



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 6, 2026 – 10:42 AM UTC

PDB ID : 4L6V / pdb_00004l6v
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	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

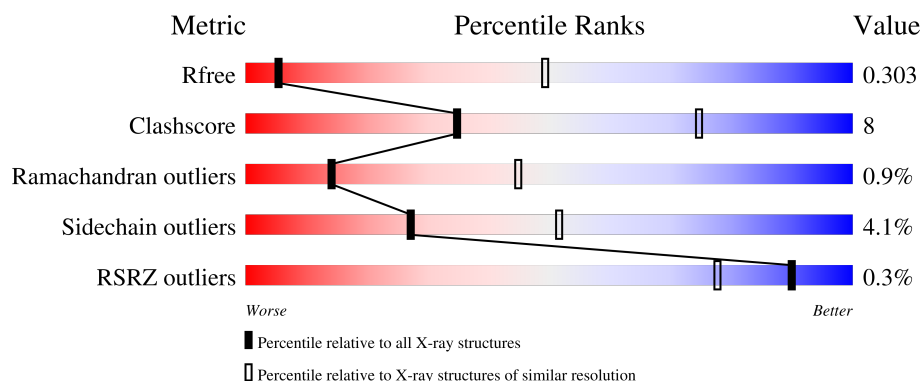
1 Overall quality at a glance

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.



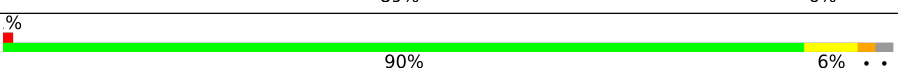
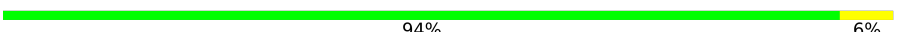
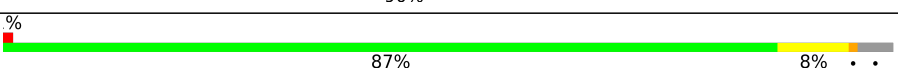
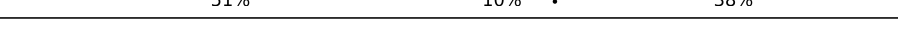
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1065 (3.96-3.64)
Clashscore	190562	1012 (3.94-3.66)
Ramachandran outliers	187476	1048 (3.96-3.64)
Sidechain outliers	187428	1043 (3.96-3.64)
RSRZ outliers	180081	1064 (3.96-3.64)

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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	1	751	89% 9% .
1	A	751	88% 10% .
1	a	751	89% 9% .
2	2	731	88% 11% .
2	B	731	87% 12% .

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Mol	Chain	Length	Quality of chain
2	b	731	 89% 10% .
3	3	81	 4% 88% 10% ..
3	C	81	 89% 7% ..
3	c	81	 85% 11% ..
4	4	141	 90% 5% ..
4	D	141	 89% 6% ..
4	d	141	 % 90% 6% ..
5	5	74	 81% 8% . 8%
5	E	74	 85% 5% . 8%
5	e	74	 82% 8% . 8%
6	6	125	 94% 6%
6	F	125	 93% 6% .
6	f	125	 93% 7%
7	8	157	 90% . . .
7	L	157	 % 87% 8% . .
7	l	157	 92% . . .
8	7	31	 77% 19% .
8	M	31	 84% 16%
8	m	31	 87% 10% .
9	9	40	 68% 28% 5%
9	I	40	 72% 22% 5%
9	i	40	 75% 20% 5%
10	0	128	 50% 11% . 38%
10	K	128	 51% 10% . 38%
10	k	128	 48% 12% . 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	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
11	CLA	1	1139	X	-	-	-
11	CLA	1	1140	X	-	-	-
11	CLA	1	1237	X	-	-	-
11	CLA	1	1801	X	-	-	-
11	CLA	2	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	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
11	CLA	8	1502	X	-	-	-
11	CLA	8	1503	X	-	-	-
11	CLA	A	1012	X	-	-	-
11	CLA	A	1022	X	-	-	-
11	CLA	A	1101	X	-	-	-
11	CLA	A	1102	X	-	-	-
11	CLA	A	1103	X	-	-	-
11	CLA	A	1104	X	-	-	-
11	CLA	A	1105	X	-	-	-
11	CLA	A	1106	X	-	-	-
11	CLA	A	1107	X	-	-	-
11	CLA	A	1108	X	-	-	-
11	CLA	A	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	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
11	CLA	A	1140	X	-	-	-
11	CLA	A	1237	X	-	-	-
11	CLA	A	1801	X	-	-	-
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	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
11	CLA	L	1501	X	-	-	-
11	CLA	L	1502	X	-	-	-
11	CLA	L	1503	X	-	-	-
11	CLA	a	1012	X	-	-	-
11	CLA	a	1022	X	-	-	-
11	CLA	a	1101	X	-	-	-
11	CLA	a	1102	X	-	-	-
11	CLA	a	1103	X	-	-	-
11	CLA	a	1104	X	-	-	-
11	CLA	a	1105	X	-	-	-
11	CLA	a	1106	X	-	-	-
11	CLA	a	1107	X	-	-	-
11	CLA	a	1108	X	-	-	-
11	CLA	a	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	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
11	CLA	a	1237	X	-	-	-
11	CLA	a	1801	X	-	-	-
11	CLA	b	1021	X	-	-	-
11	CLA	b	1023	X	-	-	-
11	CLA	b	1201	X	-	-	-
11	CLA	b	1202	X	-	-	-
11	CLA	b	1203	X	-	-	-
11	CLA	b	1204	X	-	-	-
11	CLA	b	1205	X	-	-	-
11	CLA	b	1206	X	-	-	-
11	CLA	b	1207	X	-	-	-
11	CLA	b	1208	X	-	-	-
11	CLA	b	1209	X	-	-	-
11	CLA	b	1210	X	-	-	-
11	CLA	b	1211	X	-	-	-
11	CLA	b	1212	X	-	-	-
11	CLA	b	1213	X	-	-	-
11	CLA	b	1214	X	-	-	-
11	CLA	b	1215	X	-	-	-
11	CLA	b	1216	X	-	-	-
11	CLA	b	1217	X	-	-	-
11	CLA	b	1218	X	-	-	-
11	CLA	b	1219	X	-	-	-
11	CLA	b	1220	X	-	-	-
11	CLA	b	1221	X	-	-	-
11	CLA	b	1222	X	-	-	-
11	CLA	b	1223	X	-	-	-
11	CLA	b	1224	X	-	-	-
11	CLA	b	1225	X	-	-	-
11	CLA	b	1226	X	-	-	-
11	CLA	b	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	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
11	CLA	k	1402	X	-	-	-
11	CLA	l	1502	X	-	-	-
11	CLA	l	1503	X	-	-	-
13	SF4	3	3002	-	-	X	-
13	SF4	3	3003	-	-	X	-
13	SF4	A	3001	-	-	X	-
13	SF4	C	3002	-	-	X	-
13	SF4	C	3003	-	-	X	-
13	SF4	a	3001	-	-	X	-
13	SF4	c	3002	-	-	X	-
13	SF4	c	3003	-	-	X	-

2 Entry composition

There are 16 unique types of molecules in this entry. The entry contains 68370 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	739	Total	C	N	O	S	0	0	0
			5772	3783	982	980	27			
1	a	739	Total	C	N	O	S	0	0	0
			5772	3783	982	980	27			
1	1	739	Total	C	N	O	S	0	0	0
			5772	3783	982	980	27			

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

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

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

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

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

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

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

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

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

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

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

There are 12 discrepancies between the modelled and reference sequences:

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

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

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

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

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

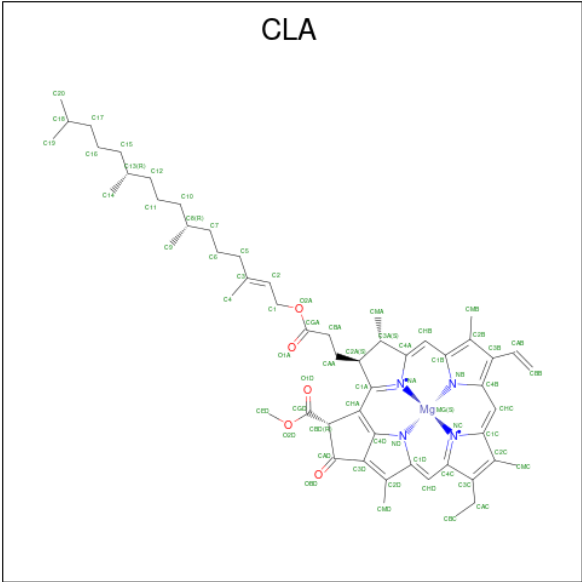
- Molecule 9 is a protein called Photosystem I subunit III.

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

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

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

- Molecule 11 is CHLOROPHYLL A (CCD ID: 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
			48	38	1	4	5		
11	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
11	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
11	A	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
11	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
11	A	1	Total	C	Mg	N	O	0	0
			54	44	1	4	5		
11	A	1	Total	C	Mg	N	O	0	0
			60	50	1	4	5		

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

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

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

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

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
11	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
11	b	1	Total 55	C 45	Mg 1	N 4	O 5	0	0
11	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
11	b	1	Total 45	C 35	Mg 1	N 4	O 5	0	0
11	b	1	Total 45	C 35	Mg 1	N 4	O 5	0	0
11	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
11	b	1	Total 45	C 35	Mg 1	N 4	O 5	0	0
11	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
11	b	1	Total 59	C 49	Mg 1	N 4	O 5	0	0
11	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
11	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
11	b	1	Total 47	C 37	Mg 1	N 4	O 5	0	0
11	b	1	Total 45	C 35	Mg 1	N 4	O 5	0	0
11	b	1	Total 55	C 45	Mg 1	N 4	O 5	0	0
11	b	1	Total 46	C 36	Mg 1	N 4	O 5	0	0
11	b	1	Total 54	C 44	Mg 1	N 4	O 5	0	0
11	b	1	Total 56	C 46	Mg 1	N 4	O 5	0	0
11	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
11	b	1	Total 55	C 45	Mg 1	N 4	O 5	0	0
11	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
11	b	1	Total 65	C 55	Mg 1	N 4	O 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
			50	40	1	4	5		
11	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
11	b	1	Total	C	Mg	N	O	0	0
			58	48	1	4	5		
11	b	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
11	b	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
11	b	1	Total	C	Mg	N	O	0	0
			60	50	1	4	5		
11	b	1	Total	C	Mg	N	O	0	0
			60	50	1	4	5		
11	b	1	Total	C	Mg	N	O	0	0
			47	37	1	4	5		
11	b	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
11	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
11	b	1	Total	C	Mg	N	O	0	0
			46	36	1	4	5		
11	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
11	b	1	Total	C	Mg	N	O	0	0
			46	36	1	4	5		
11	l	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
11	l	1	Total	C	Mg	N	O	0	0
			46	36	1	4	5		
11	l	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
11	1	1	Total	C	Mg	N	O	0	0
			52	42	1	4	5		
11	1	1	Total	C	Mg	N	O	0	0
			55	45	1	4	5		
11	1	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
11	1	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		

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

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

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

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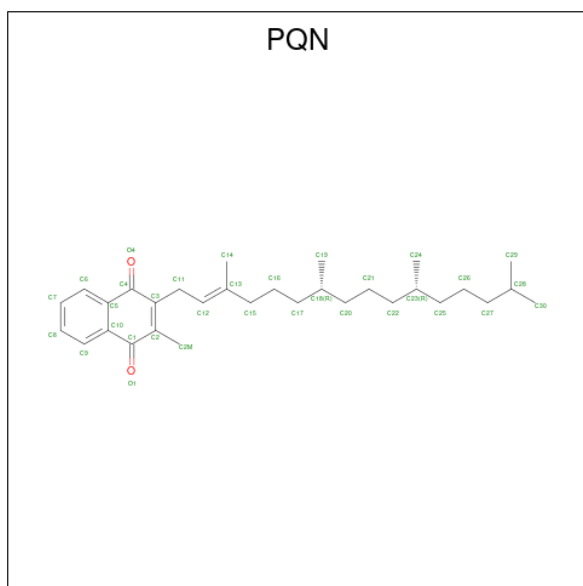
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
11	2	1	Total	C	Mg	N	O	0	0
			54	44	1	4	5		
11	2	1	Total	C	Mg	N	O	0	0
			56	46	1	4	5		
11	2	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
11	2	1	Total	C	Mg	N	O	0	0
			55	45	1	4	5		
11	2	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
11	2	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5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

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

- Molecule 12 is PHYLLOQUINONE (CCD ID: PQN) (formula: $C_{31}H_{46}O_2$).



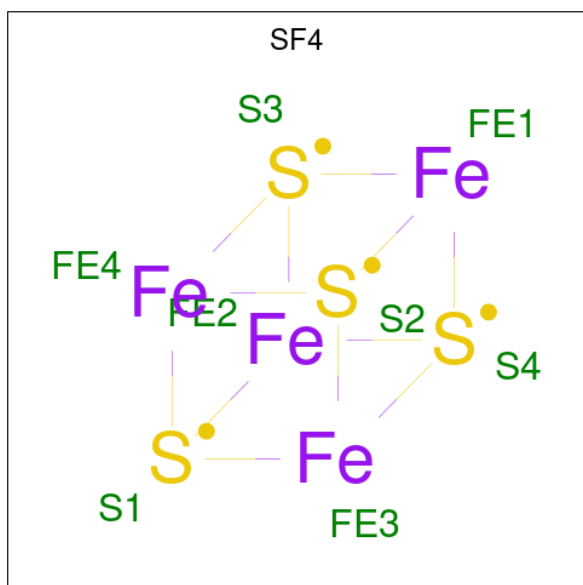
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
12	A	1	Total	C	O	0	0
			33	31	2		
12	B	1	Total	C	O	0	0
			33	31	2		
12	a	1	Total	C	O	0	0
			33	31	2		
12	b	1	Total	C	O	0	0
			33	31	2		

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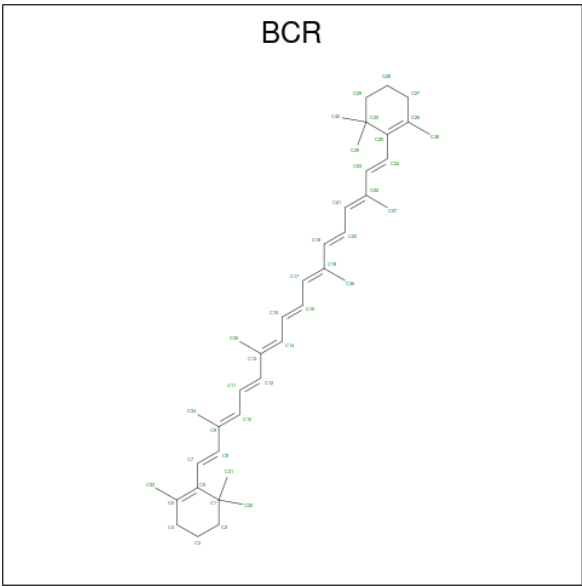
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
12	1	1	Total	C	O	0	0
			33	31	2		
12	2	1	Total	C	O	0	0
			33	31	2		

- Molecule 13 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe_4S_4).



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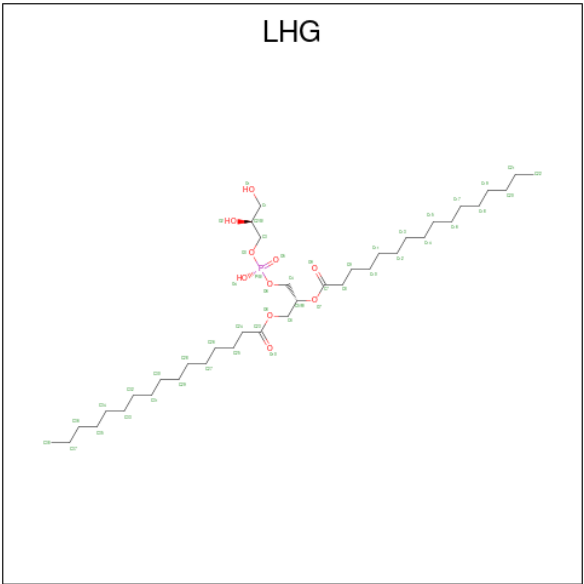
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
14	f	1	Total C 40 40	0	0
14	l	1	Total C 40 40	0	0
14	l	1	Total C 40 40	0	0
14	m	1	Total C 40 40	0	0
14	1	1	Total C 40 40	0	0
14	1	1	Total C 40 40	0	0
14	1	1	Total C 40 40	0	0
14	1	1	Total C 40 40	0	0
14	1	1	Total C 40 40	0	0
14	2	1	Total C 40 40	0	0
14	2	1	Total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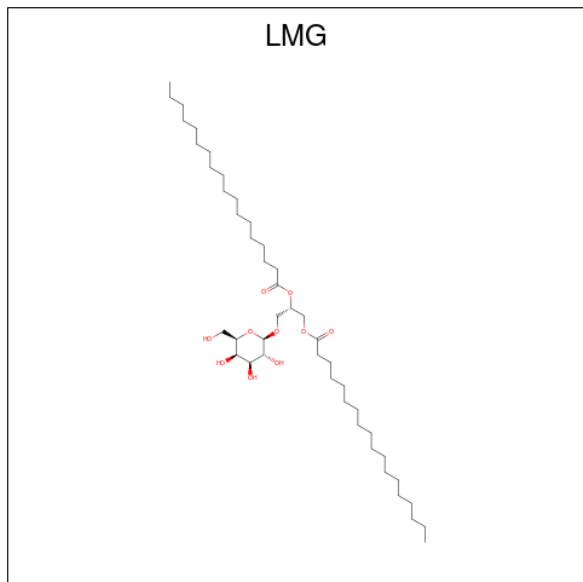
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
14	8	1	Total C 40 40	0	0
14	7	1	Total C 40 40	0	0

- Molecule 15 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (CCD ID: LHG) (formula: C₃₈H₇₅O₁₀P).



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 (CCD ID: LMG) (formula: $C_{45}H_{86}O_{10}$).

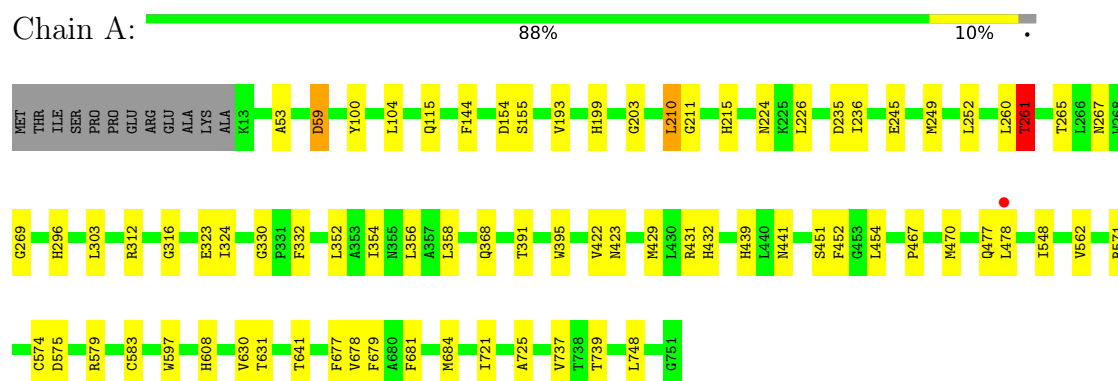


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
16	B	1	Total	C	O	0	0
			55	45	10		
16	b	1	Total	C	O	0	0
			55	45	10		
16	2	1	Total	C	O	0	0
			55	45	10		

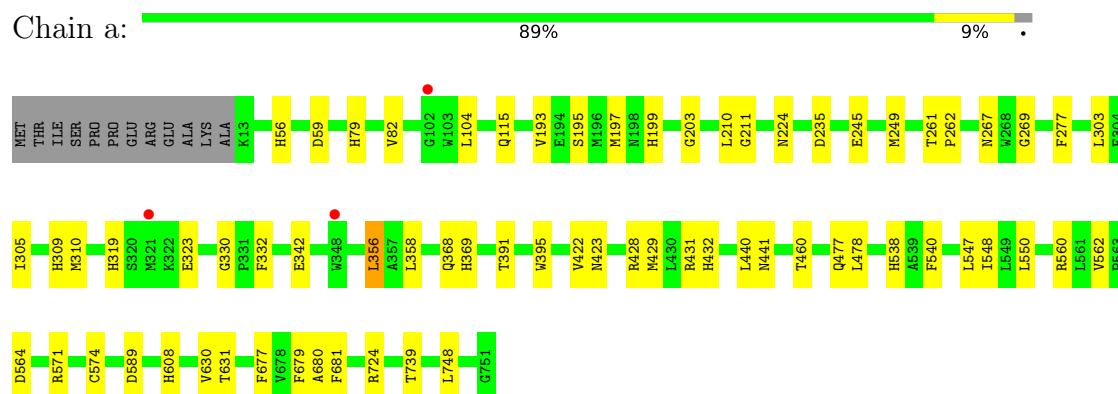
3 Residue-property plots

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

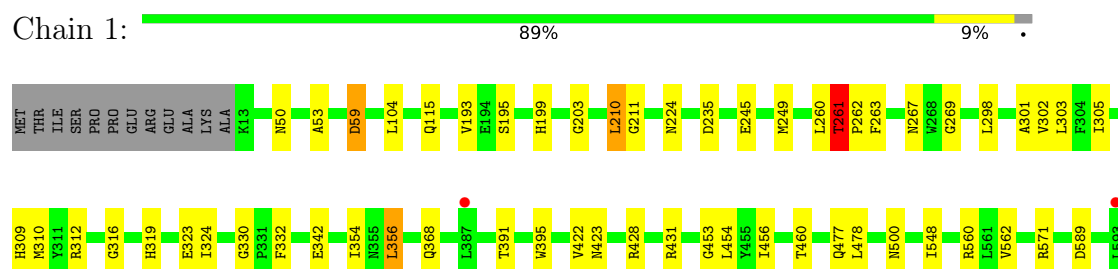
- Molecule 1: Photosystem I P700 chlorophyll a apoprotein A1



- Molecule 1: Photosystem I P700 chlorophyll a apoprotein A1



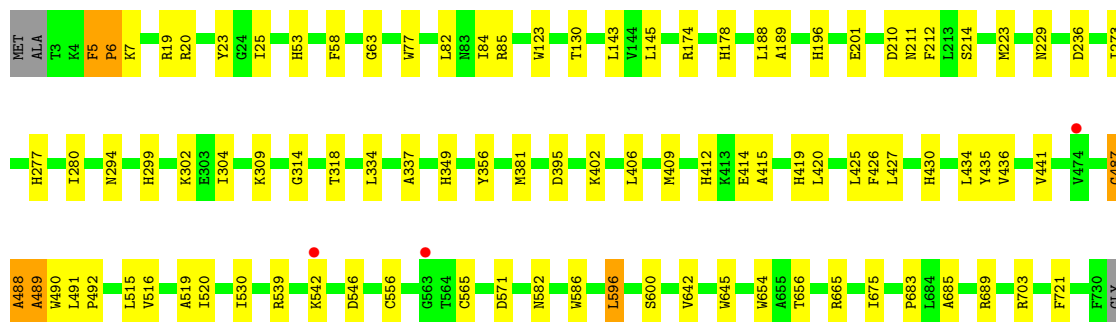
- Molecule 1: Photosystem I P700 chlorophyll a apoprotein A1





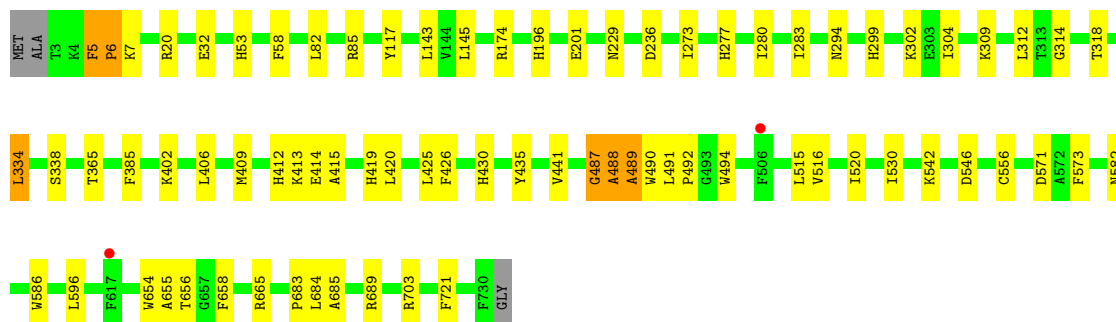
- Molecule 2: Photosystem I P700 chlorophyll a apoprotein A2

Chain B: 87% 12% .



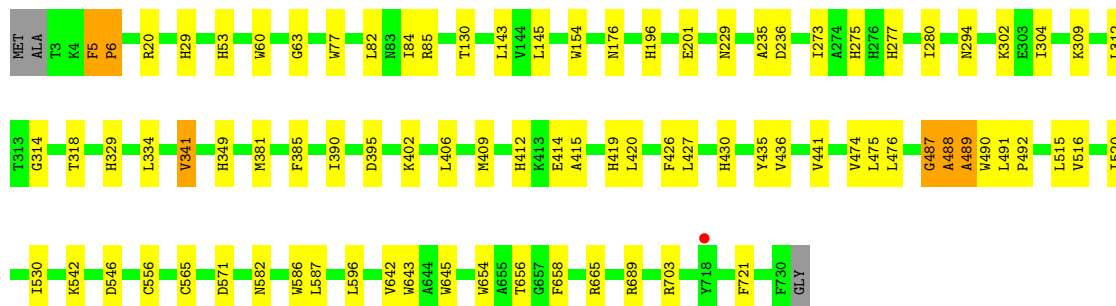
- Molecule 2: Photosystem I P700 chlorophyll a apoprotein A2

Chain b: 89% 10% .



- Molecule 2: Photosystem I P700 chlorophyll a apoprotein A2

Chain 2: 88% 11% .



- Molecule 3: Photosystem I iron-sulfur center

Chain C: 89% 7% ..



- Molecule 3: Photosystem I iron-sulfur center

Chain c: 85% 11% ..



- Molecule 3: Photosystem I iron-sulfur center

Chain 3: 4% 88% 10% ..



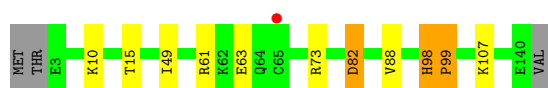
- Molecule 4: Photosystem I subunit II

Chain D: 89% 6% ..



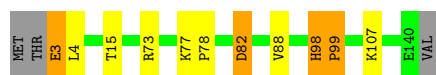
- Molecule 4: Photosystem I subunit II

Chain d: 90% 6% ..



- Molecule 4: Photosystem I subunit II

Chain 4: 90% 5% ..



- Molecule 5: Photosystem I reaction center subunit IV

Chain E: 85% 5% 8%



- Molecule 5: Photosystem I reaction center subunit IV

Chain e: 82% 8% 8%



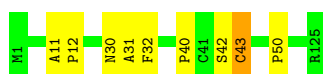
- Molecule 5: Photosystem I reaction center subunit IV

Chain 5: 81% 8% 8%



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

Chain F: 93% 6%



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

Chain f: 93% 7%



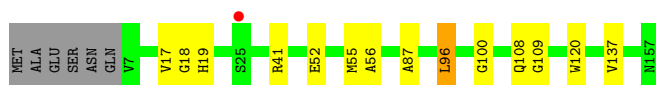
- Molecule 6: Fusion protein of Photosystem I subunit III and subunit IX

Chain 6: 94% 6%



- Molecule 7: Photosystem I reaction center subunit XI

Chain L: 87% 8%



- Molecule 7: Photosystem I reaction center subunit XI

Chain l: 92%

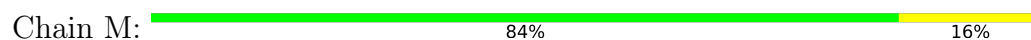


- Molecule 7: Photosystem I reaction center subunit XI

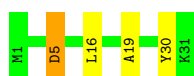
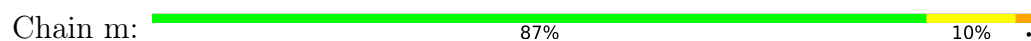
Chain 8: 90%



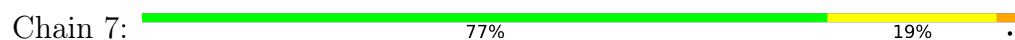
- Molecule 8: Photosystem I reaction center subunit XII



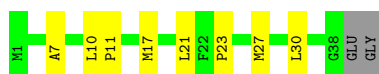
- Molecule 8: Photosystem I reaction center subunit XII



- Molecule 8: Photosystem I reaction center subunit XII



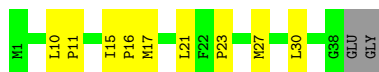
- Molecule 9: Photosystem I subunit III



- Molecule 9: Photosystem I subunit III

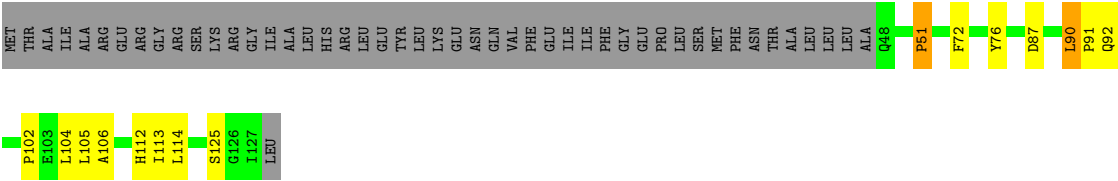


- Molecule 9: Photosystem I subunit III

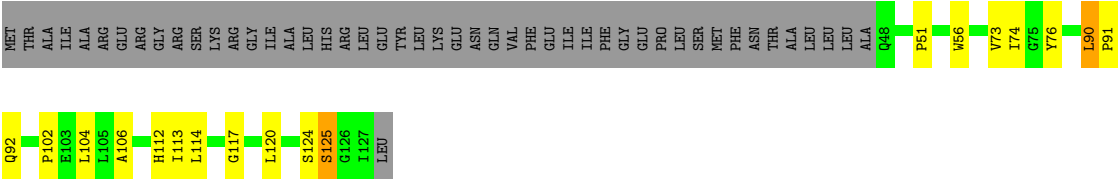


- Molecule 10: Photosystem I reaction center subunit VIII

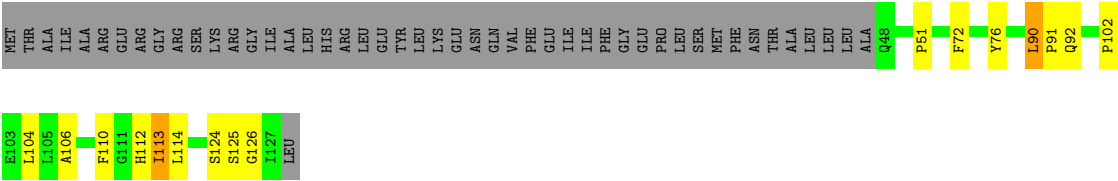




• Molecule 10: Photosystem I reaction center subunit VIII



• 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 30.00 – 3.80	Depositor EDS
% Data completeness (in resolution range)	95.4 (30.00-3.80) 77.5 (30.00-3.80)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	-0.02 (at 3.40Å)	Xtriage
Refinement program	PHENIX 1.8.2-1309, REFMAC 5.7.0032	Depositor
R, R_{free}	0.253 , 0.297 0.265 , 0.303	Depositor DCC
R_{free} test set	7809 reflections (4.89%)	wwPDB-VP
Wilson B-factor (Å ²)	93.5	Xtriage
Anisotropy	0.250	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.25 , 105.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	0.038 for l,k,h	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	68370	wwPDB-VP
Average B, all atoms (Å ²)	173.0	wwPDB-VP

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

¹Intensities estimated from amplitudes.

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

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

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	0.30	0/5970	0.66	2/8138 (0.0%)
1	A	0.31	0/5970	0.65	2/8138 (0.0%)
1	a	0.30	0/5970	0.66	0/8138
2	2	0.30	0/5976	0.64	1/8173 (0.0%)
2	B	0.31	0/5976	0.64	1/8173 (0.0%)
2	b	0.30	0/5976	0.64	1/8173 (0.0%)
3	3	0.34	0/610	0.67	0/826
3	C	0.33	0/610	0.66	0/826
3	c	0.34	0/610	0.64	0/826
4	4	0.31	0/1103	0.61	0/1487
4	D	0.30	0/1103	0.61	0/1487
4	d	0.30	0/1103	0.61	0/1487
5	5	0.30	0/538	0.67	0/729
5	E	0.29	0/538	0.63	0/729
5	e	0.29	0/538	0.64	0/729
6	6	0.36	0/700	0.92	1/976 (0.1%)
6	F	0.41	0/690	0.97	0/963
6	f	0.36	0/700	0.90	0/976
7	8	0.31	0/1163	0.67	0/1580
7	L	0.31	0/1163	0.67	0/1580
7	l	0.30	0/1163	0.67	0/1580
8	7	0.38	0/238	0.66	0/323
8	M	0.37	0/238	0.67	0/323
8	m	0.34	0/238	0.68	0/323
9	9	0.37	0/308	0.71	0/421
9	I	0.36	0/308	0.69	0/421
9	i	0.34	0/308	0.64	0/421
10	0	0.35	0/504	0.84	0/688
10	K	0.36	0/504	0.81	0/688
10	k	0.34	0/504	0.83	1/688 (0.1%)
All	All	0.31	0/51320	0.67	9/70010 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
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.

The worst 5 of 9 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	6	47	PHE	N-CA-C	-5.47	106.38	113.16
1	1	261	THR	CA-C-N	-5.18	113.58	119.28
1	1	261	THR	C-N-CA	-5.18	113.58	119.28
2	B	665	ARG	N-CA-C	5.15	116.58	110.97
2	2	665	ARG	N-CA-C	5.12	116.55	110.97

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

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	1	5772	0	5621	58	0
1	A	5772	0	5621	61	0
1	a	5772	0	5621	67	0
2	2	5765	0	5546	54	0
2	B	5765	0	5546	60	0
2	b	5765	0	5545	44	0
3	3	600	0	588	21	0
3	C	600	0	586	14	0
3	c	600	0	587	23	0
4	4	1079	0	1073	5	0
4	D	1079	0	1073	6	0
4	d	1079	0	1073	6	0
5	5	529	0	506	4	0
5	E	529	0	506	1	0
5	e	529	0	506	2	0
6	6	685	0	411	3	0
6	F	676	0	395	5	0
6	f	685	0	411	6	0
7	8	1133	0	1108	6	0
7	L	1133	0	1108	7	0
7	l	1133	0	1108	5	0
8	7	235	0	253	9	0
8	M	235	0	253	7	0
8	m	235	0	253	5	0
9	9	297	0	295	10	0
9	I	297	0	295	6	0
9	i	297	0	295	4	0
10	0	496	0	439	5	0
10	K	496	0	439	5	0
10	k	496	0	439	8	0
11	0	115	0	111	4	0
11	1	2546	0	2430	95	0
11	2	2313	0	2213	97	0
11	8	176	0	177	7	0
11	A	2546	0	2435	96	0
11	B	2313	0	2213	85	0
11	K	115	0	111	3	0
11	L	176	0	177	4	0
11	a	2546	0	2434	94	0
11	b	2313	0	2213	97	0
11	k	115	0	111	5	0
11	l	176	0	177	7	0
12	1	33	0	45	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
12	2	33	0	45	1	0
12	A	33	0	45	2	0
12	B	33	0	45	1	0
12	a	33	0	46	3	0
12	b	33	0	45	1	0
13	1	8	0	0	1	0
13	3	16	0	0	20	0
13	A	8	0	0	3	0
13	C	16	0	0	13	0
13	a	8	0	0	3	0
13	c	16	0	0	20	0
14	1	200	0	242	23	0
14	2	320	0	391	43	0
14	6	120	0	147	20	0
14	7	40	0	49	5	0
14	8	80	0	97	15	0
14	A	200	0	244	26	0
14	B	320	0	390	44	0
14	F	120	0	146	15	0
14	L	80	0	97	14	0
14	M	40	0	49	5	0
14	a	200	0	243	16	0
14	b	320	0	389	38	0
14	f	120	0	147	15	0
14	l	80	0	97	11	0
14	m	40	0	49	4	0
15	1	98	0	148	16	0
15	2	49	0	74	7	0
15	A	98	0	148	9	0
15	B	49	0	74	4	0
15	a	98	0	148	11	0
15	b	49	0	74	5	0
16	2	55	0	86	2	0
16	B	55	0	86	1	0
16	b	55	0	86	0	0
All	All	68370	0	66274	1011	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 8.

The worst 5 of 1011 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:48:CYS:SG	13:C:3002:SF4:FE4	0.75	1.74
3:3:48:CYS:SG	13:3:3002:SF4:FE4	0.87	1.64
1:a:56:HIS:CG	11:a:1103:CLA:HBB2	1.23	1.62
3:3:11:CYS:SG	13:3:3003:SF4:FE3	0.88	1.61
3:c:58:CYS:SG	13:c:3003:SF4:FE1	0.94	1.57

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	1	737/751 (98%)	697 (95%)	38 (5%)	2 (0%)	36	67
1	A	737/751 (98%)	693 (94%)	42 (6%)	2 (0%)	36	67
1	a	737/751 (98%)	698 (95%)	37 (5%)	2 (0%)	36	67
2	2	726/731 (99%)	691 (95%)	28 (4%)	7 (1%)	12	43
2	B	726/731 (99%)	690 (95%)	30 (4%)	6 (1%)	16	48
2	b	726/731 (99%)	692 (95%)	28 (4%)	6 (1%)	16	48
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%)	18	51
4	D	136/141 (96%)	122 (90%)	13 (10%)	1 (1%)	18	51
4	d	136/141 (96%)	122 (90%)	13 (10%)	1 (1%)	18	51
5	5	66/74 (89%)	58 (88%)	7 (11%)	1 (2%)	8	36
5	E	66/74 (89%)	57 (86%)	8 (12%)	1 (2%)	8	36
5	e	66/74 (89%)	58 (88%)	7 (11%)	1 (2%)	8	36
6	6	123/125 (98%)	115 (94%)	6 (5%)	2 (2%)	7	35

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
6	F	123/125 (98%)	114 (93%)	6 (5%)	3 (2%)	4	29
6	f	123/125 (98%)	115 (94%)	6 (5%)	2 (2%)	7	35
7	8	149/157 (95%)	135 (91%)	12 (8%)	2 (1%)	9	38
7	L	149/157 (95%)	135 (91%)	11 (7%)	3 (2%)	6	32
7	l	149/157 (95%)	135 (91%)	12 (8%)	2 (1%)	9	38
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%)	1	17
10	K	78/128 (61%)	66 (85%)	7 (9%)	5 (6%)	1	14
10	k	78/128 (61%)	66 (85%)	9 (12%)	3 (4%)	2	21
All	All	6474/6777 (96%)	6056 (94%)	361 (6%)	57 (1%)	14	45

5 of 57 Ramachandran outliers are listed below:

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

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	1	588/603 (98%)	568 (97%)	20 (3%)	32	55
1	A	588/603 (98%)	568 (97%)	20 (3%)	32	55

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	a	588/603 (98%)	569 (97%)	19 (3%)	34	56
2	2	582/583 (100%)	557 (96%)	25 (4%)	26	50
2	B	582/583 (100%)	559 (96%)	23 (4%)	28	52
2	b	582/583 (100%)	557 (96%)	25 (4%)	26	50
3	3	68/69 (99%)	66 (97%)	2 (3%)	37	58
3	C	68/69 (99%)	63 (93%)	5 (7%)	13	38
3	c	68/69 (99%)	65 (96%)	3 (4%)	25	49
4	4	113/116 (97%)	108 (96%)	5 (4%)	25	49
4	D	113/116 (97%)	109 (96%)	4 (4%)	32	54
4	d	113/116 (97%)	109 (96%)	4 (4%)	32	54
5	5	56/60 (93%)	53 (95%)	3 (5%)	20	45
5	E	56/60 (93%)	53 (95%)	3 (5%)	20	45
5	e	56/60 (93%)	53 (95%)	3 (5%)	20	45
6	6	21/106 (20%)	21 (100%)	0	100	100
6	F	19/106 (18%)	19 (100%)	0	100	100
6	f	21/106 (20%)	20 (95%)	1 (5%)	23	47
7	8	113/118 (96%)	111 (98%)	2 (2%)	51	67
7	L	113/118 (96%)	111 (98%)	2 (2%)	51	67
7	l	113/118 (96%)	111 (98%)	2 (2%)	51	67
8	7	24/25 (96%)	23 (96%)	1 (4%)	26	50
8	M	24/25 (96%)	23 (96%)	1 (4%)	26	50
8	m	24/25 (96%)	23 (96%)	1 (4%)	26	50
9	9	31/32 (97%)	27 (87%)	4 (13%)	4	20
9	I	31/32 (97%)	27 (87%)	4 (13%)	4	20
9	i	31/32 (97%)	27 (87%)	4 (13%)	4	20
10	0	37/100 (37%)	31 (84%)	6 (16%)	2	14
10	K	37/100 (37%)	31 (84%)	6 (16%)	2	14
10	k	37/100 (37%)	32 (86%)	5 (14%)	4	19
All	All	4897/5436 (90%)	4694 (96%)	203 (4%)	27	51

5 of 203 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
9	i	27	MET
2	2	145	LEU
10	0	104	LEU
8	m	5	ASP
1	1	368	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 65 such sidechains are listed below:

Mol	Chain	Res	Type
2	2	317	HIS
2	2	373	HIS
7	L	105	GLN
4	D	64	GLN
2	2	437	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides 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	A	1126	-	69,73,73	2.38	21 (30%)	82,113,113	2.56	26 (31%)
11	CLA	a	1105	-	52,56,73	2.74	21 (40%)	61,92,113	2.81	23 (37%)
11	CLA	2	1206	2	69,73,73	2.35	21 (30%)	82,113,113	2.39	24 (29%)
14	BCR	L	4019	-	41,41,41	2.53	6 (14%)	56,56,56	6.74	24 (42%)
11	CLA	1	1105	-	52,56,73	2.72	22 (42%)	61,92,113	2.78	23 (37%)
14	BCR	1	4001	-	41,41,41	2.57	6 (14%)	56,56,56	6.70	27 (48%)
14	BCR	B	4005	-	41,41,41	2.61	7 (17%)	56,56,56	6.69	25 (44%)
11	CLA	A	1131	-	69,73,73	2.38	21 (30%)	82,113,113	2.43	27 (32%)
11	CLA	A	1121	-	50,54,73	2.85	22 (44%)	59,90,113	2.71	20 (33%)
14	BCR	b	4010	-	41,41,41	2.61	6 (14%)	56,56,56	6.86	21 (37%)
11	CLA	2	1236	-	51,55,73	2.72	23 (45%)	60,91,113	2.84	22 (36%)
11	CLA	1	1127	-	69,73,73	2.38	22 (31%)	82,113,113	2.39	25 (30%)
14	BCR	m	4021	-	41,41,41	2.64	6 (14%)	56,56,56	6.66	24 (42%)
11	CLA	a	1108	-	49,53,73	2.70	21 (42%)	58,89,113	2.76	22 (37%)
11	CLA	b	1201	-	58,62,73	2.57	22 (37%)	68,99,113	2.70	26 (38%)
13	SF4	A	3001	1,2	0,12,12	-	-	-	-	-
11	CLA	A	1114	-	50,54,73	2.84	22 (44%)	59,90,113	2.66	21 (35%)
15	LHG	b	5004	-	48,48,48	0.94	2 (4%)	51,54,54	1.06	4 (7%)
11	CLA	A	1106	1	69,73,73	2.38	21 (30%)	82,113,113	2.46	23 (28%)
11	CLA	B	1228	-	54,58,73	2.69	22 (40%)	64,95,113	2.71	23 (35%)
11	CLA	b	1202	-	69,73,73	2.36	22 (31%)	82,113,113	2.49	24 (29%)
11	CLA	a	1134	-	50,54,73	2.83	22 (44%)	59,90,113	2.75	24 (40%)
11	CLA	A	1122	-	63,67,73	2.46	21 (33%)	74,105,113	2.70	26 (35%)
11	CLA	1	1107	-	69,73,73	2.37	22 (31%)	82,113,113	2.48	25 (30%)
11	CLA	1	1132	-	69,73,73	2.35	22 (31%)	82,113,113	2.40	24 (29%)
11	CLA	2	1211	-	50,54,73	2.81	21 (42%)	59,90,113	2.76	21 (35%)
11	CLA	A	1107	1	69,73,73	2.33	21 (30%)	82,113,113	2.52	26 (31%)
11	CLA	A	1103	-	69,73,73	2.36	22 (31%)	82,113,113	2.51	26 (31%)
12	PQN	B	2002	-	34,34,34	1.68	2 (5%)	43,45,45	1.17	4 (9%)
11	CLA	a	1107	1	69,73,73	2.35	21 (30%)	82,113,113	2.61	29 (35%)
12	PQN	1	2001	-	34,34,34	1.70	2 (5%)	43,45,45	1.12	4 (9%)
14	BCR	B	4009	-	41,41,41	2.58	6 (14%)	56,56,56	6.86	21 (37%)
11	CLA	A	1101	-	69,73,73	2.34	22 (31%)	82,113,113	2.44	26 (31%)
11	CLA	1	1101	-	69,73,73	2.36	21 (30%)	82,113,113	2.47	28 (34%)
11	CLA	A	1109	11	69,73,73	2.38	22 (31%)	82,113,113	2.52	24 (29%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
11	CLA	b	1234	-	64,68,73	2.46	21 (32%)	76,107,113	2.53	25 (32%)
11	CLA	1	1237	-	59,63,73	2.52	22 (37%)	70,101,113	2.67	27 (38%)
14	BCR	B	4017	-	41,41,41	2.60	7 (17%)	56,56,56	6.76	29 (51%)
11	CLA	a	1123	-	69,73,73	2.37	21 (30%)	82,113,113	2.43	25 (30%)
11	CLA	A	1134	1	50,54,73	2.83	22 (44%)	59,90,113	2.72	23 (38%)
11	CLA	l	1503	-	69,73,73	2.36	22 (31%)	82,113,113	2.44	24 (29%)
14	BCR	A	4002	-	41,41,41	2.57	7 (17%)	56,56,56	6.45	23 (41%)
11	CLA	b	1213	-	69,73,73	2.37	23 (33%)	82,113,113	2.48	25 (30%)
11	CLA	1	1114	-	50,54,73	2.85	22 (44%)	59,90,113	2.70	21 (35%)
11	CLA	a	1114	-	50,54,73	2.84	21 (42%)	59,90,113	2.69	21 (35%)
11	CLA	2	1217	-	51,55,73	2.73	21 (41%)	60,91,113	2.80	25 (41%)
11	CLA	A	1129	-	50,54,73	2.82	22 (44%)	59,90,113	2.67	23 (38%)
11	CLA	A	1112	-	49,53,73	2.71	21 (42%)	58,89,113	2.84	24 (41%)
14	BCR	a	4001	-	41,41,41	2.57	6 (14%)	56,56,56	6.67	25 (44%)
14	BCR	B	4010	-	41,41,41	2.57	6 (14%)	56,56,56	6.56	26 (46%)
11	CLA	K	1402	-	54,58,73	2.66	22 (40%)	64,95,113	2.68	23 (35%)
11	CLA	b	1209	-	49,53,73	2.71	21 (42%)	58,89,113	2.76	22 (37%)
11	CLA	8	1503	-	69,73,73	2.39	22 (31%)	82,113,113	2.41	24 (29%)
13	SF4	3	3002	3	0,12,12	-	-	-	-	-
11	CLA	k	1402	-	54,58,73	2.68	22 (40%)	64,95,113	2.71	24 (37%)
11	CLA	a	1139	-	54,58,73	2.70	21 (38%)	64,95,113	2.69	23 (35%)
11	CLA	b	1222	-	60,64,73	2.54	22 (36%)	71,102,113	2.76	26 (36%)
11	CLA	L	1501	7	69,73,73	2.37	22 (31%)	82,113,113	2.47	25 (30%)
11	CLA	a	1116	-	58,62,73	2.60	22 (37%)	68,99,113	2.66	27 (39%)
11	CLA	B	1227	-	49,53,73	2.68	20 (40%)	58,89,113	2.86	22 (37%)
11	CLA	1	1128	-	69,73,73	2.36	21 (30%)	82,113,113	2.37	25 (30%)
11	CLA	a	1128	-	69,73,73	2.37	21 (30%)	82,113,113	2.43	26 (31%)
14	BCR	7	4021	-	41,41,41	2.60	6 (14%)	56,56,56	6.77	21 (37%)
11	CLA	1	1124	-	59,63,73	2.55	22 (37%)	70,101,113	2.67	25 (35%)
11	CLA	B	1023	-	69,73,73	2.32	22 (31%)	82,113,113	2.51	30 (36%)
11	CLA	a	1126	-	69,73,73	2.38	23 (33%)	82,113,113	2.49	25 (30%)
11	CLA	b	1208	-	49,53,73	2.71	21 (42%)	58,89,113	2.76	21 (36%)
11	CLA	2	1013	-	69,73,73	2.37	22 (31%)	82,113,113	2.51	28 (34%)
11	CLA	1	1126	-	69,73,73	2.38	23 (33%)	82,113,113	2.50	29 (35%)
11	CLA	1	1112	-	49,53,73	2.70	21 (42%)	58,89,113	2.80	24 (41%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
11	CLA	K	1401	-	69,73,73	2.37	21 (30%)	82,113,113	2.55	29 (35%)
11	CLA	a	1110	-	58,62,73	2.59	22 (37%)	68,99,113	2.64	27 (39%)
11	CLA	1	1104	-	69,73,73	2.34	21 (30%)	82,113,113	2.52	27 (32%)
11	CLA	1	1137	-	69,73,73	2.36	22 (31%)	82,113,113	2.60	25 (30%)
11	CLA	1	1801	15	56,60,73	2.65	22 (39%)	65,97,113	2.78	26 (40%)
11	CLA	2	1212	-	49,53,73	2.69	21 (42%)	58,89,113	2.71	22 (37%)
11	CLA	1	1131	-	69,73,73	2.36	22 (31%)	82,113,113	2.46	25 (30%)
15	LHG	a	5003	11	48,48,48	0.94	2 (4%)	51,54,54	1.05	3 (5%)
11	CLA	a	1104	-	69,73,73	2.34	22 (31%)	82,113,113	2.51	28 (34%)
11	CLA	A	1108	-	49,53,73	2.68	21 (42%)	58,89,113	2.76	23 (39%)
11	CLA	1	1140	-	69,73,73	2.38	22 (31%)	82,113,113	2.55	27 (32%)
11	CLA	B	1214	-	63,67,73	2.46	22 (34%)	74,105,113	2.72	28 (37%)
14	BCR	B	4011	-	41,41,41	2.63	7 (17%)	56,56,56	6.86	27 (48%)
11	CLA	0	1402	-	54,58,73	2.70	22 (40%)	64,95,113	2.72	22 (34%)
11	CLA	1	1106	1	69,73,73	2.37	22 (31%)	82,113,113	2.41	26 (31%)
11	CLA	2	1228	-	54,58,73	2.68	22 (40%)	64,95,113	2.72	25 (39%)
13	SF4	3	3003	-	0,12,12	-	-	-	-	-
11	CLA	0	1401	-	69,73,73	2.37	21 (30%)	82,113,113	2.56	29 (35%)
12	PQN	a	2001	-	34,34,34	1.66	2 (5%)	43,45,45	1.06	4 (9%)
11	CLA	A	1119	-	69,73,73	2.36	22 (31%)	82,113,113	2.38	28 (34%)
11	CLA	a	1801	15	56,60,73	2.65	22 (39%)	65,97,113	2.74	24 (36%)
13	SF4	c	3003	3	0,12,12	-	-	-	-	-
14	BCR	2	4005	-	41,41,41	2.58	7 (17%)	56,56,56	6.53	20 (35%)
11	CLA	a	1101	-	69,73,73	2.38	22 (31%)	82,113,113	2.47	26 (31%)
11	CLA	B	1211	-	50,54,73	2.82	21 (42%)	59,90,113	2.71	21 (35%)
11	CLA	1	1139	-	54,58,73	2.69	23 (42%)	64,95,113	2.71	24 (37%)
12	PQN	2	2002	-	34,34,34	1.67	2 (5%)	43,45,45	1.12	7 (16%)
14	BCR	2	4009	-	41,41,41	2.55	6 (14%)	56,56,56	6.91	23 (41%)
11	CLA	A	1104	-	69,73,73	2.31	21 (30%)	82,113,113	2.62	28 (34%)
11	CLA	A	1137	-	69,73,73	2.37	23 (33%)	82,113,113	2.61	28 (34%)
11	CLA	1	1122	-	63,67,73	2.49	22 (34%)	74,105,113	2.58	25 (33%)
11	CLA	b	1211	-	50,54,73	2.84	22 (44%)	59,90,113	2.72	22 (37%)
11	CLA	A	1116	-	58,62,73	2.60	23 (39%)	68,99,113	2.67	27 (39%)
11	CLA	a	1103	-	69,73,73	2.39	22 (31%)	82,113,113	2.43	25 (30%)
14	BCR	1	4007	-	41,41,41	2.55	6 (14%)	56,56,56	6.82	25 (44%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
11	CLA	A	1133	-	50,54,73	2.82	21 (42%)	59,90,113	2.76	24 (40%)
11	CLA	A	1127	-	69,73,73	2.35	21 (30%)	82,113,113	2.47	26 (31%)
11	CLA	b	1212	-	49,53,73	2.68	22 (44%)	58,89,113	2.81	20 (34%)
11	CLA	B	1222	-	60,64,73	2.56	22 (36%)	71,102,113	2.74	28 (39%)
11	CLA	1	1130	-	50,54,73	2.85	22 (44%)	59,90,113	2.66	21 (35%)
14	BCR	f	4020	-	41,41,41	2.61	6 (14%)	56,56,56	6.73	22 (39%)
11	CLA	A	1118	-	65,69,73	2.40	20 (30%)	77,108,113	2.56	25 (32%)
14	BCR	a	4002	-	41,41,41	2.59	7 (17%)	56,56,56	6.74	24 (42%)
11	CLA	1	1022	-	69,73,73	2.38	22 (31%)	82,113,113	2.38	28 (34%)
11	CLA	b	1216	-	69,73,73	2.39	22 (31%)	82,113,113	2.43	29 (35%)
14	BCR	1	4002	-	41,41,41	2.56	7 (17%)	56,56,56	7.09	22 (39%)
14	BCR	b	4004	-	41,41,41	2.56	6 (14%)	56,56,56	6.72	25 (44%)
14	BCR	f	4018	-	41,41,41	2.66	7 (17%)	56,56,56	6.50	25 (44%)
11	CLA	b	1230	-	62,66,73	2.53	21 (33%)	73,104,113	2.64	27 (36%)
11	CLA	2	1023	-	69,73,73	2.35	22 (31%)	82,113,113	2.59	30 (36%)
11	CLA	B	1238	-	69,73,73	2.34	20 (28%)	82,113,113	2.43	23 (28%)
14	BCR	2	4010	-	41,41,41	2.65	7 (17%)	56,56,56	6.55	27 (48%)
11	CLA	B	1217	-	51,55,73	2.71	22 (43%)	60,91,113	2.79	23 (38%)
11	CLA	2	1232	-	49,53,73	2.71	22 (44%)	58,89,113	2.72	22 (37%)
11	CLA	b	1210	-	69,73,73	2.38	22 (31%)	82,113,113	2.48	31 (37%)
11	CLA	a	1109	11	69,73,73	2.39	22 (31%)	82,113,113	2.51	25 (30%)
15	LHG	1	5001	-	48,48,48	0.95	2 (4%)	51,54,54	1.10	4 (7%)
11	CLA	a	1130	-	50,54,73	2.86	22 (44%)	59,90,113	2.69	21 (35%)
11	CLA	b	1021	-	69,73,73	2.38	22 (31%)	82,113,113	2.54	32 (39%)
11	CLA	b	1231	-	49,53,73	2.69	21 (42%)	58,89,113	2.78	23 (39%)
11	CLA	B	1203	-	69,73,73	2.35	21 (30%)	82,113,113	2.47	23 (28%)
11	CLA	1	1109	-	69,73,73	2.36	21 (30%)	82,113,113	2.49	25 (30%)
11	CLA	2	1224	-	59,63,73	2.53	21 (35%)	70,101,113	2.81	27 (38%)
11	CLA	A	1136	-	50,54,73	2.81	22 (44%)	59,90,113	2.76	23 (38%)
11	CLA	1	1108	-	49,53,73	2.70	21 (42%)	58,89,113	2.76	20 (34%)
11	CLA	1	1118	-	65,69,73	2.41	21 (32%)	77,108,113	2.49	27 (35%)
14	BCR	6	4013	-	41,41,41	2.56	6 (14%)	56,56,56	6.77	23 (41%)
14	BCR	b	4011	-	41,41,41	2.58	7 (17%)	56,56,56	6.94	25 (44%)
14	BCR	F	4020	-	41,41,41	2.61	6 (14%)	56,56,56	6.57	23 (41%)
11	CLA	2	1223	-	69,73,73	2.38	22 (31%)	82,113,113	2.47	29 (35%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
11	CLA	A	1130	-	50,54,73	2.83	21 (42%)	59,90,113	2.70	20 (33%)
11	CLA	2	1213	-	69,73,73	2.41	23 (33%)	82,113,113	2.56	27 (32%)
16	LMG	b	5002	-	55,55,55	0.89	2 (3%)	63,63,63	1.04	4 (6%)
11	CLA	b	1023	-	69,73,73	2.34	21 (30%)	82,113,113	2.51	29 (35%)
14	BCR	B	4014	-	41,41,41	2.59	7 (17%)	56,56,56	6.44	24 (42%)
11	CLA	a	1140	-	69,73,73	2.36	21 (30%)	82,113,113	2.46	26 (31%)
11	CLA	b	1221	-	58,62,73	2.58	23 (39%)	68,99,113	2.80	27 (39%)
15	LHG	1	5003	11	48,48,48	0.96	2 (4%)	51,54,54	1.05	3 (5%)
11	CLA	2	1226	-	69,73,73	2.35	21 (30%)	82,113,113	2.51	24 (29%)
11	CLA	2	1209	-	49,53,73	2.71	21 (42%)	58,89,113	2.75	23 (39%)
11	CLA	b	1203	-	69,73,73	2.36	23 (33%)	82,113,113	2.47	24 (29%)
11	CLA	A	1125	-	56,60,73	2.65	21 (37%)	65,97,113	2.81	29 (44%)
11	CLA	2	1240	15	49,53,73	2.71	21 (42%)	58,89,113	2.70	21 (36%)
11	CLA	2	1208	-	49,53,73	2.69	21 (42%)	58,89,113	2.72	19 (32%)
11	CLA	2	1219	-	59,63,73	2.58	23 (38%)	70,101,113	2.67	25 (35%)
14	BCR	2	4006	-	41,41,41	2.56	6 (14%)	56,56,56	6.98	28 (50%)
11	CLA	B	1210	-	69,73,73	2.37	22 (31%)	82,113,113	2.49	27 (32%)
14	BCR	b	4006	-	41,41,41	2.59	6 (14%)	56,56,56	7.09	26 (46%)
11	CLA	2	1231	-	49,53,73	2.71	21 (42%)	58,89,113	2.83	26 (44%)
11	CLA	1	1119	-	69,73,73	2.36	21 (30%)	82,113,113	2.48	27 (32%)
11	CLA	2	1220	-	50,54,73	2.83	21 (42%)	59,90,113	2.73	21 (35%)
11	CLA	2	1205	-	59,63,73	2.50	20 (33%)	70,101,113	2.69	24 (34%)
11	CLA	B	1201	-	58,62,73	2.56	22 (37%)	68,99,113	2.72	28 (41%)
11	CLA	a	1112	-	49,53,73	2.70	20 (40%)	58,89,113	2.75	23 (39%)
11	CLA	b	1217	-	51,55,73	2.72	23 (45%)	60,91,113	2.79	21 (35%)
11	CLA	B	1215	-	69,73,73	2.36	22 (31%)	82,113,113	2.57	27 (32%)
11	CLA	b	1205	-	59,63,73	2.53	21 (35%)	70,101,113	2.65	25 (35%)
14	BCR	a	4007	-	41,41,41	2.55	6 (14%)	56,56,56	6.90	23 (41%)
11	CLA	A	1128	-	69,73,73	2.34	20 (28%)	82,113,113	2.40	25 (30%)
11	CLA	1	1011	-	69,73,73	2.35	22 (31%)	82,113,113	2.67	26 (31%)
11	CLA	2	1214	-	63,67,73	2.48	21 (33%)	74,105,113	2.53	26 (35%)
11	CLA	A	1115	-	50,54,73	2.86	23 (46%)	59,90,113	2.75	23 (38%)
11	CLA	a	1115	-	50,54,73	2.84	23 (46%)	59,90,113	2.71	23 (38%)
13	SF4	c	3002	3	0,12,12	-	-	-	-	-
11	CLA	A	1132	-	69,73,73	2.37	21 (30%)	82,113,113	2.53	25 (30%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
11	CLA	b	1235	-	64,68,73	2.47	23 (35%)	76,107,113	2.60	29 (38%)
14	BCR	l	4022	-	41,41,41	2.57	6 (14%)	56,56,56	6.56	26 (46%)
14	BCR	A	4008	-	41,41,41	2.55	7 (17%)	56,56,56	6.83	29 (51%)
11	CLA	b	1223	-	69,73,73	2.38	21 (30%)	82,113,113	2.40	26 (31%)
11	CLA	B	1224	-	59,63,73	2.53	22 (37%)	70,101,113	2.82	25 (35%)
12	PQN	A	2001	-	34,34,34	1.68	2 (5%)	43,45,45	1.16	5 (11%)
11	CLA	b	1228	-	54,58,73	2.68	22 (40%)	64,95,113	2.71	24 (37%)
14	BCR	M	4021	-	41,41,41	2.60	6 (14%)	56,56,56	6.73	19 (33%)
11	CLA	2	1238	-	69,73,73	2.36	22 (31%)	82,113,113	2.40	25 (30%)
11	CLA	1	1125	-	56,60,73	2.62	22 (39%)	65,97,113	2.77	27 (41%)
14	BCR	f	4013	-	41,41,41	2.62	6 (14%)	56,56,56	6.76	22 (39%)
15	LHG	a	5001	-	48,48,48	0.96	2 (4%)	51,54,54	1.08	4 (7%)
11	CLA	b	1240	-	49,53,73	2.72	22 (44%)	58,89,113	2.75	21 (36%)
11	CLA	B	1218	-	49,53,73	2.69	21 (42%)	58,89,113	2.77	21 (36%)
14	BCR	B	4004	-	41,41,41	2.61	6 (14%)	56,56,56	6.71	27 (48%)
11	CLA	a	1011	-	69,73,73	2.38	23 (33%)	82,113,113	2.47	26 (31%)
11	CLA	a	1131	-	69,73,73	2.37	21 (30%)	82,113,113	2.44	29 (35%)
11	CLA	B	1234	-	64,68,73	2.43	21 (32%)	76,107,113	2.60	29 (38%)
11	CLA	2	1229	-	69,73,73	2.37	23 (33%)	82,113,113	2.46	27 (32%)
11	CLA	k	1401	-	69,73,73	2.37	21 (30%)	82,113,113	2.56	29 (35%)
11	CLA	1	1111	-	64,68,73	2.41	21 (32%)	76,107,113	2.68	30 (39%)
11	CLA	a	1118	-	65,69,73	2.41	22 (33%)	77,108,113	2.54	26 (33%)
11	CLA	1	1116	-	58,62,73	2.59	22 (37%)	68,99,113	2.68	26 (38%)
11	CLA	b	1236	-	51,55,73	2.71	23 (45%)	60,91,113	2.87	21 (35%)
11	CLA	1	1117	-	69,73,73	2.38	22 (31%)	82,113,113	2.43	26 (31%)
11	CLA	a	1111	-	64,68,73	2.41	23 (35%)	76,107,113	2.62	29 (38%)
14	BCR	b	4005	-	41,41,41	2.58	6 (14%)	56,56,56	6.74	25 (44%)
11	CLA	b	1226	-	69,73,73	2.35	22 (31%)	82,113,113	2.44	27 (32%)
11	CLA	1	1133	-	50,54,73	2.84	21 (42%)	59,90,113	2.70	22 (37%)
11	CLA	A	1801	15	56,60,73	2.68	22 (39%)	65,97,113	2.75	28 (43%)
11	CLA	B	1240	15	49,53,73	2.72	22 (44%)	58,89,113	2.74	23 (39%)
11	CLA	a	1125	-	56,60,73	2.60	22 (39%)	65,97,113	2.70	24 (36%)
14	BCR	l	4019	-	41,41,41	2.59	6 (14%)	56,56,56	6.87	20 (35%)
11	CLA	a	1117	-	69,73,73	2.37	22 (31%)	82,113,113	2.47	26 (31%)
11	CLA	A	1012	-	69,73,73	2.35	22 (31%)	82,113,113	2.56	27 (32%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
11	CLA	B	1232	-	49,53,73	2.70	20 (40%)	58,89,113	2.74	21 (36%)
13	SF4	C	3002	3	0,12,12	-	-	-		
11	CLA	B	1223	-	69,73,73	2.38	22 (31%)	82,113,113	2.48	28 (34%)
11	CLA	2	1235	-	64,68,73	2.46	23 (35%)	76,107,113	2.58	29 (38%)
11	CLA	B	1213	-	69,73,73	2.37	22 (31%)	82,113,113	2.48	25 (30%)
11	CLA	1	1121	-	50,54,73	2.84	22 (44%)	59,90,113	2.76	22 (37%)
11	CLA	2	1021	-	69,73,73	2.36	22 (31%)	82,113,113	2.53	30 (36%)
11	CLA	A	1124	-	59,63,73	2.56	22 (37%)	70,101,113	2.66	29 (41%)
11	CLA	L	1502	-	50,54,73	2.81	20 (40%)	59,90,113	2.80	21 (35%)
14	BCR	8	4019	-	41,41,41	2.58	6 (14%)	56,56,56	6.80	22 (39%)
11	CLA	b	1239	-	50,54,73	2.84	22 (44%)	59,90,113	2.76	23 (38%)
11	CLA	2	1227	-	49,53,73	2.68	20 (40%)	58,89,113	2.82	22 (37%)
11	CLA	B	1219	-	59,63,73	2.56	22 (37%)	70,101,113	2.57	25 (35%)
11	CLA	a	1127	-	69,73,73	2.37	22 (31%)	82,113,113	2.45	31 (37%)
11	CLA	a	1022	-	69,73,73	2.37	21 (30%)	82,113,113	2.35	24 (29%)
11	CLA	a	1129	-	50,54,73	2.82	22 (44%)	59,90,113	2.78	21 (35%)
11	CLA	B	1209	-	49,53,73	2.70	21 (42%)	58,89,113	2.74	22 (37%)
11	CLA	B	1231	-	49,53,73	2.70	21 (42%)	58,89,113	2.79	24 (41%)
11	CLA	B	1220	-	50,54,73	2.82	21 (42%)	59,90,113	2.65	21 (35%)
11	CLA	A	1102	11	69,73,73	2.38	22 (31%)	82,113,113	2.48	27 (32%)
11	CLA	2	1221	-	58,62,73	2.57	23 (39%)	68,99,113	2.72	26 (38%)
11	CLA	B	1208	-	49,53,73	2.70	22 (44%)	58,89,113	2.76	21 (36%)
11	CLA	b	1220	-	50,54,73	2.87	21 (42%)	59,90,113	2.68	22 (37%)
11	CLA	8	1501	-	69,73,73	2.35	22 (31%)	82,113,113	2.53	27 (32%)
11	CLA	2	1202	-	69,73,73	2.38	22 (31%)	82,113,113	2.48	24 (29%)
16	LMG	2	5002	-	55,55,55	0.91	2 (3%)	63,63,63	1.07	4 (6%)
11	CLA	B	1212	-	49,53,73	2.70	22 (44%)	58,89,113	2.74	21 (36%)
11	CLA	b	1215	-	69,73,73	2.39	22 (31%)	82,113,113	2.53	29 (35%)
11	CLA	A	1111	-	64,68,73	2.43	22 (34%)	76,107,113	2.56	25 (32%)
11	CLA	b	1238	-	69,73,73	2.36	22 (31%)	82,113,113	2.41	25 (30%)
14	BCR	1	4003	-	41,41,41	2.60	6 (14%)	56,56,56	6.53	27 (48%)
11	CLA	1	1012	-	69,73,73	2.37	21 (30%)	82,113,113	2.52	26 (31%)
15	LHG	A	5001	-	48,48,48	0.93	2 (4%)	51,54,54	1.15	4 (7%)
11	CLA	A	1011	-	69,73,73	2.34	22 (31%)	82,113,113	2.49	25 (30%)
11	CLA	b	1206	2	69,73,73	2.36	21 (30%)	82,113,113	2.42	25 (30%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
11	CLA	1	1110	-	58,62,73	2.59	22 (37%)	68,99,113	2.70	26 (38%)
11	CLA	a	1135	-	55,59,73	2.65	21 (38%)	64,96,113	2.74	25 (39%)
15	LHG	A	5003	11	48,48,48	0.95	2 (4%)	51,54,54	1.15	4 (7%)
11	CLA	a	1124	-	59,63,73	2.56	22 (37%)	70,101,113	2.71	27 (38%)
11	CLA	2	1230	-	62,66,73	2.51	22 (35%)	73,104,113	2.62	27 (36%)
11	CLA	B	1229	-	69,73,73	2.37	22 (31%)	82,113,113	2.45	28 (34%)
11	CLA	l	1501	7	69,73,73	2.37	23 (33%)	82,113,113	2.50	25 (30%)
11	CLA	1	1129	-	50,54,73	2.84	22 (44%)	59,90,113	2.77	21 (35%)
14	BCR	2	4011	-	41,41,41	2.62	7 (17%)	56,56,56	6.92	25 (44%)
11	CLA	B	1225	-	69,73,73	2.37	22 (31%)	82,113,113	2.37	25 (30%)
15	LHG	2	5004	11	48,48,48	0.96	2 (4%)	51,54,54	1.07	3 (5%)
14	BCR	1	4008	-	41,41,41	2.58	7 (17%)	56,56,56	6.94	26 (46%)
11	CLA	A	1120	-	50,54,73	2.86	22 (44%)	59,90,113	2.75	22 (37%)
11	CLA	A	1139	-	54,58,73	2.68	23 (42%)	64,95,113	2.71	24 (37%)
14	BCR	8	4022	-	41,41,41	2.59	6 (14%)	56,56,56	6.65	30 (53%)
11	CLA	b	1207	-	69,73,73	2.34	21 (30%)	82,113,113	2.53	26 (31%)
14	BCR	a	4008	-	41,41,41	2.60	7 (17%)	56,56,56	6.71	28 (50%)
14	BCR	A	4007	-	41,41,41	2.59	7 (17%)	56,56,56	6.97	21 (37%)
14	BCR	a	4003	-	41,41,41	2.60	6 (14%)	56,56,56	6.33	27 (48%)
12	PQN	b	2002	-	34,34,34	1.67	2 (5%)	43,45,45	1.14	5 (11%)
11	CLA	2	1239	-	50,54,73	2.86	22 (44%)	59,90,113	2.73	22 (37%)
11	CLA	2	1218	-	49,53,73	2.68	21 (42%)	58,89,113	2.79	22 (37%)
14	BCR	2	4004	-	41,41,41	2.55	6 (14%)	56,56,56	6.62	29 (51%)
14	BCR	F	4013	-	41,41,41	2.60	6 (14%)	56,56,56	6.93	21 (37%)
11	CLA	2	1203	-	69,73,73	2.34	21 (30%)	82,113,113	2.50	28 (34%)
11	CLA	B	1204	-	69,73,73	2.33	21 (30%)	82,113,113	2.49	27 (32%)
11	CLA	B	1216	-	69,73,73	2.37	22 (31%)	82,113,113	2.41	27 (32%)
11	CLA	2	1234	-	64,68,73	2.43	21 (32%)	76,107,113	2.56	27 (35%)
14	BCR	L	4022	-	41,41,41	2.56	6 (14%)	56,56,56	6.25	25 (44%)
11	CLA	a	1106	1	69,73,73	2.37	22 (31%)	82,113,113	2.45	27 (32%)
11	CLA	a	1132	-	69,73,73	2.38	22 (31%)	82,113,113	2.45	26 (31%)
11	CLA	a	1119	-	69,73,73	2.36	22 (31%)	82,113,113	2.45	26 (31%)
11	CLA	b	1218	-	49,53,73	2.71	21 (42%)	58,89,113	2.75	22 (37%)
11	CLA	A	1022	-	69,73,73	2.36	21 (30%)	82,113,113	2.40	28 (34%)
11	CLA	B	1230	-	62,66,73	2.49	20 (32%)	73,104,113	2.60	27 (36%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
11	CLA	a	1137	-	69,73,73	2.37	21 (30%)	82,113,113	2.57	27 (32%)
11	CLA	B	1206	2	69,73,73	2.34	21 (30%)	82,113,113	2.42	26 (31%)
11	CLA	B	1207	-	69,73,73	2.34	21 (30%)	82,113,113	2.57	24 (29%)
11	CLA	A	1110	-	58,62,73	2.58	22 (37%)	68,99,113	2.71	26 (38%)
11	CLA	2	1201	-	58,62,73	2.59	21 (36%)	68,99,113	2.63	24 (35%)
11	CLA	B	1235	-	64,68,73	2.47	23 (35%)	76,107,113	2.55	23 (30%)
14	BCR	b	4009	-	41,41,41	2.50	6 (14%)	56,56,56	7.08	24 (42%)
11	CLA	1	1115	-	50,54,73	2.83	21 (42%)	59,90,113	2.75	22 (37%)
11	CLA	b	1232	-	49,53,73	2.71	21 (42%)	58,89,113	2.71	21 (36%)
11	CLA	1	1103	-	69,73,73	2.36	21 (30%)	82,113,113	2.55	27 (32%)
11	CLA	1	1135	-	55,59,73	2.65	23 (41%)	64,96,113	2.80	25 (39%)
11	CLA	A	1138	-	50,54,73	2.80	22 (44%)	59,90,113	2.83	22 (37%)
11	CLA	l	1502	-	50,54,73	2.81	22 (44%)	59,90,113	2.77	21 (35%)
14	BCR	b	4017	-	41,41,41	2.63	7 (17%)	56,56,56	6.81	27 (48%)
11	CLA	2	1222	-	60,64,73	2.54	22 (36%)	71,102,113	2.67	27 (38%)
11	CLA	B	1021	-	69,73,73	2.33	21 (30%)	82,113,113	2.61	30 (36%)
11	CLA	2	1207	-	69,73,73	2.34	21 (30%)	82,113,113	2.53	27 (32%)
11	CLA	b	1227	-	49,53,73	2.70	20 (40%)	58,89,113	2.83	22 (37%)
13	SF4	C	3003	3	0,12,12	-	-	-	-	-
11	CLA	b	1219	-	59,63,73	2.58	22 (37%)	70,101,113	2.58	25 (35%)
11	CLA	a	1113	-	49,53,73	2.70	21 (42%)	58,89,113	2.73	22 (37%)
11	CLA	A	1105	-	52,56,73	2.71	22 (42%)	61,92,113	2.75	23 (37%)
15	LHG	B	5004	11	48,48,48	0.96	2 (4%)	51,54,54	1.14	4 (7%)
11	CLA	a	1133	-	50,54,73	2.83	21 (42%)	59,90,113	2.75	23 (38%)
11	CLA	A	1117	-	69,73,73	2.41	22 (31%)	82,113,113	2.39	25 (30%)
11	CLA	1	1113	-	49,53,73	2.70	21 (42%)	58,89,113	2.75	22 (37%)
11	CLA	b	1224	-	59,63,73	2.56	23 (38%)	70,101,113	2.71	26 (37%)
11	CLA	1	1102	-	69,73,73	2.38	23 (33%)	82,113,113	2.40	23 (28%)
14	BCR	A	4003	-	41,41,41	2.66	6 (14%)	56,56,56	6.43	24 (42%)
11	CLA	A	1237	-	59,63,73	2.54	22 (37%)	70,101,113	2.63	25 (35%)
11	CLA	a	1012	-	69,73,73	2.38	23 (33%)	82,113,113	2.45	23 (28%)
11	CLA	B	1013	-	69,73,73	2.36	22 (31%)	82,113,113	2.47	27 (32%)
11	CLA	2	1210	-	69,73,73	2.34	22 (31%)	82,113,113	2.54	29 (35%)
16	LMG	B	5002	-	55,55,55	0.90	2 (3%)	63,63,63	1.08	4 (6%)
11	CLA	b	1013	-	69,73,73	2.38	22 (31%)	82,113,113	2.45	28 (34%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
11	CLA	B	1236	-	51,55,73	2.67	22 (43%)	60,91,113	2.88	23 (38%)
11	CLA	A	1123	-	69,73,73	2.35	22 (31%)	82,113,113	2.52	28 (34%)
11	CLA	B	1239	-	50,54,73	2.82	22 (44%)	59,90,113	2.76	20 (33%)
14	BCR	2	4017	-	41,41,41	2.61	7 (17%)	56,56,56	6.69	27 (48%)
11	CLA	2	1225	-	69,73,73	2.38	22 (31%)	82,113,113	2.44	25 (30%)
11	CLA	B	1226	-	69,73,73	2.34	22 (31%)	82,113,113	2.52	27 (32%)
11	CLA	L	1503	-	69,73,73	2.33	20 (28%)	82,113,113	2.50	23 (28%)
14	BCR	2	4014	-	41,41,41	2.61	6 (14%)	56,56,56	6.58	23 (41%)
11	CLA	A	1140	-	69,73,73	2.36	22 (31%)	82,113,113	2.49	26 (31%)
11	CLA	a	1122	-	63,67,73	2.49	22 (34%)	74,105,113	2.63	26 (35%)
11	CLA	b	1214	-	63,67,73	2.47	22 (34%)	74,105,113	2.59	30 (40%)
11	CLA	b	1229	-	69,73,73	2.37	22 (31%)	82,113,113	2.44	26 (31%)
14	BCR	F	4018	-	41,41,41	2.70	7 (17%)	56,56,56	6.72	24 (42%)
11	CLA	a	1120	-	50,54,73	2.84	23 (46%)	59,90,113	2.81	22 (37%)
11	CLA	b	1225	-	69,73,73	2.39	22 (31%)	82,113,113	2.38	24 (29%)
14	BCR	B	4006	-	41,41,41	2.57	6 (14%)	56,56,56	6.97	26 (46%)
13	SF4	1	3001	1,2	0,12,12	-	-	-	-	-
11	CLA	1	1120	-	50,54,73	2.85	23 (46%)	59,90,113	2.76	22 (37%)
13	SF4	a	3001	1,2	0,12,12	-	-	-	-	-
11	CLA	1	1136	-	50,54,73	2.82	21 (42%)	59,90,113	2.76	22 (37%)
14	BCR	A	4001	-	41,41,41	2.60	7 (17%)	56,56,56	6.54	25 (44%)
11	CLA	a	1102	11	69,73,73	2.37	22 (31%)	82,113,113	2.46	25 (30%)
11	CLA	B	1221	-	58,62,73	2.56	21 (36%)	68,99,113	2.73	25 (36%)
11	CLA	a	1121	-	50,54,73	2.85	22 (44%)	59,90,113	2.77	23 (38%)
14	BCR	b	4014	-	41,41,41	2.58	7 (17%)	56,56,56	6.64	23 (41%)
11	CLA	a	1136	-	50,54,73	2.82	21 (42%)	59,90,113	2.77	21 (35%)
11	CLA	a	1237	-	59,63,73	2.53	22 (37%)	70,101,113	2.61	25 (35%)
11	CLA	1	1138	-	50,54,73	2.81	22 (44%)	59,90,113	2.72	20 (33%)
11	CLA	2	1216	-	69,73,73	2.38	23 (33%)	82,113,113	2.44	25 (30%)
11	CLA	B	1202	-	69,73,73	2.39	22 (31%)	82,113,113	2.47	25 (30%)
11	CLA	2	1204	-	69,73,73	2.37	22 (31%)	82,113,113	2.42	26 (31%)
11	CLA	8	1502	-	50,54,73	2.81	22 (44%)	59,90,113	2.80	22 (37%)
14	BCR	6	4020	-	41,41,41	2.67	7 (17%)	56,56,56	6.68	24 (42%)
11	CLA	1	1123	-	69,73,73	2.38	22 (31%)	82,113,113	2.47	24 (29%)
11	CLA	a	1138	-	50,54,73	2.84	22 (44%)	59,90,113	2.81	23 (38%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
11	CLA	b	1204	-	69,73,73	2.35	22 (31%)	82,113,113	2.42	23 (28%)
11	CLA	A	1113	-	49,53,73	2.68	21 (42%)	58,89,113	2.77	22 (37%)
11	CLA	A	1135	-	55,59,73	2.64	22 (40%)	64,96,113	2.78	27 (42%)
11	CLA	1	1134	-	50,54,73	2.84	22 (44%)	59,90,113	2.76	22 (37%)
11	CLA	B	1205	-	59,63,73	2.51	19 (32%)	70,101,113	2.77	24 (34%)
11	CLA	2	1215	-	69,73,73	2.38	21 (30%)	82,113,113	2.56	28 (34%)
14	BCR	6	4018	-	41,41,41	2.68	7 (17%)	56,56,56	6.44	26 (46%)

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	A	1126	-	1/1/15/20	14/39/115/115	-
11	CLA	a	1105	-	1/1/11/20	6/19/95/115	-
11	CLA	2	1206	2	1/1/15/20	16/39/115/115	-
14	BCR	L	4019	-	-	13/29/63/63	0/2/2/2
11	CLA	1	1105	-	1/1/11/20	5/19/95/115	-
14	BCR	1	4001	-	-	11/29/63/63	0/2/2/2
14	BCR	B	4005	-	-	8/29/63/63	0/2/2/2
11	CLA	A	1131	-	1/1/15/20	14/39/115/115	-
11	CLA	A	1121	-	1/1/11/20	5/17/93/115	-
14	BCR	b	4010	-	-	11/29/63/63	0/2/2/2
11	CLA	2	1236	-	1/1/11/20	8/18/94/115	-
11	CLA	1	1127	-	1/1/15/20	17/39/115/115	-
14	BCR	m	4021	-	-	11/29/63/63	0/2/2/2
11	CLA	a	1108	-	1/1/11/20	4/15/91/115	-
11	CLA	b	1201	-	1/1/12/20	10/26/102/115	-
13	SF4	A	3001	1,2	-	-	0/6/5/5
11	CLA	A	1114	-	1/1/11/20	7/17/93/115	-
15	LHG	b	5004	-	-	24/53/53/53	-
11	CLA	A	1106	1	1/1/15/20	17/39/115/115	-
11	CLA	B	1228	-	1/1/12/20	8/21/97/115	-
11	CLA	b	1202	-	1/1/15/20	17/39/115/115	-
11	CLA	a	1134	-	1/1/11/20	5/17/93/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
11	CLA	A	1122	-	1/1/13/20	10/32/108/115	-
11	CLA	1	1107	-	1/1/15/20	14/39/115/115	-
11	CLA	1	1132	-	1/1/15/20	9/39/115/115	-
11	CLA	2	1211	-	1/1/11/20	9/17/93/115	-
11	CLA	A	1107	1	1/1/15/20	13/39/115/115	-
11	CLA	A	1103	-	1/1/15/20	14/39/115/115	-
12	PQN	B	2002	-	-	8/23/43/43	0/2/2/2
11	CLA	a	1107	1	1/1/15/20	11/39/115/115	-
12	PQN	1	2001	-	-	7/23/43/43	0/2/2/2
14	BCR	B	4009	-	-	13/29/63/63	0/2/2/2
11	CLA	A	1101	-	1/1/15/20	17/39/115/115	-
11	CLA	1	1101	-	1/1/15/20	21/39/115/115	-
11	CLA	A	1109	11	-	15/39/115/115	-
11	CLA	b	1234	-	1/1/14/20	14/33/109/115	-
11	CLA	1	1237	-	1/1/13/20	9/27/103/115	-
14	BCR	B	4017	-	-	6/29/63/63	0/2/2/2
11	CLA	a	1123	-	1/1/15/20	16/39/115/115	-
11	CLA	A	1134	1	1/1/11/20	5/17/93/115	-
11	CLA	l	1503	-	1/1/15/20	18/39/115/115	-
14	BCR	A	4002	-	-	13/29/63/63	0/2/2/2
11	CLA	b	1213	-	1/1/15/20	14/39/115/115	-
11	CLA	1	1114	-	1/1/11/20	10/17/93/115	-
11	CLA	a	1114	-	1/1/11/20	6/17/93/115	-
11	CLA	2	1217	-	1/1/11/20	14/18/94/115	-
11	CLA	A	1129	-	1/1/11/20	5/17/93/115	-
11	CLA	A	1112	-	1/1/11/20	9/15/91/115	-
14	BCR	a	4001	-	-	10/29/63/63	0/2/2/2
14	BCR	B	4010	-	-	13/29/63/63	0/2/2/2
11	CLA	K	1402	-	1/1/12/20	6/21/97/115	-
11	CLA	b	1209	-	1/1/11/20	7/15/91/115	-
11	CLA	8	1503	-	1/1/15/20	12/39/115/115	-
13	SF4	3	3002	3	-	-	0/6/5/5
11	CLA	k	1402	-	1/1/12/20	5/21/97/115	-
11	CLA	a	1139	-	1/1/12/20	9/21/97/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
11	CLA	b	1222	-	1/1/13/20	14/29/105/115	-
11	CLA	L	1501	7	1/1/15/20	14/39/115/115	-
11	CLA	a	1116	-	1/1/12/20	9/26/102/115	-
11	CLA	B	1227	-	1/1/11/20	6/15/91/115	-
11	CLA	1	1128	-	1/1/15/20	12/39/115/115	-
11	CLA	a	1128	-	1/1/15/20	10/39/115/115	-
14	BCR	7	4021	-	-	13/29/63/63	0/2/2/2
11	CLA	1	1124	-	1/1/13/20	13/27/103/115	-
11	CLA	B	1023	-	1/1/15/20	14/39/115/115	-
11	CLA	a	1126	-	1/1/15/20	18/39/115/115	-
11	CLA	b	1208	-	1/1/11/20	4/15/91/115	-
11	CLA	2	1013	-	-	15/39/115/115	-
11	CLA	1	1126	-	1/1/15/20	20/39/115/115	-
11	CLA	1	1112	-	1/1/11/20	2/15/91/115	-
11	CLA	K	1401	-	1/1/15/20	22/39/115/115	-
11	CLA	a	1110	-	1/1/12/20	10/26/102/115	-
11	CLA	1	1104	-	1/1/15/20	14/39/115/115	-
11	CLA	1	1137	-	1/1/15/20	18/39/115/115	-
11	CLA	1	1801	15	1/1/12/20	15/24/100/115	-
11	CLA	2	1212	-	1/1/11/20	2/15/91/115	-
11	CLA	1	1131	-	1/1/15/20	22/39/115/115	-
15	LHG	a	5003	11	-	24/53/53/53	-
11	CLA	a	1104	-	1/1/15/20	14/39/115/115	-
11	CLA	A	1108	-	1/1/11/20	3/15/91/115	-
11	CLA	1	1140	-	1/1/15/20	16/39/115/115	-
11	CLA	B	1214	-	1/1/13/20	13/32/108/115	-
14	BCR	B	4011	-	-	13/29/63/63	0/2/2/2
11	CLA	0	1402	-	1/1/12/20	5/21/97/115	-
11	CLA	1	1106	1	1/1/15/20	23/39/115/115	-
11	CLA	2	1228	-	1/1/12/20	5/21/97/115	-
13	SF4	3	3003	-	-	-	0/6/5/5
11	CLA	0	1401	-	1/1/15/20	22/39/115/115	-
12	PQN	a	2001	-	-	6/23/43/43	0/2/2/2
11	CLA	A	1119	-	1/1/15/20	16/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
11	CLA	a	1801	15	1/1/12/20	13/24/100/115	-
13	SF4	c	3003	3	-	-	0/6/5/5
14	BCR	2	4005	-	-	9/29/63/63	0/2/2/2
11	CLA	a	1101	-	1/1/15/20	19/39/115/115	-
11	CLA	B	1211	-	1/1/11/20	7/17/93/115	-
11	CLA	1	1139	-	1/1/12/20	10/21/97/115	-
12	PQN	2	2002	-	-	8/23/43/43	0/2/2/2
14	BCR	2	4009	-	-	15/29/63/63	0/2/2/2
11	CLA	A	1104	-	1/1/15/20	22/39/115/115	-
11	CLA	A	1137	-	1/1/15/20	11/39/115/115	-
11	CLA	1	1122	-	1/1/13/20	18/32/108/115	-
11	CLA	b	1211	-	1/1/11/20	6/17/93/115	-
11	CLA	A	1116	-	1/1/12/20	10/26/102/115	-
11	CLA	a	1103	-	1/1/15/20	19/39/115/115	-
14	BCR	1	4007	-	-	12/29/63/63	0/2/2/2
11	CLA	A	1133	-	1/1/11/20	4/17/93/115	-
11	CLA	A	1127	-	1/1/15/20	12/39/115/115	-
11	CLA	b	1212	-	1/1/11/20	5/15/91/115	-
11	CLA	B	1222	-	1/1/13/20	15/29/105/115	-
11	CLA	1	1130	-	-	5/17/93/115	-
14	BCR	f	4020	-	-	15/29/63/63	0/2/2/2
11	CLA	A	1118	-	1/1/14/20	17/35/111/115	-
14	BCR	a	4002	-	-	15/29/63/63	0/2/2/2
11	CLA	1	1022	-	1/1/15/20	16/39/115/115	-
11	CLA	b	1216	-	1/1/15/20	15/39/115/115	-
14	BCR	1	4002	-	-	13/29/63/63	0/2/2/2
14	BCR	b	4004	-	-	11/29/63/63	0/2/2/2
14	BCR	f	4018	-	-	6/29/63/63	0/2/2/2
11	CLA	b	1230	-	1/1/13/20	12/31/107/115	-
11	CLA	2	1023	-	1/1/15/20	14/39/115/115	-
11	CLA	B	1238	-	1/1/15/20	11/39/115/115	-
14	BCR	2	4010	-	-	10/29/63/63	0/2/2/2
11	CLA	B	1217	-	1/1/11/20	12/18/94/115	-
11	CLA	2	1232	-	1/1/11/20	7/15/91/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
11	CLA	b	1210	-	1/1/15/20	18/39/115/115	-
11	CLA	a	1109	11	-	19/39/115/115	-
15	LHG	1	5001	-	-	25/53/53/53	-
11	CLA	a	1130	-	-	7/17/93/115	-
11	CLA	b	1021	-	1/1/15/20	23/39/115/115	-
11	CLA	b	1231	-	1/1/11/20	7/15/91/115	-
11	CLA	B	1203	-	-	16/39/115/115	-
11	CLA	1	1109	-	-	16/39/115/115	-
11	CLA	2	1224	-	1/1/13/20	10/27/103/115	-
11	CLA	A	1136	-	1/1/11/20	4/17/93/115	-
11	CLA	1	1108	-	1/1/11/20	7/15/91/115	-
11	CLA	1	1118	-	1/1/14/20	21/35/111/115	-
14	BCR	6	4013	-	-	16/29/63/63	0/2/2/2
14	BCR	b	4011	-	-	15/29/63/63	0/2/2/2
14	BCR	F	4020	-	-	12/29/63/63	0/2/2/2
11	CLA	2	1223	-	1/1/15/20	19/39/115/115	-
11	CLA	A	1130	-	1/1/11/20	7/17/93/115	-
11	CLA	2	1213	-	1/1/15/20	17/39/115/115	-
16	LMG	b	5002	-	-	27/50/70/70	0/1/1/1
11	CLA	b	1023	-	1/1/15/20	17/39/115/115	-
14	BCR	B	4014	-	-	11/29/63/63	0/2/2/2
11	CLA	a	1140	-	1/1/15/20	14/39/115/115	-
11	CLA	b	1221	-	1/1/12/20	9/26/102/115	-
15	LHG	1	5003	11	-	31/53/53/53	-
11	CLA	2	1226	-	1/1/15/20	13/39/115/115	-
11	CLA	2	1209	-	1/1/11/20	6/15/91/115	-
11	CLA	b	1203	-	1/1/15/20	14/39/115/115	-
11	CLA	A	1125	-	1/1/12/20	11/24/100/115	-
11	CLA	2	1208	-	1/1/11/20	3/15/91/115	-
11	CLA	2	1219	-	1/1/13/20	10/27/103/115	-
11	CLA	2	1240	15	1/1/11/20	5/15/91/115	-
14	BCR	2	4006	-	-	13/29/63/63	0/2/2/2
11	CLA	B	1210	-	1/1/15/20	25/39/115/115	-
14	BCR	b	4006	-	-	15/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
11	CLA	2	1231	-	1/1/11/20	4/15/91/115	-
11	CLA	1	1119	-	1/1/15/20	17/39/115/115	-
11	CLA	2	1220	-	1/1/11/20	6/17/93/115	-
11	CLA	2	1205	-	1/1/13/20	8/27/103/115	-
11	CLA	B	1201	-	1/1/12/20	10/26/102/115	-
11	CLA	a	1112	-	1/1/11/20	2/15/91/115	-
11	CLA	b	1217	-	1/1/11/20	6/18/94/115	-
11	CLA	B	1215	-	1/1/15/20	14/39/115/115	-
11	CLA	b	1205	-	1/1/13/20	10/27/103/115	-
14	BCR	a	4007	-	-	11/29/63/63	0/2/2/2
11	CLA	A	1128	-	1/1/15/20	13/39/115/115	-
11	CLA	1	1011	-	-	12/39/115/115	-
11	CLA	2	1214	-	1/1/13/20	13/32/108/115	-
11	CLA	A	1115	-	1/1/11/20	7/17/93/115	-
11	CLA	a	1115	-	-	4/17/93/115	-
13	SF4	c	3002	3	-	-	0/6/5/5
11	CLA	A	1132	-	1/1/15/20	18/39/115/115	-
11	CLA	b	1235	-	1/1/14/20	13/33/109/115	-
14	BCR	l	4022	-	-	11/29/63/63	0/2/2/2
14	BCR	A	4008	-	-	11/29/63/63	0/2/2/2
11	CLA	b	1223	-	1/1/15/20	19/39/115/115	-
11	CLA	B	1224	-	1/1/13/20	11/27/103/115	-
12	PQN	A	2001	-	-	10/23/43/43	0/2/2/2
11	CLA	b	1228	-	1/1/12/20	5/21/97/115	-
14	BCR	M	4021	-	-	8/29/63/63	0/2/2/2
11	CLA	2	1238	-	1/1/15/20	12/39/115/115	-
11	CLA	1	1125	-	1/1/12/20	10/24/100/115	-
14	BCR	f	4013	-	-	17/29/63/63	0/2/2/2
15	LHG	a	5001	-	-	29/53/53/53	-
11	CLA	b	1240	-	1/1/11/20	9/15/91/115	-
11	CLA	B	1218	-	1/1/11/20	4/15/91/115	-
14	BCR	B	4004	-	-	10/29/63/63	0/2/2/2
11	CLA	a	1011	-	-	11/39/115/115	-
11	CLA	a	1131	-	1/1/15/20	18/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
11	CLA	B	1234	-	1/1/14/20	15/33/109/115	-
11	CLA	2	1229	-	1/1/15/20	16/39/115/115	-
11	CLA	k	1401	-	1/1/15/20	22/39/115/115	-
11	CLA	1	1111	-	1/1/14/20	17/33/109/115	-
11	CLA	a	1118	-	1/1/14/20	10/35/111/115	-
11	CLA	1	1116	-	1/1/12/20	11/26/102/115	-
11	CLA	b	1236	-	1/1/11/20	10/18/94/115	-
11	CLA	1	1117	-	1/1/15/20	13/39/115/115	-
11	CLA	a	1111	-	1/1/14/20	17/33/109/115	-
14	BCR	b	4005	-	-	13/29/63/63	0/2/2/2
11	CLA	b	1226	-	1/1/15/20	13/39/115/115	-
11	CLA	1	1133	-	1/1/11/20	6/17/93/115	-
11	CLA	A	1801	15	1/1/12/20	13/24/100/115	-
11	CLA	B	1240	15	1/1/11/20	8/15/91/115	-
11	CLA	a	1125	-	1/1/12/20	7/24/100/115	-
14	BCR	l	4019	-	-	17/29/63/63	0/2/2/2
11	CLA	a	1117	-	1/1/15/20	18/39/115/115	-
11	CLA	A	1012	-	1/1/15/20	17/39/115/115	-
11	CLA	B	1232	-	1/1/11/20	7/15/91/115	-
13	SF4	C	3002	3	-	-	0/6/5/5
11	CLA	B	1223	-	1/1/15/20	10/39/115/115	-
11	CLA	2	1235	-	1/1/14/20	14/33/109/115	-
11	CLA	B	1213	-	1/1/15/20	18/39/115/115	-
11	CLA	1	1121	-	1/1/11/20	8/17/93/115	-
11	CLA	2	1021	-	1/1/15/20	19/39/115/115	-
11	CLA	A	1124	-	1/1/13/20	14/27/103/115	-
11	CLA	L	1502	-	1/1/11/20	7/17/93/115	-
14	BCR	8	4019	-	-	15/29/63/63	0/2/2/2
11	CLA	b	1239	-	1/1/11/20	7/17/93/115	-
11	CLA	2	1227	-	-	9/15/91/115	-
11	CLA	B	1219	-	1/1/13/20	10/27/103/115	-
11	CLA	a	1127	-	1/1/15/20	12/39/115/115	-
11	CLA	a	1022	-	1/1/15/20	12/39/115/115	-
11	CLA	a	1129	-	1/1/11/20	8/17/93/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
11	CLA	B	1209	-	1/1/11/20	6/15/91/115	-
11	CLA	B	1231	-	1/1/11/20	9/15/91/115	-
11	CLA	B	1220	-	-	6/17/93/115	-
11	CLA	A	1102	11	1/1/15/20	19/39/115/115	-
11	CLA	2	1221	-	1/1/12/20	8/26/102/115	-
11	CLA	B	1208	-	1/1/11/20	5/15/91/115	-
11	CLA	b	1220	-	1/1/11/20	6/17/93/115	-
11	CLA	8	1501	-	1/1/15/20	14/39/115/115	-
11	CLA	2	1202	-	1/1/15/20	14/39/115/115	-
16	LMG	2	5002	-	-	30/50/70/70	0/1/1/1
11	CLA	B	1212	-	1/1/11/20	9/15/91/115	-
11	CLA	b	1215	-	1/1/15/20	12/39/115/115	-
11	CLA	A	1111	-	1/1/14/20	16/33/109/115	-
11	CLA	b	1238	-	1/1/15/20	13/39/115/115	-
14	BCR	1	4003	-	-	12/29/63/63	0/2/2/2
11	CLA	1	1012	-	1/1/15/20	19/39/115/115	-
15	LHG	A	5001	-	-	29/53/53/53	-
11	CLA	A	1011	-	-	16/39/115/115	-
11	CLA	b	1206	2	1/1/15/20	14/39/115/115	-
11	CLA	1	1110	-	1/1/12/20	14/26/102/115	-
11	CLA	a	1135	-	1/1/12/20	9/23/99/115	-
15	LHG	A	5003	11	-	30/53/53/53	-
11	CLA	a	1124	-	1/1/13/20	10/27/103/115	-
11	CLA	2	1230	-	-	9/31/107/115	-
11	CLA	B	1229	-	1/1/15/20	20/39/115/115	-
11	CLA	l	1501	7	-	16/39/115/115	-
11	CLA	1	1129	-	1/1/11/20	7/17/93/115	-
14	BCR	2	4011	-	-	13/29/63/63	0/2/2/2
11	CLA	B	1225	-	1/1/15/20	14/39/115/115	-
15	LHG	2	5004	11	-	28/53/53/53	-
14	BCR	1	4008	-	-	10/29/63/63	0/2/2/2
11	CLA	A	1120	-	1/1/11/20	6/17/93/115	-
11	CLA	A	1139	-	1/1/12/20	9/21/97/115	-
14	BCR	8	4022	-	-	6/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
11	CLA	b	1207	-	1/1/15/20	14/39/115/115	-
14	BCR	a	4008	-	-	11/29/63/63	0/2/2/2
14	BCR	A	4007	-	-	13/29/63/63	0/2/2/2
14	BCR	a	4003	-	-	14/29/63/63	0/2/2/2
12	PQN	b	2002	-	-	8/23/43/43	0/2/2/2
11	CLA	2	1239	-	1/1/11/20	10/17/93/115	-
11	CLA	2	1218	-	1/1/11/20	5/15/91/115	-
14	BCR	2	4004	-	-	10/29/63/63	0/2/2/2
14	BCR	F	4013	-	-	15/29/63/63	0/2/2/2
11	CLA	2	1203	-	1/1/15/20	16/39/115/115	-
11	CLA	B	1204	-	1/1/15/20	14/39/115/115	-
11	CLA	B	1216	-	1/1/15/20	10/39/115/115	-
11	CLA	2	1234	-	1/1/14/20	17/33/109/115	-
14	BCR	L	4022	-	-	10/29/63/63	0/2/2/2
11	CLA	a	1106	1	1/1/15/20	19/39/115/115	-
11	CLA	a	1132	-	1/1/15/20	17/39/115/115	-
11	CLA	a	1119	-	1/1/15/20	14/39/115/115	-
11	CLA	b	1218	-	1/1/11/20	4/15/91/115	-
11	CLA	A	1022	-	1/1/15/20	15/39/115/115	-
11	CLA	B	1230	-	-	9/31/107/115	-
11	CLA	a	1137	-	1/1/15/20	13/39/115/115	-
11	CLA	B	1206	2	1/1/15/20	13/39/115/115	-
11	CLA	B	1207	-	1/1/15/20	12/39/115/115	-
11	CLA	A	1110	-	1/1/12/20	11/26/102/115	-
11	CLA	2	1201	-	1/1/12/20	8/26/102/115	-
11	CLA	B	1235	-	1/1/14/20	14/33/109/115	-
14	BCR	b	4009	-	-	14/29/63/63	0/2/2/2
11	CLA	1	1115	-	1/1/11/20	4/17/93/115	-
11	CLA	b	1232	-	1/1/11/20	6/15/91/115	-
11	CLA	1	1103	-	1/1/15/20	19/39/115/115	-
11	CLA	1	1135	-	1/1/12/20	9/23/99/115	-
11	CLA	A	1138	-	1/1/11/20	0/17/93/115	-
11	CLA	l	1502	-	1/1/11/20	4/17/93/115	-
14	BCR	b	4017	-	-	6/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
11	CLA	2	1222	-	1/1/13/20	13/29/105/115	-
11	CLA	B	1021	-	1/1/15/20	22/39/115/115	-
11	CLA	2	1207	-	-	14/39/115/115	-
11	CLA	b	1227	-	-	10/15/91/115	-
13	SF4	C	3003	3	-	-	0/6/5/5
11	CLA	b	1219	-	1/1/13/20	9/27/103/115	-
11	CLA	a	1113	-	1/1/11/20	4/15/91/115	-
11	CLA	A	1105	-	1/1/11/20	7/19/95/115	-
15	LHG	B	5004	11	-	24/53/53/53	-
11	CLA	a	1133	-	1/1/11/20	4/17/93/115	-
11	CLA	A	1117	-	1/1/15/20	12/39/115/115	-
11	CLA	1	1113	-	1/1/11/20	7/15/91/115	-
11	CLA	b	1224	-	1/1/13/20	12/27/103/115	-
11	CLA	1	1102	-	1/1/15/20	14/39/115/115	-
14	BCR	A	4003	-	-	13/29/63/63	0/2/2/2
11	CLA	A	1237	-	1/1/13/20	11/27/103/115	-
11	CLA	a	1012	-	1/1/15/20	21/39/115/115	-
11	CLA	2	1210	-	1/1/15/20	15/39/115/115	-
11	CLA	B	1013	-	-	18/39/115/115	-
16	LMG	B	5002	-	-	27/50/70/70	0/1/1/1
11	CLA	b	1013	-	-	12/39/115/115	-
11	CLA	B	1236	-	1/1/11/20	8/18/94/115	-
11	CLA	A	1123	-	1/1/15/20	15/39/115/115	-
11	CLA	B	1239	-	1/1/11/20	10/17/93/115	-
14	BCR	2	4017	-	-	6/29/63/63	0/2/2/2
11	CLA	2	1225	-	1/1/15/20	12/39/115/115	-
11	CLA	B	1226	-	1/1/15/20	13/39/115/115	-
11	CLA	L	1503	-	1/1/15/20	15/39/115/115	-
14	BCR	2	4014	-	-	14/29/63/63	0/2/2/2
11	CLA	A	1140	-	1/1/15/20	16/39/115/115	-
11	CLA	a	1122	-	1/1/13/20	13/32/108/115	-
11	CLA	b	1214	-	1/1/13/20	10/32/108/115	-
11	CLA	b	1229	-	1/1/15/20	20/39/115/115	-
14	BCR	F	4018	-	-	5/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
11	CLA	a	1120	-	1/1/11/20	9/17/93/115	-
11	CLA	b	1225	-	1/1/15/20	14/39/115/115	-
14	BCR	B	4006	-	-	15/29/63/63	0/2/2/2
13	SF4	1	3001	1,2	-	-	0/6/5/5
11	CLA	1	1120	-	1/1/11/20	9/17/93/115	-
13	SF4	a	3001	1,2	-	-	0/6/5/5
11	CLA	1	1136	-	1/1/11/20	8/17/93/115	-
14	BCR	A	4001	-	-	9/29/63/63	0/2/2/2
11	CLA	a	1102	11	1/1/15/20	13/39/115/115	-
11	CLA	B	1221	-	1/1/12/20	10/26/102/115	-
11	CLA	a	1121	-	1/1/11/20	5/17/93/115	-
14	BCR	b	4014	-	-	13/29/63/63	0/2/2/2
11	CLA	a	1136	-	1/1/11/20	5/17/93/115	-
11	CLA	a	1237	-	1/1/13/20	10/27/103/115	-
11	CLA	1	1138	-	1/1/11/20	6/17/93/115	-
11	CLA	2	1216	-	1/1/15/20	17/39/115/115	-
11	CLA	B	1202	-	1/1/15/20	17/39/115/115	-
11	CLA	2	1204	-	1/1/15/20	10/39/115/115	-
11	CLA	8	1502	-	1/1/11/20	5/17/93/115	-
14	BCR	6	4020	-	-	15/29/63/63	0/2/2/2
11	CLA	1	1123	-	1/1/15/20	16/39/115/115	-
11	CLA	a	1138	-	1/1/11/20	7/17/93/115	-
11	CLA	b	1204	-	1/1/15/20	15/39/115/115	-
11	CLA	A	1113	-	1/1/11/20	7/15/91/115	-
11	CLA	A	1135	-	1/1/12/20	8/23/99/115	-
11	CLA	1	1134	-	1/1/11/20	5/17/93/115	-
11	CLA	B	1205	-	1/1/13/20	11/27/103/115	-
11	CLA	2	1215	-	1/1/15/20	17/39/115/115	-
14	BCR	6	4018	-	-	10/29/63/63	0/2/2/2

The worst 5 of 6320 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

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
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 8272 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	1	4002	BCR	C16-C17-C18	29.07	168.05	127.28
14	b	4009	BCR	C16-C17-C18	28.37	167.07	127.28
14	6	4013	BCR	C20-C21-C22	26.49	164.43	127.28
14	F	4013	BCR	C20-C21-C22	26.21	164.03	127.28
14	f	4013	BCR	C20-C21-C22	25.83	163.51	127.28

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 4221 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
11	A	1237	CLA	C1A-C2A-CAA-CBA
11	A	1237	CLA	O2A-C1-C2-C3
11	A	1022	CLA	C2-C1-O2A-CGA
11	A	1022	CLA	CBD-CGD-O2D-CED
11	A	1101	CLA	C3A-C2A-CAA-CBA

There are no ring outliers.

303 monomers are involved in 843 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
11	A	1126	CLA	9	0
11	a	1105	CLA	1	0
11	2	1206	CLA	7	0
14	L	4019	BCR	8	0
11	1	1105	CLA	1	0
14	1	4001	BCR	8	0
14	B	4005	BCR	6	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
11	A	1131	CLA	2	0
11	A	1121	CLA	2	0
14	b	4010	BCR	10	0
11	1	1127	CLA	1	0
14	m	4021	BCR	4	0
11	a	1108	CLA	2	0
11	b	1201	CLA	3	0
13	A	3001	SF4	3	0
11	A	1114	CLA	2	0
15	b	5004	LHG	5	0
11	A	1106	CLA	4	0
11	B	1228	CLA	2	0
11	b	1202	CLA	1	0
11	a	1134	CLA	1	0
11	A	1122	CLA	2	0
11	1	1107	CLA	3	0
11	1	1132	CLA	6	0
11	2	1211	CLA	1	0
11	A	1107	CLA	2	0
11	A	1103	CLA	2	0
12	B	2002	PQN	1	0
11	a	1107	CLA	1	0
14	B	4009	BCR	5	0
11	A	1101	CLA	2	0
11	1	1101	CLA	3	0
11	b	1234	CLA	1	0
11	1	1237	CLA	4	0
14	B	4017	BCR	8	0
11	a	1123	CLA	7	0
11	A	1134	CLA	1	0
11	l	1503	CLA	4	0
14	A	4002	BCR	5	0
11	2	1217	CLA	1	0
11	A	1129	CLA	5	0
11	A	1112	CLA	3	0
14	a	4001	BCR	4	0
14	B	4010	BCR	7	0
11	K	1402	CLA	3	0
11	b	1209	CLA	2	0
11	8	1503	CLA	2	0
13	3	3002	SF4	8	0
11	k	1402	CLA	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
11	b	1222	CLA	4	0
11	L	1501	CLA	4	0
11	a	1116	CLA	3	0
11	B	1227	CLA	5	0
11	1	1128	CLA	9	0
11	a	1128	CLA	2	0
14	7	4021	BCR	5	0
11	1	1124	CLA	2	0
11	B	1023	CLA	7	0
11	a	1126	CLA	4	0
11	b	1208	CLA	2	0
11	2	1013	CLA	8	0
11	1	1126	CLA	5	0
11	1	1112	CLA	3	0
11	a	1110	CLA	2	0
11	1	1104	CLA	1	0
11	1	1137	CLA	4	0
11	1	1801	CLA	5	0
11	2	1212	CLA	3	0
11	1	1131	CLA	2	0
15	a	5003	LHG	9	0
11	a	1104	CLA	1	0
11	1	1140	CLA	2	0
11	B	1214	CLA	1	0
14	B	4011	BCR	6	0
11	0	1402	CLA	1	0
11	1	1106	CLA	8	0
11	2	1228	CLA	1	0
13	3	3003	SF4	12	0
11	0	1401	CLA	3	0
12	a	2001	PQN	3	0
11	A	1119	CLA	6	0
11	a	1801	CLA	7	0
13	c	3003	SF4	13	0
14	2	4005	BCR	4	0
11	a	1101	CLA	2	0
11	B	1211	CLA	4	0
12	2	2002	PQN	1	0
14	2	4009	BCR	5	0
11	A	1104	CLA	7	0
11	A	1137	CLA	4	0
11	1	1122	CLA	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
11	b	1211	CLA	3	0
11	a	1103	CLA	16	0
14	1	4007	BCR	7	0
11	A	1133	CLA	1	0
11	b	1212	CLA	2	0
11	B	1222	CLA	3	0
11	1	1130	CLA	3	0
14	f	4020	BCR	4	0
11	A	1118	CLA	3	0
14	a	4002	BCR	5	0
11	1	1022	CLA	5	0
14	1	4002	BCR	5	0
14	b	4004	BCR	3	0
14	f	4018	BCR	7	0
11	b	1230	CLA	1	0
11	2	1023	CLA	4	0
11	B	1238	CLA	4	0
14	2	4010	BCR	6	0
11	2	1232	CLA	3	0
11	b	1210	CLA	2	0
15	1	5001	LHG	10	0
11	b	1021	CLA	5	0
11	b	1231	CLA	1	0
11	1	1109	CLA	2	0
11	2	1224	CLA	1	0
11	A	1136	CLA	3	0
11	1	1118	CLA	3	0
14	6	4013	BCR	7	0
14	b	4011	BCR	7	0
14	F	4020	BCR	4	0
11	2	1223	CLA	1	0
11	b	1023	CLA	8	0
14	B	4014	BCR	6	0
11	b	1221	CLA	6	0
15	1	5003	LHG	6	0
11	2	1209	CLA	2	0
11	b	1203	CLA	3	0
11	A	1125	CLA	4	0
11	2	1240	CLA	2	0
11	2	1208	CLA	1	0
14	2	4006	BCR	1	0
11	B	1210	CLA	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
14	b	4006	BCR	2	0
11	2	1231	CLA	7	0
11	1	1119	CLA	2	0
11	2	1220	CLA	2	0
11	2	1205	CLA	4	0
11	B	1201	CLA	3	0
11	a	1112	CLA	4	0
11	b	1217	CLA	2	0
11	B	1215	CLA	1	0
11	b	1205	CLA	5	0
14	a	4007	BCR	3	0
11	A	1128	CLA	3	0
11	1	1011	CLA	1	0
11	2	1214	CLA	3	0
11	A	1115	CLA	2	0
13	c	3002	SF4	7	0
11	A	1132	CLA	2	0
11	b	1235	CLA	3	0
14	l	4022	BCR	4	0
14	A	4008	BCR	5	0
11	b	1223	CLA	14	0
11	B	1224	CLA	1	0
12	A	2001	PQN	2	0
11	b	1228	CLA	3	0
14	M	4021	BCR	5	0
11	2	1238	CLA	5	0
11	1	1125	CLA	3	0
14	f	4013	BCR	5	0
15	a	5001	LHG	2	0
11	b	1240	CLA	3	0
14	B	4004	BCR	3	0
11	a	1011	CLA	1	0
11	a	1131	CLA	2	0
11	B	1234	CLA	2	0
11	2	1229	CLA	4	0
11	k	1401	CLA	4	0
11	1	1111	CLA	1	0
11	a	1118	CLA	4	0
11	b	1236	CLA	2	0
11	1	1117	CLA	2	0
11	a	1111	CLA	3	0
14	b	4005	BCR	3	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
11	1	1133	CLA	3	0
11	A	1801	CLA	3	0
11	a	1125	CLA	4	0
14	l	4019	BCR	7	0
11	a	1117	CLA	1	0
11	A	1012	CLA	2	0
13	C	3002	SF4	10	0
11	B	1223	CLA	8	0
11	2	1235	CLA	3	0
11	1	1121	CLA	1	0
11	2	1021	CLA	8	0
11	A	1124	CLA	4	0
14	8	4019	BCR	7	0
11	2	1227	CLA	3	0
11	B	1219	CLA	1	0
11	a	1127	CLA	1	0
11	a	1022	CLA	2	0
11	a	1129	CLA	1	0
11	B	1209	CLA	3	0
11	B	1231	CLA	2	0
11	B	1220	CLA	1	0
11	A	1102	CLA	3	0
11	2	1221	CLA	1	0
11	b	1220	CLA	6	0
11	8	1501	CLA	6	0
11	2	1202	CLA	4	0
16	2	5002	LMG	2	0
11	B	1212	CLA	3	0
11	A	1111	CLA	1	0
11	b	1238	CLA	3	0
14	1	4003	BCR	2	0
11	1	1012	CLA	4	0
15	A	5001	LHG	5	0
11	A	1011	CLA	3	0
11	b	1206	CLA	3	0
11	1	1110	CLA	2	0
11	a	1135	CLA	4	0
15	A	5003	LHG	4	0
11	a	1124	CLA	3	0
11	2	1230	CLA	4	0
11	B	1229	CLA	5	0
11	l	1501	CLA	5	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
11	1	1129	CLA	2	0
14	2	4011	BCR	8	0
11	B	1225	CLA	2	0
15	2	5004	LHG	7	0
14	1	4008	BCR	4	0
14	8	4022	BCR	8	0
11	b	1207	CLA	2	0
14	a	4008	BCR	2	0
14	A	4007	BCR	7	0
14	a	4003	BCR	4	0
12	b	2002	PQN	1	0
11	2	1239	CLA	4	0
14	2	4004	BCR	2	0
14	F	4013	BCR	3	0
11	2	1203	CLA	1	0
11	B	1204	CLA	3	0
11	2	1234	CLA	4	0
14	L	4022	BCR	6	0
11	a	1106	CLA	1	0
11	a	1132	CLA	2	0
11	a	1119	CLA	11	0
11	A	1022	CLA	5	0
11	B	1230	CLA	2	0
11	a	1137	CLA	1	0
11	B	1206	CLA	3	0
11	B	1207	CLA	3	0
11	A	1110	CLA	1	0
11	2	1201	CLA	3	0
11	B	1235	CLA	2	0
14	b	4009	BCR	4	0
11	1	1115	CLA	5	0
11	1	1103	CLA	2	0
11	A	1138	CLA	5	0
11	l	1502	CLA	1	0
14	b	4017	BCR	5	0
11	2	1222	CLA	2	0
11	B	1021	CLA	8	0
11	2	1207	CLA	4	0
11	b	1227	CLA	3	0
13	C	3003	SF4	3	0
11	b	1219	CLA	3	0
11	a	1113	CLA	2	0

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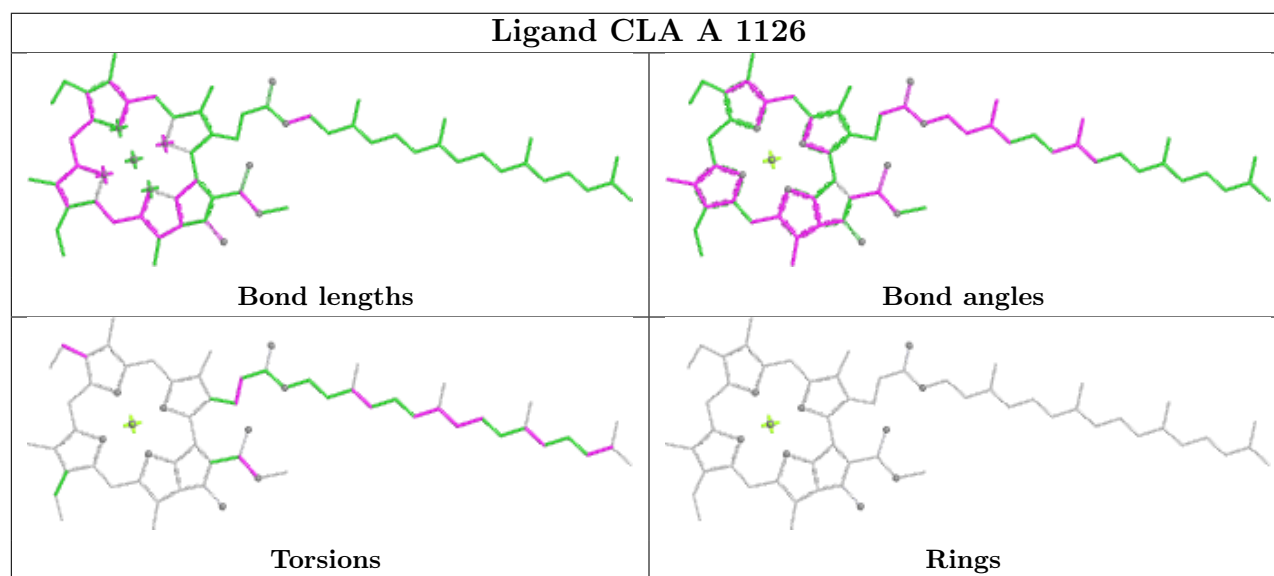
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15	B	5004	LHG	4	0
11	a	1133	CLA	4	0
11	A	1117	CLA	1	0
11	1	1113	CLA	3	0
11	1	1102	CLA	1	0
14	A	4003	BCR	7	0
11	A	1237	CLA	3	0
11	a	1012	CLA	2	0
11	B	1013	CLA	6	0
11	2	1210	CLA	1	0
16	B	5002	LMG	1	0
11	b	1013	CLA	10	0
11	B	1236	CLA	1	0
11	A	1123	CLA	9	0
11	B	1239	CLA	1	0
14	2	4017	BCR	10	0
11	2	1225	CLA	1	0
11	B	1226	CLA	2	0
14	2	4014	BCR	7	0
11	A	1140	CLA	2	0
11	a	1122	CLA	2	0
11	b	1214	CLA	2	0
11	b	1229	CLA	3	0
14	F	4018	BCR	9	0
11	b	1225	CLA	2	0
14	B	4006	BCR	3	0
13	1	3001	SF4	1	0
13	a	3001	SF4	3	0
14	A	4001	BCR	3	0
11	B	1221	CLA	3	0
11	a	1121	CLA	4	0
14	b	4014	BCR	4	0
11	a	1237	CLA	2	0
11	1	1138	CLA	2	0
11	B	1202	CLA	2	0
11	2	1204	CLA	3	0
14	6	4020	BCR	4	0
11	1	1123	CLA	5	0
11	a	1138	CLA	3	0
11	b	1204	CLA	3	0
11	A	1135	CLA	2	0
11	1	1134	CLA	3	0

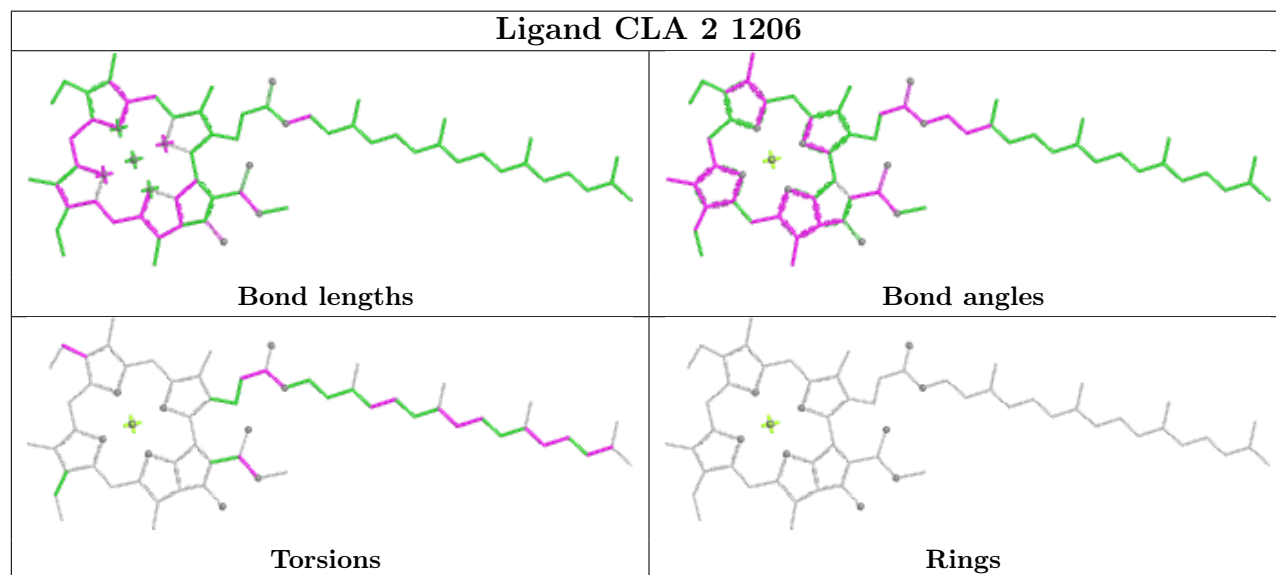
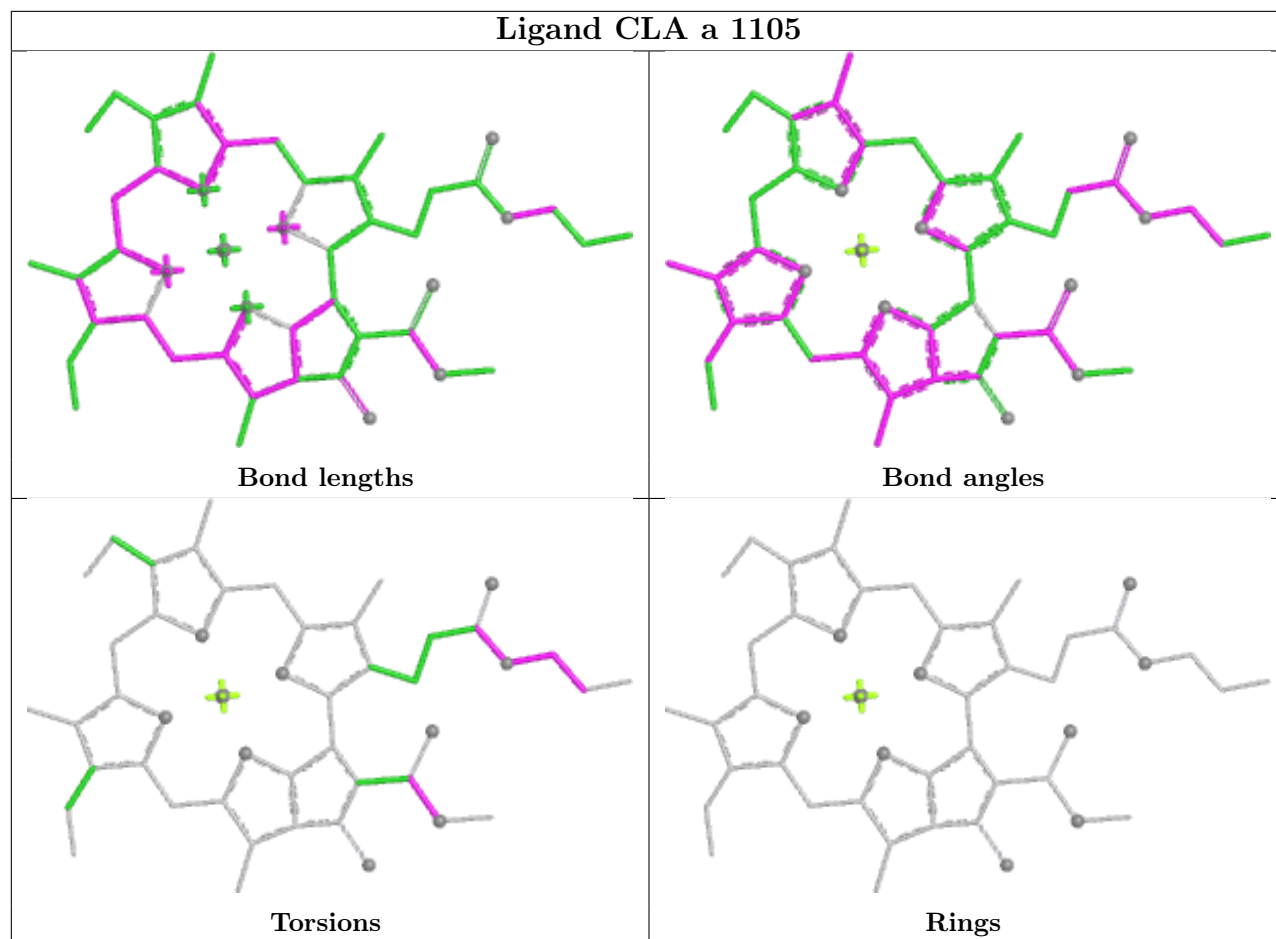
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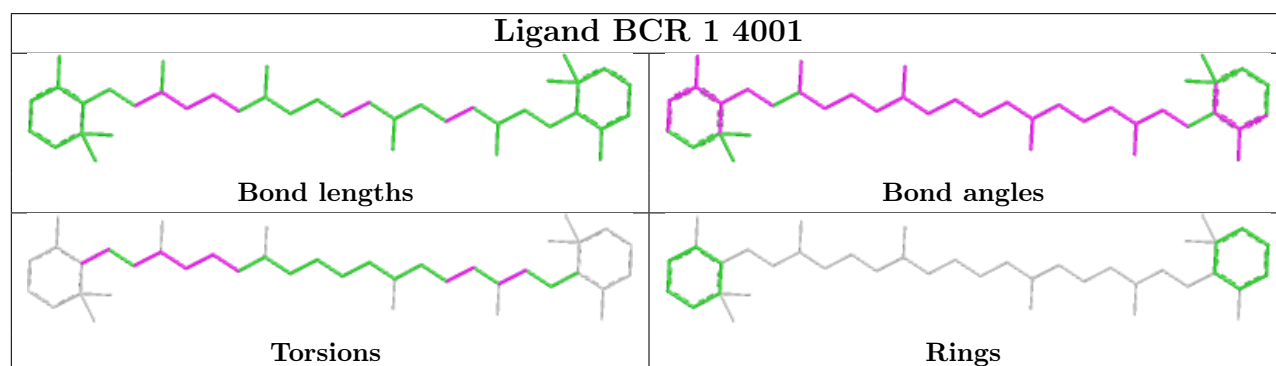
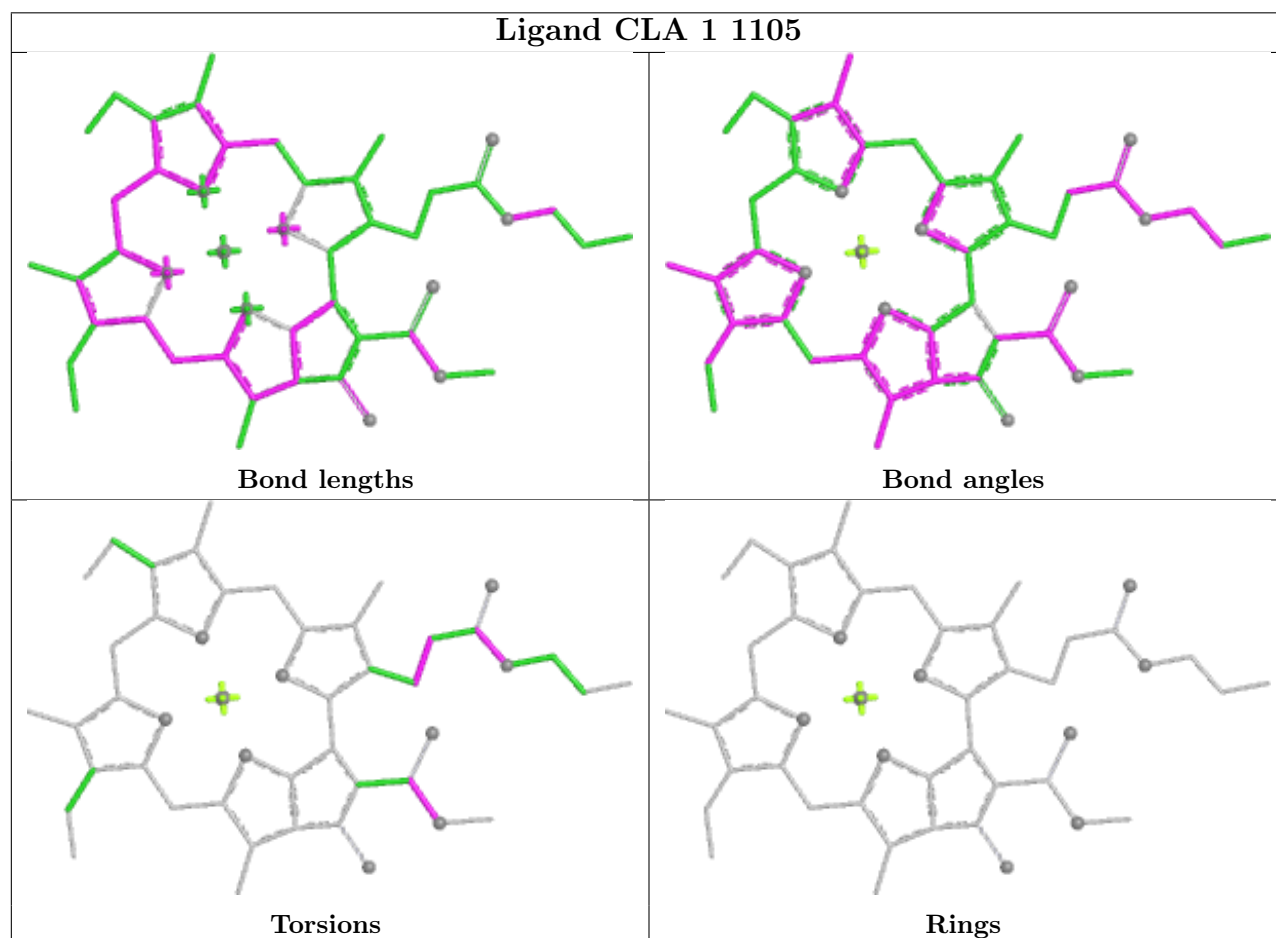
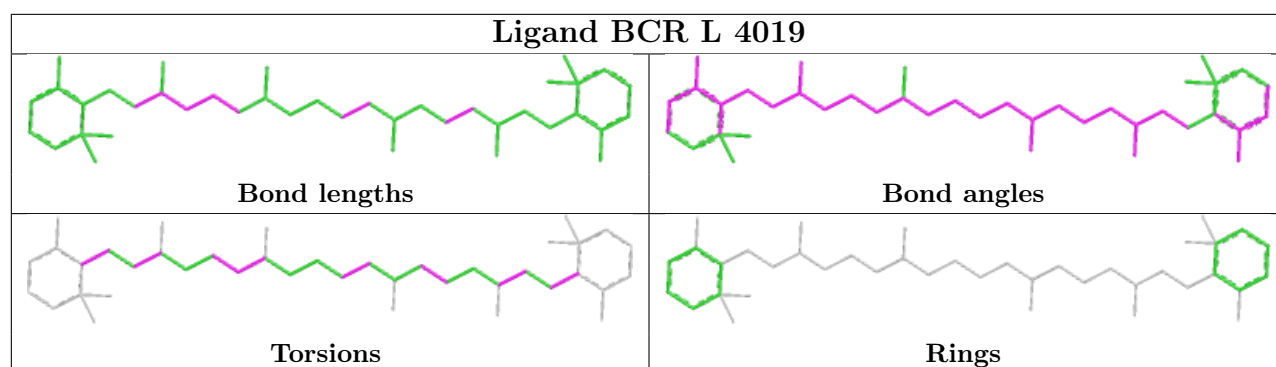
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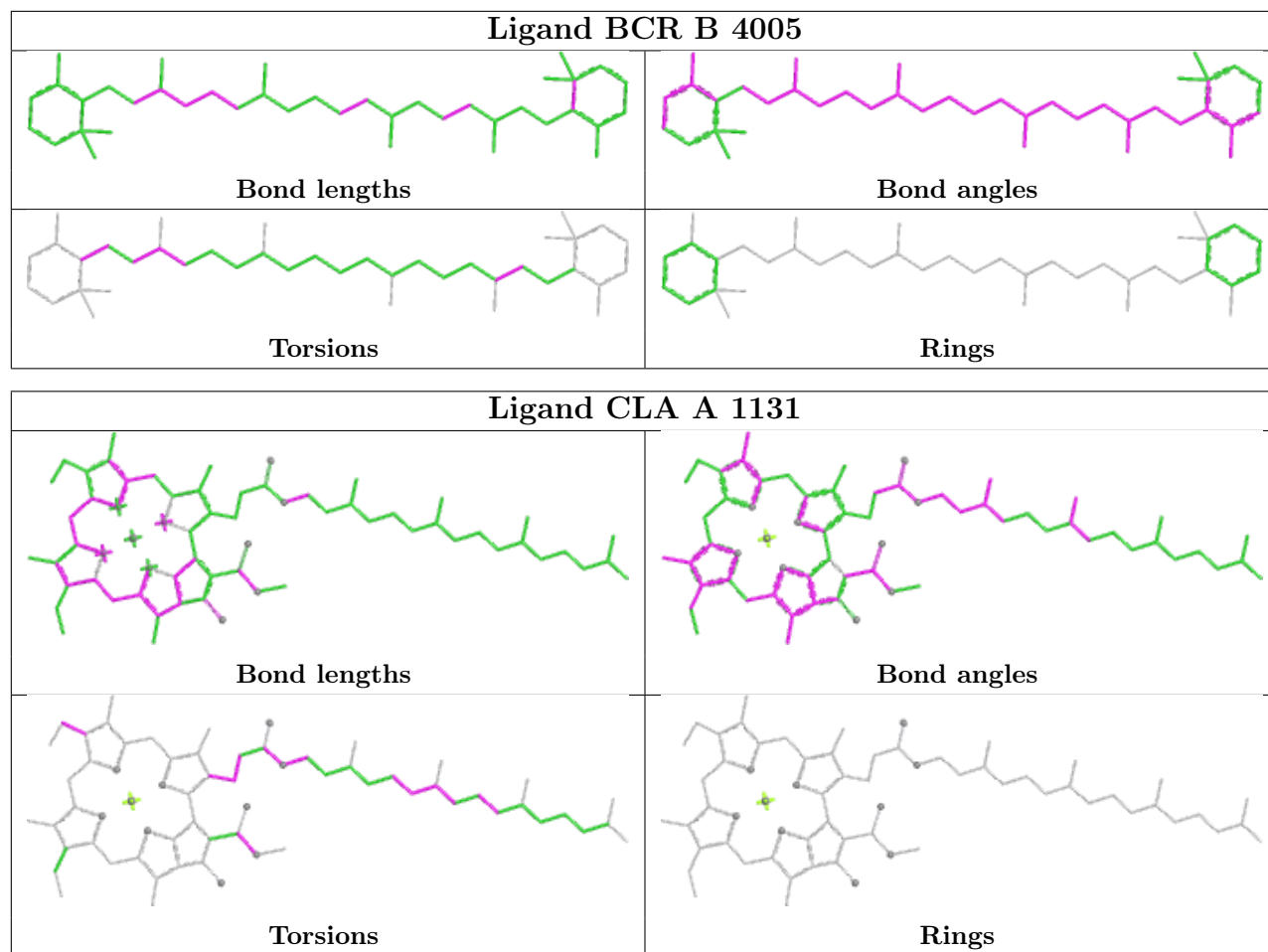
Mol	Chain	Res	Type	Clashes	Symm-Clashes
11	B	1205	CLA	4	0
14	6	4018	BCR	9	0

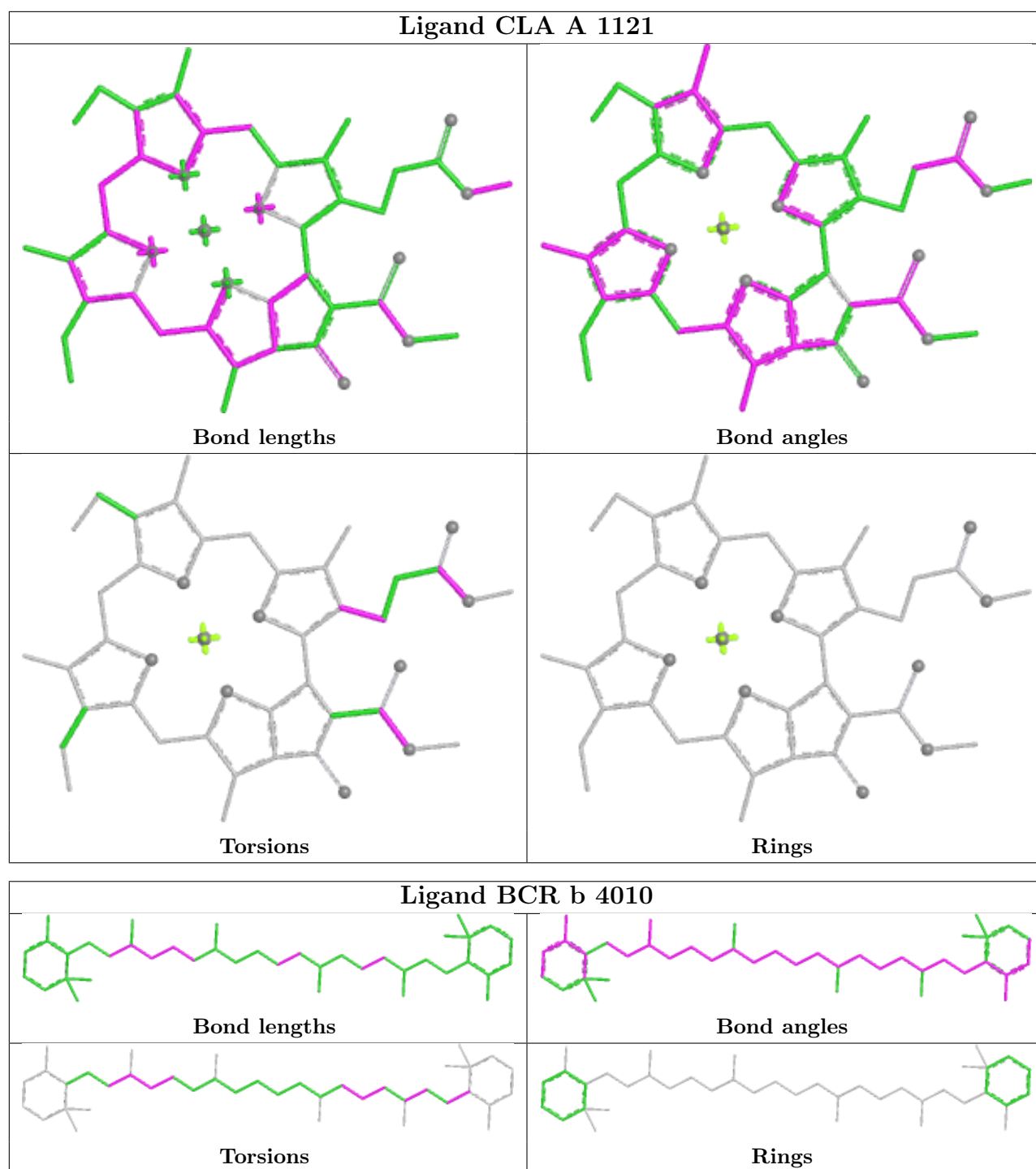
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

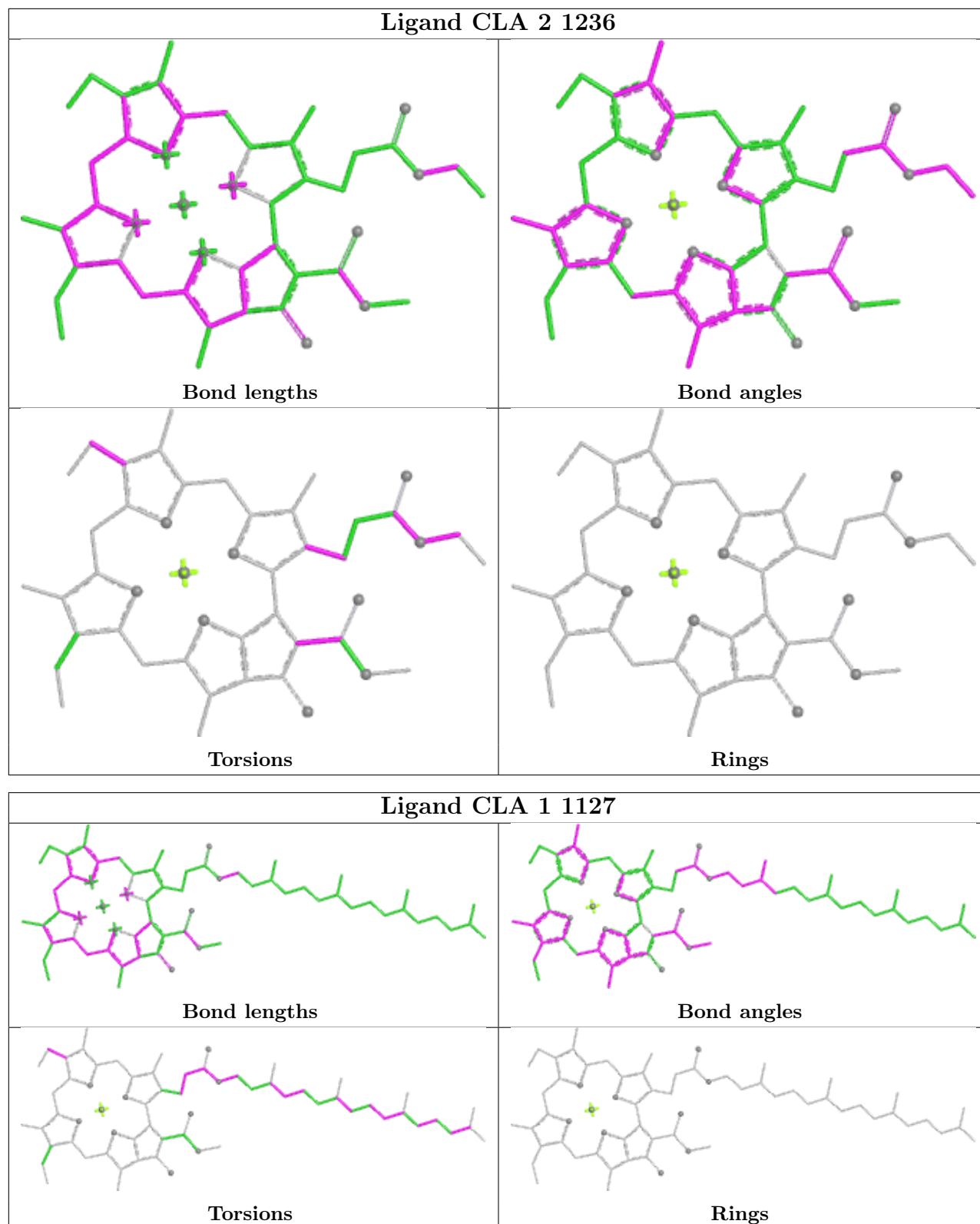


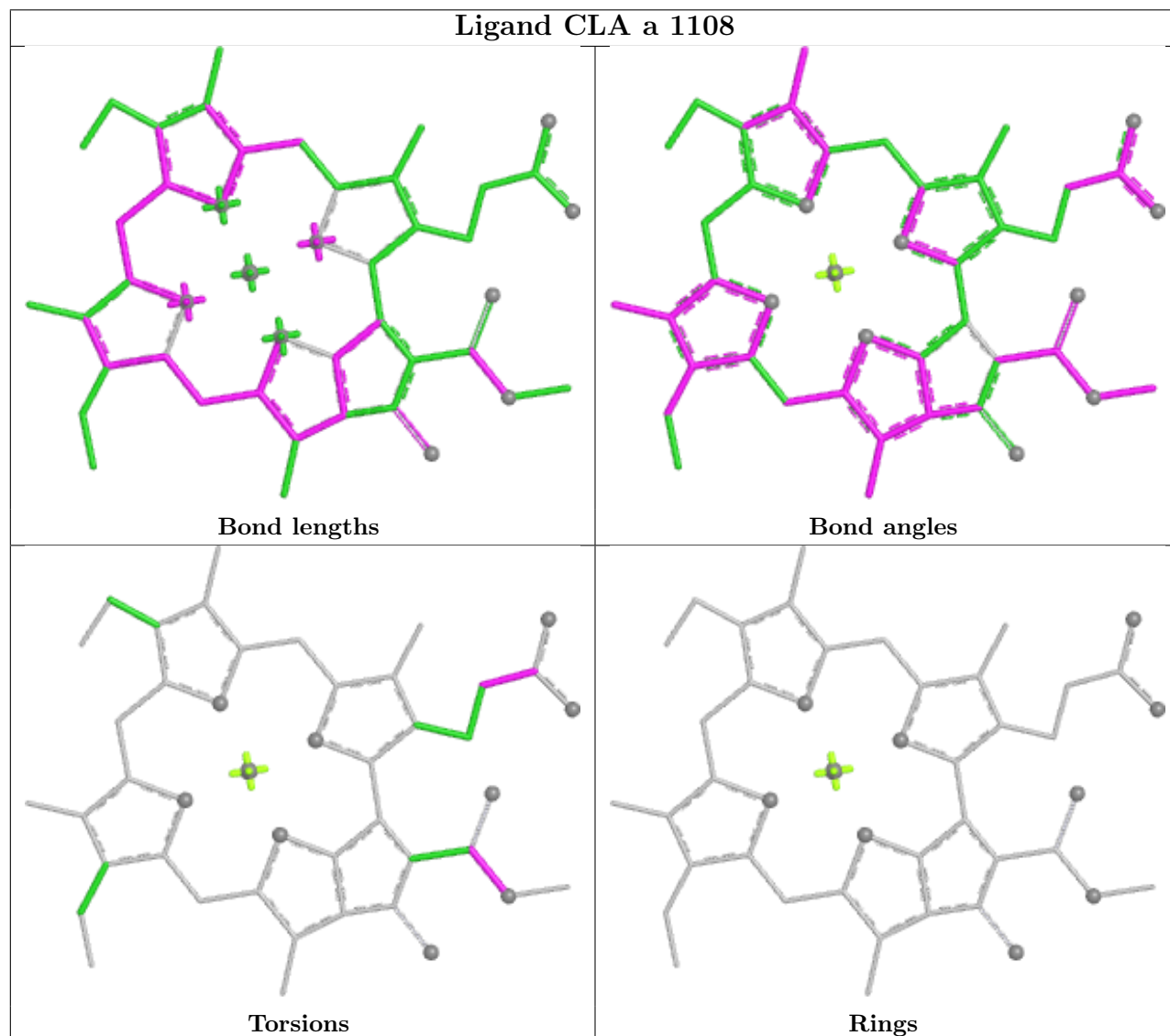
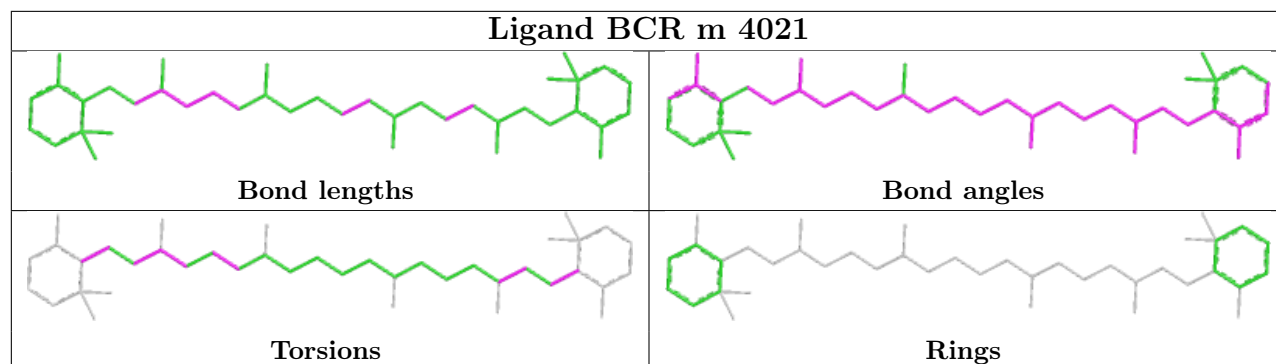


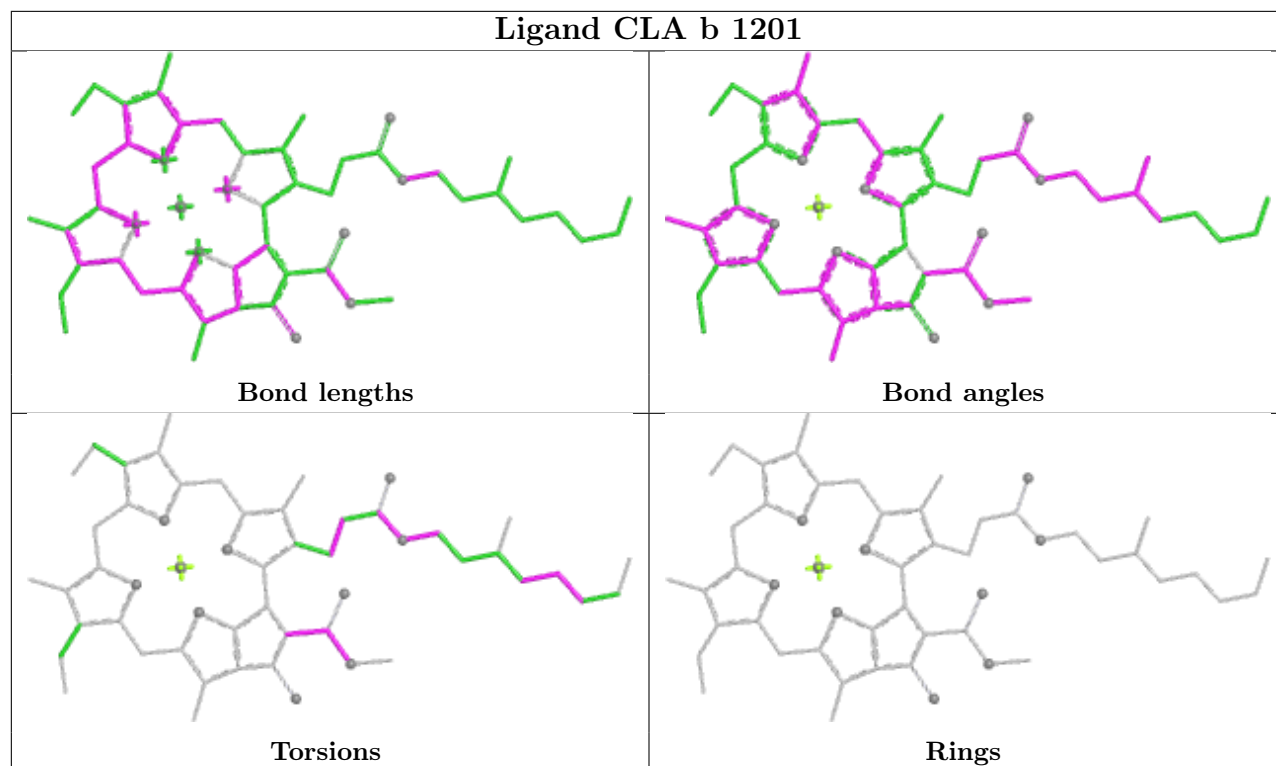




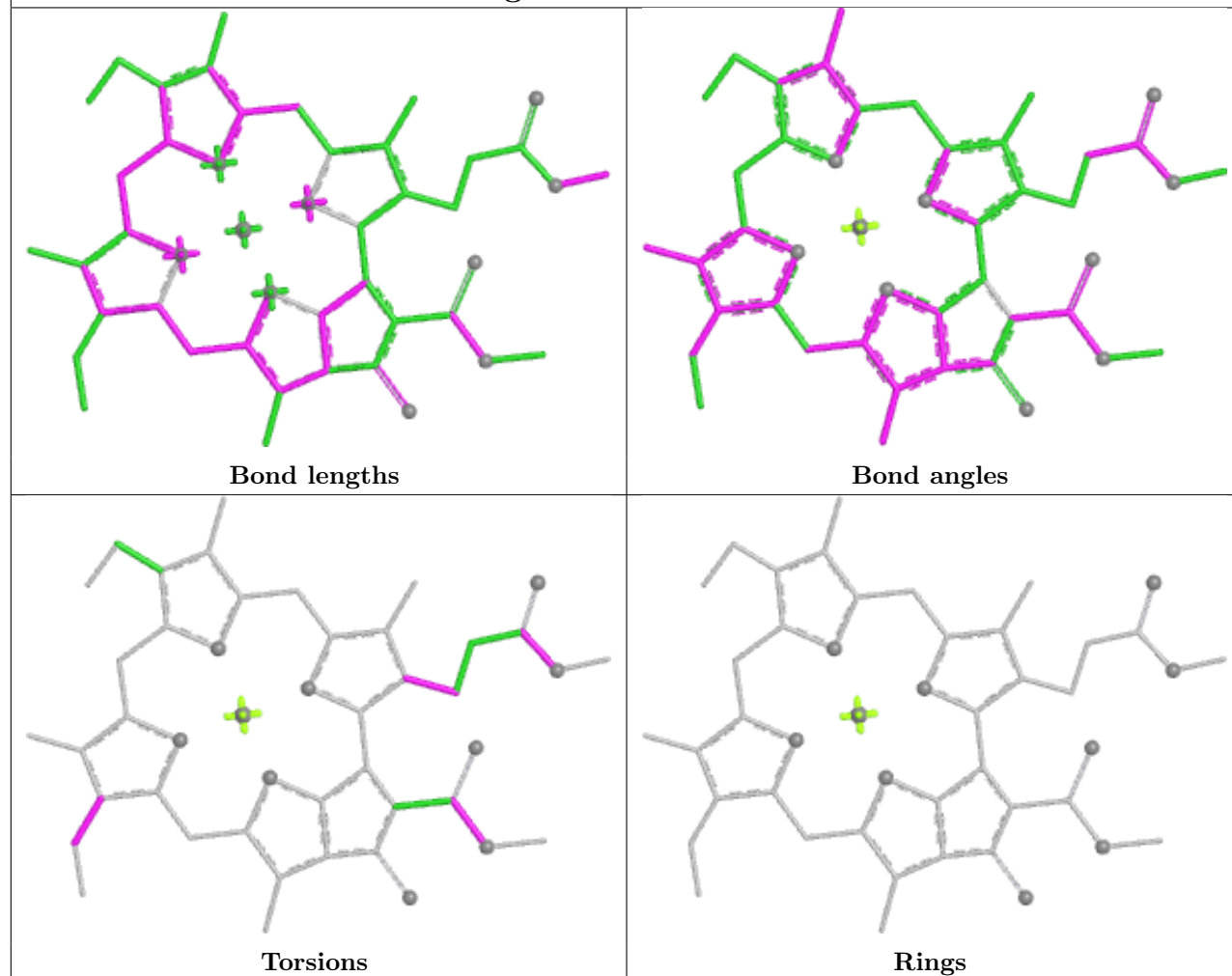


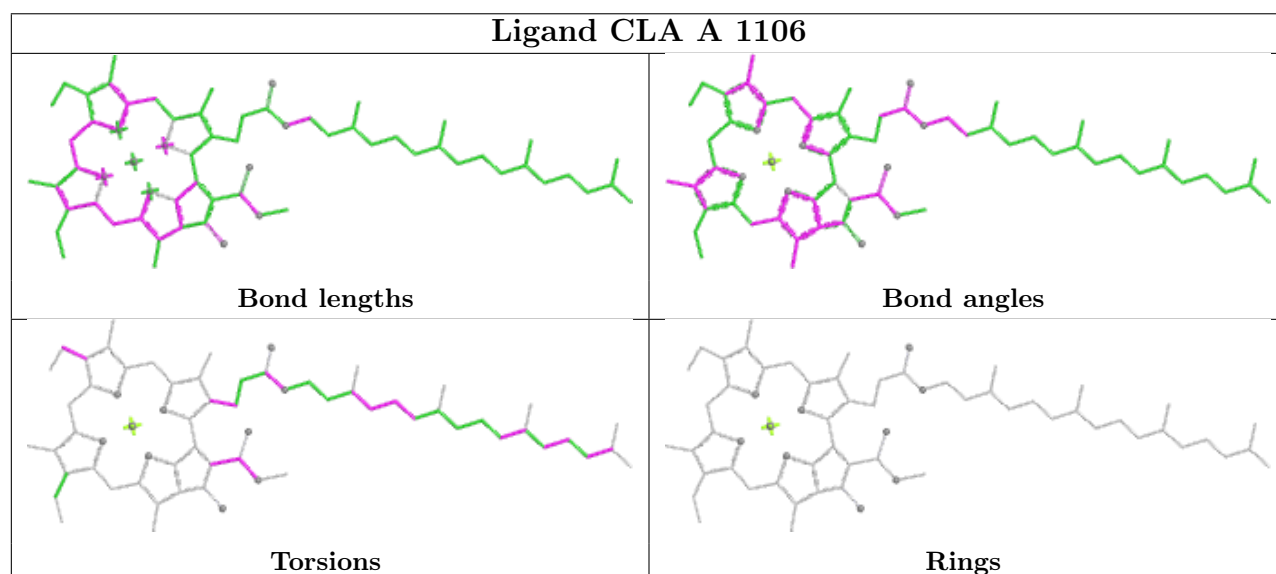
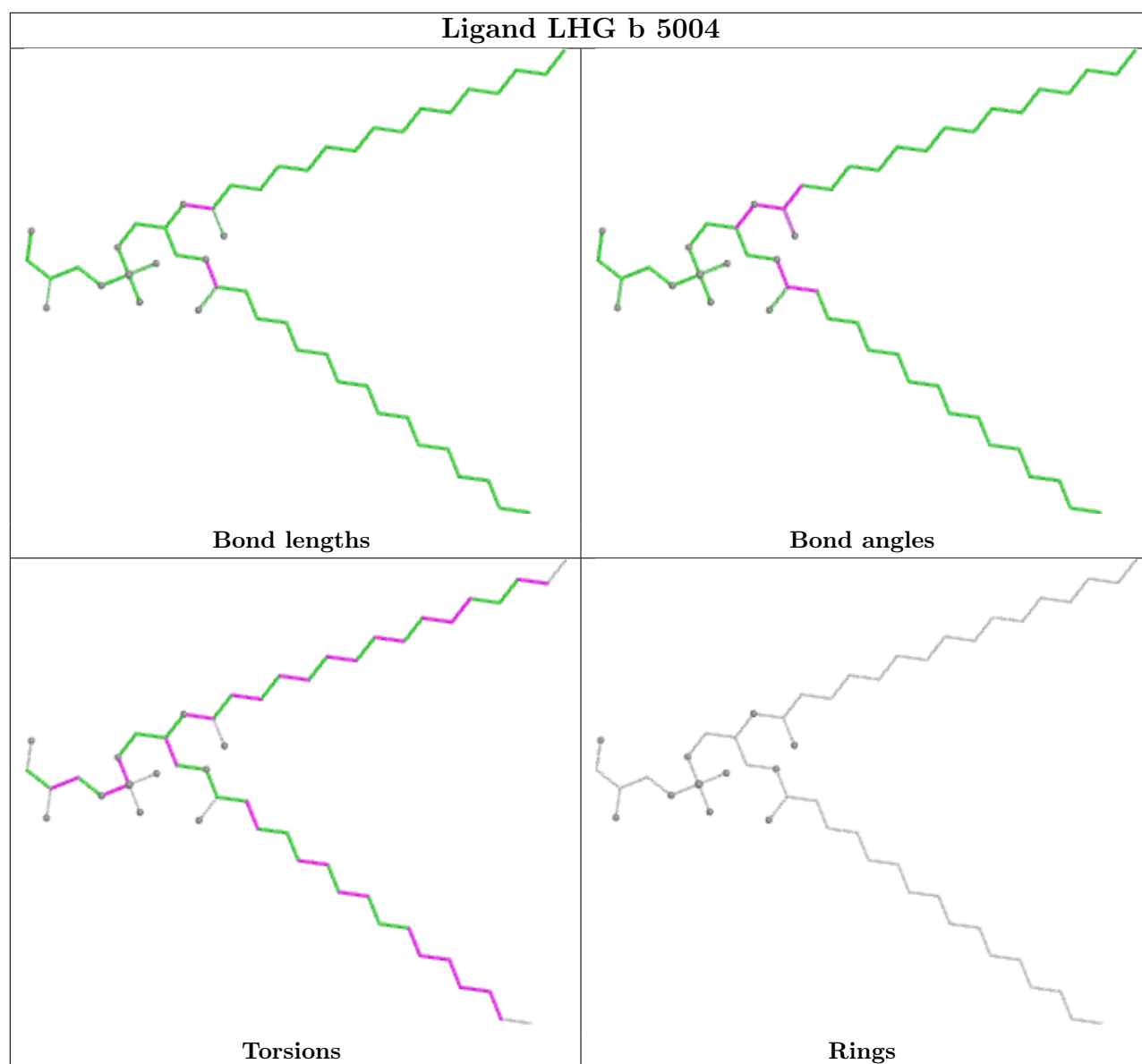




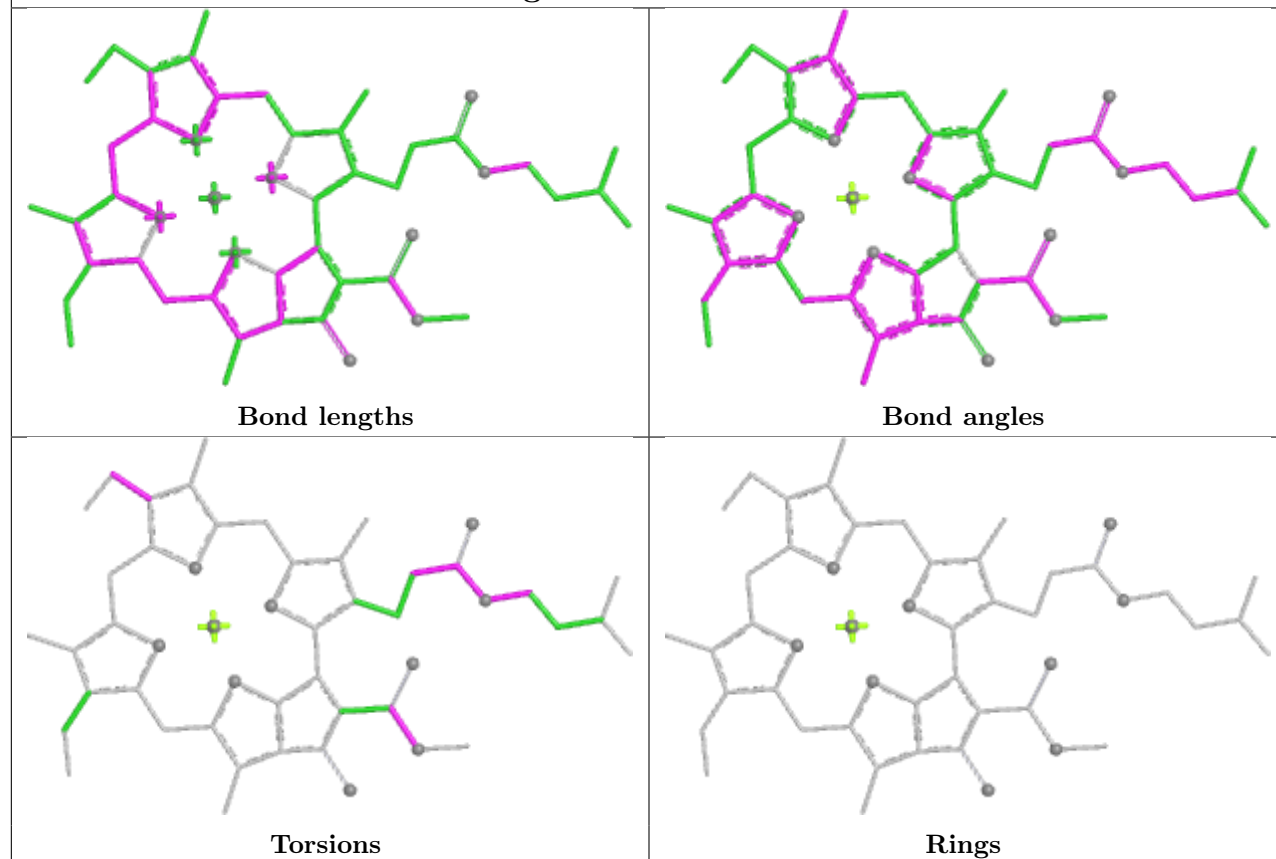


Ligand CLA A 1114

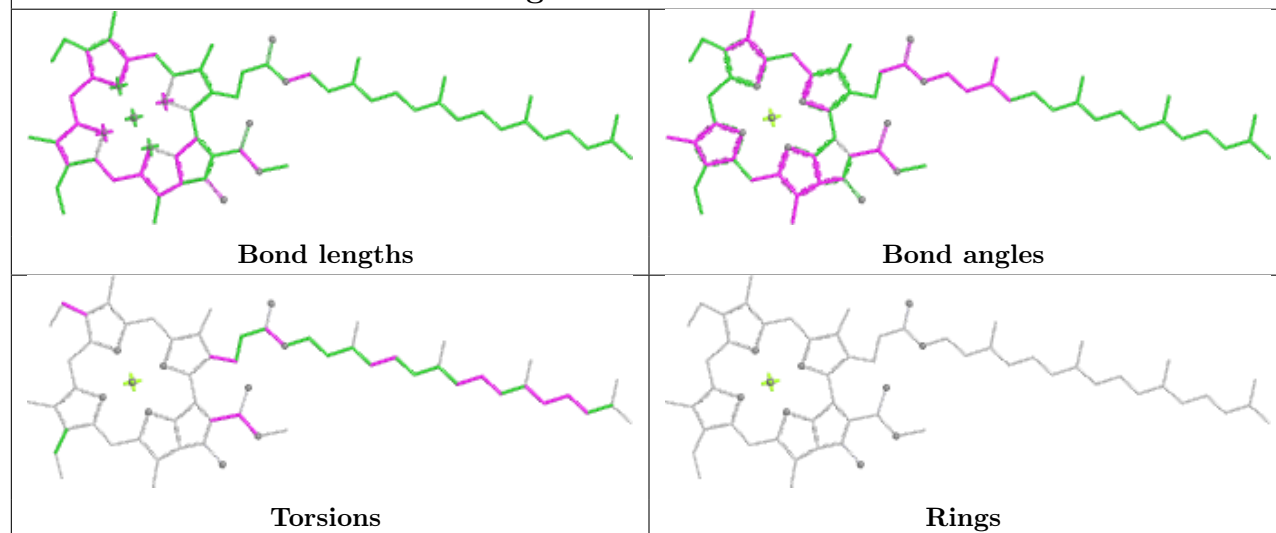


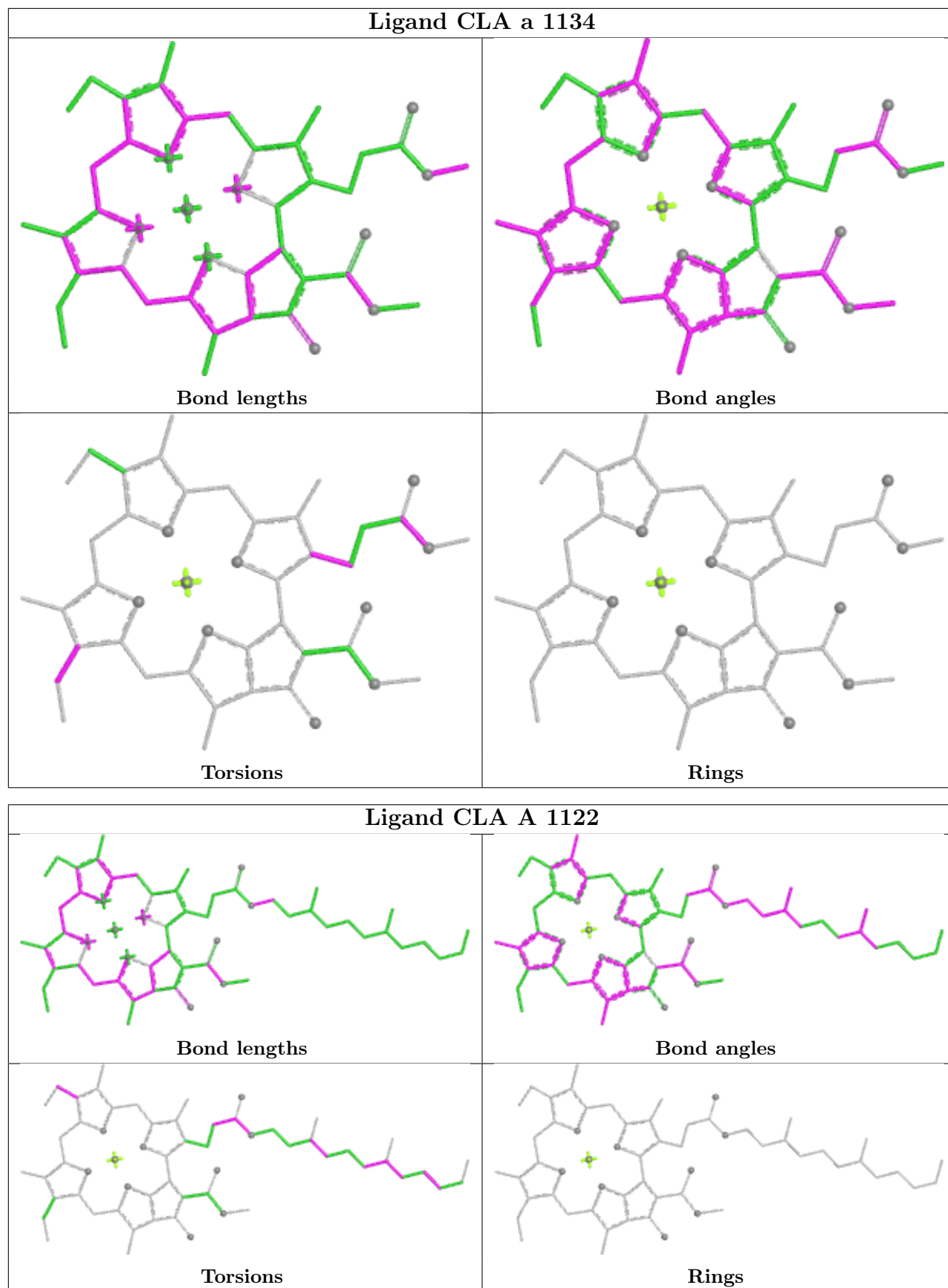


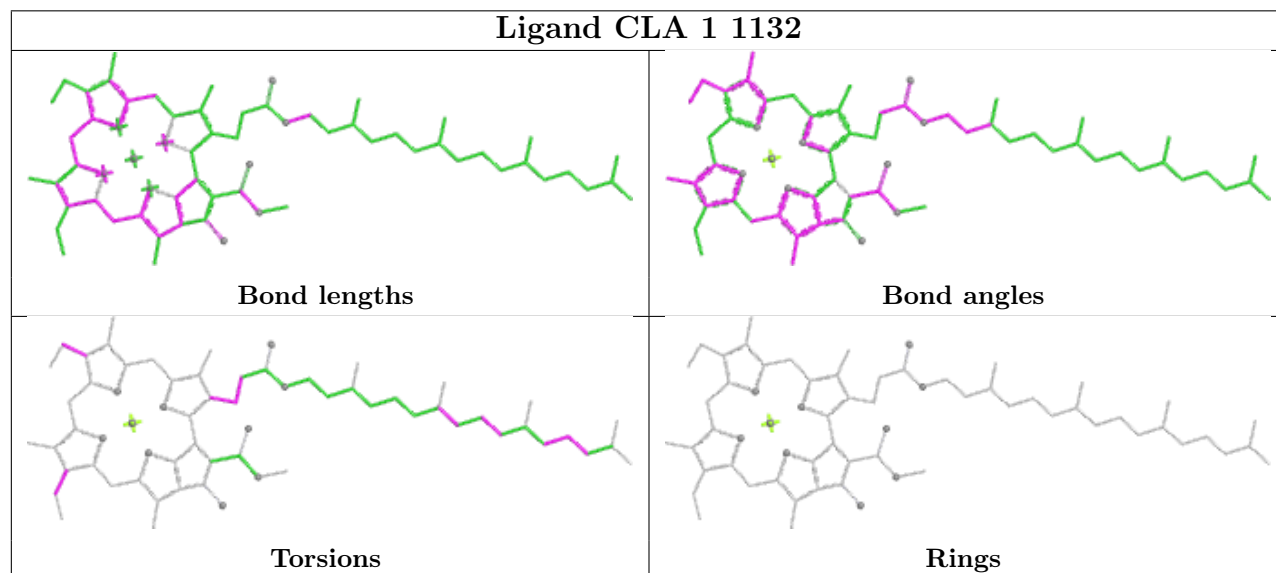
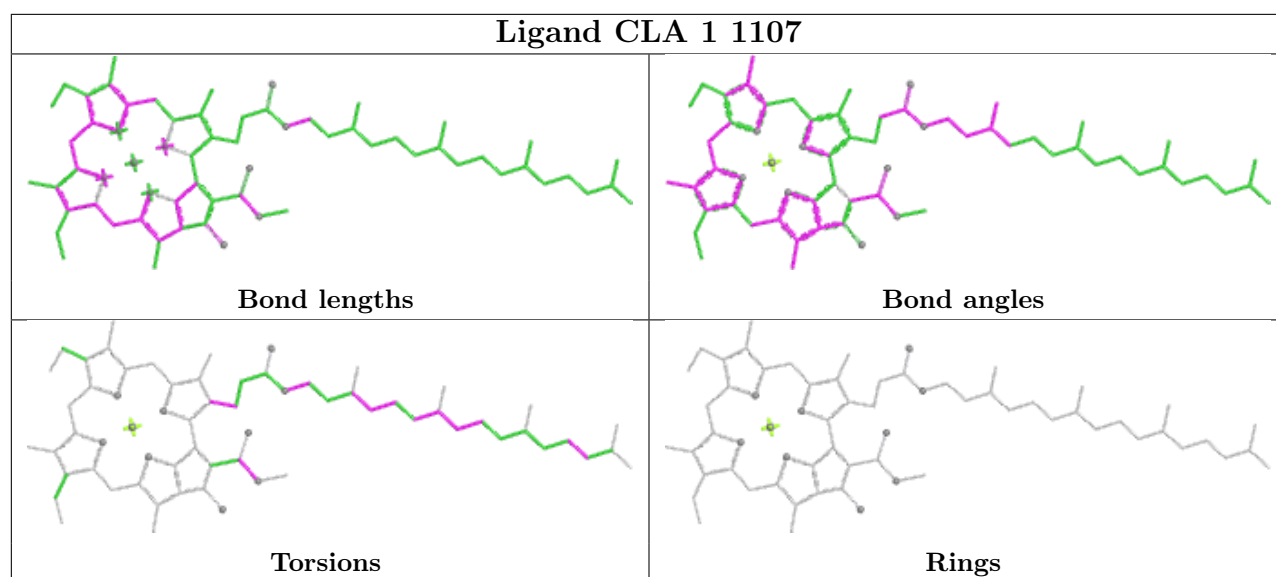
Ligand CLA B 1228

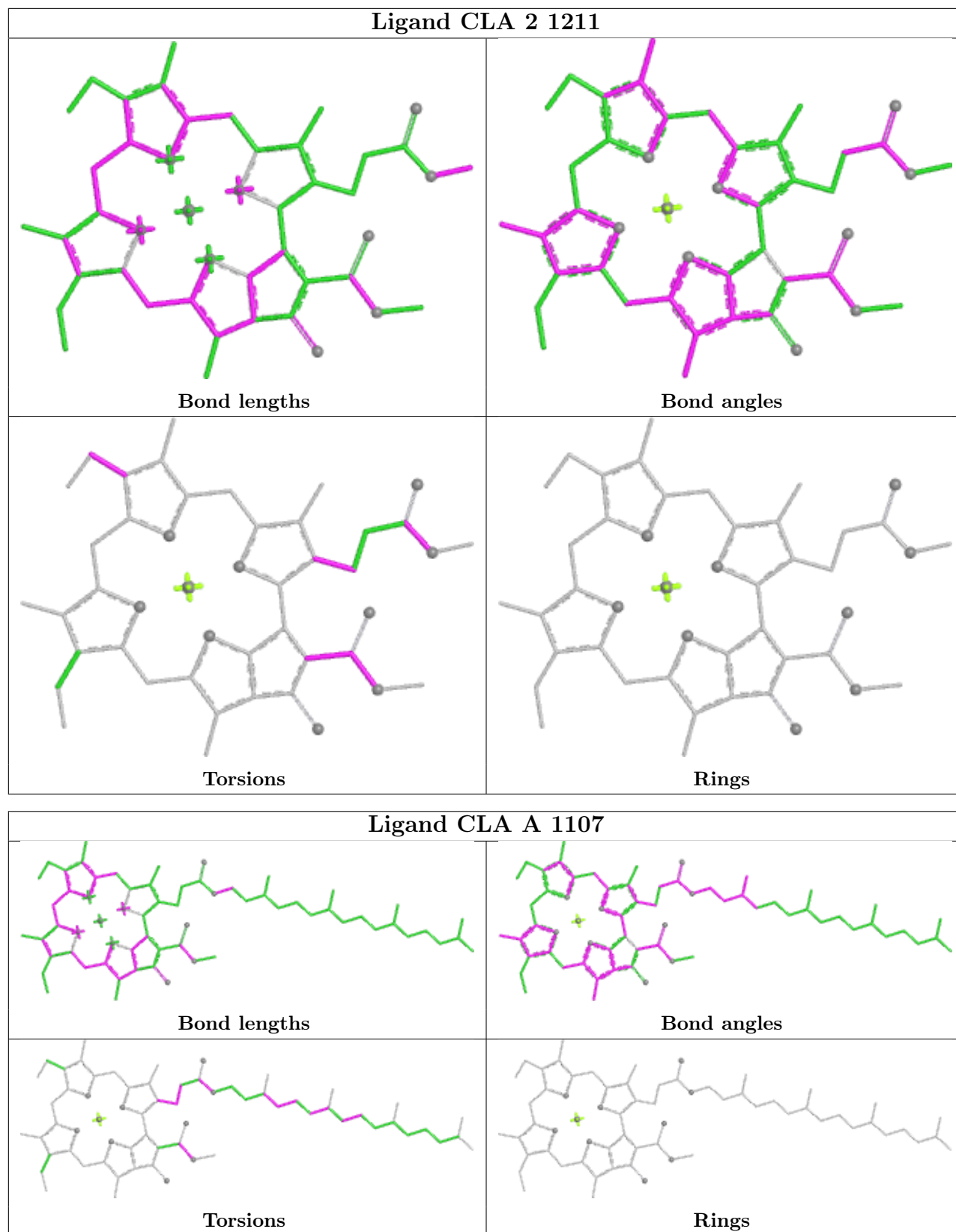


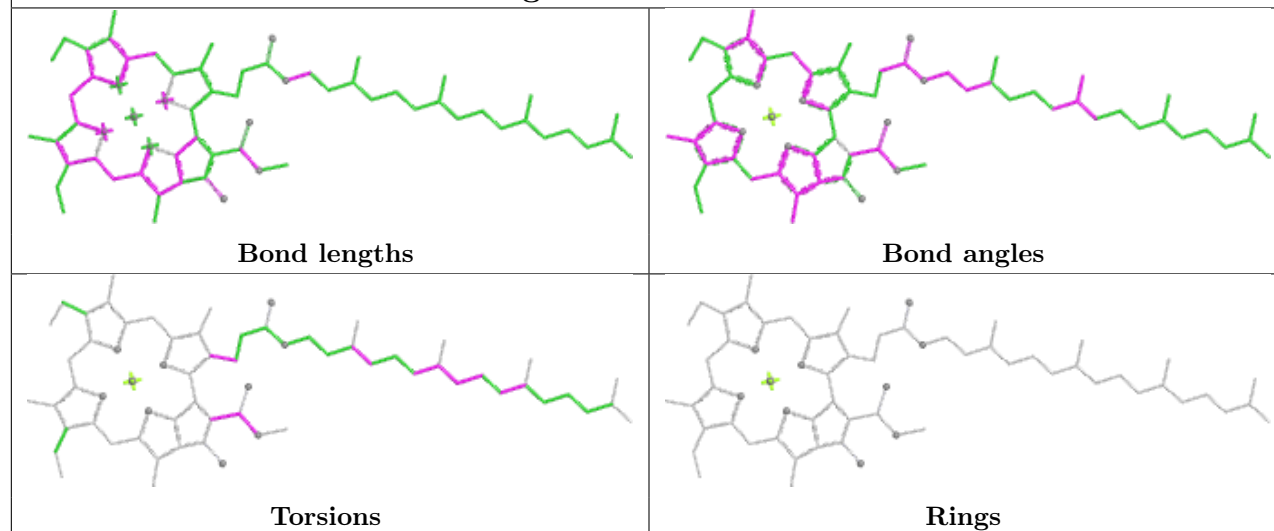
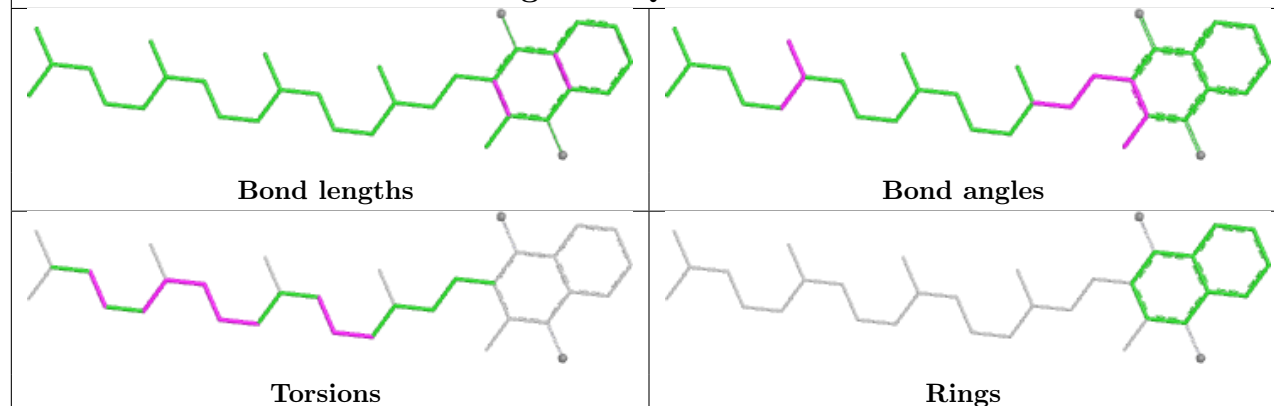
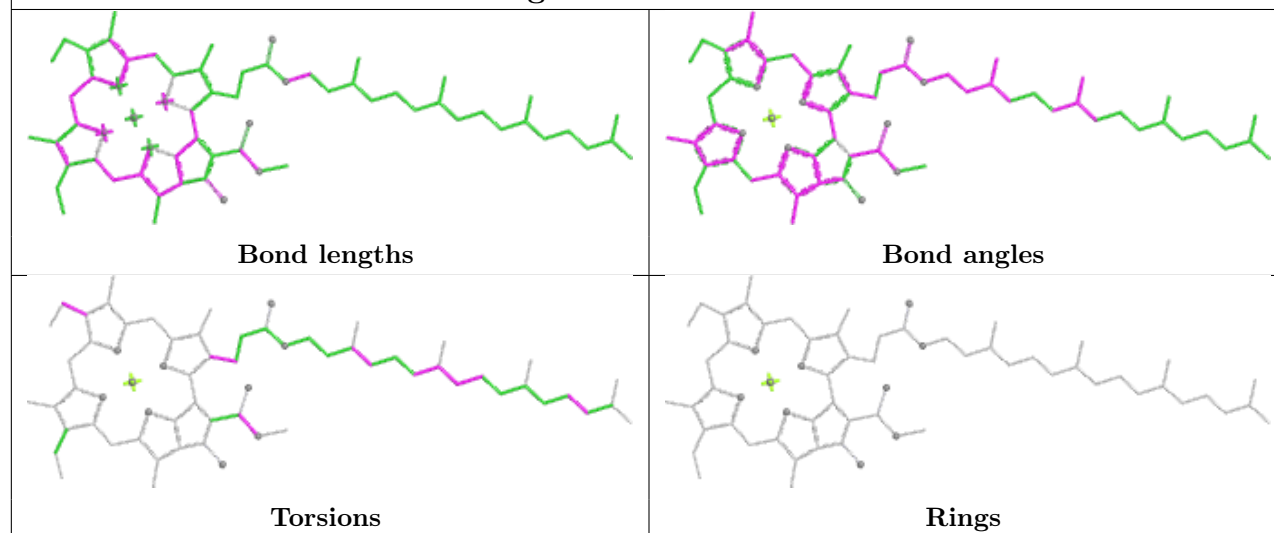
Ligand CLA b 1202

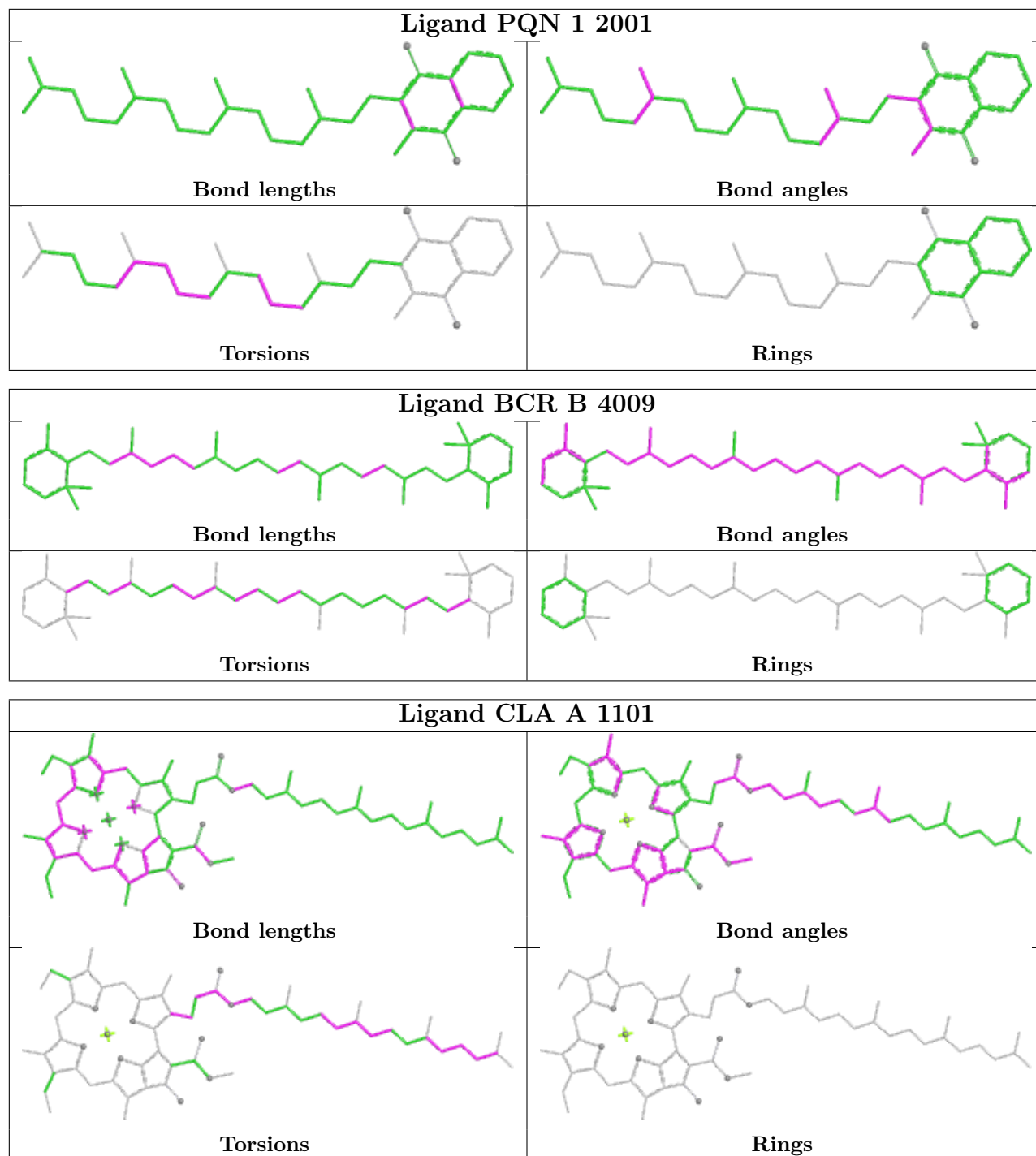


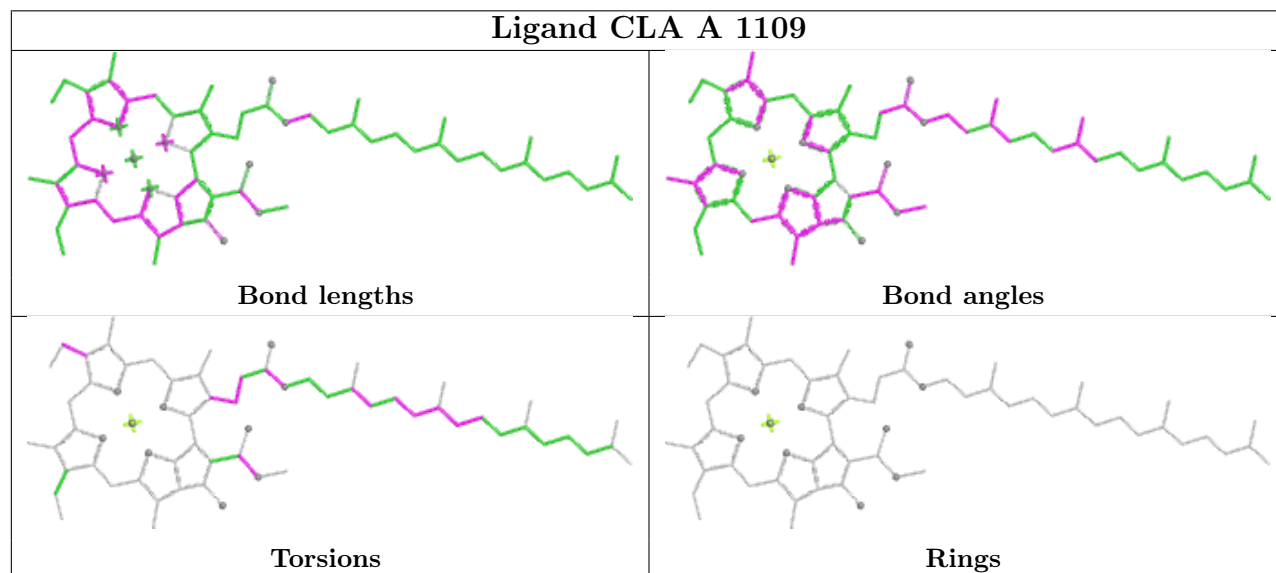
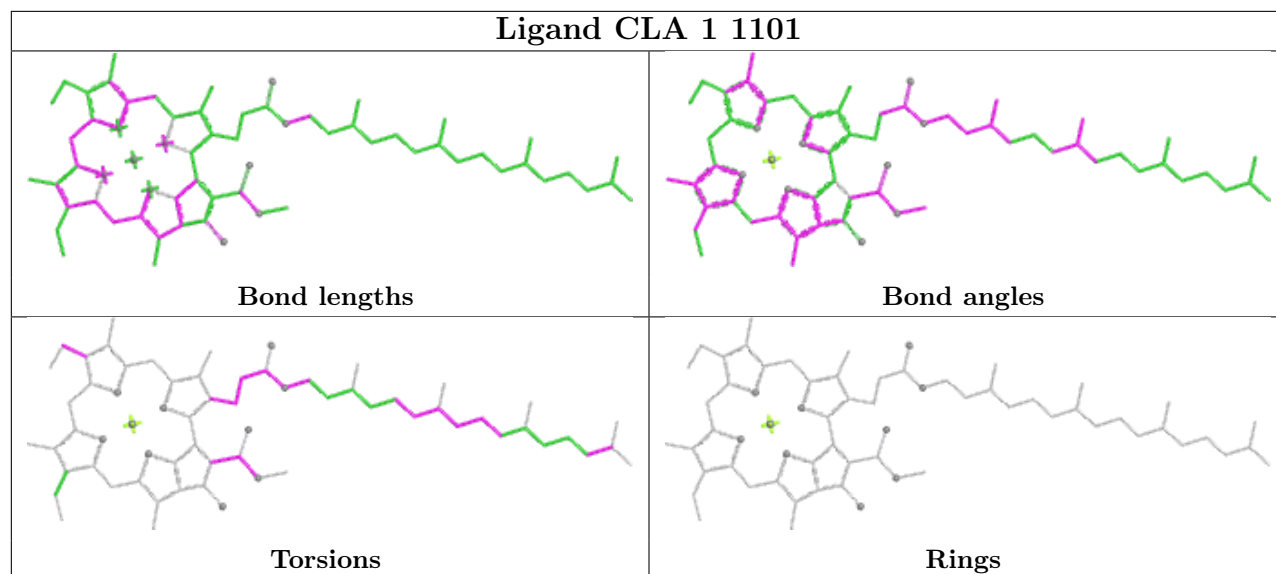


