



wwPDB X-ray Structure Validation Summary Report ⓘ

Oct 28, 2024 – 04:08 pm GMT

PDB ID : 4Y28
Title : The structure of plant photosystem I super-complex at 2.8 angstrom resolution.
Authors : Mazor, Y.; Brovikov, A.; Nelson, N.
Deposited on : 2015-02-09
Resolution : 2.80 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity : 4.02b-467
Mogul : 1.8.4, CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 3.0
buster-report : 1.1.7 (2018)
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4 : 9.0.003 (Gargrove)
Density-Fitness : 1.0.11
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.39

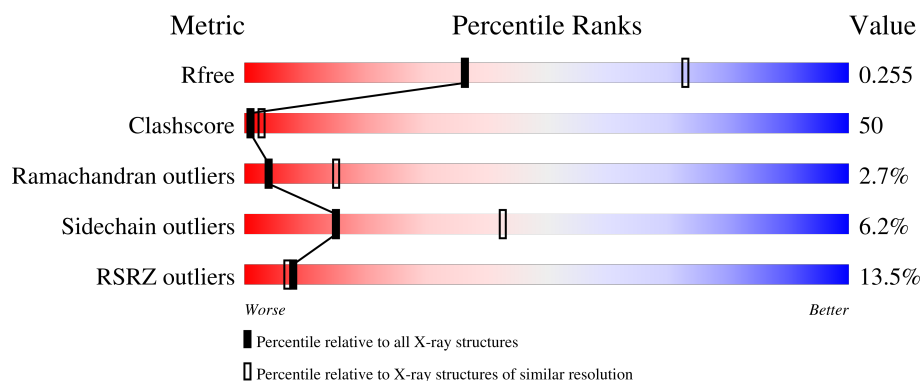
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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}	164625	3657 (2.80-2.80)
Clashscore	180529	4123 (2.80-2.80)
Ramachandran outliers	177936	4071 (2.80-2.80)
Sidechain outliers	177891	4073 (2.80-2.80)
RSRZ outliers	164620	3659 (2.80-2.80)

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	A	758	<div> <div>7%</div> <div> <div></div> <div>74%</div> <div>23%</div> <div>..</div> </div> </div>
2	B	733	<div> <div>8%</div> <div> <div></div> <div>75%</div> <div>24%</div> <div>.</div> </div> </div>
3	I	30	<div> <div>13%</div> <div> <div></div> <div>33%</div> <div>53%</div> <div>10%</div> <div>.</div> </div> </div>
4	J	42	<div> <div>14%</div> <div> <div></div> <div>33%</div> <div>52%</div> <div>7%</div> <div>5%</div> <div>.</div> </div> </div>
5	F	154	<div> <div>10%</div> <div> <div></div> <div>67%</div> <div>27%</div> <div>..</div> </div> </div>

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Mol	Chain	Length	Quality of chain
6	G	97	
7	L	167	
8	C	81	
9	D	147	
10	E	66	
11	H	90	
12	K	129	
13	2	269	
14	4	252	
15	1	202	
16	3	275	

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
17	CL0	A	1011	X	-	-	-
18	CLA	1	1001	X	-	X	-
18	CLA	1	1002	X	-	X	-
18	CLA	1	1003	X	-	X	-
18	CLA	1	1004	X	-	X	-
18	CLA	1	1005	X	-	-	-
18	CLA	1	1006	X	-	-	-
18	CLA	1	1007	X	-	-	-
18	CLA	1	1008	X	-	X	-
18	CLA	1	1011	X	-	-	-
18	CLA	1	1012	X	-	-	-
18	CLA	1	1013	X	-	-	-
18	CLA	1	1014	X	-	-	-
18	CLA	2	2001	X	-	X	-
18	CLA	2	2002	X	-	X	-
18	CLA	2	2003	X	-	X	-
18	CLA	2	2004	X	-	X	-
18	CLA	2	2005	X	-	X	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
18	CLA	2	2006	X	-	X	-
18	CLA	2	2007	X	-	X	-
18	CLA	2	2008	X	-	-	-
18	CLA	2	2009	X	-	-	-
18	CLA	2	2012	X	-	X	-
18	CLA	2	2016	X	-	X	-
18	CLA	2	2019	X	-	-	-
18	CLA	3	3001	X	-	X	-
18	CLA	3	3002	X	-	-	-
18	CLA	3	3003	X	-	X	-
18	CLA	3	3004	X	-	-	-
18	CLA	3	3005	X	-	-	-
18	CLA	3	3006	X	-	X	-
18	CLA	3	3007	X	-	-	-
18	CLA	3	3008	X	-	-	-
18	CLA	3	3010	X	-	X	-
18	CLA	3	3012	X	-	X	-
18	CLA	3	3013	X	-	X	-
18	CLA	3	3017	X	-	-	-
18	CLA	3	3018	X	-	-	-
18	CLA	3	3019	X	-	-	-
18	CLA	4	4001	X	-	X	-
18	CLA	4	4002	X	-	-	-
18	CLA	4	4003	X	-	-	-
18	CLA	4	4004	X	-	-	-
18	CLA	4	4005	X	-	-	-
18	CLA	4	4006	X	-	X	-
18	CLA	4	4007	X	-	-	-
18	CLA	4	4008	X	-	-	-
18	CLA	4	4009	X	-	-	-
18	CLA	4	4012	X	-	X	-
18	CLA	4	4016	X	-	X	-
18	CLA	4	4017	X	-	-	-
18	CLA	A	1013	X	-	-	-
18	CLA	A	1022	X	-	-	-
18	CLA	A	1101	X	-	-	-
18	CLA	A	1102	X	-	-	-
18	CLA	A	1103	X	-	-	-
18	CLA	A	1104	X	-	-	-
18	CLA	A	1105	X	-	-	-
18	CLA	A	1106	X	-	-	-
18	CLA	A	1107	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
18	CLA	A	1108	X	-	-	-
18	CLA	A	1109	X	-	-	-
18	CLA	A	1110	X	-	-	-
18	CLA	A	1111	X	-	-	-
18	CLA	A	1112	X	-	-	-
18	CLA	A	1113	X	-	-	-
18	CLA	A	1114	X	-	-	-
18	CLA	A	1115	X	-	-	-
18	CLA	A	1116	X	-	-	-
18	CLA	A	1117	X	-	-	-
18	CLA	A	1118	X	-	-	-
18	CLA	A	1119	X	-	-	-
18	CLA	A	1120	X	-	-	-
18	CLA	A	1121	X	-	-	-
18	CLA	A	1122	X	-	-	-
18	CLA	A	1123	X	-	-	-
18	CLA	A	1124	X	-	-	-
18	CLA	A	1125	X	-	-	-
18	CLA	A	1126	X	-	-	-
18	CLA	A	1127	X	-	-	-
18	CLA	A	1128	X	-	-	-
18	CLA	A	1129	X	-	-	-
18	CLA	A	1131	X	-	-	-
18	CLA	A	1132	X	-	-	-
18	CLA	A	1134	X	-	-	-
18	CLA	A	1135	X	-	-	-
18	CLA	A	1136	X	-	-	-
18	CLA	A	1137	X	-	-	-
18	CLA	A	1138	X	-	-	-
18	CLA	A	1139	X	-	-	-
18	CLA	A	1140	X	-	-	-
18	CLA	A	1151	X	-	-	-
18	CLA	A	1237	X	-	-	-
18	CLA	B	1012	X	-	-	-
18	CLA	B	1021	X	-	-	-
18	CLA	B	1023	X	-	-	-
18	CLA	B	1201	X	-	-	-
18	CLA	B	1202	X	-	-	-
18	CLA	B	1203	X	-	-	-
18	CLA	B	1204	X	-	-	-
18	CLA	B	1205	X	-	-	-
18	CLA	B	1206	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
18	CLA	B	1208	X	-	-	-
18	CLA	B	1209	X	-	-	-
18	CLA	B	1210	X	-	-	-
18	CLA	B	1211	X	-	-	-
18	CLA	B	1212	X	-	-	-
18	CLA	B	1214	X	-	-	-
18	CLA	B	1215	X	-	-	-
18	CLA	B	1216	X	-	-	-
18	CLA	B	1217	X	-	-	-
18	CLA	B	1218	X	-	-	-
18	CLA	B	1219	X	-	-	-
18	CLA	B	1221	X	-	-	-
18	CLA	B	1222	X	-	-	-
18	CLA	B	1224	X	-	-	-
18	CLA	B	1225	X	-	-	-
18	CLA	B	1226	X	-	-	-
18	CLA	B	1227	X	-	-	-
18	CLA	B	1228	X	-	-	-
18	CLA	B	1229	X	-	-	-
18	CLA	B	1230	X	-	-	-
18	CLA	B	1231	X	-	-	-
18	CLA	B	1232	X	-	-	-
18	CLA	B	1234	X	-	-	-
18	CLA	B	1235	X	-	-	-
18	CLA	B	1236	X	-	-	-
18	CLA	B	1238	X	-	-	-
18	CLA	B	1239	X	-	-	-
18	CLA	B	1240	X	-	-	-
18	CLA	F	1301	X	-	-	-
18	CLA	F	1302	X	-	-	-
18	CLA	G	1001	X	-	X	-
18	CLA	G	1002	X	-	X	-
18	CLA	G	1003	X	-	X	-
18	CLA	H	1000	X	-	-	-
18	CLA	J	1302	X	-	-	-
18	CLA	K	1001	X	-	-	-
18	CLA	L	1501	X	-	-	-
18	CLA	L	1502	X	-	-	-
18	CLA	L	1503	X	-	-	-
22	BCR	3	3503	-	-	X	-
22	BCR	G	2011	-	-	X	-
22	BCR	L	6019	-	-	X	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
27	LUT	1	1501	X	-	X	-
27	LUT	1	1502	X	-	-	-
27	LUT	2	2501	X	-	X	-
27	LUT	2	2502	X	-	X	-
27	LUT	3	3501	X	-	X	-
27	LUT	3	3502	X	-	X	-
27	LUT	4	4501	X	-	X	-
27	LUT	4	4502	X	-	X	-
27	LUT	4	4503	X	-	X	-
27	LUT	I	6018	X	-	-	-
28	CHL	1	1009	X	-	X	-
28	CHL	1	1010	X	-	-	-
28	CHL	2	2010	X	-	-	-
28	CHL	2	2011	X	-	-	-
28	CHL	2	2013	X	-	-	-
28	CHL	3	3011	X	-	X	-
28	CHL	4	4010	X	-	-	-
28	CHL	4	4011	X	-	-	-
28	CHL	4	4013	X	-	-	-

2 Entry composition

There are 29 unique types of molecules in this entry. The entry contains 35653 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	742	5852	3833	997	1004	18	0	0	0

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	21	ILE	LEU	engineered mutation	UNP P05310
A	22	LEU	VAL	engineered mutation	UNP P05310
A	117	ARG	GLY	engineered mutation	UNP P05310
A	220	GLY	ARG	engineered mutation	UNP P05310

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	732	5856	3851	995	996	14	0	0	0

There are 7 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	5	LEU	ILE	engineered mutation	UNP P05311
B	115	ILE	ASN	engineered mutation	UNP P05311
B	273	MET	VAL	engineered mutation	UNP P05311
B	471	SER	THR	engineered mutation	UNP P05311
B	476	VAL	ILE	engineered mutation	UNP P05311
B	477	LEU	PRO	engineered mutation	UNP P05311
B	635	TYR	ILE	engineered mutation	UNP P05311

- Molecule 3 is a protein called Photosystem I reaction center subunit VIII.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	I	29	Total	C	N	O	S	0	0	0
			224	155	35	33	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	J	41	Total	C	N	O	S	0	0	0
			321	217	50	54				

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	F	150	Total	C	N	O	S	0	0	0
			1187	770	207	208	2			

- Molecule 6 is a protein called photosystem I reaction center.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	G	91	Total	C	N	O	S	0	0	0
			689	444	117	128				

- Molecule 7 is a protein called Putative uncharacterized protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	L	160	Total	C	N	O	S	0	0	0
			1197	791	190	215	1			

- Molecule 8 is a protein called Photosystem I iron-sulfur center.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	C	80	Total	C	N	O	S	0	0	0
			612	379	107	115	11			

- Molecule 9 is a protein called Photosystem I reaction center subunit II, chloroplastic.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	D	141	Total	C	N	O	S	0	0	0
			1116	720	192	201	3			

- Molecule 10 is a protein called Photosystem I reaction center subunit IV A, chloroplastic.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
10	E	66	Total	C	N	O	0	0	0
			530	337	93	100			

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
11	H	84	Total	C	N	O	0	0	0
			642	425	97	120			

- Molecule 12 is a protein called Photosystem I reaction center subunit X psaK.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	K	57	Total	C	N	O	S	0	0	0
			379	241	64	71	3			

- Molecule 13 is a protein called Type II chlorophyll a/b binding protein from photosystem I.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	2	207	Total	C	N	O	S	0	0	0
			1613	1057	263	289	4			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
2	133	LEU	ASN	engineered mutation	UNP Q41038

- Molecule 14 is a protein called Chlorophyll a-b binding protein P4, chloroplastic.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	4	198	Total	C	N	O	S	0	0	0
			1544	1007	252	282	3			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
4	128	ASP	ALA	engineered mutation	UNP Q9SQL2

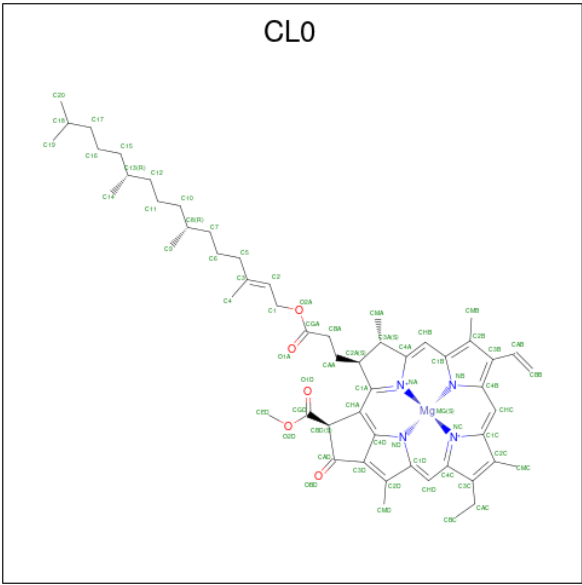
- Molecule 15 is a protein called Light-harvesting complex I chlorophyll A/B-binding protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
15	1	194	Total	C	N	O	S	0	0	0
			1513	986	254	268	5			

- Molecule 16 is a protein called Chlorophyll a-b binding protein 3, chloroplastic.

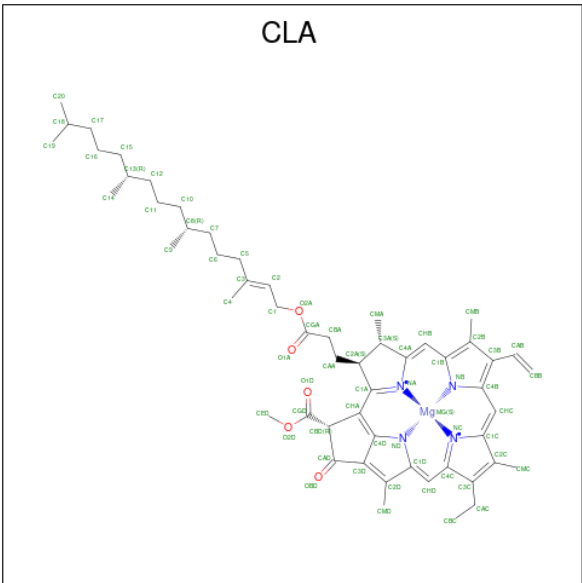
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
16	3	215	1619	1053	263	298	5	0	0	0

- Molecule 17 is CHLOROPHYLL A ISOMER (three-letter code: CL0) (formula: C₅₅H₇₂MgN₄O₅).



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

- Molecule 18 is CHLOROPHYLL A (three-letter code: CLA) (formula: C₅₅H₇₂MgN₄O₅).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
18	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
18	A	1	Total	C	Mg	N	O	0	0
			50	40	1	4	5		
18	A	1	Total	C	Mg	N	O	0	0
			60	50	1	4	5		
18	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
18	A	1	Total	C	Mg	N	O	0	0
			50	40	1	4	5		
18	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
18	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
18	A	1	Total	C	Mg	N	O	0	0
			51	41	1	4	5		
18	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
18	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
18	A	1	Total	C	Mg	N	O	0	0
			46	36	1	4	5		
18	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
18	A	1	Total	C	Mg	N	O	0	0
			55	45	1	4	5		
18	A	1	Total	C	Mg	N	O	0	0
			60	50	1	4	5		
18	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
18	A	1	Total	C	Mg	N	O	0	0
			46	36	1	4	5		
18	A	1	Total	C	Mg	N	O	0	0
			46	36	1	4	5		
18	A	1	Total	C	Mg	N	O	0	0
			60	50	1	4	5		
18	A	1	Total	C	Mg	N	O	0	0
			55	45	1	4	5		
18	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
18	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
18	A	1	Total	C	Mg	N	O	0	0
			55	45	1	4	5		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
18	A	1	Total 60	C 50	Mg 1	N 4	O 5	0	0
18	A	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
18	A	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
18	A	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
18	A	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
18	A	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
18	A	1	Total 55	C 45	Mg 1	N 4	O 5	0	0
18	A	1	Total 55	C 45	Mg 1	N 4	O 5	0	0
18	A	1	Total 51	C 41	Mg 1	N 4	O 5	0	0
18	A	1	Total 56	C 46	Mg 1	N 4	O 5	0	0
18	A	1	Total 55	C 45	Mg 1	N 4	O 5	0	0
18	A	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
18	A	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
18	A	1	Total 46	C 36	Mg 1	N 4	O 5	0	0
18	A	1	Total 60	C 50	Mg 1	N 4	O 5	0	0
18	A	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
18	A	1	Total 46	C 36	Mg 1	N 4	O 5	0	0
18	A	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
18	A	1	Total 50	C 40	Mg 1	N 4	O 5	0	0
18	A	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
18	A	1	Total 65	C 55	Mg 1	N 4	O 5	0	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
18	A	1	Total	C	Mg	N	O	0	0
			50	40	1	4	5		
18	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
18	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
18	B	1	Total	C	Mg	N	O	0	0
			60	50	1	4	5		
18	B	1	Total	C	Mg	N	O	0	0
			55	45	1	4	5		
18	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
18	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
18	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
18	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
18	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
18	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
18	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
18	B	1	Total	C	Mg	N	O	0	0
			46	36	1	4	5		
18	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
18	B	1	Total	C	Mg	N	O	0	0
			60	50	1	4	5		
18	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
18	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
18	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
18	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
18	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
18	B	1	Total	C	Mg	N	O	0	0
			50	40	1	4	5		
18	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
18	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
18	B	1	Total	C	Mg	N	O	0	0
			55	45	1	4	5		
18	B	1	Total	C	Mg	N	O	0	0
			46	36	1	4	5		
18	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
18	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
18	B	1	Total	C	Mg	N	O	0	0
			55	45	1	4	5		
18	B	1	Total	C	Mg	N	O	0	0
			60	50	1	4	5		
18	B	1	Total	C	Mg	N	O	0	0
			59	49	1	4	5		
18	B	1	Total	C	Mg	N	O	0	0
			60	50	1	4	5		
18	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
18	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
18	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
18	B	1	Total	C	Mg	N	O	0	0
			60	50	1	4	5		
18	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
18	B	1	Total	C	Mg	N	O	0	0
			58	48	1	4	5		
18	B	1	Total	C	Mg	N	O	0	0
			55	45	1	4	5		
18	B	1	Total	C	Mg	N	O	0	0
			60	50	1	4	5		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
18	J	1	Total	C	Mg	N	O	0	0
			50	40	1	4	5		
18	F	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
18	F	1	Total	C	Mg	N	O	0	0
			50	40	1	4	5		
18	G	1	Total	C	Mg	N	O	0	0
			55	45	1	4	5		
18	G	1	Total	C	Mg	N	O	0	0
			46	36	1	4	5		
18	G	1	Total	C	Mg	N	O	0	0
			60	50	1	4	5		
18	L	1	Total	C	Mg	N	O	0	0
			50	40	1	4	5		
18	L	1	Total	C	Mg	N	O	0	0
			60	50	1	4	5		
18	L	1	Total	C	Mg	N	O	0	0
			50	40	1	4	5		
18	H	1	Total	C	Mg	N	O	0	0
			46	36	1	4	5		
18	K	1	Total	C	Mg	N	O	0	0
			46	36	1	4	5		
18	2	1	Total	C	Mg	N	O	0	0
			60	50	1	4	5		
18	2	1	Total	C	Mg	N	O	0	0
			46	36	1	4	5		
18	2	1	Total	C	Mg	N	O	0	0
			55	45	1	4	5		
18	2	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
18	2	1	Total	C	Mg	N	O	0	0
			55	45	1	4	5		
18	2	1	Total	C	Mg	N	O	0	0
			60	50	1	4	5		
18	2	1	Total	C	Mg	N	O	0	0
			50	40	1	4	5		
18	2	1	Total	C	Mg	N	O	0	0
			55	45	1	4	5		
18	2	1	Total	C	Mg	N	O	0	0
			50	40	1	4	5		

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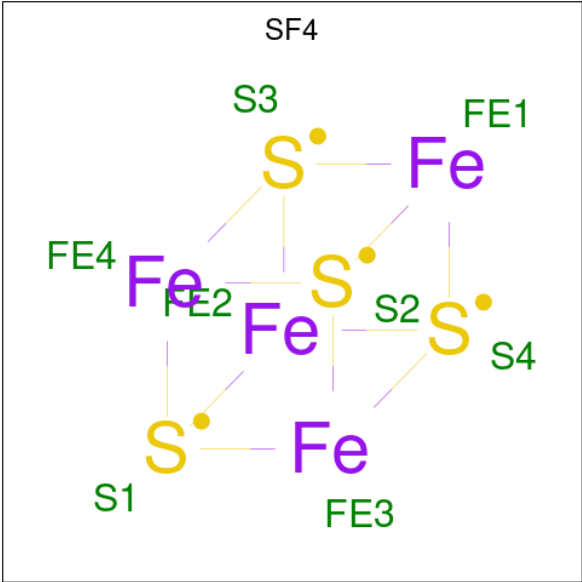
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
18	2	1	Total 27	C 22	Mg 1	N 4	0	0
18	2	1	Total 50	C 40	Mg 1	N 4 O 5	0	0
18	4	1	Total 50	C 40	Mg 1	N 4 O 5	0	0
18	4	1	Total 60	C 50	Mg 1	N 4 O 5	0	0
18	4	1	Total 50	C 40	Mg 1	N 4 O 5	0	0
18	4	1	Total 65	C 55	Mg 1	N 4 O 5	0	0
18	4	1	Total 60	C 50	Mg 1	N 4 O 5	0	0
18	4	1	Total 60	C 50	Mg 1	N 4 O 5	0	0
18	4	1	Total 50	C 40	Mg 1	N 4 O 5	0	0
18	4	1	Total 60	C 50	Mg 1	N 4 O 5	0	0
18	4	1	Total 46	C 36	Mg 1	N 4 O 5	0	0
18	4	1	Total 65	C 55	Mg 1	N 4 O 5	0	0
18	4	1	Total 46	C 36	Mg 1	N 4 O 5	0	0
18	4	1	Total 65	C 55	Mg 1	N 4 O 5	0	0
18	1	1	Total 60	C 50	Mg 1	N 4 O 5	0	0
18	1	1	Total 46	C 36	Mg 1	N 4 O 5	0	0
18	1	1	Total 55	C 45	Mg 1	N 4 O 5	0	0
18	1	1	Total 65	C 55	Mg 1	N 4 O 5	0	0
18	1	1	Total 55	C 45	Mg 1	N 4 O 5	0	0
18	1	1	Total 50	C 40	Mg 1	N 4 O 5	0	0
18	1	1	Total 46	C 36	Mg 1	N 4 O 5	0	0

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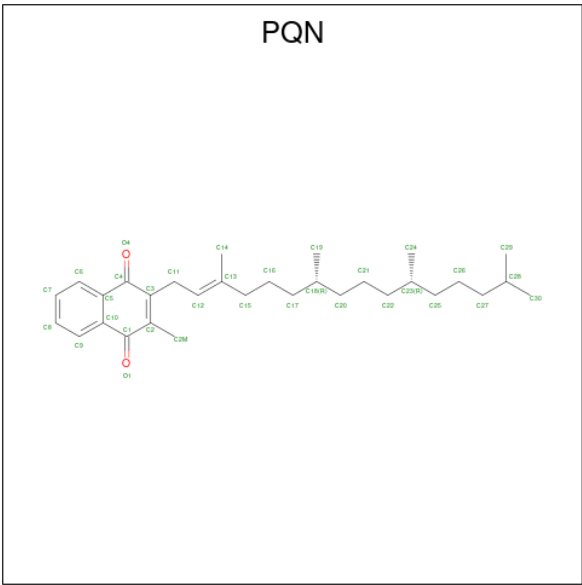
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
18	1	1	Total	C	Mg	N	O	0	0
			46	36	1	4	5		
18	1	1	Total	C	Mg	N	O	0	0
			50	40	1	4	5		
18	1	1	Total	C	Mg	N	O	0	0
			50	40	1	4	5		
18	1	1	Total	C	Mg	N	O	0	0
			46	36	1	4	5		
18	1	1	Total	C	Mg	N	O	0	0
			46	36	1	4	5		
18	3	1	Total	C	Mg	N	O	0	0
			50	40	1	4	5		
18	3	1	Total	C	Mg	N	O	0	0
			46	36	1	4	5		
18	3	1	Total	C	Mg	N	O	0	0
			60	50	1	4	5		
18	3	1	Total	C	Mg	N	O	0	0
			60	50	1	4	5		
18	3	1	Total	C	Mg	N	O	0	0
			55	45	1	4	5		
18	3	1	Total	C	Mg	N	O	0	0
			50	40	1	4	5		
18	3	1	Total	C	Mg	N	O	0	0
			50	40	1	4	5		
18	3	1	Total	C	Mg	N	O	0	0
			48	38	1	4	5		
18	3	1	Total	C	Mg	N	O	0	0
			60	50	1	4	5		
18	3	1	Total	C	Mg	N	O	0	0
			50	40	1	4	5		
18	3	1	Total	C	Mg	N	O	0	0
			46	36	1	4	5		
18	3	1	Total	C	Mg	N	O	0	0
			46	36	1	4	5		
18	3	1	Total	C	Mg	N	O	0	0
			50	40	1	4	5		
18	3	1	Total	C	Mg	N		0	0
			27	22	1	4			

- Molecule 19 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe₄S₄).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
19	A	1	Total	Fe	S	0	0
			8	4	4		
19	C	1	Total	Fe	S	0	0
			8	4	4		
19	C	1	Total	Fe	S	0	0
			8	4	4		

- Molecule 20 is PHYLLOQUINONE (three-letter code: PQN) (formula: C₃₁H₄₆O₂).



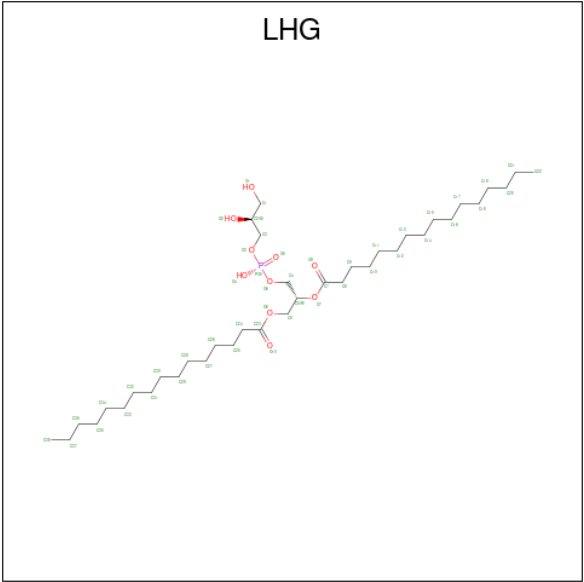
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
20	A	1	Total	C	O	0	0
			33	31	2		

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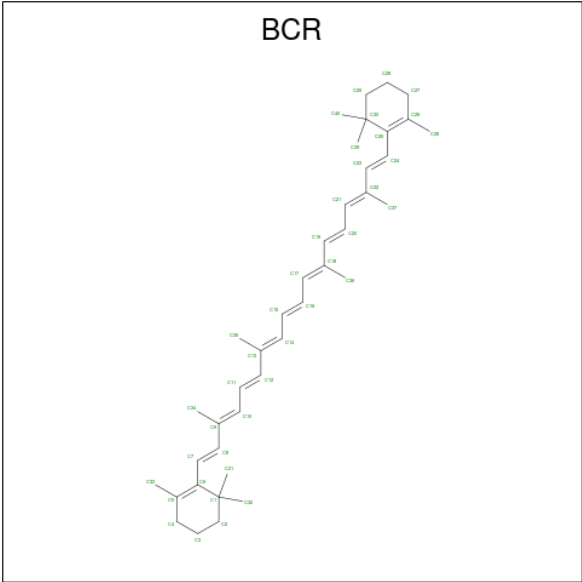
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
20	B	1	Total	C	O	0	0
			33	31	2		

- Molecule 21 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (three-letter code: LHG) (formula: C₃₈H₇₅O₁₀P).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
21	A	1	Total	C	O	P	0	0
			40	29	10	1		
21	A	1	Total	C	O	P	0	0
			49	38	10	1		
21	B	1	Total	C	O	P	0	0
			21	10	10	1		
21	2	1	Total	C	O	P	0	0
			24	13	10	1		
21	1	1	Total	C	O	P	0	0
			49	38	10	1		

- Molecule 22 is BETA-CAROTENE (three-letter code: BCR) (formula: C₄₀H₅₆).



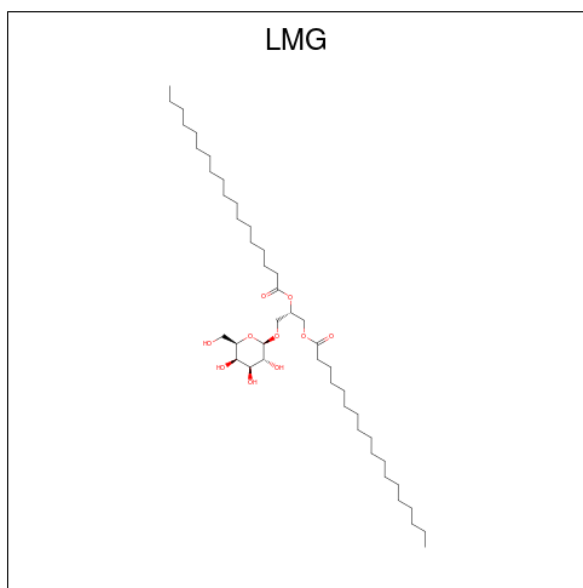
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
22	A	1	Total C 40 40	0	0
22	A	1	Total C 40 40	0	0
22	A	1	Total C 40 40	0	0
22	A	1	Total C 40 40	0	0
22	A	1	Total C 40 40	0	0
22	A	1	Total C 40 40	0	0
22	B	1	Total C 40 40	0	0
22	B	1	Total C 40 40	0	0
22	B	1	Total C 40 40	0	0
22	B	1	Total C 40 40	0	0
22	B	1	Total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

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
22	F	1	Total C 40 40	0	0
22	F	1	Total C 40 40	0	0
22	G	1	Total C 40 40	0	0
22	L	1	Total C 40 40	0	0
22	L	1	Total C 40 40	0	0
22	K	1	Total C 40 40	0	0
22	3	1	Total C 40 40	0	0

- Molecule 23 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (three-letter code: LMG) (formula: $C_{45}H_{86}O_{10}$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
23	B	1	Total C O 38 28 10	0	0
23	J	1	Total C O 55 45 10	0	0
23	F	1	Total C O 23 13 10	0	0
23	F	1	Total C O 37 27 10	0	0

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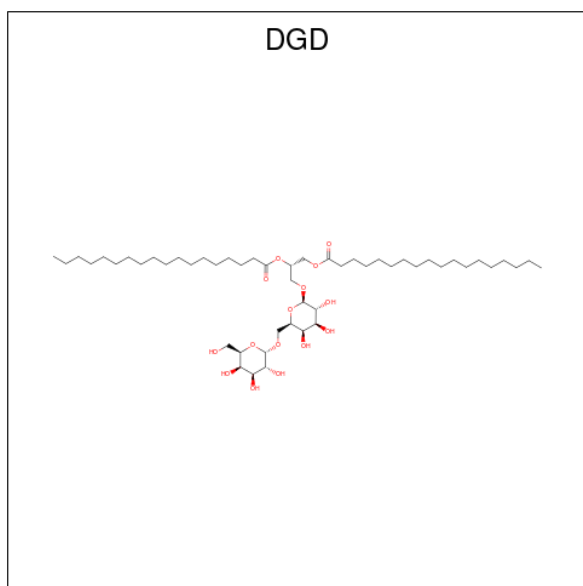
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
23	G	1	Total	C	O	0	0
			41	31	10		
23	2	1	Total	C	O	0	0
			35	25	10		
23	4	1	Total	C	O	0	0
			35	25	10		

- Molecule 24 is CALCIUM ION (three-letter code: CA) (formula: Ca).

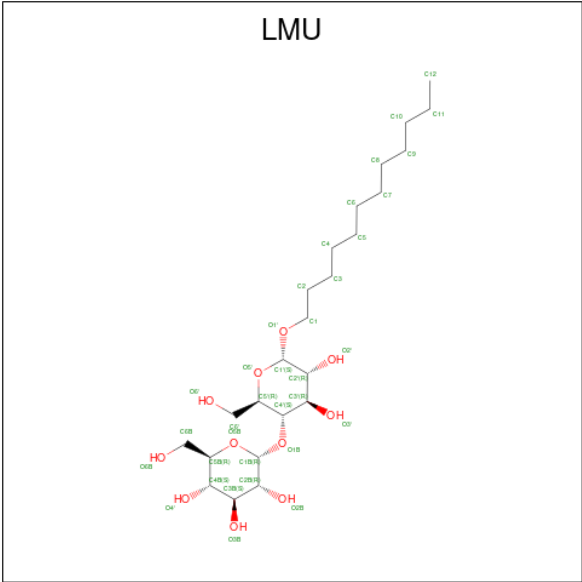
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
24	B	1	Total	Ca	0	0
			1	1		

- Molecule 25 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (three-letter code: DGD) (formula: C₅₁H₉₆O₁₅).



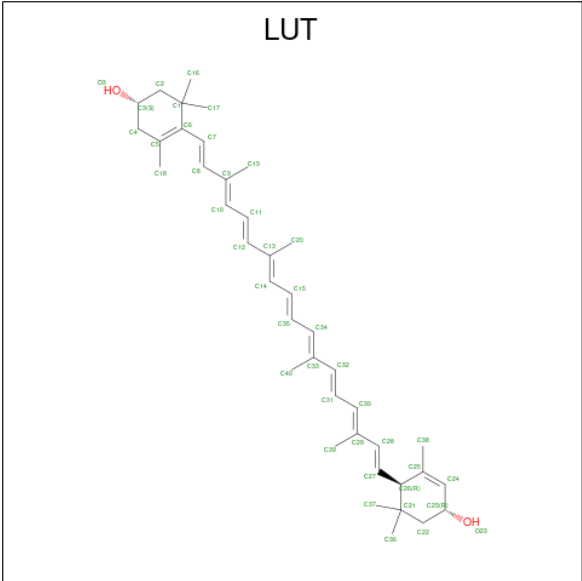
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
25	B	1	Total	C	O	0	0
			61	46	15		

- Molecule 26 is DODECYL-ALPHA-D-MALTOSIDE (three-letter code: LMU) (formula: C₂₄H₄₆O₁₁).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
26	B	1	Total	C	O	0	0
			35	24	11		
26	B	1	Total	C	O	0	0
			35	24	11		

- Molecule 27 is (3R,3'R,6S)-4,5-DIDEHYDRO-5,6-DIHYDRO-BETA,BETA-CAROTENE-3,3'-DIOL (three-letter code: LUT) (formula: C₄₀H₅₆O₂).



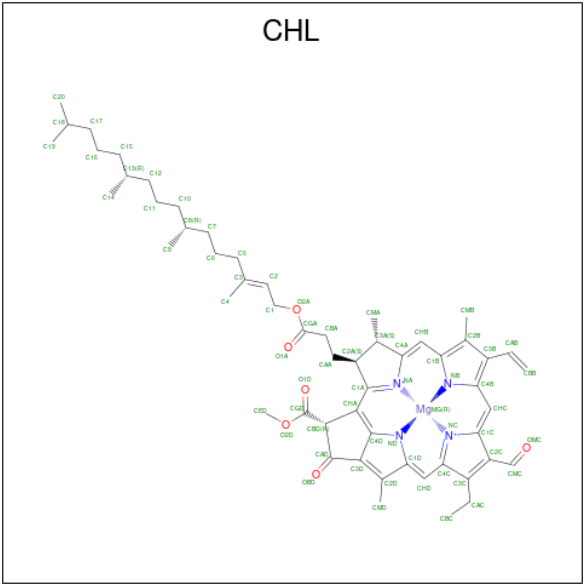
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
27	I	1	Total	C	O	0	0
			42	40	2		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
27	2	1	Total	C	O	0	0
			42	40	2		
27	2	1	Total	C	O	0	0
			42	40	2		
27	4	1	Total	C	O	0	0
			42	40	2		
27	4	1	Total	C	O	0	0
			42	40	2		
27	4	1	Total	C	O	0	0
			42	40	2		
27	1	1	Total	C	O	0	0
			42	40	2		
27	1	1	Total	C	O	0	0
			42	40	2		
27	3	1	Total	C	O	0	0
			42	40	2		
27	3	1	Total	C	O	0	0
			42	40	2		

- Molecule 28 is CHLOROPHYLL B (three-letter code: CHL) (formula: C₅₅H₇₀MgN₄O₆).



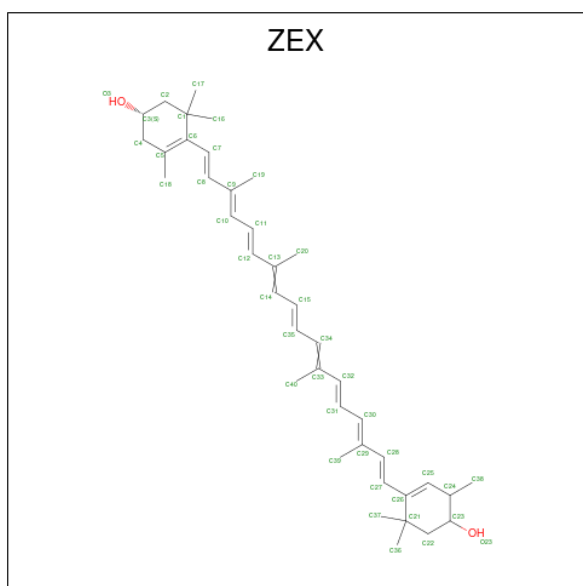
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
28	2	1	Total	C	Mg	N	O	0	0
			47	36	1	4	6		
28	2	1	Total	C	Mg	N	O	0	0
			48	37	1	4	6		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
28	2	1	Total	C	Mg	N	O	0	0
			46	35	1	4	6		
28	4	1	Total	C	Mg	N	O	0	0
			47	36	1	4	6		
28	4	1	Total	C	Mg	N	O	0	0
			51	40	1	4	6		
28	4	1	Total	C	Mg	N	O	0	0
			47	36	1	4	6		
28	1	1	Total	C	Mg	N	O	0	0
			56	45	1	4	6		
28	1	1	Total	C	Mg	N	O	0	0
			47	36	1	4	6		
28	3	1	Total	C	Mg	N	O	0	0
			56	45	1	4	6		

- Molecule 29 is (1R,2S)-4-[(1E,3E,5E,7E,9E,11E,13E,15E,17E)-18-[(4S)-4-hydroxy-2,6,6-trimethylcyclohex-1-en-1-yl]-3,7,12,16-tetramethyloctadeca-1,3,5,7,9,11,13,15,17-nonaen-1-yl]-2,5,5-trimethylcyclohex-3-en-1-ol (three-letter code: ZEX) (formula: C₄₀H₅₆O₂).

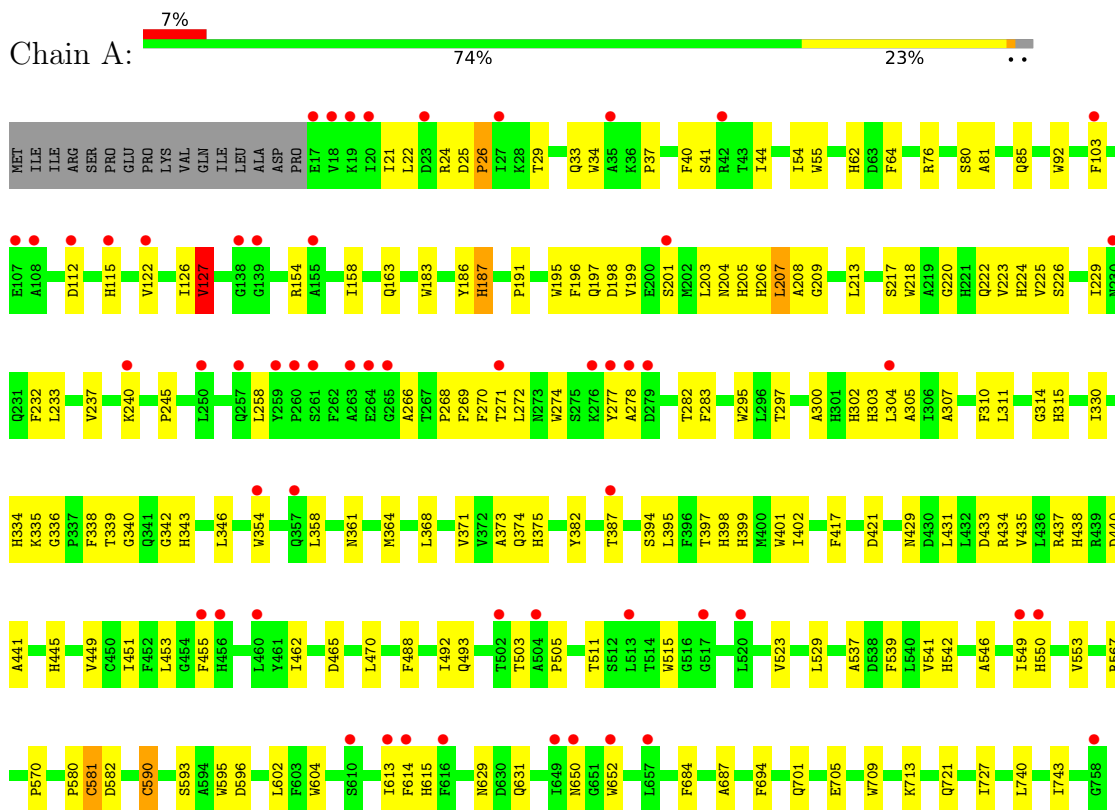


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
29	4	1	Total	C	O	0	0
			42	40	2		

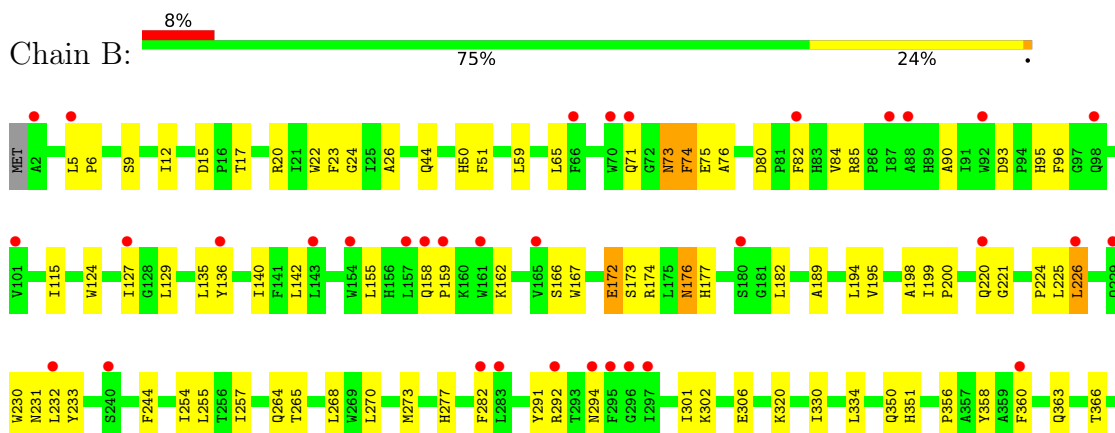
3 Residue-property plots [i](#)

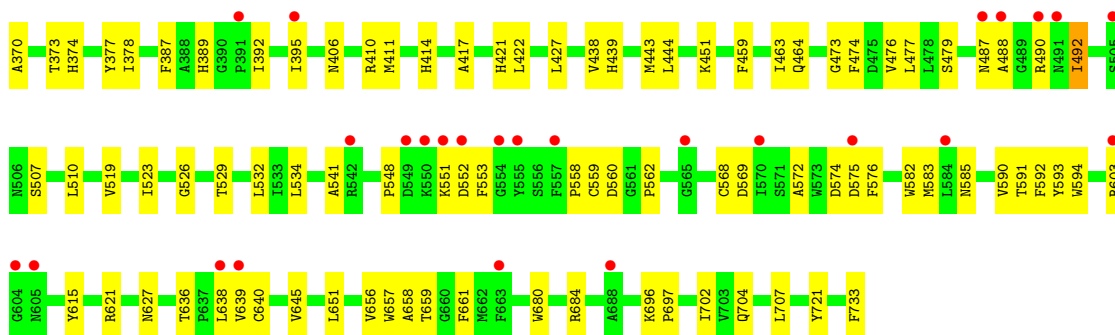
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

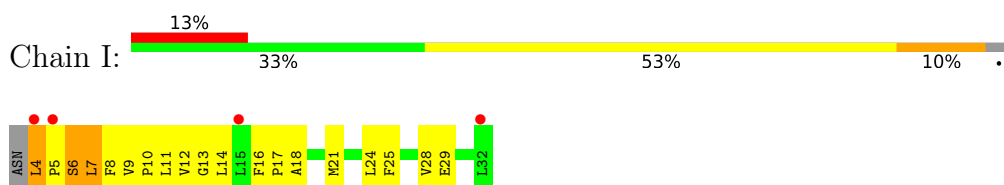


- Molecule 2: Photosystem I P700 chlorophyll a apoprotein A2

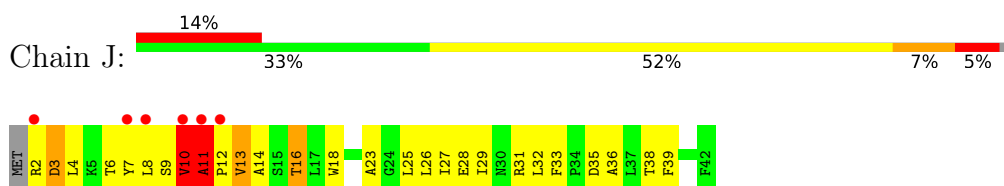




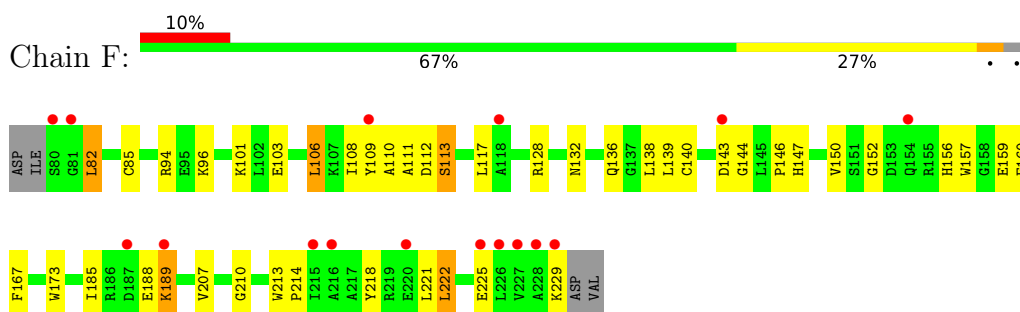
• Molecule 3: Photosystem I reaction center subunit VIII



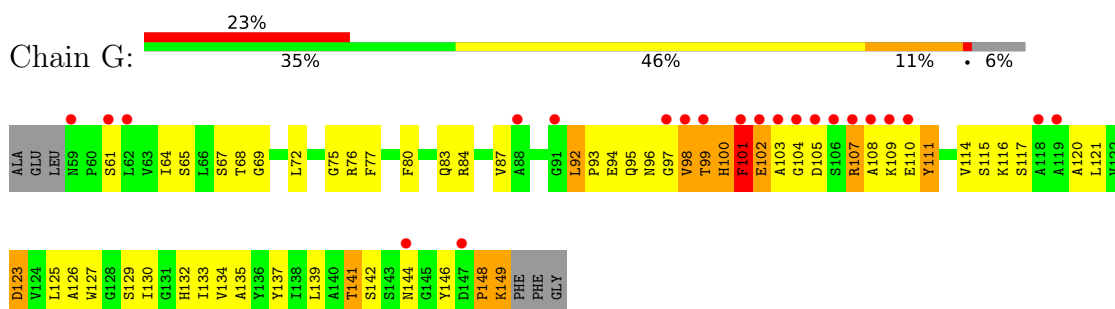
• Molecule 4: Photosystem I reaction center subunit IX



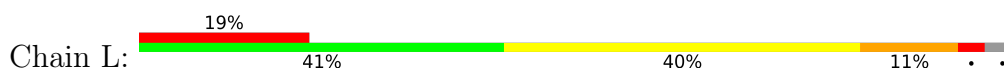
• Molecule 5: Photosystem I reaction center subunit III

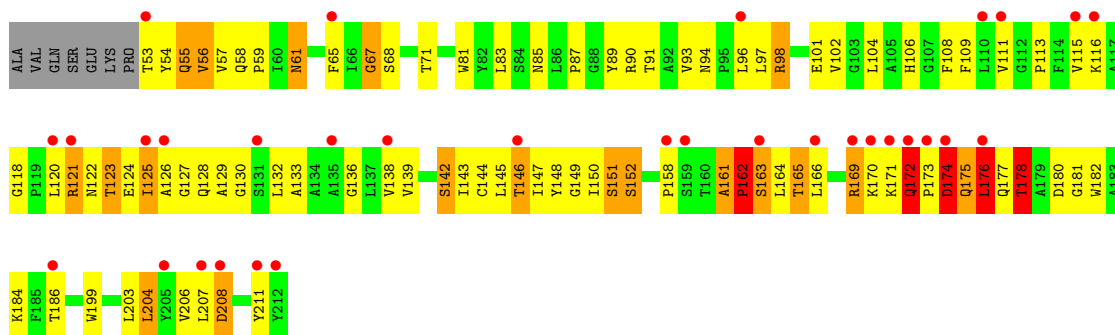


• Molecule 6: photosystem I reaction center

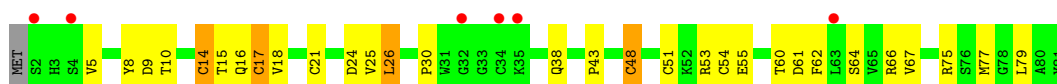


• Molecule 7: Putative uncharacterized protein

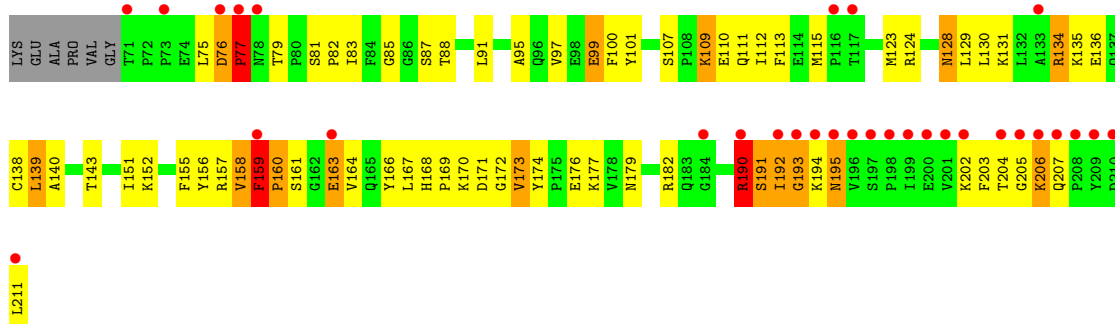




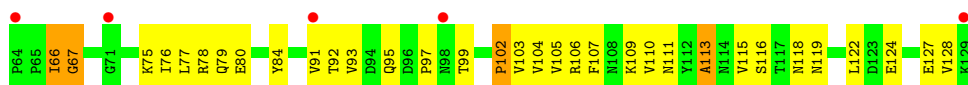
• Molecule 8: Photosystem I iron-sulfur center



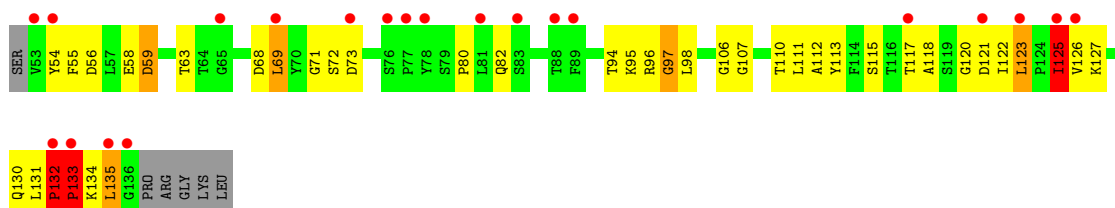
• Molecule 9: Photosystem I reaction center subunit II, chloroplastic



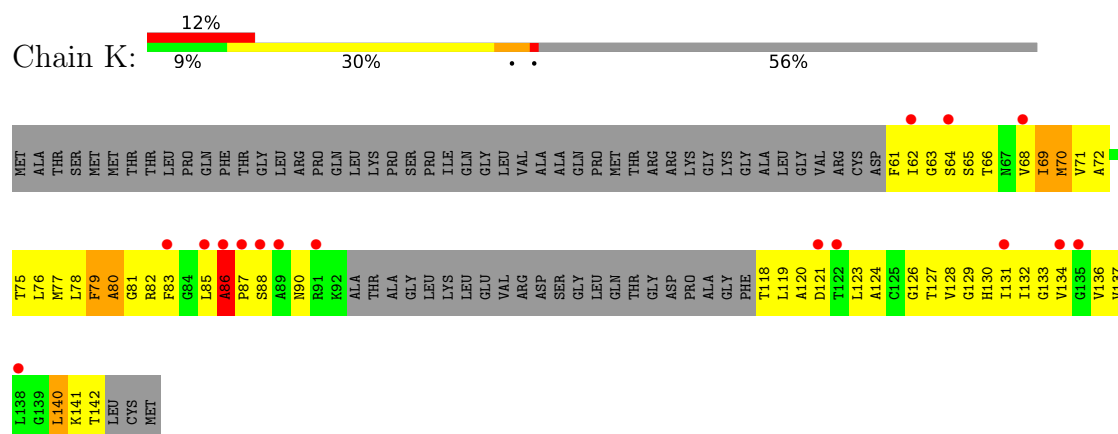
• Molecule 10: Photosystem I reaction center subunit IV A, chloroplastic



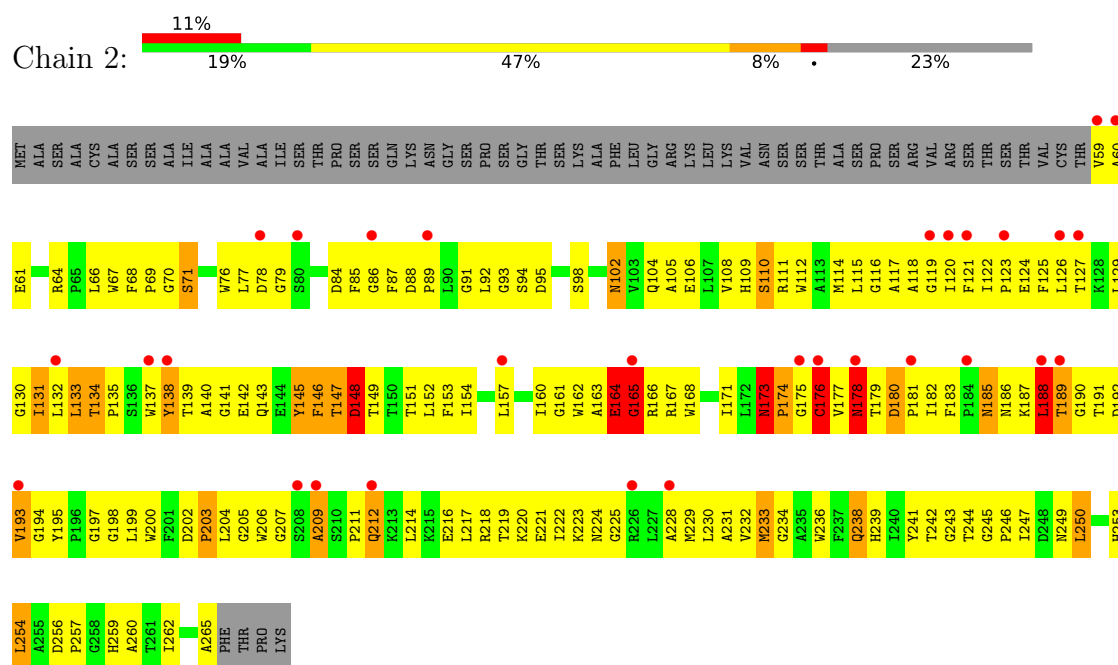
• Molecule 11: Photosystem I reaction center subunit VI



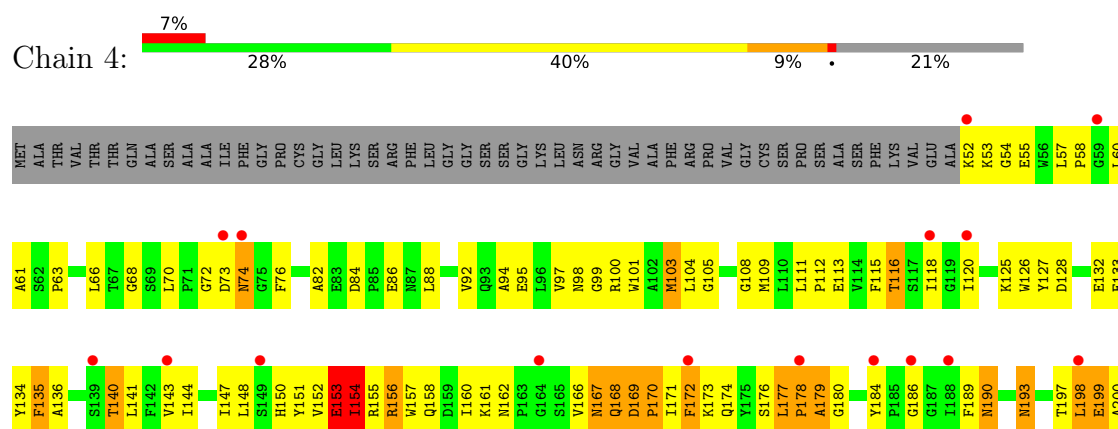
● Molecule 12: Photosystem I reaction center subunit X psaK



● Molecule 13: Type II chlorophyll a/b binding protein from photosystem I

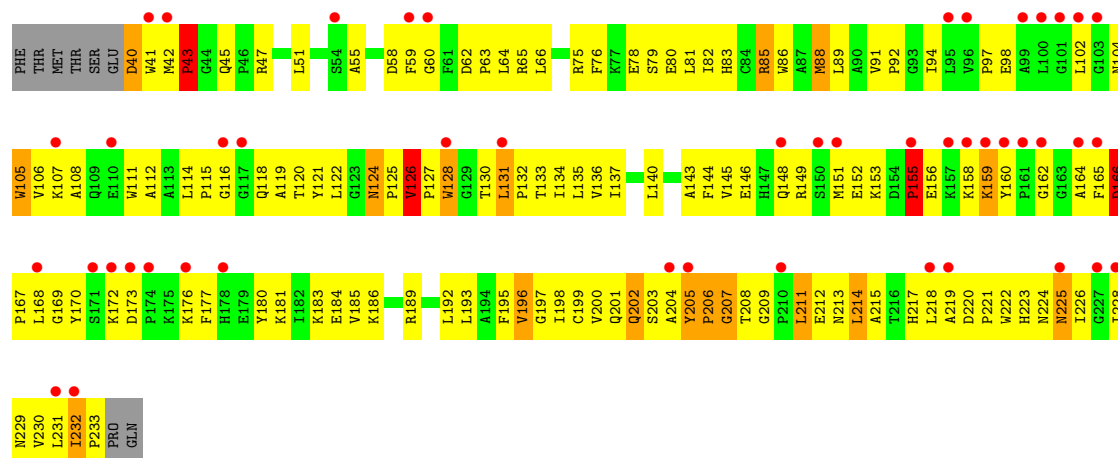


● Molecule 14: Chlorophyll a-b binding protein P4, chloroplastic

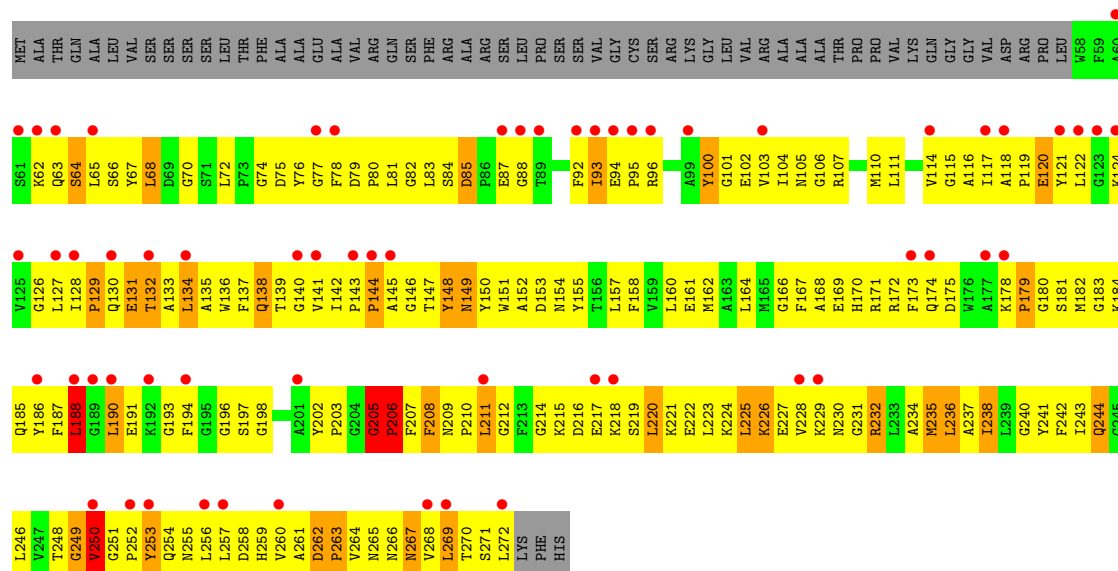
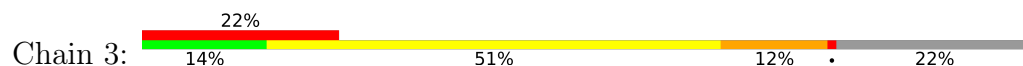




• Molecule 15: Light-harvesting complex I chlorophyll A/B-binding protein



• Molecule 16: Chlorophyll a-b binding protein 3, chloroplastic



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	189.00Å 201.90Å 213.20Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.65 – 2.80 48.65 – 2.80	Depositor EDS
% Data completeness (in resolution range)	100.0 (48.65-2.80) 89.2 (48.65-2.80)	Depositor EDS
R_{merge}	0.26	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.29 (at 2.81Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.259 , 0.268 0.243 , 0.255	Depositor DCC
R_{free} test set	3970 reflections (2.00%)	wwPDB-VP
Wilson B-factor (Å ²)	78.1	Xtriage
Anisotropy	0.306	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.24 , 53.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	35653	wwPDB-VP
Average B, all atoms (Å ²)	113.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.92% 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: BCR, LMG, ZEX, CL0, PQN, DGD, CLA, LMU, CA, SF4, LUT, LHG, CHL

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	A	0.23	0/6049	0.40	0/8253
2	B	0.24	0/6067	0.40	0/8287
3	I	0.92	0/230	1.02	2/313 (0.6%)
4	J	0.76	0/330	0.90	2/452 (0.4%)
5	F	0.62	0/1214	0.64	0/1638
6	G	0.78	0/705	1.01	3/956 (0.3%)
7	L	0.76	0/1233	0.94	7/1690 (0.4%)
8	C	0.82	0/625	0.81	1/846 (0.1%)
9	D	1.00	0/1146	1.06	7/1550 (0.5%)
10	E	0.89	0/542	0.90	3/737 (0.4%)
11	H	0.62	0/662	0.85	4/902 (0.4%)
12	K	0.48	0/381	0.87	1/517 (0.2%)
13	2	0.94	2/1672 (0.1%)	1.09	11/2292 (0.5%)
14	4	0.93	2/1592 (0.1%)	0.99	10/2174 (0.5%)
15	1	0.86	0/1563	1.04	6/2132 (0.3%)
16	3	0.86	2/1666 (0.1%)	1.08	11/2265 (0.5%)
All	All	0.63	6/25677 (0.0%)	0.76	68/35004 (0.2%)

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
6	G	0	1
7	L	0	1
13	2	0	1
14	4	0	1
16	3	0	1
All	All	0	5

The worst 5 of 6 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	4	153	GLU	C-O	-10.68	1.03	1.23
13	2	164	GLU	C-O	-10.38	1.03	1.23
16	3	205	GLY	C-N	7.70	1.48	1.34
16	3	205	GLY	C-O	-7.23	1.12	1.23
13	2	164	GLU	C-N	6.29	1.44	1.33

The worst 5 of 68 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	G	101	PHE	C-N-CA	11.02	149.25	121.70
6	G	100	HIS	N-CA-C	-10.25	83.33	111.00
13	2	165	GLY	N-CA-C	-9.45	89.48	113.10
11	H	120	GLY	N-CA-C	-8.68	91.41	113.10
16	3	206	PRO	CA-N-CD	-8.59	99.47	111.50

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
13	2	164	GLU	Mainchain
16	3	205	GLY	Mainchain
14	4	153	GLU	Mainchain
6	G	101	PHE	Peptide
7	L	98	ARG	Sidechain

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	A	5852	0	5710	169	0
2	B	5856	0	5666	146	0
3	I	224	0	247	34	0
4	J	321	0	328	48	0
5	F	1187	0	1226	39	3
6	G	689	0	675	112	0
7	L	1197	0	1187	165	3

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	C	612	0	594	36	0
9	D	1116	0	1126	103	0
10	E	530	0	530	44	0
11	H	642	0	637	48	0
12	K	379	0	386	92	0
13	2	1613	0	1554	371	0
14	4	1544	0	1489	230	0
15	1	1513	0	1495	379	0
16	3	1619	0	1554	472	0
17	A	65	0	72	6	0
18	1	615	0	511	235	0
18	2	628	0	538	255	0
18	3	698	0	559	265	0
18	4	677	0	635	195	0
18	A	2583	0	2555	197	0
18	B	2519	0	2617	217	0
18	F	95	0	72	20	0
18	G	161	0	141	92	0
18	H	46	0	33	4	0
18	J	50	0	39	7	0
18	K	46	0	33	12	0
18	L	160	0	137	39	0
19	A	8	0	0	1	0
19	C	16	0	0	0	0
20	A	33	0	46	3	0
20	B	33	0	46	5	0
21	1	49	0	74	15	0
21	2	24	0	18	6	0
21	A	89	0	127	12	0
21	B	21	0	12	1	0
22	3	40	0	48	21	0
22	A	240	0	292	21	0
22	B	200	0	245	24	0
22	F	80	0	98	19	0
22	G	40	0	49	29	0
22	I	40	0	49	3	0
22	J	80	0	98	15	0
22	K	40	0	49	17	0
22	L	80	0	98	28	0
23	2	35	0	40	9	0
23	4	35	0	40	6	0
23	B	38	0	46	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
23	F	60	0	60	13	0
23	G	41	0	52	20	0
23	J	55	0	86	9	0
24	B	1	0	0	0	0
25	B	61	0	83	4	0
26	B	70	0	92	4	0
27	1	84	0	110	48	0
27	2	84	0	110	55	0
27	3	84	0	110	62	0
27	4	126	0	165	84	0
27	I	42	0	55	14	0
28	1	103	0	78	35	0
28	2	141	0	95	39	0
28	3	56	0	47	22	0
28	4	145	0	99	44	0
29	4	42	0	56	12	0
All	All	35653	0	35119	3560	3

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 50.

The worst 5 of 3560 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)
16:3:138:GLN:HB2	16:3:145:ALA:HB2	1.25	1.18
18:3:3012:CLA:HBB1	18:3:3012:CLA:HMB1	1.18	1.17
16:3:268:VAL:HG21	18:3:3003:CLA:H43	1.17	1.16
18:3:3004:CLA:HMB1	18:3:3004:CLA:HBB1	1.25	1.15
16:3:111:LEU:HD22	18:3:3006:CLA:CBB	1.74	1.15

All (3) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:96:LYS:CD	7:L:170:LYS:NZ[3_555]	1.69	0.51
5:F:96:LYS:CE	7:L:170:LYS:NZ[3_555]	1.86	0.34
5:F:96:LYS:CG	7:L:170:LYS:NZ[3_555]	1.99	0.21

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	740/758 (98%)	691 (93%)	45 (6%)	4 (0%)	25	56
2	B	730/733 (100%)	695 (95%)	30 (4%)	5 (1%)	19	48
3	I	27/30 (90%)	25 (93%)	1 (4%)	1 (4%)	2	9
4	J	39/42 (93%)	34 (87%)	3 (8%)	2 (5%)	1	5
5	F	148/154 (96%)	138 (93%)	8 (5%)	2 (1%)	9	30
6	G	89/97 (92%)	76 (85%)	8 (9%)	5 (6%)	1	4
7	L	158/167 (95%)	133 (84%)	15 (10%)	10 (6%)	1	3
8	C	78/81 (96%)	72 (92%)	6 (8%)	0	100	100
9	D	139/147 (95%)	116 (84%)	14 (10%)	9 (6%)	1	3
10	E	64/66 (97%)	57 (89%)	6 (9%)	1 (2%)	8	27
11	H	82/90 (91%)	65 (79%)	10 (12%)	7 (8%)	0	1
12	K	53/129 (41%)	49 (92%)	2 (4%)	2 (4%)	2	9
13	2	205/269 (76%)	184 (90%)	7 (3%)	14 (7%)	1	2
14	4	196/252 (78%)	174 (89%)	15 (8%)	7 (4%)	3	10
15	1	192/202 (95%)	168 (88%)	17 (9%)	7 (4%)	3	10
16	3	213/275 (78%)	189 (89%)	15 (7%)	9 (4%)	2	8
All	All	3153/3492 (90%)	2866 (91%)	202 (6%)	85 (3%)	4	15

5 of 85 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	127	VAL
3	I	6	SER
4	J	11	ALA
6	G	101	PHE
6	G	102	GLU

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	603/619 (97%)	595 (99%)	8 (1%)	65	88
2	B	599/600 (100%)	587 (98%)	12 (2%)	50	81
3	I	25/26 (96%)	23 (92%)	2 (8%)	10	30
4	J	33/35 (94%)	29 (88%)	4 (12%)	4	13
5	F	123/127 (97%)	115 (94%)	8 (6%)	14	40
6	G	71/76 (93%)	65 (92%)	6 (8%)	8	27
7	L	124/133 (93%)	107 (86%)	17 (14%)	3	10
8	C	69/70 (99%)	65 (94%)	4 (6%)	17	45
9	D	120/125 (96%)	110 (92%)	10 (8%)	9	28
10	E	59/59 (100%)	57 (97%)	2 (3%)	32	66
11	H	69/74 (93%)	63 (91%)	6 (9%)	8	26
12	K	38/99 (38%)	32 (84%)	6 (16%)	2	7
13	2	166/216 (77%)	148 (89%)	18 (11%)	5	17
14	4	161/202 (80%)	145 (90%)	16 (10%)	6	21
15	1	158/167 (95%)	141 (89%)	17 (11%)	5	17
16	3	159/213 (75%)	135 (85%)	24 (15%)	2	8
All	All	2577/2841 (91%)	2417 (94%)	160 (6%)	15	43

5 of 160 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
14	4	221	GLN
16	3	148	TYR
15	1	40	ASP
15	1	159	LYS
16	3	225	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 59 such sidechains are listed below:

Mol	Chain	Res	Type
8	C	71	HIS
16	3	185	GLN
12	K	130	HIS
16	3	174	GLN
15	1	201	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 209 ligands modelled in this entry, 1 is monoatomic - leaving 208 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
27	LUT	1	1502	-	42,43,43	2.47	4 (9%)	51,60,60	2.21	18 (35%)
18	CLA	3	3001	16	50,58,73	2.56	19 (38%)	58,95,113	2.97	21 (36%)
22	BCR	K	2011	-	41,41,41	2.71	6 (14%)	56,56,56	6.74	27 (48%)
22	BCR	J	6013	-	41,41,41	2.89	8 (19%)	56,56,56	6.55	30 (53%)
18	CLA	1	1002	-	46,54,73	2.63	18 (39%)	53,90,113	3.08	22 (41%)
18	CLA	A	1131	-	65,73,73	2.37	20 (30%)	76,113,113	2.56	21 (27%)
18	CLA	L	1503	-	50,58,73	2.56	18 (36%)	58,95,113	2.97	22 (37%)
26	LMU	B	8001	-	36,36,36	0.49	0	47,47,47	1.18	5 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
18	CLA	2	2003	-	55,63,73	2.38	18 (32%)	64,101,113	3.05	24 (37%)
18	CLA	3	3013	-	46,54,73	2.77	20 (43%)	53,90,113	2.67	20 (37%)
18	CLA	B	1204	-	55,63,73	2.61	19 (34%)	64,101,113	2.78	21 (32%)
18	CLA	2	2019	-	29,35,73	3.22	14 (48%)	28,60,113	3.34	16 (57%)
18	CLA	A	1140	-	65,73,73	2.39	20 (30%)	76,113,113	2.55	23 (30%)
18	CLA	G	1001	-	55,63,73	2.43	18 (32%)	64,101,113	2.88	28 (43%)
18	CLA	4	4007	-	60,68,73	2.27	17 (28%)	70,107,113	2.88	23 (32%)
18	CLA	3	3017	-	46,54,73	2.73	18 (39%)	53,90,113	2.84	21 (39%)
18	CLA	B	1012	-	65,73,73	2.36	19 (29%)	76,113,113	2.50	22 (28%)
18	CLA	4	4017	-	65,73,73	2.21	19 (29%)	76,113,113	2.60	25 (32%)
18	CLA	B	1203	2	65,73,73	2.33	19 (29%)	76,113,113	2.60	22 (28%)
18	CLA	A	1114	-	46,54,73	2.89	19 (41%)	53,90,113	2.86	20 (37%)
18	CLA	A	1130	-	50,58,73	2.74	20 (40%)	58,95,113	2.94	21 (36%)
18	CLA	L	1501	7	50,58,73	2.57	18 (36%)	58,95,113	2.94	25 (43%)
29	ZEX	4	4505	-	42,43,43	1.08	3 (7%)	55,60,60	2.17	19 (34%)
18	CLA	B	1207	-	65,73,73	2.37	20 (30%)	76,113,113	2.62	23 (30%)
18	CLA	A	1117	-	65,73,73	2.38	19 (29%)	76,113,113	2.54	22 (28%)
18	CLA	B	1234	-	60,68,73	2.49	20 (33%)	70,107,113	2.72	24 (34%)
22	BCR	B	6004	-	41,41,41	2.78	6 (14%)	56,56,56	6.67	29 (51%)
18	CLA	1	1014	15	46,54,73	2.70	19 (41%)	53,90,113	3.07	22 (41%)
23	LMG	G	2021	-	41,41,55	0.95	2 (4%)	49,49,63	1.16	5 (10%)
18	CLA	2	2002	-	46,54,73	2.65	19 (41%)	53,90,113	2.99	24 (45%)
18	CLA	A	1104	-	65,73,73	2.37	20 (30%)	76,113,113	2.61	22 (28%)
18	CLA	1	1003	15	55,63,73	2.42	21 (38%)	64,101,113	2.83	26 (40%)
18	CLA	2	2001	13	60,68,73	2.29	19 (31%)	70,107,113	2.81	27 (38%)
23	LMG	2	2802	-	35,35,55	1.08	2 (5%)	43,43,63	1.33	7 (16%)
22	BCR	G	2011	-	41,41,41	3.05	7 (17%)	56,56,56	6.73	29 (51%)
18	CLA	A	1102	-	50,58,73	2.71	19 (38%)	58,95,113	2.86	21 (36%)
18	CLA	A	1120	-	60,68,73	2.46	19 (31%)	70,107,113	2.70	21 (30%)
18	CLA	B	1206	2	65,73,73	2.39	19 (29%)	76,113,113	2.60	24 (31%)
23	LMG	J	5001	-	55,55,55	0.88	2 (3%)	63,63,63	1.44	7 (11%)
18	CLA	A	1151	21	50,58,73	2.76	20 (40%)	58,95,113	2.90	20 (34%)
18	CLA	A	1115	-	46,54,73	2.89	20 (43%)	53,90,113	2.79	19 (35%)
18	CLA	3	3012	16	50,58,73	2.50	19 (38%)	58,95,113	3.08	23 (39%)
18	CLA	B	1213	-	60,68,73	2.47	18 (30%)	70,107,113	2.67	22 (31%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
18	CLA	B	1228	-	60,68,73	2.48	19 (31%)	70,107,113	2.65	22 (31%)
18	CLA	B	1232	-	55,63,73	2.58	20 (36%)	64,101,113	2.74	21 (32%)
18	CLA	2	2012	13	55,63,73	2.39	18 (32%)	64,101,113	2.85	23 (35%)
22	BCR	A	6007	-	41,41,41	2.75	7 (17%)	56,56,56	6.52	23 (41%)
19	SF4	A	3001	1,2	0,12,12	-	-	-	-	-
18	CLA	A	1128	-	65,73,73	2.37	19 (29%)	76,113,113	2.51	21 (27%)
25	DGD	B	7101	-	62,62,67	0.91	1 (1%)	76,76,81	1.33	11 (14%)
18	CLA	A	1138	-	65,73,73	2.40	20 (30%)	76,113,113	2.48	24 (31%)
19	SF4	C	3003	8	0,12,12	-	-	-	-	-
18	CLA	2	2006	-	55,63,73	2.49	18 (32%)	64,101,113	2.80	22 (34%)
18	CLA	4	4009	14	50,58,73	2.48	19 (38%)	58,95,113	2.93	22 (37%)
22	BCR	3	3503	-	41,41,41	2.95	9 (21%)	56,56,56	6.43	31 (55%)
18	CLA	1	1008	-	46,54,73	2.67	18 (39%)	53,90,113	2.98	24 (45%)
23	LMG	F	5001	-	23,23,55	1.24	3 (13%)	31,31,63	1.72	6 (19%)
22	BCR	B	6005	-	41,41,41	2.71	6 (14%)	56,56,56	6.79	23 (41%)
18	CLA	A	1133	-	55,63,73	2.58	20 (36%)	64,101,113	2.77	22 (34%)
18	CLA	1	1007	21	46,54,73	2.65	19 (41%)	53,90,113	3.16	21 (39%)
28	CHL	1	1009	-	56,64,74	1.57	8 (14%)	61,102,114	1.33	11 (18%)
18	CLA	B	1240	21	65,73,73	2.36	19 (29%)	76,113,113	2.60	25 (32%)
18	CLA	3	3008	-	48,56,73	2.54	18 (37%)	55,92,113	3.48	27 (49%)
18	CLA	B	1239	-	65,73,73	2.37	20 (30%)	76,113,113	2.58	22 (28%)
22	BCR	A	6003	-	41,41,41	2.79	6 (14%)	56,56,56	6.48	20 (35%)
28	CHL	3	3011	-	56,64,74	1.87	9 (16%)	61,102,114	1.51	12 (19%)
27	LUT	3	3502	-	42,43,43	2.39	3 (7%)	51,60,60	2.28	17 (33%)
18	CLA	4	4002	-	50,58,73	2.56	17 (34%)	58,95,113	2.97	26 (44%)
27	LUT	I	6018	-	42,43,43	2.46	1 (2%)	51,60,60	2.21	18 (35%)
27	LUT	4	4501	-	42,43,43	2.44	3 (7%)	51,60,60	2.19	16 (31%)
18	CLA	A	1237	-	60,68,73	2.46	19 (31%)	70,107,113	2.80	23 (32%)
18	CLA	B	1209	-	46,54,73	2.91	19 (41%)	53,90,113	2.85	19 (35%)
18	CLA	A	1101	-	65,73,73	2.36	19 (29%)	76,113,113	2.65	22 (28%)
18	CLA	A	1013	-	65,73,73	2.36	20 (30%)	76,113,113	2.58	23 (30%)
19	SF4	C	3002	8	0,12,12	-	-	-	-	-
22	BCR	L	6019	-	41,41,41	2.93	7 (17%)	56,56,56	6.55	24 (42%)
26	LMU	B	8002	-	36,36,36	0.45	0	47,47,47	1.06	3 (6%)
18	CLA	G	1002	-	46,54,73	2.74	20 (43%)	53,90,113	2.93	22 (41%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
18	CLA	B	1219	-	60,68,73	2.48	20 (33%)	70,107,113	2.60	21 (30%)
21	LHG	B	5004	18	20,20,48	1.34	2 (10%)	23,26,54	1.53	3 (13%)
18	CLA	K	1001	-	46,54,73	2.73	19 (41%)	53,90,113	3.10	20 (37%)
18	CLA	B	1227	-	65,73,73	2.37	20 (30%)	76,113,113	2.59	24 (31%)
20	PQN	A	5001	-	34,34,34	1.62	2 (5%)	42,45,45	1.19	3 (7%)
22	BCR	A	6017	-	41,41,41	2.67	6 (14%)	56,56,56	7.12	27 (48%)
18	CLA	B	1212	-	55,63,73	2.57	20 (36%)	64,101,113	2.83	23 (35%)
18	CLA	2	2016	13	50,58,73	2.62	18 (36%)	58,95,113	3.57	29 (50%)
18	CLA	A	1108	-	46,54,73	2.90	20 (43%)	53,90,113	2.84	21 (39%)
22	BCR	A	6002	-	41,41,41	2.74	6 (14%)	56,56,56	6.45	22 (39%)
22	BCR	F	6014	-	41,41,41	3.05	7 (17%)	56,56,56	6.69	23 (41%)
18	CLA	B	1235	-	65,73,73	2.36	19 (29%)	76,113,113	2.64	22 (28%)
18	CLA	A	1113	-	46,54,73	2.87	19 (41%)	53,90,113	2.83	21 (39%)
18	CLA	3	3007	-	50,58,73	2.58	20 (40%)	58,95,113	2.93	24 (41%)
18	CLA	B	1218	-	65,73,73	2.37	20 (30%)	76,113,113	2.63	22 (28%)
23	LMG	B	5005	-	38,38,55	1.08	2 (5%)	46,46,63	1.04	3 (6%)
18	CLA	A	1135	-	51,59,73	2.68	19 (37%)	59,96,113	2.93	22 (37%)
18	CLA	4	4008	-	46,54,73	2.60	18 (39%)	53,90,113	3.32	26 (49%)
28	CHL	4	4013	-	47,55,74	1.98	9 (19%)	50,91,114	1.64	11 (22%)
18	CLA	2	2007	-	60,68,73	2.37	19 (31%)	70,107,113	2.67	22 (31%)
18	CLA	B	1202	-	65,73,73	2.35	19 (29%)	76,113,113	2.65	23 (30%)
18	CLA	A	1110	-	55,63,73	2.60	20 (36%)	64,101,113	2.73	23 (35%)
18	CLA	2	2008	-	50,58,73	2.48	19 (38%)	58,95,113	3.32	30 (51%)
27	LUT	1	1501	-	42,43,43	2.50	4 (9%)	51,60,60	2.31	14 (27%)
18	CLA	F	1301	-	45,53,73	2.64	17 (37%)	52,89,113	2.91	18 (34%)
18	CLA	F	1302	5	50,58,73	2.62	18 (36%)	58,95,113	2.94	21 (36%)
18	CLA	A	1129	-	50,58,73	2.71	19 (38%)	58,95,113	2.92	23 (39%)
18	CLA	A	1132	-	65,73,73	2.37	20 (30%)	76,113,113	2.56	23 (30%)
18	CLA	B	1216	-	65,73,73	2.38	20 (30%)	76,113,113	2.56	23 (30%)
18	CLA	B	1226	-	65,73,73	2.35	19 (29%)	76,113,113	2.55	22 (28%)
18	CLA	A	1106	1	65,73,73	2.39	20 (30%)	76,113,113	2.61	23 (30%)
18	CLA	1	1013	-	46,54,73	2.74	20 (43%)	53,90,113	2.98	19 (35%)
18	CLA	A	1124	-	55,63,73	2.59	20 (36%)	64,101,113	2.85	23 (35%)
18	CLA	2	2009	13	50,58,73	2.57	20 (40%)	58,95,113	2.94	23 (39%)
27	LUT	4	4503	-	42,43,43	2.41	3 (7%)	51,60,60	2.42	15 (29%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
18	CLA	1	1011	-	50,58,73	2.52	18 (36%)	58,95,113	2.93	24 (41%)
18	CLA	B	1210	-	65,73,73	2.34	19 (29%)	76,113,113	2.56	23 (30%)
28	CHL	2	2011	-	48,56,74	2.02	10 (20%)	51,92,114	1.57	11 (21%)
18	CLA	A	1123	-	65,73,73	2.39	20 (30%)	76,113,113	2.59	23 (30%)
23	LMG	F	5002	-	37,37,55	1.07	2 (5%)	45,45,63	1.27	5 (11%)
18	CLA	4	4003	14	65,73,73	2.25	20 (30%)	76,113,113	2.59	24 (31%)
18	CLA	A	1109	-	65,73,73	2.37	19 (29%)	76,113,113	2.58	22 (28%)
18	CLA	B	1221	-	65,73,73	2.38	20 (30%)	76,113,113	2.62	25 (32%)
18	CLA	4	4004	14	60,68,73	2.31	18 (30%)	70,107,113	2.68	24 (34%)
18	CLA	A	1127	-	65,73,73	2.39	19 (29%)	76,113,113	2.53	22 (28%)
18	CLA	B	1214	-	59,67,73	2.50	19 (32%)	68,105,113	2.73	23 (33%)
18	CLA	3	3002	-	46,54,73	2.68	20 (43%)	53,90,113	3.03	25 (47%)
20	PQN	B	5002	-	34,34,34	1.69	2 (5%)	42,45,45	1.07	3 (7%)
18	CLA	B	1224	-	65,73,73	2.36	19 (29%)	76,113,113	2.58	23 (30%)
18	CLA	4	4005	14	60,68,73	2.28	18 (30%)	70,107,113	2.84	27 (38%)
18	CLA	A	1125	-	60,68,73	2.43	19 (31%)	70,107,113	2.69	24 (34%)
18	CLA	3	3004	16	60,68,73	2.32	19 (31%)	70,107,113	2.67	20 (28%)
18	CLA	B	1231	-	60,68,73	2.50	20 (33%)	70,107,113	2.60	23 (32%)
18	CLA	A	1139	-	65,73,73	2.37	20 (30%)	76,113,113	2.56	23 (30%)
18	CLA	B	1023	-	65,73,73	2.36	19 (29%)	76,113,113	2.55	24 (31%)
18	CLA	B	1211	-	65,73,73	2.34	19 (29%)	76,113,113	2.63	25 (32%)
27	LUT	2	2502	-	42,43,43	2.47	3 (7%)	51,60,60	2.10	16 (31%)
18	CLA	B	1222	-	65,73,73	2.36	19 (29%)	76,113,113	2.64	25 (32%)
18	CLA	4	4016	-	46,54,73	2.76	18 (39%)	53,90,113	2.93	23 (43%)
17	CL0	A	1011	-	65,73,73	2.38	20 (30%)	76,113,113	2.55	22 (28%)
18	CLA	3	3018	16	50,58,73	2.57	21 (42%)	58,95,113	3.03	25 (43%)
22	BCR	A	6008	-	41,41,41	2.83	6 (14%)	56,56,56	6.57	26 (46%)
28	CHL	2	2013	-	46,54,74	1.60	7 (15%)	49,90,114	1.45	9 (18%)
18	CLA	A	1022	-	65,73,73	2.39	19 (29%)	76,113,113	2.48	23 (30%)
18	CLA	2	2004	13	65,73,73	2.36	17 (26%)	76,113,113	2.51	23 (30%)
18	CLA	A	1122	-	65,73,73	2.37	19 (29%)	76,113,113	2.53	22 (28%)
18	CLA	1	1001	15	60,68,73	2.30	19 (31%)	70,107,113	2.74	21 (30%)
18	CLA	1	1006	-	50,58,73	2.59	21 (42%)	58,95,113	2.95	23 (39%)
27	LUT	2	2501	-	42,43,43	2.43	1 (2%)	51,60,60	2.11	14 (27%)
22	BCR	B	6010	-	41,41,41	2.73	6 (14%)	56,56,56	6.56	23 (41%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
18	CLA	A	1111	-	60,68,73	2.46	19 (31%)	70,107,113	2.64	24 (34%)
18	CLA	4	4001	14	60,68,73	2.30	19 (31%)	70,107,113	2.76	26 (37%)
18	CLA	G	1003	-	60,68,73	2.35	19 (31%)	70,107,113	2.74	25 (35%)
18	CLA	B	1021	-	65,73,73	2.37	18 (27%)	76,113,113	2.64	23 (30%)
18	CLA	L	1502	-	60,68,73	2.34	18 (30%)	70,107,113	2.73	24 (34%)
18	CLA	A	1121	-	55,63,73	2.58	20 (36%)	64,101,113	2.86	24 (37%)
22	BCR	J	6012	-	41,41,41	2.91	8 (19%)	56,56,56	6.56	29 (51%)
18	CLA	A	1136	-	56,64,73	2.56	20 (35%)	65,102,113	2.78	25 (38%)
18	CLA	A	1116	-	60,68,73	2.47	19 (31%)	70,107,113	2.75	22 (31%)
18	CLA	B	1238	-	65,73,73	2.39	20 (30%)	76,113,113	2.55	21 (27%)
18	CLA	A	1105	-	51,59,73	2.70	20 (39%)	59,96,113	2.89	25 (42%)
22	BCR	L	6020	-	41,41,41	2.83	7 (17%)	56,56,56	6.55	29 (51%)
18	CLA	B	1205	-	65,73,73	2.36	19 (29%)	76,113,113	2.46	23 (30%)
18	CLA	J	1302	4	50,58,73	2.73	20 (40%)	58,95,113	2.96	23 (39%)
18	CLA	B	1201	-	50,58,73	2.70	20 (40%)	58,95,113	2.86	24 (41%)
27	LUT	4	4502	-	42,43,43	2.38	3 (7%)	51,60,60	1.95	15 (29%)
18	CLA	B	1220	-	65,73,73	2.37	20 (30%)	76,113,113	2.47	23 (30%)
18	CLA	3	3010	-	60,68,73	2.34	18 (30%)	70,107,113	2.78	23 (32%)
18	CLA	A	1103	-	65,73,73	2.34	20 (30%)	76,113,113	2.61	24 (31%)
18	CLA	B	1230	-	58,66,73	2.48	17 (29%)	67,104,113	2.86	22 (32%)
21	LHG	A	7001	-	48,48,48	0.96	2 (4%)	51,54,54	1.13	4 (7%)
18	CLA	A	1118	-	46,54,73	2.86	18 (39%)	53,90,113	2.91	20 (37%)
22	BCR	I	6020	-	41,41,41	2.77	7 (17%)	56,56,56	6.64	20 (35%)
21	LHG	A	5003	18	39,39,48	1.04	2 (5%)	42,45,54	1.18	4 (9%)
18	CLA	4	4006	-	50,58,73	2.51	18 (36%)	58,95,113	2.85	23 (39%)
18	CLA	A	1134	-	55,63,73	2.59	19 (34%)	64,101,113	2.78	22 (34%)
18	CLA	3	3003	16	60,68,73	2.36	19 (31%)	70,107,113	2.73	24 (34%)
18	CLA	B	1223	-	65,73,73	2.34	19 (29%)	76,113,113	2.60	24 (31%)
18	CLA	B	1208	-	55,63,73	2.60	20 (36%)	64,101,113	2.82	22 (34%)
18	CLA	2	2005	-	55,63,73	2.49	18 (32%)	64,101,113	2.76	24 (37%)
28	CHL	2	2010	-	47,55,74	1.97	9 (19%)	50,91,114	1.47	9 (18%)
18	CLA	B	1229	-	65,73,73	2.37	20 (30%)	76,113,113	2.60	23 (30%)
18	CLA	4	4012	14	65,73,73	2.21	18 (27%)	76,113,113	2.68	26 (34%)
18	CLA	B	1236	-	55,63,73	2.58	19 (34%)	64,101,113	2.84	22 (34%)
18	CLA	A	1107	1	65,73,73	2.38	20 (30%)	76,113,113	2.58	23 (30%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
18	CLA	A	1112	-	65,73,73	2.36	20 (30%)	76,113,113	2.54	22 (28%)
18	CLA	A	1119	-	65,73,73	2.37	19 (29%)	76,113,113	2.54	23 (30%)
18	CLA	3	3006	-	50,58,73	2.57	20 (40%)	58,95,113	2.97	24 (41%)
18	CLA	1	1005	-	55,63,73	2.39	19 (34%)	64,101,113	2.89	26 (40%)
22	BCR	B	6009	-	41,41,41	2.81	6 (14%)	56,56,56	6.39	23 (41%)
28	CHL	1	1010	15	47,55,74	1.64	7 (14%)	50,91,114	1.41	8 (16%)
22	BCR	F	6016	-	41,41,41	3.07	9 (21%)	56,56,56	6.70	24 (42%)
18	CLA	B	1215	-	60,68,73	2.50	20 (33%)	70,107,113	2.68	22 (31%)
18	CLA	3	3005	-	55,63,73	2.45	19 (34%)	64,101,113	2.89	24 (37%)
18	CLA	A	1126	-	65,73,73	2.38	20 (30%)	76,113,113	2.56	23 (30%)
23	LMG	4	4801	-	35,35,55	1.04	2 (5%)	43,43,63	1.63	10 (23%)
21	LHG	2	2801	-	23,23,48	1.32	2 (8%)	26,29,54	1.21	4 (15%)
18	CLA	B	1217	-	46,54,73	2.88	20 (43%)	53,90,113	2.84	19 (35%)
28	CHL	4	4011	-	51,59,74	1.89	10 (19%)	55,96,114	1.56	11 (20%)
22	BCR	A	6011	-	41,41,41	2.89	6 (14%)	56,56,56	6.72	24 (42%)
18	CLA	1	1012	15	50,58,73	2.57	20 (40%)	58,95,113	2.89	23 (39%)
21	LHG	1	1801	18	48,48,48	0.91	2 (4%)	51,54,54	1.20	5 (9%)
27	LUT	3	3501	-	42,43,43	2.34	1 (2%)	51,60,60	2.37	19 (37%)
18	CLA	B	1225	-	65,73,73	2.38	20 (30%)	76,113,113	2.52	21 (27%)
18	CLA	1	1004	15	65,73,73	2.22	19 (29%)	76,113,113	2.65	23 (30%)
18	CLA	H	1000	11	46,54,73	2.88	19 (41%)	53,90,113	2.84	19 (35%)
22	BCR	B	6006	-	41,41,41	2.79	6 (14%)	56,56,56	6.86	28 (50%)
28	CHL	4	4010	-	47,55,74	2.11	12 (25%)	50,91,114	1.74	13 (26%)
18	CLA	3	3019	-	29,35,73	3.33	15 (51%)	28,60,113	3.29	15 (53%)
18	CLA	A	1137	-	55,63,73	2.58	20 (36%)	64,101,113	2.74	22 (34%)

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
27	LUT	1	1502	-	1/1/12/27	3/29/67/67	0/2/2/2
18	CLA	3	3001	16	1/1/12/20	4/19/97/115	-
22	BCR	K	2011	-	-	11/29/63/63	0/2/2/2
22	BCR	J	6013	-	-	13/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
18	CLA	1	1002	-	1/1/11/20	6/15/93/115	-
18	CLA	A	1131	-	1/1/15/20	12/37/115/115	-
18	CLA	L	1503	-	1/1/12/20	5/19/97/115	-
26	LMU	B	8001	-	-	8/21/61/61	0/2/2/2
18	CLA	2	2003	-	1/1/13/20	11/25/103/115	-
18	CLA	3	3013	-	1/1/11/20	11/15/93/115	-
18	CLA	B	1204	-	1/1/13/20	12/25/103/115	-
18	CLA	2	2019	-	1/1/5/20	-	-
18	CLA	A	1140	-	1/1/15/20	16/37/115/115	-
18	CLA	G	1001	-	1/1/13/20	18/25/103/115	-
18	CLA	4	4007	-	1/1/14/20	14/31/109/115	-
18	CLA	3	3017	-	1/1/11/20	9/15/93/115	-
18	CLA	B	1012	-	1/1/15/20	15/37/115/115	-
18	CLA	4	4017	-	1/1/15/20	19/37/115/115	-
18	CLA	B	1203	2	1/1/15/20	14/37/115/115	-
18	CLA	A	1114	-	1/1/11/20	6/15/93/115	-
18	CLA	A	1130	-	-	7/19/97/115	-
18	CLA	L	1501	7	1/1/12/20	7/19/97/115	-
29	ZEX	4	4505	-	-	2/29/67/67	0/2/2/2
18	CLA	B	1207	-	-	18/37/115/115	-
18	CLA	A	1117	-	1/1/15/20	13/37/115/115	-
18	CLA	B	1234	-	1/1/14/20	11/31/109/115	-
22	BCR	B	6004	-	-	10/29/63/63	0/2/2/2
18	CLA	1	1014	15	1/1/11/20	9/15/93/115	-
23	LMG	G	2021	-	-	24/36/56/70	0/1/1/1
18	CLA	2	2002	-	1/1/11/20	8/15/93/115	-
18	CLA	A	1104	-	1/1/15/20	16/37/115/115	-
18	CLA	1	1003	15	1/1/13/20	7/25/103/115	-
18	CLA	2	2001	13	1/1/14/20	18/31/109/115	-
23	LMG	2	2802	-	-	12/30/50/70	0/1/1/1
22	BCR	G	2011	-	-	11/29/63/63	0/2/2/2
18	CLA	A	1102	-	1/1/12/20	7/19/97/115	-
18	CLA	A	1120	-	1/1/14/20	16/31/109/115	-
18	CLA	B	1206	2	1/1/15/20	15/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
23	LMG	J	5001	-	-	36/50/70/70	0/1/1/1
18	CLA	A	1151	21	1/1/12/20	11/19/97/115	-
18	CLA	A	1115	-	1/1/11/20	6/15/93/115	-
18	CLA	3	3012	16	1/1/12/20	7/19/97/115	-
18	CLA	B	1228	-	1/1/14/20	15/31/109/115	-
18	CLA	B	1232	-	1/1/13/20	6/25/103/115	-
18	CLA	B	1213	-	-	13/31/109/115	-
18	CLA	2	2012	13	1/1/13/20	9/25/103/115	-
22	BCR	A	6007	-	-	6/29/63/63	0/2/2/2
19	SF4	A	3001	1,2	-	-	0/6/5/5
18	CLA	A	1128	-	1/1/15/20	13/37/115/115	-
25	DGD	B	7101	-	-	23/50/90/95	0/2/2/2
18	CLA	A	1138	-	1/1/15/20	19/37/115/115	-
19	SF4	C	3003	8	-	-	0/6/5/5
18	CLA	2	2006	-	1/1/13/20	10/25/103/115	-
18	CLA	4	4009	14	1/1/12/20	4/19/97/115	-
22	BCR	3	3503	-	-	14/29/63/63	0/2/2/2
18	CLA	1	1008	-	1/1/11/20	9/15/93/115	-
23	LMG	F	5001	-	-	9/16/36/70	0/1/1/1
22	BCR	B	6005	-	-	13/29/63/63	0/2/2/2
18	CLA	A	1133	-	-	10/25/103/115	-
18	CLA	1	1007	21	1/1/11/20	8/15/93/115	-
28	CHL	1	1009	-	4/4/18/26	8/27/125/137	-
18	CLA	B	1240	21	1/1/15/20	17/37/115/115	-
18	CLA	3	3008	-	1/1/11/20	12/17/95/115	-
18	CLA	B	1239	-	1/1/15/20	18/37/115/115	-
28	CHL	3	3011	-	4/4/18/26	6/27/125/137	-
22	BCR	A	6003	-	-	13/29/63/63	0/2/2/2
27	LUT	3	3502	-	1/1/12/27	8/29/67/67	0/2/2/2
18	CLA	4	4002	-	1/1/12/20	7/19/97/115	-
27	LUT	I	6018	-	1/1/12/27	3/29/67/67	0/2/2/2
27	LUT	4	4501	-	1/1/12/27	4/29/67/67	0/2/2/2
18	CLA	A	1237	-	1/1/14/20	13/31/109/115	-
18	CLA	B	1209	-	1/1/11/20	5/15/93/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
18	CLA	A	1101	-	1/1/15/20	15/37/115/115	-
18	CLA	A	1013	-	1/1/15/20	12/37/115/115	-
22	BCR	L	6019	-	-	11/29/63/63	0/2/2/2
19	SF4	C	3002	8	-	-	0/6/5/5
26	LMU	B	8002	-	-	14/21/61/61	0/2/2/2
18	CLA	G	1002	-	1/1/11/20	8/15/93/115	-
18	CLA	B	1219	-	1/1/14/20	17/31/109/115	-
21	LHG	B	5004	18	-	15/23/23/53	-
18	CLA	K	1001	-	1/1/11/20	11/15/93/115	-
18	CLA	B	1227	-	1/1/15/20	11/37/115/115	-
20	PQN	A	5001	-	-	10/23/43/43	0/2/2/2
22	BCR	A	6017	-	-	10/29/63/63	0/2/2/2
18	CLA	B	1212	-	1/1/13/20	7/25/103/115	-
18	CLA	2	2016	13	1/1/12/20	9/19/97/115	-
18	CLA	A	1108	-	1/1/11/20	6/15/93/115	-
22	BCR	A	6002	-	-	11/29/63/63	0/2/2/2
22	BCR	F	6014	-	-	12/29/63/63	0/2/2/2
18	CLA	B	1235	-	1/1/15/20	17/37/115/115	-
18	CLA	A	1113	-	1/1/11/20	11/15/93/115	-
18	CLA	3	3007	-	1/1/12/20	6/19/97/115	-
18	CLA	B	1218	-	1/1/15/20	16/37/115/115	-
23	LMG	B	5005	-	-	17/33/53/70	0/1/1/1
18	CLA	A	1135	-	1/1/12/20	6/21/99/115	-
18	CLA	4	4008	-	1/1/11/20	12/15/93/115	-
18	CLA	2	2007	-	1/1/14/20	13/31/109/115	-
18	CLA	B	1202	-	1/1/15/20	18/37/115/115	-
18	CLA	A	1110	-	1/1/13/20	10/25/103/115	-
18	CLA	2	2008	-	1/1/12/20	9/19/97/115	-
27	LUT	1	1501	-	1/1/12/27	8/29/67/67	0/2/2/2
18	CLA	F	1301	-	1/1/11/20	2/13/91/115	-
18	CLA	F	1302	5	1/1/12/20	10/19/97/115	-
18	CLA	A	1129	-	1/1/12/20	9/19/97/115	-
18	CLA	A	1132	-	1/1/15/20	13/37/115/115	-
18	CLA	B	1216	-	1/1/15/20	13/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
18	CLA	B	1226	-	1/1/15/20	19/37/115/115	-
18	CLA	A	1106	1	1/1/15/20	14/37/115/115	-
18	CLA	1	1013	-	1/1/11/20	8/15/93/115	-
18	CLA	A	1124	-	1/1/13/20	10/25/103/115	-
18	CLA	2	2009	13	1/1/12/20	7/19/97/115	-
27	LUT	4	4503	-	1/1/12/27	10/29/67/67	0/2/2/2
18	CLA	1	1011	-	1/1/12/20	10/19/97/115	-
18	CLA	B	1210	-	1/1/15/20	15/37/115/115	-
28	CHL	2	2011	-	3/3/16/26	2/18/116/137	-
18	CLA	A	1123	-	1/1/15/20	16/37/115/115	-
23	LMG	F	5002	-	-	15/32/52/70	0/1/1/1
18	CLA	4	4003	14	1/1/15/20	17/37/115/115	-
18	CLA	A	1109	-	1/1/15/20	11/37/115/115	-
18	CLA	B	1221	-	1/1/15/20	19/37/115/115	-
18	CLA	4	4004	14	1/1/14/20	10/31/109/115	-
18	CLA	A	1127	-	1/1/15/20	19/37/115/115	-
18	CLA	B	1214	-	1/1/13/20	10/30/108/115	-
18	CLA	3	3002	-	1/1/11/20	6/15/93/115	-
20	PQN	B	5002	-	-	13/23/43/43	0/2/2/2
18	CLA	B	1224	-	1/1/15/20	21/37/115/115	-
18	CLA	4	4005	14	1/1/14/20	12/31/109/115	-
18	CLA	A	1125	-	1/1/14/20	19/31/109/115	-
18	CLA	3	3004	16	1/1/14/20	10/31/109/115	-
18	CLA	B	1231	-	1/1/14/20	11/31/109/115	-
18	CLA	A	1139	-	1/1/15/20	14/37/115/115	-
18	CLA	B	1023	-	1/1/15/20	10/37/115/115	-
18	CLA	B	1211	-	1/1/15/20	11/37/115/115	-
27	LUT	2	2502	-	1/1/12/27	4/29/67/67	0/2/2/2
18	CLA	B	1222	-	1/1/15/20	16/37/115/115	-
18	CLA	4	4016	-	1/1/11/20	11/15/93/115	-
17	CL0	A	1011	-	3/3/20/25	8/37/135/135	-
18	CLA	3	3018	16	1/1/12/20	7/19/97/115	-
22	BCR	A	6008	-	-	9/29/63/63	0/2/2/2
28	CHL	2	2013	-	3/3/16/26	4/15/113/137	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
18	CLA	A	1022	-	1/1/15/20	12/37/115/115	-
18	CLA	2	2004	13	1/1/15/20	13/37/115/115	-
18	CLA	A	1122	-	1/1/15/20	24/37/115/115	-
18	CLA	1	1001	15	1/1/14/20	14/31/109/115	-
18	CLA	1	1006	-	1/1/12/20	8/19/97/115	-
27	LUT	2	2501	-	1/1/12/27	3/29/67/67	0/2/2/2
22	BCR	B	6010	-	-	10/29/63/63	0/2/2/2
18	CLA	A	1111	-	1/1/14/20	11/31/109/115	-
18	CLA	4	4001	14	1/1/14/20	13/31/109/115	-
18	CLA	G	1003	-	1/1/14/20	13/31/109/115	-
18	CLA	B	1021	-	1/1/15/20	14/37/115/115	-
18	CLA	L	1502	-	1/1/14/20	15/31/109/115	-
18	CLA	A	1121	-	1/1/13/20	15/25/103/115	-
22	BCR	J	6012	-	-	11/29/63/63	0/2/2/2
18	CLA	A	1136	-	1/1/13/20	9/27/105/115	-
18	CLA	A	1116	-	1/1/14/20	17/31/109/115	-
18	CLA	B	1238	-	1/1/15/20	15/37/115/115	-
18	CLA	A	1105	-	1/1/12/20	12/21/99/115	-
22	BCR	L	6020	-	-	9/29/63/63	0/2/2/2
18	CLA	B	1205	-	1/1/15/20	10/37/115/115	-
18	CLA	J	1302	4	1/1/12/20	11/19/97/115	-
18	CLA	B	1201	-	1/1/12/20	10/19/97/115	-
27	LUT	4	4502	-	1/1/12/27	8/29/67/67	0/2/2/2
18	CLA	B	1220	-	-	16/37/115/115	-
18	CLA	3	3010	-	1/1/14/20	17/31/109/115	-
18	CLA	A	1103	-	1/1/15/20	21/37/115/115	-
18	CLA	B	1230	-	1/1/13/20	16/29/107/115	-
21	LHG	A	7001	-	-	30/53/53/53	-
18	CLA	A	1118	-	1/1/11/20	8/15/93/115	-
22	BCR	I	6020	-	-	10/29/63/63	0/2/2/2
21	LHG	A	5003	18	-	21/44/44/53	-
18	CLA	4	4006	-	1/1/12/20	6/19/97/115	-
18	CLA	A	1134	-	1/1/13/20	15/25/103/115	-
18	CLA	3	3003	16	1/1/14/20	10/31/109/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
18	CLA	B	1223	-	-	14/37/115/115	-
18	CLA	B	1208	-	1/1/13/20	15/25/103/115	-
18	CLA	2	2005	-	1/1/13/20	14/25/103/115	-
28	CHL	2	2010	-	3/3/16/26	2/17/115/137	-
18	CLA	B	1229	-	1/1/15/20	15/37/115/115	-
18	CLA	4	4012	14	1/1/15/20	17/37/115/115	-
18	CLA	B	1236	-	1/1/13/20	10/25/103/115	-
18	CLA	A	1107	1	1/1/15/20	14/37/115/115	-
18	CLA	A	1112	-	1/1/15/20	14/37/115/115	-
18	CLA	A	1119	-	1/1/15/20	24/37/115/115	-
18	CLA	3	3006	-	1/1/12/20	6/19/97/115	-
18	CLA	1	1005	-	1/1/13/20	10/25/103/115	-
28	CHL	1	1010	15	3/3/16/26	5/17/115/137	-
22	BCR	B	6009	-	-	7/29/63/63	0/2/2/2
22	BCR	F	6016	-	-	8/29/63/63	0/2/2/2
18	CLA	B	1215	-	1/1/14/20	15/31/109/115	-
18	CLA	3	3005	-	1/1/13/20	17/25/103/115	-
18	CLA	A	1126	-	1/1/15/20	15/37/115/115	-
23	LMG	4	4801	-	-	16/30/50/70	0/1/1/1
21	LHG	2	2801	-	-	15/28/28/53	-
18	CLA	B	1217	-	1/1/11/20	8/15/93/115	-
28	CHL	4	4011	-	3/3/17/26	3/21/119/137	-
22	BCR	A	6011	-	-	18/29/63/63	0/2/2/2
18	CLA	1	1012	15	1/1/12/20	8/19/97/115	-
27	LUT	3	3501	-	1/1/12/27	5/29/67/67	0/2/2/2
21	LHG	1	1801	18	-	24/53/53/53	-
18	CLA	B	1225	-	1/1/15/20	16/37/115/115	-
18	CLA	1	1004	15	1/1/15/20	18/37/115/115	-
18	CLA	H	1000	11	1/1/11/20	10/15/93/115	-
28	CHL	4	4013	-	3/3/16/26	4/17/115/137	-
28	CHL	4	4010	-	3/3/16/26	4/17/115/137	-
22	BCR	B	6006	-	-	10/29/63/63	0/2/2/2
18	CLA	3	3019	-	1/1/5/20	-	-
18	CLA	A	1137	-	1/1/13/20	12/25/103/115	-

The worst 5 of 3091 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	2	2502	LUT	C24-C25	14.89	1.51	1.33
27	I	6018	LUT	C24-C25	14.89	1.51	1.33
27	2	2501	LUT	C24-C25	14.81	1.51	1.33
27	1	1501	LUT	C24-C25	14.74	1.51	1.33
27	1	1502	LUT	C24-C25	14.31	1.51	1.33

The worst 5 of 4248 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	A	6017	BCR	C16-C17-C18	29.85	169.91	127.31
22	G	2011	BCR	C16-C17-C18	27.95	167.20	127.31
22	B	6005	BCR	C16-C17-C18	27.71	166.86	127.31
22	K	2011	BCR	C16-C17-C18	27.60	166.70	127.31
22	I	6020	BCR	C16-C17-C18	27.15	166.06	127.31

5 of 182 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
17	A	1011	CL0	ND
17	A	1011	CL0	NA
17	A	1011	CL0	NC
18	A	1013	CLA	ND
18	A	1151	CLA	ND

5 of 2380 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
18	A	1013	CLA	CHA-CBD-CGD-O1D
18	A	1151	CLA	CHA-CBD-CGD-O1D
18	A	1151	CLA	CHA-CBD-CGD-O2D
18	A	1151	CLA	CBD-CGD-O2D-CED
18	A	1022	CLA	CBD-CGD-O2D-CED

There are no ring outliers.

205 monomers are involved in 1953 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
27	1	1502	LUT	17	0
18	3	3001	CLA	24	0
22	K	2011	BCR	17	0
22	J	6013	BCR	8	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
18	1	1002	CLA	21	0
18	A	1131	CLA	3	0
18	L	1503	CLA	11	0
26	B	8001	LMU	1	0
18	2	2003	CLA	30	0
18	3	3013	CLA	23	0
18	B	1204	CLA	10	0
18	A	1140	CLA	5	0
18	G	1001	CLA	36	0
18	4	4007	CLA	20	0
18	3	3017	CLA	11	0
18	B	1012	CLA	6	0
18	4	4017	CLA	11	0
18	B	1203	CLA	3	0
18	A	1114	CLA	3	0
18	A	1130	CLA	4	0
18	L	1501	CLA	15	0
29	4	4505	ZEX	12	0
18	B	1207	CLA	12	0
18	A	1117	CLA	4	0
18	B	1234	CLA	8	0
22	B	6004	BCR	10	0
18	1	1014	CLA	14	0
23	G	2021	LMG	20	0
18	2	2002	CLA	38	0
18	A	1104	CLA	4	0
18	1	1003	CLA	32	0
18	2	2001	CLA	33	0
23	2	2802	LMG	9	0
22	G	2011	BCR	29	0
18	A	1102	CLA	4	0
18	A	1120	CLA	3	0
18	B	1206	CLA	6	0
23	J	5001	LMG	9	0
18	A	1151	CLA	4	0
18	A	1115	CLA	3	0
18	3	3012	CLA	32	0
18	B	1213	CLA	6	0
18	B	1228	CLA	1	0
18	B	1232	CLA	3	0
18	2	2012	CLA	24	0
22	A	6007	BCR	3	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
19	A	3001	SF4	1	0
18	A	1128	CLA	11	0
25	B	7101	DGD	4	0
18	A	1138	CLA	4	0
18	2	2006	CLA	22	0
18	4	4009	CLA	9	0
22	3	3503	BCR	21	0
18	1	1008	CLA	34	0
23	F	5001	LMG	7	0
22	B	6005	BCR	2	0
18	A	1133	CLA	3	0
18	1	1007	CLA	10	0
28	1	1009	CHL	27	0
18	B	1240	CLA	10	0
18	3	3008	CLA	19	0
18	B	1239	CLA	5	0
22	A	6003	BCR	2	0
28	3	3011	CHL	22	0
27	3	3502	LUT	24	0
18	4	4002	CLA	11	0
27	I	6018	LUT	14	0
27	4	4501	LUT	21	0
18	A	1237	CLA	5	0
18	B	1209	CLA	3	0
18	A	1101	CLA	6	0
18	A	1013	CLA	8	0
22	L	6019	BCR	22	0
26	B	8002	LMU	3	0
18	G	1002	CLA	26	0
18	B	1219	CLA	2	0
21	B	5004	LHG	1	0
18	K	1001	CLA	12	0
18	B	1227	CLA	8	0
20	A	5001	PQN	3	0
22	A	6017	BCR	5	0
18	B	1212	CLA	5	0
18	2	2016	CLA	36	0
18	A	1108	CLA	3	0
22	A	6002	BCR	4	0
22	F	6014	BCR	8	0
18	B	1235	CLA	5	0
18	A	1113	CLA	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
18	3	3007	CLA	8	0
18	B	1218	CLA	11	0
23	B	5005	LMG	3	0
18	A	1135	CLA	4	0
18	4	4008	CLA	15	0
28	4	4013	CHL	19	0
18	2	2007	CLA	26	0
18	B	1202	CLA	7	0
18	A	1110	CLA	10	0
18	2	2008	CLA	16	0
27	1	1501	LUT	31	0
18	F	1301	CLA	6	0
18	F	1302	CLA	14	0
18	A	1129	CLA	1	0
18	A	1132	CLA	7	0
18	B	1216	CLA	7	0
18	B	1226	CLA	7	0
18	A	1106	CLA	9	0
18	1	1013	CLA	16	0
18	A	1124	CLA	4	0
18	2	2009	CLA	15	0
27	4	4503	LUT	32	0
18	1	1011	CLA	18	0
18	B	1210	CLA	9	0
28	2	2011	CHL	6	0
18	A	1123	CLA	4	0
23	F	5002	LMG	6	0
18	4	4003	CLA	13	0
18	A	1109	CLA	8	0
18	B	1221	CLA	14	0
18	4	4004	CLA	19	0
18	A	1127	CLA	6	0
18	B	1214	CLA	3	0
18	3	3002	CLA	10	0
20	B	5002	PQN	5	0
18	B	1224	CLA	7	0
18	4	4005	CLA	16	0
18	A	1125	CLA	3	0
18	3	3004	CLA	20	0
18	B	1231	CLA	3	0
18	A	1139	CLA	5	0
18	B	1023	CLA	5	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
18	B	1211	CLA	7	0
27	2	2502	LUT	32	0
18	B	1222	CLA	8	0
18	4	4016	CLA	24	0
17	A	1011	CL0	6	0
18	3	3018	CLA	19	0
22	A	6008	BCR	2	0
28	2	2013	CHL	18	0
18	A	1022	CLA	7	0
18	2	2004	CLA	23	0
18	A	1122	CLA	6	0
18	1	1001	CLA	48	0
18	1	1006	CLA	11	0
27	2	2501	LUT	23	0
22	B	6010	BCR	1	0
18	A	1111	CLA	8	0
18	4	4001	CLA	25	0
18	G	1003	CLA	30	0
18	B	1021	CLA	9	0
18	L	1502	CLA	13	0
18	A	1121	CLA	4	0
22	J	6012	BCR	7	0
18	A	1136	CLA	7	0
18	A	1116	CLA	7	0
18	B	1238	CLA	9	0
18	A	1105	CLA	3	0
22	L	6020	BCR	6	0
18	B	1205	CLA	8	0
18	J	1302	CLA	7	0
18	B	1201	CLA	2	0
27	4	4502	LUT	31	0
18	B	1220	CLA	11	0
18	3	3010	CLA	34	0
18	A	1103	CLA	6	0
18	B	1230	CLA	8	0
21	A	7001	LHG	7	0
18	A	1118	CLA	3	0
22	I	6020	BCR	3	0
21	A	5003	LHG	5	0
18	4	4006	CLA	21	0
18	A	1134	CLA	2	0
18	3	3003	CLA	51	0

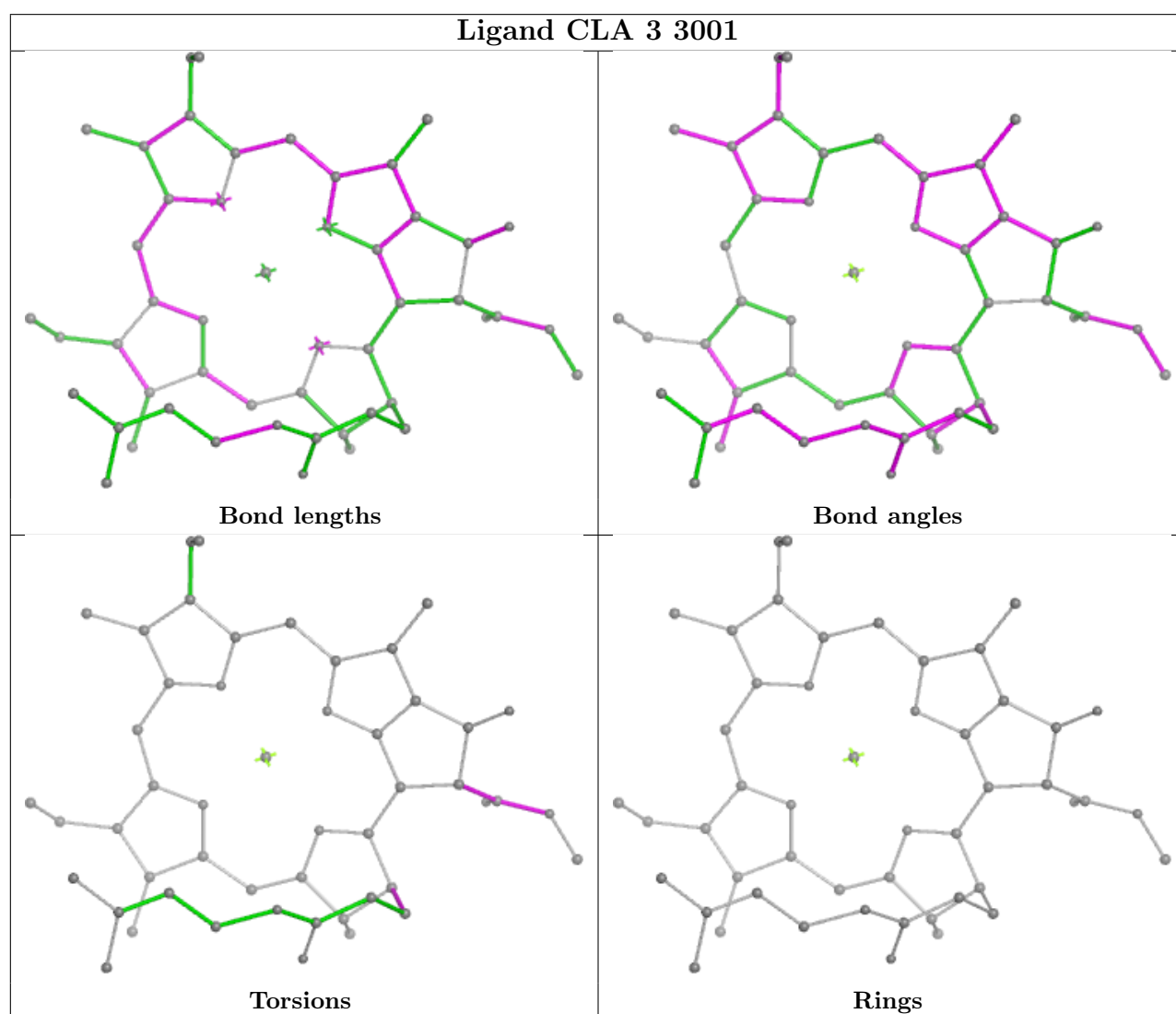
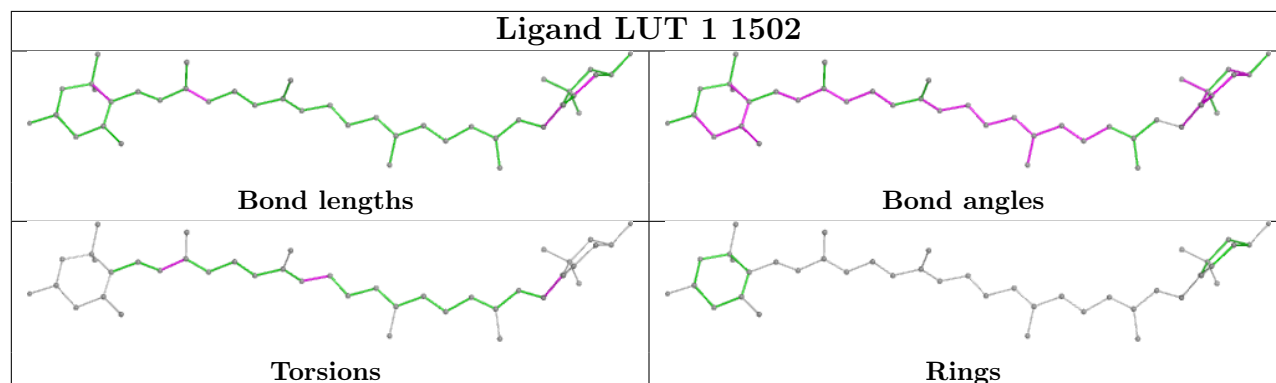
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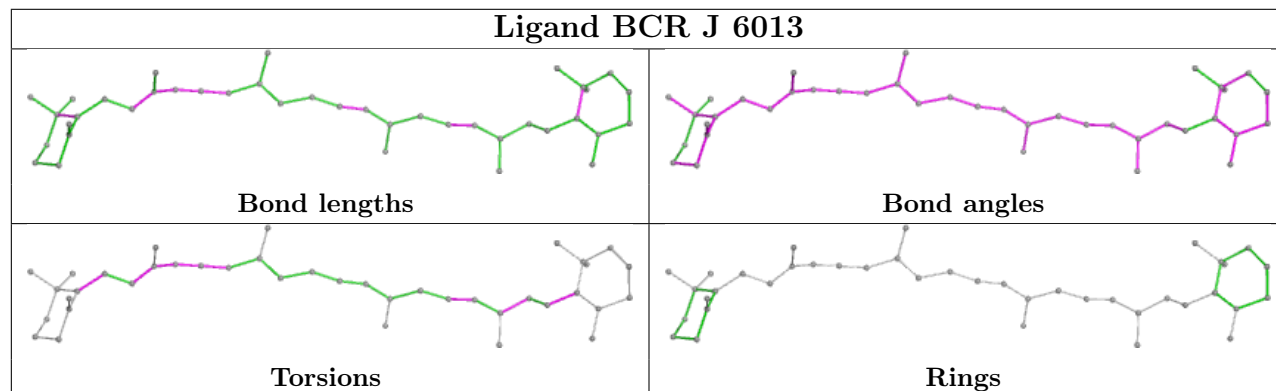
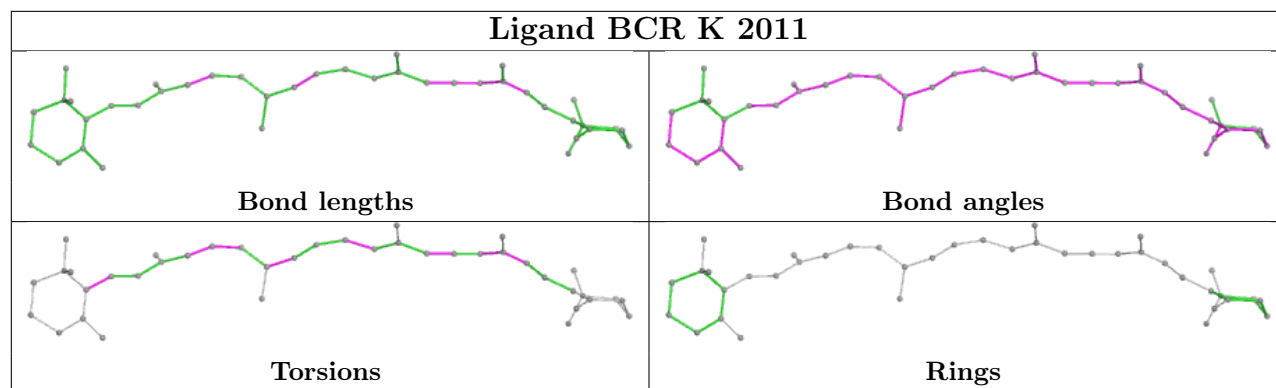
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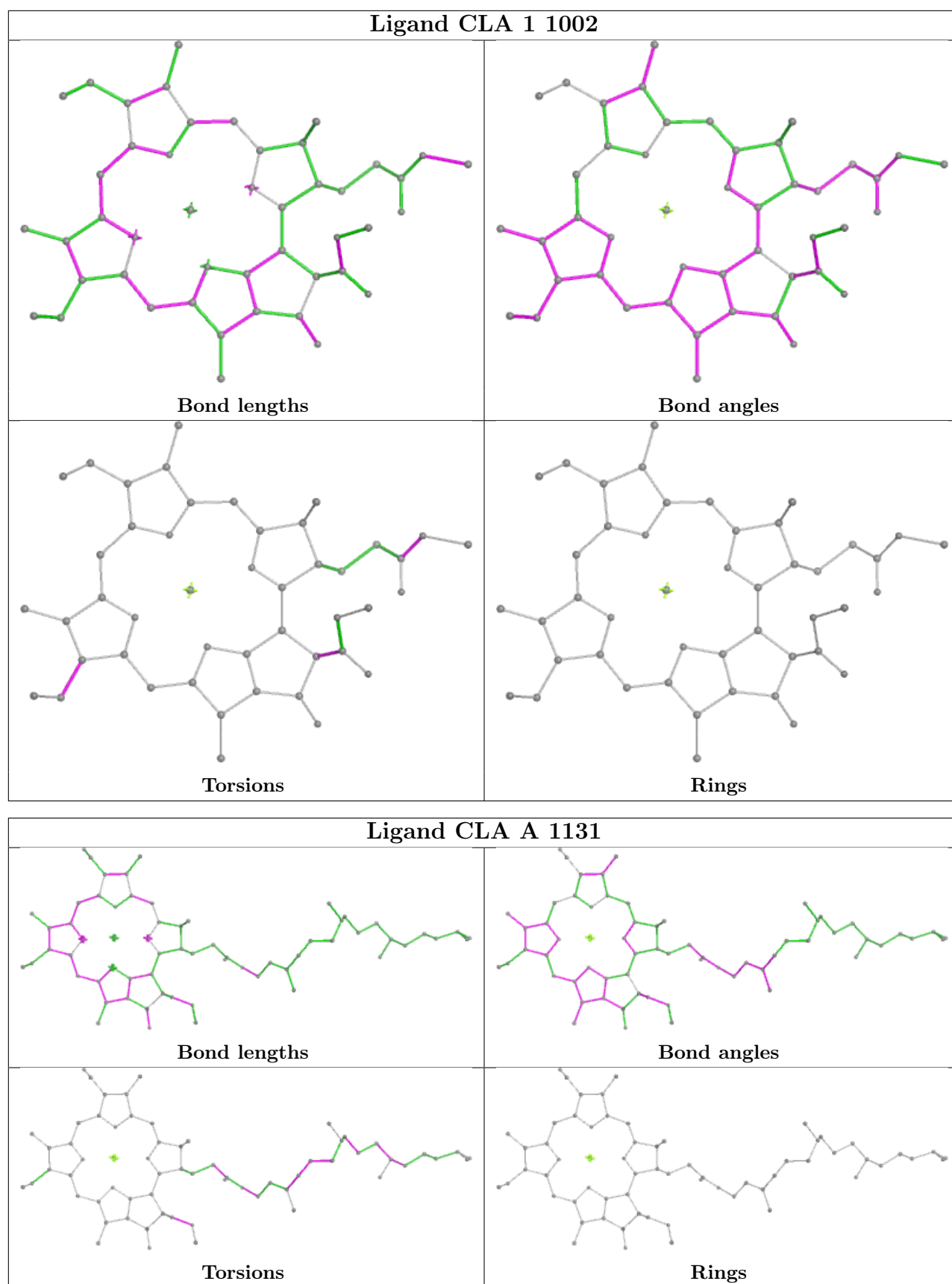
Mol	Chain	Res	Type	Clashes	Symm-Clashes
18	B	1223	CLA	4	0
18	B	1208	CLA	7	0
18	2	2005	CLA	24	0
28	2	2010	CHL	18	0
18	B	1229	CLA	6	0
18	4	4012	CLA	28	0
18	B	1236	CLA	5	0
18	A	1107	CLA	3	0
18	A	1112	CLA	13	0
18	A	1119	CLA	7	0
18	3	3006	CLA	36	0
18	1	1005	CLA	15	0
22	B	6009	BCR	6	0
28	1	1010	CHL	8	0
22	F	6016	BCR	11	0
18	B	1215	CLA	4	0
18	3	3005	CLA	18	0
18	A	1126	CLA	10	0
23	4	4801	LMG	6	0
21	2	2801	LHG	6	0
18	B	1217	CLA	1	0
28	4	4011	CHL	20	0
22	A	6011	BCR	5	0
18	1	1012	CLA	16	0
21	1	1801	LHG	15	0
27	3	3501	LUT	38	0
18	B	1225	CLA	4	0
18	1	1004	CLA	26	0
18	H	1000	CLA	4	0
22	B	6006	BCR	5	0
28	4	4010	CHL	8	0
18	3	3019	CLA	1	0
18	A	1137	CLA	3	0

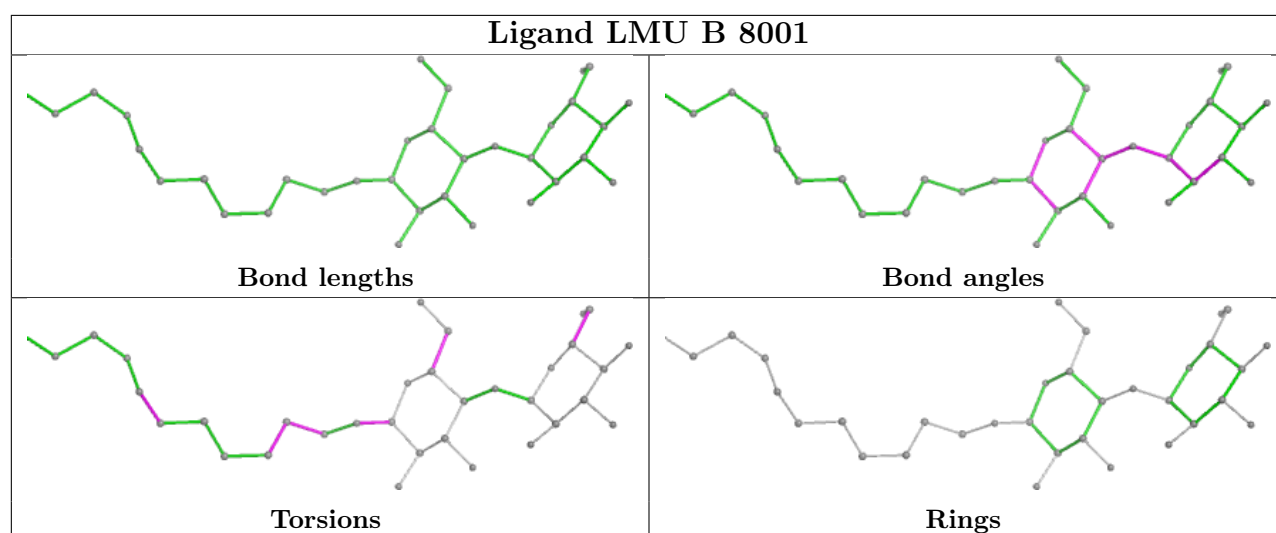
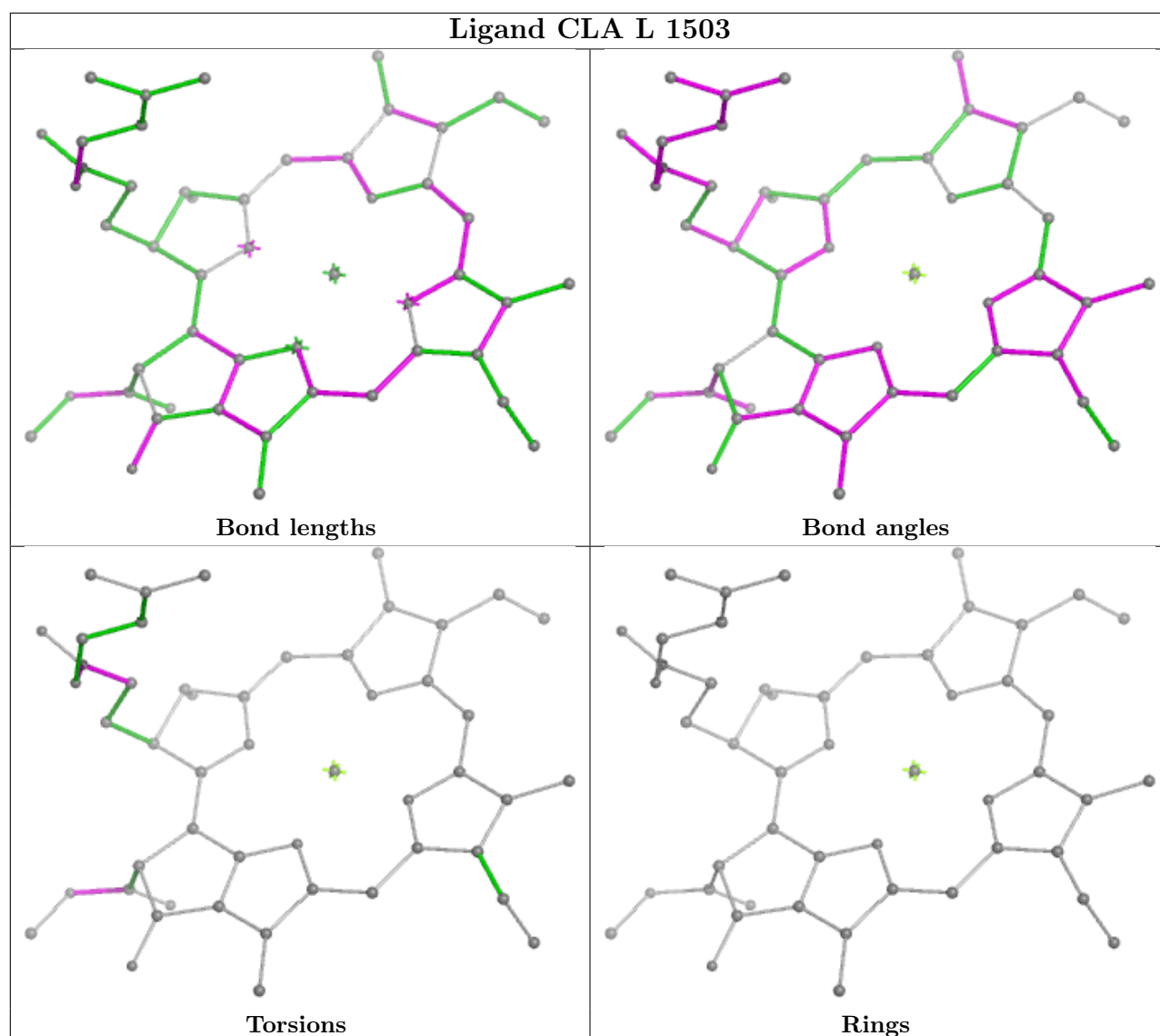
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

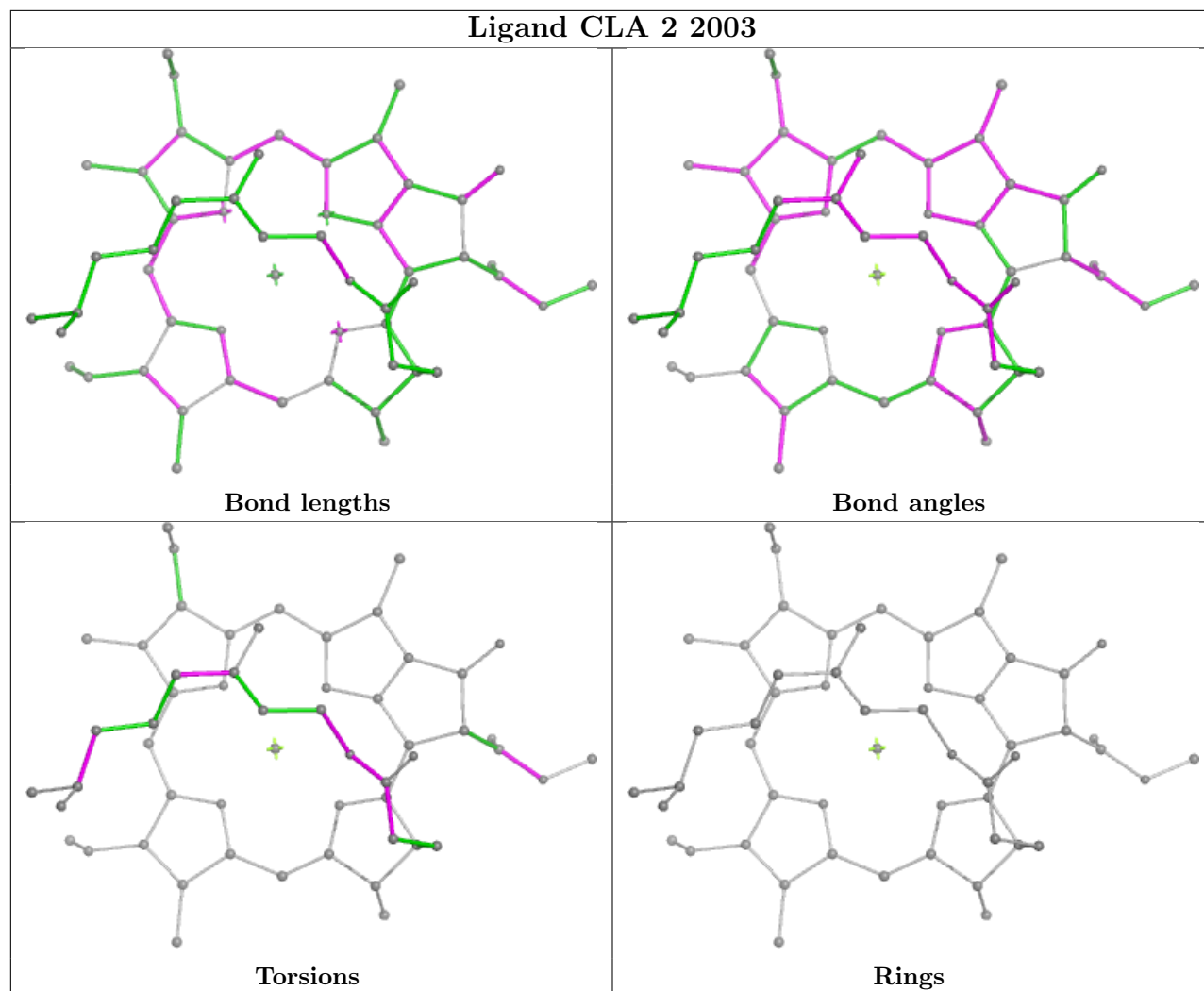
any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

