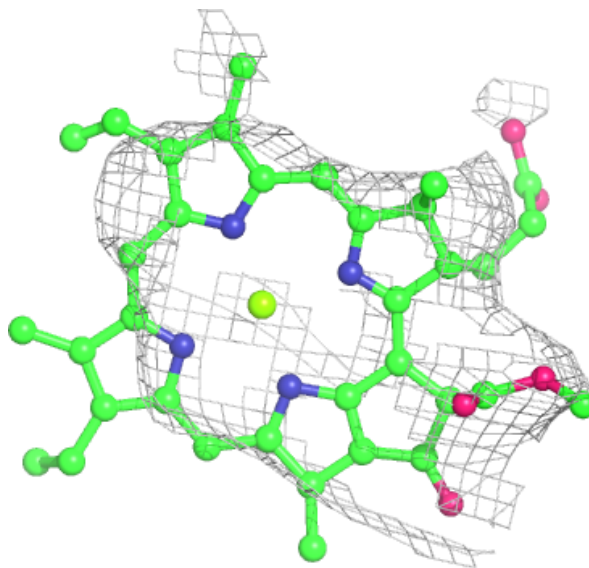
**Electron density around CLA b 1208:**

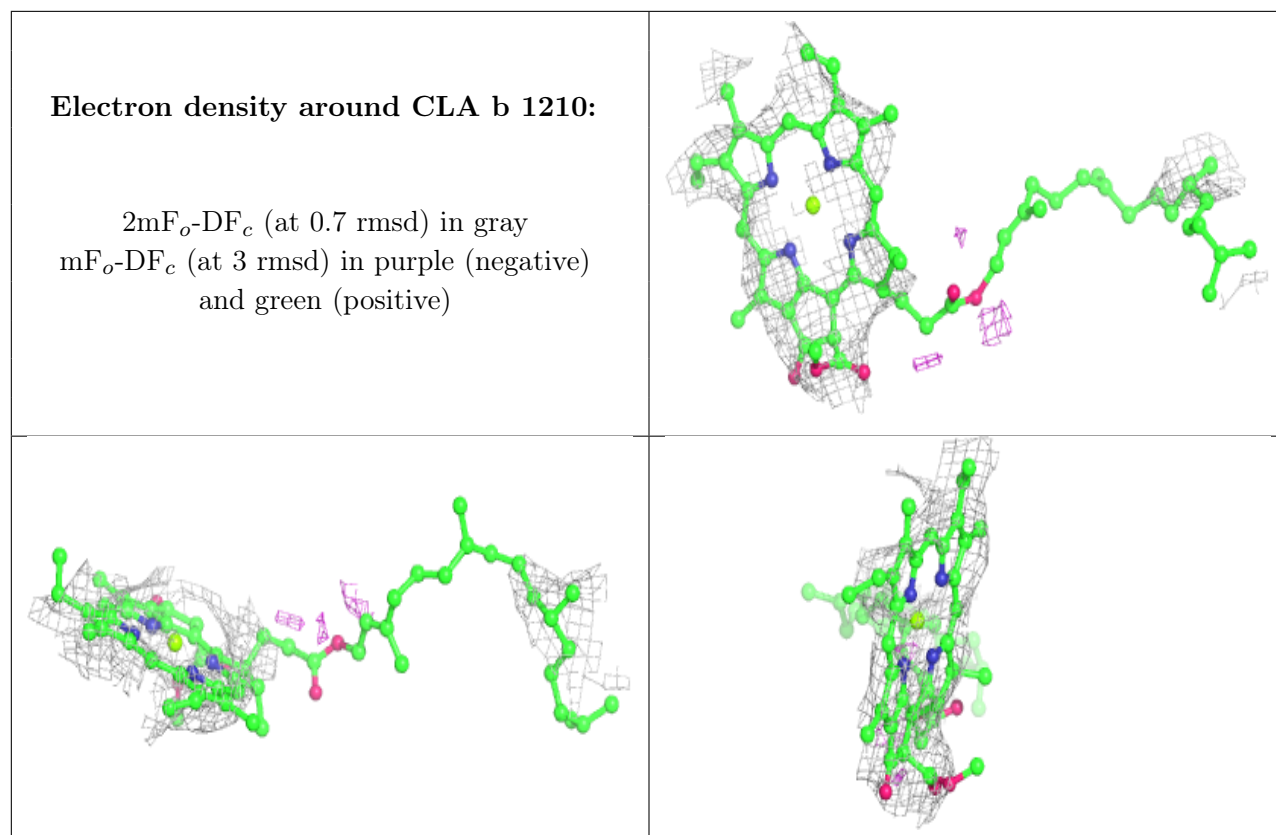
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around CLA b 1209:

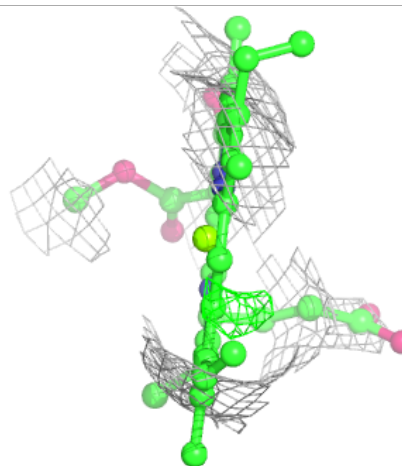
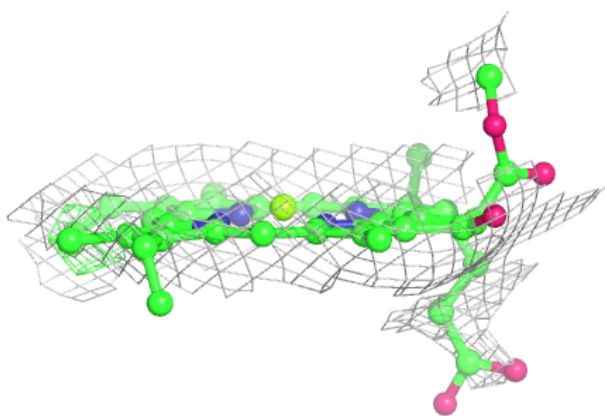
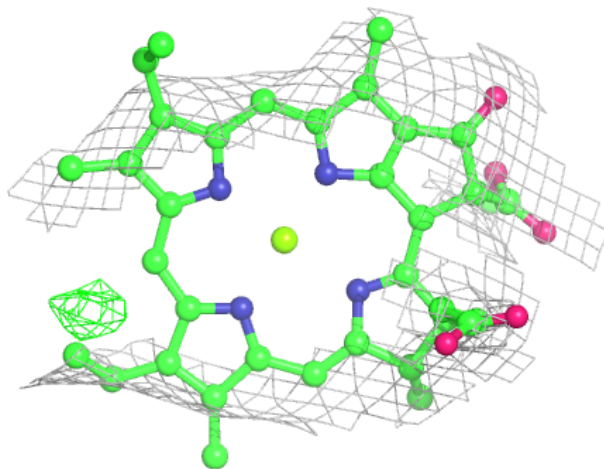
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

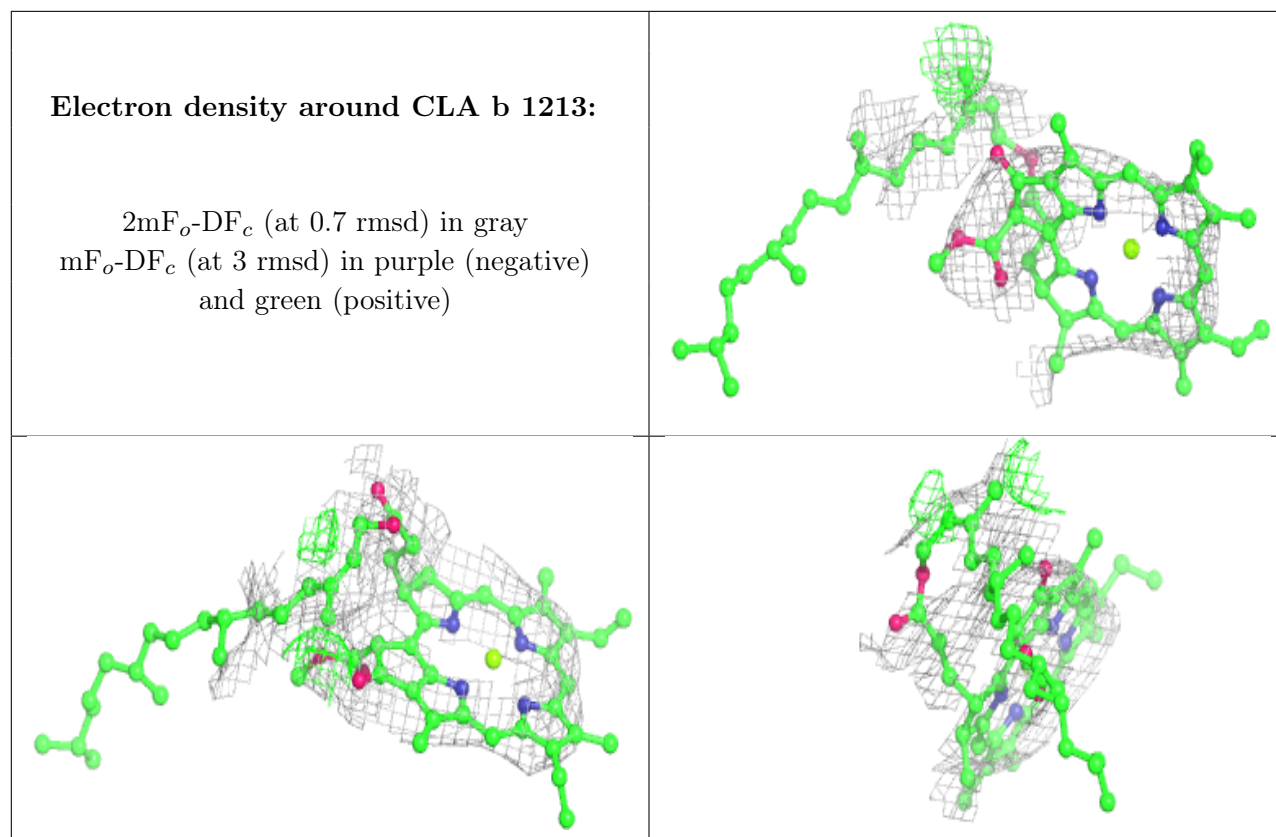




Electron density around CLA b 1212:

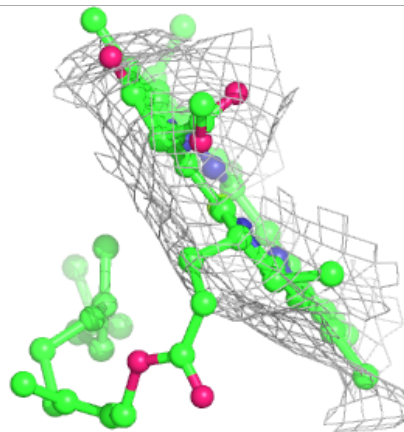
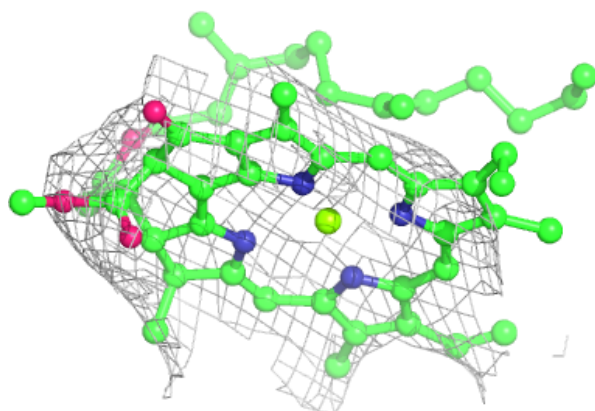
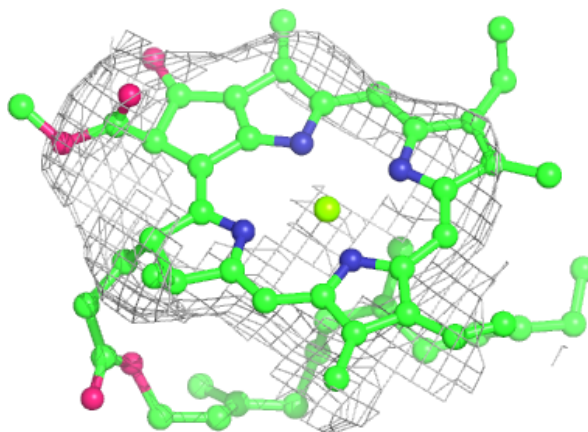
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





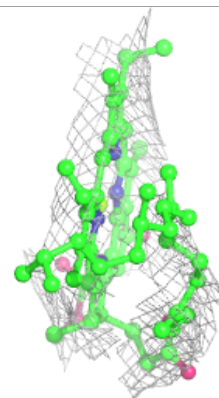
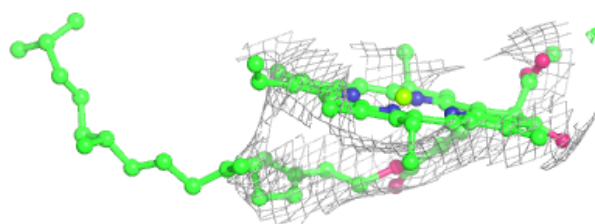
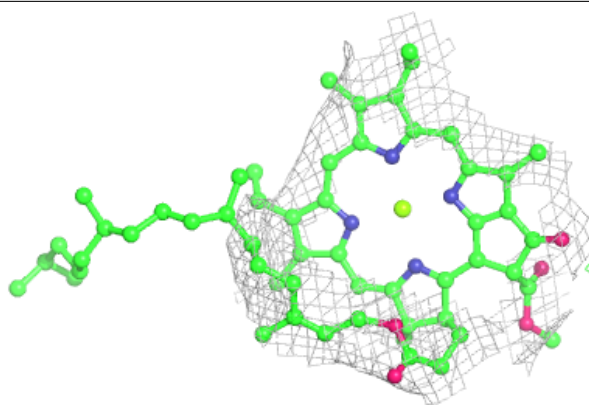
Electron density around CLA b 1214:

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

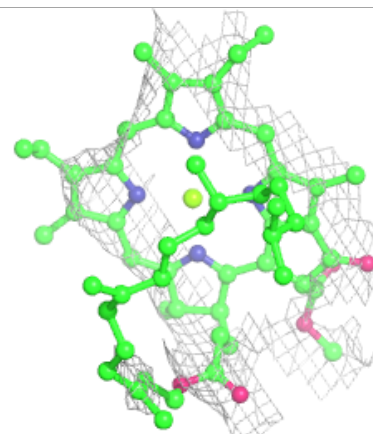
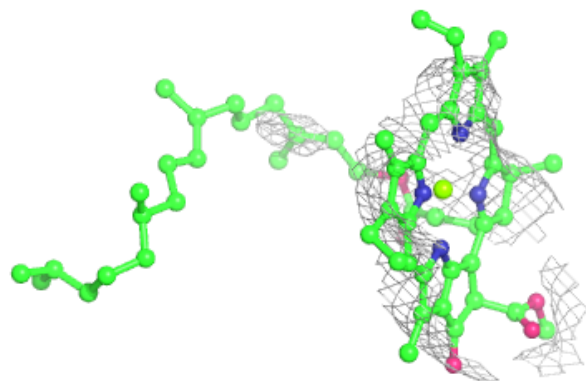
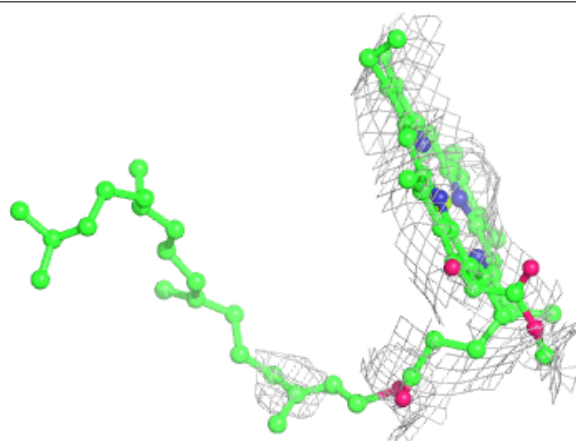


Electron density around CLA b 1215:

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

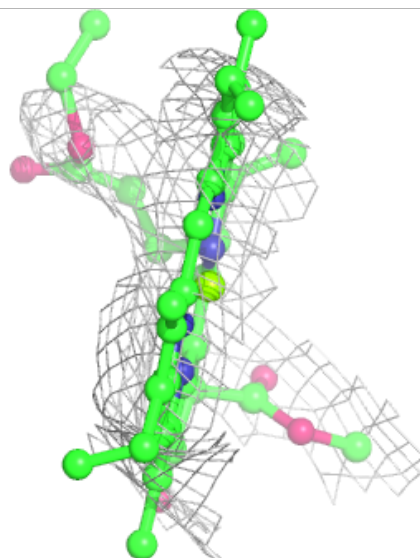
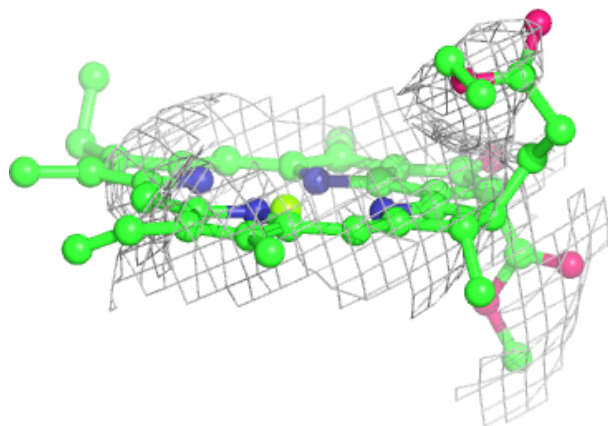
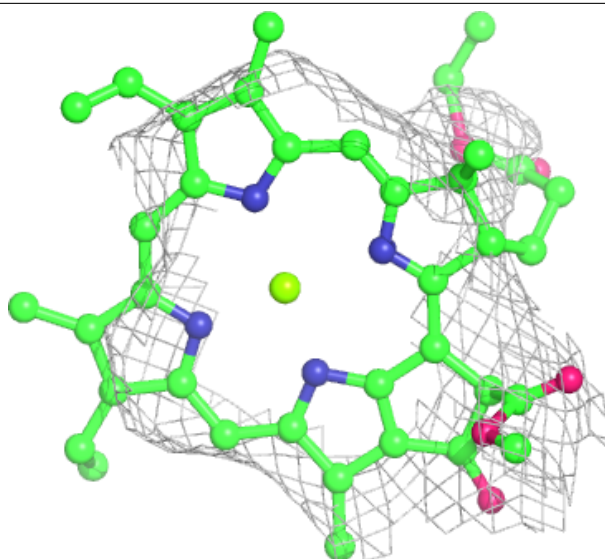
**Electron density around CLA b 1216:**

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



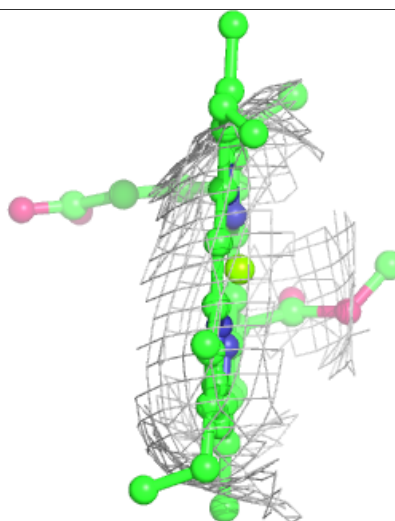
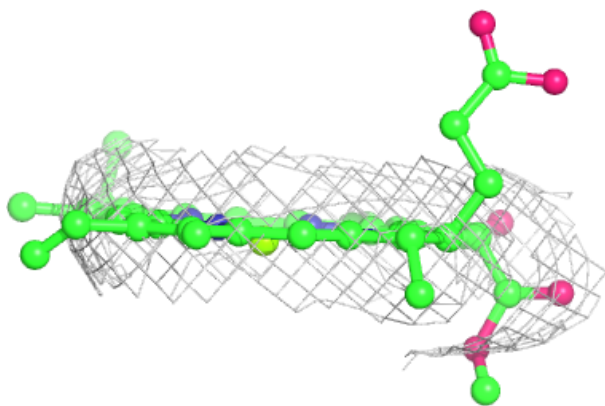
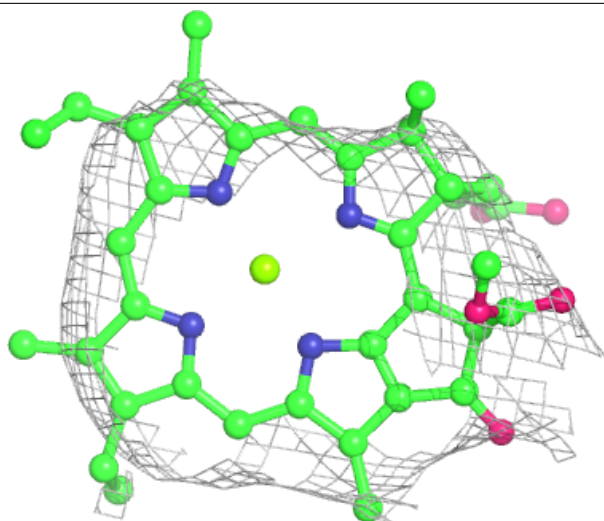
Electron density around CLA b 1217:

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



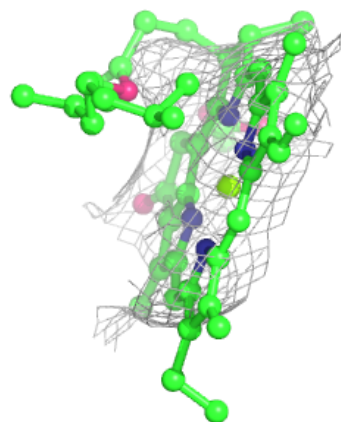
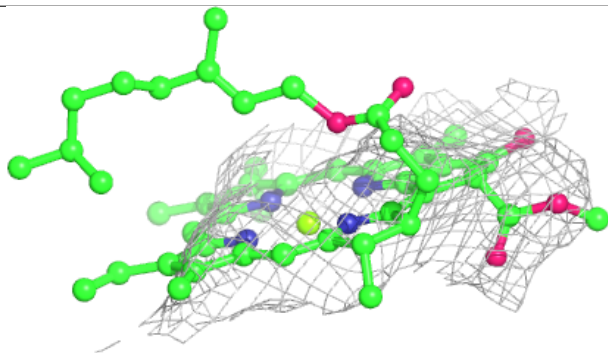
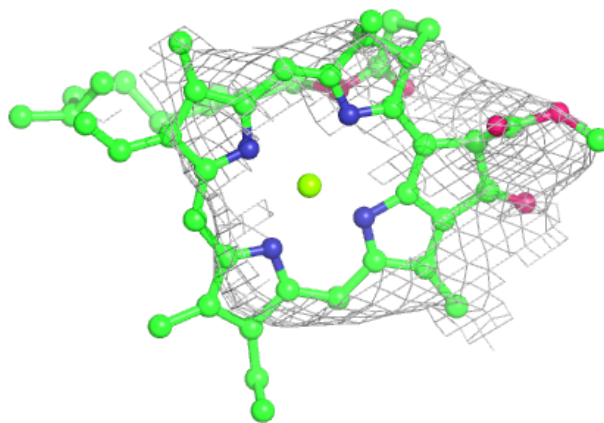
Electron density around CLA b 1218:

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



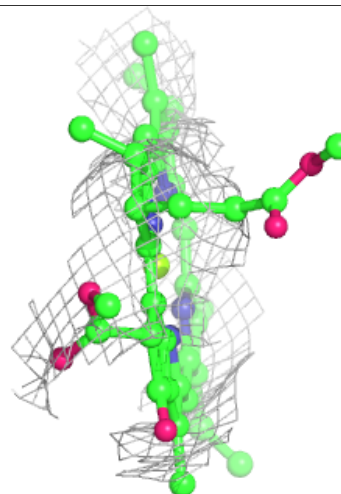
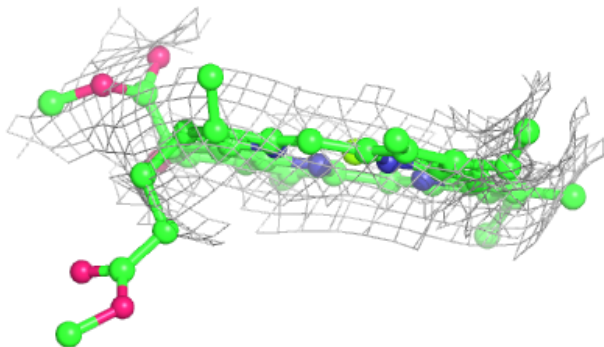
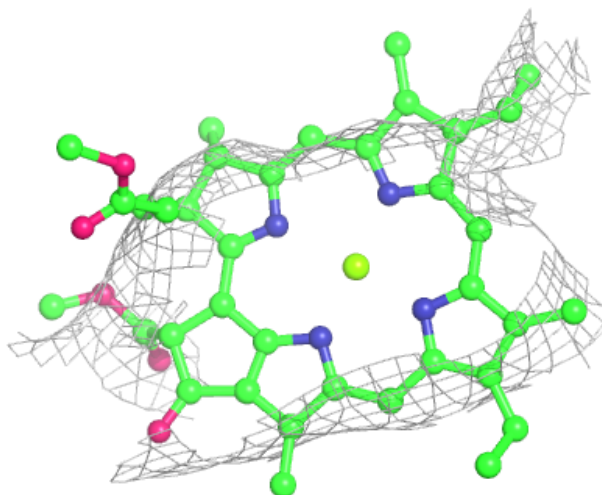
Electron density around CLA b 1219:

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



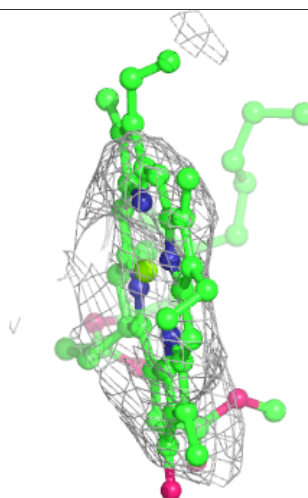
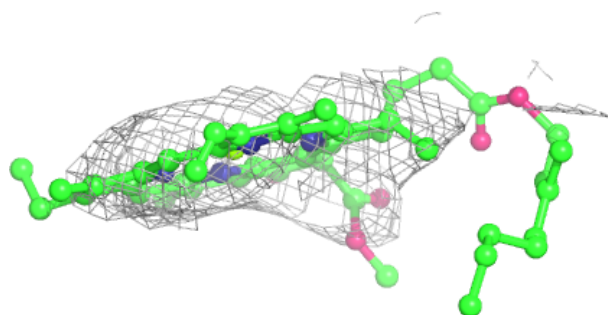
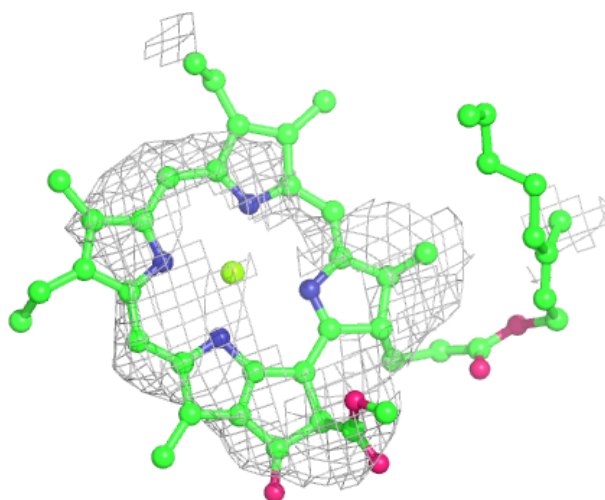
Electron density around CLA b 1220:

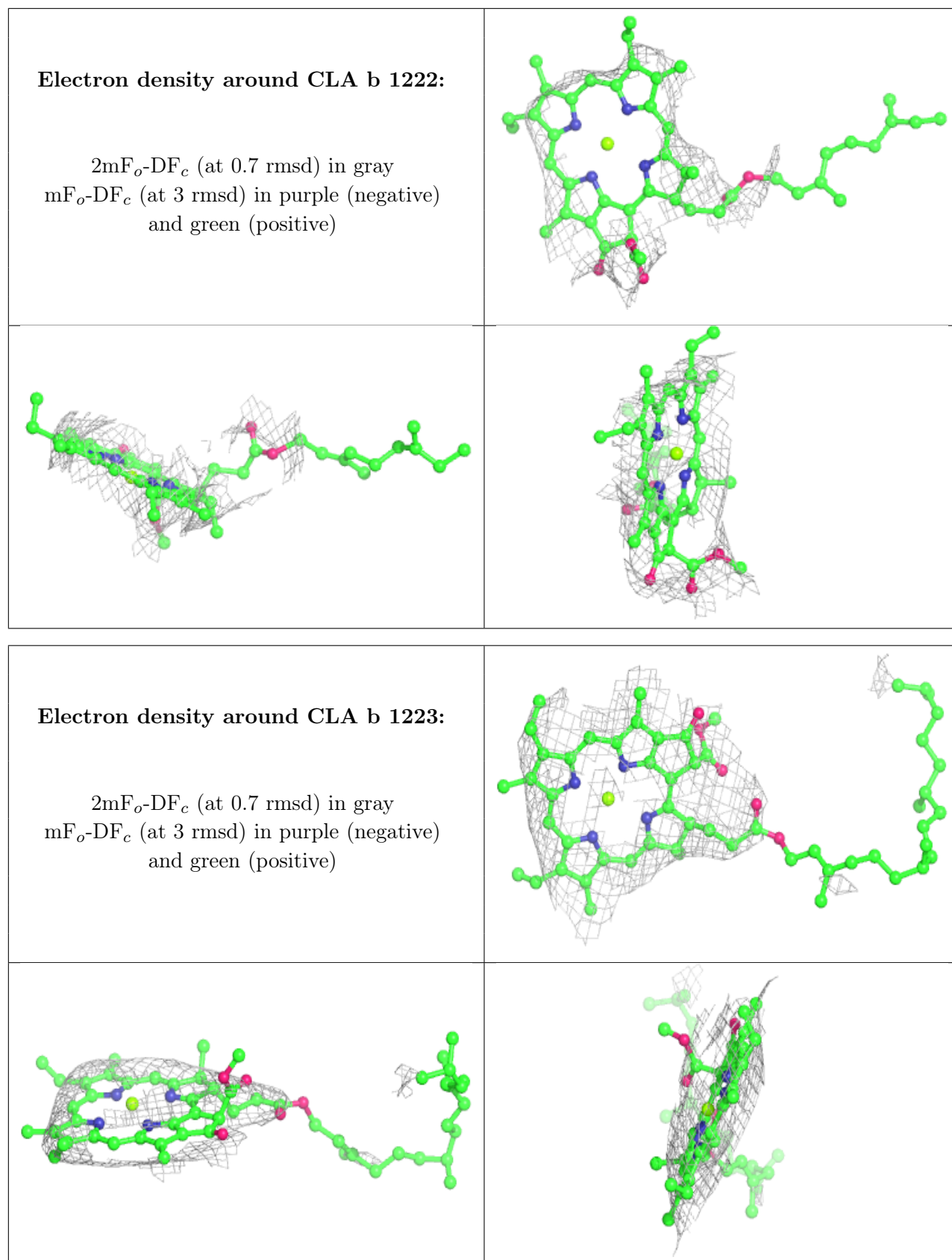
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around CLA b 1221:

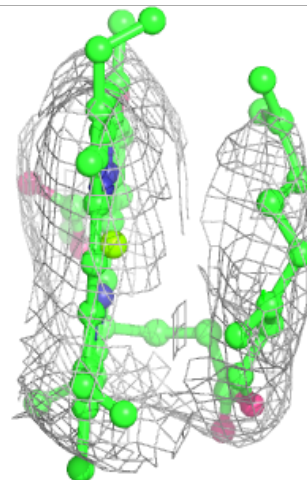
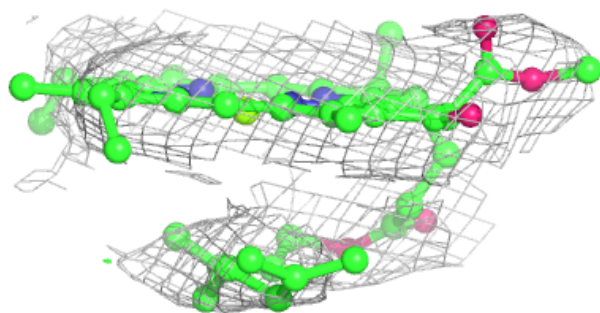
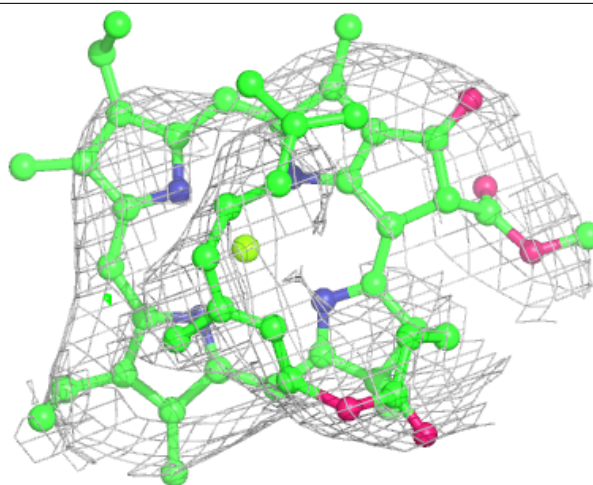
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





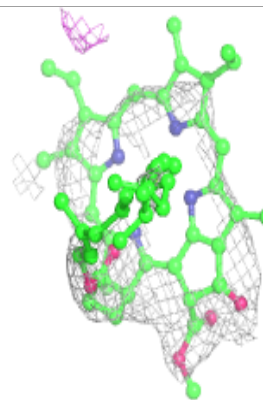
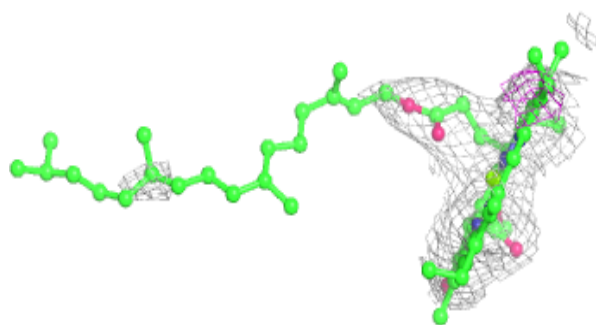
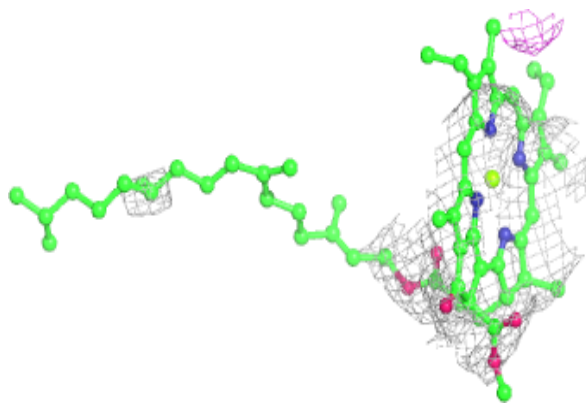
Electron density around CLA b 1224:

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

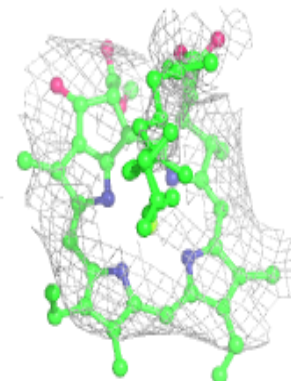
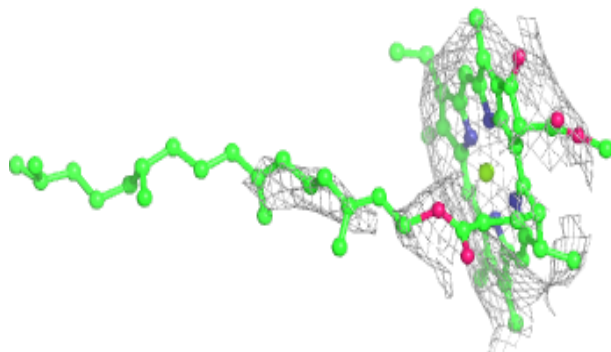
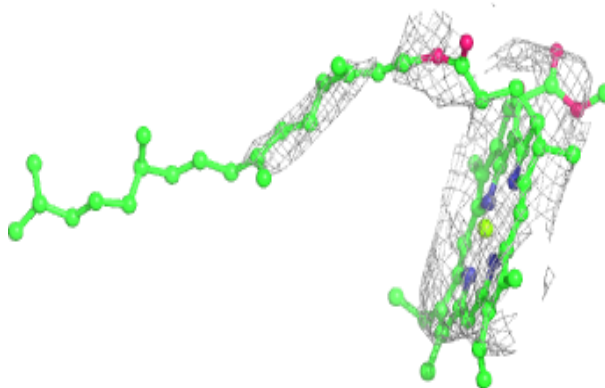


Electron density around CLA b 1225:

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

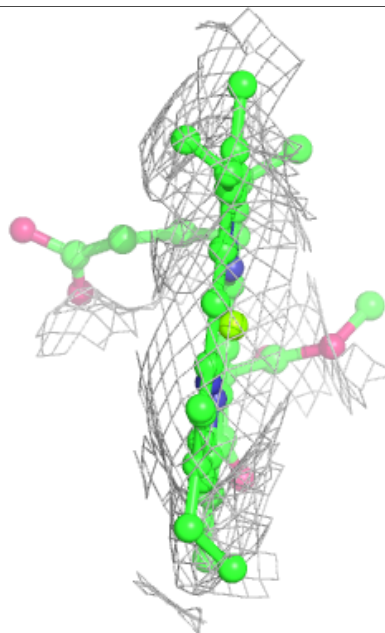
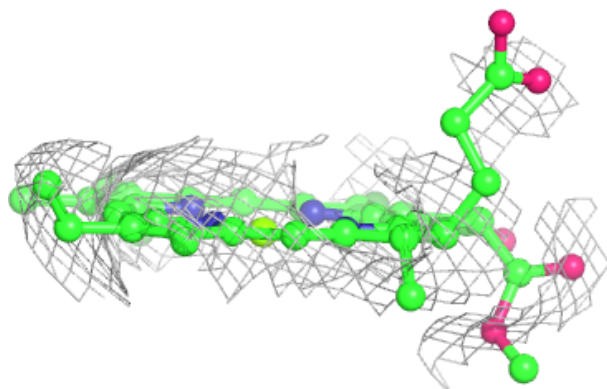
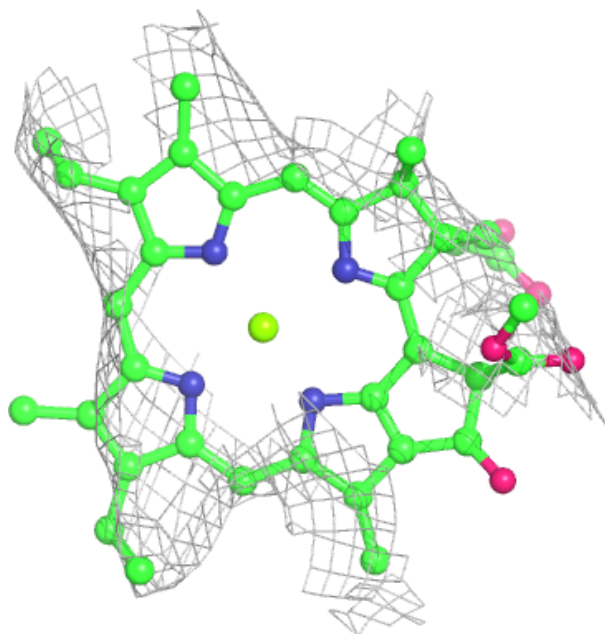
**Electron density around CLA b 1226:**

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



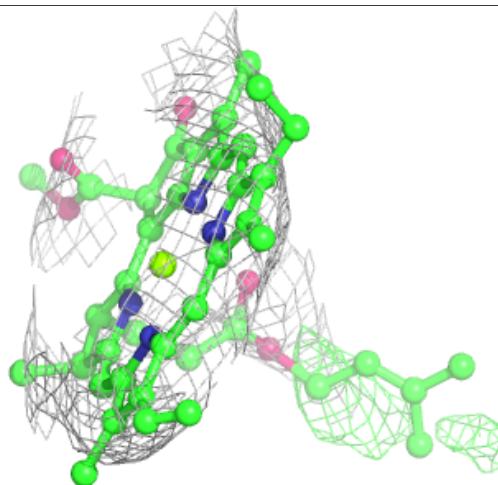
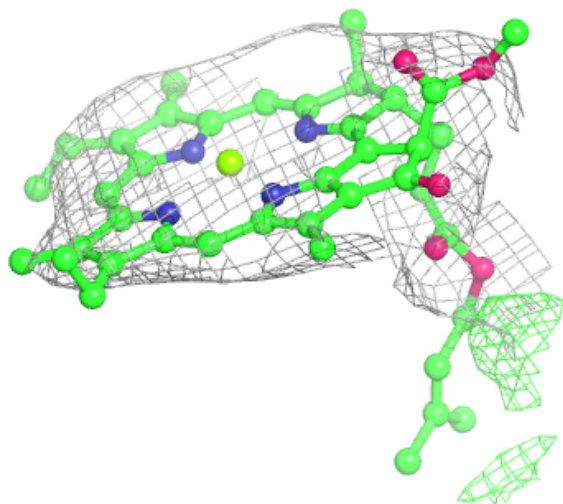
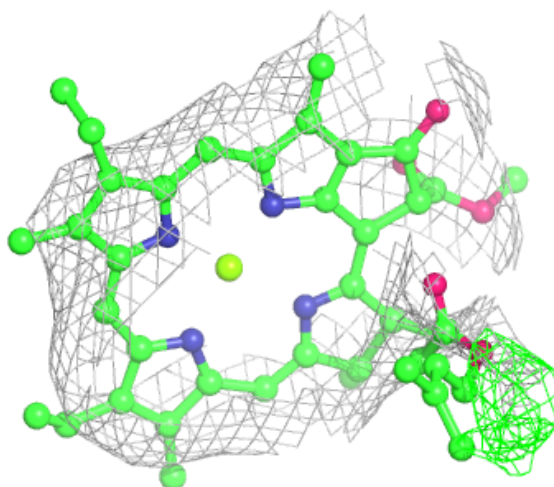
Electron density around CLA b 1227:

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



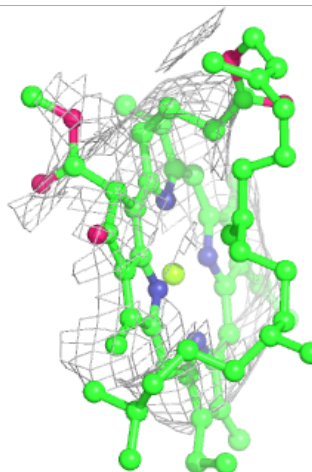
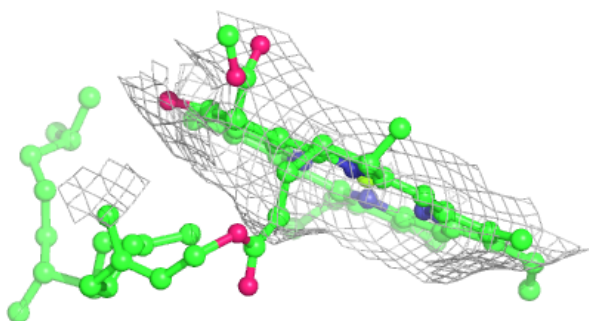
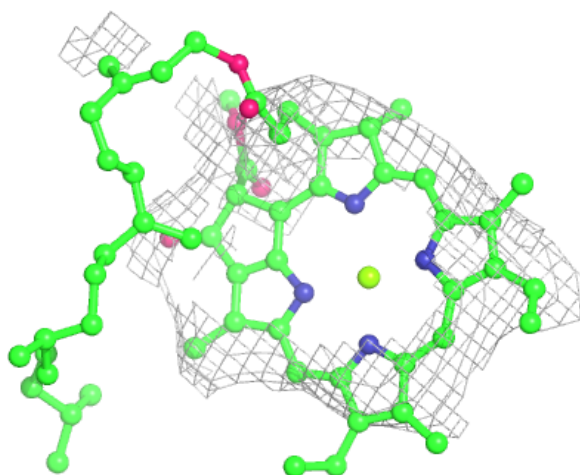
Electron density around CLA b 1228:

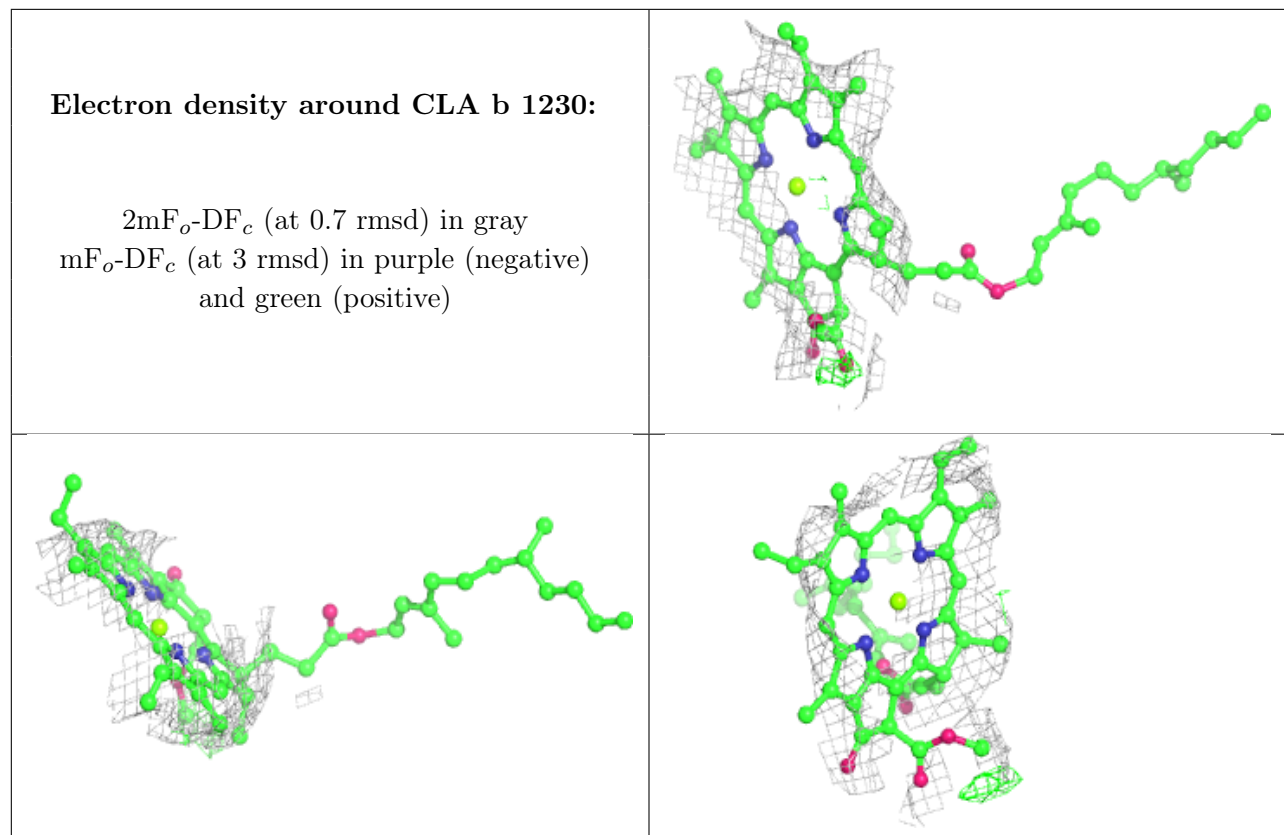
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around CLA b 1229:

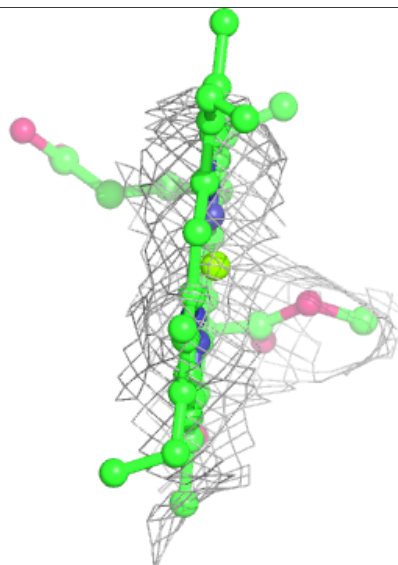
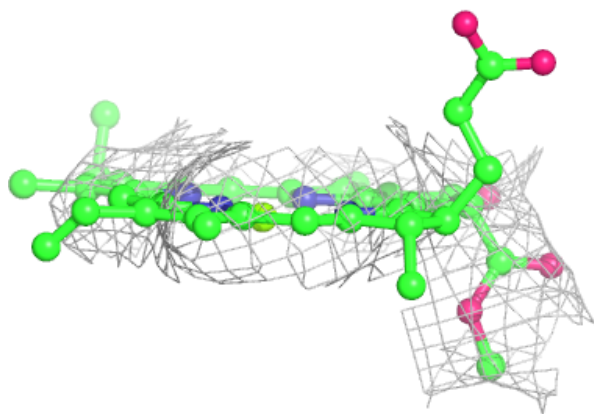
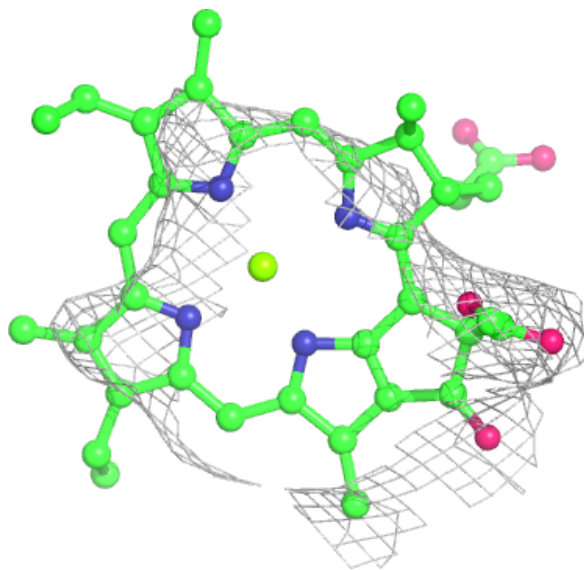
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





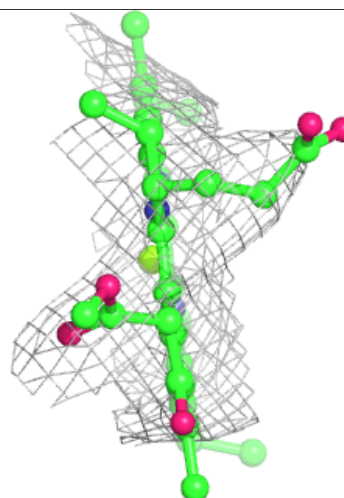
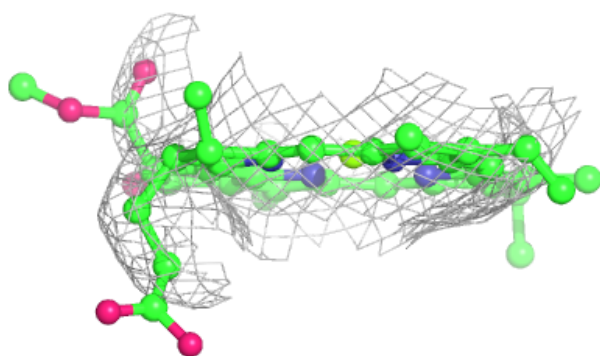
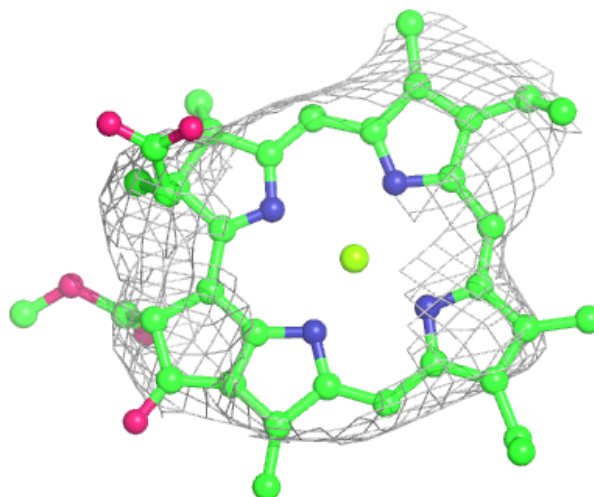
Electron density around CLA b 1231:

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



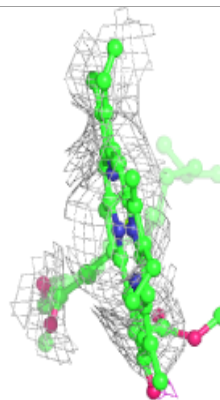
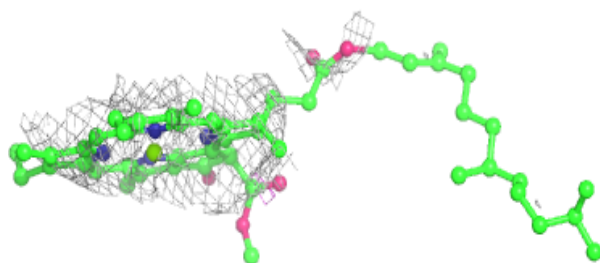
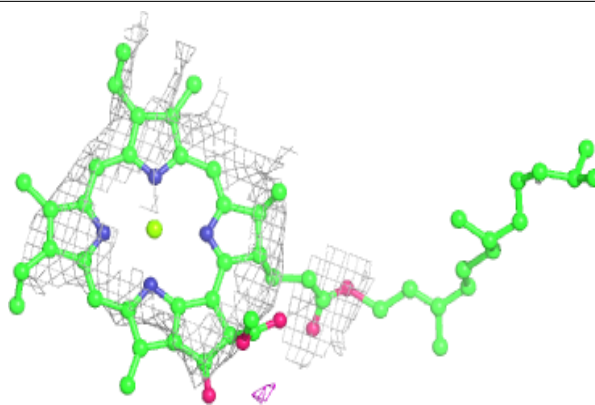
Electron density around CLA b 1232:

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

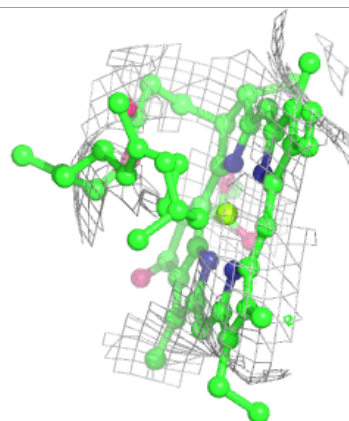
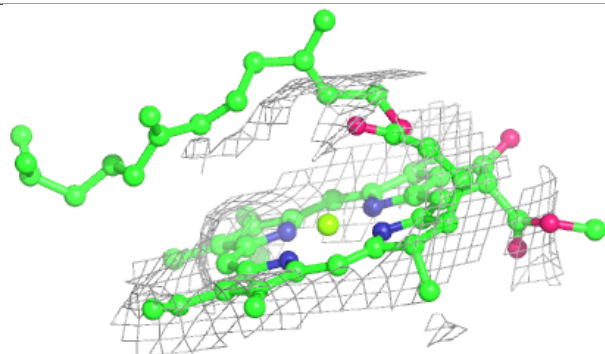
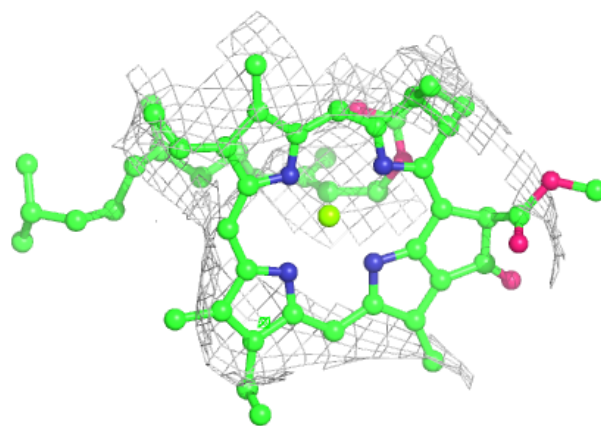


Electron density around CLA b 1234:

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

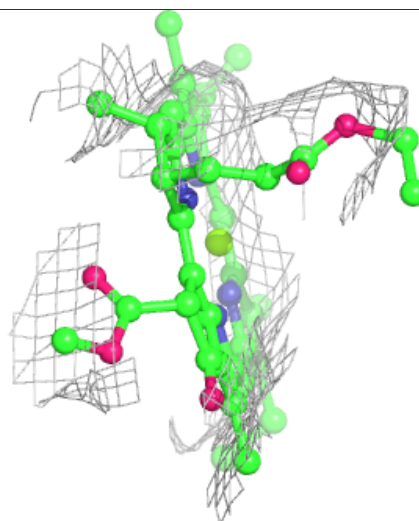
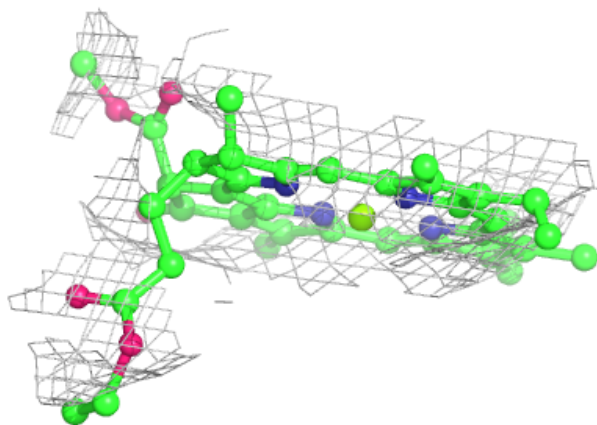
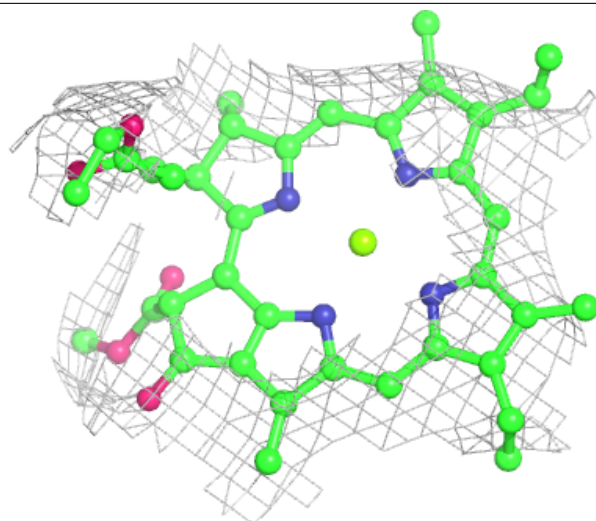
**Electron density around CLA b 1235:**

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



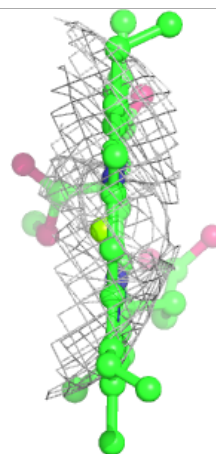
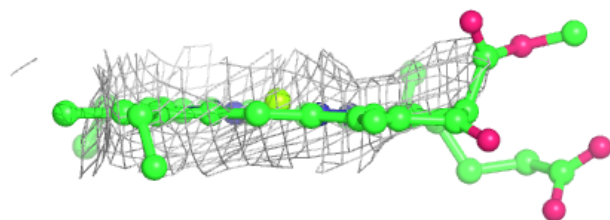
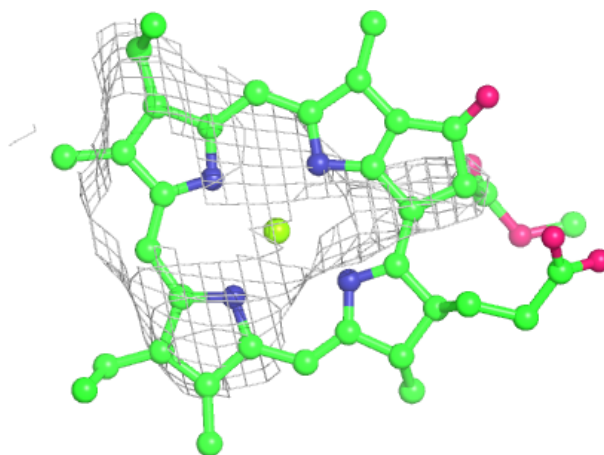
Electron density around CLA b 1236:

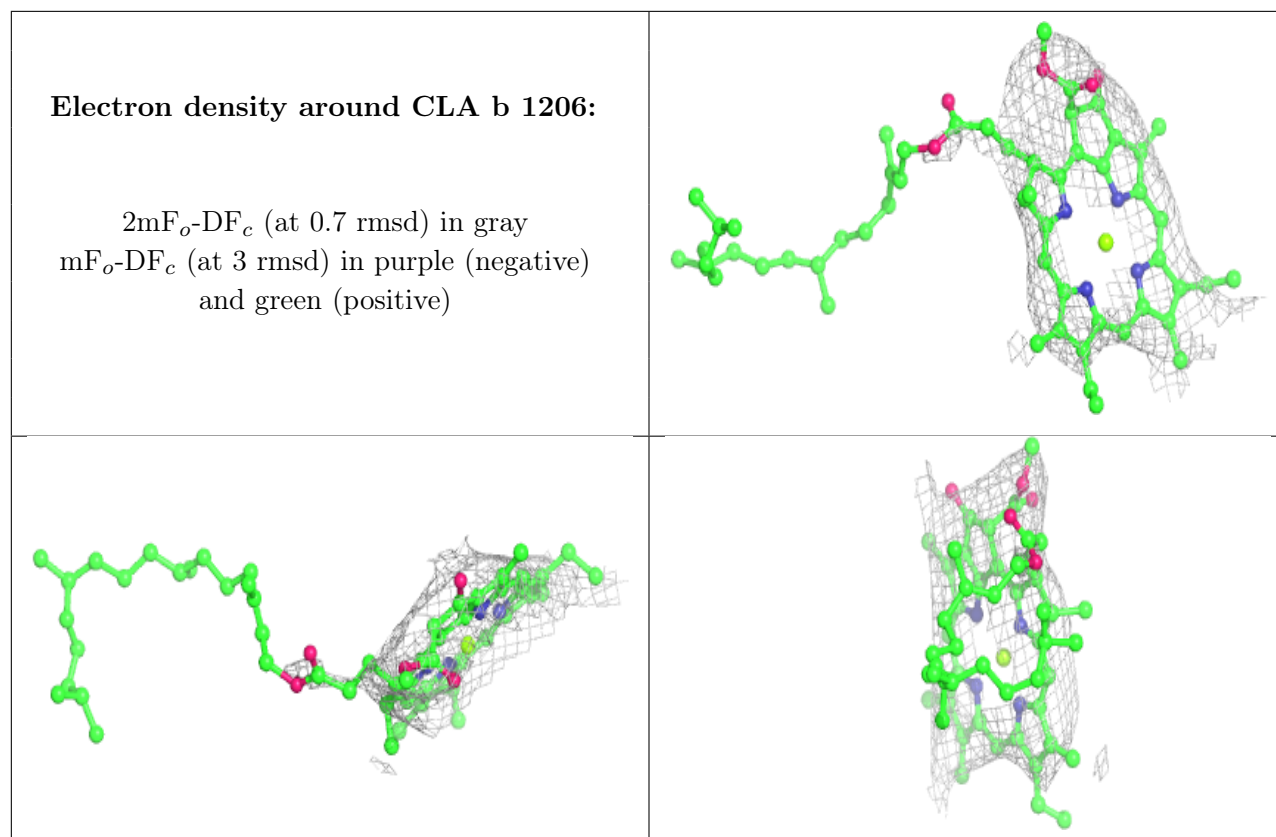
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around CLA b 1240:

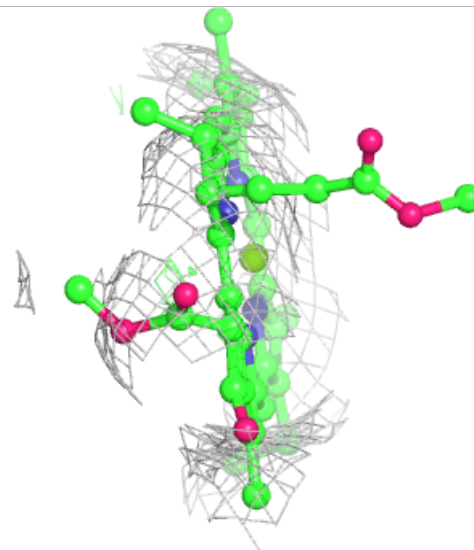
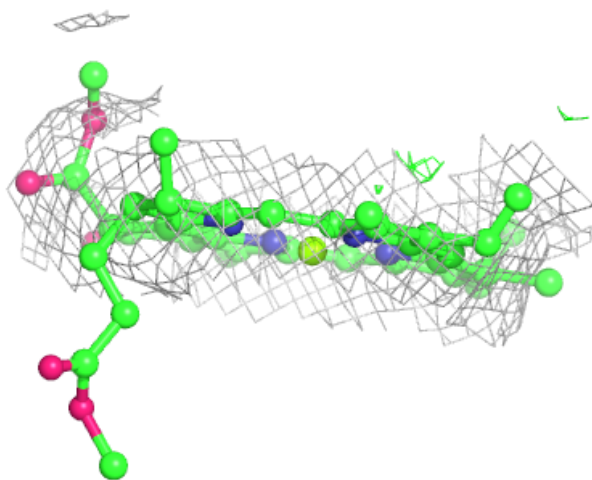
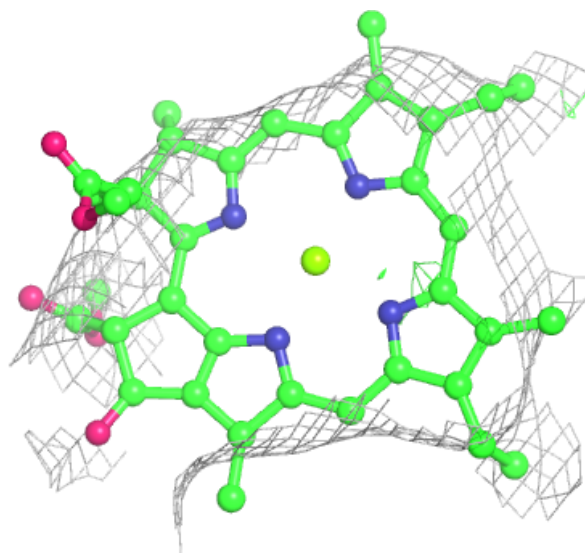
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

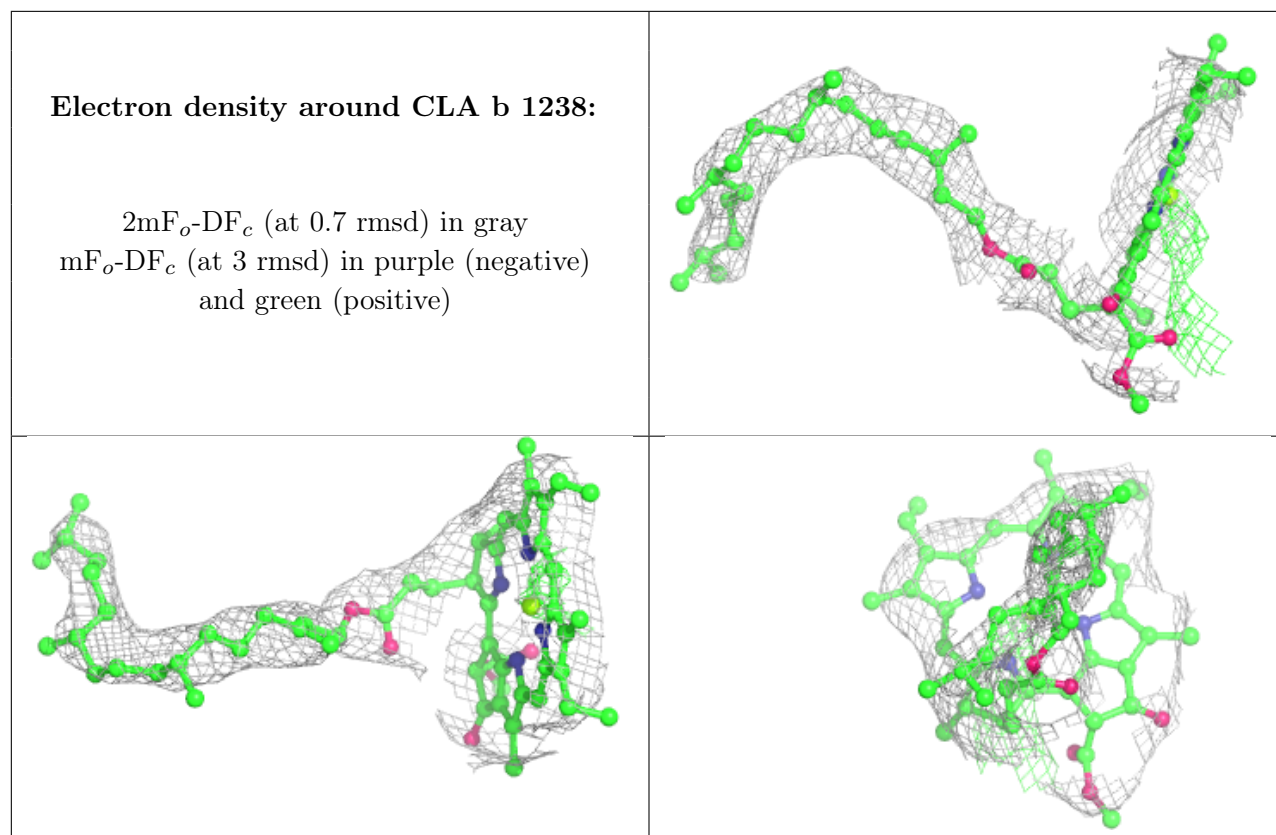




Electron density around CLA b 1211:

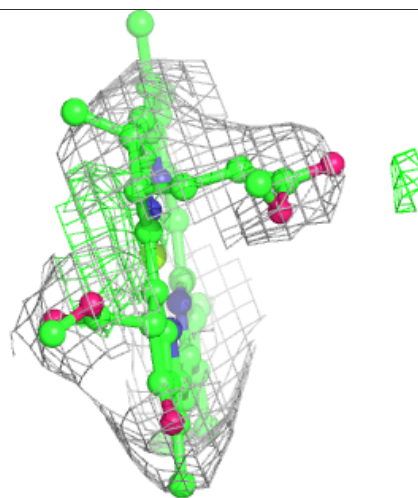
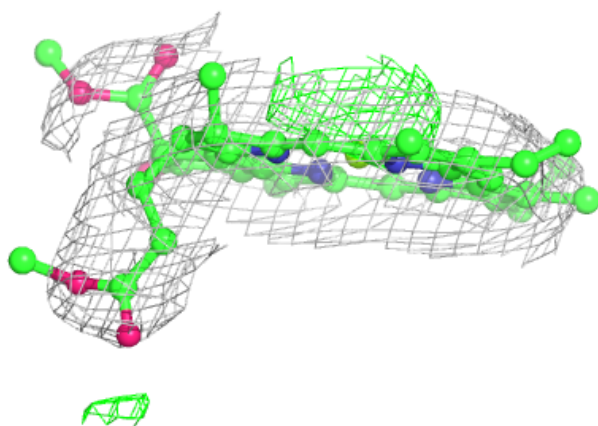
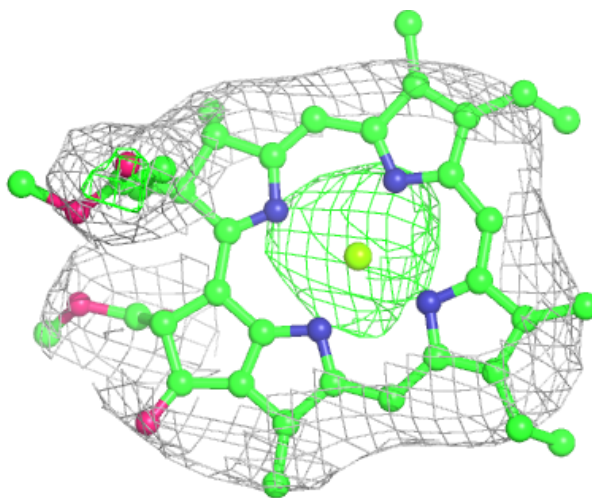
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

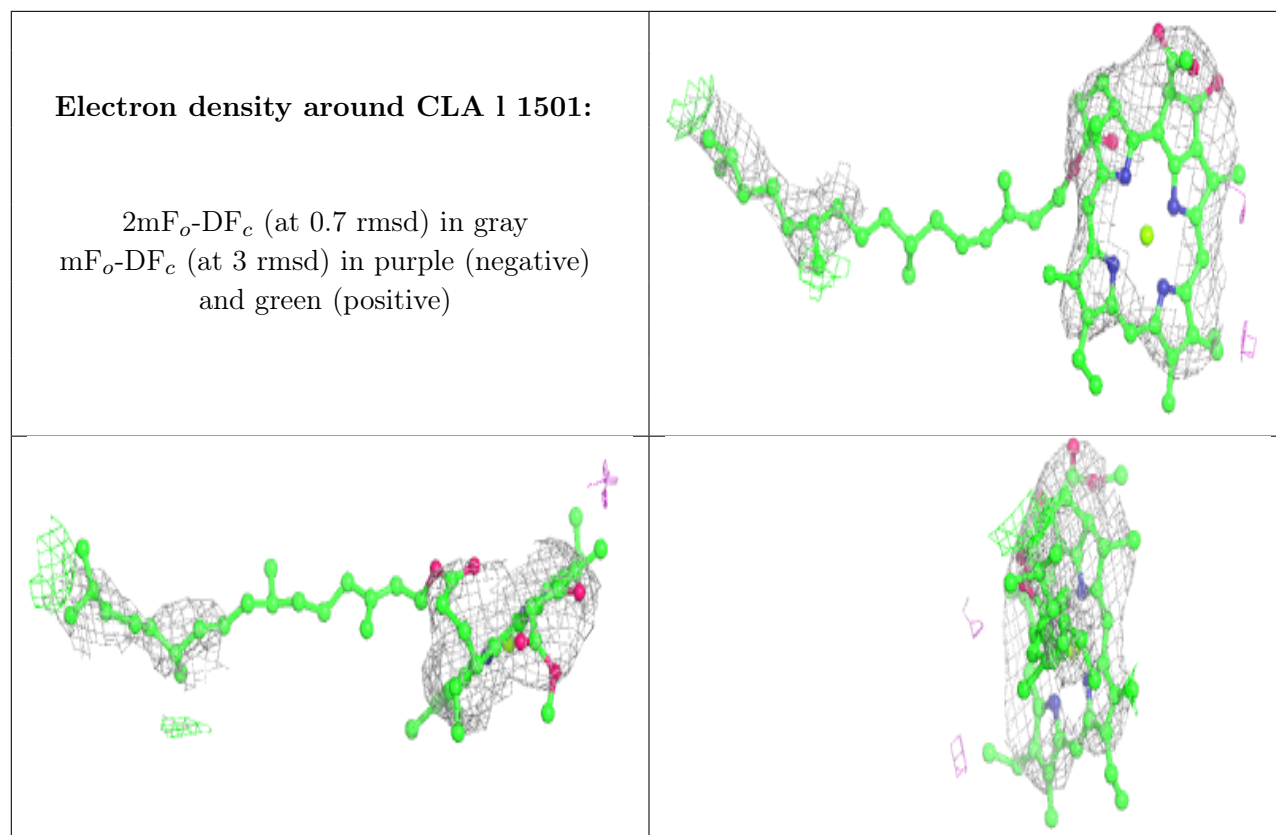


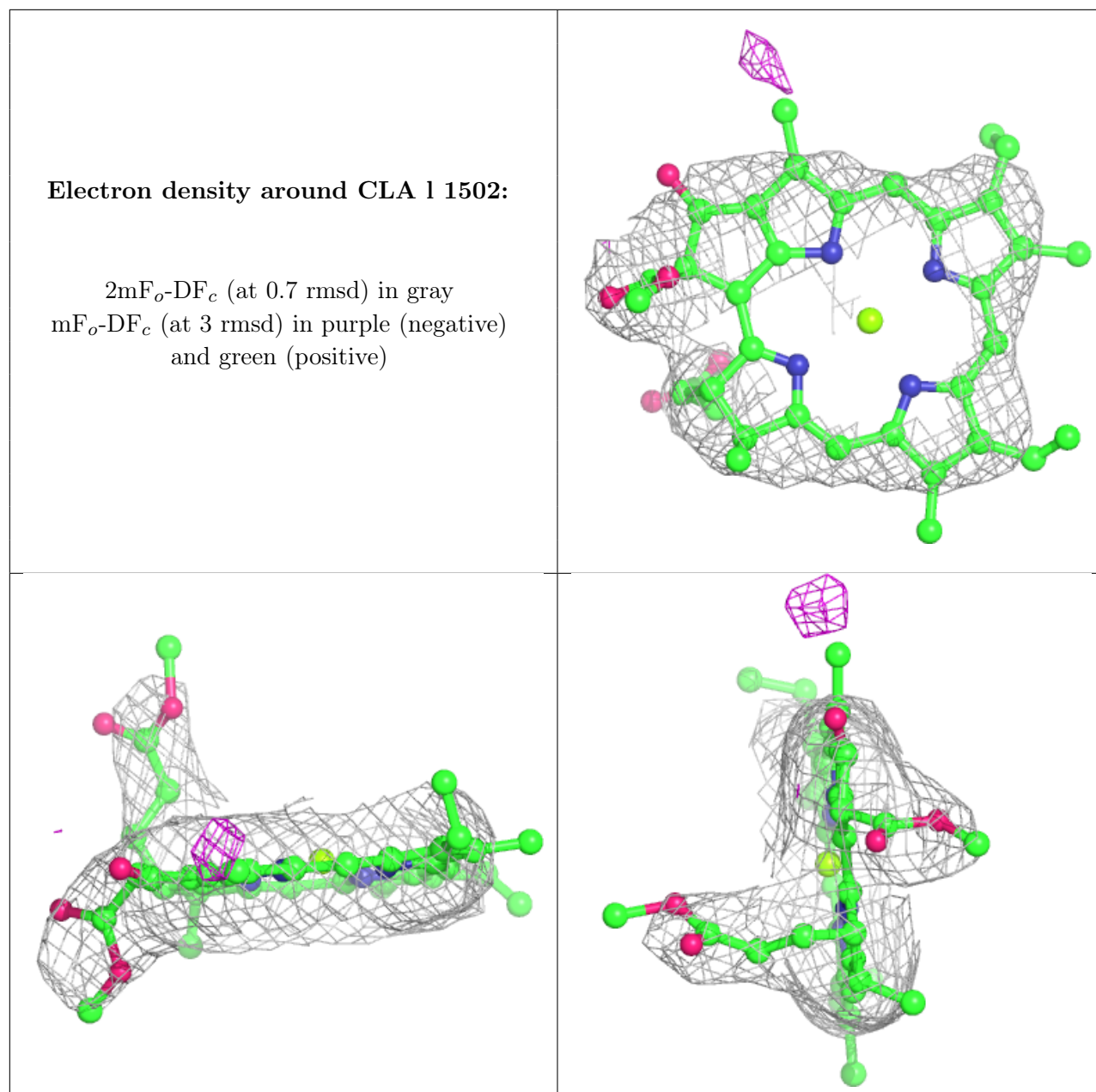


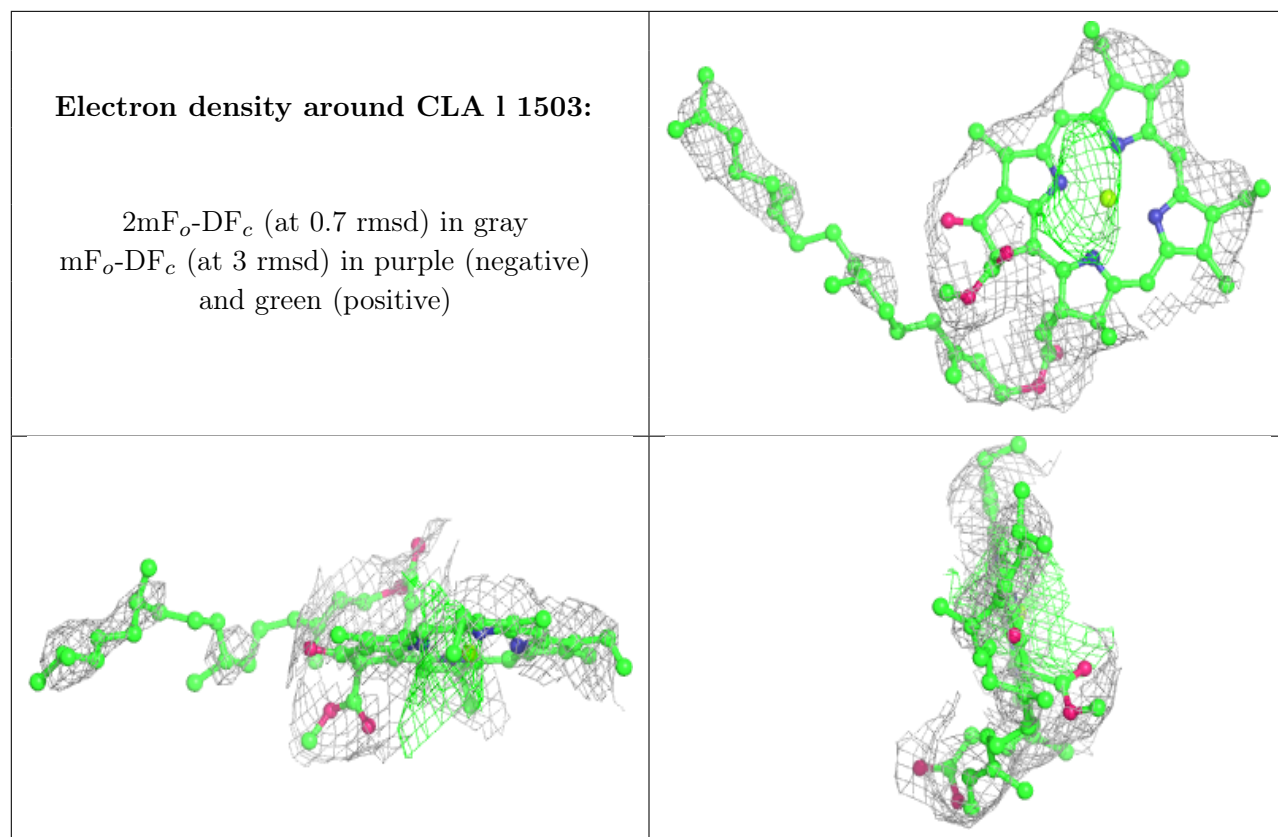
Electron density around CLA b 1239:

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



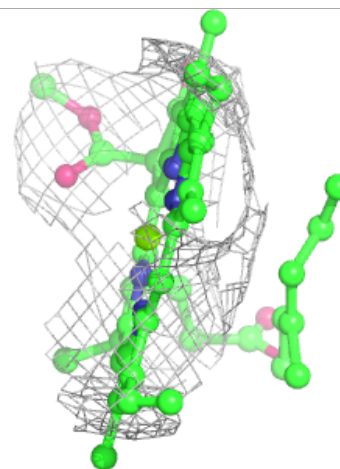
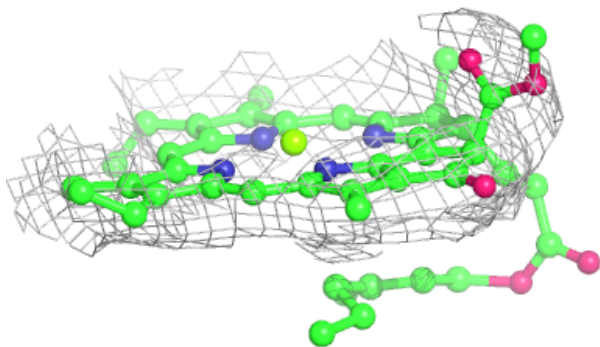
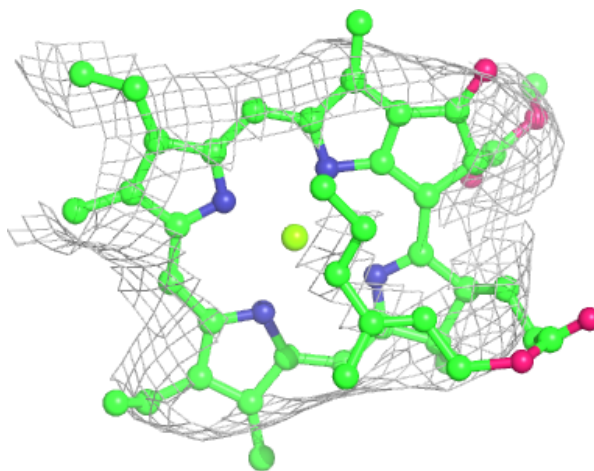






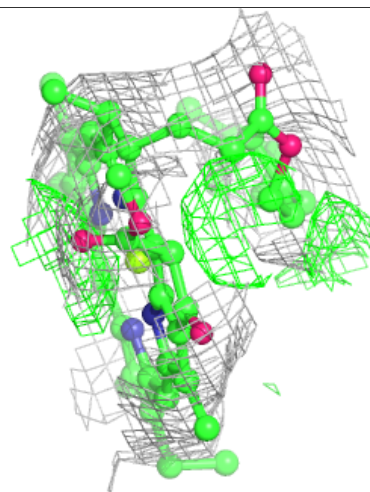
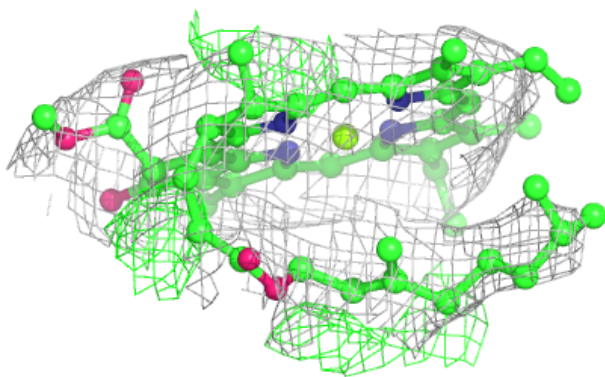
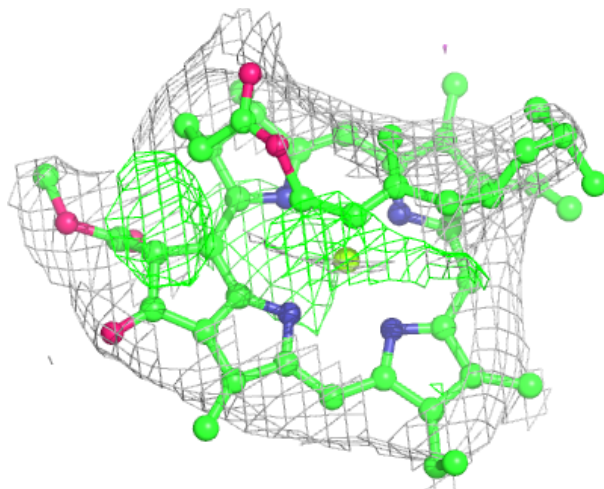
Electron density around CLA 1 1801:

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



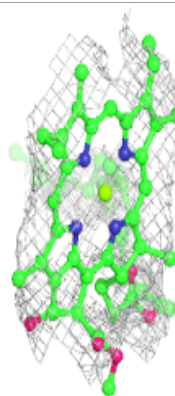
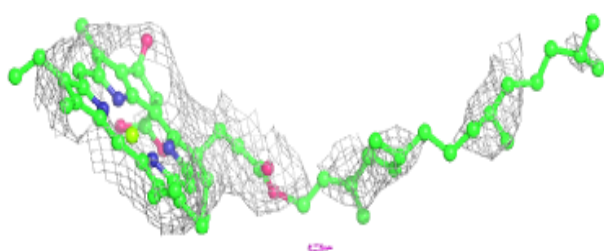
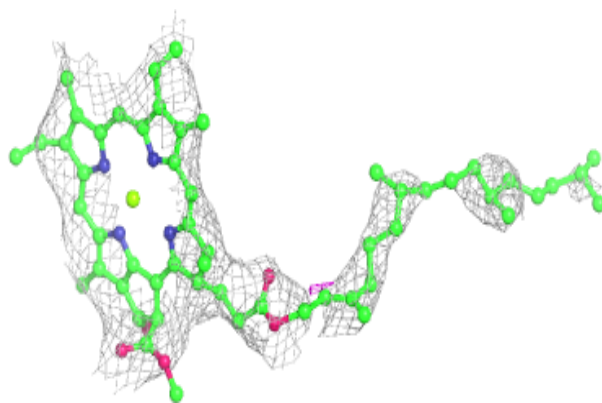
Electron density around CLA 1 1237:

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

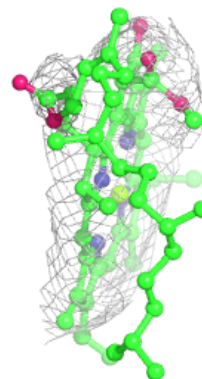
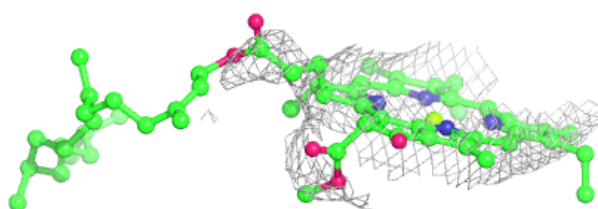
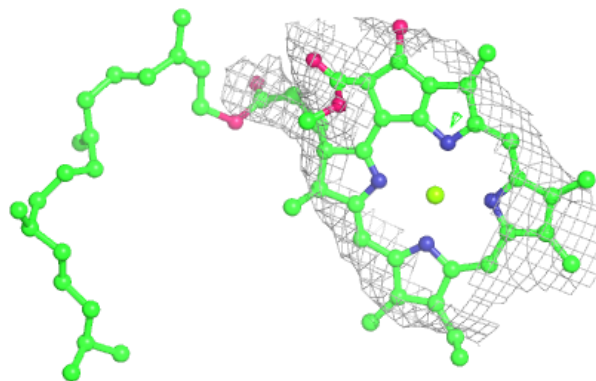


Electron density around CLA 1 1022:

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

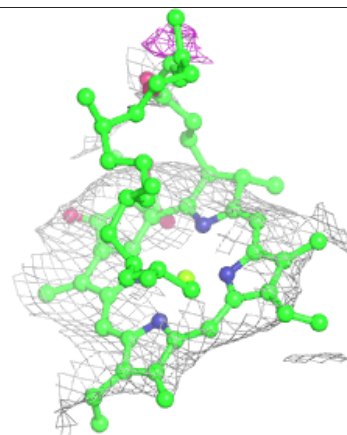
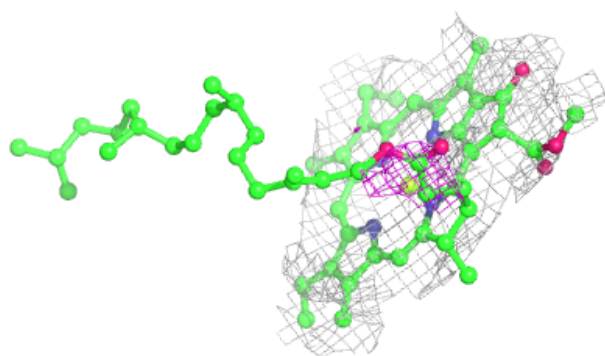
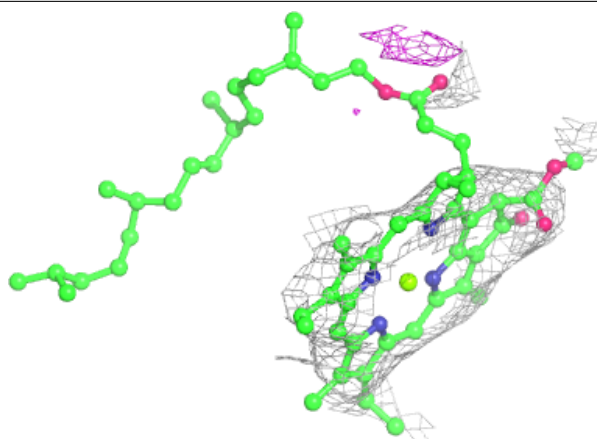
**Electron density around CLA 1 1101:**

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

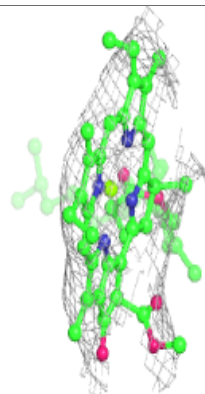
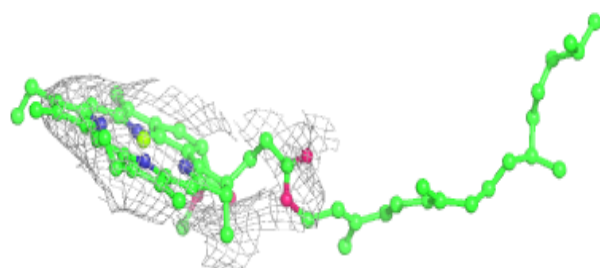
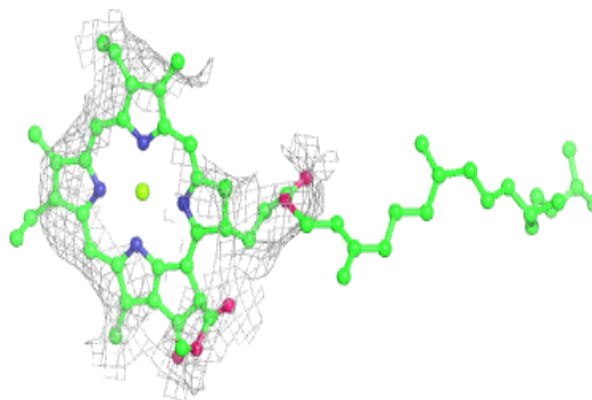


Electron density around CLA 1 1102:

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

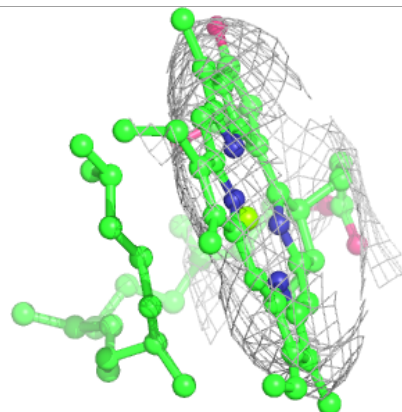
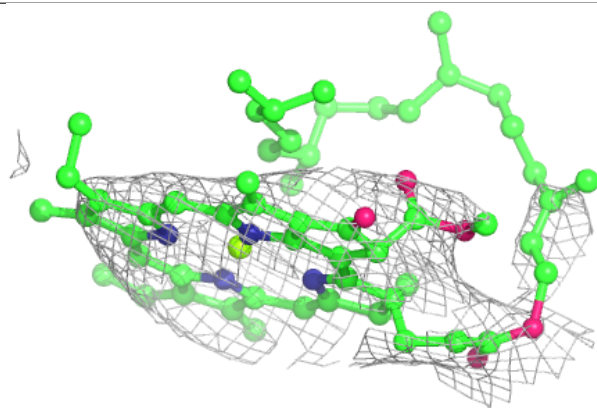
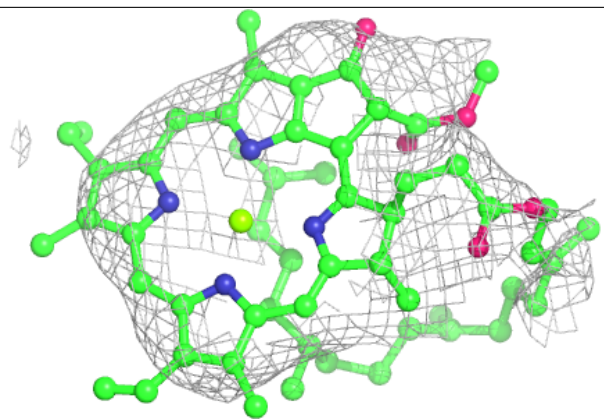
**Electron density around CLA 1 1103:**

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



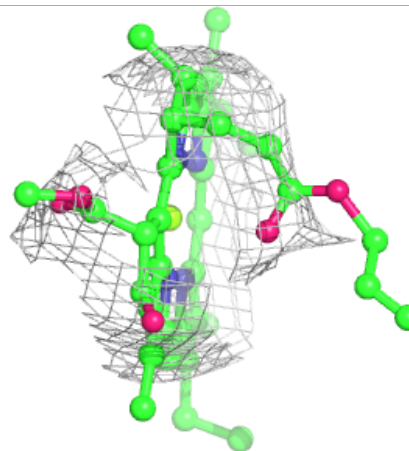
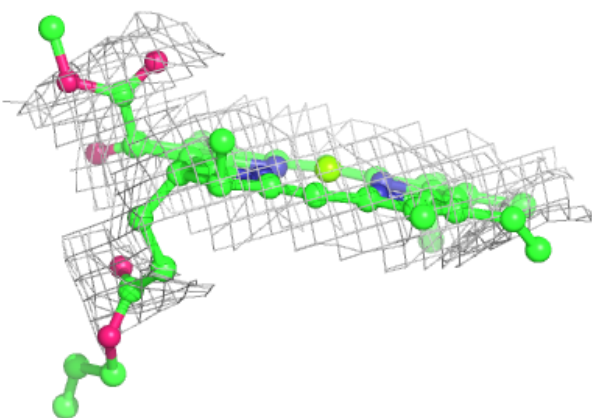
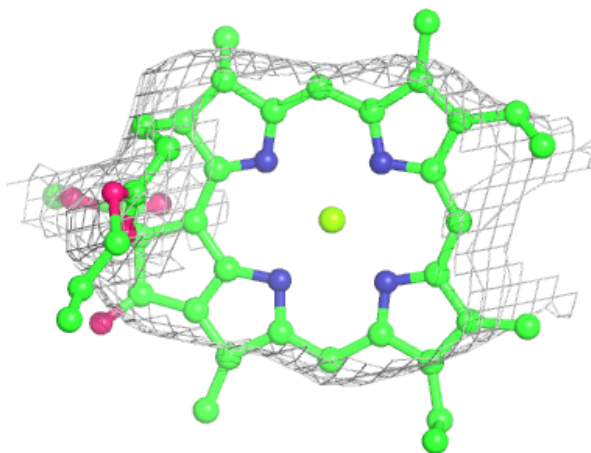
Electron density around CLA 1 1104:

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



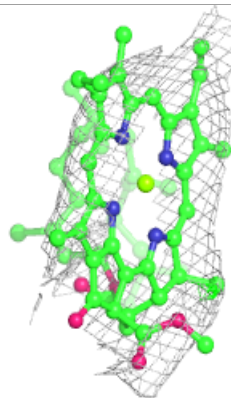
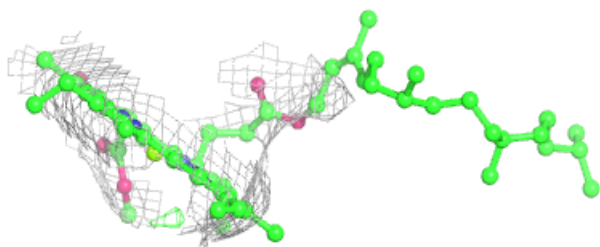
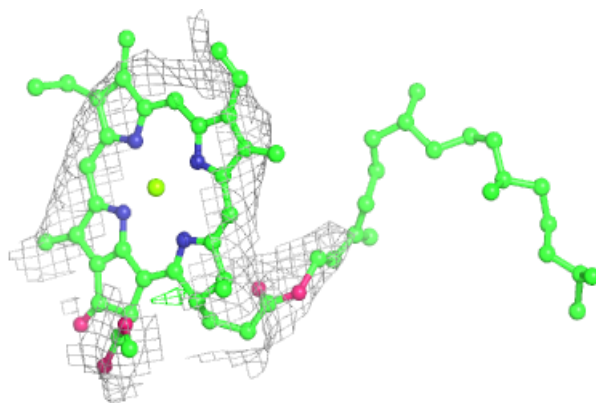
Electron density around CLA 1 1105:

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

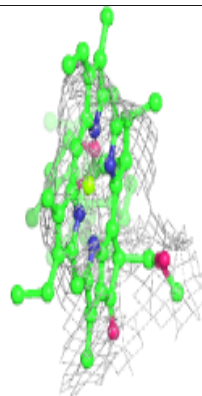
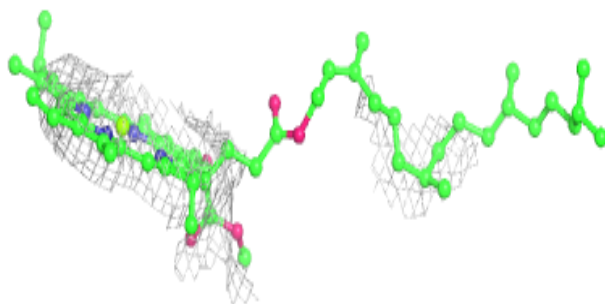
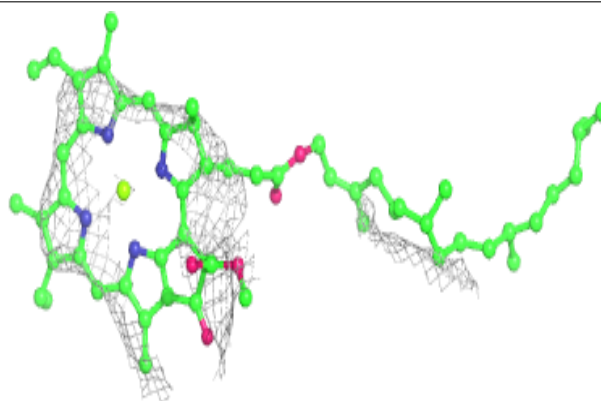


Electron density around CLA 1 1106:

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

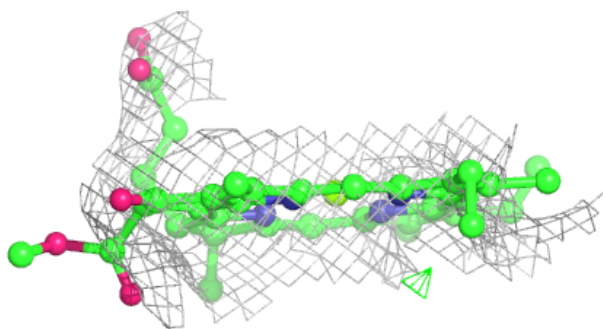
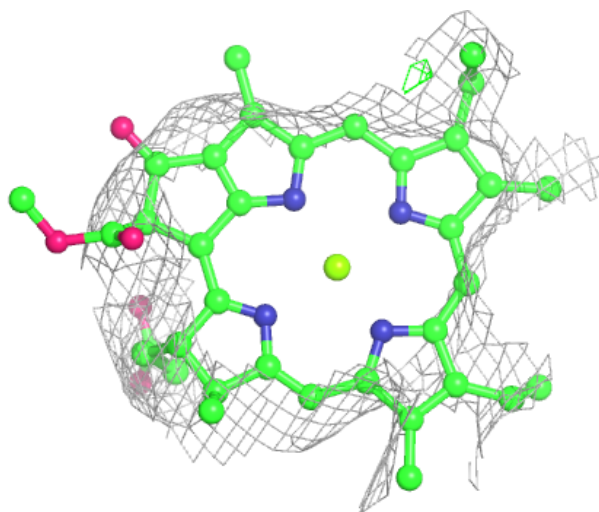
**Electron density around CLA 1 1107:**

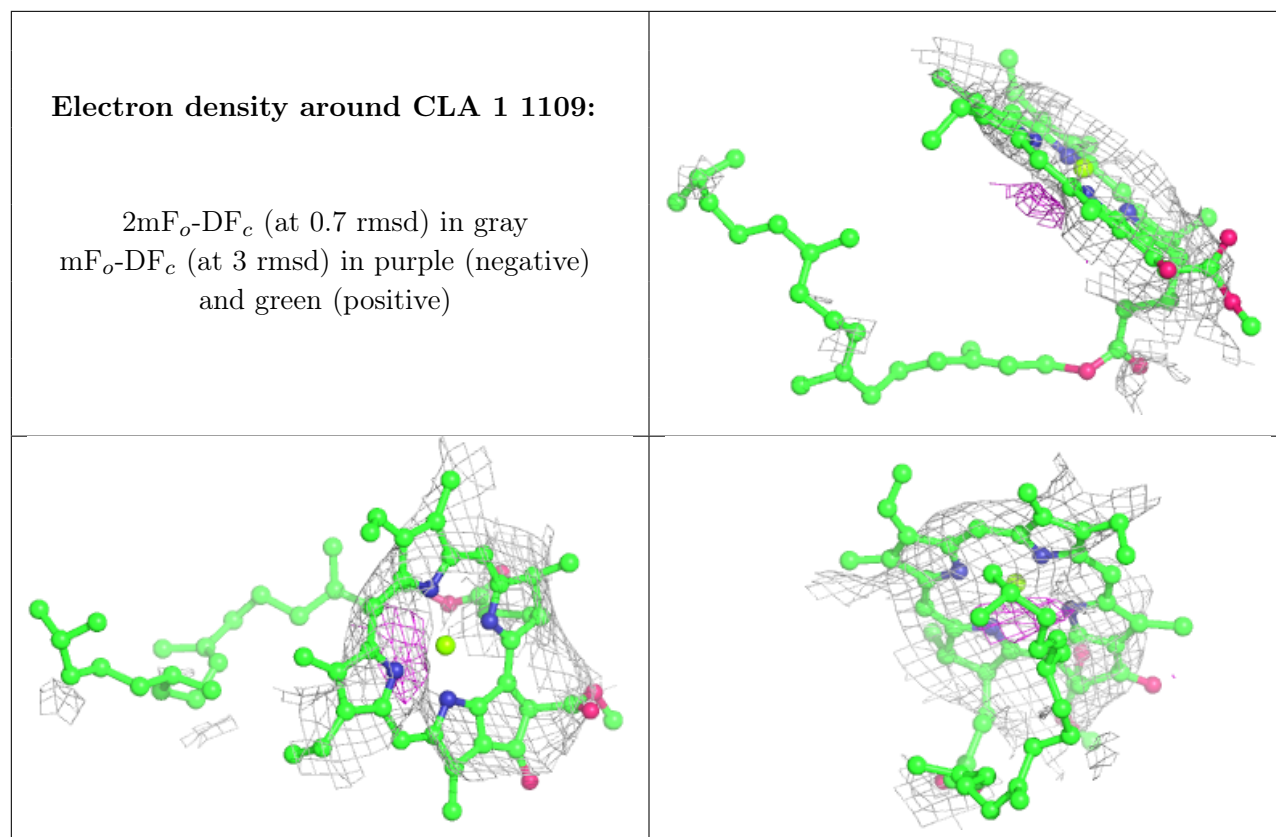
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around CLA 1 1108:

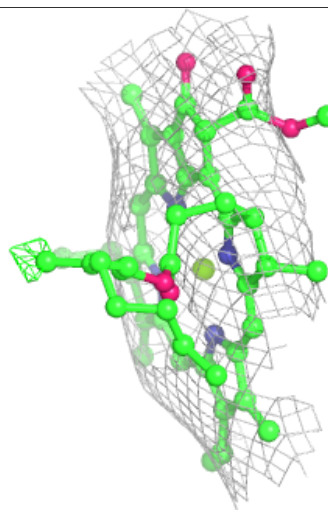
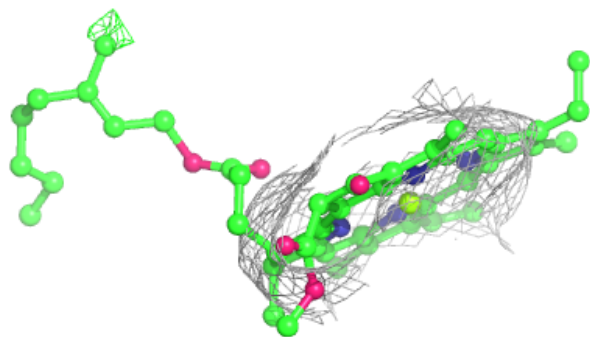
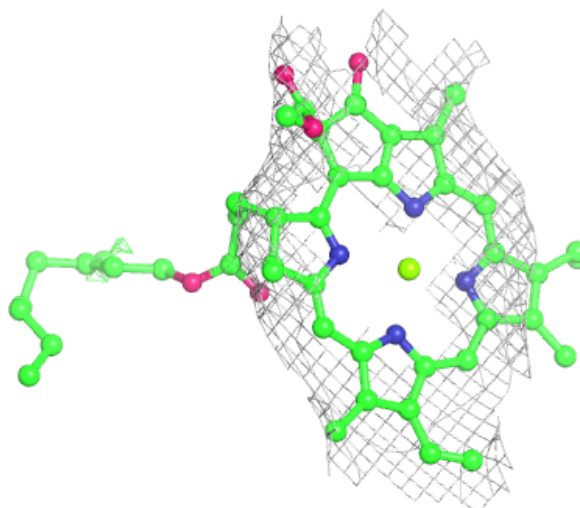
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





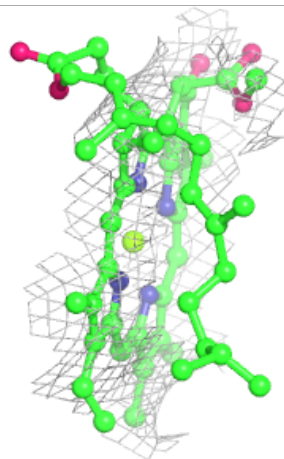
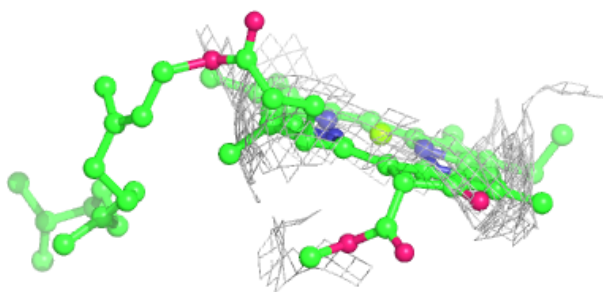
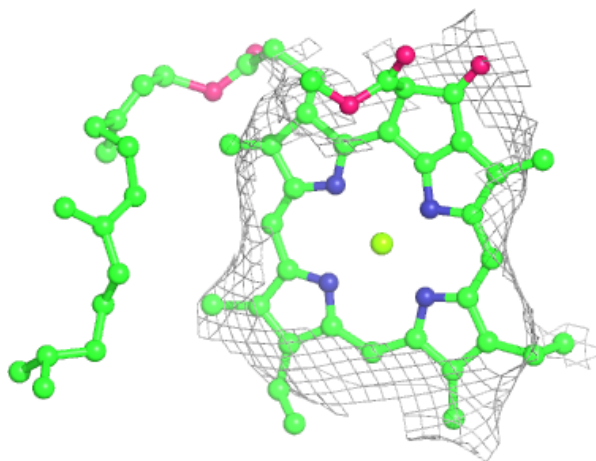
Electron density around CLA 1 1110:

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



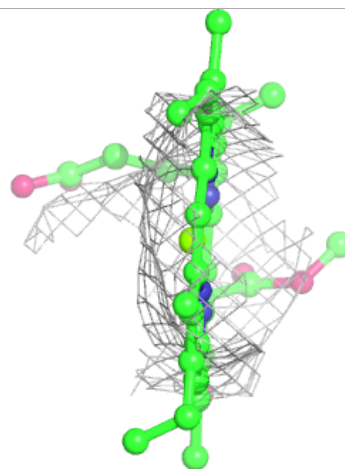
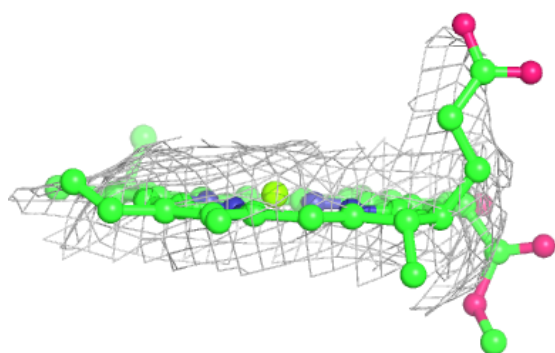
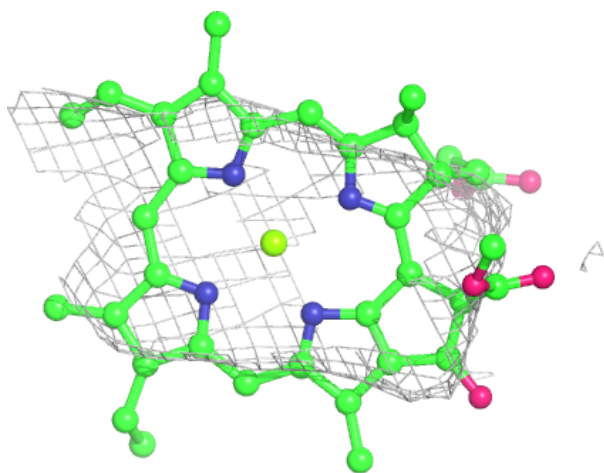
Electron density around CLA 1 1111:

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



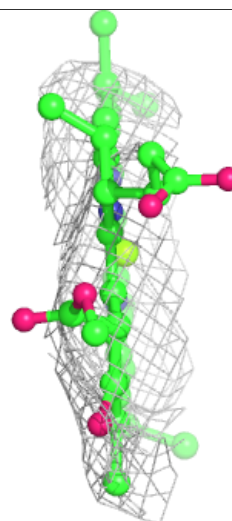
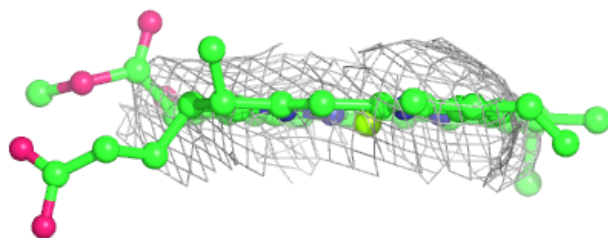
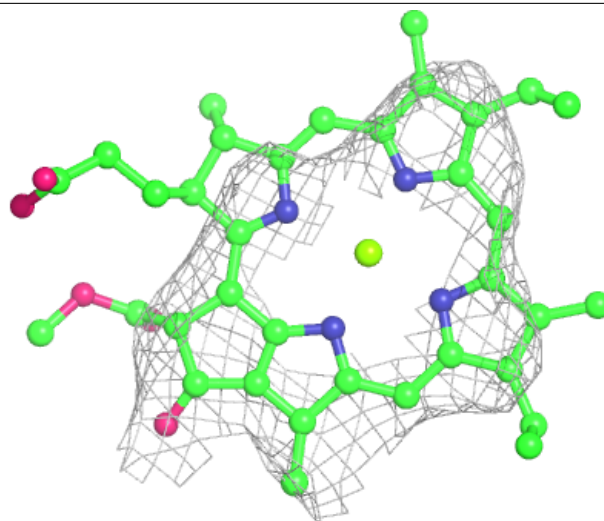
Electron density around CLA 1 1112:

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



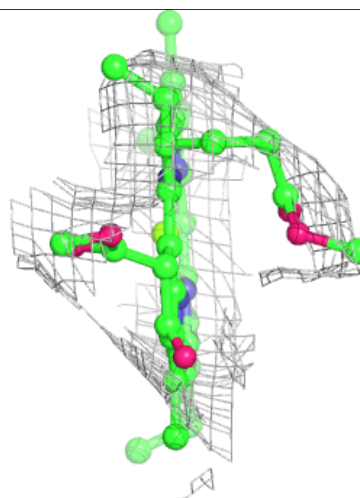
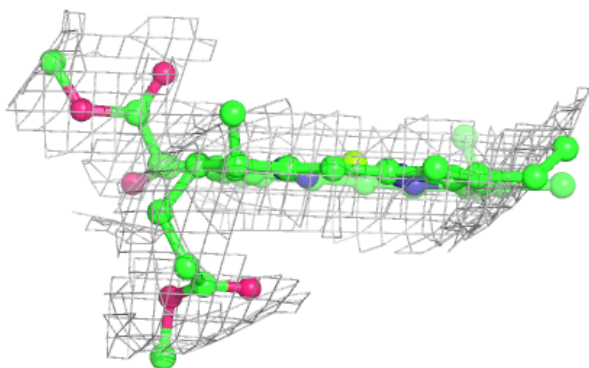
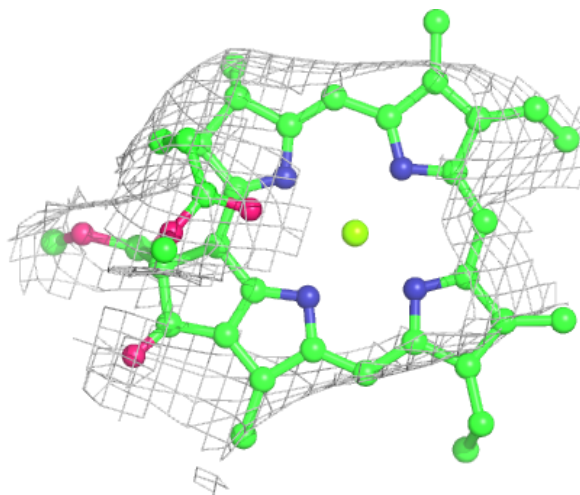
Electron density around CLA 1 1113:

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



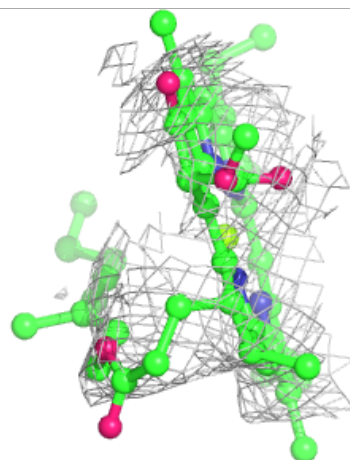
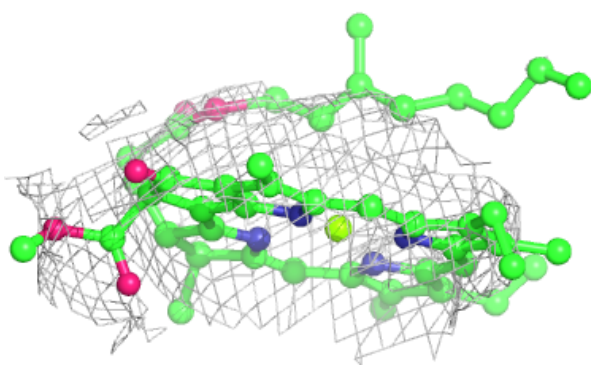
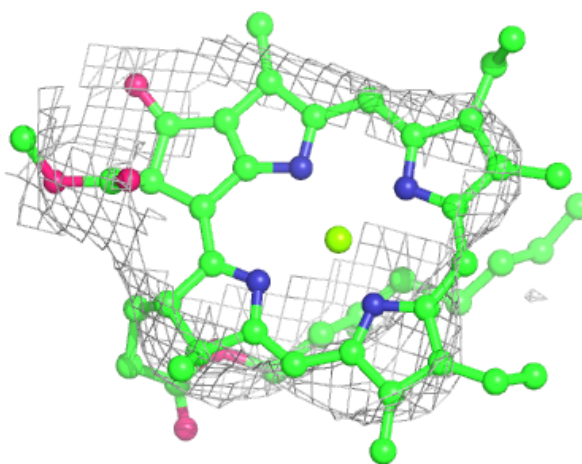
Electron density around CLA 1 1115:

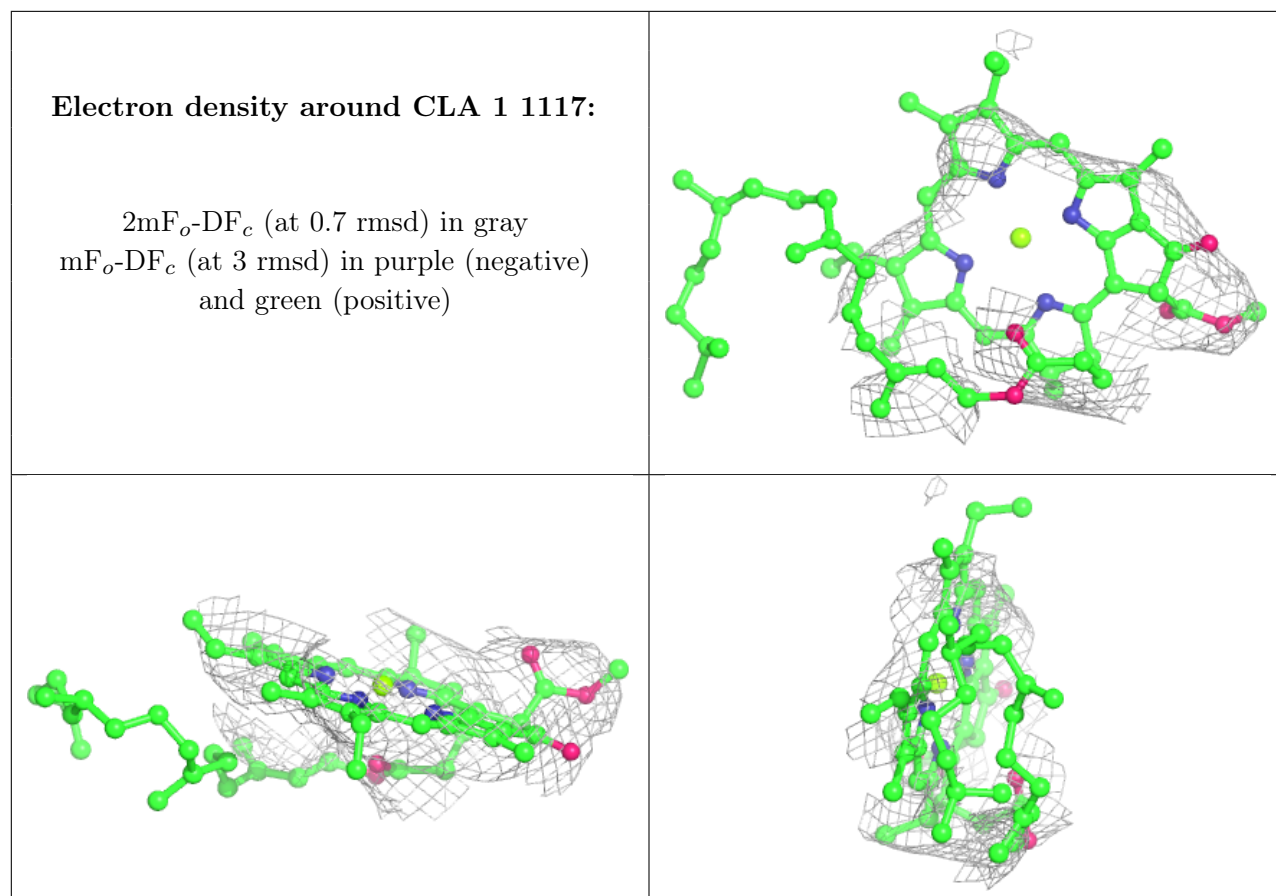
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around CLA 1 1116:

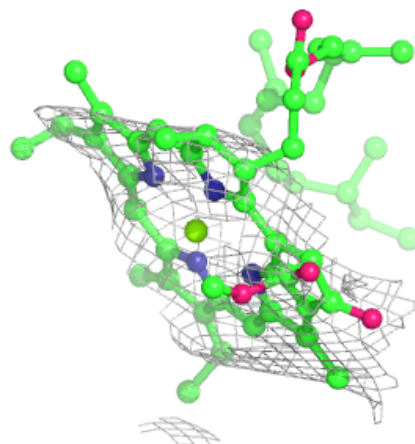
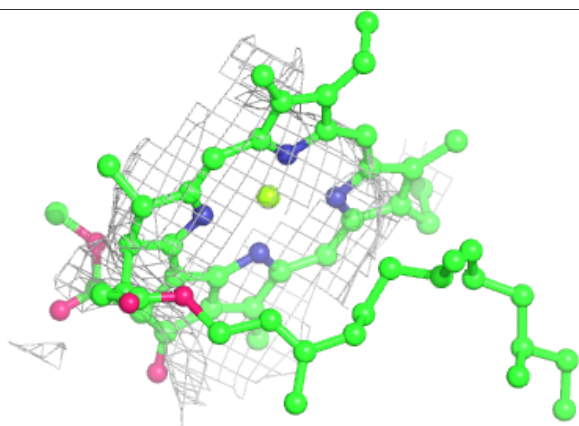
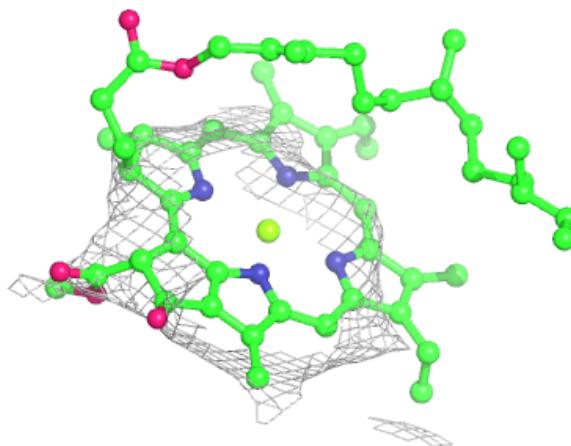
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

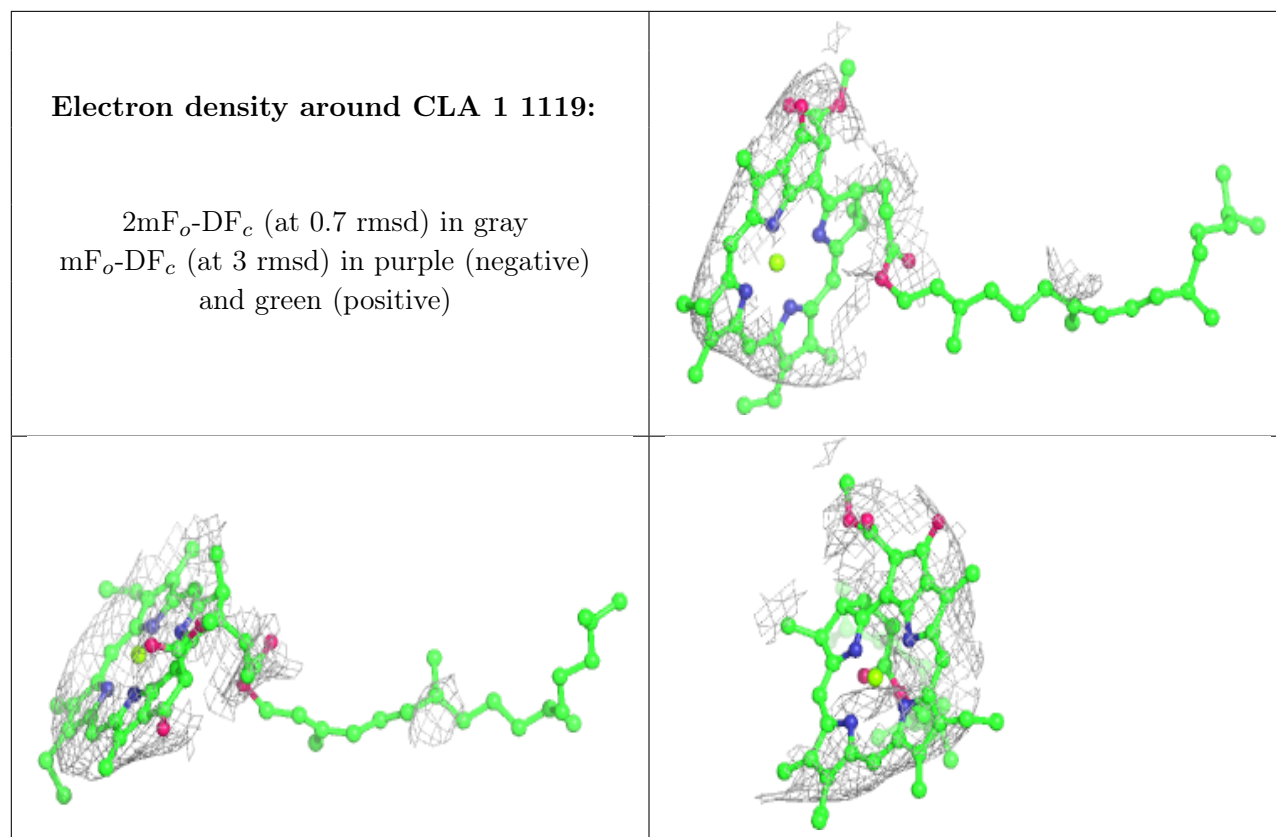




Electron density around CLA 1 1118:

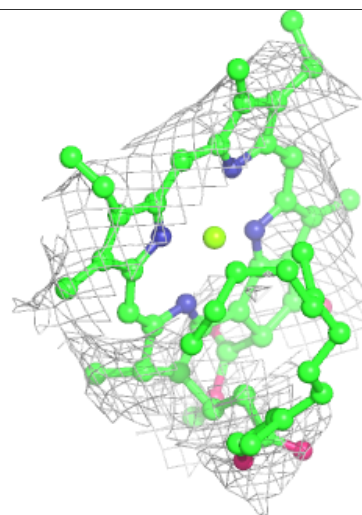
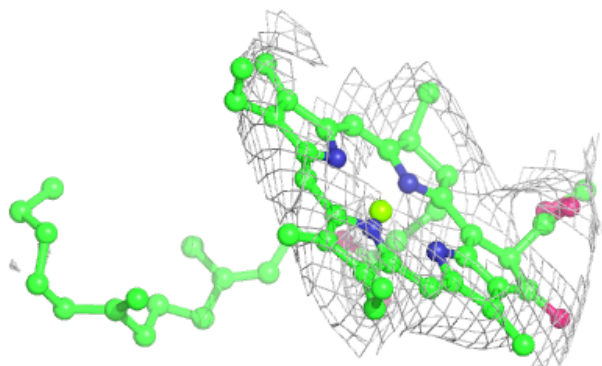
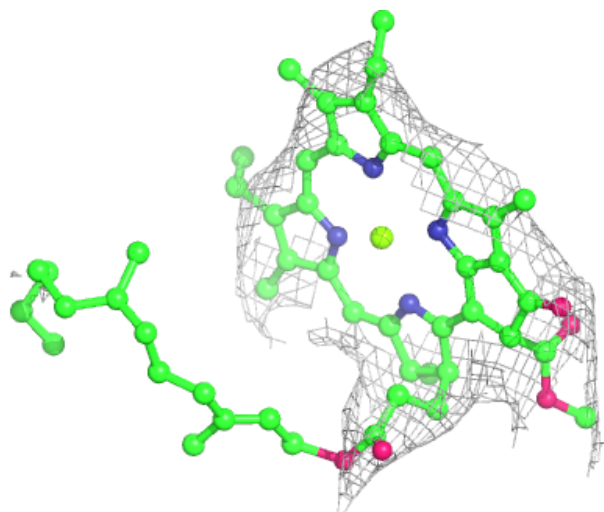
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





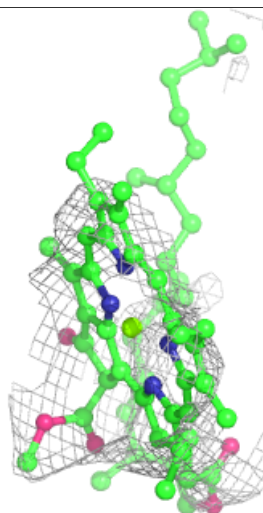
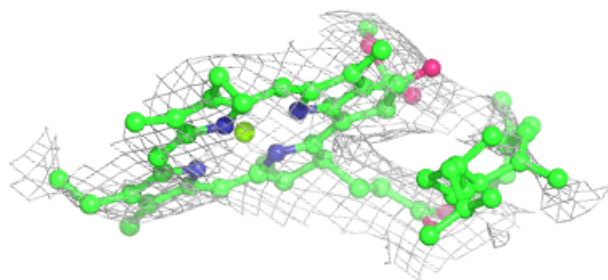
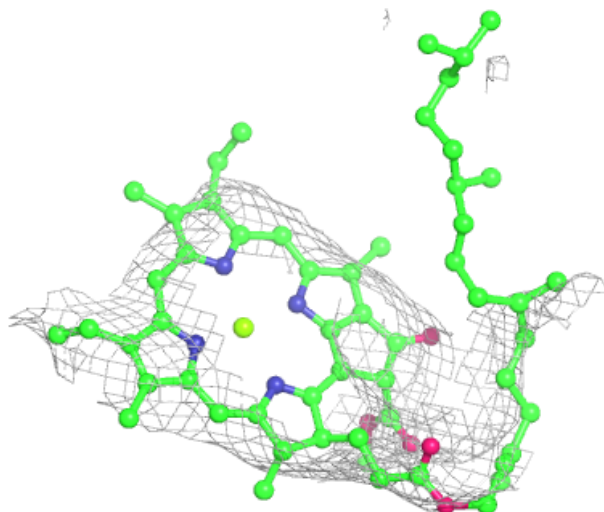
Electron density around CLA 1 1122:

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



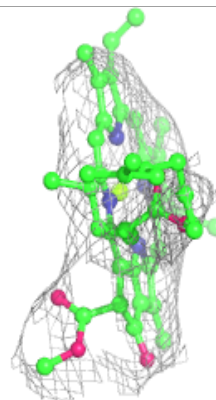
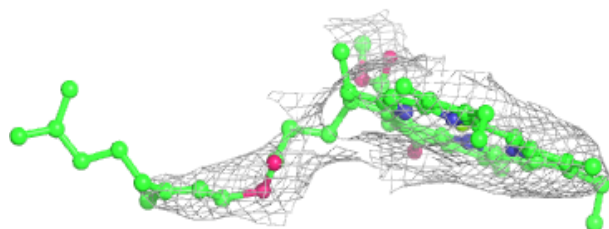
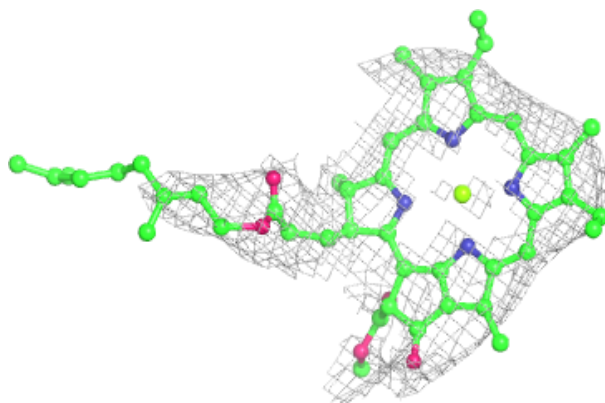
Electron density around CLA 1 1123:

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

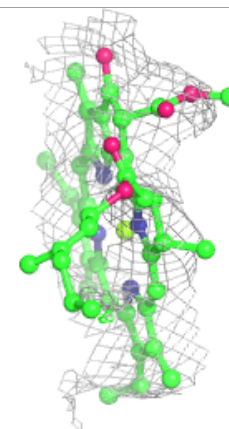
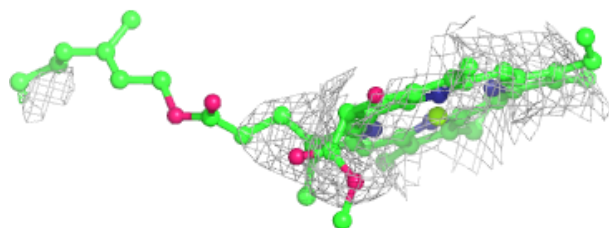
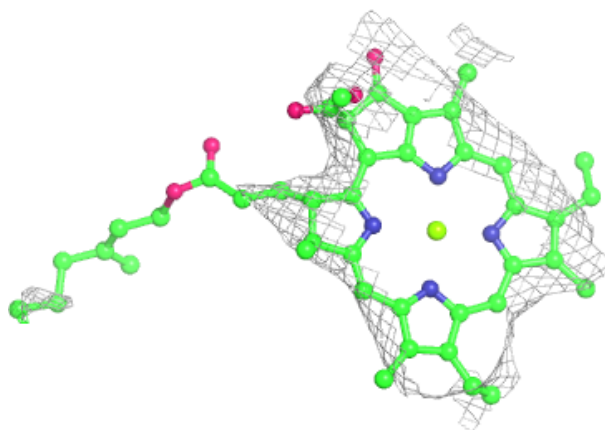


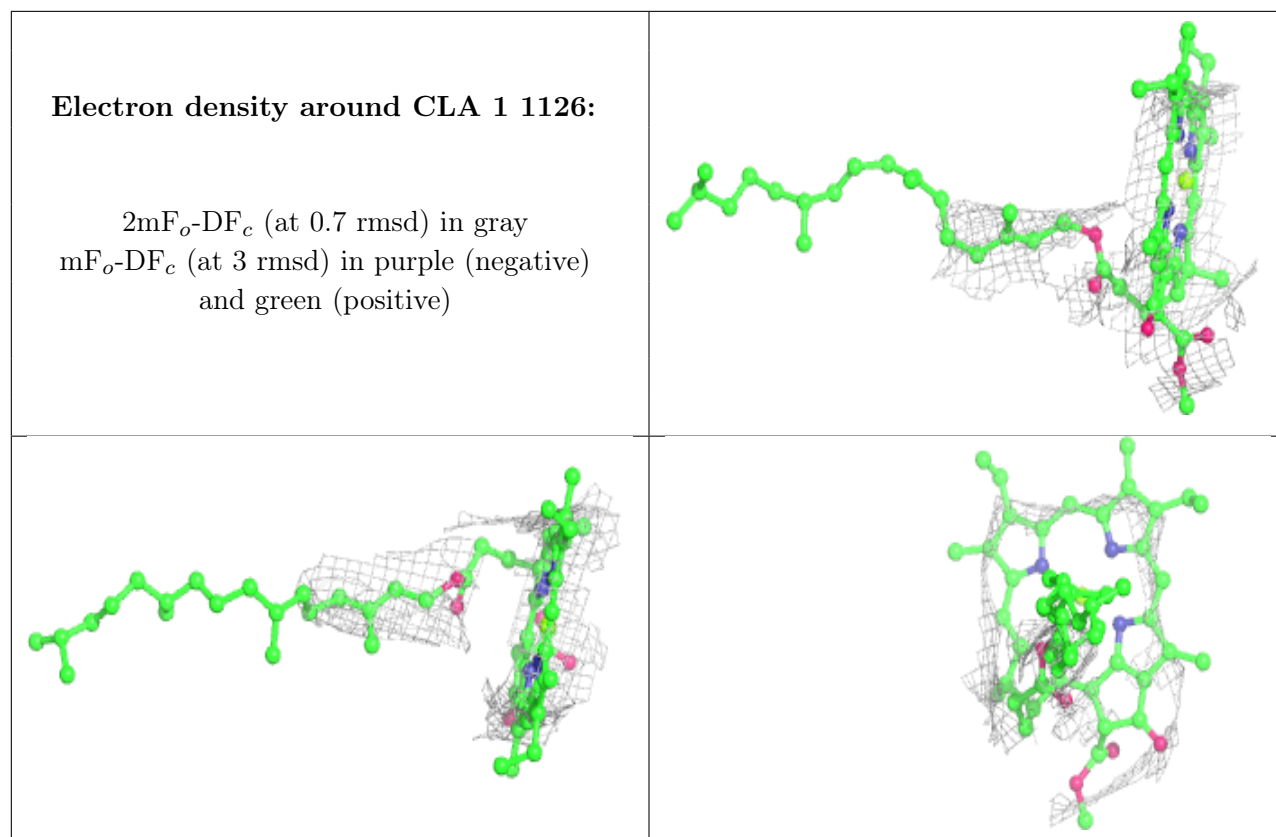
Electron density around CLA 1 1124:

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

**Electron density around CLA 1 1125:**

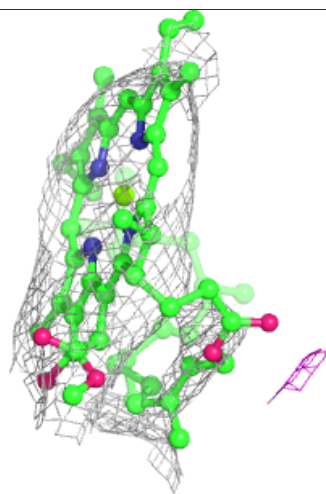
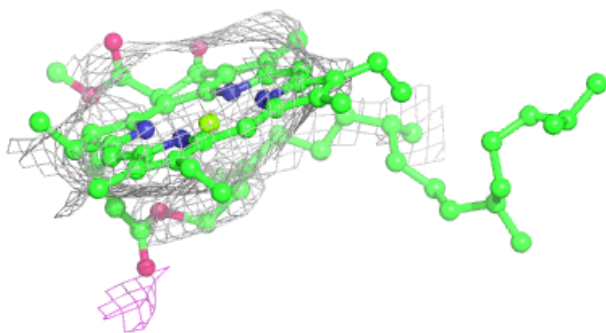
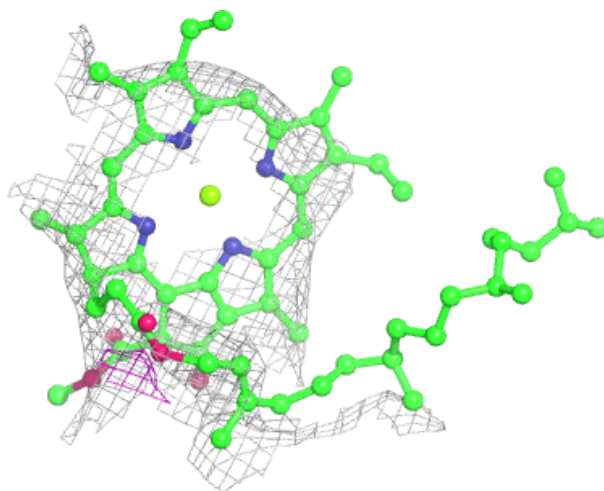
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

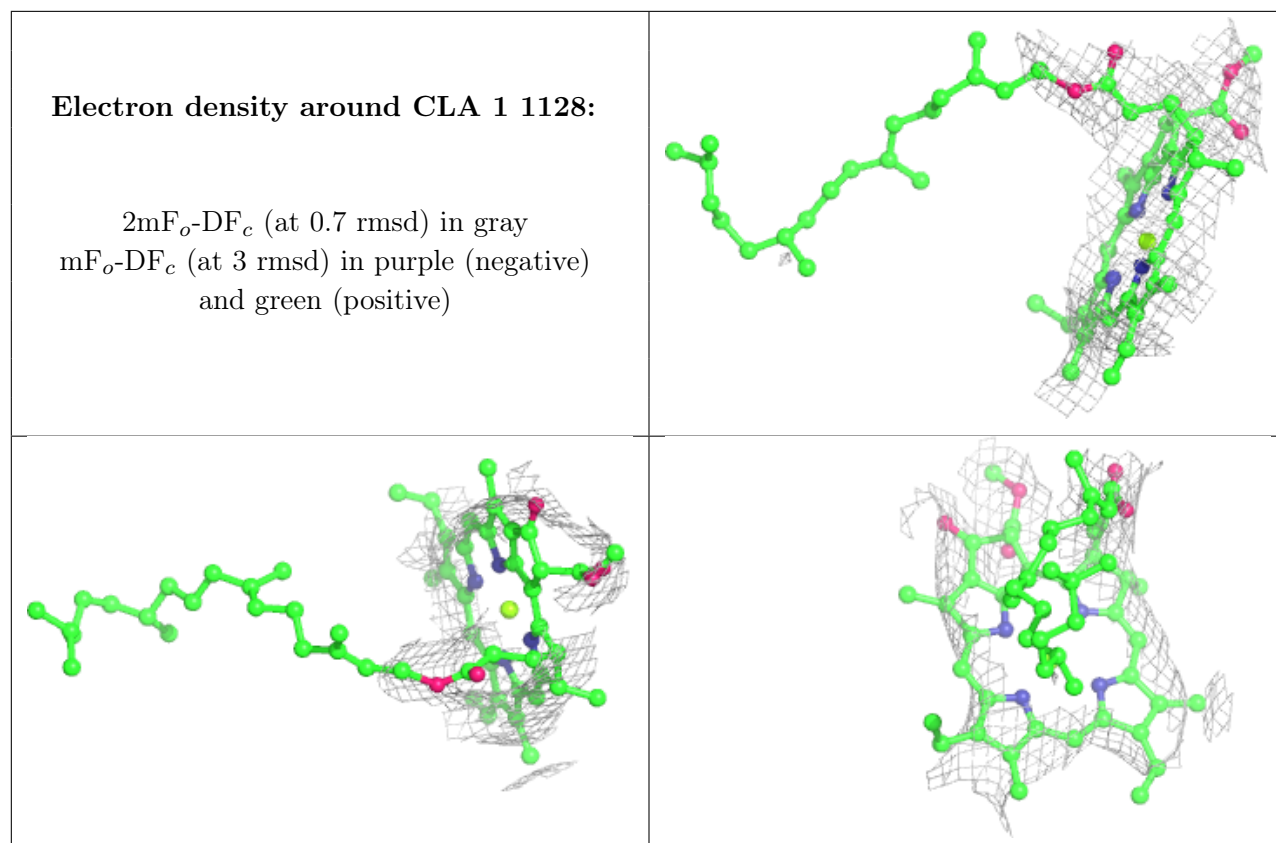




Electron density around CLA 1 1127:

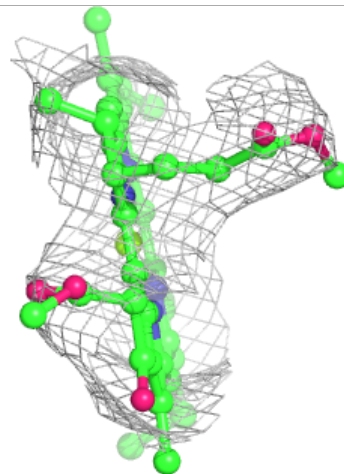
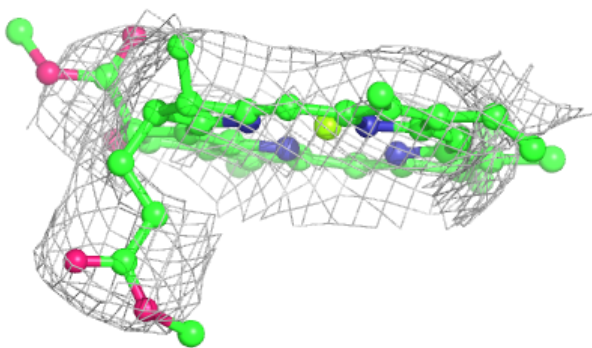
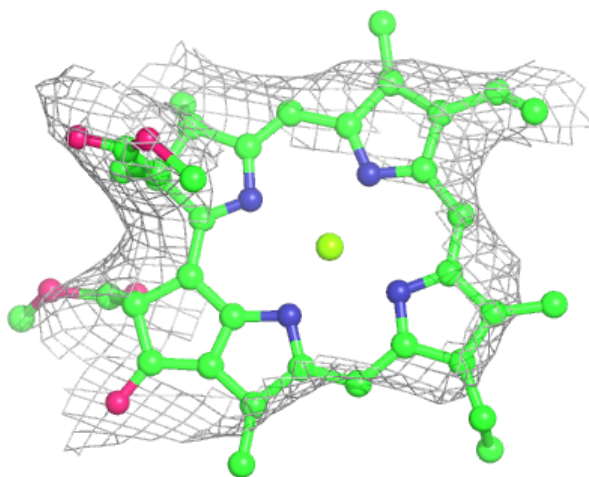
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





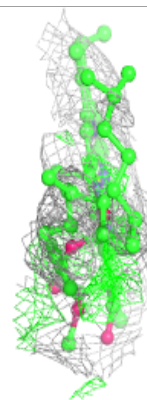
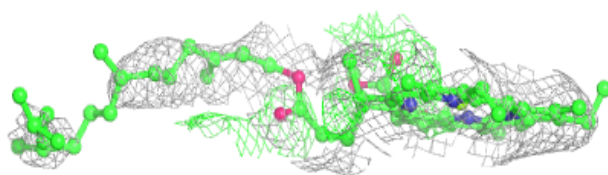
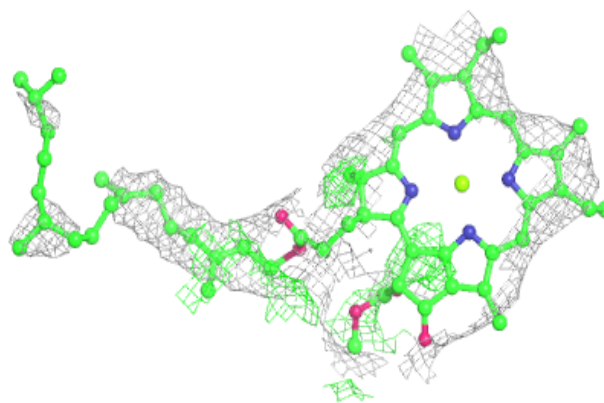
Electron density around CLA 1 1130:

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

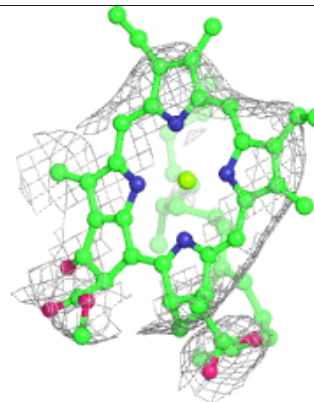
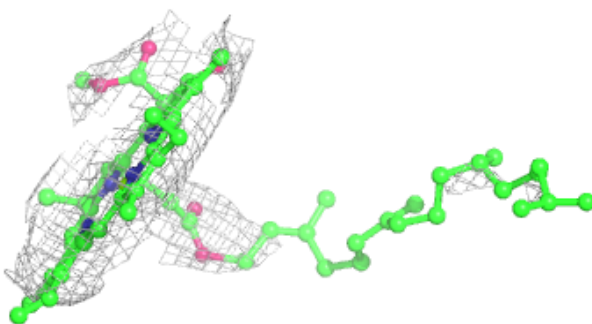
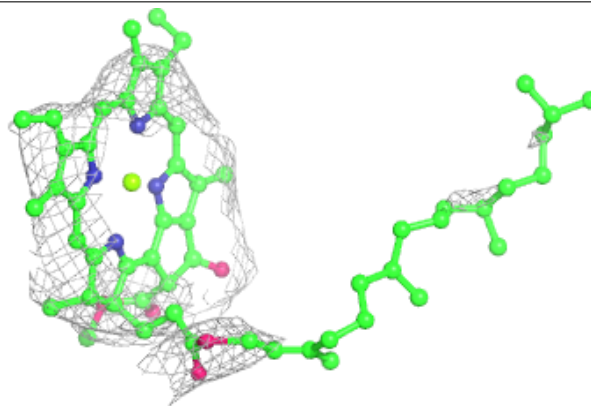


Electron density around CLA 1 1131:

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

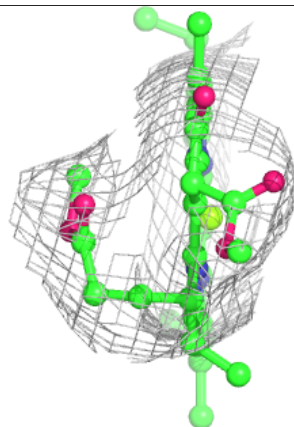
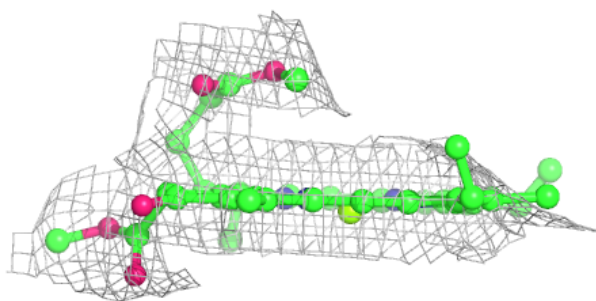
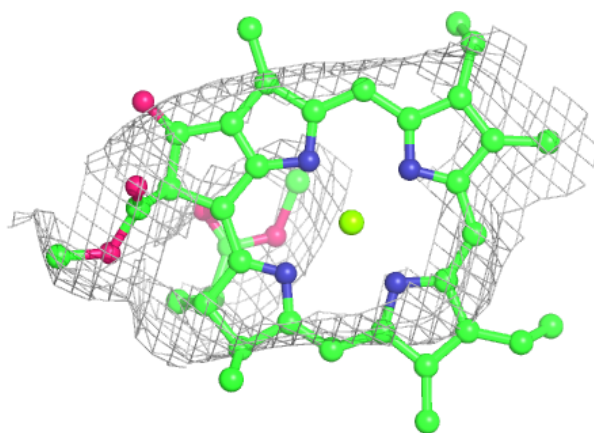
**Electron density around CLA 1 1137:**

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

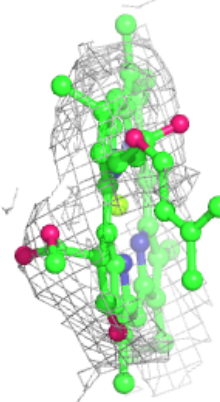
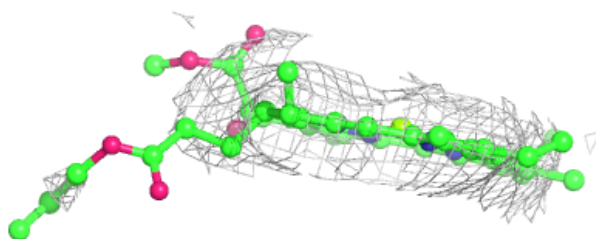
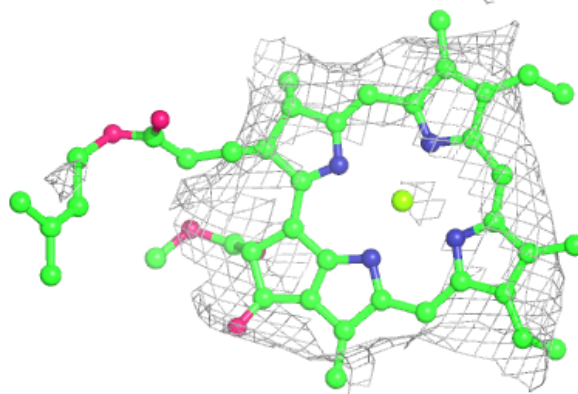


Electron density around CLA 1 1138:

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

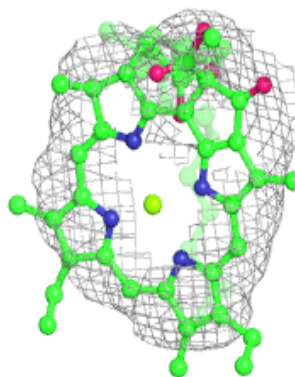
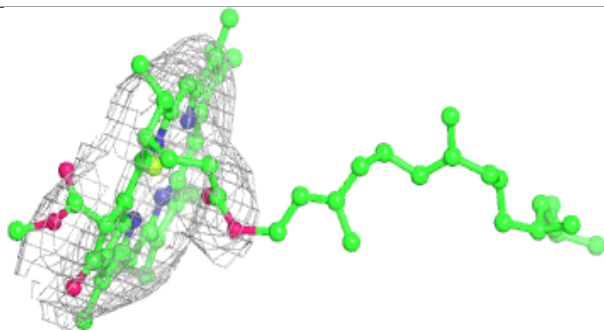
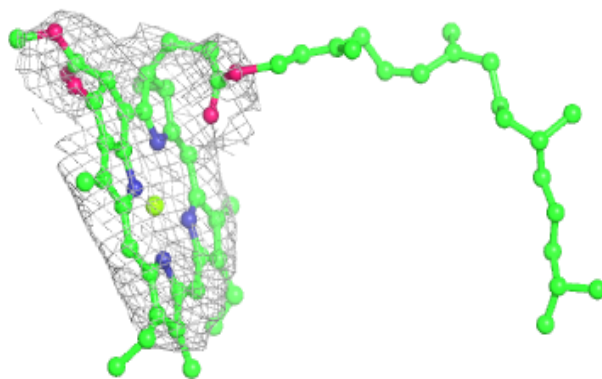
**Electron density around CLA 1 1139:**

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

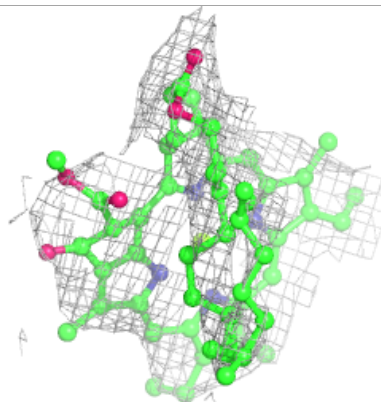
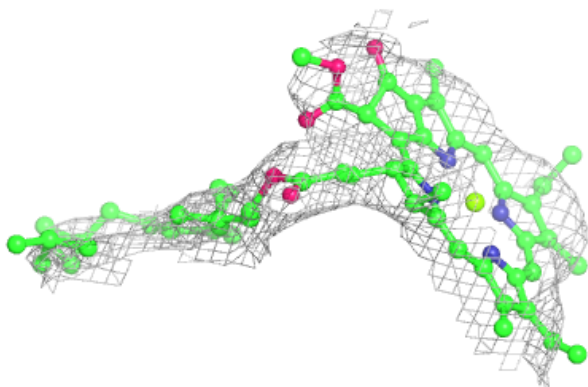
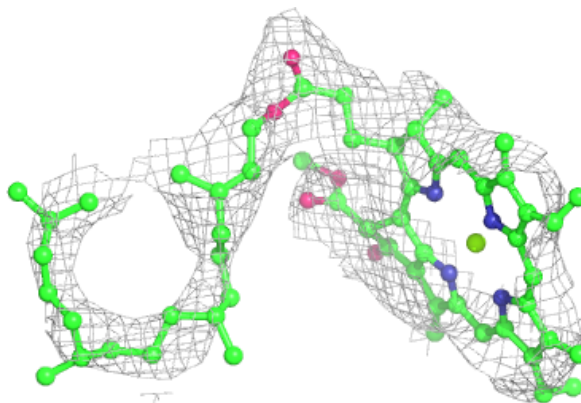


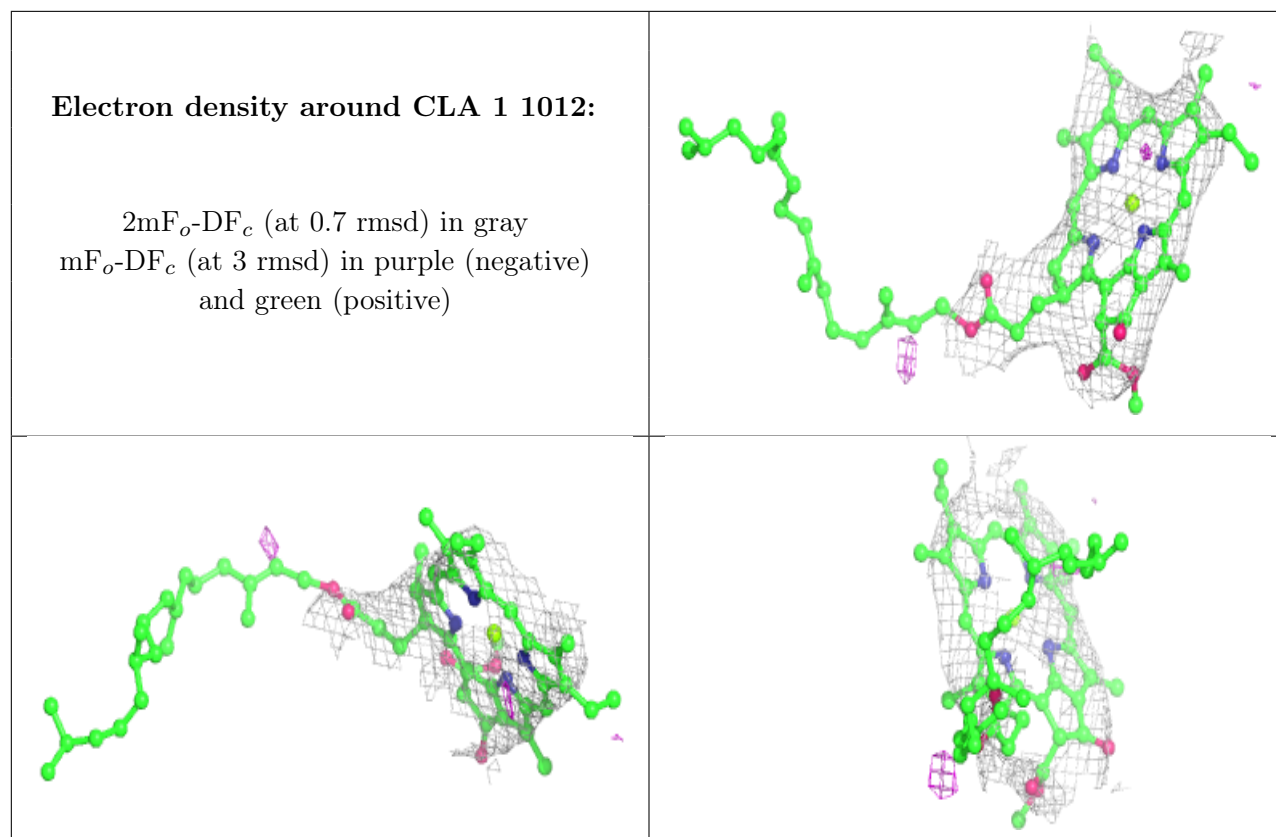
Electron density around CLA 1 1140:

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

**Electron density around CLA 1 1011:**

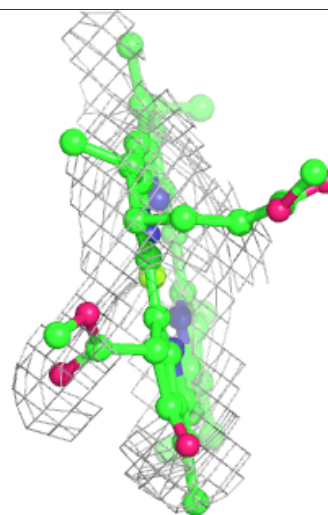
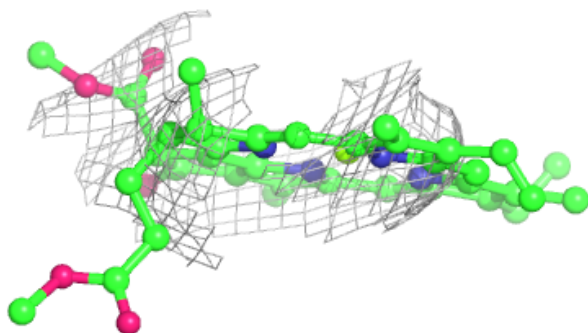
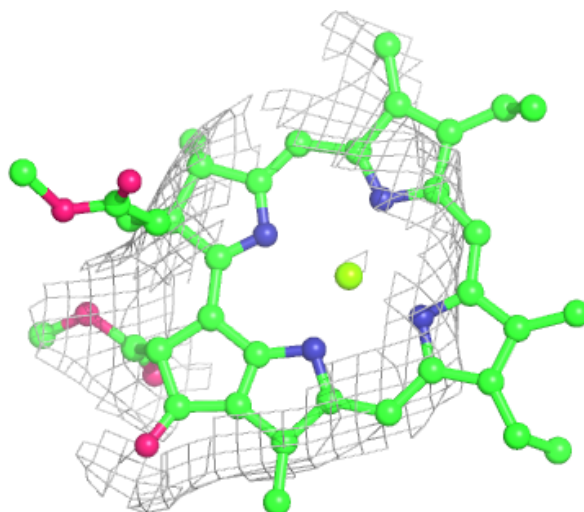
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





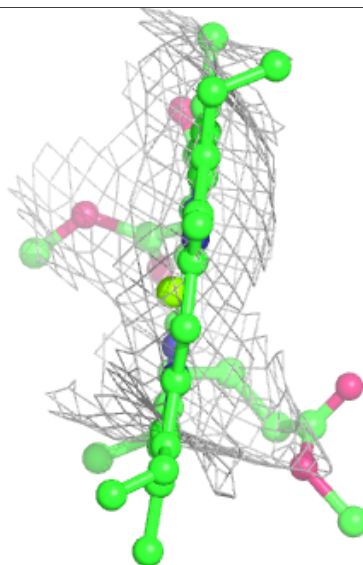
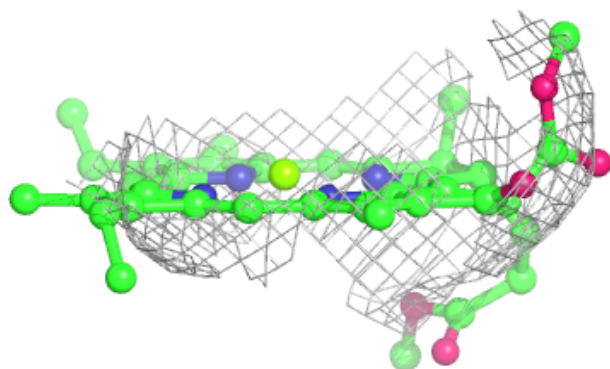
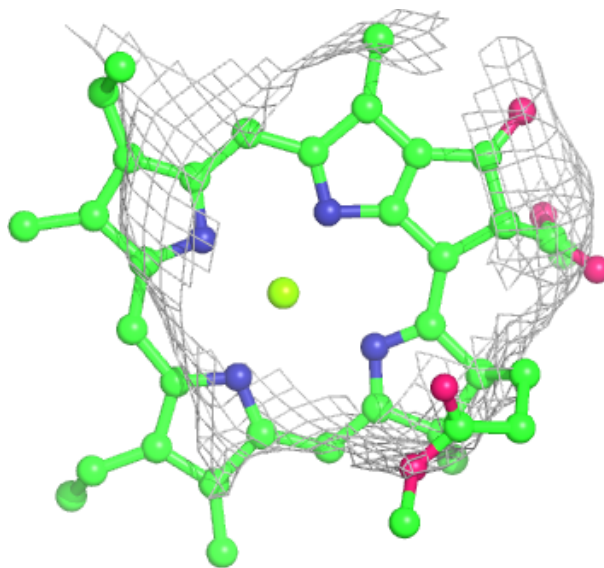
Electron density around CLA 1 1114:

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



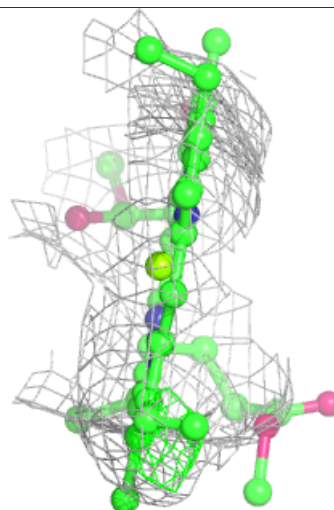
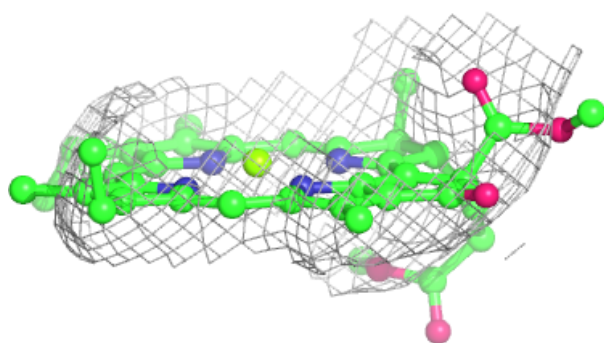
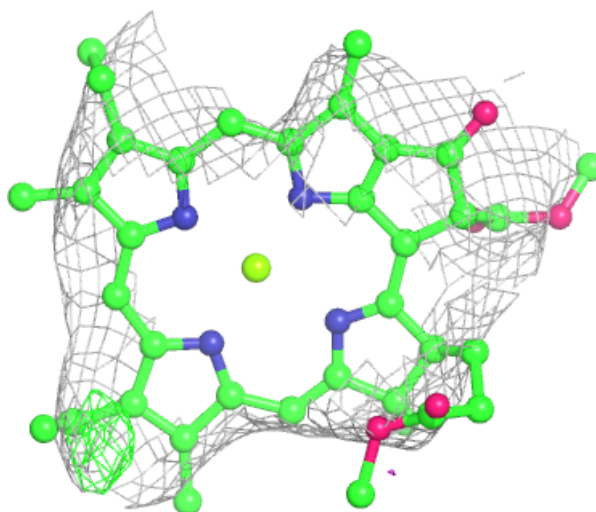
Electron density around CLA 1 1120:

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



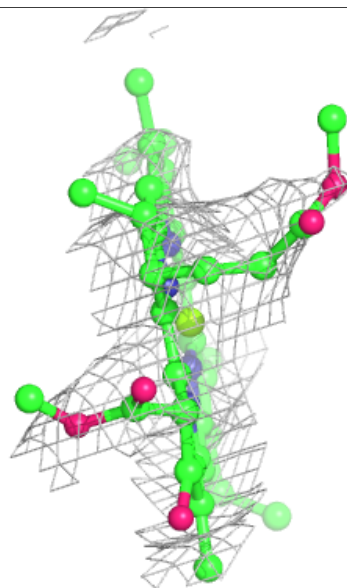
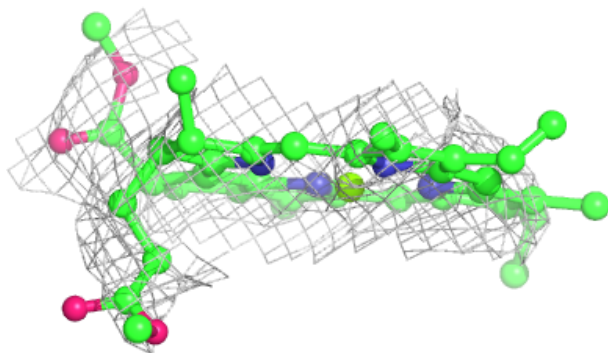
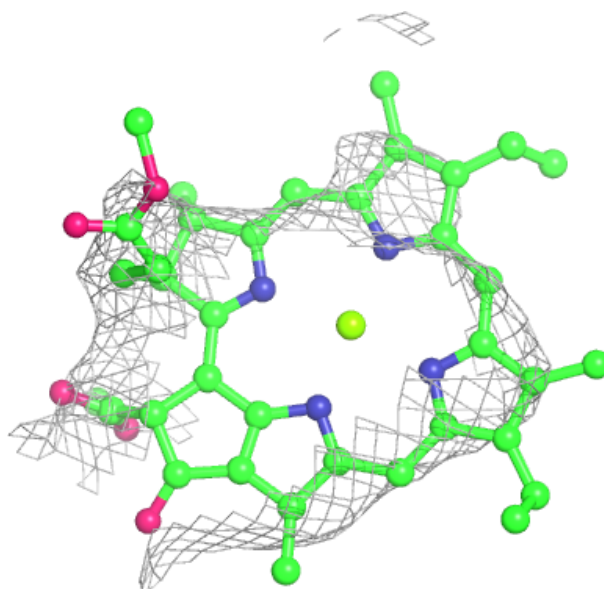
Electron density around CLA 1 1121:

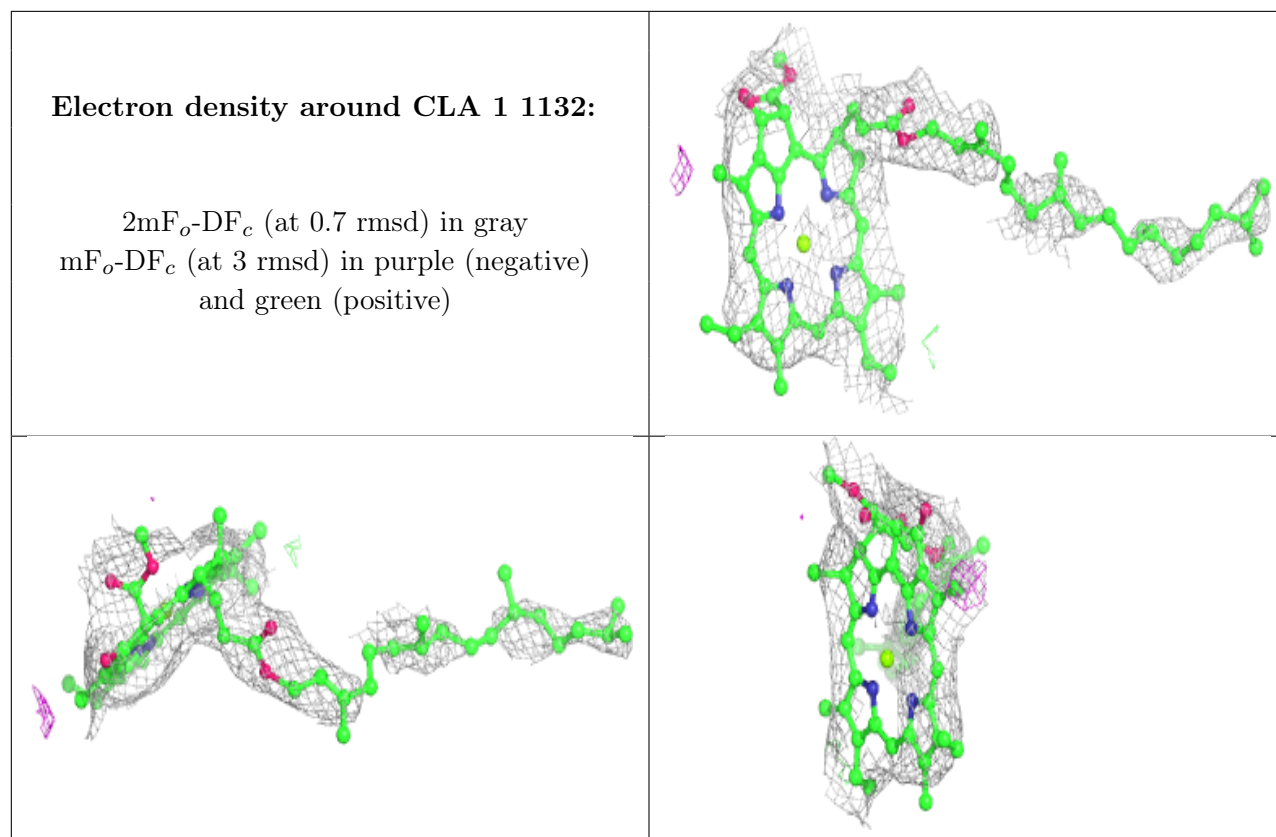
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around CLA 1 1129:

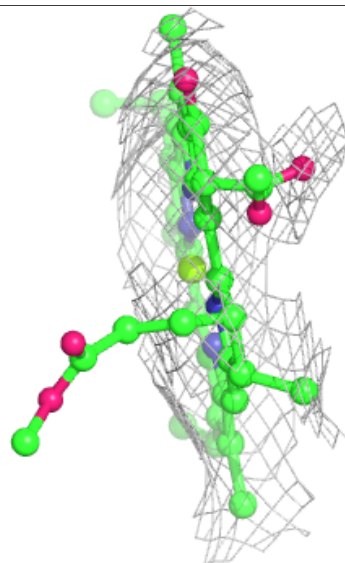
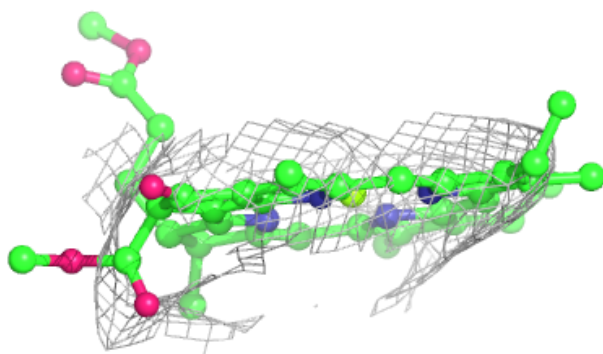
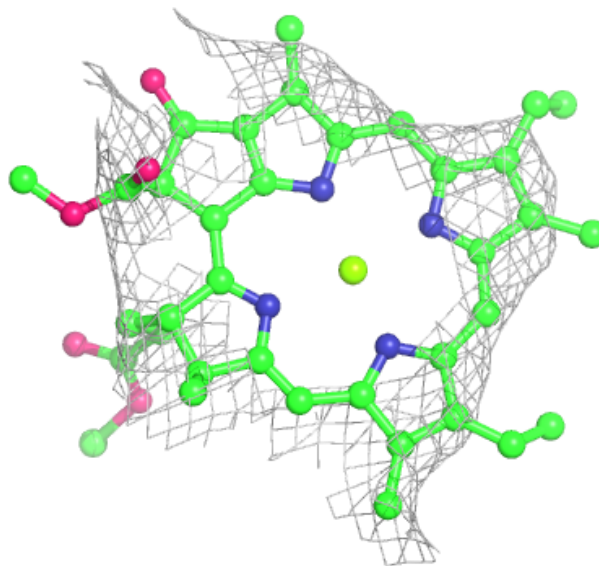
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





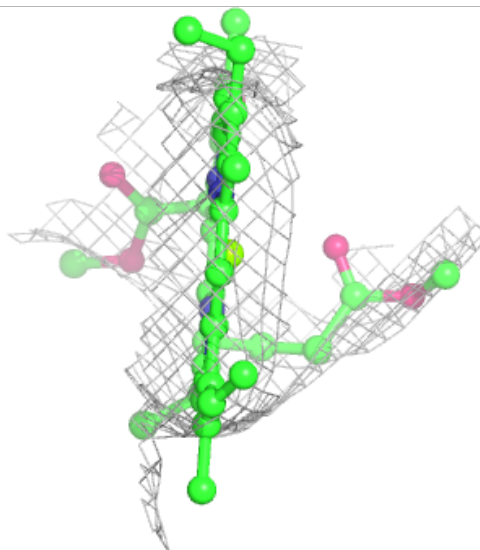
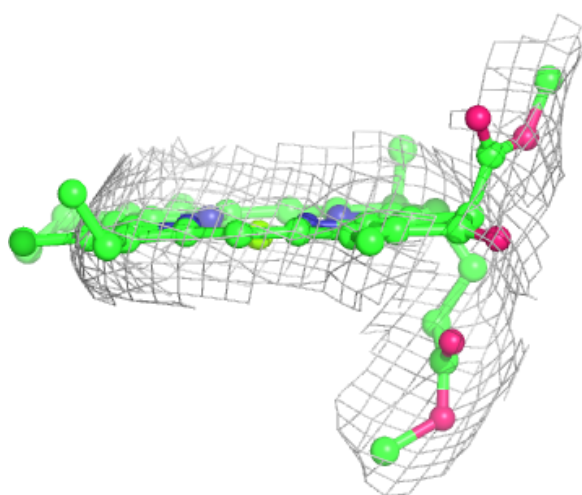
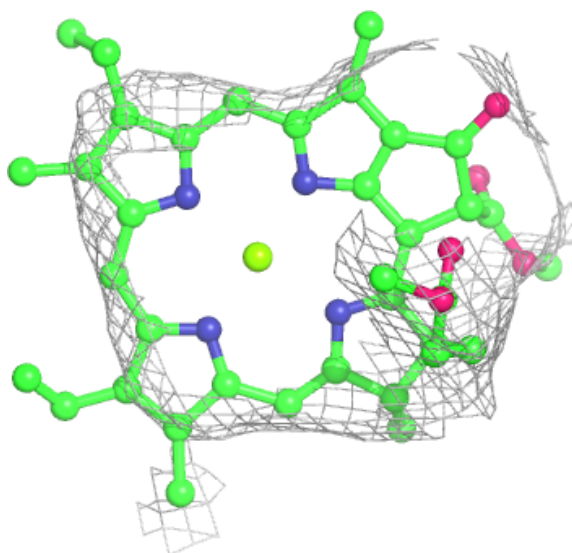
Electron density around CLA 1 1133:

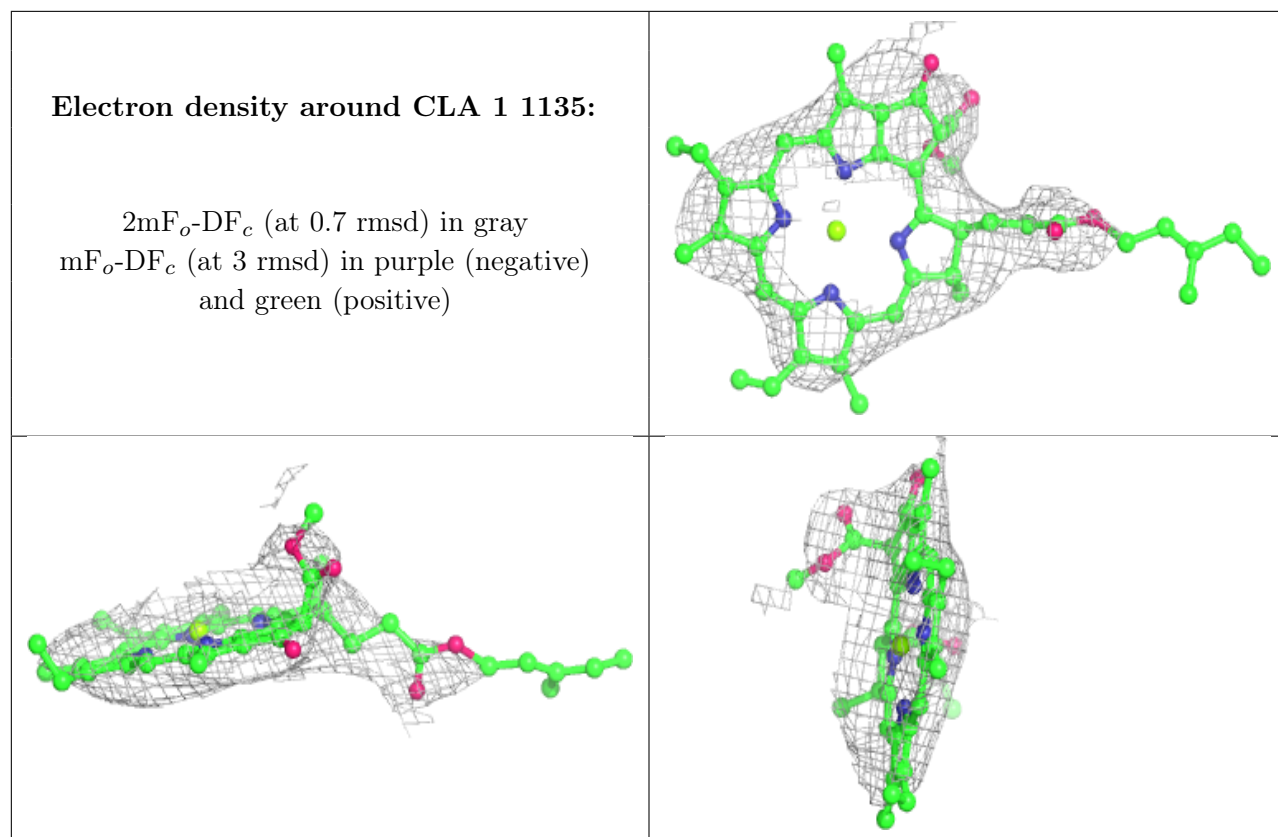
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around CLA 1 1134:

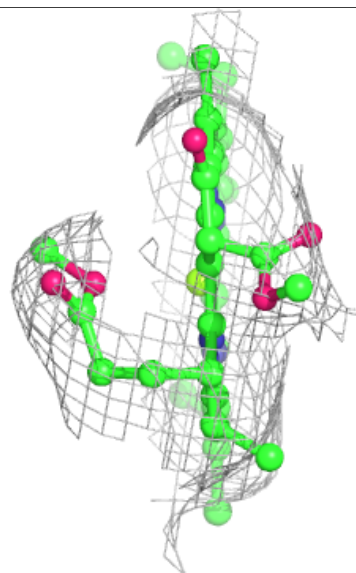
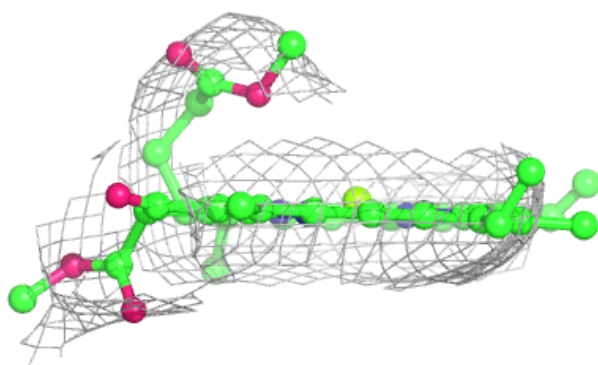
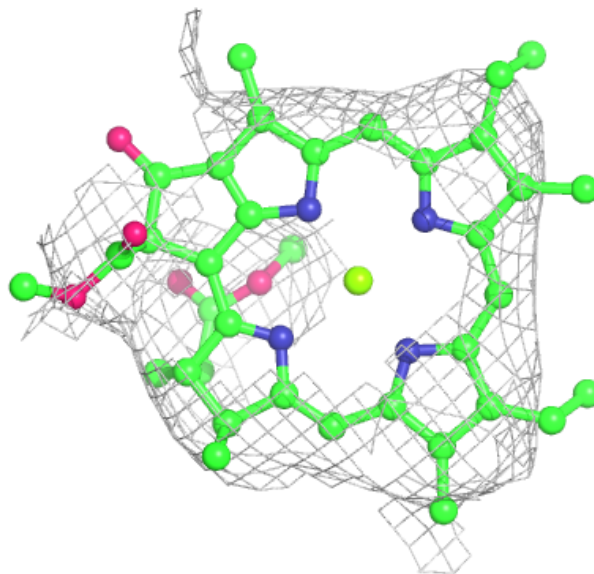
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





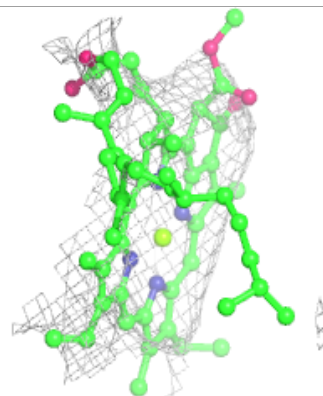
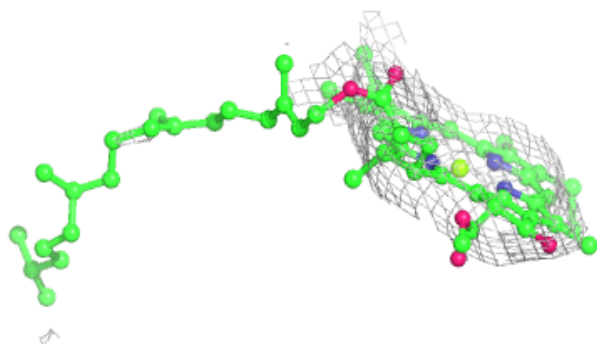
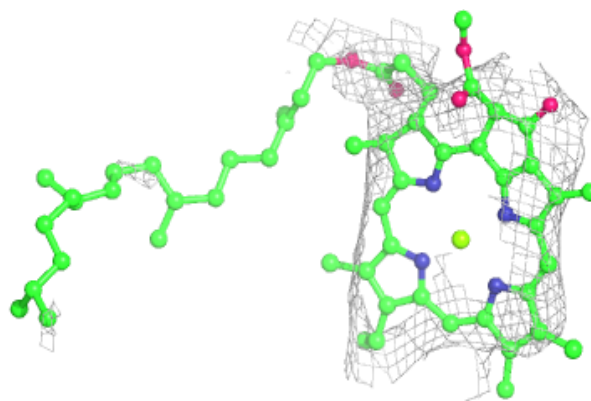
Electron density around CLA 1 1136:

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

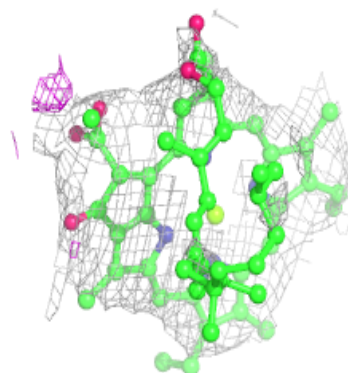
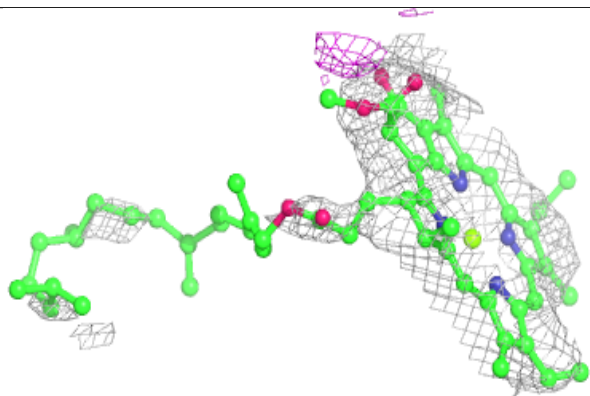
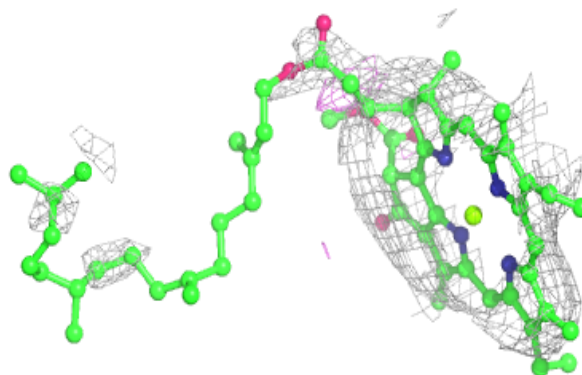


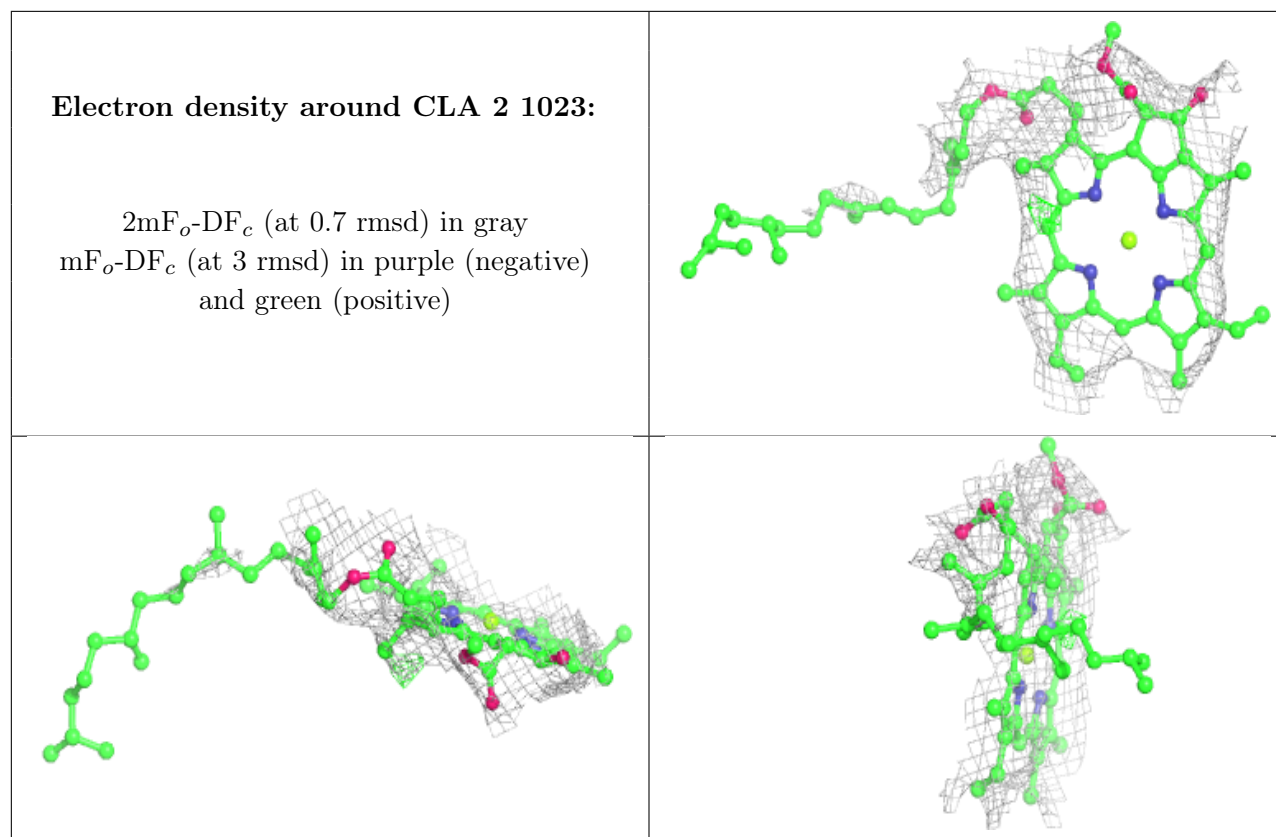
Electron density around CLA 2 1013:

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

**Electron density around CLA 2 1021:**

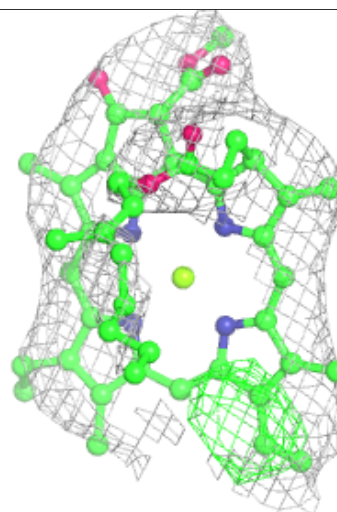
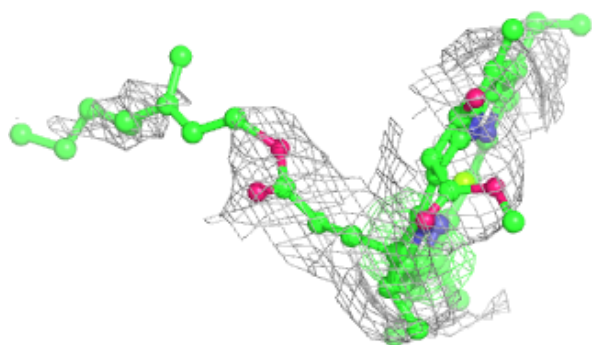
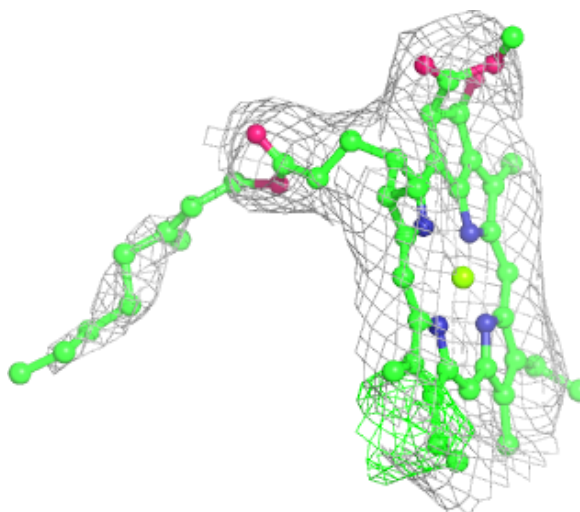
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





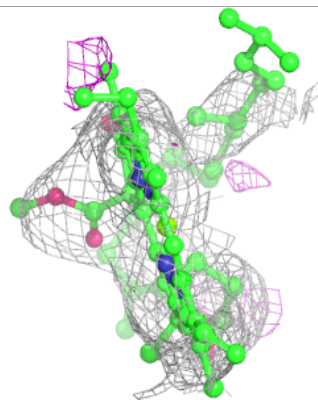
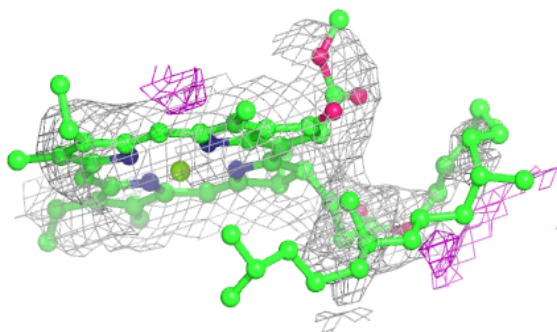
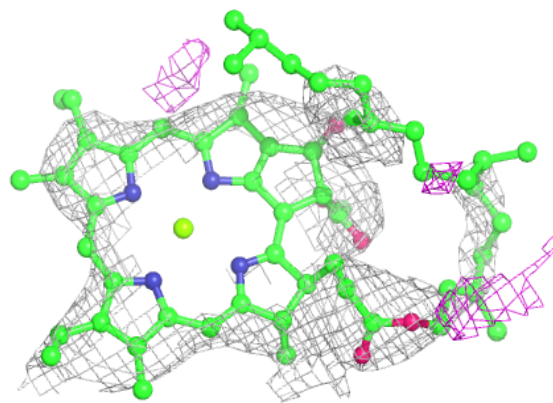
Electron density around CLA 2 1201:

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



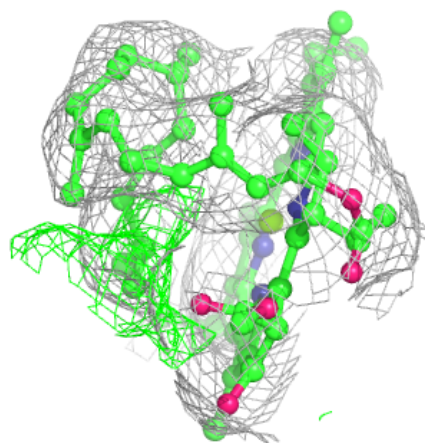
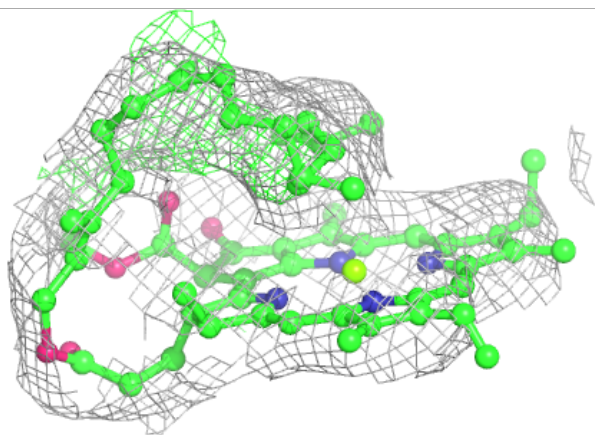
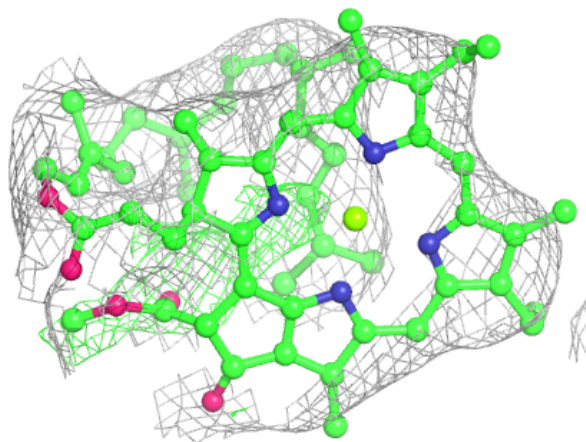
Electron density around CLA 2 1202:

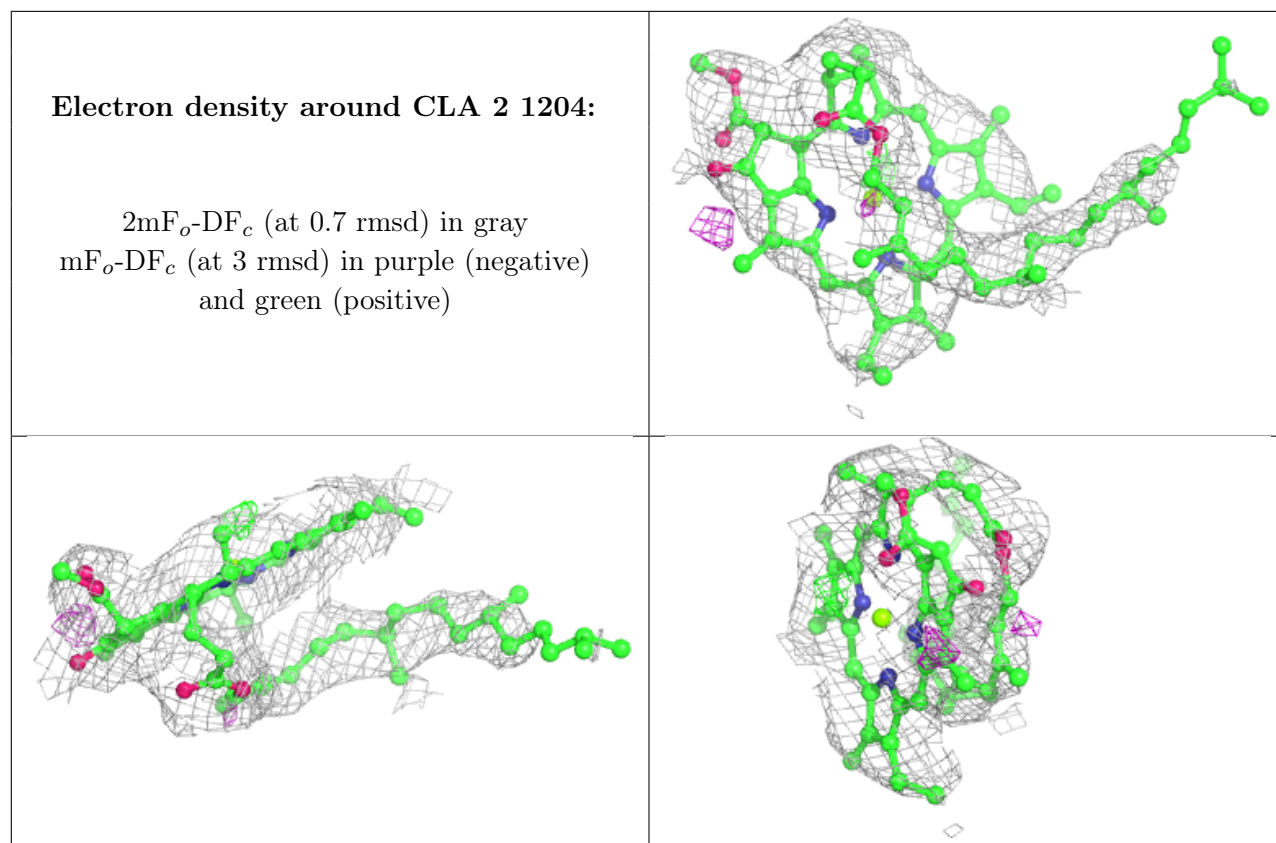
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around CLA 2 1203:

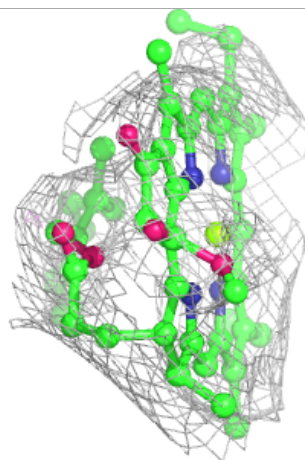
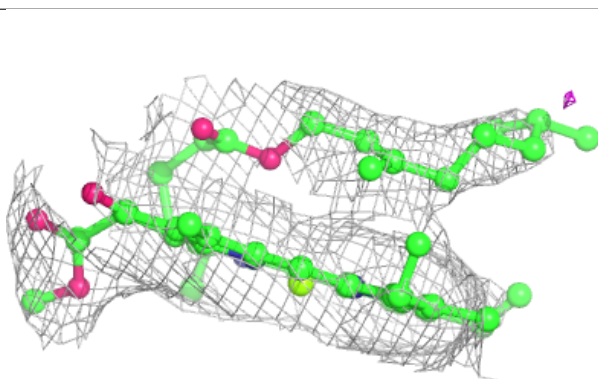
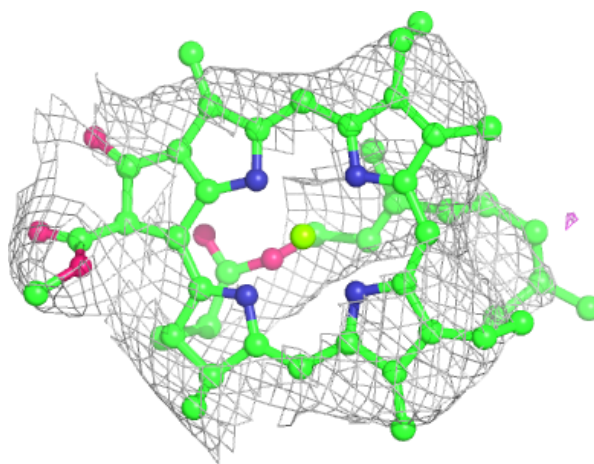
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





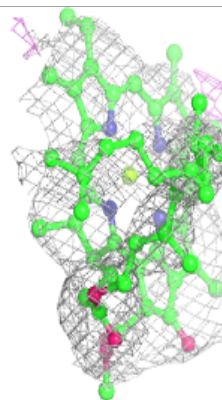
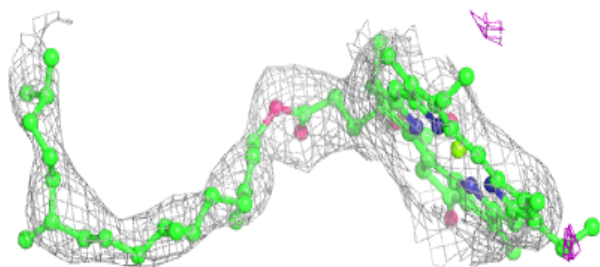
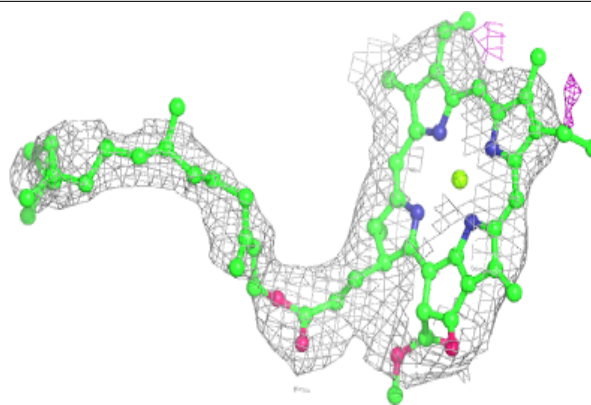
Electron density around CLA 2 1205:

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

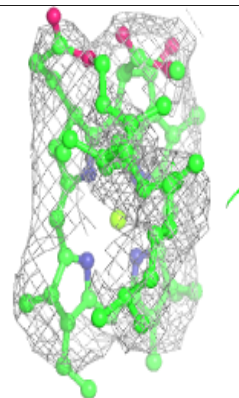
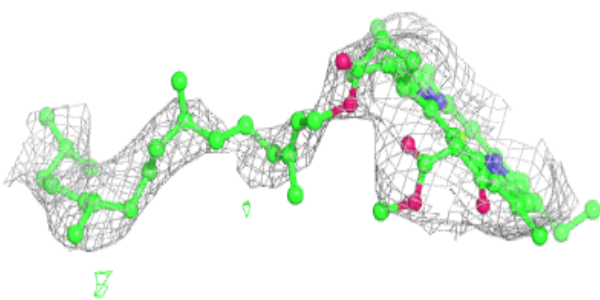
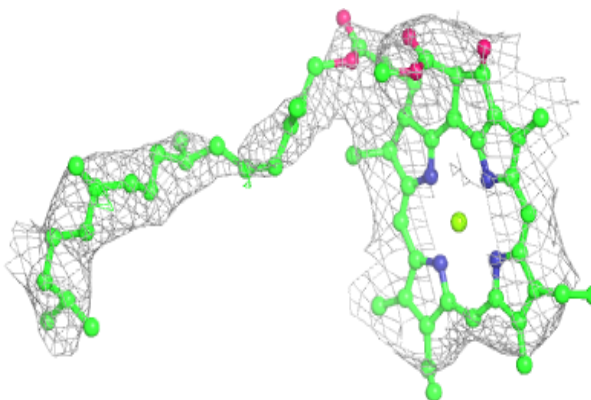


Electron density around CLA 2 1206:

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

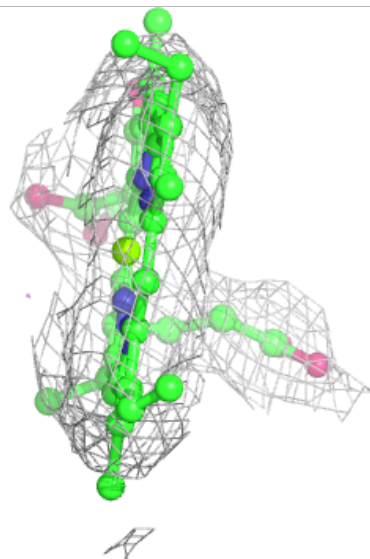
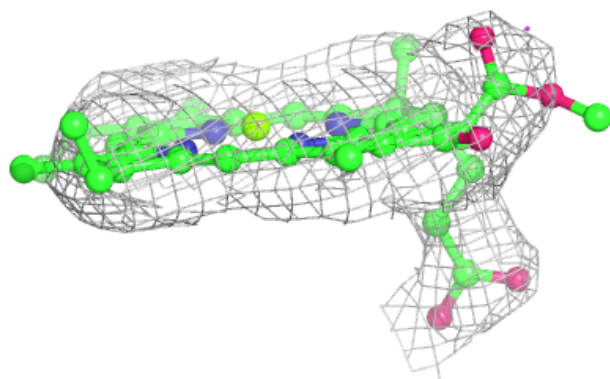
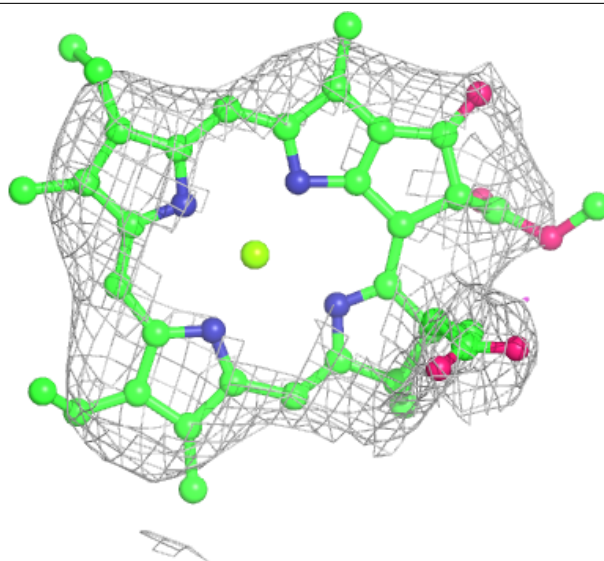
**Electron density around CLA 2 1207:**

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



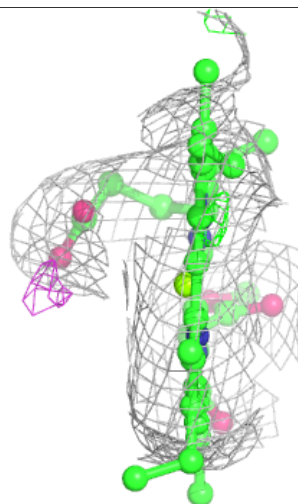
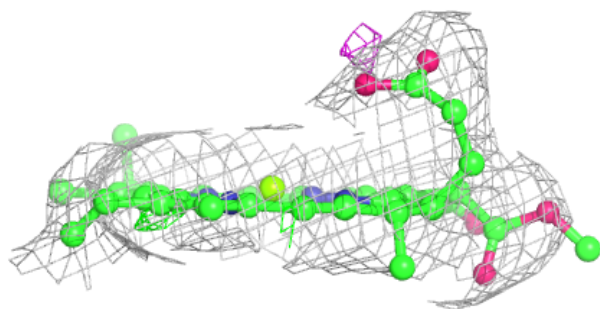
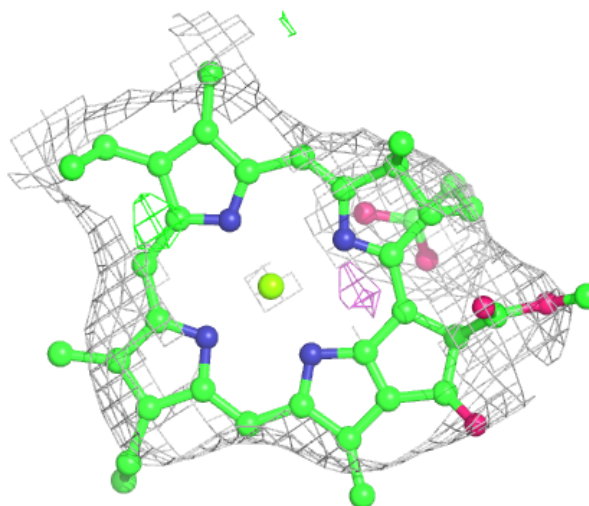
Electron density around CLA 2 1208:

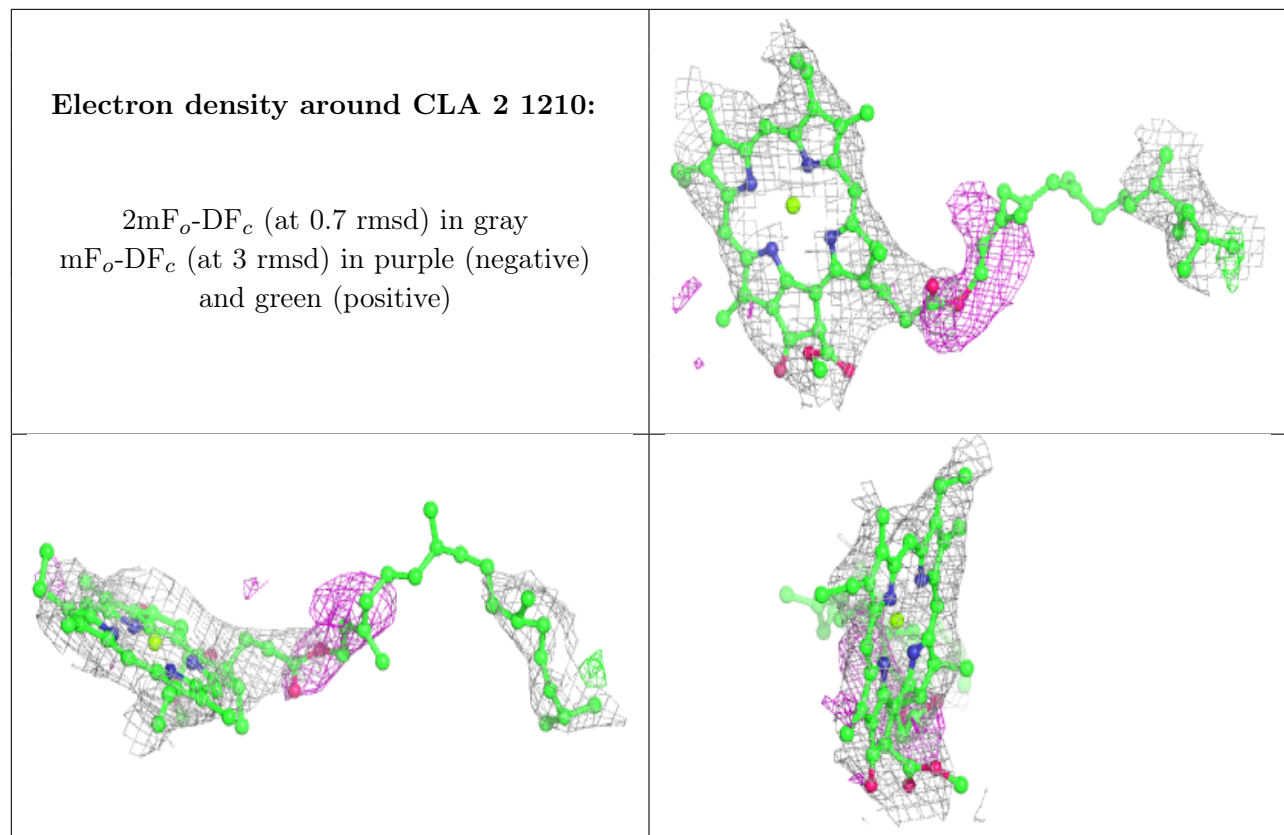
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around CLA 2 1209:

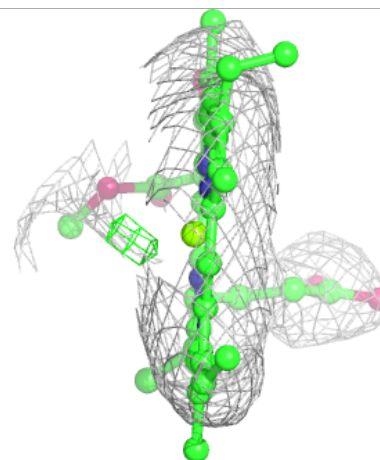
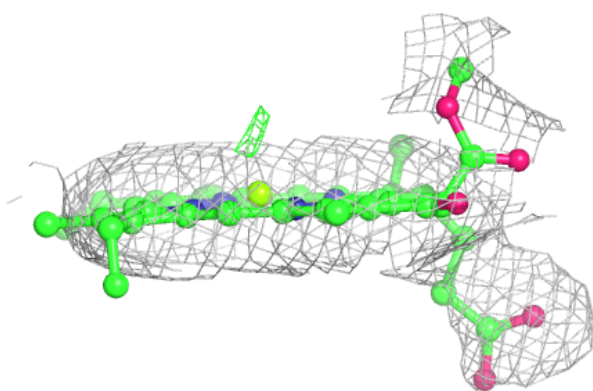
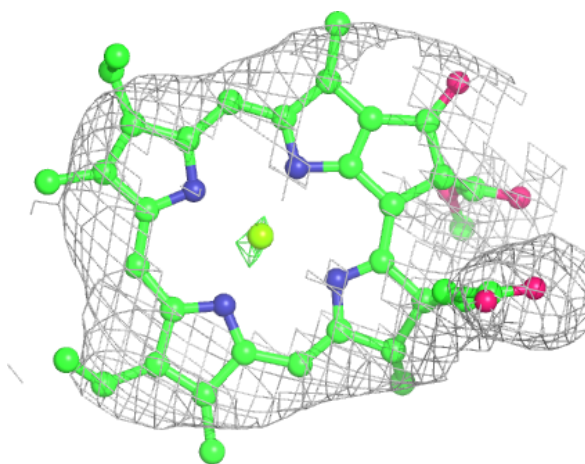
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

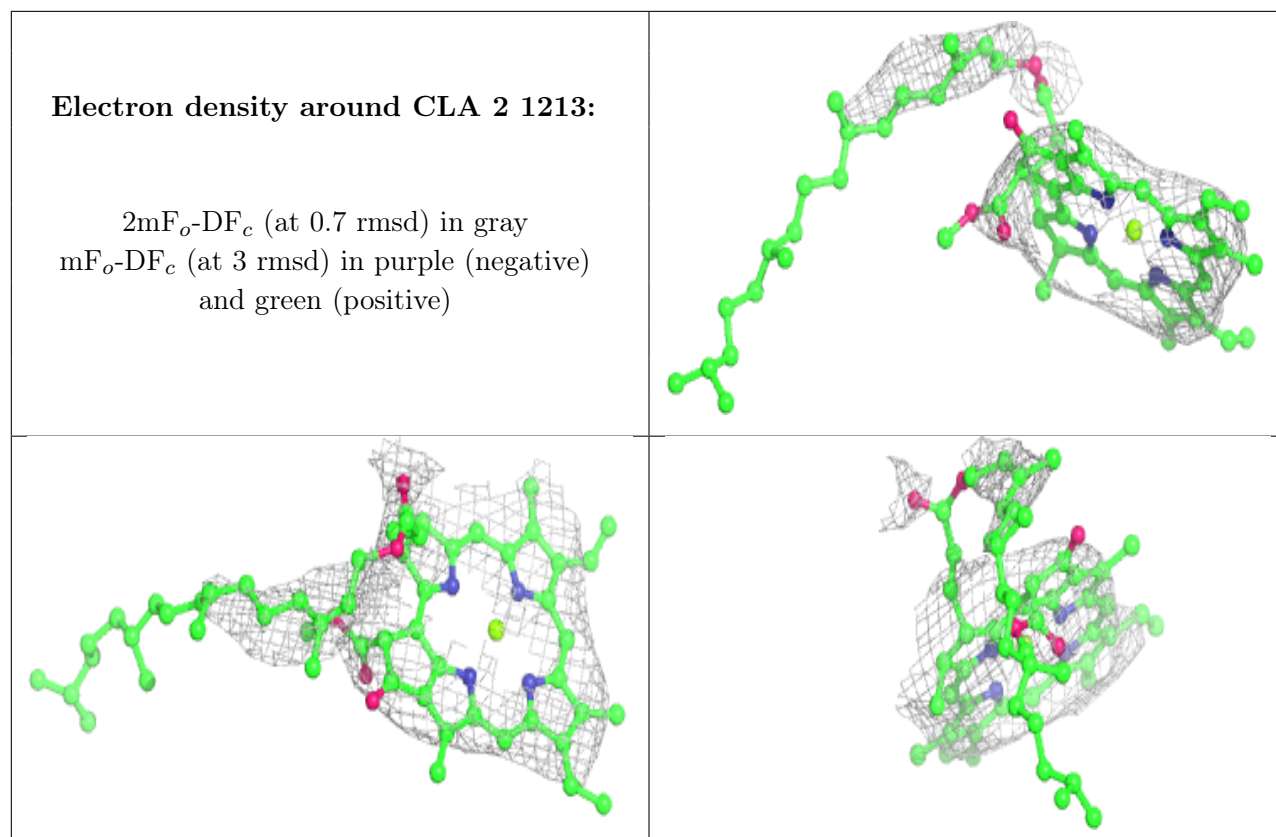




Electron density around CLA 2 1212:

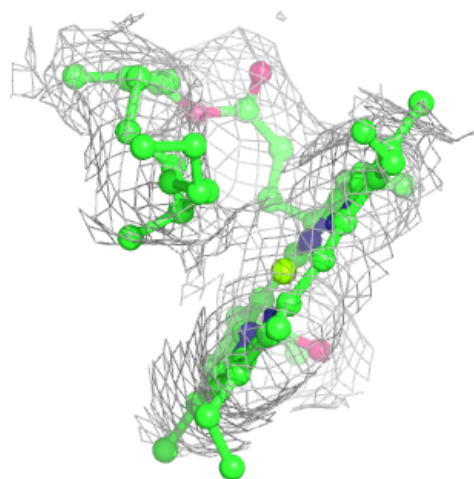
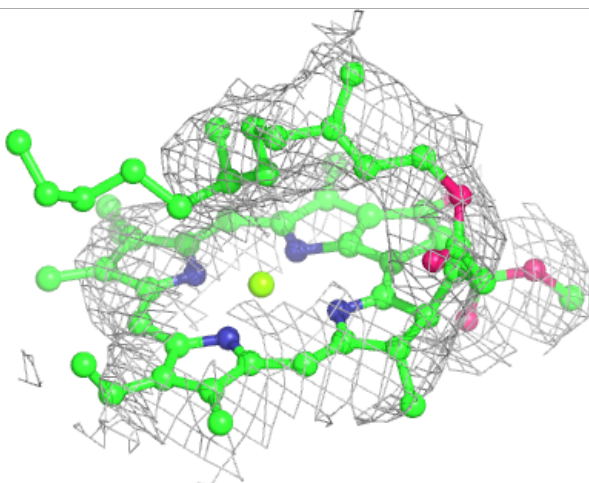
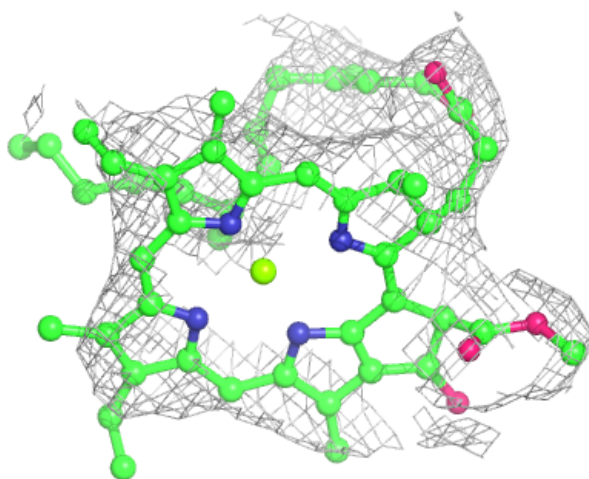
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





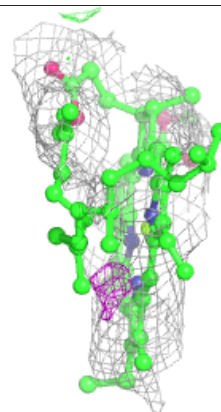
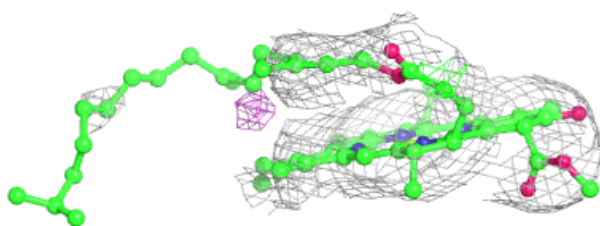
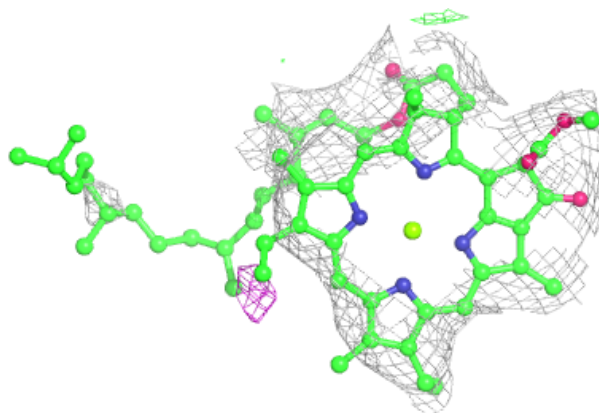
Electron density around CLA 2 1214:

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

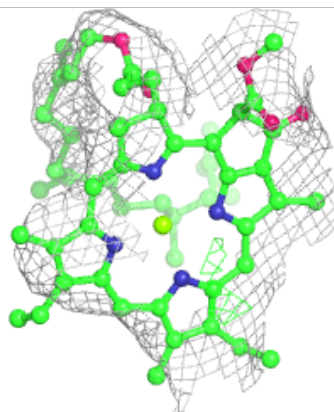
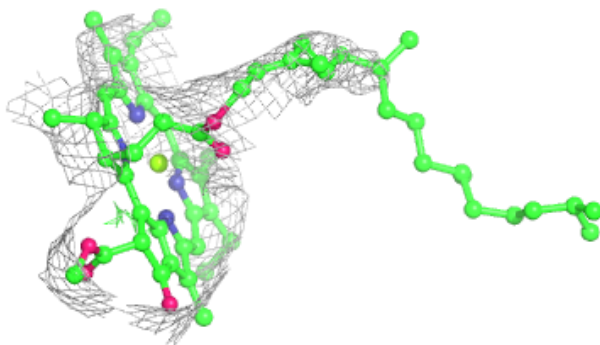
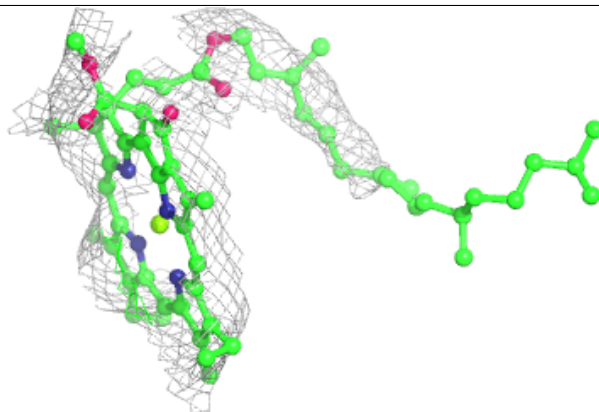


Electron density around CLA 2 1215:

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

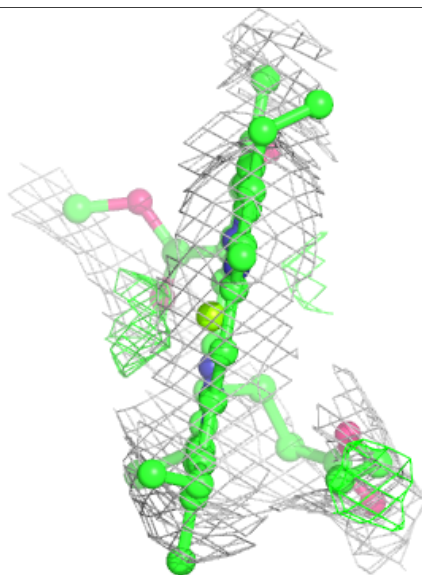
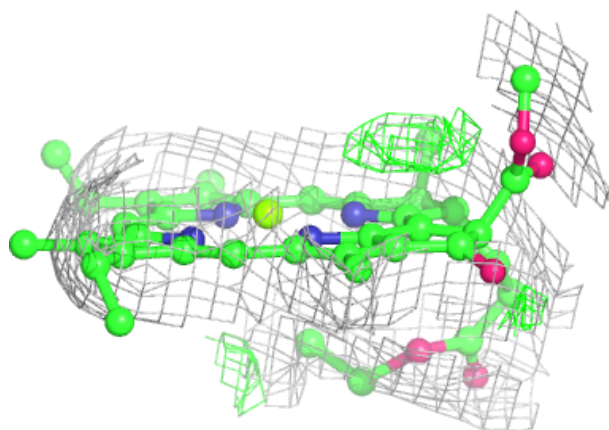
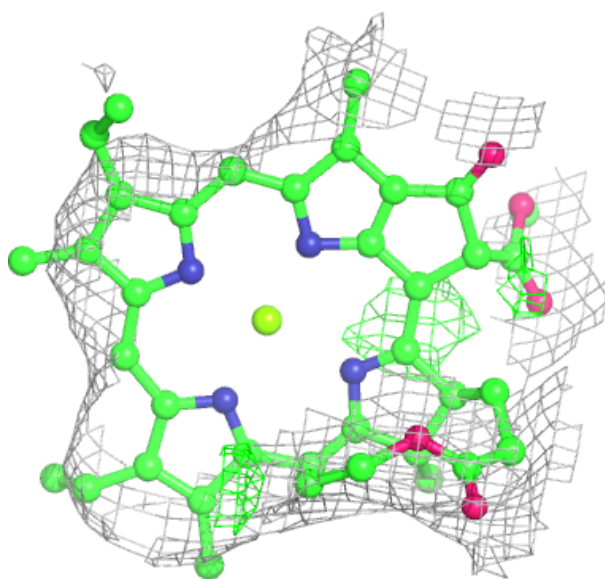
**Electron density around CLA 2 1216:**

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



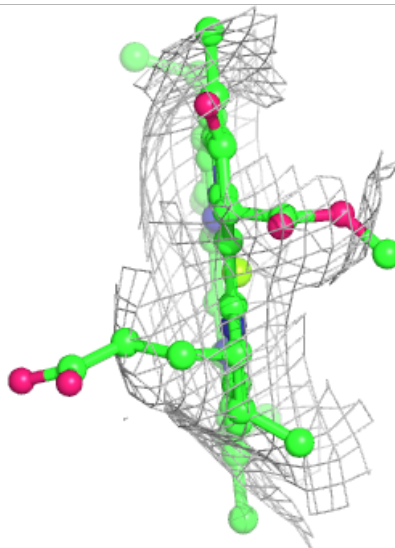
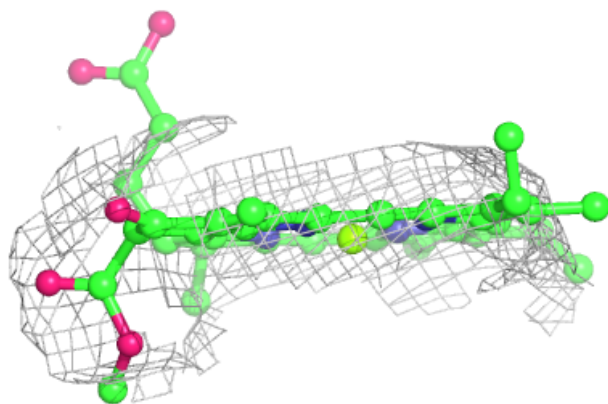
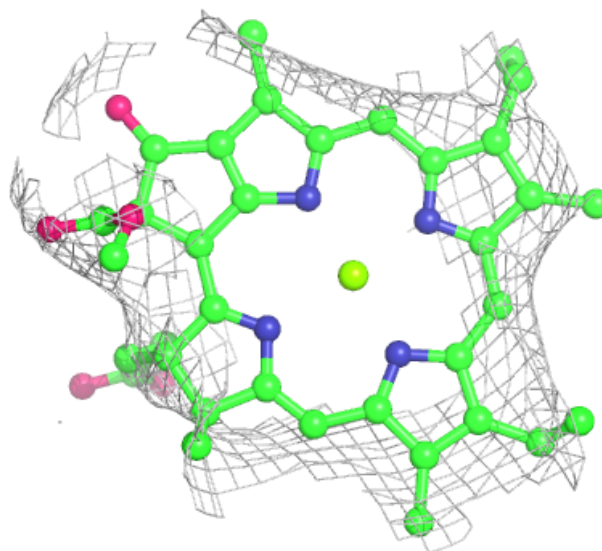
Electron density around CLA 2 1217:

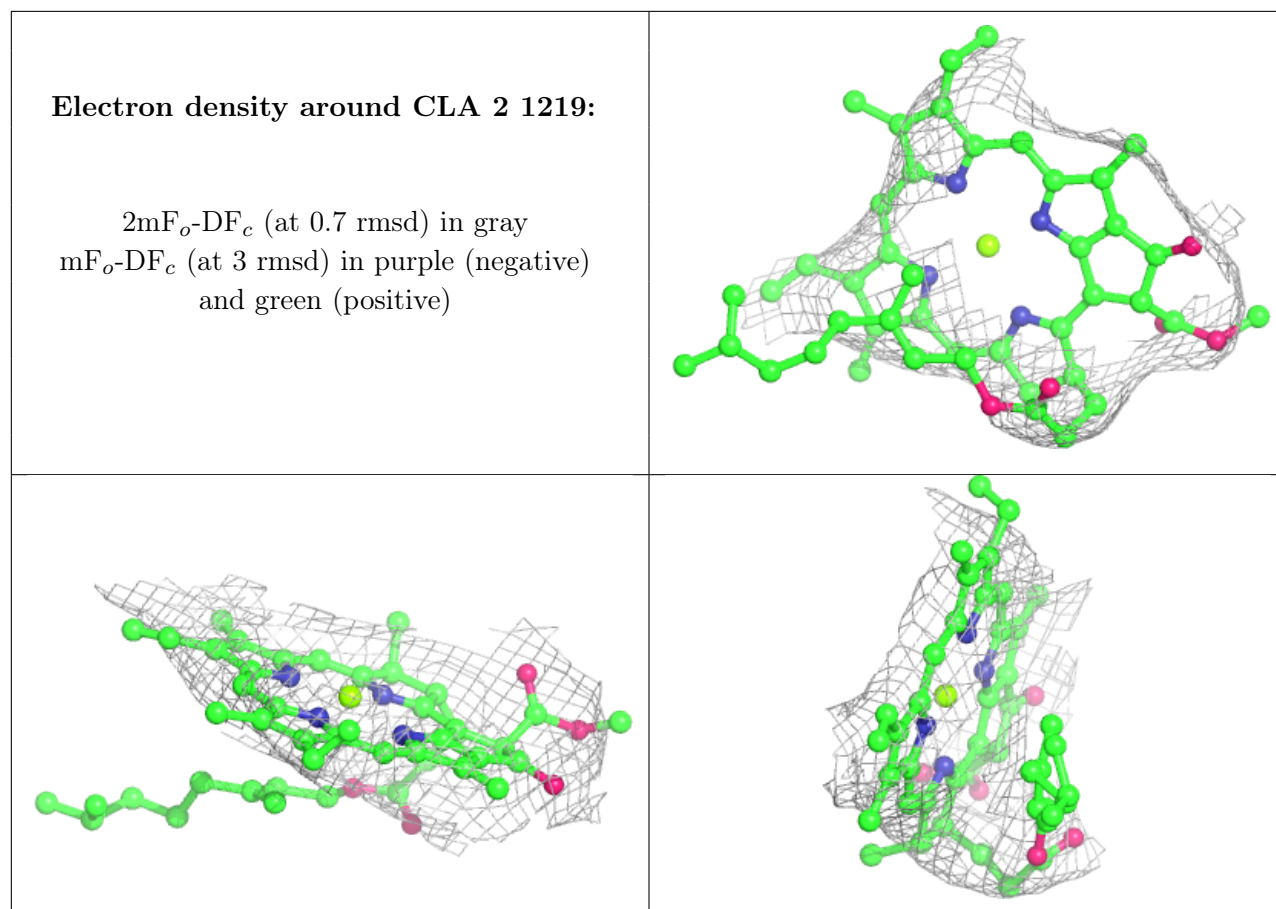
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around CLA 2 1218:

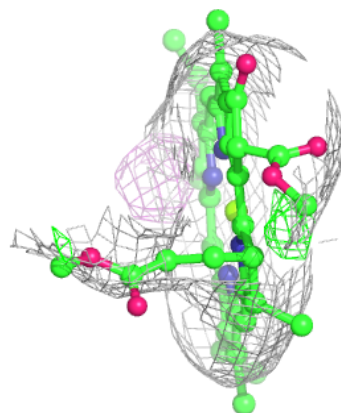
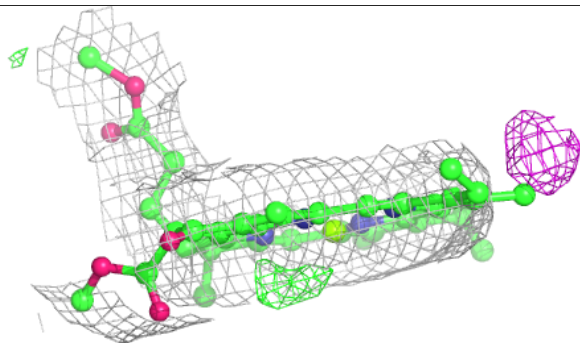
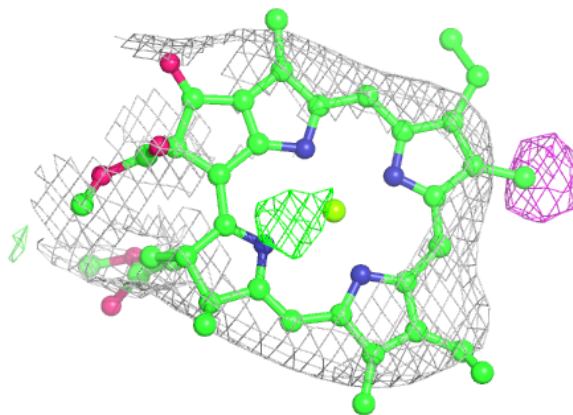
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





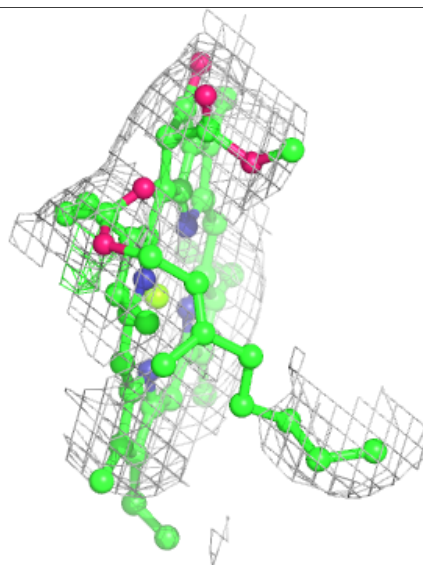
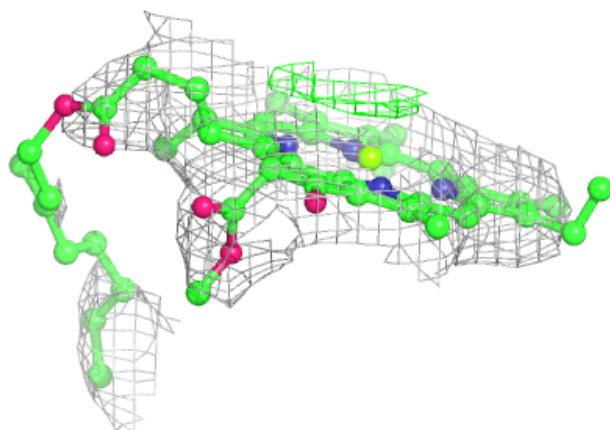
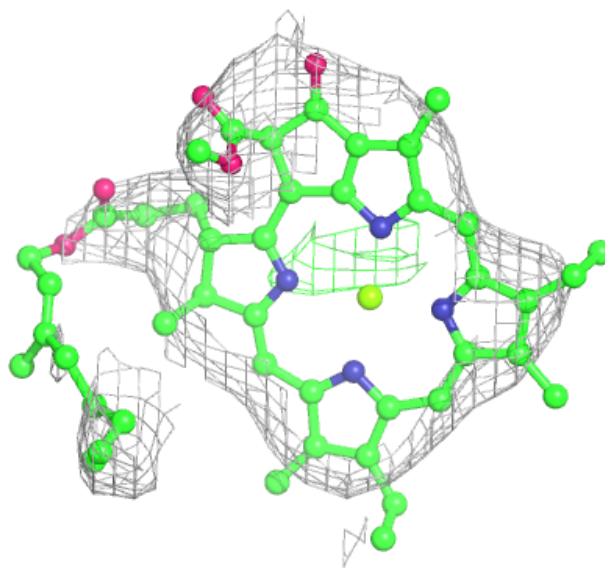
Electron density around CLA 2 1220:

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



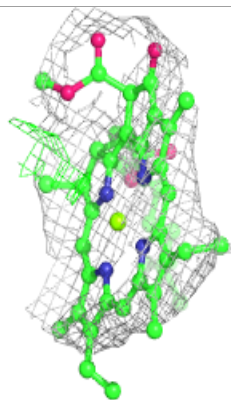
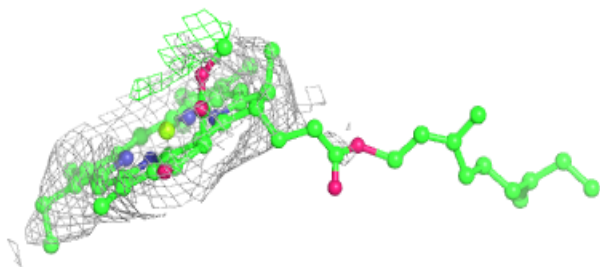
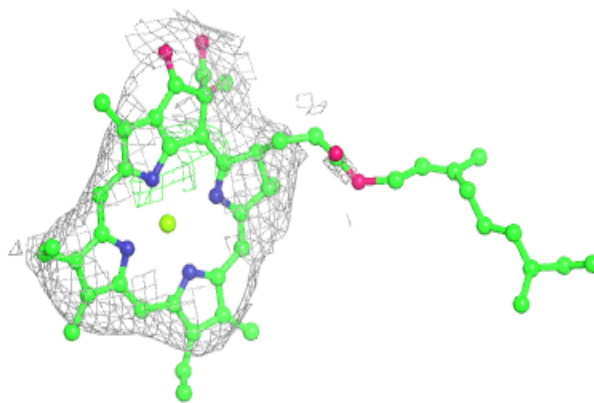
Electron density around CLA 2 1221:

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

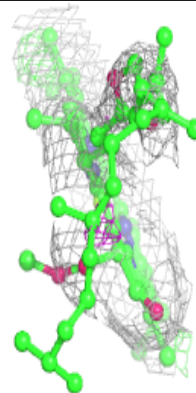
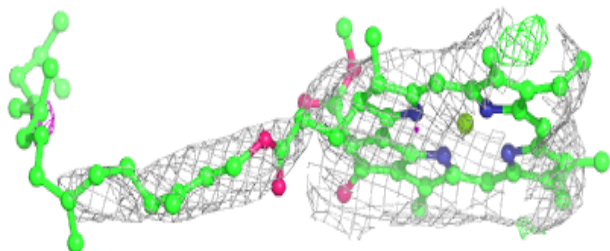
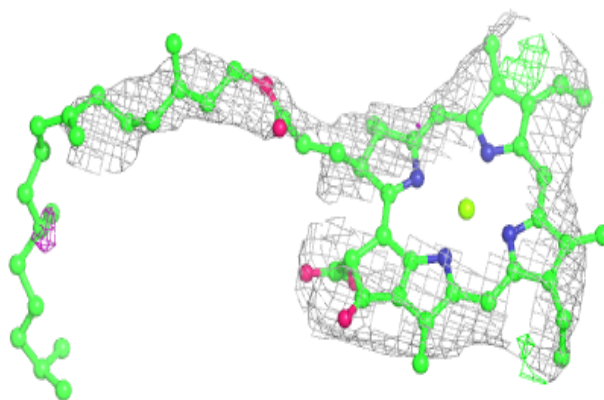


Electron density around CLA 2 1222:

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

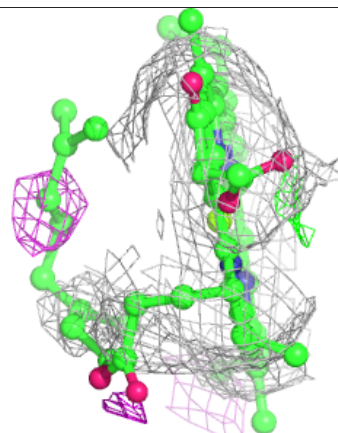
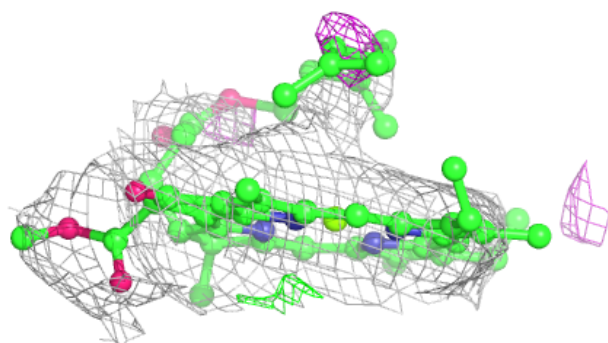
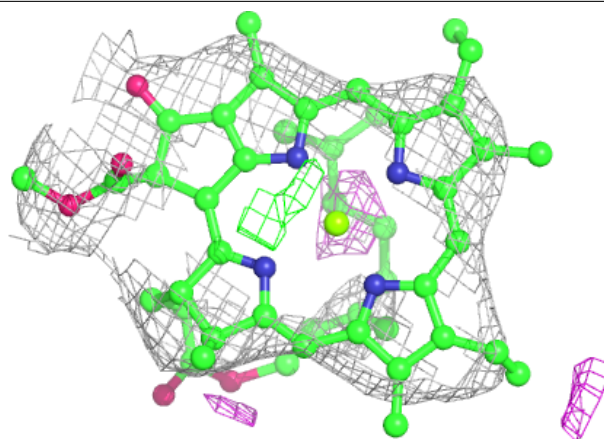
**Electron density around CLA 2 1223:**

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

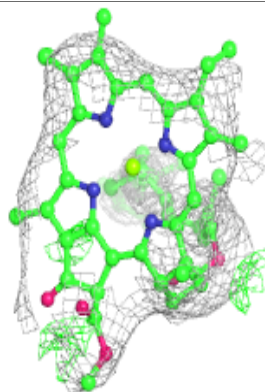
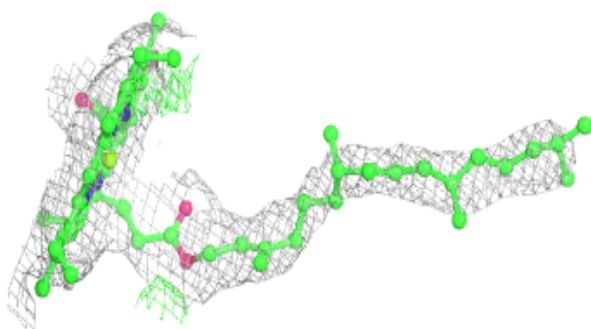
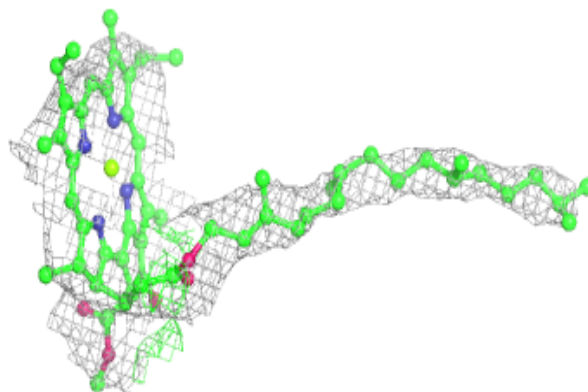


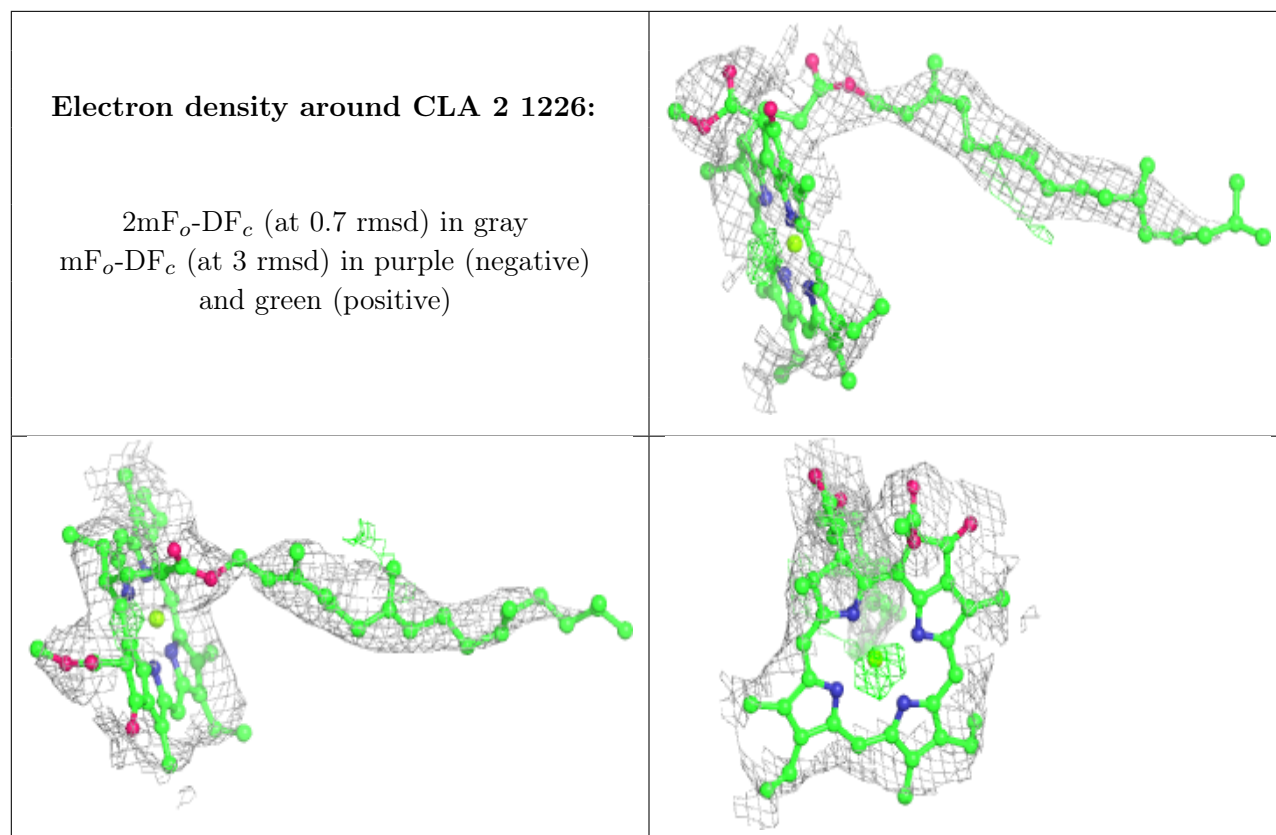
Electron density around CLA 2 1224:

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

**Electron density around CLA 2 1225:**

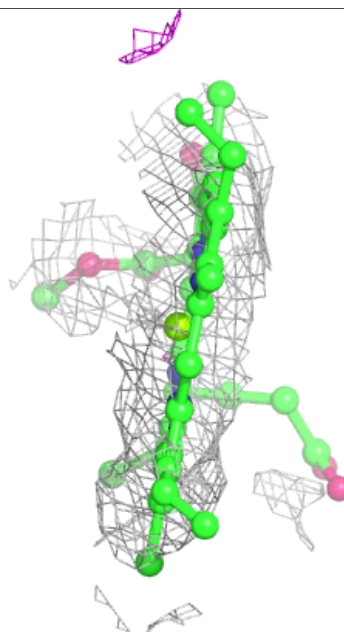
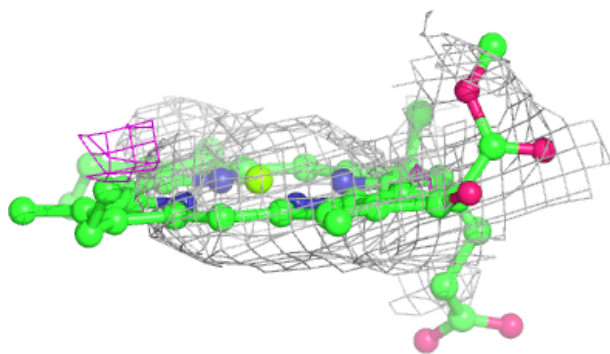
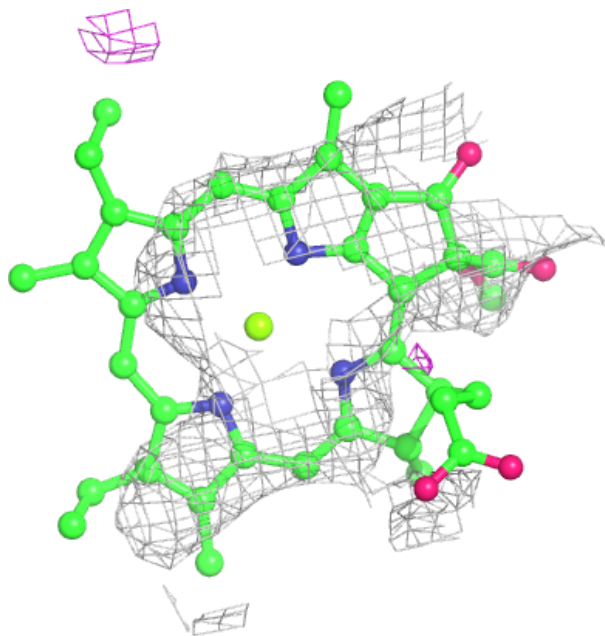
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





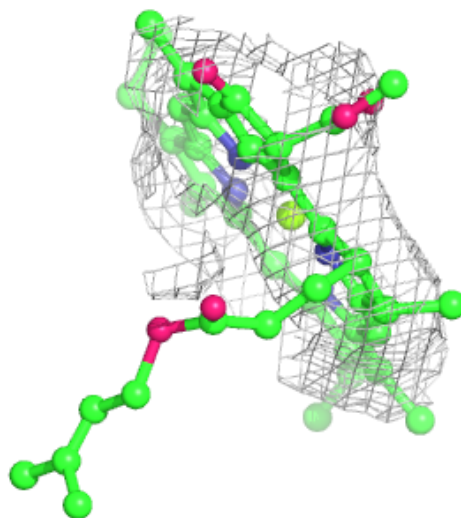
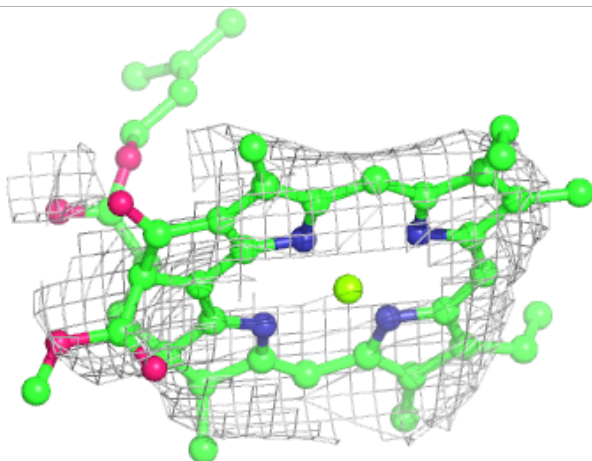
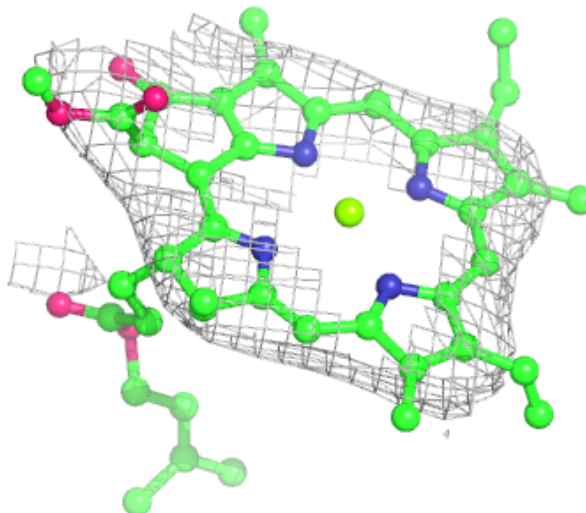
Electron density around CLA 2 1227:

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



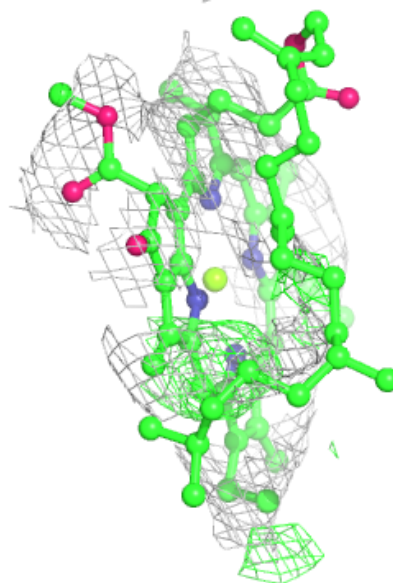
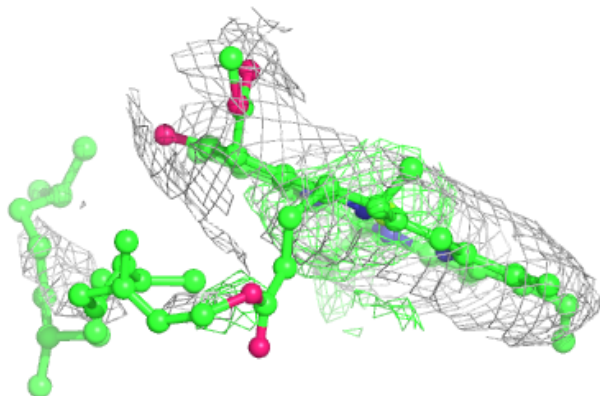
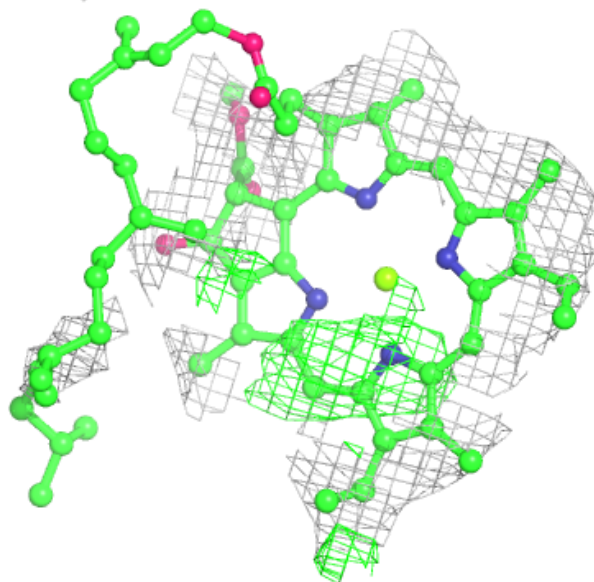
Electron density around CLA 2 1228:

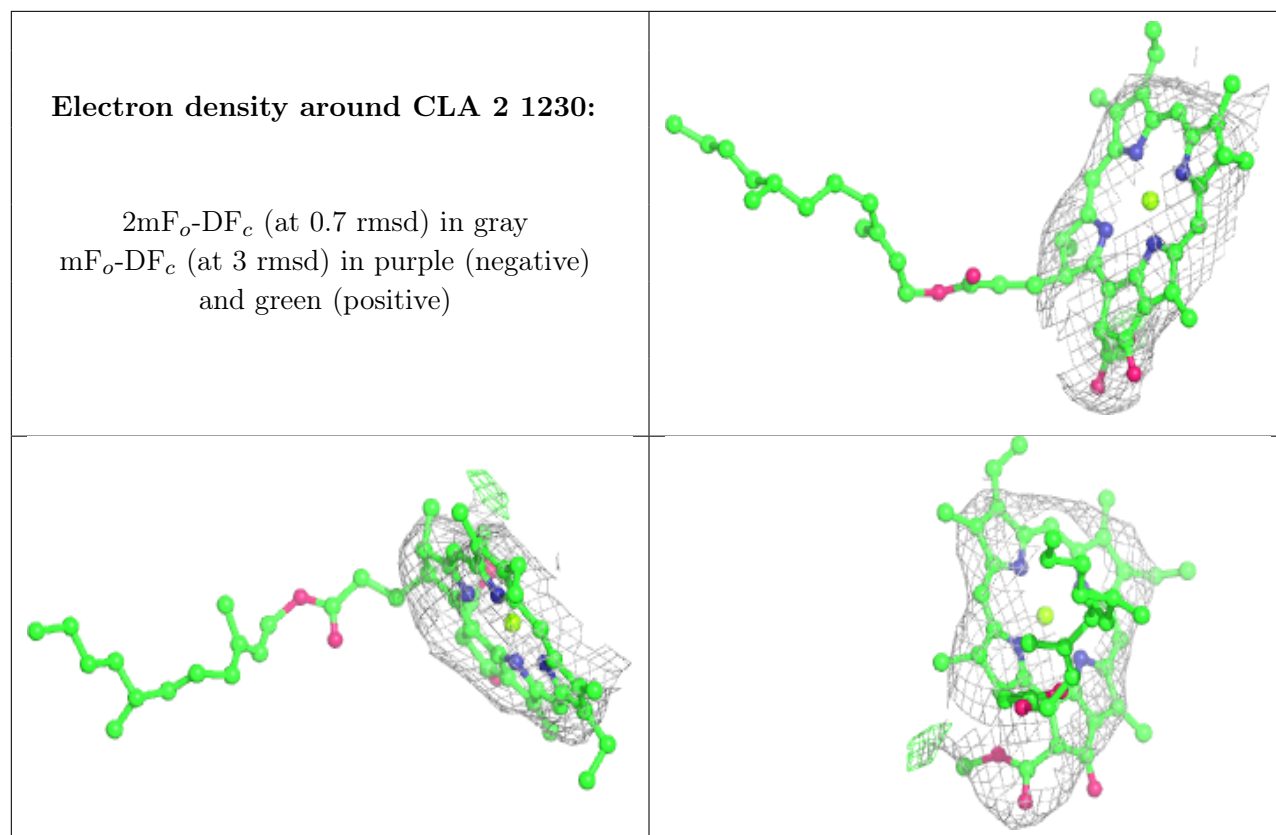
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around CLA 2 1229:

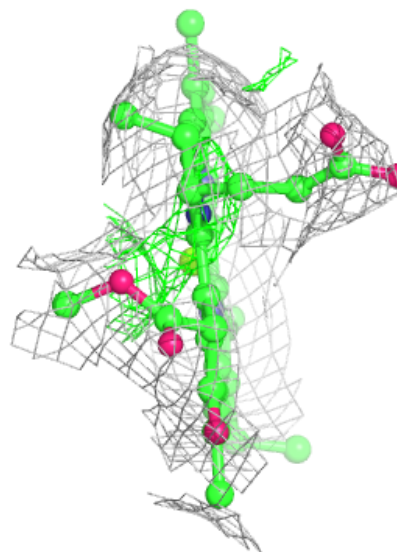
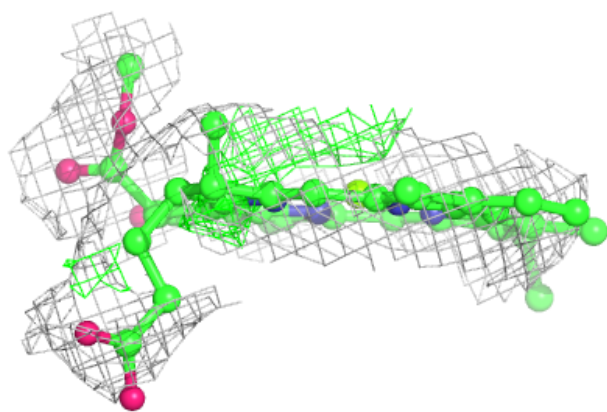
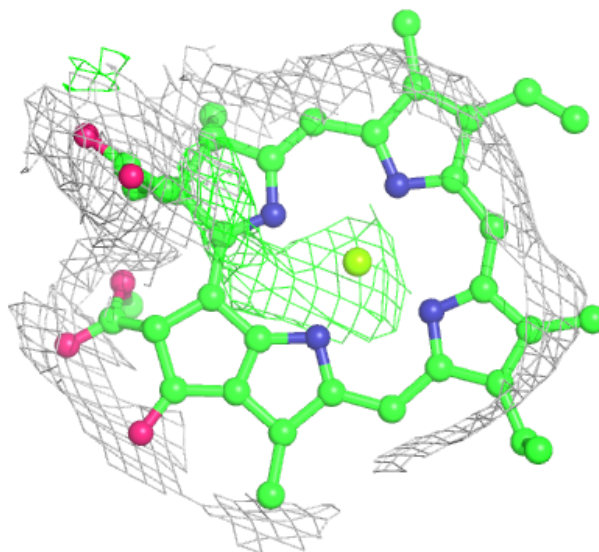
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





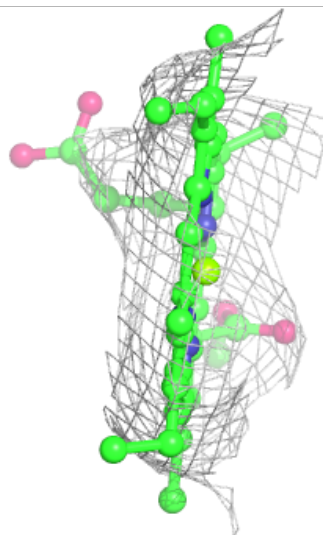
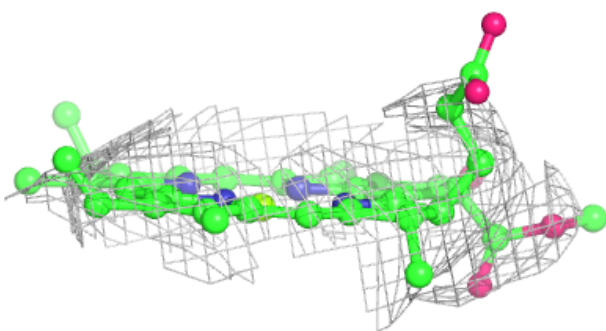
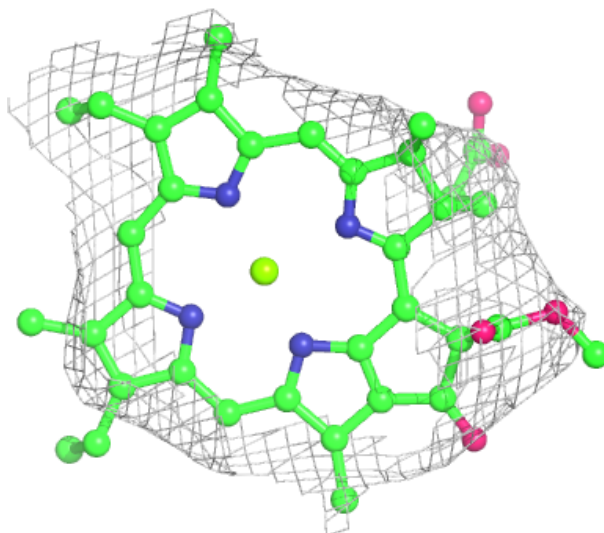
Electron density around CLA 2 1231:

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



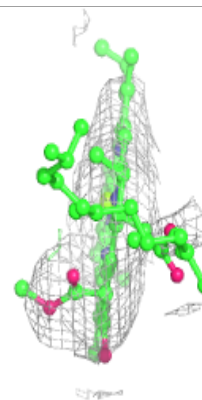
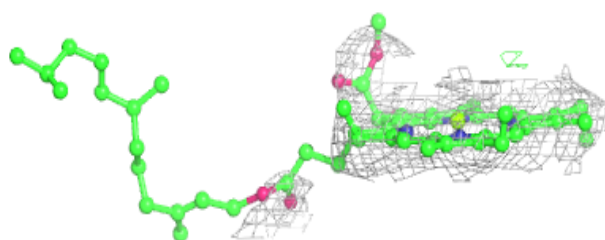
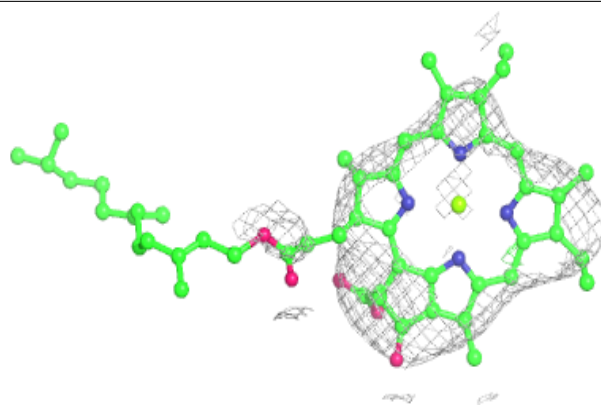
Electron density around CLA 2 1232:

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

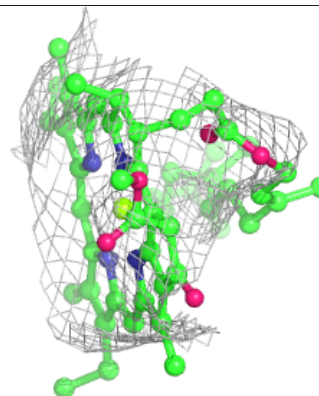
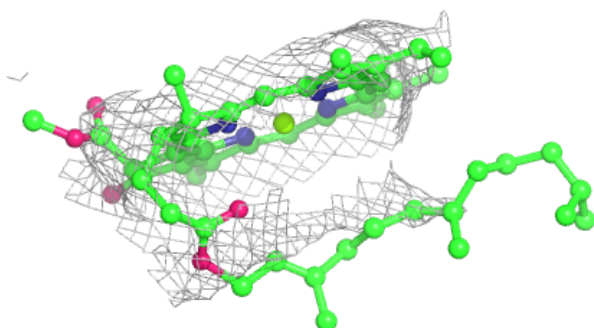
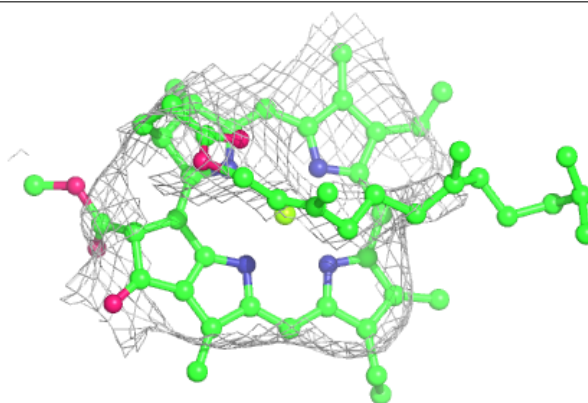


Electron density around CLA 2 1234:

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

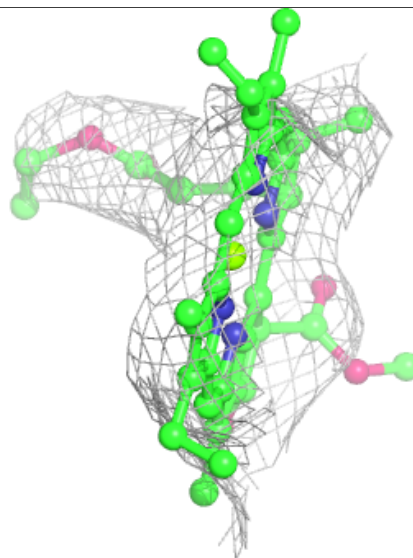
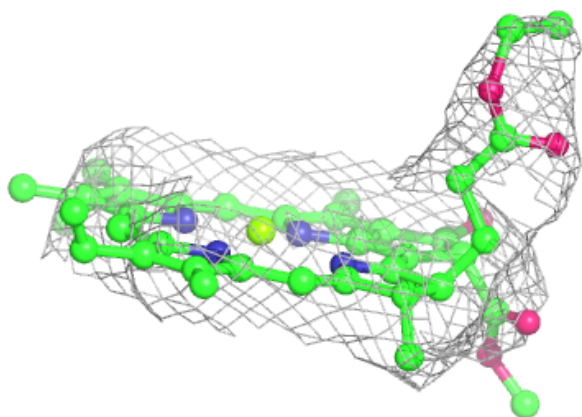
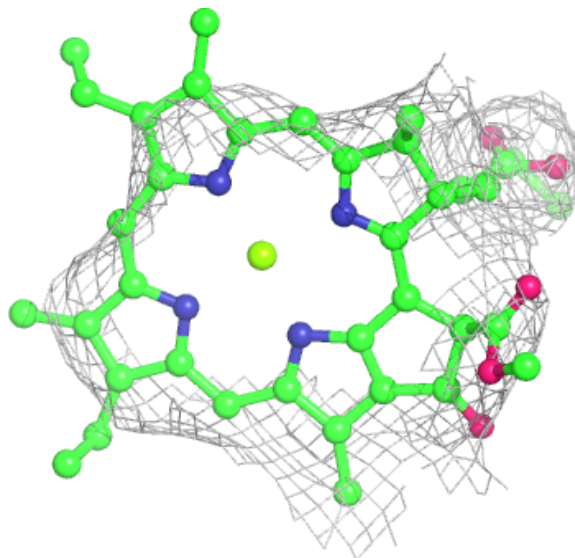
**Electron density around CLA 2 1235:**

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



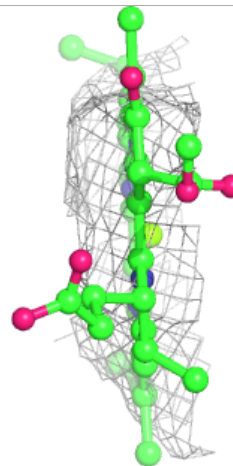
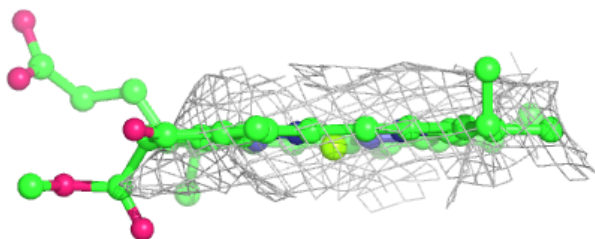
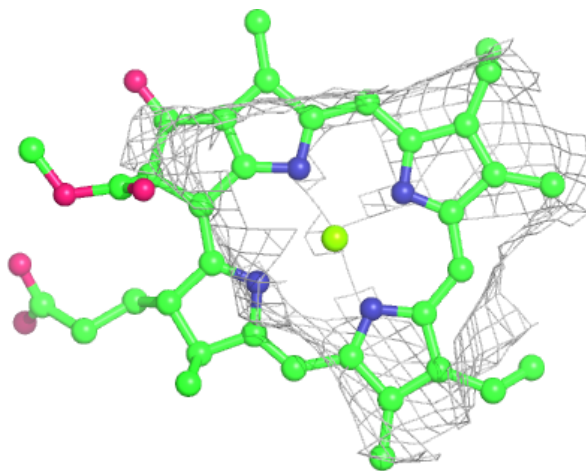
Electron density around CLA 2 1236:

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



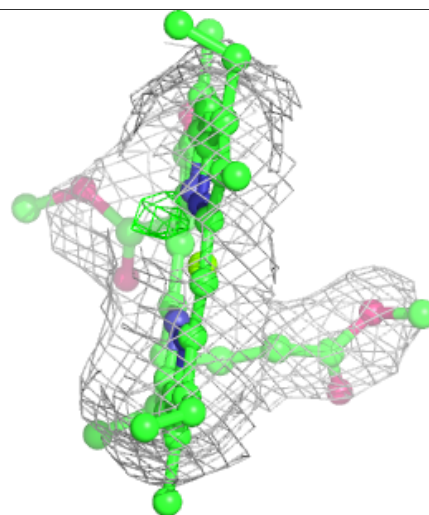
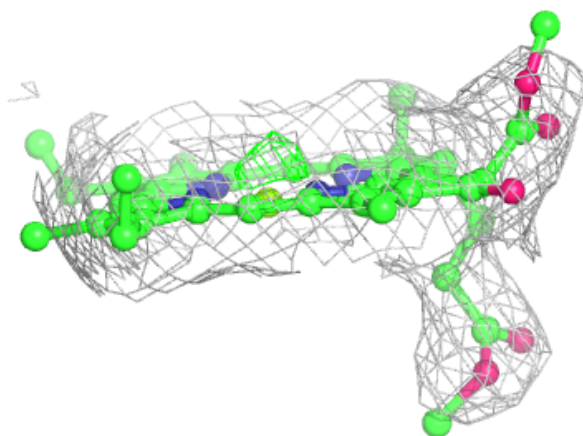
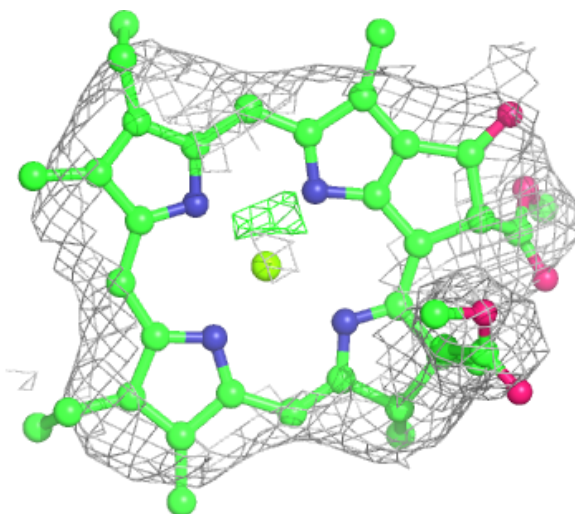
Electron density around CLA 2 1240:

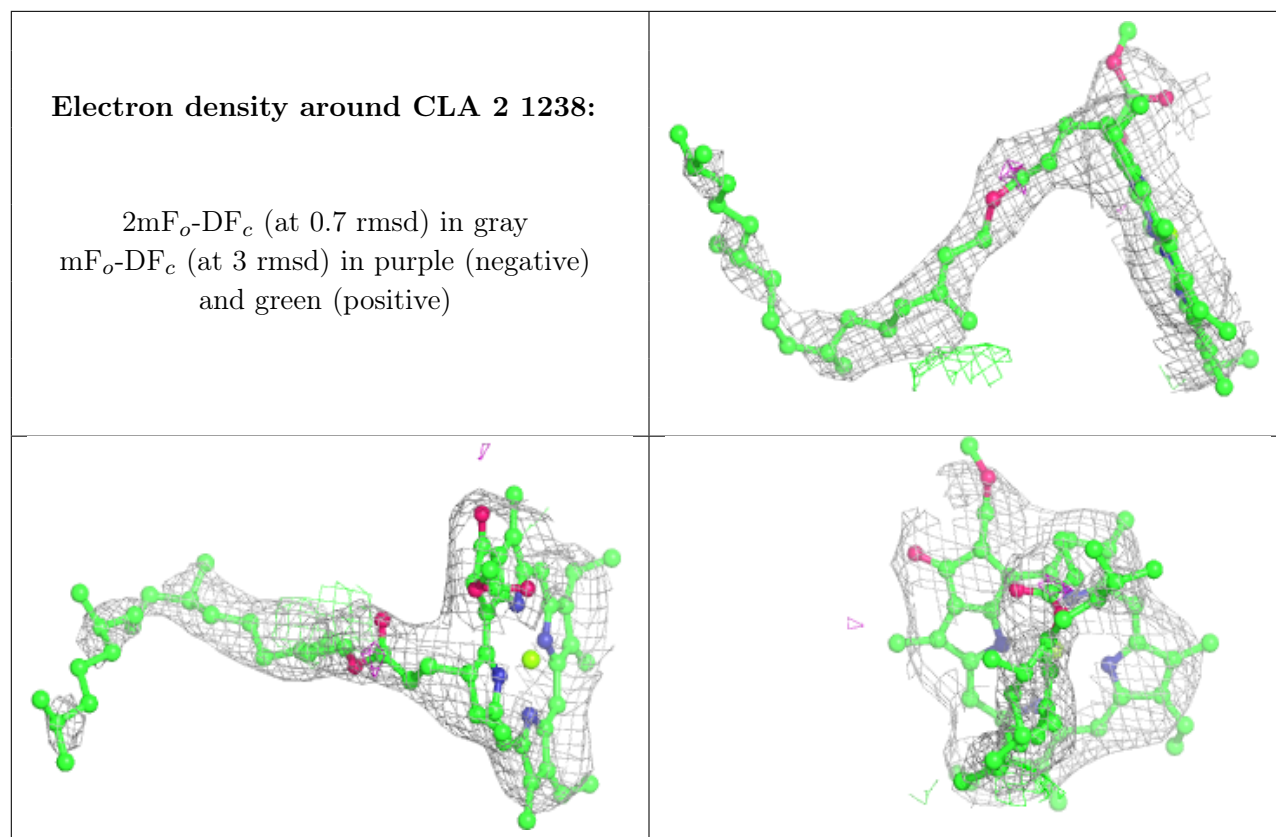
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around CLA 2 1211:

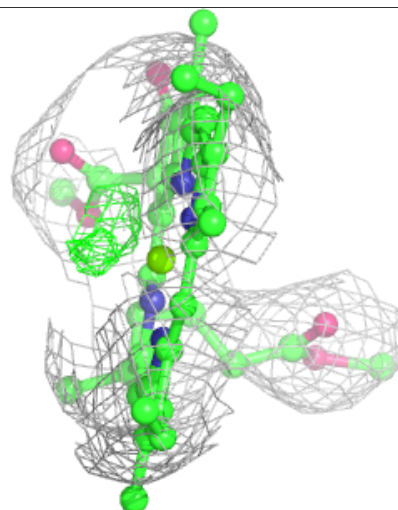
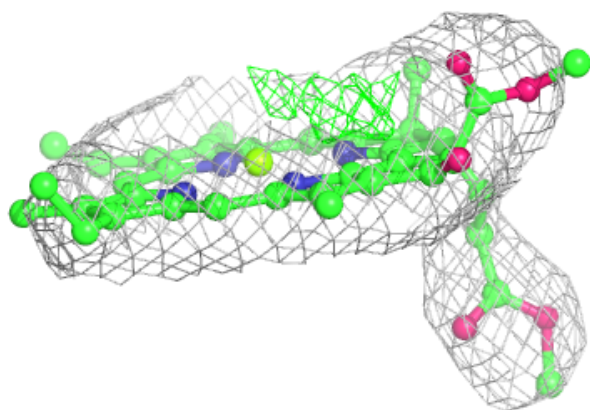
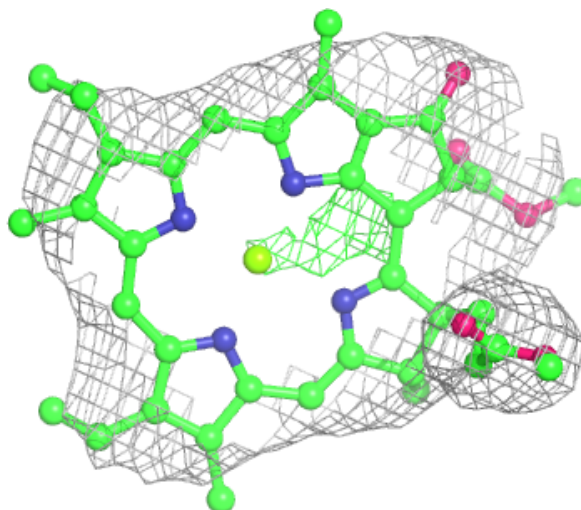
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