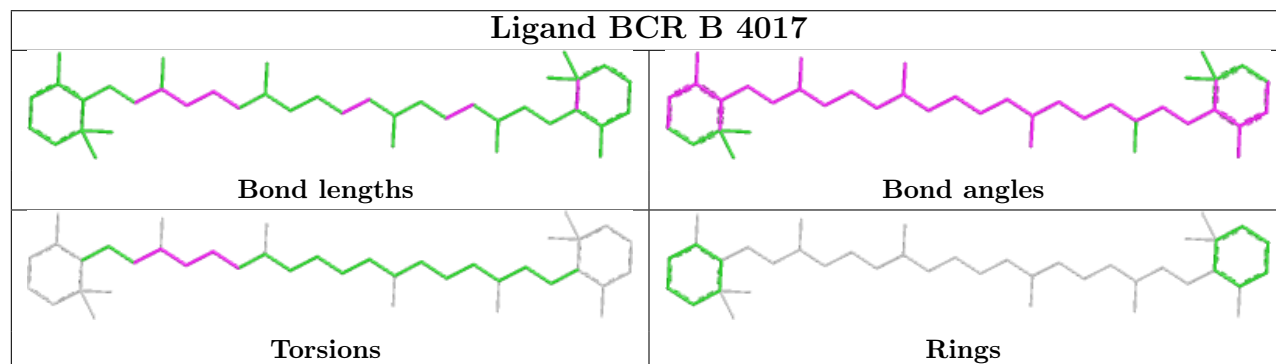
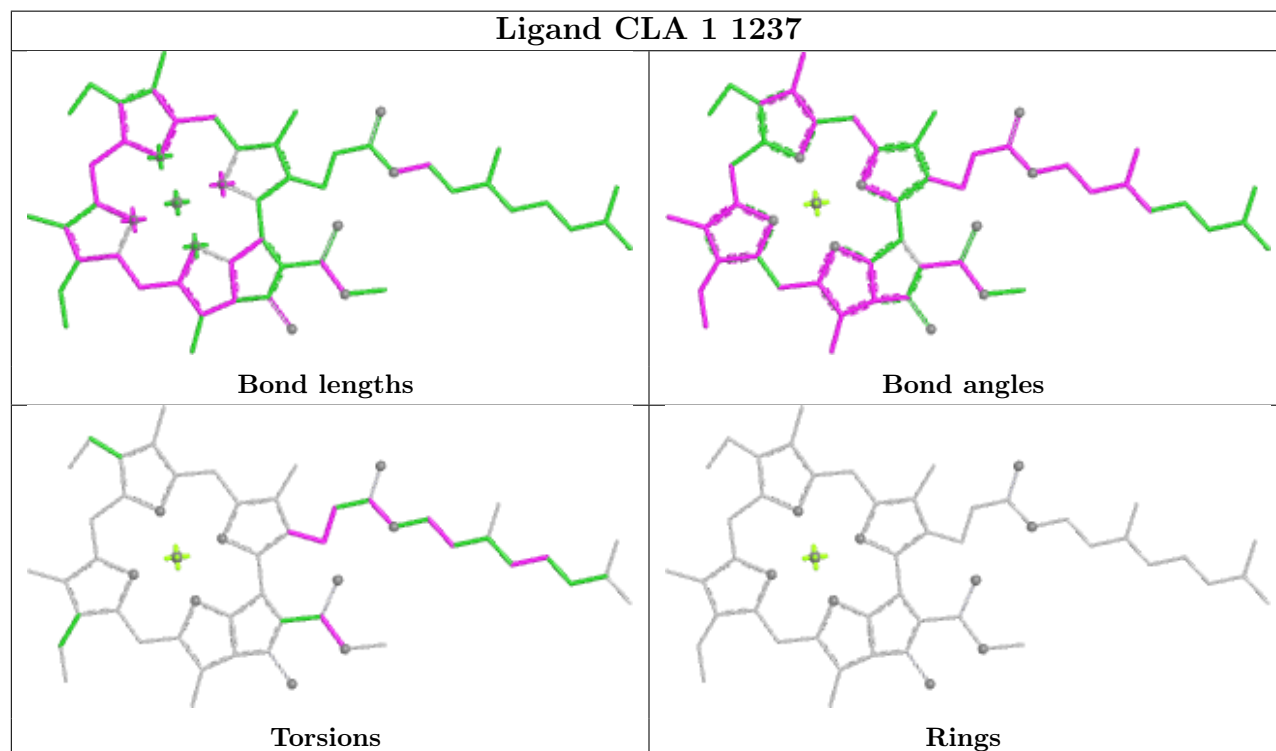
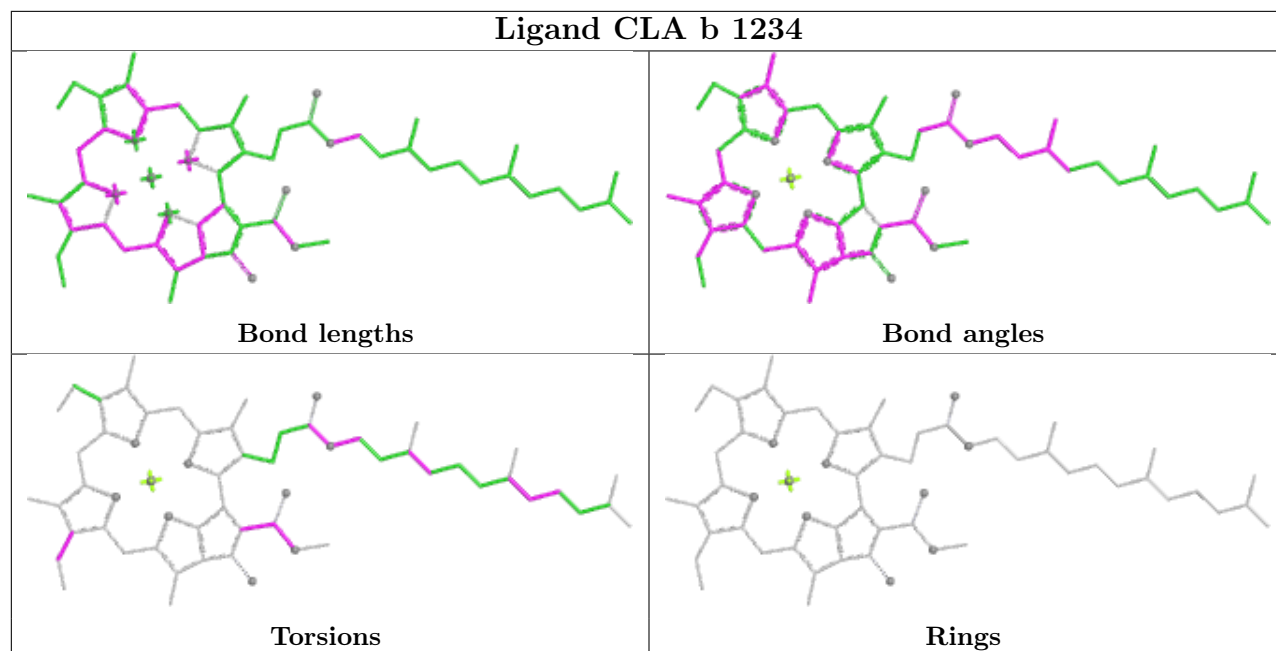


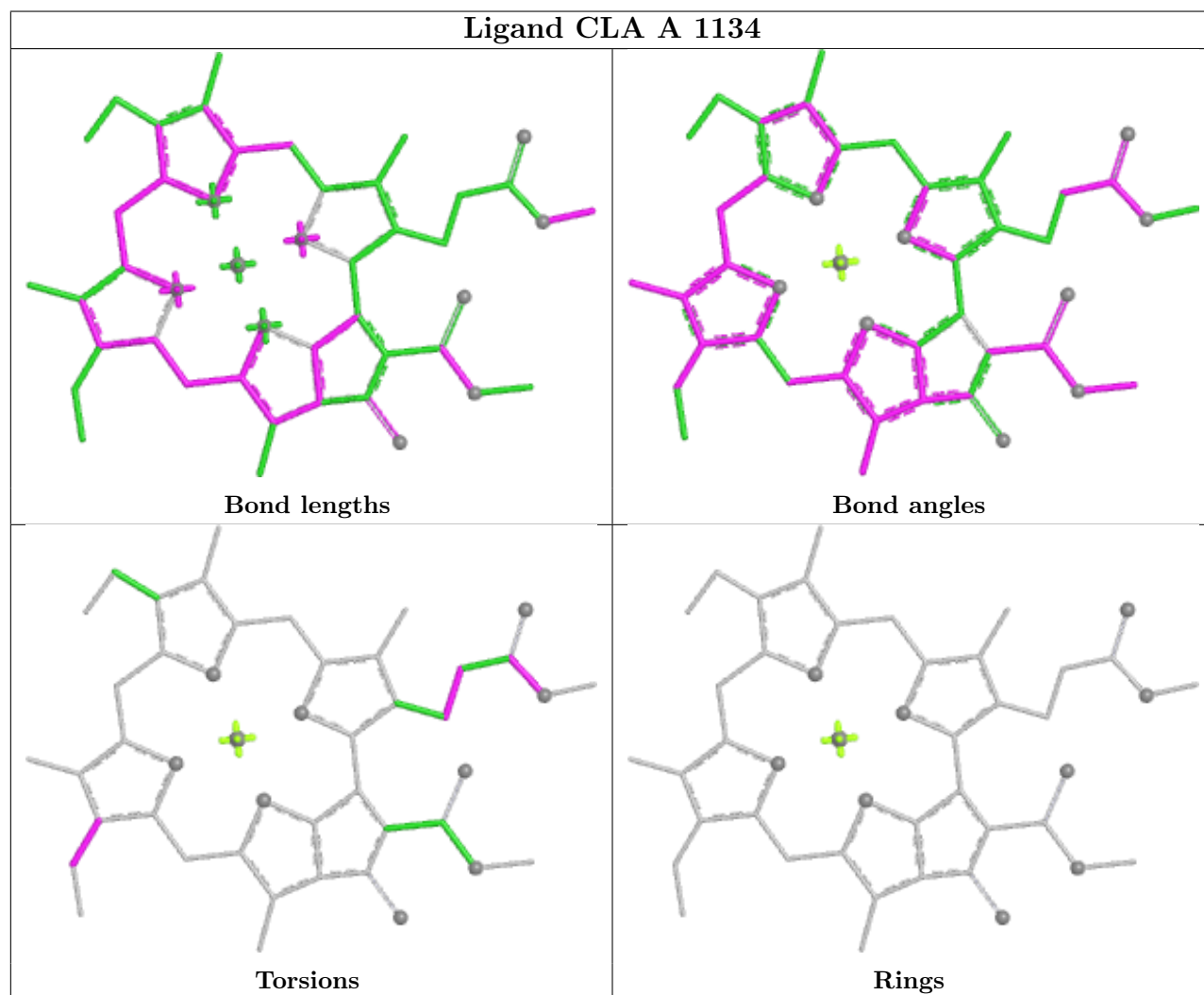
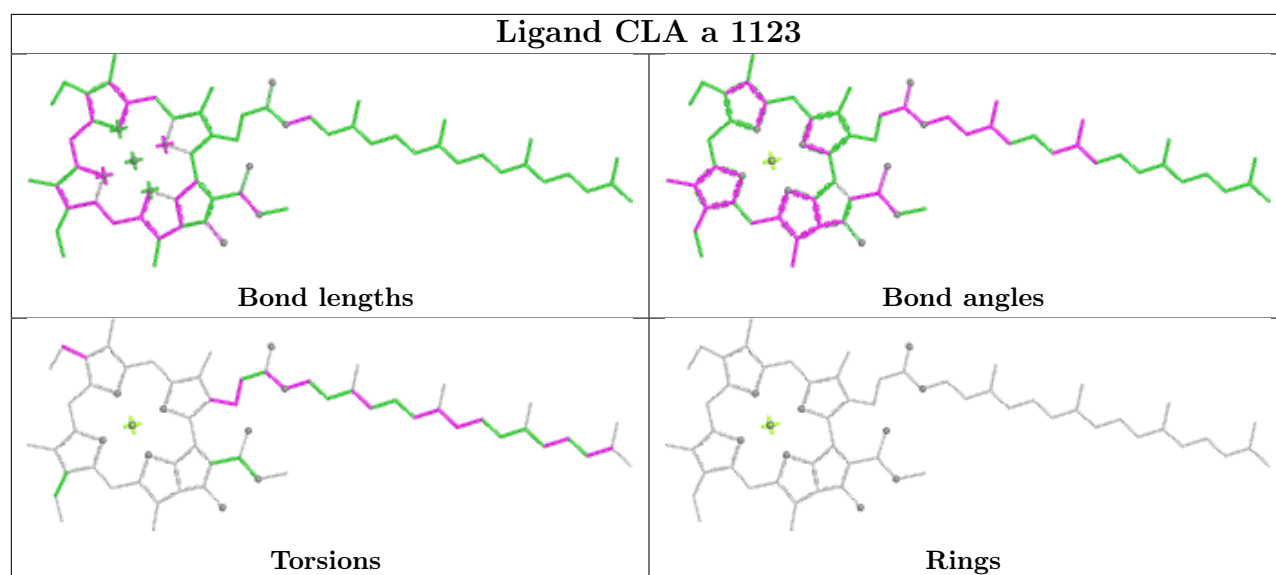


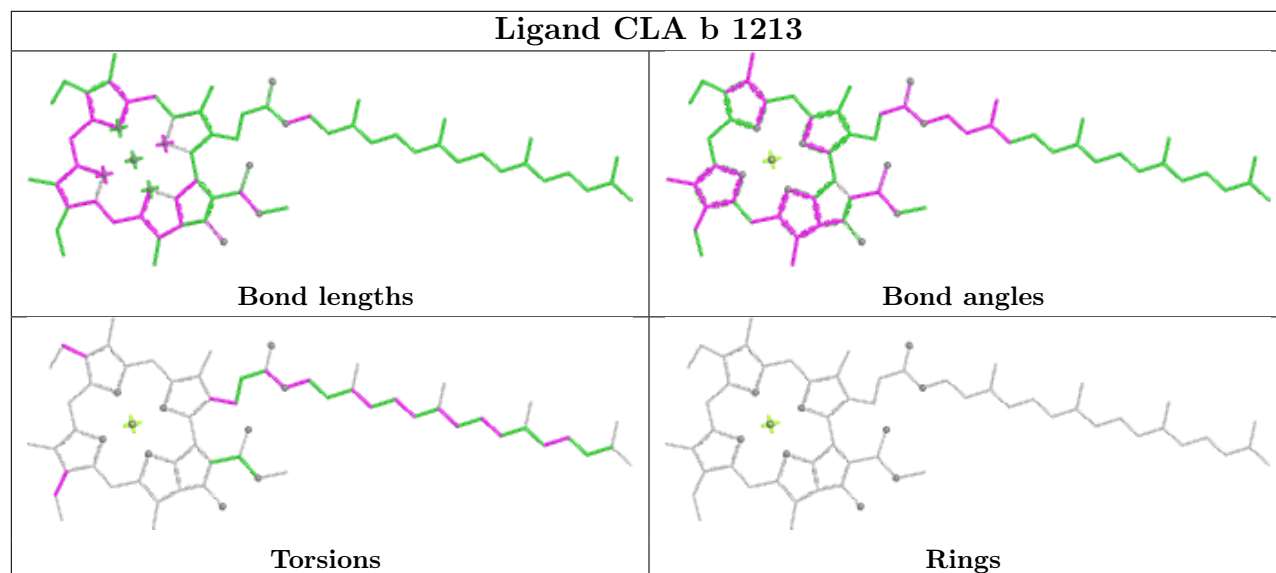
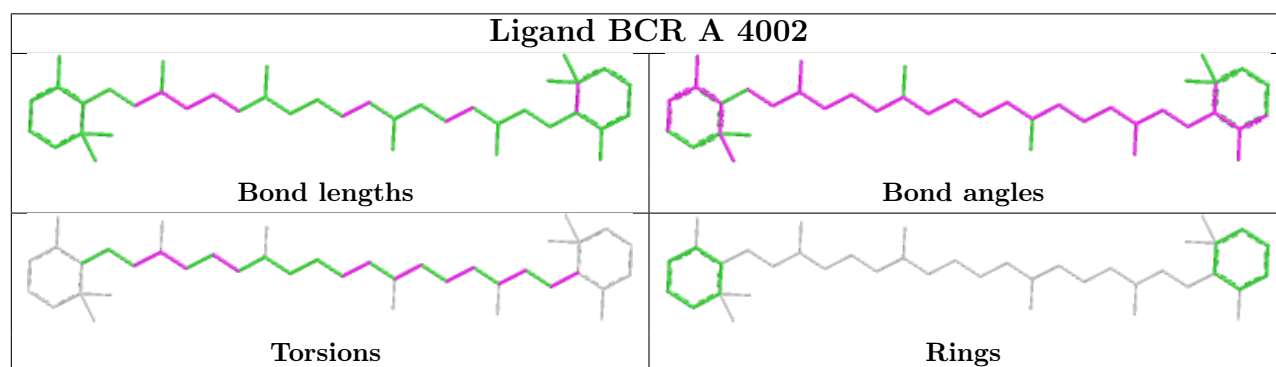
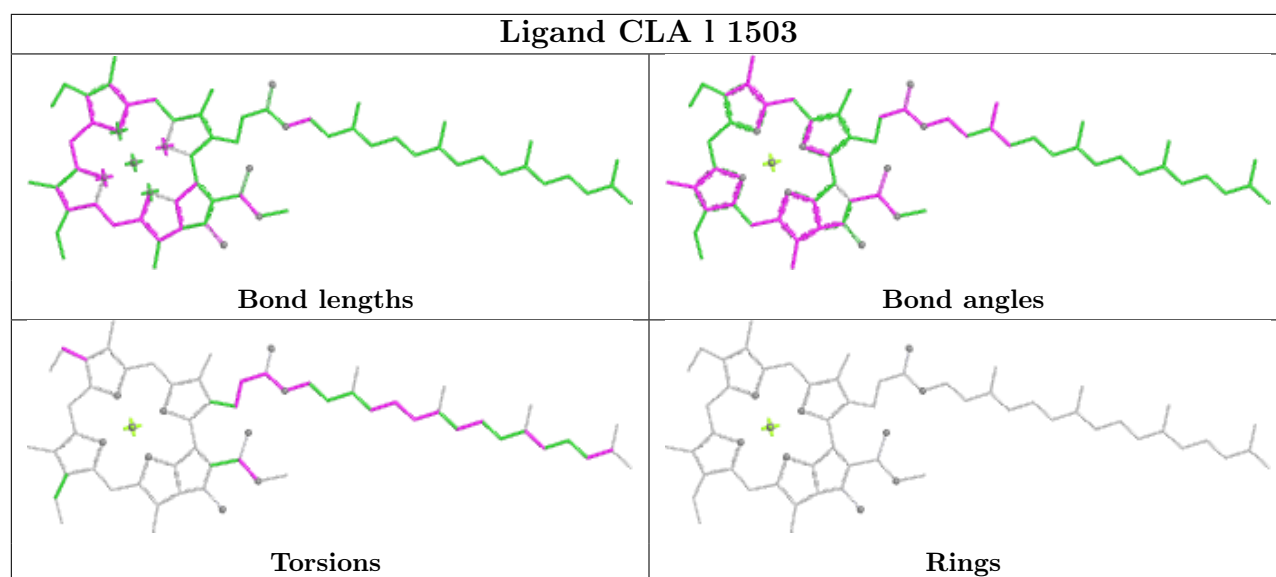
Ligand CLA A 1103**Ligand PQN B 2002****Ligand CLA a 1107**

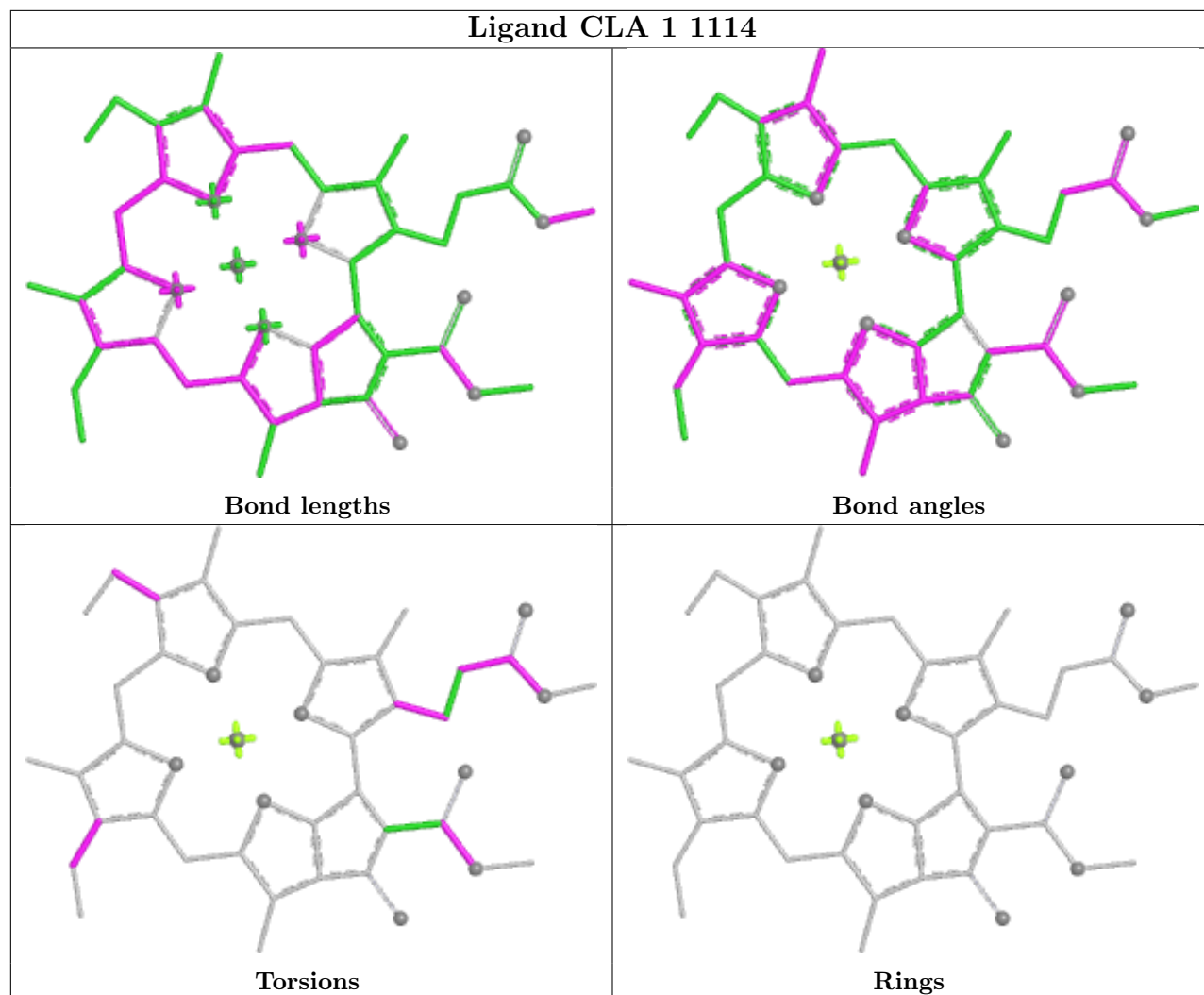


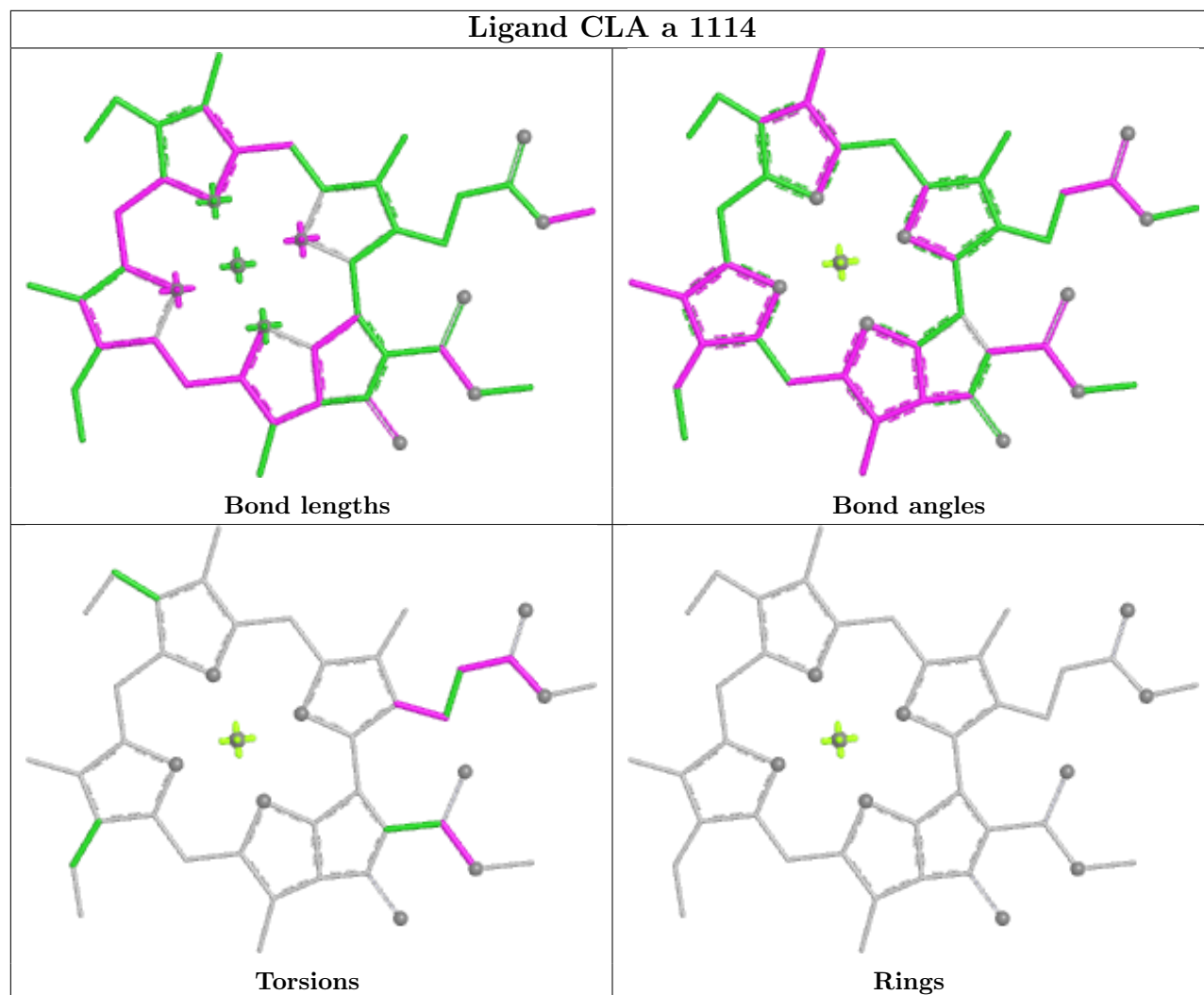


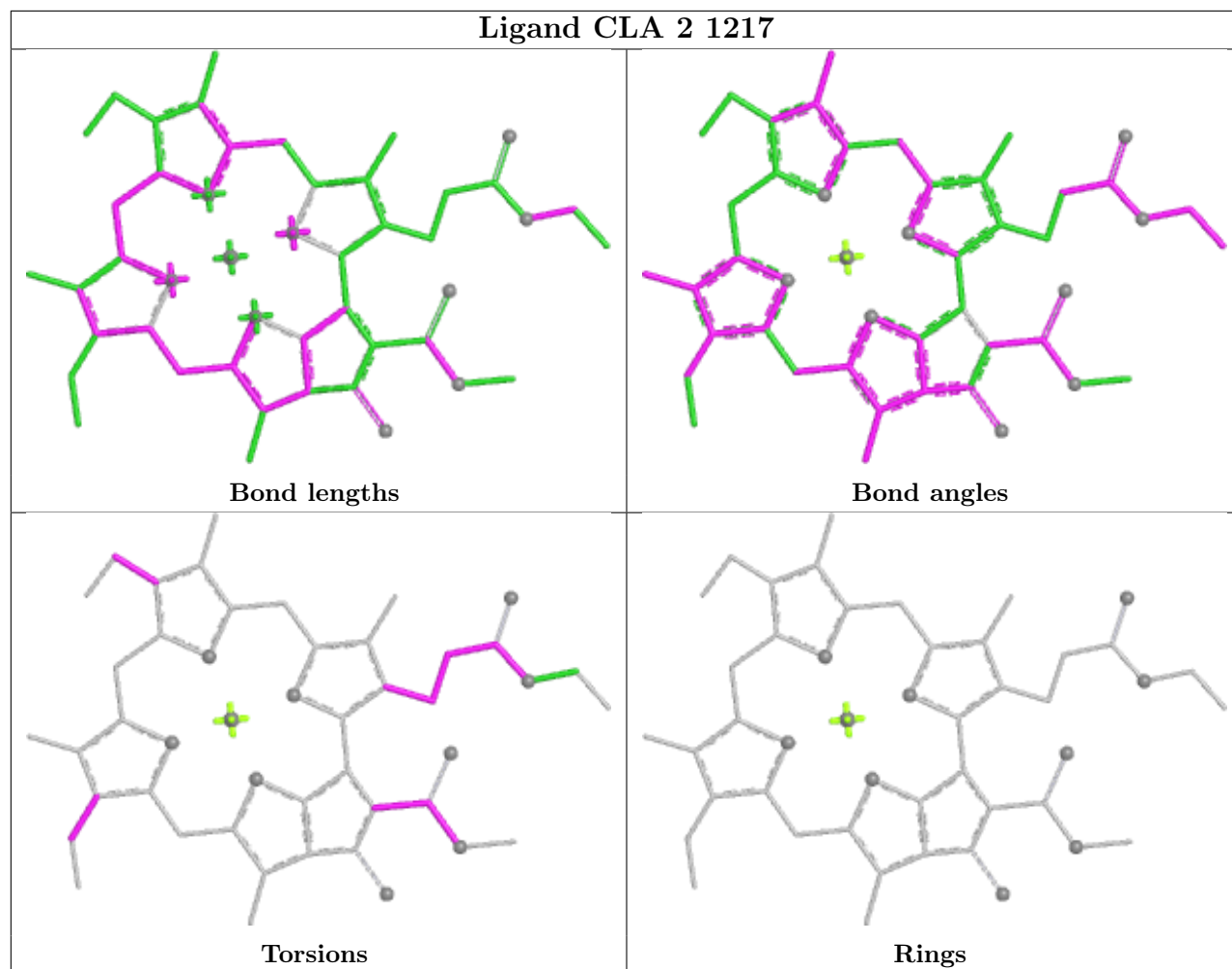




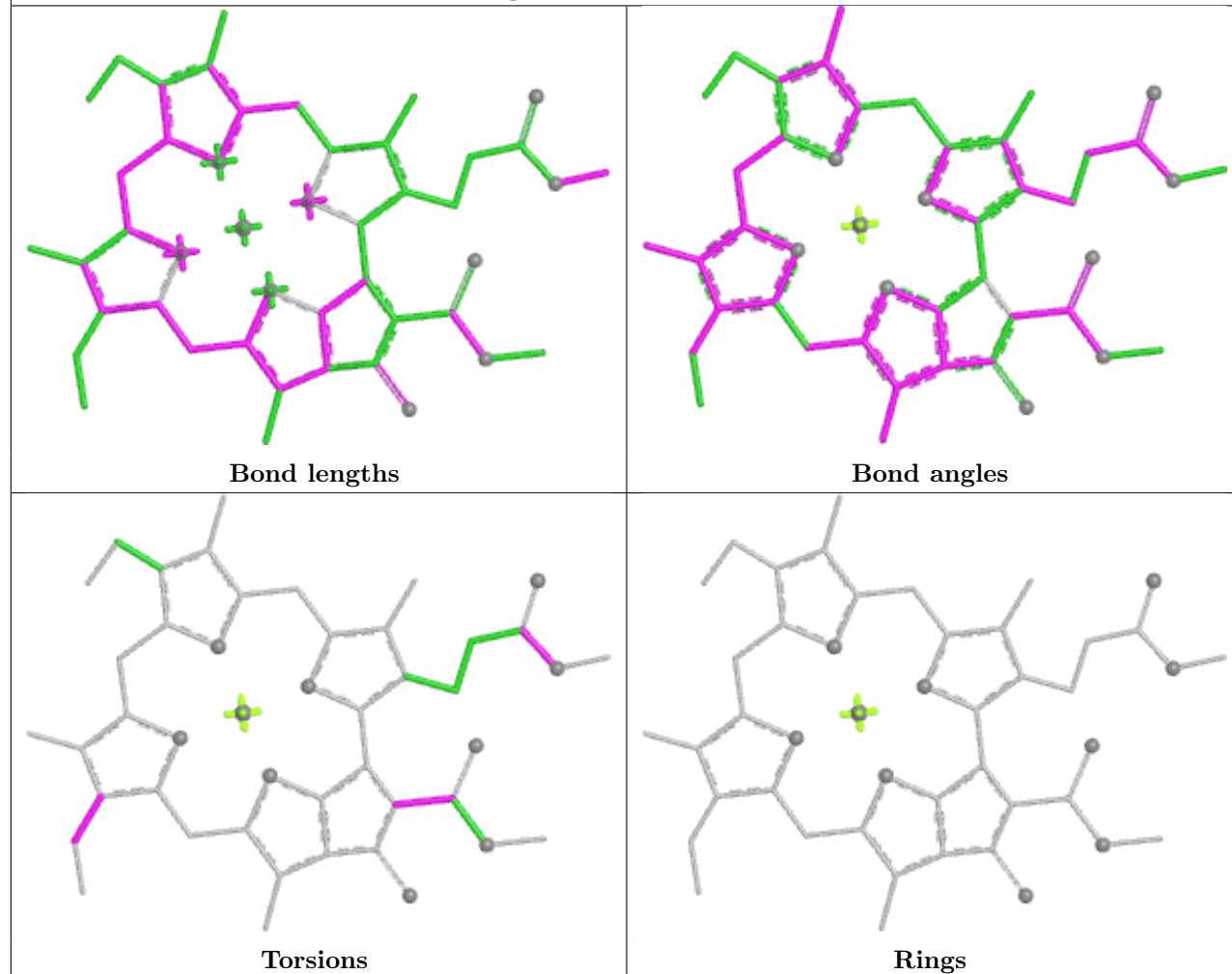




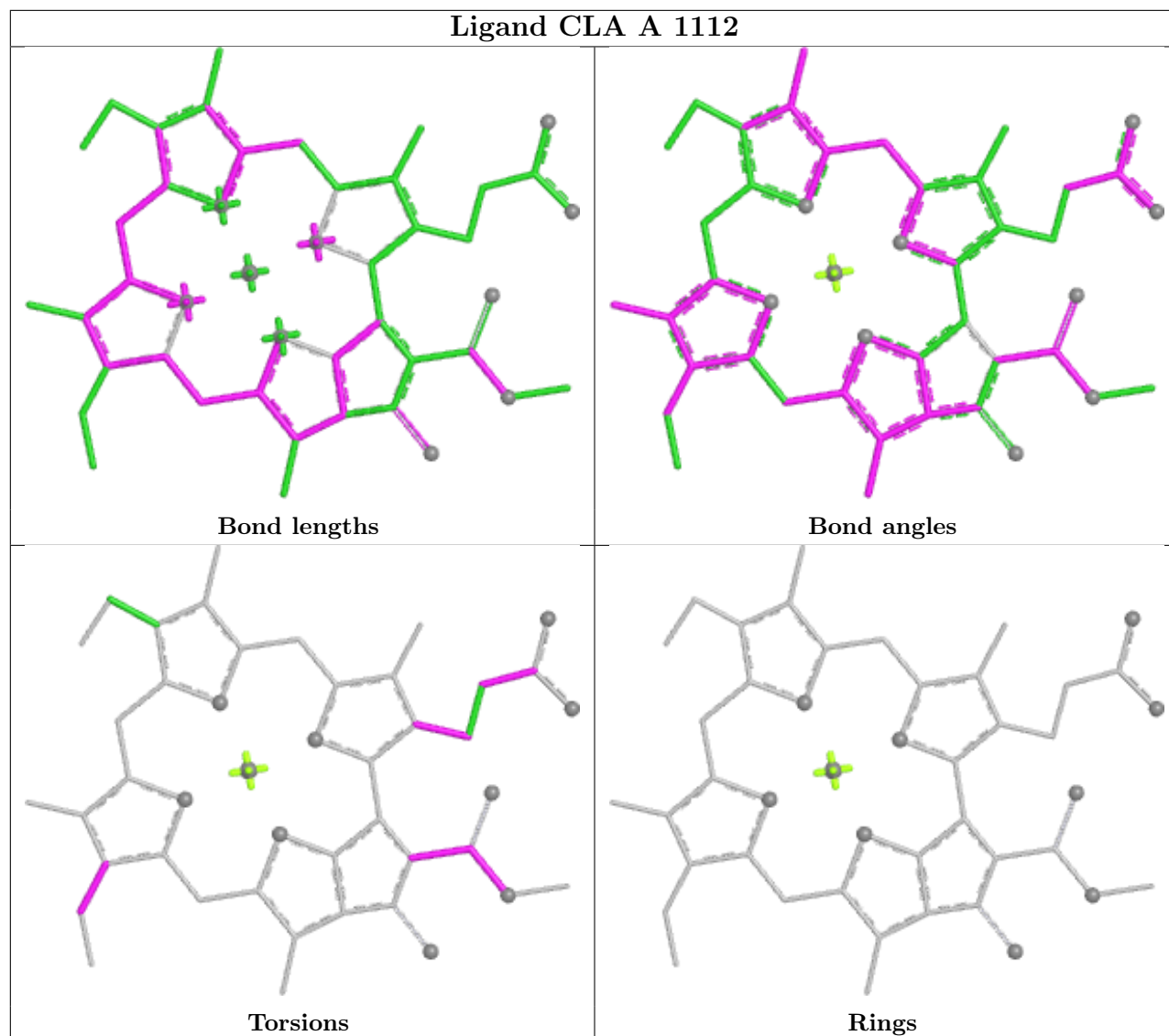




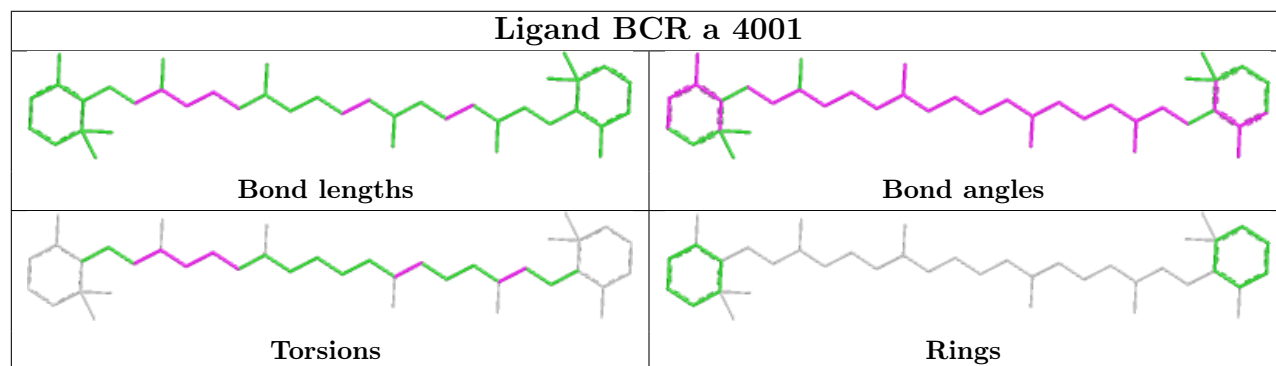
Ligand CLA A 1129

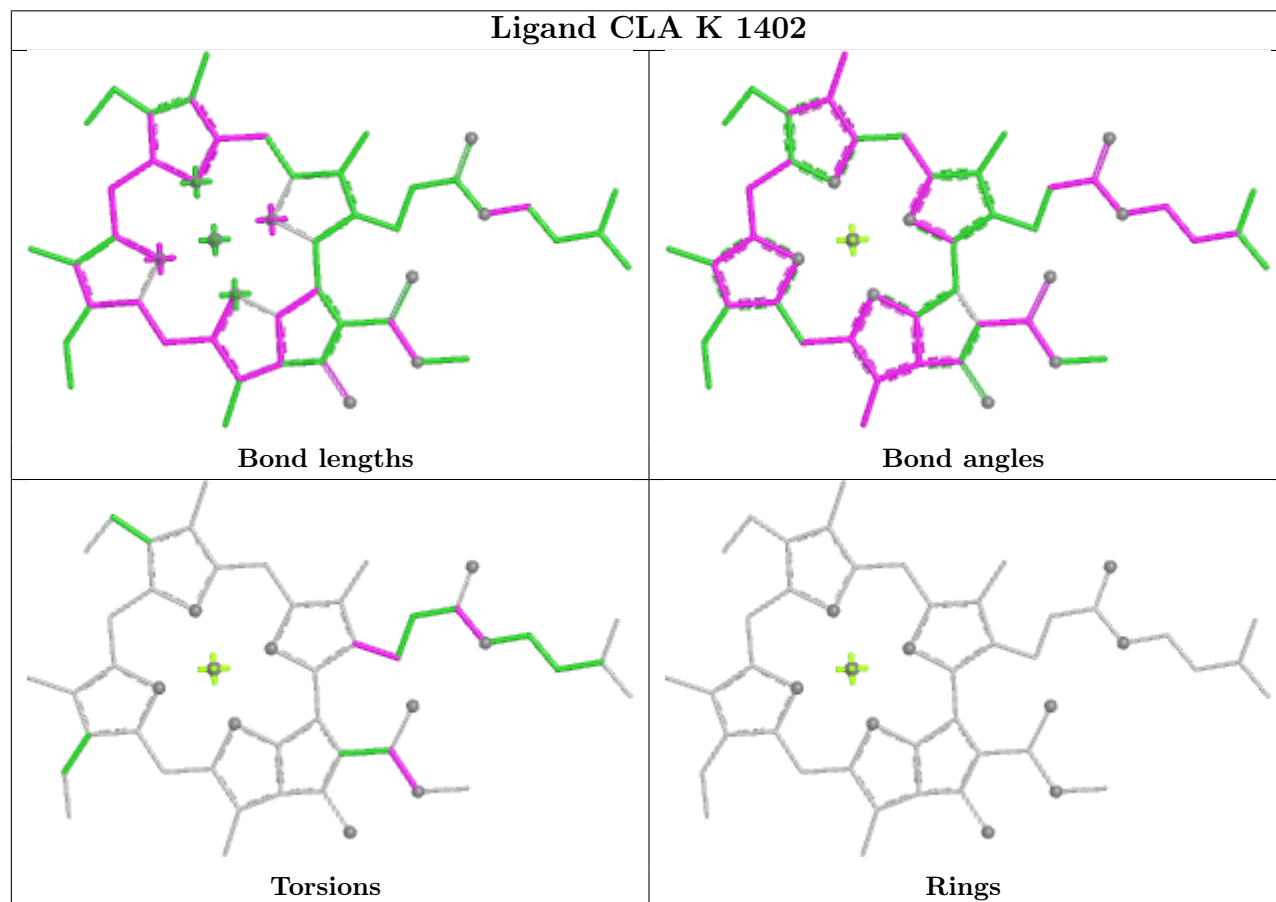
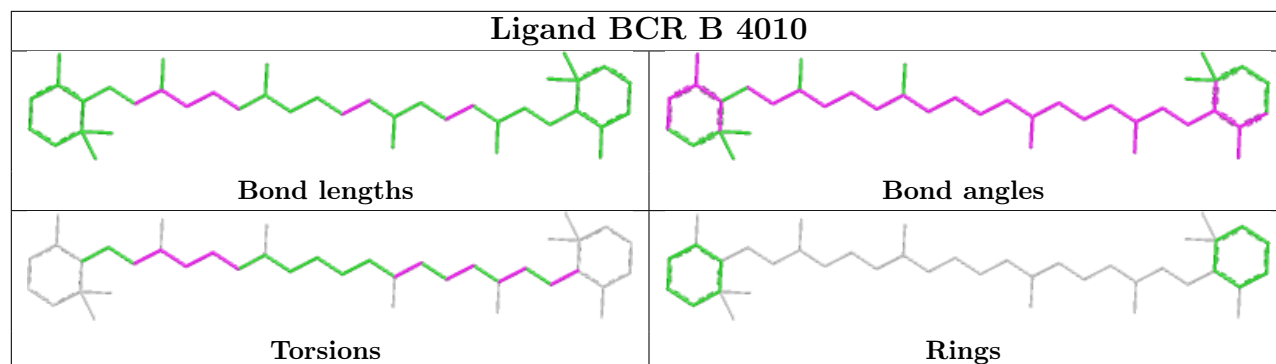


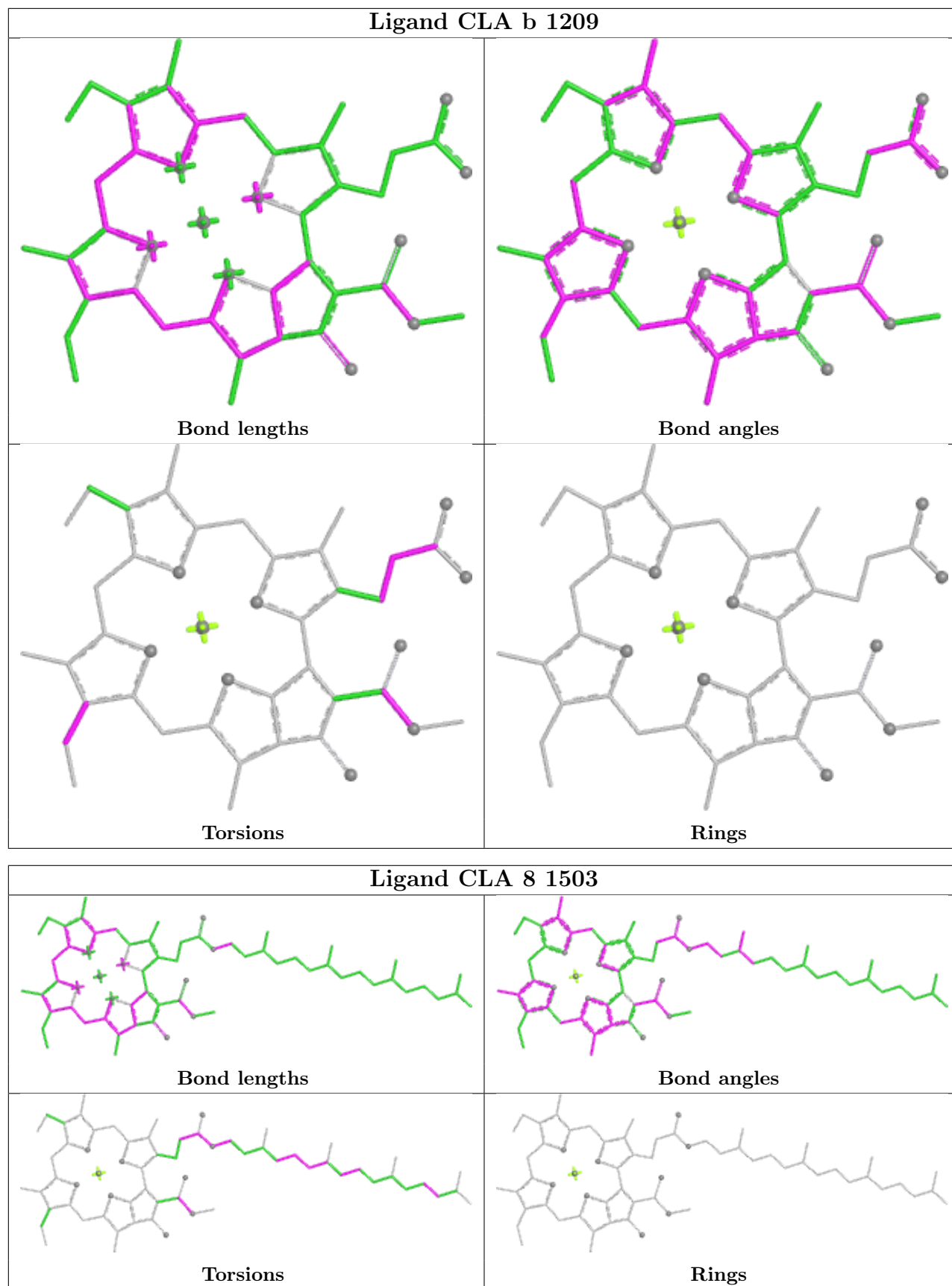
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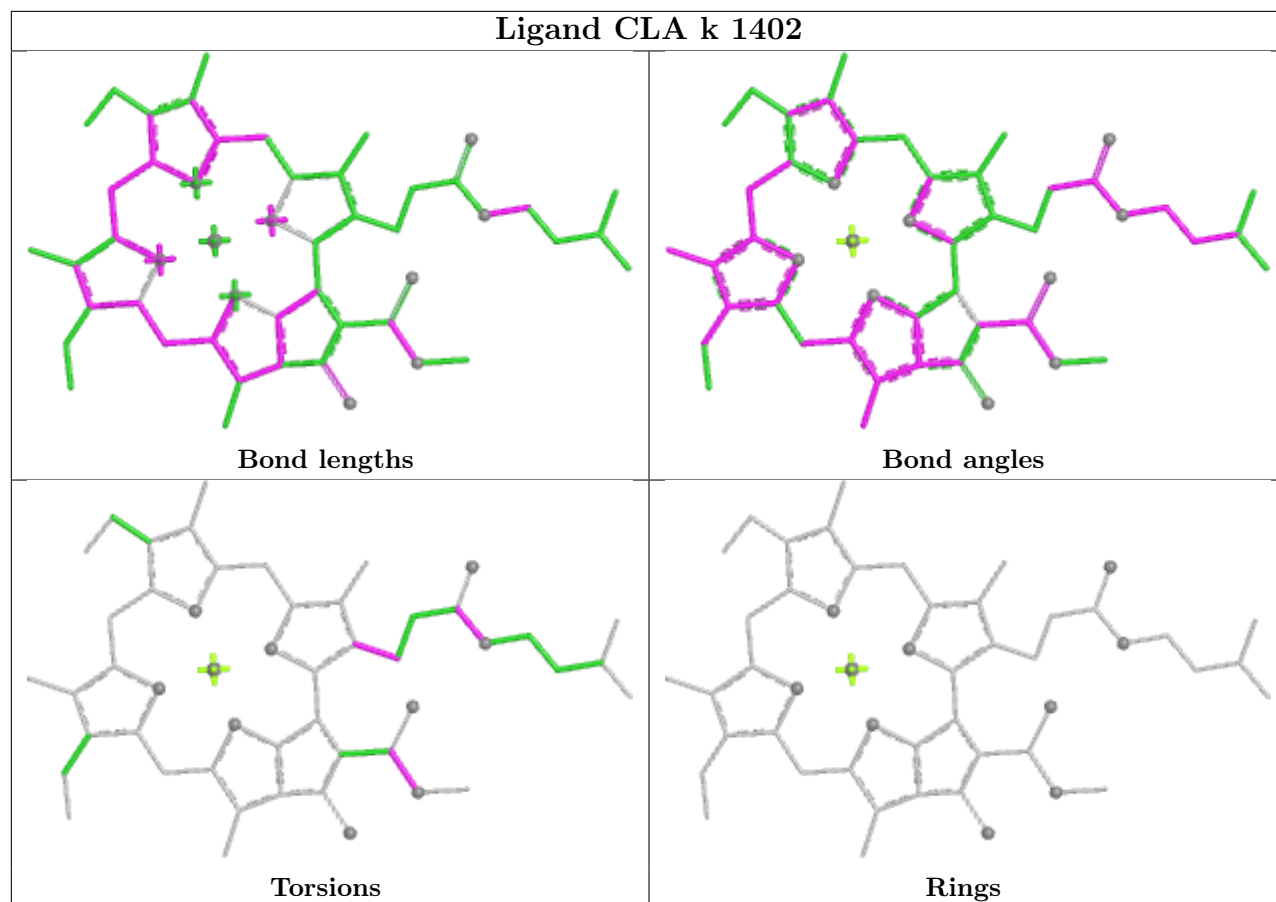


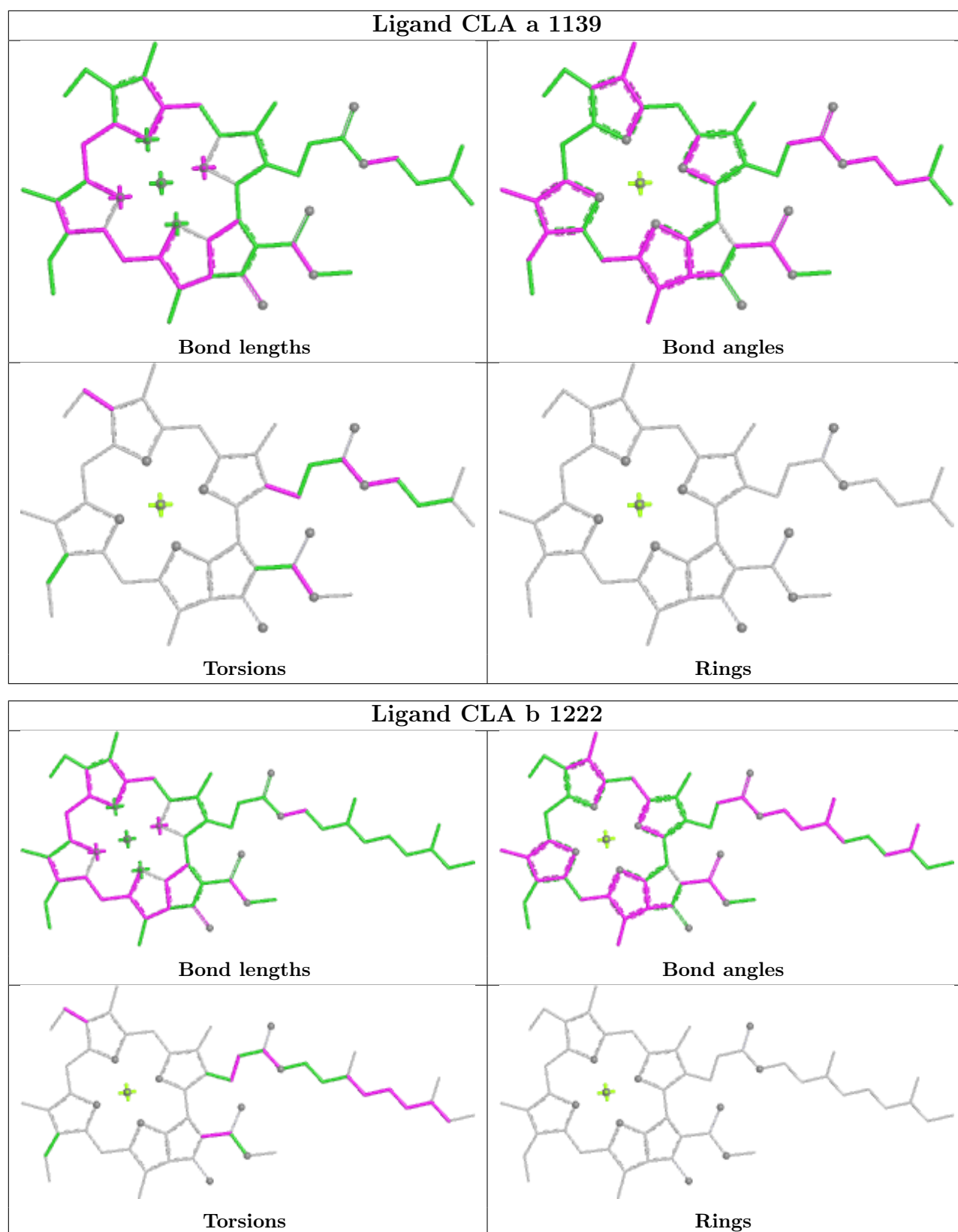
Ligand BCR a 4001

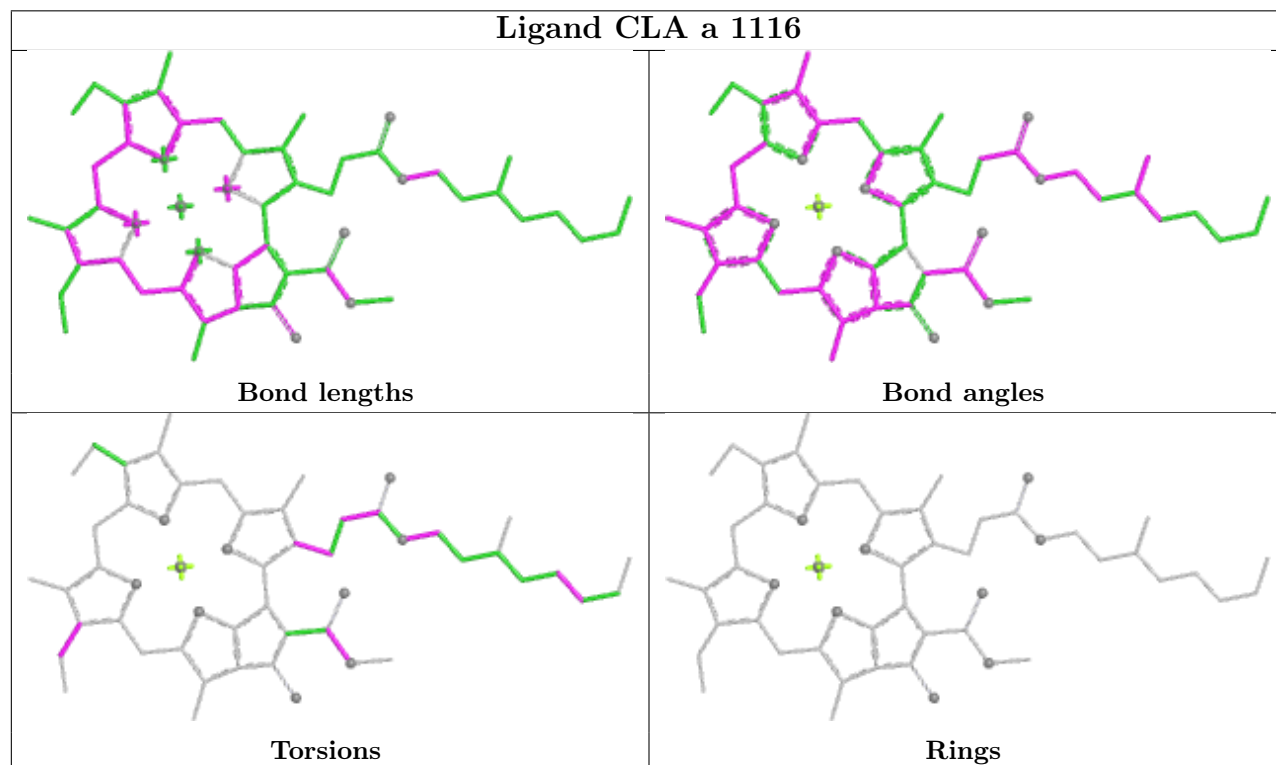
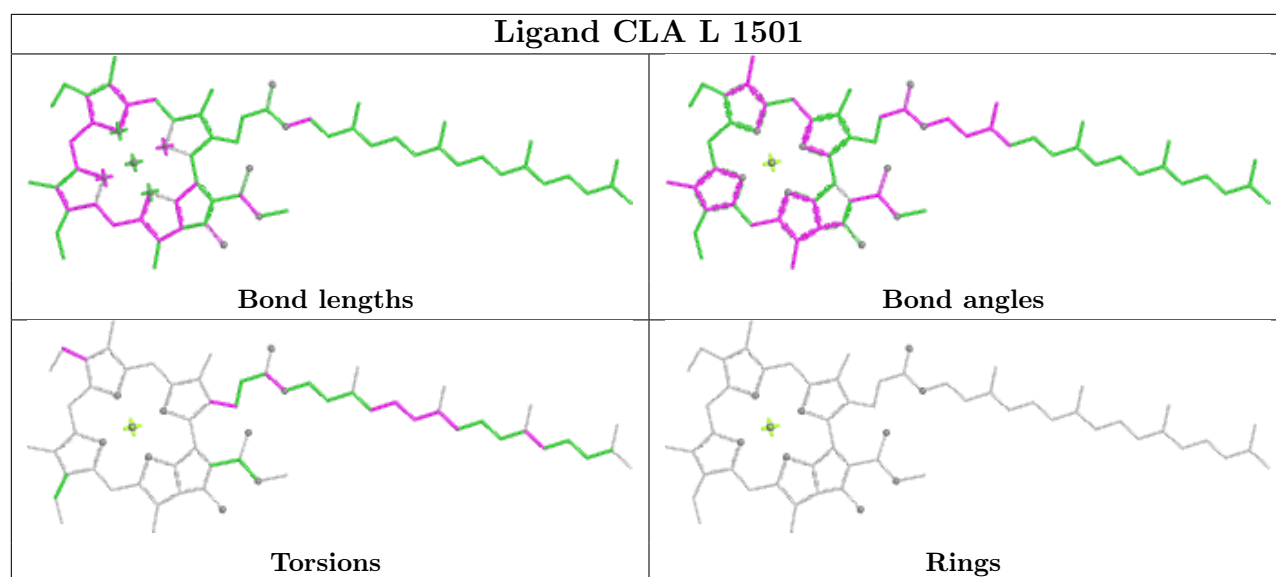




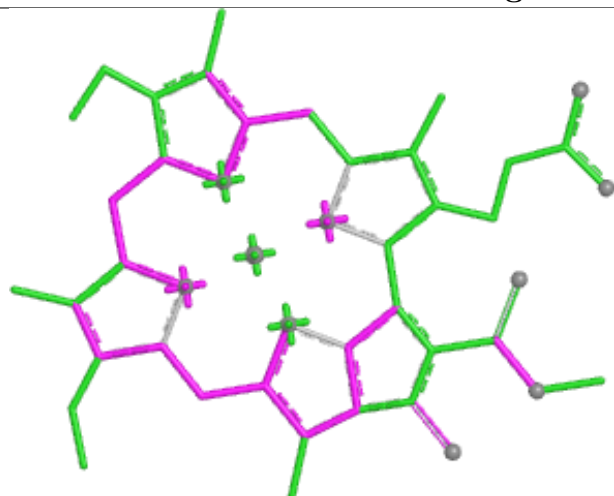




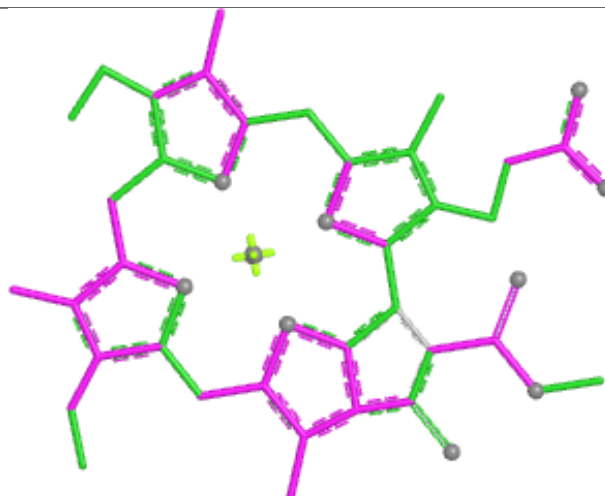




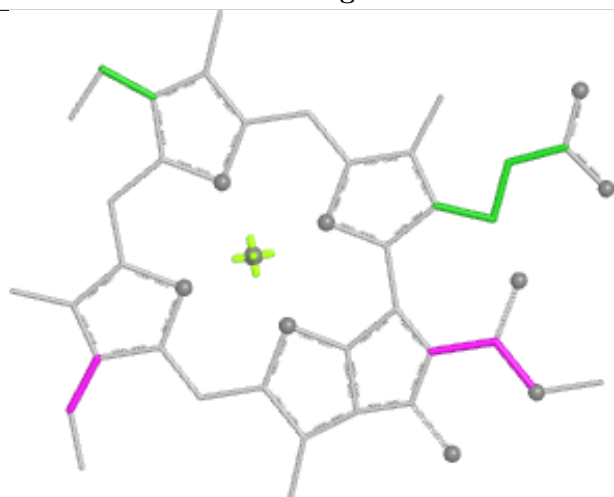
Ligand CLA B 1227



Bond lengths



Bond angles

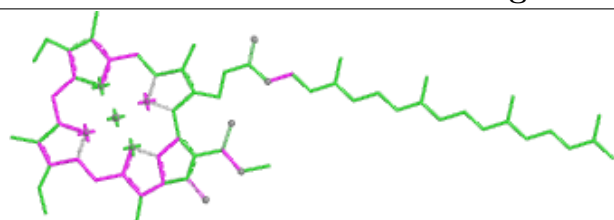


Torsions

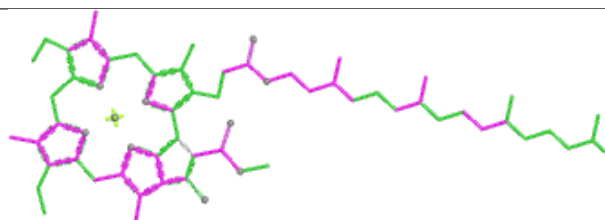


Rings

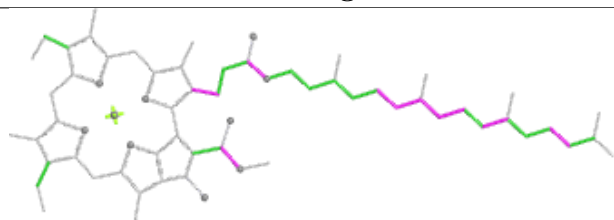
Ligand CLA 1 1128



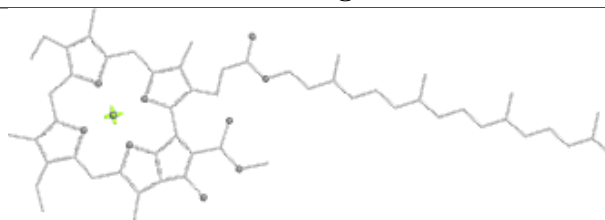
Bond lengths



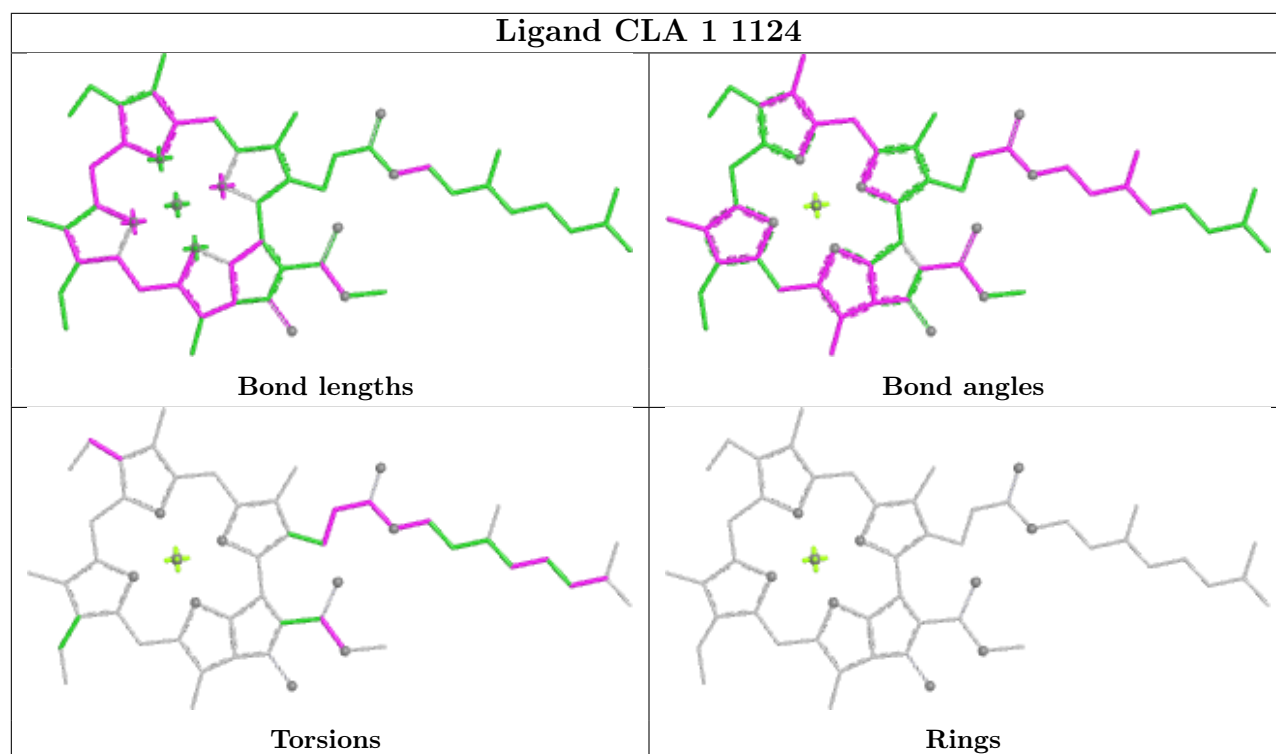
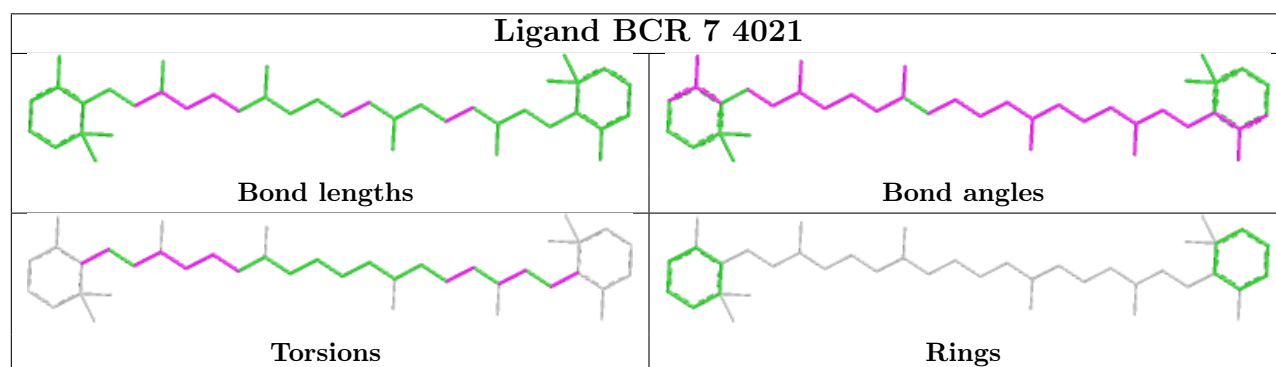
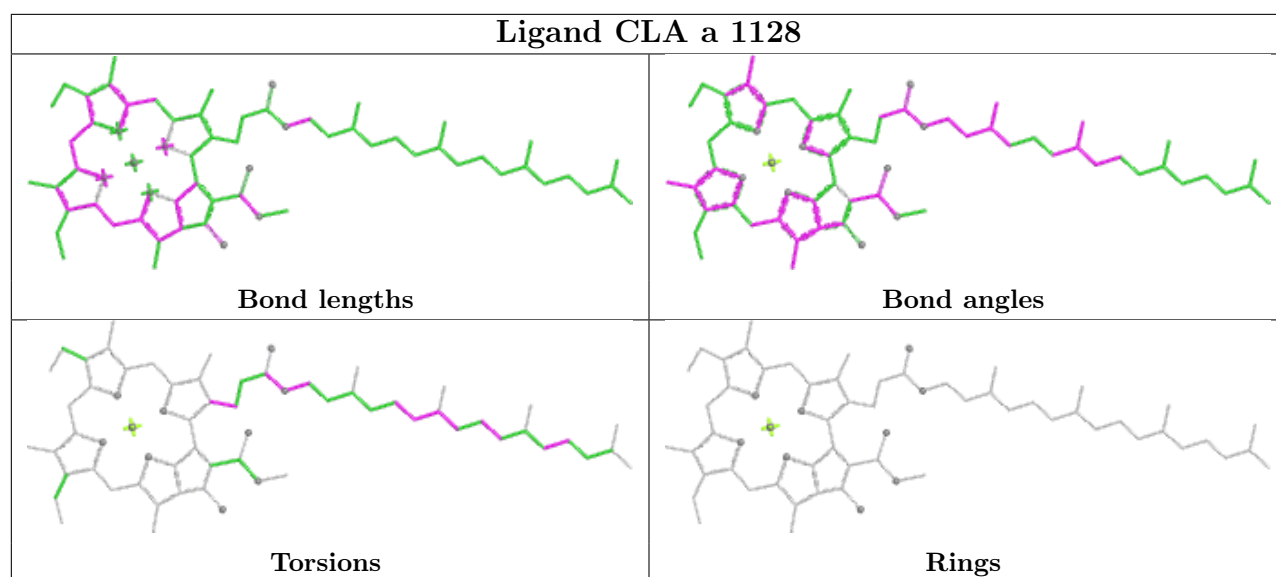
Bond angles

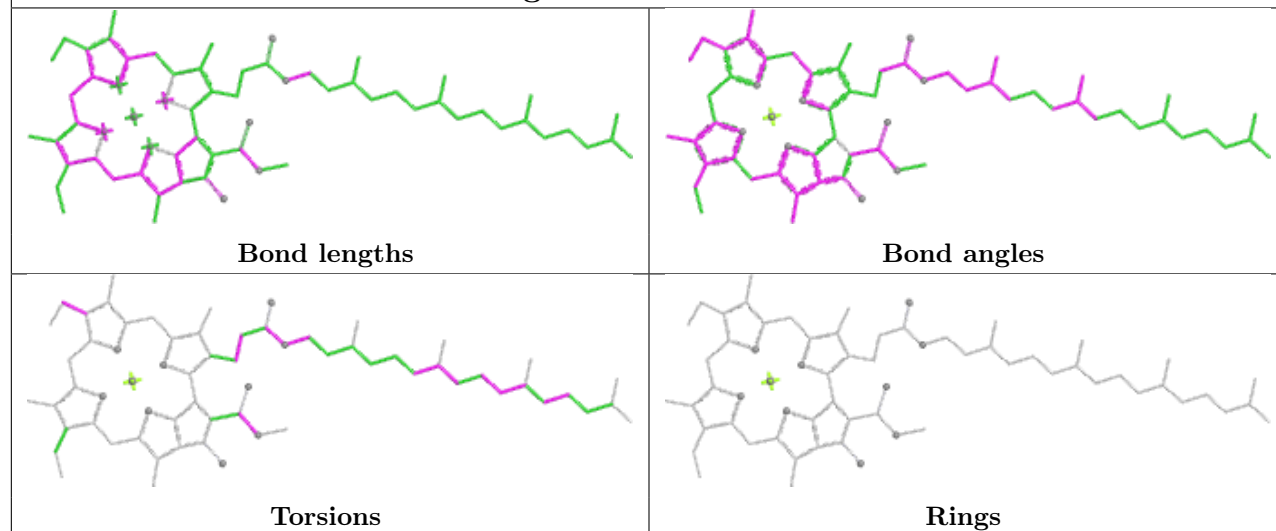
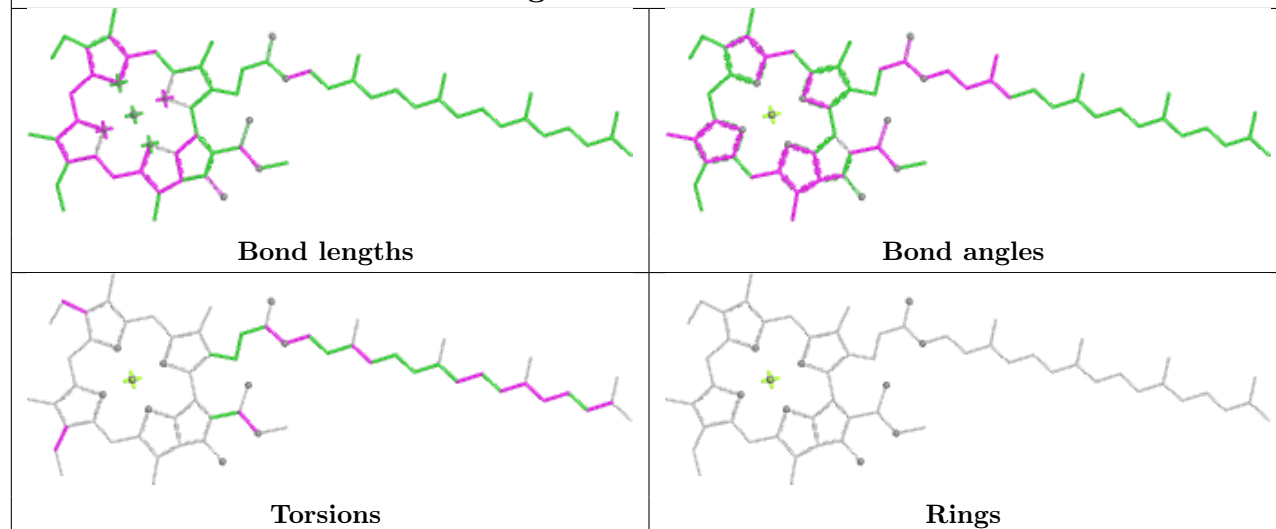


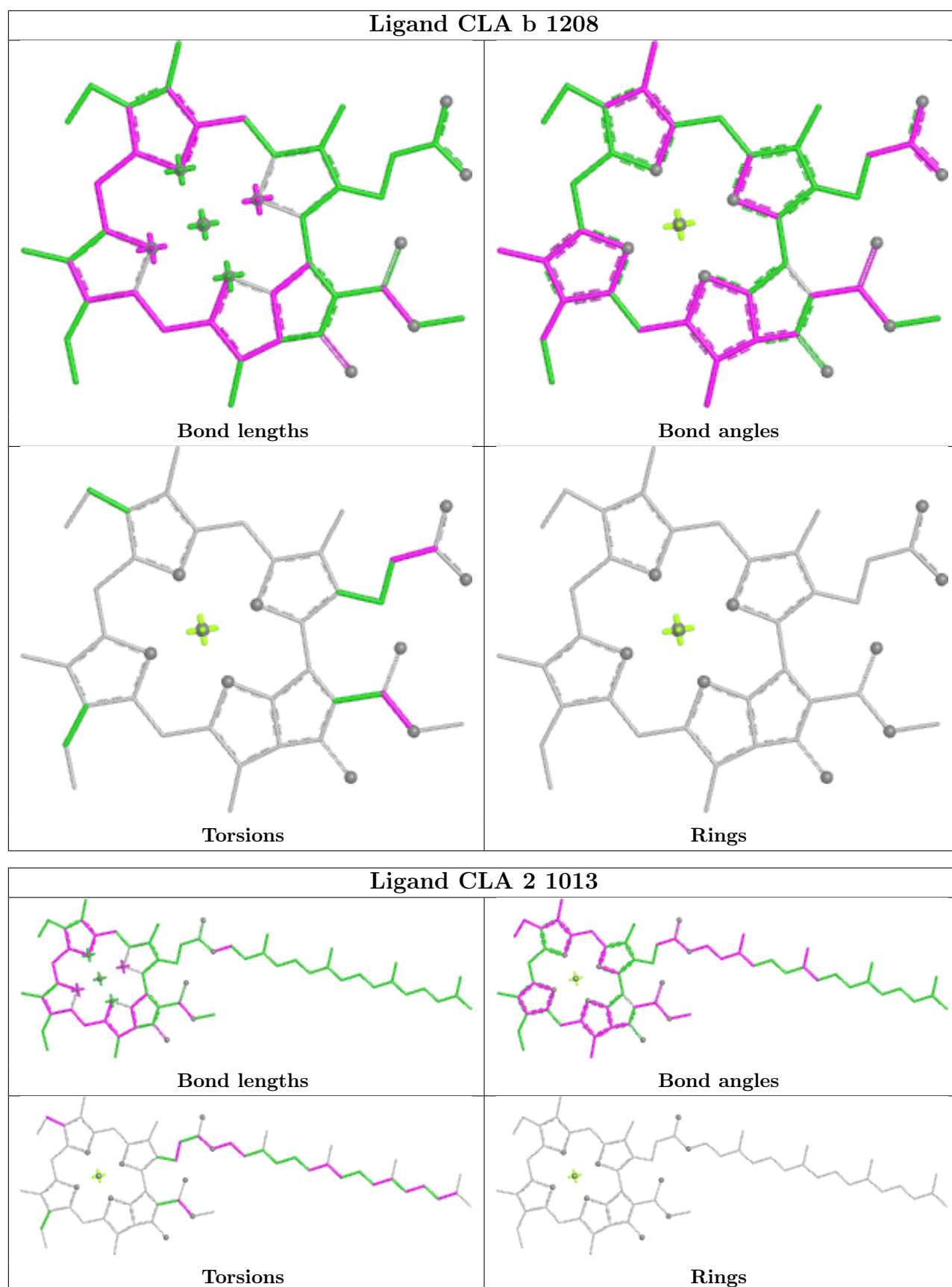
Torsions

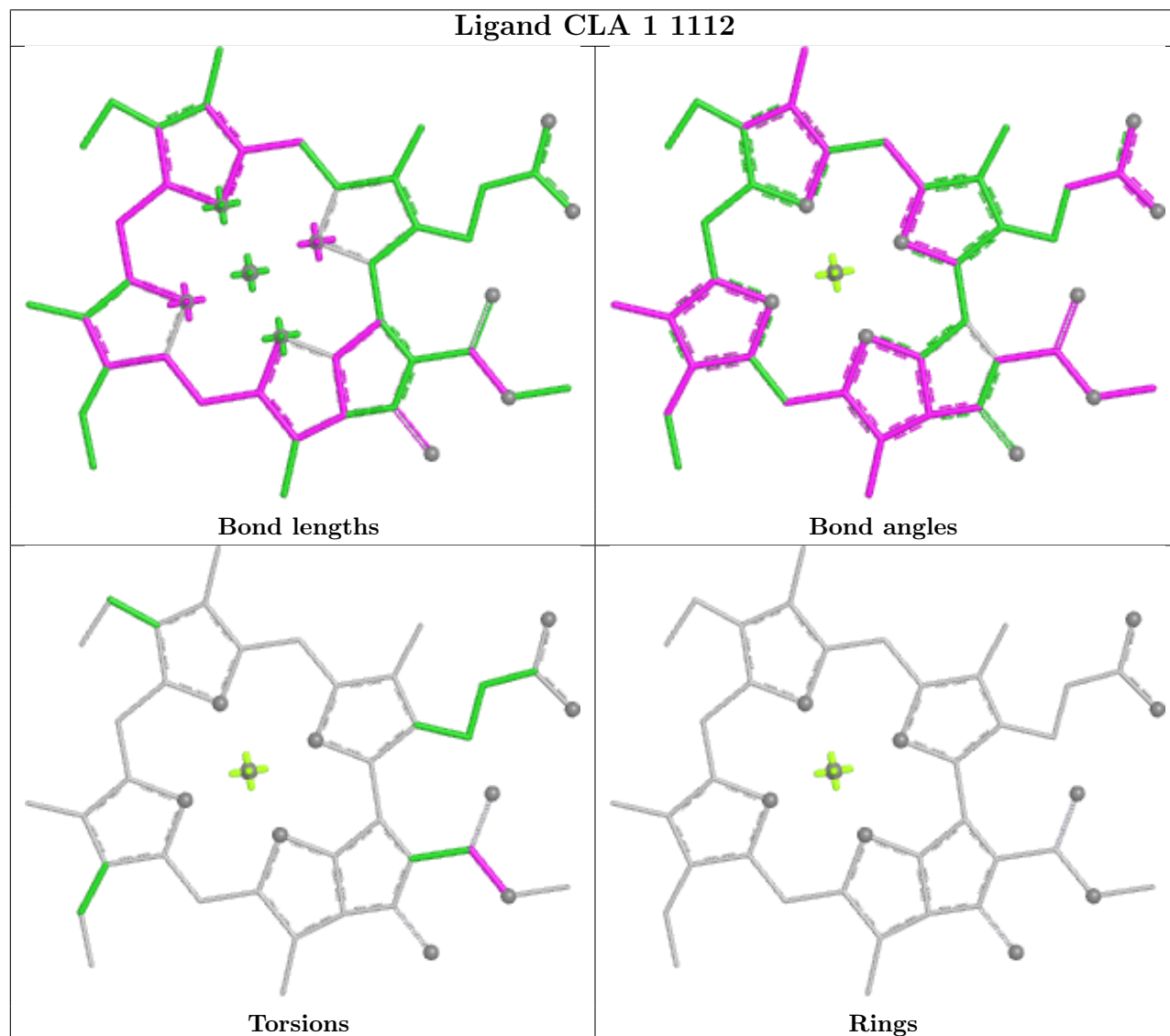
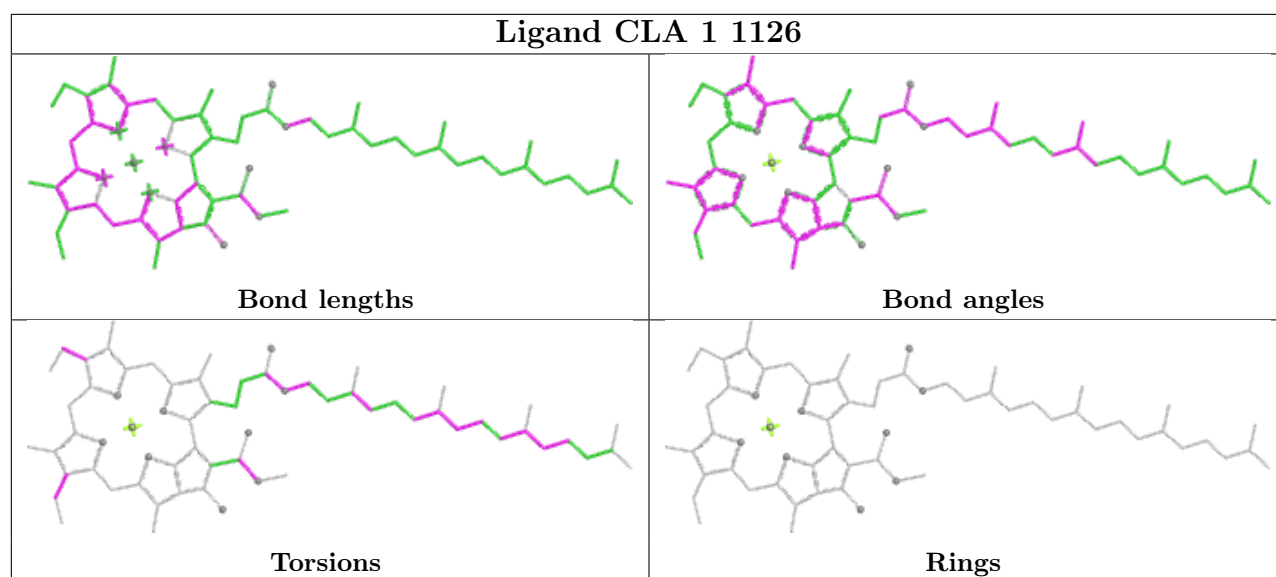


Rings

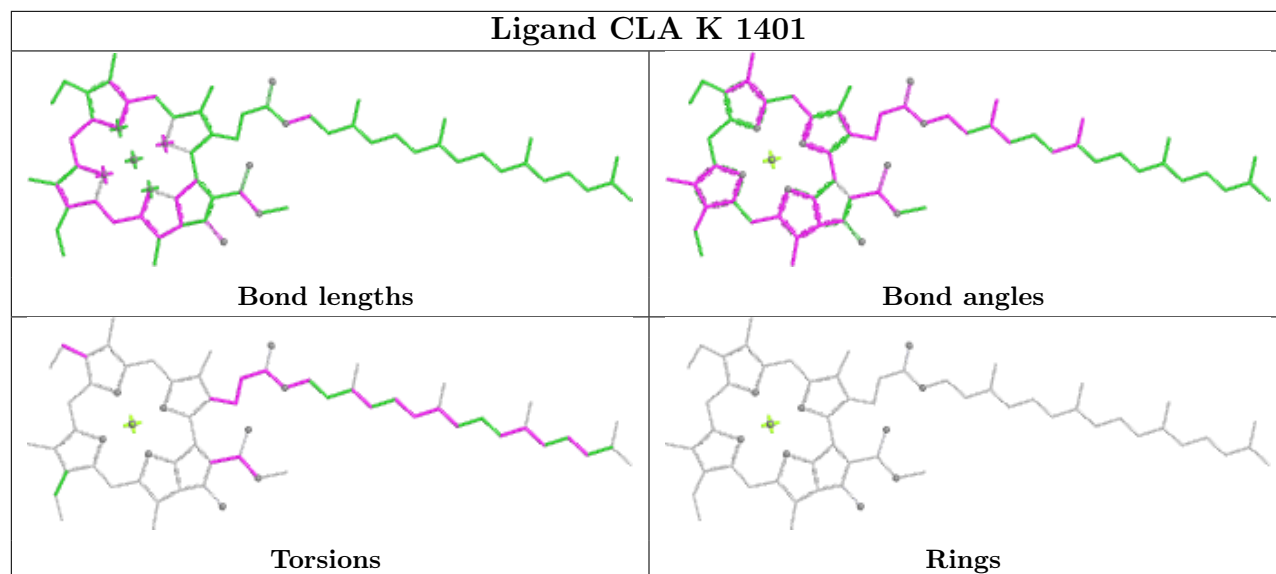


Ligand CLA B 1023**Ligand CLA a 1126**

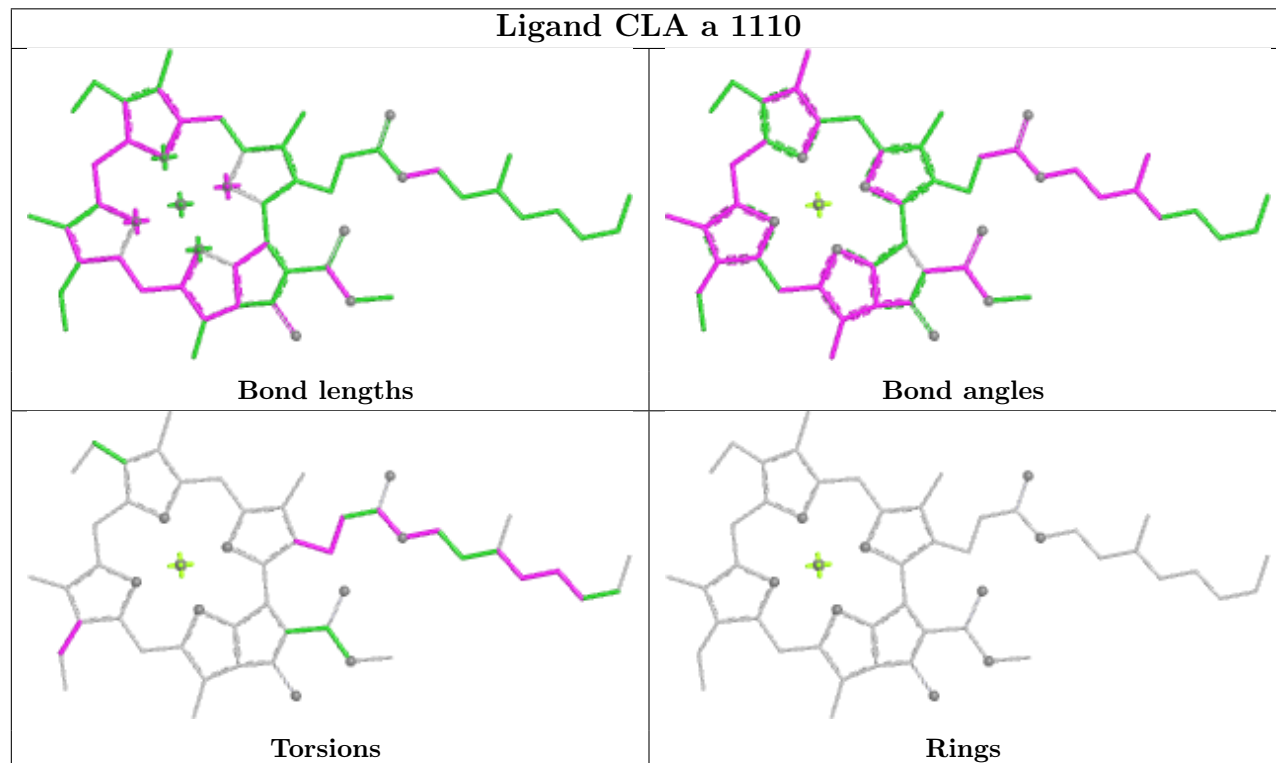


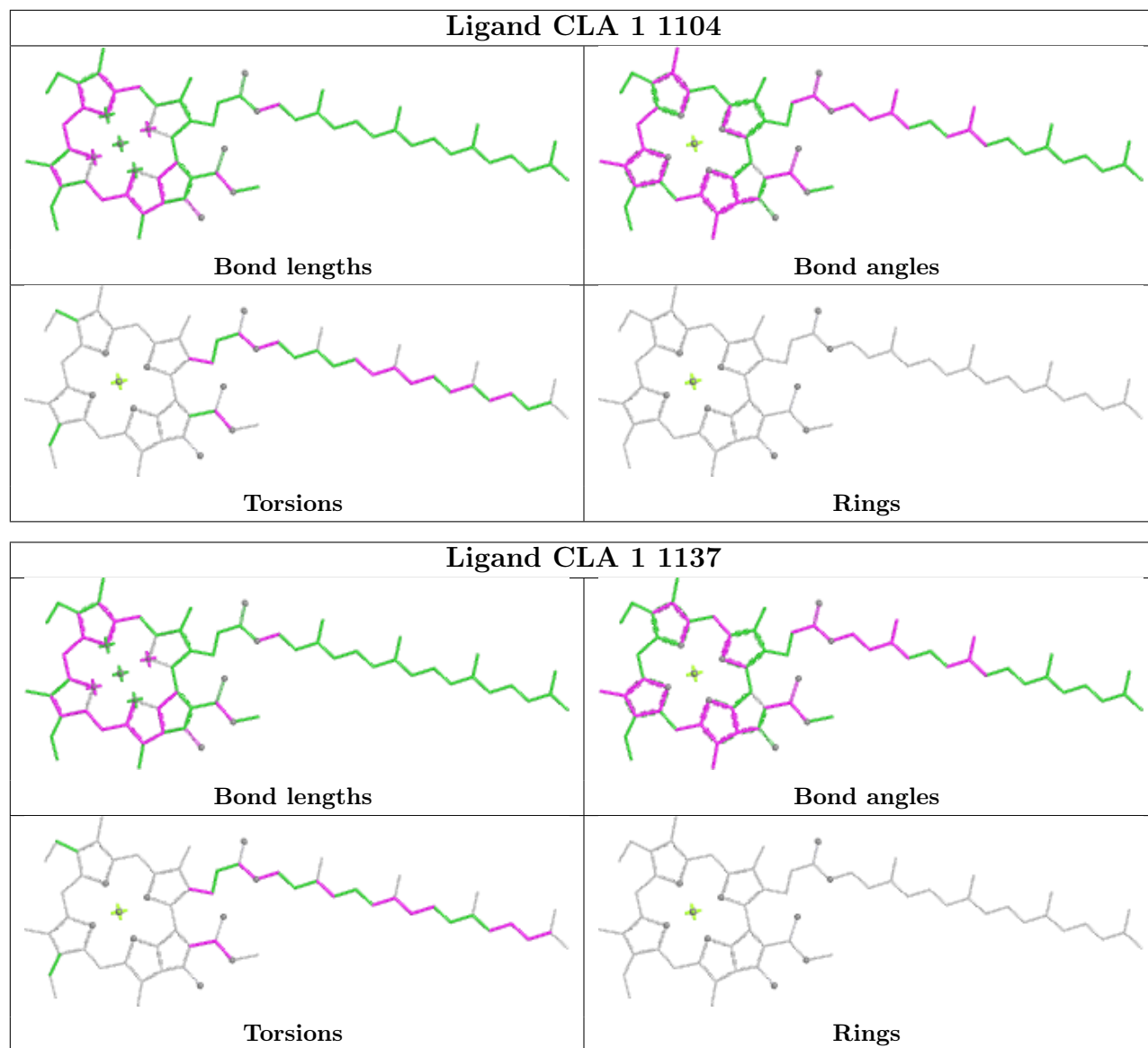


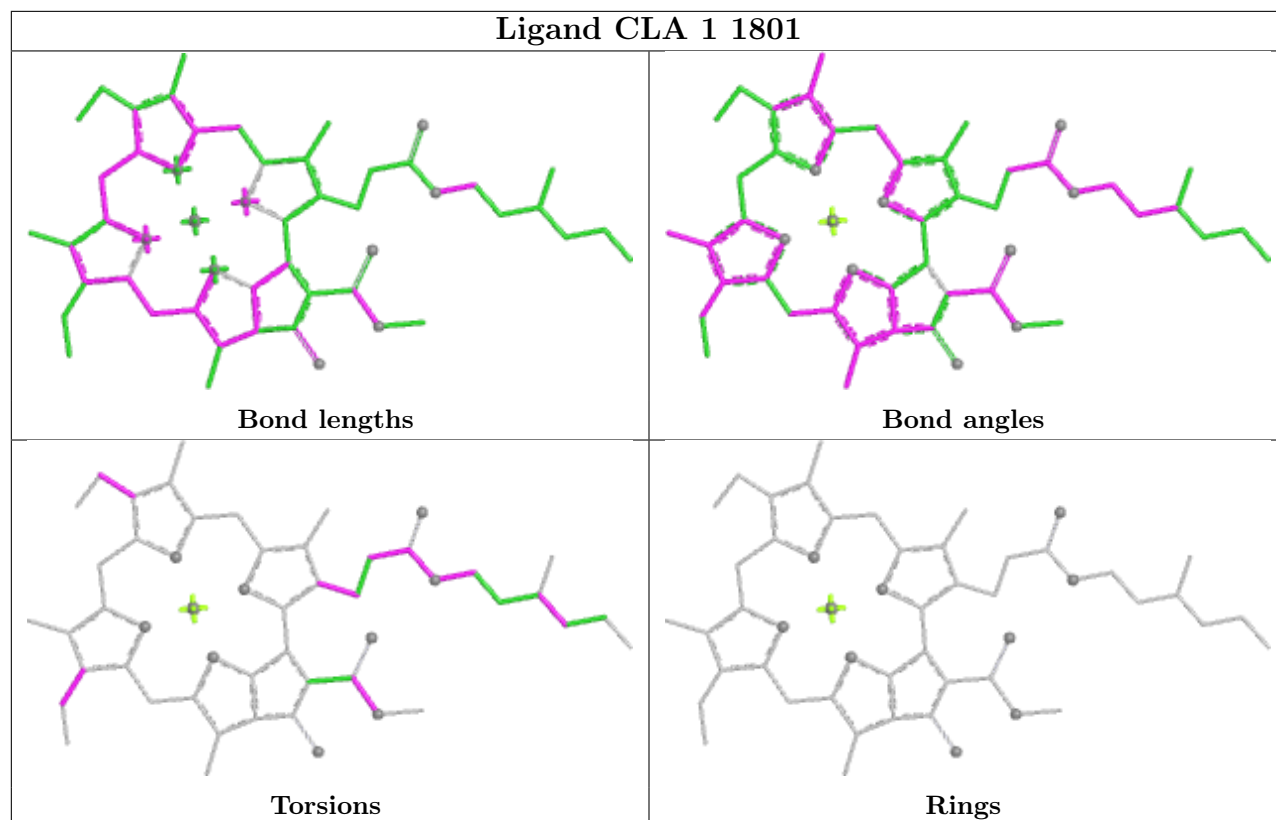
Ligand CLA K 1401

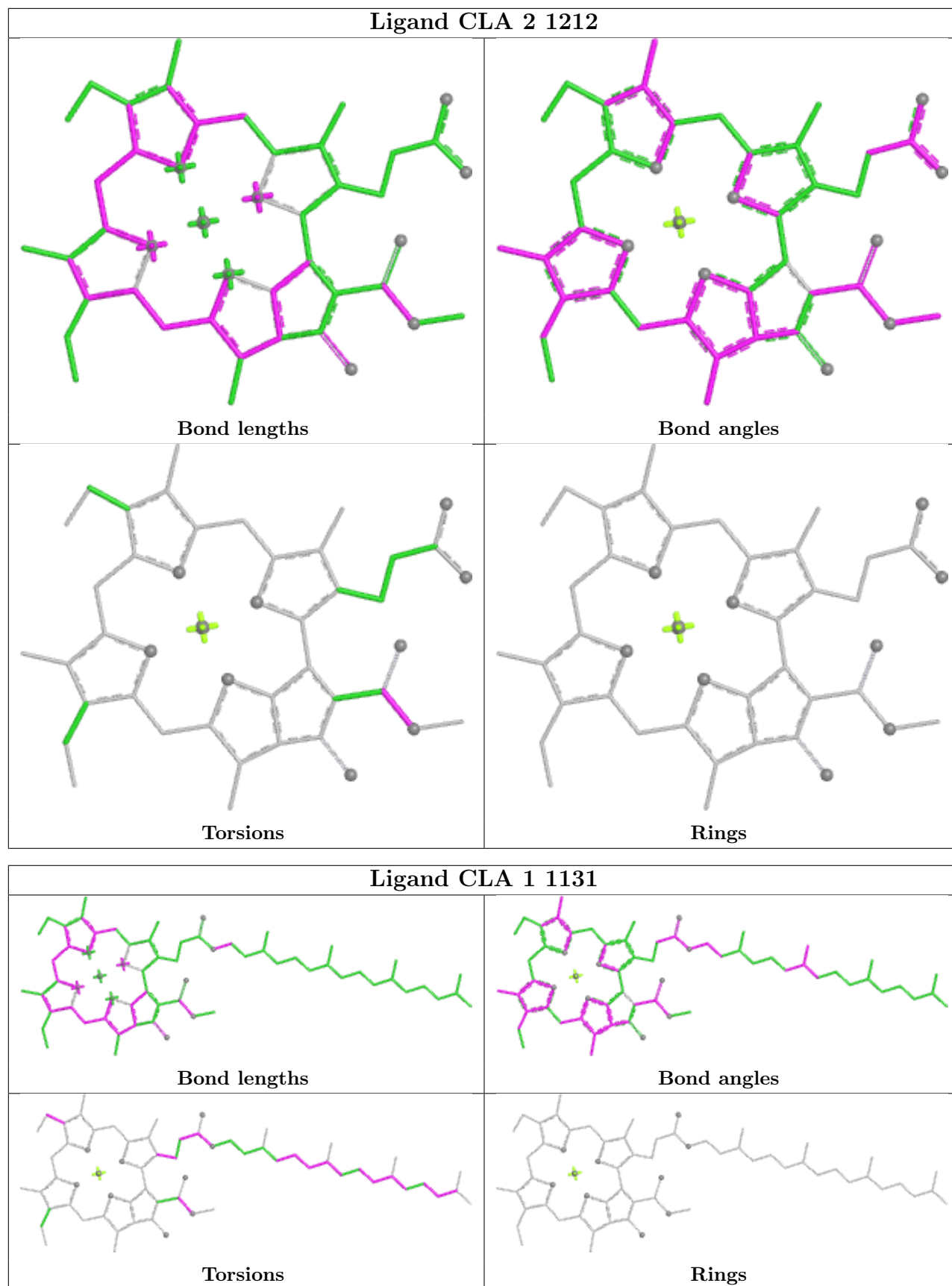


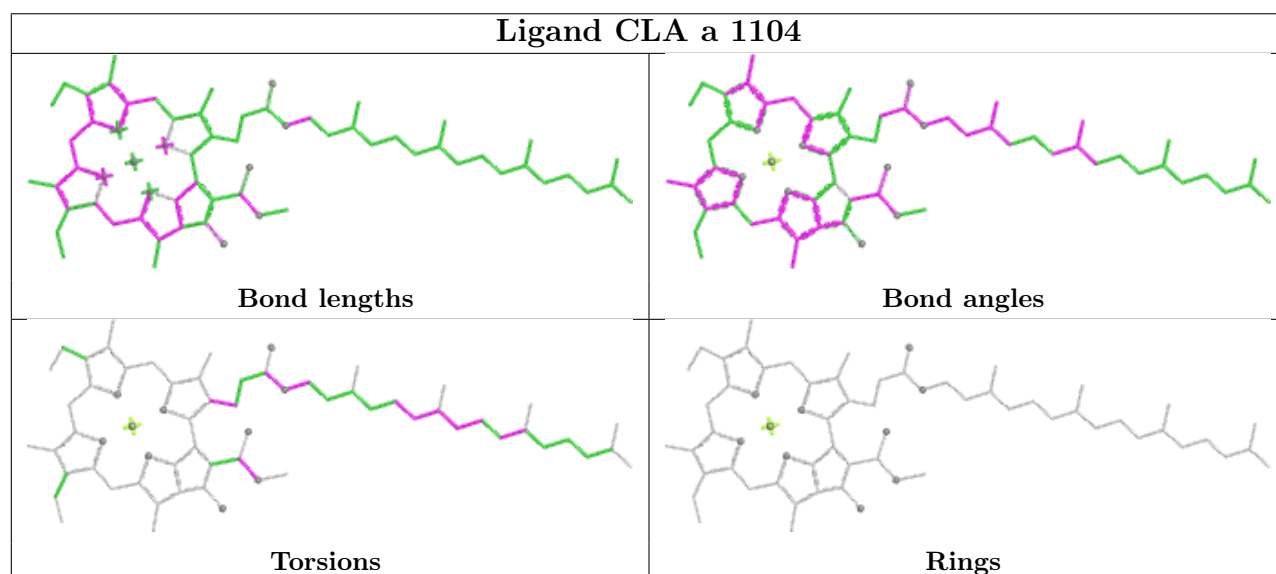
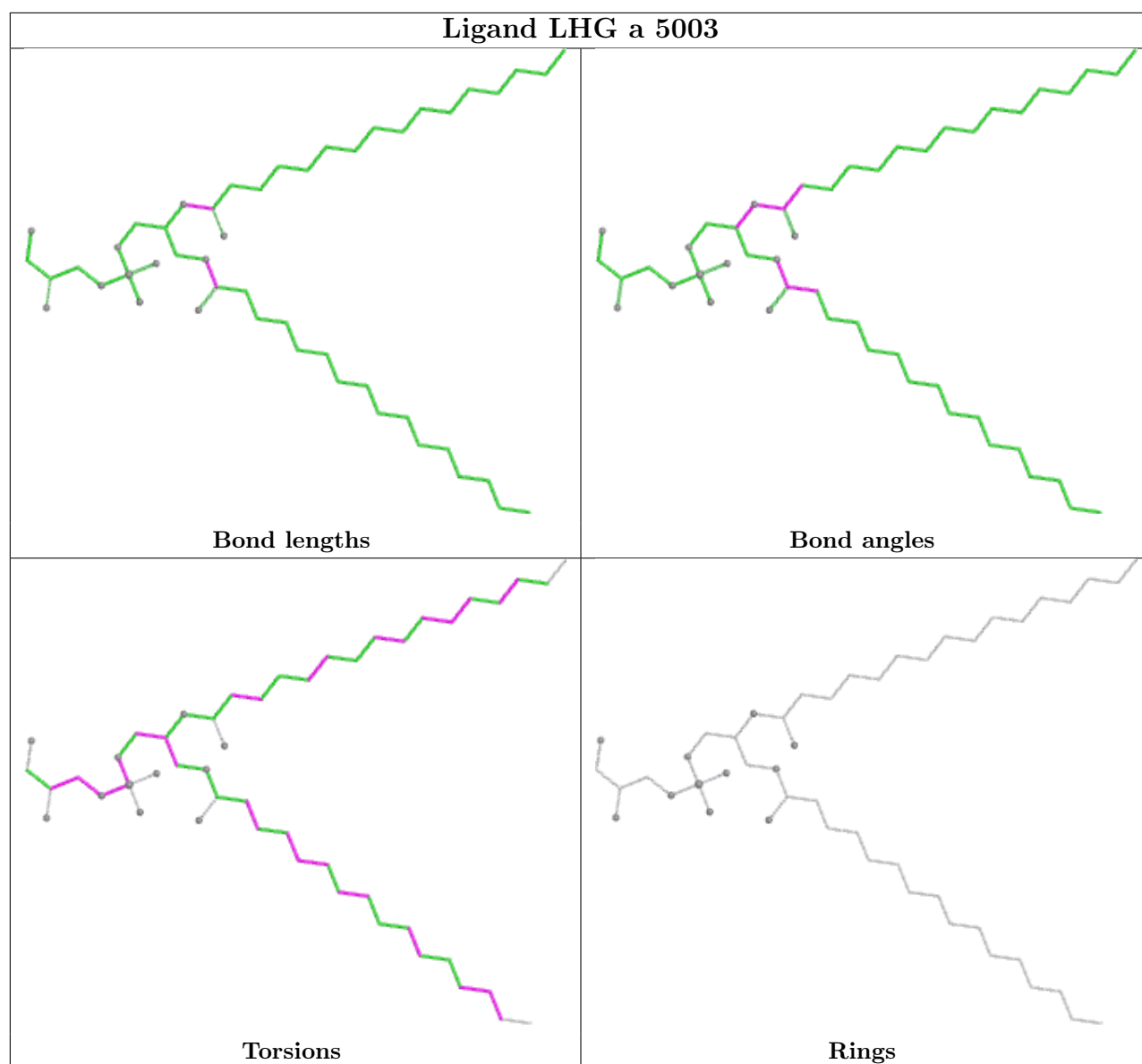
Ligand CLA a 1110



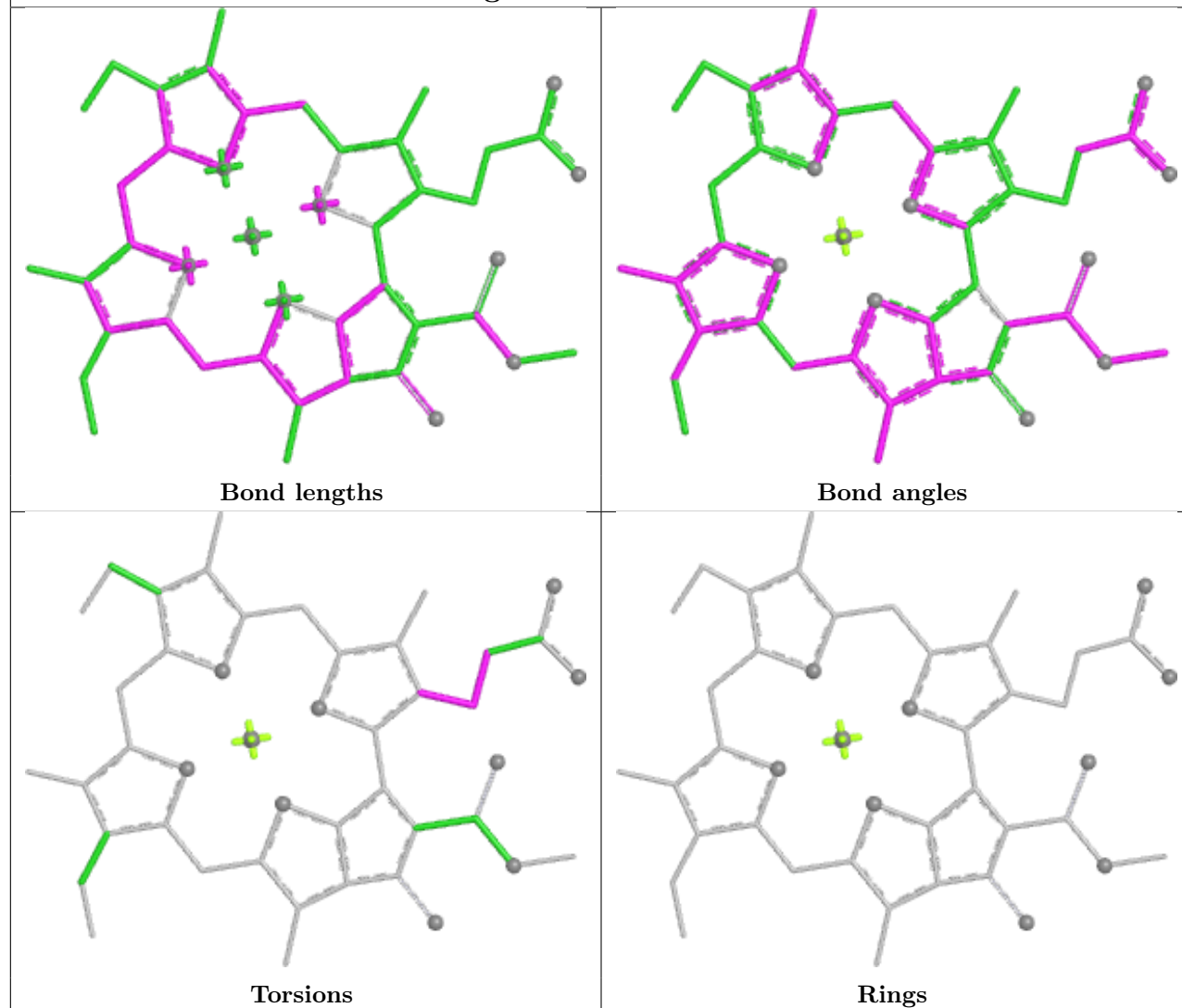




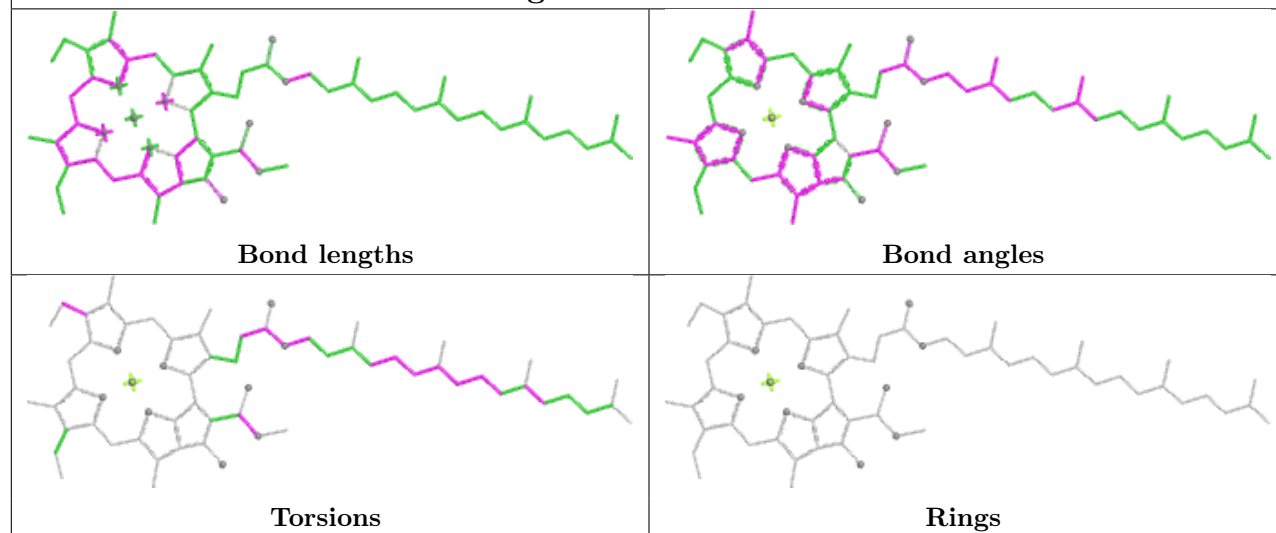


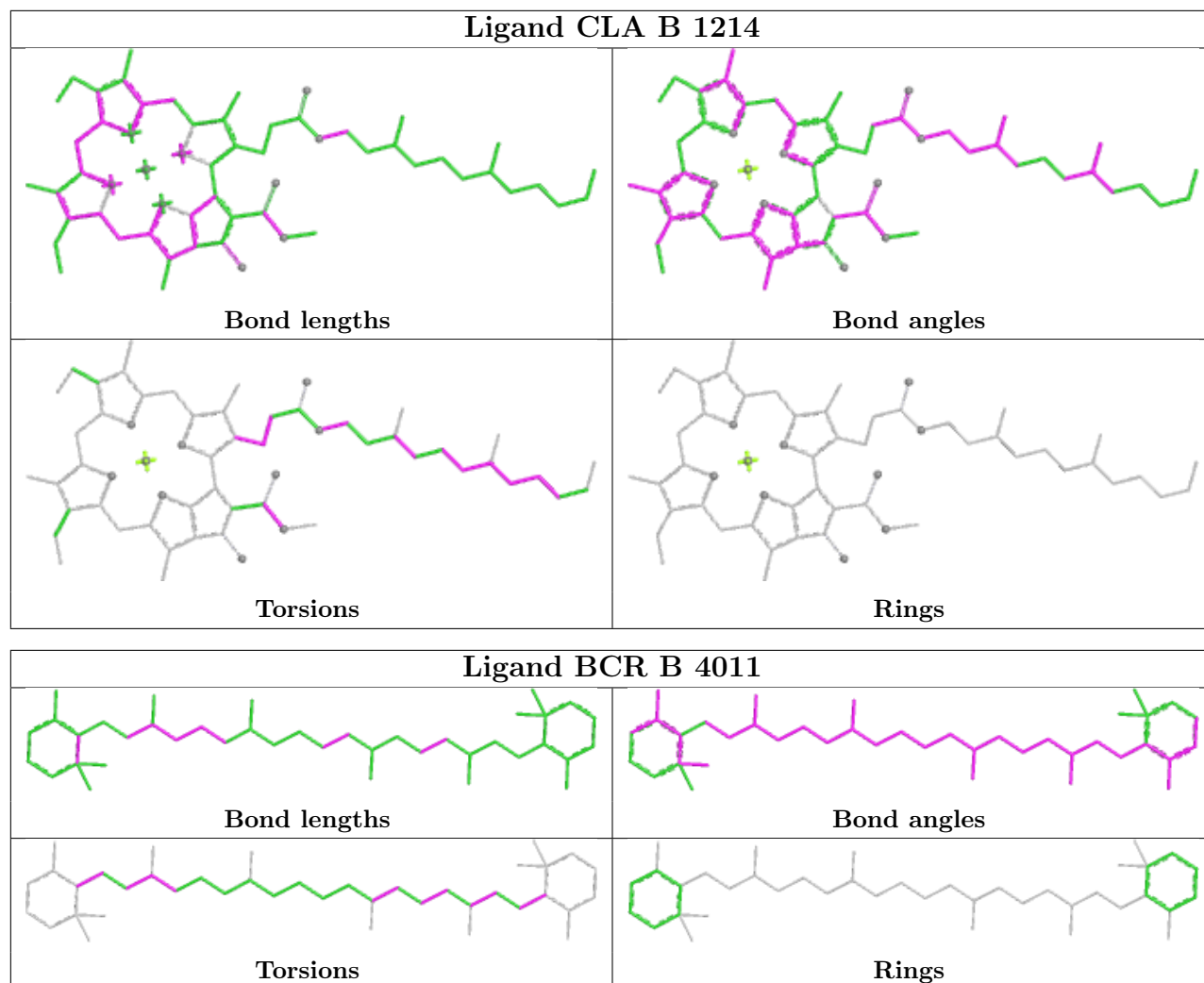


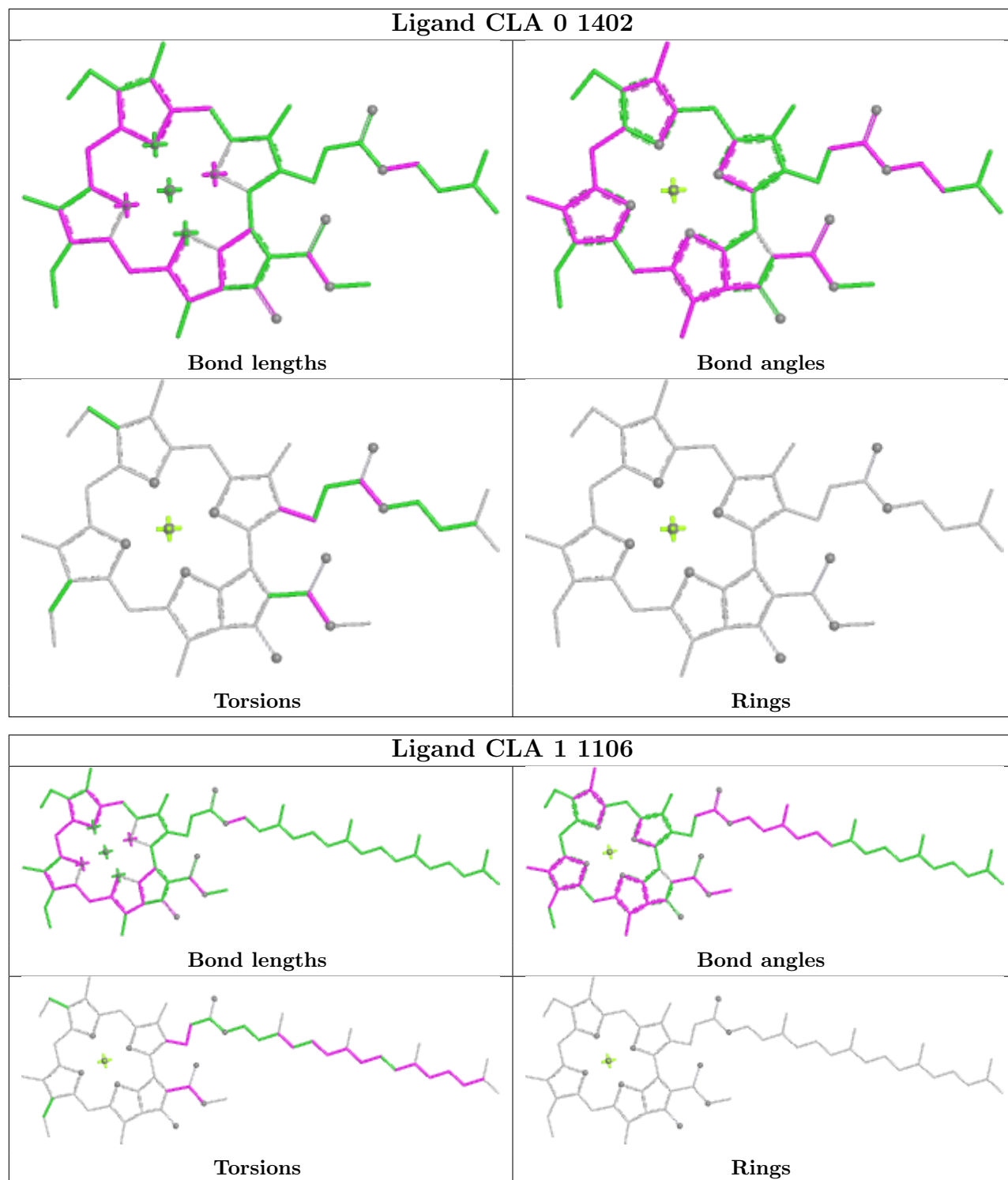
Ligand CLA A 1108

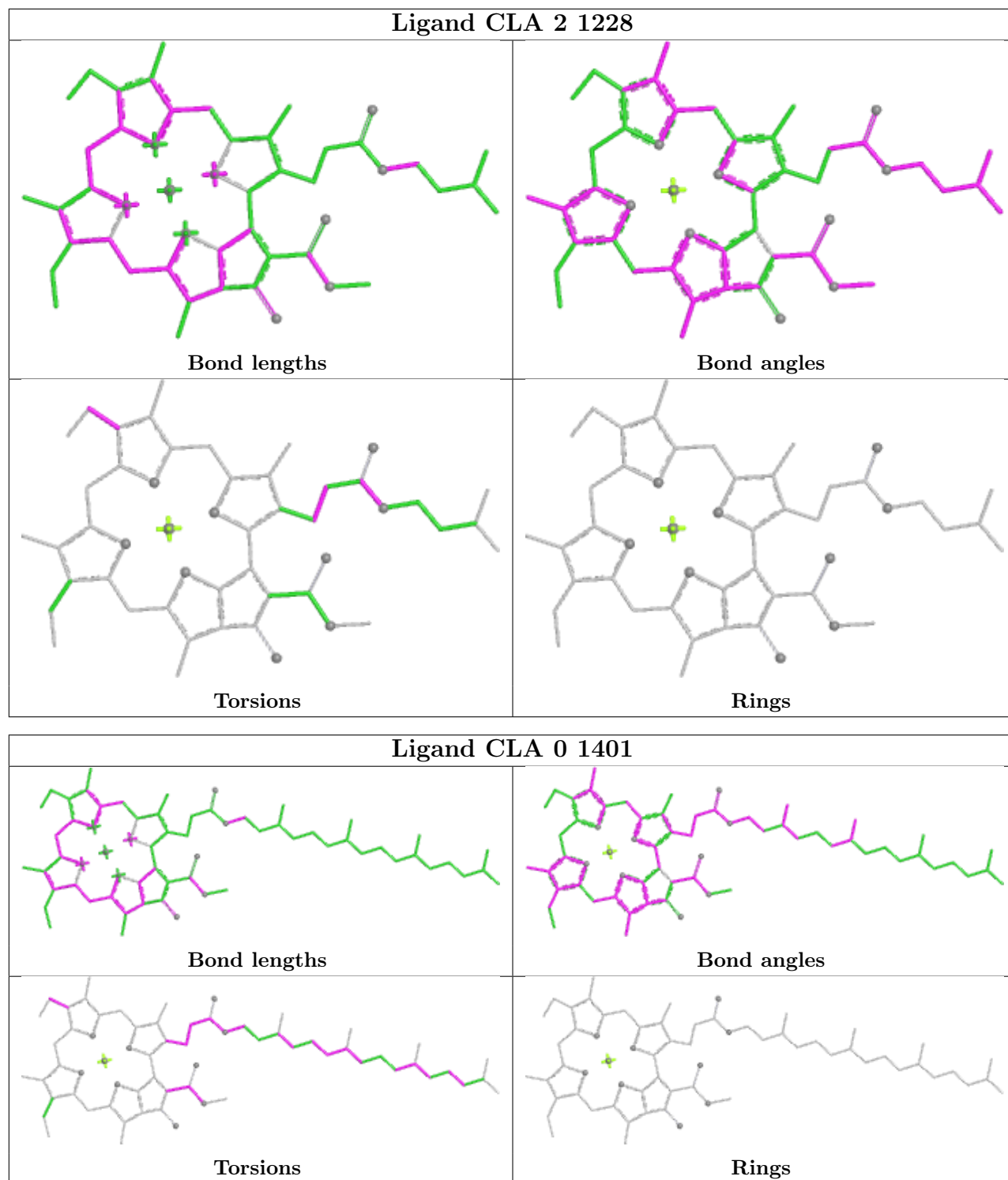


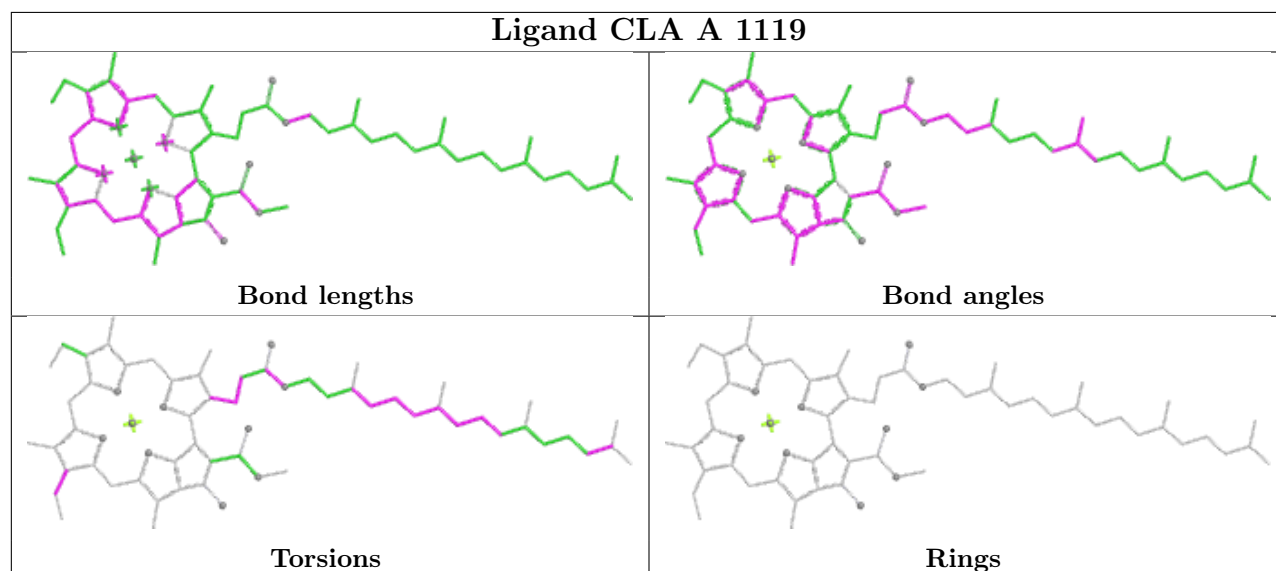
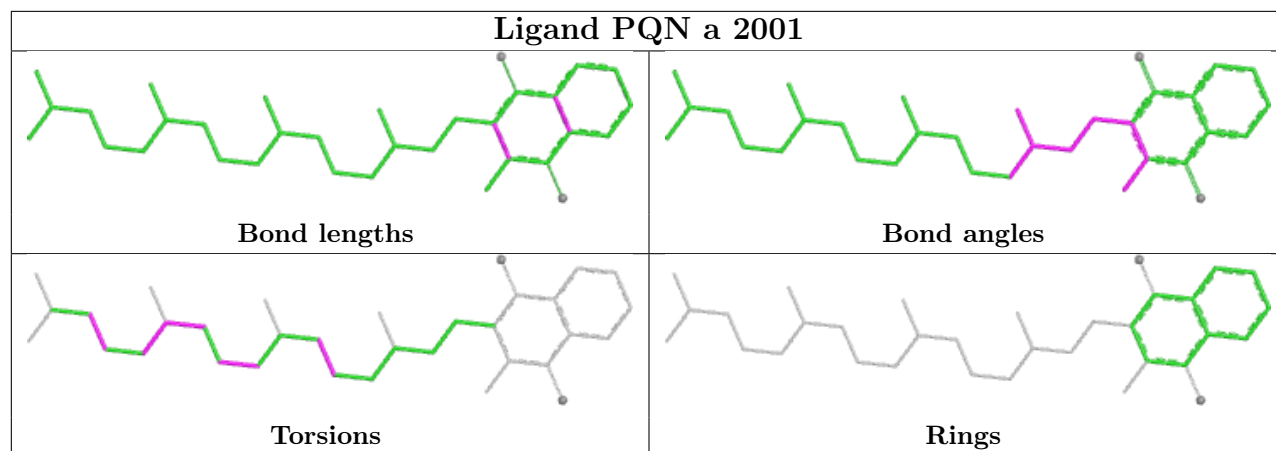
Ligand CLA 1 1140

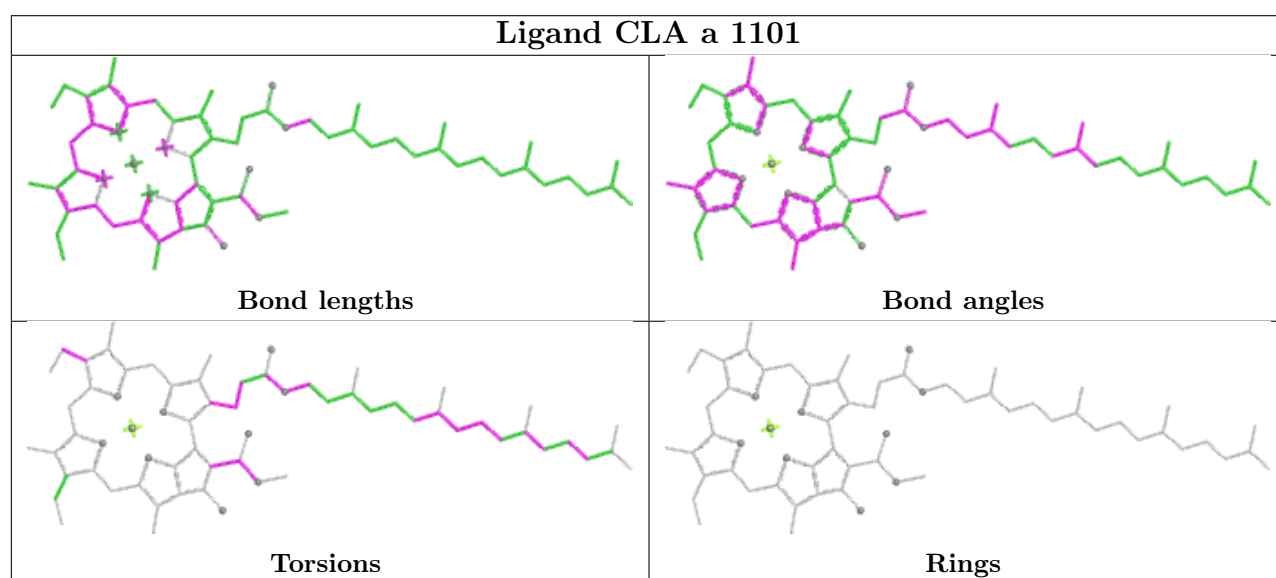
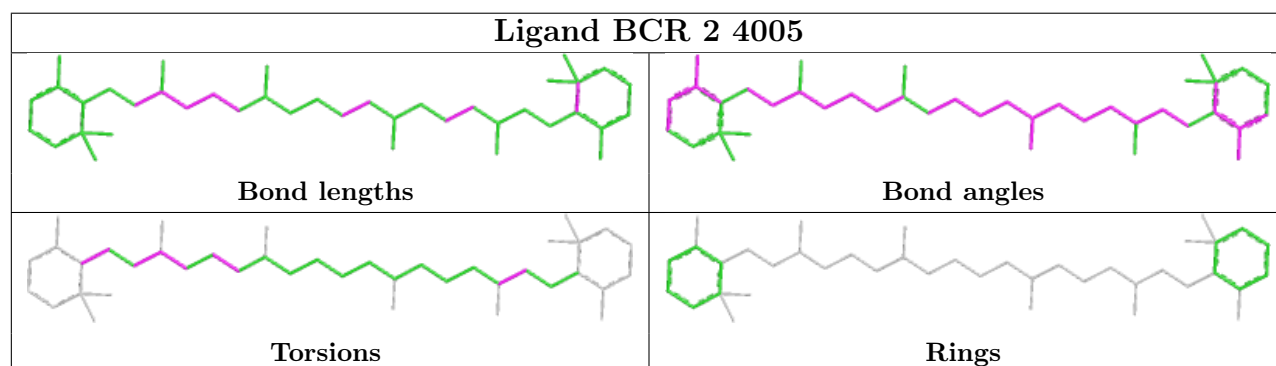
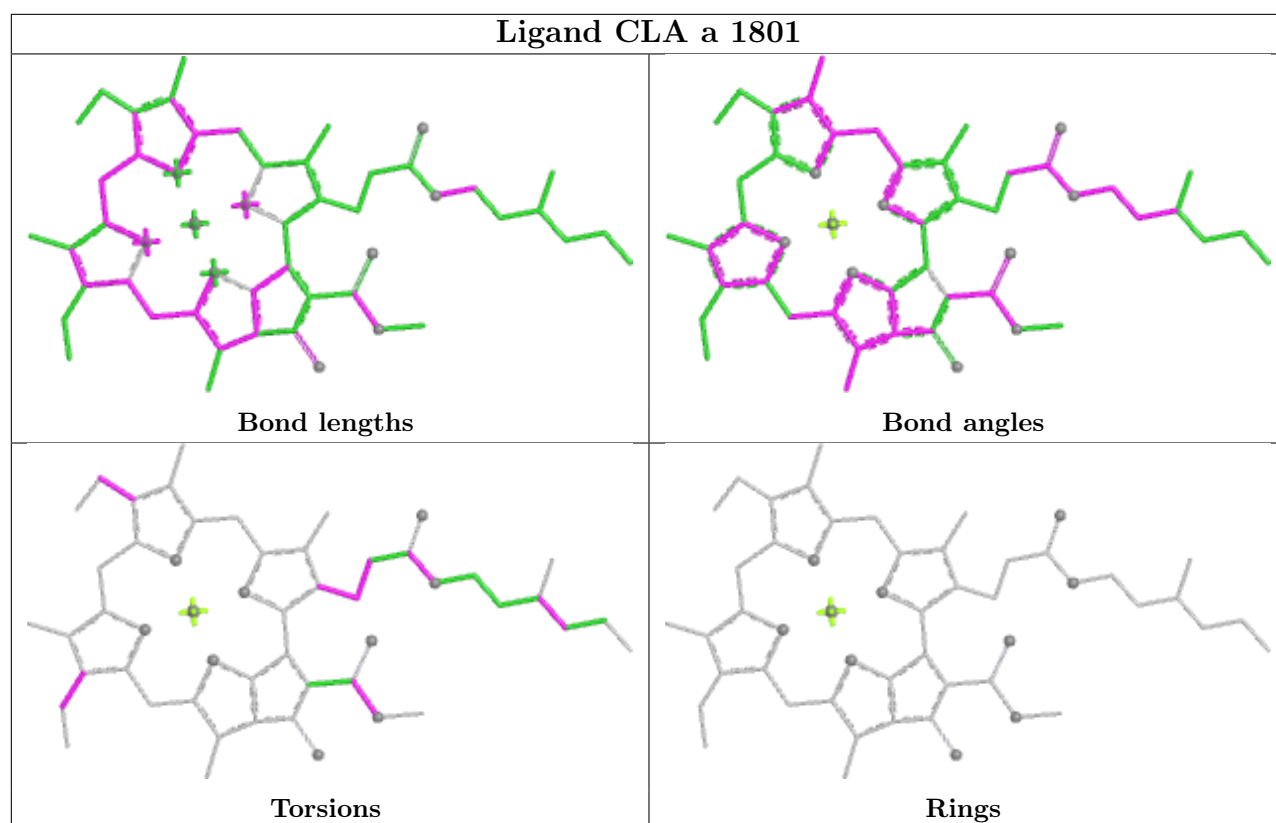




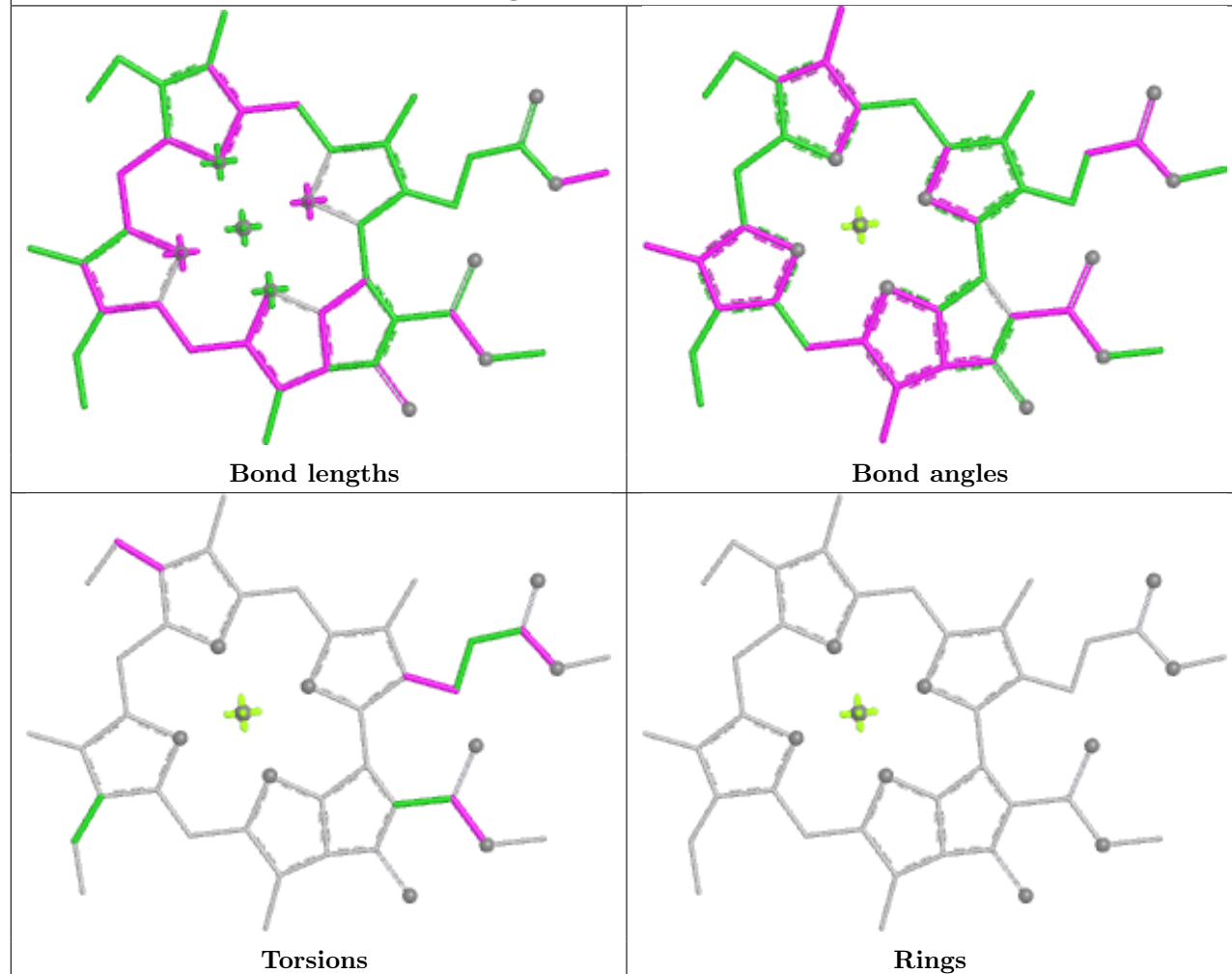


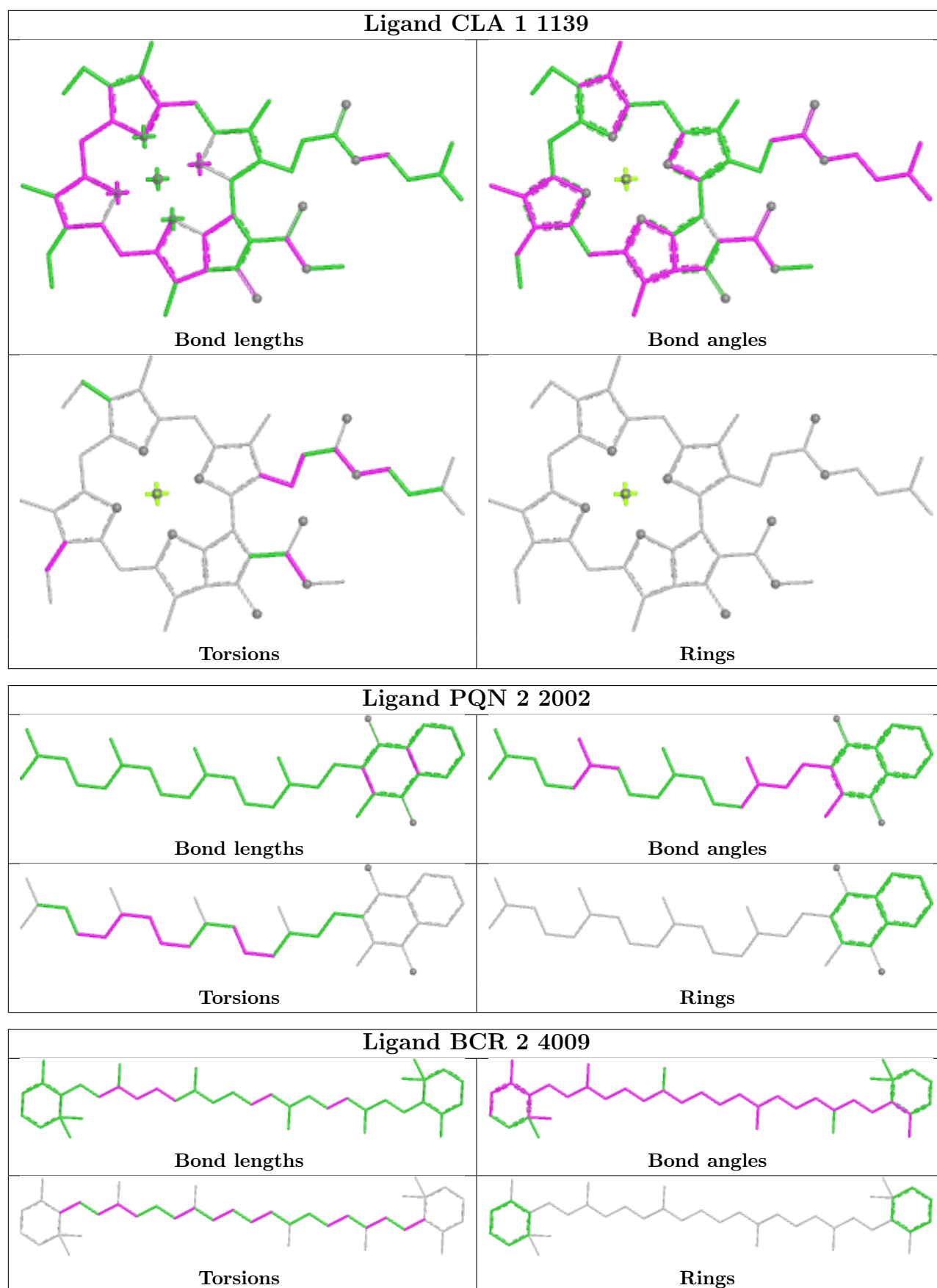


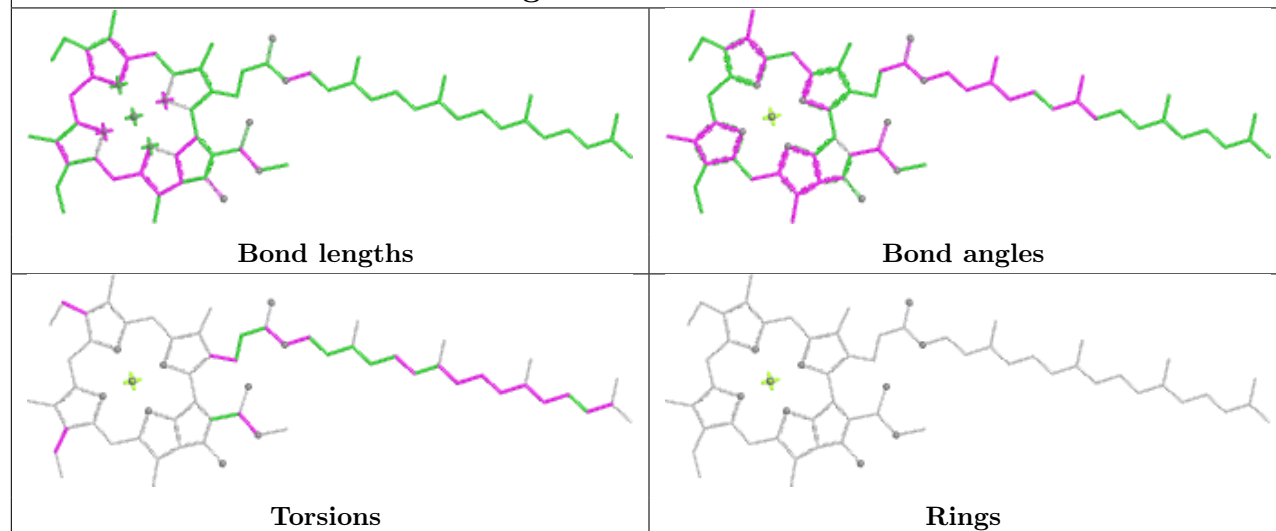
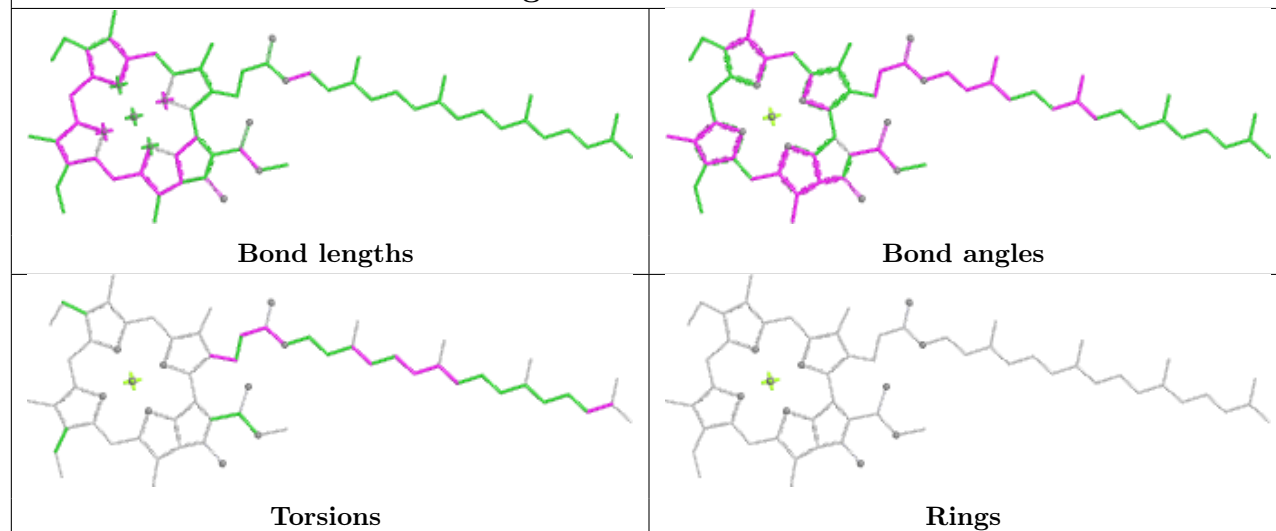


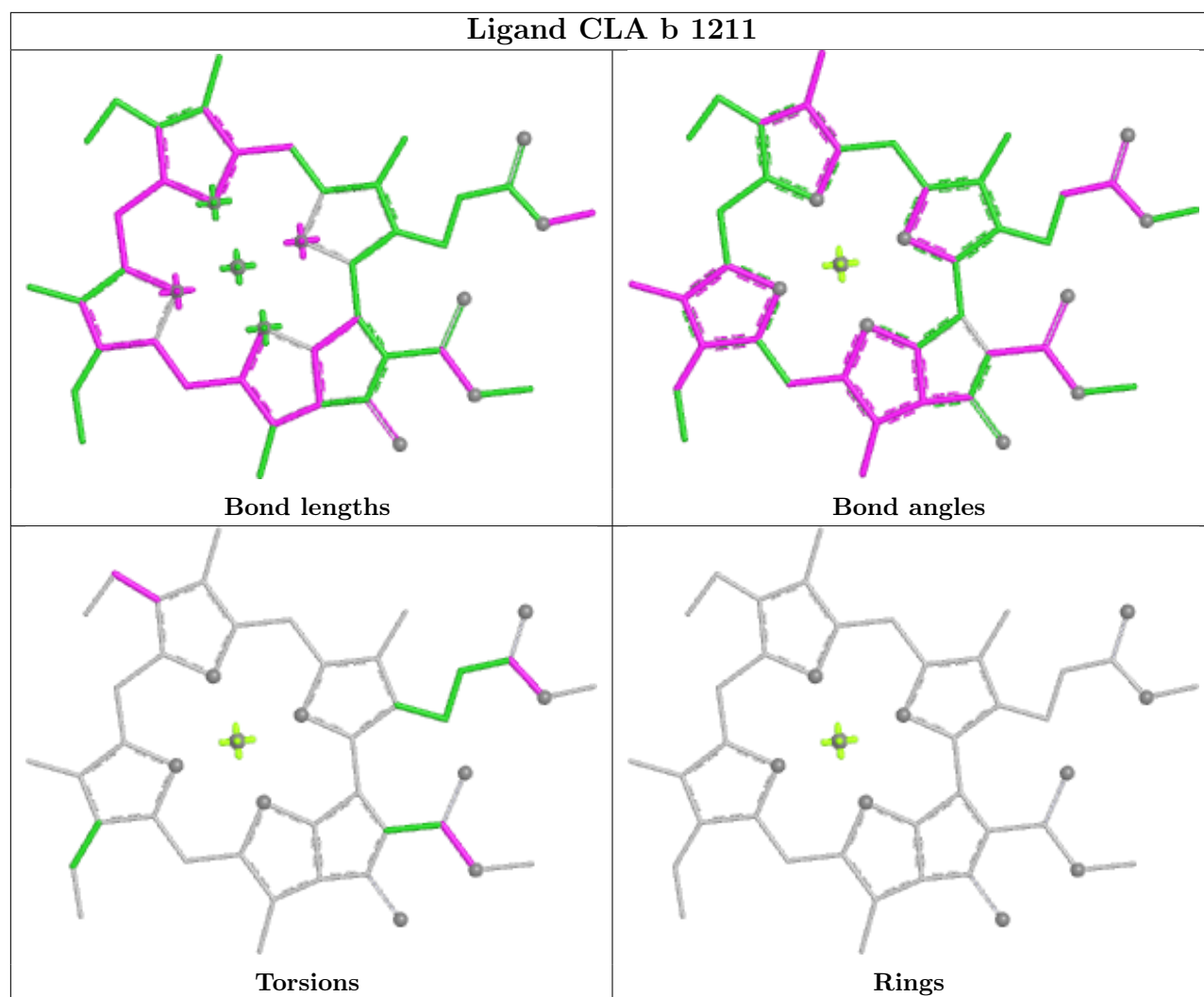
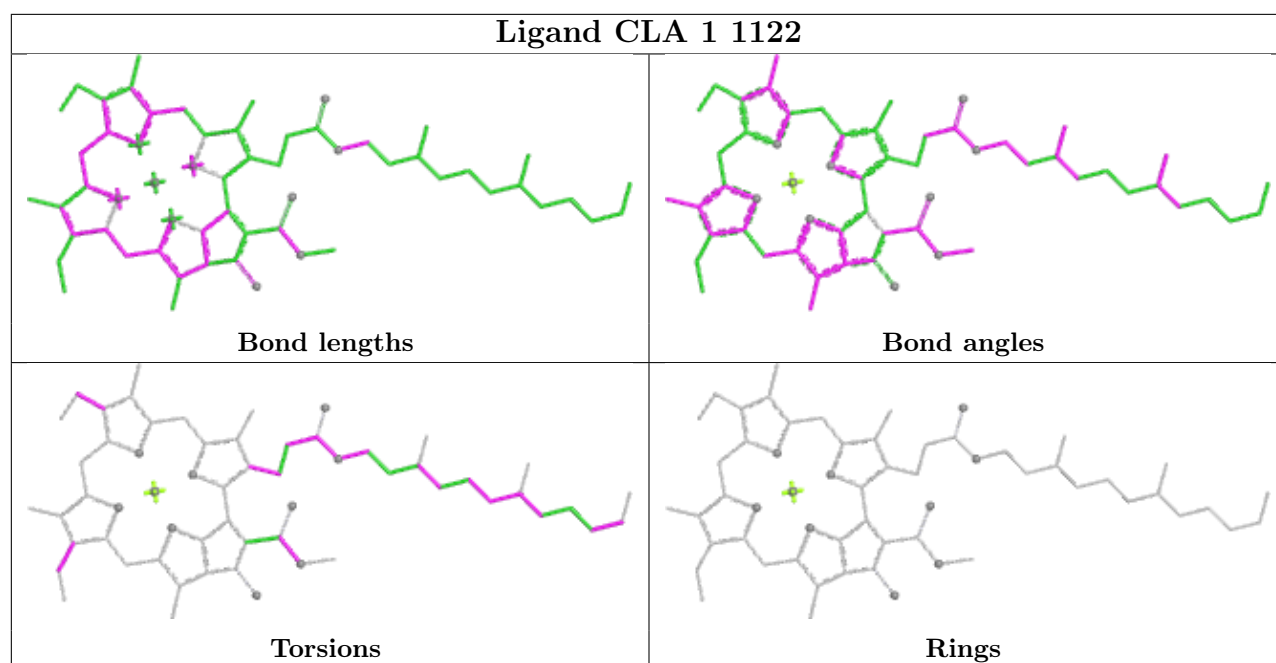


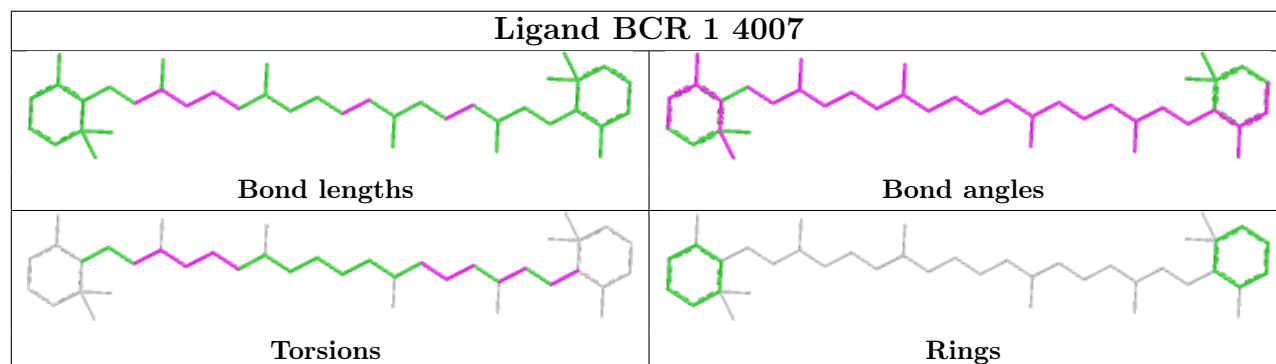
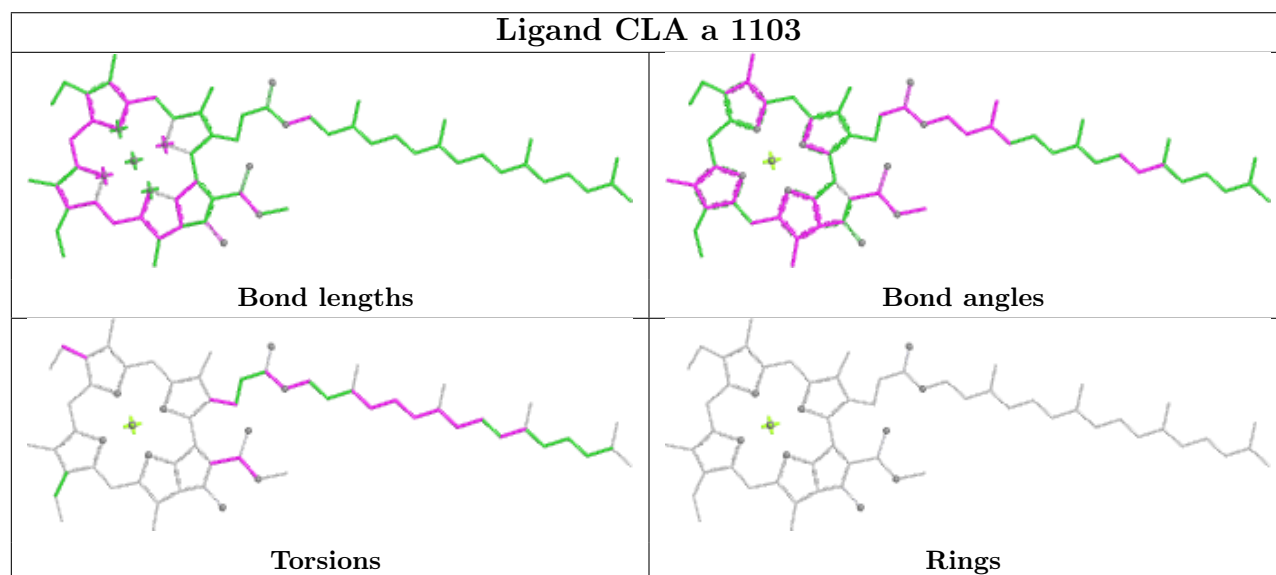
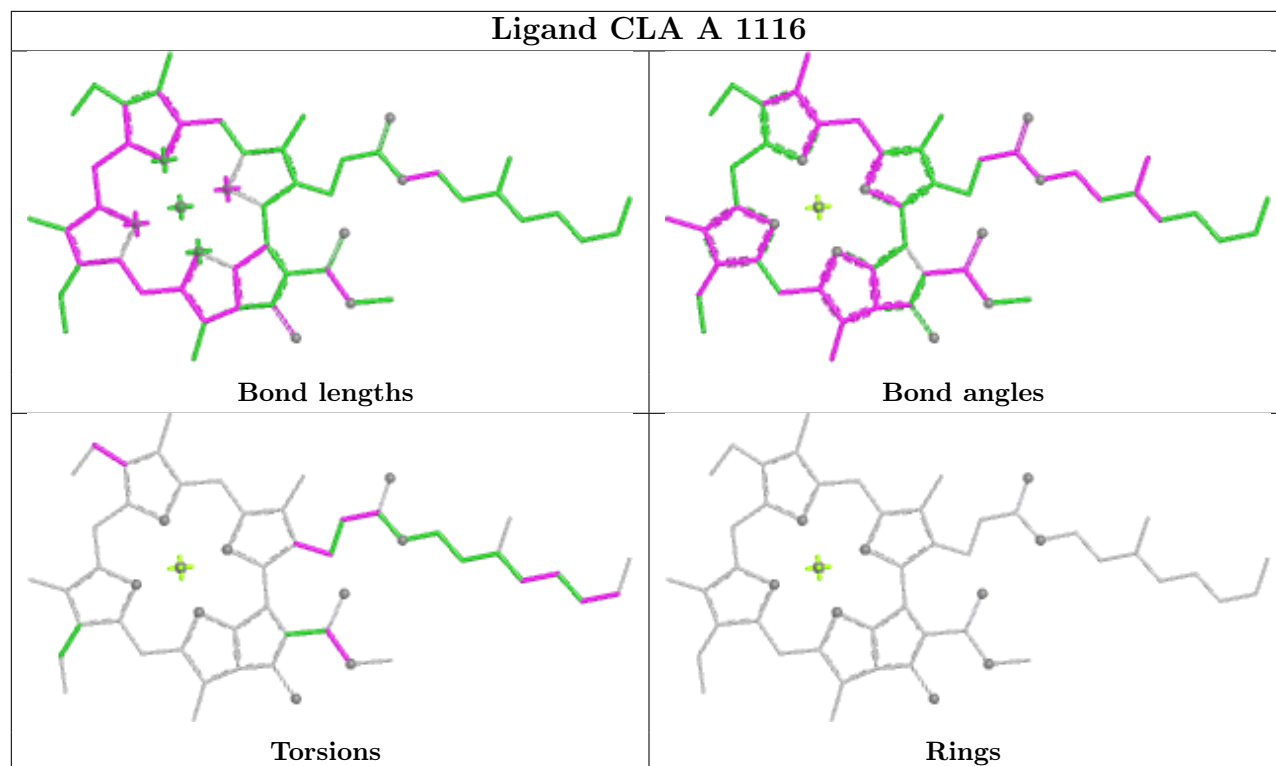
Ligand CLA B 1211



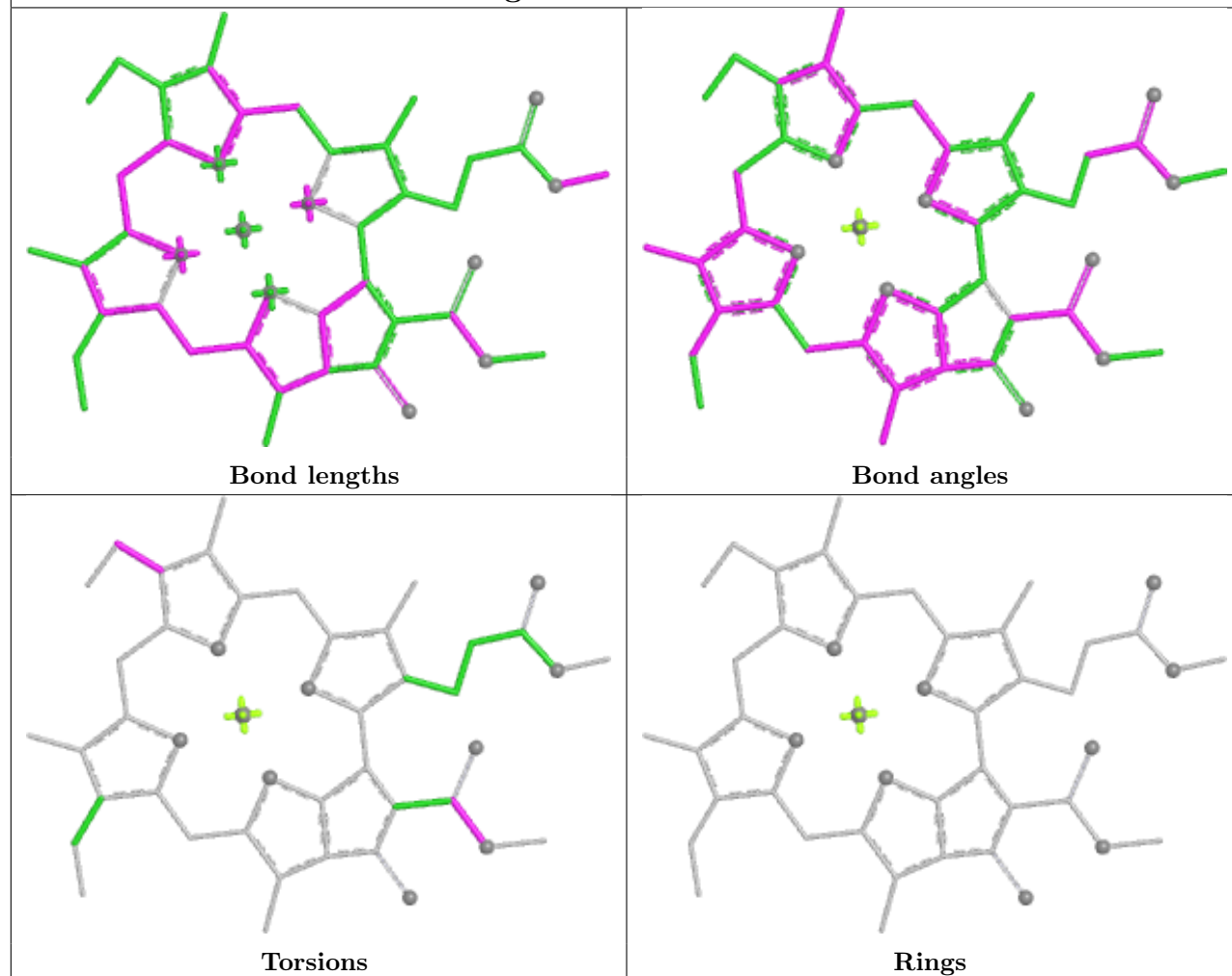


Ligand CLA A 1104**Ligand CLA A 1137**

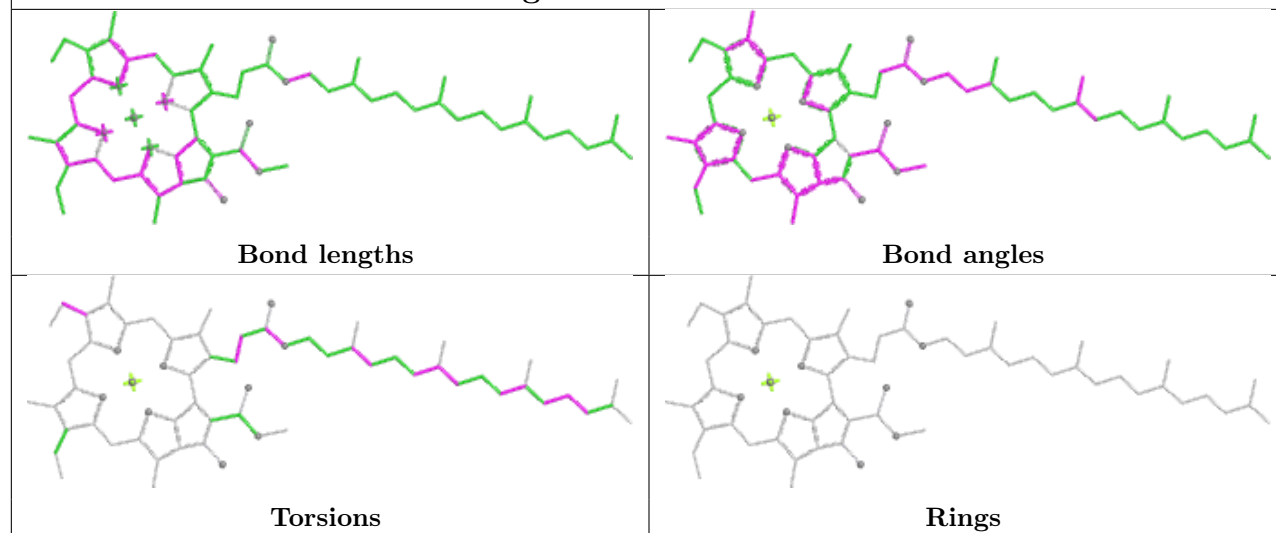


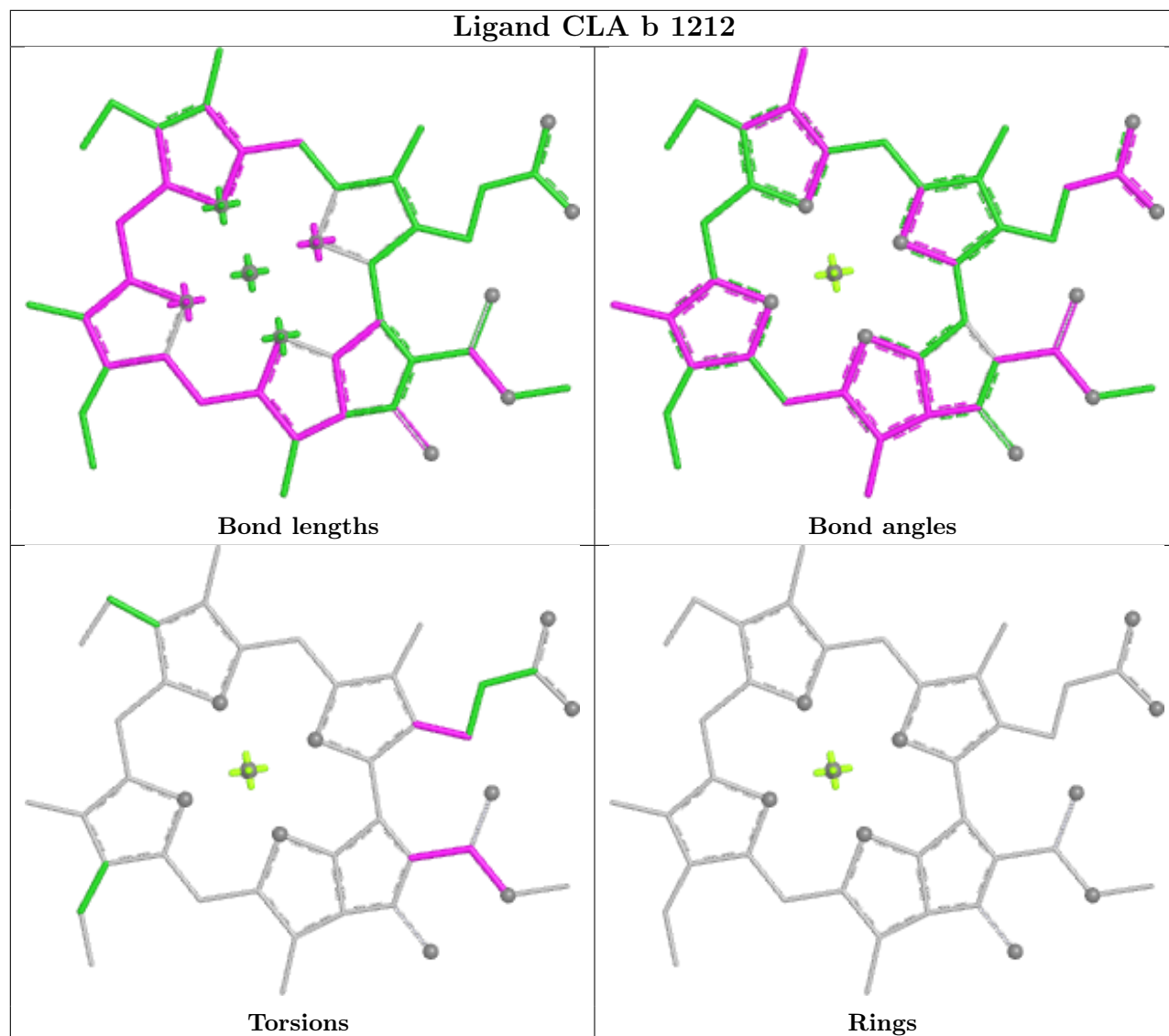


Ligand CLA A 1133

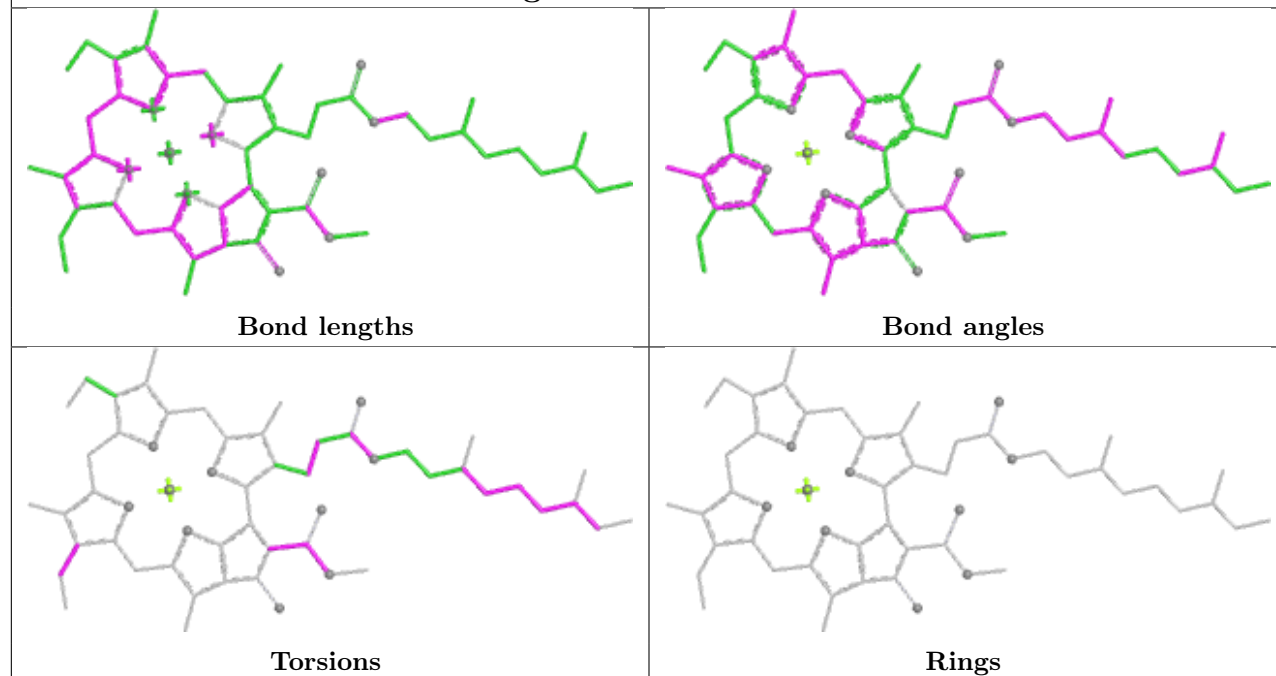


Ligand CLA A 1127

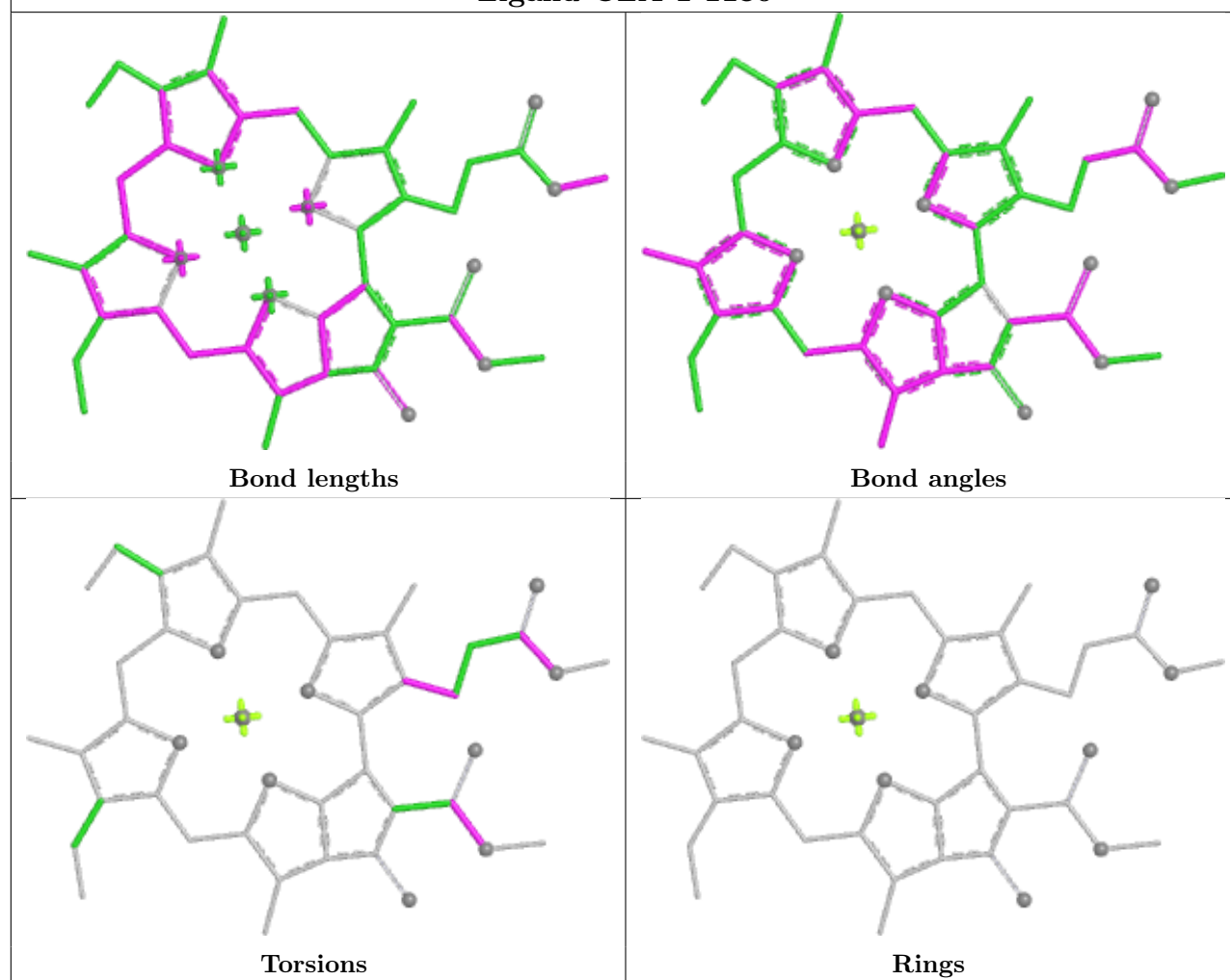


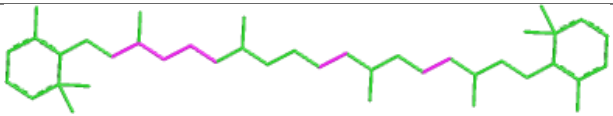
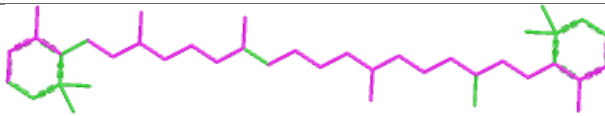
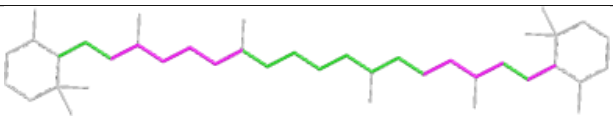
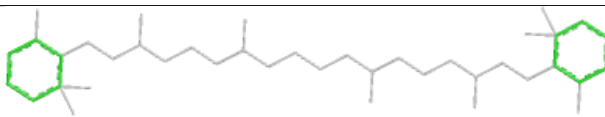


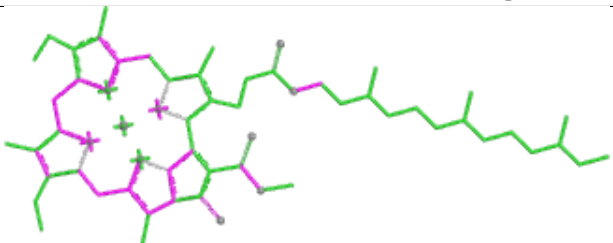
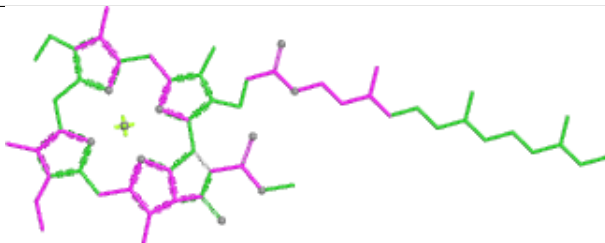
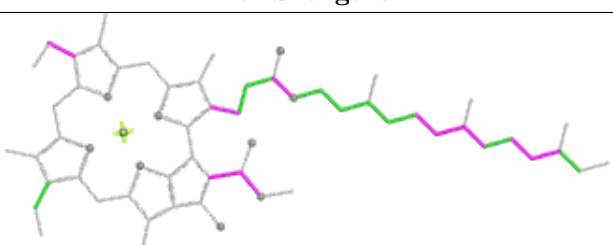
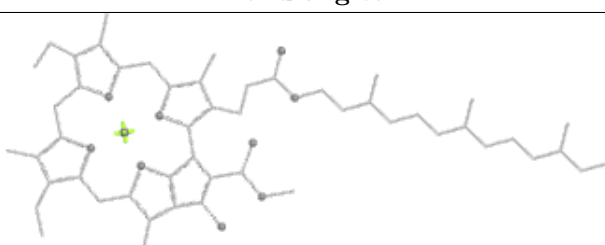
Ligand CLA B 1222

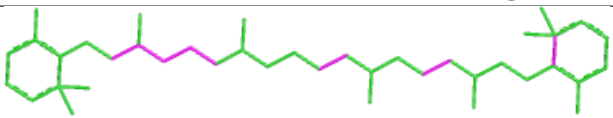
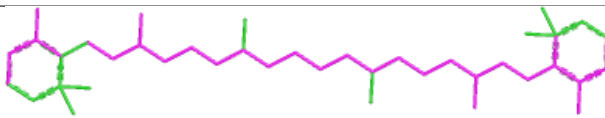
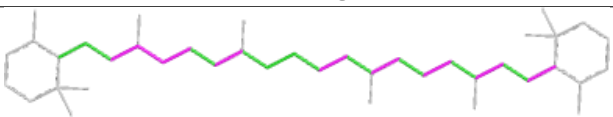
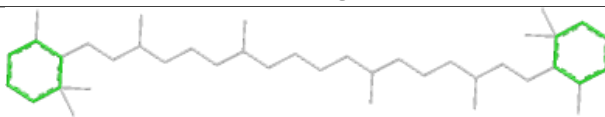


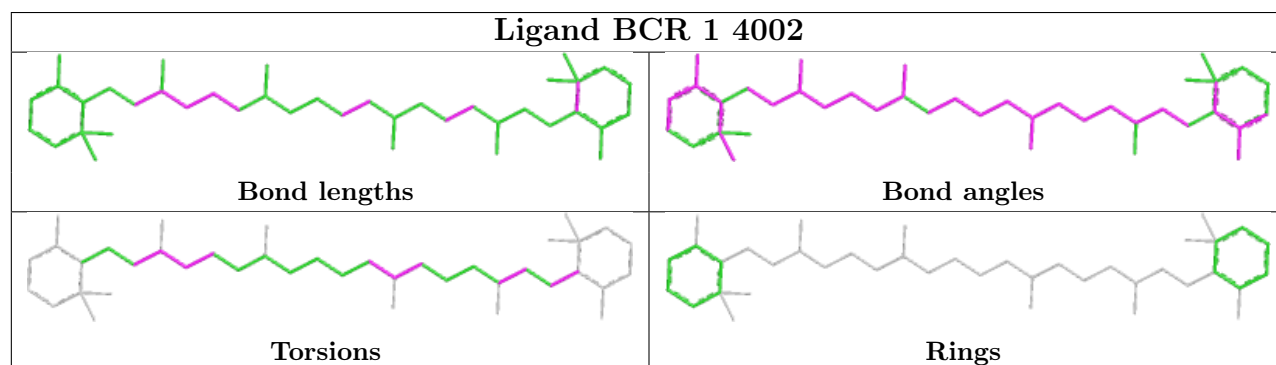
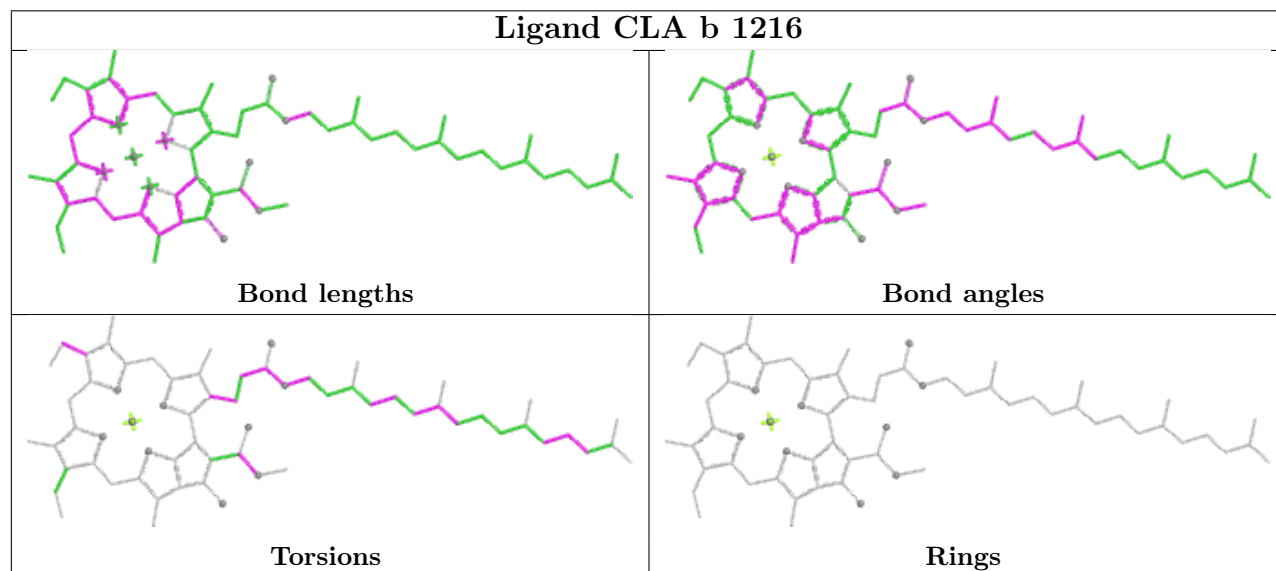
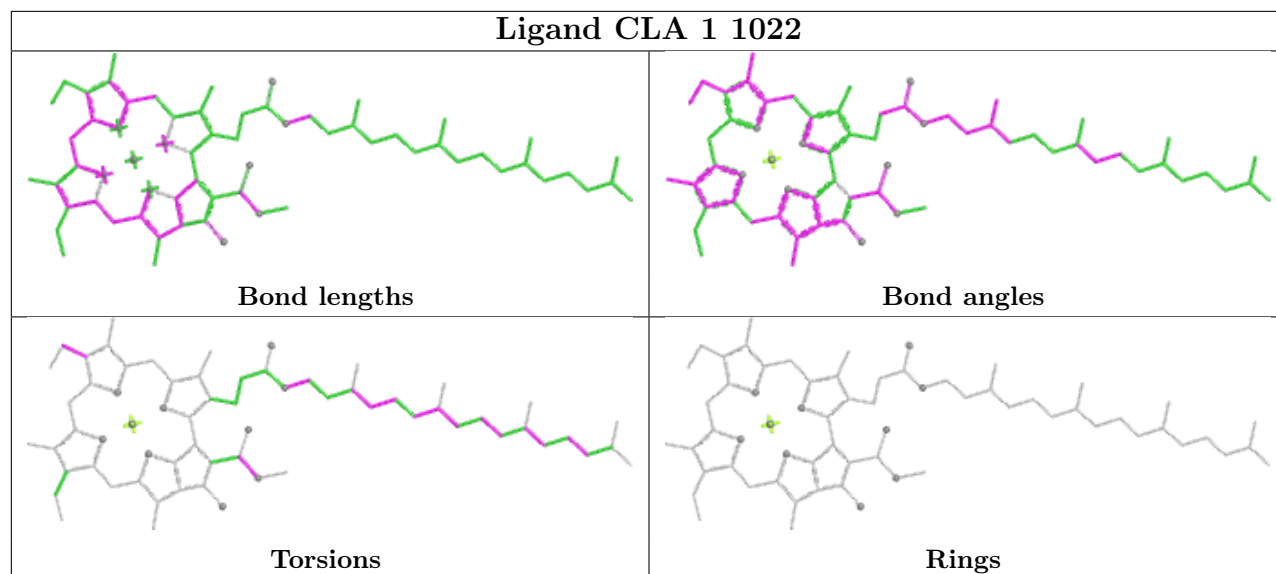
Ligand CLA 1 1130