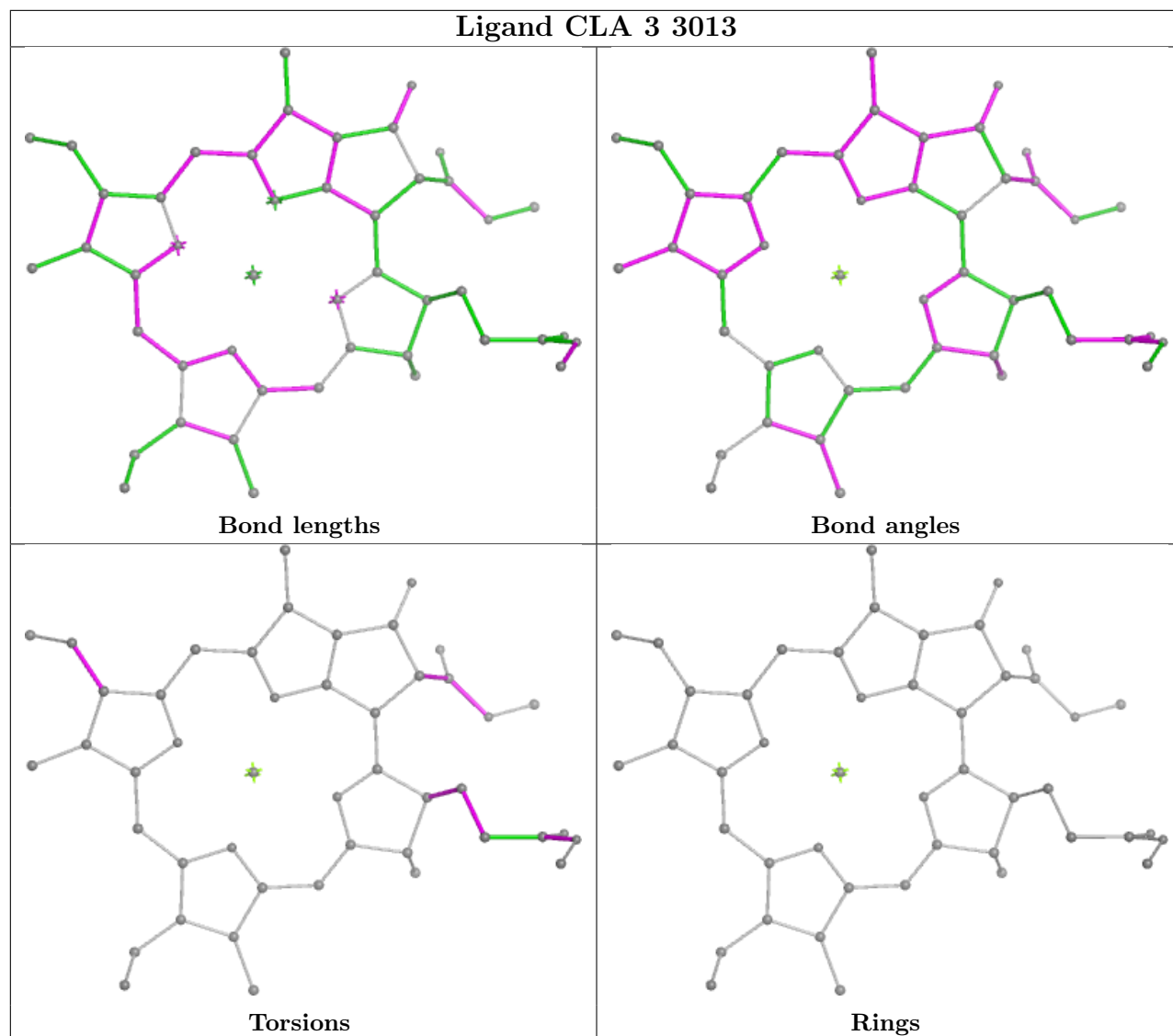


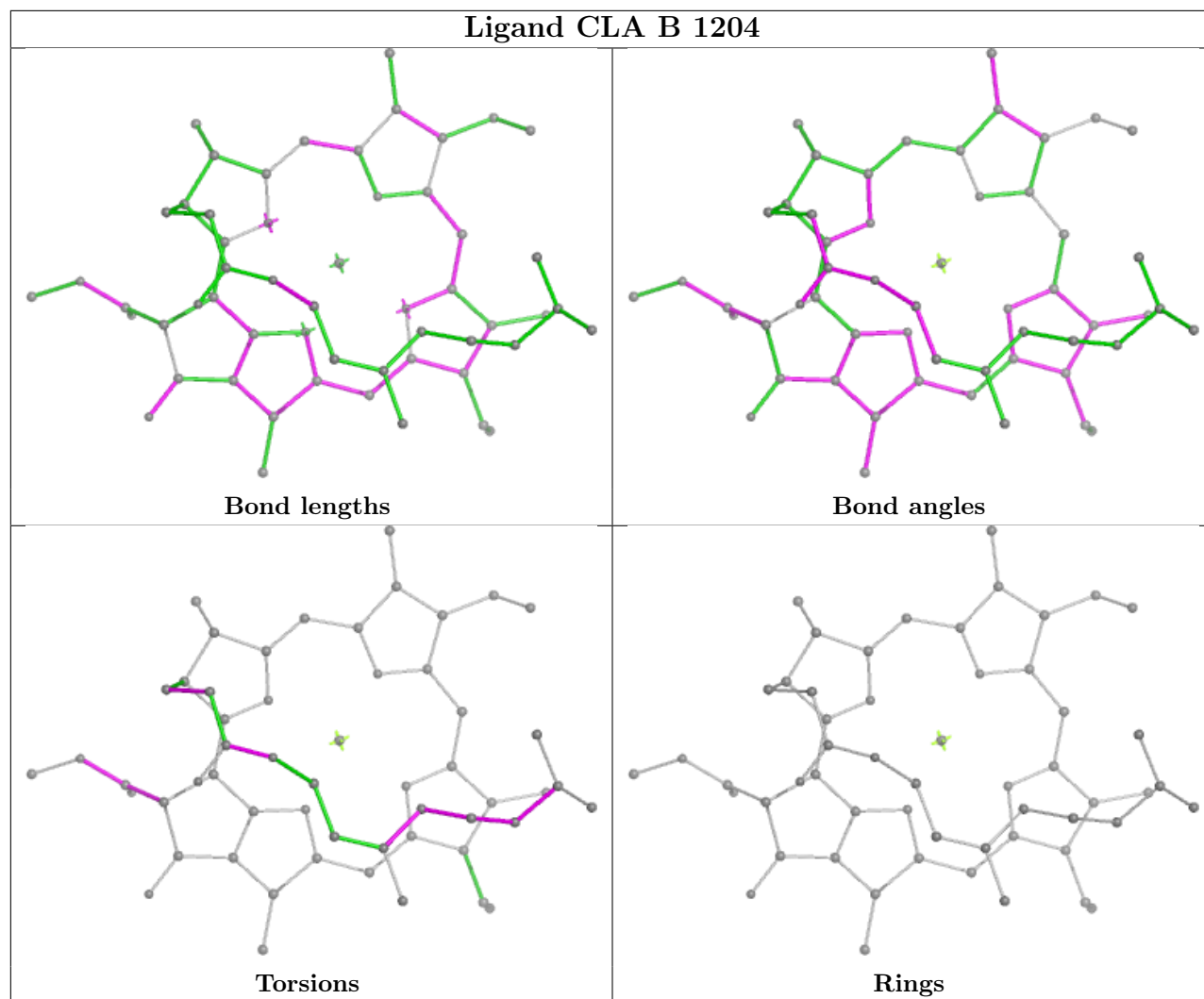


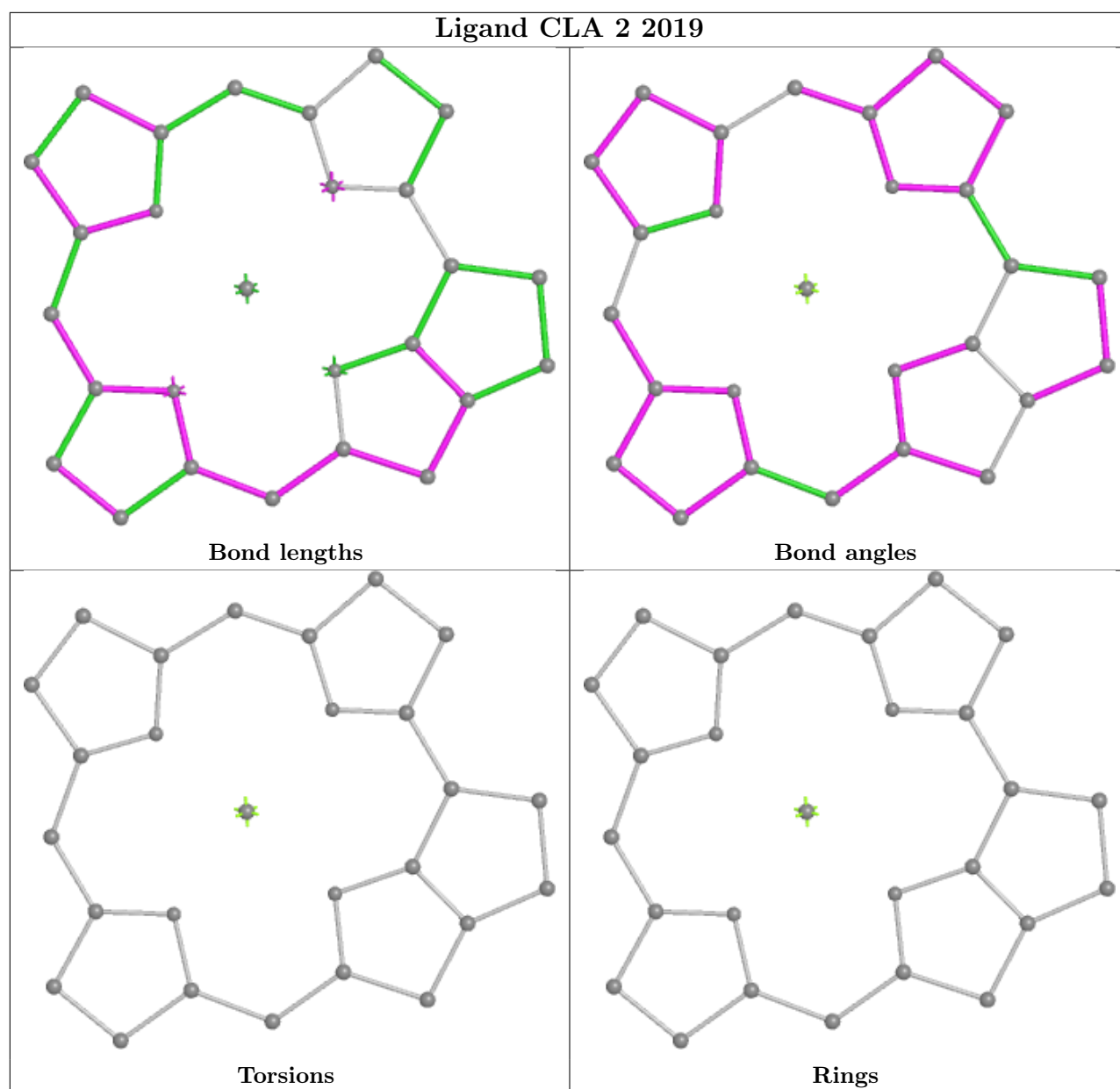


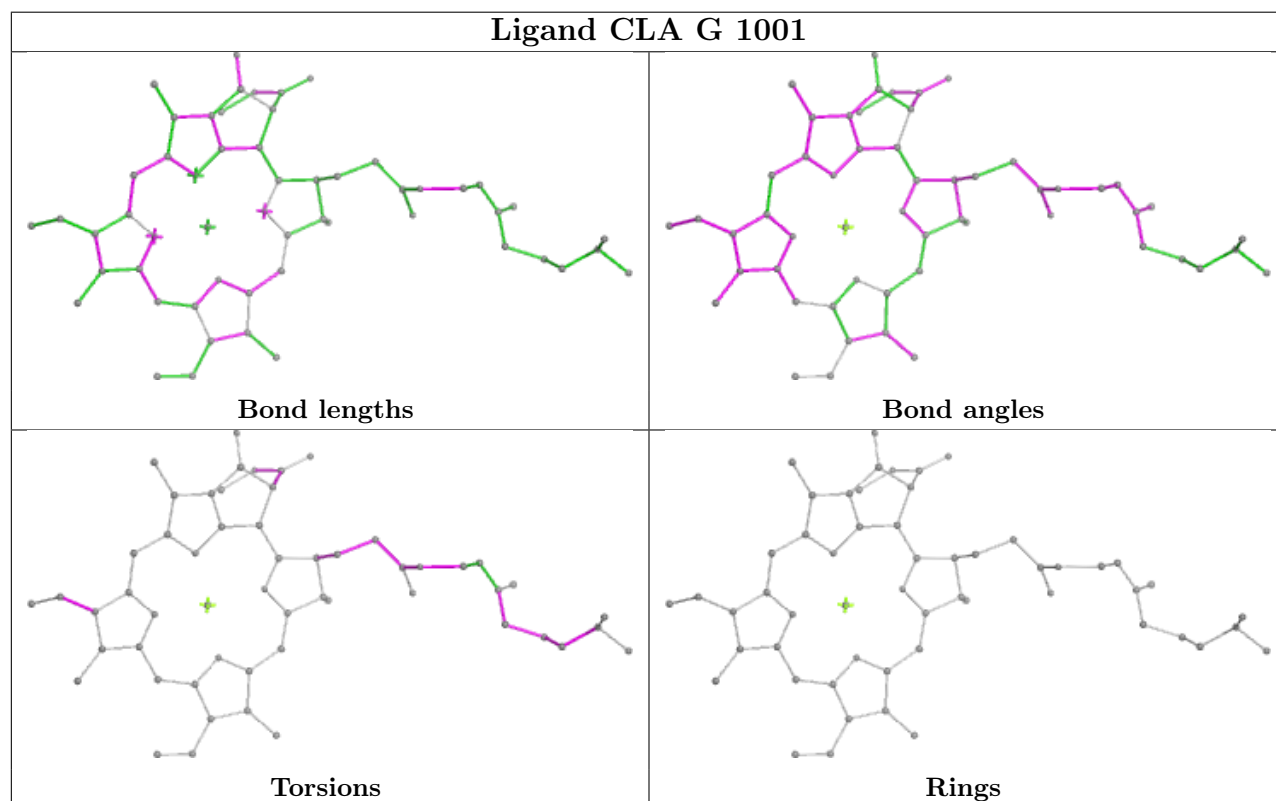
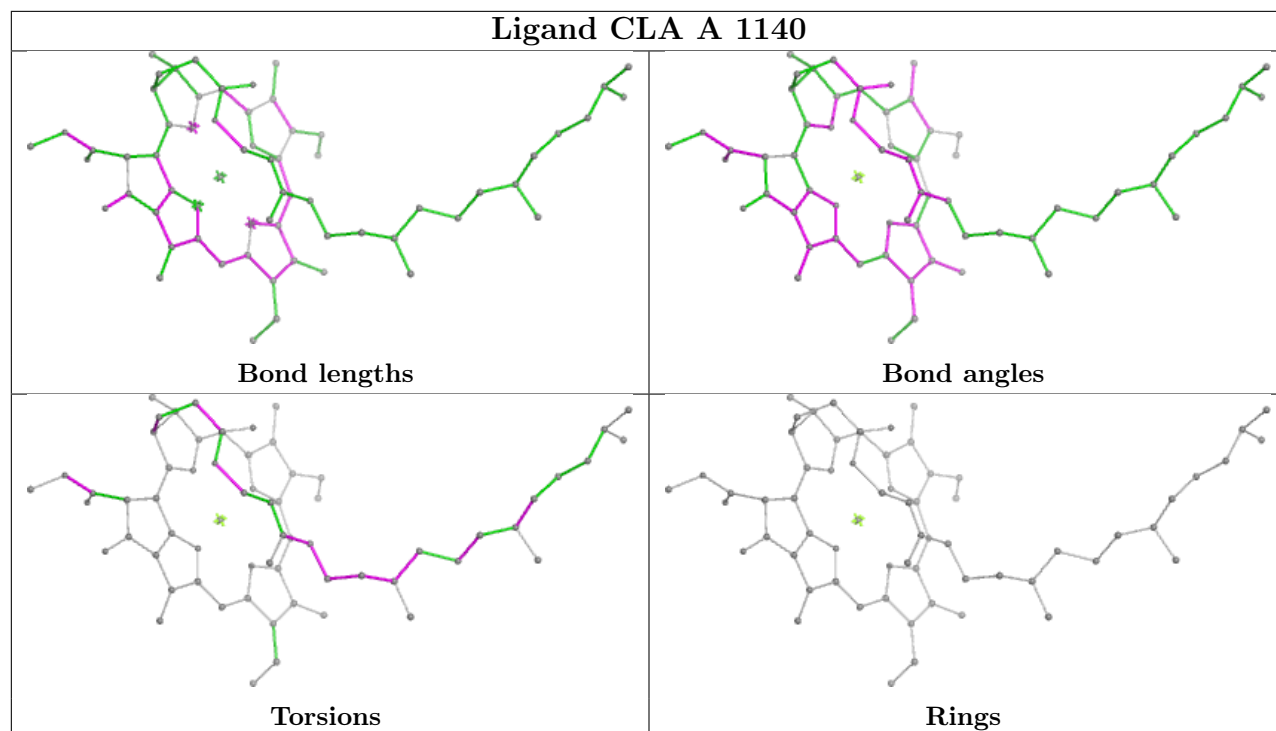


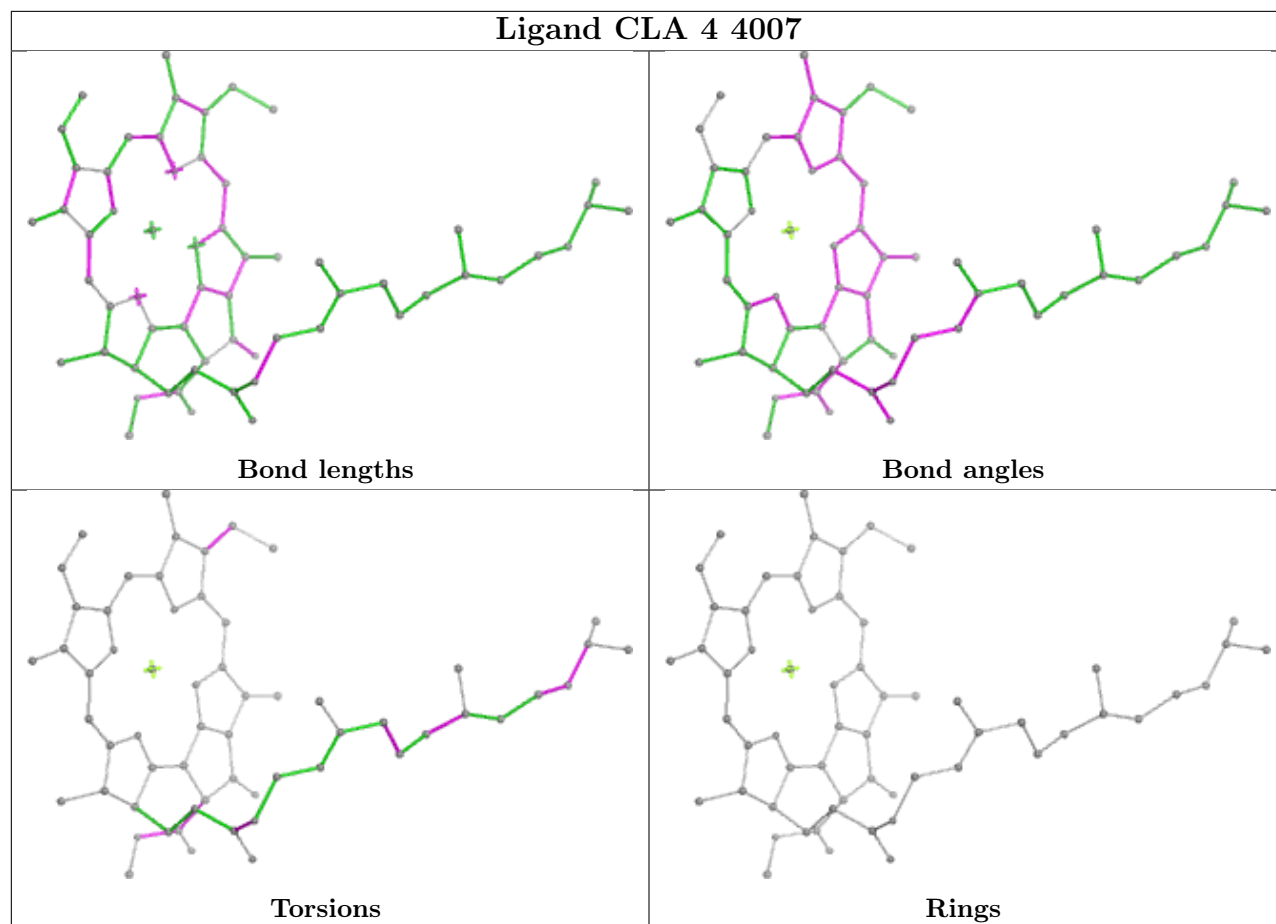


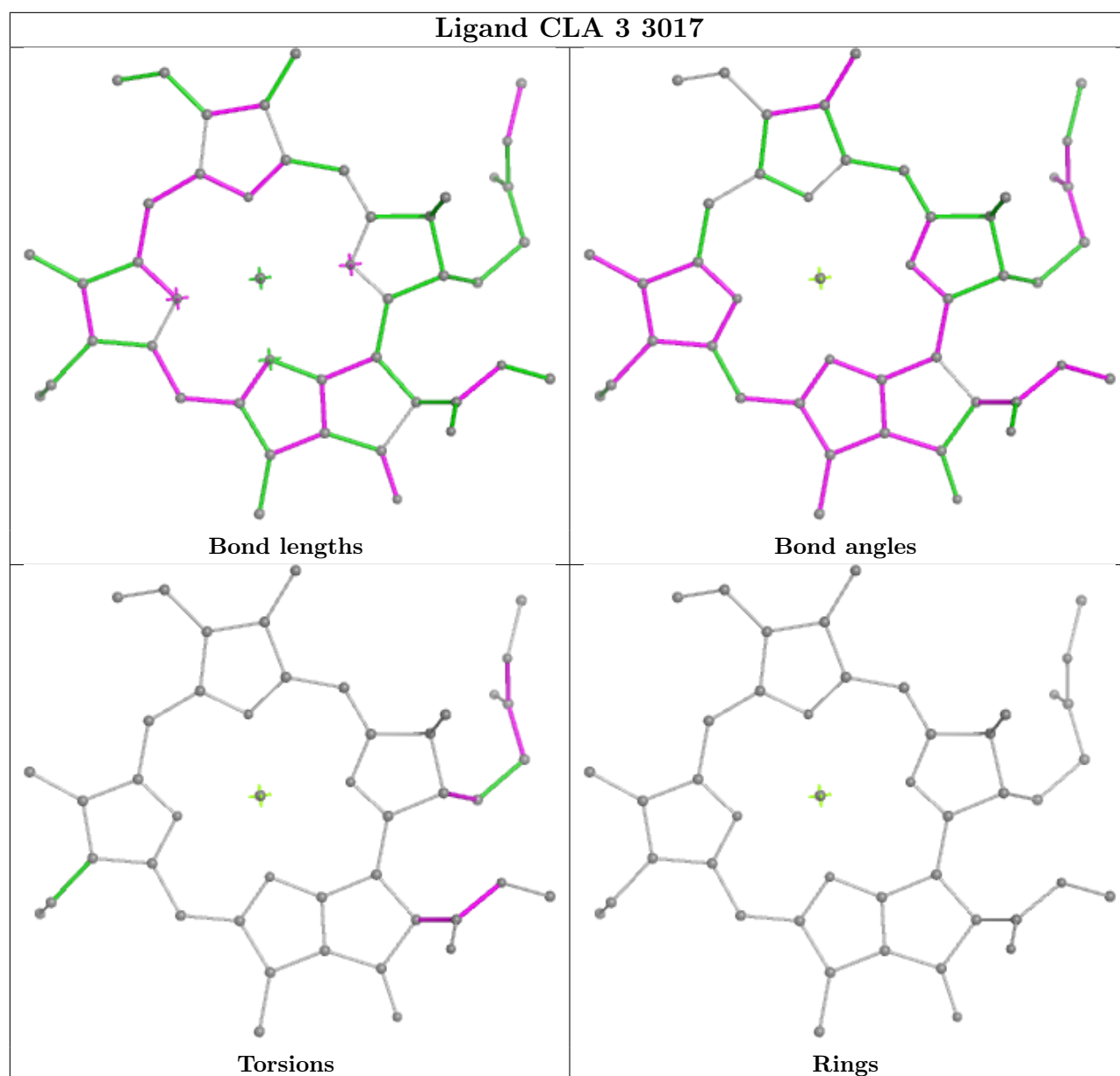


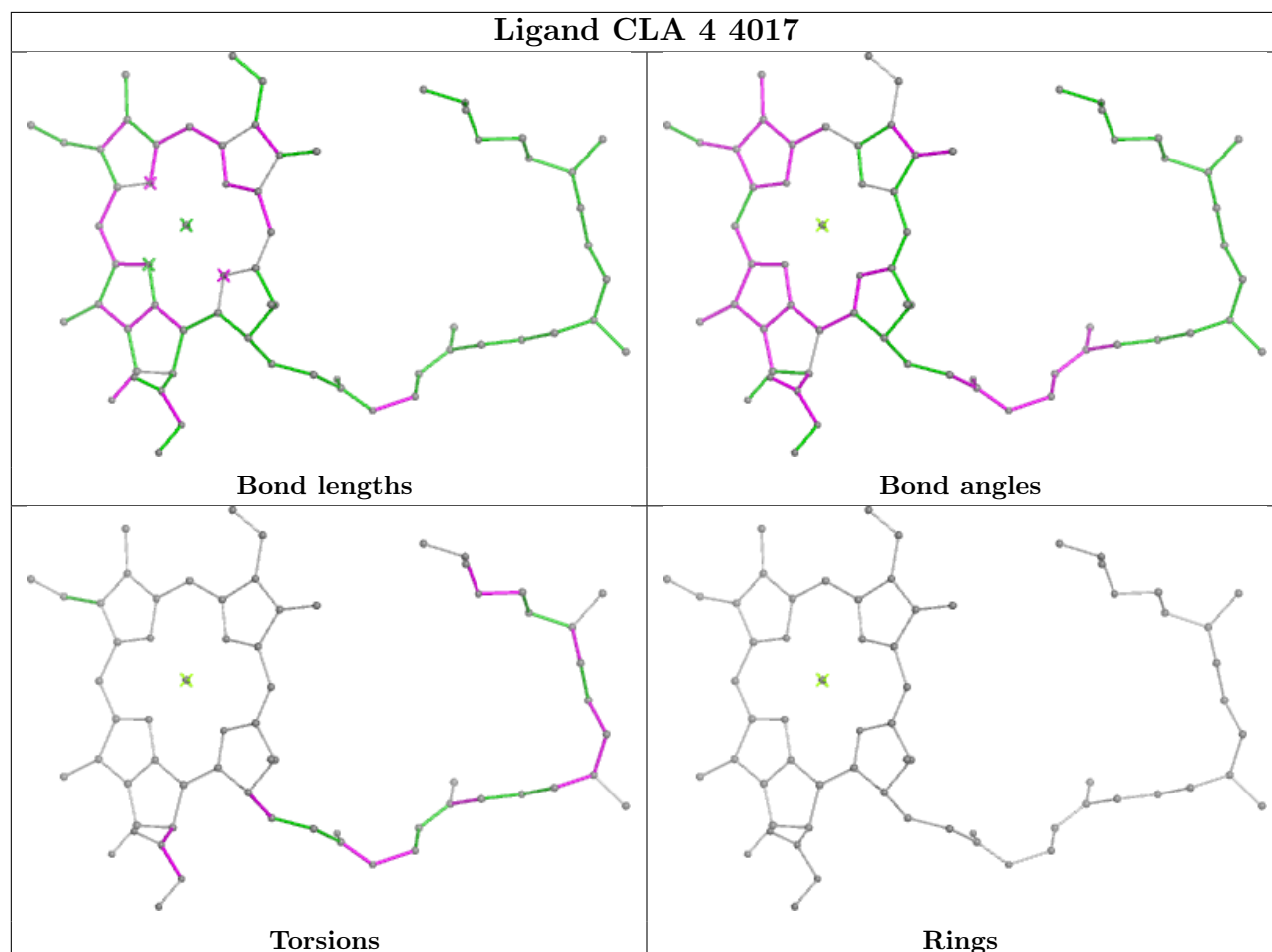
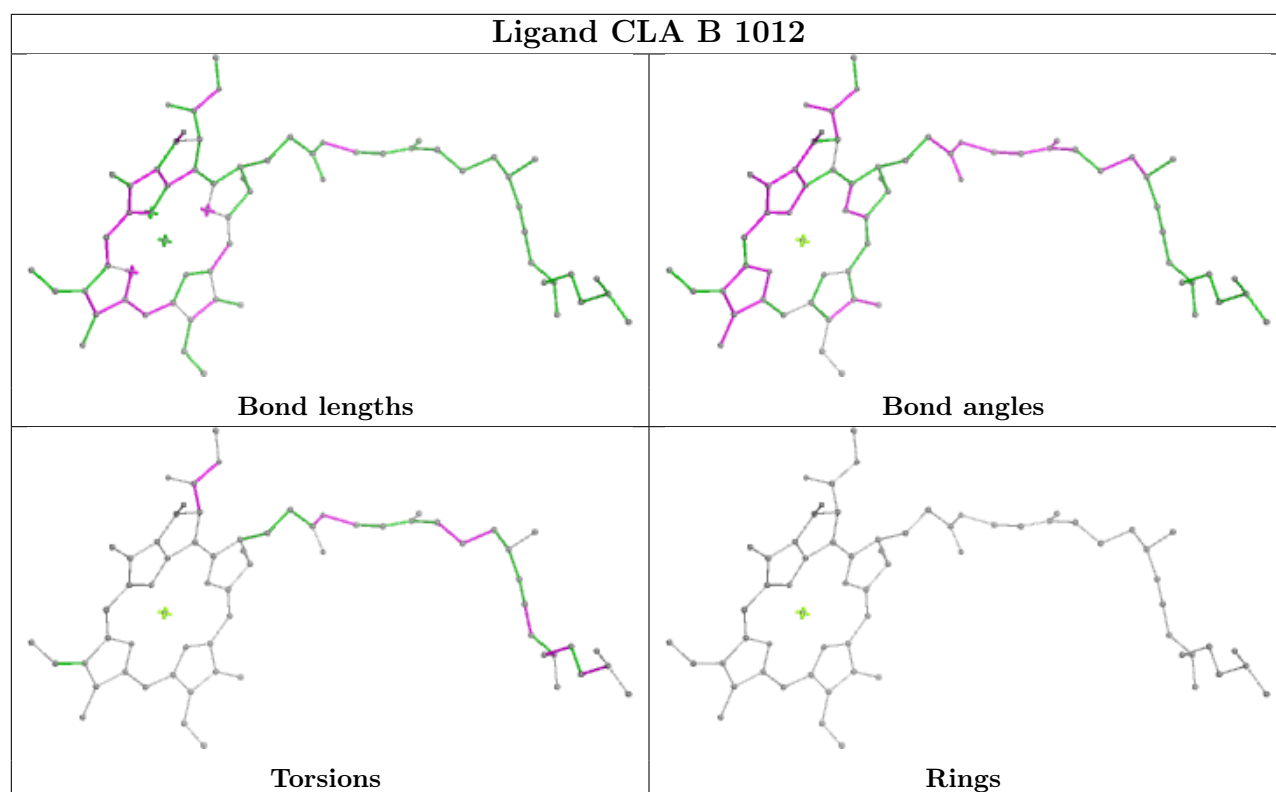




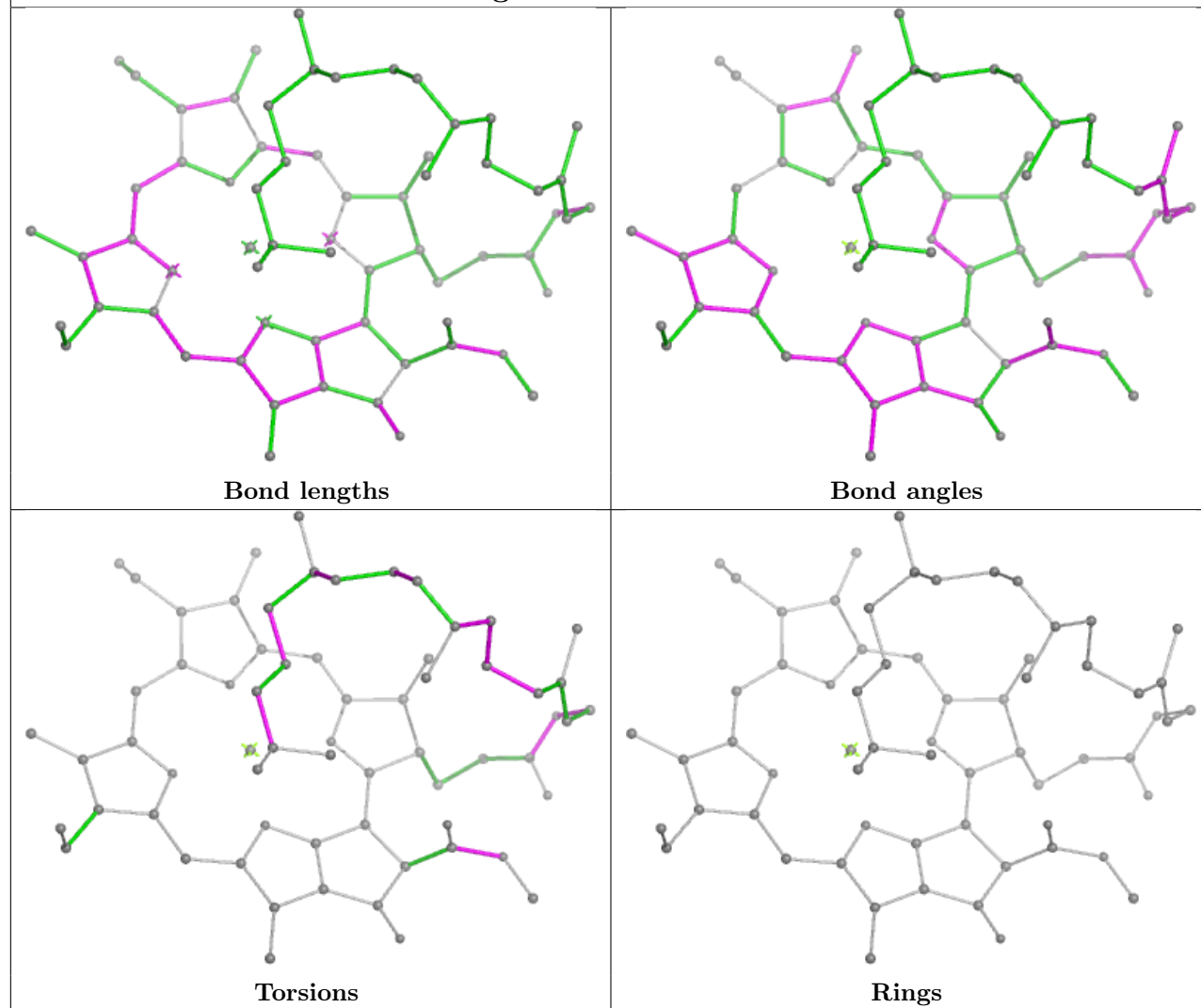


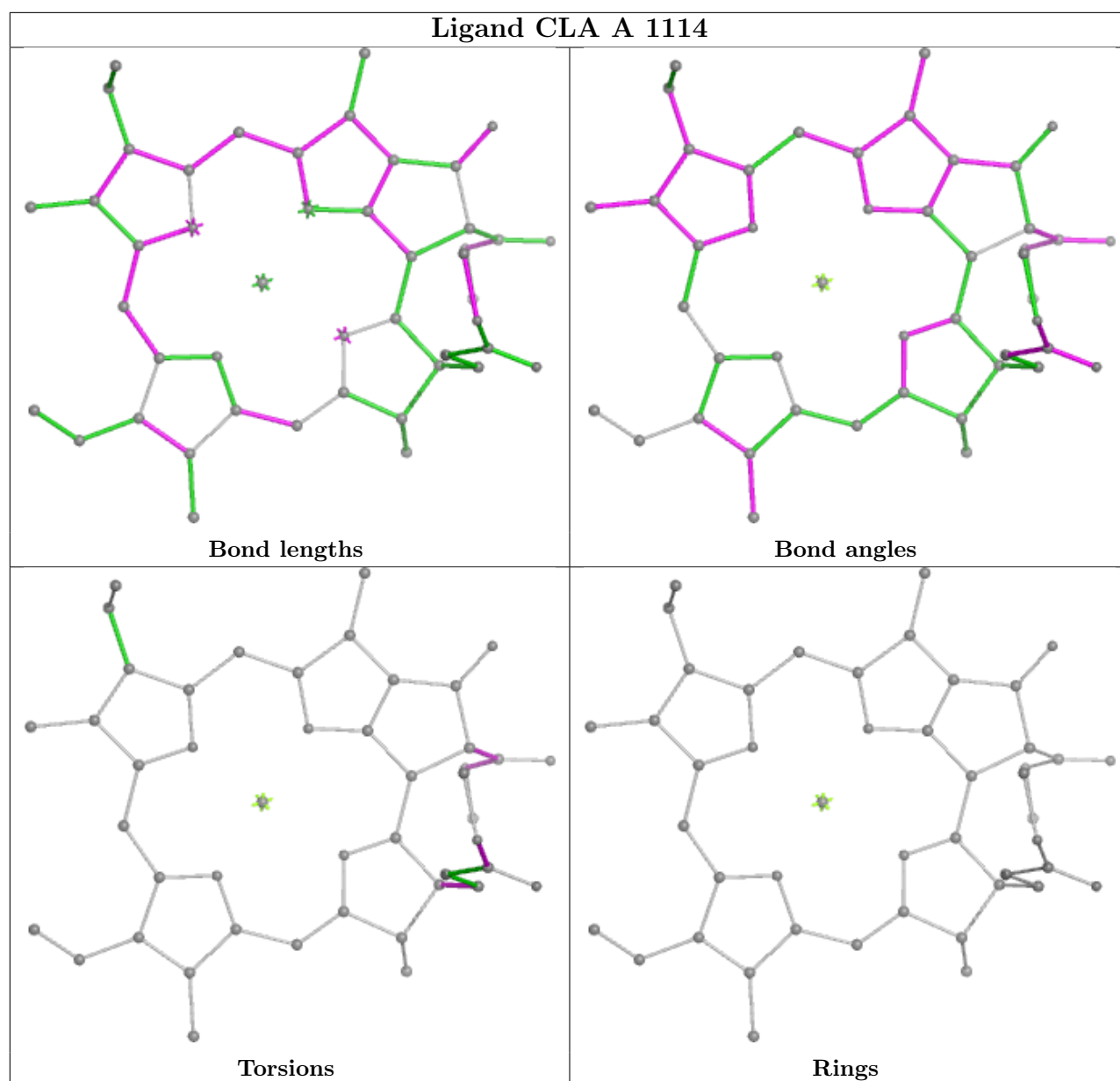


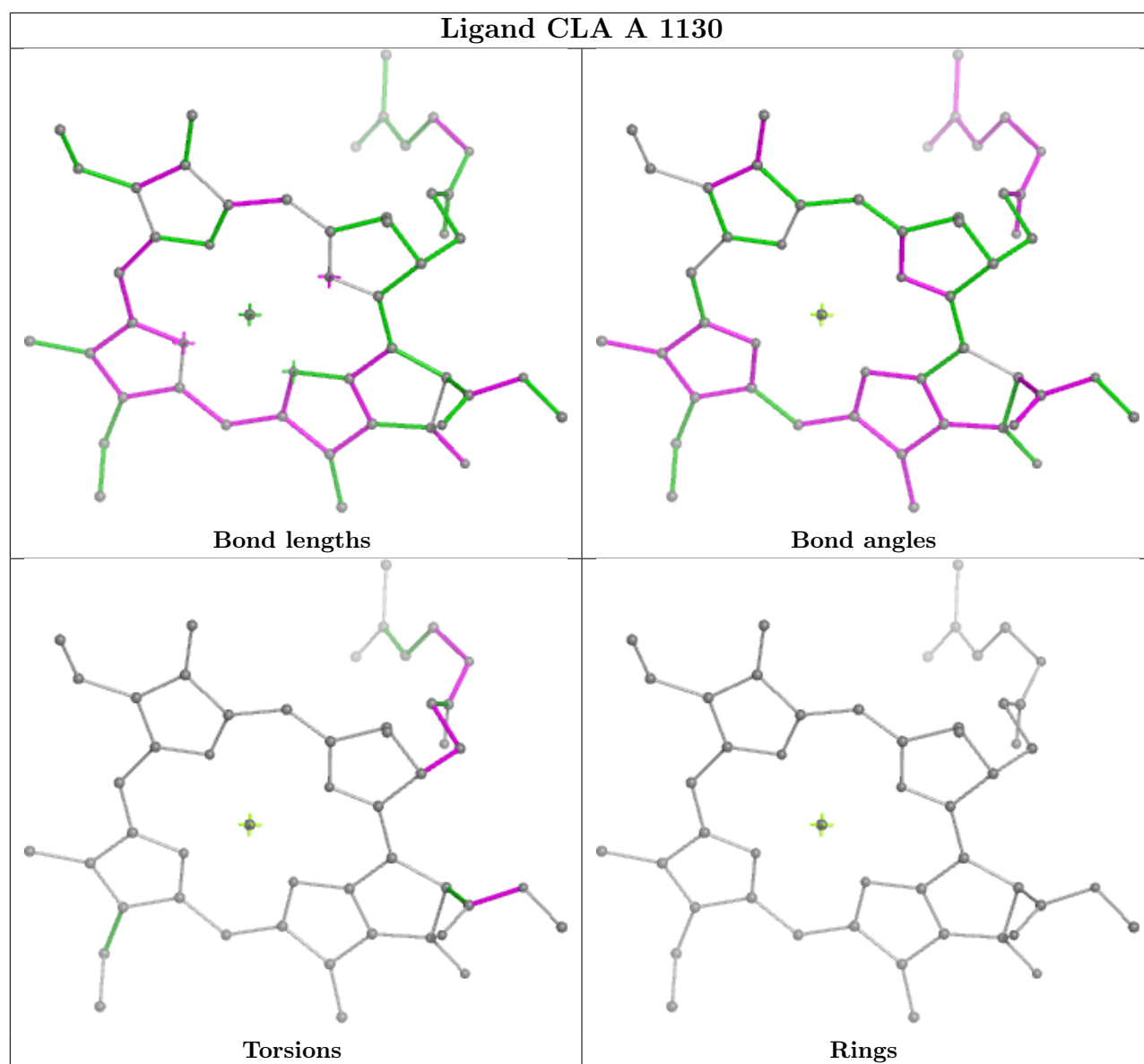


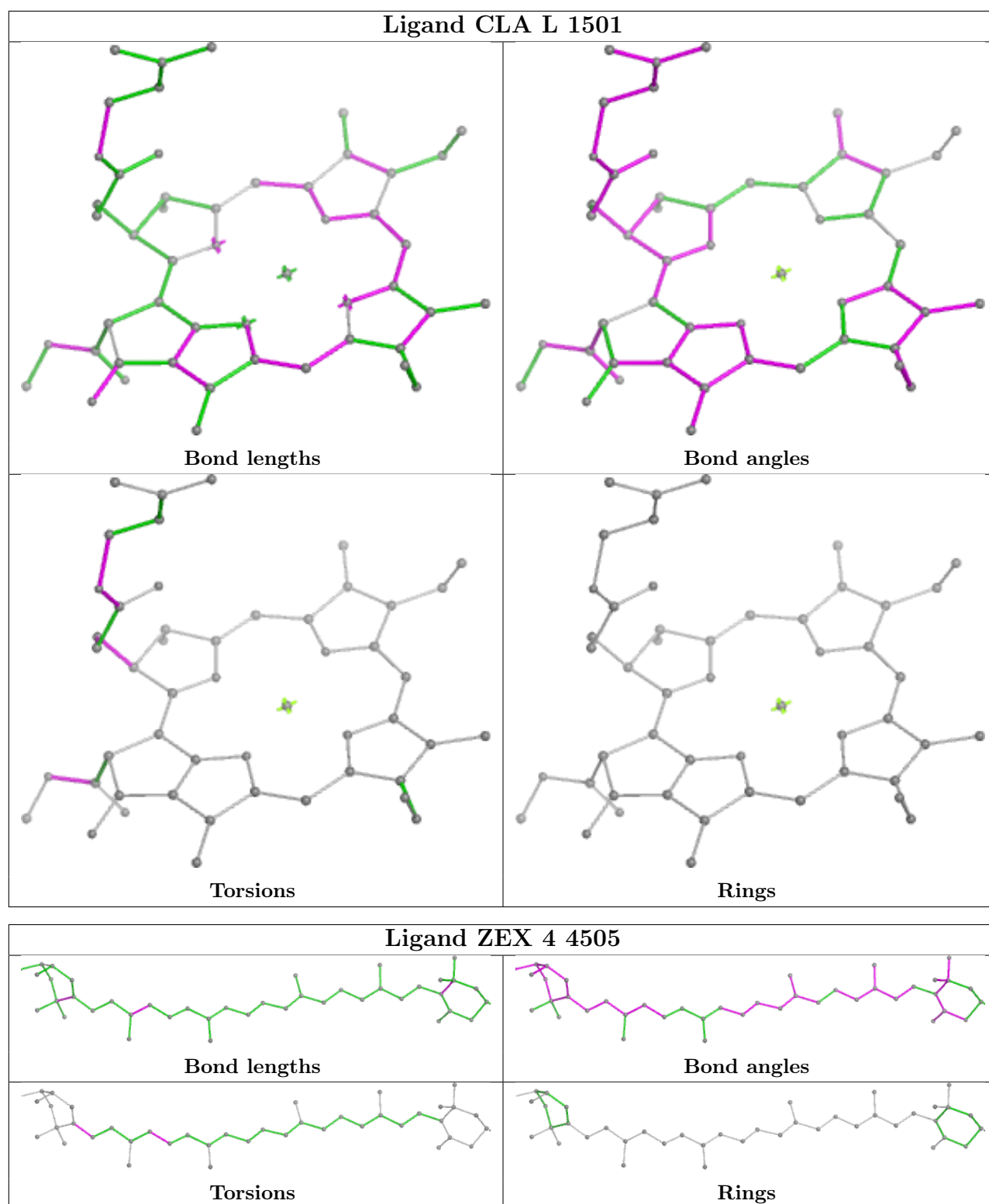


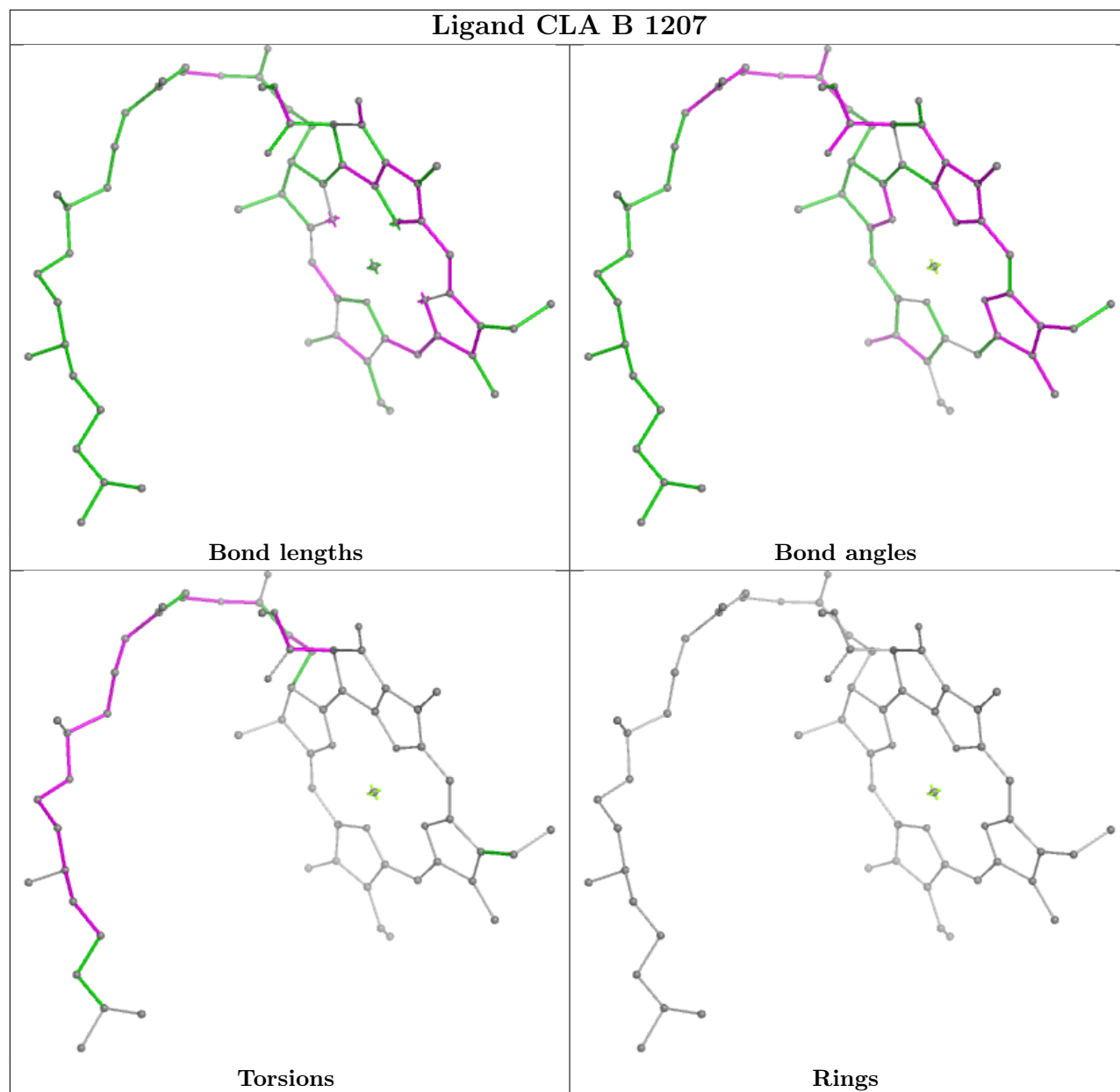
Ligand CLA B 1203

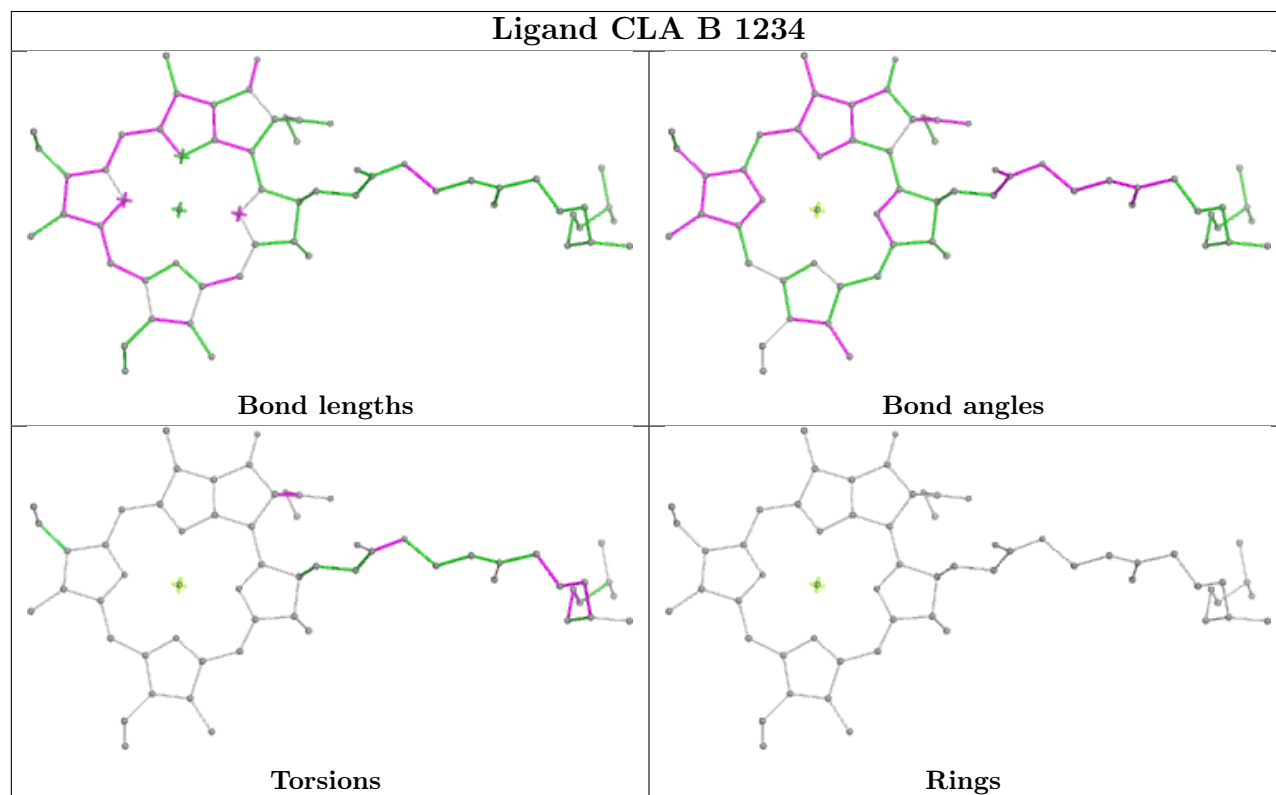
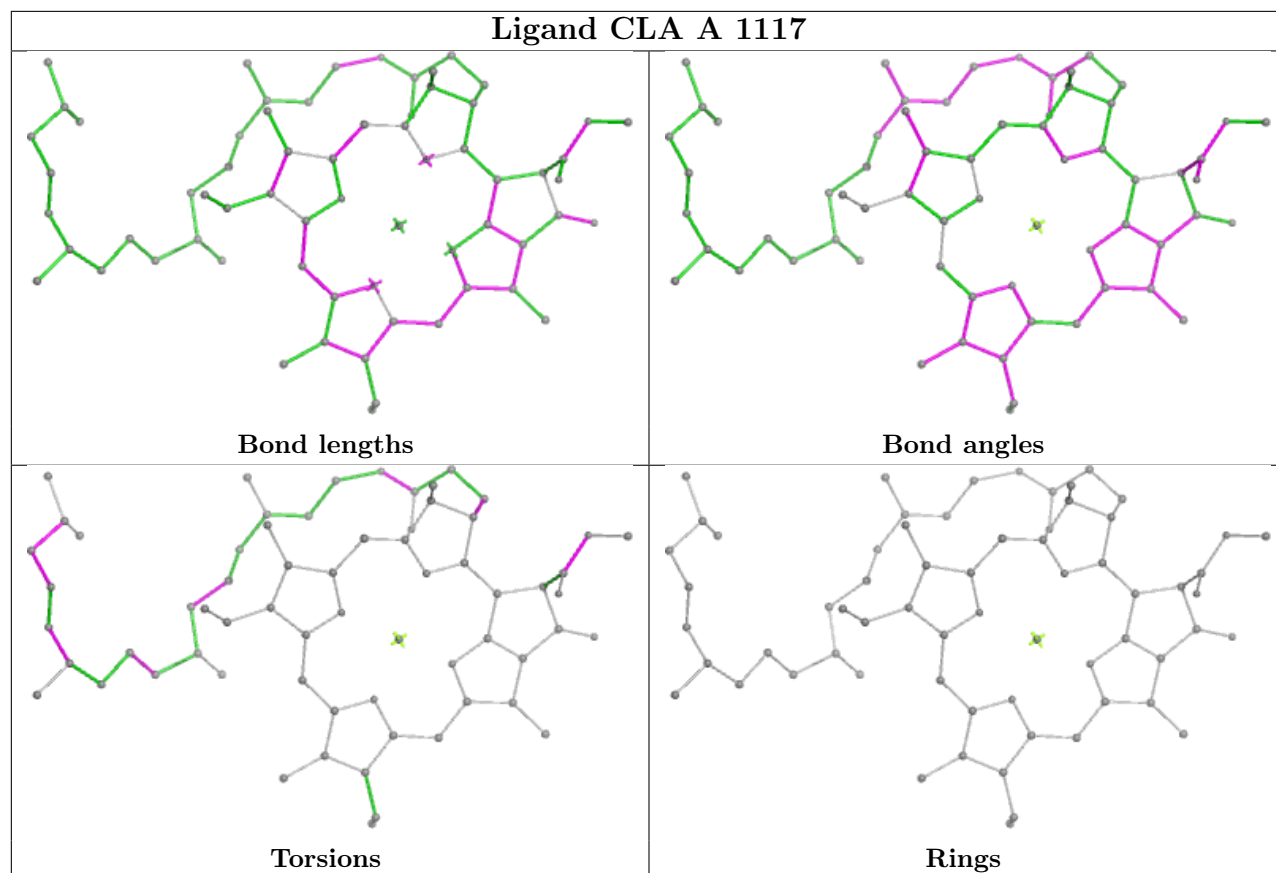


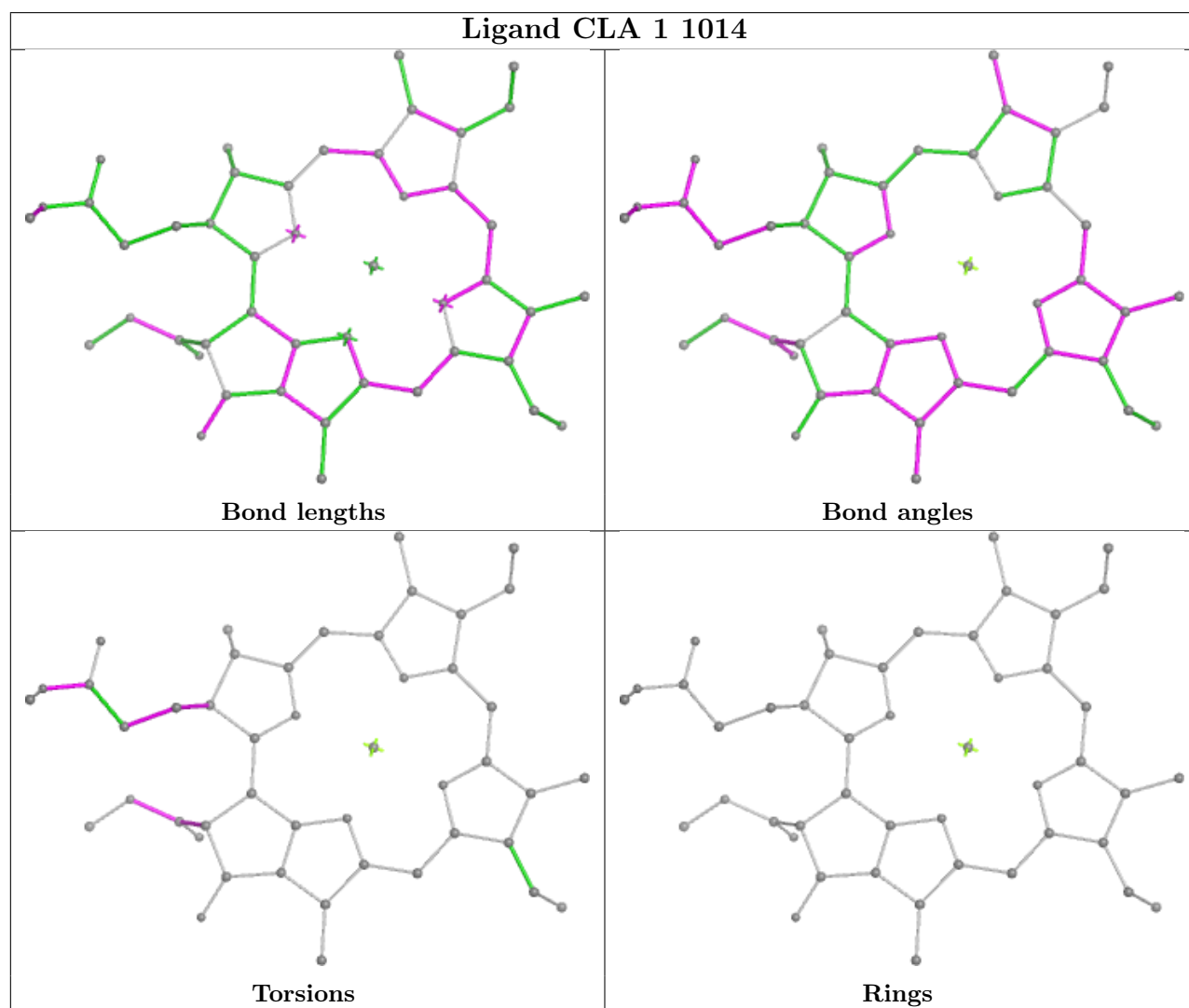
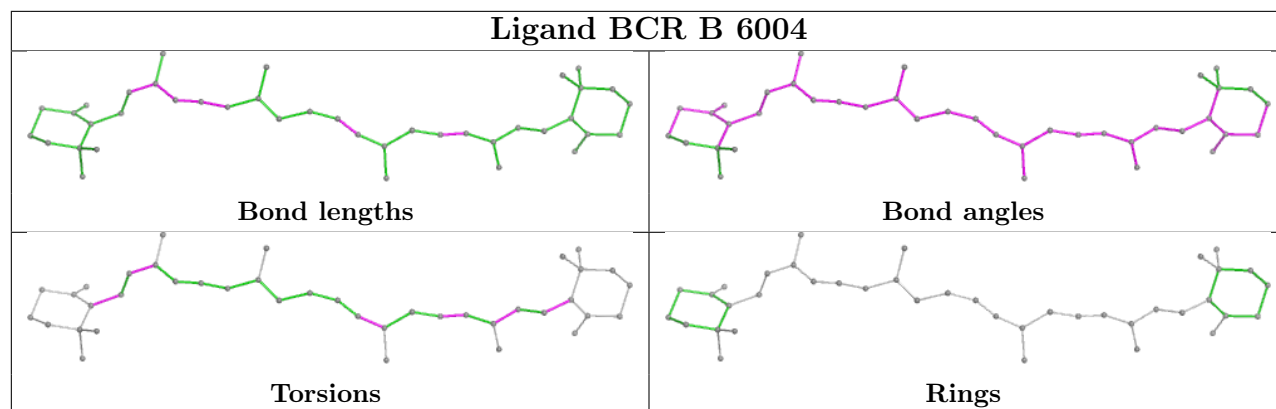


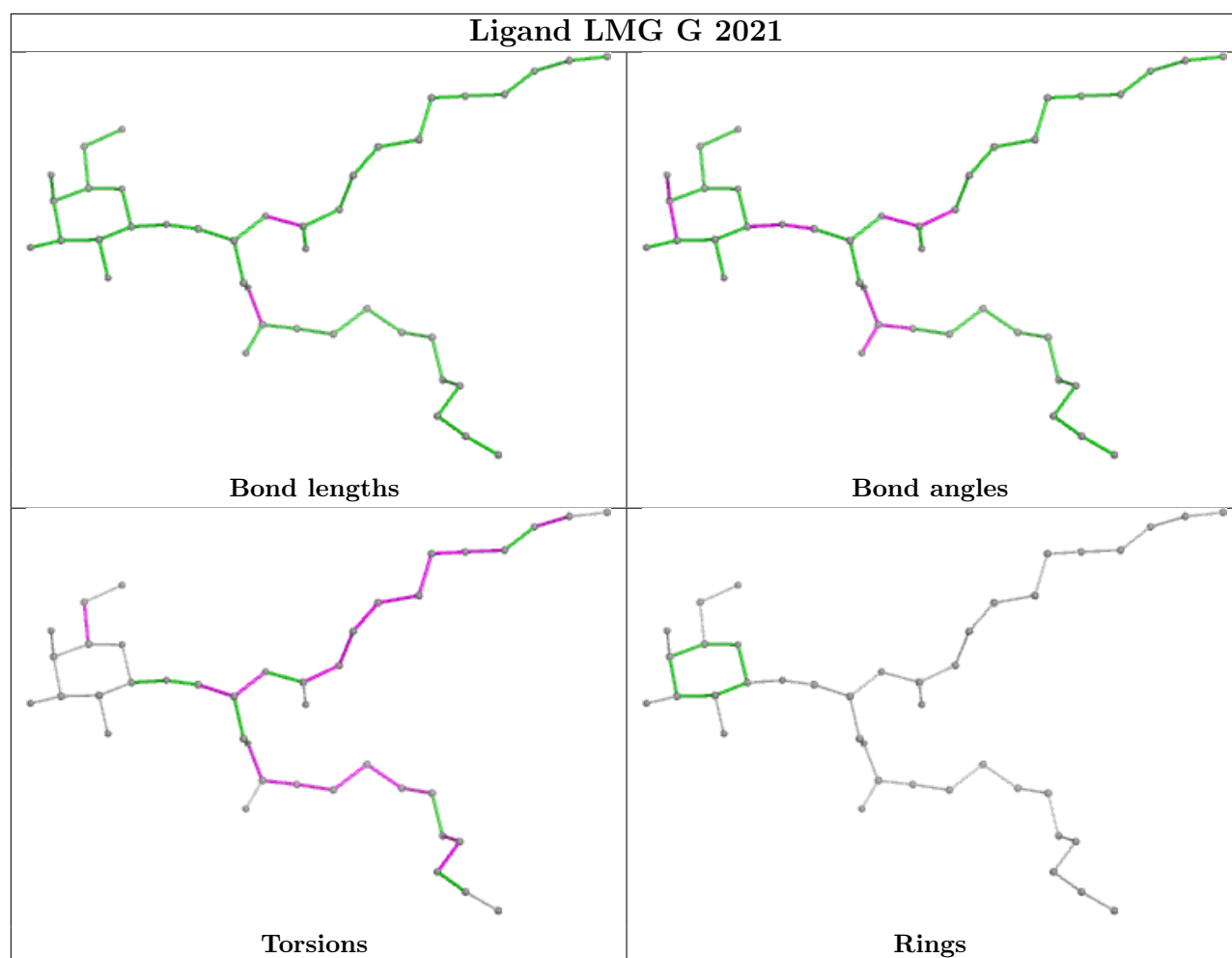


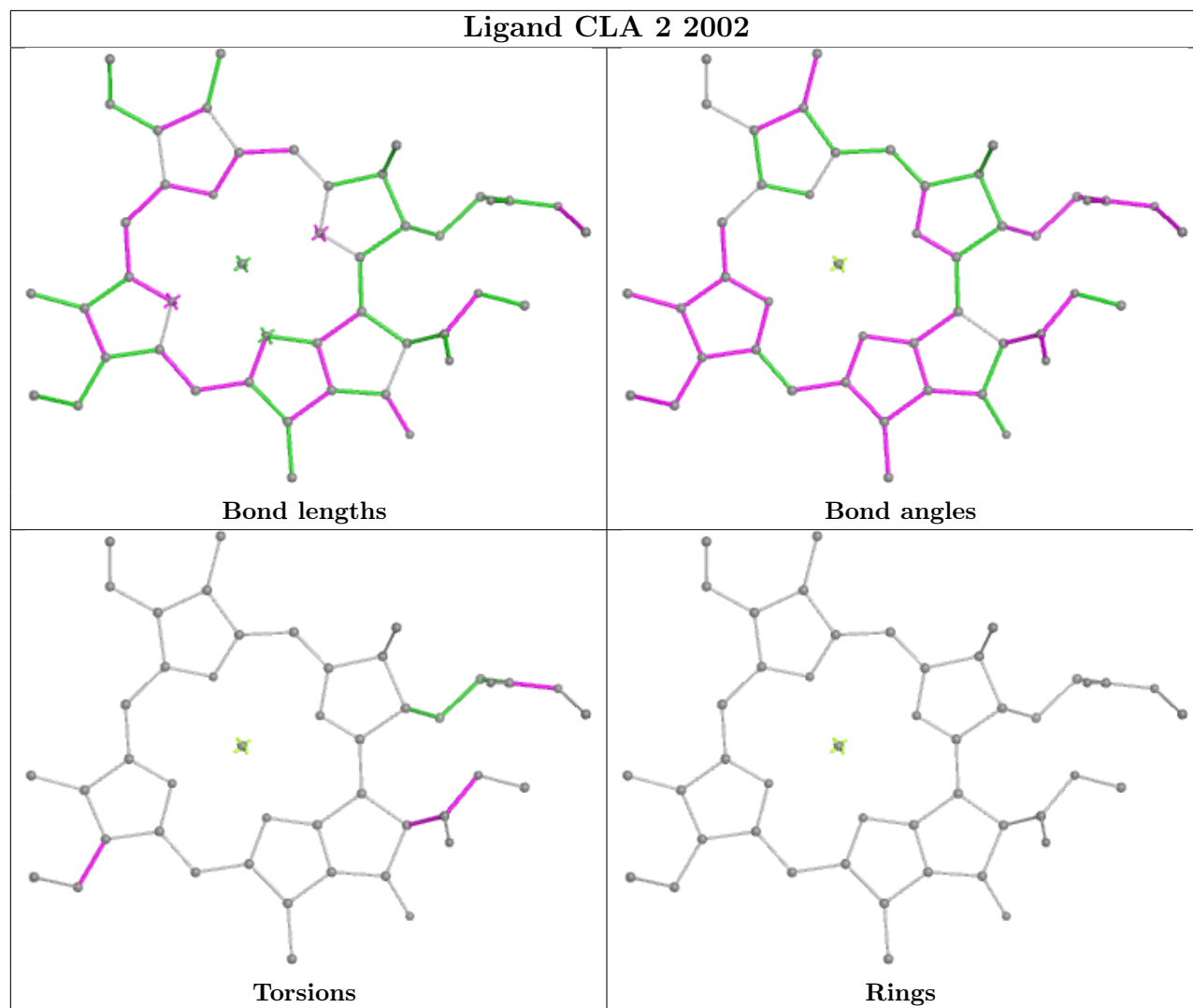


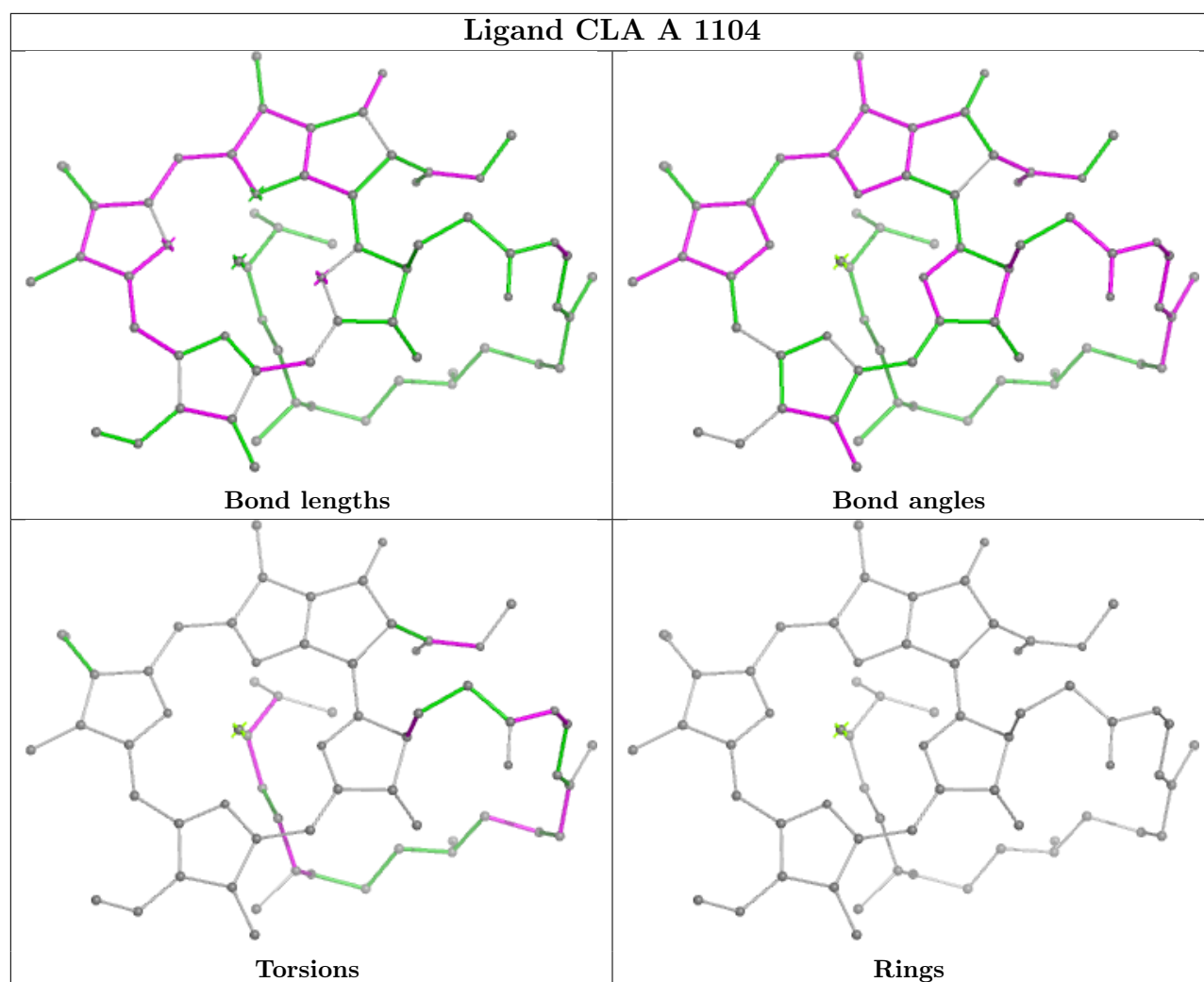


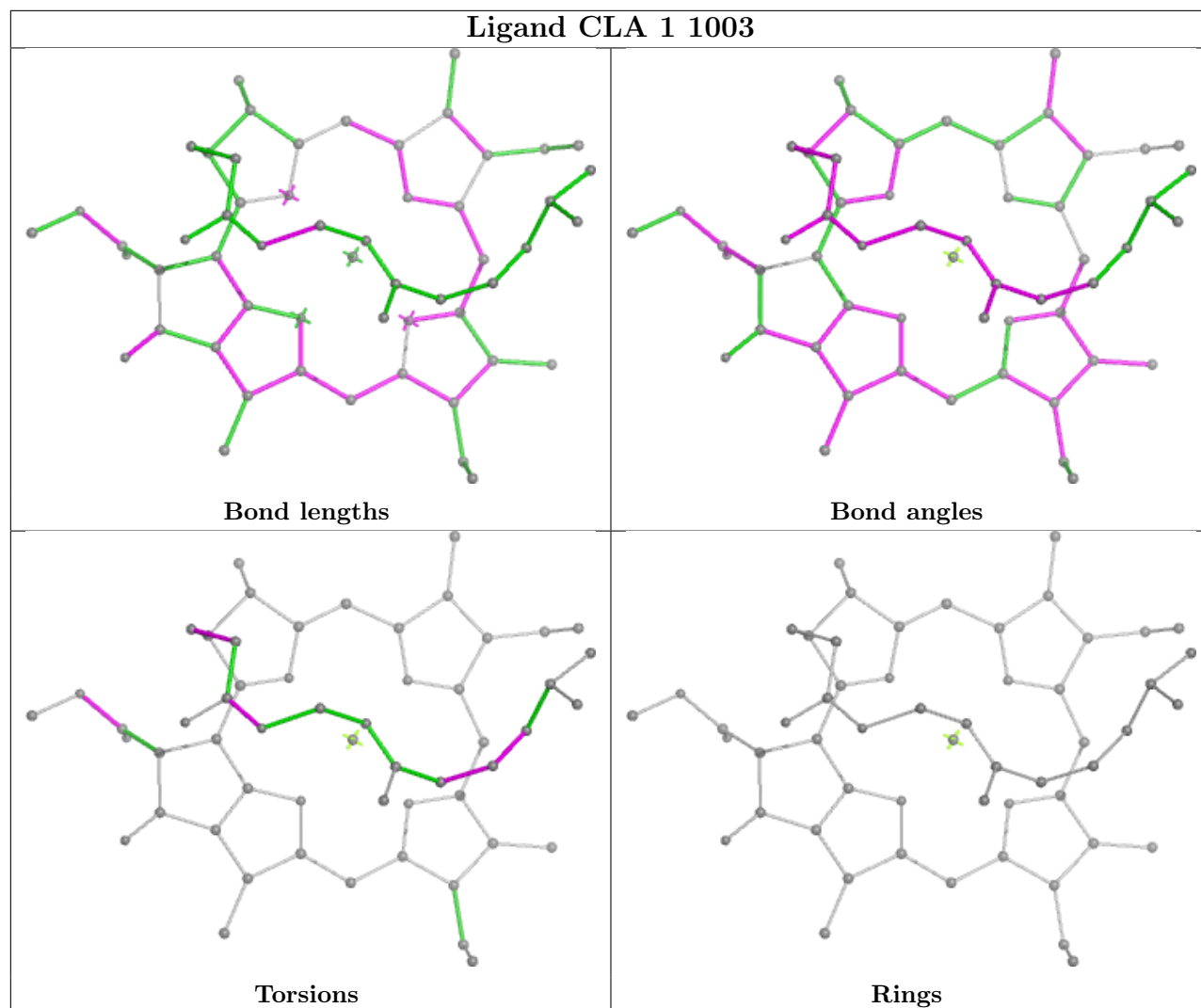


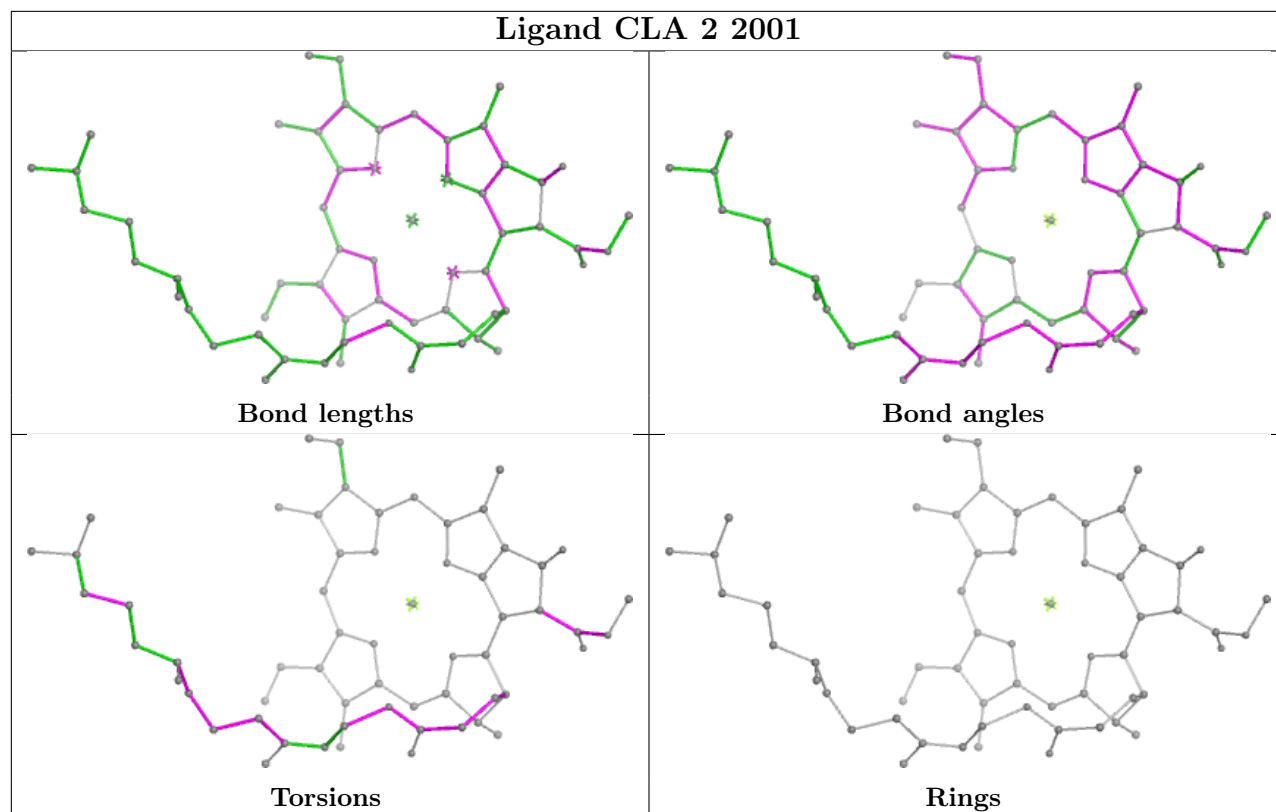


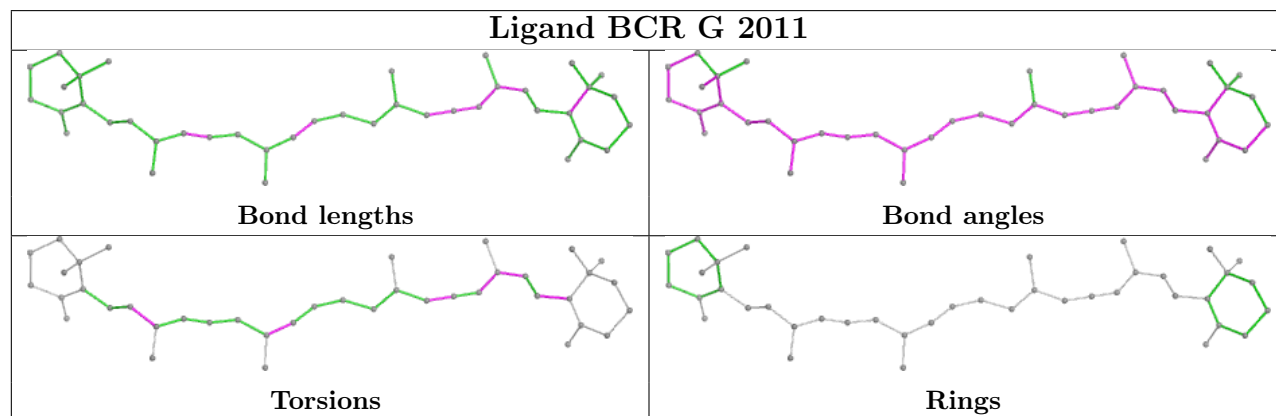
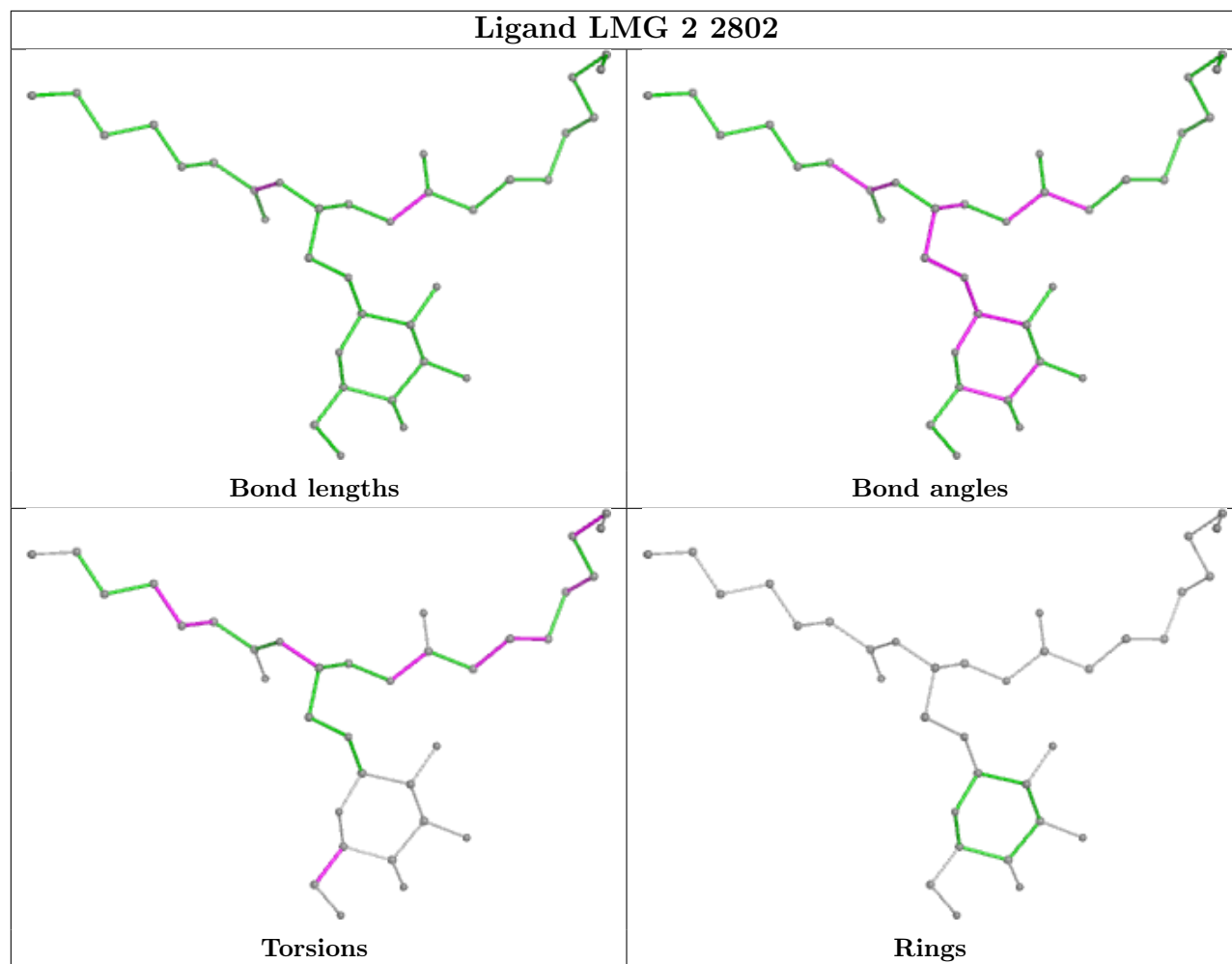




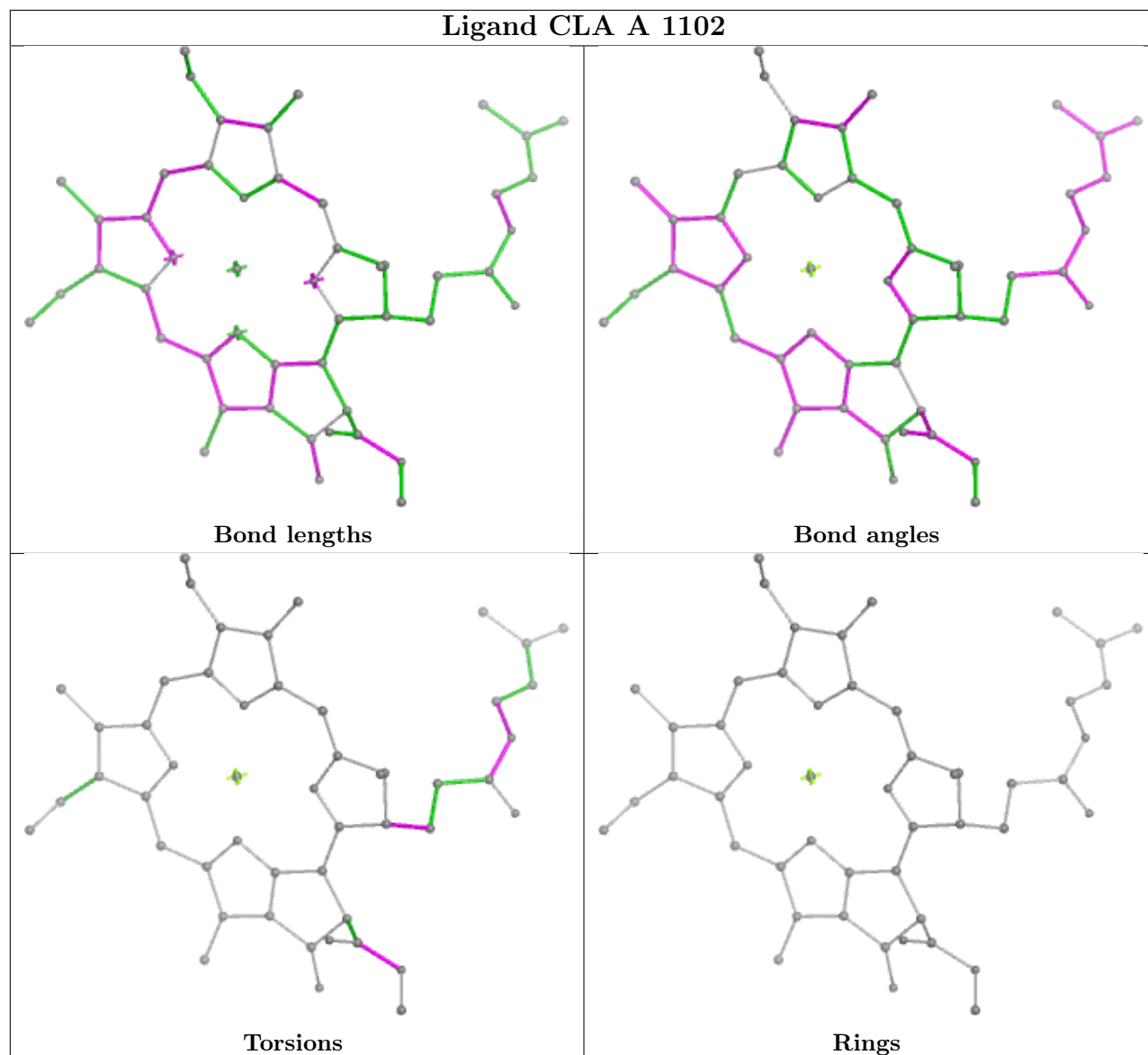


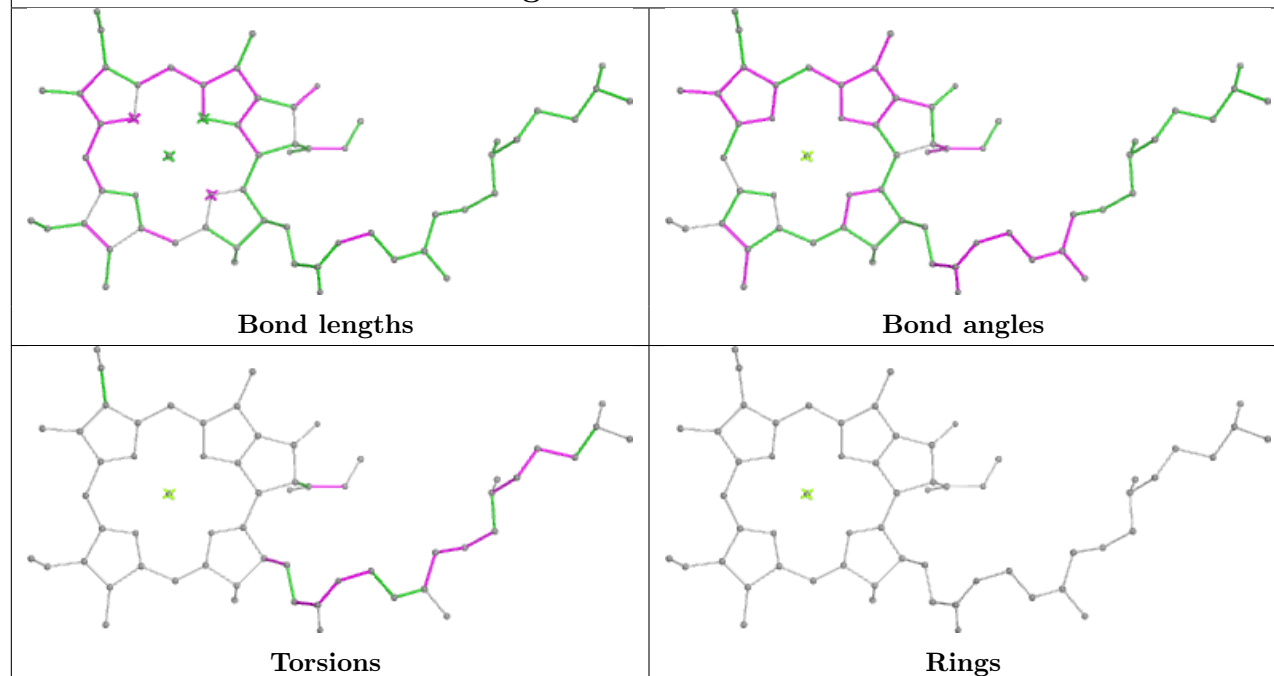
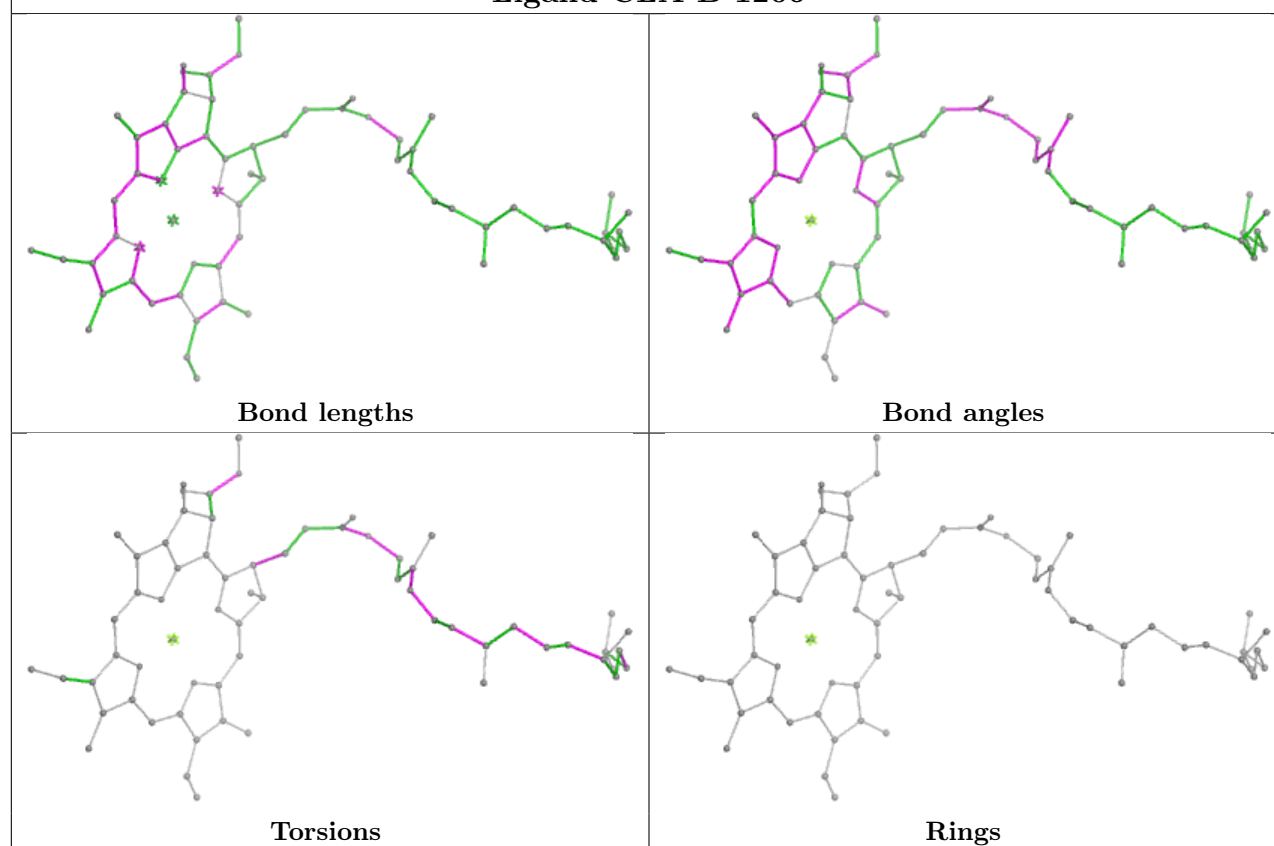


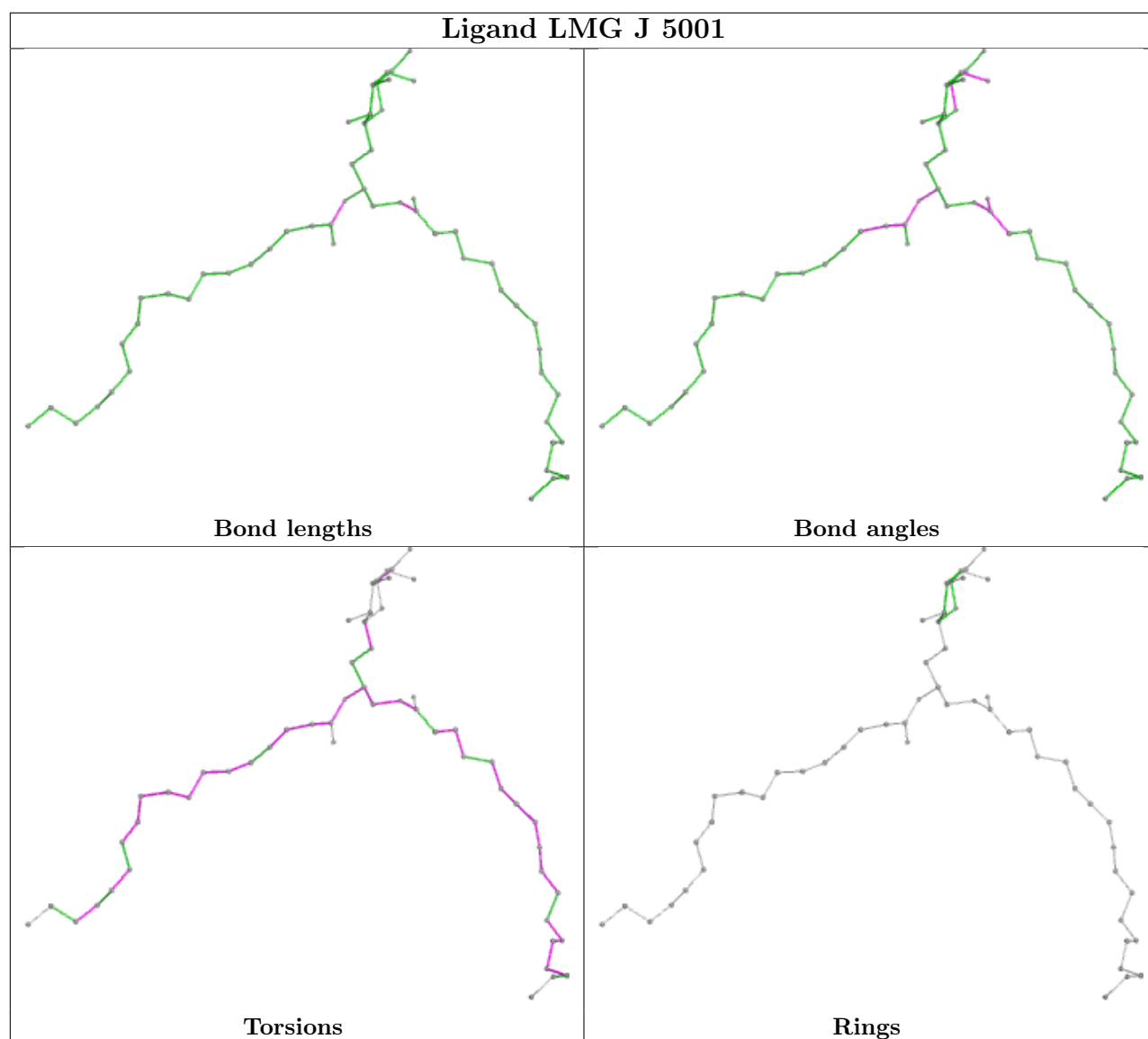




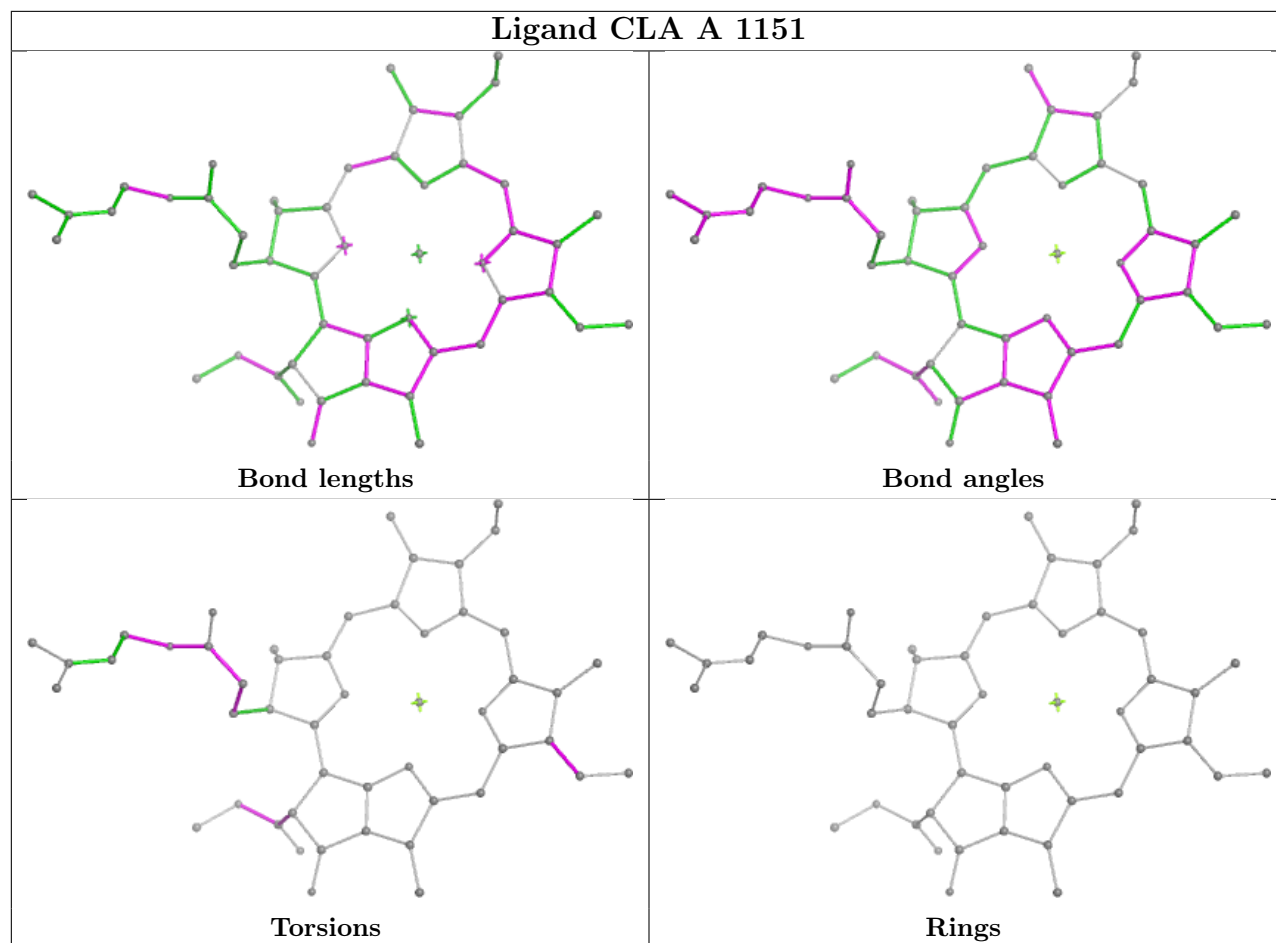
Ligand CLA A 1102



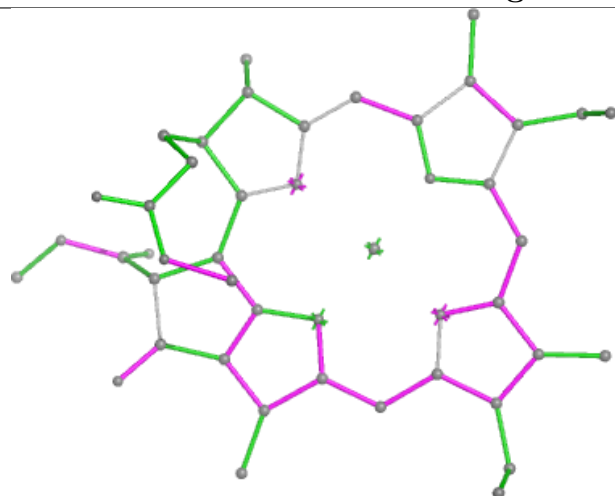
Ligand CLA A 1120**Ligand CLA B 1206**



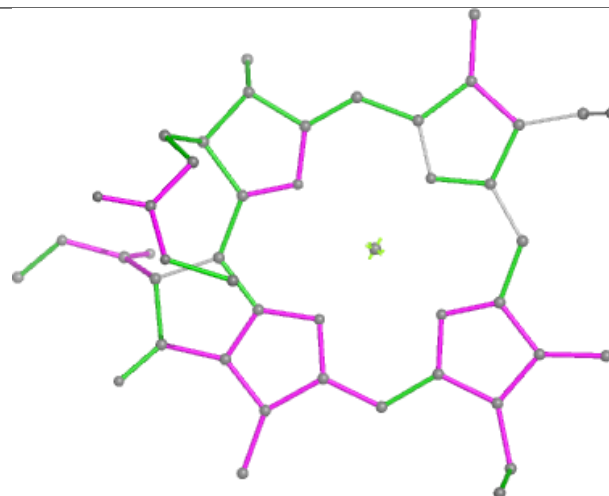
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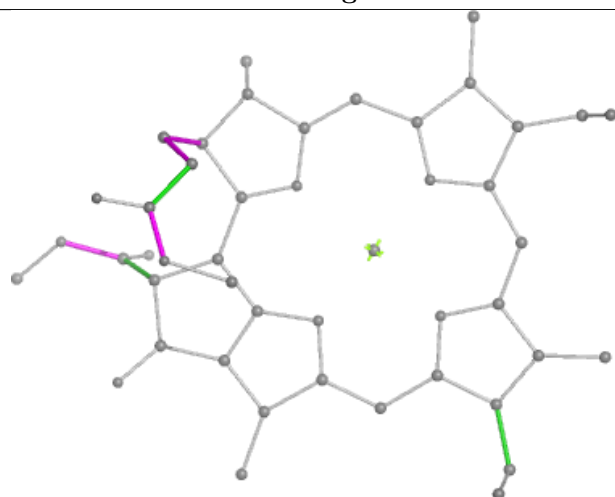
Ligand CLA A 1115



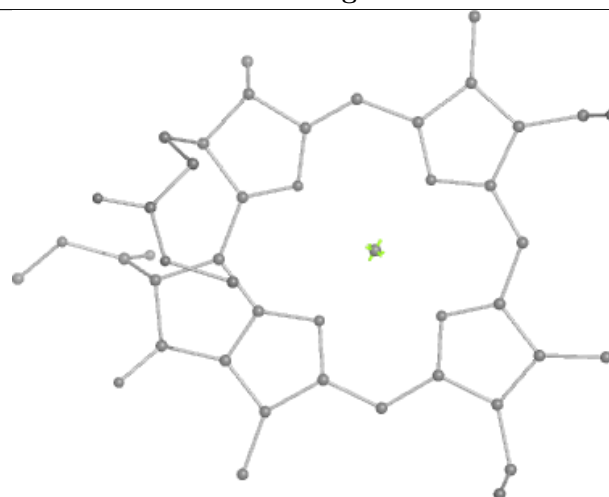
Bond lengths



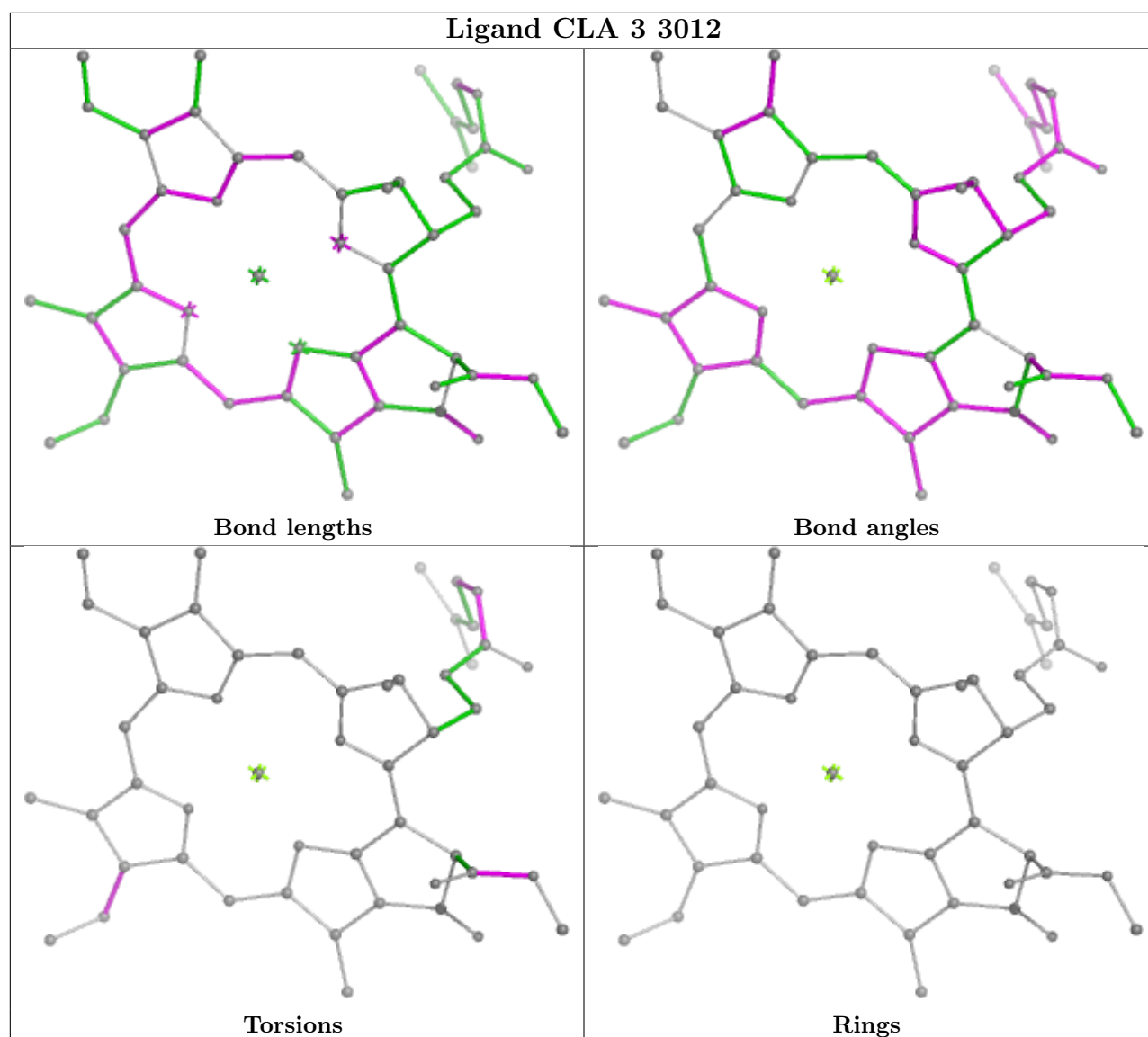
Bond angles

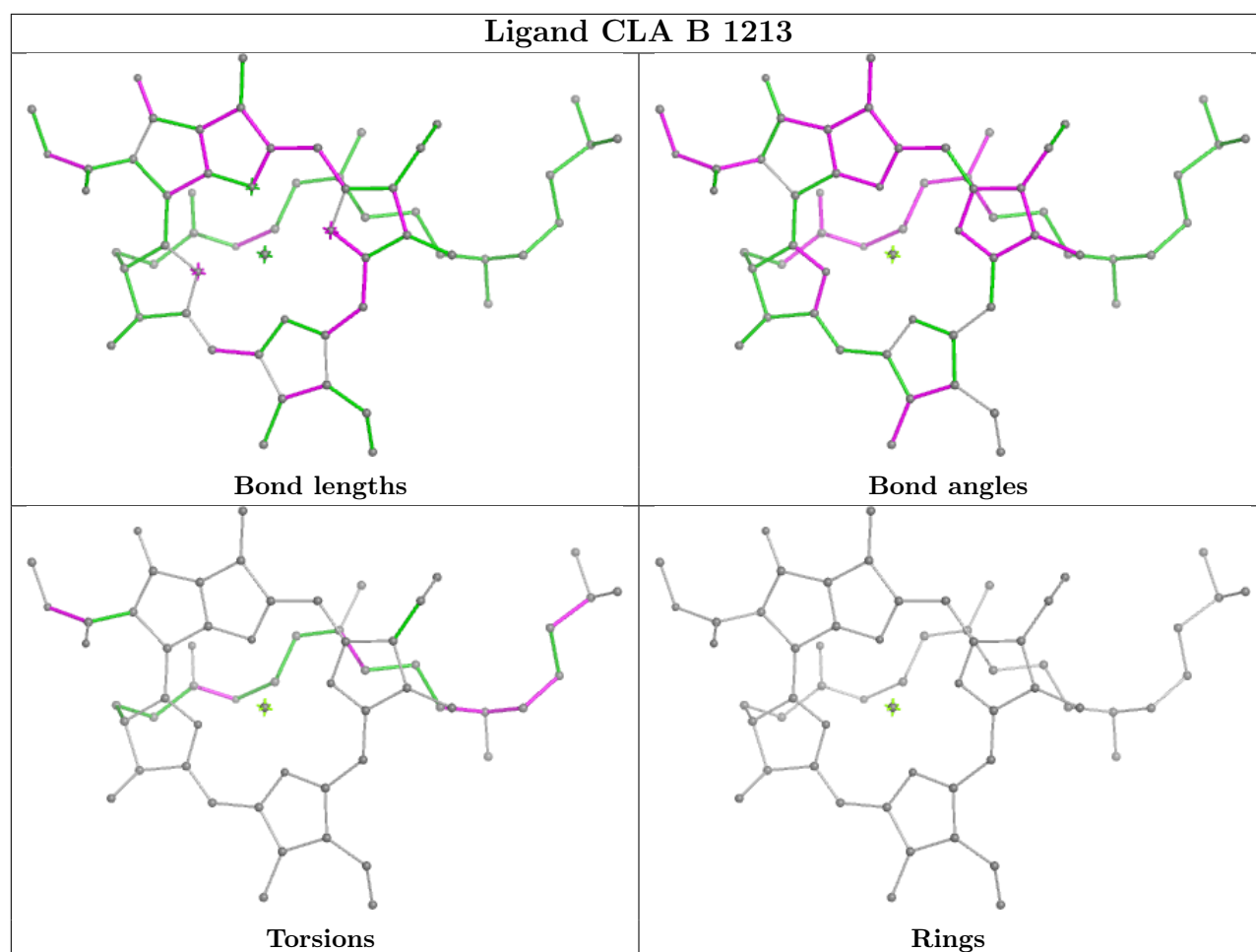


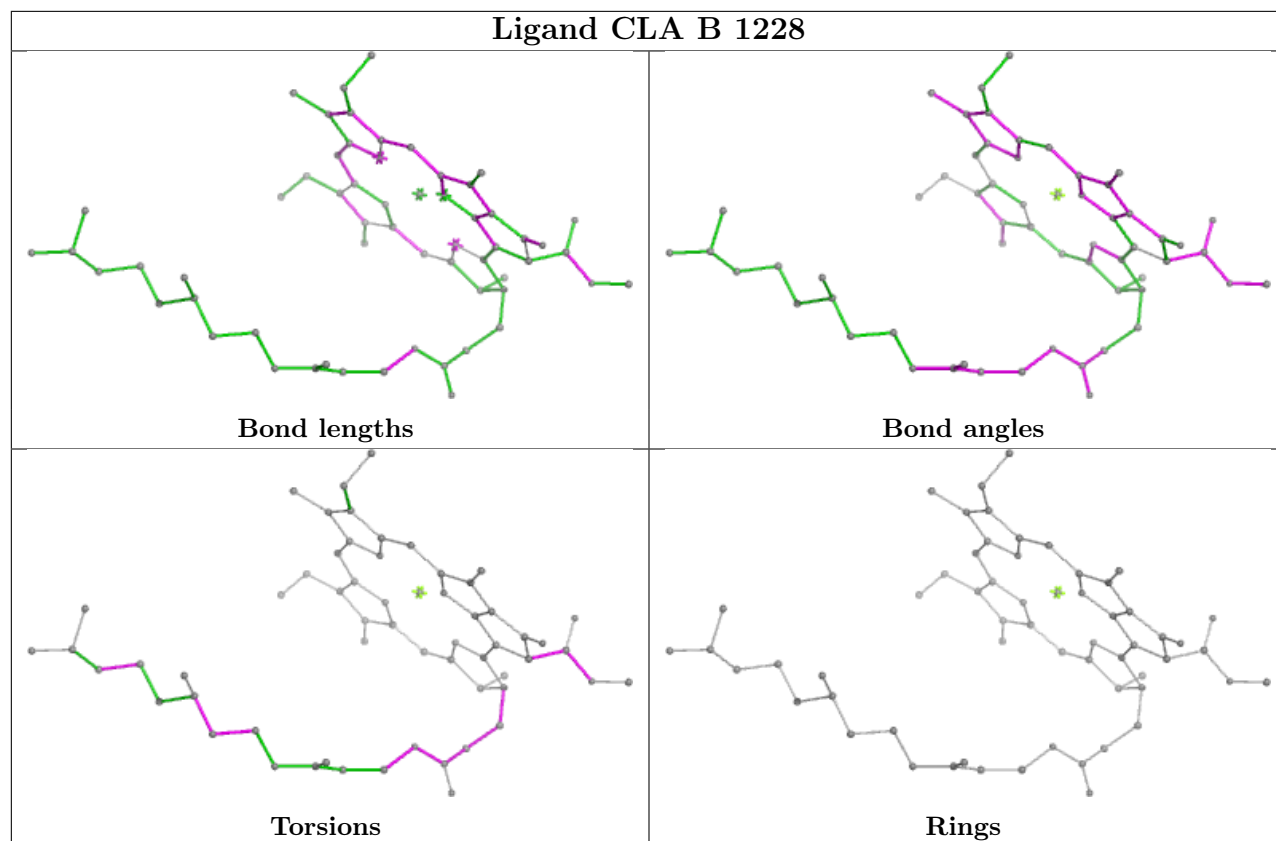
Torsions

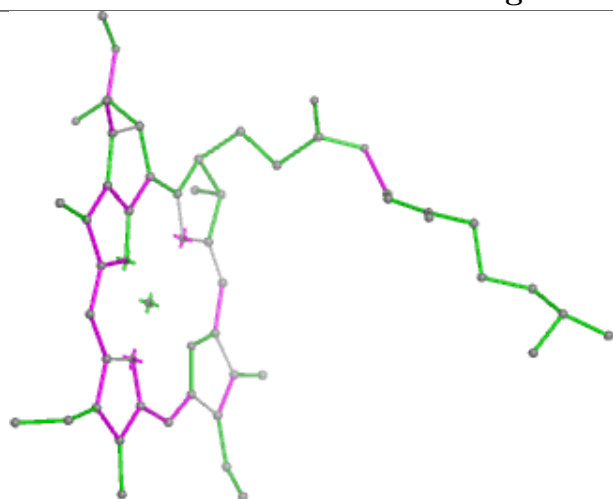
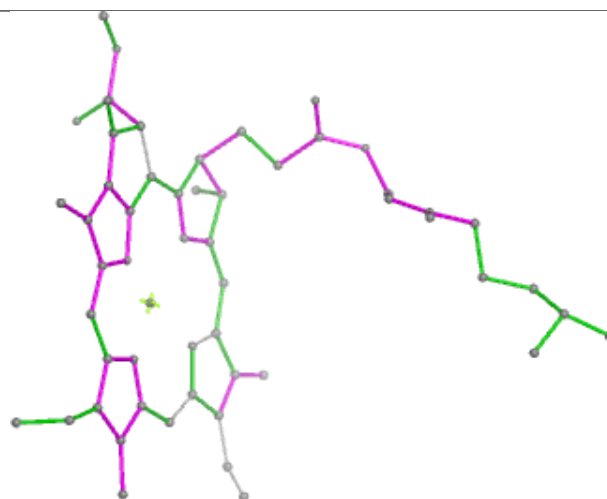
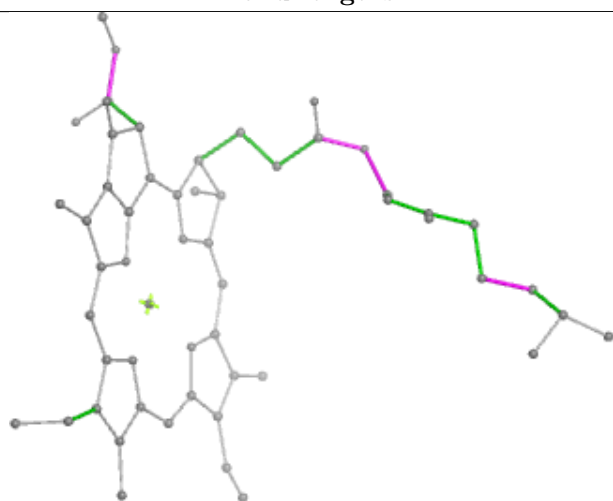
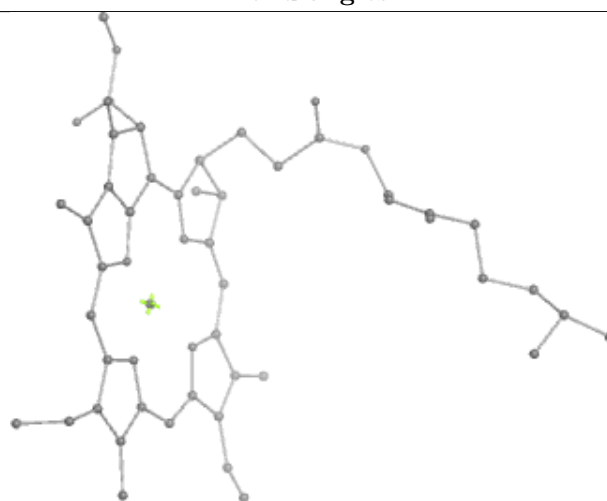


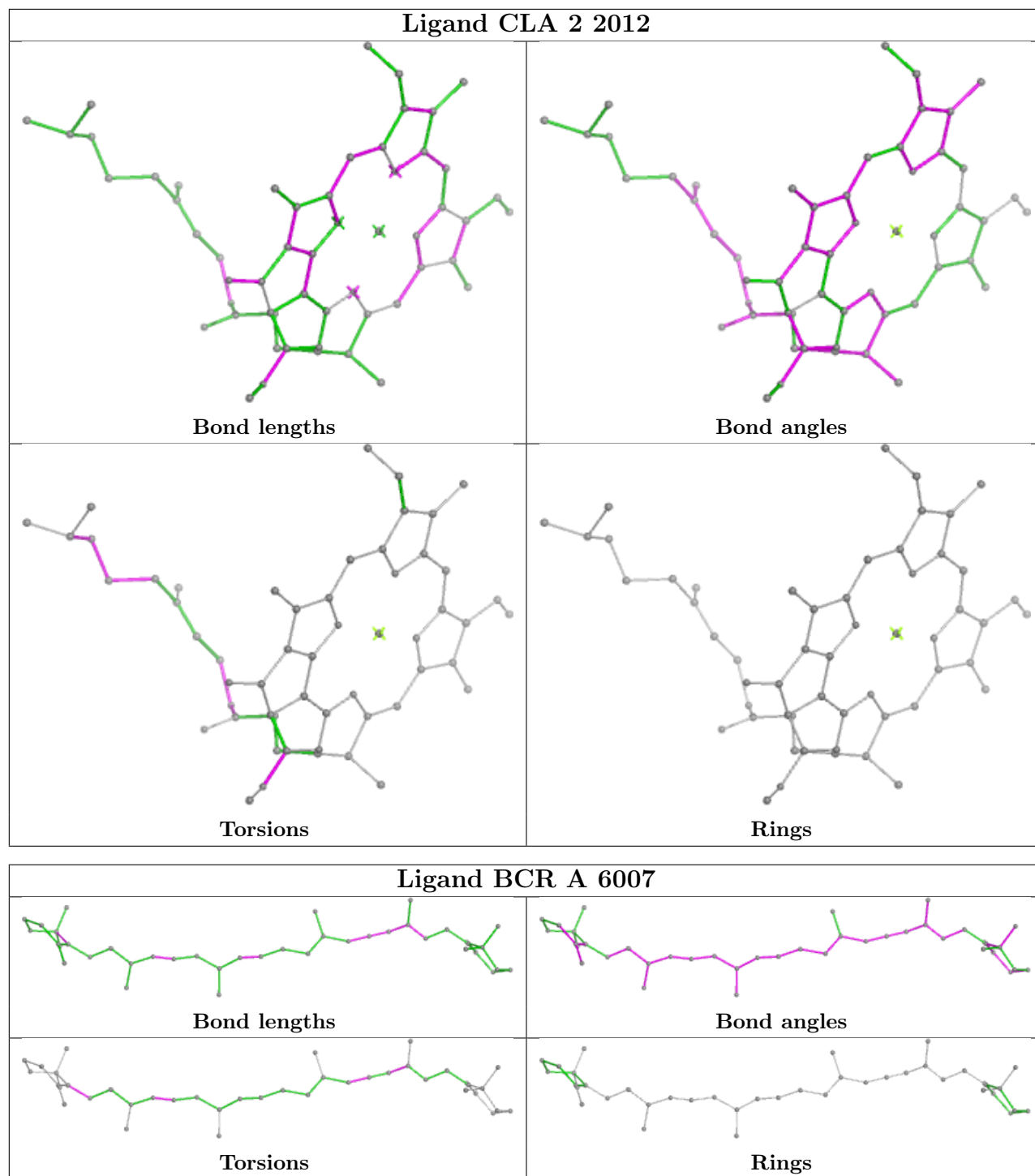
Rings

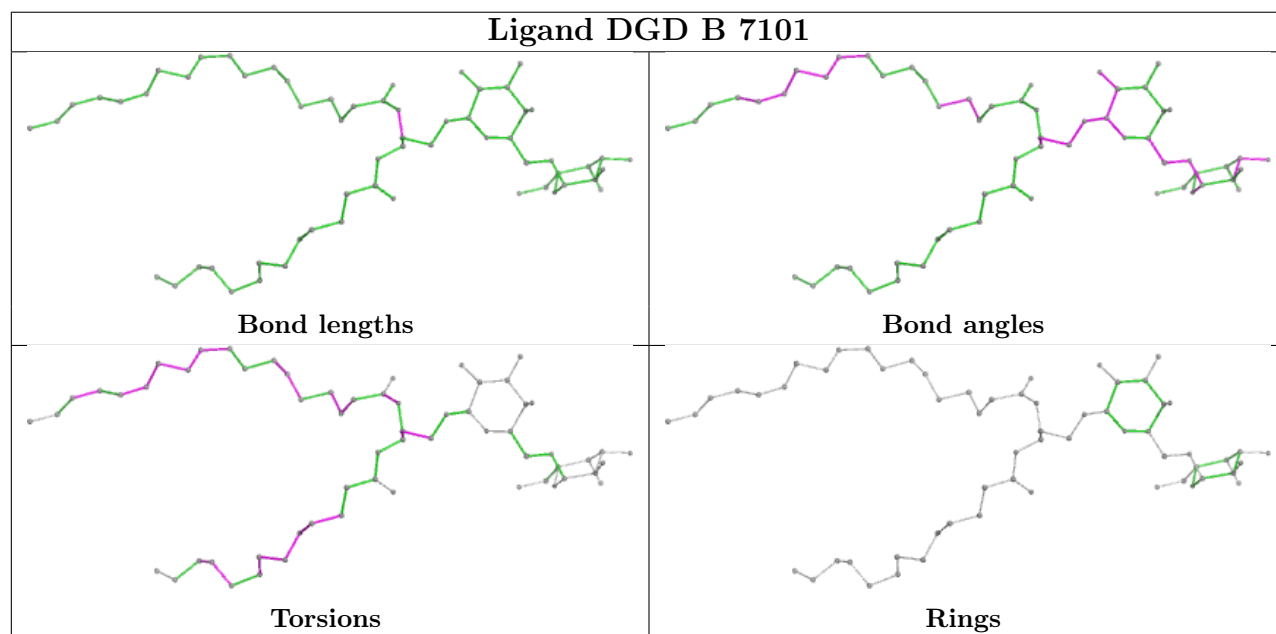
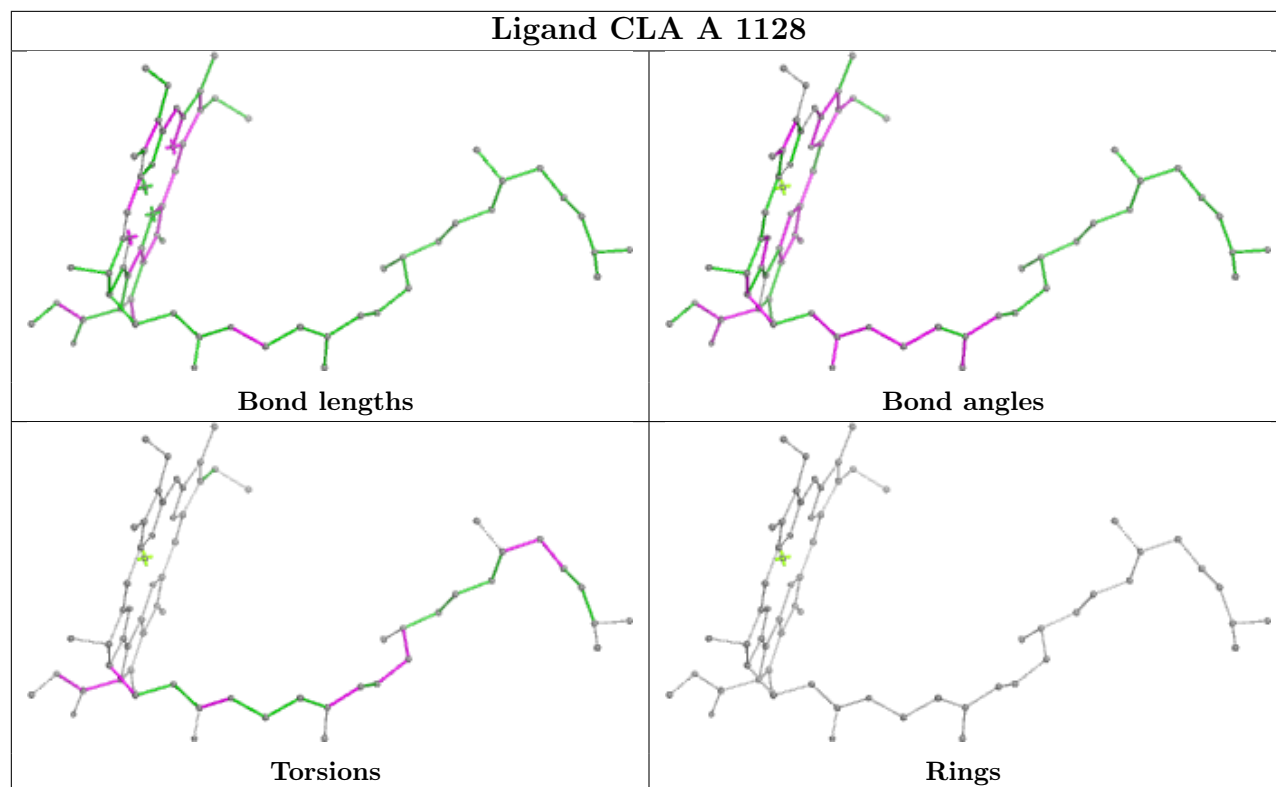