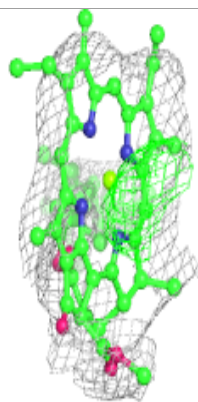
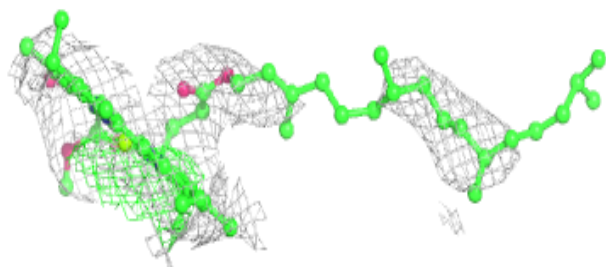
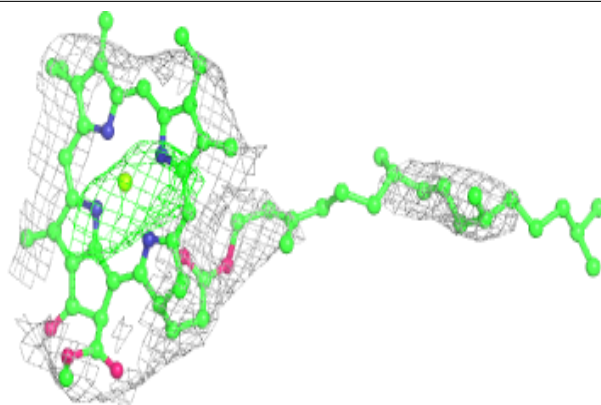
Electron density around CLA 2 1239:

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

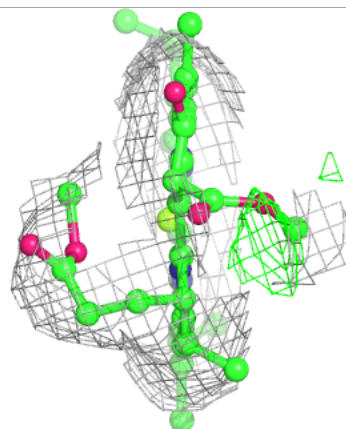
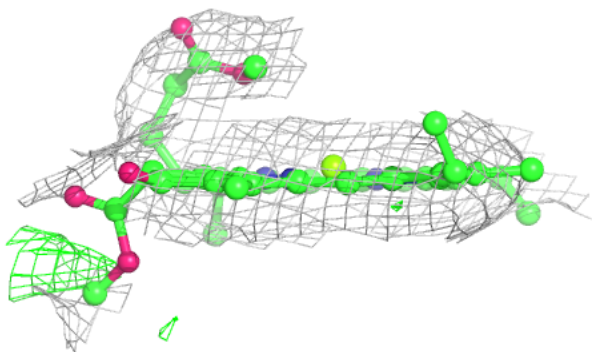
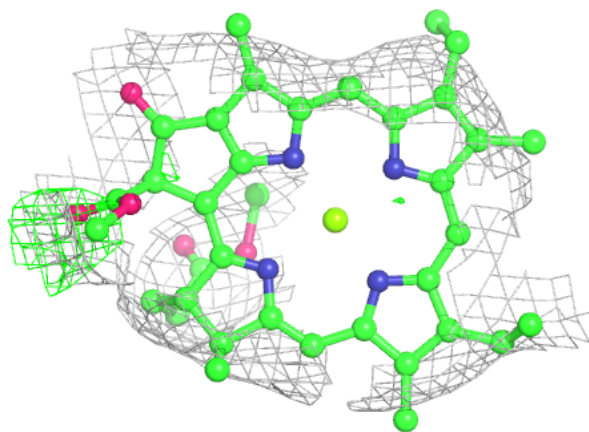


Electron density around CLA 8 1501:

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

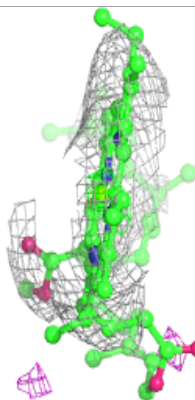
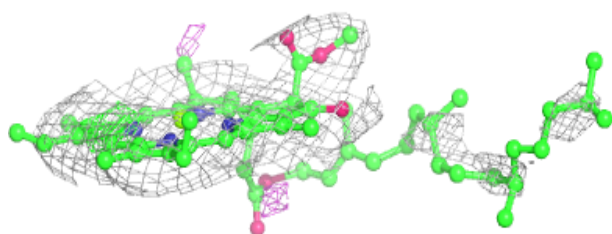
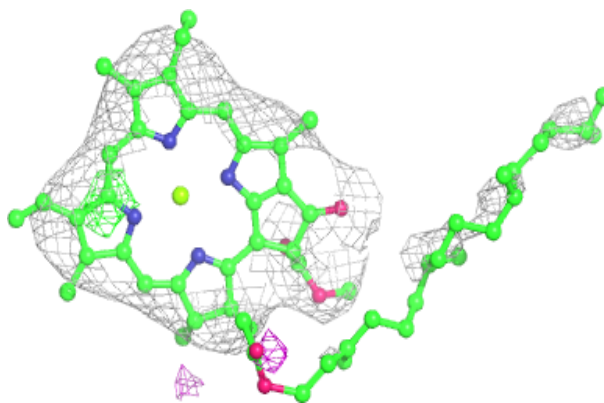
**Electron density around CLA 8 1502:**

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

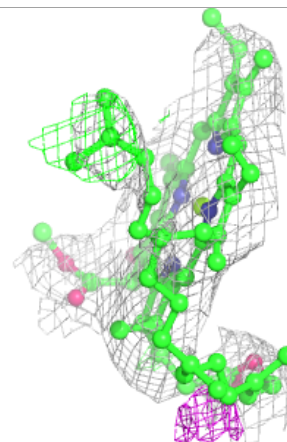
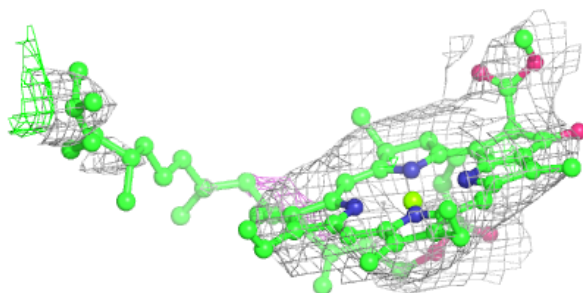
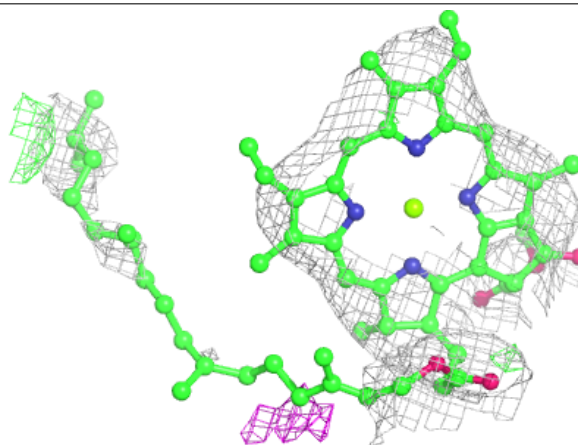


Electron density around CLA 8 1503:

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

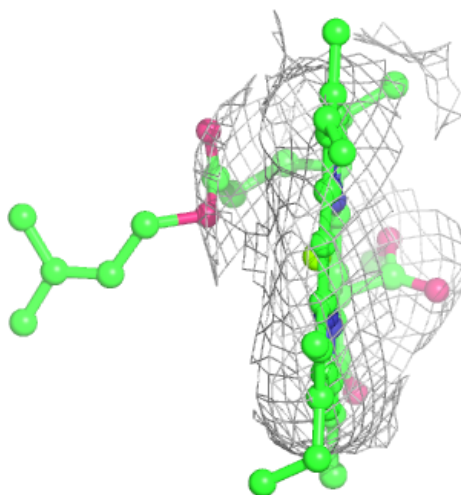
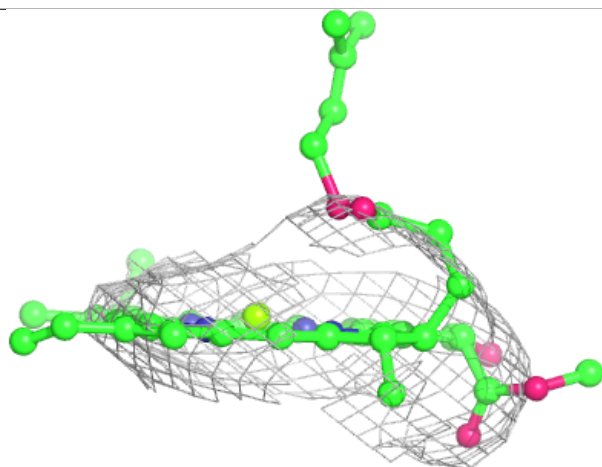
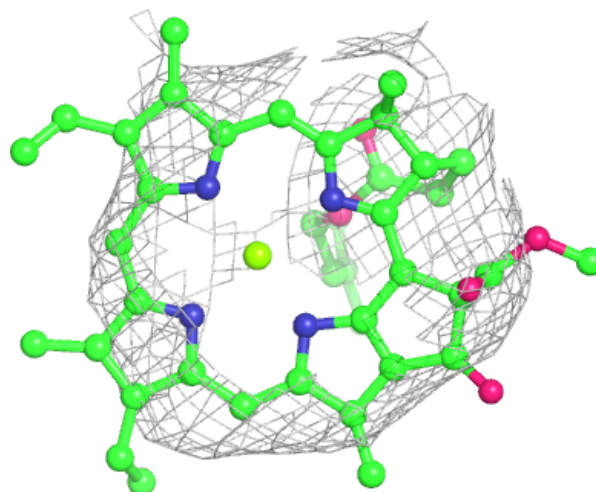
**Electron density around CLA K 1401:**

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



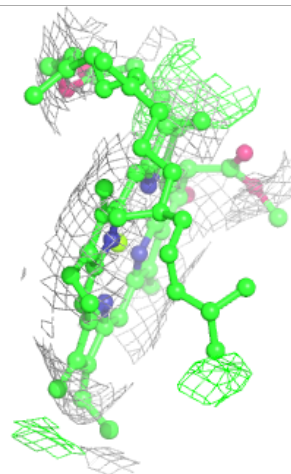
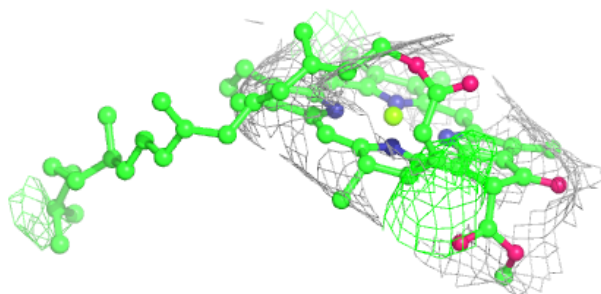
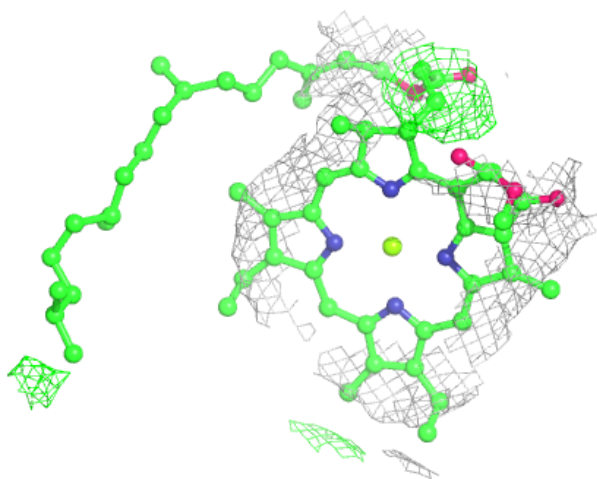
Electron density around CLA K 1402:

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



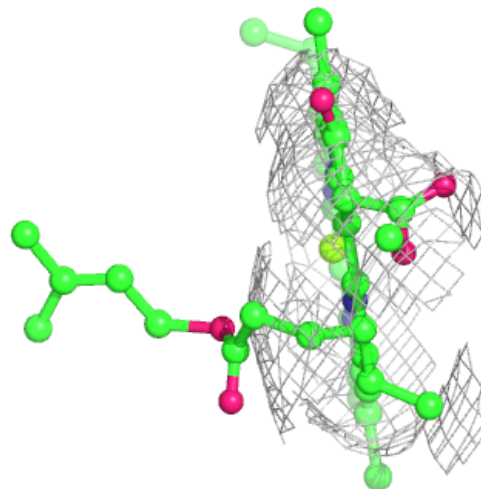
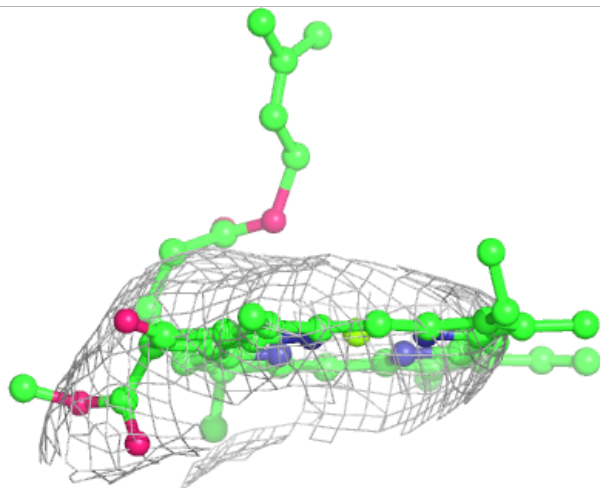
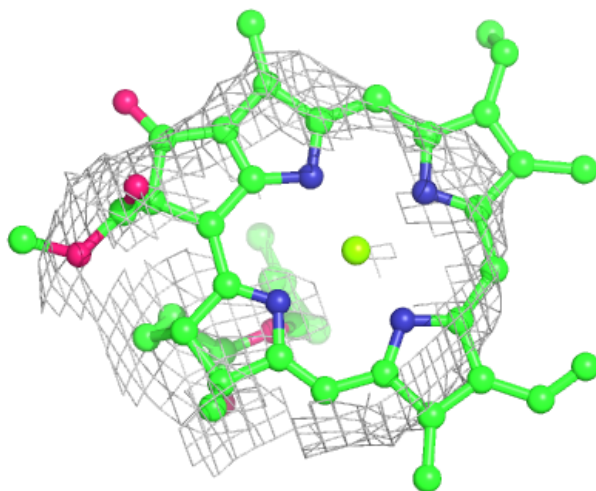
Electron density around CLA k 1401:

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



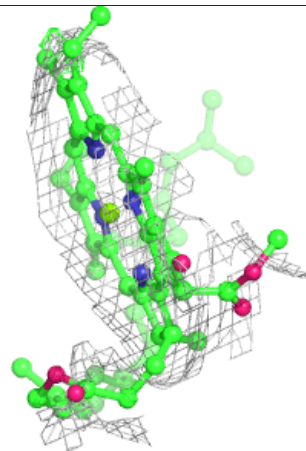
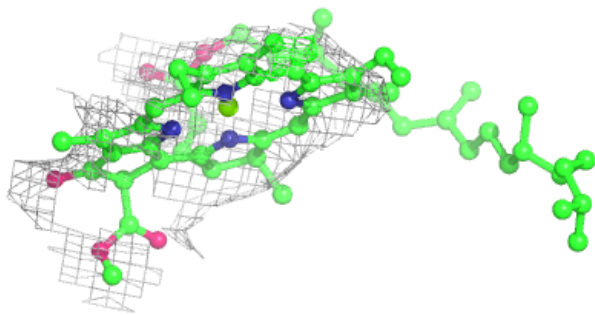
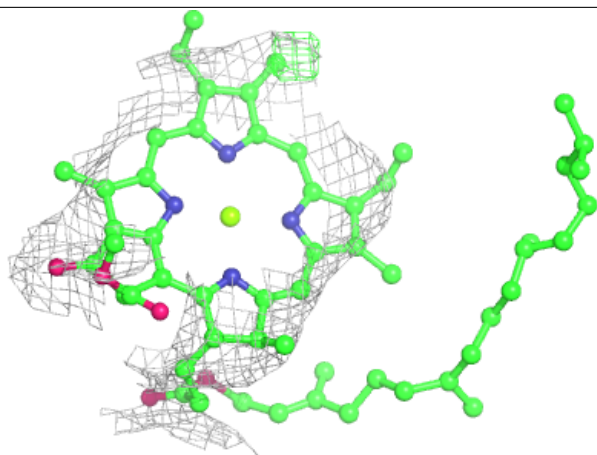
Electron density around CLA k 1402:

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



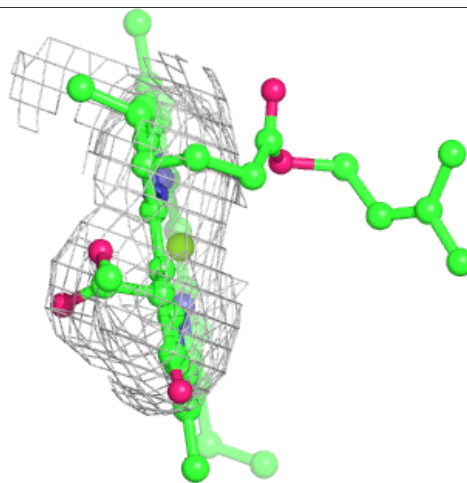
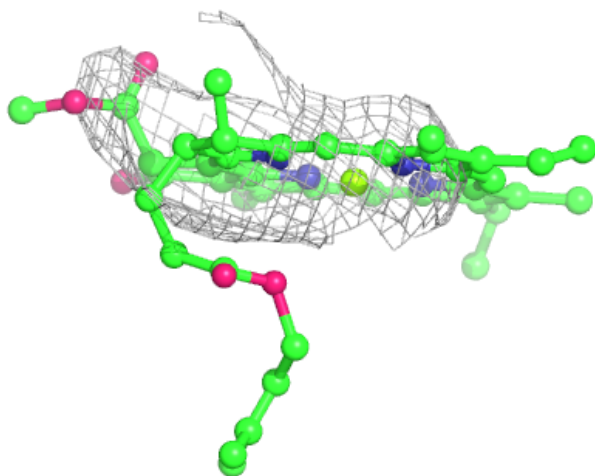
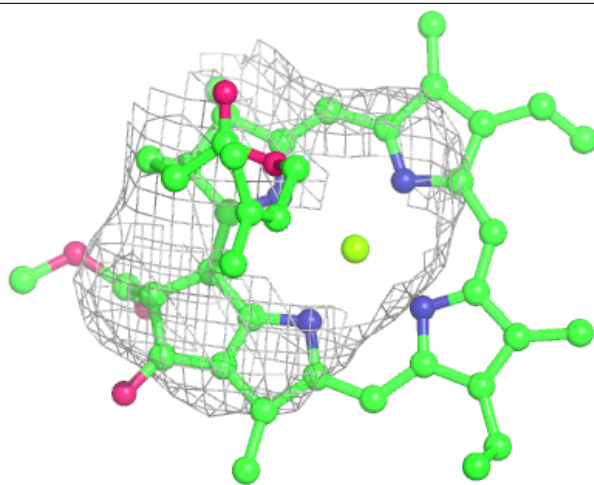
Electron density around CLA 0 1401:

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



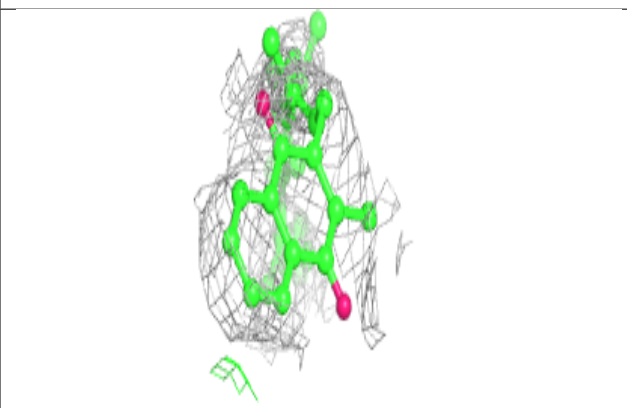
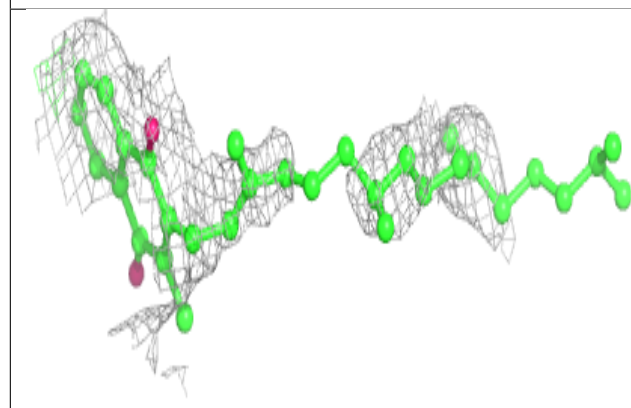
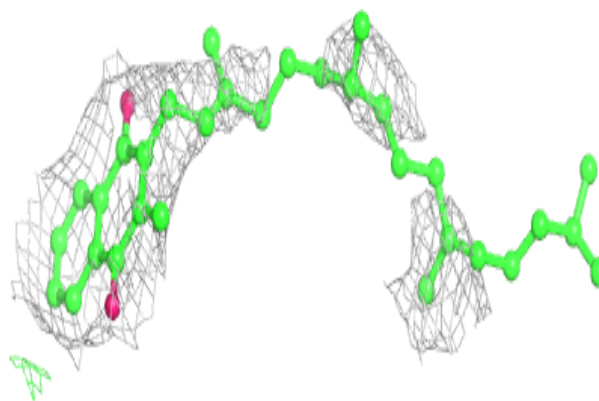
Electron density around CLA 0 1402:

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

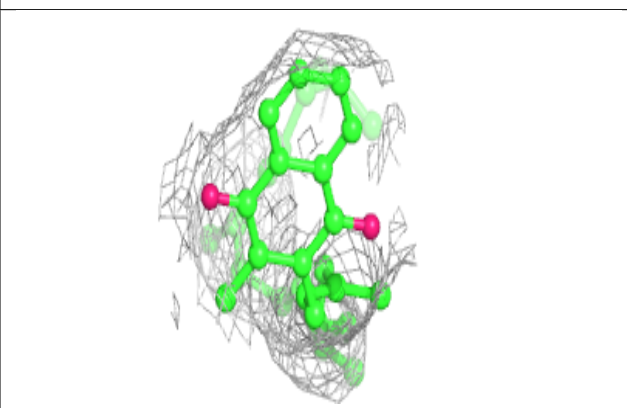
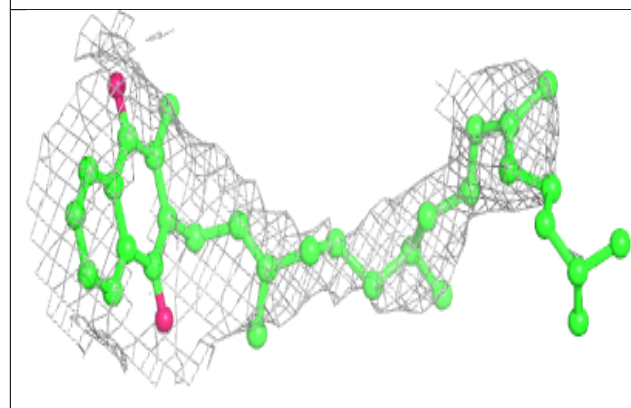
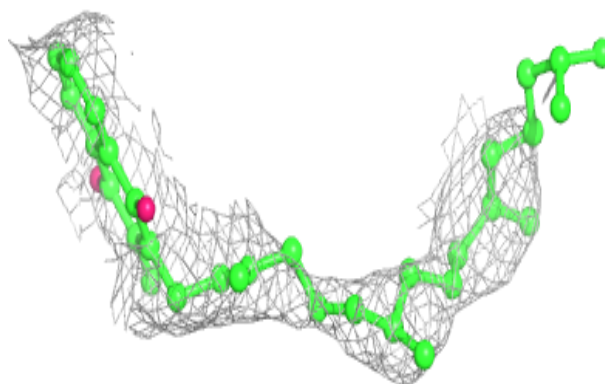


Electron density around PQN A 2001:

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

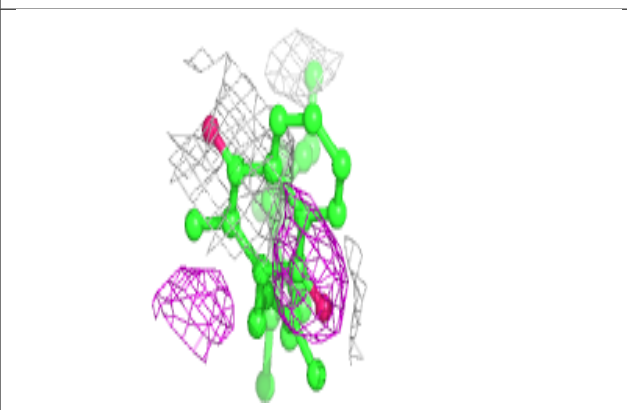
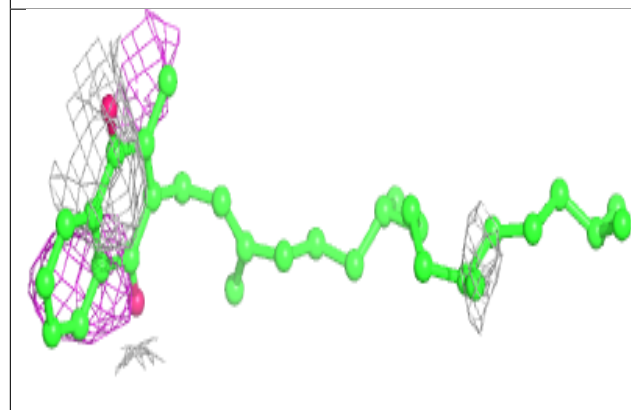
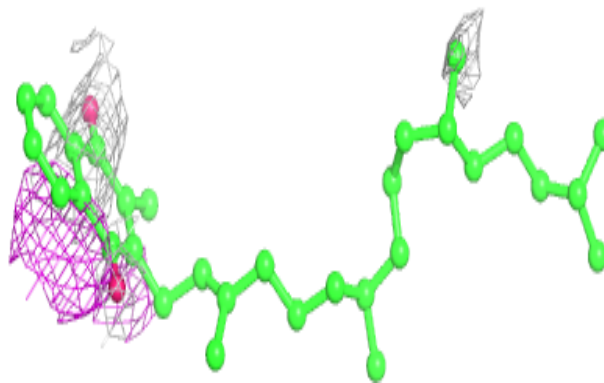
**Electron density around PQN B 2002:**

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

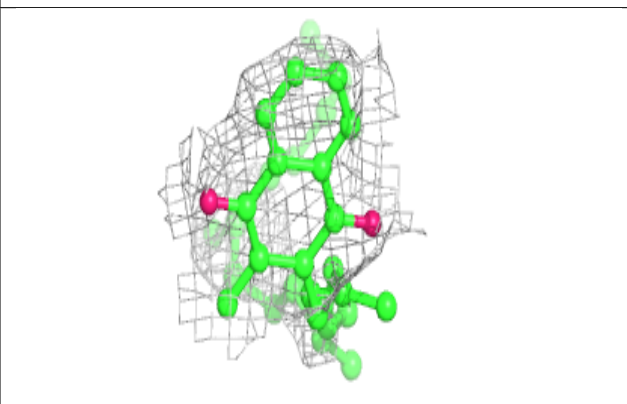
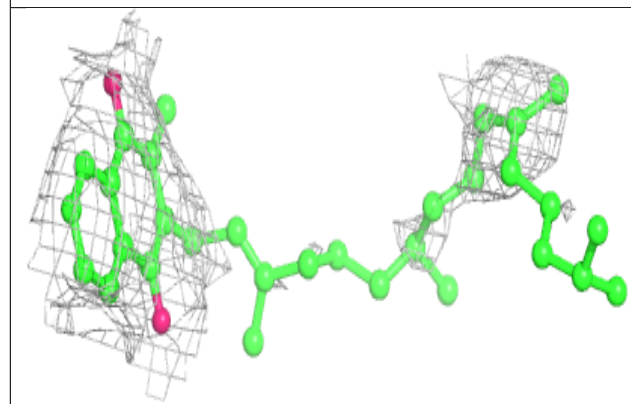
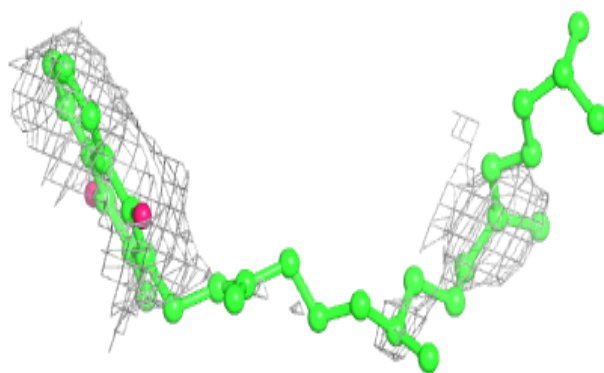


Electron density around PQN a 2001:

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

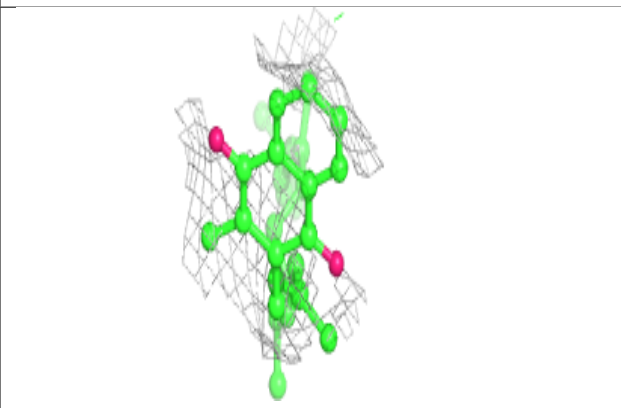
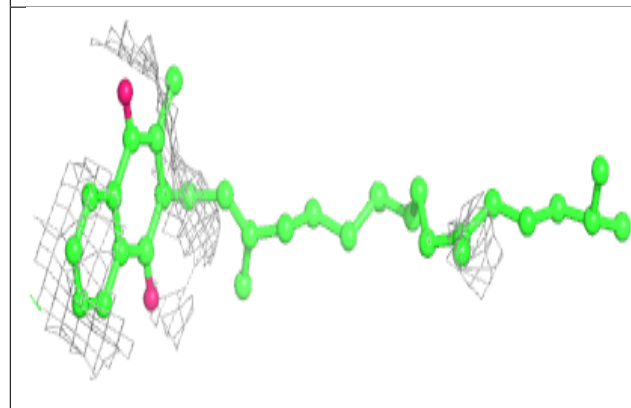
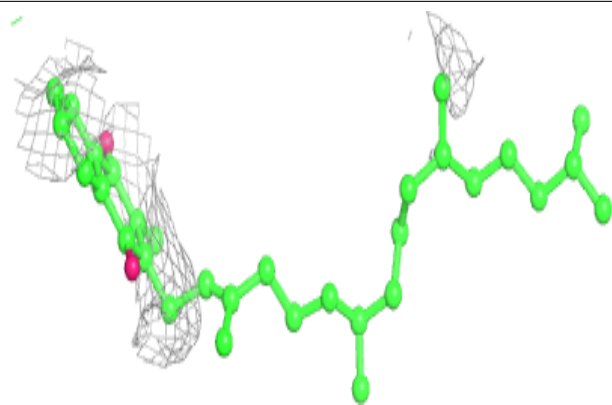
**Electron density around PQN b 2002:**

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

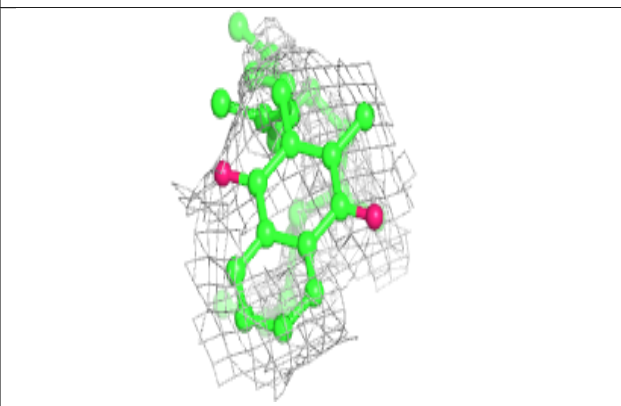
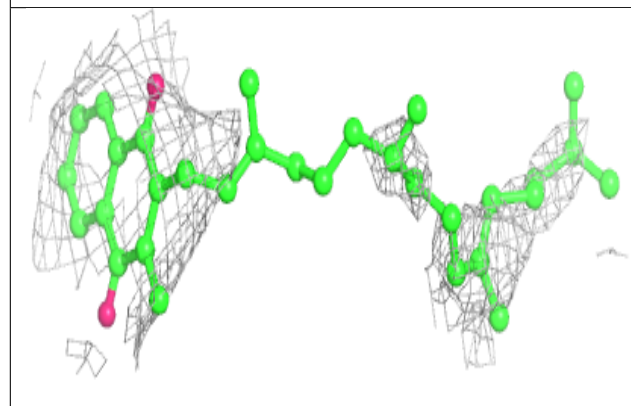
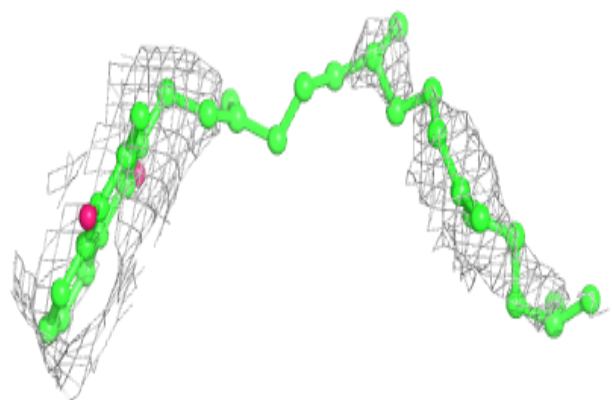


Electron density around PQN 1 2001:

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

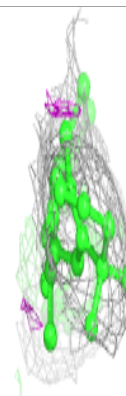
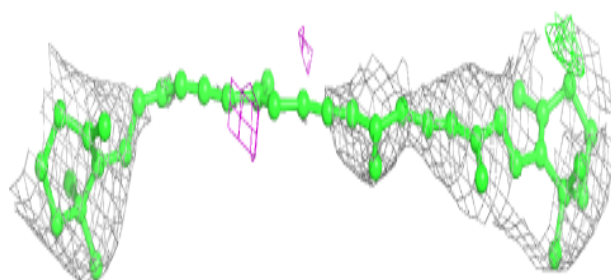
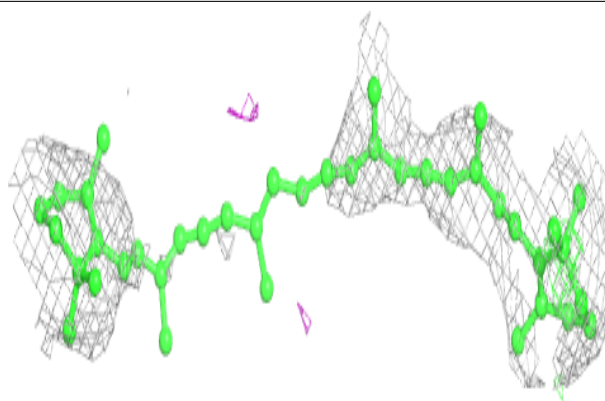
**Electron density around PQN 2 2002:**

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

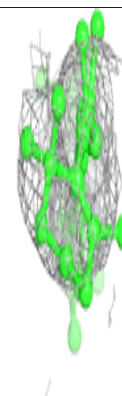
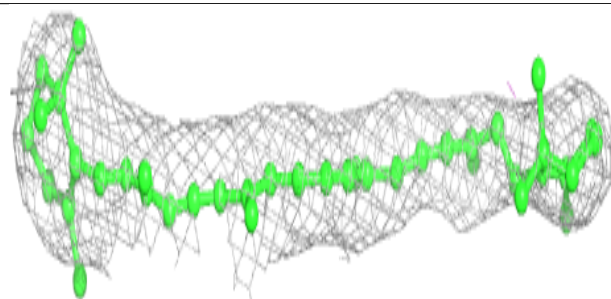
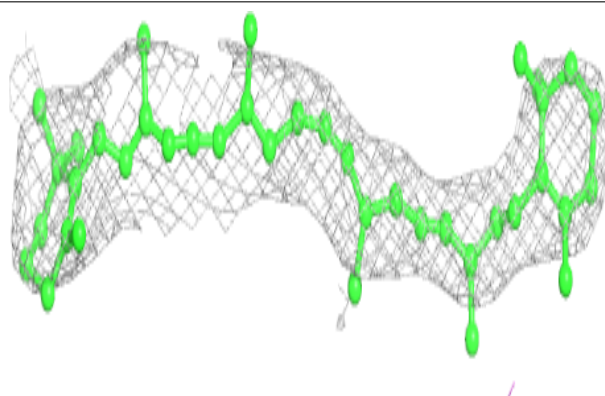


Electron density around BCR A 4001:

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

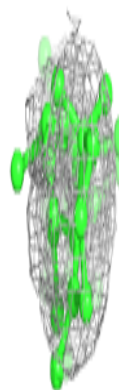
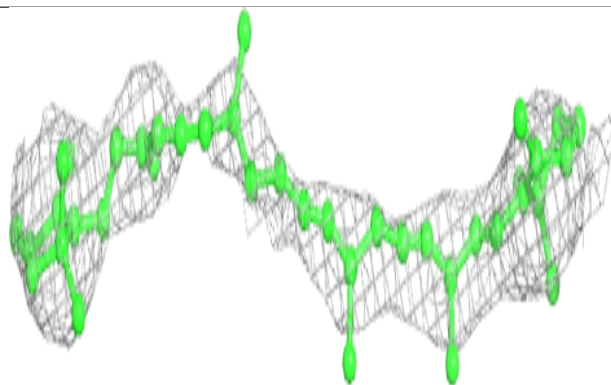
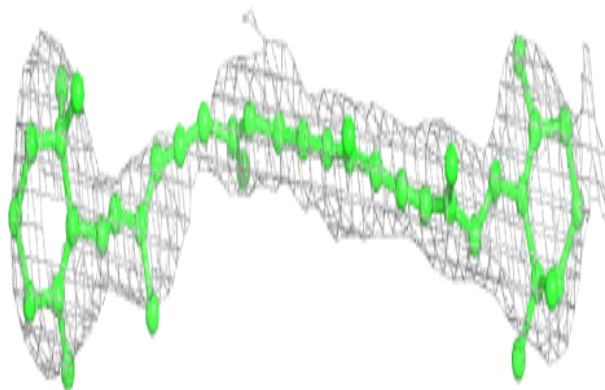
**Electron density around BCR A 4002:**

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

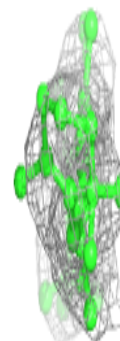
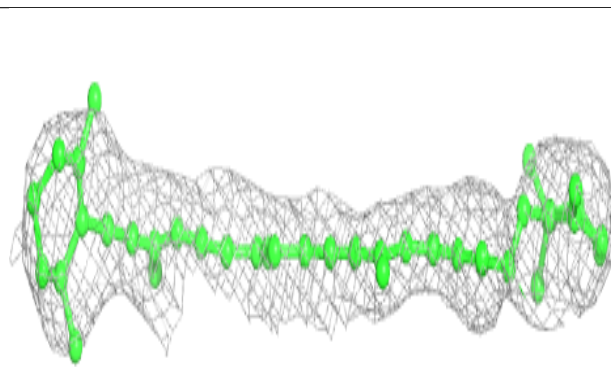
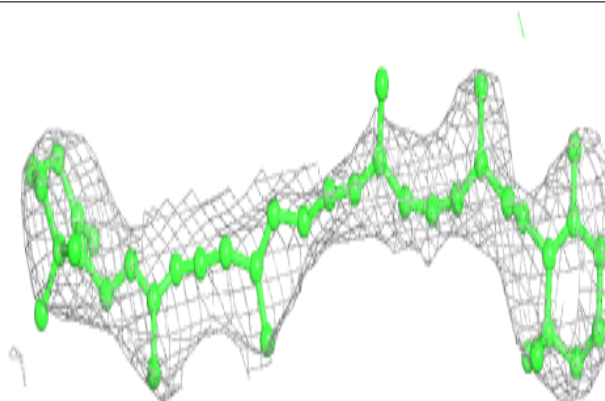


Electron density around BCR A 4003:

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

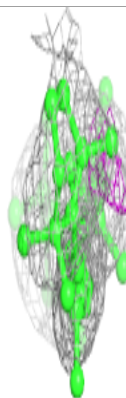
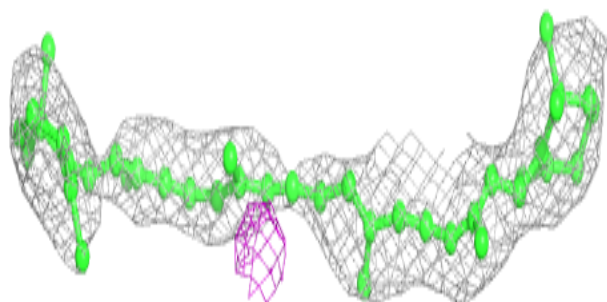
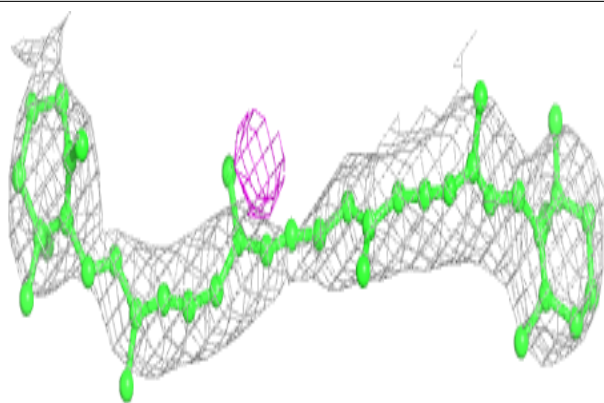
**Electron density around BCR A 4007:**

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

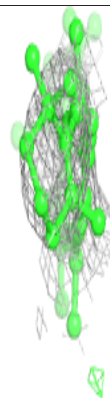
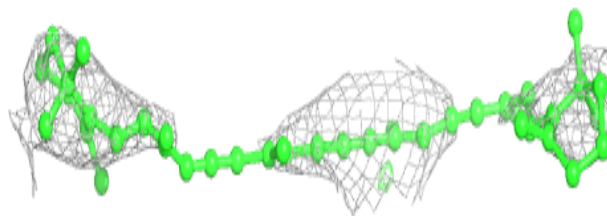
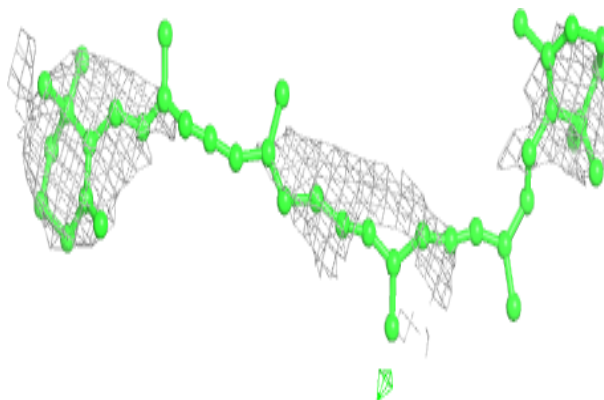


Electron density around BCR A 4008:

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

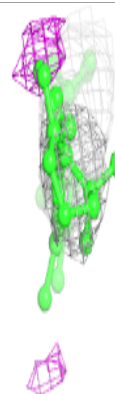
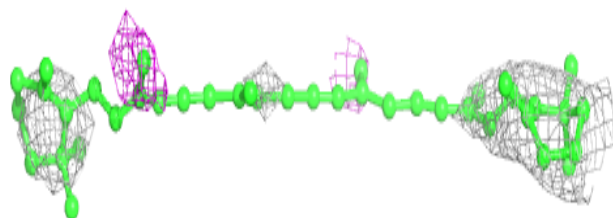
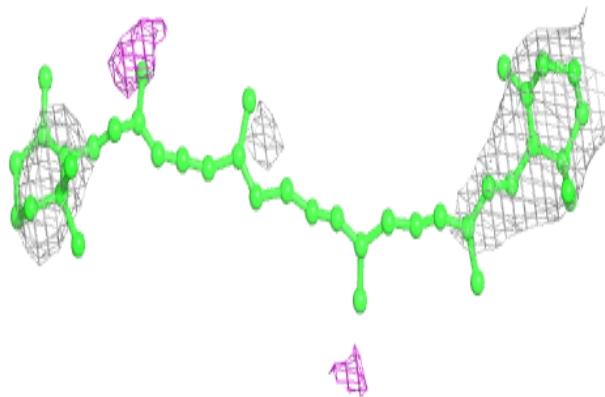
**Electron density around BCR B 4004:**

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

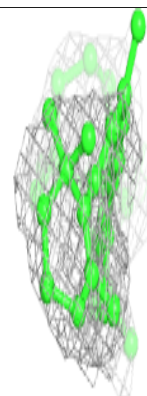
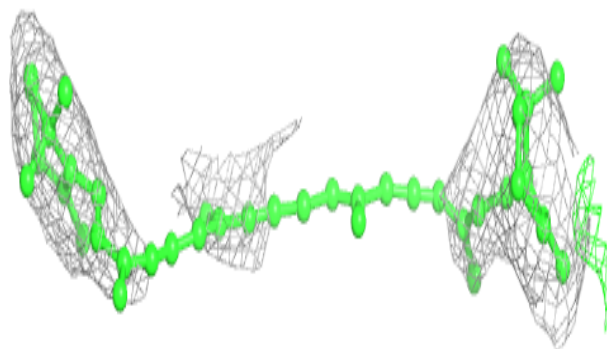
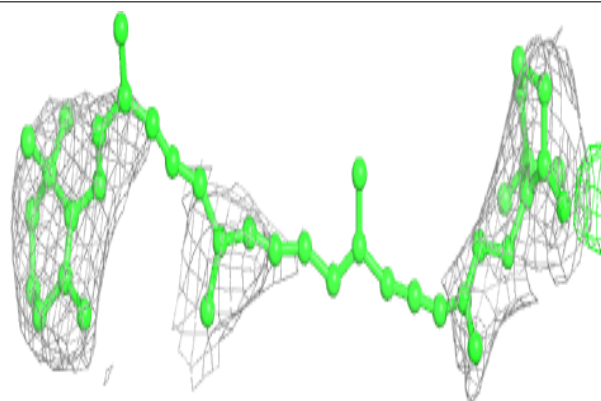


Electron density around BCR B 4005:

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

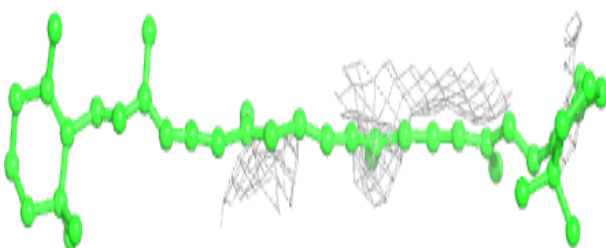
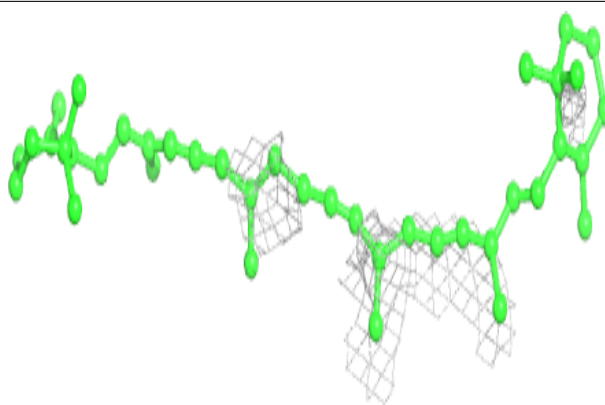
**Electron density around BCR B 4006:**

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

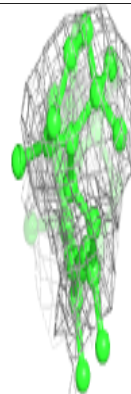
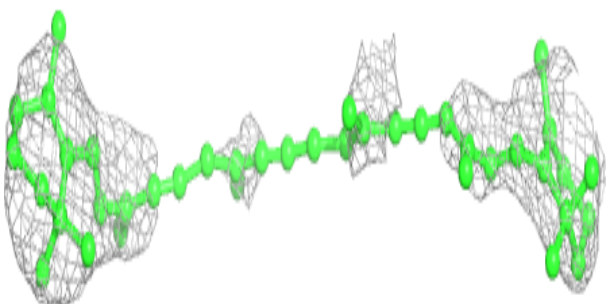
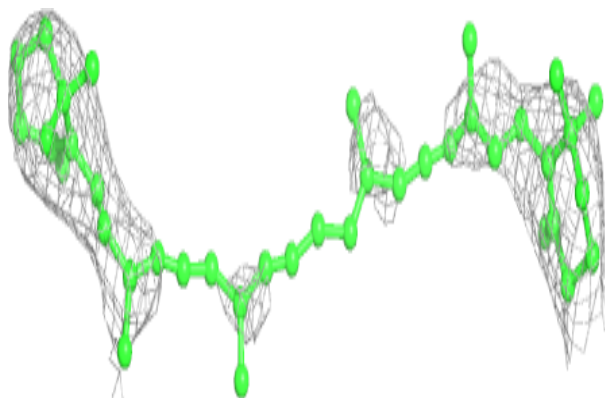


Electron density around BCR B 4009:

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

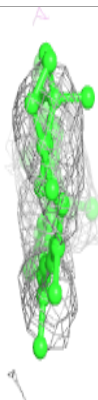
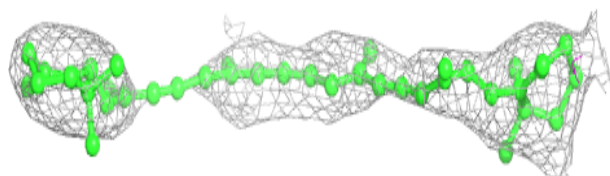
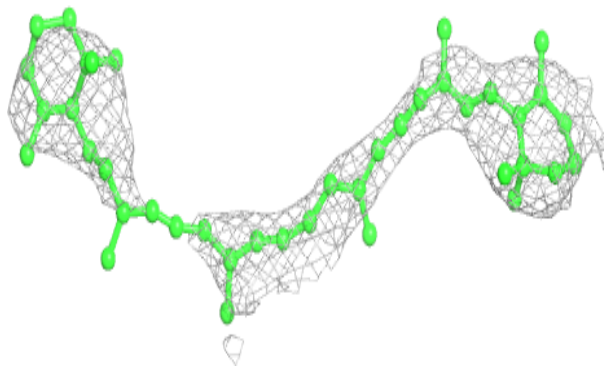
**Electron density around BCR B 4010:**

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

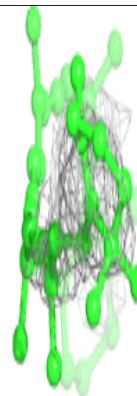
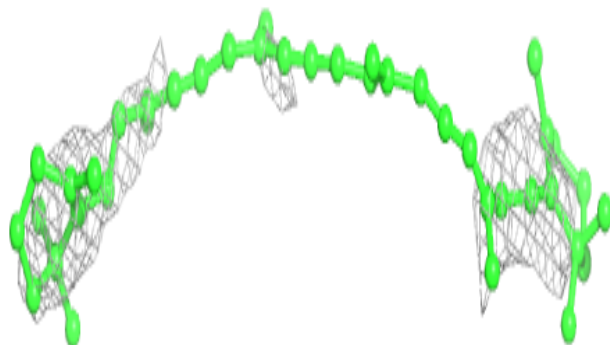
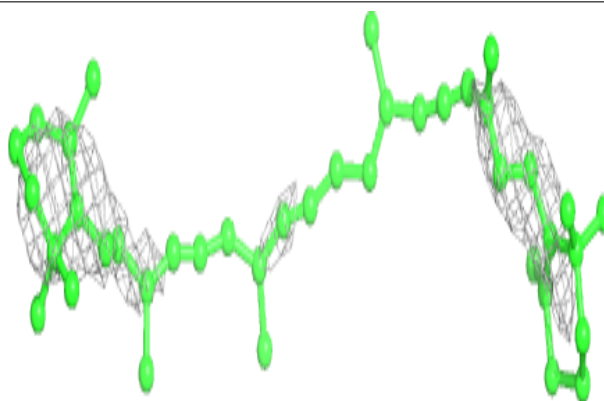


Electron density around BCR B 4011:

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

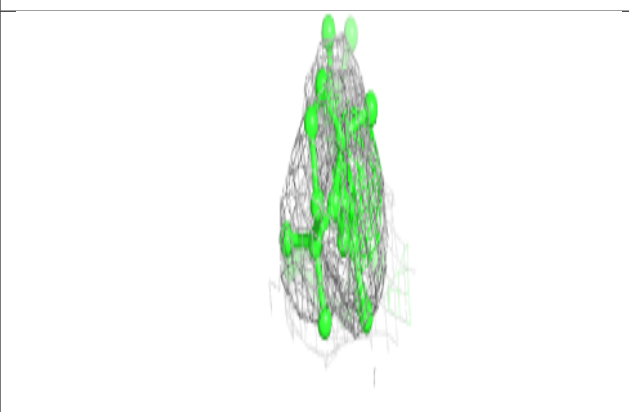
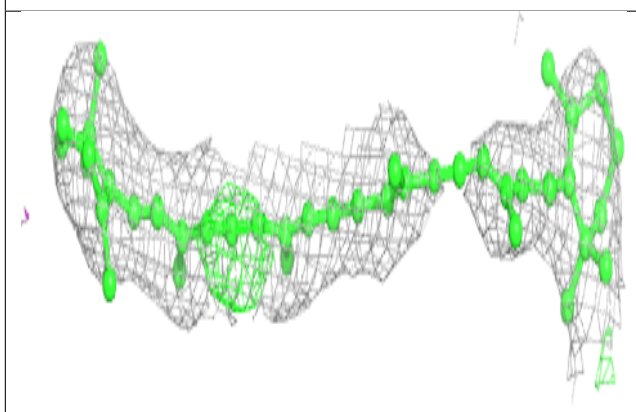
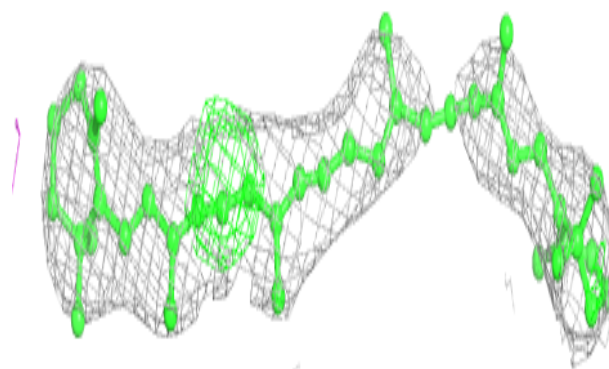
**Electron density around BCR B 4014:**