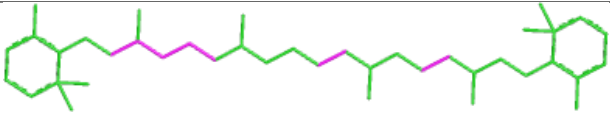
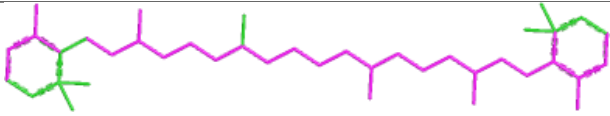
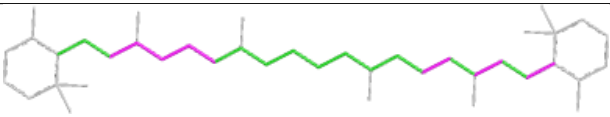
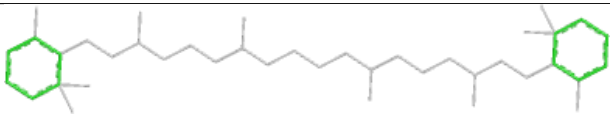
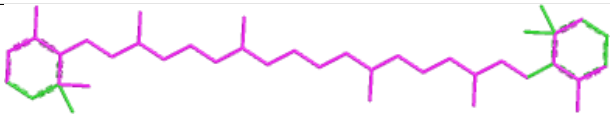
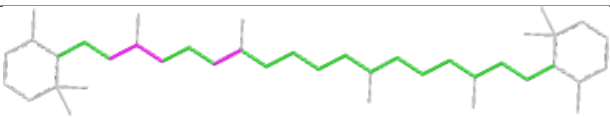
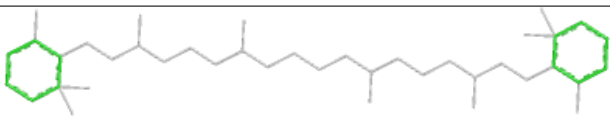
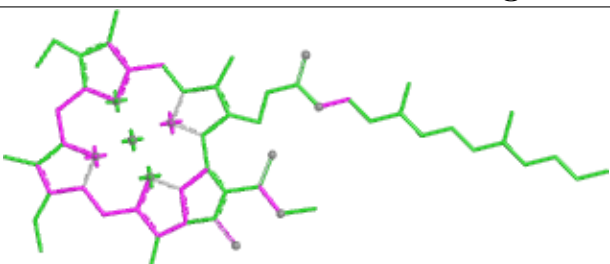
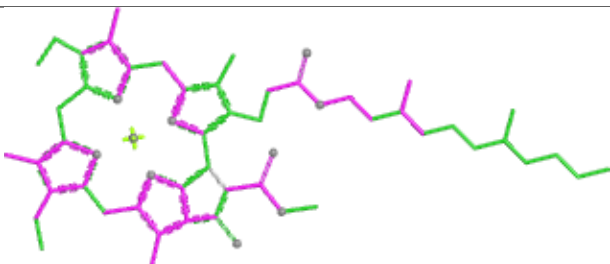
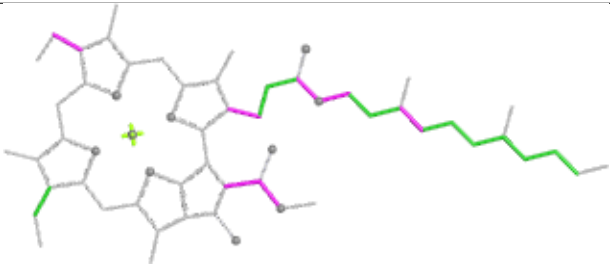
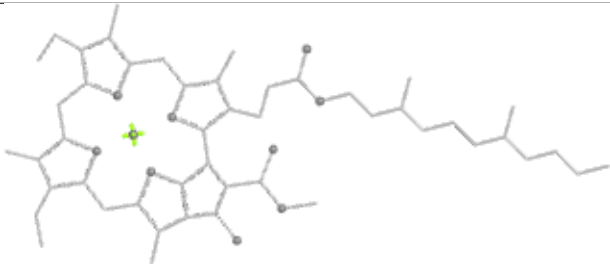


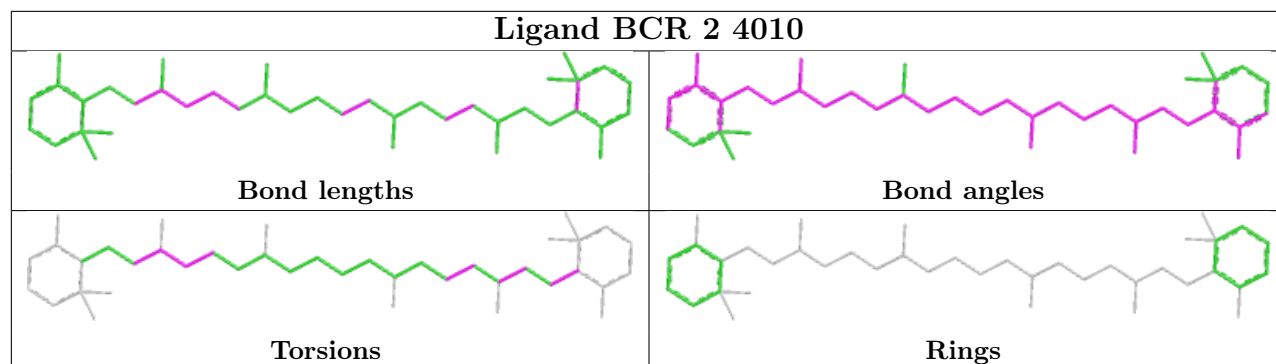
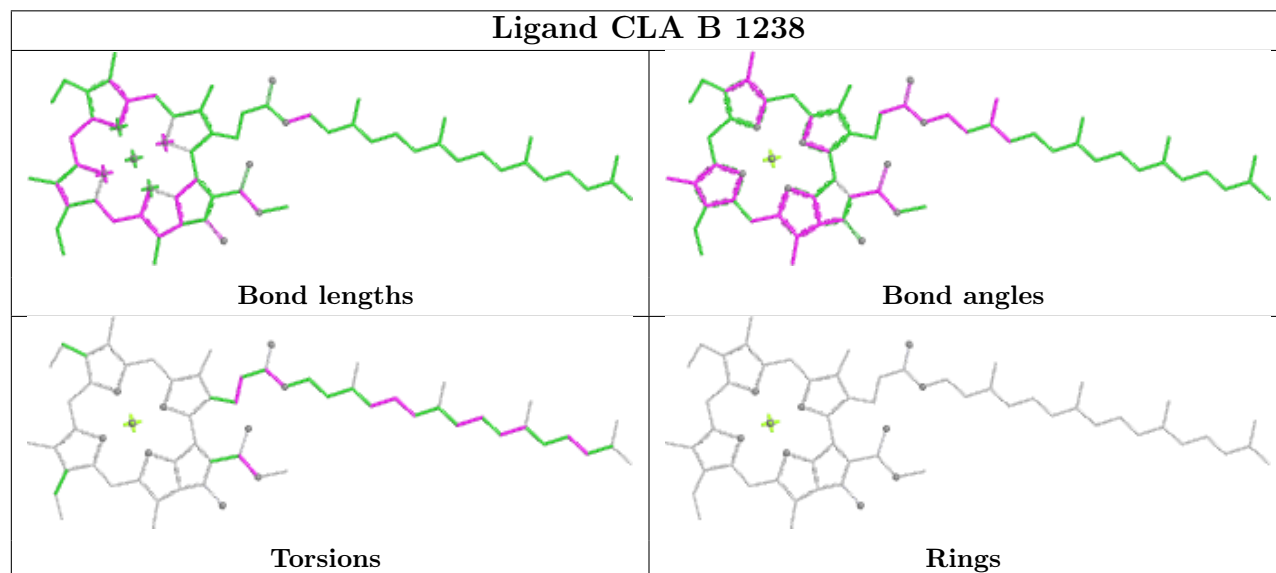
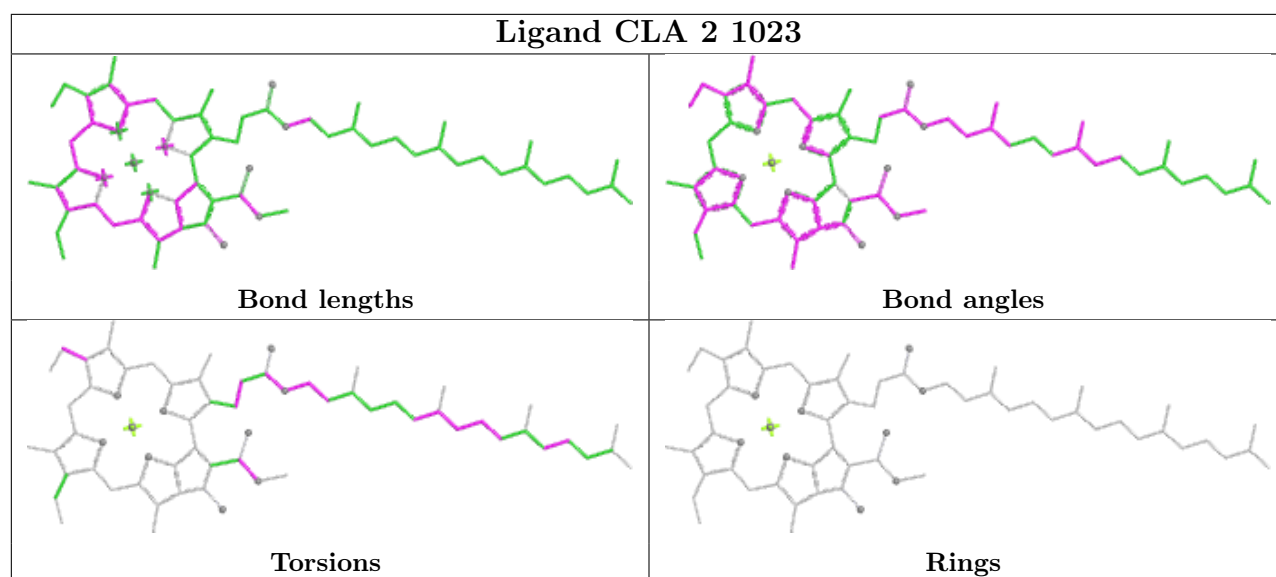
Ligand BCR f 4020	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA A 1118	
	
Bond lengths	Bond angles
	
Torsions	Rings

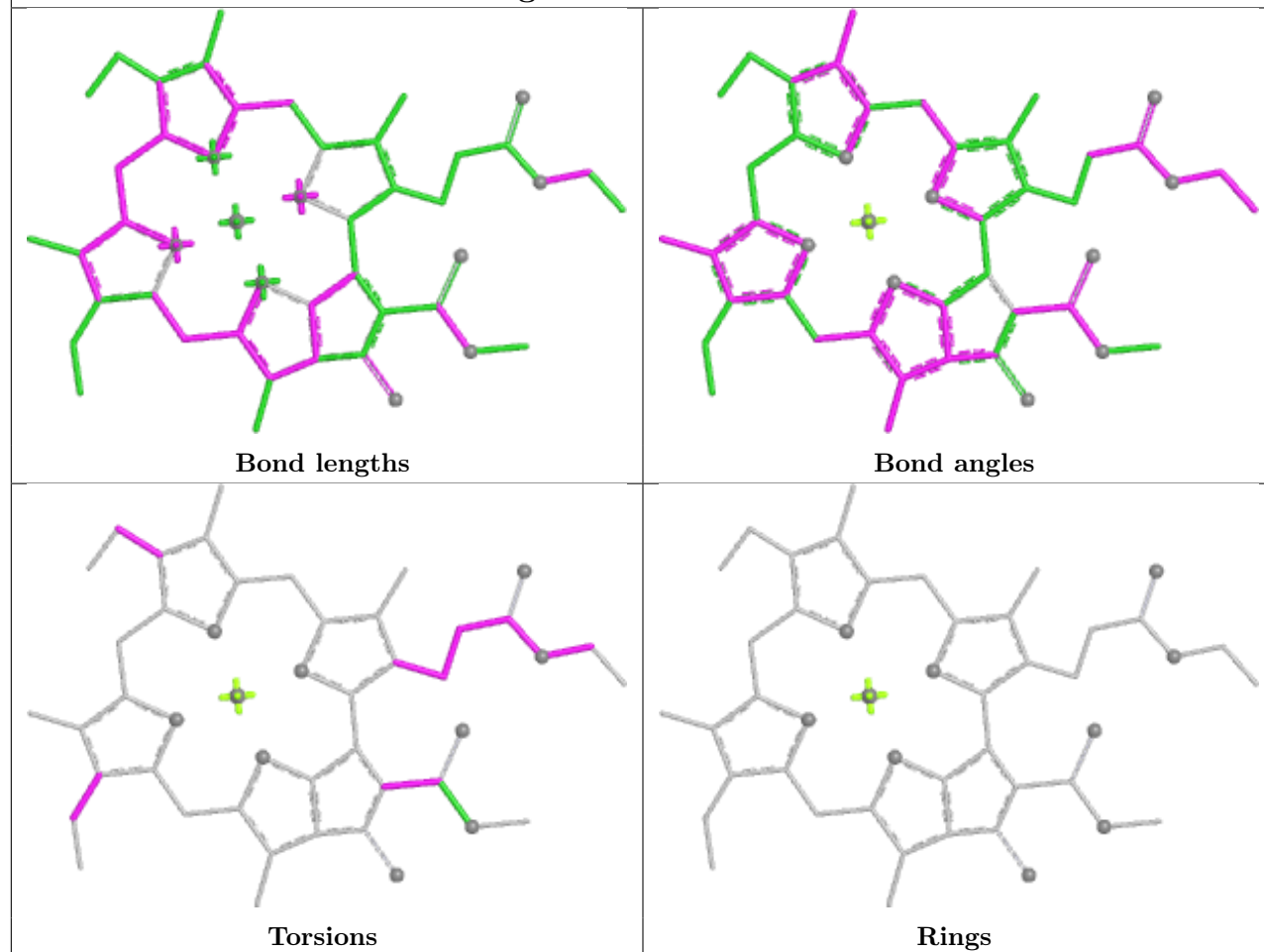
Ligand BCR a 4002	
	
Bond lengths	Bond angles
	
Torsions	Rings

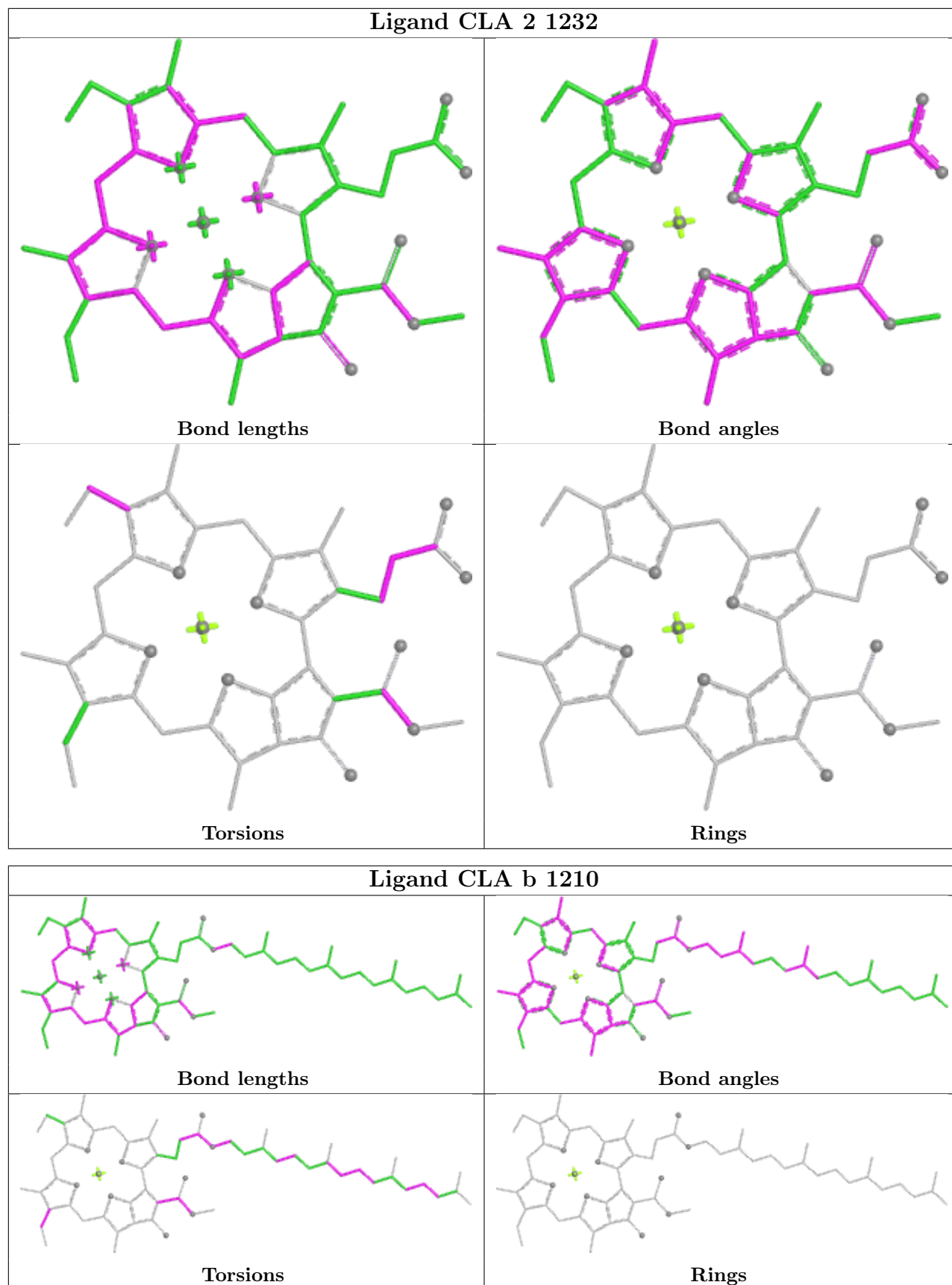


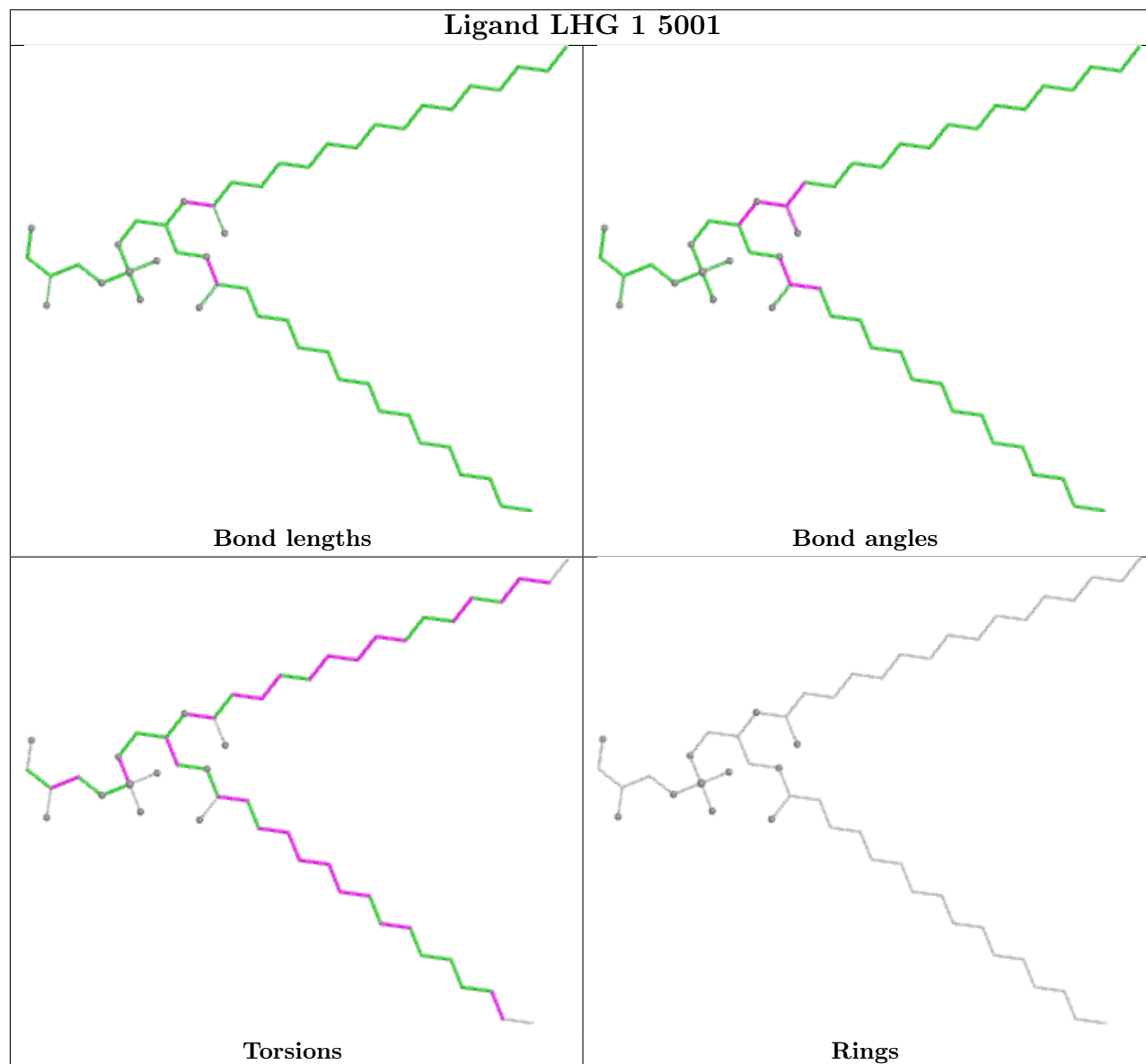
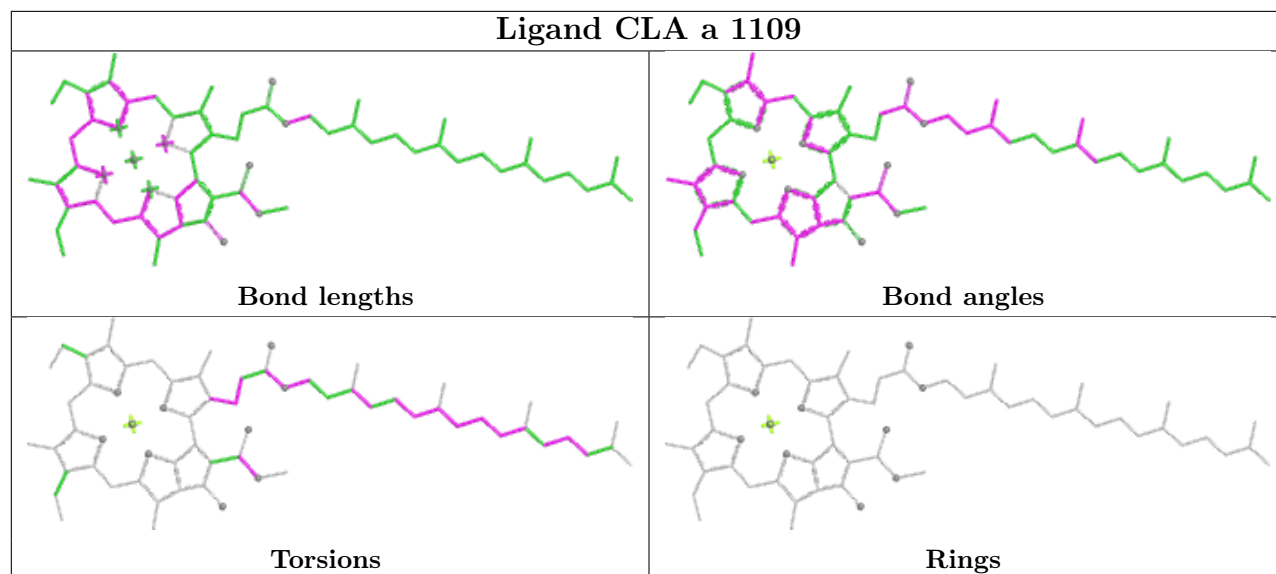
Ligand BCR b 4004	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand BCR f 4018	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand CLA b 1230	
 Bond lengths	 Bond angles
 Torsions	 Rings

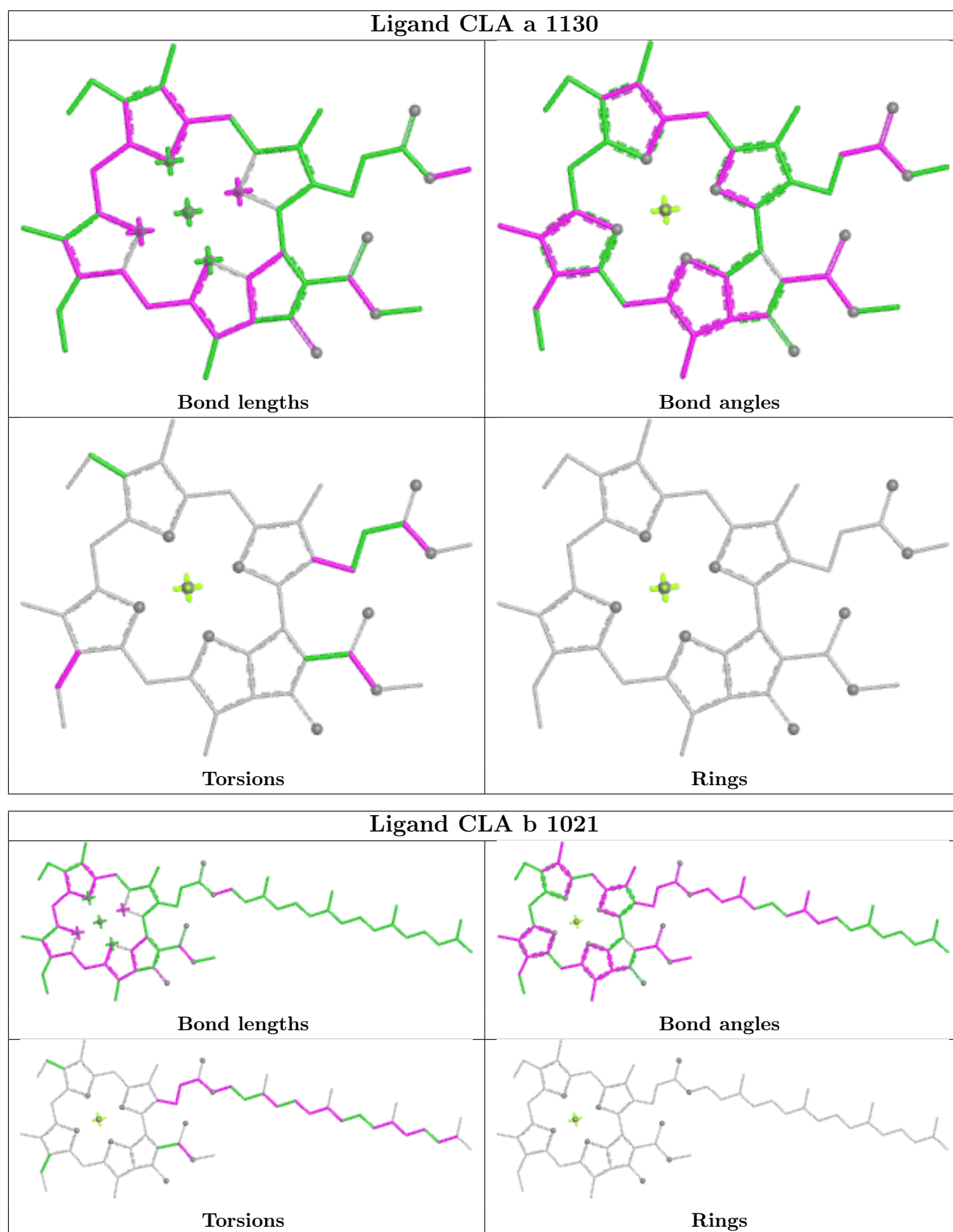


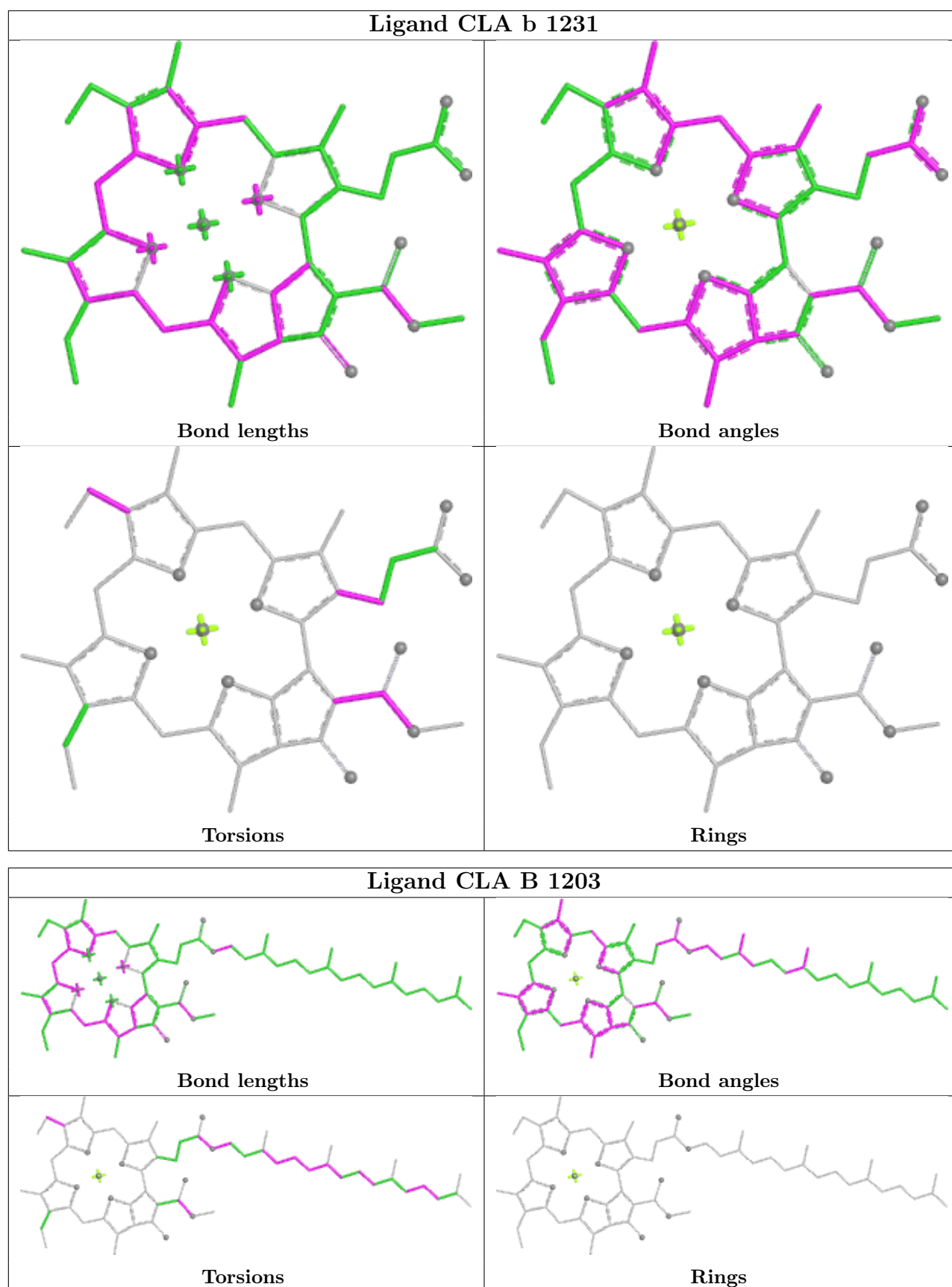
Ligand CLA B 1217

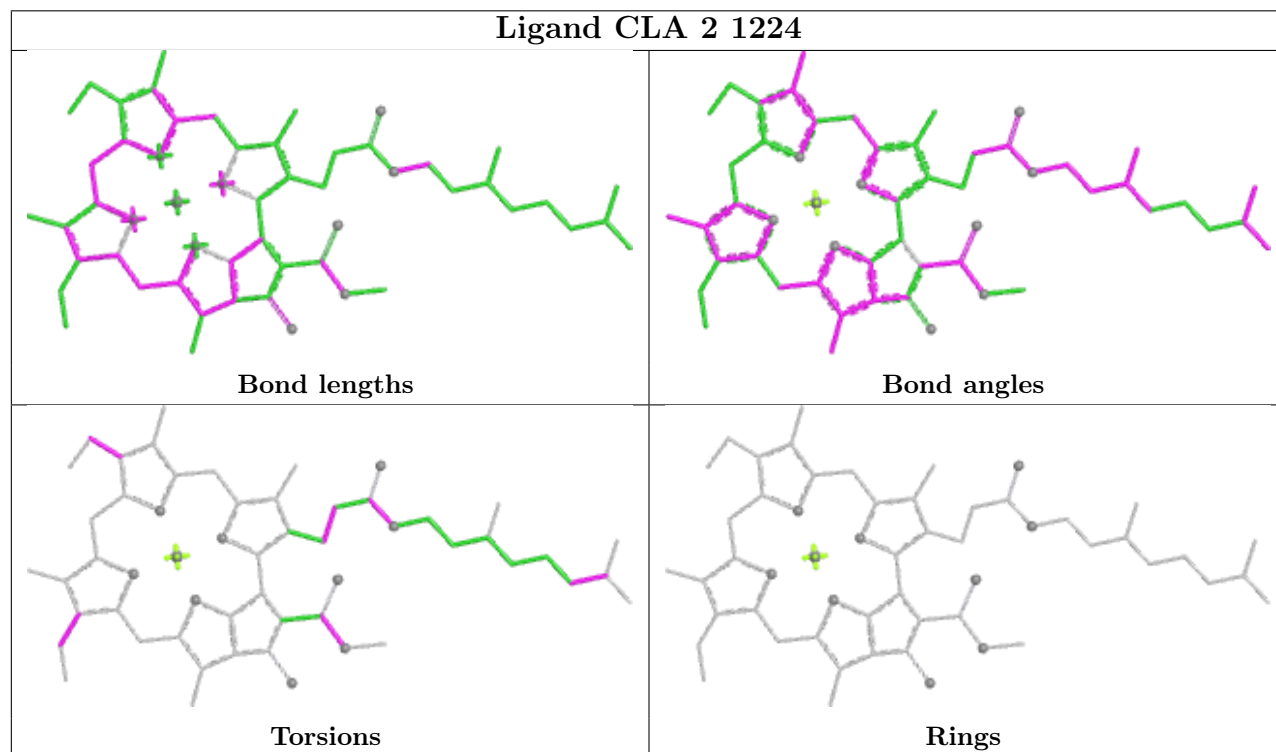
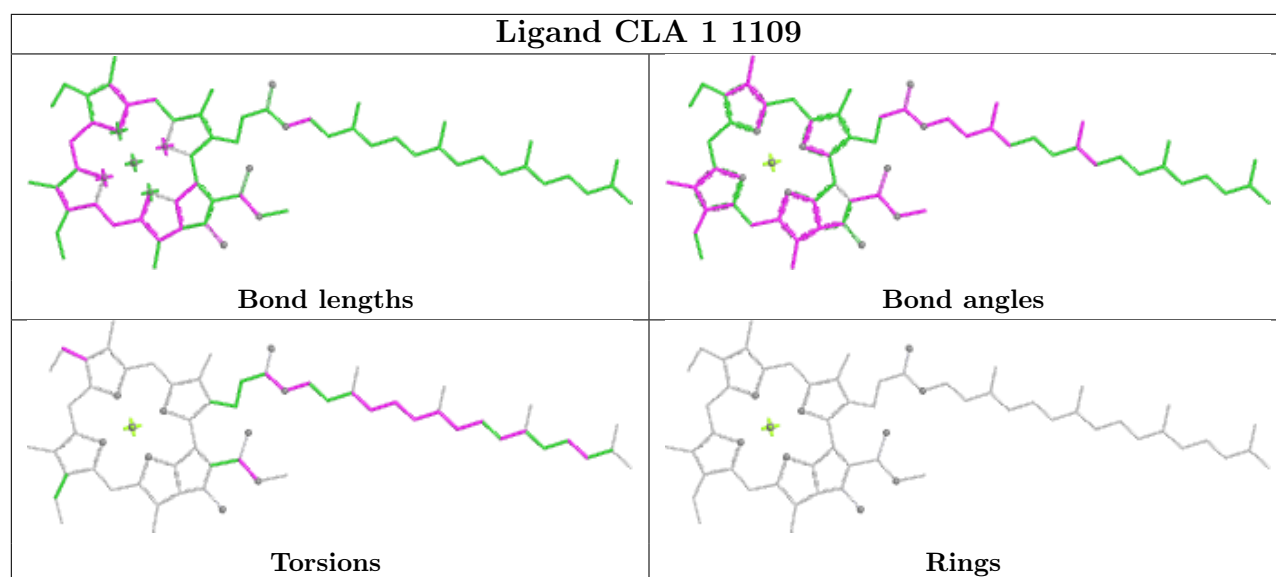




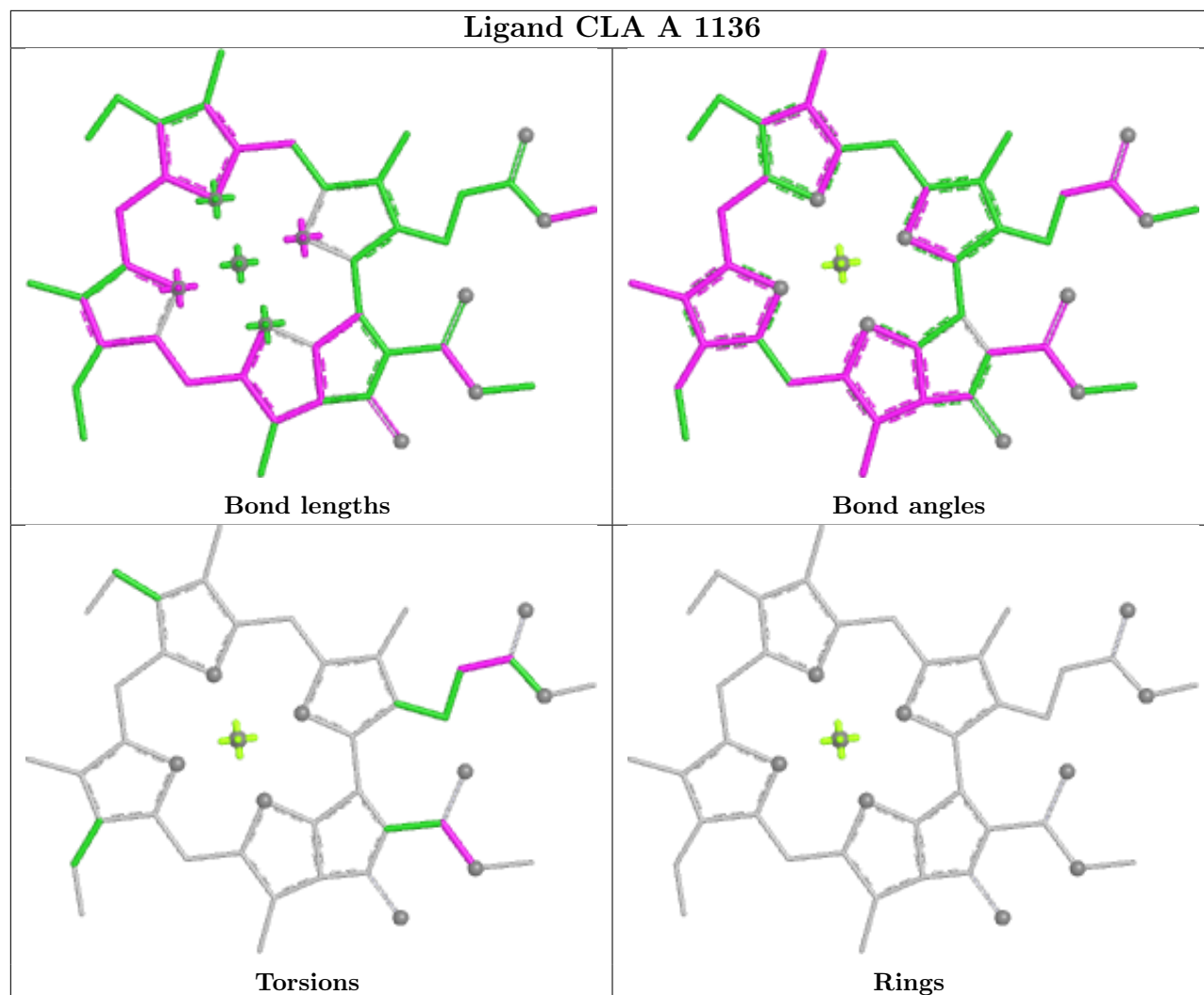


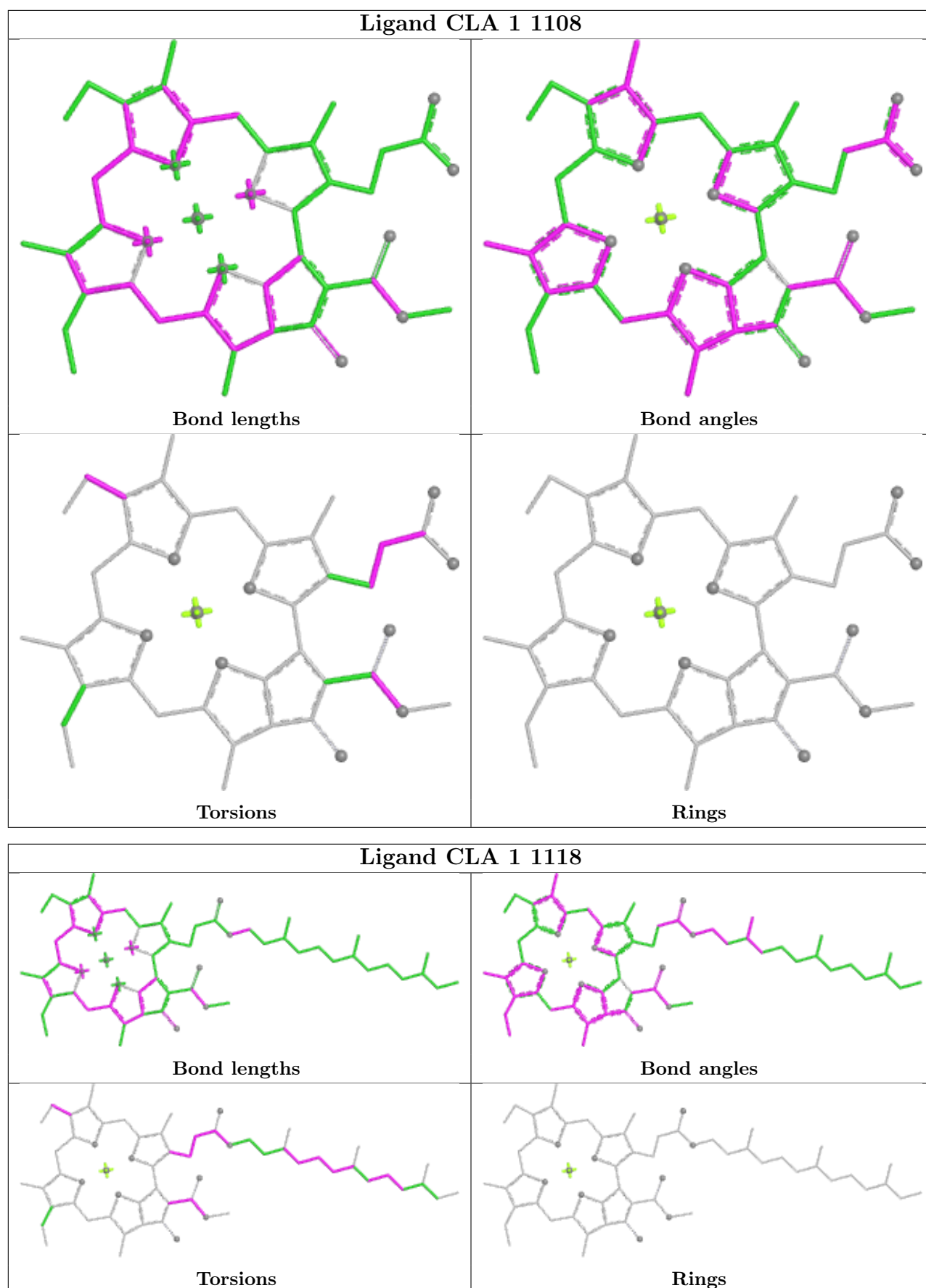


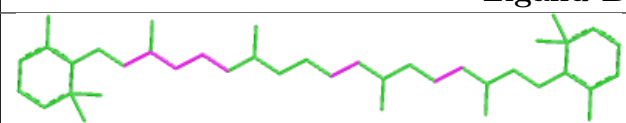
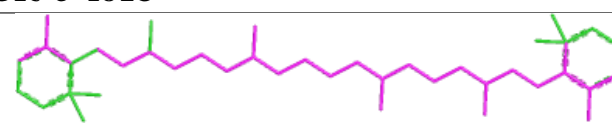
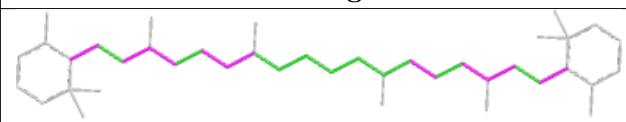
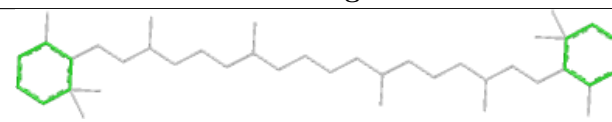


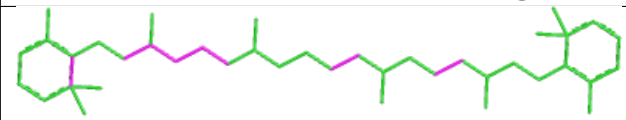
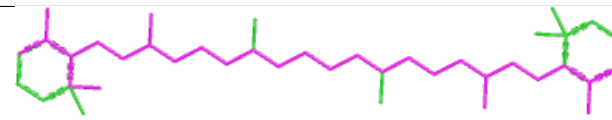
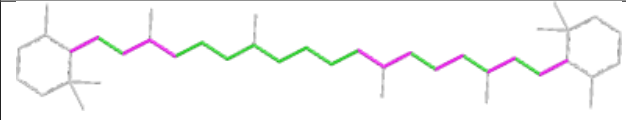
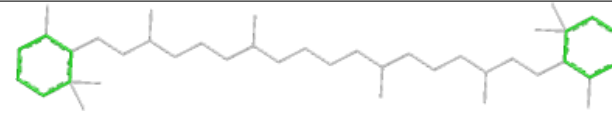


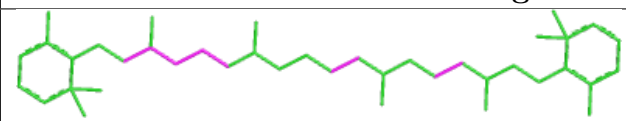
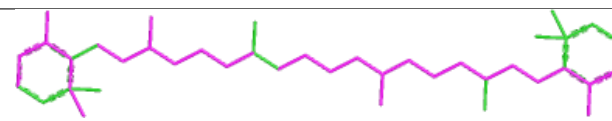
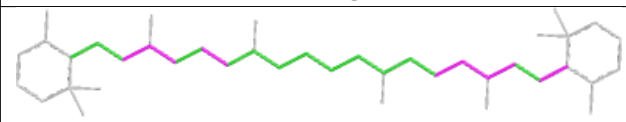
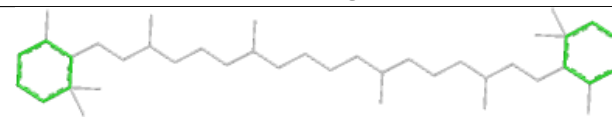
Ligand CLA A 1136

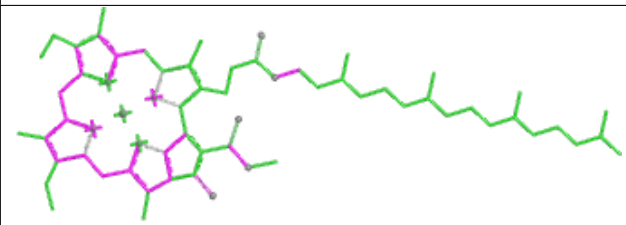
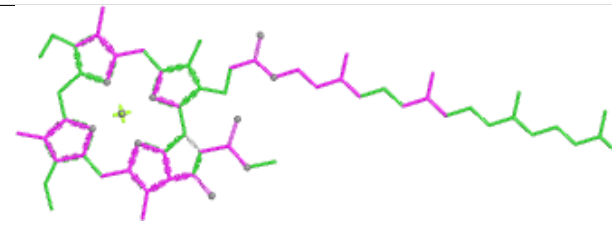
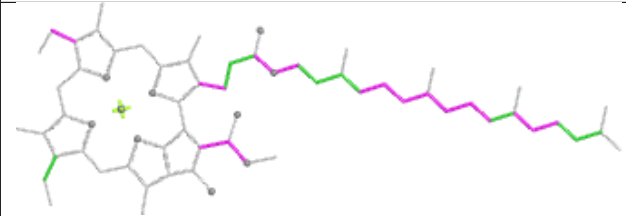
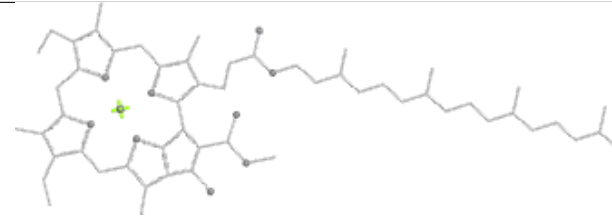




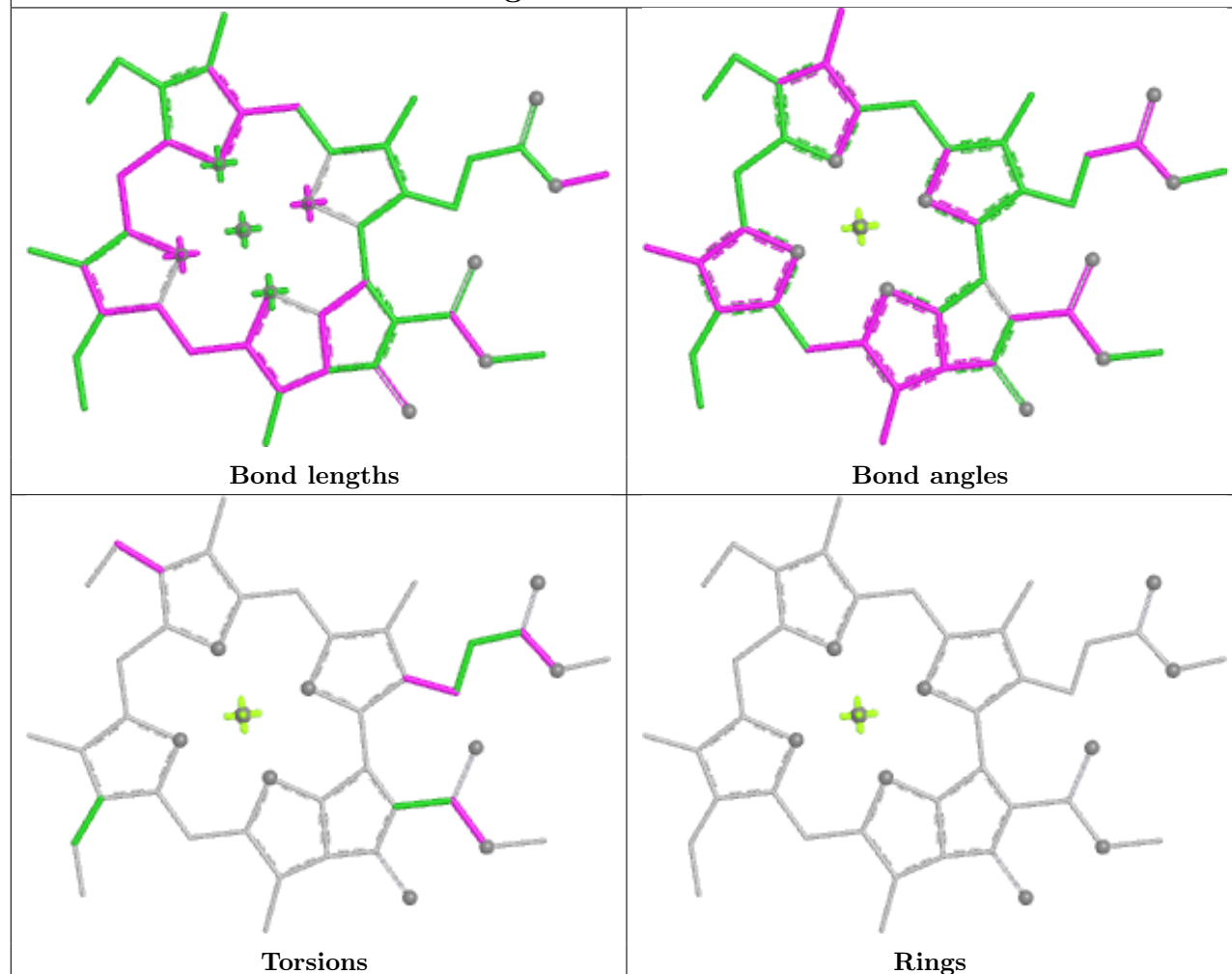
Ligand BCR 6 4013	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand BCR b 4011	
	
Bond lengths	Bond angles
	
Torsions	Rings

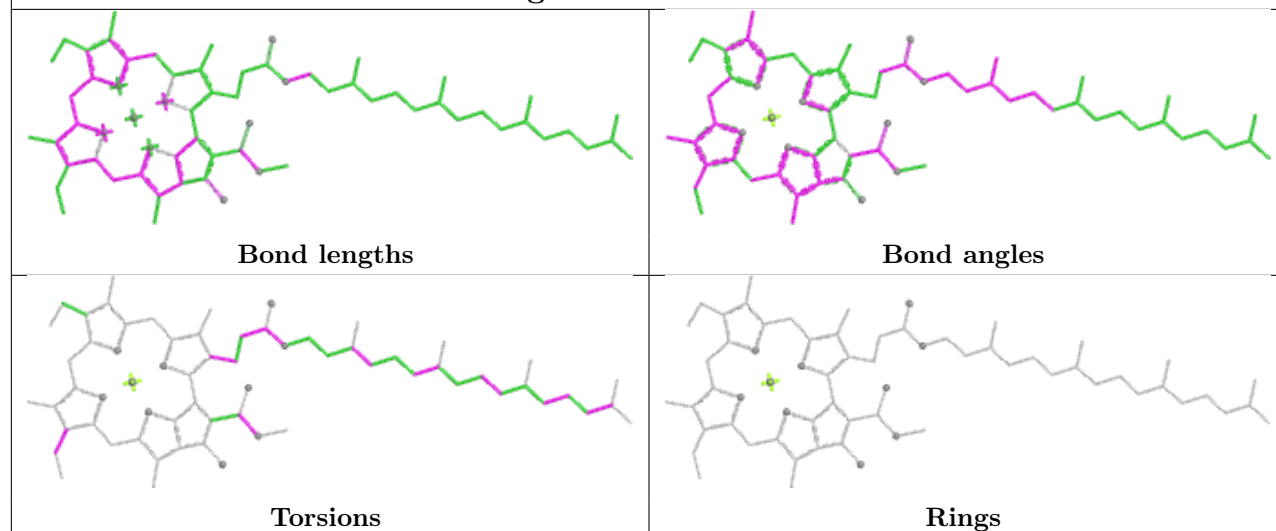
Ligand BCR F 4020	
	
Bond lengths	Bond angles
	
Torsions	Rings

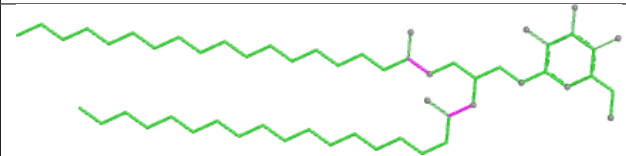
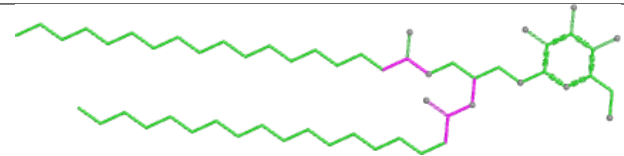
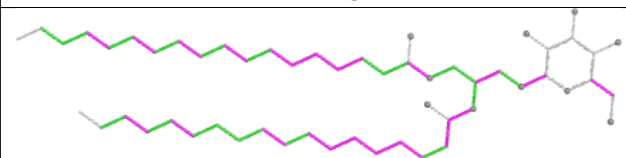
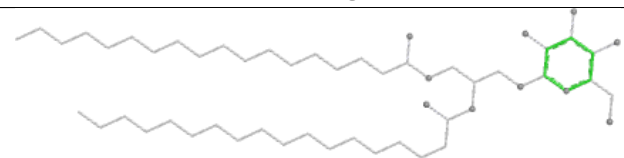
Ligand CLA 2 1223	
	
Bond lengths	Bond angles
	
Torsions	Rings

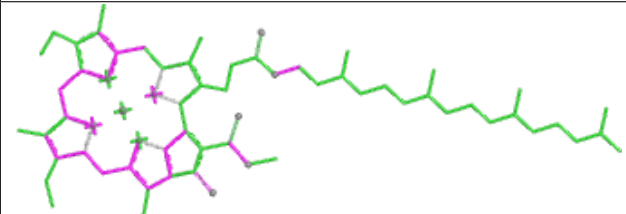
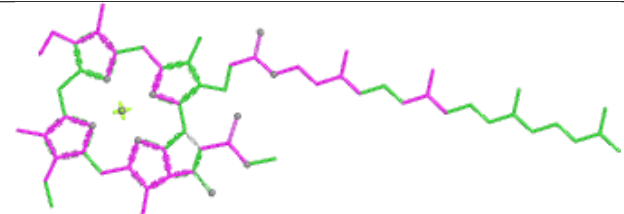
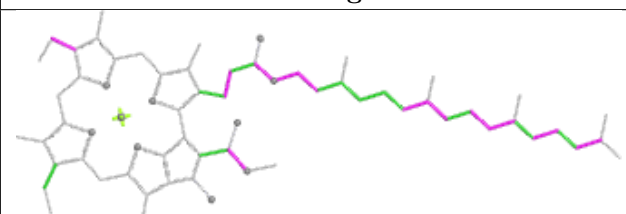
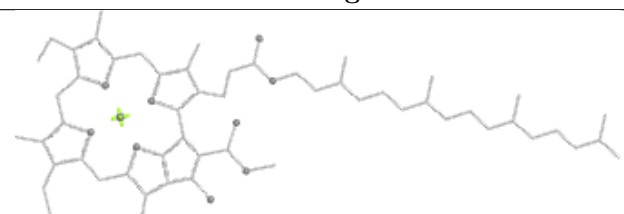
Ligand CLA A 1130

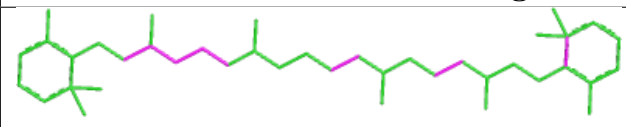
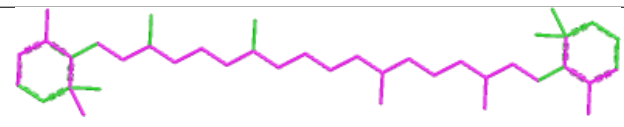
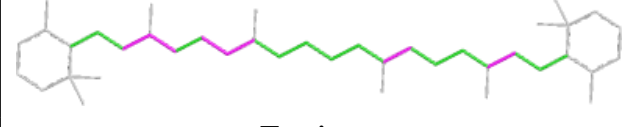
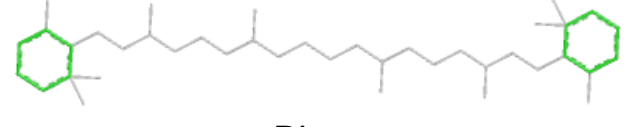


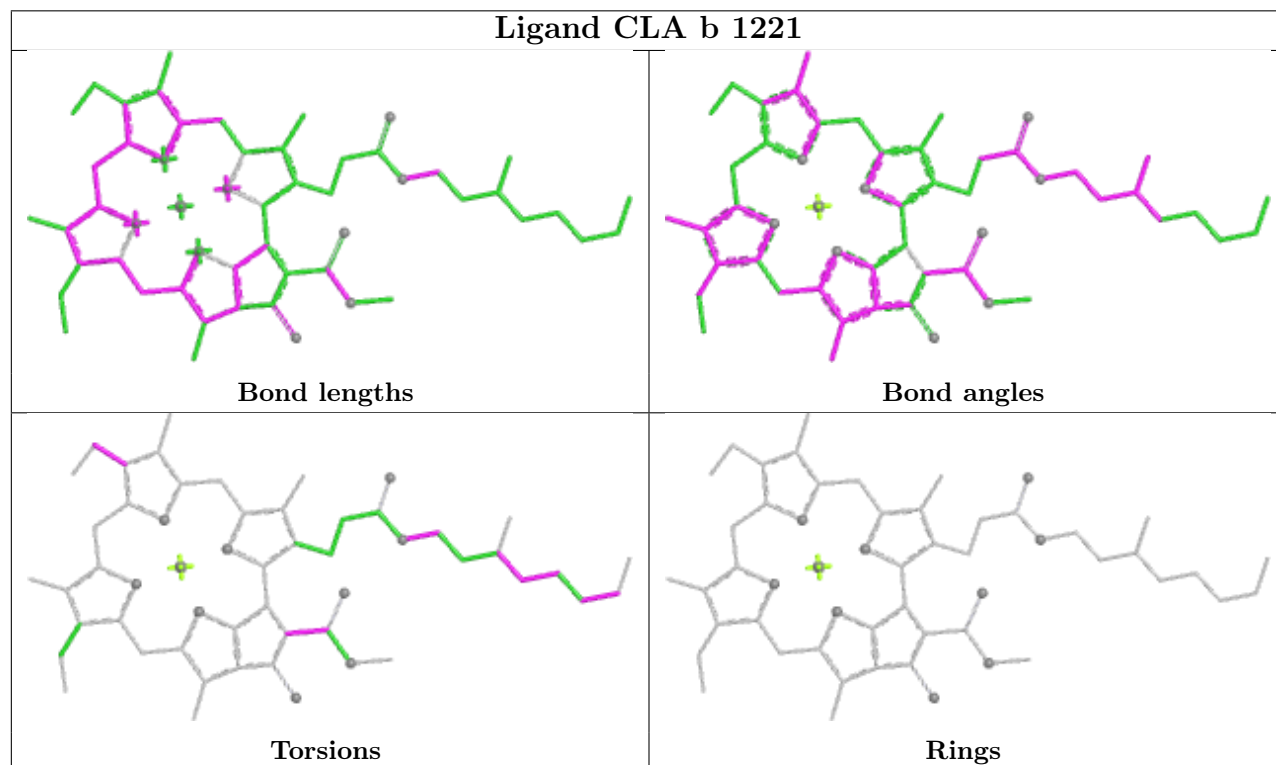
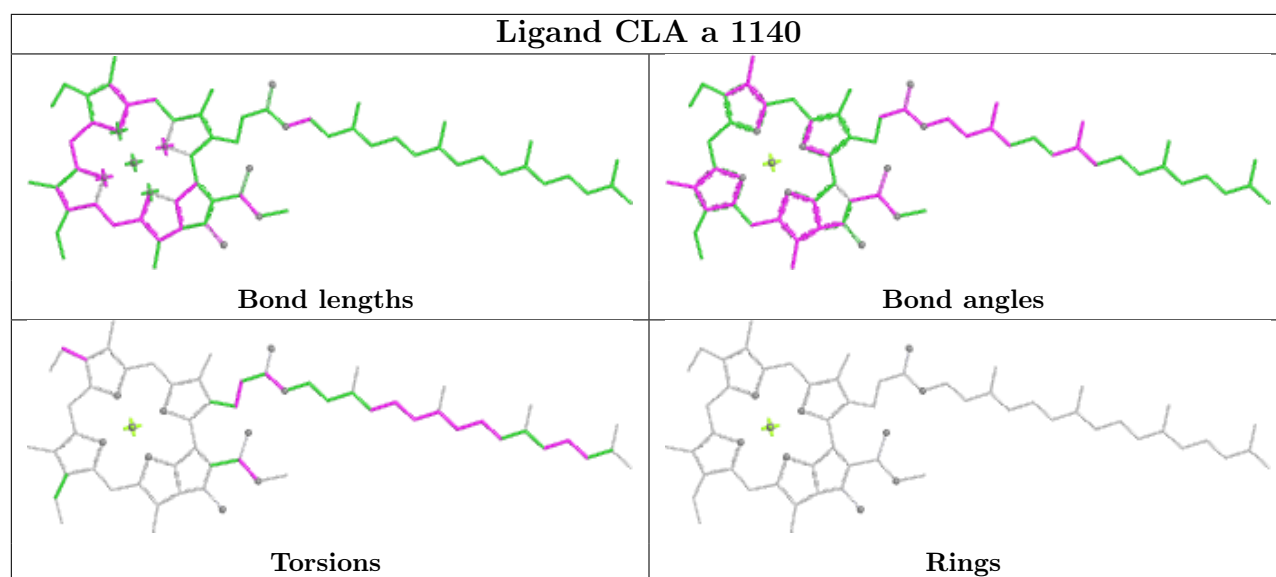
Ligand CLA 2 1213

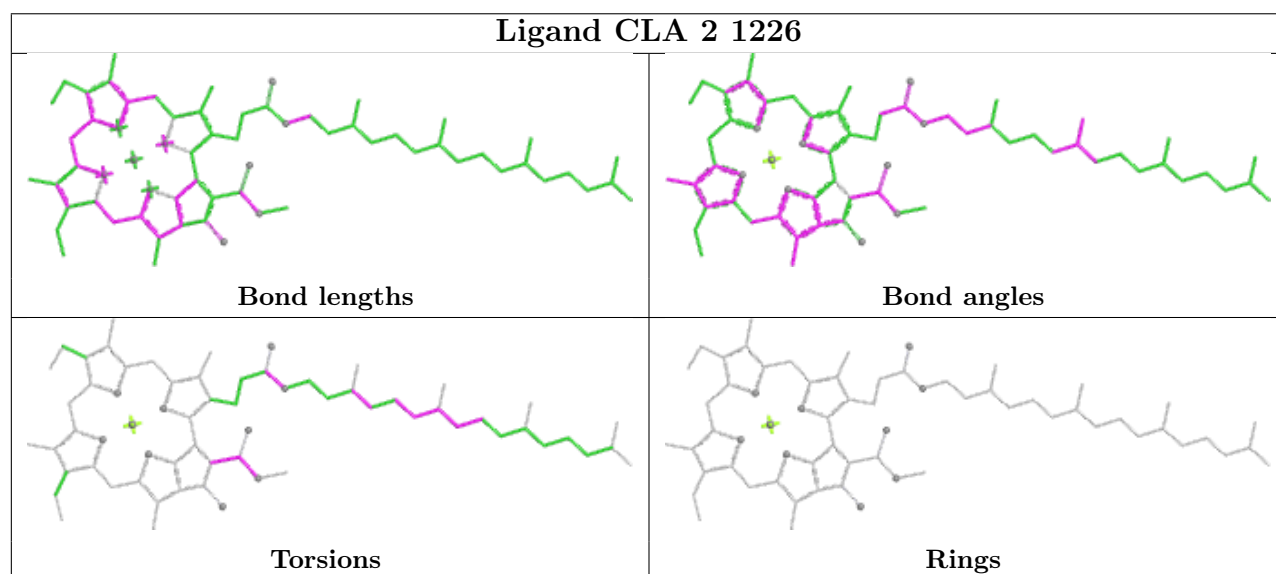
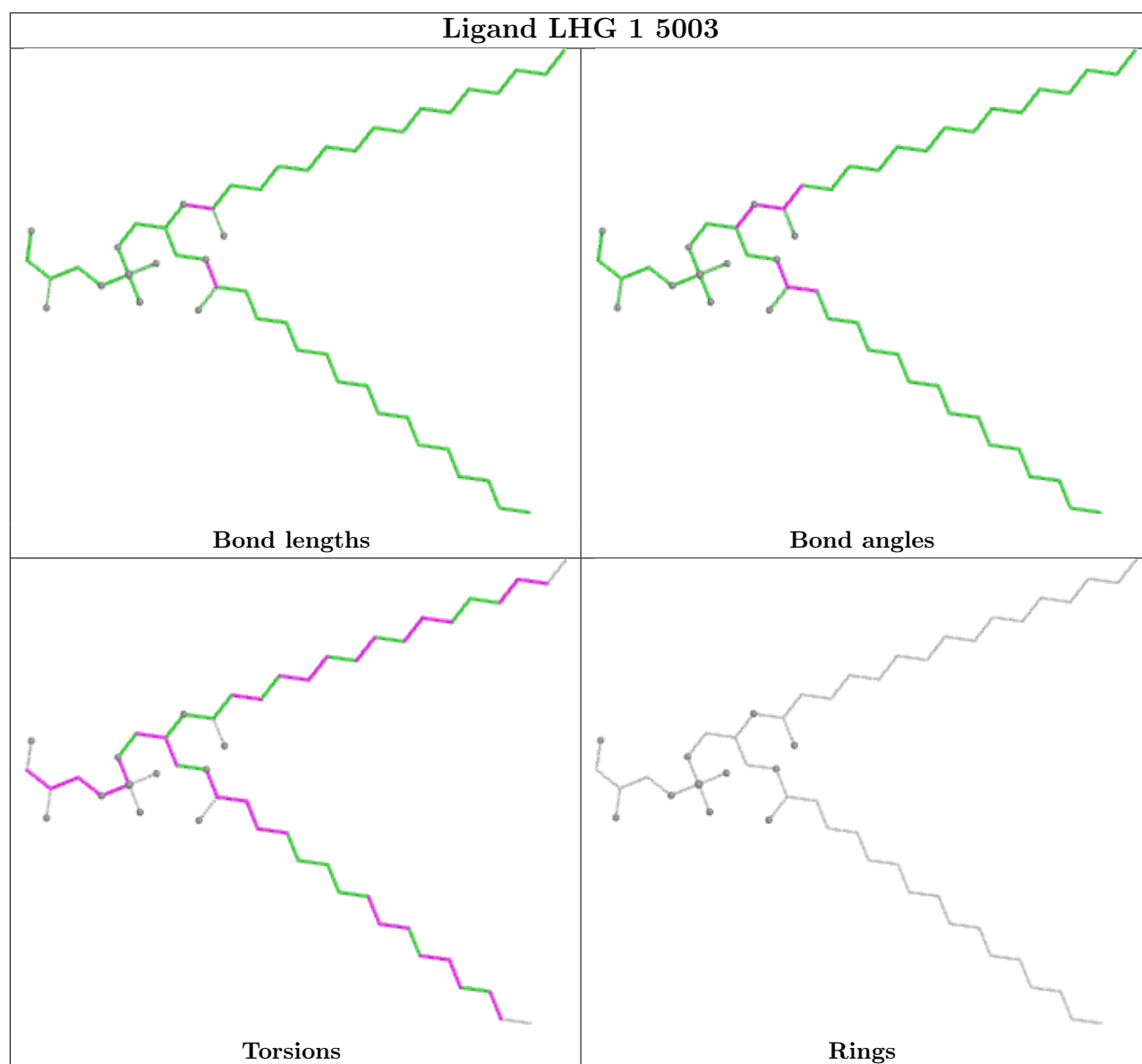


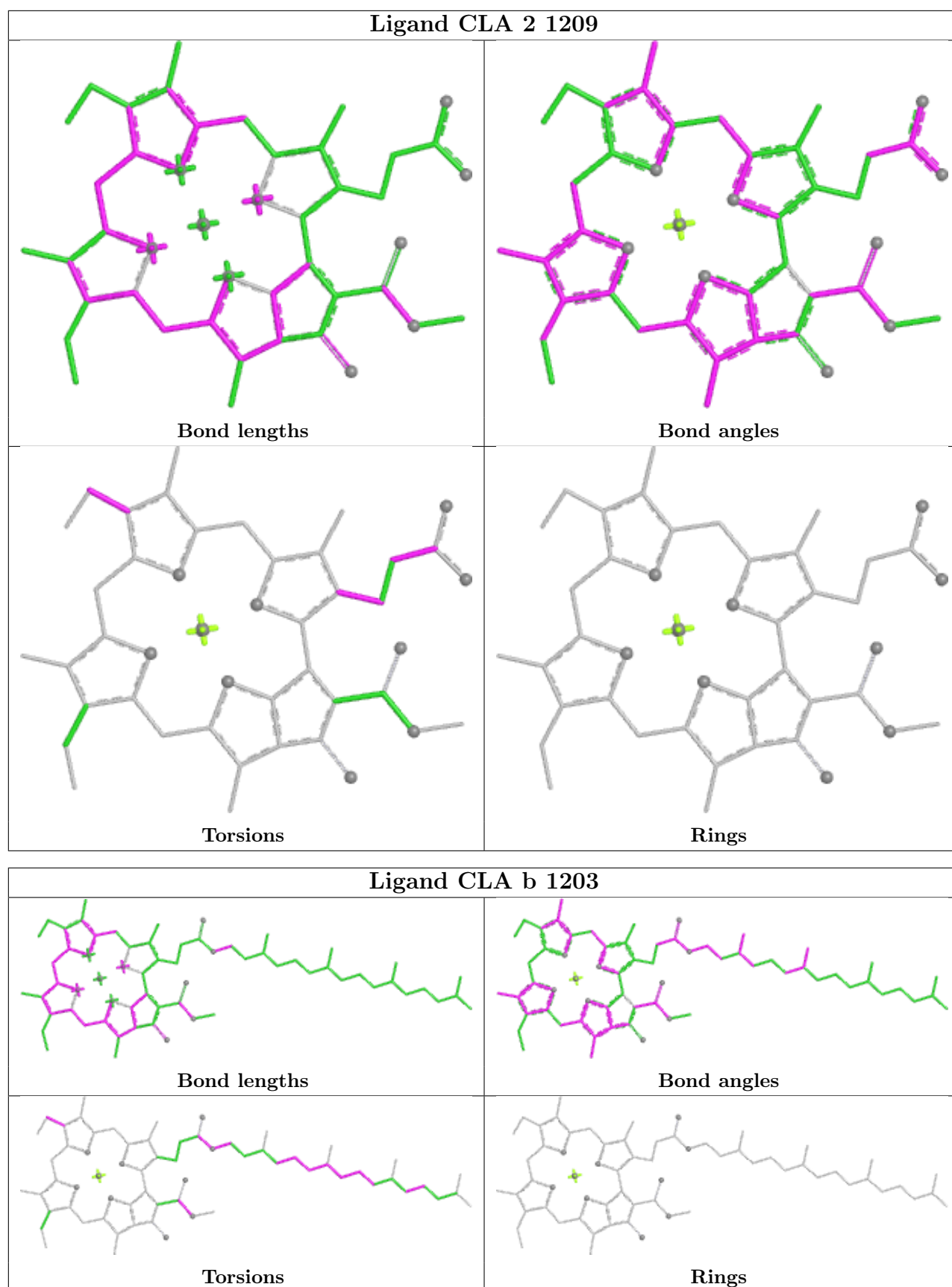
Ligand LMG b 5002	
	Bond lengths
	Bond angles
	Torsions
	Rings

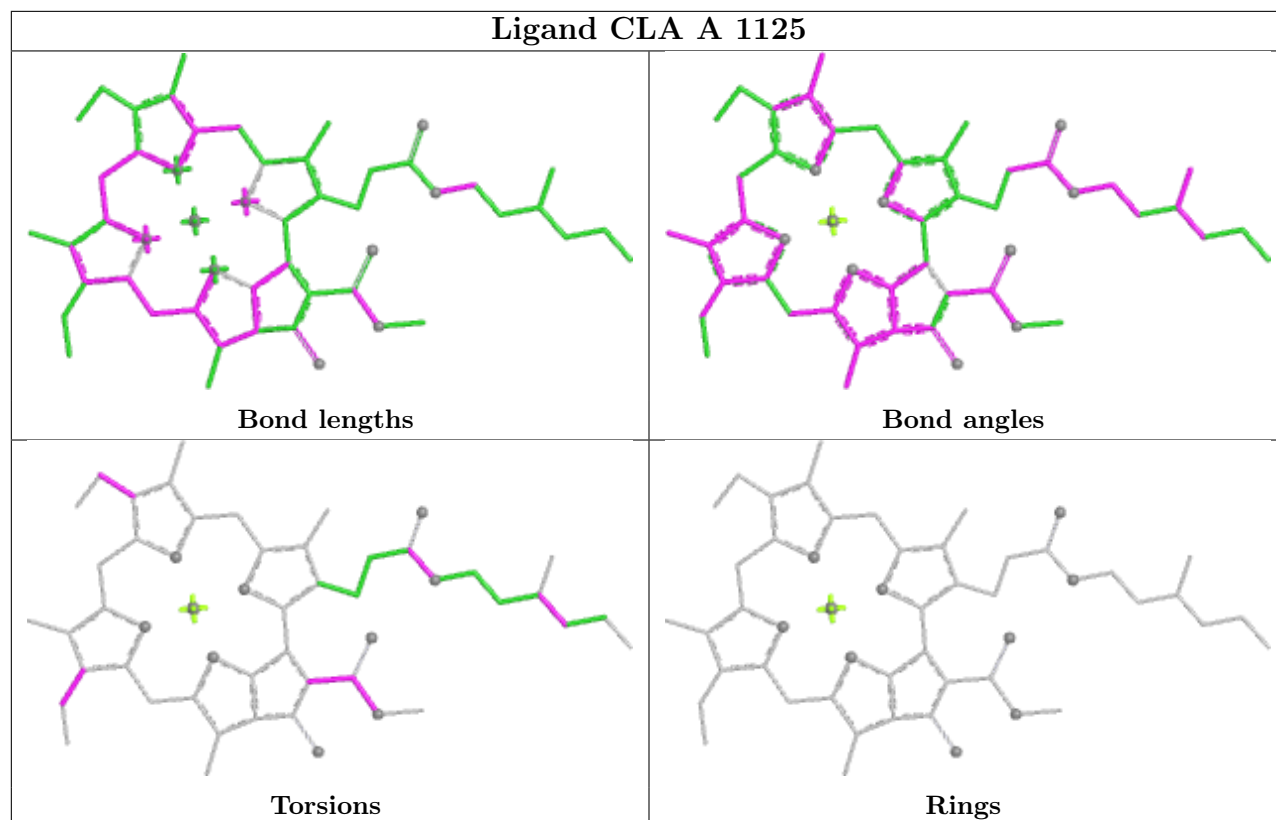
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	Bond lengths
	Bond angles
	Torsions
	Rings

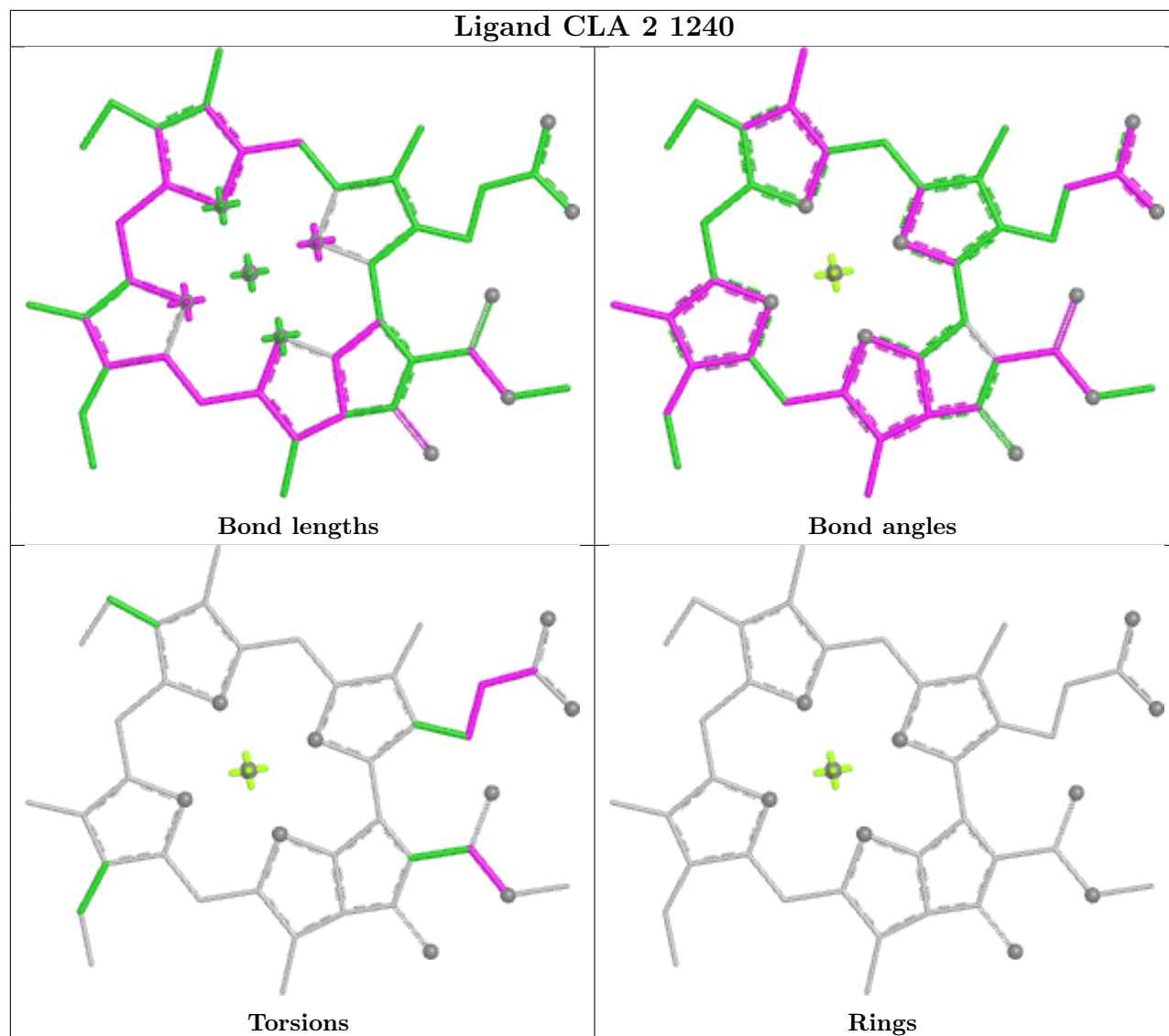
Ligand BCR B 4014	
	Bond lengths
	Bond angles
	Torsions
	Rings

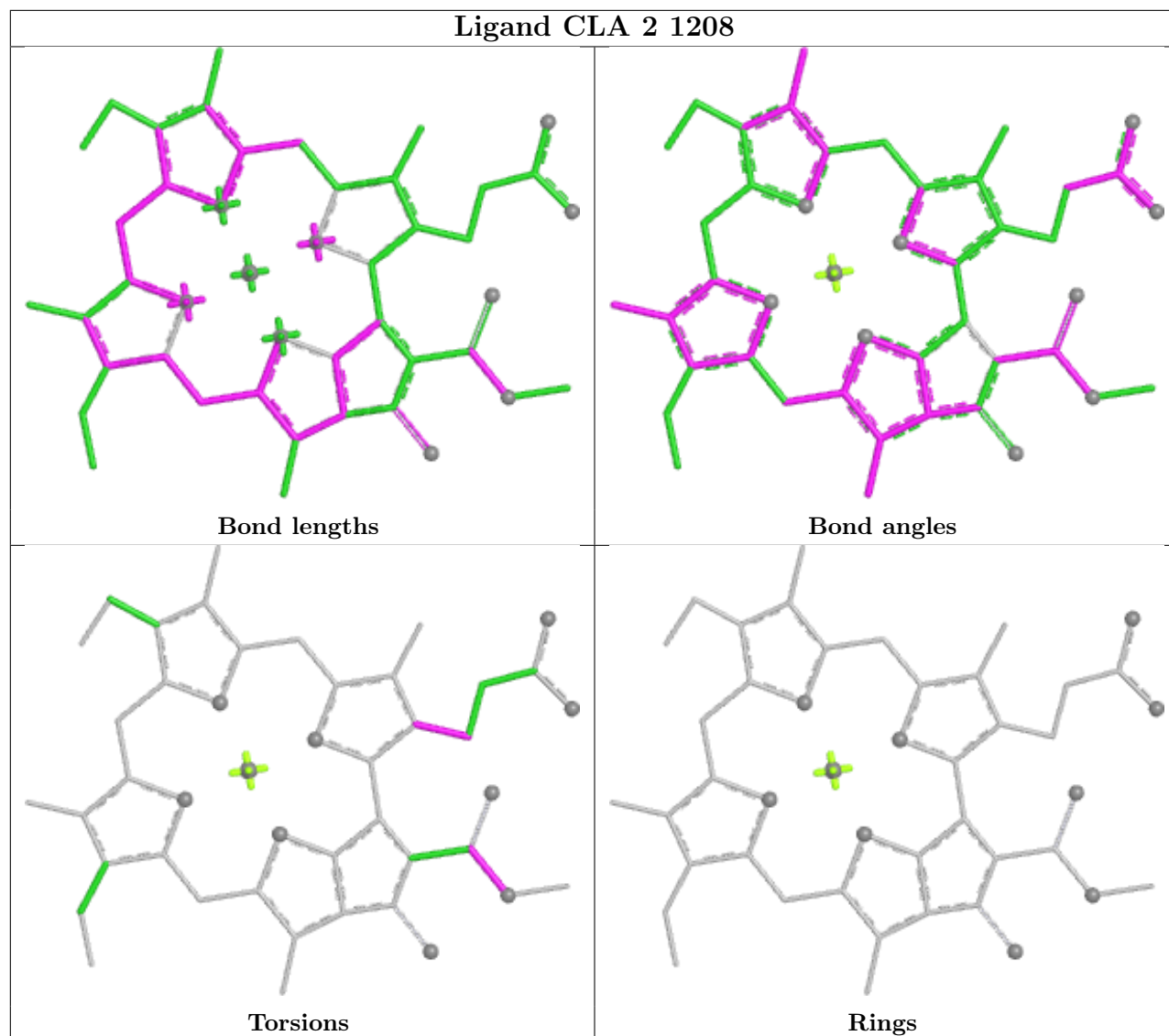


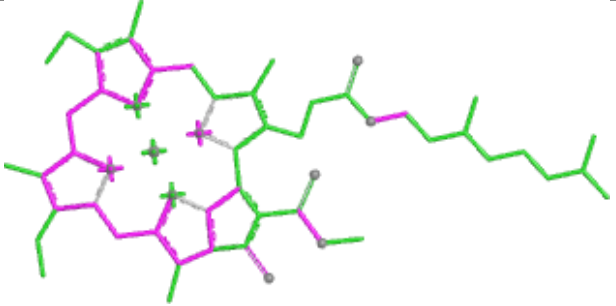
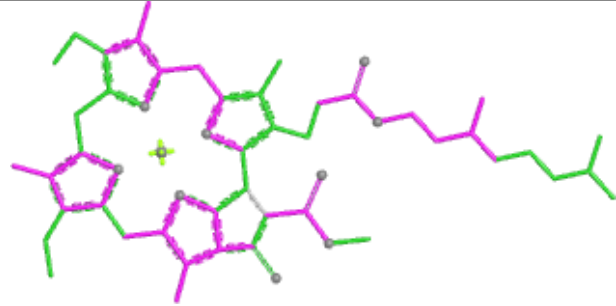
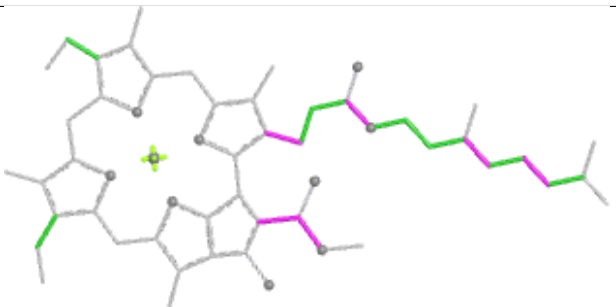
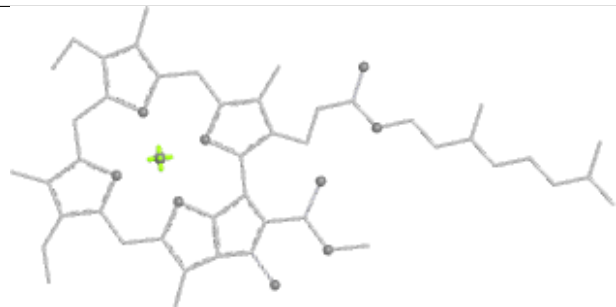


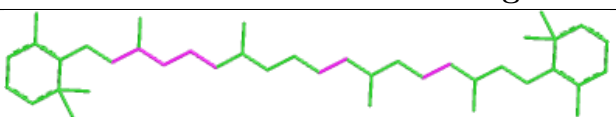
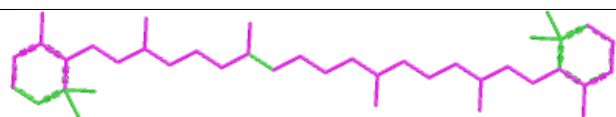
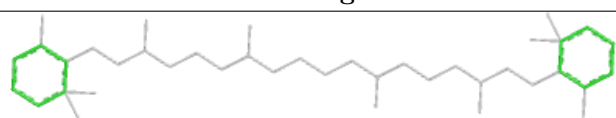


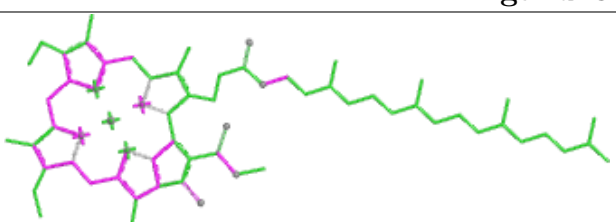
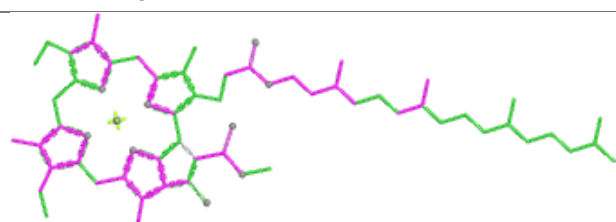
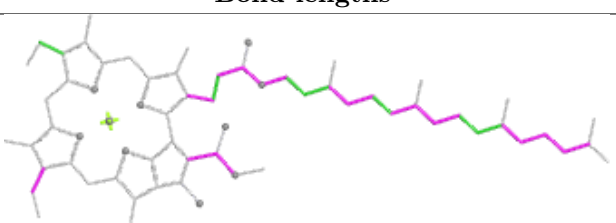
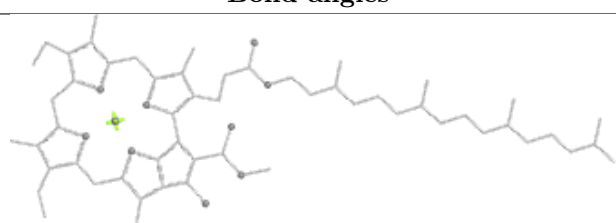


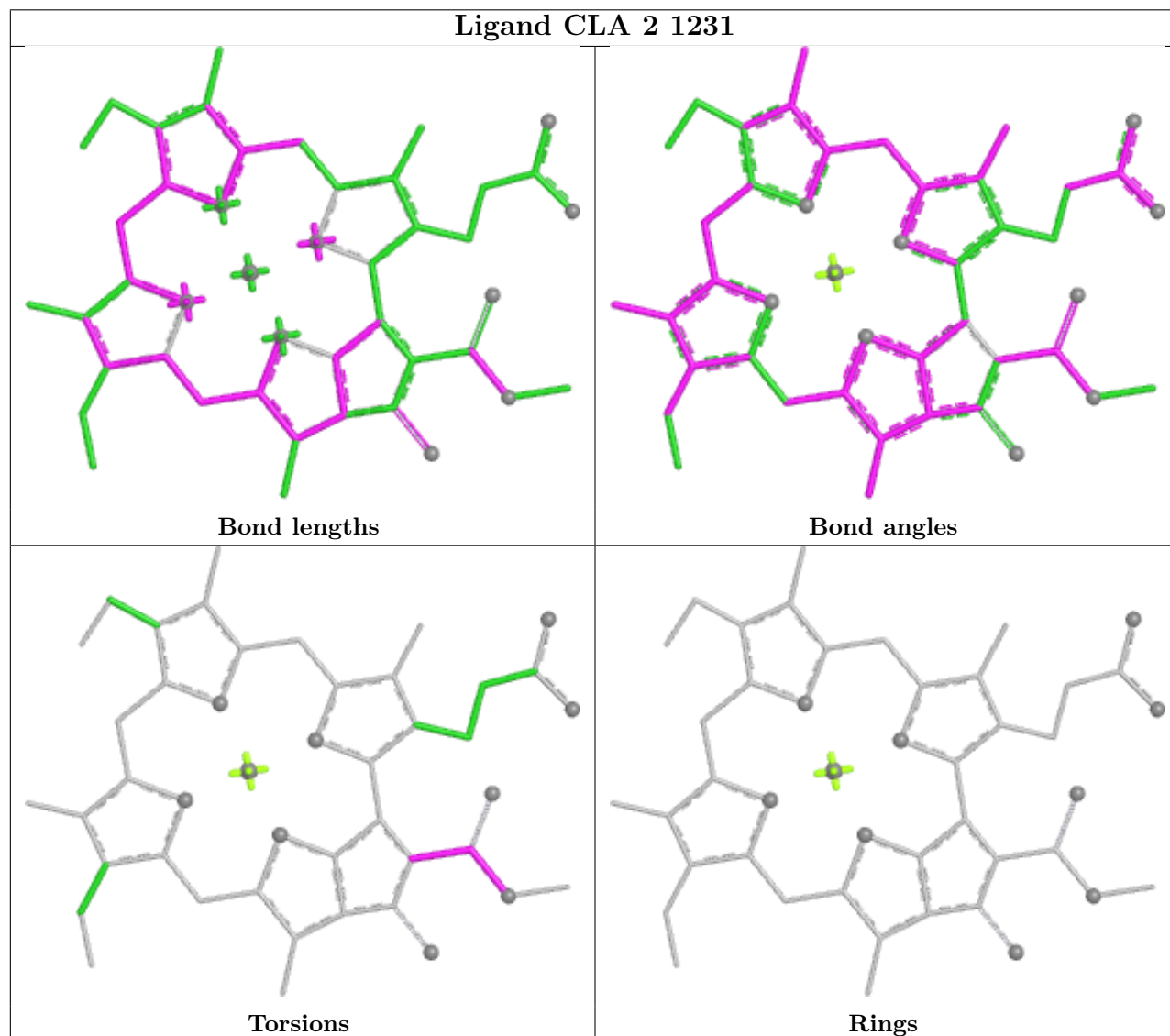
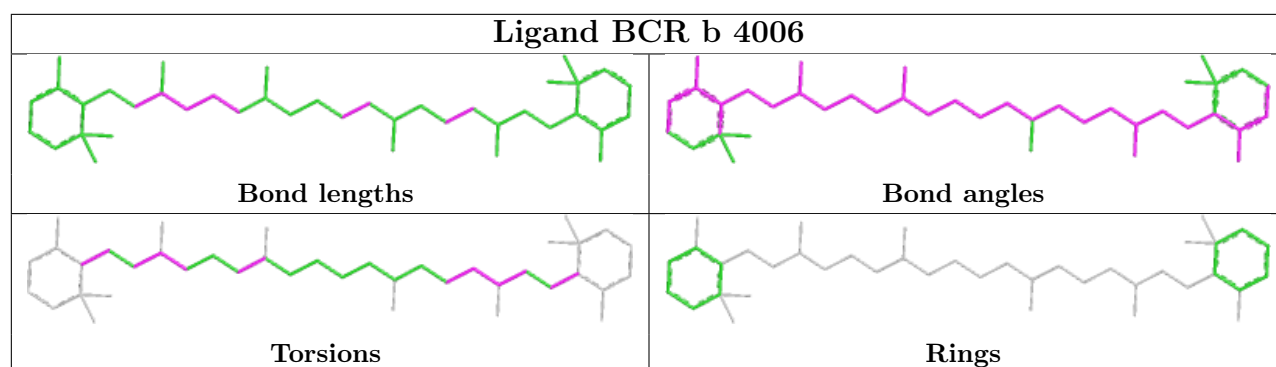


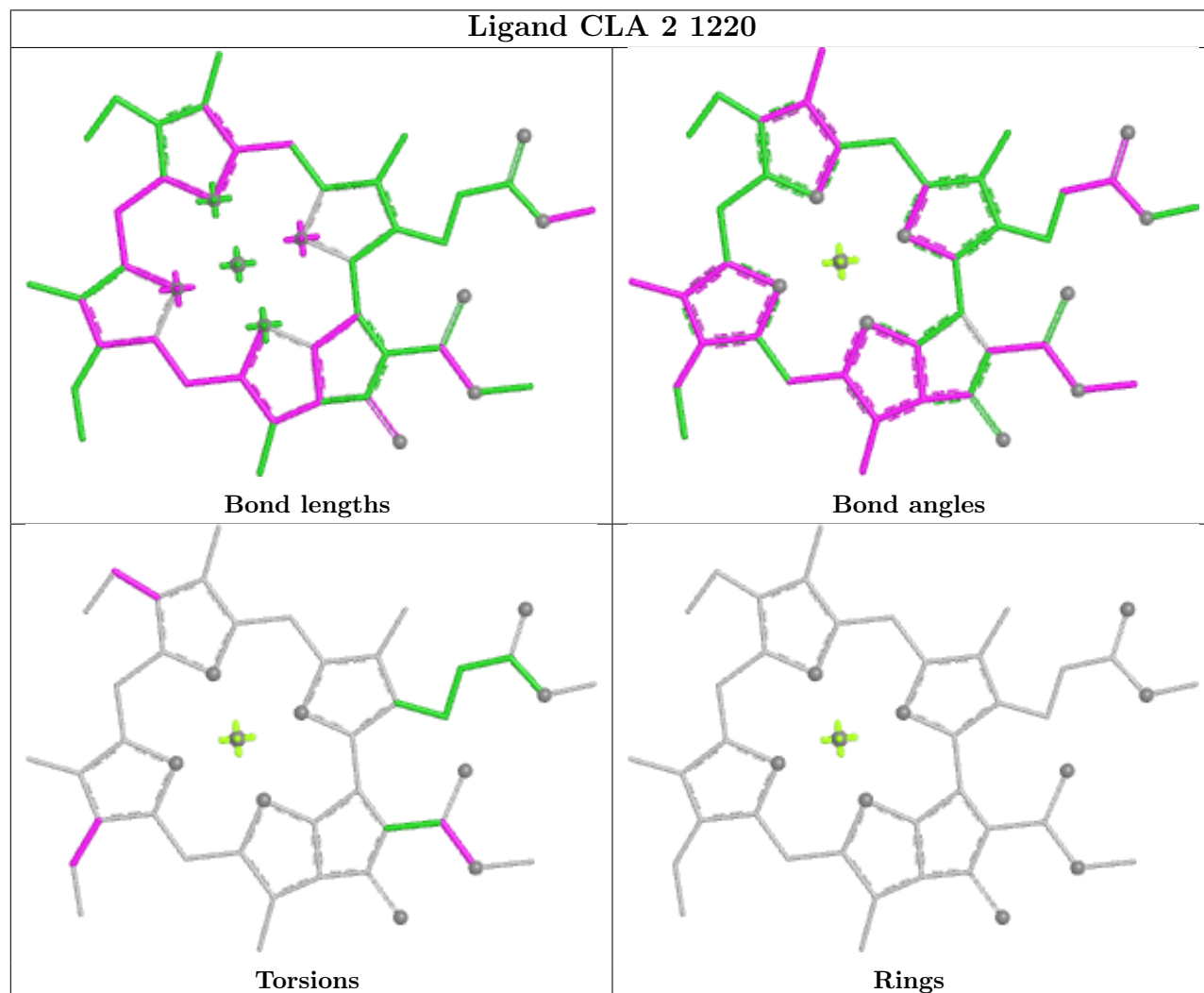
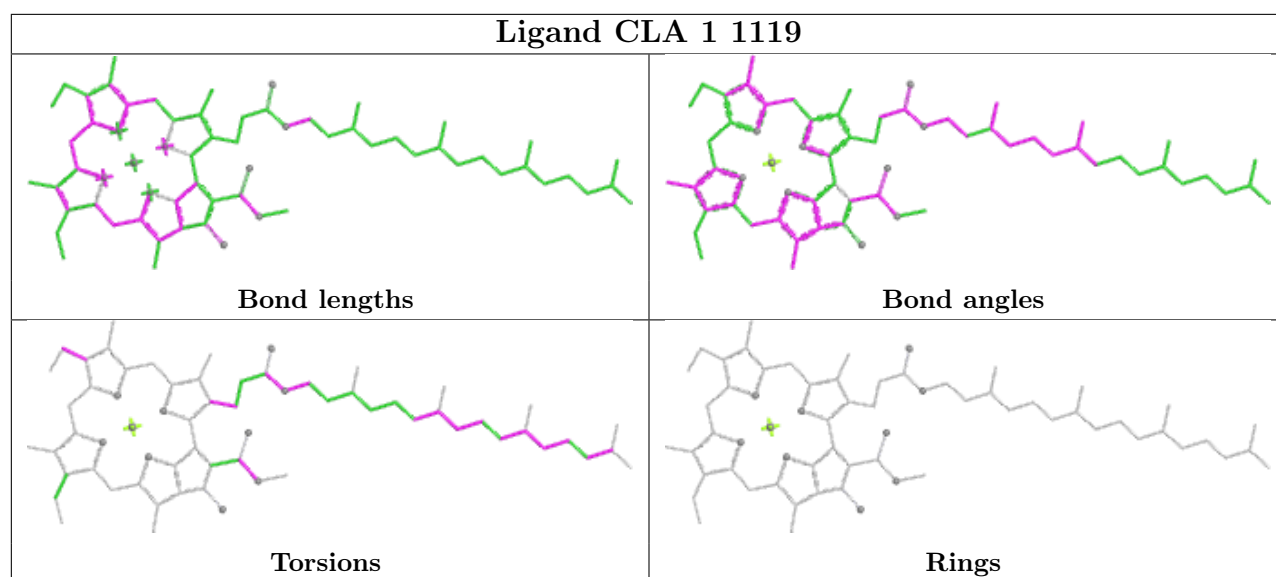


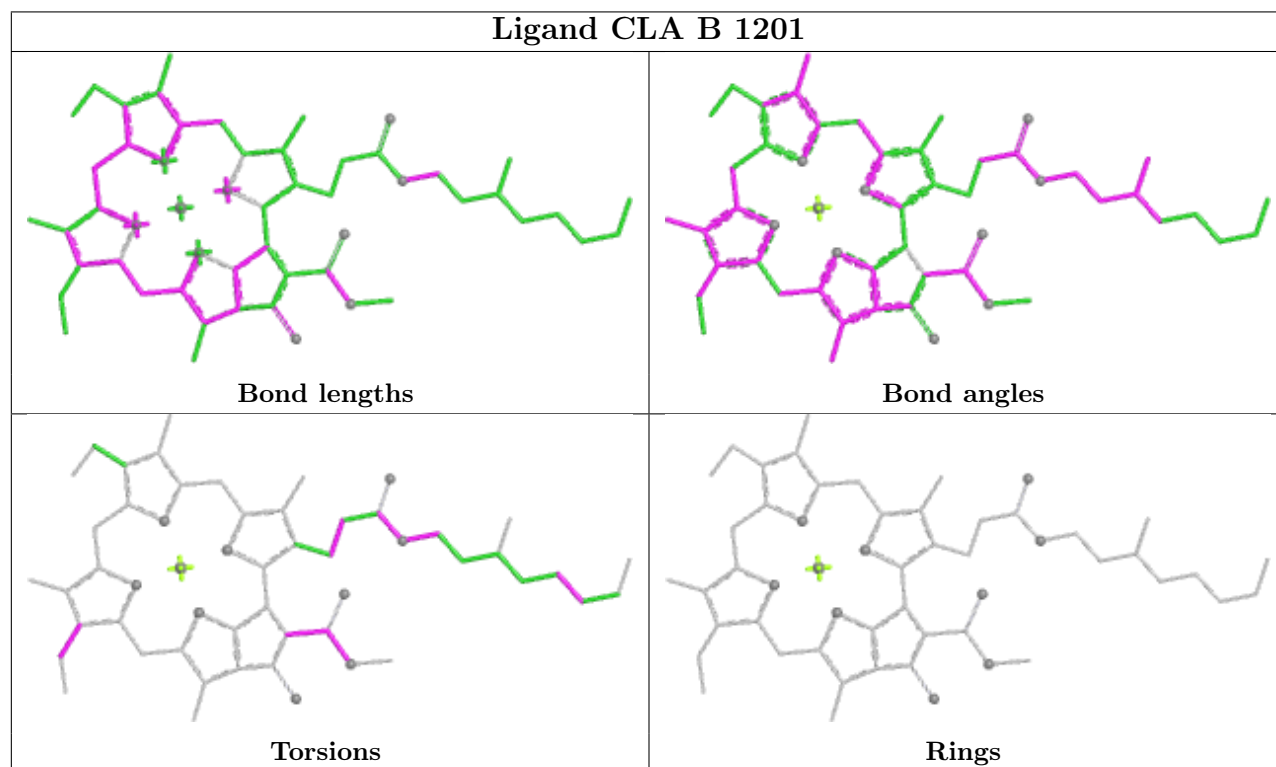
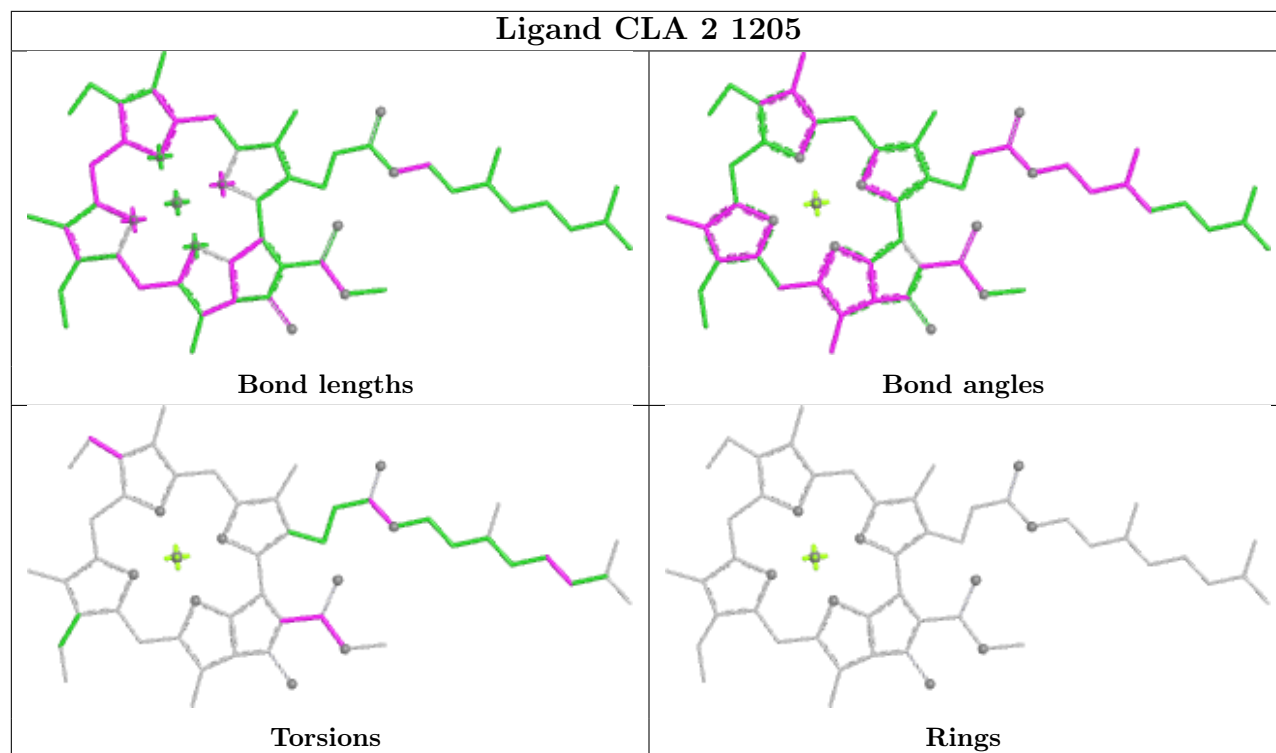
Ligand CLA 2 1219	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand BCR 2 4006	
	
Bond lengths	Bond angles
	
Torsions	Rings

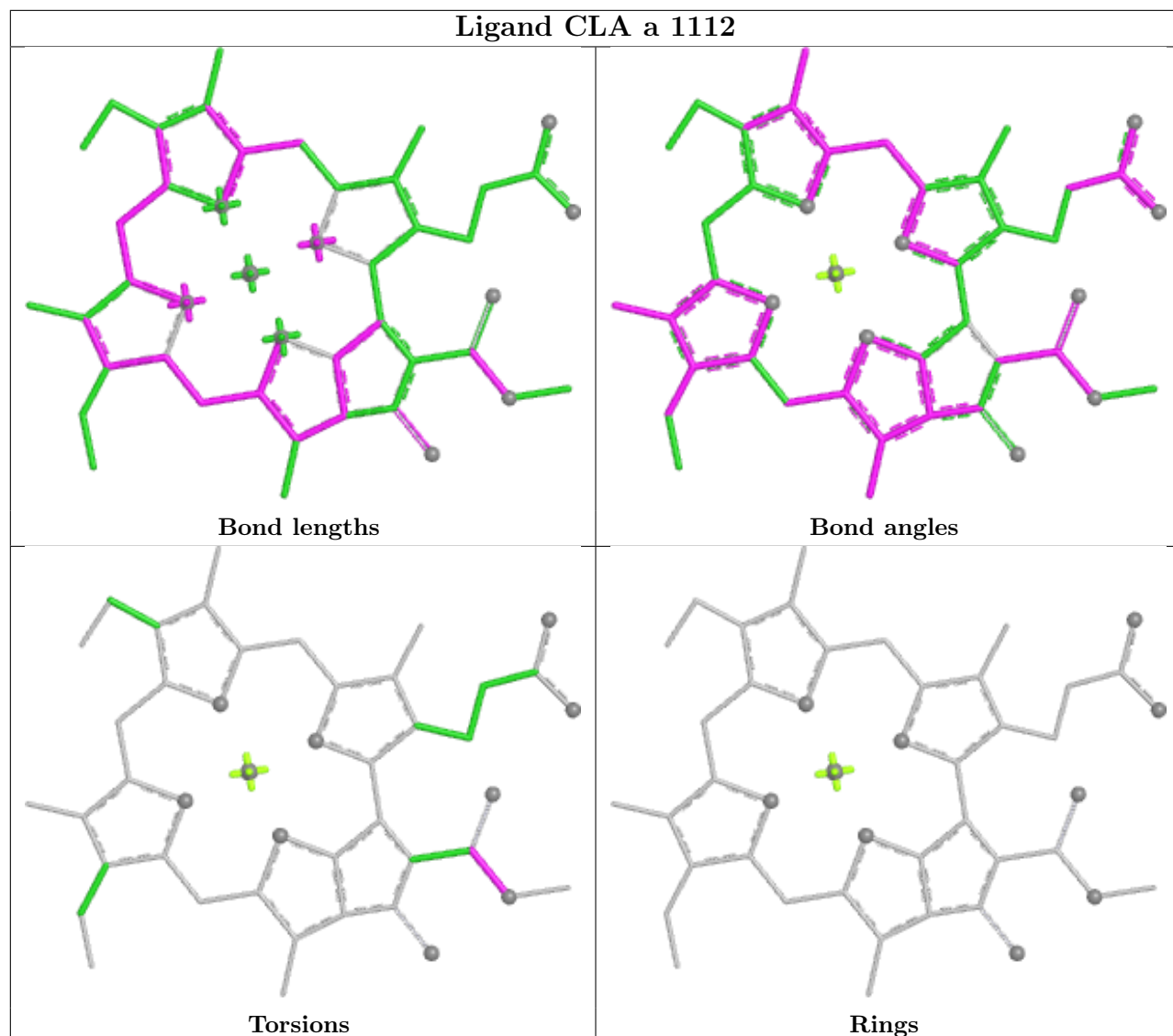
Ligand CLA B 1210	
	
Bond lengths	Bond angles
	
Torsions	Rings

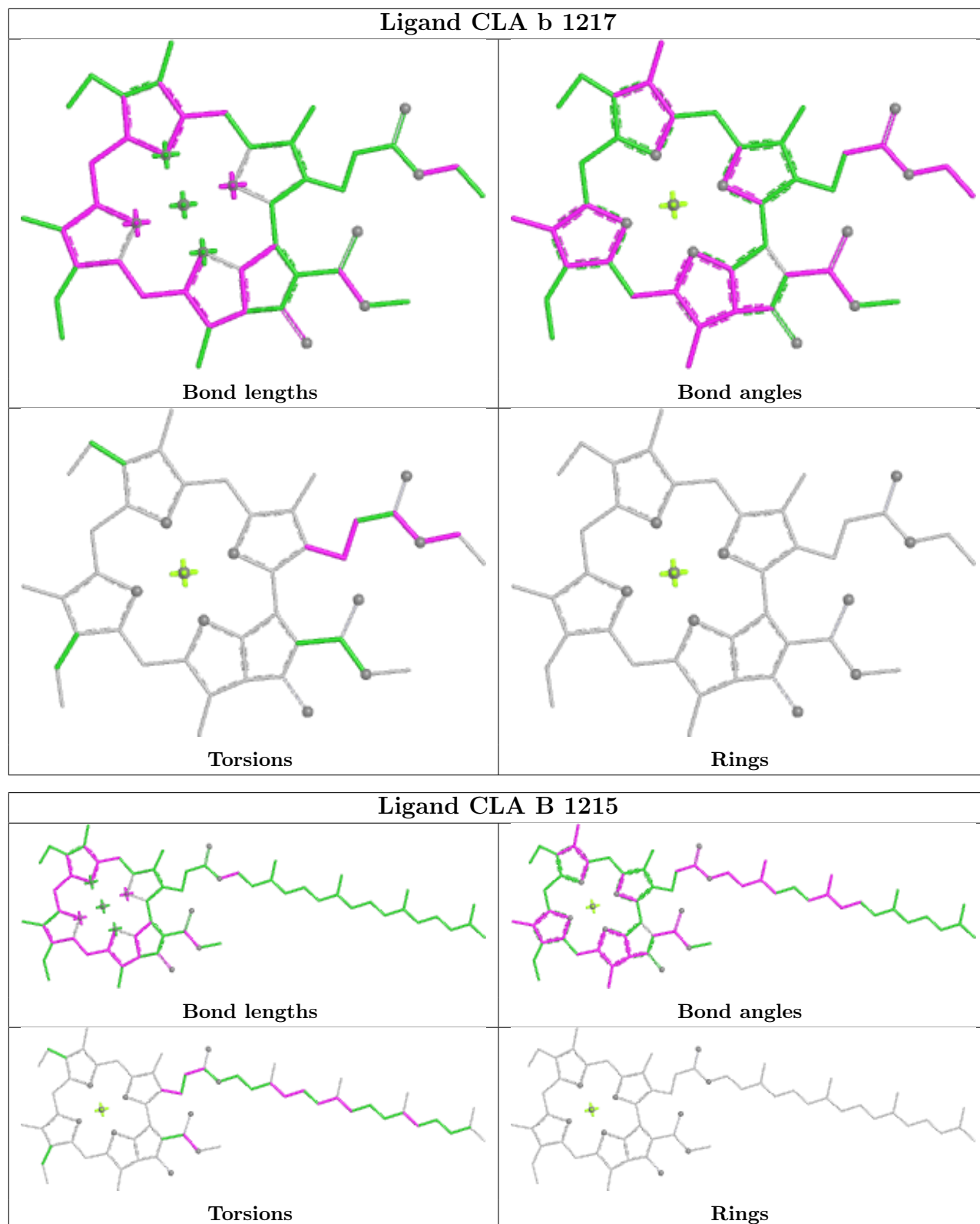


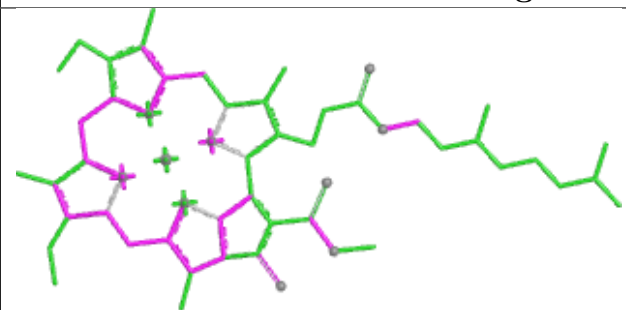
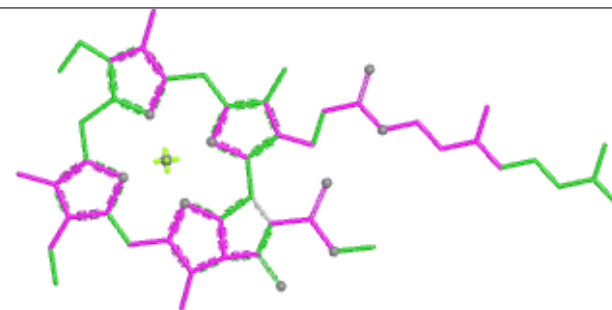
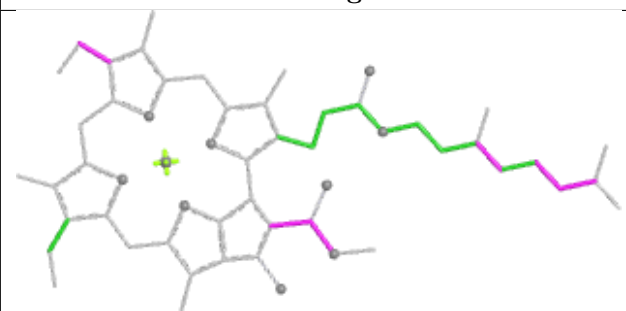
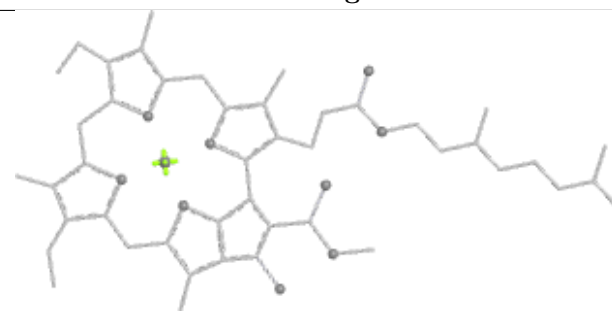


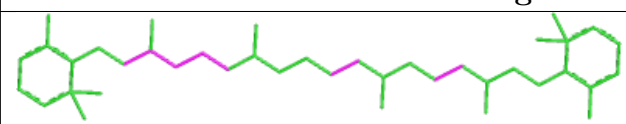
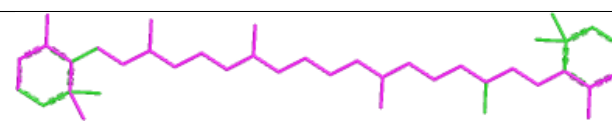
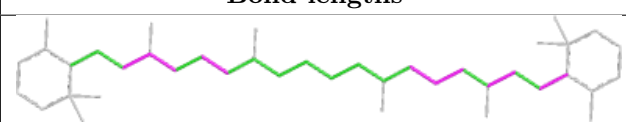
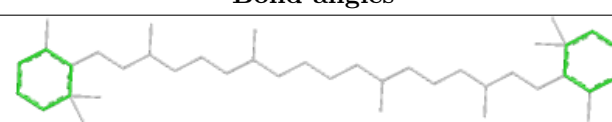


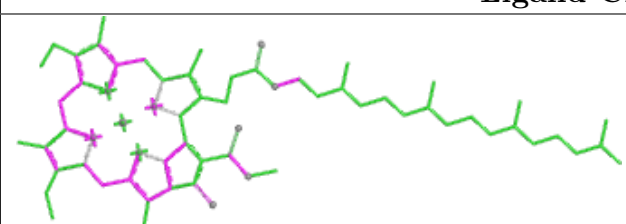
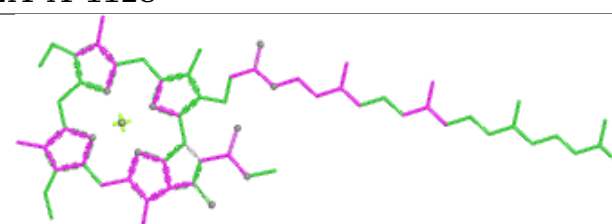
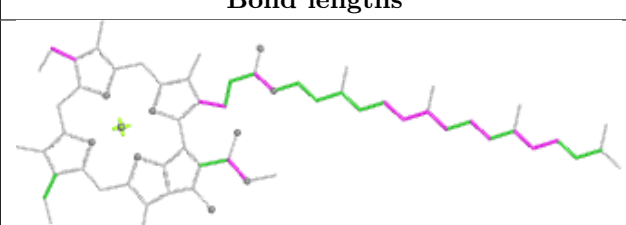
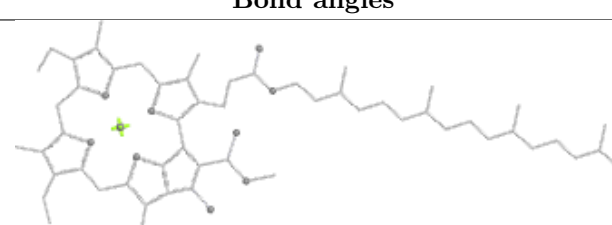
Ligand CLA a 1112

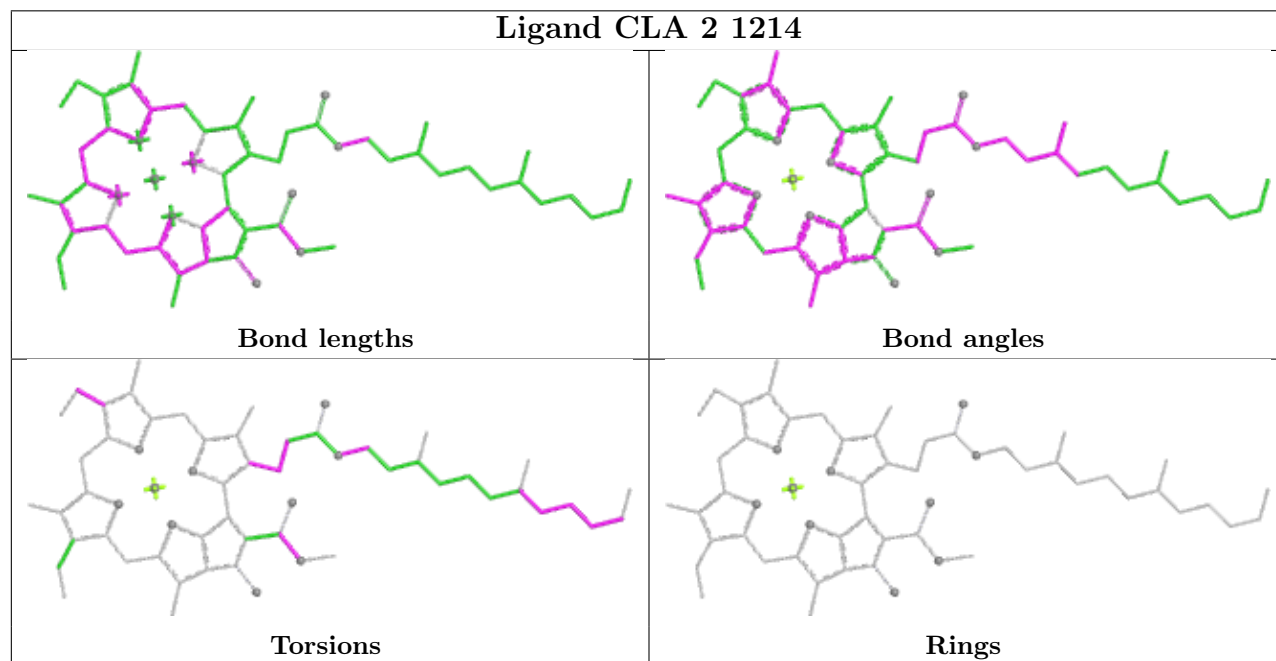
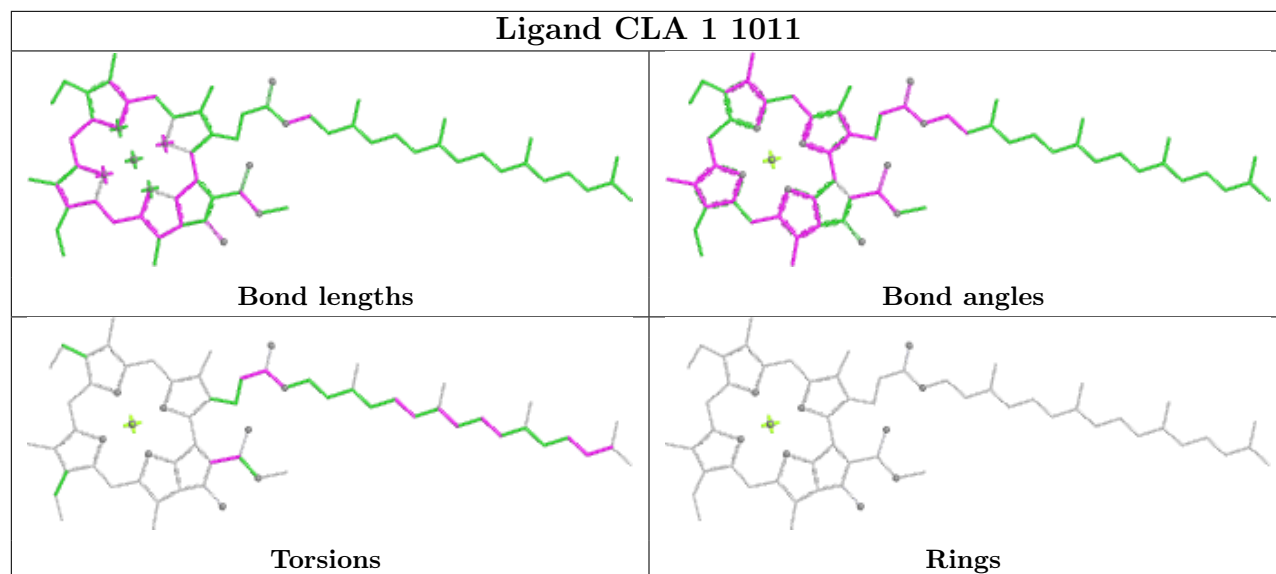




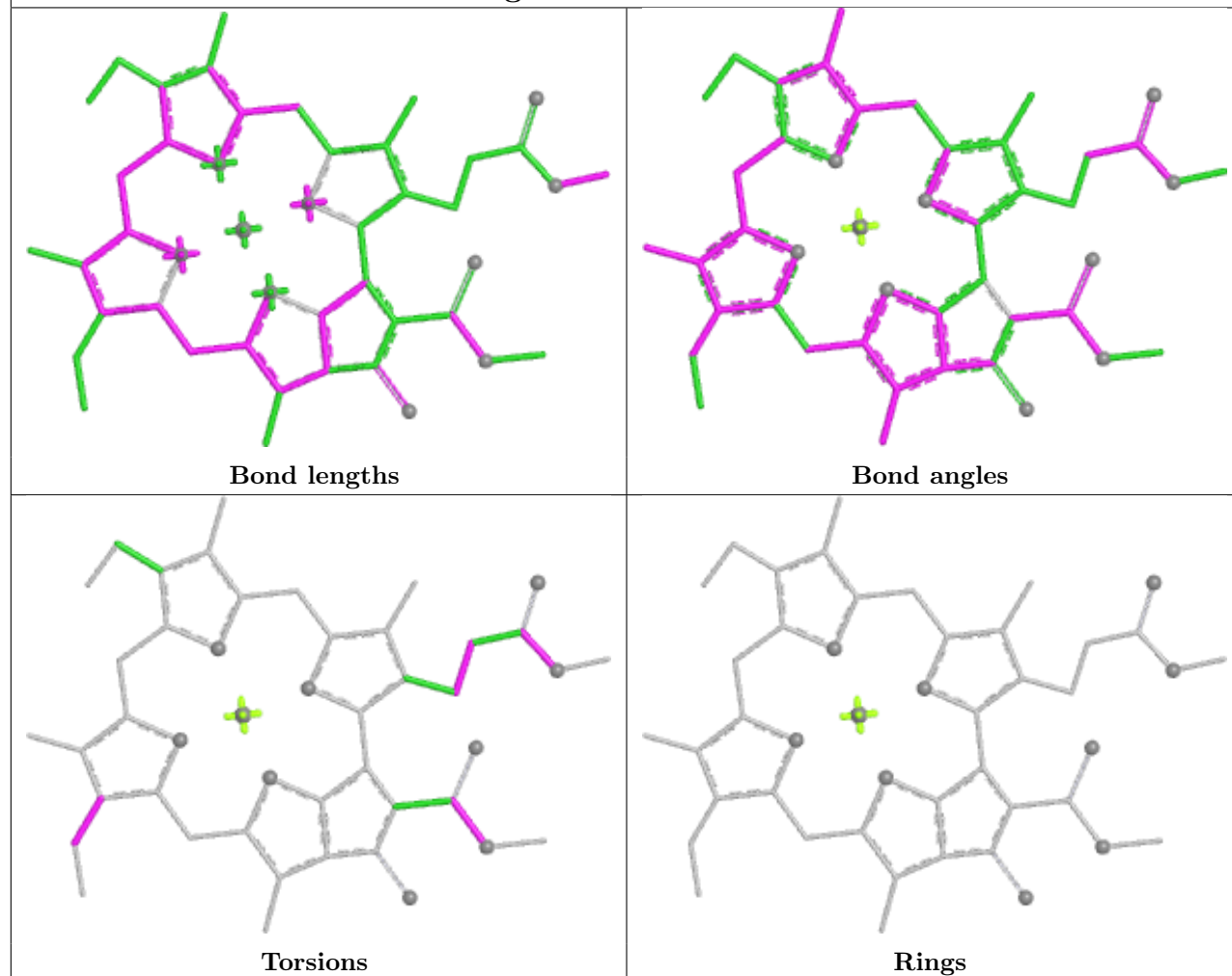
Ligand CLA b 1205	
	
Bond lengths	Bond angles
	
Torsions	Rings

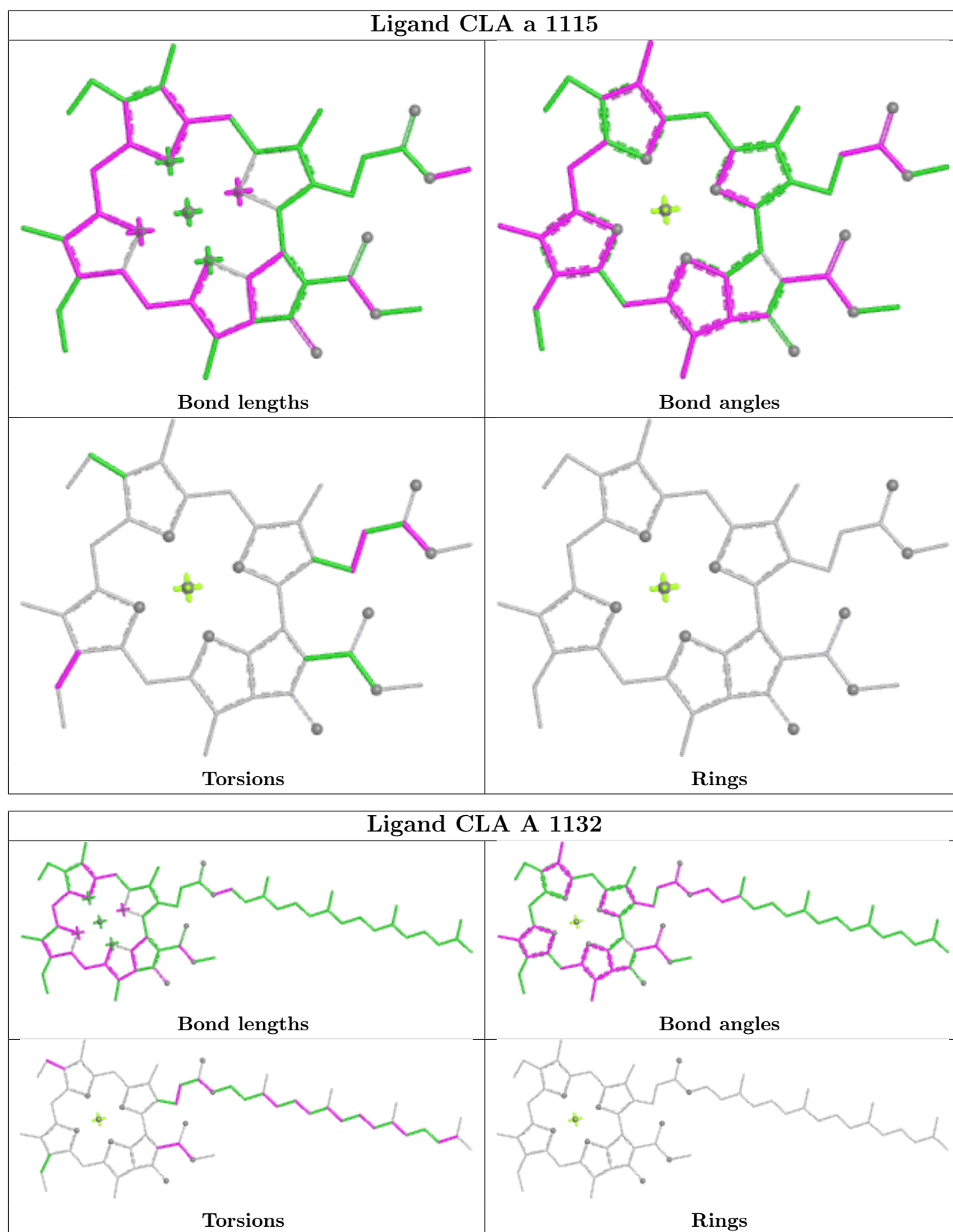
Ligand BCR a 4007	
	
Bond lengths	Bond angles
	
Torsions	Rings

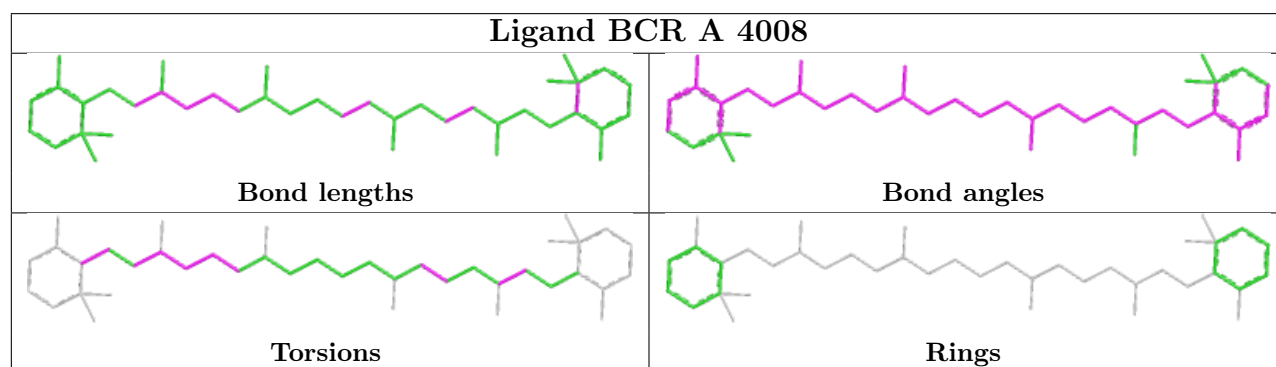
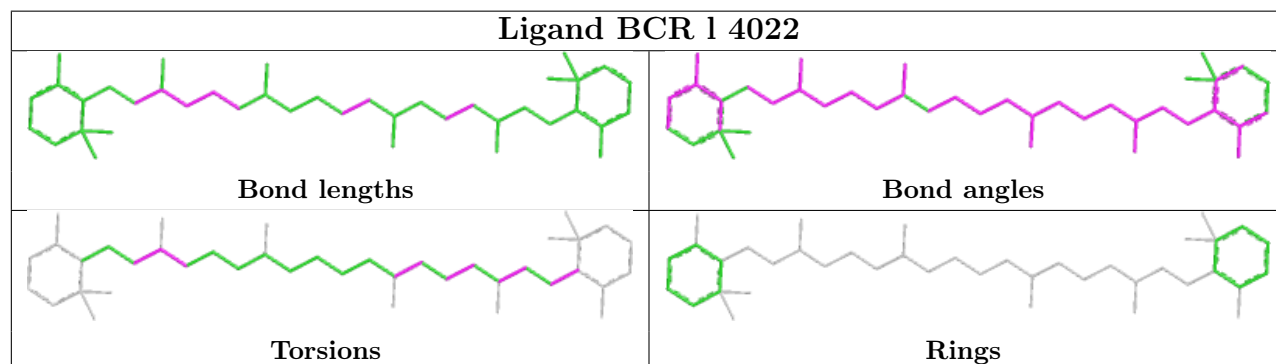
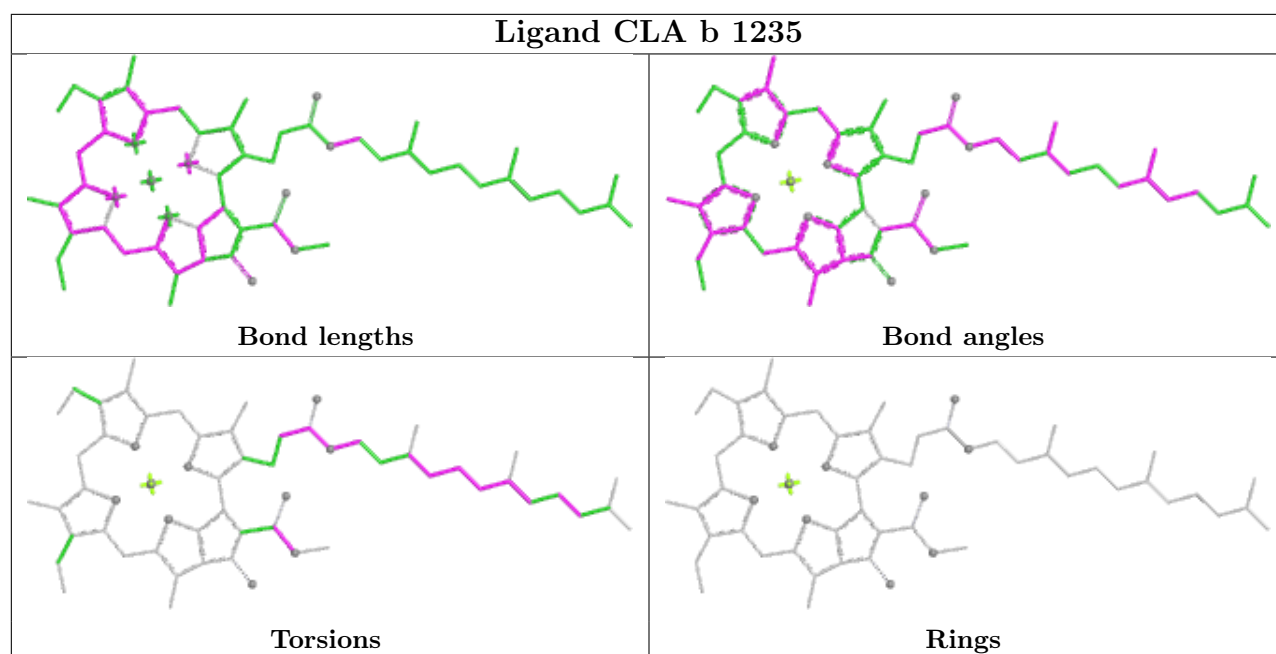
Ligand CLA A 1128	
	
Bond lengths	Bond angles
	
Torsions	Rings

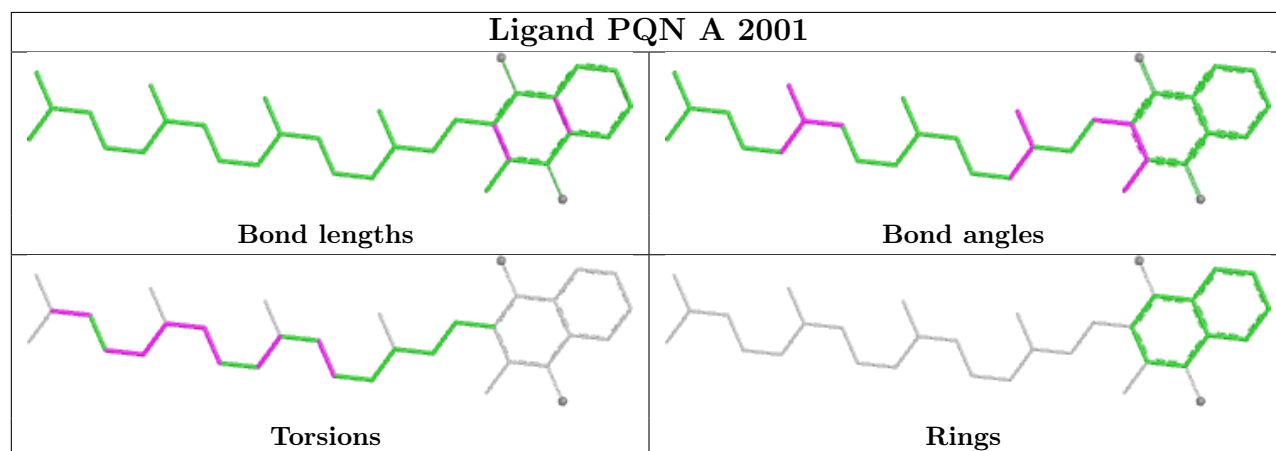
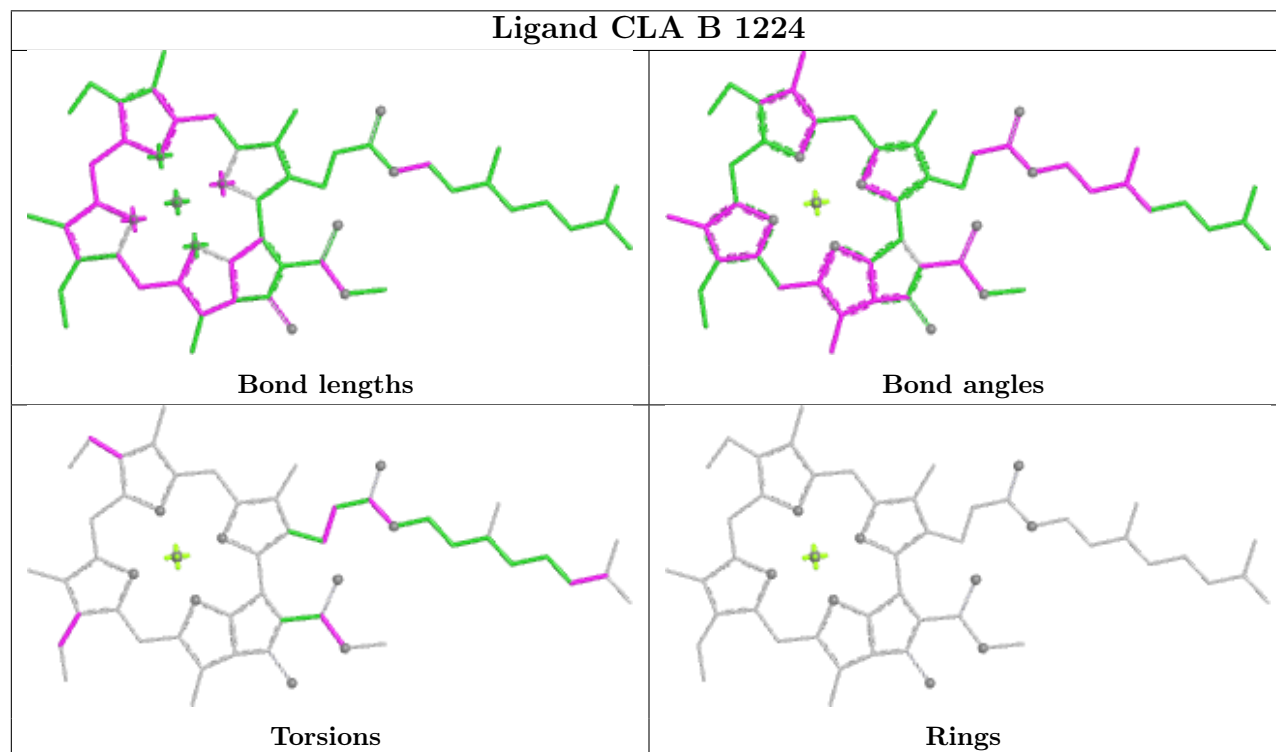
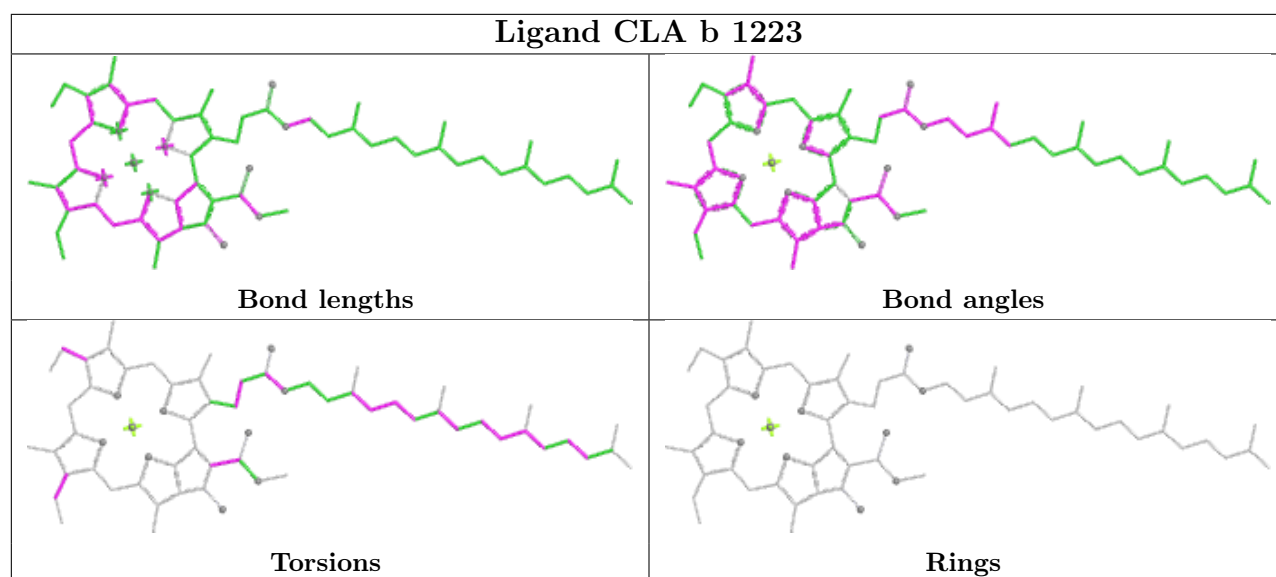


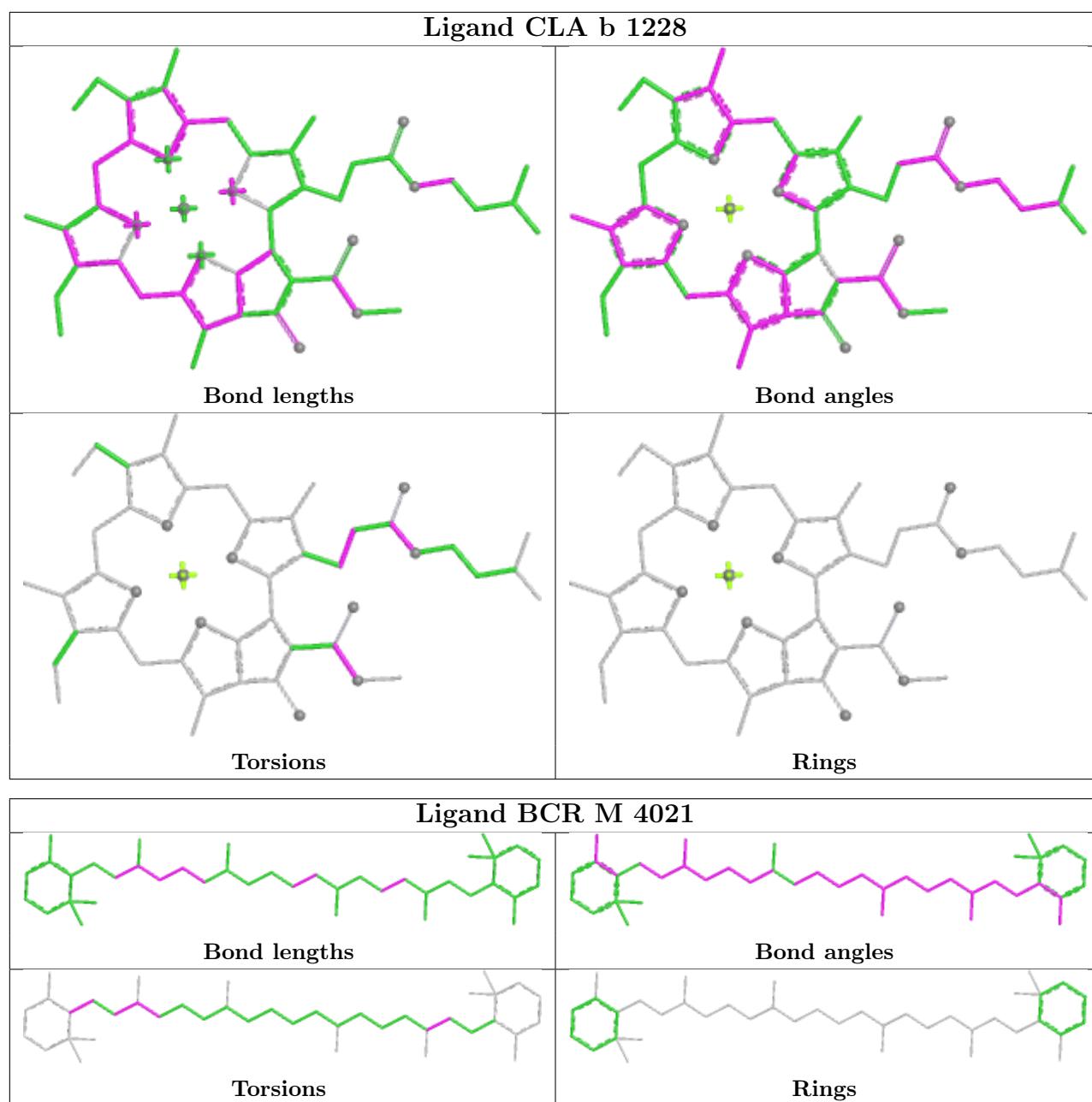
Ligand CLA A 1115

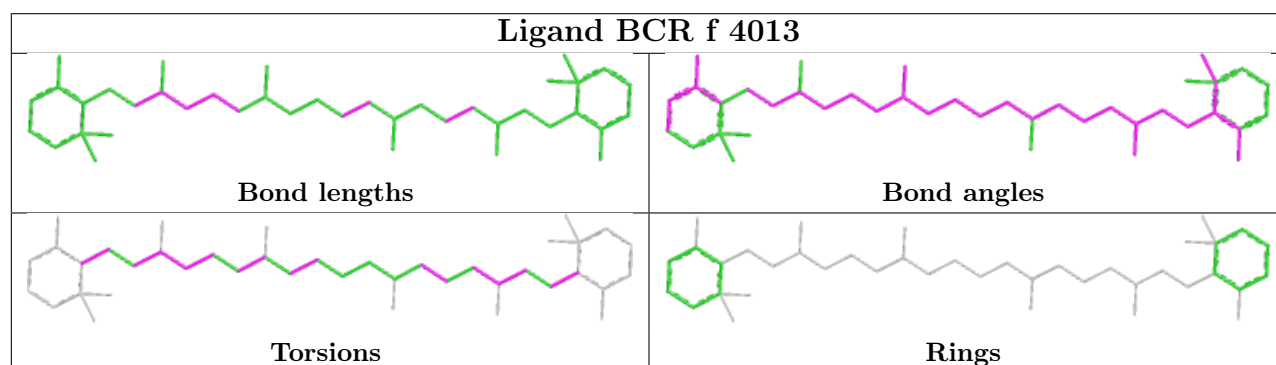
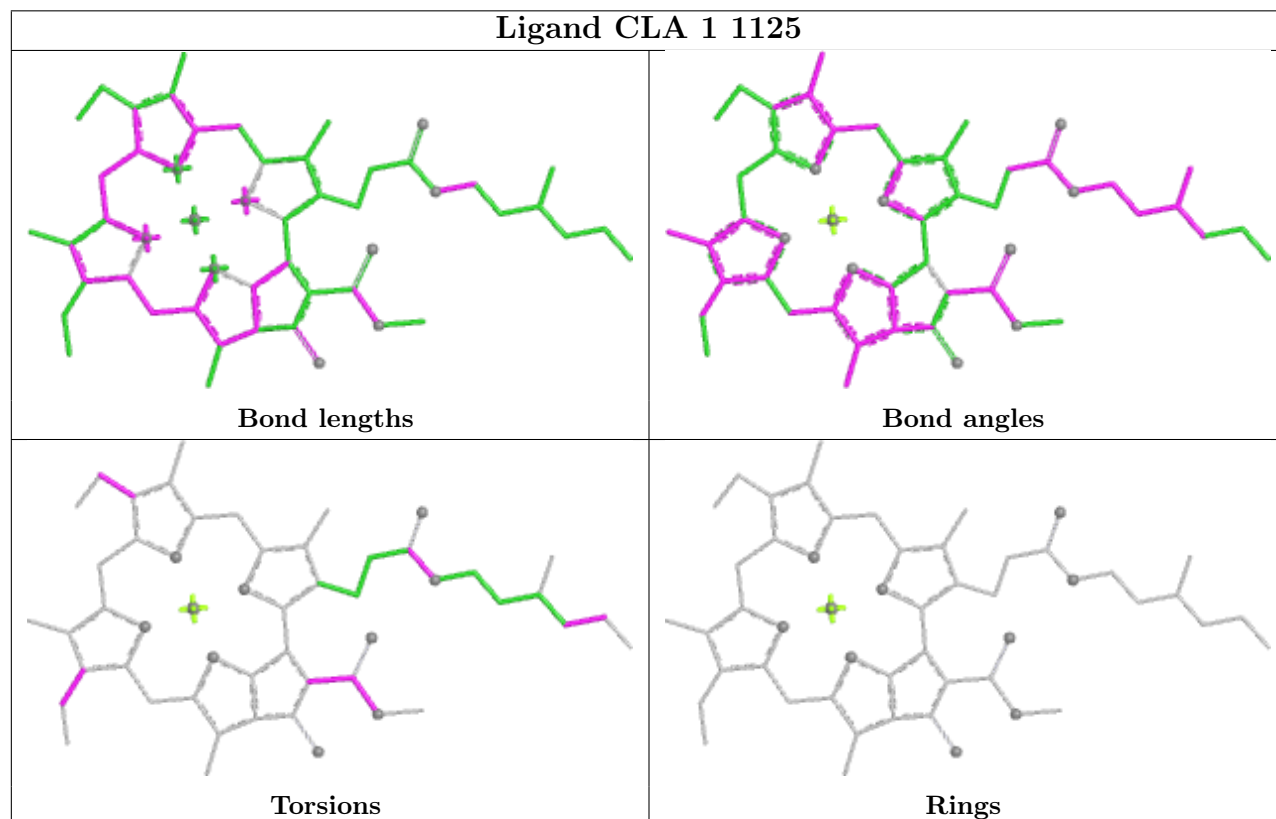
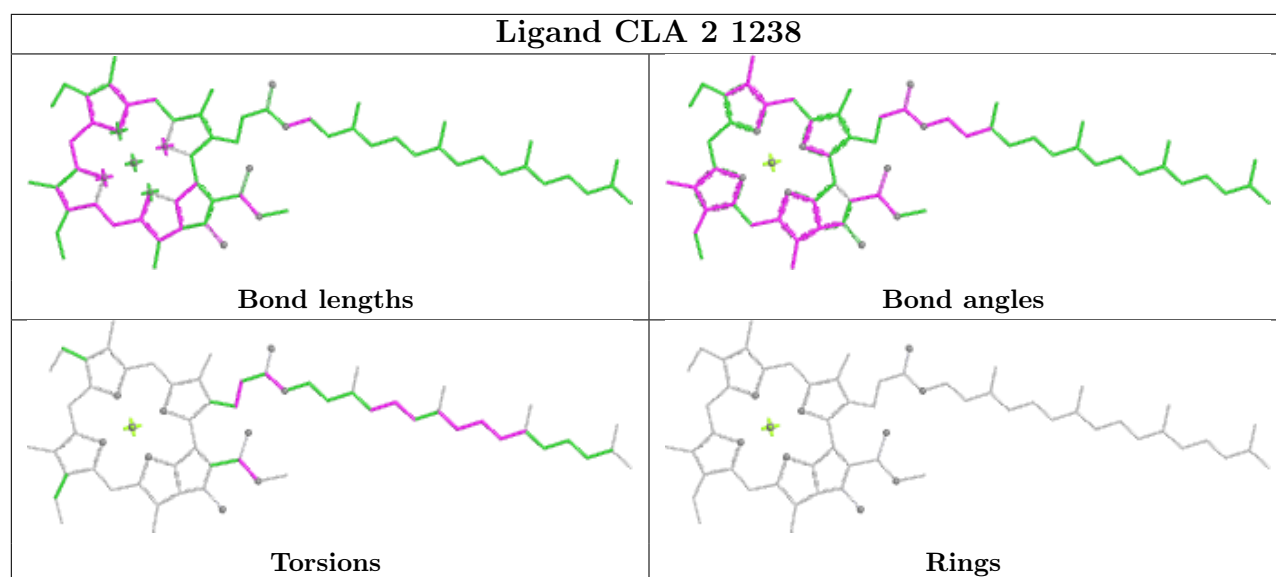


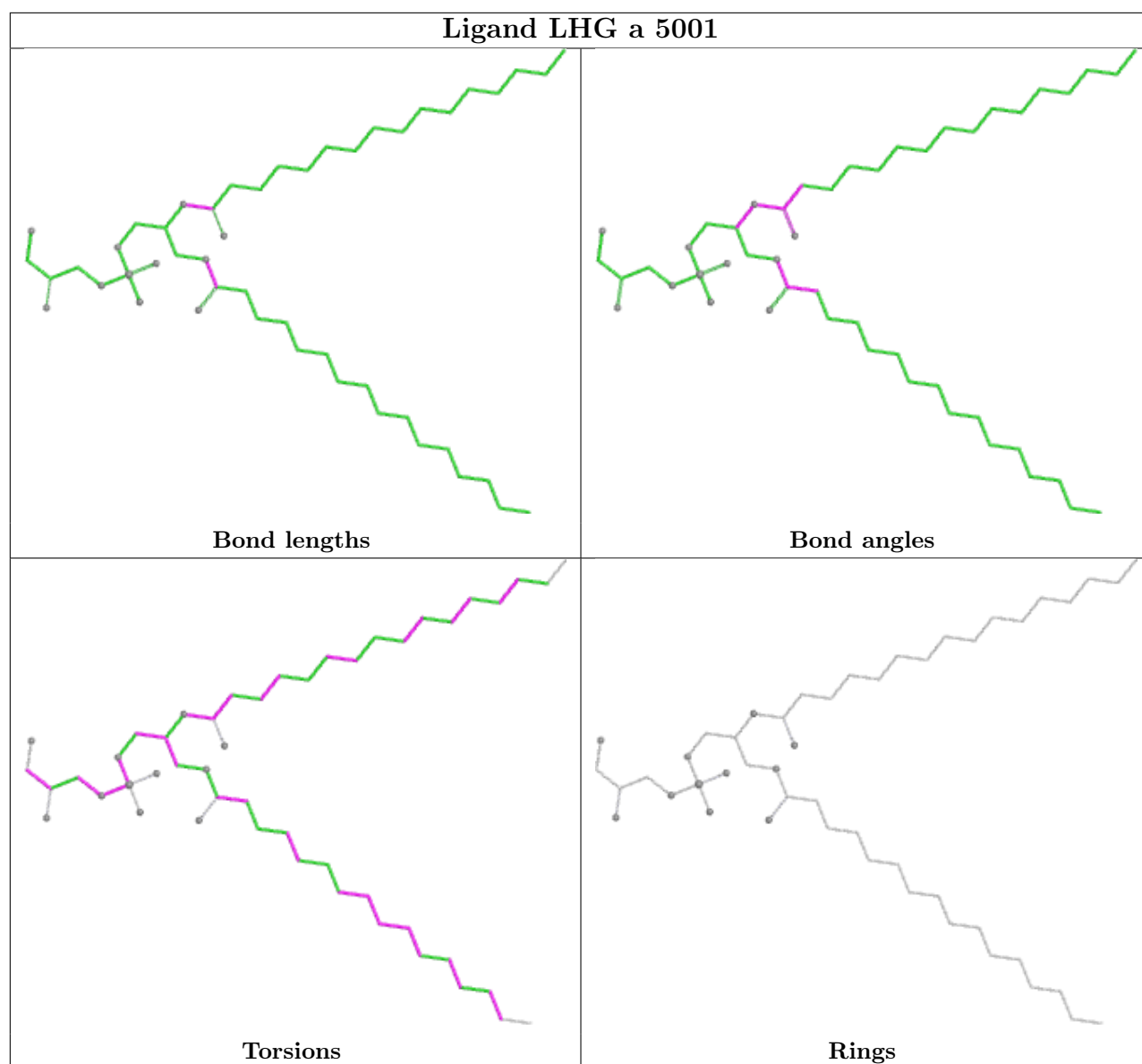


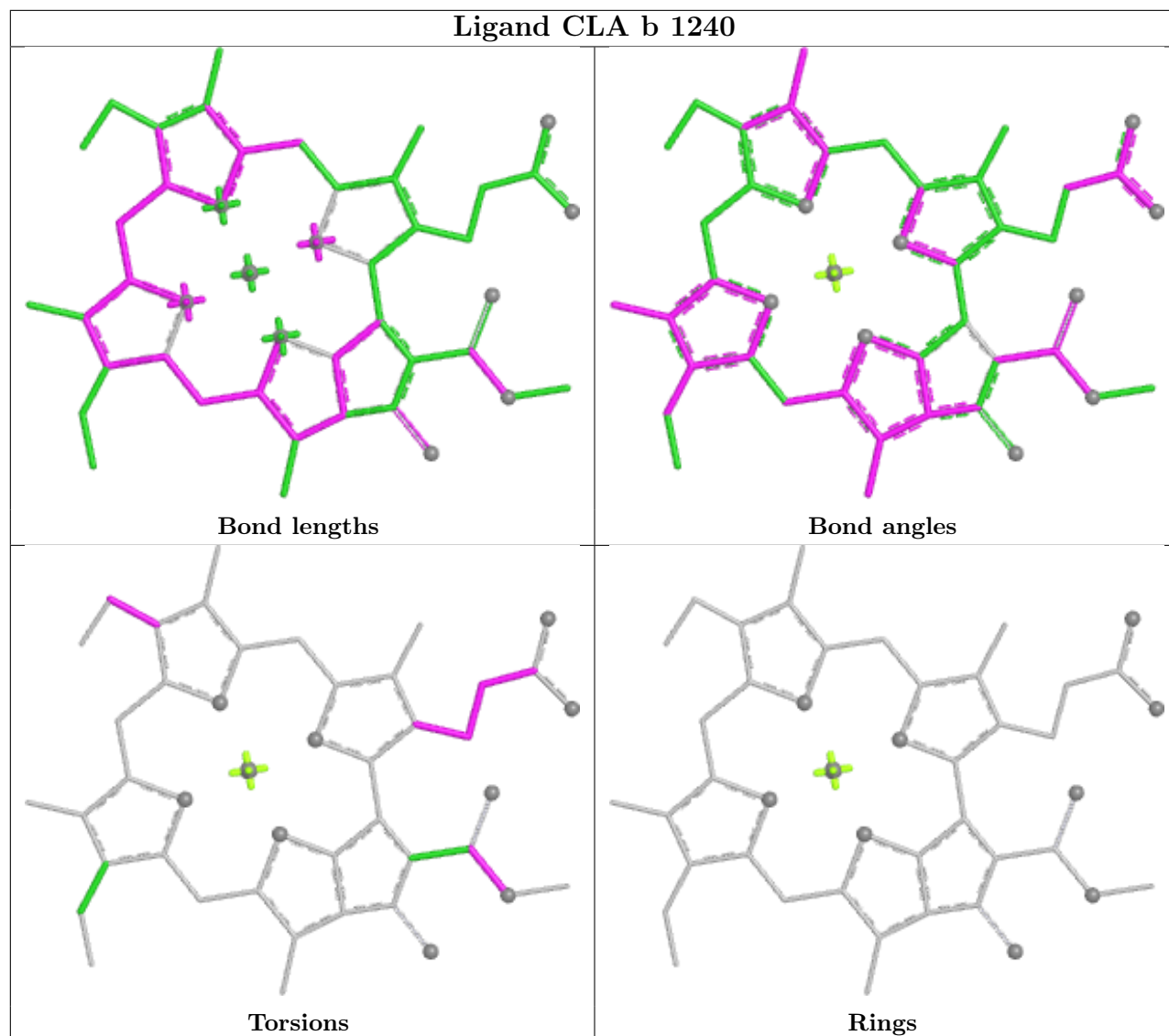




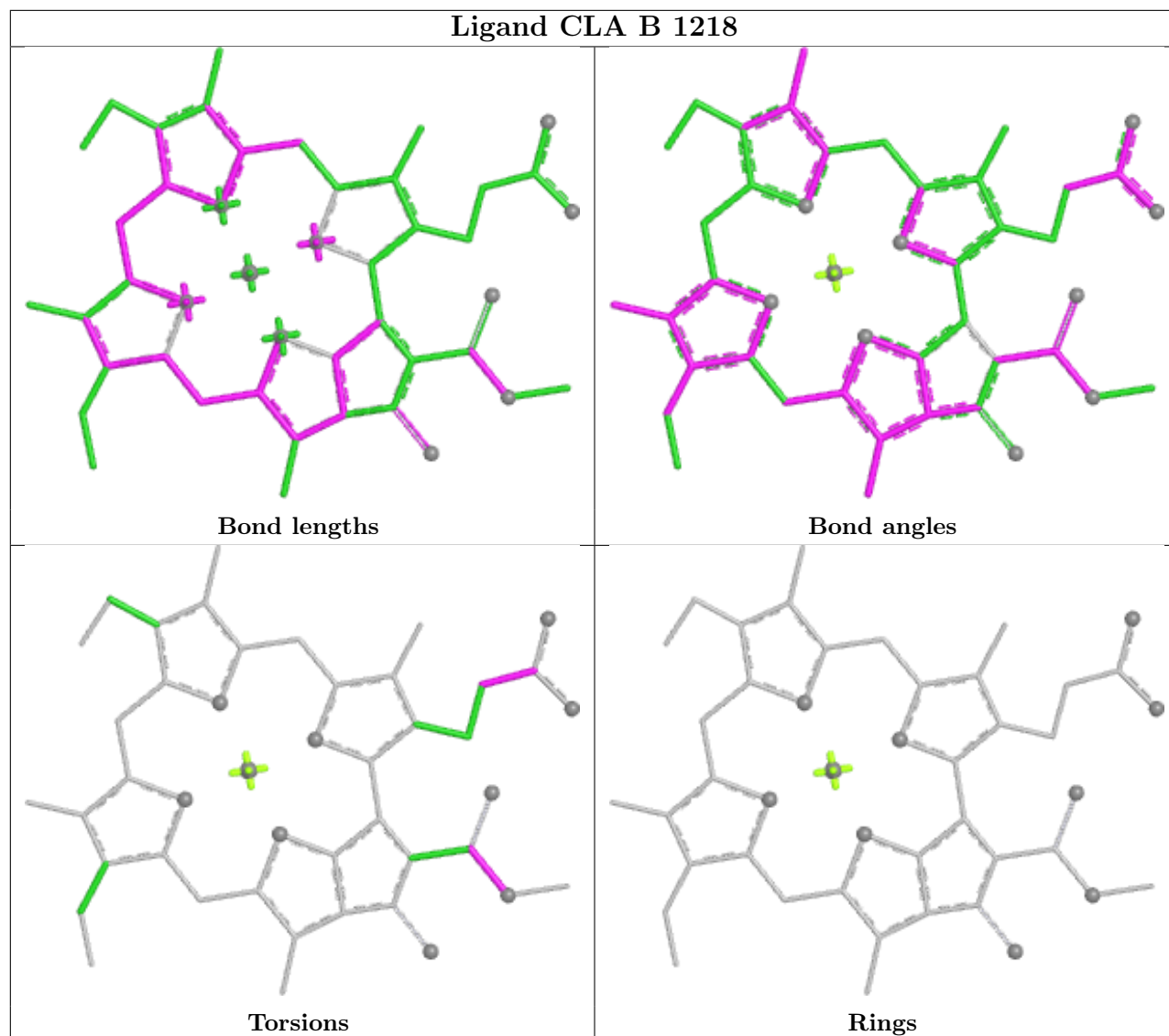




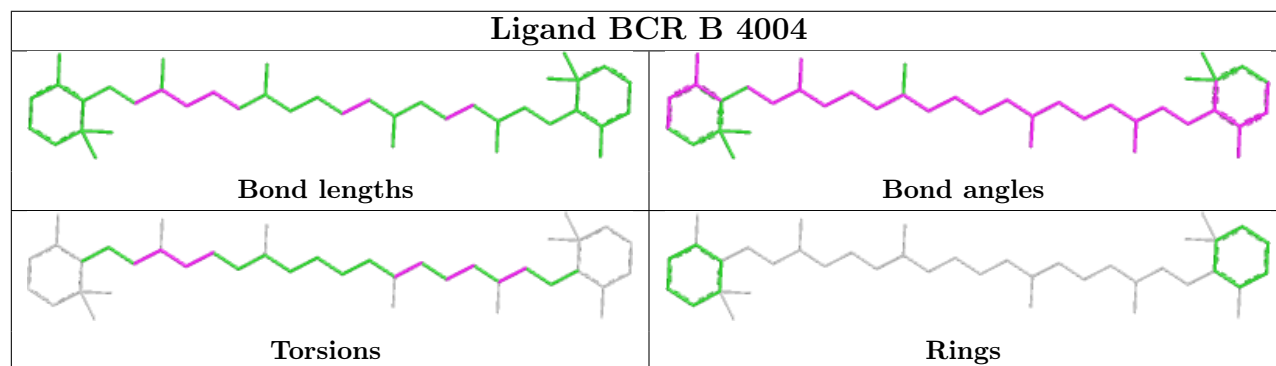


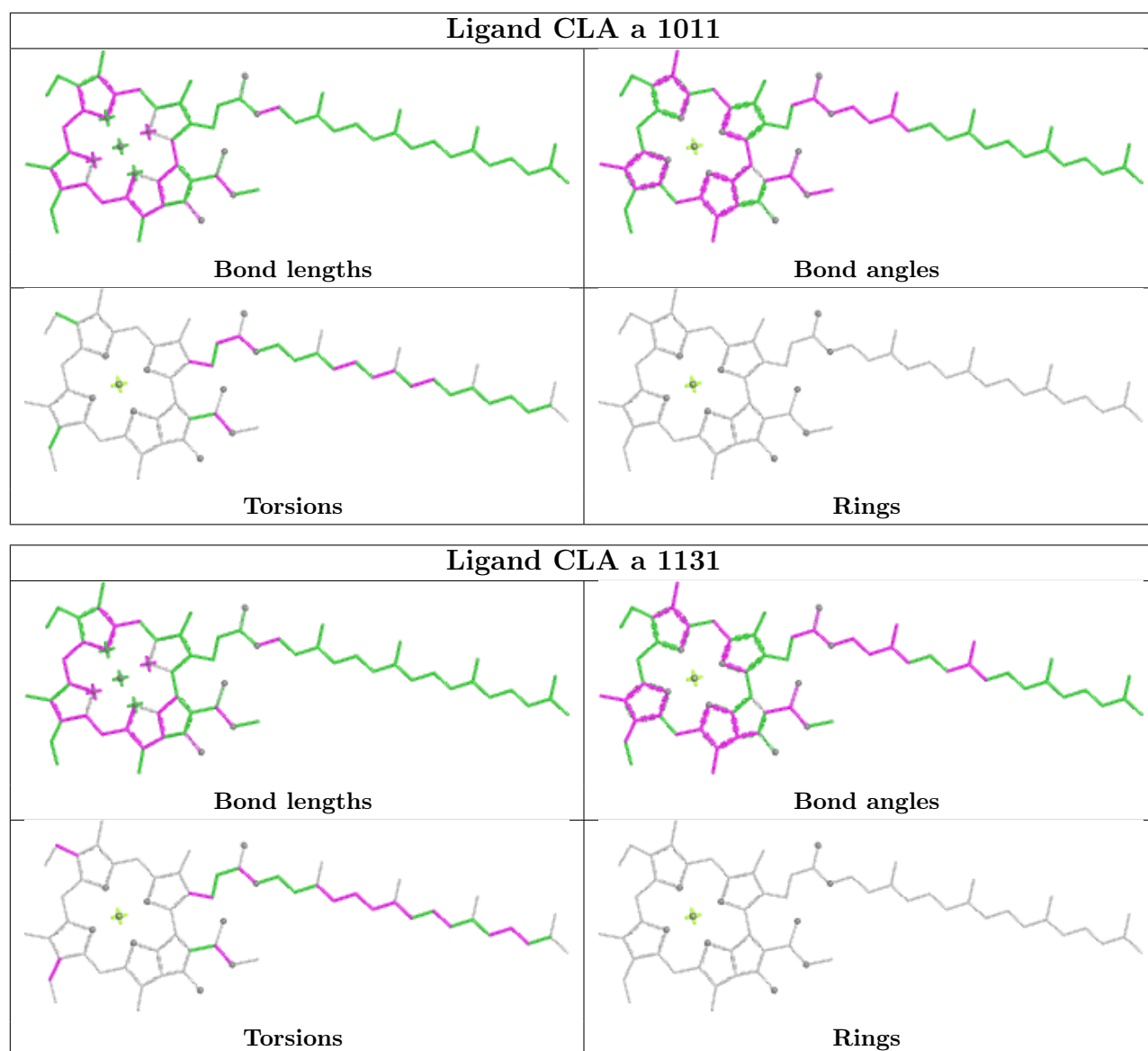


Ligand CLA B 1218

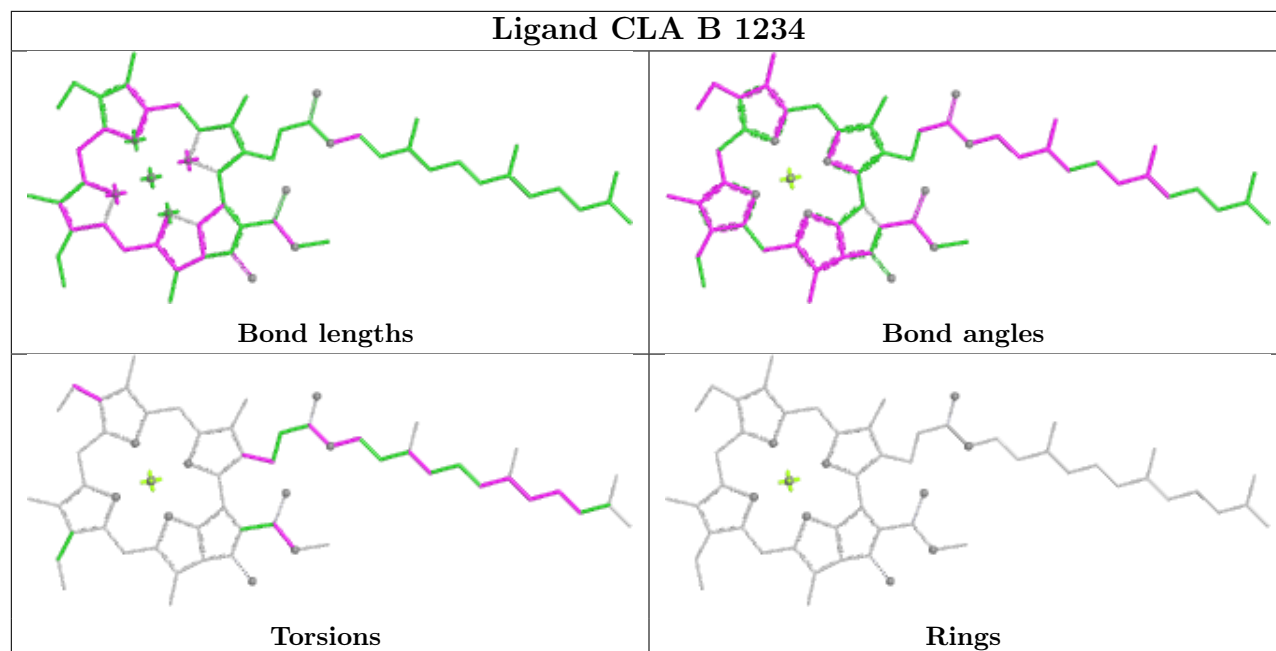


Ligand BCR B 4004

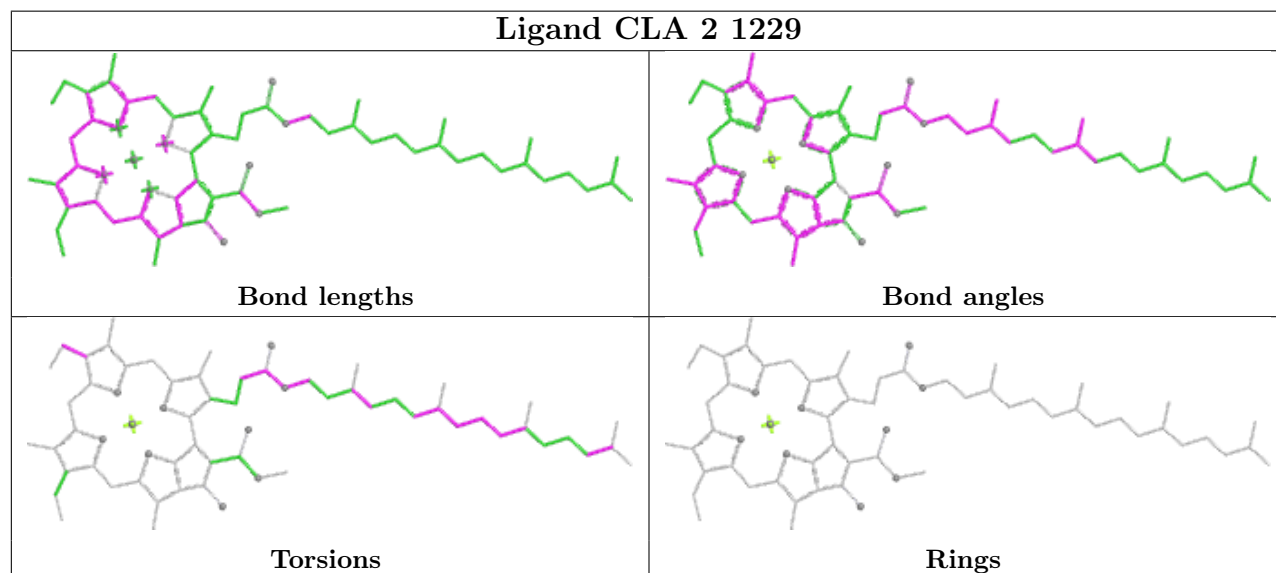


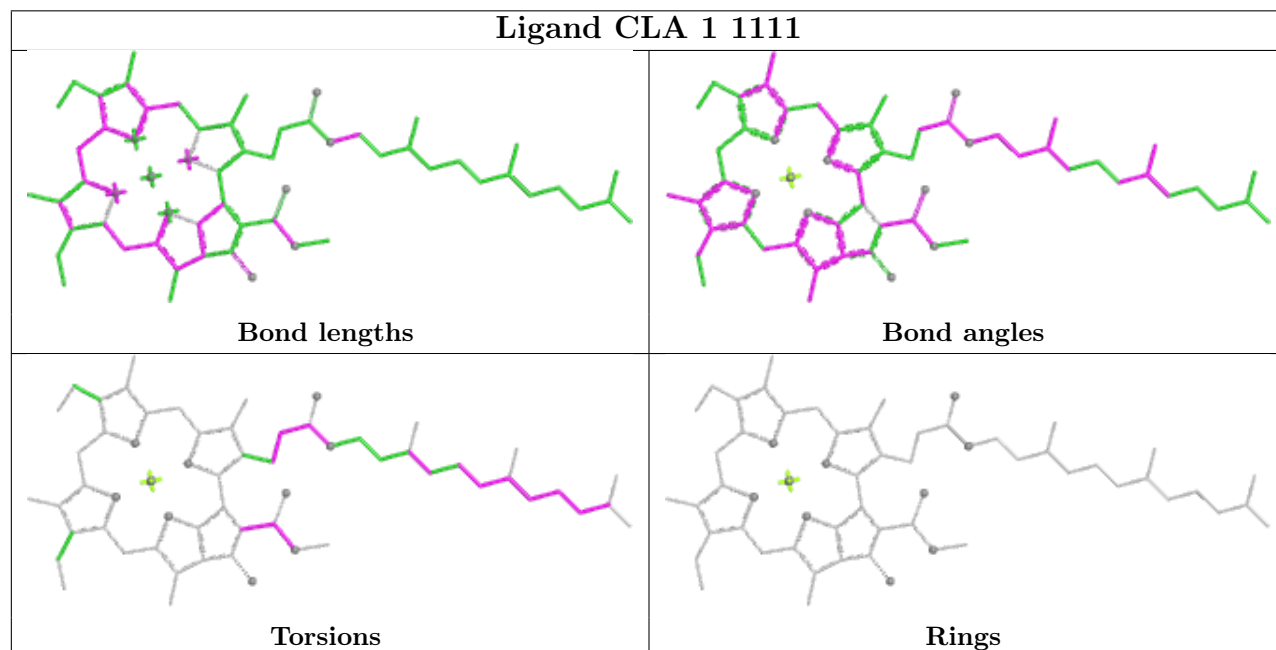
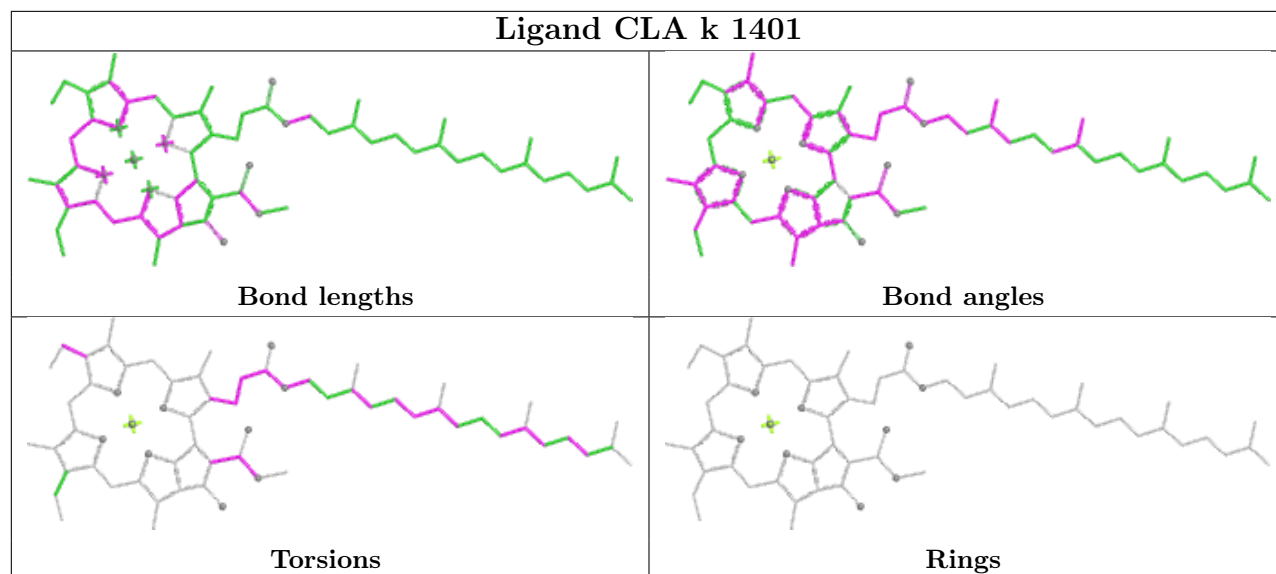


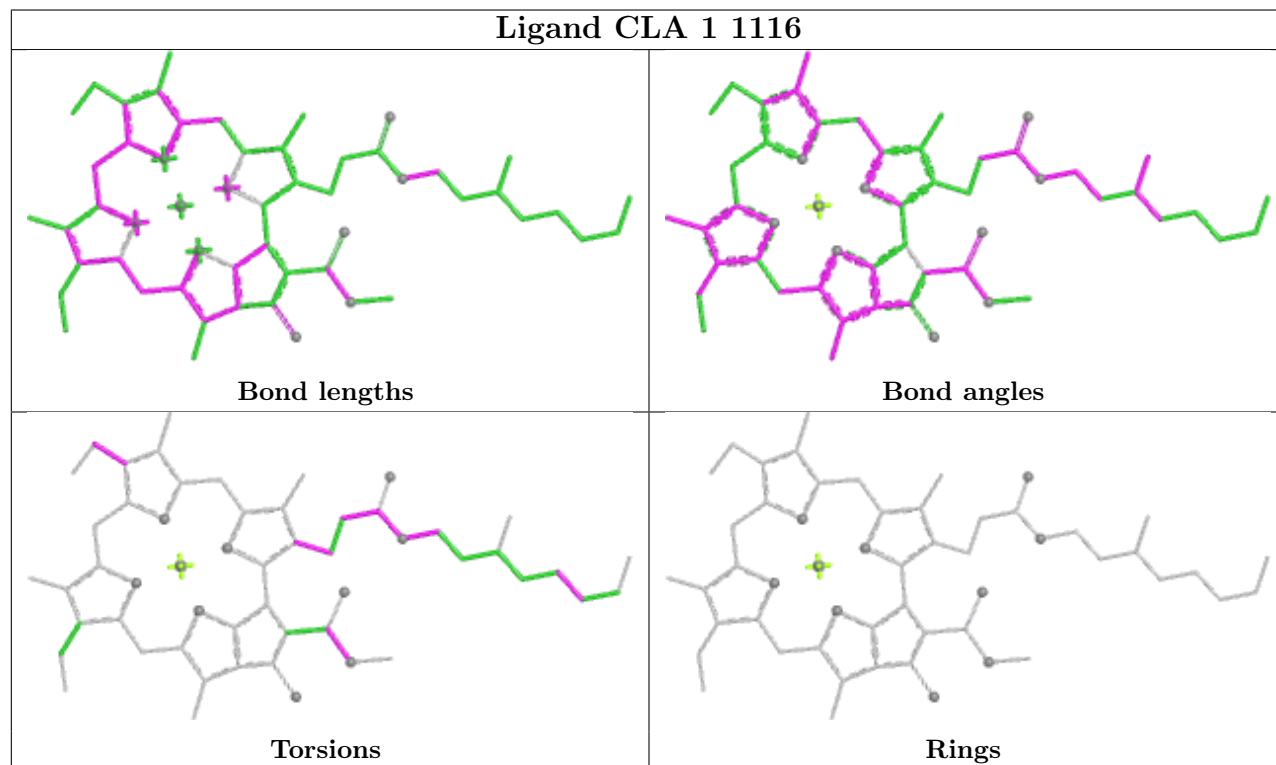
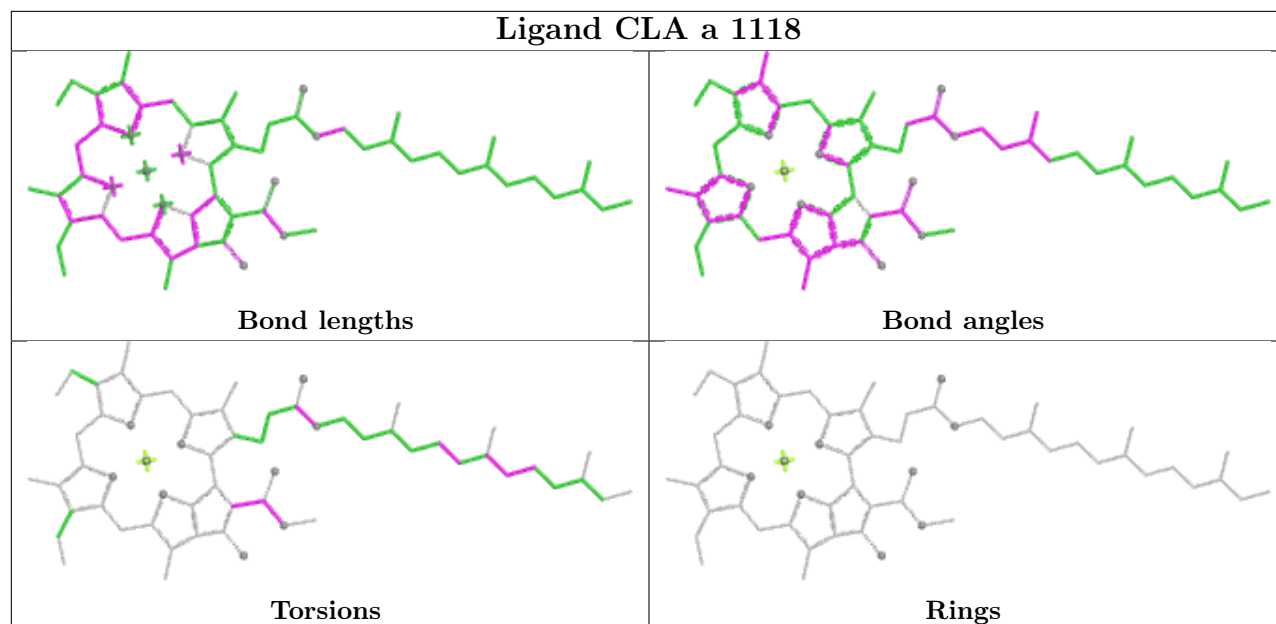
Ligand CLA B 1234