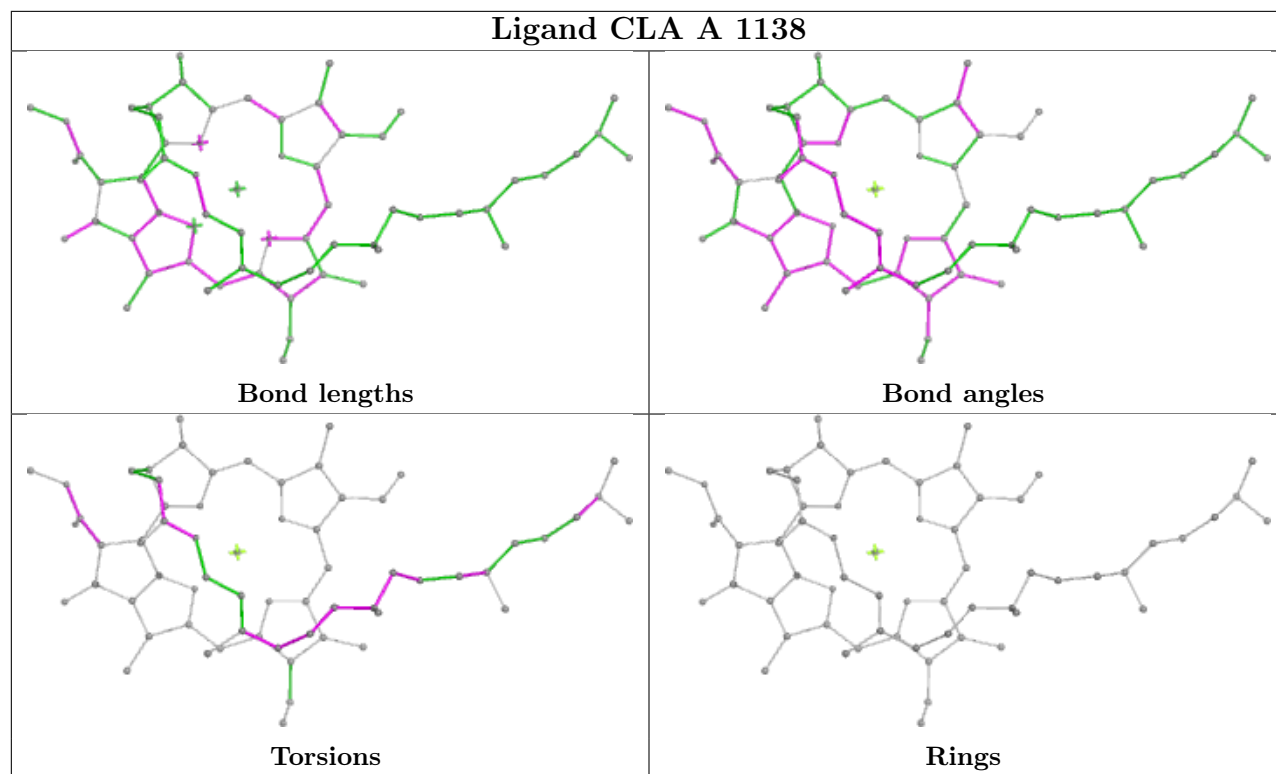


Ligand CLA B 1232**Bond lengths****Bond angles****Torsions****Rings**

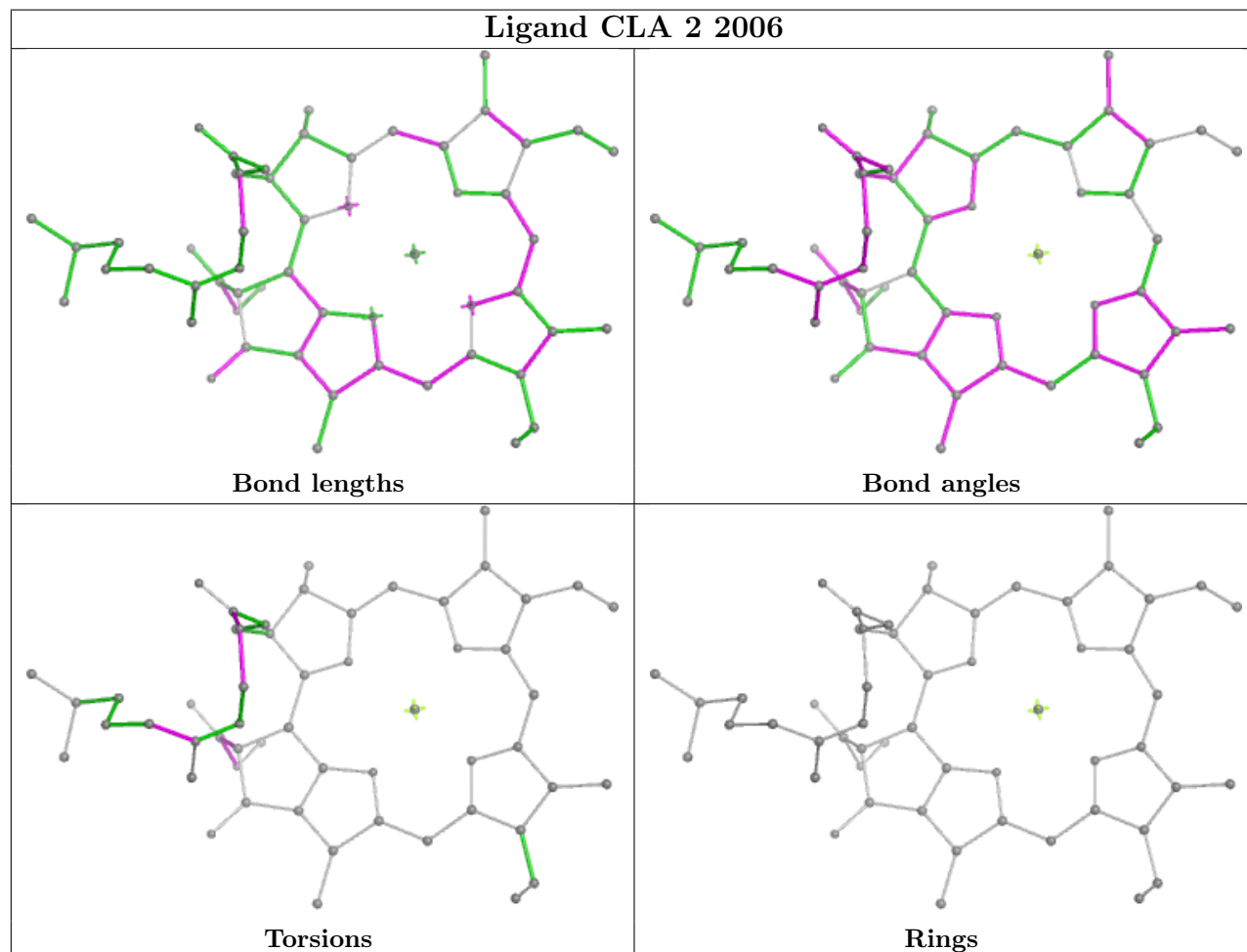


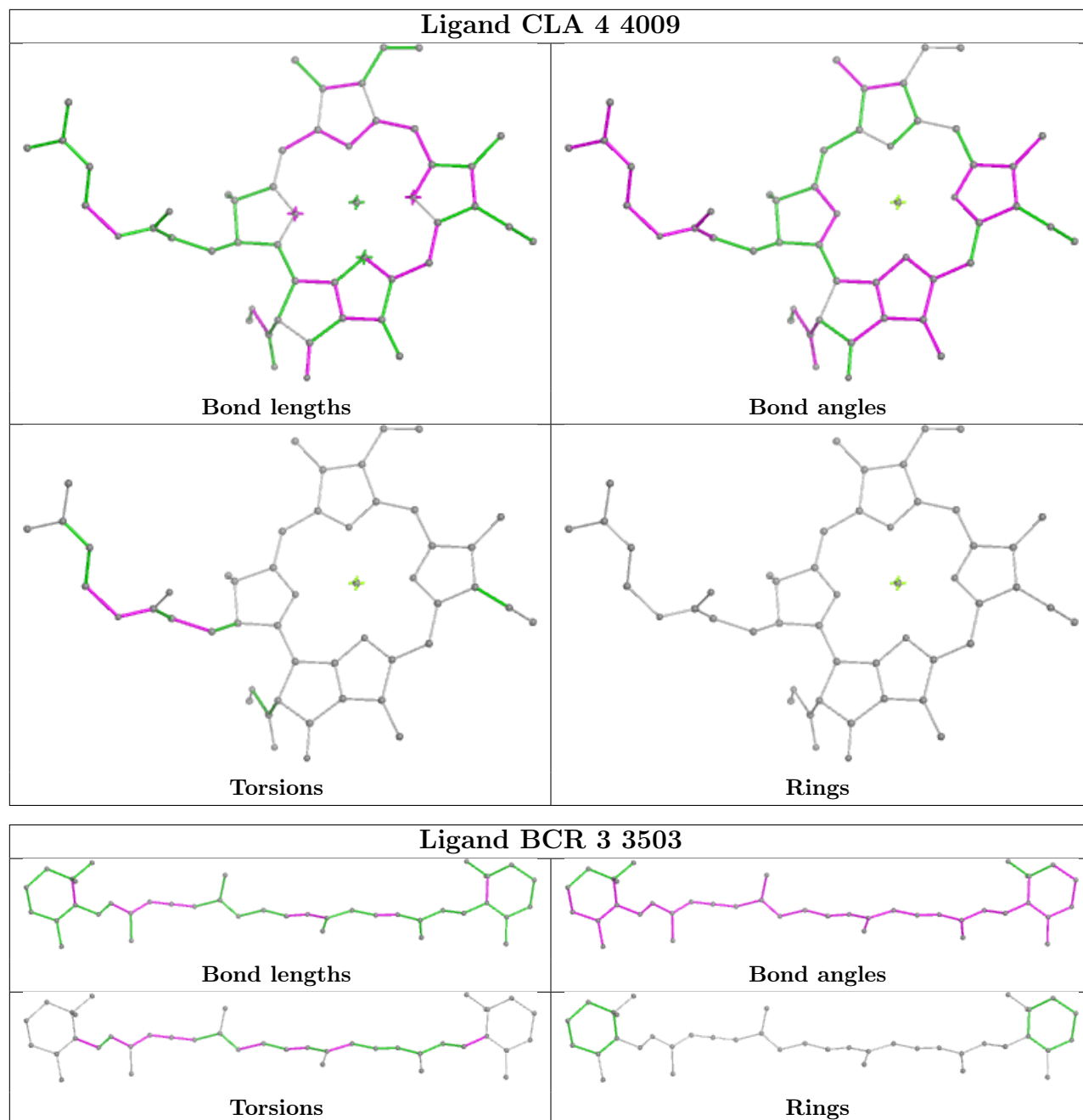


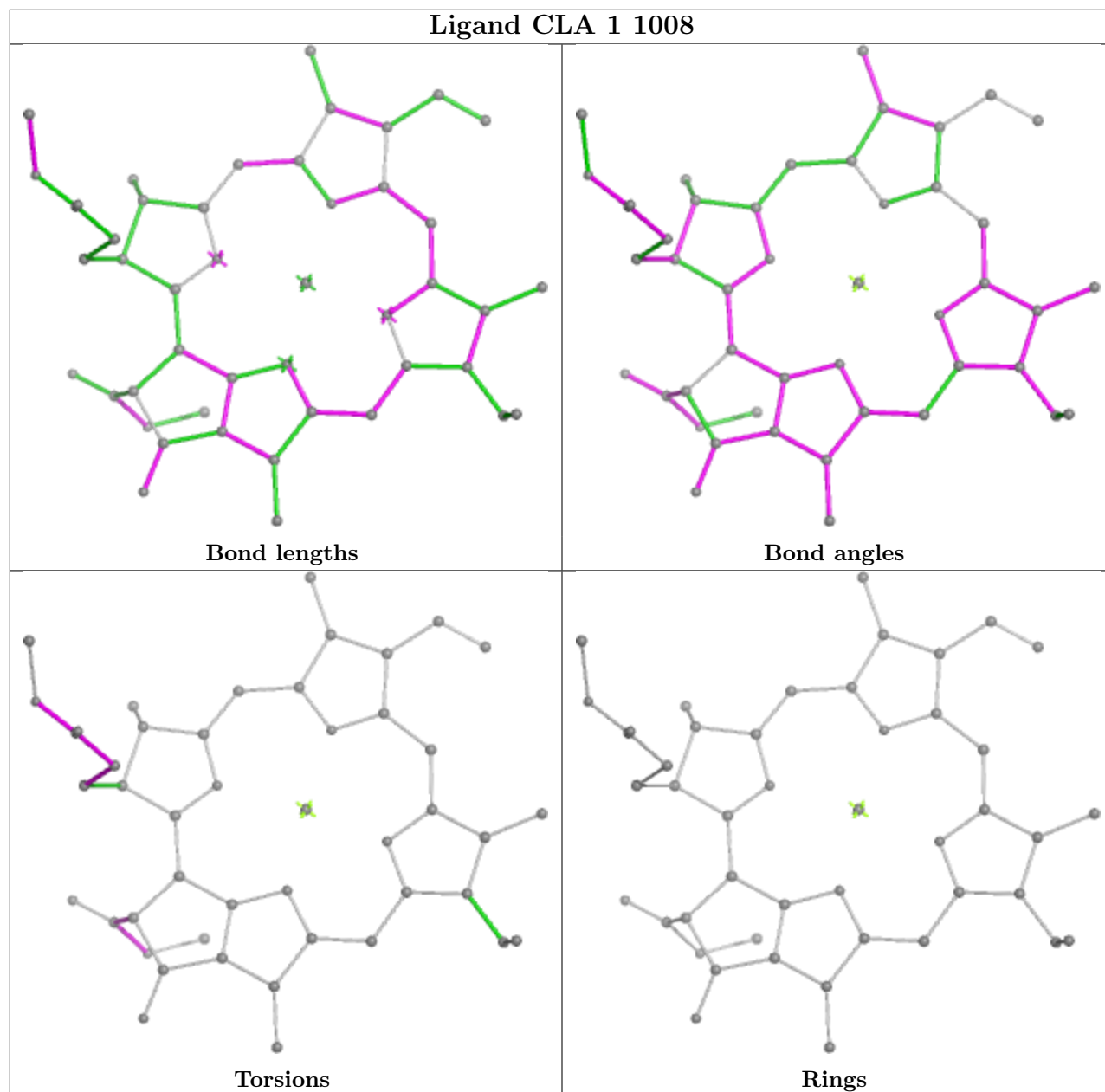
Ligand CLA A 1138

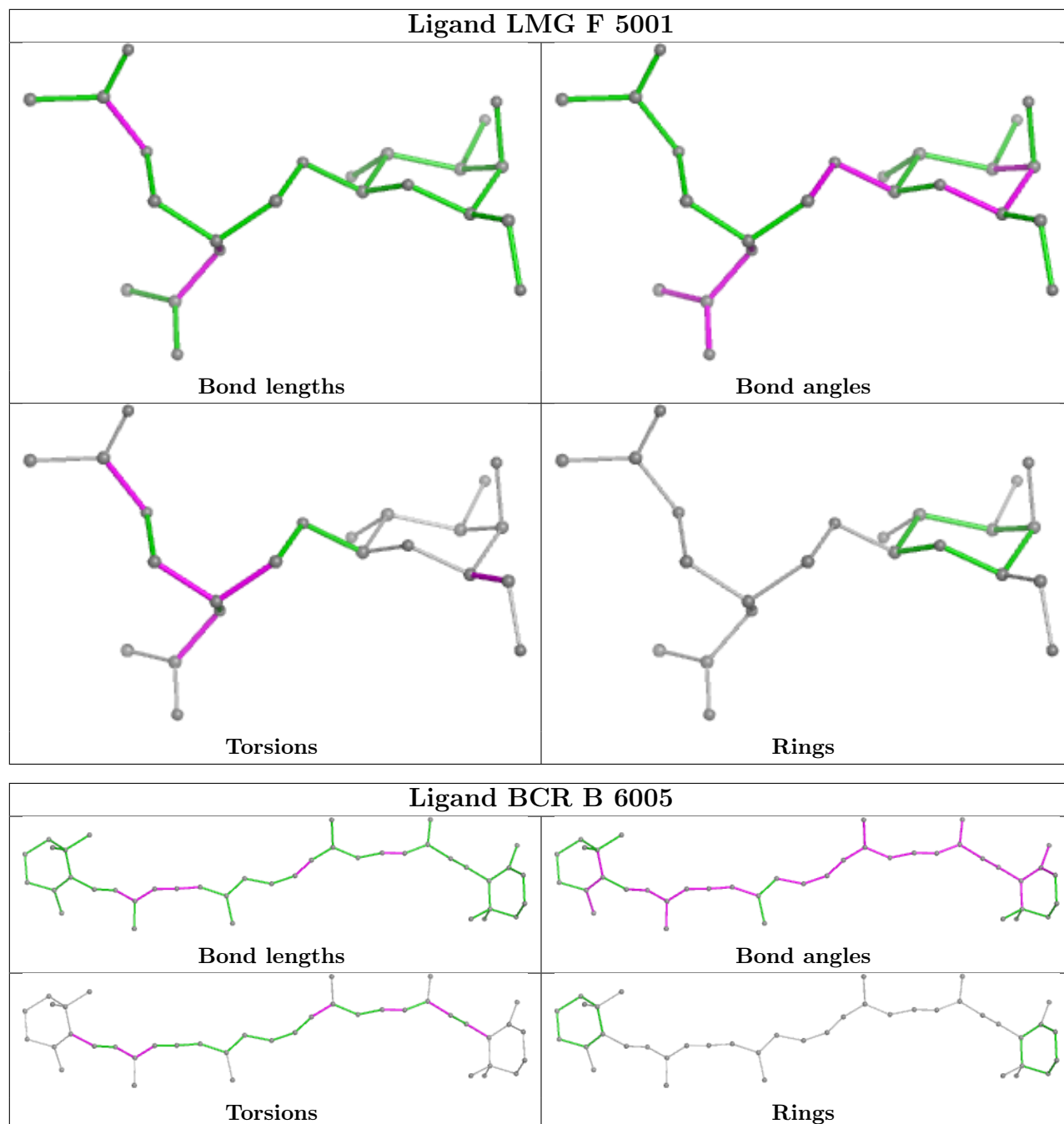


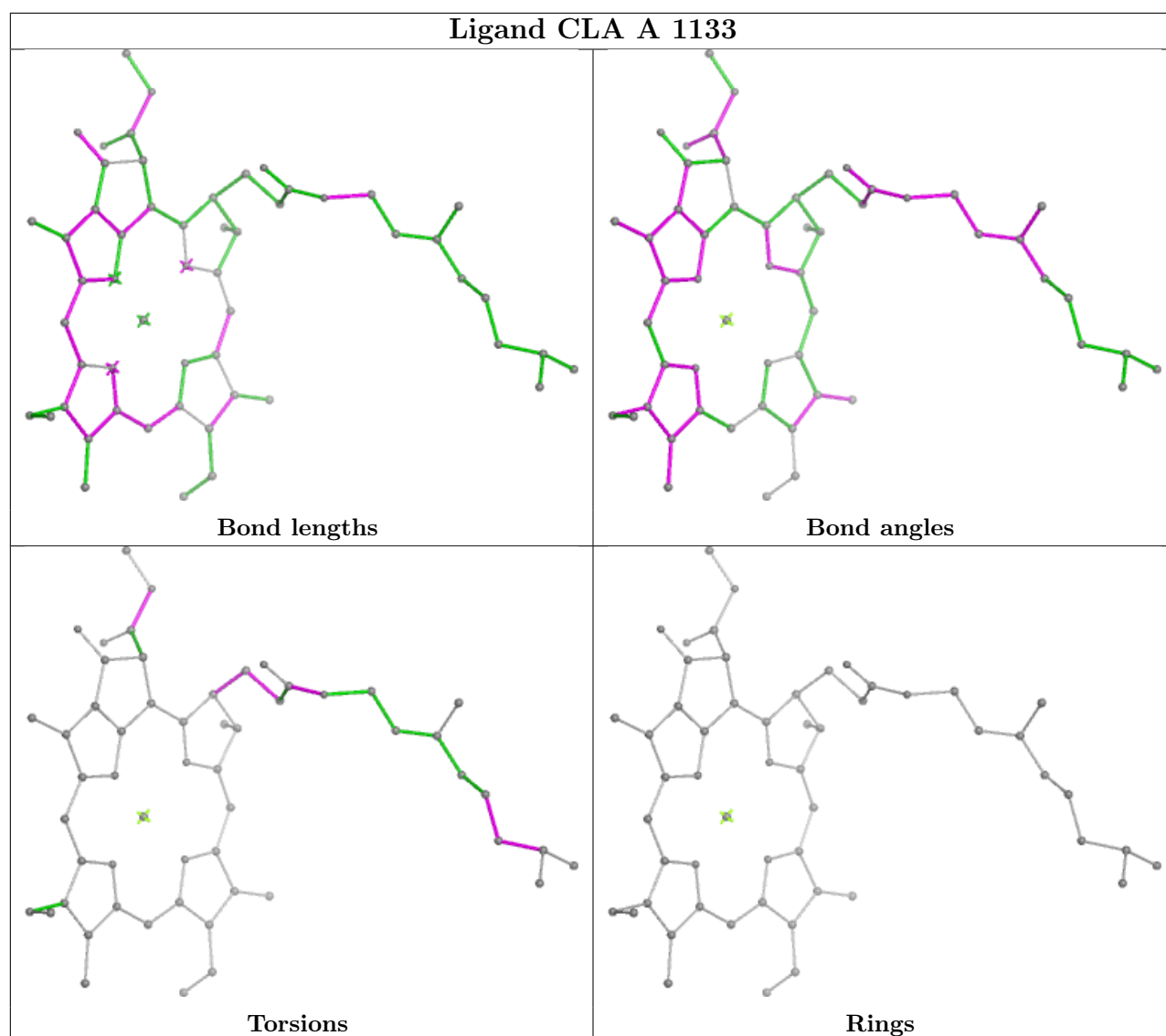
Ligand CLA 2 2006

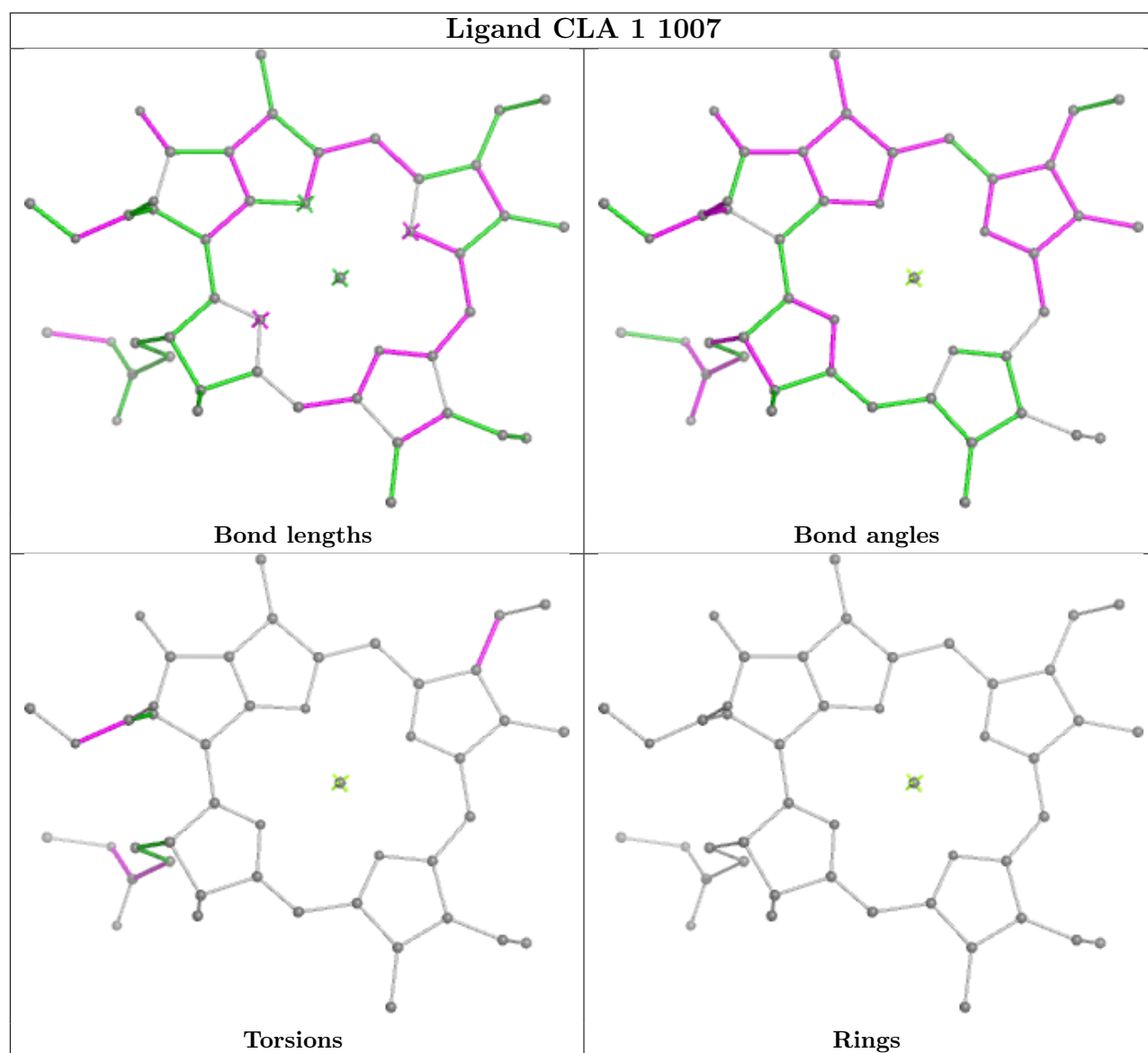


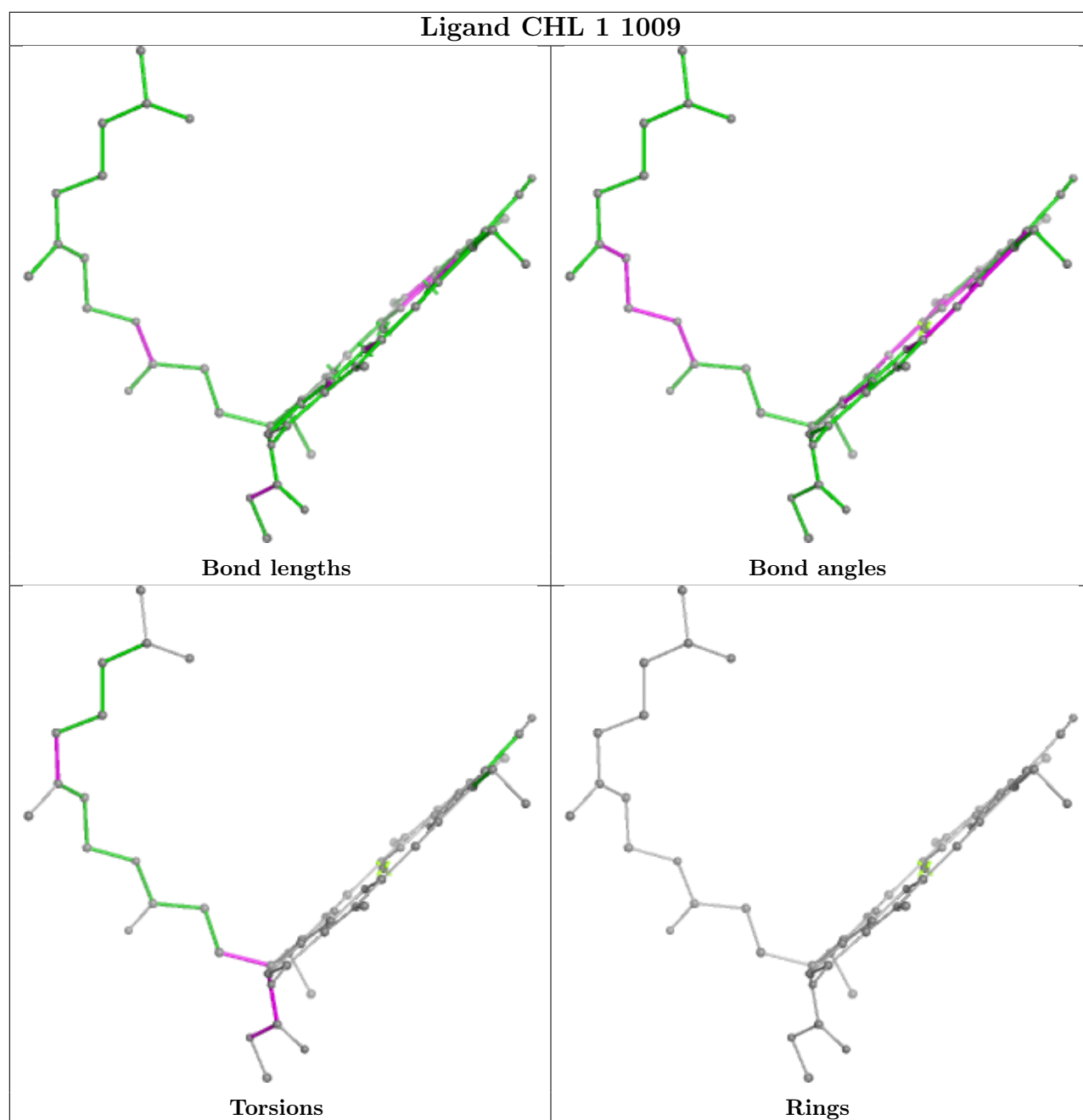


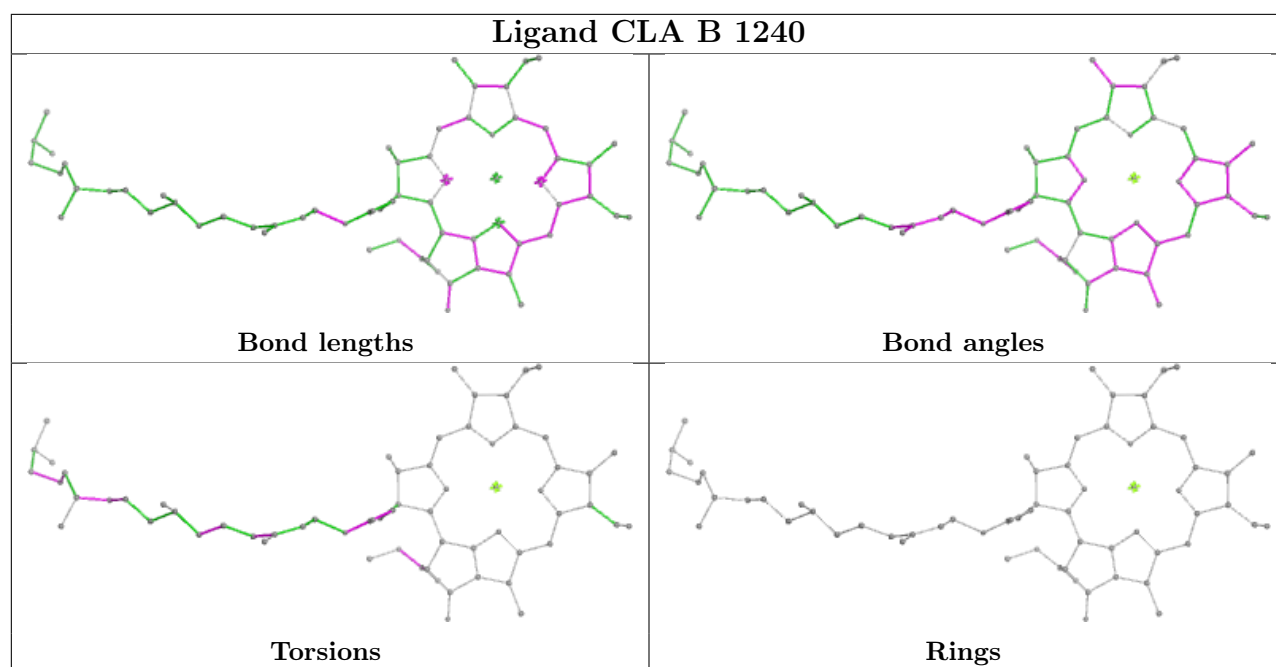


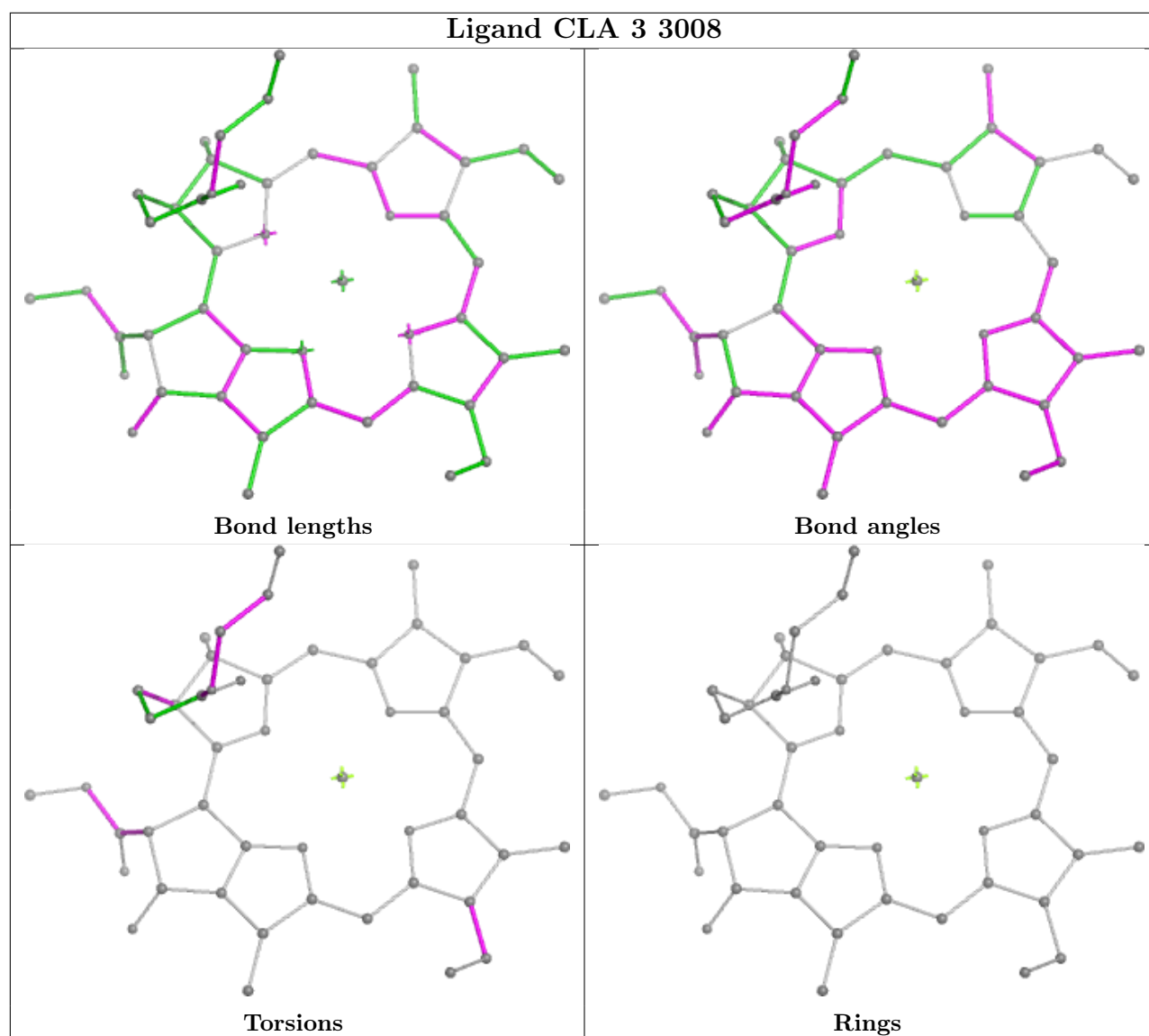


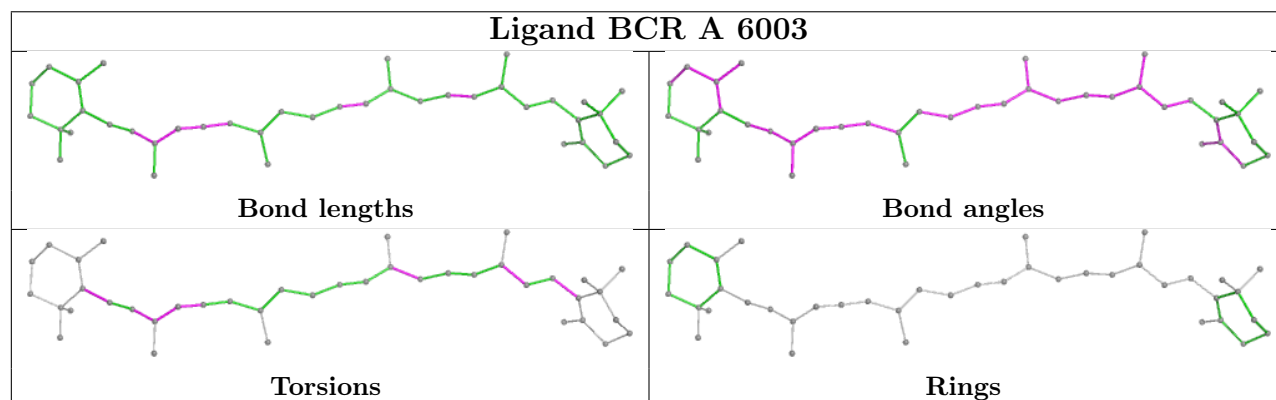
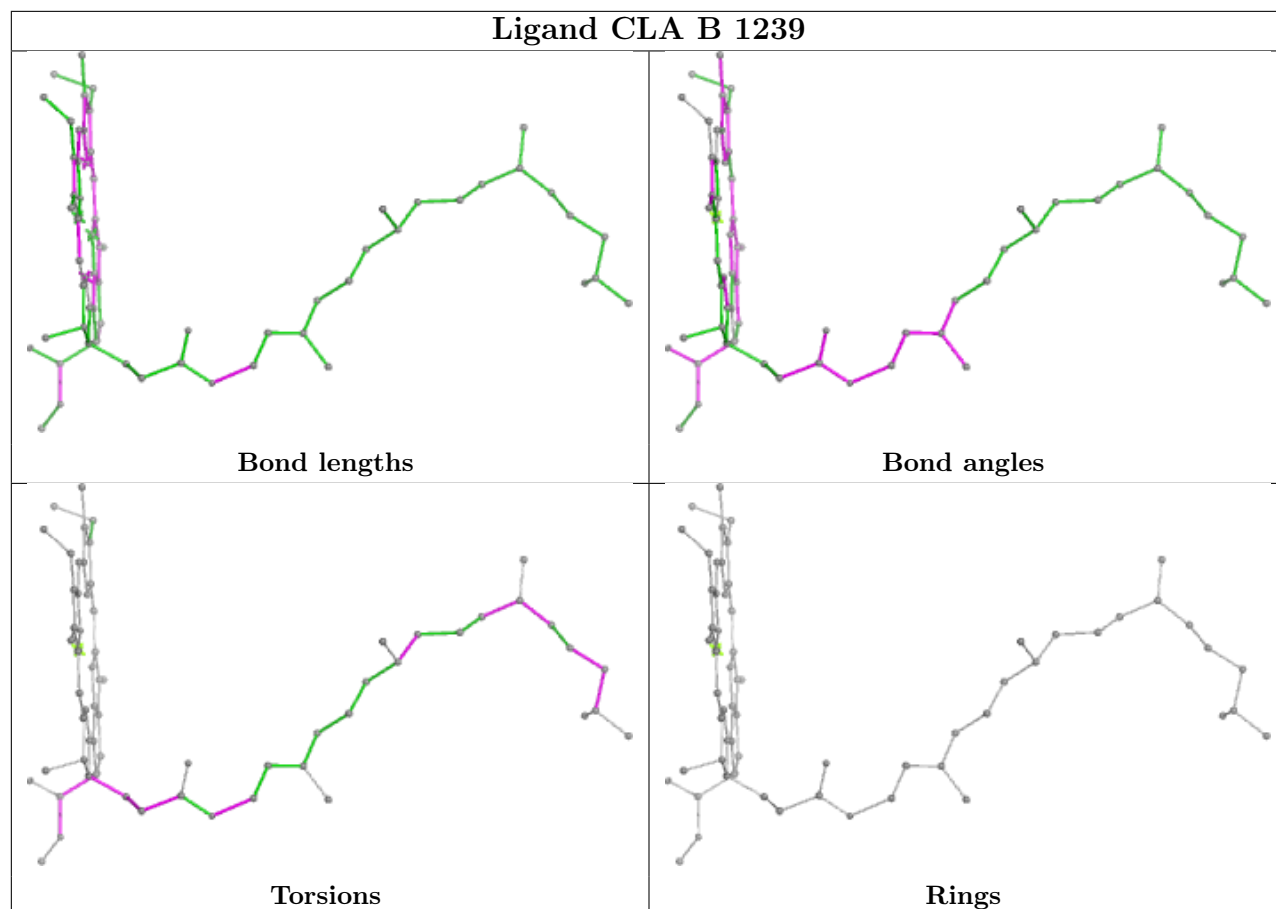


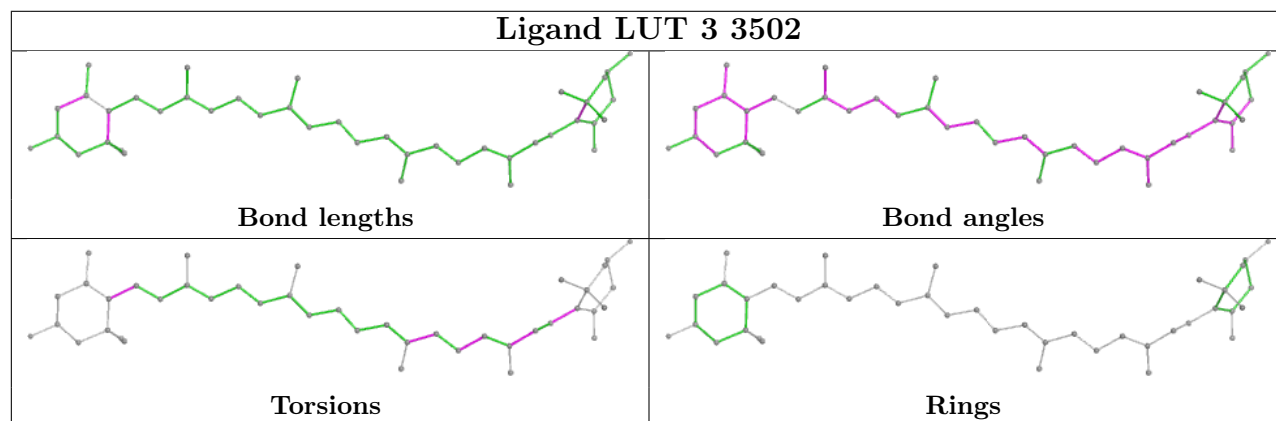
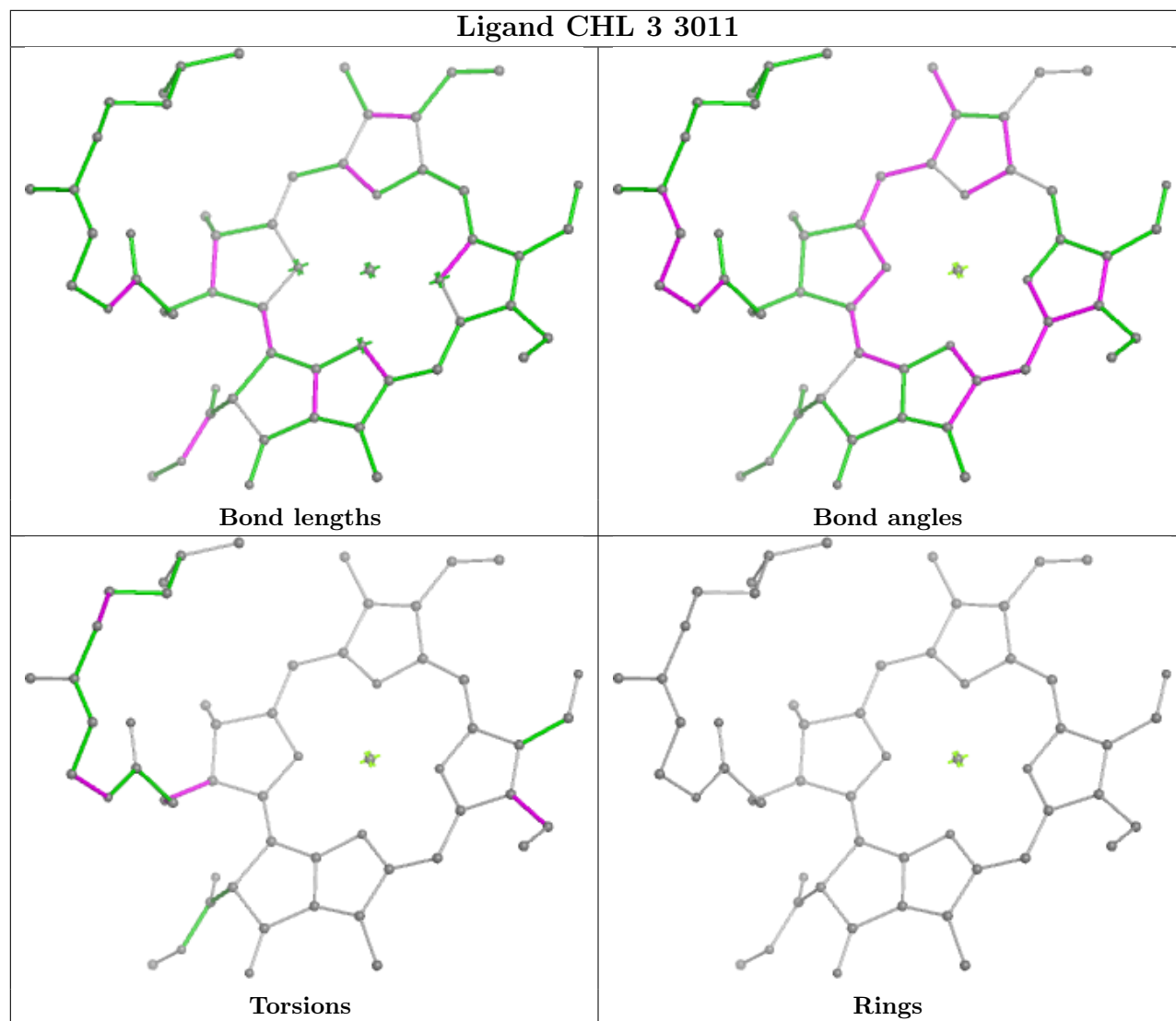


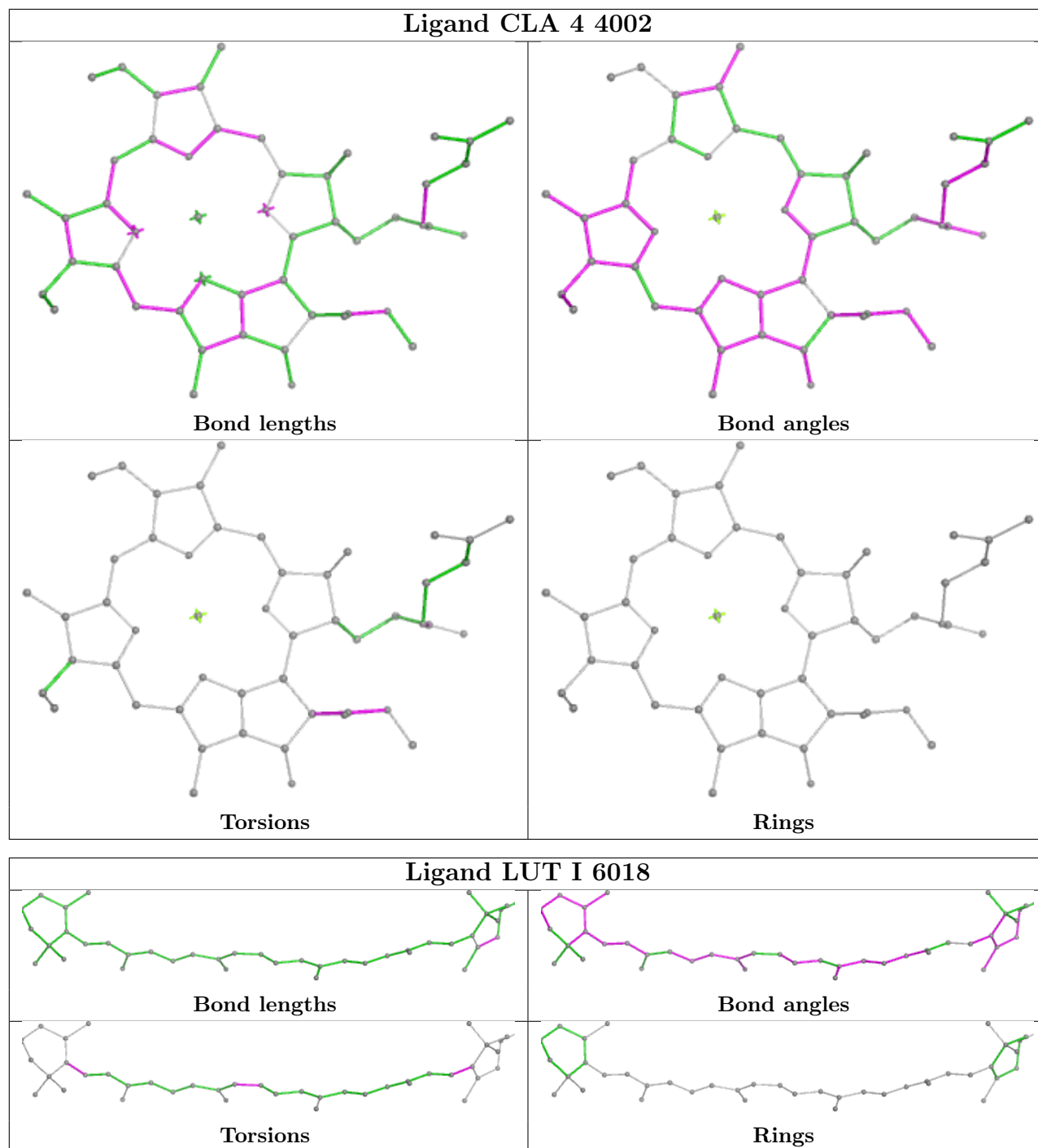


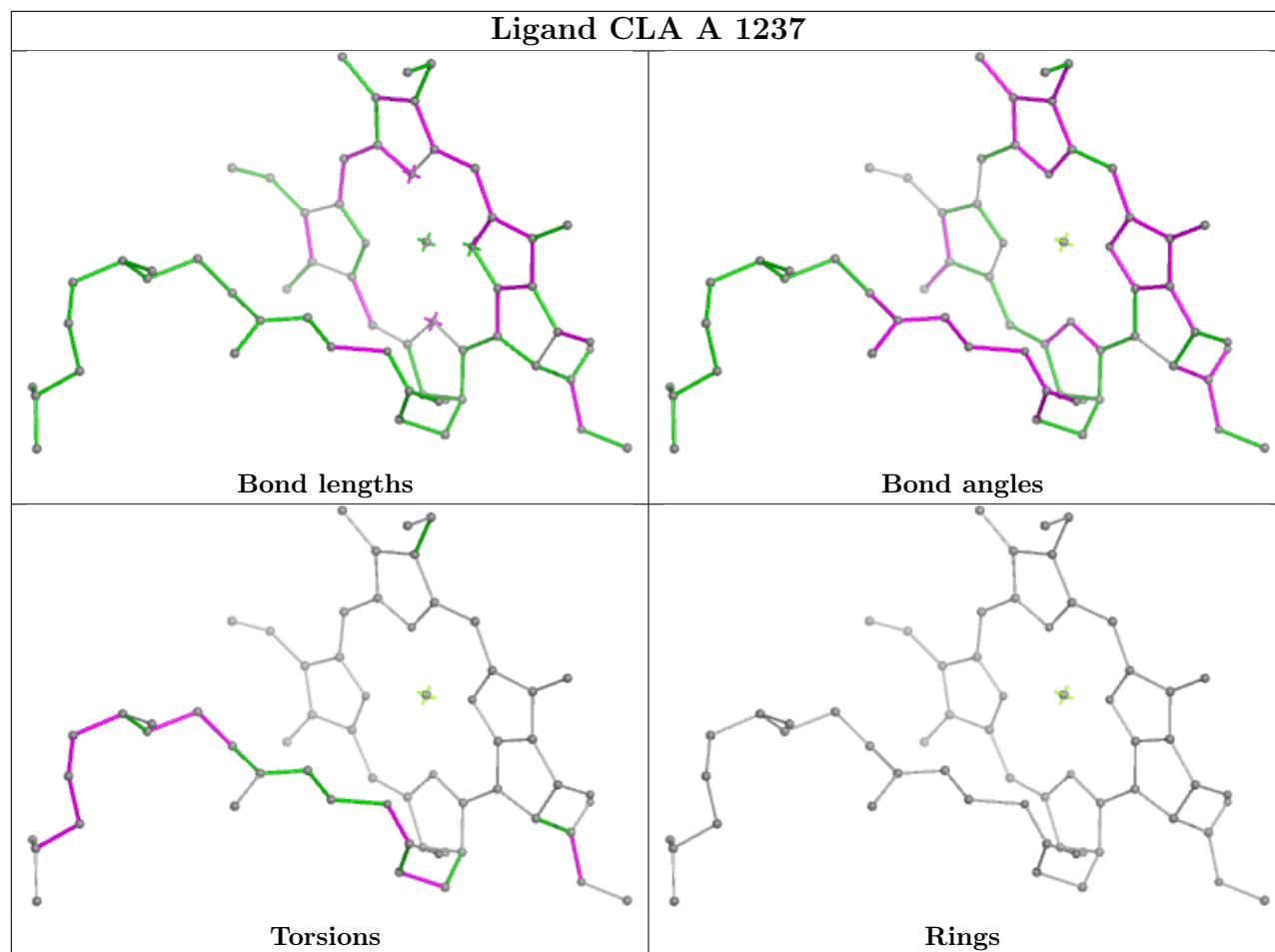
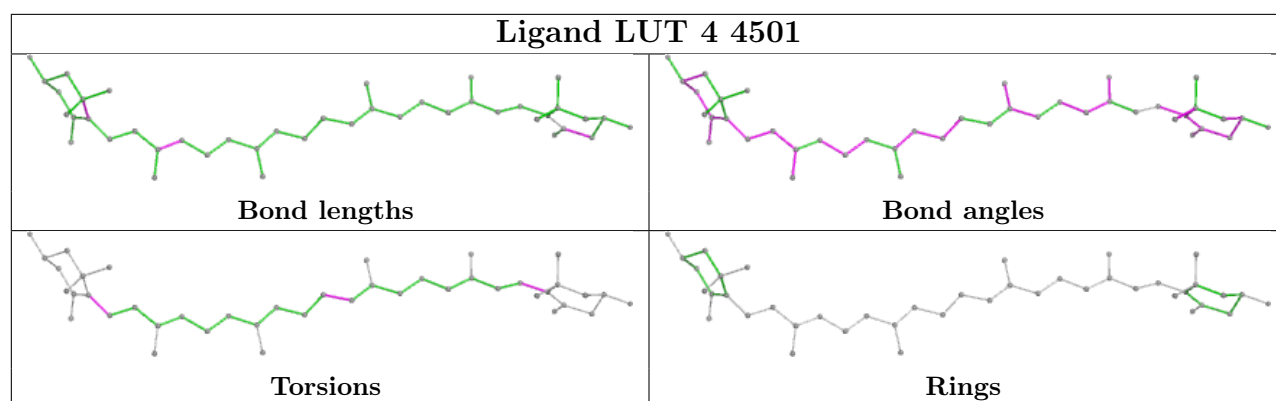




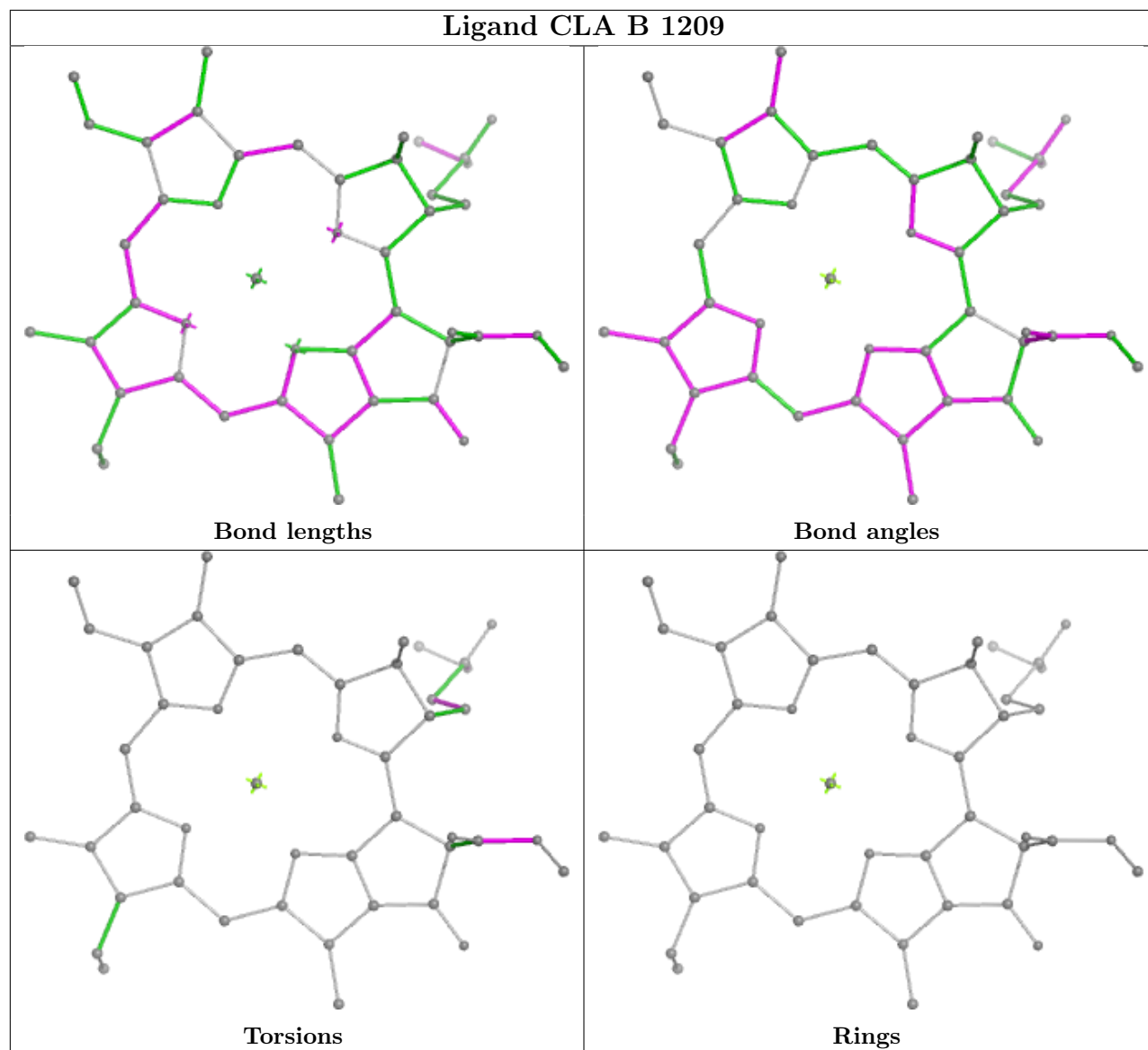


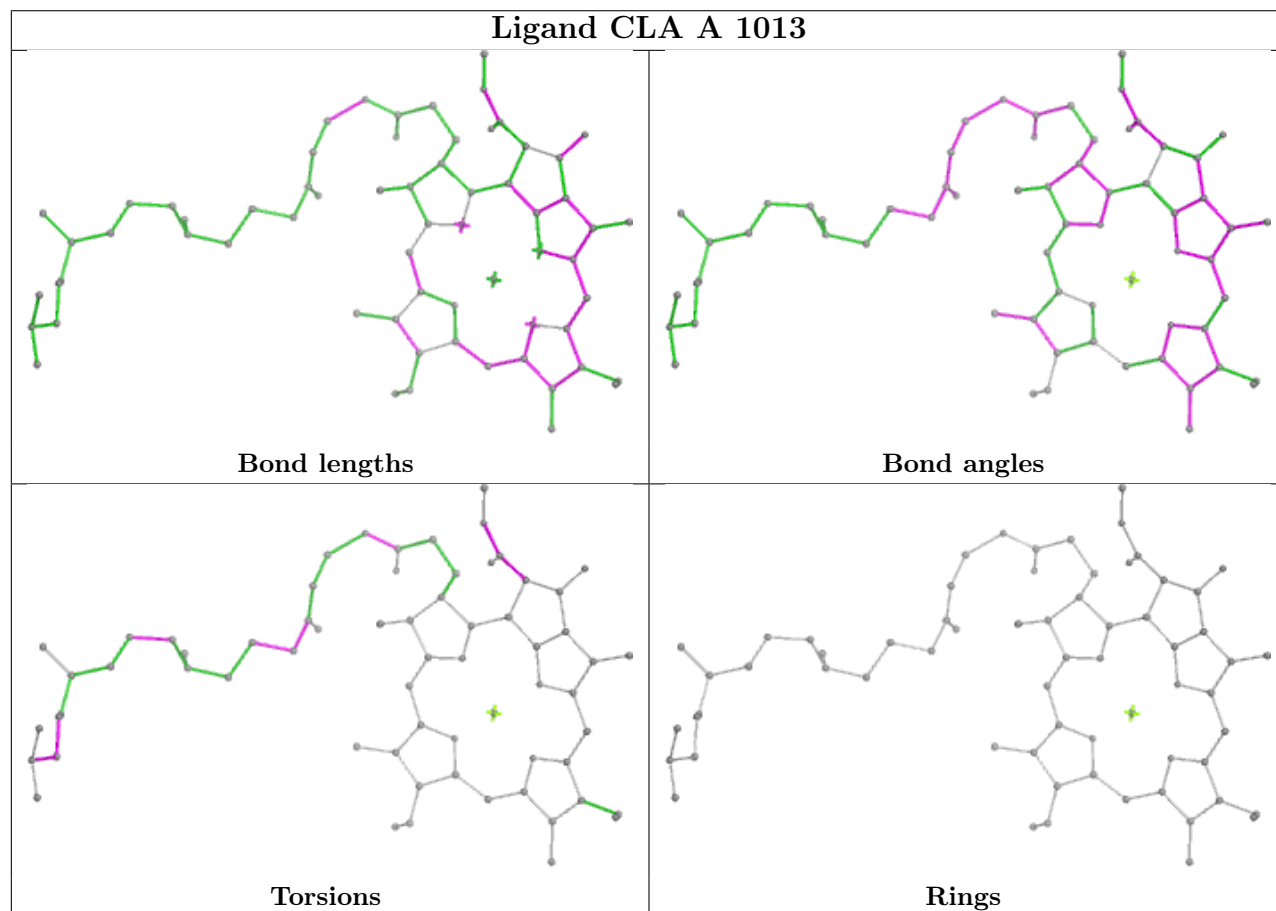
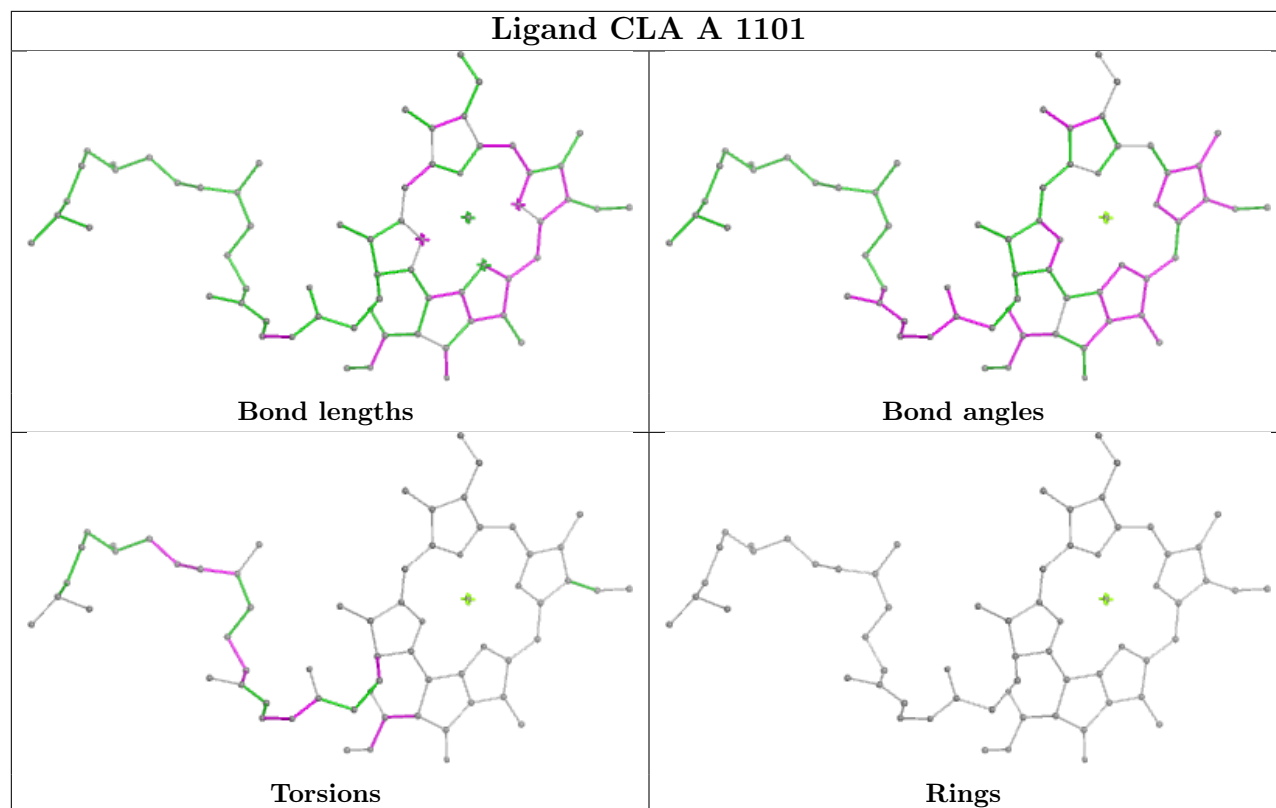


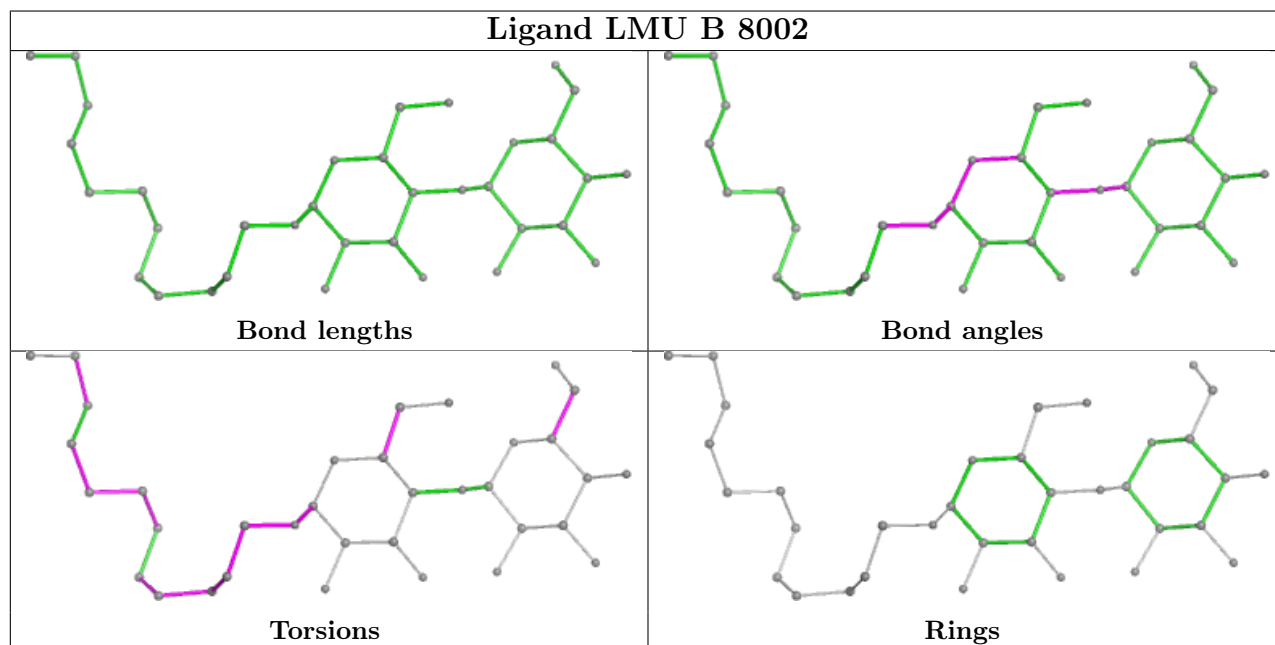
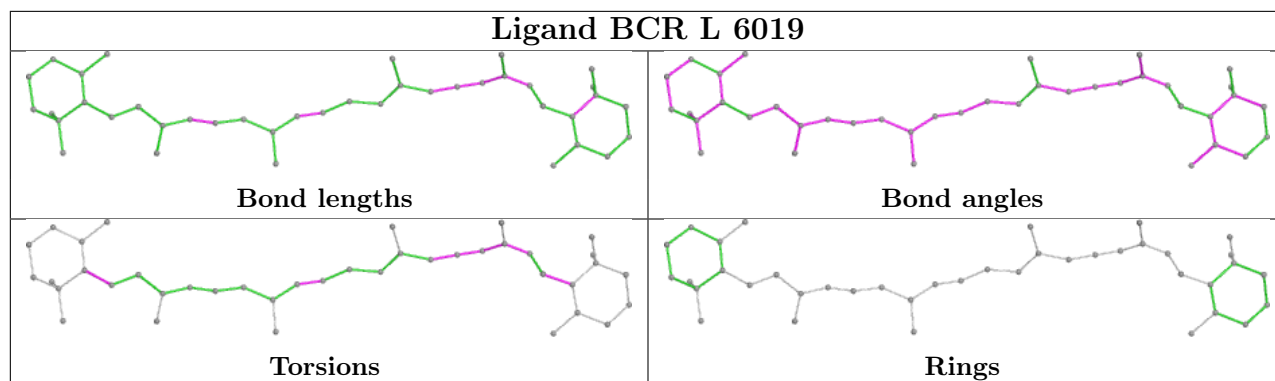


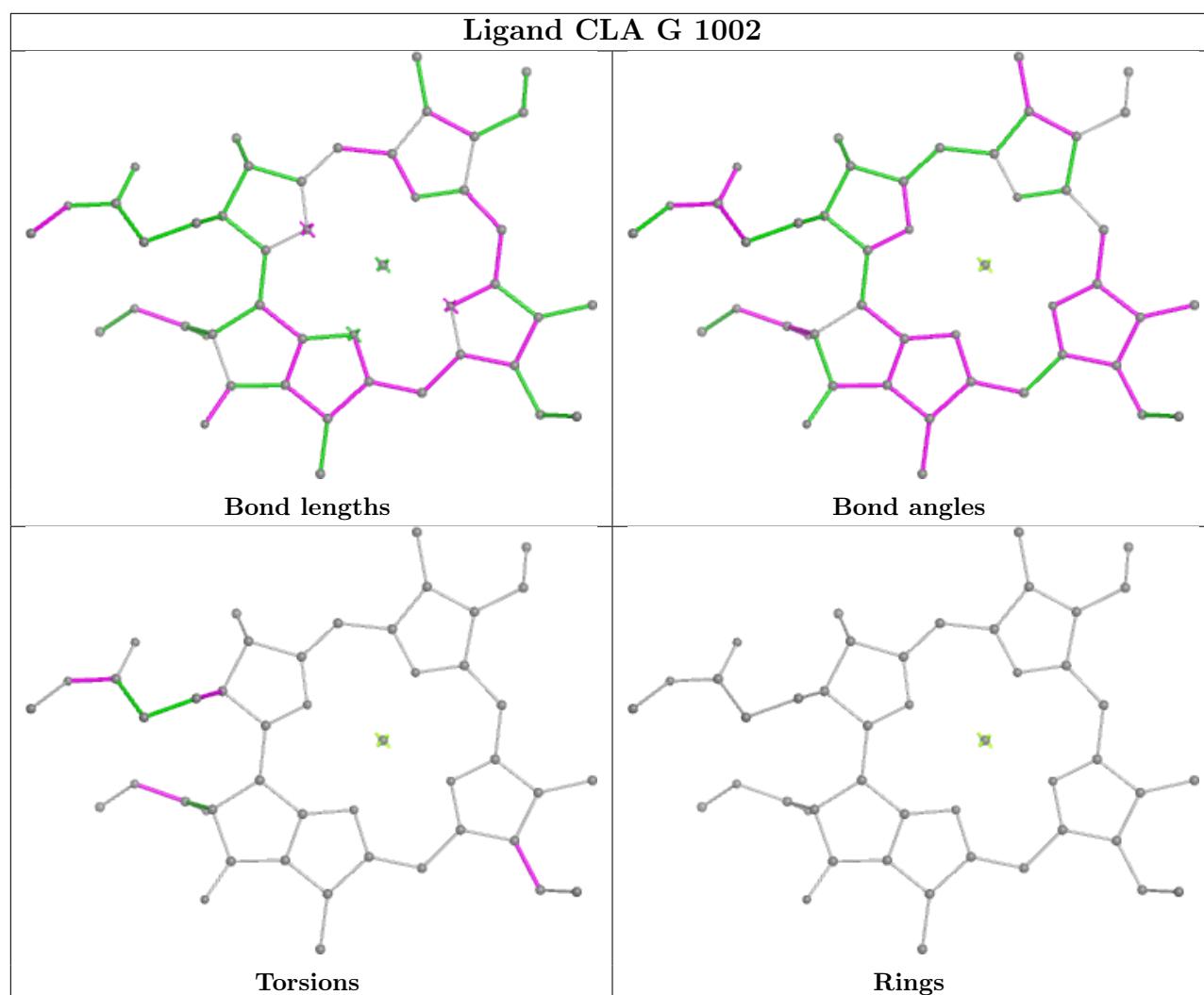


Ligand CLA B 1209

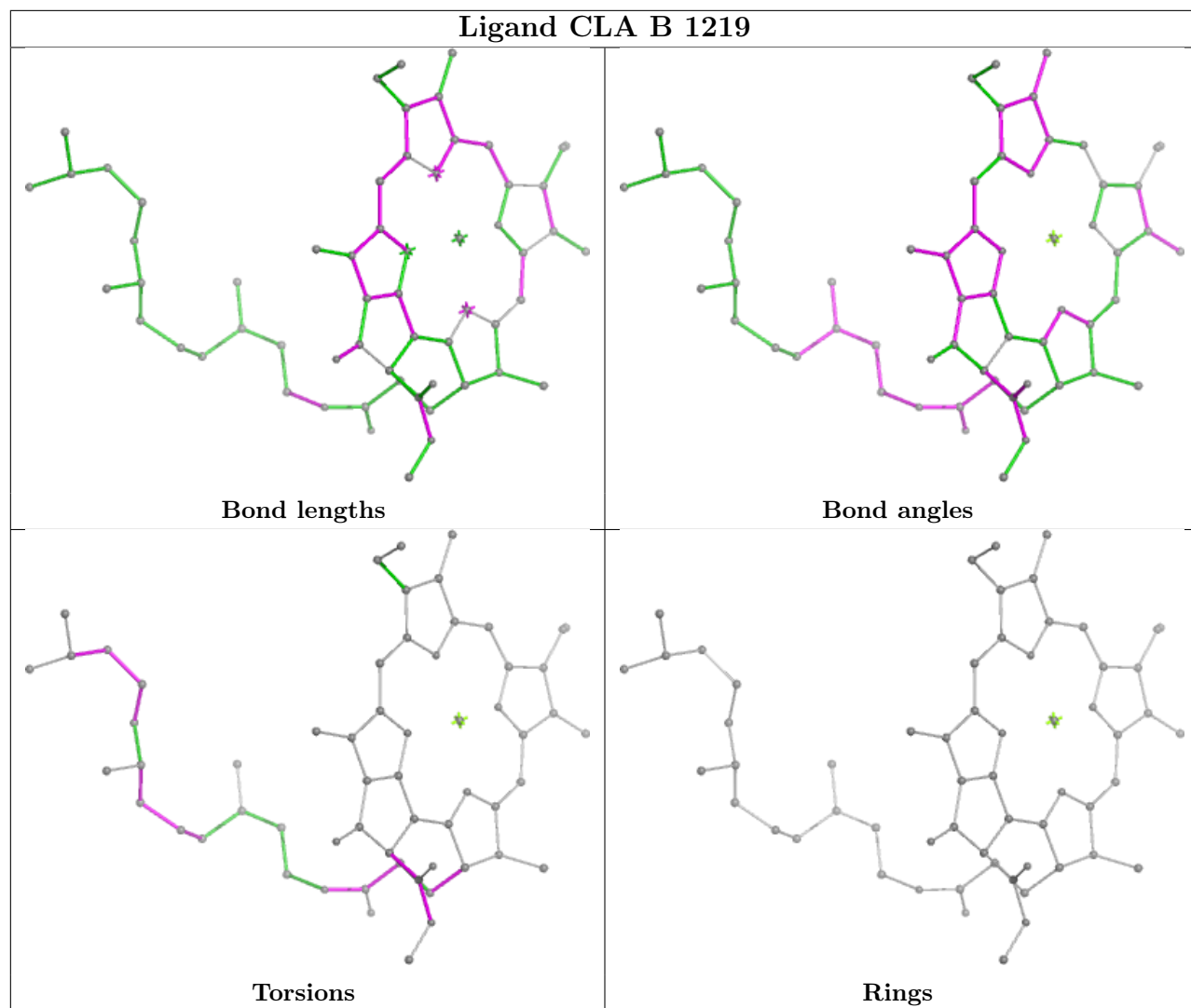


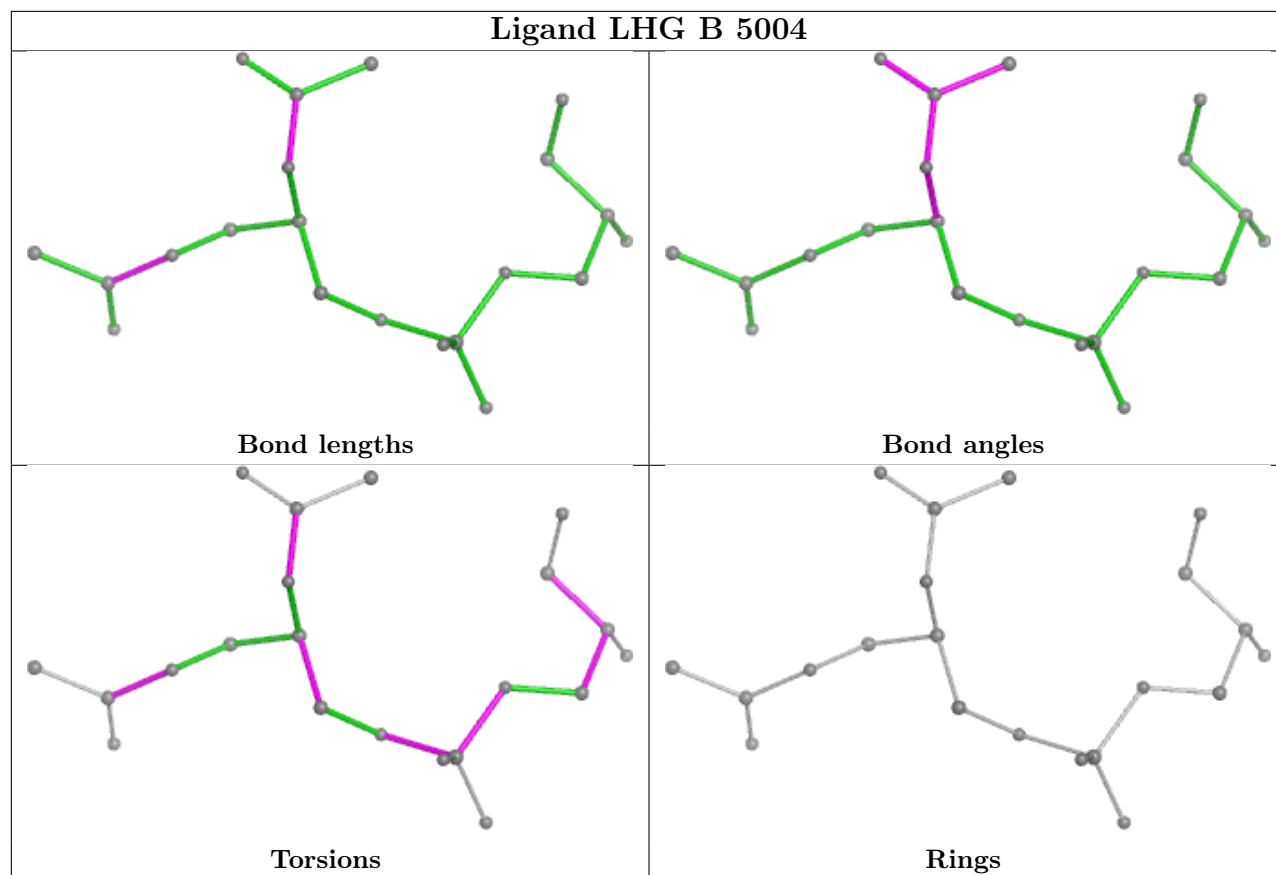




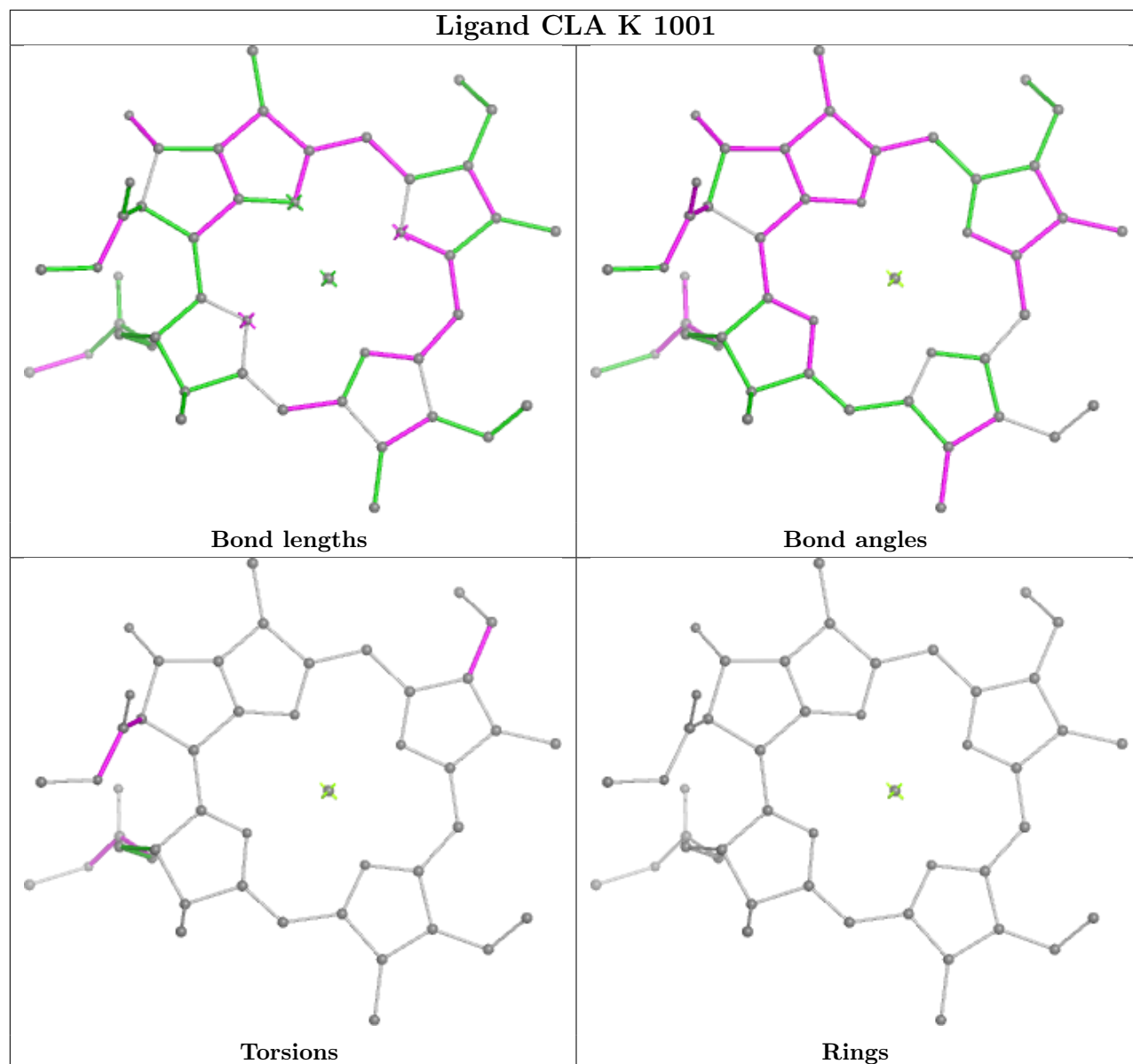


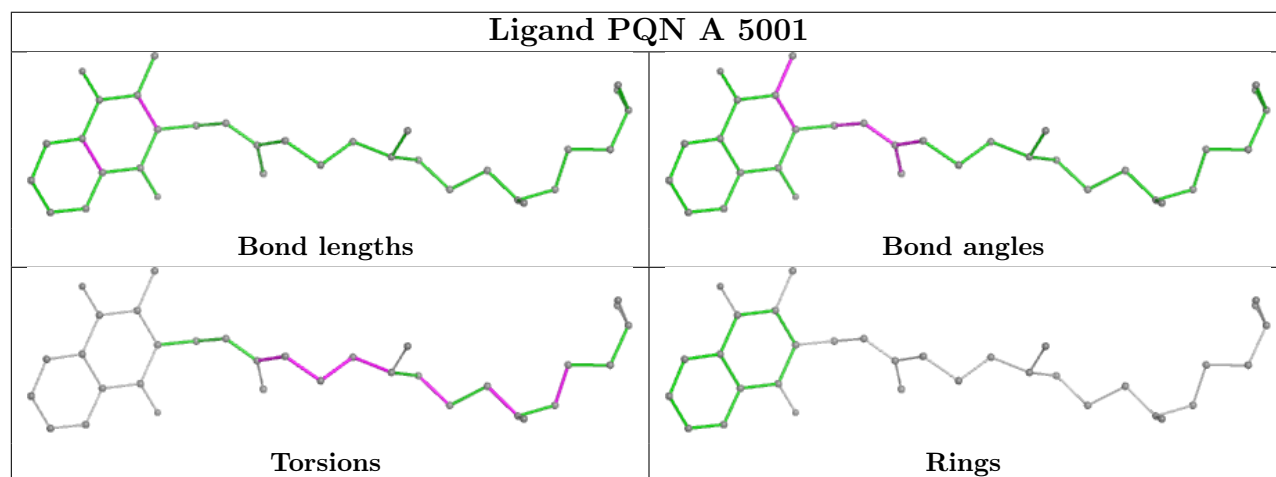
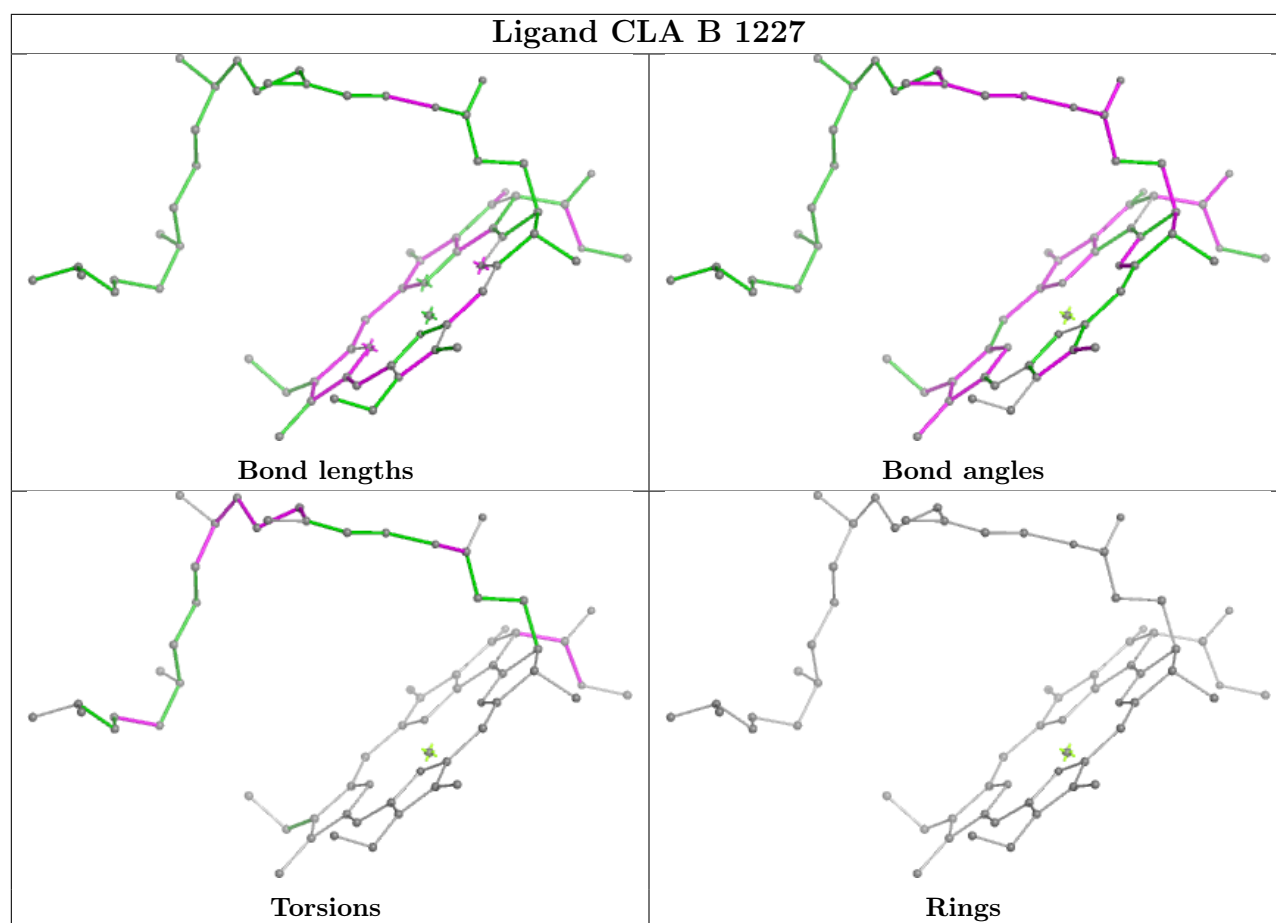
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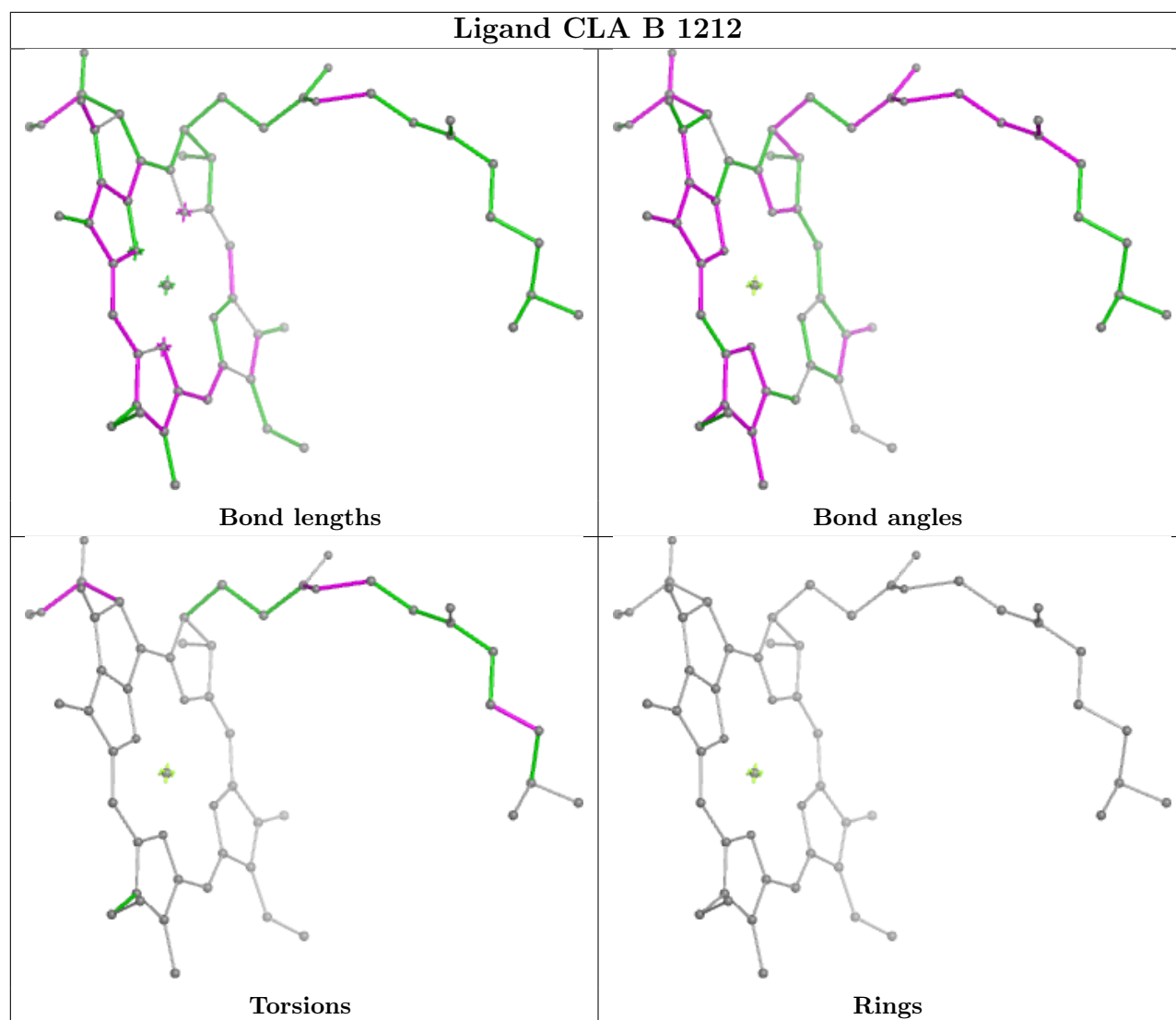
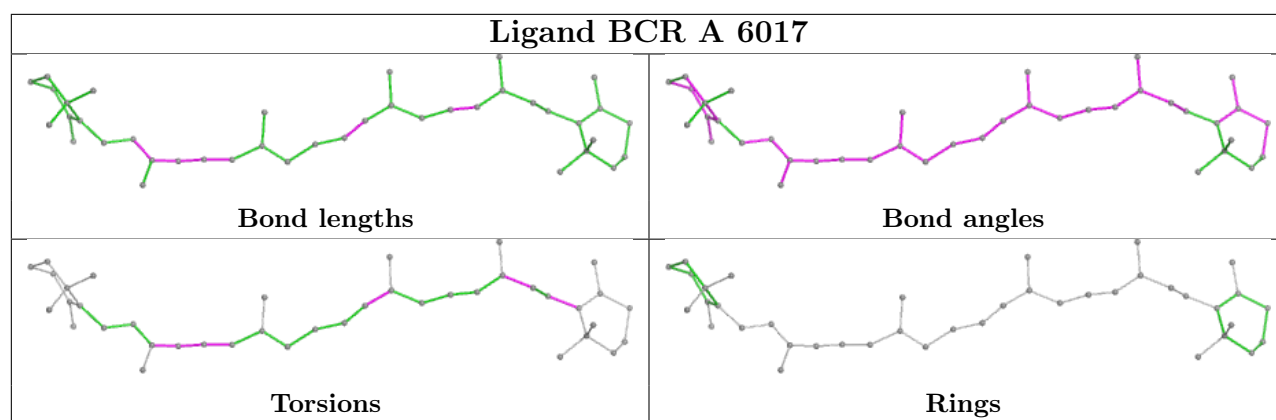


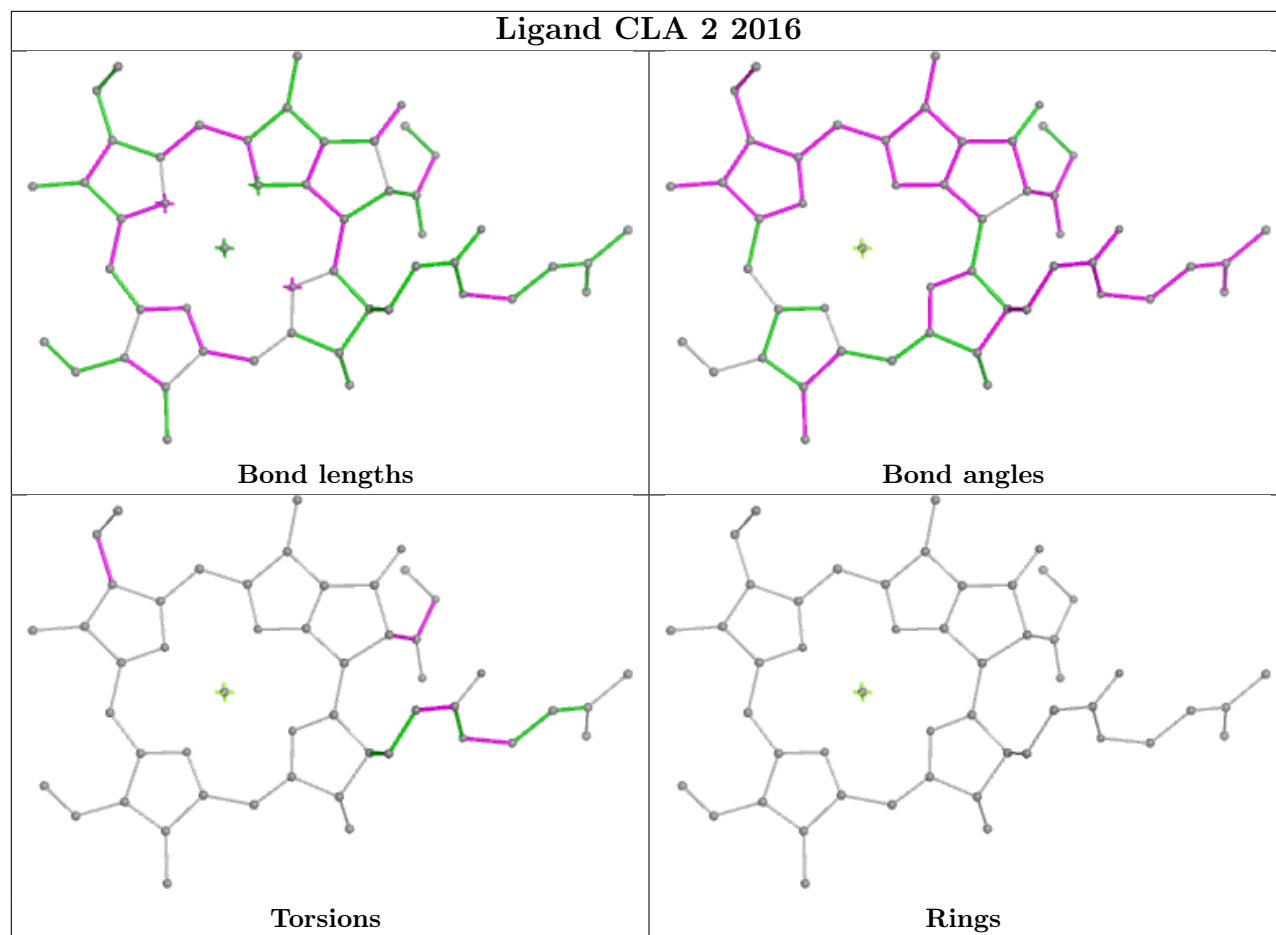


Ligand CLA K 1001

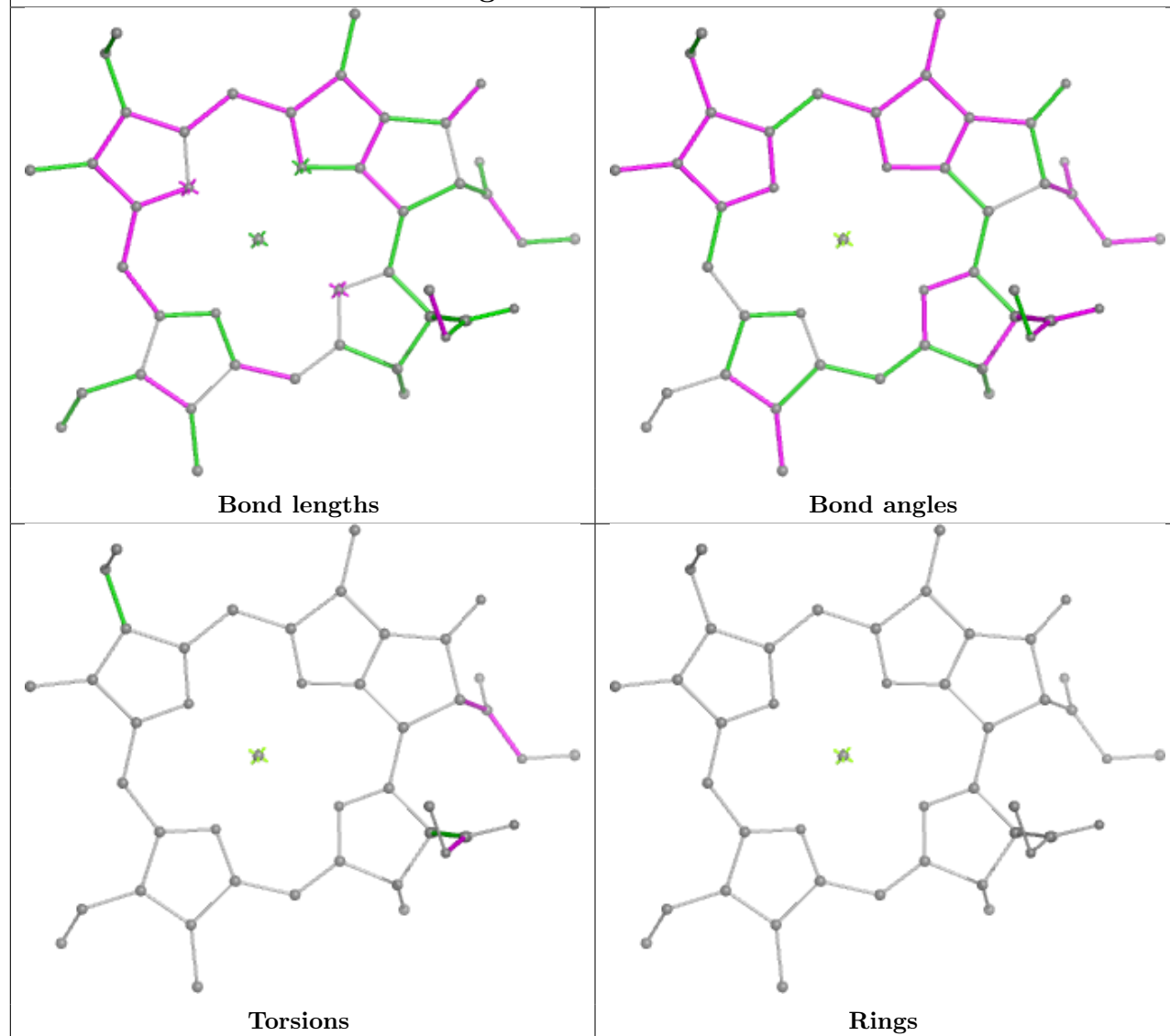




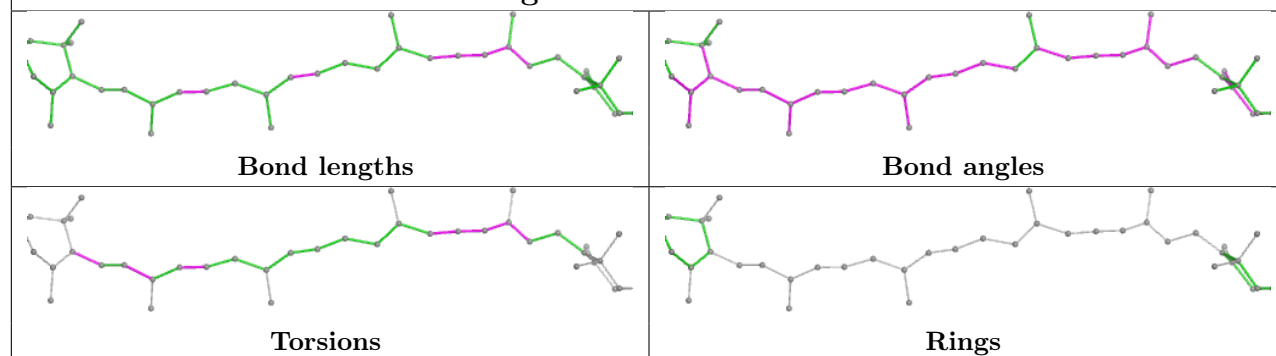


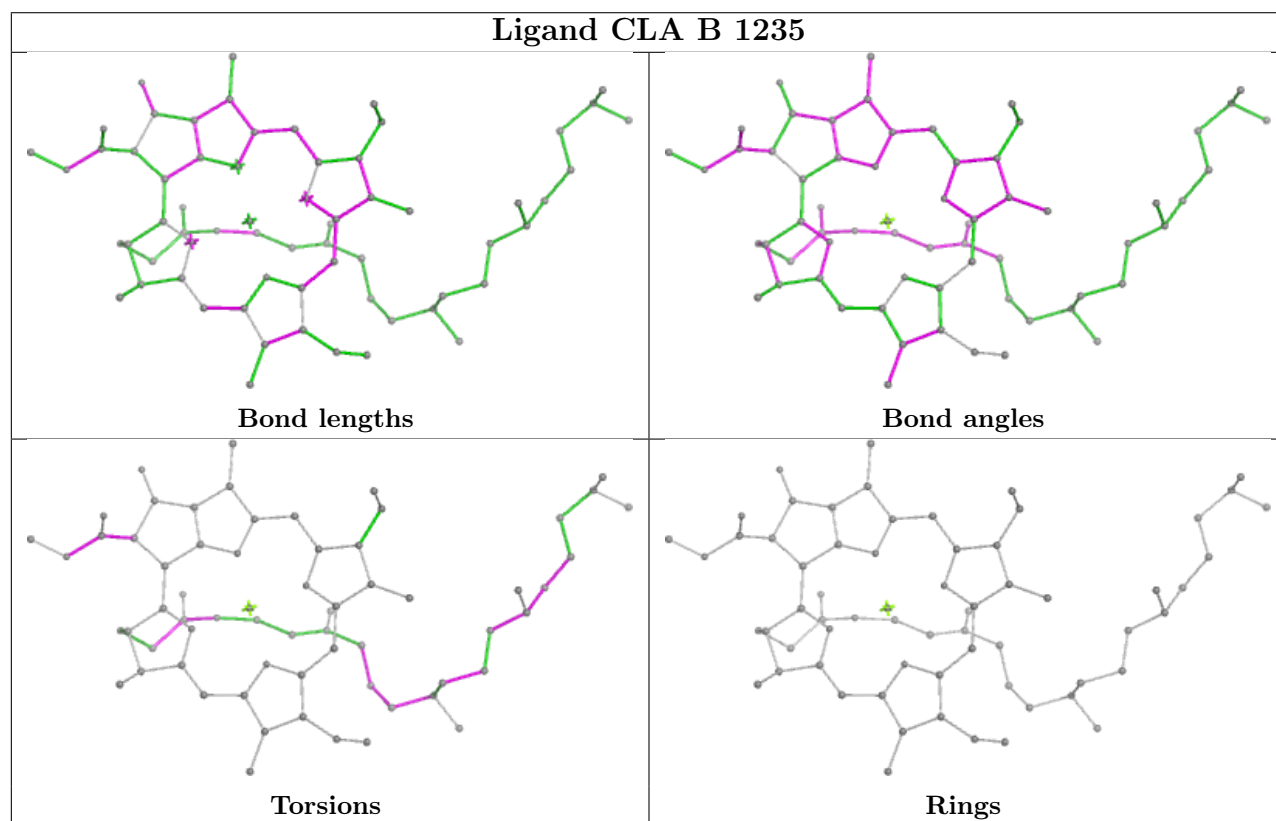
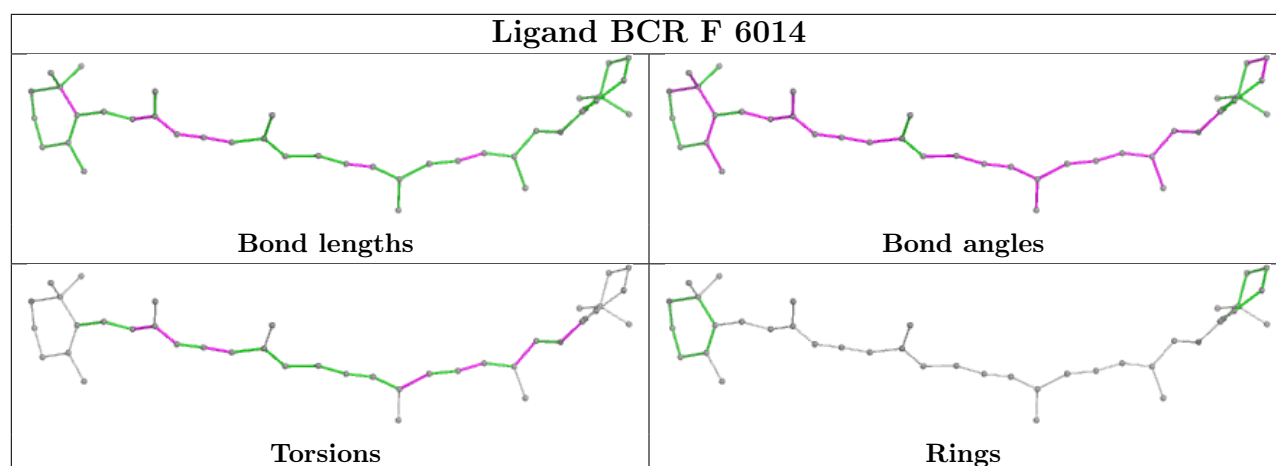


Ligand CLA A 1108

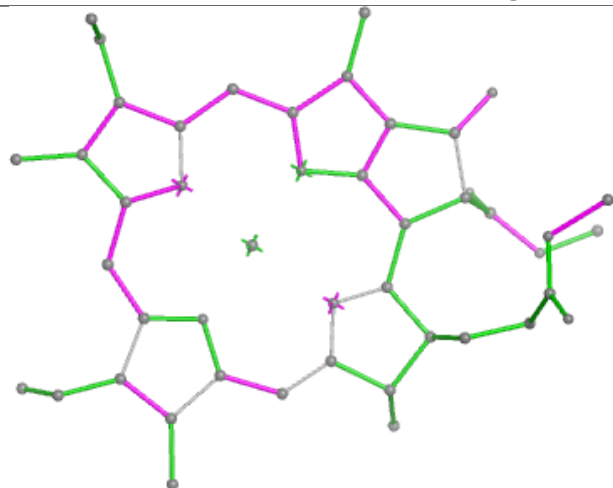


Ligand BCR A 6002

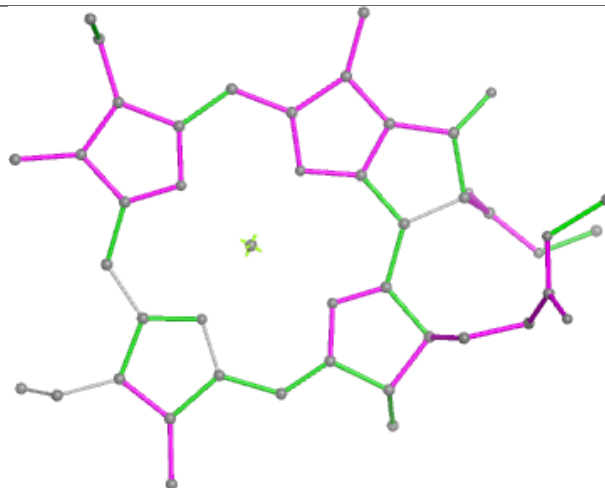




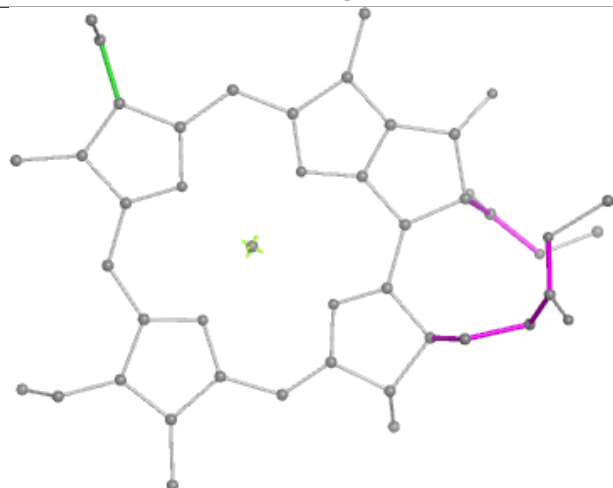
Ligand CLA A 1113



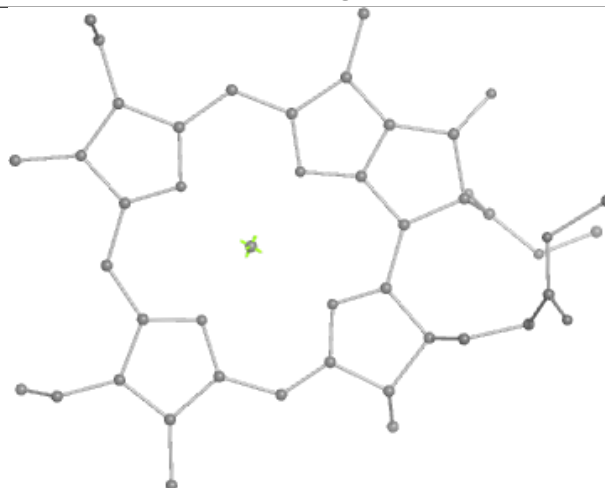
Bond lengths



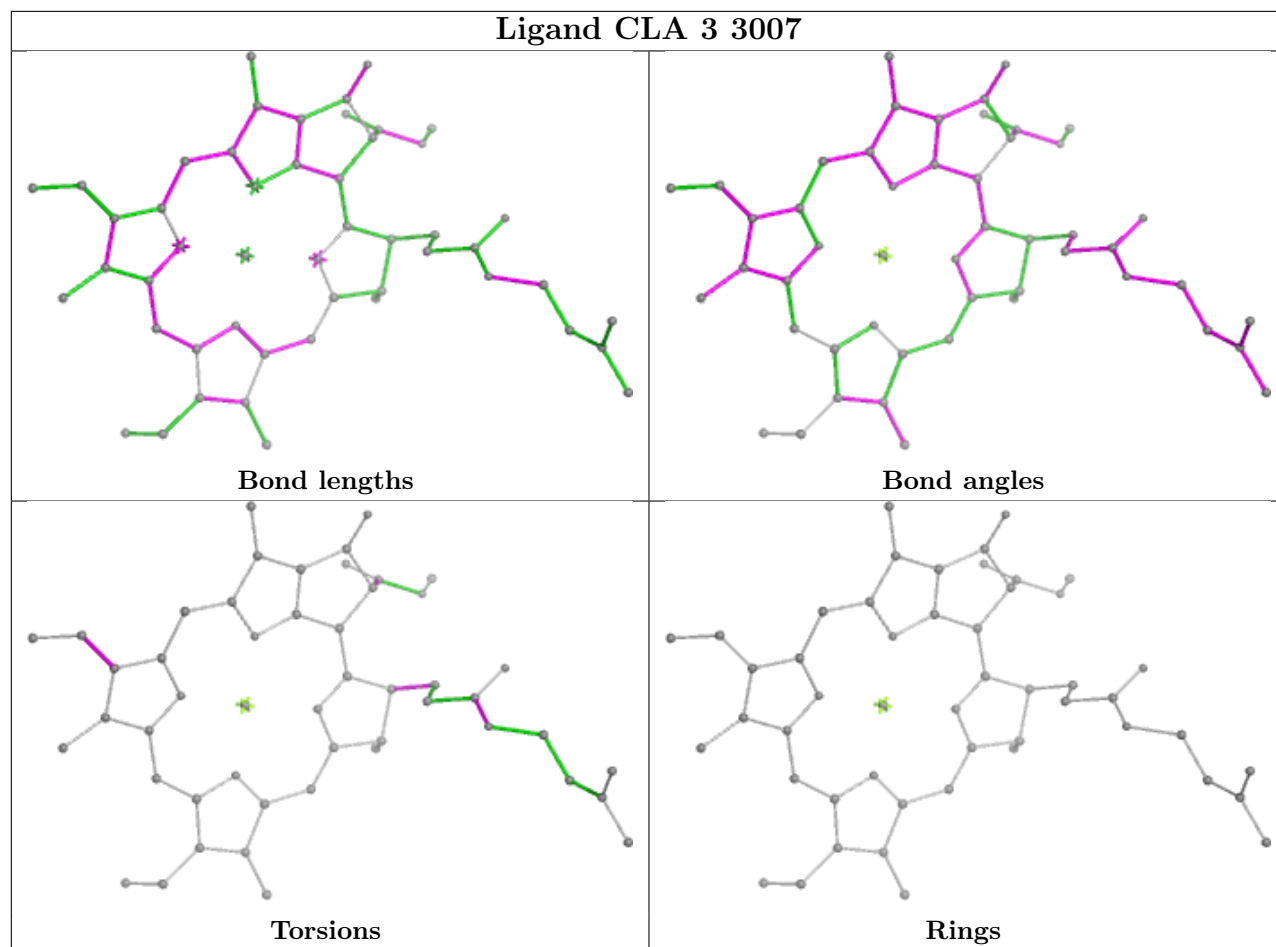
Bond angles

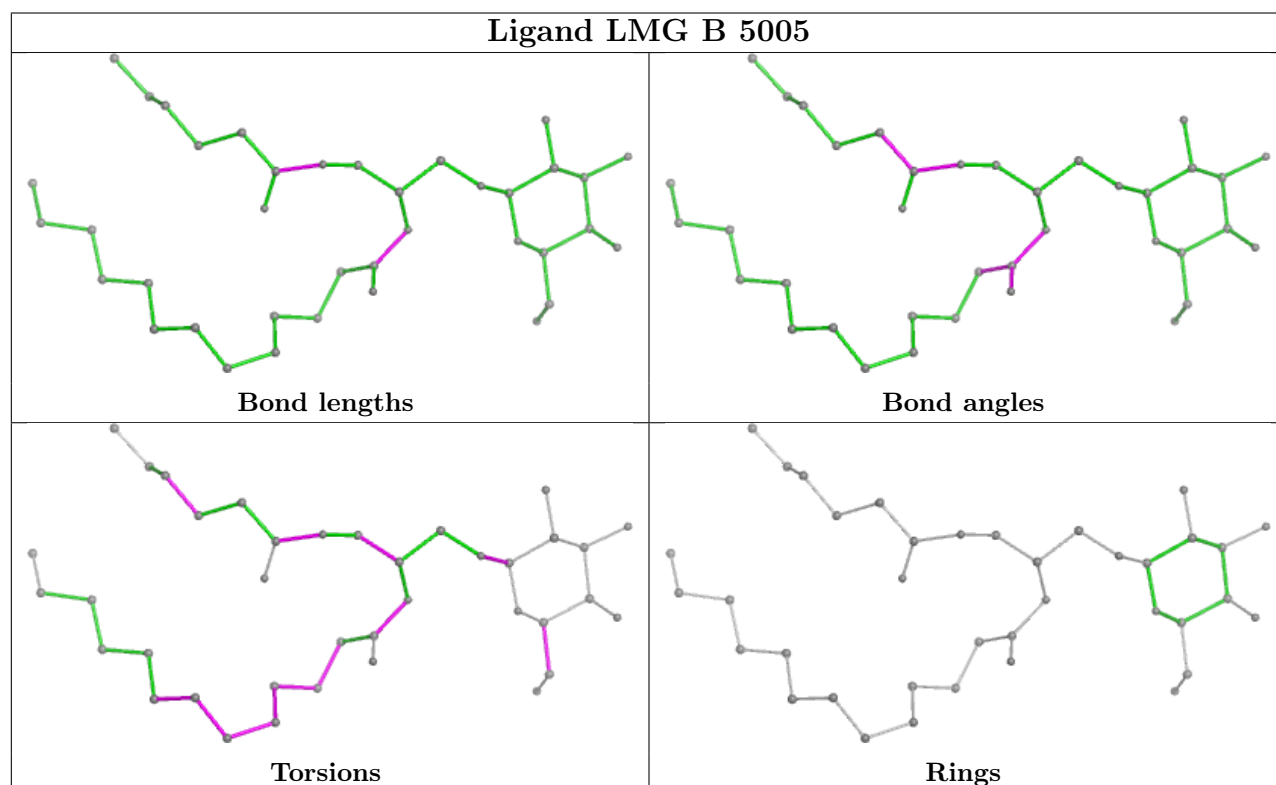
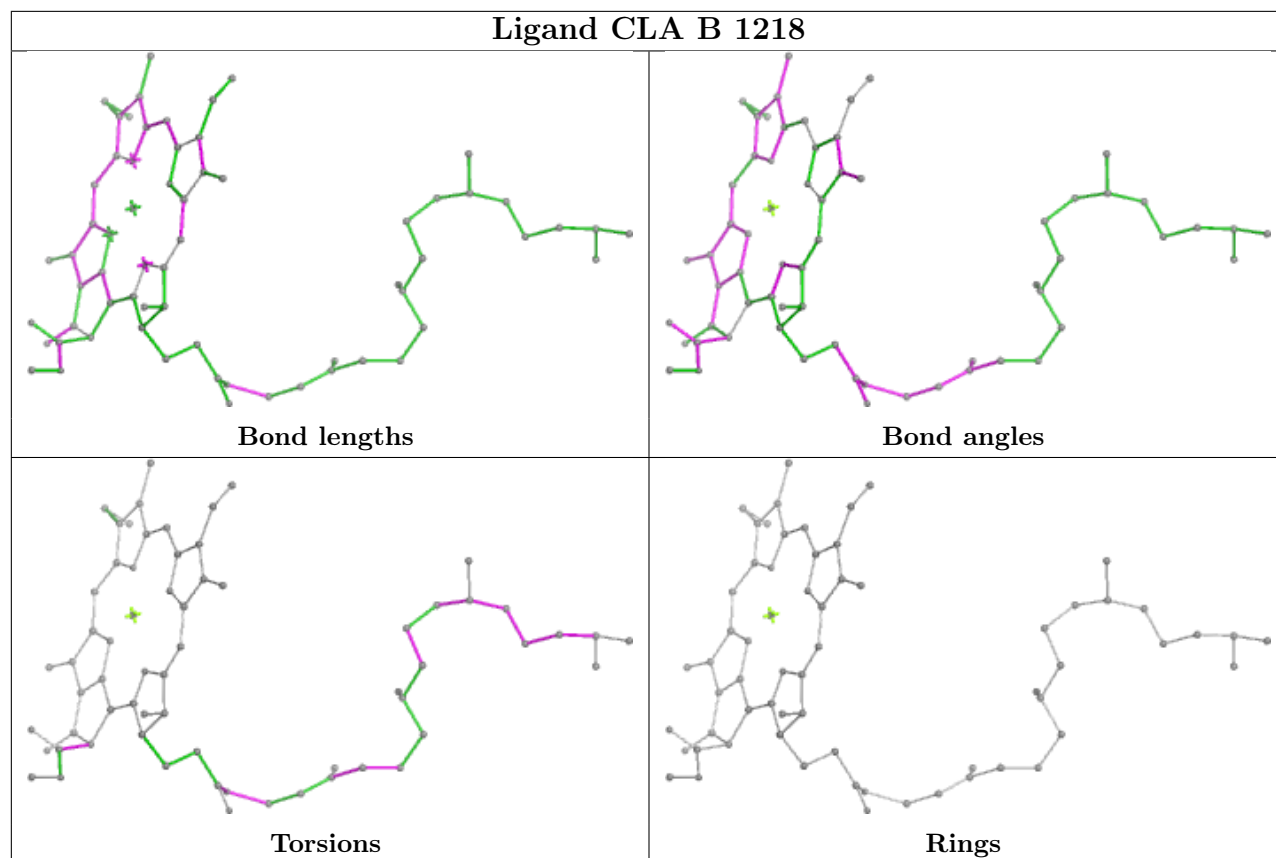


