



wwPDB X-ray Structure Validation Summary Report ⓘ

Sep 13, 2021 – 08:33 PM EDT

PDB ID : 3LW5
Title : Improved model of plant photosystem I
Authors : Nelson, N.; Toporik, H.
Deposited on : 2010-02-23
Resolution : 3.30 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.23.1
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.23.1

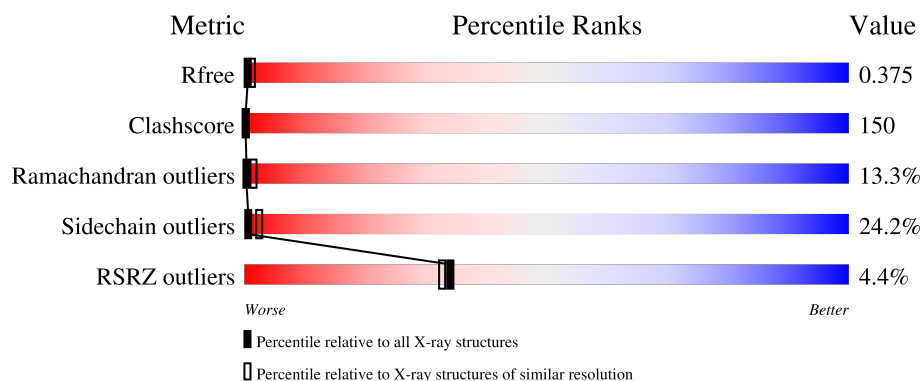
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.30 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1149 (3.34-3.26)
Clashscore	141614	1205 (3.34-3.26)
Ramachandran outliers	138981	1183 (3.34-3.26)
Sidechain outliers	138945	1182 (3.34-3.26)
RSRZ outliers	127900	1115 (3.34-3.26)

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	738	
2	B	733	
3	C	81	
4	D	138	
5	E	64	

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Mol	Chain	Length	Quality of chain
6	F	154	
7	G	95	
8	H	69	
9	I	30	
10	J	42	
11	K	84	
12	L	161	
13	N	85	
14	R	53	
15	1	170	
16	2	176	
17	3	172	
18	4	166	

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
19	CLA	1	1001	X	-	-	-
19	CLA	1	1002	X	-	-	-
19	CLA	1	1003	X	-	-	-
19	CLA	1	1005	X	-	-	-
19	CLA	1	1006	X	-	-	X
19	CLA	1	1007	X	-	-	-
19	CLA	1	1008	X	-	-	-
19	CLA	1	1010	X	-	-	-
19	CLA	1	1011	X	-	-	-
19	CLA	1	1012	X	-	-	-
19	CLA	1	1013	X	-	-	X
19	CLA	1	1014	X	-	-	-
19	CLA	1	1015	X	-	-	-
19	CLA	1	1303	X	-	-	-
19	CLA	1	1310	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
19	CLA	2	1307	X	-	-	X
19	CLA	2	2001	X	-	-	-
19	CLA	2	2002	X	-	-	-
19	CLA	2	2003	X	-	-	-
19	CLA	2	2004	X	-	-	-
19	CLA	2	2005	X	-	-	-
19	CLA	2	2006	X	-	-	-
19	CLA	2	2007	X	-	-	-
19	CLA	2	2008	X	-	-	-
19	CLA	2	2010	X	-	-	-
19	CLA	2	2011	X	-	-	-
19	CLA	2	2012	X	-	-	-
19	CLA	2	2013	X	-	-	-
19	CLA	2	2014	X	-	X	-
19	CLA	2	4009	X	-	-	-
19	CLA	3	1118	X	-	-	-
19	CLA	3	1147	X	-	-	-
19	CLA	3	2009	X	-	X	-
19	CLA	3	3001	X	-	-	-
19	CLA	3	3002	X	-	-	-
19	CLA	3	3003	X	-	-	-
19	CLA	3	3004	X	-	-	-
19	CLA	3	3005	X	-	-	-
19	CLA	3	3006	X	-	-	-
19	CLA	3	3007	X	-	-	-
19	CLA	3	3008	X	-	-	-
19	CLA	3	3010	X	-	-	-
19	CLA	3	3011	X	-	-	-
19	CLA	3	3012	X	-	-	-
19	CLA	3	3013	X	-	-	-
19	CLA	3	3014	X	-	-	X
19	CLA	3	3015	X	-	-	X
19	CLA	3	3016	X	-	-	X
19	CLA	3	3017	X	-	-	-
19	CLA	4	1004	X	-	X	-
19	CLA	4	1009	X	-	-	-
19	CLA	4	1304	X	-	X	-
19	CLA	4	1306	X	-	-	-
19	CLA	4	4001	X	-	-	X
19	CLA	4	4002	X	-	X	-
19	CLA	4	4003	X	-	-	-
19	CLA	4	4004	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
19	CLA	4	4005	X	-	-	-
19	CLA	4	4006	X	-	-	-
19	CLA	4	4007	X	-	-	-
19	CLA	4	4010	X	-	-	-
19	CLA	4	4011	X	-	-	-
19	CLA	4	4012	X	-	-	-
19	CLA	4	4013	X	-	-	-
19	CLA	4	4014	X	-	-	-
19	CLA	4	4015	X	-	-	-
19	CLA	A	1101	X	-	-	-
19	CLA	A	1102	X	-	-	-
19	CLA	A	1103	X	-	-	-
19	CLA	A	1104	X	-	-	-
19	CLA	A	1105	X	-	X	-
19	CLA	A	1106	X	-	X	-
19	CLA	A	1107	X	-	X	-
19	CLA	A	1108	X	-	-	-
19	CLA	A	1109	X	-	-	-
19	CLA	A	1110	X	-	-	-
19	CLA	A	1111	X	-	X	-
19	CLA	A	1112	X	-	X	X
19	CLA	A	1113	X	-	-	-
19	CLA	A	1115	X	-	X	-
19	CLA	A	1116	X	-	-	-
19	CLA	A	1117	X	-	X	-
19	CLA	A	1119	X	-	X	-
19	CLA	A	1120	X	-	-	-
19	CLA	A	1121	X	-	-	-
19	CLA	A	1122	X	-	X	-
19	CLA	A	1123	X	-	X	-
19	CLA	A	1124	X	-	X	-
19	CLA	A	1125	X	-	X	-
19	CLA	A	1126	X	-	X	-
19	CLA	A	1127	X	-	-	-
19	CLA	A	1128	X	-	X	-
19	CLA	A	1129	X	-	-	-
19	CLA	A	1131	X	-	X	-
19	CLA	A	1132	X	-	-	-
19	CLA	A	1133	X	-	X	-
19	CLA	A	1134	X	-	-	-
19	CLA	A	1135	X	-	X	-
19	CLA	A	1136	X	-	X	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
19	CLA	A	1137	X	-	-	-
19	CLA	A	1138	X	-	X	-
19	CLA	A	1139	X	-	X	-
19	CLA	A	1140	X	-	X	-
19	CLA	A	1141	X	-	X	-
19	CLA	A	1149	X	-	-	-
19	CLA	A	1151	X	-	-	-
19	CLA	A	1237	X	-	X	-
19	CLA	A	1309	X	-	-	X
19	CLA	A	9011	X	-	-	-
19	CLA	A	9012	X	-	X	-
19	CLA	A	9013	X	-	X	-
19	CLA	A	9022	X	-	X	-
19	CLA	A	9023	X	-	X	-
19	CLA	B	1201	X	-	-	-
19	CLA	B	1202	X	-	X	-
19	CLA	B	1203	X	-	-	-
19	CLA	B	1205	X	-	X	-
19	CLA	B	1206	X	-	-	-
19	CLA	B	1208	X	-	-	-
19	CLA	B	1209	X	-	-	-
19	CLA	B	1210	X	-	X	-
19	CLA	B	1211	X	-	-	-
19	CLA	B	1212	X	-	-	-
19	CLA	B	1213	X	-	-	-
19	CLA	B	1214	X	-	X	-
19	CLA	B	1215	X	-	-	-
19	CLA	B	1216	X	-	-	-
19	CLA	B	1217	X	-	-	-
19	CLA	B	1218	X	-	-	-
19	CLA	B	1219	X	-	-	-
19	CLA	B	1220	X	-	X	-
19	CLA	B	1221	X	-	X	-
19	CLA	B	1222	X	-	X	-
19	CLA	B	1223	X	-	X	-
19	CLA	B	1224	X	-	-	-
19	CLA	B	1225	X	-	X	-
19	CLA	B	1226	X	-	X	-
19	CLA	B	1227	X	-	-	-
19	CLA	B	1228	X	-	-	-
19	CLA	B	1229	X	-	-	-
19	CLA	B	1230	X	-	X	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
19	CLA	B	1231	X	-	-	-
19	CLA	B	1232	X	-	-	X
19	CLA	B	1233	X	-	-	-
19	CLA	B	1234	X	-	-	-
19	CLA	B	1235	X	-	X	-
19	CLA	B	1236	X	-	X	-
19	CLA	B	1238	X	-	X	-
19	CLA	B	1239	X	-	X	-
19	CLA	B	1301	X	-	-	-
19	CLA	B	9010	X	-	-	-
19	CLA	F	1240	X	-	-	-
19	CLA	F	1302	X	-	-	-
19	CLA	F	1305	X	-	-	-
19	CLA	G	1242	X	-	-	-
19	CLA	H	1145	X	-	X	-
19	CLA	H	1207	X	-	X	-
19	CLA	H	1241	X	-	-	-
19	CLA	H	1505	X	-	-	-
19	CLA	I	1204	X	-	-	-
19	CLA	J	1308	X	-	X	-
19	CLA	J	1311	X	-	-	-
19	CLA	K	1142	X	-	-	-
19	CLA	K	1143	X	-	X	-
19	CLA	K	1146	X	-	-	-
19	CLA	K	3009	X	-	-	-
19	CLA	L	1130	X	-	X	-
19	CLA	L	1148	X	-	X	-
19	CLA	L	1501	X	-	-	-
19	CLA	L	1502	X	-	X	-
19	CLA	L	1503	X	-	-	-
19	CLA	L	1504	X	-	X	X
19	CLA	R	1144	X	-	-	-
19	CLA	R	1150	X	-	-	-
20	PQN	A	5001	X	-	-	-
20	PQN	B	5002	X	-	X	-
21	BCR	1	6023	-	-	-	X
21	BCR	A	6002	-	-	X	-
21	BCR	A	6007	-	-	X	-
21	BCR	A	6008	-	-	X	-
21	BCR	A	6011	-	-	X	-
21	BCR	B	6010	-	-	X	-
21	BCR	B	6017	-	-	X	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
21	BCR	B	6020	-	-	X	-
21	BCR	F	6014	-	-	X	-
21	BCR	F	6016	-	-	X	-
21	BCR	I	6021	-	-	X	-
21	BCR	J	6012	-	-	X	-
21	BCR	L	6019	-	-	X	-
22	LMU	1	7004	-	-	-	X
22	LMU	3	7005	-	-	X	-
22	LMU	4	7034	-	-	X	-
22	LMU	4	7052	-	-	X	-
22	LMU	B	7038	-	-	-	X
22	LMU	D	7050	-	-	X	-
23	SF4	A	8001	-	-	X	-
23	SF4	C	8002	-	-	X	-
23	SF4	C	8003	-	-	X	-

2 Entry composition

There are 24 unique types of molecules in this entry. The entry contains 36370 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	730	Total	C	N	O	S	0	0	0
			5739	3762	974	985	18			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	733	Total	C	N	O	S	0	0	0
			5844	3841	997	993	13			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	81	Total	C	N	O	S	0	0	0
			619	384	108	115	12			

- Molecule 4 is a protein called Putative uncharacterized protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	138	Total	C	N	O	S	0	0	0
			1097	704	191	199	3			

- Molecule 5 is a protein called Putative uncharacterized protein.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
5	E	64	Total	C	N	O	0	0	0
			513	327	90	96			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	F	154	Total	C	N	O	S	0	0	0
			1221	794	207	217	3			

- Molecule 7 is a protein called Putative uncharacterized protein.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
7	G	95	Total	C	N	O	0	0	0
			738	481	120	137			

- Molecule 8 is a protein called Putative uncharacterized protein.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
8	H	69	Total	C	N	O	0	0	0
			517	334	80	103			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	I	30	Total	C	N	O	S	0	0	0
			229	158	34	35	2			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	J	42	Total	C	N	O	S	0	0	0
			334	228	51	54	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	K	84	Total	C	N	O	S	0	0	0
			592	377	102	110	3			

- Molecule 12 is a protein called Putative uncharacterized protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	L	161	Total	C	N	O	S	0	0	0
			1209	797	192	219	1			

- Molecule 13 is a protein called Photosystem I-N subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	N	85	Total	C	N	O	S	0	0	0
			685	436	113	132	4			

- Molecule 14 is a protein called CHAIN R.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
14	R	53	Total	C	N	O	0	0	0
			265	159	53	53			

- Molecule 15 is a protein called AT3g54890.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
15	1	165	Total	C	N	O	S	0	0	0
			1257	816	208	229	4			

- Molecule 16 is a protein called Type II chlorophyll a/b binding protein from photosystem I.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
16	2	176	Total	C	N	O	S	0	0	0
			1367	895	223	245	4			

- Molecule 17 is a protein called Chlorophyll a-b binding protein 3, chloroplastic.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
17	3	156	Total	C	N	O	S	0	0	0
			1197	784	199	209	5			

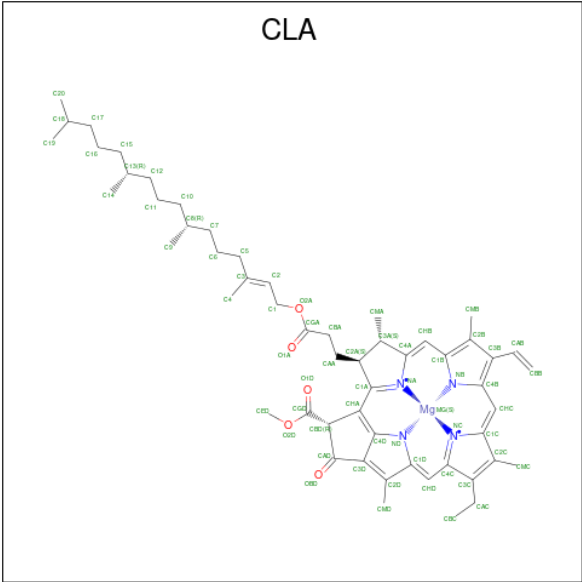
- Molecule 18 is a protein called Chlorophyll a-b binding protein P4, chloroplastic.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
18	4	166	Total	C	N	O	S	0	0	0
			1309	856	216	234	3			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
4	?	-	ALA	SEE REMARK 999	UNP Q9SQL2

- Molecule 19 is CHLOROPHYLL A (three-letter code: CLA) (formula: C₅₅H₇₂MgN₄O₅).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
19	A	1	Total	C	Mg	N	O	0	0
			50	40	1	4	5		
19	A	1	Total	C	Mg	N	O	0	0
			55	45	1	4	5		
19	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
19	A	1	Total	C	Mg	N	O	0	0
			57	47	1	4	5		
19	A	1	Total	C	Mg	N	O	0	0
			46	36	1	4	5		
19	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
19	A	1	Total	C	Mg	N	O	0	0
			55	45	1	4	5		
19	A	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
19	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
19	A	1	Total	C	Mg	N	O	0	0
			54	44	1	4	5		
19	A	1	Total	C	Mg	N	O	0	0
			54	44	1	4	5		
19	A	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
19	A	1	Total	C	Mg	N	O	0	0
			50	40	1	4	5		
19	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
19	A	1	Total	C	Mg	N	O	0	0
			52	42	1	4	5		
19	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
19	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
19	A	1	Total	C	Mg	N	O	0	0
			51	41	1	4	5		
19	A	1	Total	C	Mg	N	O	0	0
			42	34	1	4	3		
19	A	1	Total	C	Mg	N	O	0	0
			55	45	1	4	5		
19	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
19	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
19	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
19	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
19	A	1	Total	C	Mg	N	O	0	0
			55	45	1	4	5		
19	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
19	A	1	Total	C	Mg	N	O	0	0
			50	40	1	4	5		
19	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
19	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
19	A	1	Total	C	Mg	N	O	0	0
			50	40	1	4	5		
19	A	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
19	A	1	Total	C	Mg	N	O	0	0
			51	41	1	4	5		
19	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
19	A	1	Total	C	Mg	N	O	0	0
			47	37	1	4	5		
19	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
19	A	1	Total	C	Mg	N	O	0	0
			51	41	1	4	5		
19	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
19	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
19	A	1	Total	C	Mg	N	O	0	0
			46	36	1	4	5		
19	A	1	Total	C	Mg	N	O	0	0
			50	40	1	4	5		
19	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
19	A	1	Total	C	Mg	N		0	0
			25	20	1	4			
19	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
19	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
19	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
19	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
19	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
19	B	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
19	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
19	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
19	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
19	B	1	Total	C	Mg	N	O	0	0
			54	44	1	4	5		
19	B	1	Total	C	Mg	N	O	0	0
			55	45	1	4	5		
19	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
19	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
19	B	1	Total	C	Mg	N	O	0	0
			60	50	1	4	5		
19	B	1	Total	C	Mg	N	O	0	0
			46	36	1	4	5		
19	B	1	Total	C	Mg	N	O	0	0
			59	49	1	4	5		
19	B	1	Total	C	Mg	N	O	0	0
			60	50	1	4	5		
19	B	1	Total	C	Mg	N	O	0	0
			61	51	1	4	5		
19	B	1	Total	C	Mg	N	O	0	0
			50	40	1	4	5		
19	B	1	Total	C	Mg	N	O	0	0
			46	36	1	4	5		
19	B	1	Total	C	Mg	N	O	0	0
			55	45	1	4	5		
19	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
19	B	1	Total	C	Mg	N	O	0	0
			54	44	1	4	5		
19	B	1	Total	C	Mg	N	O	0	0
			58	48	1	4	5		
19	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
19	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
19	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
19	B	1	Total	C	Mg	N	O	0	0
			50	40	1	4	5		
19	B	1	Total	C	Mg	N	O	0	0
			50	40	1	4	5		
19	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
19	B	1	Total	C	Mg	N	O	0	0
			50	40	1	4	5		
19	B	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
19	B	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
19	B	1	Total	C	Mg	N	O	0	0
			51	41	1	4	5		
19	B	1	Total	C	Mg	N	O	0	0
			60	50	1	4	5		
19	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
19	B	1	Total	C	Mg	N	O	0	0
			47	37	1	4	5		
19	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
19	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
19	B	1	Total	C	Mg	N	O	0	0
			36	30	1	4	1		
19	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
19	F	1	Total	C	Mg	N	O	0	0
			36	30	1	4	1		
19	F	1	Total	C	Mg	N	O	0	0
			41	33	1	4	3		
19	F	1	Total	C	Mg	N	O	0	0
			53	43	1	4	5		
19	G	1	Total	C	Mg	N	O	0	0
			51	41	1	4	5		
19	H	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
19	H	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
19	H	1	Total	C	Mg	N	O	0	0
			55	45	1	4	5		
19	H	1	Total	C	Mg	N	O	0	0
			55	45	1	4	5		
19	I	1	Total	C	Mg	N	O	0	0
			60	50	1	4	5		
19	J	1	Total	C	Mg	N	O	0	0
			55	45	1	4	5		
19	J	1	Total	C	Mg	N	O	0	0
			61	51	1	4	5		
19	K	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
19	K	1	Total	C	Mg	N	O	0	0
			50	40	1	4	5		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
19	K	1	Total	C	Mg	N	O	0	0
			50	40	1	4	5		
19	K	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
19	L	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
19	L	1	Total	C	Mg	N	O	0	0
			55	45	1	4	5		
19	L	1	Total	C	Mg	N	O	0	0
			50	40	1	4	5		
19	L	1	Total	C	Mg	N	O	0	0
			47	37	1	4	5		
19	L	1	Total	C	Mg	N	O	0	0
			50	40	1	4	5		
19	L	1	Total	C	Mg	N	O	0	0
			55	45	1	4	5		
19	R	1	Total	C	Mg	N	O	0	0
			57	47	1	4	5		
19	R	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
19	1	1	Total	C	Mg	N	O	0	0
			46	36	1	4	5		
19	1	1	Total	C	Mg	N	O	0	0
			47	37	1	4	5		
19	1	1	Total	C	Mg	N	O	0	0
			47	37	1	4	5		
19	1	1	Total	C	Mg	N	O	0	0
			46	36	1	4	5		
19	1	1	Total	C	Mg	N	O	0	0
			36	30	1	4	1		
19	1	1	Total	C	Mg	N	O	0	0
			61	51	1	4	5		
19	1	1	Total	C	Mg	N	O	0	0
			51	41	1	4	5		
19	1	1	Total	C	Mg	N	O	0	0
			46	36	1	4	5		
19	1	1	Total	C	Mg	N	O	0	0
			36	30	1	4	1		
19	1	1	Total	C	Mg	N	O	0	0
			36	30	1	4	1		
19	1	1	Total	C	Mg	N	O	0	0
			51	41	1	4	5		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
19	1	1	Total	C	Mg	N	O	0	0
			61	51	1	4	5		
19	1	1	Total	C	Mg	N		0	0
			25	20	1	4			
19	1	1	Total	C	Mg	N	O	0	0
			51	41	1	4	5		
19	1	1	Total	C	Mg	N		0	0
			25	20	1	4			
19	2	1	Total	C	Mg	N		0	0
			25	20	1	4			
19	2	1	Total	C	Mg	N	O	0	0
			51	41	1	4	5		
19	2	1	Total	C	Mg	N	O	0	0
			56	46	1	4	5		
19	2	1	Total	C	Mg	N		0	0
			25	20	1	4			
19	2	1	Total	C	Mg	N	O	0	0
			50	40	1	4	5		
19	2	1	Total	C	Mg	N		0	0
			25	20	1	4			
19	2	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
19	2	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
19	2	1	Total	C	Mg	N		0	0
			25	20	1	4			
19	2	1	Total	C	Mg	N		0	0
			25	20	1	4			
19	2	1	Total	C	Mg	N	O	0	0
			50	40	1	4	5		
19	2	1	Total	C	Mg	N	O	0	0
			50	40	1	4	5		
19	2	1	Total	C	Mg	N	O	0	0
			61	51	1	4	5		
19	2	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
19	3	1	Total	C	Mg	N	O	0	0
			36	30	1	4	1		
19	3	1	Total	C	Mg	N	O	0	0
			46	36	1	4	5		

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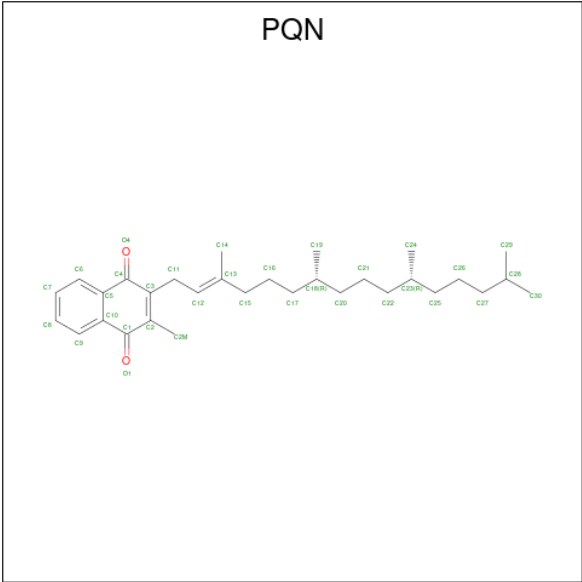
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
19	3	1	Total	C	Mg	N	O	0	0
			56	46	1	4	5		
19	3	1	Total	C	Mg	N		0	0
			25	20	1	4			
19	3	1	Total	C	Mg	N		0	0
			25	20	1	4			
19	3	1	Total	C	Mg	N	O	0	0
			36	30	1	4	1		
19	3	1	Total	C	Mg	N		0	0
			25	20	1	4			
19	3	1	Total	C	Mg	N		0	0
			25	20	1	4			
19	3	1	Total	C	Mg	N		0	0
			25	20	1	4			
19	3	1	Total	C	Mg	N	O	0	0
			42	34	1	4	3		
19	3	1	Total	C	Mg	N	O	0	0
			50	40	1	4	5		
19	3	1	Total	C	Mg	N		0	0
			25	20	1	4			
19	3	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
19	3	1	Total	C	Mg	N		0	0
			25	20	1	4			
19	3	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
19	3	1	Total	C	Mg	N		0	0
			25	20	1	4			
19	3	1	Total	C	Mg	N		0	0
			25	20	1	4			
19	3	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
19	3	1	Total	C	Mg	N	O	0	0
			50	40	1	4	5		
19	4	1	Total	C	Mg	N	O	0	0
			55	45	1	4	5		
19	4	1	Total	C	Mg	N	O	0	0
			36	30	1	4	1		
19	4	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
19	4	1	Total	C	Mg	N	O	0	0
			55	45	1	4	5		

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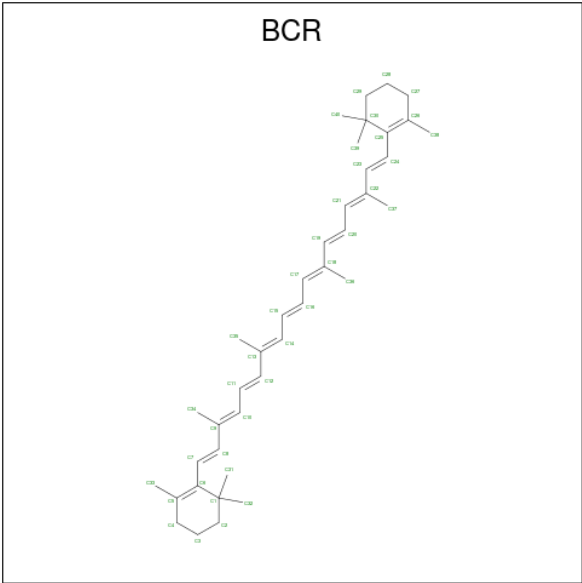
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
19	4	1	Total	C	Mg	N	O	0	0
			50	40	1	4	5		
19	4	1	Total	C	Mg	N	O	0	0
			52	42	1	4	5		
19	4	1	Total	C	Mg	N	O	0	0
			55	45	1	4	5		
19	4	1	Total	C	Mg	N		0	0
			25	20	1	4			
19	4	1	Total	C	Mg	N		0	0
			25	20	1	4			
19	4	1	Total	C	Mg	N	O	0	0
			55	45	1	4	5		
19	4	1	Total	C	Mg	N	O	0	0
			52	42	1	4	5		
19	4	1	Total	C	Mg	N		0	0
			25	20	1	4			
19	4	1	Total	C	Mg	N		0	0
			25	20	1	4			
19	4	1	Total	C	Mg	N	O	0	0
			36	30	1	4	1		
19	4	1	Total	C	Mg	N		0	0
			25	20	1	4			
19	4	1	Total	C	Mg	N	O	0	0
			47	37	1	4	5		
19	4	1	Total	C	Mg	N	O	0	0
			46	36	1	4	5		

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



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

- Molecule 21 is BETA-CAROTENE (three-letter code: BCR) (formula: C₄₀H₅₆).



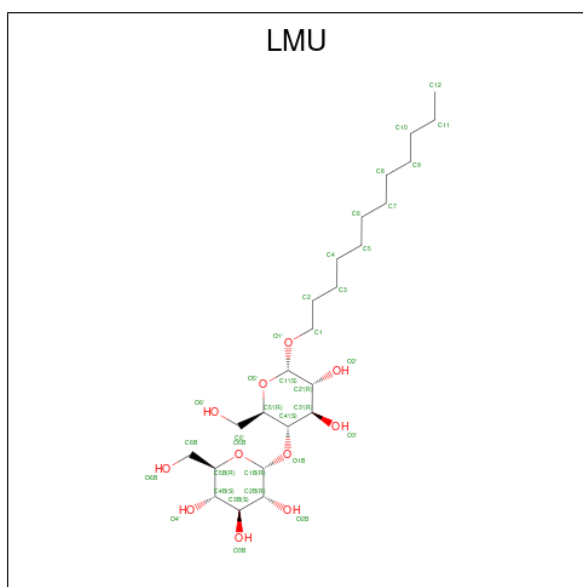
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
21	A	1	Total	C		0
			40	40		
21	A	1	Total	C		0
			40	40		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
21	A	1	Total C 40 40	0	0
21	A	1	Total C 40 40	0	0
21	A	1	Total C 40 40	0	0
21	B	1	Total C 40 40	0	0
21	B	1	Total C 40 40	0	0
21	B	1	Total C 40 40	0	0
21	B	1	Total C 40 40	0	0
21	B	1	Total C 40 40	0	0
21	B	1	Total C 40 40	0	0
21	F	1	Total C 40 40	0	0
21	F	1	Total C 40 40	0	0
21	I	1	Total C 40 40	0	0
21	I	1	Total C 40 40	0	0
21	J	1	Total C 40 40	0	0
21	L	1	Total C 40 40	0	0
21	1	1	Total C 40 40	0	0
21	3	1	Total C 40 40	0	0

- Molecule 22 is DODECYL-ALPHA-D-MALTOSIDE (three-letter code: LMU) (formula: $C_{24}H_{46}O_{11}$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
22	A	1	Total 35	C 24	O 11	0	0
22	A	1	Total 35	C 24	O 11	0	0
22	A	1	Total 35	C 24	O 11	0	0
22	A	1	Total 35	C 24	O 11	0	0
22	A	1	Total 35	C 24	O 11	0	0
22	A	1	Total 35	C 24	O 11	0	0
22	B	1	Total 25	C 14	O 11	0	0
22	B	1	Total 35	C 24	O 11	0	0
22	B	1	Total 35	C 24	O 11	0	0
22	C	1	Total 35	C 24	O 11	0	0
22	D	1	Total 35	C 24	O 11	0	0
22	E	1	Total 35	C 24	O 11	0	0
22	E	1	Total 35	C 24	O 11	0	0
22	F	1	Total 34	C 23	O 11	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
22	G	1	Total	C	O	0	0
			35	24	11		
22	G	1	Total	C	O	0	0
			35	24	11		
22	G	1	Total	C	O	0	0
			35	24	11		
22	H	1	Total	C	O	0	0
			35	24	11		
22	H	1	Total	C	O	0	0
			35	24	11		
22	H	1	Total	C	O	0	0
			35	24	11		
22	H	1	Total	C	O	0	0
			35	24	11		
22	H	1	Total	C	O	0	0
			35	24	11		
22	H	1	Total	C	O	0	0
			35	24	11		
22	K	1	Total	C	O	0	0
			35	24	11		
22	K	1	Total	C	O	0	0
			35	24	11		
22	K	1	Total	C	O	0	0
			35	24	11		
22	K	1	Total	C	O	0	0
			35	24	11		
22	L	1	Total	C	O	0	0
			35	24	11		
22	N	1	Total	C	O	0	0
			35	24	11		
22	R	1	Total	C	O	0	0
			35	24	11		
22	R	1	Total	C	O	0	0
			35	24	11		
22	R	1	Total	C	O	0	0
			35	24	11		
22	R	1	Total	C	O	0	0
			35	24	11		

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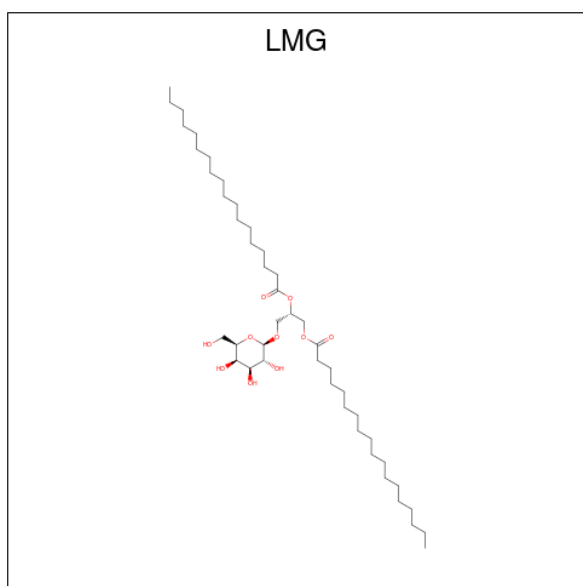
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
22	R	1	Total	C	O	0	0
			35	24	11		
22	R	1	Total	C	O	0	0
			35	24	11		
22	1	1	Total	C	O	0	0
			35	24	11		
22	1	1	Total	C	O	0	0
			35	24	11		
22	2	1	Total	C	O	0	0
			35	24	11		
22	2	1	Total	C	O	0	0
			35	24	11		
22	2	1	Total	C	O	0	0
			35	24	11		
22	2	1	Total	C	O	0	0
			35	24	11		
22	3	1	Total	C	O	0	0
			35	24	11		
22	3	1	Total	C	O	0	0
			35	24	11		
22	4	1	Total	C	O	0	0
			35	24	11		
22	4	1	Total	C	O	0	0
			34	23	11		
22	4	1	Total	C	O	0	0
			35	24	11		
22	4	1	Total	C	O	0	0
			35	24	11		
22	4	1	Total	C	O	0	0
			35	24	11		
22	4	1	Total	C	O	0	0
			35	24	11		
22	4	1	Total	C	O	0	0
			34	23	11		

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



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

- Molecule 24 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (three-letter code: LMG) (formula: C₄₅H₈₆O₁₀).

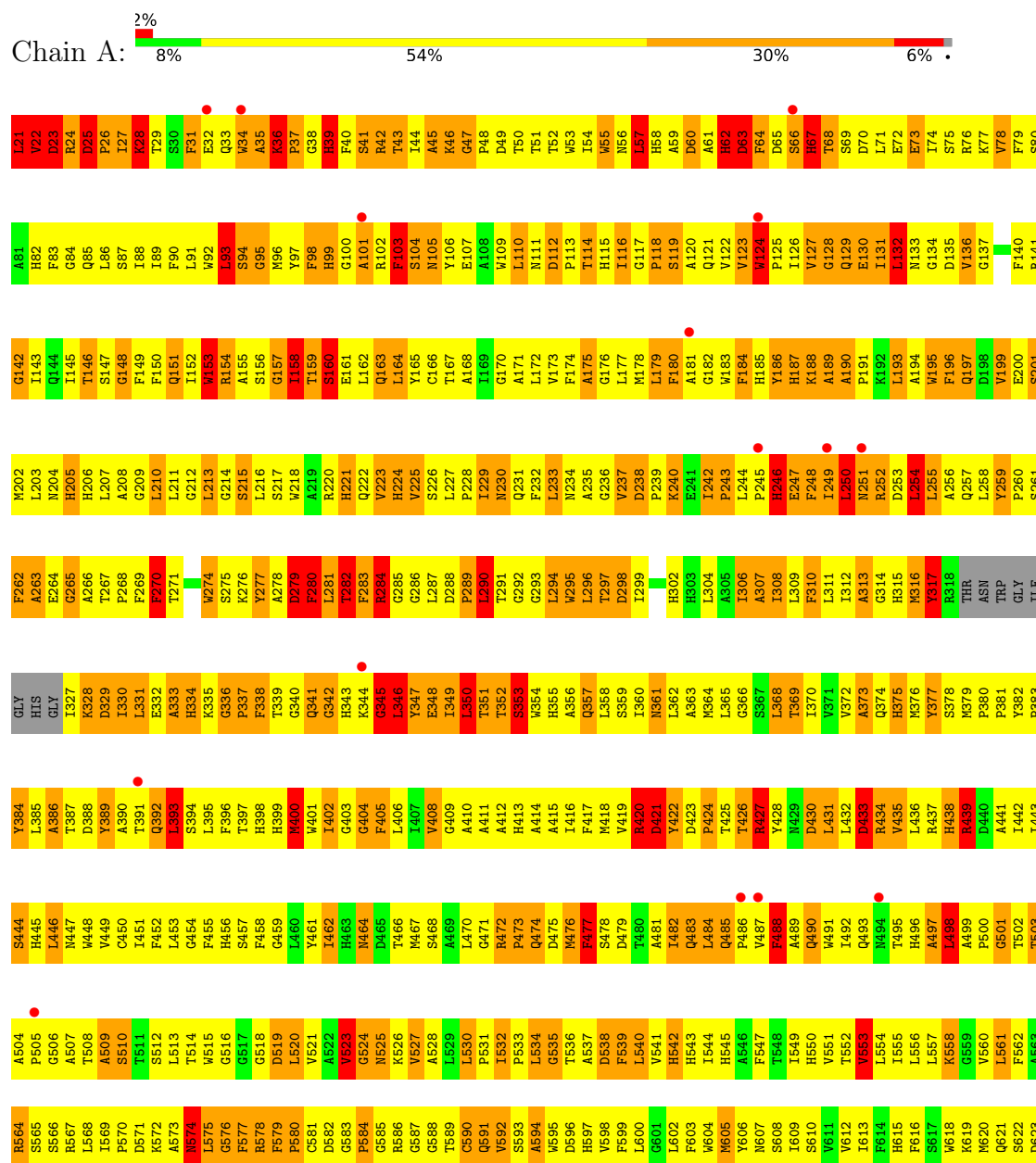


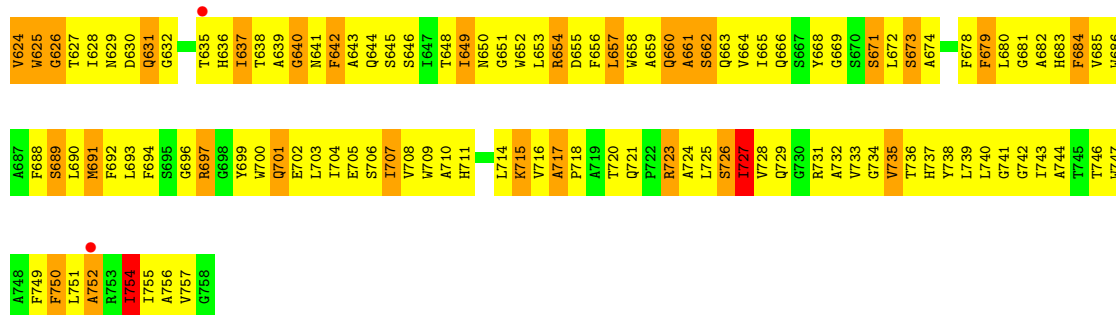
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
24	B	1	Total	C	O	0	0
			49	39	10		

3 Residue-property plots

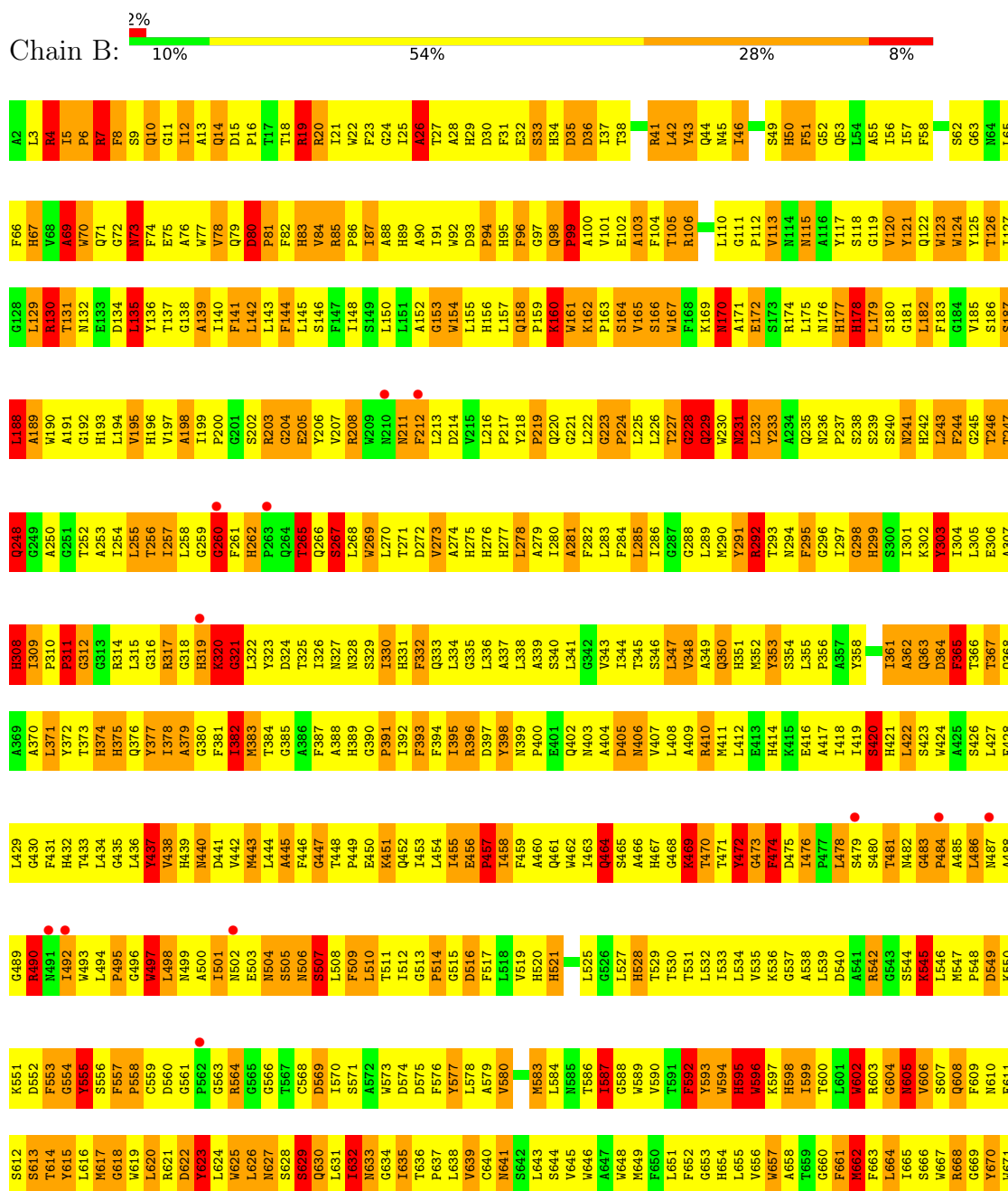
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

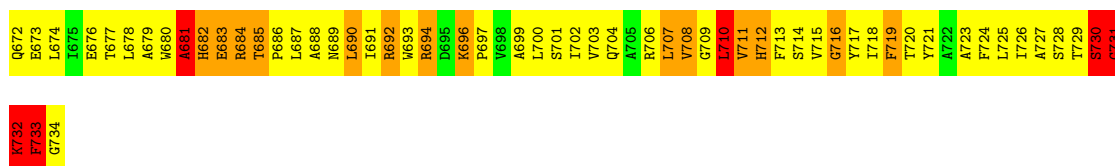
- Molecule 1: Photosystem I P700 chlorophyll a apoprotein A1



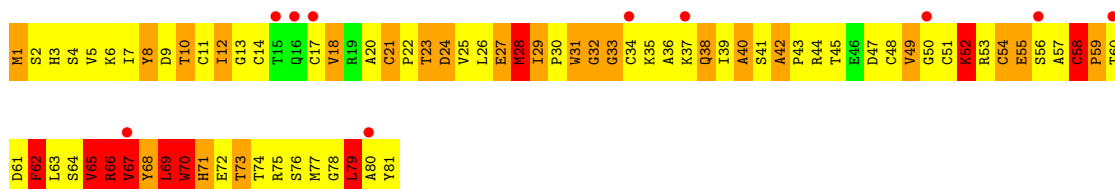


● Molecule 2: Photosystem I P700 chlorophyll a apoprotein A2

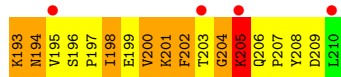
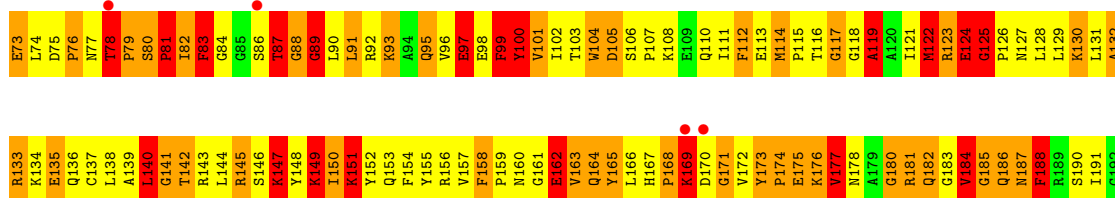




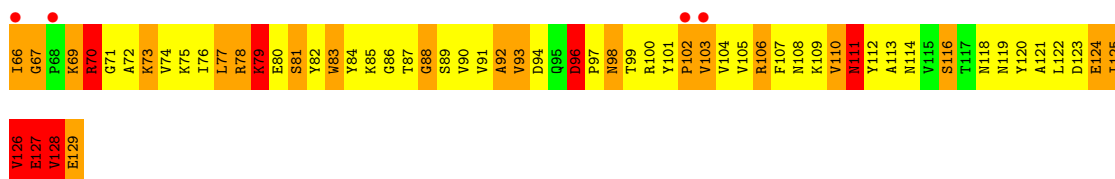
• Molecule 3: Photosystem I iron-sulfur center



• Molecule 4: Putative uncharacterized protein

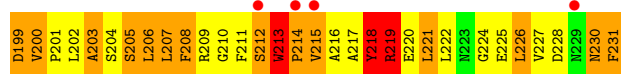


• Molecule 5: Putative uncharacterized protein

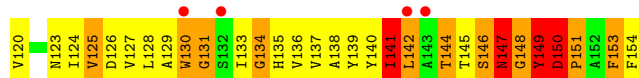
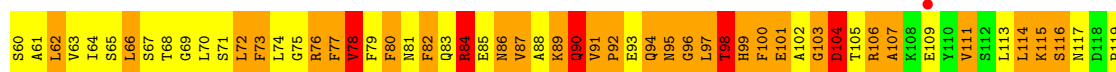


• Molecule 6: Photosystem I reaction center subunit III, chloroplastic





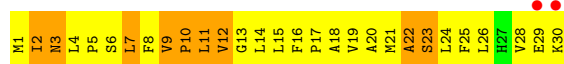
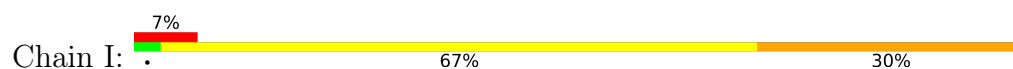
• Molecule 7: Putative uncharacterized protein



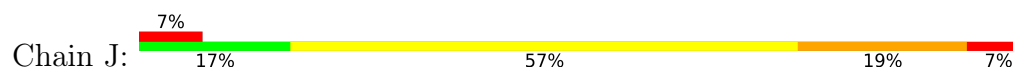
• Molecule 8: Putative uncharacterized protein



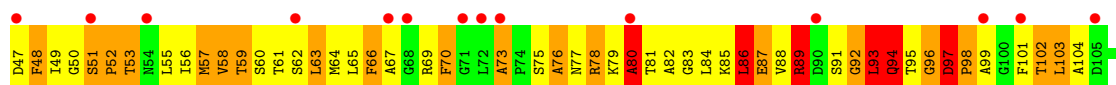
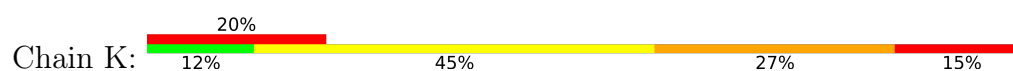
• Molecule 9: Photosystem I reaction center subunit VIII



• Molecule 10: Photosystem I reaction center subunit IX



• Molecule 11: Photosystem I reaction center subunit X psaK





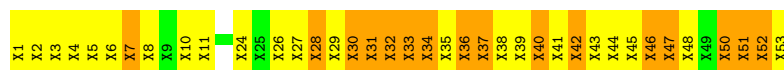
• Molecule 12: Putative uncharacterized protein



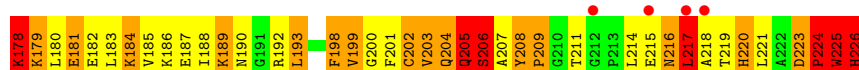
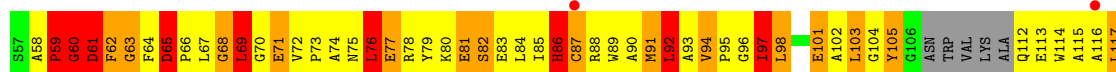
• Molecule 13: Photosystem I-N subunit



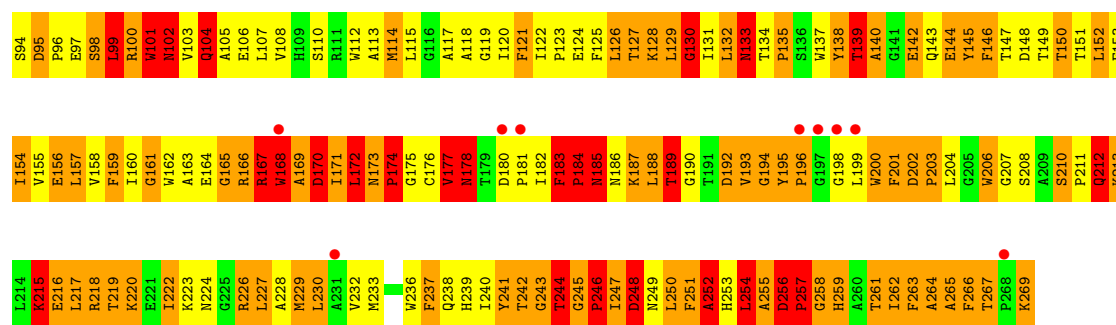
• Molecule 14: CHAIN R



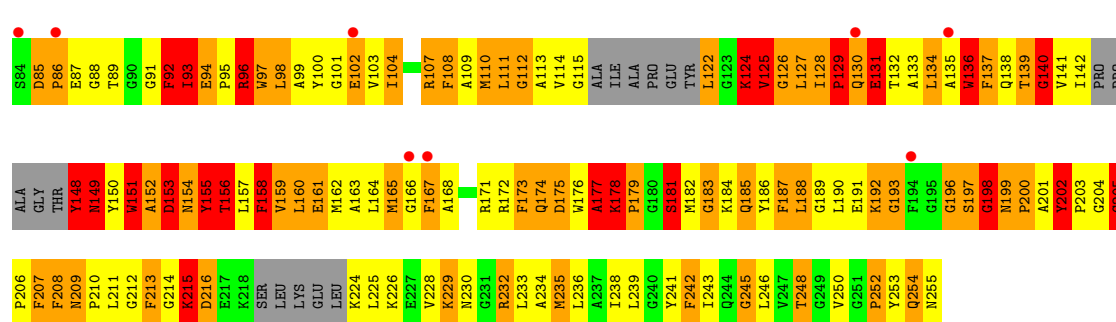
• Molecule 15: AT3g54890



• Molecule 16: Type II chlorophyll a/b binding protein from photosystem I



• Molecule 17: Chlorophyll a-b binding protein 3, chloroplastic



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	120.66Å 189.09Å 129.39Å 90.00° 91.24° 90.00°	Depositor
Resolution (Å)	30.00 – 3.30 49.14 – 3.21	Depositor EDS
% Data completeness (in resolution range)	99.5 (30.00-3.30) 99.0 (49.14-3.21)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.56 (at 3.19Å)	Xtriage
Refinement program	REFMAC 5.5.0072	Depositor
R, R_{free}	0.349 , 0.383 0.353 , 0.375	Depositor DCC
R_{free} test set	4705 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	77.2	Xtriage
Anisotropy	0.691	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.16 , 93.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.024 for h,-k,-l	Xtriage
F_o, F_c correlation	0.79	EDS
Total number of atoms	36370	wwPDB-VP
Average B, all atoms (Å ²)	24.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.09% 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: PQN, SF4, CLA, BCR, LMG, LMU

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	0.88	5/5932 (0.1%)	1.20	49/8096 (0.6%)
2	B	0.96	8/6054 (0.1%)	1.16	35/8273 (0.4%)
3	C	1.10	1/632 (0.2%)	1.35	5/856 (0.6%)
4	D	1.13	2/1124 (0.2%)	1.49	15/1516 (1.0%)
5	E	1.26	2/523 (0.4%)	1.38	7/710 (1.0%)
6	F	0.98	0/1250	1.29	10/1687 (0.6%)
7	G	1.00	3/757 (0.4%)	1.41	5/1031 (0.5%)
8	H	1.12	3/530 (0.6%)	1.58	11/722 (1.5%)
9	I	0.82	0/235	0.88	0/320
10	J	0.83	0/344	0.99	0/469
11	K	1.14	4/599 (0.7%)	1.50	8/811 (1.0%)
12	L	1.07	3/1244 (0.2%)	1.32	10/1703 (0.6%)
13	N	1.11	3/699 (0.4%)	1.51	10/936 (1.1%)
15	1	1.50	20/1295 (1.5%)	1.51	21/1763 (1.2%)
16	2	1.16	9/1413 (0.6%)	1.51	30/1934 (1.6%)
17	3	1.09	9/1231 (0.7%)	1.37	18/1658 (1.1%)
18	4	1.13	6/1349 (0.4%)	1.56	13/1839 (0.7%)
All	All	1.04	78/25211 (0.3%)	1.32	247/34324 (0.7%)

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
1	A	0	81
2	B	0	83
3	C	0	14
4	D	0	37
5	E	0	10
6	F	0	27

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Mol	Chain	#Chirality outliers	#Planarity outliers
7	G	1	24
8	H	2	22
11	K	0	21
12	L	0	23
13	N	0	40
14	R	0	17
15	1	0	37
16	2	0	45
17	3	0	35
18	4	0	28
All	All	3	544

The worst 5 of 78 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	1	119	GLY	N-CA	13.83	1.66	1.46
15	1	172	GLY	C-O	12.76	1.44	1.23
15	1	63	GLY	C-O	11.60	1.42	1.23
15	1	225	TRP	C-N	10.48	1.58	1.34
2	B	94	PRO	N-CD	-10.34	1.33	1.47

The worst 5 of 247 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	4	84	ASP	C-N-CD	-31.95	50.30	120.60
16	2	184	PRO	O-C-N	11.36	140.88	122.70
16	2	258	GLY	N-CA-C	10.50	139.35	113.10
4	D	123	ARG	NE-CZ-NH2	-10.44	115.08	120.30
18	4	186	GLY	N-CA-C	10.00	138.11	113.10

All (3) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
7	G	77	PHE	CA
8	H	60	ASN	CA
8	H	68	TYR	CA

5 of 544 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	21	LEU	Peptide
1	A	22	VAL	Peptide

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Mol	Chain	Res	Type	Group
1	A	23	ASP	Peptide
1	A	25	ASP	Peptide
1	A	26	PRO	Peptide

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5739	0	5574	1922	6
2	B	5844	0	5648	1926	14
3	C	619	0	605	325	0
4	D	1097	0	1101	436	4
5	E	513	0	514	252	0
6	F	1221	0	1247	373	28
7	G	738	0	709	337	6
8	H	517	0	503	208	2
9	I	229	0	252	53	1
10	J	334	0	344	84	0
11	K	592	0	618	270	5
12	L	1209	0	1220	435	64
13	N	685	0	667	344	0
14	R	265	0	67	79	0
15	1	1257	0	1220	592	37
16	2	1367	0	1312	644	35
17	3	1197	0	1137	516	2
18	4	1309	0	1264	532	45
19	1	665	0	453	123	1
19	2	663	0	494	142	0
19	3	736	0	453	158	0
19	4	729	0	496	154	0
19	A	2676	0	2544	1037	0
19	B	2177	0	2072	680	0
19	F	130	0	85	21	0
19	G	51	0	40	9	0
19	H	240	0	237	61	0
19	I	60	0	58	7	0
19	J	116	0	107	51	0
19	K	210	0	179	40	8

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
19	L	322	0	275	118	0
19	R	122	0	123	13	0
20	A	33	0	45	9	0
20	B	33	0	46	22	0
21	1	40	0	54	6	0
21	3	40	0	54	6	0
21	A	200	0	271	162	0
21	B	240	0	323	116	0
21	F	80	0	107	61	0
21	I	80	0	111	46	0
21	J	40	0	52	32	0
21	L	40	0	53	34	0
22	1	70	0	92	10	0
22	2	140	0	184	14	0
22	3	70	0	90	38	0
22	4	278	0	357	69	0
22	A	210	0	275	27	0
22	B	95	0	115	11	0
22	C	35	0	46	0	0
22	D	35	0	45	21	0
22	E	70	0	92	24	0
22	F	34	0	41	12	0
22	G	105	0	138	14	0
22	H	245	0	322	40	0
22	K	140	0	184	37	2
22	L	35	0	46	11	0
22	N	35	0	46	9	0
22	R	245	0	322	34	0
23	A	8	0	0	2	0
23	C	16	0	0	9	0
24	B	49	0	71	19	0
All	All	36370	0	35200	10756	130

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 150.