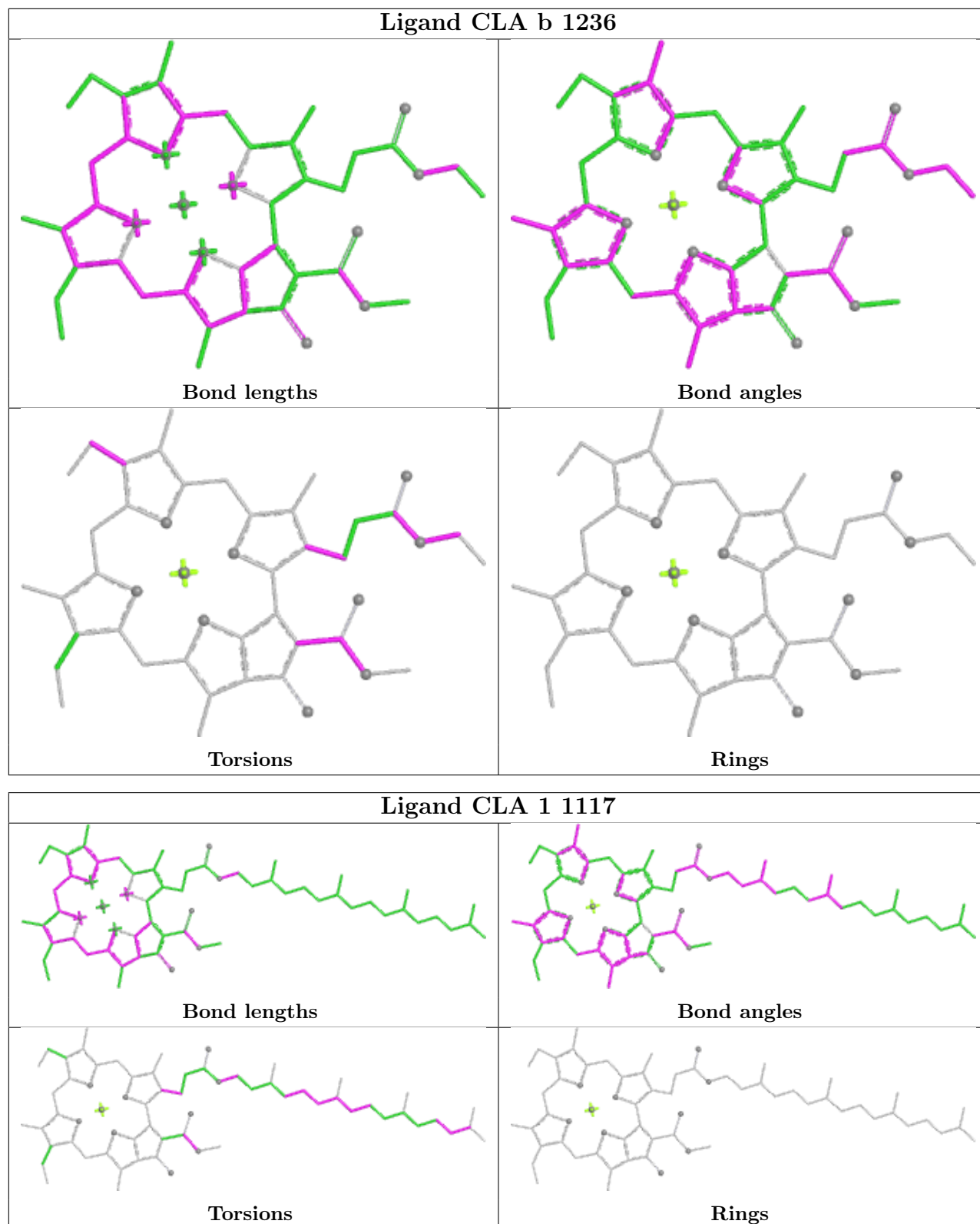


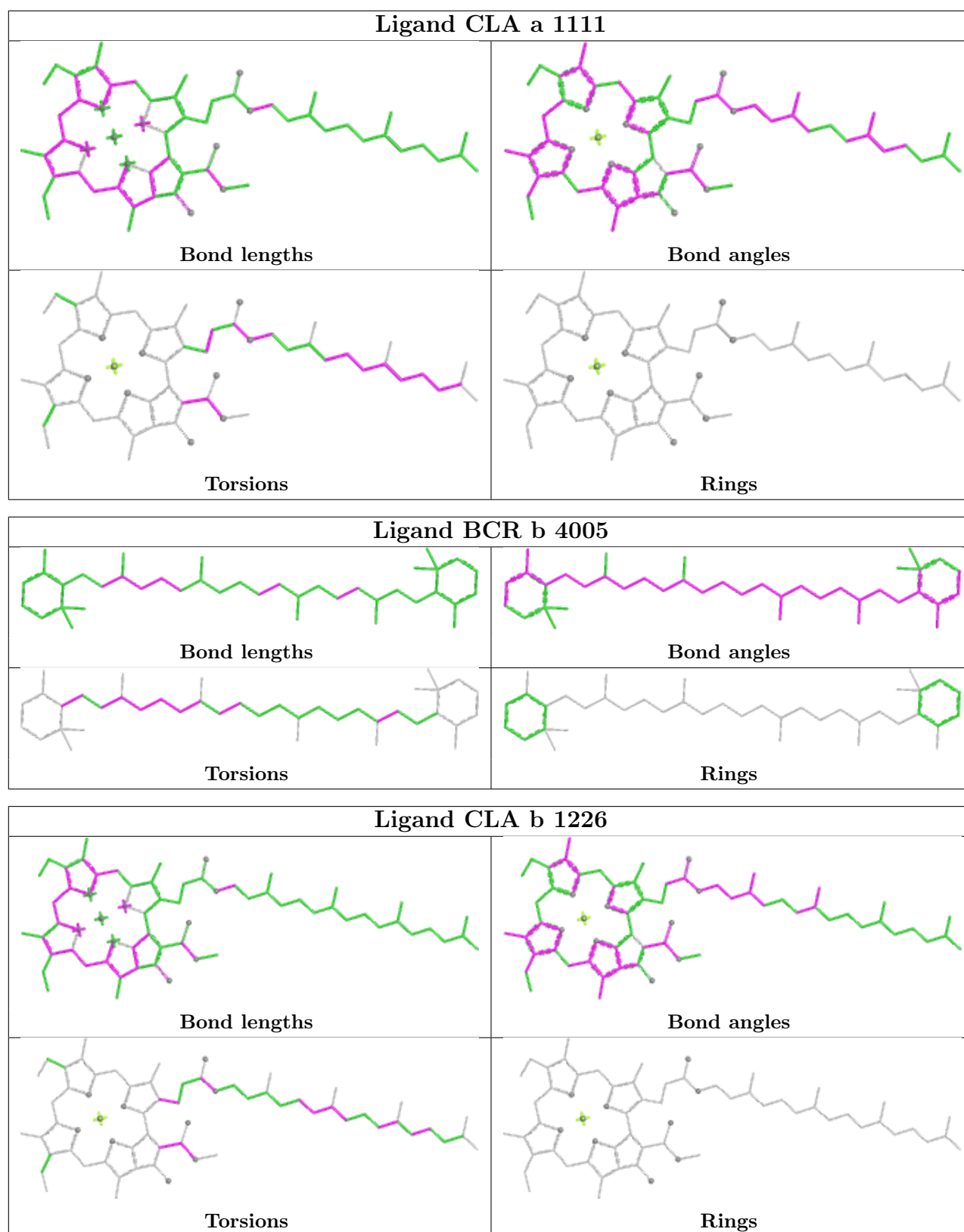
Ligand CLA 2 1229



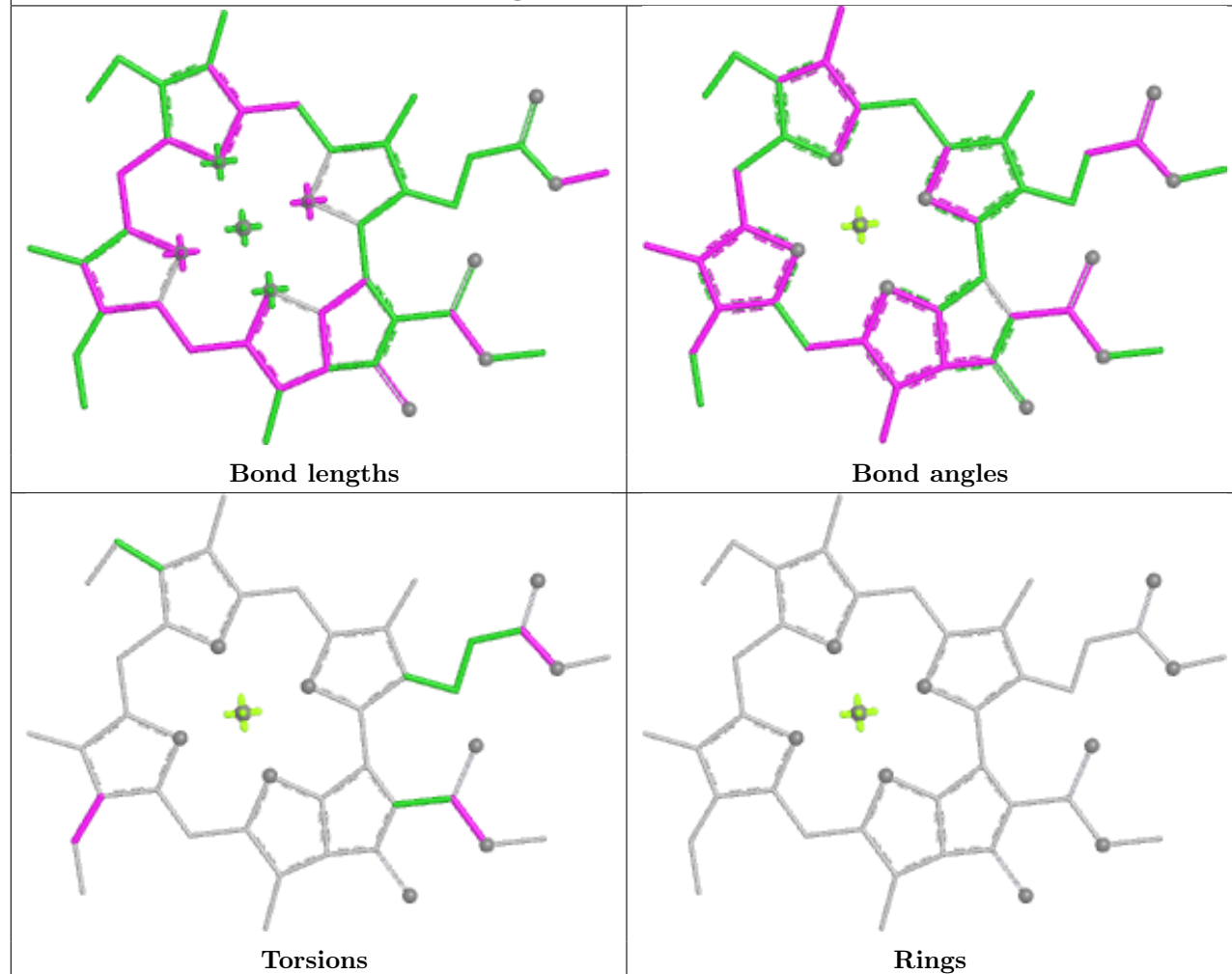


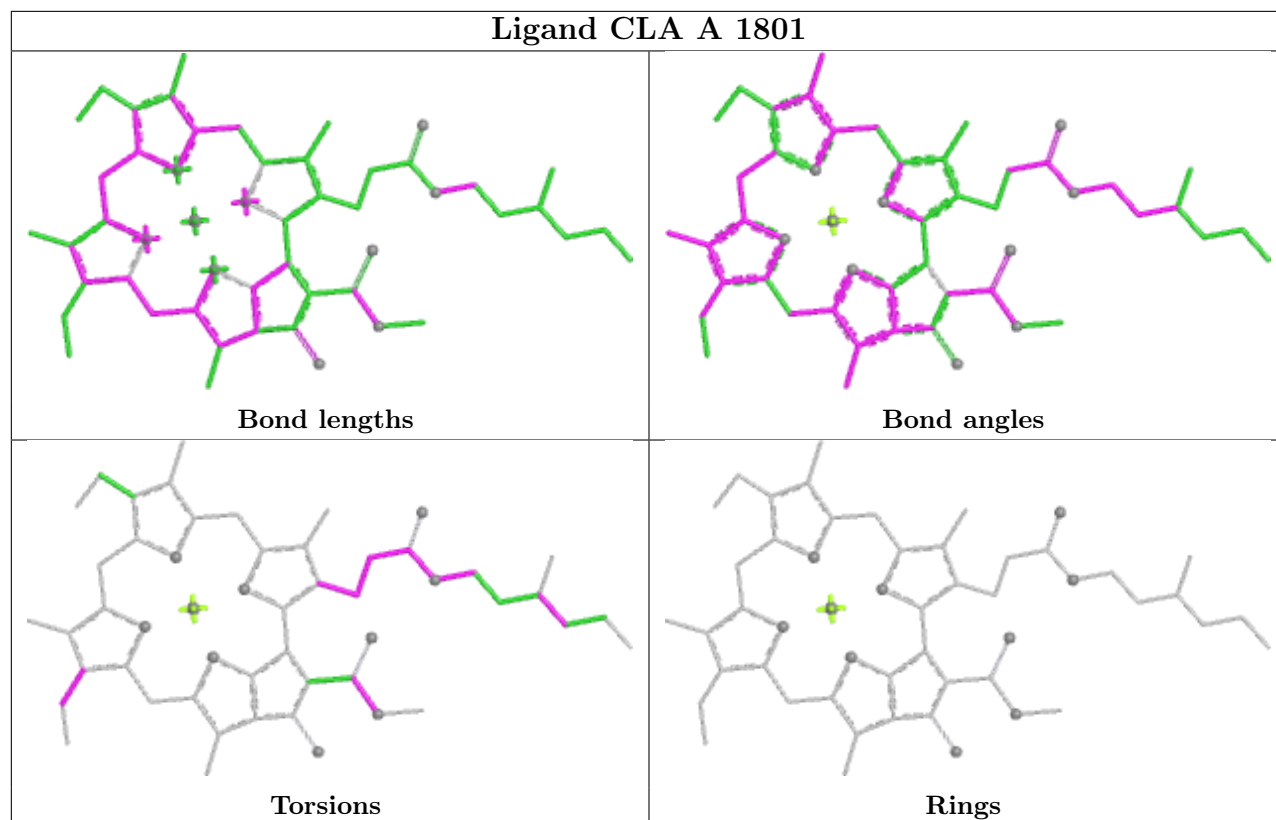




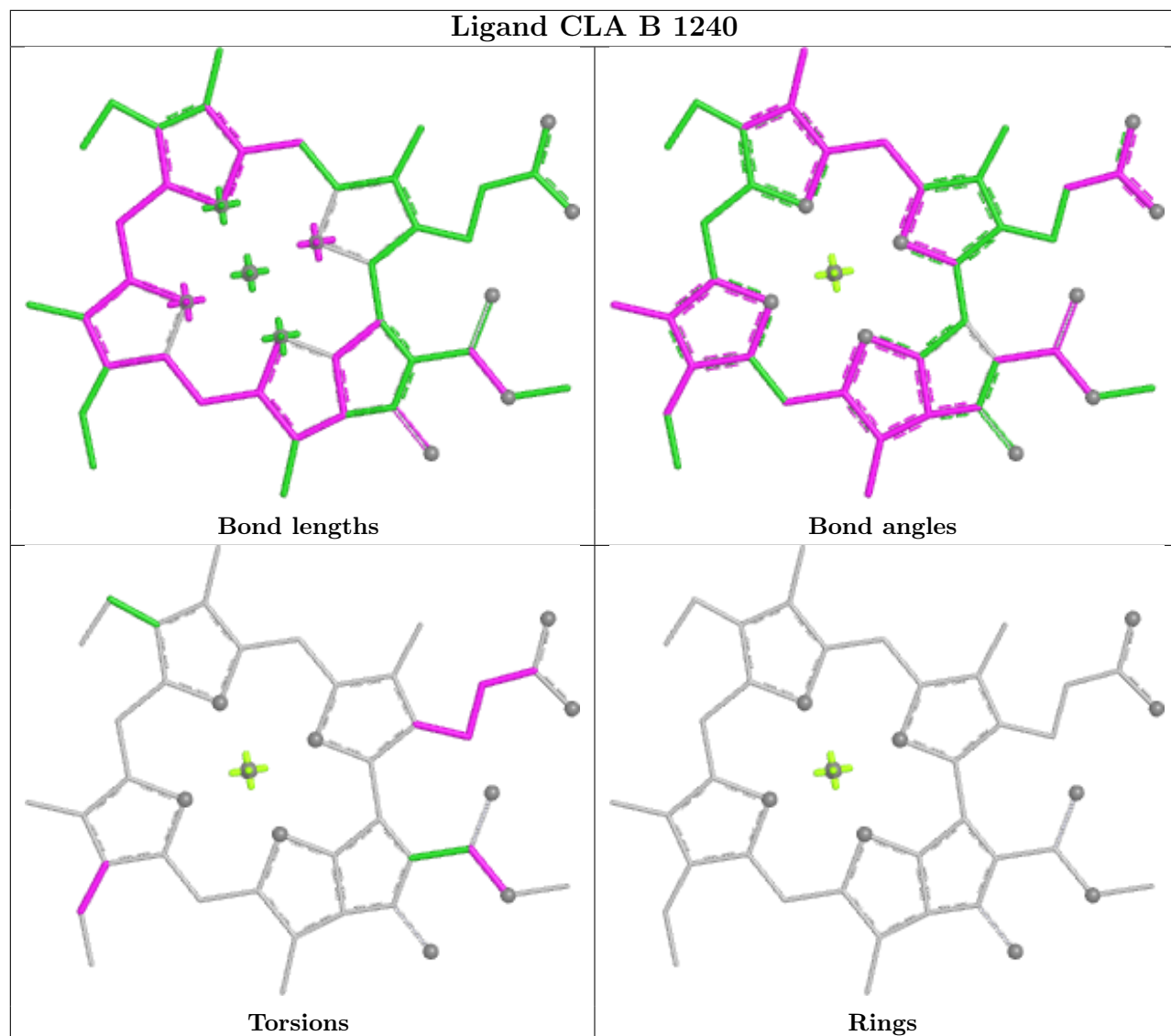


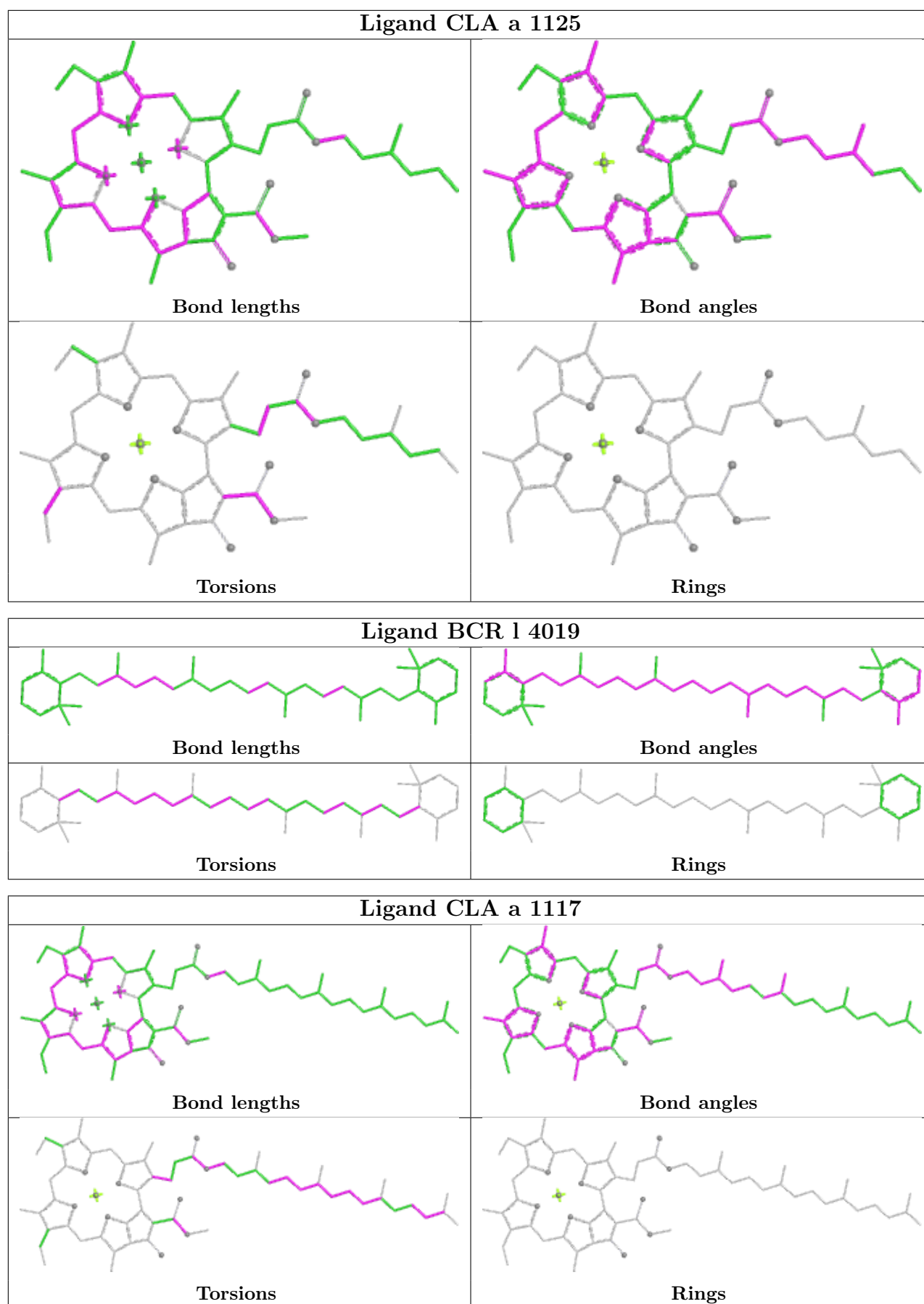
Ligand CLA 1 1133



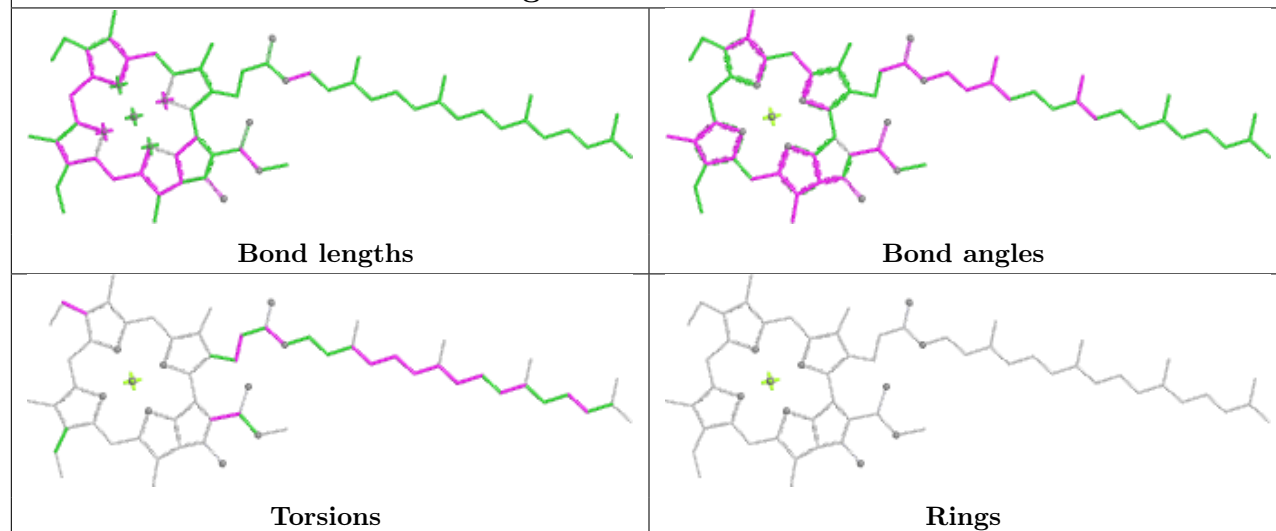


Ligand CLA B 1240

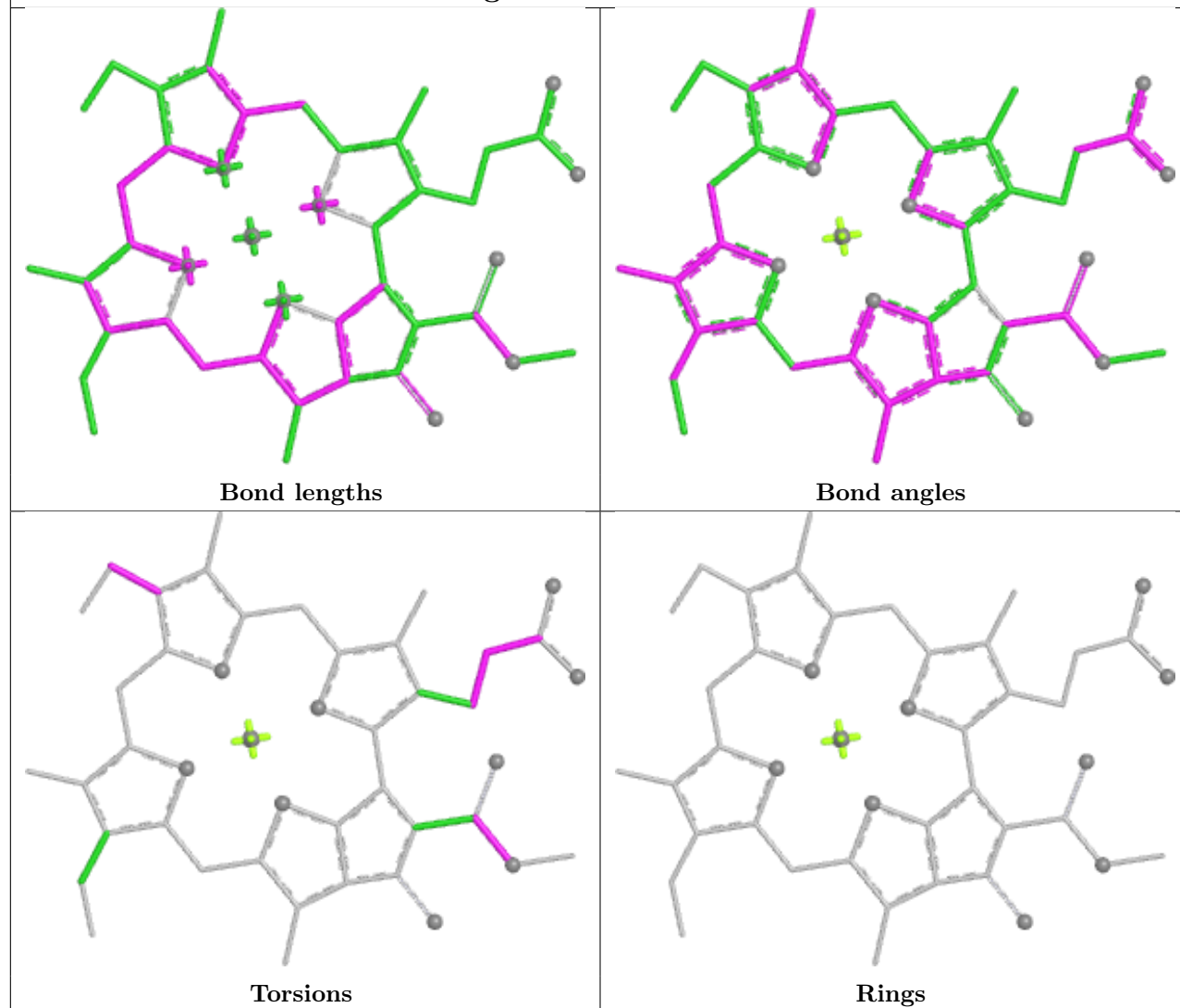


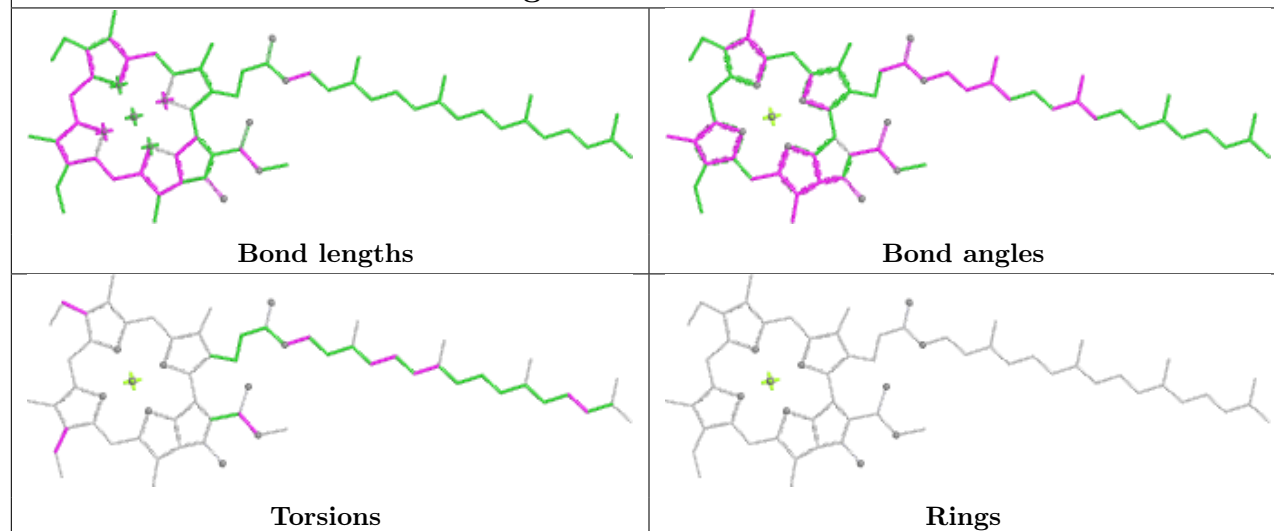
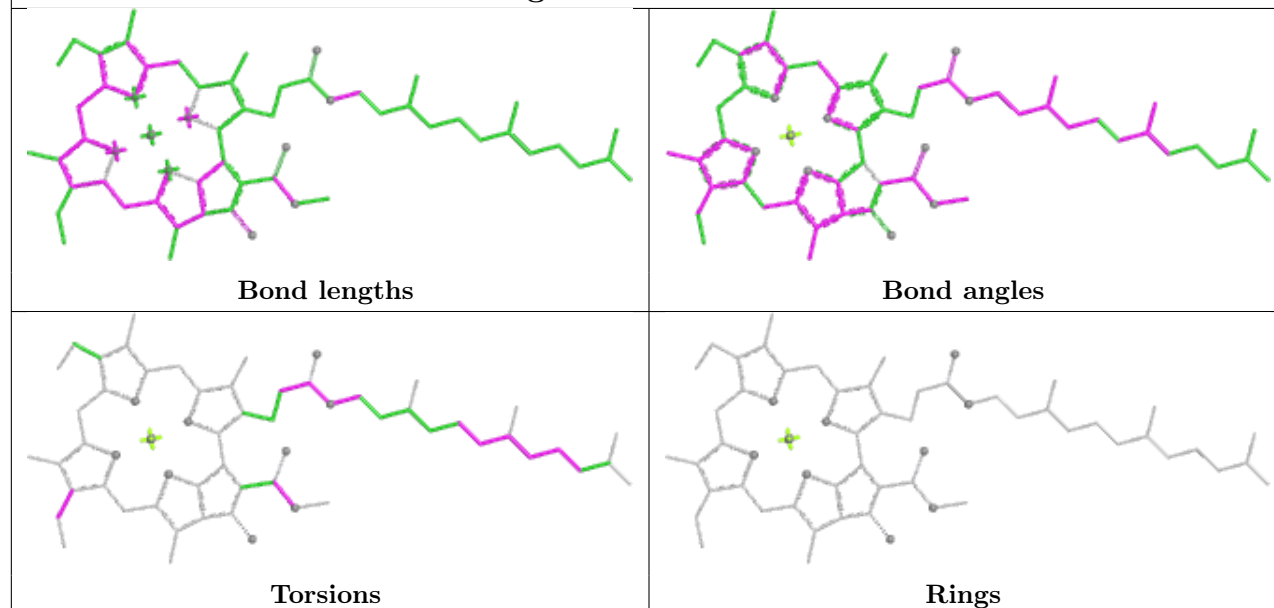


Ligand CLA A 1012

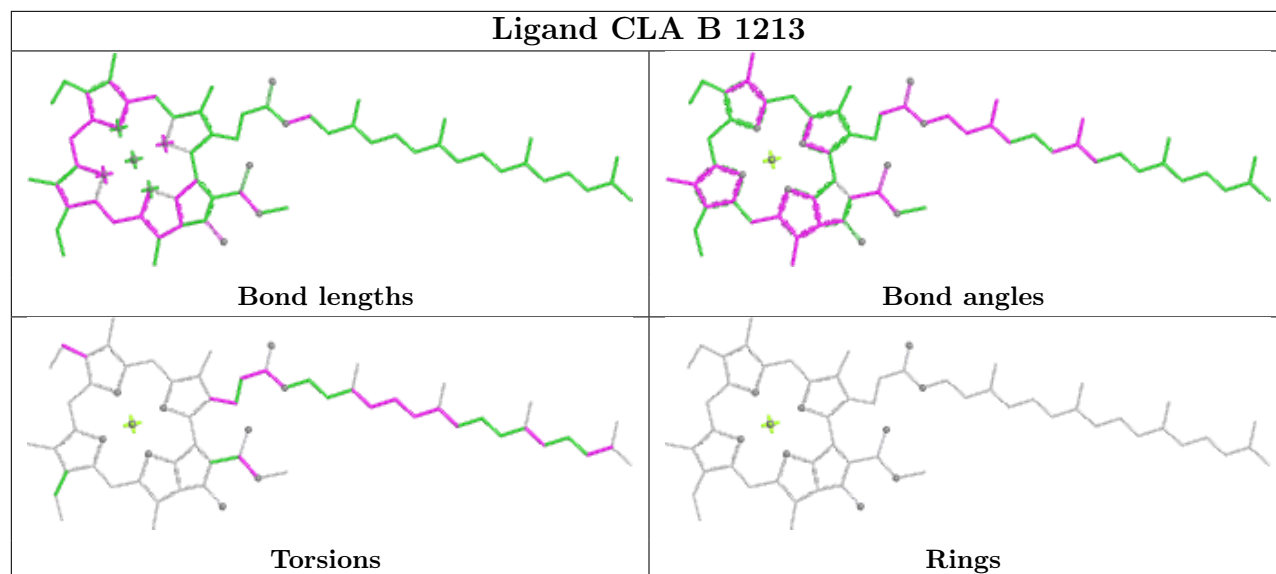


Ligand CLA B 1232

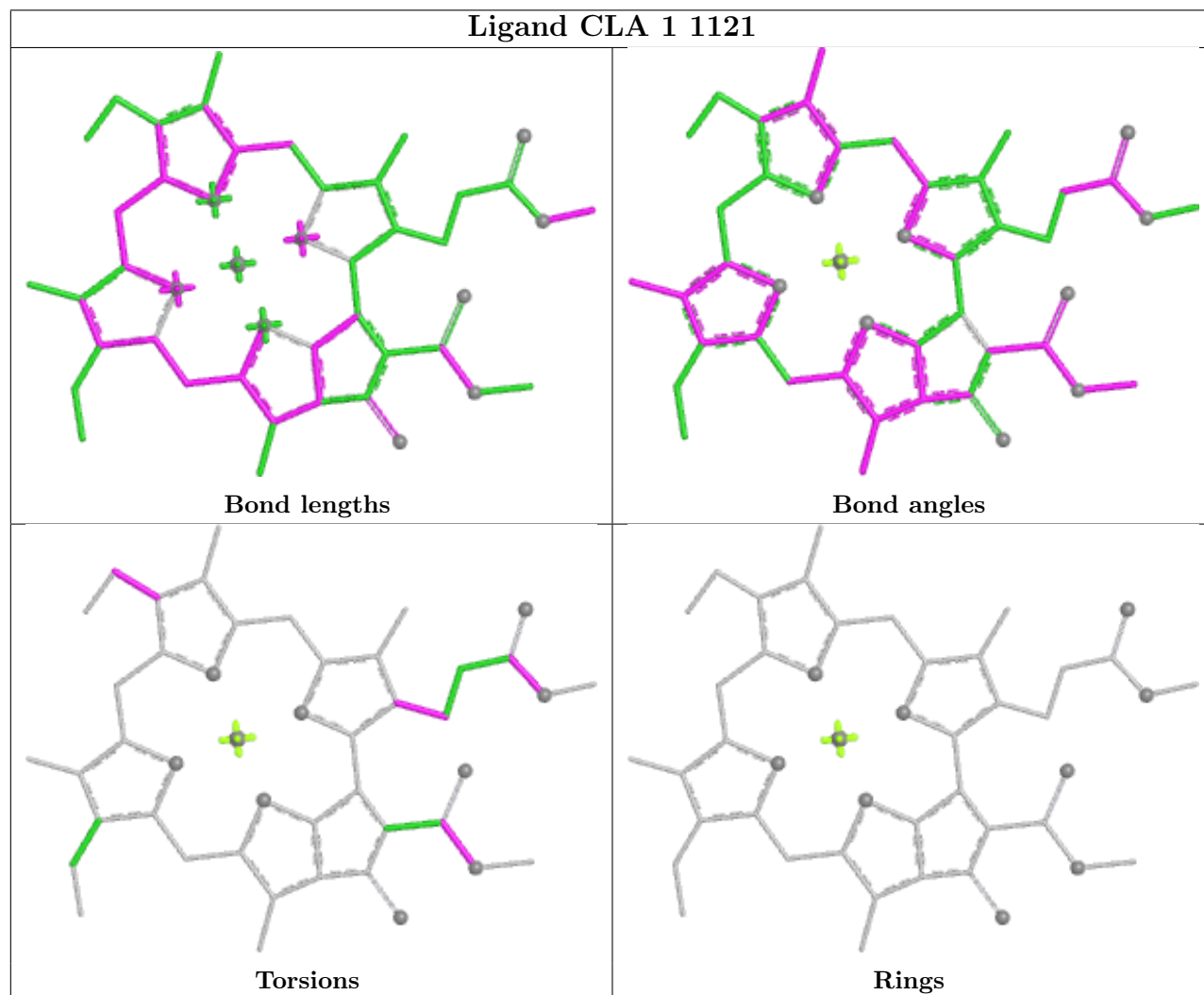


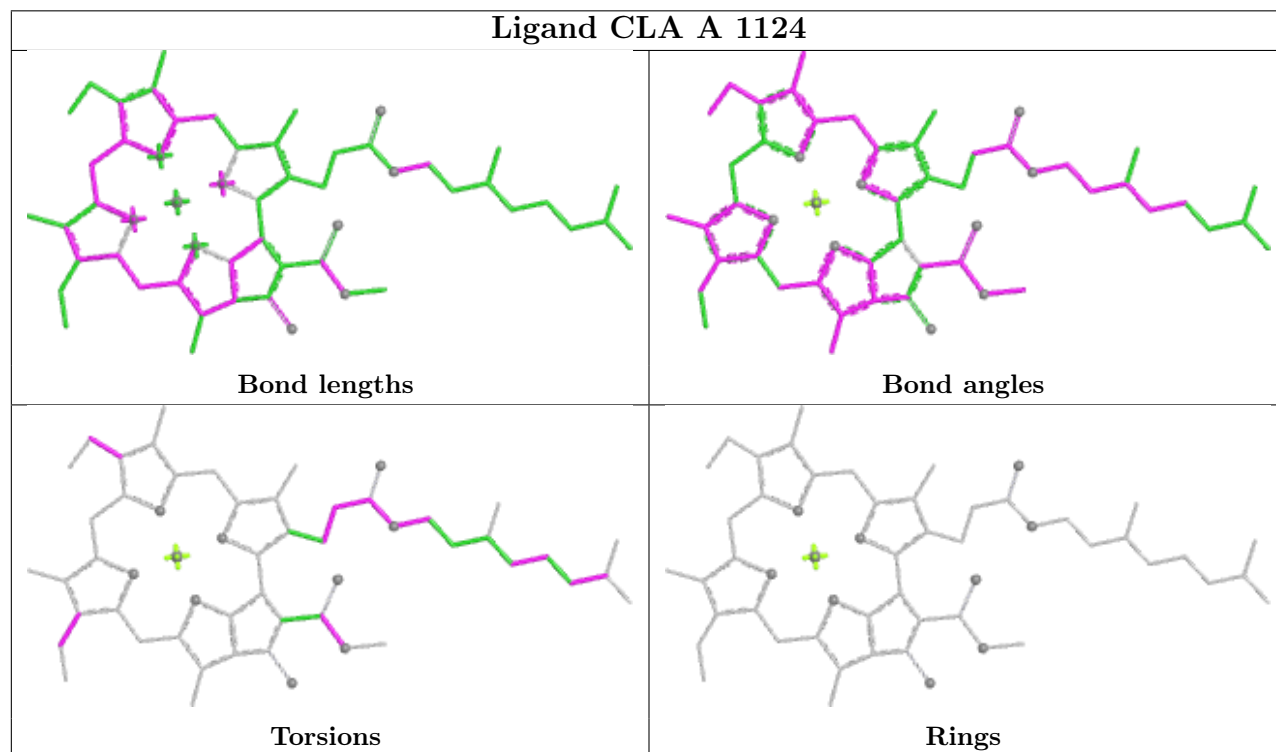
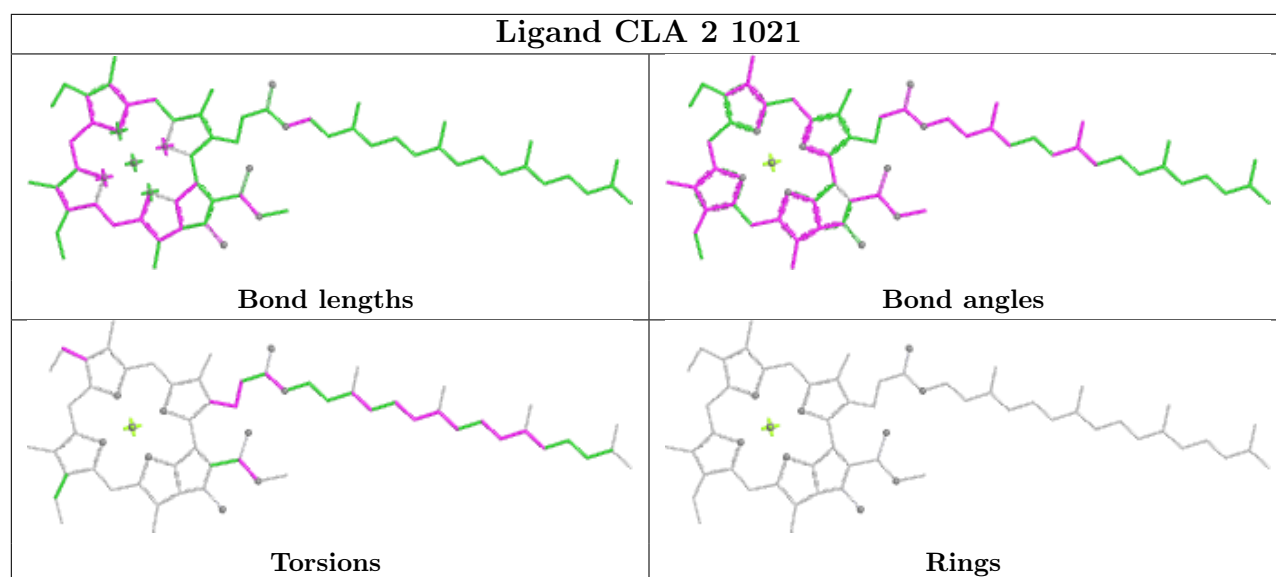
Ligand CLA B 1223**Ligand CLA 2 1235**

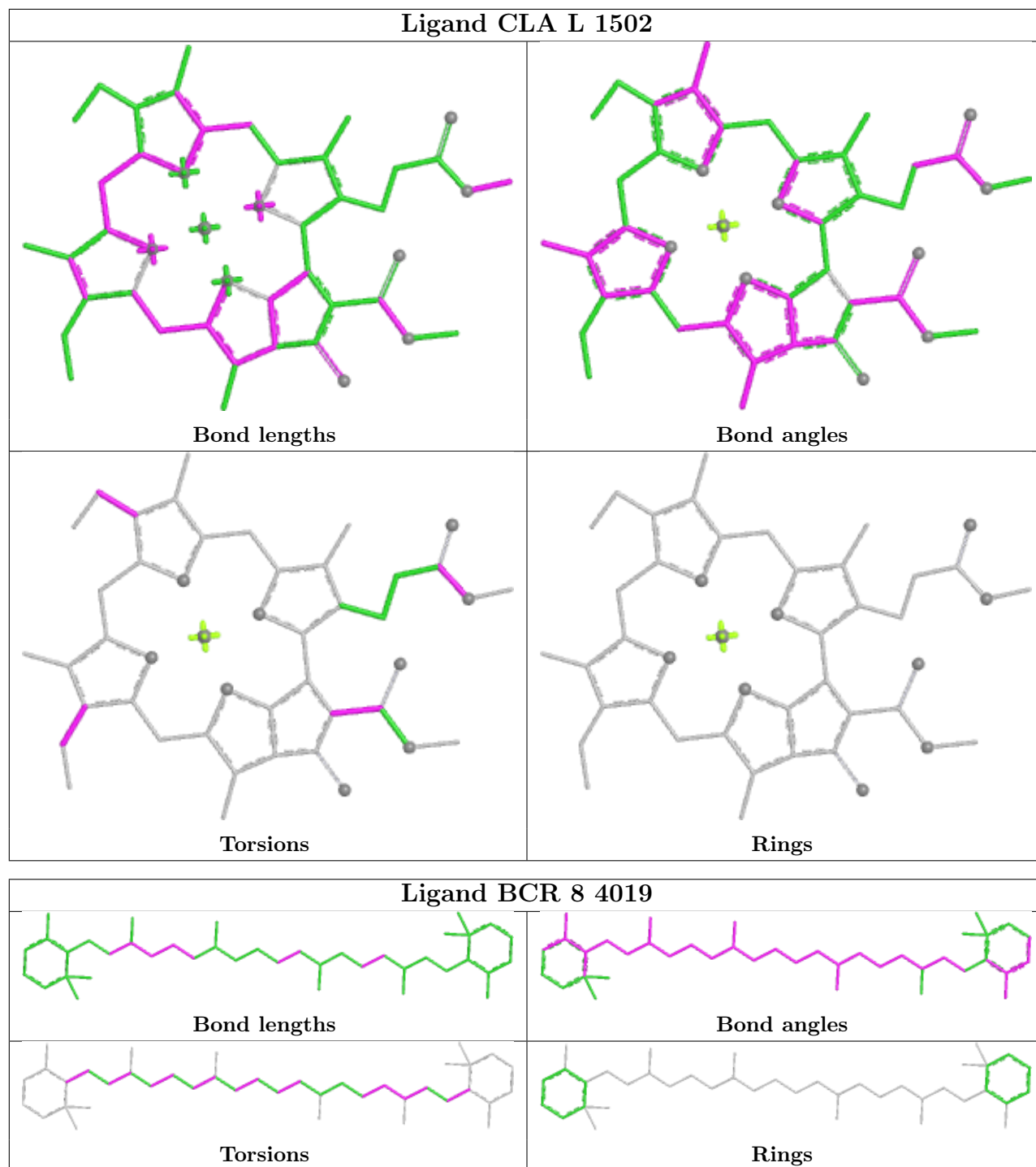
Ligand CLA B 1213

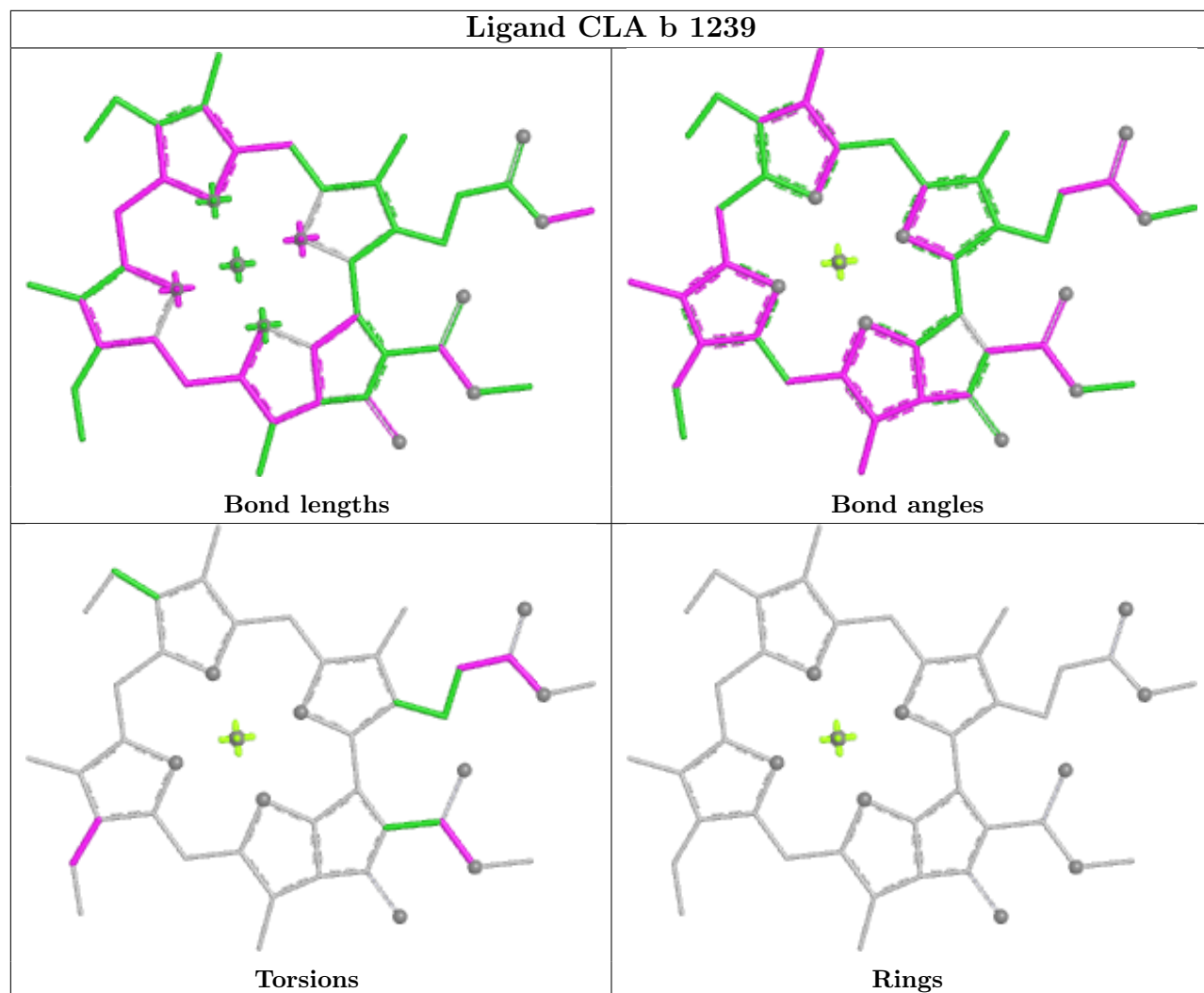


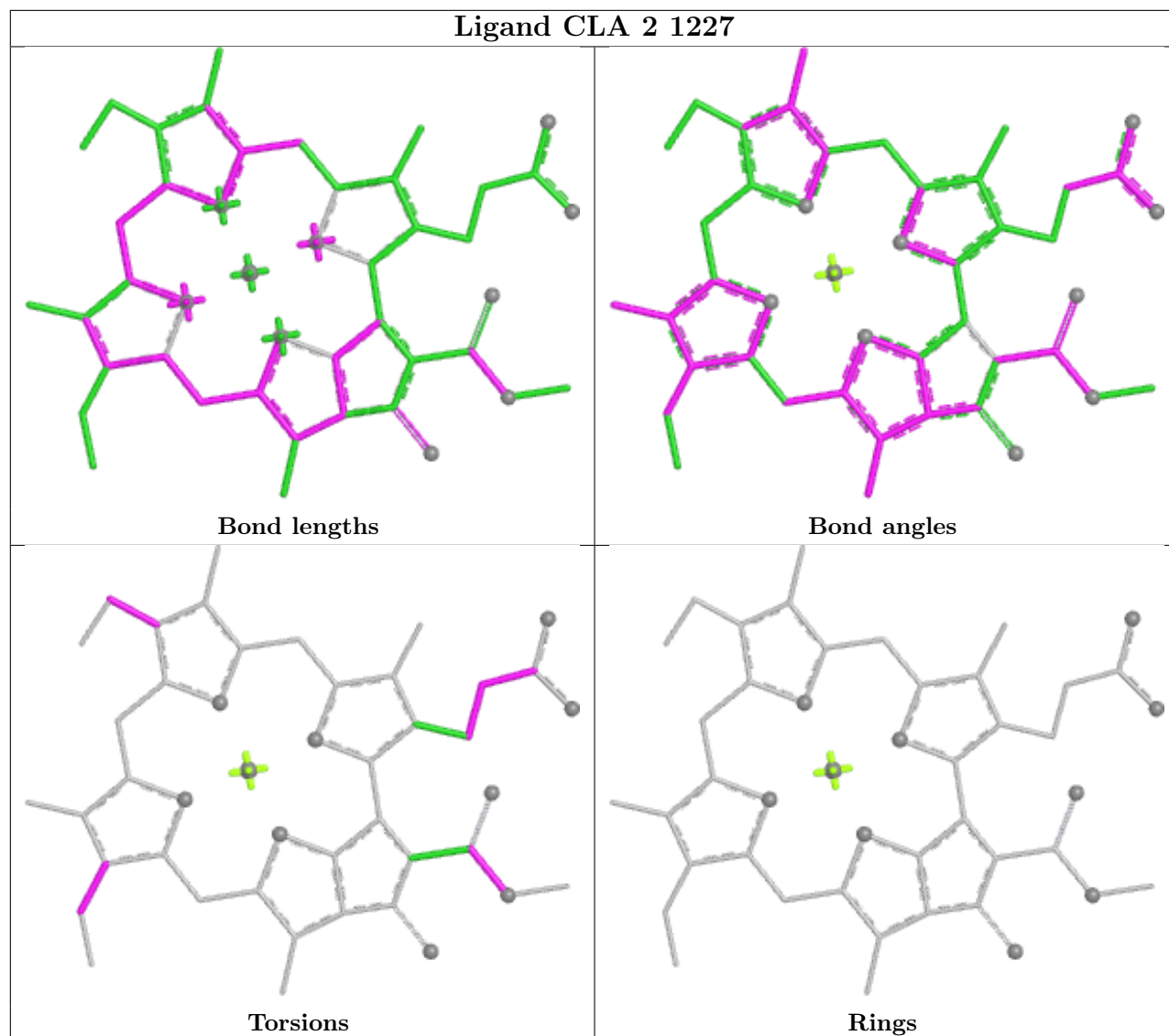
Ligand CLA 1 1121



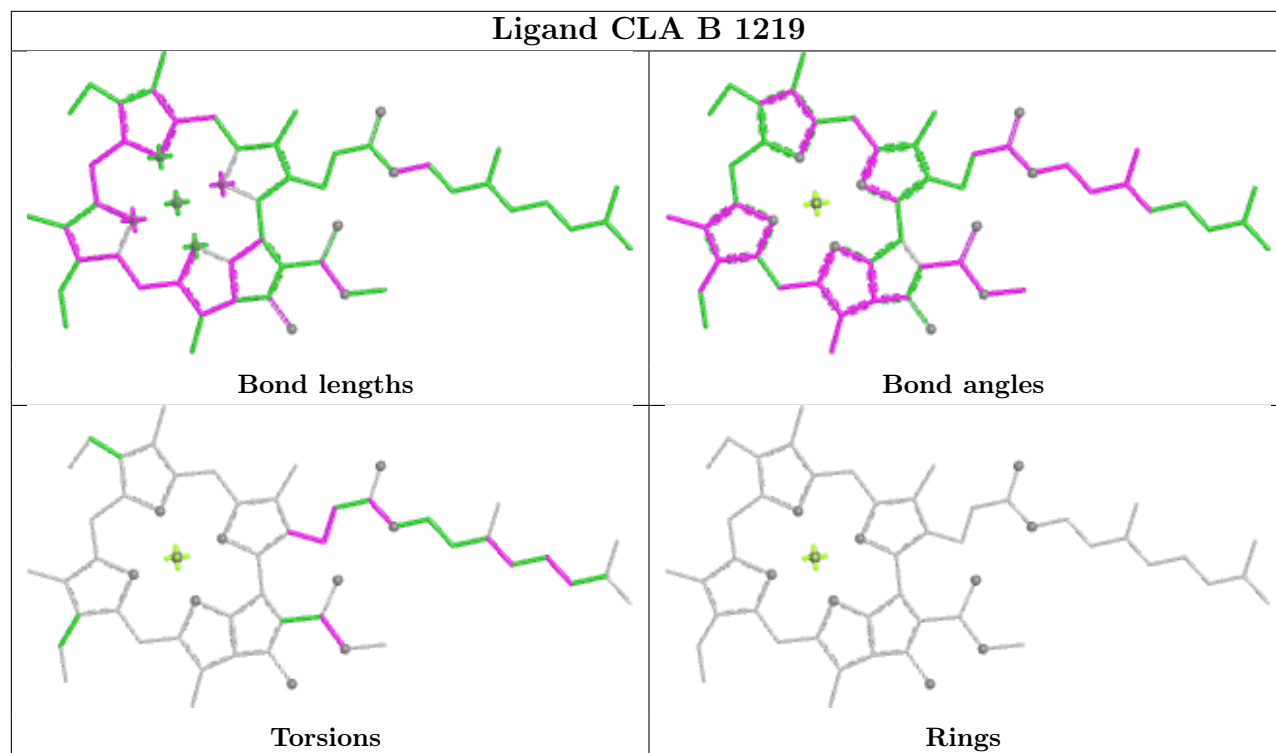




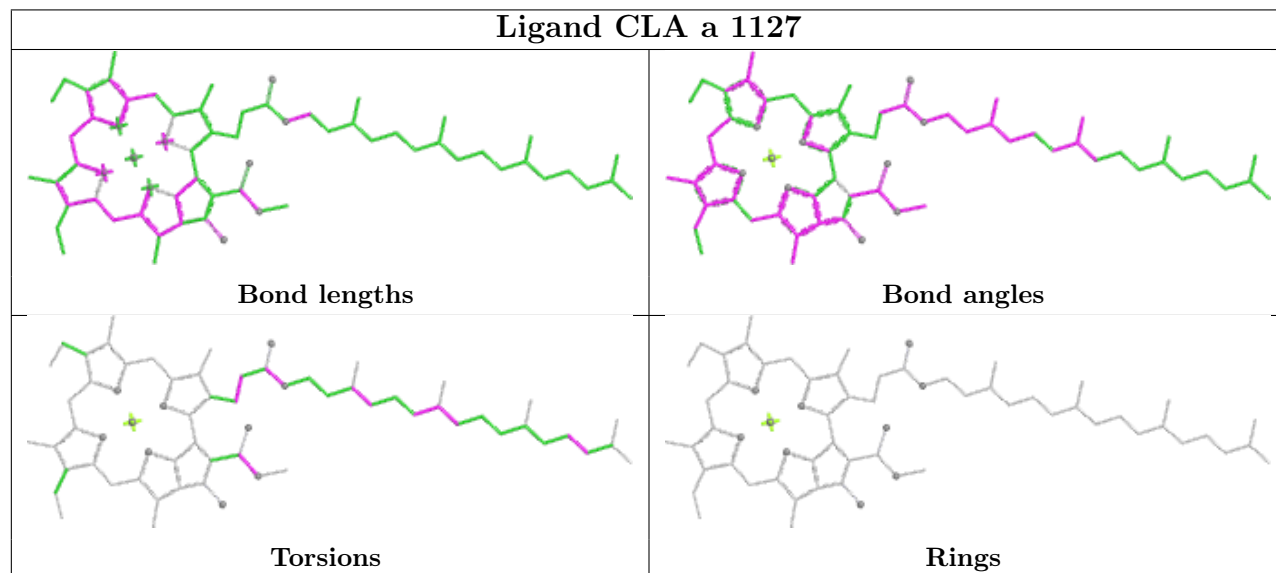


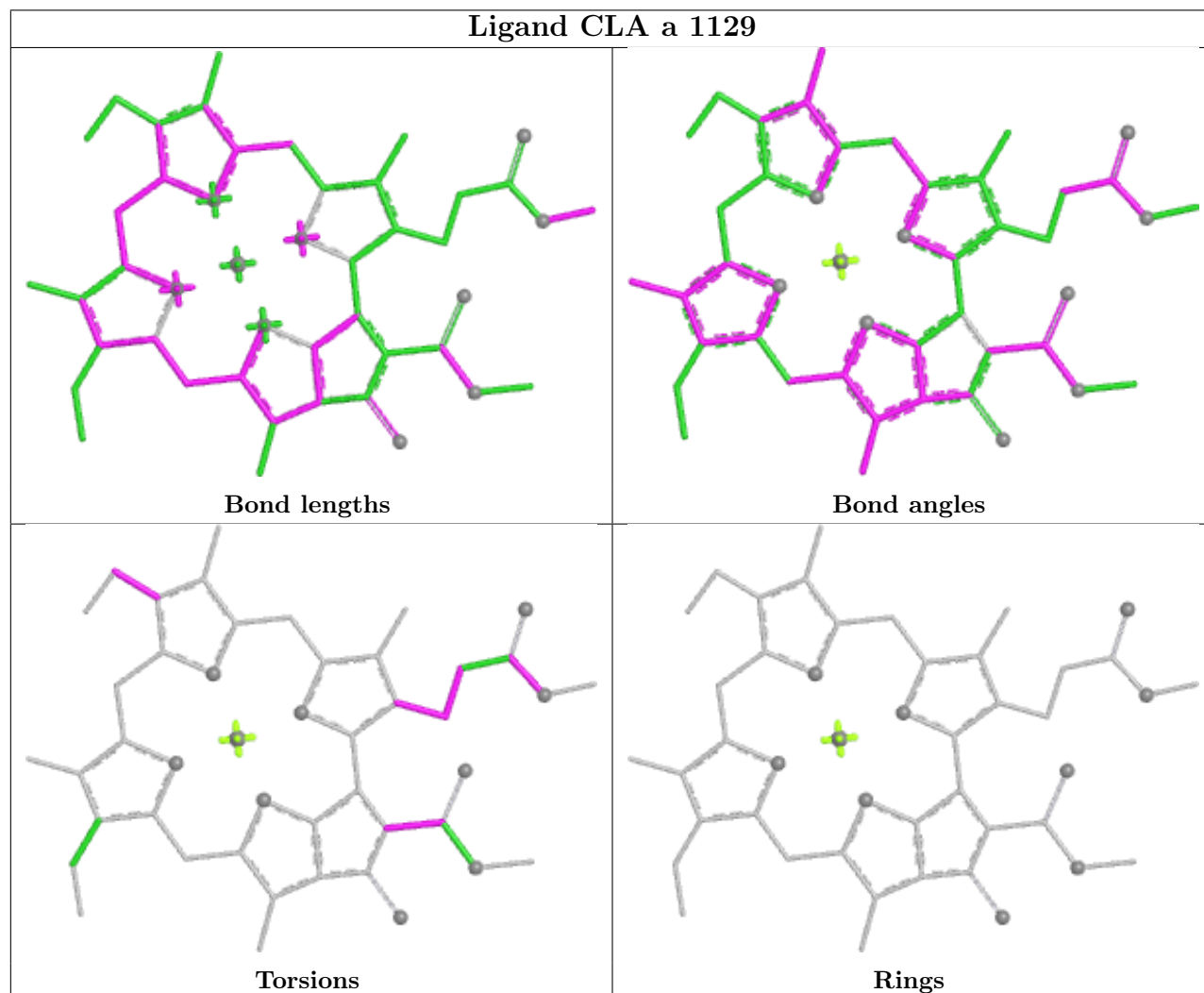
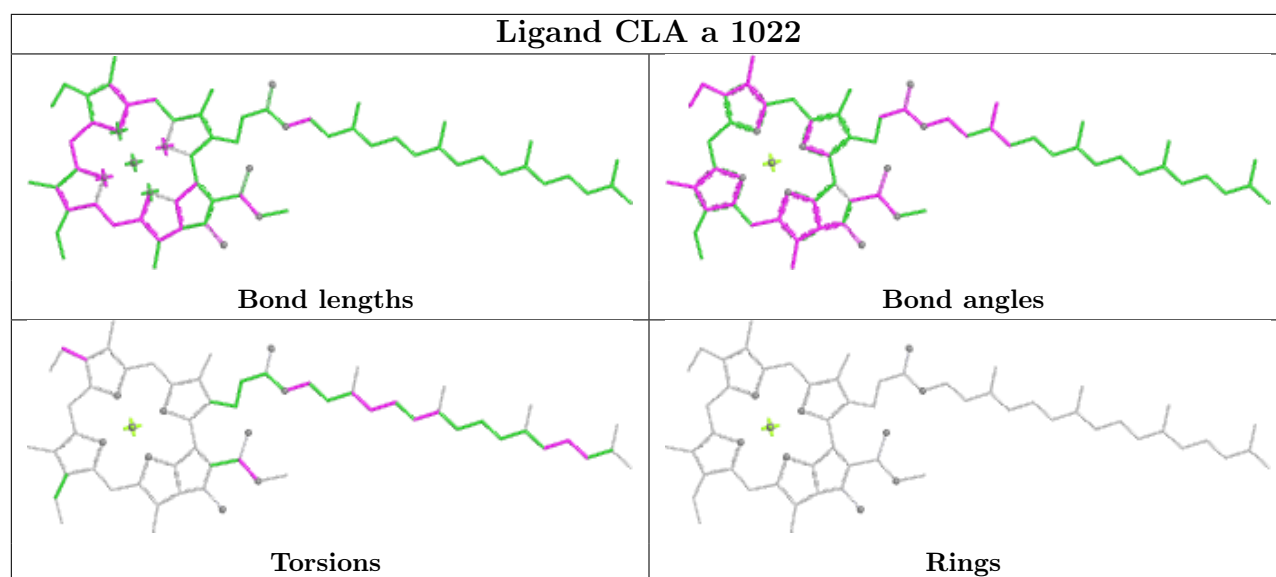


Ligand CLA B 1219

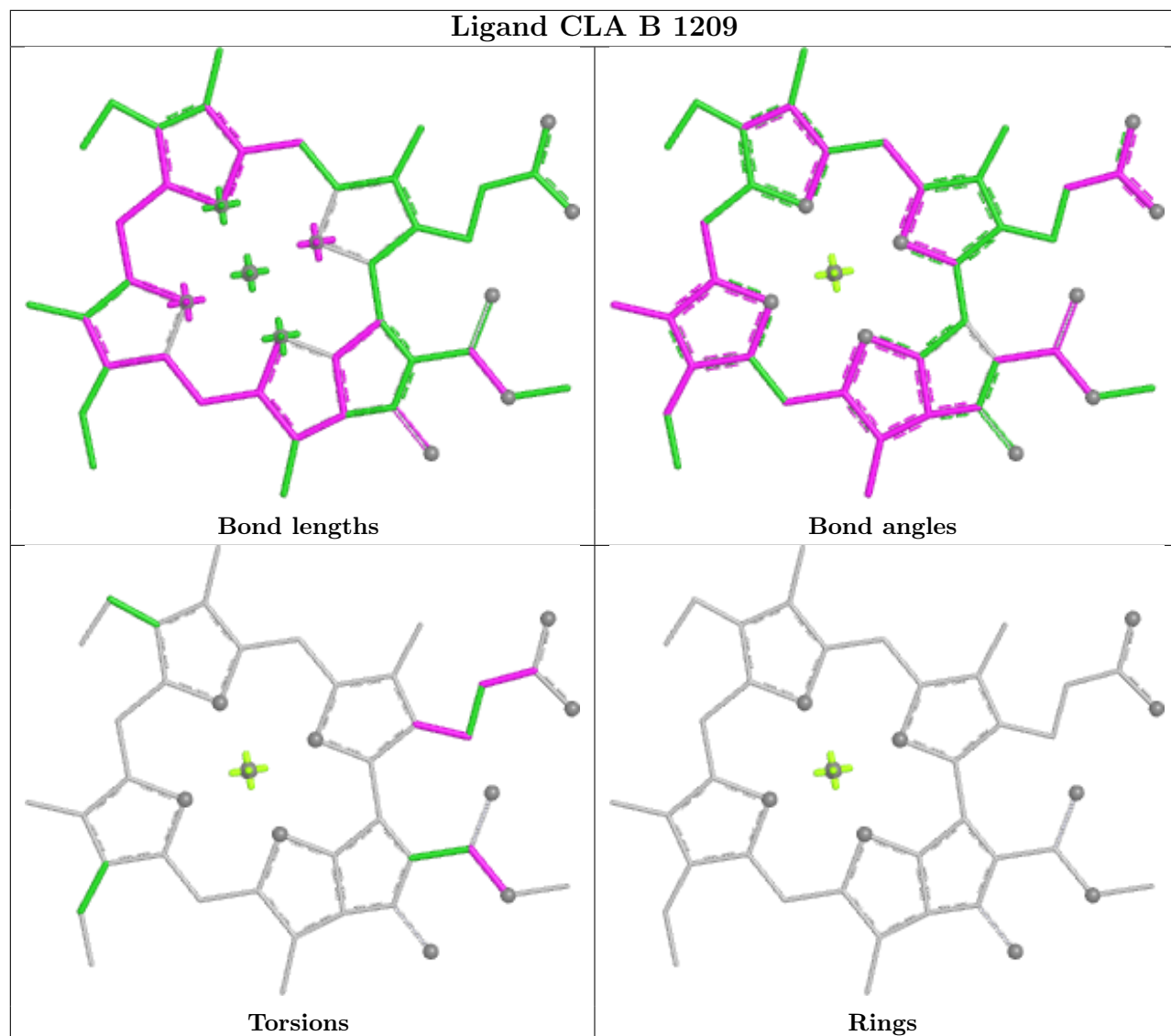


Ligand CLA a 1127

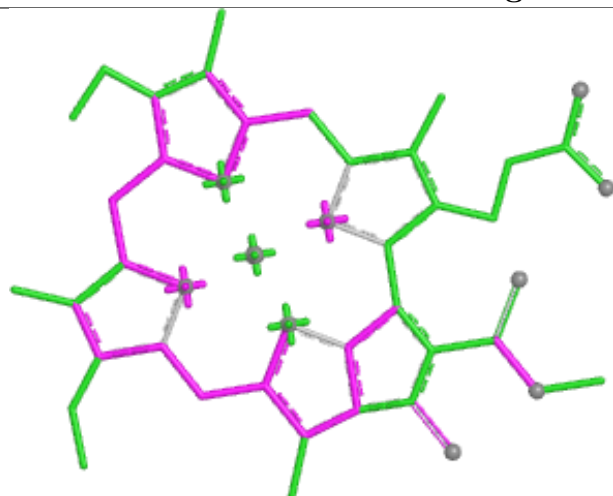




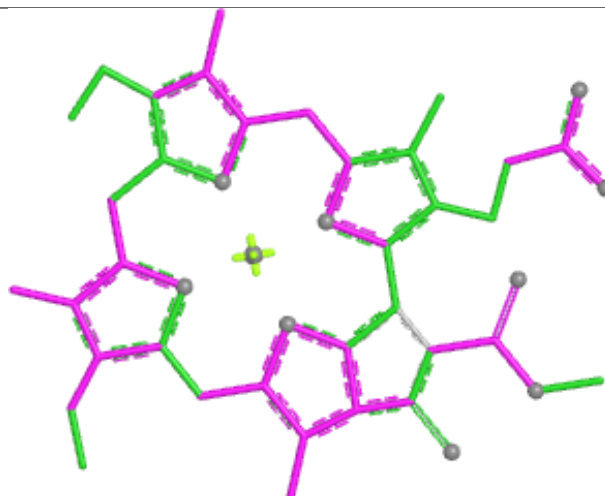
Ligand CLA B 1209



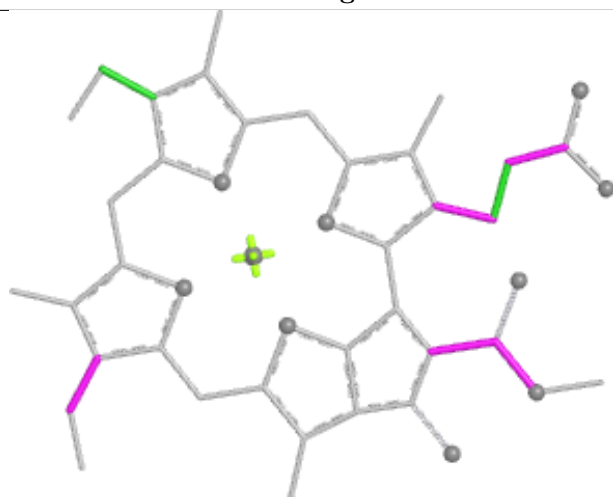
Ligand CLA B 1231



Bond lengths



Bond angles

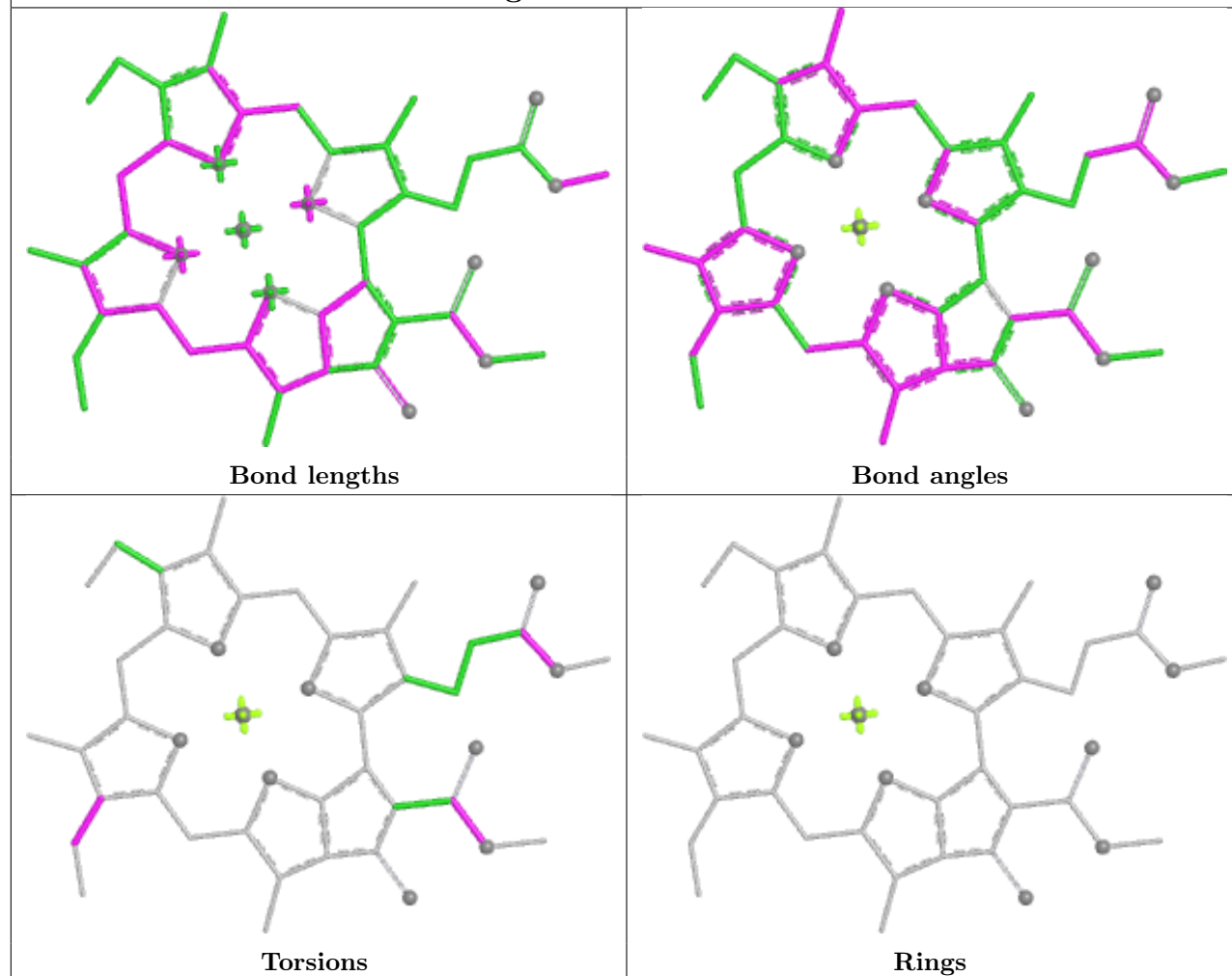


Torsions

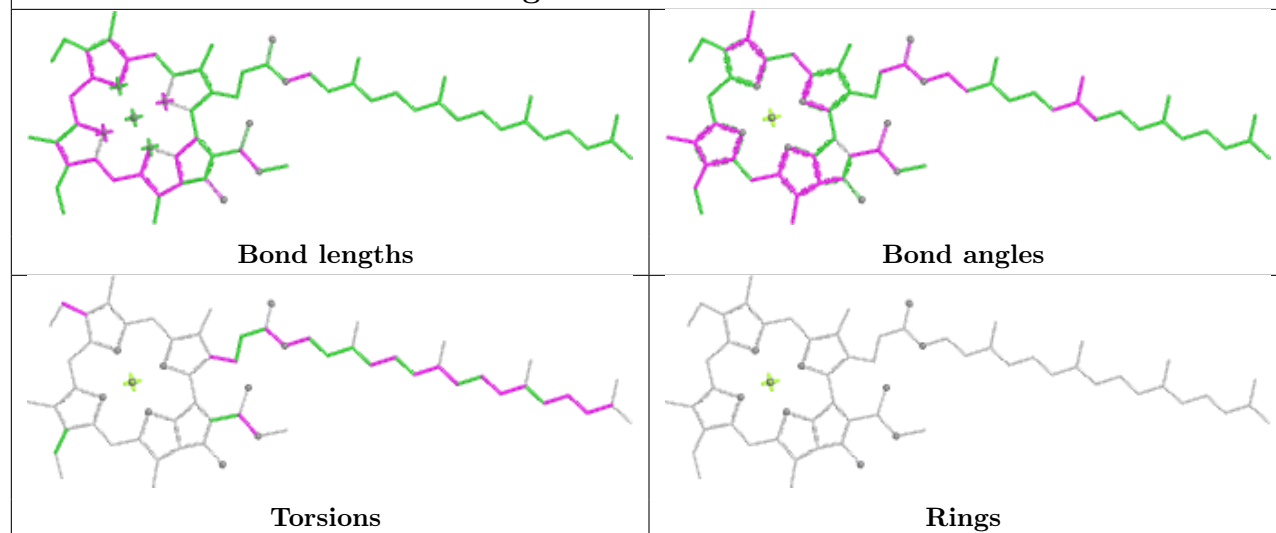


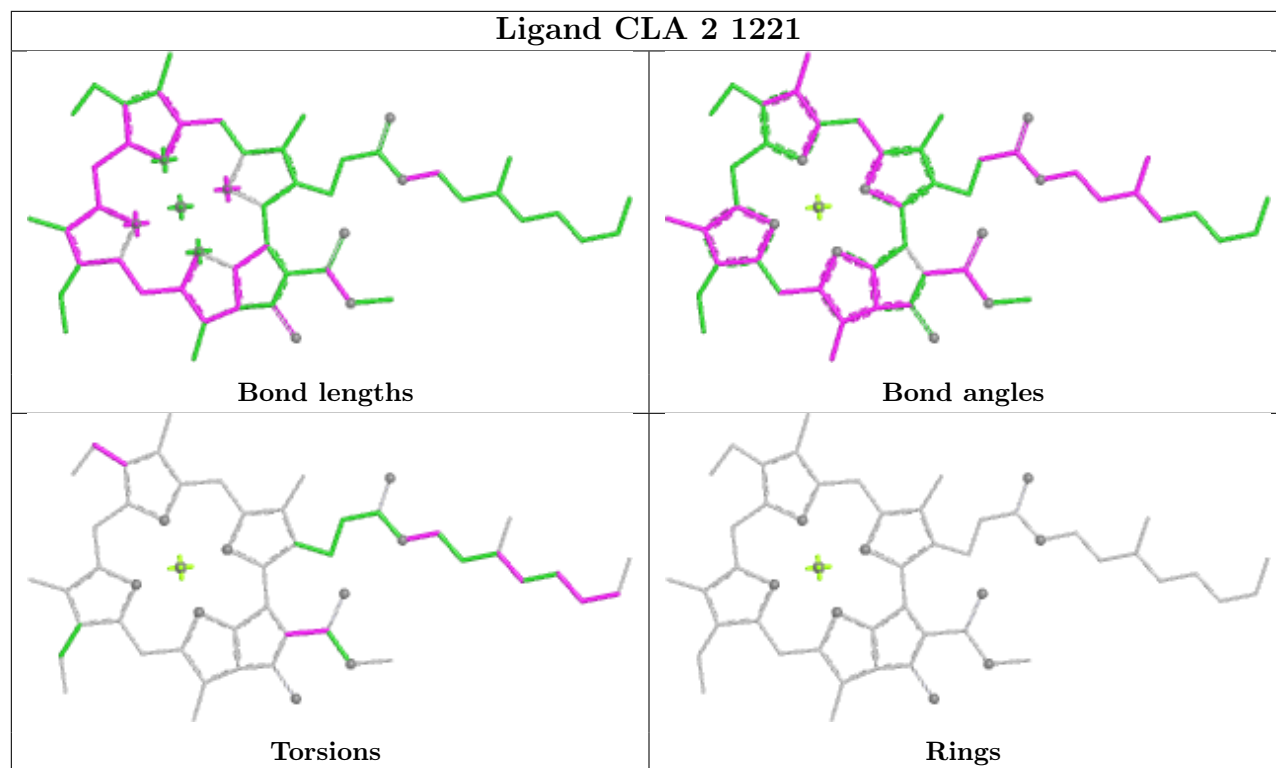
Rings

Ligand CLA B 1220

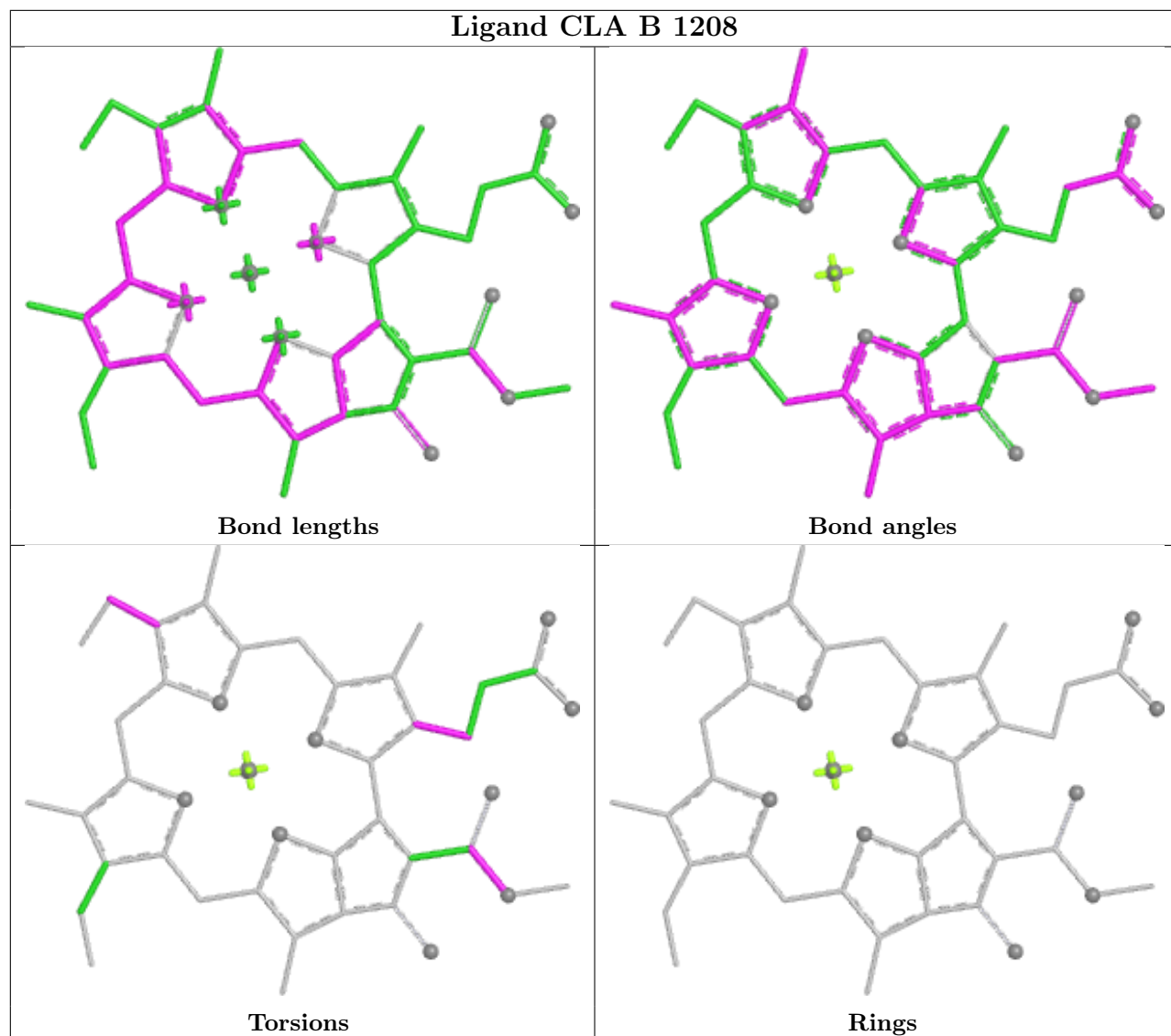


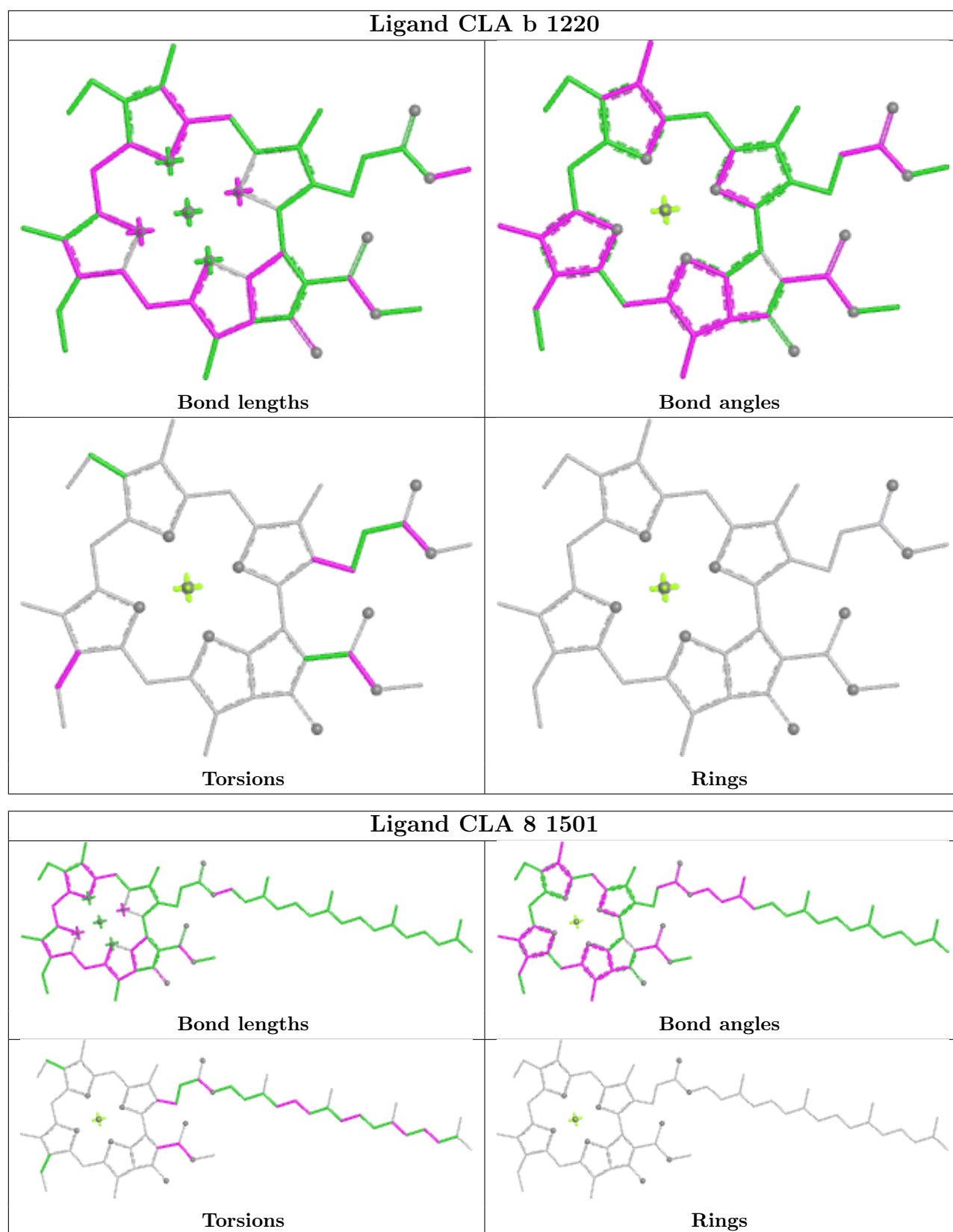
Ligand CLA A 1102

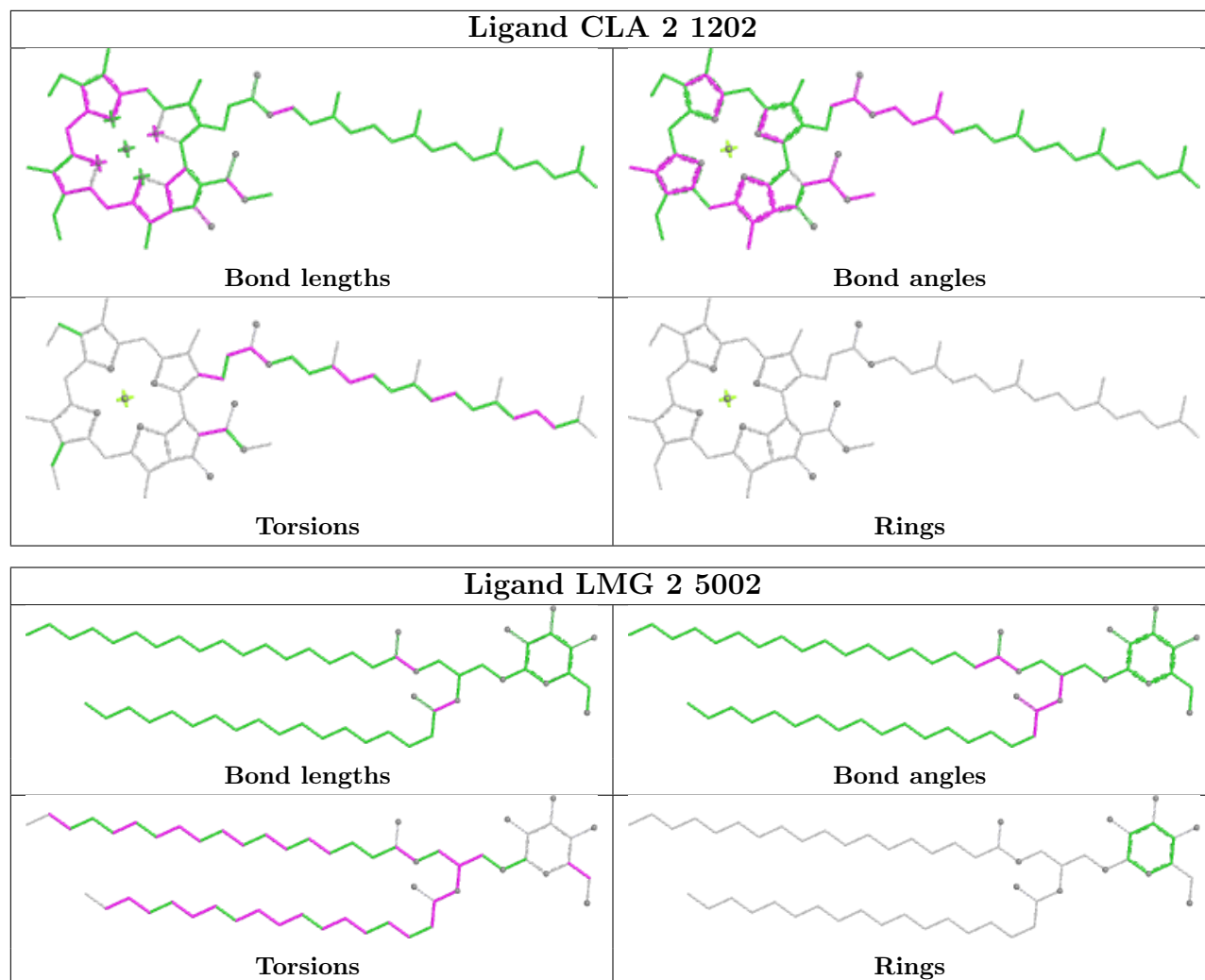




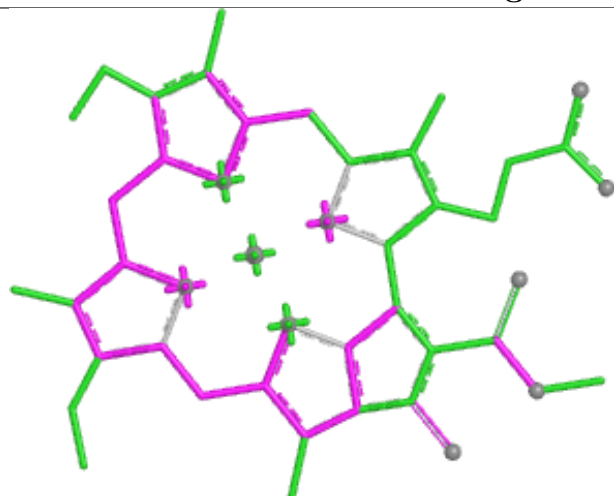
Ligand CLA B 1208



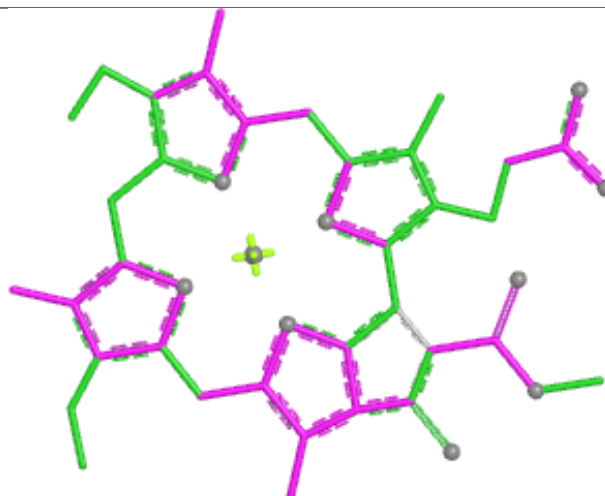




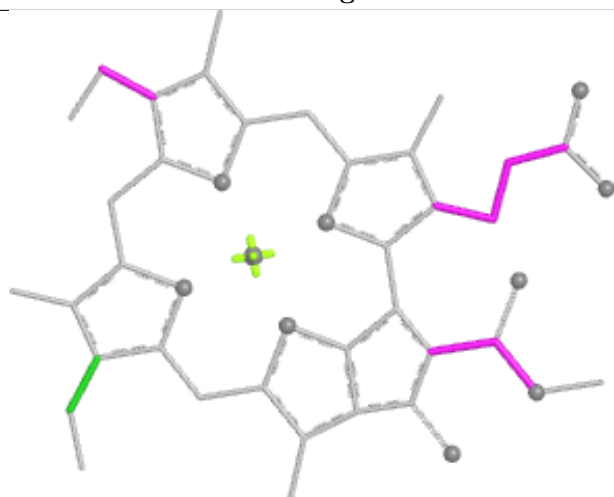
Ligand CLA B 1212



Bond lengths



Bond angles

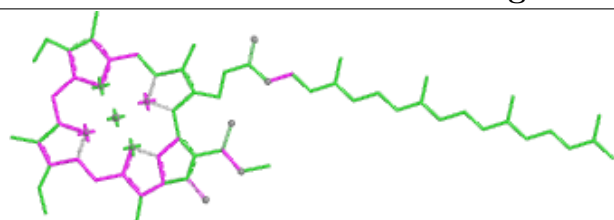


Torsions

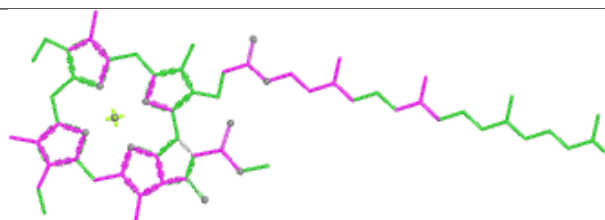


Rings

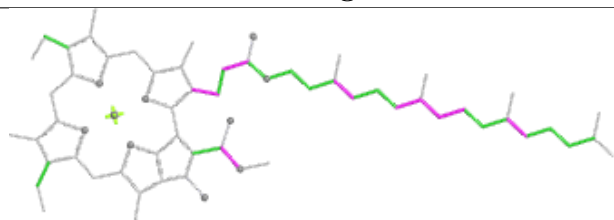
Ligand CLA b 1215



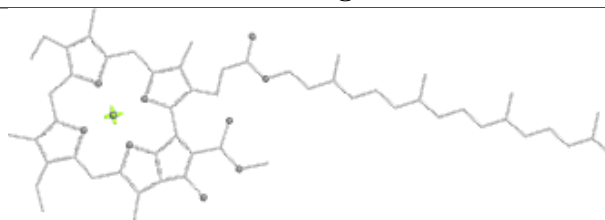
Bond lengths



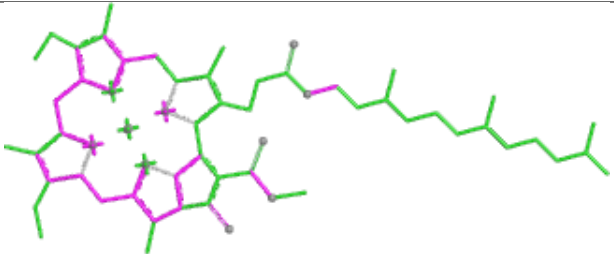
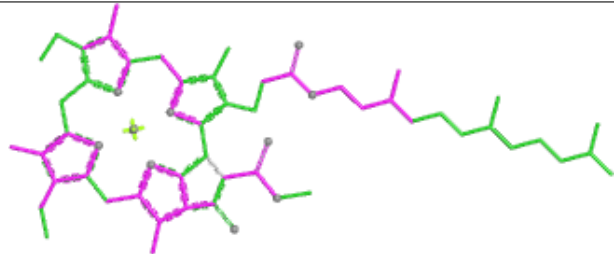
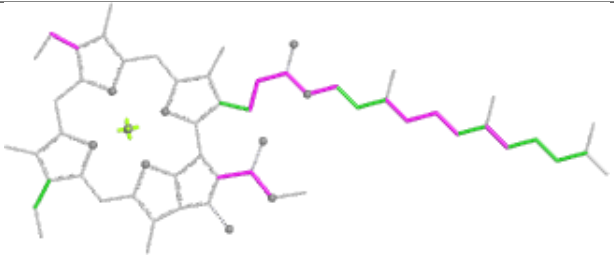
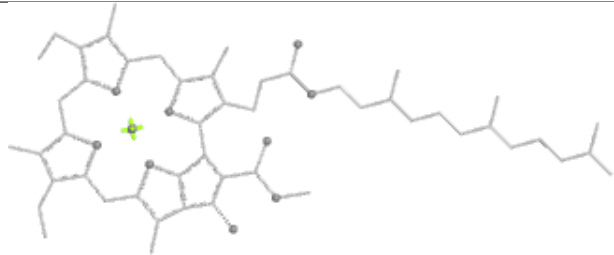
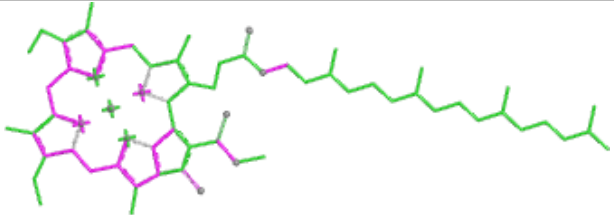
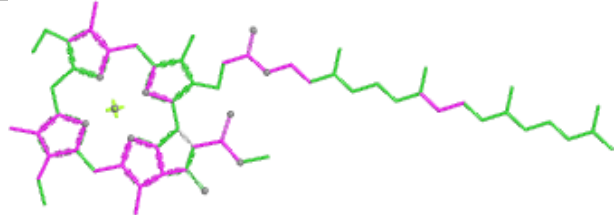
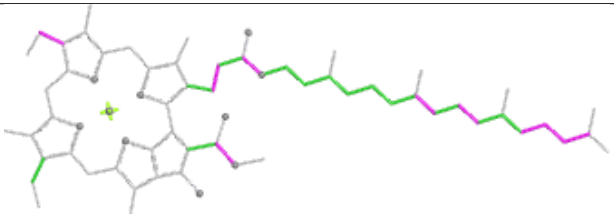
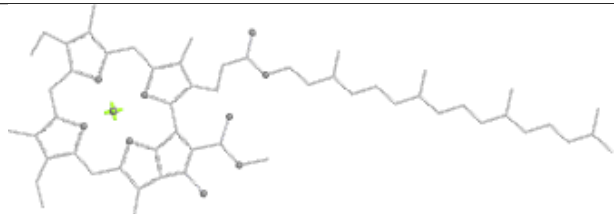
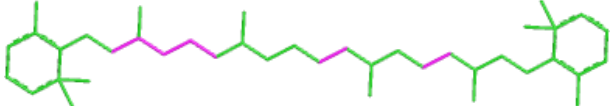
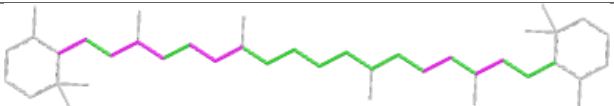
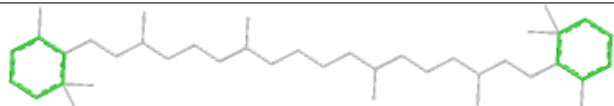
Bond angles

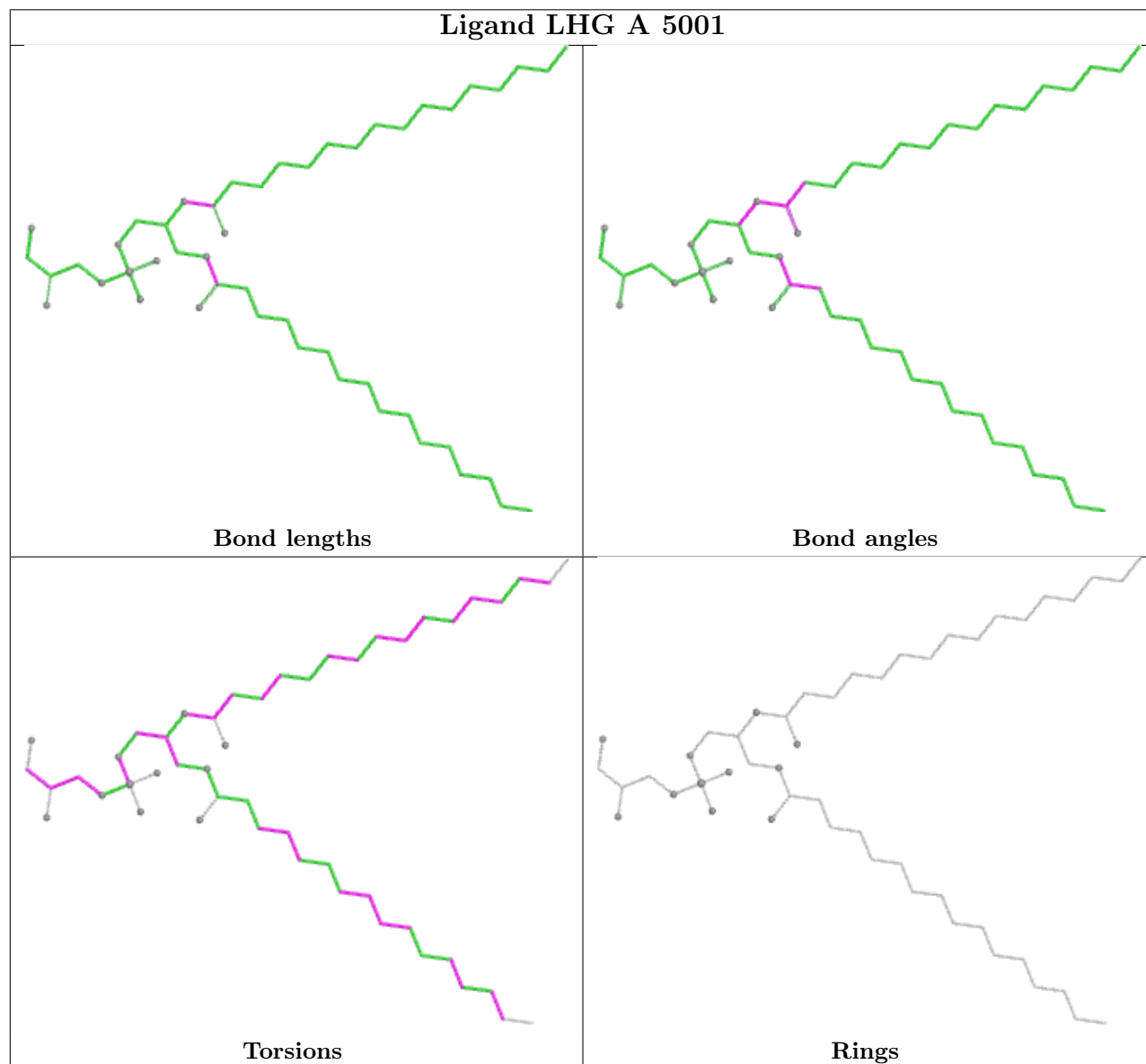
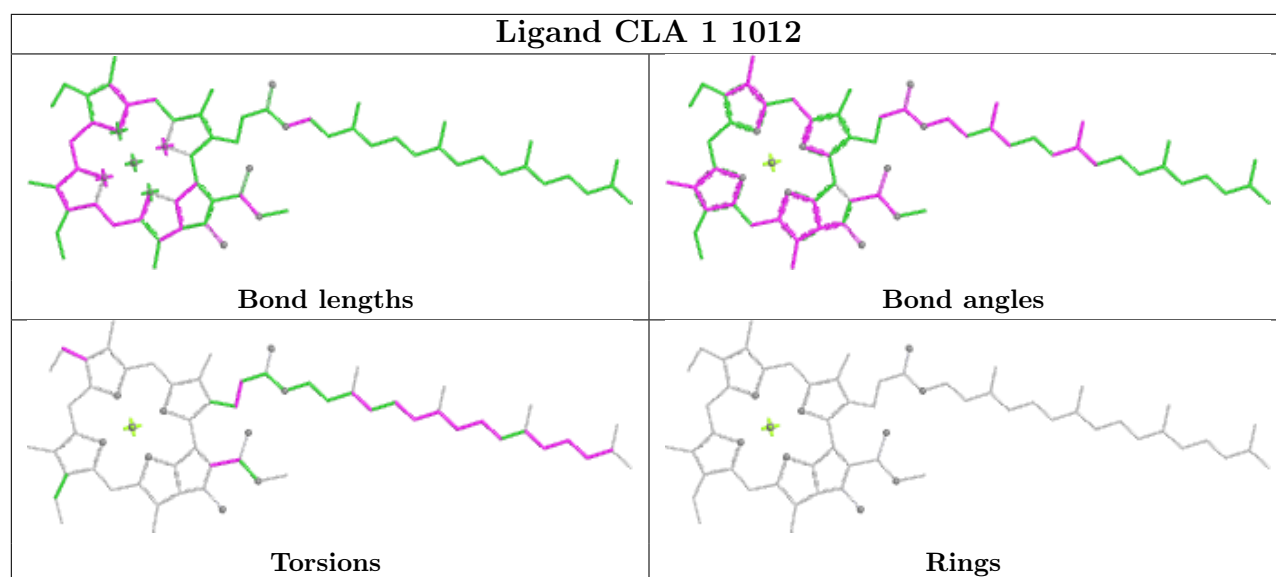


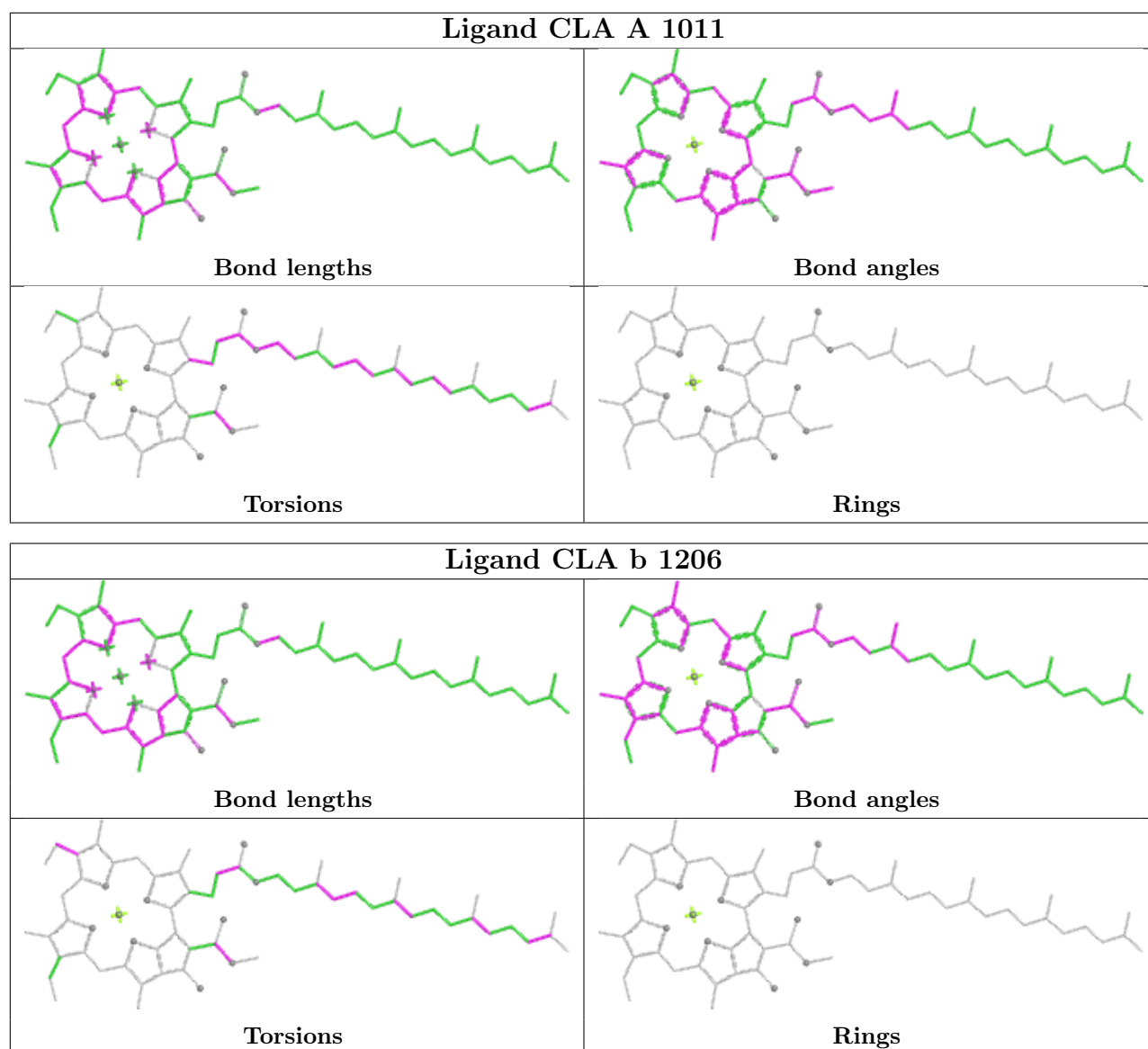
Torsions

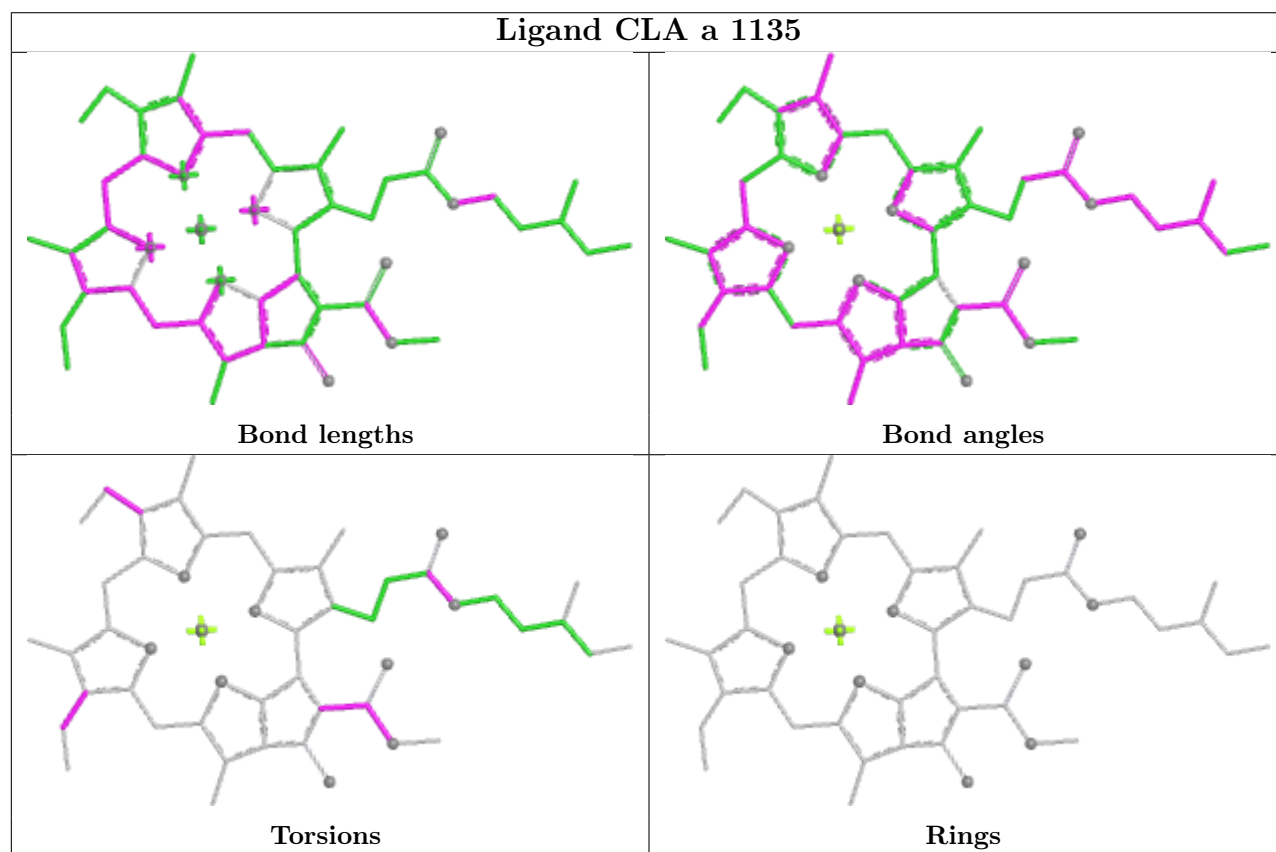
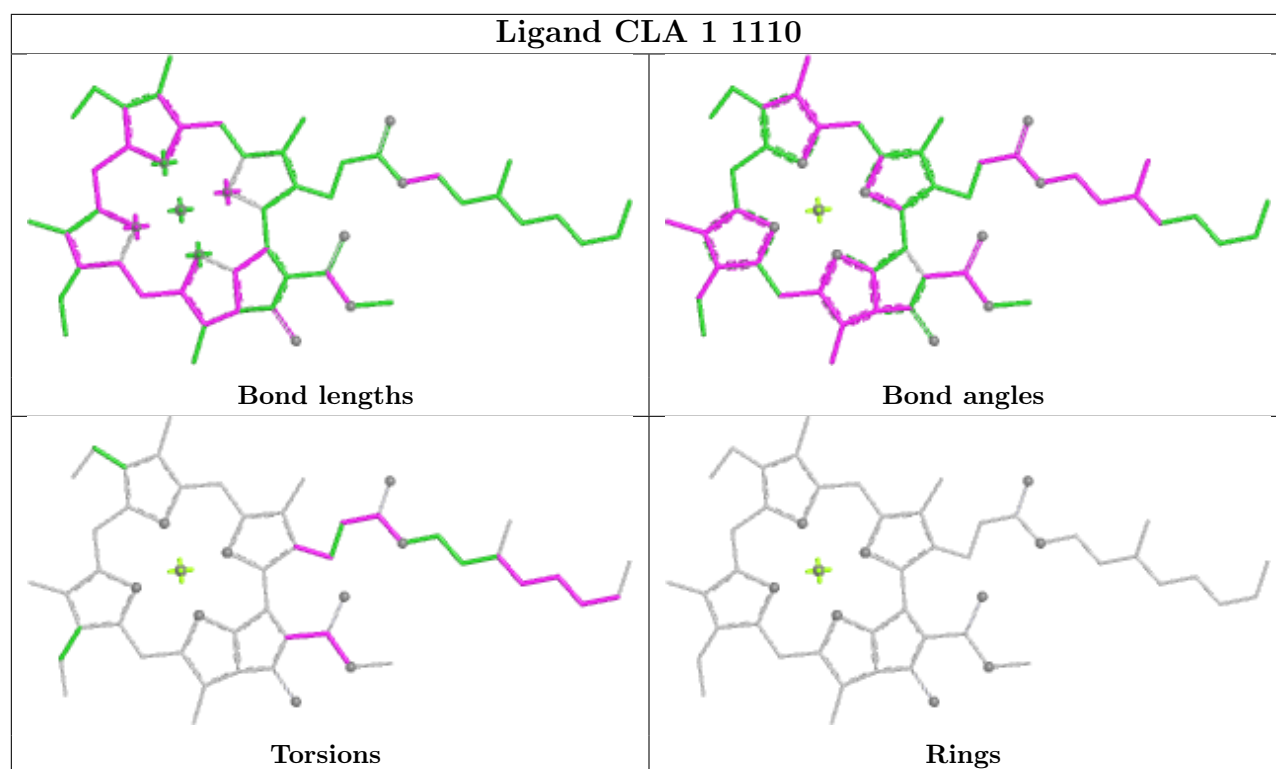


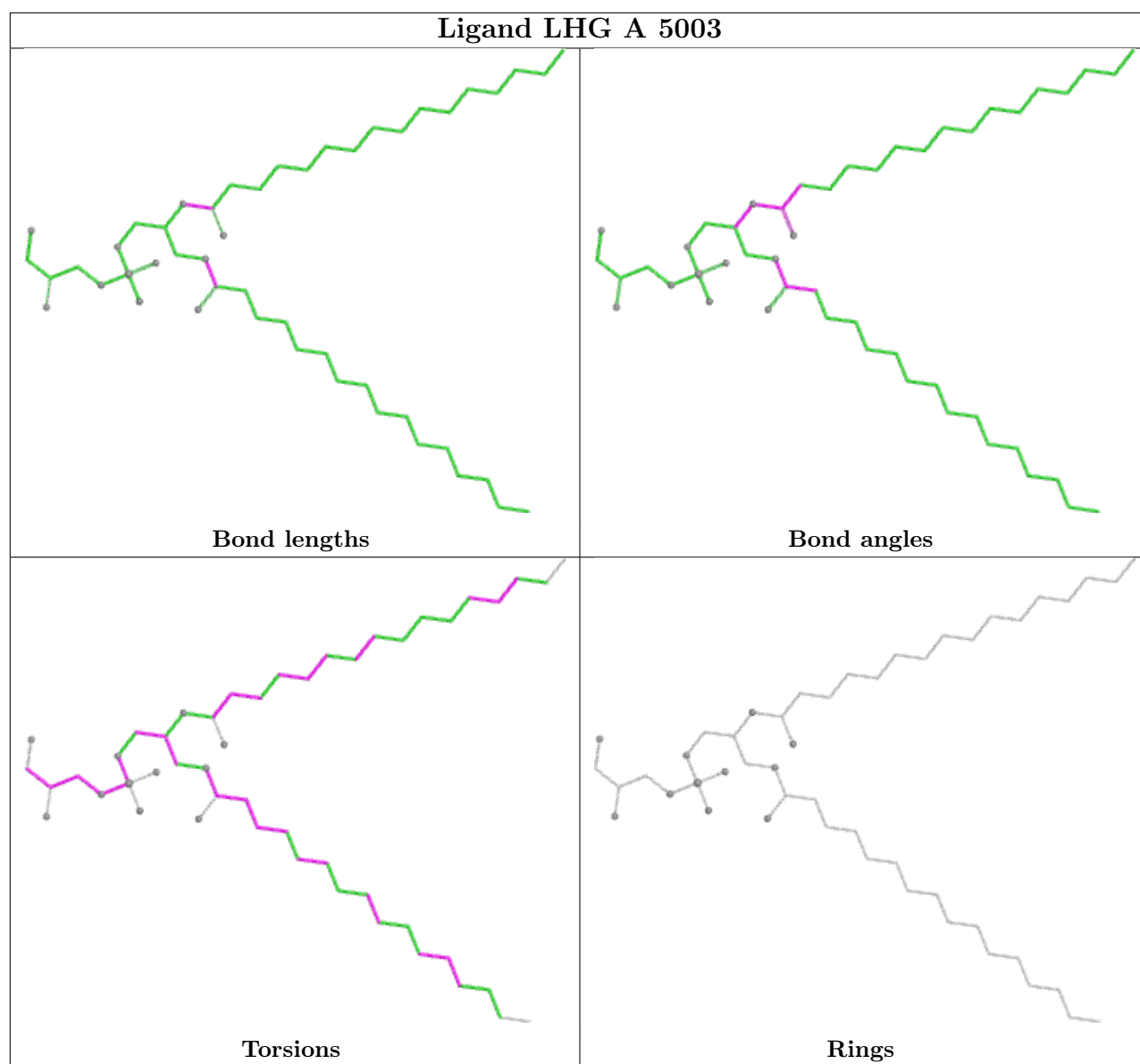
Rings

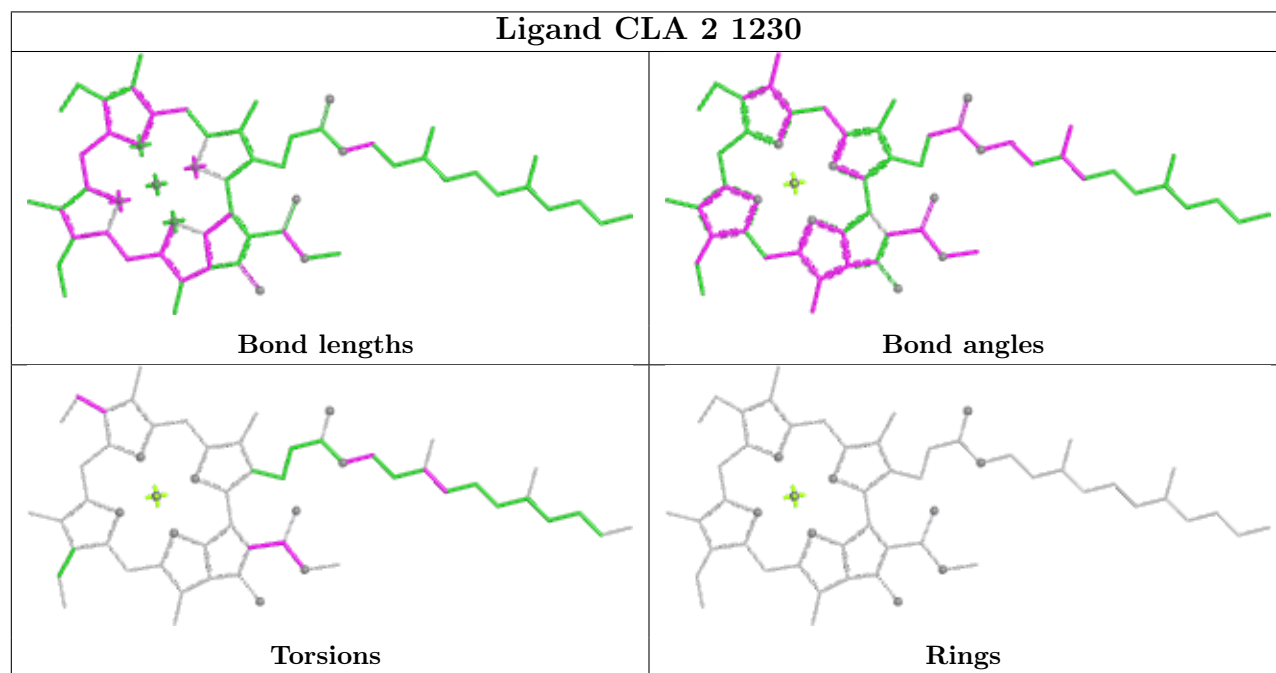
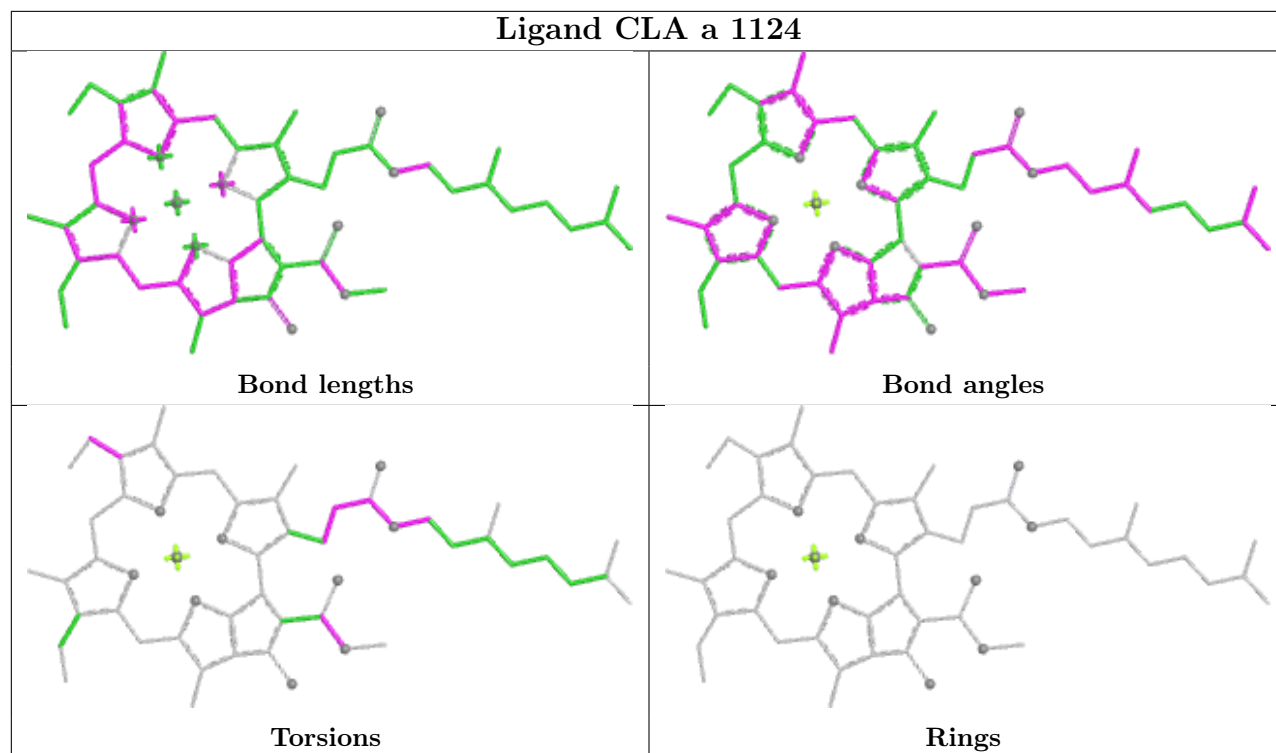
Ligand CLA A 1111	
	
Bond lengths	Bond angles
	
Torsions	Rings
Ligand CLA b 1238	
	
Bond lengths	Bond angles
	
Torsions	Rings
Ligand BCR 1 4003	
	
Bond lengths	Bond angles
	
Torsions	Rings

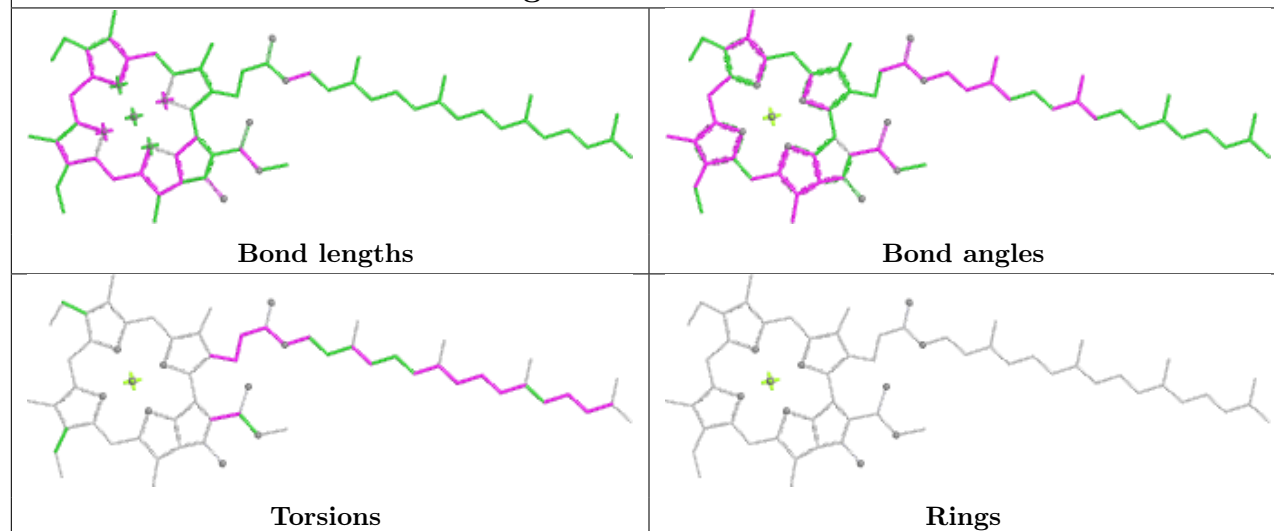
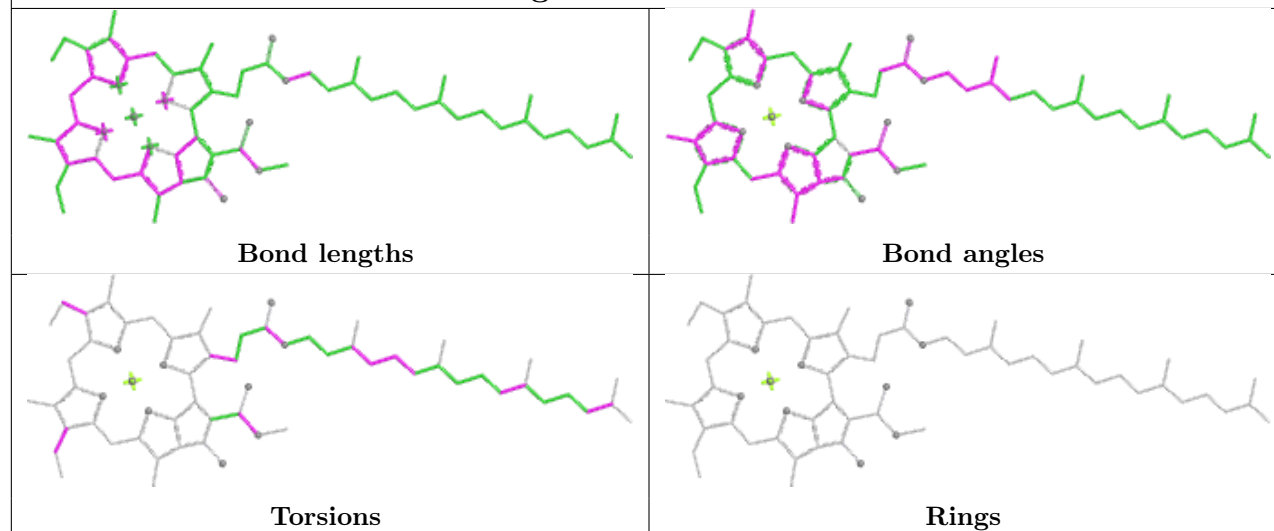


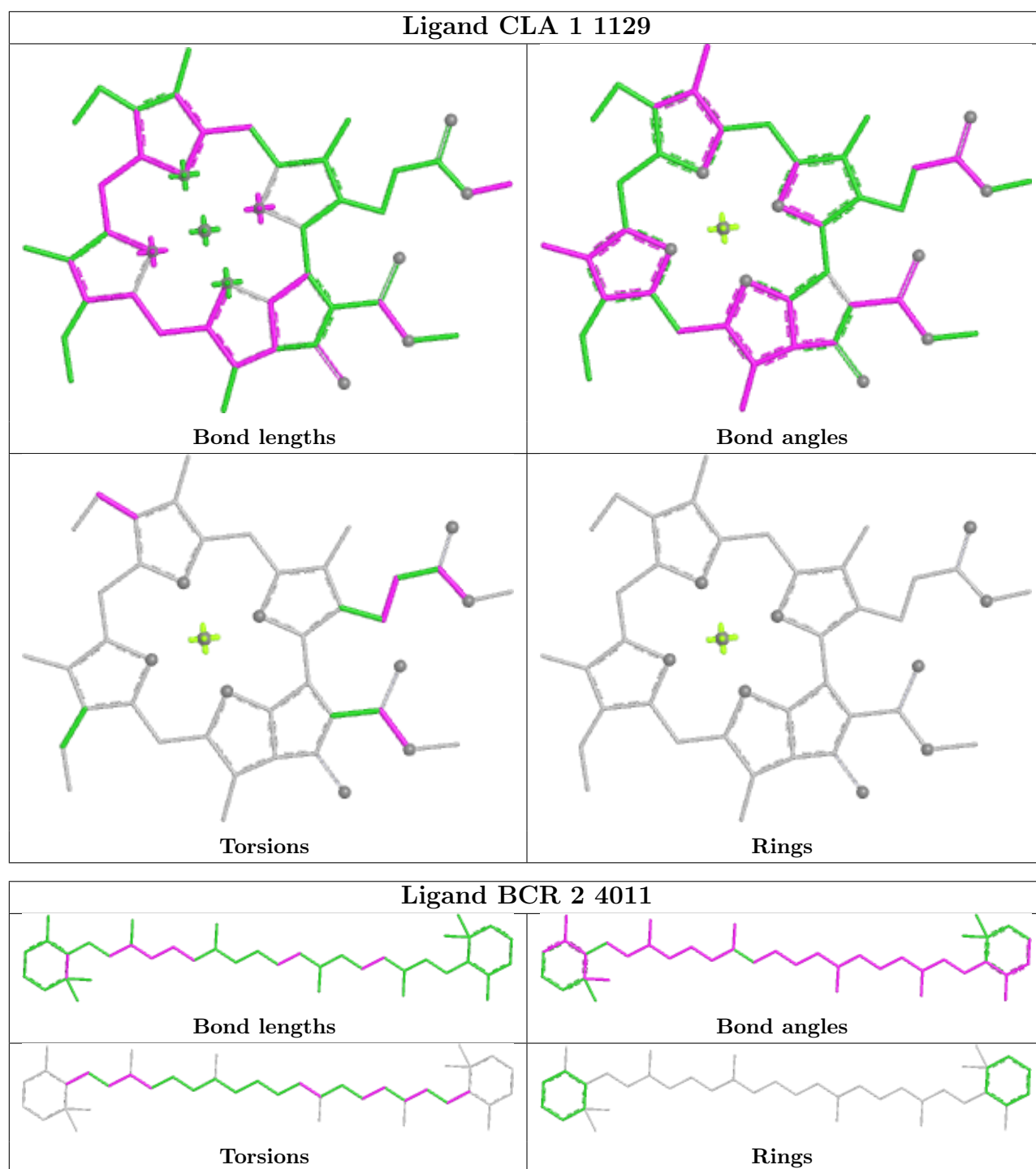


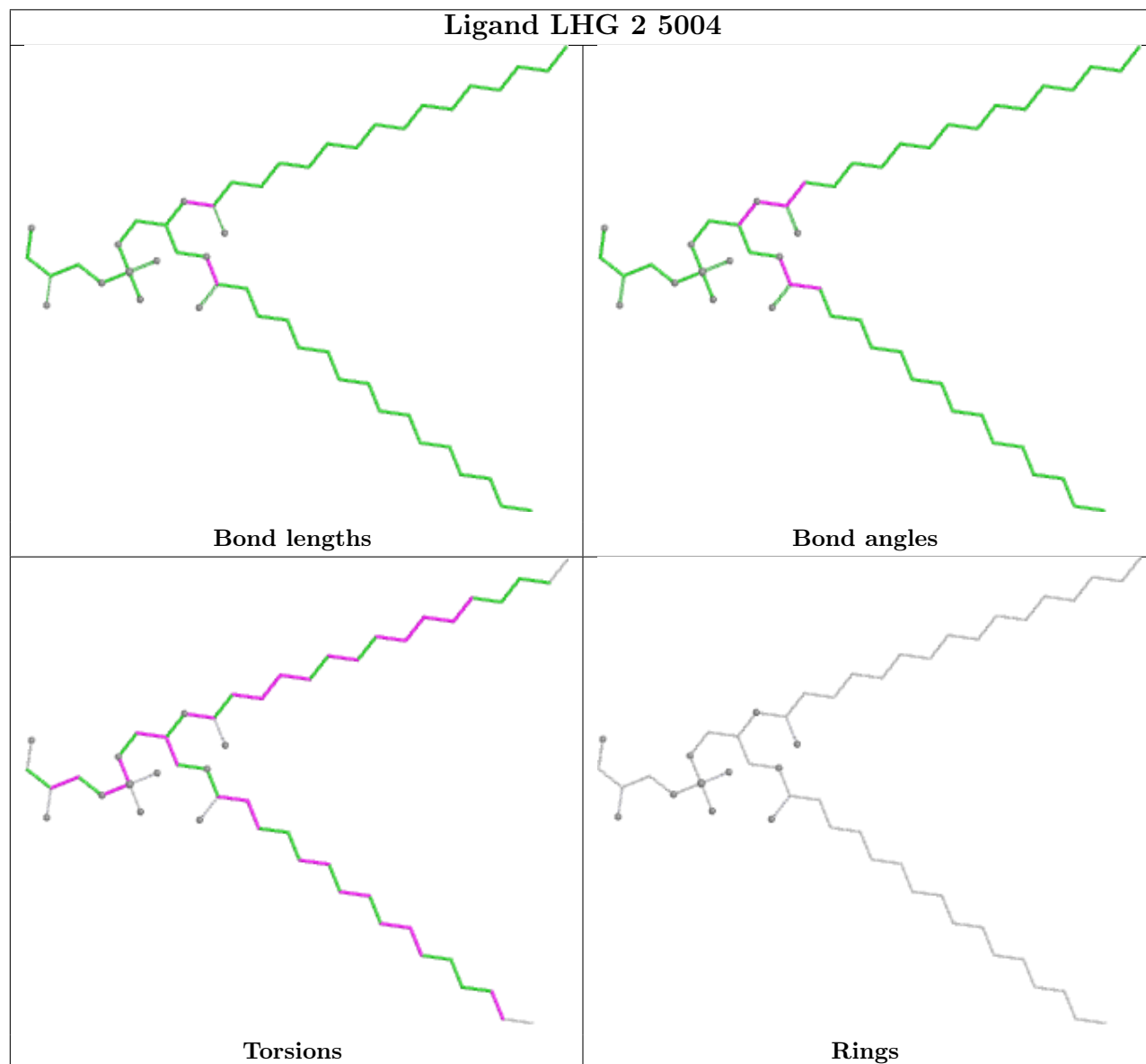
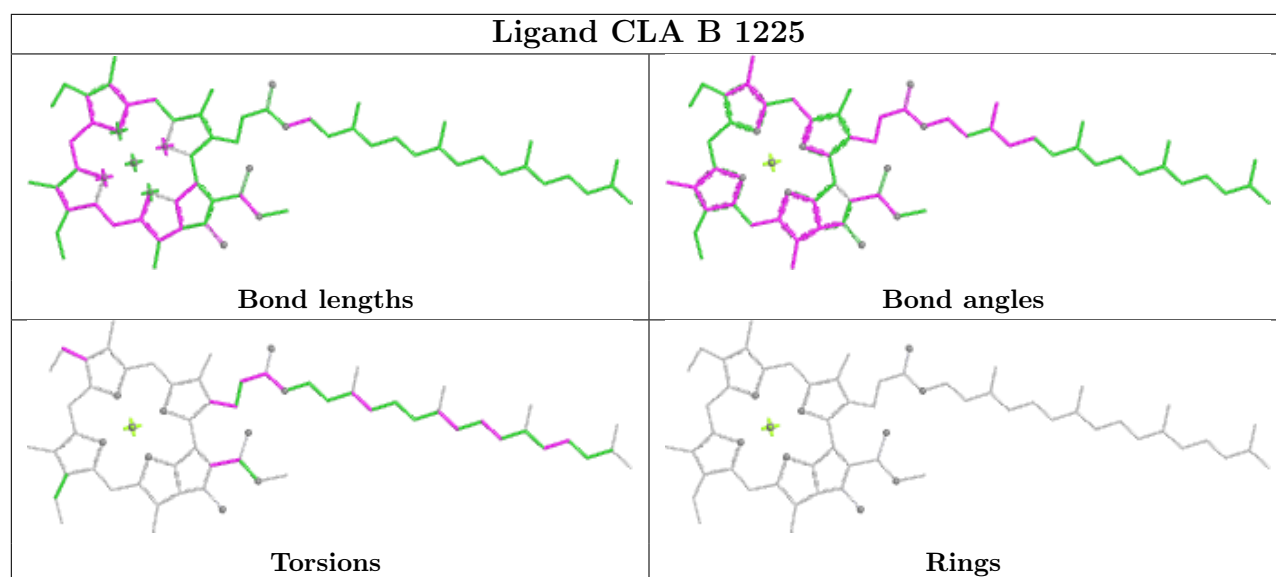


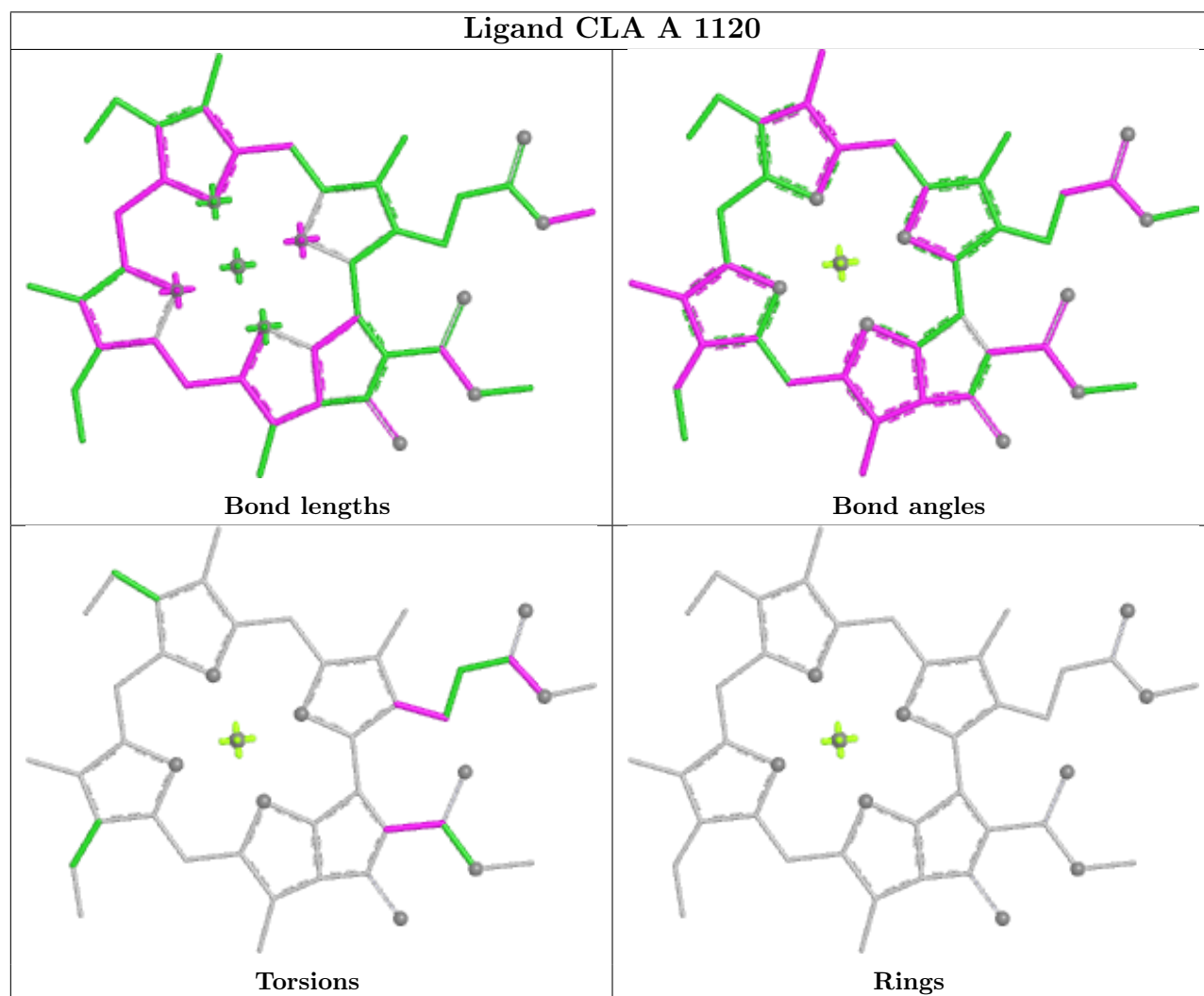
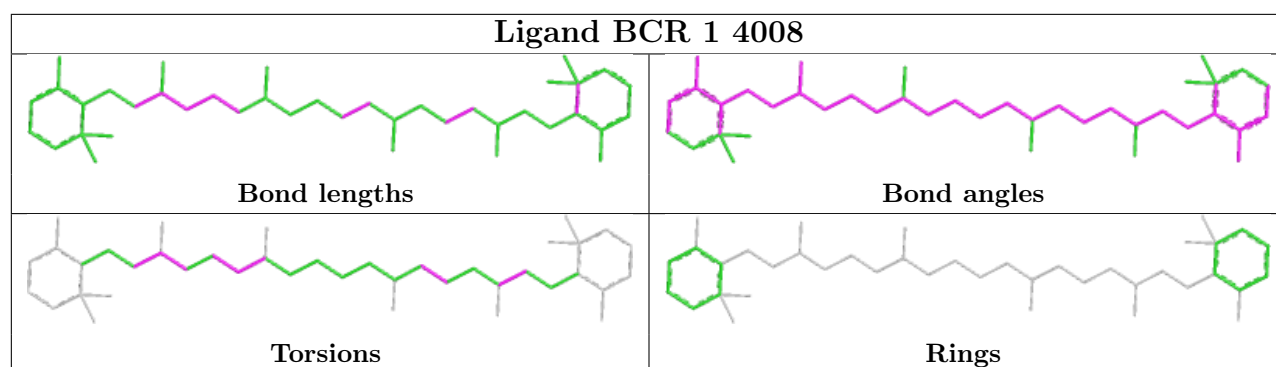




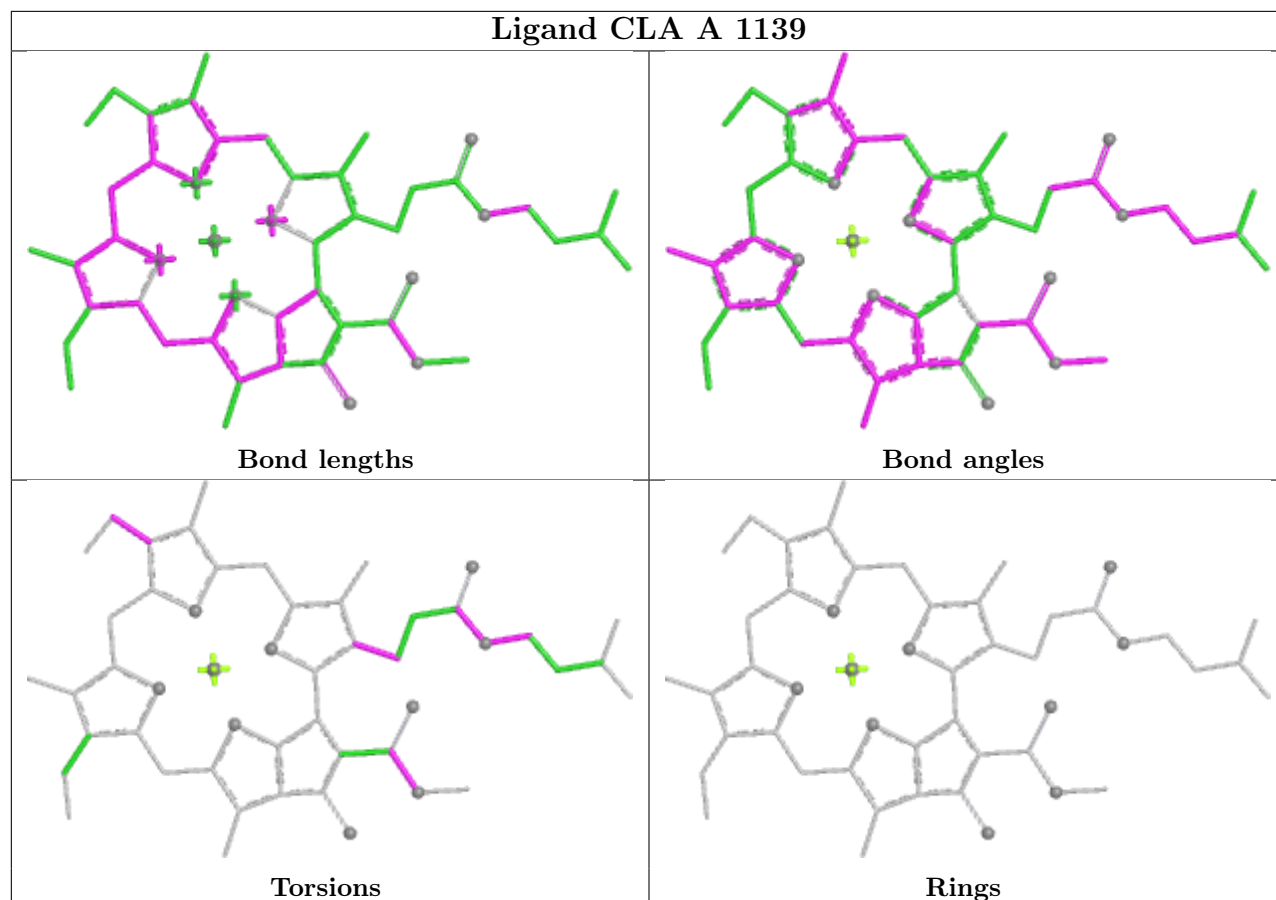
Ligand CLA B 1229**Ligand CLA I 1501**



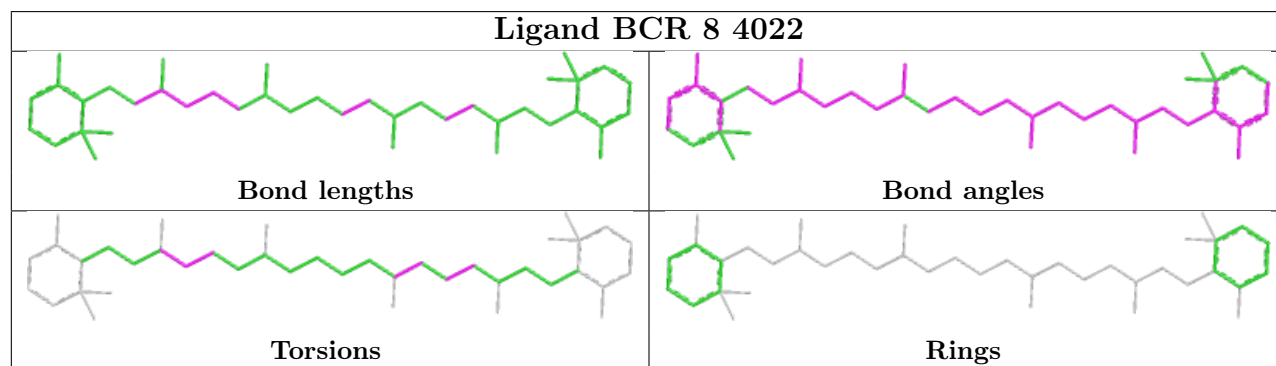


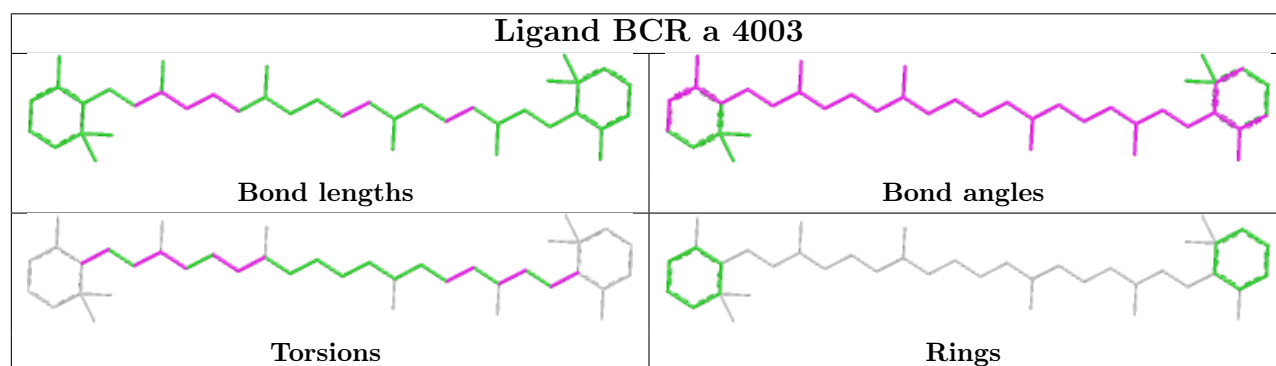
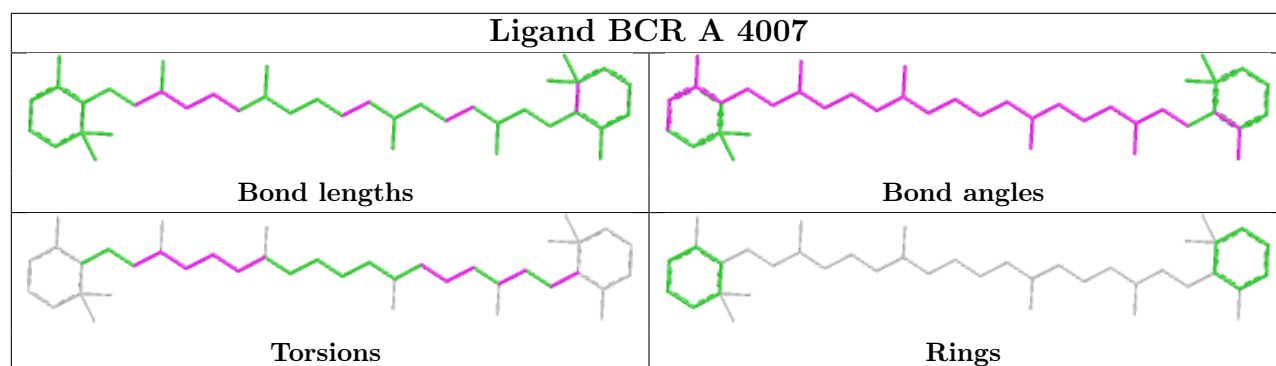
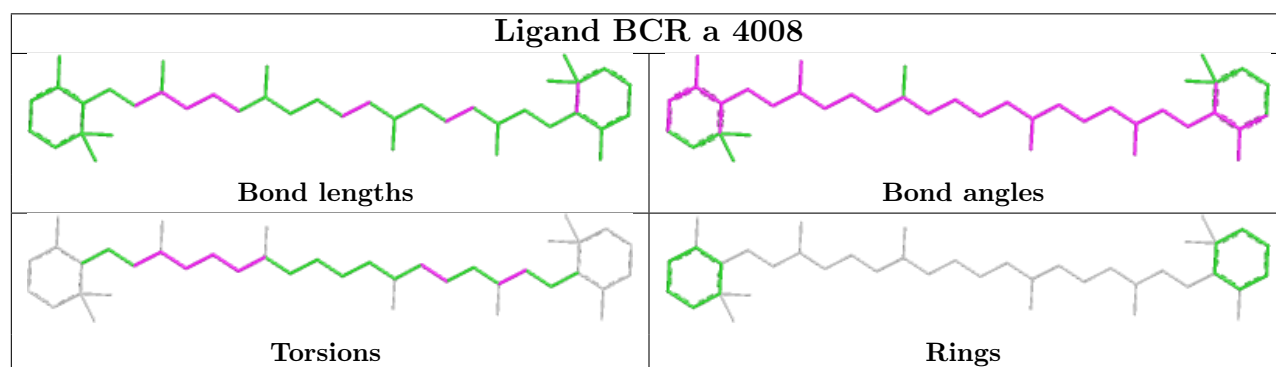
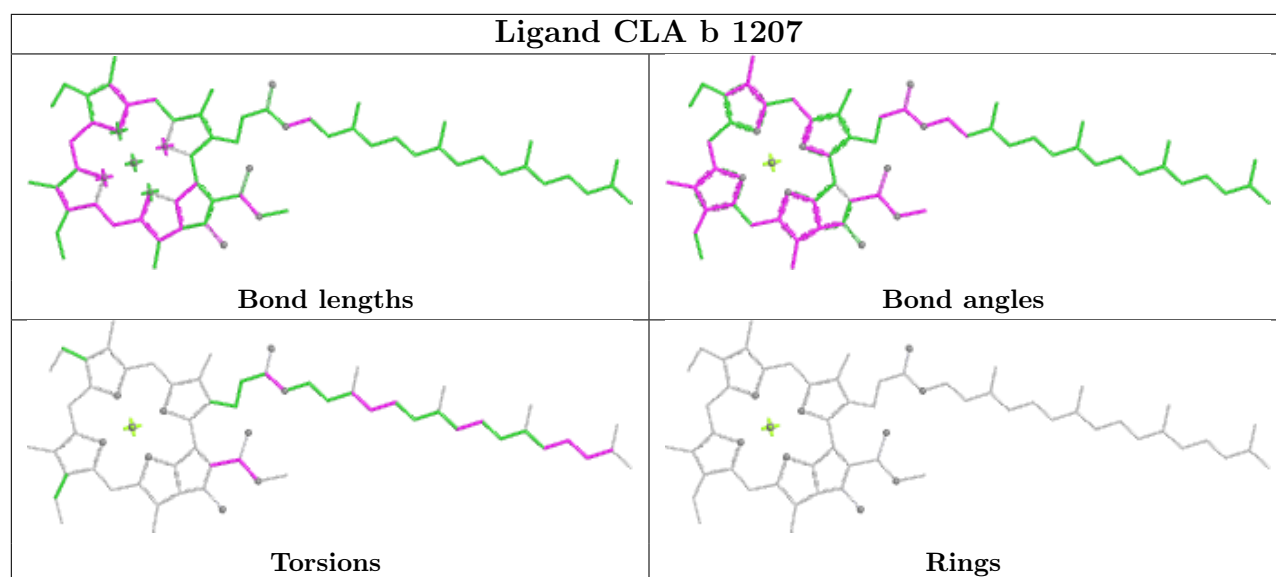


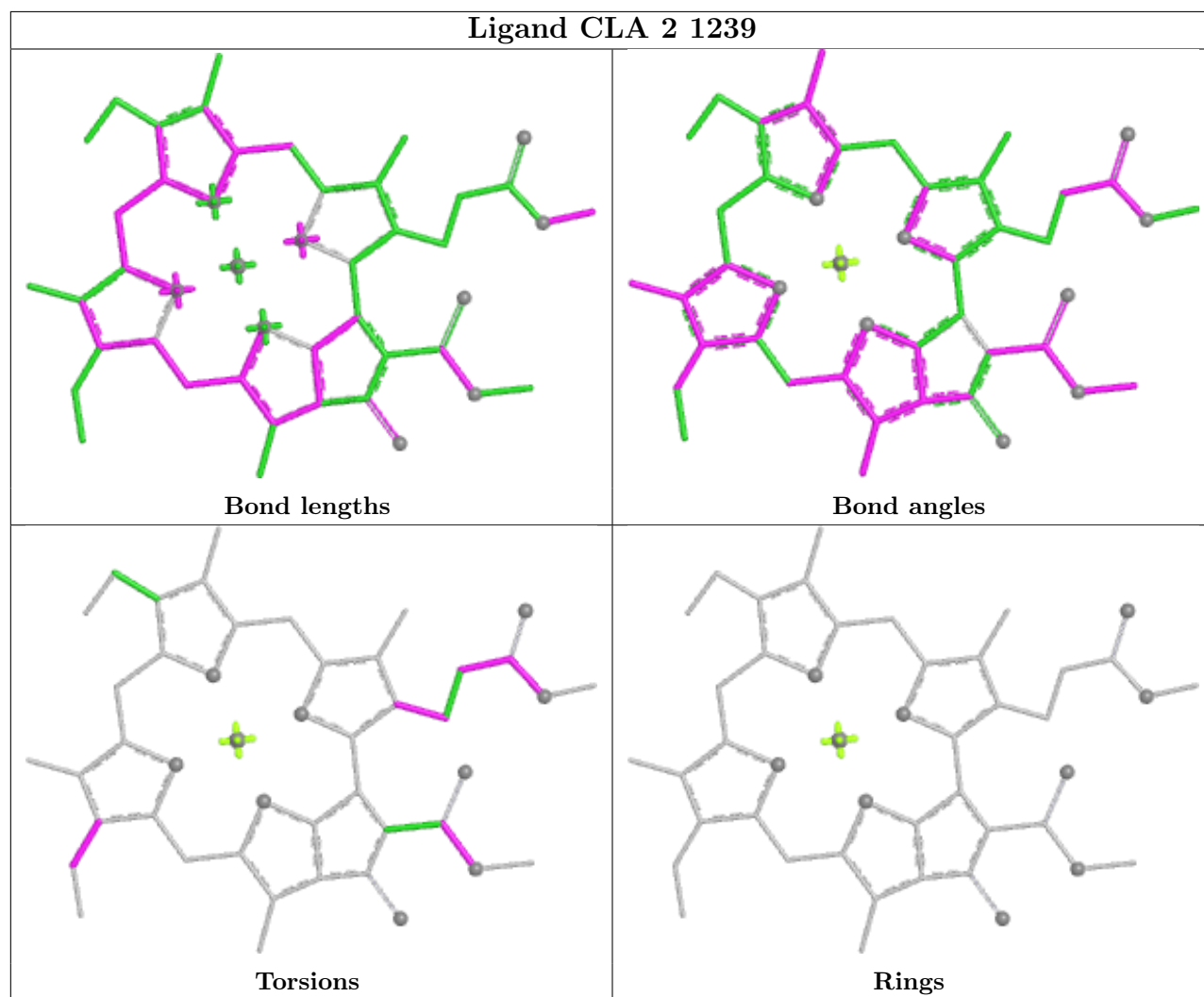
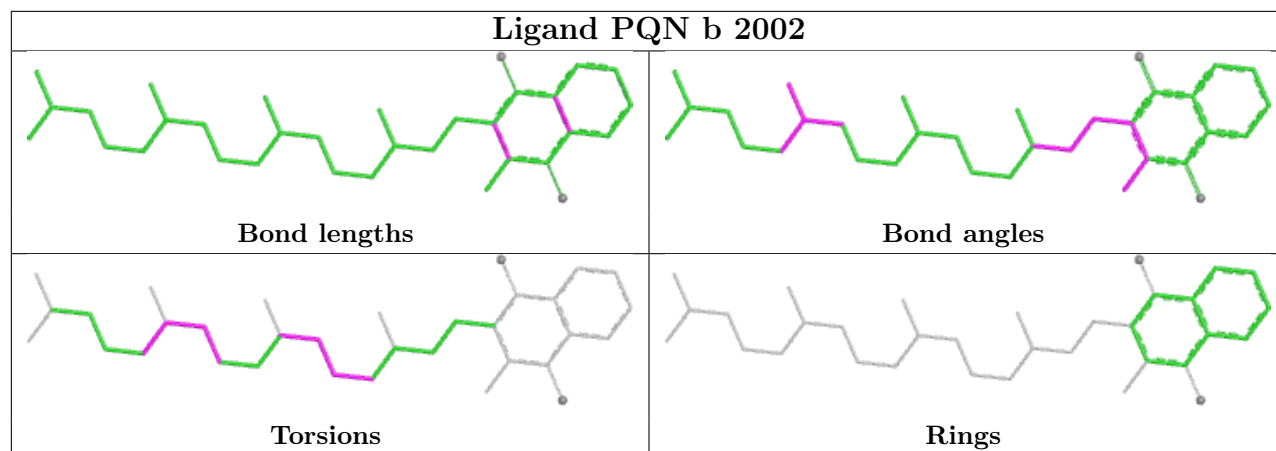
Ligand CLA A 1139

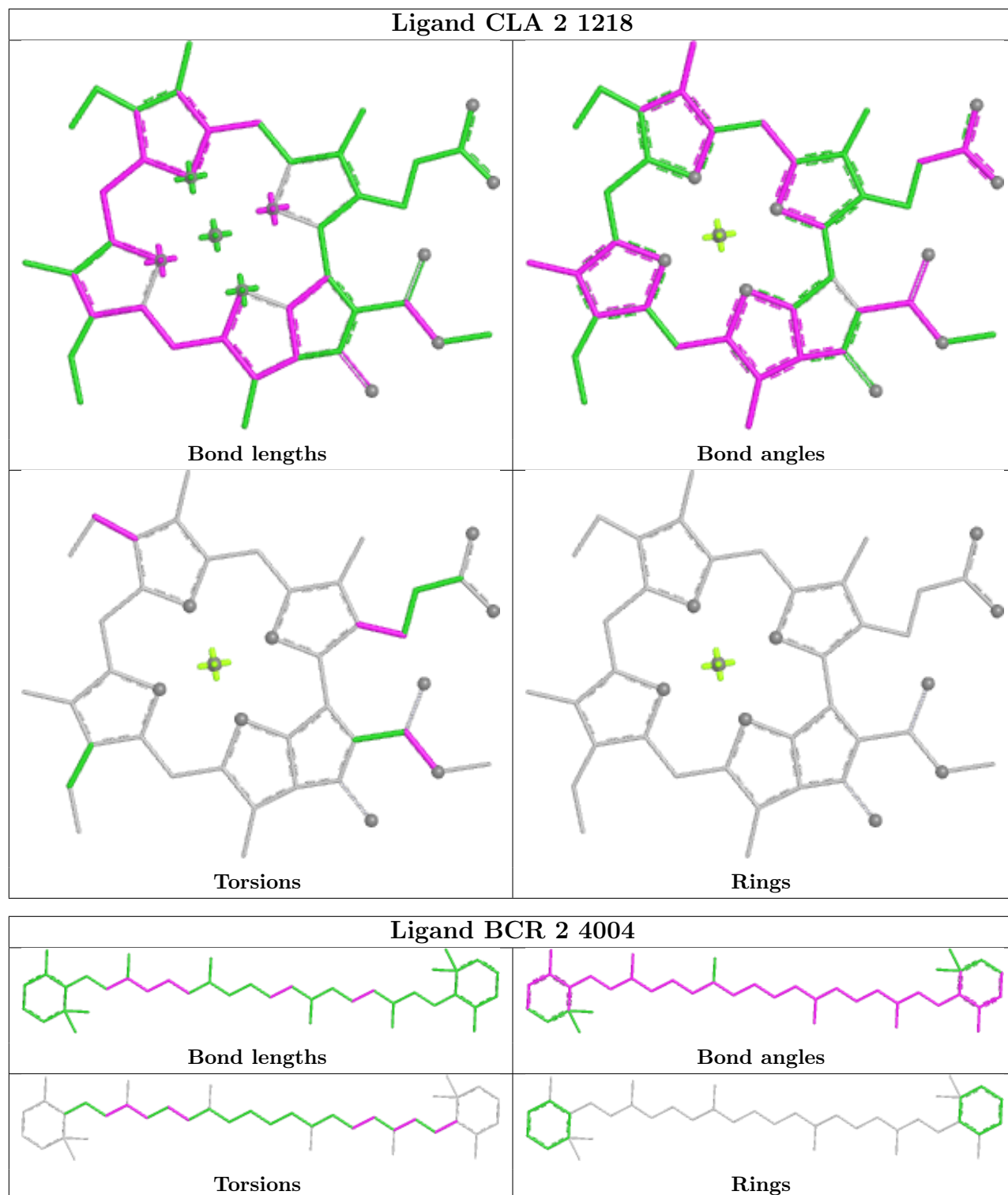


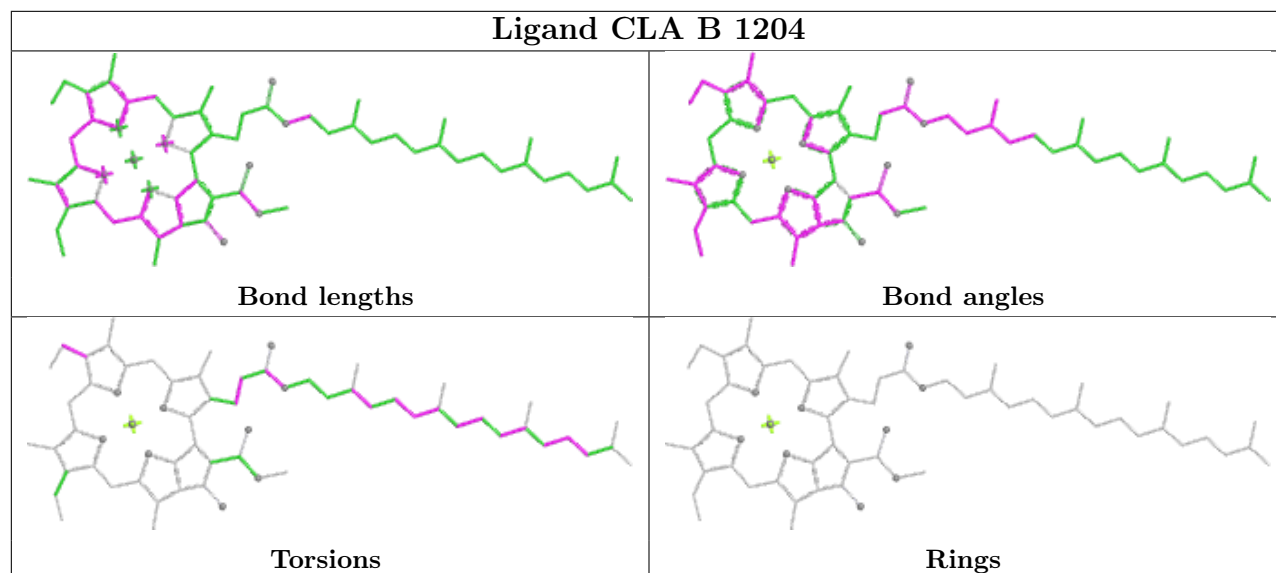
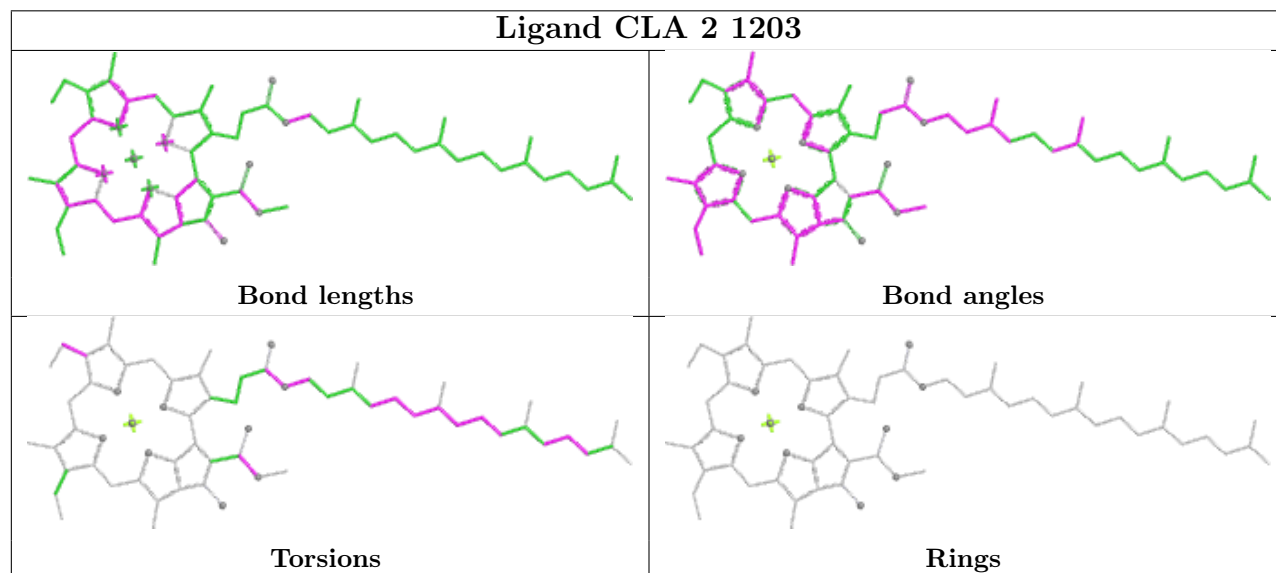
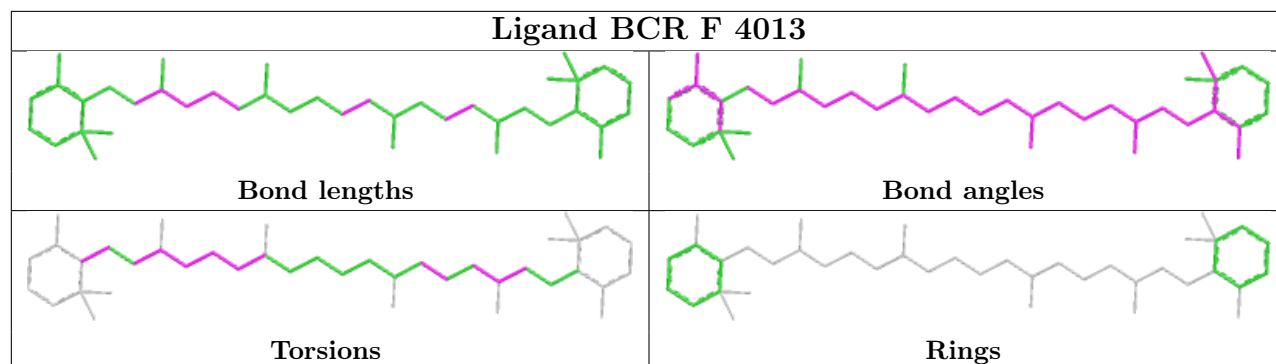
Ligand BCR 8 4022

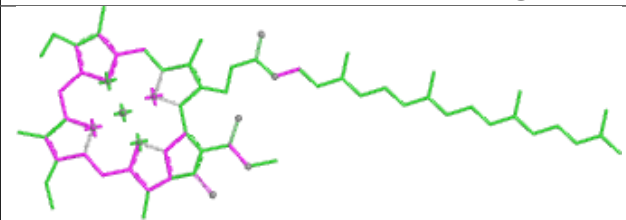
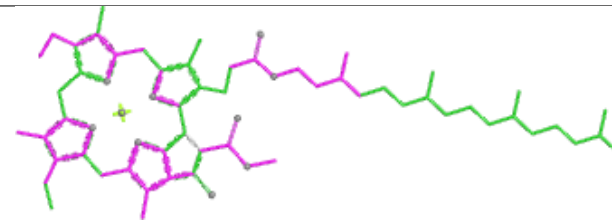
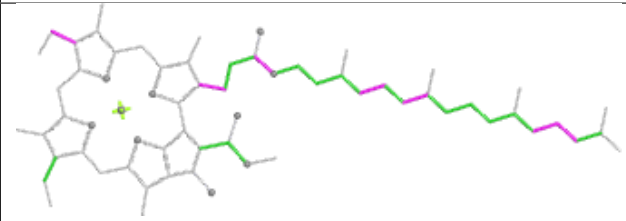
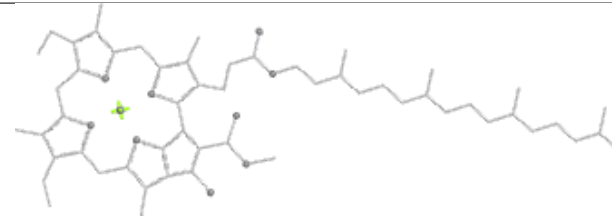


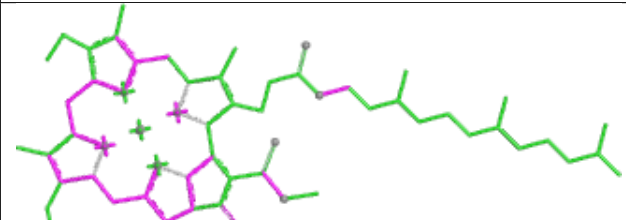
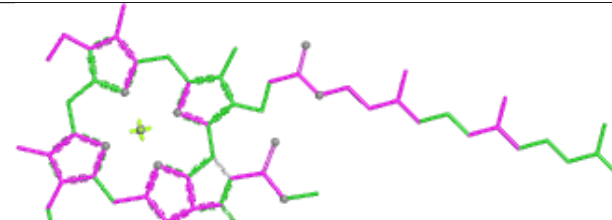
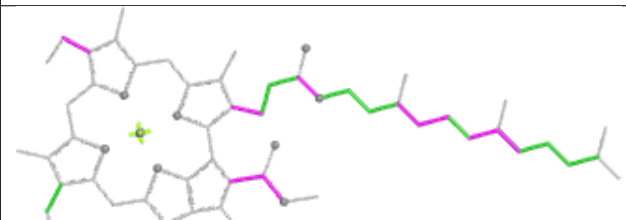
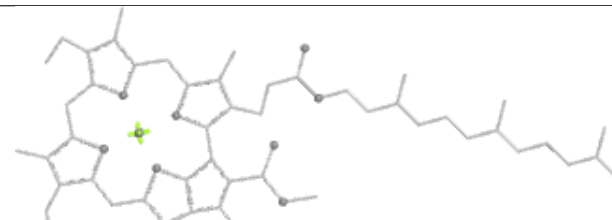


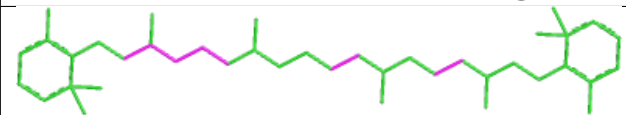
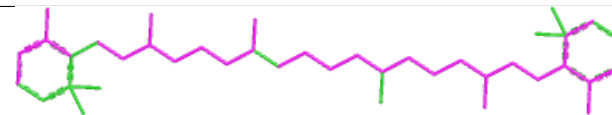
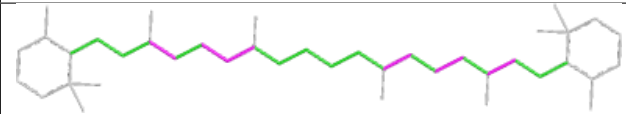
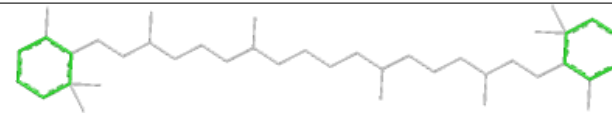


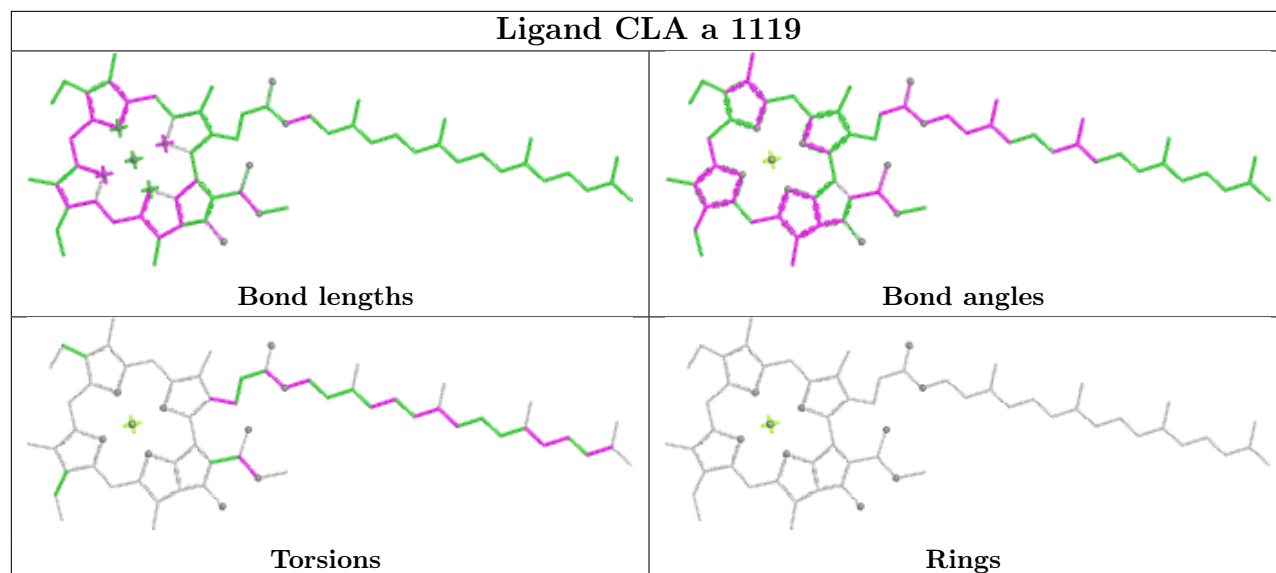
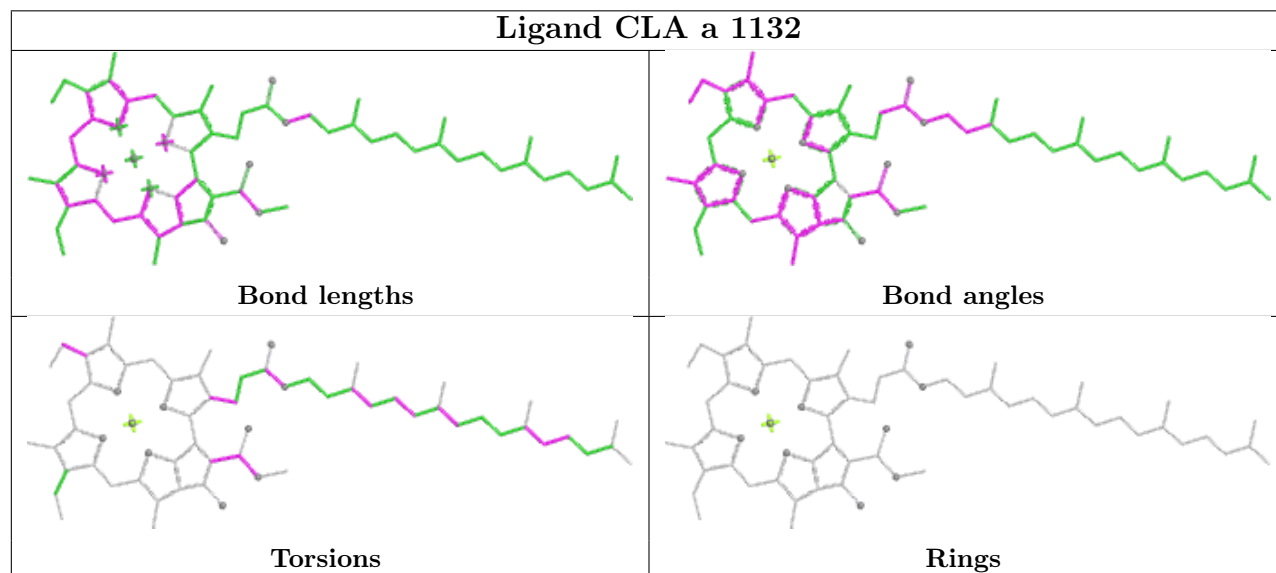
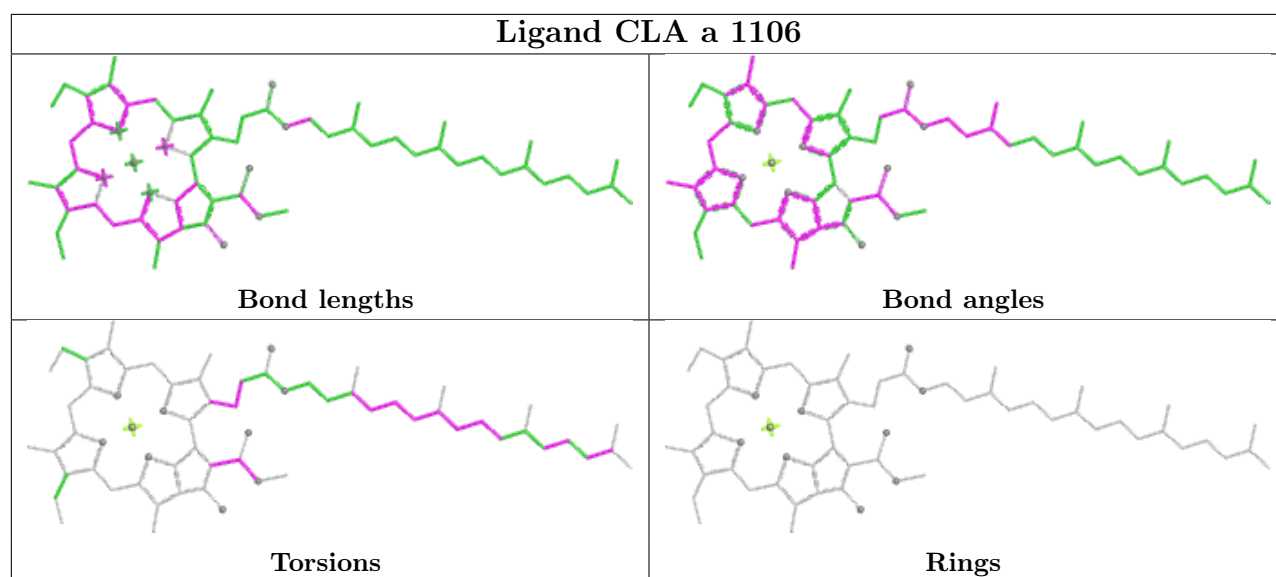


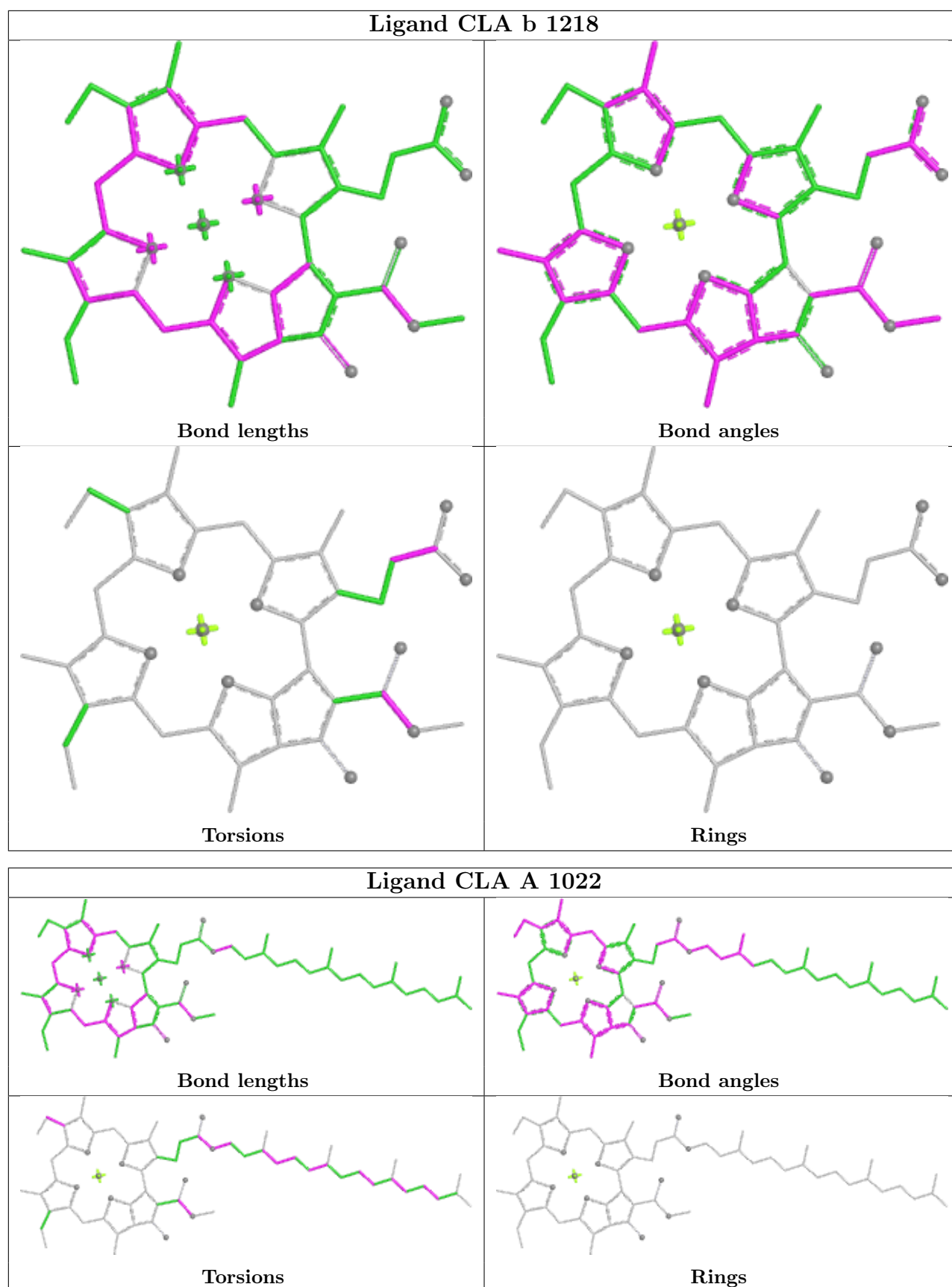


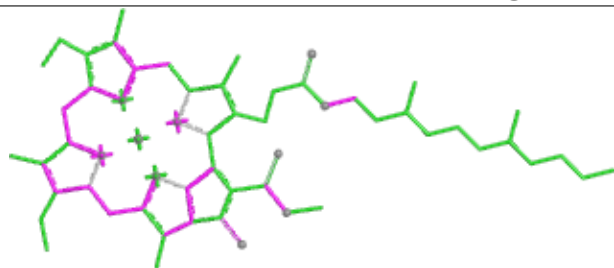
Ligand CLA B 1216	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA 2 1234	
	