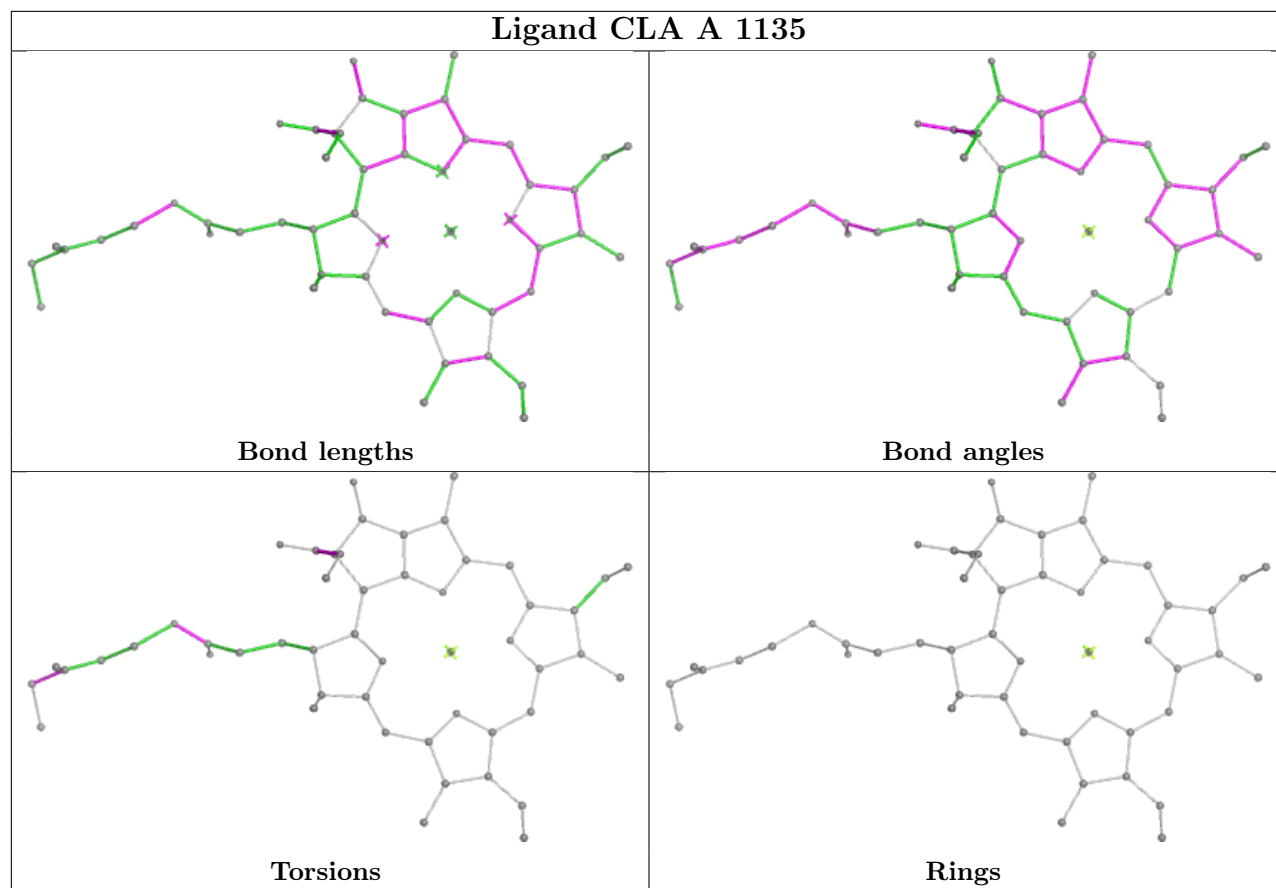
Torsions

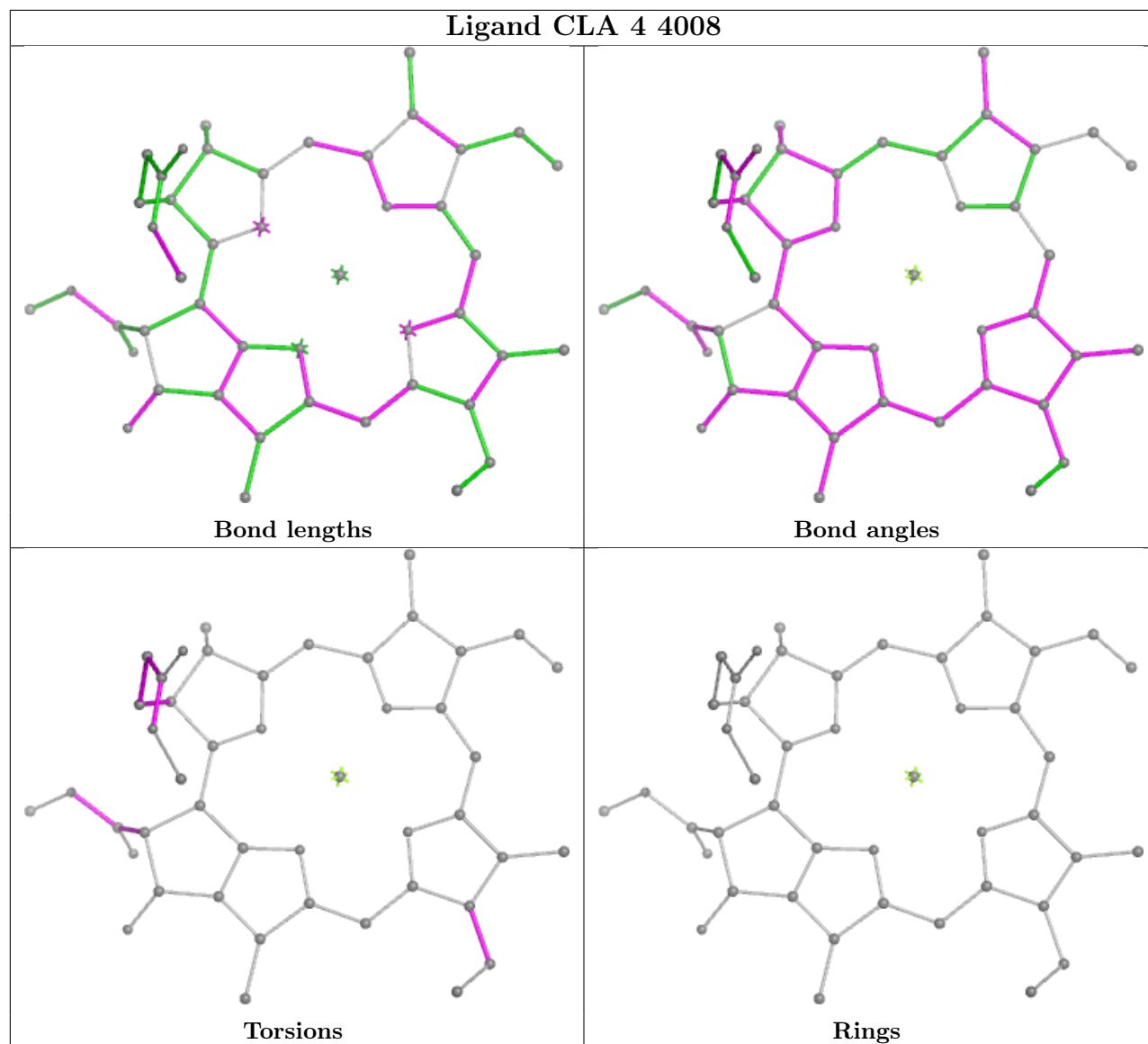


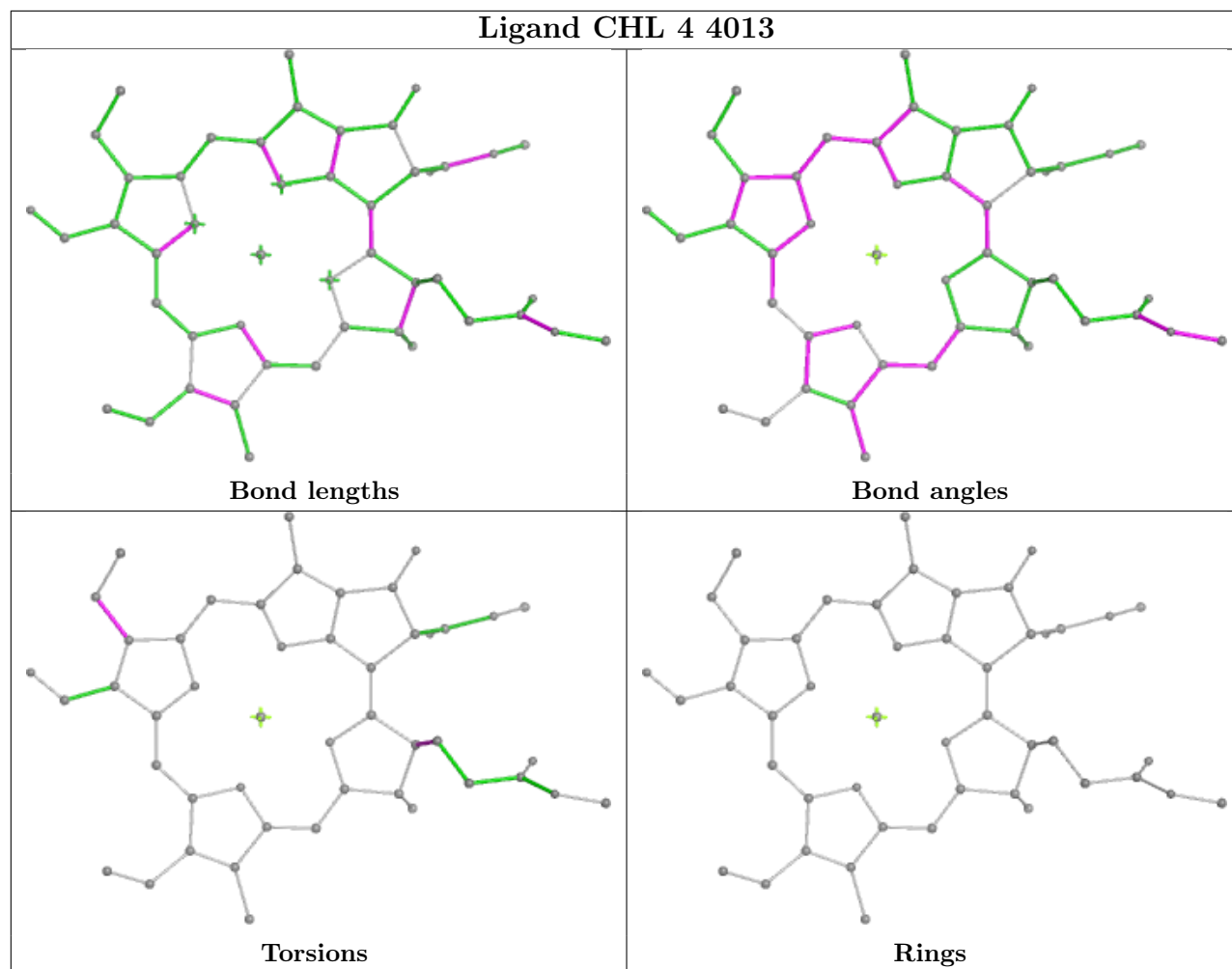
Rings

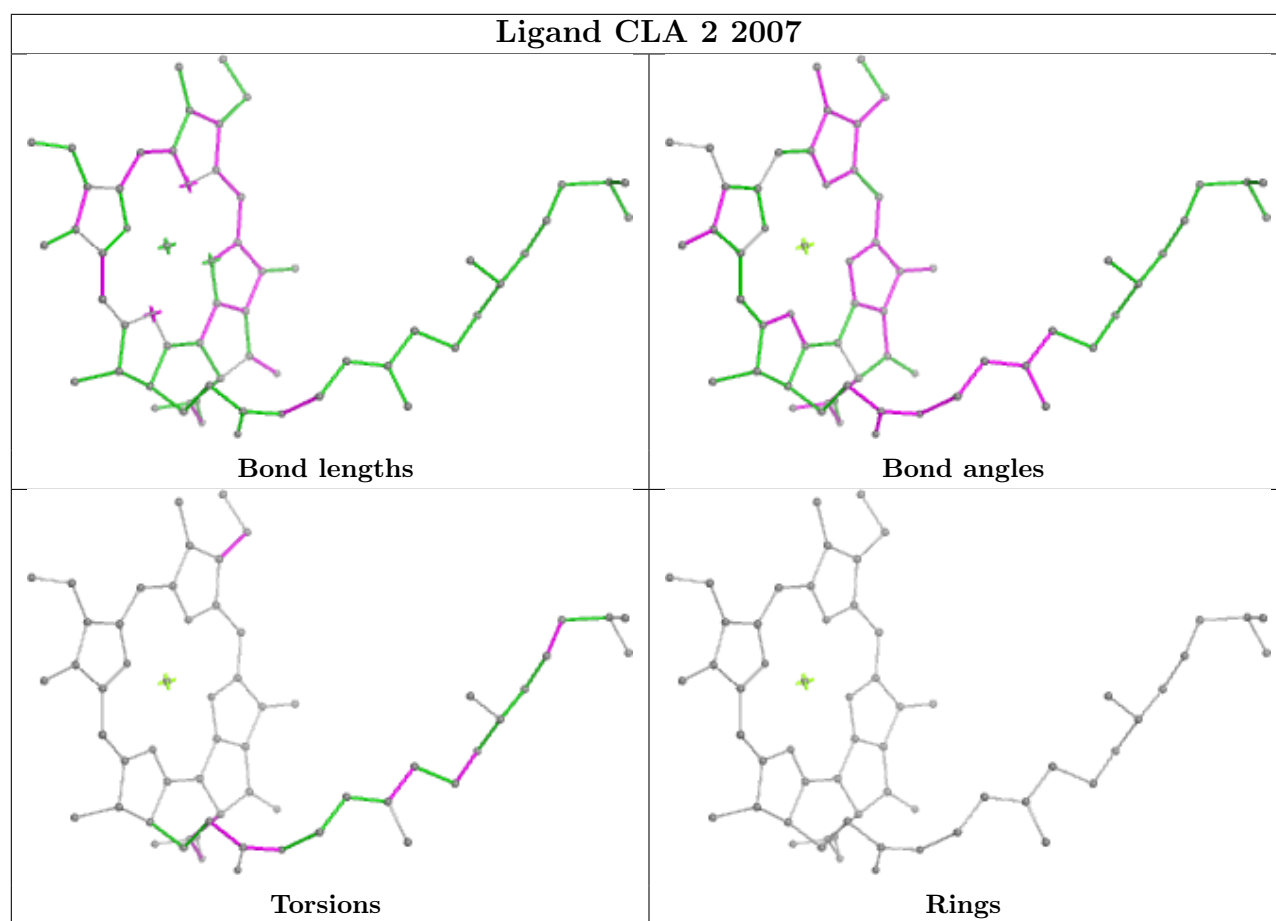




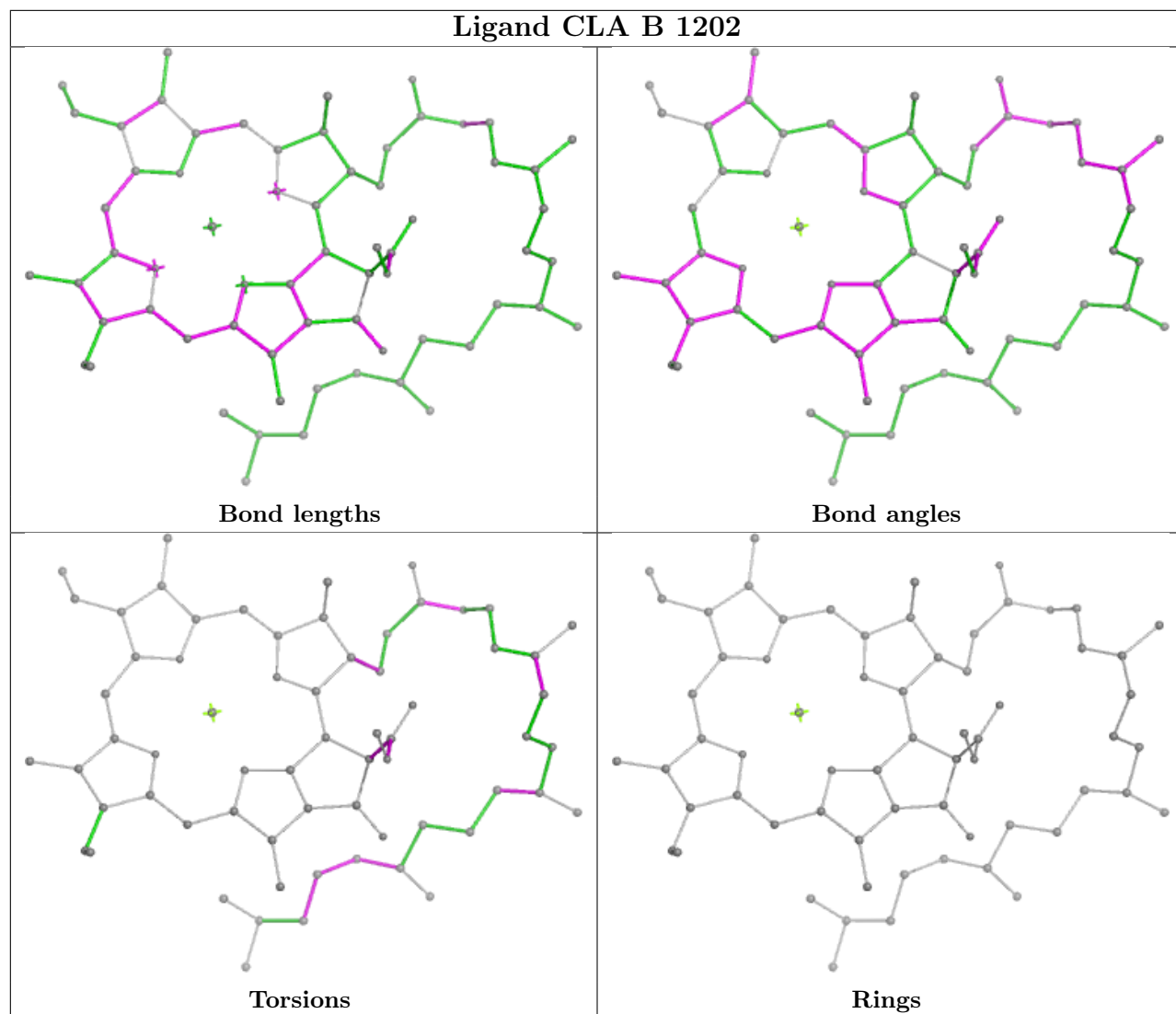




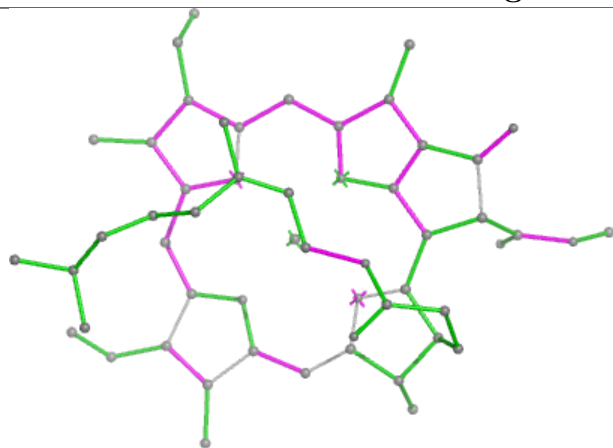




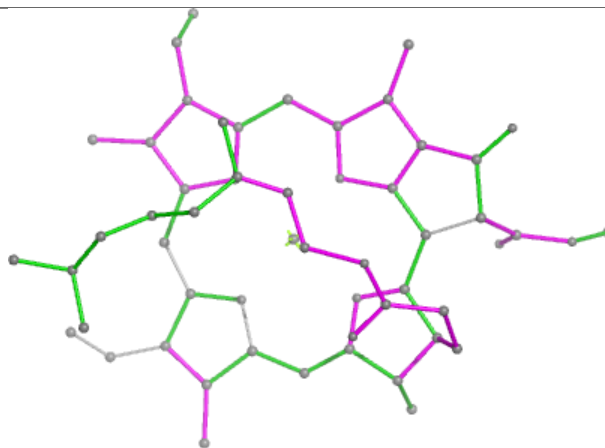
Ligand CLA B 1202



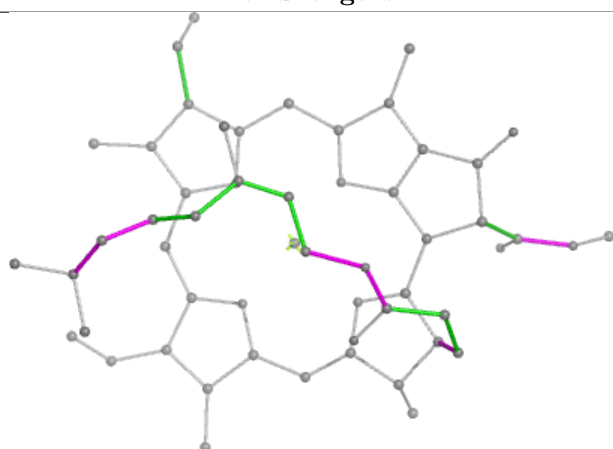
Ligand CLA A 1110



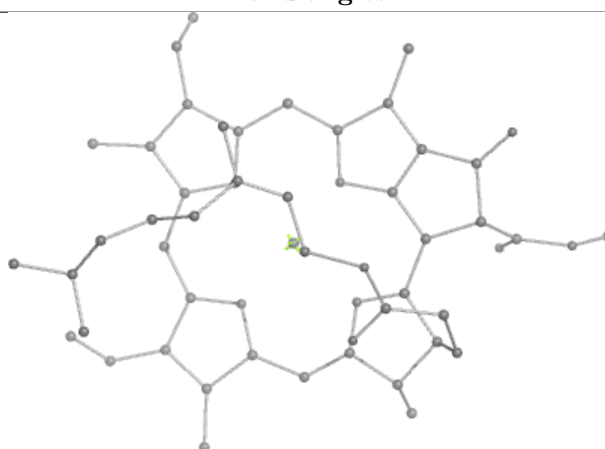
Bond lengths



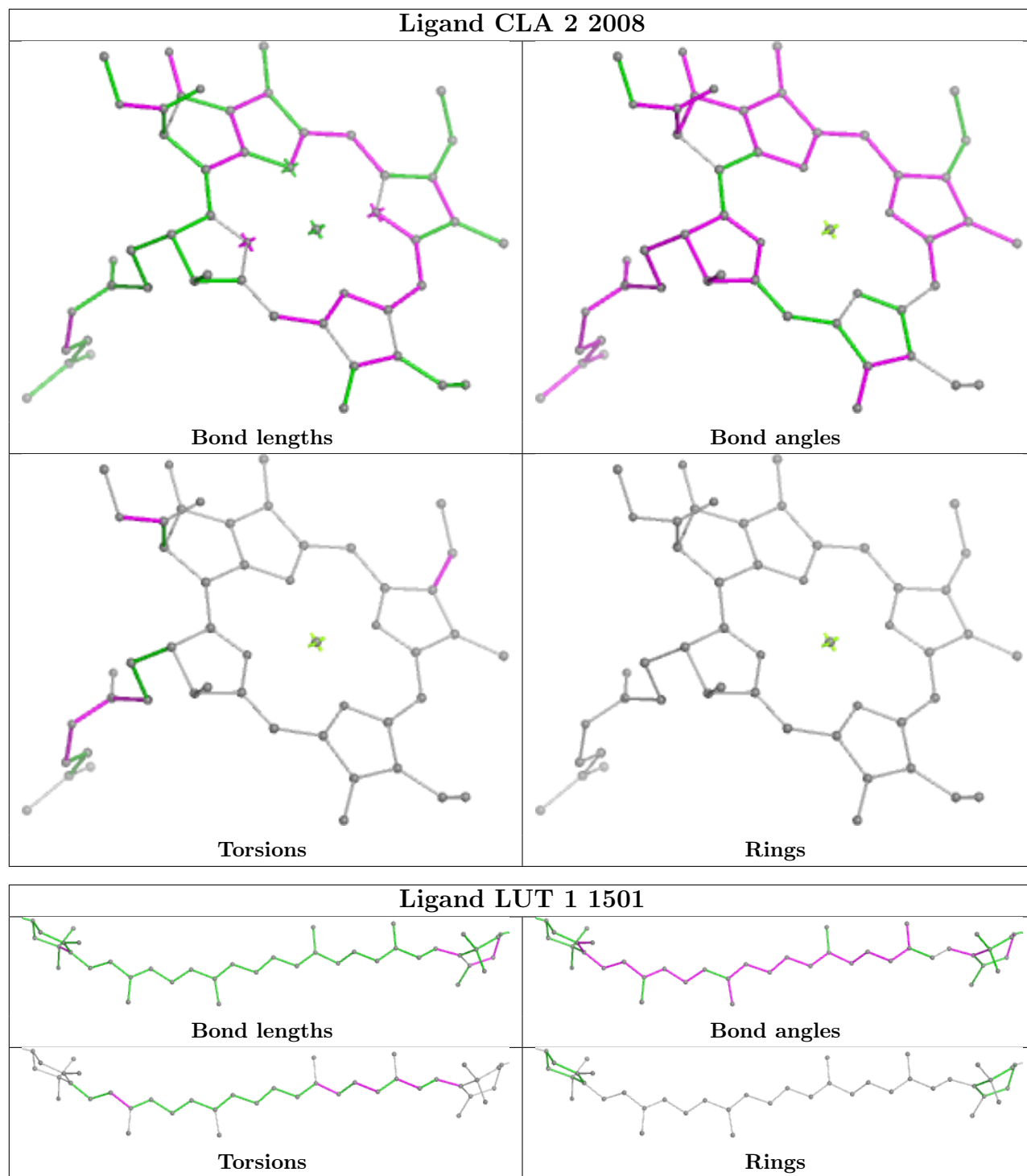
Bond angles

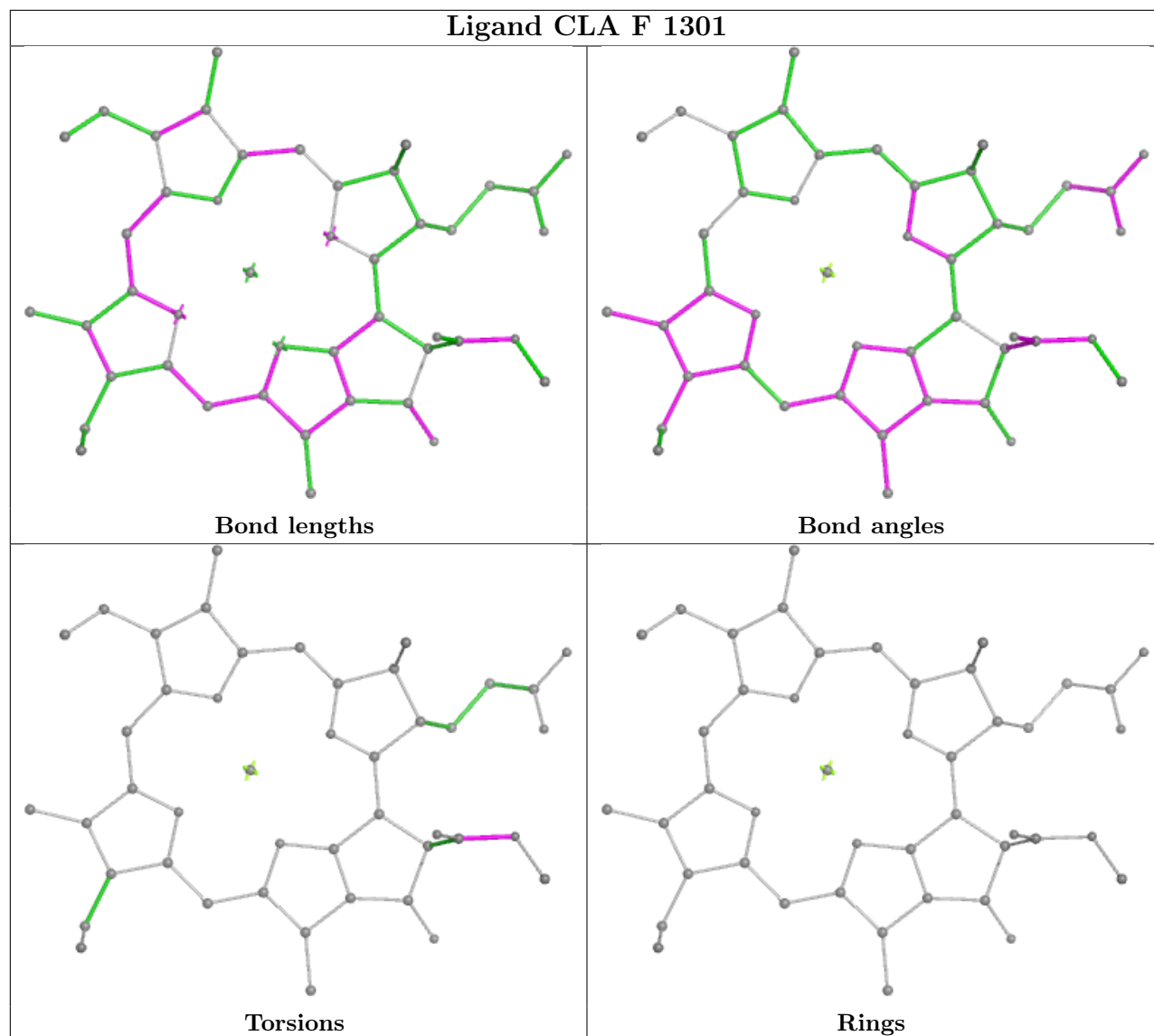


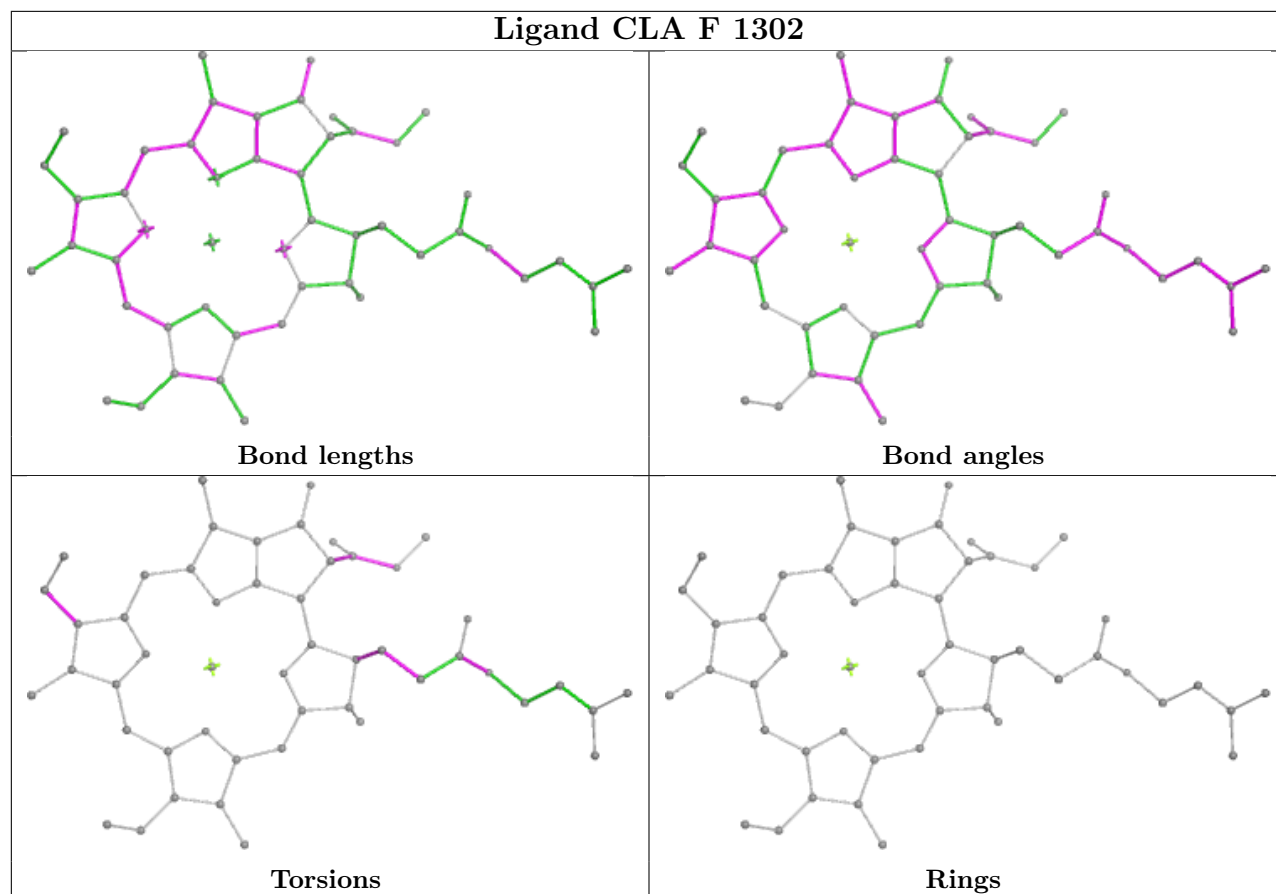
Torsions

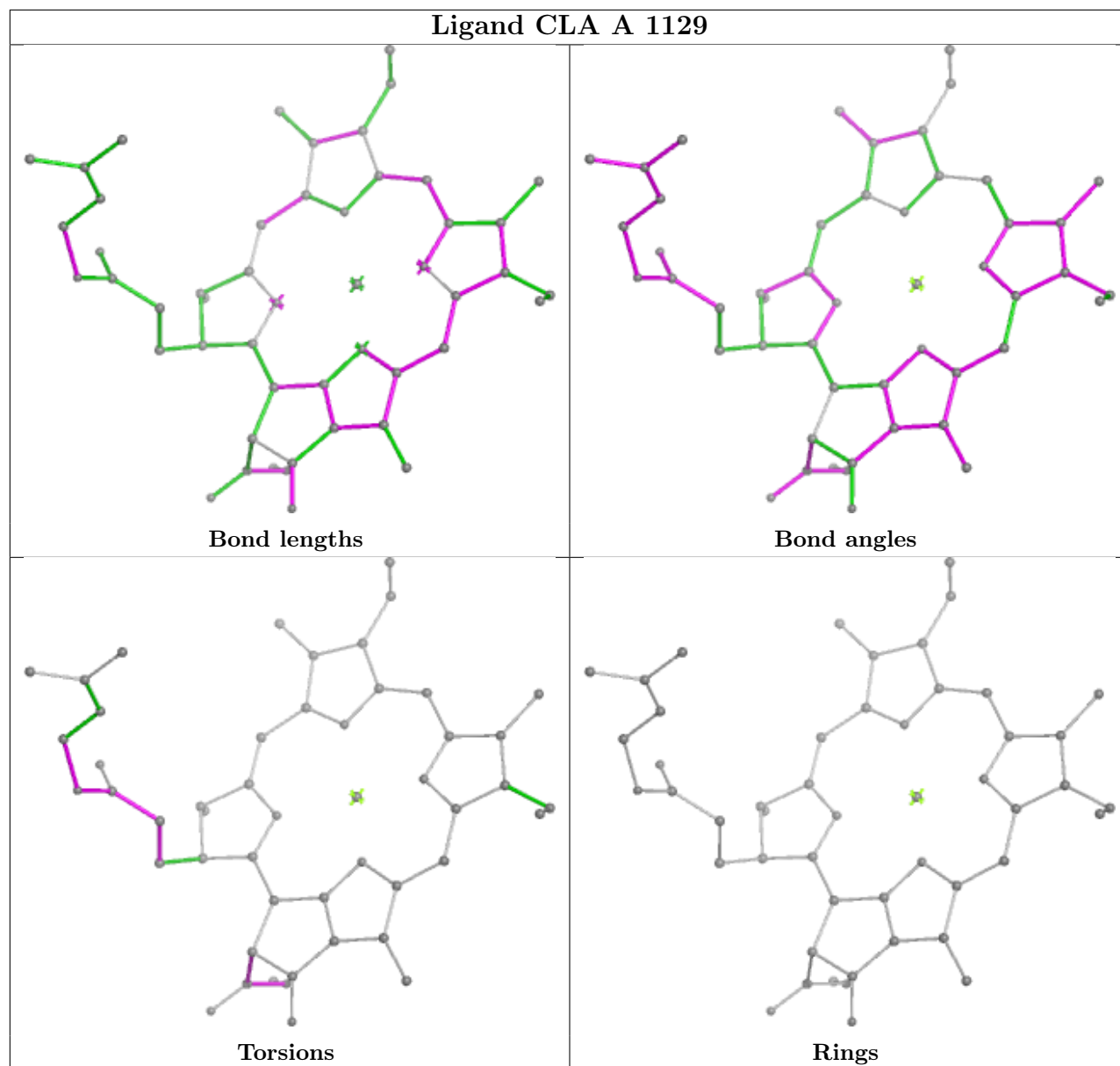


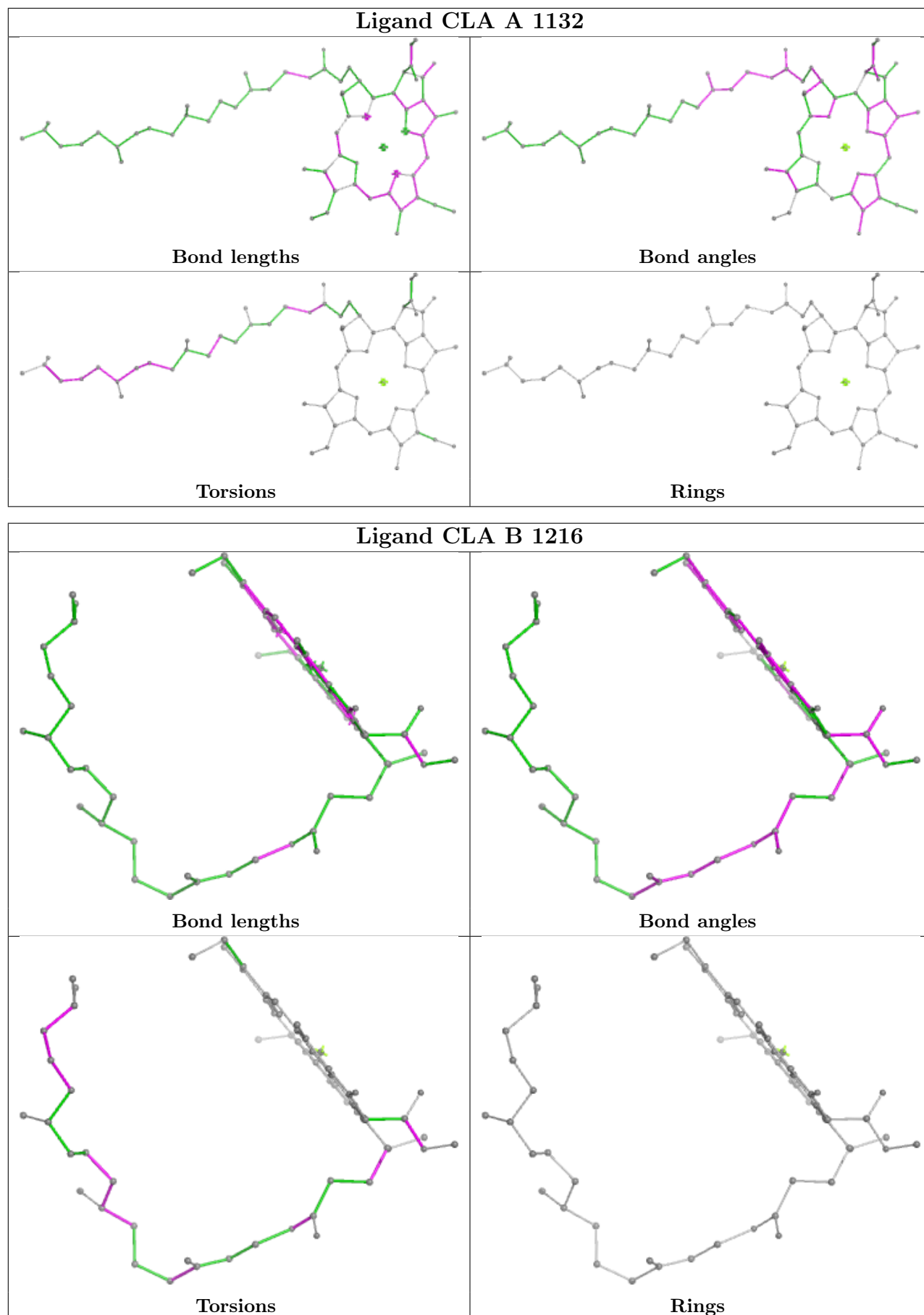
Rings

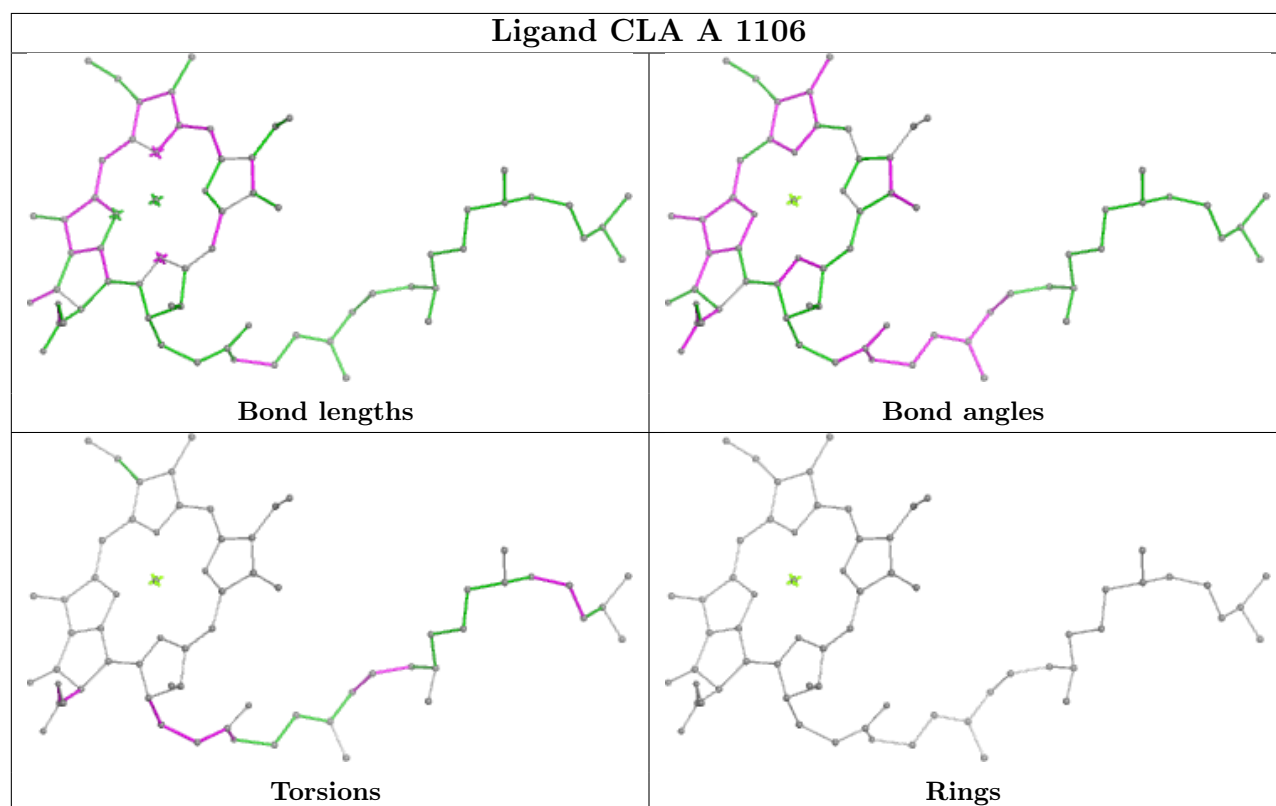
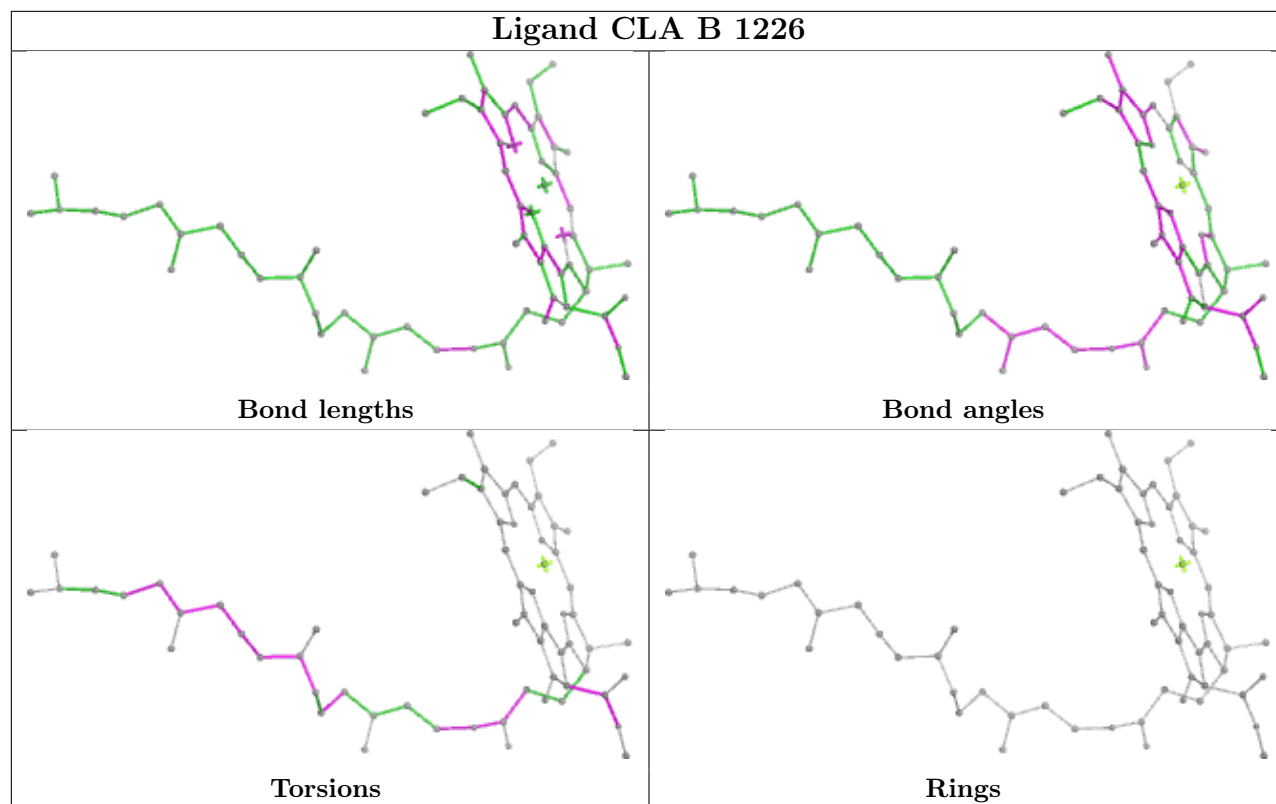


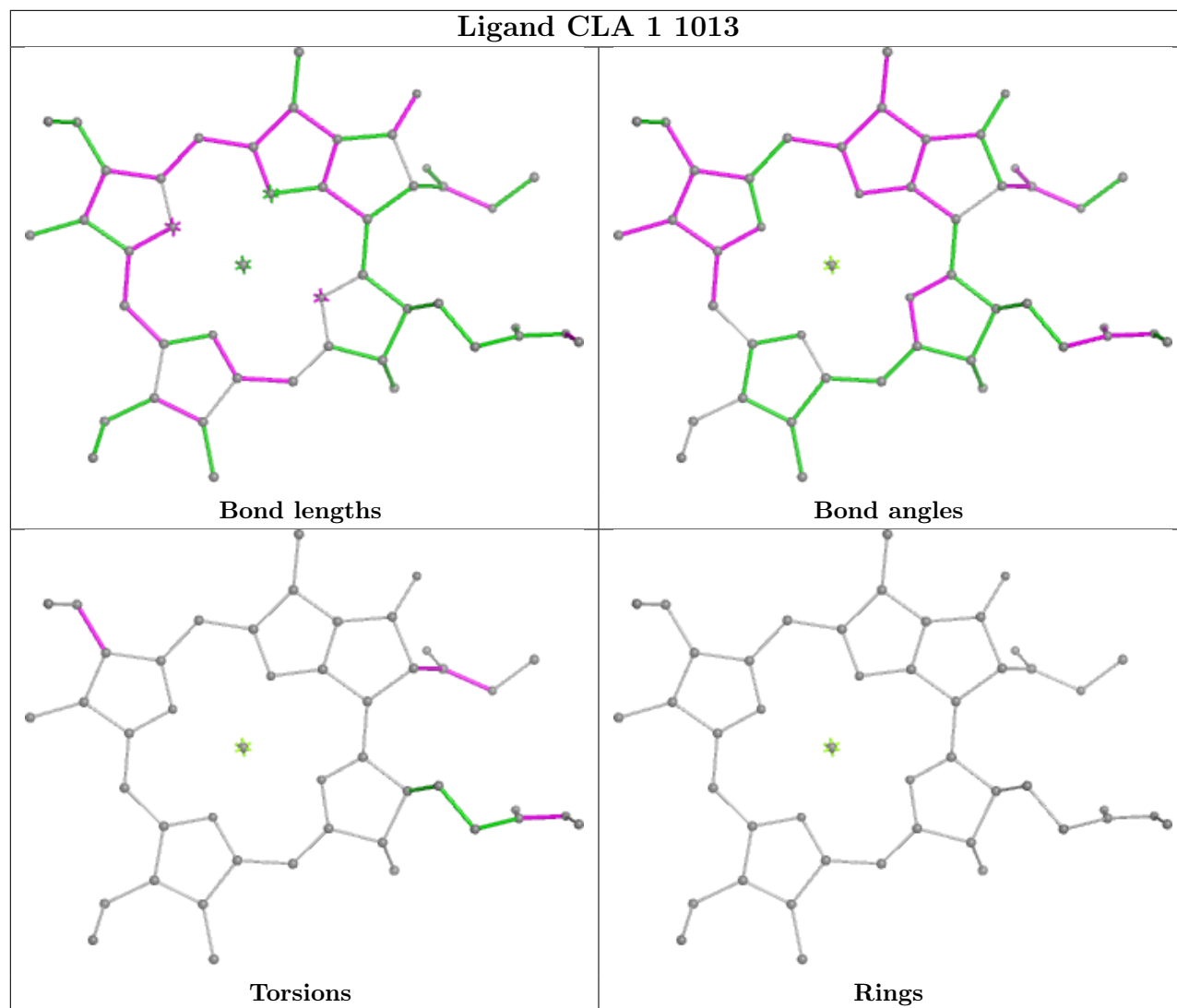


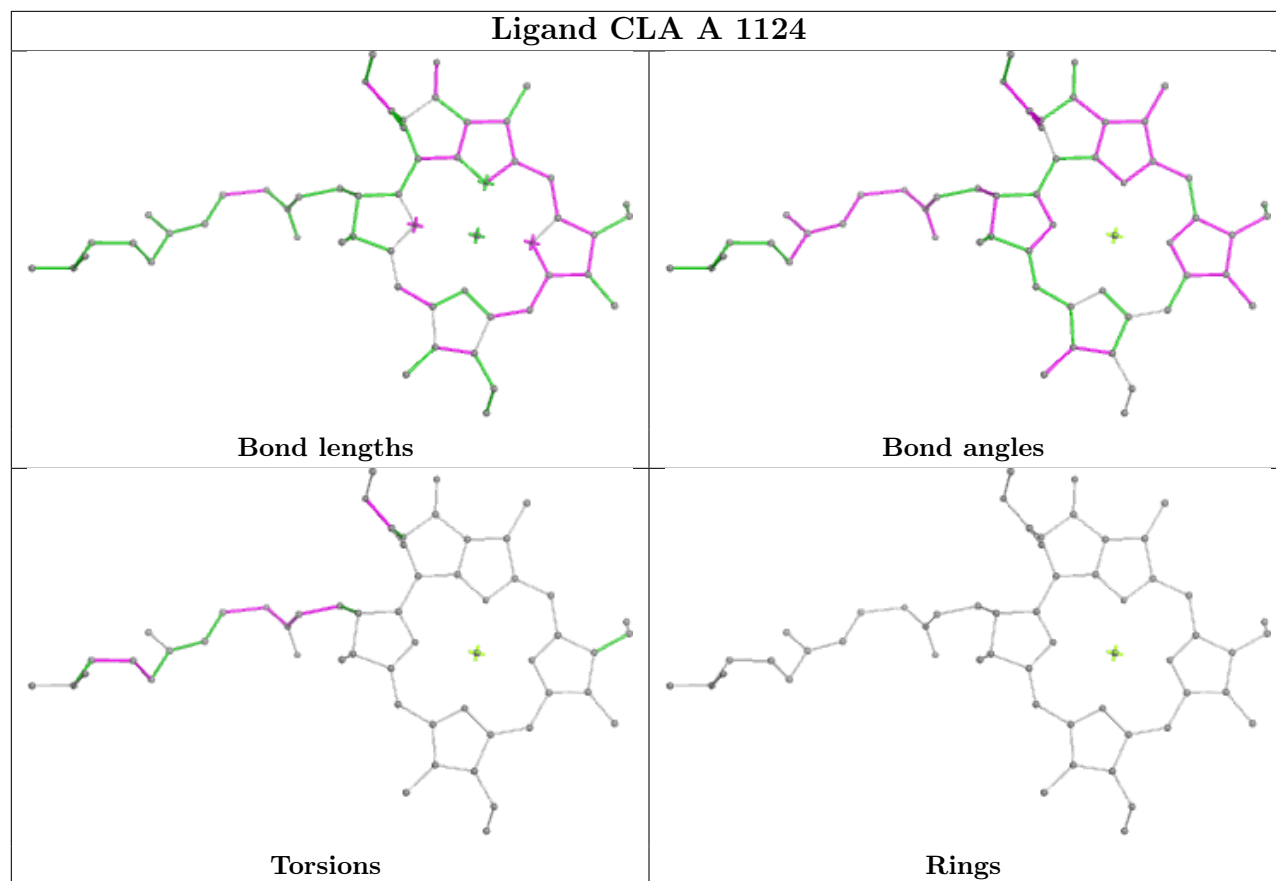


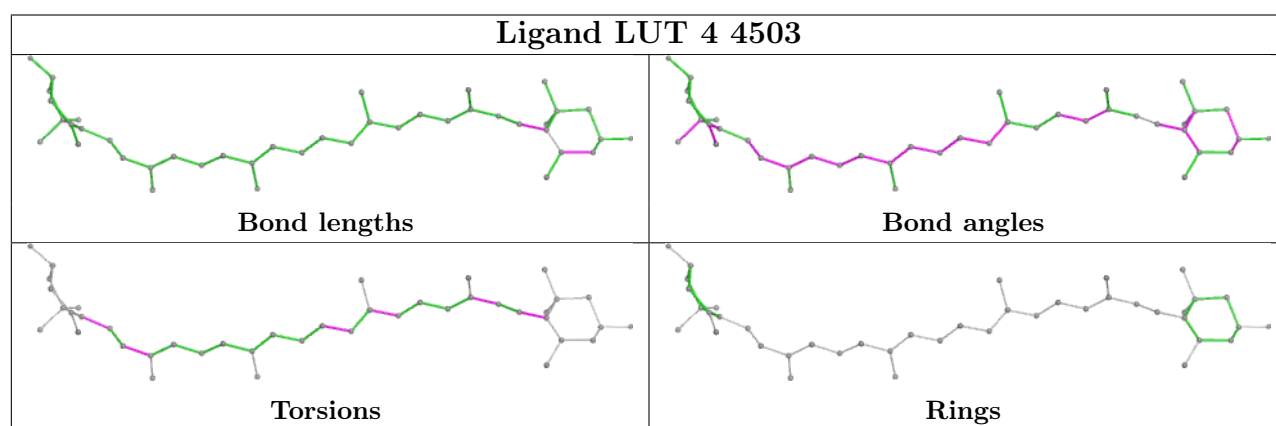
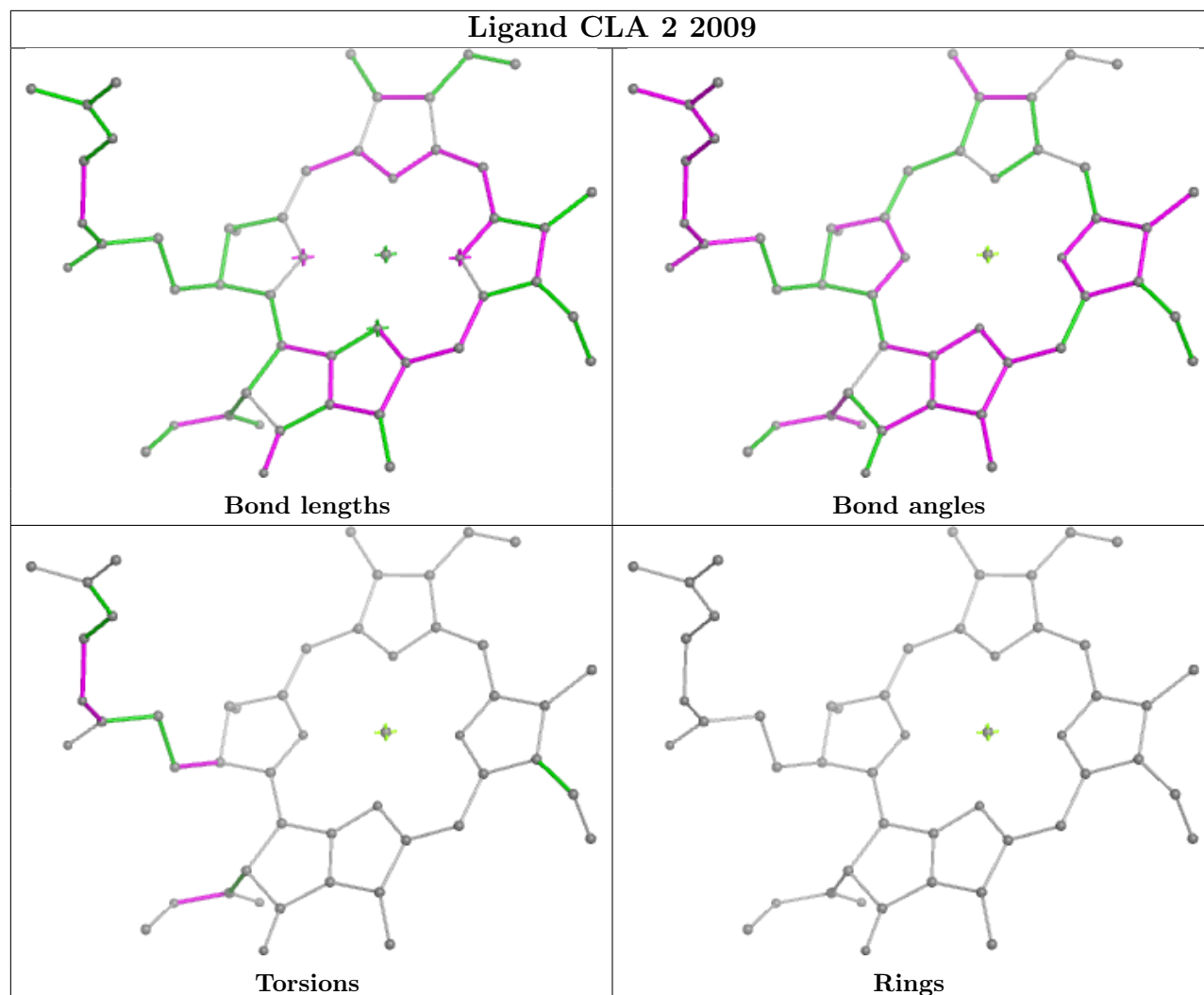




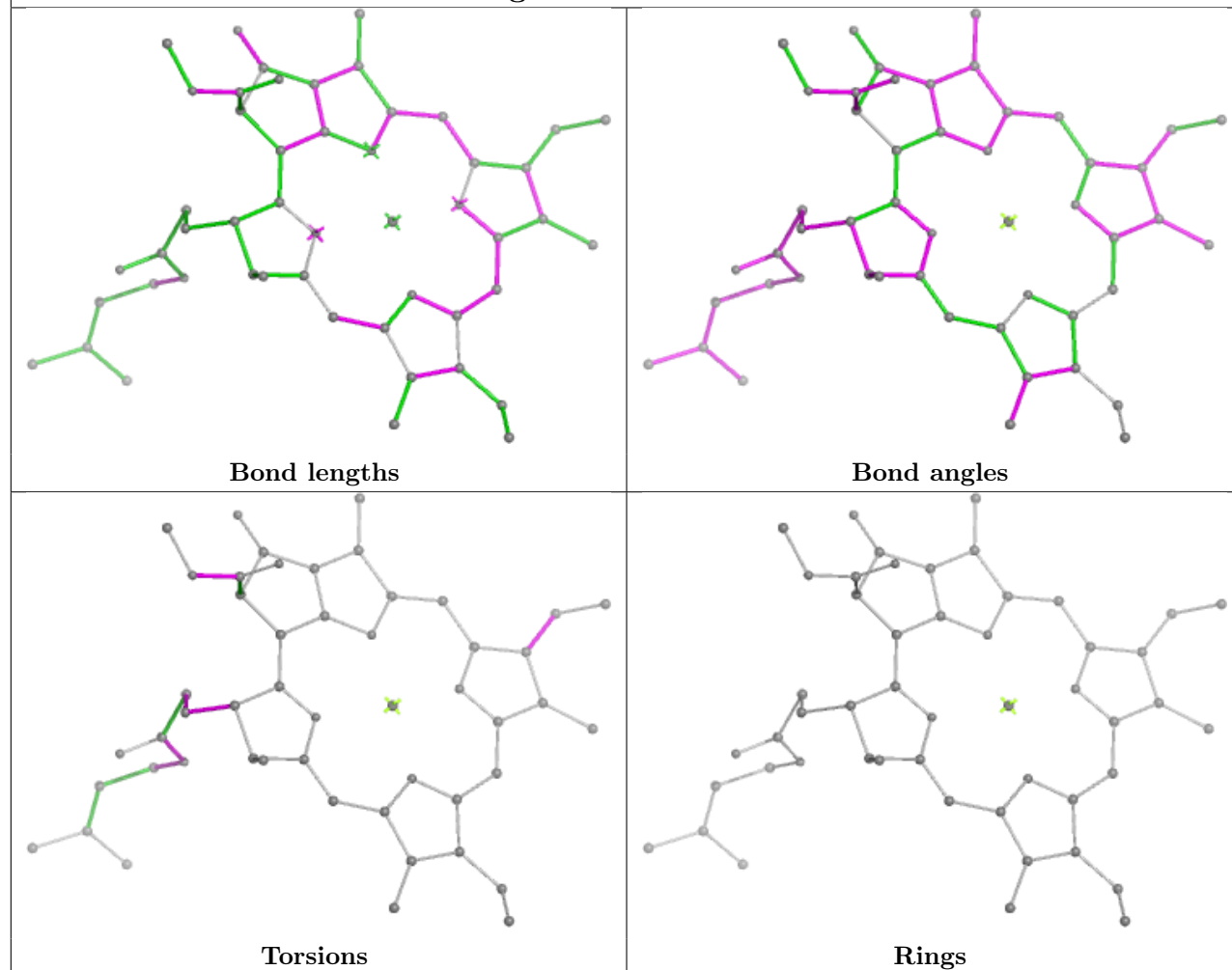


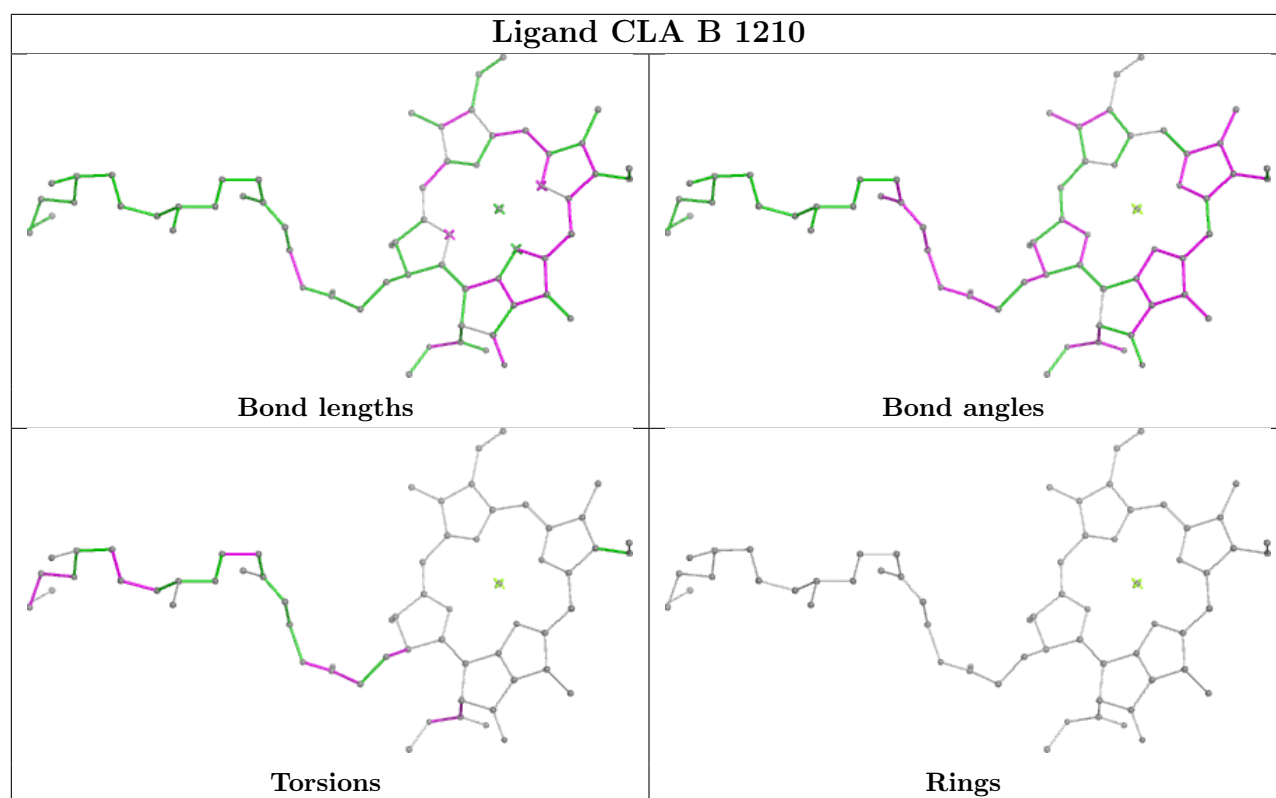


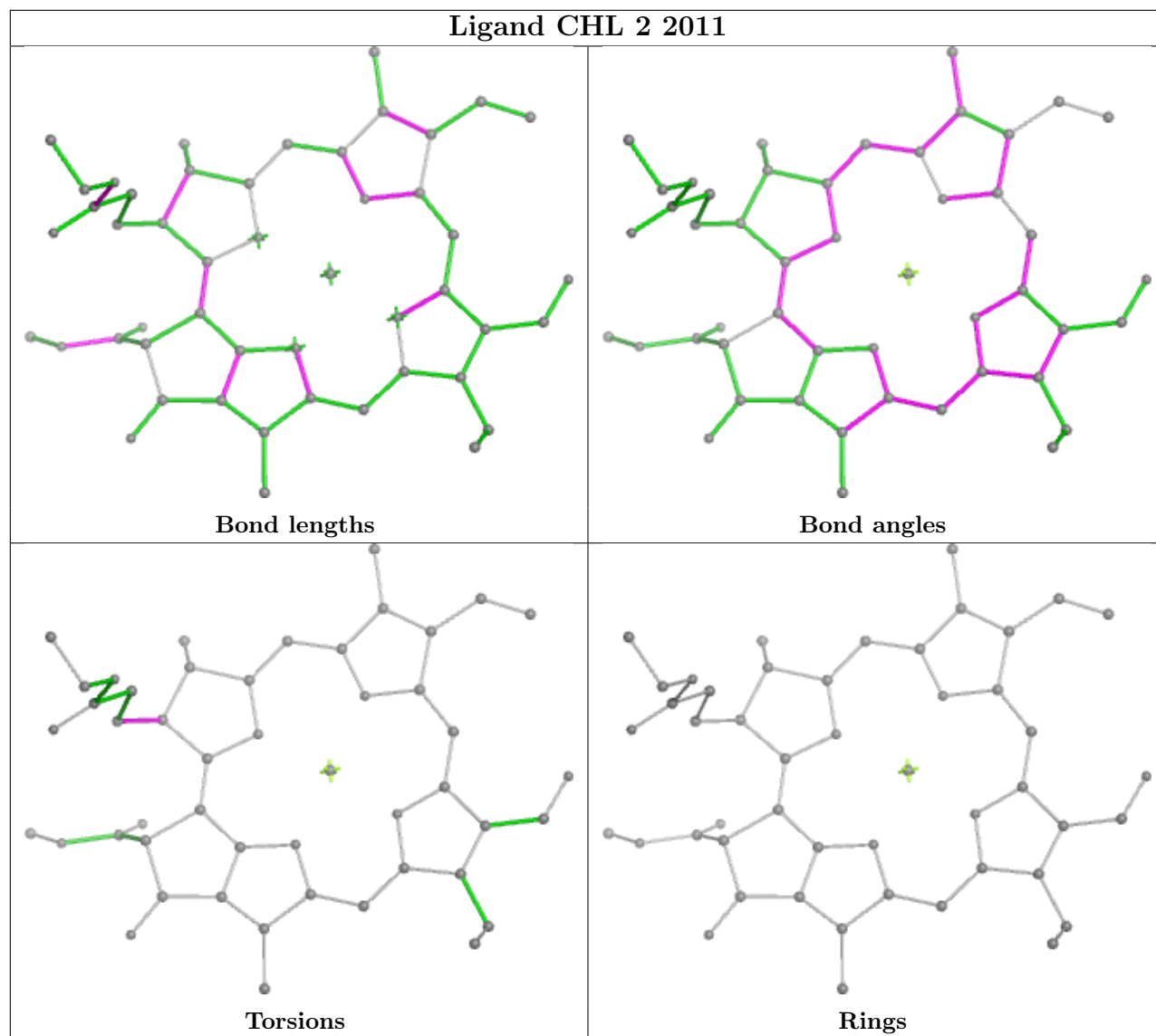


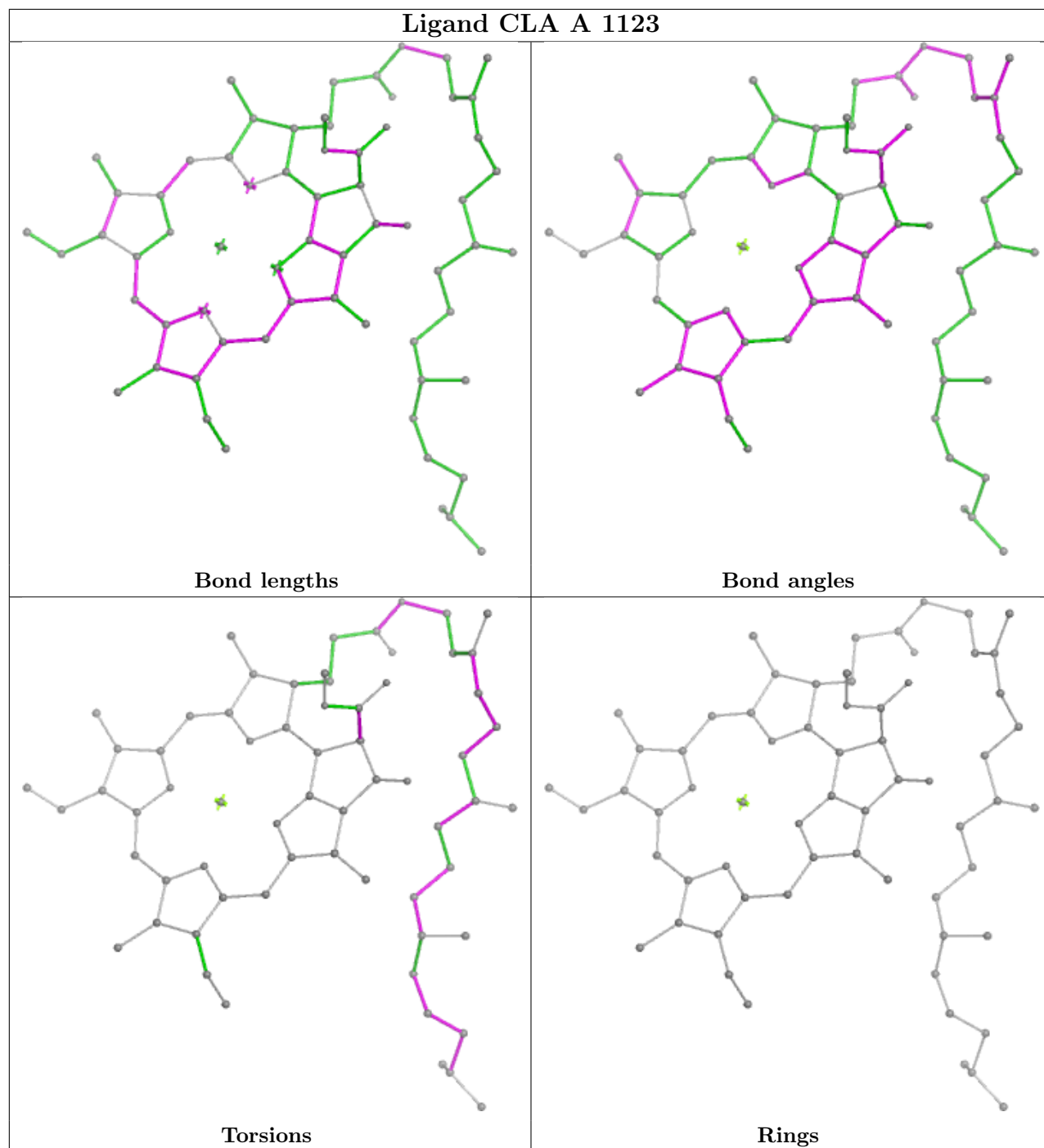


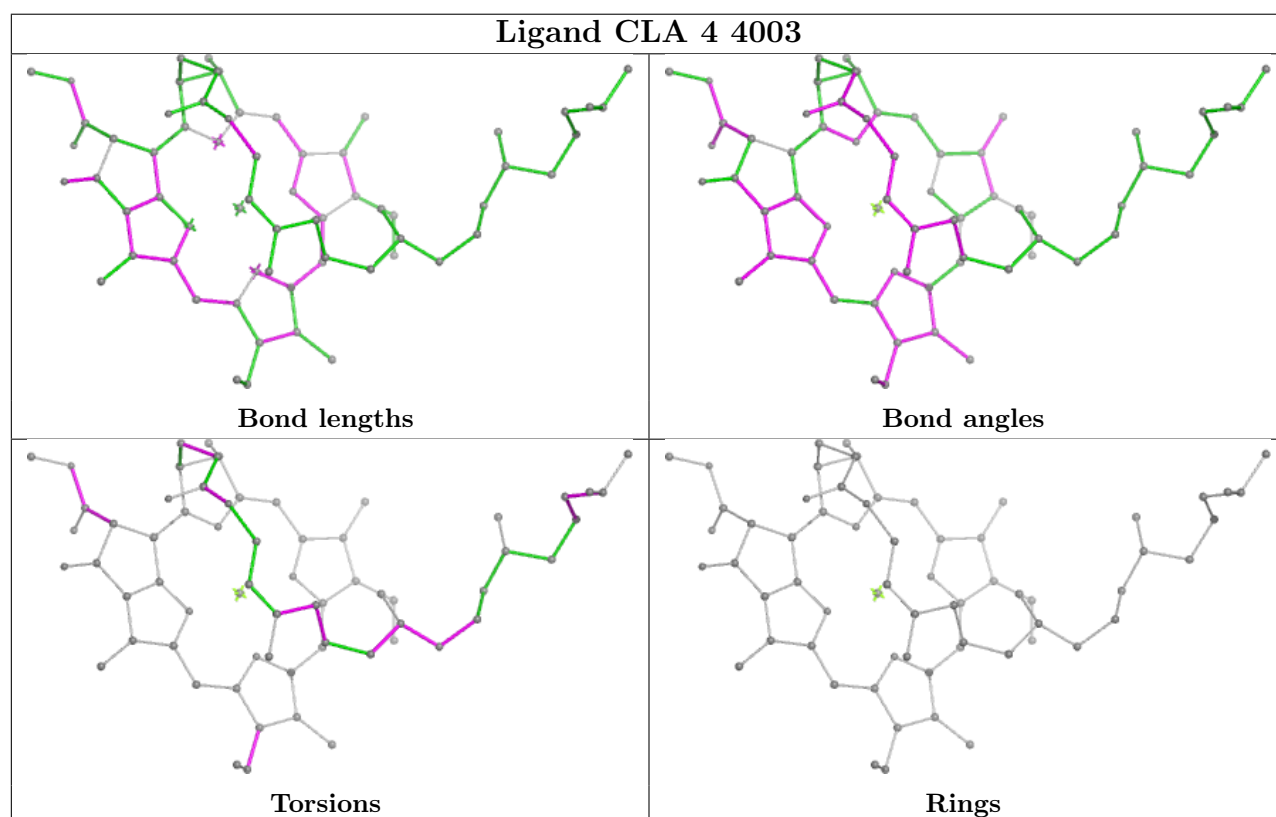
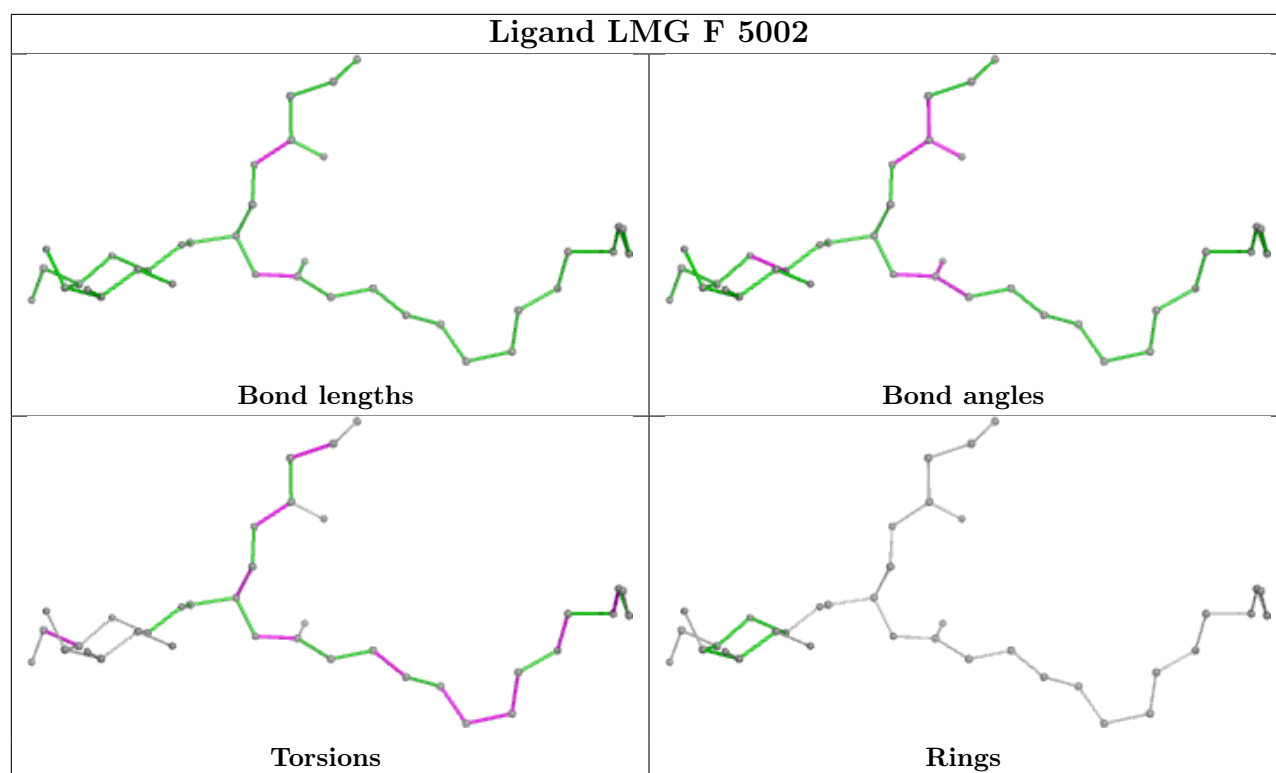
Ligand CLA 1 1011

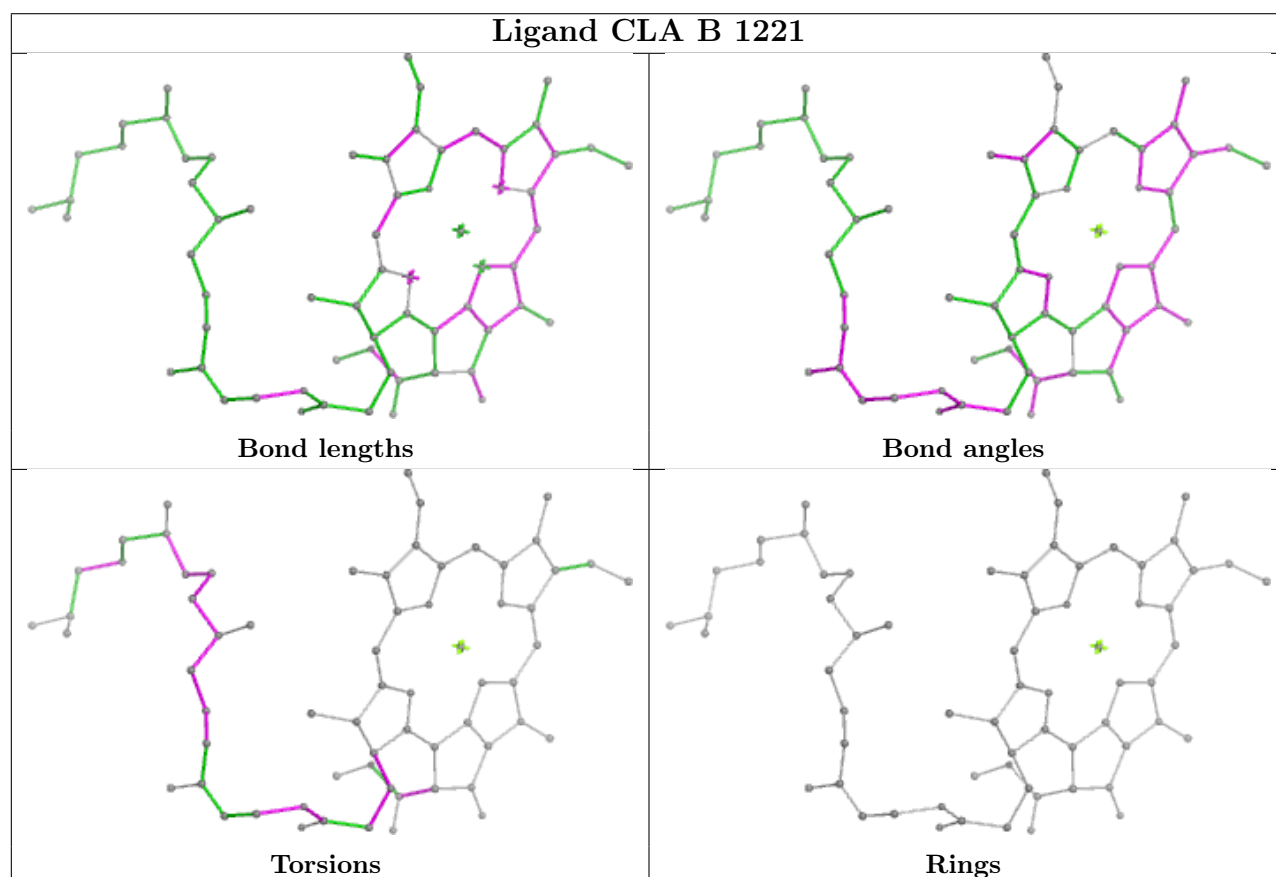
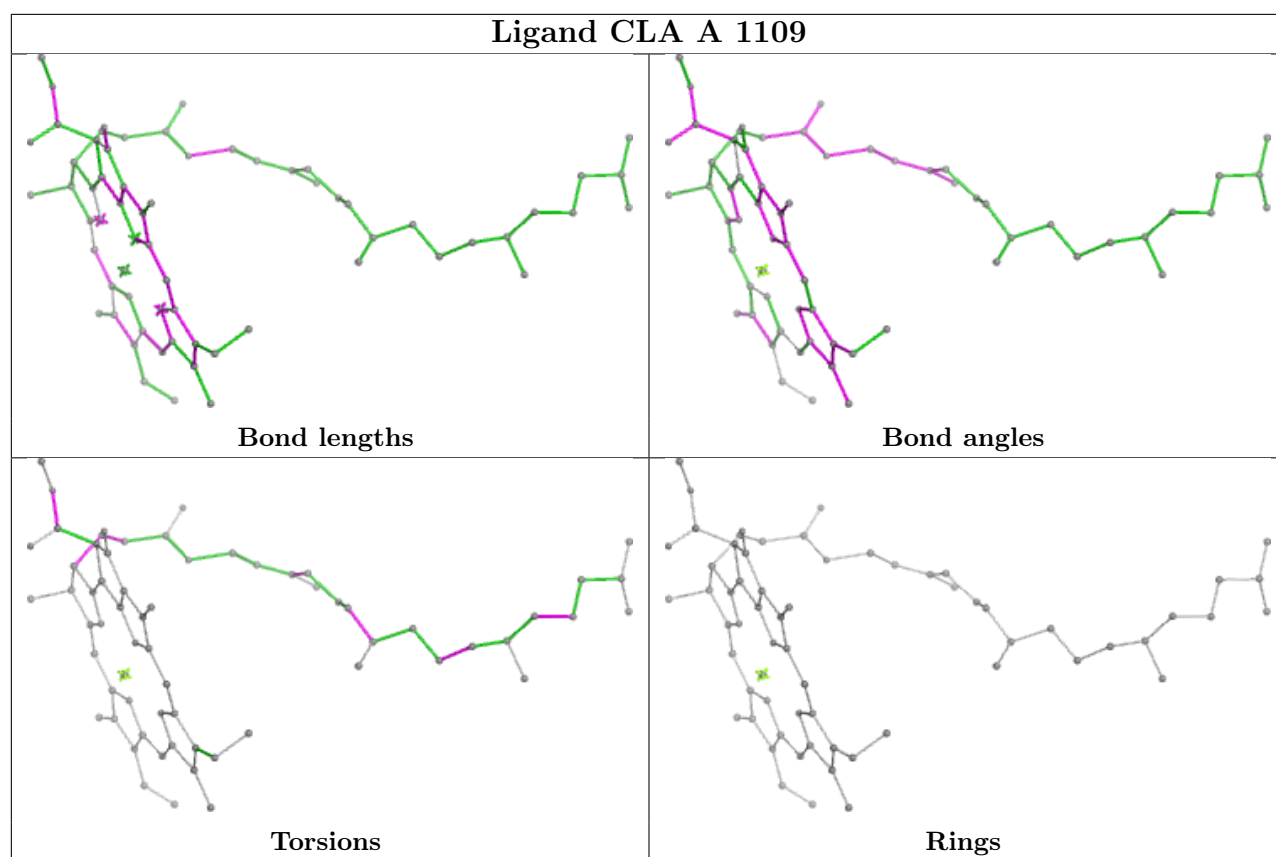


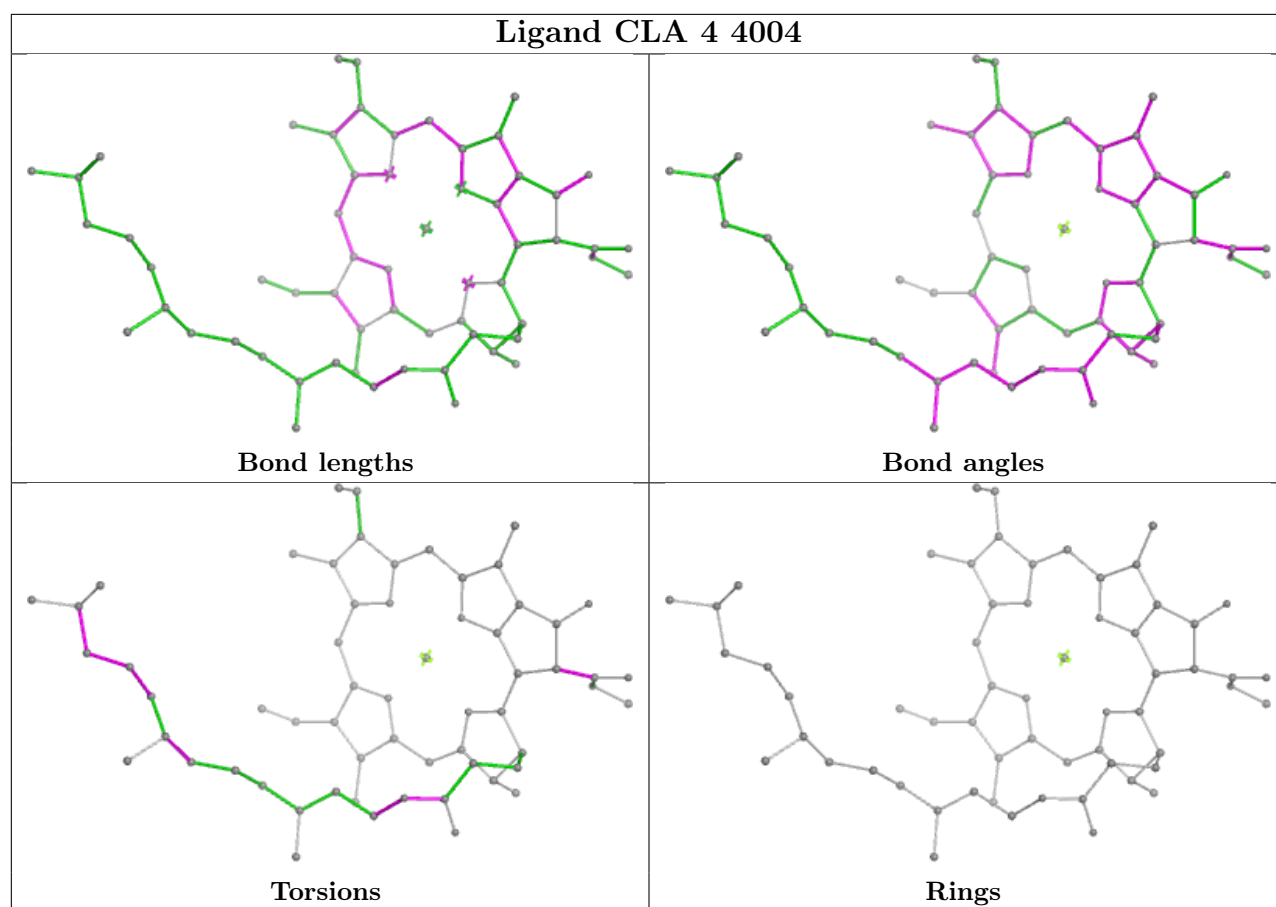


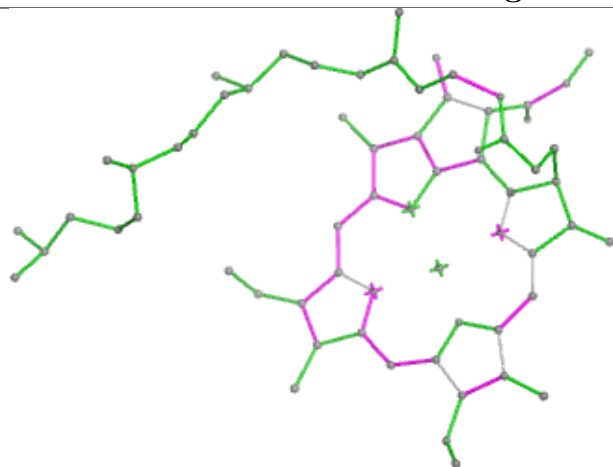
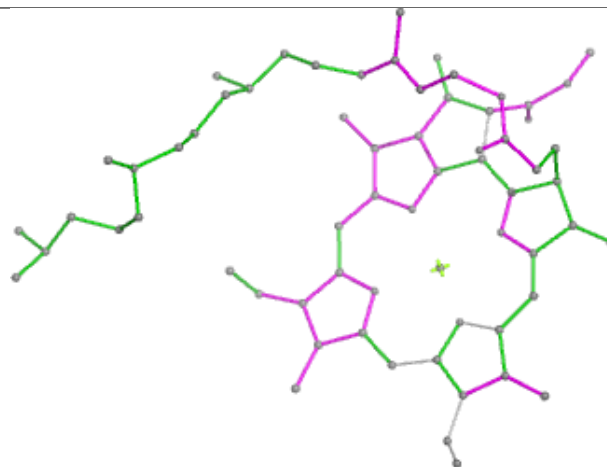
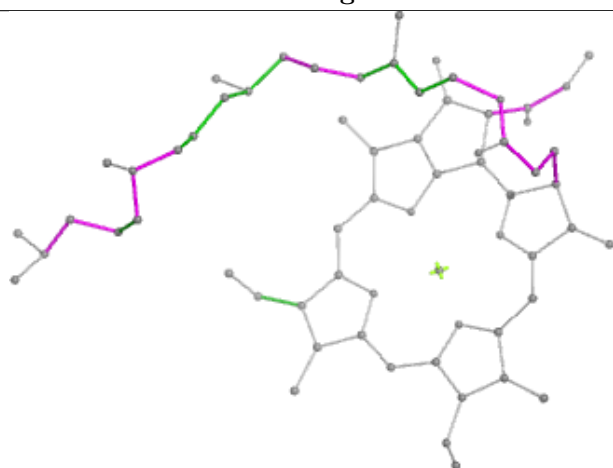
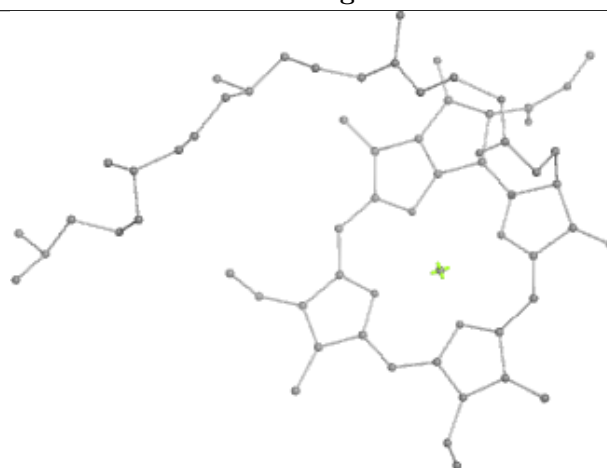


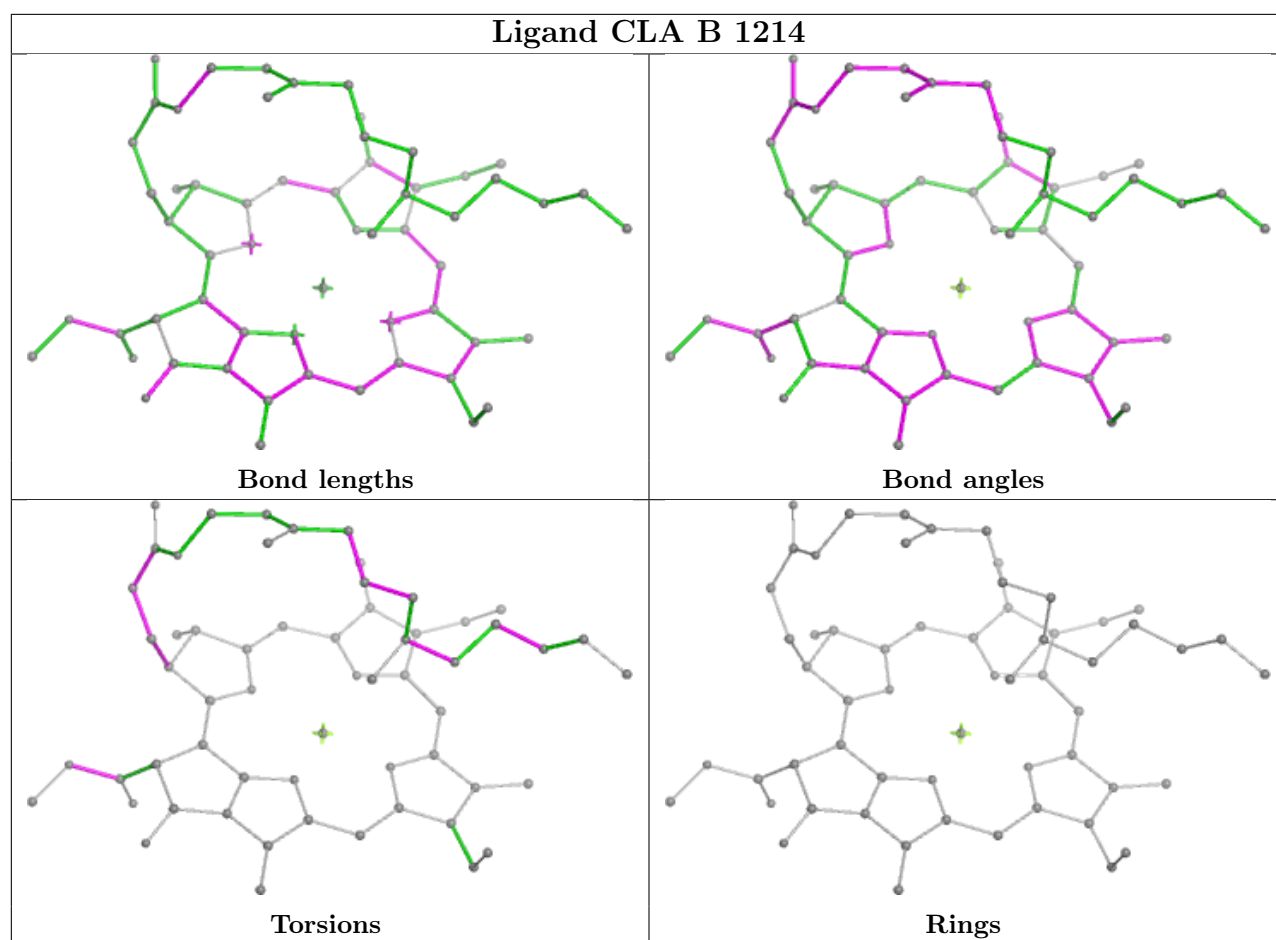


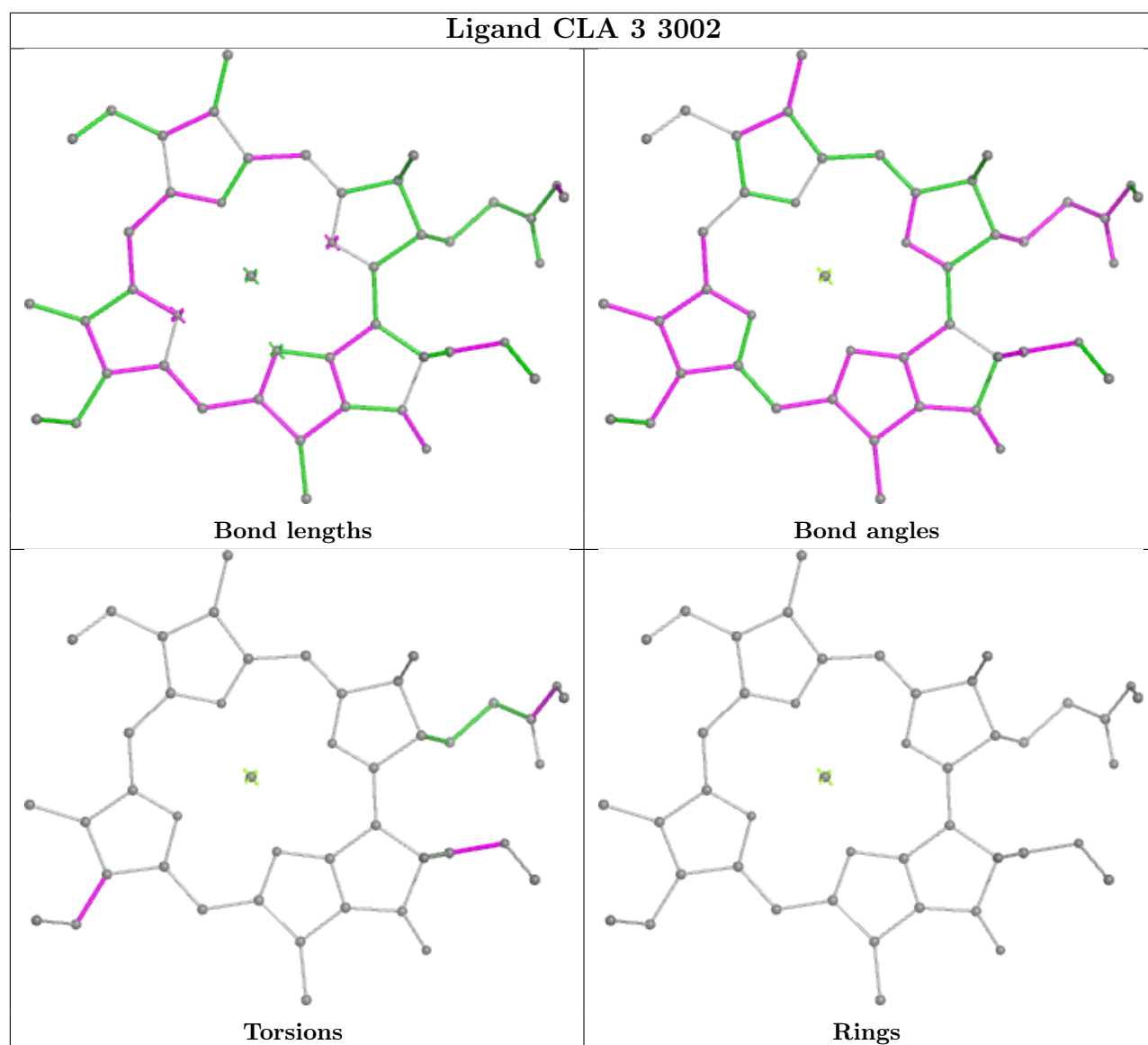


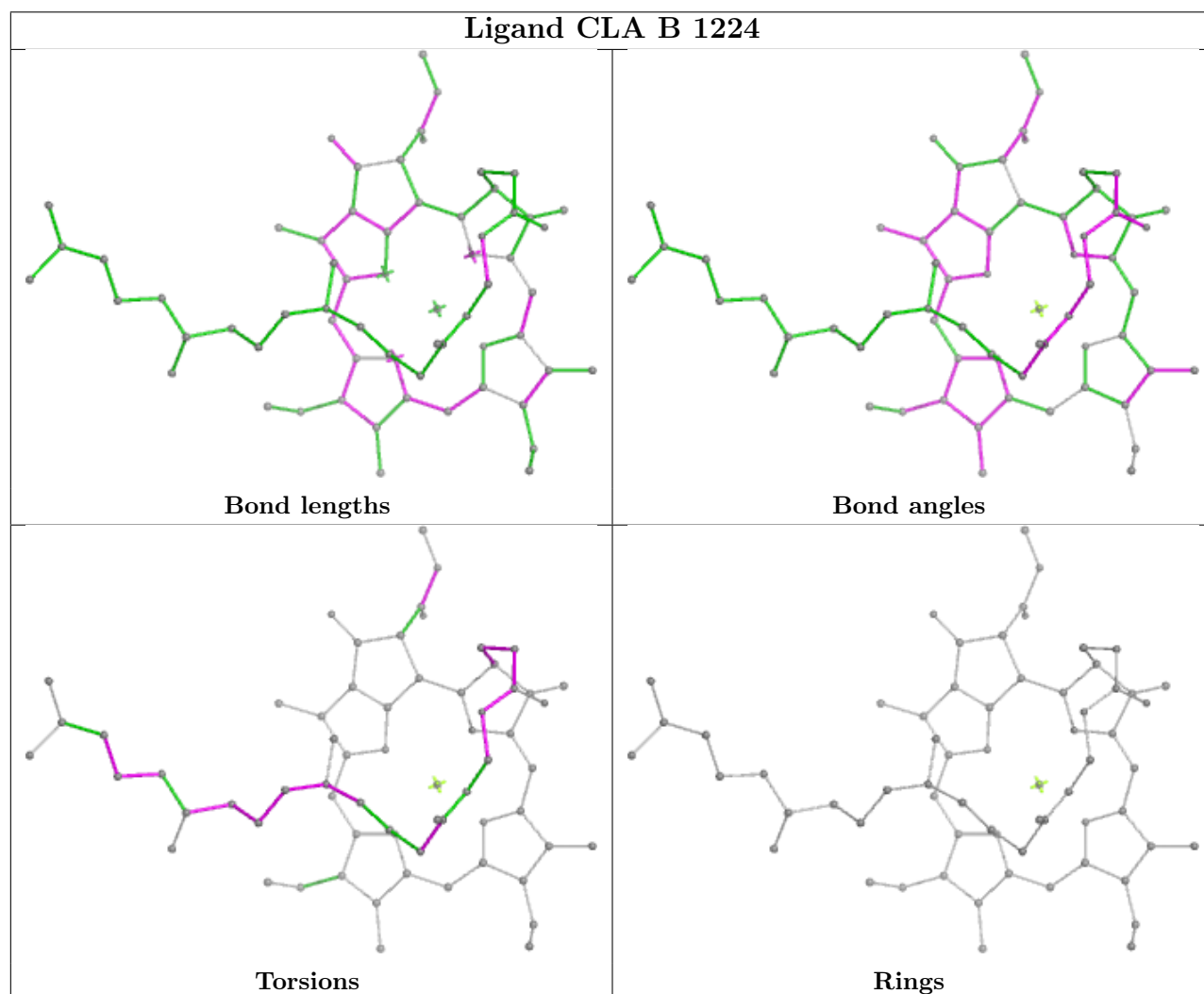
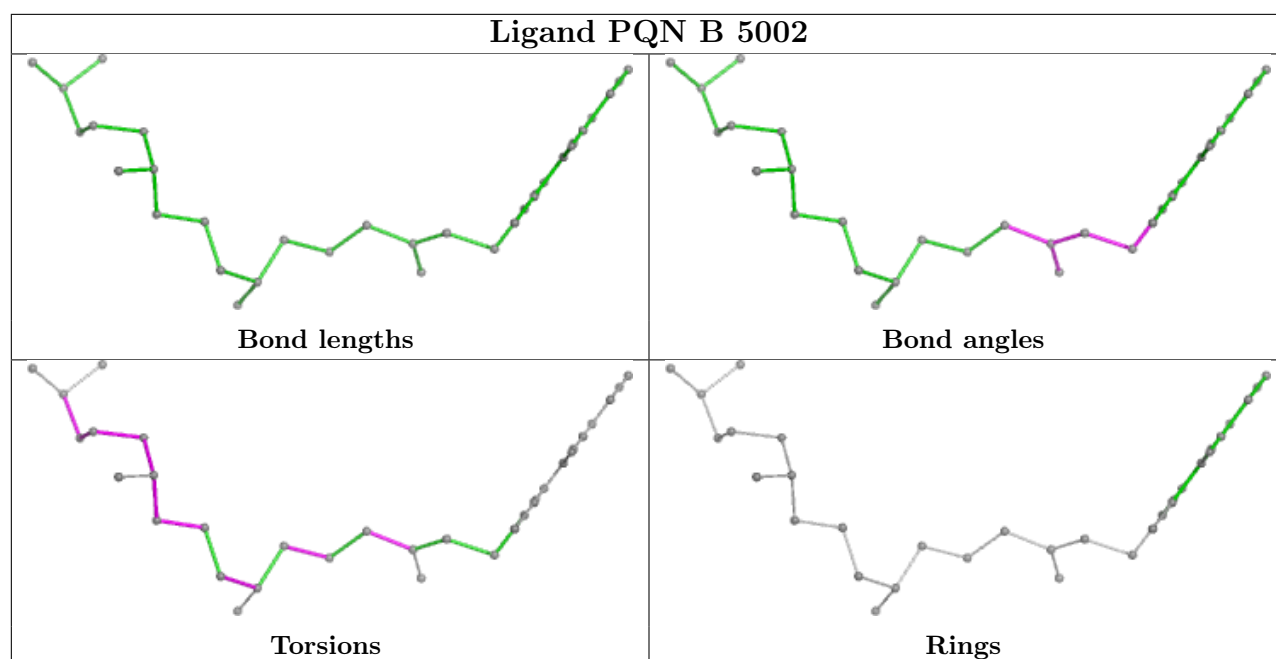


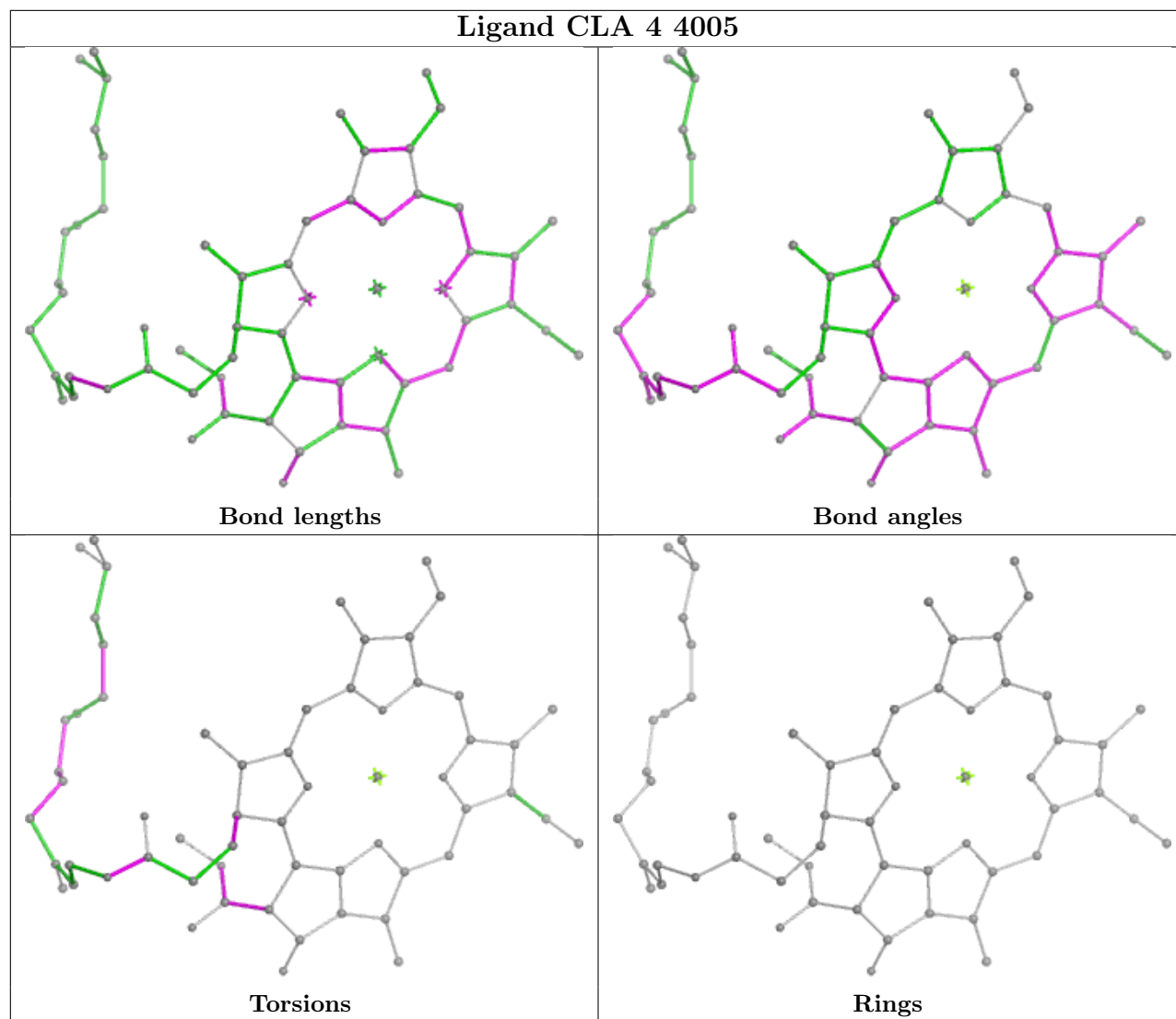


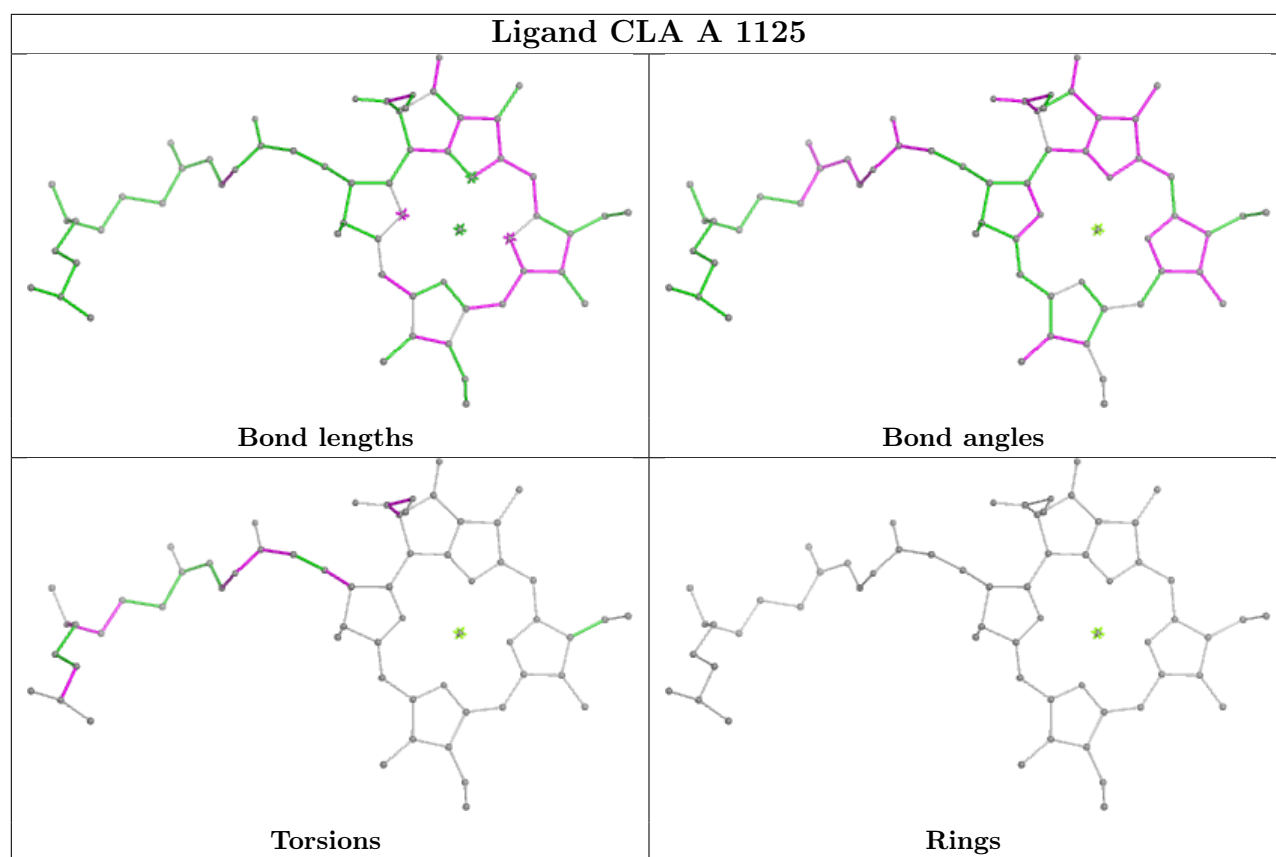
Ligand CLA A 1127**Bond lengths****Bond angles****Torsions****Rings**

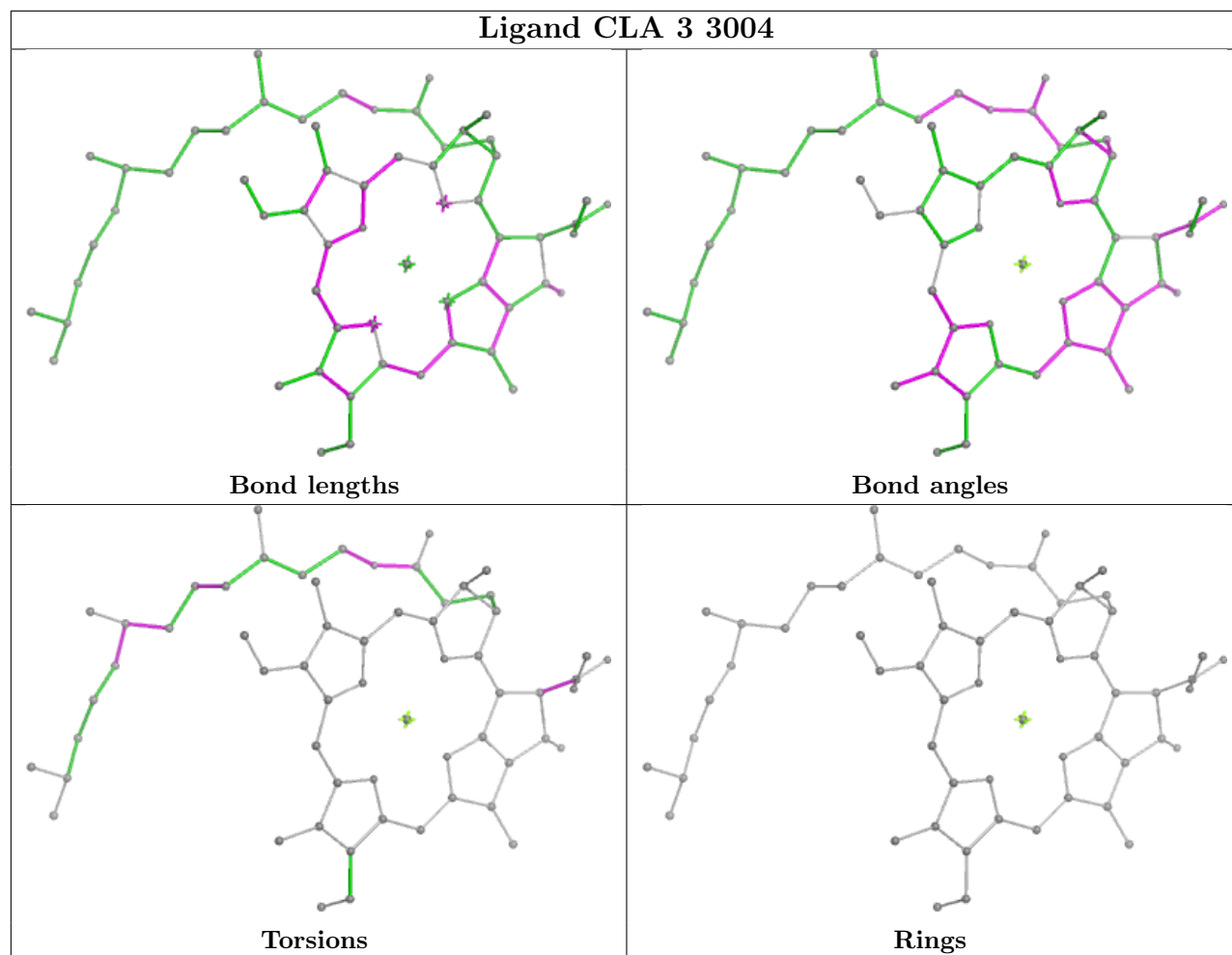




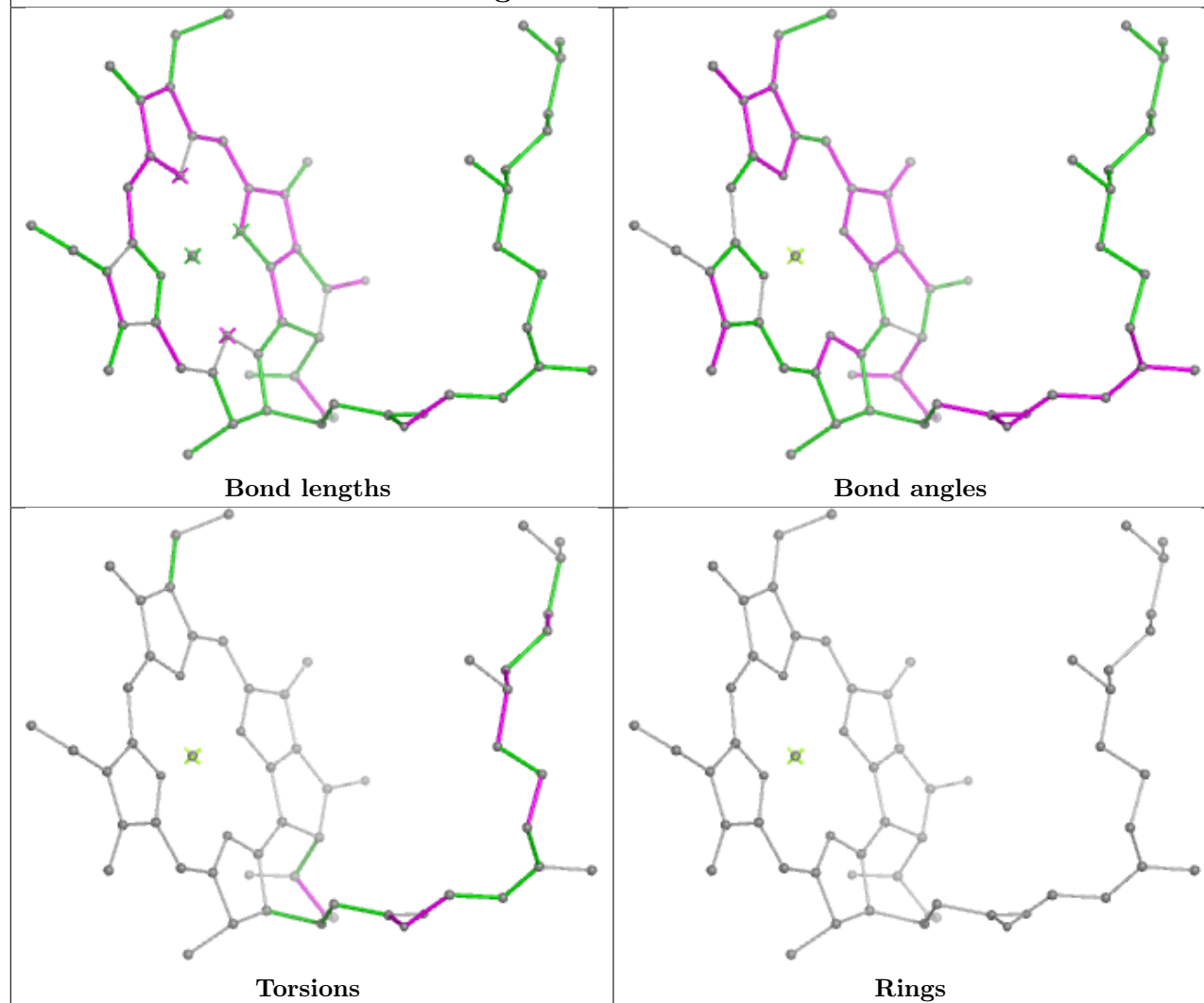




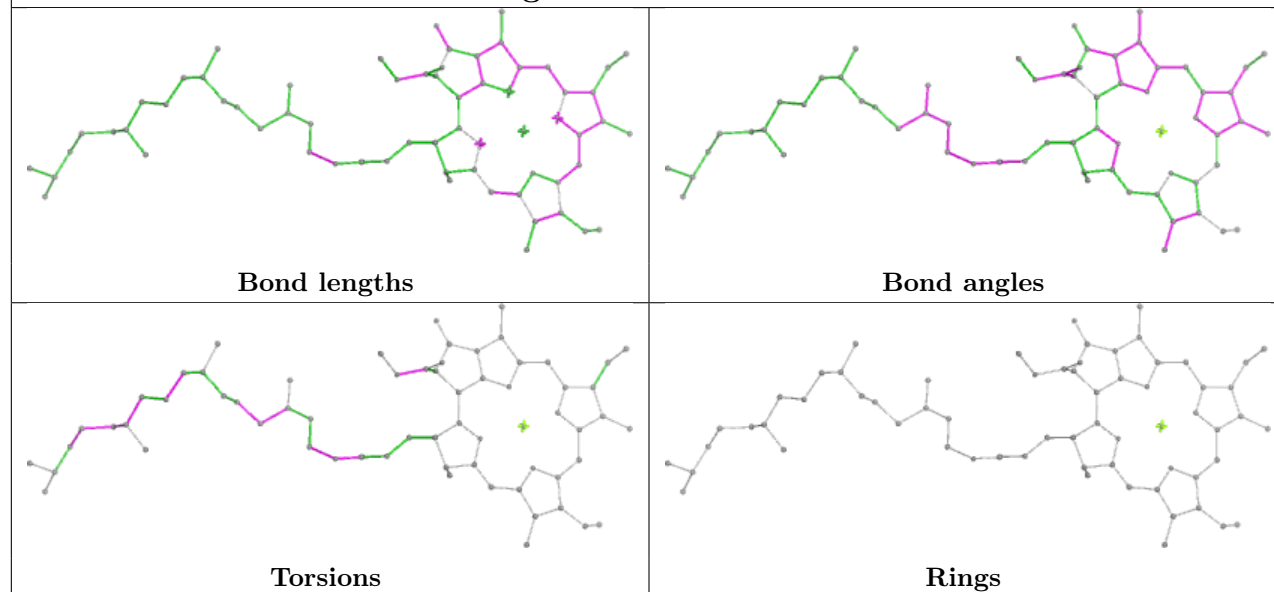


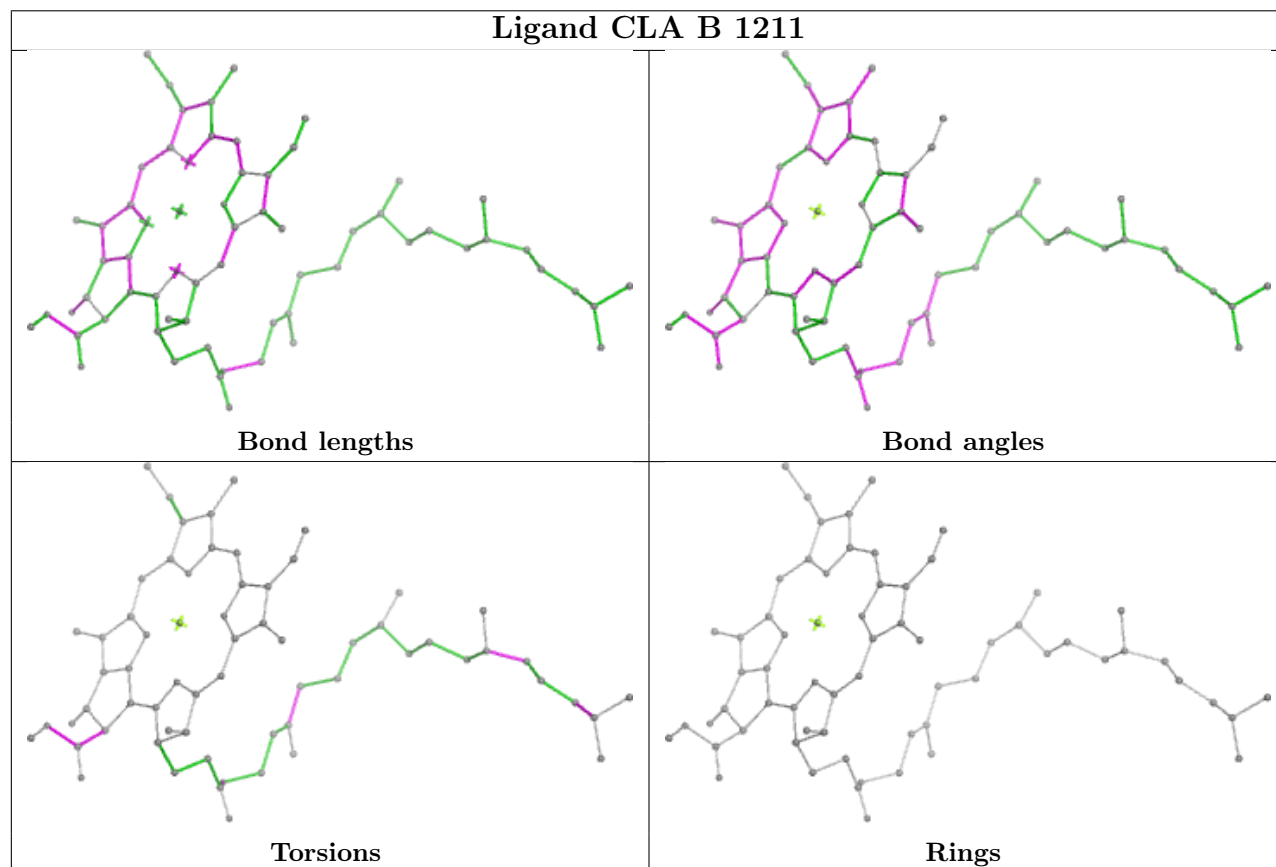
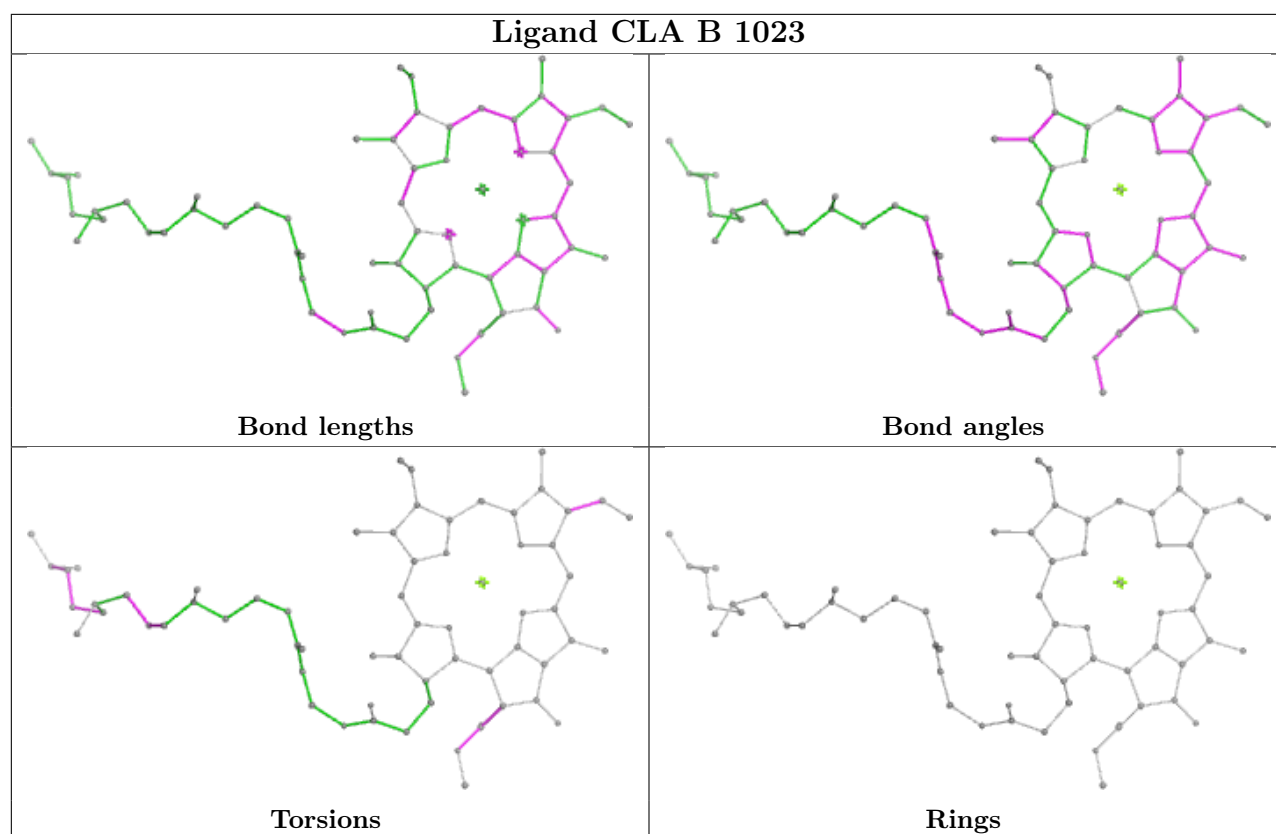


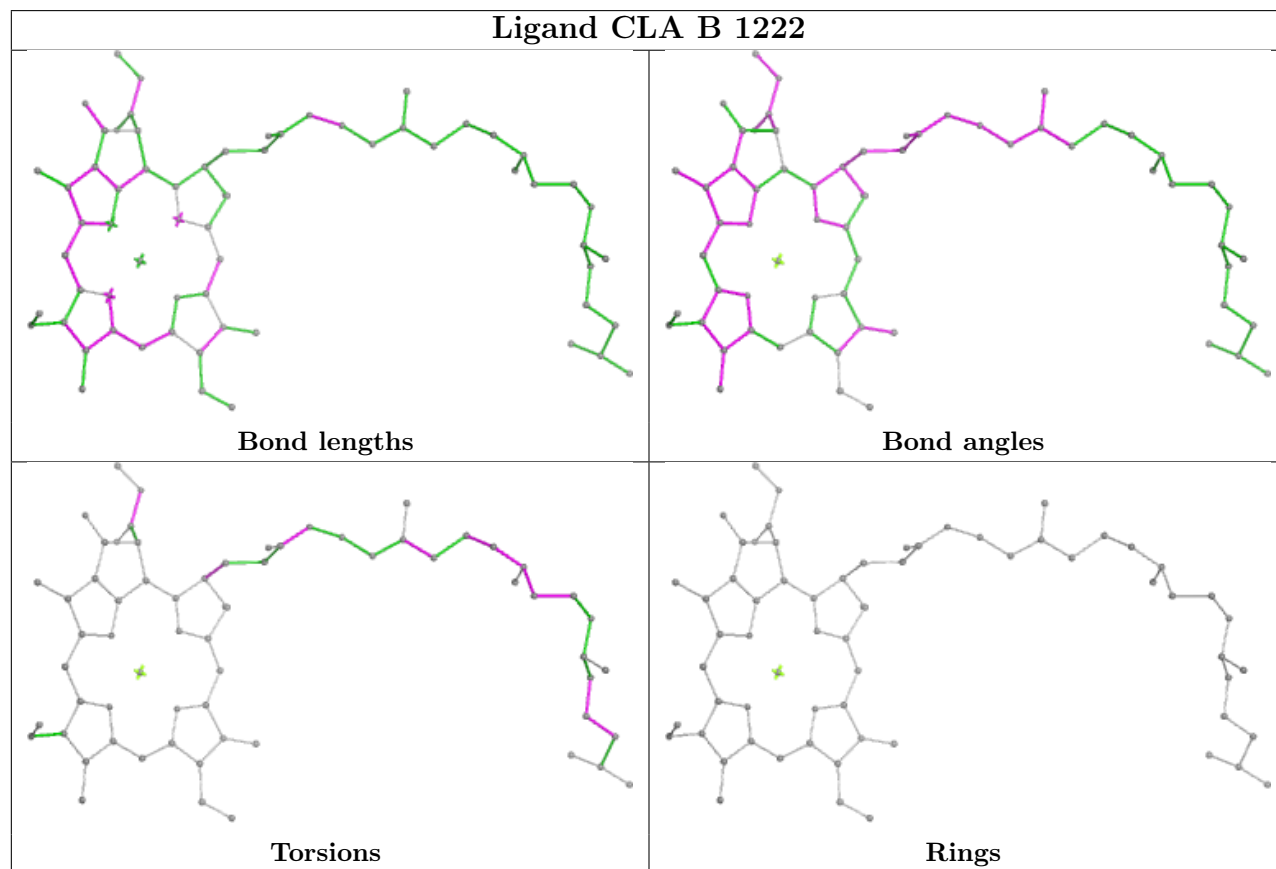
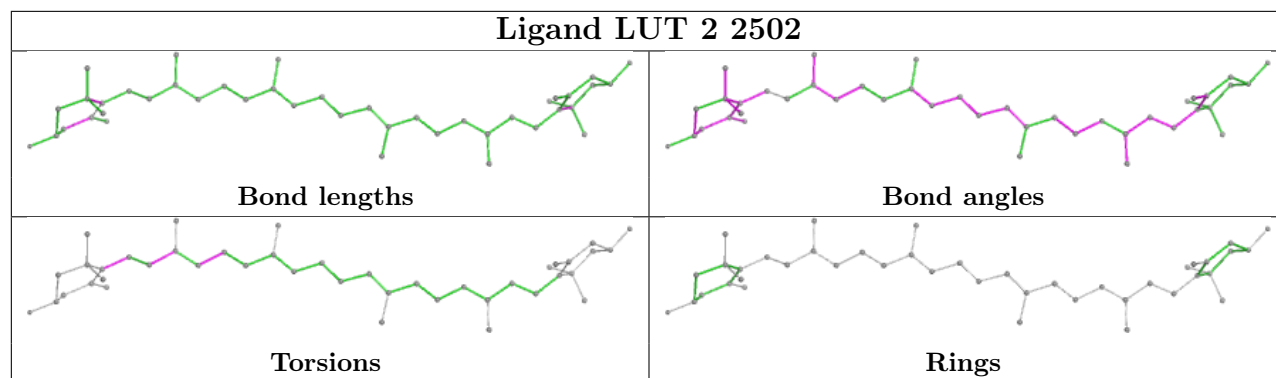
Ligand CLA B 1231

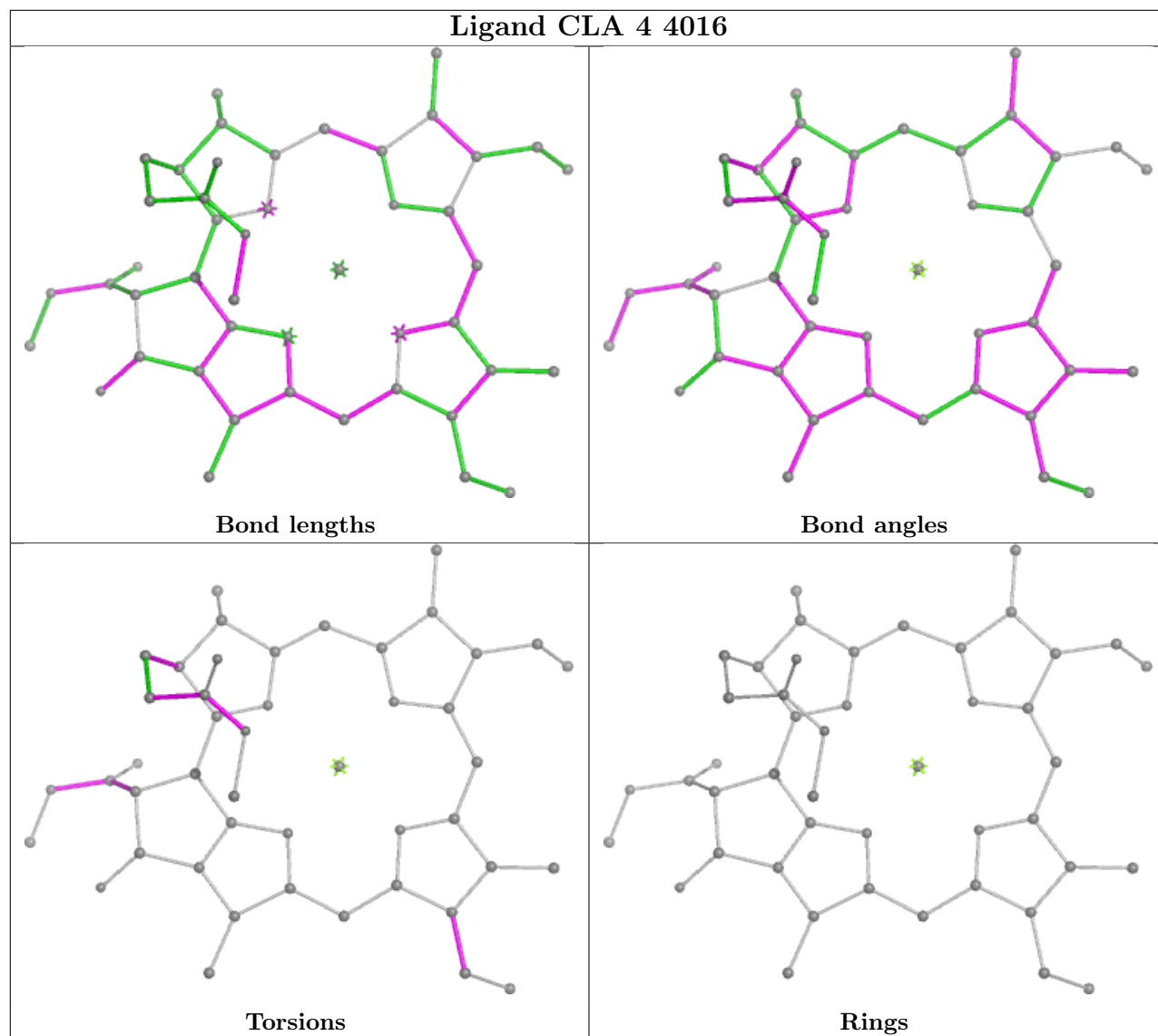


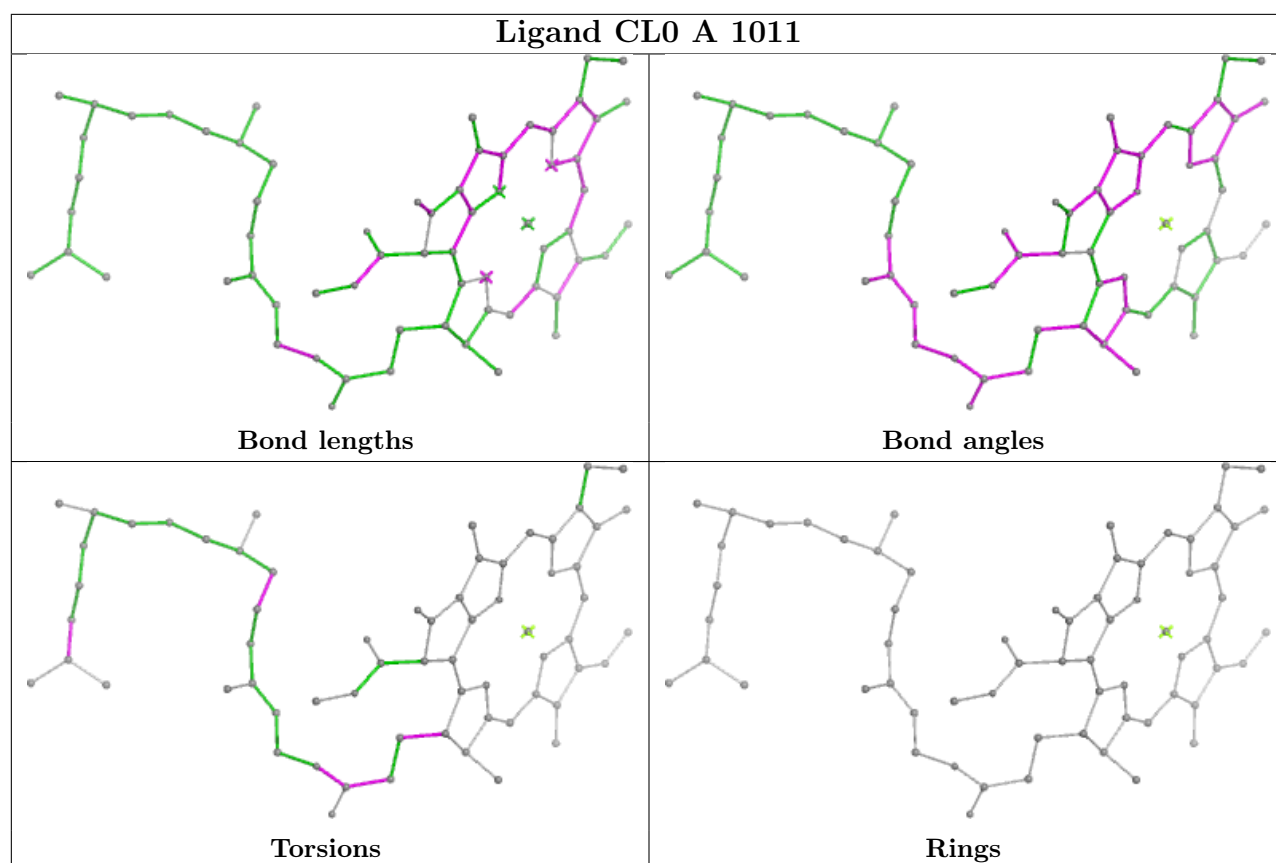
Ligand CLA A 1139

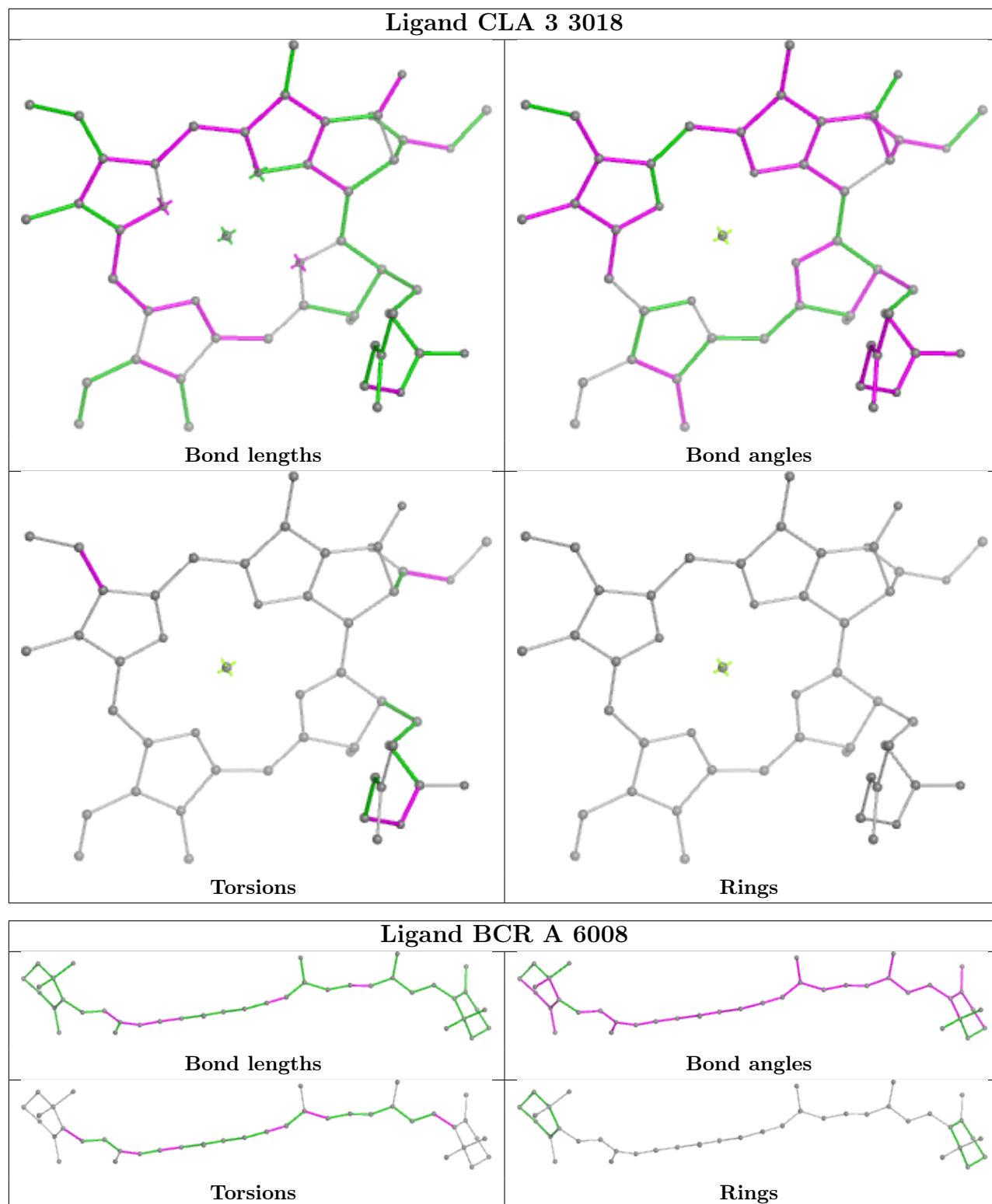


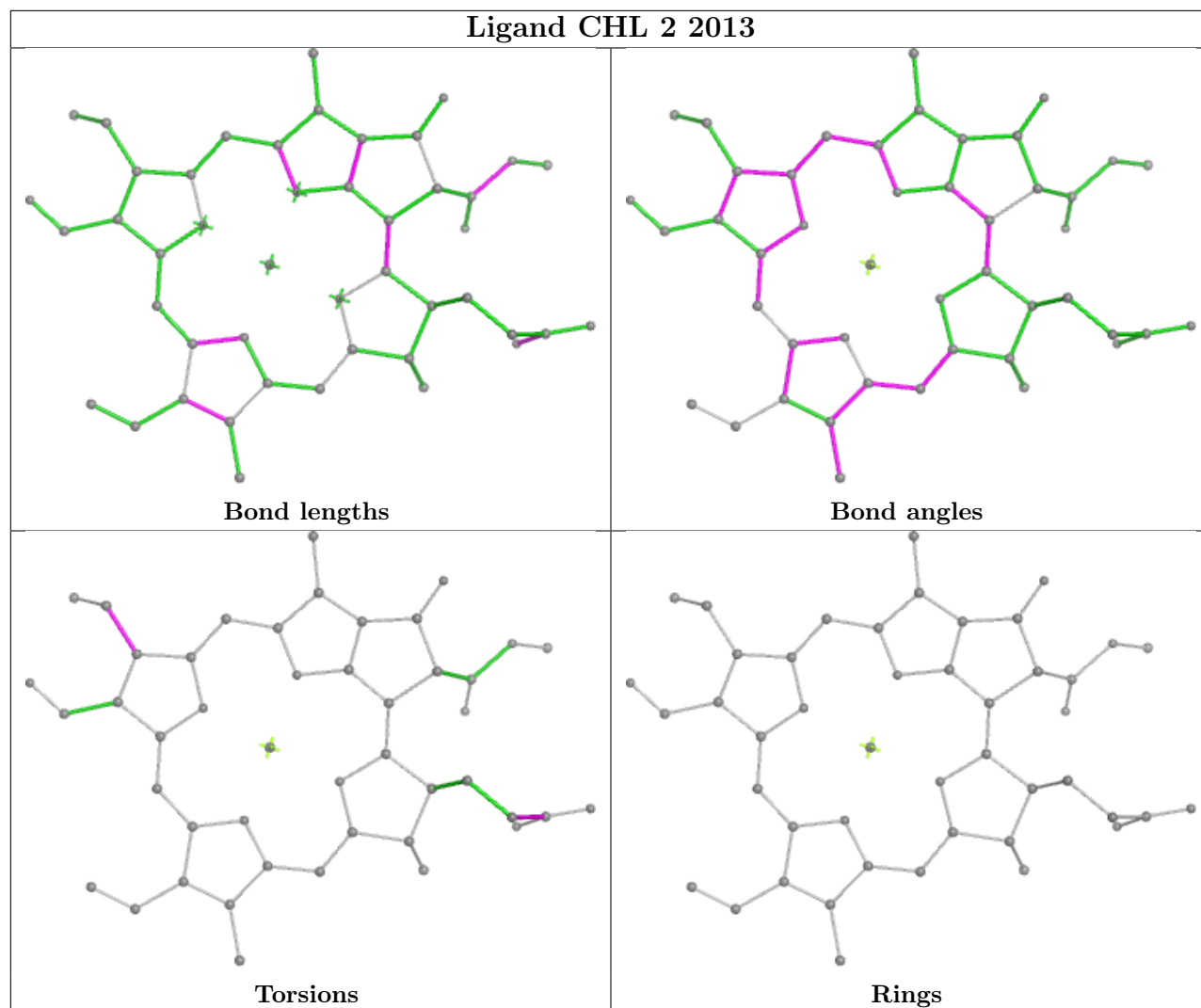


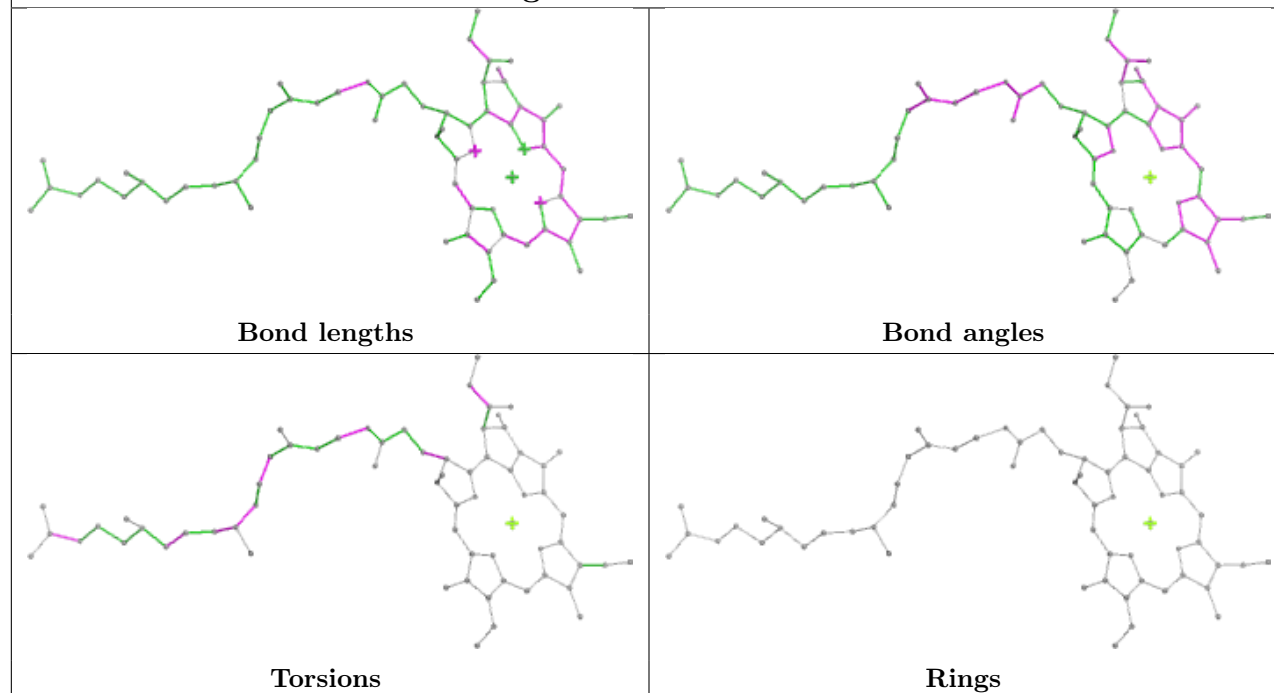
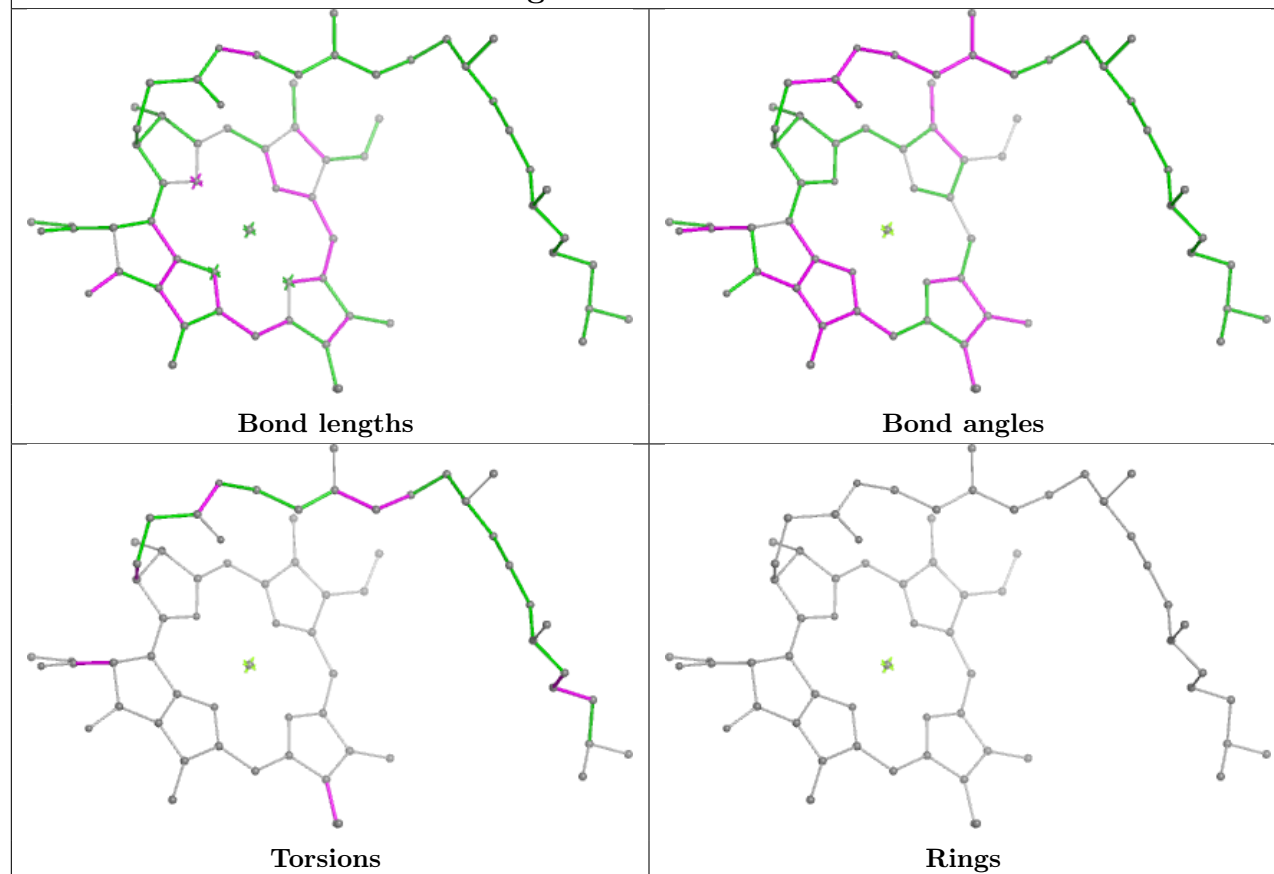