The worst 5 of 10756 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)
22:4:7034:LMU:C9	22:4:7052:LMU:H1'	1.24	1.64
2:B:459:PHE:CE2	19:B:1235:CLA:C2D	1.76	1.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:A:1125:CLA:HBB2	19:A:1133:CLA:CMA	1.18	1.60
1:A:244:LEU:CB	1:A:247:GLU:HG3	1.25	1.60
16:2:130:GLY:CA	16:2:131:ILE:HG13	1.29	1.60

The worst 5 of 130 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)
15:1:173:TYR:OH	16:2:132:LEU:C[2_646]	0.71	1.49
6:F:130:PHE:CG	12:L:170:LYS:NZ[2_556]	0.72	1.48
2:B:205:GLU:OE2	11:K:69:ARG:NH1[1_554]	0.79	1.41
12:L:123:THR:O	18:4:180:GLY:CA[1_455]	0.88	1.32
15:1:171:LEU:N	16:2:132:LEU:N[2_646]	0.98	1.22

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	726/738 (98%)	483 (66%)	139 (19%)	104 (14%)	0	1
2	B	731/733 (100%)	527 (72%)	111 (15%)	93 (13%)	0	1
3	C	79/81 (98%)	42 (53%)	18 (23%)	19 (24%)	0	0
4	D	136/138 (99%)	94 (69%)	24 (18%)	18 (13%)	0	1
5	E	62/64 (97%)	44 (71%)	11 (18%)	7 (11%)	0	2
6	F	152/154 (99%)	105 (69%)	27 (18%)	20 (13%)	0	1
7	G	93/95 (98%)	60 (64%)	22 (24%)	11 (12%)	0	2
8	H	67/69 (97%)	49 (73%)	9 (13%)	9 (13%)	0	1
9	I	28/30 (93%)	11 (39%)	9 (32%)	8 (29%)	0	0
10	J	40/42 (95%)	19 (48%)	11 (28%)	10 (25%)	0	0

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
11	K	82/84 (98%)	66 (80%)	9 (11%)	7 (8%)	1	5
12	L	159/161 (99%)	110 (69%)	23 (14%)	26 (16%)	0	1
13	N	83/85 (98%)	50 (60%)	19 (23%)	14 (17%)	0	1
15	1	161/170 (95%)	119 (74%)	28 (17%)	14 (9%)	1	5
16	2	174/176 (99%)	129 (74%)	26 (15%)	19 (11%)	0	2
17	3	148/172 (86%)	111 (75%)	20 (14%)	17 (12%)	0	2
18	4	164/166 (99%)	129 (79%)	21 (13%)	14 (8%)	1	5
All	All	3085/3158 (98%)	2148 (70%)	527 (17%)	410 (13%)	0	1

5 of 410 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	28	LYS
1	A	41	SER
1	A	98	PHE
1	A	99	HIS
1	A	158	ILE

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	590/599 (98%)	475 (80%)	115 (20%)	1	5
2	B	597/599 (100%)	468 (78%)	129 (22%)	1	4
3	C	70/70 (100%)	60 (86%)	10 (14%)	3	15
4	D	117/117 (100%)	83 (71%)	34 (29%)	0	1
5	E	56/56 (100%)	42 (75%)	14 (25%)	0	2
6	F	127/127 (100%)	91 (72%)	36 (28%)	0	1
7	G	78/79 (99%)	60 (77%)	18 (23%)	1	3
8	H	55/55 (100%)	42 (76%)	13 (24%)	1	3
9	I	26/26 (100%)	23 (88%)	3 (12%)	5	22

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
10	J	35/36 (97%)	26 (74%)	9 (26%)	0	2
11	K	62/62 (100%)	45 (73%)	17 (27%)	0	1
12	L	127/127 (100%)	105 (83%)	22 (17%)	2	8
13	N	74/74 (100%)	49 (66%)	25 (34%)	0	1
15	1	126/134 (94%)	76 (60%)	50 (40%)	0	0
16	2	139/142 (98%)	91 (66%)	48 (34%)	0	1
17	3	113/129 (88%)	74 (66%)	39 (34%)	0	1
18	4	136/140 (97%)	107 (79%)	29 (21%)	1	4
All	All	2528/2572 (98%)	1917 (76%)	611 (24%)	0	2

5 of 611 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
15	1	133	THR
17	3	207	PHE
15	1	168	PHE
15	1	131	TRP
16	2	192	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 85 such sidechains are listed below:

Mol	Chain	Res	Type
5	E	111	ASN
15	1	190	ASN
6	F	193	GLN
12	L	122	ASN
16	2	133	ASN

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 [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

252 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
22	LMU	H	7002	-	36,36,36	0.61	0	47,47,47	1.50	7 (14%)
22	LMU	E	7048	-	36,36,36	0.83	1 (2%)	47,47,47	2.04	10 (21%)
19	CLA	B	1201	-	33,53,73	2.29	9 (27%)	27,89,113	4.10	10 (37%)
19	CLA	B	1230	-	41,58,73	2.15	11 (26%)	37,95,113	4.12	14 (37%)
22	LMU	H	7030	-	36,36,36	0.75	2 (5%)	47,47,47	1.19	4 (8%)
19	CLA	A	1110	-	45,62,73	2.02	9 (20%)	41,99,113	3.26	12 (29%)
19	CLA	2	2004	-	41,58,73	2.08	9 (21%)	37,95,113	3.93	14 (37%)
19	CLA	A	1125	-	56,73,73	1.80	9 (16%)	55,113,113	3.07	11 (20%)
19	CLA	4	4010	-	18,32,73	1.77	6 (33%)	22,54,113	3.98	13 (59%)
21	BCR	A	6007	-	41,41,41	1.55	4 (9%)	56,56,56	3.81	31 (55%)
19	CLA	A	1120	-	42,59,73	2.14	10 (23%)	38,96,113	3.76	15 (39%)
21	BCR	I	6018	-	41,41,41	1.47	4 (9%)	56,56,56	4.70	32 (57%)
22	LMU	B	7038	-	36,36,36	0.74	0	47,47,47	1.68	10 (21%)
19	CLA	B	1235	-	56,73,73	1.73	10 (17%)	55,113,113	2.69	11 (20%)
22	LMU	E	7037	-	36,36,36	0.72	1 (2%)	47,47,47	1.75	11 (23%)
19	CLA	3	3006	-	18,32,73	1.75	4 (22%)	22,54,113	4.07	14 (63%)
22	LMU	R	7024	-	36,36,36	0.76	1 (2%)	47,47,47	1.46	8 (17%)
19	CLA	A	1136	-	56,73,73	1.80	10 (17%)	55,113,113	3.23	14 (25%)
23	SF4	C	8002	3	0,12,12	0.00	-	-	-	-
19	CLA	A	1128	-	56,73,73	1.83	10 (17%)	55,113,113	3.61	17 (30%)
19	CLA	3	3012	-	18,32,73	1.76	5 (27%)	22,54,113	4.20	13 (59%)
19	CLA	A	1103	-	56,73,73	1.91	11 (19%)	55,113,113	2.98	15 (27%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
19	CLA	B	1202	-	56,73,73	1.88	11 (19%)	55,113,113	3.65	16 (29%)
19	CLA	2	2005	-	18,32,73	1.60	4 (22%)	22,54,113	3.99	11 (50%)
19	CLA	3	3004	-	18,32,73	2.01	6 (33%)	22,54,113	4.10	11 (50%)
21	BCR	B	6017	-	41,41,41	1.53	5 (12%)	56,56,56	3.97	25 (44%)
19	CLA	B	1215	-	51,68,73	1.82	10 (19%)	49,107,113	3.59	15 (30%)
19	CLA	A	1101	-	41,58,73	2.09	8 (19%)	37,95,113	3.83	15 (40%)
19	CLA	A	1137	-	38,55,73	2.18	11 (28%)	33,91,113	3.85	12 (36%)
19	CLA	L	1502	-	38,55,73	2.24	7 (18%)	33,91,113	4.16	15 (45%)
19	CLA	3	3011	-	56,73,73	1.83	10 (17%)	55,113,113	2.61	15 (27%)
22	LMU	B	7012	-	26,26,36	0.78	1 (3%)	37,37,47	1.41	7 (18%)
22	LMU	G	7039	-	36,36,36	0.68	0	47,47,47	1.35	4 (8%)
22	LMU	K	7047	-	36,36,36	0.79	1 (2%)	47,47,47	1.04	3 (6%)
19	CLA	A	1106	-	56,73,73	1.76	10 (17%)	55,113,113	3.13	18 (32%)
19	CLA	A	1123	-	56,73,73	1.77	9 (16%)	55,113,113	2.56	13 (23%)
19	CLA	B	1219	-	46,63,73	2.20	11 (23%)	43,101,113	3.63	10 (23%)
19	CLA	L	1501	12	41,58,73	2.13	9 (21%)	37,95,113	3.83	13 (35%)
19	CLA	B	1209	-	46,63,73	1.94	9 (19%)	43,101,113	3.68	13 (30%)
19	CLA	L	1504	-	46,63,73	2.10	10 (21%)	43,101,113	3.00	16 (37%)
19	CLA	A	1108	-	33,53,73	2.20	8 (24%)	27,89,113	4.77	12 (44%)
19	CLA	B	1222	-	49,66,73	1.95	11 (22%)	46,104,113	3.39	14 (30%)
19	CLA	3	3015	-	18,32,73	1.66	5 (27%)	22,54,113	3.74	11 (50%)
19	CLA	H	1241	-	46,63,73	2.19	8 (17%)	43,101,113	3.80	18 (41%)
19	CLA	B	1217	-	41,58,73	2.08	10 (24%)	37,95,113	3.82	13 (35%)
22	LMU	4	7018	-	36,36,36	0.74	1 (2%)	47,47,47	1.07	3 (6%)
21	BCR	B	6004	-	41,41,41	1.29	3 (7%)	56,56,56	4.27	29 (51%)
19	CLA	H	1505	-	46,63,73	2.13	9 (19%)	43,101,113	3.70	13 (30%)
19	CLA	3	3003	-	27,44,73	2.43	8 (29%)	27,78,113	4.14	12 (44%)
19	CLA	A	1112	-	33,53,73	2.35	8 (24%)	27,89,113	4.37	11 (40%)
19	CLA	3	3016	-	56,73,73	1.85	11 (19%)	55,113,113	3.19	15 (27%)
19	CLA	A	1138	-	56,73,73	1.85	10 (17%)	55,113,113	3.15	14 (25%)
19	CLA	A	1134	1	33,53,73	2.16	8 (24%)	27,89,113	4.44	11 (40%)
22	LMU	H	7017	-	36,36,36	0.73	1 (2%)	47,47,47	1.90	11 (23%)
19	CLA	3	1118	-	27,44,73	2.42	9 (33%)	27,78,113	4.69	10 (37%)
19	CLA	A	1127	-	46,63,73	2.06	10 (21%)	43,101,113	3.61	14 (32%)
19	CLA	A	1139	-	42,59,73	2.14	10 (23%)	38,96,113	3.81	15 (39%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
19	CLA	B	1218	-	37,54,73	2.19	9 (24%)	32,90,113	4.29	12 (37%)
21	BCR	A	6003	-	41,41,41	1.48	3 (7%)	56,56,56	4.08	27 (48%)
22	LMU	4	7034	-	36,36,36	0.62	0	47,47,47	0.70	0
23	SF4	A	8001	1,2	0,12,12	0.00	-	-		
22	LMU	4	7019	-	36,36,36	0.81	1 (2%)	47,47,47	1.35	9 (19%)
21	BCR	F	6016	-	41,41,41	1.67	11 (26%)	56,56,56	3.64	27 (48%)
19	CLA	L	1148	-	46,63,73	2.23	14 (30%)	43,101,113	4.25	21 (48%)
19	CLA	1	1011	-	27,44,73	2.80	10 (37%)	27,78,113	5.22	10 (37%)
19	CLA	J	1308	-	46,63,73	2.07	11 (23%)	43,101,113	3.53	17 (39%)
22	LMU	A	7016	-	36,36,36	0.68	0	47,47,47	1.43	6 (12%)
19	CLA	A	1109	19	56,73,73	1.85	10 (17%)	55,113,113	2.92	16 (29%)
19	CLA	1	1002	-	38,55,73	2.31	9 (23%)	33,91,113	3.68	16 (48%)
21	BCR	1	6023	-	41,41,41	1.73	3 (7%)	56,56,56	6.25	30 (53%)
19	CLA	B	1220	-	56,73,73	1.99	11 (19%)	55,113,113	3.38	16 (29%)
19	CLA	A	9011	-	56,73,73	1.81	10 (17%)	55,113,113	3.55	15 (27%)
19	CLA	1	1010	-	37,54,73	2.36	11 (29%)	32,90,113	4.84	19 (59%)
19	CLA	4	4002	18	43,60,73	2.17	13 (30%)	39,97,113	4.64	25 (64%)
22	LMU	R	7007	-	36,36,36	0.58	1 (2%)	47,47,47	0.80	2 (4%)
19	CLA	A	1119	-	56,73,73	1.85	9 (16%)	55,113,113	3.41	17 (30%)
22	LMU	4	7008	-	36,36,36	0.58	0	47,47,47	0.87	1 (2%)
22	LMU	1	7013	-	36,36,36	0.71	1 (2%)	47,47,47	1.04	1 (2%)
19	CLA	L	1503	-	41,58,73	2.37	13 (31%)	37,95,113	4.47	14 (37%)
19	CLA	4	4007	-	43,60,73	2.12	9 (20%)	39,97,113	3.68	15 (38%)
19	CLA	B	1301	-	27,44,73	2.58	9 (33%)	27,78,113	4.58	12 (44%)
19	CLA	3	3010	-	18,32,73	1.69	6 (33%)	22,54,113	3.89	12 (54%)
19	CLA	2	2011	-	18,32,73	1.71	4 (22%)	22,54,113	4.01	14 (63%)
19	CLA	3	3014	-	18,32,73	1.85	5 (27%)	22,54,113	4.25	14 (63%)
22	LMU	R	7022	-	36,36,36	0.71	1 (2%)	47,47,47	1.31	6 (12%)
19	CLA	B	1231	19	33,53,73	2.31	7 (21%)	27,89,113	4.37	12 (44%)
19	CLA	4	1304	-	56,73,73	1.98	13 (23%)	55,113,113	3.54	20 (36%)
19	CLA	1	1007	-	52,69,73	2.01	10 (19%)	50,108,113	2.98	15 (30%)
19	CLA	4	4001	-	41,58,73	2.23	10 (24%)	37,95,113	4.14	14 (37%)
23	SF4	C	8003	3	0,12,12	0.00	-	-		
22	LMU	A	7045	-	36,36,36	0.75	1 (2%)	47,47,47	1.48	8 (17%)
19	CLA	2	2001	-	42,59,73	2.09	10 (23%)	38,96,113	3.57	14 (36%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
19	CLA	3	3007	-	33,50,73	2.18	8 (24%)	27,85,113	4.67	10 (37%)
19	CLA	A	9013	-	56,73,73	1.97	10 (17%)	55,113,113	3.29	16 (29%)
19	CLA	4	1306	-	46,63,73	2.05	10 (21%)	43,101,113	3.38	13 (30%)
19	CLA	A	1113	-	41,58,73	2.22	8 (19%)	37,95,113	3.77	17 (45%)
19	CLA	A	1102	19	46,63,73	2.09	9 (19%)	43,101,113	2.80	15 (34%)
19	CLA	A	1309	-	18,32,73	1.66	5 (27%)	22,54,113	3.81	11 (50%)
22	LMU	A	7023	-	36,36,36	0.60	0	47,47,47	1.18	4 (8%)
19	CLA	J	1311	-	52,69,73	1.89	10 (19%)	50,108,113	3.41	14 (28%)
19	CLA	B	1223	-	56,73,73	1.82	11 (19%)	55,113,113	3.16	16 (29%)
19	CLA	B	1212	-	51,68,73	1.88	9 (17%)	49,107,113	2.88	13 (26%)
19	CLA	A	1140	-	56,73,73	1.77	10 (17%)	55,113,113	3.15	14 (25%)
19	CLA	A	1115	-	56,73,73	1.87	11 (19%)	55,113,113	3.19	15 (27%)
22	LMU	K	7001	-	36,36,36	0.82	2 (5%)	47,47,47	1.37	7 (14%)
19	CLA	B	1203	-	56,73,73	1.89	12 (21%)	55,113,113	3.18	19 (34%)
19	CLA	4	1004	-	46,63,73	2.17	13 (28%)	43,101,113	3.71	14 (32%)
19	CLA	B	1210	-	56,73,73	1.86	10 (17%)	55,113,113	3.20	15 (27%)
19	CLA	3	1147	-	37,54,73	2.77	12 (32%)	32,90,113	3.85	19 (59%)
19	CLA	B	9010	-	56,73,73	1.75	10 (17%)	55,113,113	3.34	18 (32%)
19	CLA	1	1005	-	37,54,73	2.74	10 (27%)	32,90,113	2.70	11 (34%)
19	CLA	4	4014	-	38,55,73	2.07	9 (23%)	33,91,113	4.70	13 (39%)
22	LMU	R	7025	-	36,36,36	0.76	1 (2%)	47,47,47	1.20	5 (10%)
22	LMU	R	7021	-	36,36,36	0.74	1 (2%)	47,47,47	1.34	5 (10%)
19	CLA	A	1149	-	37,54,73	2.57	11 (29%)	36,90,113	5.93	22 (61%)
19	CLA	A	1104	-	48,65,73	1.94	8 (16%)	45,103,113	3.57	16 (35%)
22	LMU	4	7009	-	35,35,36	1.34	2 (5%)	46,46,47	1.24	4 (8%)
19	CLA	4	4003	-	46,63,73	2.07	10 (21%)	43,101,113	3.21	13 (30%)
19	CLA	B	1236	-	38,55,73	2.13	10 (26%)	33,91,113	3.81	13 (39%)
19	CLA	L	1130	-	56,73,73	1.97	9 (16%)	55,113,113	2.63	15 (27%)
22	LMU	R	7020	-	36,36,36	0.67	0	47,47,47	1.39	6 (12%)
19	CLA	B	1211	-	56,73,73	1.94	10 (17%)	55,113,113	2.64	12 (21%)
22	LMU	C	7015	-	36,36,36	0.69	1 (2%)	47,47,47	1.27	6 (12%)
22	LMU	4	7052	-	36,36,36	1.22	4 (11%)	47,47,47	1.78	8 (17%)
19	CLA	3	3005	-	18,32,73	1.71	5 (27%)	22,54,113	4.02	13 (59%)
22	LMU	K	7041	-	36,36,36	0.57	0	47,47,47	1.06	3 (6%)
22	LMU	B	7040	-	36,36,36	0.74	1 (2%)	47,47,47	1.61	10 (21%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
19	CLA	2	2003	-	18,32,73	1.80	5 (27%)	22,54,113	3.98	12 (54%)
22	LMU	D	7050	-	36,36,36	0.62	1 (2%)	47,47,47	0.82	1 (2%)
19	CLA	B	1239	-	56,73,73	1.79	11 (19%)	55,113,113	2.83	15 (27%)
19	CLA	A	9023	-	56,73,73	1.83	8 (14%)	55,113,113	2.93	18 (32%)
19	CLA	A	9022	-	56,73,73	1.91	10 (17%)	55,113,113	3.20	14 (25%)
19	CLA	3	3017	-	41,58,73	2.18	10 (24%)	37,95,113	4.47	18 (48%)
19	CLA	1	1015	-	18,32,73	1.72	5 (27%)	22,54,113	3.94	13 (59%)
19	CLA	1	1008	-	42,59,73	2.24	11 (26%)	38,96,113	4.25	16 (42%)
22	LMU	A	7010	-	36,36,36	1.29	2 (5%)	47,47,47	1.20	5 (10%)
19	CLA	A	1133	-	41,58,73	2.14	11 (26%)	37,95,113	3.76	14 (37%)
20	PQN	A	5001	-	34,34,34	1.70	2 (5%)	42,45,45	1.43	5 (11%)
22	LMU	N	7049	-	36,36,36	0.58	1 (2%)	47,47,47	1.34	4 (8%)
19	CLA	B	1221	-	45,62,73	2.19	11 (24%)	41,99,113	2.82	14 (34%)
22	LMU	4	7053	-	35,35,36	0.70	1 (2%)	46,46,47	1.25	6 (13%)
19	CLA	1	1303	-	42,59,73	2.39	12 (28%)	38,96,113	4.91	16 (42%)
21	BCR	B	6020	-	41,41,41	2.21	11 (26%)	56,56,56	4.46	27 (48%)
19	CLA	K	1146	-	41,58,73	2.22	10 (24%)	37,95,113	4.08	17 (45%)
19	CLA	A	1126	-	56,73,73	1.86	9 (16%)	55,113,113	3.70	20 (36%)
19	CLA	F	1302	-	32,49,73	2.40	10 (31%)	26,84,113	4.37	11 (42%)
22	LMU	A	7044	-	36,36,36	0.87	1 (2%)	47,47,47	1.57	9 (19%)
19	CLA	B	1229	-	56,73,73	1.91	9 (16%)	55,113,113	3.24	16 (29%)
19	CLA	B	1208	-	45,62,73	2.27	9 (20%)	46,100,113	3.53	18 (39%)
19	CLA	1	1012	-	27,44,73	2.39	6 (22%)	27,78,113	4.18	9 (33%)
19	CLA	1	1014	-	52,69,73	1.97	9 (17%)	50,108,113	3.30	12 (24%)
19	CLA	2	2007	-	56,73,73	1.86	8 (14%)	55,113,113	3.11	17 (30%)
19	CLA	3	2009	-	47,64,73	2.09	13 (27%)	44,102,113	3.83	15 (34%)
19	CLA	B	1224	-	56,73,73	1.90	10 (17%)	55,113,113	3.63	15 (27%)
19	CLA	B	1213	-	37,54,73	2.23	9 (24%)	32,90,113	3.91	12 (37%)
19	CLA	B	1214	-	50,67,73	2.00	10 (20%)	47,105,113	2.84	14 (29%)
19	CLA	B	1227	-	41,58,73	2.15	8 (19%)	37,95,113	3.71	13 (35%)
19	CLA	1	1310	-	18,32,73	1.92	4 (22%)	22,54,113	4.29	13 (59%)
19	CLA	2	2014	-	52,69,73	1.89	10 (19%)	50,108,113	3.42	17 (34%)
19	CLA	A	1122	-	46,63,73	2.11	10 (21%)	43,101,113	3.56	13 (30%)
19	CLA	2	4009	-	56,73,73	1.84	9 (16%)	55,113,113	3.84	16 (29%)
22	LMU	2	7031	-	36,36,36	1.23	3 (8%)	47,47,47	1.32	5 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
19	CLA	B	1234	-	51,68,73	1.92	9 (17%)	49,107,113	3.51	11 (22%)
19	CLA	3	3013	-	56,73,73	1.86	10 (17%)	55,113,113	3.79	15 (27%)
19	CLA	G	1242	-	42,59,73	2.17	10 (23%)	38,96,113	3.73	17 (44%)
22	LMU	G	7051	-	36,36,36	0.86	1 (2%)	47,47,47	2.07	12 (25%)
22	LMU	R	7014	-	36,36,36	0.92	2 (5%)	47,47,47	2.02	8 (17%)
19	CLA	2	2010	-	18,32,73	1.77	6 (33%)	22,54,113	3.69	9 (40%)
19	CLA	A	1121	1	33,50,73	2.32	7 (21%)	27,85,113	4.65	11 (40%)
19	CLA	B	1228	-	41,58,73	2.10	9 (21%)	37,95,113	3.67	15 (40%)
19	CLA	4	4005	-	18,32,73	1.83	5 (27%)	22,54,113	4.00	11 (50%)
19	CLA	K	1142	-	33,53,73	2.12	9 (27%)	27,89,113	4.42	11 (40%)
22	LMU	L	7029	-	36,36,36	0.68	1 (2%)	47,47,47	0.73	0
19	CLA	K	3009	-	56,73,73	1.89	8 (14%)	55,113,113	2.95	15 (27%)
19	CLA	A	1107	-	46,63,73	2.00	10 (21%)	43,101,113	3.29	16 (37%)
19	CLA	B	1216	-	52,69,73	1.81	9 (17%)	50,108,113	3.53	14 (28%)
19	CLA	A	1151	-	41,58,73	2.25	9 (21%)	37,95,113	3.89	12 (32%)
19	CLA	B	1238	-	56,73,73	1.84	10 (17%)	55,113,113	2.94	16 (29%)
22	LMU	F	7036	-	35,35,36	0.76	1 (2%)	46,46,47	1.41	6 (13%)
19	CLA	4	4004	-	18,32,73	1.78	5 (27%)	22,54,113	4.06	14 (63%)
19	CLA	A	1237	-	56,73,73	1.85	10 (17%)	55,113,113	3.66	15 (27%)
21	BCR	B	6006	-	41,41,41	1.52	9 (21%)	56,56,56	4.50	26 (46%)
19	CLA	I	1204	-	51,68,73	1.86	9 (17%)	49,107,113	3.69	12 (24%)
19	CLA	4	4015	-	37,54,73	2.22	11 (29%)	32,90,113	3.45	12 (37%)
21	BCR	A	6008	-	41,41,41	1.38	4 (9%)	56,56,56	4.07	29 (51%)
19	CLA	R	1144	-	48,65,73	2.02	9 (18%)	45,103,113	3.93	16 (35%)
19	CLA	4	1009	-	27,44,73	2.67	9 (33%)	27,78,113	4.76	12 (44%)
19	CLA	4	4006	-	46,63,73	2.04	8 (17%)	43,101,113	3.09	14 (32%)
19	CLA	A	1111	-	45,62,73	1.95	10 (22%)	41,99,113	3.46	15 (36%)
19	CLA	F	1240	-	27,44,73	2.32	7 (25%)	27,78,113	3.72	15 (55%)
22	LMU	2	7046	-	36,36,36	0.71	1 (2%)	47,47,47	0.86	2 (4%)
22	LMU	K	7042	-	36,36,36	0.62	0	47,47,47	1.16	5 (10%)
19	CLA	2	2008	-	18,32,73	1.69	4 (22%)	22,54,113	3.98	11 (50%)
19	CLA	1	1001	-	37,54,73	2.53	13 (35%)	32,90,113	4.57	14 (43%)
21	BCR	B	6010	-	41,41,41	1.39	3 (7%)	56,56,56	4.27	28 (50%)
19	CLA	B	1233	-	42,59,73	2.24	9 (21%)	38,96,113	4.21	13 (34%)
21	BCR	B	6005	-	41,41,41	1.37	4 (9%)	56,56,56	4.72	32 (57%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
22	LMU	H	7011	-	36,36,36	0.77	2 (5%)	47,47,47	1.93	10 (21%)
22	LMU	3	7005	-	36,36,36	0.71	0	47,47,47	2.09	14 (29%)
19	CLA	2	1307	-	18,32,73	1.80	6 (33%)	22,54,113	3.96	11 (50%)
19	CLA	A	1117	-	56,73,73	1.82	10 (17%)	55,113,113	2.93	16 (29%)
19	CLA	3	3008	-	41,58,73	2.12	10 (24%)	37,95,113	4.12	15 (40%)
19	CLA	1	1013	-	42,59,73	2.50	15 (35%)	38,96,113	4.55	17 (44%)
20	PQN	B	5002	-	34,34,34	1.60	2 (5%)	42,45,45	1.53	6 (14%)
19	CLA	3	3001	-	18,32,73	1.82	6 (33%)	22,54,113	4.03	13 (59%)
19	CLA	H	1207	-	56,73,73	1.86	9 (16%)	55,113,113	3.31	13 (23%)
21	BCR	F	6014	-	41,41,41	1.34	6 (14%)	56,56,56	4.82	27 (48%)
19	CLA	A	1129	-	41,58,73	2.12	11 (26%)	37,95,113	4.11	14 (37%)
19	CLA	A	1132	-	56,73,73	1.86	9 (16%)	55,113,113	3.17	16 (29%)
19	CLA	A	1135	-	42,59,73	2.11	10 (23%)	38,96,113	3.82	14 (36%)
19	CLA	2	2013	-	41,58,73	2.19	9 (21%)	37,95,113	4.35	14 (37%)
19	CLA	2	2006	-	56,73,73	1.93	9 (16%)	55,113,113	3.37	11 (20%)
19	CLA	4	4011	-	18,32,73	1.71	5 (27%)	22,54,113	4.03	13 (59%)
22	LMU	A	7035	-	36,36,36	0.61	0	47,47,47	1.54	8 (17%)
22	LMU	4	7033	-	36,36,36	0.75	0	47,47,47	1.59	9 (19%)
22	LMU	H	7032	-	36,36,36	0.72	1 (2%)	47,47,47	1.44	6 (12%)
19	CLA	B	1226	-	56,73,73	1.72	9 (16%)	55,113,113	2.98	14 (25%)
19	CLA	2	2012	16	41,58,73	2.18	9 (21%)	37,95,113	3.79	12 (32%)
19	CLA	4	4012	-	27,44,73	2.46	8 (29%)	27,78,113	4.78	10 (37%)
19	CLA	H	1145	-	56,73,73	1.82	11 (19%)	55,113,113	3.71	16 (29%)
19	CLA	1	1006	-	27,44,73	2.64	9 (33%)	27,78,113	4.48	10 (37%)
19	CLA	A	1131	-	56,73,73	1.84	11 (19%)	55,113,113	3.16	14 (25%)
19	CLA	B	1206	2	56,73,73	1.78	9 (16%)	55,113,113	3.32	14 (25%)
21	BCR	L	6019	-	41,41,41	1.75	12 (29%)	56,56,56	4.27	25 (44%)
21	BCR	J	6012	-	41,41,41	1.47	5 (12%)	56,56,56	5.42	26 (46%)
21	BCR	A	6011	-	41,41,41	1.36	5 (12%)	56,56,56	4.17	32 (57%)
19	CLA	A	9012	-	56,73,73	1.91	11 (19%)	55,113,113	3.04	16 (29%)
24	LMG	B	7101	-	49,49,55	1.04	3 (6%)	57,57,63	1.02	3 (5%)
19	CLA	2	2002	-	47,64,73	2.05	9 (19%)	44,102,113	3.29	18 (40%)
19	CLA	B	1232	19	33,53,73	2.27	8 (24%)	27,89,113	4.29	10 (37%)
19	CLA	3	3002	-	18,32,73	1.77	5 (27%)	22,54,113	3.80	11 (50%)
19	CLA	B	1205	-	56,73,73	1.90	9 (16%)	55,113,113	3.16	15 (27%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
19	CLA	B	1225	-	56,73,73	1.81	9 (16%)	55,113,113	3.13	15 (27%)
19	CLA	R	1150	-	56,73,73	2.07	10 (17%)	55,113,113	3.09	17 (30%)
21	BCR	A	6002	-	41,41,41	1.87	6 (14%)	56,56,56	4.62	34 (60%)
22	LMU	1	7004	-	36,36,36	0.66	1 (2%)	47,47,47	0.79	1 (2%)
21	BCR	3	6022	-	41,41,41	1.35	4 (9%)	56,56,56	4.91	25 (44%)
19	CLA	4	4013	18	18,32,73	1.59	5 (27%)	22,54,113	3.60	12 (54%)
19	CLA	A	1141	-	56,73,73	1.84	10 (17%)	55,113,113	3.10	13 (23%)
22	LMU	2	7006	-	36,36,36	0.63	1 (2%)	47,47,47	0.73	0
22	LMU	3	7003	-	36,36,36	0.80	0	47,47,47	1.48	7 (14%)
19	CLA	A	1124	-	56,73,73	1.81	10 (17%)	55,113,113	3.12	13 (23%)
21	BCR	I	6021	-	41,41,41	2.04	8 (19%)	56,56,56	4.79	32 (57%)
19	CLA	F	1305	-	44,61,73	2.32	14 (31%)	40,98,113	3.78	16 (40%)
19	CLA	1	1003	-	38,55,73	2.23	9 (23%)	33,91,113	4.48	13 (39%)
22	LMU	H	7028	-	36,36,36	0.59	0	47,47,47	0.97	2 (4%)
19	CLA	A	1105	-	37,54,73	2.18	8 (21%)	32,90,113	4.71	12 (37%)
22	LMU	G	7026	-	36,36,36	0.88	2 (5%)	47,47,47	1.49	7 (14%)
22	LMU	2	7027	-	36,36,36	0.81	1 (2%)	47,47,47	1.67	10 (21%)
22	LMU	H	7043	-	36,36,36	0.83	1 (2%)	47,47,47	1.64	10 (21%)
19	CLA	A	1116	-	43,60,73	2.18	9 (20%)	39,97,113	3.95	15 (38%)
19	CLA	K	1143	-	41,58,73	2.10	10 (24%)	37,95,113	3.72	16 (43%)

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
22	LMU	H	7002	-	-	14/21/61/61	0/2/2/2
22	LMU	E	7048	-	-	12/21/61/61	0/2/2/2
19	CLA	B	1201	-	1/1/11/20	6/11/91/115	-
19	CLA	B	1230	-	1/1/12/20	6/19/97/115	-
22	LMU	H	7030	-	-	14/21/61/61	0/2/2/2
19	CLA	A	1110	-	1/1/12/20	12/24/102/115	-
19	CLA	2	2004	-	1/1/12/20	8/19/97/115	-
19	CLA	A	1125	-	2/2/15/20	23/37/115/115	-
19	CLA	4	4010	-	1/1/4/20	-	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
21	BCR	A	6007	-	-	14/29/63/63	0/2/2/2
19	CLA	A	1120	-	1/1/12/20	9/21/99/115	-
21	BCR	I	6018	-	-	14/29/63/63	0/2/2/2
22	LMU	B	7038	-	-	13/21/61/61	0/2/2/2
19	CLA	B	1235	-	2/2/15/20	13/37/115/115	-
22	LMU	E	7037	-	-	16/21/61/61	0/2/2/2
19	CLA	3	3006	-	1/1/4/20	-	-
22	LMU	R	7024	-	-	14/21/61/61	0/2/2/2
19	CLA	A	1136	-	2/2/15/20	12/37/115/115	-
23	SF4	C	8002	3	-	-	0/6/5/5
19	CLA	A	1128	-	2/2/15/20	18/37/115/115	-
19	CLA	3	3012	-	1/1/4/20	-	-
19	CLA	A	1103	-	2/2/15/20	24/37/115/115	-
19	CLA	B	1202	-	2/2/15/20	21/37/115/115	-
19	CLA	2	2005	-	1/1/4/20	-	-
19	CLA	3	3004	-	1/1/4/20	-	-
21	BCR	B	6017	-	-	14/29/63/63	0/2/2/2
19	CLA	B	1215	-	2/2/14/20	13/31/109/115	-
19	CLA	A	1101	-	1/1/12/20	5/19/97/115	-
19	CLA	A	1137	-	1/1/11/20	9/16/94/115	-
19	CLA	L	1502	-	1/1/11/20	8/16/94/115	-
19	CLA	3	3011	-	2/2/15/20	19/37/115/115	-
22	LMU	B	7012	-	-	5/11/51/61	0/2/2/2
22	LMU	G	7039	-	-	17/21/61/61	0/2/2/2
22	LMU	K	7047	-	-	9/21/61/61	0/2/2/2
19	CLA	A	1106	-	2/2/15/20	22/37/115/115	-
19	CLA	A	1123	-	2/2/15/20	20/37/115/115	-
19	CLA	B	1219	-	2/2/13/20	9/25/103/115	-
19	CLA	L	1501	12	1/1/12/20	7/19/97/115	-
19	CLA	B	1209	-	2/2/13/20	10/25/103/115	-
19	CLA	L	1504	-	2/2/13/20	7/25/103/115	-
19	CLA	A	1108	-	1/1/11/20	2/11/91/115	-
19	CLA	B	1222	-	2/2/13/20	16/29/107/115	-
19	CLA	3	3015	-	1/1/4/20	-	-
19	CLA	H	1241	-	2/2/13/20	7/25/103/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
19	CLA	B	1217	-	1/1/12/20	6/19/97/115	-
22	LMU	4	7018	-	-	13/21/61/61	0/2/2/2
21	BCR	B	6004	-	-	16/29/63/63	0/2/2/2
19	CLA	H	1505	-	2/2/13/20	13/25/103/115	-
19	CLA	3	3003	-	1/1/9/20	-	-
19	CLA	A	1112	-	1/1/11/20	7/11/91/115	-
19	CLA	3	3016	-	2/2/15/20	22/37/115/115	-
19	CLA	A	1138	-	2/2/15/20	21/37/115/115	-
19	CLA	A	1134	1	1/1/11/20	5/11/91/115	-
22	LMU	H	7017	-	-	13/21/61/61	0/2/2/2
19	CLA	3	1118	-	1/1/9/20	-	-
19	CLA	A	1127	-	2/2/13/20	11/25/103/115	-
19	CLA	A	1139	-	1/1/12/20	11/21/99/115	-
19	CLA	B	1218	-	1/1/11/20	12/15/93/115	-
21	BCR	A	6003	-	-	14/29/63/63	0/2/2/2
22	LMU	4	7034	-	-	12/21/61/61	0/2/2/2
23	SF4	A	8001	1,2	-	-	0/6/5/5
22	LMU	4	7019	-	-	15/21/61/61	0/2/2/2
21	BCR	F	6016	-	-	13/29/63/63	0/2/2/2
19	CLA	L	1148	-	3/3/13/20	12/25/103/115	-
19	CLA	1	1011	-	1/1/9/20	-	-
19	CLA	J	1308	-	2/2/13/20	16/25/103/115	-
22	LMU	A	7016	-	-	11/21/61/61	0/2/2/2
19	CLA	A	1109	19	2/2/15/20	25/37/115/115	-
19	CLA	1	1002	-	1/1/11/20	9/16/94/115	-
21	BCR	1	6023	-	-	15/29/63/63	0/2/2/2
19	CLA	B	1220	-	1/1/15/20	21/37/115/115	-
19	CLA	A	9011	-	2/2/15/20	23/37/115/115	-
19	CLA	1	1010	-	1/1/11/20	7/15/93/115	-
19	CLA	4	4002	18	2/2/12/20	6/22/100/115	-
22	LMU	R	7007	-	-	16/21/61/61	0/2/2/2
19	CLA	A	1119	-	2/2/15/20	17/37/115/115	-
22	LMU	4	7008	-	-	12/21/61/61	0/2/2/2
22	LMU	1	7013	-	-	10/21/61/61	0/2/2/2
19	CLA	L	1503	-	2/2/12/20	10/19/97/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
19	CLA	4	4007	-	1/1/12/20	9/22/100/115	-
19	CLA	B	1301	-	1/1/9/20	-	-
19	CLA	3	3010	-	1/1/4/20	-	-
19	CLA	2	2011	-	1/1/4/20	-	-
19	CLA	3	3014	-	1/1/4/20	-	-
22	LMU	R	7022	-	-	14/21/61/61	0/2/2/2
19	CLA	B	1231	19	1/1/11/20	9/11/91/115	-
19	CLA	4	1304	-	3/3/15/20	20/37/115/115	-
19	CLA	1	1007	-	2/2/14/20	20/33/111/115	-
19	CLA	4	4001	-	1/1/12/20	6/19/97/115	-
23	SF4	C	8003	3	-	-	0/6/5/5
22	LMU	A	7045	-	-	14/21/61/61	0/2/2/2
19	CLA	2	2001	-	1/1/12/20	9/21/99/115	-
19	CLA	3	3007	-	1/1/10/20	5/10/88/115	-
19	CLA	A	9013	-	2/2/15/20	25/37/115/115	-
19	CLA	4	1306	-	2/2/13/20	12/25/103/115	-
19	CLA	A	1113	-	1/1/12/20	10/19/97/115	-
19	CLA	A	1102	19	2/2/13/20	12/25/103/115	-
19	CLA	A	1309	-	1/1/4/20	-	-
22	LMU	A	7023	-	-	17/21/61/61	0/2/2/2
19	CLA	J	1311	-	2/2/14/20	24/33/111/115	-
19	CLA	B	1223	-	2/2/15/20	18/37/115/115	-
19	CLA	B	1212	-	2/2/14/20	14/31/109/115	-
19	CLA	A	1140	-	2/2/15/20	17/37/115/115	-
19	CLA	A	1115	-	2/2/15/20	17/37/115/115	-
22	LMU	K	7001	-	-	13/21/61/61	0/2/2/2
19	CLA	B	1203	-	2/2/15/20	16/37/115/115	-
19	CLA	4	1004	-	2/2/13/20	9/25/103/115	-
19	CLA	B	1210	-	2/2/15/20	23/37/115/115	-
19	CLA	3	1147	-	1/1/11/20	8/15/93/115	-
19	CLA	B	9010	-	2/2/15/20	20/37/115/115	-
19	CLA	1	1005	-	1/1/11/20	6/15/93/115	-
19	CLA	4	4014	-	1/1/11/20	13/16/94/115	-
22	LMU	R	7025	-	-	13/21/61/61	0/2/2/2
22	LMU	R	7021	-	-	14/21/61/61	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
19	CLA	A	1149	-	3/3/11/20	12/16/92/115	-
19	CLA	A	1104	-	2/2/13/20	7/28/106/115	-
22	LMU	4	7009	-	-	13/20/60/61	0/2/2/2
19	CLA	4	4003	-	2/2/13/20	15/25/103/115	-
19	CLA	B	1236	-	1/1/11/20	8/16/94/115	-
19	CLA	L	1130	-	2/2/15/20	18/37/115/115	-
22	LMU	R	7020	-	-	10/21/61/61	0/2/2/2
19	CLA	B	1211	-	2/2/15/20	23/37/115/115	-
22	LMU	C	7015	-	-	14/21/61/61	0/2/2/2
22	LMU	4	7052	-	-	19/21/61/61	0/2/2/2
19	CLA	3	3005	-	1/1/4/20	-	-
22	LMU	K	7041	-	-	12/21/61/61	0/2/2/2
22	LMU	B	7040	-	-	13/21/61/61	0/2/2/2
19	CLA	2	2003	-	1/1/4/20	-	-
22	LMU	D	7050	-	-	11/21/61/61	0/2/2/2
19	CLA	B	1239	-	2/2/15/20	18/37/115/115	-
19	CLA	A	9023	-	2/2/15/20	17/37/115/115	-
19	CLA	A	9022	-	2/2/15/20	16/37/115/115	-
19	CLA	3	3017	-	1/1/12/20	7/19/97/115	-
19	CLA	1	1015	-	1/1/4/20	-	-
19	CLA	1	1008	-	2/2/12/20	9/21/99/115	-
22	LMU	A	7010	-	-	18/21/61/61	0/2/2/2
19	CLA	A	1133	-	1/1/12/20	11/19/97/115	-
20	PQN	A	5001	-	1/1/8/9	11/23/43/43	0/2/2/2
22	LMU	N	7049	-	-	16/21/61/61	0/2/2/2
19	CLA	B	1221	-	1/1/12/20	9/24/102/115	-
22	LMU	4	7053	-	-	13/20/60/61	0/2/2/2
19	CLA	1	1303	-	3/3/12/20	11/21/99/115	-
21	BCR	B	6020	-	-	14/29/63/63	0/2/2/2
19	CLA	K	1146	-	1/1/12/20	8/19/97/115	-
19	CLA	A	1126	-	2/2/15/20	14/37/115/115	-
19	CLA	F	1302	-	1/1/10/20	5/8/86/115	-
22	LMU	A	7044	-	-	15/21/61/61	0/2/2/2
19	CLA	B	1229	-	2/2/15/20	18/37/115/115	-
19	CLA	B	1208	-	2/2/13/20	9/25/101/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
19	CLA	1	1012	-	1/1/9/20	-	-
19	CLA	1	1014	-	2/2/14/20	15/33/111/115	-
19	CLA	2	2007	-	2/2/15/20	16/37/115/115	-
19	CLA	3	2009	-	2/2/13/20	13/27/105/115	-
19	CLA	B	1224	-	2/2/15/20	16/37/115/115	-
19	CLA	B	1213	-	1/1/11/20	11/15/93/115	-
19	CLA	B	1214	-	2/2/13/20	11/30/108/115	-
19	CLA	B	1227	-	1/1/12/20	9/19/97/115	-
19	CLA	1	1310	-	1/1/4/20	-	-
19	CLA	2	2014	-	2/2/14/20	20/33/111/115	-
19	CLA	A	1122	-	2/2/13/20	8/25/103/115	-
19	CLA	2	4009	-	2/2/15/20	16/37/115/115	-
22	LMU	2	7031	-	-	11/21/61/61	0/2/2/2
19	CLA	B	1234	-	2/2/14/20	13/31/109/115	-
19	CLA	3	3013	-	2/2/15/20	17/37/115/115	-
19	CLA	G	1242	-	1/1/12/20	10/21/99/115	-
22	LMU	G	7051	-	-	13/21/61/61	0/2/2/2
22	LMU	R	7014	-	-	12/21/61/61	0/2/2/2
19	CLA	2	2010	-	1/1/4/20	-	-
19	CLA	A	1121	1	1/1/10/20	2/10/88/115	-
19	CLA	B	1228	-	1/1/12/20	12/19/97/115	-
19	CLA	4	4005	-	1/1/4/20	-	-
19	CLA	K	1142	-	1/1/11/20	3/11/91/115	-
22	LMU	L	7029	-	-	16/21/61/61	0/2/2/2
19	CLA	K	3009	-	2/2/15/20	21/37/115/115	-
19	CLA	A	1107	-	2/2/13/20	11/25/103/115	-
19	CLA	B	1216	-	2/2/14/20	16/33/111/115	-
19	CLA	A	1151	-	1/1/12/20	10/19/97/115	-
19	CLA	B	1238	-	2/2/15/20	19/37/115/115	-
22	LMU	F	7036	-	-	11/20/60/61	0/2/2/2
19	CLA	4	4004	-	1/1/4/20	-	-
19	CLA	A	1237	-	2/2/15/20	19/37/115/115	-
21	BCR	B	6006	-	-	12/29/63/63	0/2/2/2
19	CLA	I	1204	-	2/2/14/20	13/31/109/115	-
19	CLA	4	4015	-	1/1/11/20	11/15/93/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
21	BCR	A	6008	-	-	15/29/63/63	0/2/2/2
19	CLA	R	1144	-	2/2/13/20	13/28/106/115	-
19	CLA	4	1009	-	1/1/9/20	-	-
19	CLA	4	4006	-	2/2/13/20	12/25/103/115	-
19	CLA	A	1111	-	1/1/12/20	13/24/102/115	-
19	CLA	F	1240	-	1/1/9/20	-	-
22	LMU	2	7046	-	-	16/21/61/61	0/2/2/2
22	LMU	K	7042	-	-	18/21/61/61	0/2/2/2
19	CLA	2	2008	-	1/1/4/20	-	-
19	CLA	1	1001	-	1/1/11/20	10/15/93/115	-
21	BCR	B	6010	-	-	13/29/63/63	0/2/2/2
19	CLA	B	1233	-	1/1/12/20	10/21/99/115	-
21	BCR	B	6005	-	-	9/29/63/63	0/2/2/2
22	LMU	H	7011	-	-	17/21/61/61	0/2/2/2
22	LMU	3	7005	-	-	15/21/61/61	0/2/2/2
19	CLA	2	1307	-	1/1/4/20	-	-
19	CLA	A	1117	-	2/2/15/20	18/37/115/115	-
19	CLA	3	3008	-	1/1/12/20	6/19/97/115	-
19	CLA	1	1013	-	2/2/12/20	8/21/99/115	-
20	PQN	B	5002	-	1/1/8/9	9/23/43/43	0/2/2/2
19	CLA	3	3001	-	1/1/4/20	-	-
19	CLA	H	1207	-	2/2/15/20	19/37/115/115	-
21	BCR	F	6014	-	-	17/29/63/63	0/2/2/2
19	CLA	A	1129	-	1/1/12/20	3/19/97/115	-
19	CLA	A	1132	-	2/2/15/20	24/37/115/115	-
19	CLA	A	1135	-	1/1/12/20	9/21/99/115	-
19	CLA	2	2013	-	1/1/12/20	11/19/97/115	-
19	CLA	2	2006	-	2/2/15/20	17/37/115/115	-
19	CLA	4	4011	-	1/1/4/20	-	-
22	LMU	A	7035	-	-	13/21/61/61	0/2/2/2
22	LMU	4	7033	-	-	12/21/61/61	0/2/2/2
22	LMU	H	7032	-	-	17/21/61/61	0/2/2/2
19	CLA	B	1226	-	2/2/15/20	26/37/115/115	-
19	CLA	2	2012	16	1/1/12/20	6/19/97/115	-
19	CLA	4	4012	-	1/1/9/20	-	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
19	CLA	H	1145	-	3/3/15/20	20/37/115/115	-
19	CLA	1	1006	-	1/1/9/20	-	-
19	CLA	A	1131	-	2/2/15/20	19/37/115/115	-
19	CLA	B	1206	2	2/2/15/20	17/37/115/115	-
21	BCR	L	6019	-	-	13/29/63/63	0/2/2/2
21	BCR	J	6012	-	-	13/29/63/63	0/2/2/2
21	BCR	A	6011	-	-	11/29/63/63	0/2/2/2
19	CLA	A	9012	-	2/2/15/20	20/37/115/115	-
24	LMG	B	7101	-	-	24/44/64/70	0/1/1/1
19	CLA	2	2002	-	2/2/13/20	9/27/105/115	-
19	CLA	B	1232	19	1/1/11/20	6/11/91/115	-
19	CLA	3	3002	-	1/1/4/20	-	-
19	CLA	B	1205	-	2/2/15/20	11/37/115/115	-
19	CLA	B	1225	-	2/2/15/20	15/37/115/115	-
19	CLA	R	1150	-	2/2/15/20	19/37/115/115	-
21	BCR	A	6002	-	-	16/29/63/63	0/2/2/2
22	LMU	1	7004	-	-	16/21/61/61	0/2/2/2
21	BCR	3	6022	-	-	19/29/63/63	0/2/2/2
19	CLA	4	4013	18	1/1/4/20	-	-
19	CLA	A	1141	-	2/2/15/20	19/37/115/115	-
22	LMU	2	7006	-	-	14/21/61/61	0/2/2/2
22	LMU	3	7003	-	-	14/21/61/61	0/2/2/2
19	CLA	A	1124	-	2/2/15/20	19/37/115/115	-
21	BCR	I	6021	-	-	13/29/63/63	0/2/2/2
19	CLA	F	1305	-	4/4/12/20	10/23/101/115	-
19	CLA	1	1003	-	1/1/11/20	8/16/94/115	-
22	LMU	H	7028	-	-	13/21/61/61	0/2/2/2
19	CLA	A	1105	-	1/1/11/20	7/15/93/115	-
22	LMU	G	7026	-	-	15/21/61/61	0/2/2/2
22	LMU	2	7027	-	-	11/21/61/61	0/2/2/2
22	LMU	H	7043	-	-	11/21/61/61	0/2/2/2
19	CLA	A	1116	-	1/1/12/20	13/22/100/115	-
19	CLA	K	1143	-	1/1/12/20	4/19/97/115	-

The worst 5 of 1756 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	1	1005	CLA	OBD-CAD	10.52	1.37	1.22
19	1	1011	CLA	CAB-C3B	-8.86	1.33	1.51
19	1	1006	CLA	CAB-C3B	-8.85	1.33	1.51
19	4	1009	CLA	CAB-C3B	-8.52	1.33	1.51
19	B	1208	CLA	CAB-C3B	-8.25	1.34	1.51

The worst 5 of 3333 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	J	6012	BCR	C20-C21-C22	30.06	170.21	127.31
21	A	6002	BCR	C20-C21-C22	24.71	162.58	127.31
21	3	6022	BCR	C20-C21-C22	24.52	162.30	127.31
21	F	6014	BCR	C20-C21-C22	22.67	159.67	127.31
21	B	6005	BCR	C20-C21-C22	22.24	159.05	127.31

5 of 271 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
19	A	1101	CLA	ND
19	A	1102	CLA	ND
19	A	1102	CLA	C8
19	A	1103	CLA	ND
19	A	1103	CLA	C8

5 of 2879 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
19	A	1101	CLA	C3A-C2A-CAA-CBA
19	A	1102	CLA	C3A-C2A-CAA-CBA
19	A	1102	CLA	CBA-CGA-O2A-C1
19	A	1102	CLA	O1A-CGA-O2A-C1
19	A	1102	CLA	CBD-CGD-O2D-CED

There are no ring outliers.