Bond lengths	Bond angles
	
Torsions	Rings

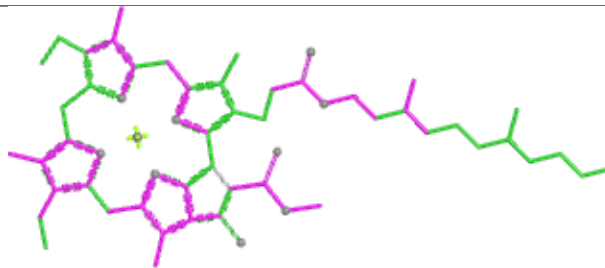
Ligand BCR L 4022	
	
Bond lengths	Bond angles
	
Torsions	Rings



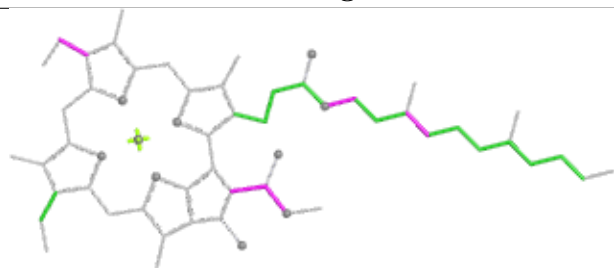


Ligand CLA B 1230

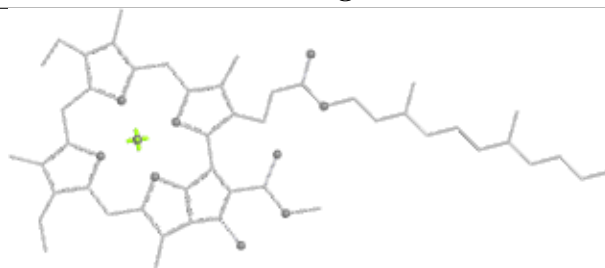
Bond lengths



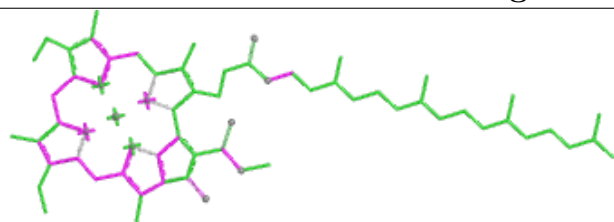
Bond angles



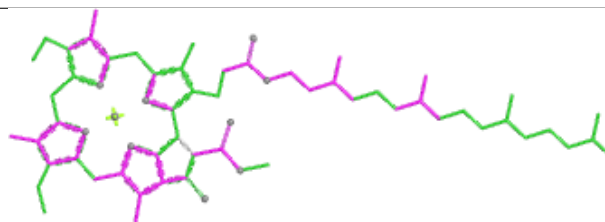
Torsions



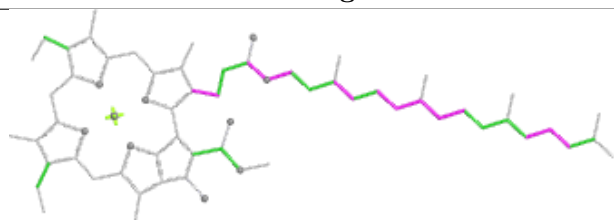
Rings

Ligand CLA a 1137

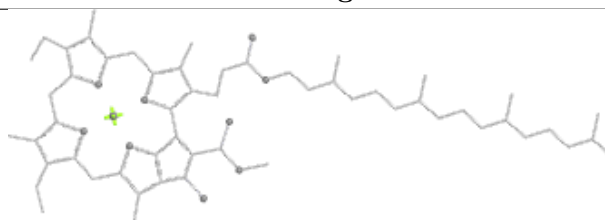
Bond lengths



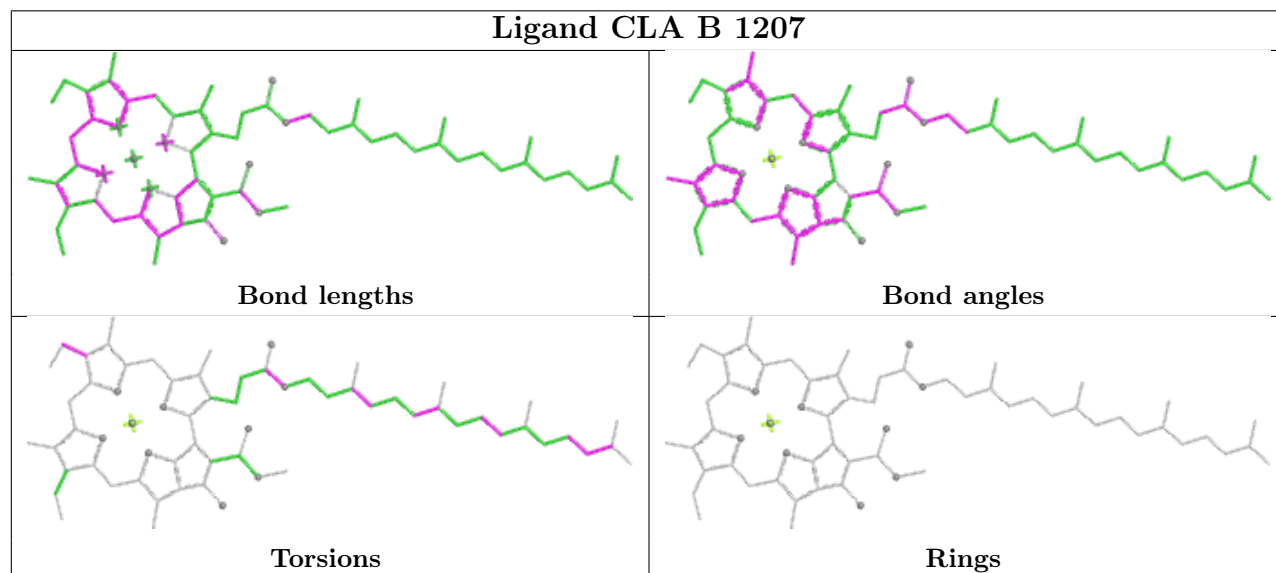
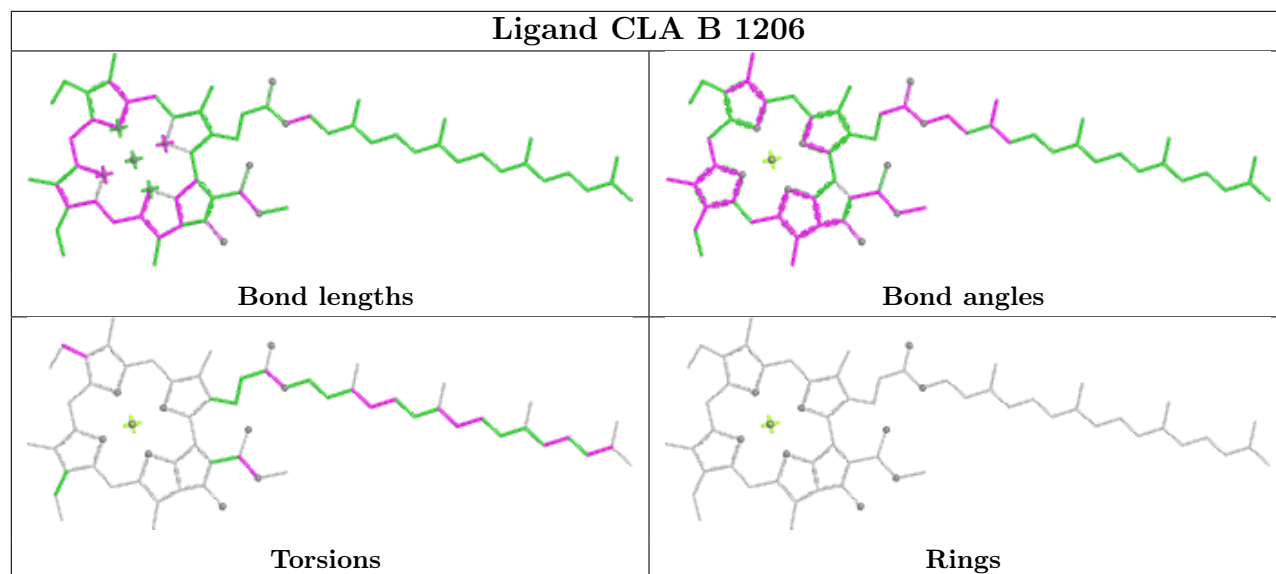
Bond angles



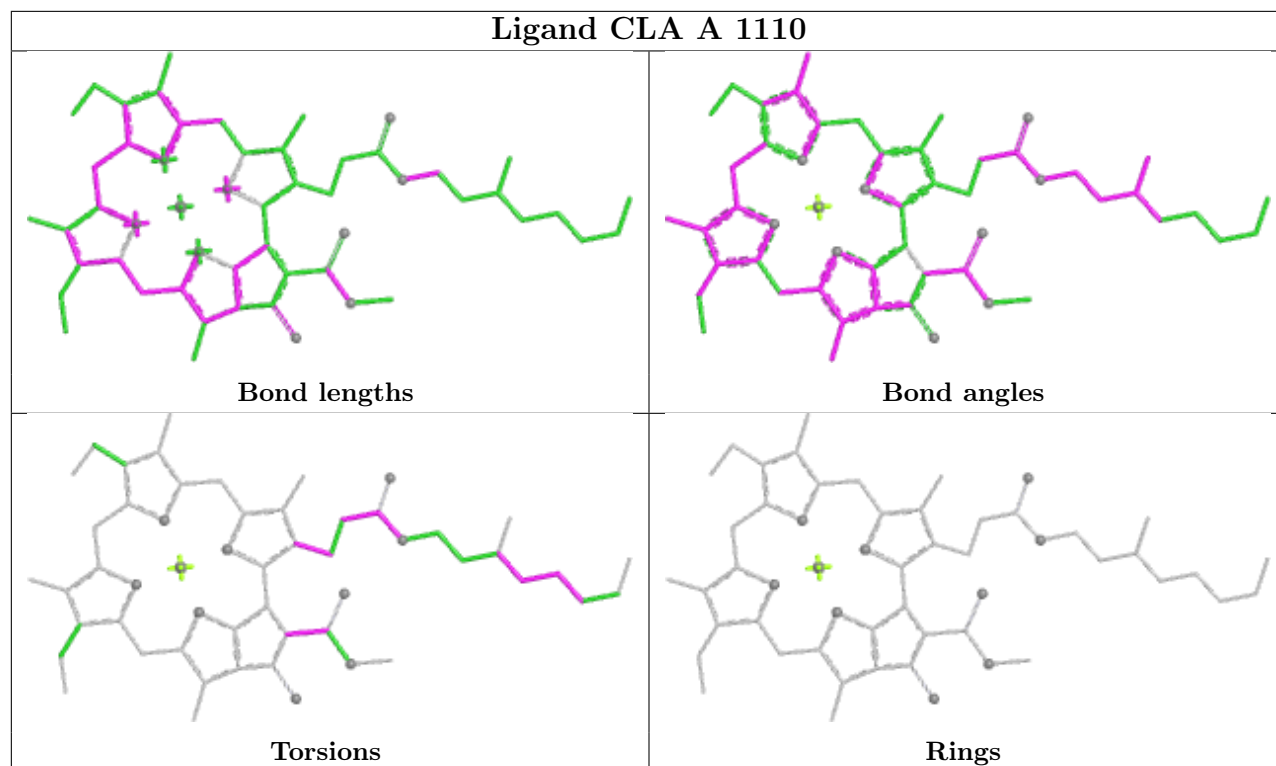
Torsions



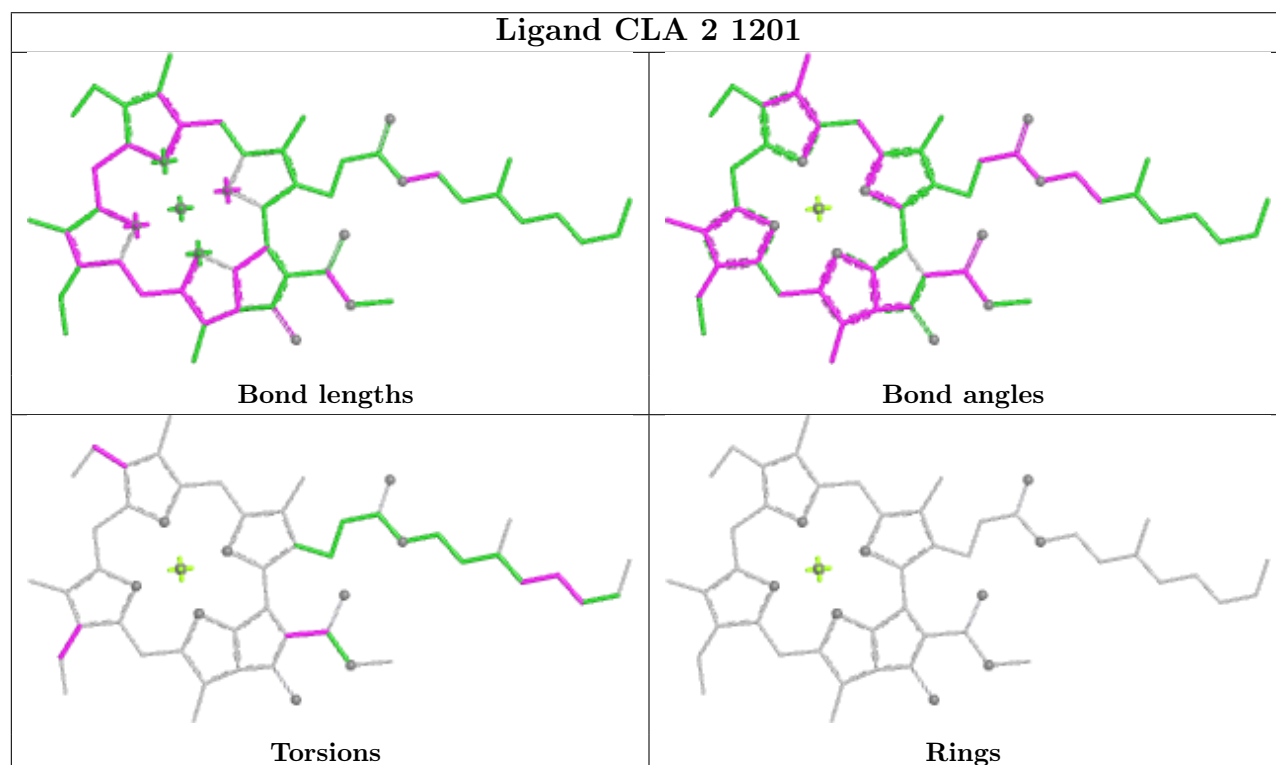
Rings

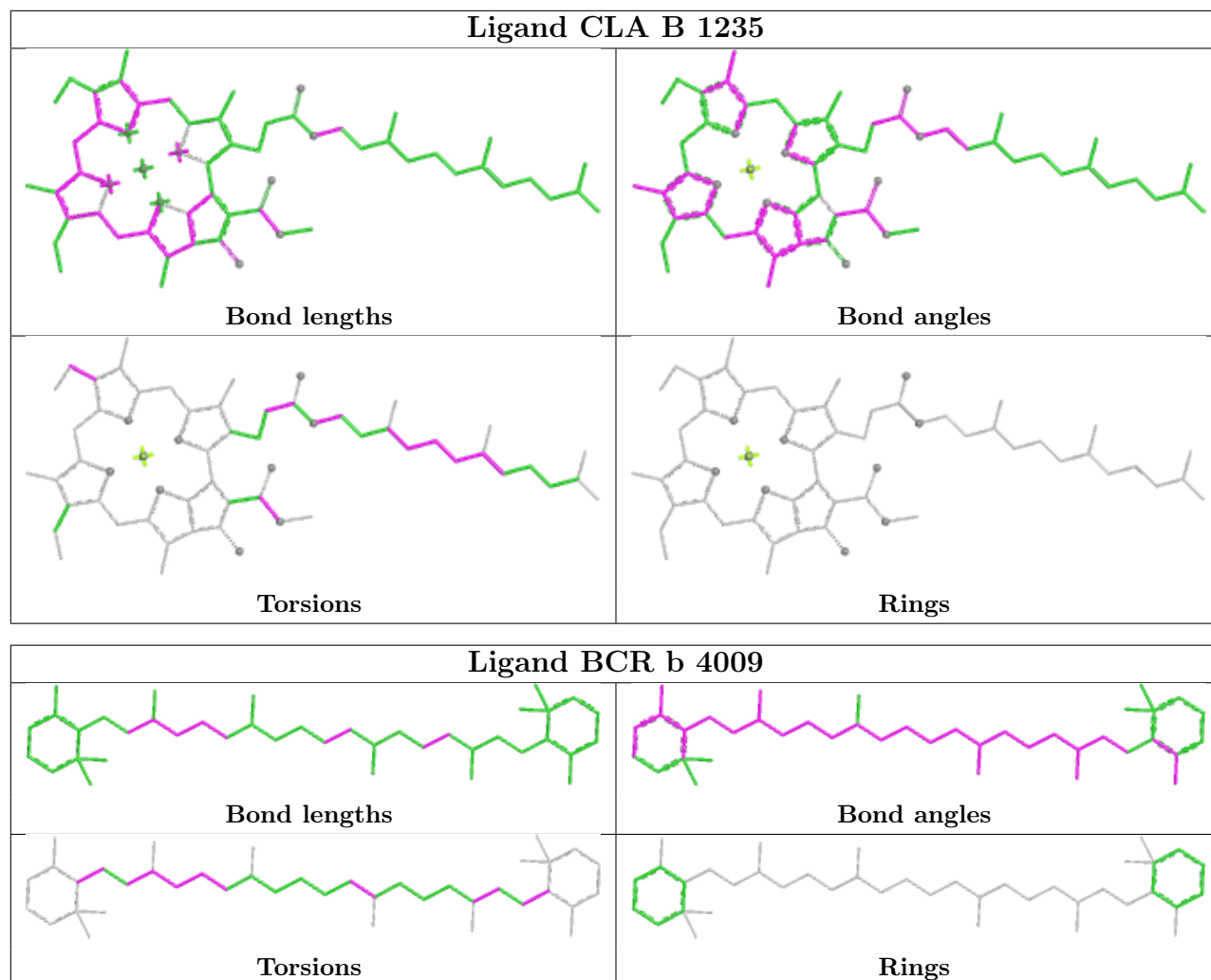


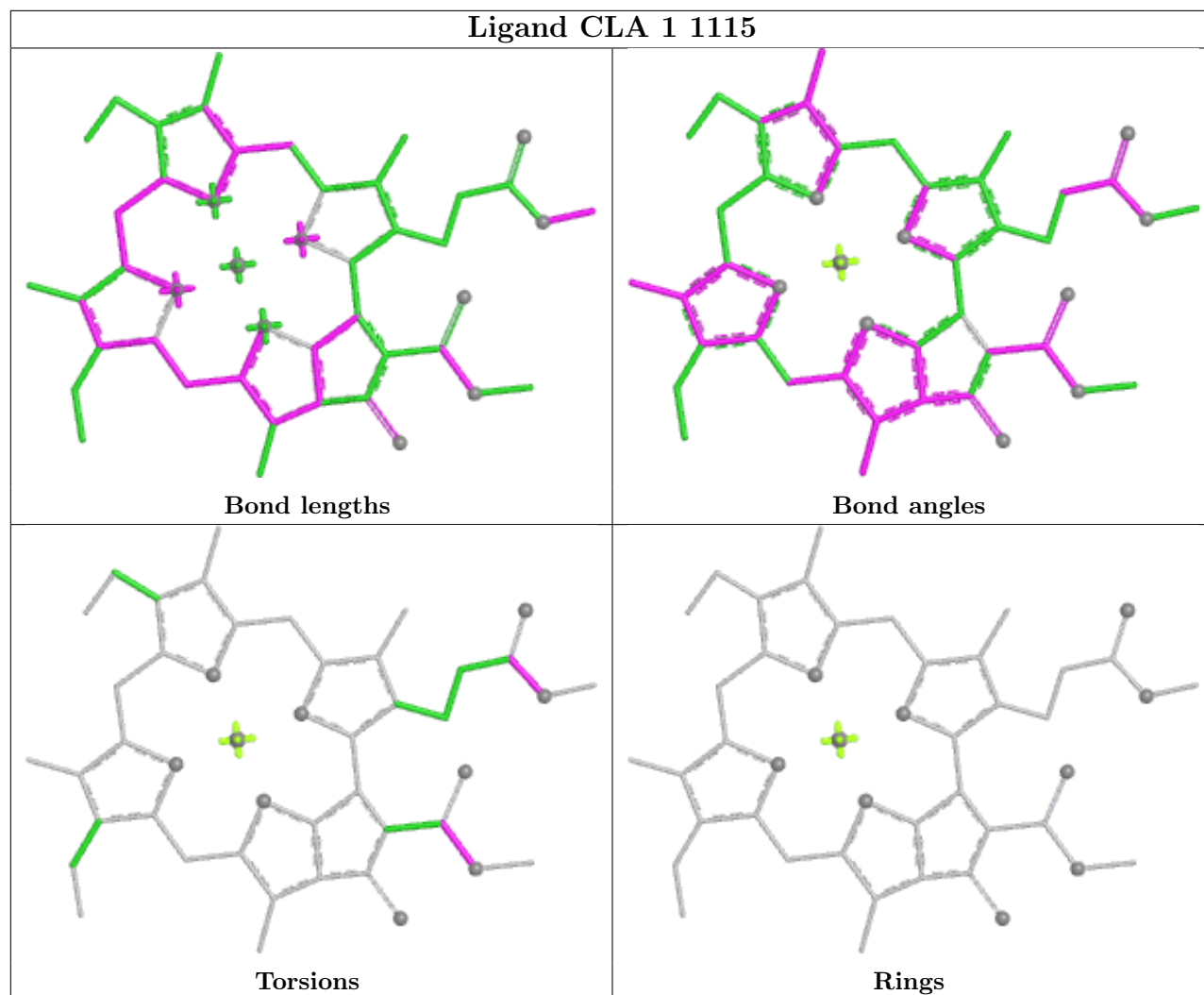
Ligand CLA A 1110

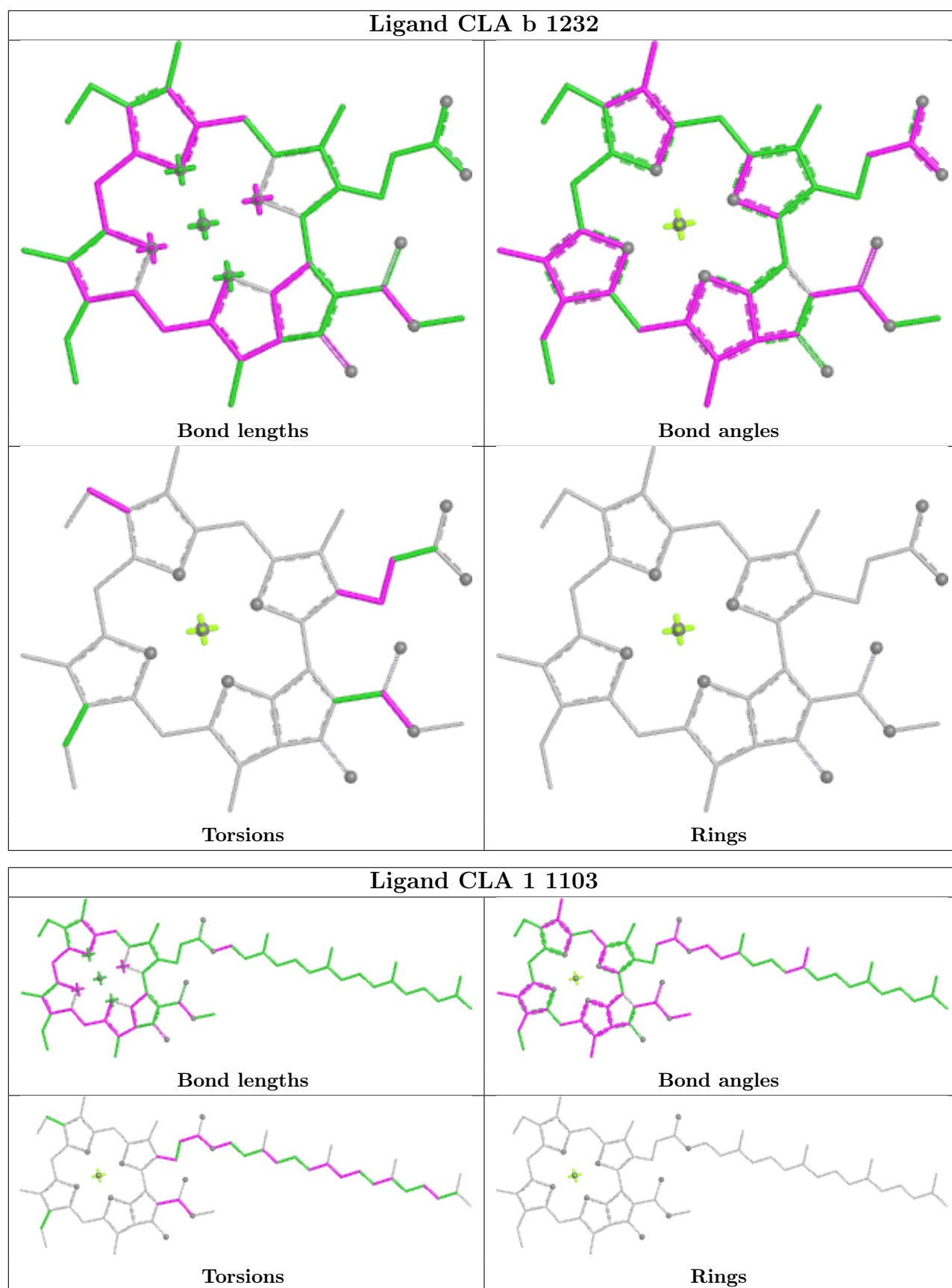


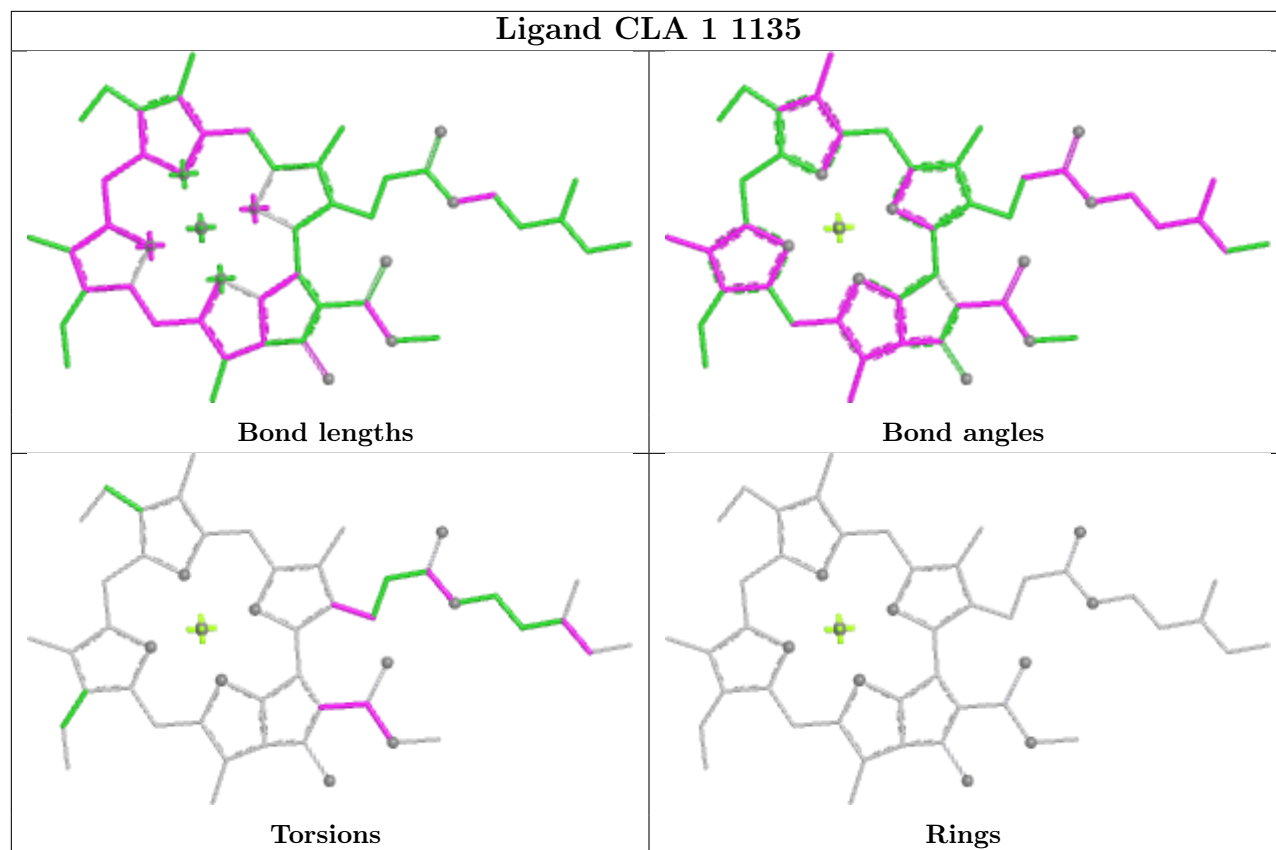
Ligand CLA 2 1201



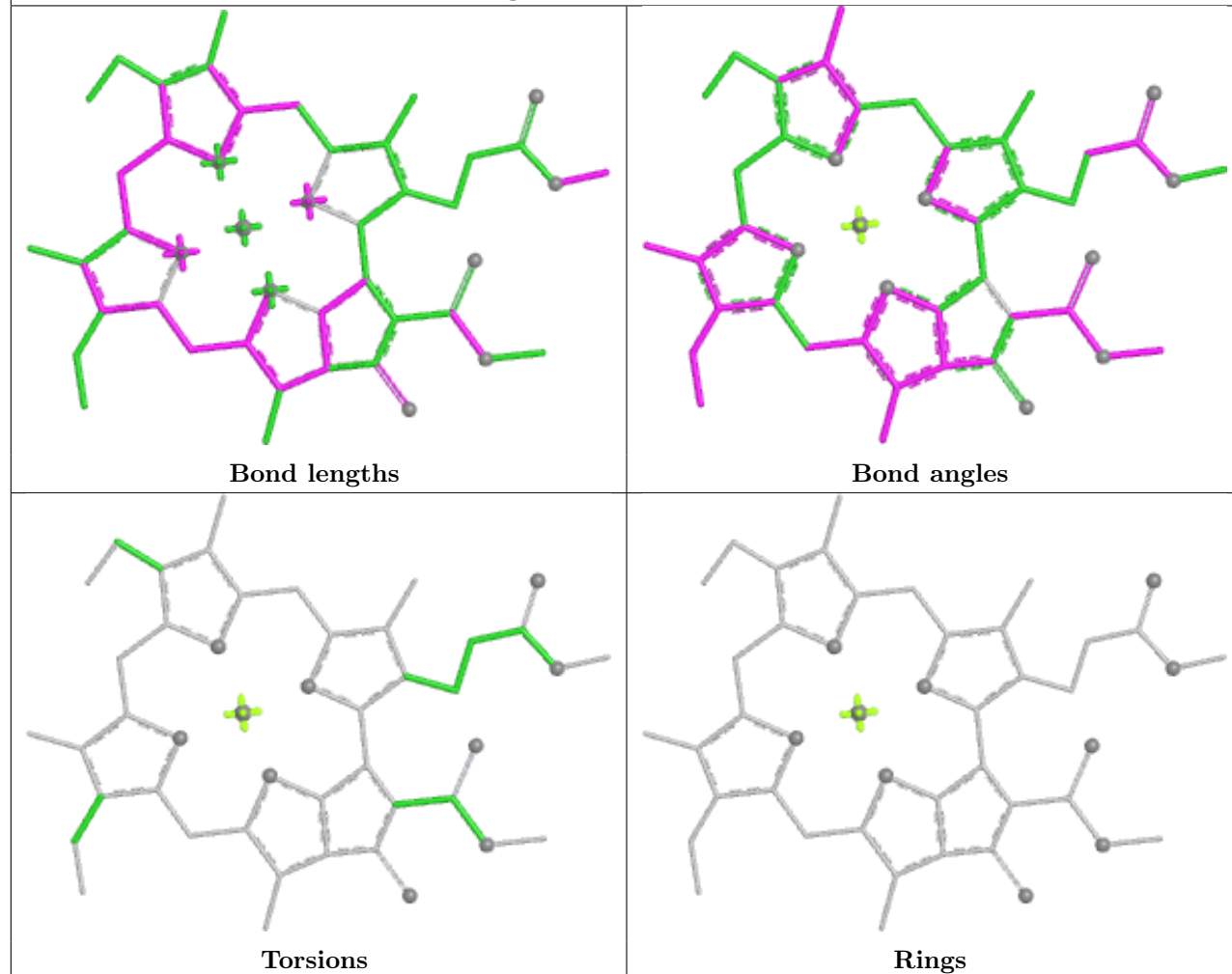


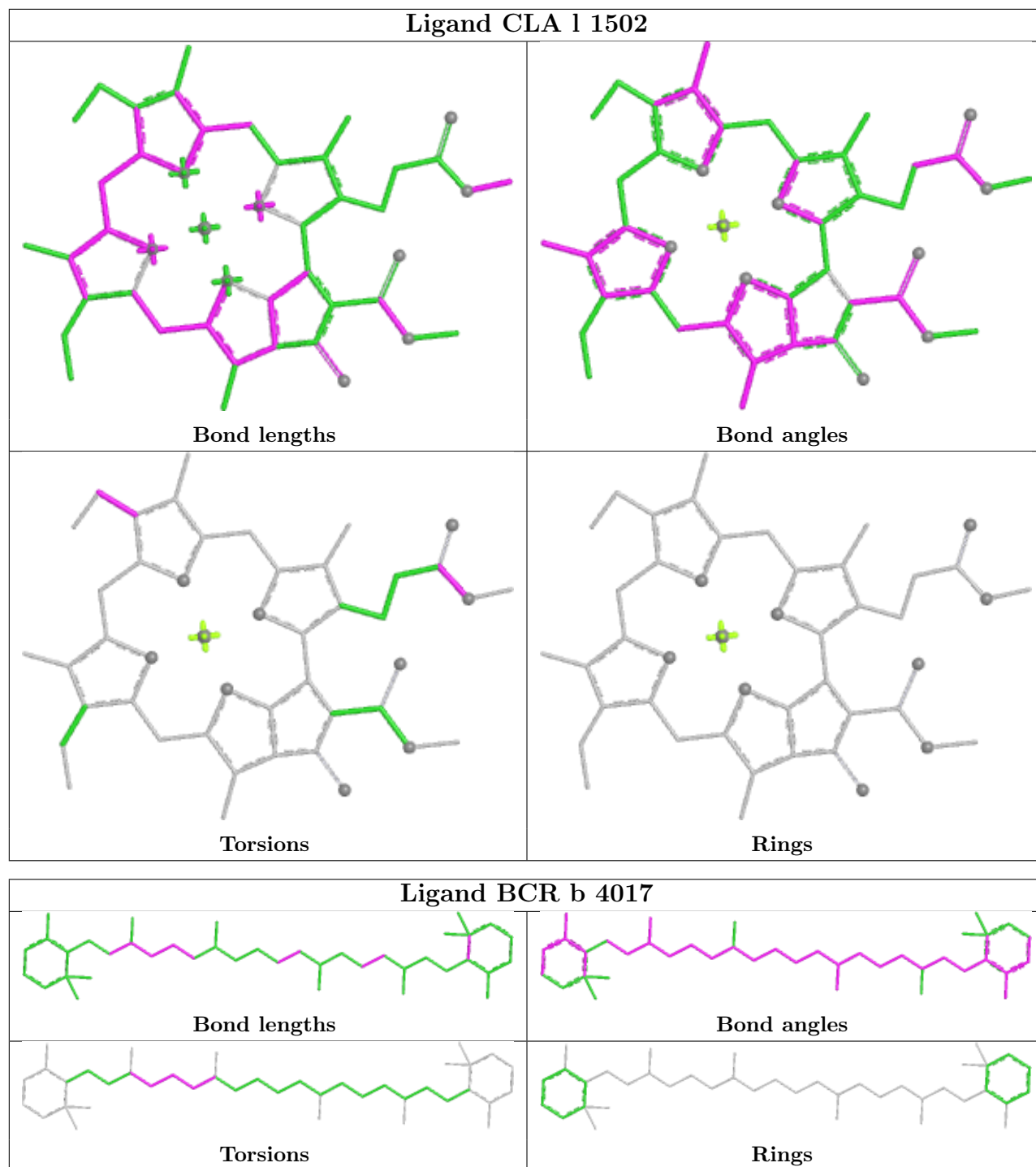


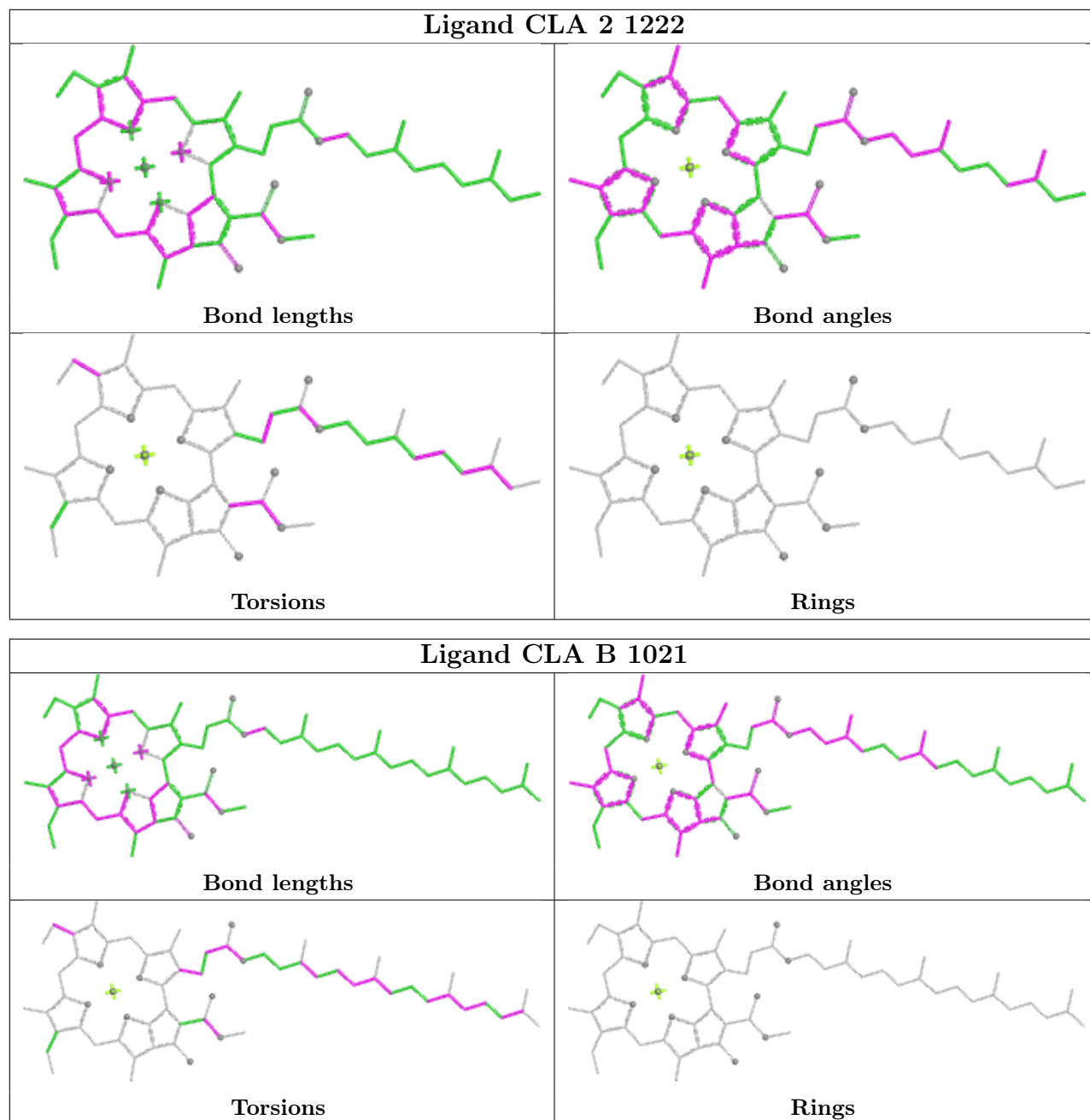


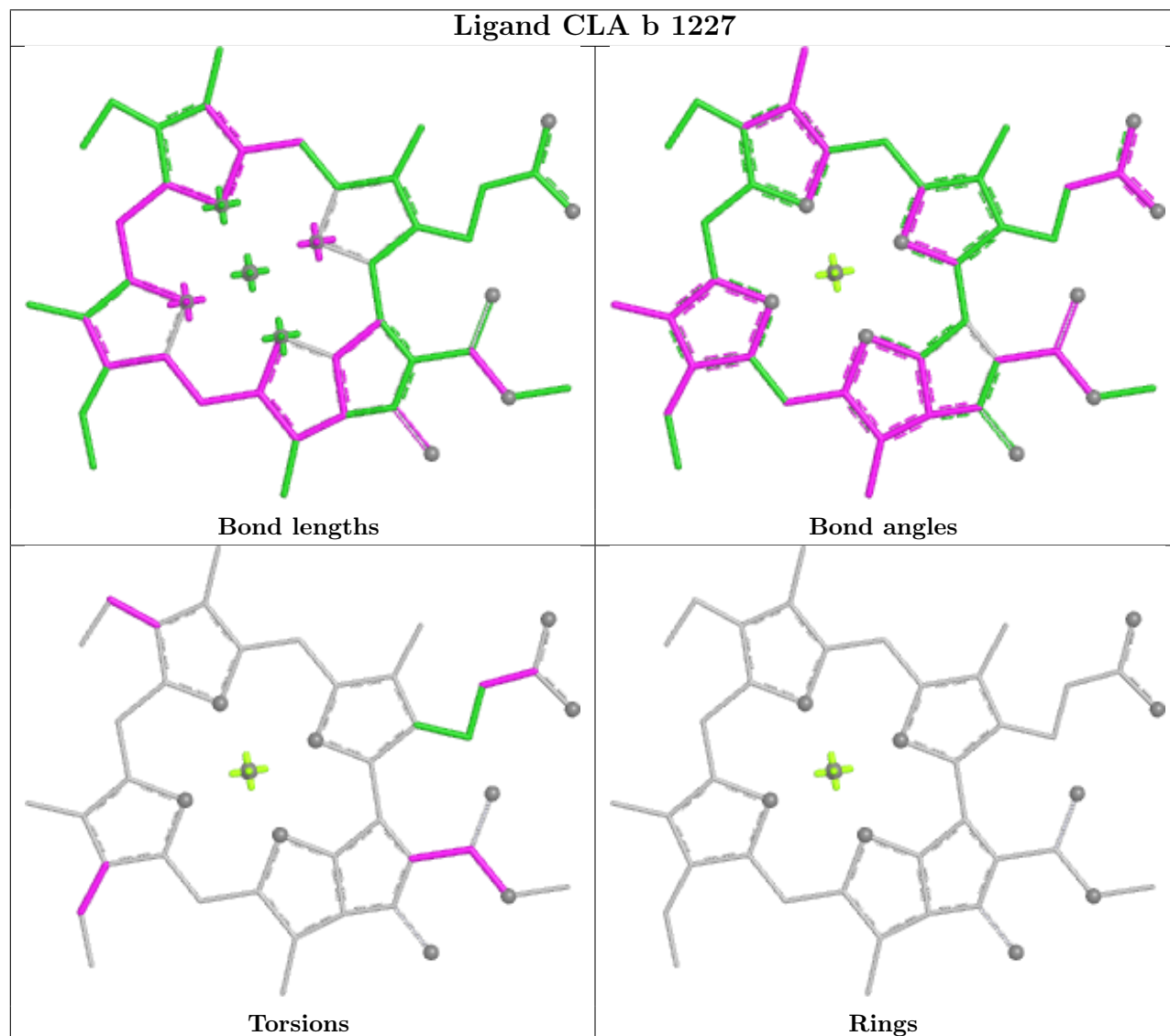
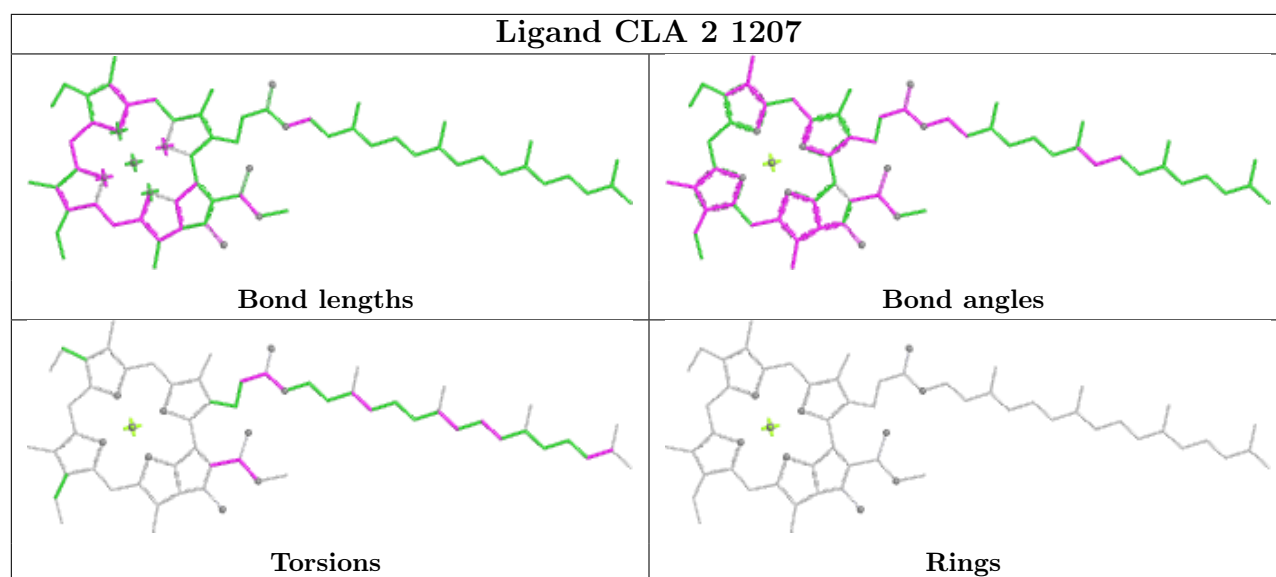


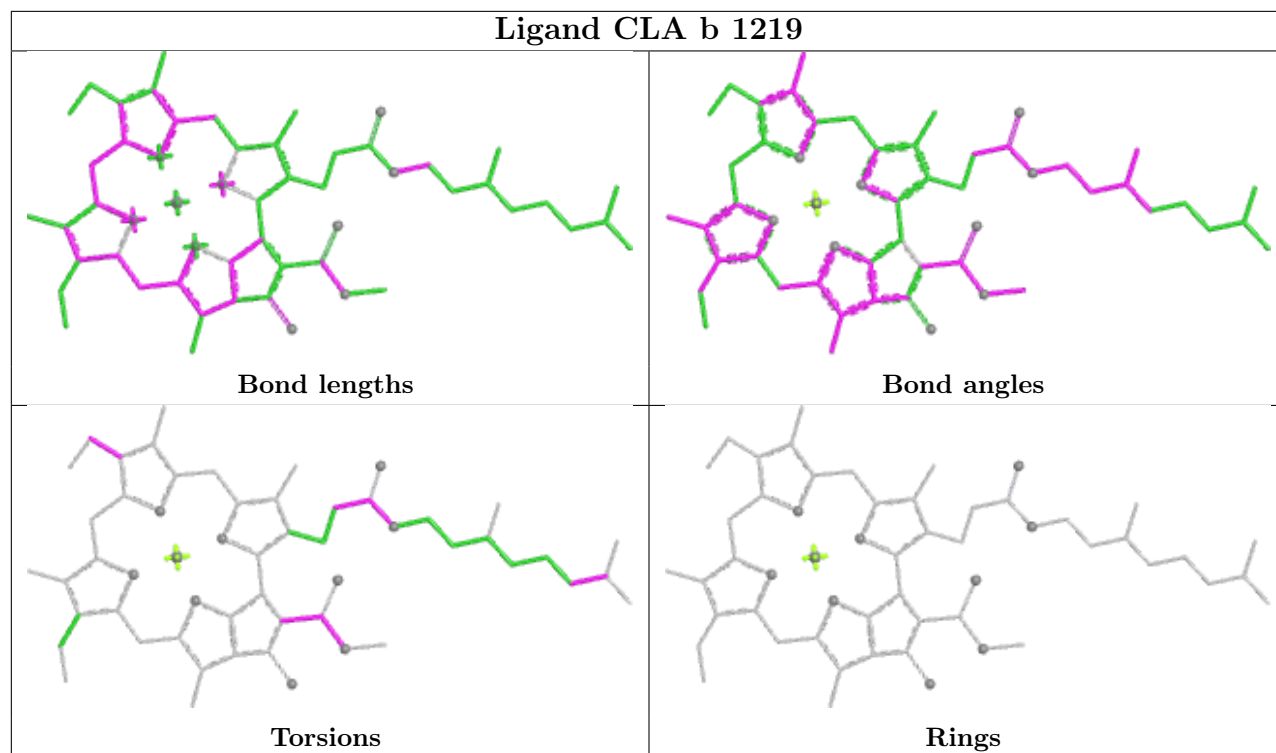
Ligand CLA A 1138

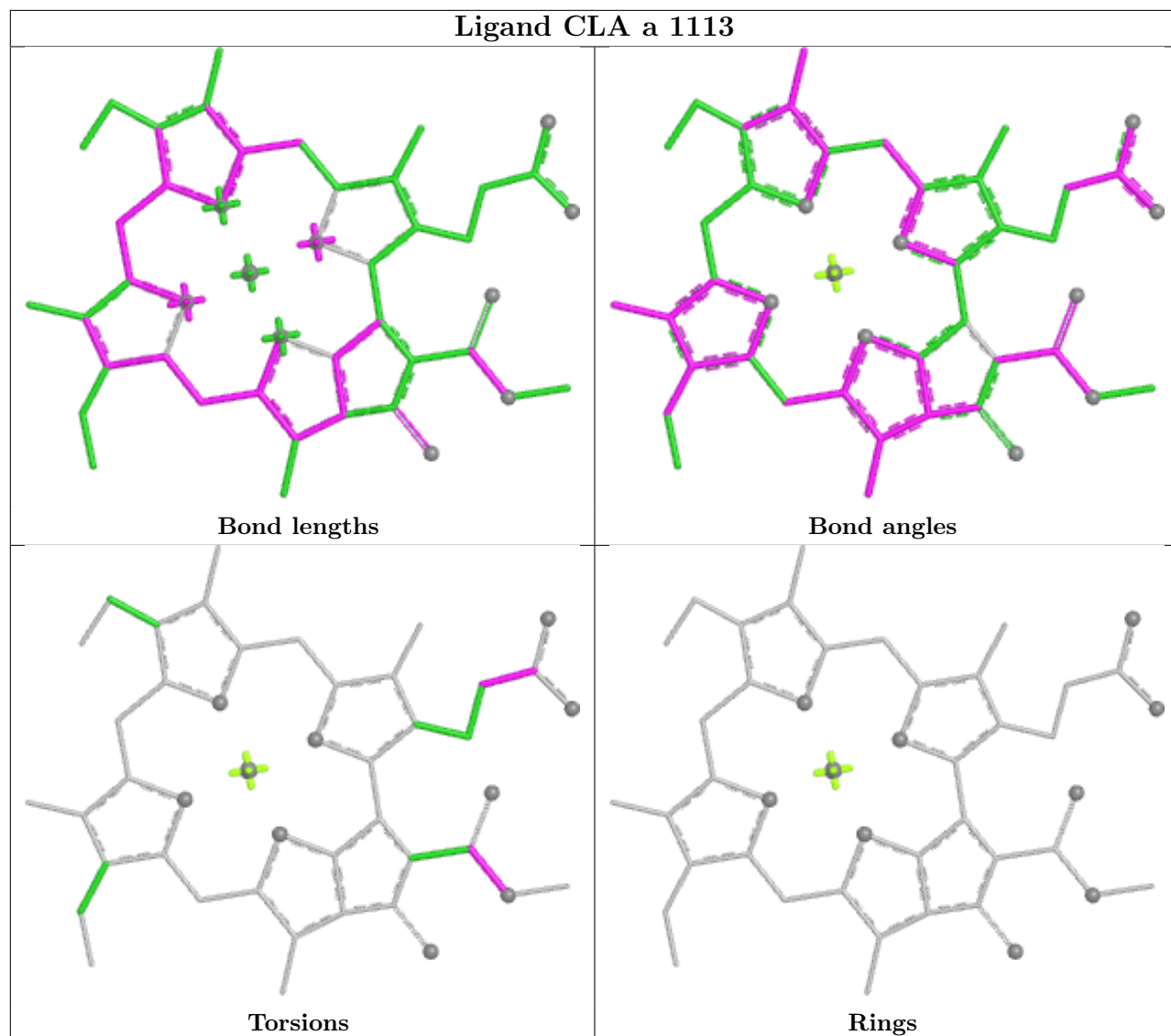




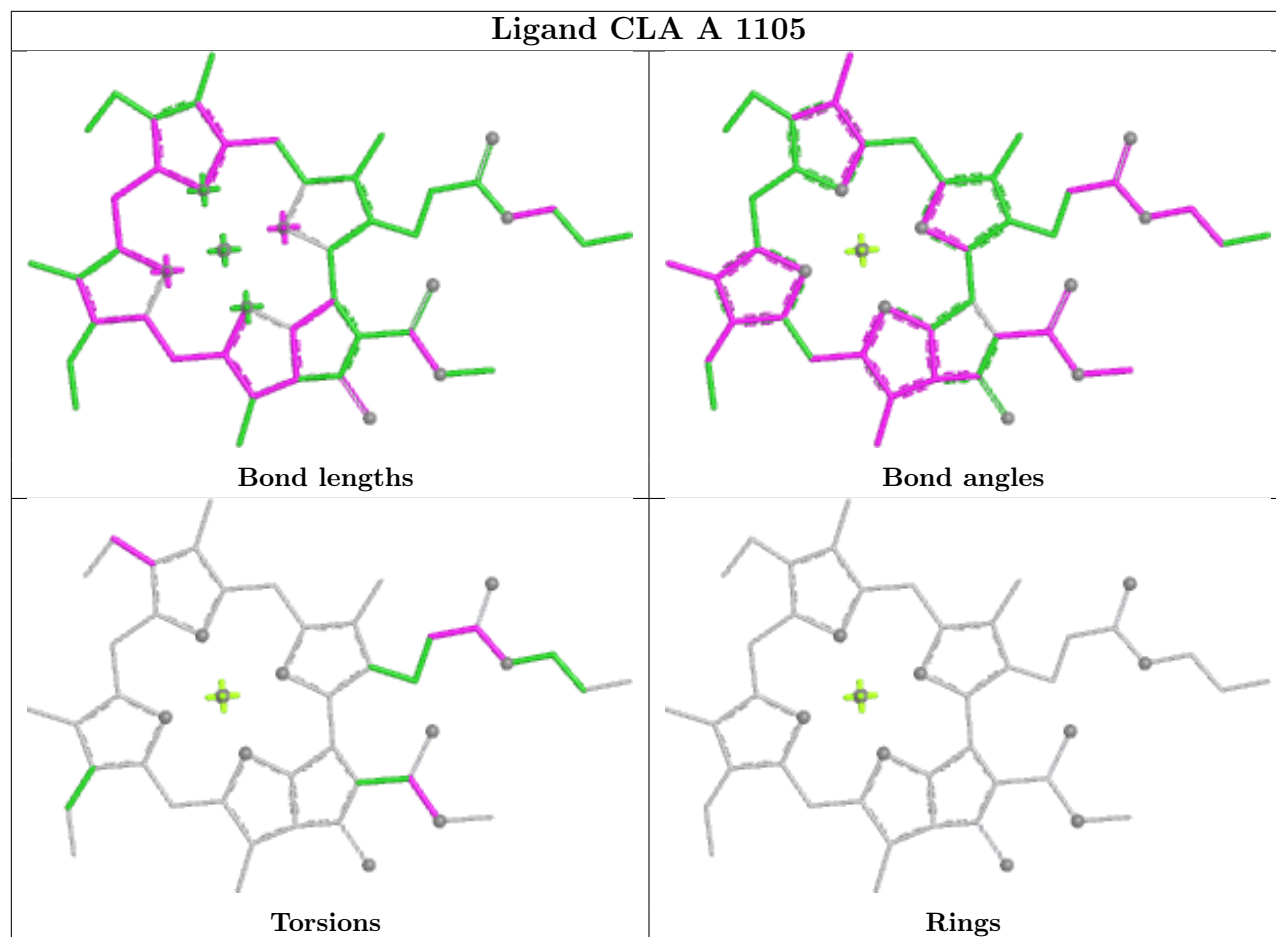


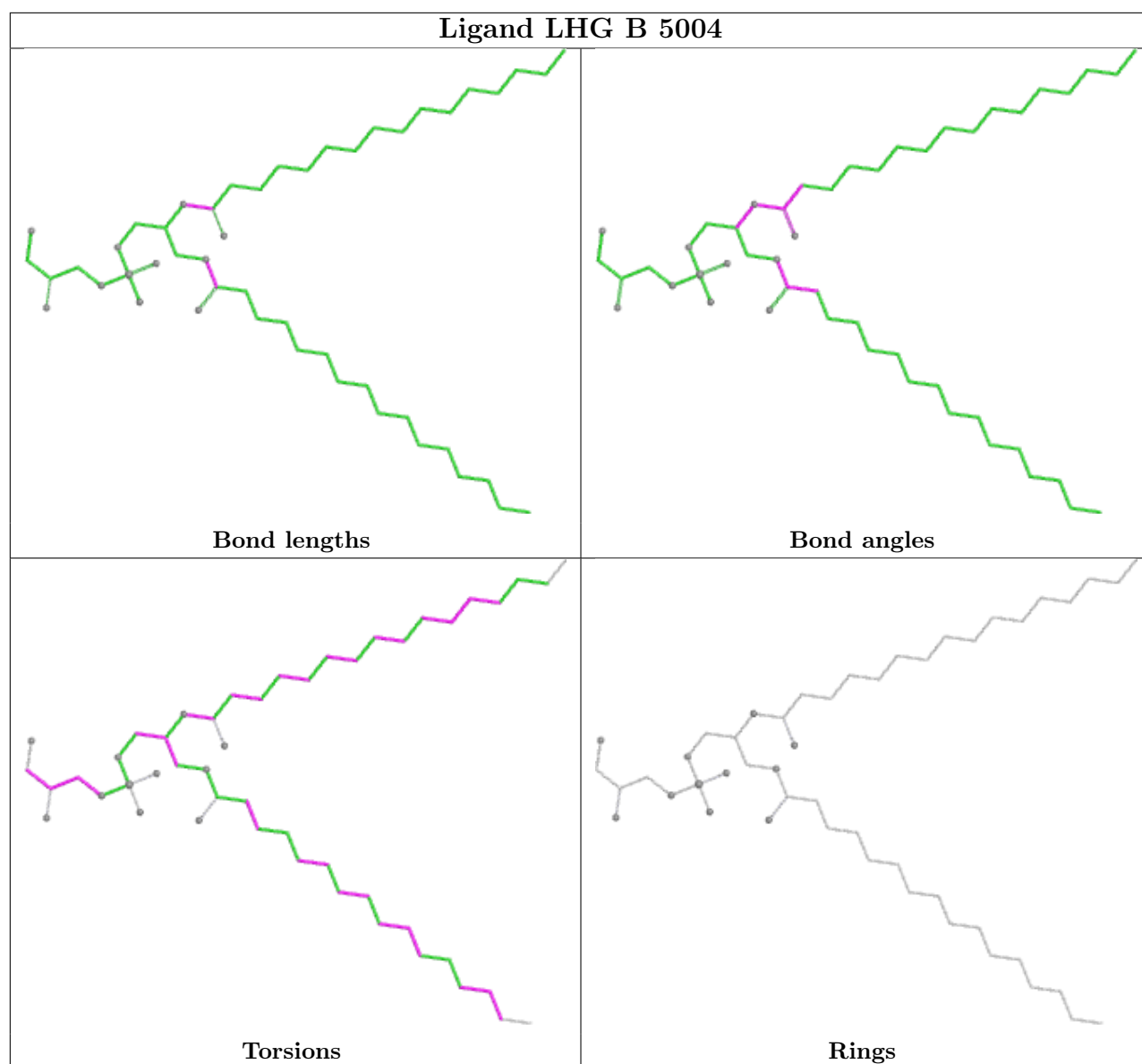


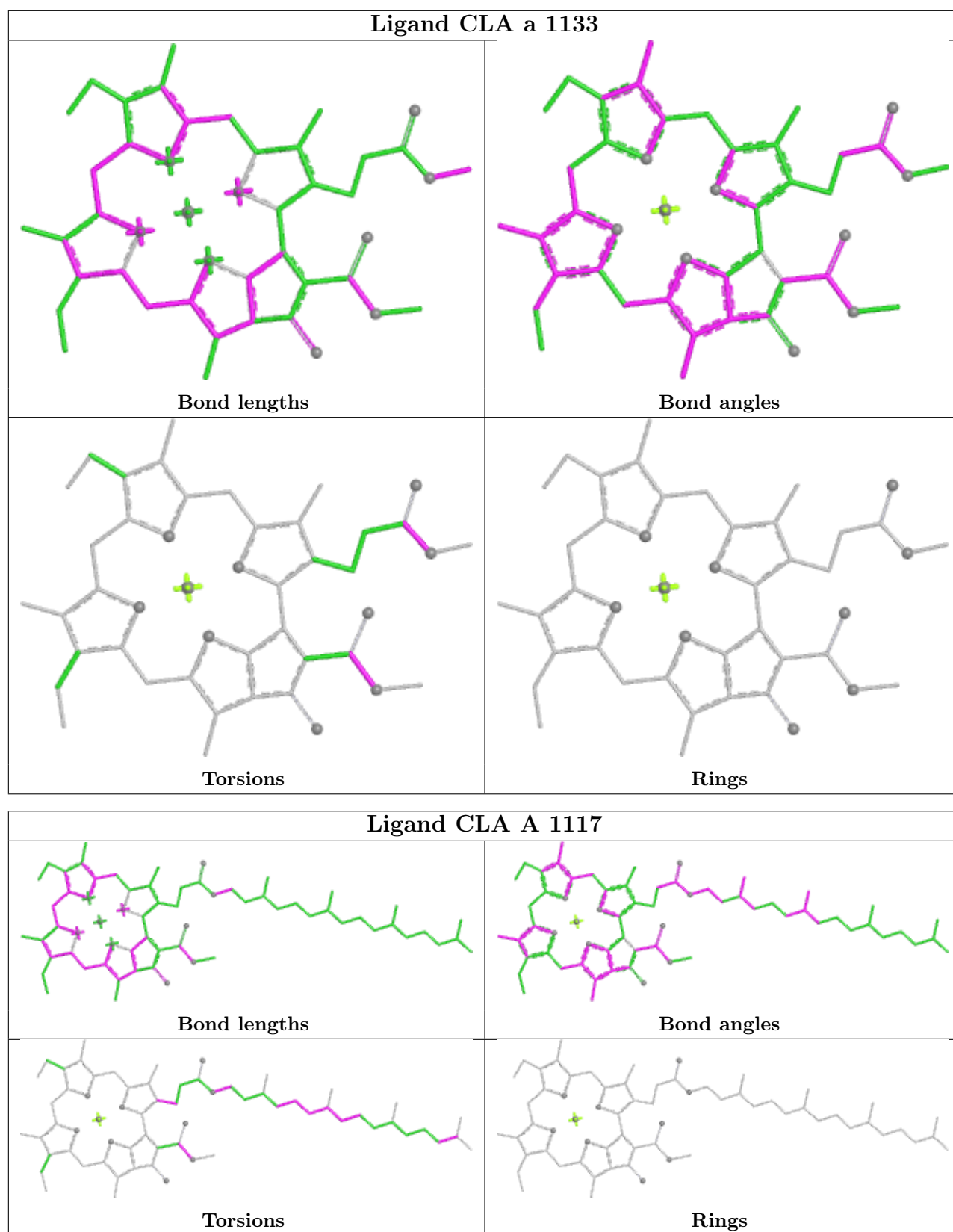


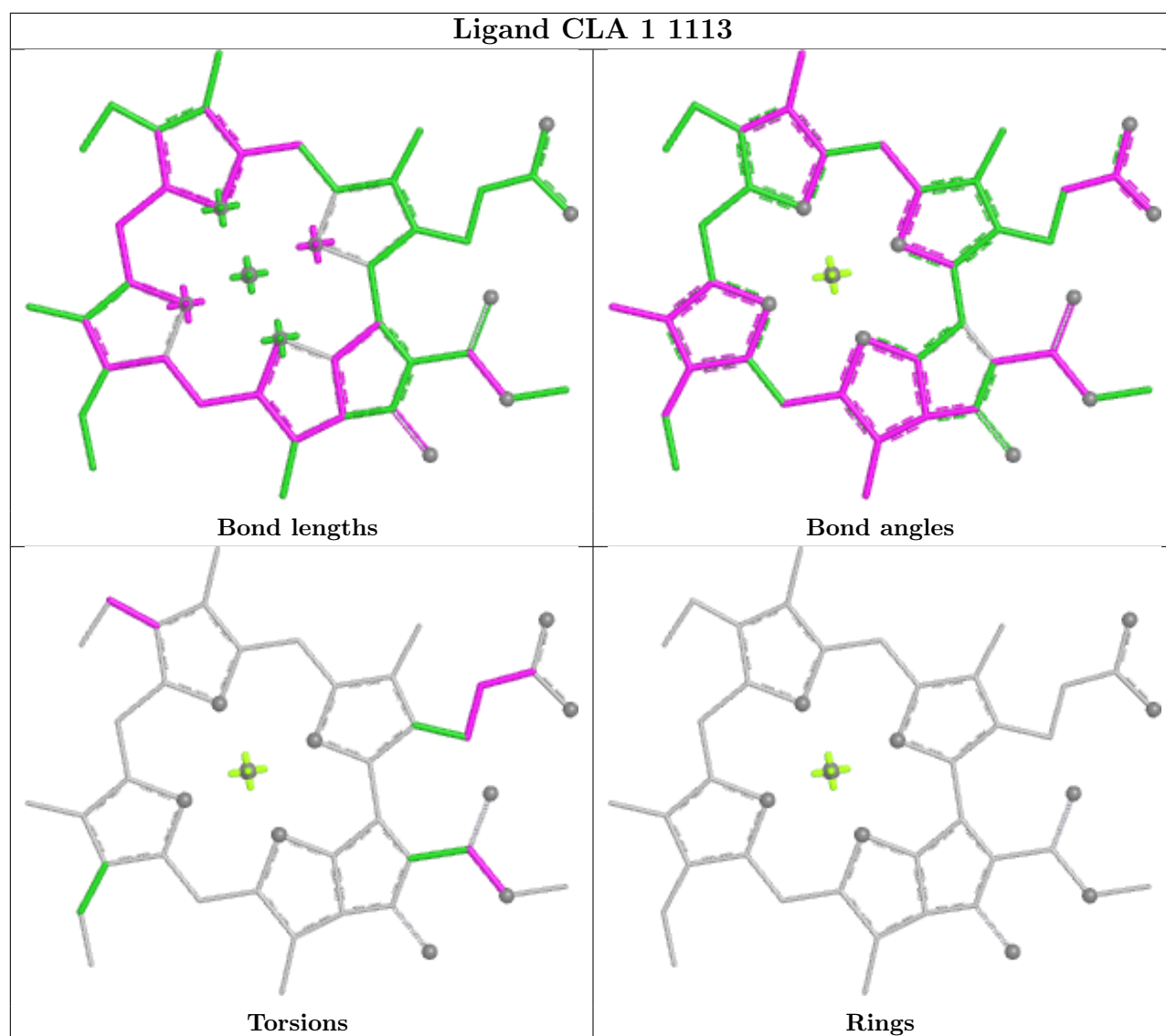


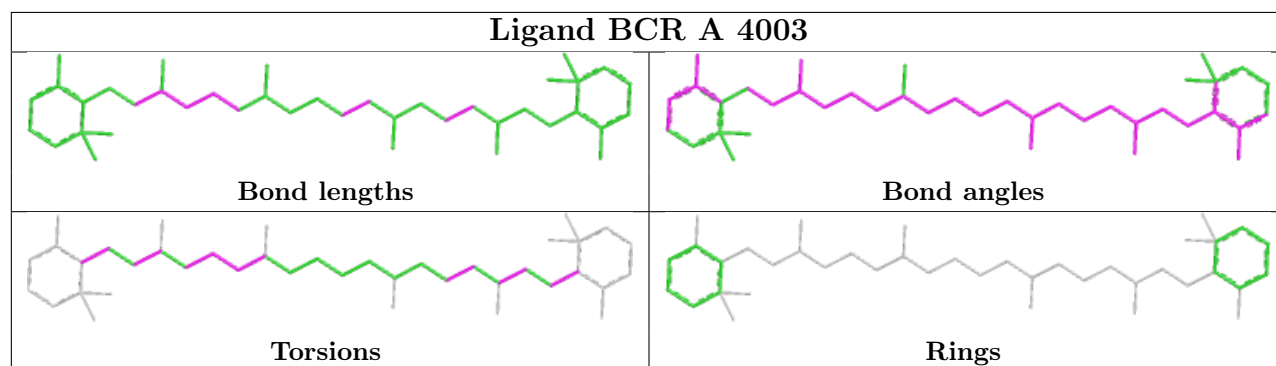
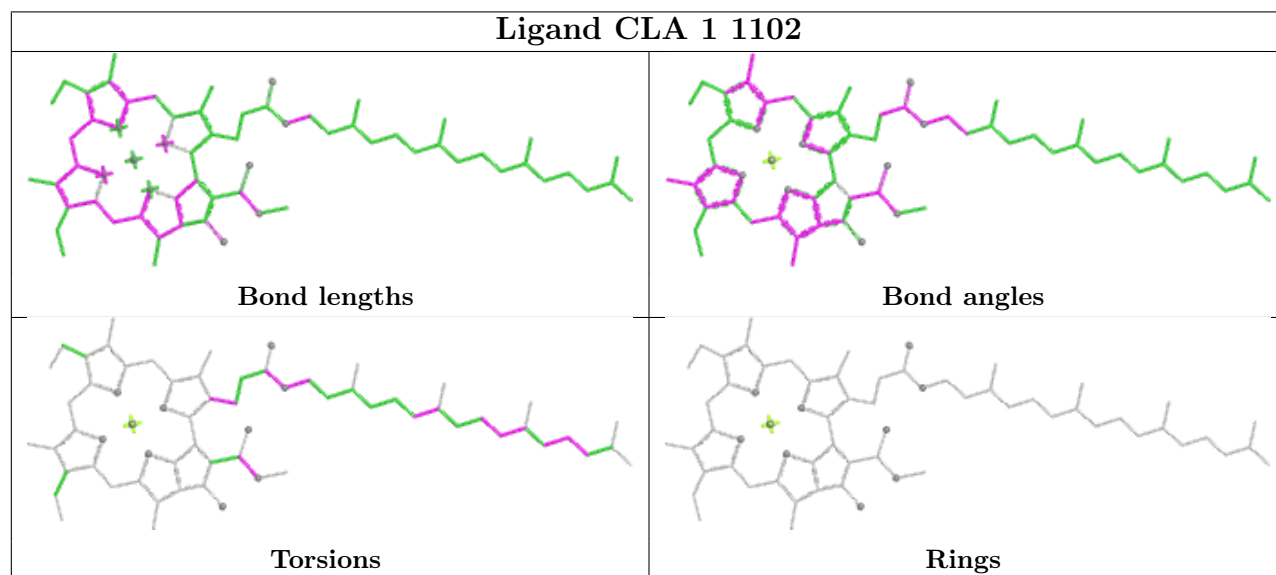
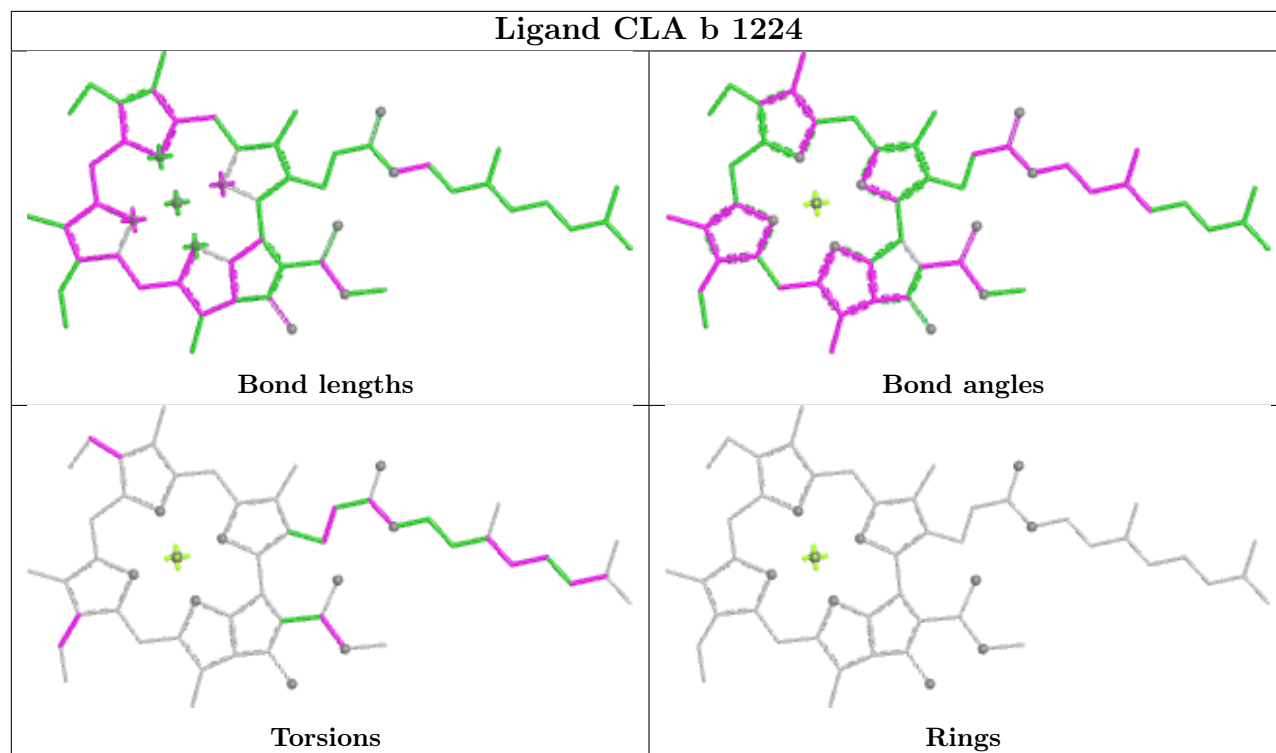
Ligand CLA A 1105



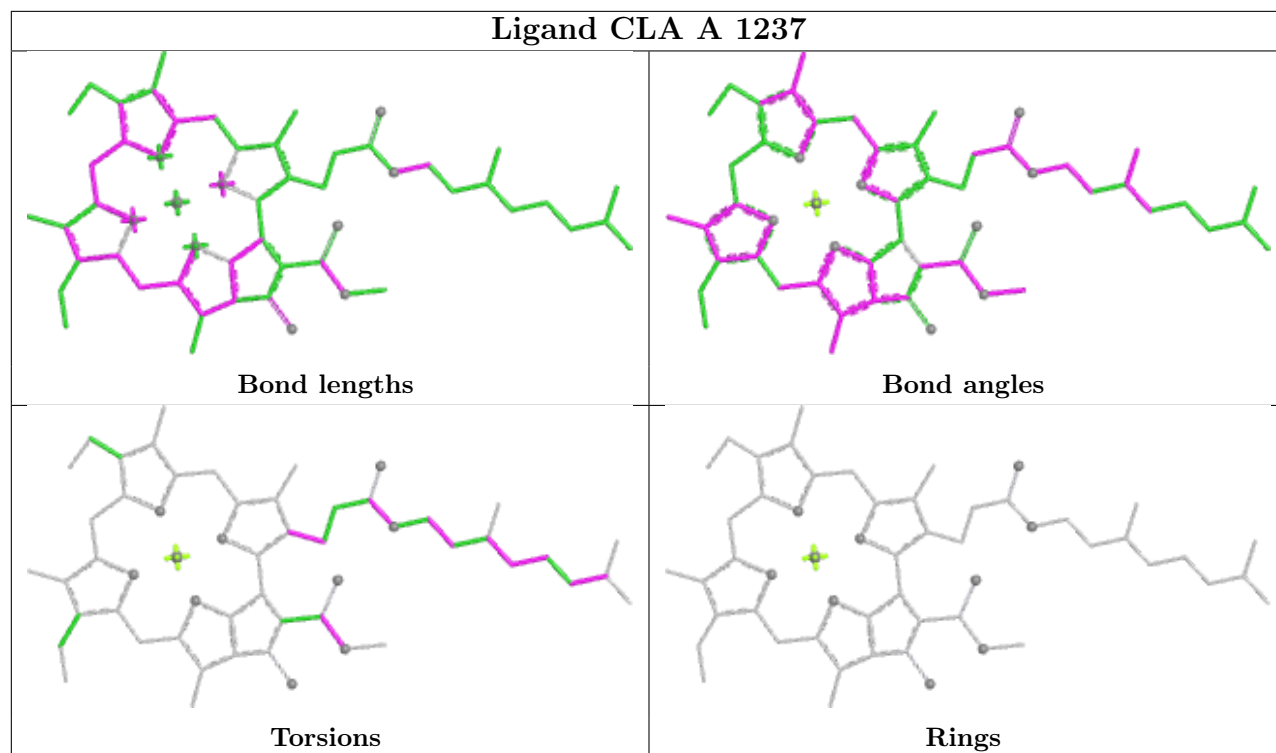




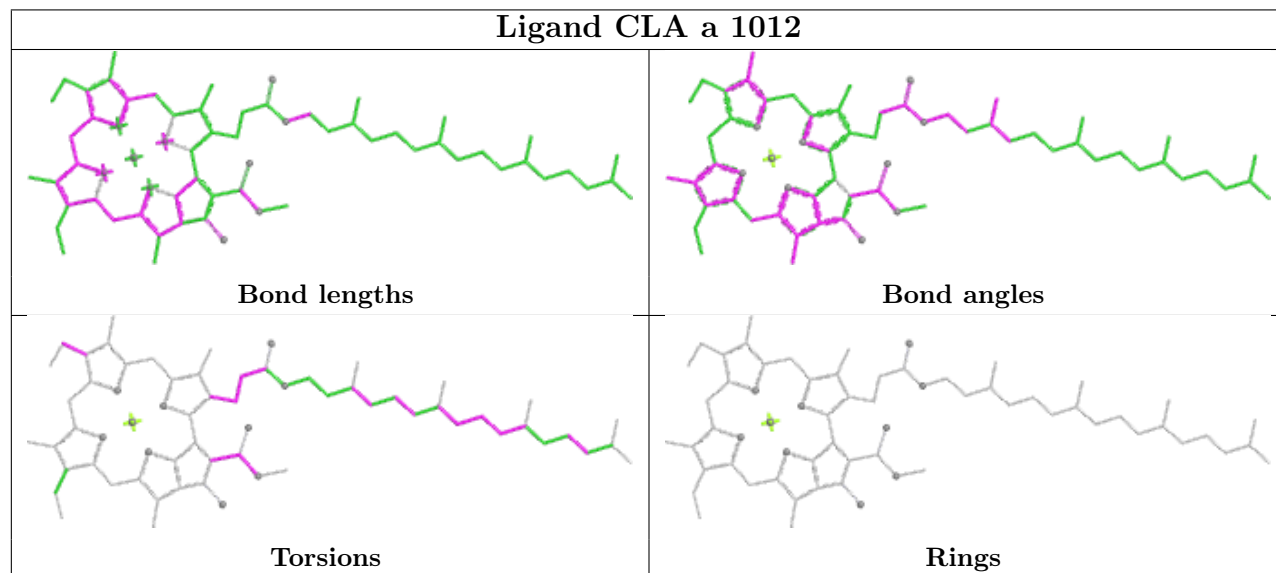


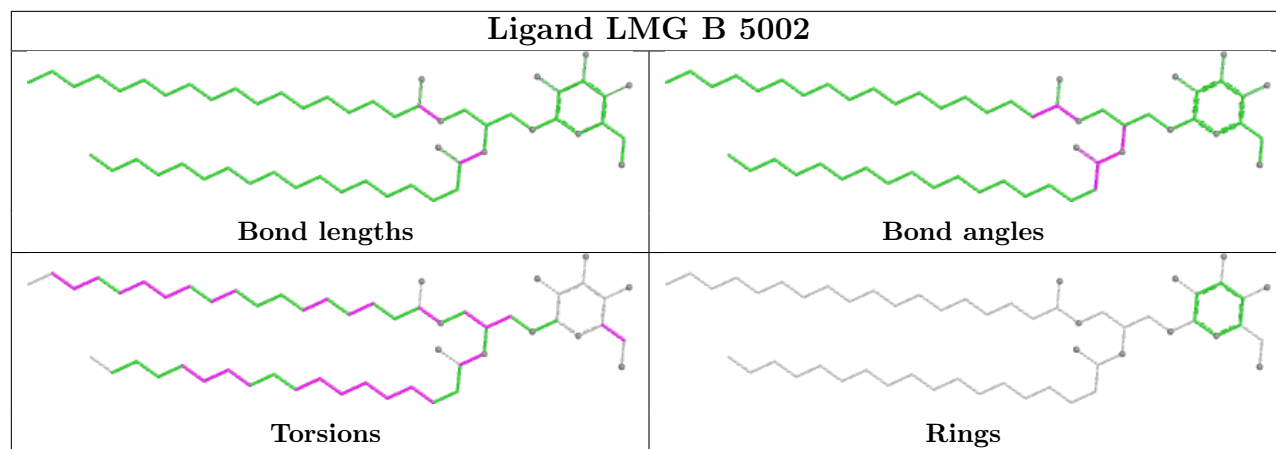
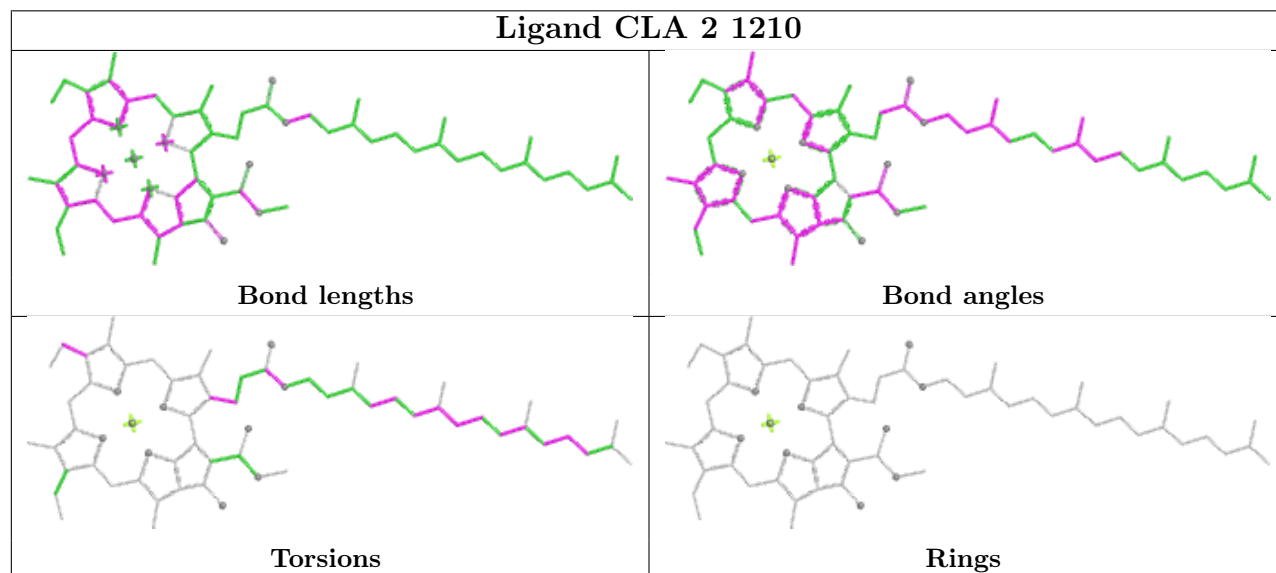
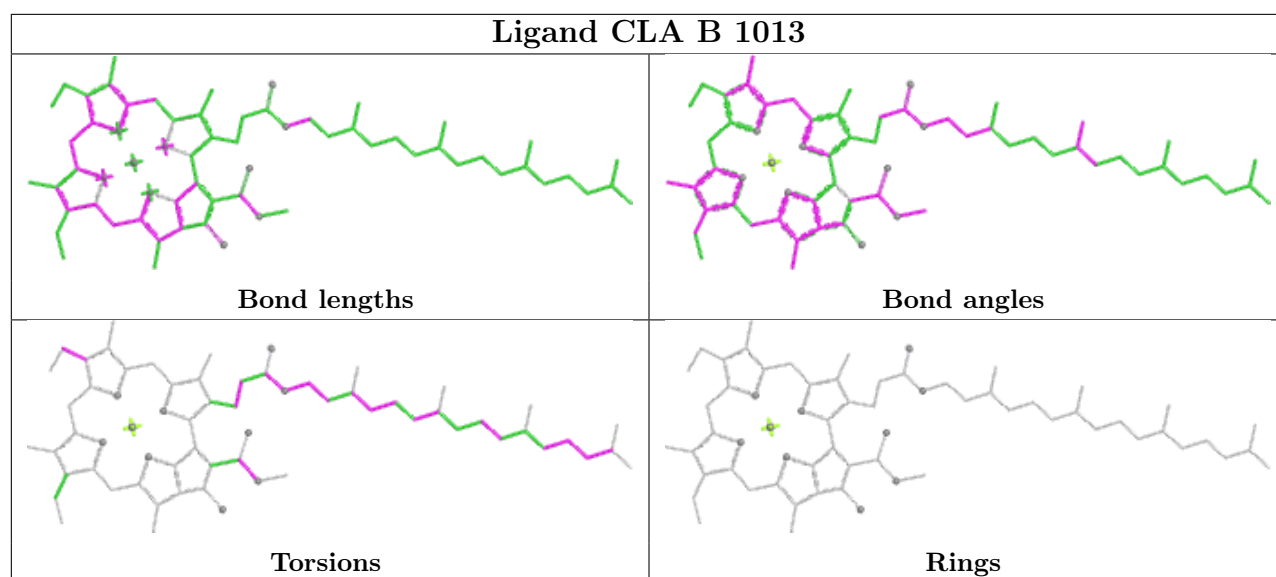


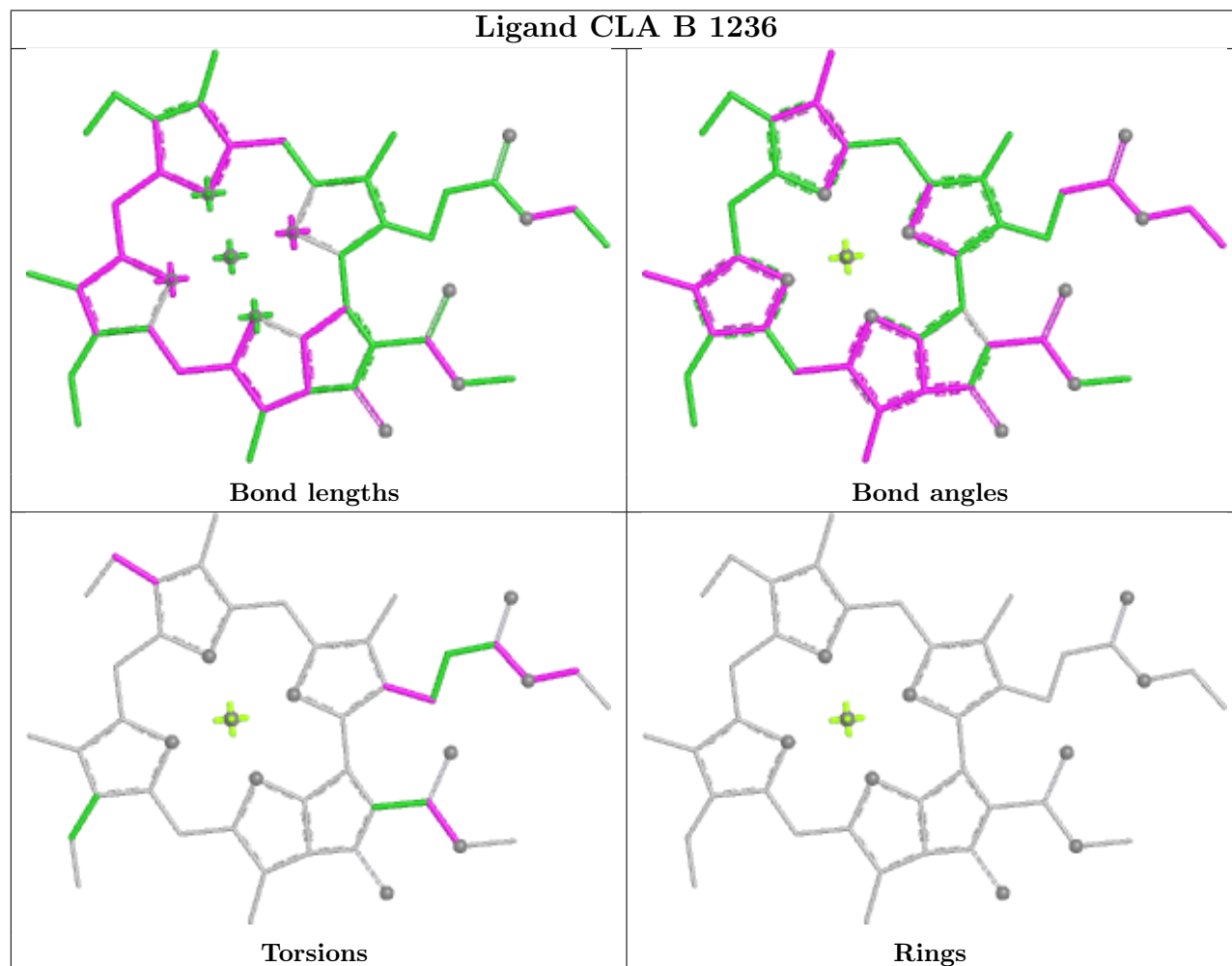
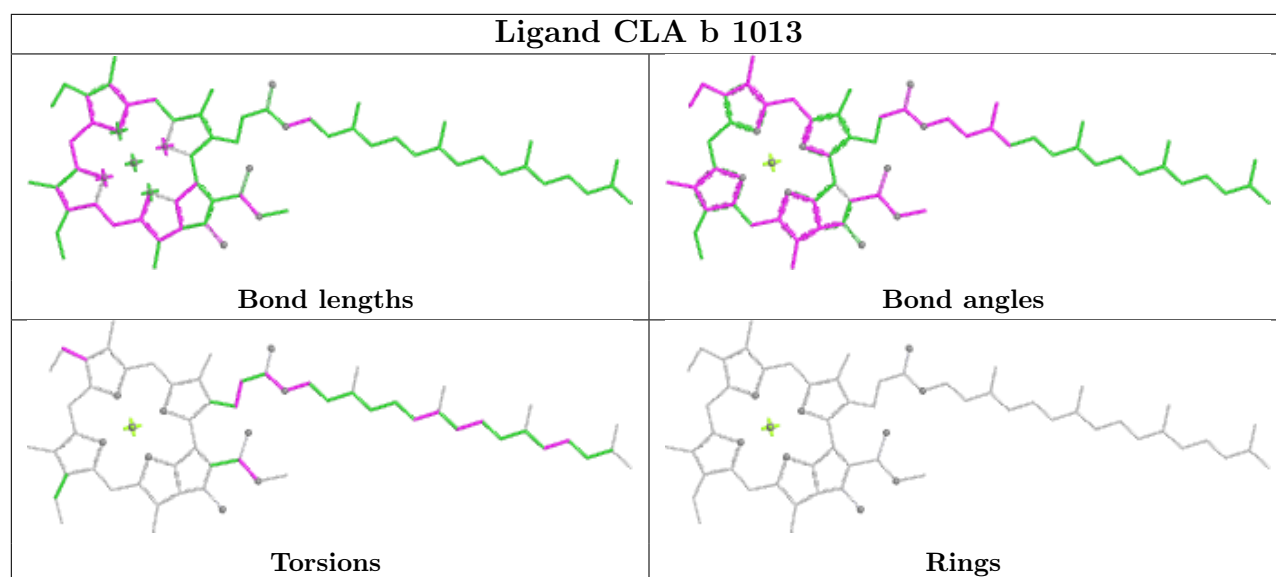
Ligand CLA A 1237



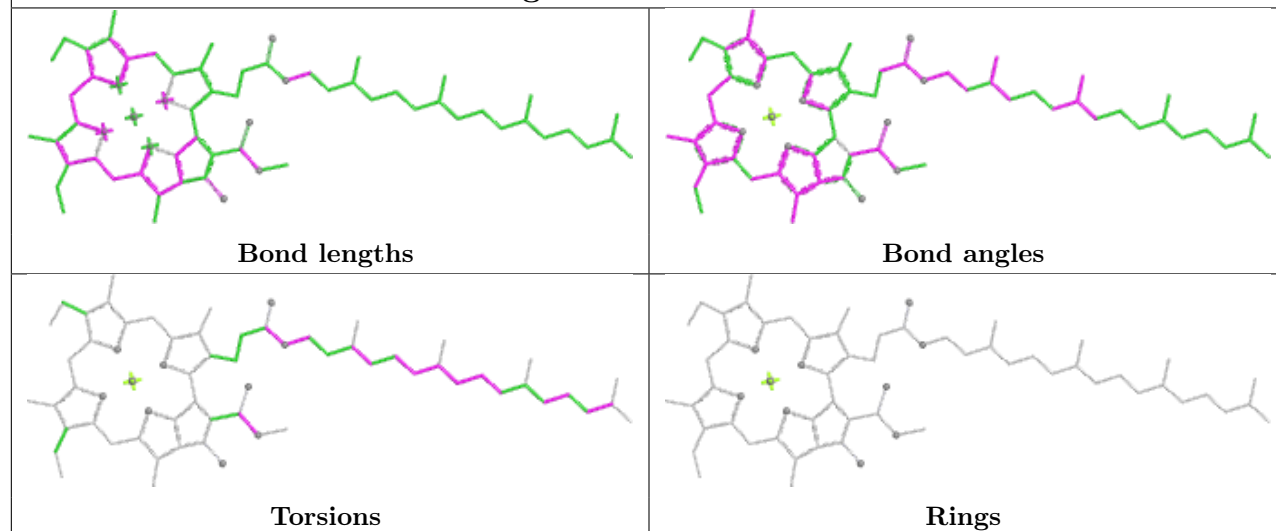
Ligand CLA a 1012



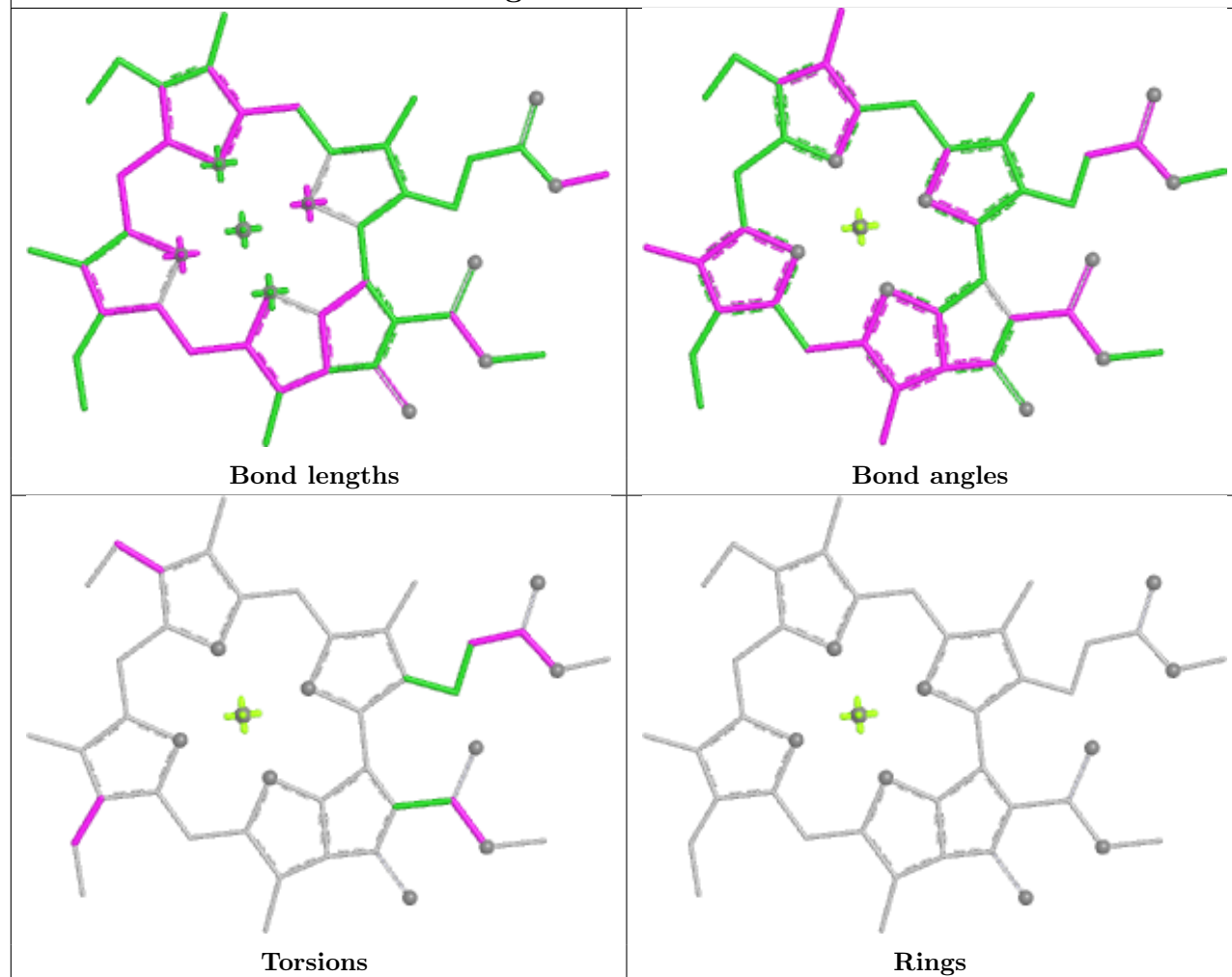


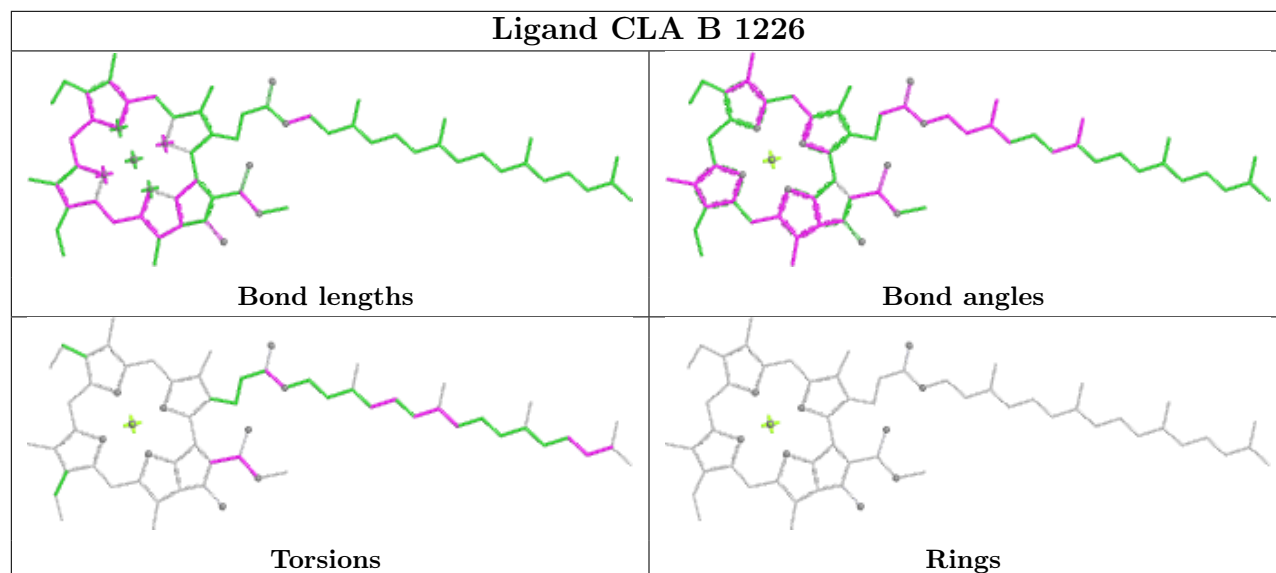
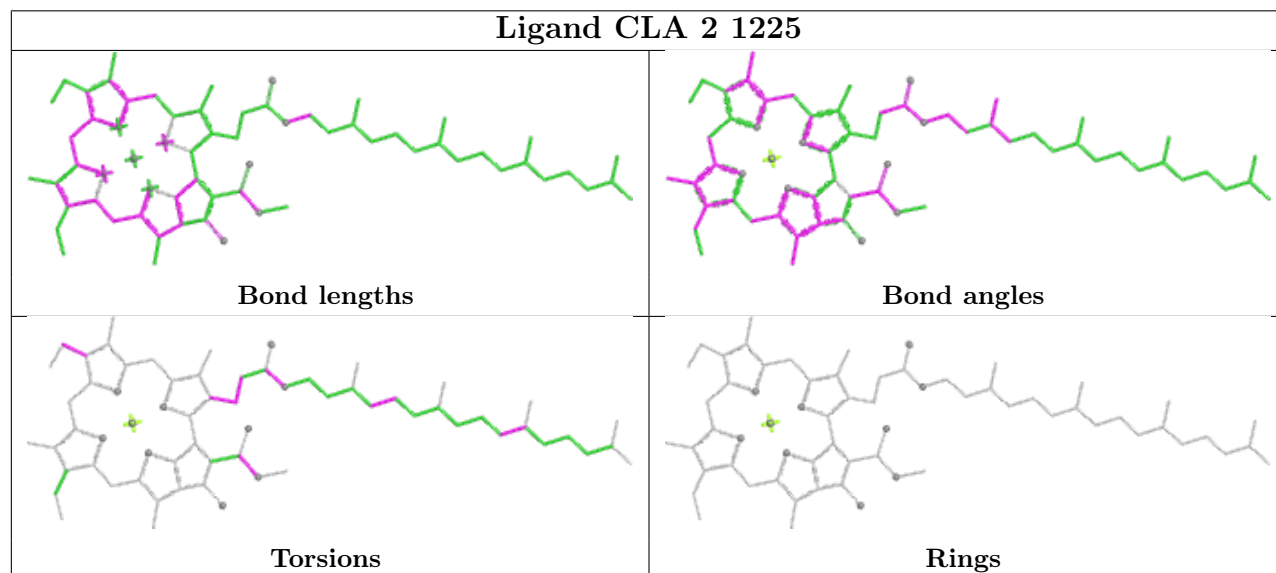
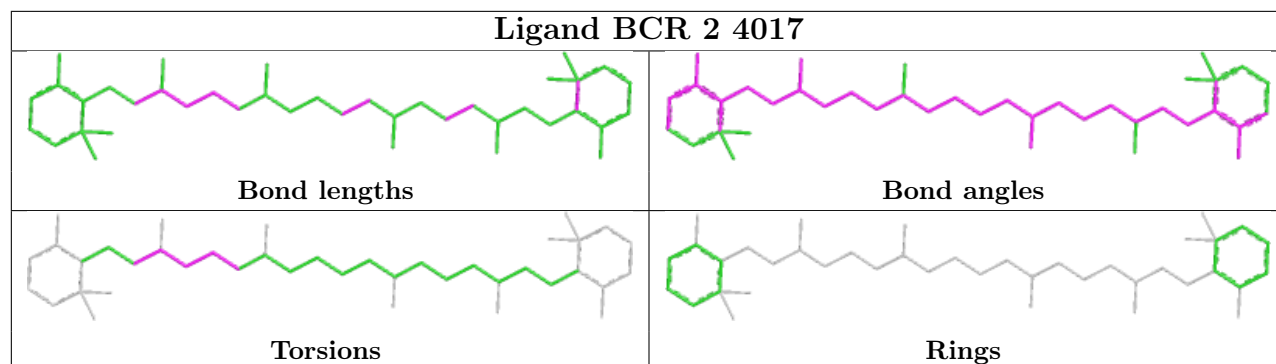


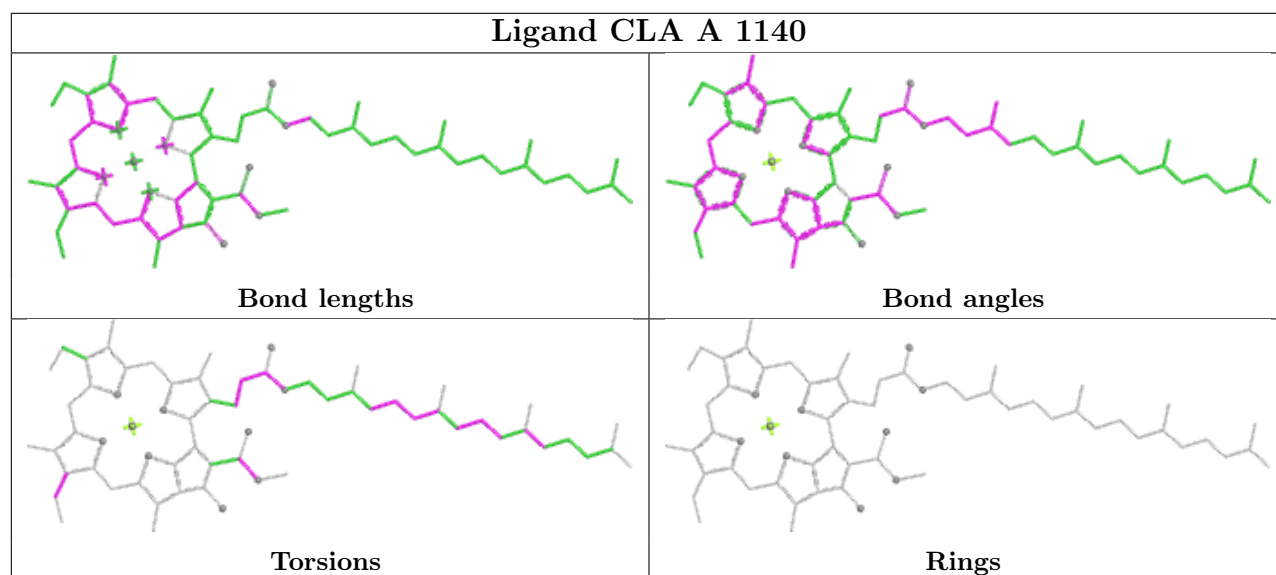
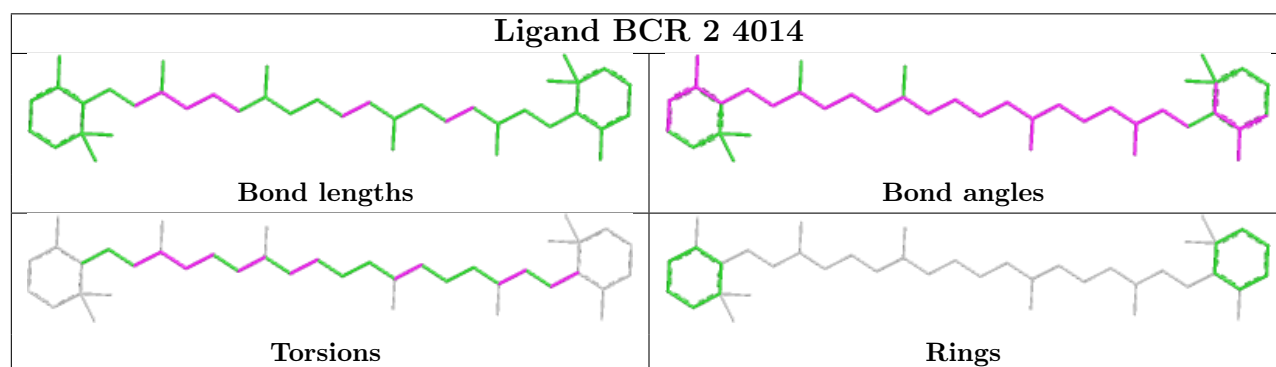
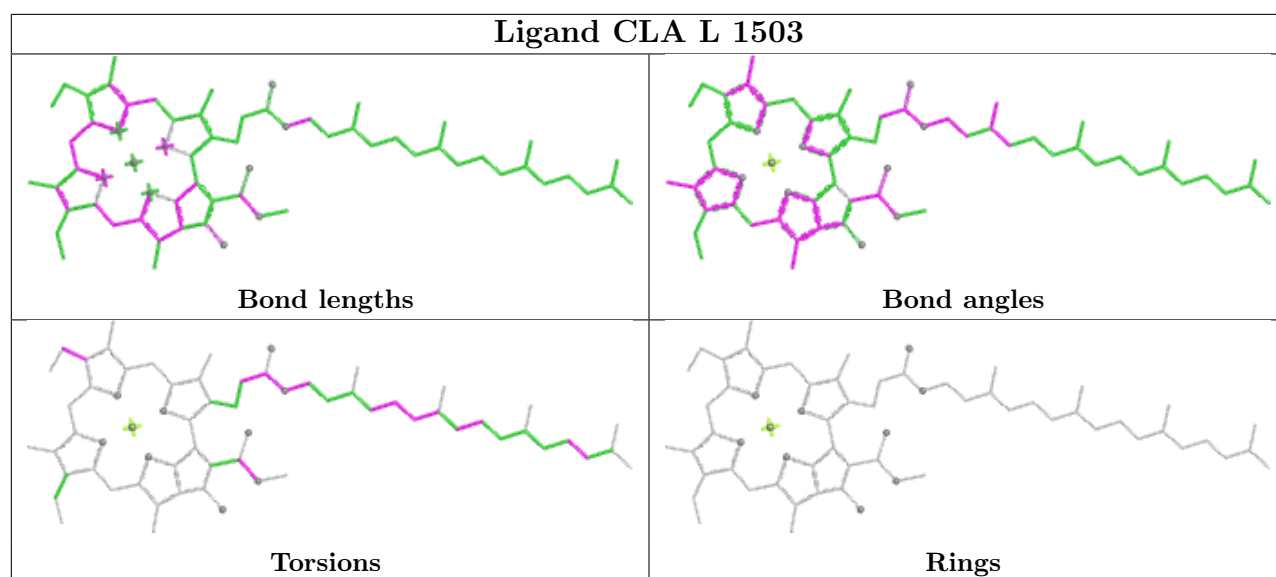
Ligand CLA A 1123

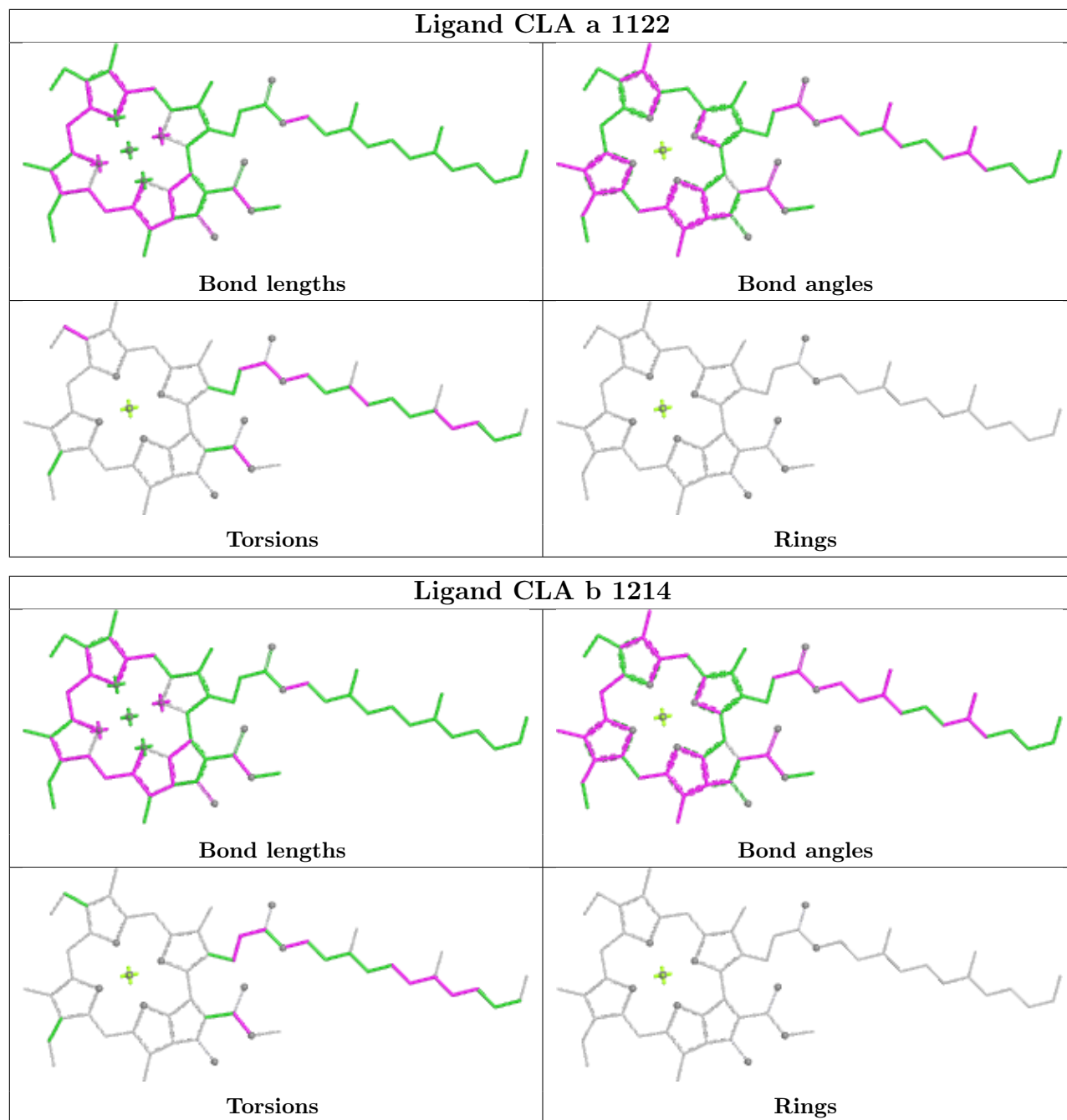


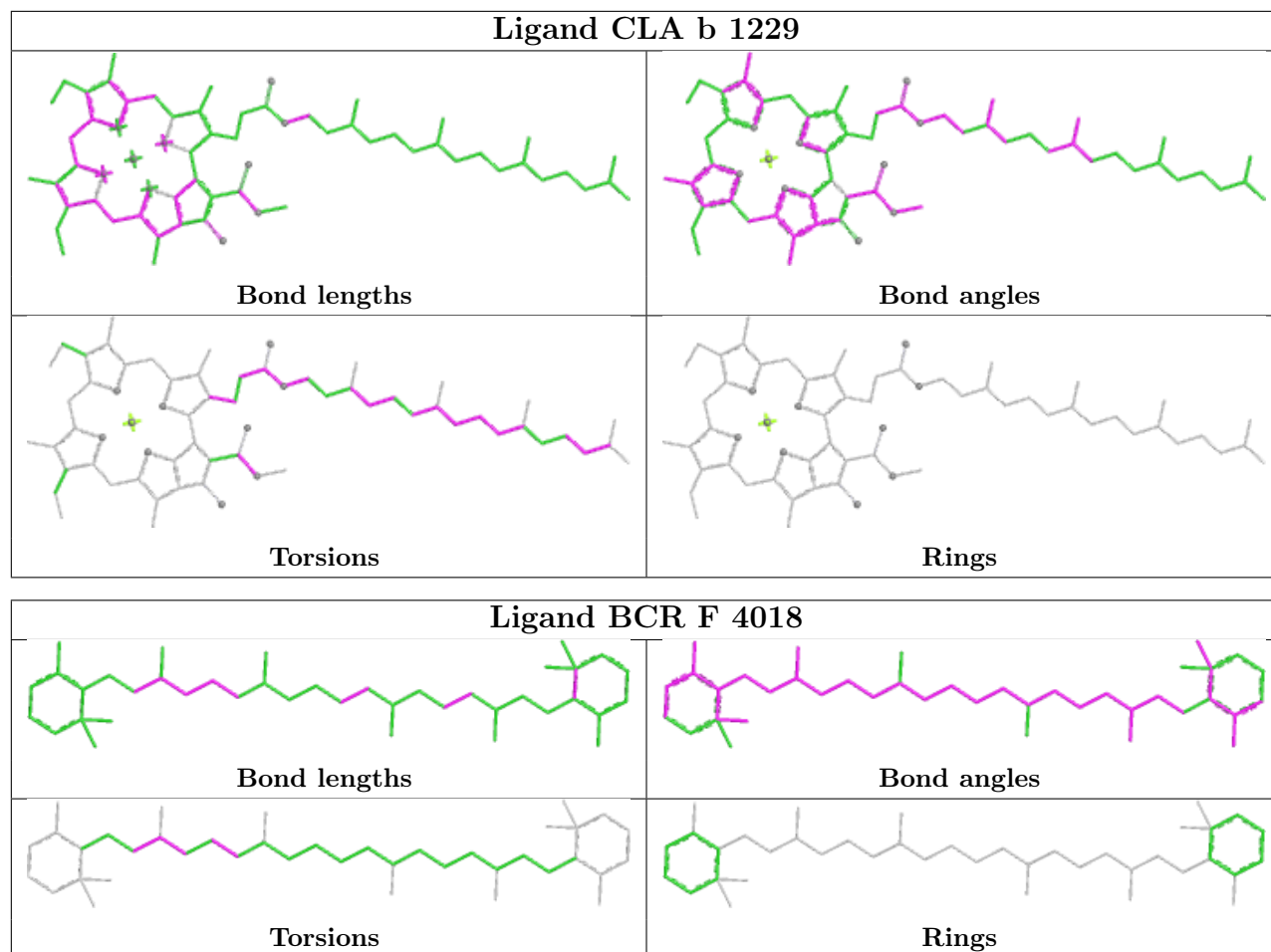
Ligand CLA B 1239

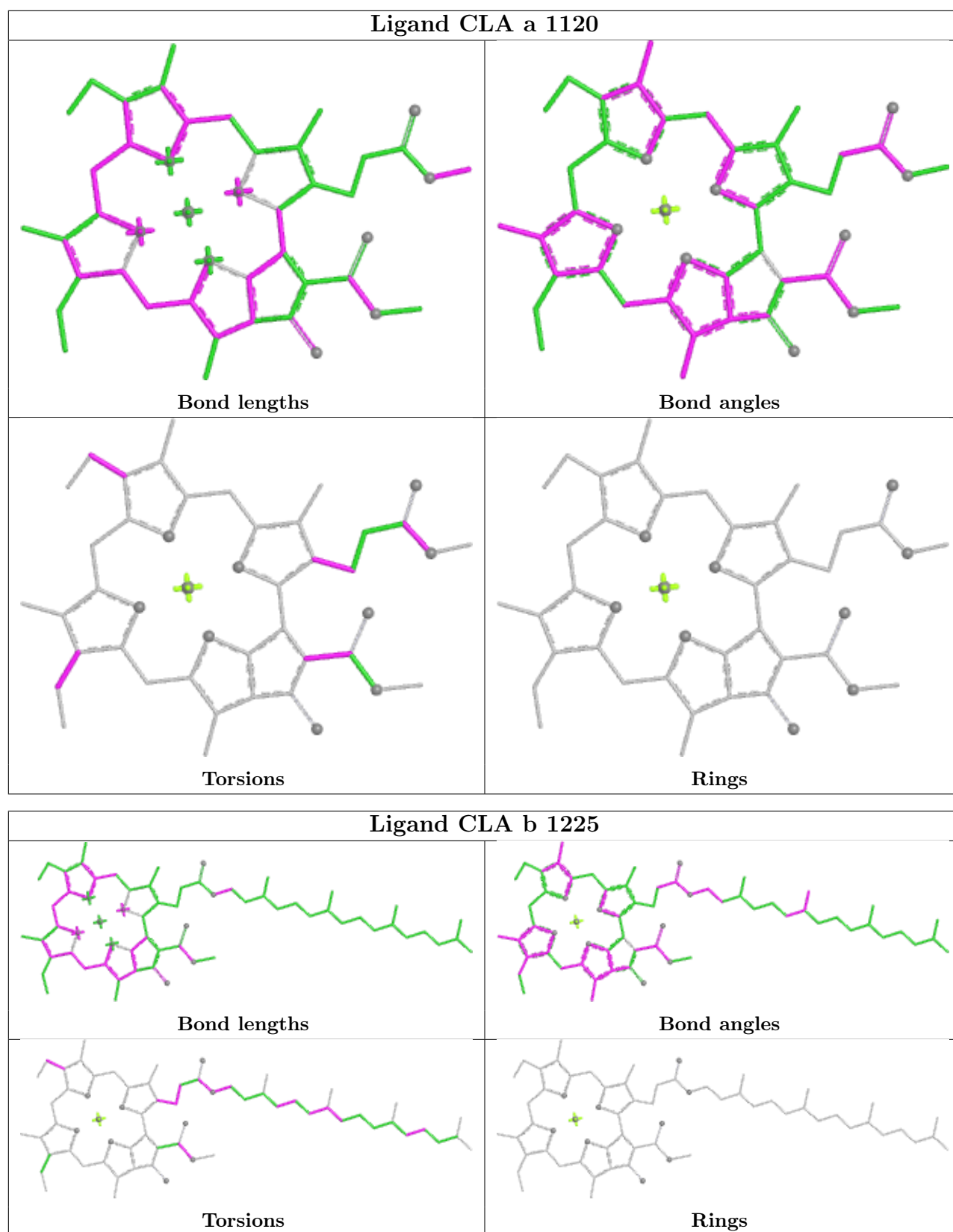


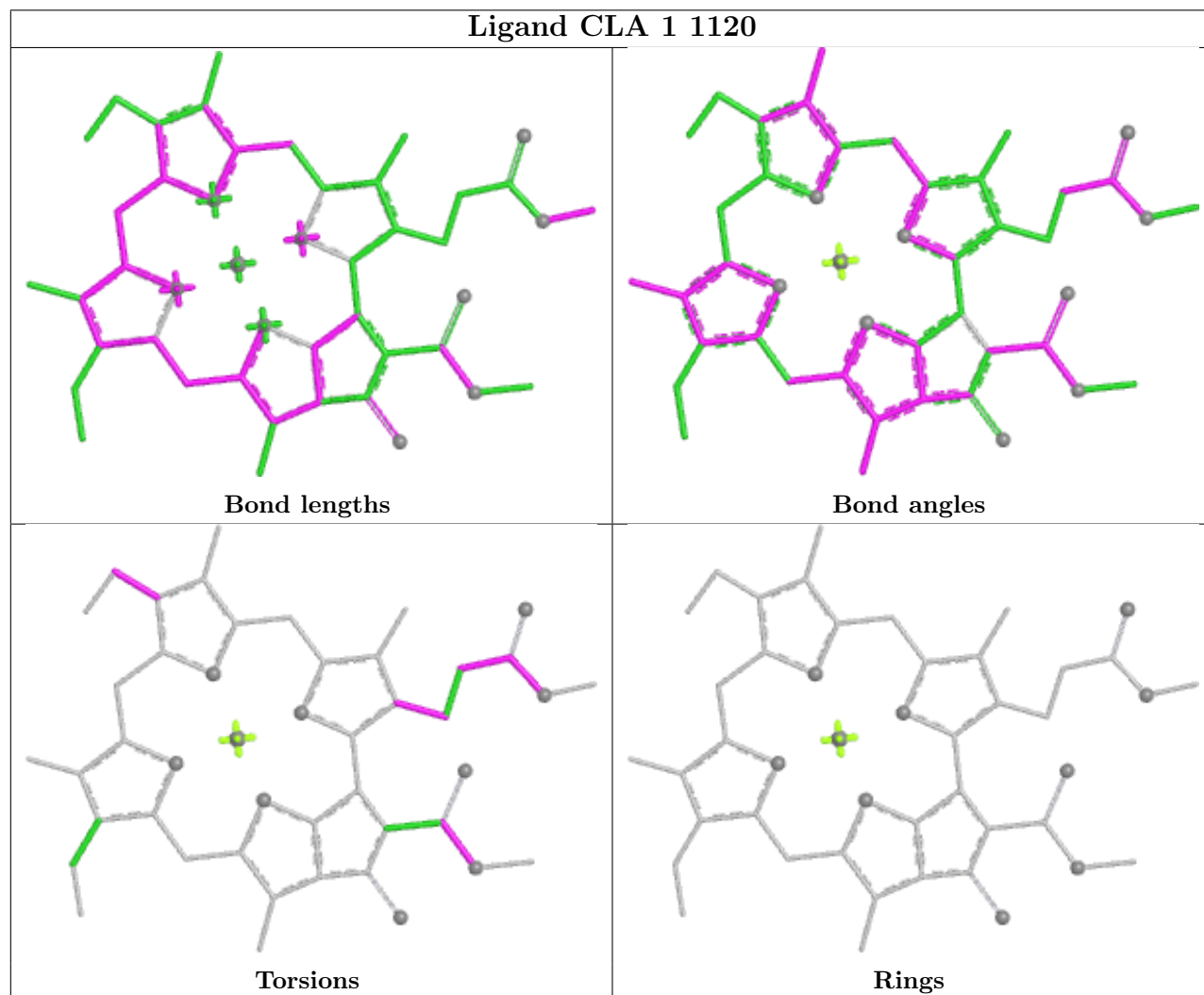
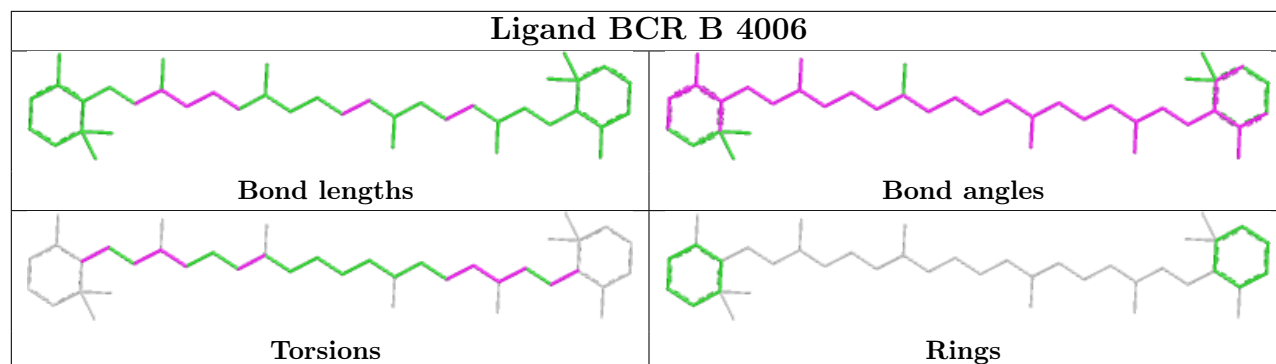


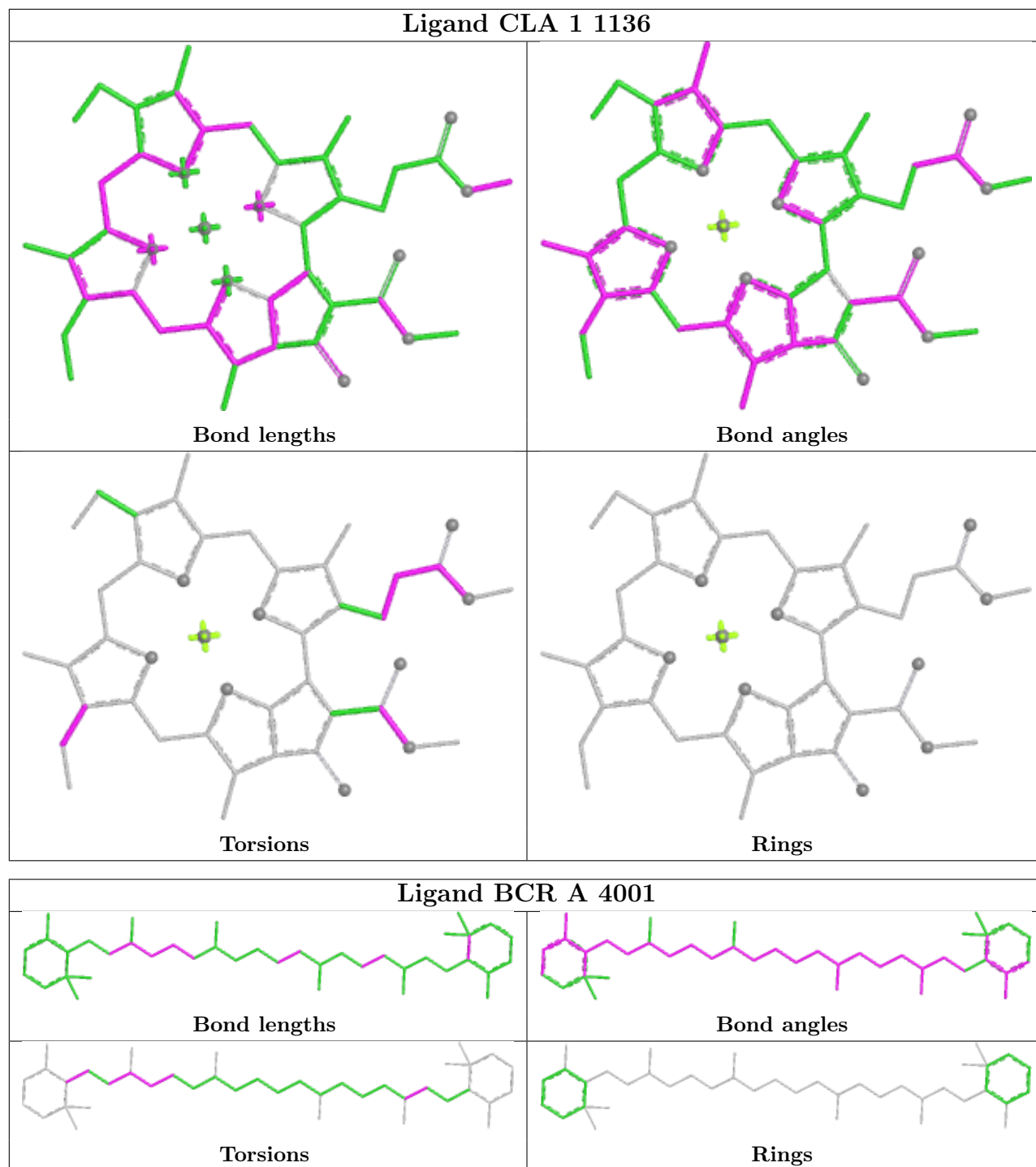


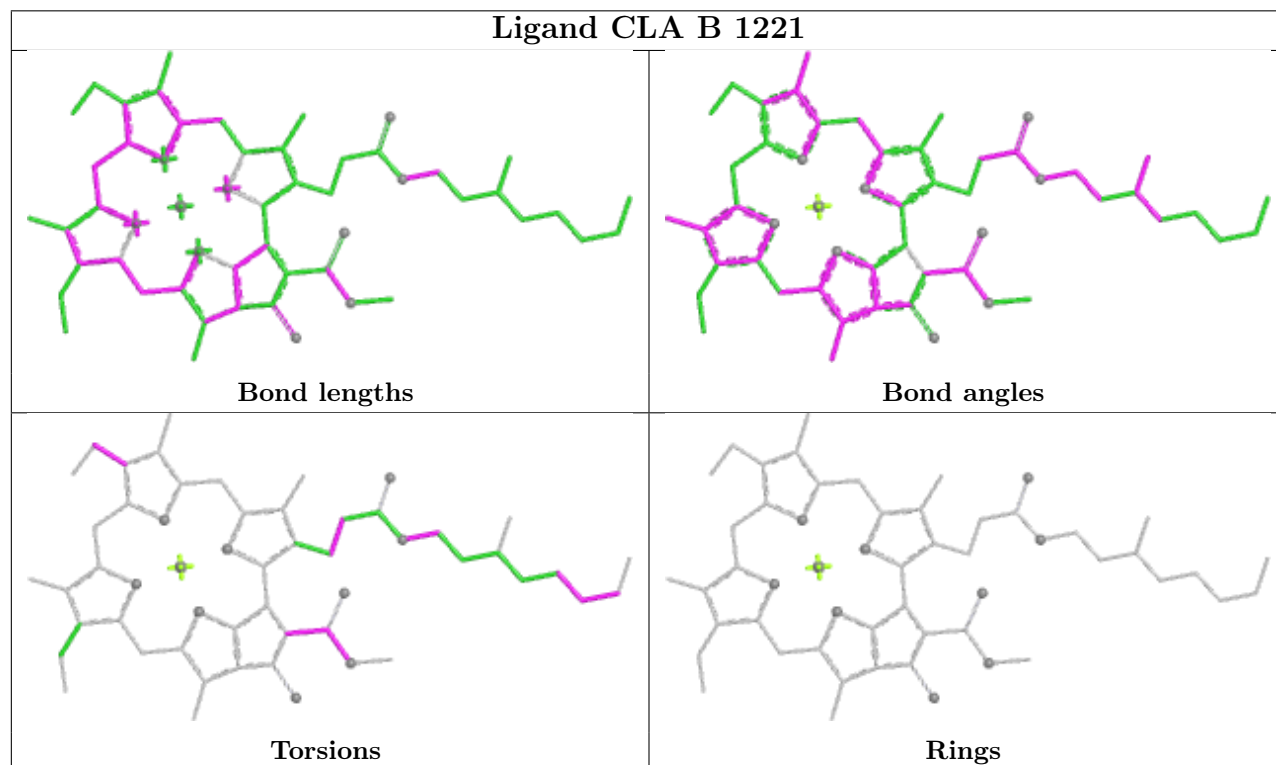
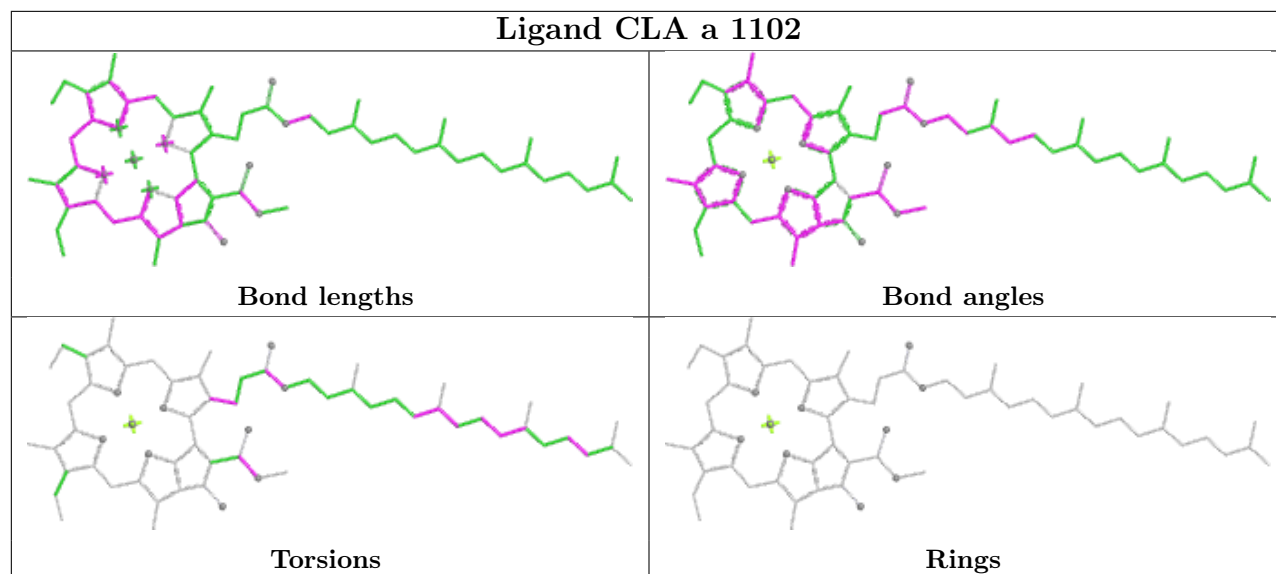


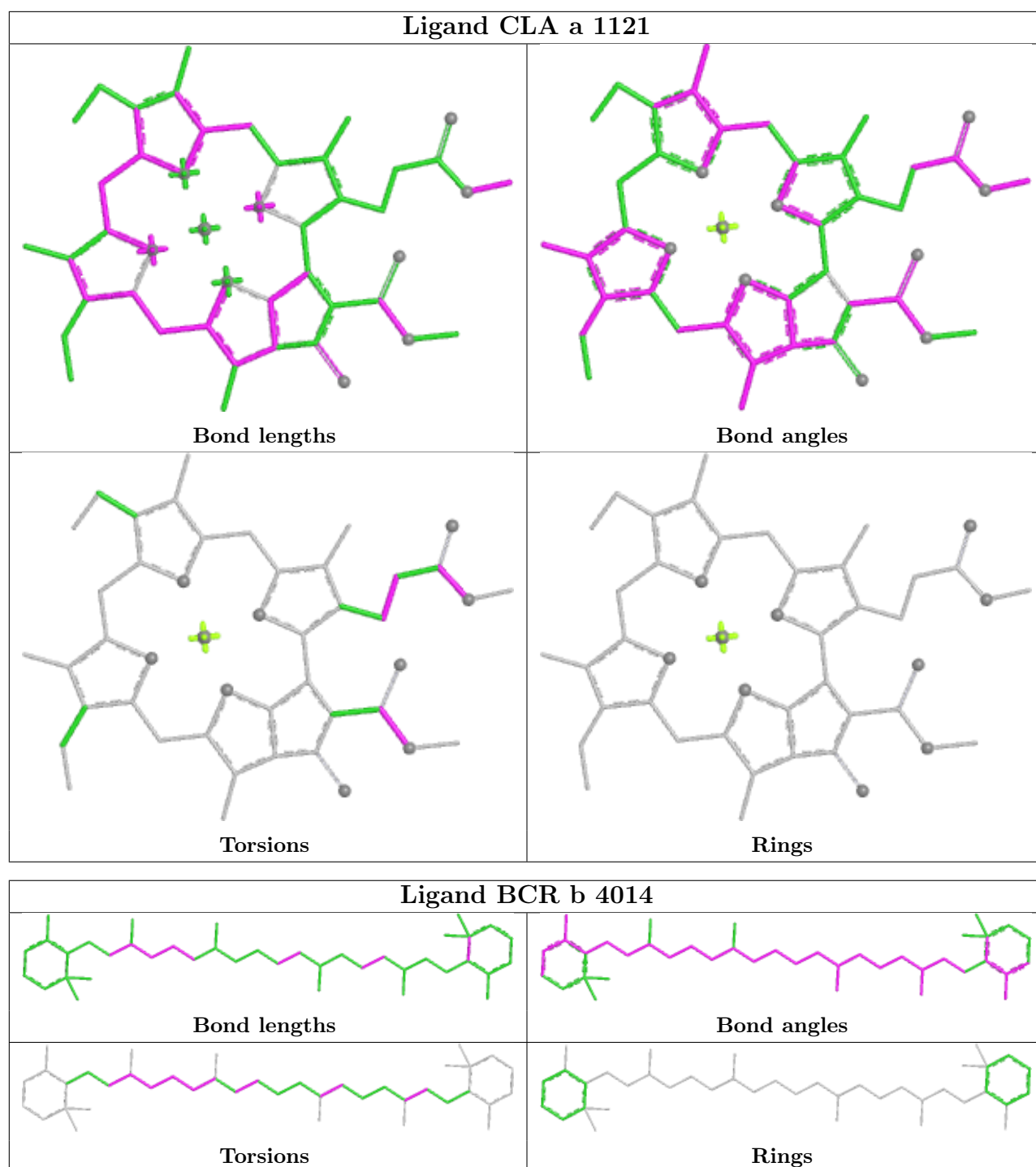


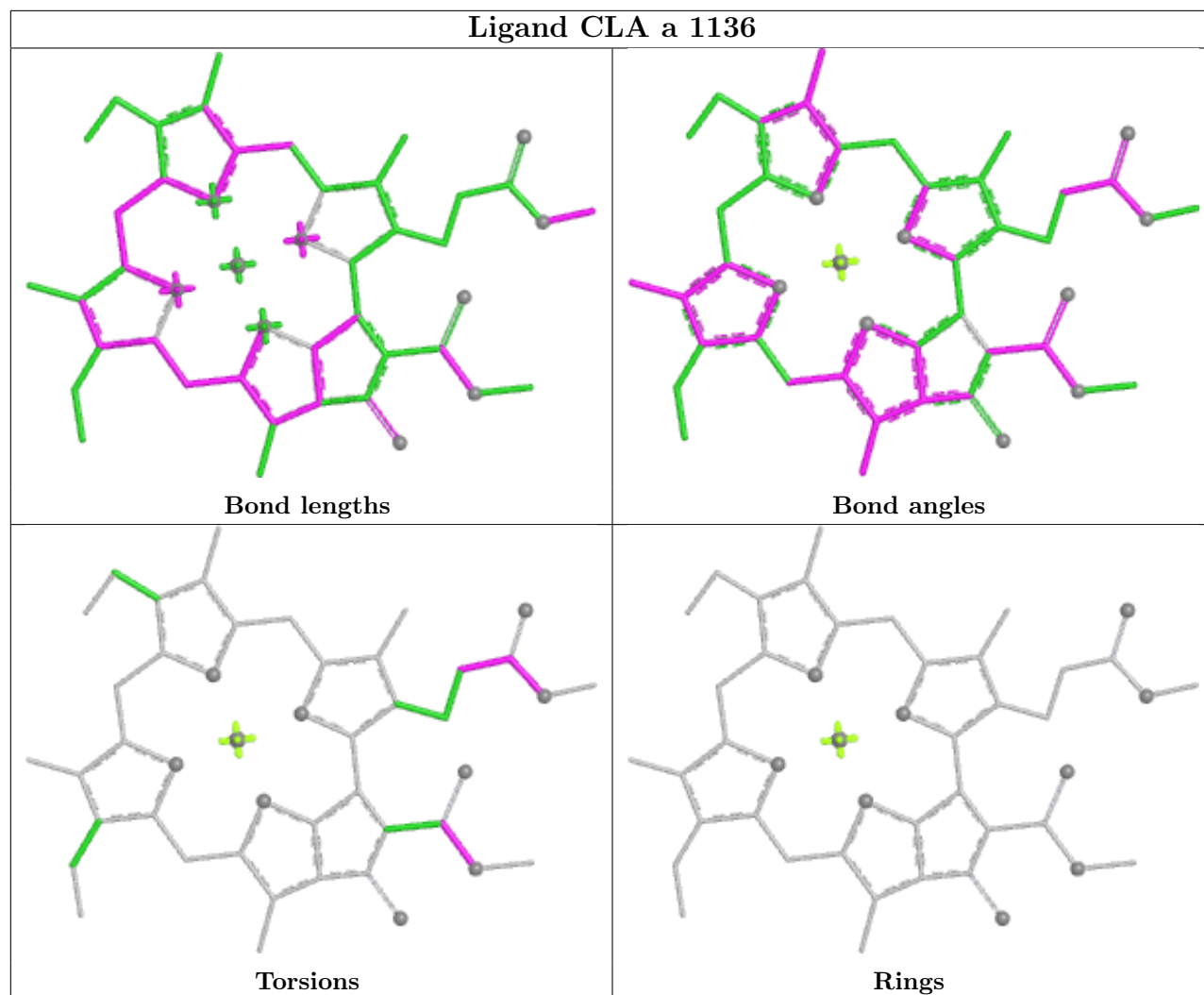


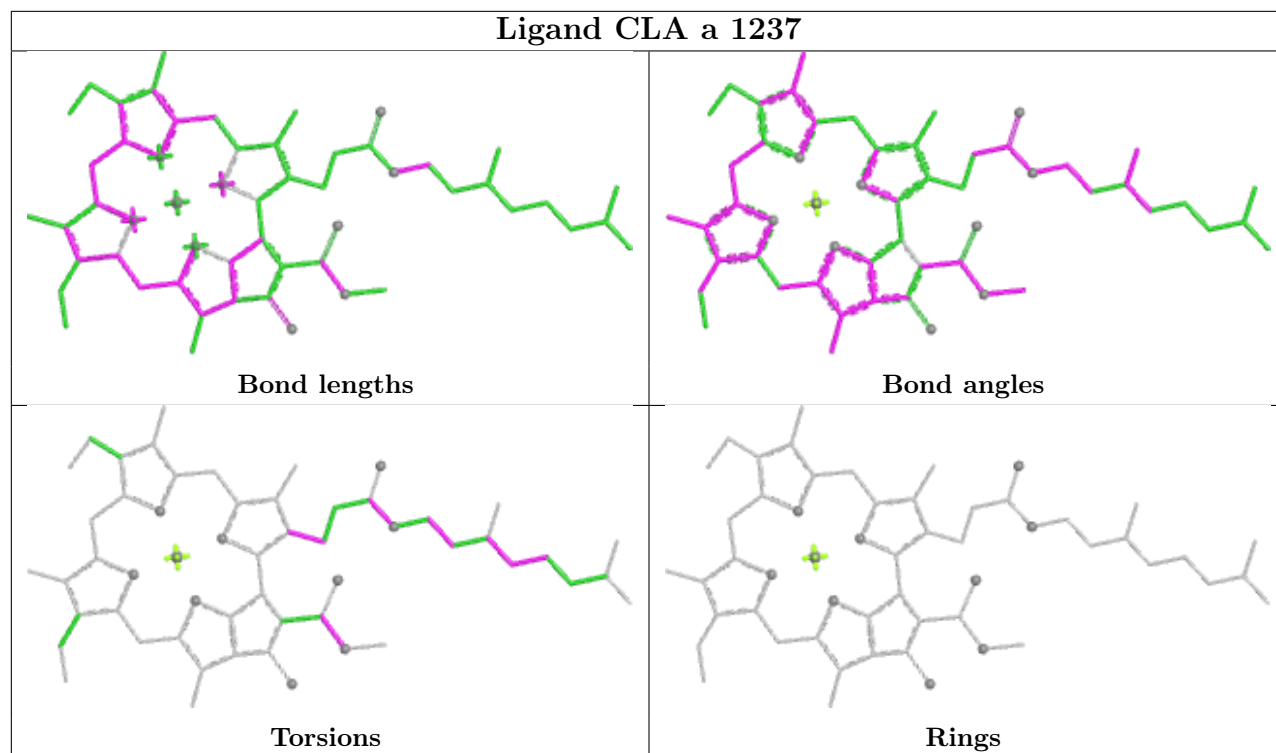


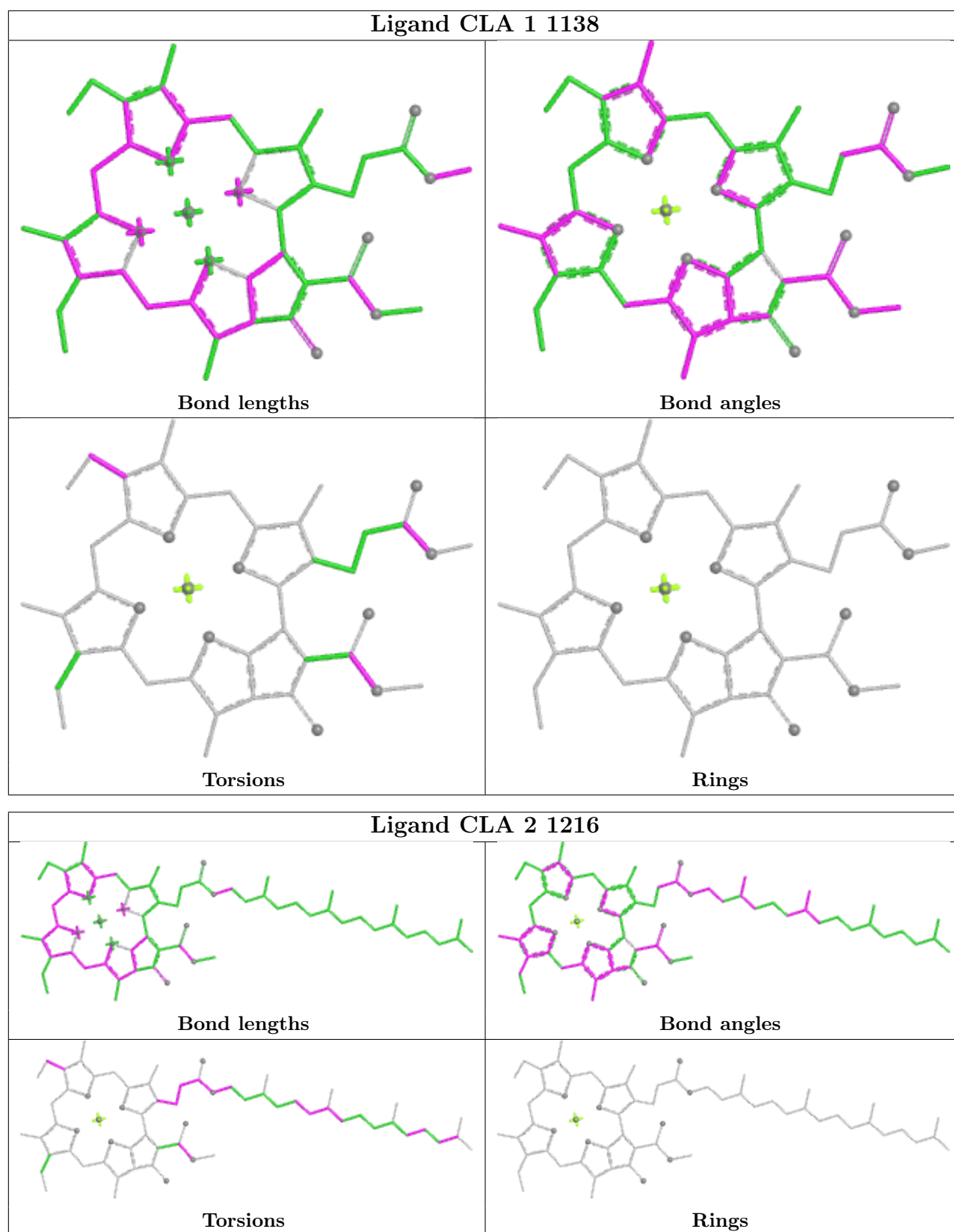


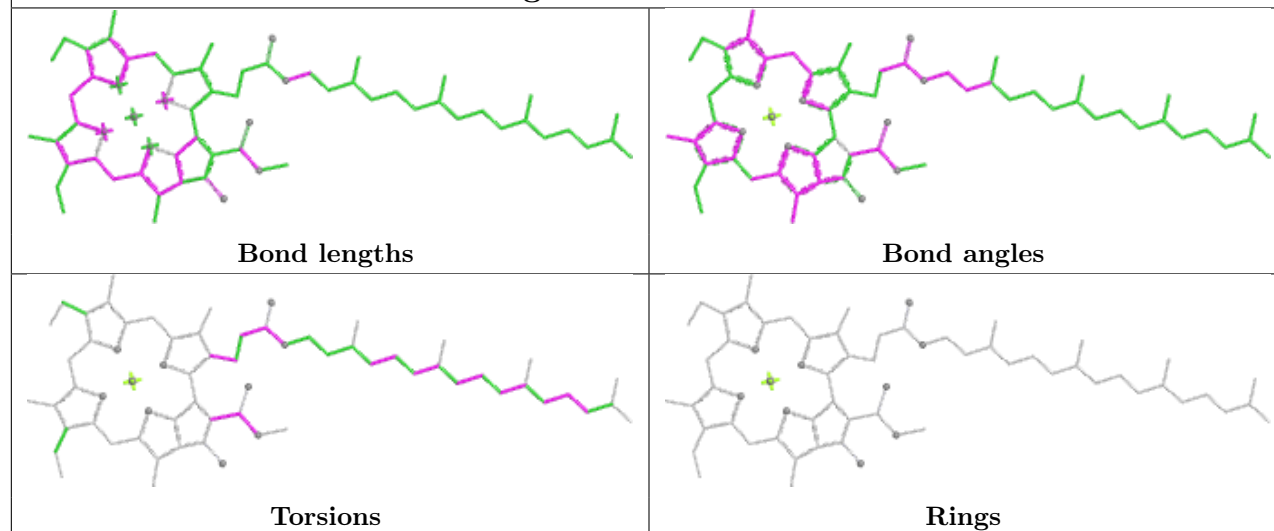
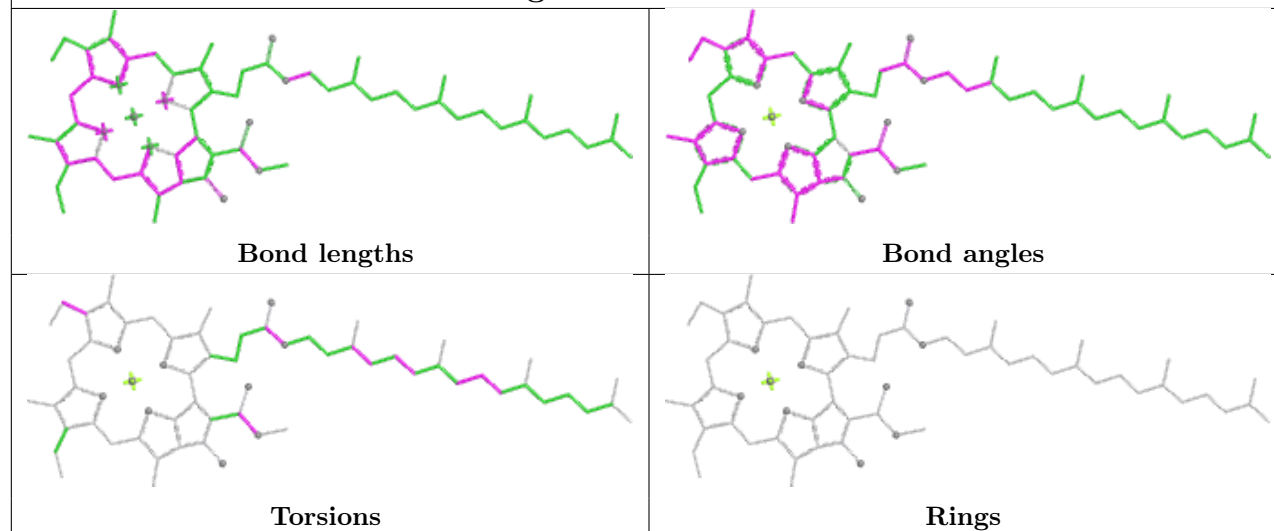


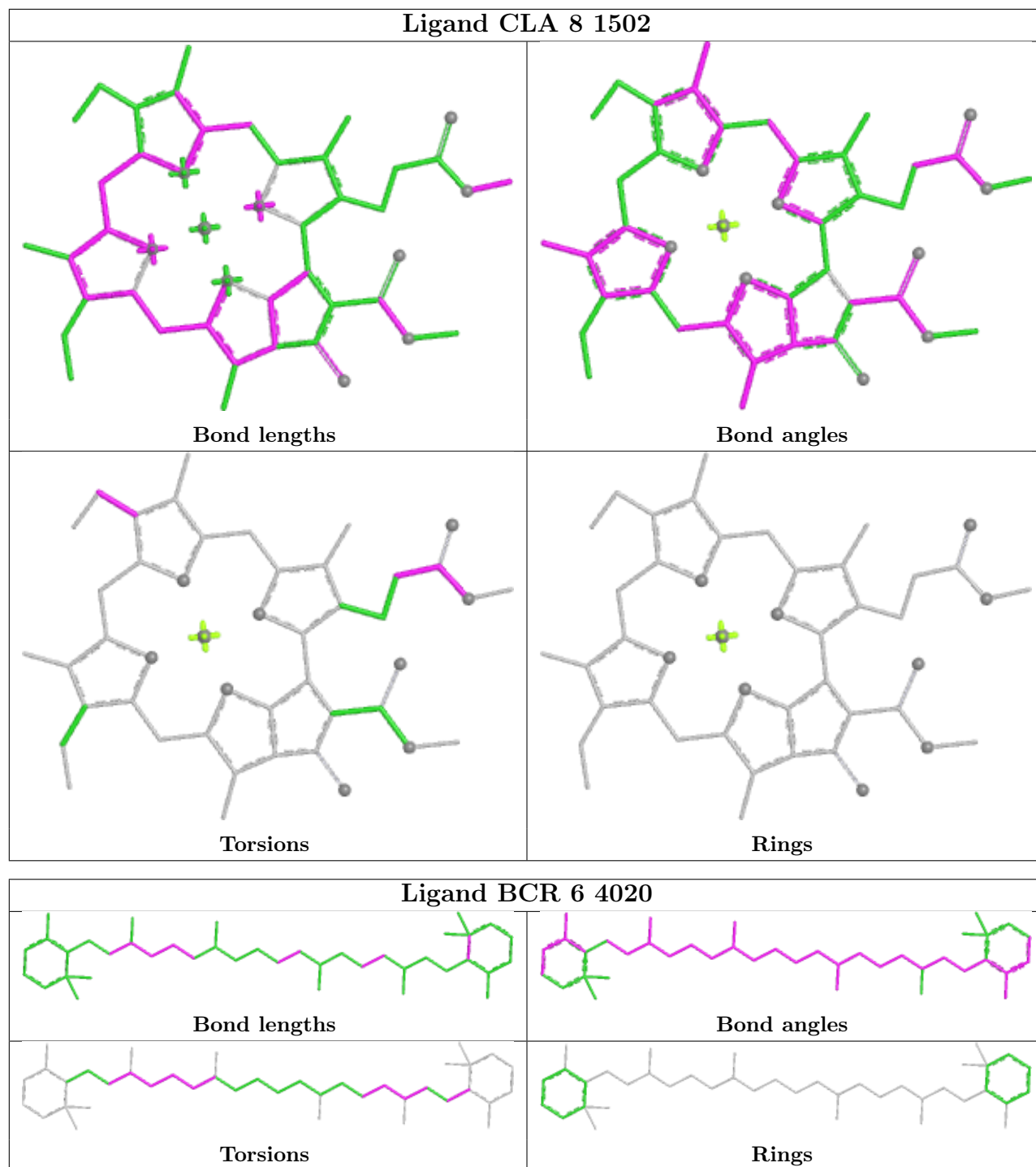


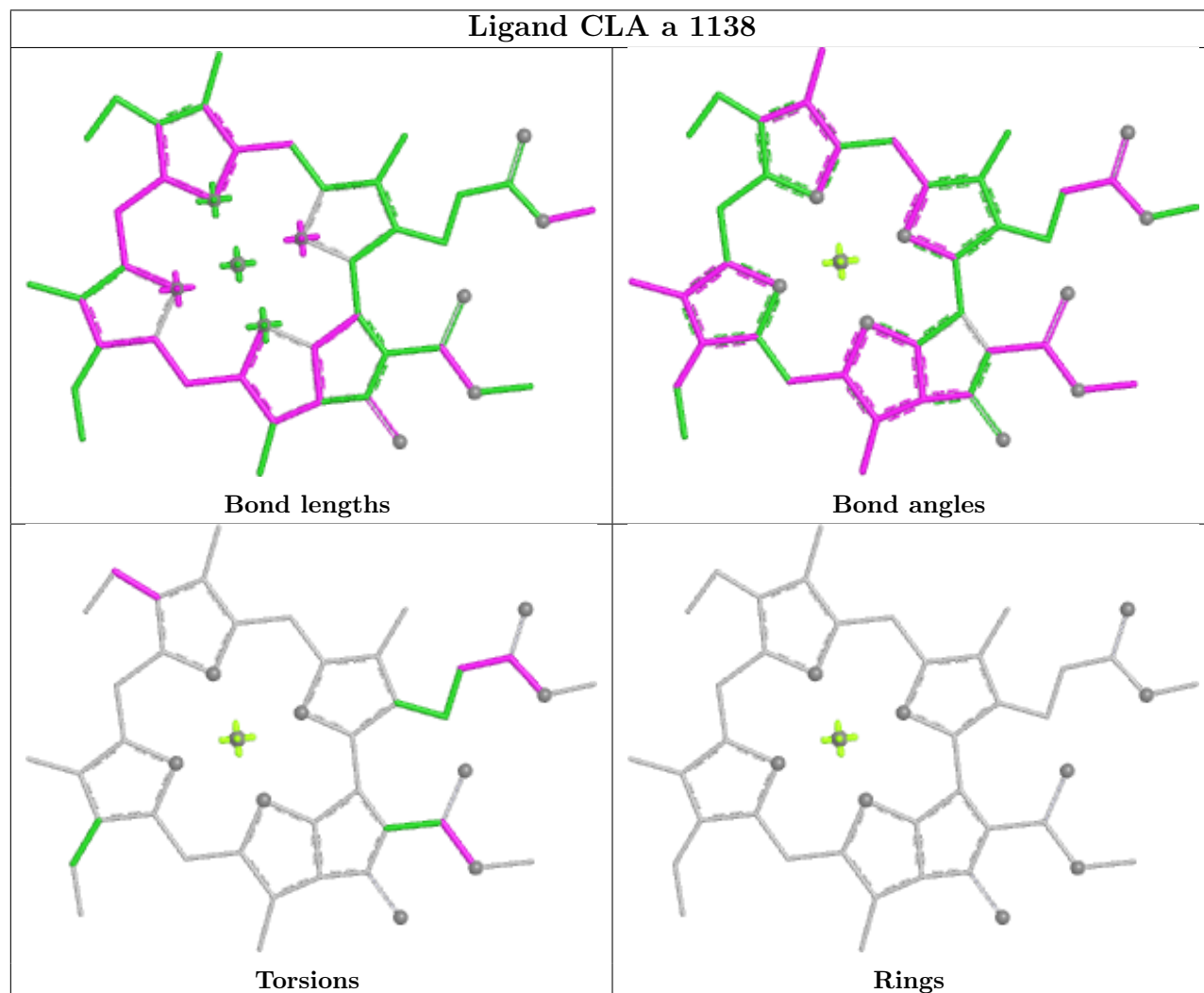
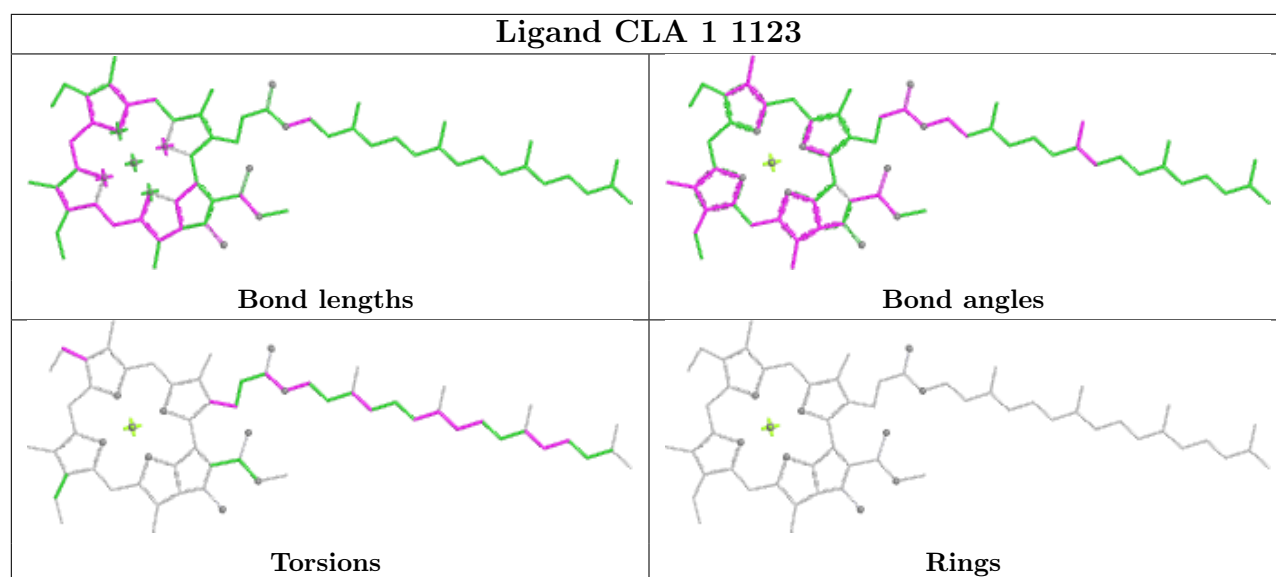


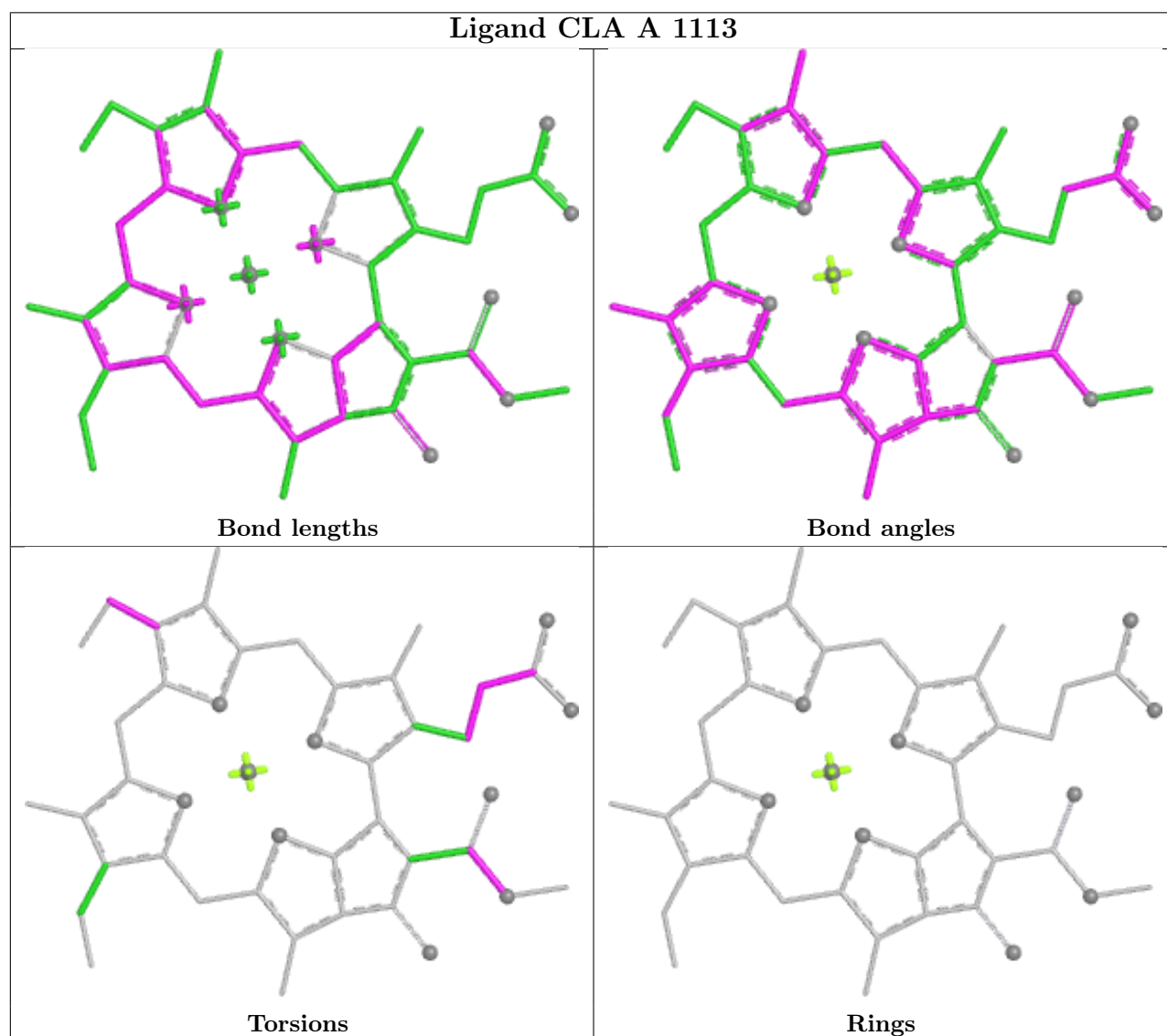
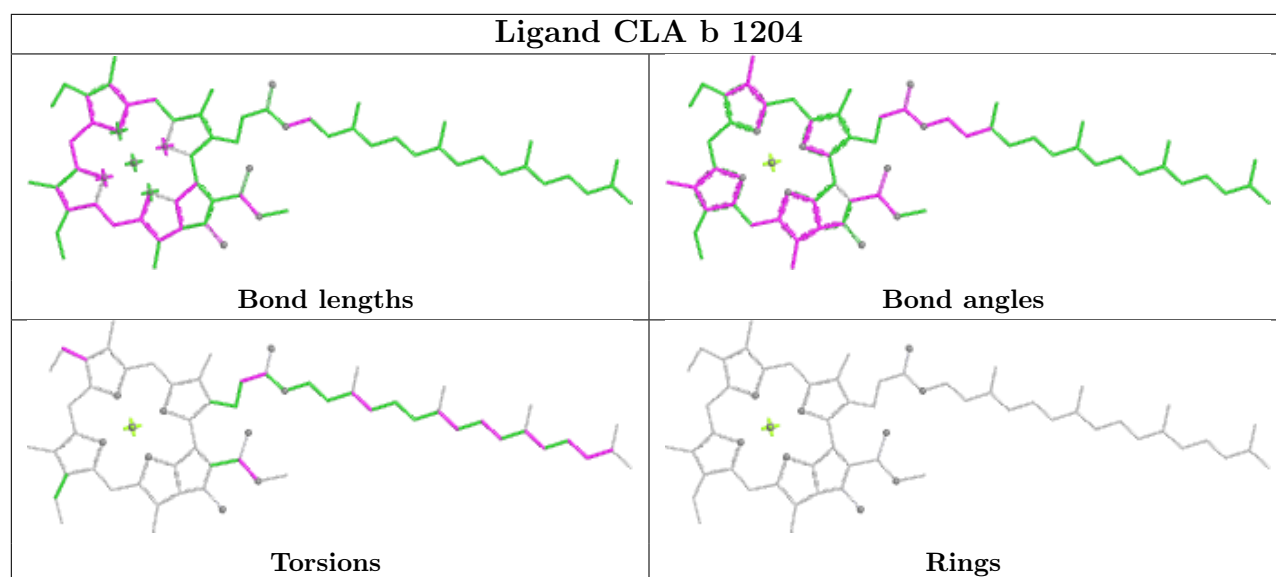




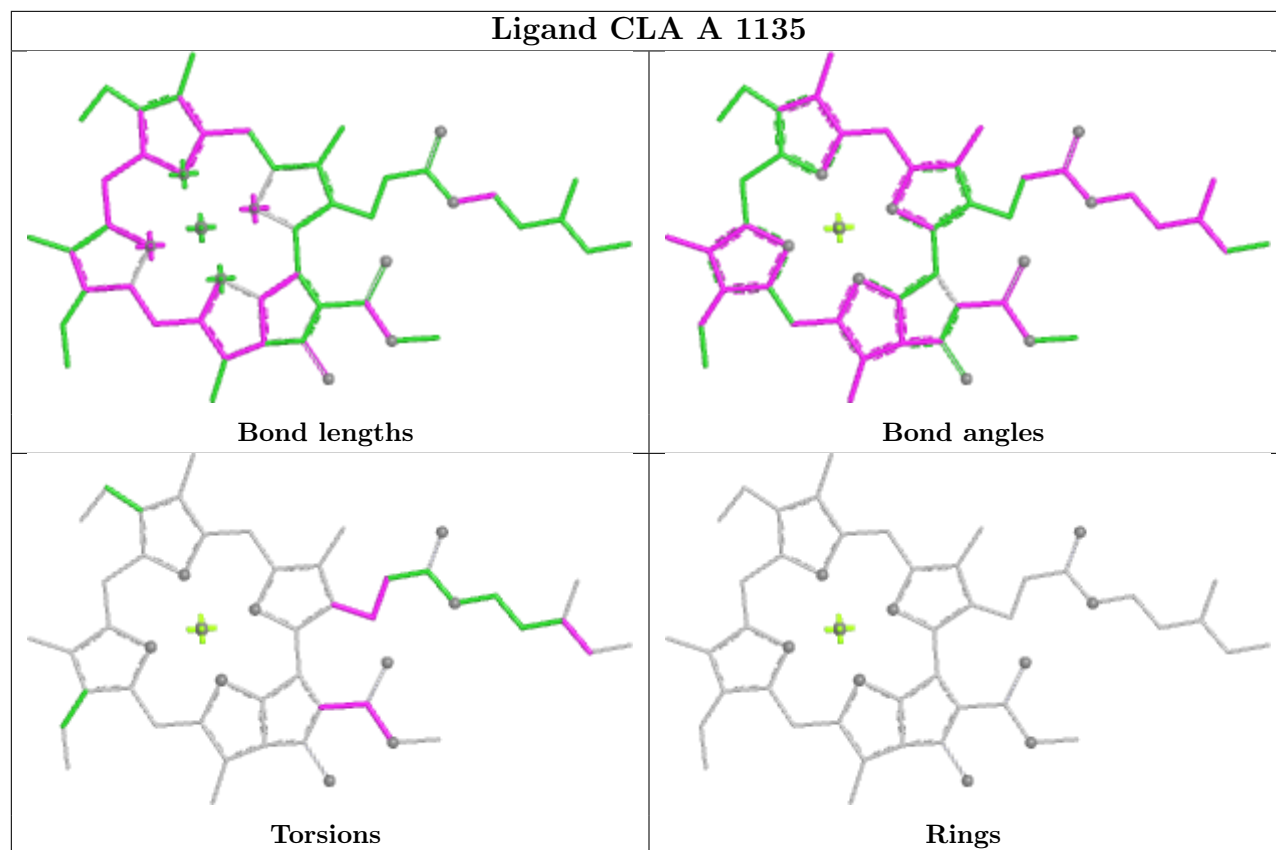
Ligand CLA B 1202**Ligand CLA 2 1204**



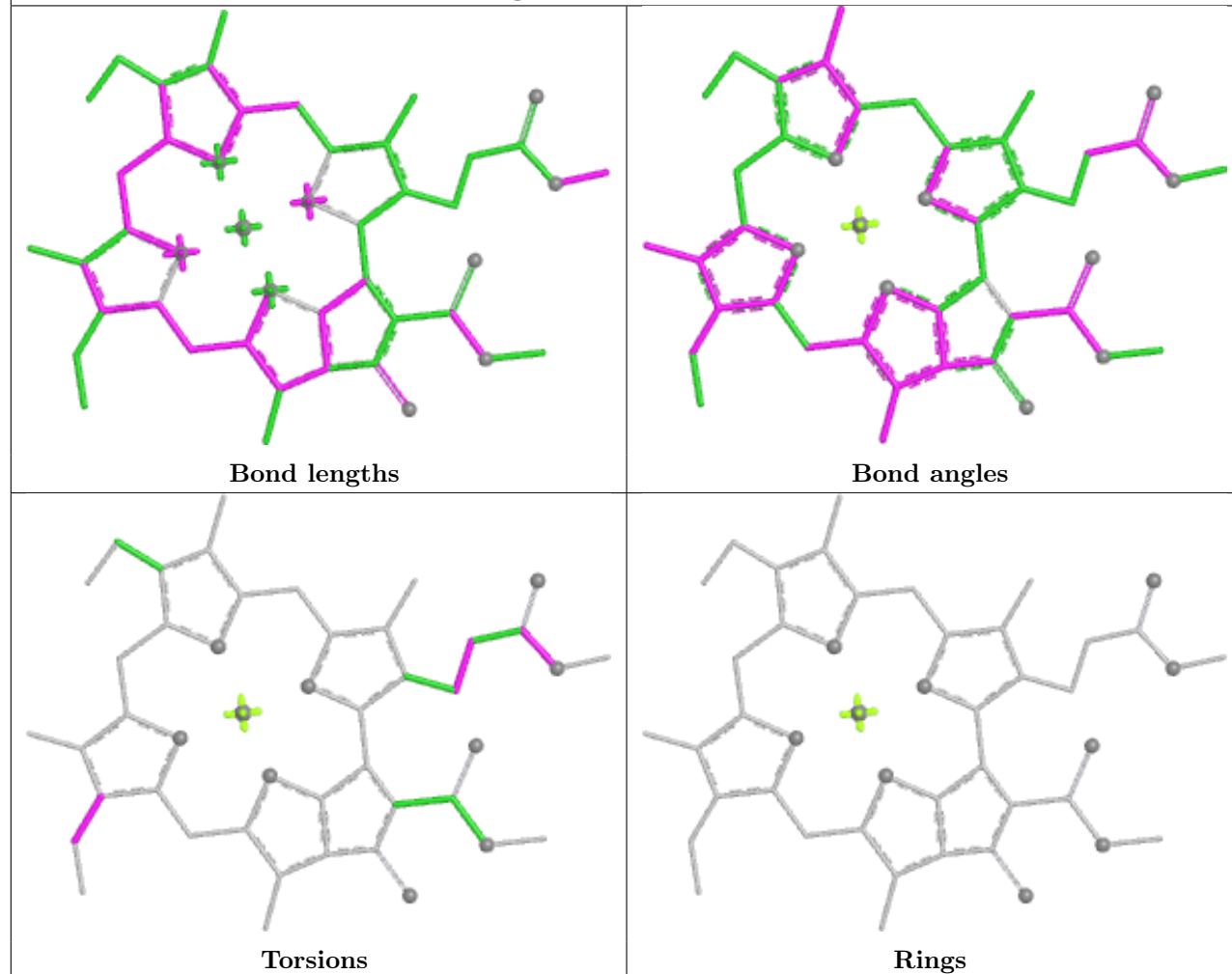




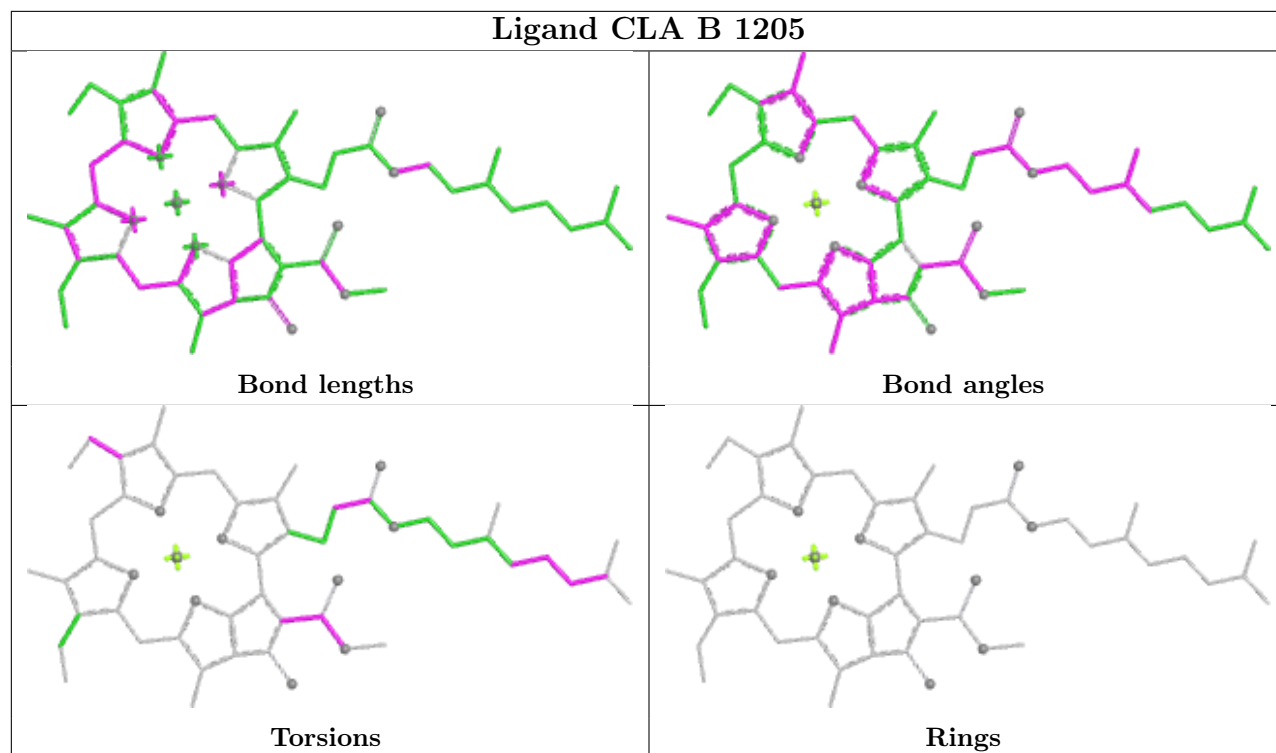
Ligand CLA A 1135



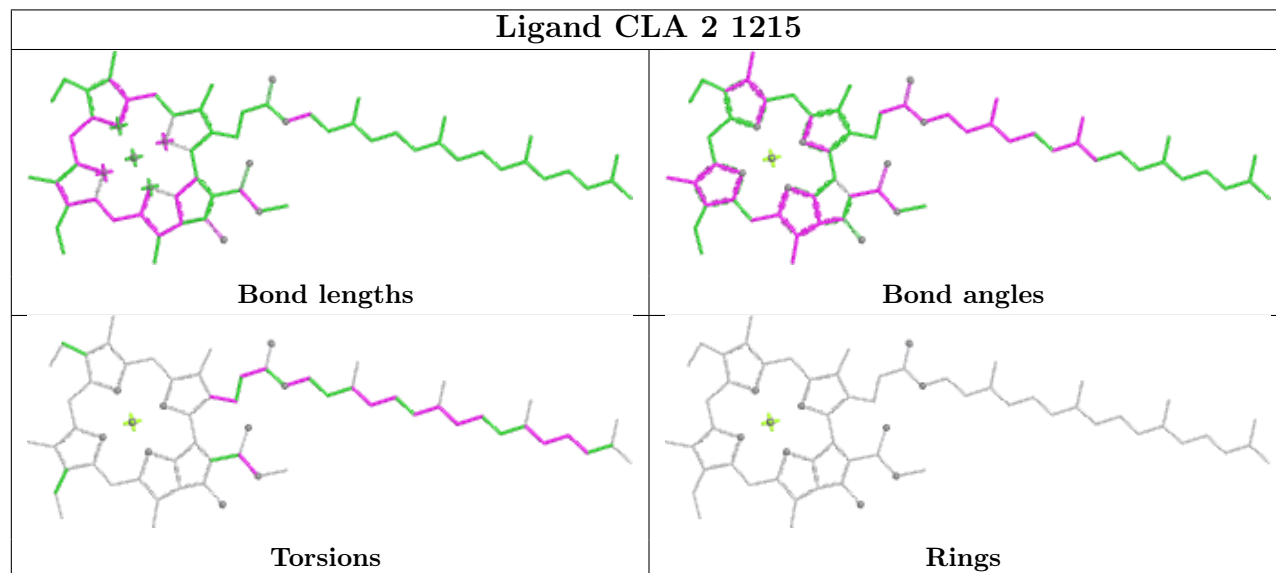
Ligand CLA 1 1134



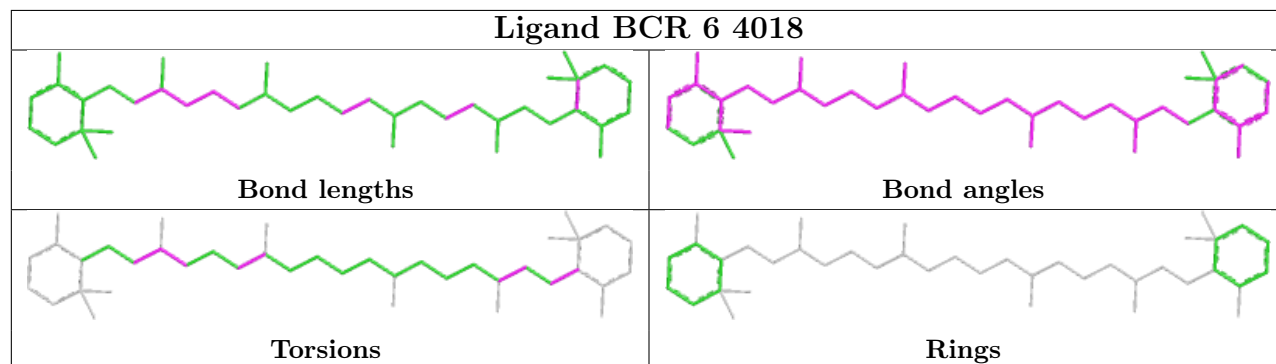
Ligand CLA B 1205



Ligand CLA 2 1215



Ligand BCR 6 4018



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	1	739/751 (98%)	-0.45	2 (0%) 90 78	100, 203, 296, 388	0
1	A	739/751 (98%)	-0.41	1 (0%) 92 87	80, 112, 176, 250	0
1	a	739/751 (98%)	-0.45	3 (0%) 88 74	125, 205, 289, 372	0
2	2	728/731 (99%)	-0.46	1 (0%) 92 87	91, 133, 197, 293	0
2	B	728/731 (99%)	-0.43	3 (0%) 88 74	81, 133, 213, 297	0
2	b	728/731 (99%)	-0.51	2 (0%) 90 78	112, 221, 302, 414	0
3	3	80/81 (98%)	-0.13	3 (3%) 44 31	143, 185, 231, 268	0
3	C	80/81 (98%)	-0.19	0 100 100	100, 116, 140, 196	0
3	c	80/81 (98%)	-0.20	0 100 100	149, 205, 255, 292	0
4	4	138/141 (97%)	-0.50	0 100 100	93, 195, 240, 290	0
4	D	138/141 (97%)	-0.41	0 100 100	88, 119, 165, 202	0
4	d	138/141 (97%)	-0.51	1 (0%) 84 65	83, 185, 253, 282	0
5	5	68/74 (91%)	-0.61	0 100 100	175, 220, 285, 372	0
5	E	68/74 (91%)	-0.43	0 100 100	111, 151, 185, 210	0
5	e	68/74 (91%)	-0.51	0 100 100	198, 253, 319, 365	0
6	6	125/125 (100%)	-0.48	0 100 100	188, 307, 389, 486	0
6	F	125/125 (100%)	-0.52	0 100 100	154, 241, 336, 388	0
6	f	125/125 (100%)	-0.38	0 100 100	245, 333, 408, 478	0
7	8	151/157 (96%)	-0.46	0 100 100	97, 125, 211, 294	0
7	L	151/157 (96%)	-0.38	1 (0%) 84 65	88, 109, 163, 229	0
7	l	151/157 (96%)	-0.44	0 100 100	107, 122, 165, 258	0
8	7	31/31 (100%)	-0.70	0 100 100	89, 95, 139, 147	0
8	M	31/31 (100%)	-0.57	0 100 100	108, 124, 158, 172	0
8	m	31/31 (100%)	-0.48	0 100 100	150, 174, 211, 233	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å²)	Q<0.9
9	9	38/40 (95%)	-0.53	0	100	100	89, 97, 152, 208	0
9	I	38/40 (95%)	-0.65	0	100	100	92, 112, 198, 208	0
9	i	38/40 (95%)	-0.62	0	100	100	125, 151, 224, 233	0
10	0	80/128 (62%)	-0.41	0	100	100	220, 289, 383, 449	0
10	K	80/128 (62%)	-0.30	0	100	100	118, 160, 246, 314	0
10	k	80/128 (62%)	-0.29	0	100	100	189, 227, 344, 404	0
All	All	6534/6777 (96%)	-0.45	17 (0%)	90	78	80, 168, 303, 486	0

The worst 5 of 17 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	1	593	LEU	5.1
1	a	321	MET	3.9
1	1	387	LEU	3.9
1	a	348	TRP	3.6
2	b	617	PHE	3.6