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

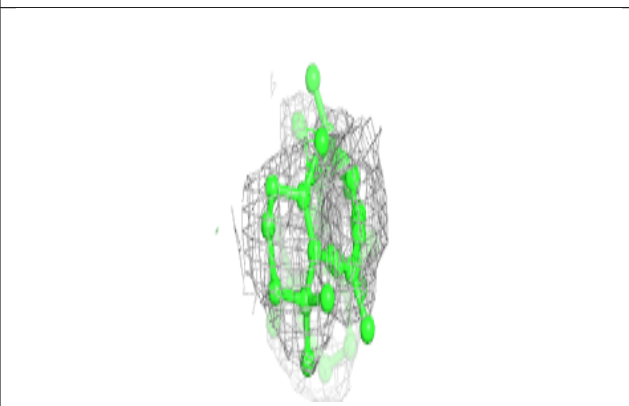
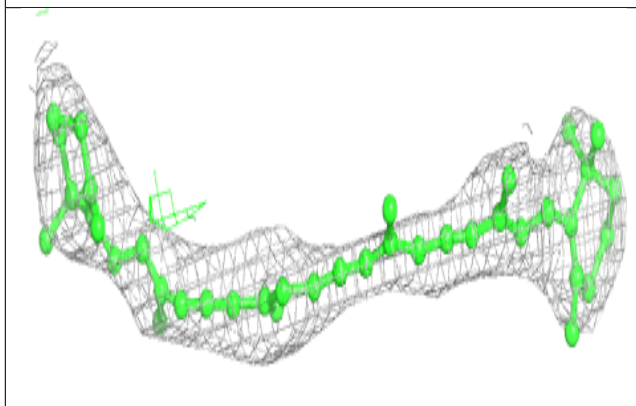
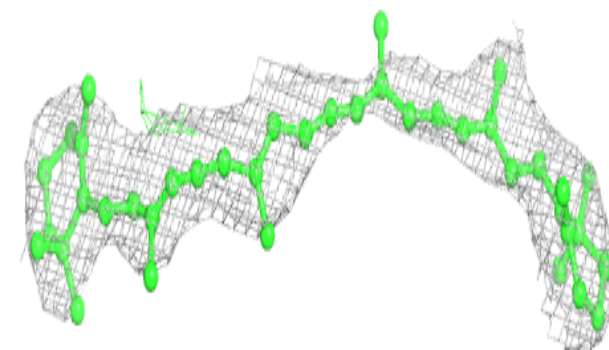


Electron density around BCR B 4017:

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

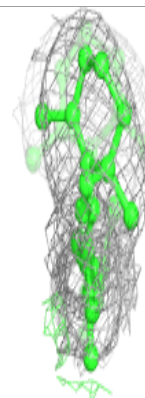
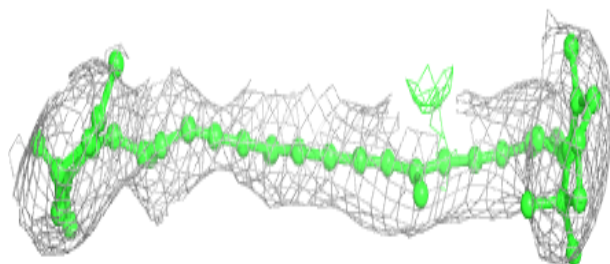
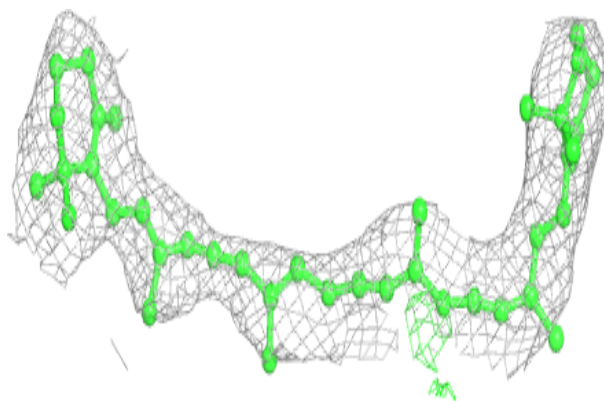
**Electron density around BCR F 4018:**

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

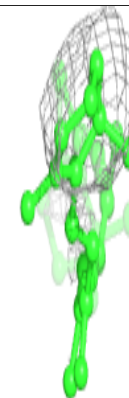
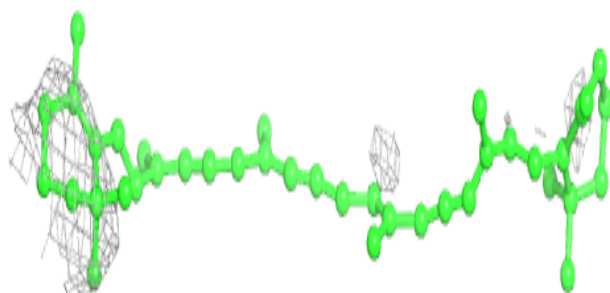
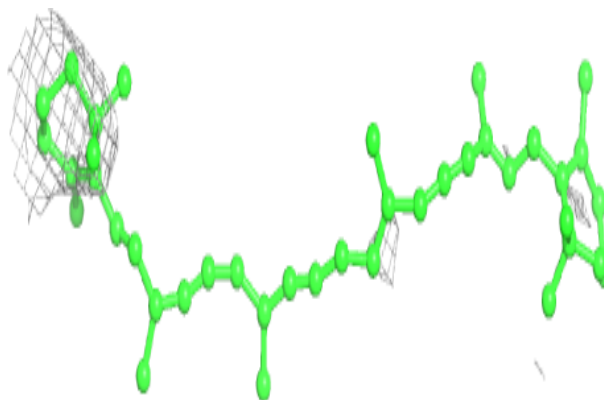


Electron density around BCR F 4020:

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

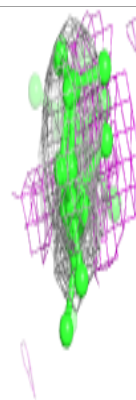
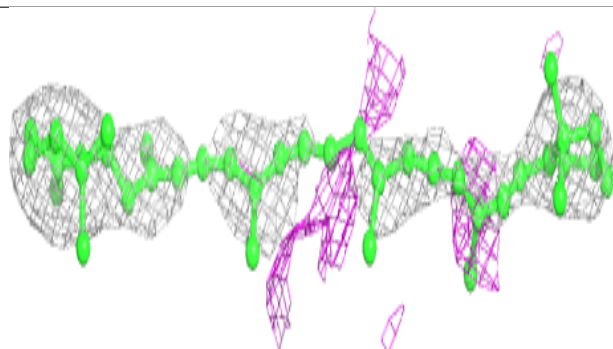
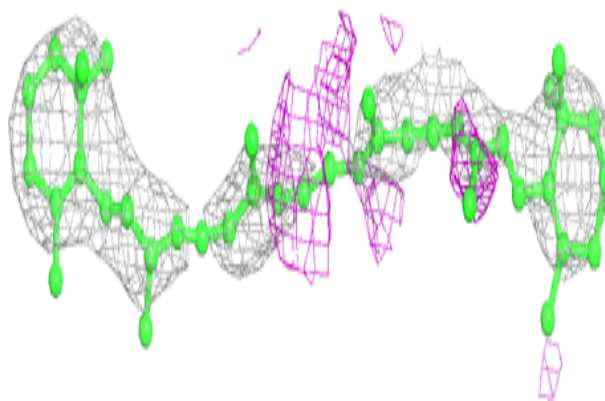
**Electron density around BCR F 4013:**

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

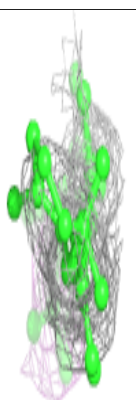
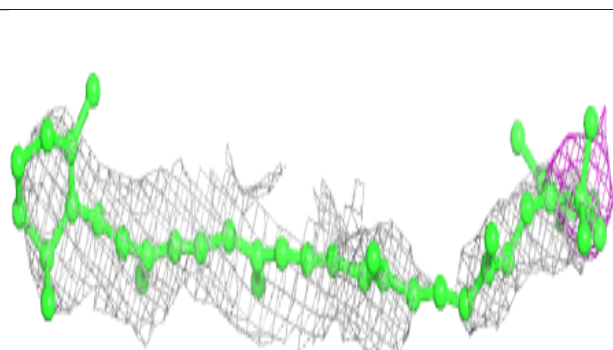
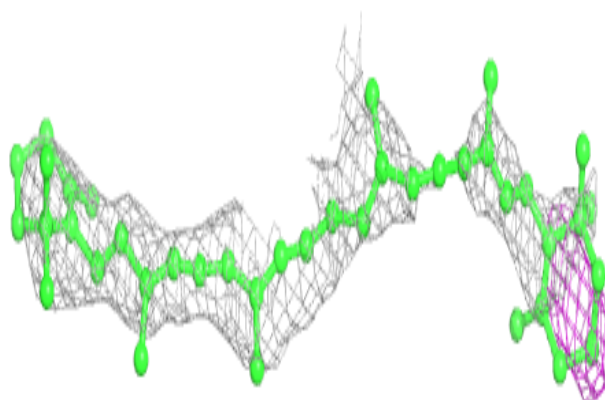


Electron density around BCR L 4019:

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

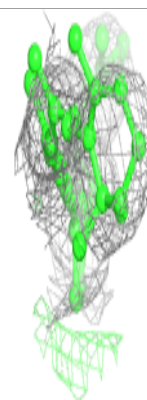
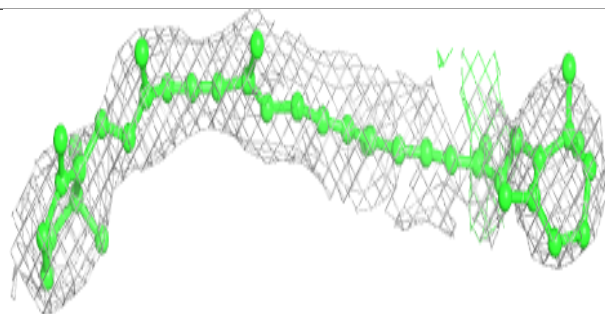
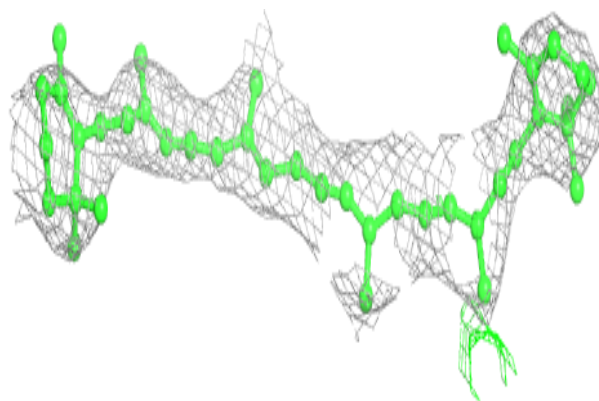
**Electron density around BCR L 4022:**

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

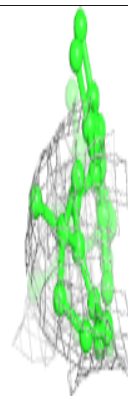
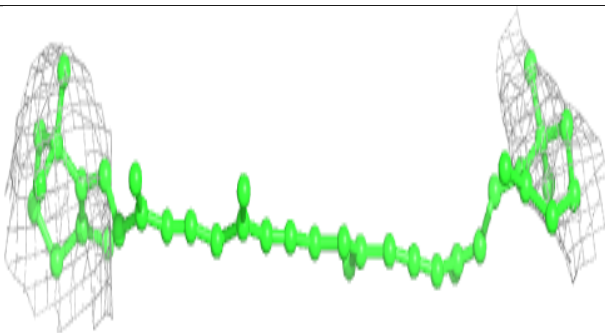
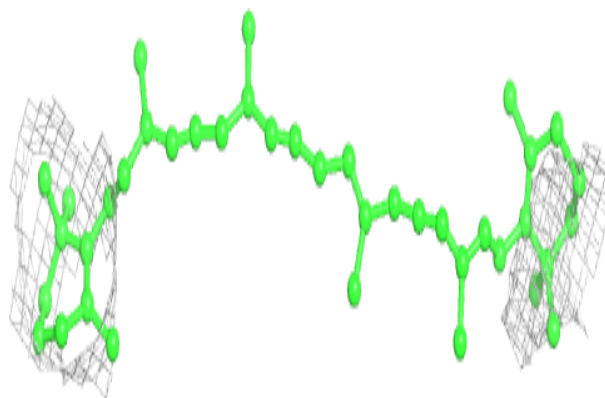


Electron density around BCR M 4021:

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

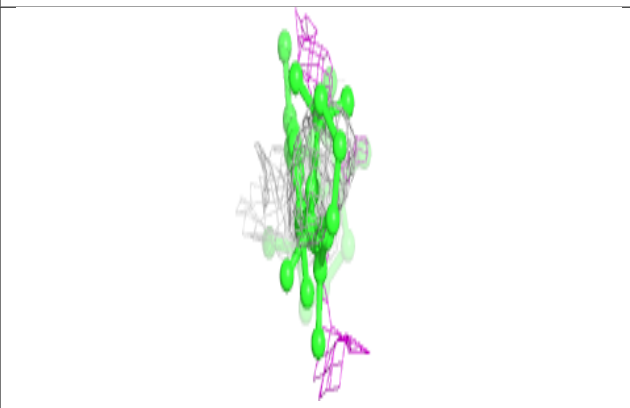
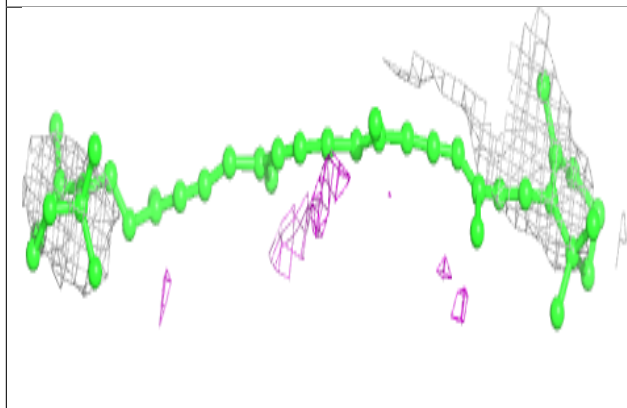
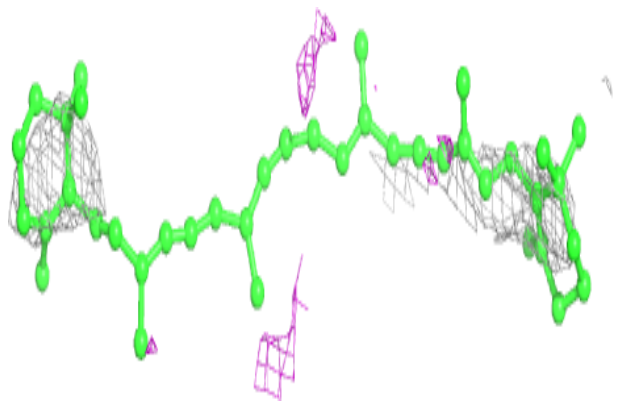
**Electron density around BCR a 4001:**

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

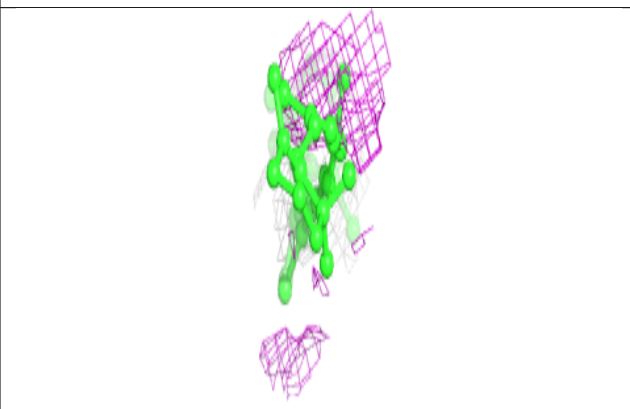
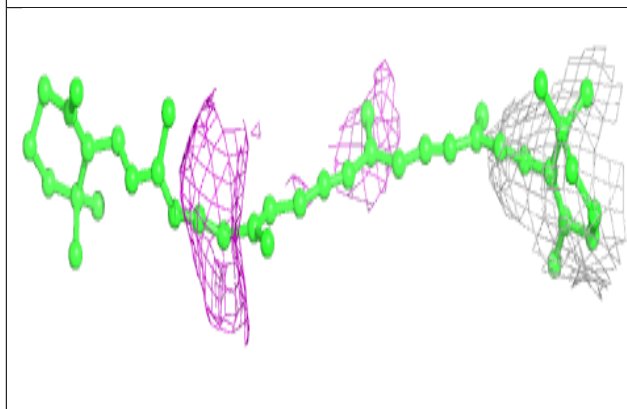
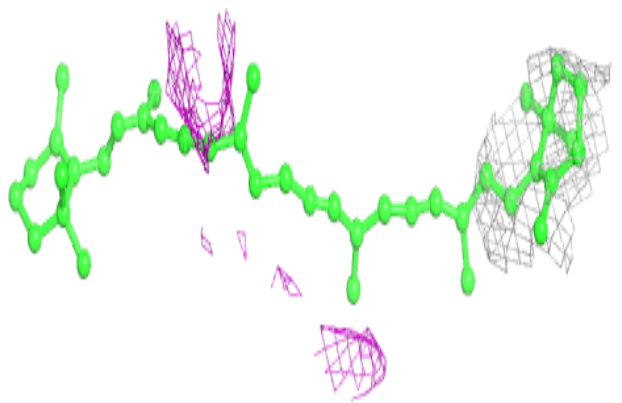


Electron density around BCR a 4002:

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

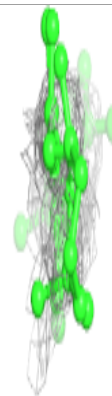
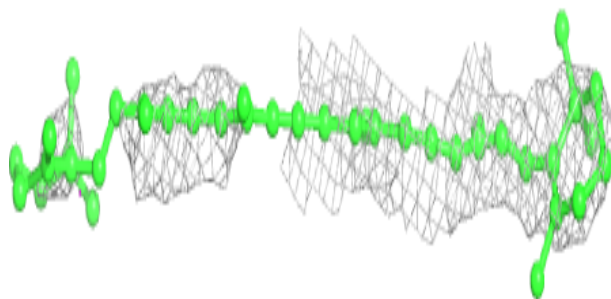
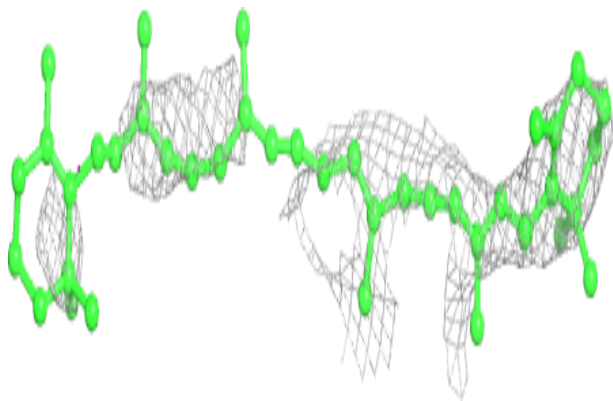
**Electron density around BCR a 4003:**

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

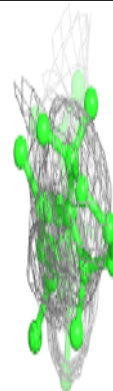
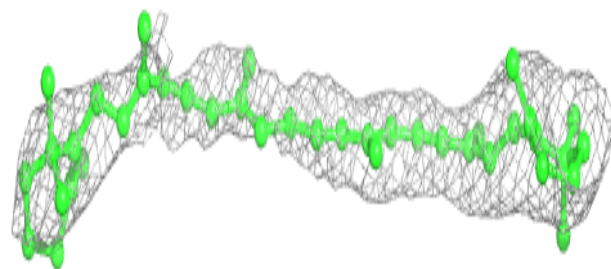
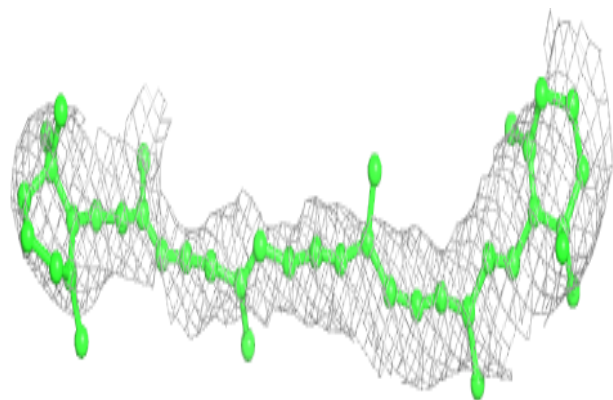


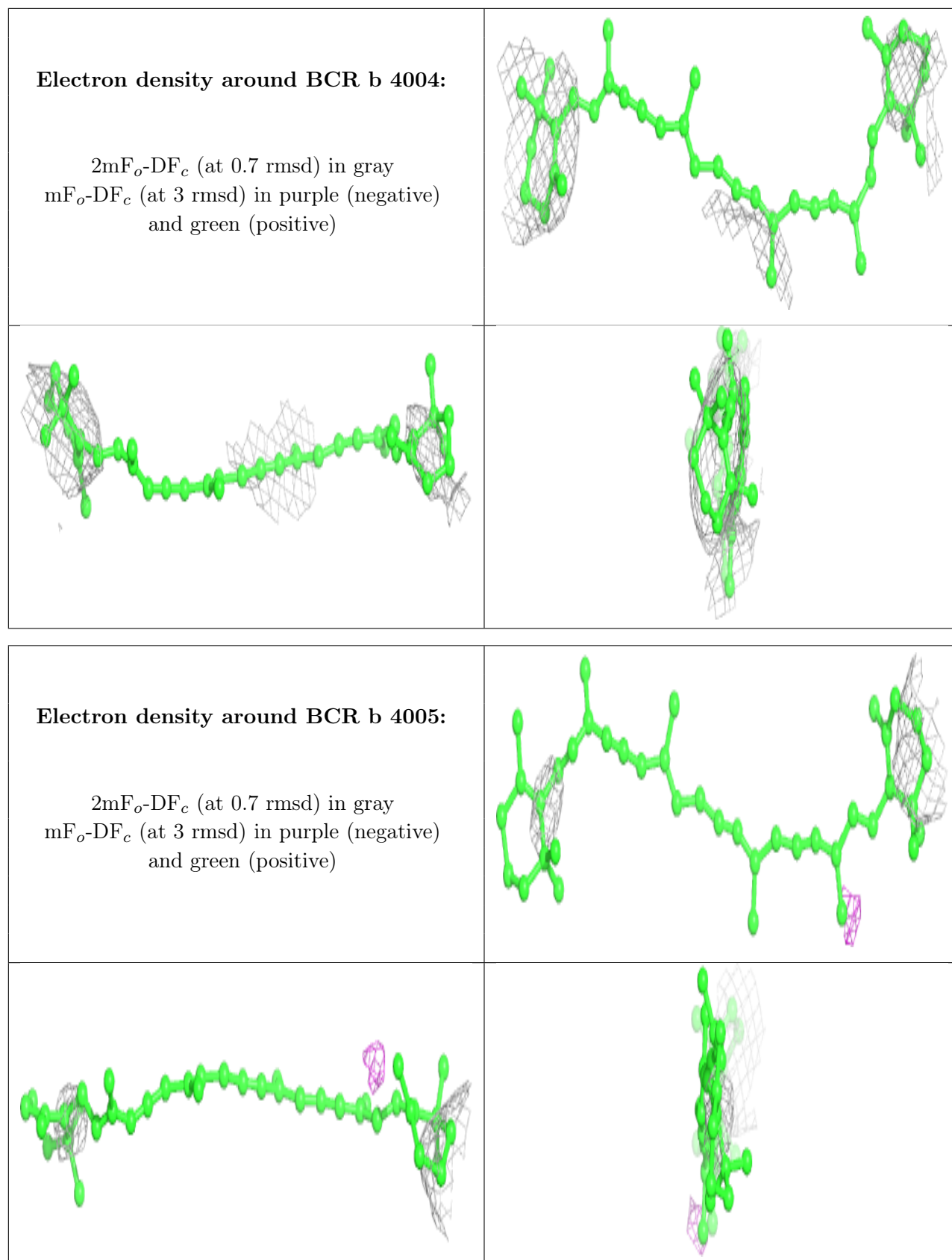
Electron density around BCR a 4007:

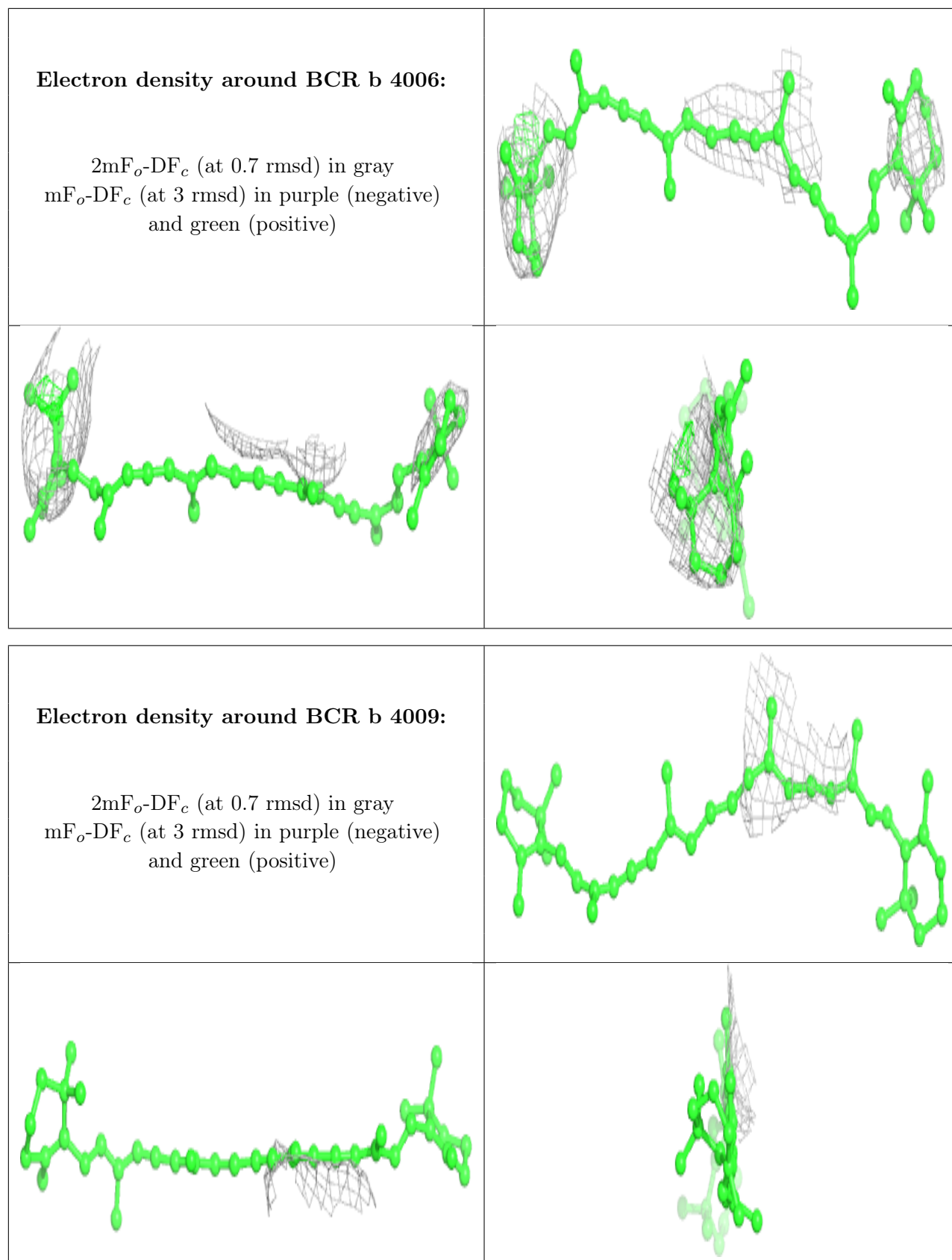
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

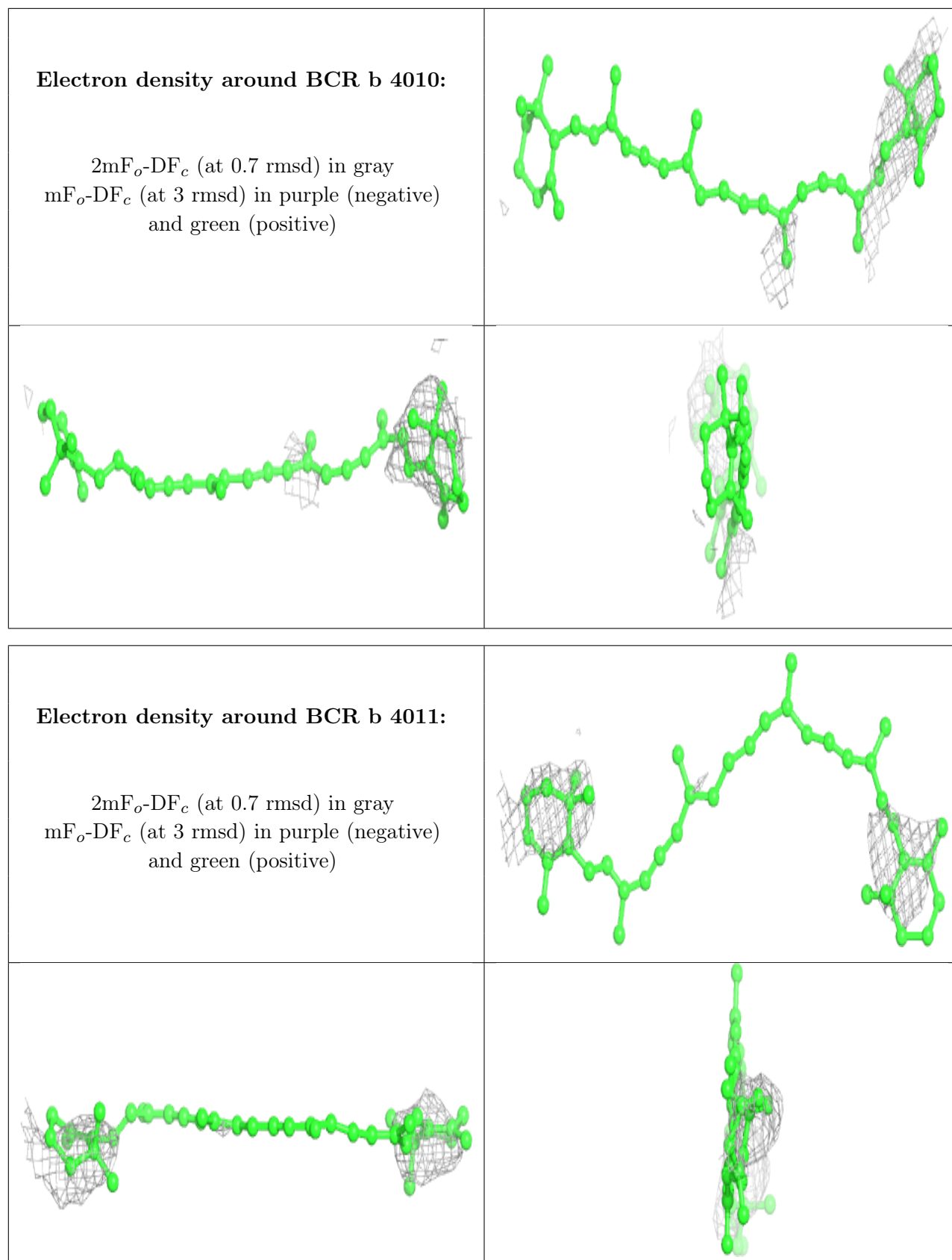
**Electron density around BCR a 4008:**

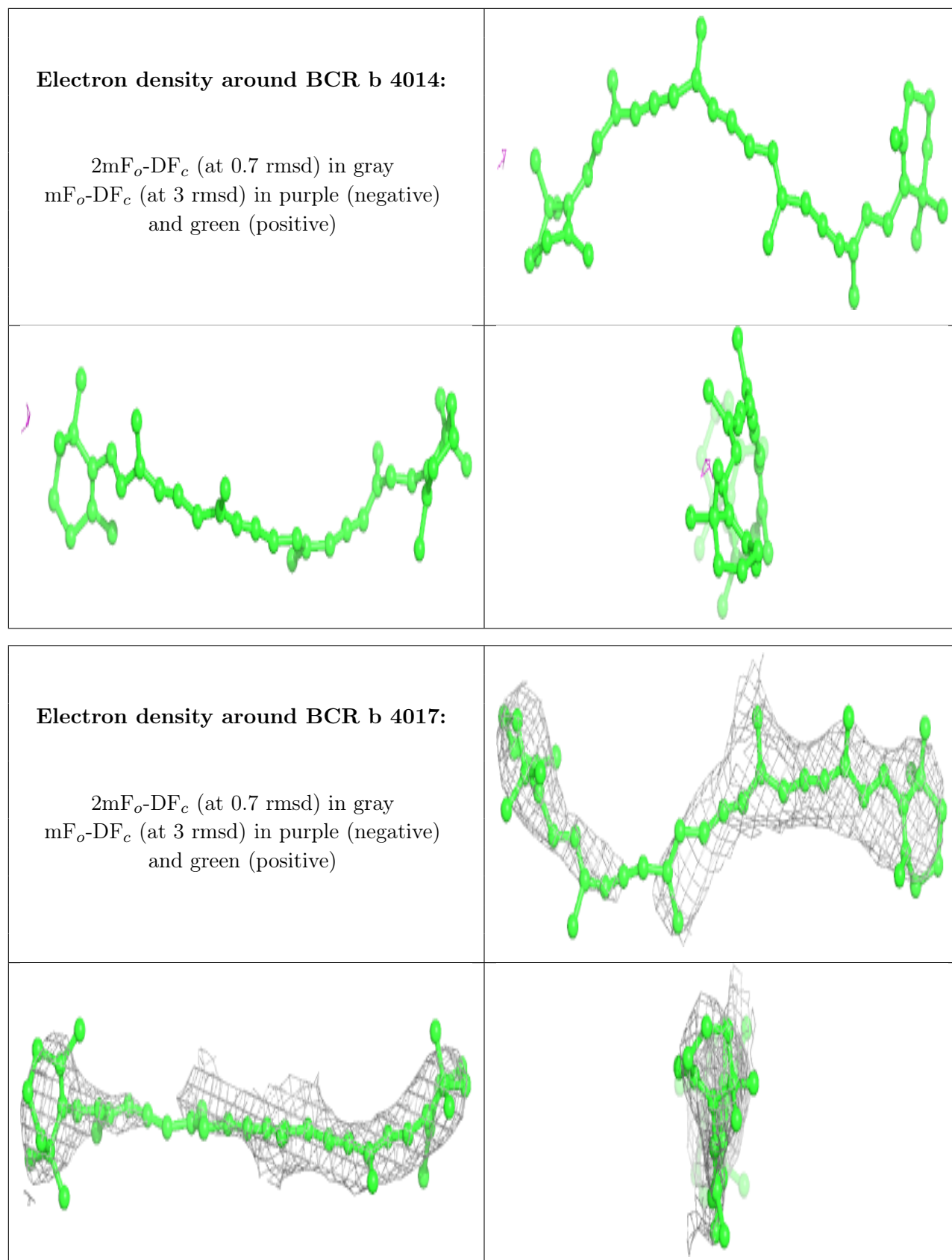
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





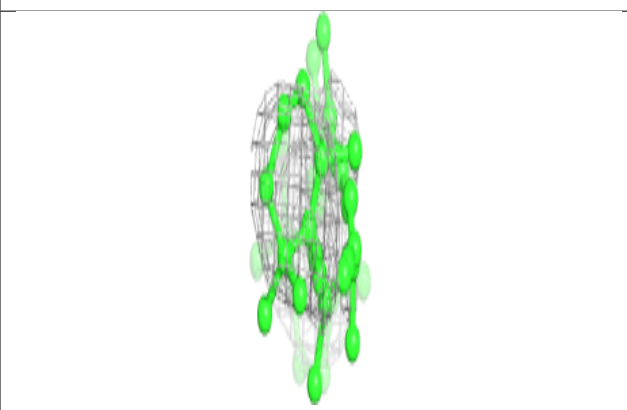
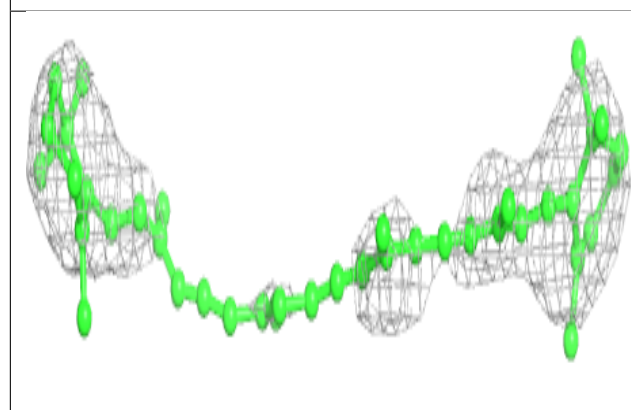
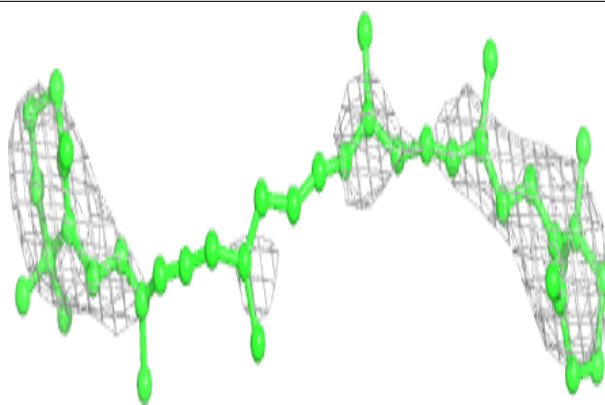




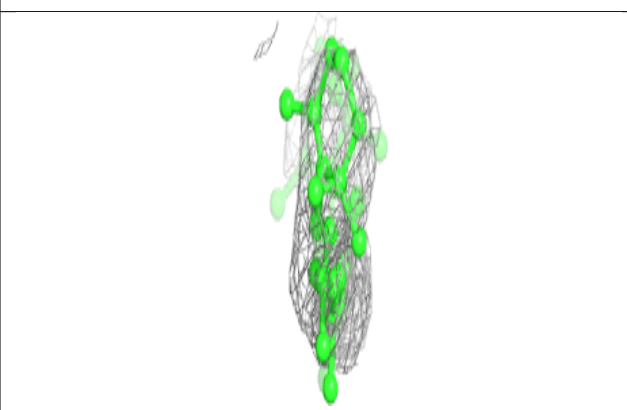
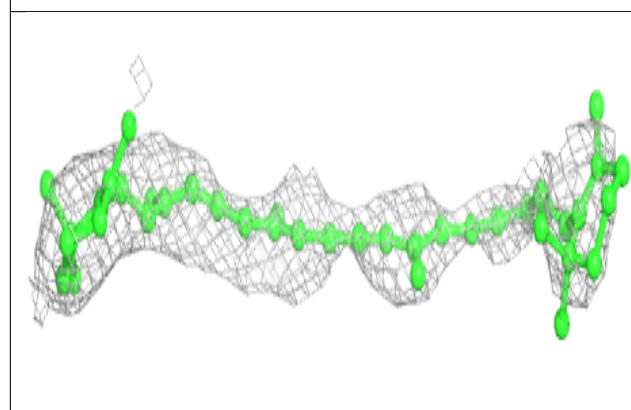
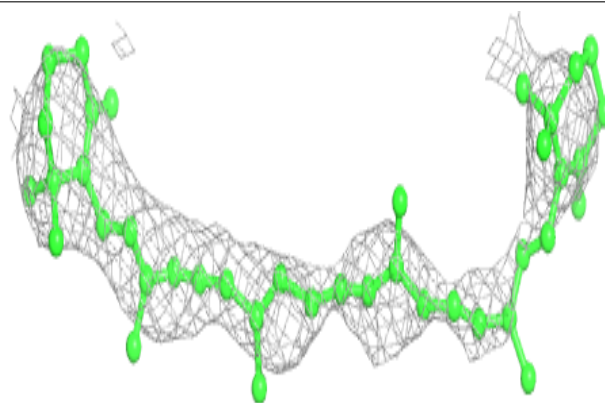


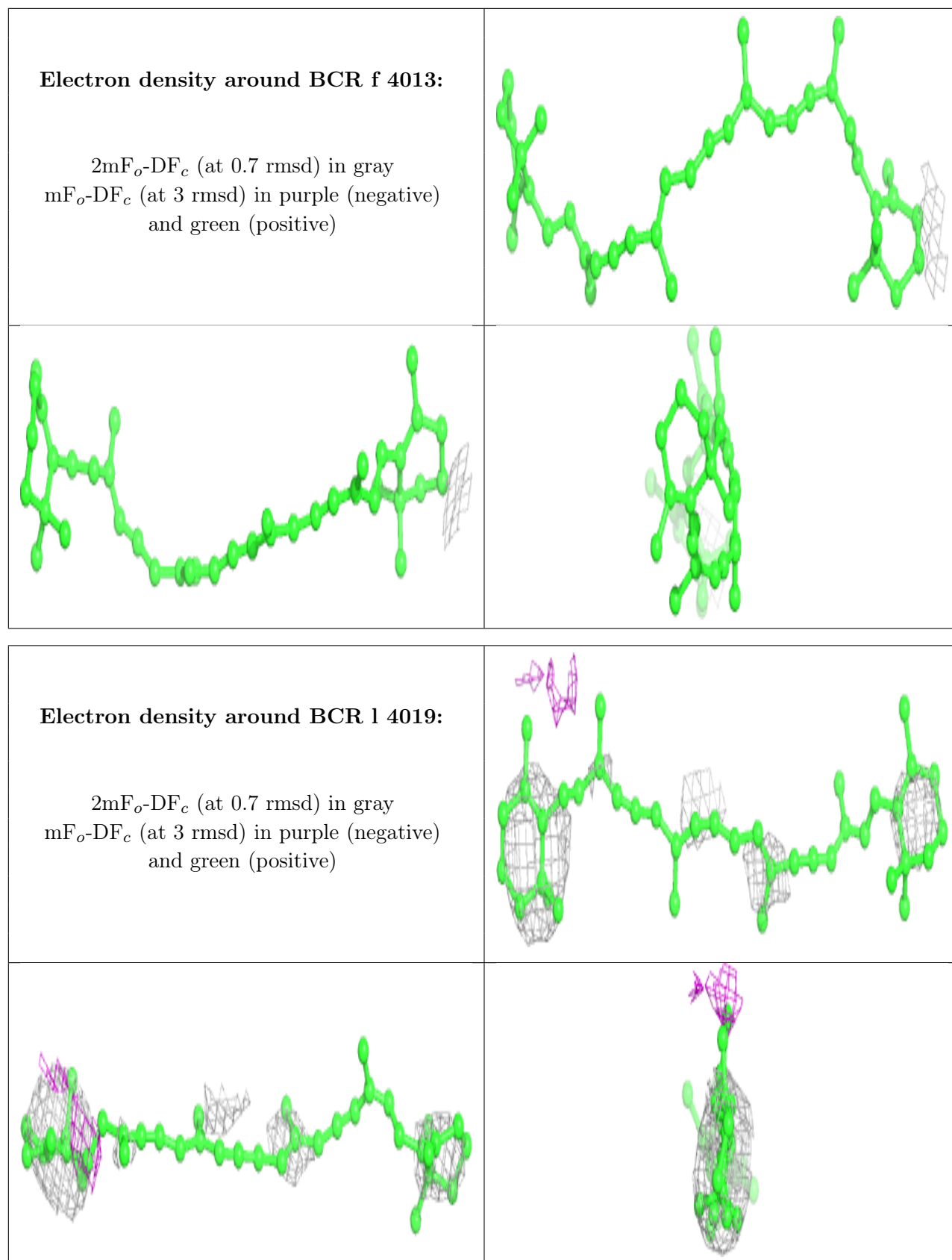
Electron density around BCR f 4018:

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

**Electron density around BCR f 4020:**

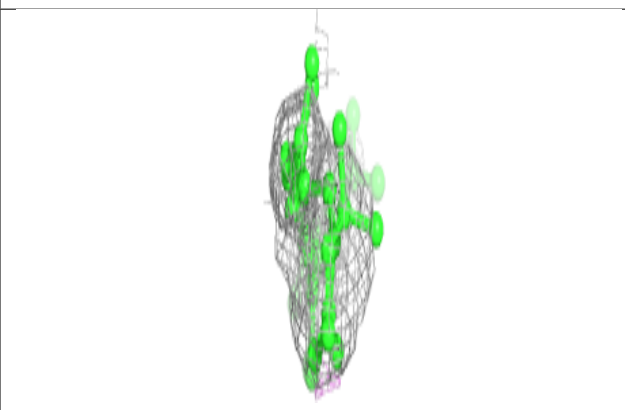
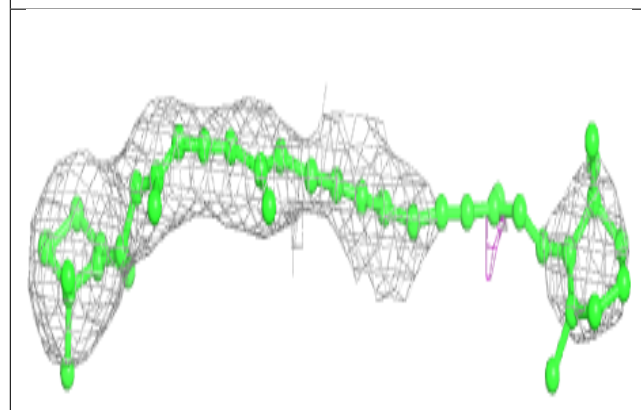
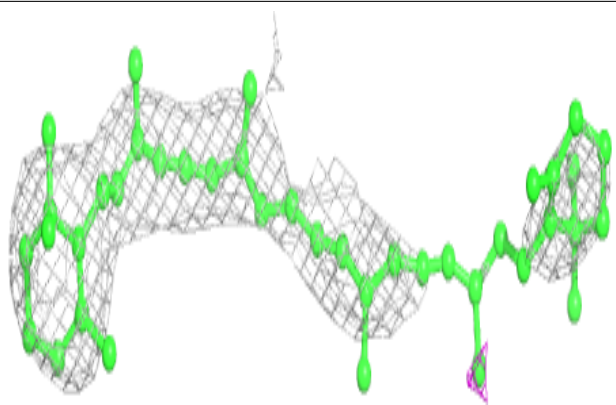
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



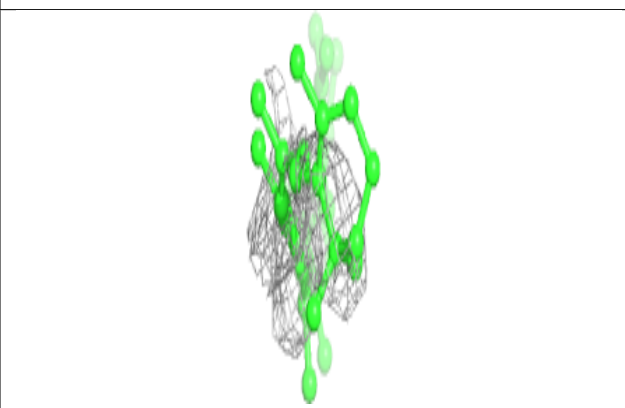
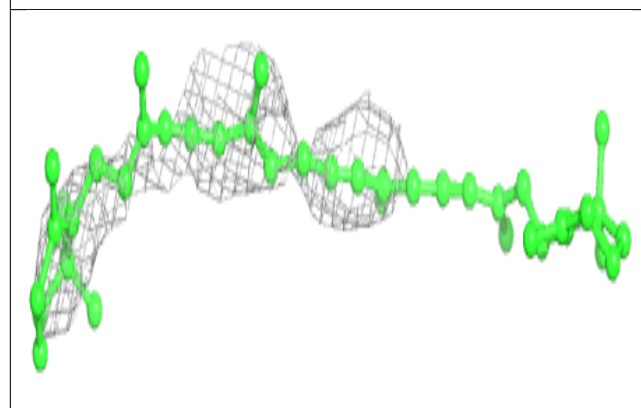
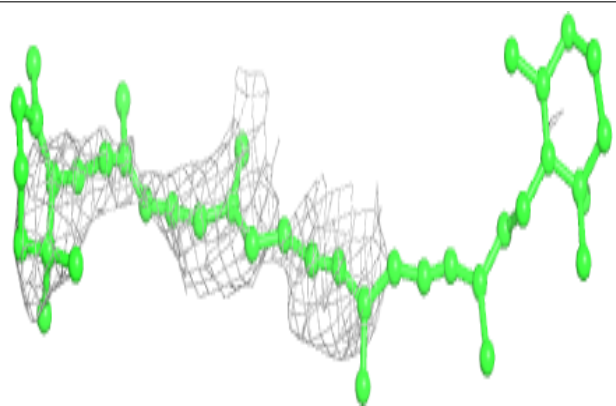


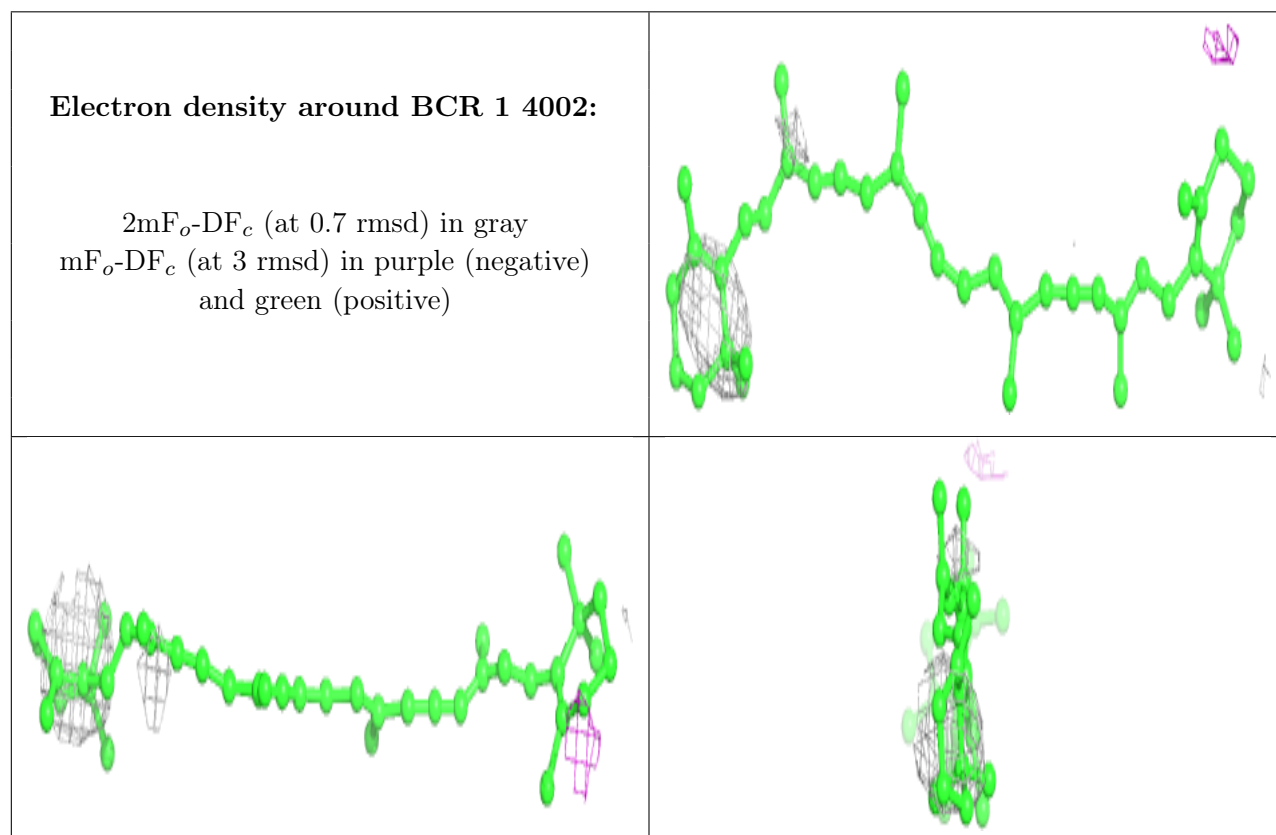
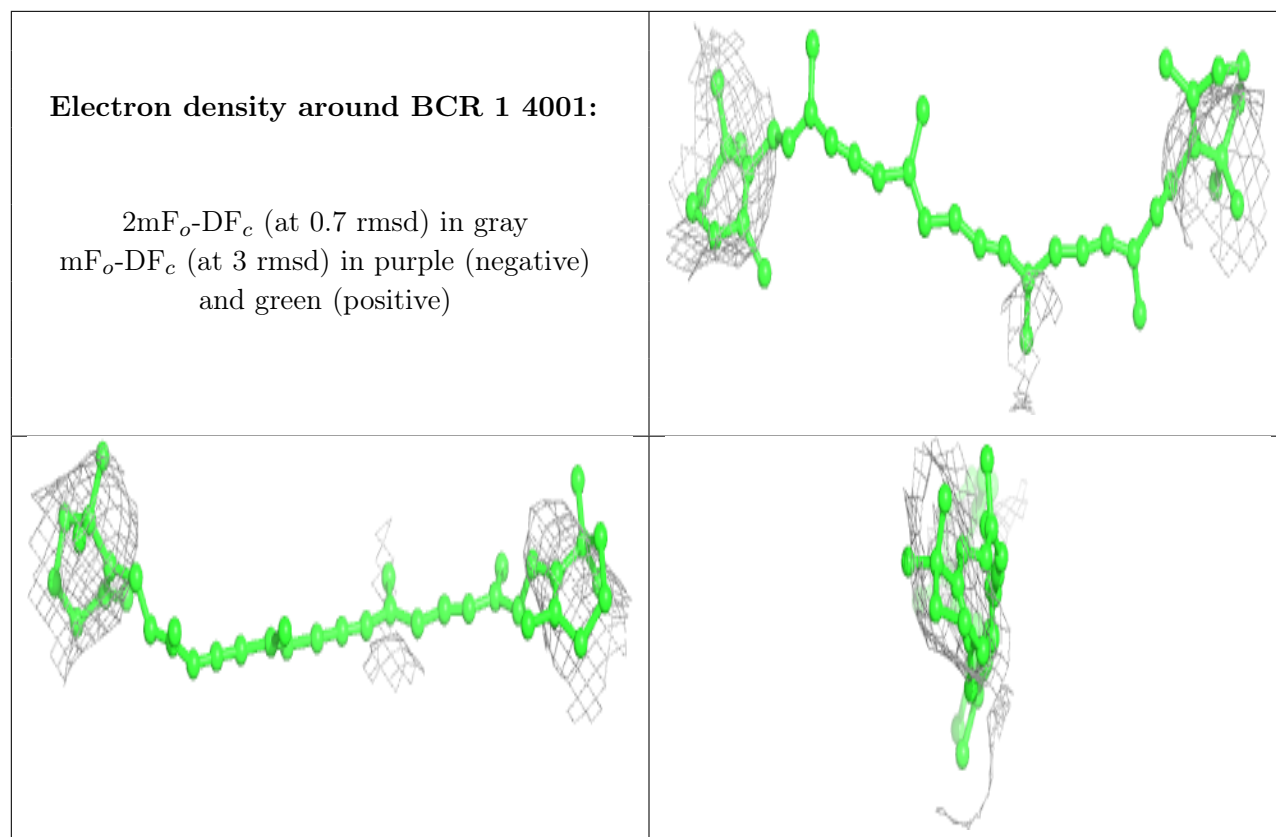
Electron density around BCR 1 4022:

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

**Electron density around BCR m 4021:**

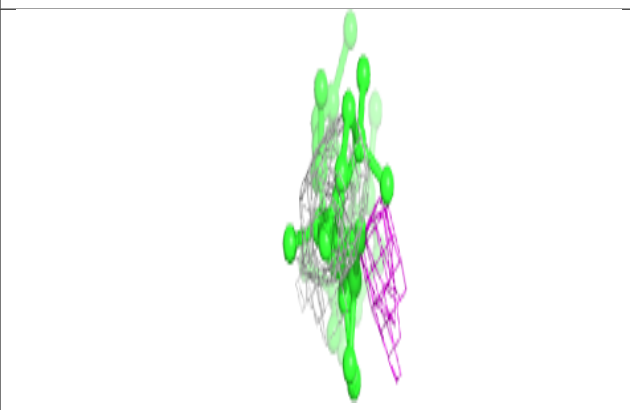
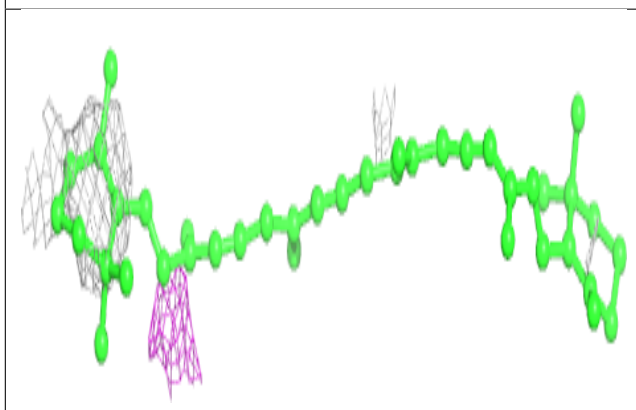
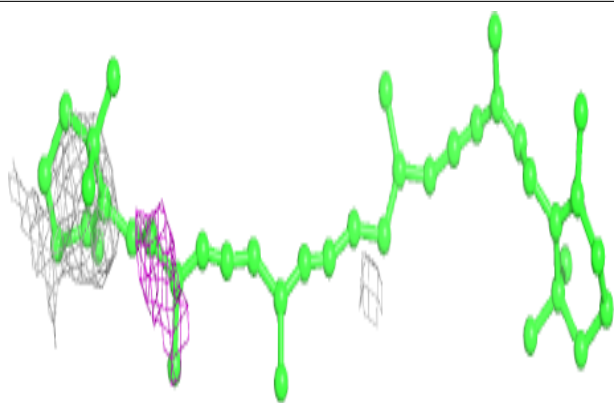
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