234 monomers are involved in 3097 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
22	H	7002	LMU	3	0
22	E	7048	LMU	17	0
19	B	1201	CLA	11	0
19	B	1230	CLA	21	0
22	H	7030	LMU	4	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
19	A	1110	CLA	3	0
19	2	2004	CLA	18	0
19	A	1125	CLA	65	0
19	4	4010	CLA	2	0
21	A	6007	BCR	32	0
19	A	1120	CLA	10	0
21	I	6018	BCR	15	0
22	B	7038	LMU	7	0
19	B	1235	CLA	62	0
22	E	7037	LMU	7	0
19	3	3006	CLA	9	0
19	A	1136	CLA	24	0
23	C	8002	SF4	6	0
19	A	1128	CLA	21	0
19	3	3012	CLA	11	0
19	A	1103	CLA	19	0
19	B	1202	CLA	31	0
19	3	3004	CLA	7	0
21	B	6017	BCR	42	0
19	B	1215	CLA	10	0
19	A	1101	CLA	15	0
19	A	1137	CLA	8	0
19	L	1502	CLA	27	0
19	3	3011	CLA	12	0
22	B	7012	LMU	1	0
22	G	7039	LMU	4	0
22	K	7047	LMU	5	2
19	A	1106	CLA	27	0
19	A	1123	CLA	29	0
19	B	1219	CLA	13	0
19	L	1501	CLA	17	0
19	B	1209	CLA	14	0
19	L	1504	CLA	21	0
19	A	1108	CLA	7	0
19	B	1222	CLA	43	0
19	H	1241	CLA	11	0
19	B	1217	CLA	9	0
21	B	6004	BCR	6	0
19	H	1505	CLA	3	0
19	3	3003	CLA	7	0
19	A	1112	CLA	31	0
19	3	3016	CLA	14	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
19	A	1138	CLA	29	0
19	A	1134	CLA	20	0
22	H	7017	LMU	2	0
19	A	1127	CLA	16	0
19	A	1139	CLA	31	0
19	B	1218	CLA	20	0
21	A	6003	BCR	14	0
22	4	7034	LMU	36	0
23	A	8001	SF4	2	0
22	4	7019	LMU	1	0
21	F	6016	BCR	37	0
19	L	1148	CLA	21	0
19	1	1011	CLA	6	0
19	J	1308	CLA	31	0
22	A	7016	LMU	12	0
19	A	1109	CLA	18	0
19	1	1002	CLA	10	0
21	1	6023	BCR	6	0
19	B	1220	CLA	44	0
19	A	9011	CLA	13	0
19	1	1010	CLA	8	0
19	4	4002	CLA	23	0
22	R	7007	LMU	5	0
19	A	1119	CLA	43	0
22	4	7008	LMU	3	0
22	1	7013	LMU	4	0
19	L	1503	CLA	9	0
19	B	1301	CLA	6	0
19	3	3010	CLA	5	0
19	2	2011	CLA	1	0
22	R	7022	LMU	5	0
19	B	1231	CLA	16	0
19	4	1304	CLA	23	0
19	1	1007	CLA	19	0
19	4	4001	CLA	4	0
23	C	8003	SF4	3	0
22	A	7045	LMU	2	0
19	2	2001	CLA	13	0
19	3	3007	CLA	2	0
19	A	9013	CLA	29	0
19	4	1306	CLA	19	0
19	A	1113	CLA	9	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
19	A	1102	CLA	19	0
22	A	7023	LMU	6	0
19	J	1311	CLA	20	0
19	B	1223	CLA	38	0
19	B	1212	CLA	14	0
19	A	1140	CLA	47	0
19	A	1115	CLA	76	0
22	K	7001	LMU	11	0
19	B	1203	CLA	19	0
19	4	1004	CLA	33	0
19	B	1210	CLA	21	0
19	3	1147	CLA	15	0
19	B	9010	CLA	17	0
19	1	1005	CLA	5	0
19	4	4014	CLA	8	0
22	R	7025	LMU	1	0
22	R	7021	LMU	9	0
19	A	1149	CLA	7	0
19	A	1104	CLA	15	0
22	4	7009	LMU	3	0
19	4	4003	CLA	2	0
19	B	1236	CLA	24	0
19	L	1130	CLA	29	0
22	R	7020	LMU	10	0
19	B	1211	CLA	19	0
22	4	7052	LMU	36	0
19	3	3005	CLA	9	0
22	K	7041	LMU	6	0
22	B	7040	LMU	3	0
19	2	2003	CLA	1	0
22	D	7050	LMU	21	0
19	B	1239	CLA	22	0
19	A	9023	CLA	53	0
19	A	9022	CLA	39	0
19	3	3017	CLA	4	0
19	1	1015	CLA	3	0
19	1	1008	CLA	8	1
22	A	7010	LMU	6	0
19	A	1133	CLA	31	0
20	A	5001	PQN	9	0
22	N	7049	LMU	9	0
19	B	1221	CLA	21	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
22	4	7053	LMU	13	0
19	1	1303	CLA	10	0
21	B	6020	BCR	24	0
19	K	1146	CLA	7	0
19	A	1126	CLA	43	0
19	F	1302	CLA	10	0
22	A	7044	LMU	1	0
19	B	1229	CLA	20	0
19	B	1208	CLA	6	0
19	1	1012	CLA	2	0
19	1	1014	CLA	17	0
19	2	2007	CLA	18	0
19	3	2009	CLA	37	0
19	B	1224	CLA	19	0
19	B	1213	CLA	19	0
19	B	1214	CLA	23	0
19	B	1227	CLA	11	0
19	2	2014	CLA	35	0
19	A	1122	CLA	24	0
19	2	4009	CLA	6	0
22	2	7031	LMU	2	0
19	B	1234	CLA	11	0
19	3	3013	CLA	18	0
19	G	1242	CLA	9	0
22	G	7051	LMU	1	0
22	R	7014	LMU	4	0
19	A	1121	CLA	8	0
19	B	1228	CLA	14	0
19	K	1142	CLA	15	1
22	L	7029	LMU	11	0
19	K	3009	CLA	3	7
19	A	1107	CLA	40	0
19	B	1216	CLA	15	0
19	A	1151	CLA	18	0
19	B	1238	CLA	24	0
22	F	7036	LMU	12	0
19	4	4004	CLA	2	0
19	A	1237	CLA	31	0
21	B	6006	BCR	14	0
19	I	1204	CLA	7	0
19	4	4015	CLA	4	0
21	A	6008	BCR	27	0

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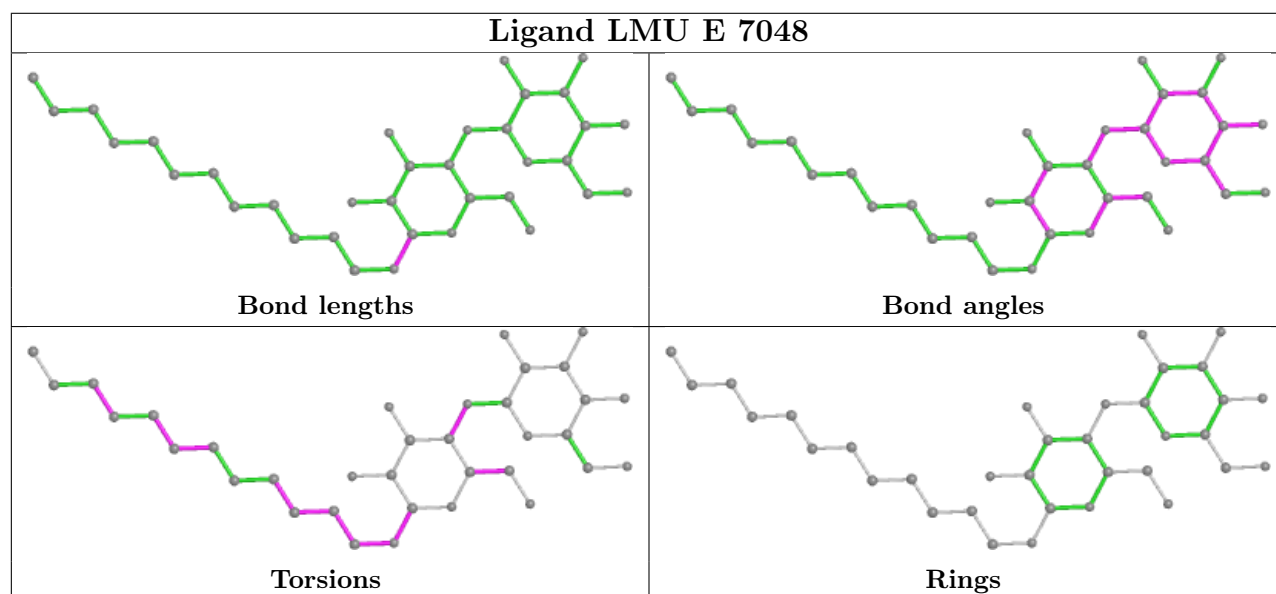
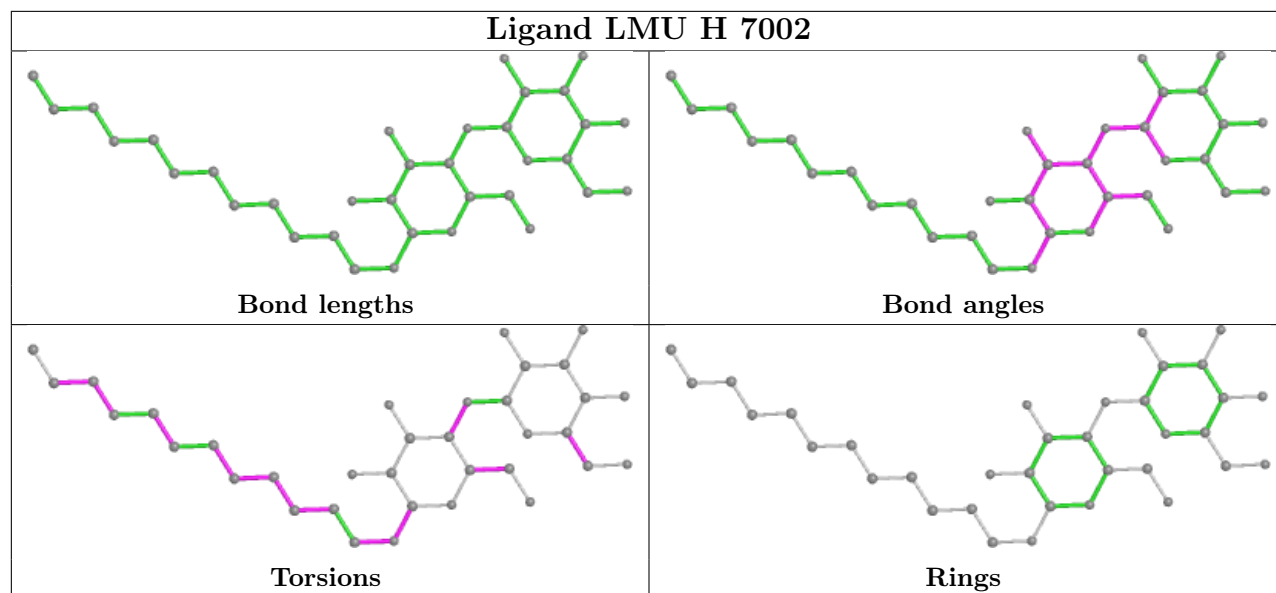
Mol	Chain	Res	Type	Clashes	Symm-Clashes
19	R	1144	CLA	10	0
19	4	1009	CLA	3	0
19	4	4006	CLA	11	0
19	A	1111	CLA	21	0
22	2	7046	LMU	1	0
22	K	7042	LMU	16	0
19	1	1001	CLA	11	0
21	B	6010	BCR	23	0
19	B	1233	CLA	6	0
21	B	6005	BCR	7	0
22	H	7011	LMU	15	0
22	3	7005	LMU	38	0
19	A	1117	CLA	27	0
19	3	3008	CLA	15	0
19	1	1013	CLA	13	0
20	B	5002	PQN	22	0
19	H	1207	CLA	25	0
21	F	6014	BCR	24	0
19	A	1129	CLA	8	0
19	A	1132	CLA	18	0
19	A	1135	CLA	23	0
19	2	2013	CLA	5	0
19	2	2006	CLA	7	0
19	4	4011	CLA	2	0
22	4	7033	LMU	7	0
22	H	7032	LMU	11	0
19	B	1226	CLA	21	0
19	2	2012	CLA	20	0
19	4	4012	CLA	7	0
19	H	1145	CLA	22	0
19	1	1006	CLA	15	0
19	A	1131	CLA	36	0
19	B	1206	CLA	20	0
21	L	6019	BCR	34	0
21	J	6012	BCR	32	0
21	A	6011	BCR	46	0
19	A	9012	CLA	39	0
24	B	7101	LMG	19	0
19	2	2002	CLA	19	0
19	B	1232	CLA	18	0
19	B	1205	CLA	25	0
19	B	1225	CLA	28	0

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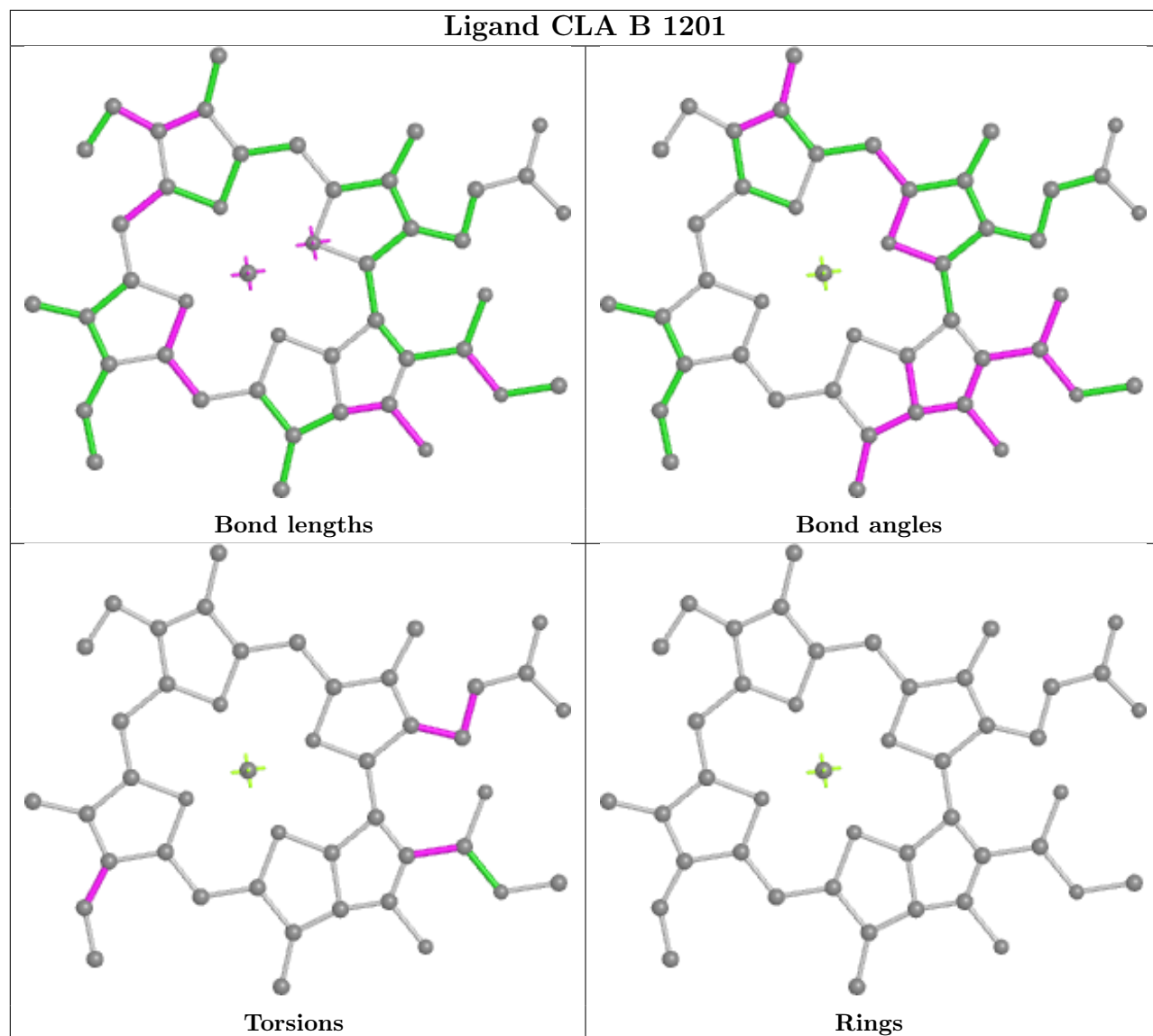
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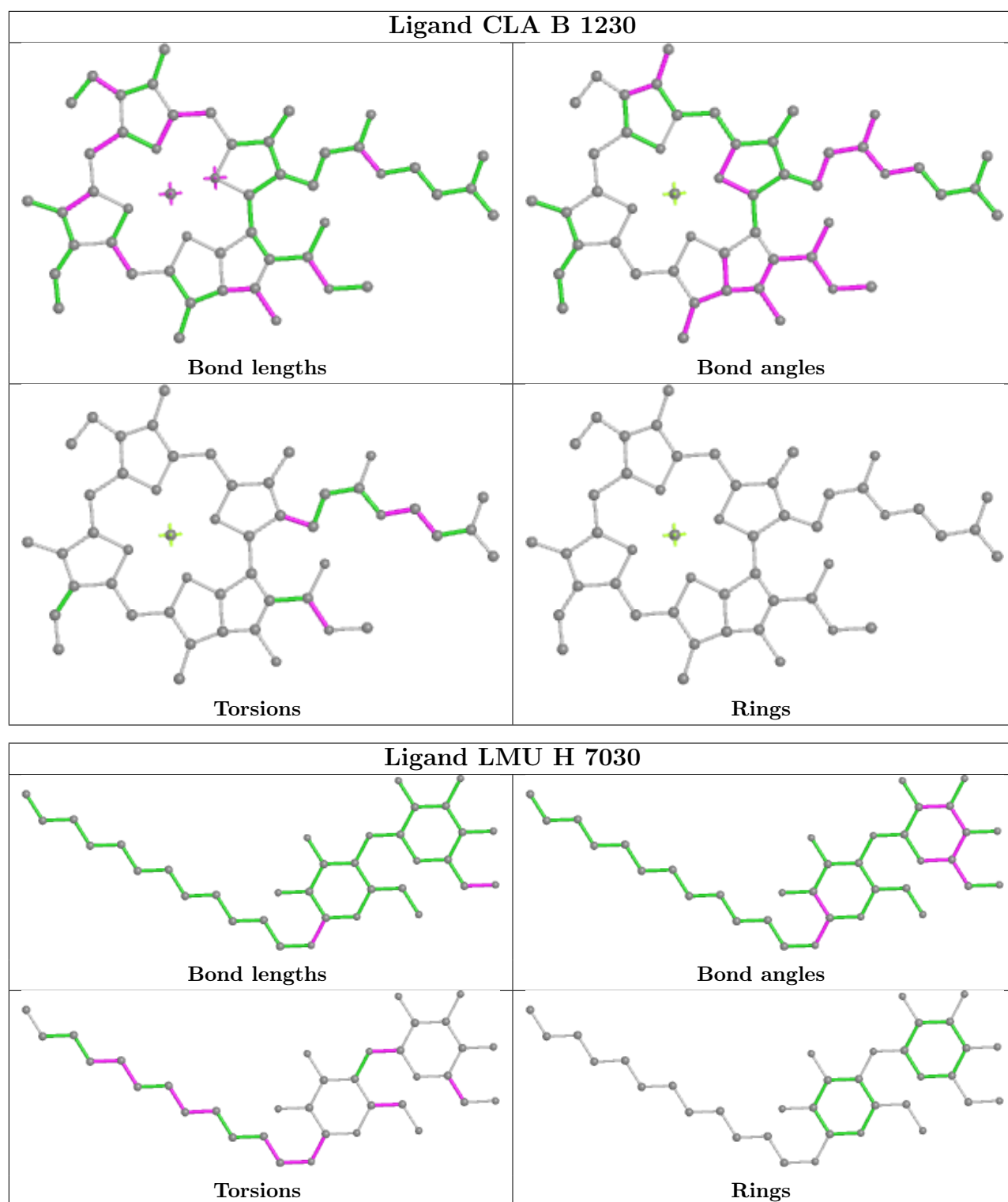
Mol	Chain	Res	Type	Clashes	Symm-Clashes
19	R	1150	CLA	3	0
21	A	6002	BCR	43	0
22	1	7004	LMU	6	0
21	3	6022	BCR	6	0
19	4	4013	CLA	11	0
19	A	1141	CLA	29	0
22	2	7006	LMU	8	0
22	3	7003	LMU	20	0
19	A	1124	CLA	59	0
21	I	6021	BCR	32	0
19	F	1305	CLA	13	0
19	1	1003	CLA	5	0
22	H	7028	LMU	2	0
19	A	1105	CLA	26	0
22	G	7026	LMU	9	0
22	2	7027	LMU	3	0
22	H	7043	LMU	3	0
19	A	1116	CLA	9	0
19	K	1143	CLA	29	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.

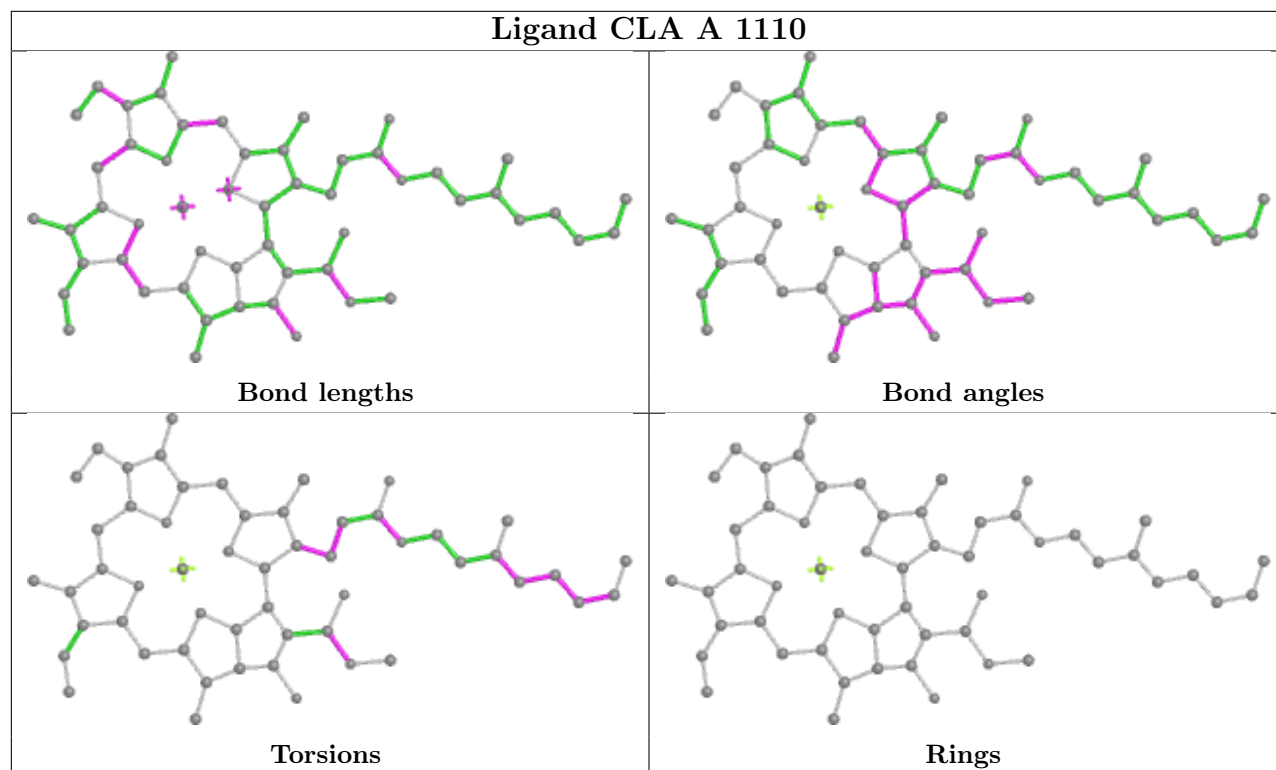


Ligand CLA B 1201

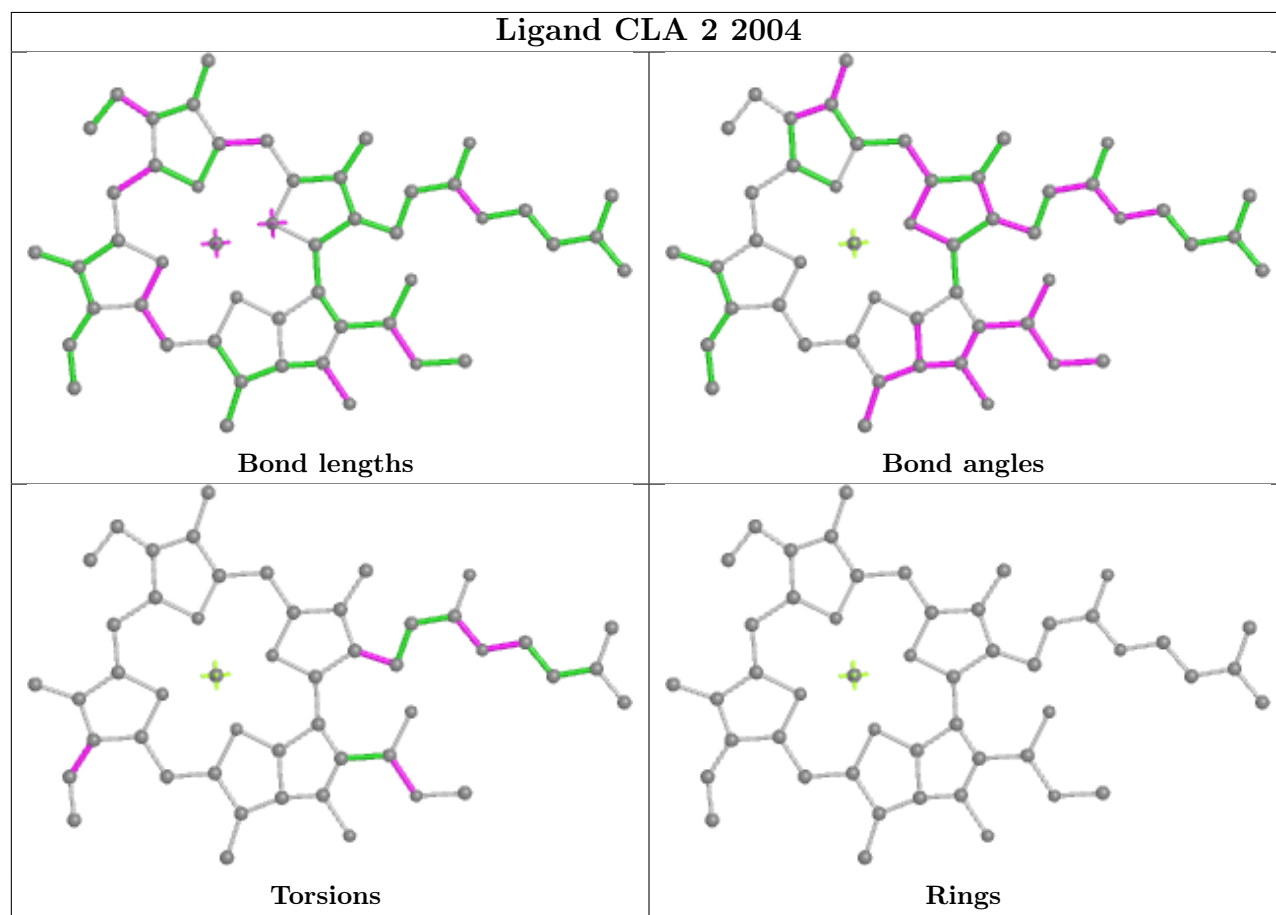


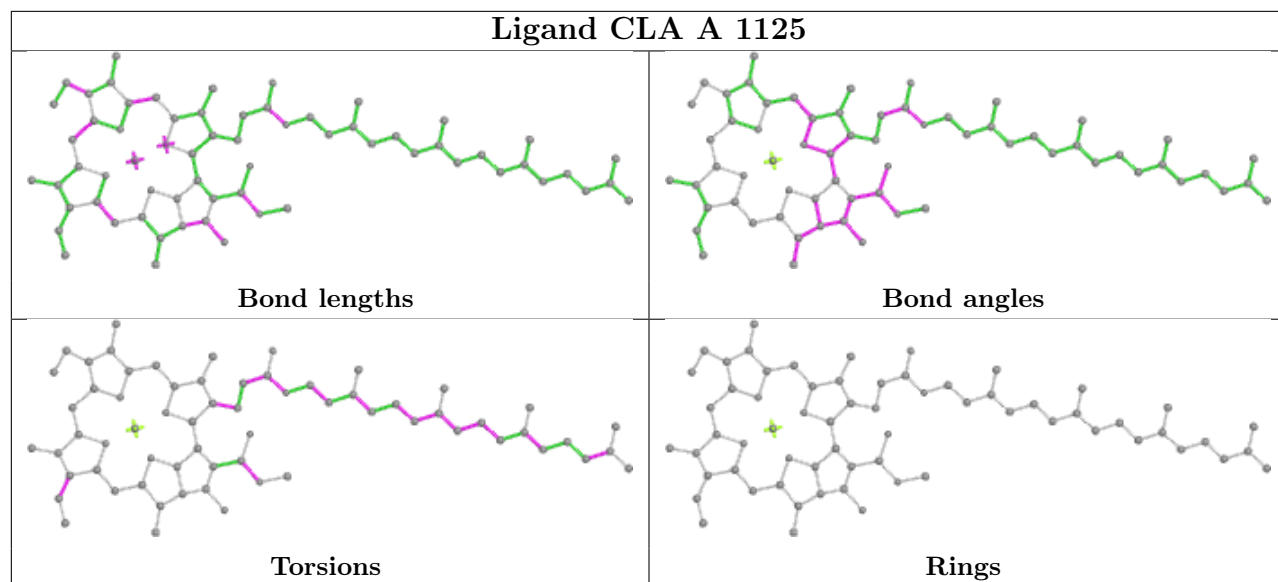


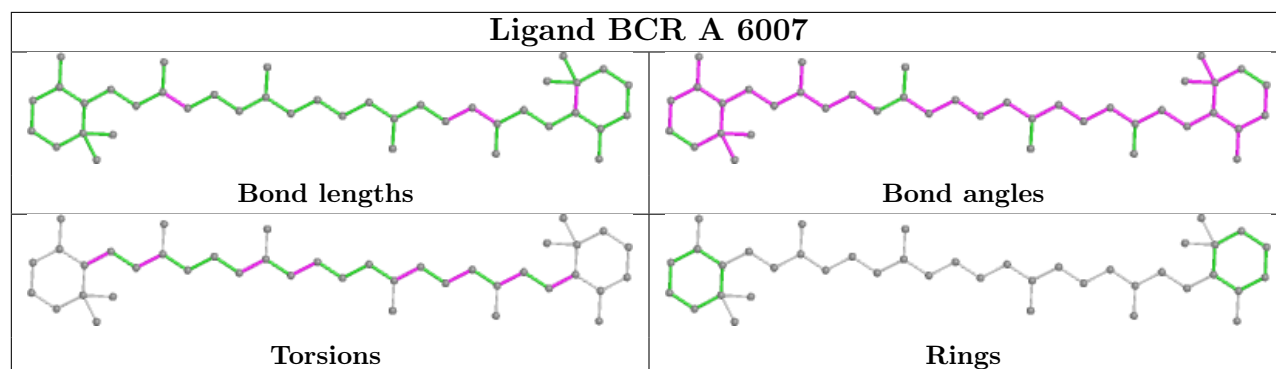
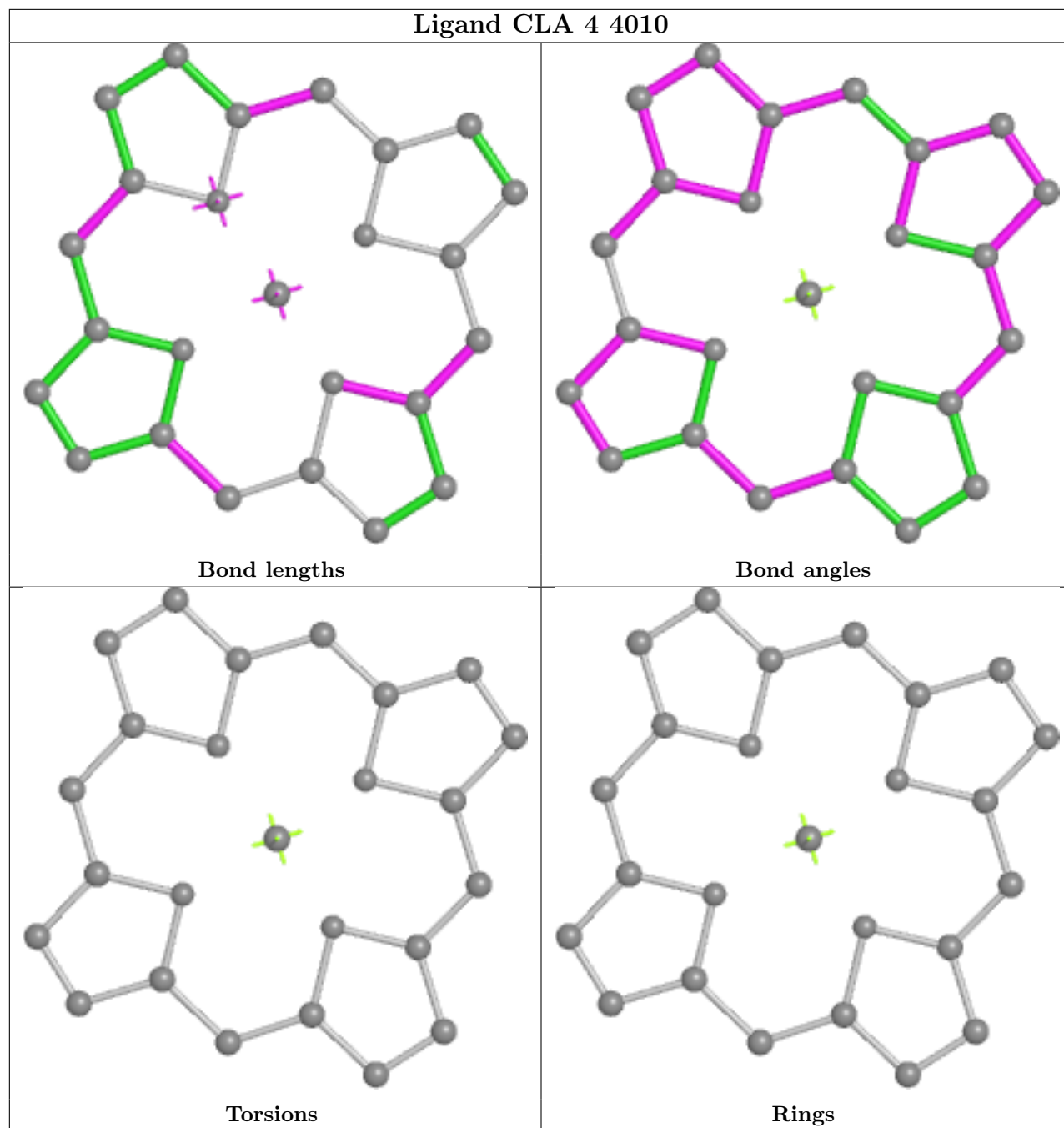
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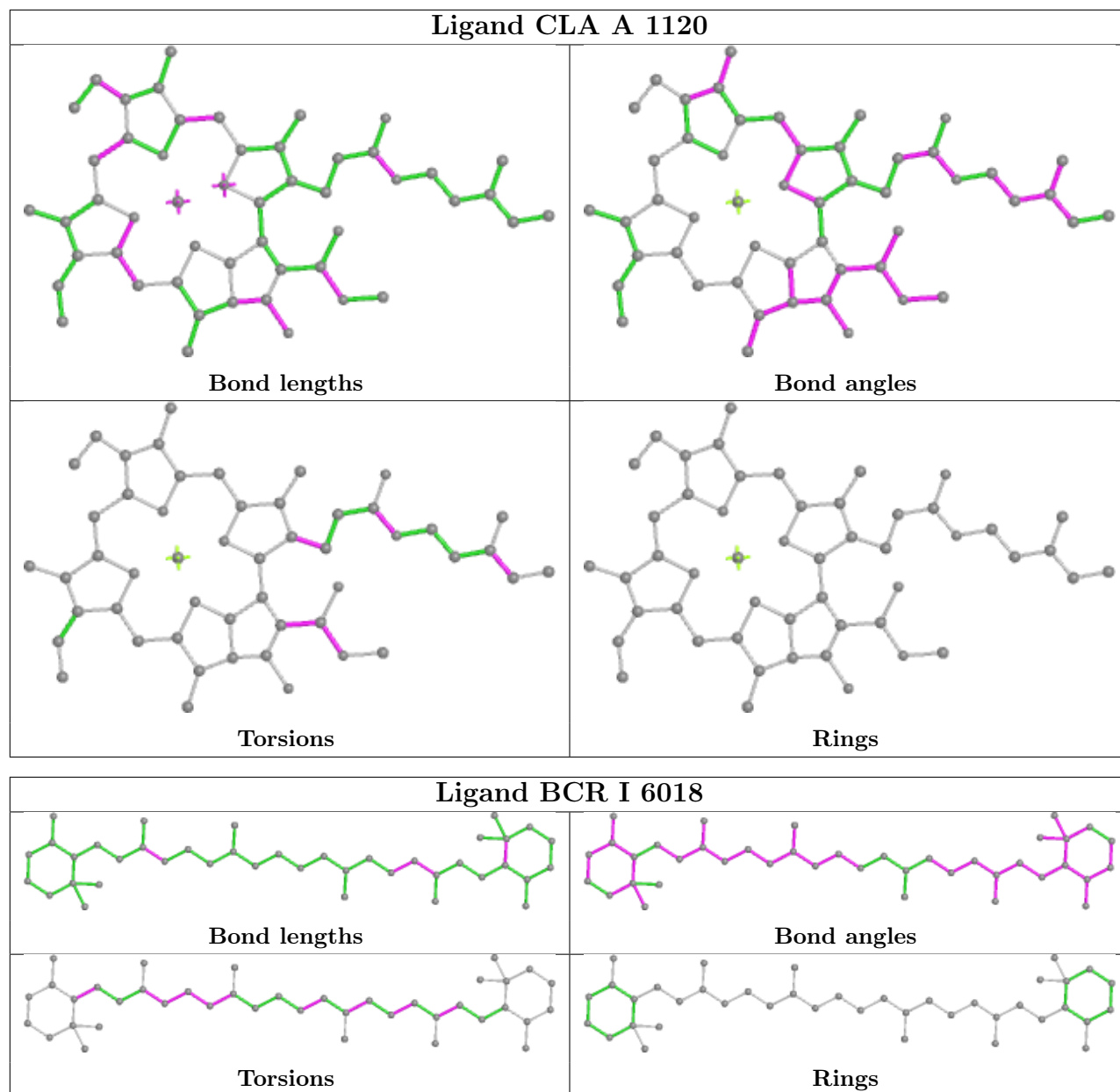


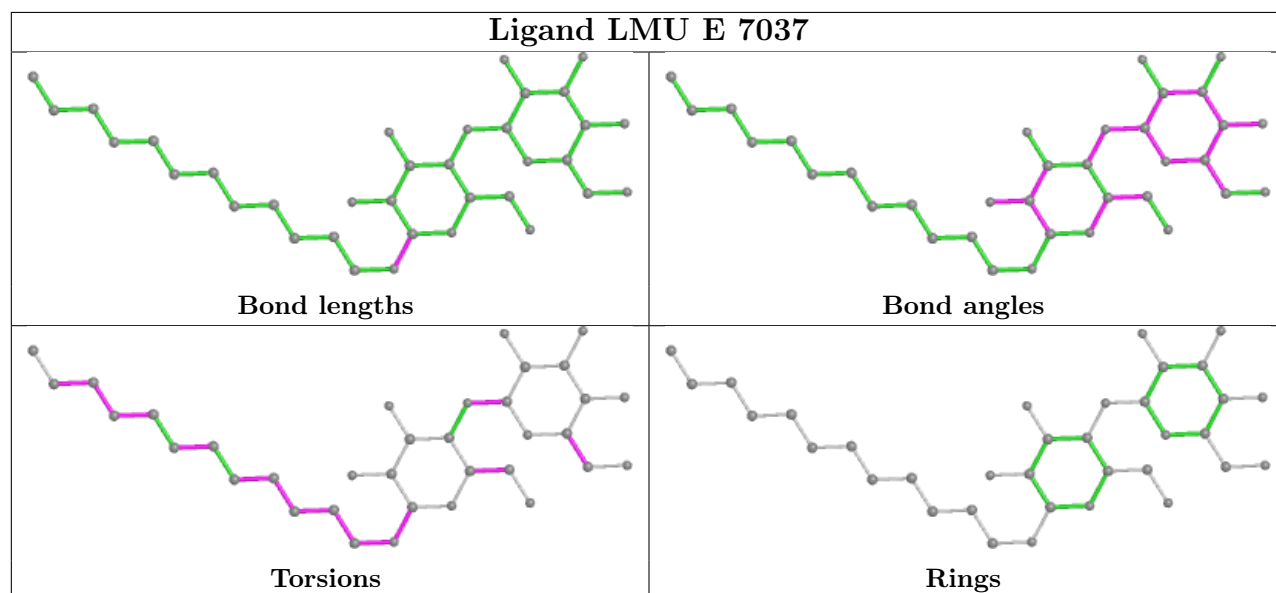
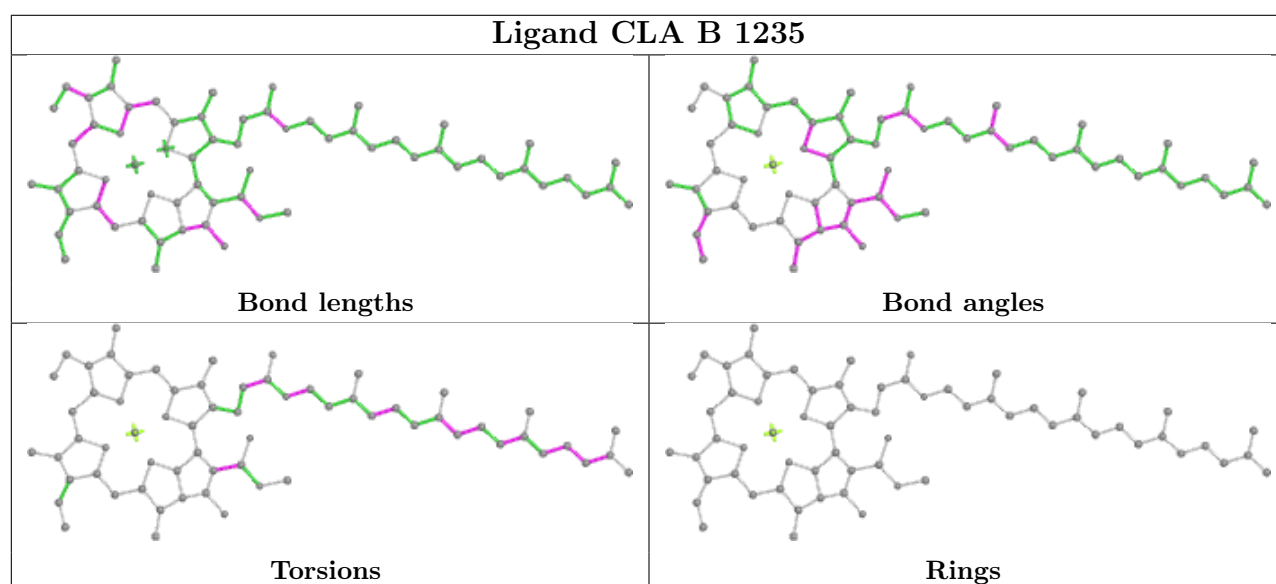
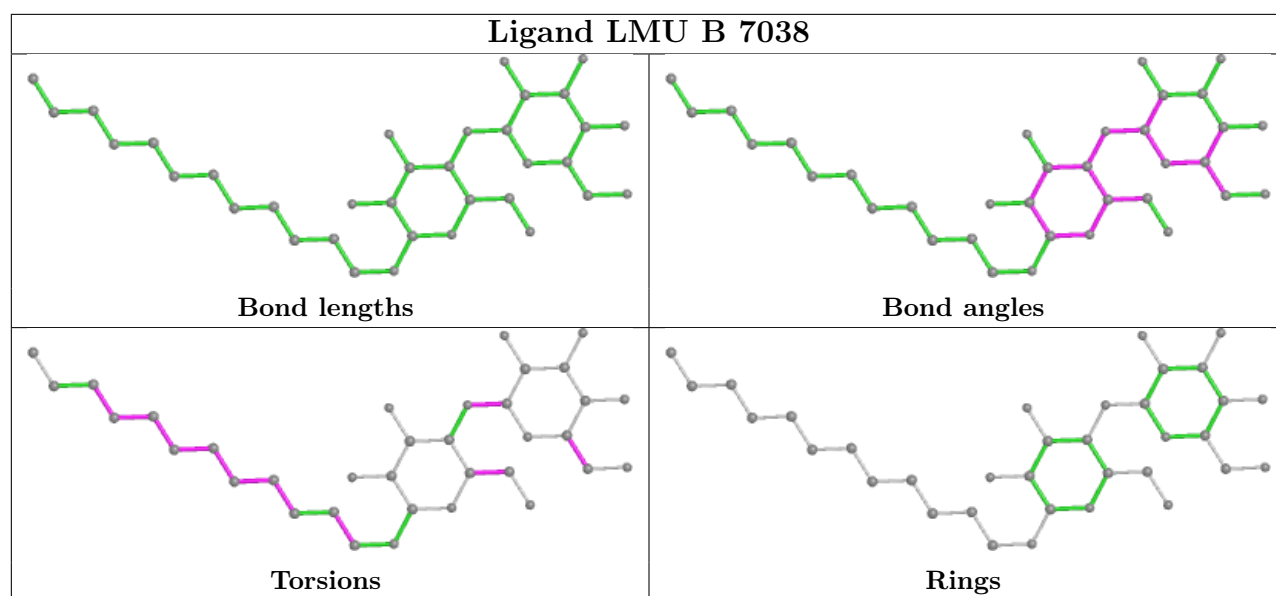
Ligand CLA 2 2004