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

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

6.3 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
11	CLA	2	1240	45/65	0.59	0.09	224,246,269,289	0
11	CLA	b	1240	45/65	0.62	0.09	286,304,319,324	0
11	CLA	1	1110	54/65	0.64	0.11	258,268,295,299	0
11	CLA	B	1240	45/65	0.65	0.09	211,230,239,242	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
14	BCR	6	4013	40/40	0.65	0.10	254,275,285,291	0
11	CLA	a	1114	46/65	0.68	0.10	248,267,279,284	0
14	BCR	f	4013	40/40	0.70	0.10	275,292,321,326	0
14	BCR	1	4002	40/40	0.72	0.15	220,241,266,270	0
11	CLA	b	1218	45/65	0.73	0.09	273,286,303,305	0
11	CLA	b	1227	45/65	0.73	0.08	277,302,310,314	0
11	CLA	1	1113	45/65	0.73	0.11	235,255,277,284	0
11	CLA	1	1121	46/65	0.73	0.10	195,211,221,226	0
14	BCR	2	4011	40/40	0.74	0.12	187,207,215,220	0
11	CLA	B	1213	65/65	0.74	0.17	190,205,222,228	0
14	BCR	b	4011	40/40	0.75	0.14	204,219,248,251	0
11	CLA	1	1118	61/65	0.75	0.13	279,308,317,321	0
11	CLA	b	1209	45/65	0.75	0.10	226,238,250,254	0
11	CLA	1	1108	45/65	0.75	0.09	247,270,284,289	0
14	BCR	a	4002	40/40	0.75	0.16	214,227,233,235	0
11	CLA	0	1402	50/65	0.76	0.09	282,304,319,325	0
11	CLA	b	1208	45/65	0.76	0.11	227,240,247,250	0
14	BCR	m	4021	40/40	0.76	0.16	175,183,191,194	0
14	BCR	1	4003	40/40	0.77	0.18	193,227,269,270	0
14	BCR	F	4013	40/40	0.77	0.10	163,191,214,225	0
11	CLA	B	1227	45/65	0.77	0.09	168,175,199,212	0
15	LHG	B	5004	49/49	0.77	0.12	158,169,178,183	0
12	PQN	a	2001	33/33	0.78	0.13	181,201,225,229	0
11	CLA	b	1230	58/65	0.79	0.10	250,275,310,317	0
11	CLA	b	1234	60/65	0.79	0.11	220,242,268,270	0
11	CLA	b	1228	50/65	0.79	0.10	262,267,290,297	0
11	CLA	b	1219	55/65	0.80	0.09	267,284,296,299	0
15	LHG	b	5004	49/49	0.80	0.10	270,283,301,308	0
11	CLA	1	1114	46/65	0.81	0.08	262,279,288,293	0
11	CLA	b	1213	65/65	0.81	0.13	261,273,288,291	0
11	CLA	A	1114	46/65	0.82	0.10	150,165,173,175	0
11	CLA	1	1105	48/65	0.82	0.10	208,225,238,242	0
14	BCR	a	4003	40/40	0.83	0.14	192,210,235,238	0
11	CLA	a	1109	65/65	0.83	0.12	224,238,254,259	0
11	CLA	b	1232	45/65	0.83	0.06	249,265,277,284	0
11	CLA	b	1216	65/65	0.83	0.10	221,239,260,264	0
11	CLA	b	1201	54/65	0.83	0.10	150,157,164,166	0
11	CLA	a	1105	48/65	0.84	0.08	249,270,280,285	0
11	CLA	2	1219	55/65	0.84	0.09	177,196,211,233	0
14	BCR	b	4005	40/40	0.84	0.10	193,207,227,230	0
14	BCR	L	4022	40/40	0.85	0.15	110,121,132,133	0
14	BCR	M	4021	40/40	0.85	0.10	103,111,125,126	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
11	CLA	k	1401	65/65	0.85	0.11	196,201,206,207	0
11	CLA	k	1402	50/65	0.85	0.09	225,232,238,242	0
11	CLA	a	1126	65/65	0.85	0.12	210,232,258,266	0
15	LHG	A	5003	49/49	0.85	0.09	92,97,104,115	0
11	CLA	b	1229	65/65	0.85	0.10	249,269,282,289	0
11	CLA	a	1110	54/65	0.85	0.09	211,224,241,244	0
15	LHG	2	5004	49/49	0.85	0.10	183,200,224,236	0
14	BCR	2	4004	40/40	0.86	0.14	123,137,161,163	0
14	BCR	B	4004	40/40	0.86	0.12	168,175,187,190	0
11	CLA	2	1229	65/65	0.86	0.11	177,187,202,209	0
11	CLA	1	1107	65/65	0.86	0.09	207,232,269,282	0
12	PQN	B	2002	33/33	0.86	0.12	86,88,98,133	0
11	CLA	b	1211	46/65	0.86	0.10	210,224,234,240	0
15	LHG	1	5003	49/49	0.86	0.12	154,173,196,198	0
14	BCR	A	4008	40/40	0.86	0.10	82,86,94,95	0
16	LMG	2	5002	55/55	0.86	0.13	122,136,148,155	0
14	BCR	b	4014	40/40	0.87	0.14	230,259,294,299	0
14	BCR	f	4018	40/40	0.87	0.11	132,138,152,154	0
11	CLA	B	1234	60/65	0.87	0.12	124,143,166,172	0
11	CLA	b	1221	54/65	0.87	0.12	241,253,261,266	0
11	CLA	b	1210	65/65	0.87	0.11	207,221,229,232	0
11	CLA	1	1102	65/65	0.87	0.10	199,219,239,246	0
11	CLA	2	1209	45/65	0.87	0.09	124,135,140,143	0
14	BCR	2	4005	40/40	0.87	0.11	102,108,118,120	0
14	BCR	2	4010	40/40	0.87	0.13	132,140,147,150	0
14	BCR	B	4005	40/40	0.87	0.10	118,135,161,162	0
11	CLA	a	1121	46/65	0.87	0.10	162,173,180,183	0
14	BCR	7	4021	40/40	0.87	0.12	106,110,121,131	0
11	CLA	a	1118	61/65	0.87	0.10	202,218,238,243	0
11	CLA	2	1230	58/65	0.87	0.09	222,240,273,278	0
11	CLA	b	1217	47/65	0.87	0.08	240,259,267,270	0
11	CLA	A	1801	52/65	0.87	0.10	89,95,98,103	0
11	CLA	1	1111	60/65	0.87	0.10	229,246,266,273	0
11	CLA	0	1401	65/65	0.87	0.10	251,268,277,306	0
14	BCR	1	4001	40/40	0.88	0.14	241,254,269,271	0
11	CLA	a	1117	65/65	0.88	0.11	167,191,206,211	0
14	BCR	F	4018	40/40	0.88	0.10	94,101,113,114	0
14	BCR	1	4008	40/40	0.88	0.09	169,180,189,192	0
11	CLA	K	1401	65/65	0.88	0.12	141,148,155,157	0
11	CLA	K	1402	50/65	0.88	0.12	169,178,200,223	0
11	CLA	B	1218	45/65	0.88	0.09	168,176,189,196	0
11	CLA	a	1102	65/65	0.88	0.12	213,223,246,250	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
11	CLA	1	1109	65/65	0.88	0.12	239,261,278,283	0
14	BCR	a	4007	40/40	0.88	0.12	144,153,167,170	0
11	CLA	2	1218	45/65	0.88	0.08	164,178,189,194	0
11	CLA	A	1107	65/65	0.88	0.09	122,130,137,141	0
15	LHG	a	5003	49/49	0.88	0.10	144,147,154,158	0
11	CLA	2	1227	45/65	0.88	0.09	197,210,223,231	0
14	BCR	A	4001	40/40	0.88	0.20	110,115,129,130	0
11	CLA	B	1230	58/65	0.88	0.09	159,178,203,214	0
11	CLA	A	1118	61/65	0.88	0.11	130,138,152,163	0
14	BCR	b	4006	40/40	0.89	0.11	193,210,237,241	0
14	BCR	b	4010	40/40	0.89	0.10	230,257,283,284	0
11	CLA	1	1115	46/65	0.89	0.10	236,256,261,267	0
11	CLA	a	1139	50/65	0.89	0.10	210,233,255,263	0
11	CLA	a	1107	65/65	0.89	0.08	235,255,266,271	0
11	CLA	1	1120	46/65	0.89	0.08	227,248,258,262	0
11	CLA	l	1501	65/65	0.89	0.10	137,139,157,168	0
11	CLA	1	1801	52/65	0.89	0.08	199,212,225,231	0
12	PQN	b	2002	33/33	0.89	0.09	140,146,156,158	0
11	CLA	B	1228	50/65	0.89	0.09	181,188,206,208	0
11	CLA	b	1013	65/65	0.89	0.13	201,226,239,244	0
11	CLA	B	1229	65/65	0.89	0.10	151,164,176,181	0
11	CLA	2	1228	50/65	0.89	0.08	191,205,224,232	0
14	BCR	B	4010	40/40	0.89	0.14	128,141,167,171	0
14	BCR	B	4011	40/40	0.89	0.12	108,121,138,141	0
14	BCR	2	4014	40/40	0.89	0.12	184,206,223,228	0
11	CLA	a	1113	45/65	0.89	0.09	233,253,273,278	0
11	CLA	L	1503	65/65	0.89	0.13	106,116,134,148	0
11	CLA	2	1232	45/65	0.89	0.08	148,157,170,176	0
11	CLA	2	1234	60/65	0.89	0.11	151,164,196,206	0
11	CLA	2	1235	60/65	0.89	0.11	154,169,185,191	0
11	CLA	B	1209	45/65	0.89	0.07	149,160,170,173	0
11	CLA	a	1125	52/65	0.89	0.10	157,167,173,177	0
14	BCR	a	4008	40/40	0.89	0.10	150,152,155,155	0
16	LMG	b	5002	55/55	0.89	0.10	149,160,167,167	0
11	CLA	B	1232	45/65	0.89	0.08	168,184,196,202	0
14	BCR	b	4004	40/40	0.90	0.10	242,256,279,281	0
11	CLA	A	1106	65/65	0.90	0.12	123,134,140,152	0
11	CLA	L	1501	65/65	0.90	0.10	116,126,140,160	0
14	BCR	b	4009	40/40	0.90	0.12	254,280,313,316	0
11	CLA	A	1105	48/65	0.90	0.08	118,132,139,142	0
11	CLA	1	1122	59/65	0.90	0.09	168,189,205,209	0
11	CLA	1	1125	52/65	0.90	0.11	168,181,193,200	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
11	CLA	1	1131	65/65	0.90	0.12	108,119,126,130	0
11	CLA	a	1801	52/65	0.90	0.11	156,164,182,184	0
11	CLA	a	1101	65/65	0.90	0.10	236,245,257,265	0
11	CLA	B	1216	65/65	0.90	0.12	151,164,179,185	0
12	PQN	1	2001	33/33	0.90	0.11	184,204,226,230	0
11	CLA	1	1132	65/65	0.90	0.10	99,105,118,123	0
14	BCR	A	4002	40/40	0.90	0.11	118,122,130,131	0
11	CLA	2	1203	65/65	0.90	0.10	97,104,108,110	0
11	CLA	a	1103	65/65	0.90	0.12	199,214,239,246	0
11	CLA	2	1213	65/65	0.90	0.12	142,149,160,181	0
14	BCR	B	4009	40/40	0.90	0.13	169,203,225,226	0
11	CLA	a	1140	65/65	0.90	0.08	203,218,260,267	0
11	CLA	1	1101	65/65	0.90	0.08	214,232,245,253	0
14	BCR	8	4022	40/40	0.90	0.11	123,131,145,146	0
14	BCR	B	4014	40/40	0.90	0.12	138,157,191,200	0
15	LHG	A	5001	49/49	0.90	0.12	94,99,108,110	0
11	CLA	B	1208	45/65	0.90	0.07	128,136,143,147	0
11	CLA	1	1104	65/65	0.90	0.11	205,230,242,264	0
11	CLA	a	1120	46/65	0.90	0.10	190,204,214,230	0
11	CLA	b	1223	65/65	0.90	0.09	218,233,240,242	0
15	LHG	1	5001	49/49	0.90	0.11	182,196,208,213	0
11	CLA	b	1224	55/65	0.90	0.10	163,171,178,179	0
11	CLA	b	1225	65/65	0.90	0.10	183,198,210,214	0
16	LMG	B	5002	55/55	0.90	0.12	110,116,120,125	0
11	CLA	B	1219	55/65	0.90	0.07	158,173,186,192	0
11	CLA	B	1222	56/65	0.90	0.11	121,136,161,169	0
14	BCR	l	4022	40/40	0.91	0.15	121,122,124,124	0
14	BCR	B	4006	40/40	0.91	0.10	128,148,172,176	0
11	CLA	A	1131	65/65	0.91	0.11	81,84,88,109	0
11	CLA	2	1236	47/65	0.91	0.10	149,159,173,177	0
11	CLA	b	1214	59/65	0.91	0.10	229,247,262,266	0
11	CLA	2	1238	65/65	0.91	0.09	93,106,113,116	0
11	CLA	8	1503	65/65	0.91	0.12	137,142,156,177	0
11	CLA	2	1201	54/65	0.91	0.12	91,100,104,107	0
14	BCR	L	4019	40/40	0.91	0.11	87,90,93,93	0
11	CLA	a	1112	45/65	0.91	0.10	233,251,261,266	0
11	CLA	A	1116	54/65	0.91	0.11	96,102,108,123	0
14	BCR	6	4018	40/40	0.91	0.09	93,97,107,113	0
14	BCR	6	4020	40/40	0.91	0.10	93,104,116,117	0
11	CLA	b	1235	60/65	0.91	0.08	235,252,263,268	0
11	CLA	B	1238	65/65	0.91	0.12	82,86,90,93	0
11	CLA	a	1134	46/65	0.91	0.08	160,175,184,187	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
12	PQN	A	2001	33/33	0.91	0.11	104,115,128,137	0
11	CLA	2	1221	54/65	0.91	0.12	120,128,140,143	0
11	CLA	2	1222	56/65	0.91	0.11	141,153,179,185	0
11	CLA	2	1223	65/65	0.91	0.11	131,134,148,153	0
11	CLA	A	1120	46/65	0.91	0.11	99,107,111,112	0
11	CLA	a	1124	55/65	0.91	0.10	156,166,174,176	0
11	CLA	b	1207	65/65	0.91	0.11	120,127,132,133	0
11	CLA	A	1101	65/65	0.91	0.10	143,151,160,175	0
11	CLA	a	1108	45/65	0.91	0.08	215,233,245,250	0
14	BCR	f	4020	40/40	0.91	0.10	113,119,125,126	0
11	CLA	A	1126	65/65	0.91	0.12	95,105,125,130	0
11	CLA	2	1204	65/65	0.92	0.12	88,90,94,99	0
11	CLA	2	1207	65/65	0.92	0.12	99,103,107,121	0
14	BCR	b	4017	40/40	0.92	0.12	143,150,160,162	0
11	CLA	2	1208	45/65	0.92	0.09	102,111,118,120	0
11	CLA	1	1103	65/65	0.92	0.09	218,234,261,272	0
11	CLA	B	1206	65/65	0.92	0.11	94,99,104,106	0
14	BCR	l	4019	40/40	0.92	0.12	122,133,149,151	0
11	CLA	a	1132	65/65	0.92	0.10	113,128,133,136	0
11	CLA	1	1106	65/65	0.92	0.10	187,201,212,222	0
14	BCR	A	4007	40/40	0.92	0.10	91,93,99,109	0
11	CLA	A	1119	65/65	0.92	0.11	82,95,99,109	0
11	CLA	B	1221	54/65	0.92	0.12	126,134,140,146	0
11	CLA	A	1122	59/65	0.92	0.11	83,88,92,94	0
11	CLA	2	1226	65/65	0.92	0.10	99,113,120,122	0
11	CLA	b	1202	65/65	0.92	0.12	169,187,198,202	0
14	BCR	2	4009	40/40	0.92	0.14	189,224,256,263	0
11	CLA	A	1121	46/65	0.92	0.09	97,103,120,155	0
11	CLA	A	1134	46/65	0.92	0.07	98,106,111,113	0
11	CLA	A	1125	52/65	0.92	0.09	95,99,105,127	0
14	BCR	B	4017	40/40	0.92	0.13	80,85,96,96	0
11	CLA	A	1102	65/65	0.92	0.10	123,130,142,144	0
11	CLA	a	1137	65/65	0.92	0.11	153,164,174,179	0
14	BCR	8	4019	40/40	0.92	0.12	125,129,144,154	0
11	CLA	A	1113	45/65	0.92	0.10	121,133,146,148	0
11	CLA	b	1206	65/65	0.92	0.10	135,142,149,151	0
11	CLA	1	1137	65/65	0.92	0.10	155,167,185,189	0
14	BCR	a	4001	40/40	0.92	0.12	173,199,227,229	0
11	CLA	2	1211	46/65	0.92	0.11	98,104,109,112	0
11	CLA	1	1139	50/65	0.92	0.08	181,204,222,225	0
11	CLA	b	1215	65/65	0.92	0.10	226,238,256,265	0
11	CLA	A	1139	50/65	0.92	0.11	112,126,138,142	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
11	CLA	a	1012	65/65	0.92	0.13	185,204,226,230	0
11	CLA	1	1237	55/65	0.92	0.10	113,120,130,133	0
11	CLA	1	1134	46/65	0.92	0.07	212,228,242,244	0
11	CLA	B	1235	60/65	0.92	0.08	141,154,163,166	0
11	CLA	A	1140	65/65	0.92	0.09	124,136,172,178	0
11	CLA	l	1503	65/65	0.93	0.11	125,130,137,187	0
11	CLA	A	1137	65/65	0.93	0.08	81,83,91,110	0
11	CLA	a	1111	60/65	0.93	0.10	198,205,225,229	0
11	CLA	2	1023	65/65	0.93	0.11	117,135,145,149	0
11	CLA	B	1231	45/65	0.93	0.08	154,169,180,185	0
11	CLA	a	1237	55/65	0.93	0.10	116,121,126,128	0
11	CLA	b	1222	56/65	0.93	0.09	230,254,284,293	0
11	CLA	a	1022	65/65	0.93	0.14	142,156,166,168	0
11	CLA	B	1204	65/65	0.93	0.10	100,109,115,117	0
11	CLA	a	1122	59/65	0.93	0.09	134,144,153,156	0
12	PQN	2	2002	33/33	0.93	0.09	106,118,130,131	0
11	CLA	2	1210	65/65	0.93	0.14	104,112,120,123	0
11	CLA	b	1226	65/65	0.93	0.10	165,186,192,194	0
14	BCR	A	4003	40/40	0.93	0.10	100,112,129,132	0
14	BCR	1	4007	40/40	0.93	0.09	202,218,231,231	0
11	CLA	2	1216	65/65	0.93	0.09	141,156,169,176	0
11	CLA	2	1217	47/65	0.93	0.08	127,139,146,149	0
11	CLA	B	1220	46/65	0.93	0.08	133,148,155,158	0
14	BCR	2	4006	40/40	0.93	0.10	98,105,120,122	0
11	CLA	b	1203	65/65	0.93	0.09	169,178,189,193	0
11	CLA	b	1204	65/65	0.93	0.10	163,169,175,177	0
11	CLA	A	1104	65/65	0.93	0.10	93,99,105,107	0
11	CLA	1	1112	45/65	0.93	0.07	263,286,301,303	0
14	BCR	2	4017	40/40	0.93	0.10	96,102,117,117	0
11	CLA	b	1231	45/65	0.93	0.07	275,294,305,311	0
11	CLA	A	1129	46/65	0.93	0.12	82,85,88,89	0
11	CLA	a	1131	65/65	0.93	0.10	121,124,131,134	0
11	CLA	a	1106	65/65	0.93	0.08	212,222,232,234	0
14	BCR	F	4020	40/40	0.93	0.10	84,87,94,94	0
11	CLA	1	1124	55/65	0.93	0.09	176,181,188,196	0
11	CLA	2	1231	45/65	0.93	0.09	139,147,159,168	0
11	CLA	b	1236	47/65	0.93	0.07	239,254,268,270	0
11	CLA	1	1126	65/65	0.93	0.08	179,200,211,215	0
15	LHG	a	5001	49/49	0.93	0.08	181,190,210,212	0
11	CLA	1	1127	65/65	0.93	0.10	214,223,233,237	0
11	CLA	a	1138	46/65	0.93	0.08	226,242,255,260	0
11	CLA	B	1212	45/65	0.93	0.10	160,174,184,187	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
11	CLA	A	1132	65/65	0.93	0.12	90,92,97,100	0
11	CLA	1	1140	65/65	0.93	0.08	180,188,218,225	0
11	CLA	8	1501	65/65	0.93	0.12	131,138,145,158	0
11	CLA	b	1238	65/65	0.93	0.10	121,126,133,135	0
11	CLA	A	1133	46/65	0.93	0.08	89,96,101,103	0
11	CLA	a	1136	46/65	0.94	0.08	140,148,157,173	0
11	CLA	B	1225	65/65	0.94	0.09	110,123,143,148	0
11	CLA	1	1012	65/65	0.94	0.11	147,161,195,201	0
11	CLA	B	1226	65/65	0.94	0.11	104,114,121,124	0
11	CLA	A	1130	46/65	0.94	0.10	88,90,93,107	0
11	CLA	a	1123	65/65	0.94	0.10	159,181,191,193	0
11	CLA	B	1210	65/65	0.94	0.10	126,135,144,149	0
11	CLA	1	1133	46/65	0.94	0.09	179,192,203,206	0
11	CLA	b	1205	55/65	0.94	0.09	146,156,165,167	0
11	CLA	A	1103	65/65	0.94	0.12	93,100,116,120	0
11	CLA	A	1124	55/65	0.94	0.11	85,89,93,93	0
11	CLA	B	1214	59/65	0.94	0.10	143,159,171,177	0
11	CLA	A	1138	46/65	0.94	0.09	121,131,139,143	0
11	CLA	2	1206	65/65	0.94	0.08	91,95,98,100	0
11	CLA	B	1217	47/65	0.94	0.08	159,172,182,186	0
11	CLA	A	1110	54/65	0.94	0.07	113,119,131,135	0
11	CLA	1	1117	65/65	0.94	0.10	185,202,216,219	0
11	CLA	A	1237	55/65	0.94	0.12	80,83,86,87	0
11	CLA	a	1011	65/65	0.94	0.14	161,188,194,198	0
11	CLA	A	1136	46/65	0.94	0.09	82,86,88,89	0
11	CLA	B	1211	46/65	0.94	0.08	137,146,156,161	0
11	CLA	A	1012	65/65	0.94	0.12	105,116,126,129	0
11	CLA	B	1239	46/65	0.94	0.08	87,91,94,95	0
11	CLA	2	1220	46/65	0.94	0.09	145,153,163,167	0
11	CLA	1	1128	65/65	0.94	0.11	197,213,223,224	0
13	SF4	C	3002	8/8	0.94	0.07	60,88,151,152	0
13	SF4	c	3002	8/8	0.94	0.09	60,88,151,152	0
11	CLA	1	1130	46/65	0.94	0.09	131,140,148,150	0
11	CLA	A	1128	65/65	0.94	0.13	102,108,118,128	0
11	CLA	2	1225	65/65	0.94	0.11	100,105,110,112	0
11	CLA	a	1115	46/65	0.94	0.08	188,200,211,232	0
11	CLA	1	1138	46/65	0.94	0.08	175,188,205,208	0
11	CLA	B	1207	65/65	0.95	0.11	99,106,116,180	0
11	CLA	b	1021	65/65	0.95	0.12	185,193,223,226	0
11	CLA	2	1202	65/65	0.95	0.13	114,123,128,130	0
11	CLA	b	1023	65/65	0.95	0.12	135,142,156,159	0
11	CLA	B	1236	47/65	0.95	0.09	136,145,152,153	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
11	CLA	2	1205	55/65	0.95	0.09	92,96,98,99	0
11	CLA	A	1108	45/65	0.95	0.07	111,120,127,130	0
11	CLA	a	1127	65/65	0.95	0.11	186,200,211,220	0
11	CLA	a	1128	65/65	0.95	0.08	185,196,213,224	0
11	CLA	1	1116	54/65	0.95	0.10	201,212,225,236	0
11	CLA	a	1130	46/65	0.95	0.09	117,123,125,128	0
11	CLA	A	1111	60/65	0.95	0.09	106,111,121,124	0
11	CLA	2	1214	59/65	0.95	0.09	120,130,139,145	0
13	SF4	c	3003	8/8	0.95	0.12	60,67,100,115	0
13	SF4	3	3002	8/8	0.95	0.06	60,88,151,152	0
11	CLA	1	1119	65/65	0.95	0.11	197,237,248,254	0
11	CLA	B	1223	65/65	0.95	0.12	154,166,176,183	0
11	CLA	1	1123	65/65	0.95	0.09	208,227,237,242	0
11	CLA	A	1109	65/65	0.95	0.10	111,119,129,132	0
11	CLA	A	1135	51/65	0.95	0.11	90,94,97,99	0
11	CLA	b	1212	45/65	0.95	0.08	248,260,269,270	0
11	CLA	A	1115	46/65	0.95	0.07	111,121,126,126	0
11	CLA	b	1239	46/65	0.95	0.08	155,159,164,171	0
11	CLA	2	1224	55/65	0.95	0.11	103,107,124,141	0
11	CLA	L	1502	46/65	0.95	0.10	86,91,96,114	0
11	CLA	l	1502	46/65	0.95	0.08	111,114,119,120	0
11	CLA	B	1023	65/65	0.95	0.10	80,82,87,88	0
11	CLA	B	1215	65/65	0.95	0.15	135,141,147,154	0
11	CLA	B	1201	54/65	0.95	0.08	99,107,110,111	0
11	CLA	1	1022	65/65	0.95	0.11	101,124,132,137	0
11	CLA	1	1011	65/65	0.95	0.12	124,133,140,142	0
11	CLA	B	1203	65/65	0.95	0.09	104,109,117,121	0
11	CLA	a	1129	46/65	0.95	0.11	141,147,154,156	0
11	CLA	a	1119	65/65	0.95	0.10	143,162,172,177	0
11	CLA	a	1133	46/65	0.95	0.07	158,171,178,183	0
11	CLA	1	1129	46/65	0.95	0.10	166,179,190,191	0
11	CLA	A	1123	65/65	0.95	0.12	89,95,99,100	0
11	CLA	a	1135	51/65	0.95	0.10	140,155,162,167	0
11	CLA	2	1239	46/65	0.95	0.08	103,112,115,119	0
11	CLA	B	1205	55/65	0.95	0.08	97,104,114,127	0
11	CLA	1	1135	51/65	0.95	0.09	174,178,184,187	0
11	CLA	2	1013	65/65	0.95	0.10	153,169,194,196	0
11	CLA	a	1104	65/65	0.96	0.10	189,200,213,217	0
11	CLA	A	1011	65/65	0.96	0.13	85,97,106,141	0
11	CLA	A	1117	65/65	0.96	0.09	92,103,111,114	0
11	CLA	a	1116	54/65	0.96	0.08	170,177,186,189	0
11	CLA	1	1136	46/65	0.96	0.08	154,164,170,176	0

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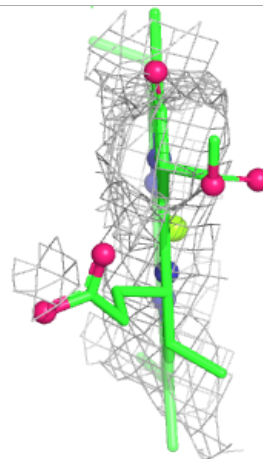
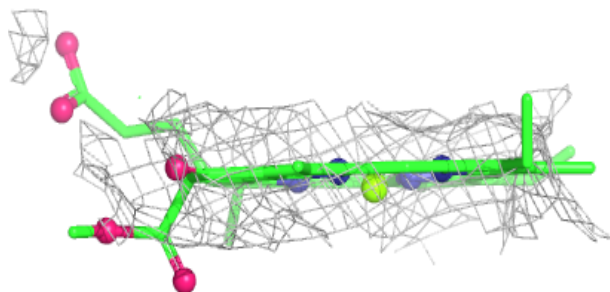
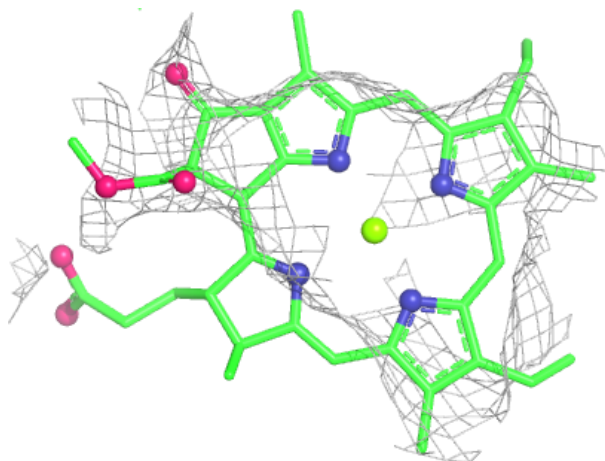
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
11	CLA	B	1224	55/65	0.96	0.12	116,122,128,136	0
11	CLA	2	1212	45/65	0.96	0.08	114,120,125,126	0
11	CLA	8	1502	46/65	0.96	0.10	153,164,178,197	0
11	CLA	2	1021	65/65	0.96	0.13	122,129,148,156	0
11	CLA	A	1112	45/65	0.96	0.09	132,143,149,153	0
13	SF4	3	3003	8/8	0.96	0.13	60,67,100,115	0
11	CLA	2	1215	65/65	0.96	0.11	107,116,134,140	0
11	CLA	b	1220	46/65	0.96	0.07	254,281,294,297	0
11	CLA	B	1013	65/65	0.96	0.09	99,112,120,139	0
11	CLA	B	1021	65/65	0.96	0.13	110,119,135,150	0
11	CLA	A	1022	65/65	0.96	0.10	82,88,92,93	0
13	SF4	1	3001	8/8	0.97	0.07	50,62,210,290	0
11	CLA	B	1202	65/65	0.97	0.10	107,117,127,130	0
13	SF4	C	3003	8/8	0.97	0.04	60,67,100,115	0
13	SF4	a	3001	8/8	0.97	0.06	50,62,210,290	0
11	CLA	A	1127	65/65	0.97	0.08	94,101,108,110	0
13	SF4	A	3001	8/8	0.97	0.07	50,62,210,290	0

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

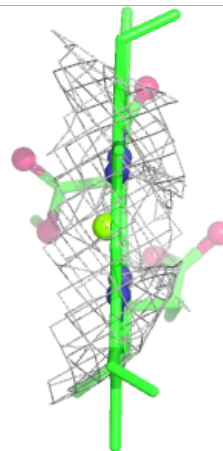
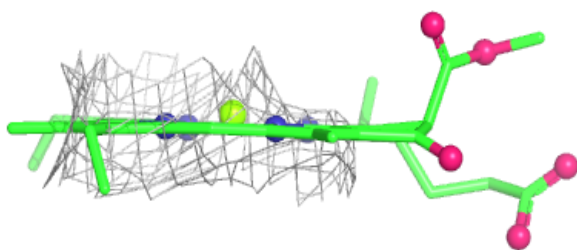
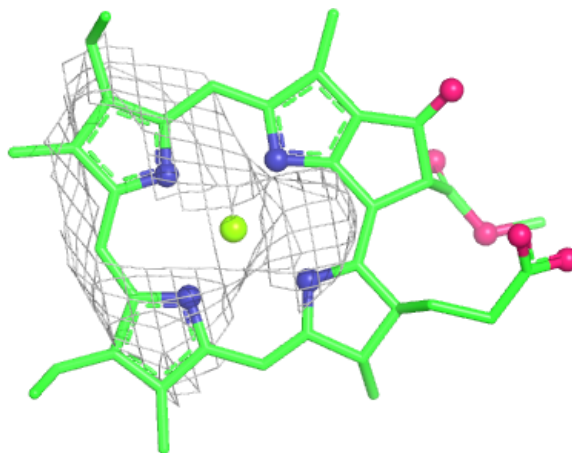
Electron density around CLA 2 1240:

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



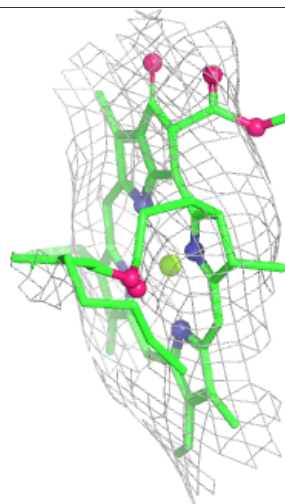
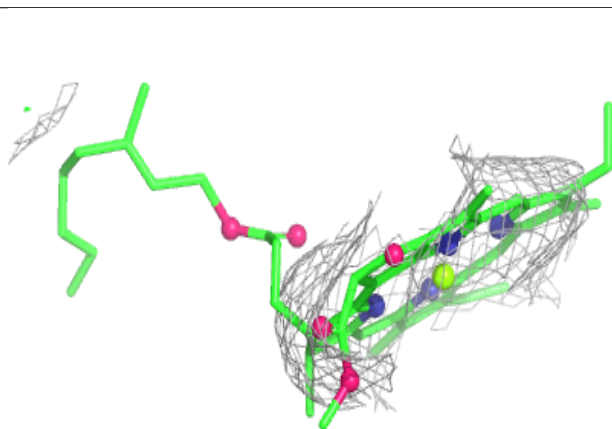
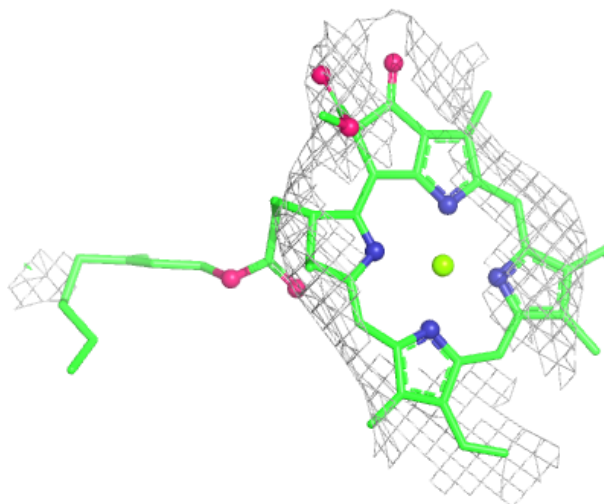
Electron density around CLA b 1240:

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



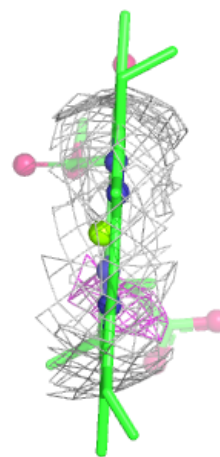
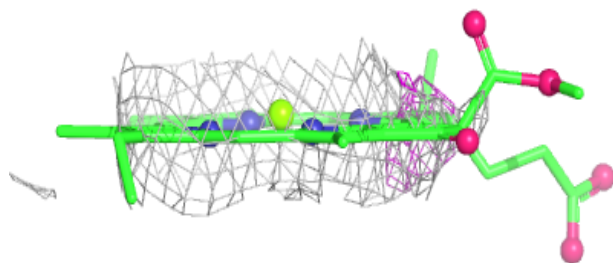
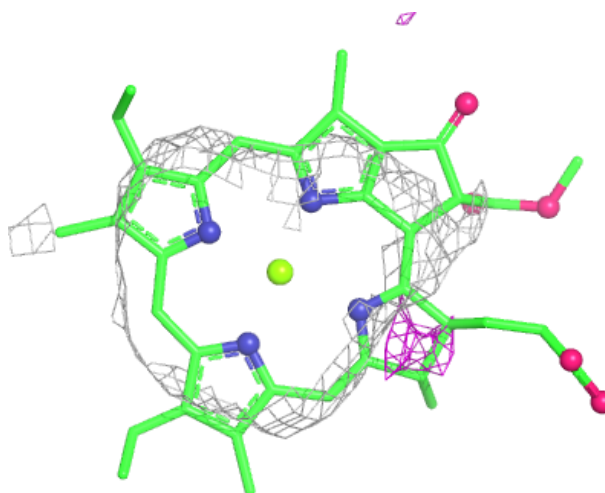
Electron density around CLA 1 1110:

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and green (positive)



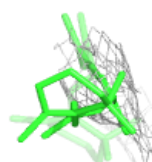
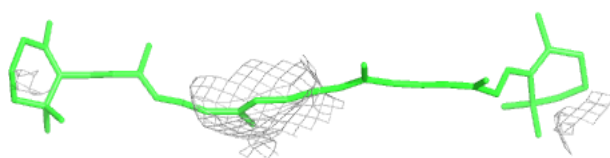
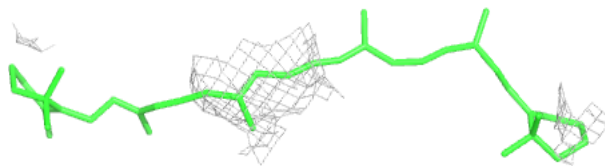
Electron density around CLA B 1240:

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and green (positive)

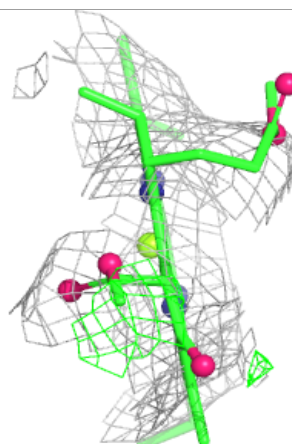
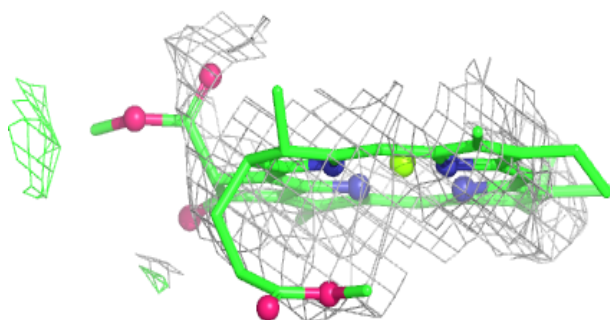
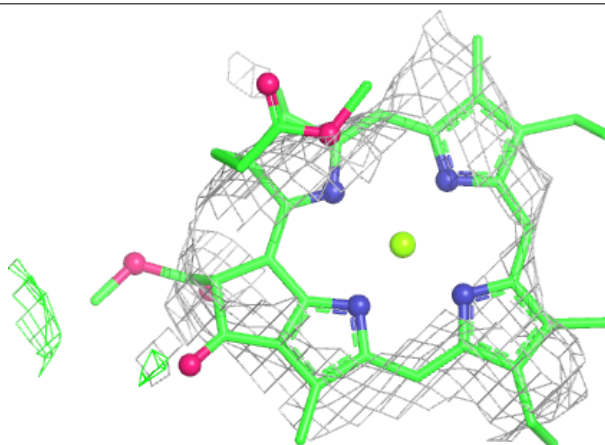


Electron density around BCR 6 4013:

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

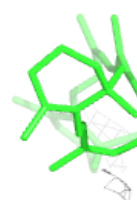
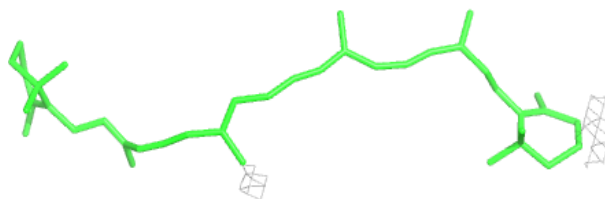
**Electron density around CLA a 1114:**

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

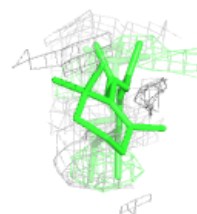
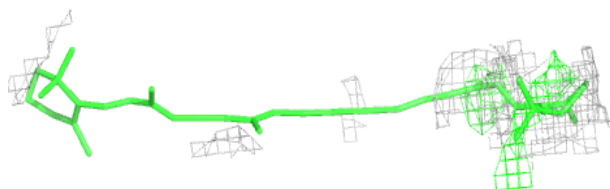
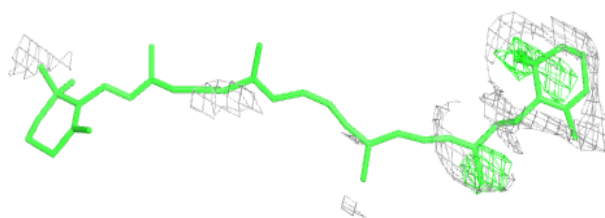


Electron density around BCR f 4013:

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

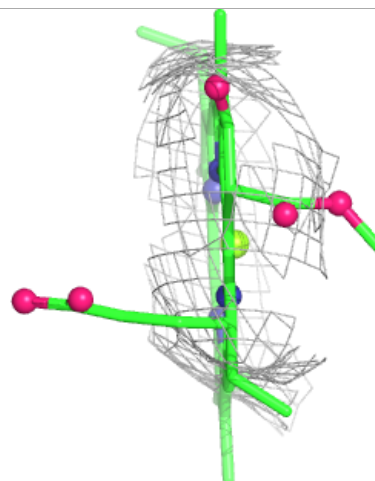
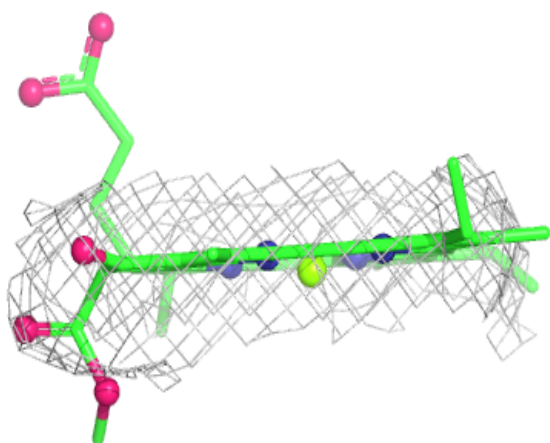
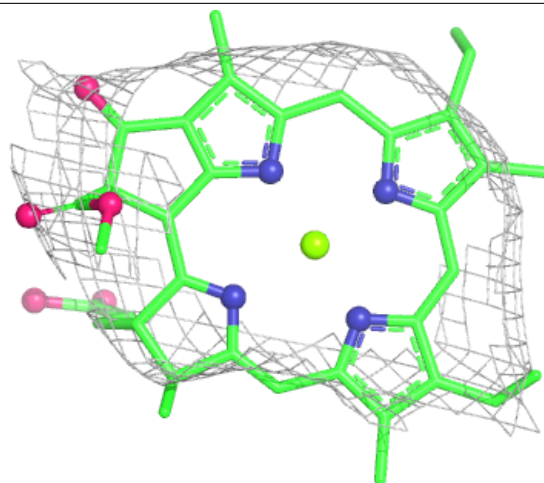
**Electron density around BCR 1 4002:**

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



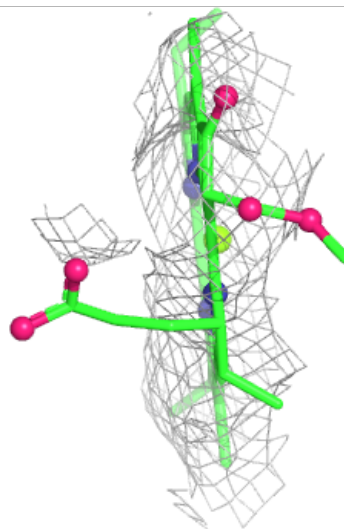
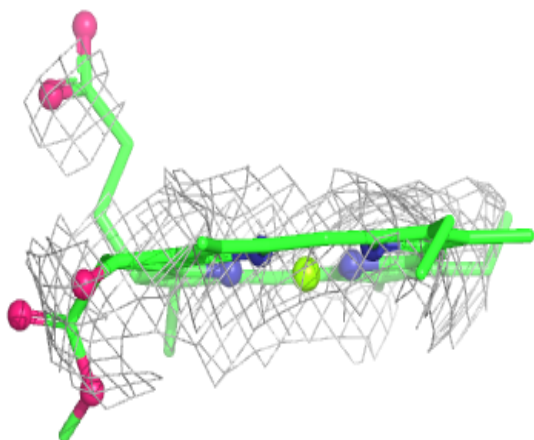
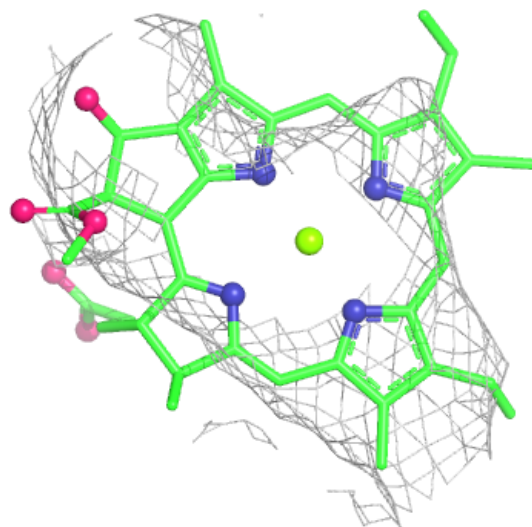
Electron density around CLA b 1218:

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and green (positive)



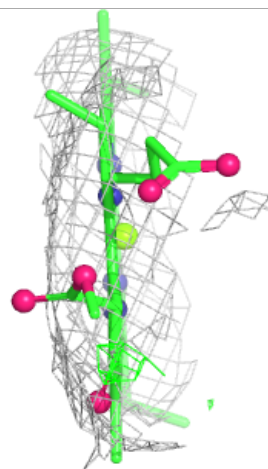
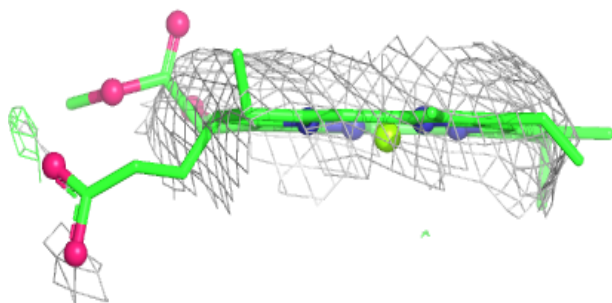
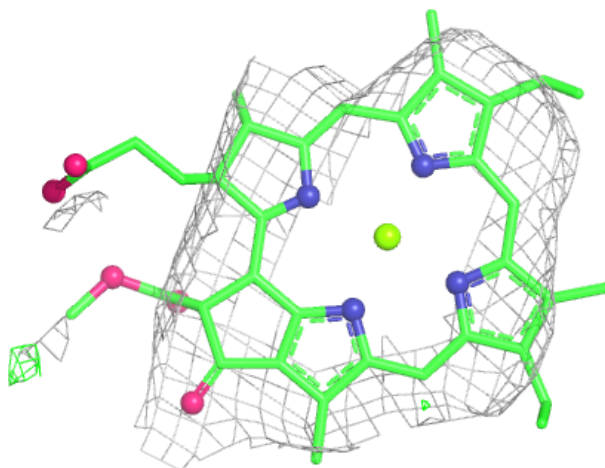
Electron density around CLA b 1227:

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and green (positive)



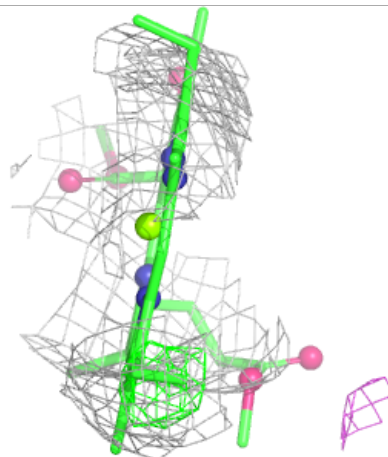
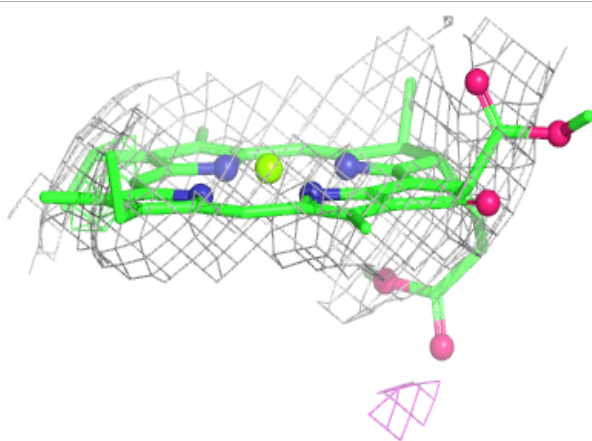
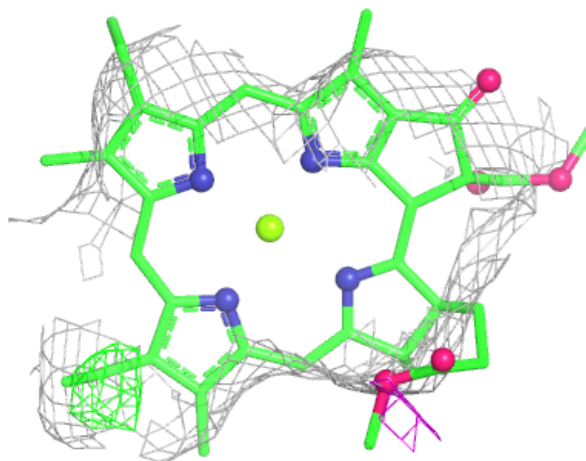
Electron density around CLA 1 1113:

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and green (positive)



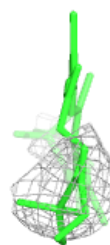
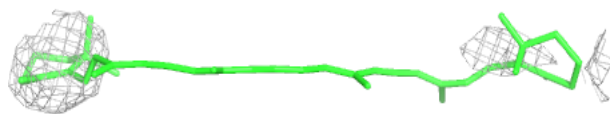
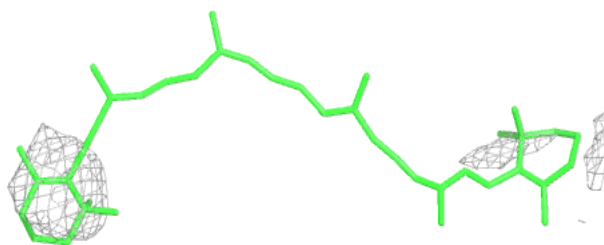
Electron density around CLA 1 1121:

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and green (positive)

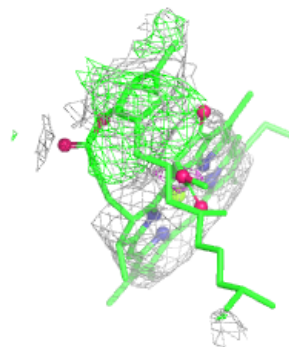
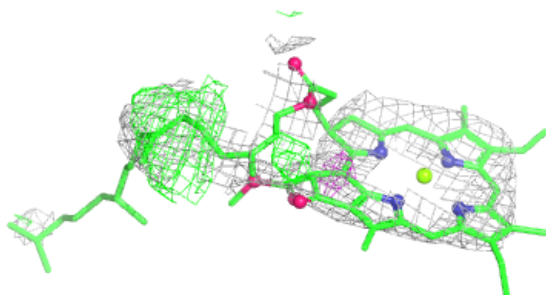
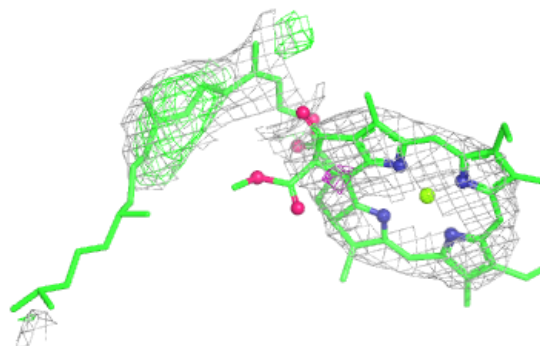


Electron density around BCR 2 4011:

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

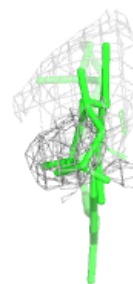
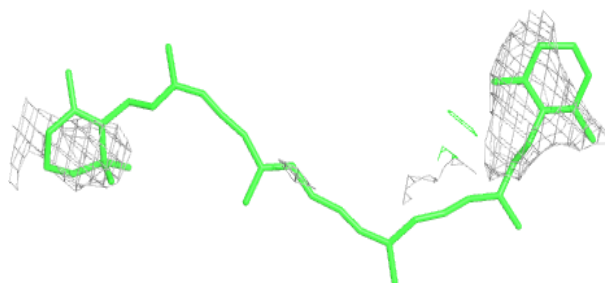
**Electron density around CLA B 1213:**

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and green (positive)

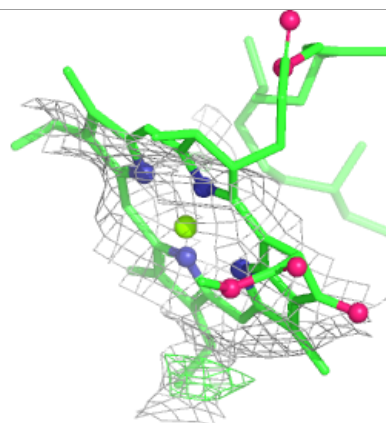
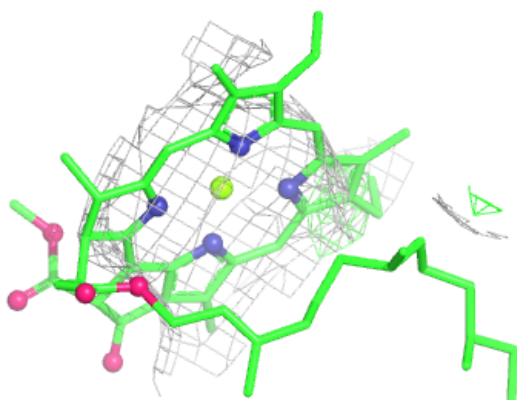
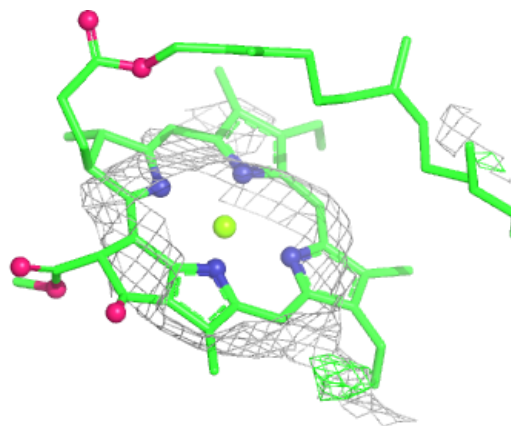


Electron density around BCR b 4011:

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

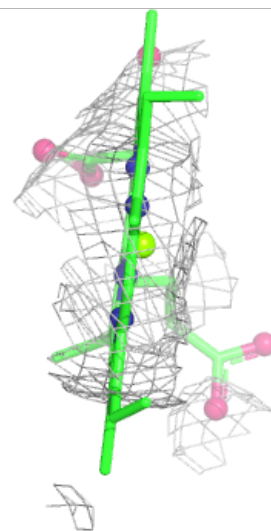
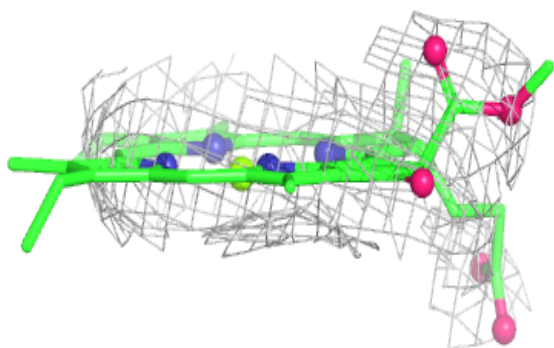
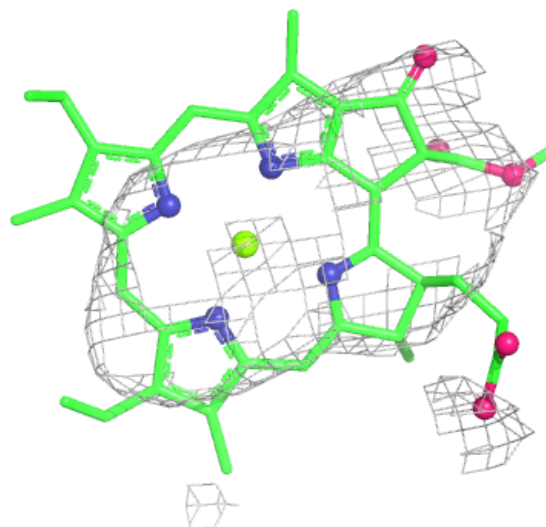
**Electron density around CLA 1 1118:**

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



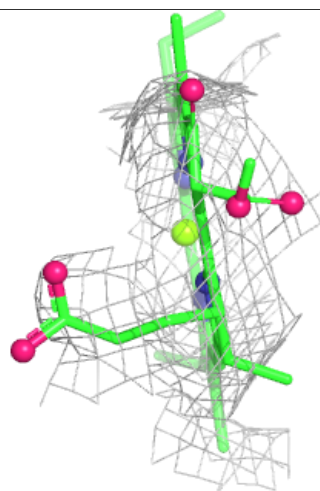
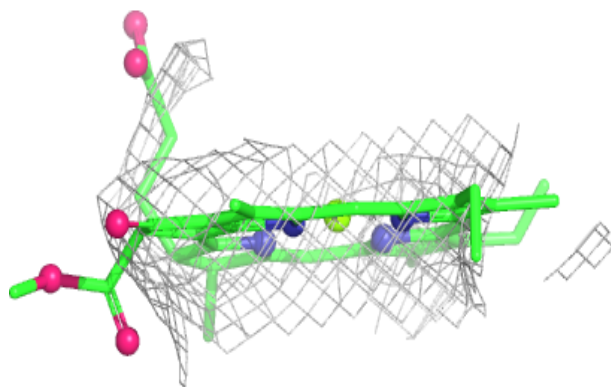
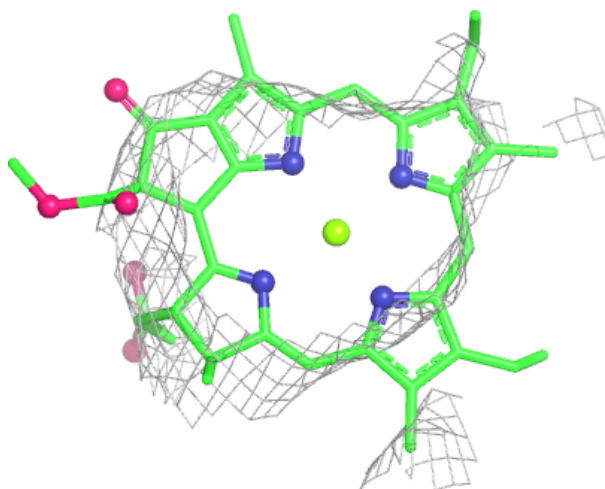
Electron density around CLA b 1209:

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and green (positive)



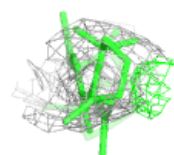
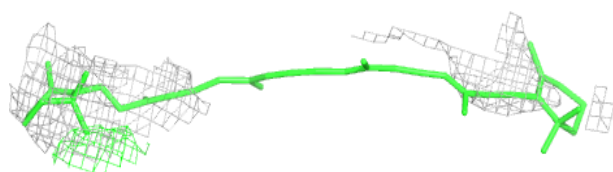
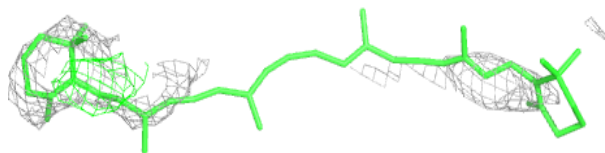
Electron density around CLA 1 1108:

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



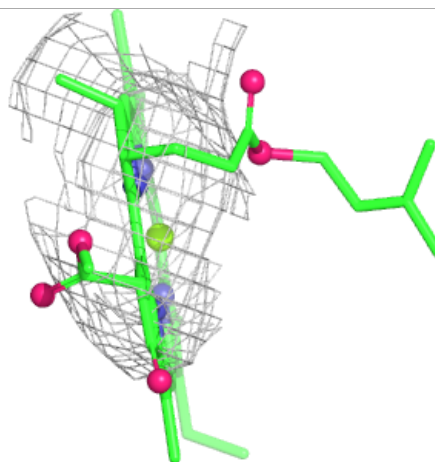
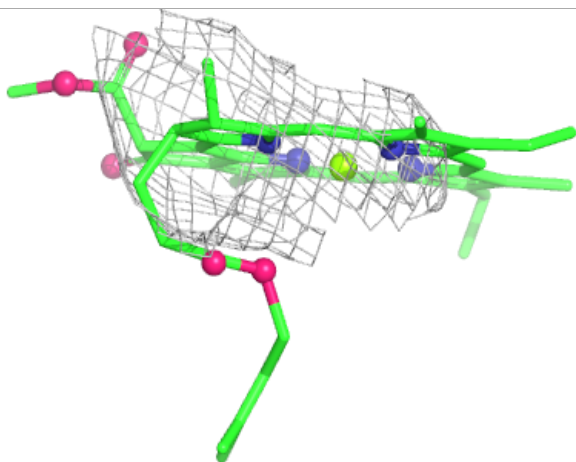
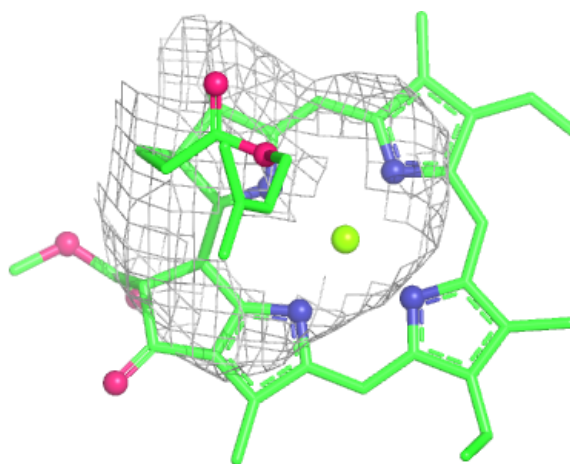
Electron density around BCR a 4002:

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



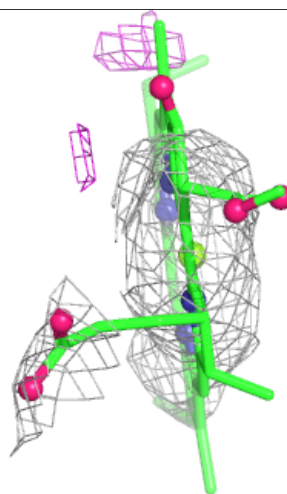
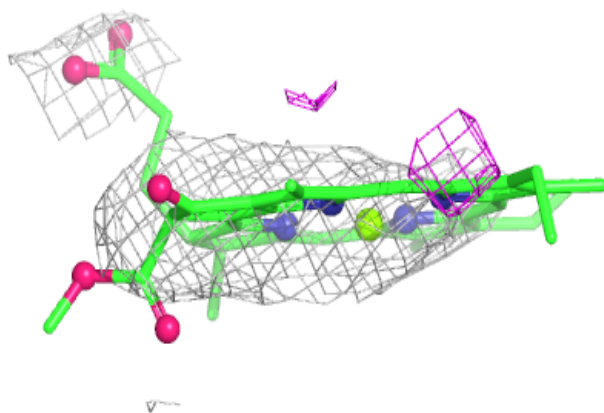
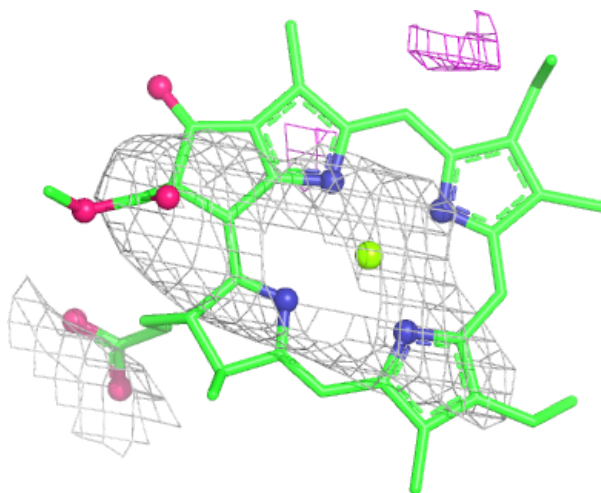
Electron density around CLA 0 1402:

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



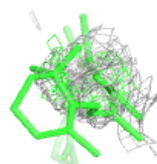
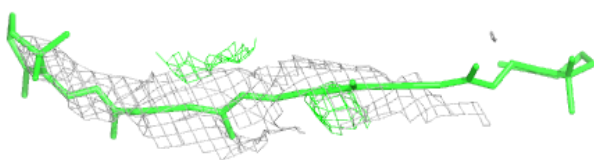
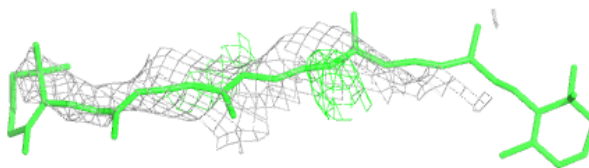
Electron density around CLA b 1208:

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

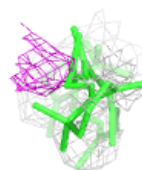
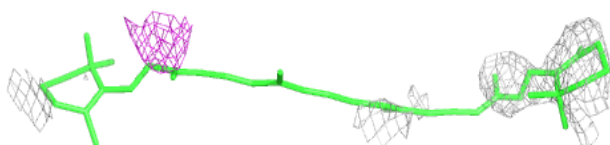
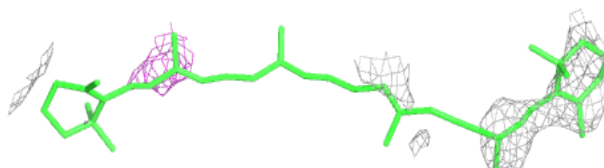


Electron density around BCR m 4021:

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

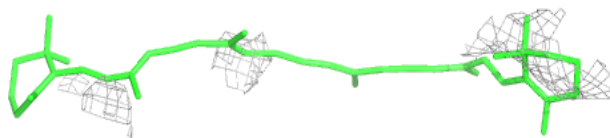
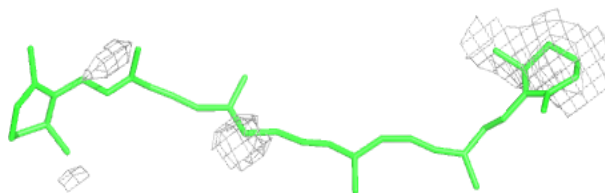
**Electron density around BCR 1 4003:**

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



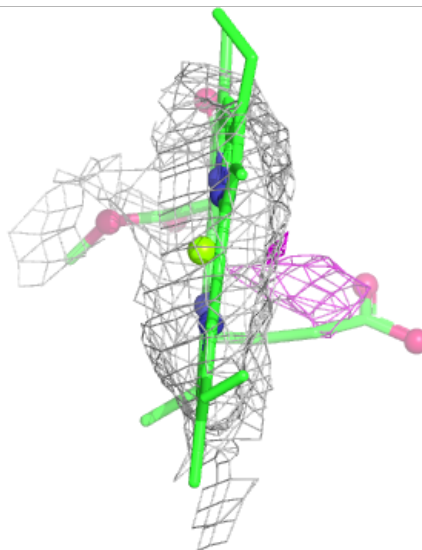
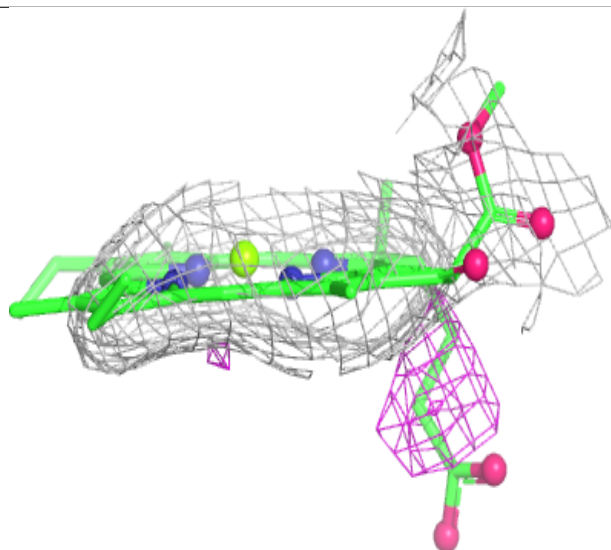
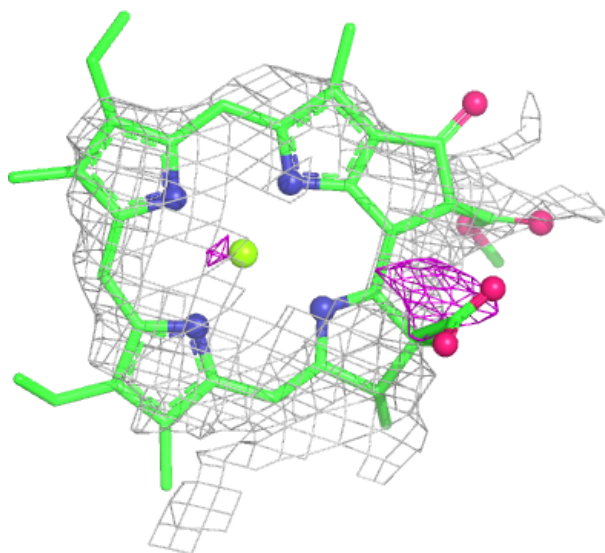
Electron density around BCR F 4013:

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



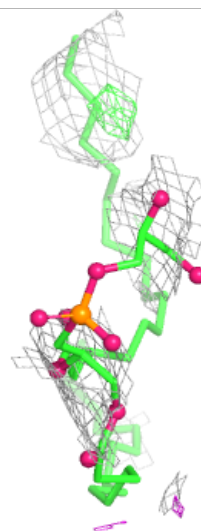
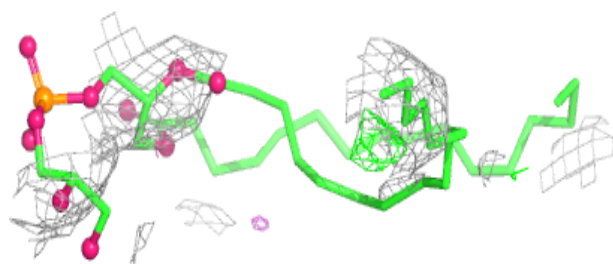
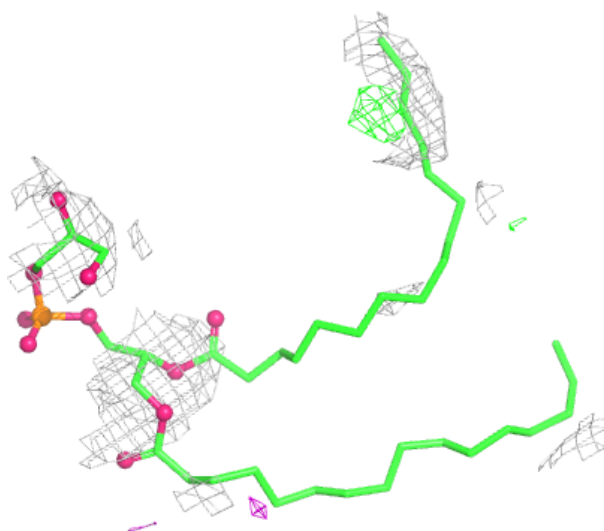
Electron density around CLA B 1227:

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



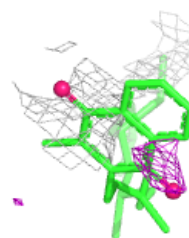
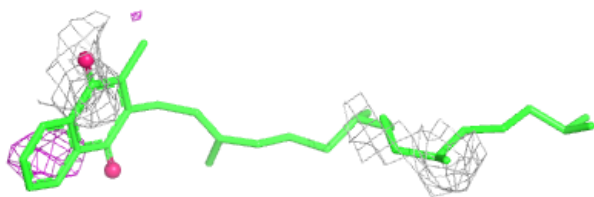
Electron density around LHG B 5004:

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

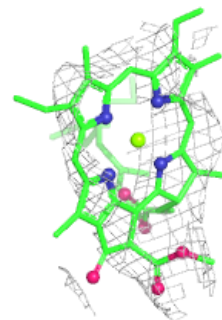
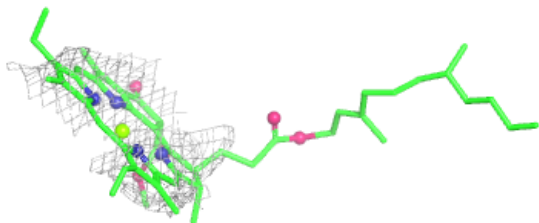
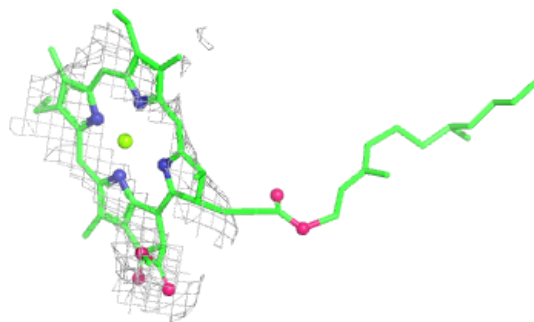


Electron density around PQN a 2001:

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

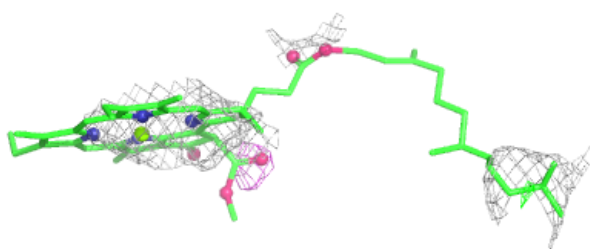
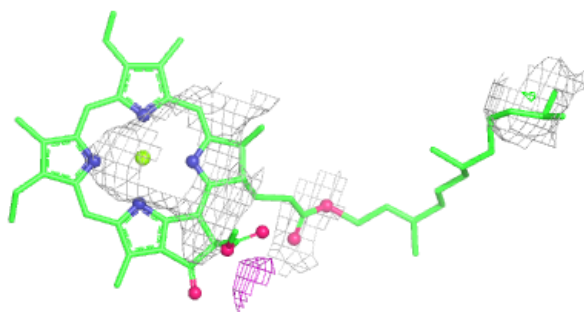
**Electron density around CLA b 1230:**

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

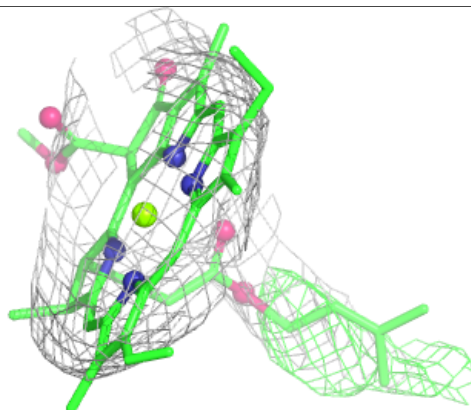
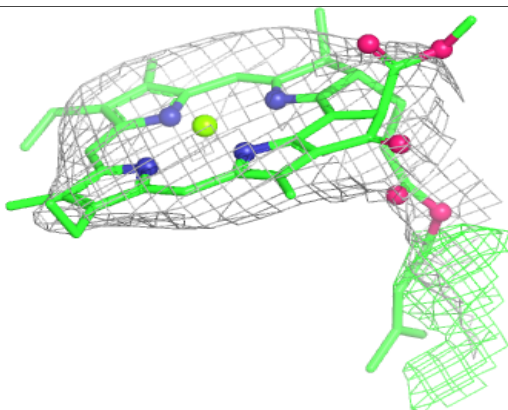
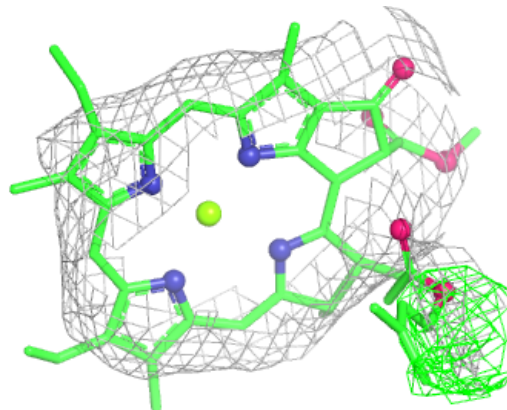


Electron density around CLA b 1234:

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

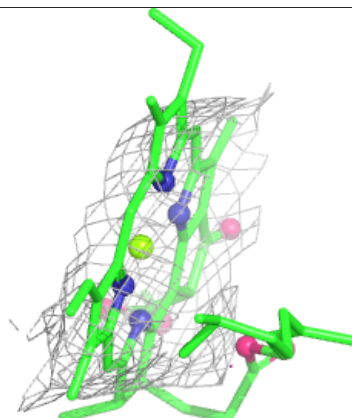
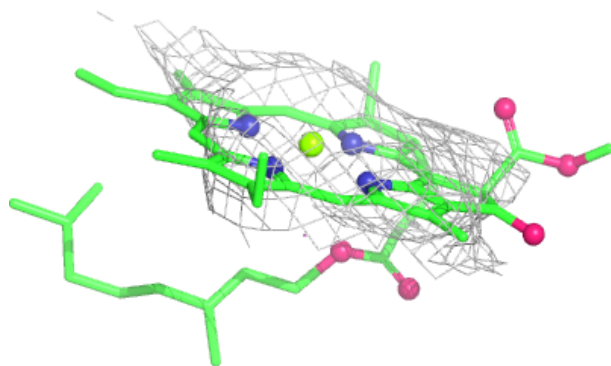
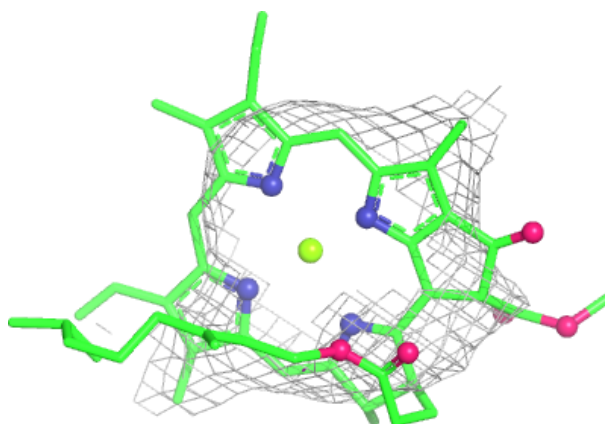
**Electron density around CLA b 1228:**

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



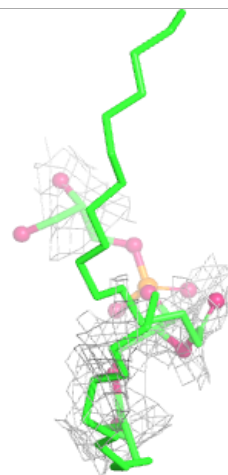
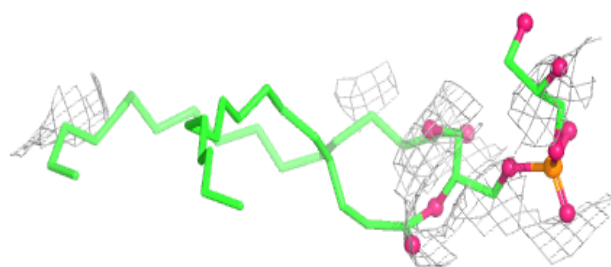
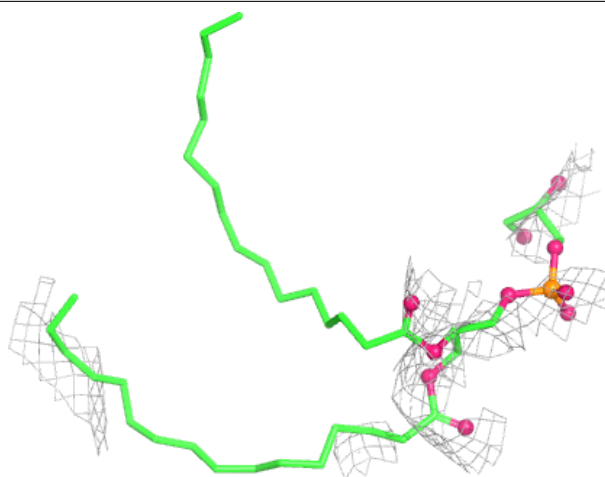
Electron density around CLA b 1219:

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



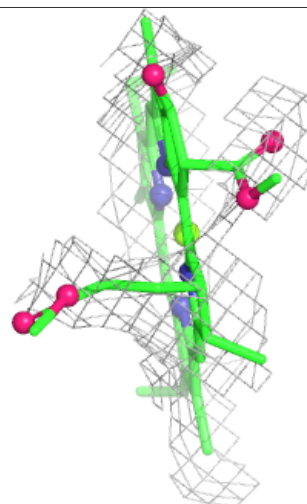
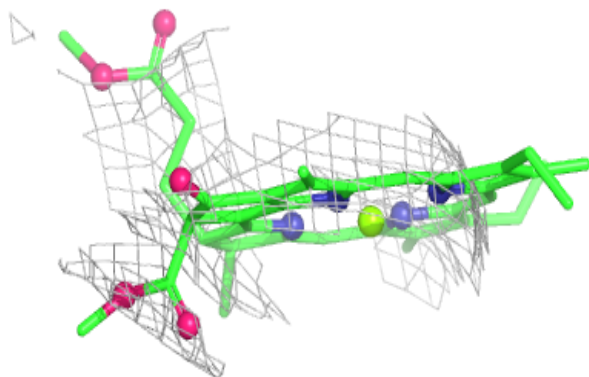
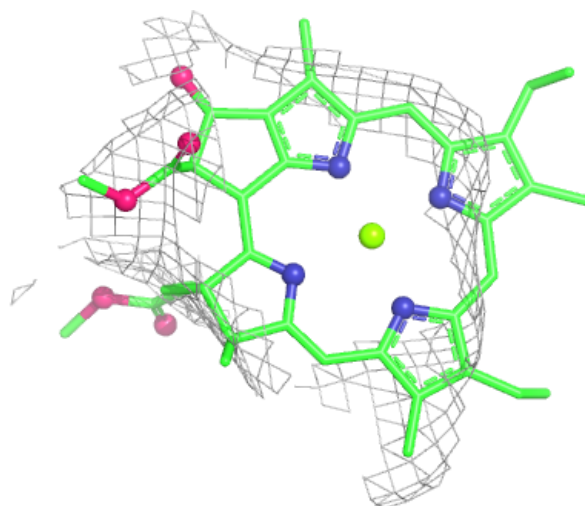
Electron density around LHG b 5004:

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



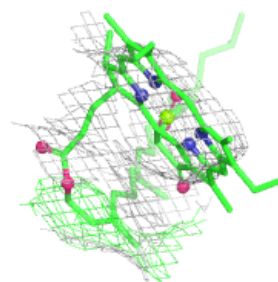
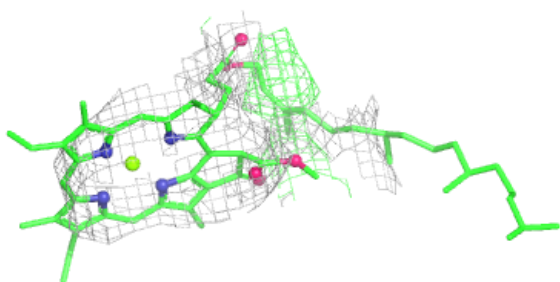
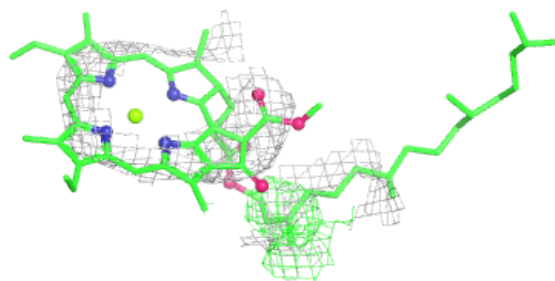
Electron density around CLA 1 1114:

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



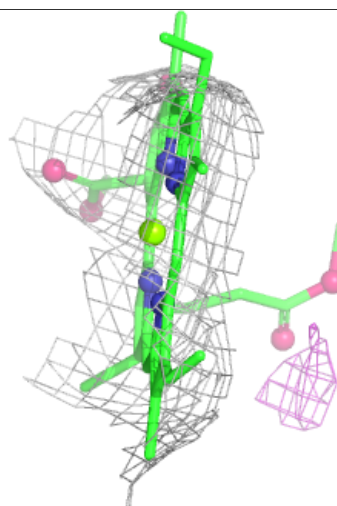
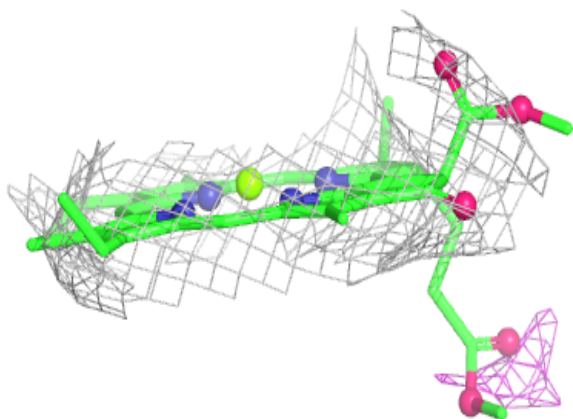
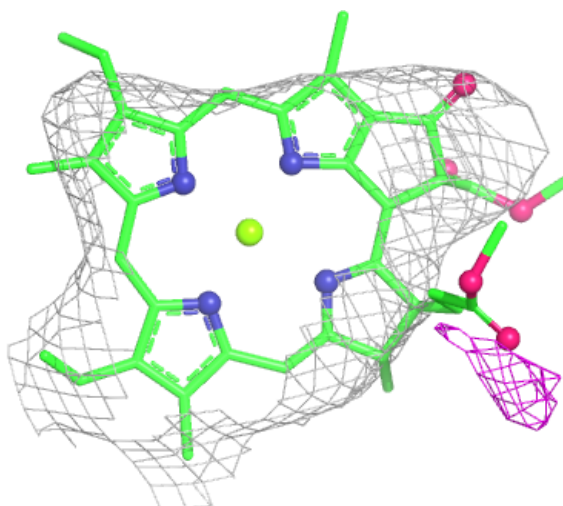
Electron density around CLA b 1213:

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



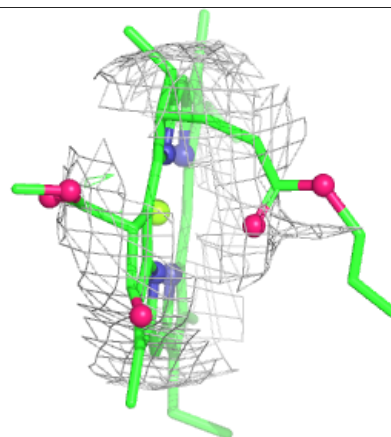
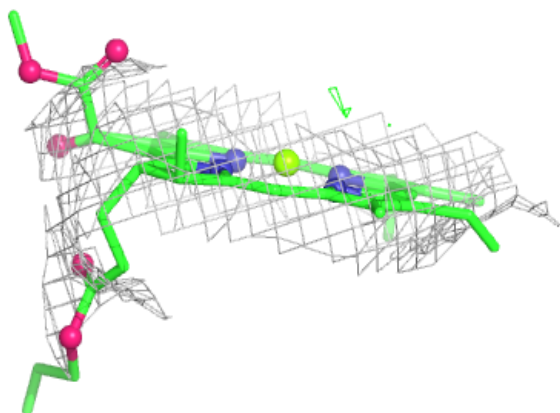
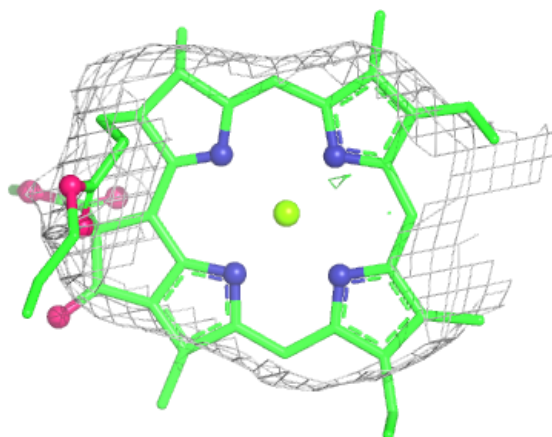
Electron density around CLA A 1114:

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

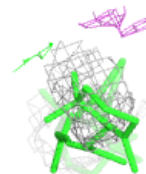
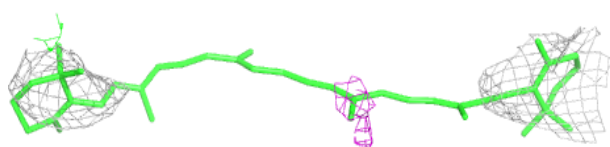
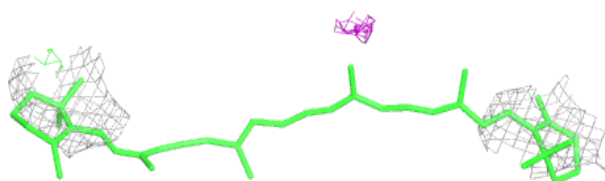


Electron density around CLA 1 1105:

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

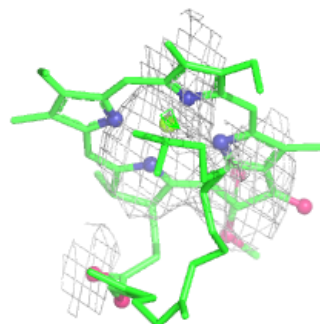
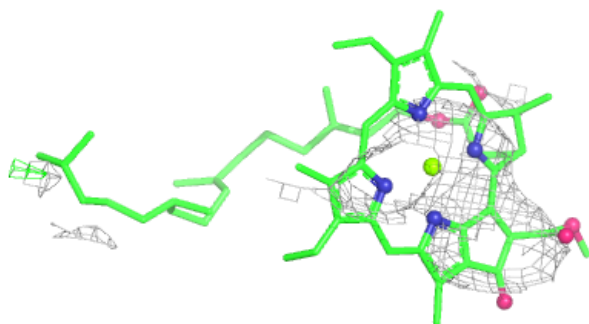
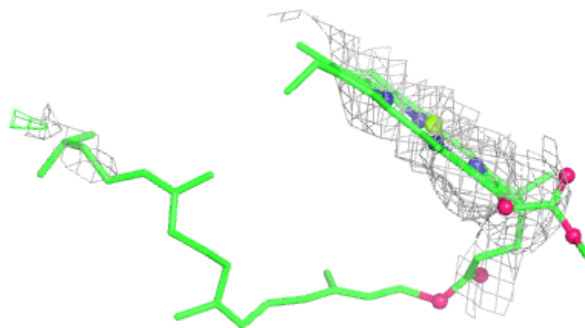
**Electron density around BCR a 4003:**

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



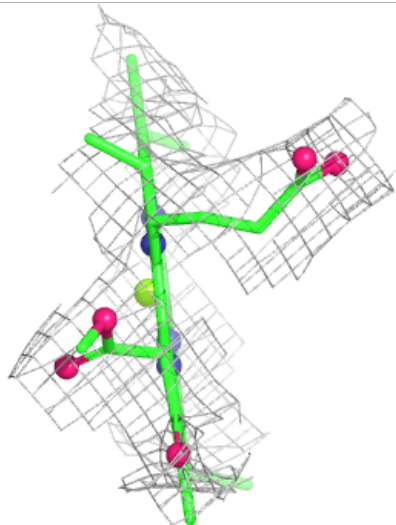
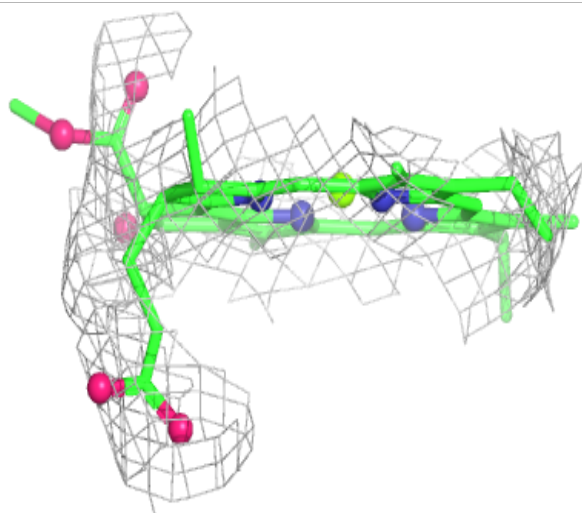
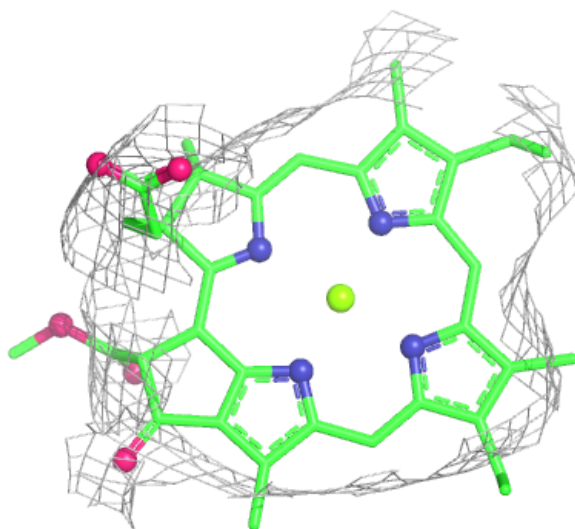
Electron density around CLA a 1109:

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



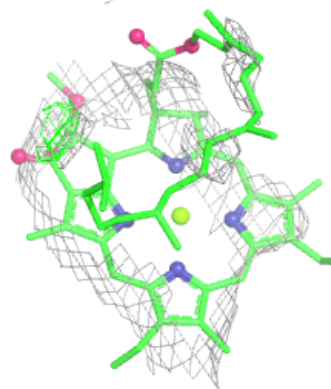
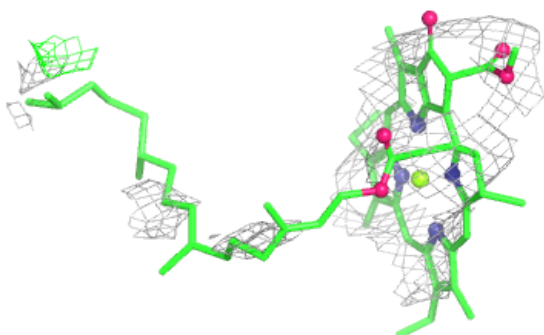
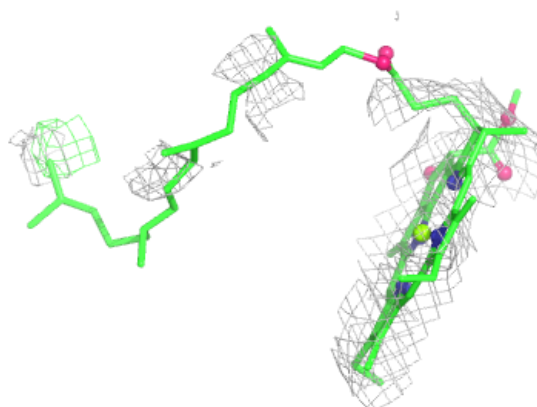
Electron density around CLA b 1232:

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

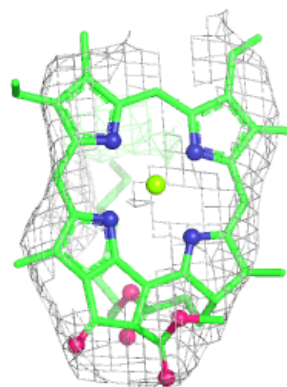
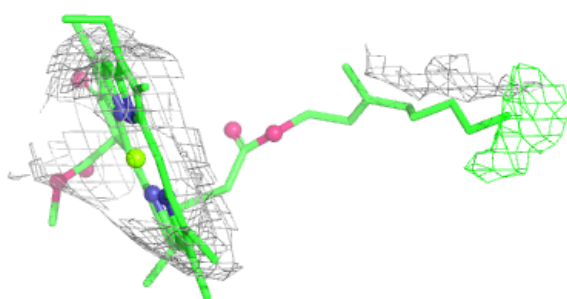
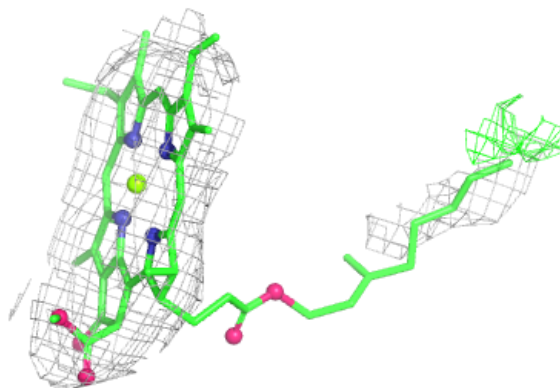


Electron density around CLA b 1216:

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

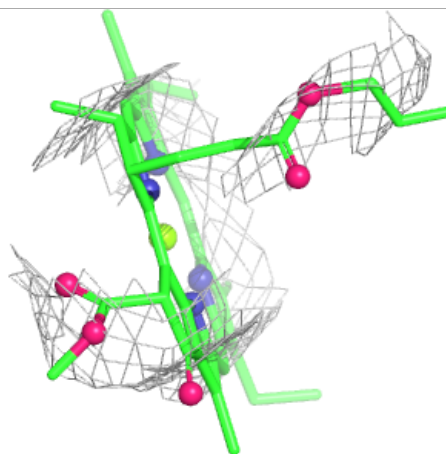
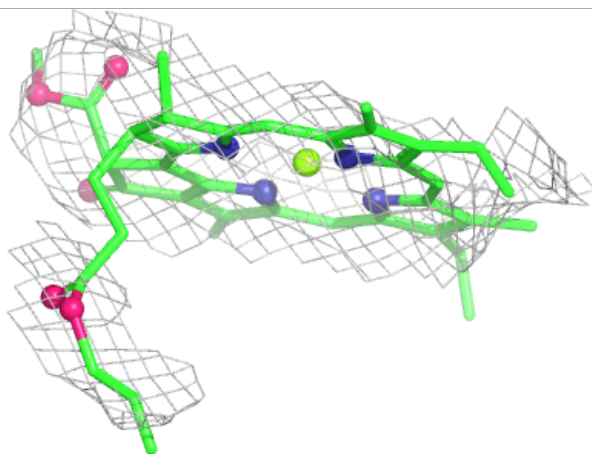
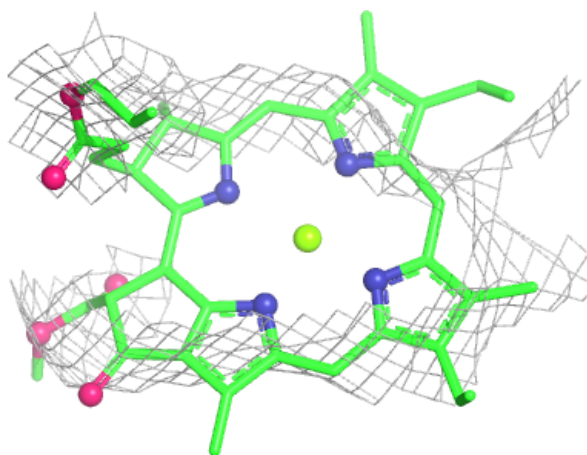
**Electron density around CLA b 1201:**

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



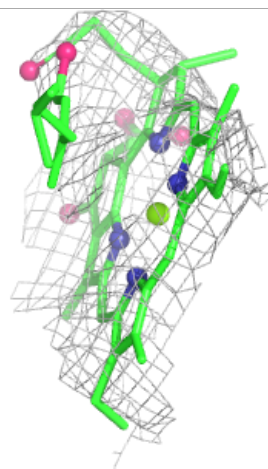
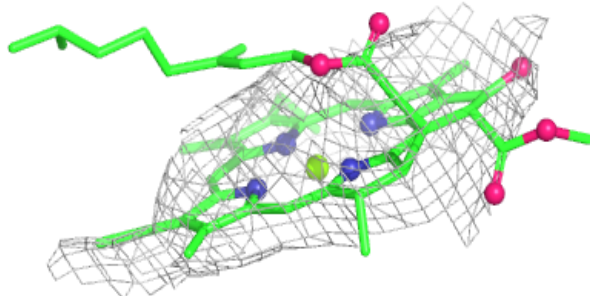
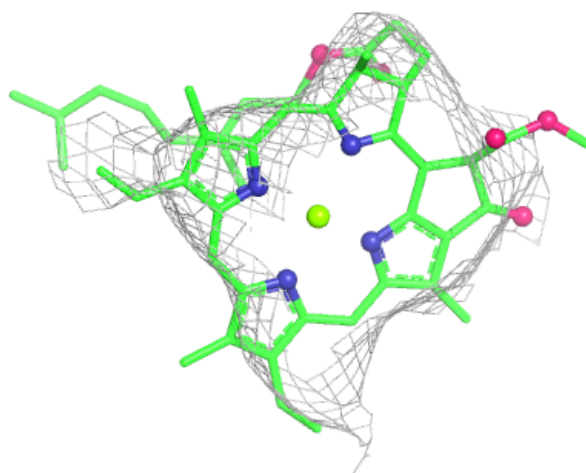
Electron density around CLA a 1105:

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



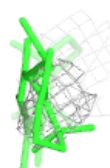
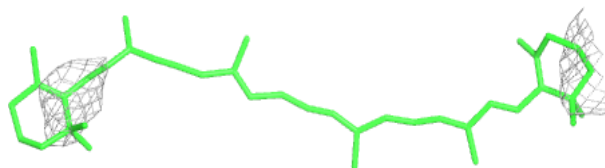
Electron density around CLA 2 1219:

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

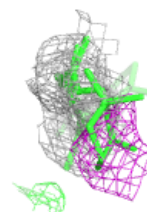
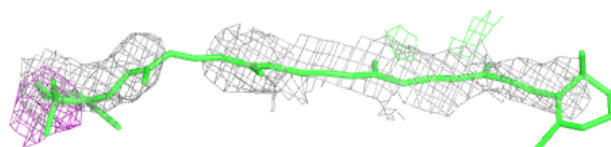
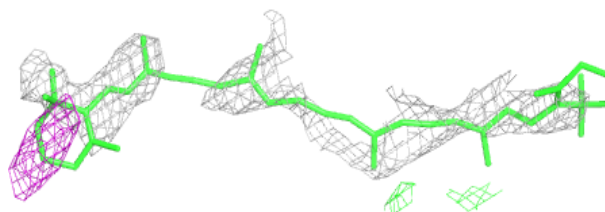


Electron density around BCR b 4005:

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

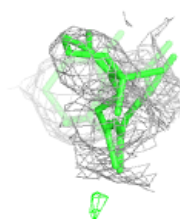
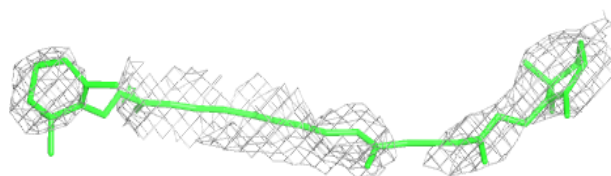
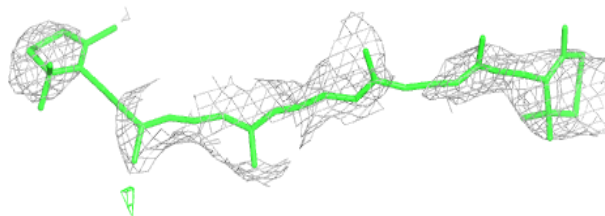
**Electron density around BCR L 4022:**

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



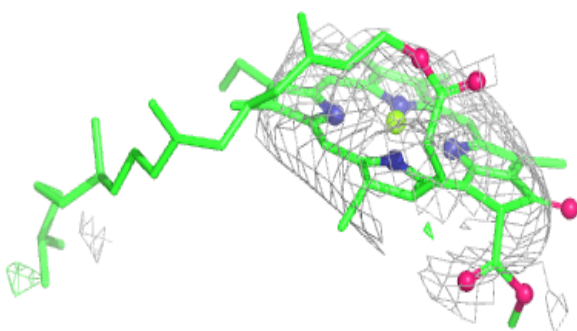
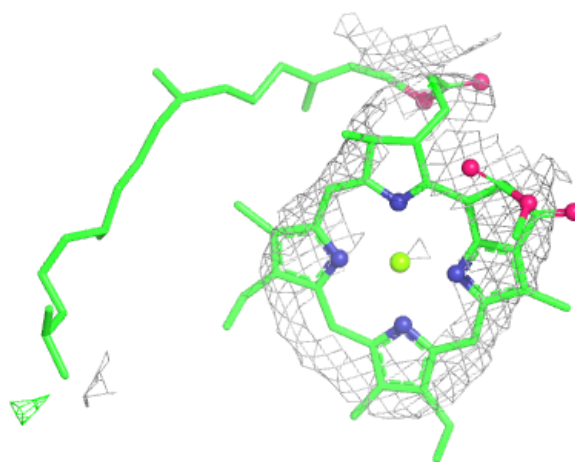
Electron density around BCR M 4021:

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



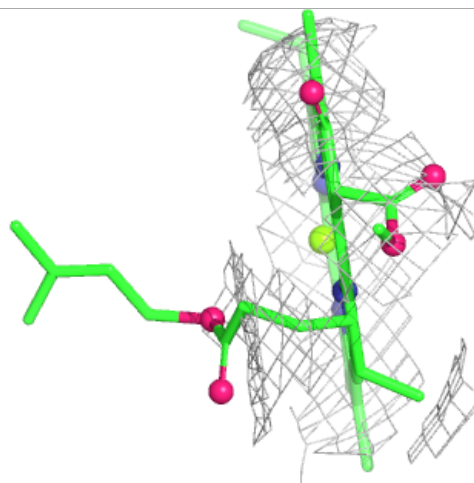
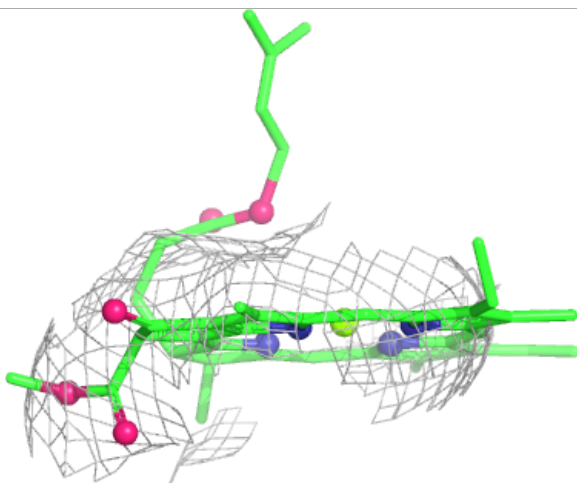
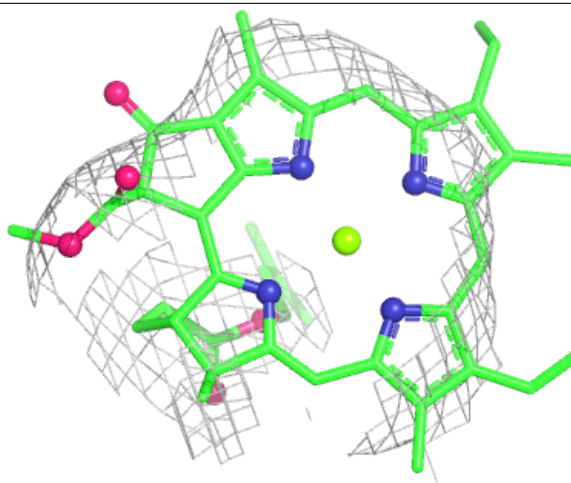
Electron density around CLA k 1401:

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



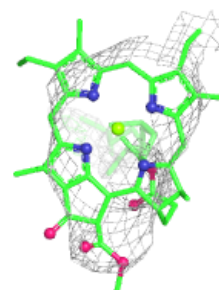
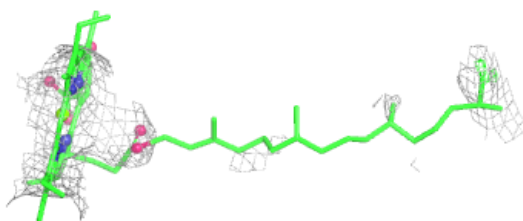
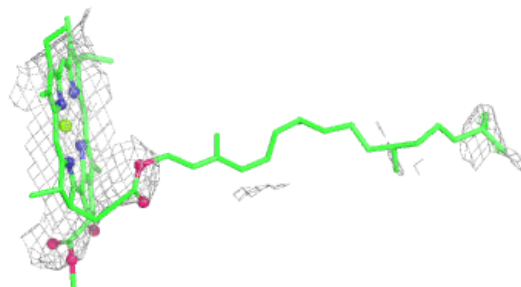
Electron density around CLA k 1402:

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

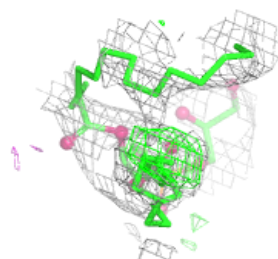
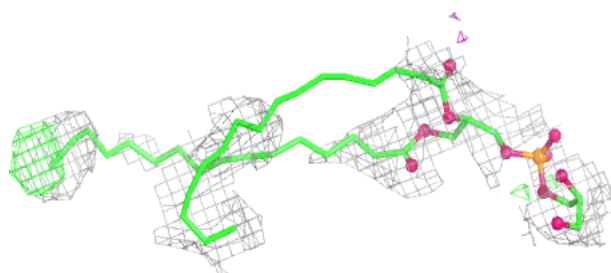
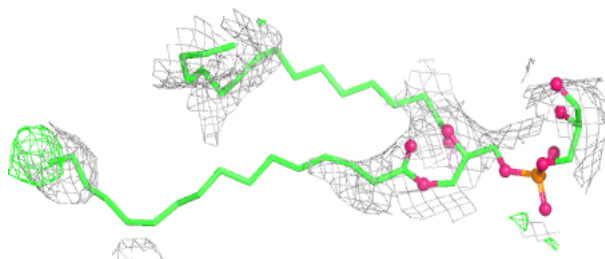


Electron density around CLA a 1126:

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

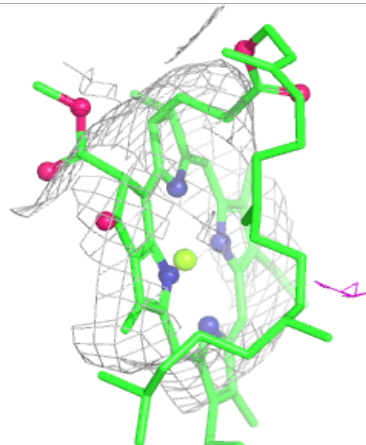
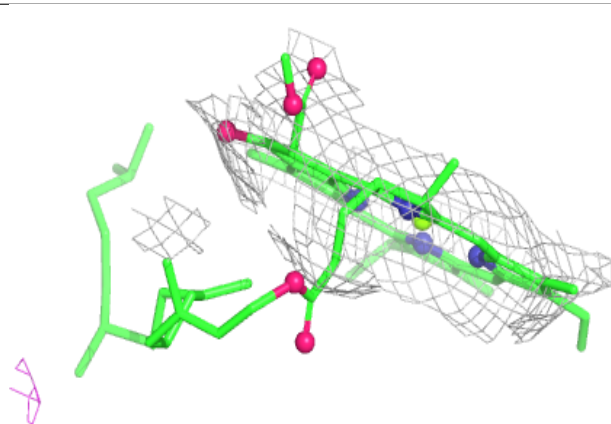
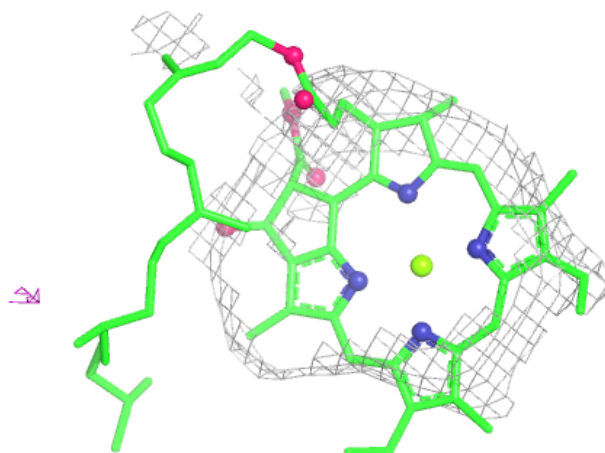
**Electron density around LHG A 5003:**

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



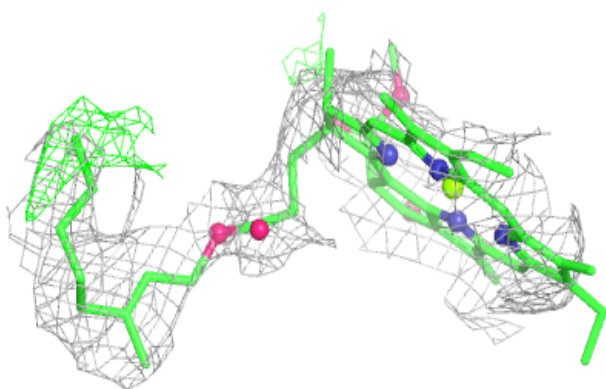
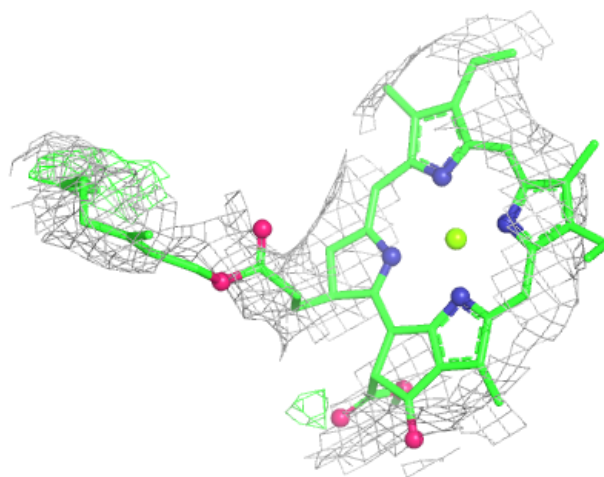
Electron density around CLA b 1229:

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



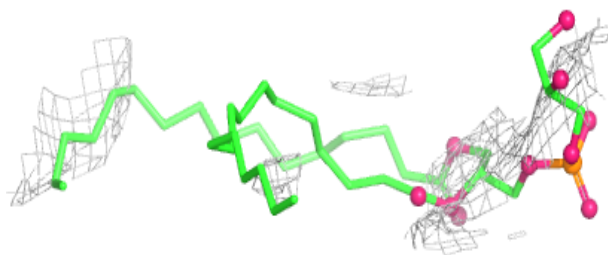
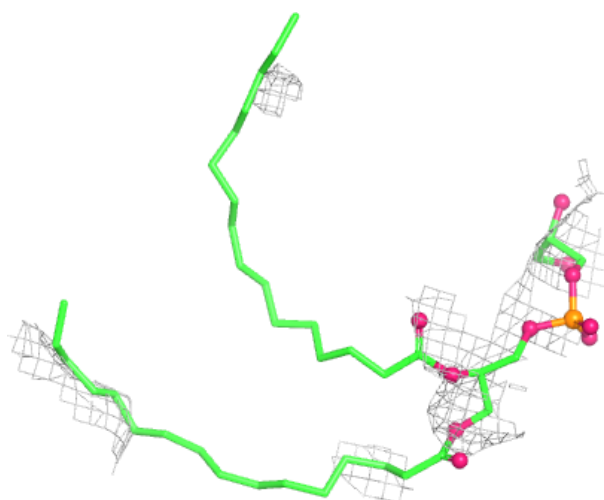
Electron density around CLA a 1110:

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



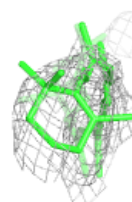
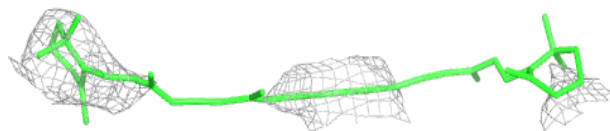
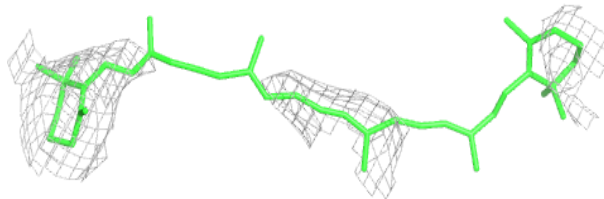
Electron density around LHG 2 5004:

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

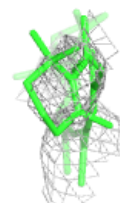
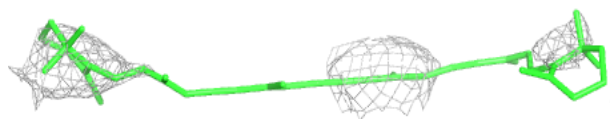
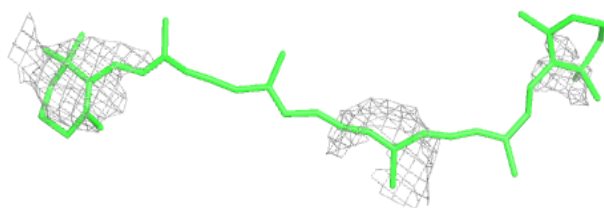


Electron density around BCR 2 4004:

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

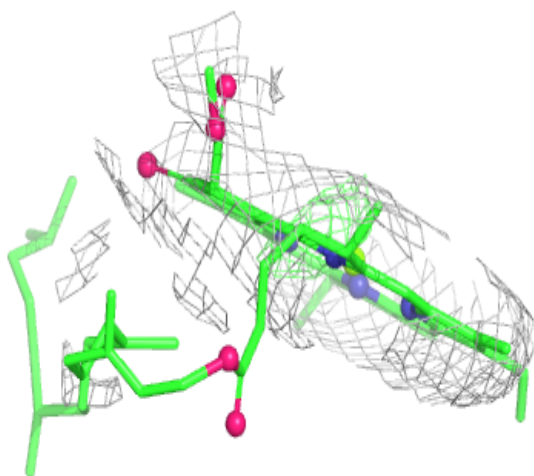
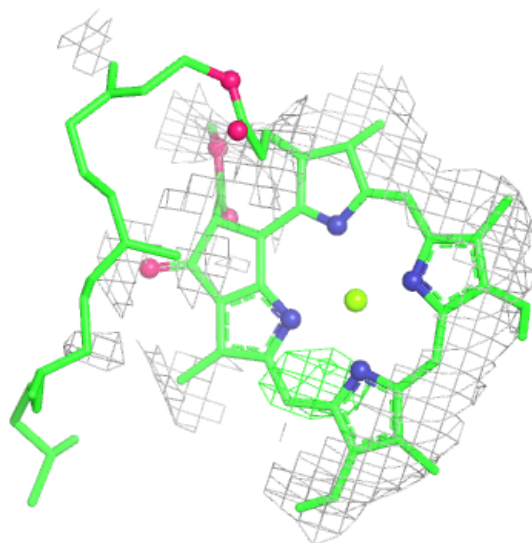
**Electron density around BCR B 4004:**

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



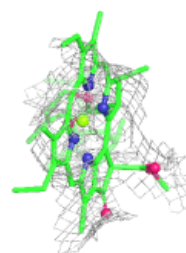
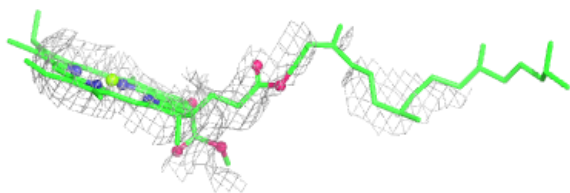
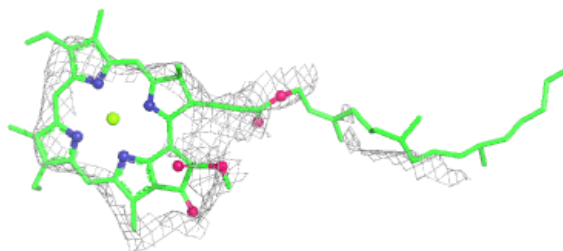
Electron density around CLA 2 1229:

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

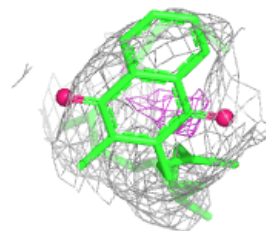
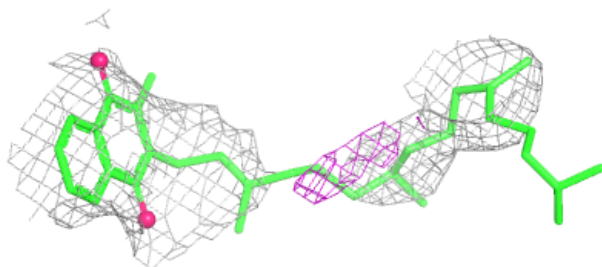
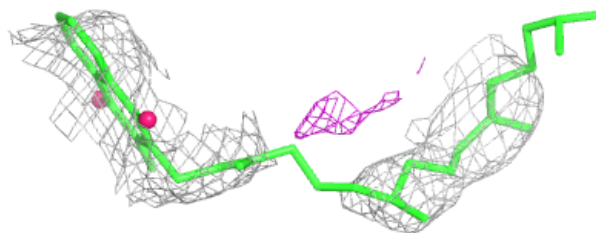


Electron density around CLA 1 1107:

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

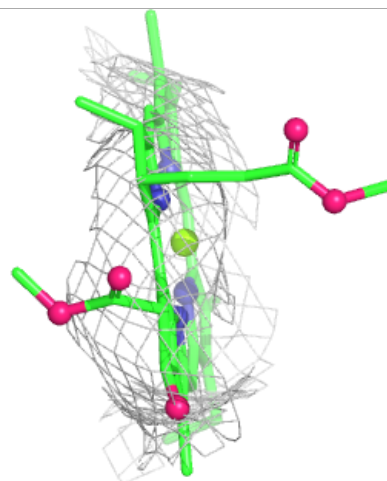
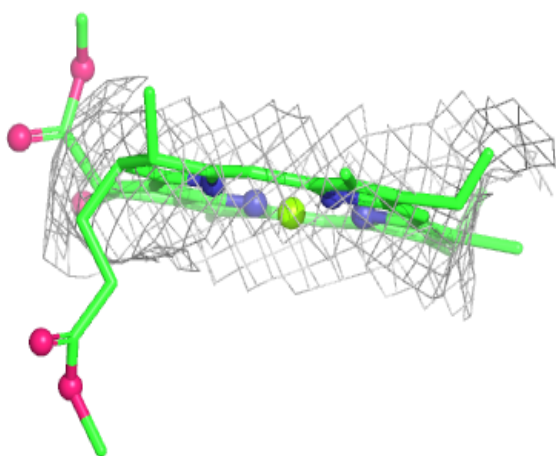
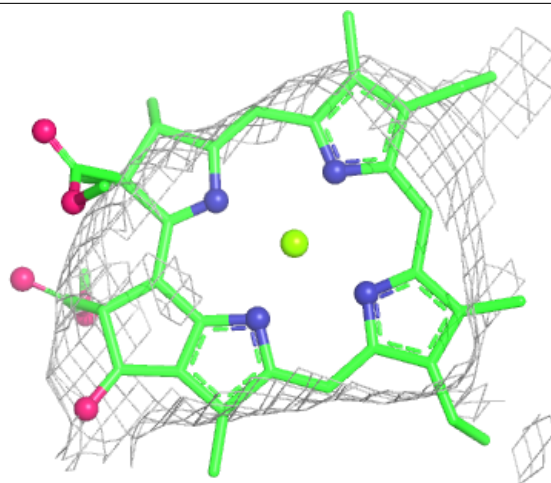
**Electron density around PQN B 2002:**

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



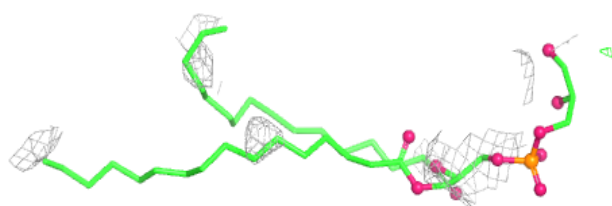
Electron density around CLA b 1211:

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

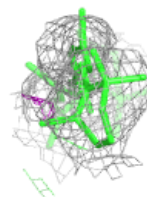
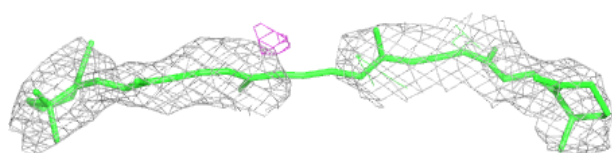
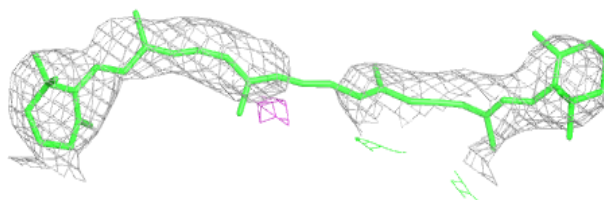


Electron density around LHG 1 5003:

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

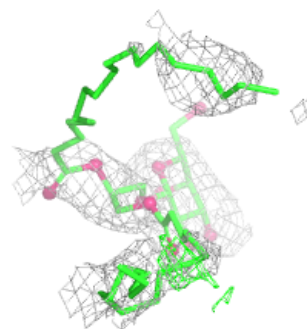
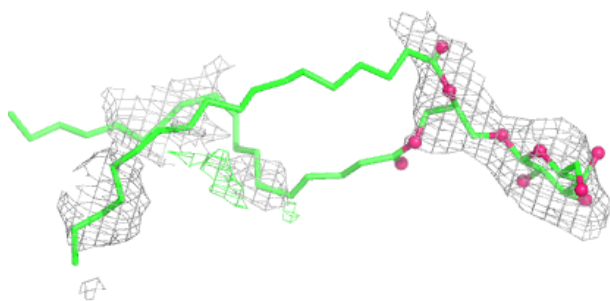
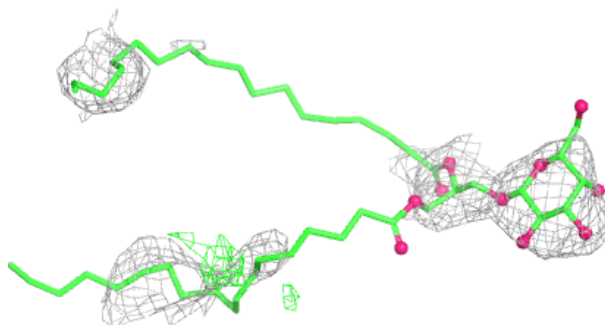
**Electron density around BCR A 4008:**

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

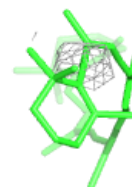
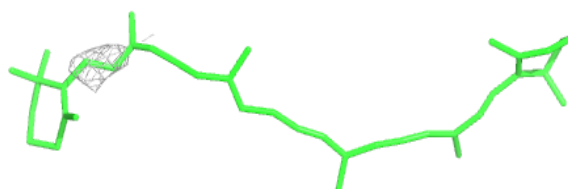


Electron density around LMG 2 5002:

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

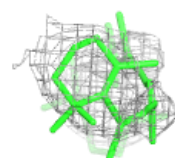
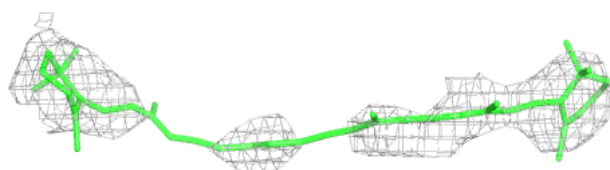
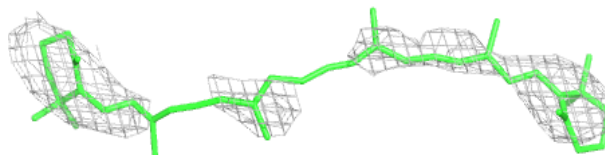
**Electron density around BCR b 4014:**

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

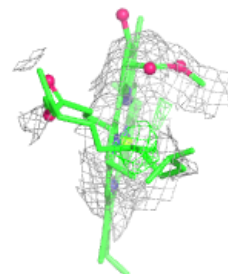
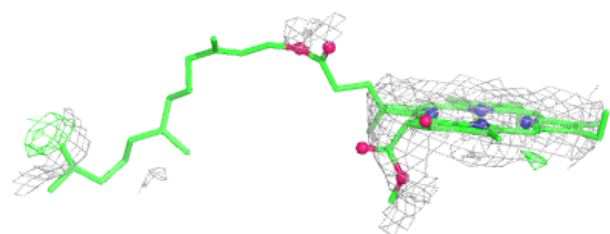
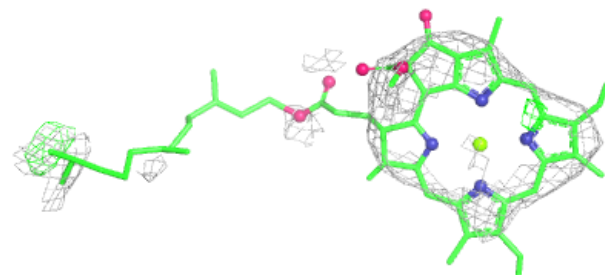


Electron density around BCR f 4018:

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

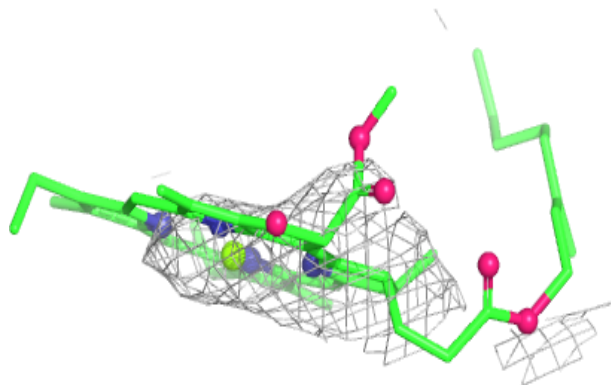
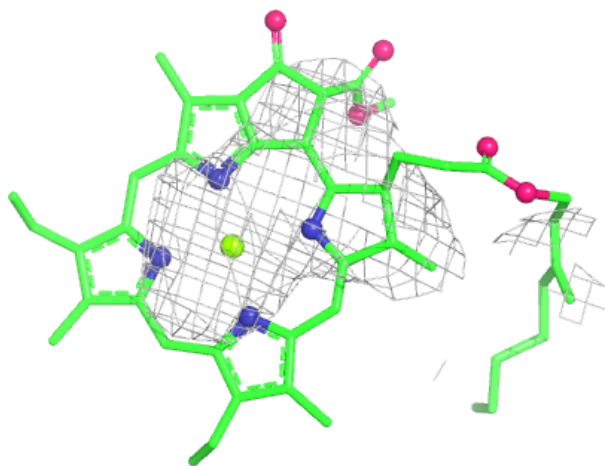
**Electron density around CLA B 1234:**

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



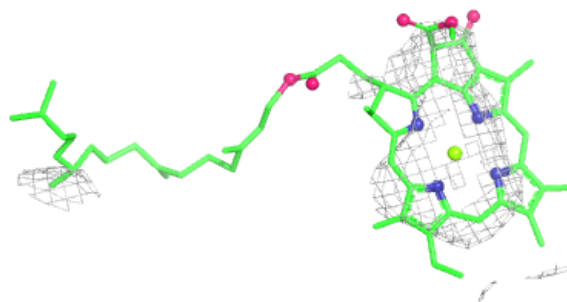
Electron density around CLA b 1221:

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

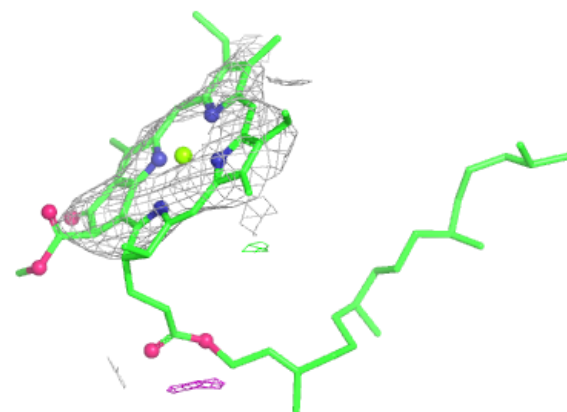


Electron density around CLA b 1210:

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

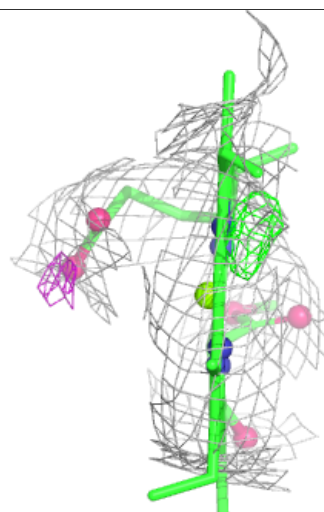
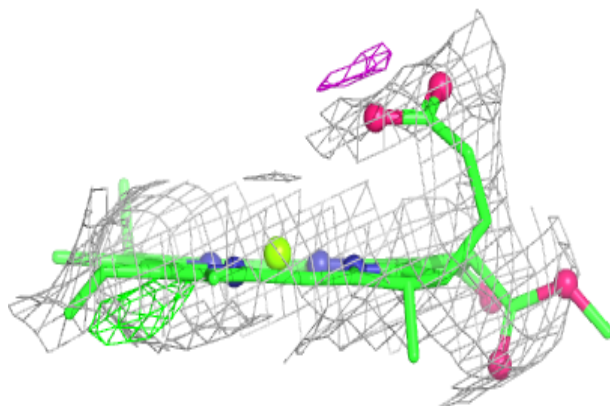
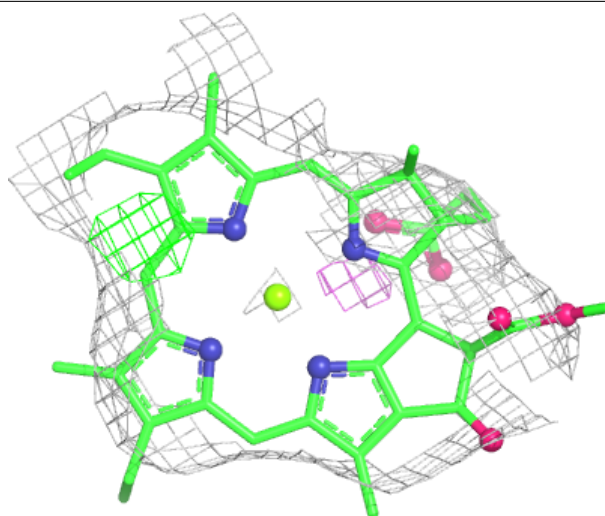
**Electron density around CLA 1 1102:**

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



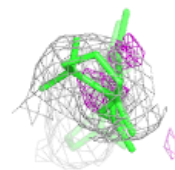
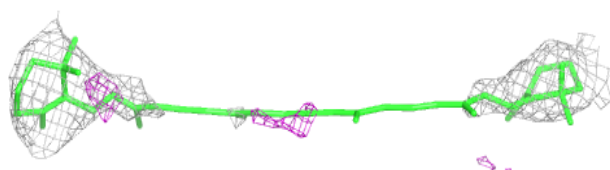
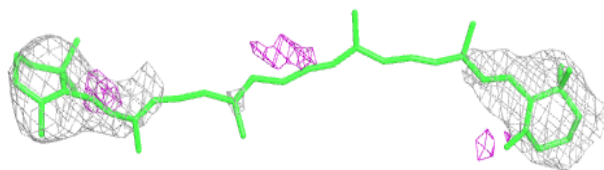
Electron density around CLA 2 1209:

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

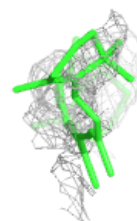
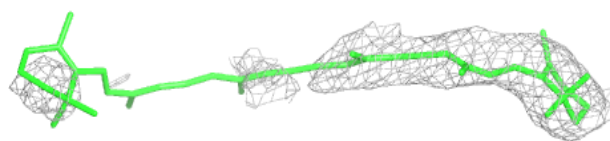
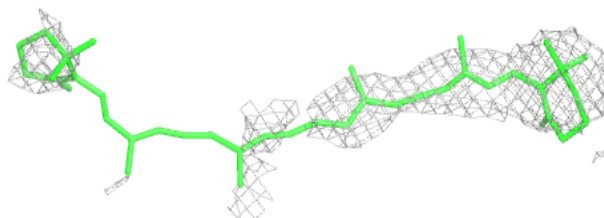


Electron density around BCR 2 4005:

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

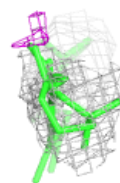
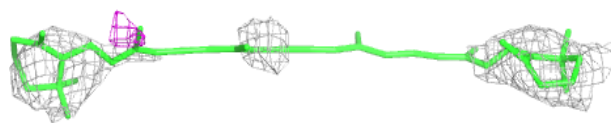
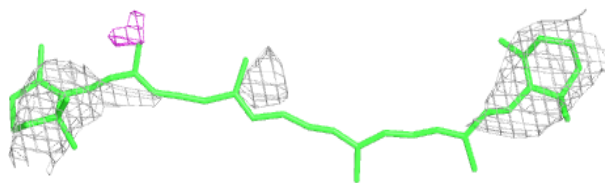
**Electron density around BCR 2 4010:**

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



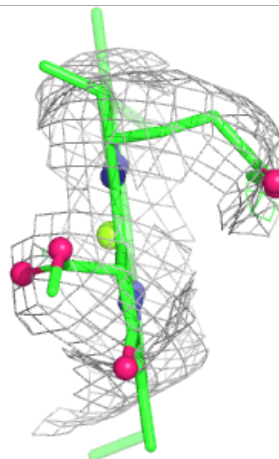
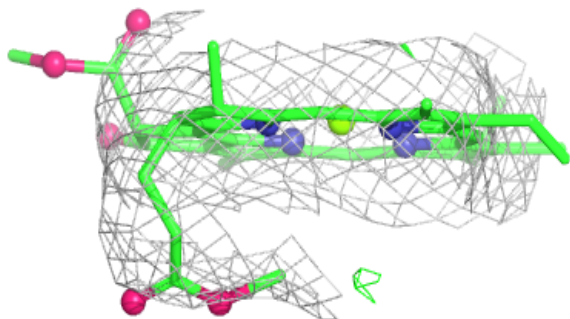
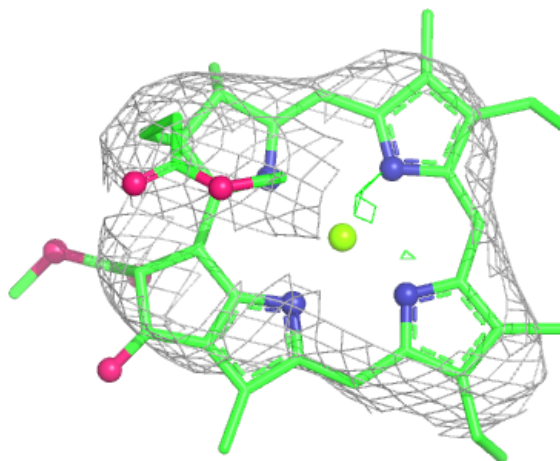
Electron density around BCR B 4005:

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



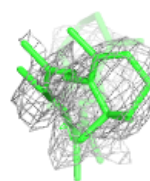
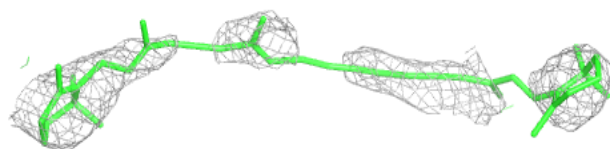
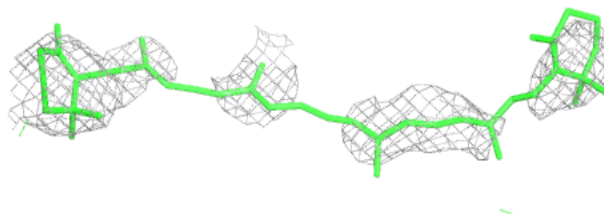
Electron density around CLA a 1121:

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

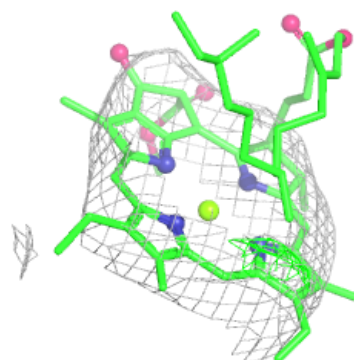
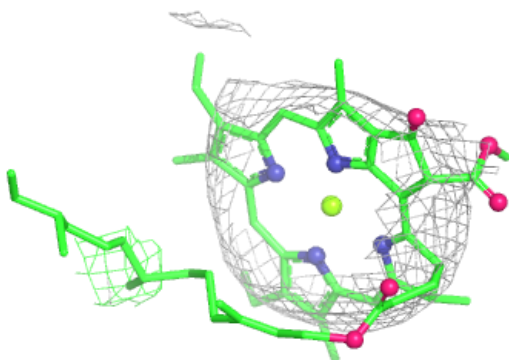
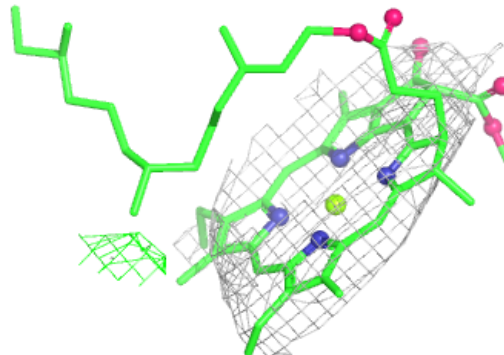


Electron density around BCR 7 4021:

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

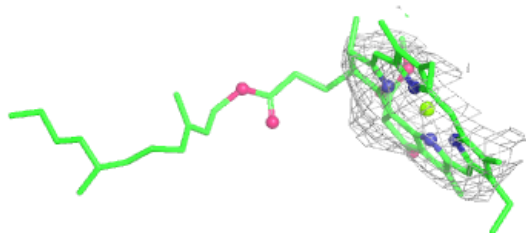
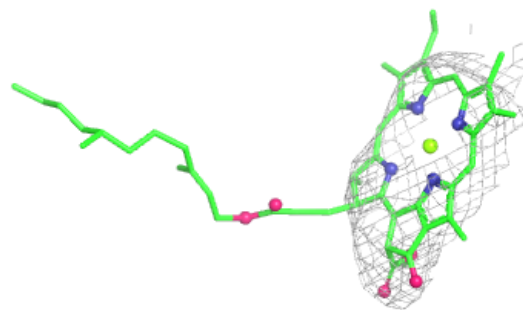
**Electron density around CLA a 1118:**

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



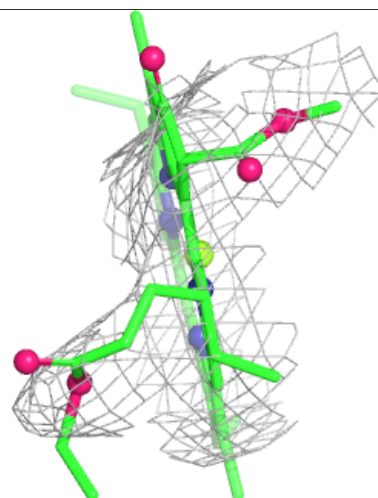
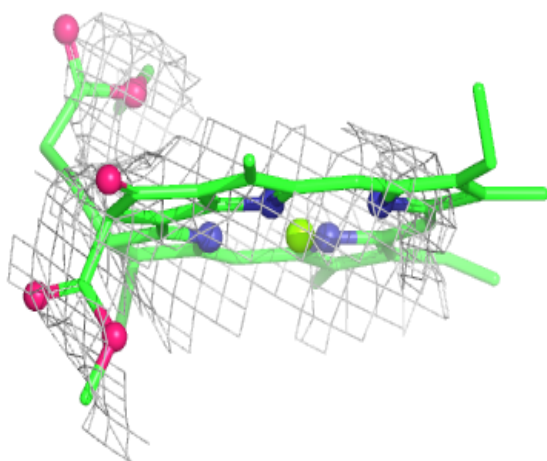
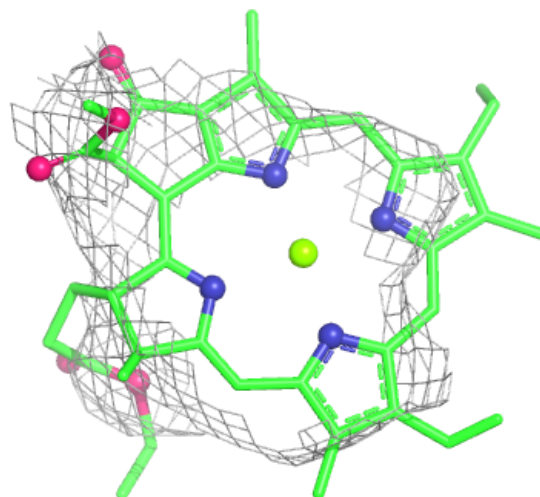
Electron density around CLA 2 1230:

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



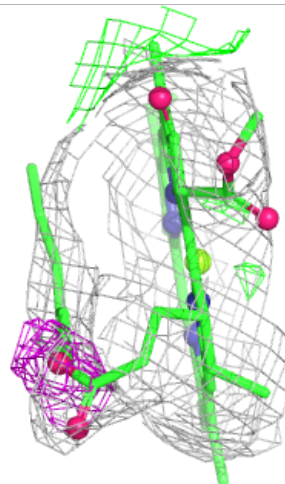
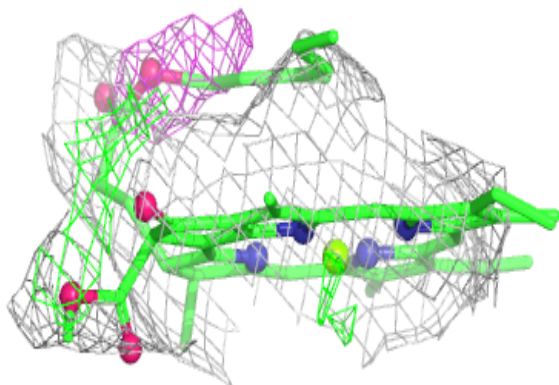
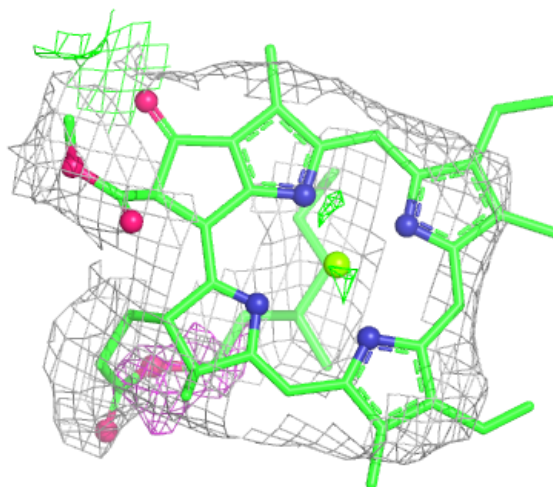
Electron density around CLA b 1217:

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



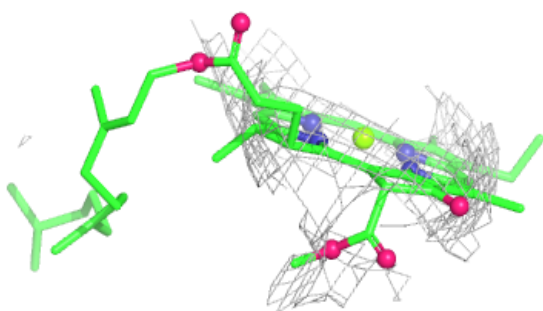
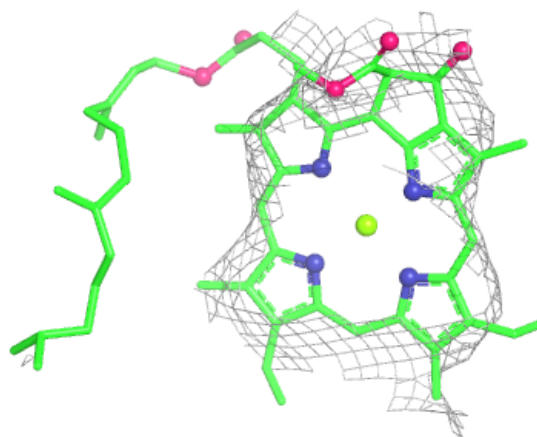
Electron density around CLA A 1801:

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



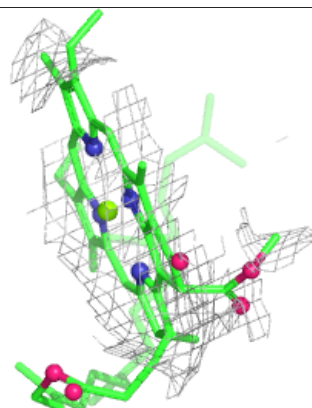
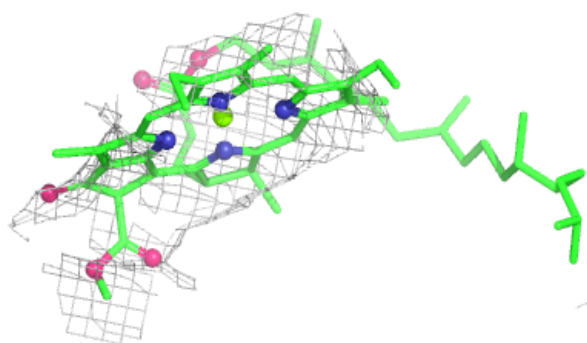
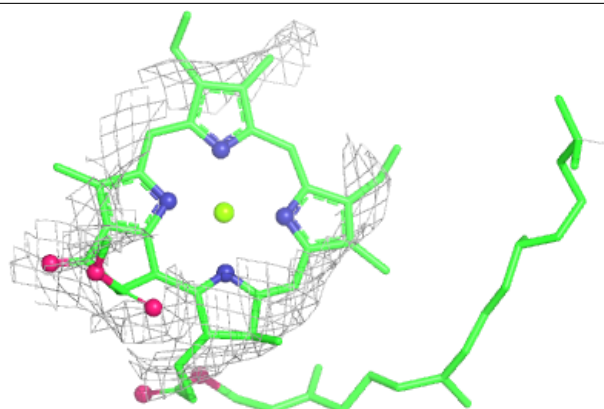
Electron density around CLA 1 1111:

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

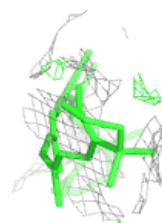
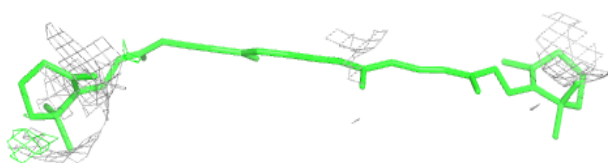
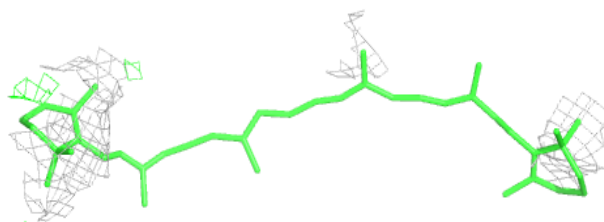


Electron density around CLA 0 1401:

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

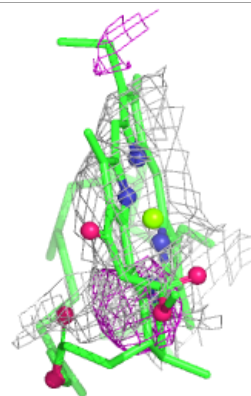
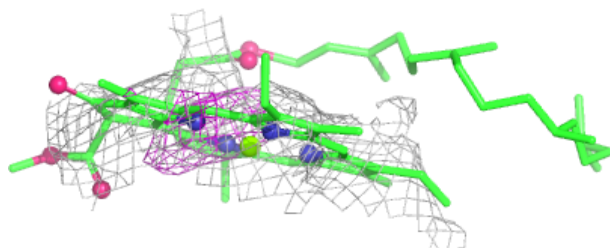
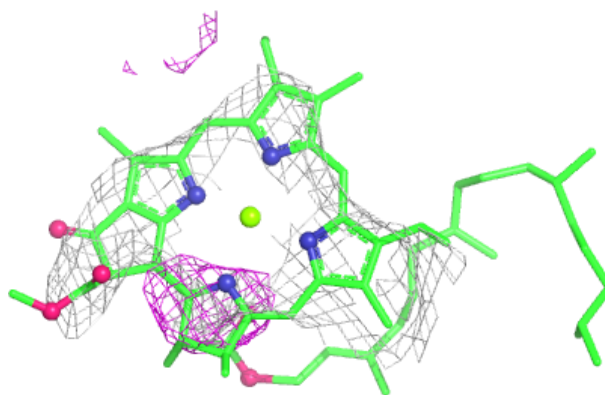
**Electron density around BCR 1 4001:**

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

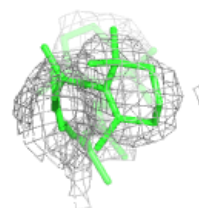
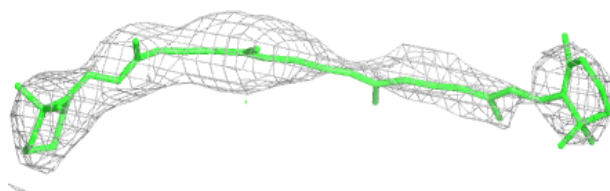
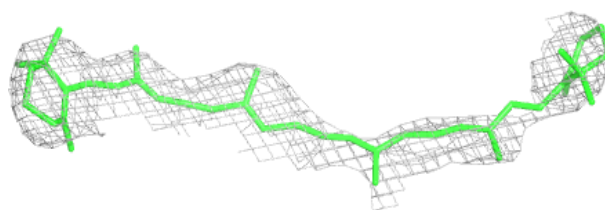


Electron density around CLA a 1117:

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

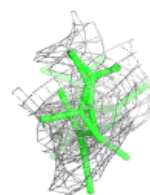
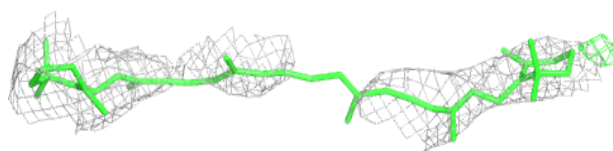
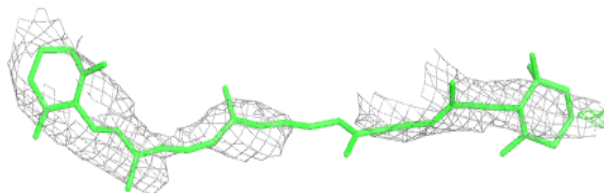
**Electron density around BCR F 4018:**

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



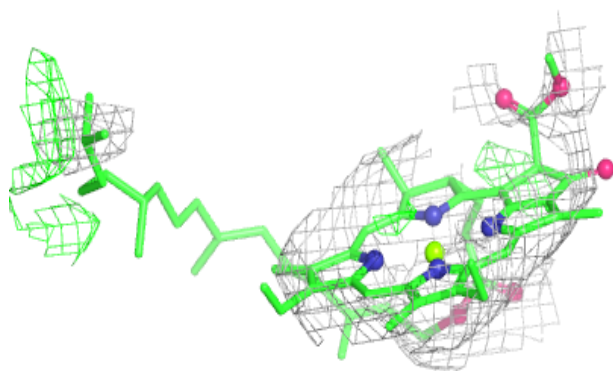
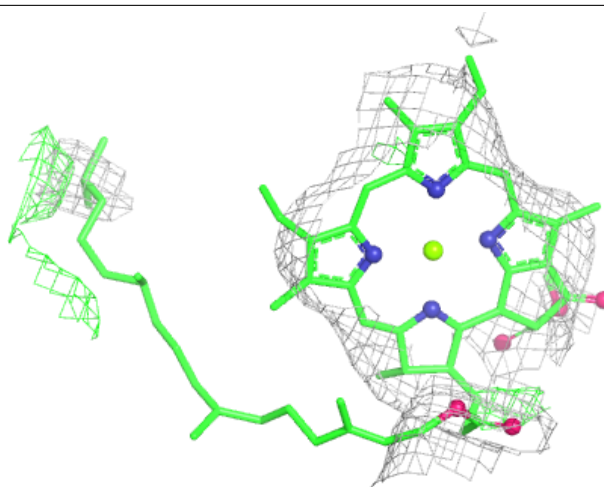
Electron density around BCR 1 4008:

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



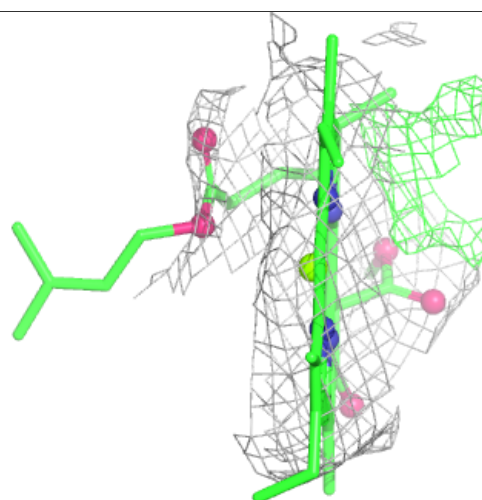
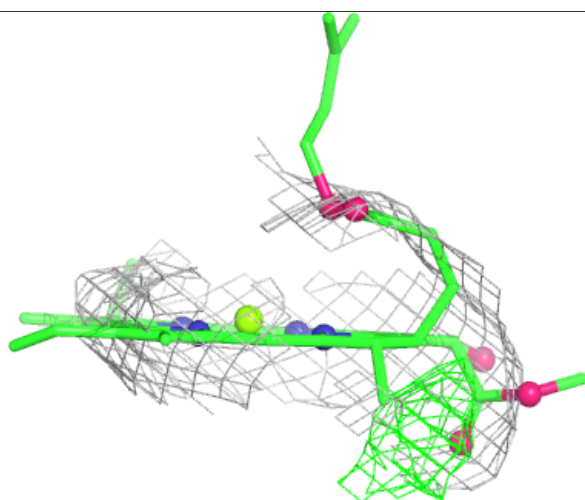
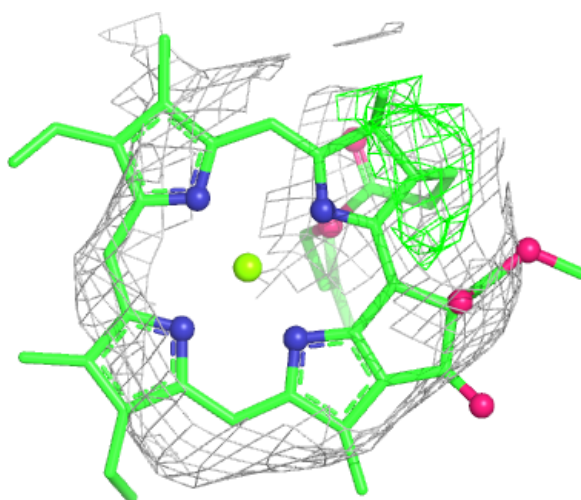
Electron density around CLA K 1401:

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



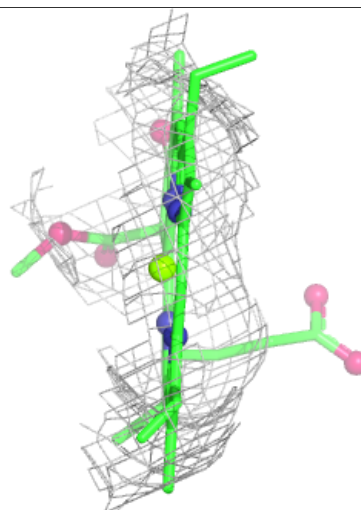
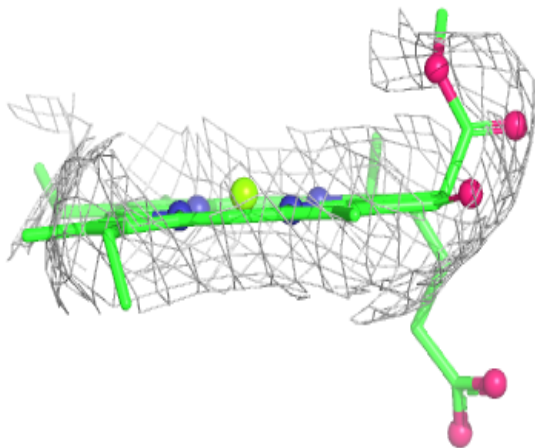
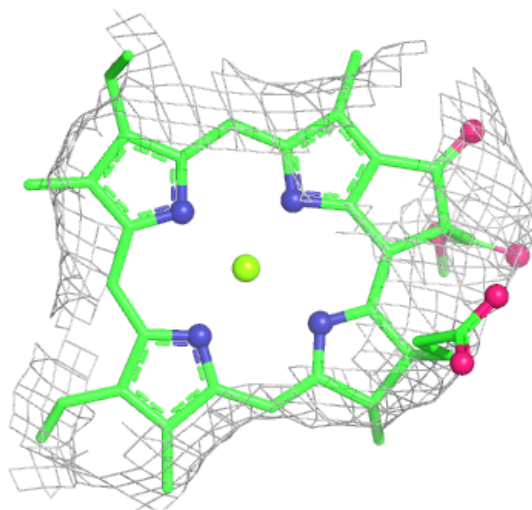
Electron density around CLA K 1402:

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



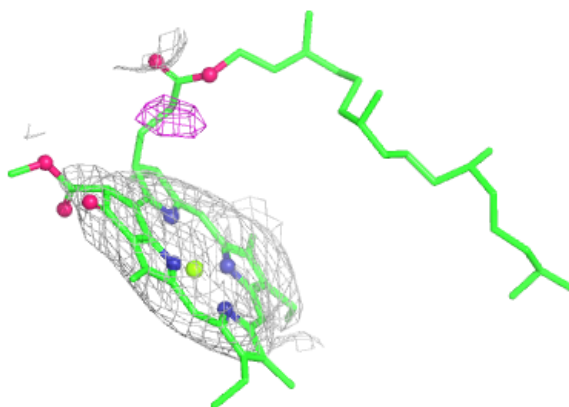
Electron density around CLA B 1218:

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

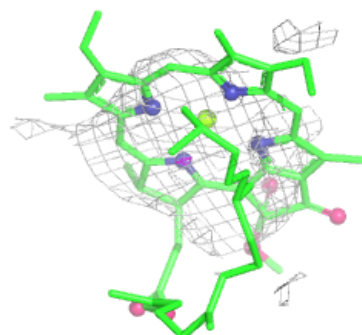
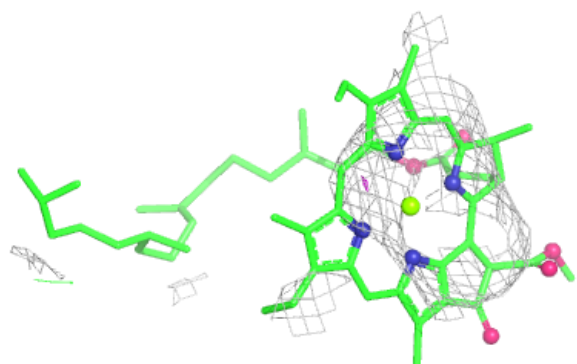
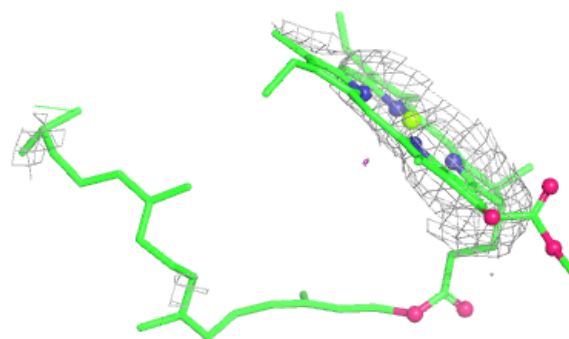


Electron density around CLA a 1102:

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

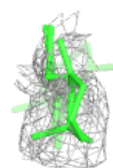
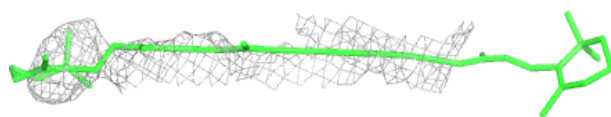
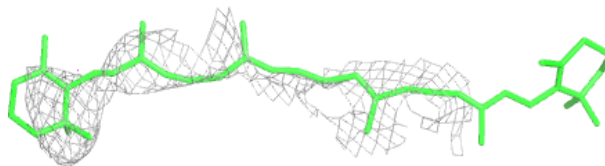
**Electron density around CLA 1 1109:**

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



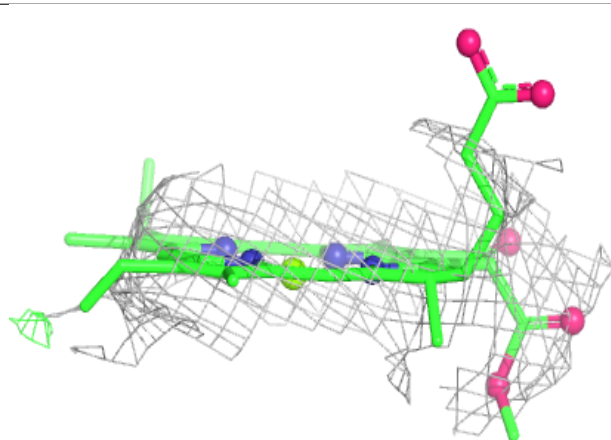
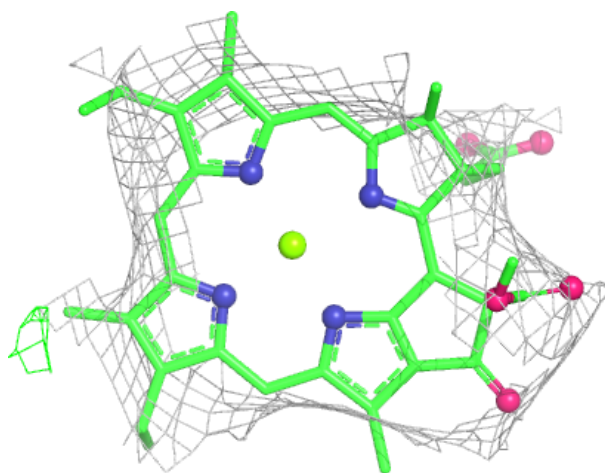
Electron density around BCR a 4007:

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



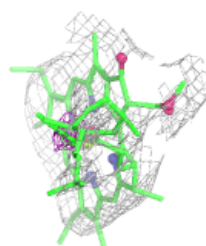
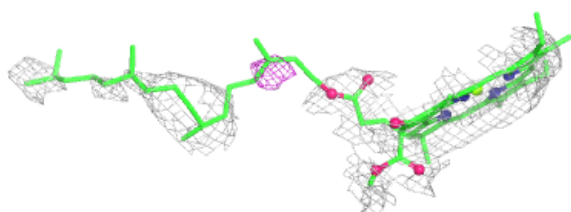
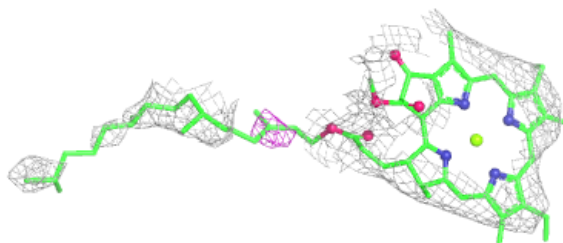
Electron density around CLA 2 1218:

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

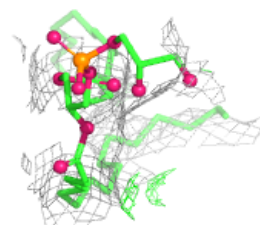
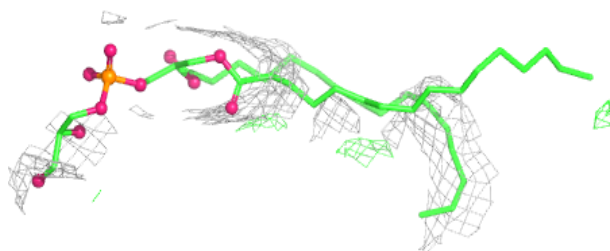
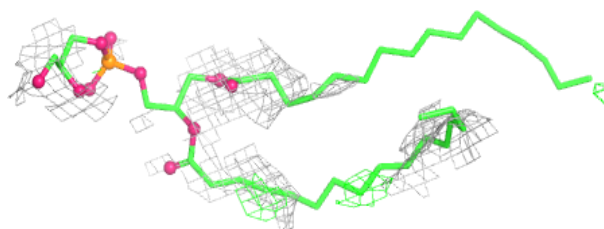


Electron density around CLA A 1107:

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

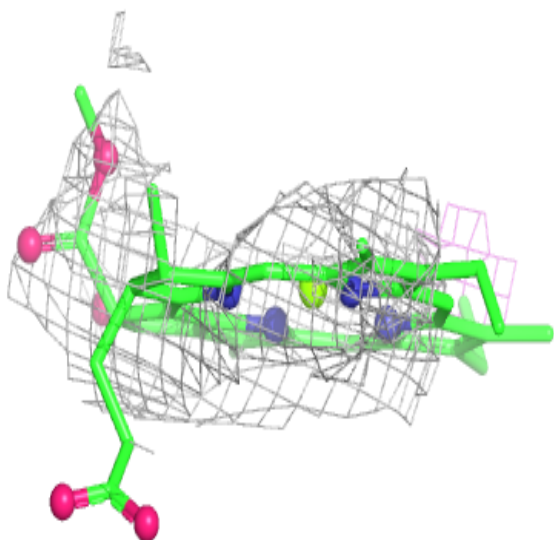
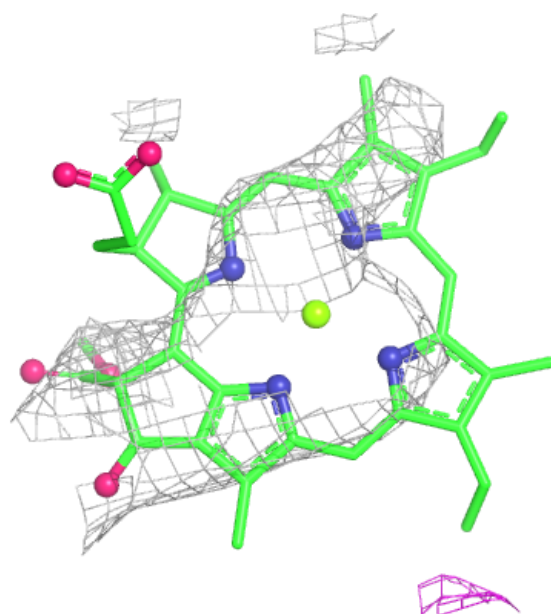
**Electron density around LHG a 5003:**

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



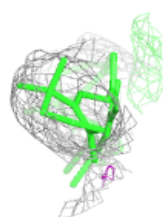
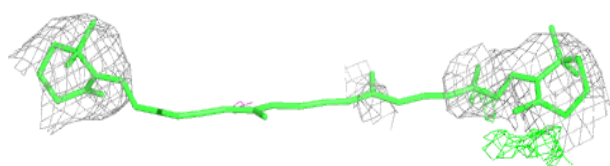
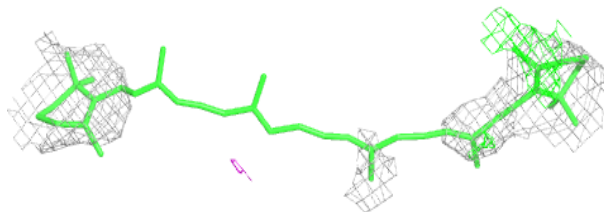
Electron density around CLA 2 1227:

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

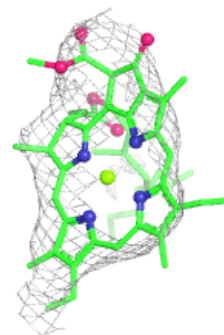
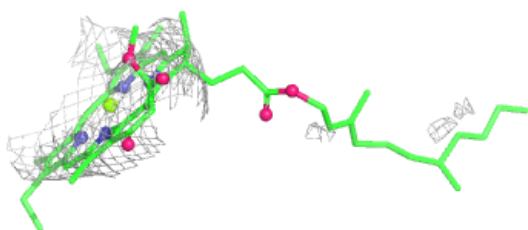
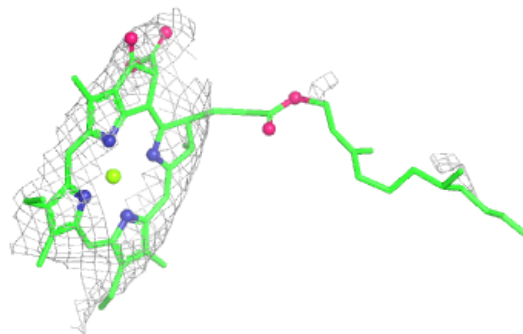


Electron density around BCR A 4001:

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

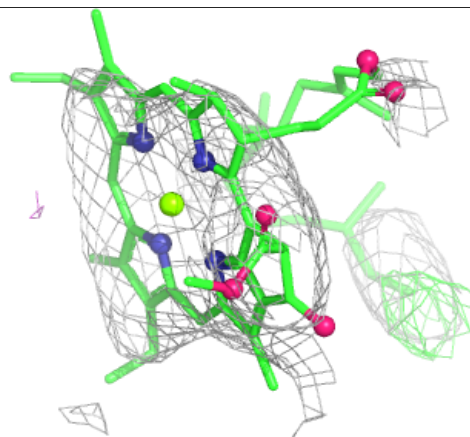
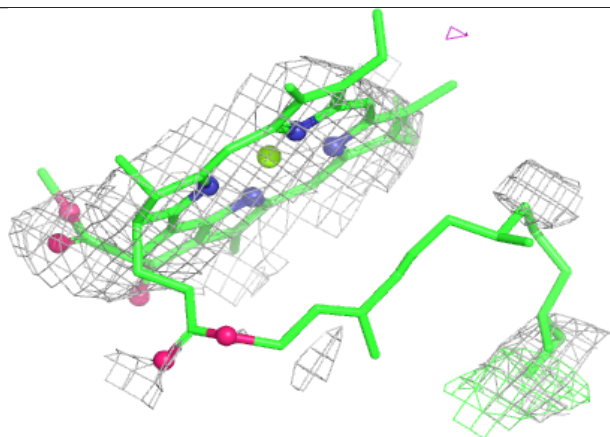
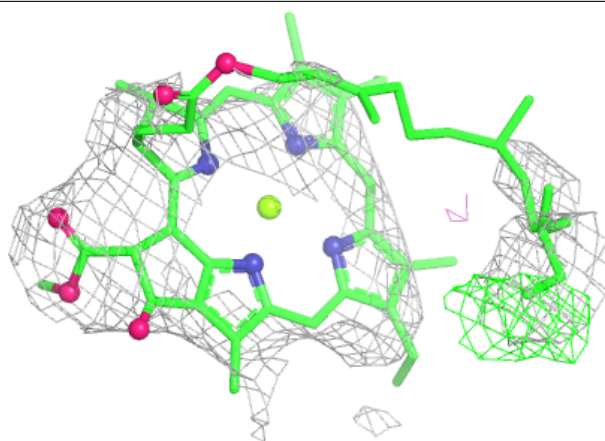
**Electron density around CLA B 1230:**

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

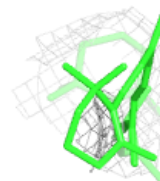
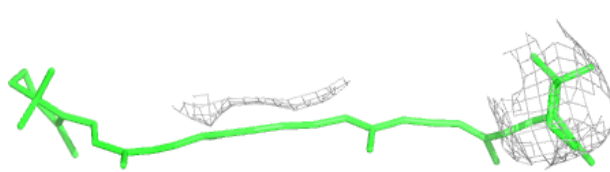
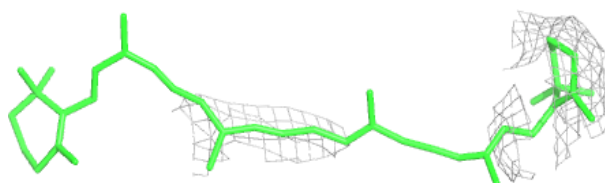


Electron density around CLA A 1118:

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

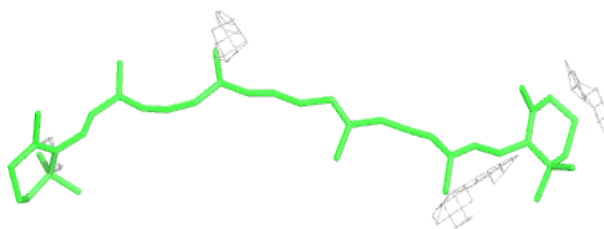
**Electron density around BCR b 4006:**

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



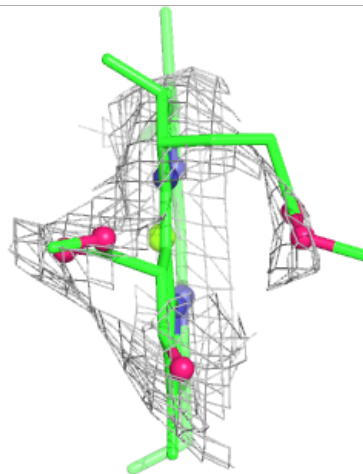
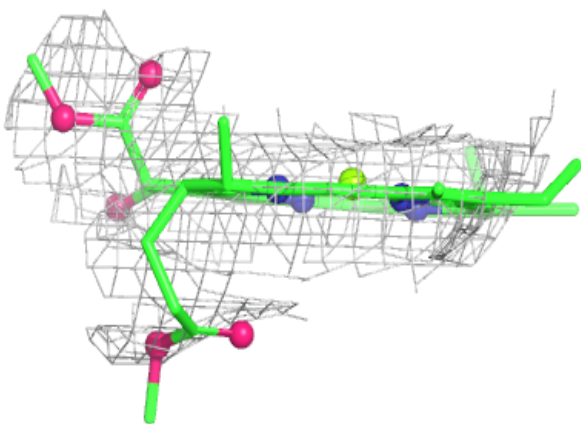
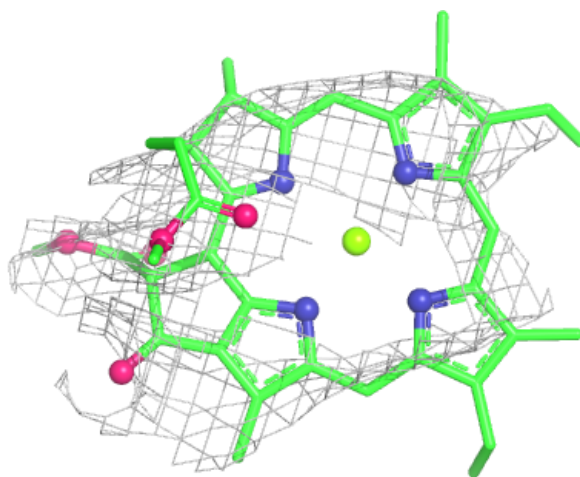
Electron density around BCR b 4010:

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



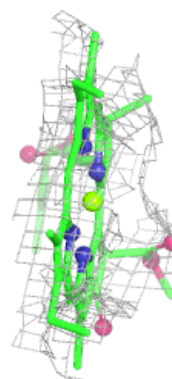
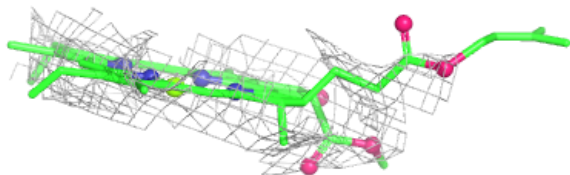
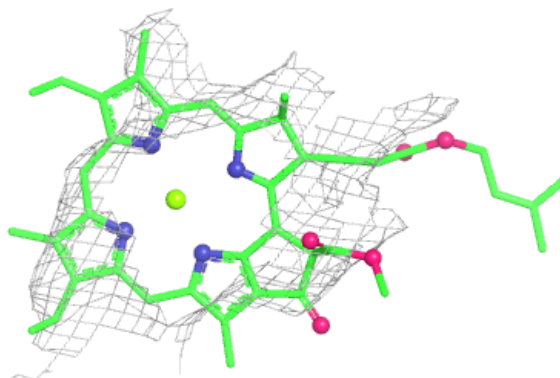
Electron density around CLA 1 1115:

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

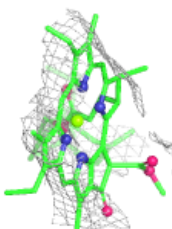
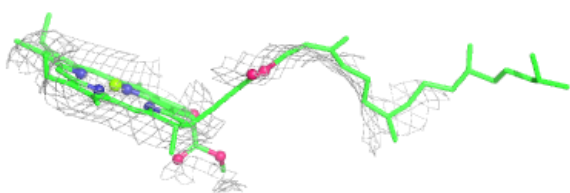
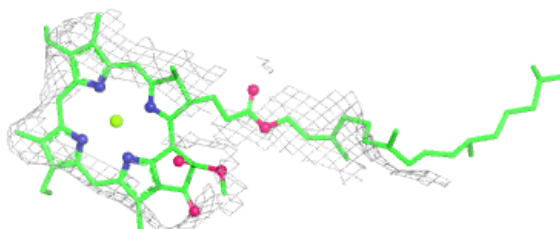


Electron density around CLA a 1139:

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

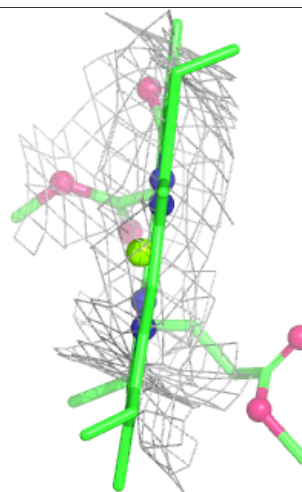
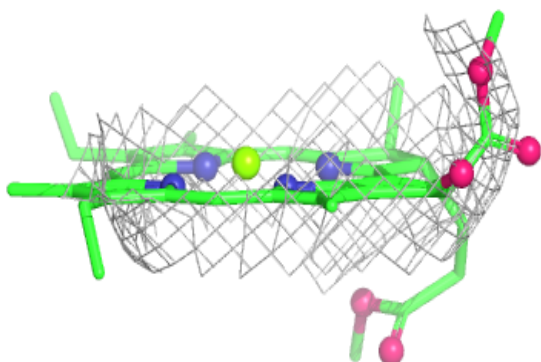
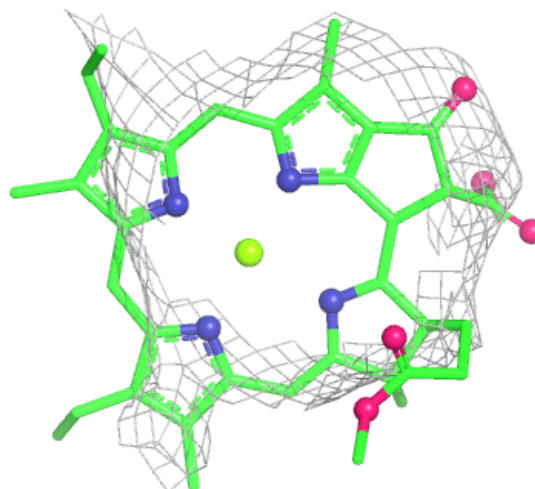
**Electron density around CLA a 1107:**

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



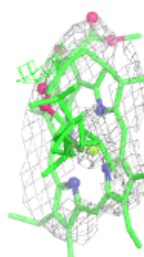
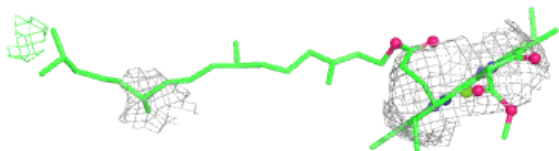
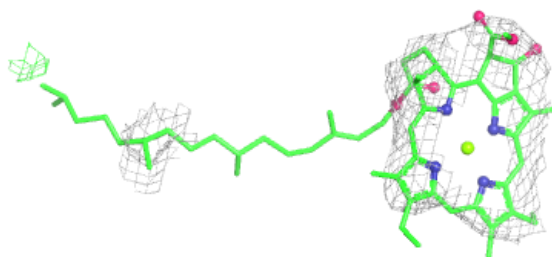
Electron density around CLA 1 1120:

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



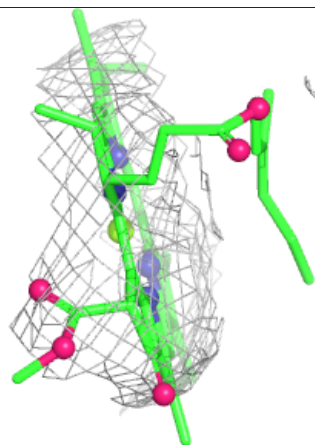
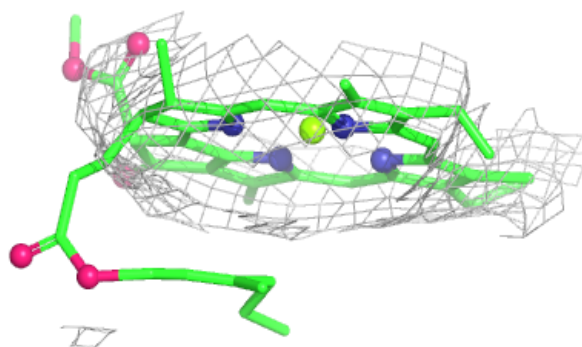
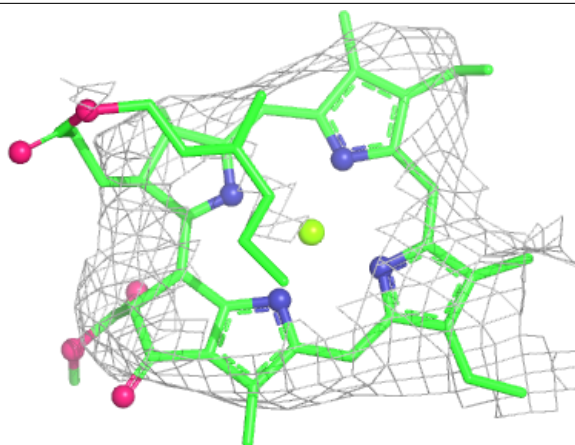
Electron density around CLA 1 1501:

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



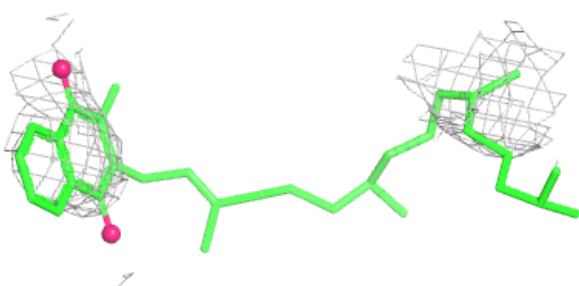
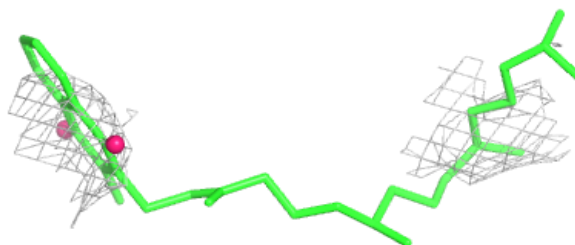
Electron density around CLA 1 1801:

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

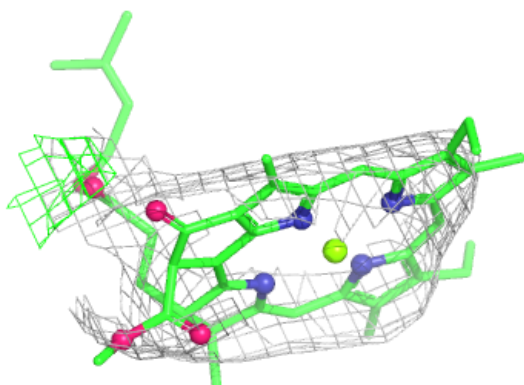
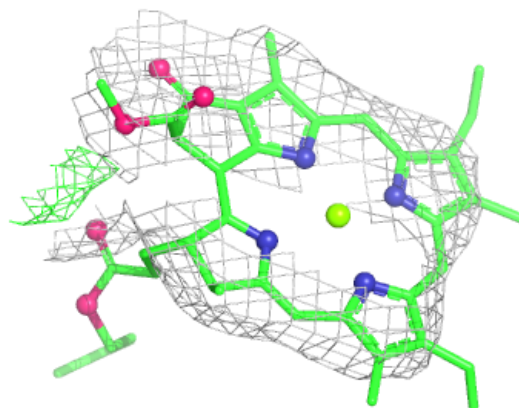


Electron density around PQN b 2002:

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

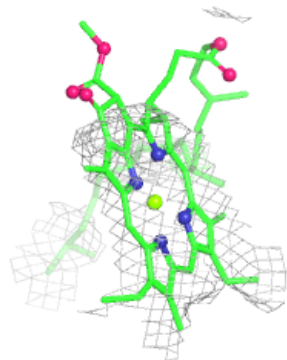
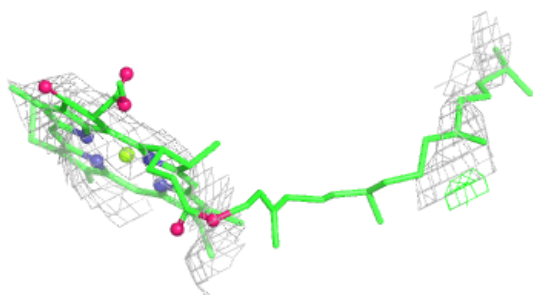
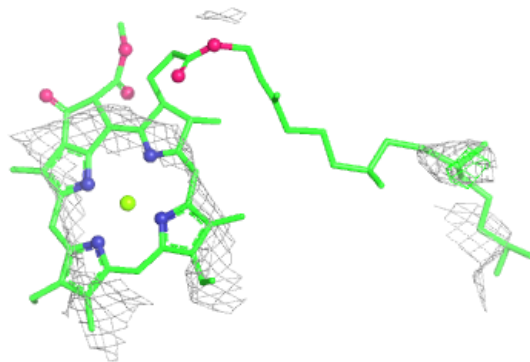
**Electron density around CLA B 1228:**

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



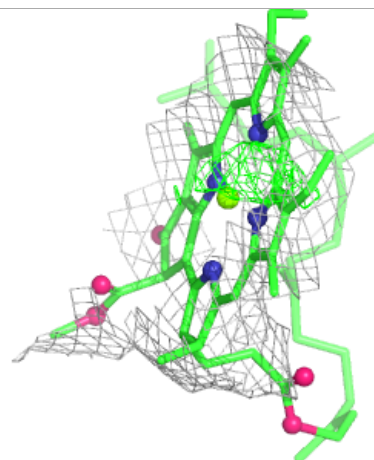
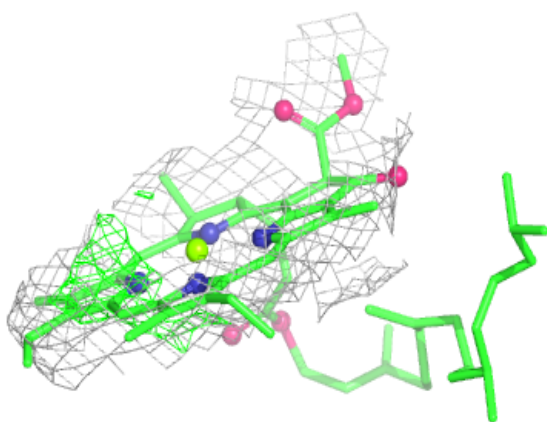
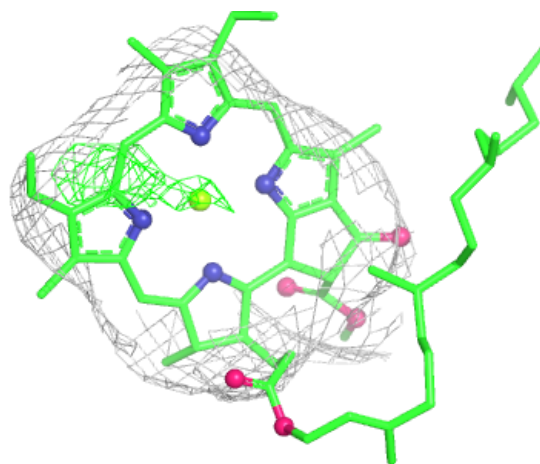
Electron density around CLA b 1013:

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



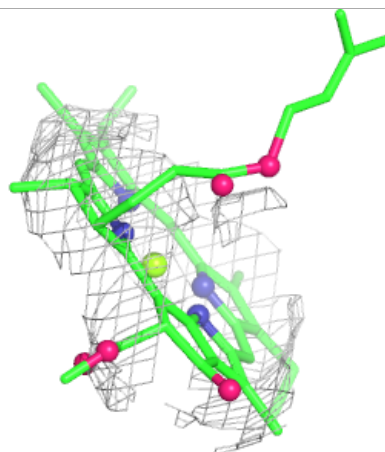
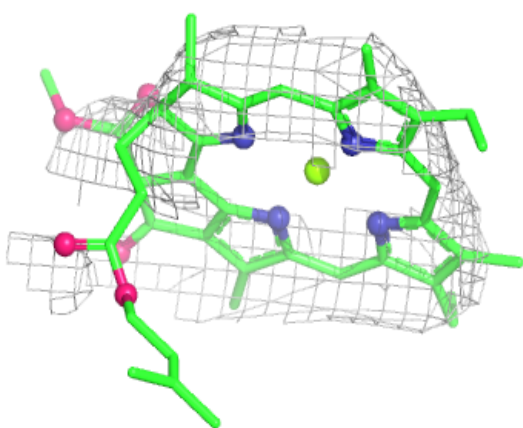
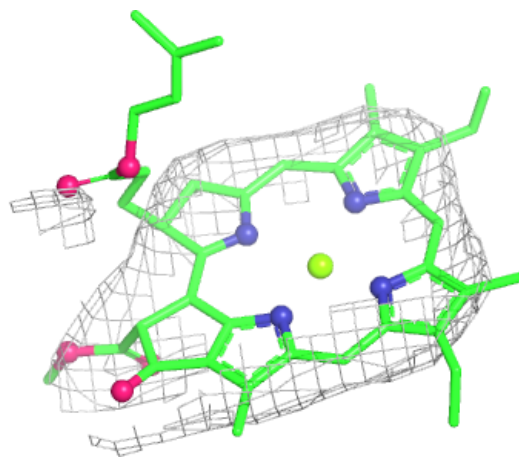
Electron density around CLA B 1229:

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



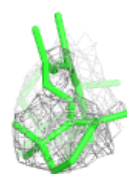
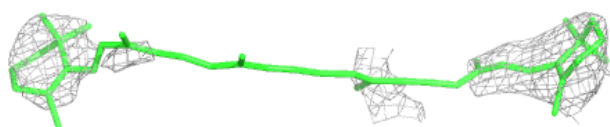
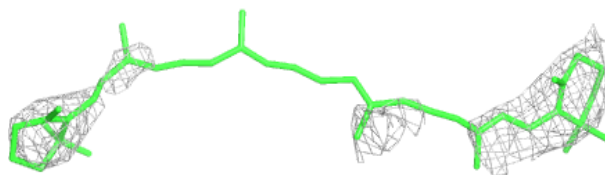
Electron density around CLA 2 1228:

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

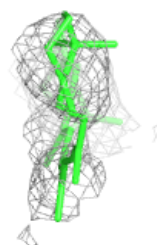
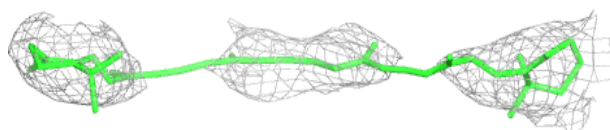
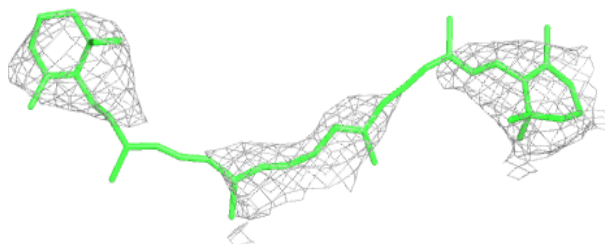


Electron density around BCR B 4010:

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

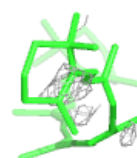
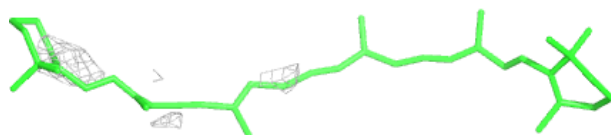
**Electron density around BCR B 4011:**

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



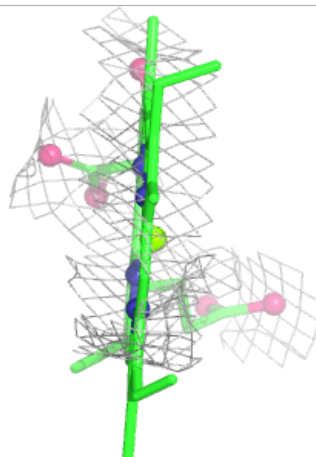
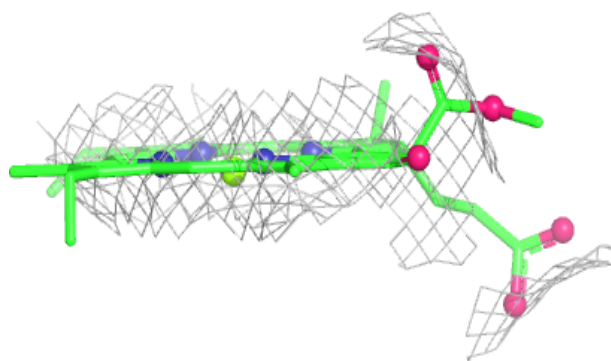
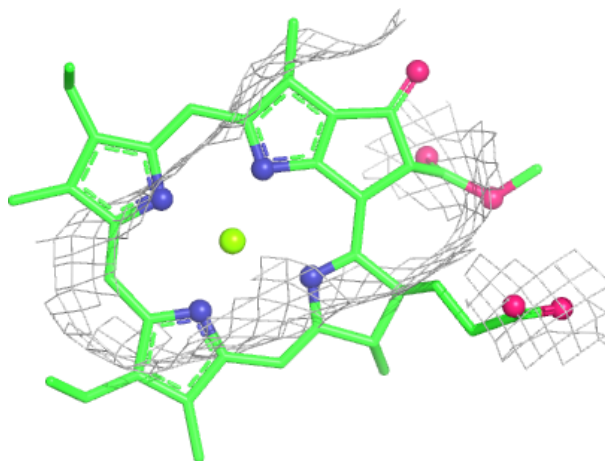
Electron density around BCR 2 4014:

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



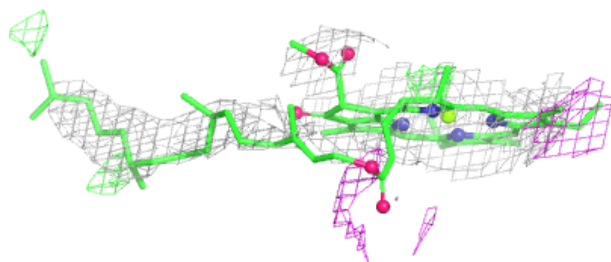
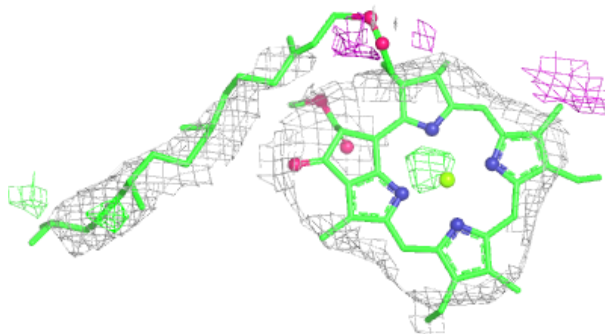
Electron density around CLA a 1113:

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



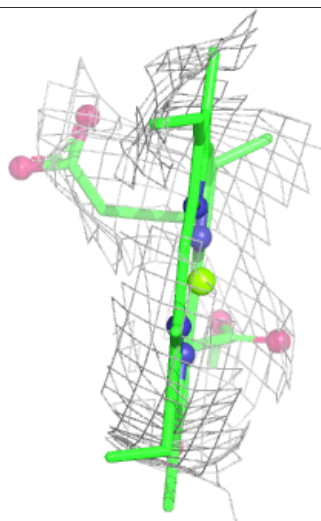
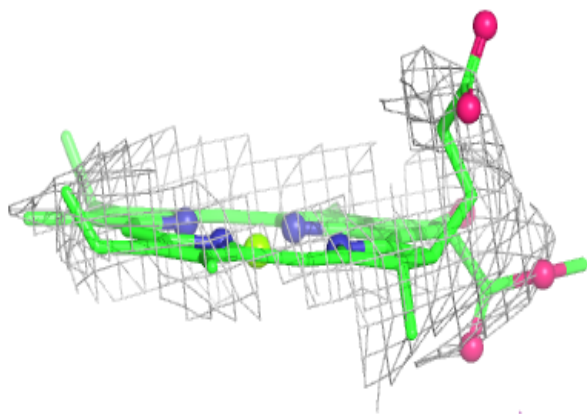
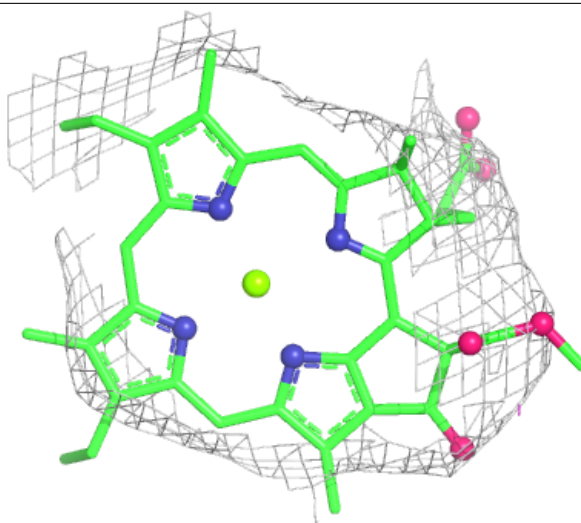
Electron density around CLA L 1503:

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



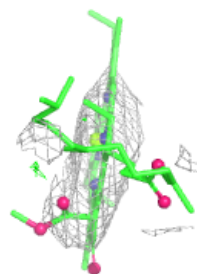
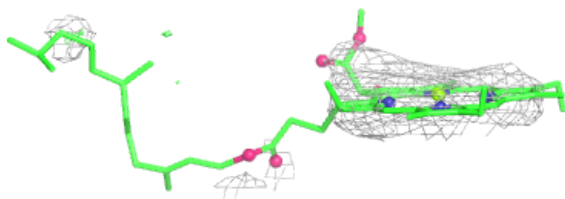
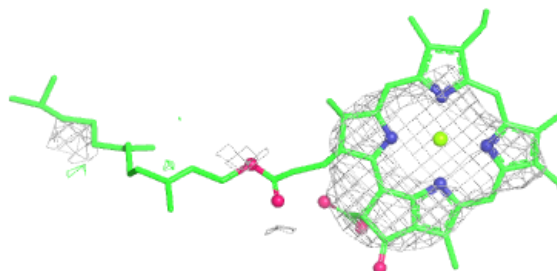
Electron density around CLA 2 1232:

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

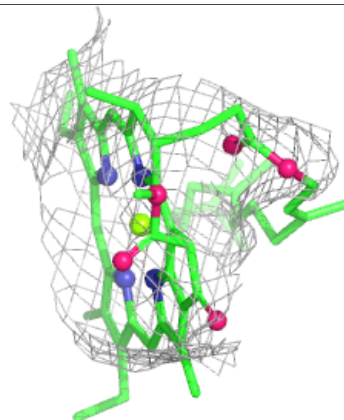
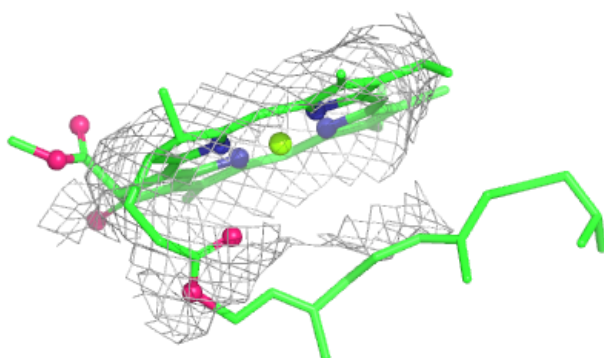
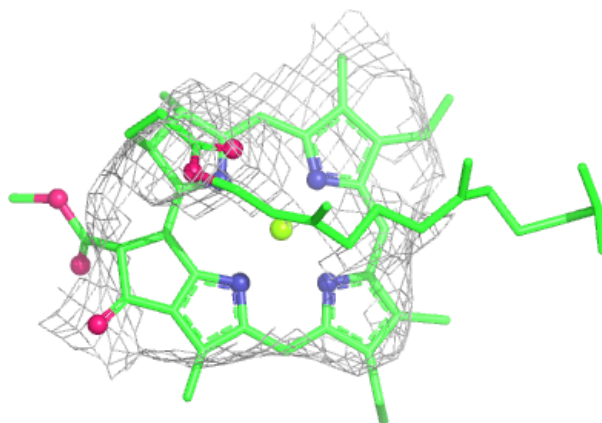


Electron density around CLA 2 1234:

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

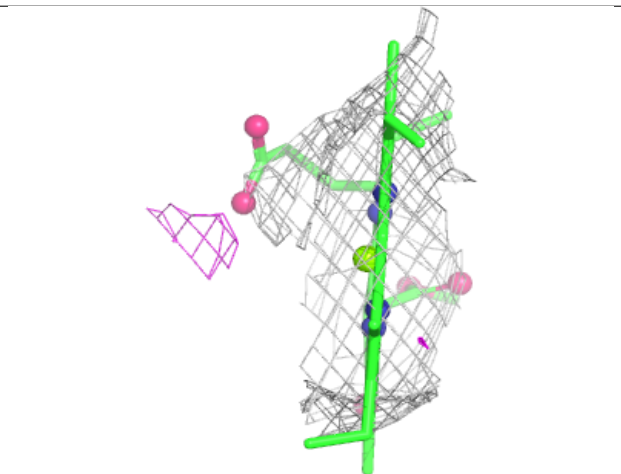
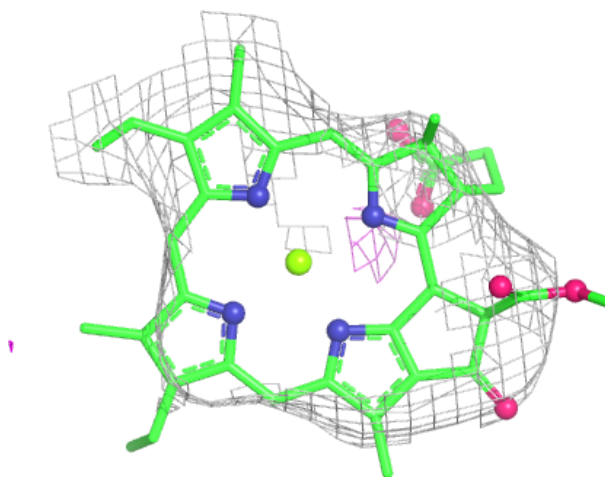
**Electron density around CLA 2 1235:**

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



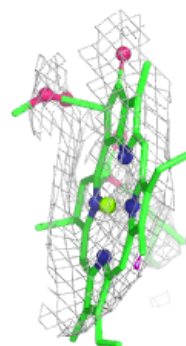
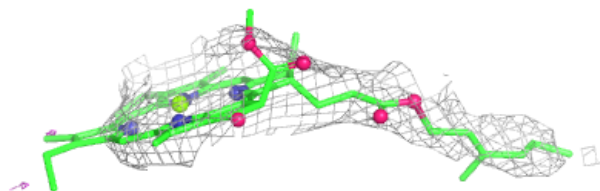
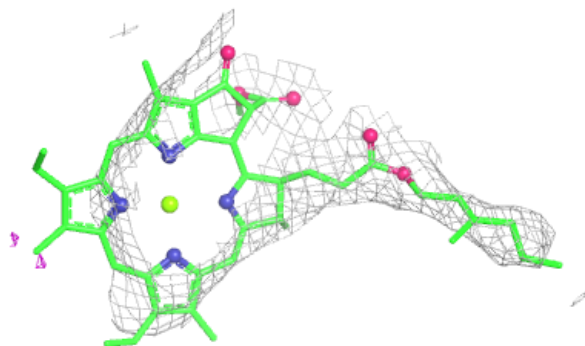
Electron density around CLA B 1209:

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

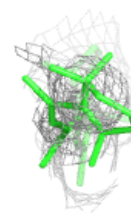
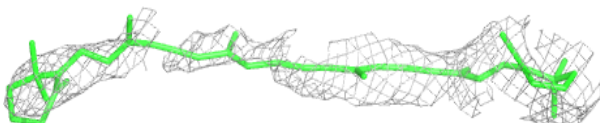
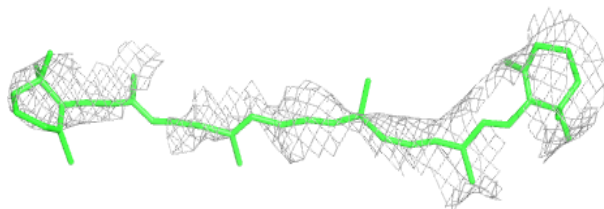


Electron density around CLA a 1125:

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

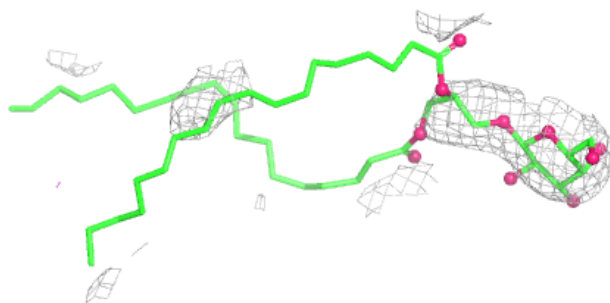
**Electron density around BCR a 4008:**

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



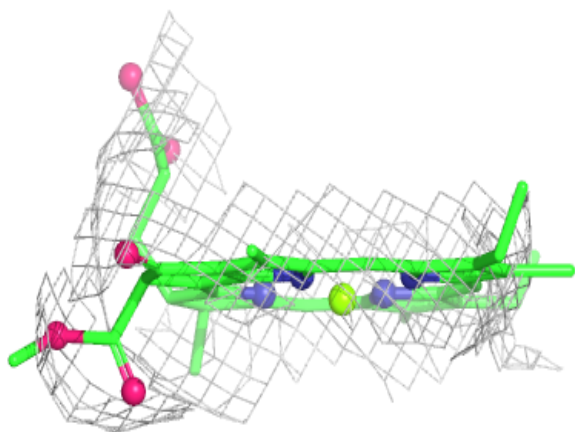
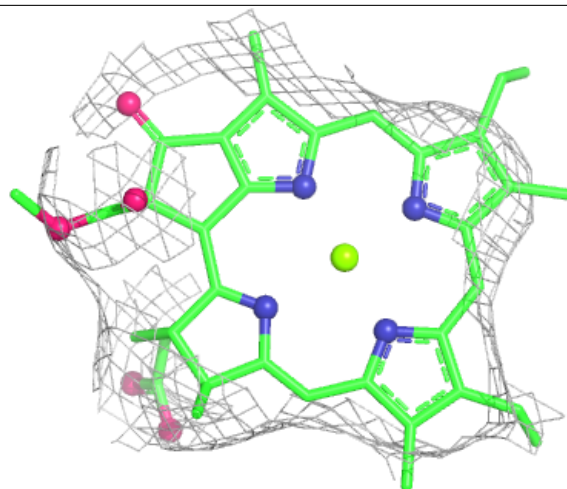
Electron density around LMG b 5002:

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



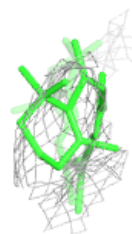
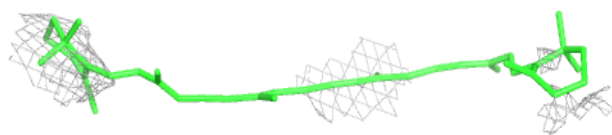
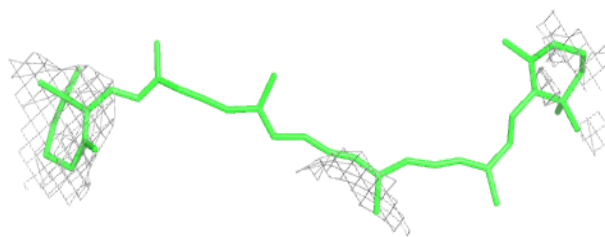
Electron density around CLA B 1232:

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

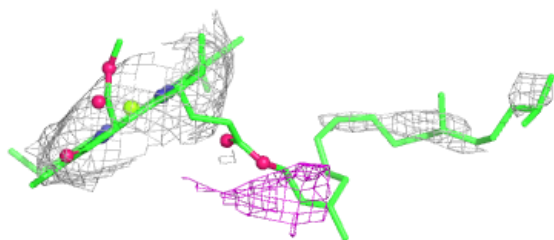
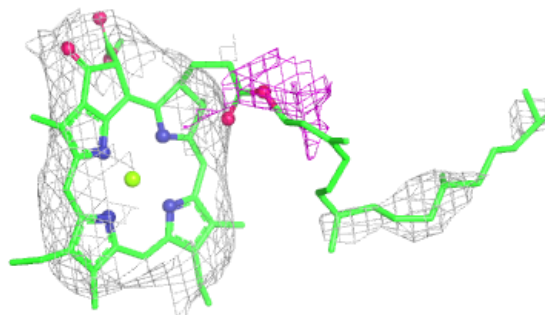


Electron density around BCR b 4004:

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

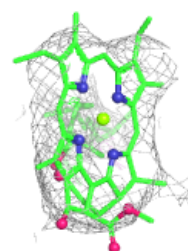
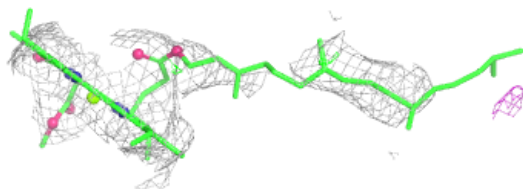
**Electron density around CLA A 1106:**

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

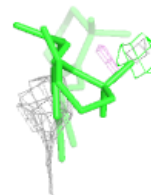
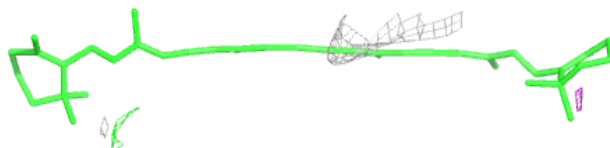
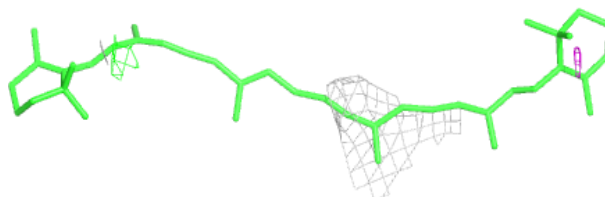


Electron density around CLA L 1501:

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

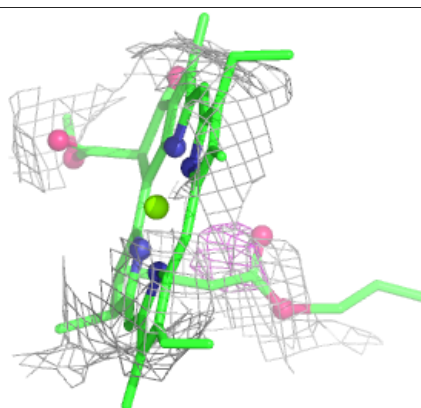
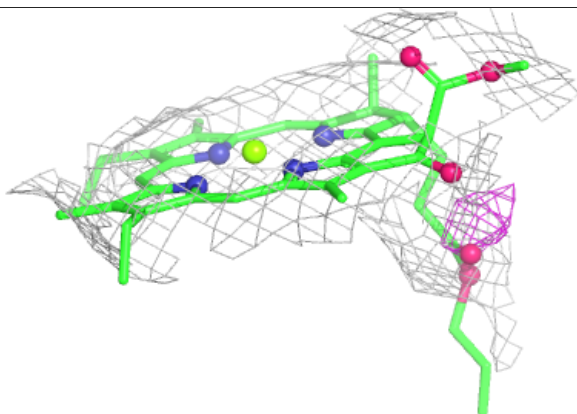
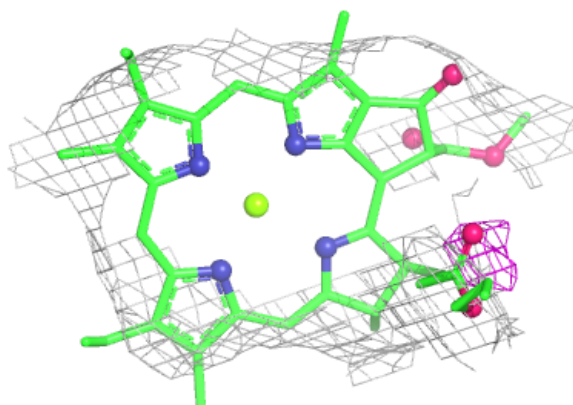
**Electron density around BCR b 4009:**

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



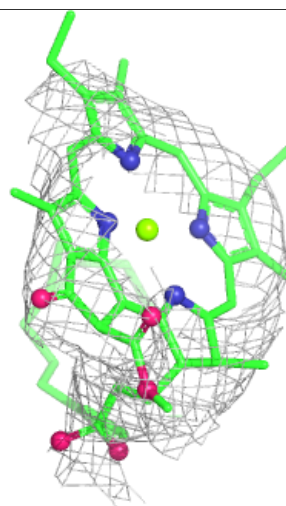
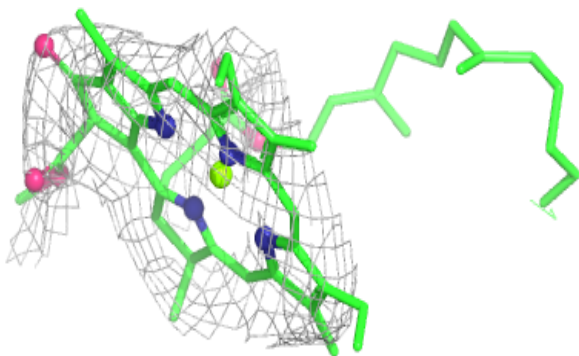
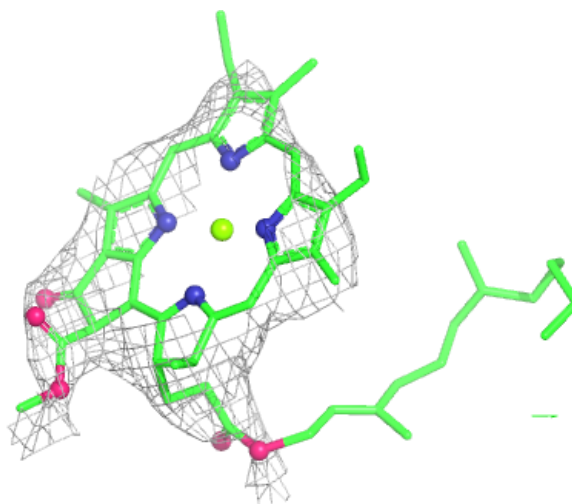
Electron density around CLA A 1105:

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



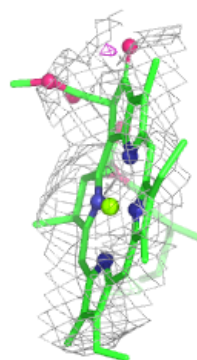
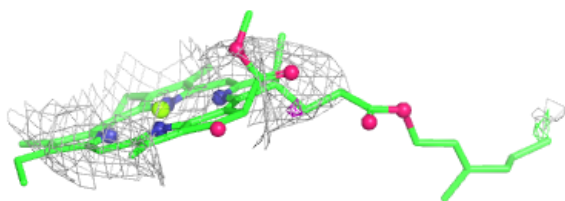
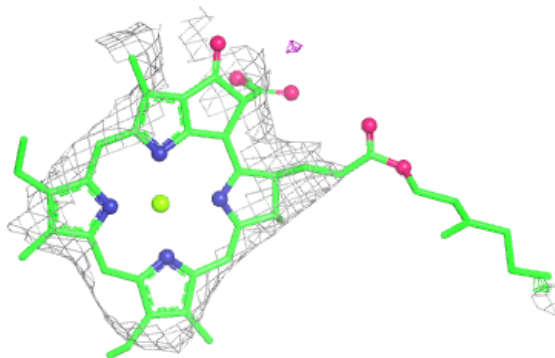
Electron density around CLA 1 1122:

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

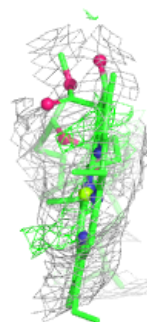
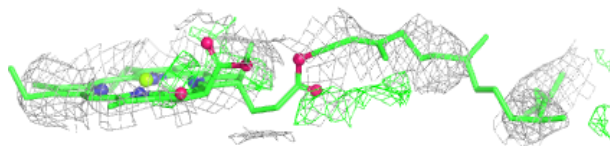
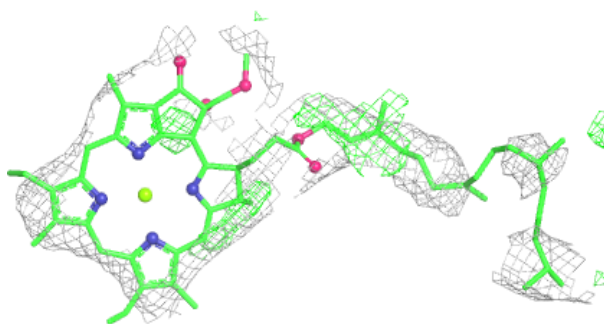


Electron density around CLA 1 1125:

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

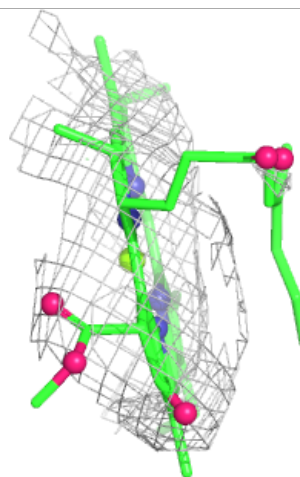
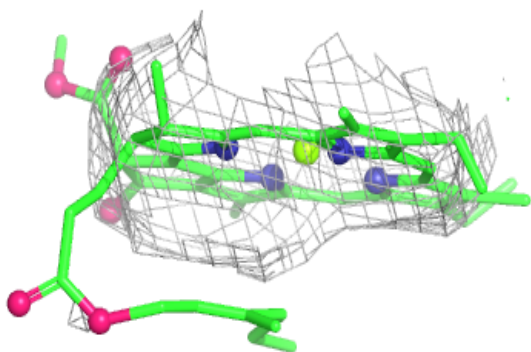
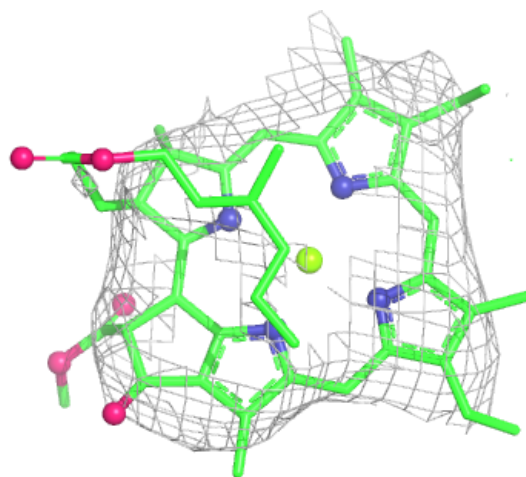
**Electron density around CLA 1 1131:**

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



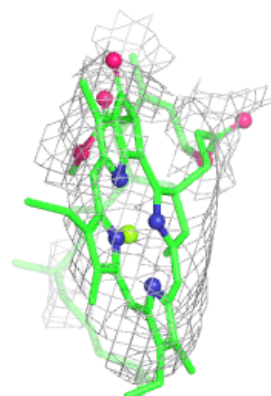
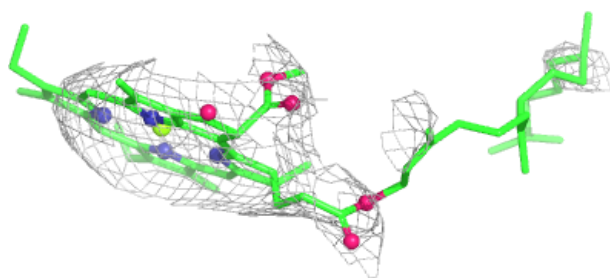
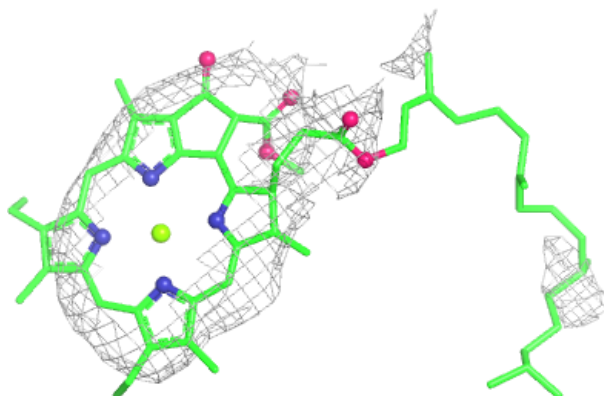
Electron density around CLA a 1801:

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

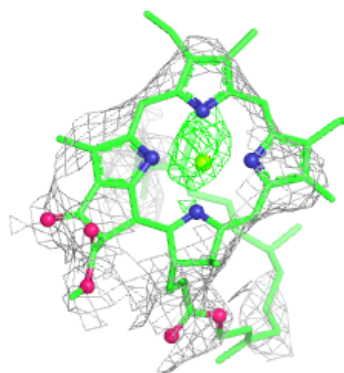
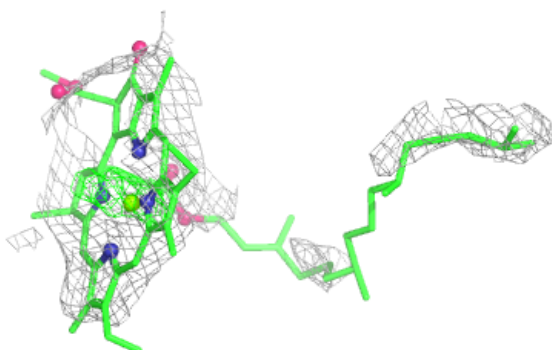
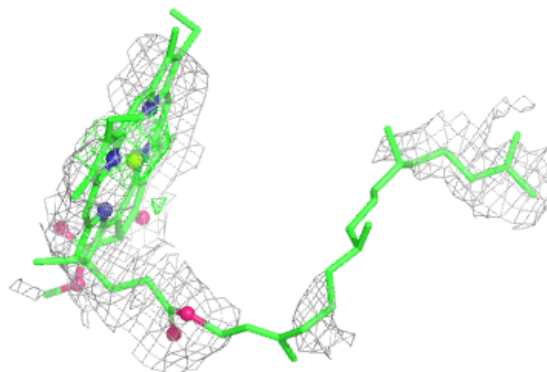


Electron density around CLA a 1101:

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

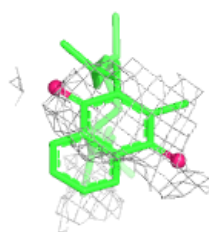
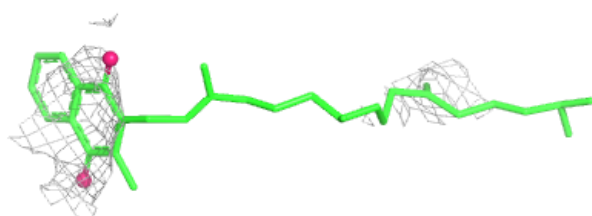
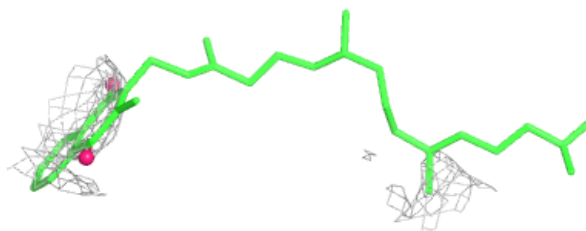
**Electron density around CLA B 1216:**

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

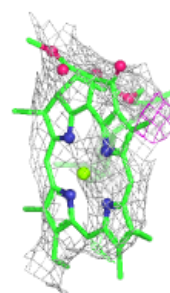
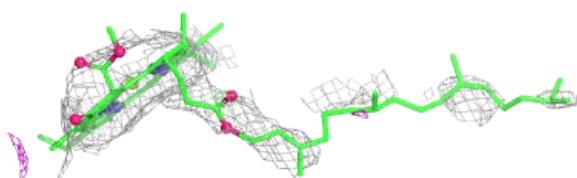


Electron density around PQN 1 2001:

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

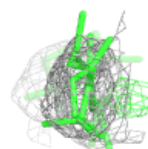
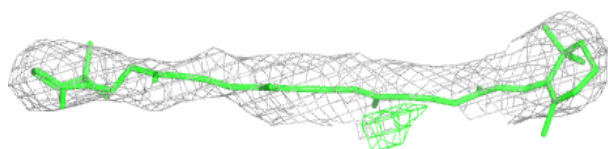
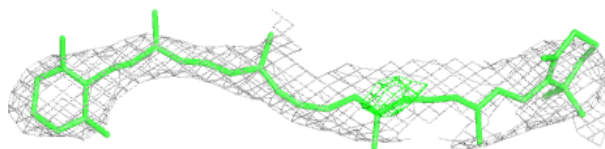
**Electron density around CLA 1 1132:**

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



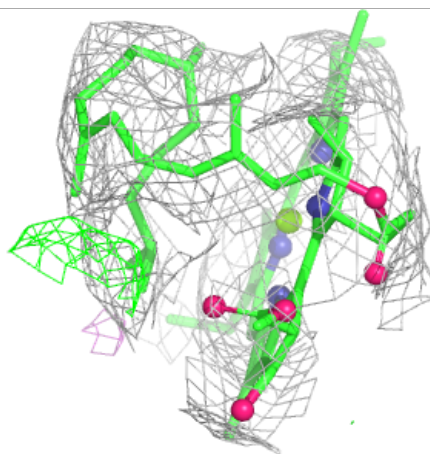
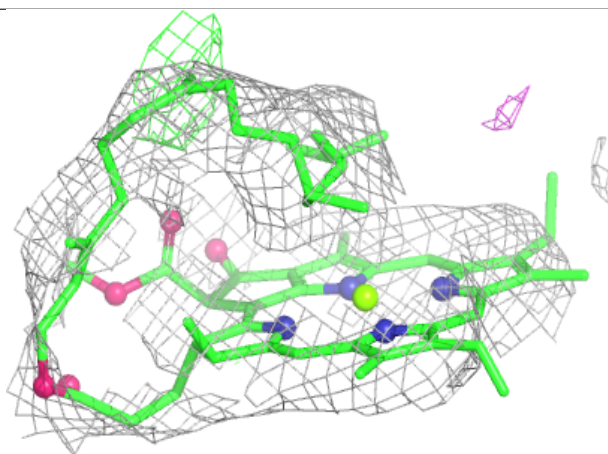
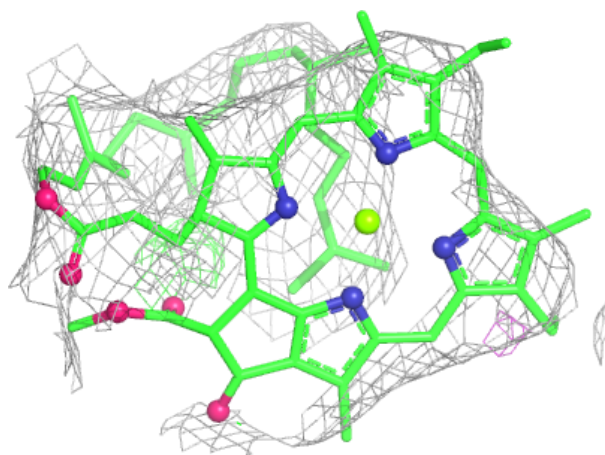
Electron density around BCR A 4002:

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



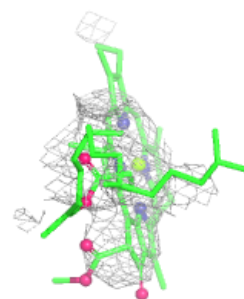
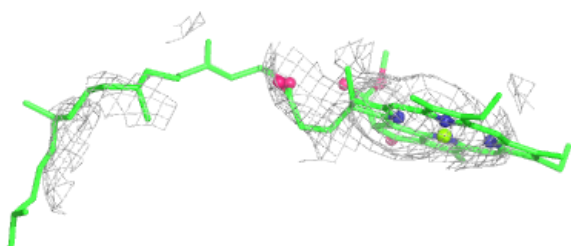
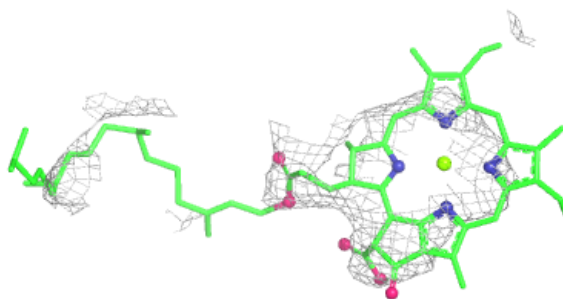
Electron density around CLA 2 1203:

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

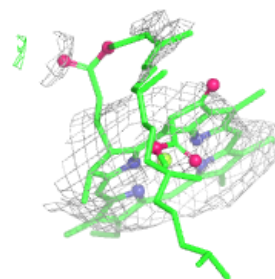
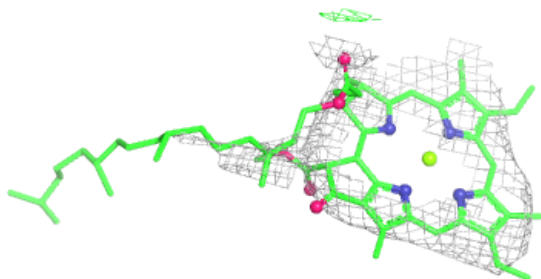
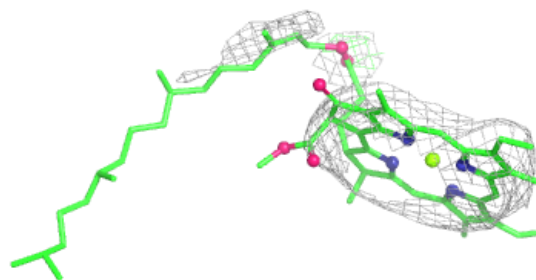


Electron density around CLA a 1103:

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

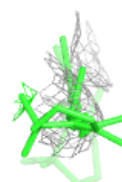
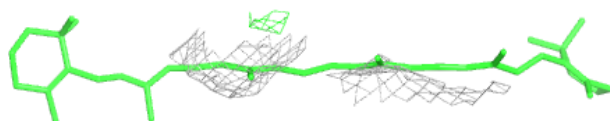
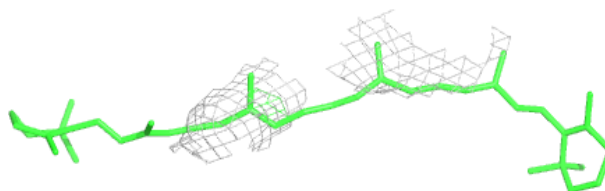
**Electron density around CLA 2 1213:**

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

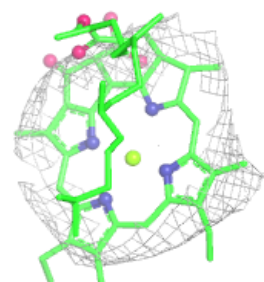
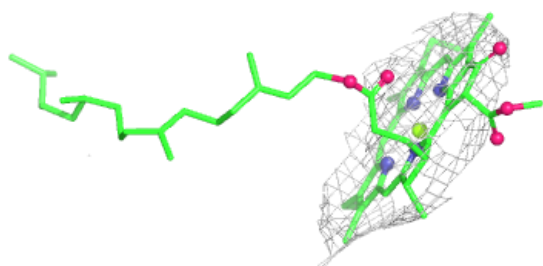
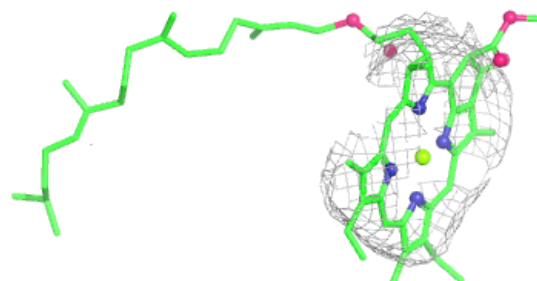


Electron density around BCR B 4009:

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

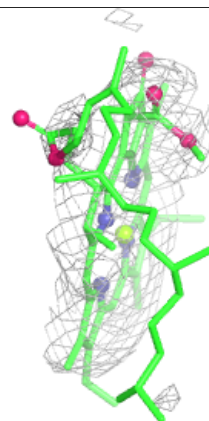
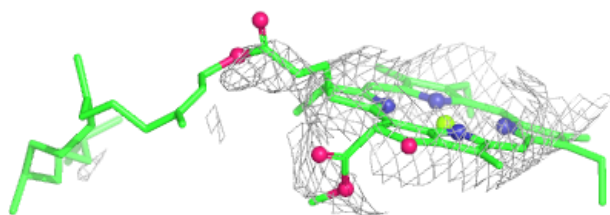
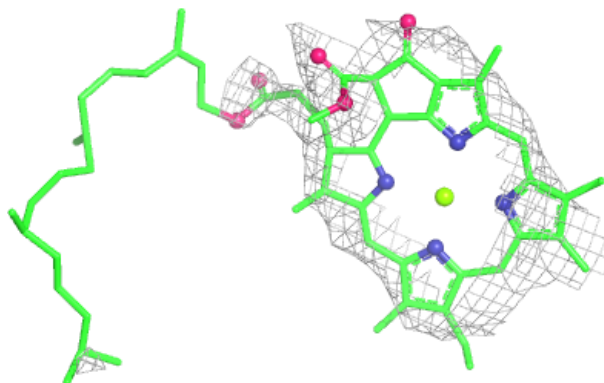
**Electron density around CLA a 1140:**

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

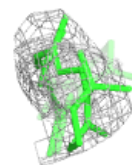
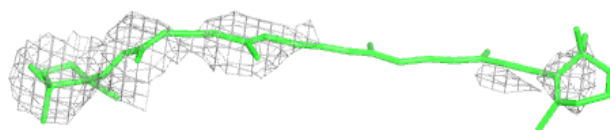
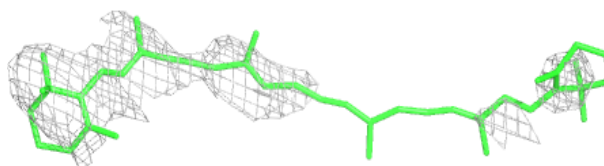


Electron density around CLA 1 1101:

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

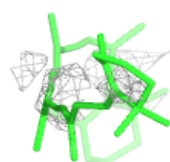
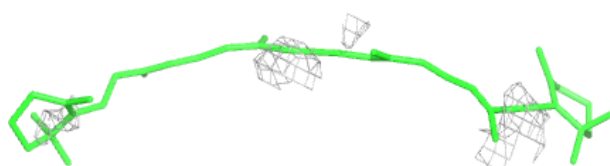
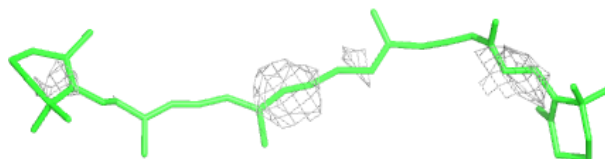
**Electron density around BCR 8 4022:**

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

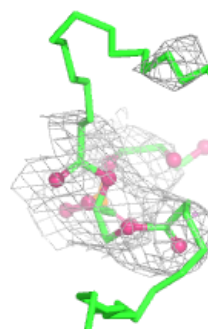
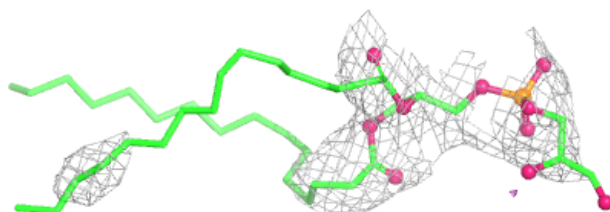
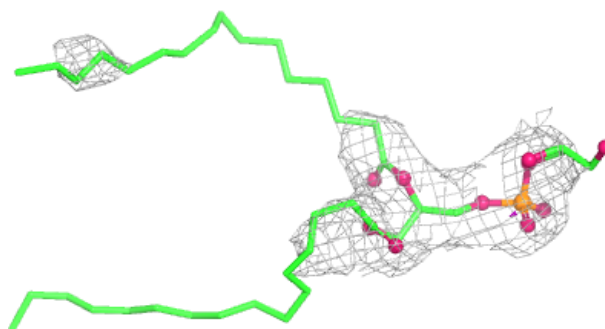


Electron density around BCR B 4014:

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

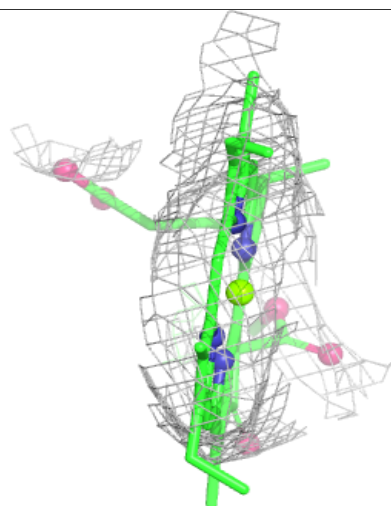
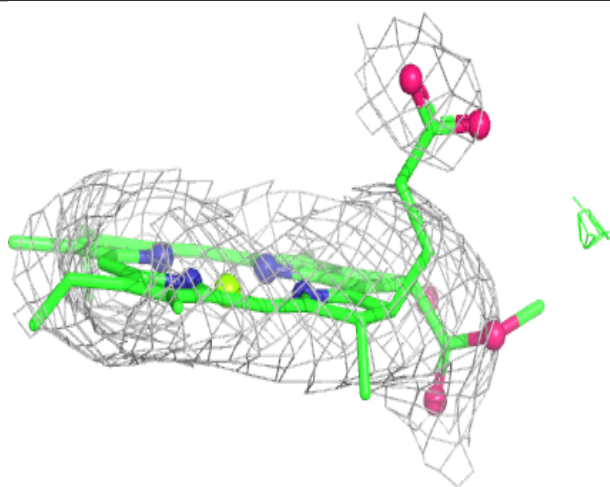
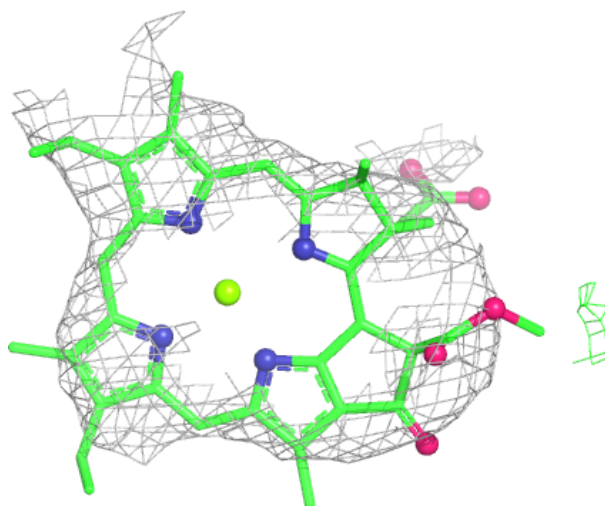
**Electron density around LHG A 5001:**

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



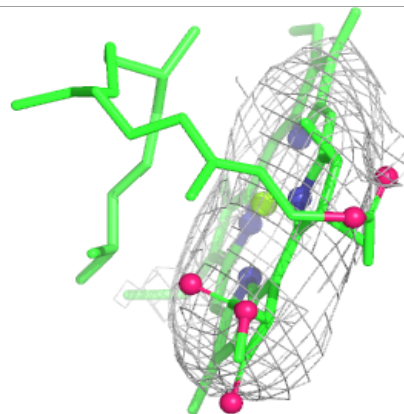
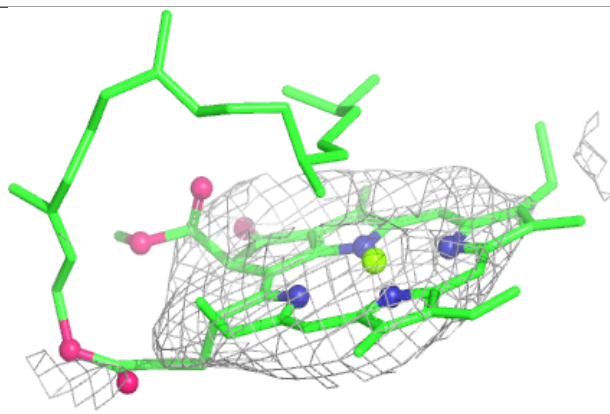
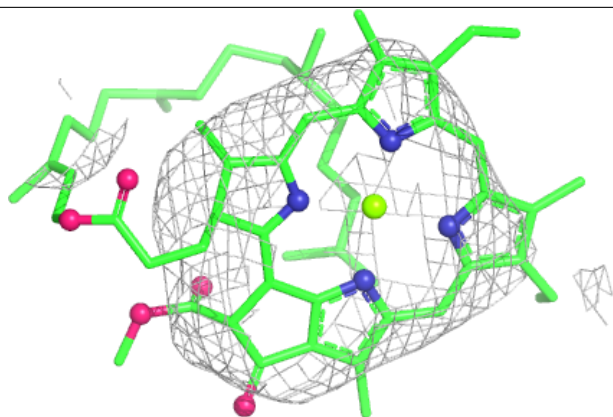
Electron density around CLA B 1208:

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



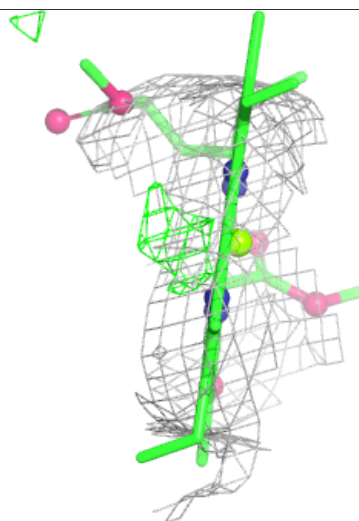
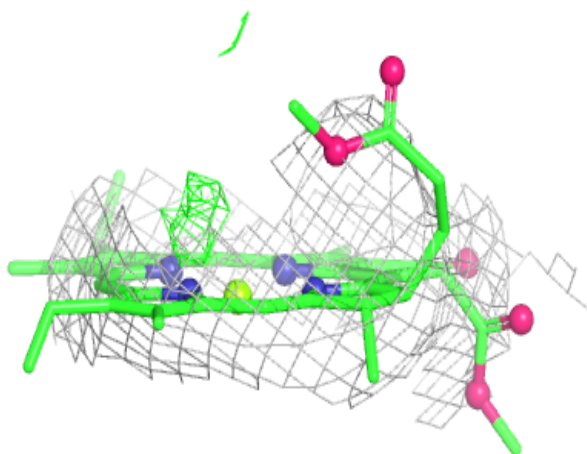
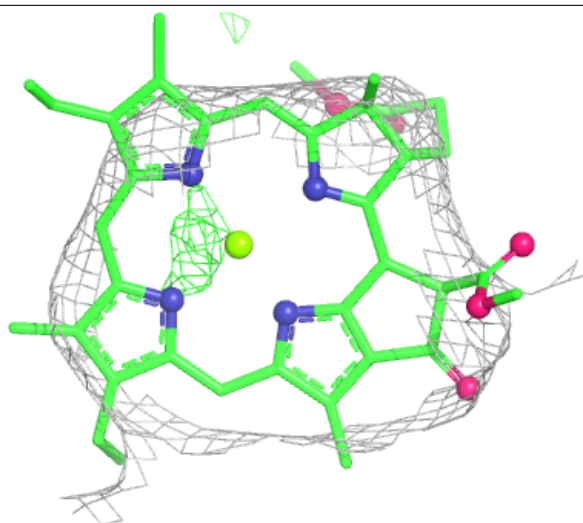
Electron density around CLA 1 1104:

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



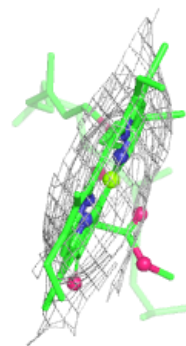
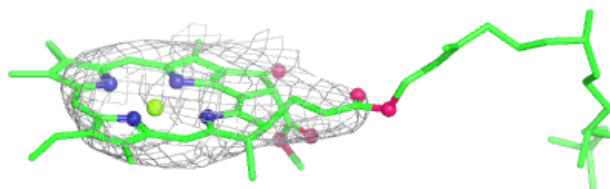
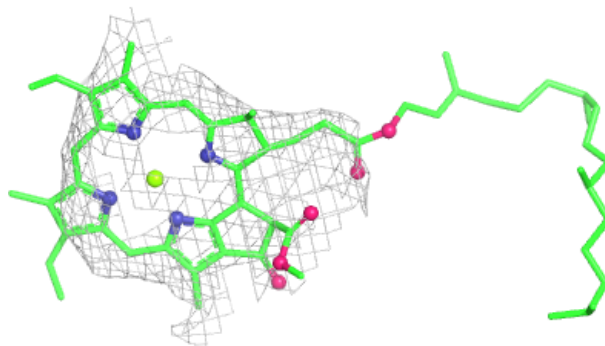
Electron density around CLA a 1120:

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

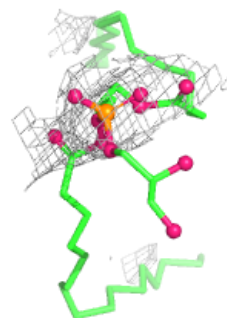
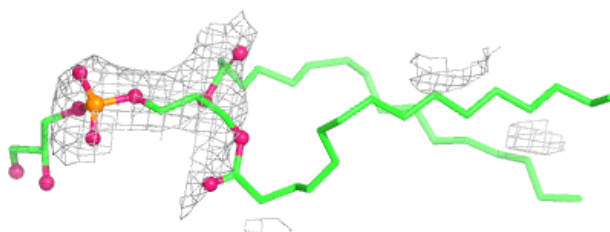
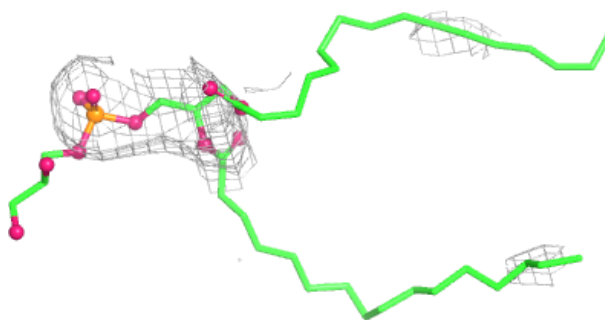


Electron density around CLA b 1223:

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

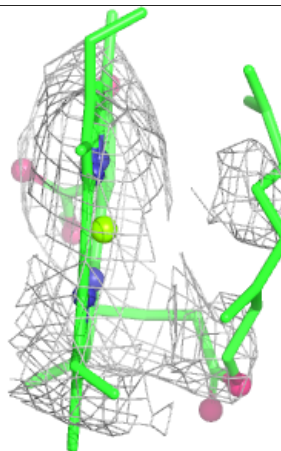
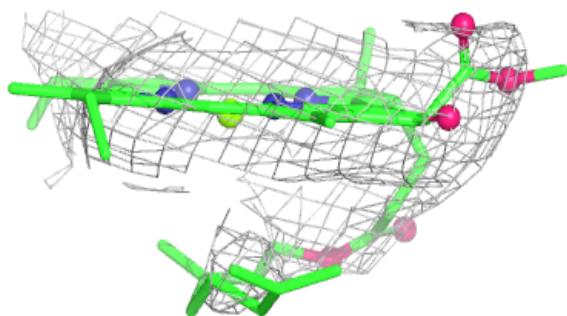
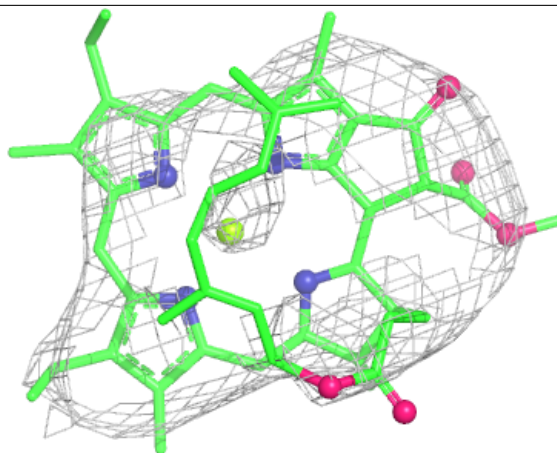
**Electron density around LHG 1 5001:**

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



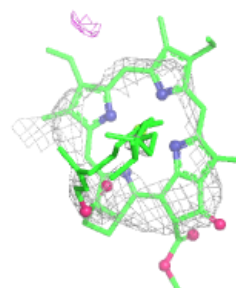
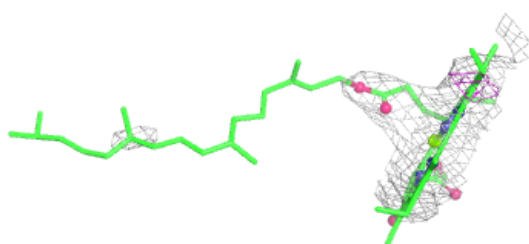
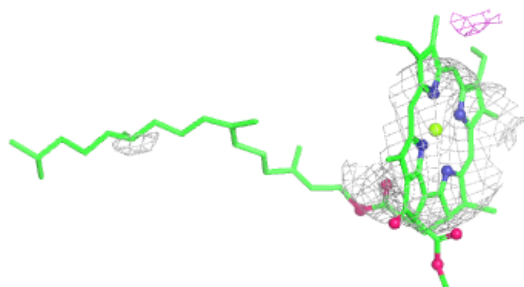
Electron density around CLA b 1224:

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

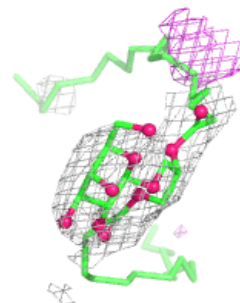
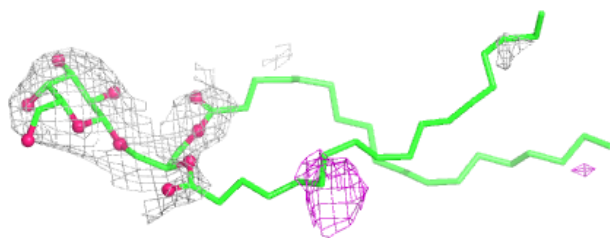
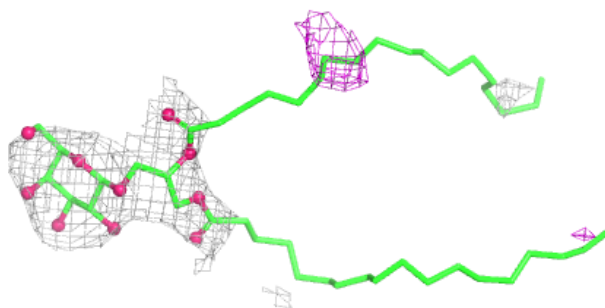


Electron density around CLA b 1225:

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

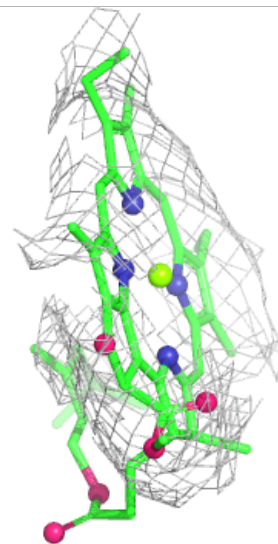
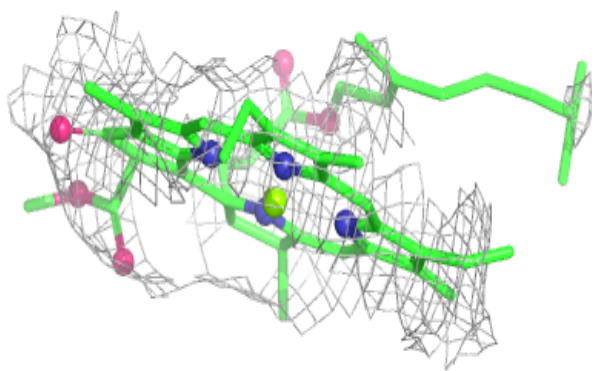
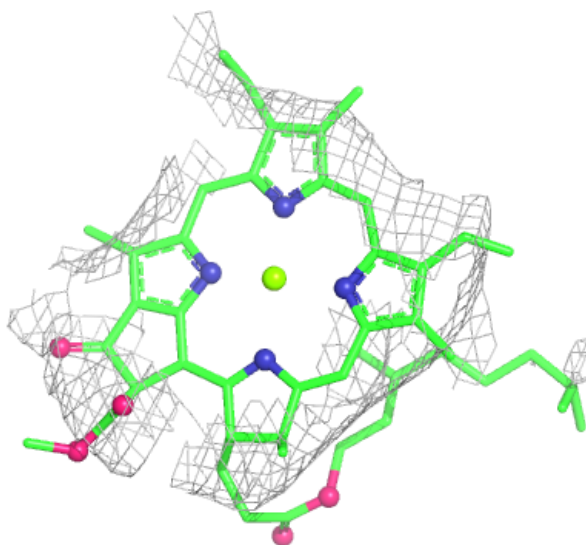
**Electron density around LMG B 5002:**

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



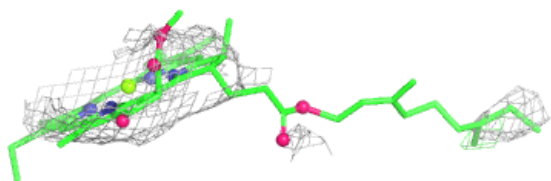
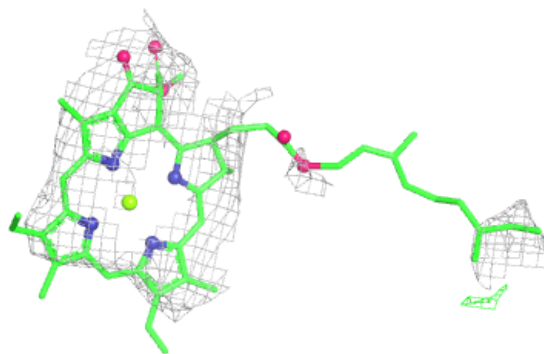
Electron density around CLA B 1219:

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

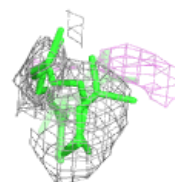
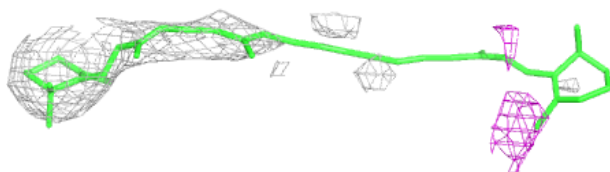
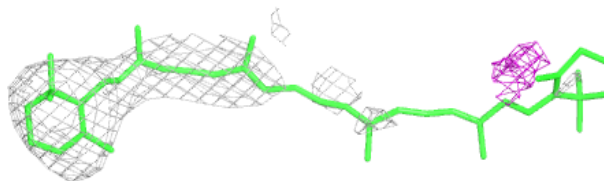


Electron density around CLA B 1222:

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

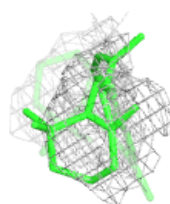
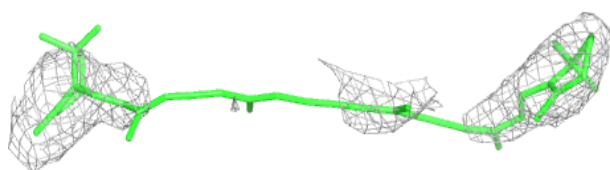
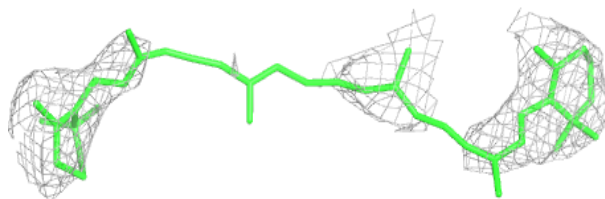
**Electron density around BCR 1 4022:**

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

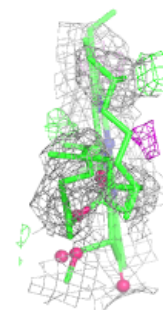
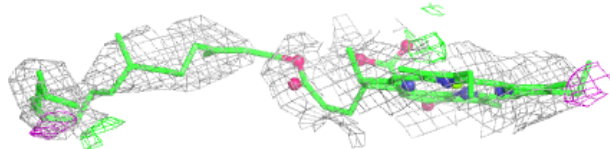
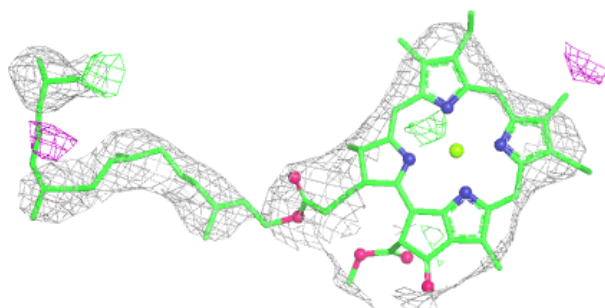


Electron density around BCR B 4006:

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

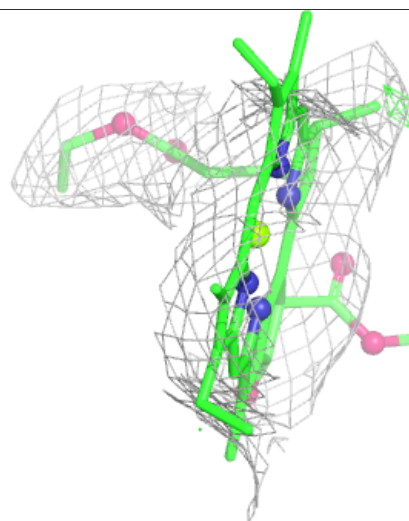
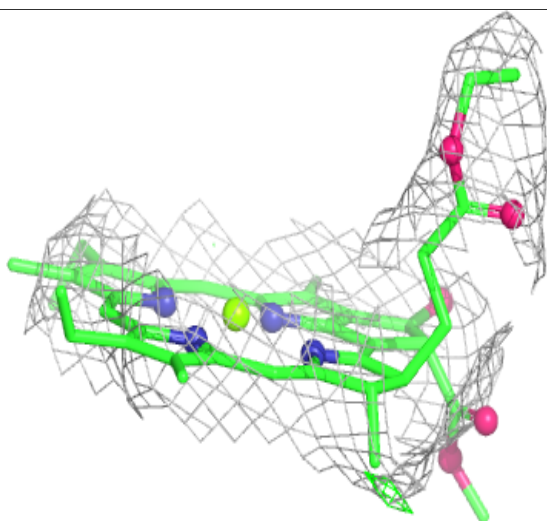
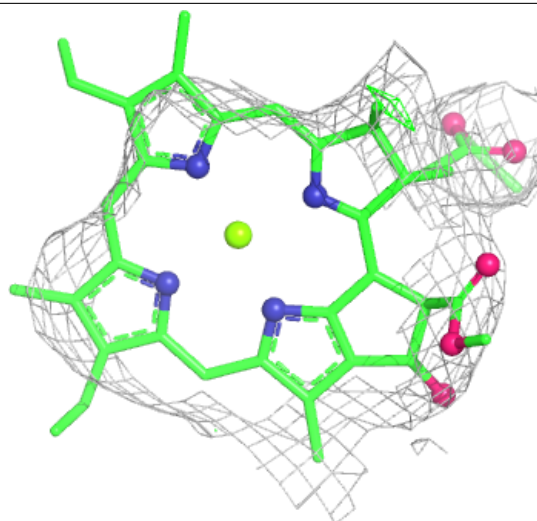
**Electron density around CLA A 1131:**

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



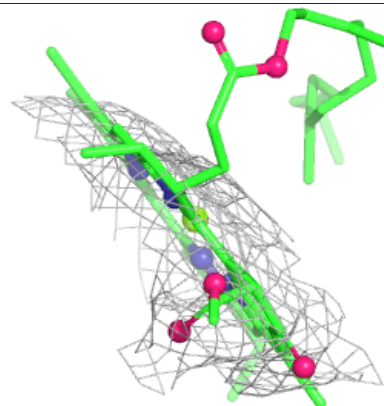
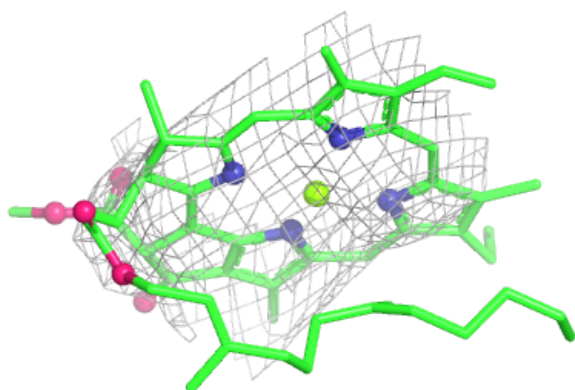
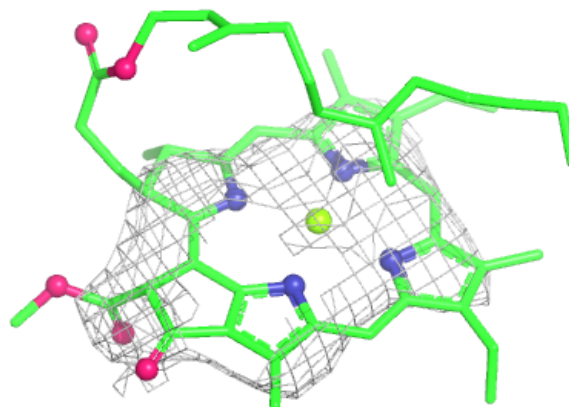
Electron density around CLA 2 1236:

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

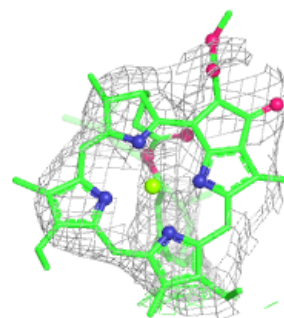
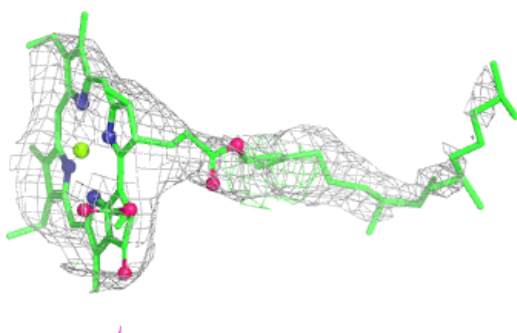
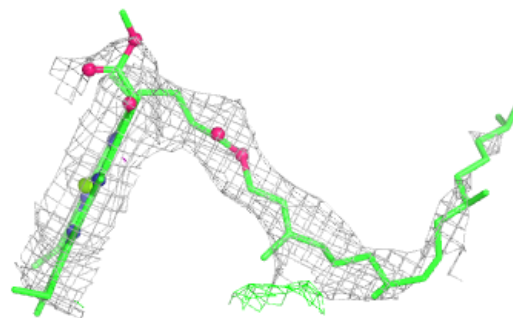


Electron density around CLA b 1214:

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

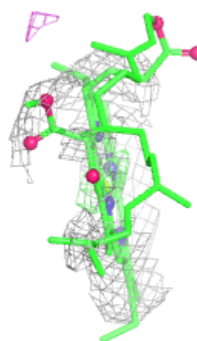
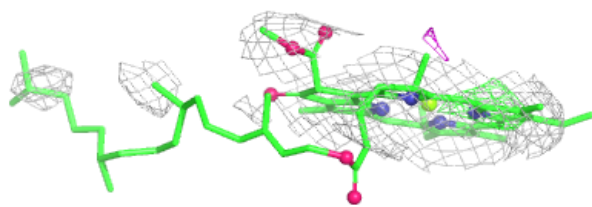
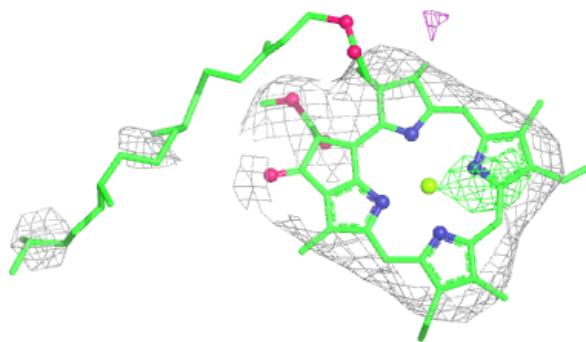
**Electron density around CLA 2 1238:**

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

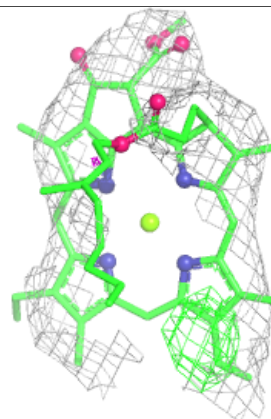
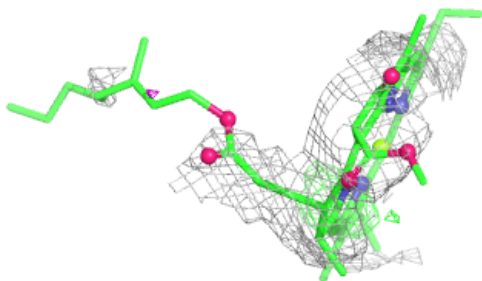
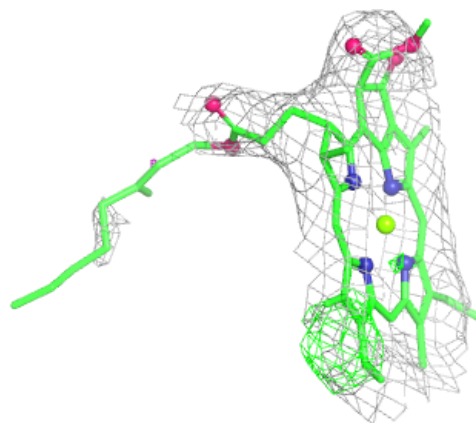


Electron density around CLA 8 1503:

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

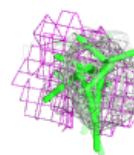
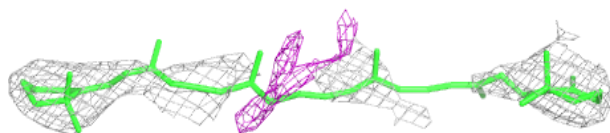
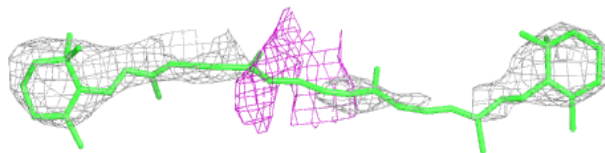
**Electron density around CLA 2 1201:**

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



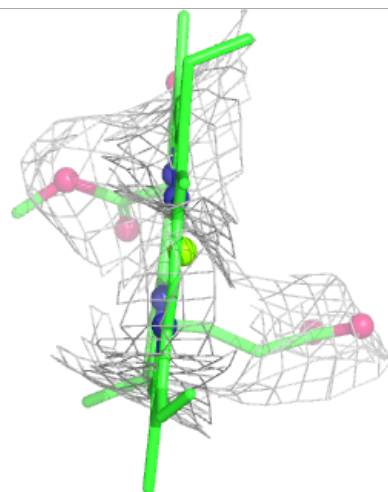
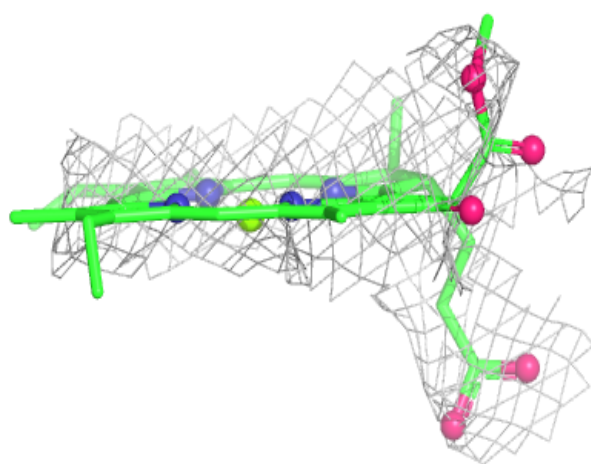
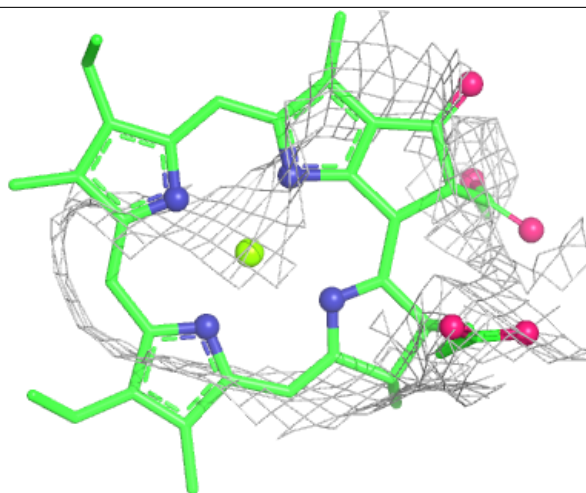
Electron density around BCR L 4019:

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



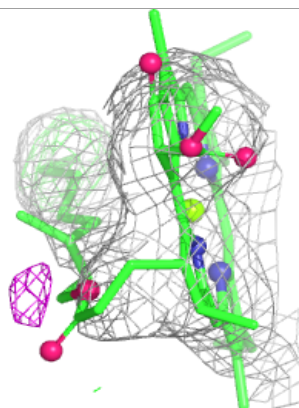
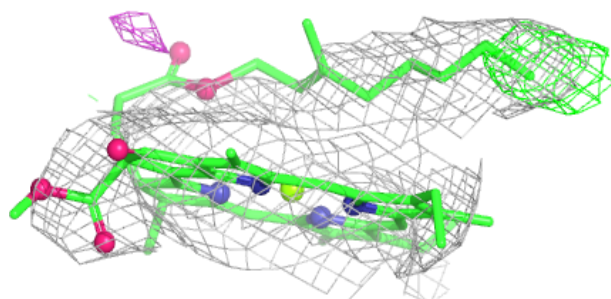
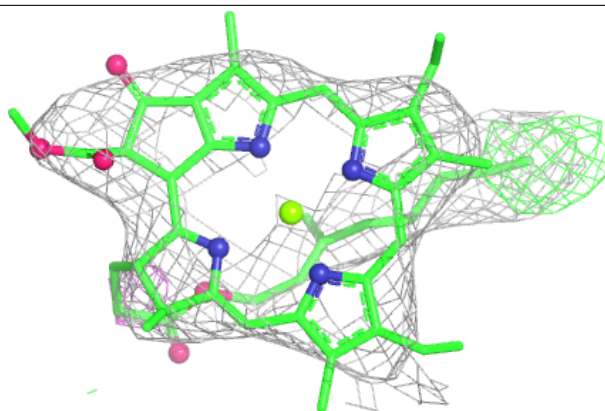
Electron density around CLA a 1112:

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

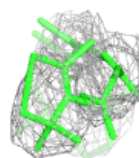
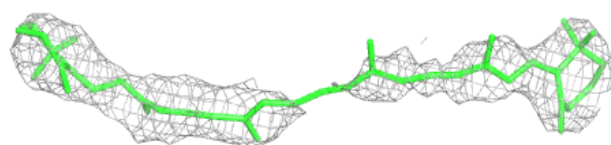
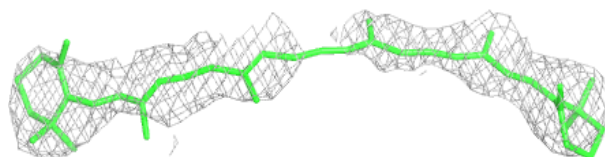


Electron density around CLA A 1116:

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

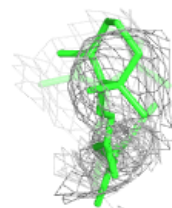
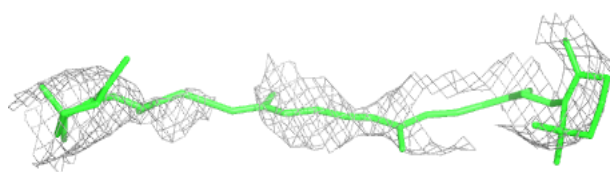
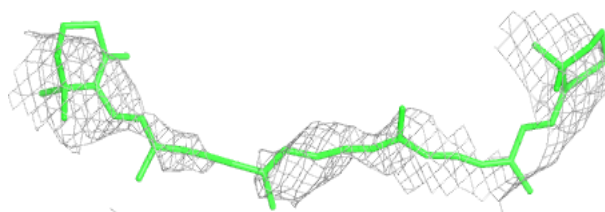
**Electron density around BCR 6 4018:**

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

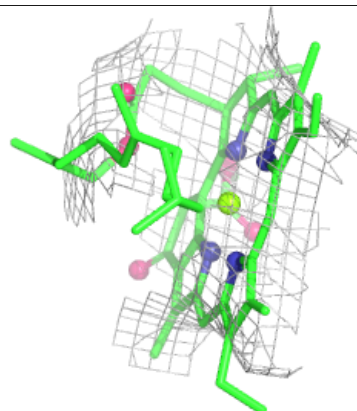
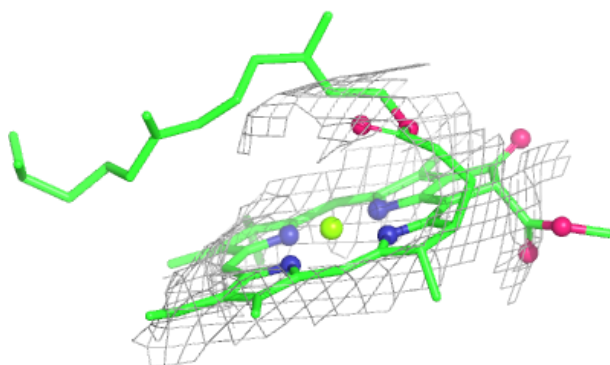
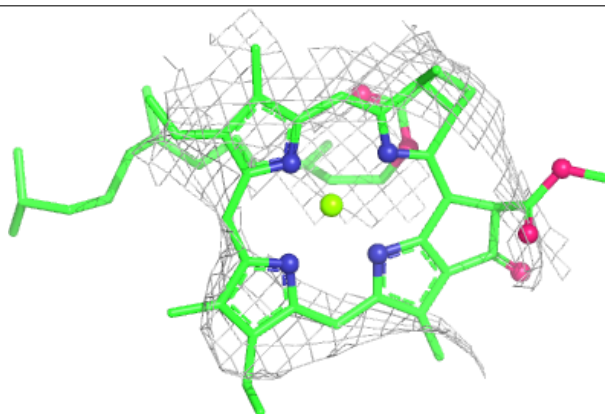


Electron density around BCR 6 4020:

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

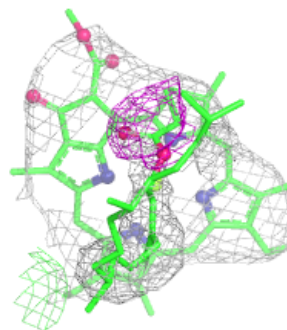
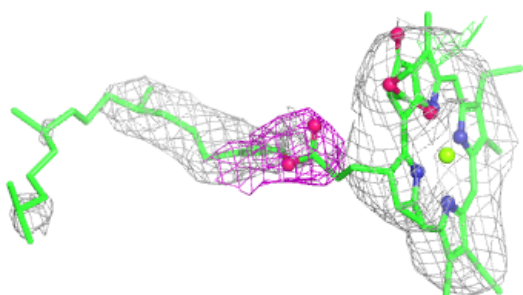
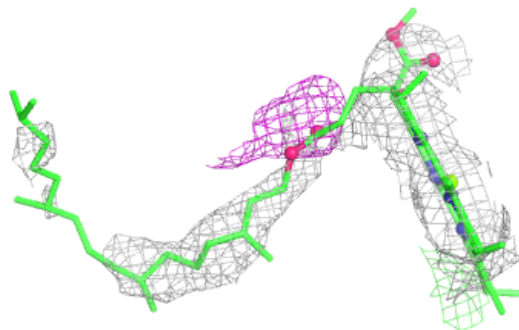
**Electron density around CLA b 1235:**

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



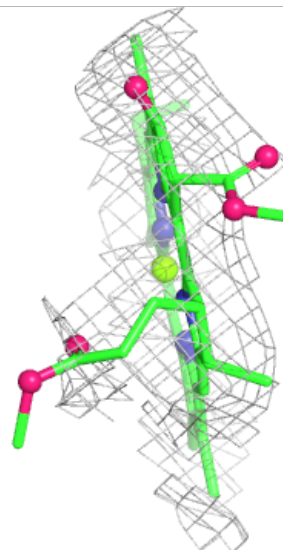
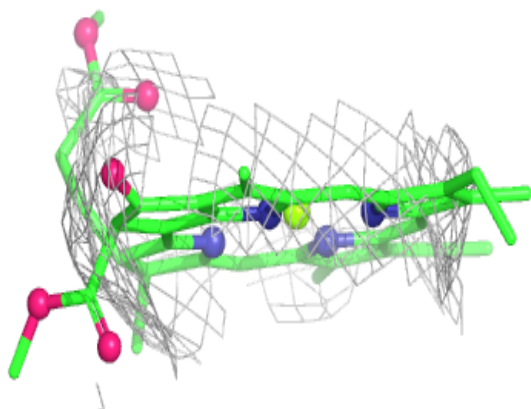
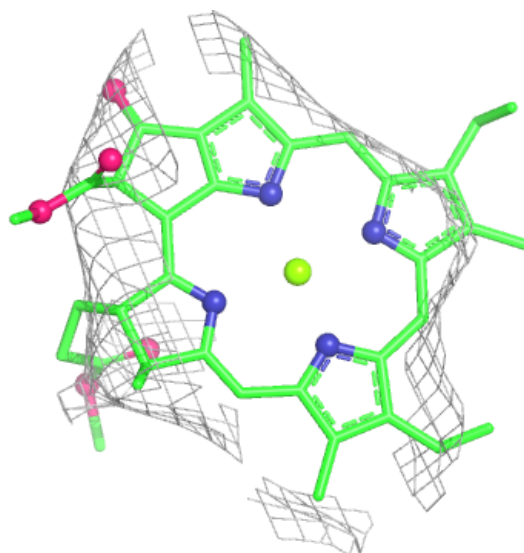
Electron density around CLA B 1238:

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



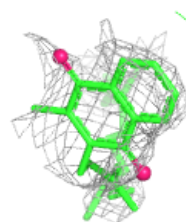
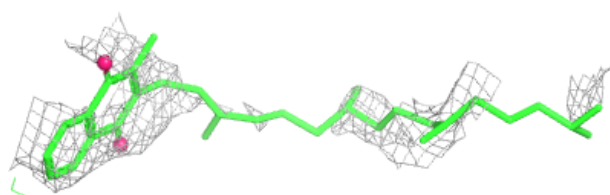
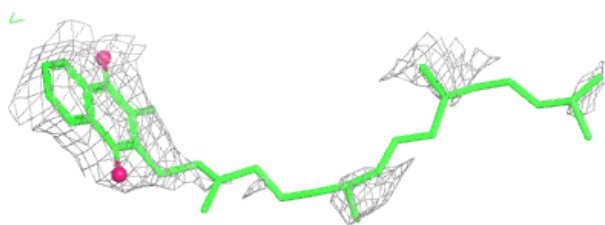
Electron density around CLA a 1134:

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



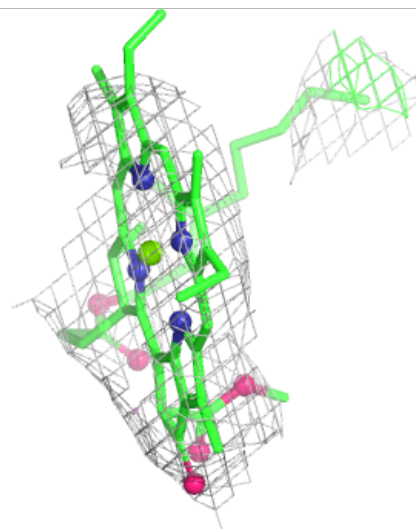
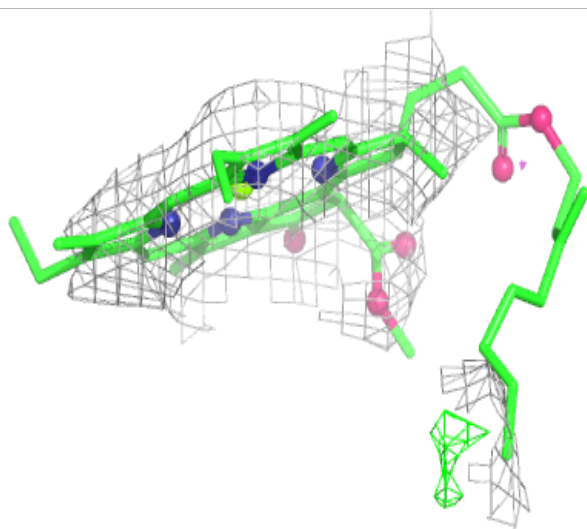
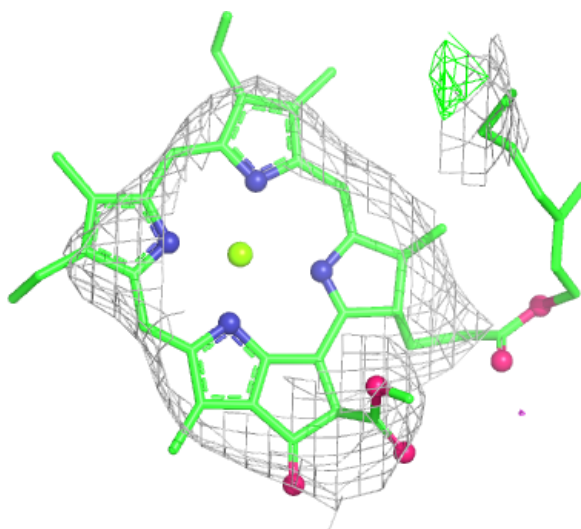
Electron density around PQN A 2001:

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



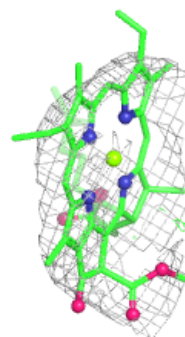
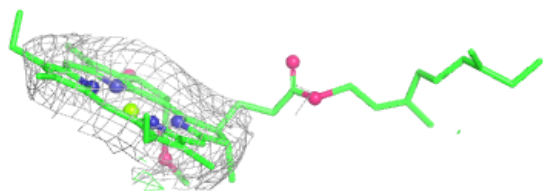
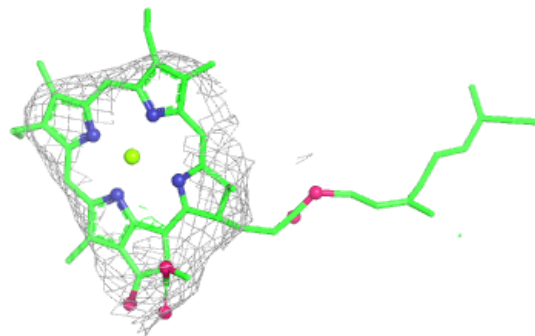
Electron density around CLA 2 1221:

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

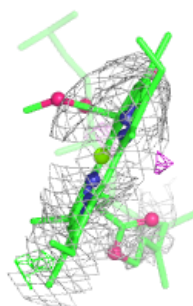
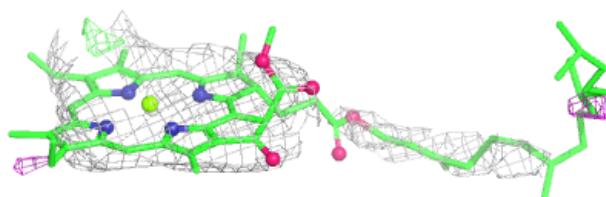
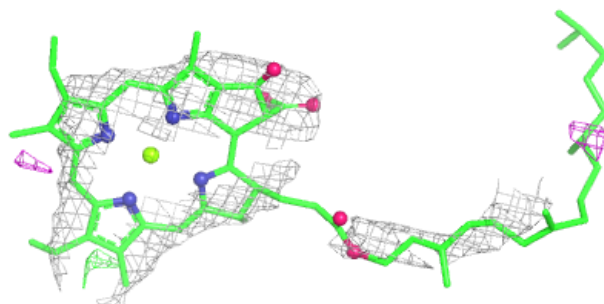


Electron density around CLA 2 1222:

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

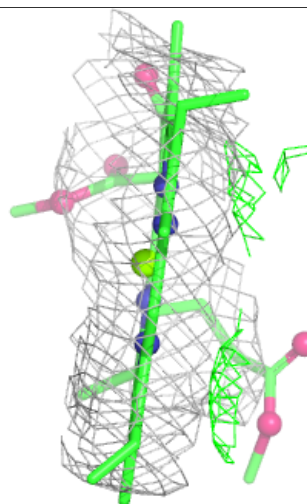
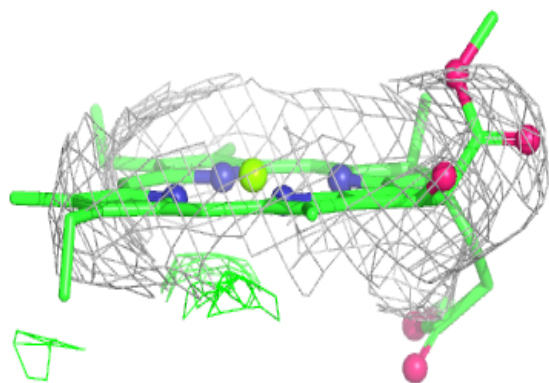
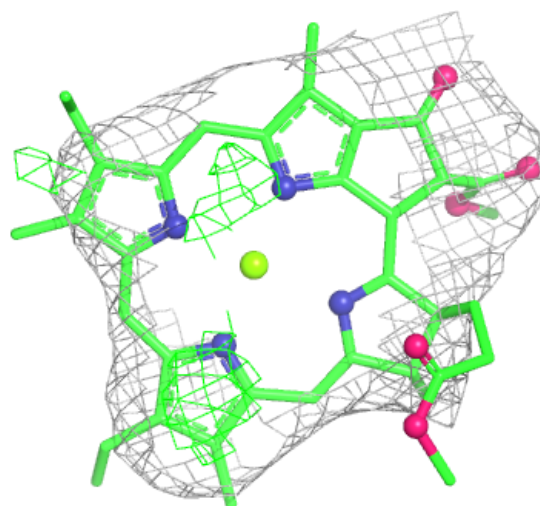
**Electron density around CLA 2 1223:**

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



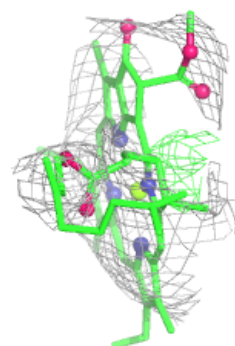
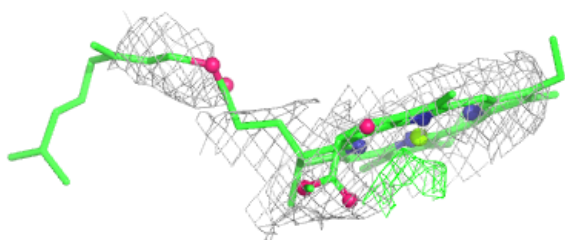
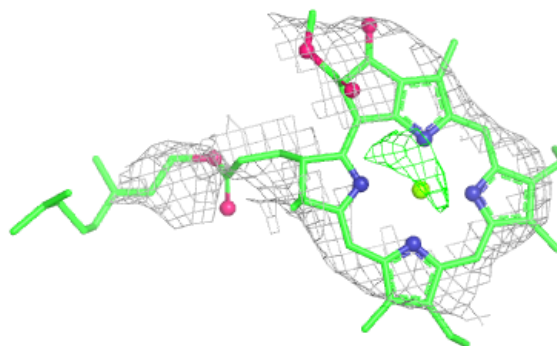
Electron density around CLA A 1120:

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

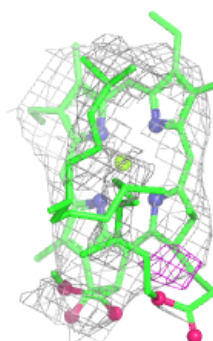
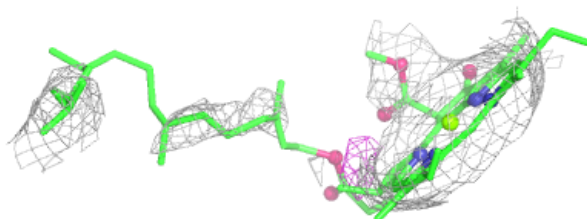
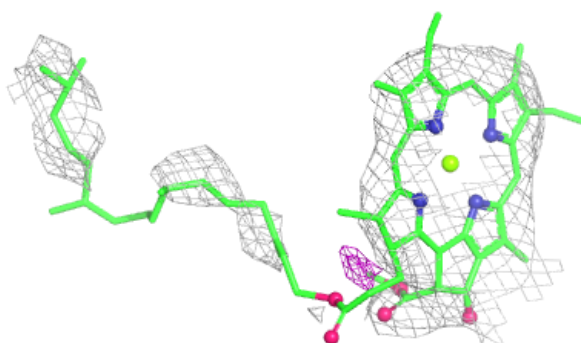


Electron density around CLA a 1124:

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

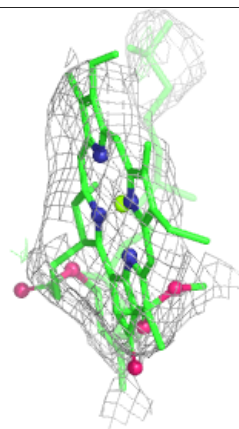
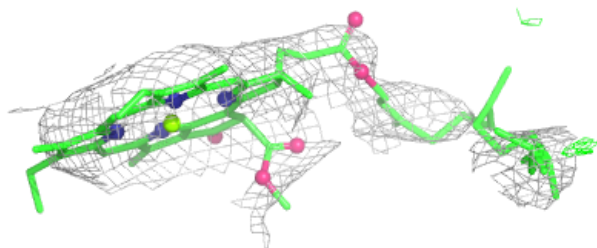
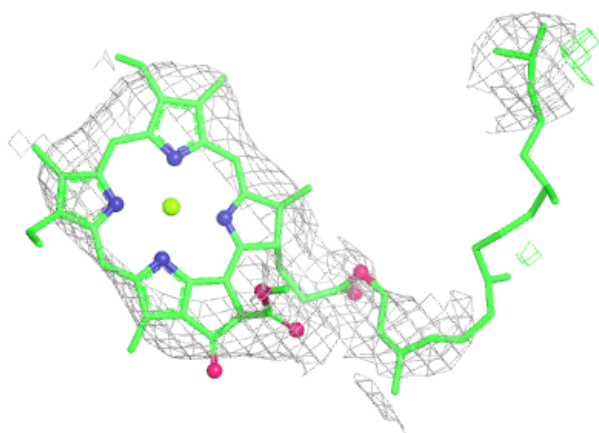
**Electron density around CLA b 1207:**

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



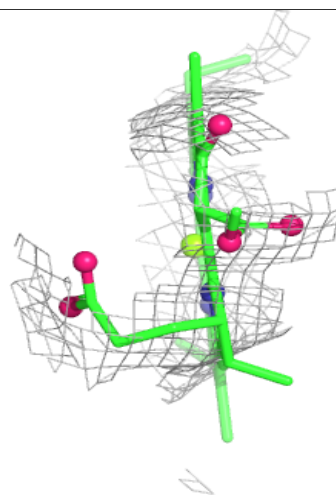
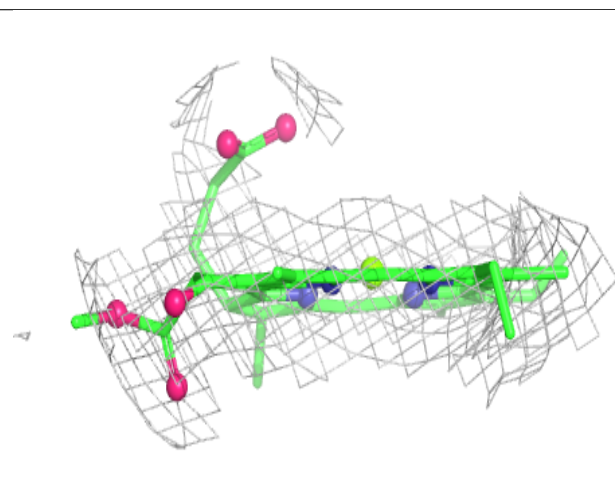
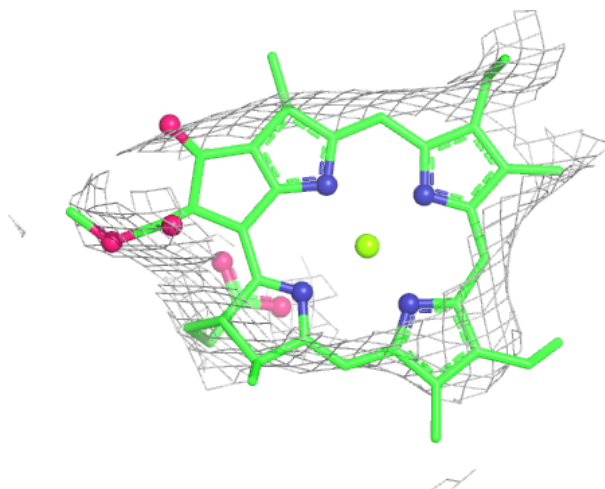
Electron density around CLA A 1101:

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



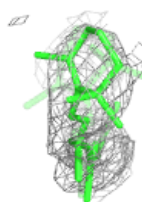
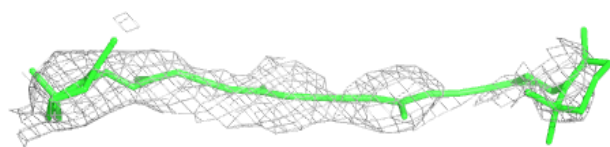
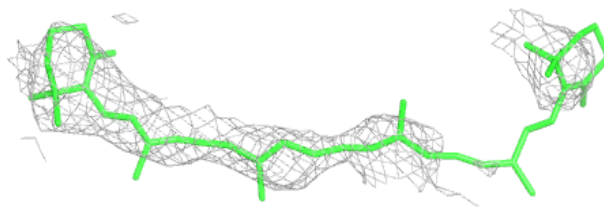
Electron density around CLA a 1108:

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

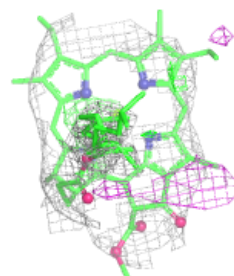
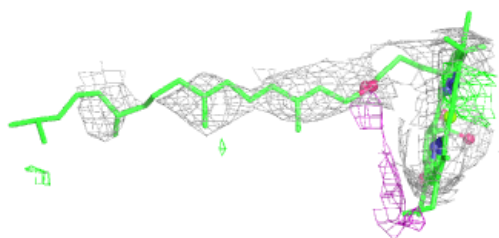
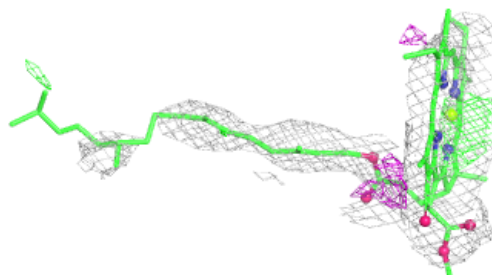


Electron density around BCR f 4020:

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

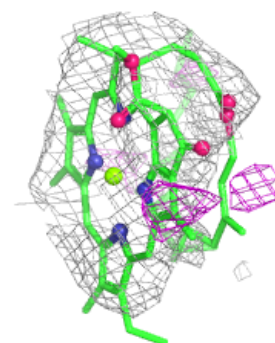
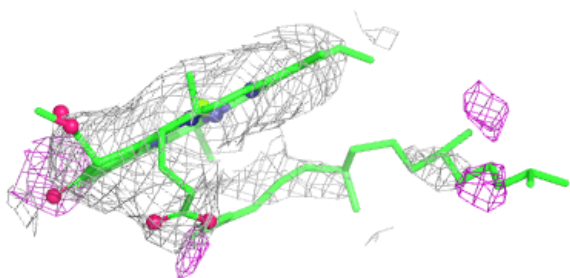
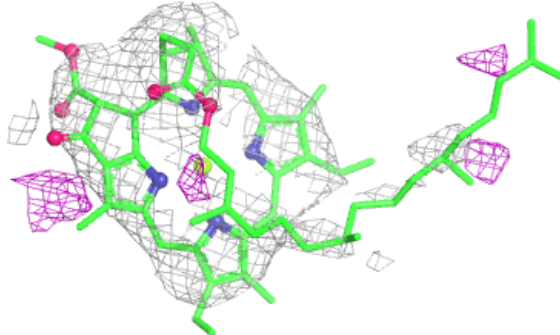
**Electron density around CLA A 1126:**

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

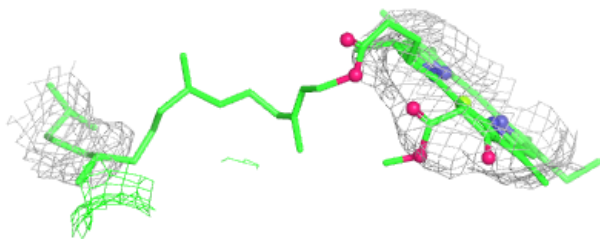
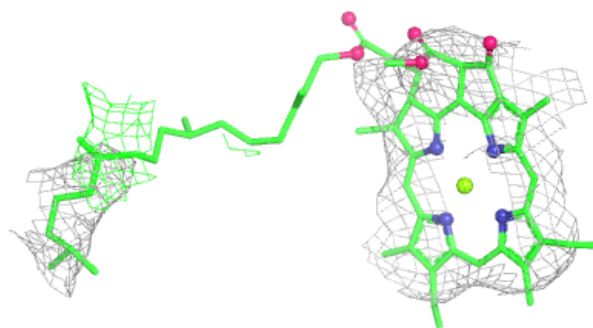


Electron density around CLA 2 1204:

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

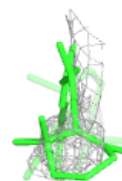
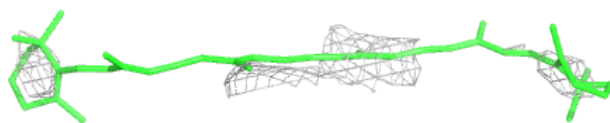
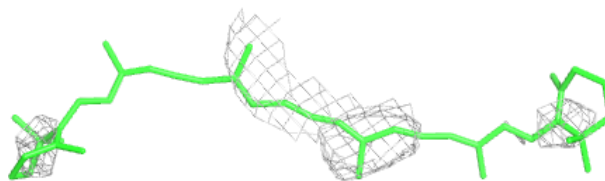
**Electron density around CLA 2 1207:**

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



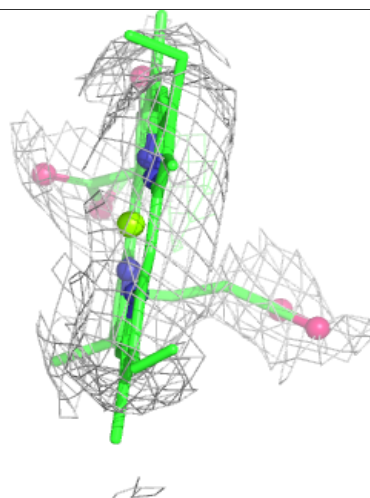
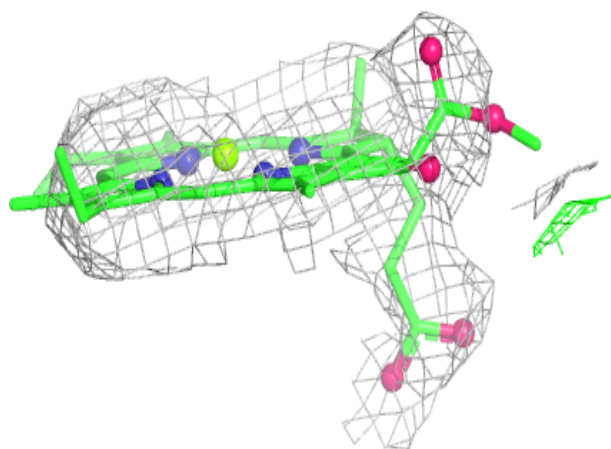
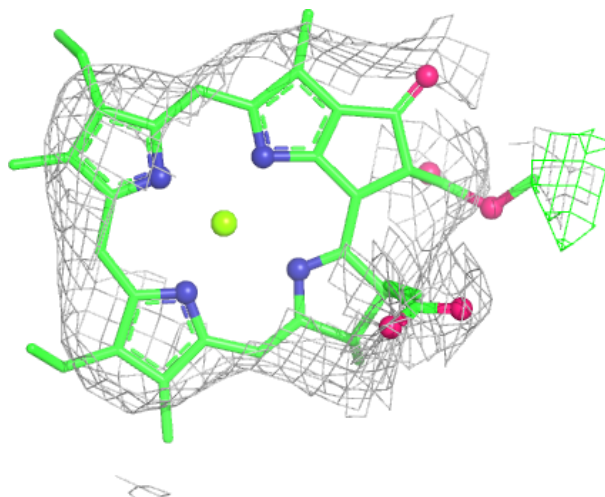
Electron density around BCR b 4017:

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



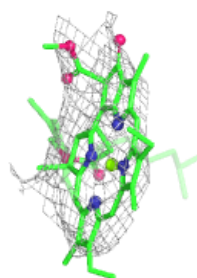
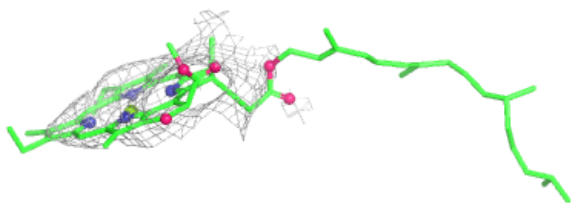
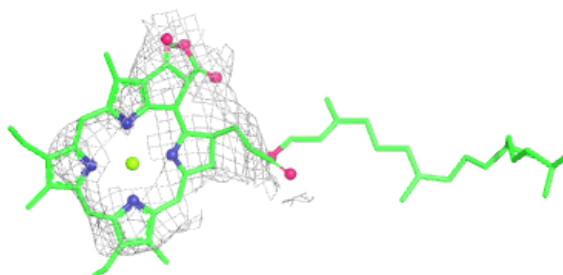
Electron density around CLA 2 1208:

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

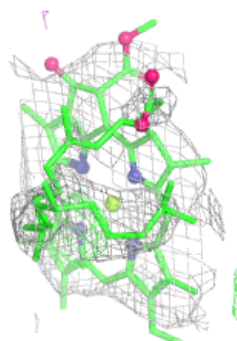
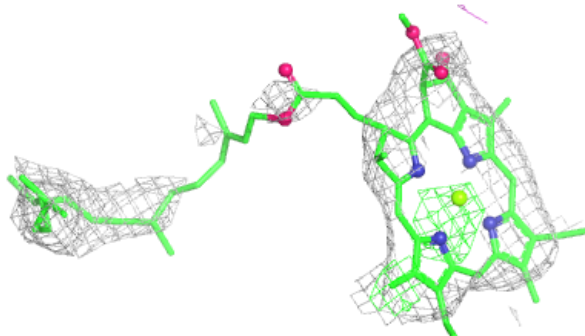


Electron density around CLA 1 1103:

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

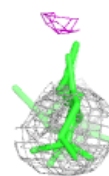
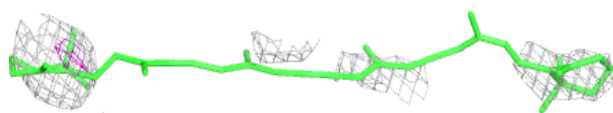
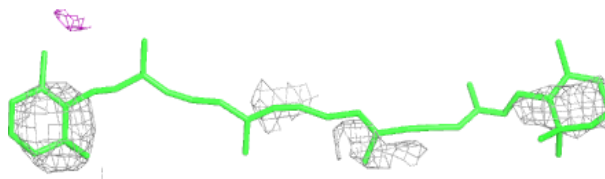
**Electron density around CLA B 1206:**

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

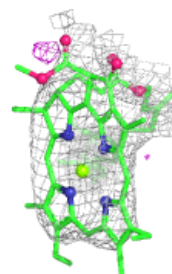
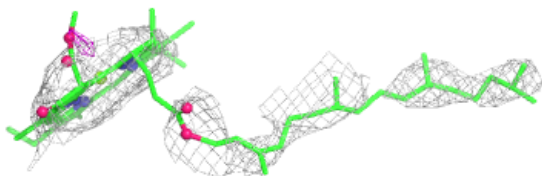
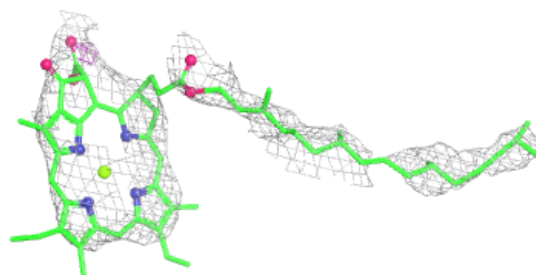


Electron density around BCR 1 4019:

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

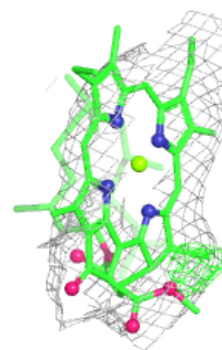
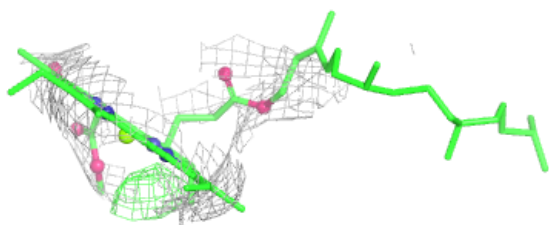
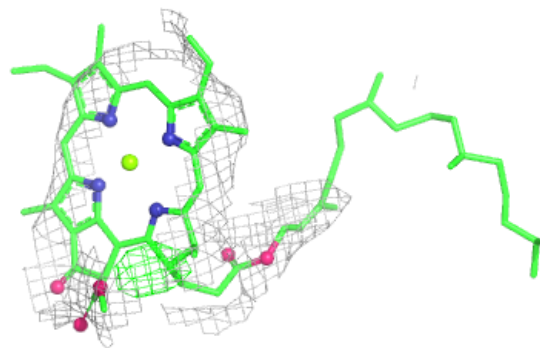
**Electron density around CLA a 1132:**

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

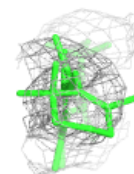
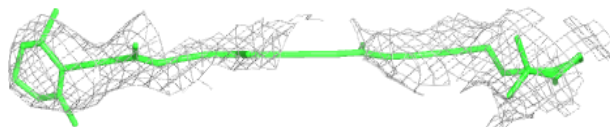
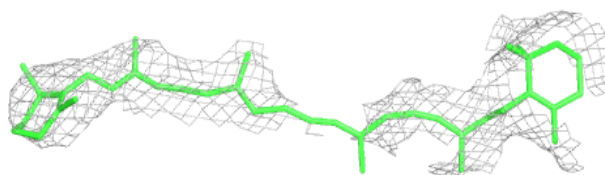


Electron density around CLA 1 1106:

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

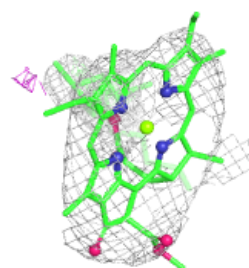
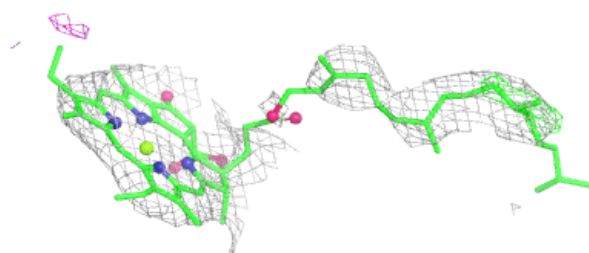
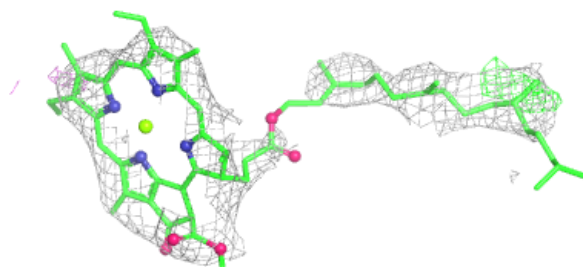
**Electron density around BCR A 4007:**

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



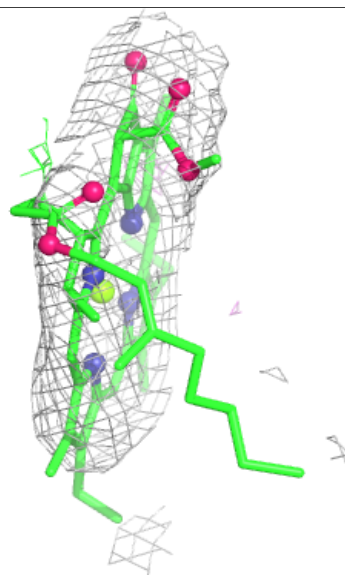
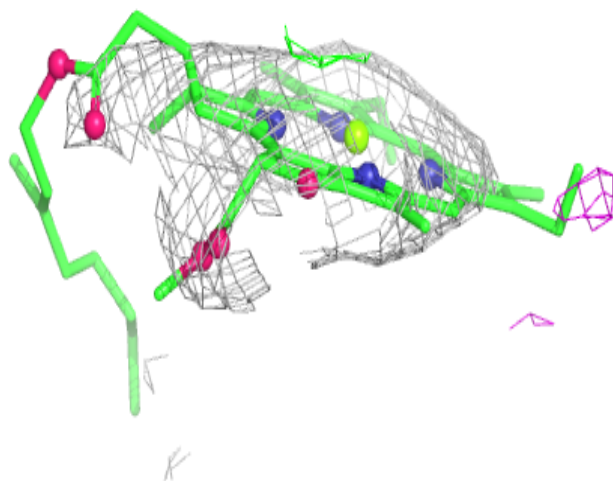
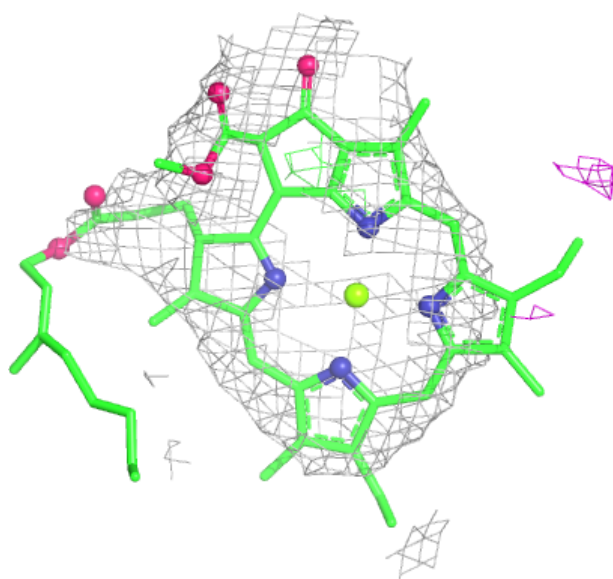
Electron density around CLA A 1119:

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



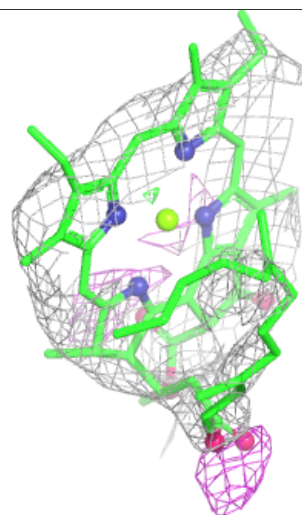
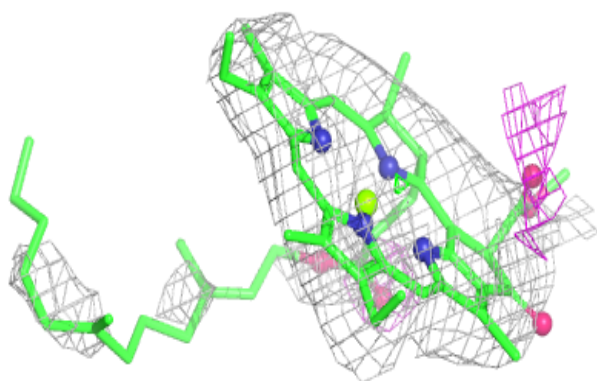
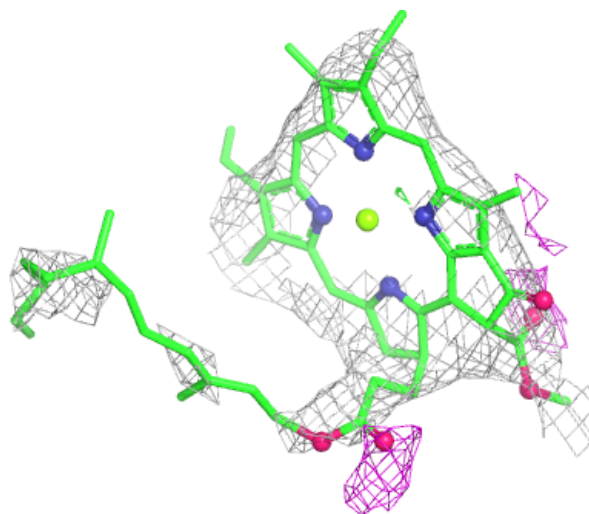
Electron density around CLA B 1221:

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



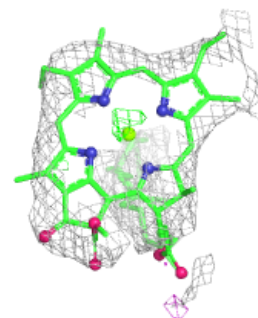
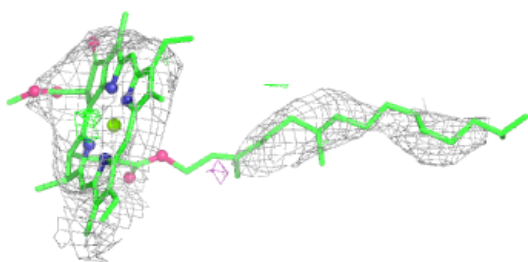
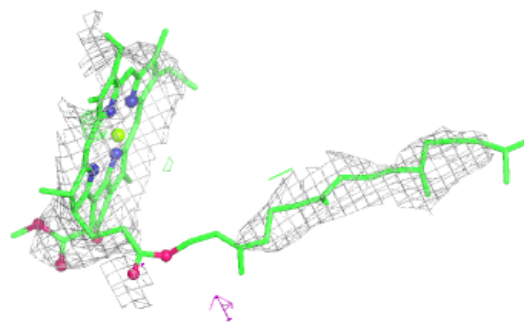
Electron density around CLA A 1122:

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



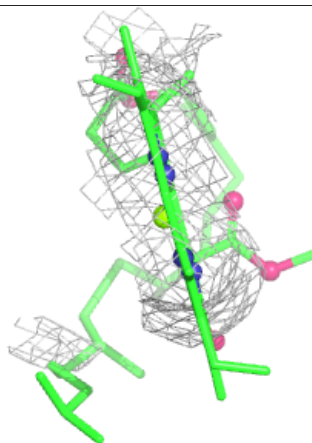
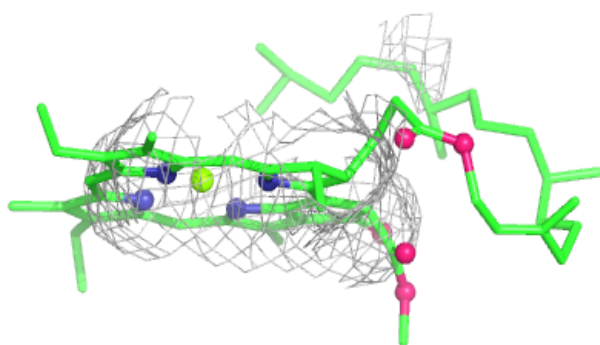
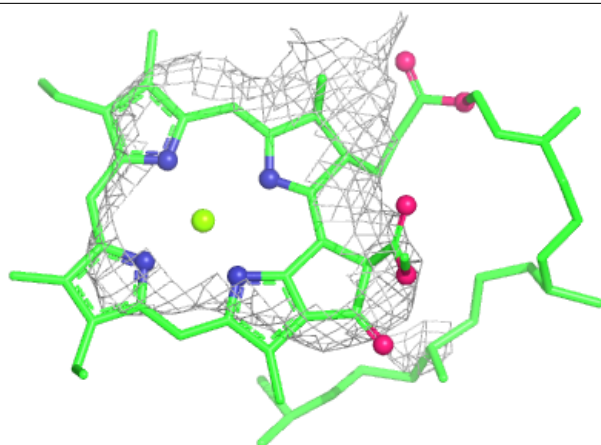
Electron density around CLA 2 1226:

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

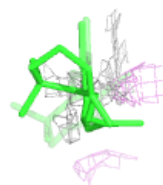
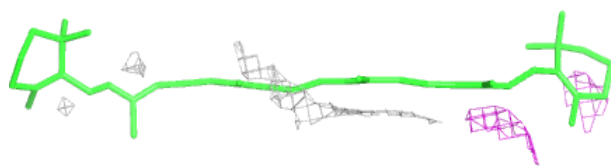
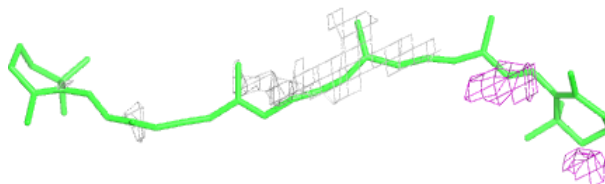


Electron density around CLA b 1202:

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

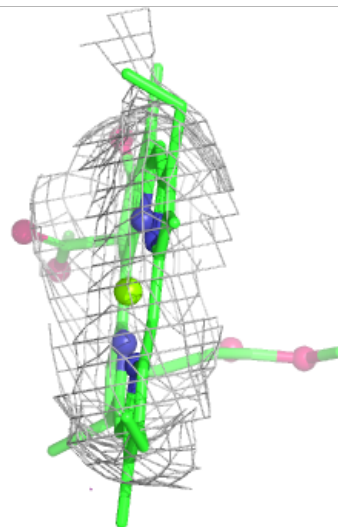
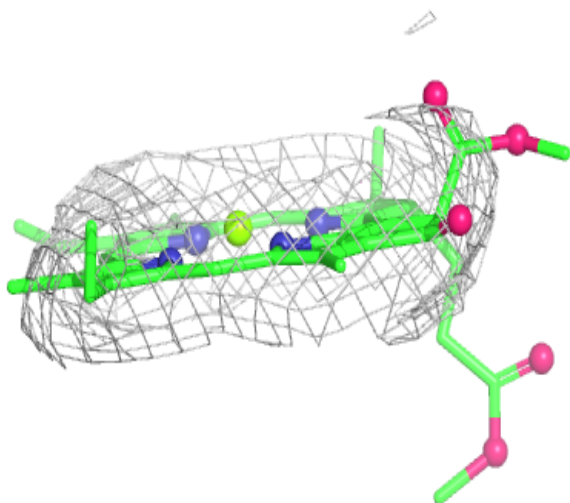
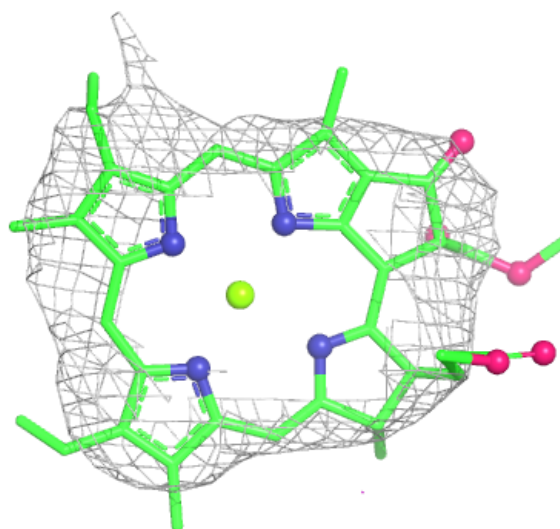
**Electron density around BCR 2 4009:**

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



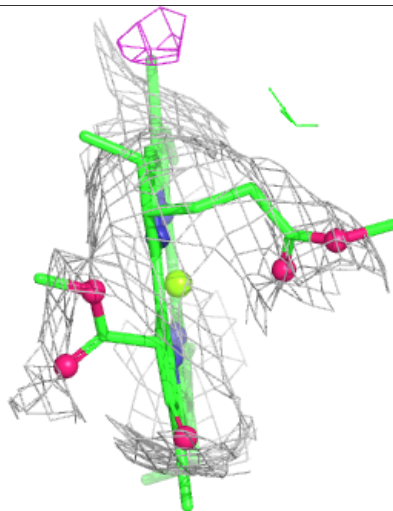
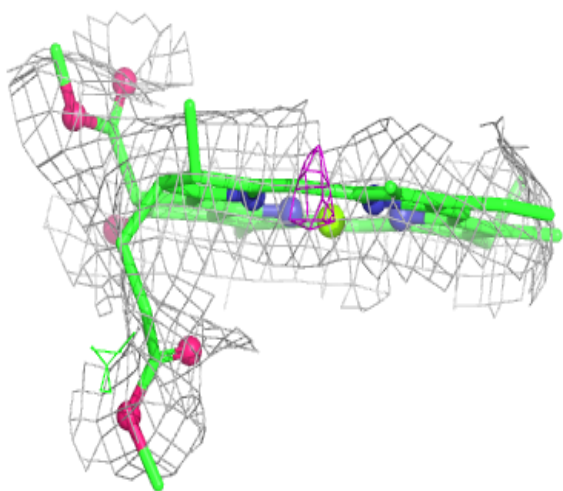
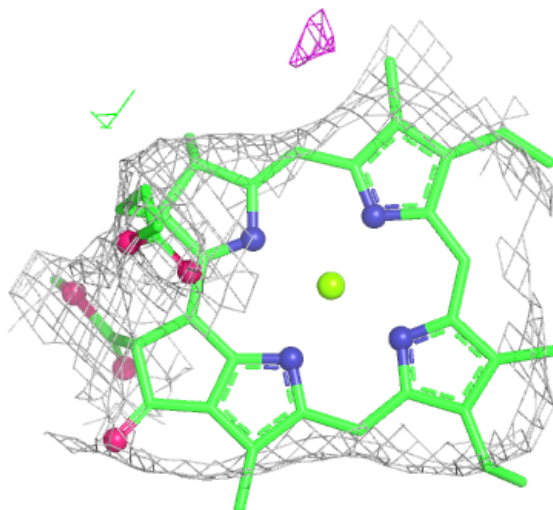
Electron density around CLA A 1121:

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



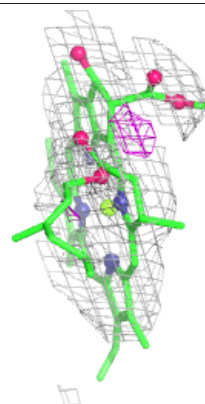
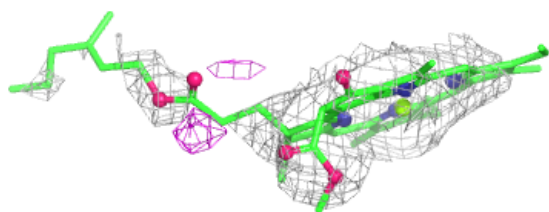
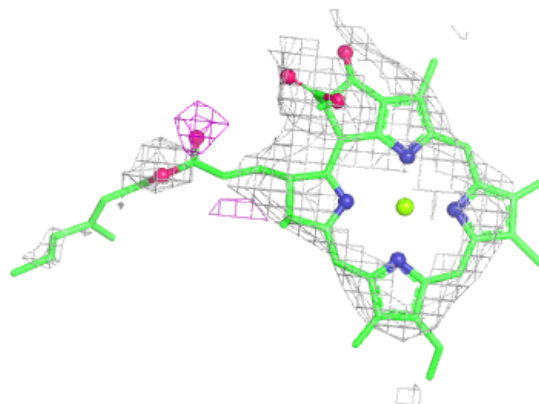
Electron density around CLA A 1134:

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

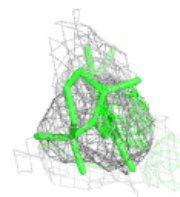
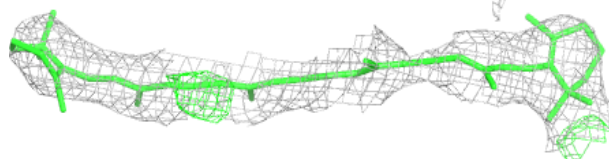
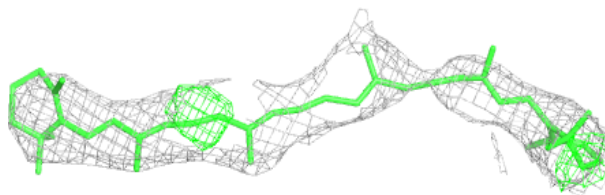


Electron density around CLA A 1125:

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

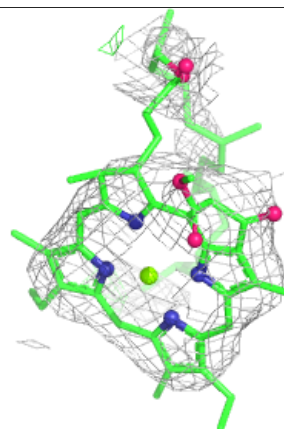
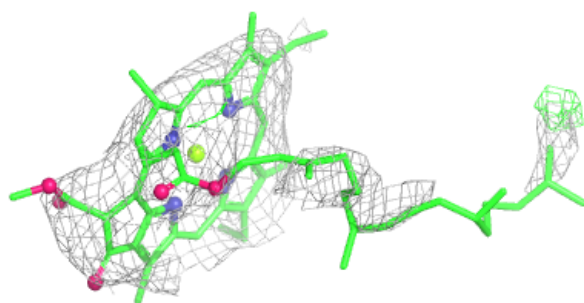
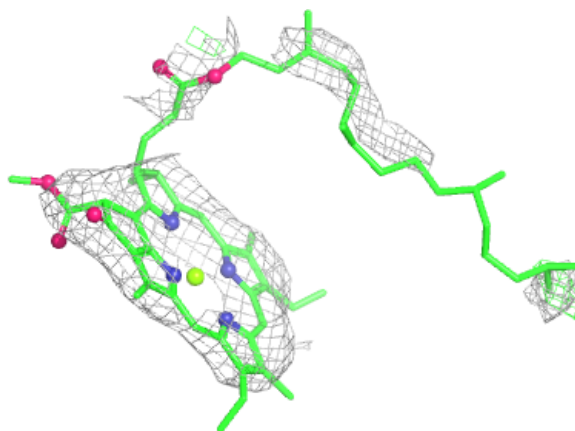
**Electron density around BCR B 4017:**

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

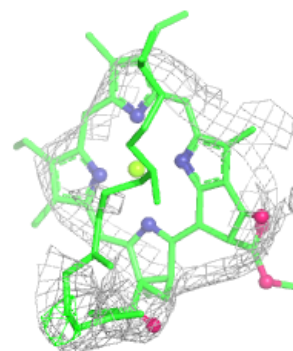
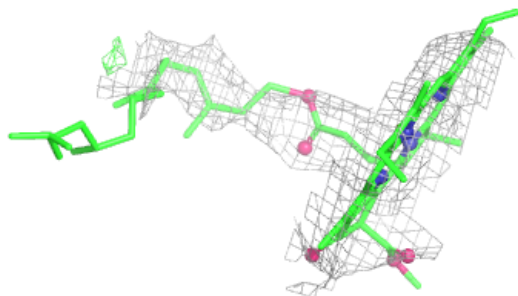
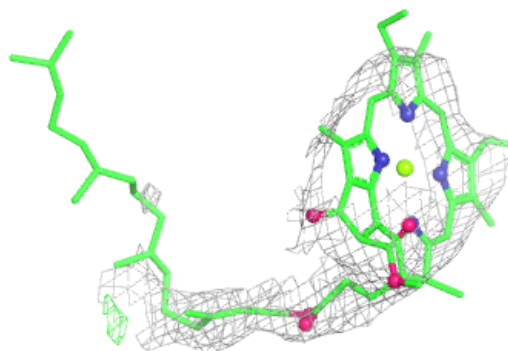


Electron density around CLA A 1102:

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

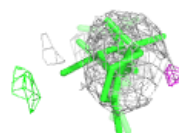
**Electron density around CLA a 1137:**

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



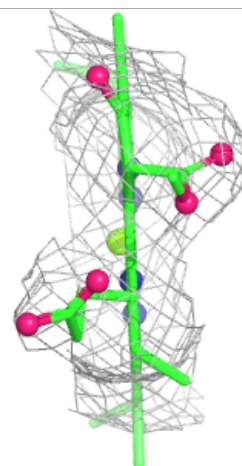
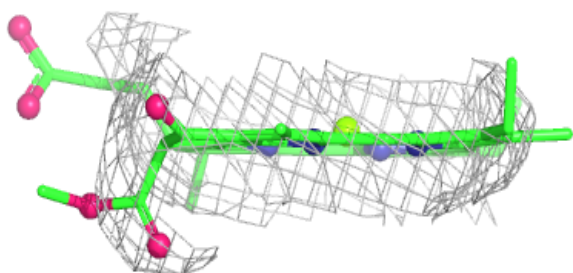
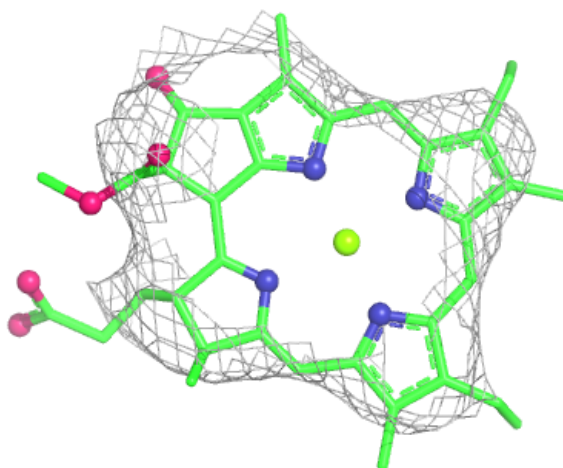
Electron density around BCR 8 4019:

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



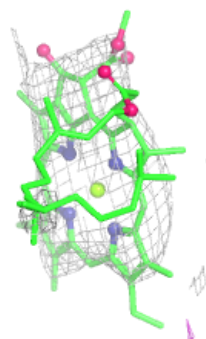
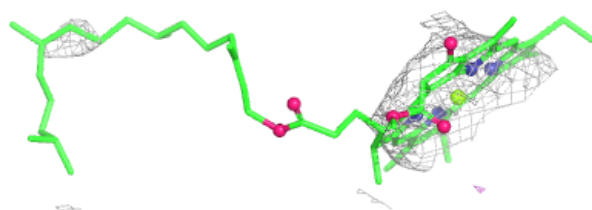
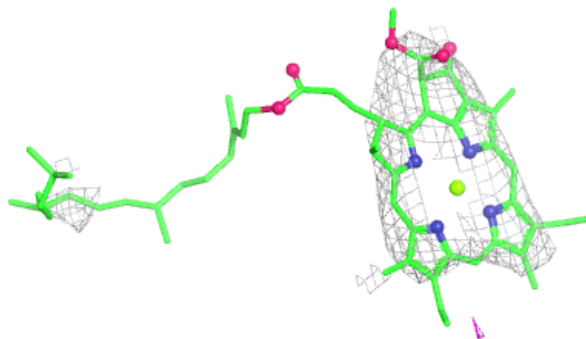
Electron density around CLA A 1113:

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

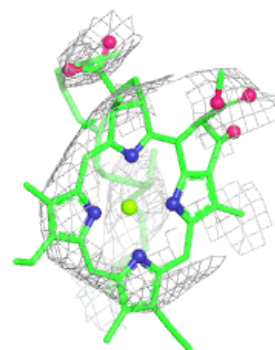
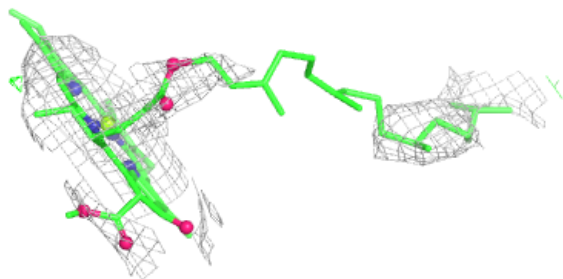
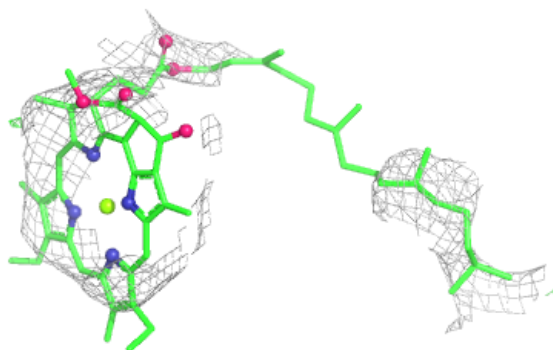


Electron density around CLA b 1206:

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

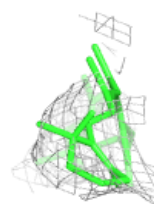
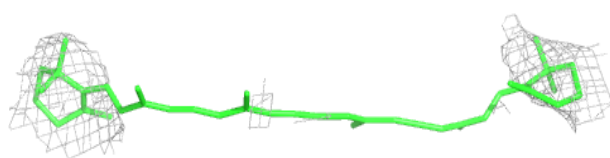
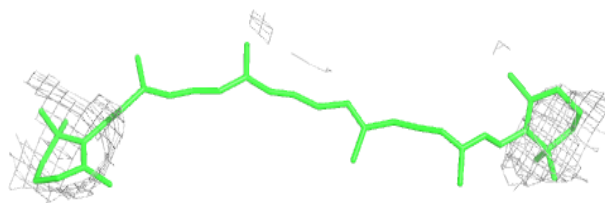
**Electron density around CLA 1 1137:**

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



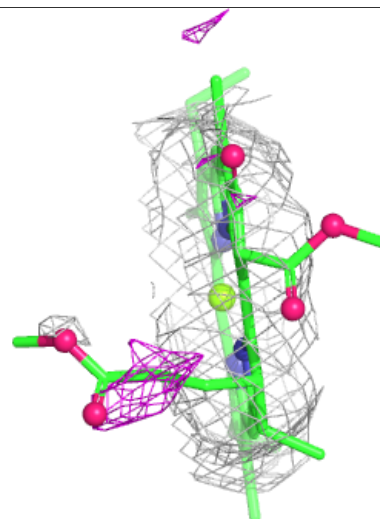
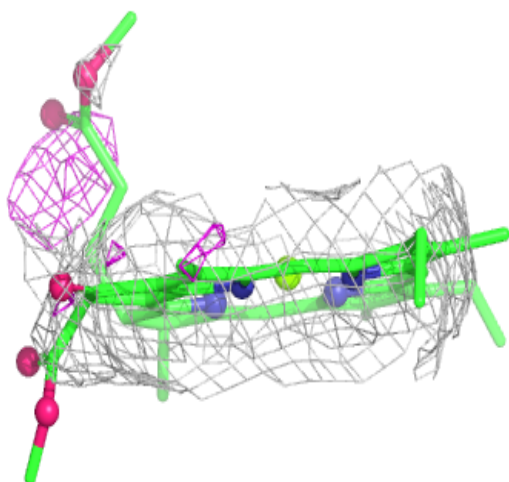
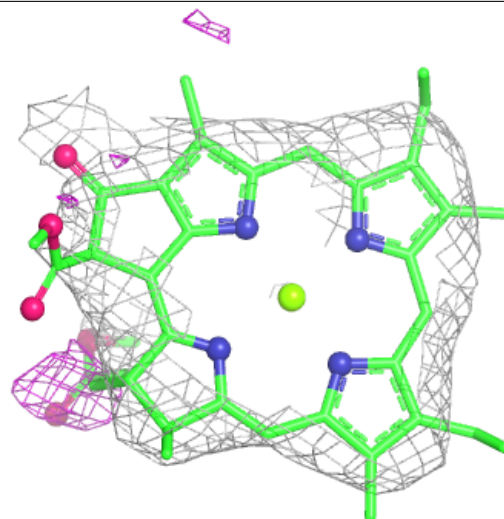
Electron density around BCR a 4001:

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



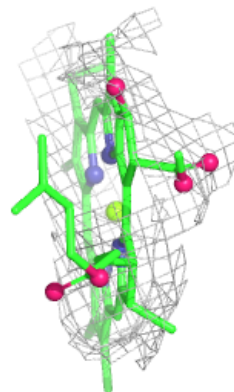
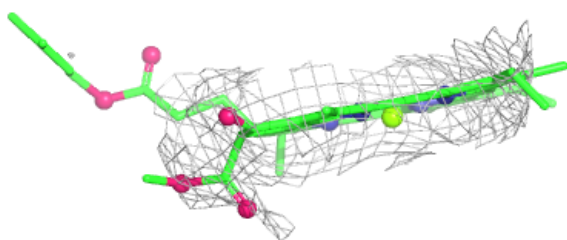
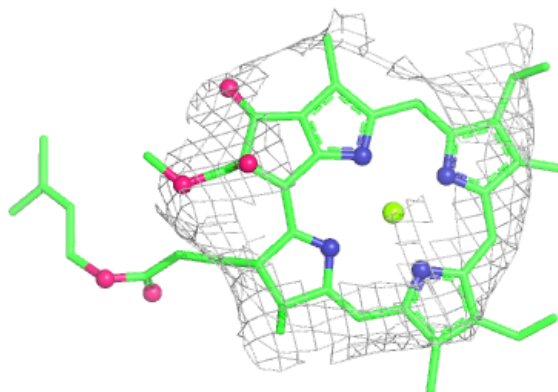
Electron density around CLA 2 1211:

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

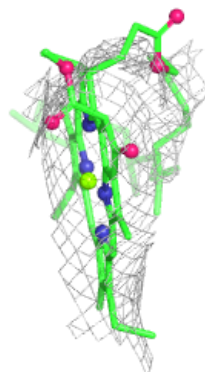
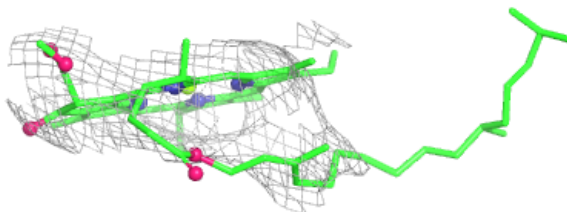
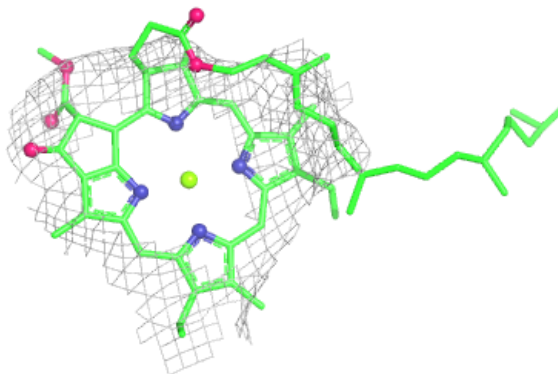


Electron density around CLA 1 1139:

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

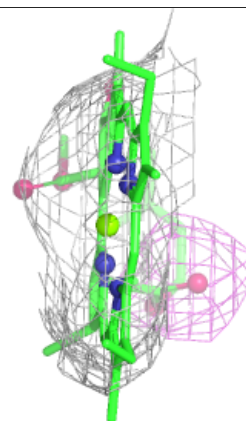
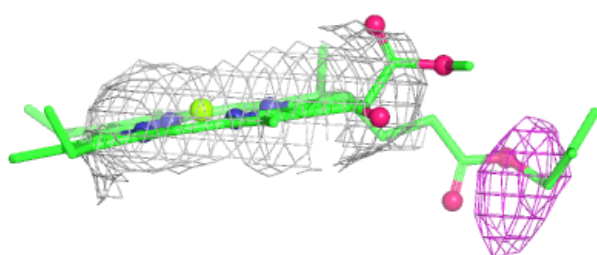
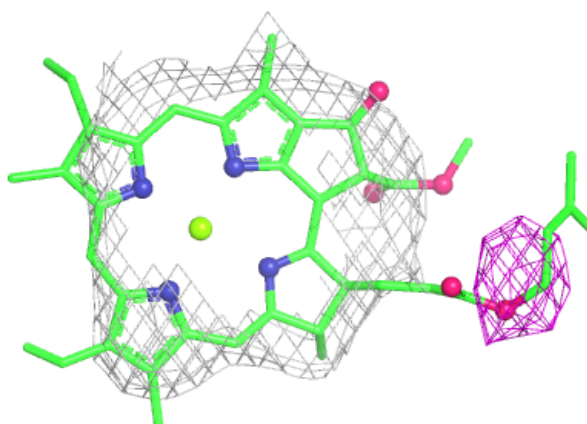
**Electron density around CLA b 1215:**

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

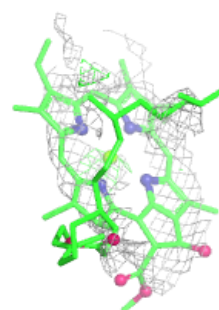
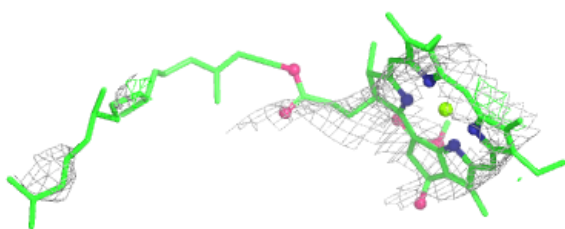
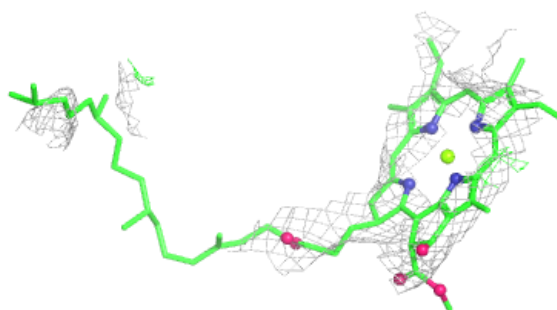


Electron density around CLA A 1139:

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

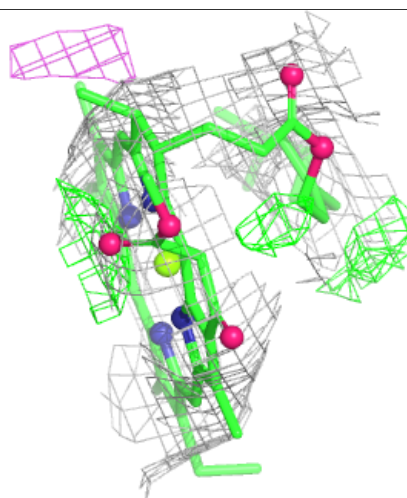
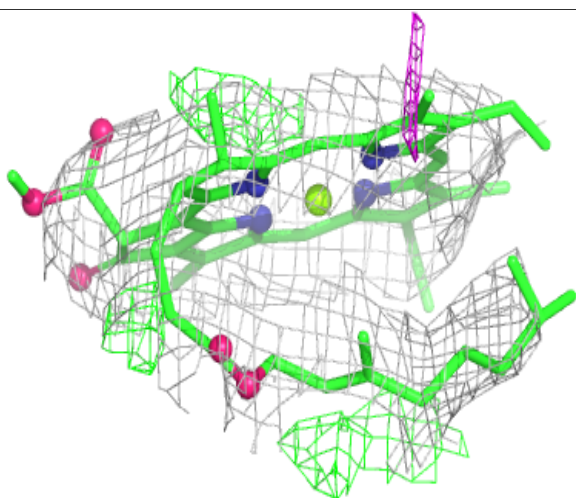
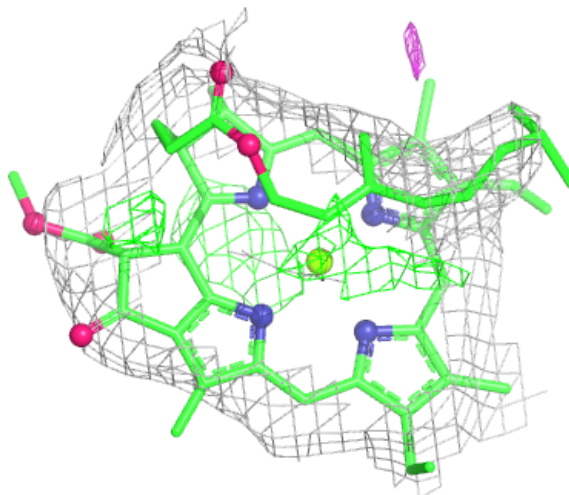
**Electron density around CLA a 1012:**

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



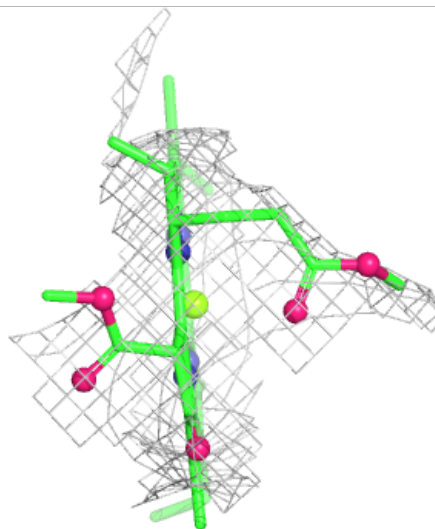
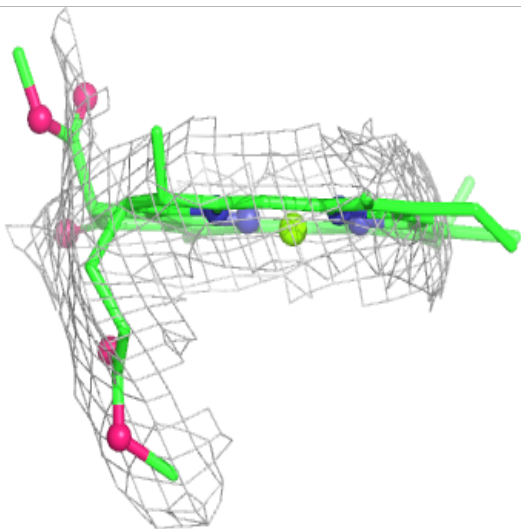
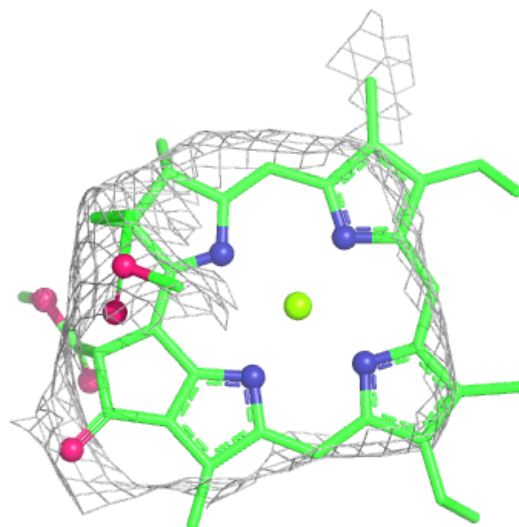
Electron density around CLA 1 1237:

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



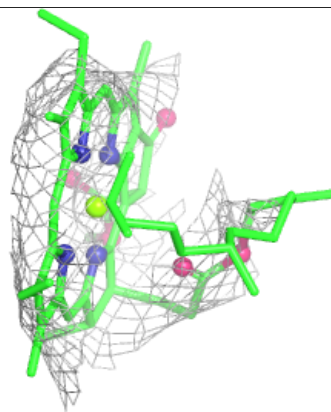
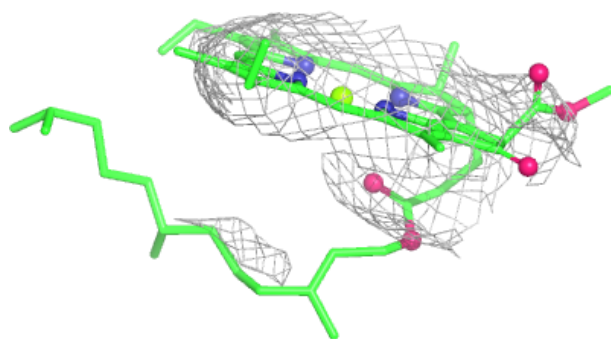
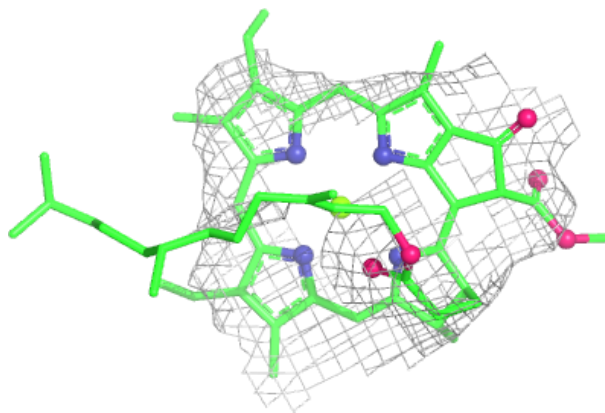
Electron density around CLA 1 1134:

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

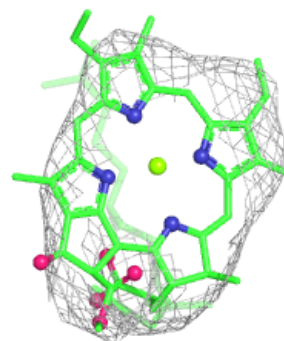
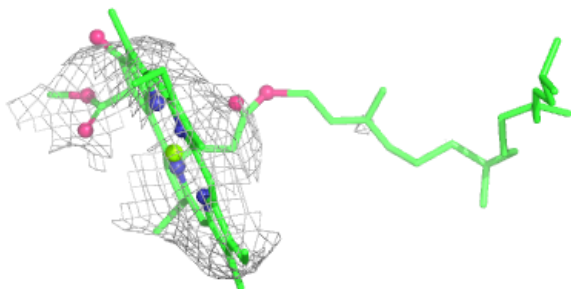
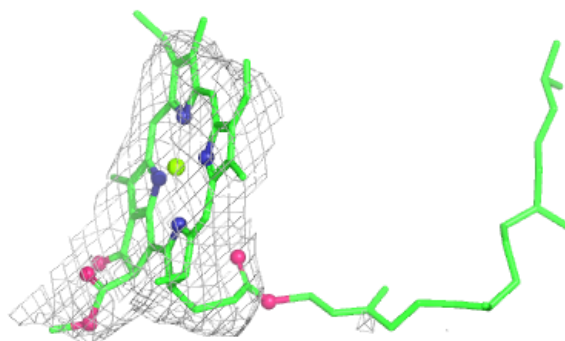


Electron density around CLA B 1235:

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

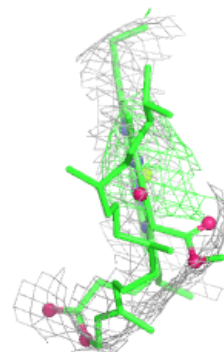
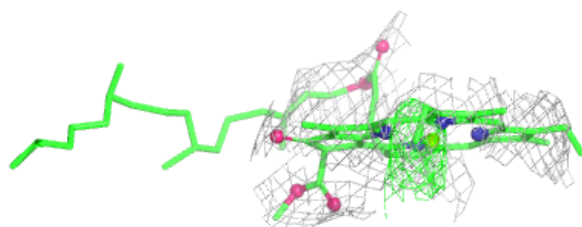
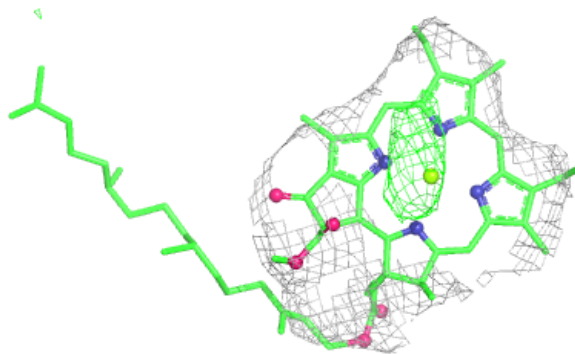
**Electron density around CLA A 1140:**

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

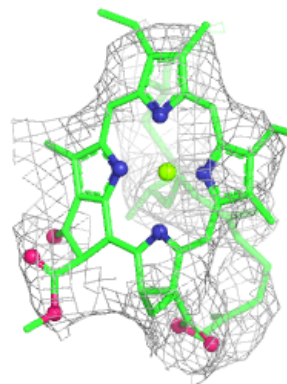
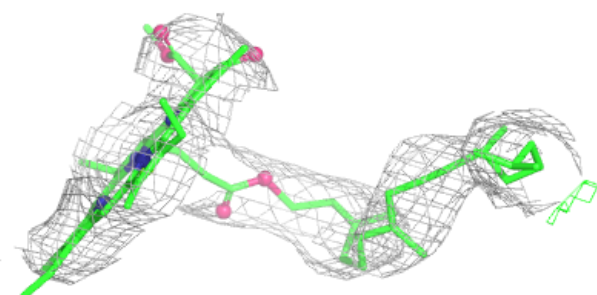
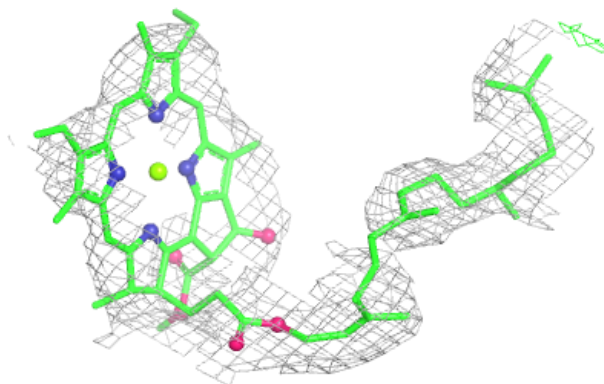


Electron density around CLA 1 1503:

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

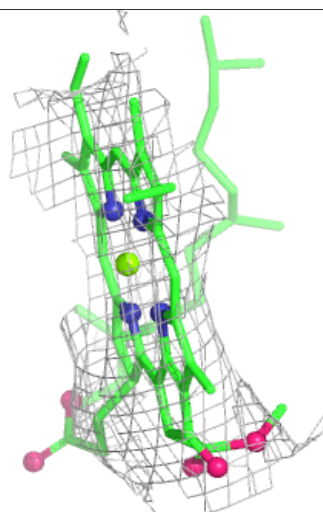
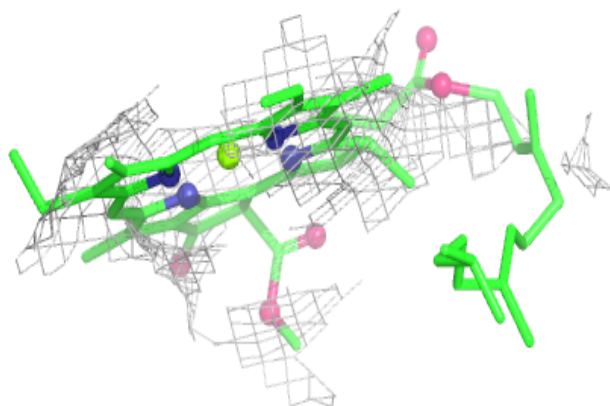
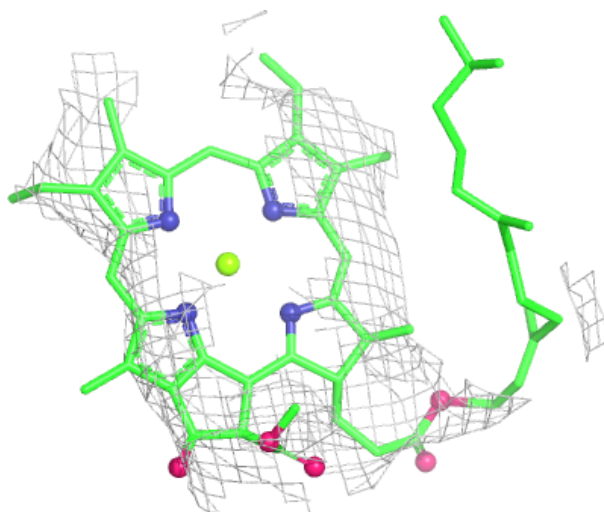
**Electron density around CLA A 1137:**

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



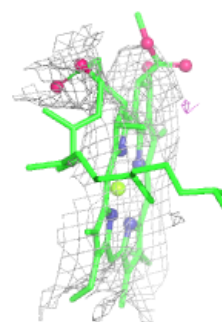
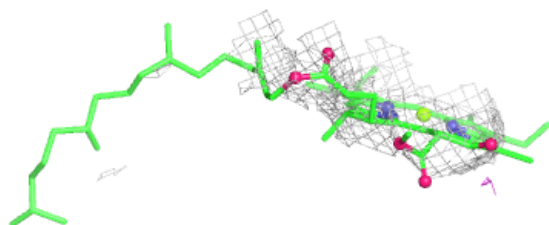
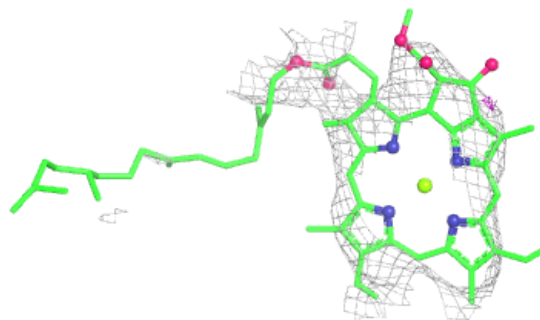
Electron density around CLA a 1111:

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



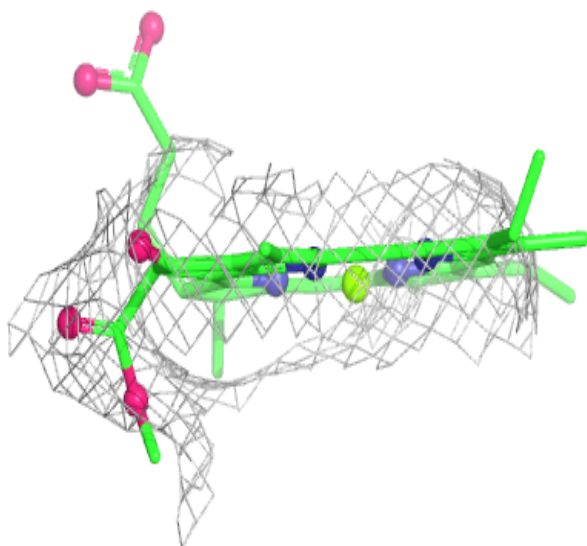
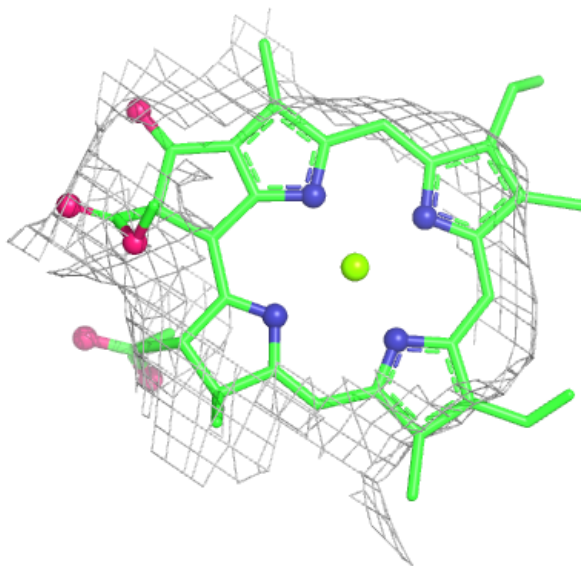
Electron density around CLA 2 1023:

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



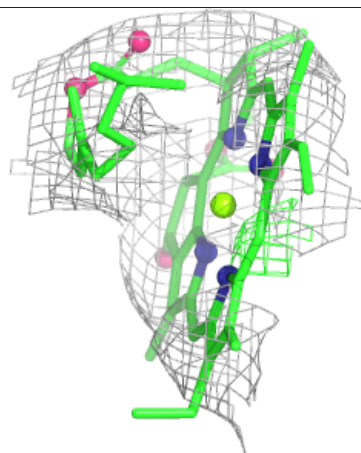
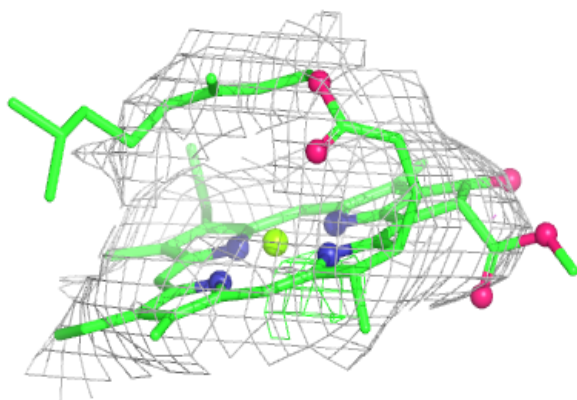
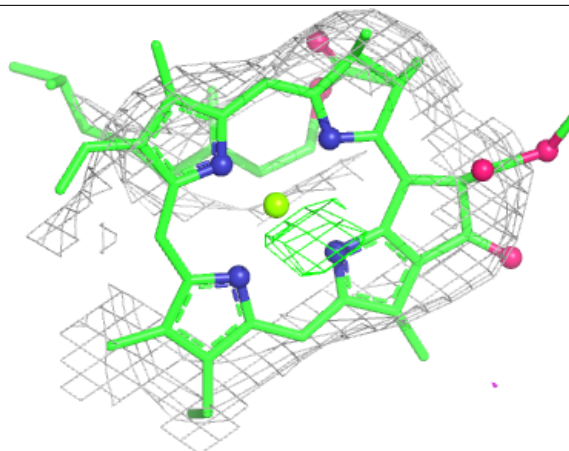
Electron density around CLA B 1231:

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



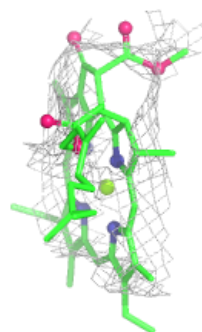
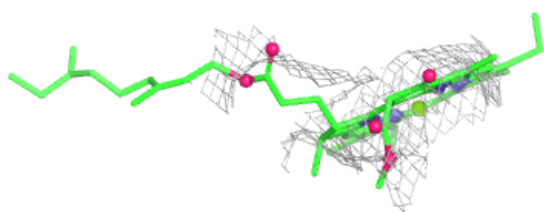
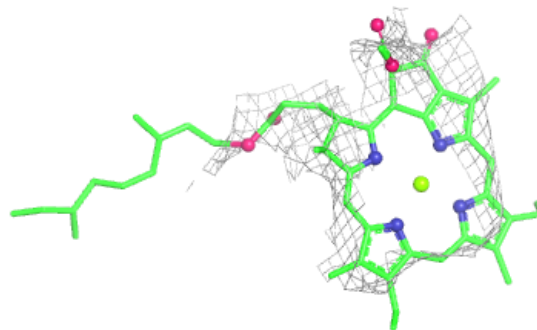
Electron density around CLA a 1237:

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

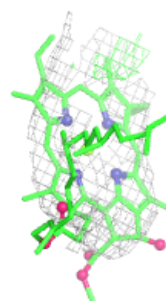
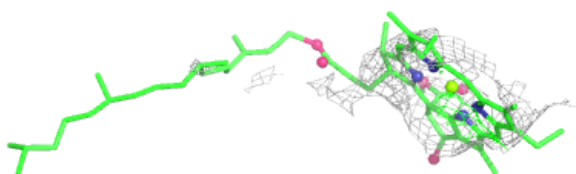
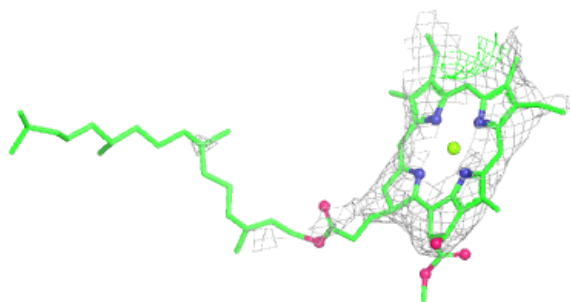


Electron density around CLA b 1222:

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

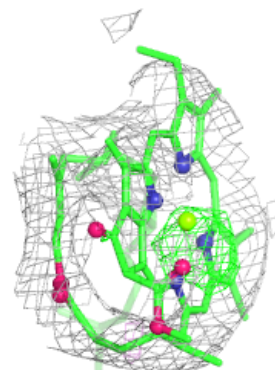
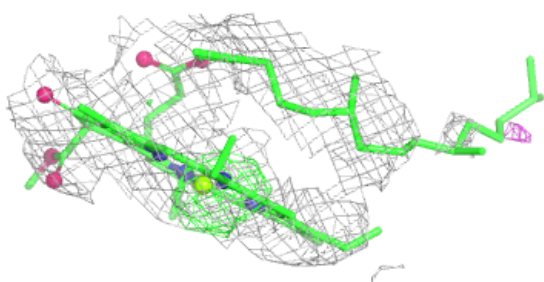
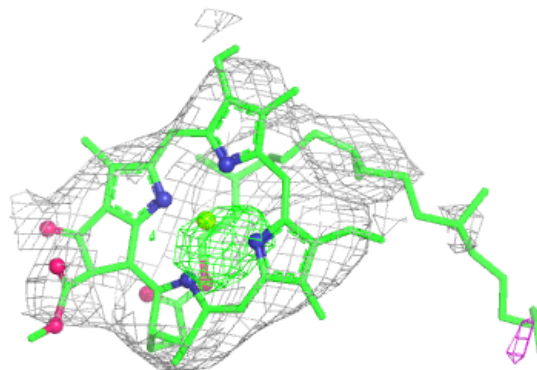
**Electron density around CLA a 1022:**

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



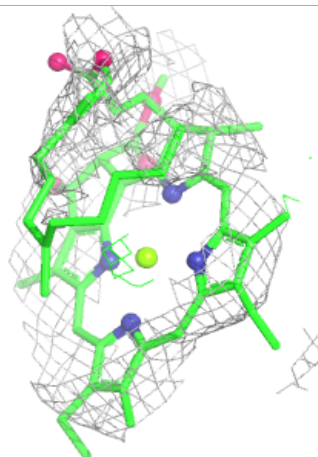
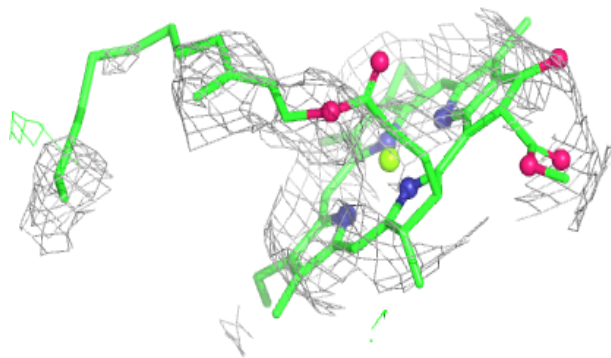
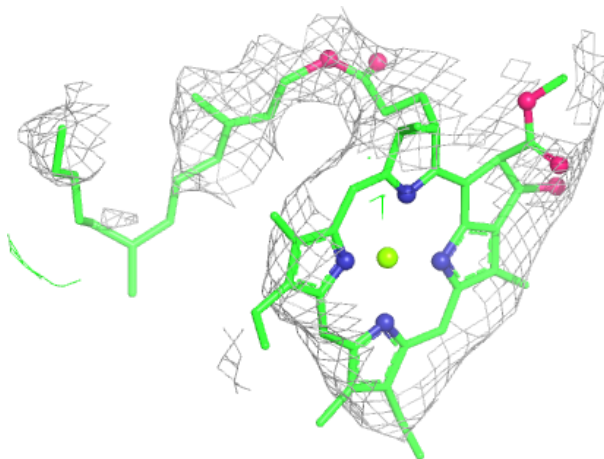
Electron density around CLA B 1204:

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



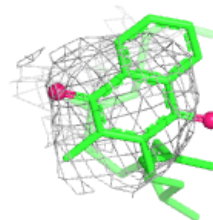
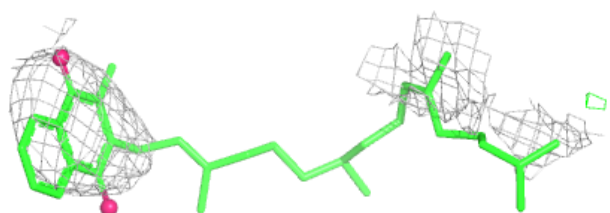
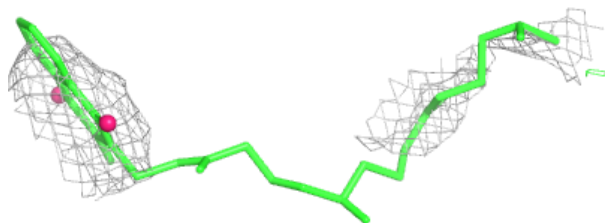
Electron density around CLA a 1122:

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

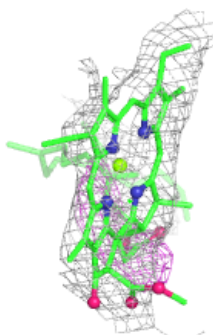
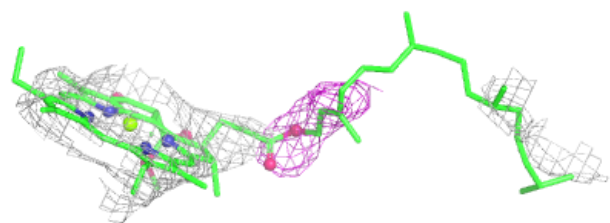
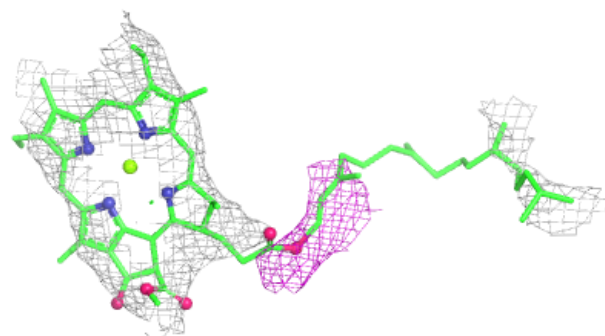


Electron density around PQN 2 2002:

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

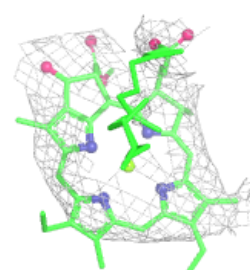
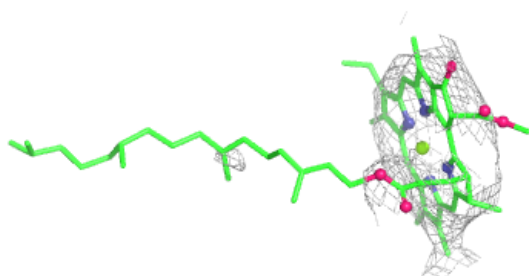
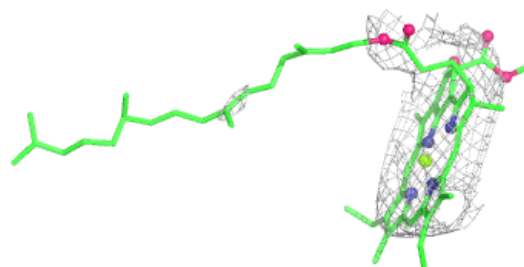
**Electron density around CLA 2 1210:**

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

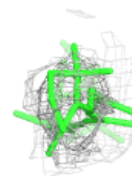
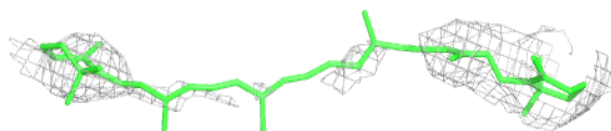
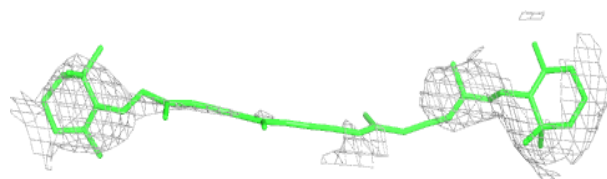


Electron density around CLA b 1226:

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

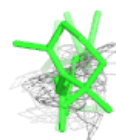
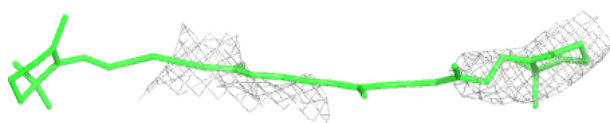
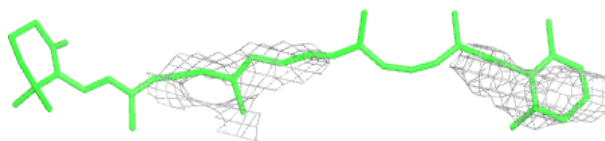
**Electron density around BCR A 4003:**

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

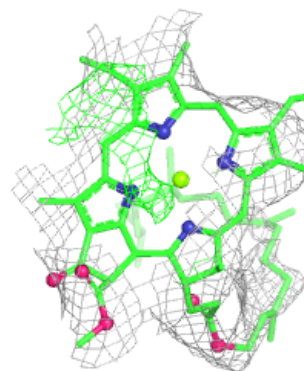
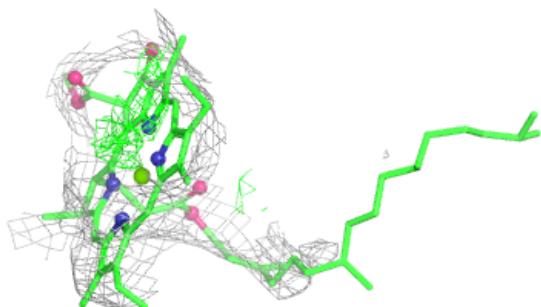
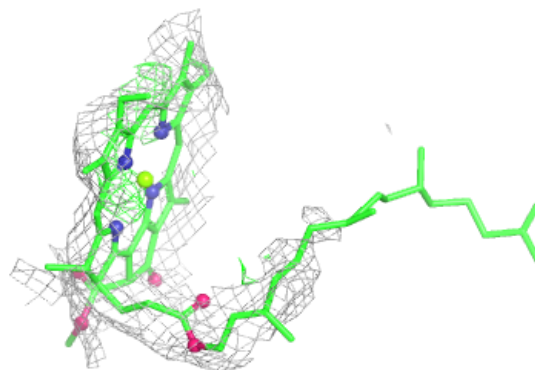


Electron density around BCR 1 4007:

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

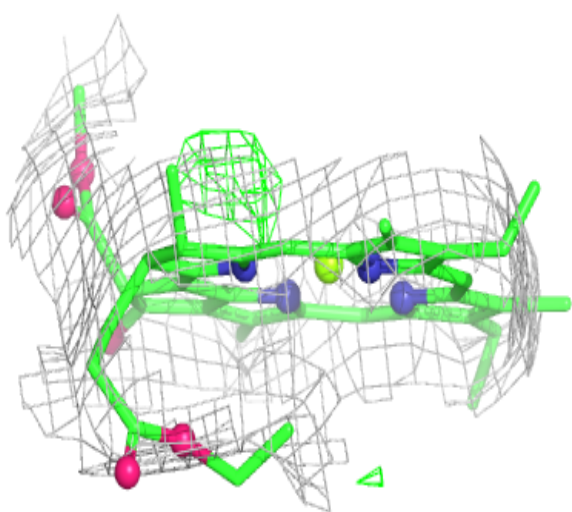
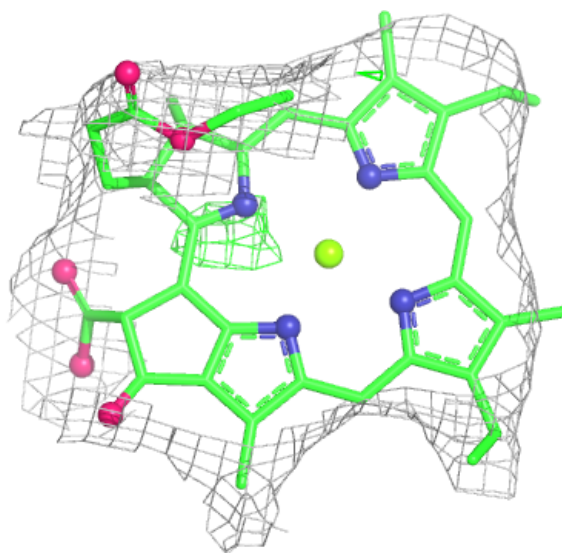
**Electron density around CLA 2 1216:**

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



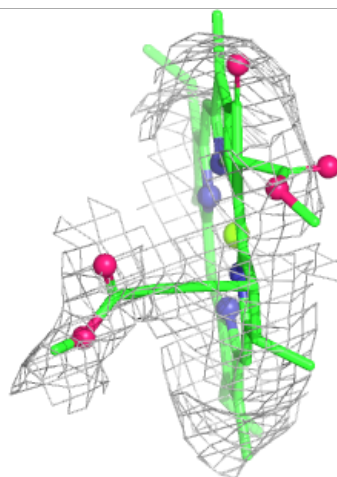
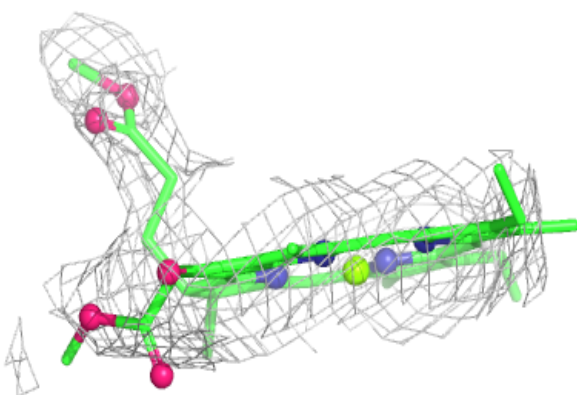
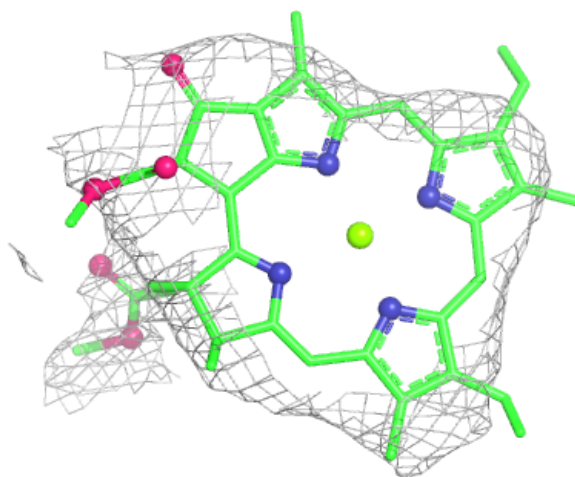
Electron density around CLA 2 1217:

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



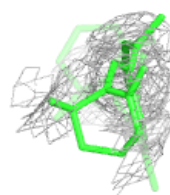
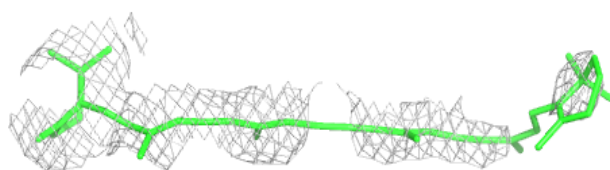
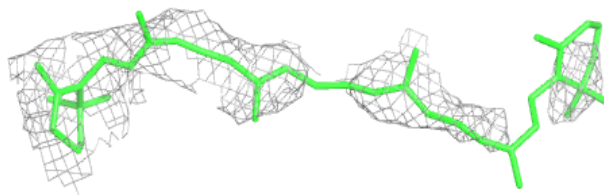
Electron density around CLA B 1220:

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



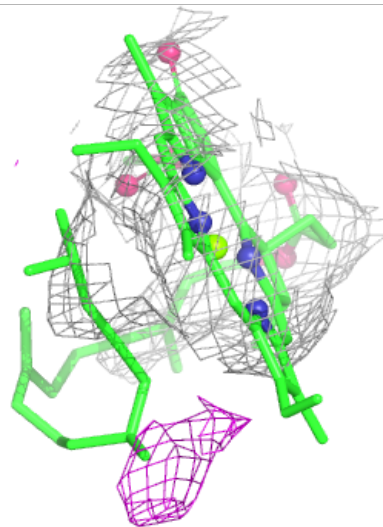
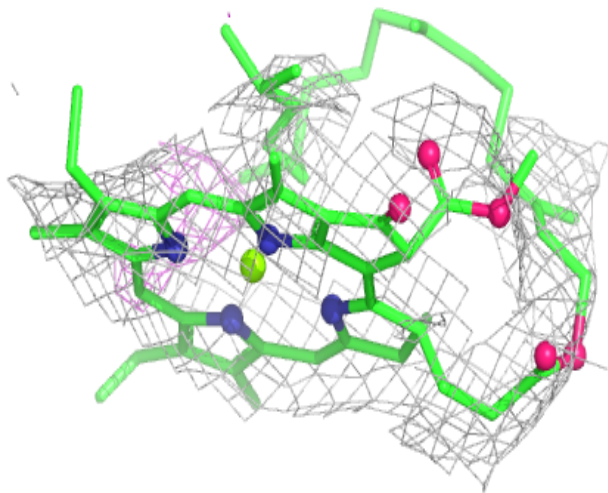
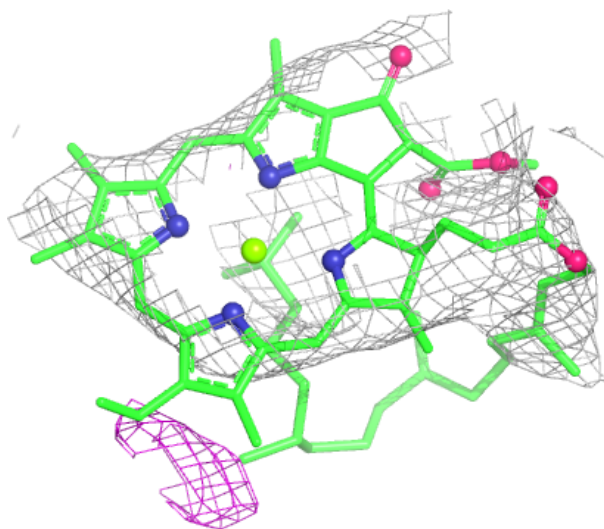
Electron density around BCR 2 4006:

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



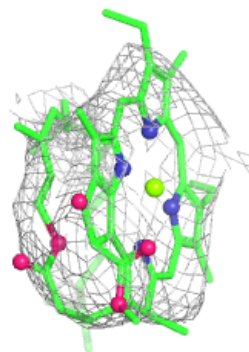
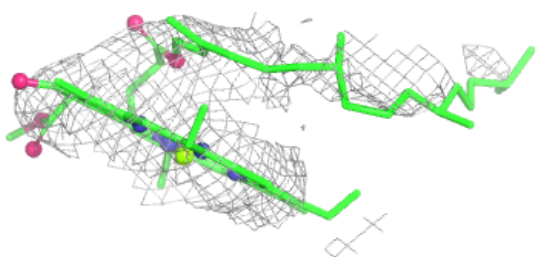
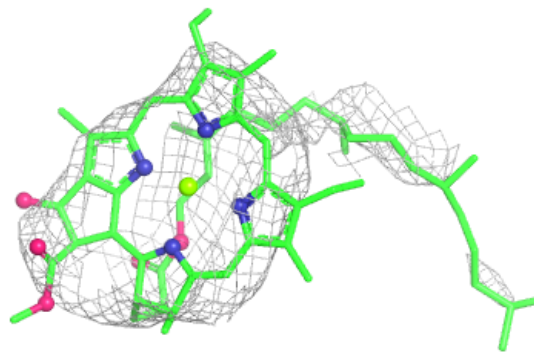
Electron density around CLA b 1203:

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

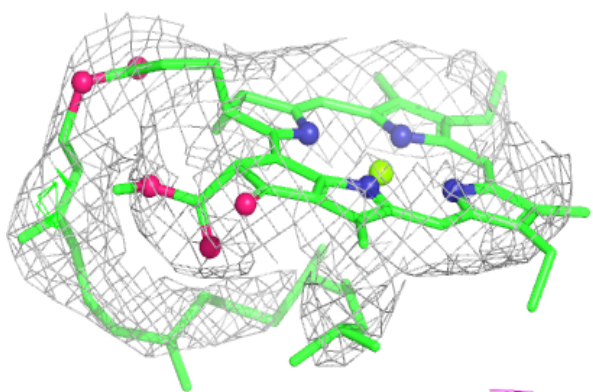
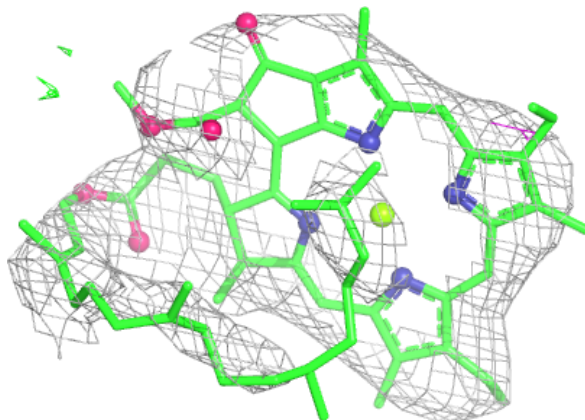


Electron density around CLA b 1204:

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

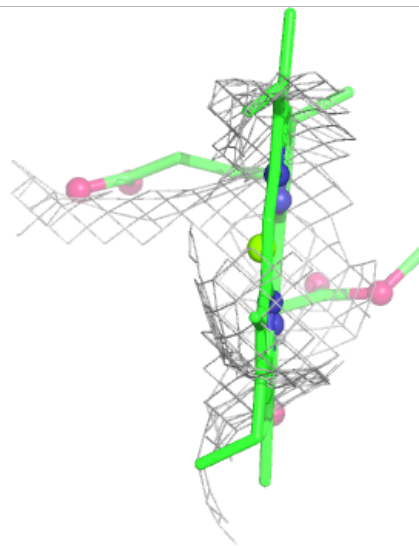
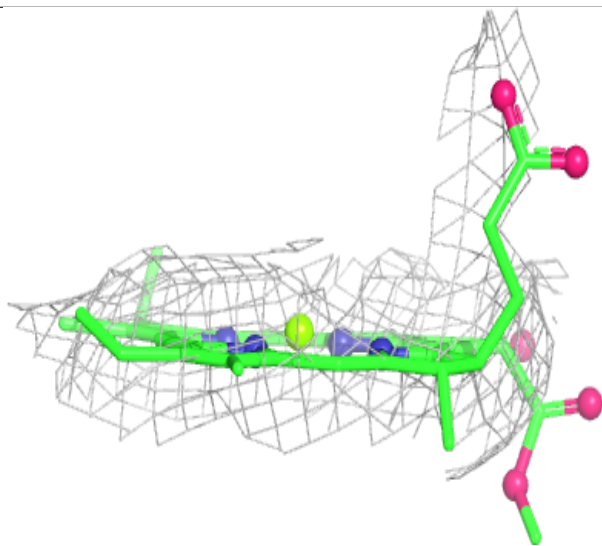
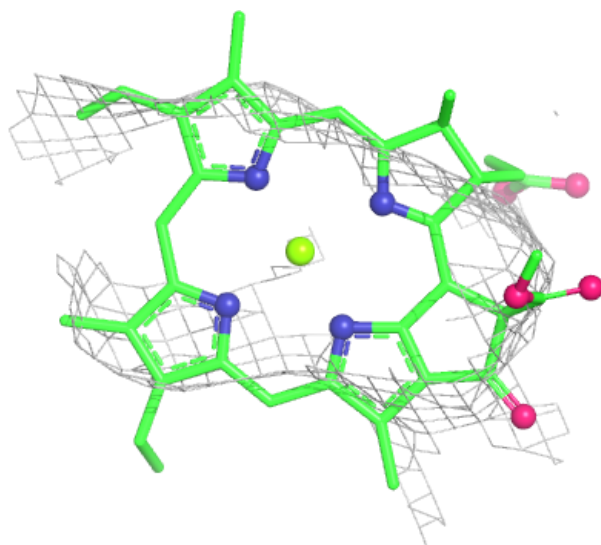
**Electron density around CLA A 1104:**

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



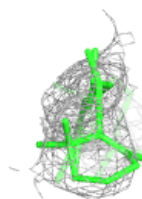
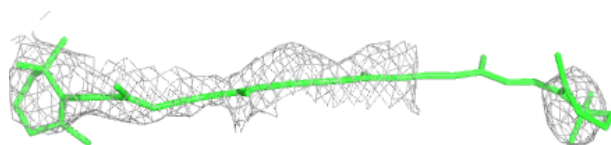
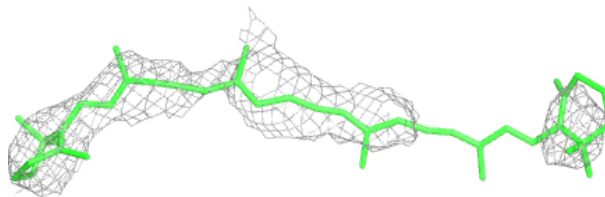
Electron density around CLA 1 1112:

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



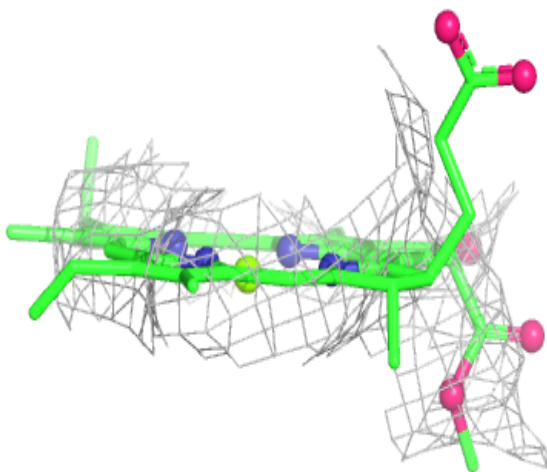
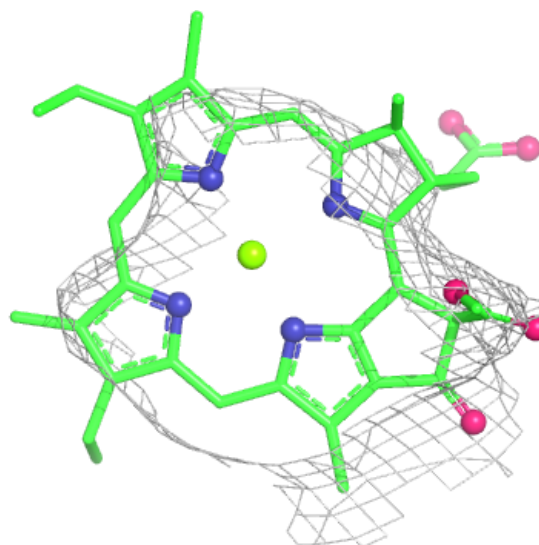
Electron density around BCR 2 4017:

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



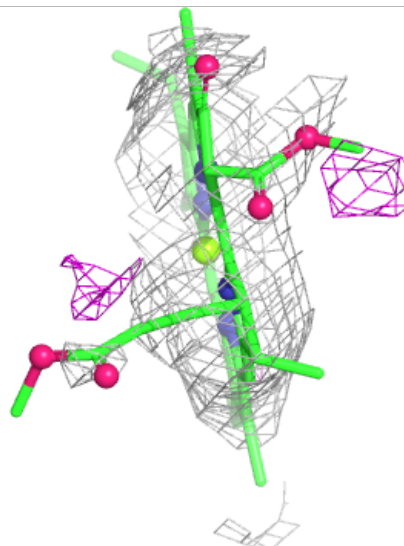
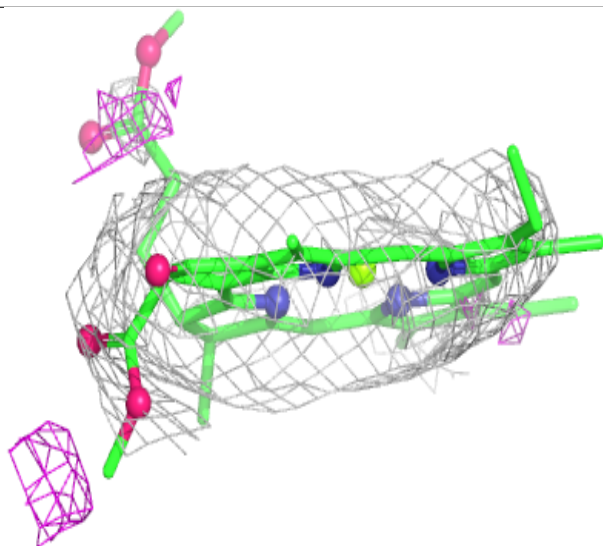
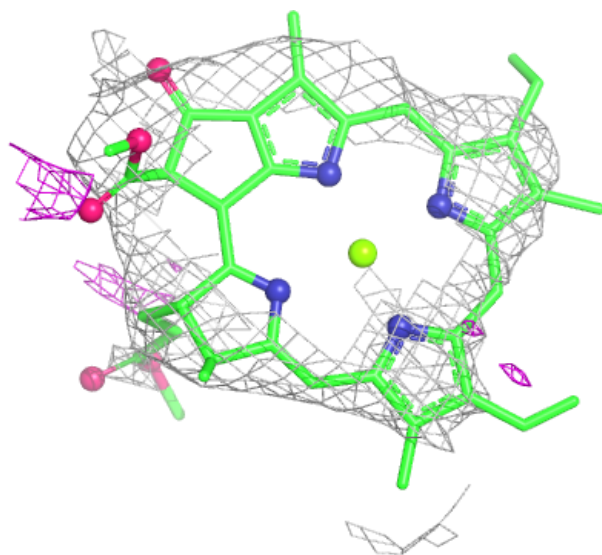
Electron density around CLA b 1231:

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



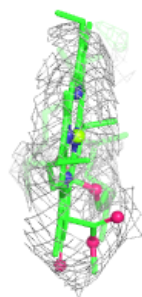
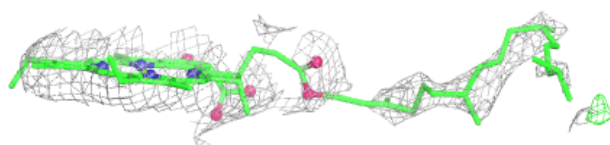
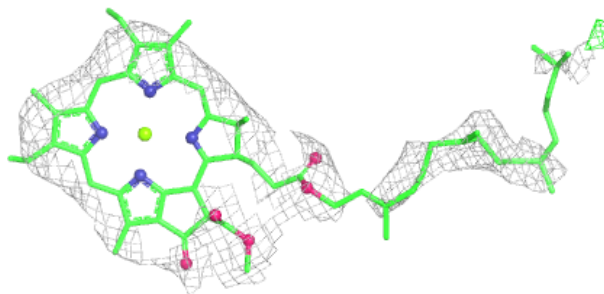
Electron density around CLA A 1129:

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

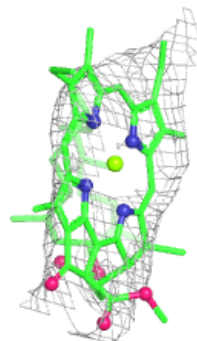
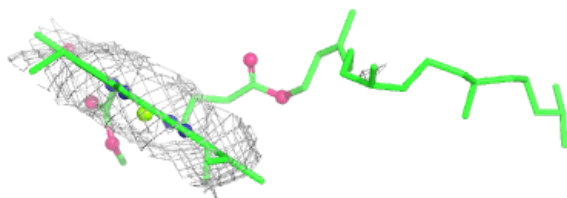
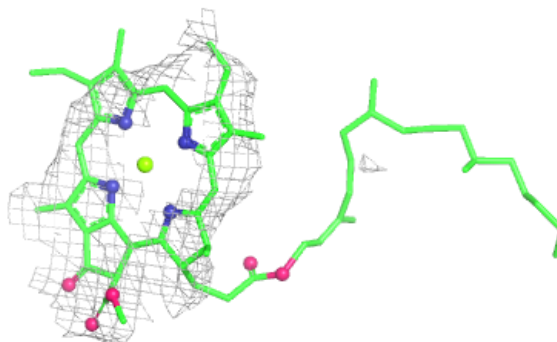


Electron density around CLA a 1131:

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

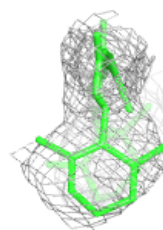
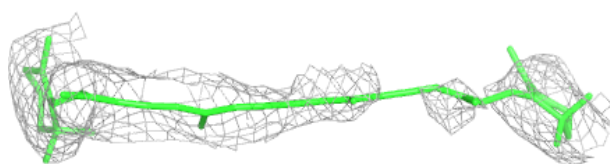
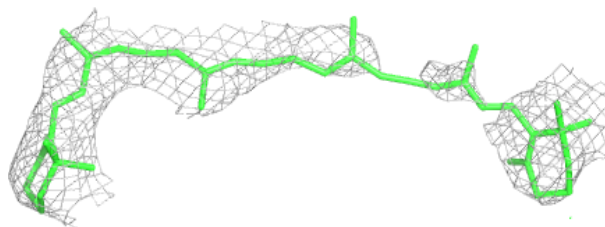
**Electron density around CLA a 1106:**

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

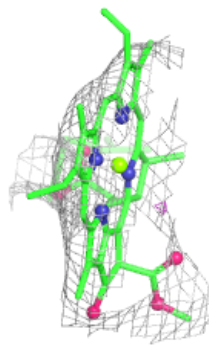
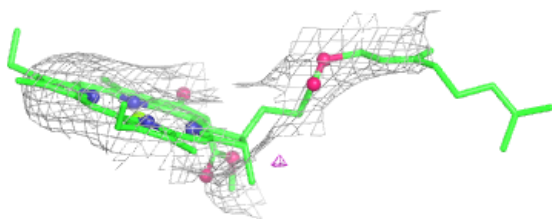
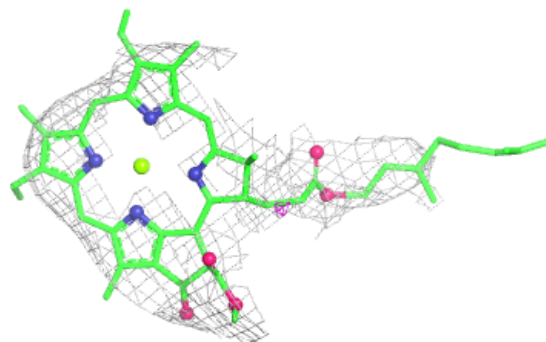


Electron density around BCR F 4020:

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

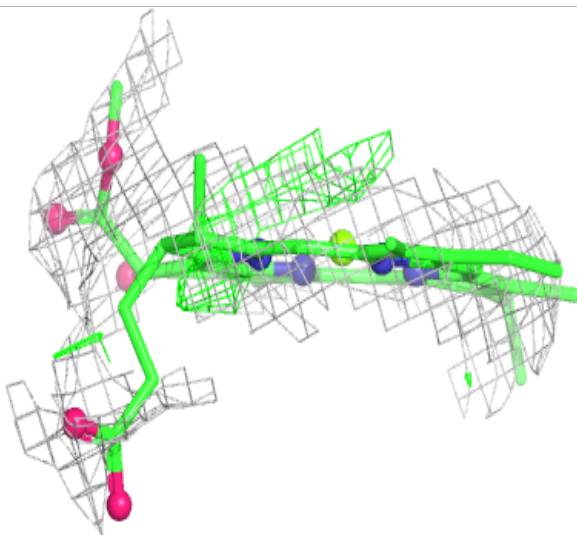
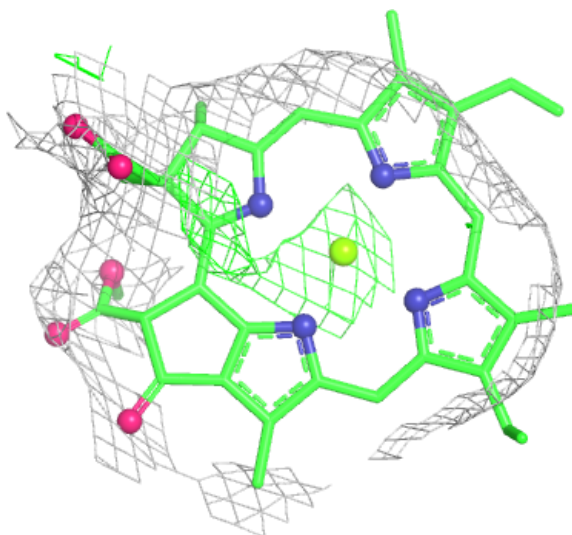
**Electron density around CLA 1 1124:**

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



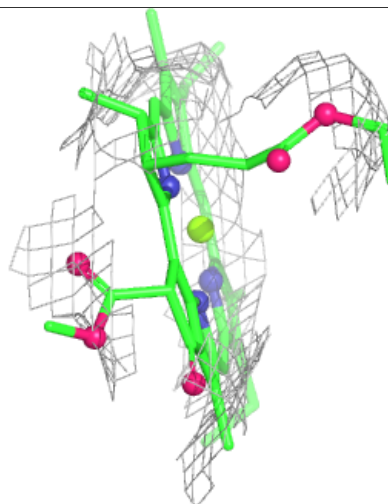
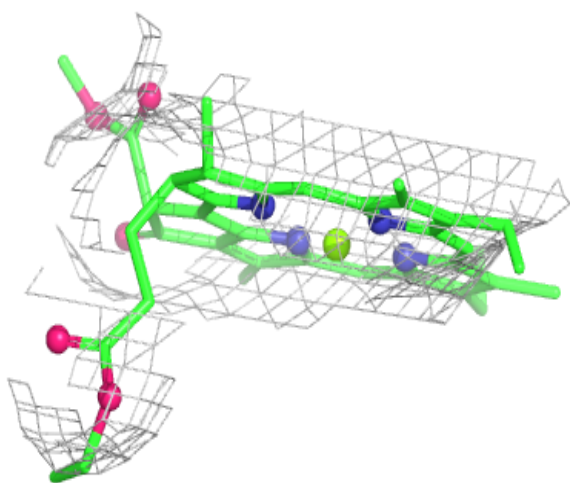
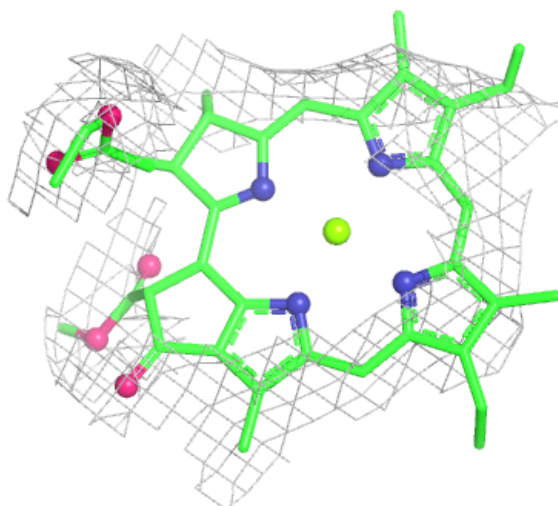
Electron density around CLA 2 1231:

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



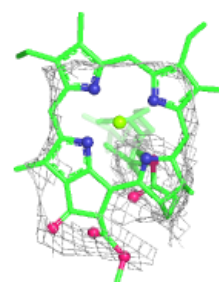
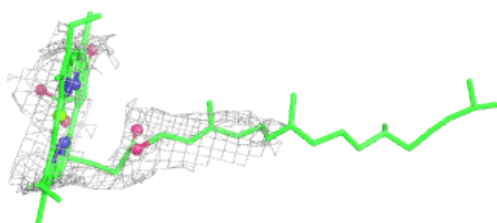
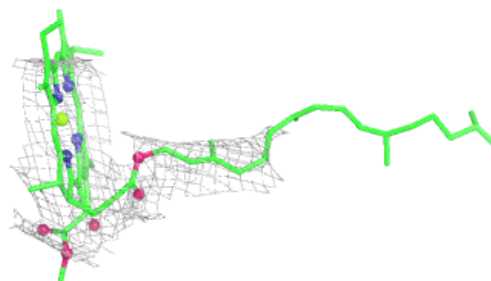
Electron density around CLA b 1236:

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

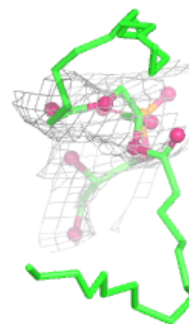
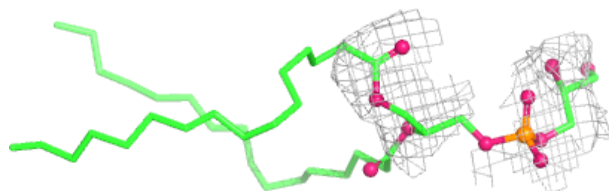
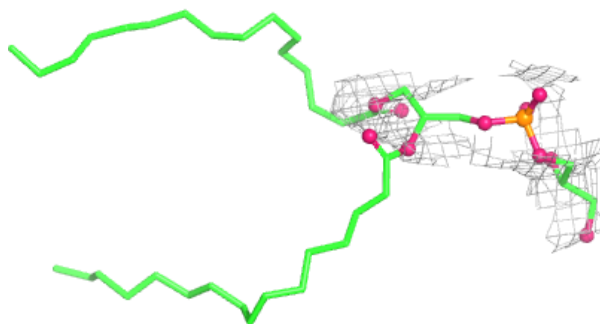


Electron density around CLA 1 1126:

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

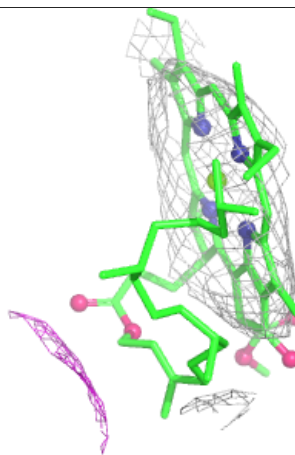
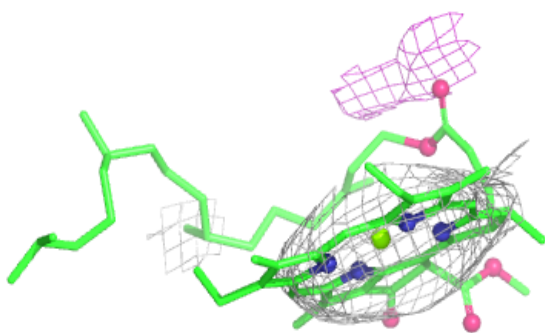
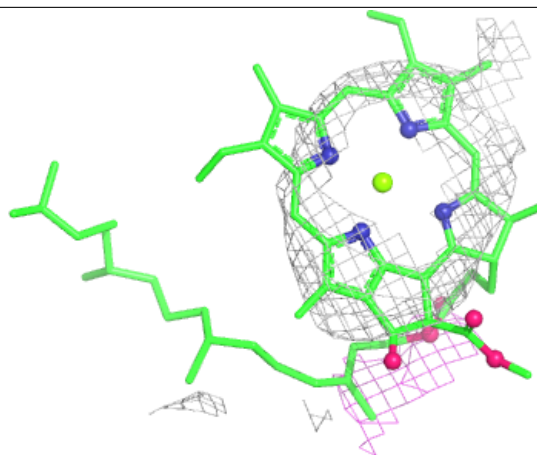
**Electron density around LHG a 5001:**

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



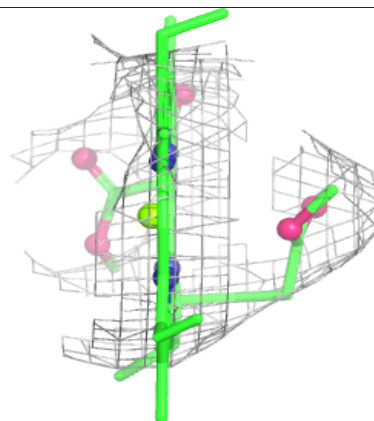
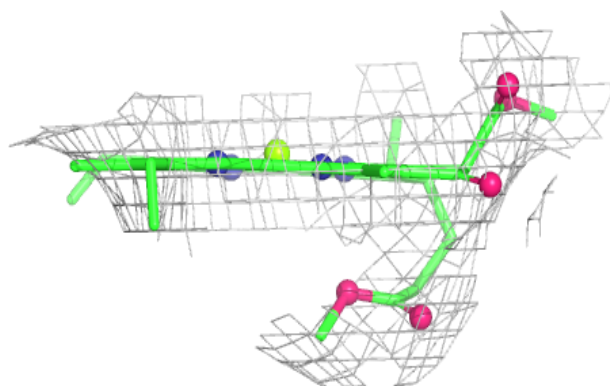
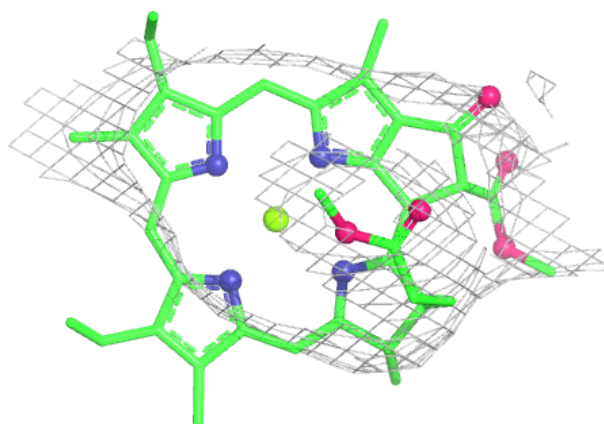
Electron density around CLA 1 1127:

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



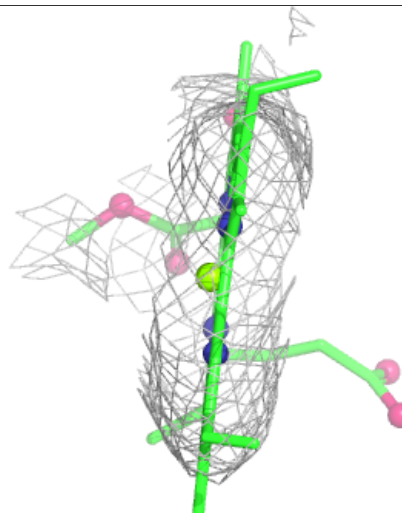
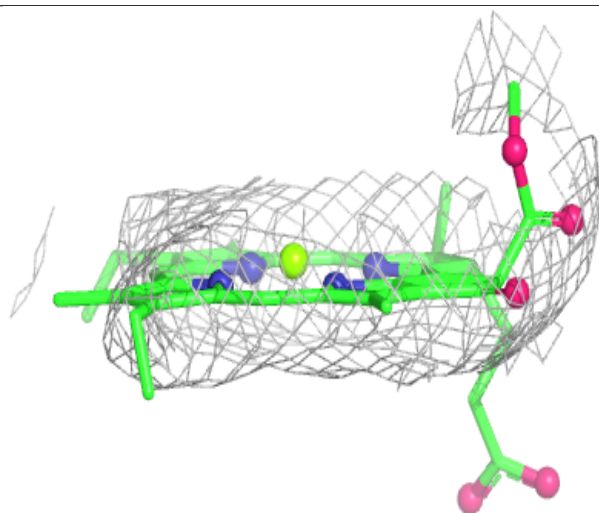
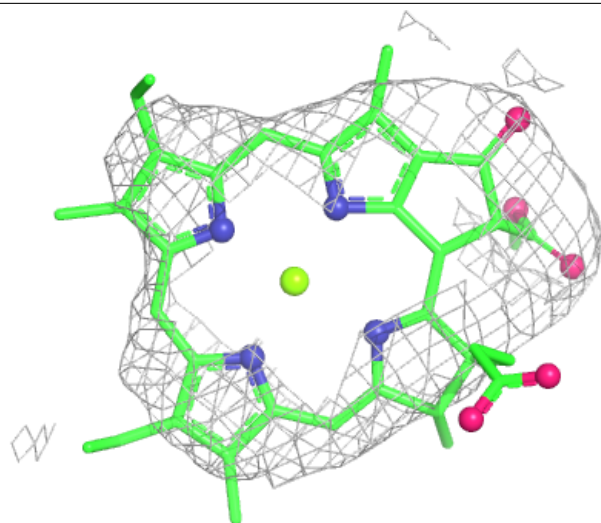
Electron density around CLA a 1138:

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



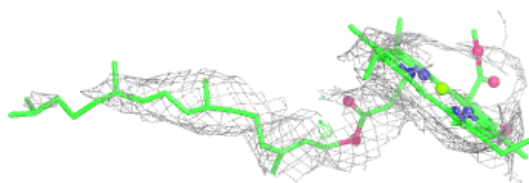
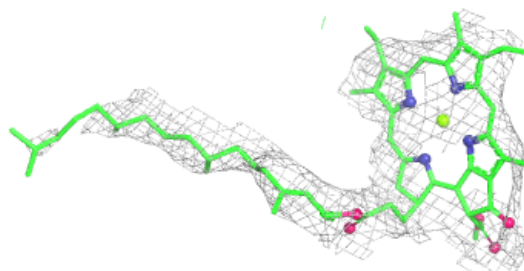
Electron density around CLA B 1212:

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

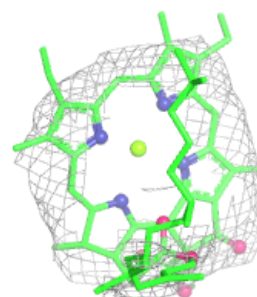
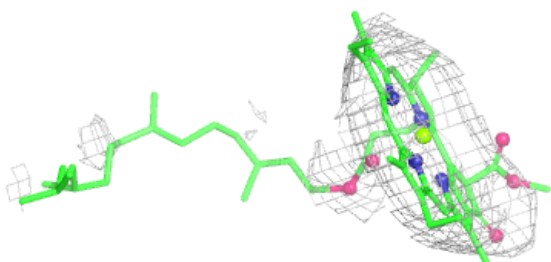
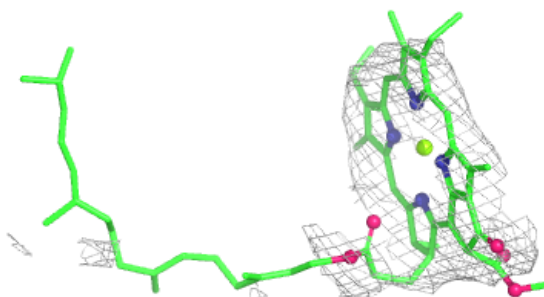


Electron density around CLA A 1132:

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

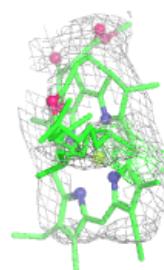
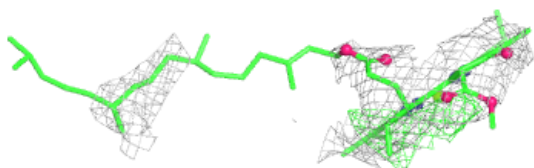
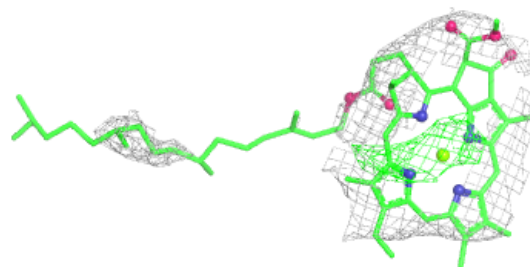
**Electron density around CLA 1 1140:**

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

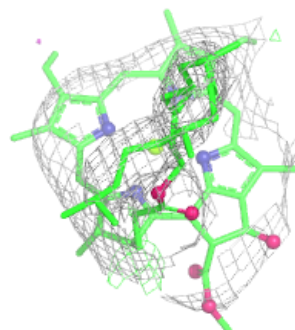
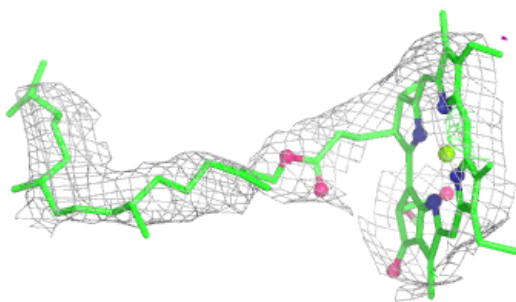
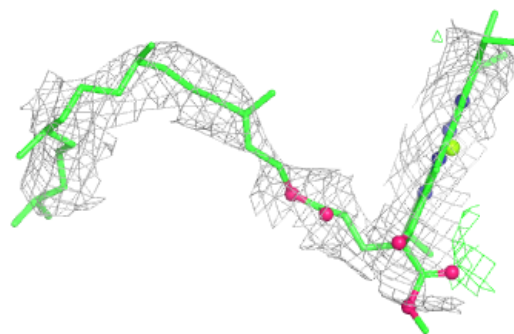


Electron density around CLA 8 1501:

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

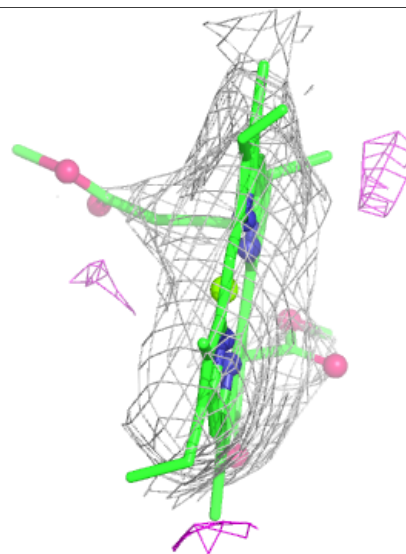
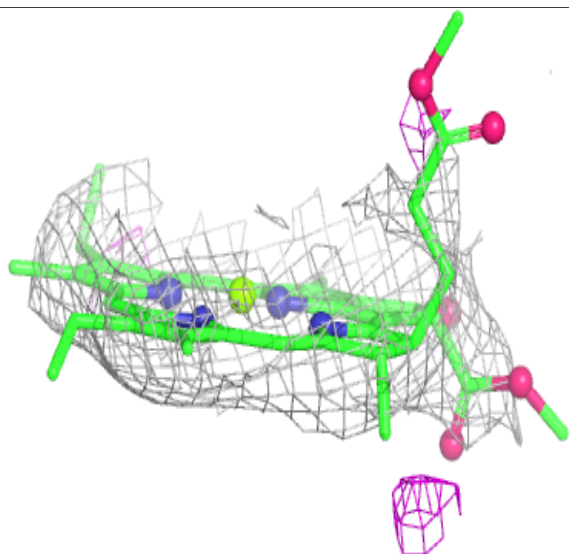
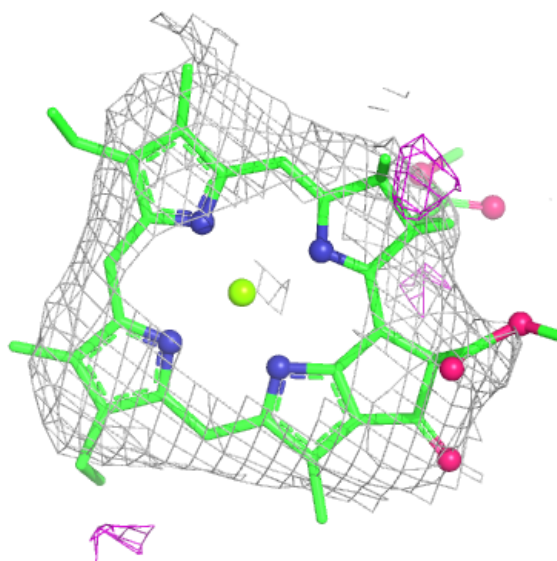
**Electron density around CLA b 1238:**

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



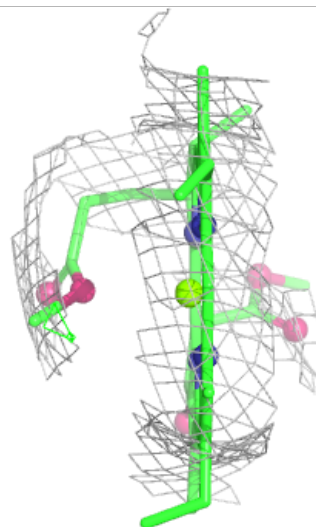
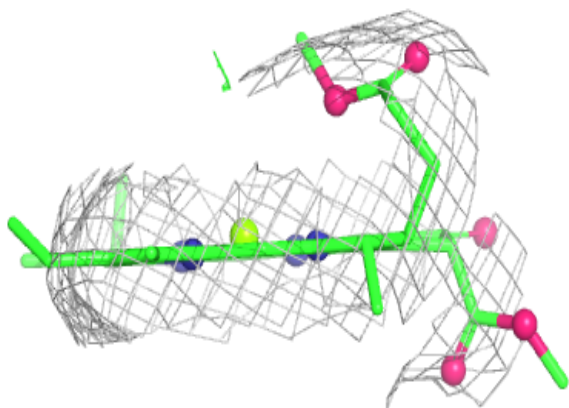
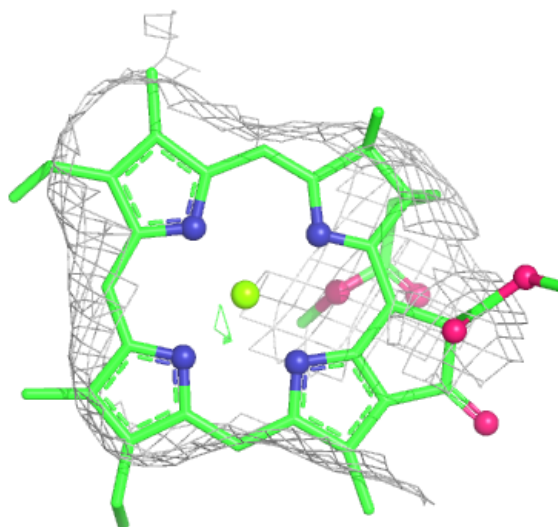
Electron density around CLA A 1133:

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



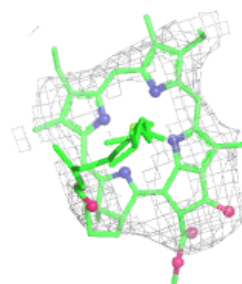
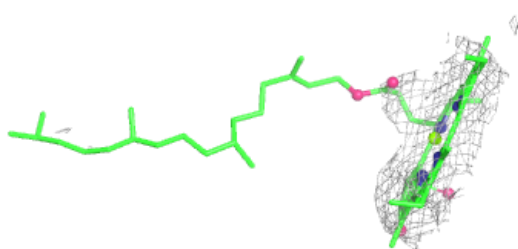
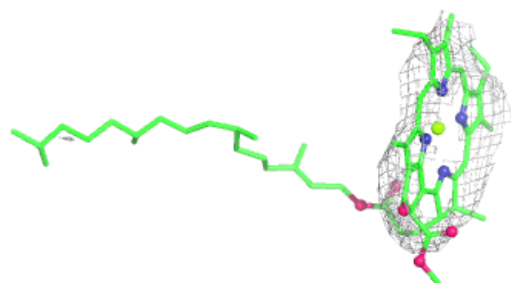
Electron density around CLA a 1136:

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

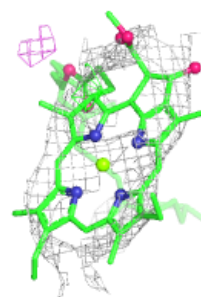
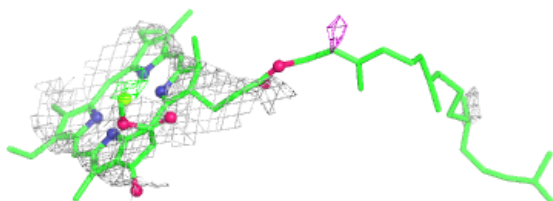
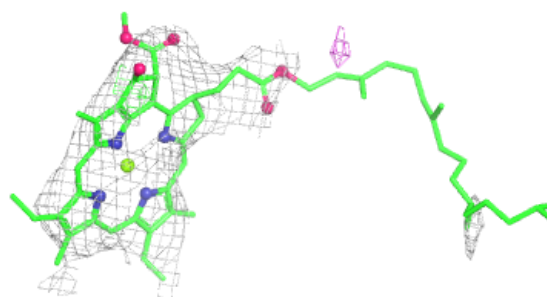


Electron density around CLA B 1225:

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

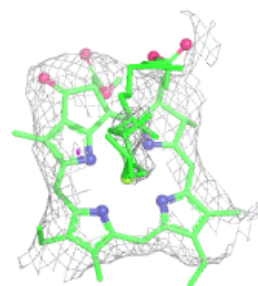
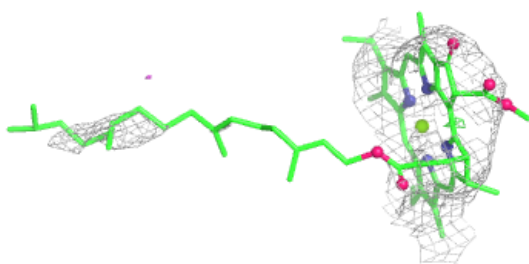
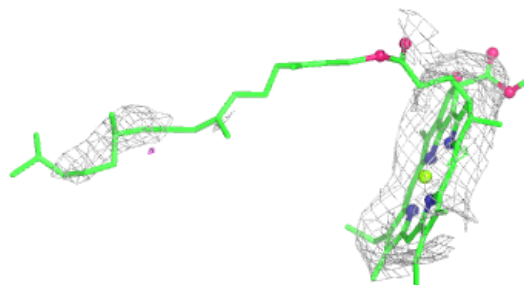
**Electron density around CLA 1 1012:**

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



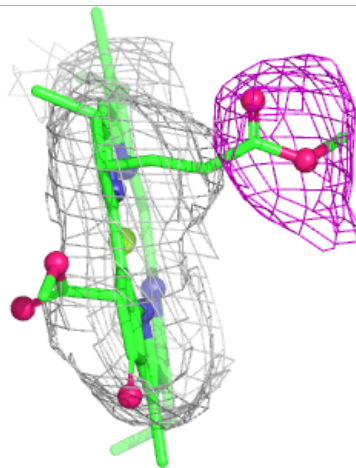
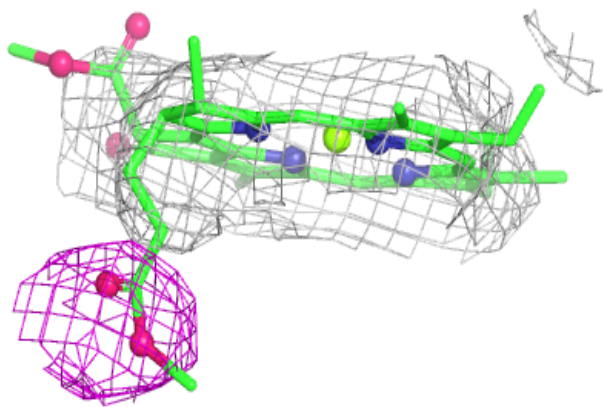
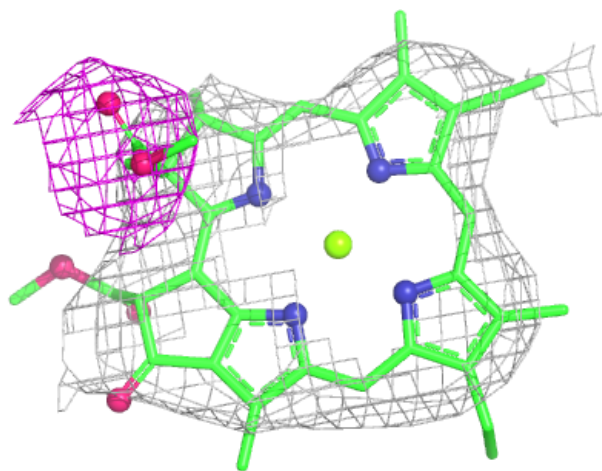
Electron density around CLA B 1226:

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



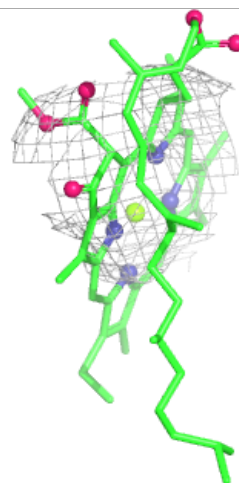
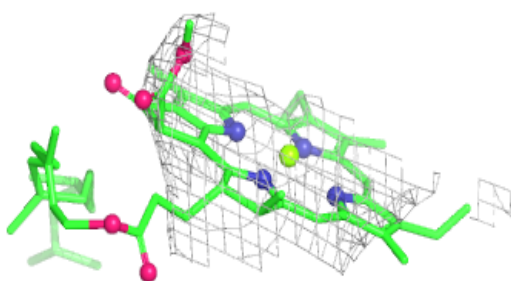
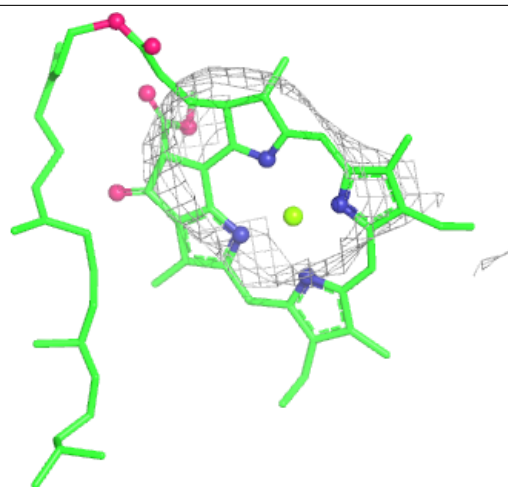
Electron density around CLA A 1130:

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



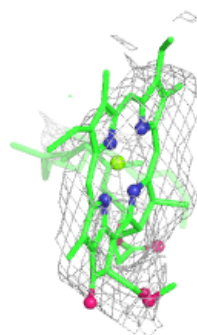
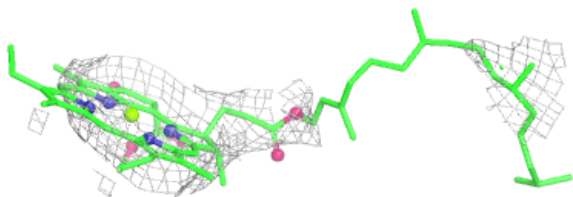
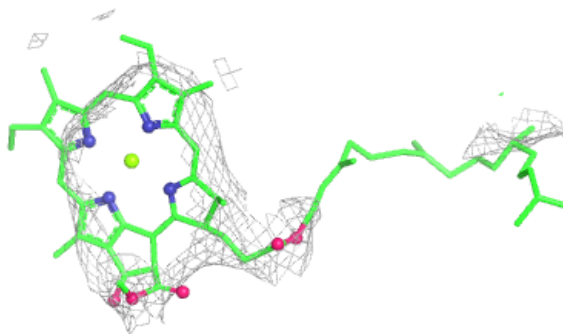
Electron density around CLA a 1123:

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



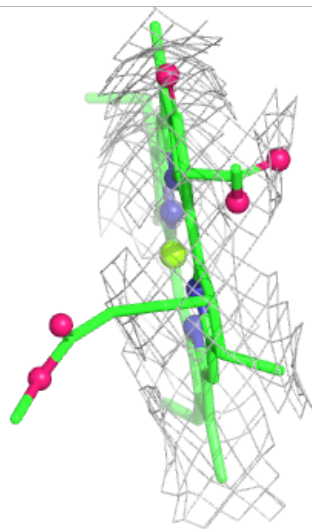
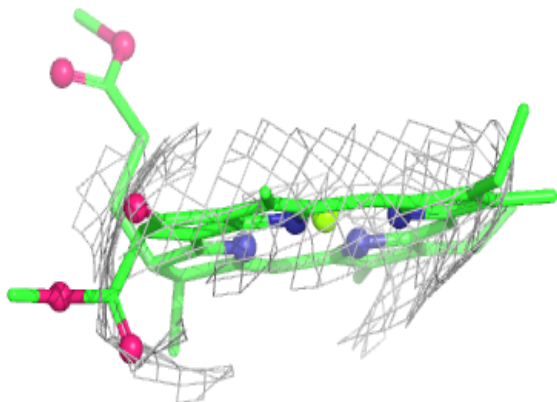
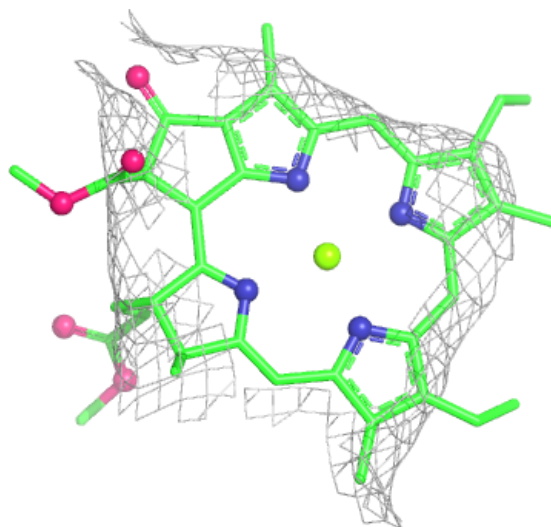
Electron density around CLA B 1210:

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



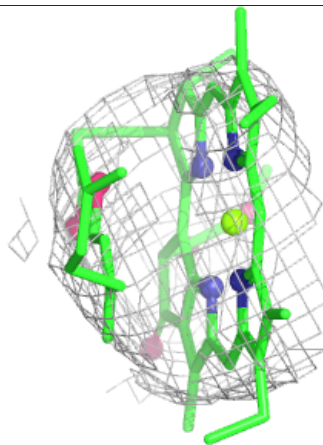
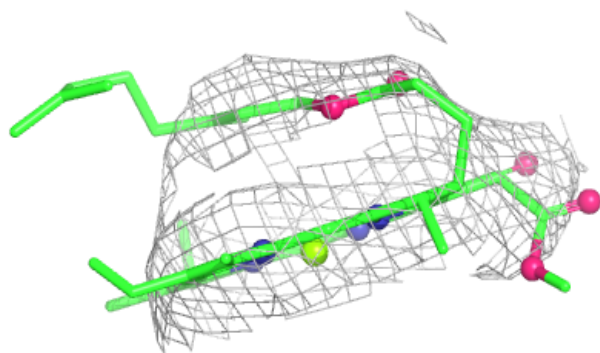
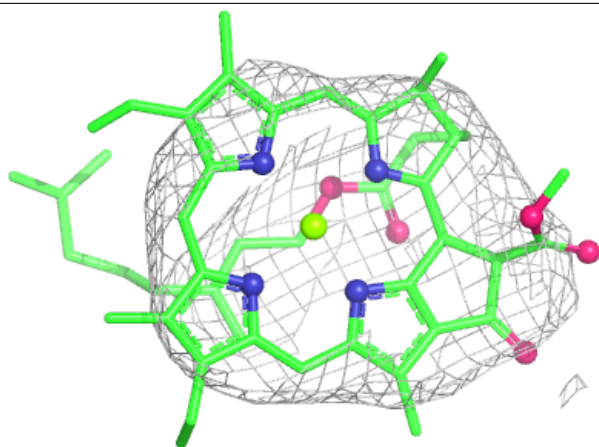
Electron density around CLA 1 1133:

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



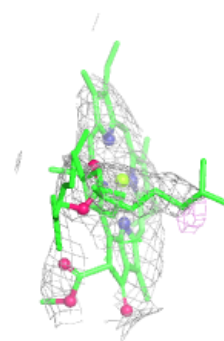
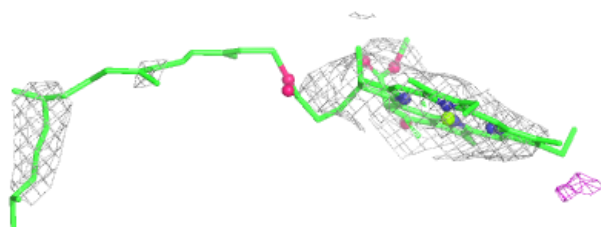
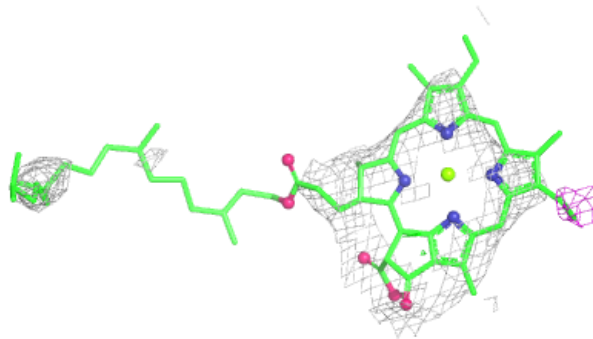
Electron density around CLA b 1205:

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

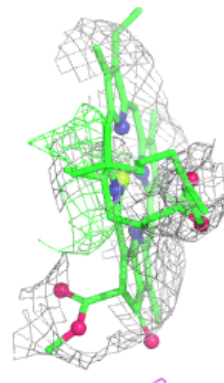
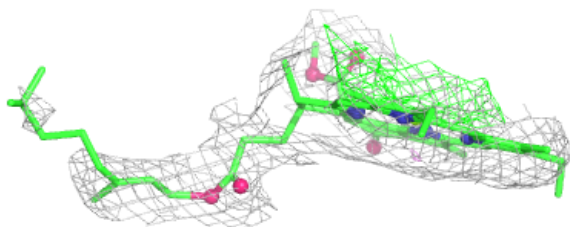
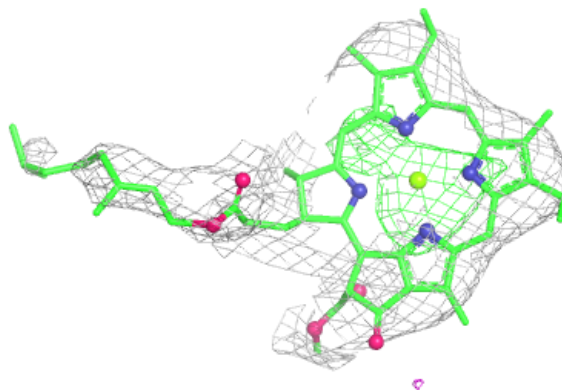


Electron density around CLA A 1103:

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

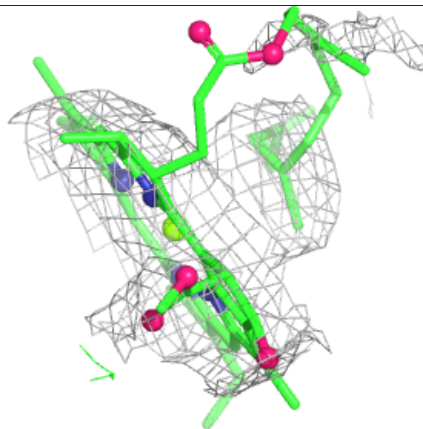
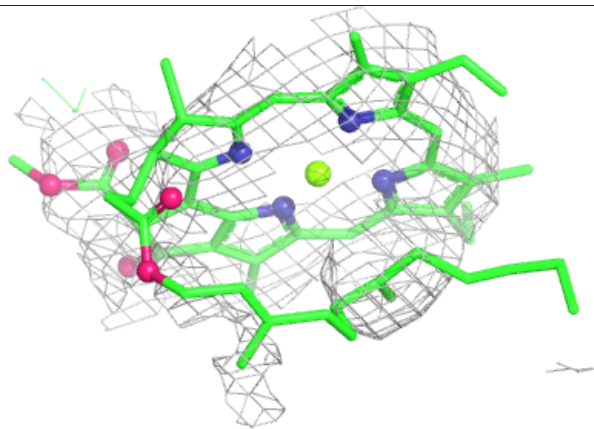
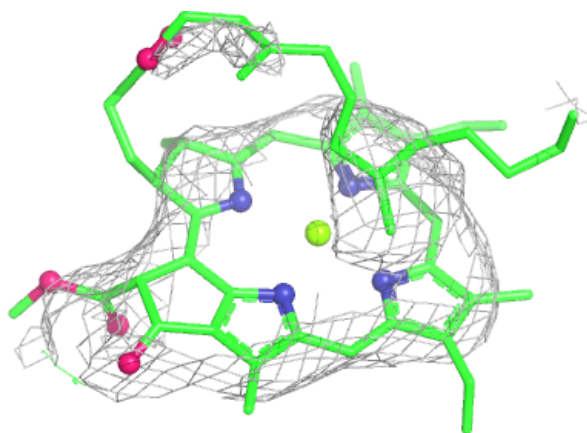
**Electron density around CLA A 1124:**

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



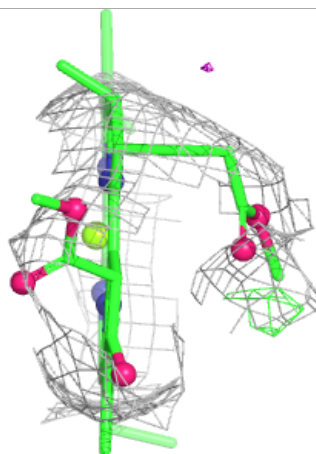
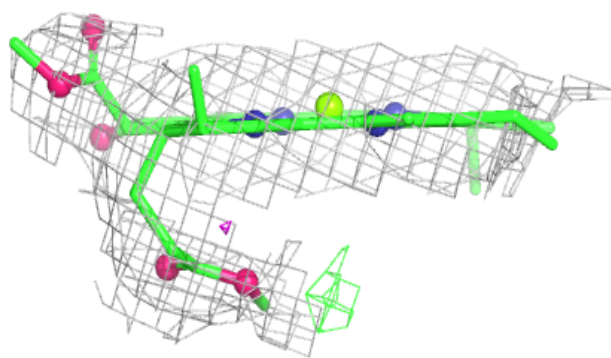
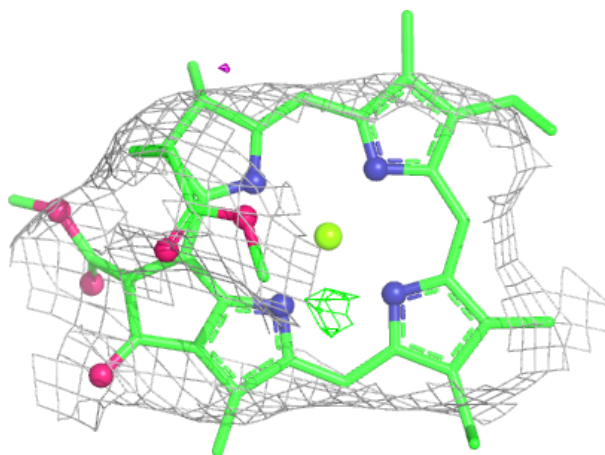
Electron density around CLA B 1214:

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



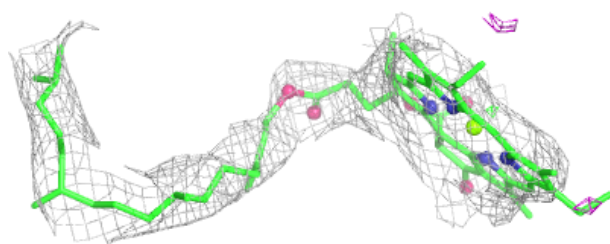
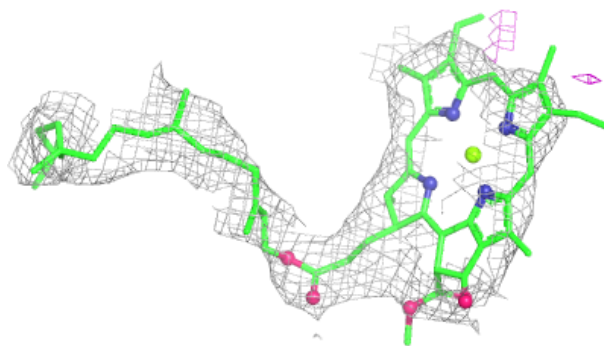
Electron density around CLA A 1138:

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



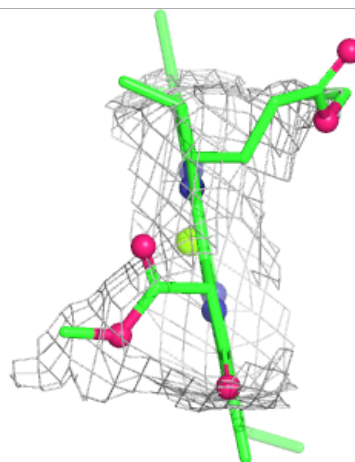
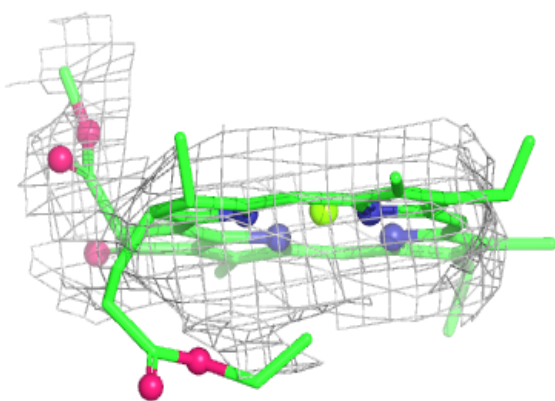
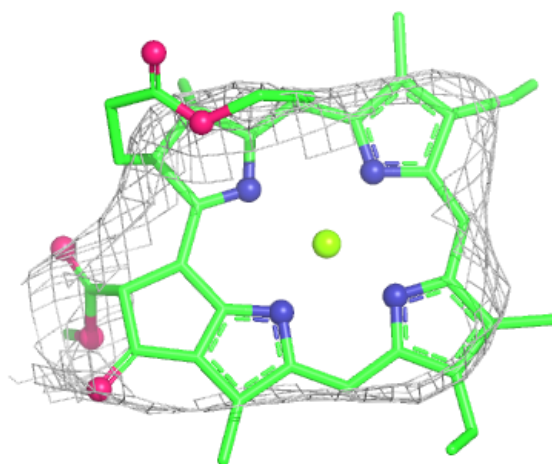
Electron density around CLA 2 1206:

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



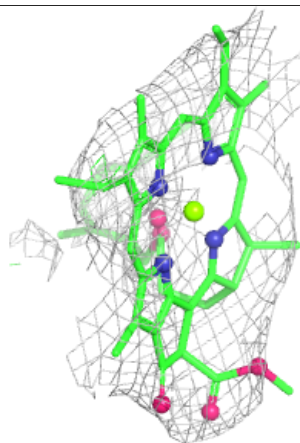
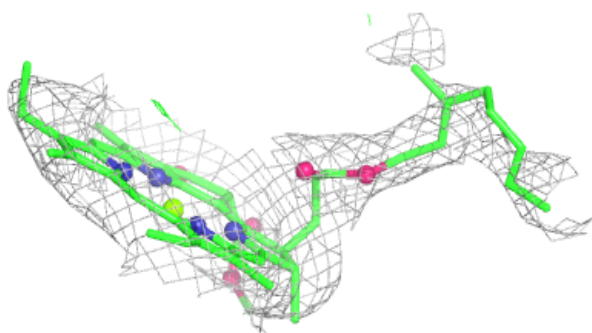
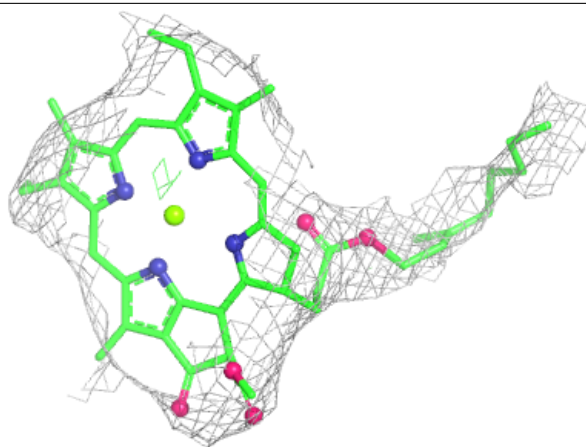
Electron density around CLA B 1217:

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



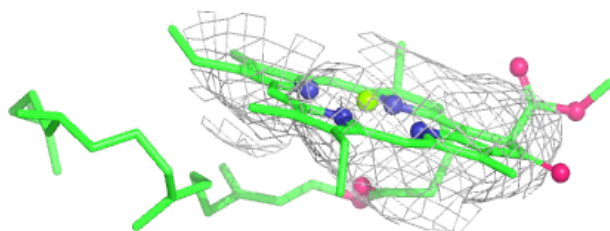
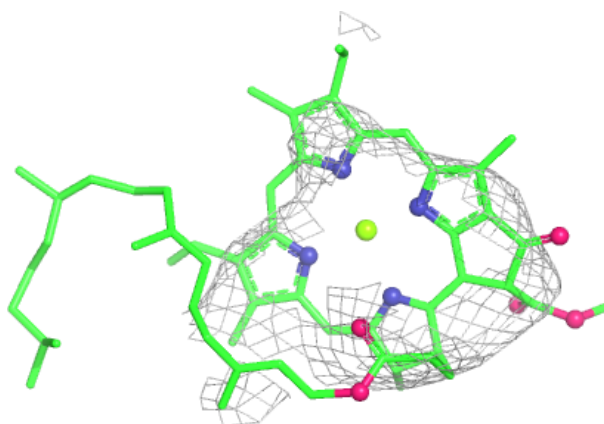
Electron density around CLA A 1110:

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

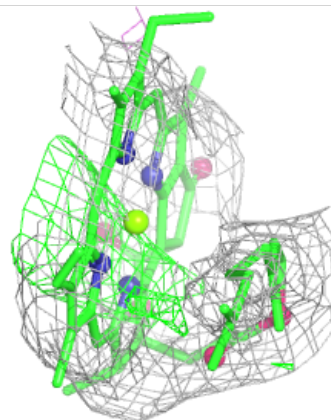
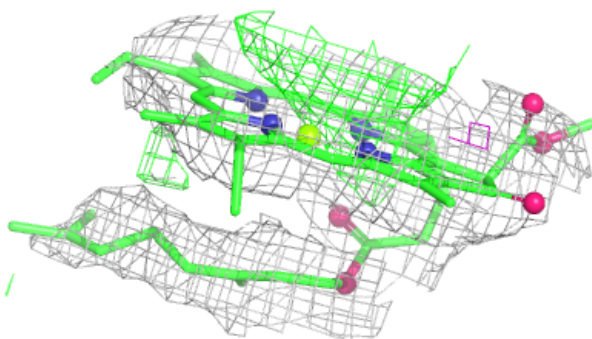
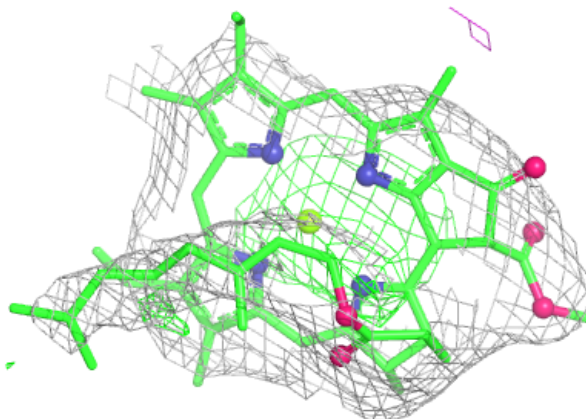


Electron density around CLA 1 1117:

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

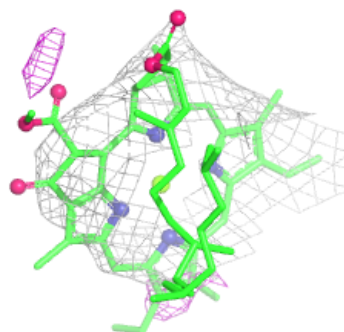
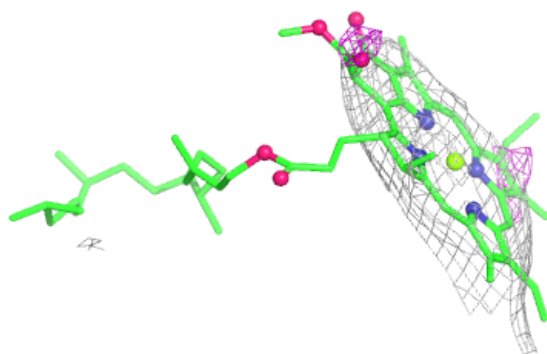
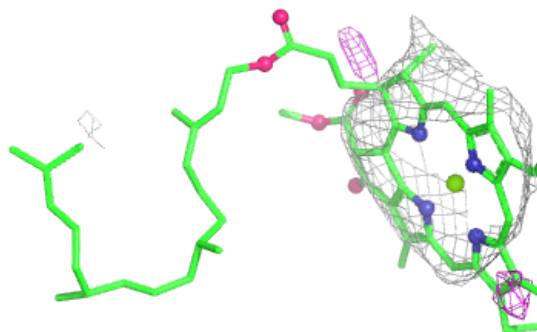
**Electron density around CLA A 1237:**

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



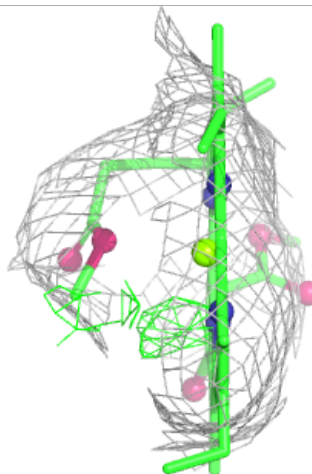
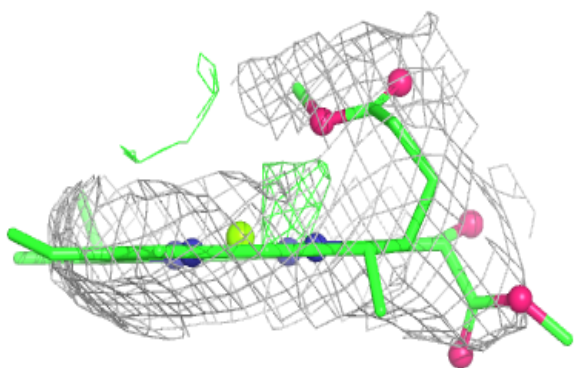
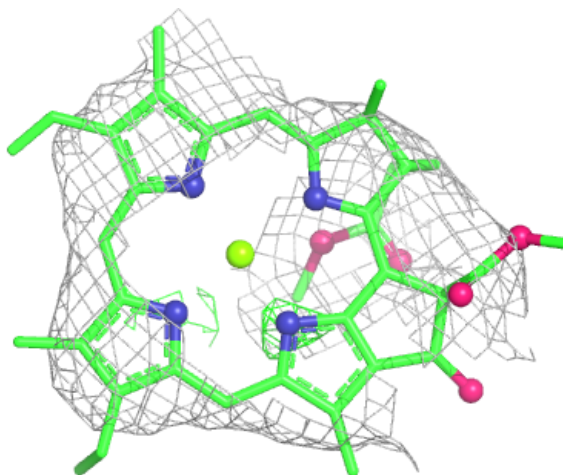
Electron density around CLA a 1011:

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



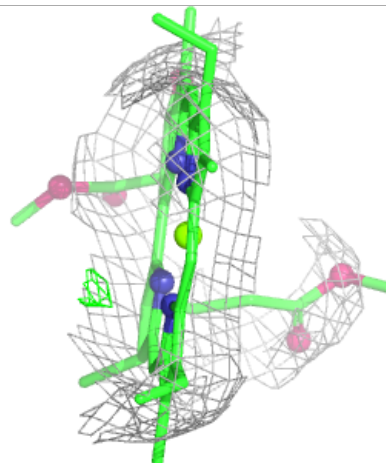
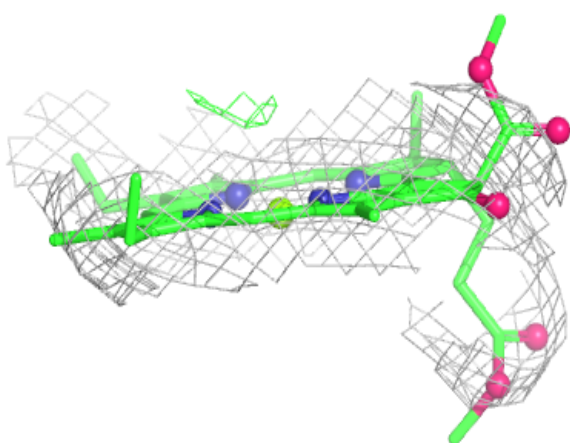
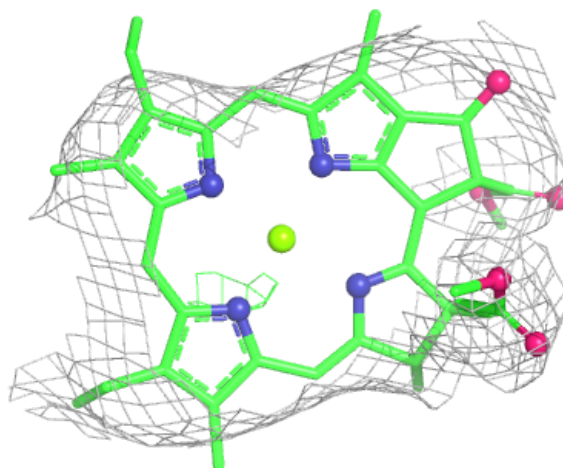
Electron density around CLA A 1136:

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



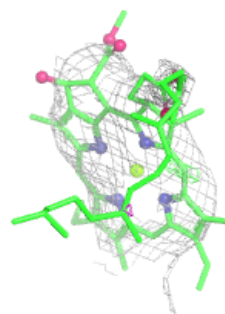
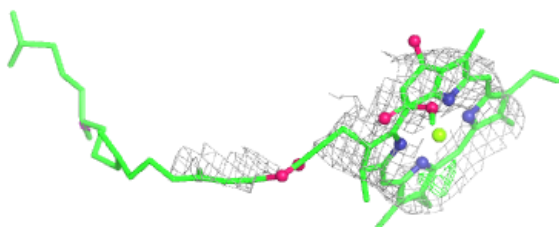
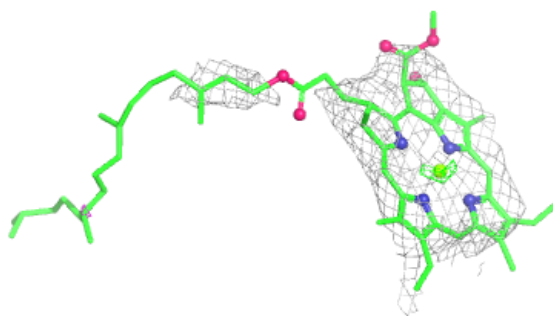
Electron density around CLA B 1211:

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



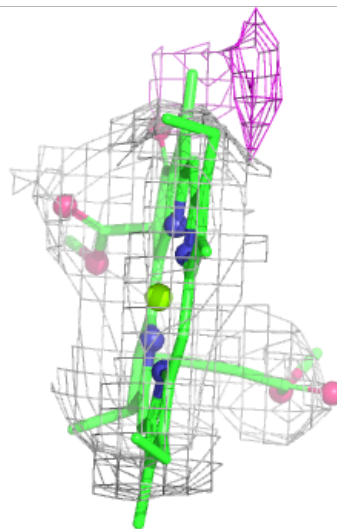
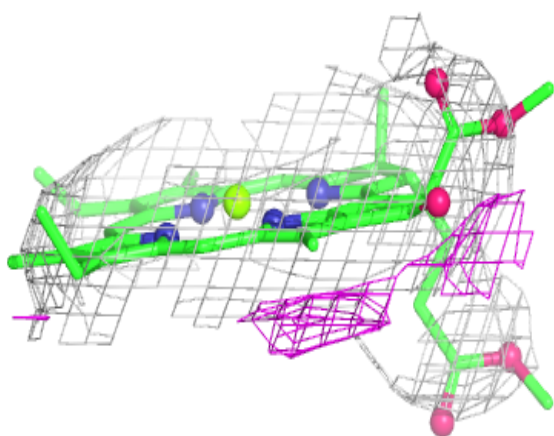
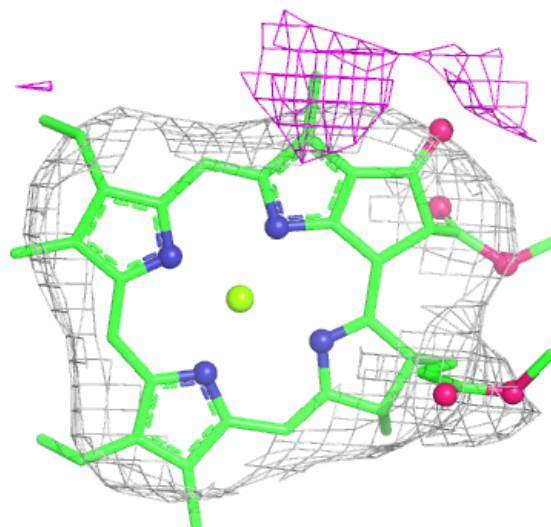
Electron density around CLA A 1012:

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



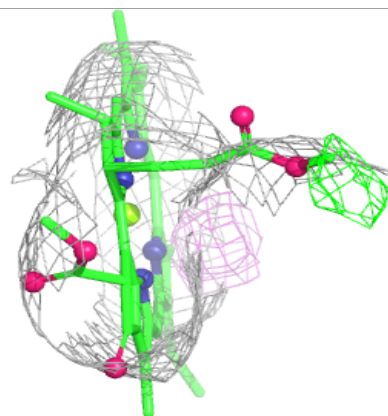
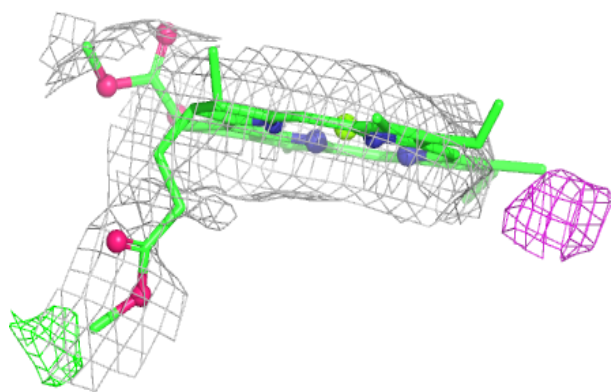
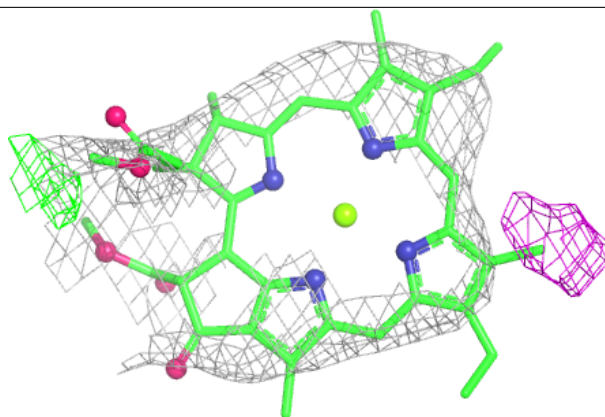
Electron density around CLA B 1239:

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

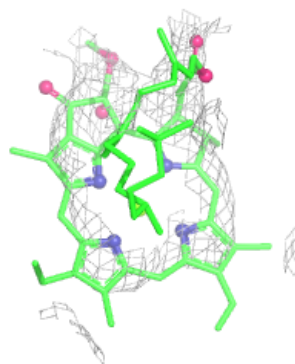
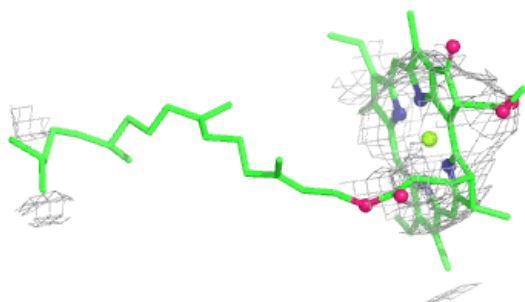
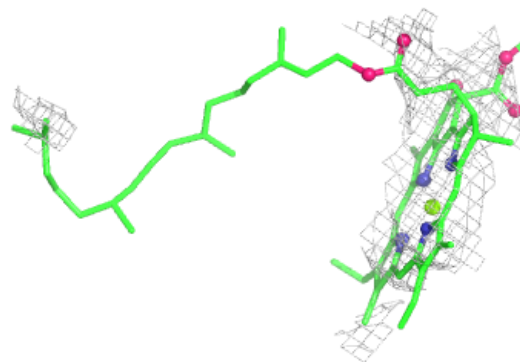


Electron density around CLA 2 1220:

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

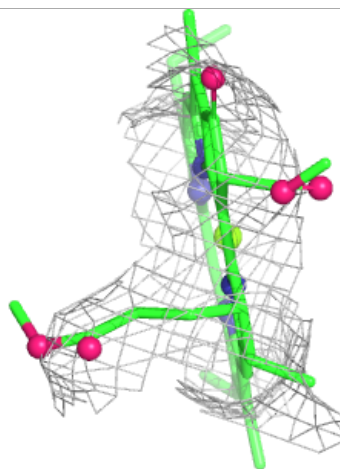
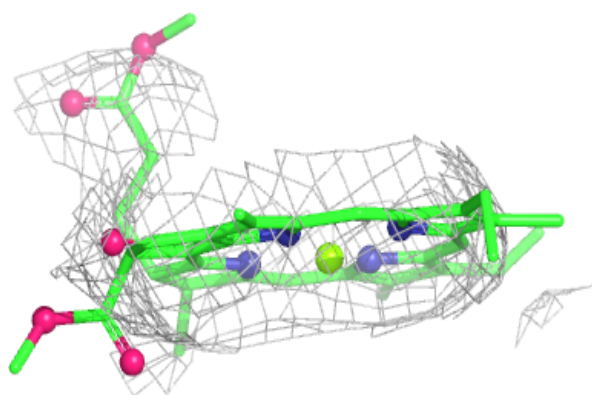
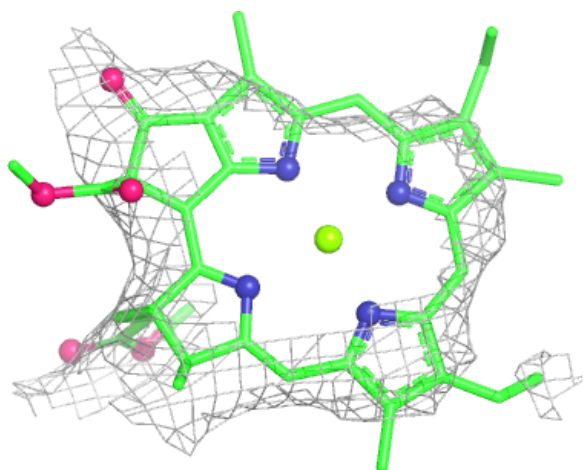
**Electron density around CLA 1 1128:**

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



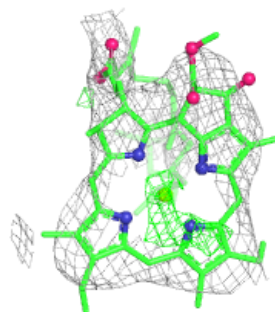
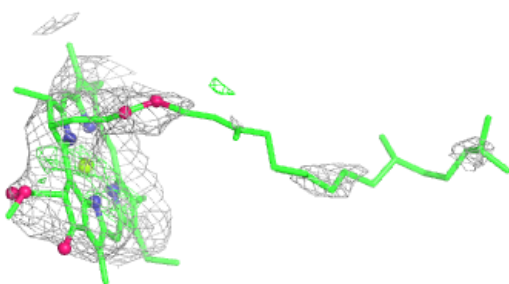
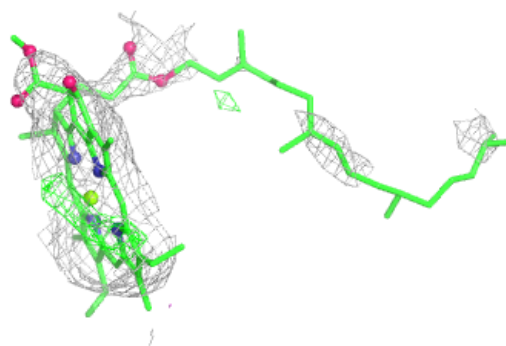
Electron density around CLA 1 1130:

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

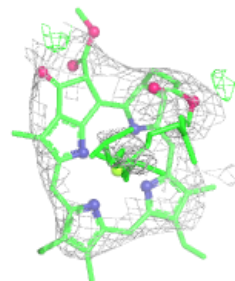
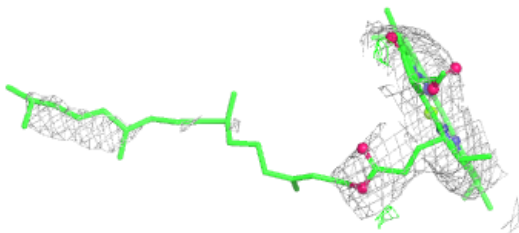
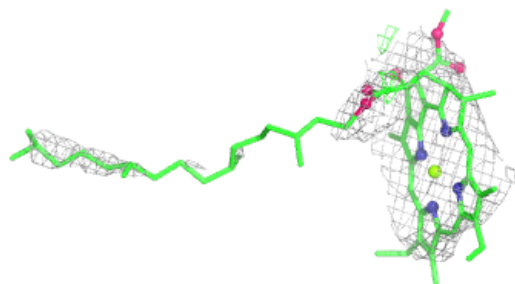


Electron density around CLA A 1128:

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

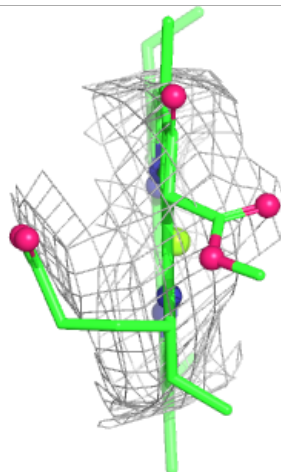
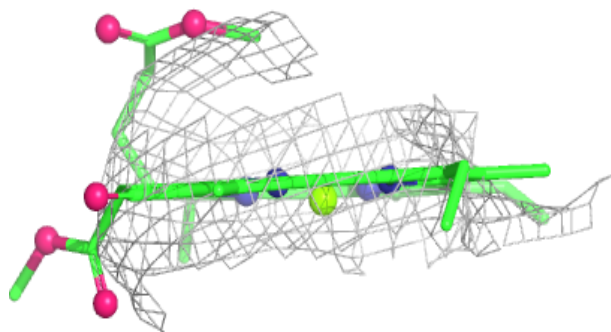
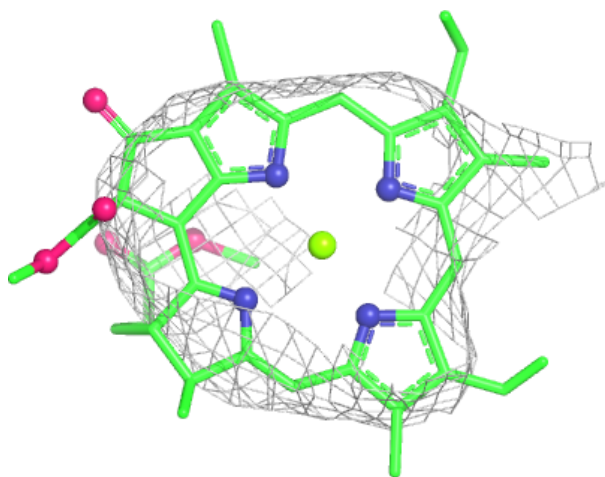
**Electron density around CLA 2 1225:**

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



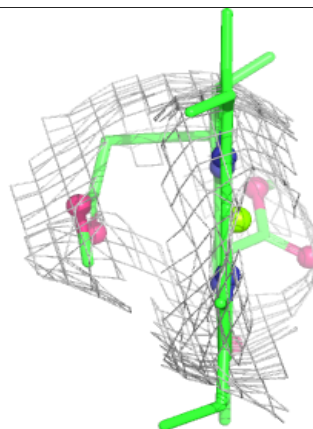
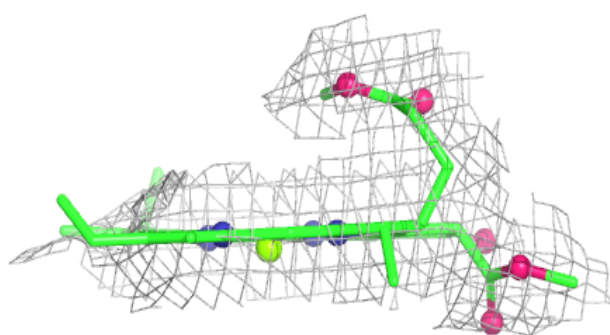
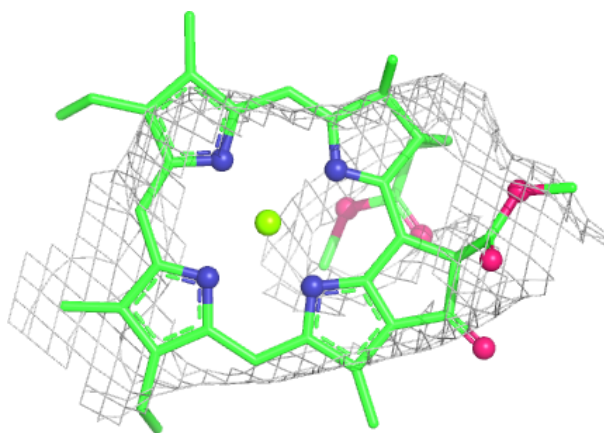
Electron density around CLA a 1115:

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

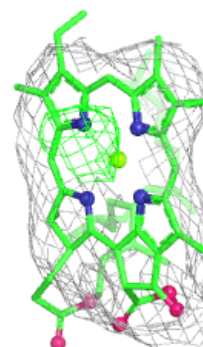
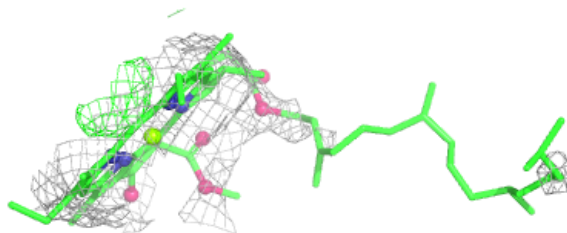
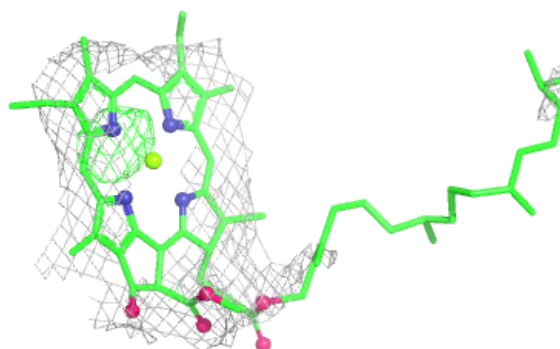


Electron density around CLA 1 1138:

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

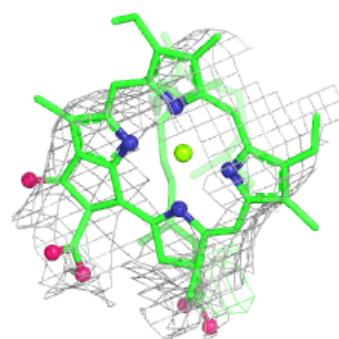
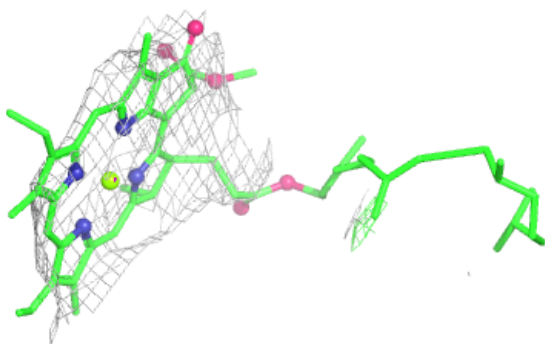
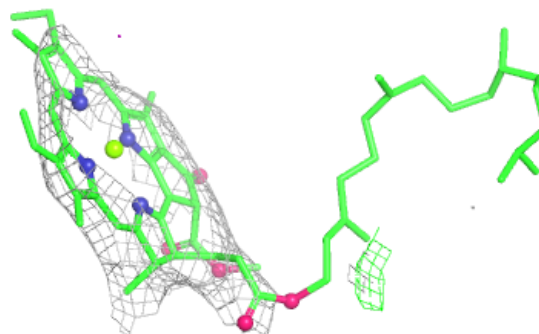
**Electron density around CLA B 1207:**

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

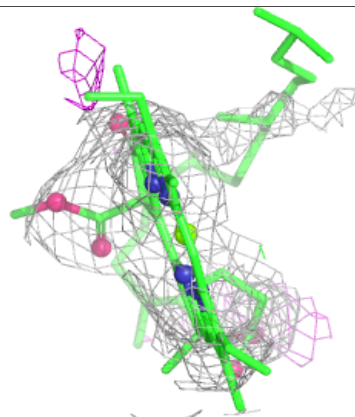
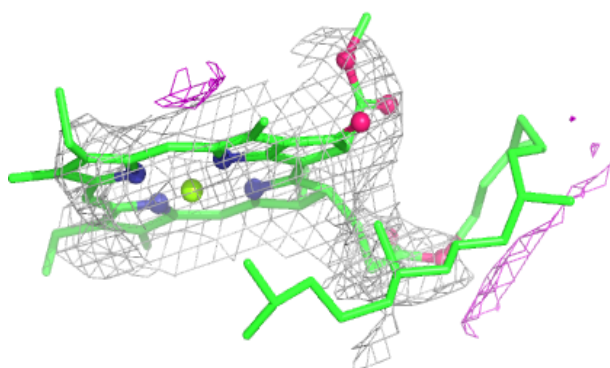
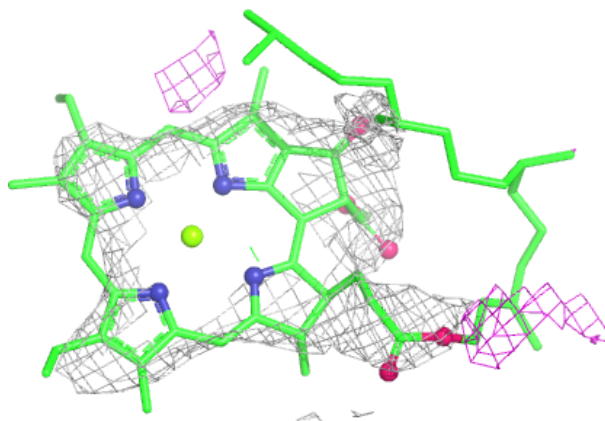


Electron density around CLA b 1021:

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

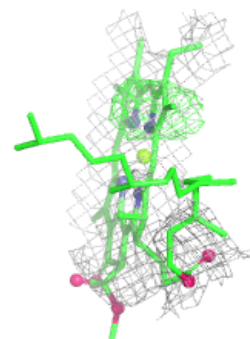
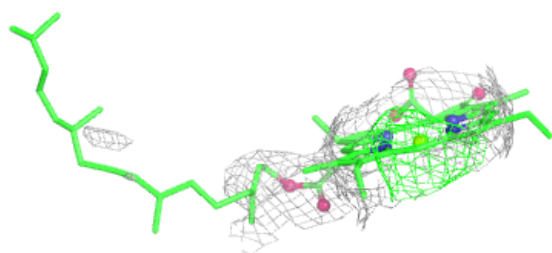
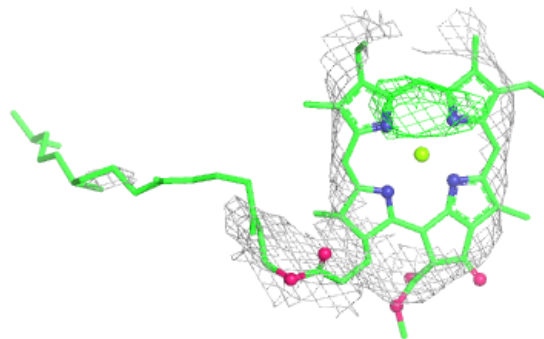
**Electron density around CLA 2 1202:**

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



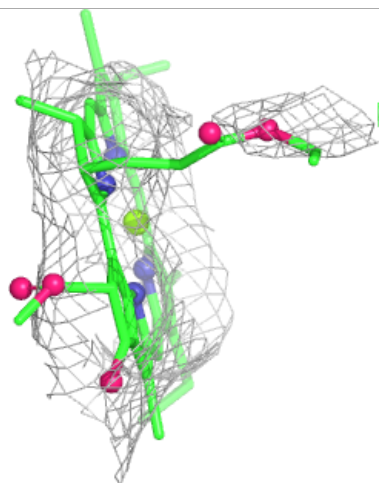
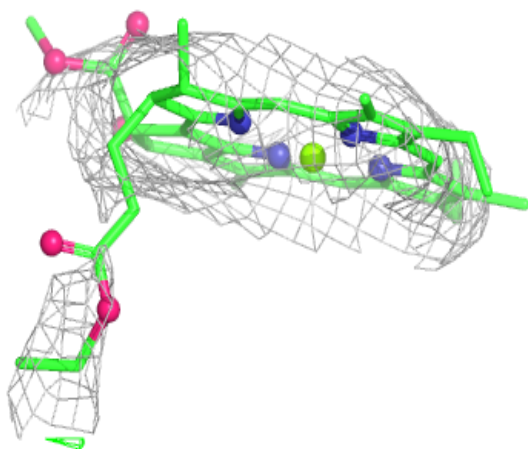
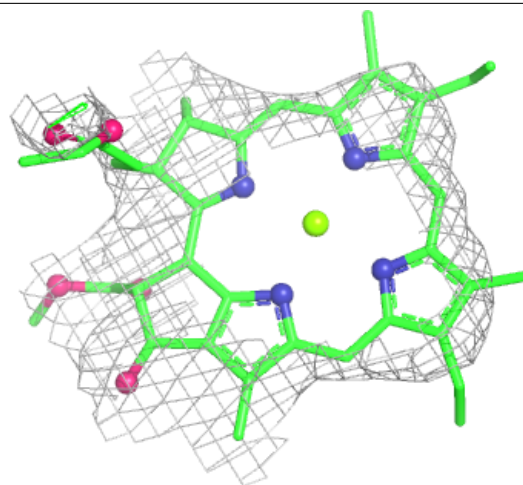
Electron density around CLA b 1023:

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



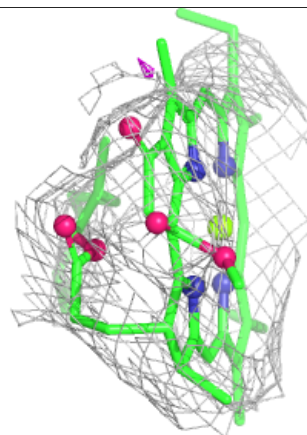
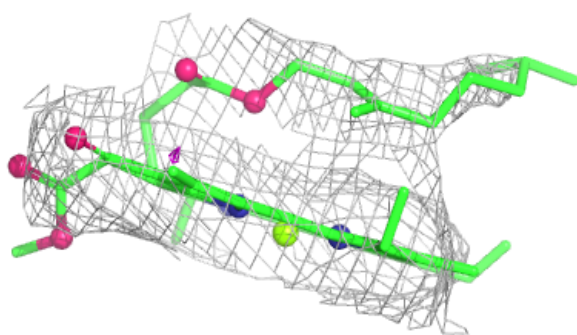
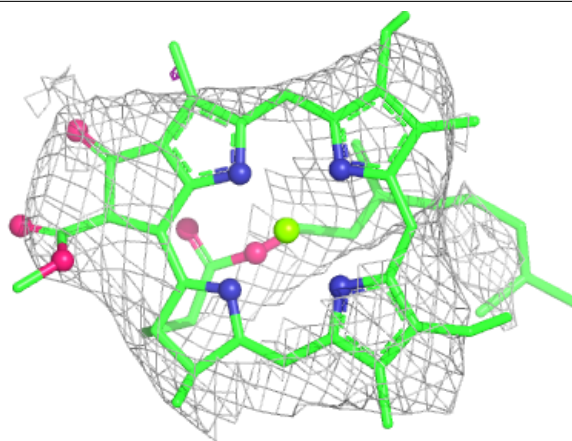
Electron density around CLA B 1236:

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



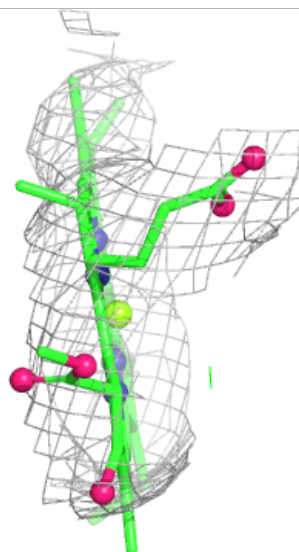
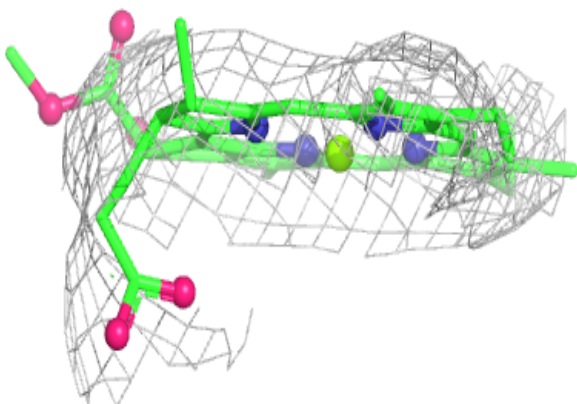
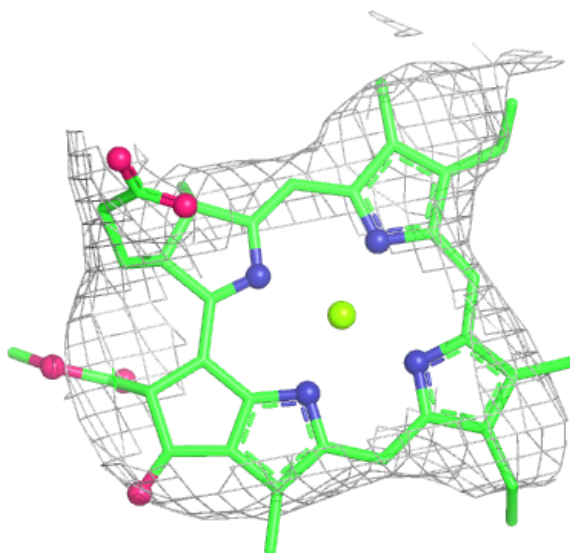
Electron density around CLA 2 1205:

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



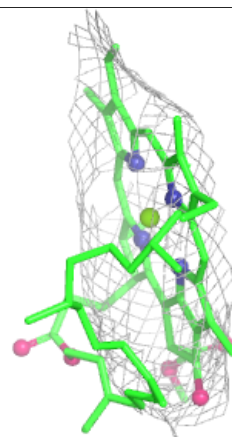
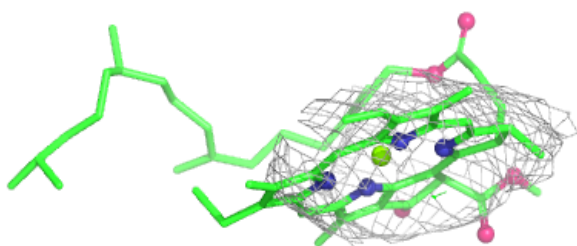
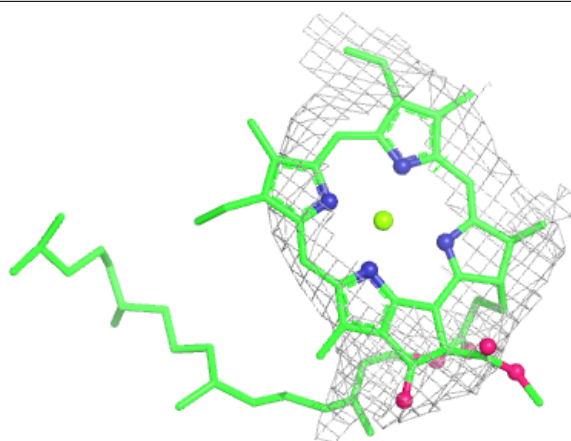
Electron density around CLA A 1108:

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



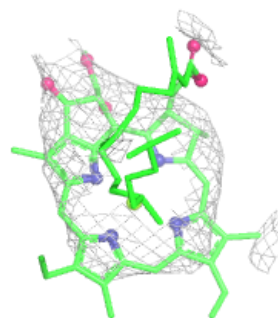
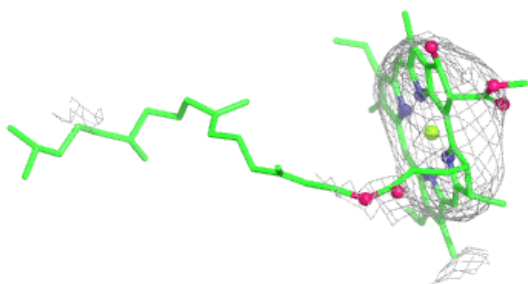
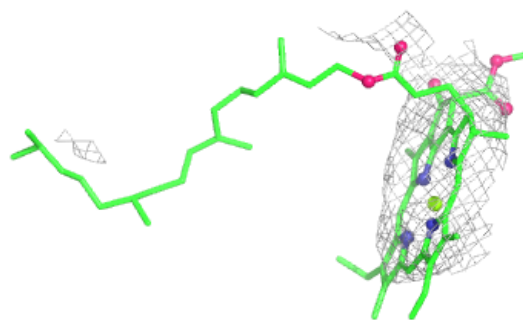
Electron density around CLA a 1127:

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



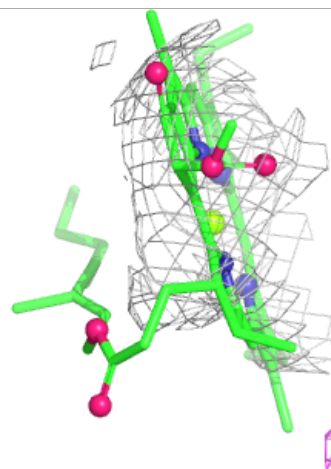
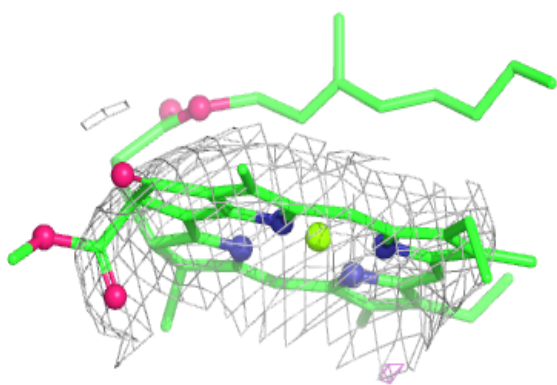
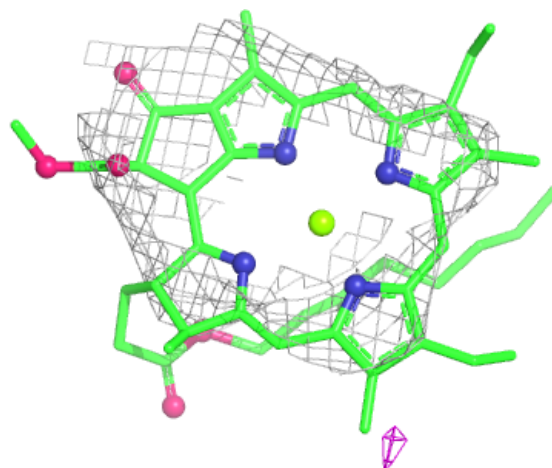
Electron density around CLA a 1128:

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



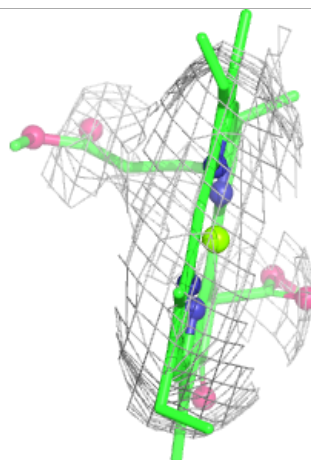
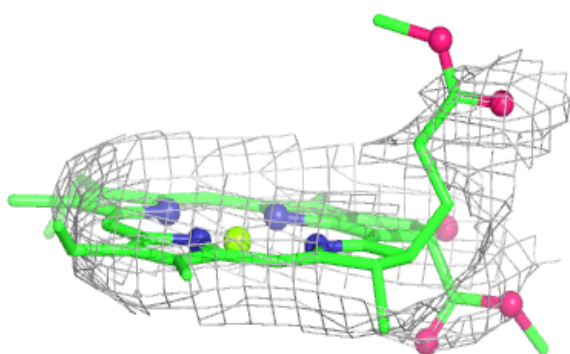
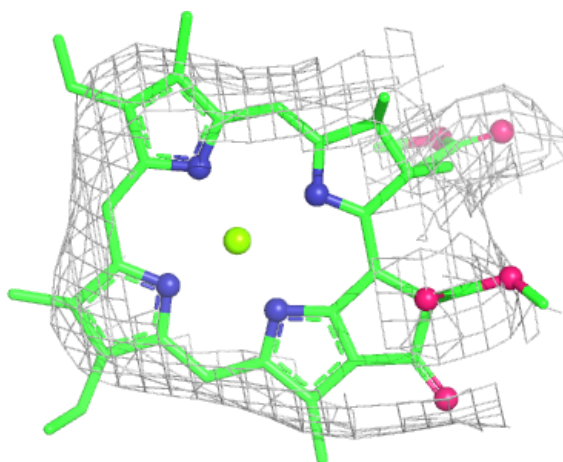
Electron density around CLA 1 1116:

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



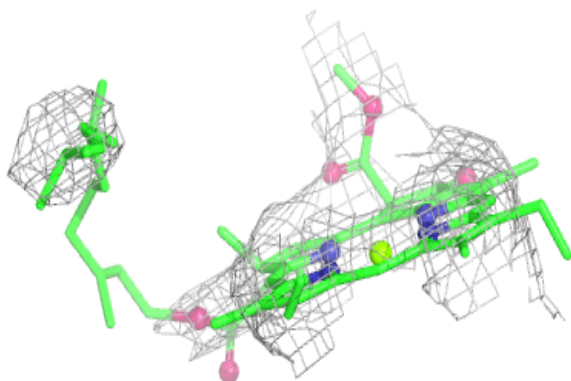
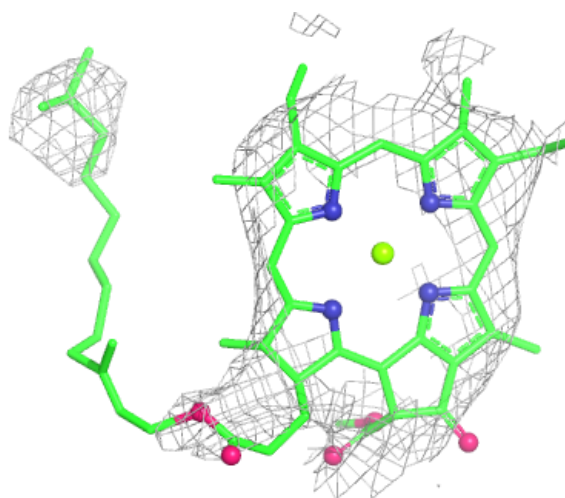
Electron density around CLA a 1130:

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



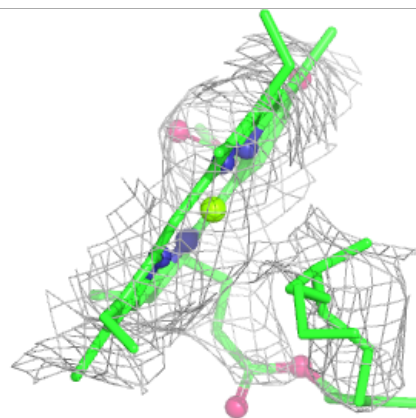
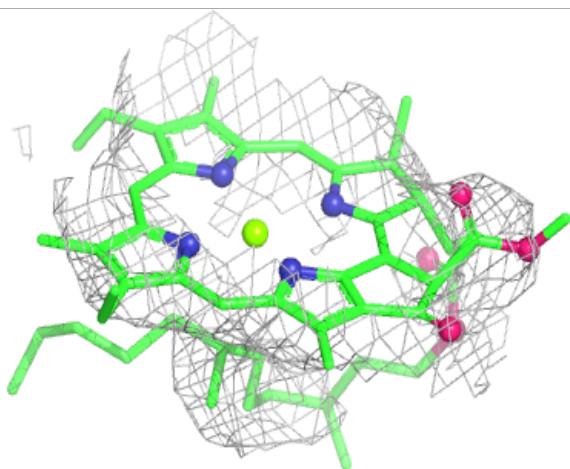
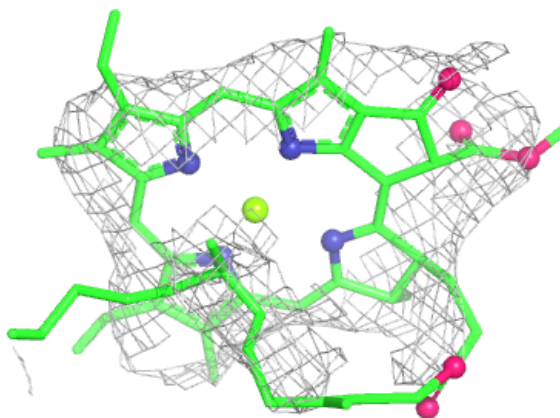
Electron density around CLA A 1111:

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



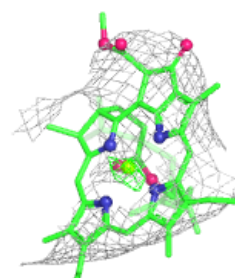
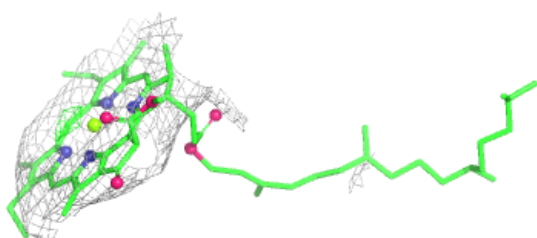
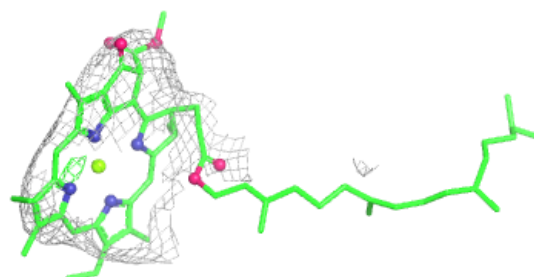
Electron density around CLA 2 1214:

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

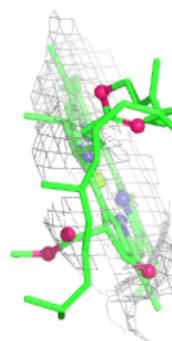
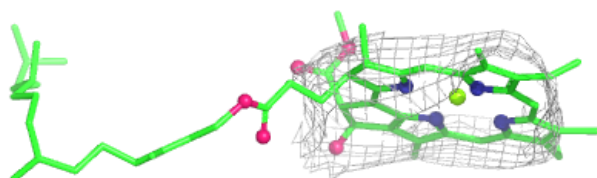
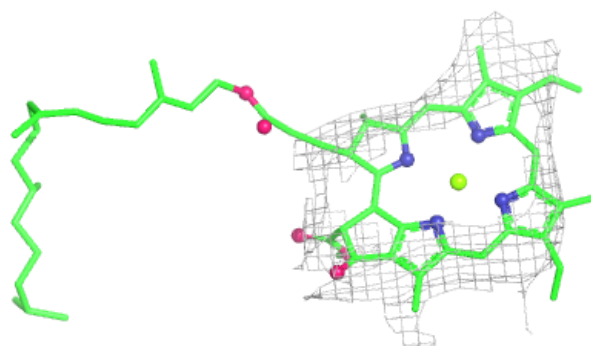


Electron density around CLA 1 1119:

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

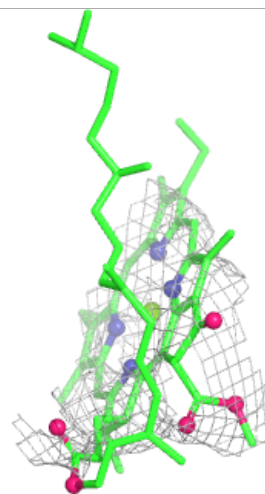
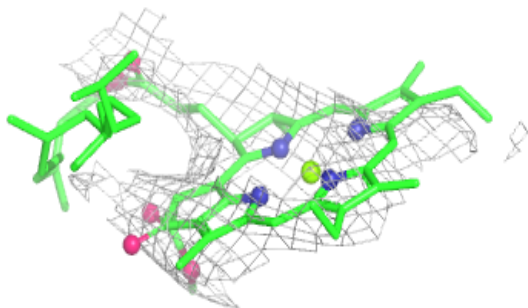
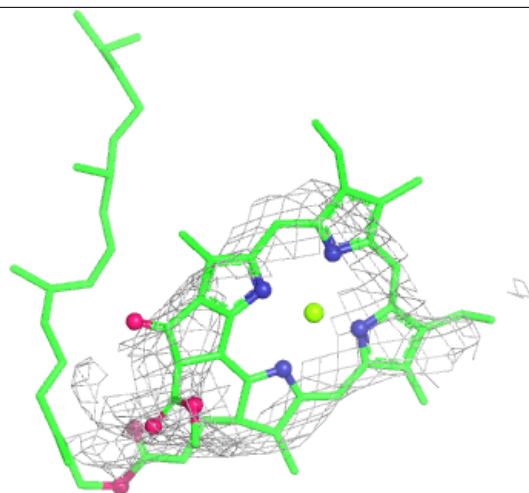
**Electron density around CLA B 1223:**

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



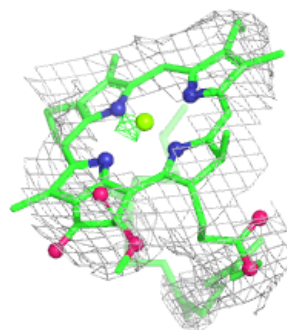
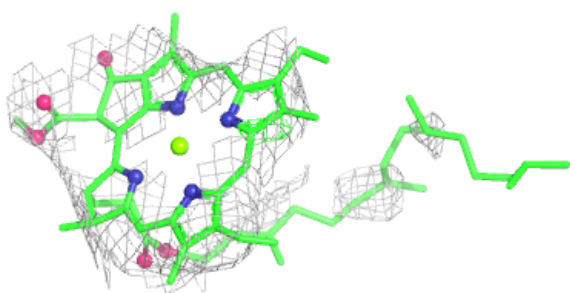
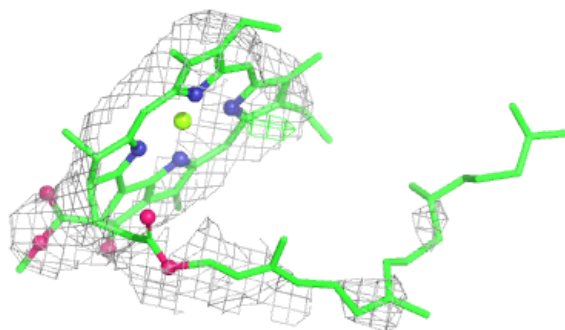
Electron density around CLA 1 1123:

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

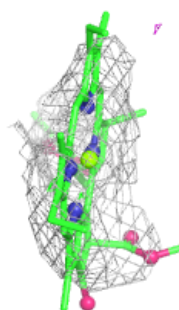
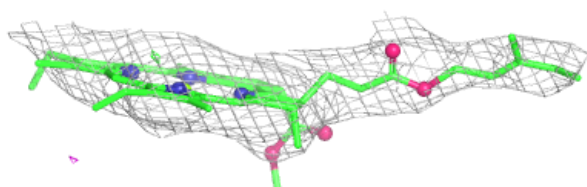
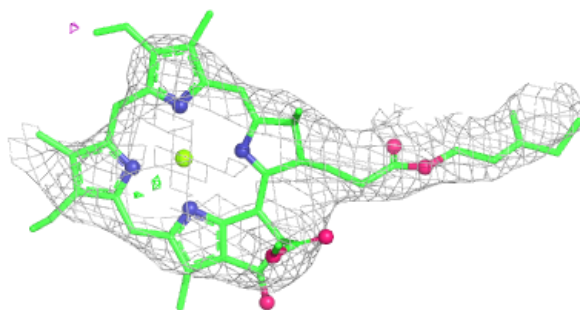


Electron density around CLA A 1109:

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

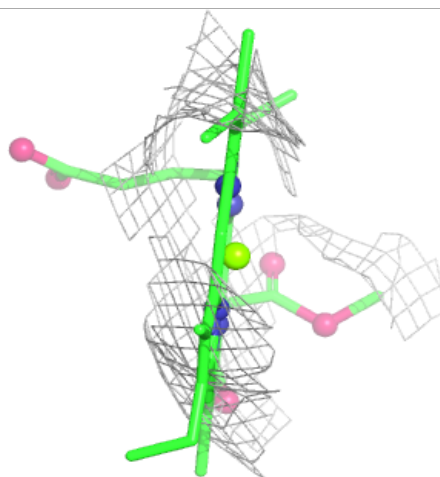
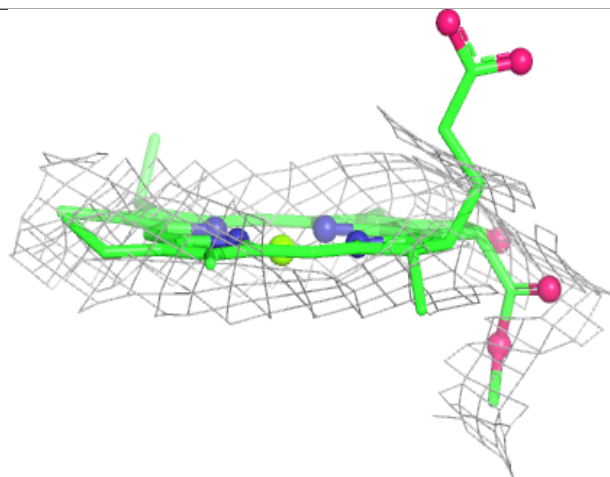
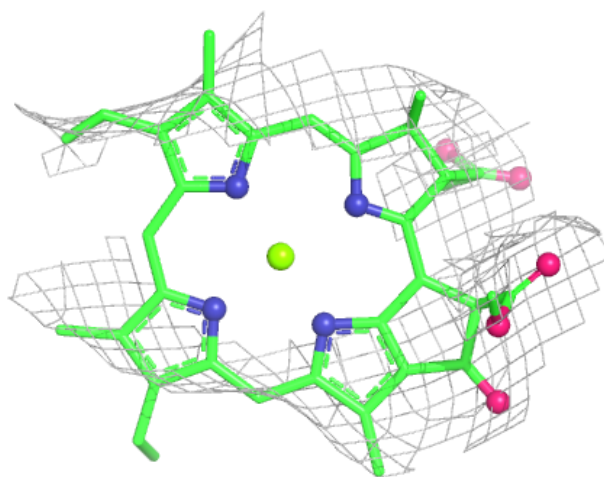
**Electron density around CLA A 1135:**

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



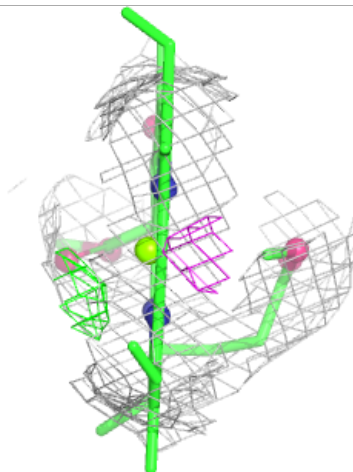
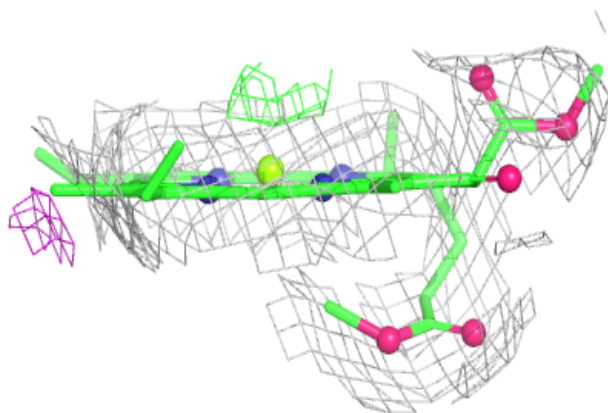
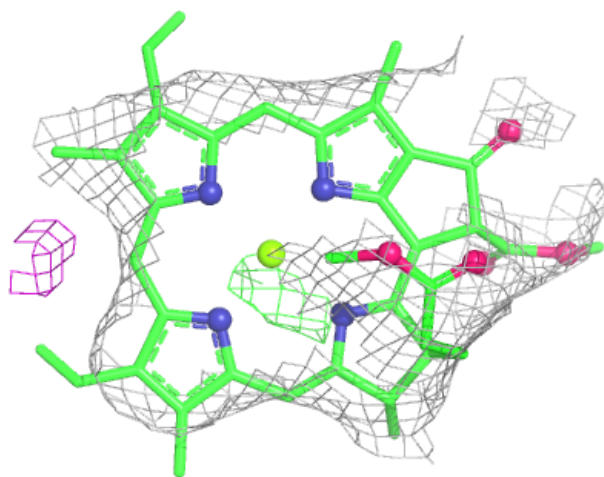
Electron density around CLA b 1212:

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



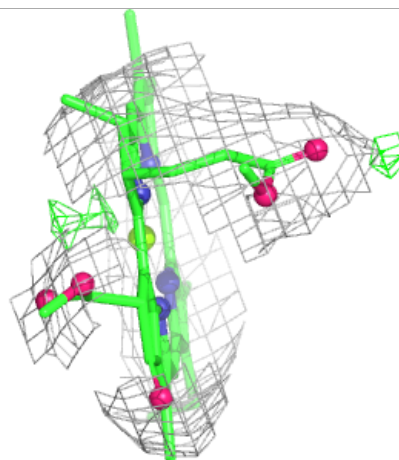
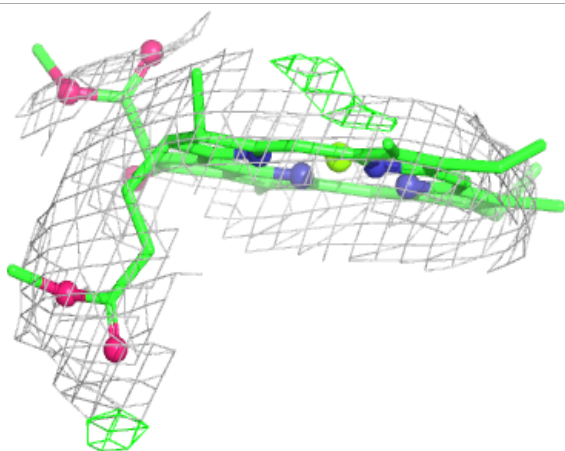
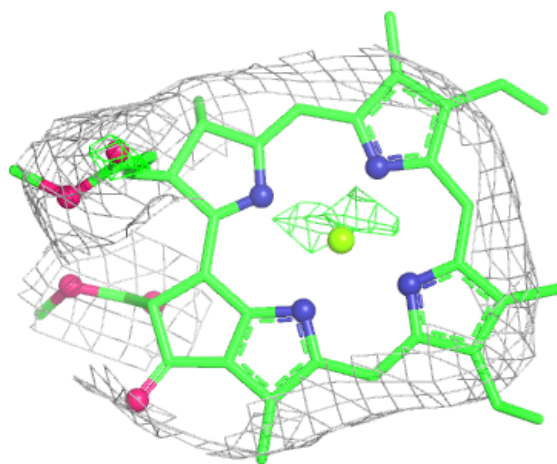
Electron density around CLA A 1115:

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



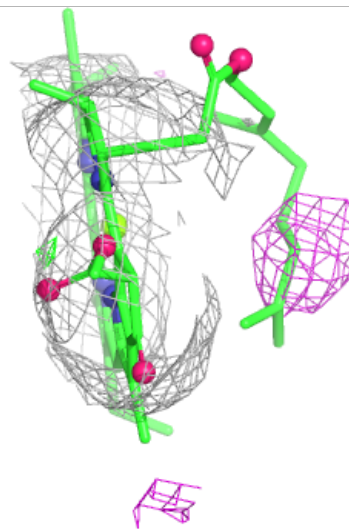
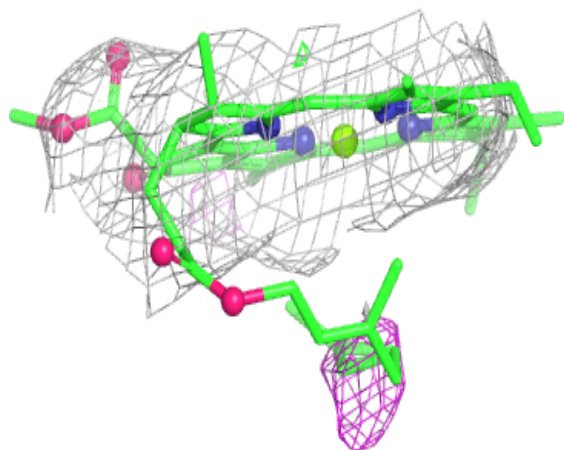
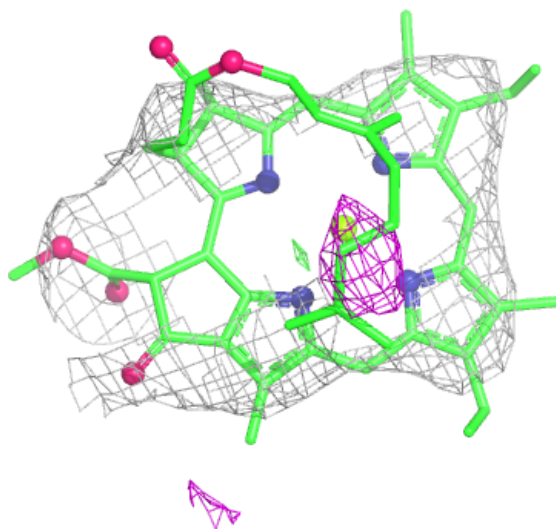
Electron density around CLA b 1239:

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



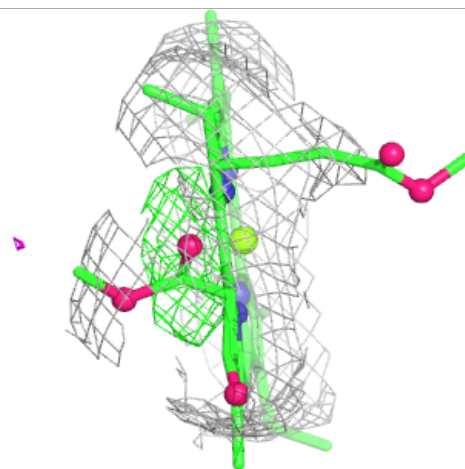
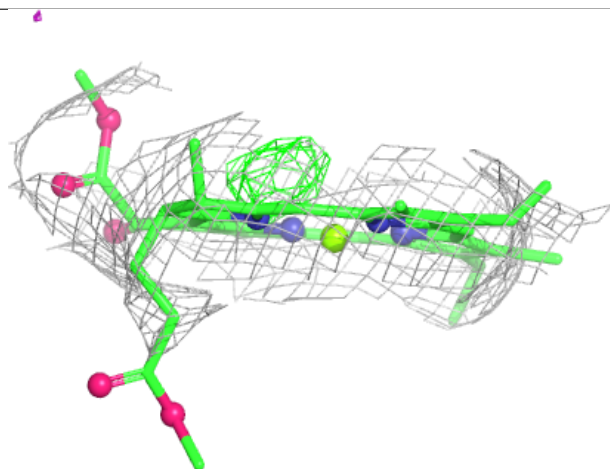
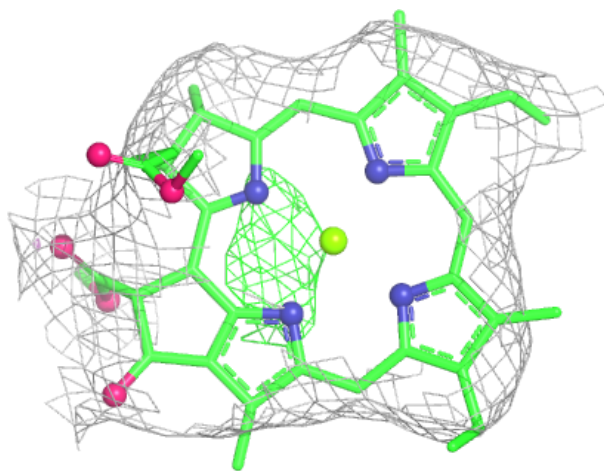
Electron density around CLA 2 1224:

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



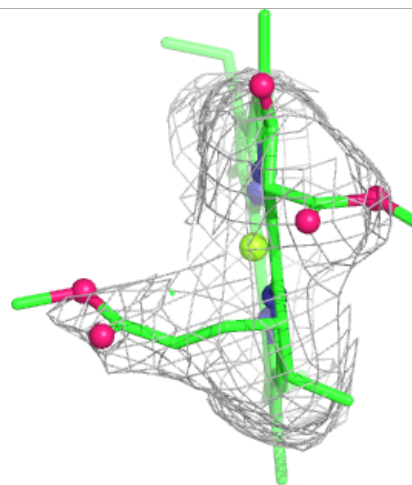
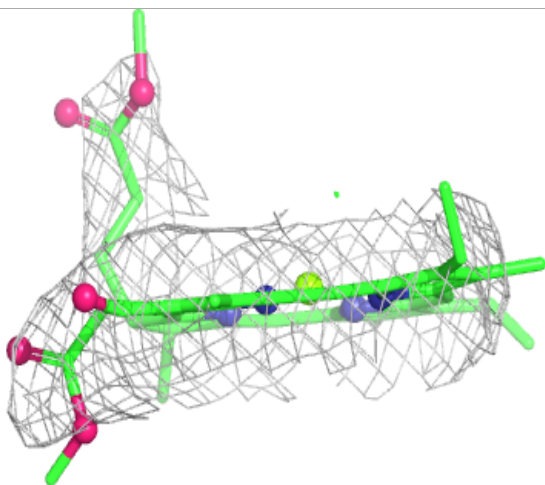
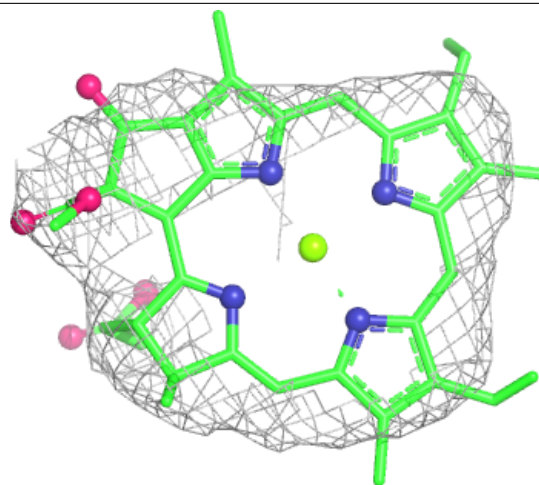
Electron density around CLA L 1502:

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



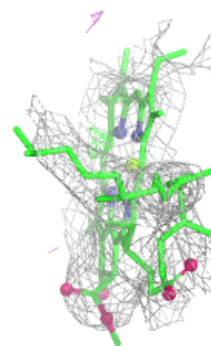
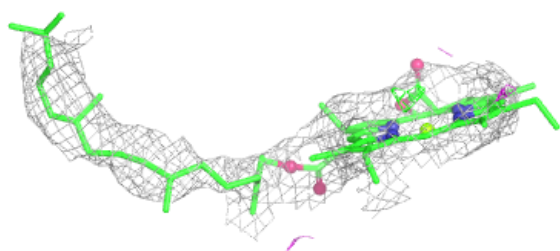
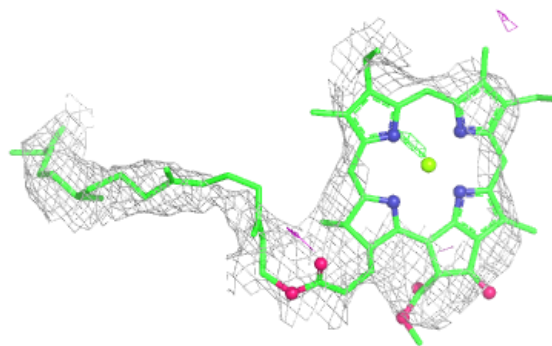
Electron density around CLA 1 1502:

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

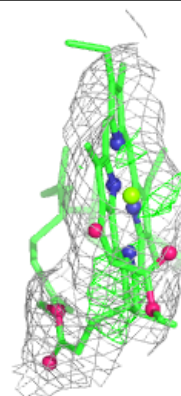
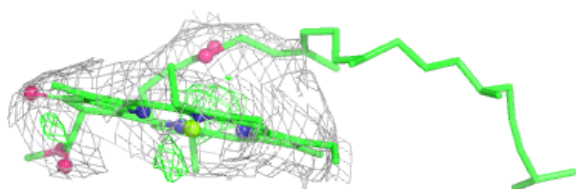
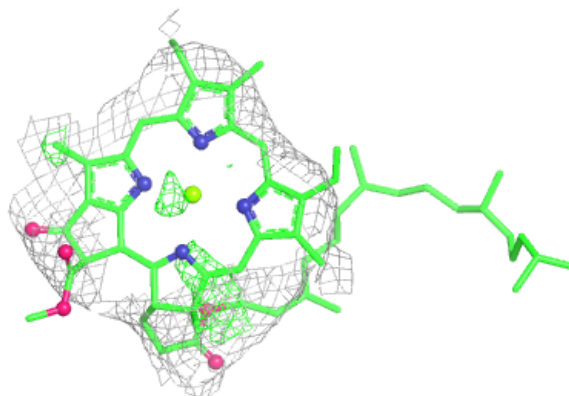


Electron density around CLA B 1023:

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

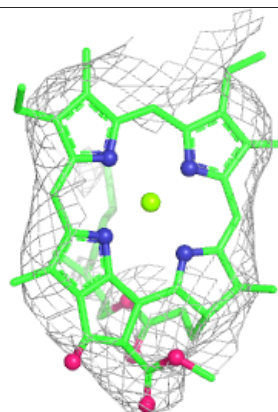
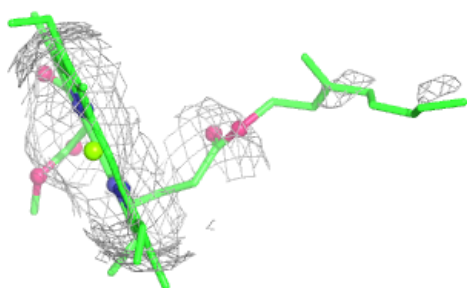
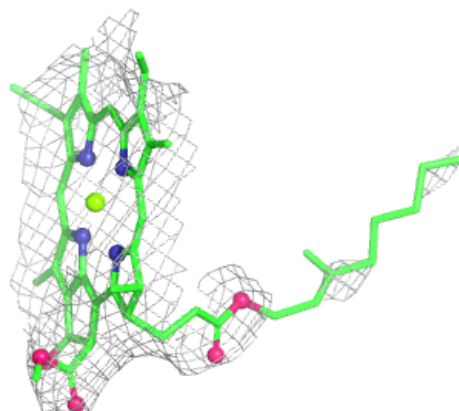
**Electron density around CLA B 1215:**

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

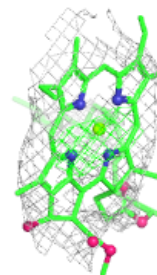
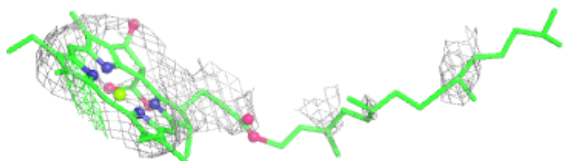
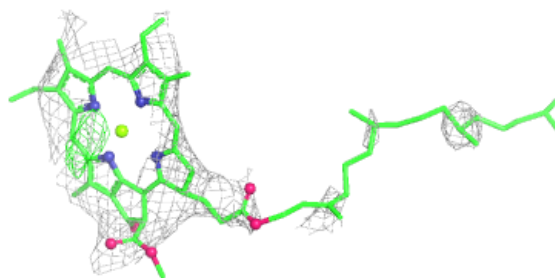


Electron density around CLA B 1201:

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

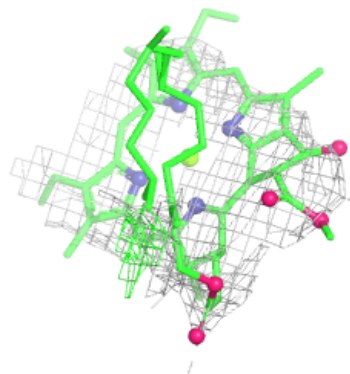
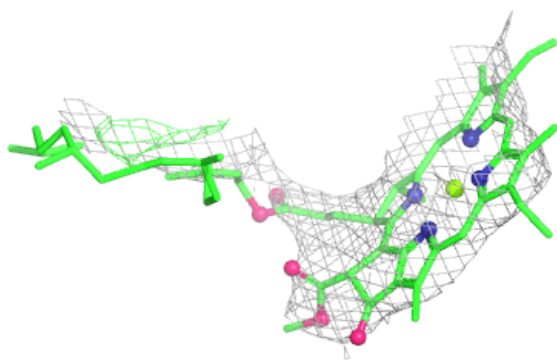
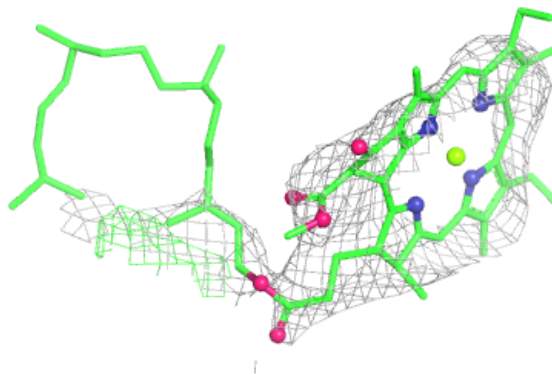
**Electron density around CLA 1 1022:**

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



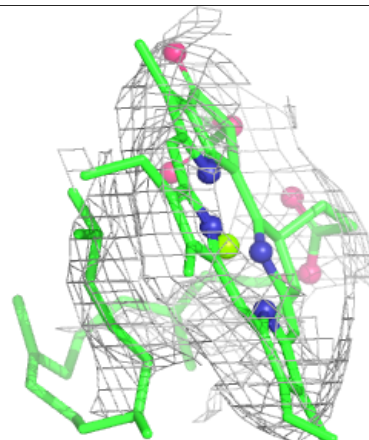
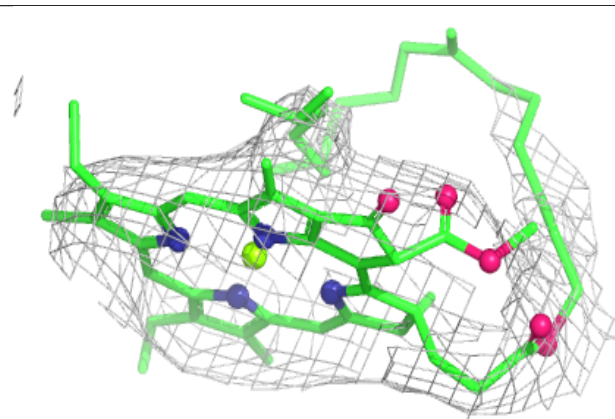
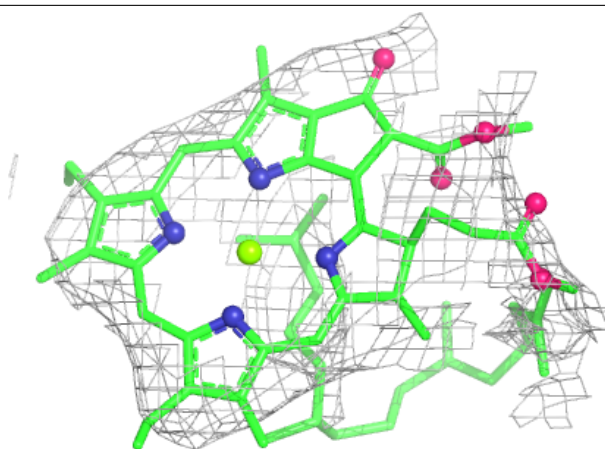
Electron density around CLA 1 1011:

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



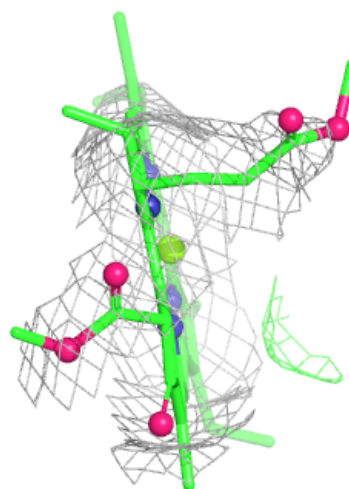
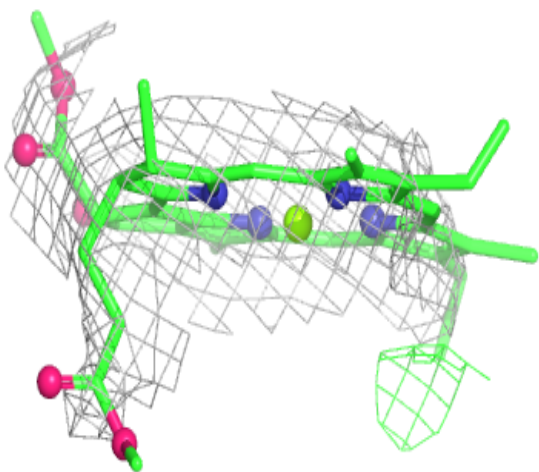
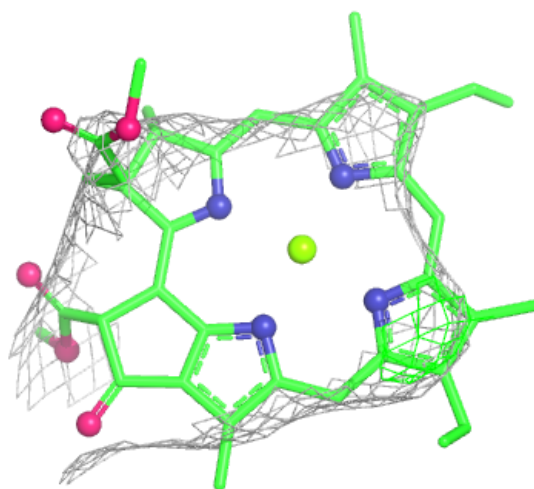
Electron density around CLA B 1203:

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



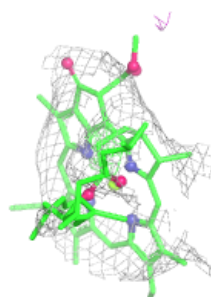
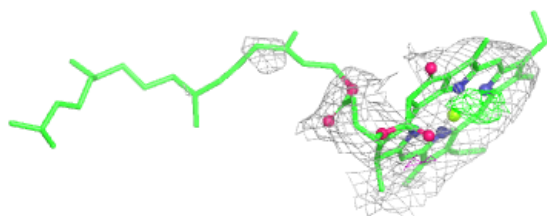
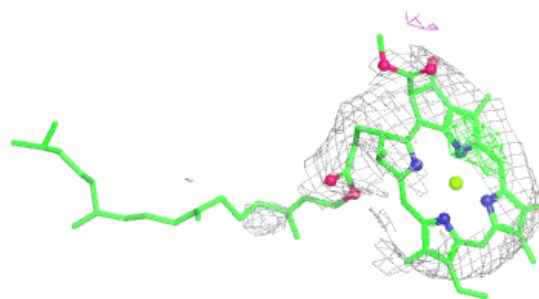
Electron density around CLA a 1129:

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



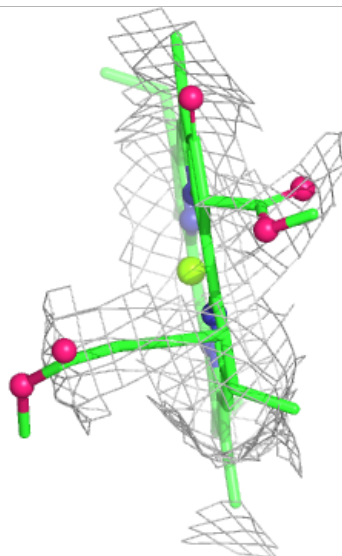
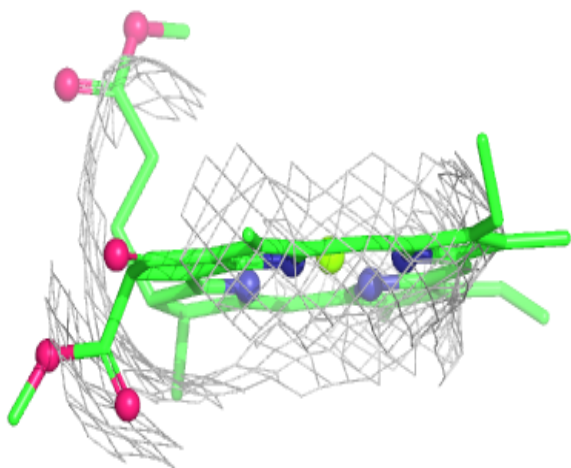
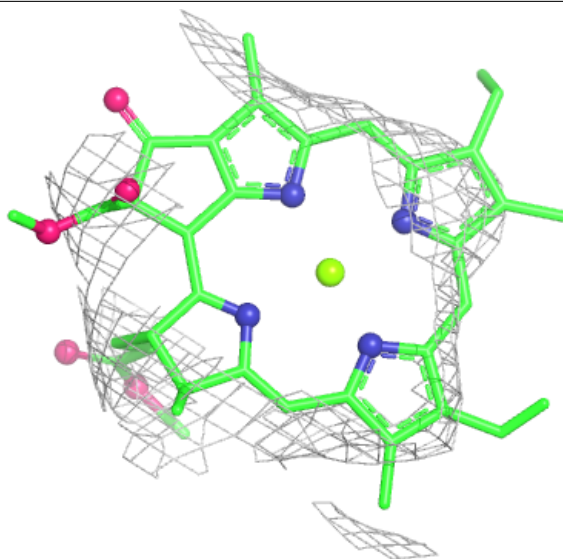
Electron density around CLA a 1119:

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



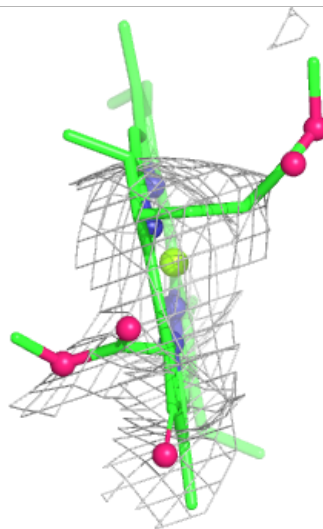
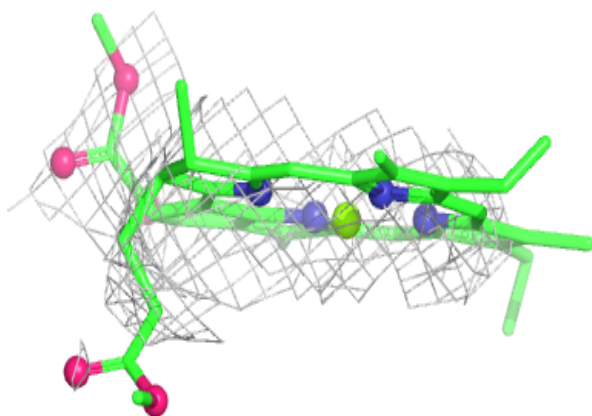
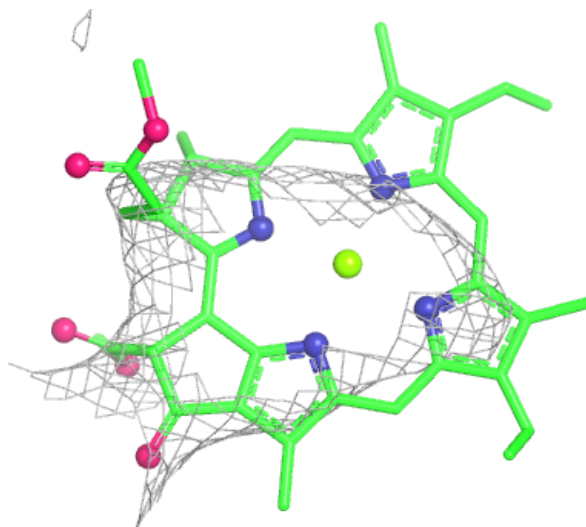
Electron density around CLA a 1133:

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



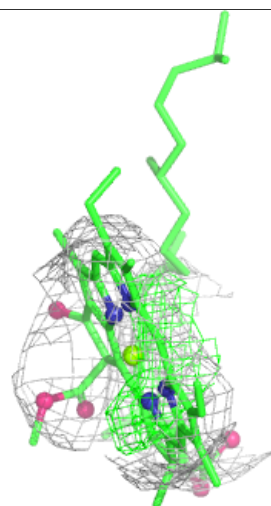
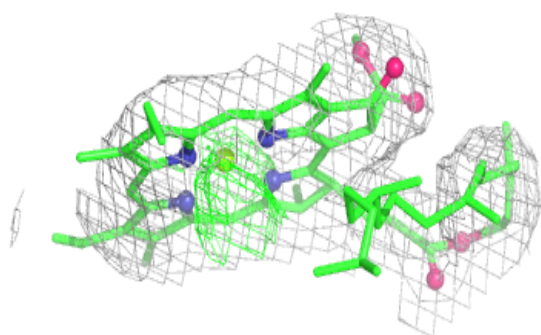
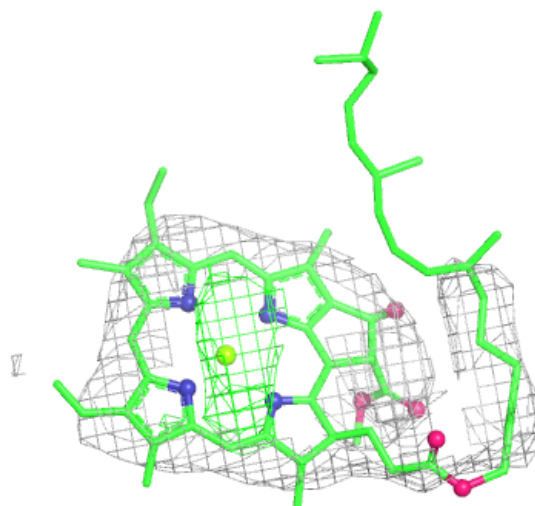
Electron density around CLA 1 1129:

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



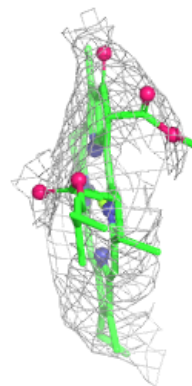
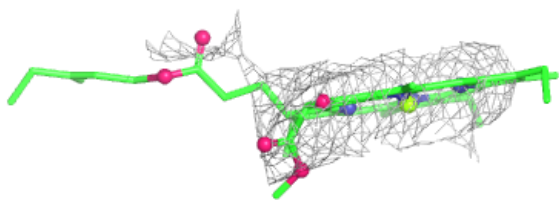
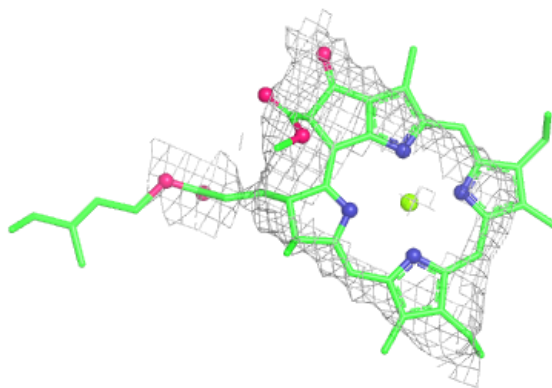
Electron density around CLA A 1123:

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



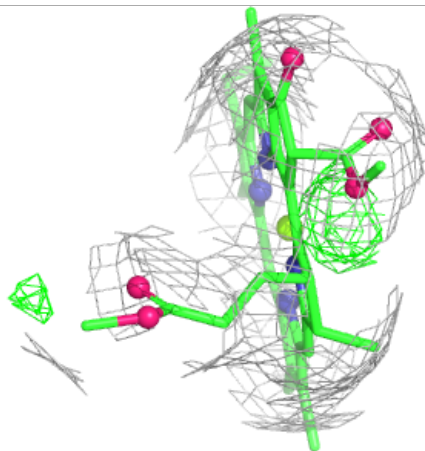
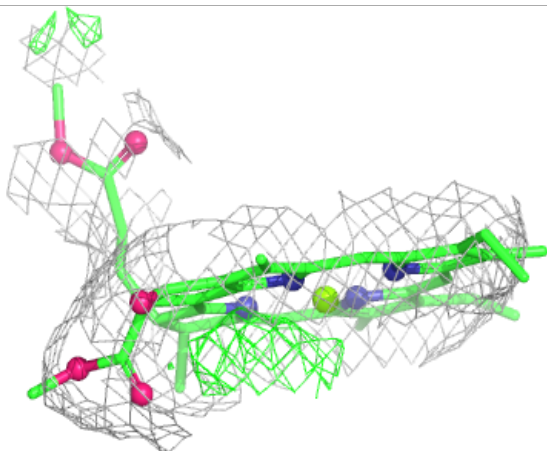
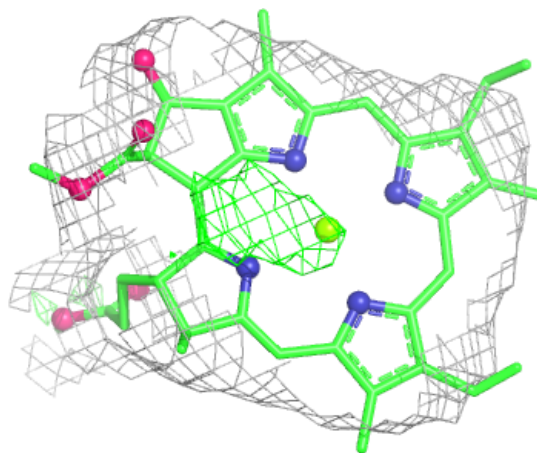
Electron density around CLA a 1135:

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



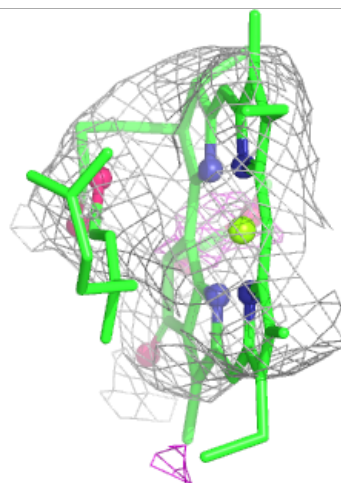
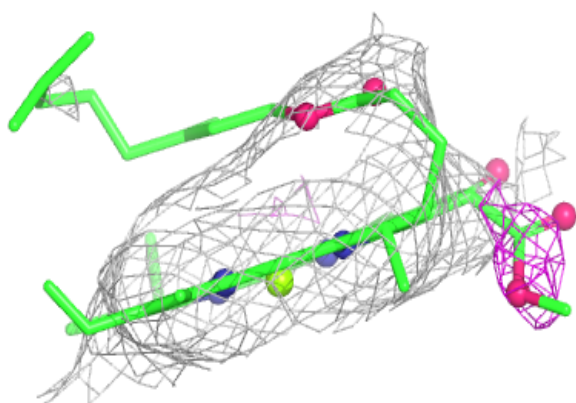
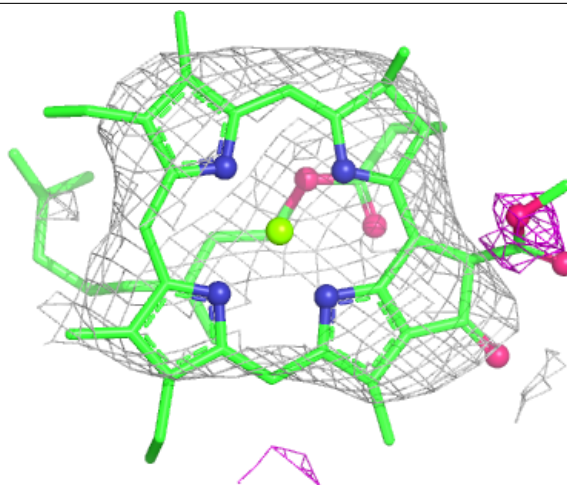
Electron density around CLA 2 1239:

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



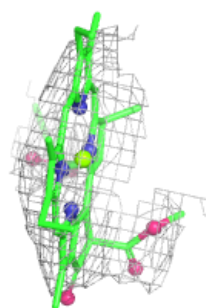
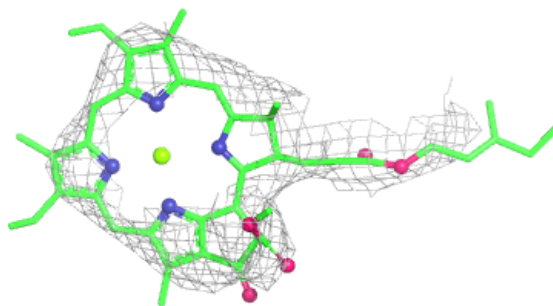
Electron density around CLA B 1205:

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

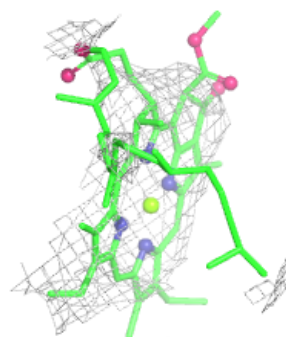
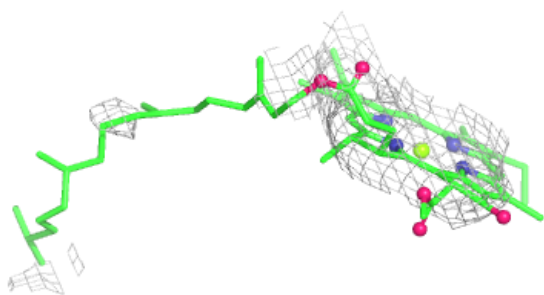
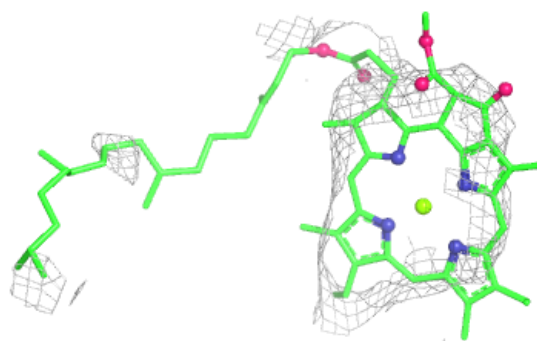


Electron density around CLA 1 1135:

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

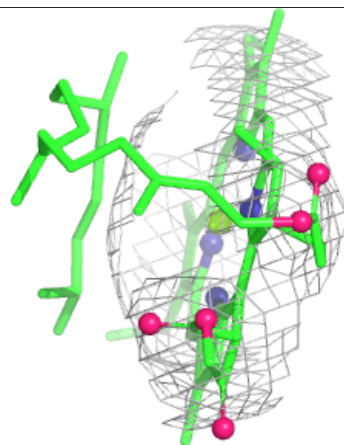
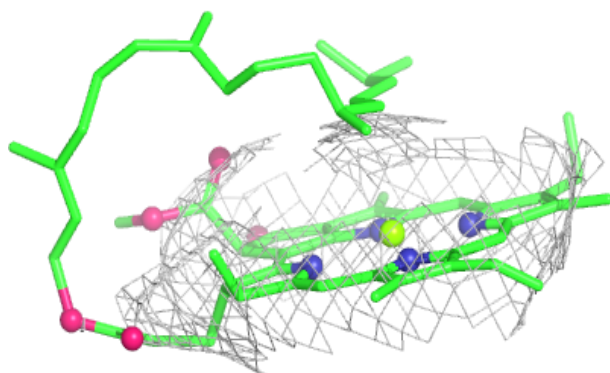
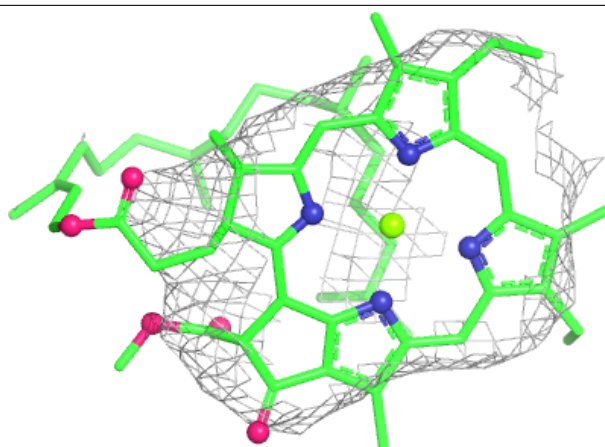
**Electron density around CLA 2 1013:**

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



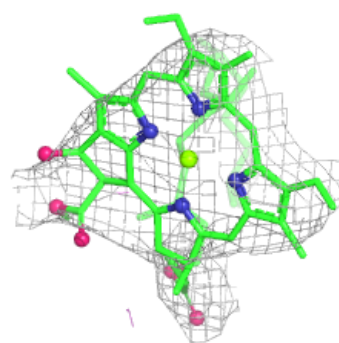
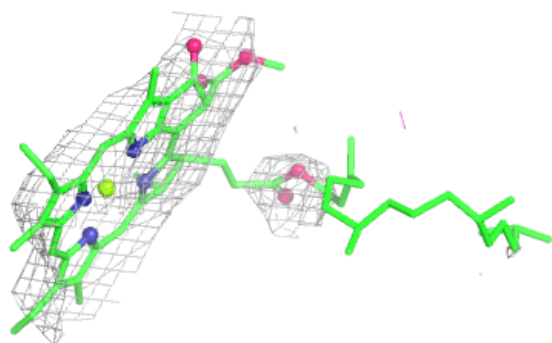
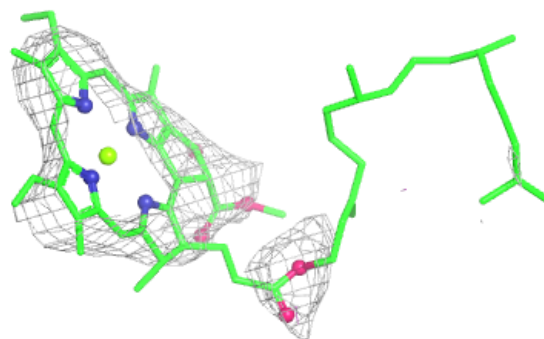
Electron density around CLA a 1104:

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

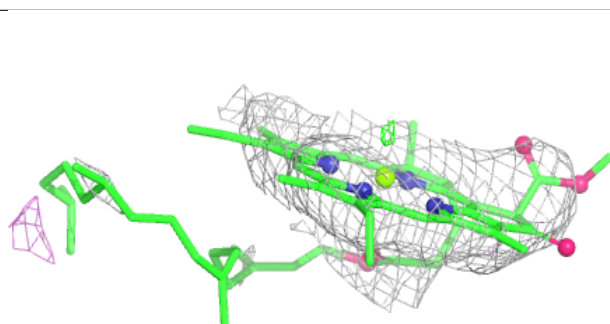
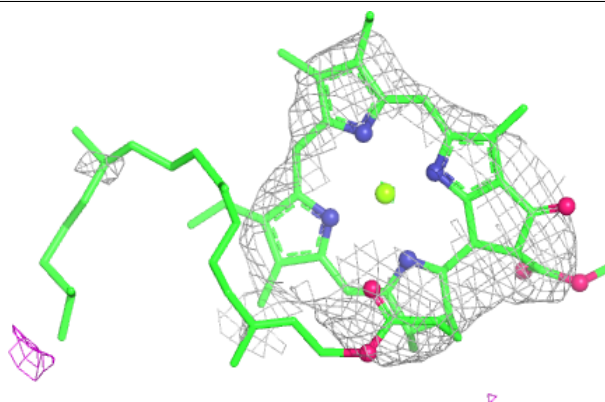


Electron density around CLA A 1011:

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

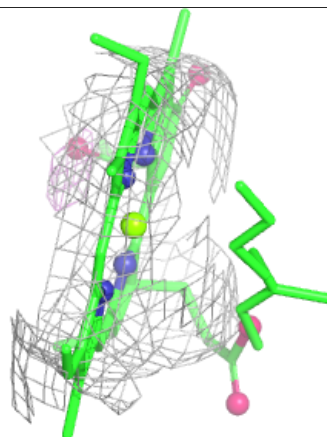
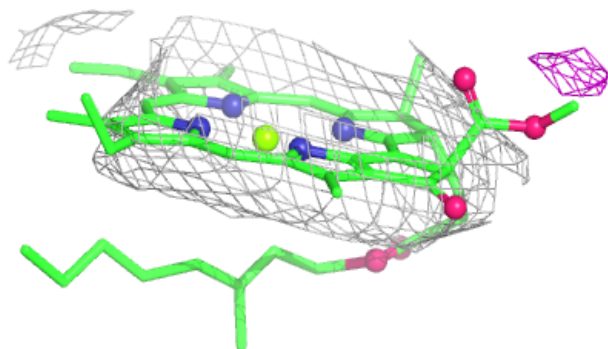
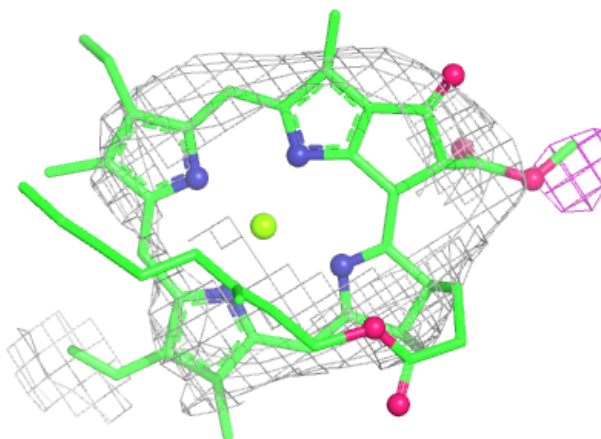
**Electron density around CLA A 1117:**

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



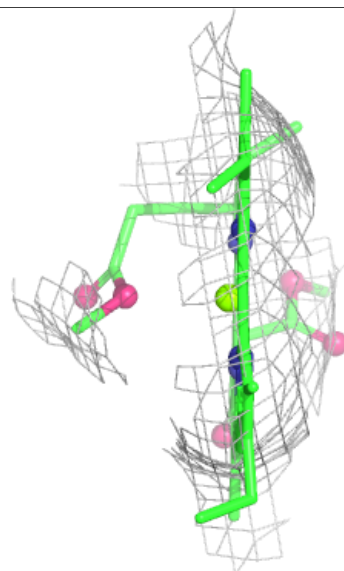
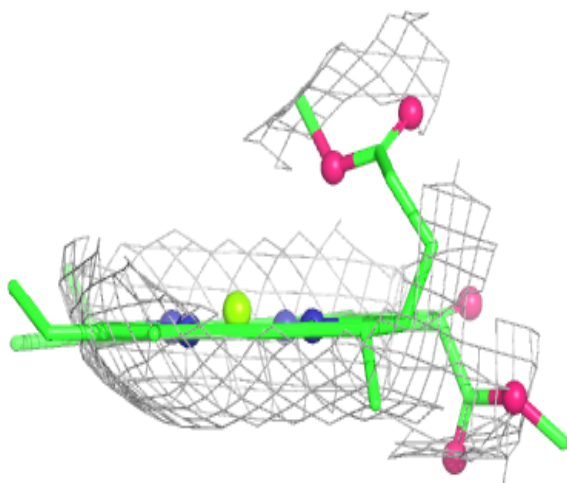
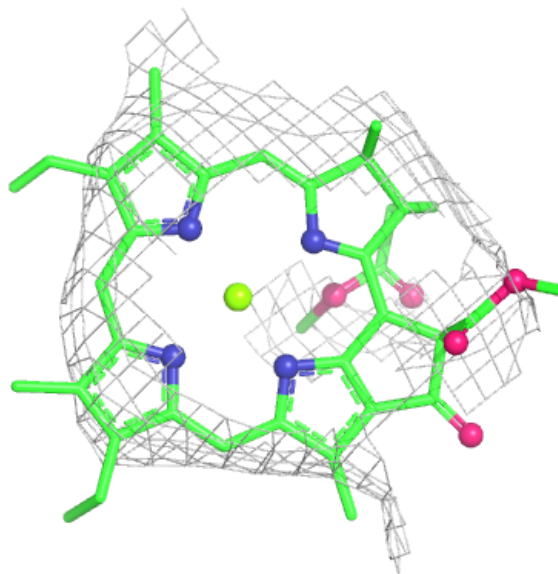
Electron density around CLA a 1116:

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



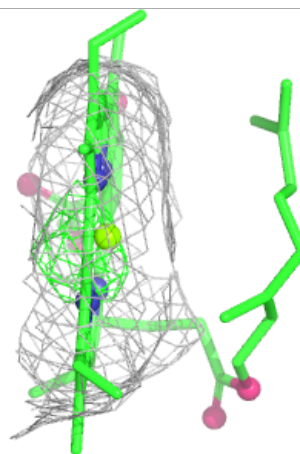
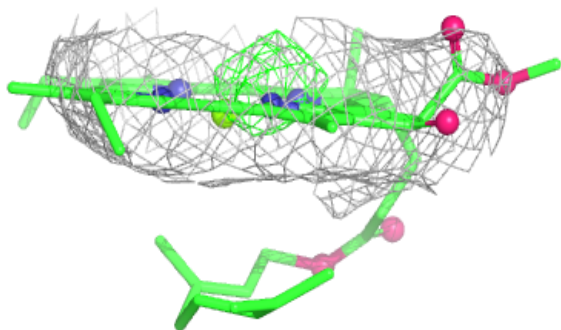
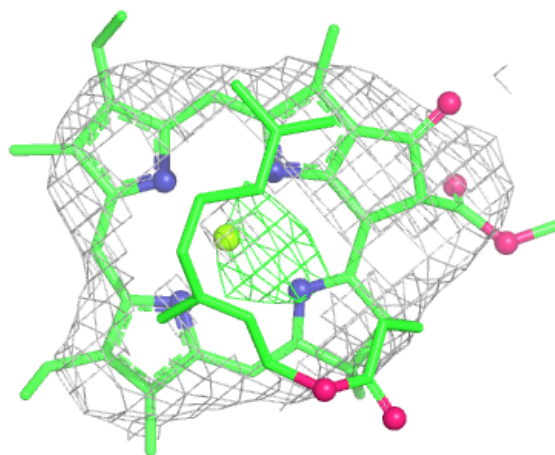
Electron density around CLA 1 1136:

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



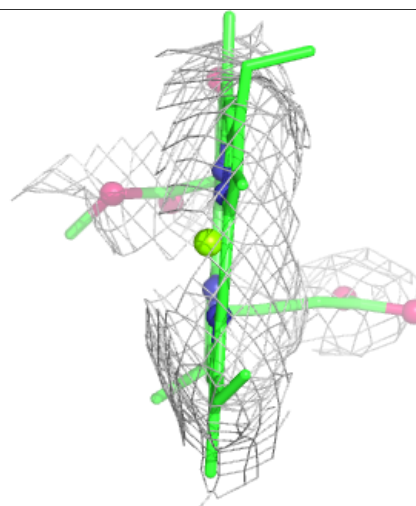
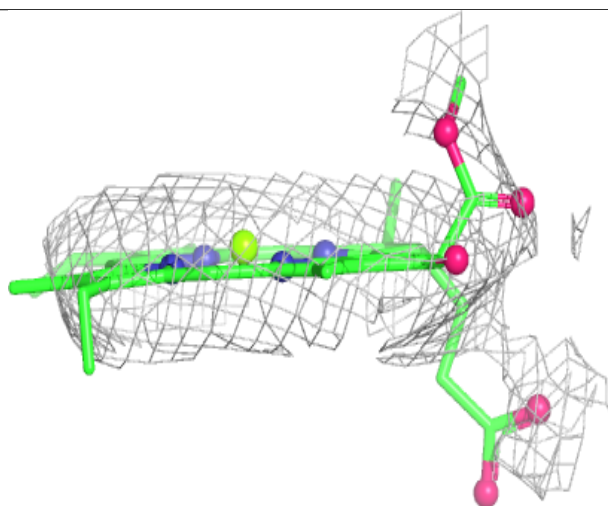
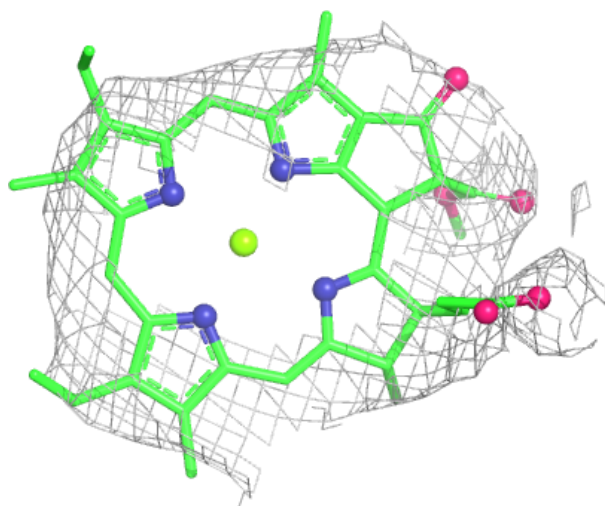
Electron density around CLA B 1224:

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



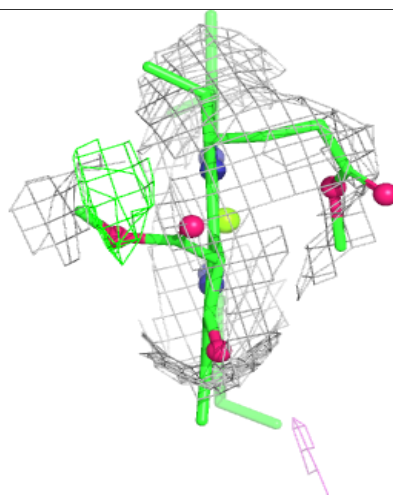
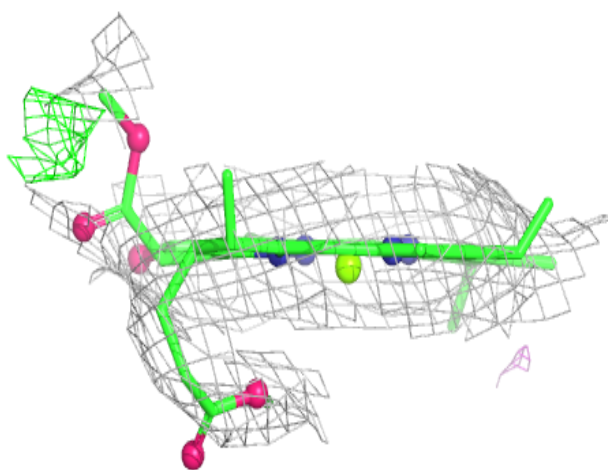
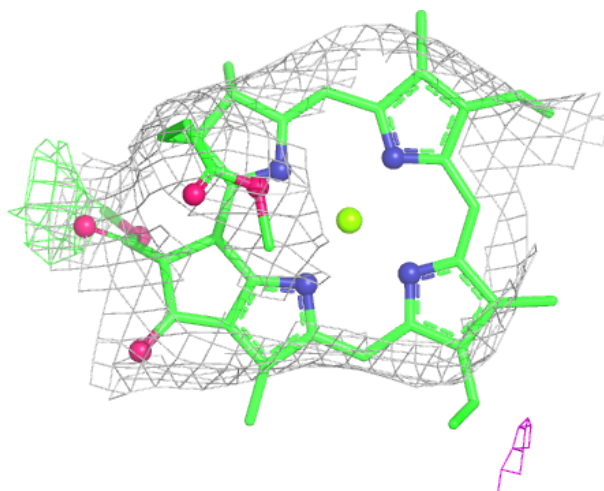
Electron density around CLA 2 1212:

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



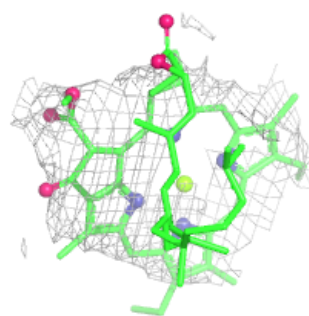
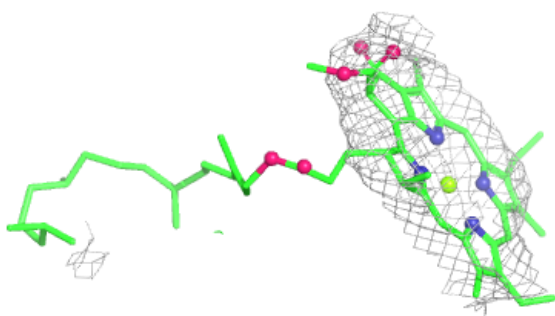
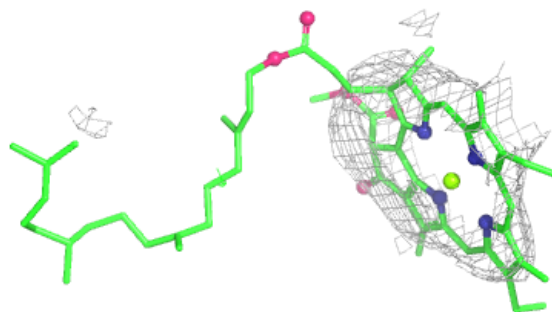
Electron density around CLA 8 1502:

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



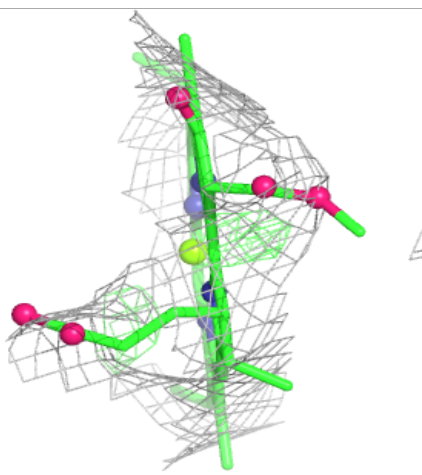
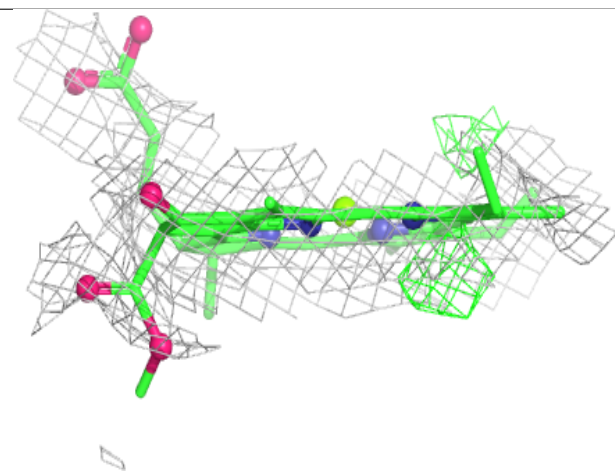
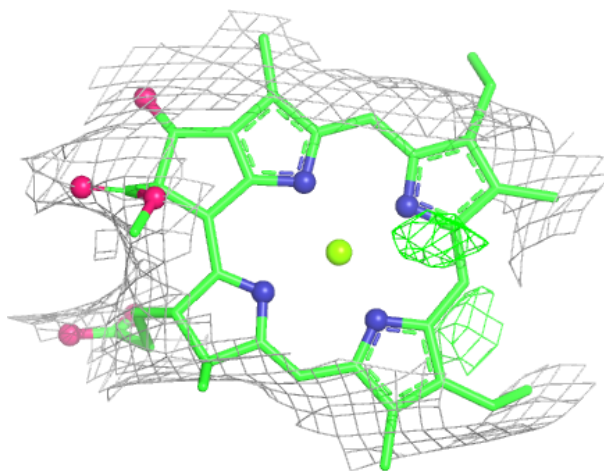
Electron density around CLA 2 1021:

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



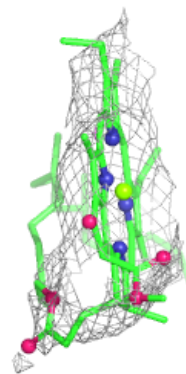
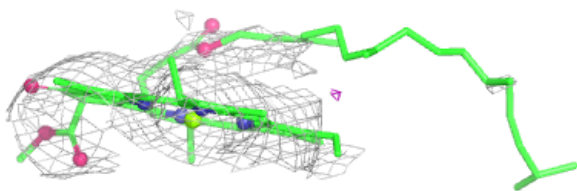
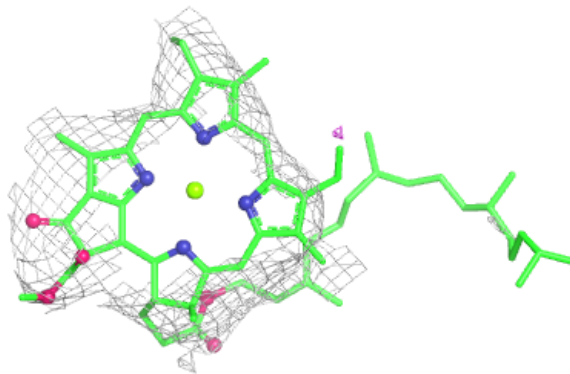
Electron density around CLA A 1112:

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



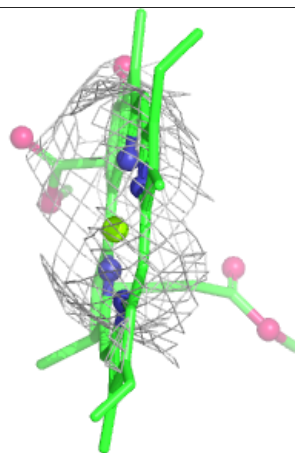
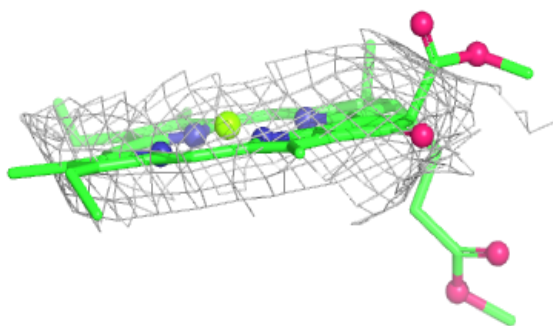
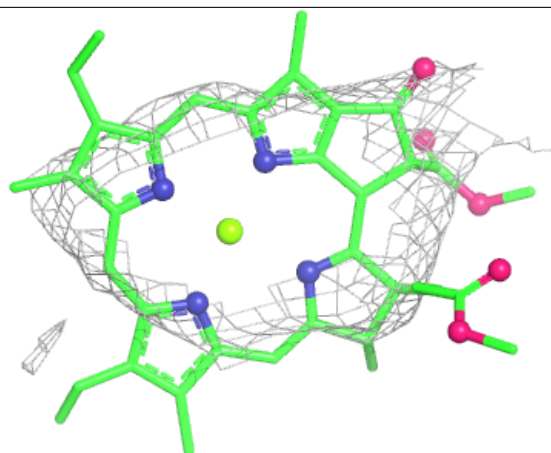
Electron density around CLA 2 1215:

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



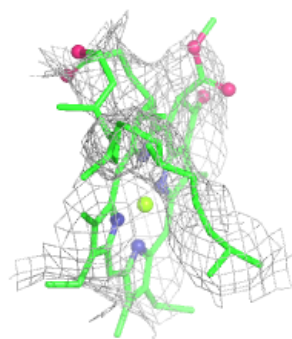
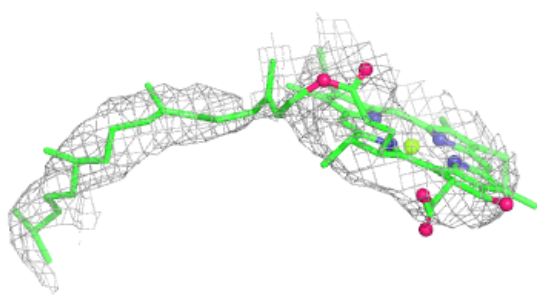
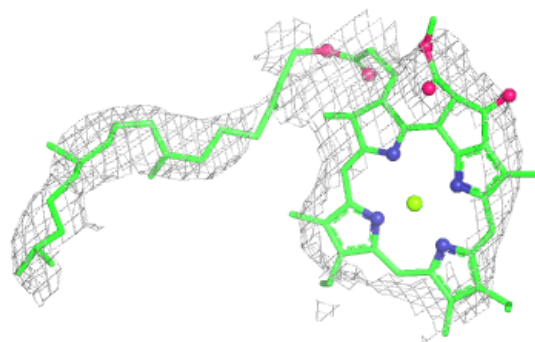
Electron density around CLA b 1220:

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

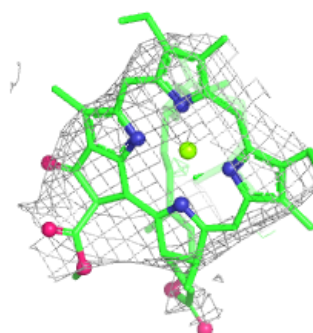
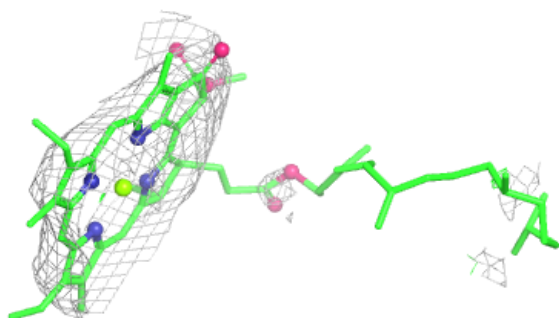
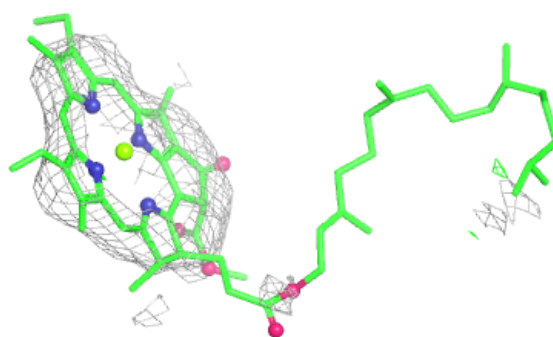


Electron density around CLA B 1013:

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

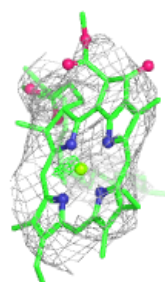
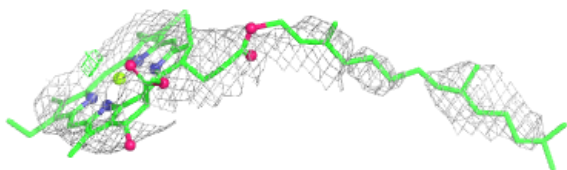
**Electron density around CLA B 1021:**

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



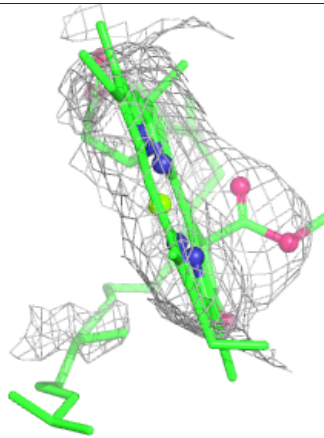
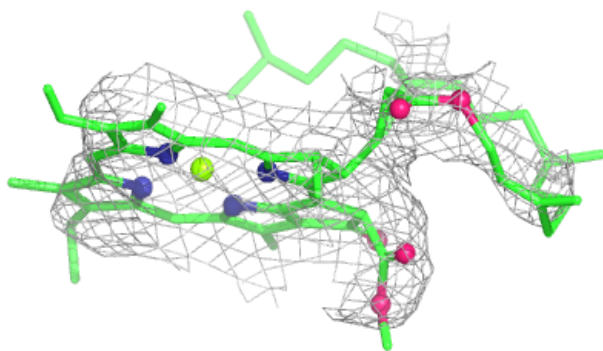
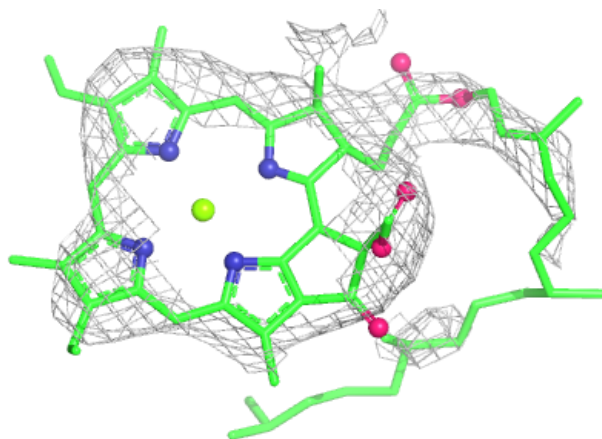
Electron density around CLA A 1022:

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



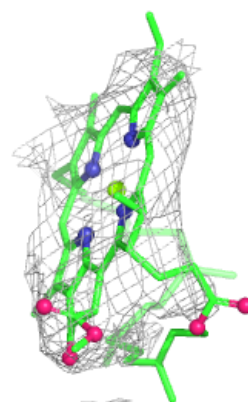
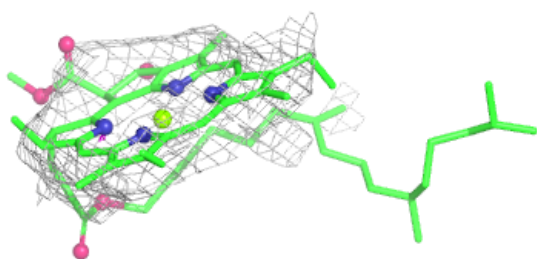
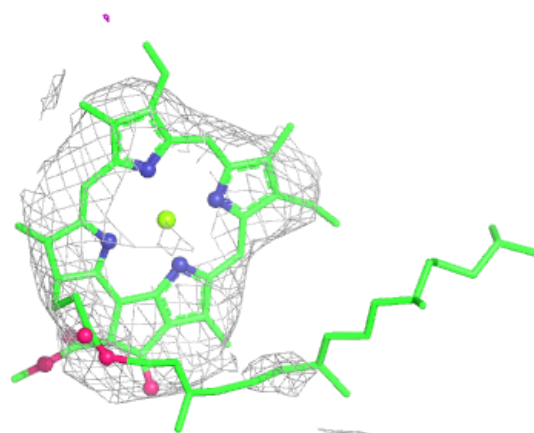
Electron density around CLA B 1202:

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



Electron density around CLA A 1127:

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



6.5 Other polymers ⓘ

There are no such residues in this entry.