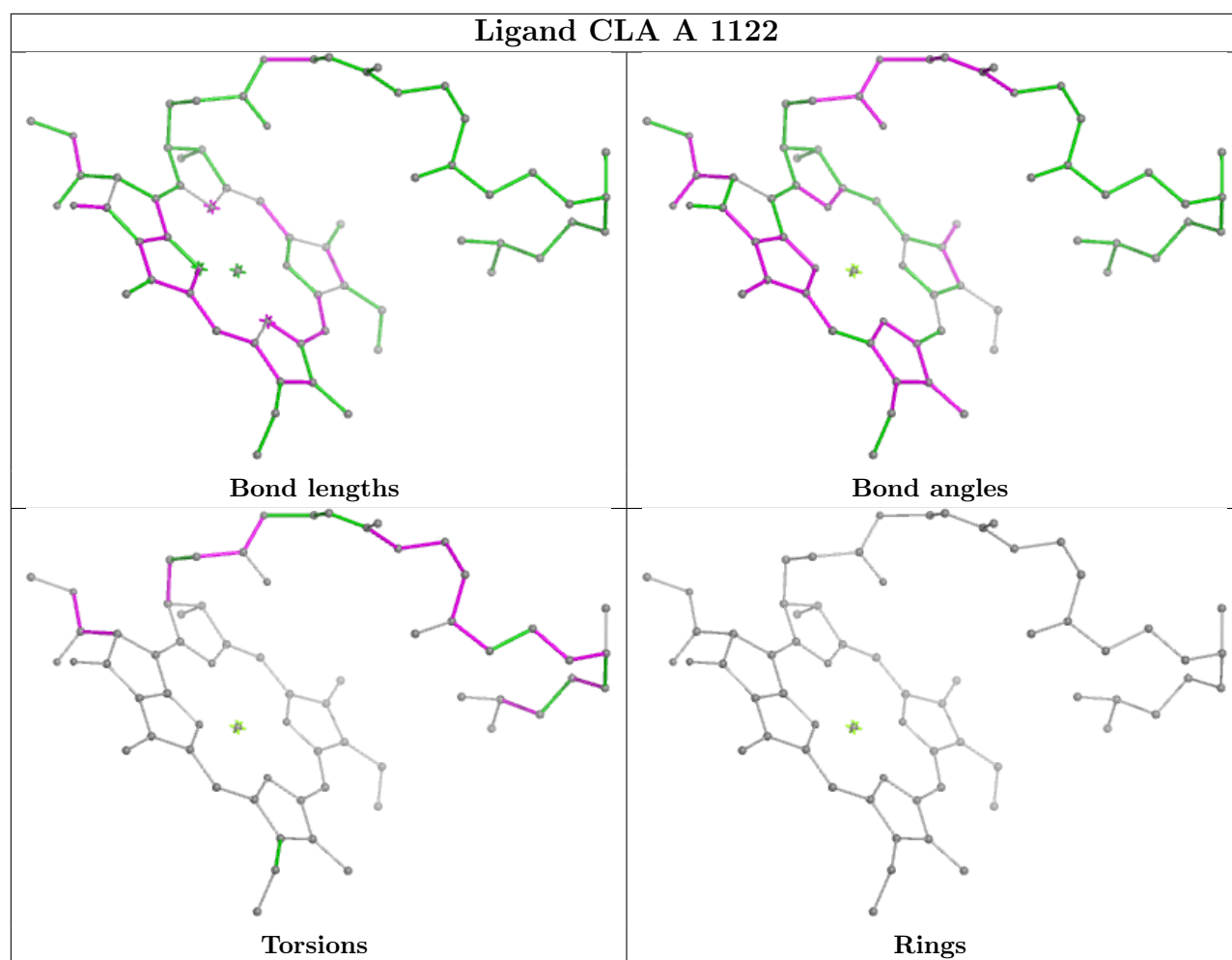


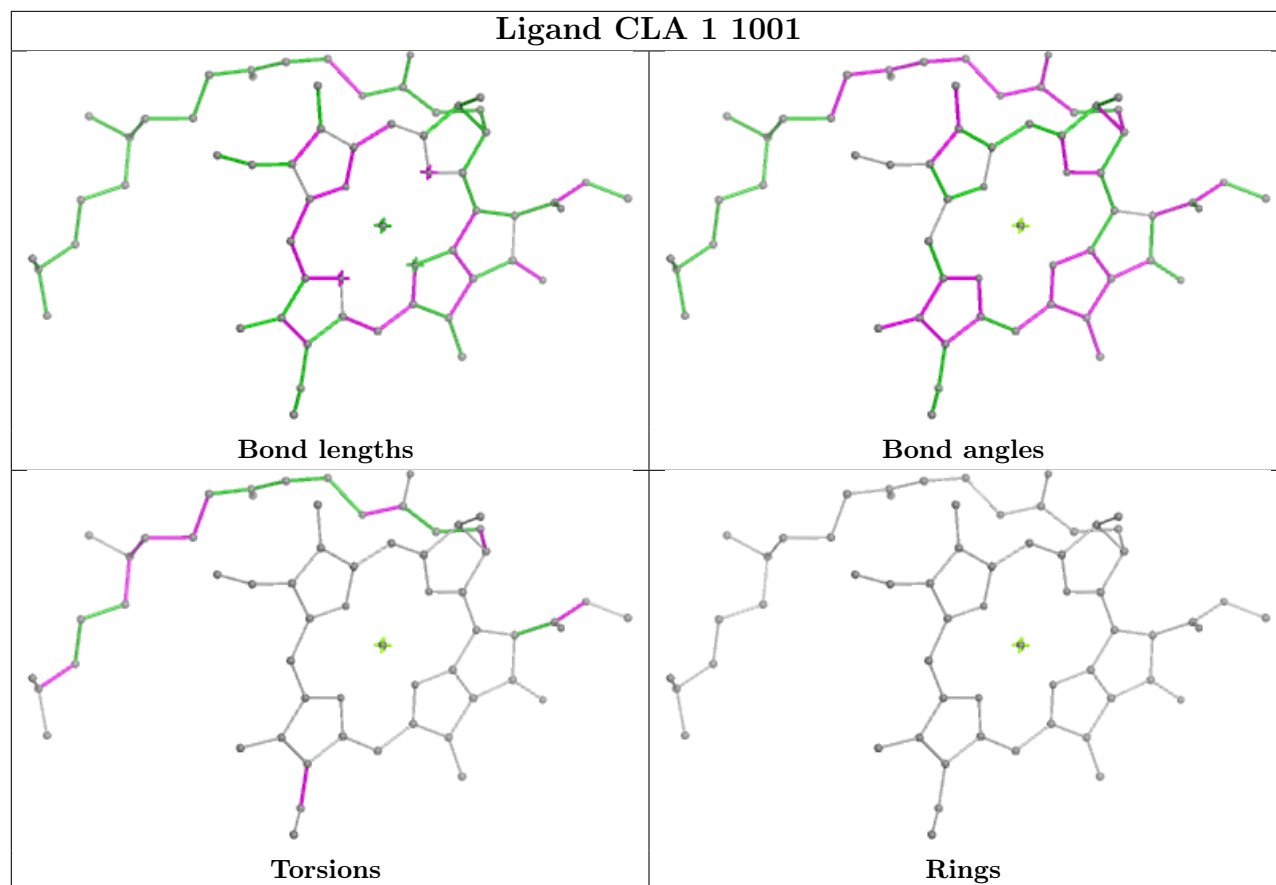


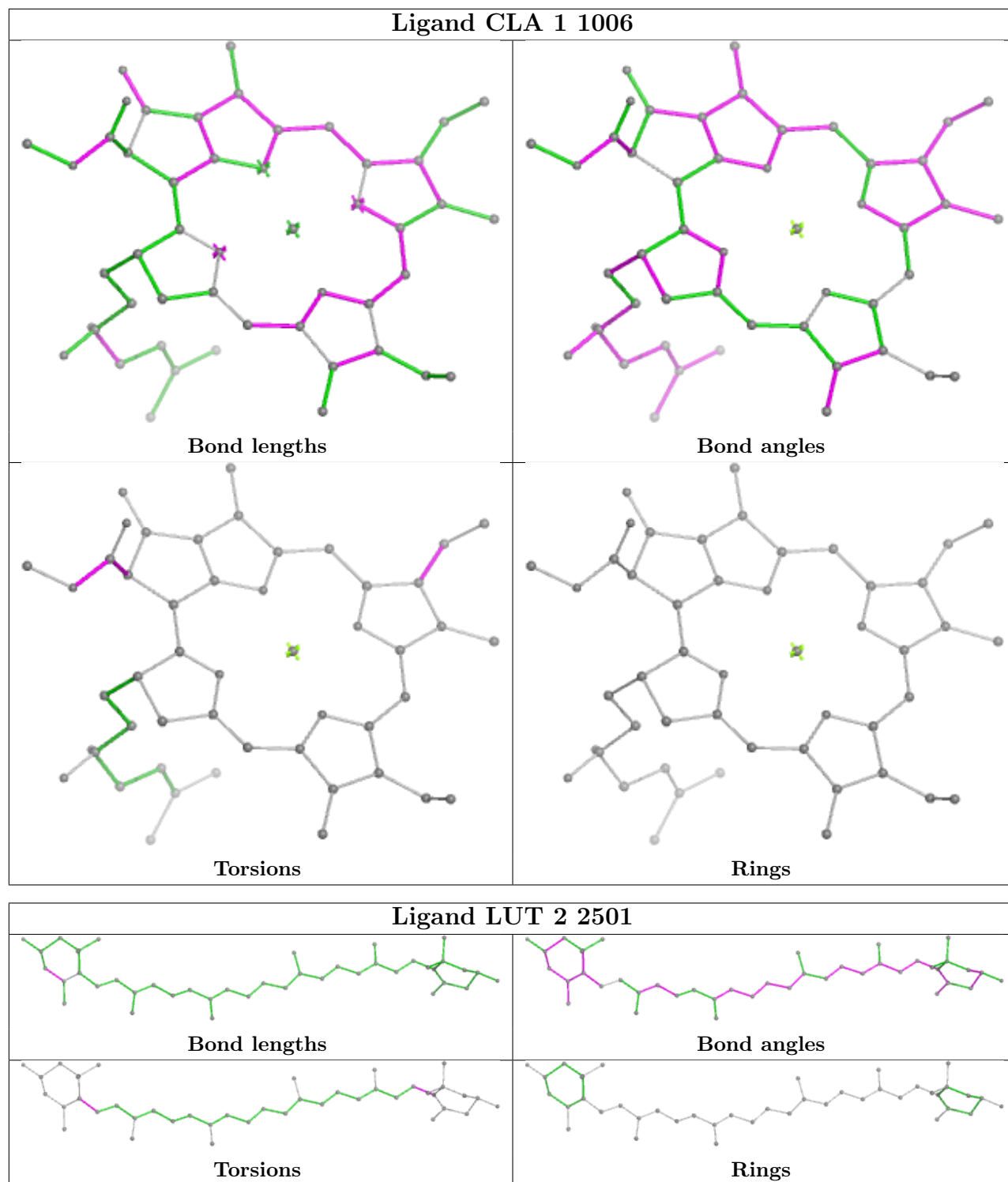


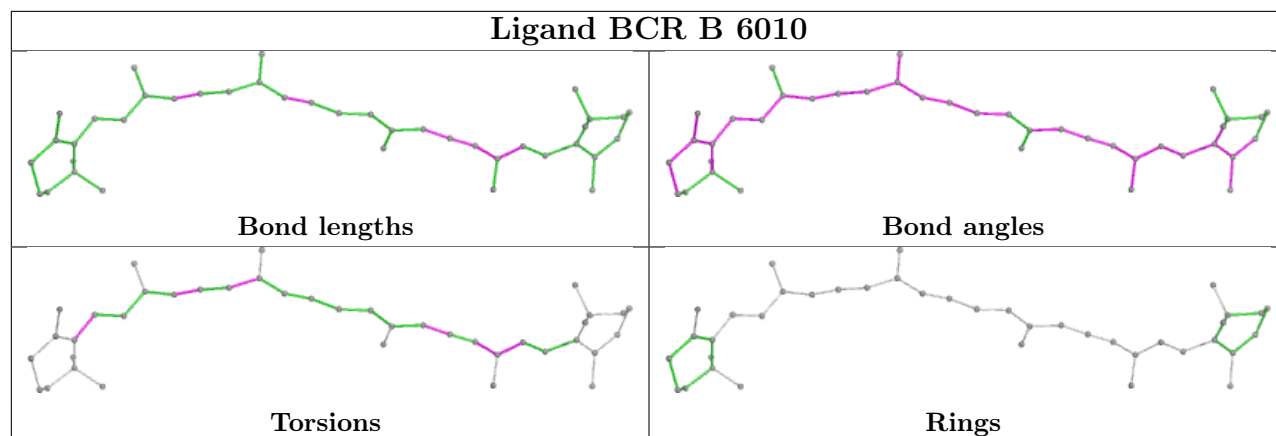
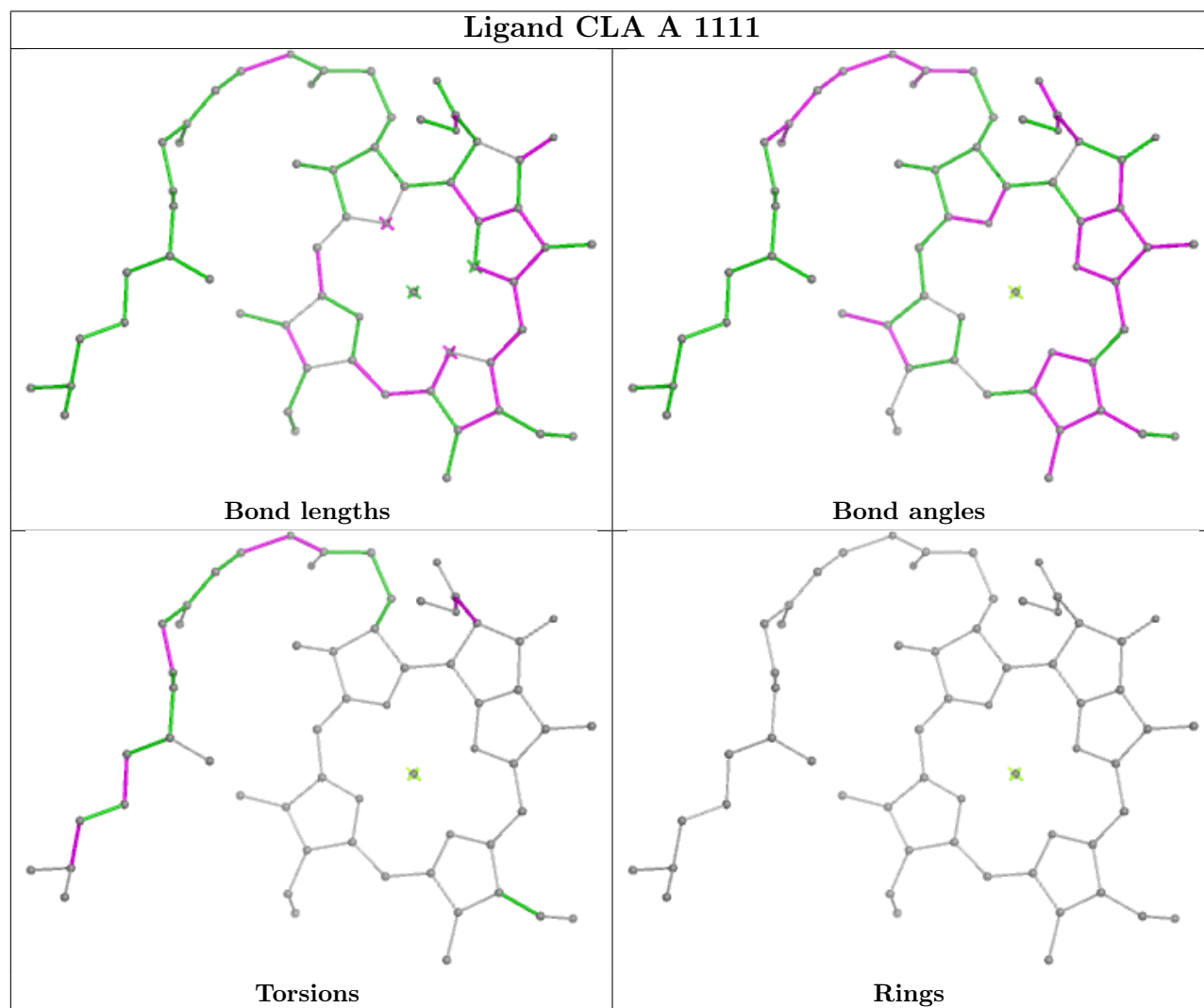


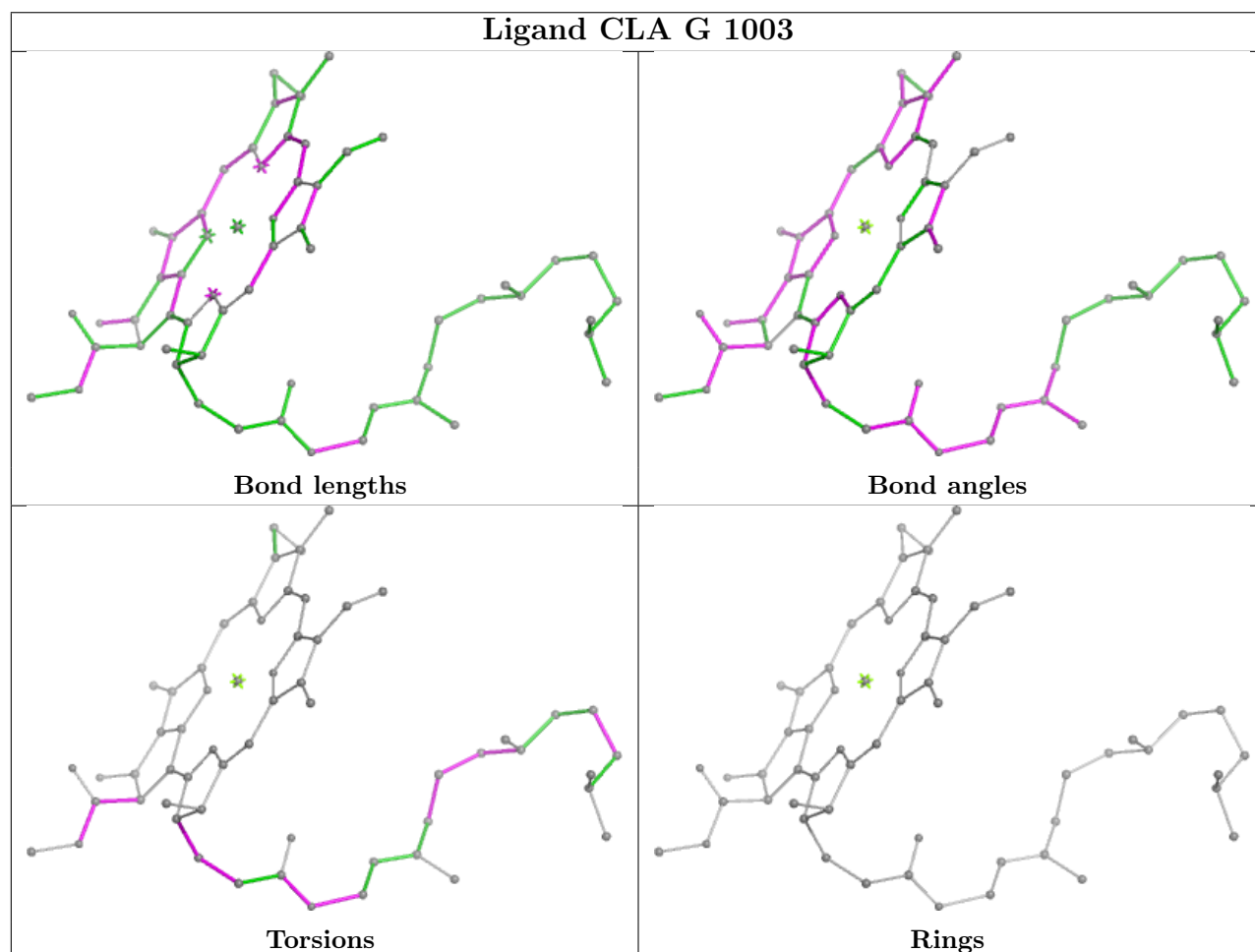
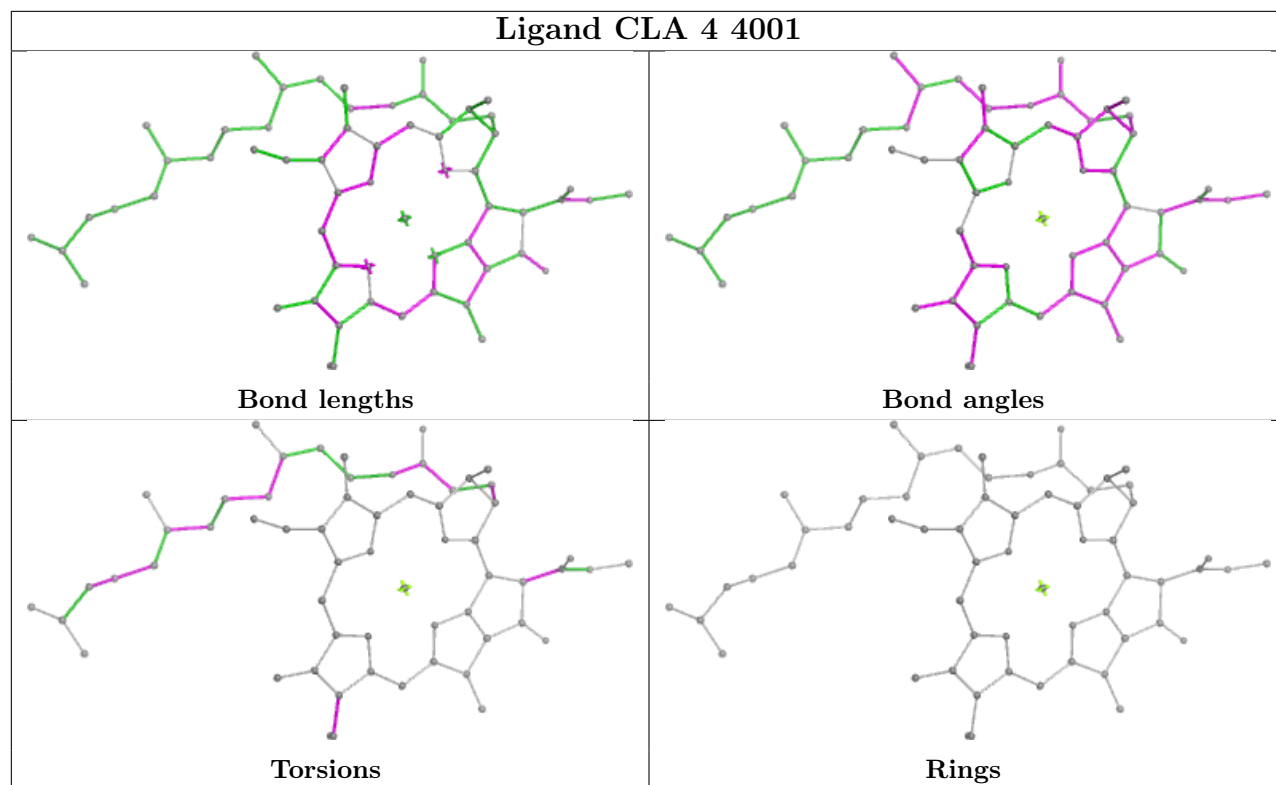
Ligand CLA A 1022**Ligand CLA 2 2004**

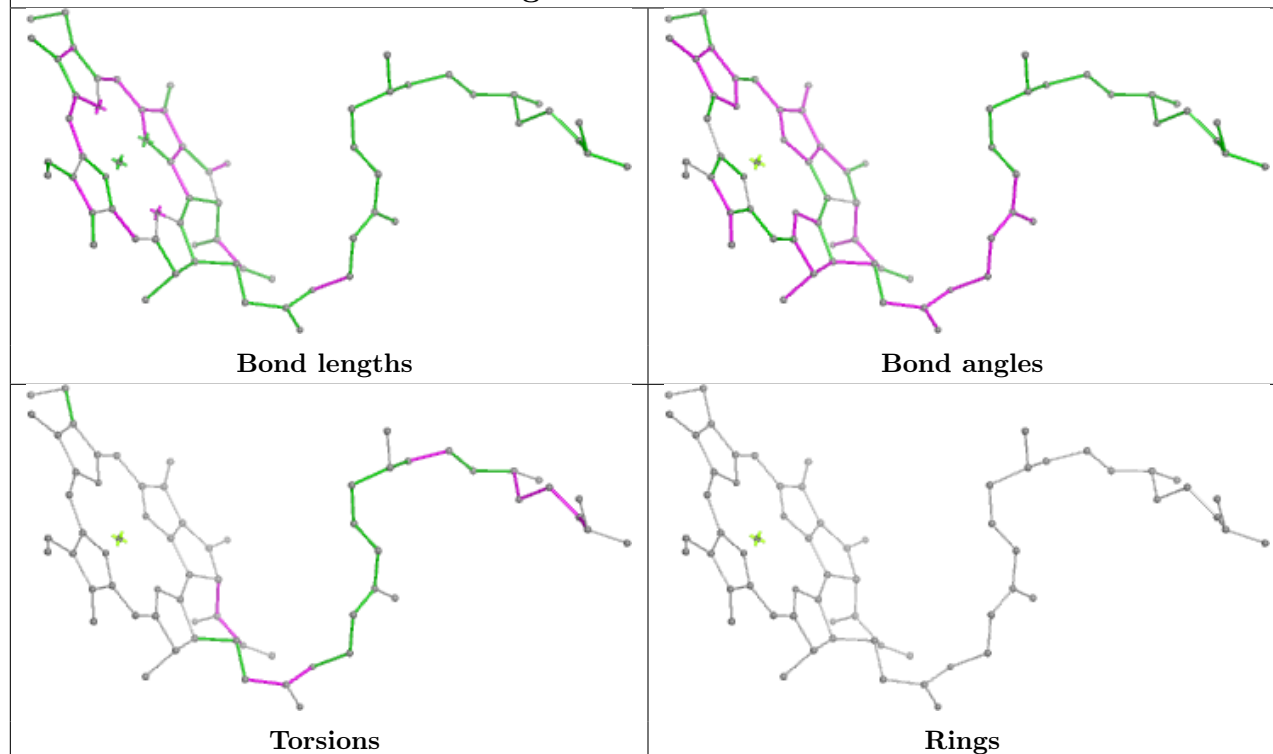
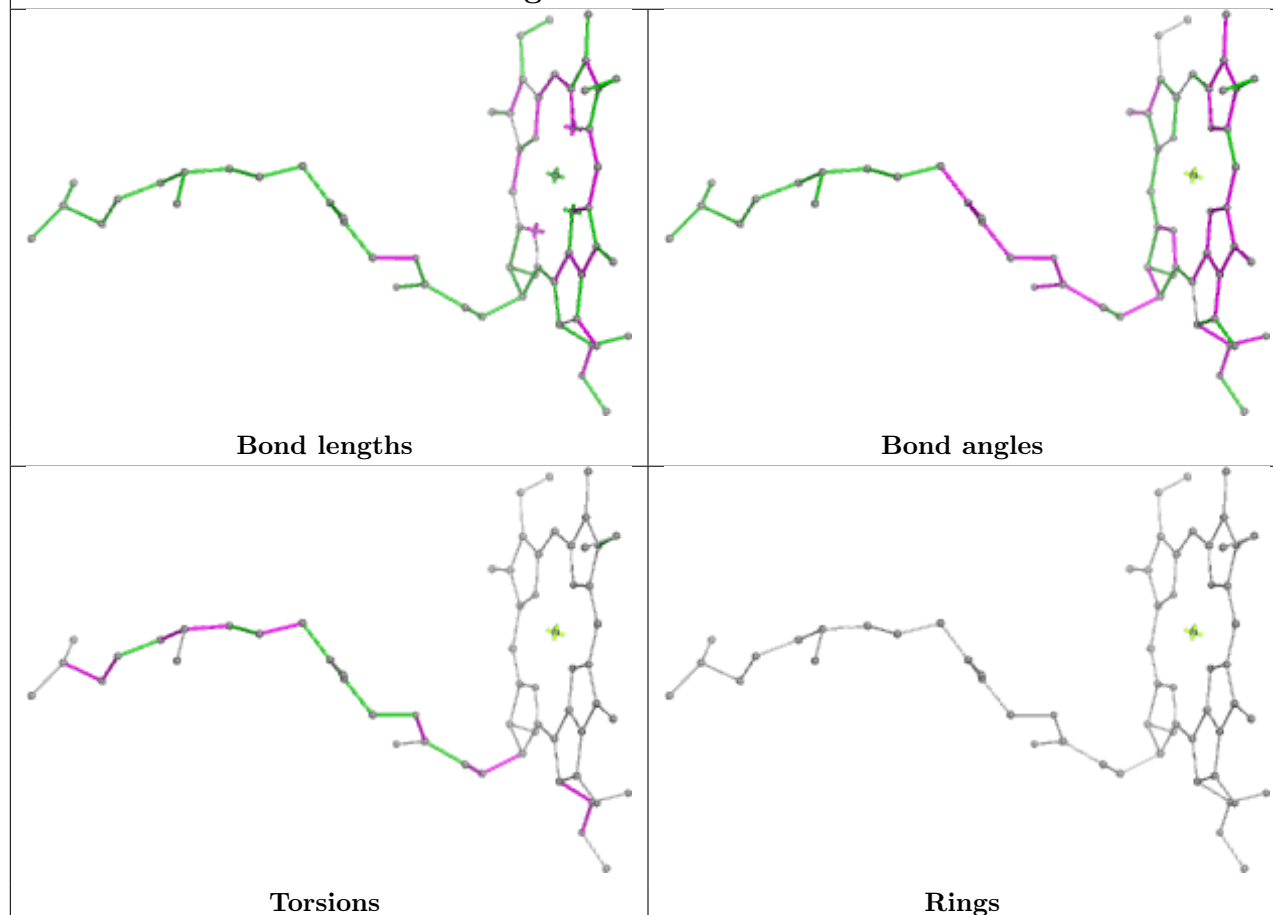


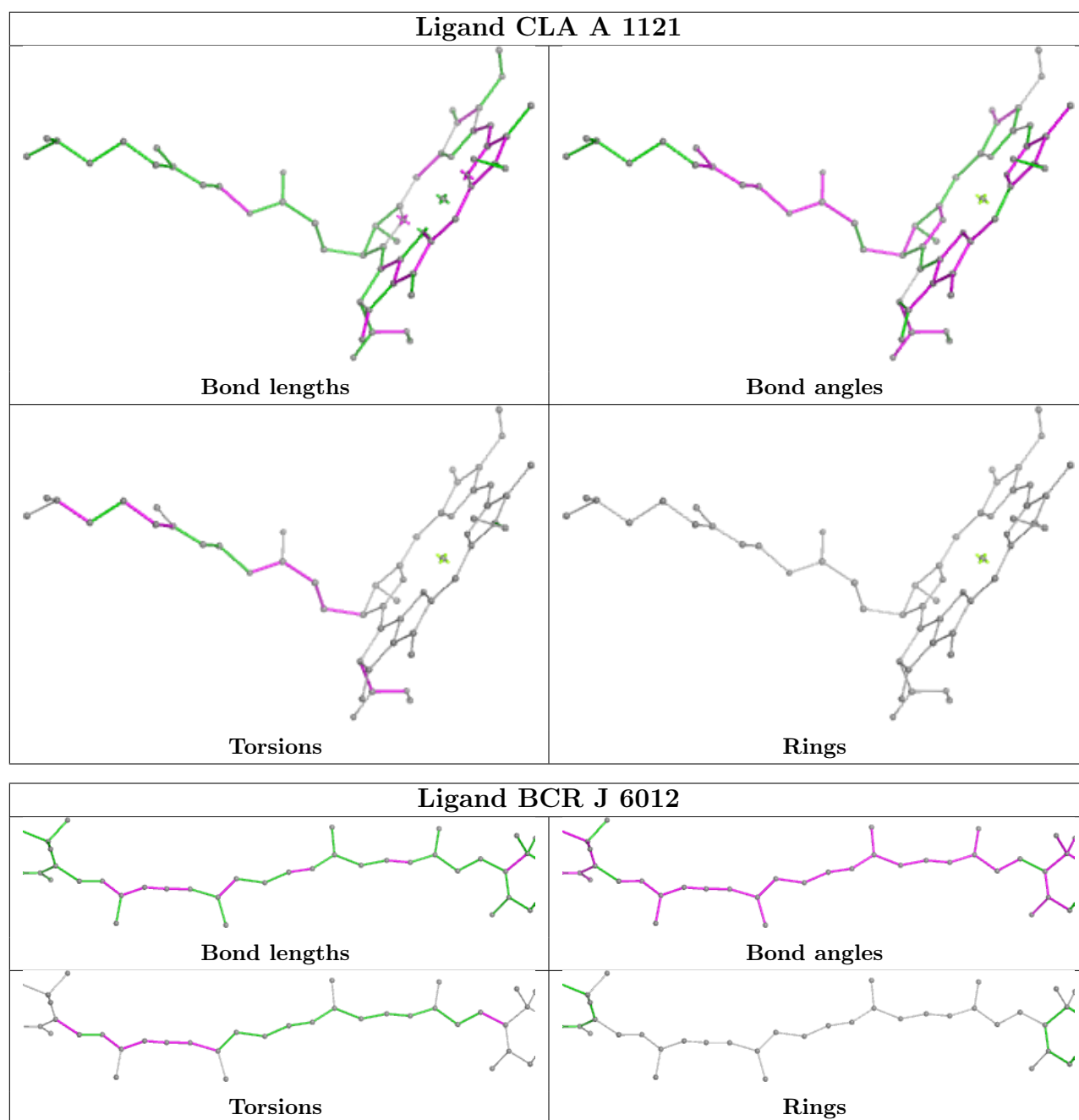




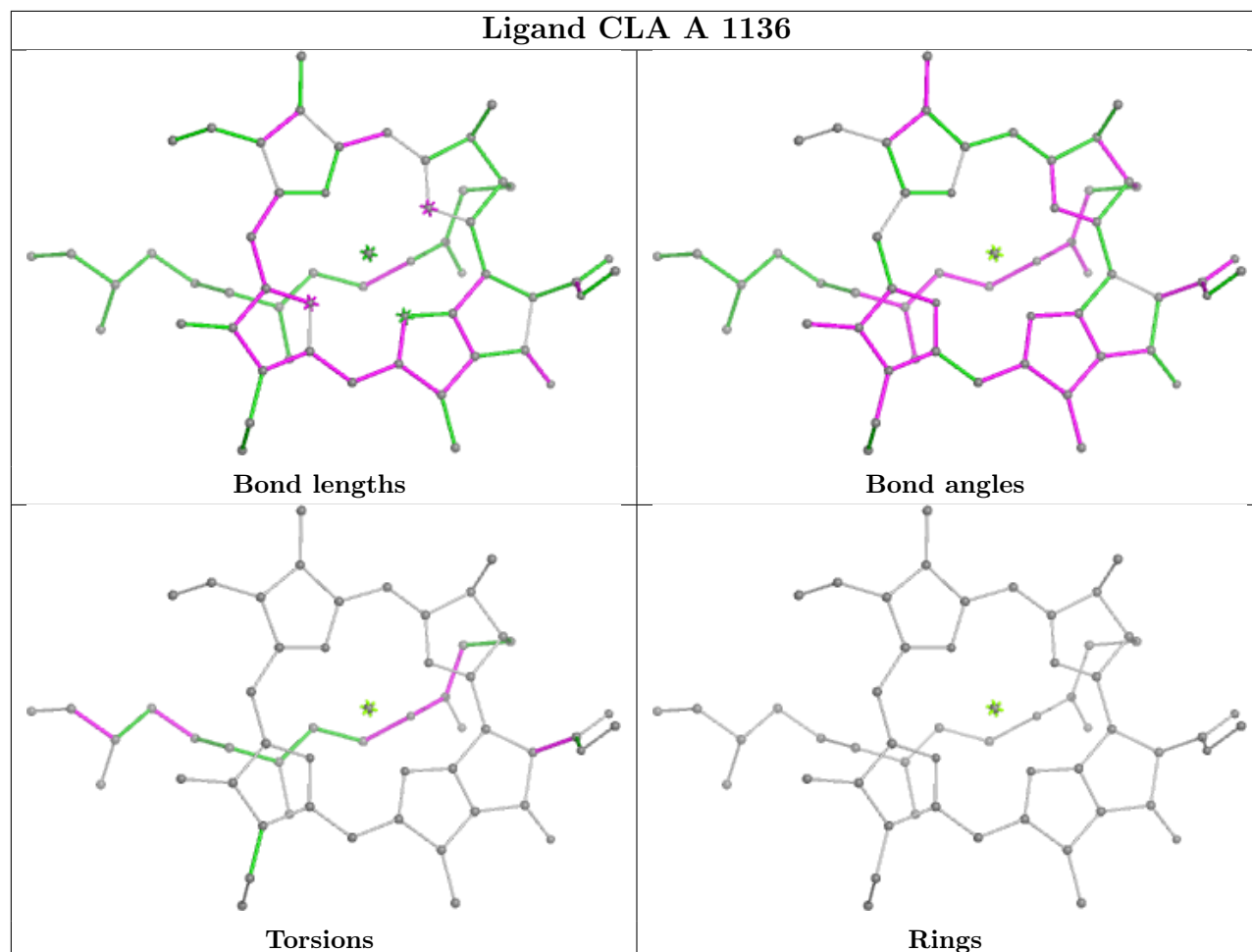
Ligand BCR B 6010**Ligand CLA A 1111**



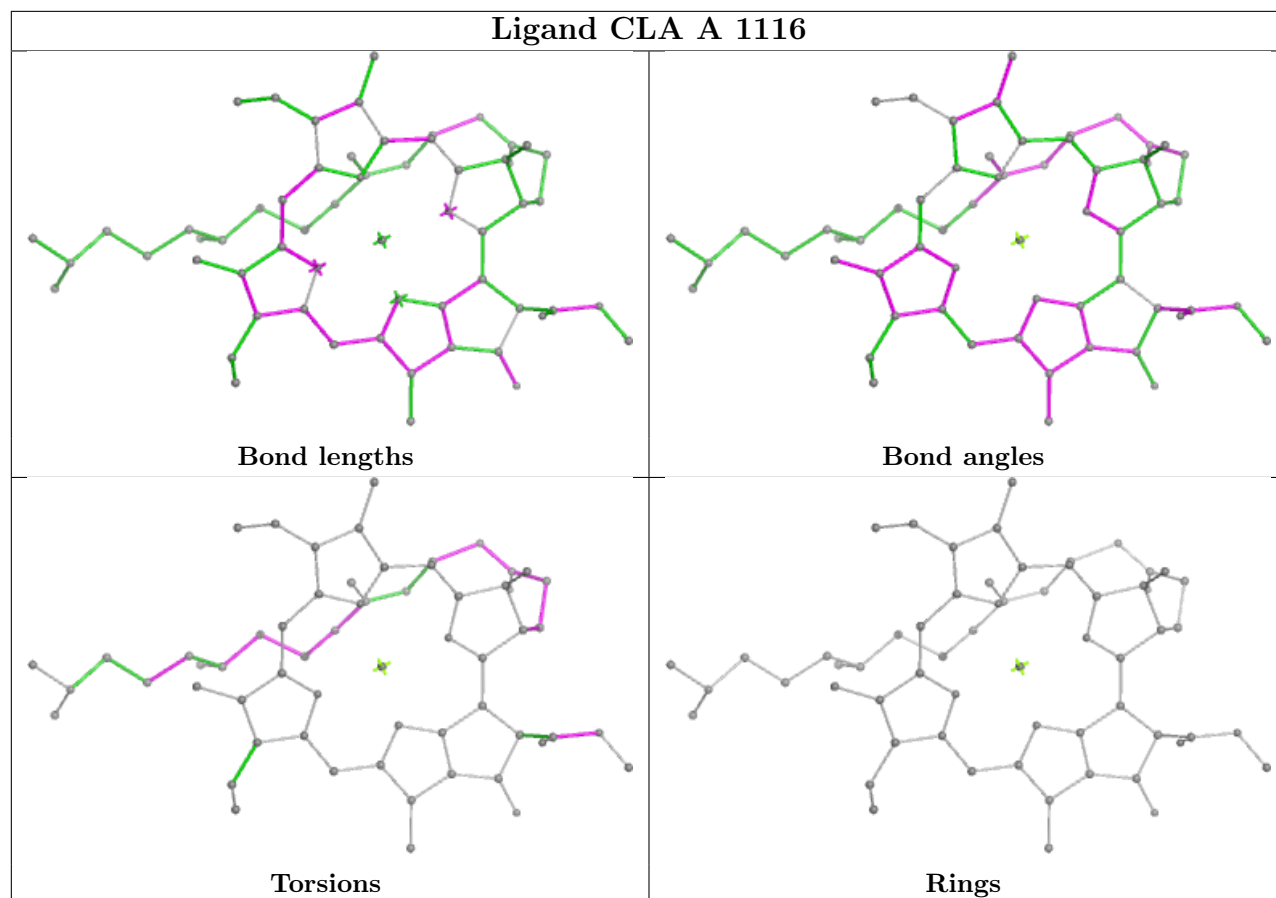
Ligand CLA B 1021**Ligand CLA L 1502**



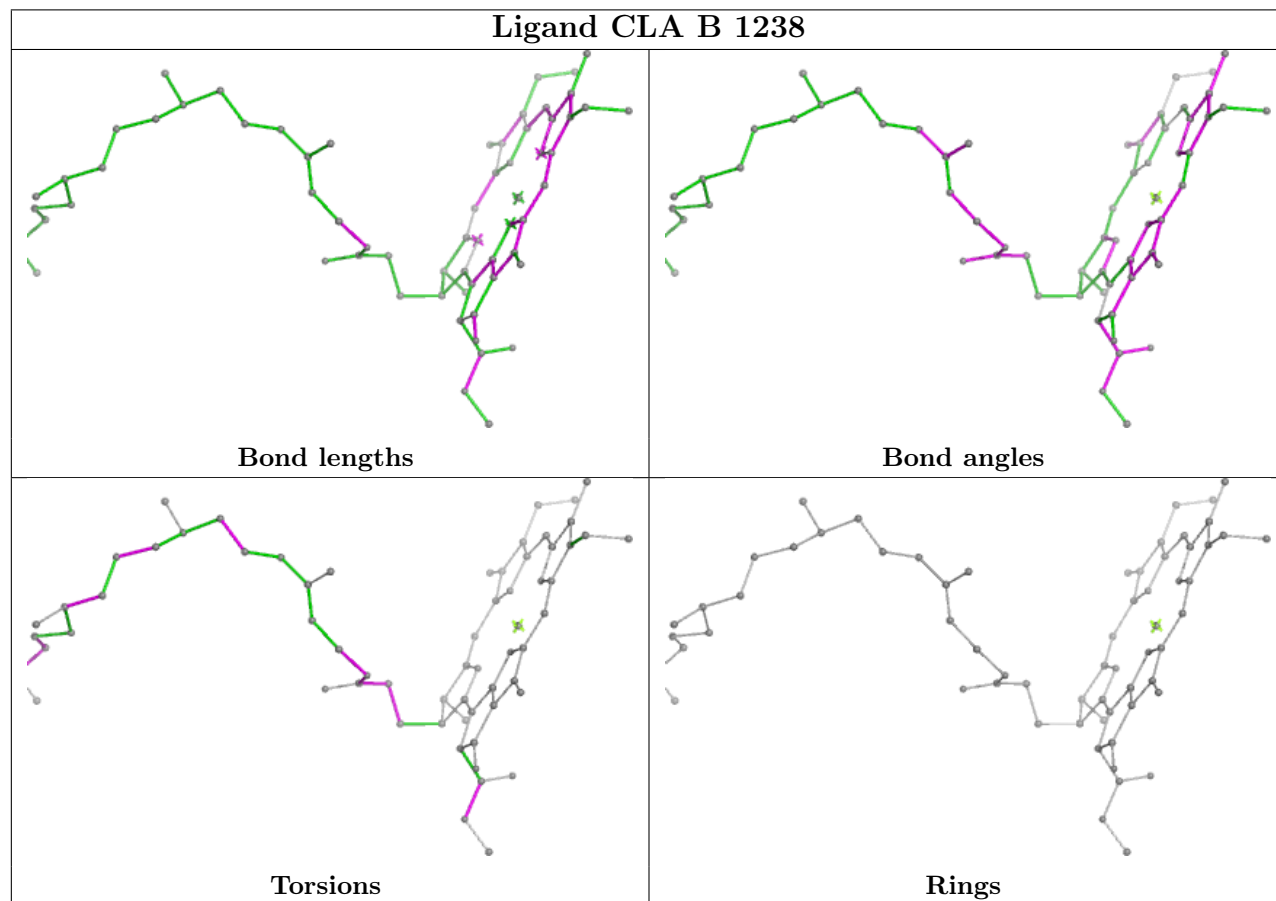
Ligand CLA A 1136



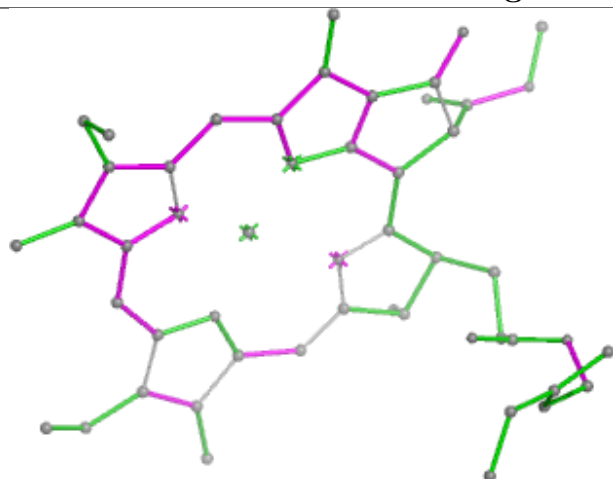
Ligand CLA A 1116



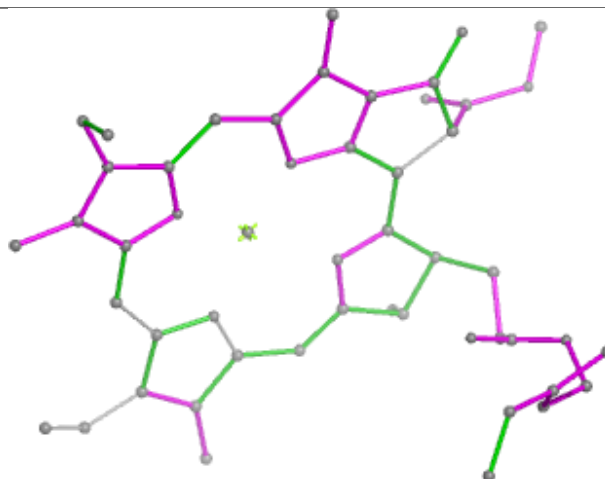
Ligand CLA B 1238



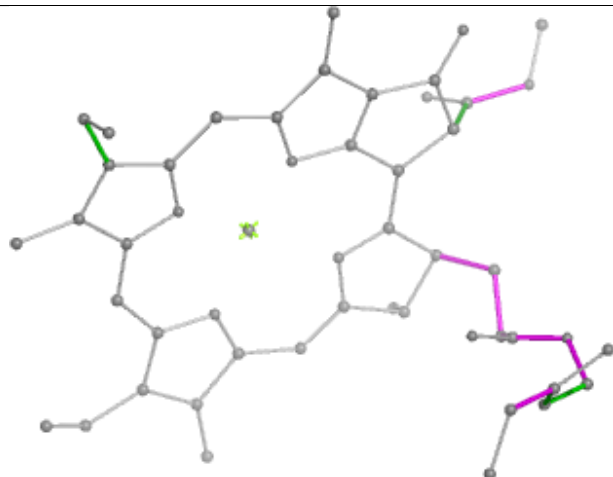
Ligand CLA A 1105



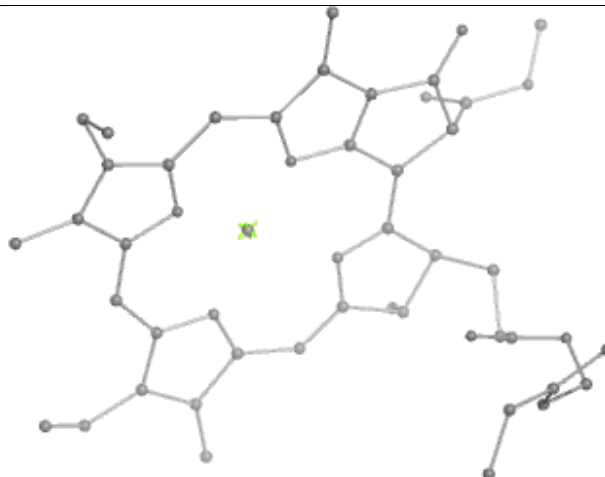
Bond lengths



Bond angles

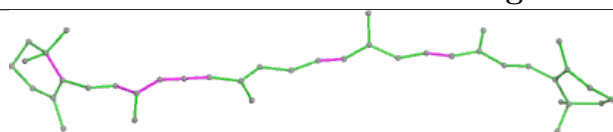


Torsions

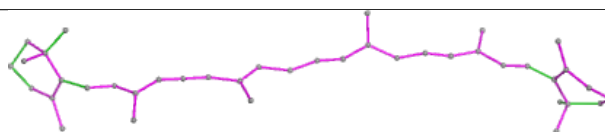


Rings

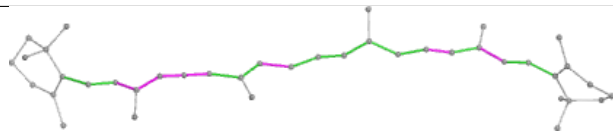
Ligand BCR L 6020



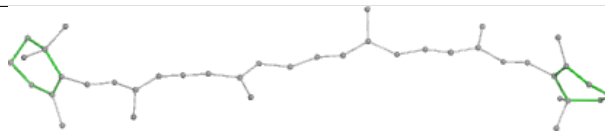
Bond lengths



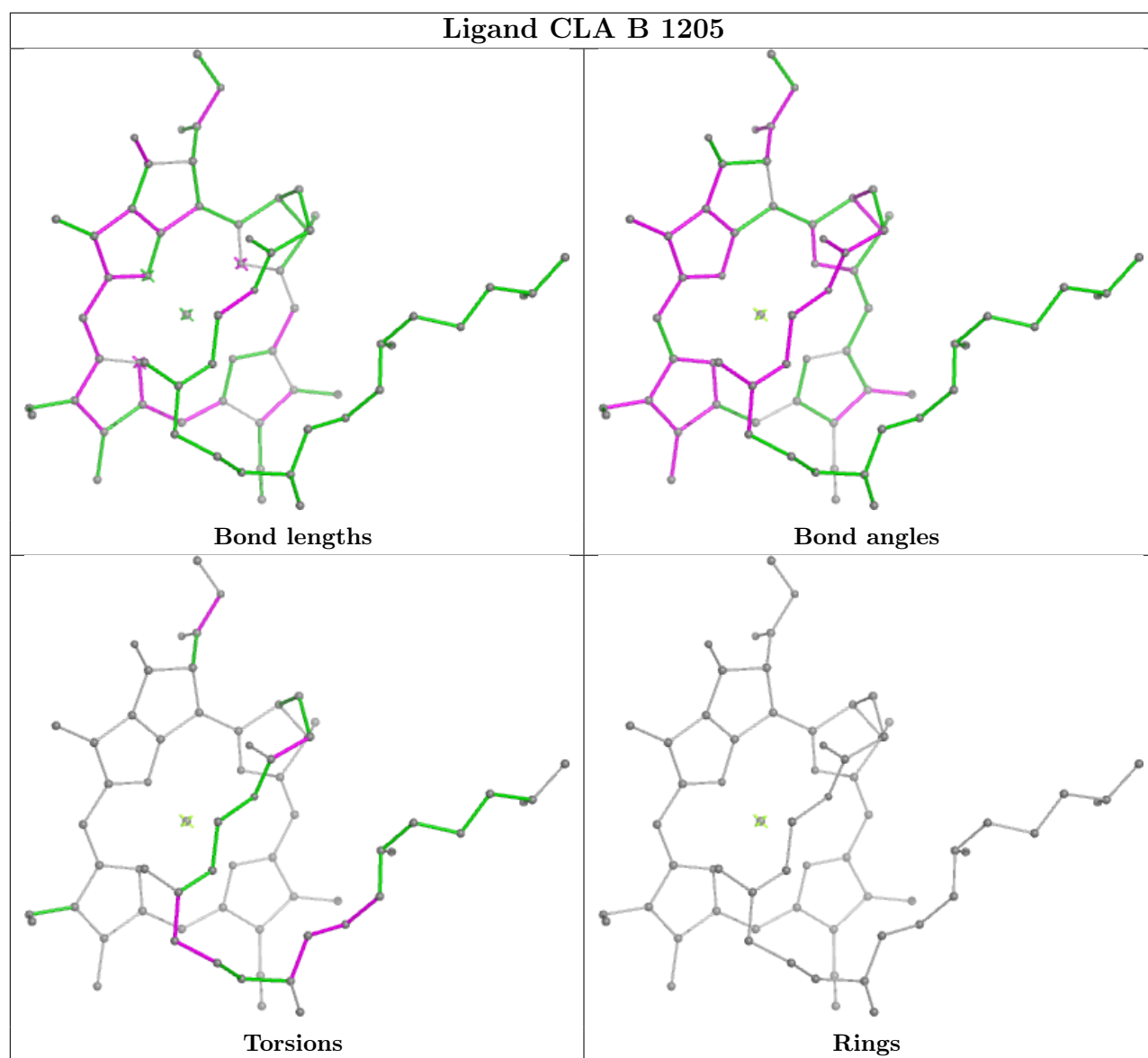
Bond angles

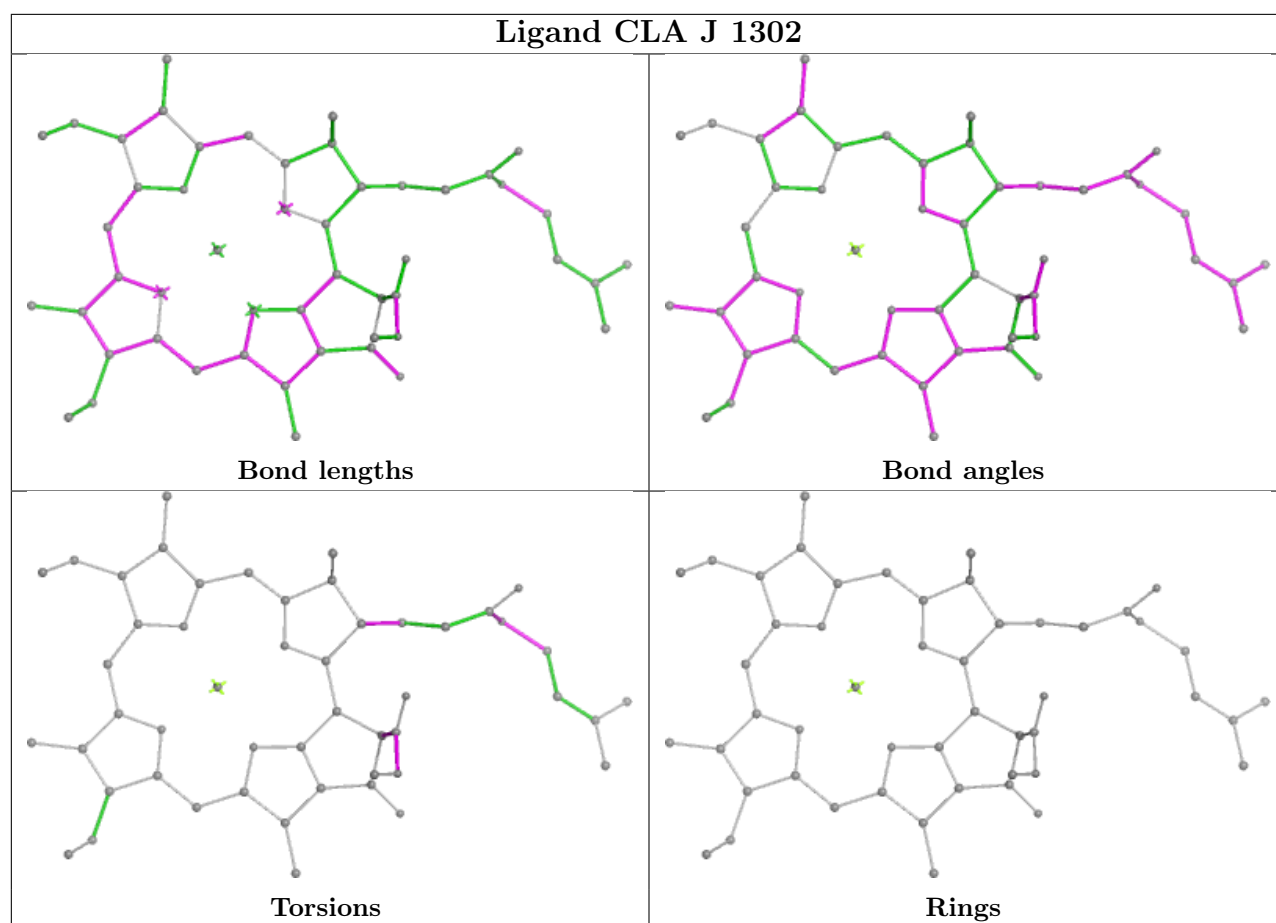


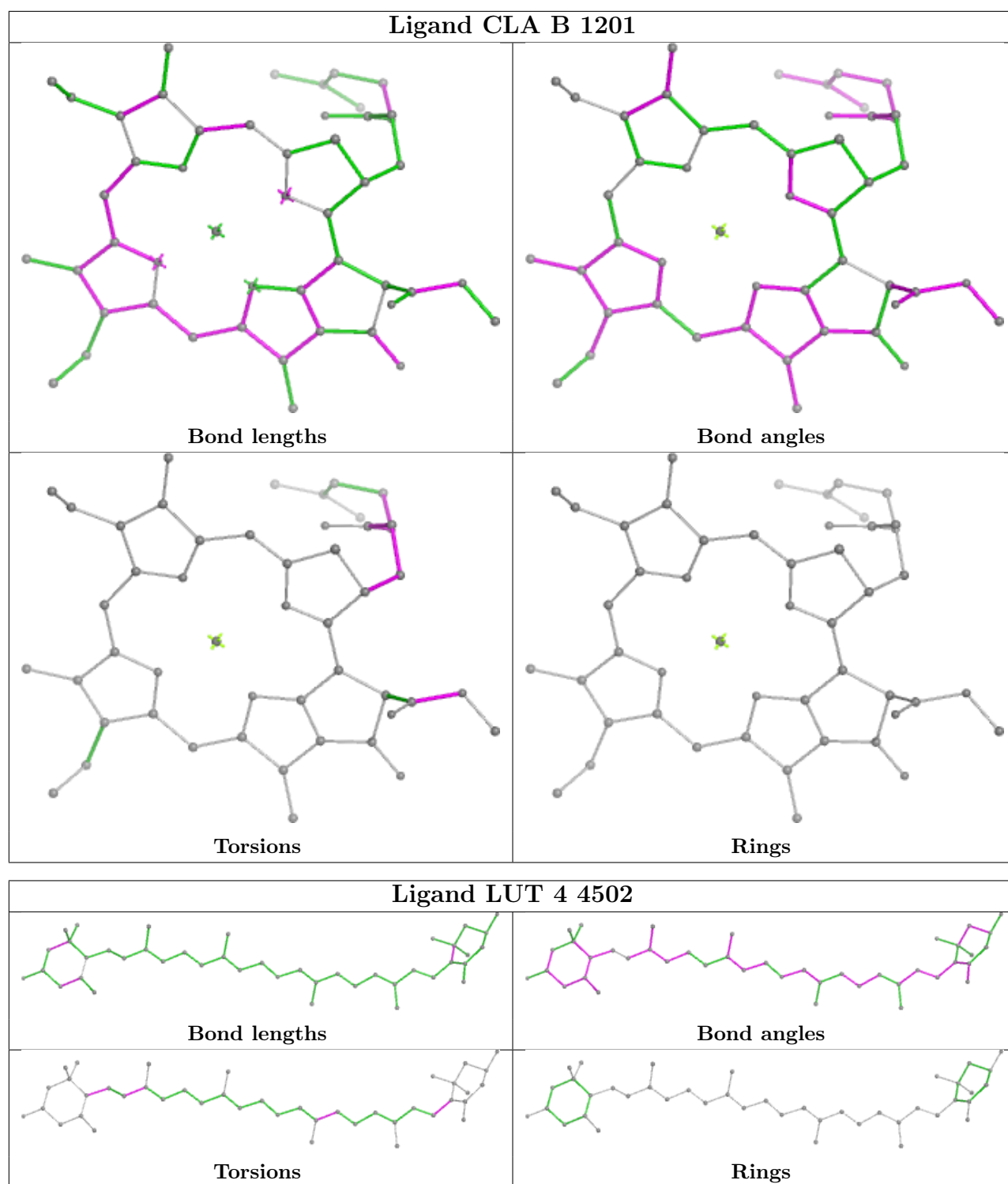
Torsions



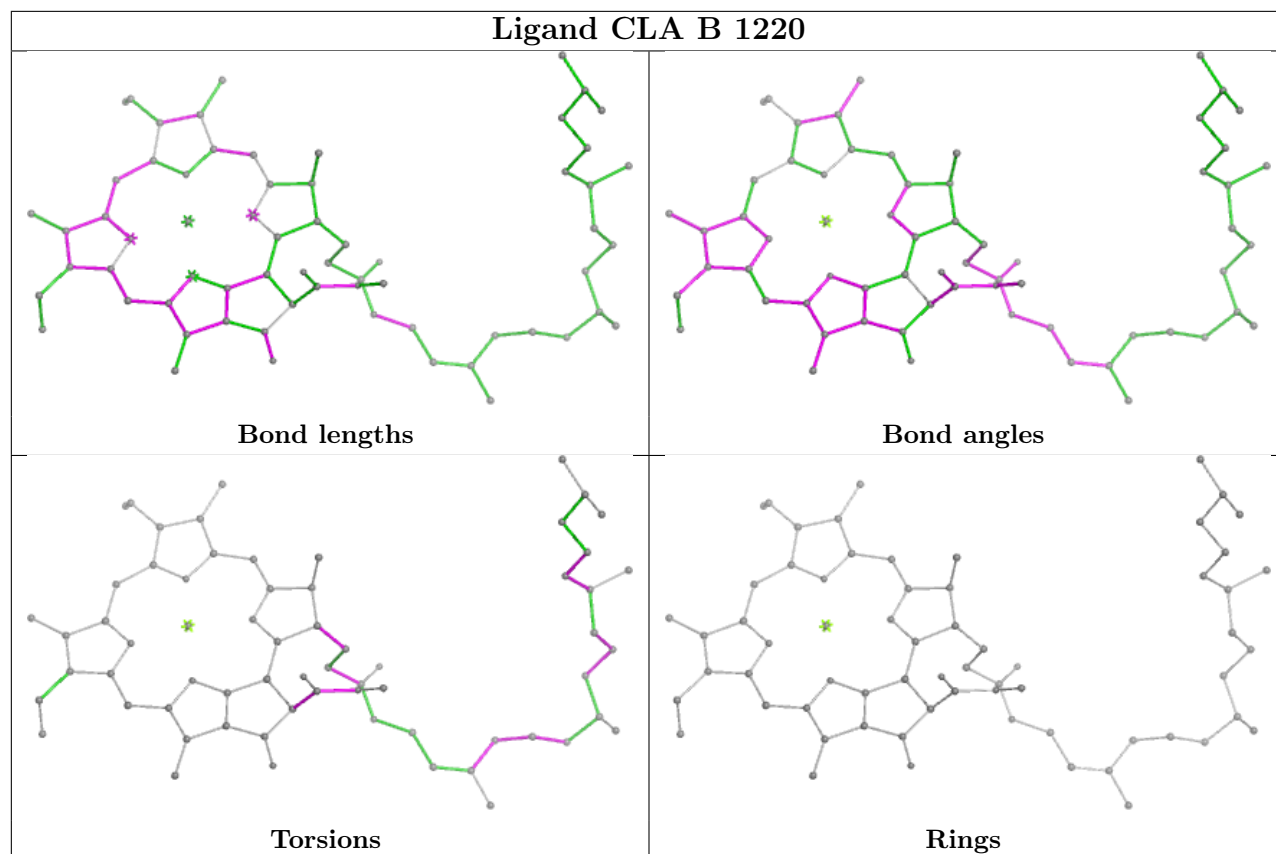
Rings



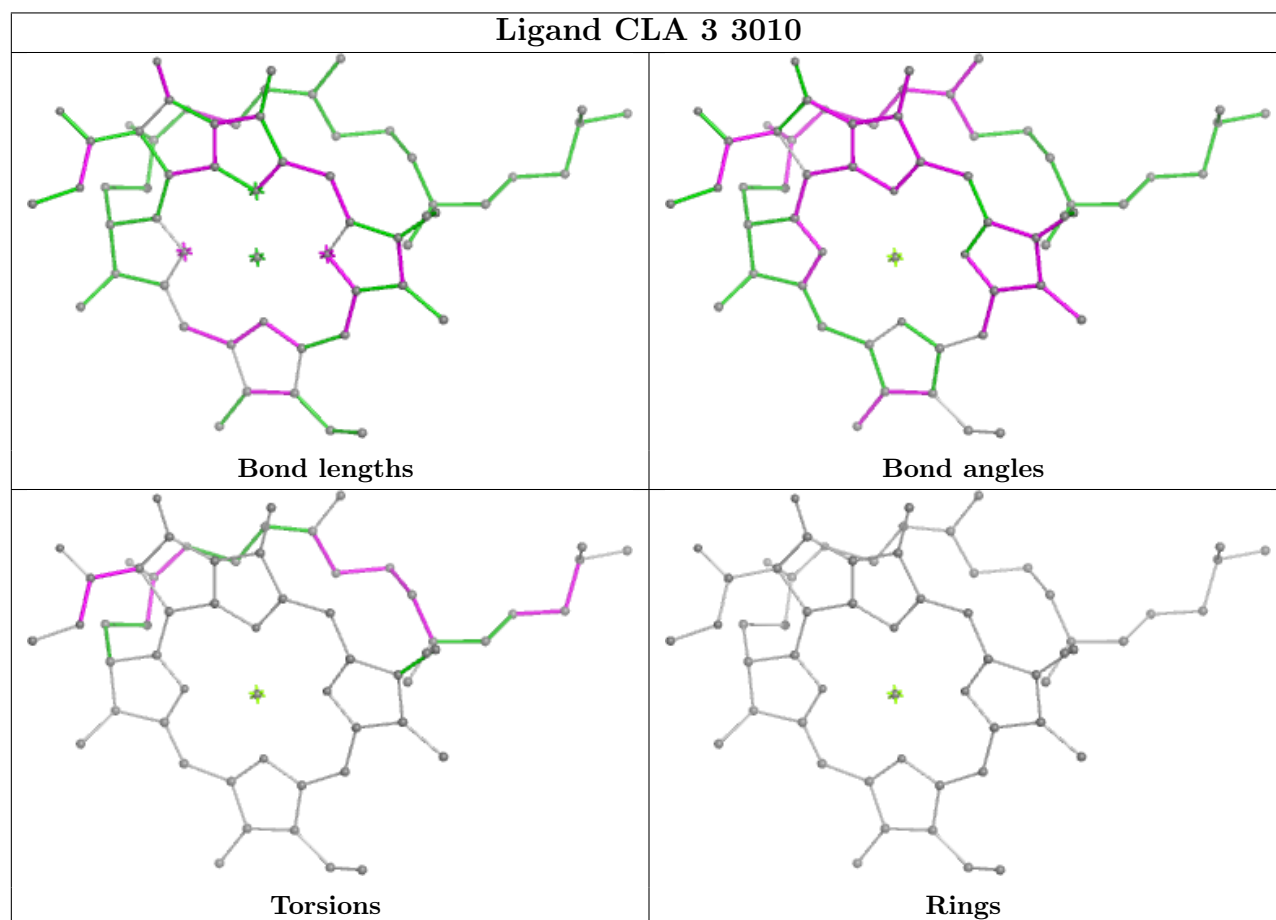


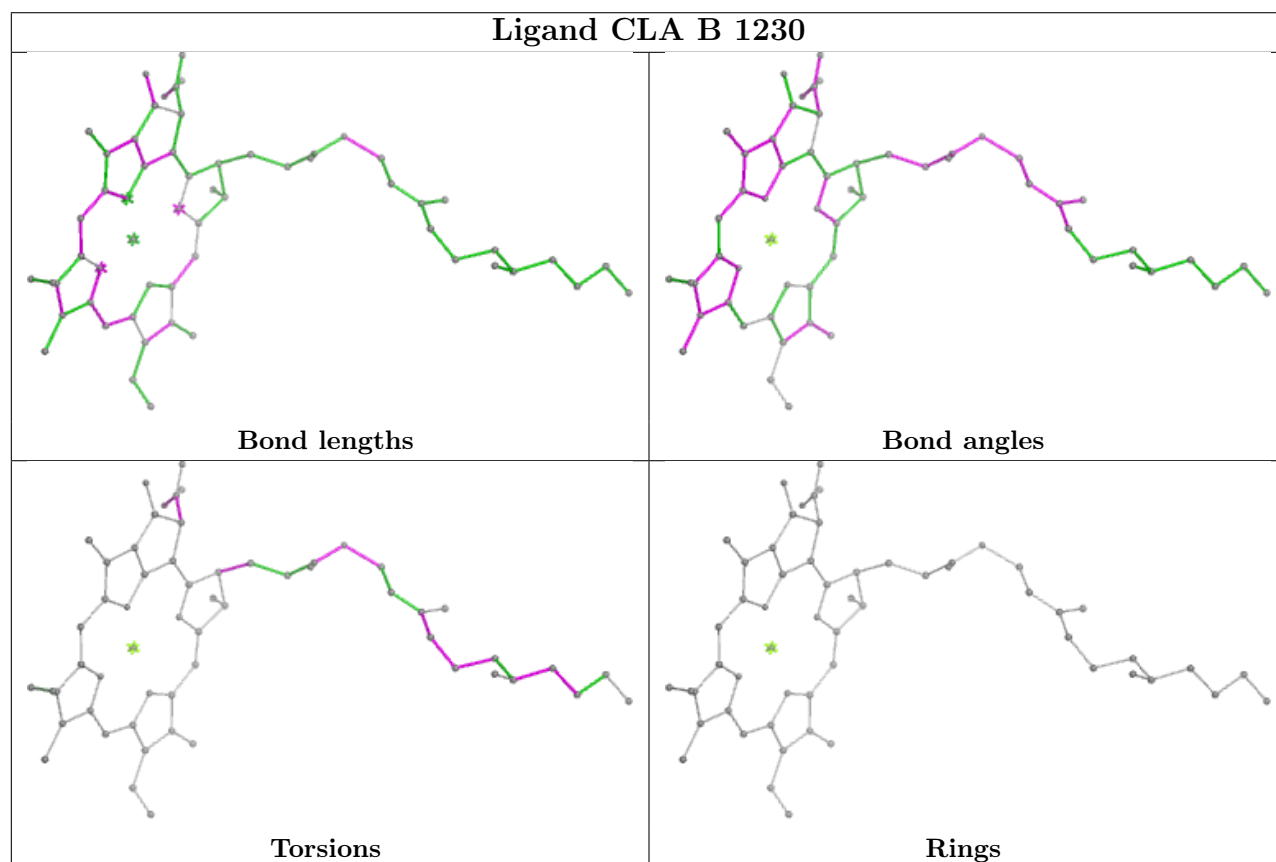
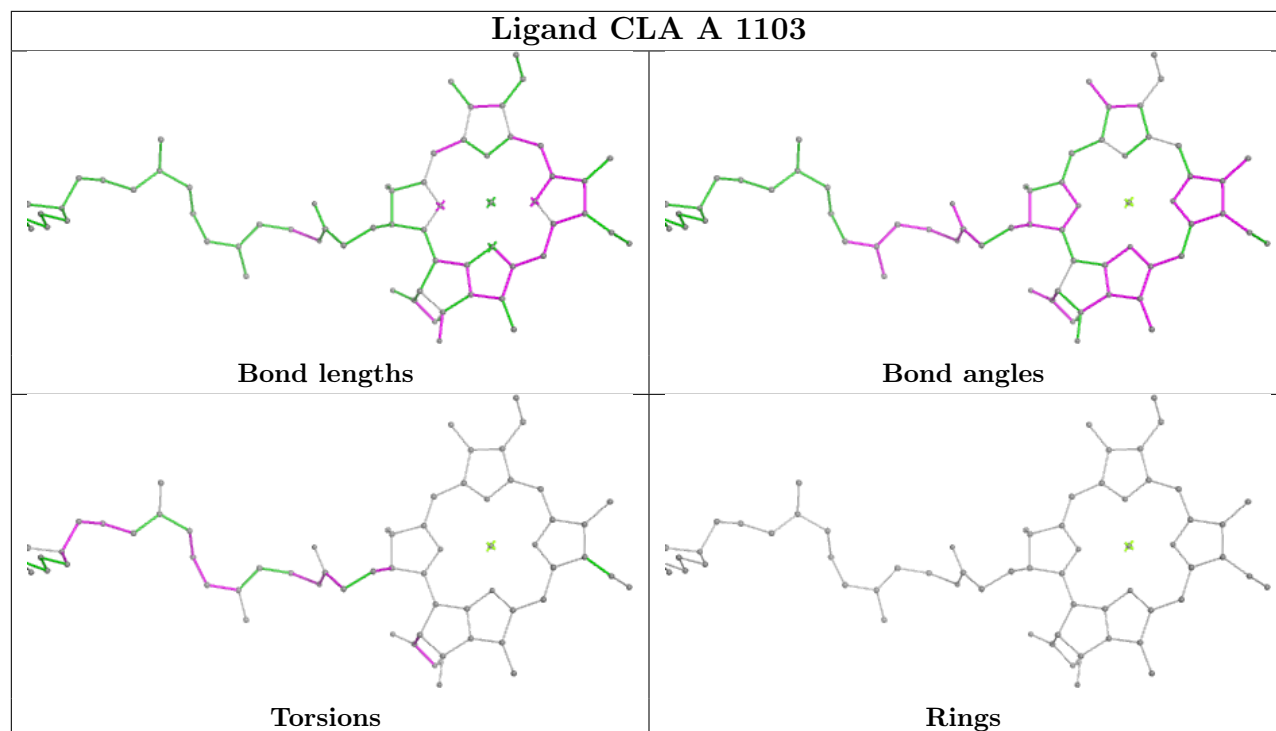


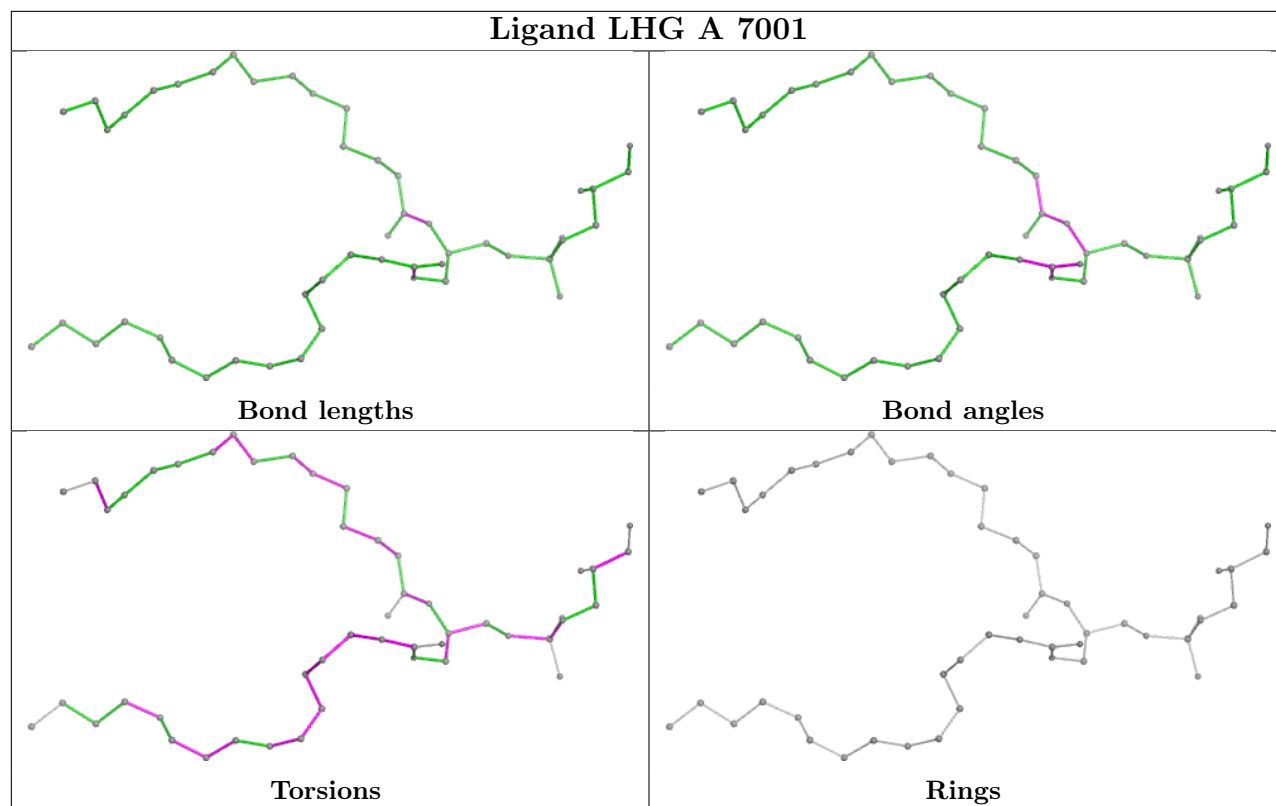
Ligand CLA B 1220



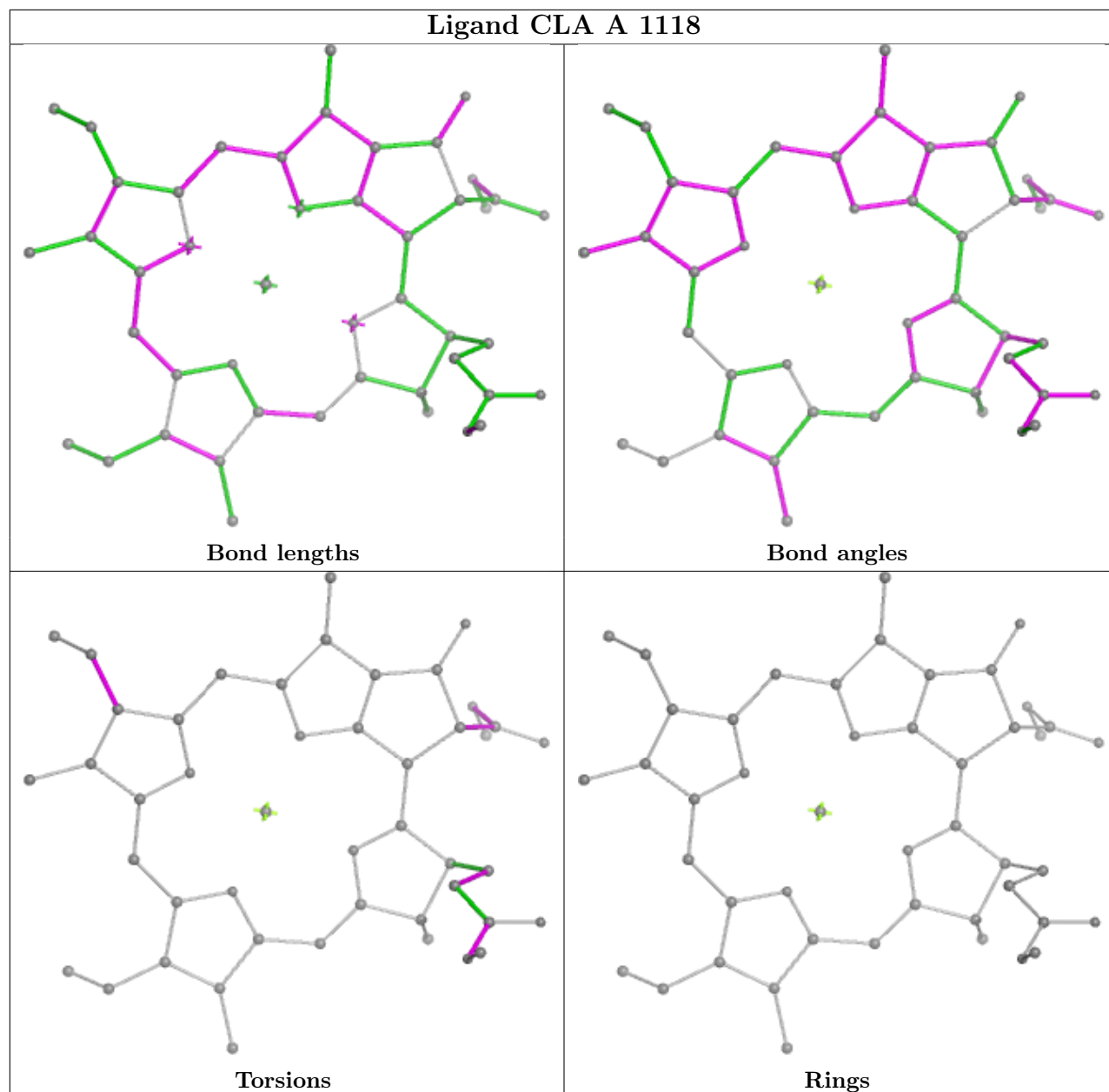
Ligand CLA 3 3010

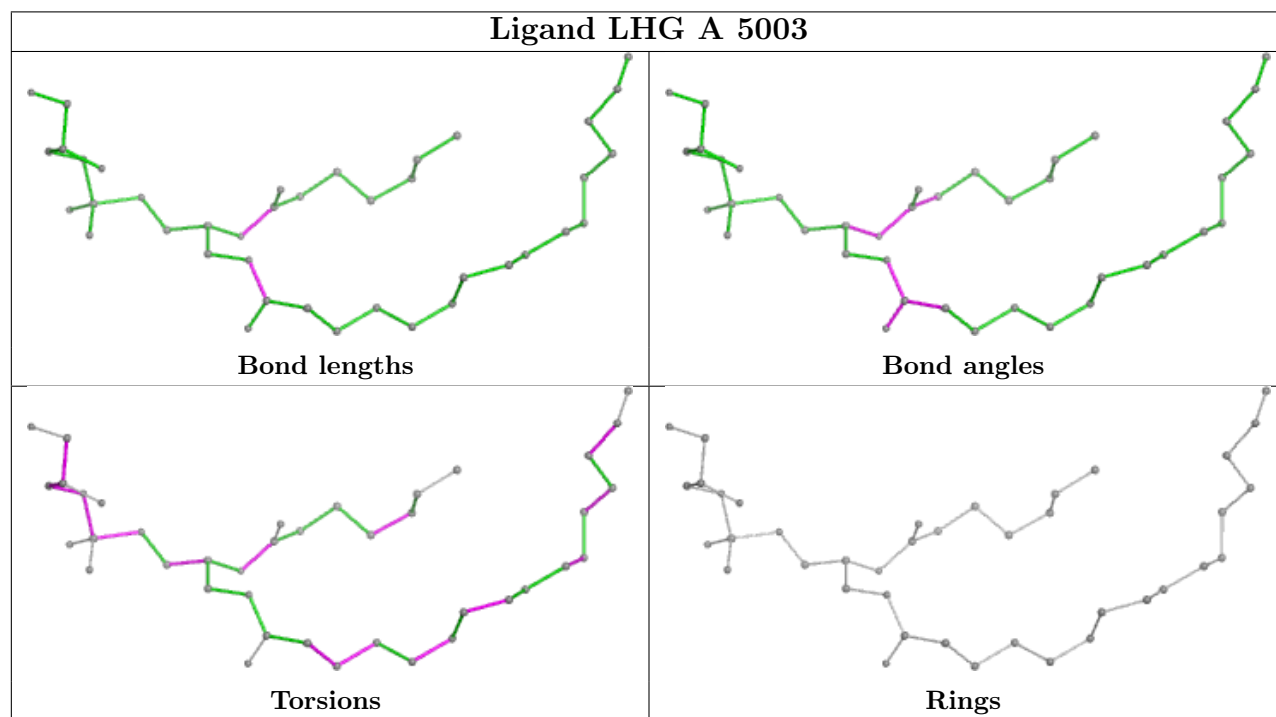
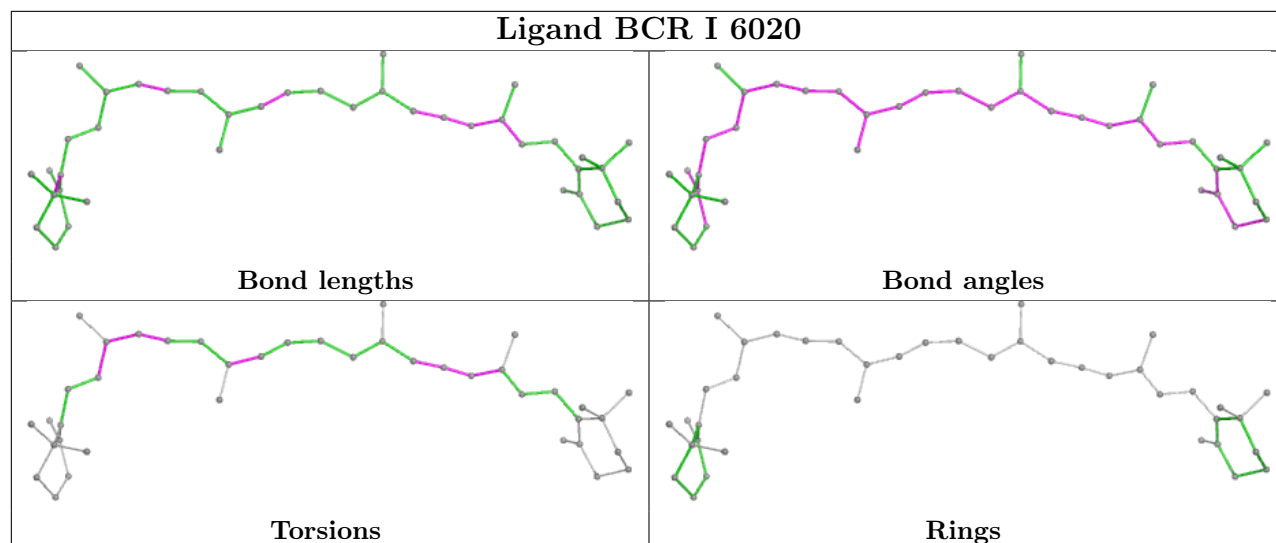


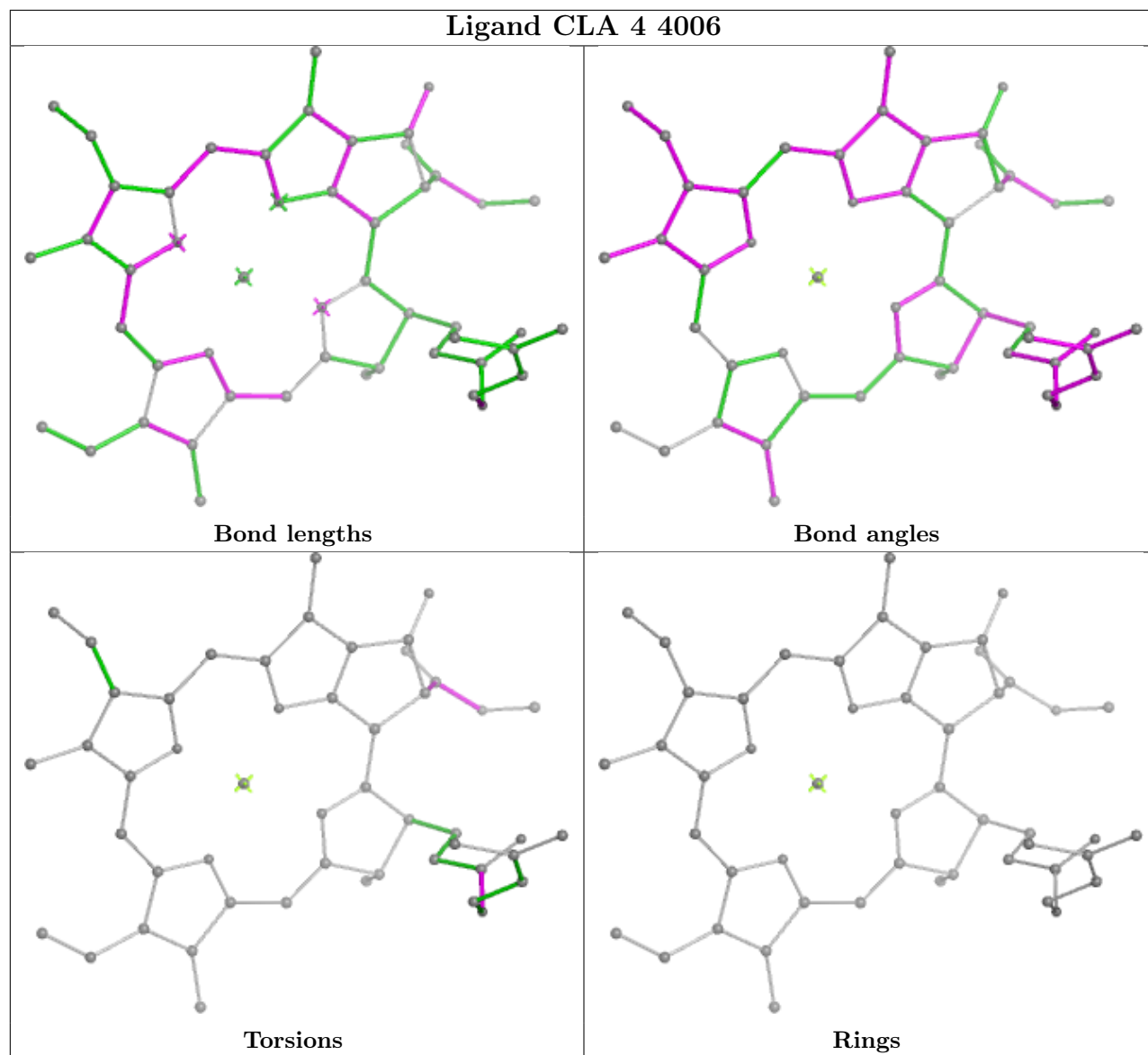




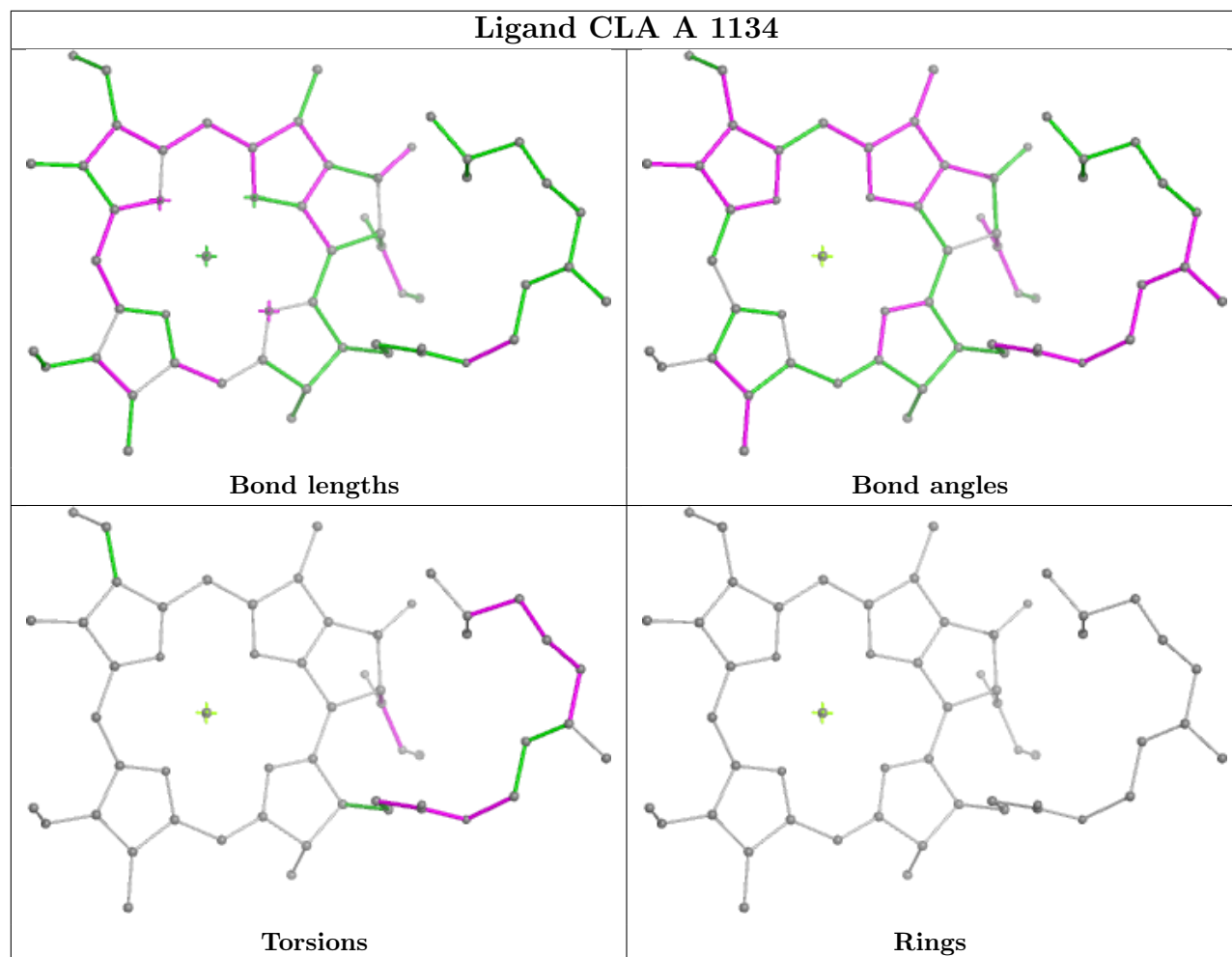
Ligand CLA A 1118

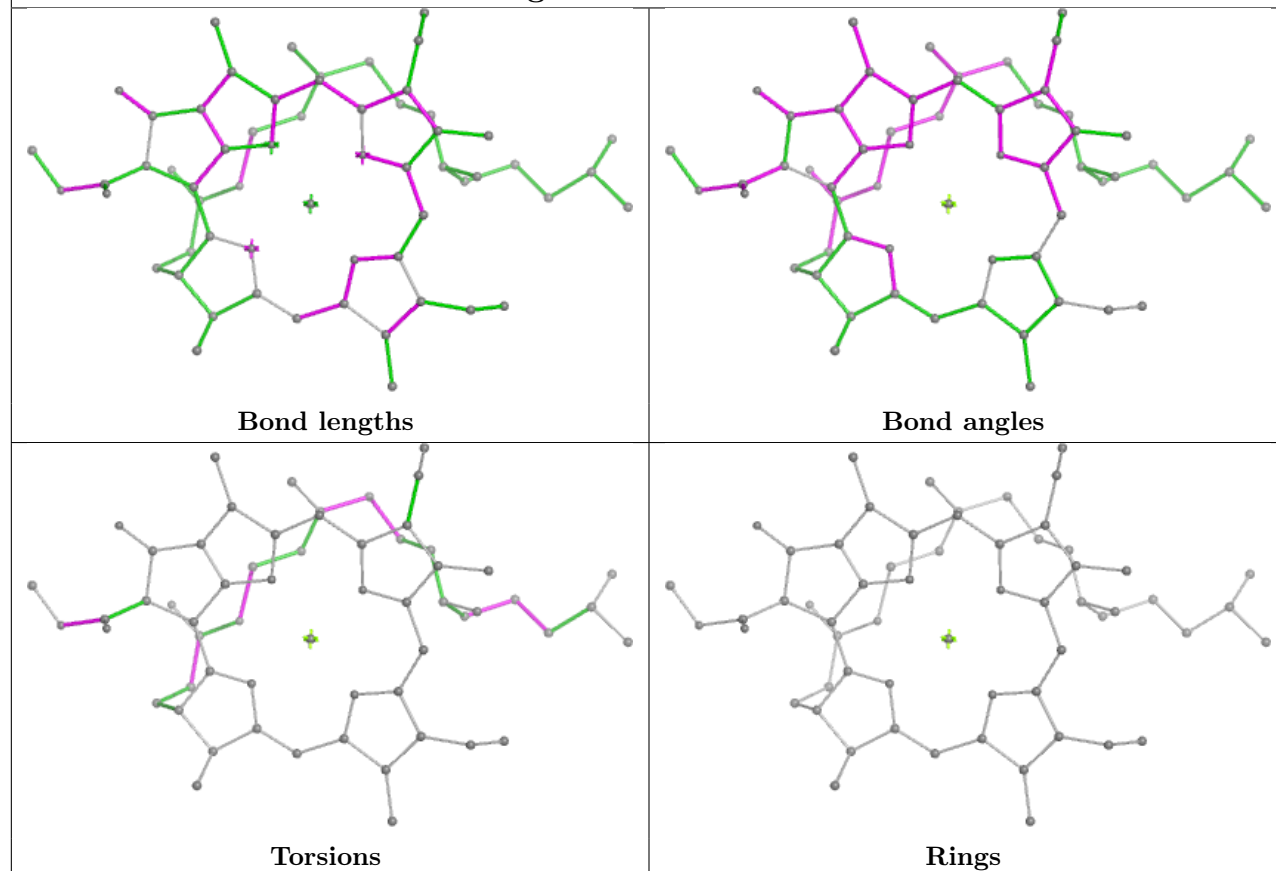
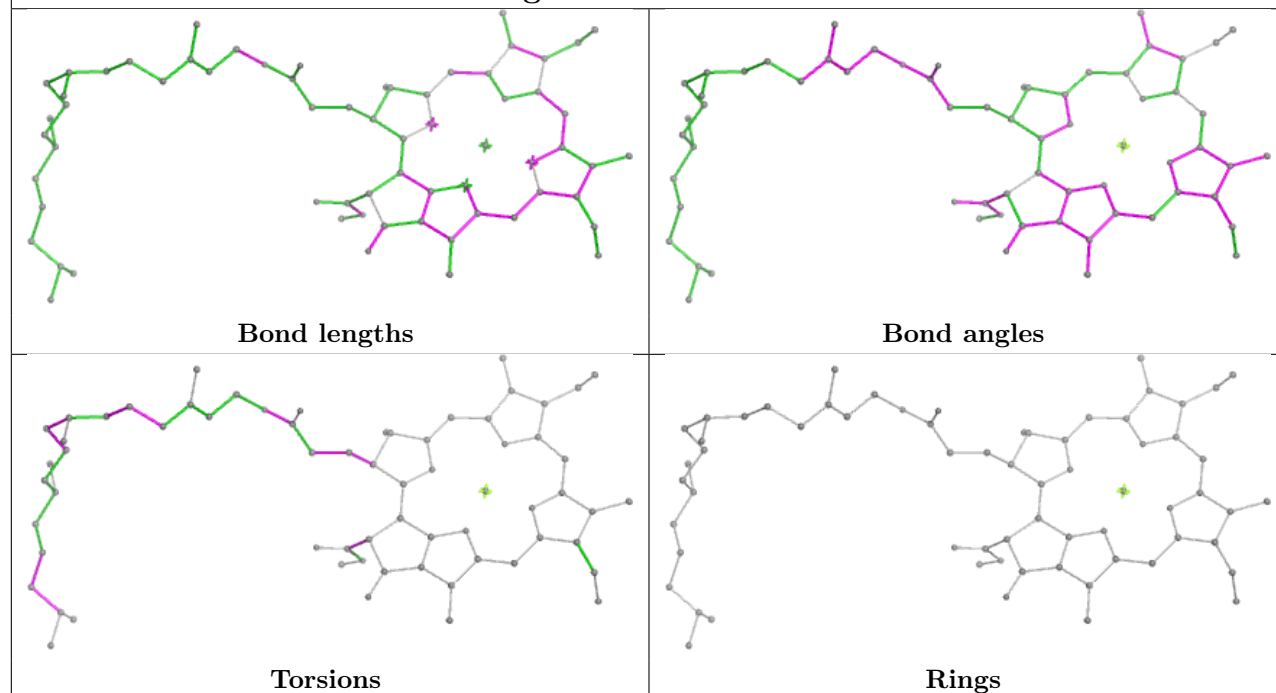


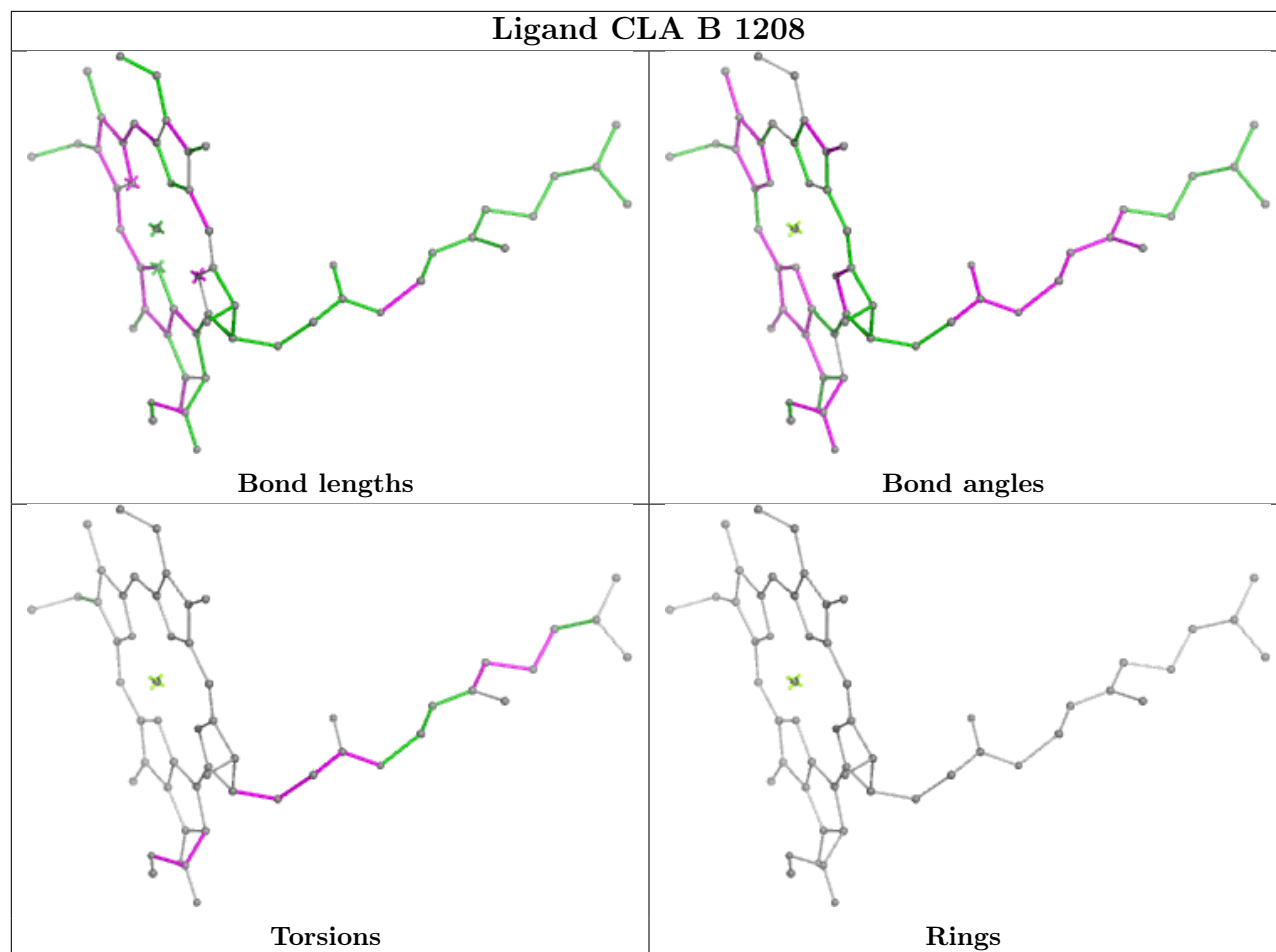


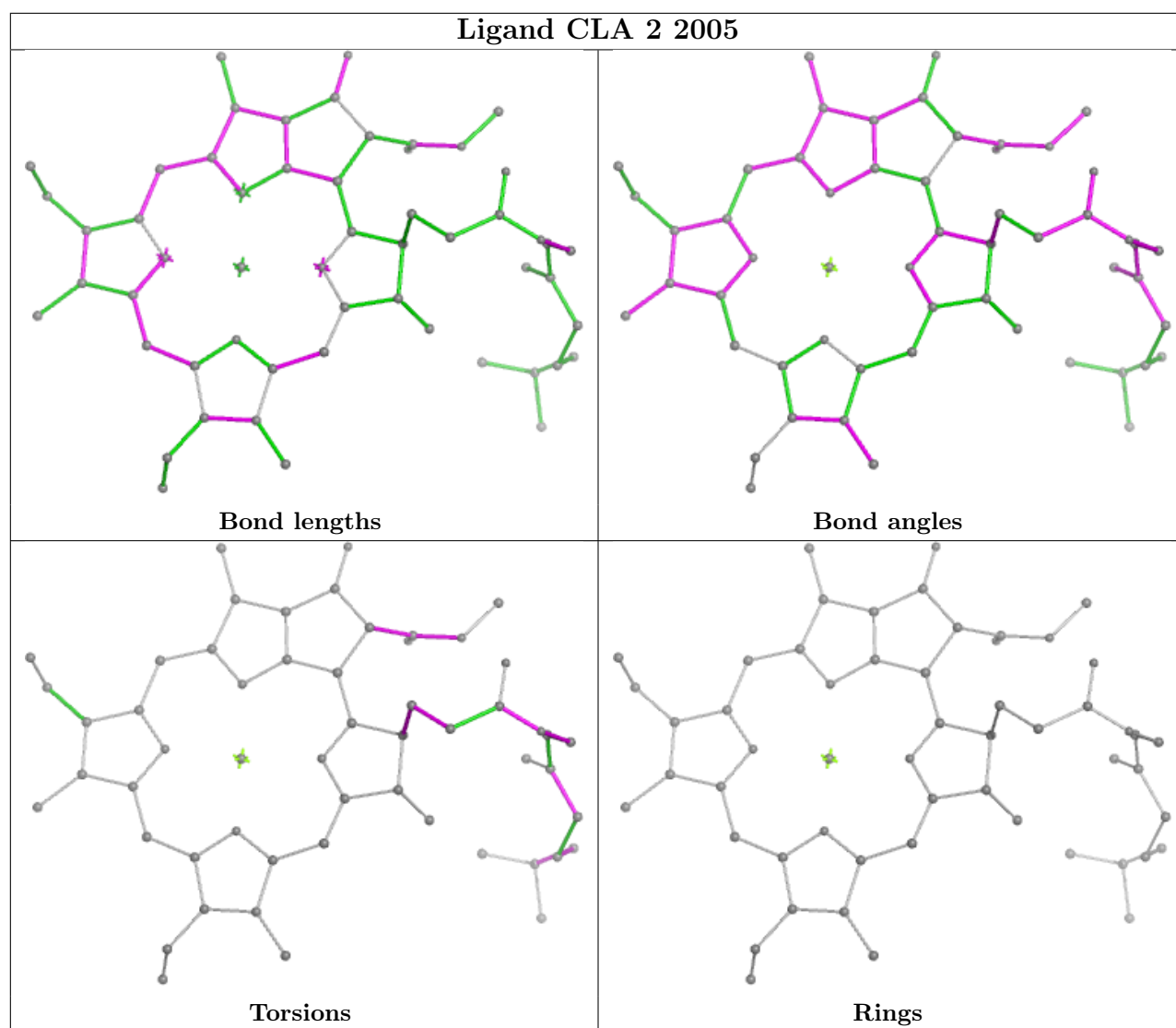


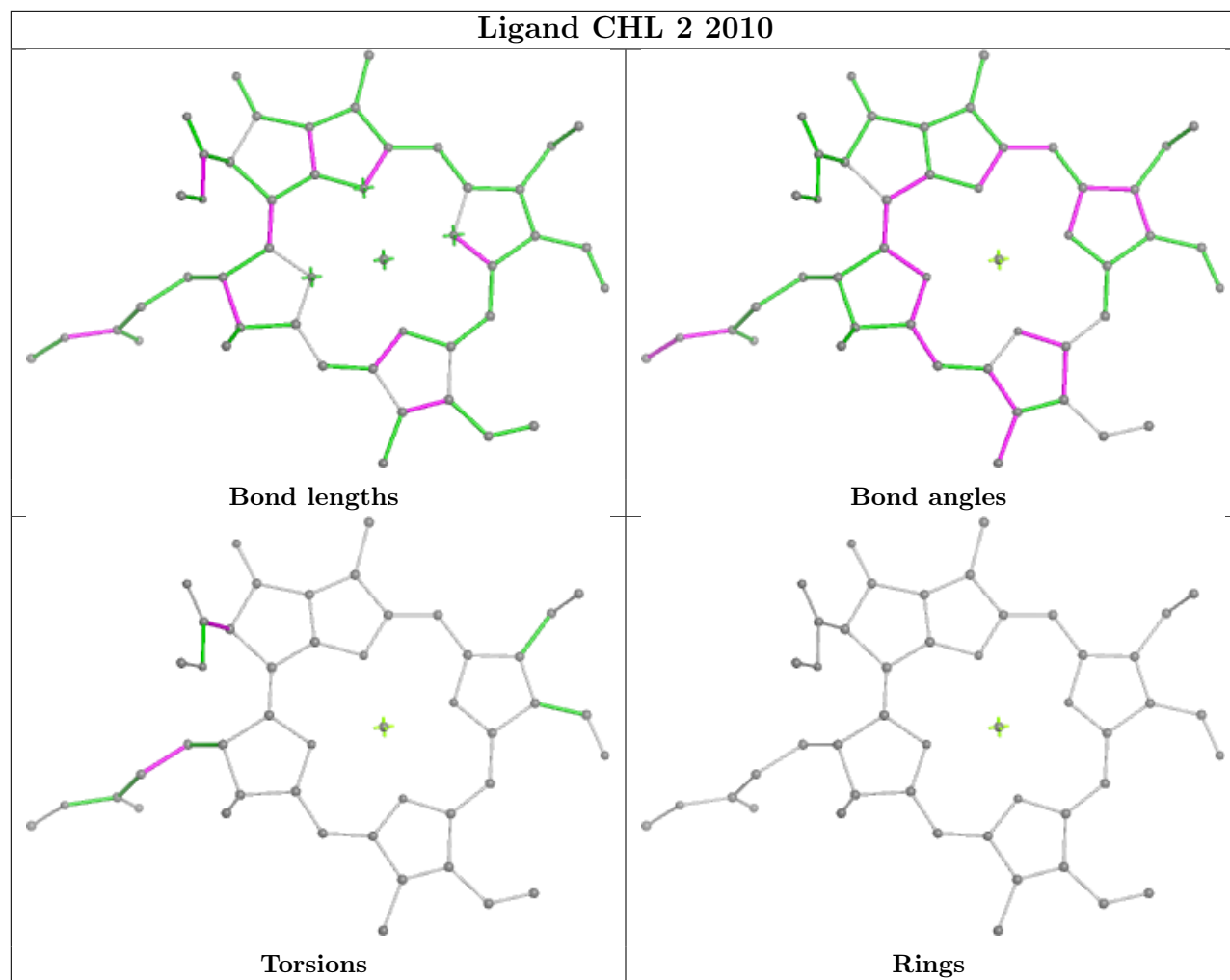
Ligand CLA A 1134

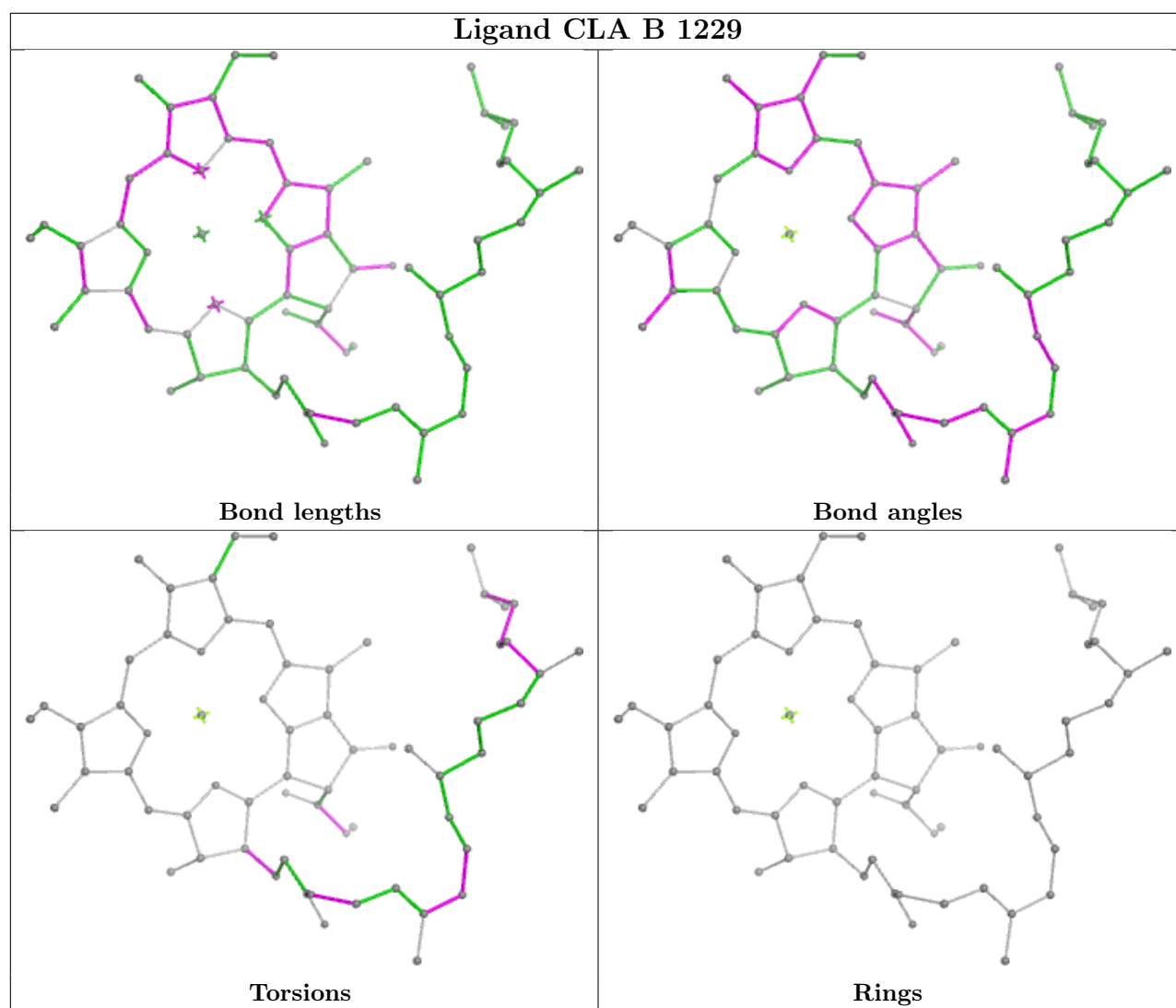


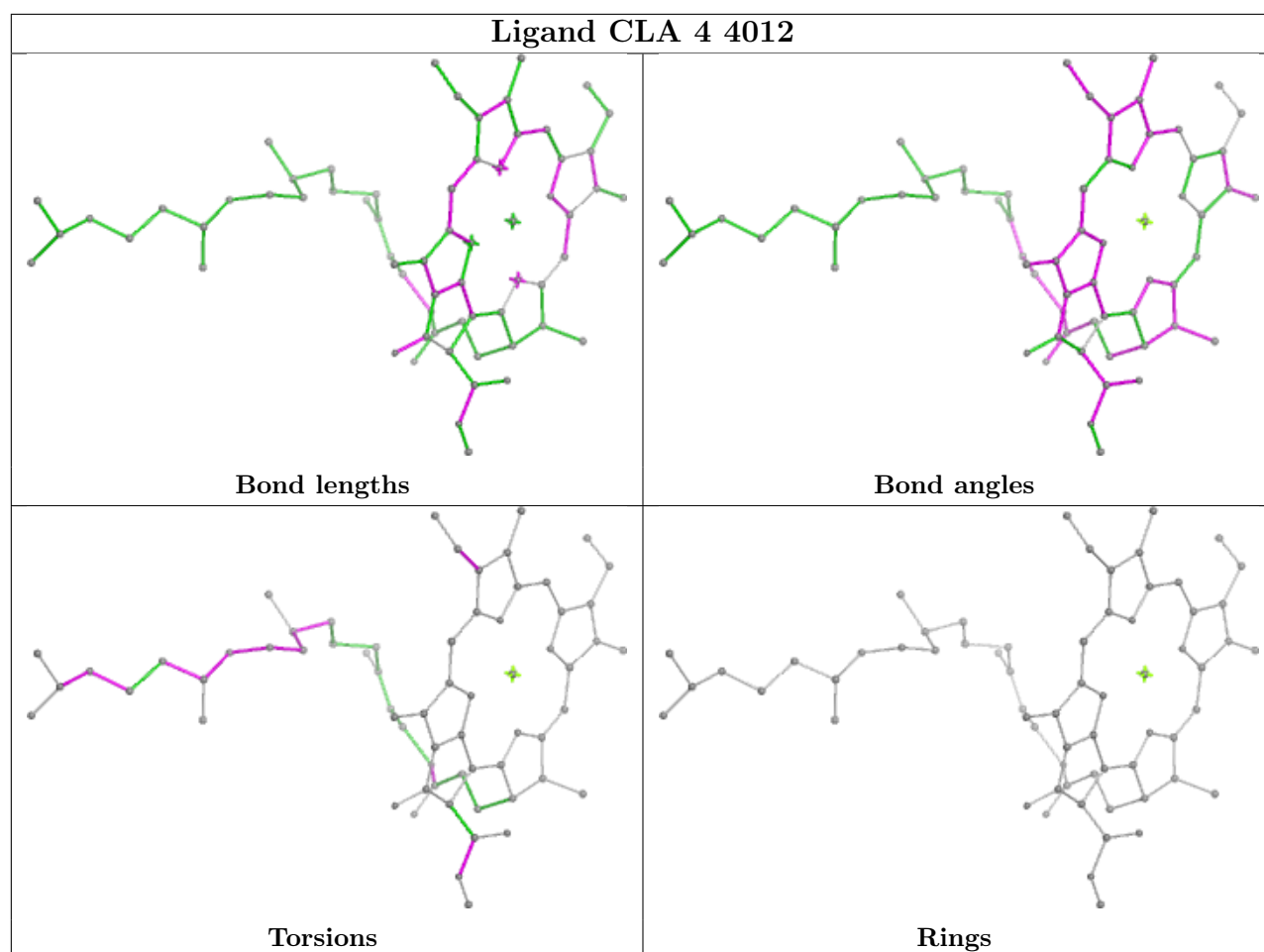
Ligand CLA 3 3003**Ligand CLA B 1223**

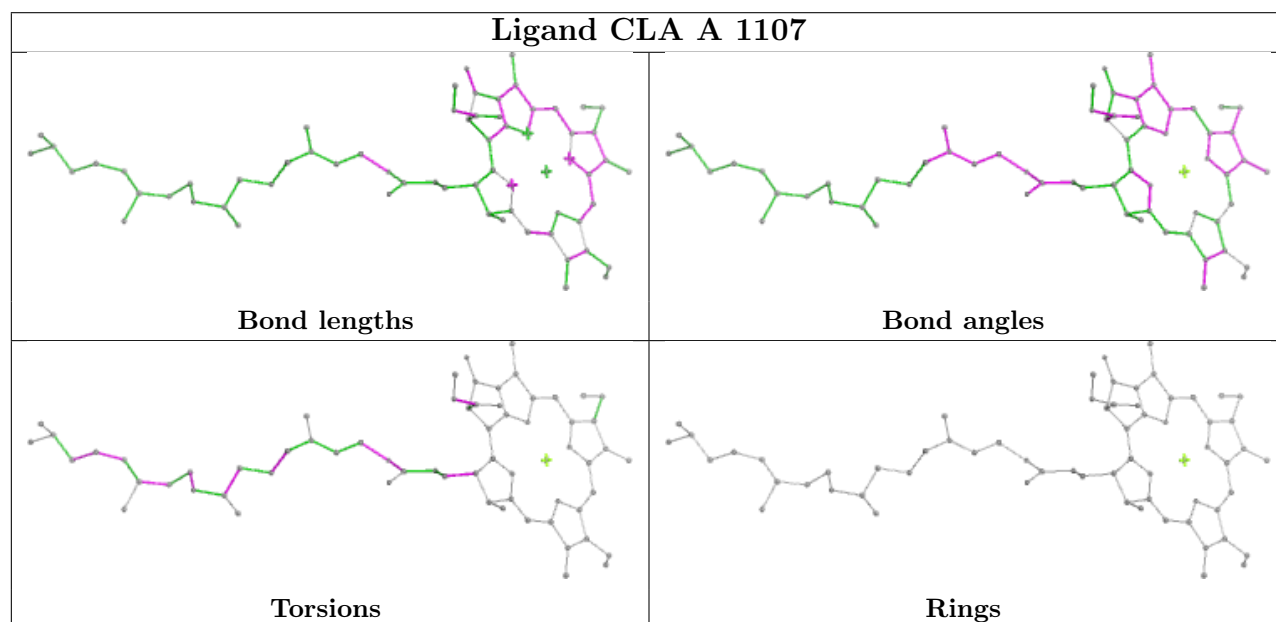
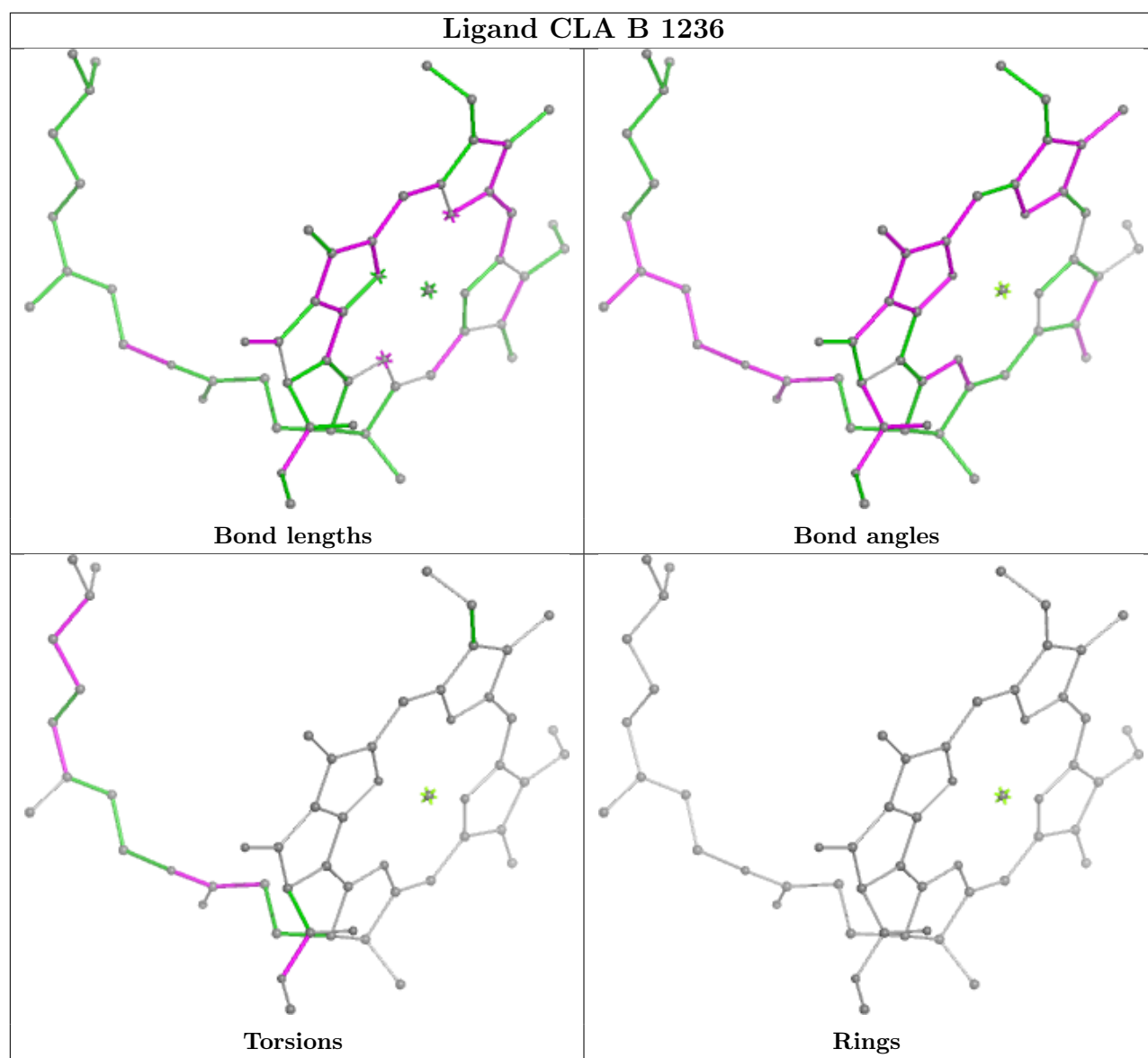


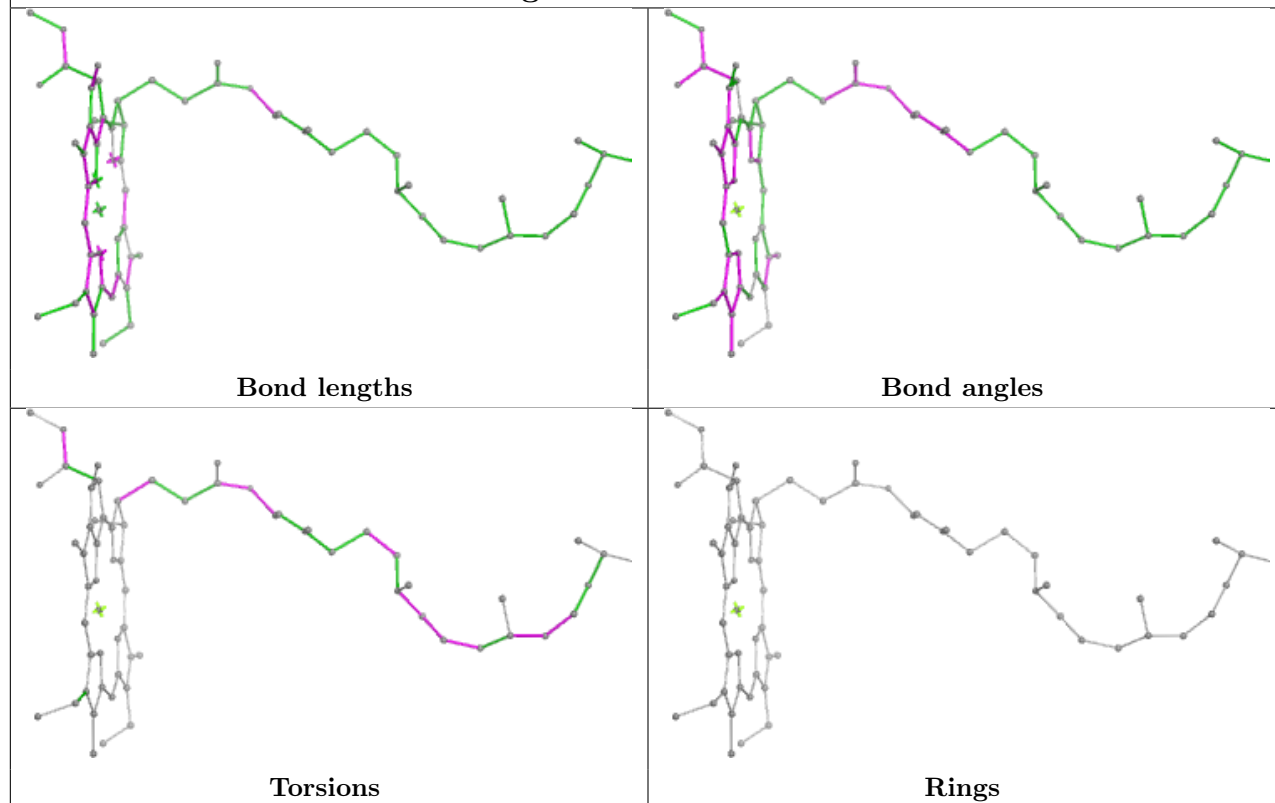
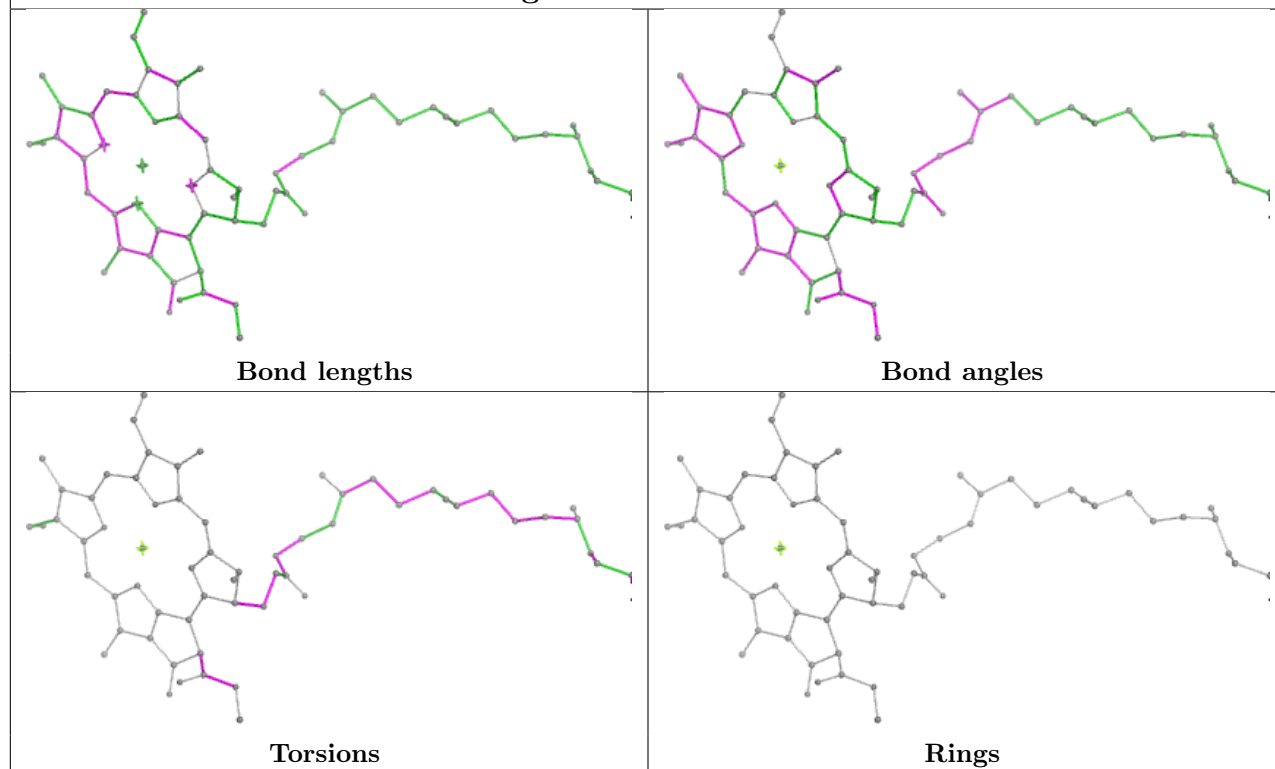


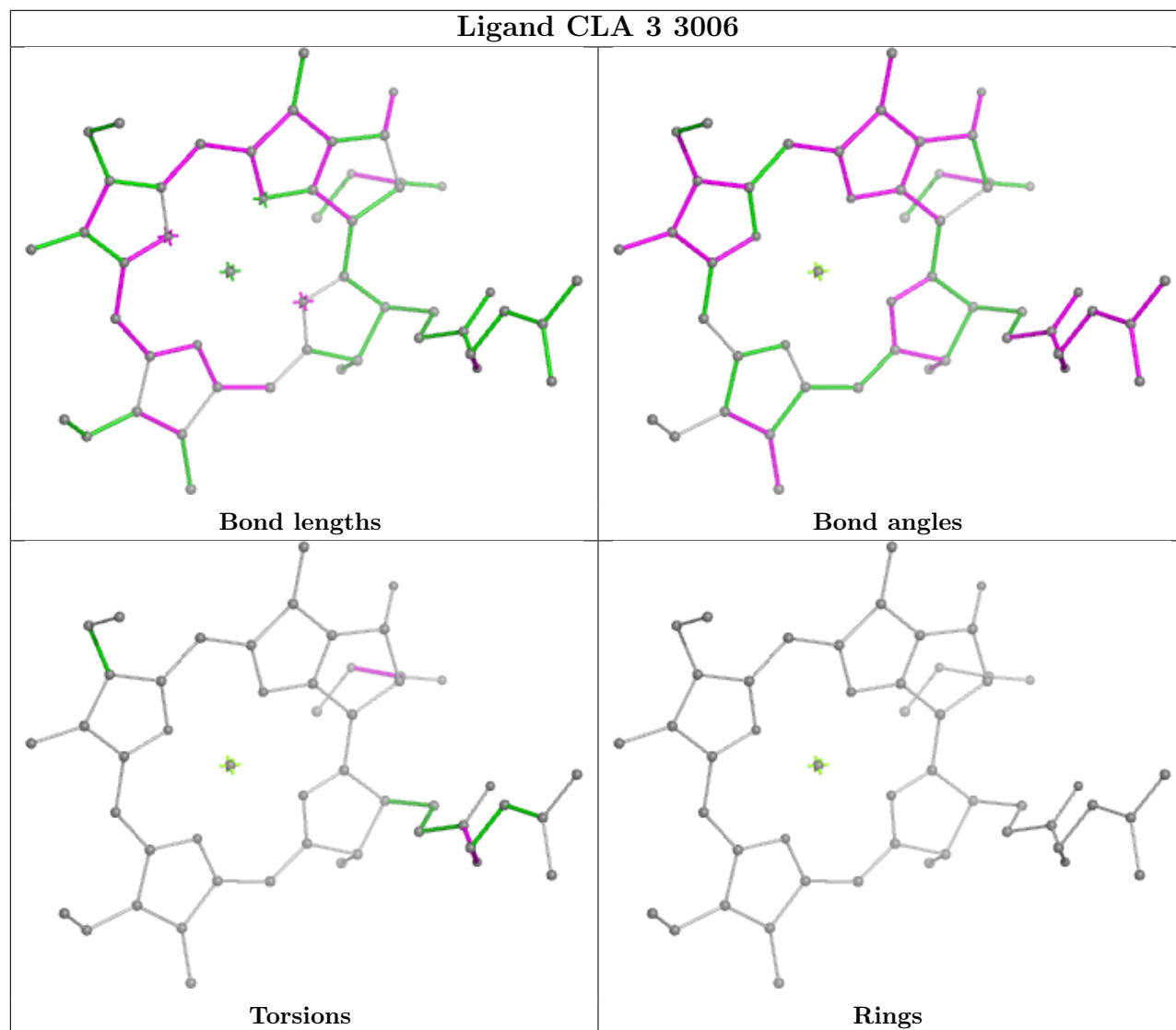


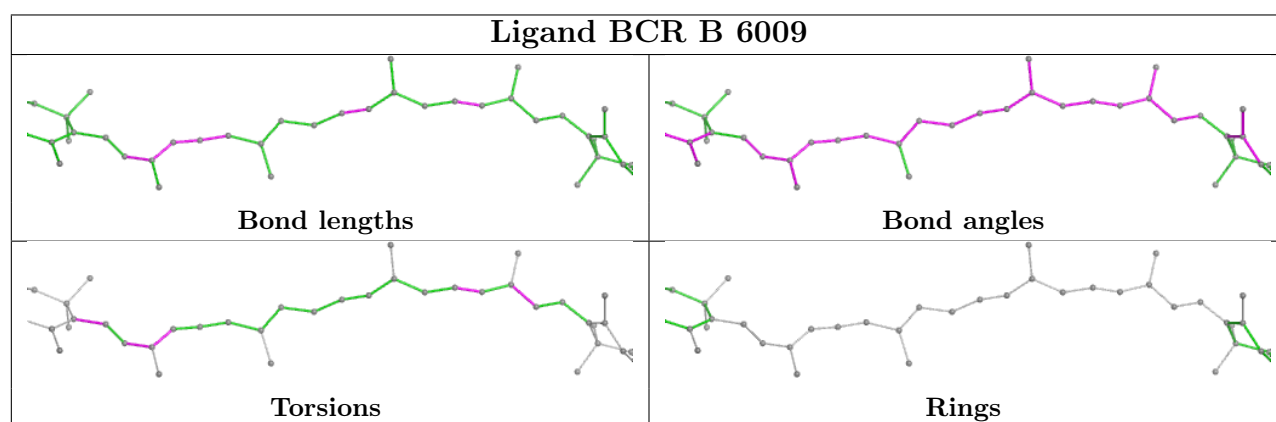
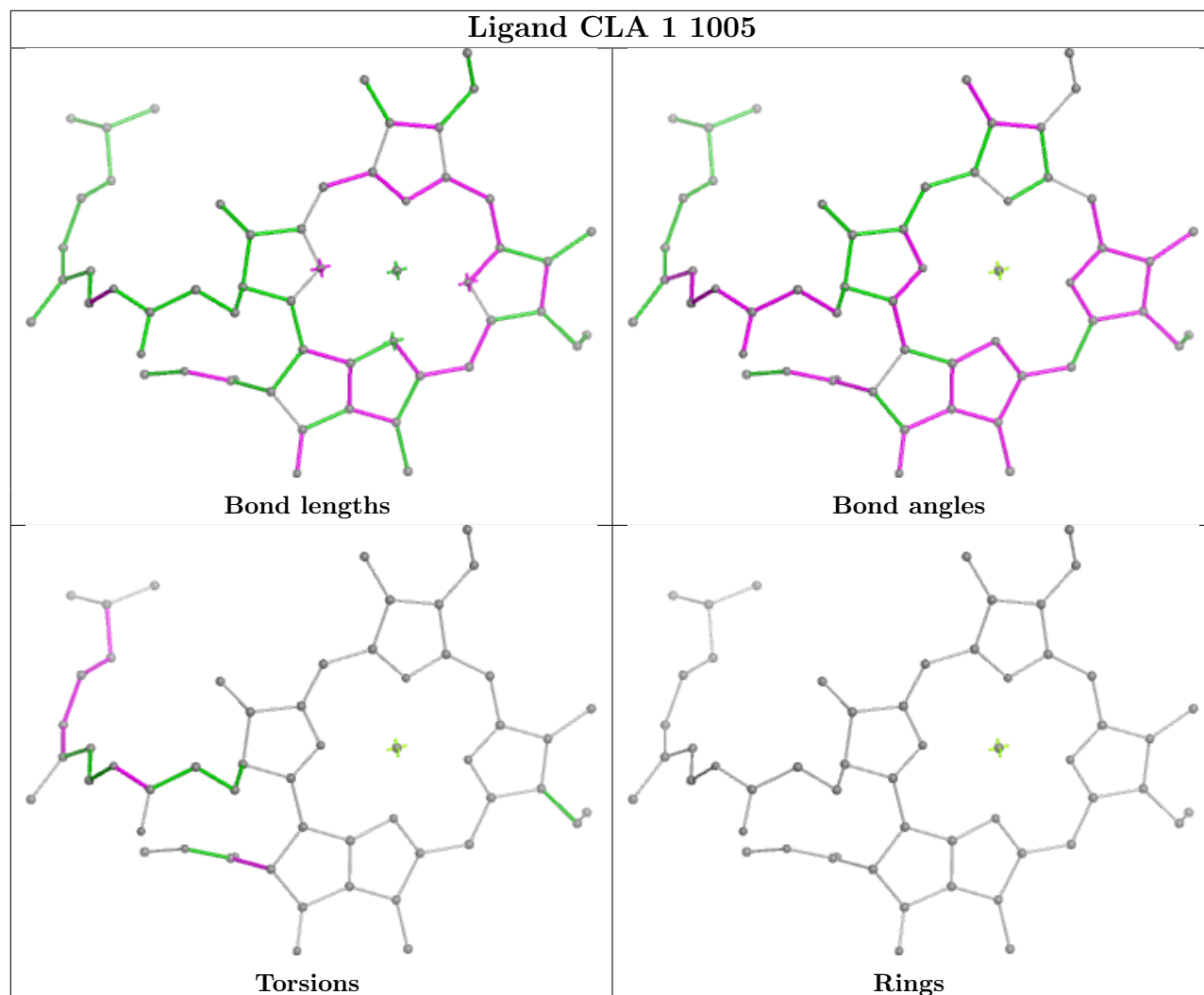


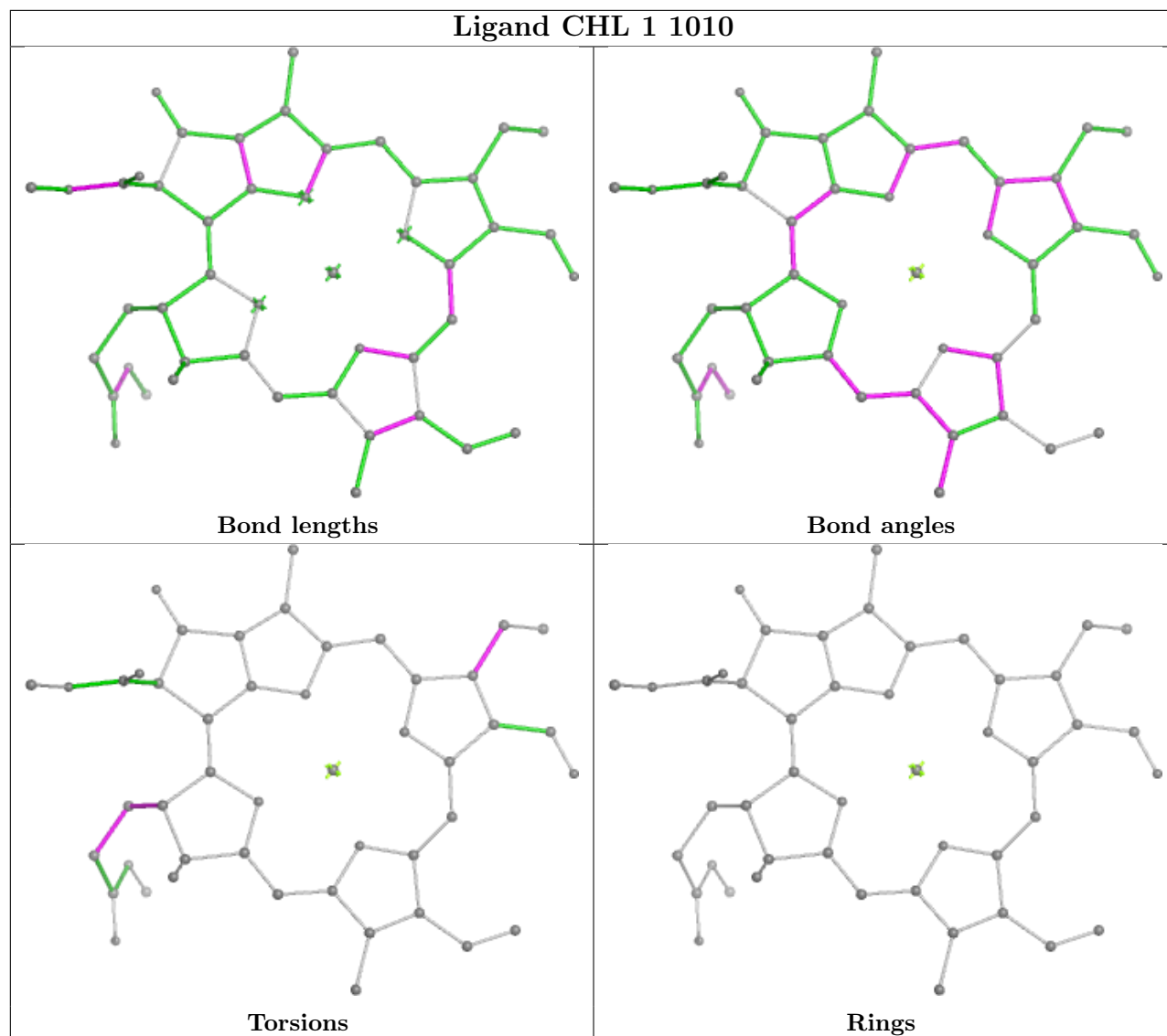


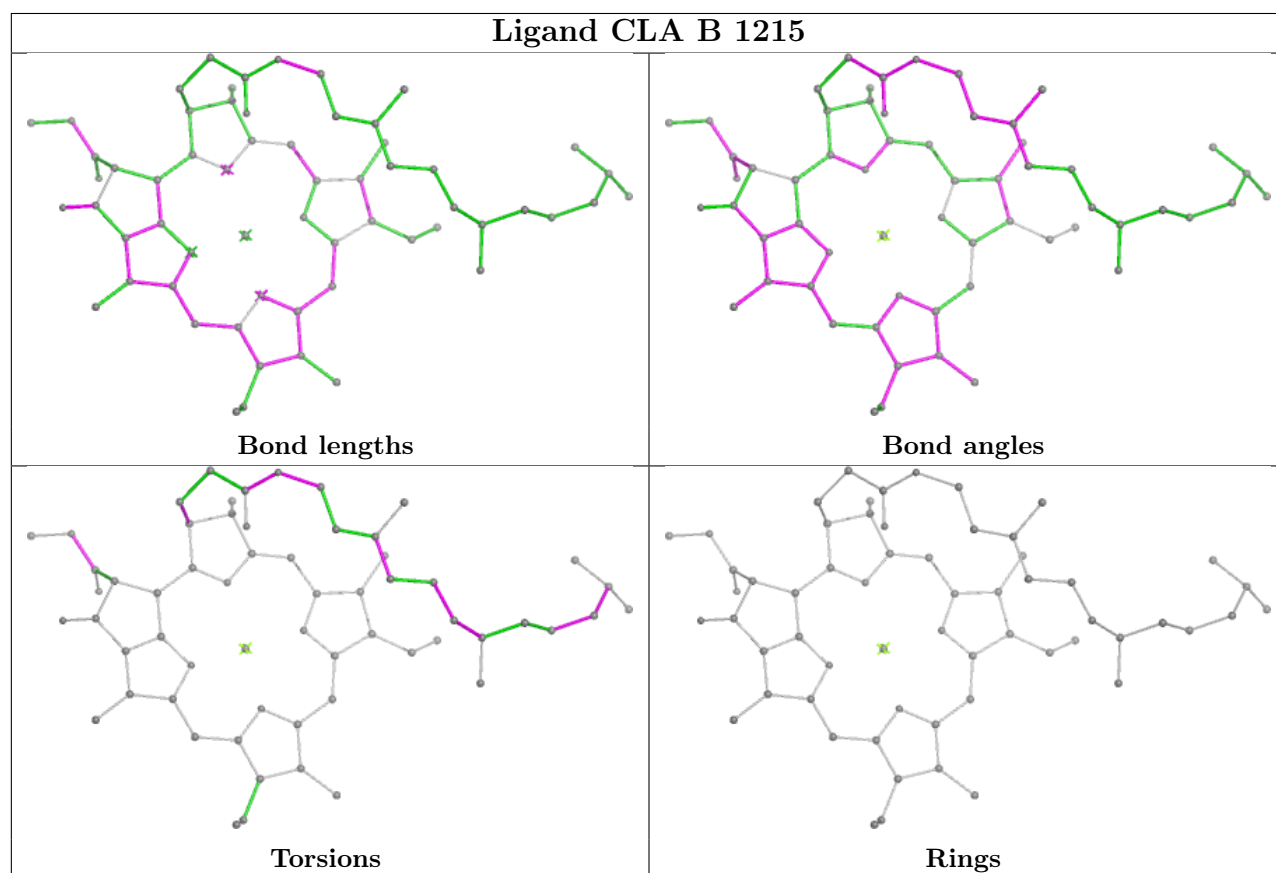
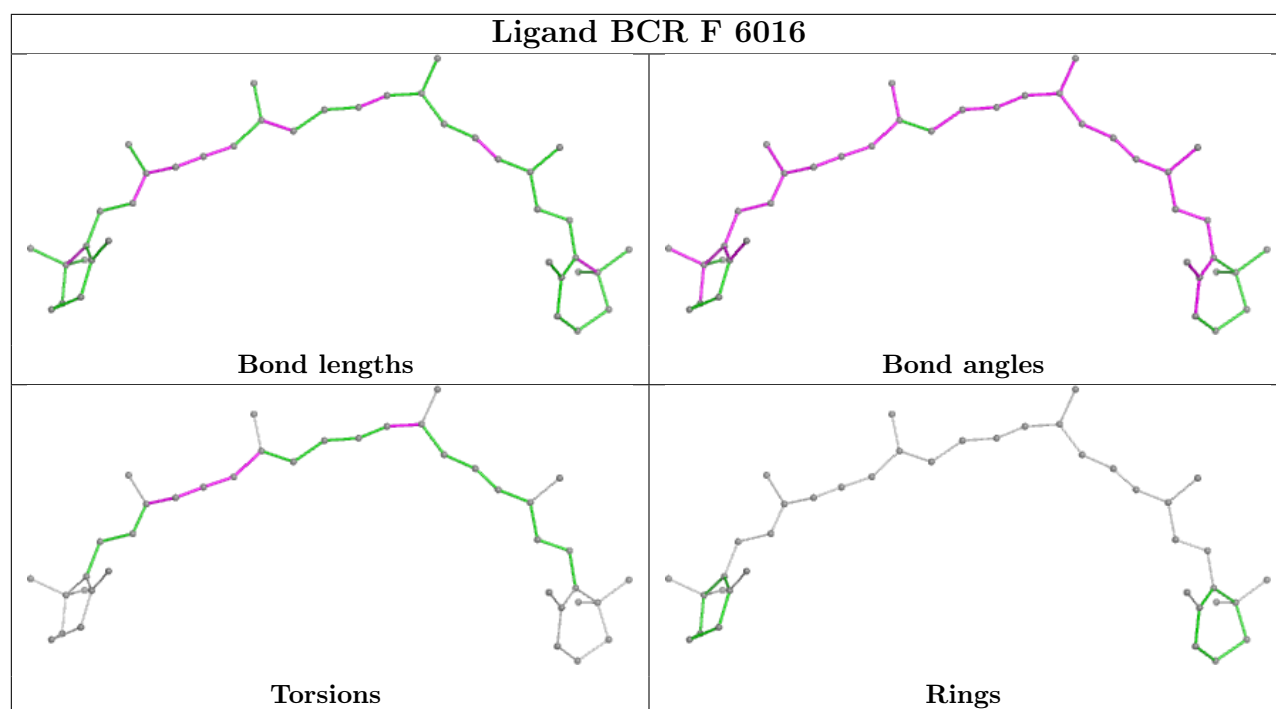