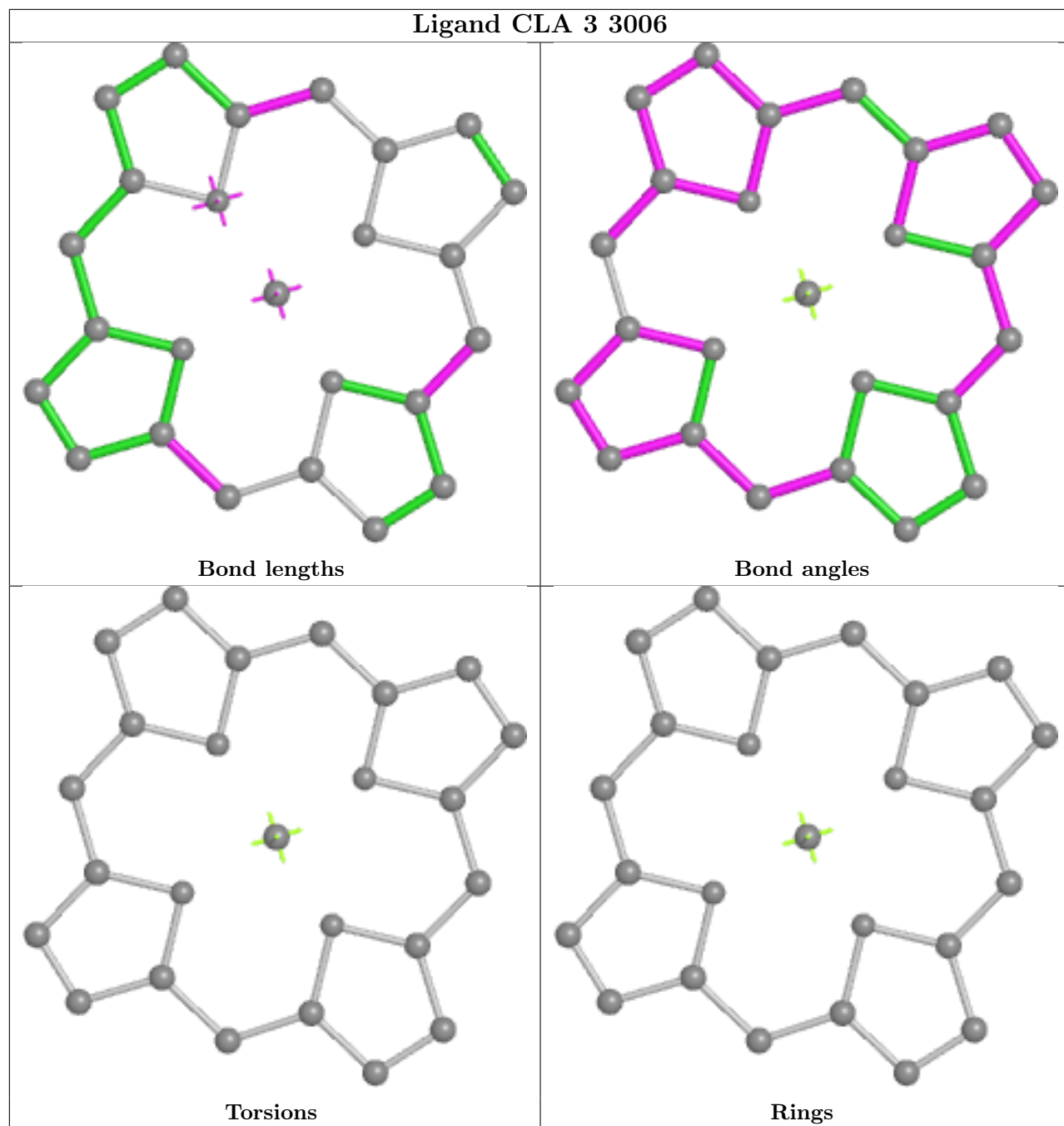


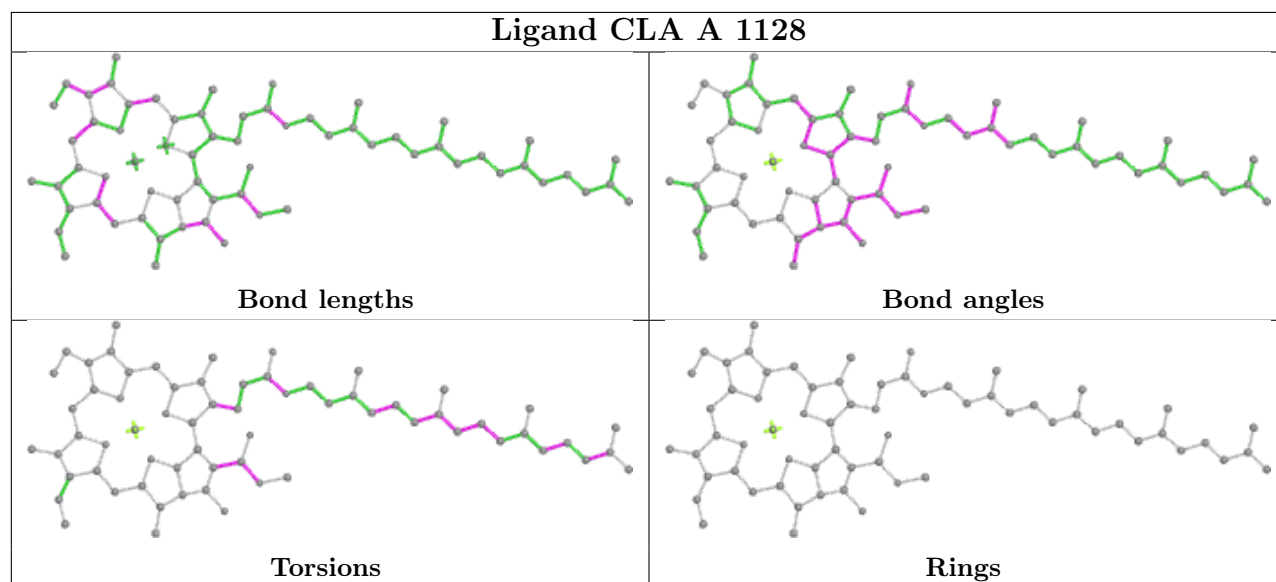
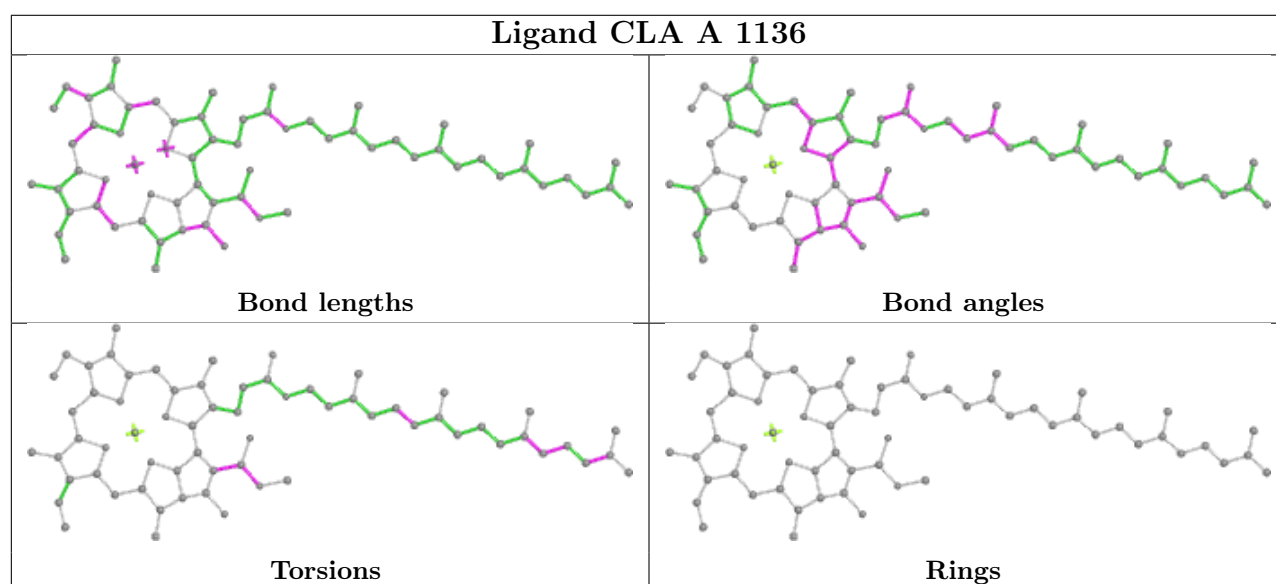
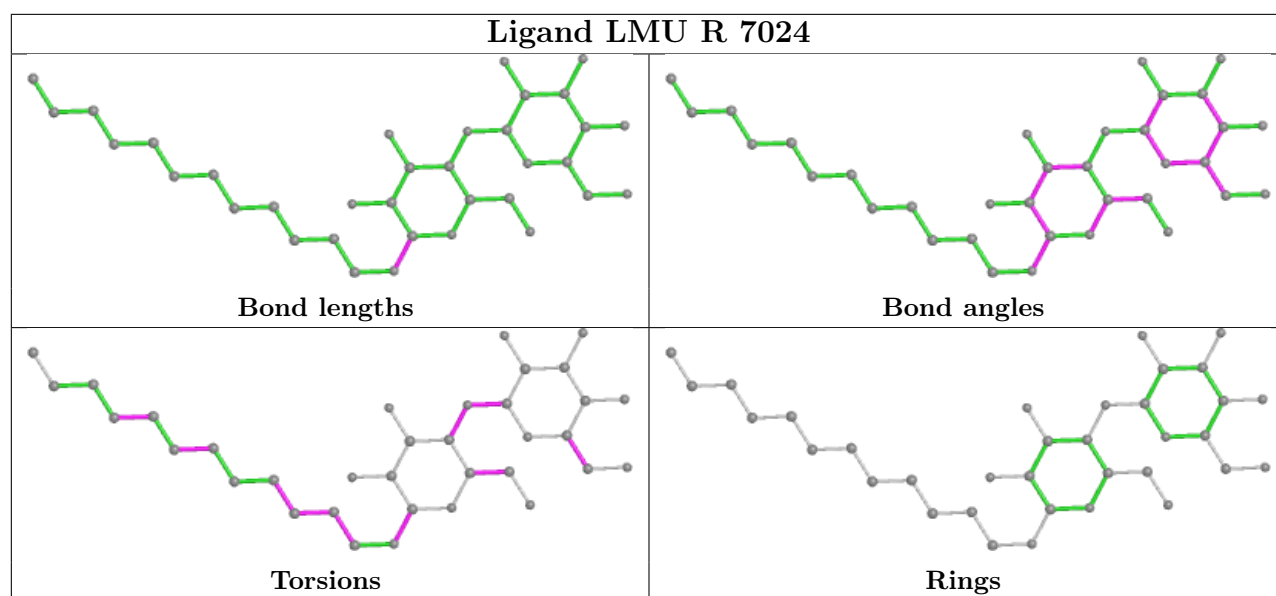


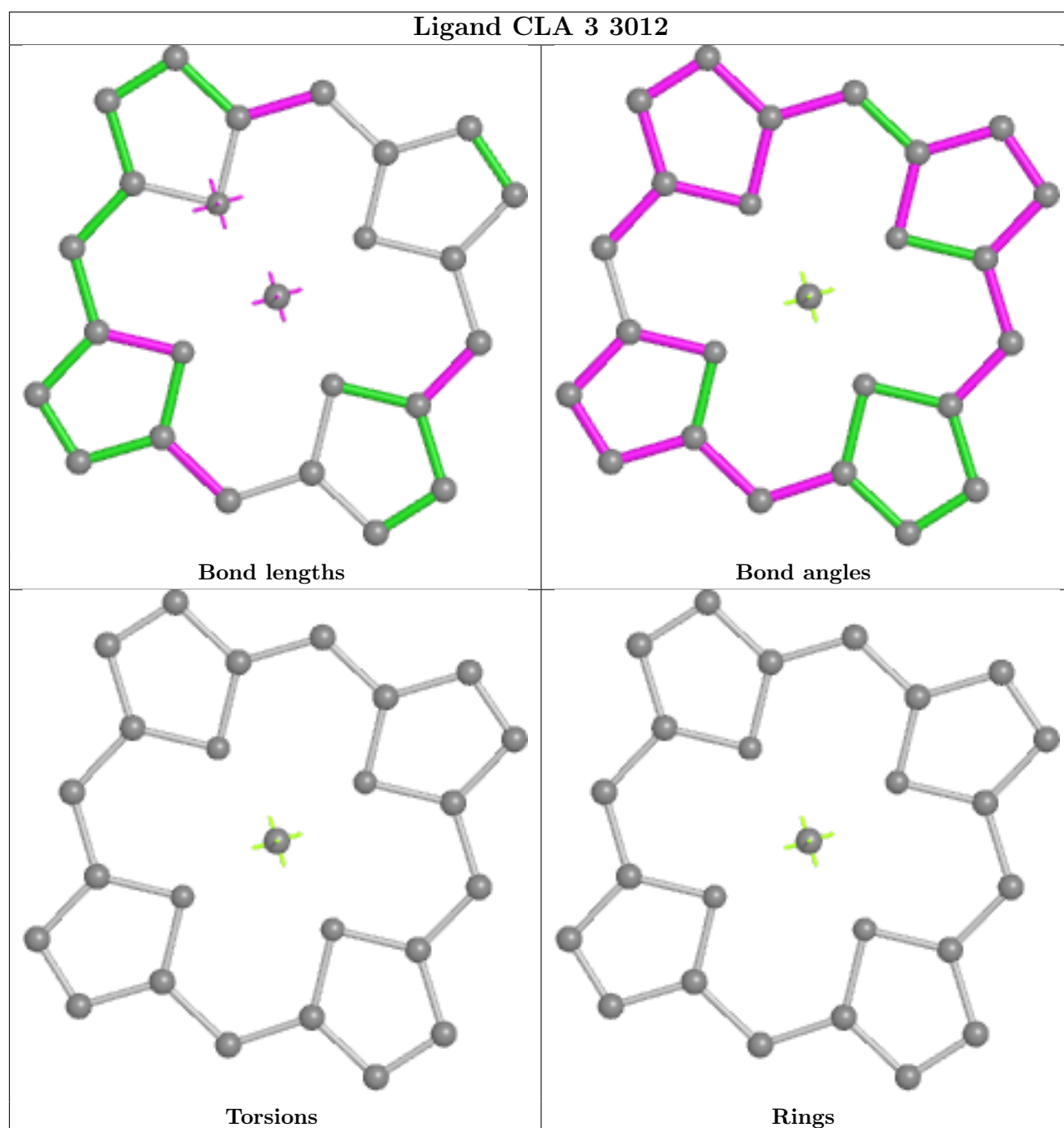


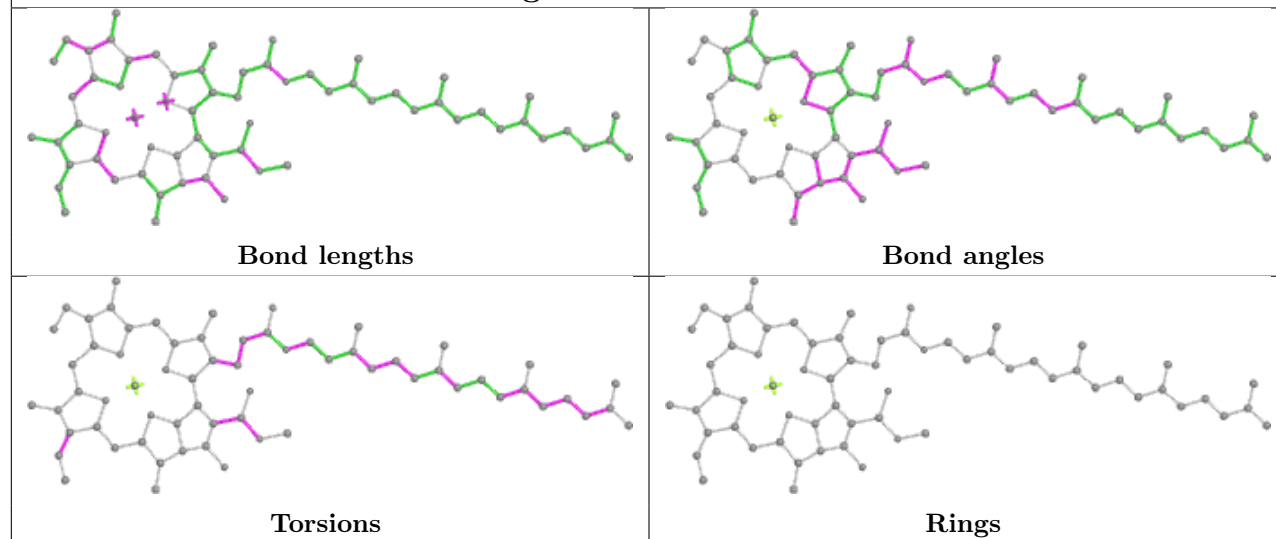
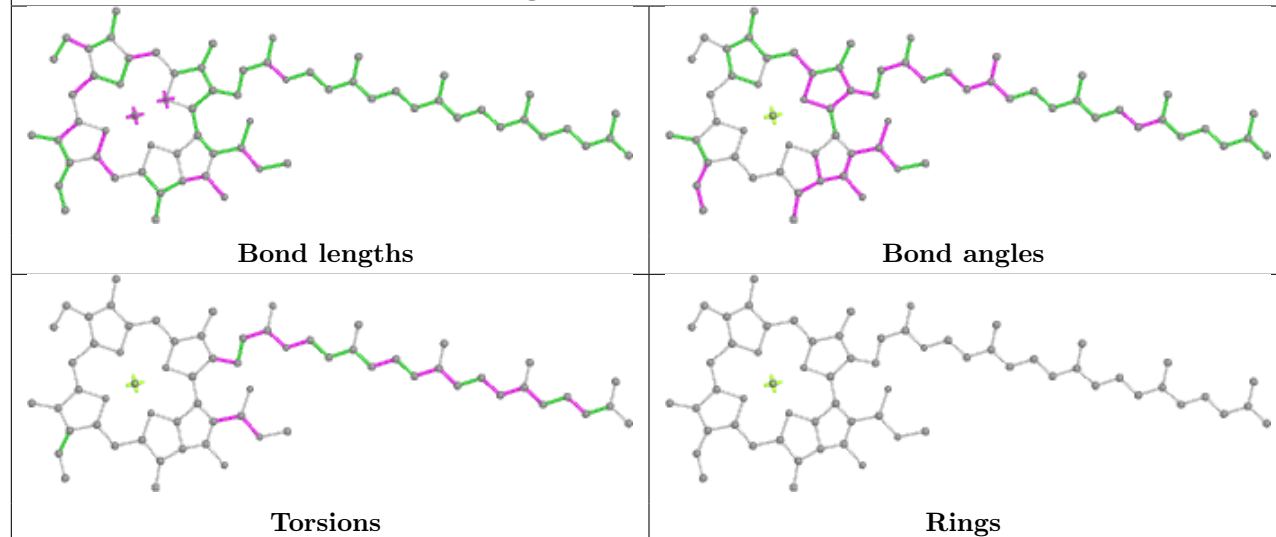


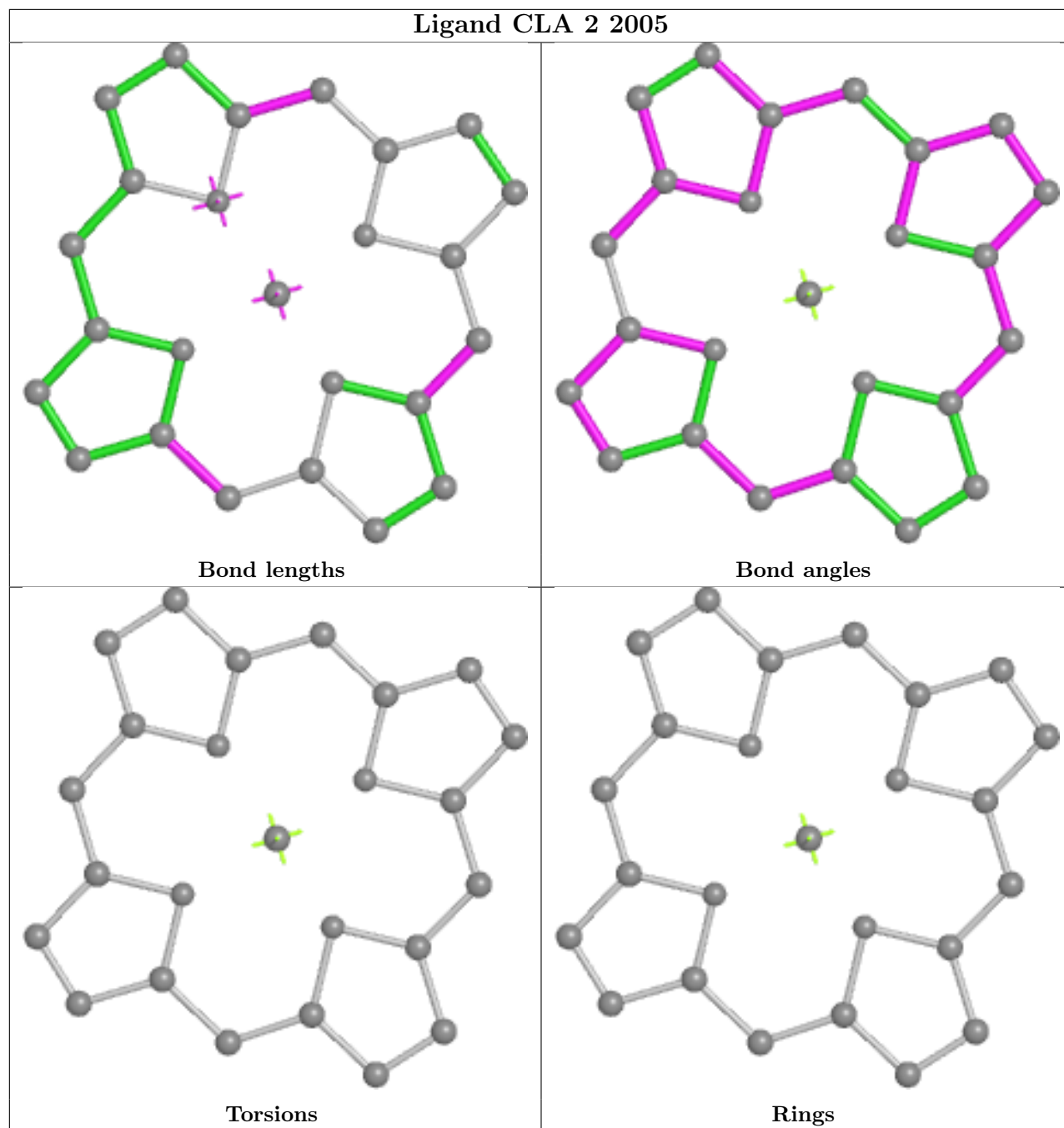


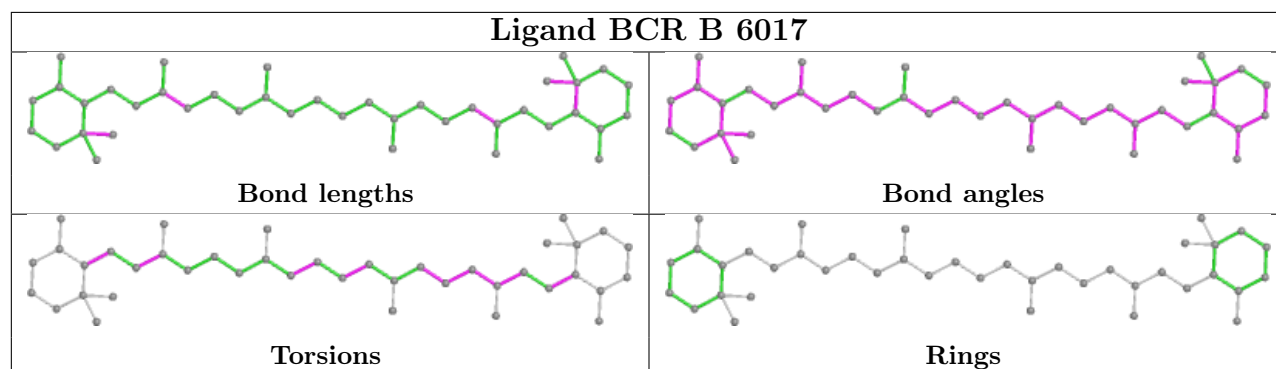
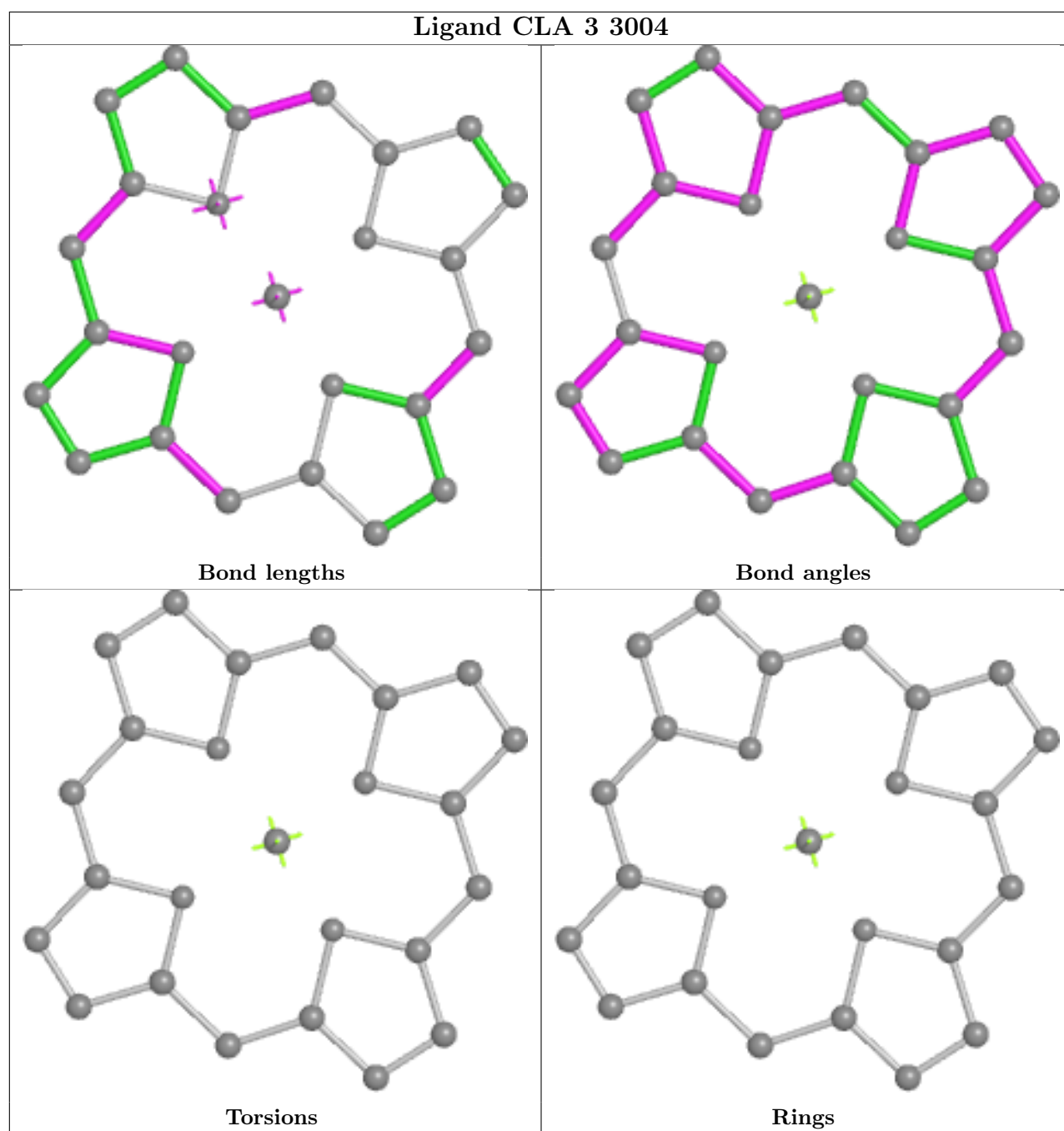




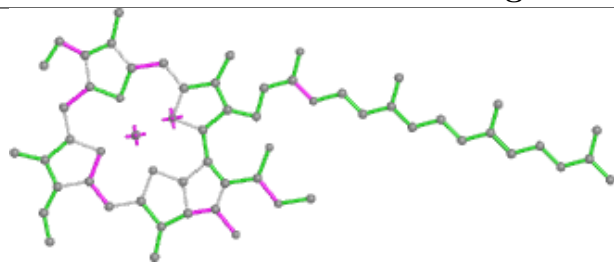


Ligand CLA A 1103**Ligand CLA B 1202**

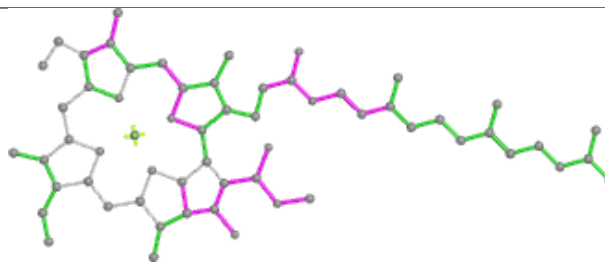




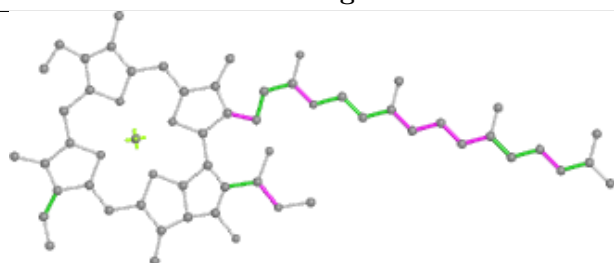
Ligand CLA B 1215



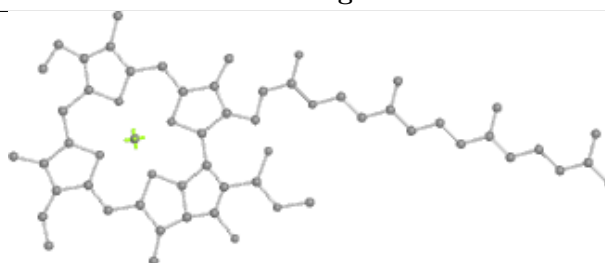
Bond lengths



Bond angles

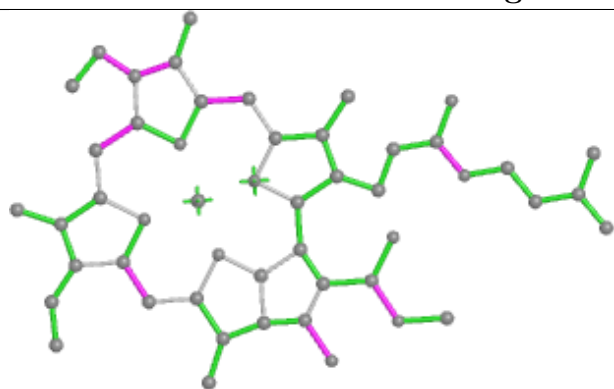


Torsions

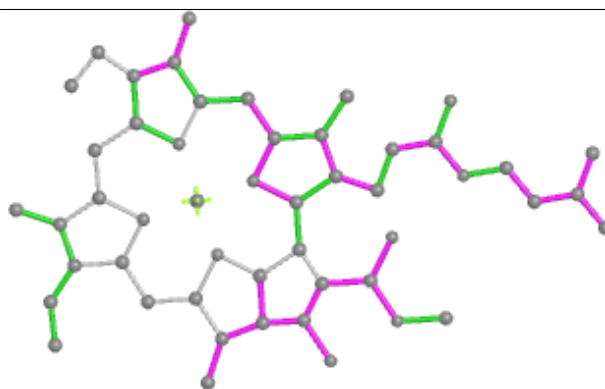


Rings

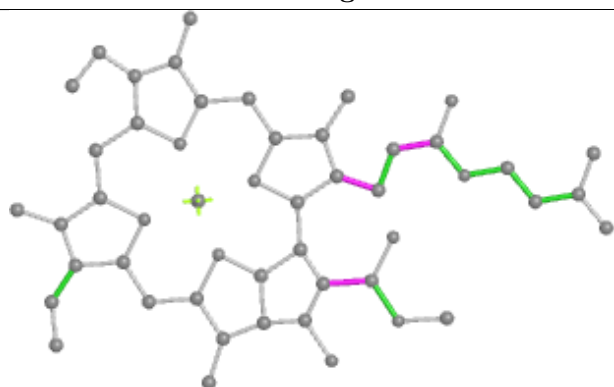
Ligand CLA A 1101



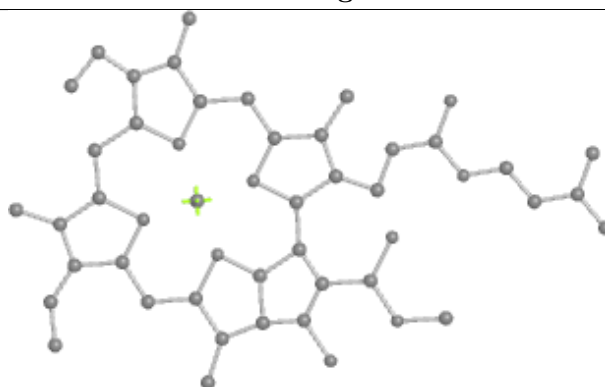
Bond lengths



Bond angles

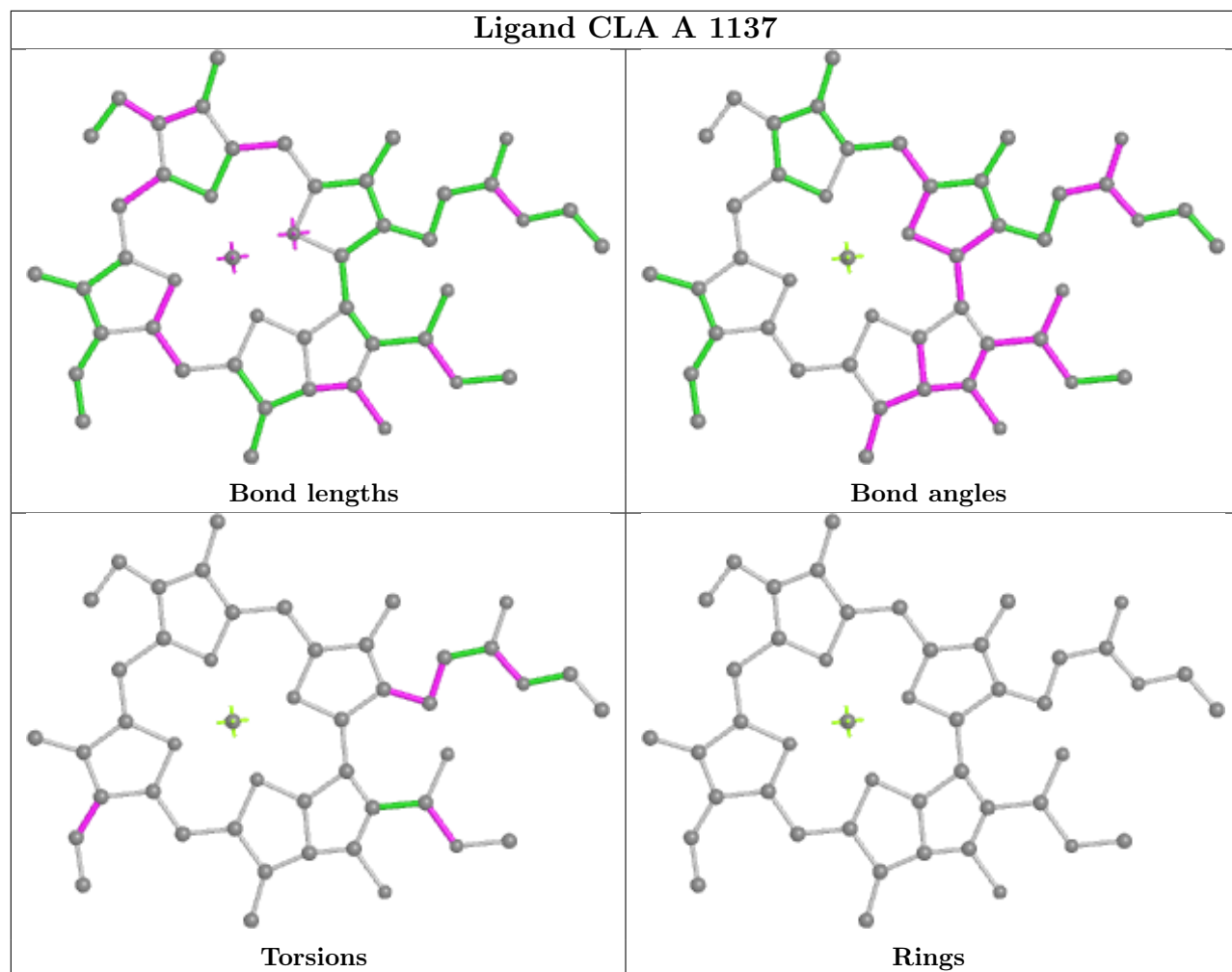


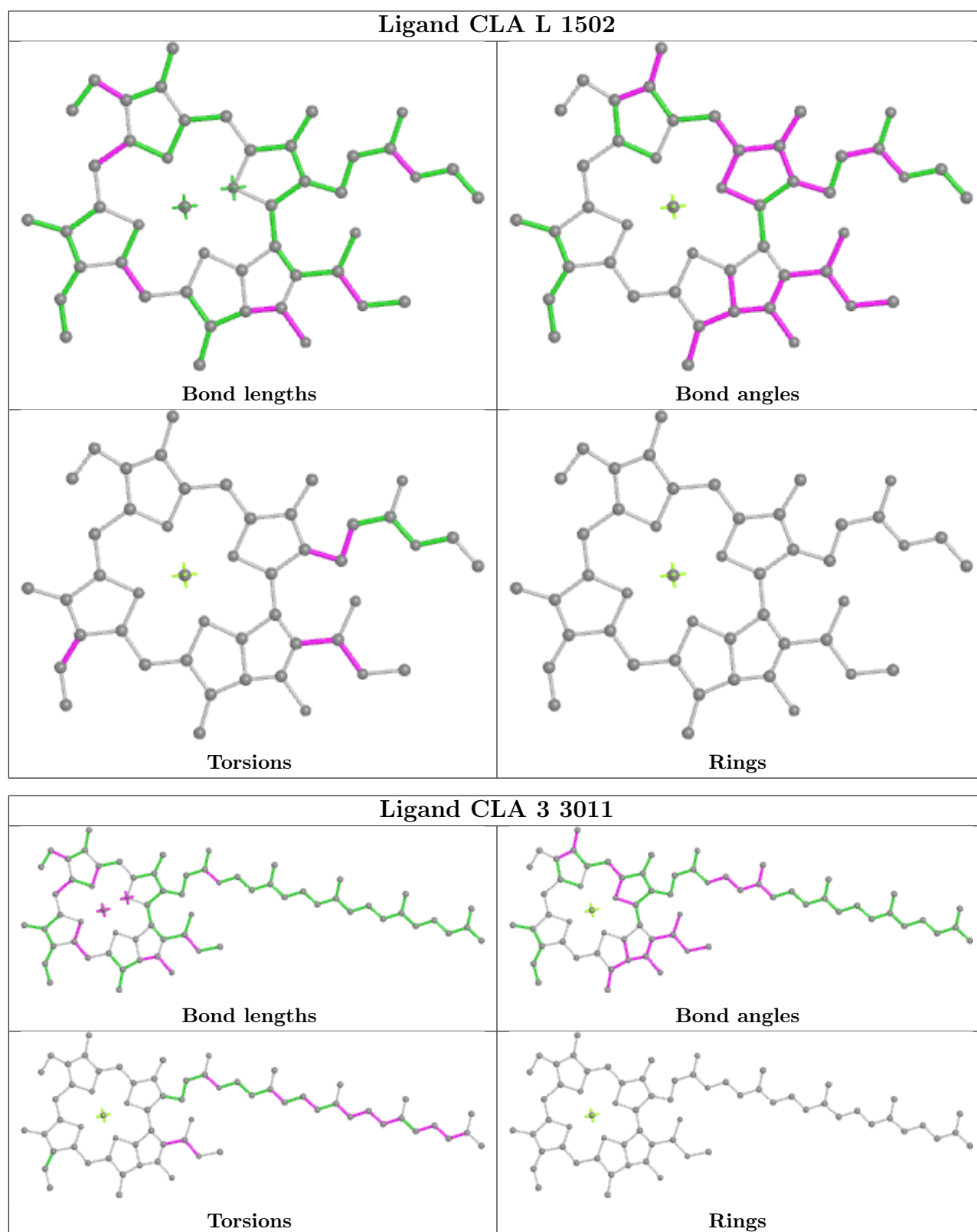
Torsions



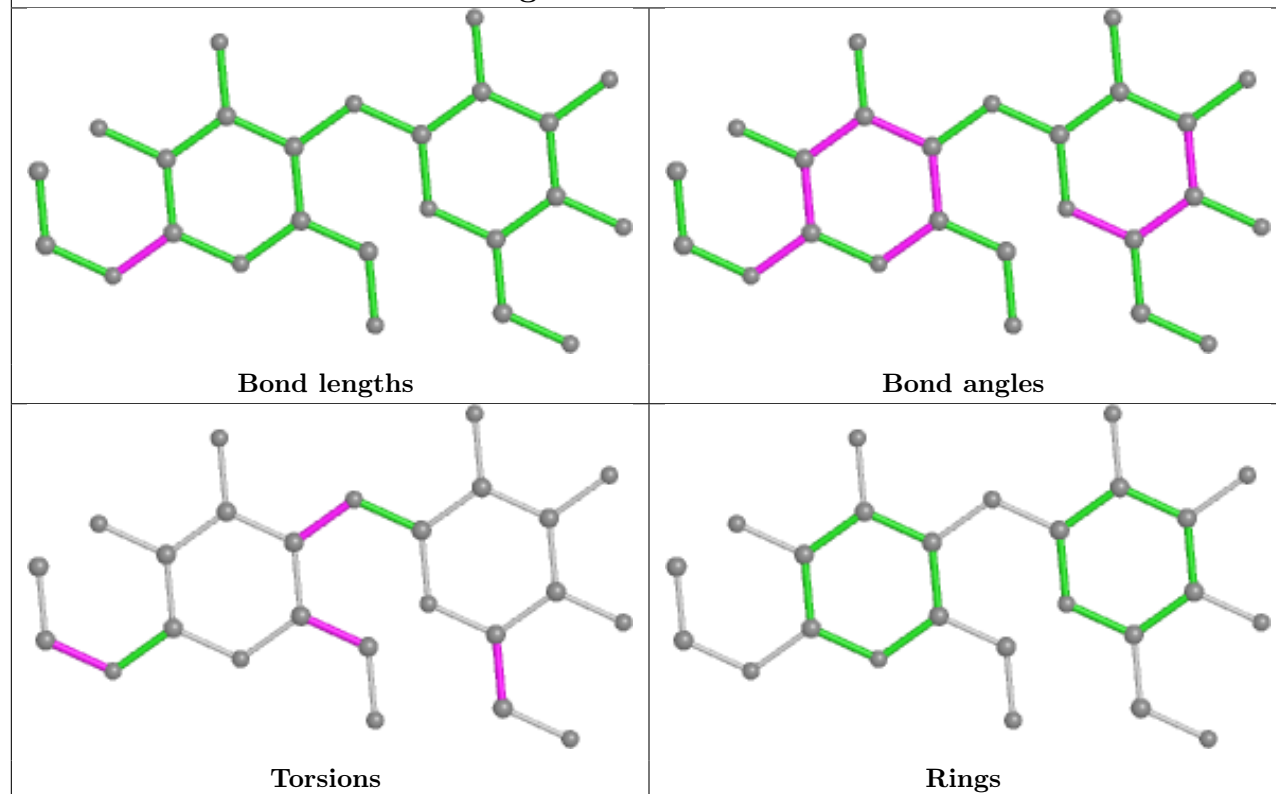
Rings

Ligand CLA A 1137

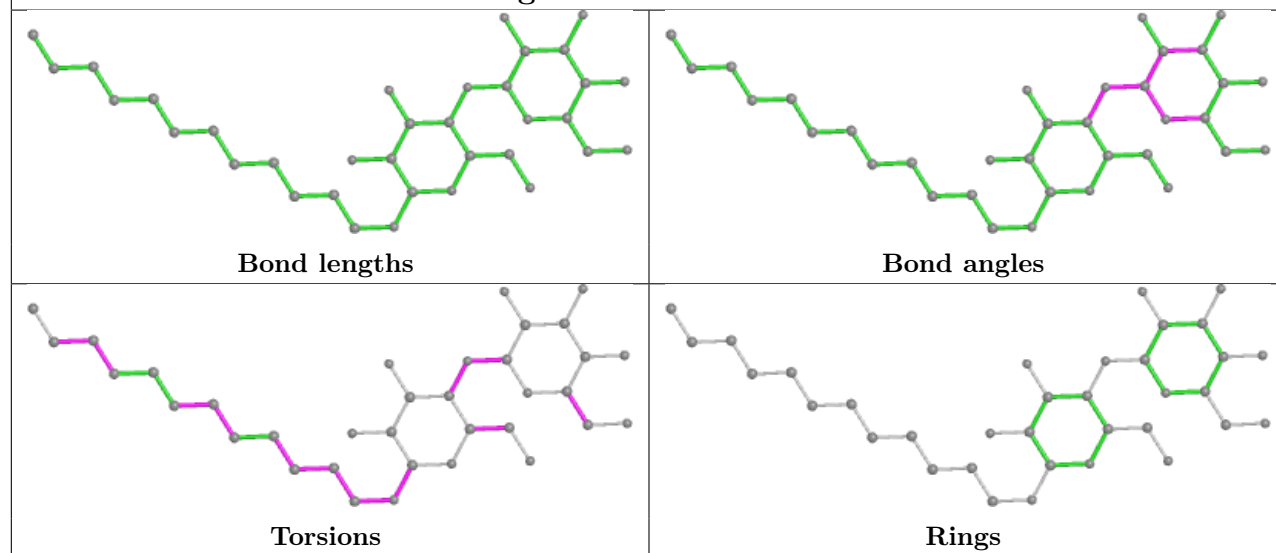


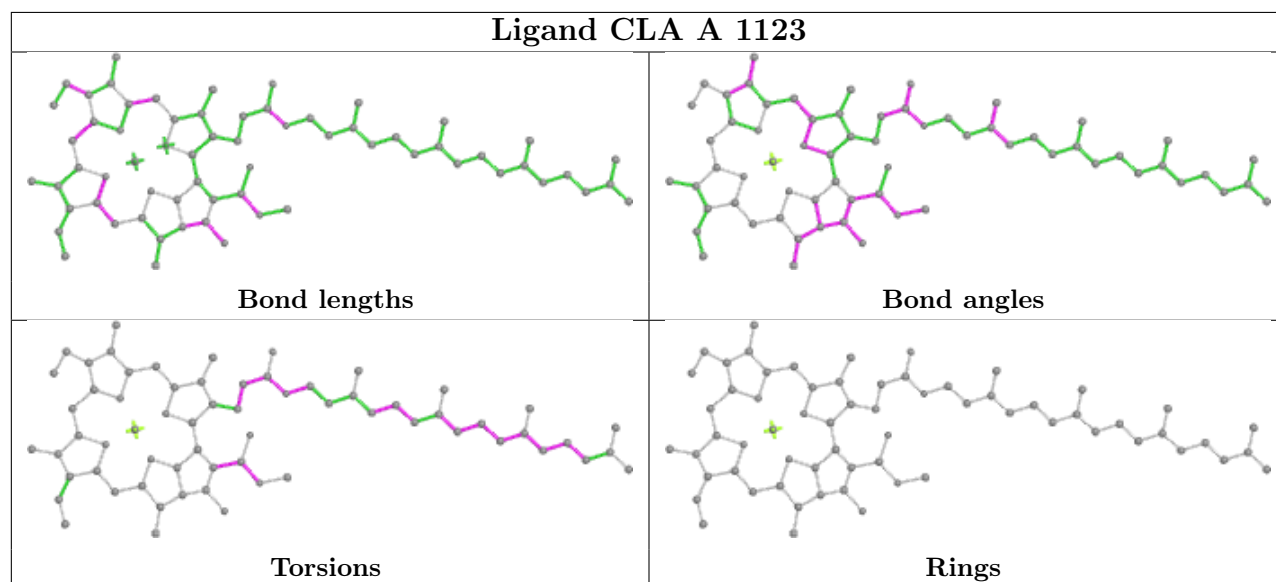
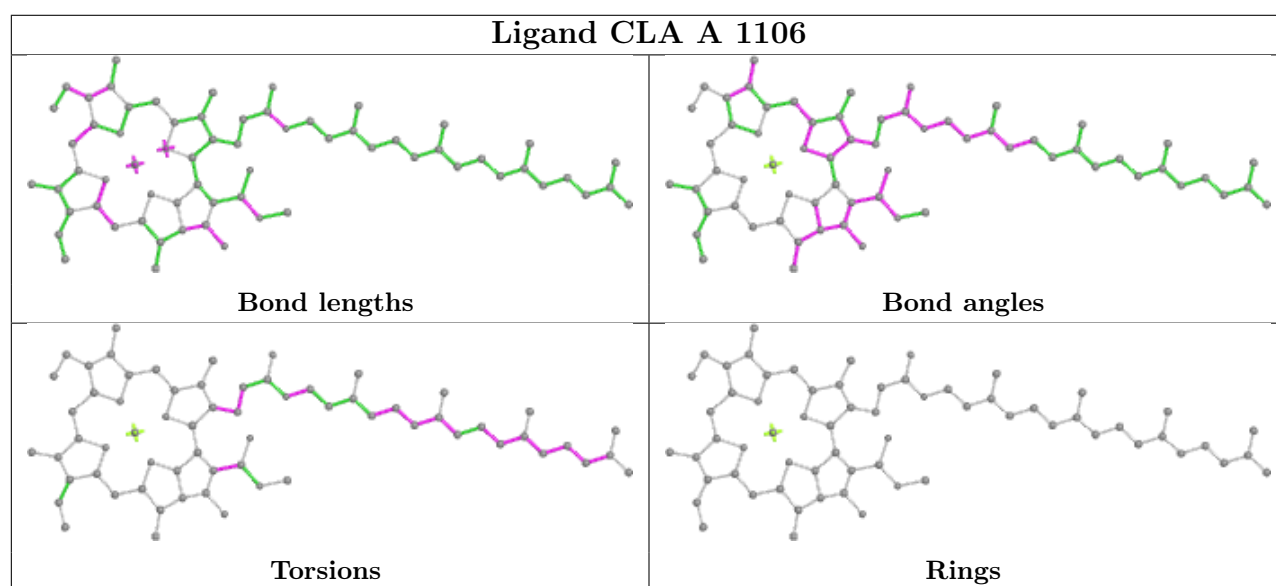
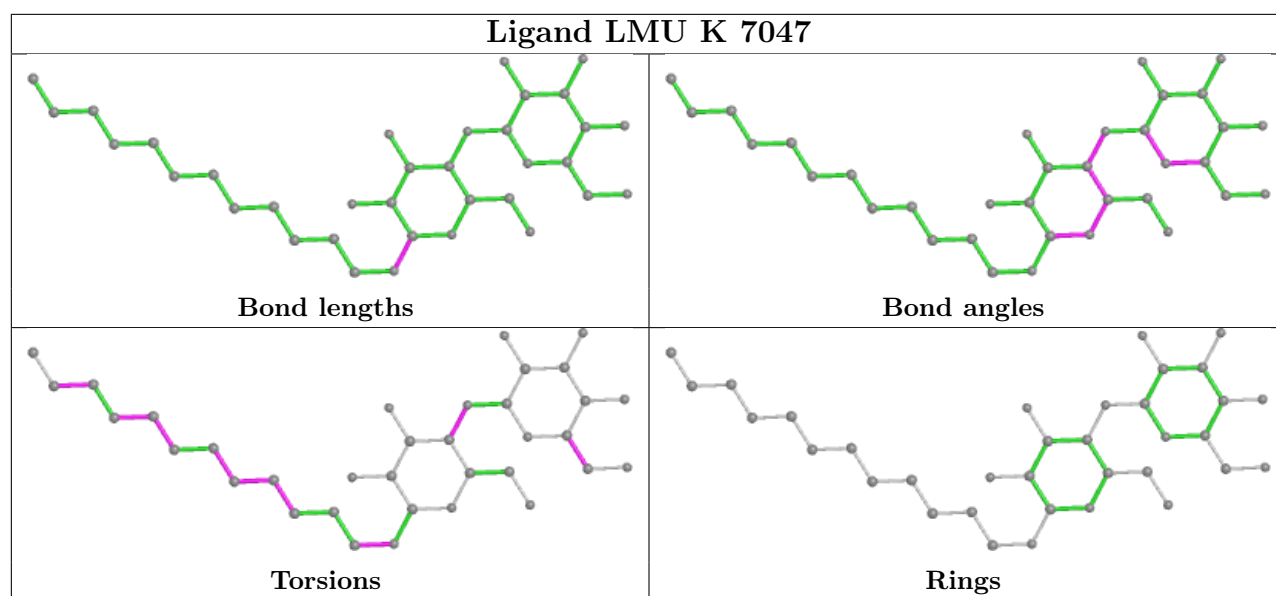