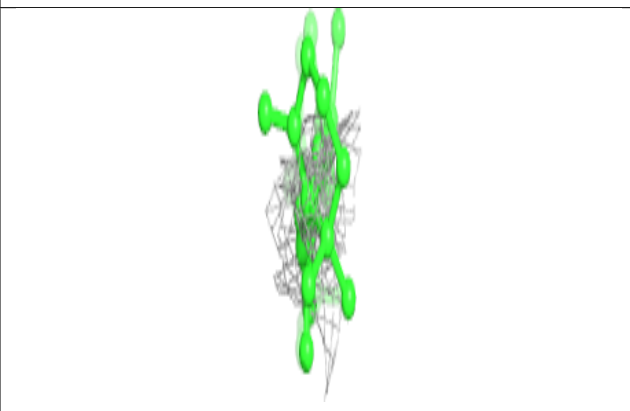
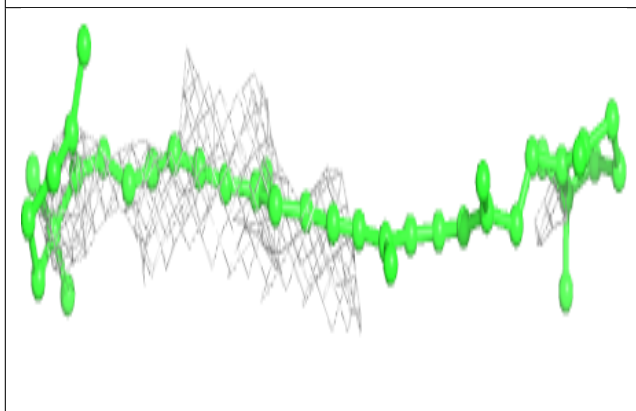
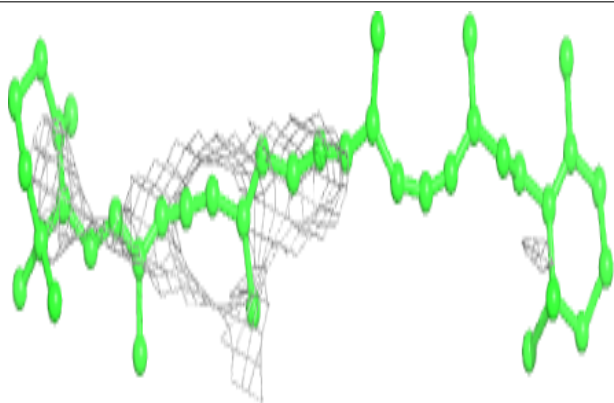


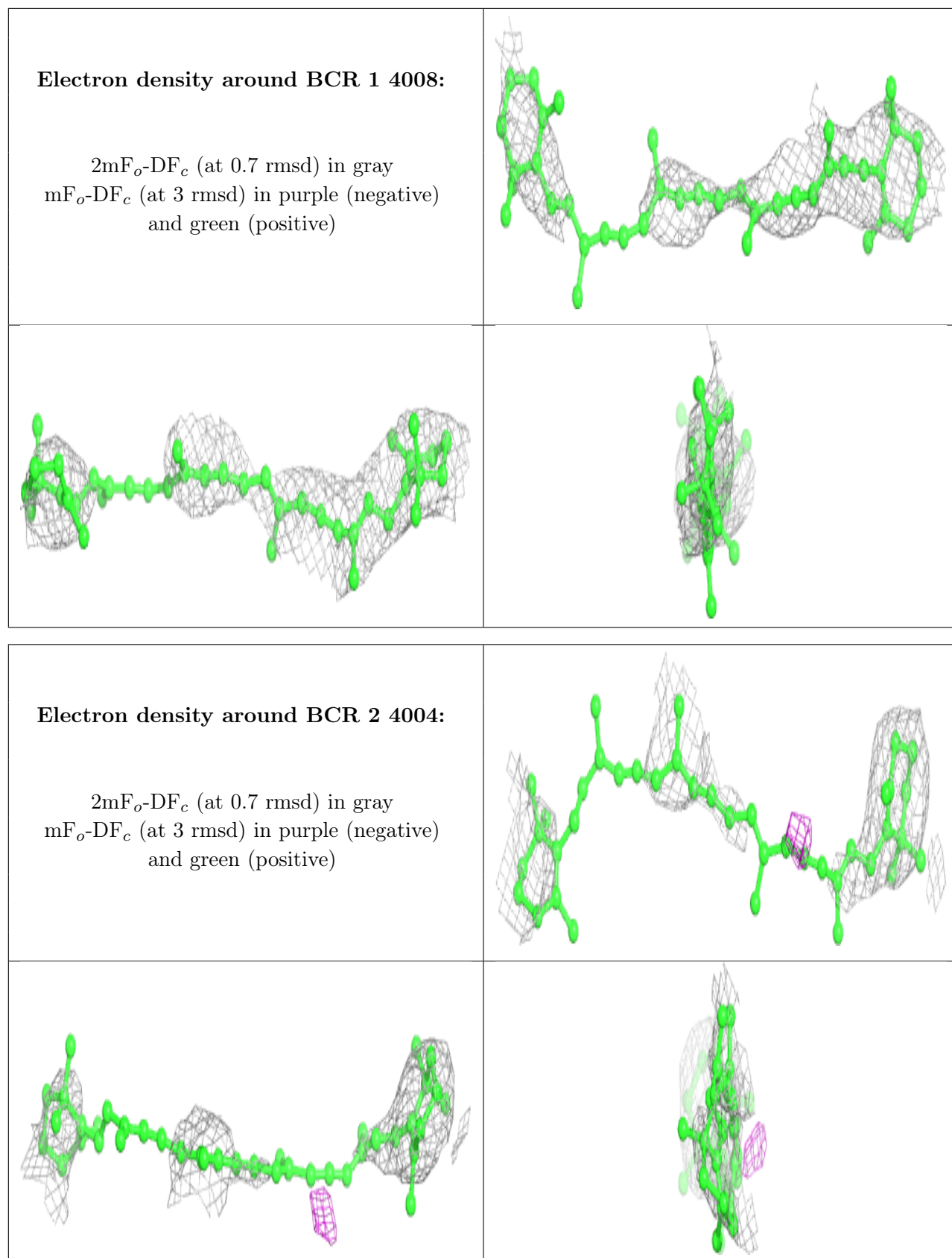
Electron density around BCR 1 4003:

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

**Electron density around BCR 1 4007:**

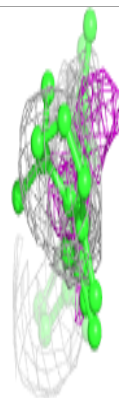
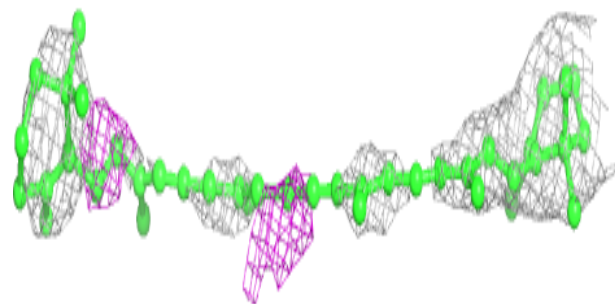
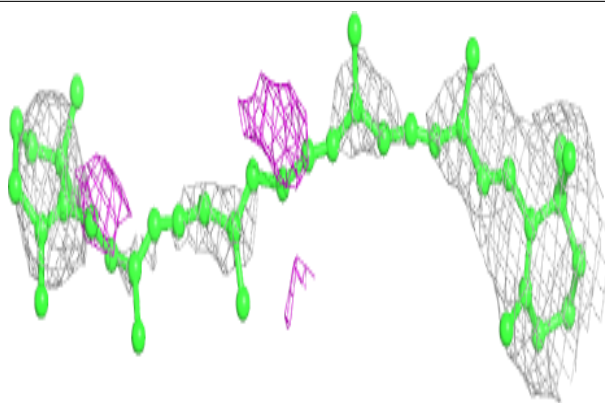
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



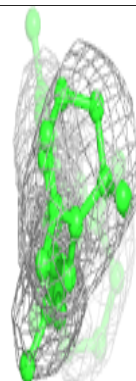
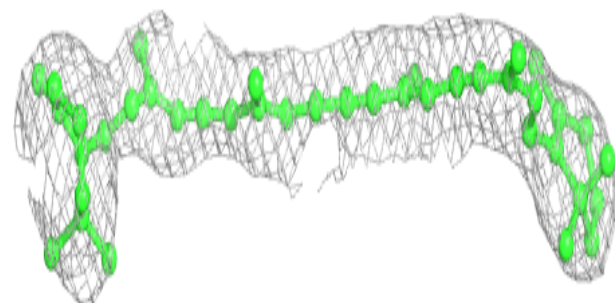
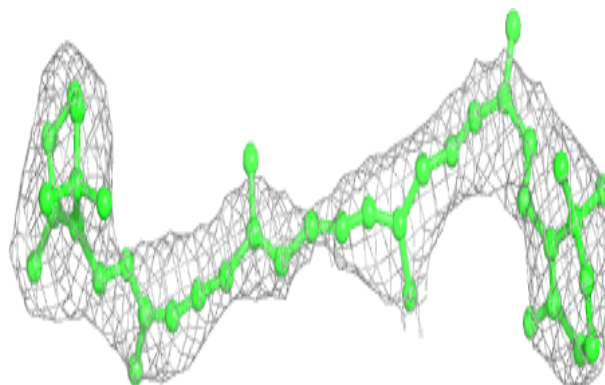


Electron density around BCR 2 4005:

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

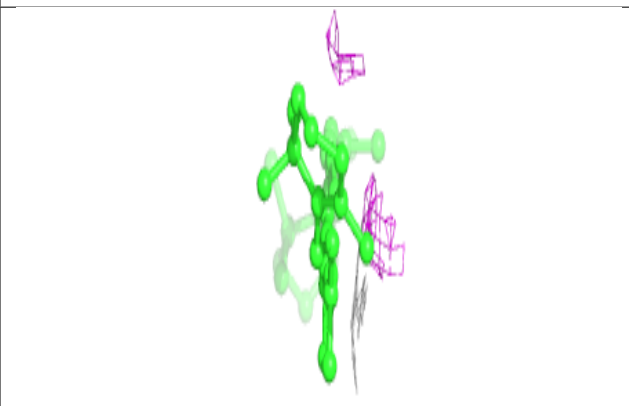
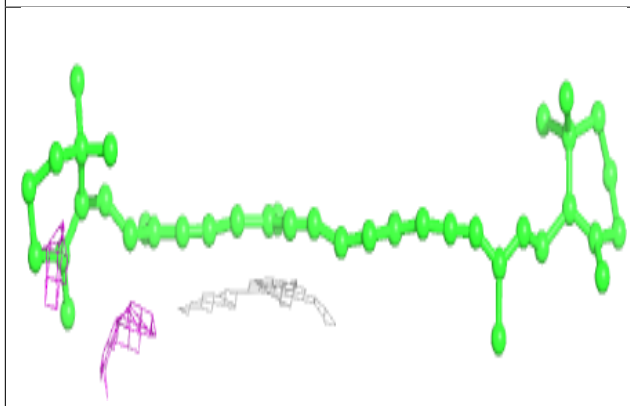
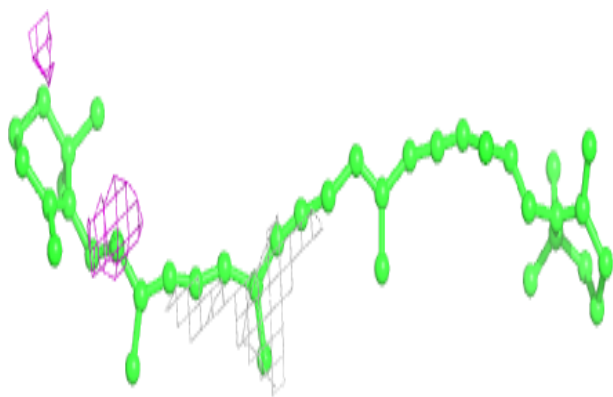
**Electron density around BCR 2 4006:**

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

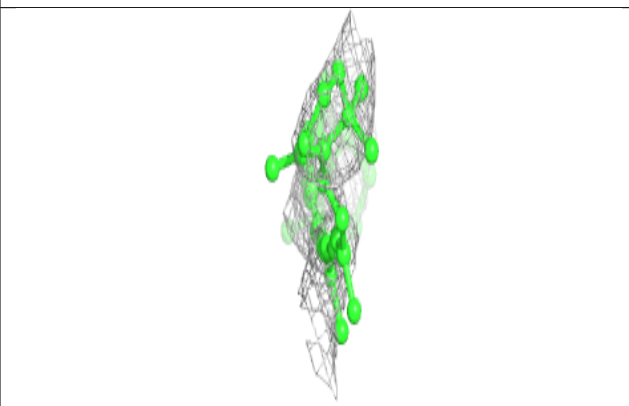
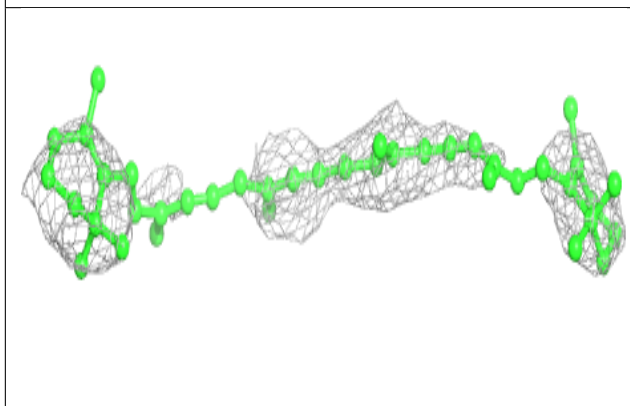
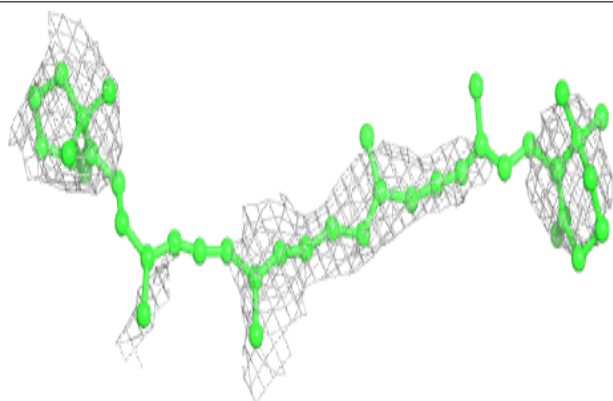


Electron density around BCR 2 4009:

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

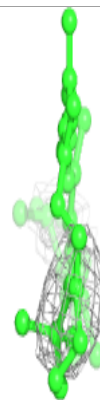
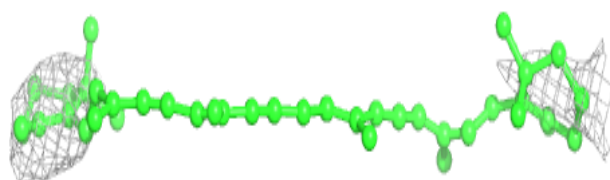
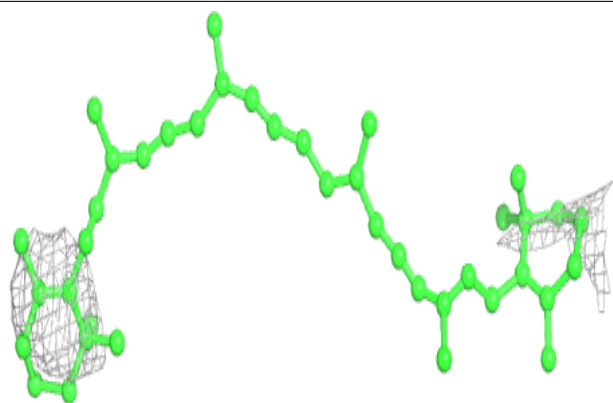
**Electron density around BCR 2 4010:**

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

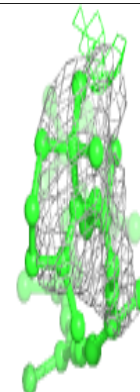
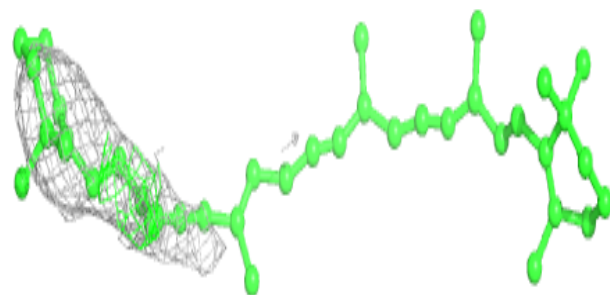
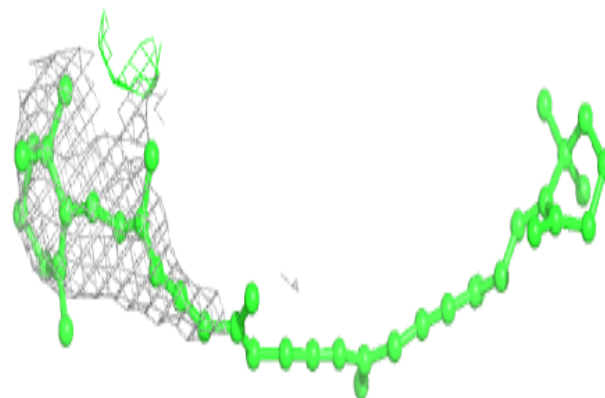


Electron density around BCR 2 4011:

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

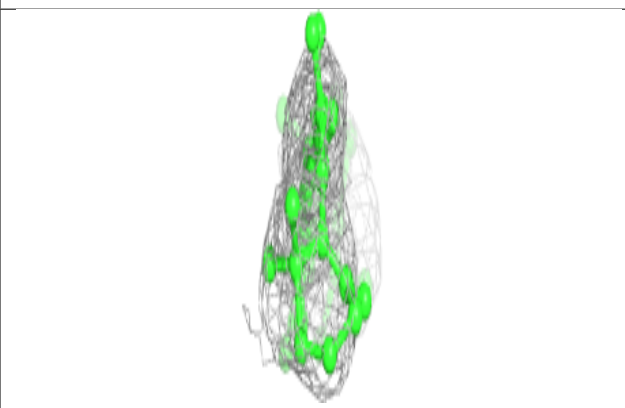
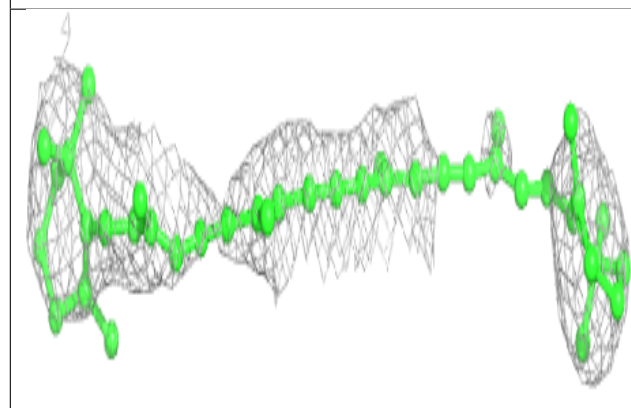
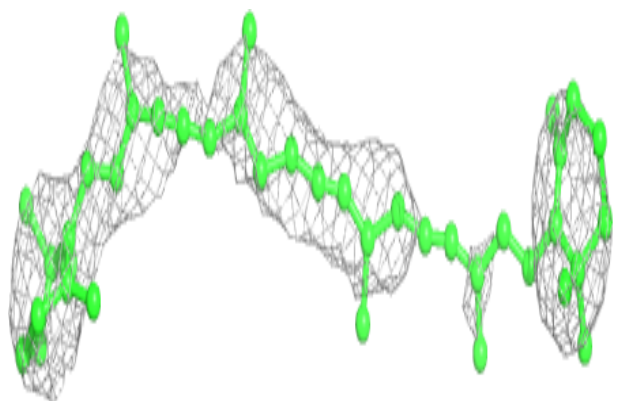
**Electron density around BCR 2 4014:**

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

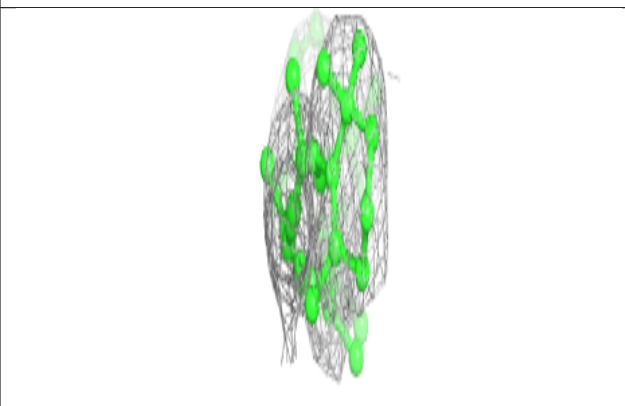
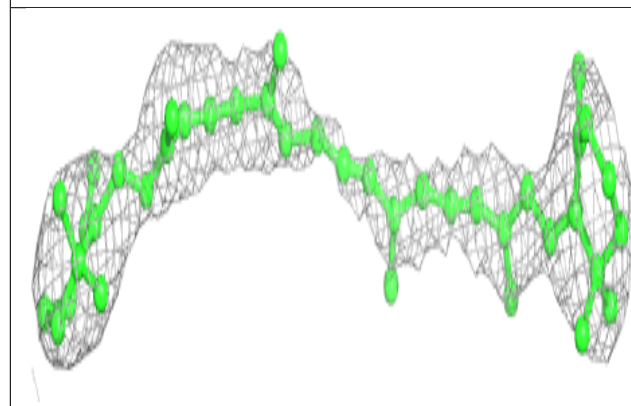
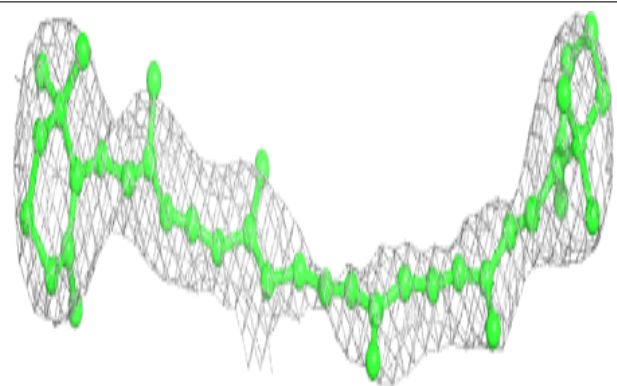


Electron density around BCR 2 4017:

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

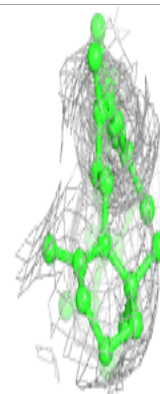
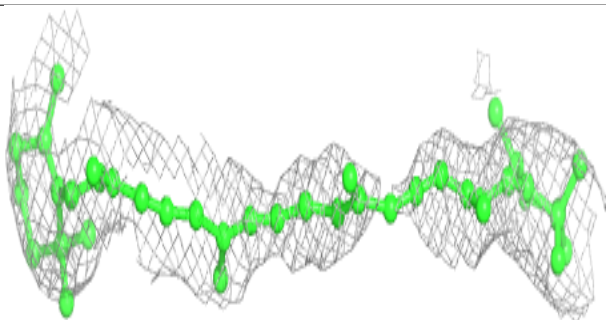
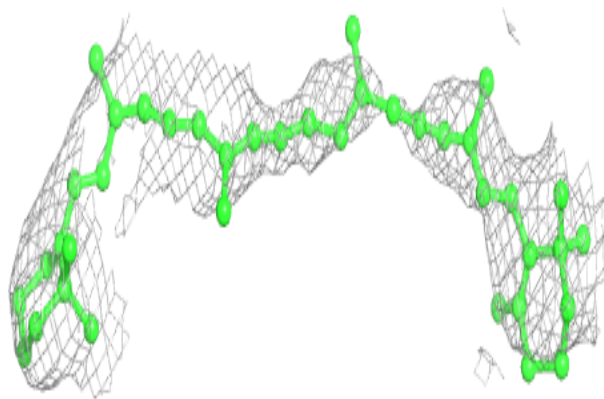
**Electron density around BCR 6 4018:**

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

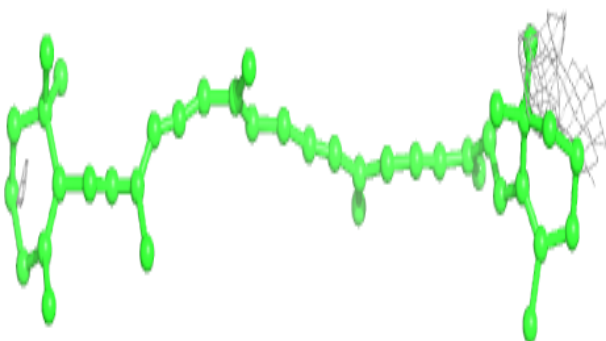
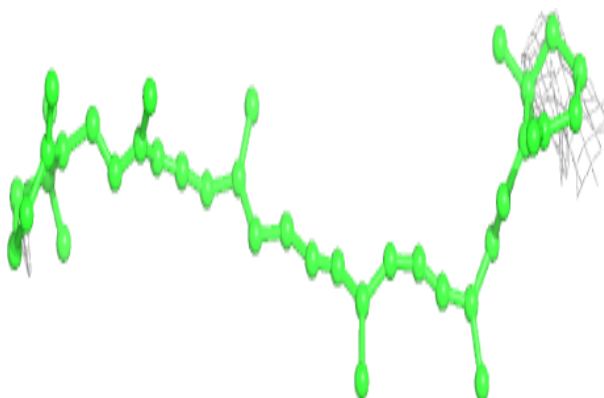


Electron density around BCR 6 4020:

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

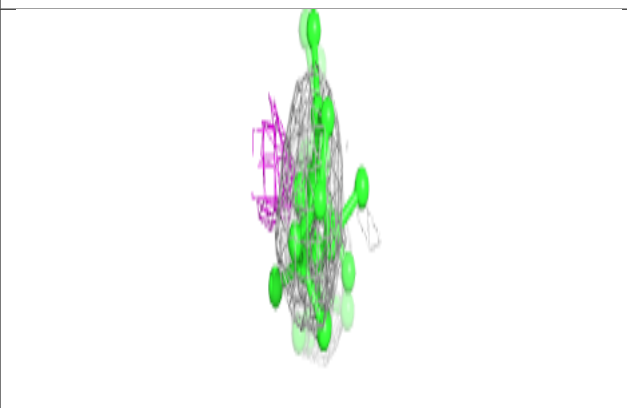
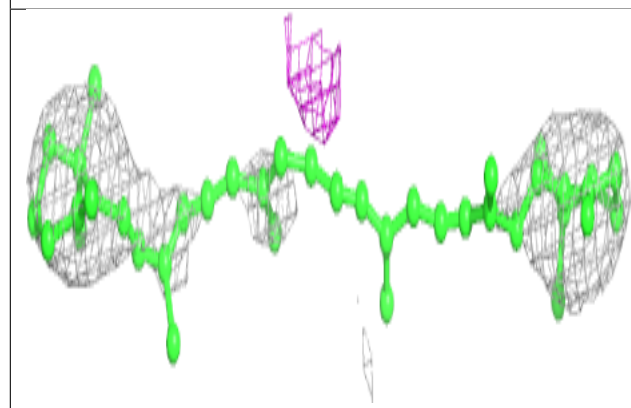
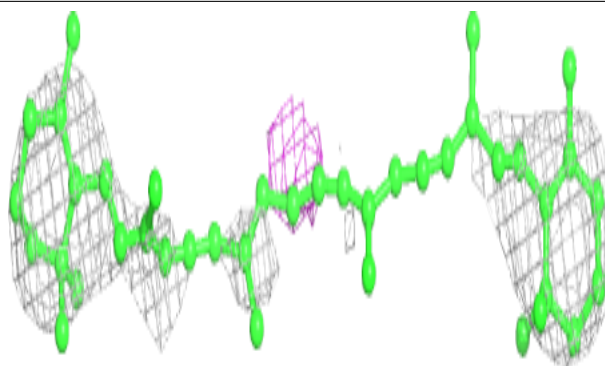
**Electron density around BCR 6 4013:**

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

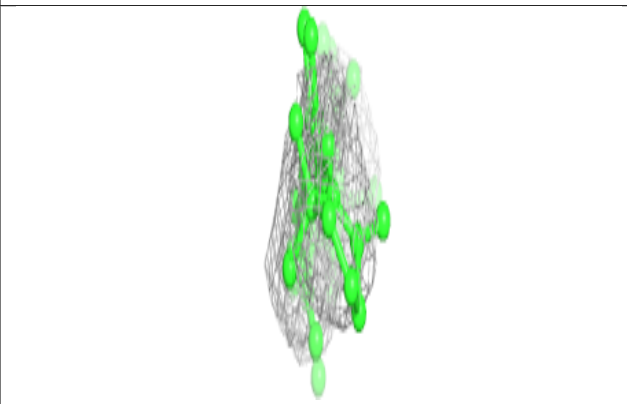
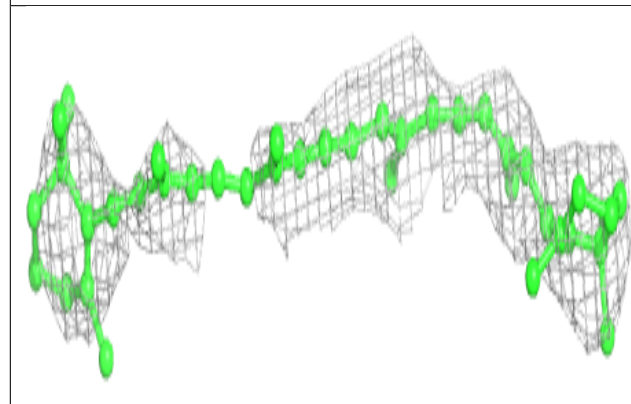
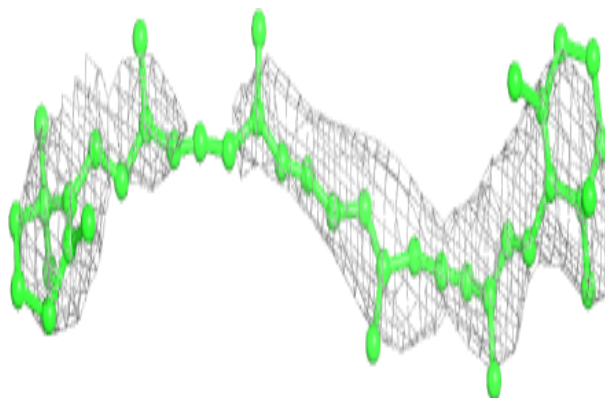


Electron density around BCR 8 4019:

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

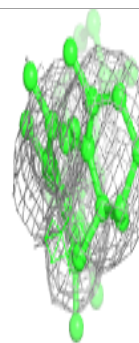
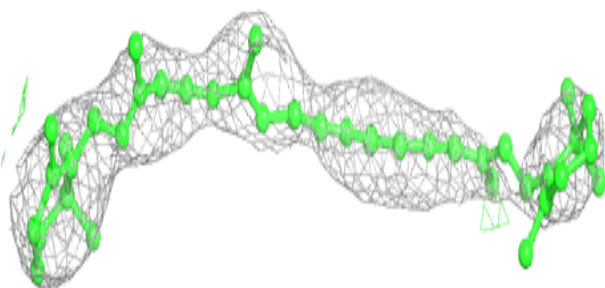
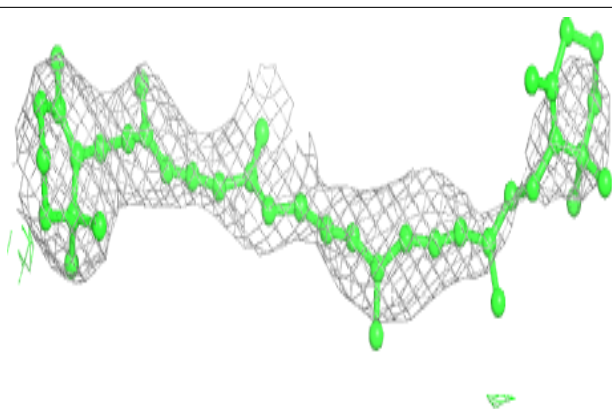
**Electron density around BCR 8 4022:**

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

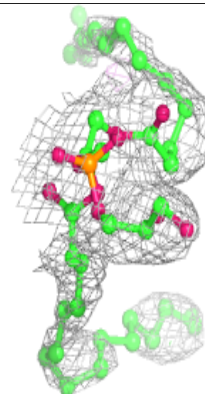
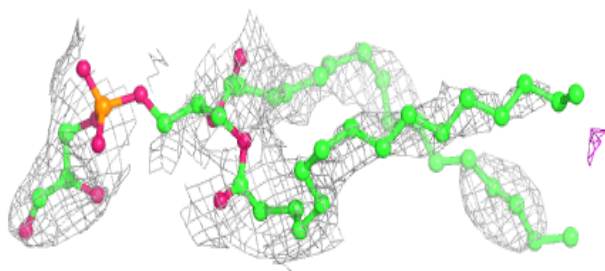
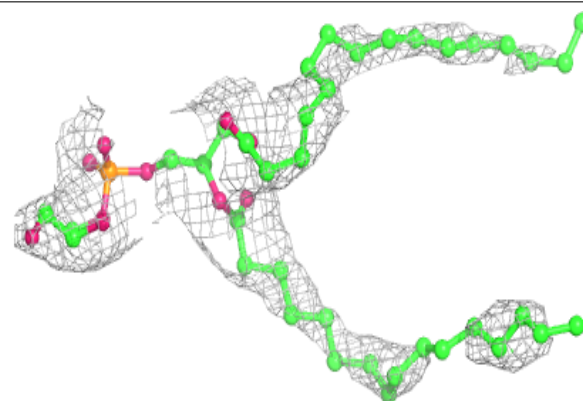


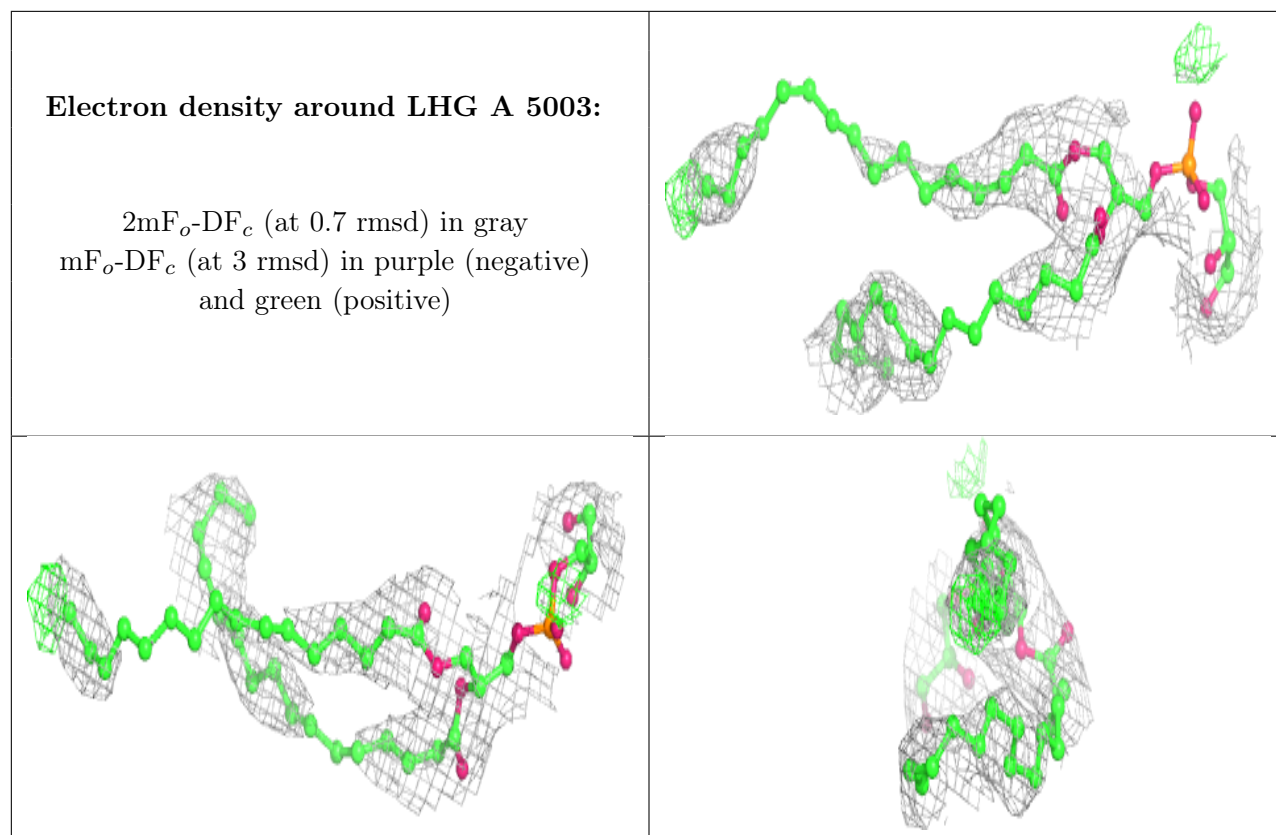
Electron density around BCR 7 4021:

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

**Electron density around LHG A 5001:**

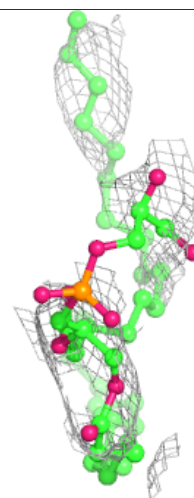
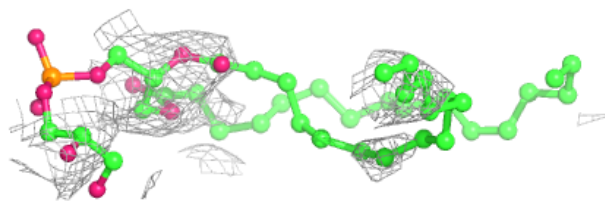
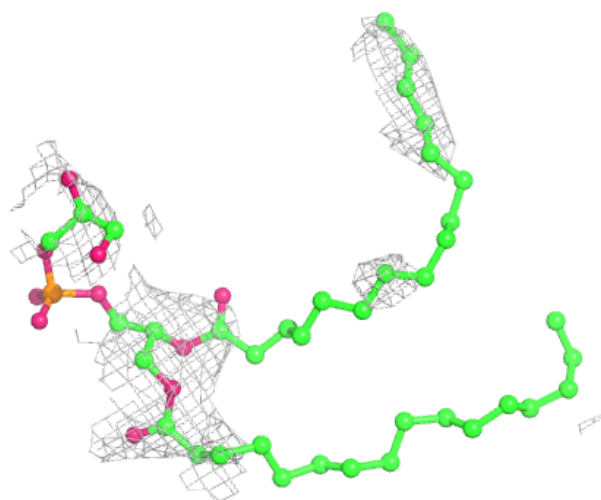
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





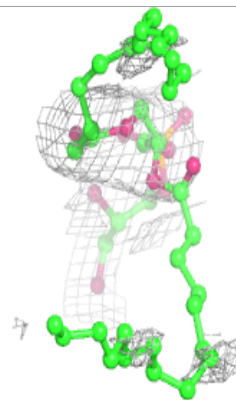
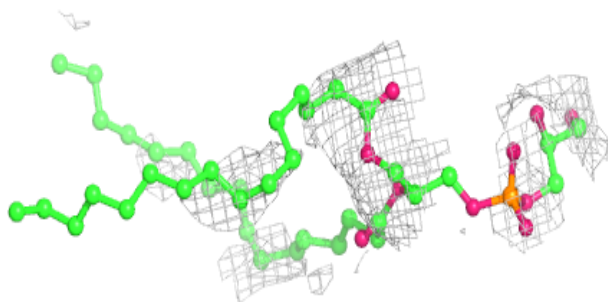
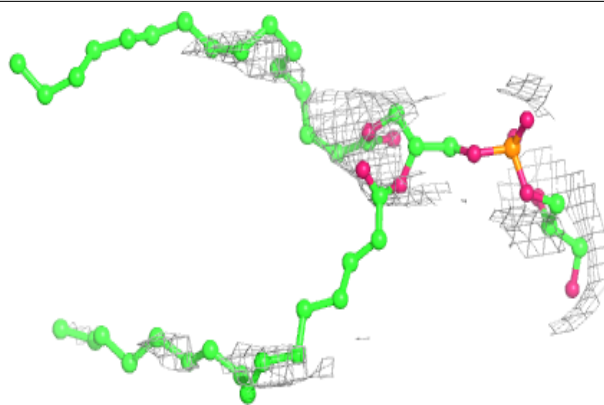
Electron density around LHG B 5004:

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

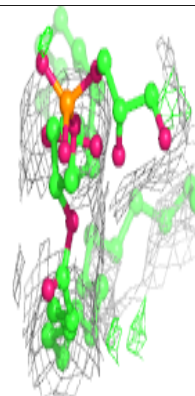
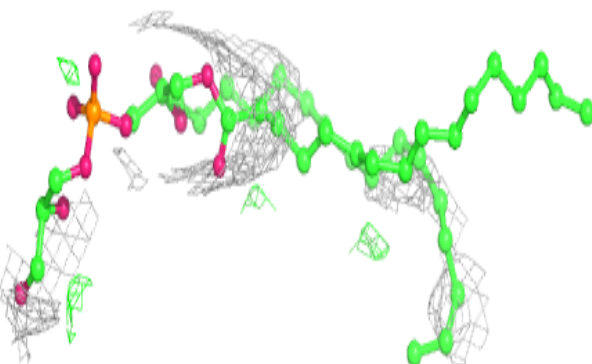
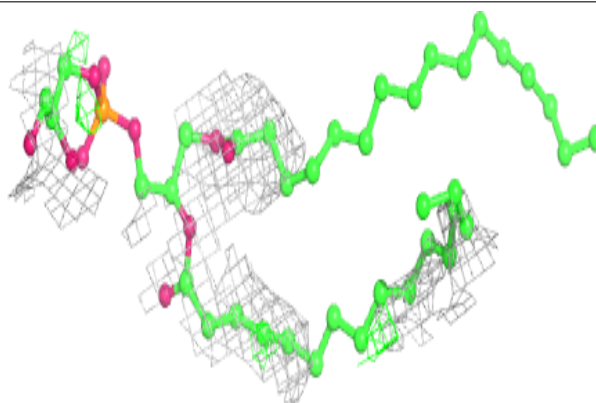


Electron density around LHG a 5001:

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

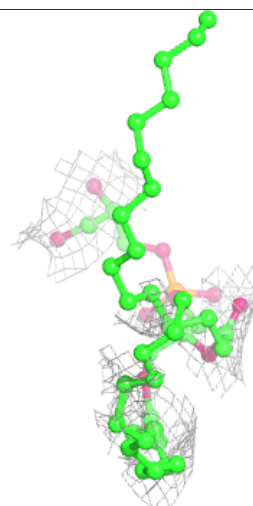
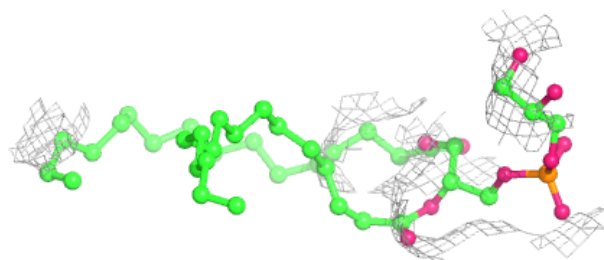
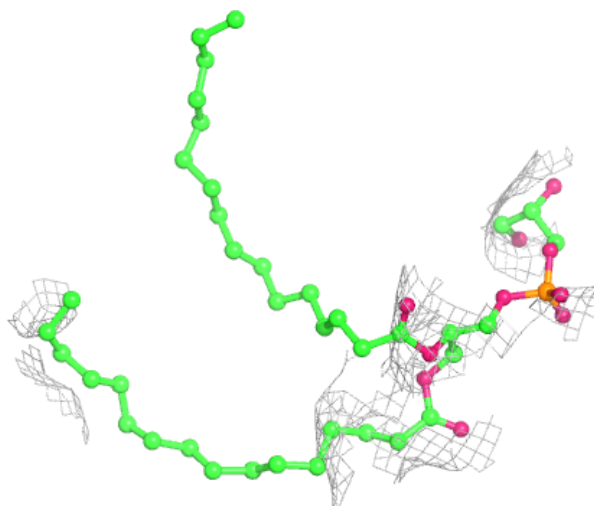
**Electron density around LHG a 5003:**

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



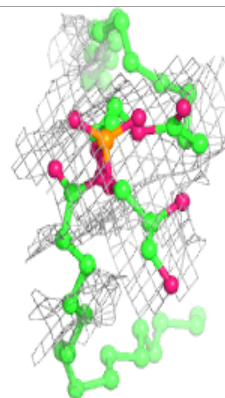
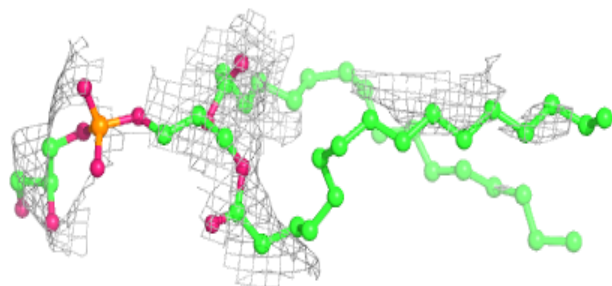
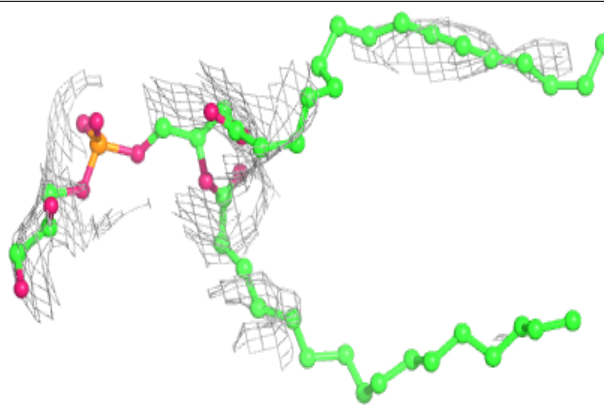
Electron density around LHG b 5004:

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

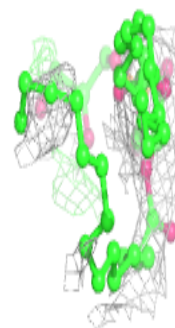
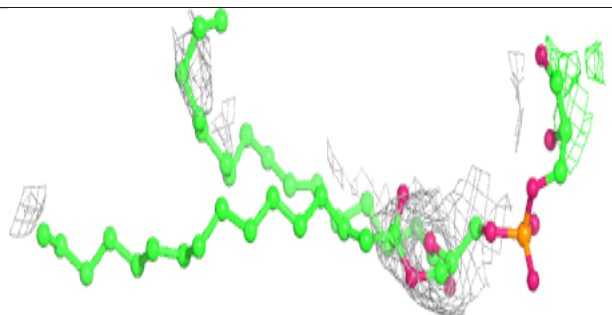
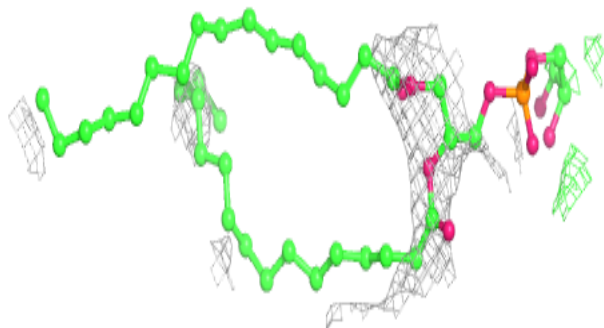


Electron density around LHG 1 5001:

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

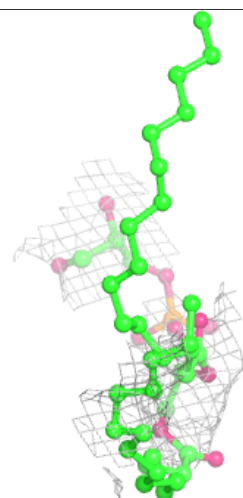
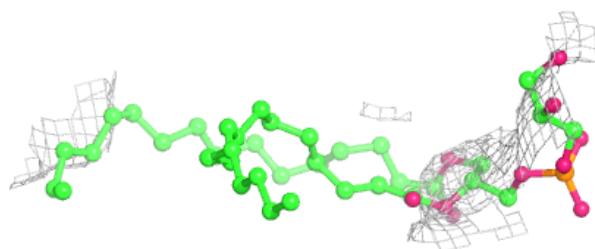
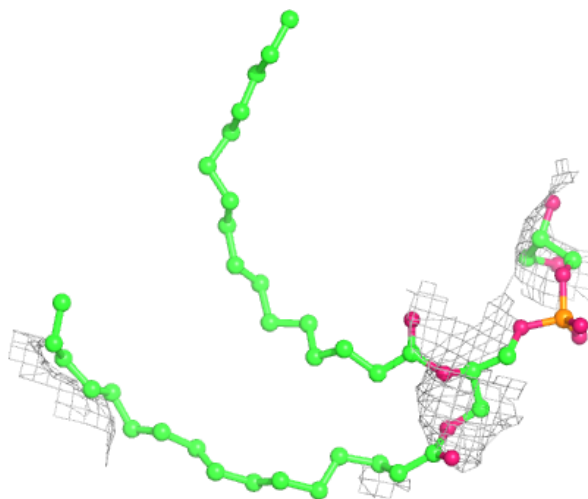
**Electron density around LHG 1 5003:**

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



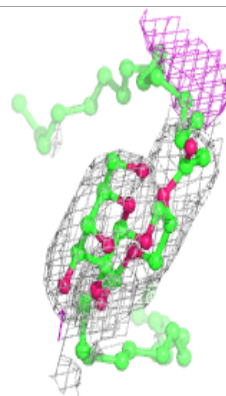
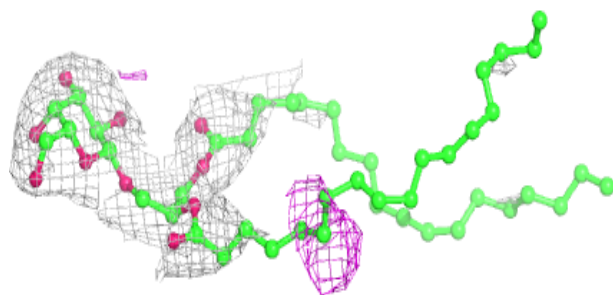
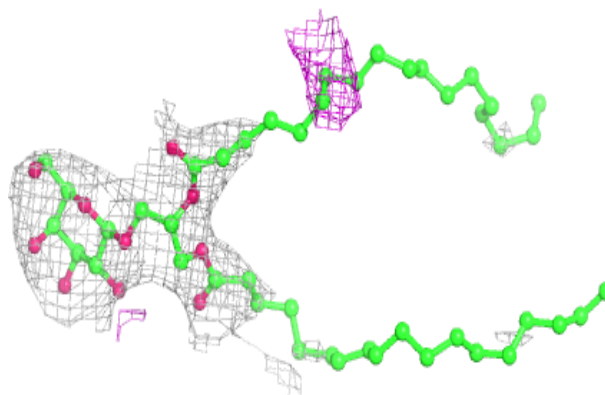
Electron density around LHG 2 5004:

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

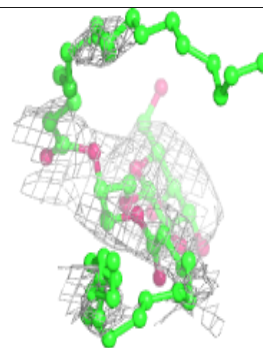
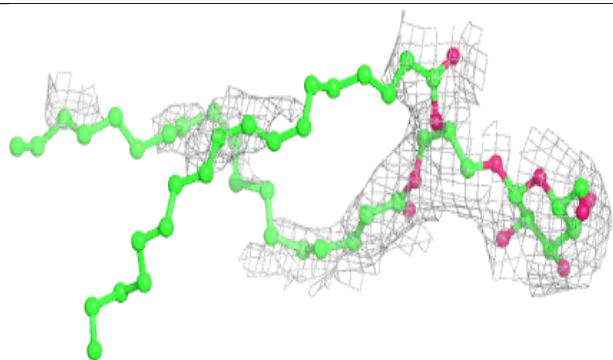
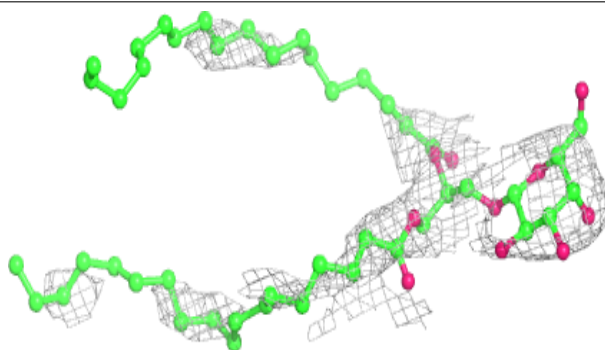


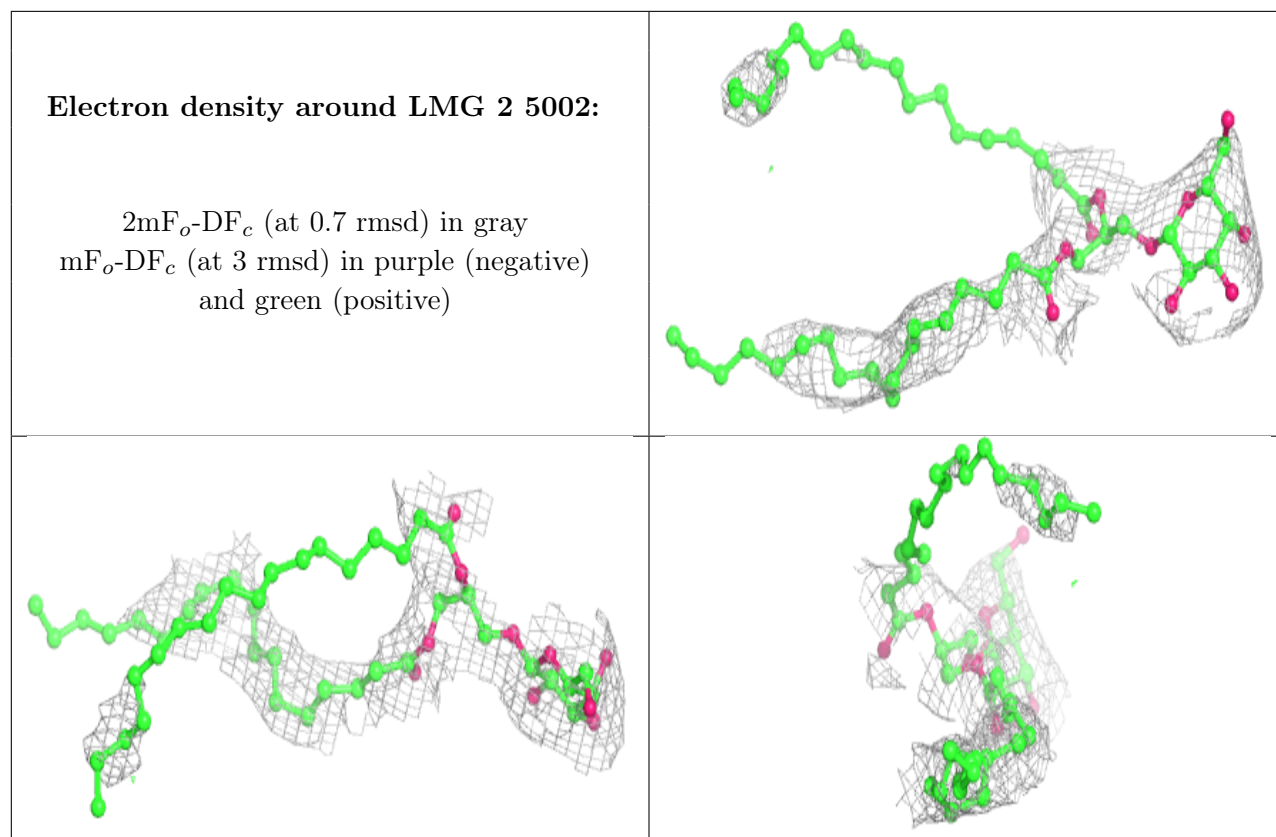
Electron density around LMG B 5002:

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

**Electron density around LMG b 5002:**

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





6.5 Other polymers [i](#)

Unable to reproduce the depositor's R factor - this section is therefore empty.