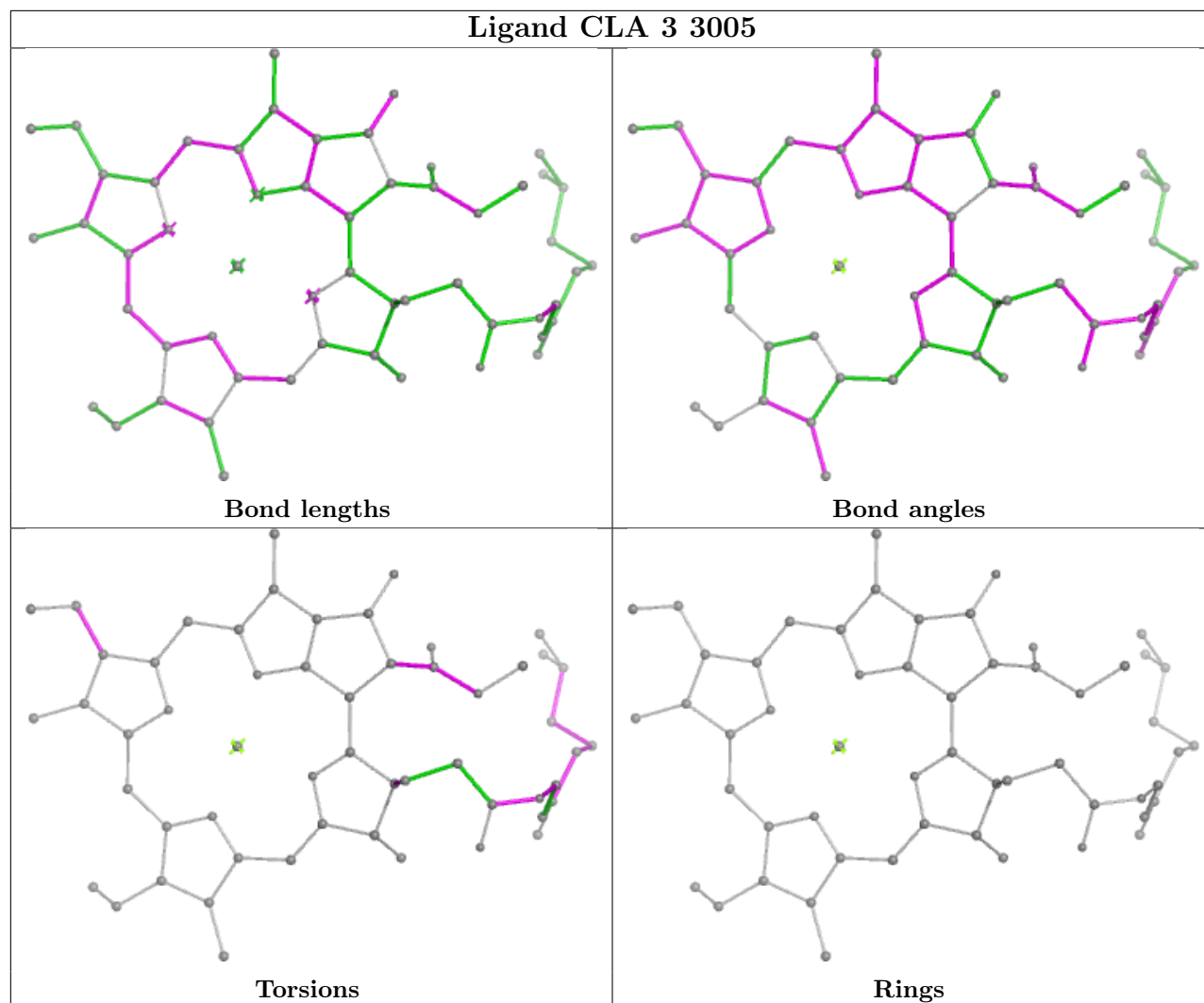
Ligand CLA A 1112**Ligand CLA A 1119**



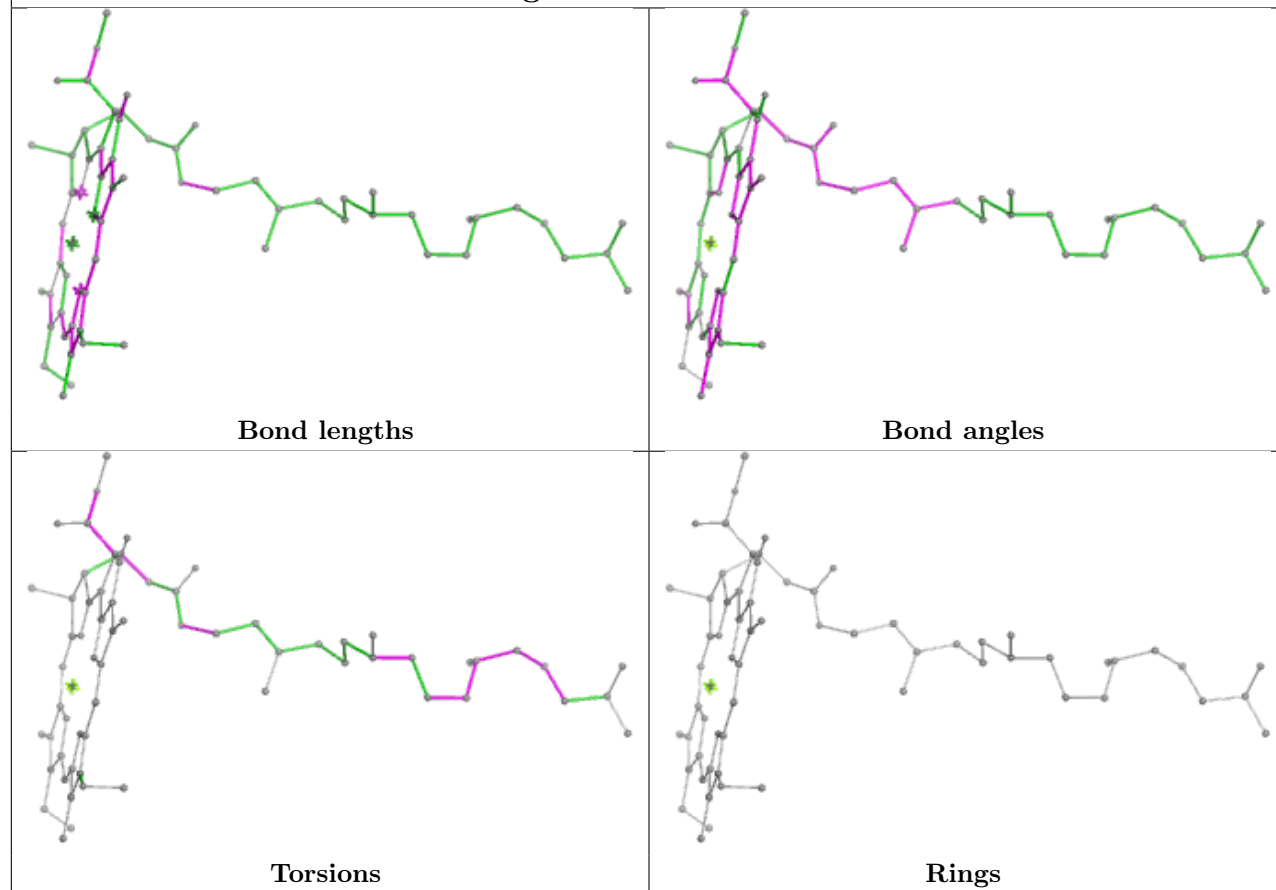




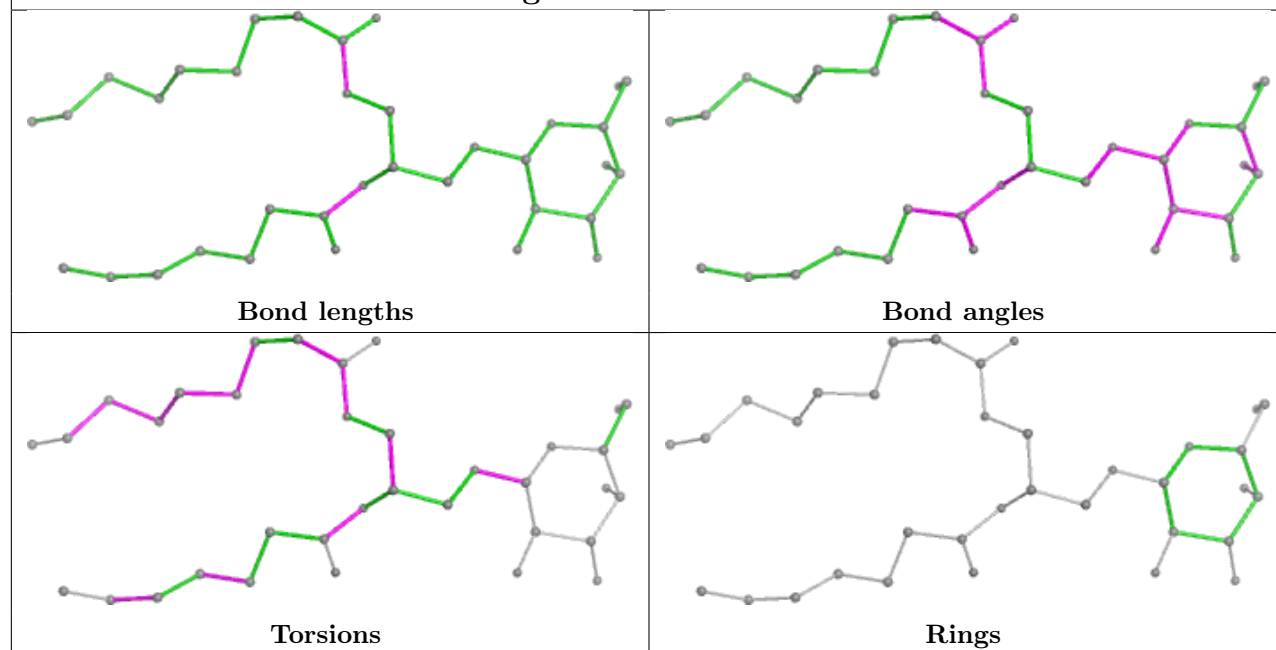


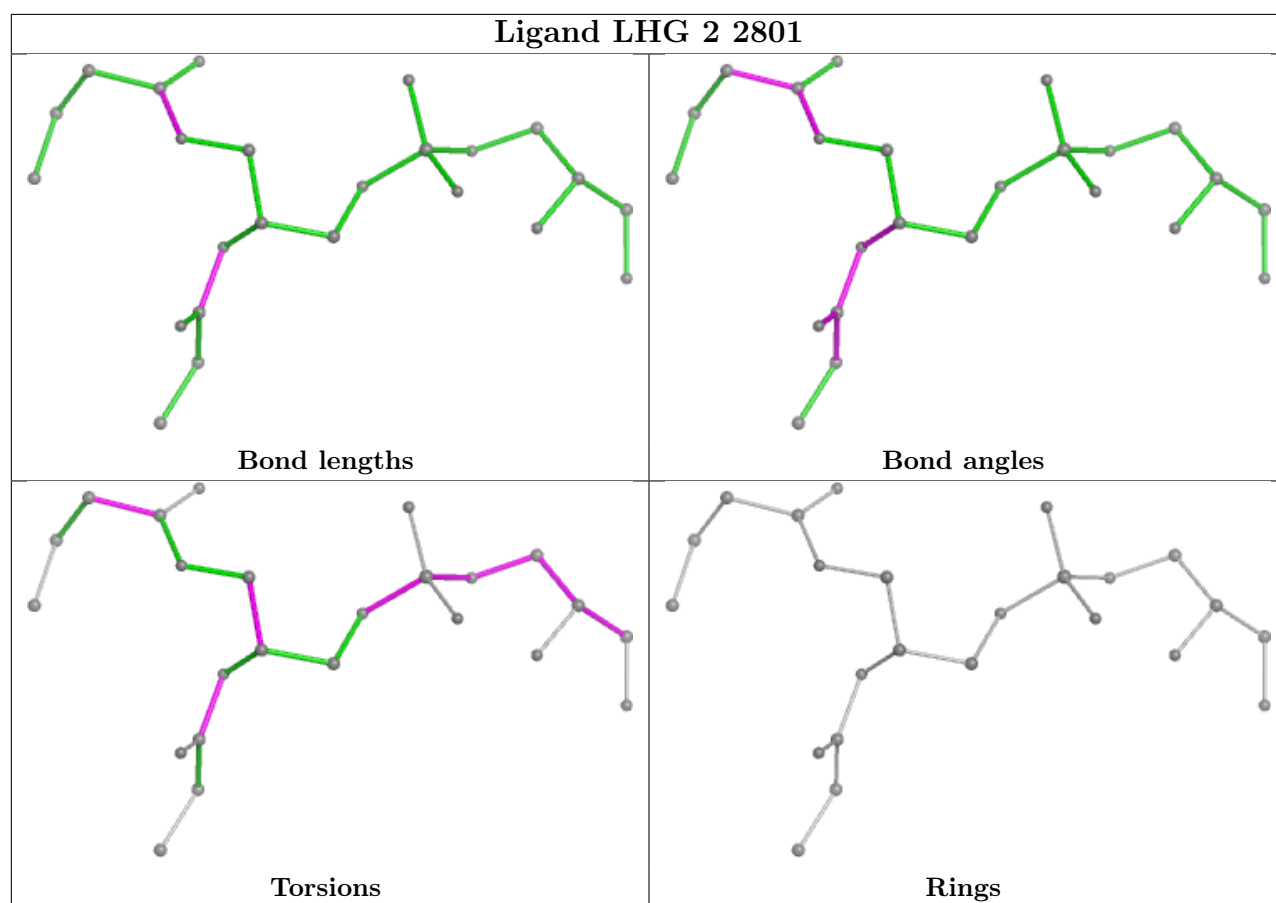


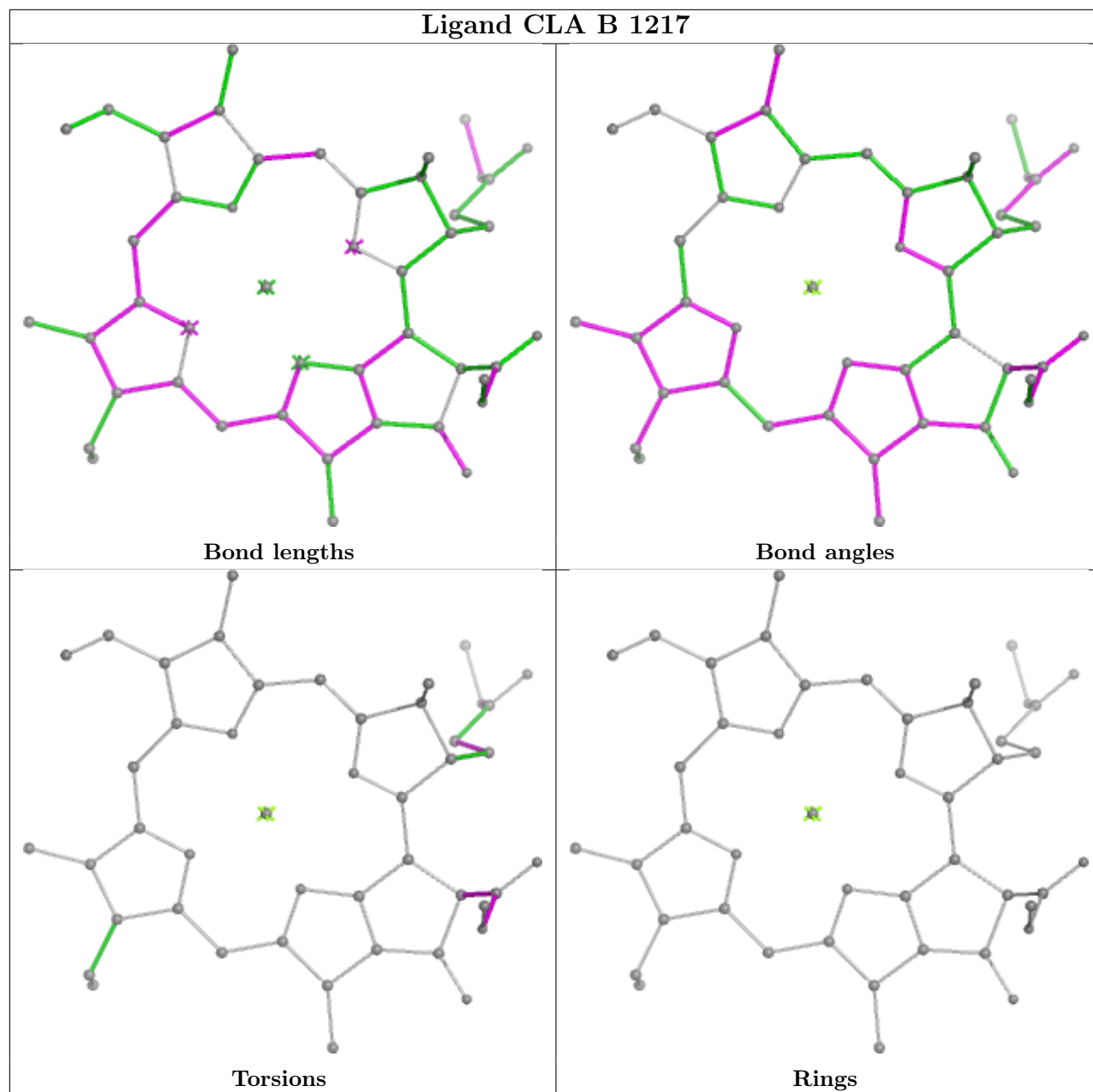
Ligand CLA A 1126

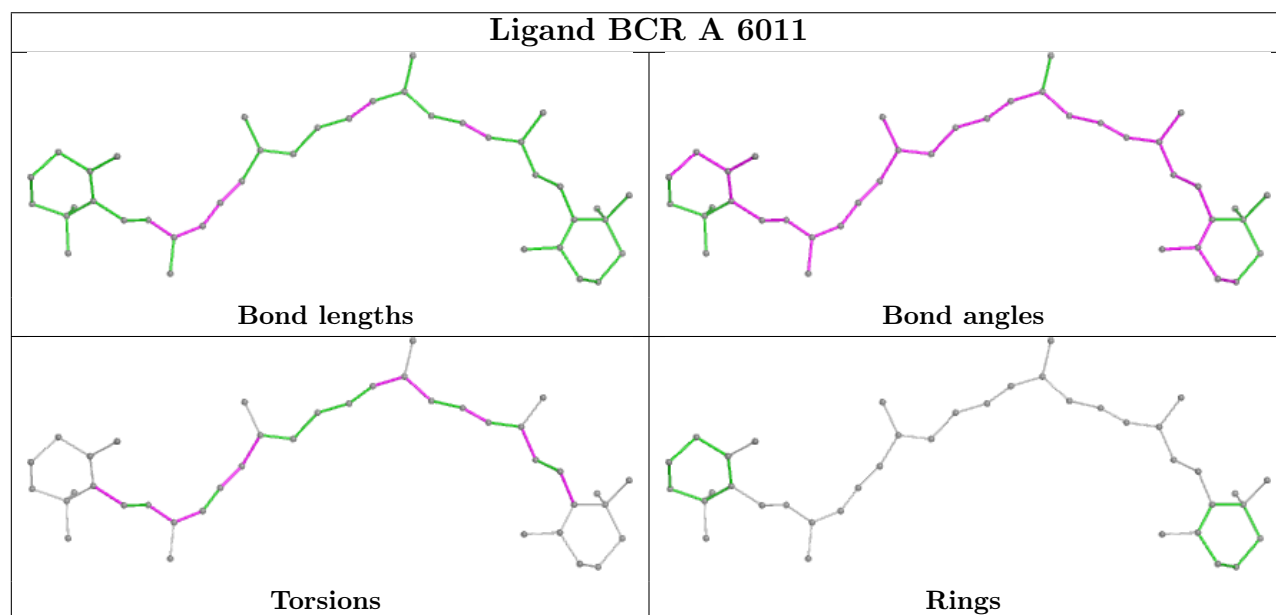
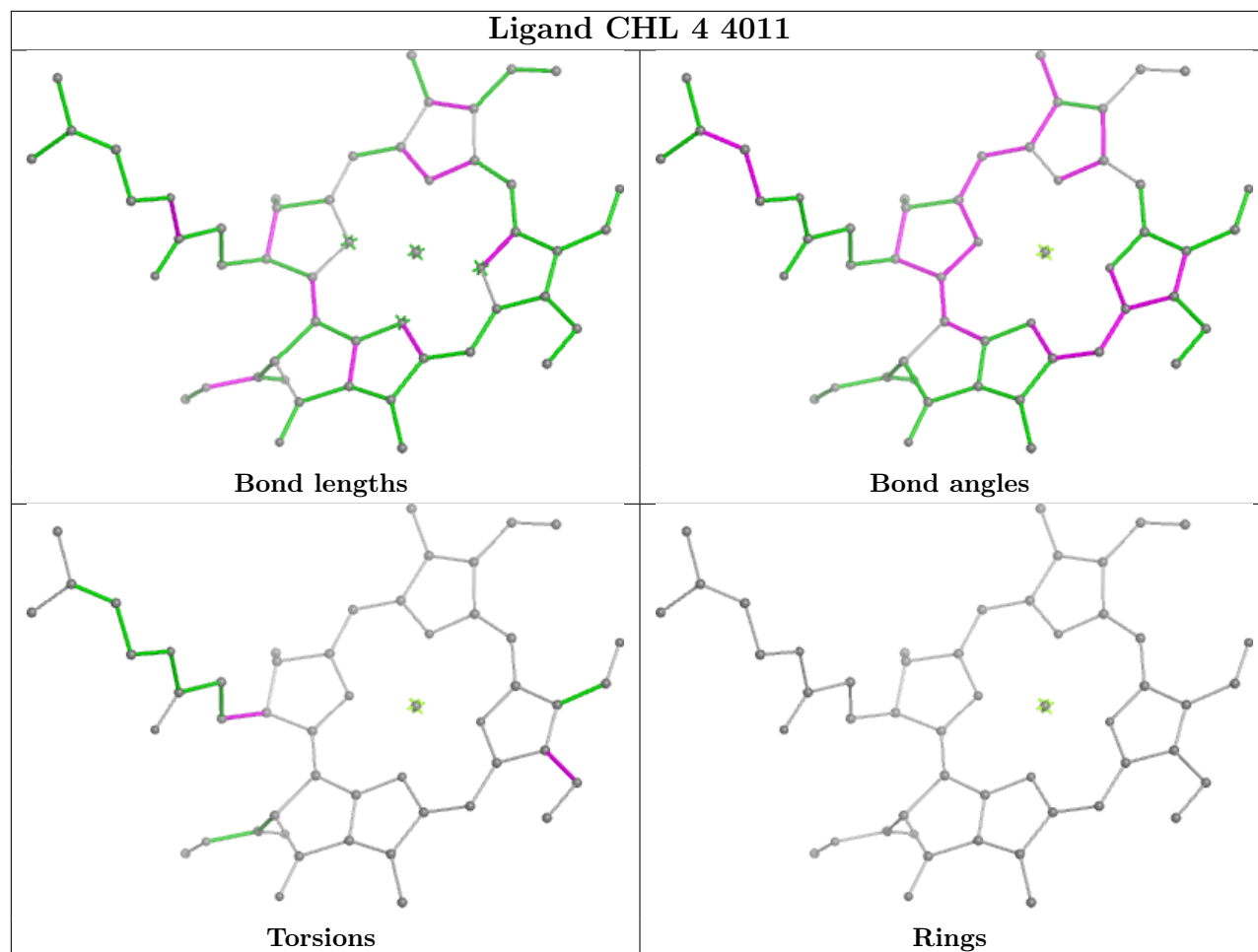


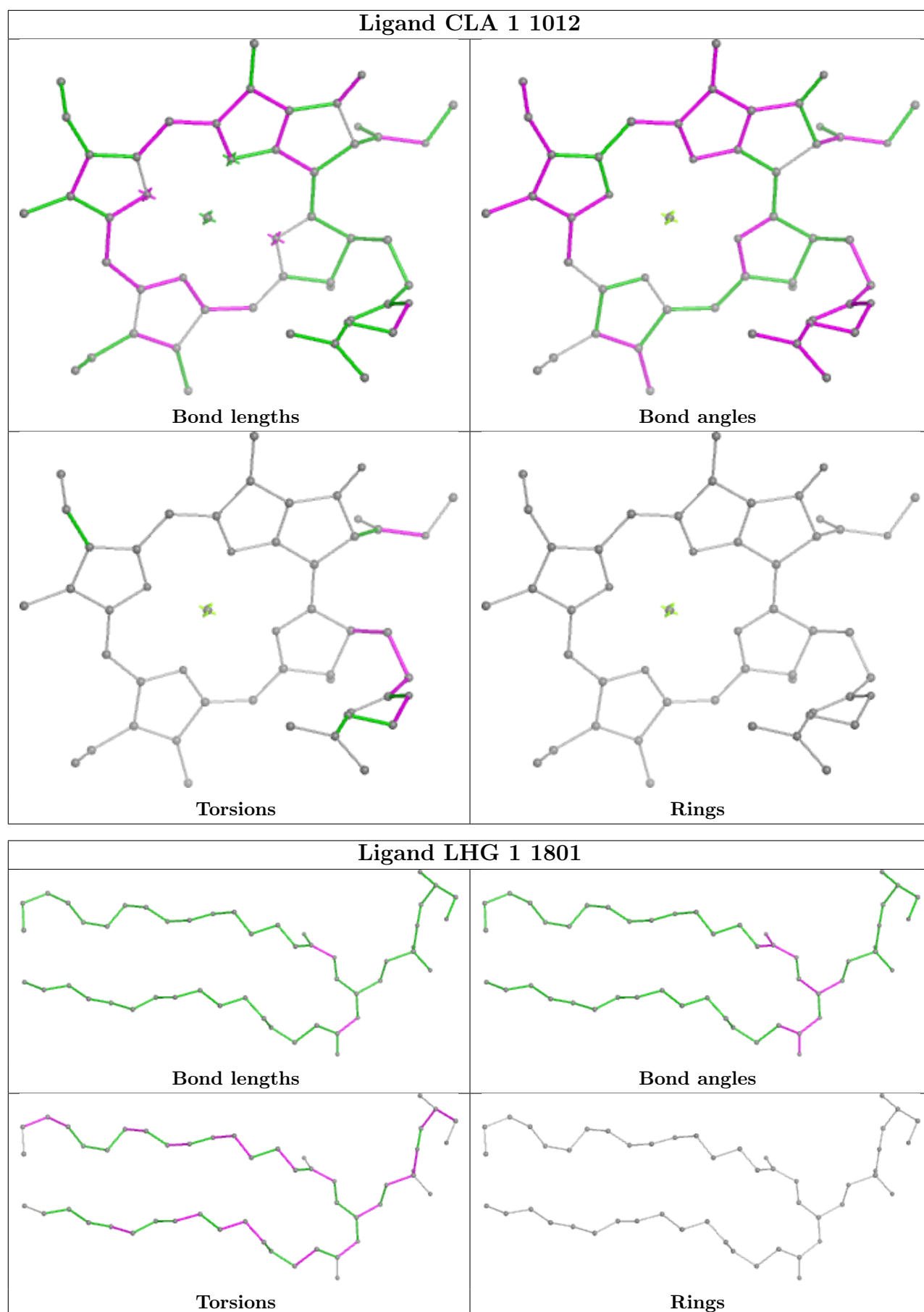
Ligand LMG 4 4801

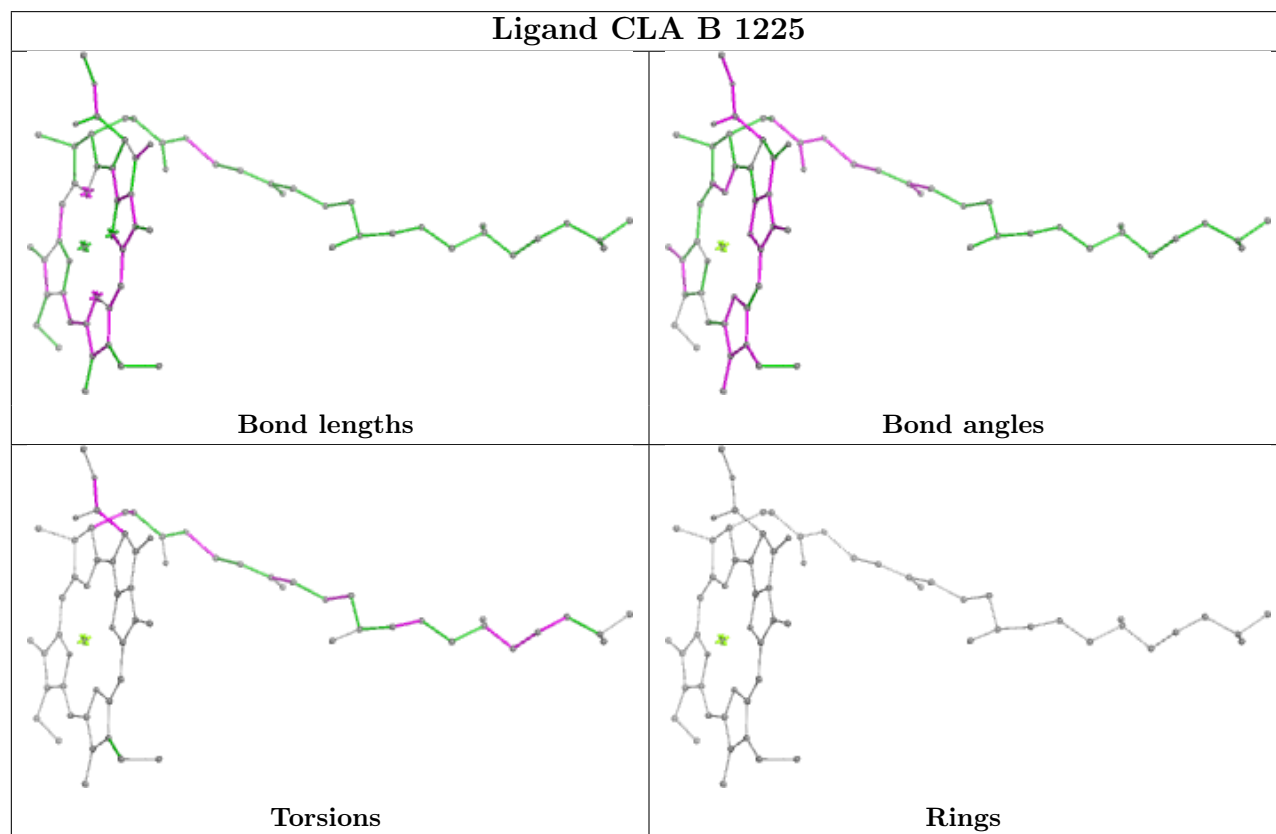
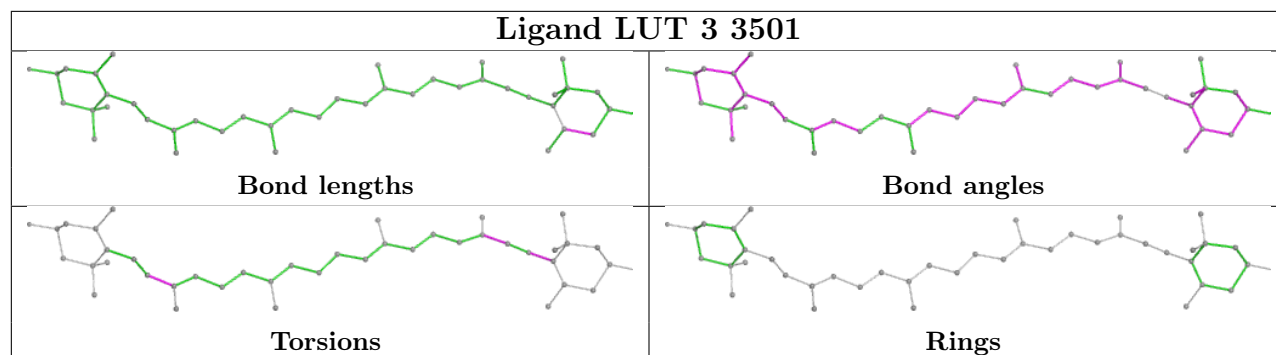


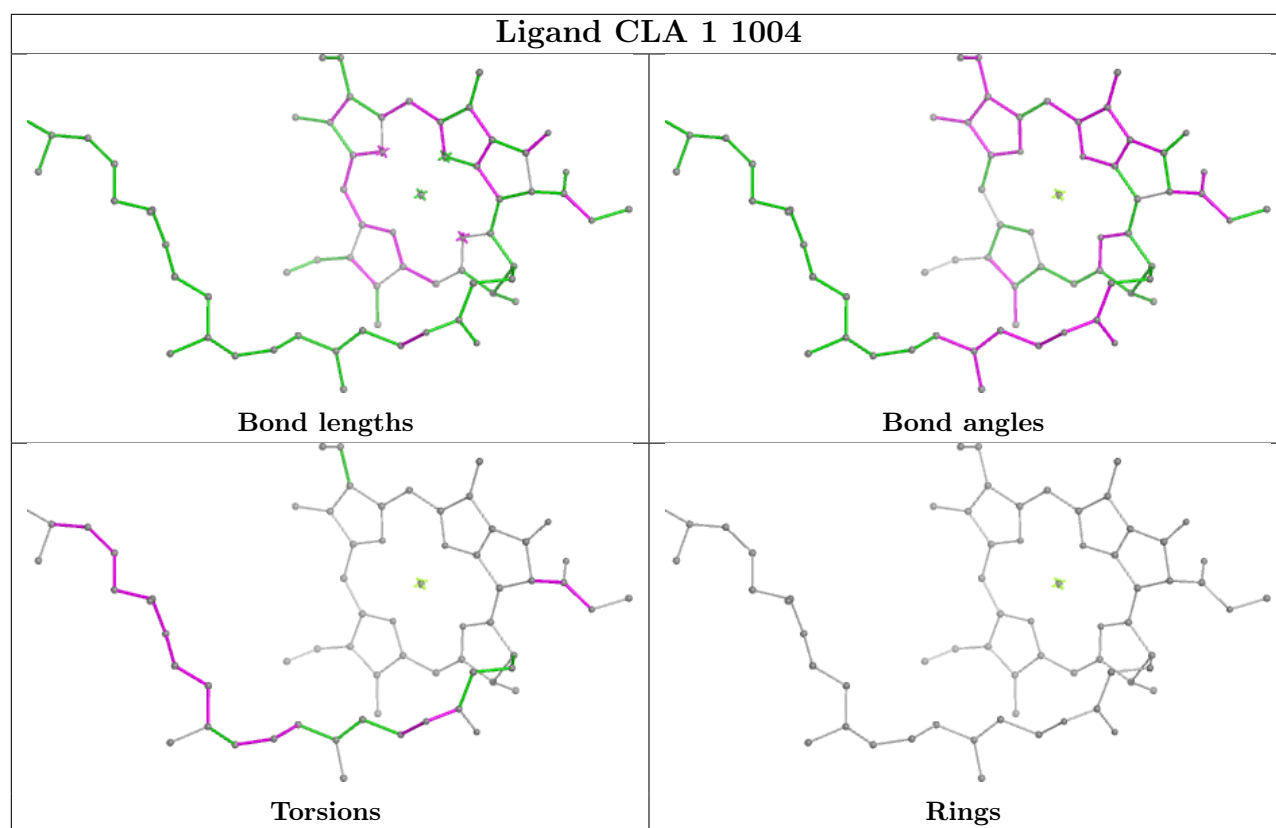




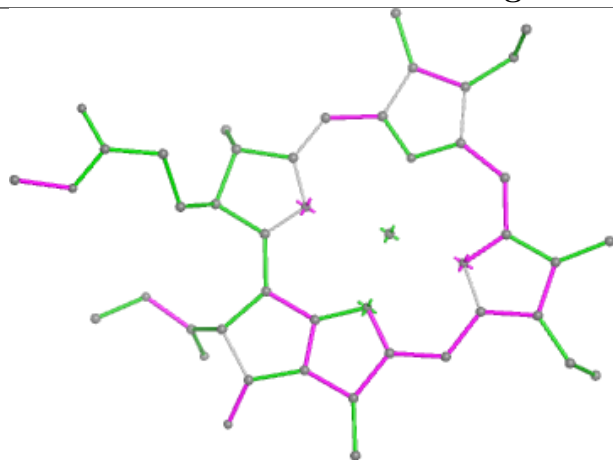




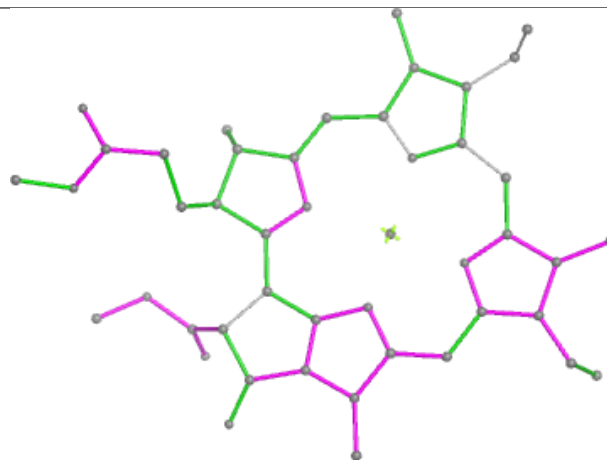




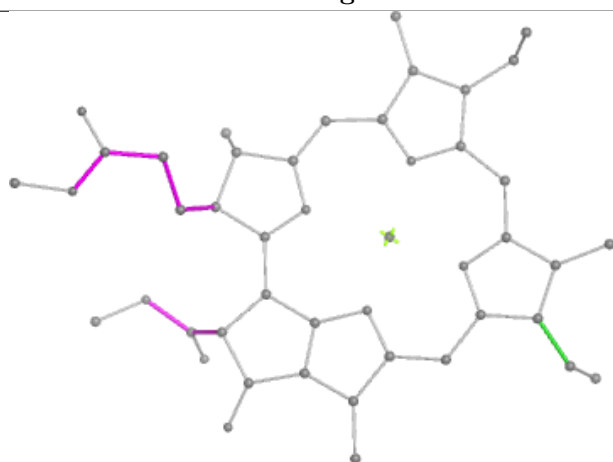
Ligand CLA H 1000



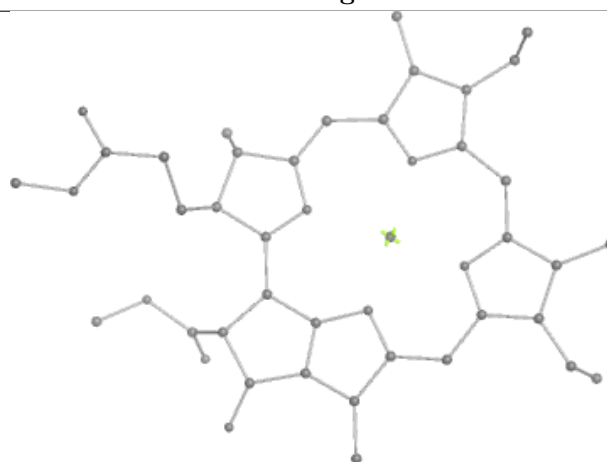
Bond lengths



Bond angles

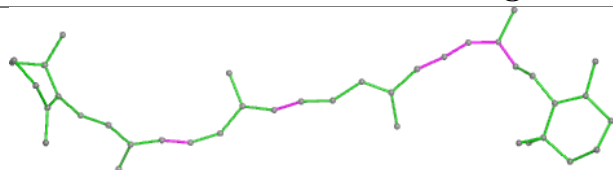


Torsions

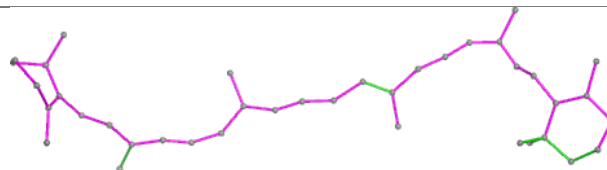


Rings

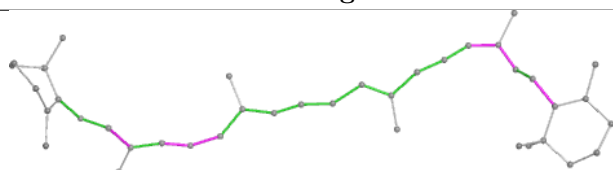
Ligand BCR B 6006



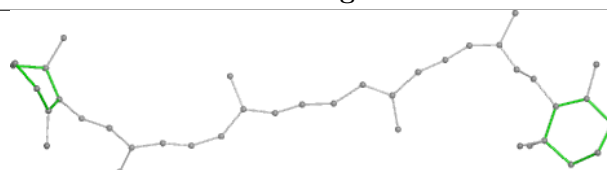
Bond lengths



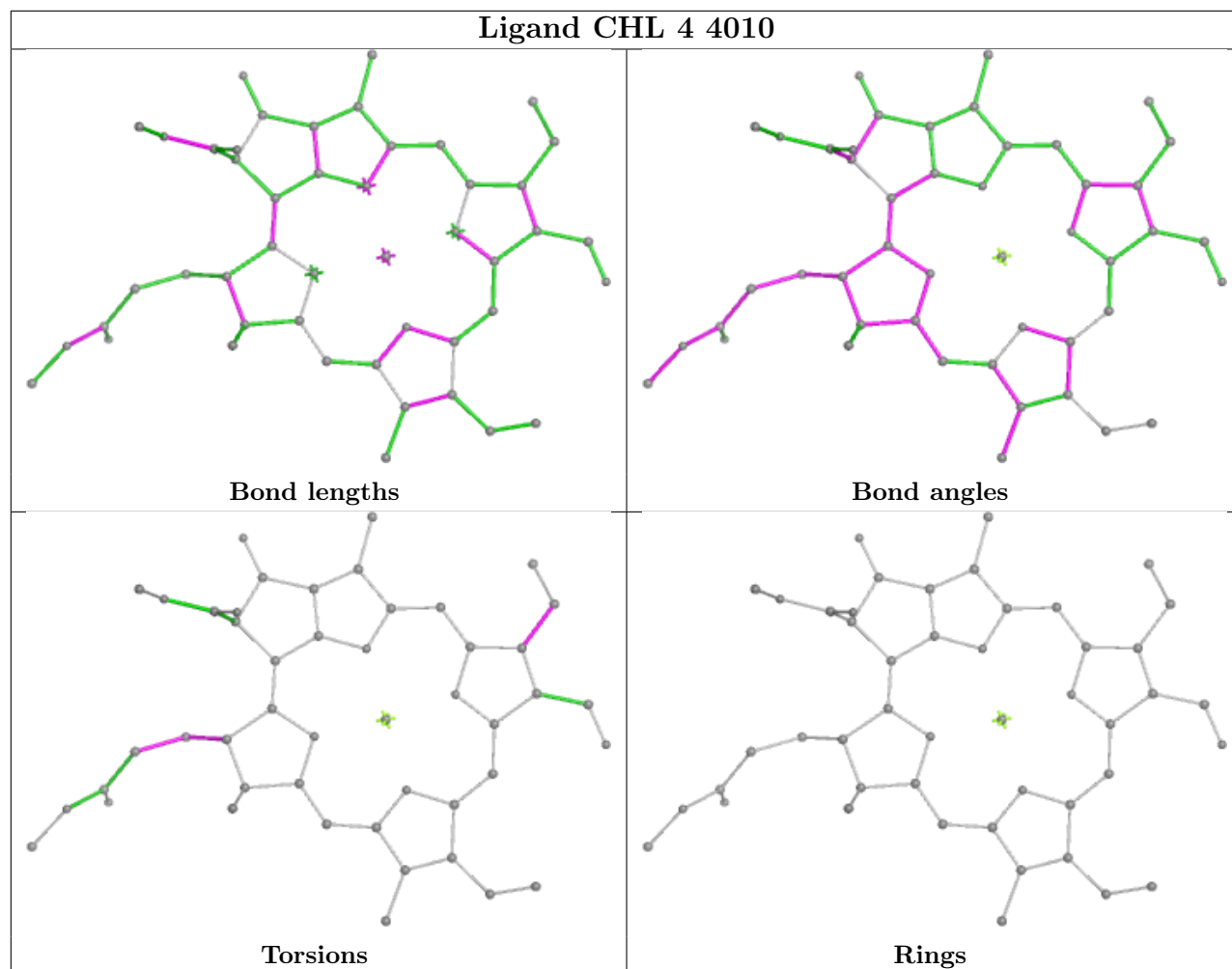
Bond angles

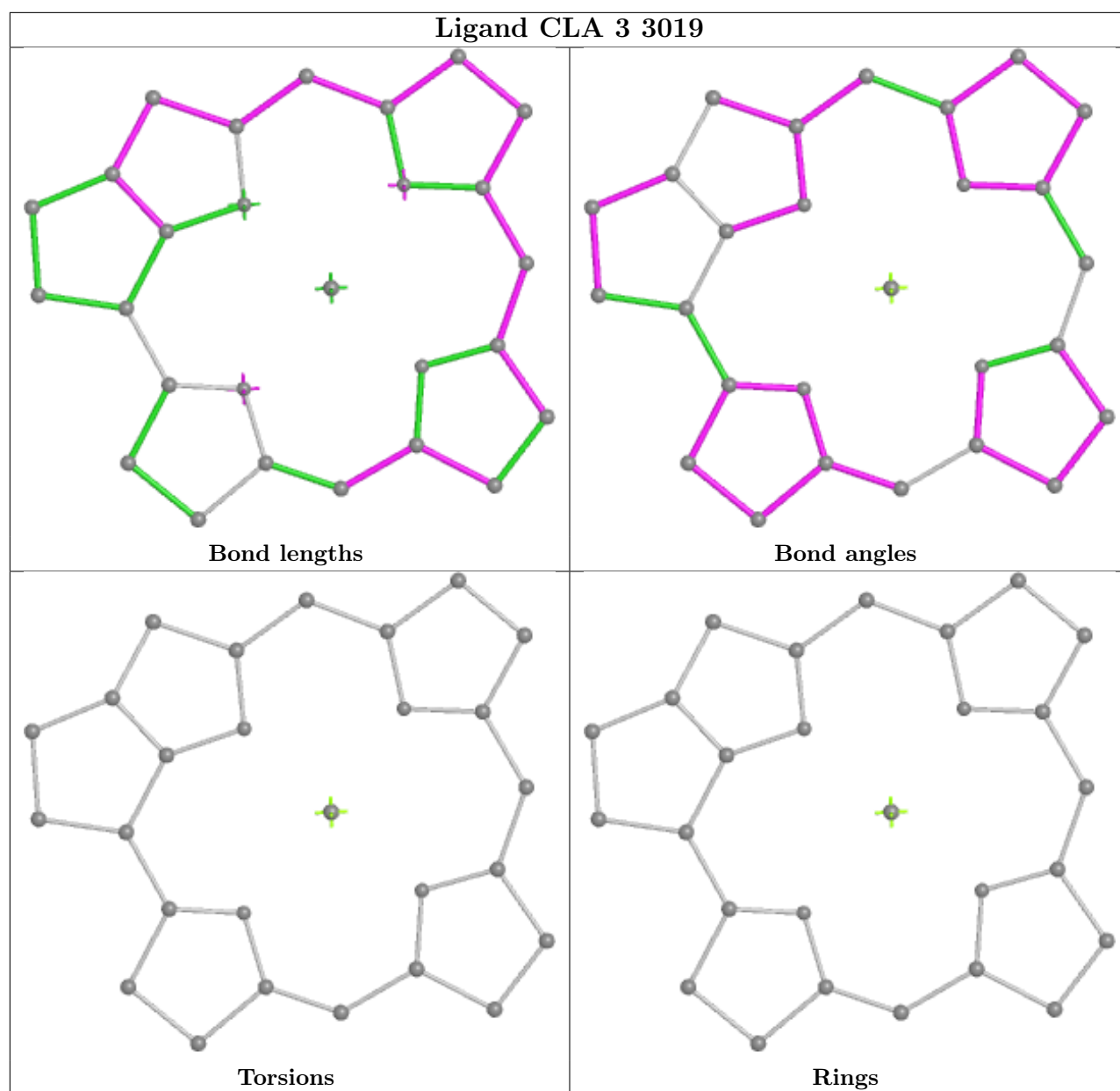


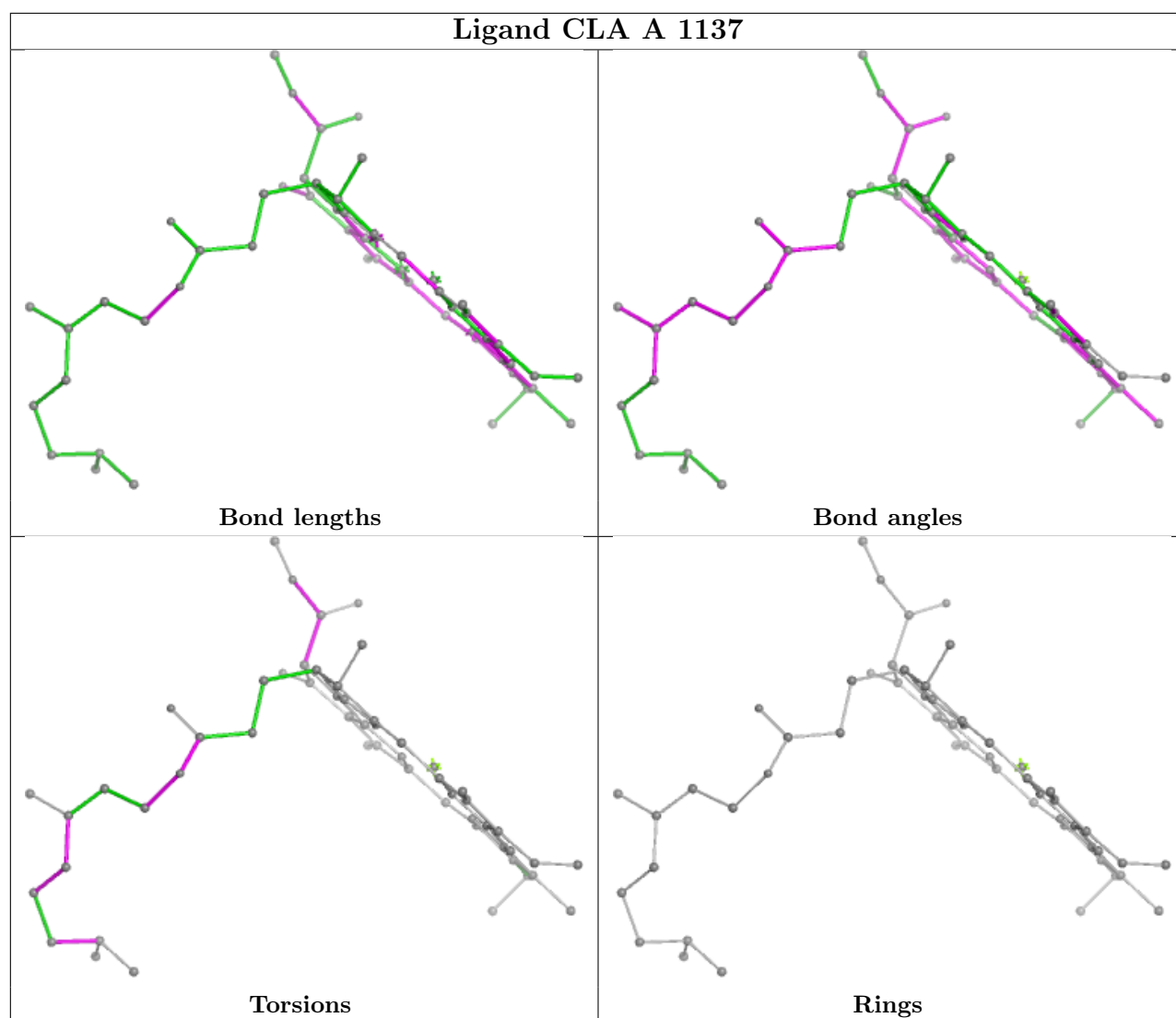
Torsions



Rings







5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å ²)	Q<0.9
1	A	742/758 (97%)	0.51	56 (7%)	22	16	56, 92, 150, 244	0
2	B	732/733 (99%)	0.52	60 (8%)	19	14	61, 89, 126, 157	0
3	I	29/30 (96%)	0.68	4 (13%)	8	7	89, 114, 148, 153	0
4	J	41/42 (97%)	0.65	6 (14%)	7	6	70, 80, 116, 164	0
5	F	150/154 (97%)	0.46	16 (10%)	12	10	66, 90, 122, 157	0
6	G	91/97 (93%)	1.31	22 (24%)	2	2	98, 129, 174, 184	0
7	L	160/167 (95%)	1.08	32 (20%)	3	3	86, 123, 172, 197	0
8	C	80/81 (98%)	0.49	6 (7%)	22	16	66, 81, 96, 106	0
9	D	141/147 (95%)	1.21	31 (21%)	3	3	77, 97, 120, 139	0
10	E	66/66 (100%)	0.41	5 (7%)	21	16	65, 91, 136, 183	0
11	H	84/90 (93%)	1.22	21 (25%)	2	2	103, 138, 178, 234	0
12	K	57/129 (44%)	1.35	16 (28%)	2	2	147, 215, 286, 324	0
13	2	207/269 (76%)	0.87	30 (14%)	7	6	85, 130, 180, 270	0
14	4	198/252 (78%)	0.58	17 (8%)	18	13	84, 121, 193, 274	0
15	1	194/202 (96%)	1.37	47 (24%)	2	2	95, 147, 225, 289	0
16	3	215/275 (78%)	1.33	60 (27%)	2	2	111, 179, 317, 368	0
All	All	3187/3492 (91%)	0.76	429 (13%)	8	7	56, 106, 205, 368	0

The worst 5 of 429 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
9	D	196	VAL	12.1
2	B	82	PHE	11.2
9	D	200	GLU	10.1
2	B	552	ASP	9.6
9	D	206	LYS	8.7

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

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

6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

6.4 Ligands [i](#)

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(\AA^2)	Q<0.9
18	CLA	3	3019	27/65	0.45	0.27	158,174,188,189	1
23	LMG	B	5005	38/55	0.63	0.20	76,120,141,143	0
18	CLA	J	1302	50/65	0.66	0.20	137,152,189,196	0
18	CLA	4	4016	46/65	0.68	0.18	126,166,177,183	0
18	CLA	3	3008	48/65	0.69	0.17	180,199,214,217	0
18	CLA	2	2019	27/65	0.71	0.17	148,159,174,174	1
18	CLA	3	3010	60/65	0.73	0.26	122,158,181,196	0
18	CLA	2	2016	50/65	0.75	0.19	114,164,207,211	0
26	LMU	B	8002	35/35	0.76	0.18	162,173,189,191	0
18	CLA	3	3018	50/65	0.78	0.16	173,190,207,213	0
23	LMG	F	5002	37/55	0.78	0.13	84,107,120,126	0
26	LMU	B	8001	35/35	0.78	0.14	104,158,168,172	0
18	CLA	K	1001	46/65	0.78	0.16	147,173,200,209	0
18	CLA	3	3007	50/65	0.79	0.18	175,193,239,246	0
18	CLA	1	1013	46/65	0.80	0.17	127,154,181,185	0
18	CLA	3	3013	46/65	0.80	0.16	127,157,166,176	0
18	CLA	G	1003	60/65	0.81	0.16	97,121,149,153	0
18	CLA	H	1000	46/65	0.82	0.14	119,150,170,176	0
22	BCR	G	2011	40/40	0.82	0.20	112,132,172,174	0
28	CHL	2	2010	47/66	0.82	0.12	111,134,142,143	0
22	BCR	J	6013	40/40	0.83	0.18	74,94,112,116	0
23	LMG	F	5001	23/55	0.83	0.10	86,94,106,109	0
18	CLA	1	1001	60/65	0.83	0.17	122,151,165,171	0
22	BCR	K	2011	40/40	0.84	0.22	125,136,144,147	0
18	CLA	3	3006	50/65	0.84	0.12	125,157,167,170	0
23	LMG	G	2021	41/55	0.84	0.19	138,156,175,176	0
28	CHL	3	3011	56/66	0.84	0.18	144,156,197,200	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
18	CLA	A	1151	50/65	0.85	0.13	99,113,187,189	0
18	CLA	A	1113	46/65	0.85	0.16	119,135,172,187	0
27	LUT	3	3501	42/42	0.85	0.26	202,209,216,218	0
18	CLA	L	1501	50/65	0.85	0.15	106,129,153,159	0
28	CHL	4	4010	47/66	0.85	0.16	105,125,180,187	0
23	LMG	2	2802	35/55	0.85	0.17	108,127,149,152	0
18	CLA	A	1134	55/65	0.86	0.16	112,124,168,172	0
22	BCR	L	6020	40/40	0.86	0.19	98,131,157,164	0
18	CLA	1	1006	50/65	0.86	0.14	125,138,144,148	0
18	CLA	1	1008	46/65	0.86	0.17	112,129,142,150	0
18	CLA	A	1114	46/65	0.86	0.12	107,117,124,136	0
18	CLA	4	4006	50/65	0.86	0.16	110,127,148,156	0
18	CLA	2	2006	55/65	0.86	0.15	105,132,173,174	0
22	BCR	A	6007	40/40	0.87	0.17	77,90,147,151	0
18	CLA	A	1115	46/65	0.87	0.15	107,141,170,178	0
28	CHL	2	2013	46/66	0.87	0.14	110,125,130,135	0
18	CLA	3	3002	46/65	0.87	0.15	173,188,195,222	0
18	CLA	G	1001	55/65	0.87	0.14	119,145,181,184	0
18	CLA	B	1218	65/65	0.88	0.17	86,100,155,160	0
18	CLA	1	1014	46/65	0.88	0.12	83,110,123,143	0
18	CLA	4	4008	46/65	0.88	0.14	93,112,129,137	0
28	CHL	1	1010	47/66	0.88	0.14	125,137,152,155	0
22	BCR	3	3503	40/40	0.88	0.21	119,136,175,177	0
27	LUT	1	1501	42/42	0.89	0.23	115,142,189,197	0
18	CLA	1	1011	50/65	0.89	0.17	126,153,175,185	0
23	LMG	4	4801	35/55	0.89	0.18	104,117,128,132	0
18	CLA	G	1002	46/65	0.89	0.11	142,160,173,181	0
22	BCR	B	6004	40/40	0.89	0.22	105,112,138,144	0
27	LUT	2	2502	42/42	0.89	0.22	102,115,124,131	0
27	LUT	4	4503	42/42	0.89	0.22	110,135,158,160	0
23	LMG	J	5001	55/55	0.90	0.17	62,96,110,122	0
18	CLA	L	1503	50/65	0.90	0.12	106,114,143,149	0
18	CLA	B	1232	55/65	0.90	0.12	80,97,118,122	0
27	LUT	1	1502	42/42	0.90	0.19	85,116,128,129	0
18	CLA	3	3001	50/65	0.90	0.11	147,169,201,206	0
27	LUT	3	3502	42/42	0.90	0.21	133,142,164,166	0
18	CLA	4	4001	60/65	0.90	0.17	113,129,158,160	0
18	CLA	A	1121	55/65	0.90	0.13	104,123,209,211	0
21	LHG	B	5004	21/49	0.90	0.11	86,102,116,119	0
28	CHL	4	4013	47/66	0.90	0.12	98,118,130,134	0
18	CLA	B	1213	60/65	0.90	0.15	85,105,118,126	0
27	LUT	2	2501	42/42	0.90	0.20	121,137,141,143	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
29	ZEX	4	4505	42/42	0.90	0.13	85,96,107,114	0
22	BCR	A	6008	40/40	0.91	0.20	76,97,137,139	0
18	CLA	1	1002	46/65	0.91	0.15	120,155,171,194	0
22	BCR	B	6009	40/40	0.91	0.17	63,78,94,95	0
18	CLA	1	1005	55/65	0.91	0.13	84,113,122,124	0
18	CLA	B	1201	50/65	0.91	0.14	80,93,131,134	0
18	CLA	B	1208	55/65	0.91	0.13	82,114,133,137	0
18	CLA	B	1238	65/65	0.91	0.15	70,85,96,116	0
18	CLA	3	3017	46/65	0.91	0.14	101,119,134,145	0
18	CLA	B	1228	60/65	0.91	0.15	63,73,111,114	0
18	CLA	B	1217	46/65	0.91	0.14	96,109,124,127	0
21	LHG	A	5003	40/49	0.91	0.16	101,117,132,134	0
18	CLA	A	1120	60/65	0.91	0.14	95,118,178,182	0
21	LHG	2	2801	24/49	0.91	0.14	109,123,148,152	0
22	BCR	A	6003	40/40	0.91	0.21	79,94,139,140	0
18	CLA	B	1219	60/65	0.91	0.16	82,97,134,135	0
25	DGD	B	7101	61/66	0.91	0.15	62,79,104,113	0
18	CLA	A	1105	51/65	0.92	0.12	66,88,97,100	0
18	CLA	2	2002	46/65	0.92	0.12	137,154,171,183	0
18	CLA	2	2004	65/65	0.92	0.14	84,105,117,125	0
18	CLA	2	2005	55/65	0.92	0.13	93,103,129,135	0
18	CLA	3	3003	60/65	0.92	0.14	137,170,188,190	0
18	CLA	3	3004	60/65	0.92	0.15	125,139,154,155	0
18	CLA	B	1209	46/65	0.92	0.13	100,109,118,145	0
18	CLA	B	1212	55/65	0.92	0.16	109,129,146,154	0
18	CLA	B	1231	60/65	0.92	0.12	65,81,101,104	0
18	CLA	A	1108	46/65	0.92	0.12	85,101,121,126	0
18	CLA	3	3012	50/65	0.92	0.13	117,135,142,144	0
18	CLA	4	4002	50/65	0.92	0.15	107,141,171,211	0
18	CLA	B	1240	65/65	0.92	0.12	66,84,103,108	0
18	CLA	4	4007	60/65	0.92	0.17	110,130,179,183	0
18	CLA	B	1021	65/65	0.92	0.15	61,72,80,83	0
18	CLA	F	1301	45/65	0.92	0.12	61,73,86,101	0
18	CLA	4	4017	65/65	0.92	0.16	93,103,120,121	0
18	CLA	B	1204	55/65	0.92	0.12	80,103,118,124	0
21	LHG	1	1801	49/49	0.92	0.17	94,113,164,170	0
22	BCR	A	6002	40/40	0.92	0.21	82,115,168,169	0
18	CLA	A	1112	65/65	0.92	0.15	101,118,138,140	0
18	CLA	A	1124	55/65	0.92	0.14	59,77,104,116	0
18	CLA	A	1022	65/65	0.92	0.14	58,76,88,99	0
18	CLA	1	1007	46/65	0.92	0.12	112,131,162,181	0
22	BCR	B	6005	40/40	0.92	0.21	87,103,182,184	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
18	CLA	B	1220	65/65	0.92	0.15	61,76,114,118	0
22	BCR	J	6012	40/40	0.92	0.15	67,80,89,91	0
18	CLA	A	1139	65/65	0.92	0.14	56,70,98,104	0
18	CLA	A	1133	55/65	0.93	0.14	83,109,120,126	0
18	CLA	2	2003	55/65	0.93	0.12	103,127,135,158	0
22	BCR	F	6016	40/40	0.93	0.12	66,75,91,94	0
18	CLA	B	1211	65/65	0.93	0.13	93,107,131,136	0
18	CLA	A	1109	65/65	0.93	0.12	71,85,94,101	0
22	BCR	L	6019	40/40	0.93	0.24	88,105,132,135	0
18	CLA	B	1239	65/65	0.93	0.14	69,82,111,116	0
18	CLA	2	2007	60/65	0.93	0.15	116,142,189,195	0
18	CLA	2	2012	55/65	0.93	0.13	86,104,149,153	0
18	CLA	B	1214	59/65	0.93	0.16	71,91,100,108	0
18	CLA	B	1227	65/65	0.93	0.13	60,74,99,105	0
18	CLA	2	2009	50/65	0.93	0.12	100,117,138,139	0
18	CLA	A	1135	51/65	0.93	0.14	72,92,114,117	0
18	CLA	A	1137	55/65	0.93	0.13	71,85,125,126	0
18	CLA	4	4003	65/65	0.93	0.13	84,106,135,143	0
18	CLA	4	4004	60/65	0.93	0.14	76,99,112,118	0
18	CLA	B	1234	60/65	0.93	0.15	64,77,106,108	0
18	CLA	A	1126	65/65	0.93	0.15	65,79,87,97	0
27	LUT	I	6018	42/42	0.93	0.15	101,109,116,121	0
18	CLA	A	1131	65/65	0.93	0.16	79,93,103,112	0
18	CLA	4	4012	65/65	0.93	0.14	92,104,117,120	0
27	LUT	4	4501	42/42	0.93	0.15	107,121,142,149	0
27	LUT	4	4502	42/42	0.93	0.16	88,106,117,121	0
18	CLA	A	1118	46/65	0.93	0.13	99,108,127,131	0
18	CLA	A	1129	50/65	0.93	0.11	71,93,115,126	0
18	CLA	A	1101	65/65	0.93	0.12	58,72,90,113	0
18	CLA	B	1222	65/65	0.93	0.15	58,74,103,110	0
18	CLA	1	1004	65/65	0.93	0.14	98,114,122,125	0
18	CLA	L	1502	60/65	0.93	0.13	86,116,125,130	0
28	CHL	2	2011	48/66	0.93	0.14	108,124,129,136	0
18	CLA	B	1012	65/65	0.93	0.15	51,69,85,92	0
18	CLA	B	1207	65/65	0.93	0.14	78,102,122,129	0
22	BCR	B	6006	40/40	0.93	0.19	94,115,164,164	0
28	CHL	1	1009	56/66	0.93	0.12	92,105,113,130	0
18	CLA	B	1216	65/65	0.93	0.14	73,86,105,108	0
22	BCR	B	6010	40/40	0.93	0.15	64,73,96,100	0
22	BCR	I	6020	40/40	0.93	0.16	85,97,110,111	0
18	CLA	A	1123	65/65	0.94	0.16	70,88,93,96	0
18	CLA	B	1221	65/65	0.94	0.14	66,78,115,122	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
18	CLA	A	1119	65/65	0.94	0.14	78,95,107,115	0
18	CLA	B	1223	65/65	0.94	0.14	59,78,90,96	0
18	CLA	A	1102	50/65	0.94	0.11	58,69,95,104	0
18	CLA	A	1110	55/65	0.94	0.15	97,114,138,143	0
24	CA	B	6000	1/1	0.94	0.09	100,100,100,100	0
18	CLA	A	1127	65/65	0.94	0.15	69,83,95,99	0
18	CLA	1	1003	55/65	0.94	0.14	100,122,134,142	0
18	CLA	2	2001	60/65	0.94	0.16	114,134,167,169	0
18	CLA	A	1111	60/65	0.94	0.13	75,91,112,118	0
18	CLA	A	1132	65/65	0.94	0.14	79,94,120,129	0
18	CLA	B	1236	55/65	0.94	0.14	56,69,117,124	0
18	CLA	A	1104	65/65	0.94	0.13	55,73,81,85	0
18	CLA	A	1237	60/65	0.94	0.14	75,94,113,116	0
18	CLA	1	1012	50/65	0.94	0.11	103,125,130,132	0
18	CLA	B	1224	65/65	0.94	0.15	65,83,100,107	0
18	CLA	B	1226	65/65	0.94	0.14	65,76,97,103	0
18	CLA	A	1106	65/65	0.94	0.13	59,74,90,106	0
18	CLA	A	1136	56/65	0.94	0.12	84,98,115,119	0
18	CLA	B	1023	65/65	0.94	0.12	57,70,94,105	0
22	BCR	F	6014	40/40	0.94	0.12	54,64,73,74	0
18	CLA	A	1107	65/65	0.94	0.13	60,77,94,105	0
18	CLA	3	3005	55/65	0.94	0.14	107,131,144,157	0
17	CL0	A	1011	65/65	0.94	0.13	52,70,82,84	0
18	CLA	A	1122	65/65	0.94	0.15	76,96,122,139	0
18	CLA	F	1302	50/65	0.94	0.09	67,84,114,124	0
18	CLA	4	4005	60/65	0.94	0.13	84,97,106,120	0
18	CLA	A	1116	60/65	0.94	0.14	89,119,137,142	0
21	LHG	A	7001	49/49	0.95	0.13	56,72,84,92	0
18	CLA	A	1130	50/65	0.95	0.13	83,100,123,127	0
18	CLA	A	1013	65/65	0.95	0.12	49,62,74,90	0
18	CLA	2	2008	50/65	0.95	0.13	109,138,148,156	0
18	CLA	A	1117	65/65	0.95	0.16	85,98,110,114	0
18	CLA	B	1215	60/65	0.95	0.13	82,91,102,109	0
18	CLA	A	1103	65/65	0.95	0.12	66,83,104,107	0
18	CLA	B	1225	65/65	0.95	0.14	66,81,98,105	0
22	BCR	A	6017	40/40	0.95	0.16	71,86,105,122	0
18	CLA	B	1235	65/65	0.95	0.09	54,68,78,92	0
18	CLA	B	1205	65/65	0.95	0.15	90,103,116,152	0
18	CLA	B	1202	65/65	0.95	0.14	71,82,91,104	0
18	CLA	B	1230	58/65	0.95	0.10	58,74,83,86	0
28	CHL	4	4011	51/66	0.95	0.13	117,131,149,154	0
18	CLA	B	1206	65/65	0.95	0.12	86,104,112,127	0

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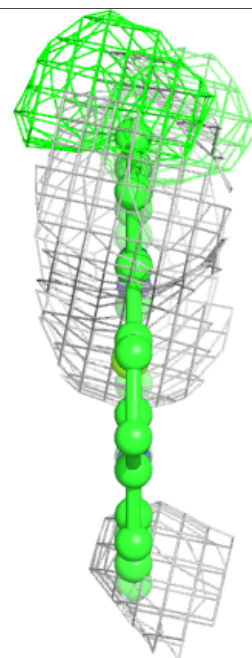
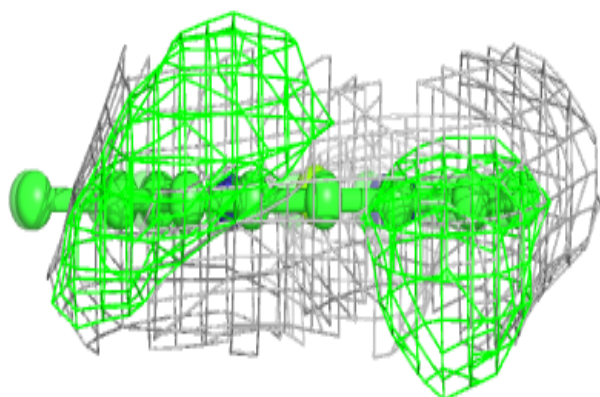
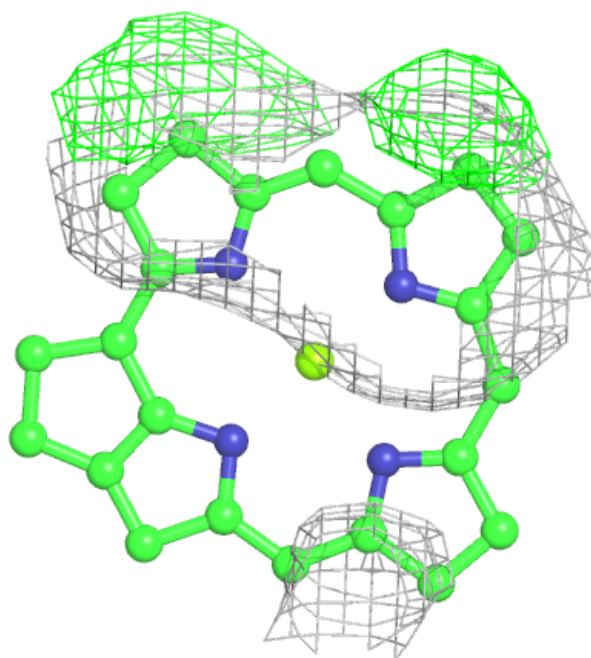
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
18	CLA	A	1128	65/65	0.95	0.12	56,66,74,85	0
18	CLA	A	1140	65/65	0.95	0.12	58,66,78,106	0
20	PQN	A	5001	33/33	0.95	0.12	53,63,76,85	0
18	CLA	A	1125	60/65	0.95	0.12	79,94,102,114	0
18	CLA	A	1138	65/65	0.96	0.11	55,65,75,82	0
22	BCR	A	6011	40/40	0.96	0.13	61,73,88,96	0
18	CLA	B	1229	65/65	0.96	0.11	60,72,82,84	0
18	CLA	B	1203	65/65	0.96	0.11	68,82,97,104	0
20	PQN	B	5002	33/33	0.96	0.11	54,72,91,93	0
18	CLA	B	1210	65/65	0.96	0.14	81,94,107,113	0
18	CLA	4	4009	50/65	0.96	0.11	85,94,116,131	0
19	SF4	C	3003	8/8	0.97	0.05	89,106,119,126	0
19	SF4	C	3002	8/8	0.97	0.05	73,103,107,107	0
19	SF4	A	3001	8/8	0.98	0.04	69,95,97,99	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.

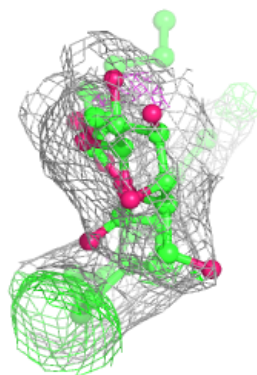
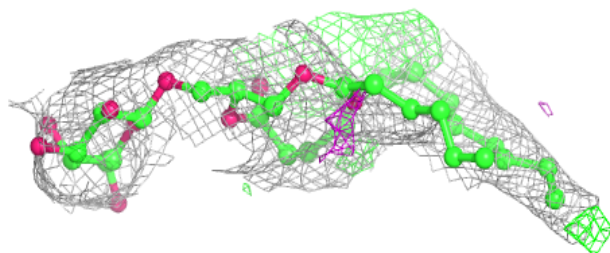
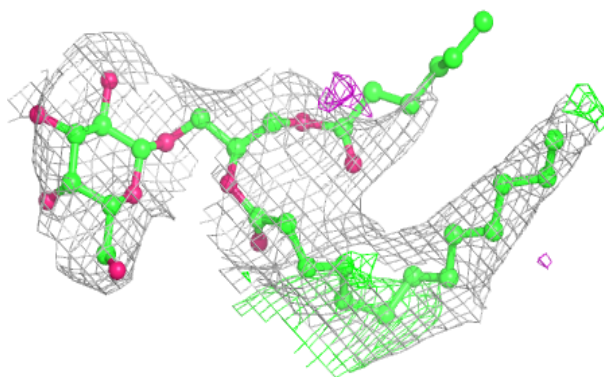
Electron density around CLA 3 3019:

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

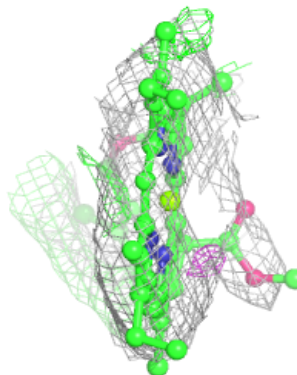
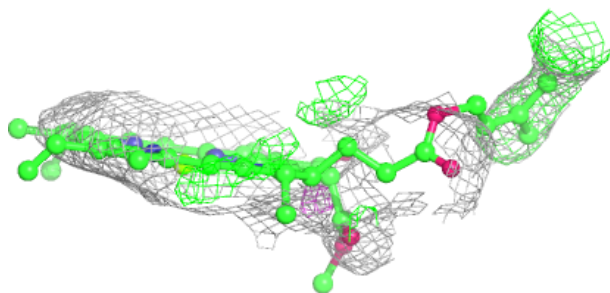
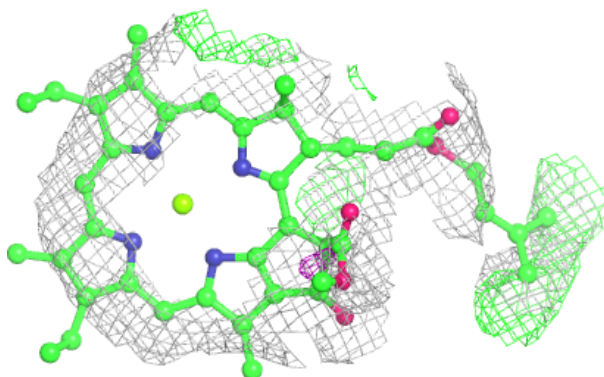


Electron density around LMG B 5005:

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

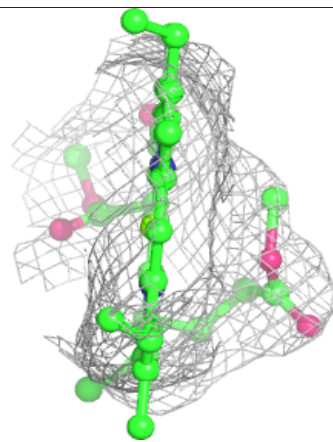
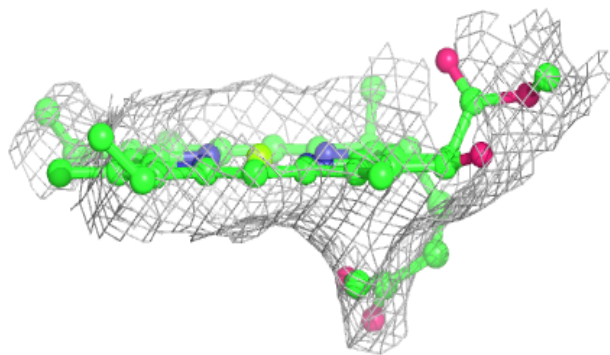
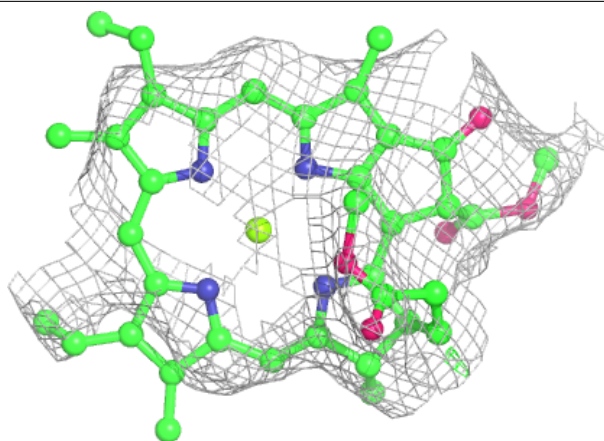
**Electron density around CLA J 1302:**

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



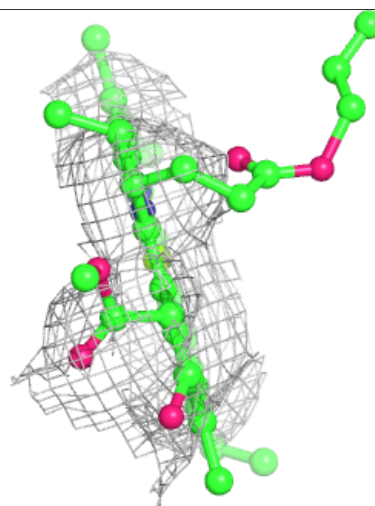
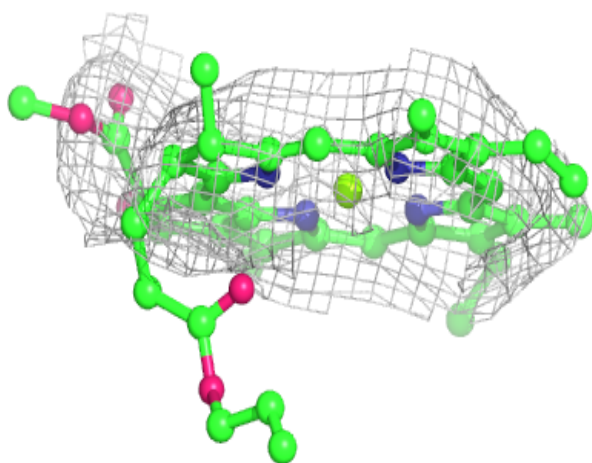
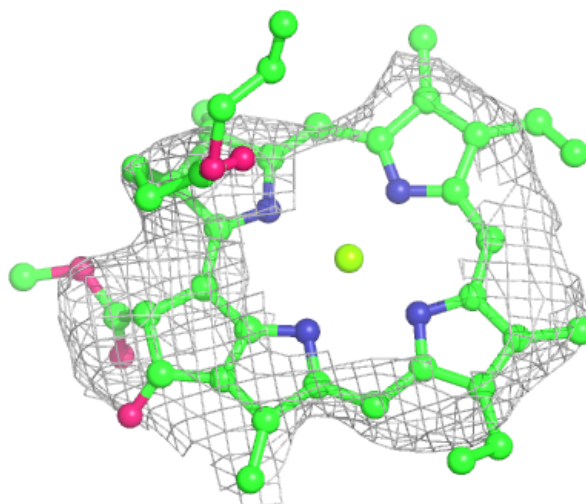
Electron density around CLA 4 4016:

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



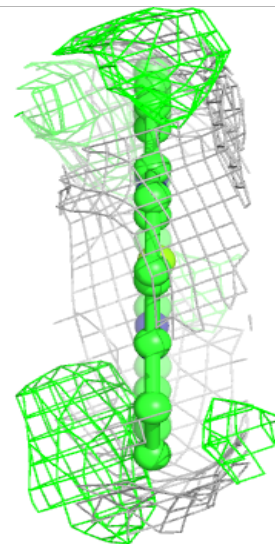
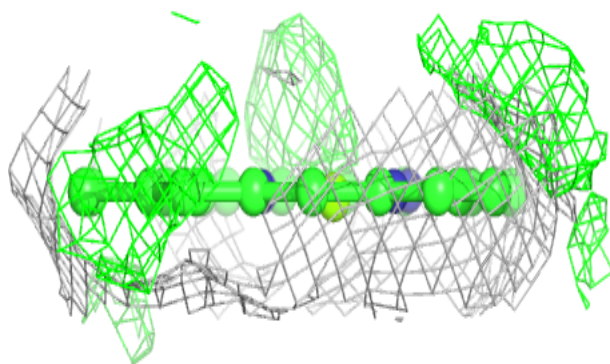
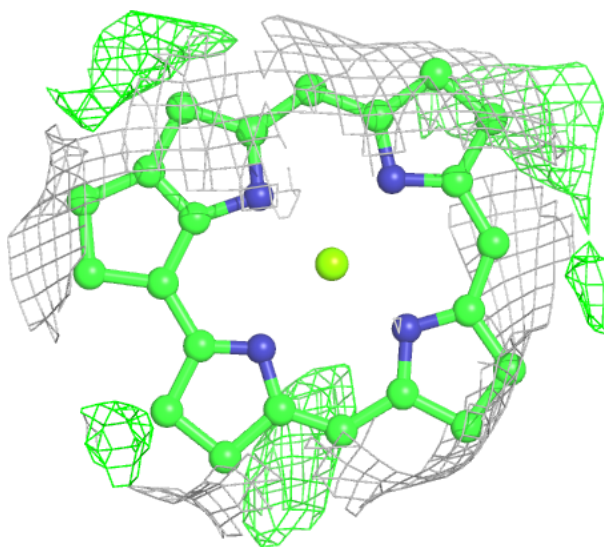
Electron density around CLA 3 3008:

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



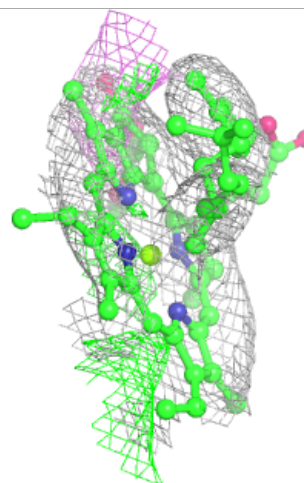
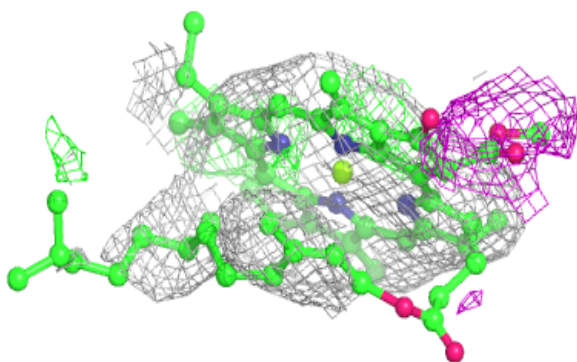
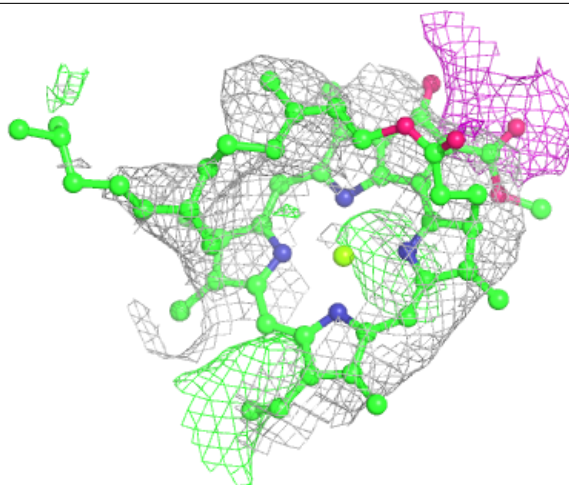
Electron density around CLA 2 2019:

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



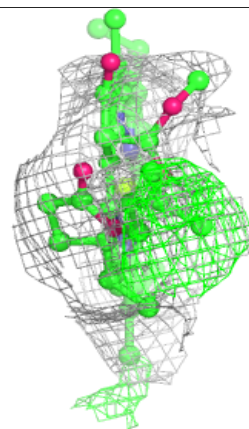
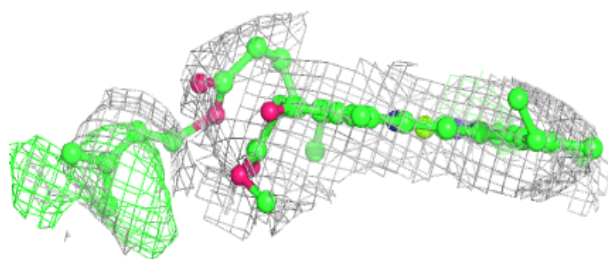
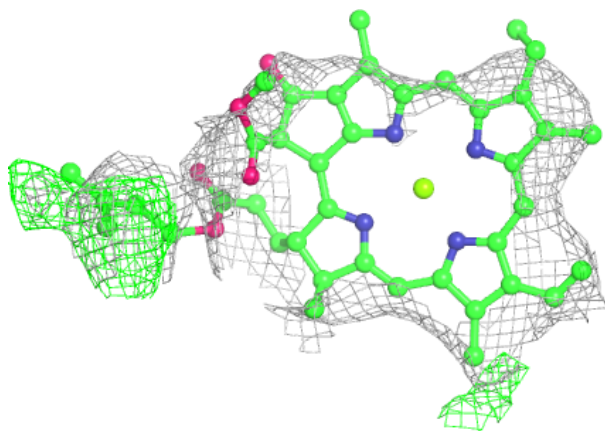
Electron density around CLA 3 3010:

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

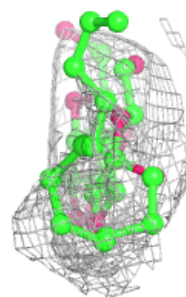
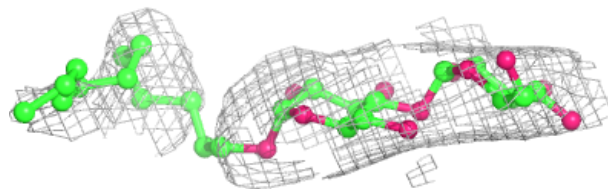
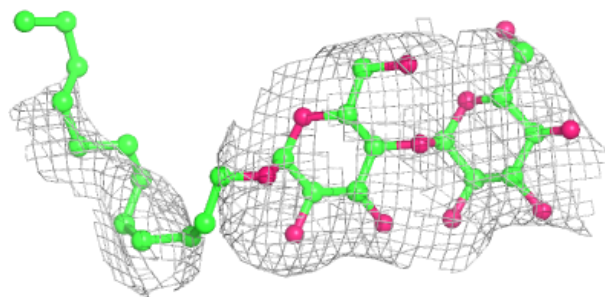


Electron density around CLA 2 2016:

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

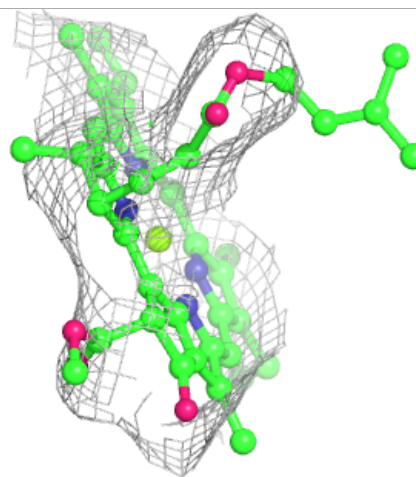
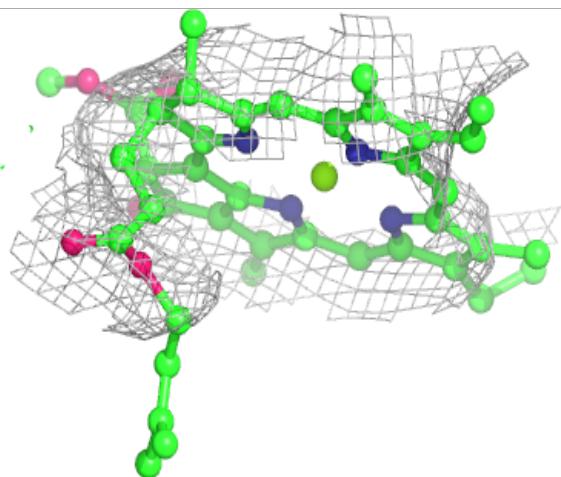
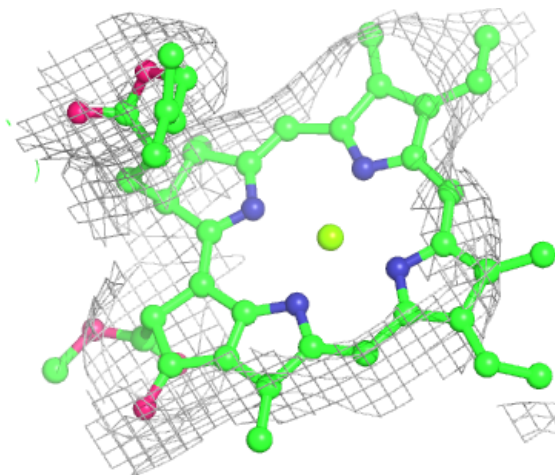
**Electron density around LMU B 8002:**

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



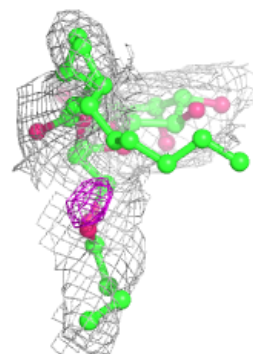
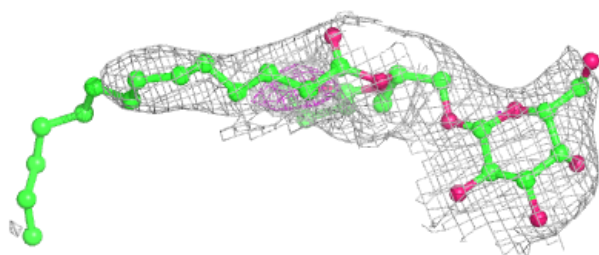
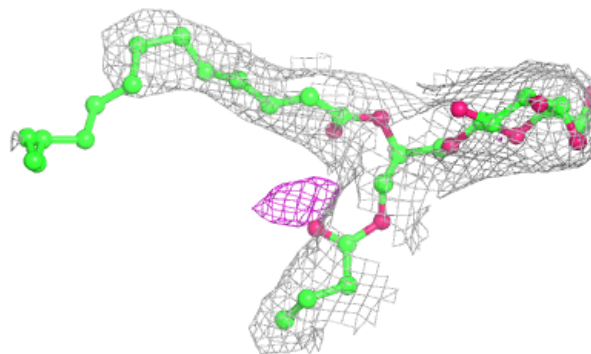
Electron density around CLA 3 3018:

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

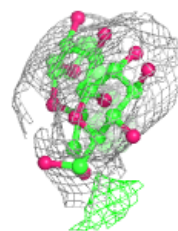
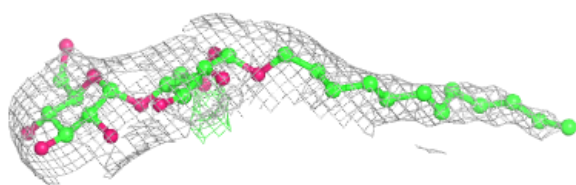
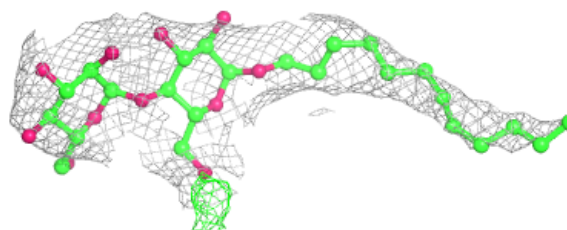


Electron density around LMG F 5002:

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

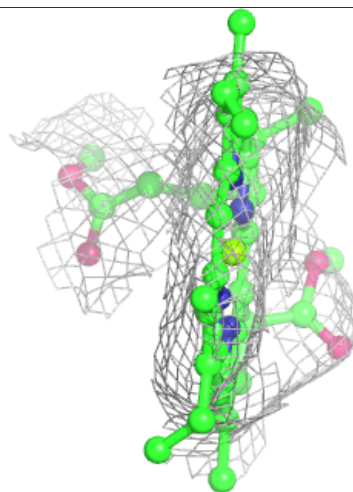
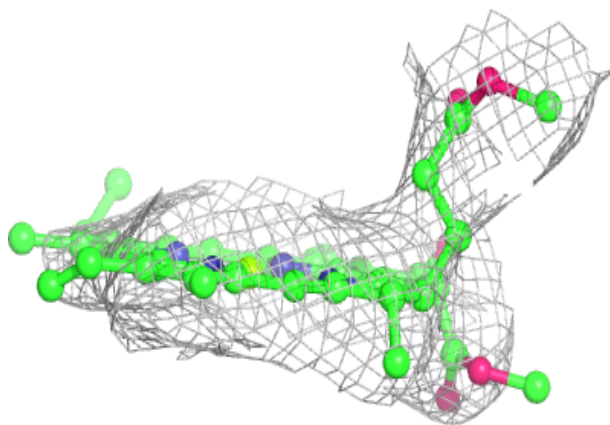
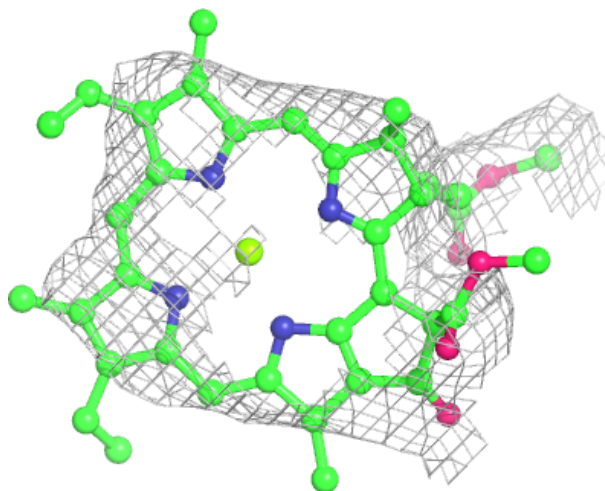
**Electron density around LMU B 8001:**

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



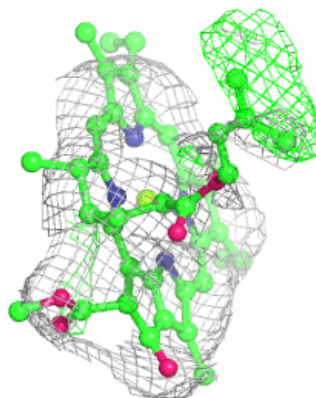
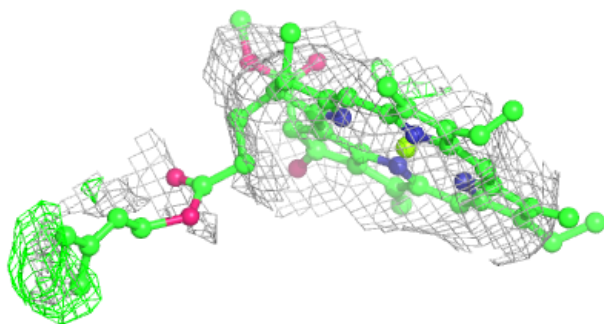
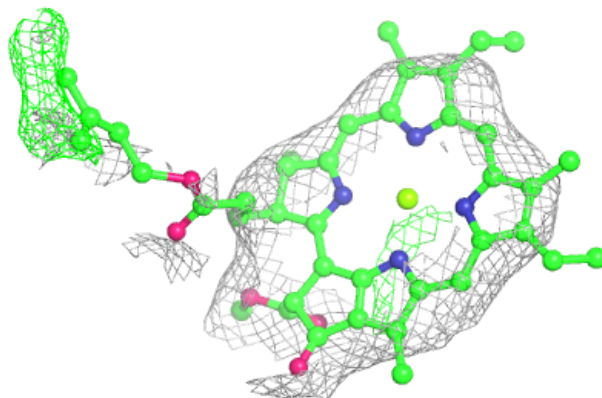
Electron density around CLA K 1001:

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



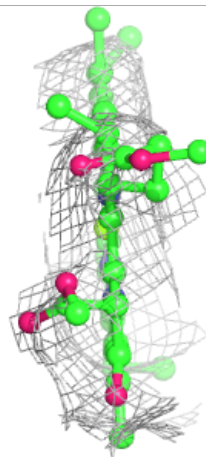
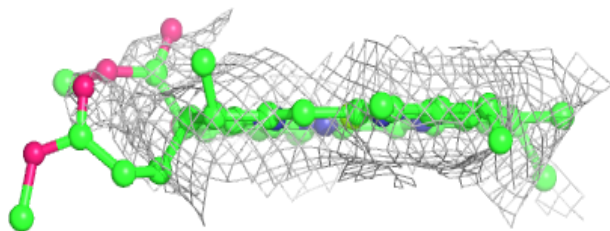
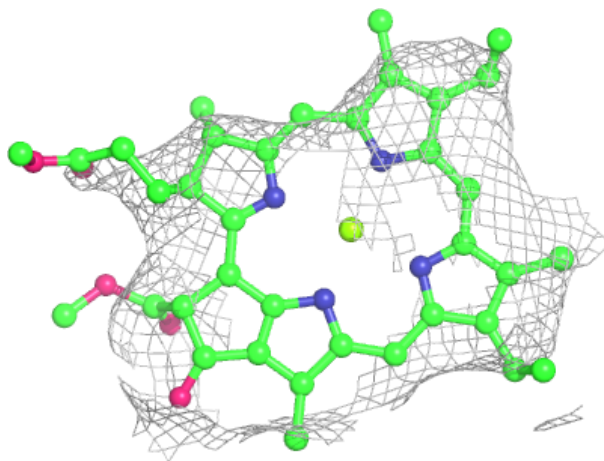
Electron density around CLA 3 3007:

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



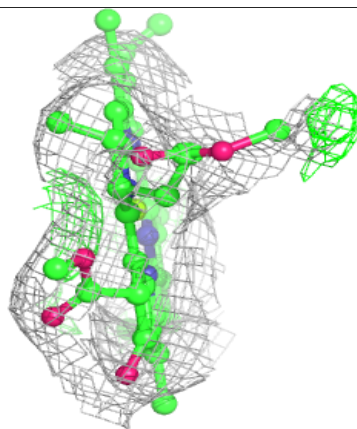
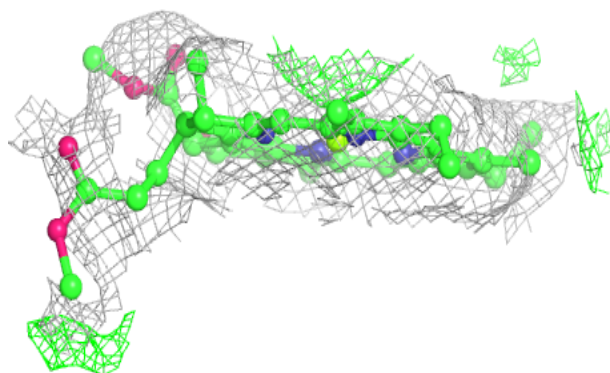
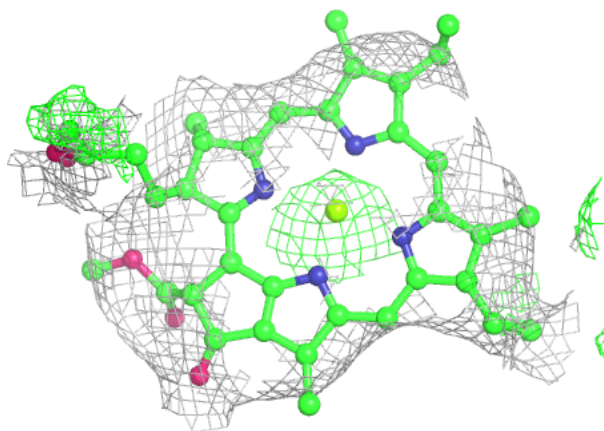
Electron density around CLA 1 1013:

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

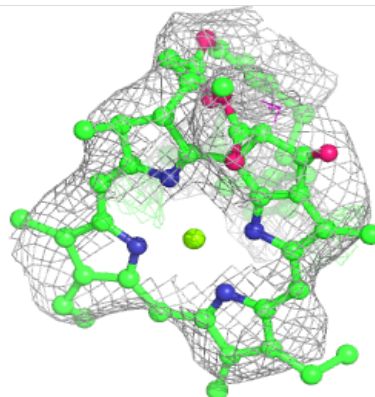
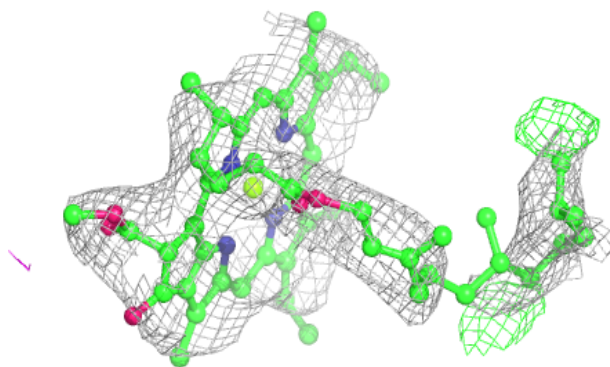
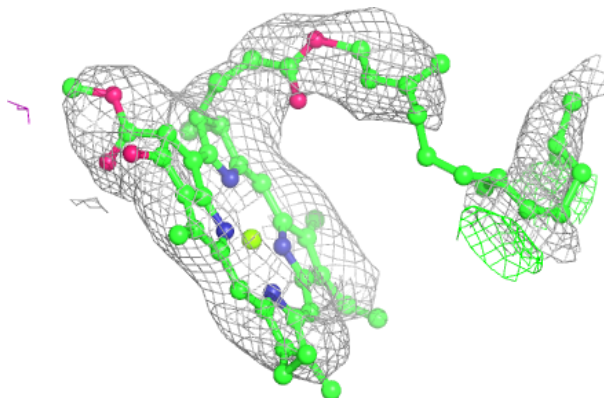


Electron density around CLA 3 3013:

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

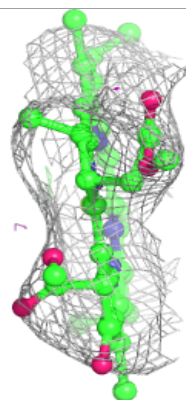
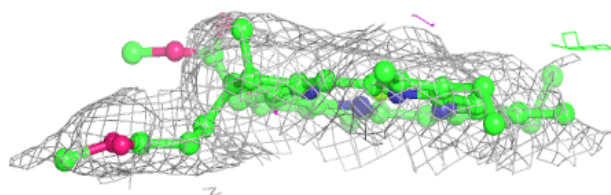
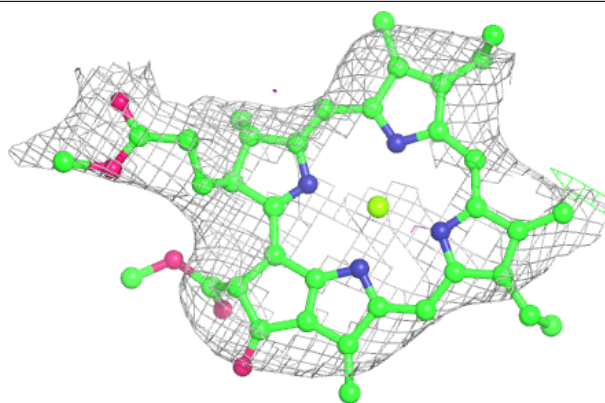
**Electron density around CLA G 1003:**

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

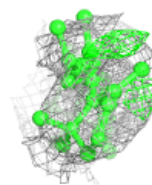
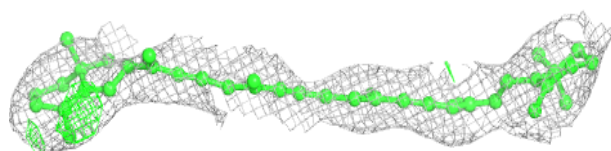
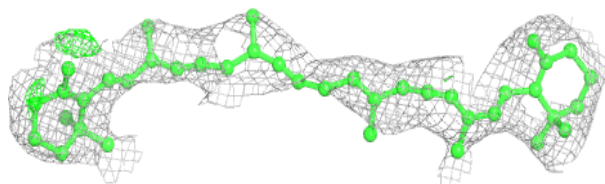


Electron density around CLA H 1000:

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

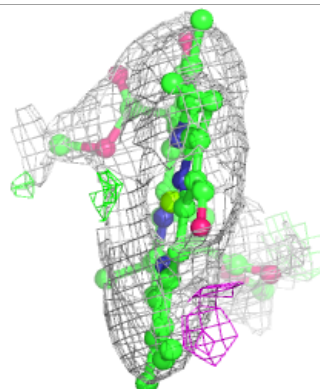
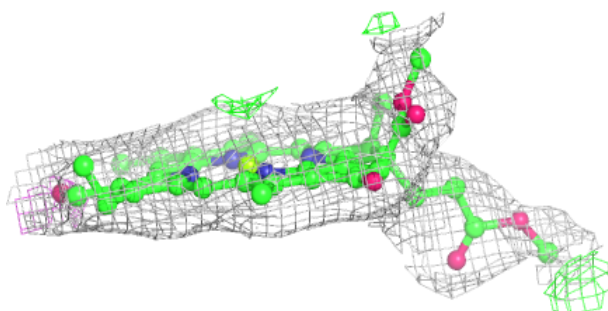
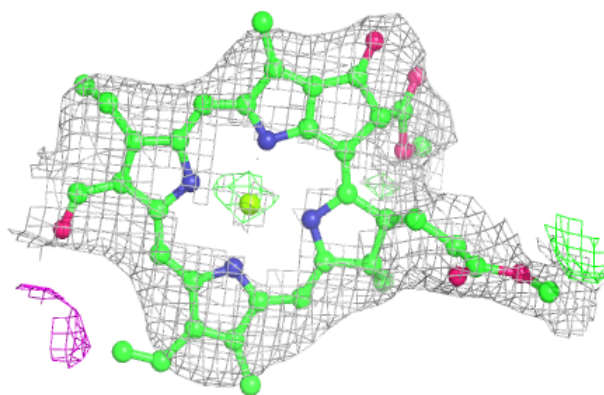
**Electron density around BCR G 2011:**

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

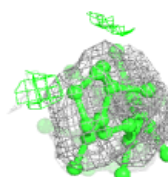
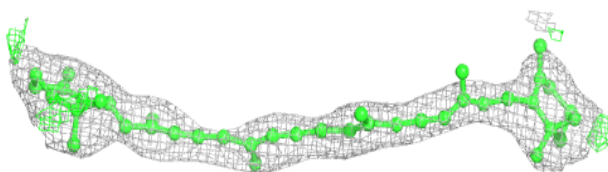
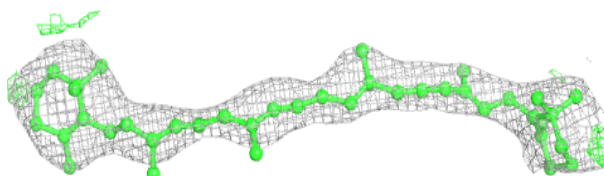


Electron density around CHL 2 2010:

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

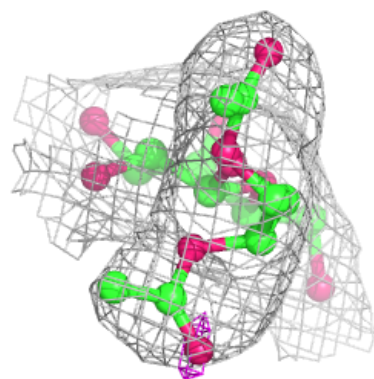
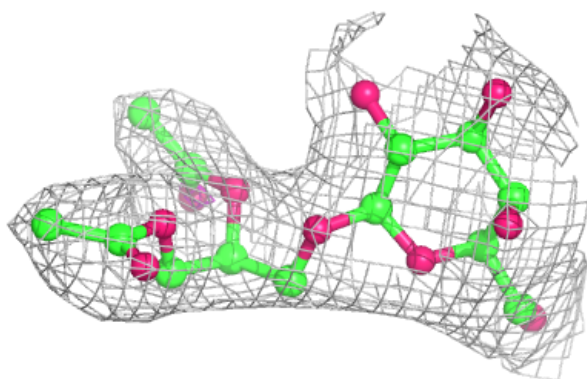
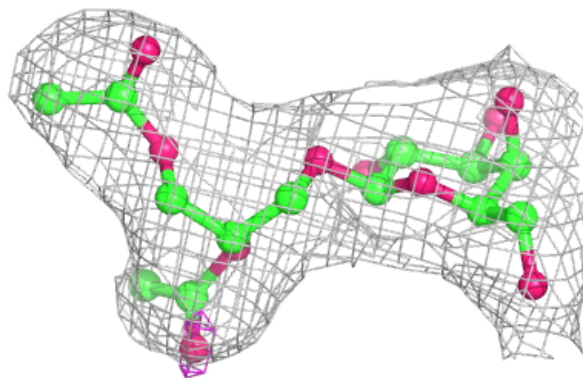
**Electron density around BCR J 6013:**

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

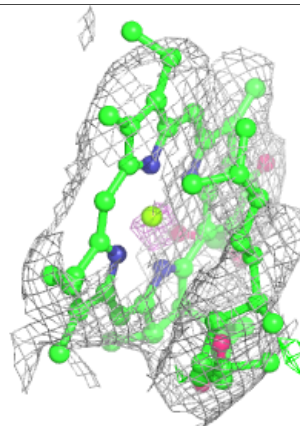
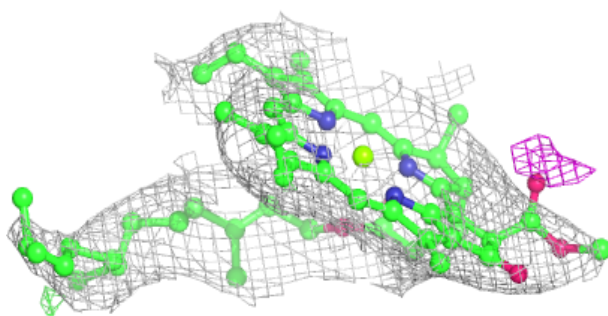
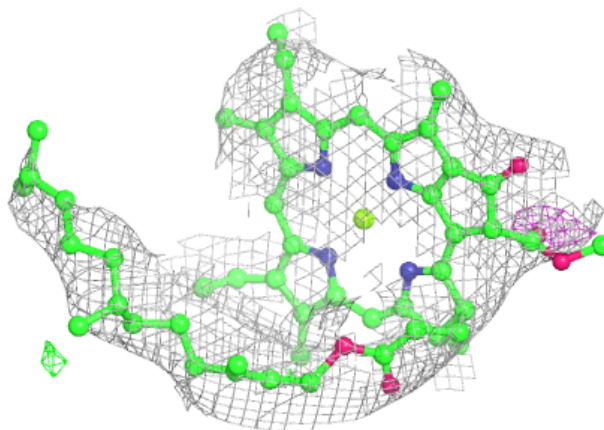


Electron density around LMG F 5001:

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

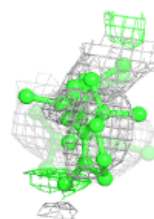
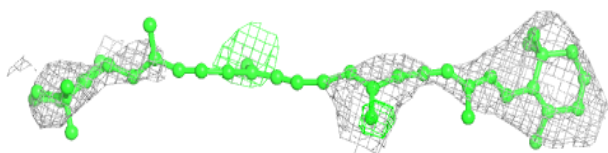
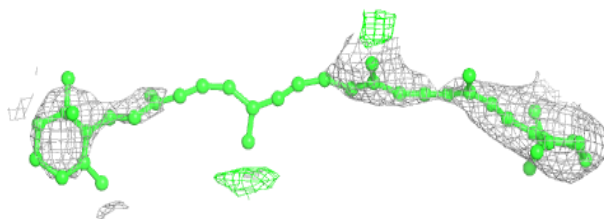
**Electron density around CLA 1 1001:**

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



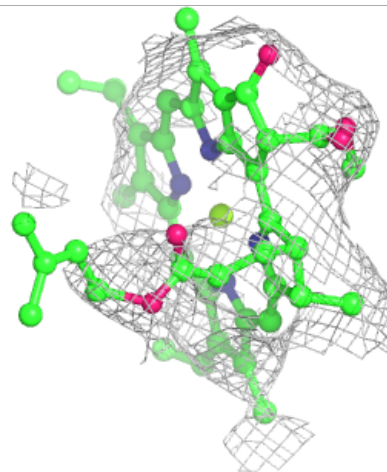
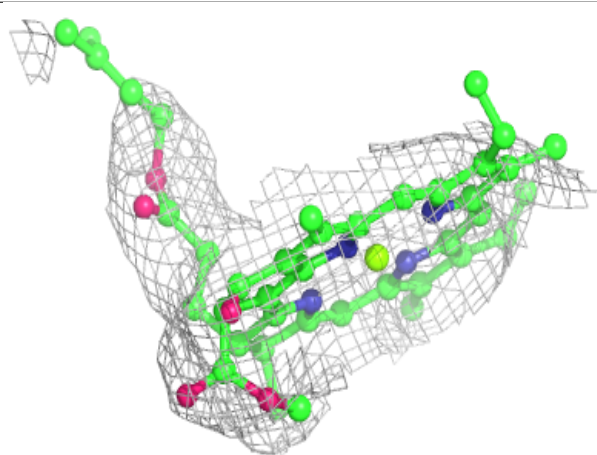
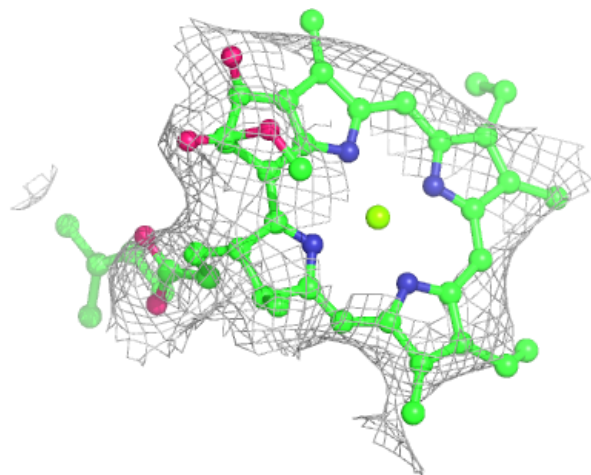
Electron density around BCR K 2011:

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



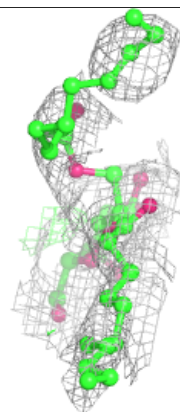
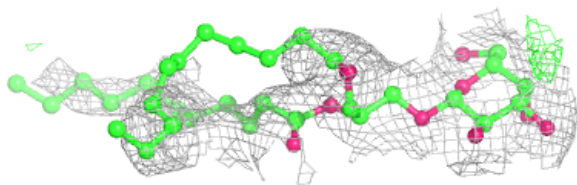
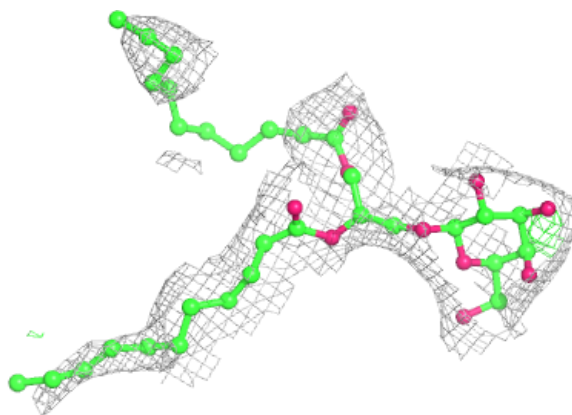
Electron density around CLA 3 3006:

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



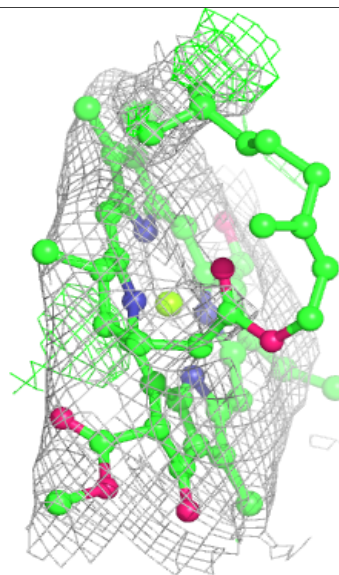
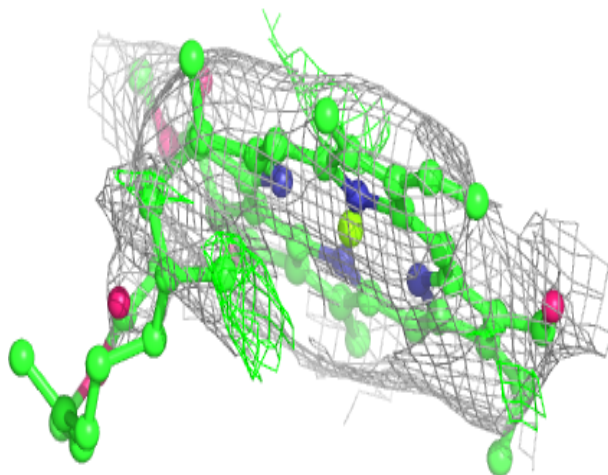
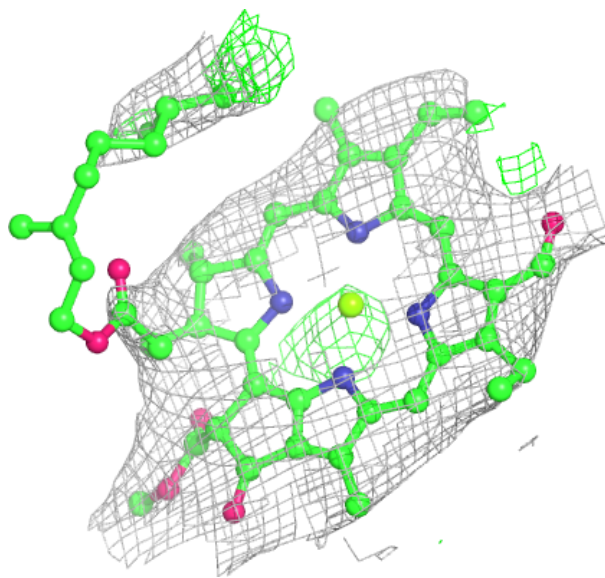
Electron density around LMG G 2021:

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



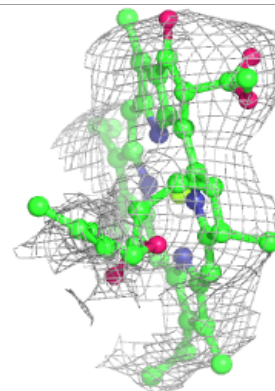
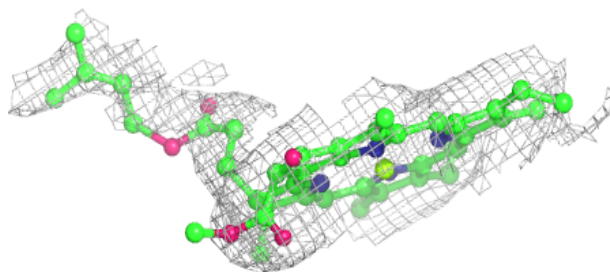
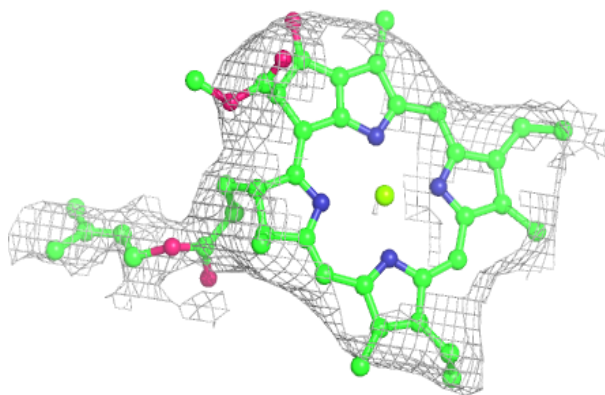
Electron density around CHL 3 3011:

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

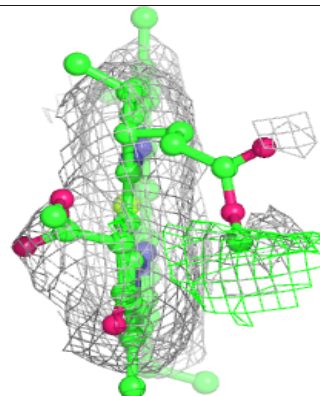
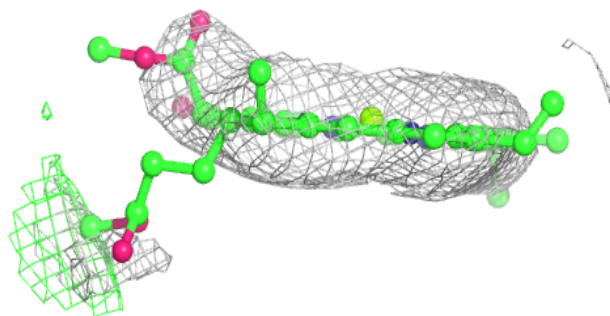
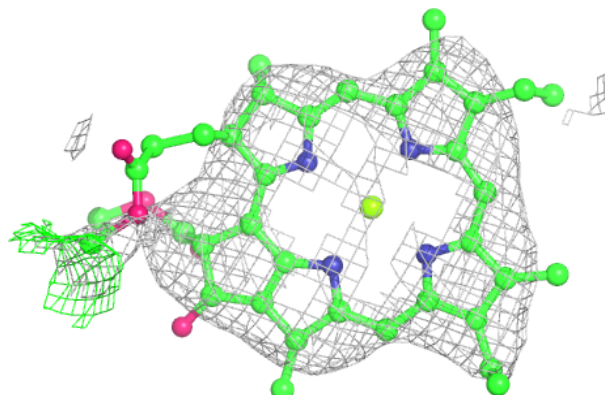


Electron density around CLA A 1151:

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

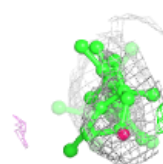
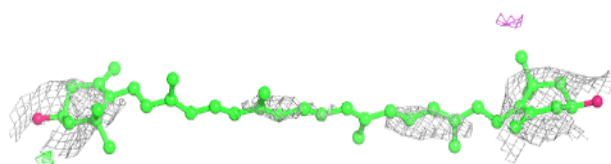
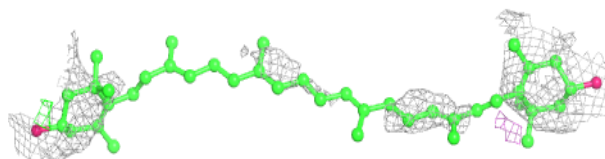
**Electron density around CLA A 1113:**

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



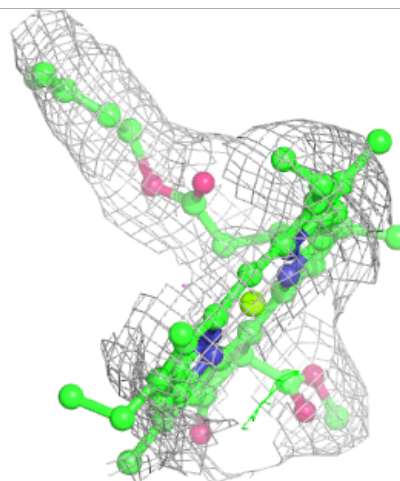
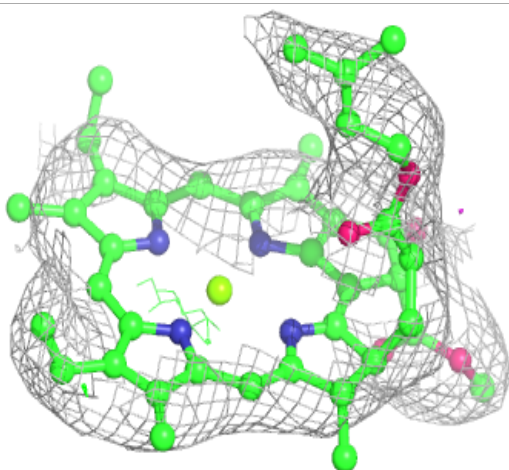
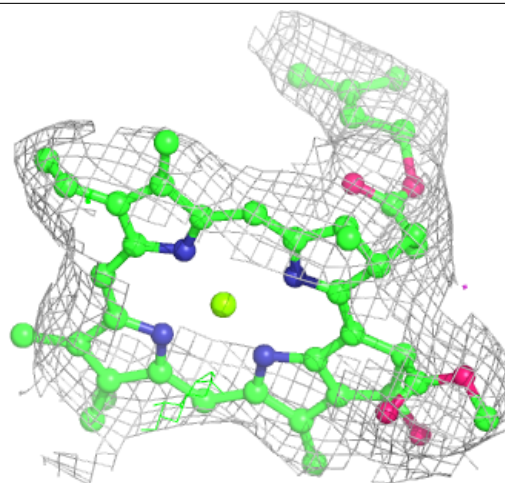
Electron density around LUT 3 3501:

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



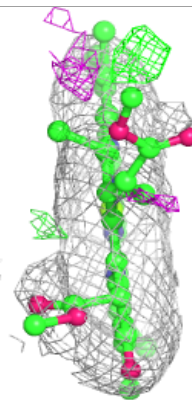
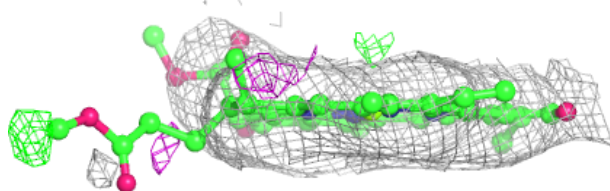
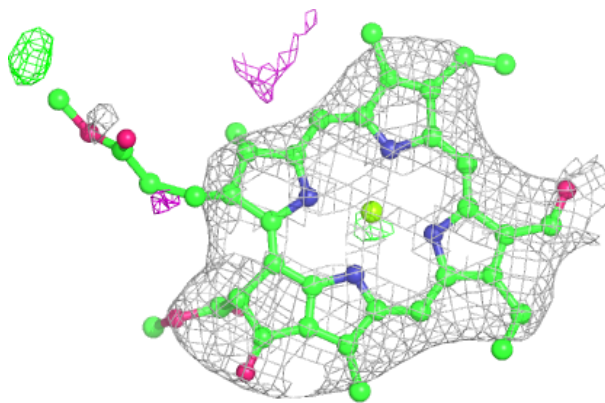
Electron density around CLA L 1501:

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

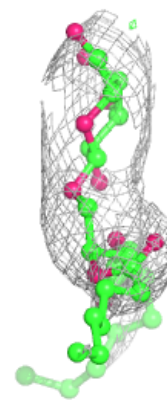
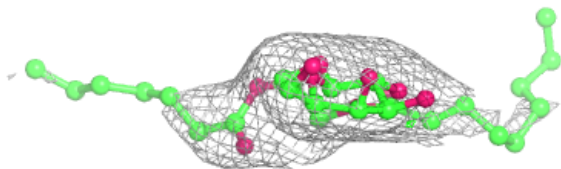
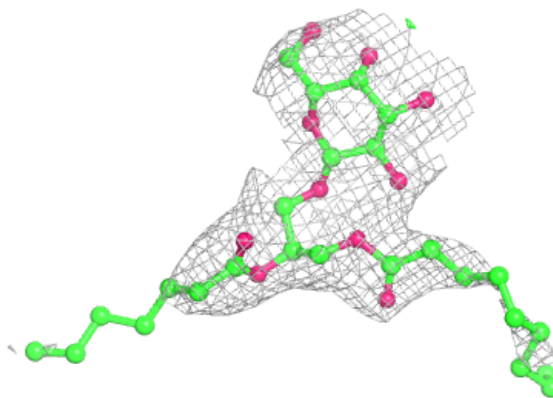


Electron density around CHL 4 4010:

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

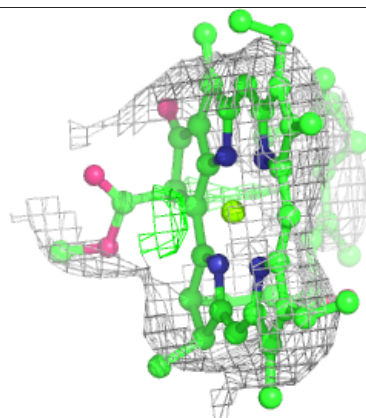
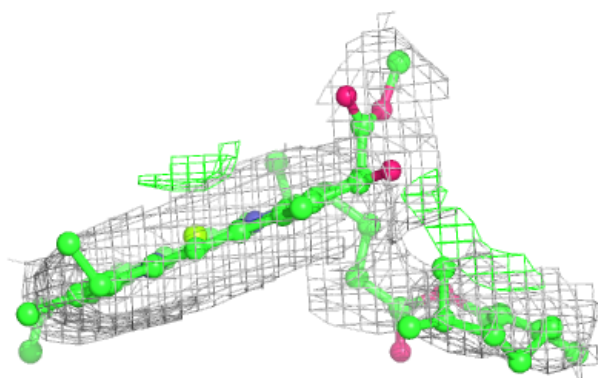
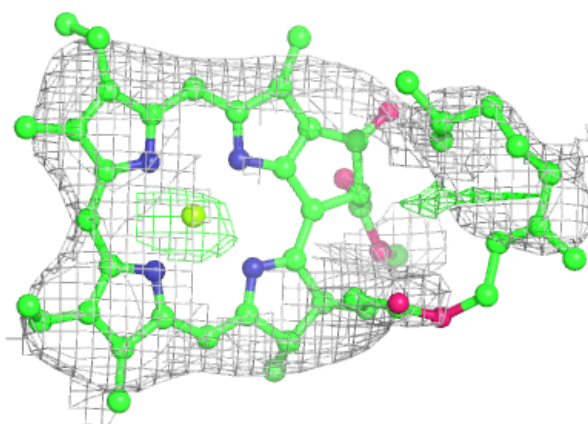
**Electron density around LMG 2 2802:**

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

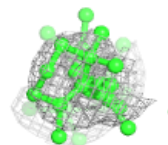
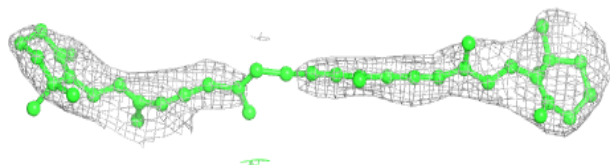
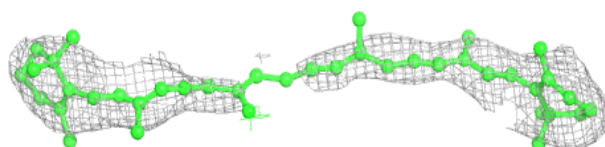


Electron density around CLA A 1134:

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

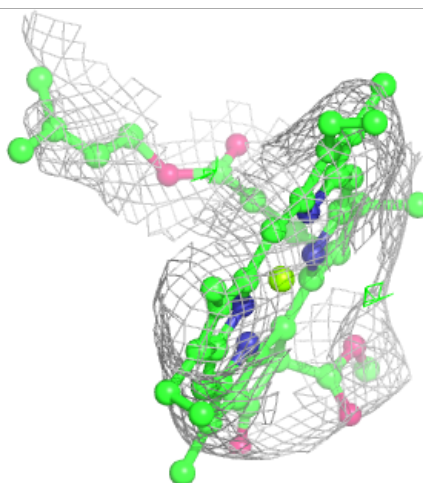
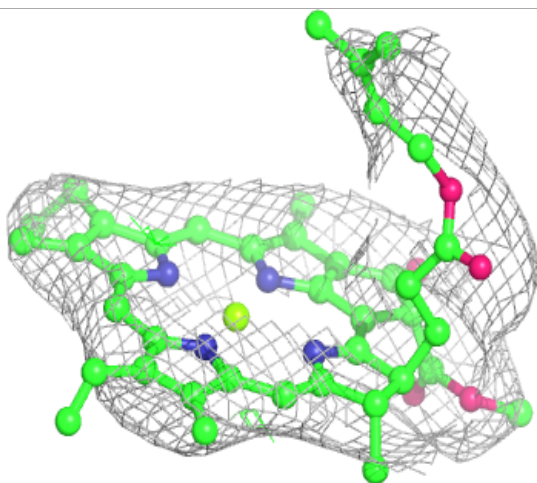
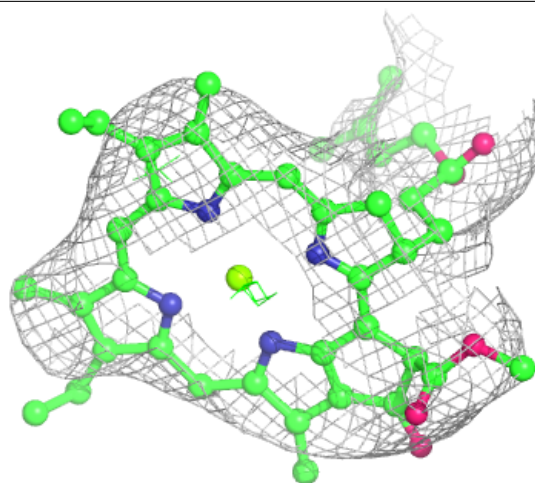
**Electron density around BCR L 6020:**

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



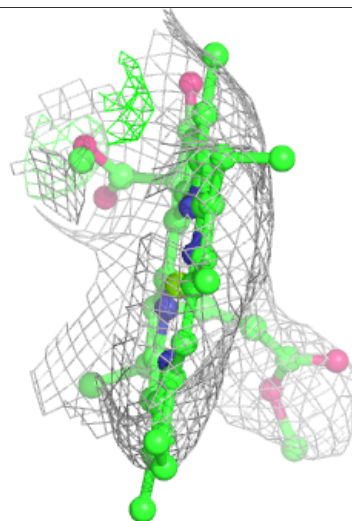
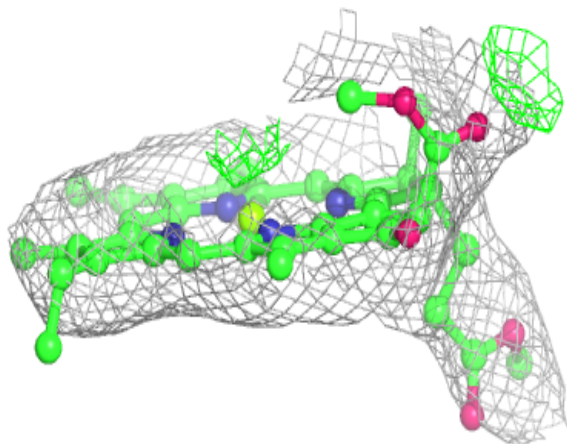
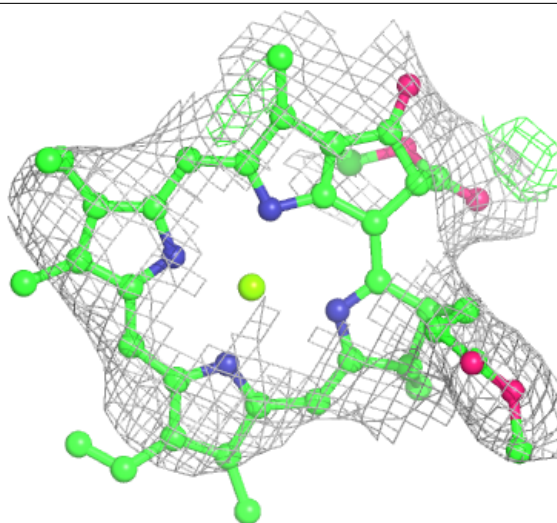
Electron density around CLA 1 1006:

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



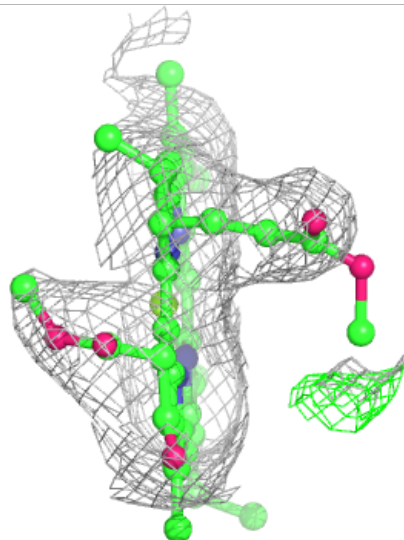
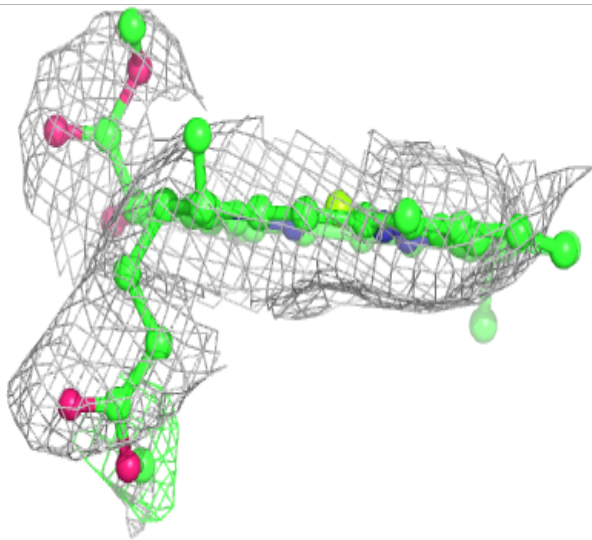
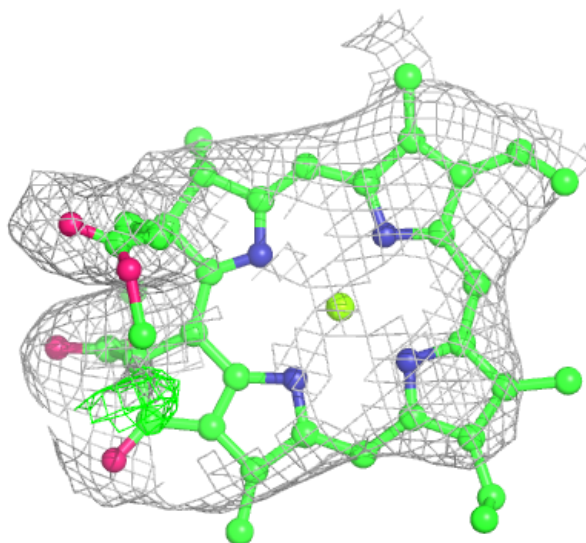
Electron density around CLA 1 1008:

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



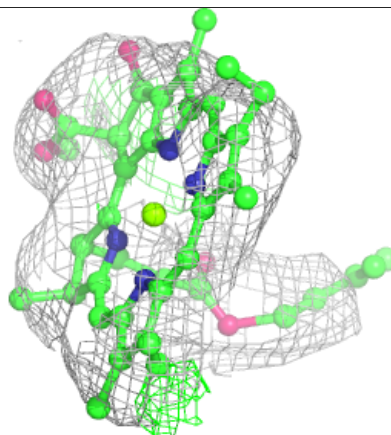
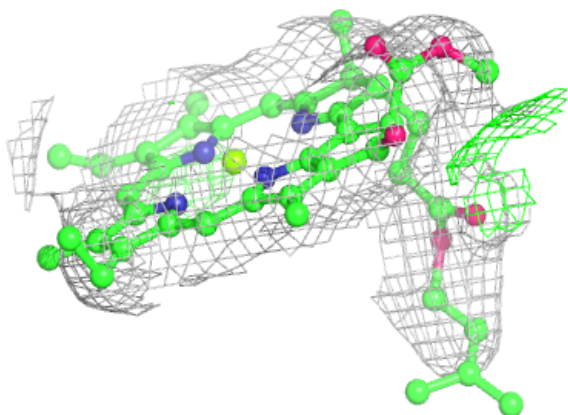
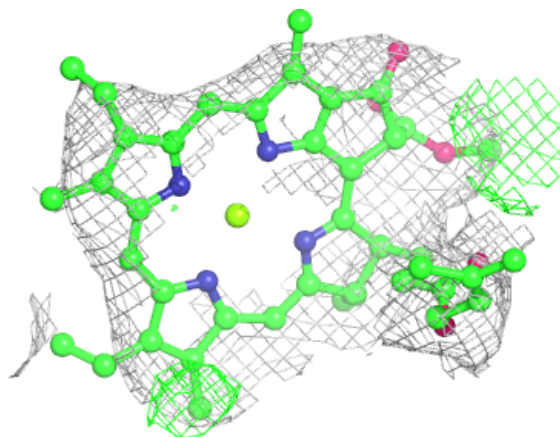
Electron density around CLA A 1114:

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

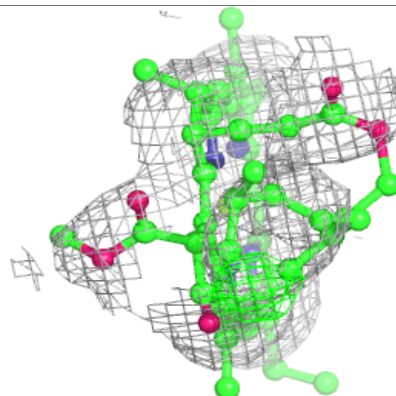
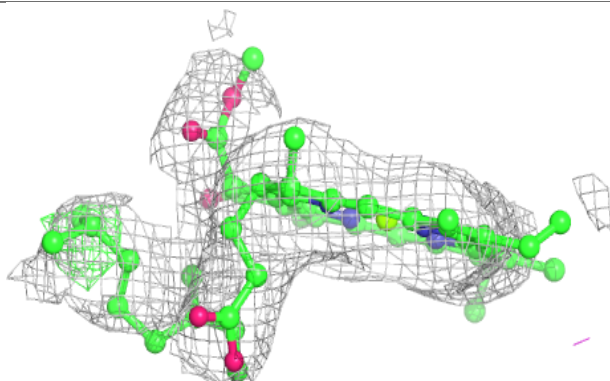
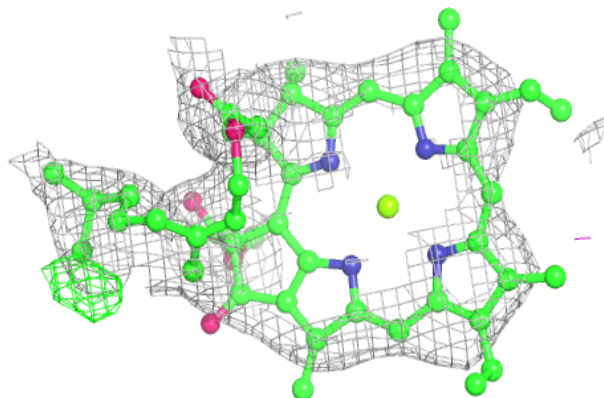


Electron density around CLA 4 4006:

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

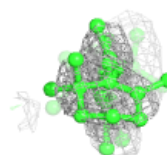
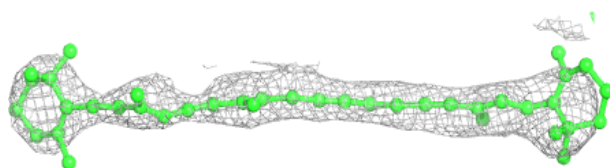
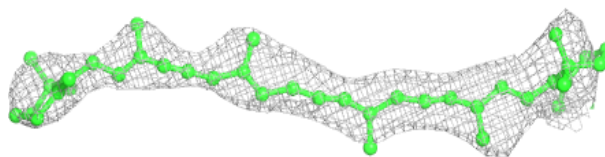
**Electron density around CLA 2 2006:**

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



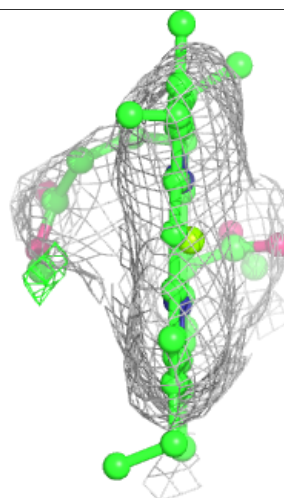
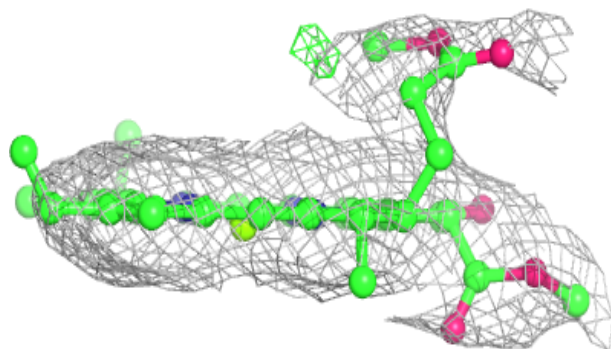
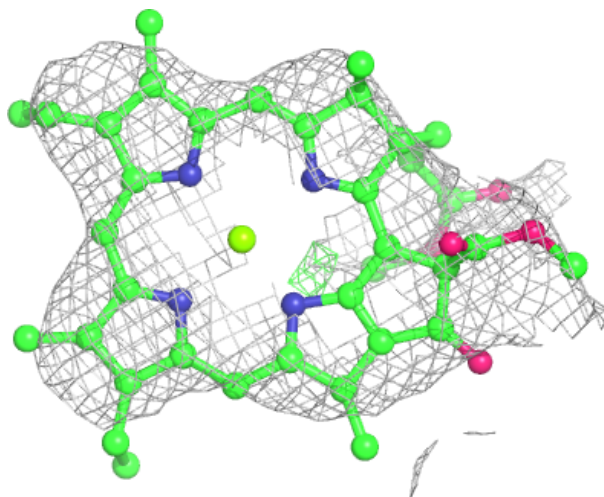
Electron density around BCR A 6007:

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



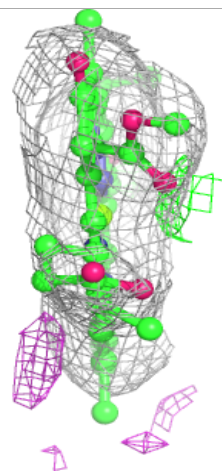
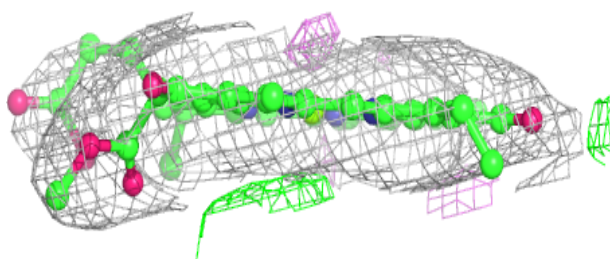
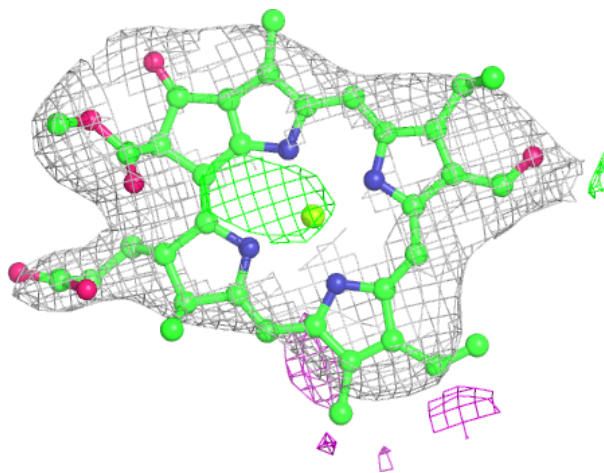
Electron density around CLA A 1115:

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



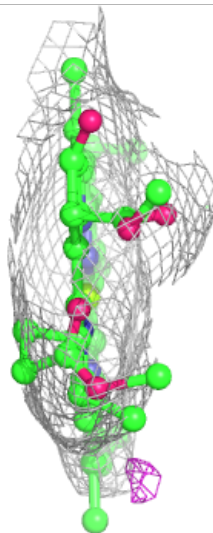
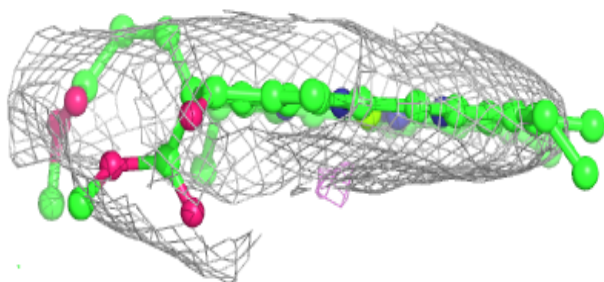
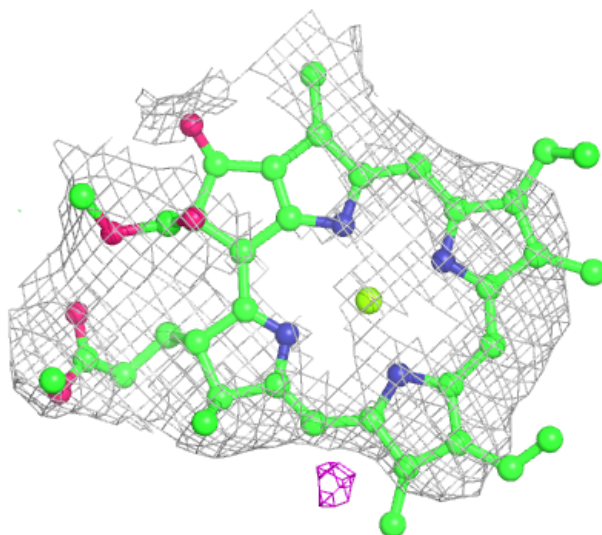
Electron density around CHL 2 2013:

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



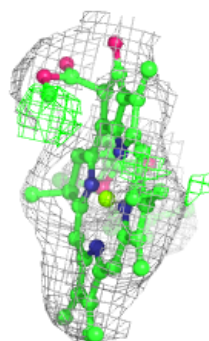
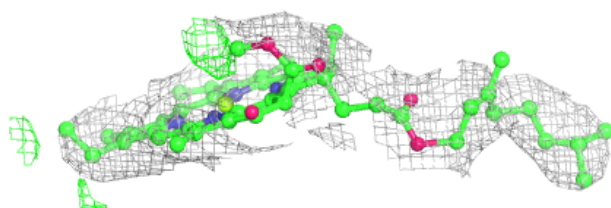
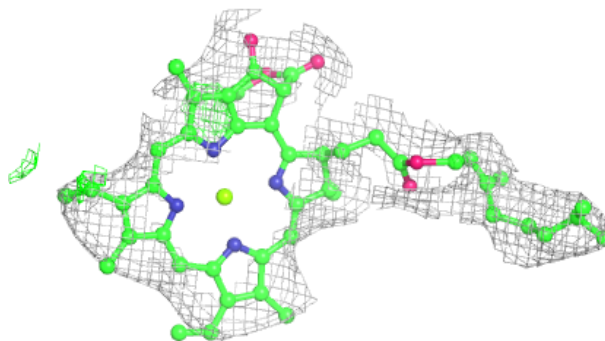
Electron density around CLA 3 3002:

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

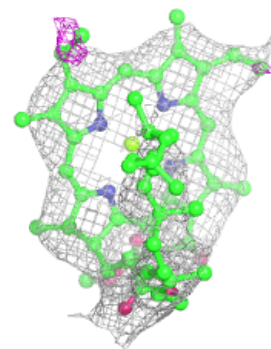
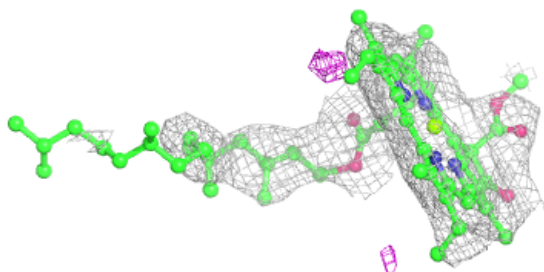
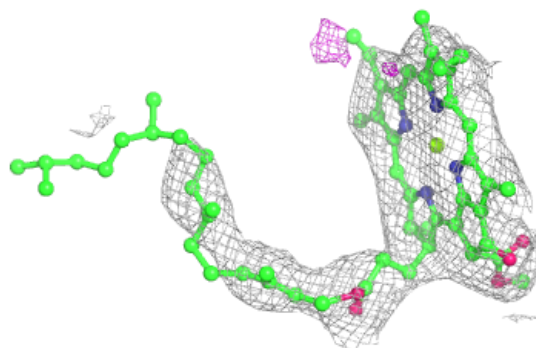


Electron density around CLA G 1001:

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

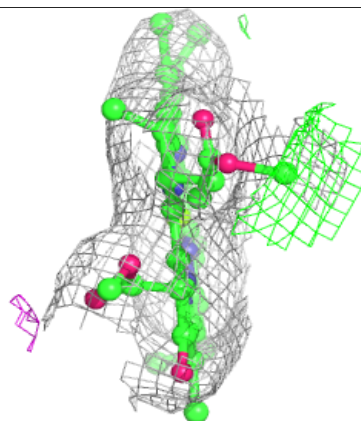
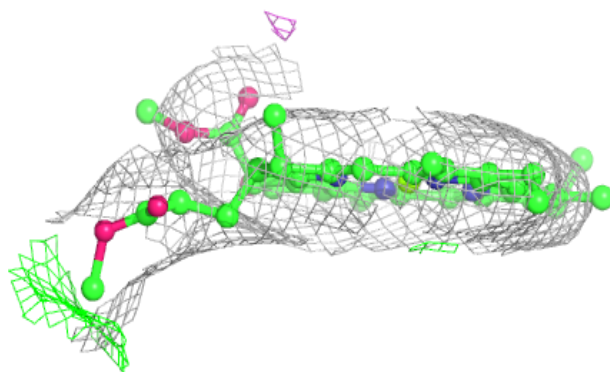
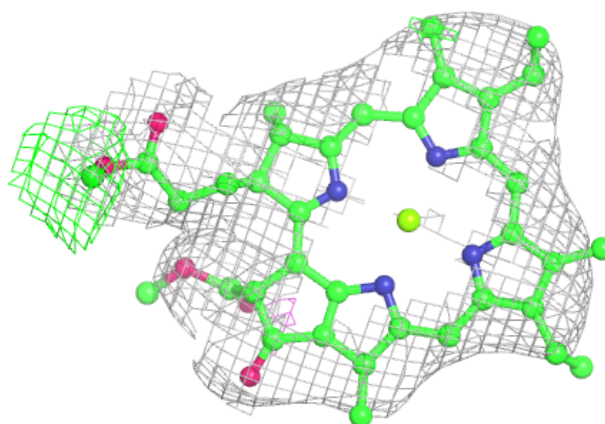
**Electron density around CLA B 1218:**

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



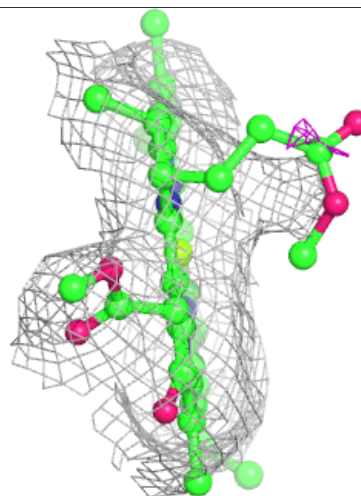
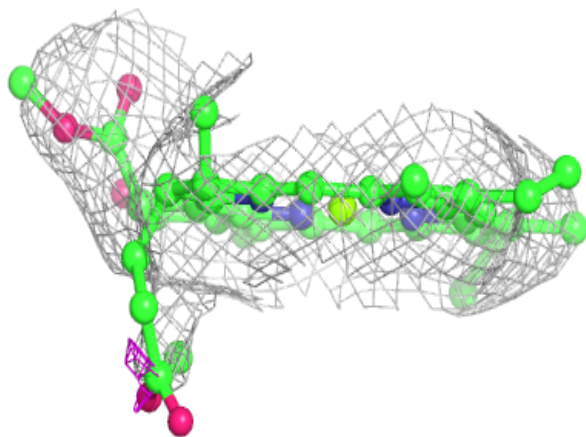
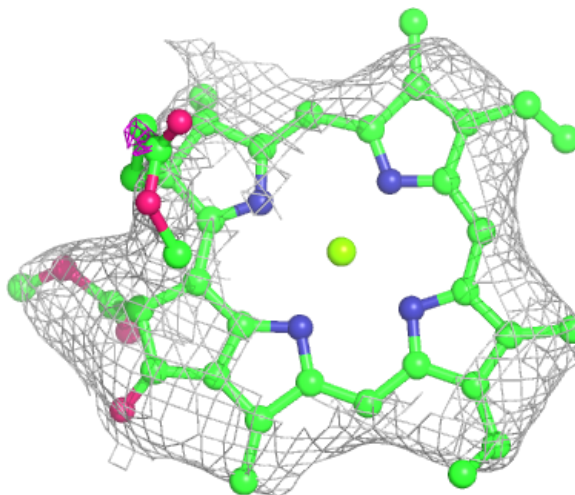
Electron density around CLA 1 1014:

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



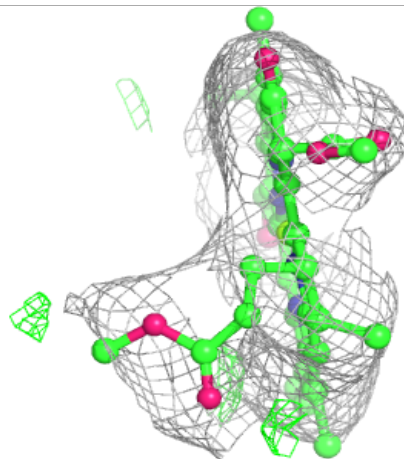
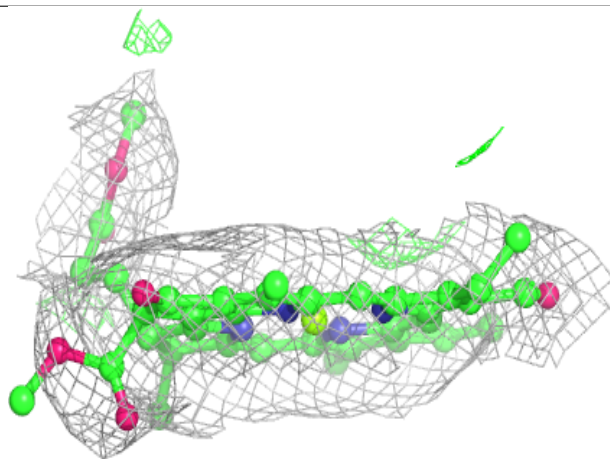
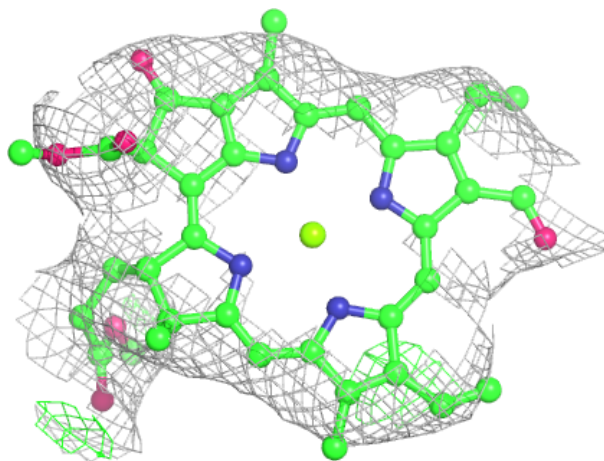
Electron density around CLA 4 4008:

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



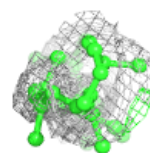
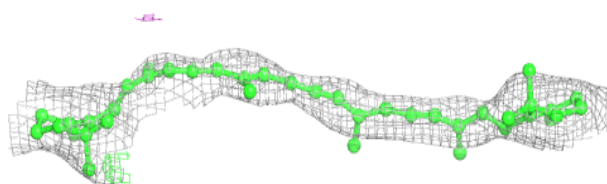
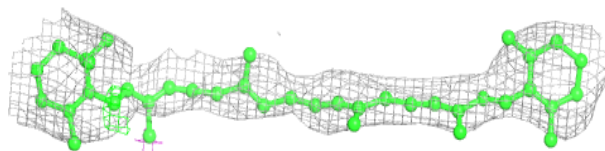
Electron density around CHL 1 1010:

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

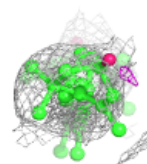
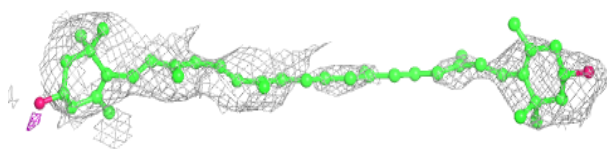
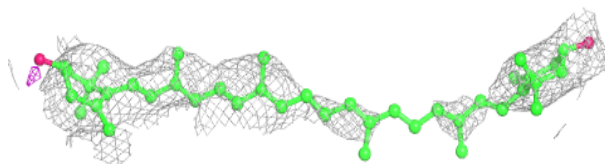


Electron density around BCR 3 3503:

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

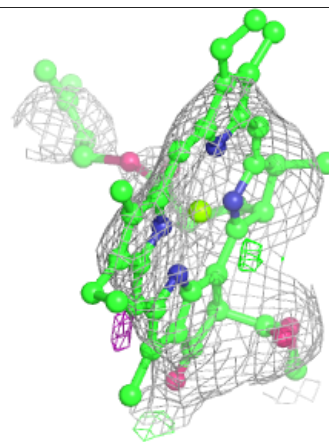
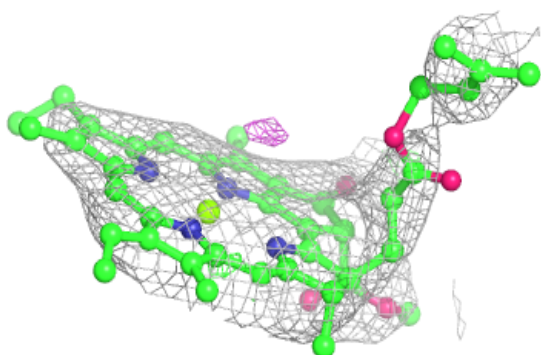
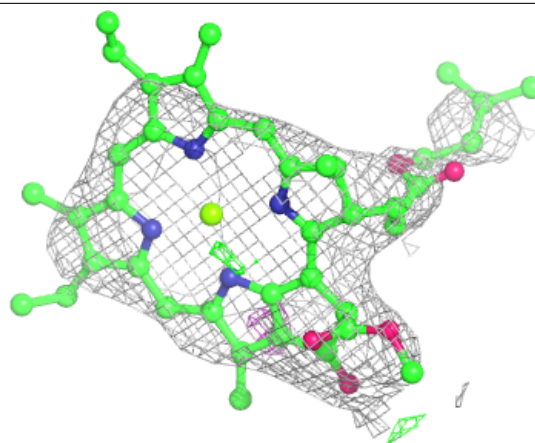
**Electron density around LUT 1 1501:**

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

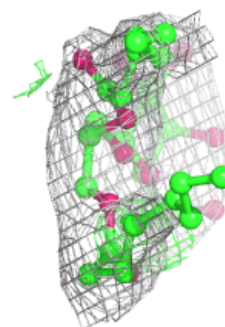
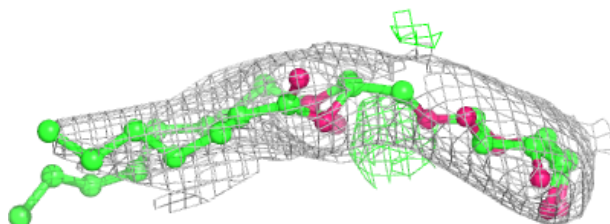
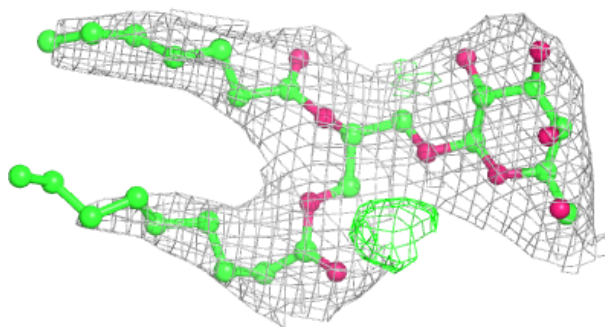


Electron density around CLA 1 1011:

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

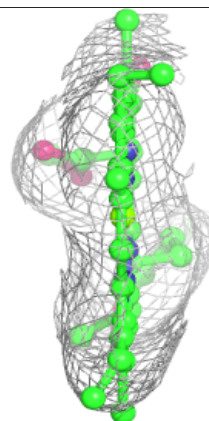
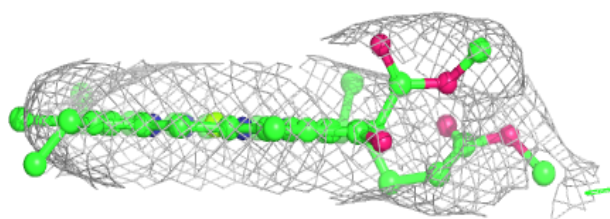
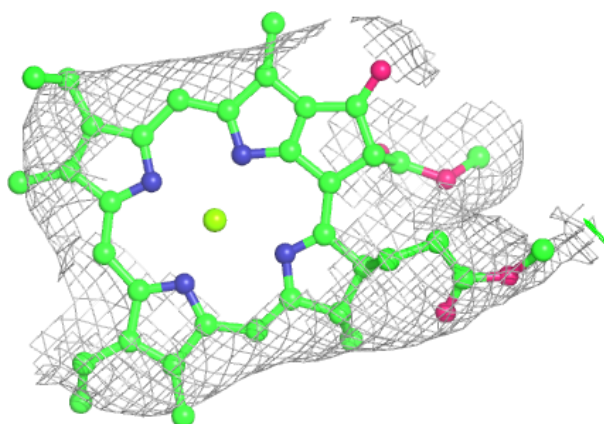
**Electron density around LMG 4 4801:**

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

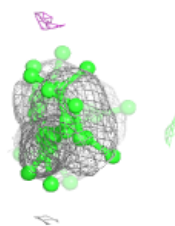
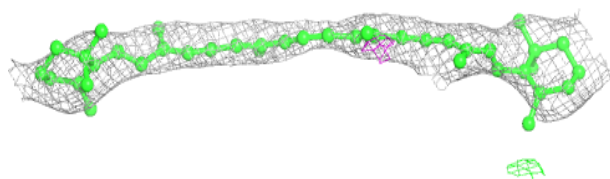
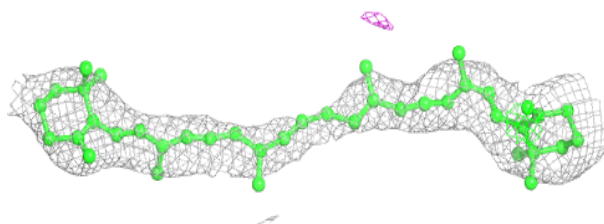


Electron density around CLA G 1002:

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

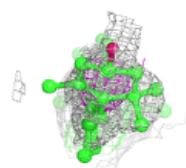
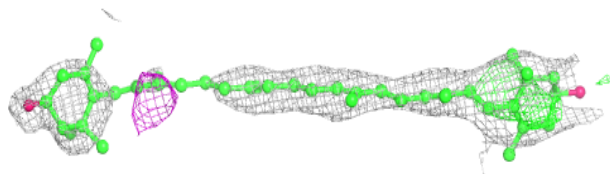
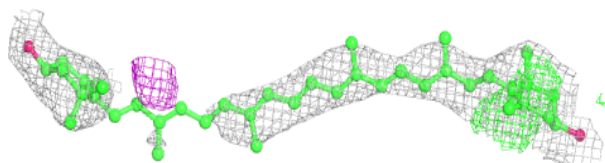
**Electron density around BCR B 6004:**

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

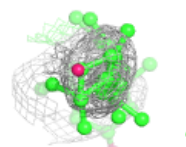
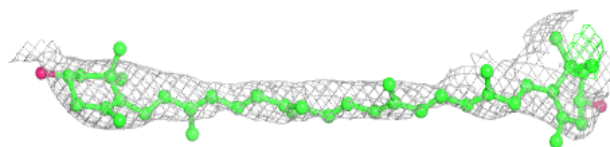
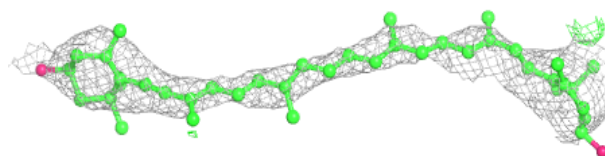


Electron density around LUT 2 2502:

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

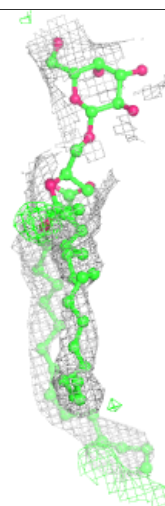
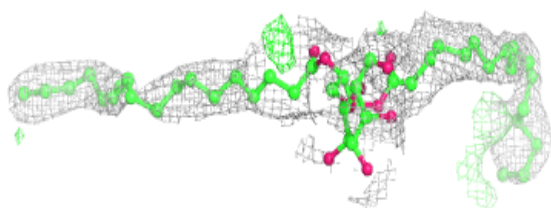
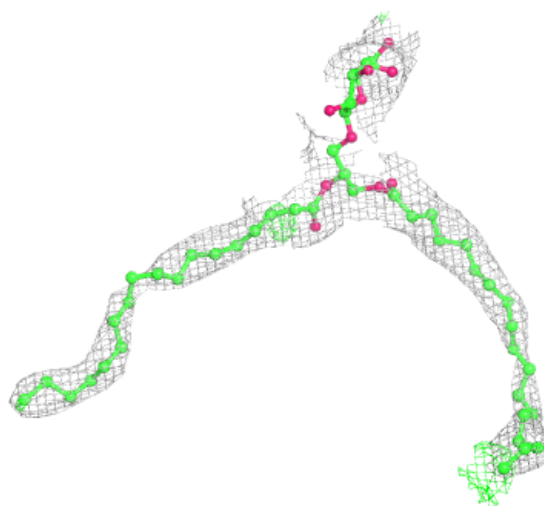
**Electron density around LUT 4 4503:**

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



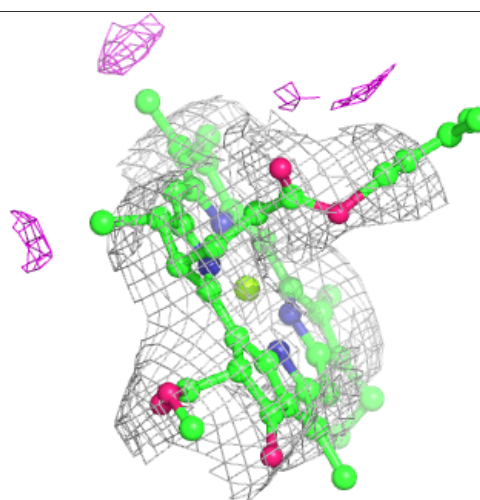
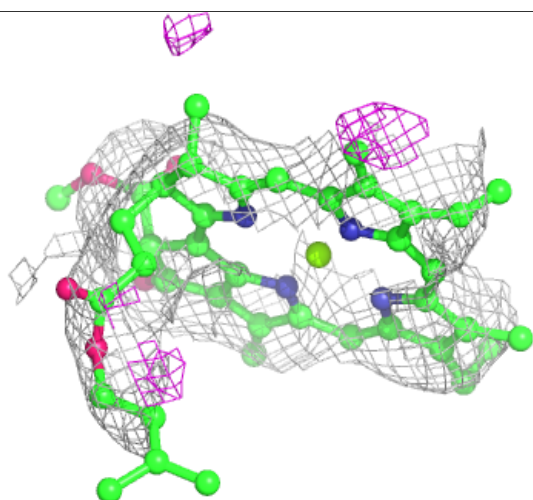
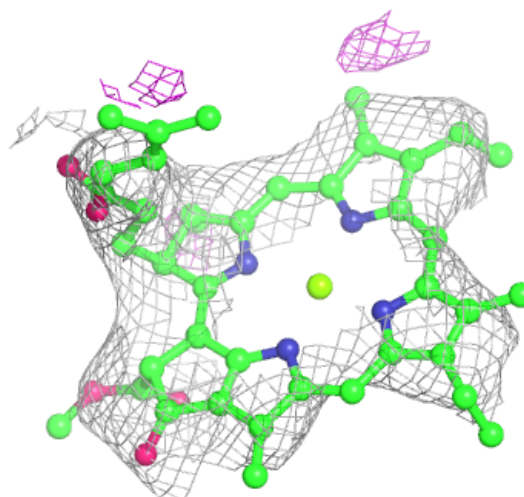
Electron density around LMG J 5001:

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



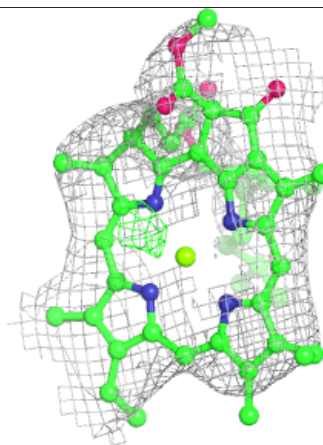
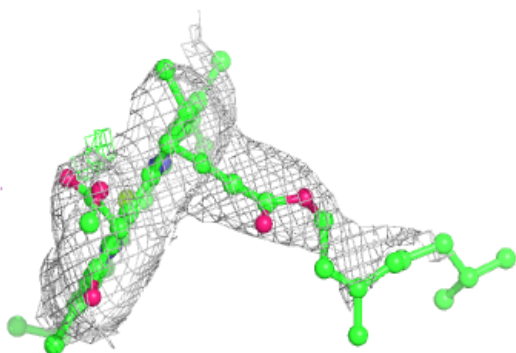
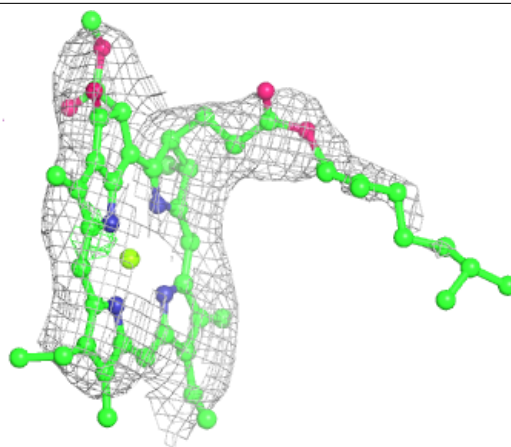
Electron density around CLA L 1503:

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

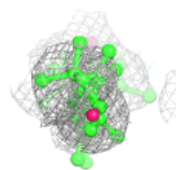
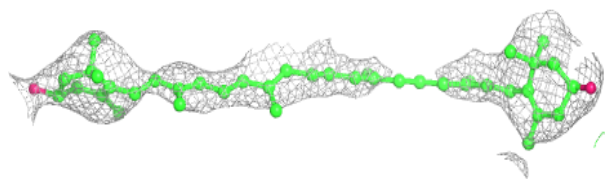
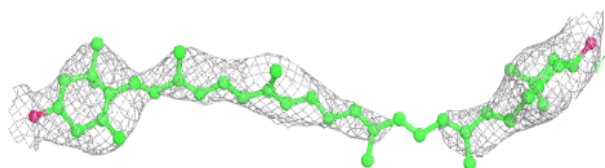


Electron density around CLA B 1232:

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

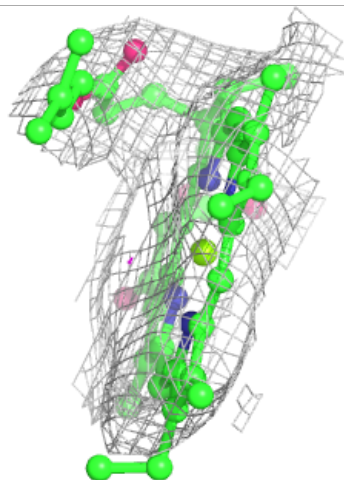
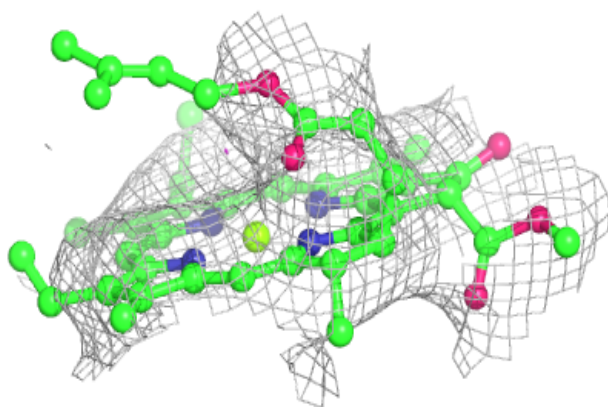
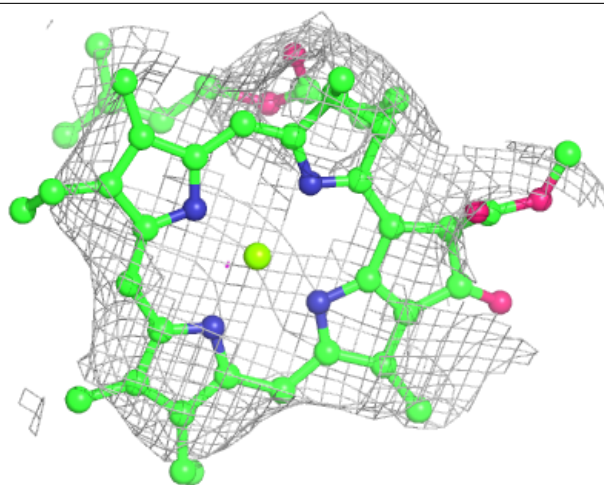
**Electron density around LUT 1 1502:**

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



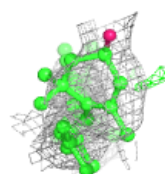
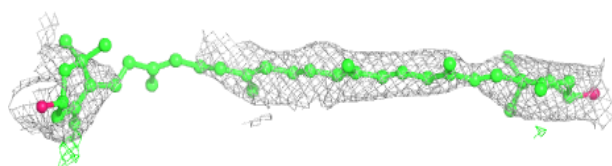
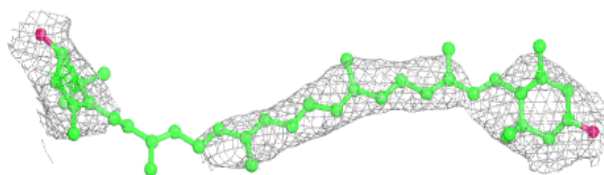
Electron density around CLA 3 3001:

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

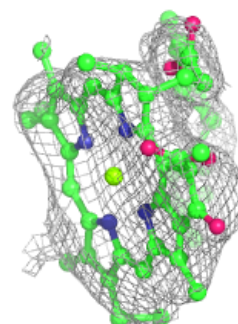
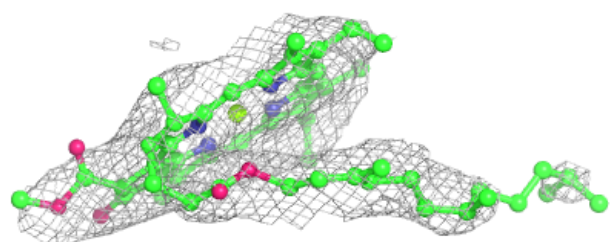
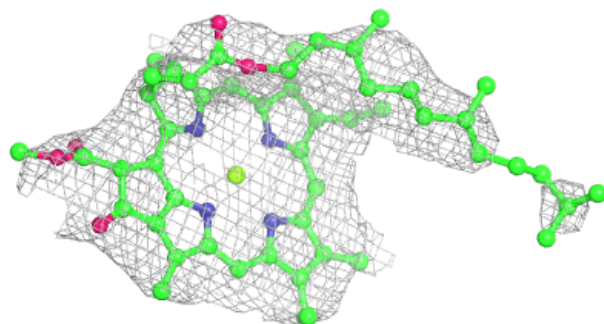


Electron density around LUT 3 3502:

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

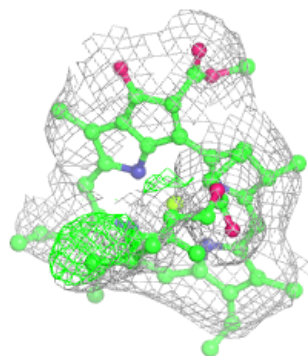
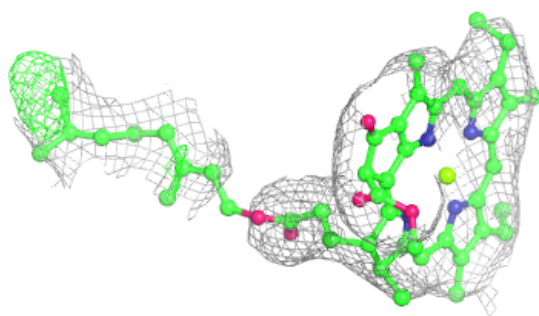
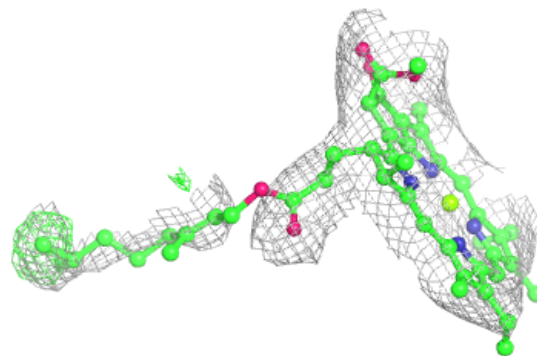
**Electron density around CLA 4 4001:**

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



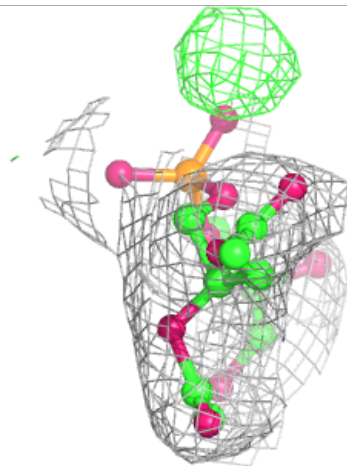
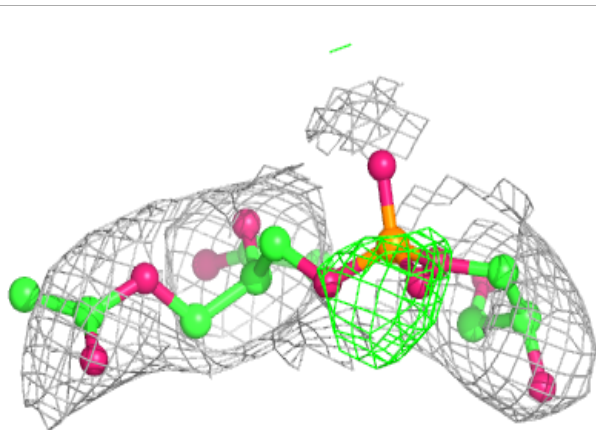
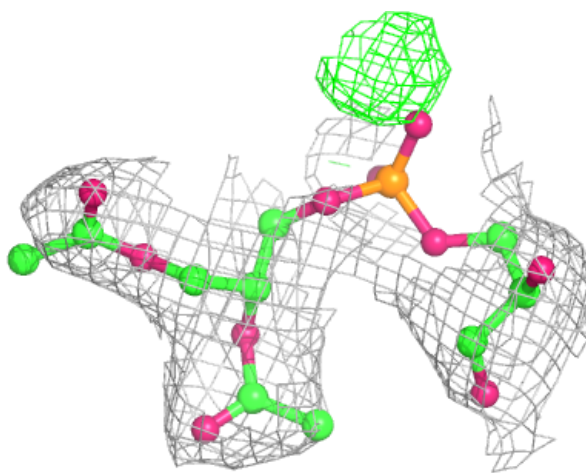
Electron density around CLA A 1121:

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



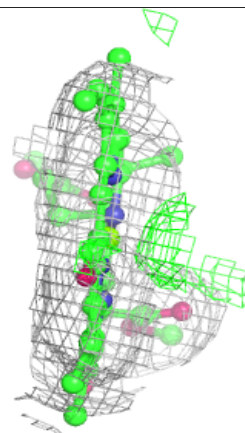
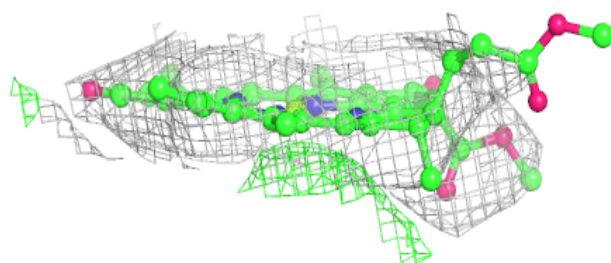
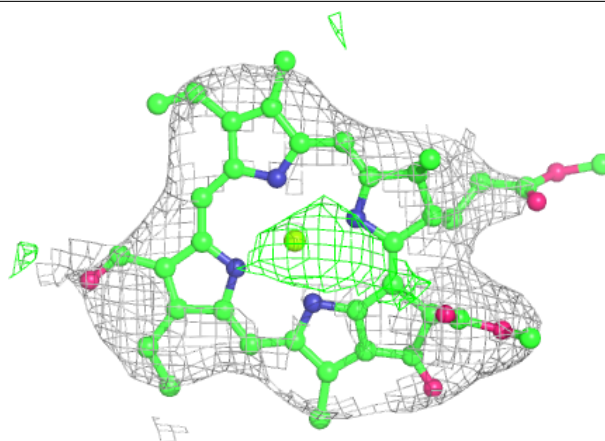
Electron density around LHG B 5004:

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



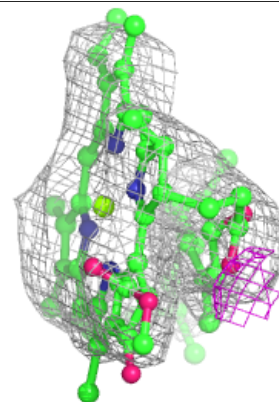
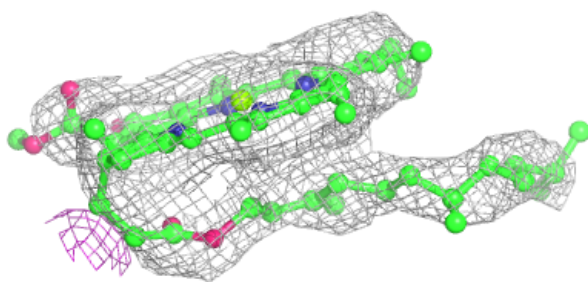
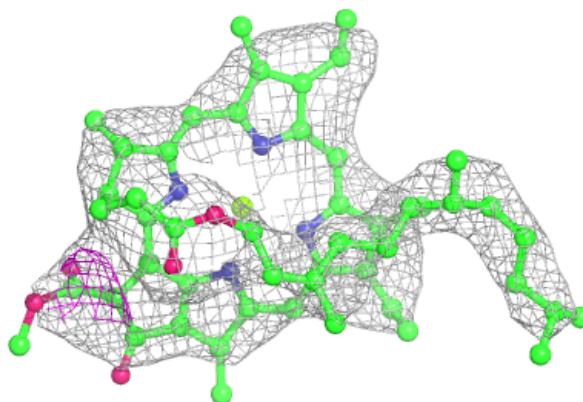
Electron density around CHL 4 4013:

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

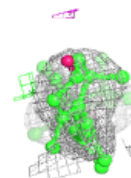
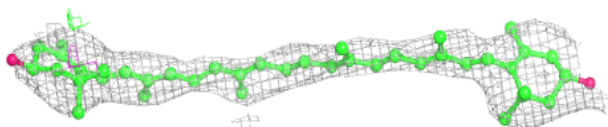
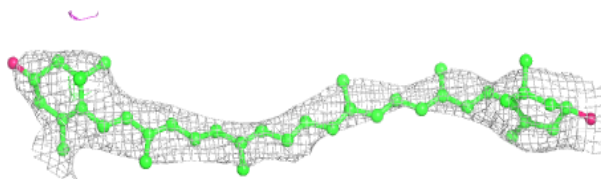


Electron density around CLA B 1213:

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

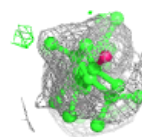
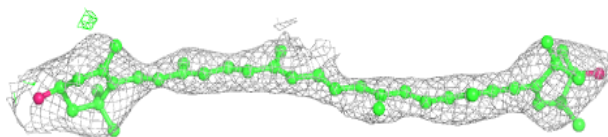
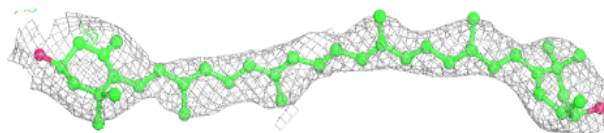
**Electron density around LUT 2 2501:**

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

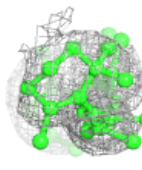
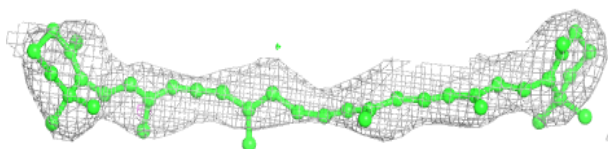
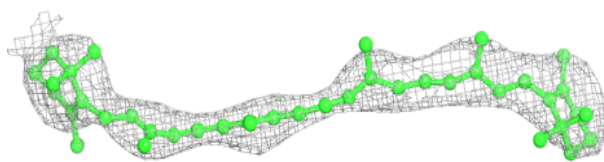


Electron density around ZEX 4 4505:

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

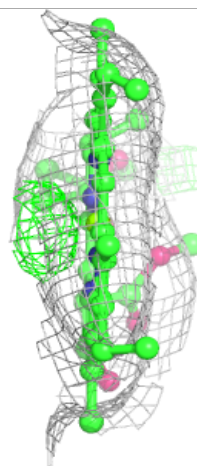
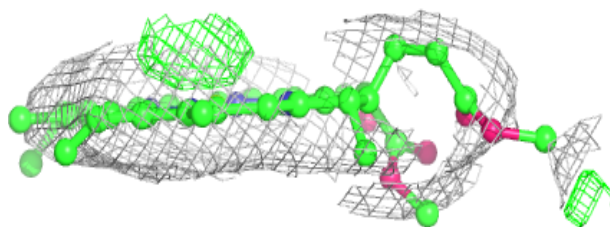
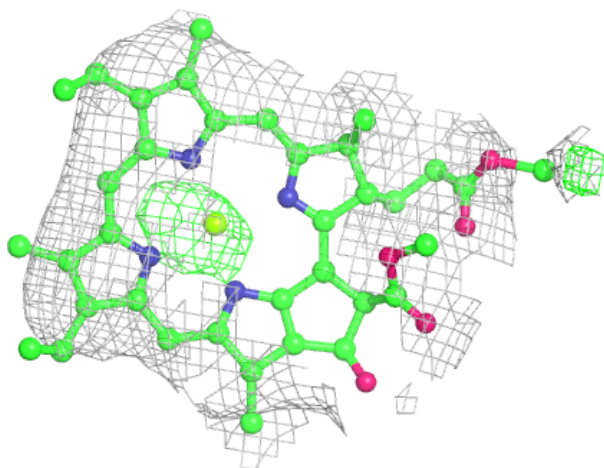
**Electron density around BCR A 6008:**

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



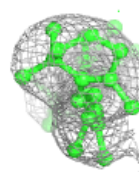
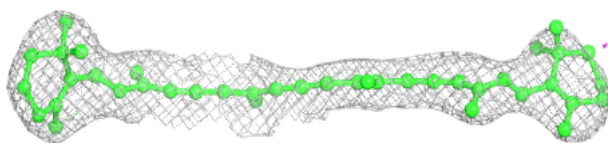
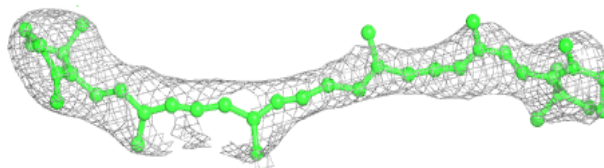
Electron density around CLA 1 1002:

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

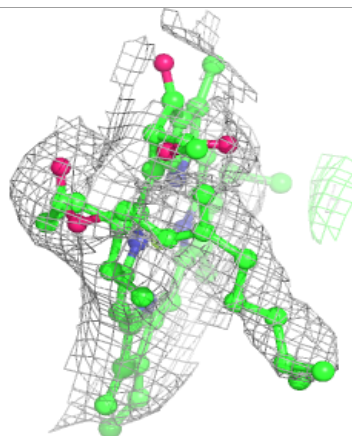
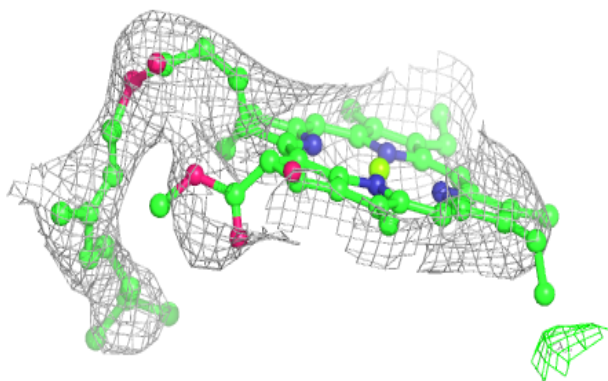
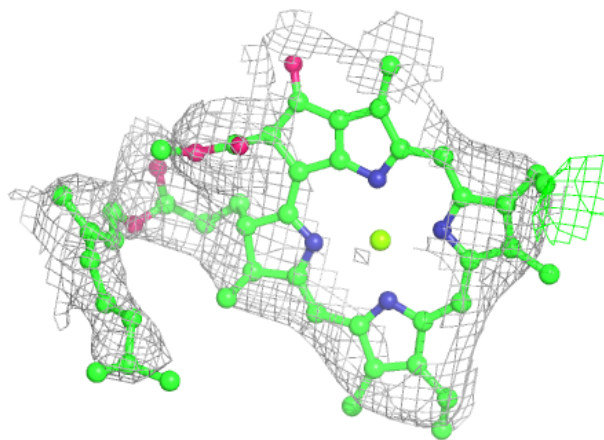


Electron density around BCR B 6009:

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

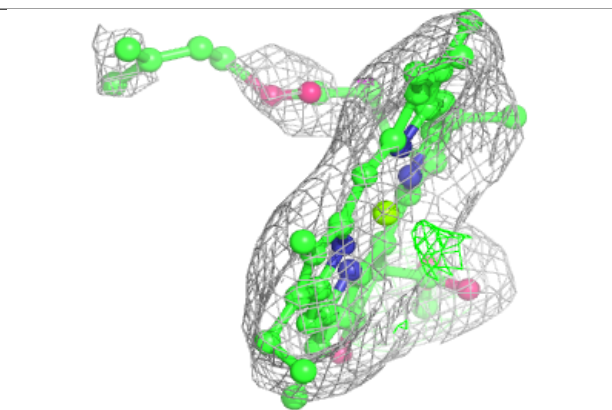
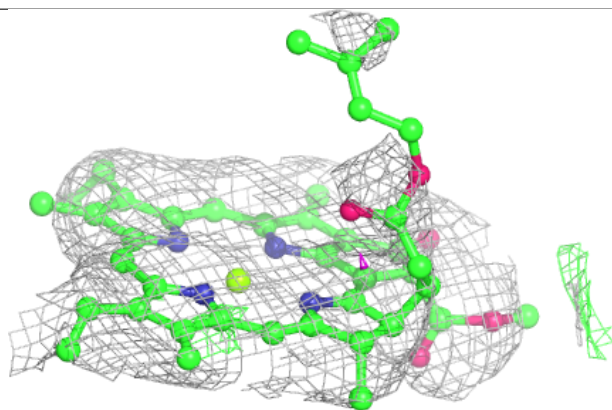
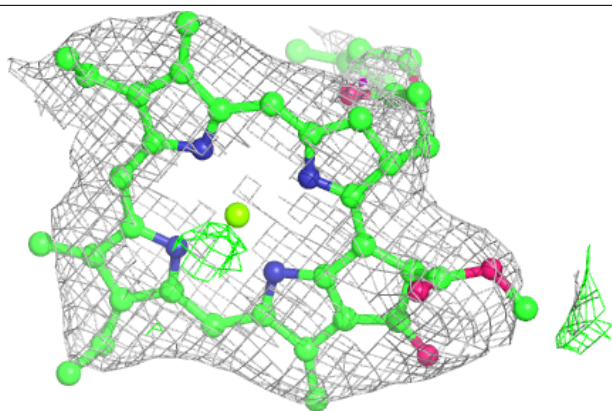
**Electron density around CLA 1 1005:**

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

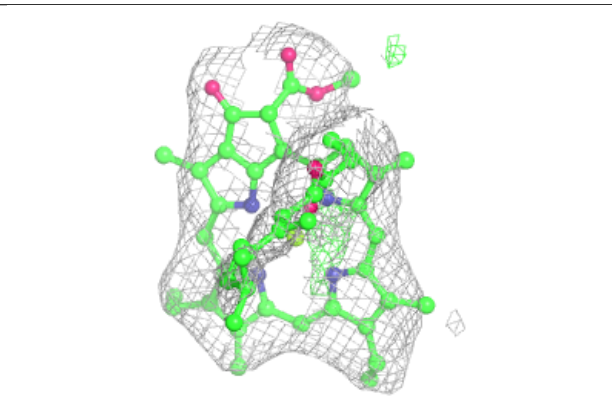
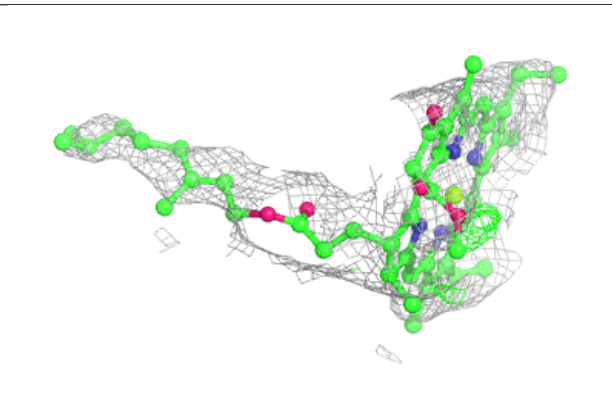
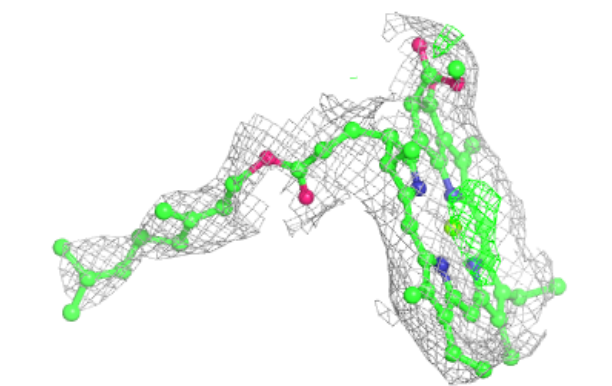


Electron density around CLA B 1201:

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

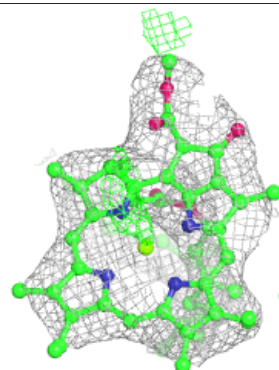
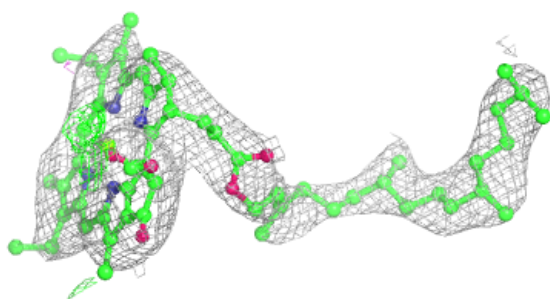
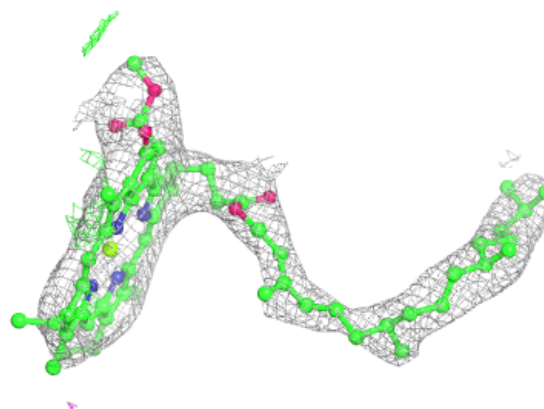
**Electron density around CLA B 1208:**

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



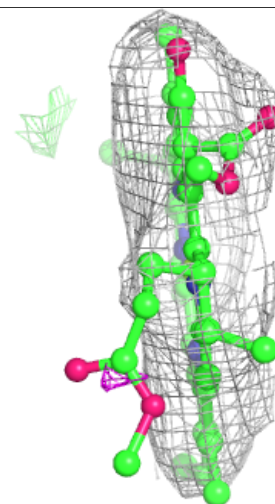
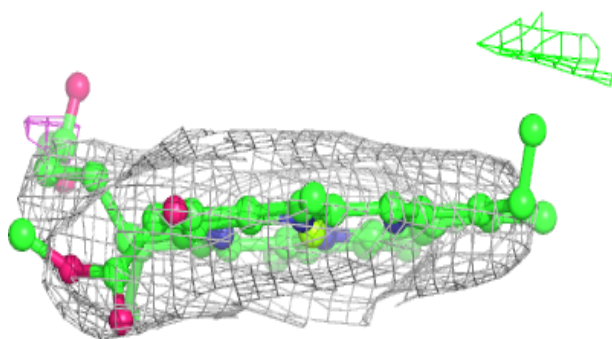
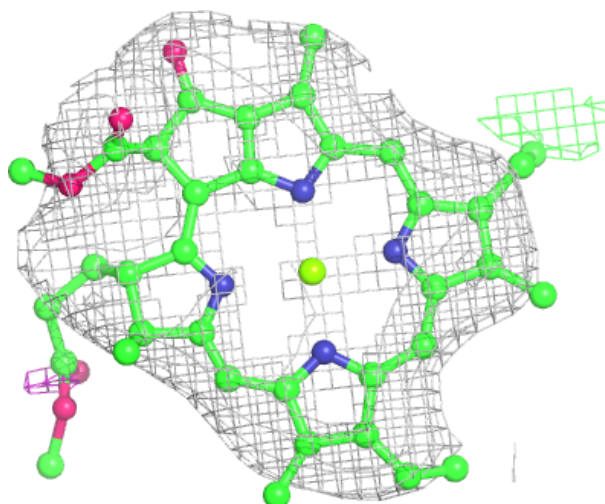
Electron density around CLA B 1238:

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



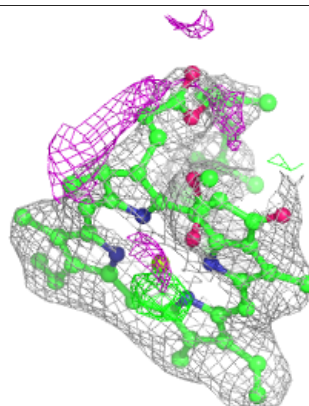
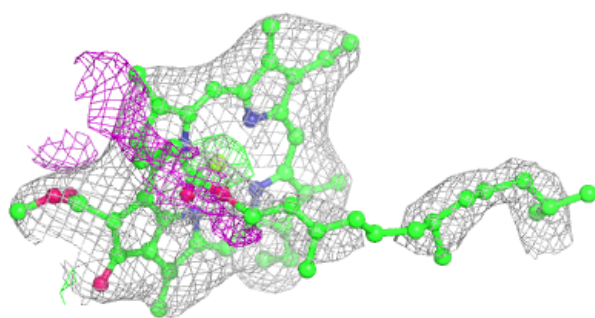
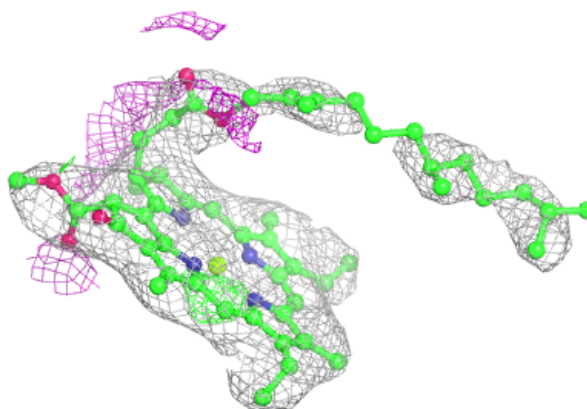
Electron density around CLA 3 3017:

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



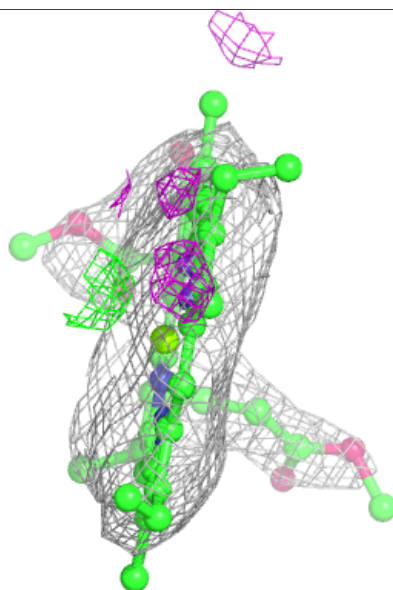
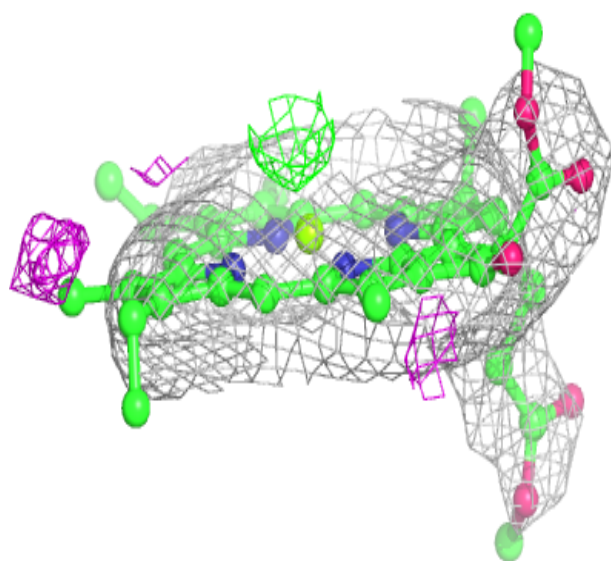
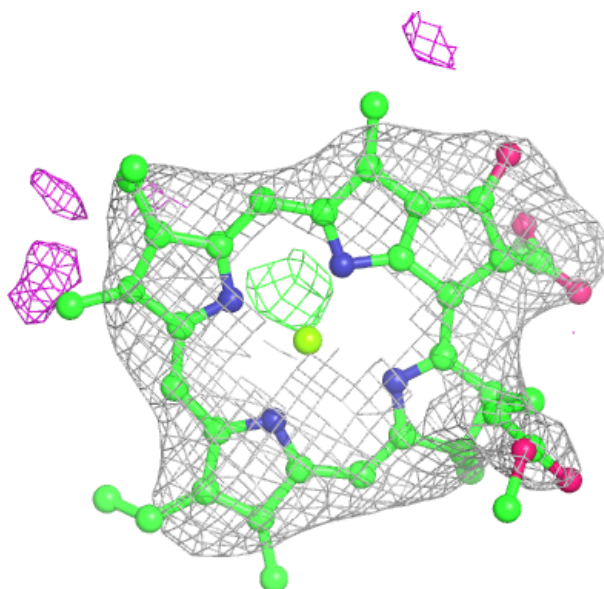
Electron density around CLA B 1228:

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



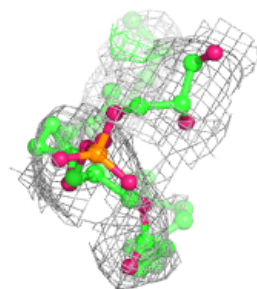
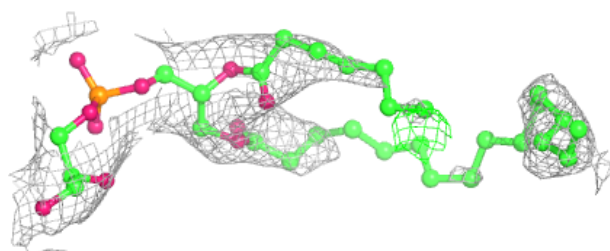
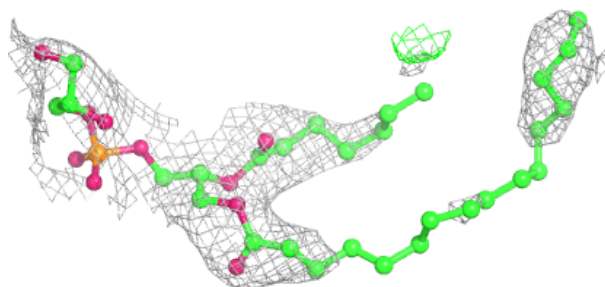
Electron density around CLA B 1217:

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

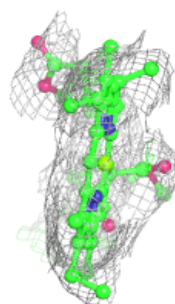
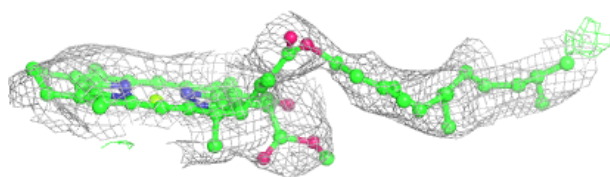
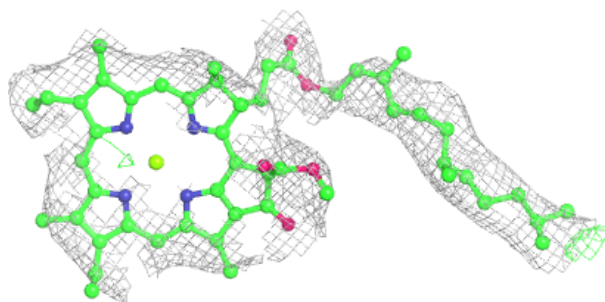


Electron density around LHG A 5003:

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

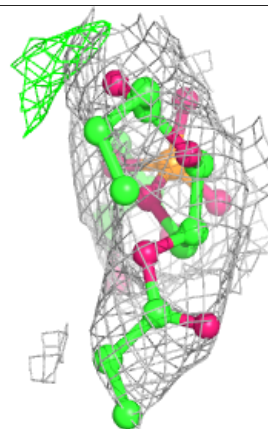
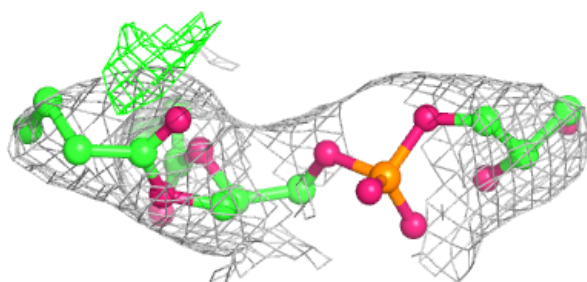
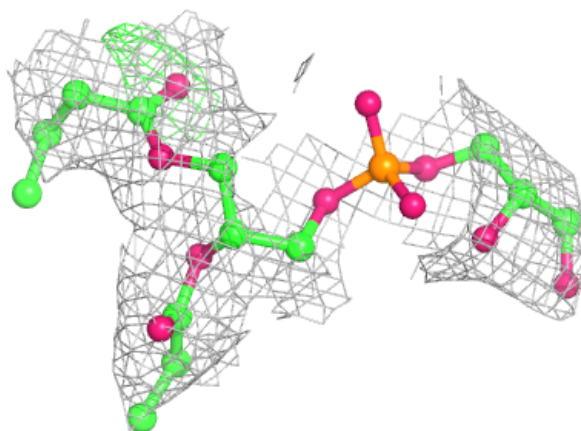
**Electron density around CLA A 1120:**

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

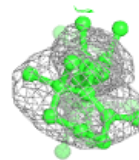
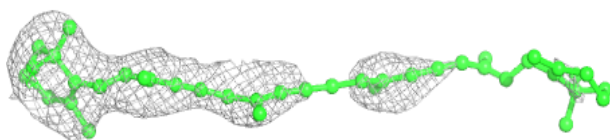
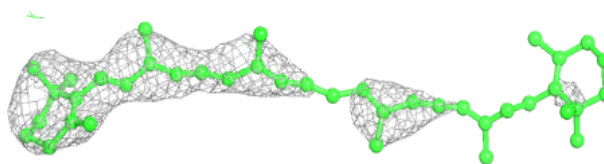


Electron density around LHG 2 2801:

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

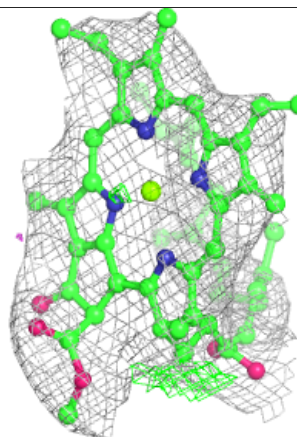
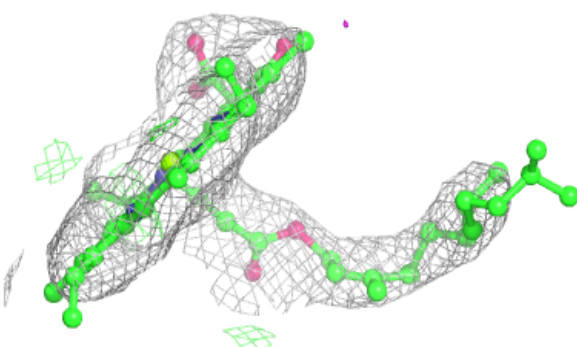
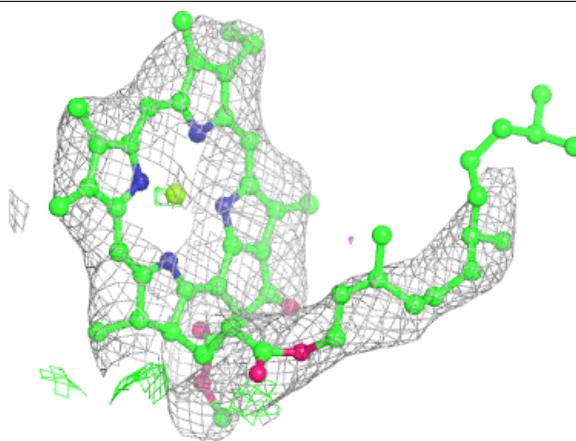
**Electron density around BCR A 6003:**

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

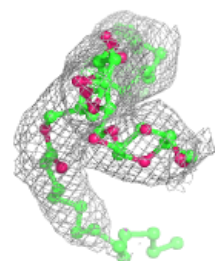
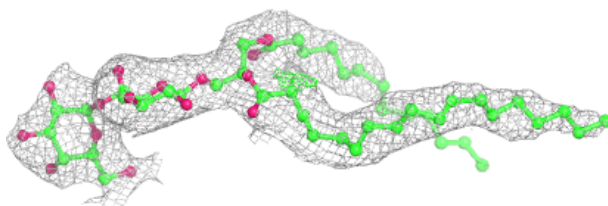
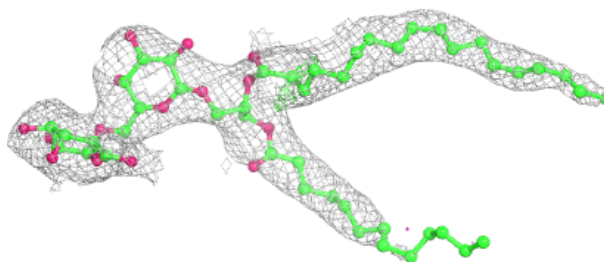


Electron density around CLA B 1219:

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

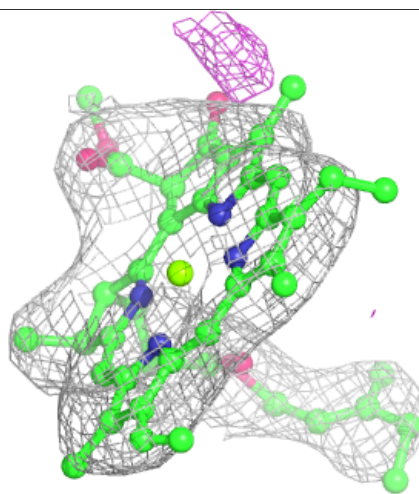
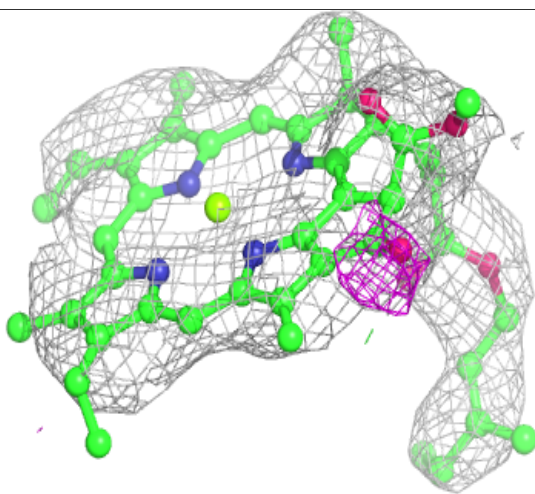
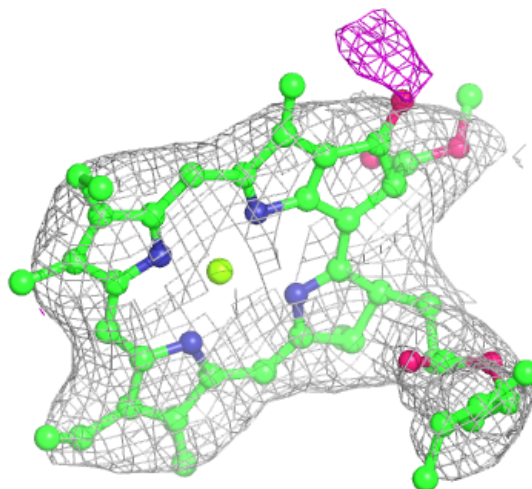
**Electron density around DGD B 7101:**

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



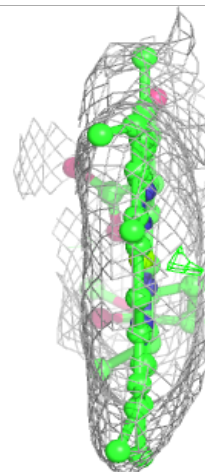
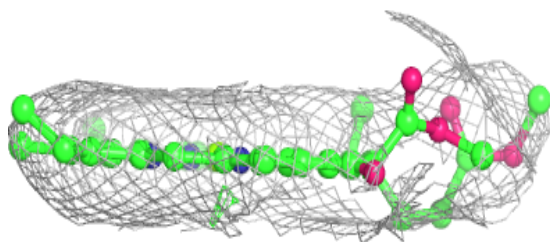
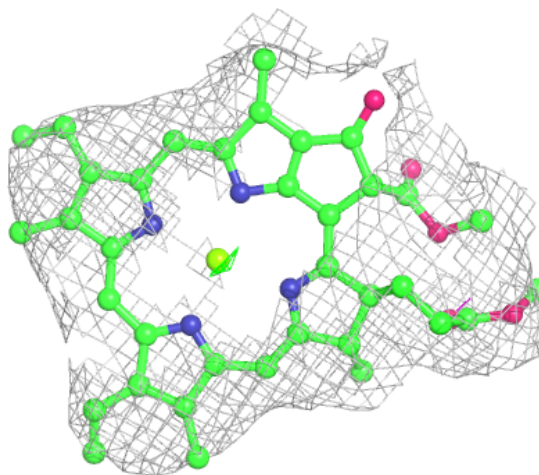
Electron density around CLA A 1105:

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



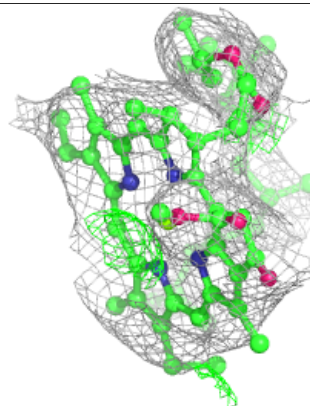
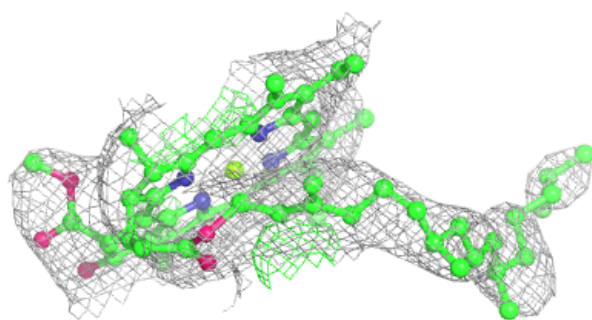
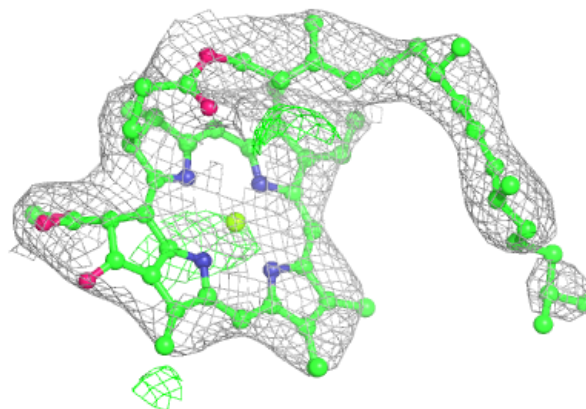
Electron density around CLA 2 2002:

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



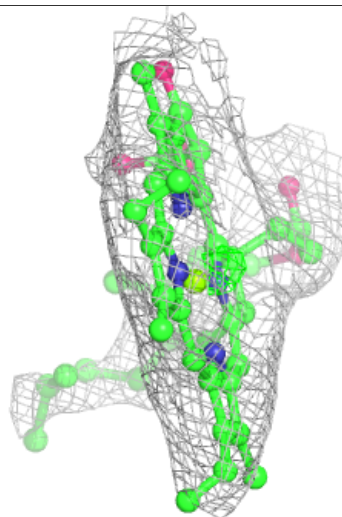
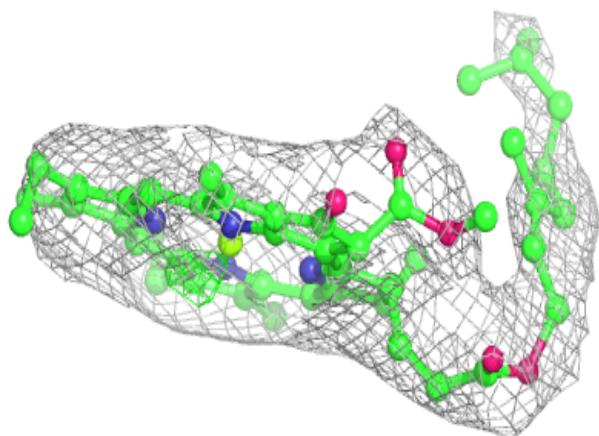
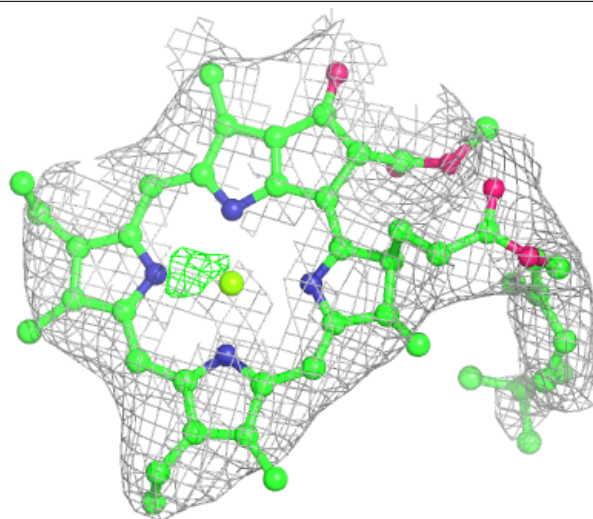
Electron density around CLA 2 2004:

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



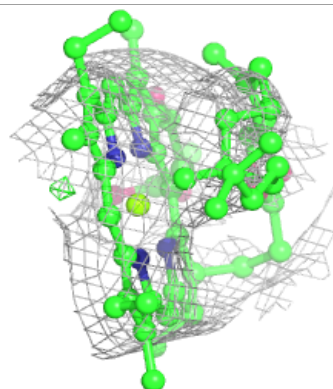
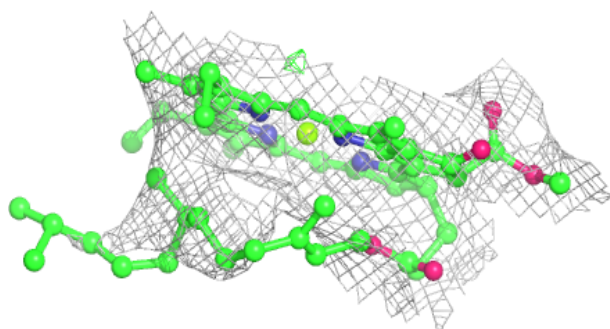
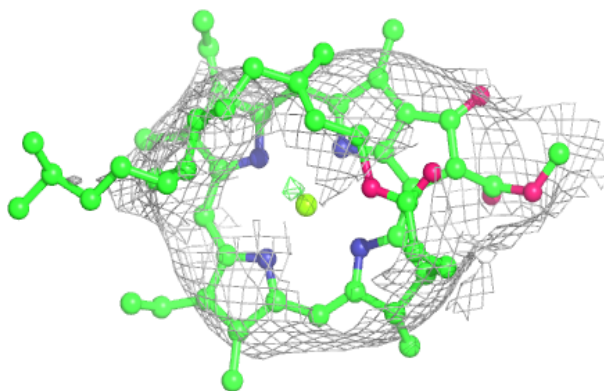
Electron density around CLA 2 2005:

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

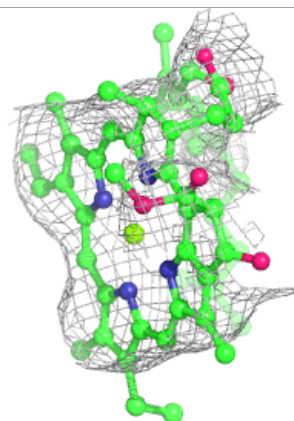
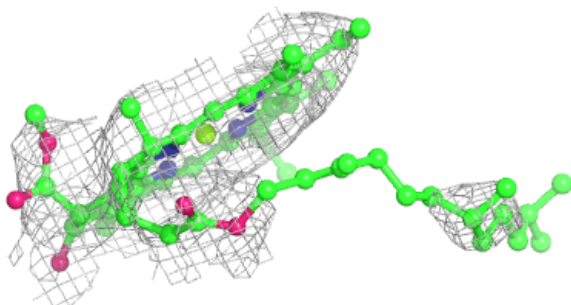
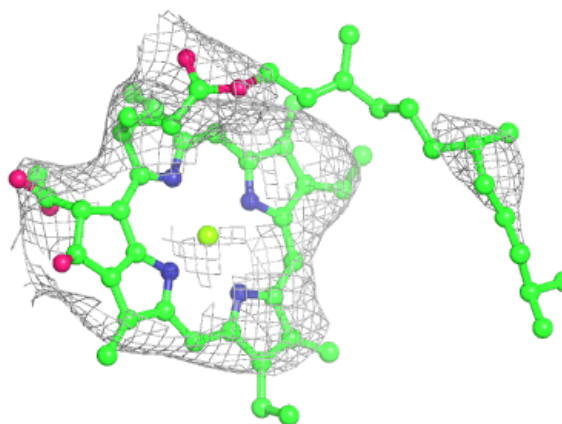


Electron density around CLA 3 3003:

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

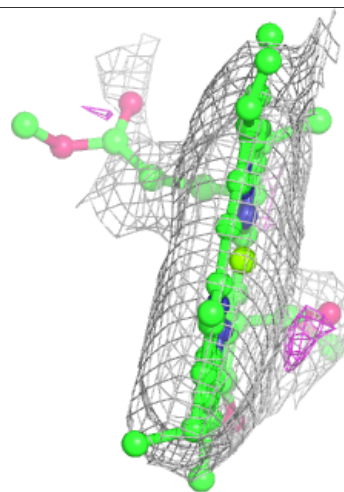
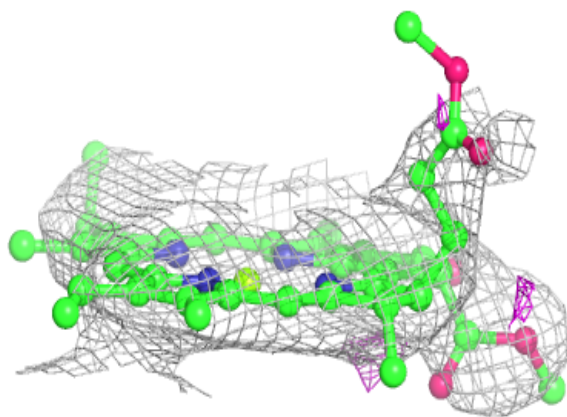
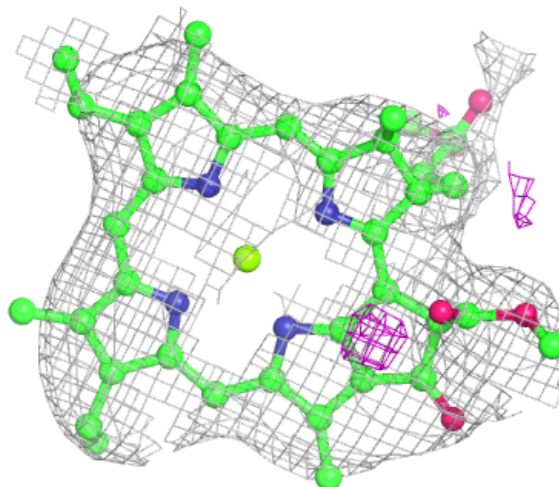
**Electron density around CLA 3 3004:**

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



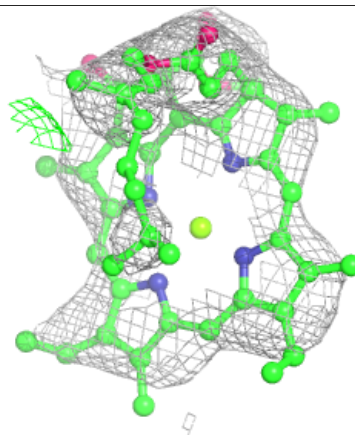
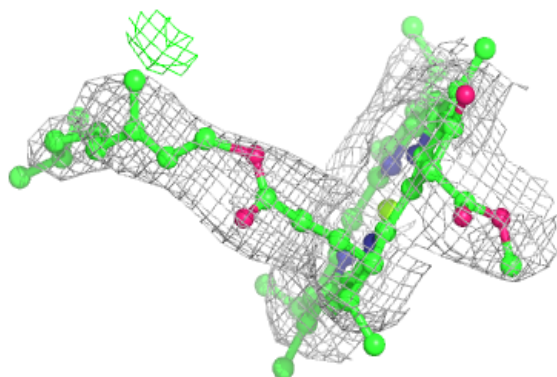
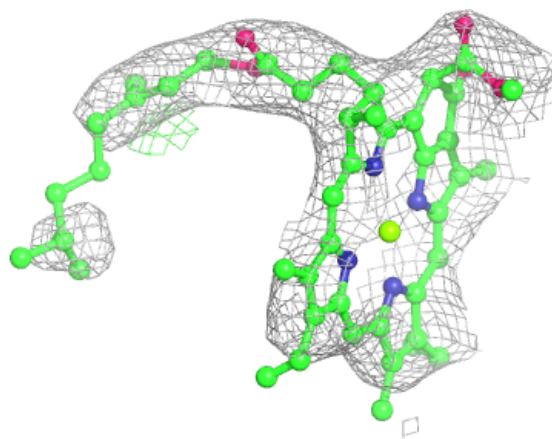
Electron density around CLA B 1209:

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



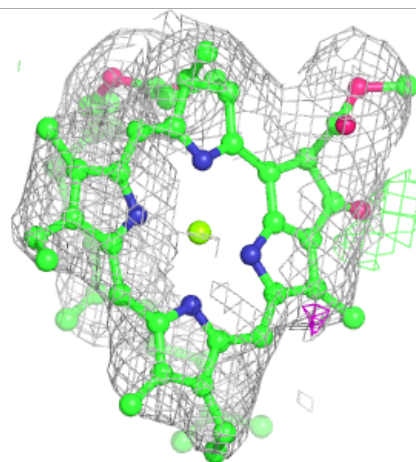
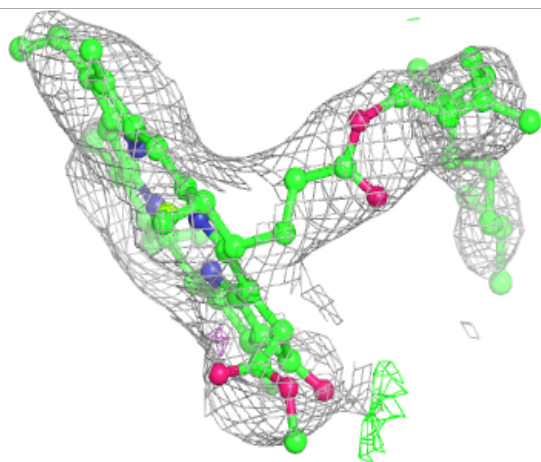
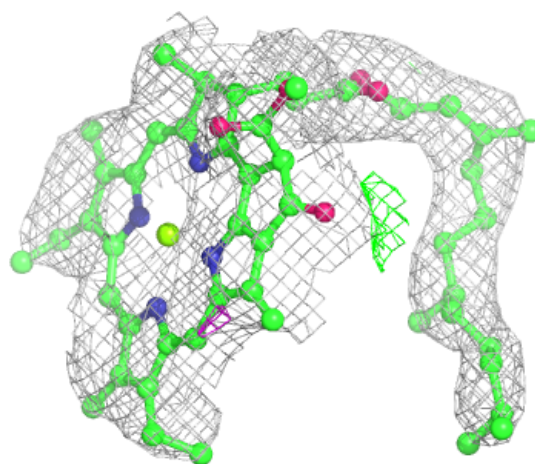
Electron density around CLA B 1212:

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



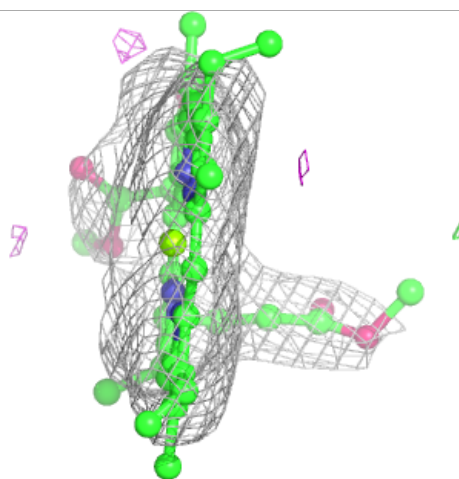
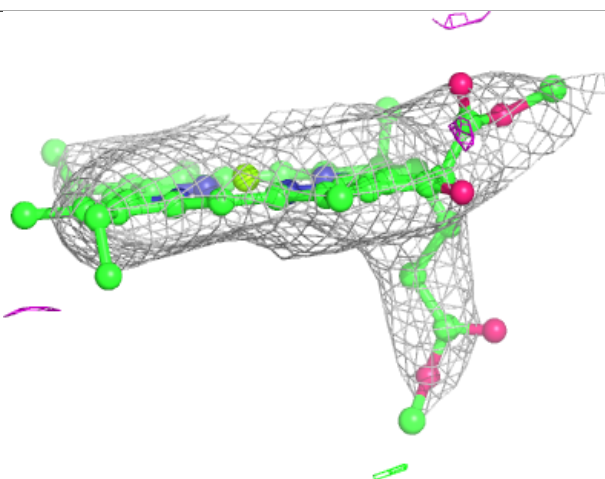
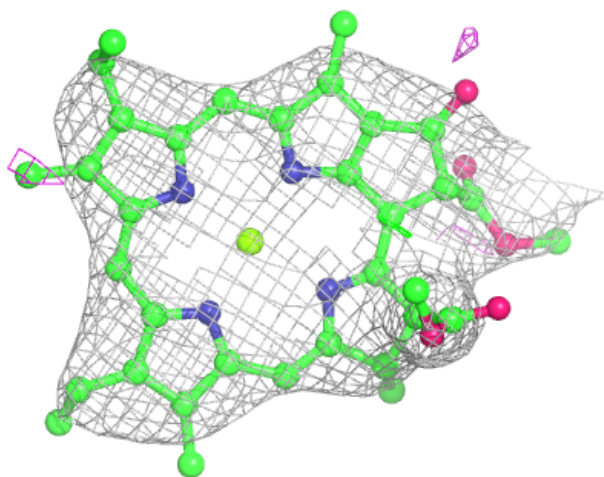
Electron density around CLA B 1231:

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



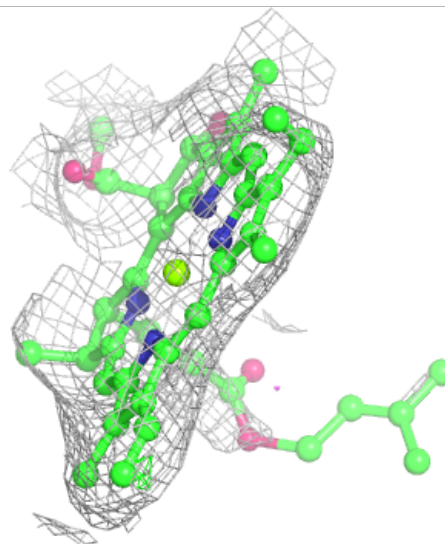
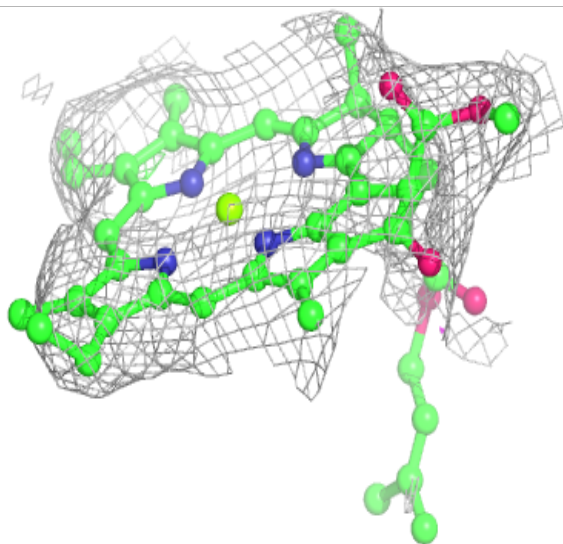
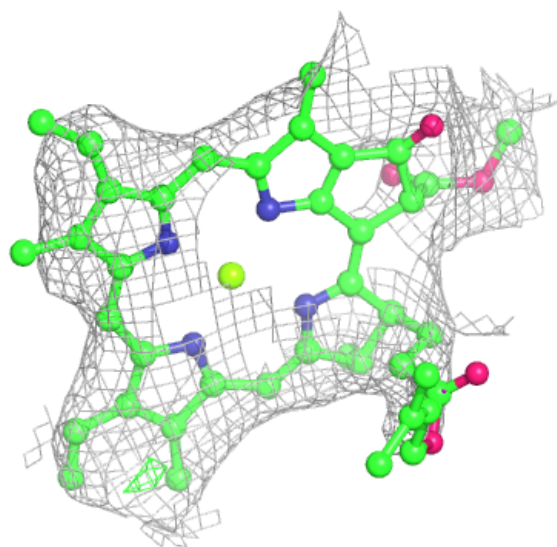
Electron density around CLA A 1108:

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



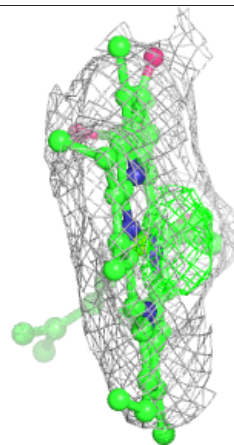
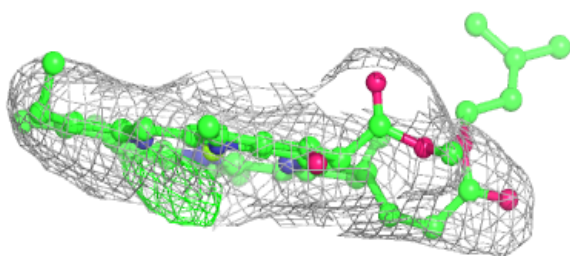
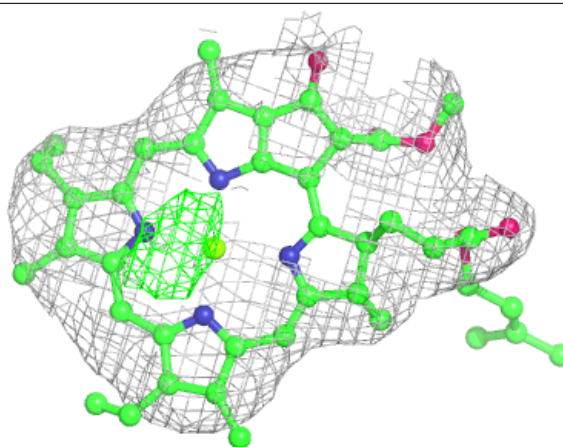
Electron density around CLA 3 3012:

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

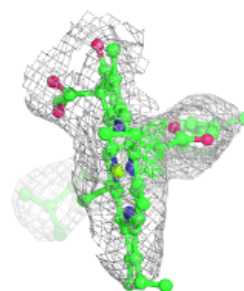
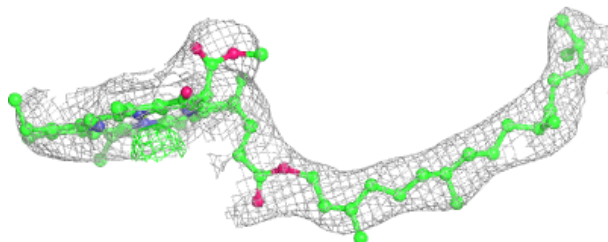
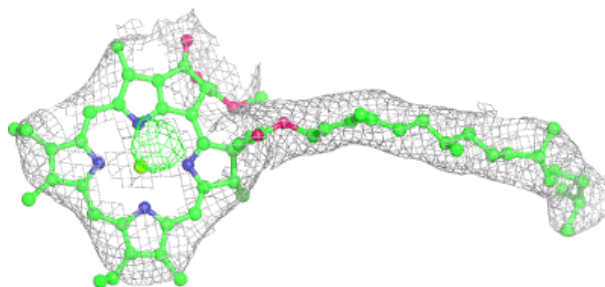


Electron density around CLA 4 4002:

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

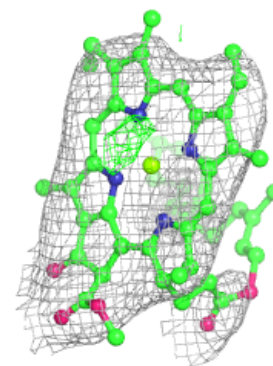
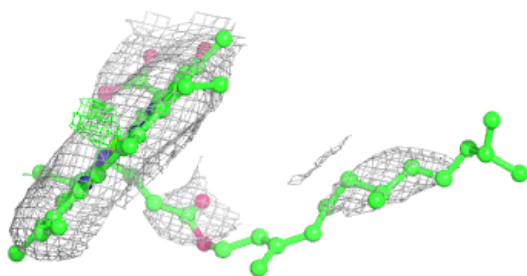
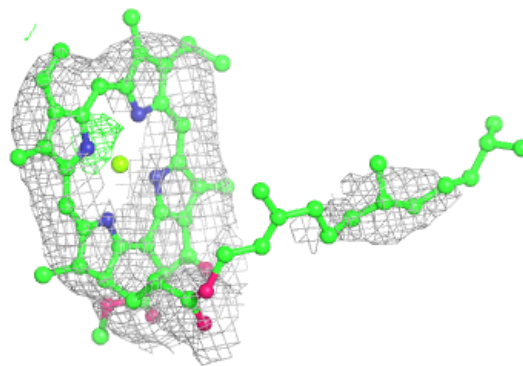
**Electron density around CLA B 1240:**

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

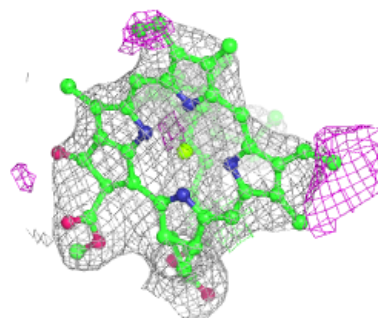
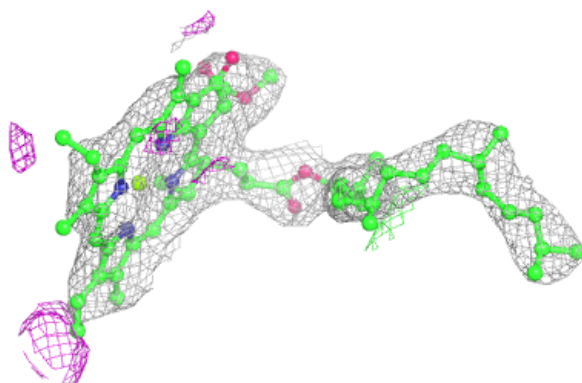
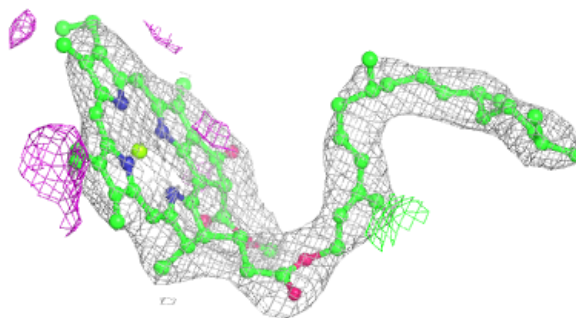


Electron density around CLA 4 4007:

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

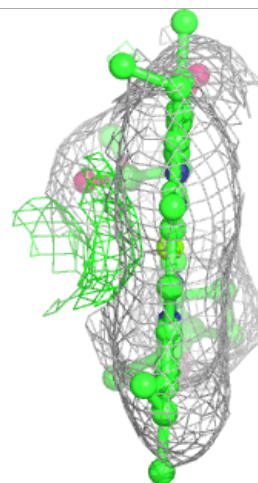
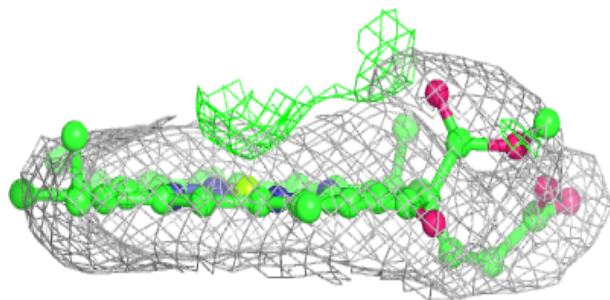
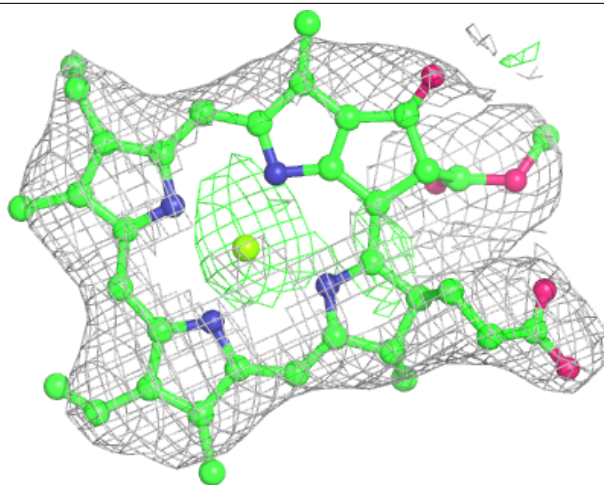
**Electron density around CLA B 1021:**

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



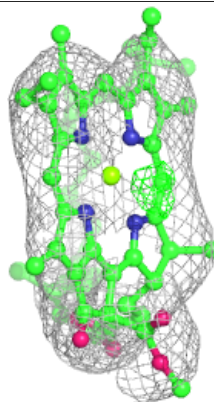
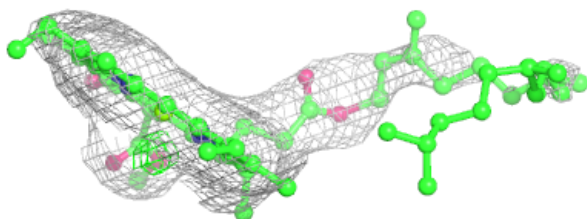
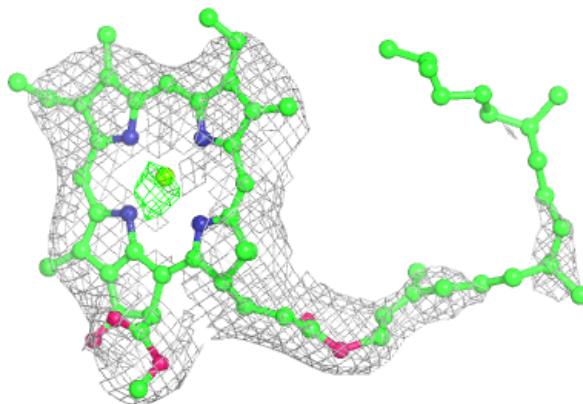
Electron density around CLA F 1301:

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

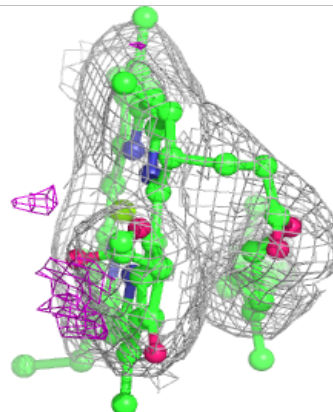
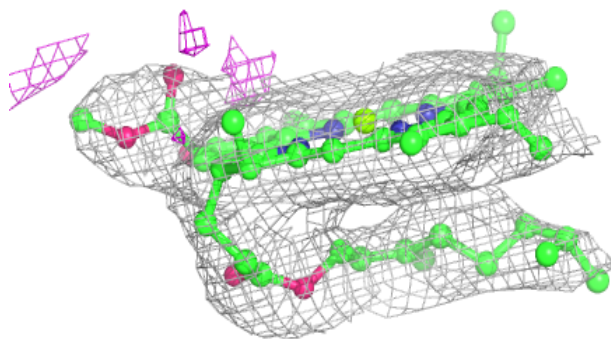
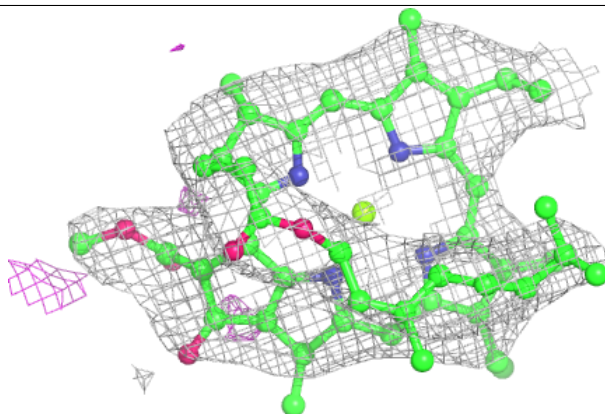


Electron density around CLA 4 4017:

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

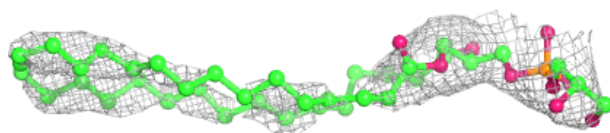
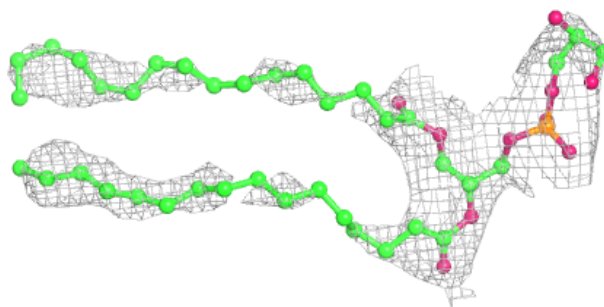
**Electron density around CLA B 1204:**

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

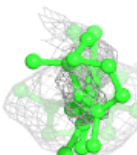
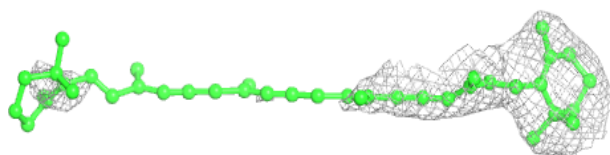
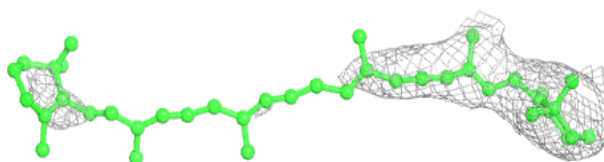


Electron density around LHG 1 1801:

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

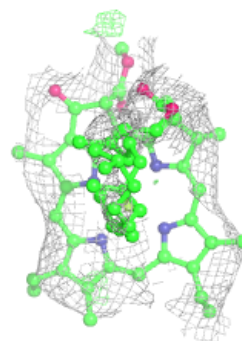
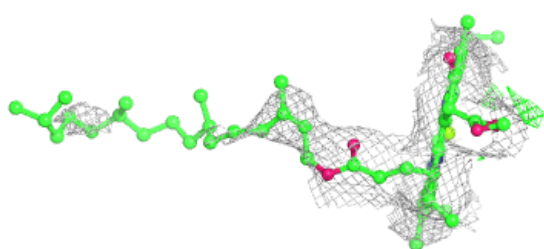
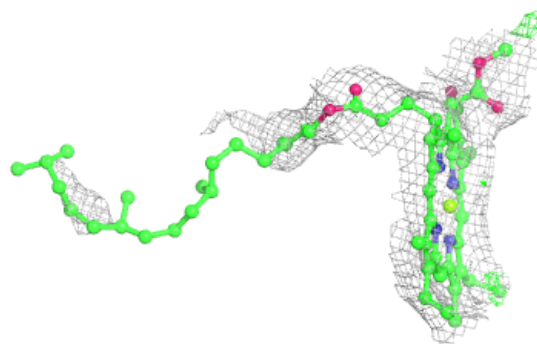
**Electron density around BCR A 6002:**

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

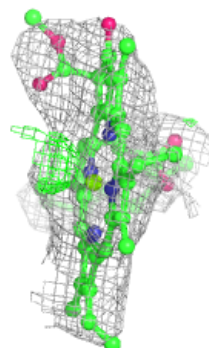
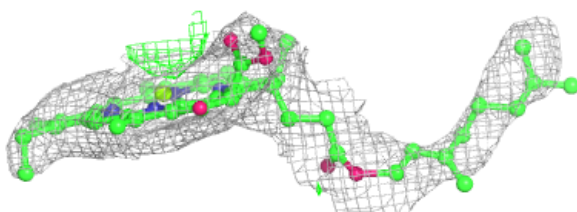
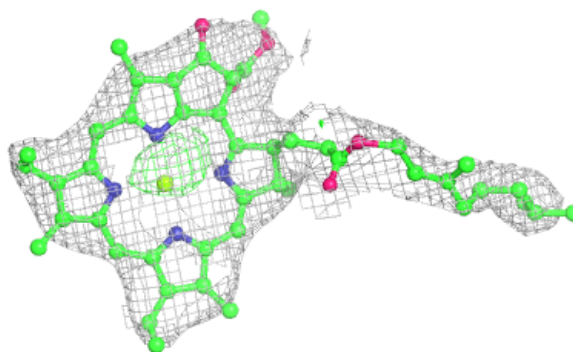


Electron density around CLA A 1112:

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

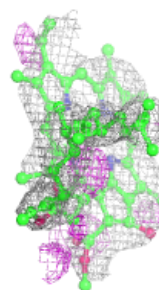
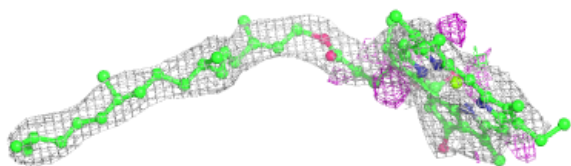
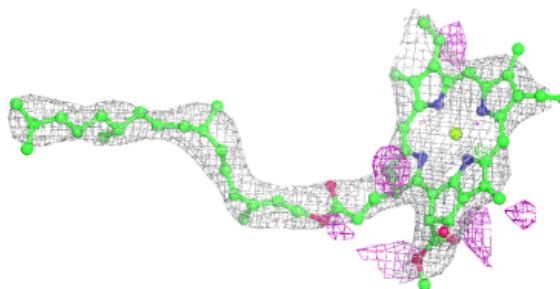
**Electron density around CLA A 1124:**

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



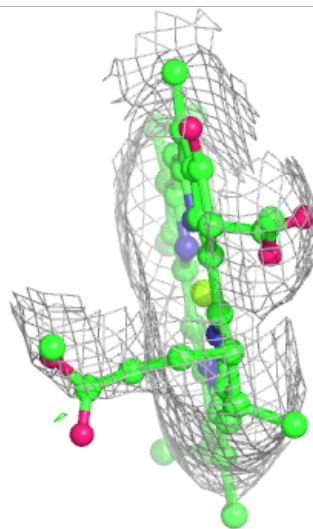
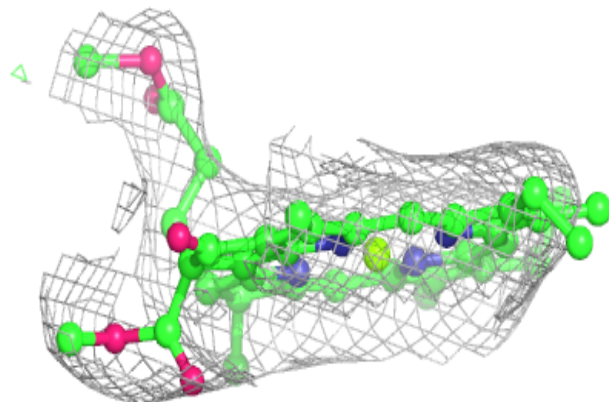
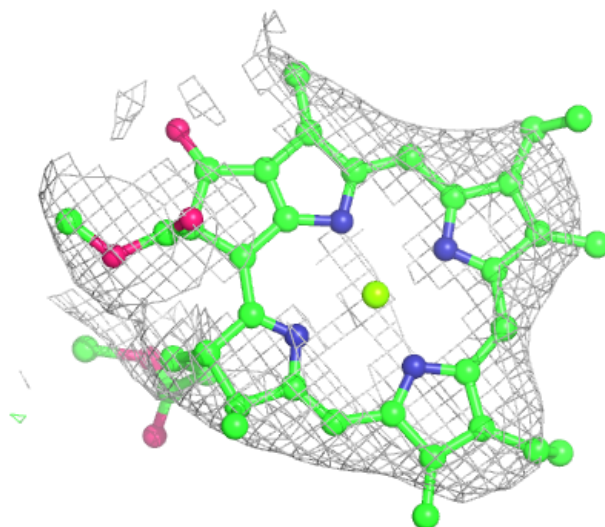
Electron density around CLA A 1022:

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



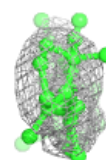
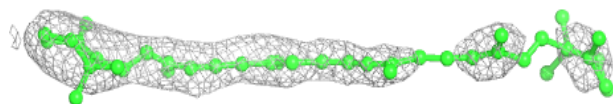
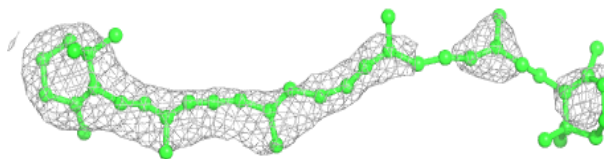
Electron density around CLA 1 1007:

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

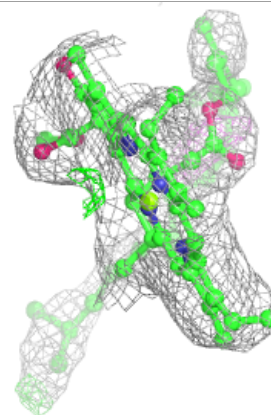
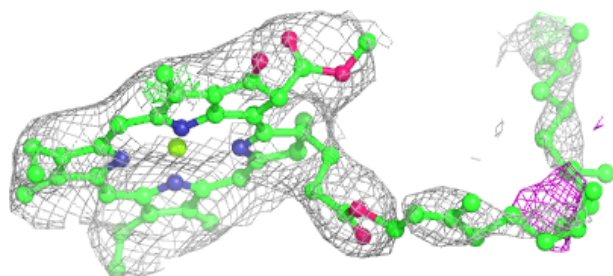
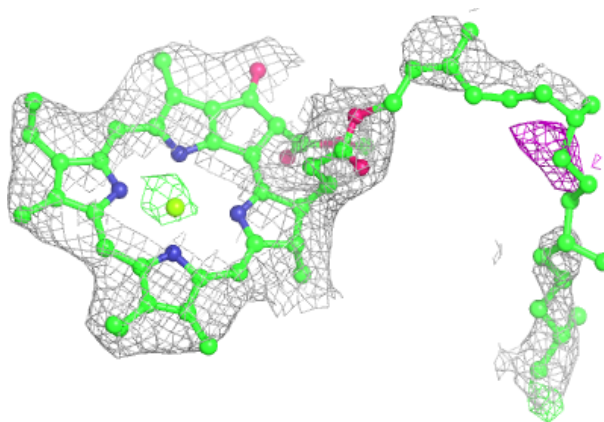


Electron density around BCR B 6005:

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

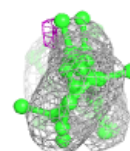
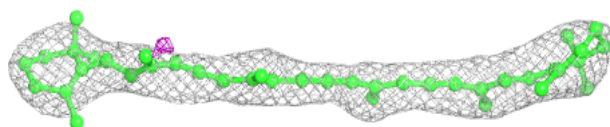
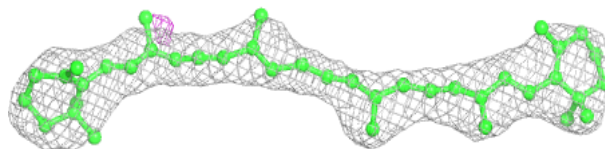
**Electron density around CLA B 1220:**

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

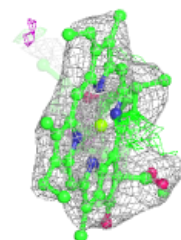
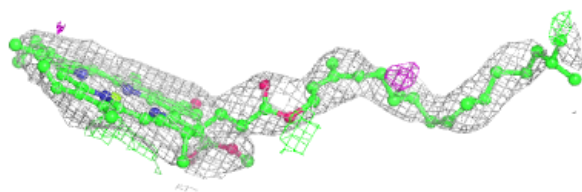
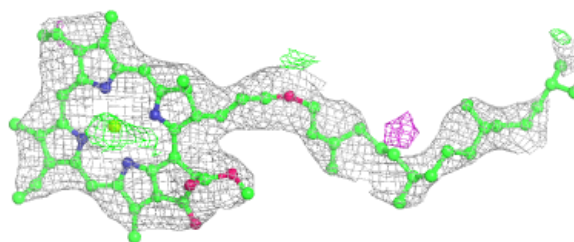


Electron density around BCR J 6012:

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

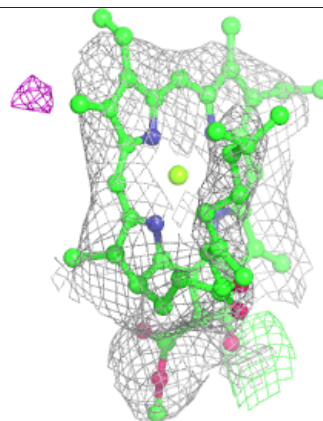
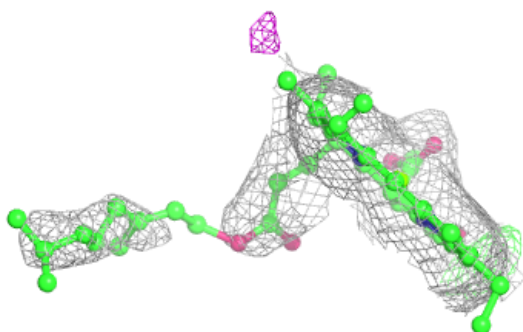
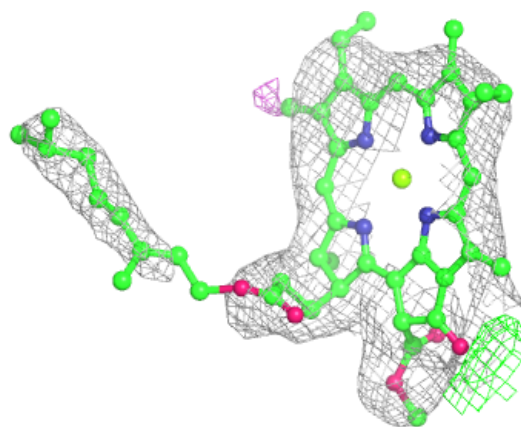
**Electron density around CLA A 1139:**

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



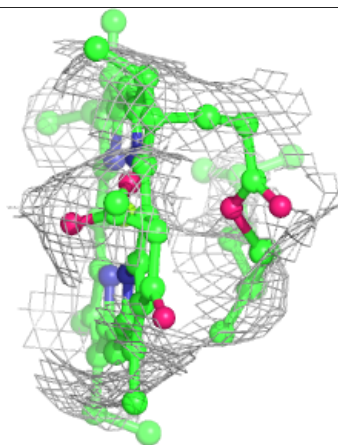
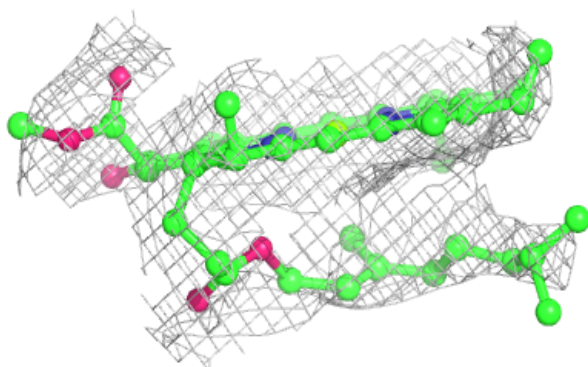
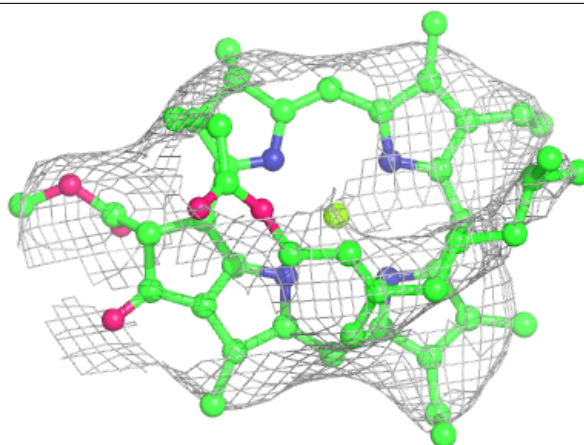
Electron density around CLA A 1133:

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

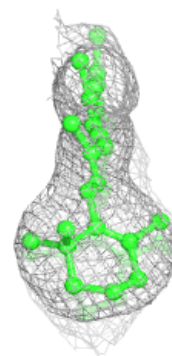
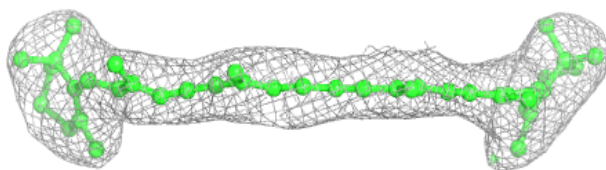
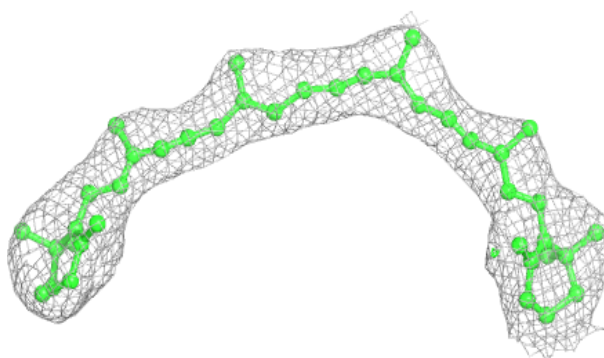


Electron density around CLA 2 2003:

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

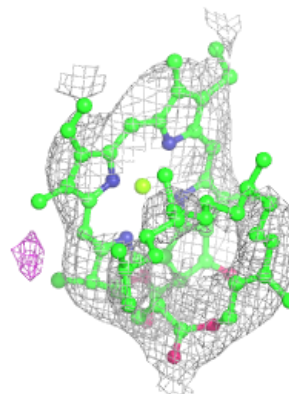
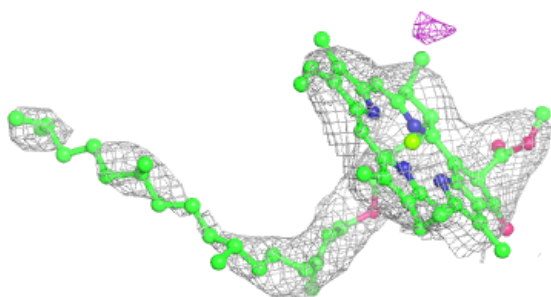
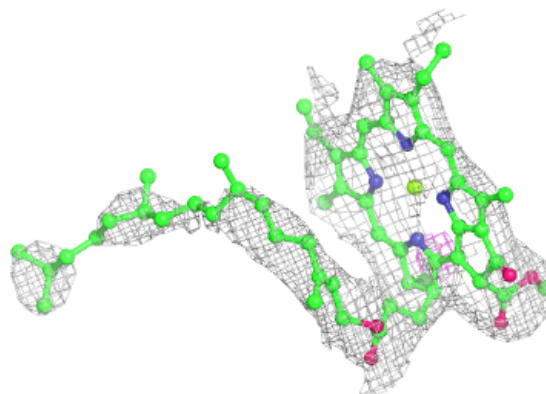
**Electron density around BCR F 6016:**

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

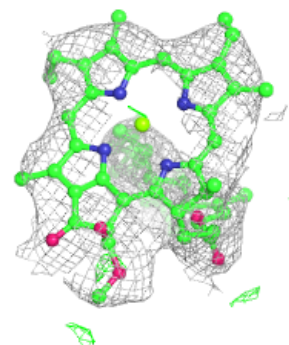
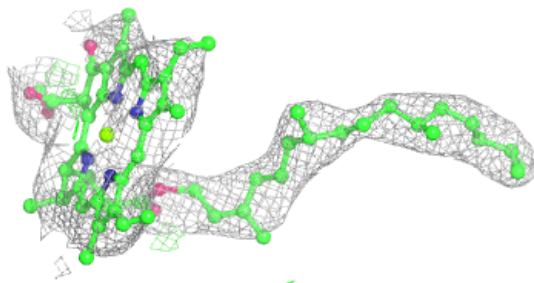
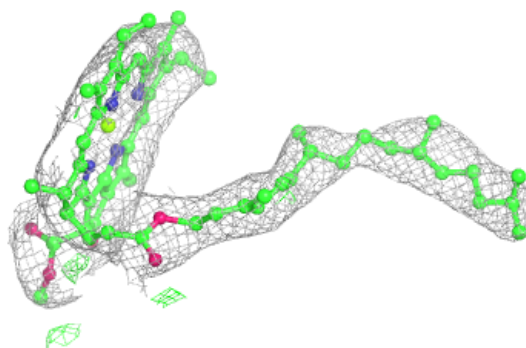


Electron density around CLA B 1211:

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

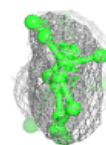
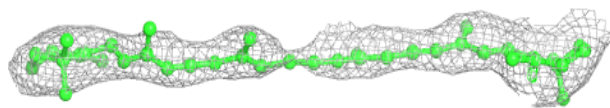
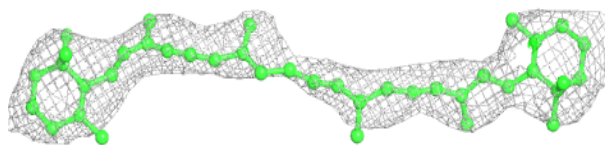
**Electron density around CLA A 1109:**

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

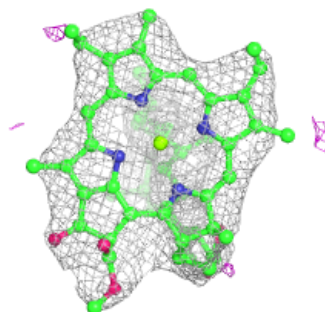
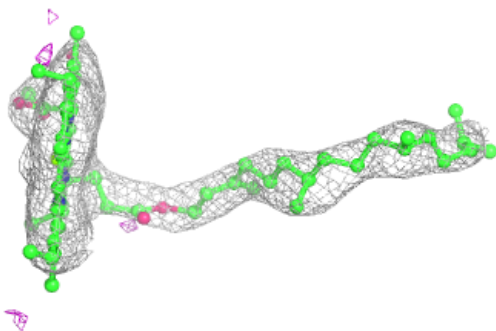
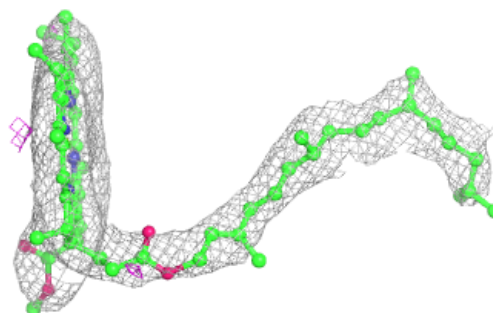


Electron density around BCR L 6019:

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

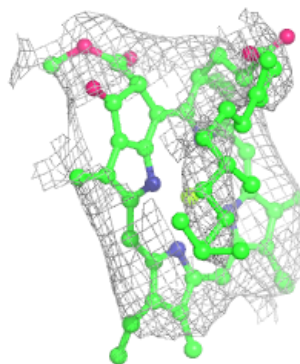
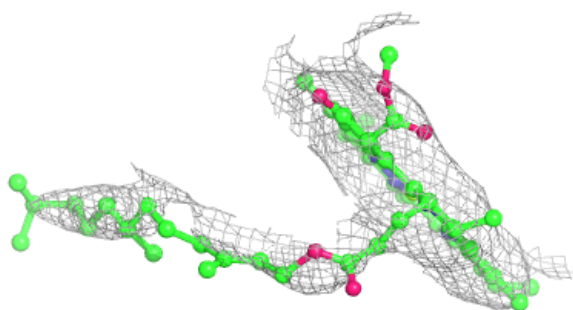
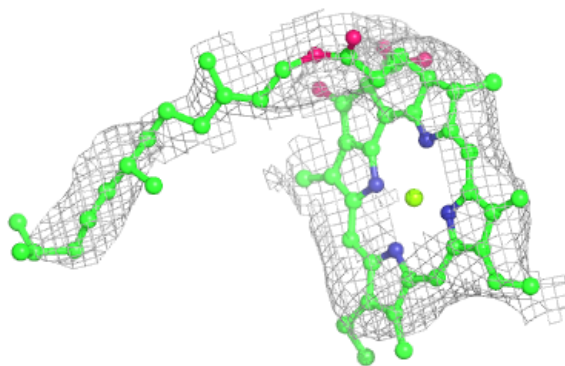
**Electron density around CLA B 1239:**

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



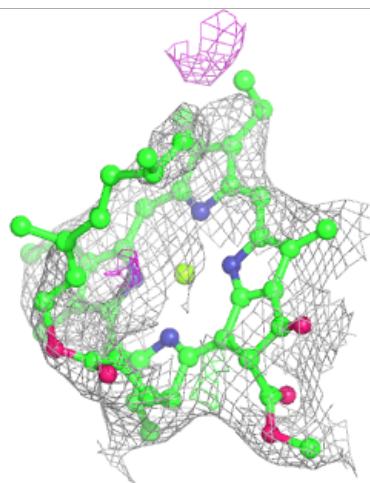
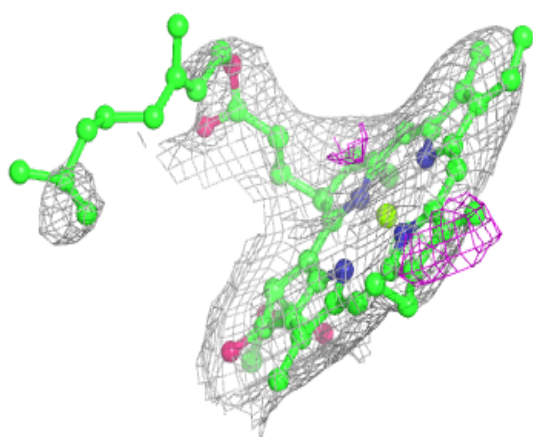
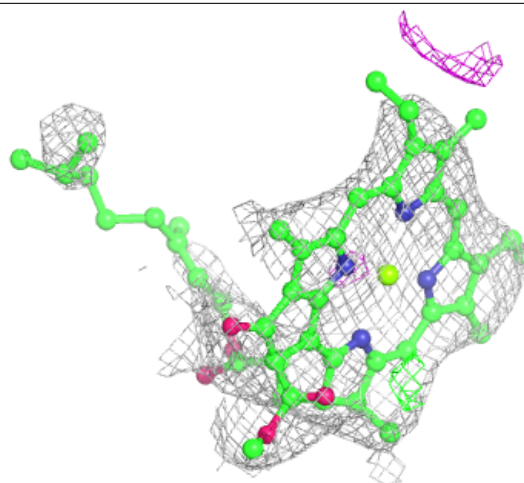
Electron density around CLA 2 2007:

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



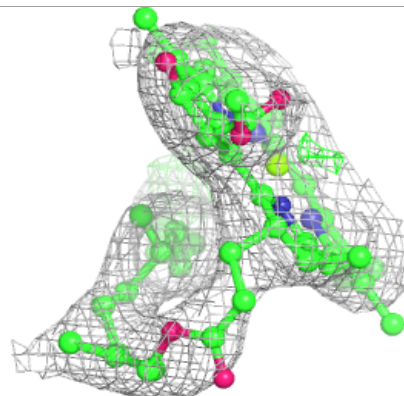
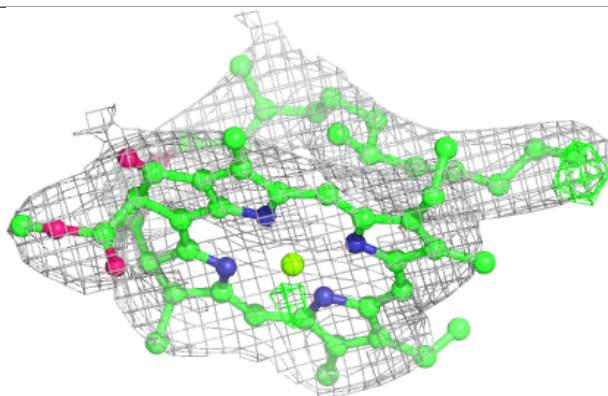
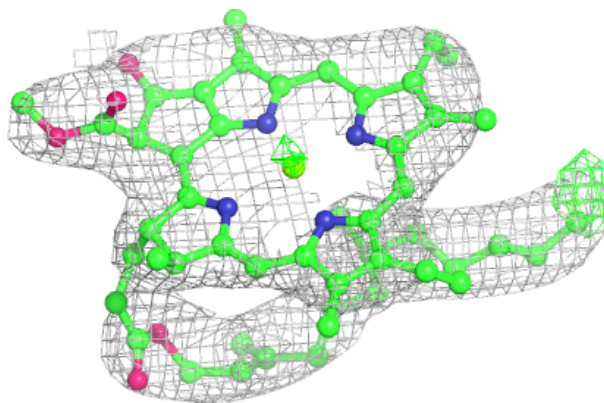
Electron density around CLA 2 2012:

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

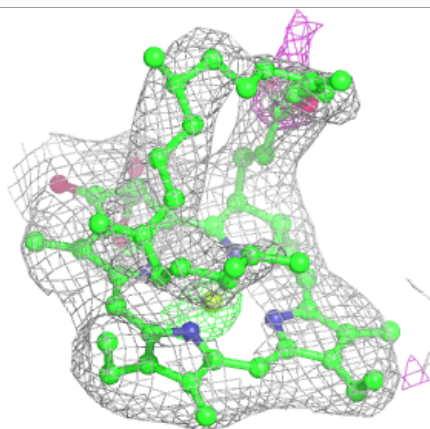
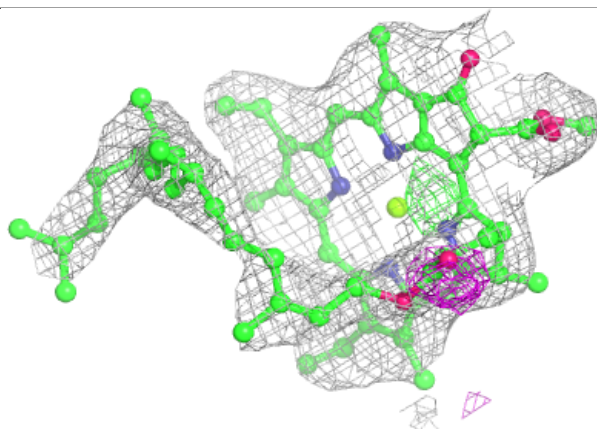
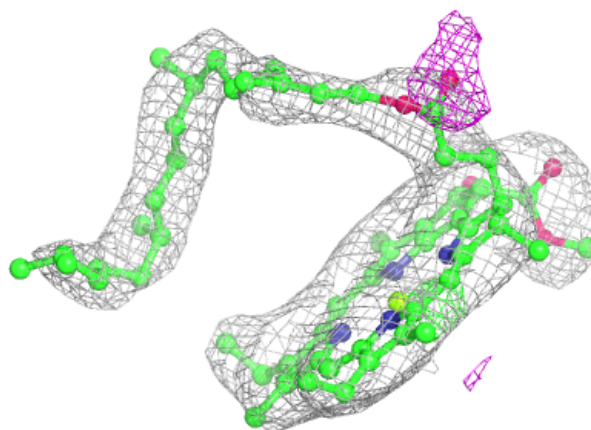


Electron density around CLA B 1214:

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

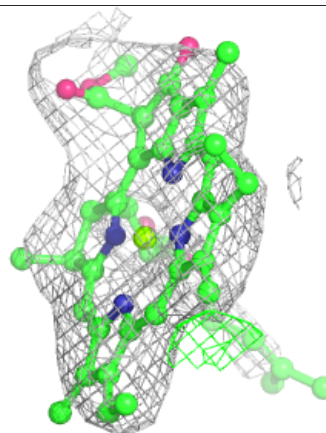
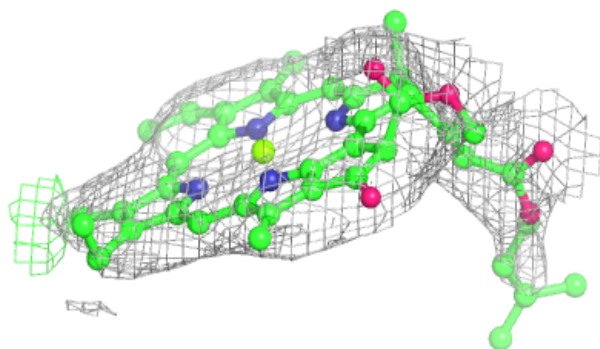
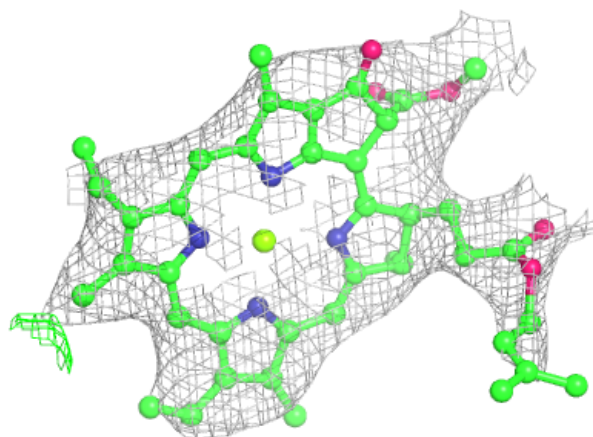
**Electron density around CLA B 1227:**

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



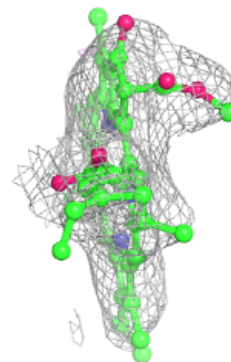
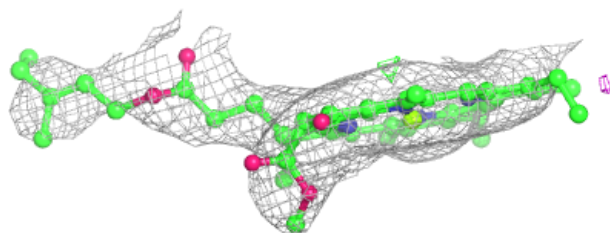
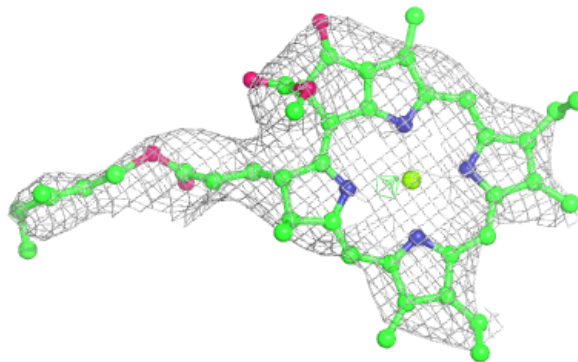
Electron density around CLA 2 2009:

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



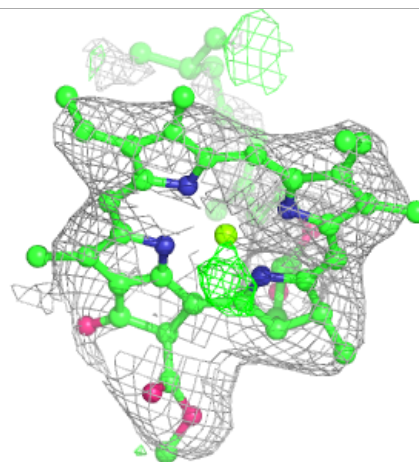
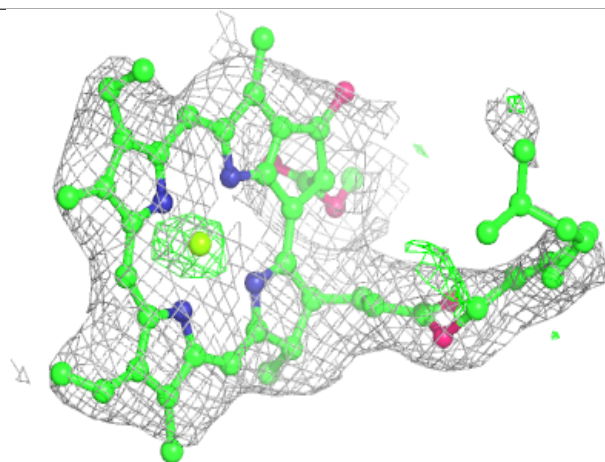
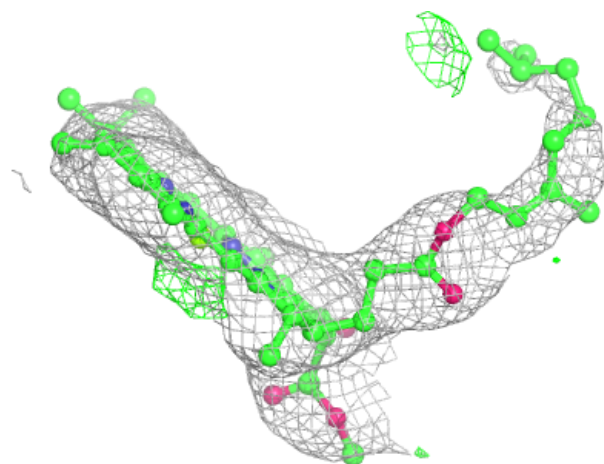
Electron density around CLA A 1135:

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



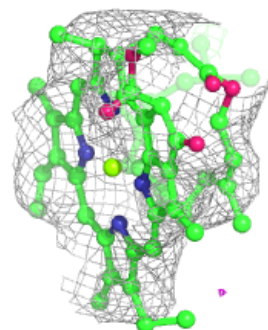
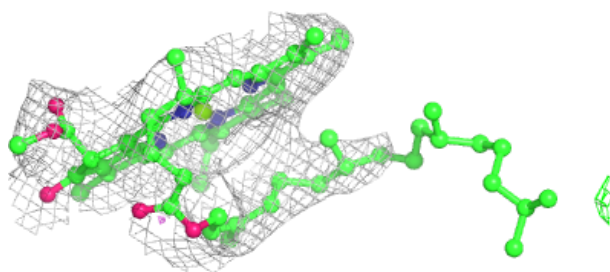
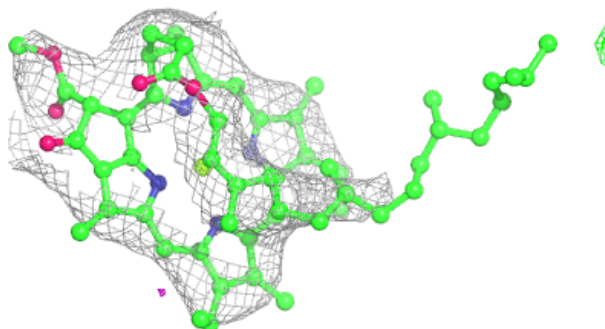
Electron density around CLA A 1137:

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

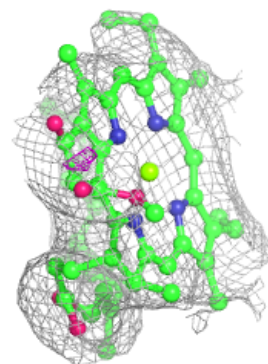
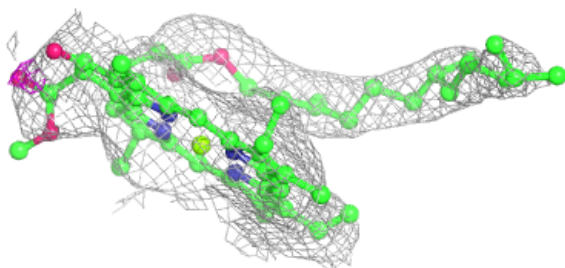
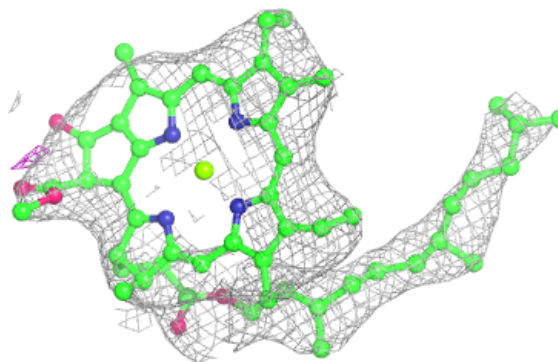


Electron density around CLA 4 4003:

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

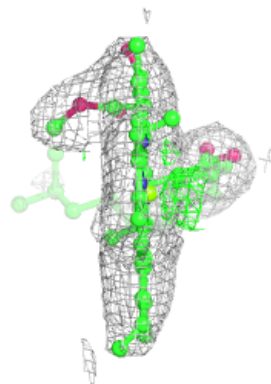
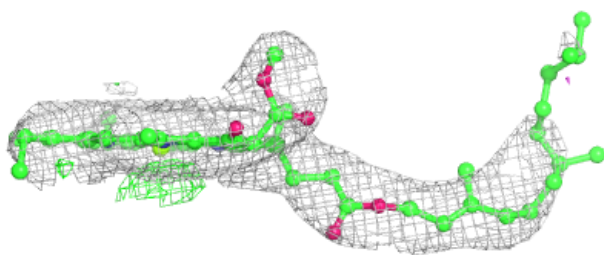
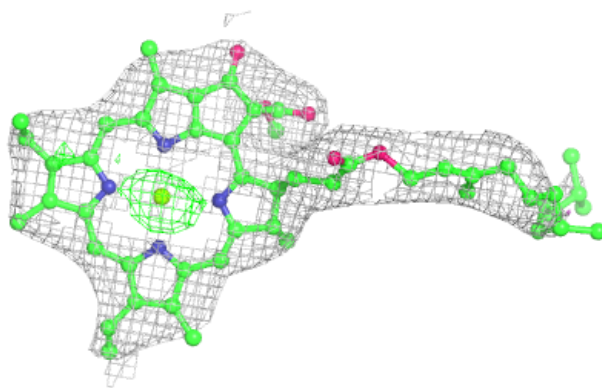
**Electron density around CLA 4 4004:**

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

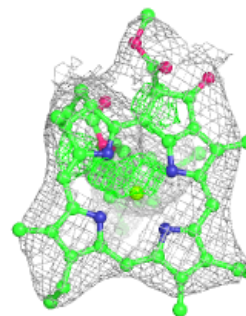
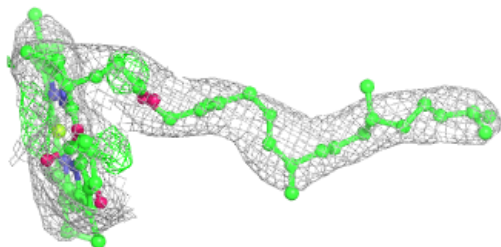
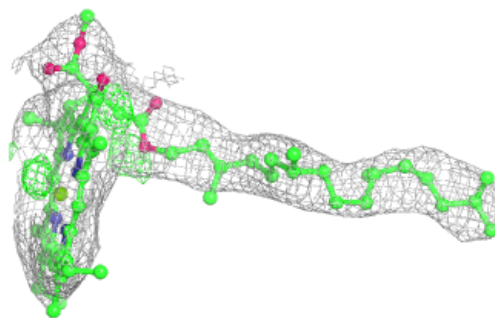


Electron density around CLA B 1234:

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

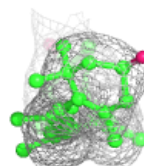
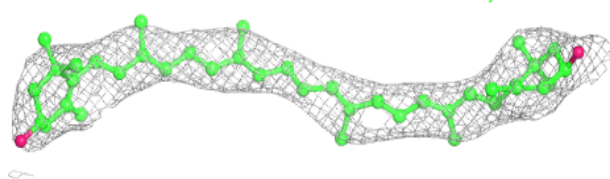
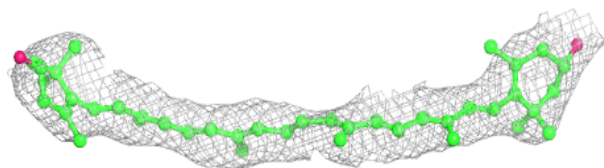
**Electron density around CLA A 1126:**

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

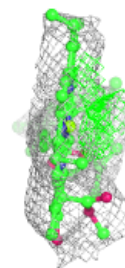
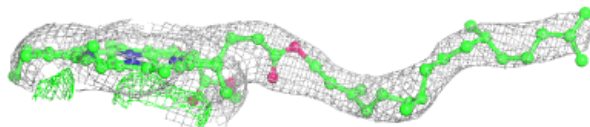
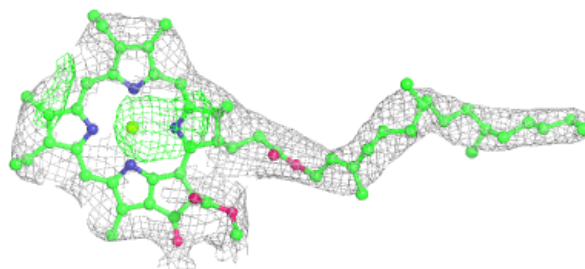


Electron density around LUT I 6018:

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

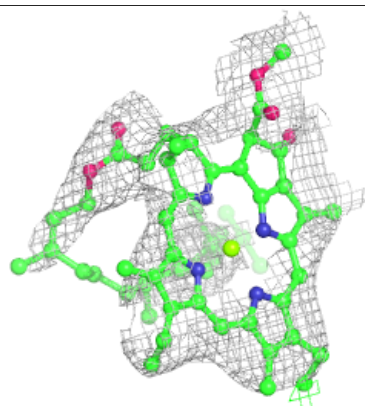
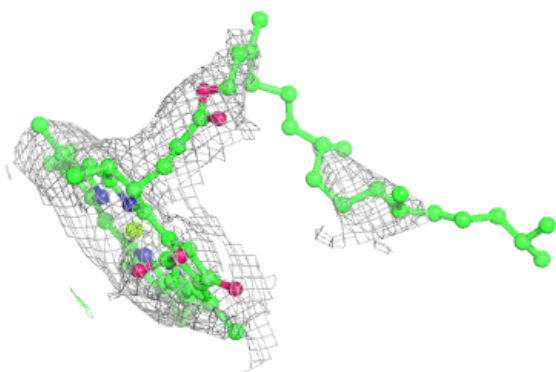
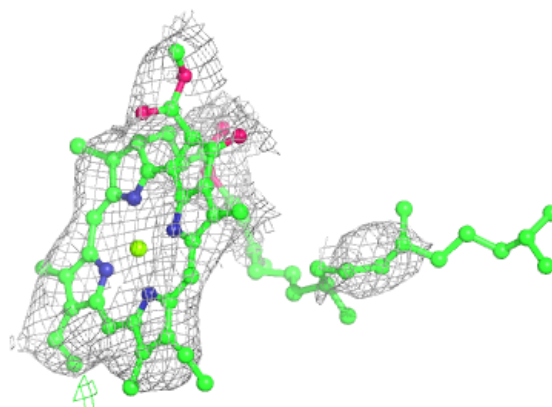
**Electron density around CLA A 1131:**

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

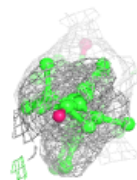
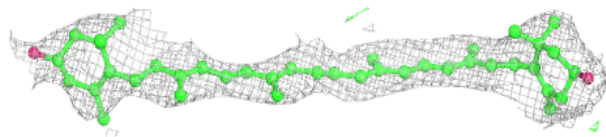
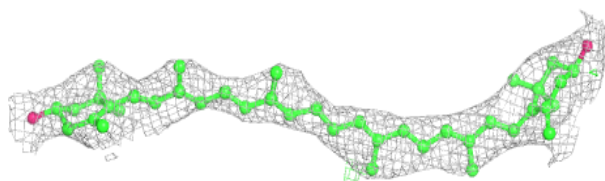


Electron density around CLA 4 4012:

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

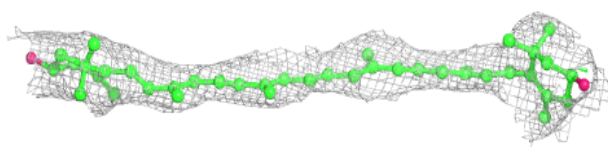
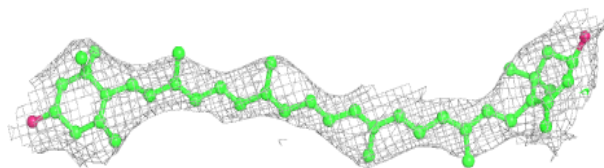
**Electron density around LUT 4 4501:**

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



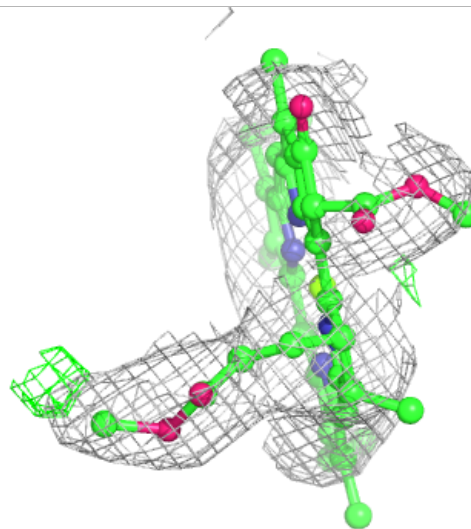
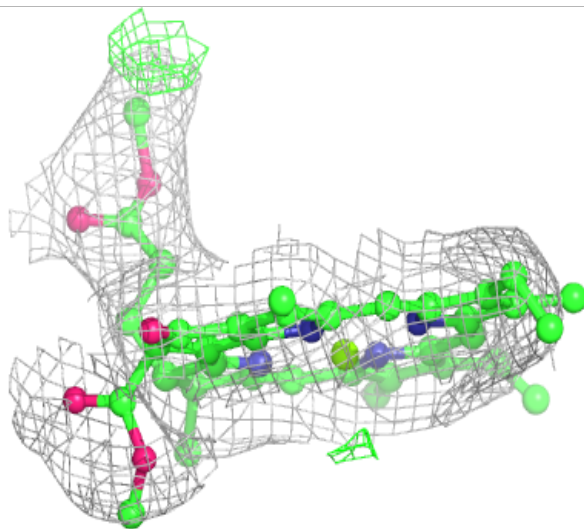
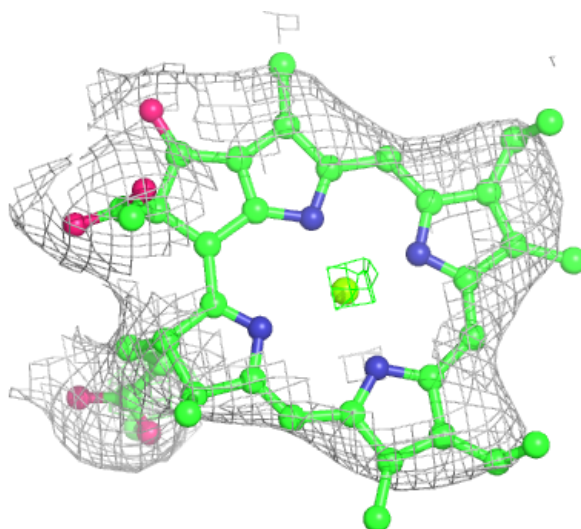
Electron density around LUT 4 4502:

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



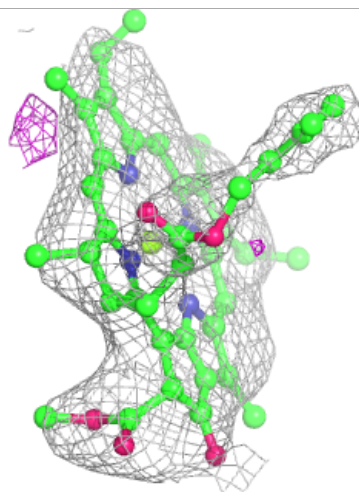
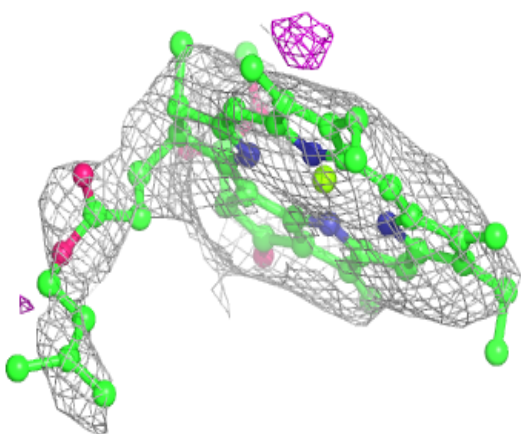
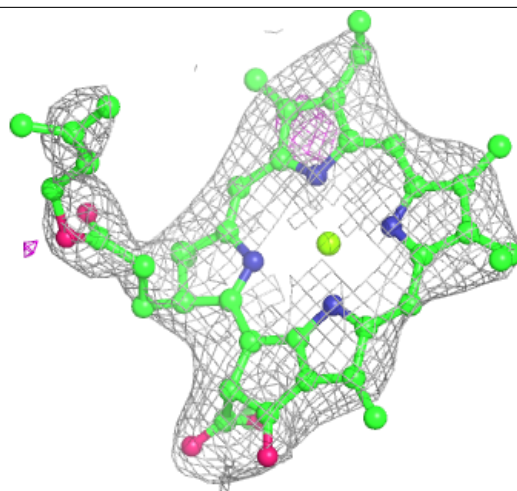
Electron density around CLA A 1118:

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



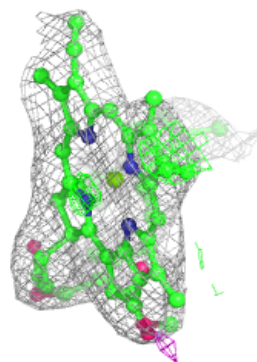
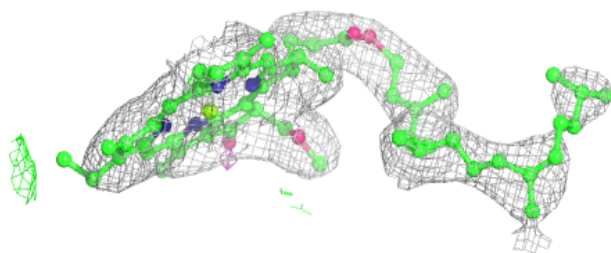
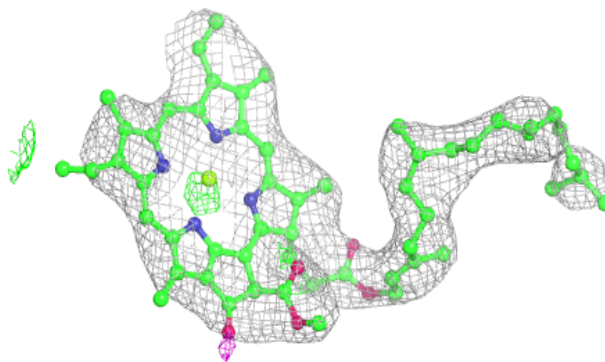
Electron density around CLA A 1129:

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

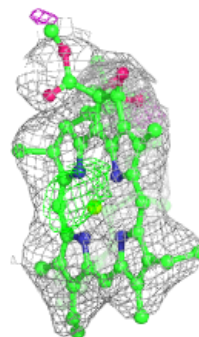
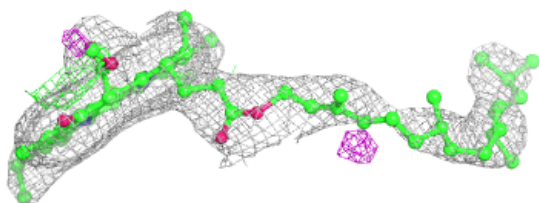
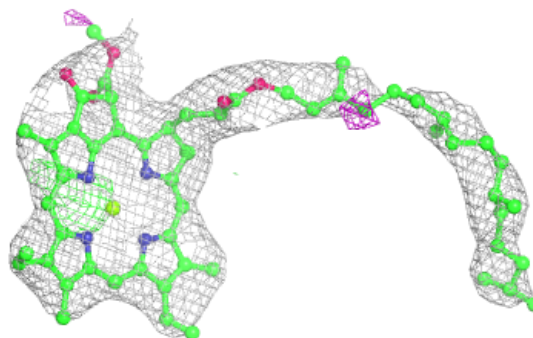


Electron density around CLA A 1101:

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

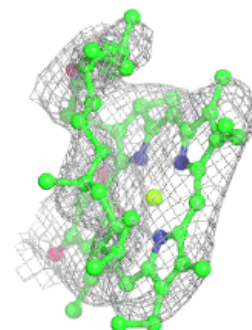
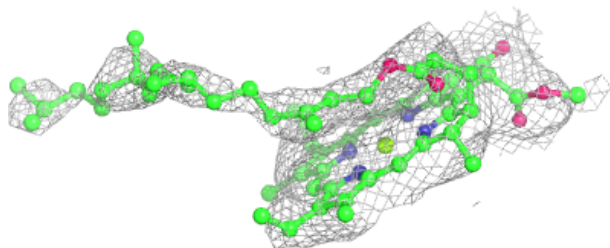
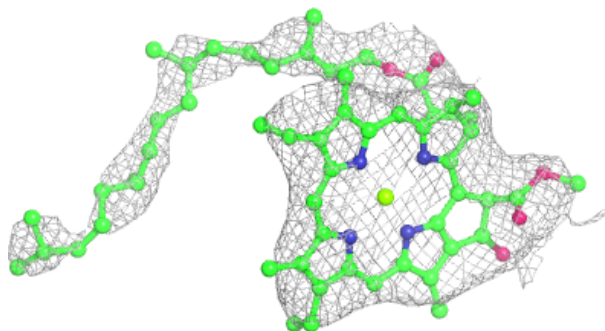
**Electron density around CLA B 1222:**

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

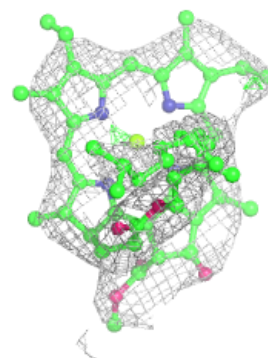
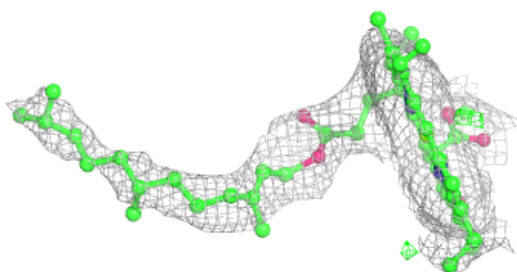
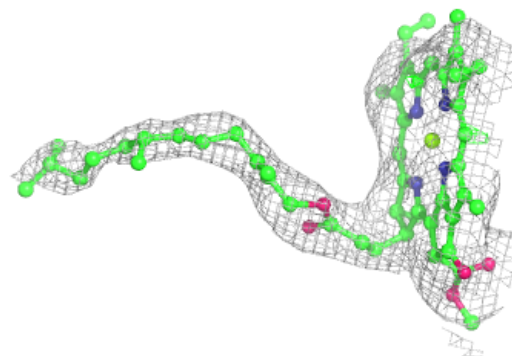


Electron density around CLA 1 1004:

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

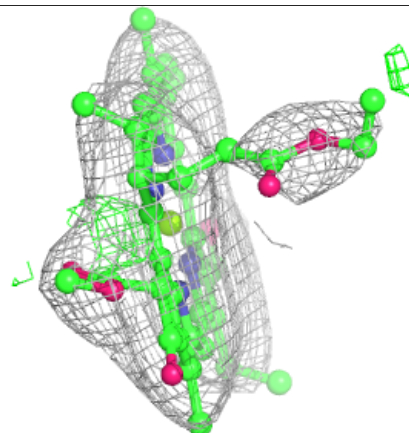
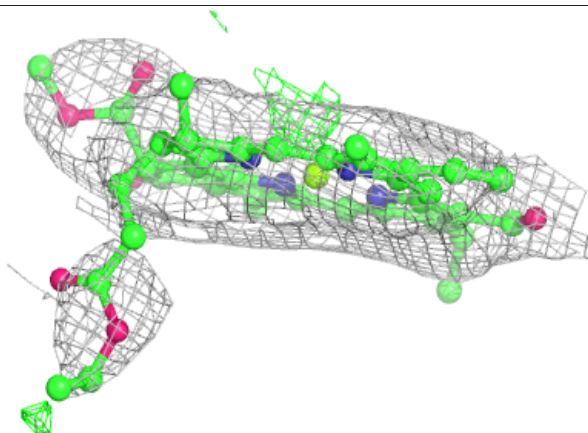
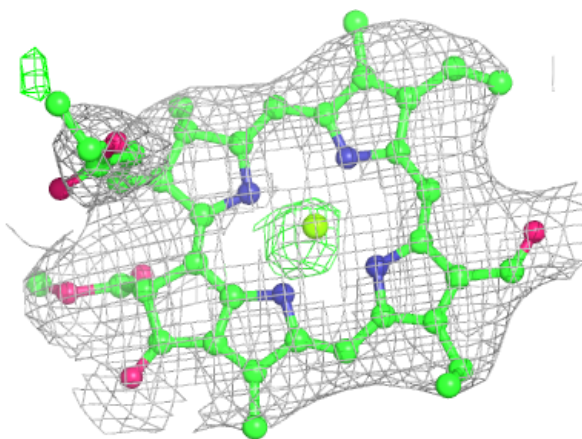
**Electron density around CLA L 1502:**

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



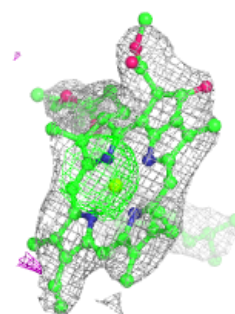
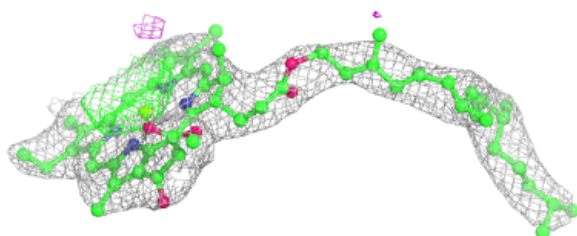
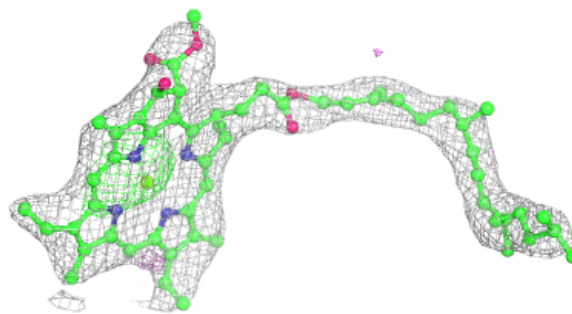
Electron density around CHL 2 2011:

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



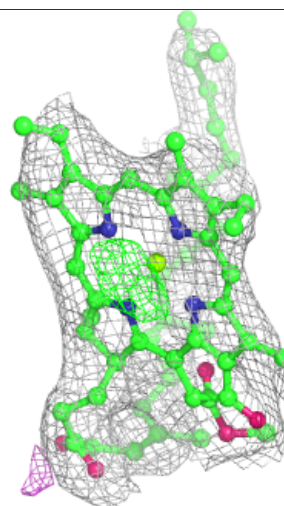
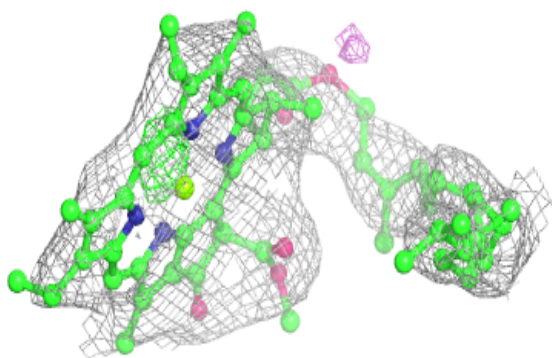
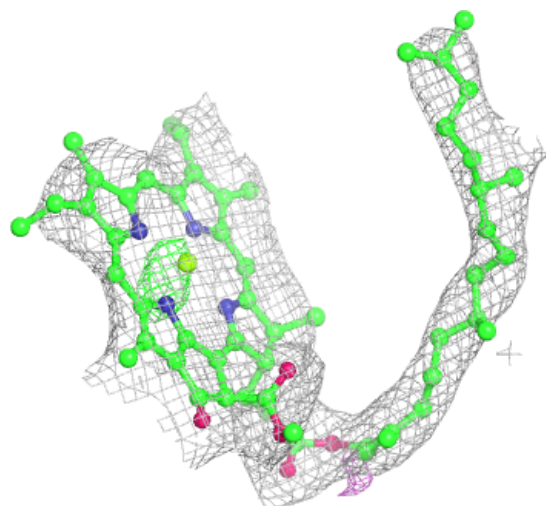
Electron density around CLA B 1012:

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



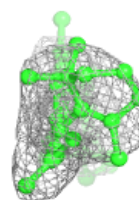
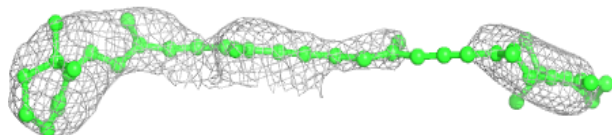
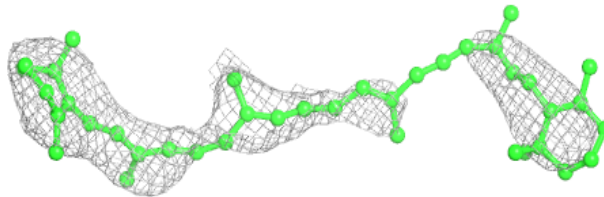
Electron density around CLA B 1207:

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



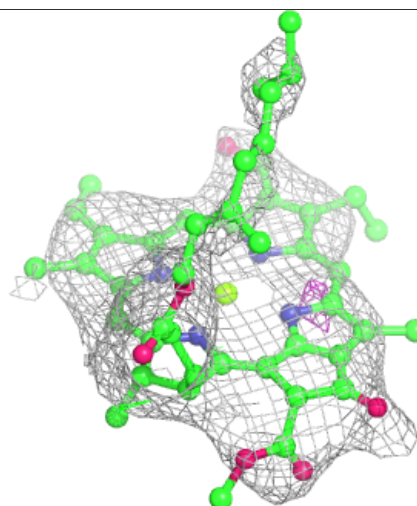
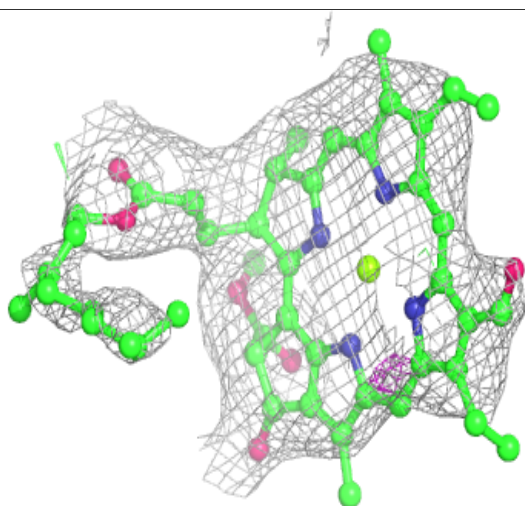
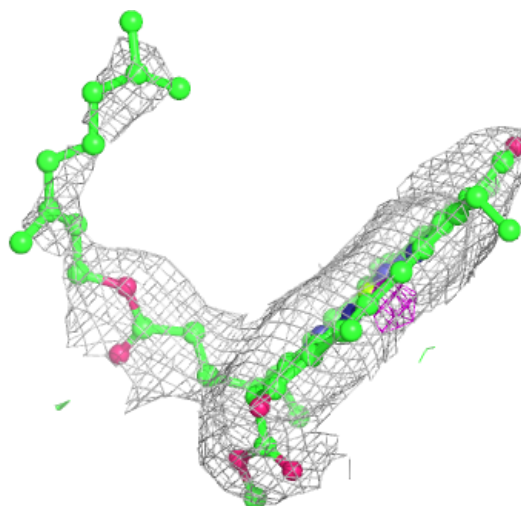
Electron density around BCR B 6006:

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



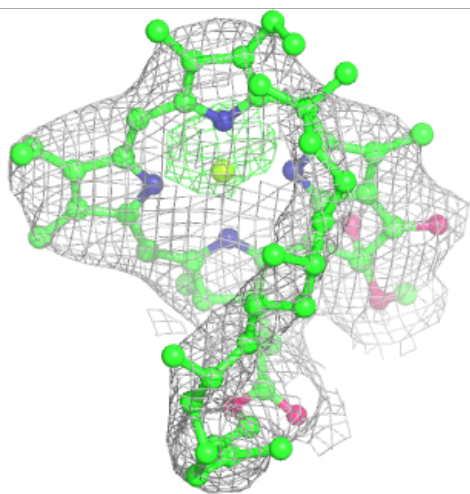
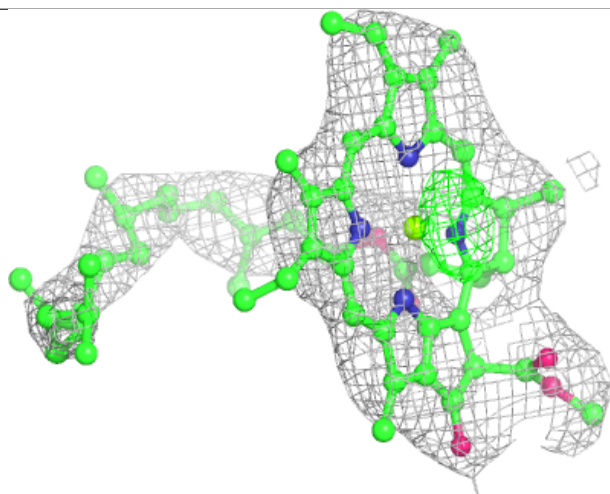
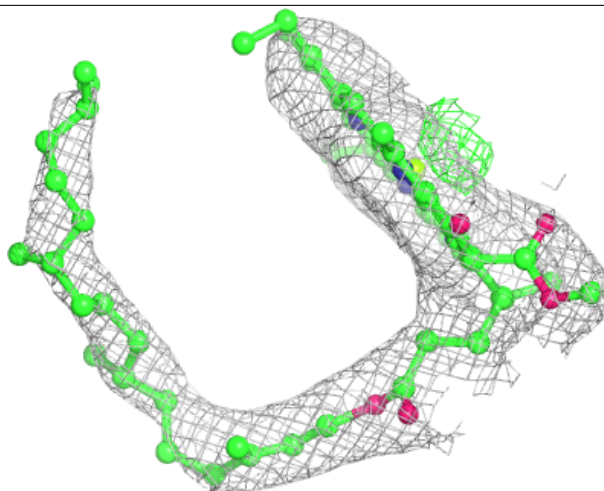
Electron density around CHL 1 1009:

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



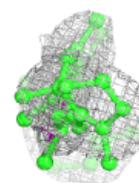
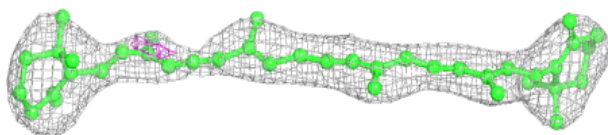
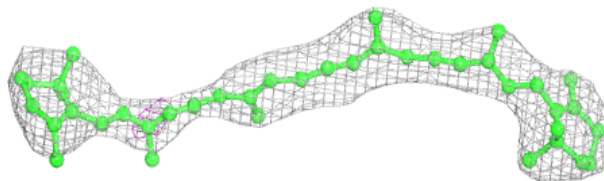
Electron density around CLA B 1216:

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

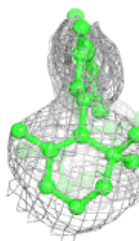
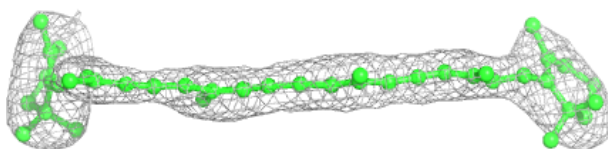
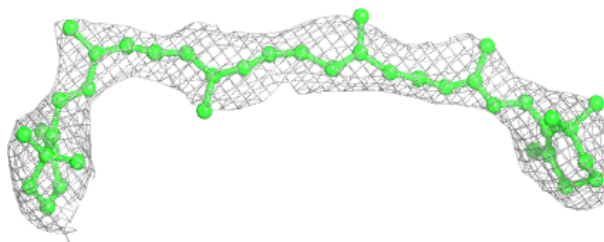


Electron density around BCR B 6010:

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

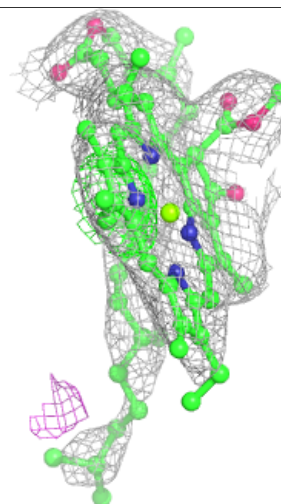
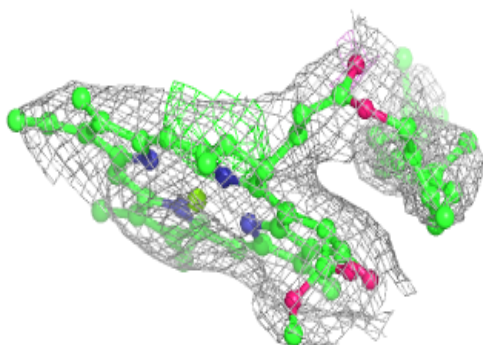
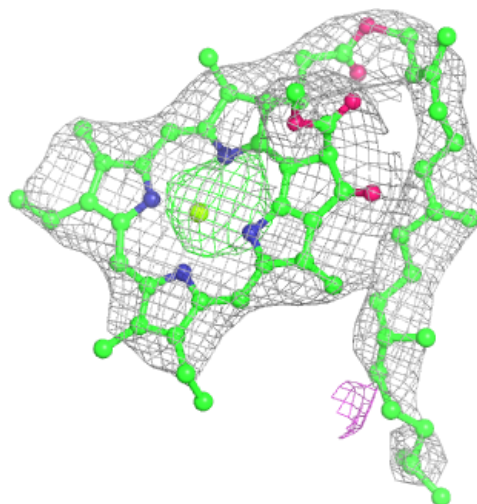
**Electron density around BCR I 6020:**

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



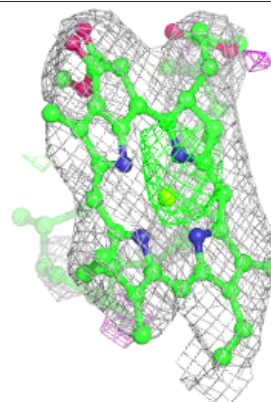
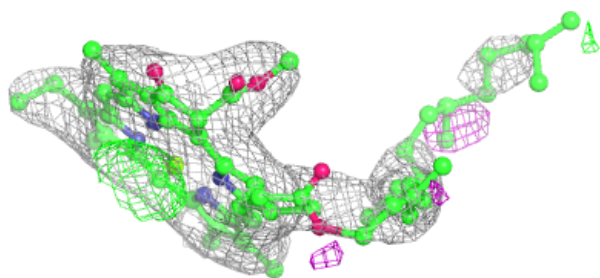
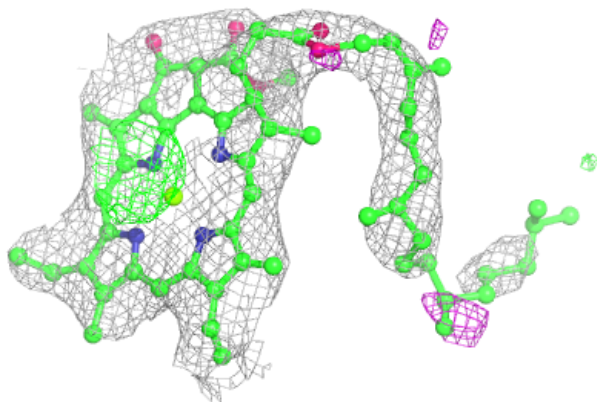
Electron density around CLA A 1123:

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

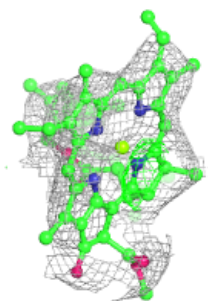
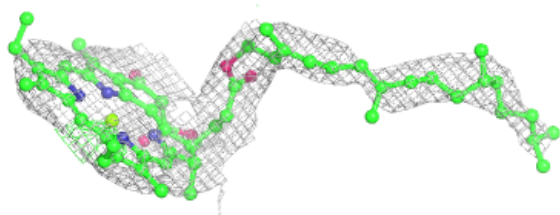
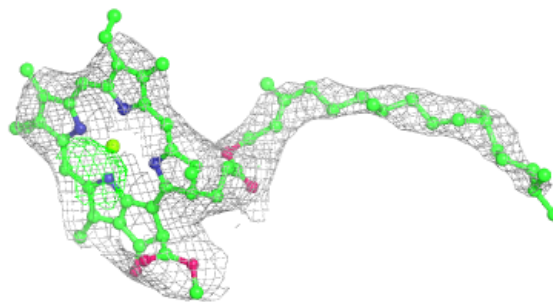


Electron density around CLA B 1221:

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

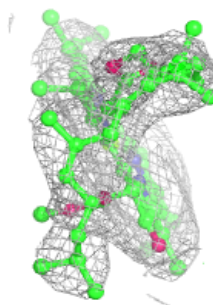
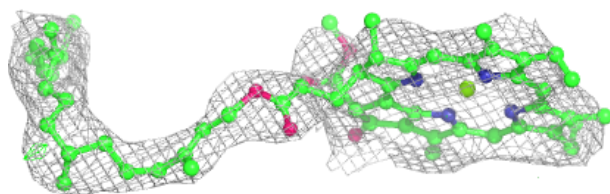
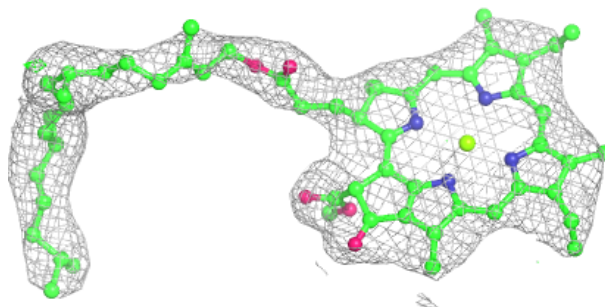
**Electron density around CLA A 1119:**

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



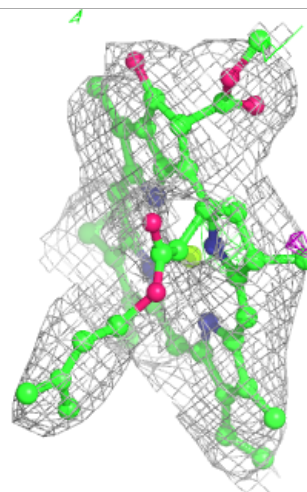
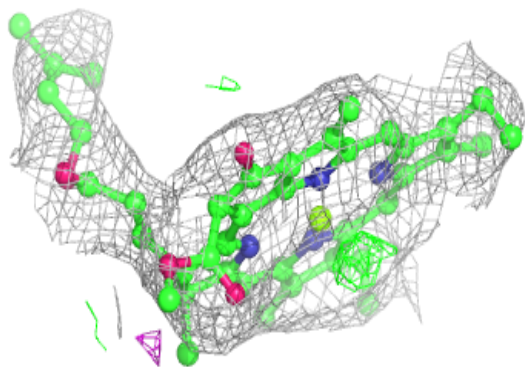
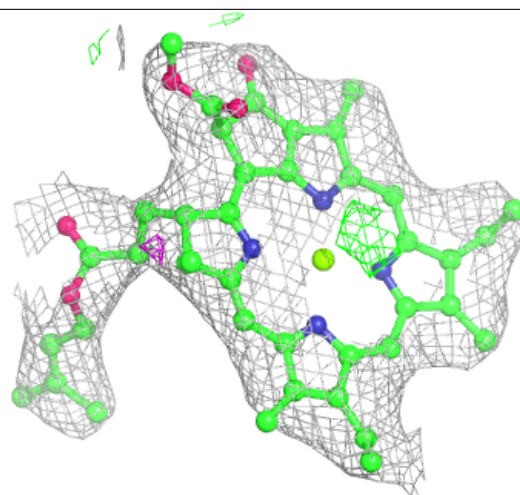
Electron density around CLA B 1223:

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



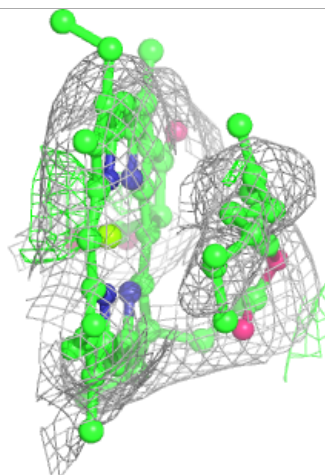
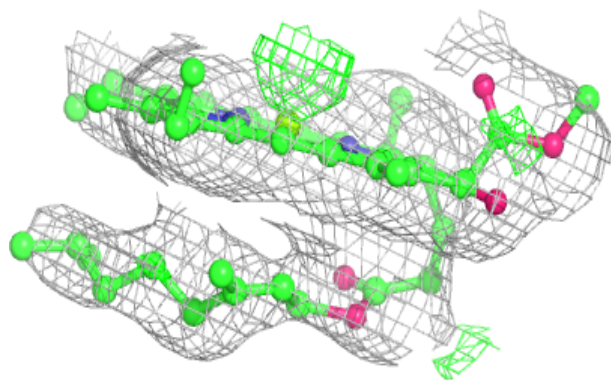
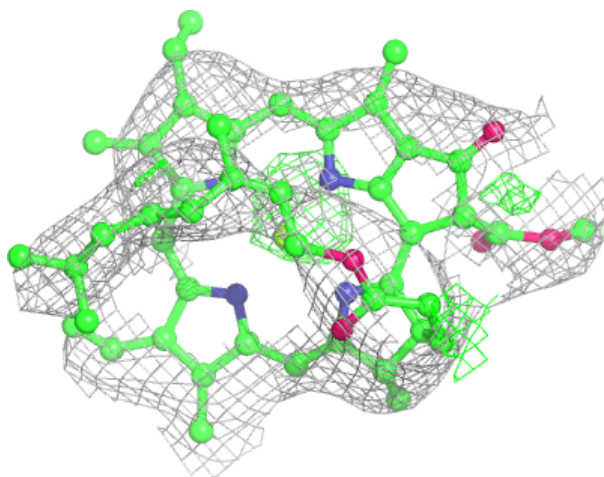
Electron density around CLA A 1102:

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



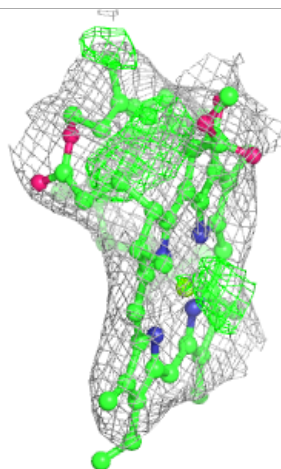
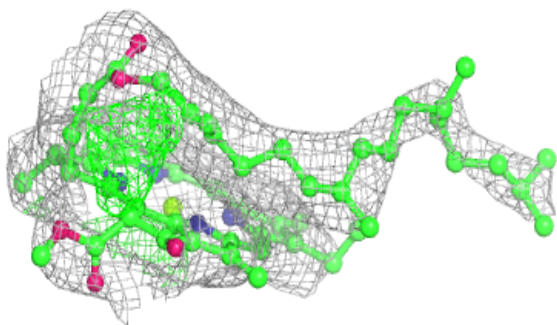
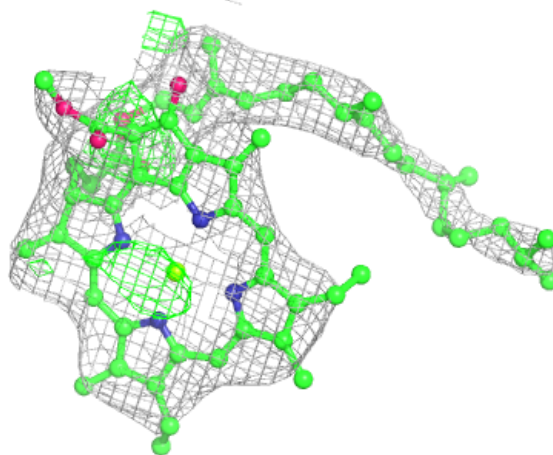
Electron density around CLA A 1110:

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



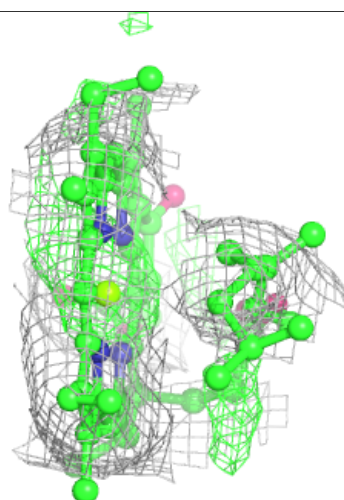
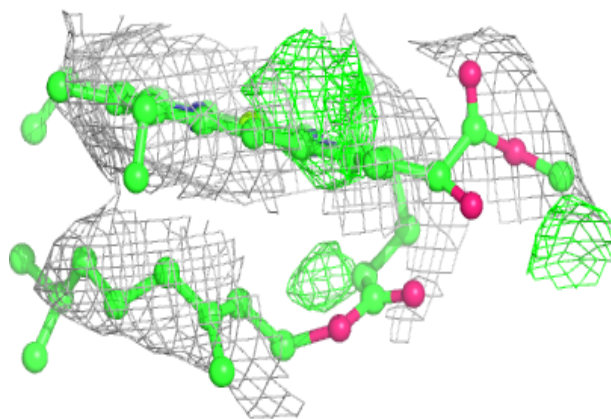
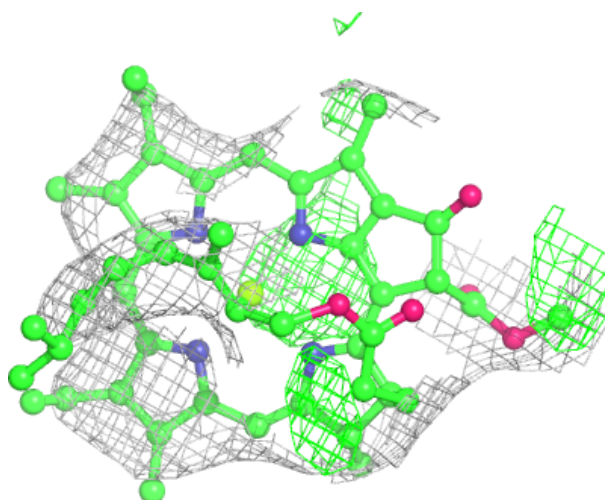
Electron density around CLA A 1127:

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



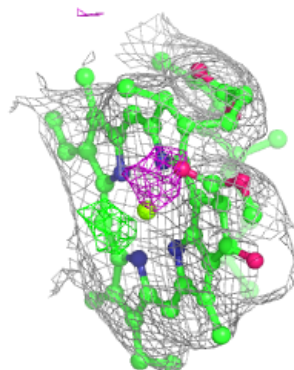
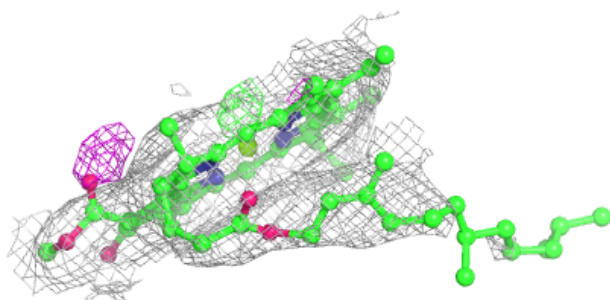
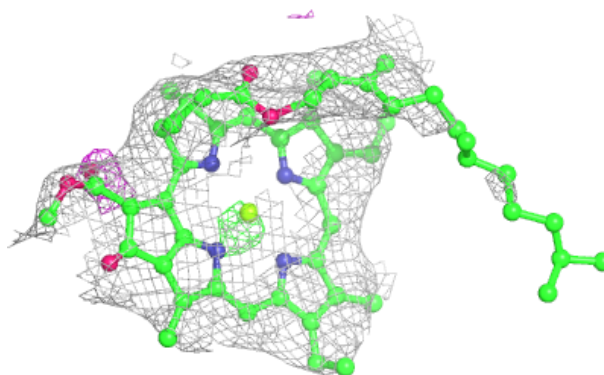
Electron density around CLA 1 1003:

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



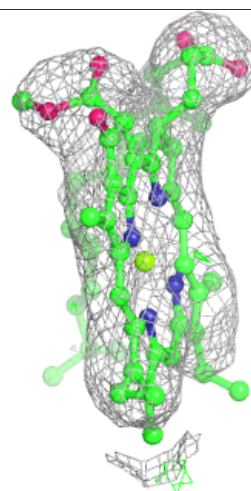
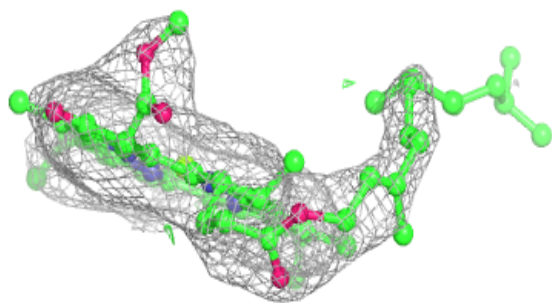
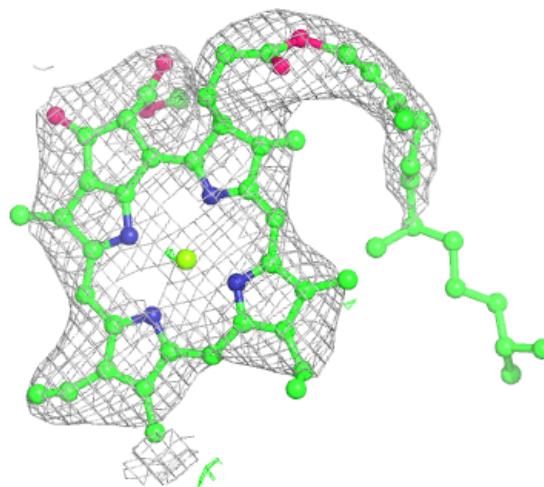
Electron density around CLA 2 2001:

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



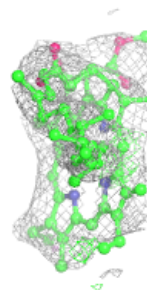
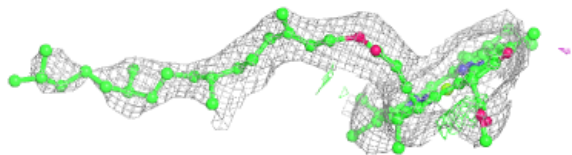
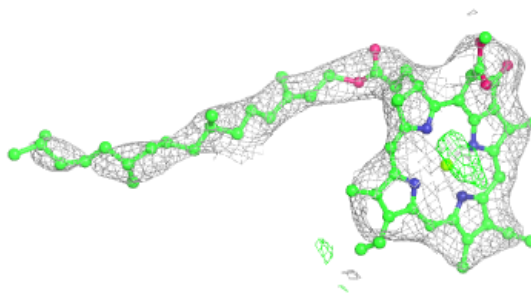
Electron density around CLA A 1111:

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



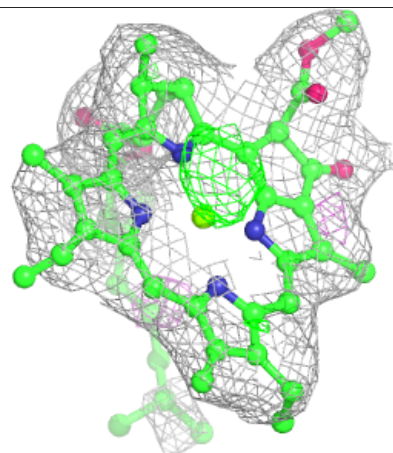
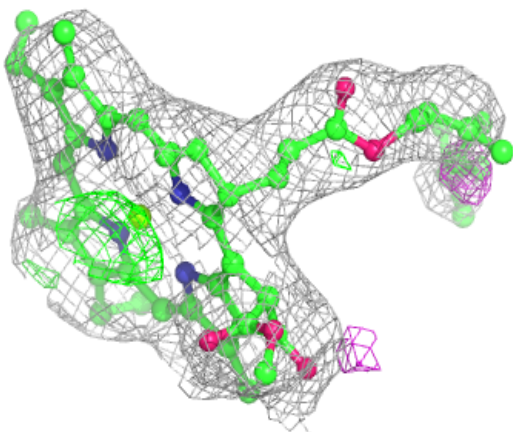
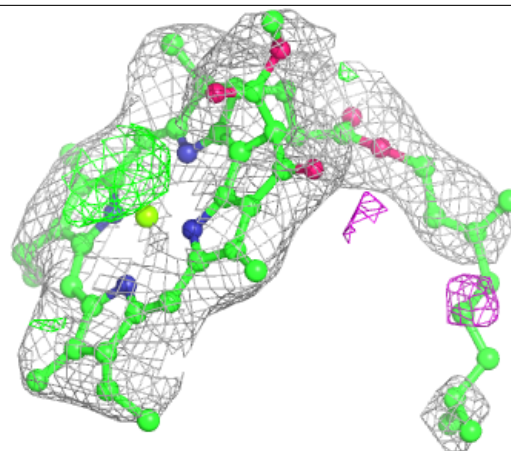
Electron density around CLA A 1132:

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

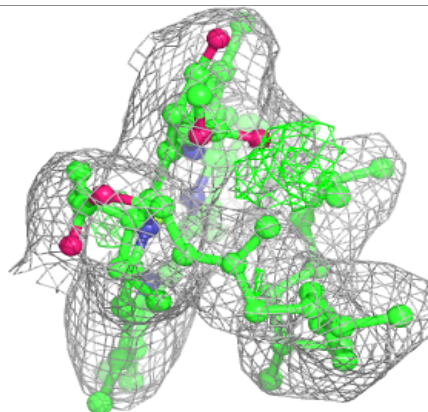
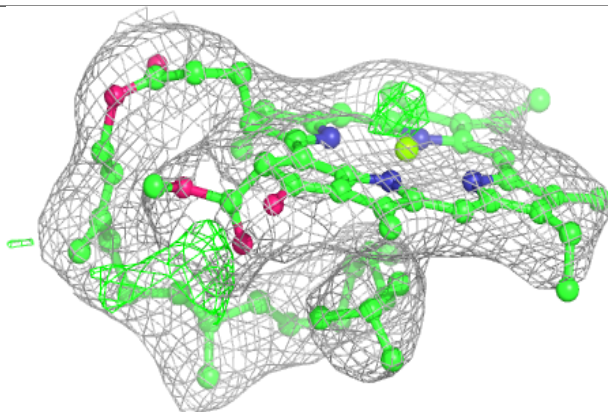
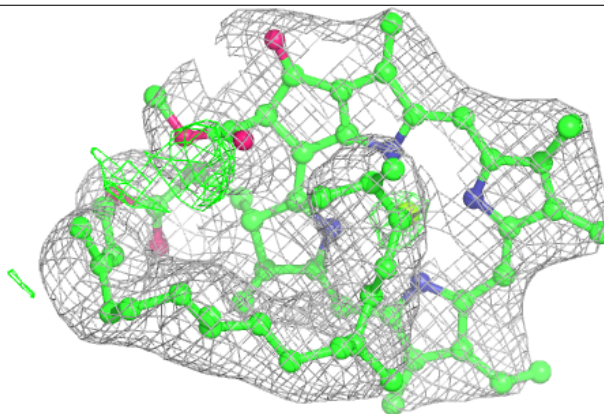


Electron density around CLA B 1236:

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

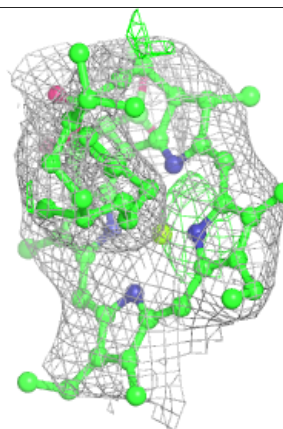
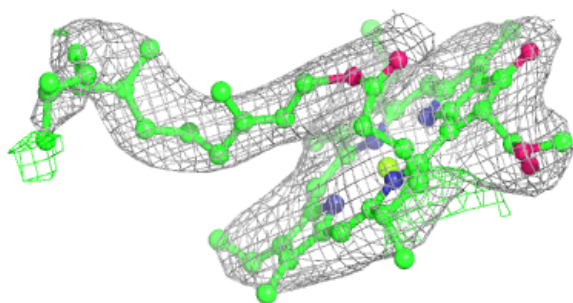
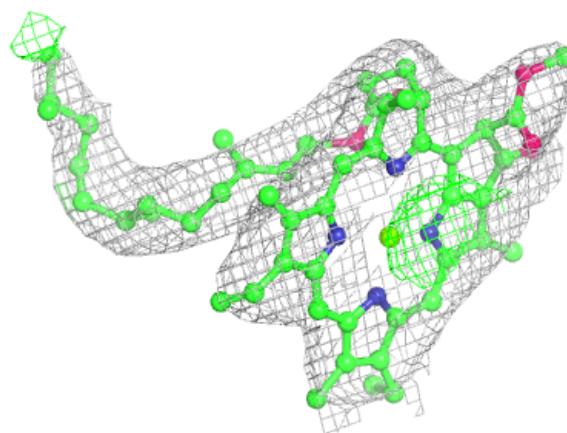
**Electron density around CLA A 1104:**

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



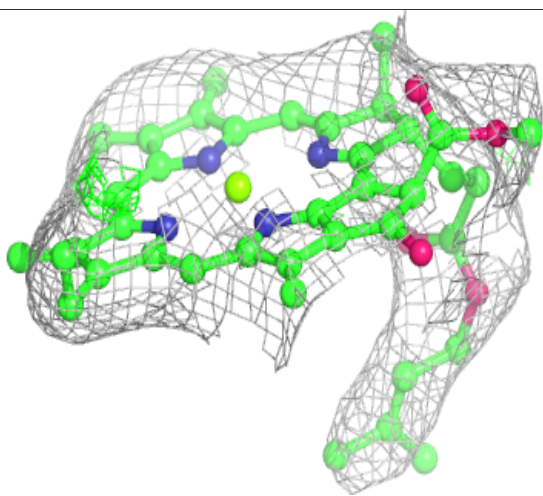
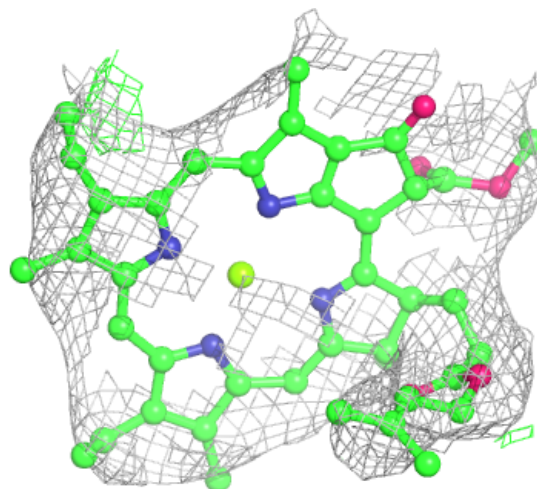
Electron density around CLA A 1237:

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



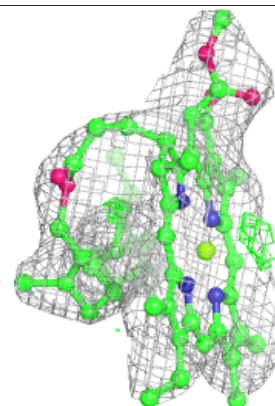
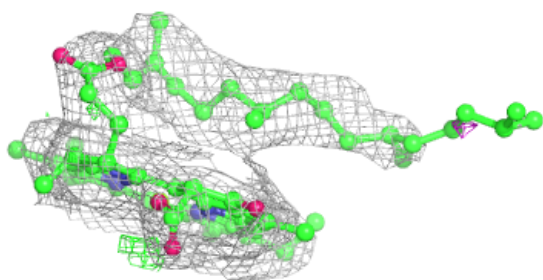
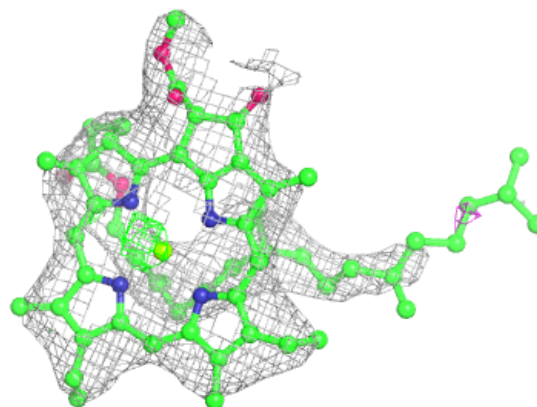
Electron density around CLA 1 1012:

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

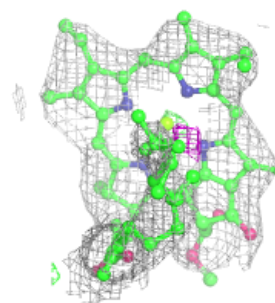
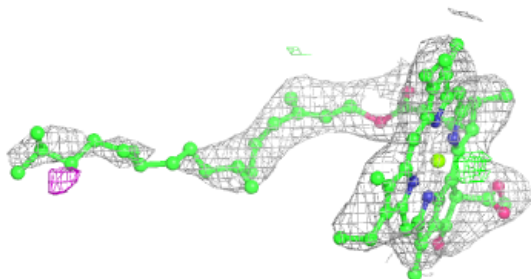
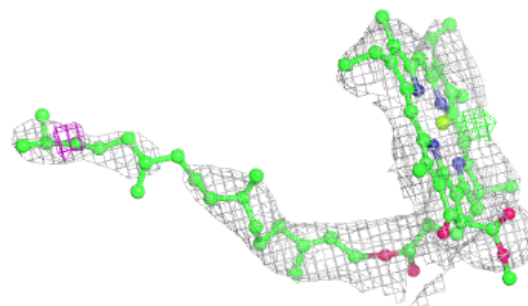


Electron density around CLA B 1224:

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

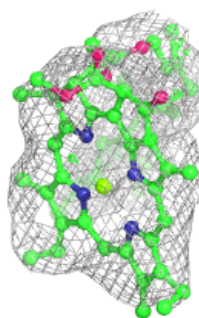
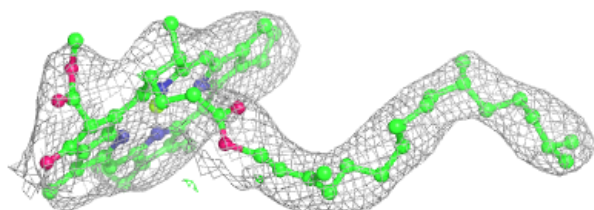
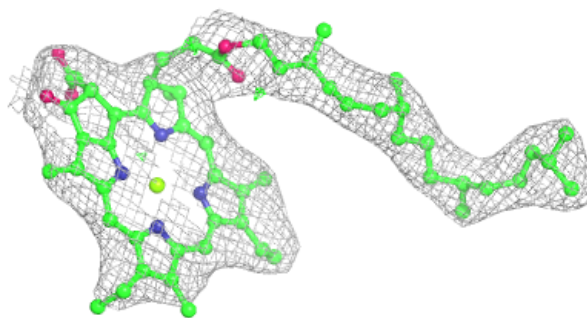
**Electron density around CLA B 1226:**

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

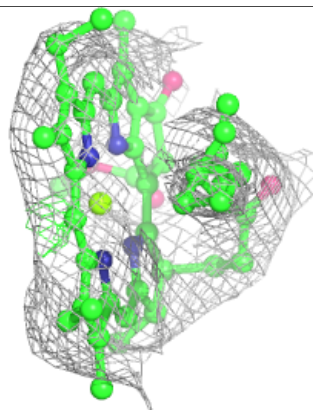
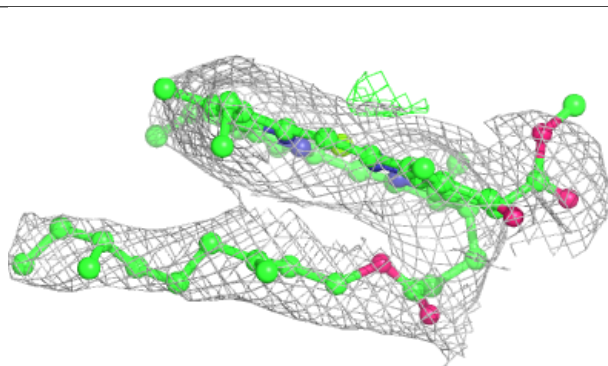
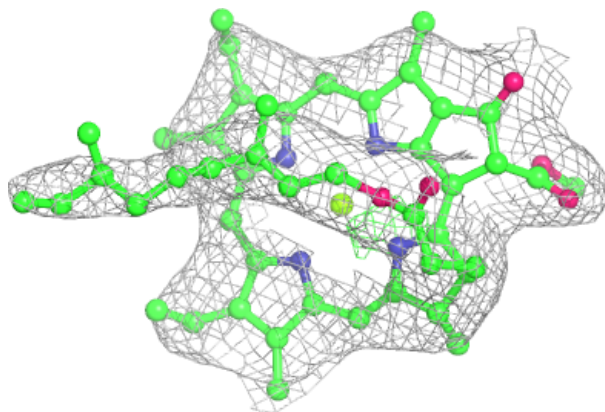


Electron density around CLA A 1106:

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

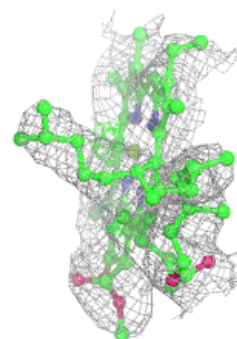
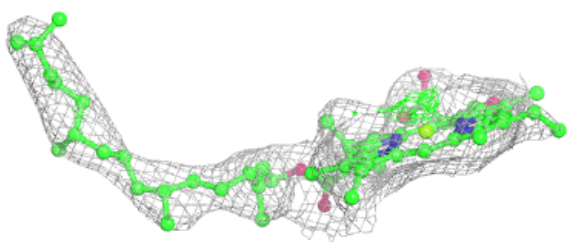
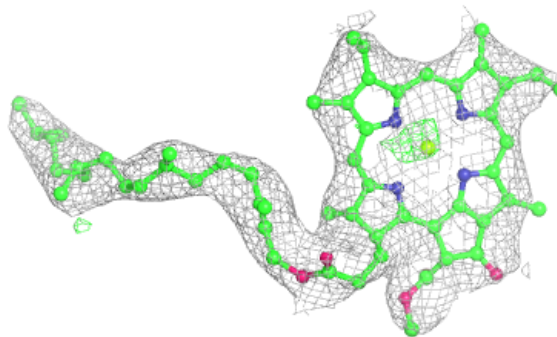
**Electron density around CLA A 1136:**

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

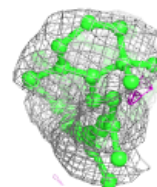
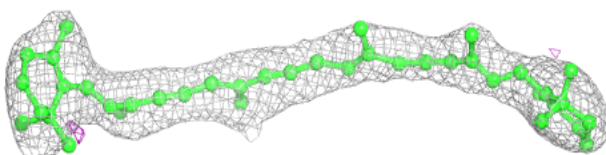
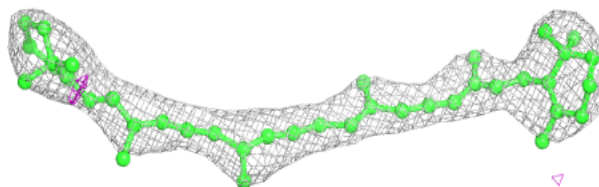


Electron density around CLA B 1023:

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

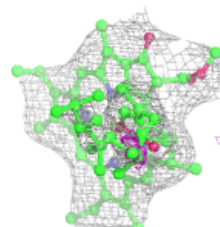
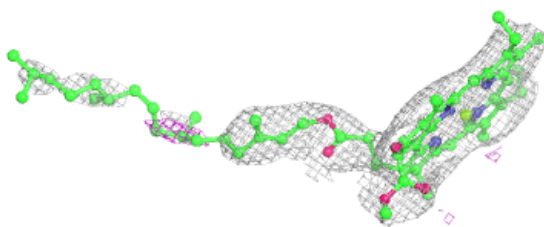
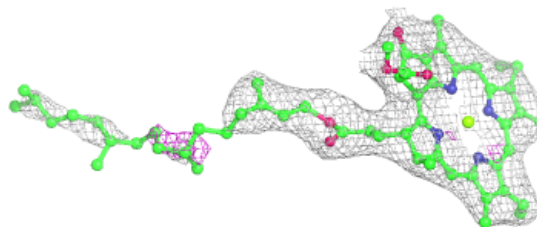
**Electron density around BCR F 6014:**

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



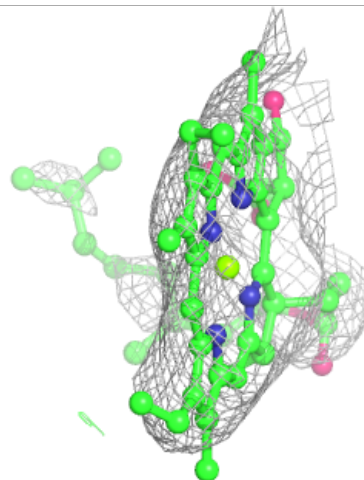
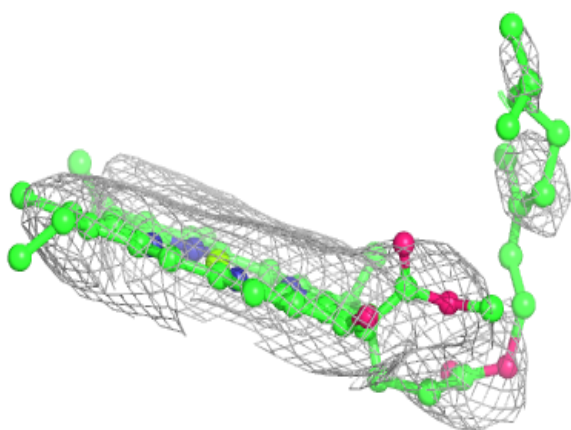
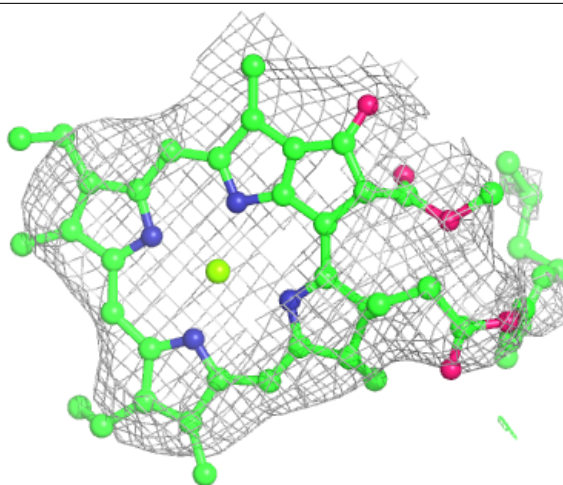
Electron density around CLA A 1107:

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



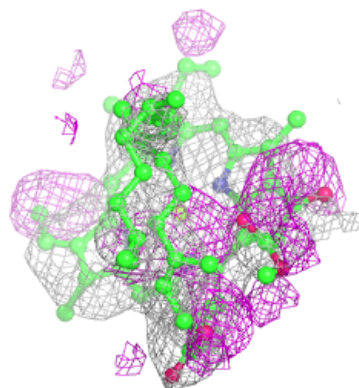
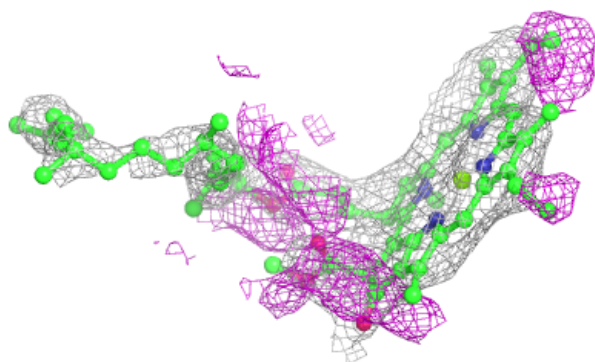
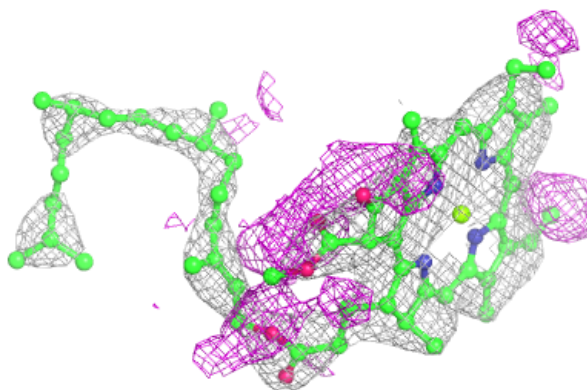
Electron density around CLA 3 3005:

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

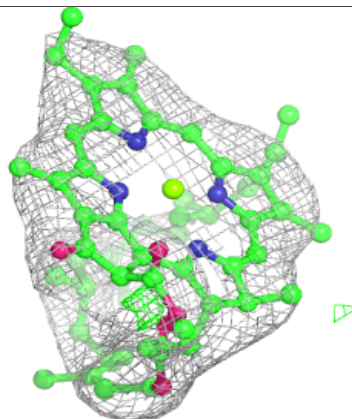
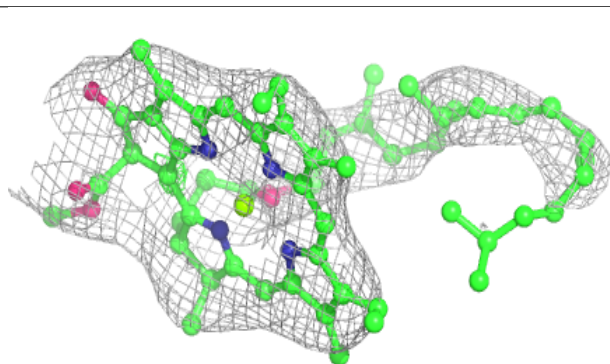
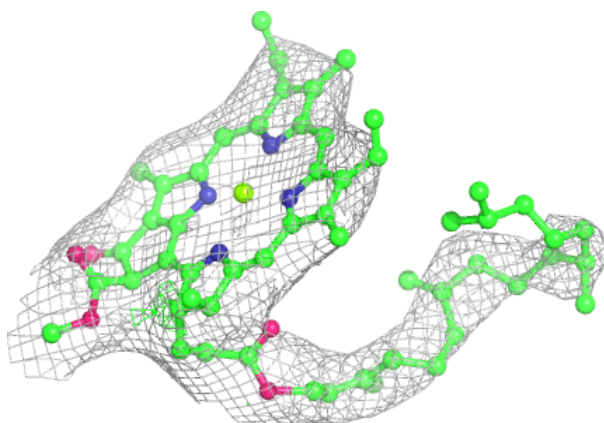


Electron density around CL0 A 1011:

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

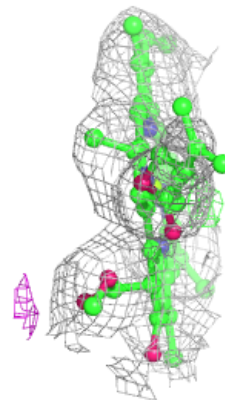
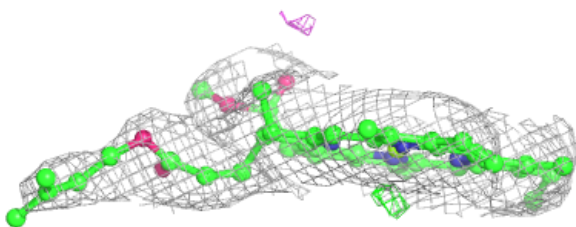
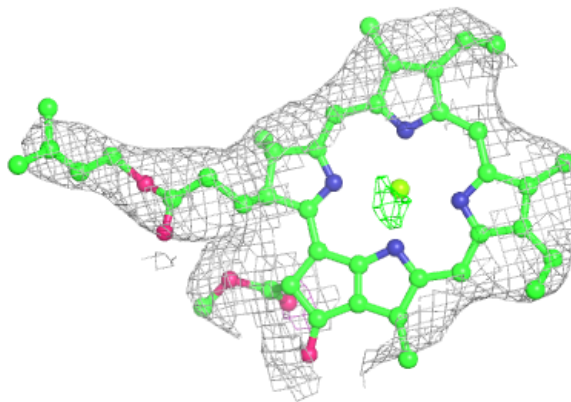
**Electron density around CLA A 1122:**

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



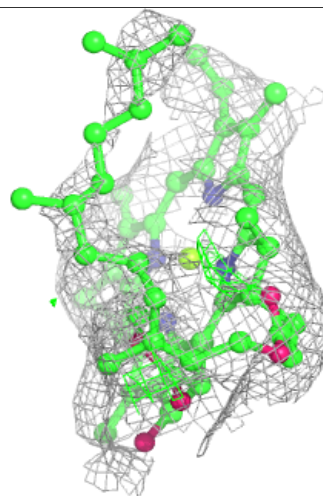
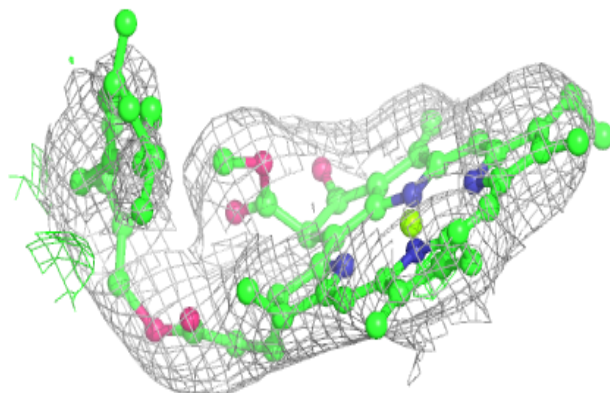
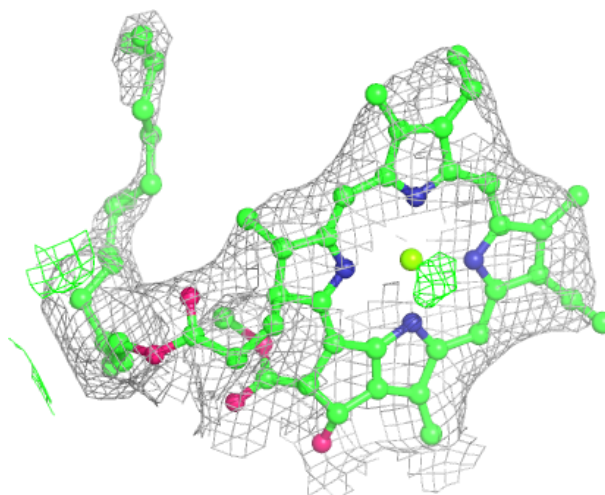
Electron density around CLA F 1302:

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



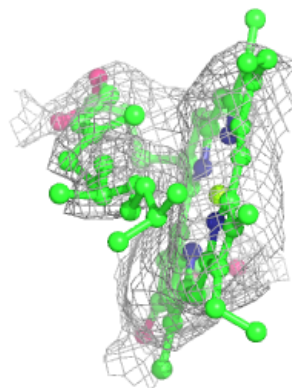
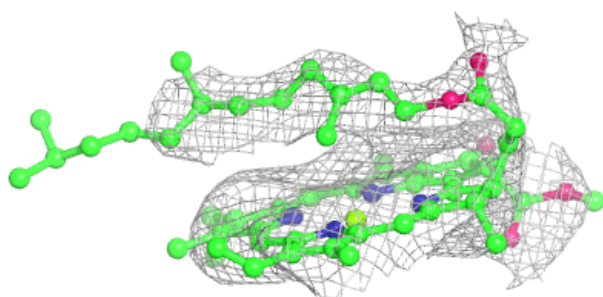
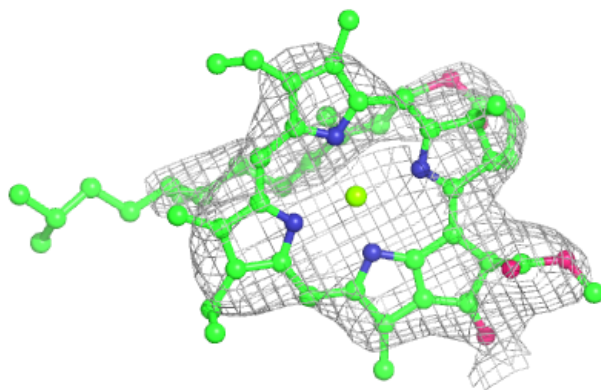
Electron density around CLA 4 4005:

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

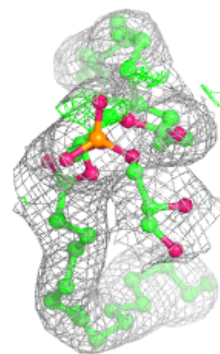
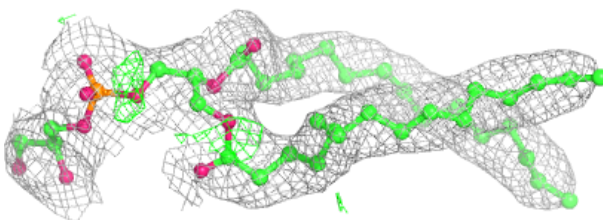
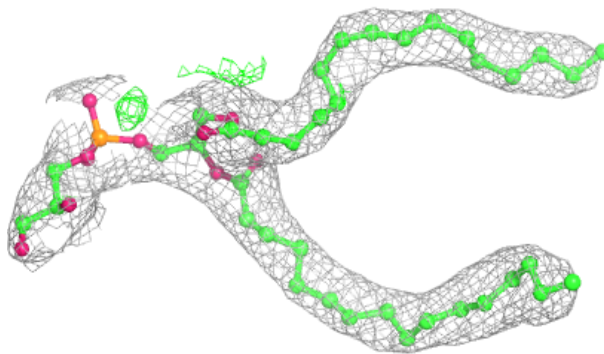


Electron density around CLA A 1116:

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

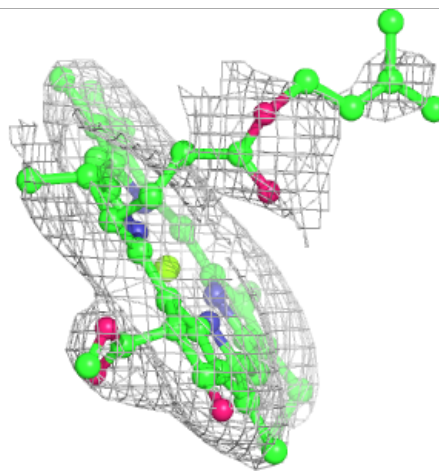
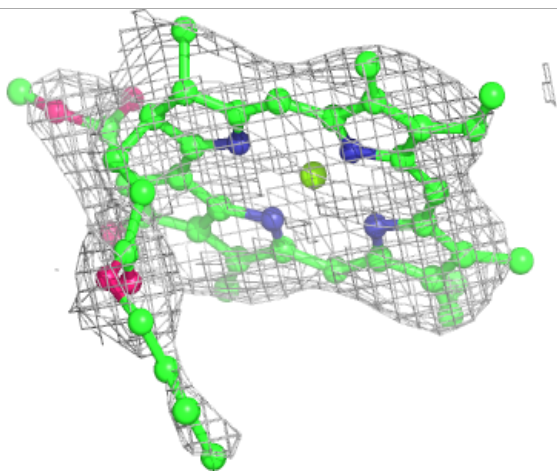
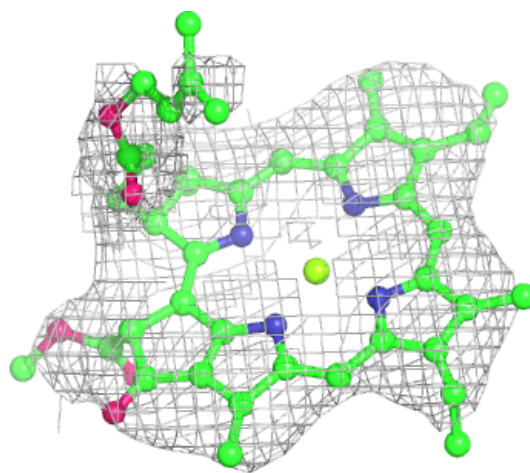
**Electron density around LHG A 7001:**

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



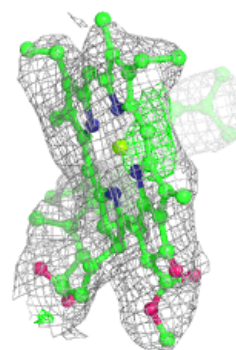
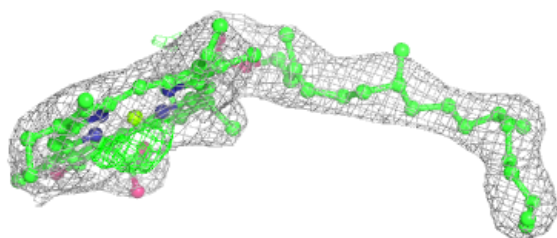
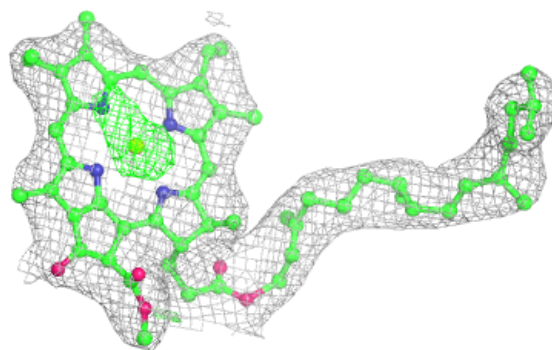
Electron density around CLA A 1130:

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

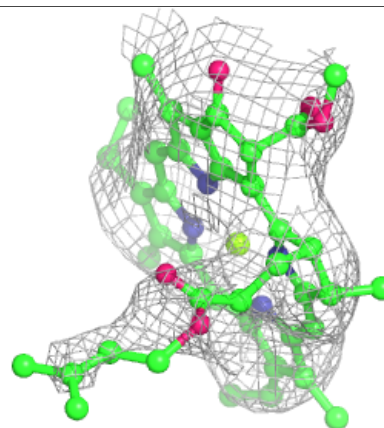
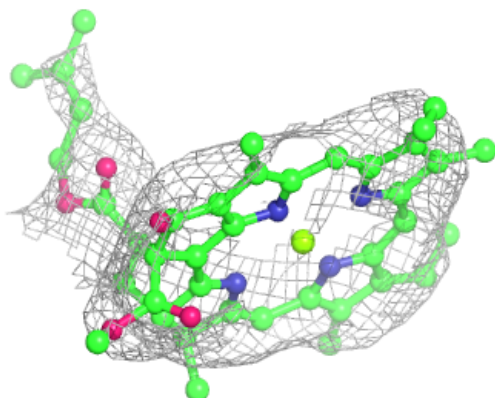
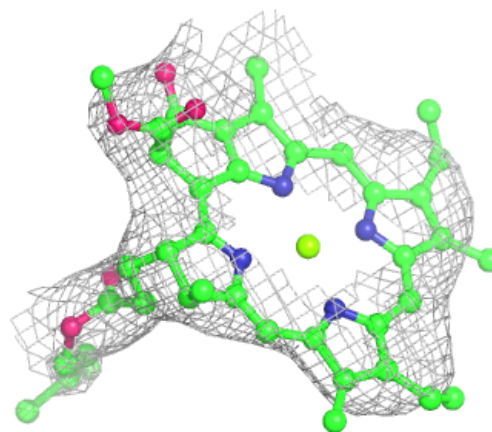


Electron density around CLA A 1013:

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

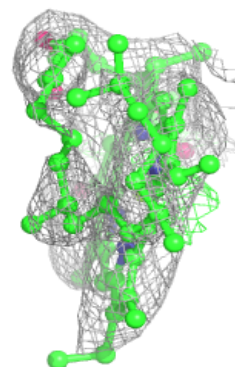
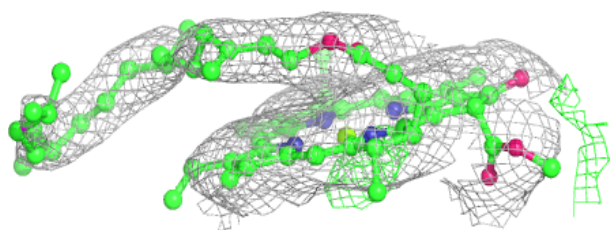
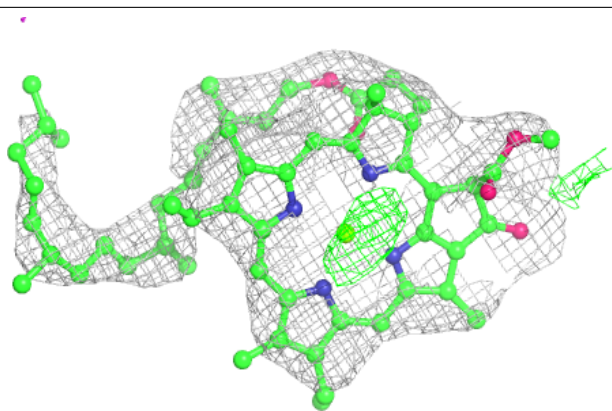
**Electron density around CLA 2 2008:**

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

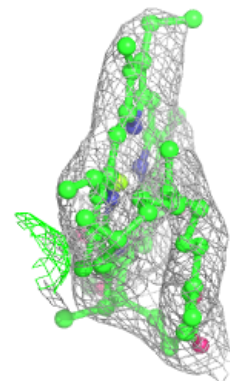
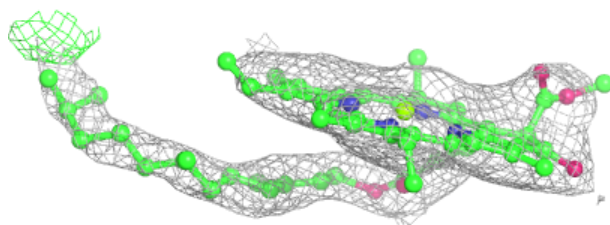
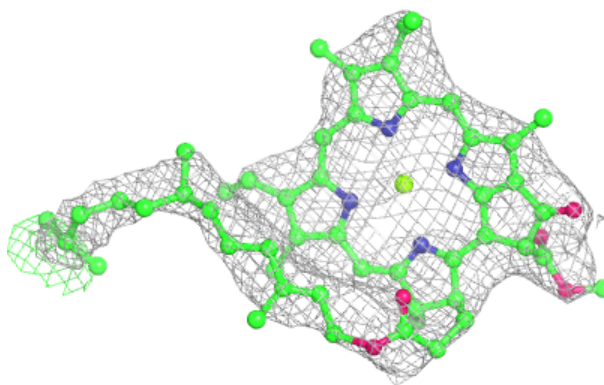


Electron density around CLA A 1117:

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

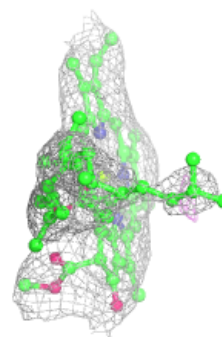
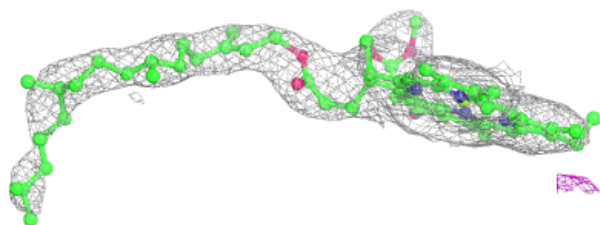
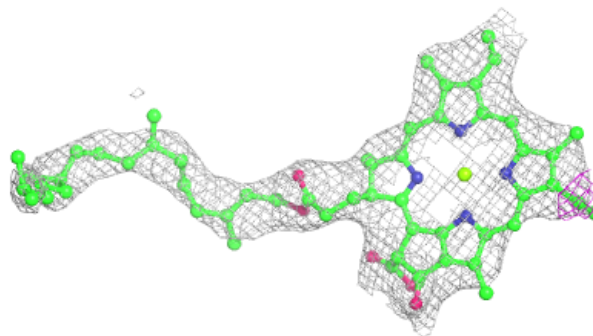
**Electron density around CLA B 1215:**

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

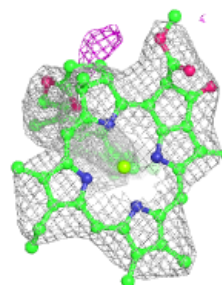
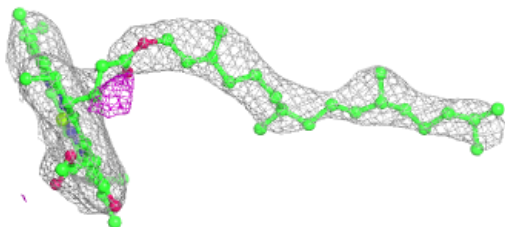
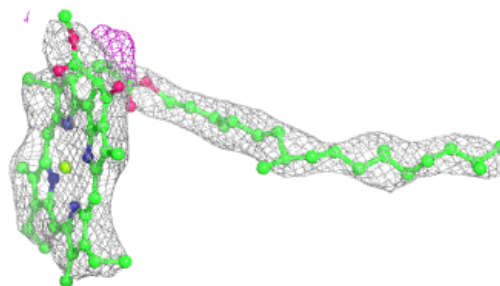


Electron density around CLA A 1103:

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

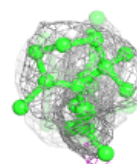
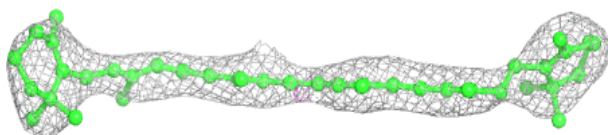
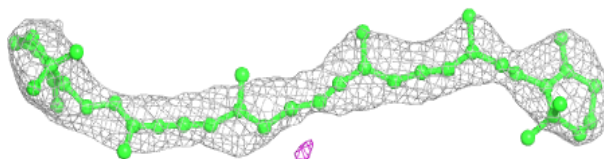
**Electron density around CLA B 1225:**

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

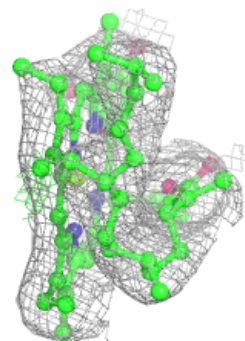
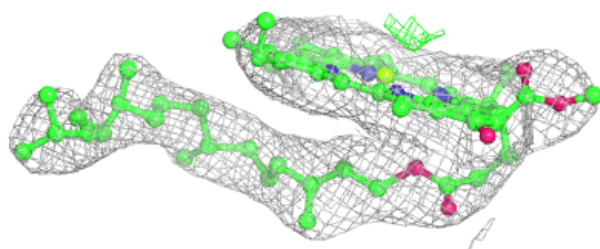
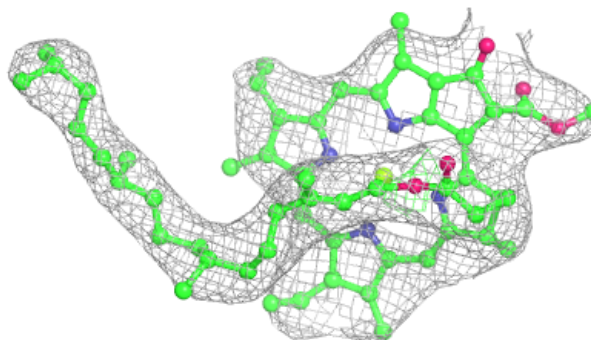


Electron density around BCR A 6017:

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

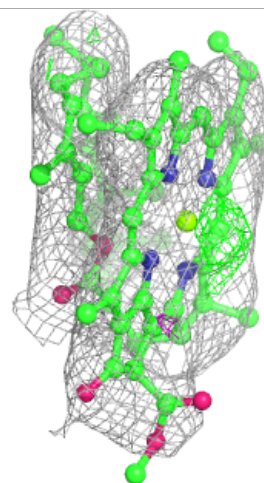
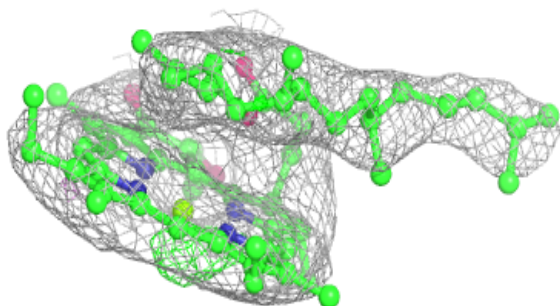
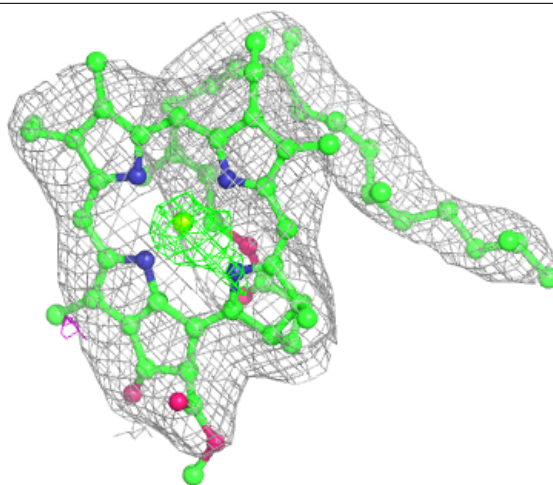
**Electron density around CLA B 1235:**

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



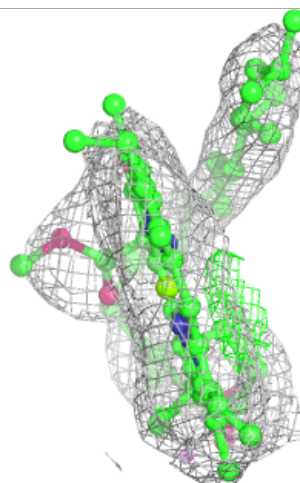
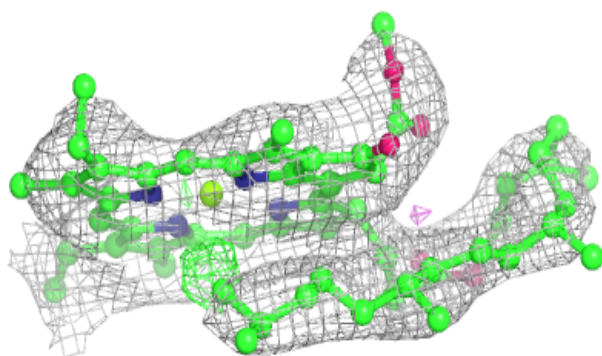
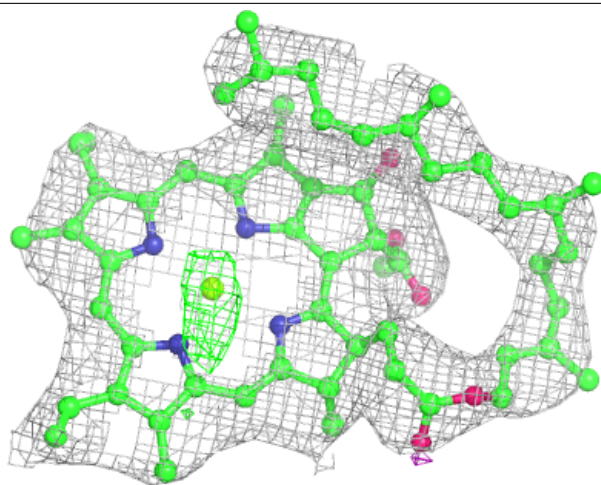
Electron density around CLA B 1205:

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



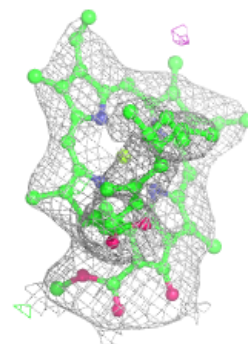
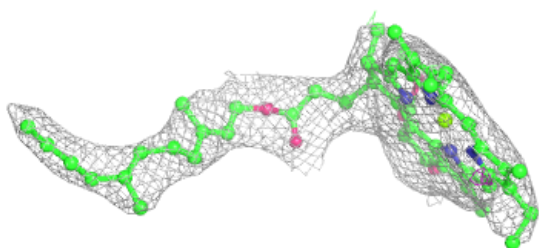
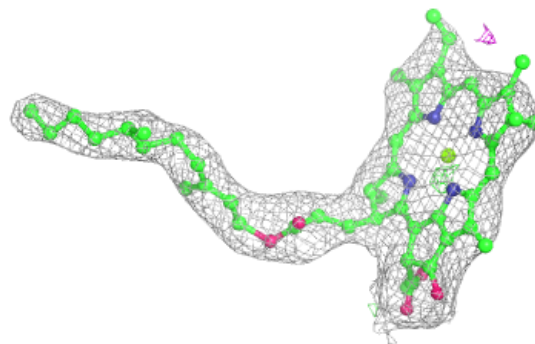
Electron density around CLA B 1202:

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



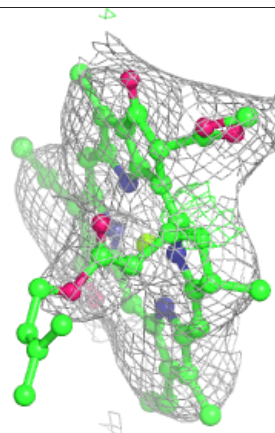
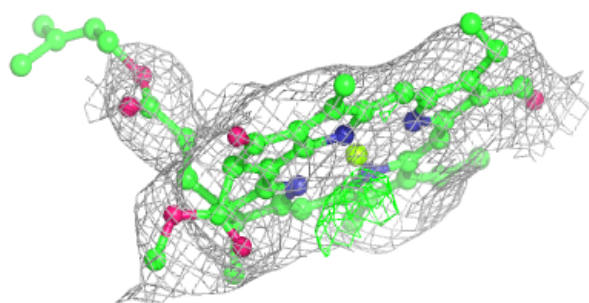
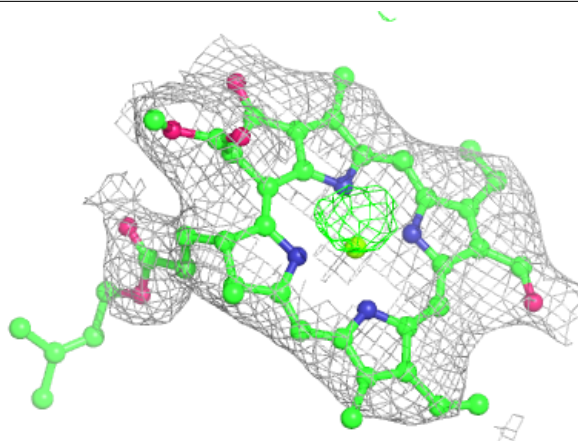
Electron density around CLA B 1230:

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



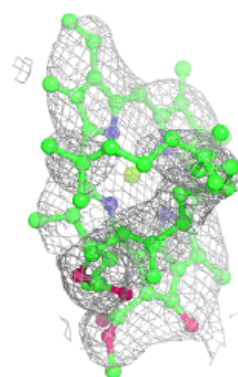
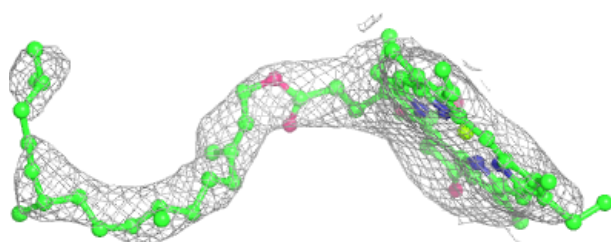
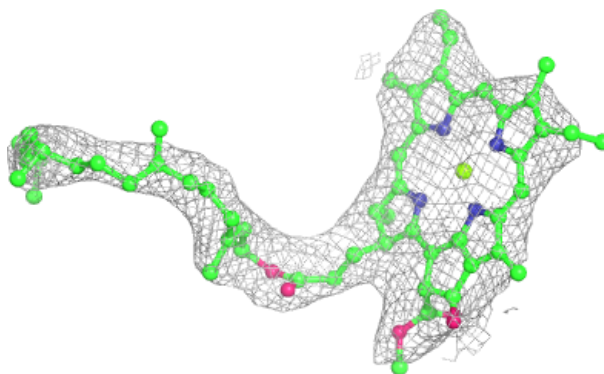
Electron density around CHL 4 4011:

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

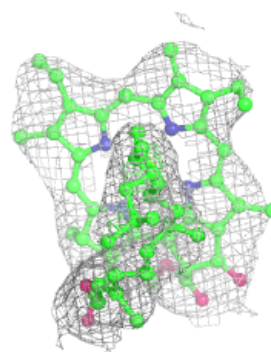
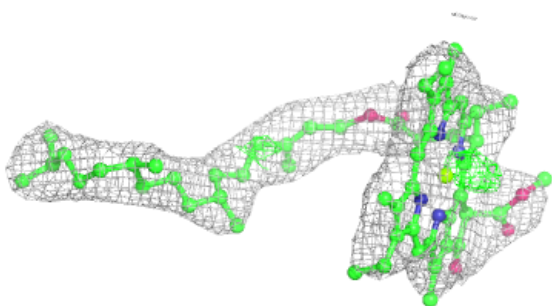
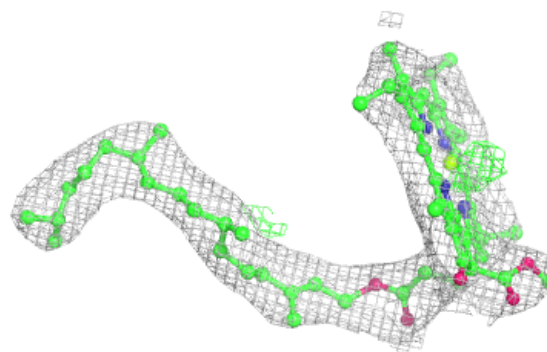


Electron density around CLA B 1206:

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

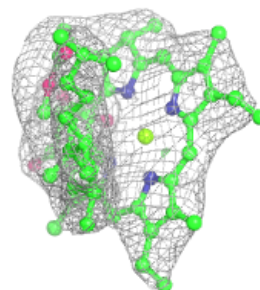
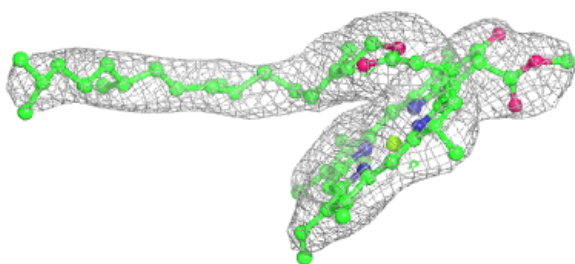
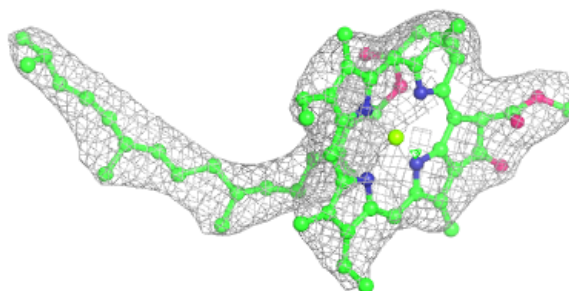
**Electron density around CLA A 1128:**

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

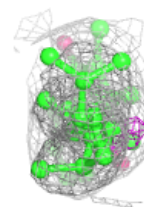
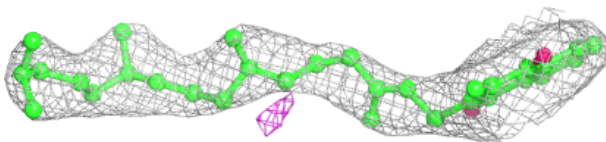
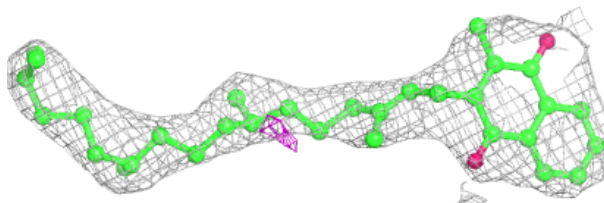


Electron density around CLA A 1140:

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

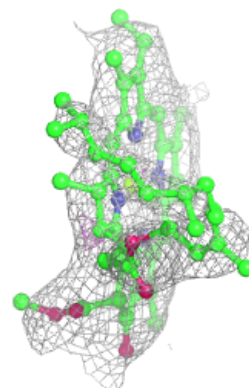
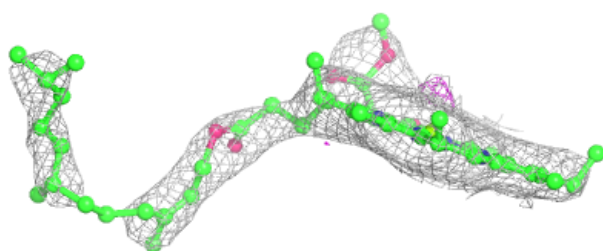
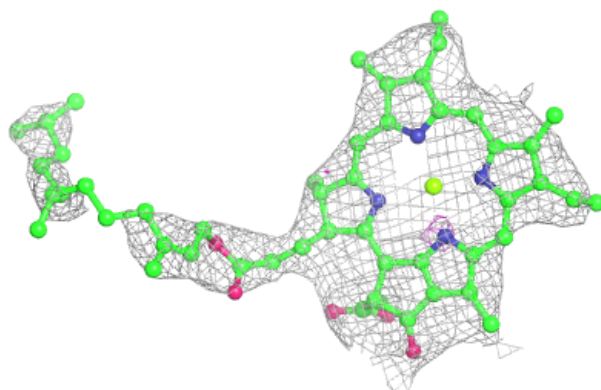
**Electron density around PQN A 5001:**

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

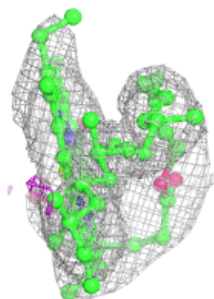
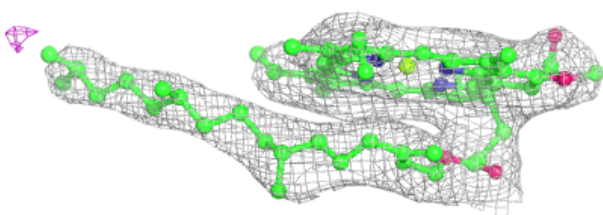
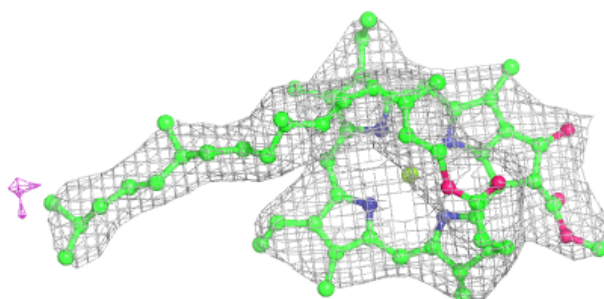


Electron density around CLA A 1125:

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

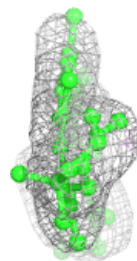
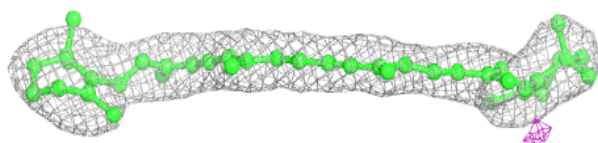
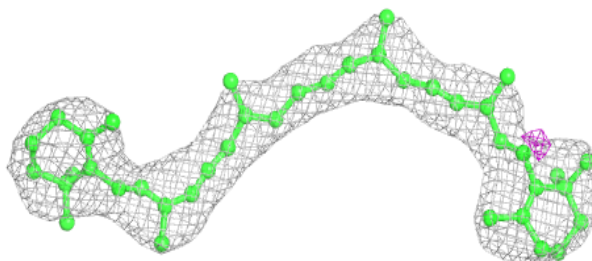
**Electron density around CLA A 1138:**

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



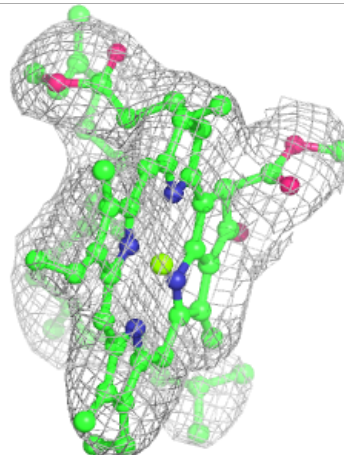
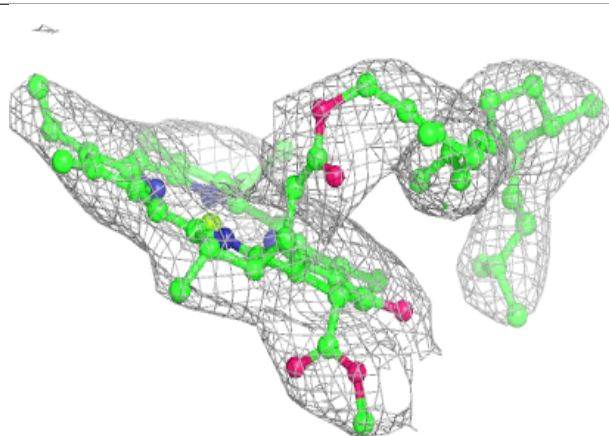
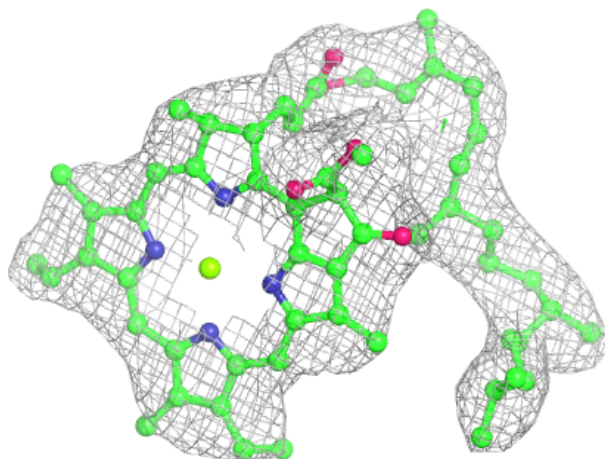
Electron density around BCR A 6011:

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



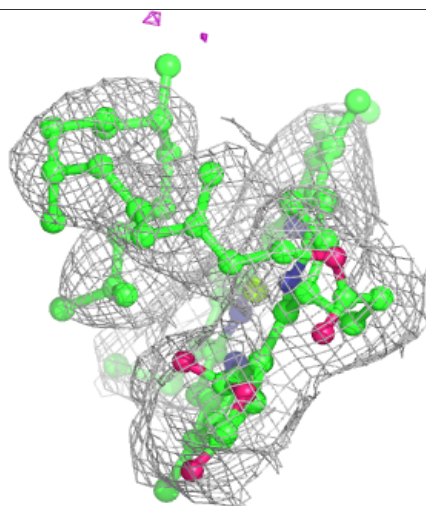
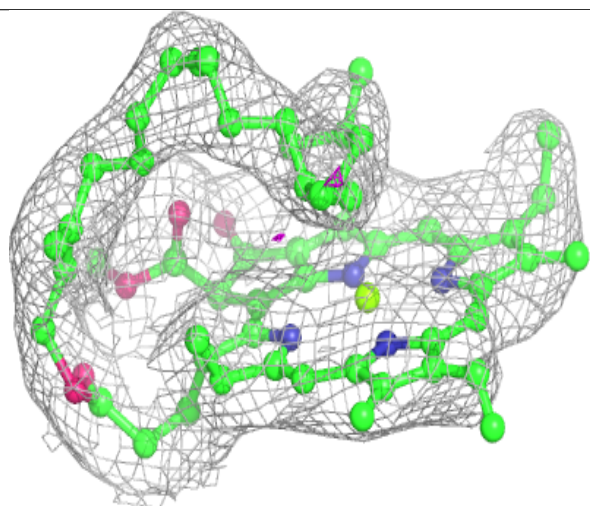
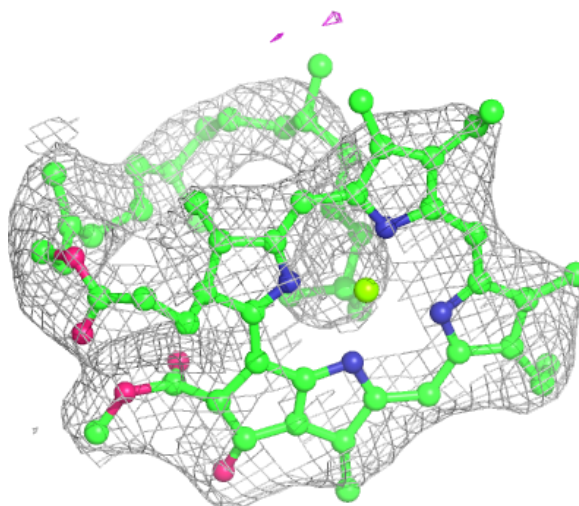
Electron density around CLA B 1229:

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



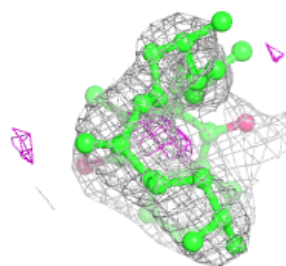
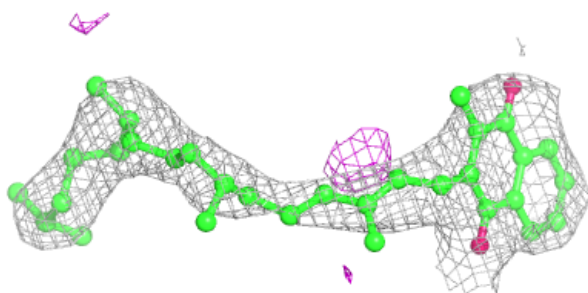
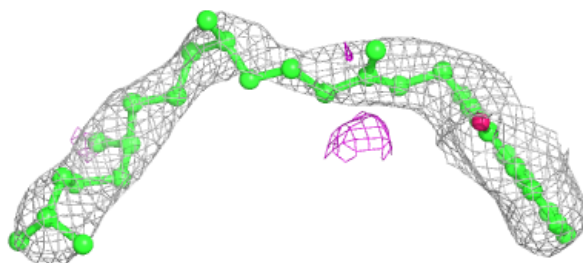
Electron density around CLA B 1203:

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

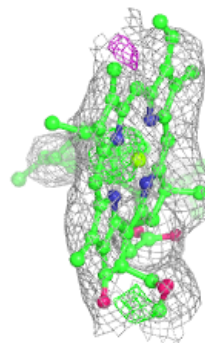
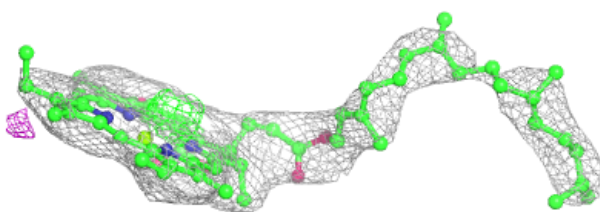
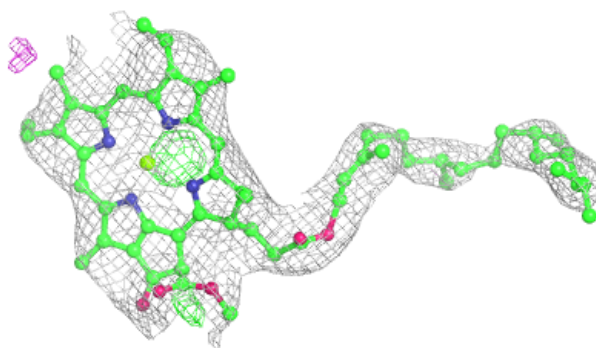


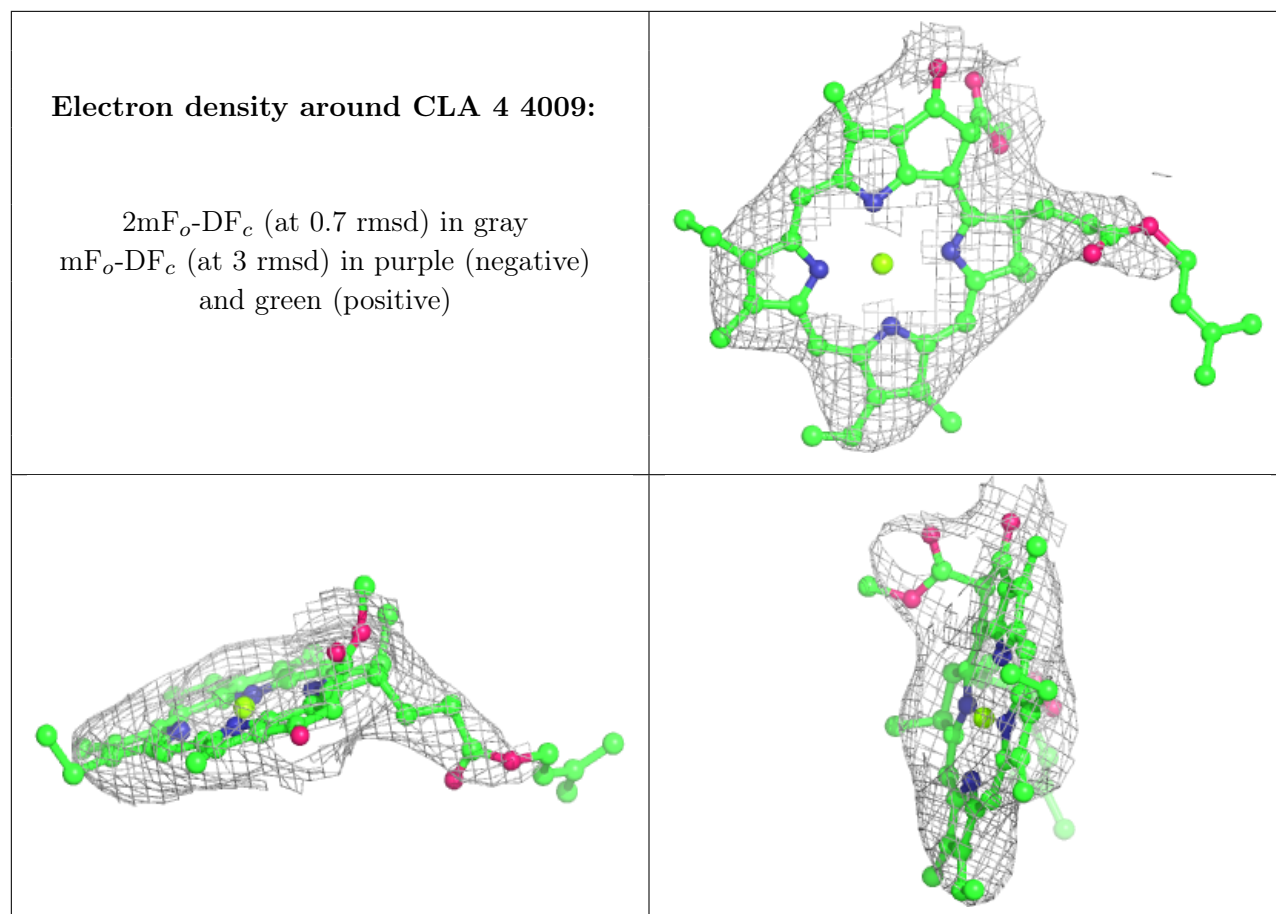
Electron density around PQN B 5002:

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

**Electron density around CLA B 1210:**

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





6.5 Other polymers [i](#)

There are no such residues in this entry.