Ligand LMU B 7012

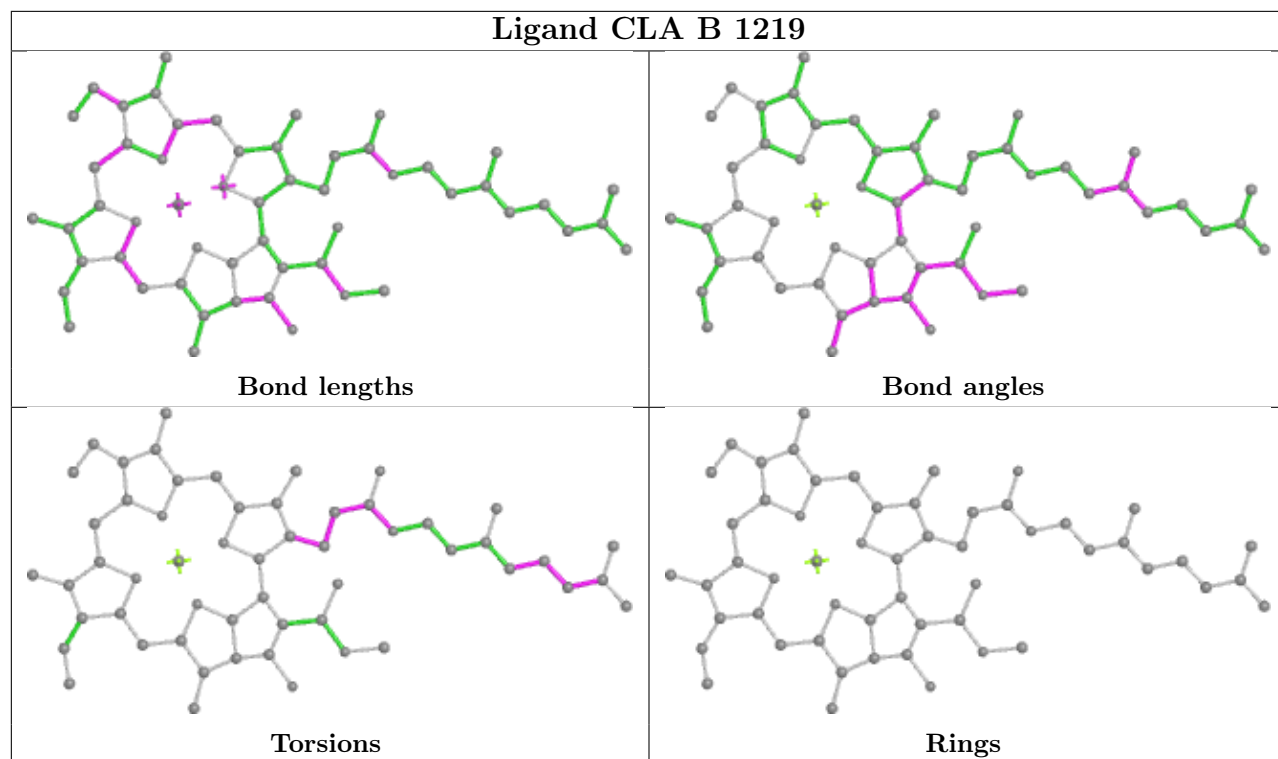


Ligand LMU G 7039

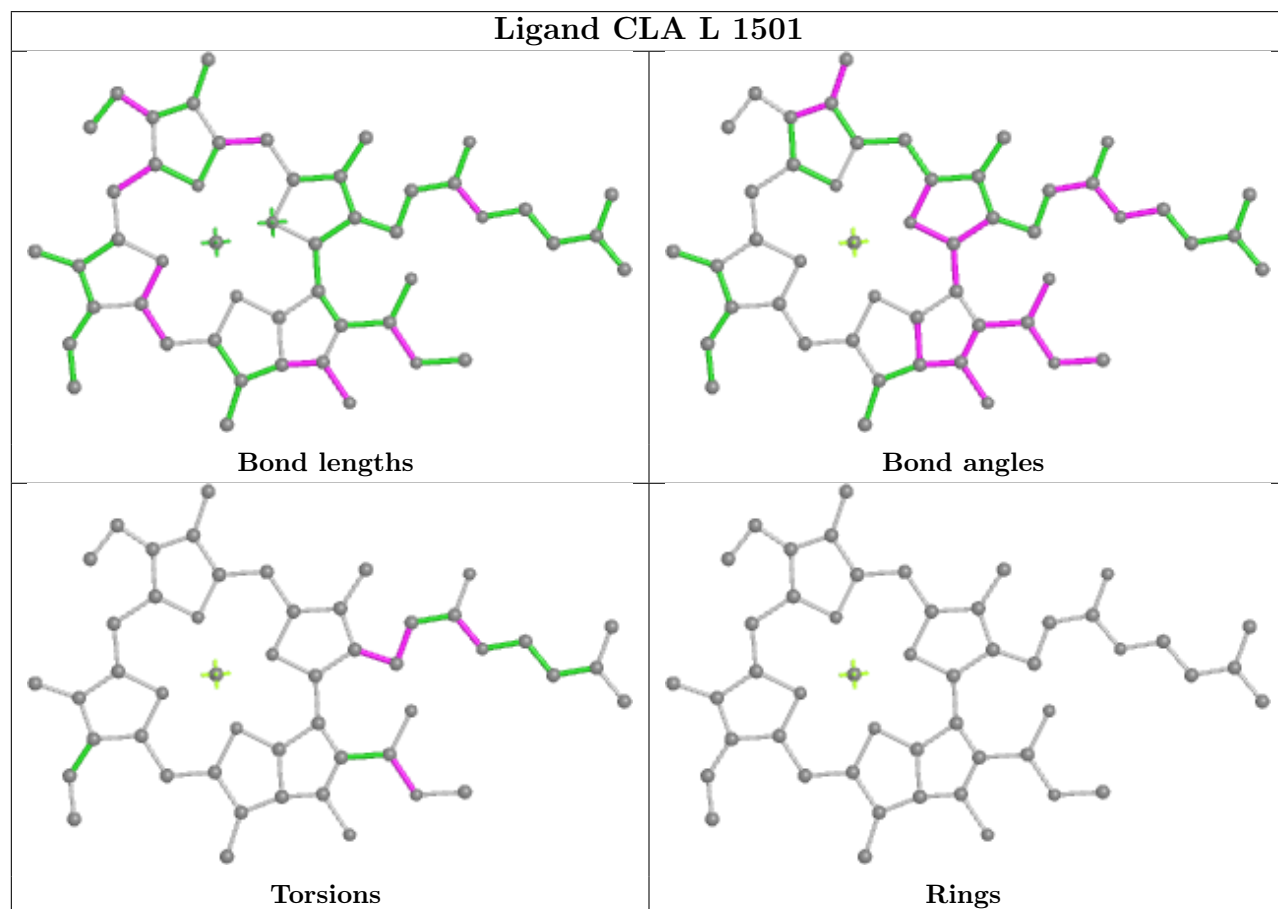




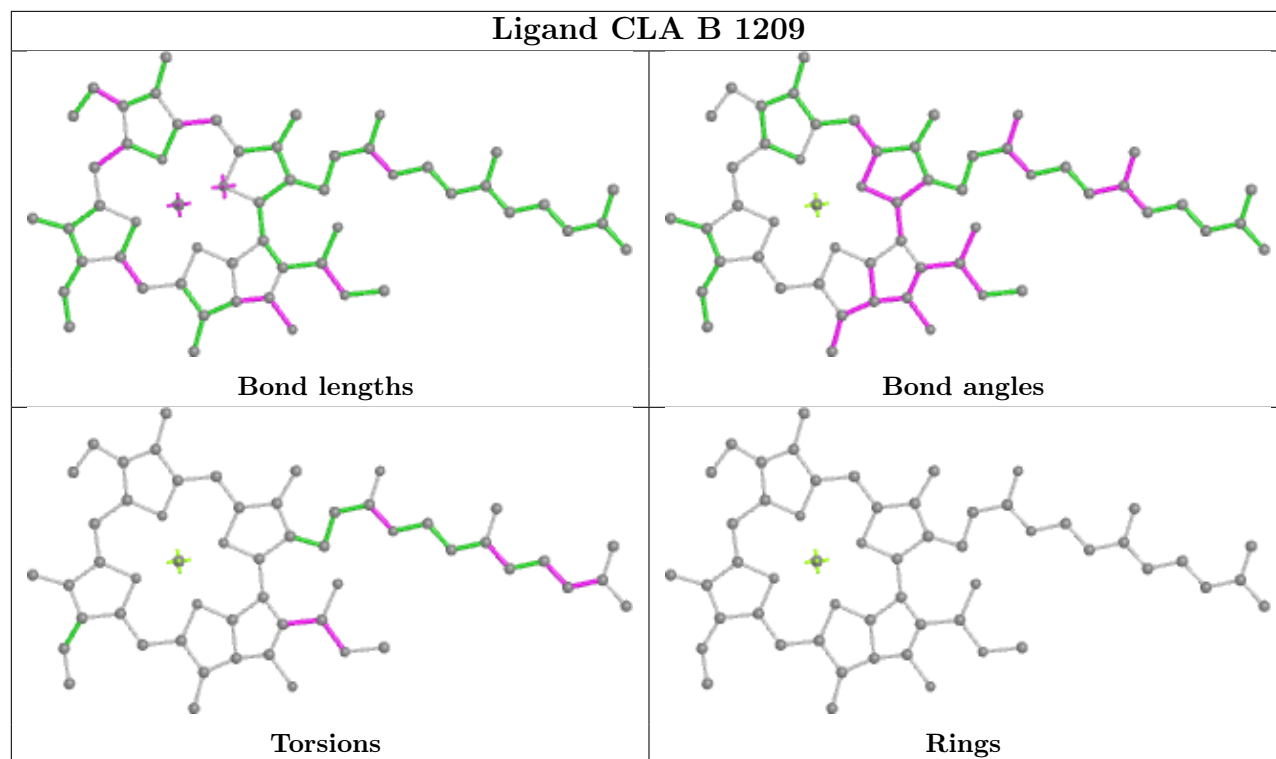
Ligand CLA B 1219



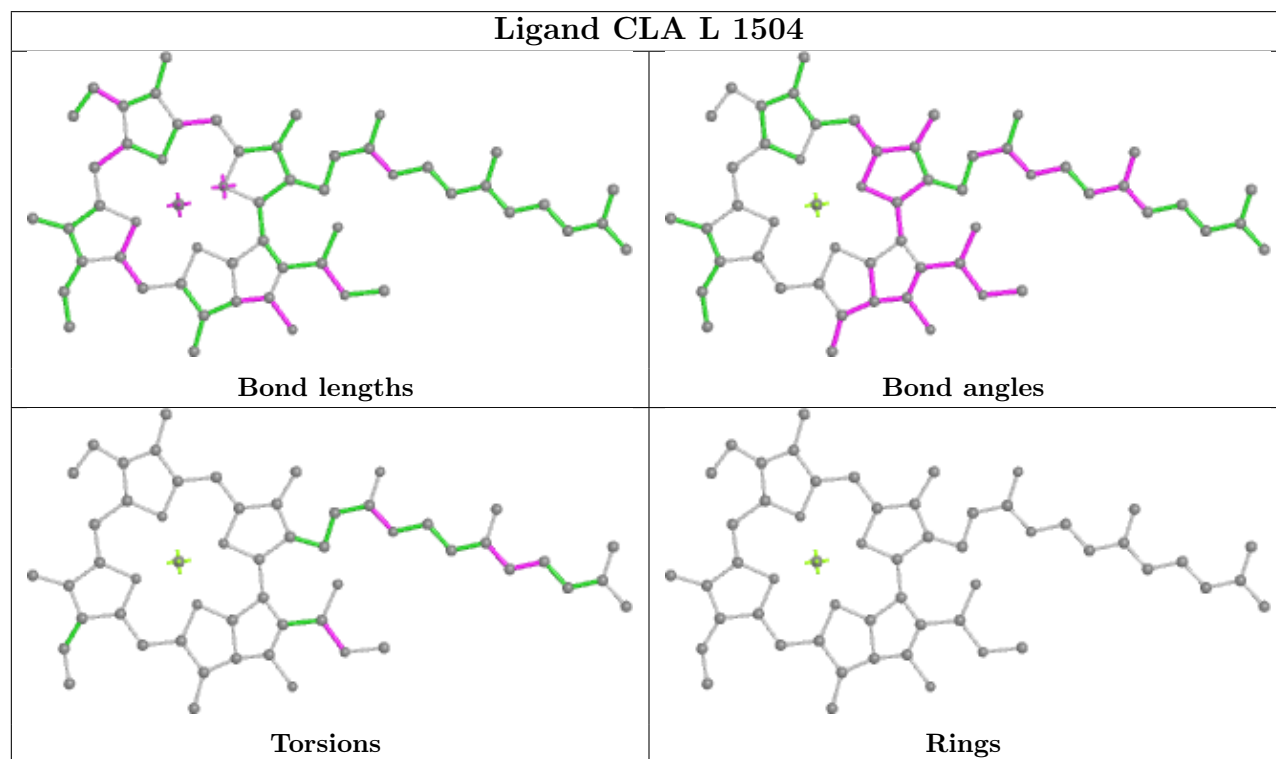
Ligand CLA L 1501



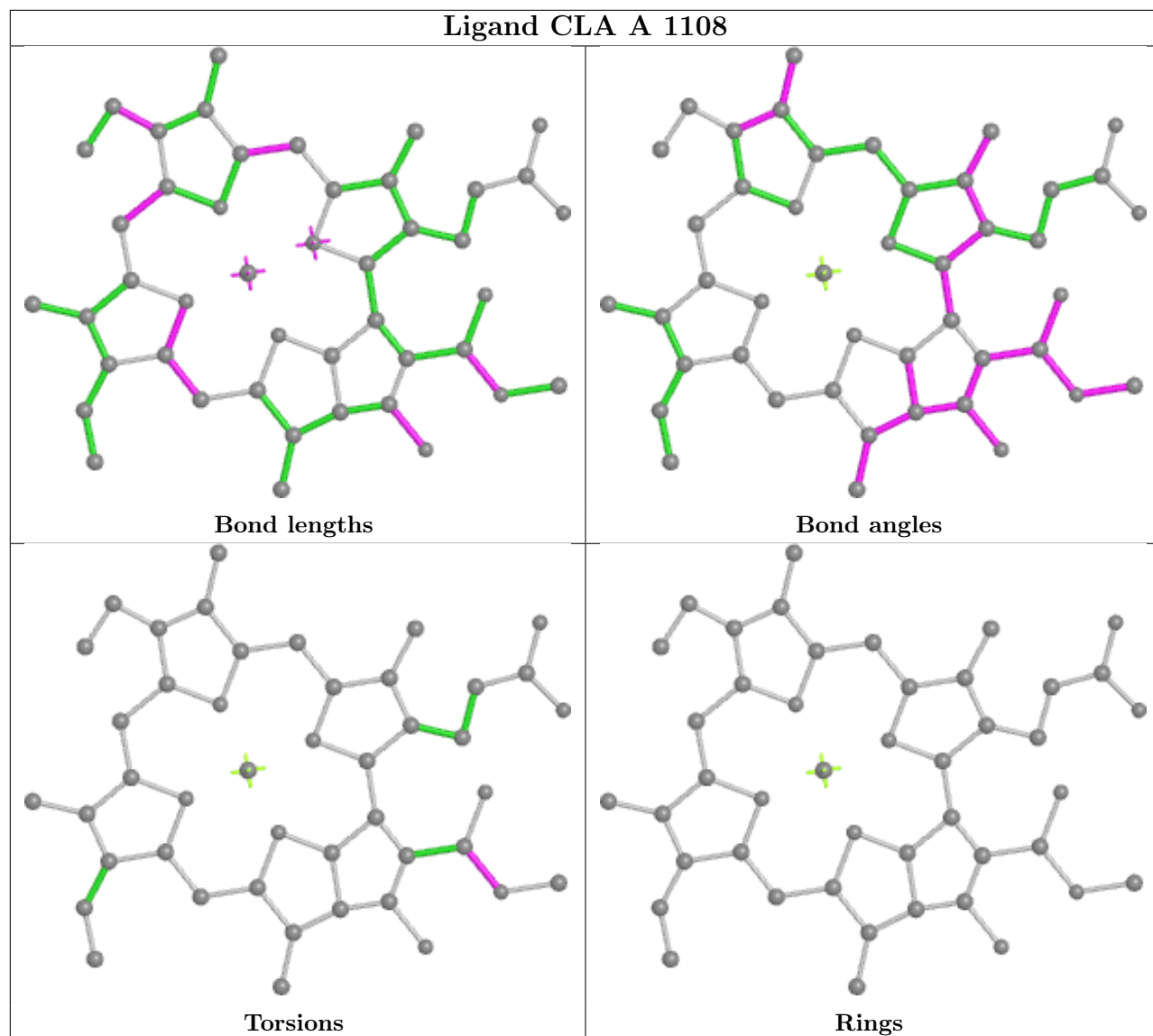
Ligand CLA B 1209

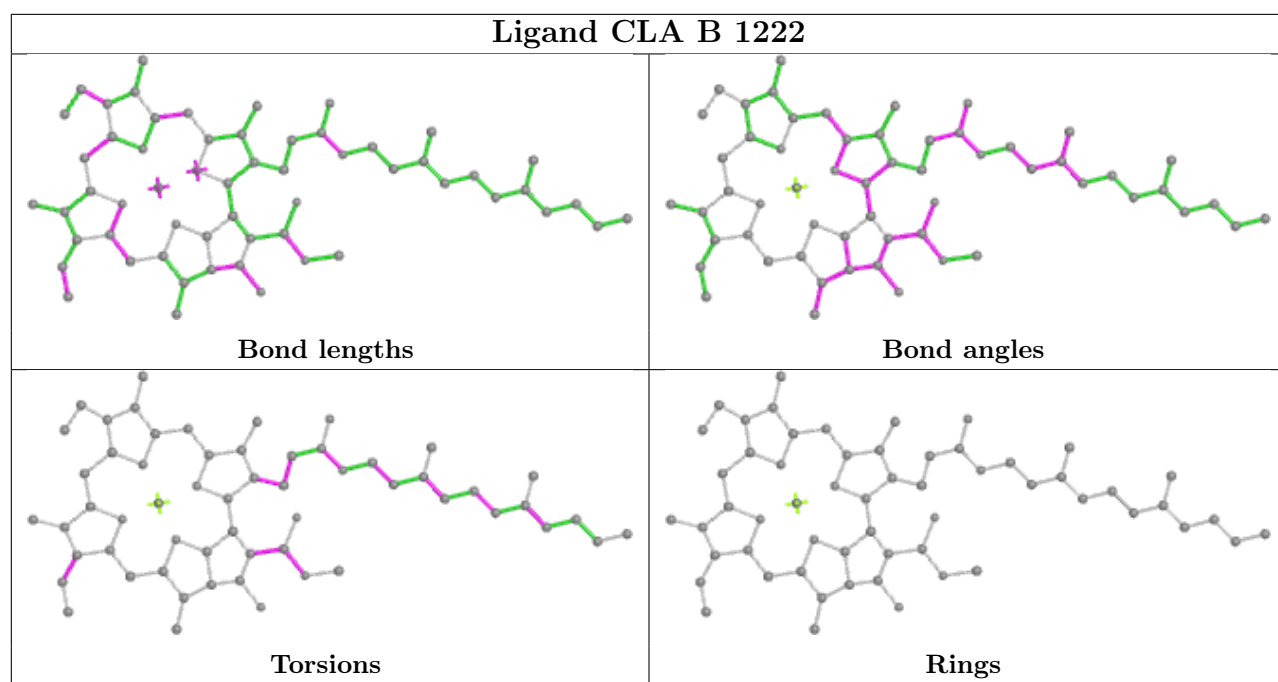


Ligand CLA L 1504

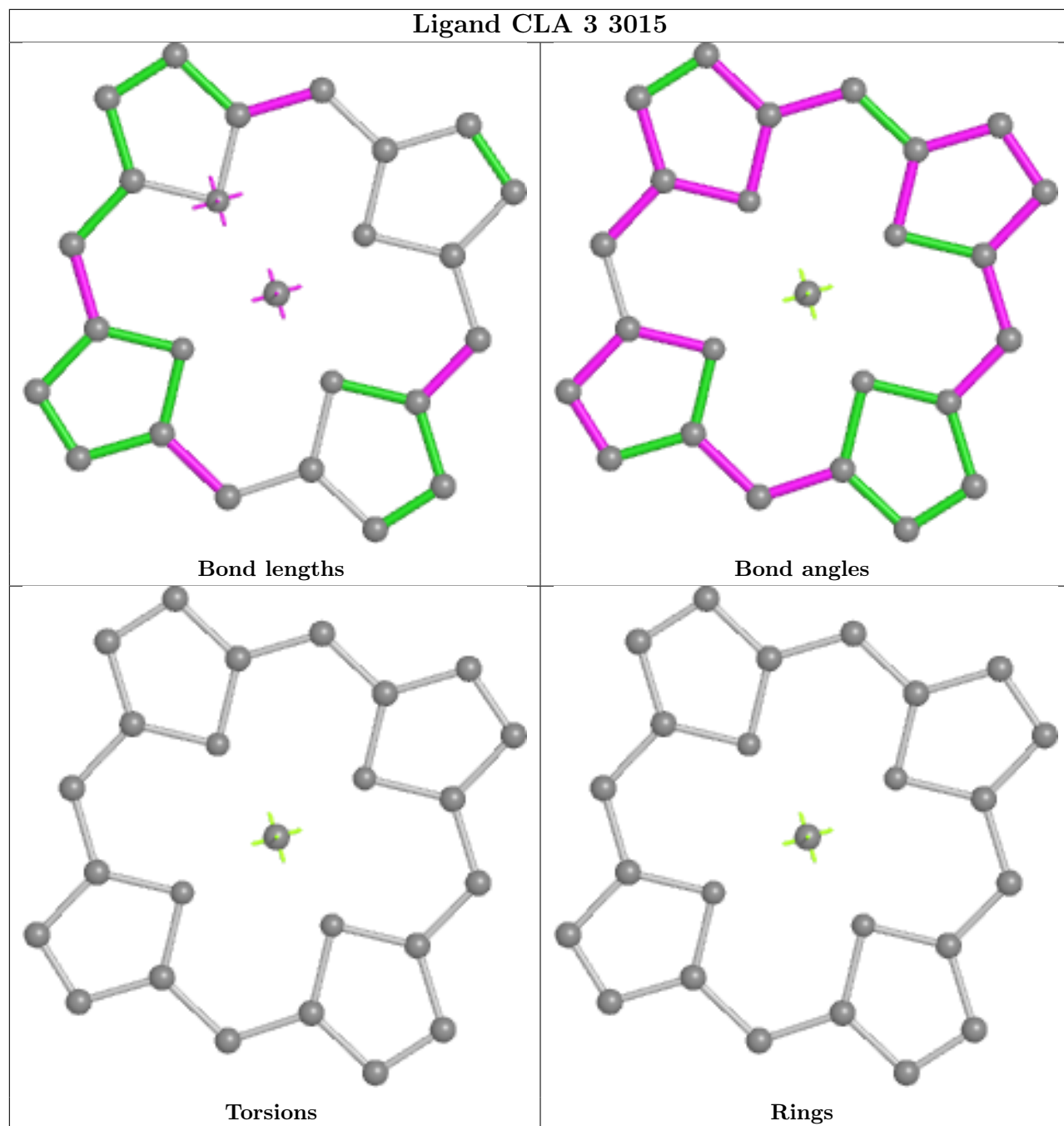


Ligand CLA A 1108

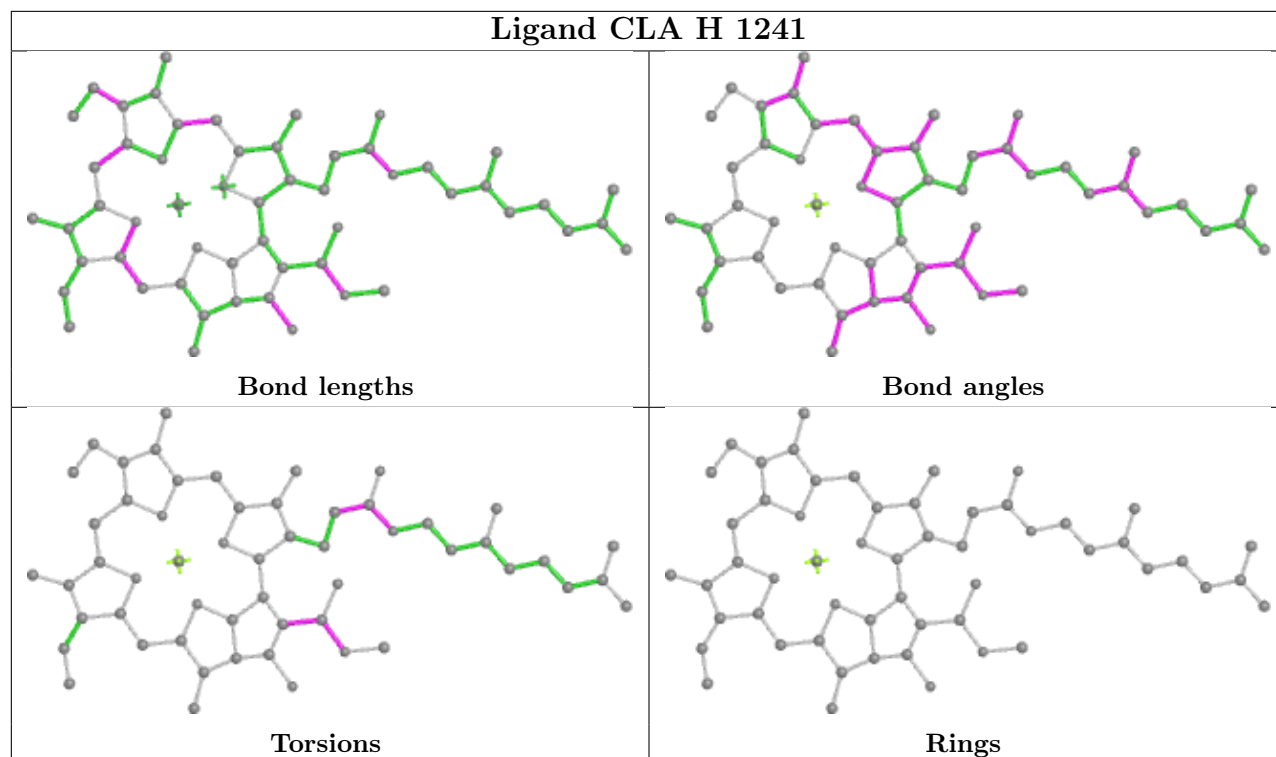




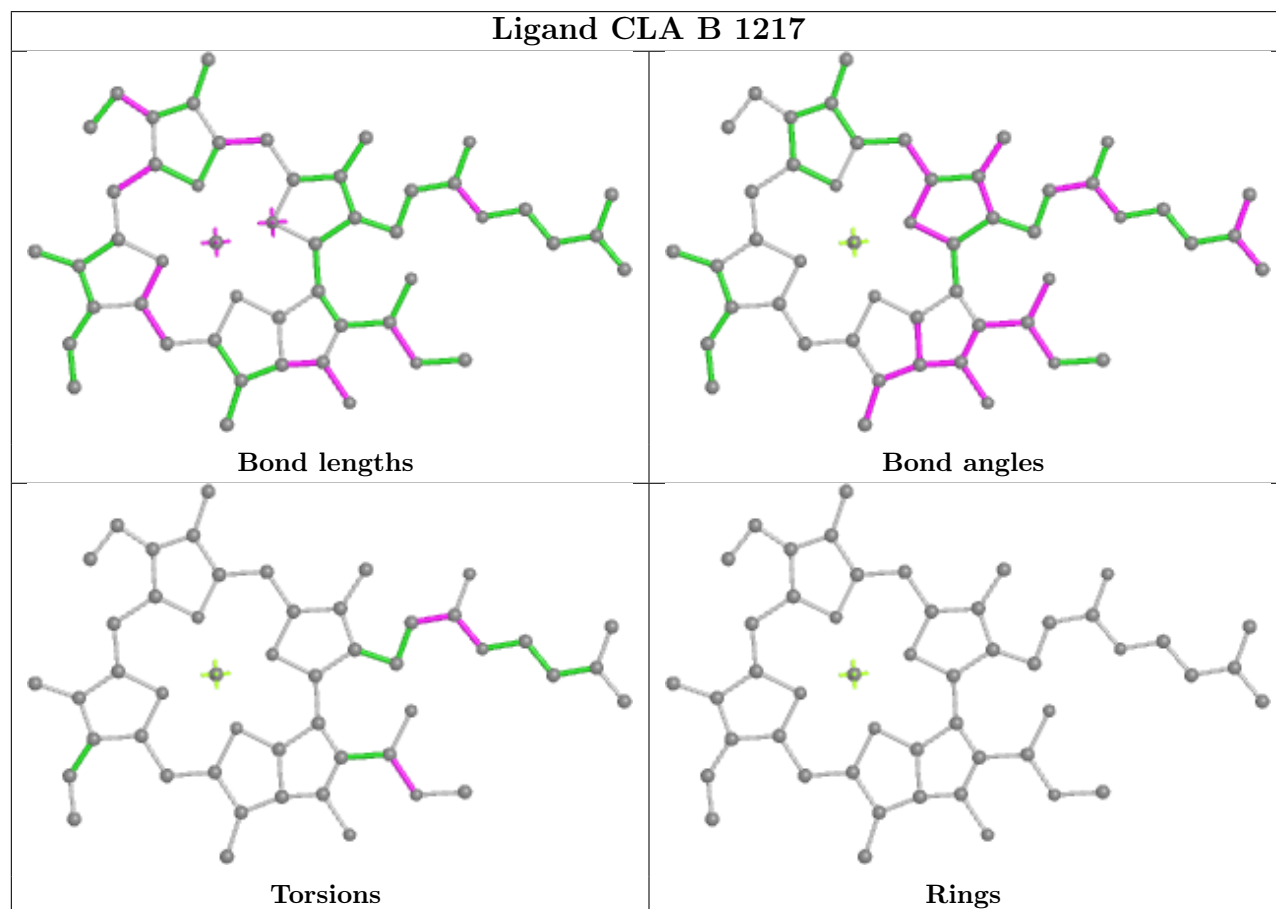
Ligand CLA 3 3015

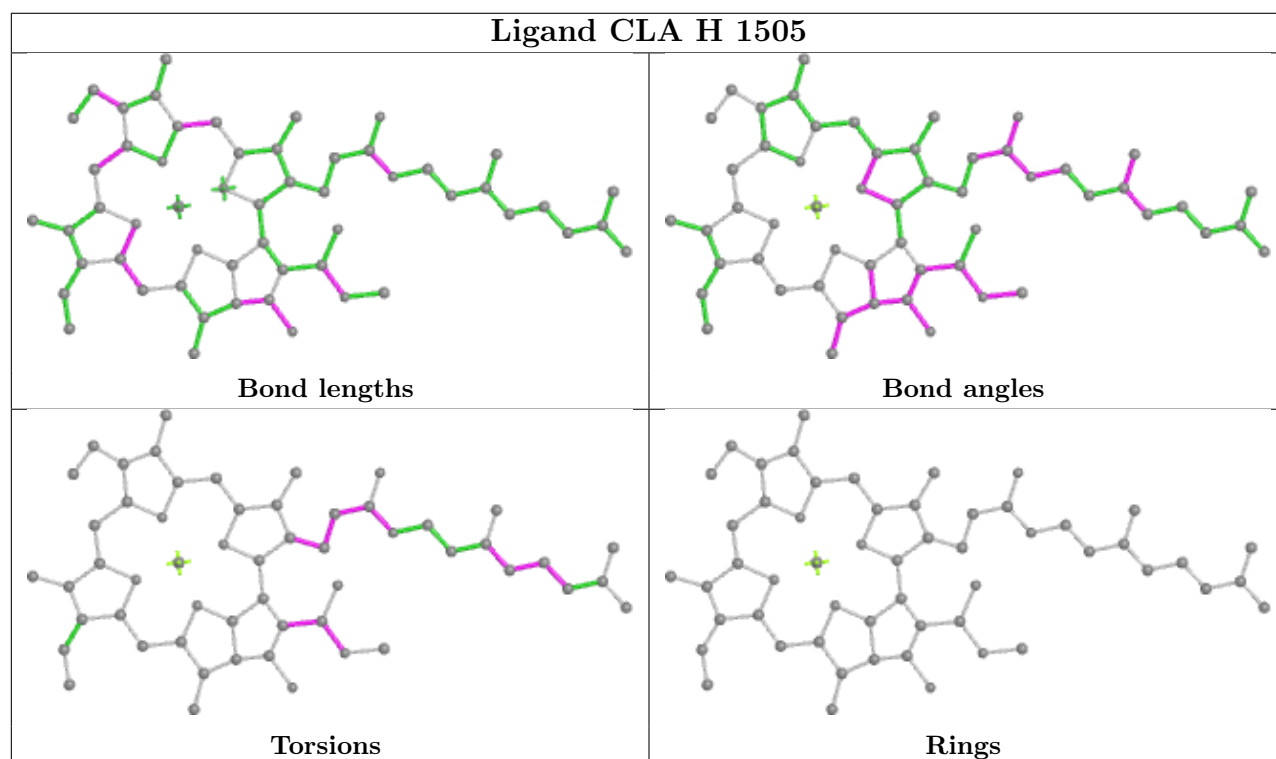
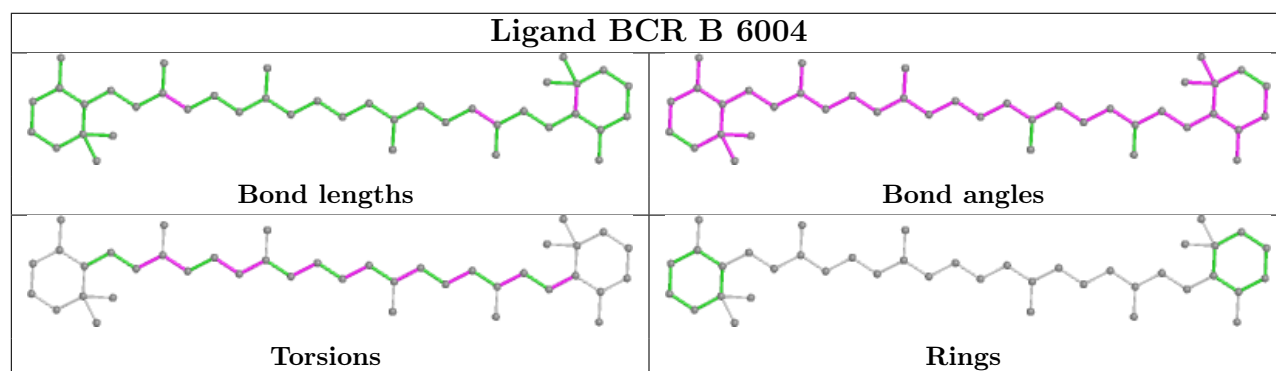
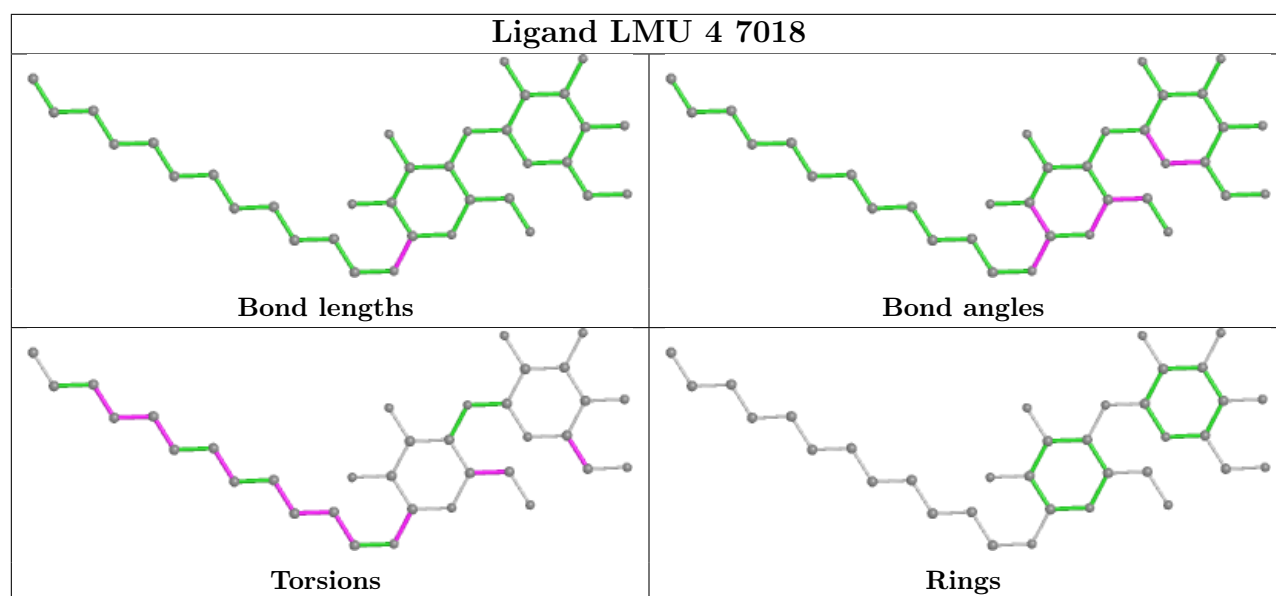


Ligand CLA H 1241

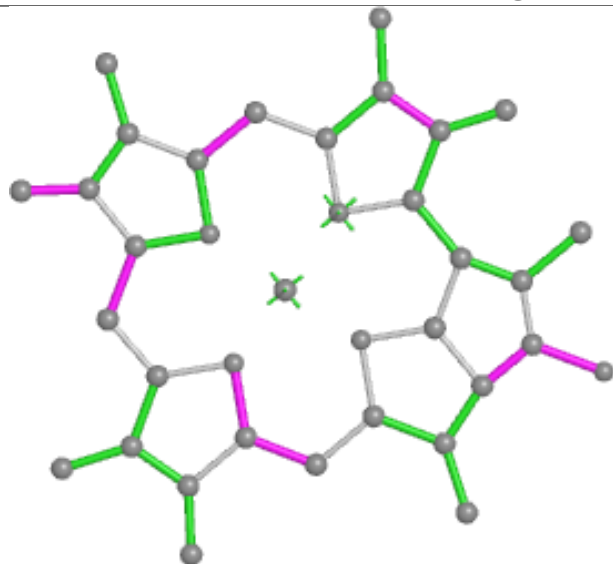


Ligand CLA B 1217

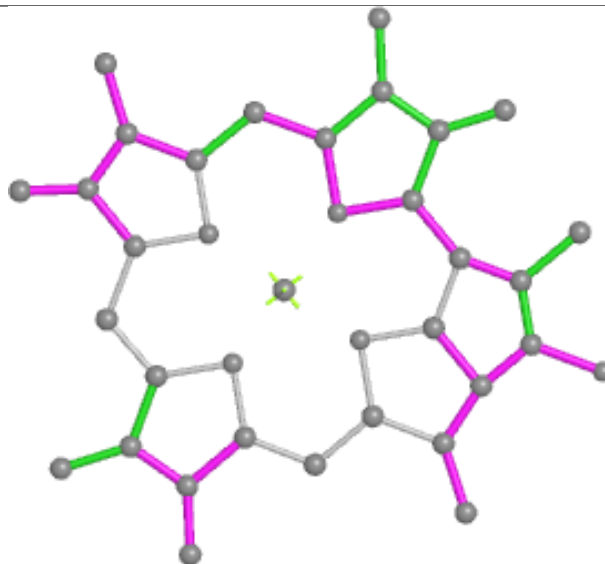




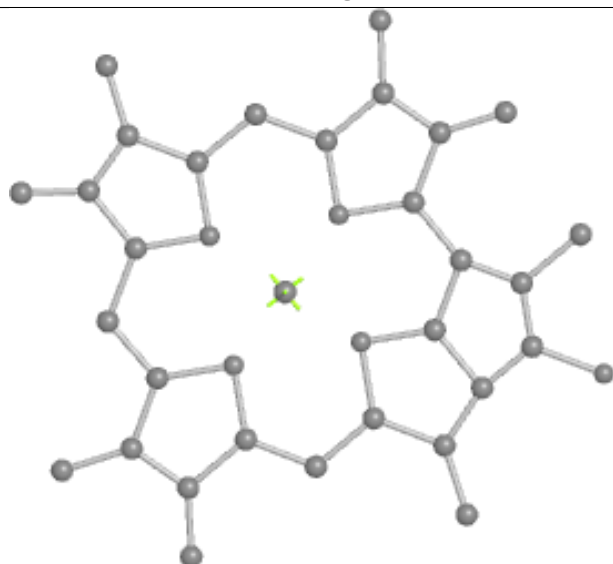
Ligand CLA 3 3003



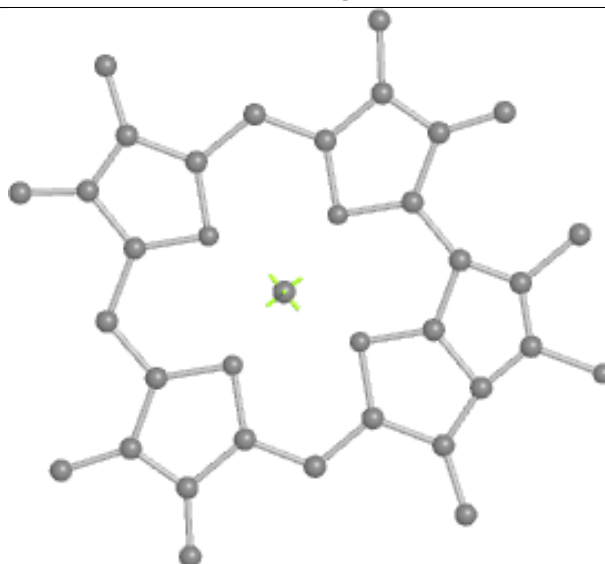
Bond lengths



Bond angles

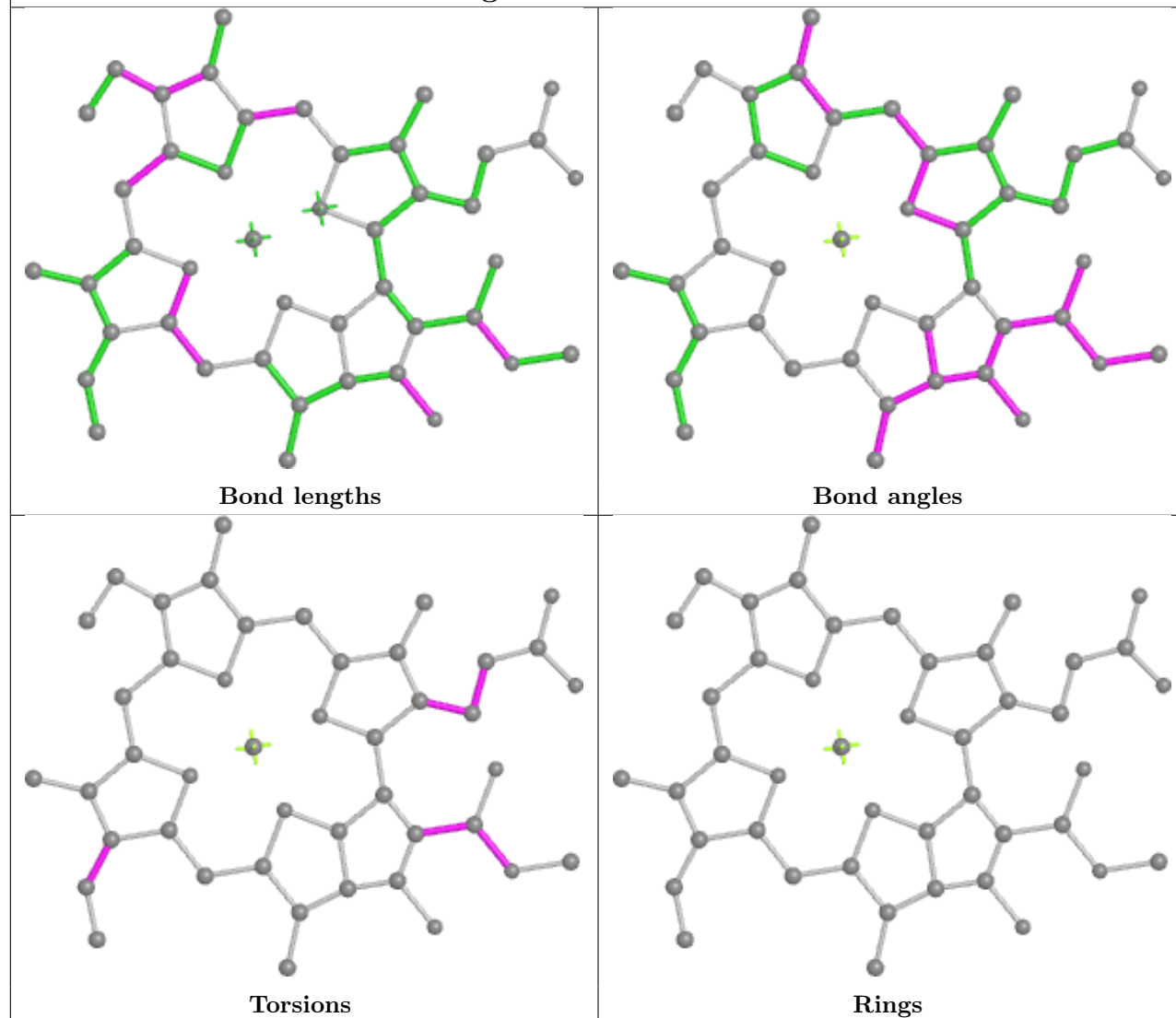


Torsions

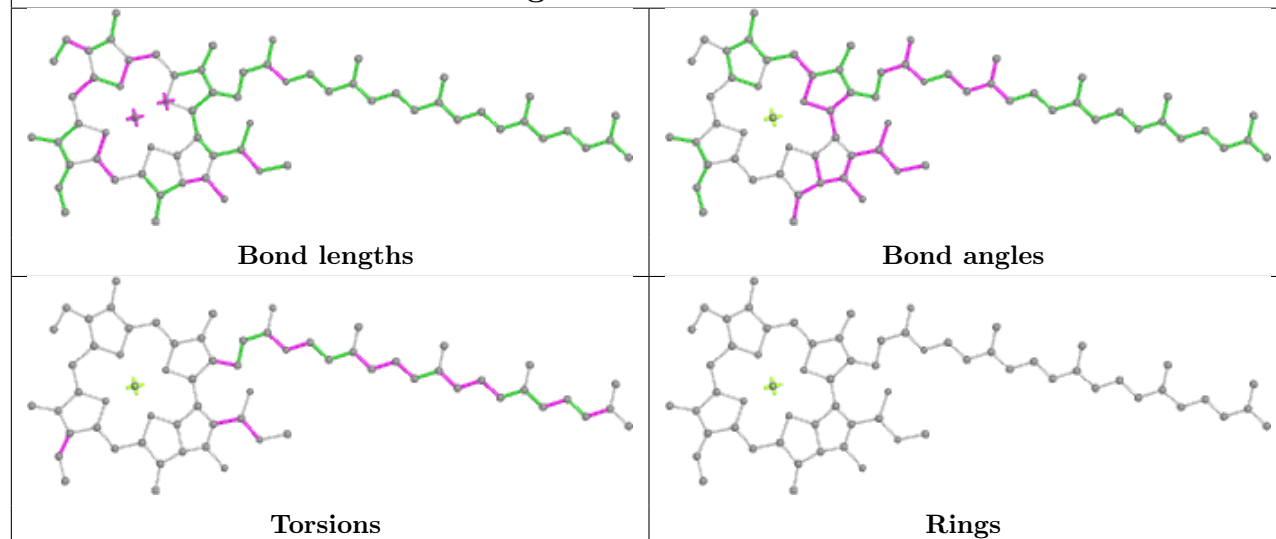


Rings

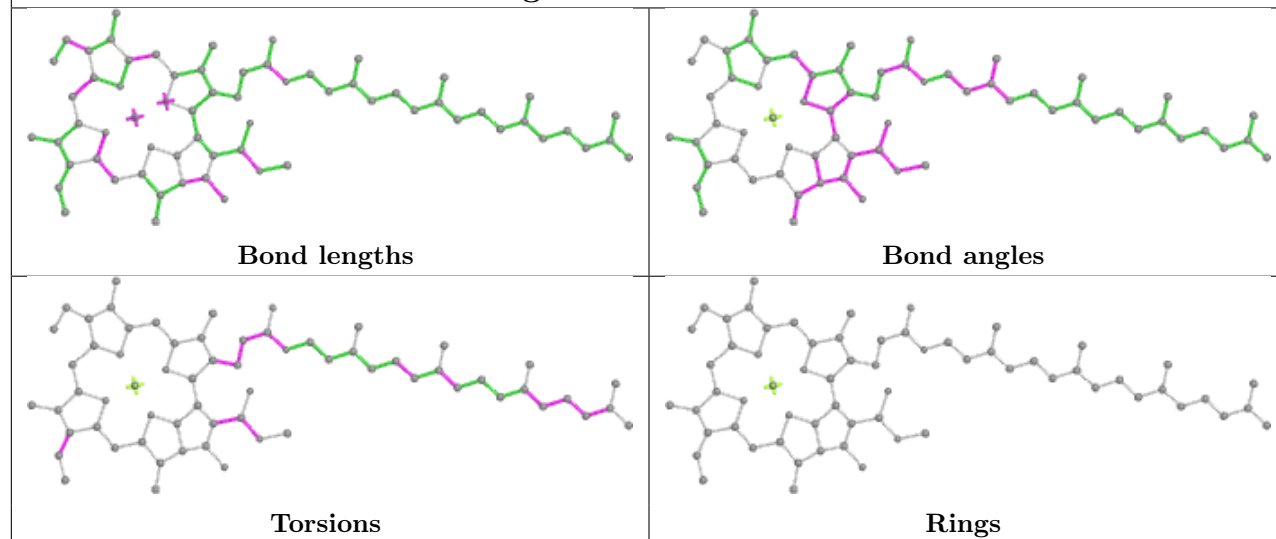
Ligand CLA A 1112



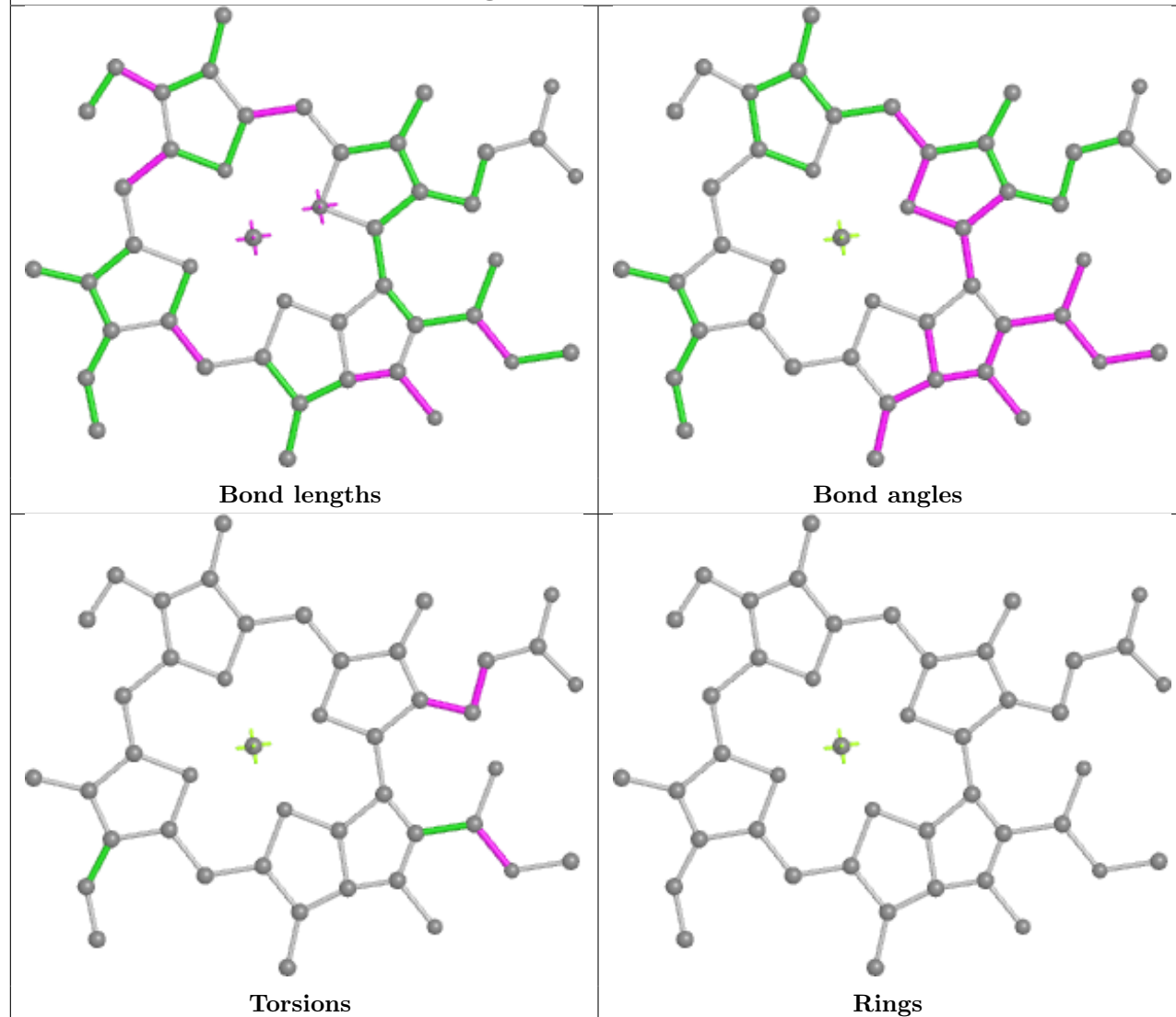
Ligand CLA 3 3016

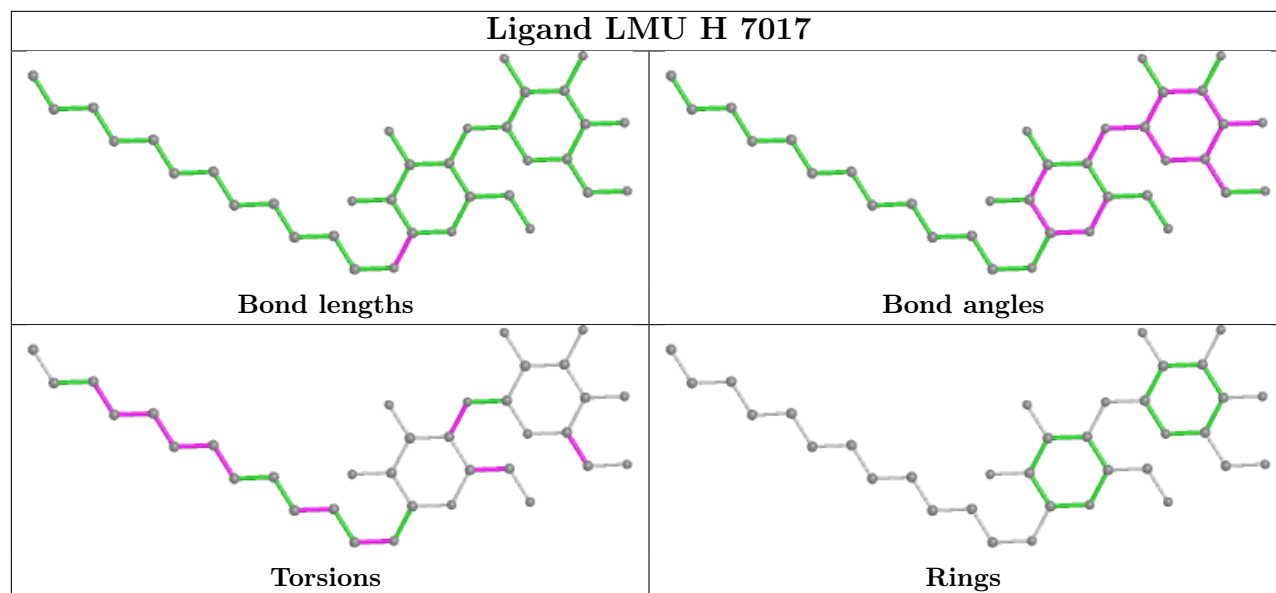


Ligand CLA A 1138

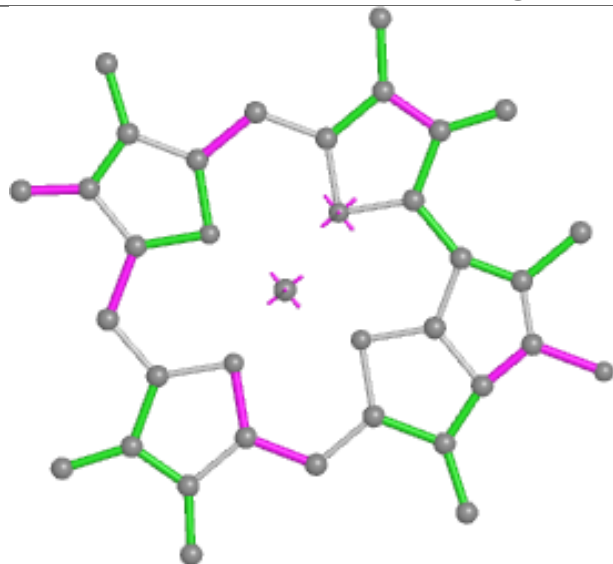


Ligand CLA A 1134

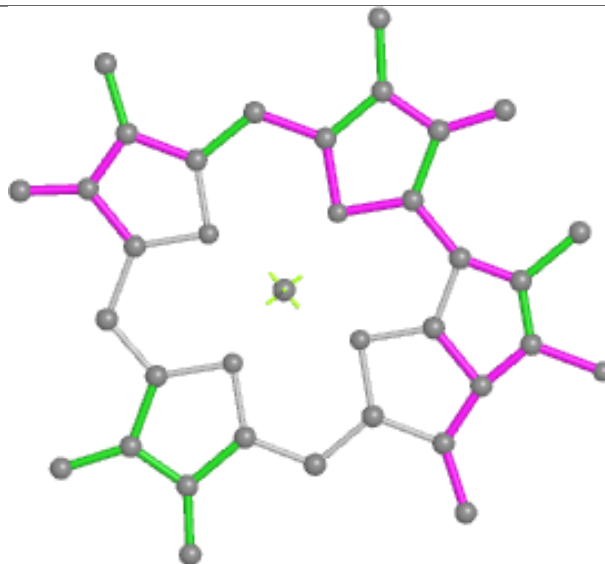




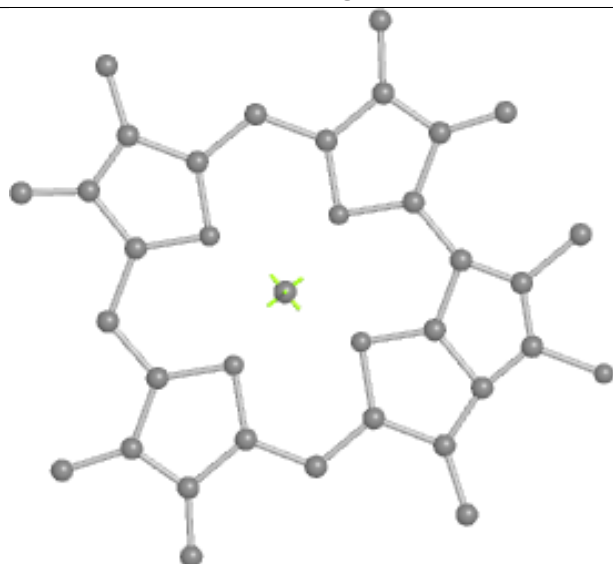
Ligand CLA 3 1118



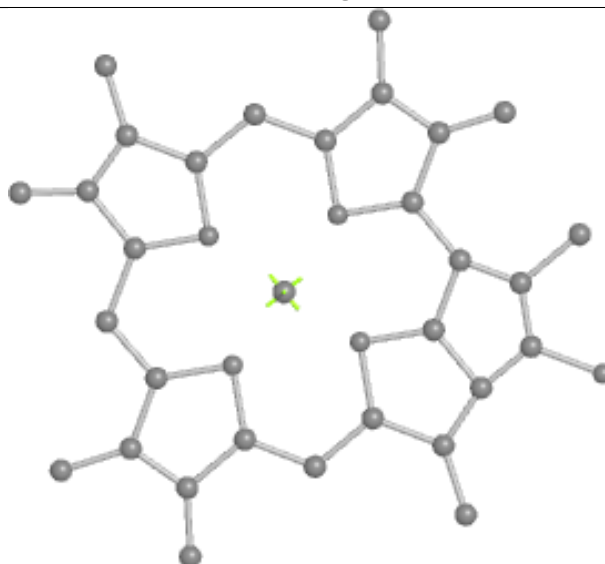
Bond lengths



Bond angles

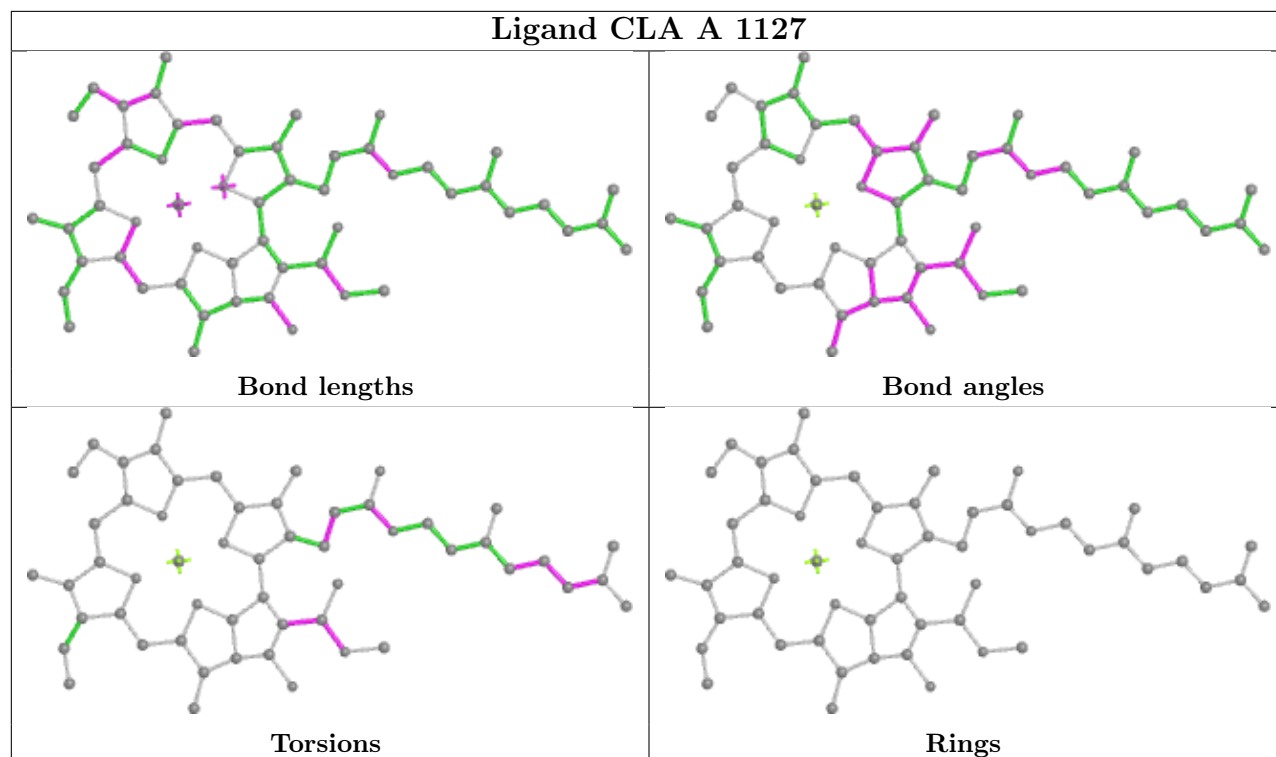


Torsions

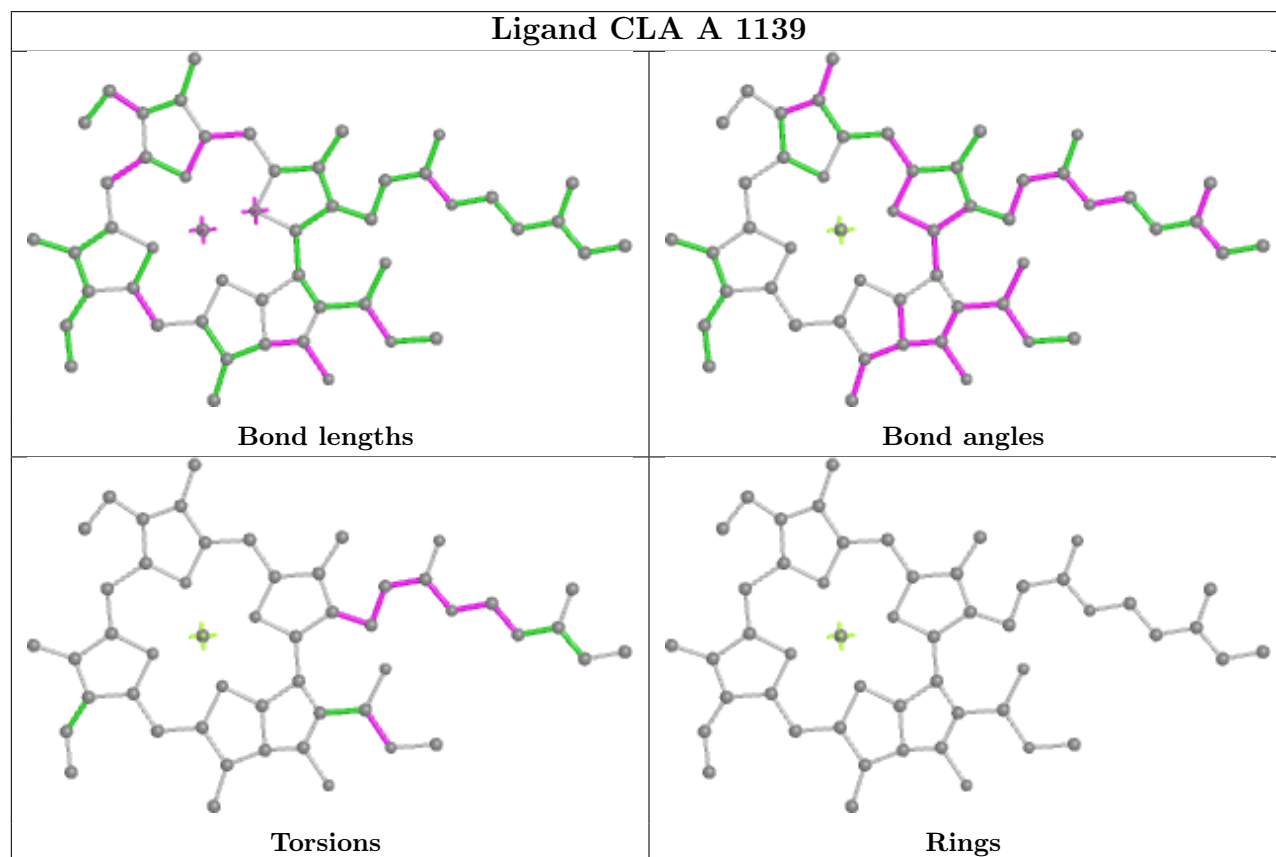


Rings

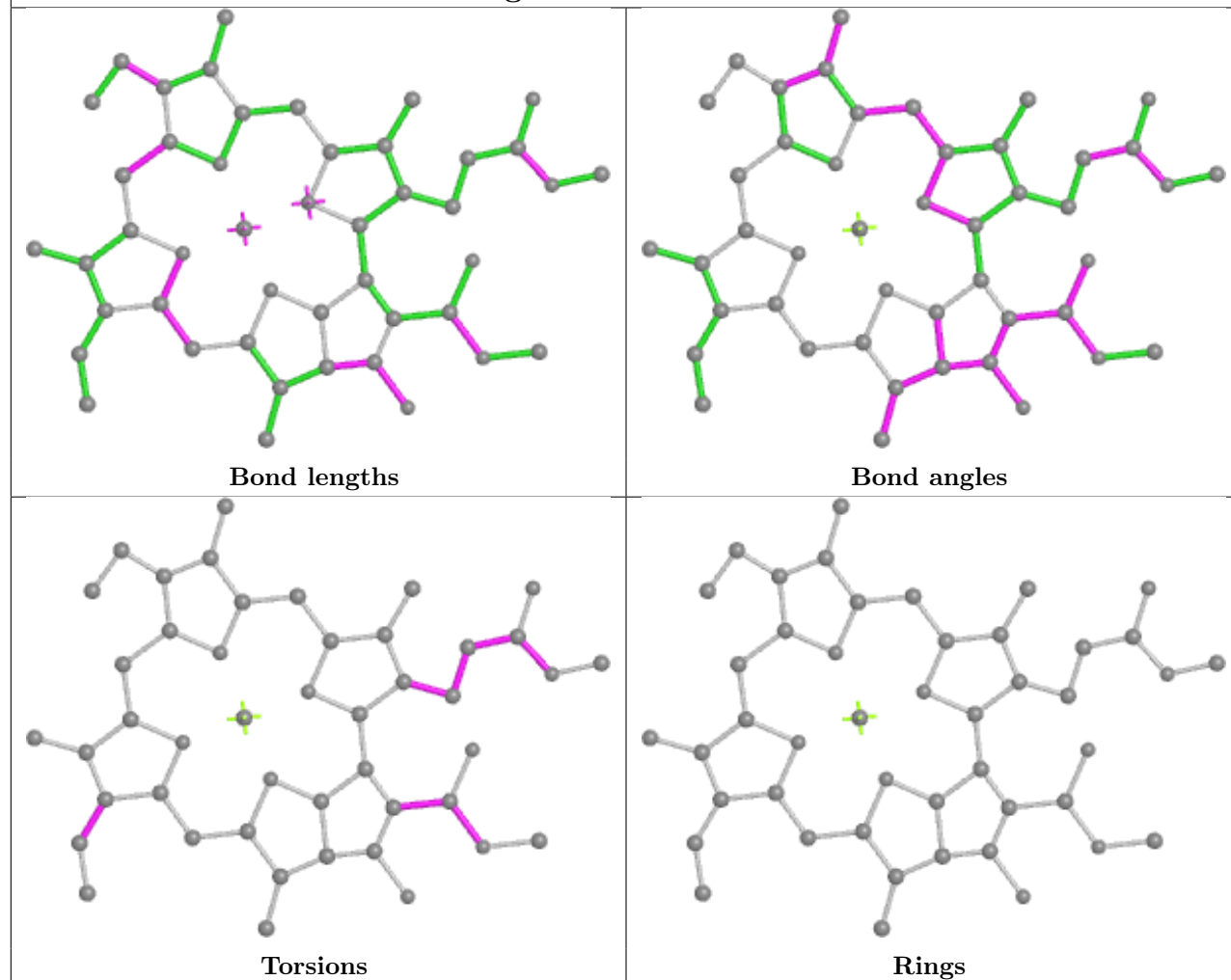
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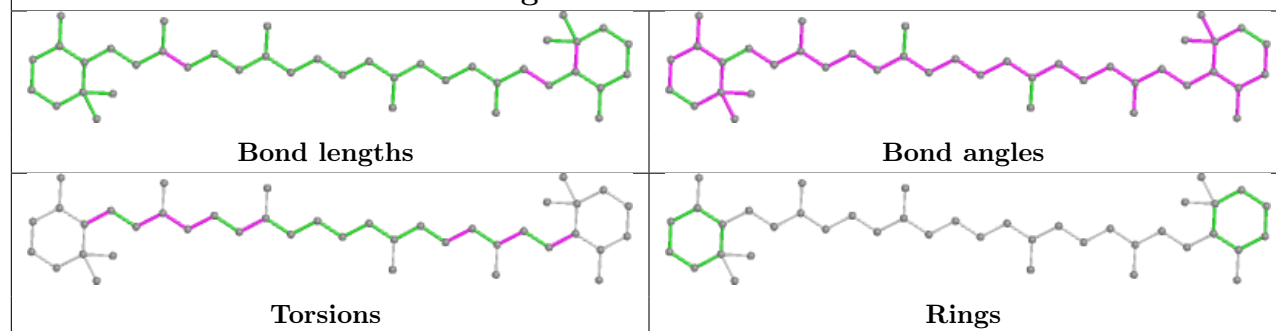
Ligand CLA A 1139

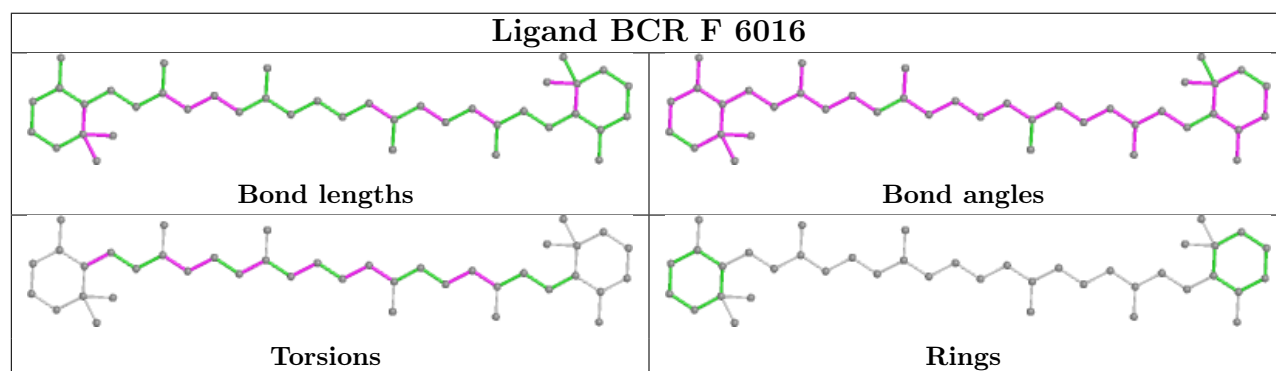
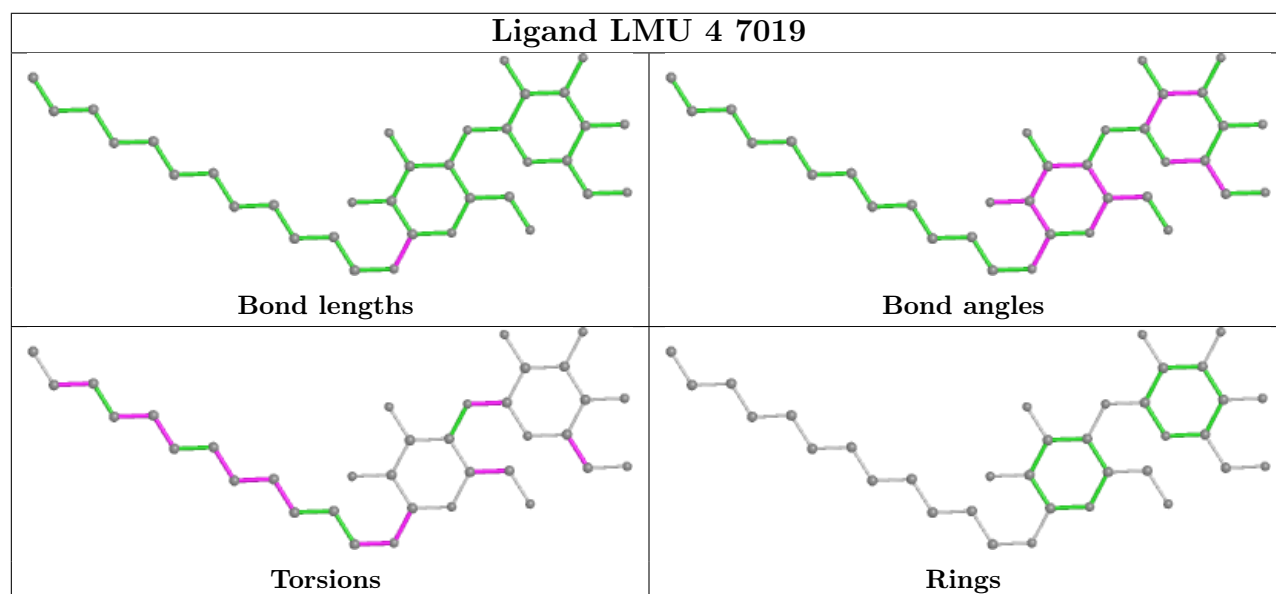
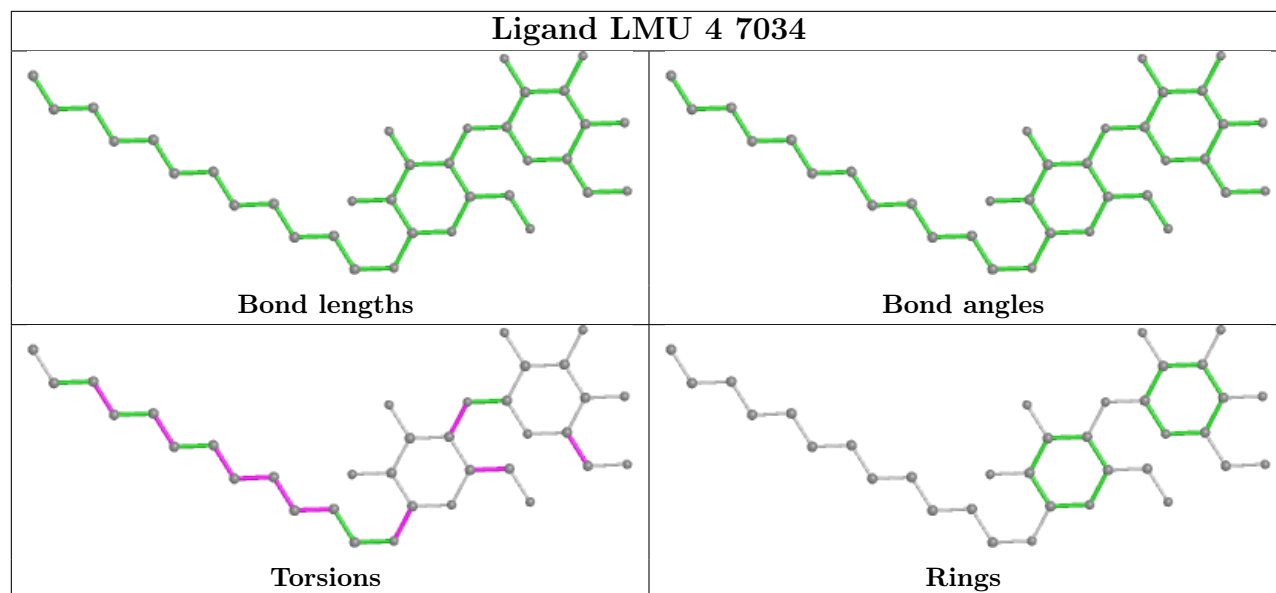


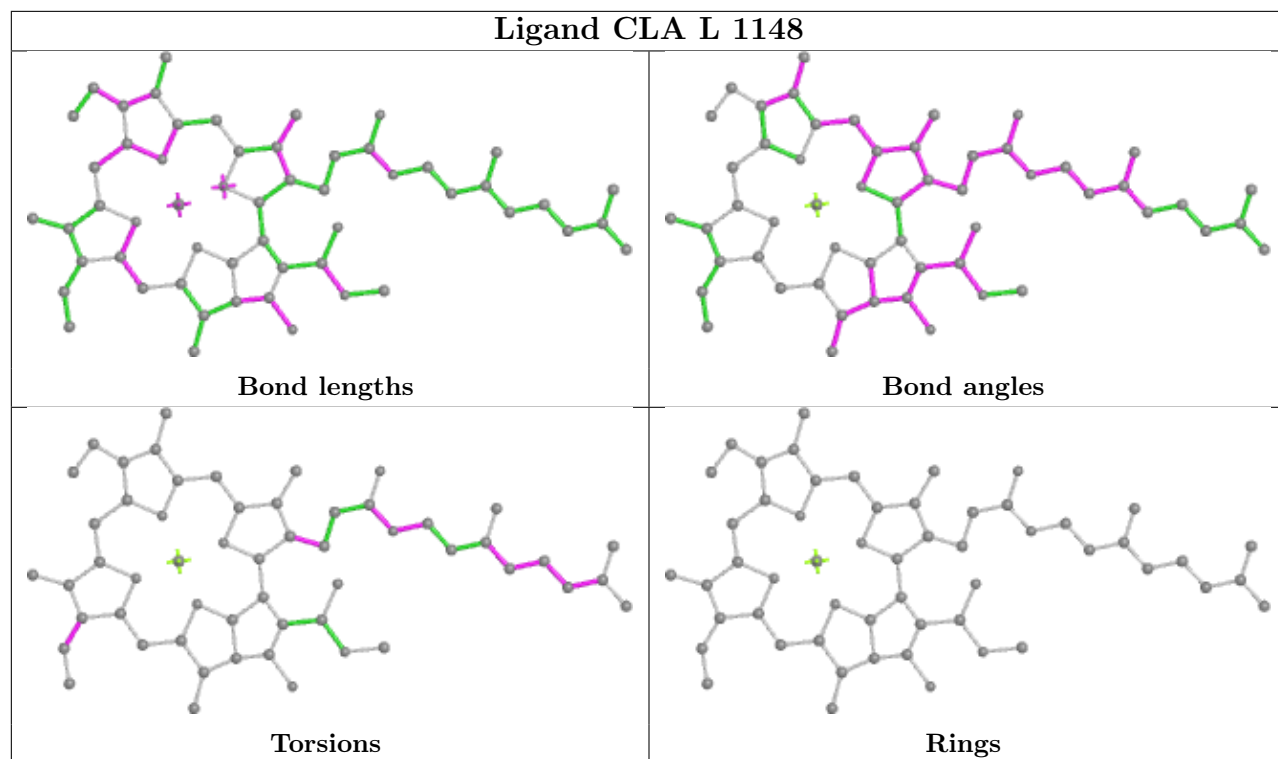
Ligand CLA B 1218



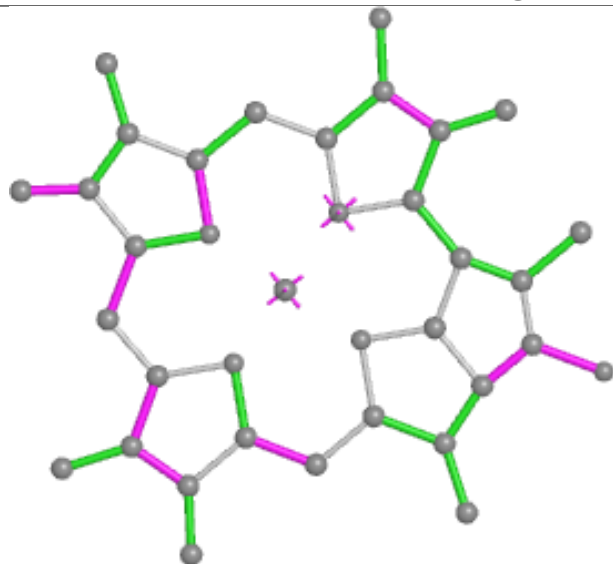
Ligand BCR A 6003



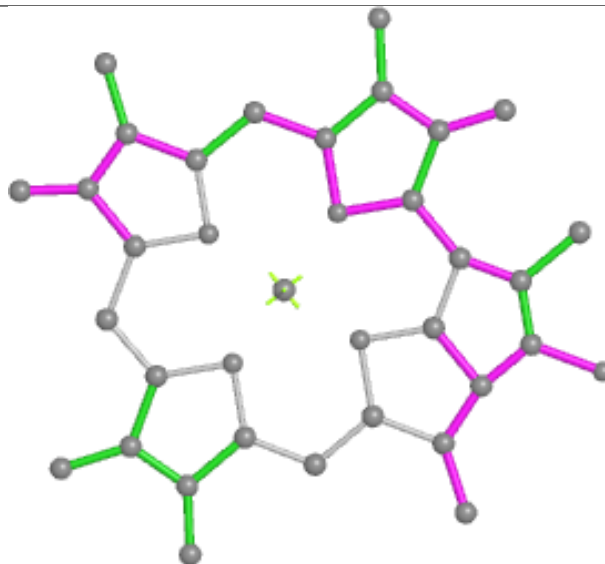




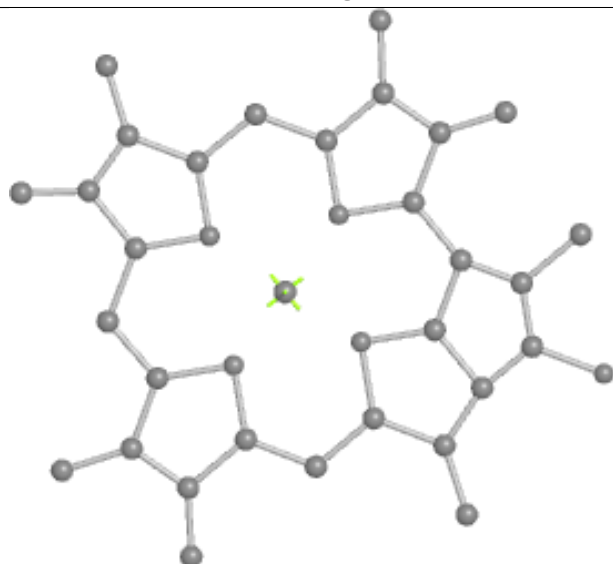
Ligand CLA 1 1011



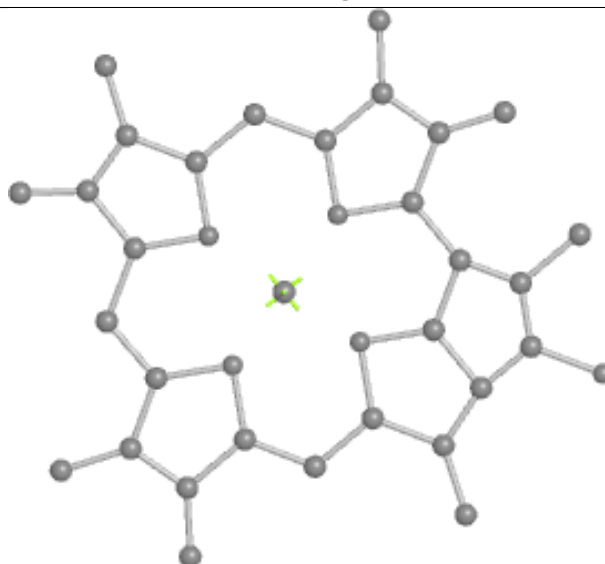
Bond lengths



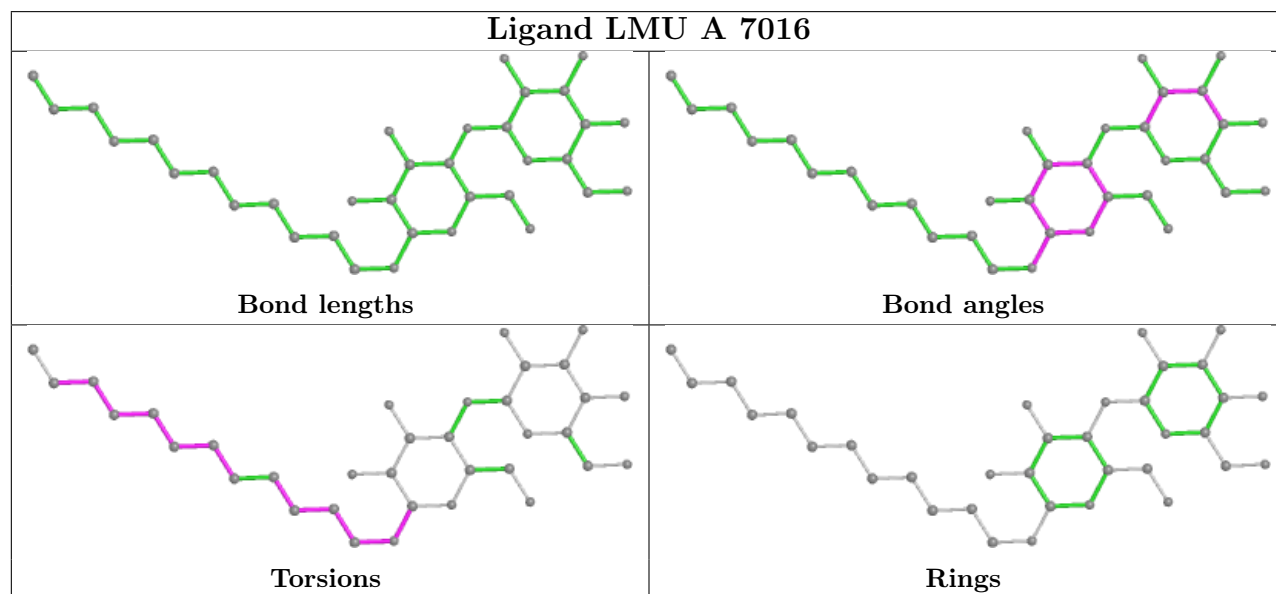
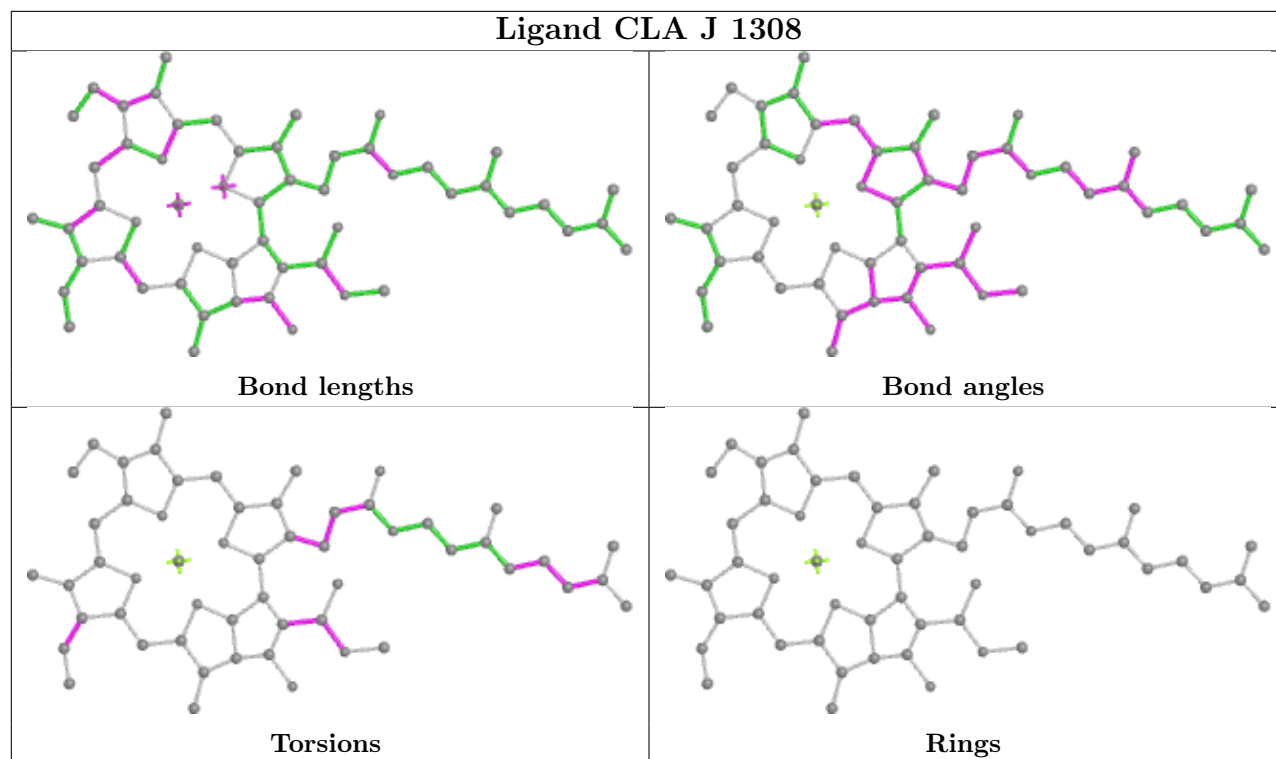
Bond angles



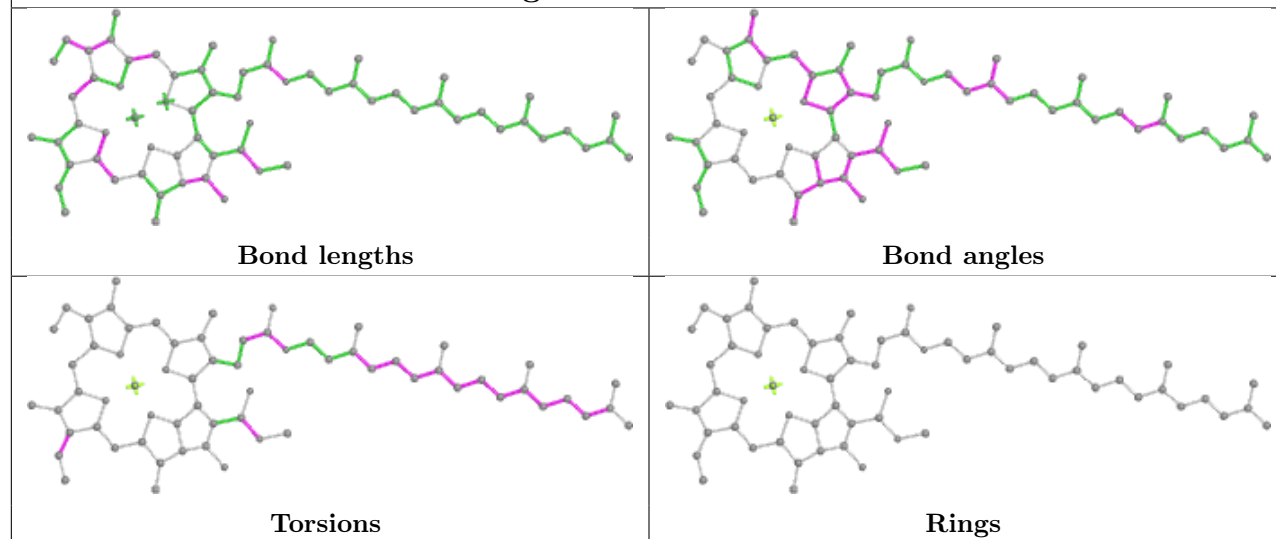
Torsions



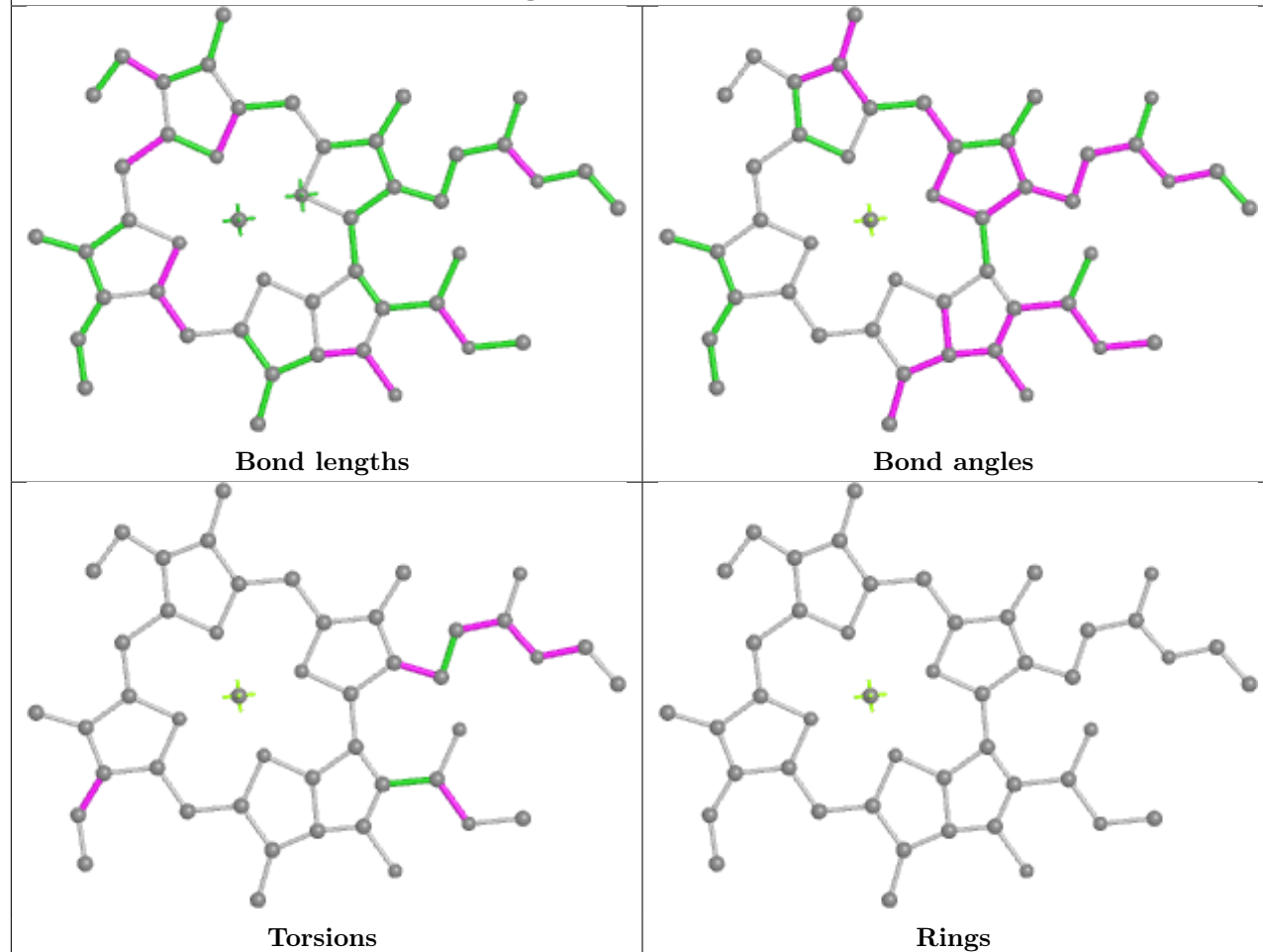
Rings

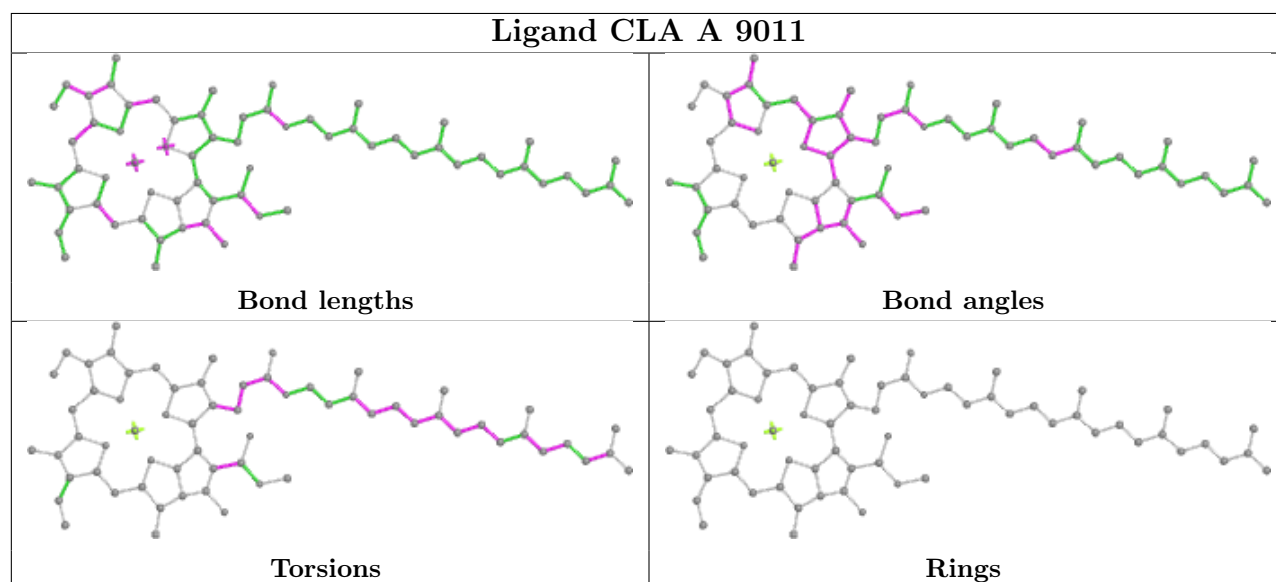
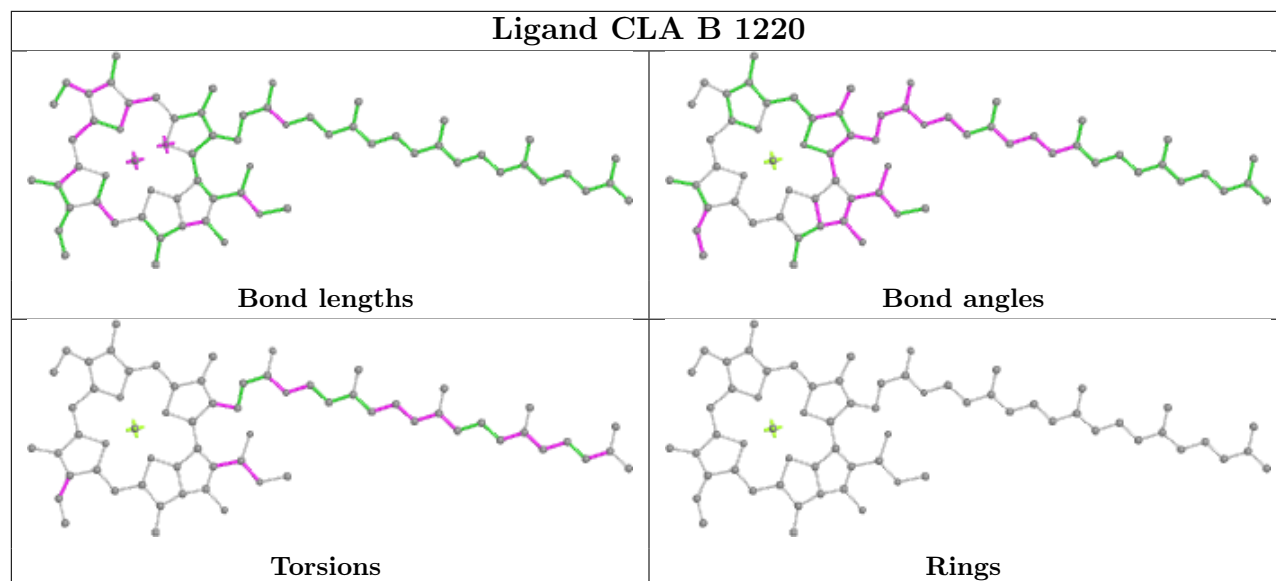
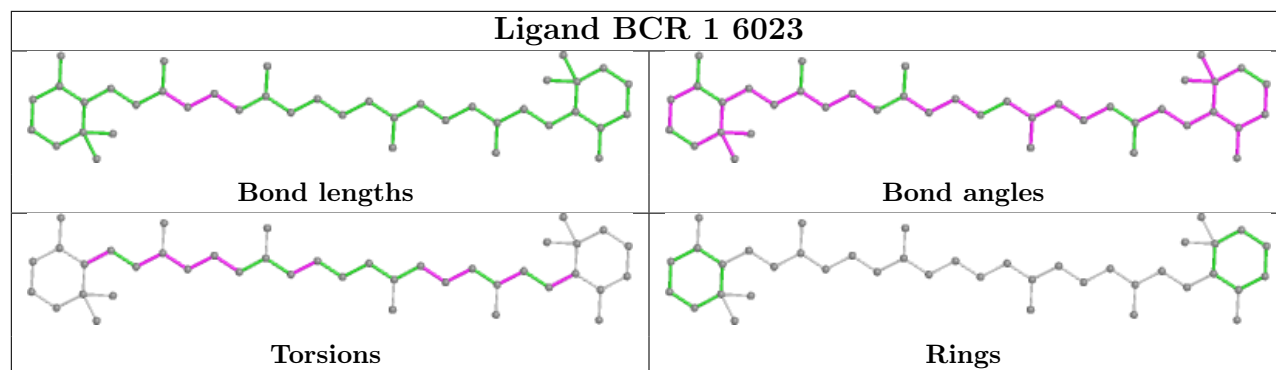


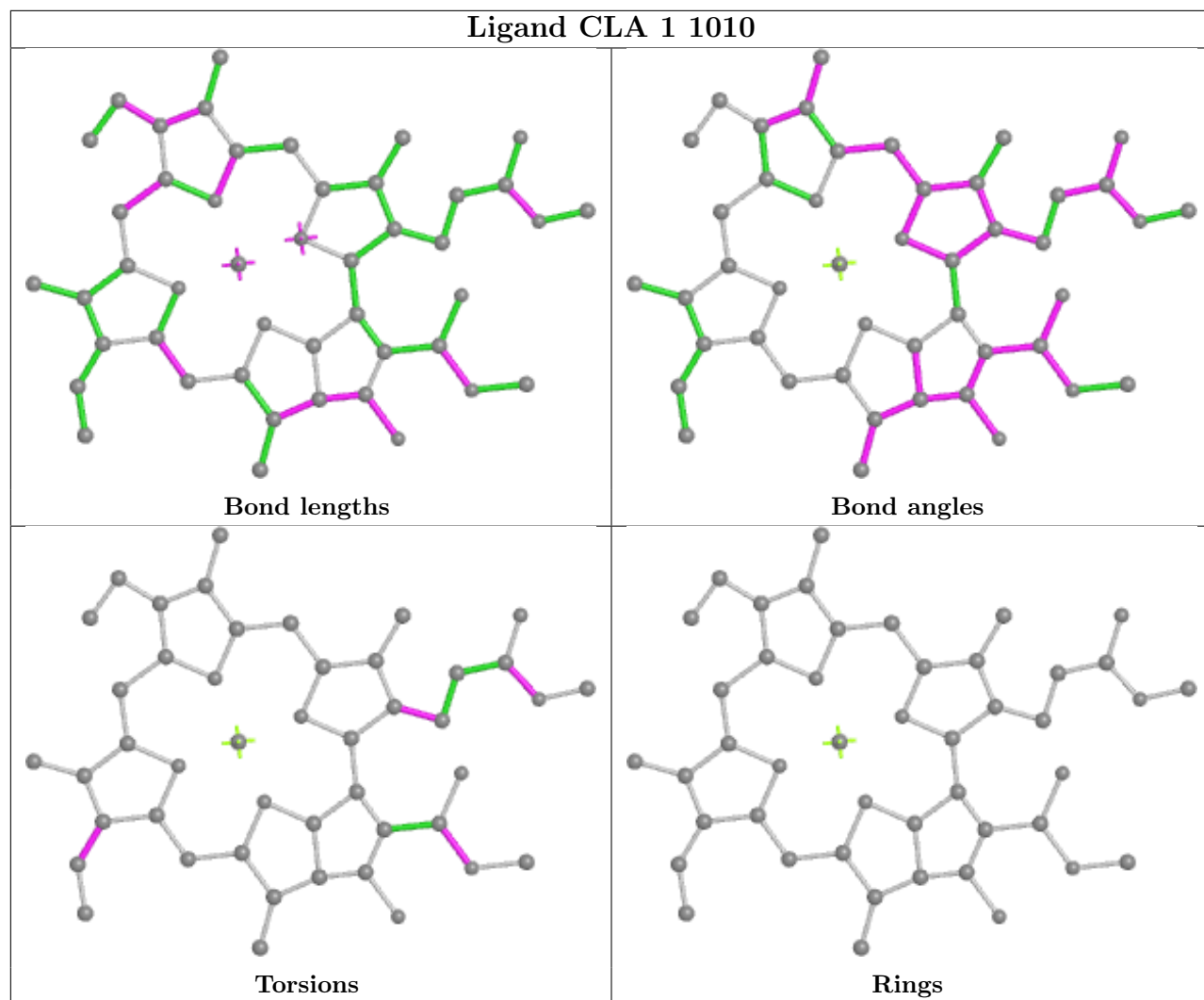
Ligand CLA A 1109

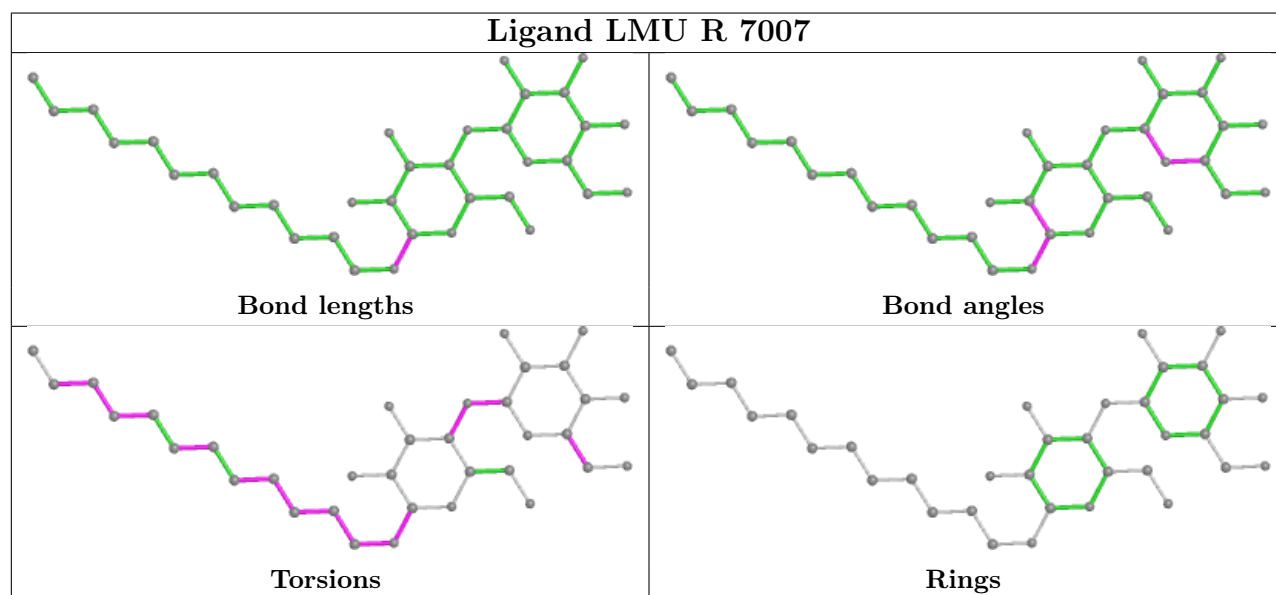
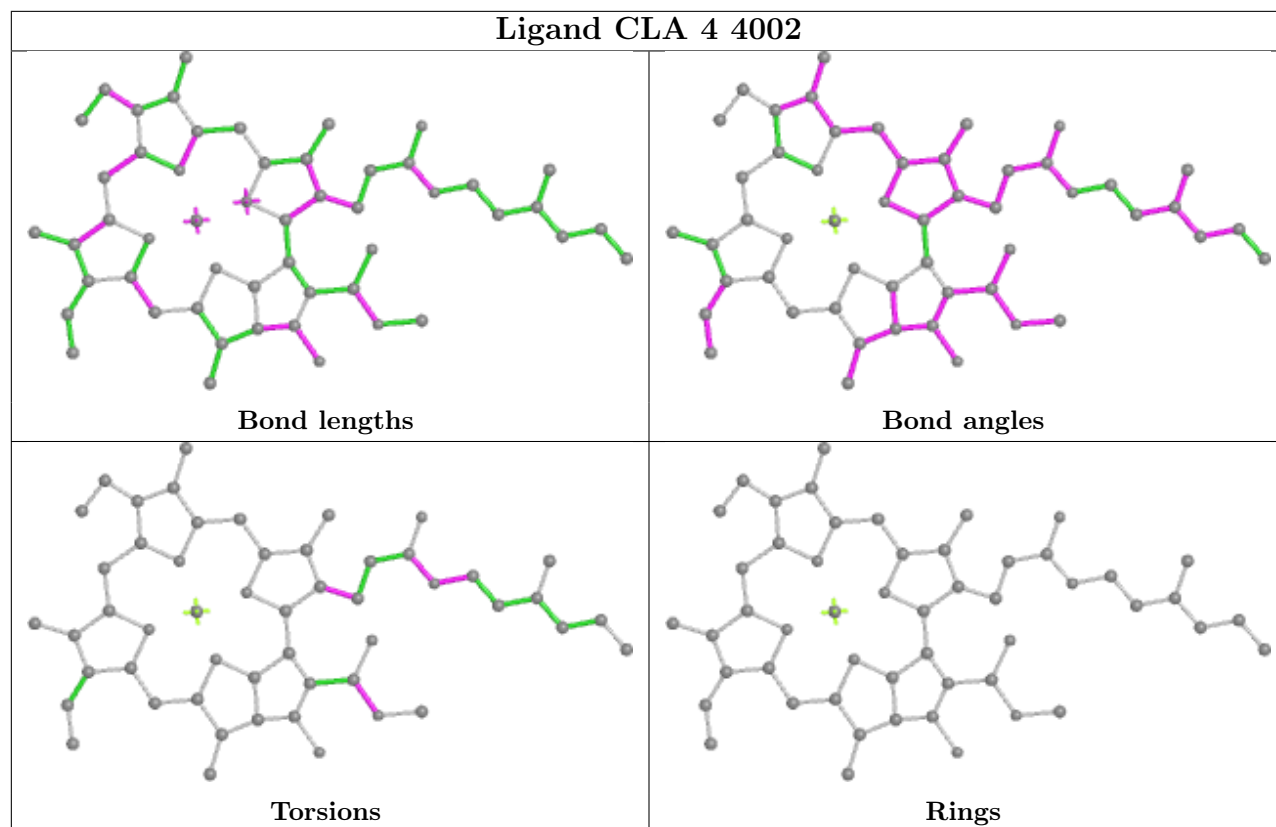


Ligand CLA 1 1002

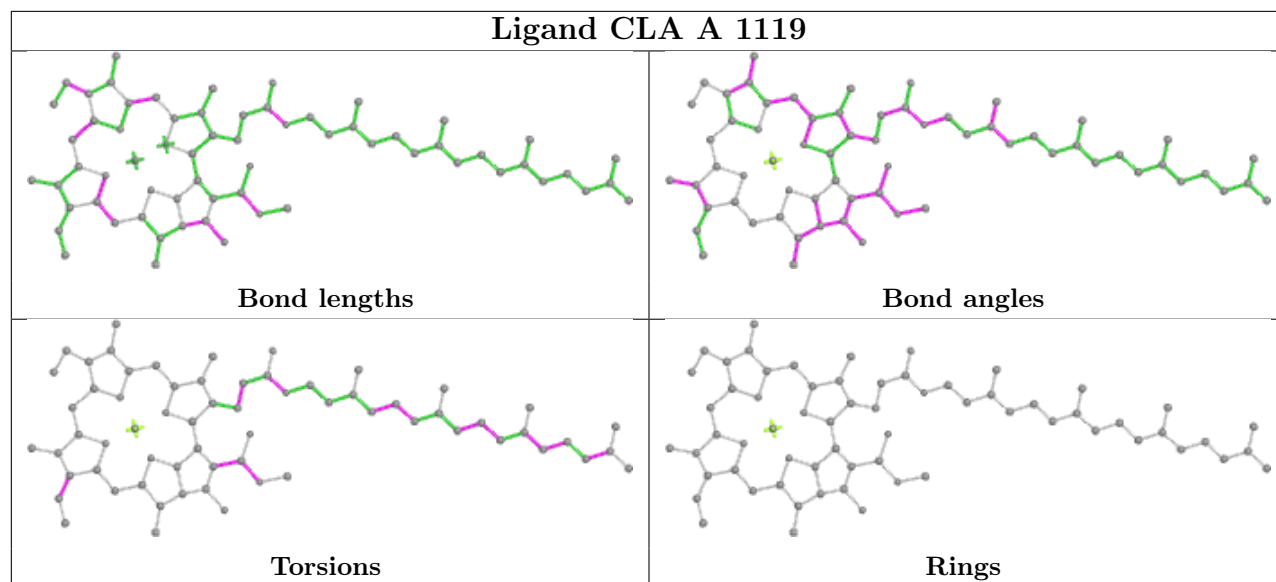




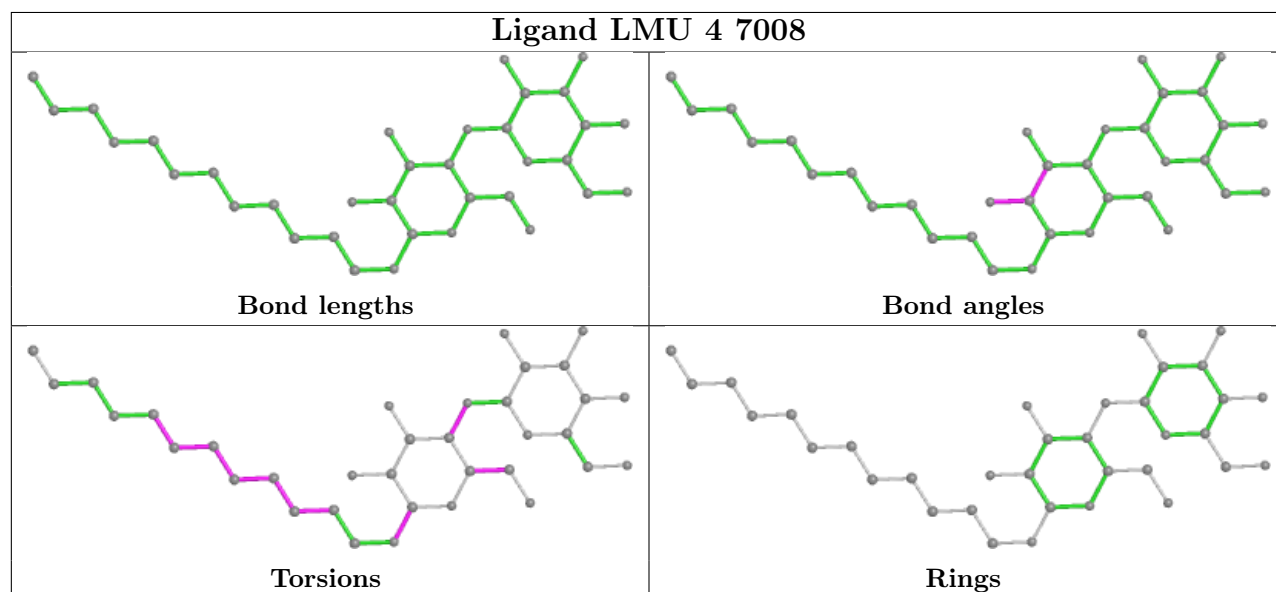




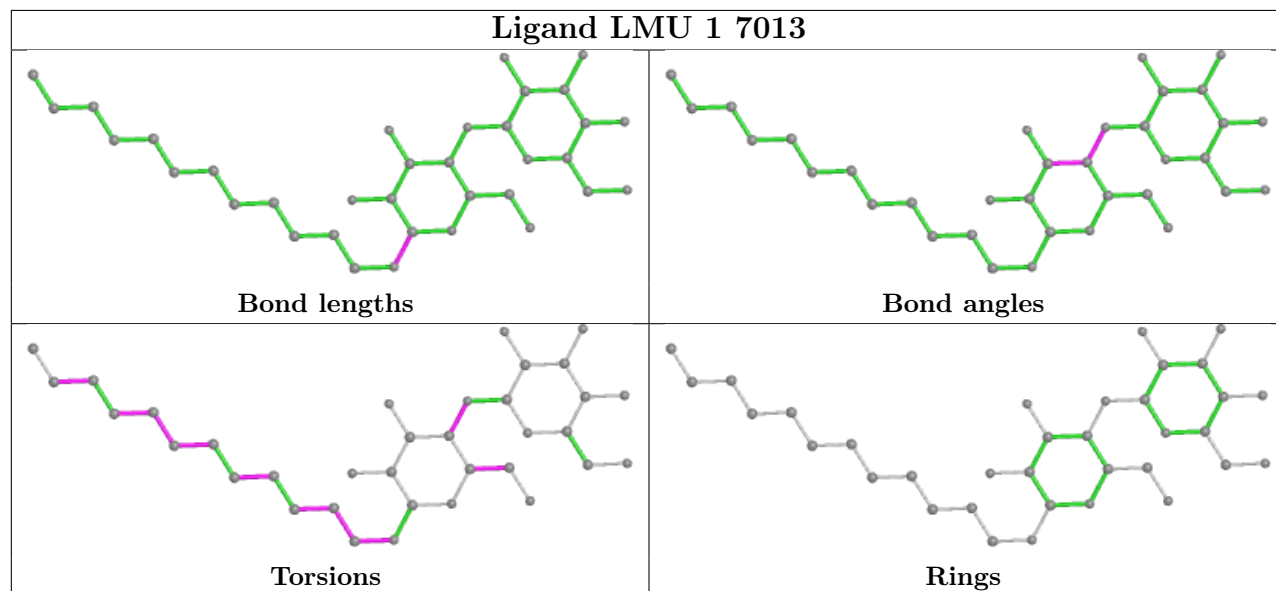
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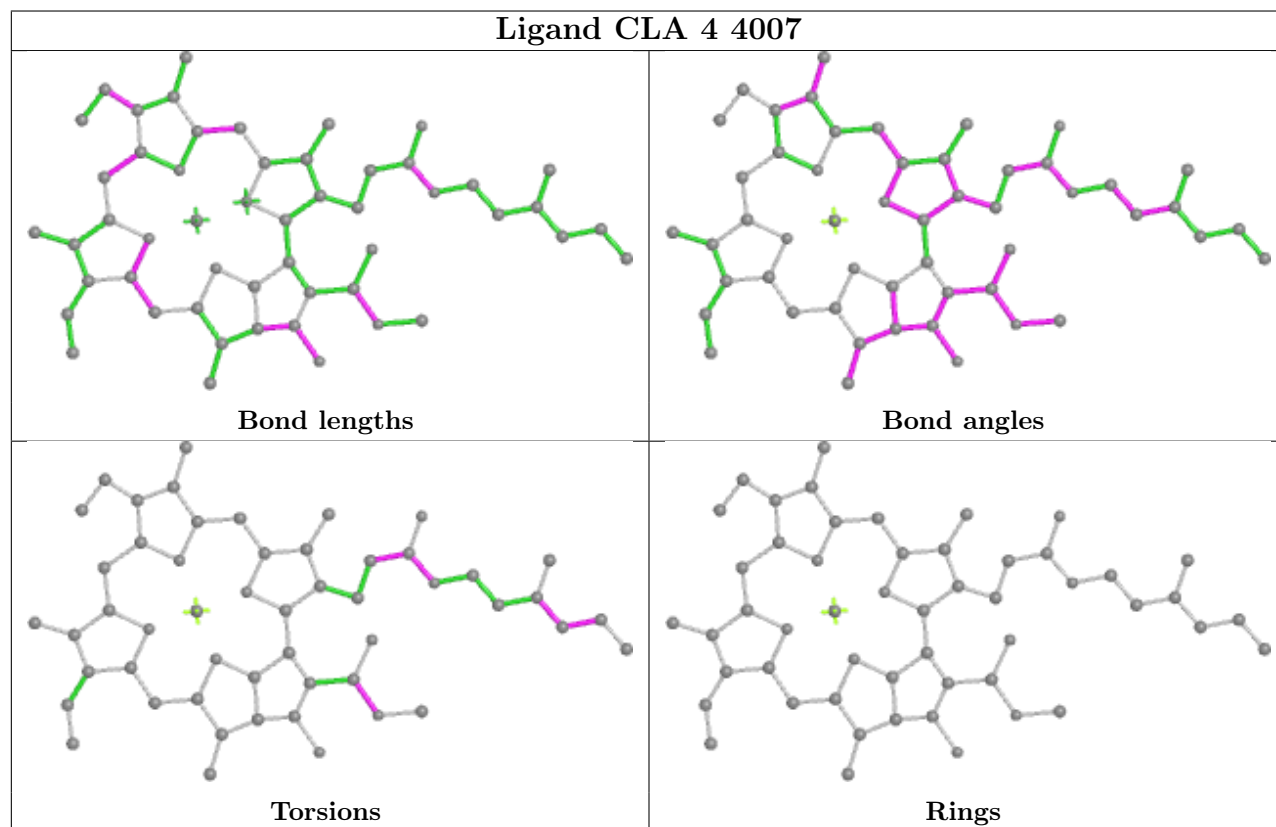
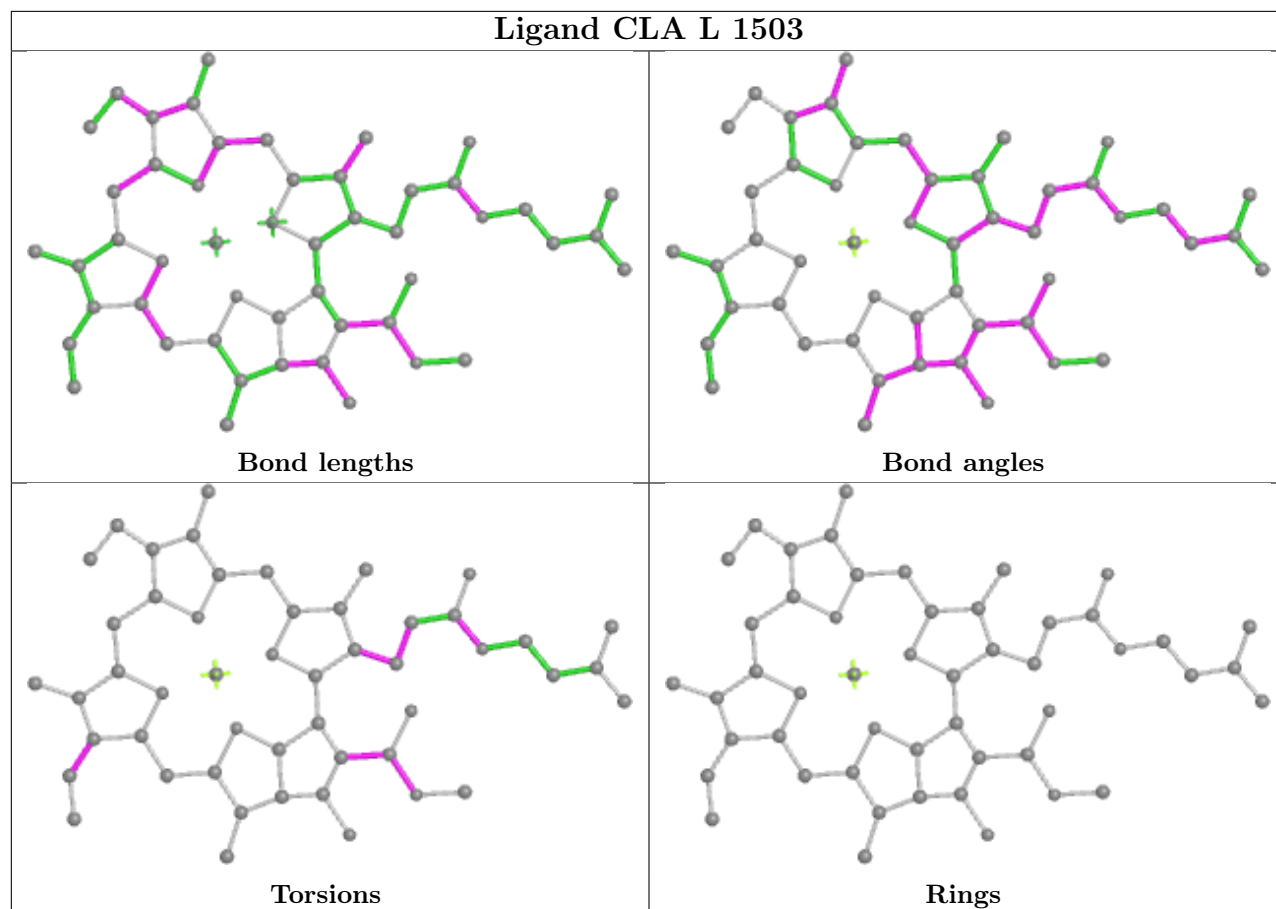


Ligand LMU 4 7008

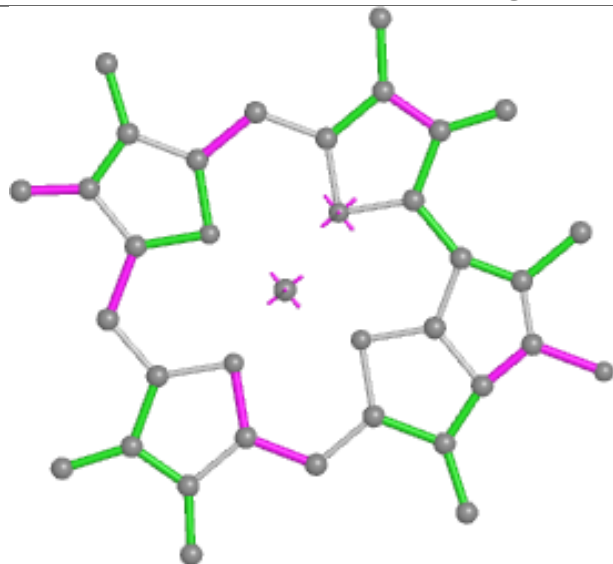


Ligand LMU 1 7013

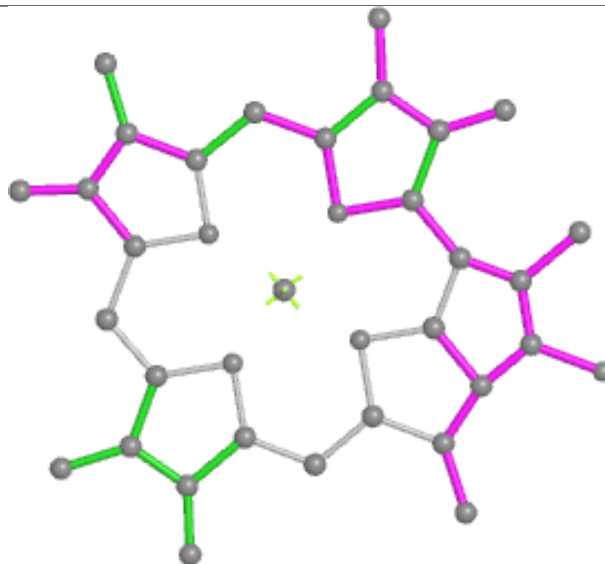




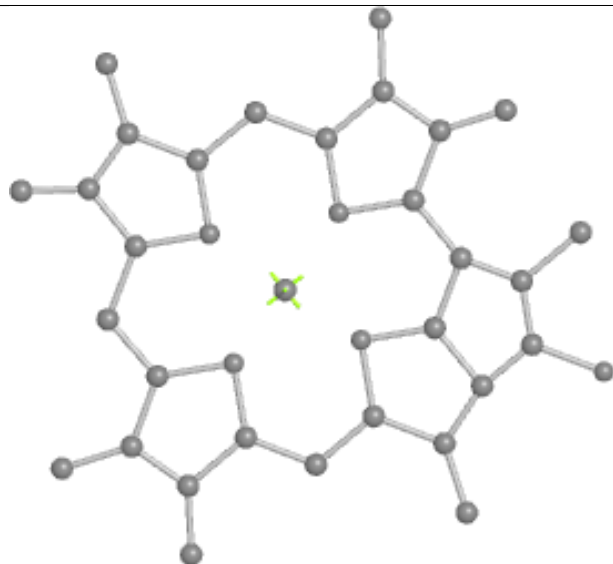
Ligand CLA B 1301



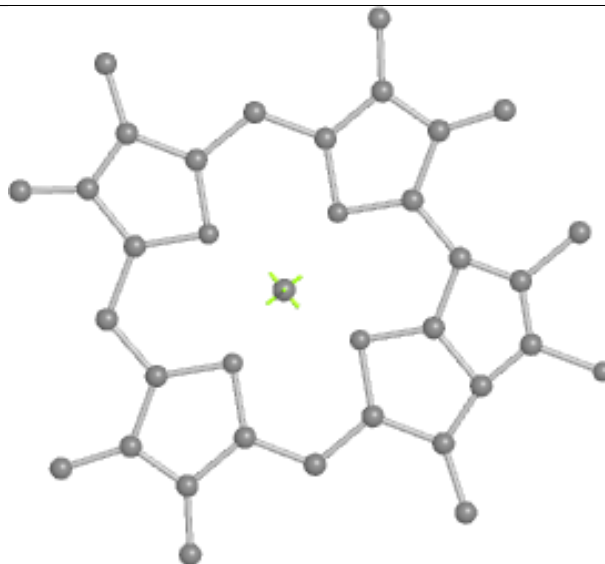
Bond lengths



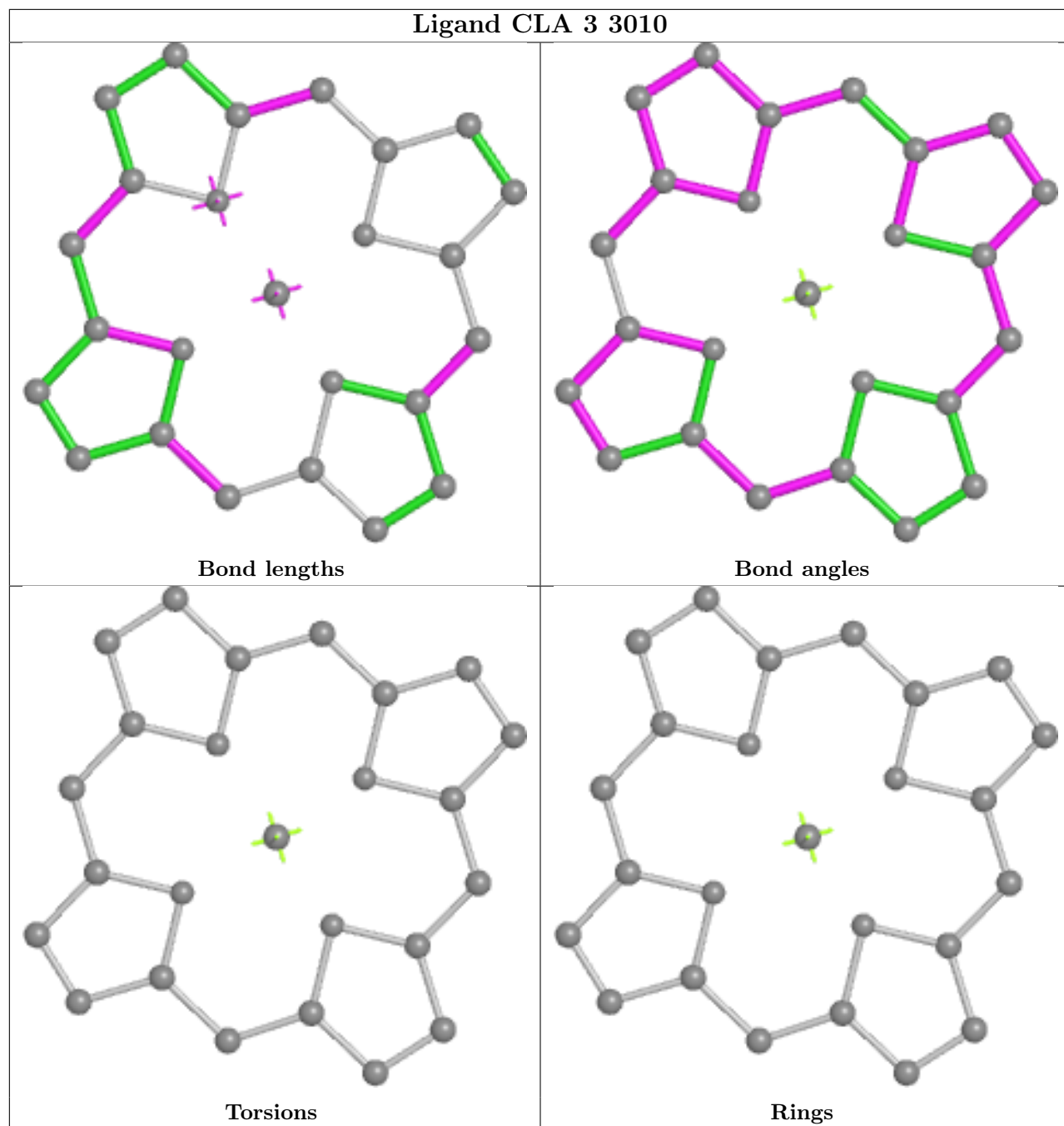
Bond angles

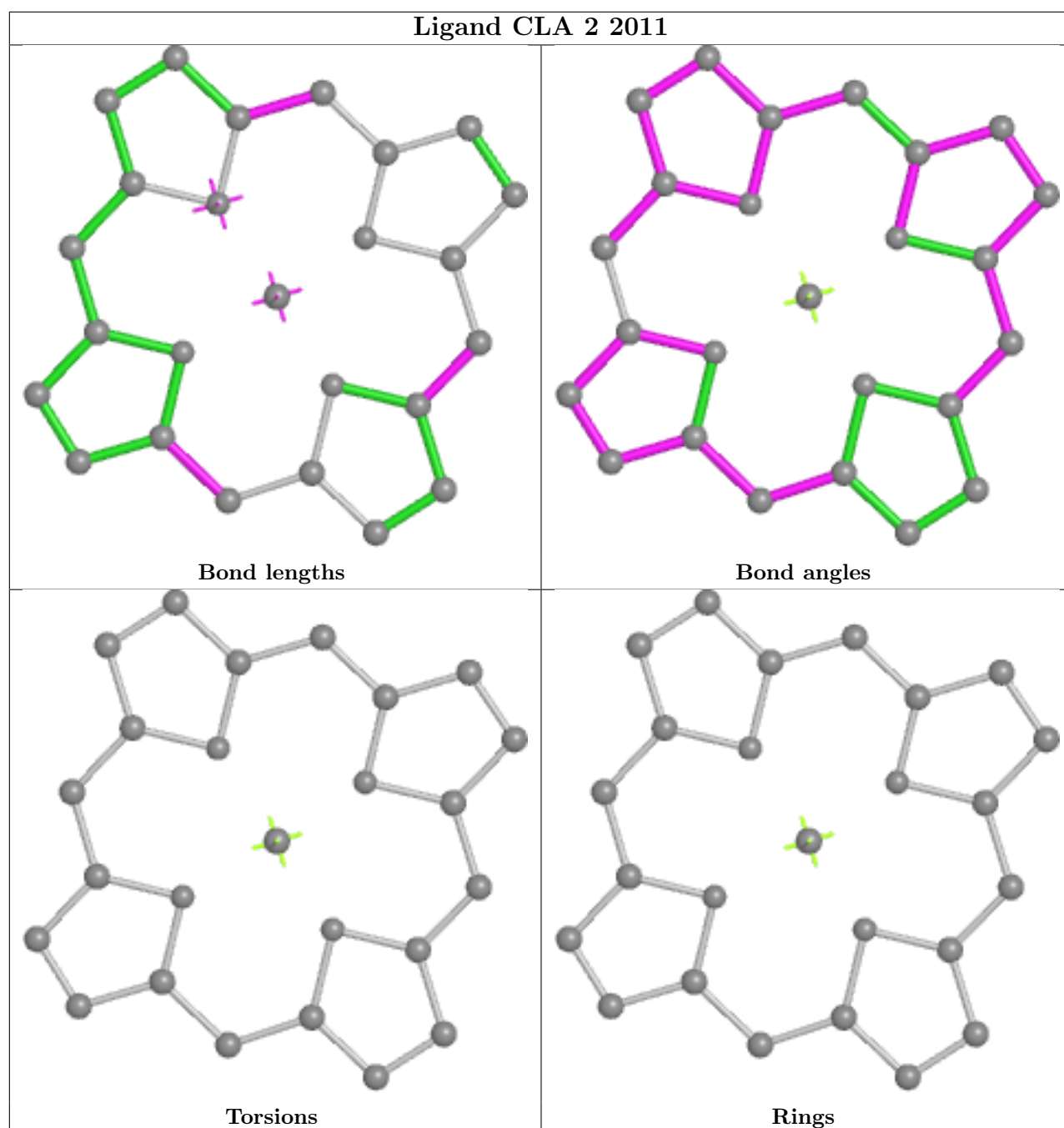


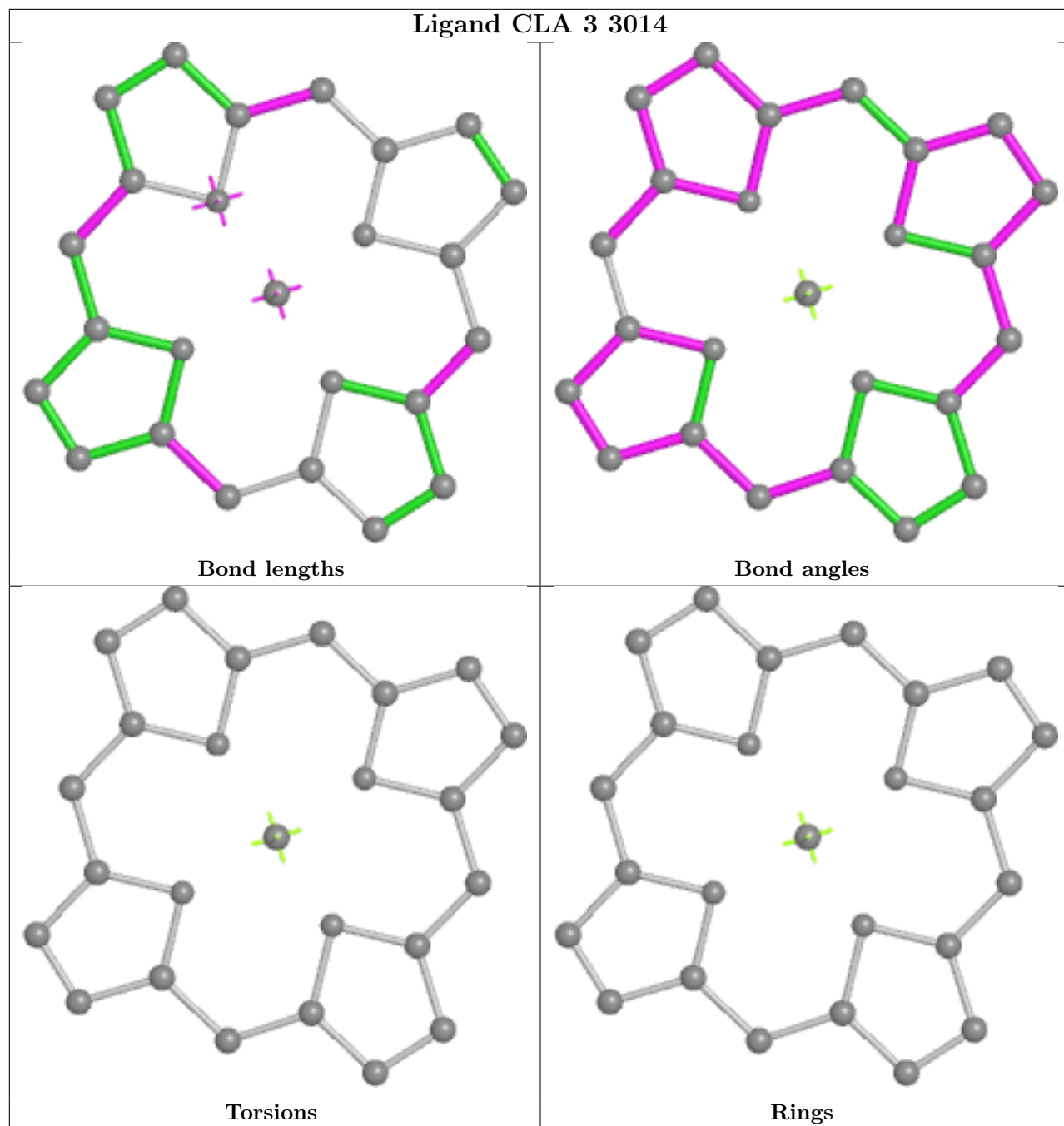
Torsions

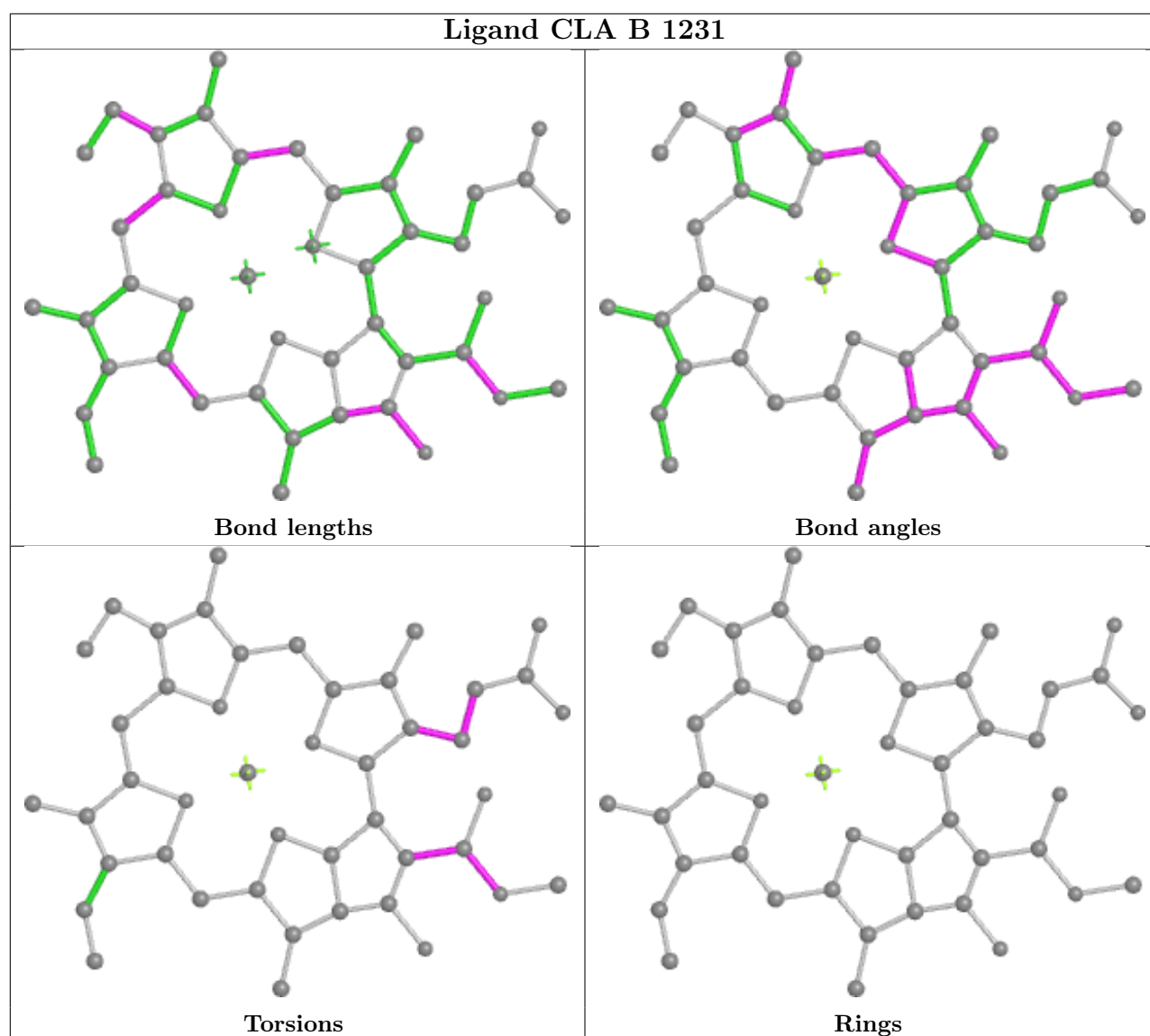
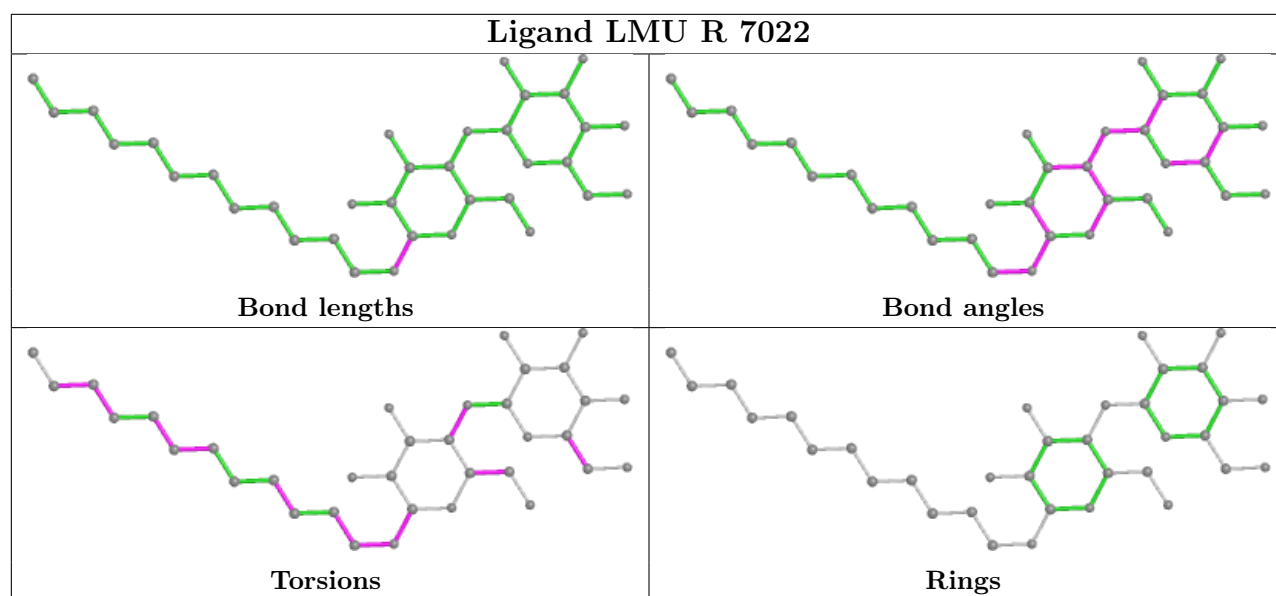


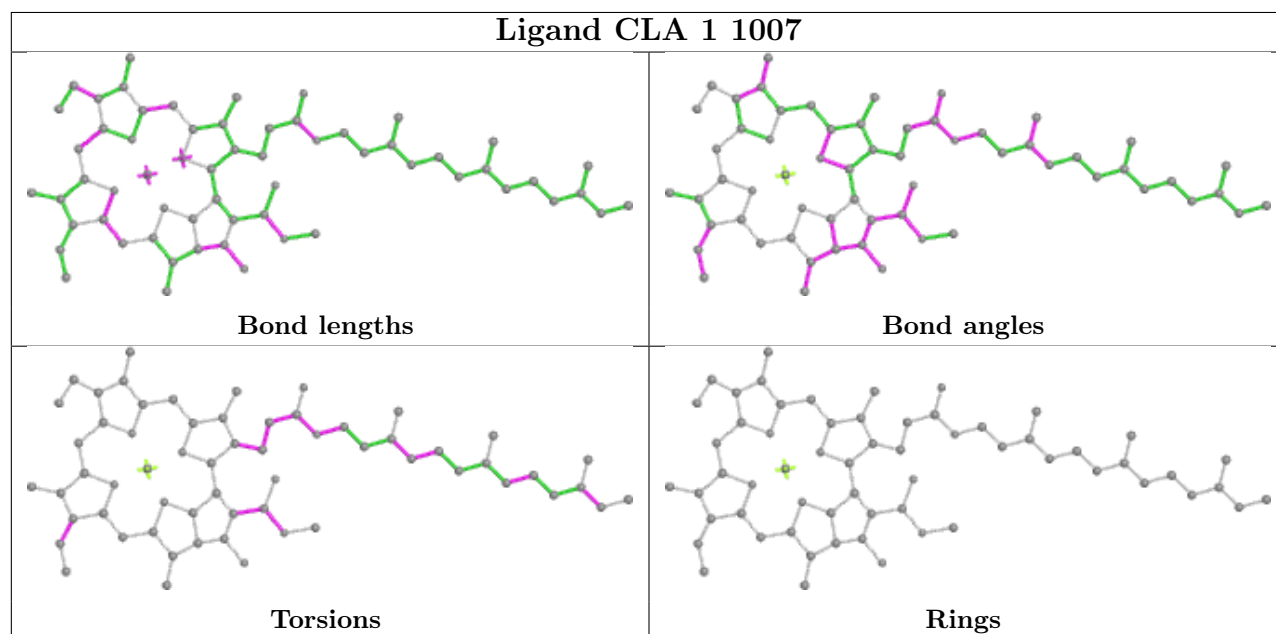
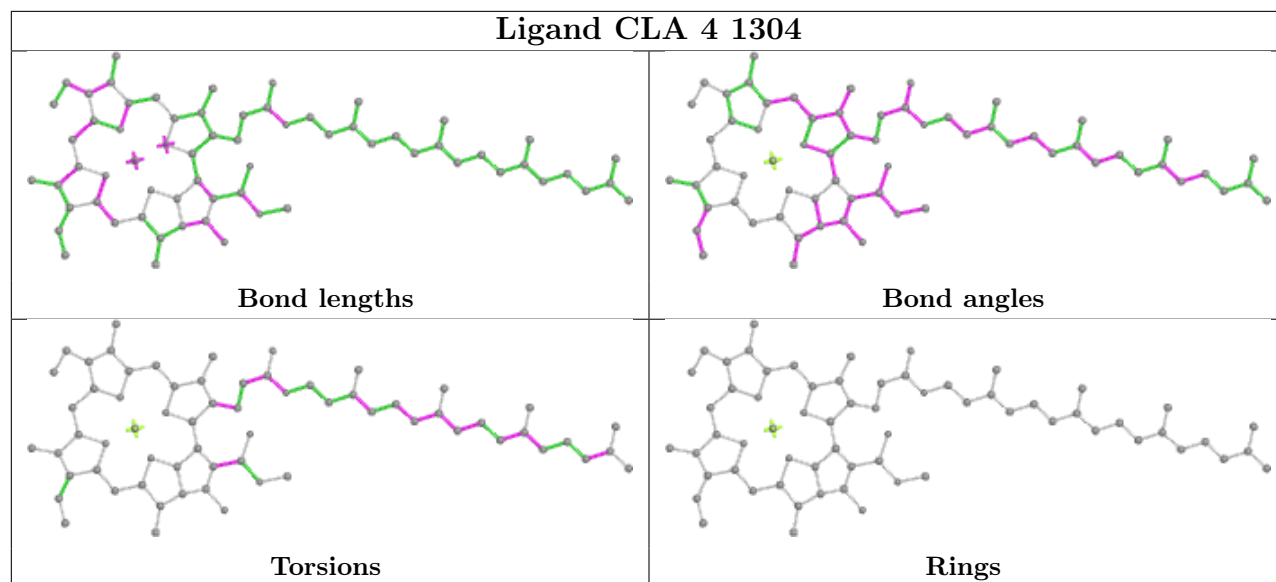
Rings

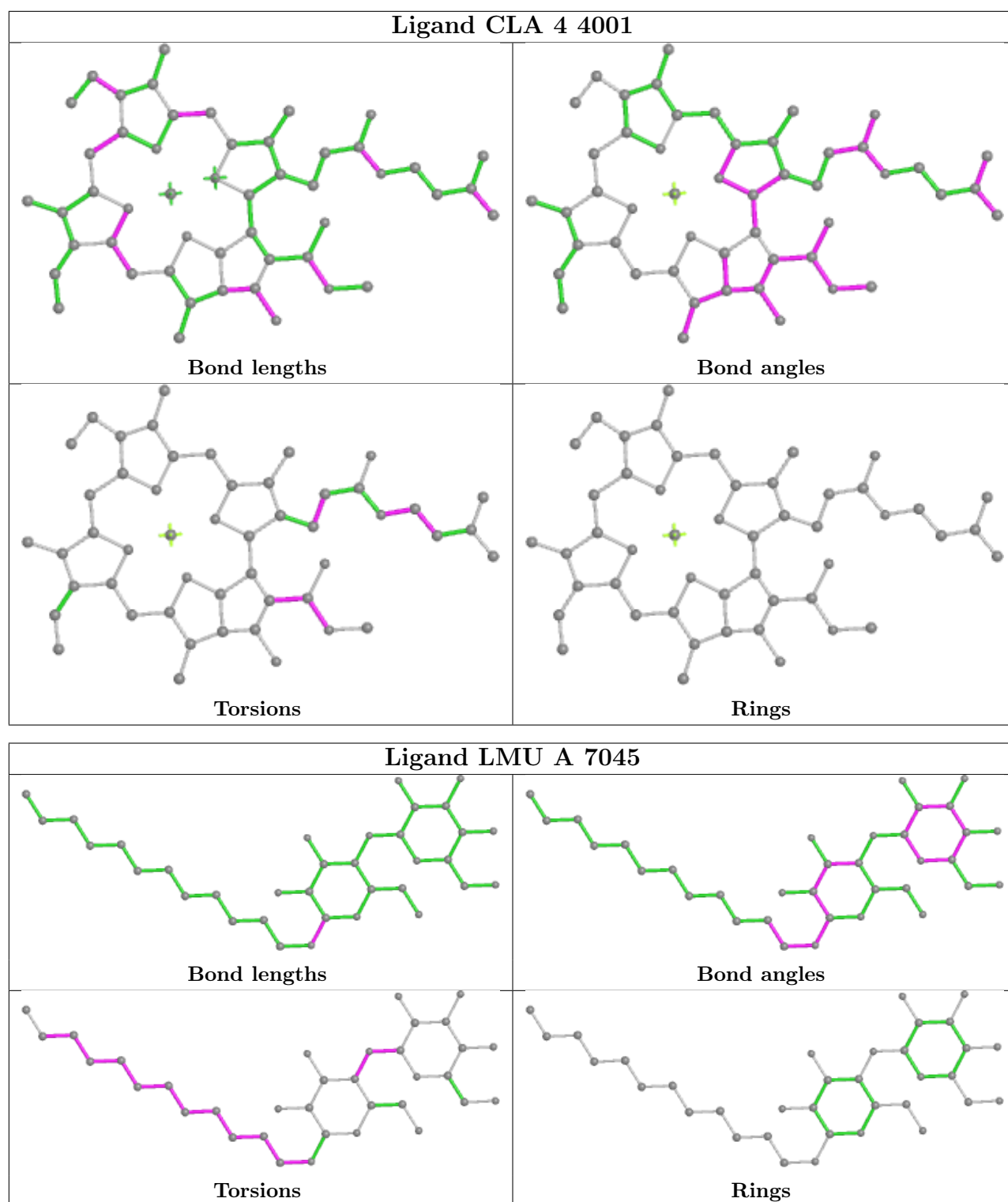


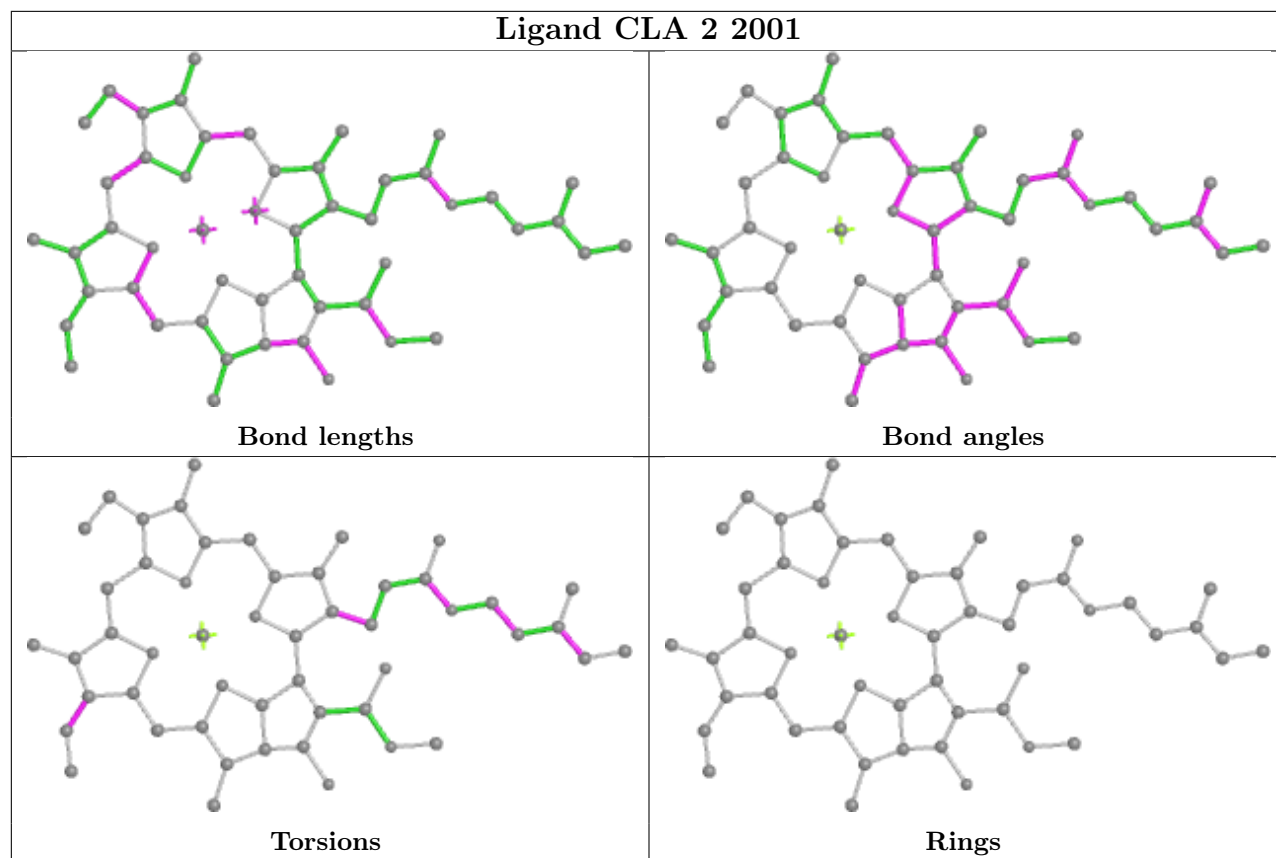


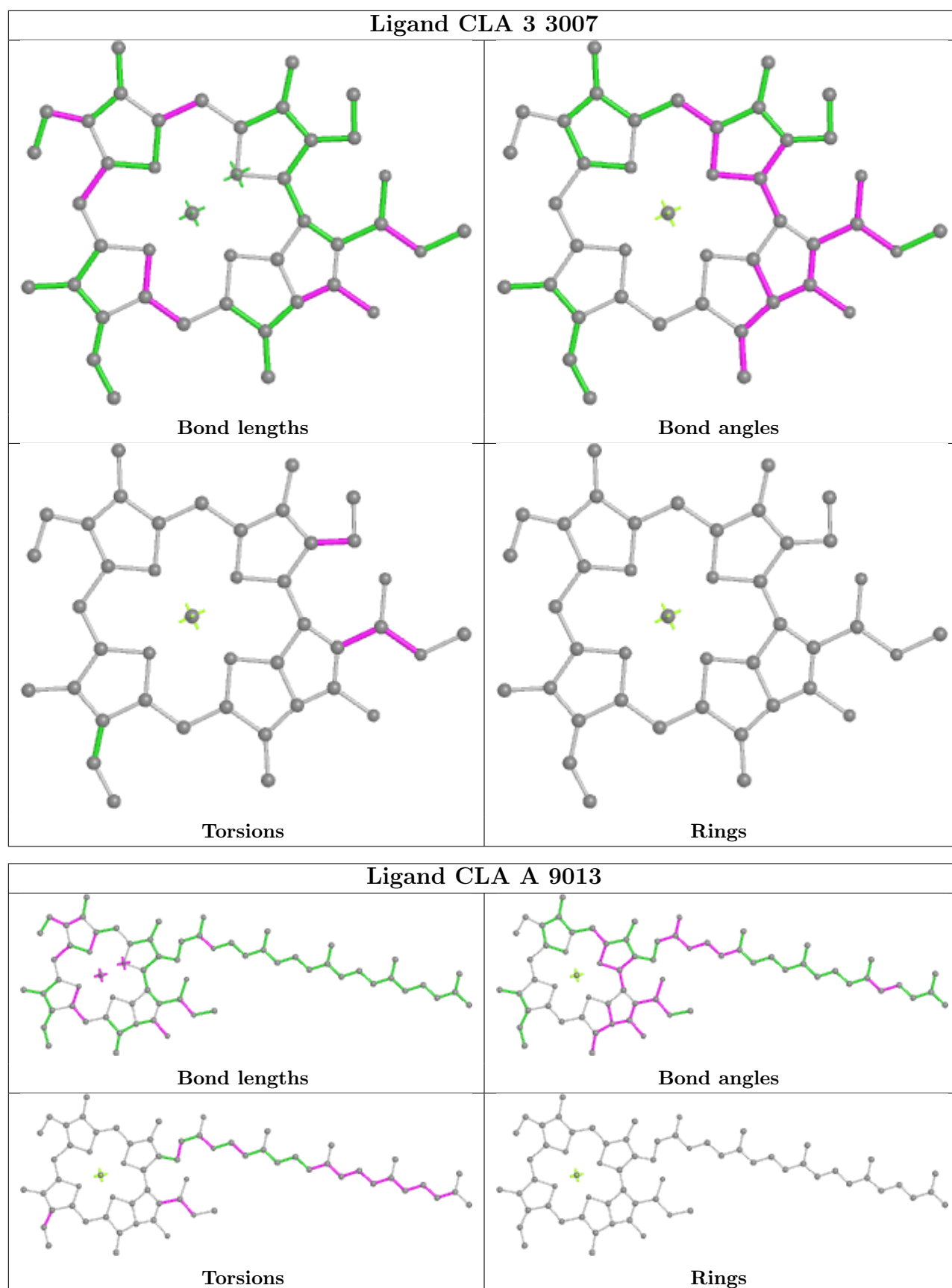


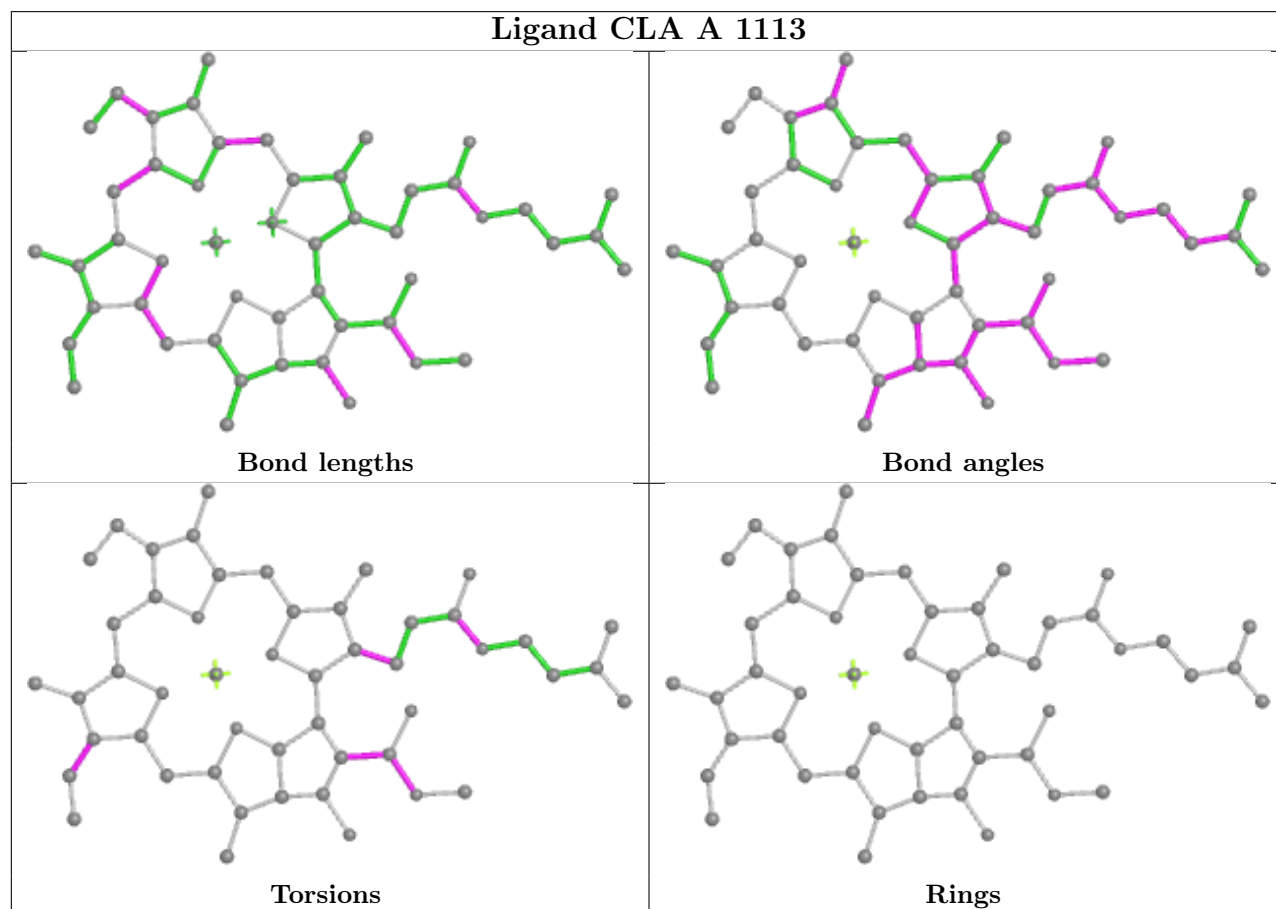
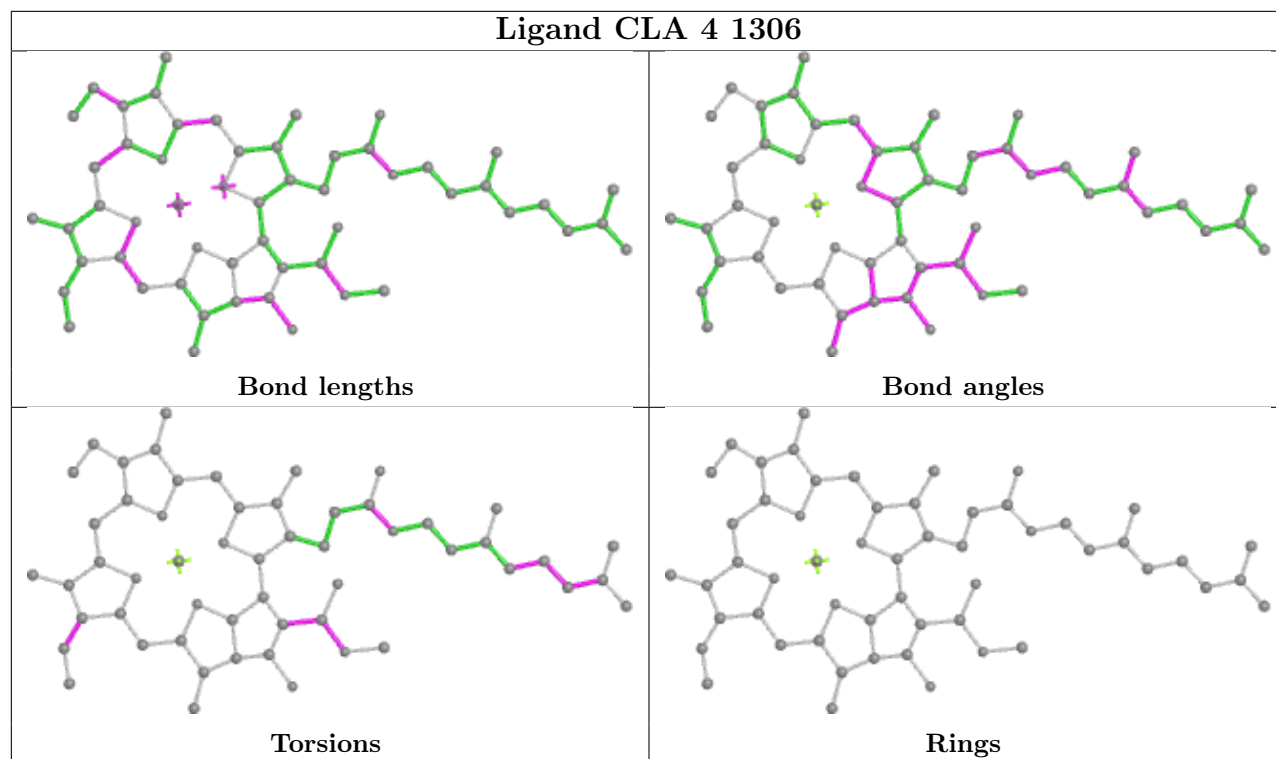


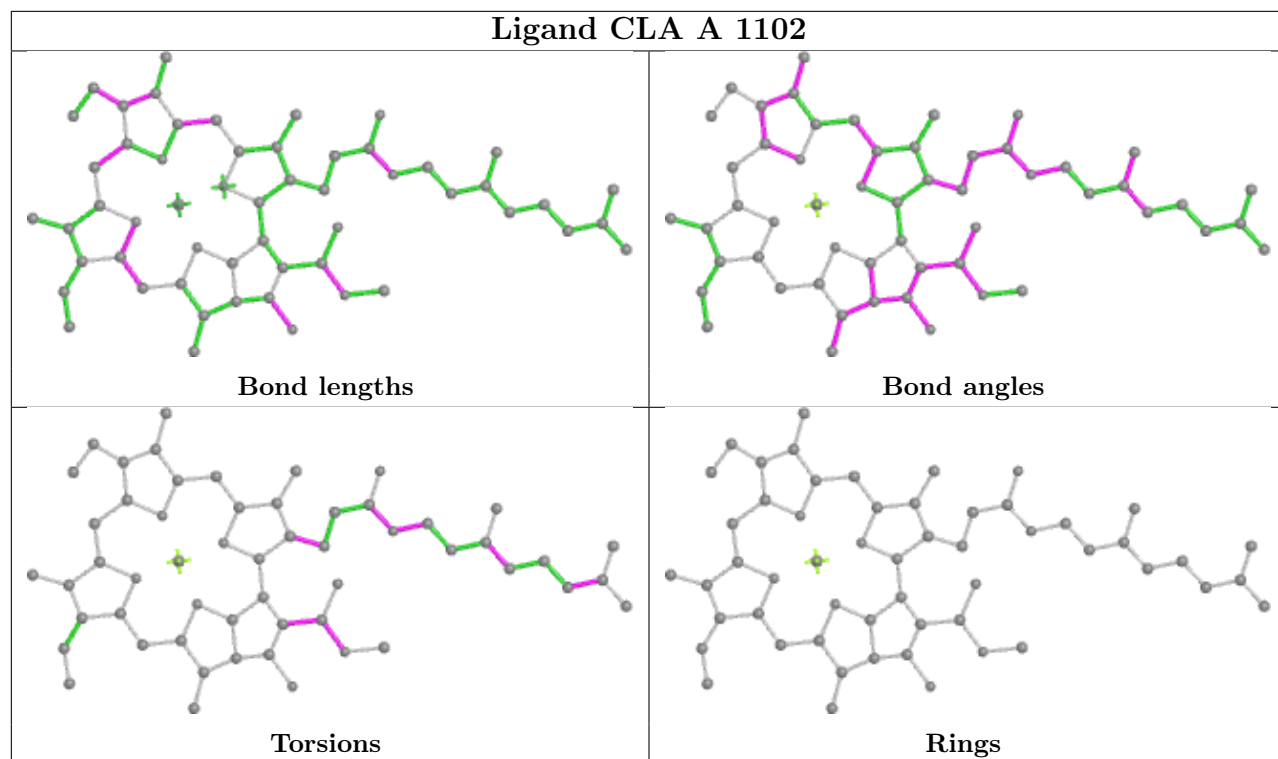




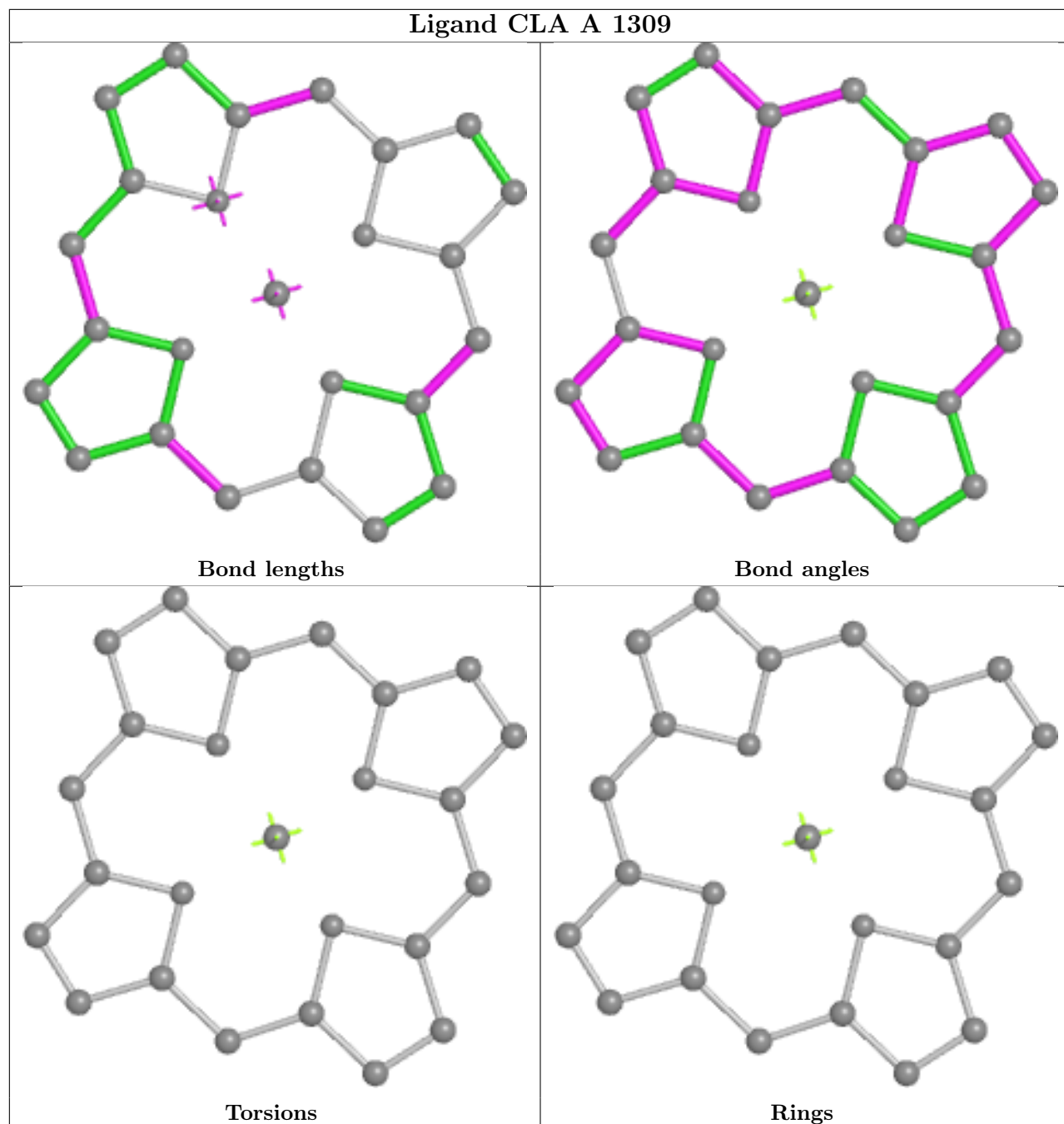




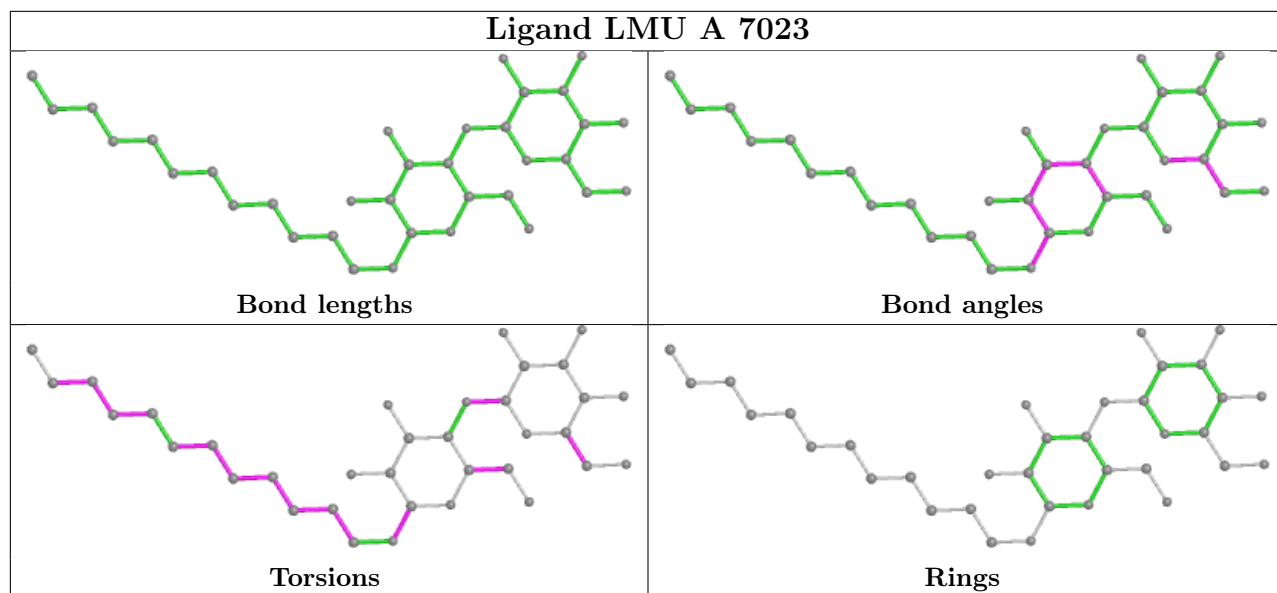




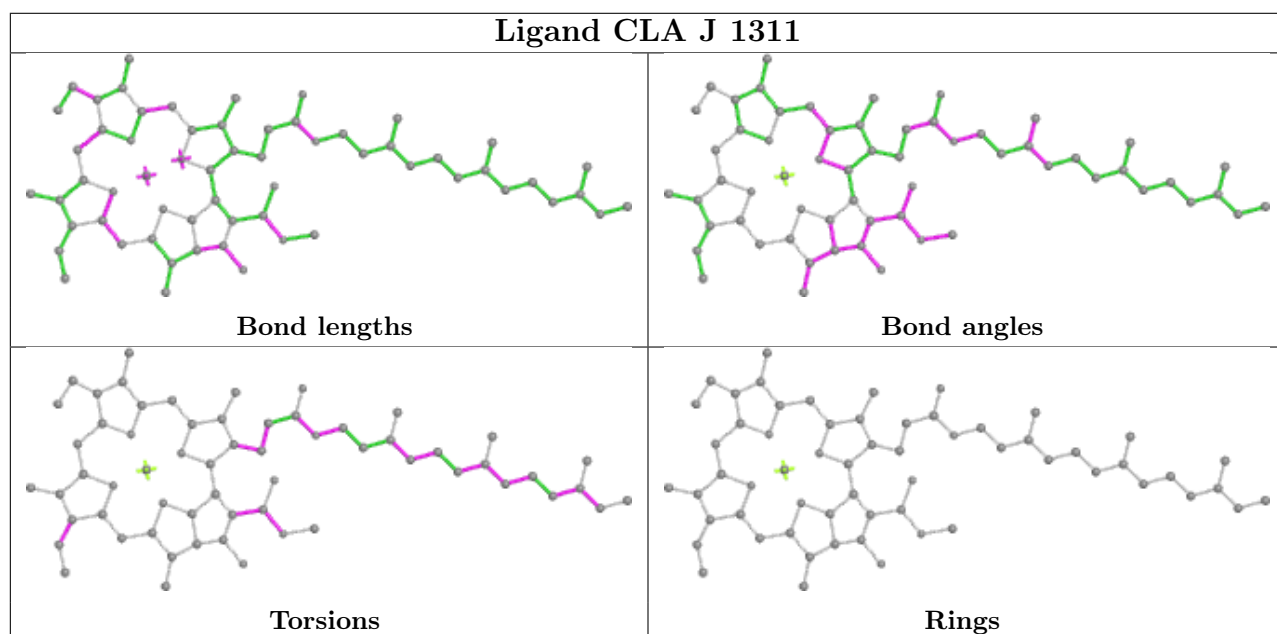
Ligand CLA A 1309

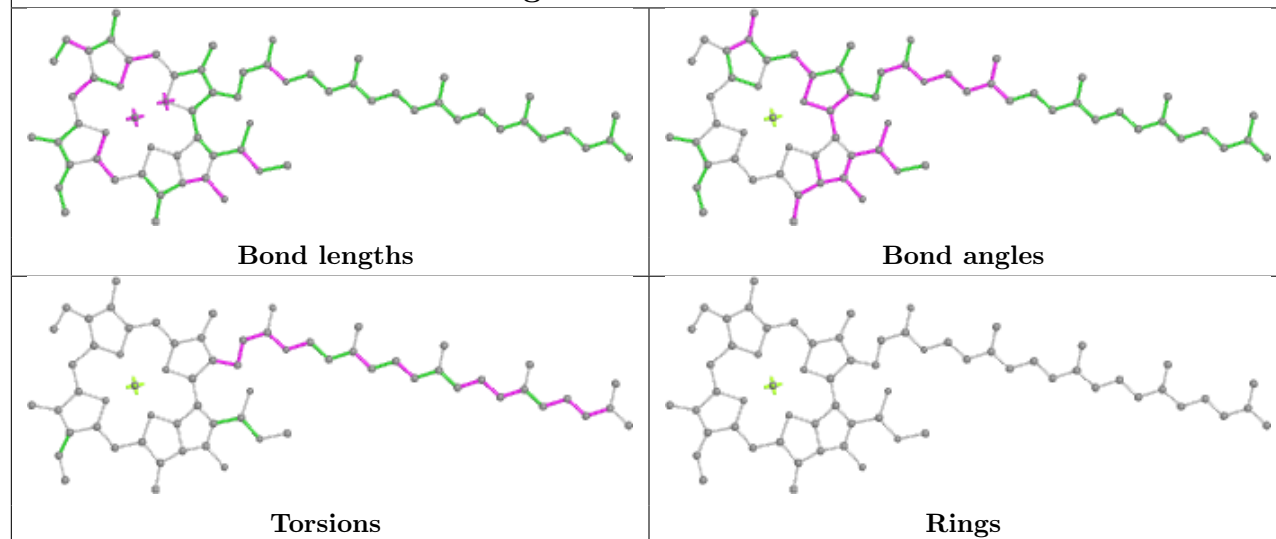
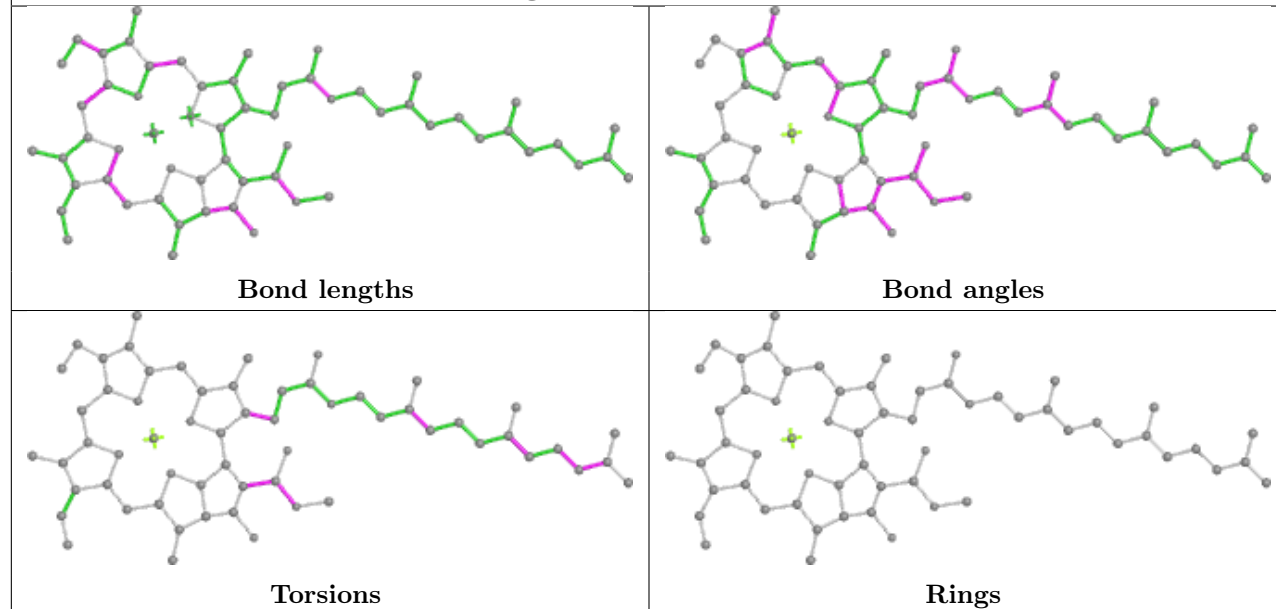


Ligand LMU A 7023

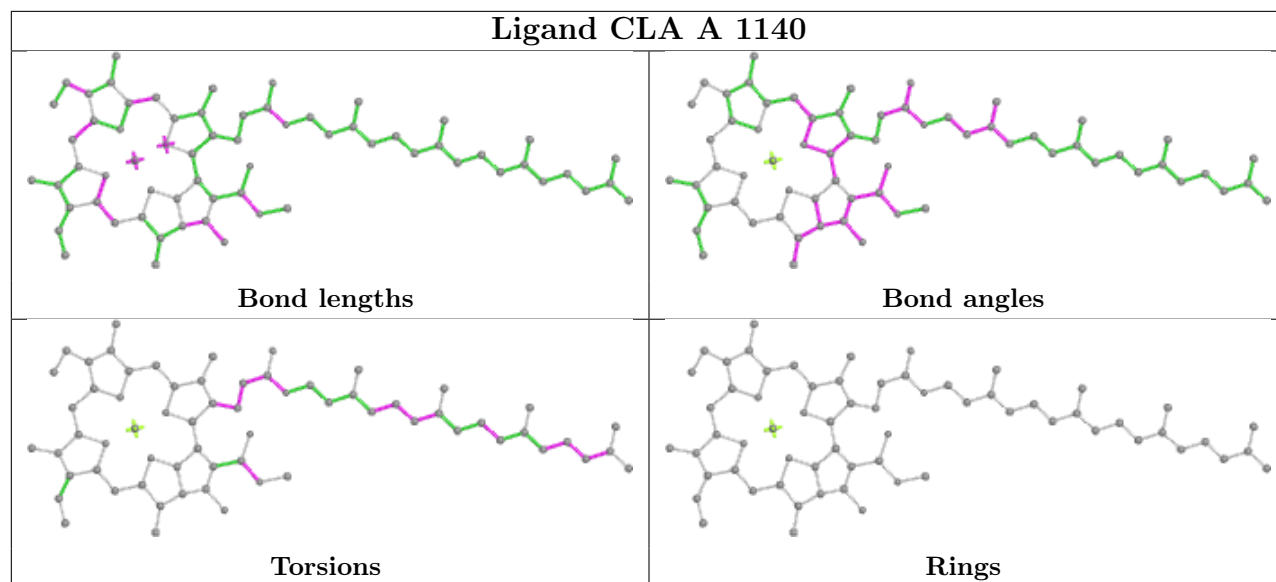


Ligand CLA J 1311

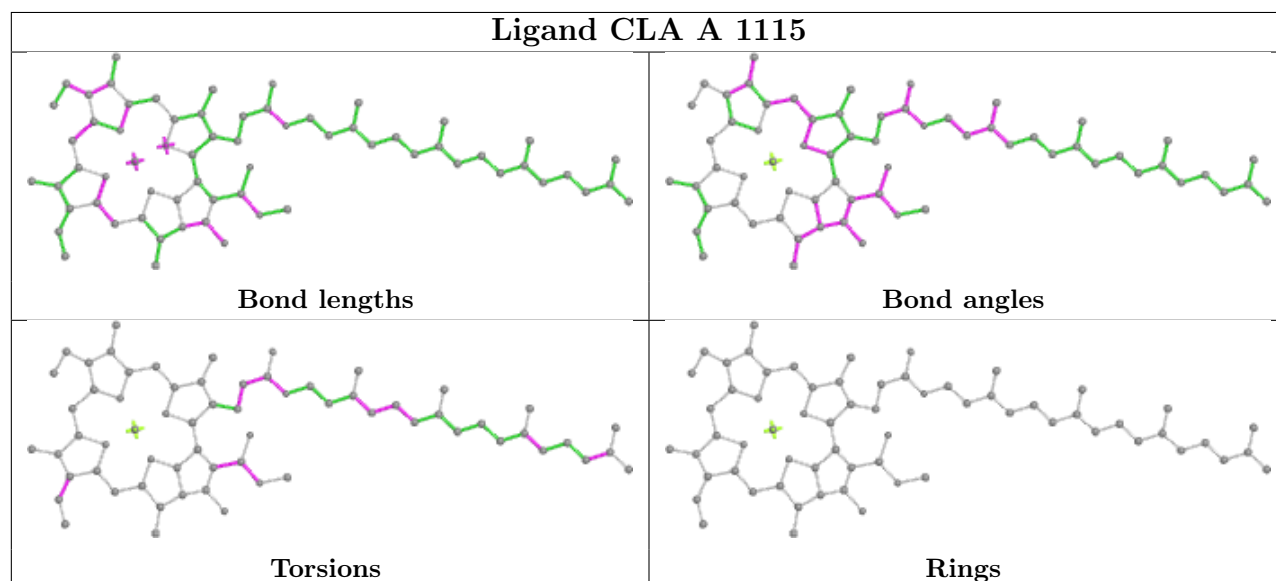


Ligand CLA B 1223**Ligand CLA B 1212**

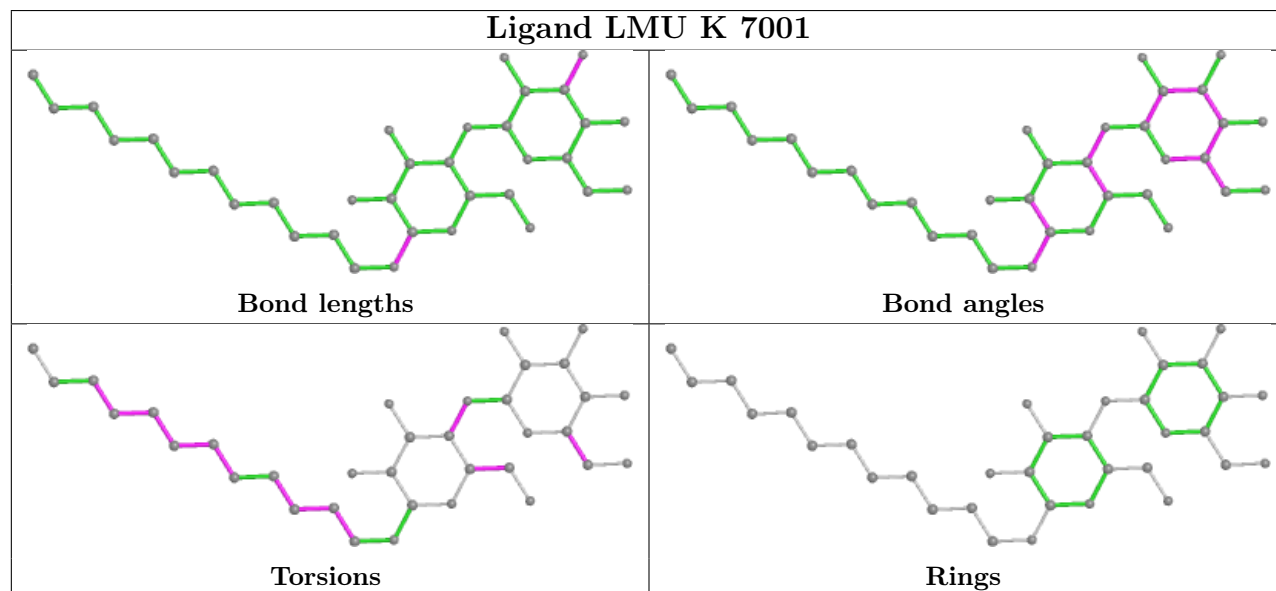
Ligand CLA A 1140



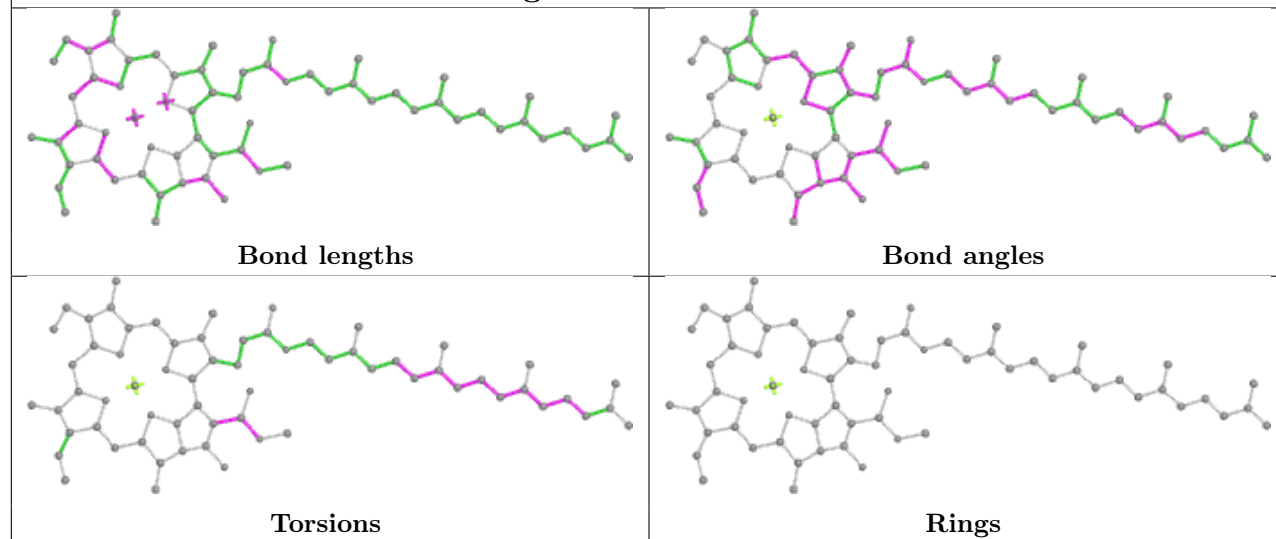
Ligand CLA A 1115



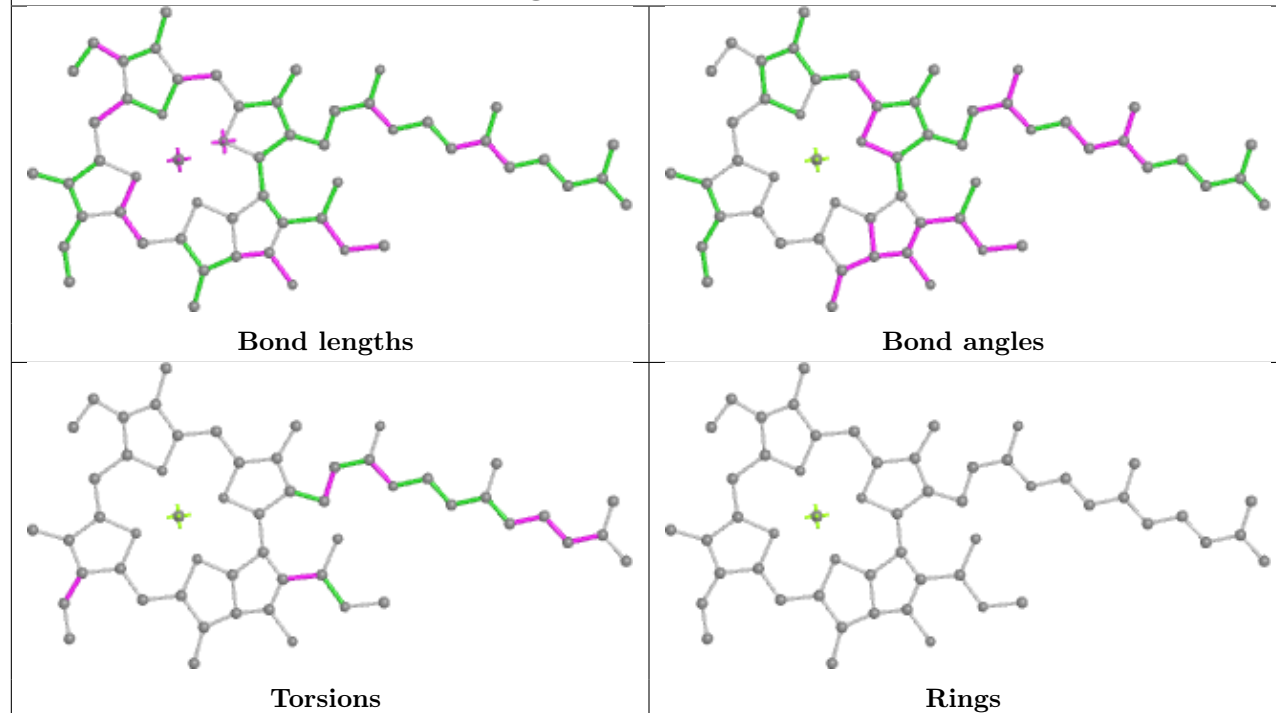
Ligand LMU K 7001



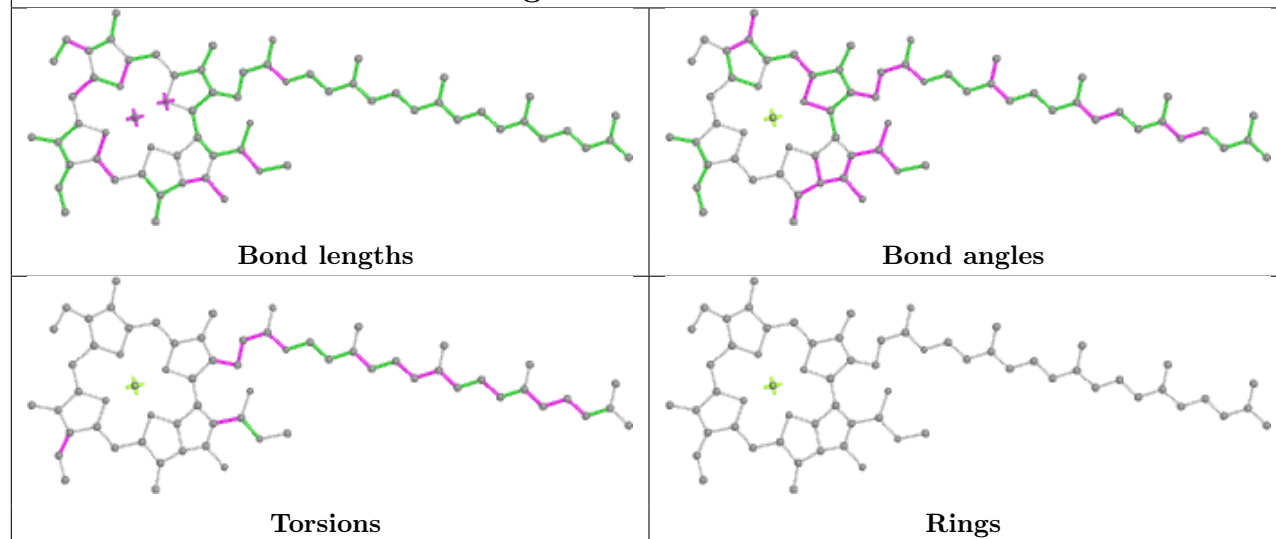
Ligand CLA B 1203



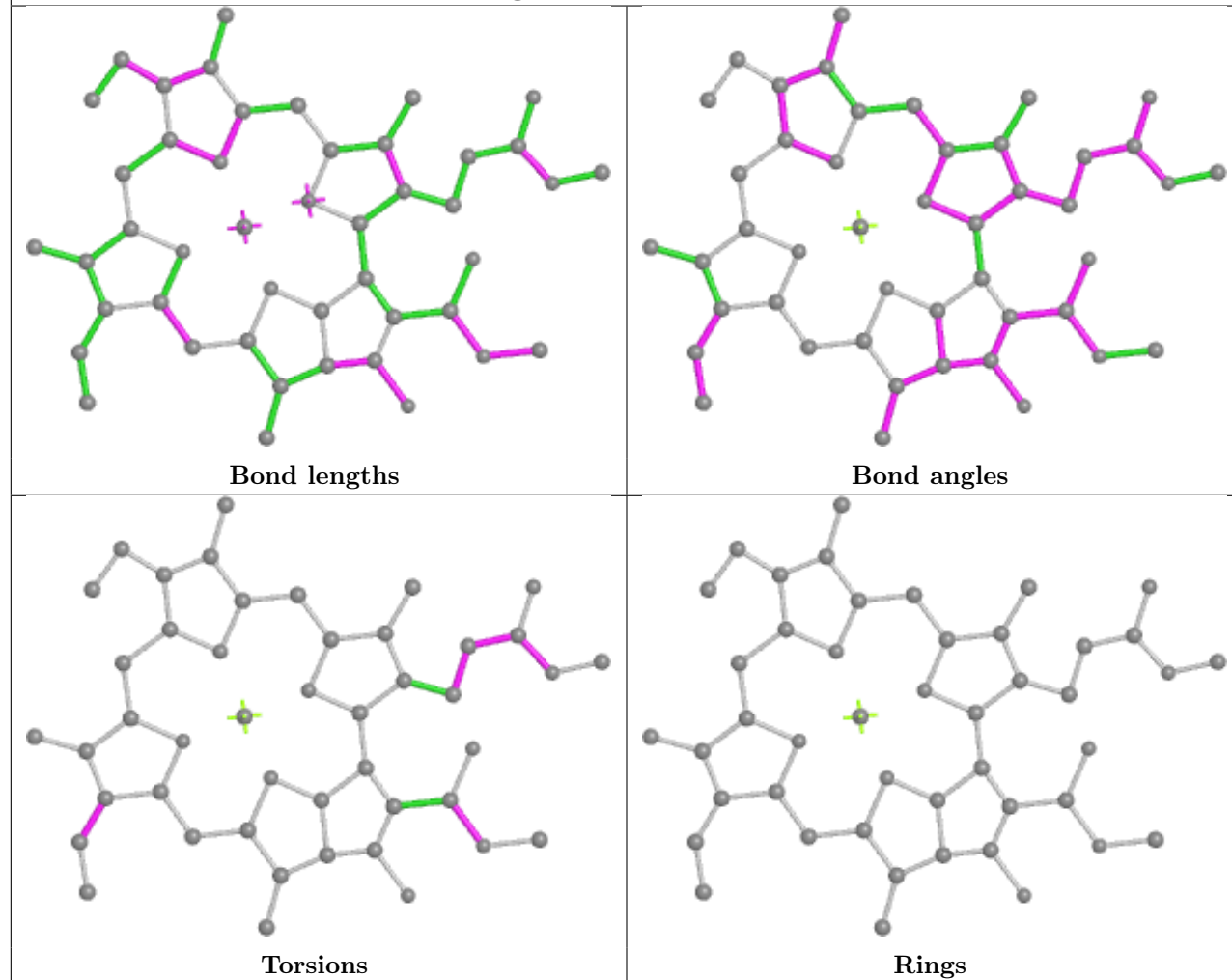
Ligand CLA 4 1004



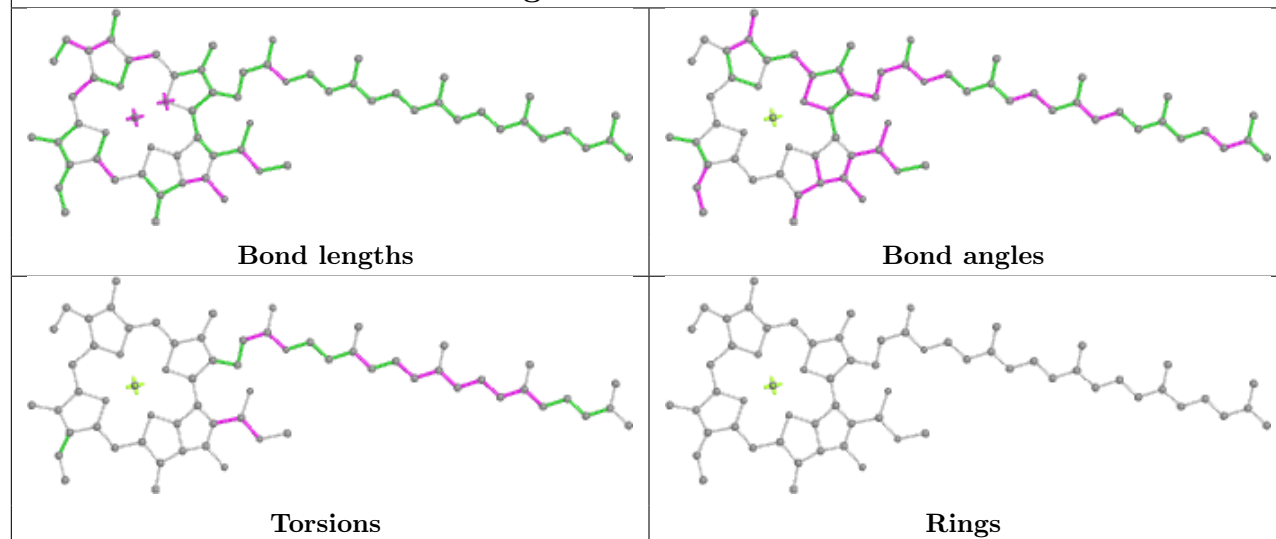
Ligand CLA B 1210



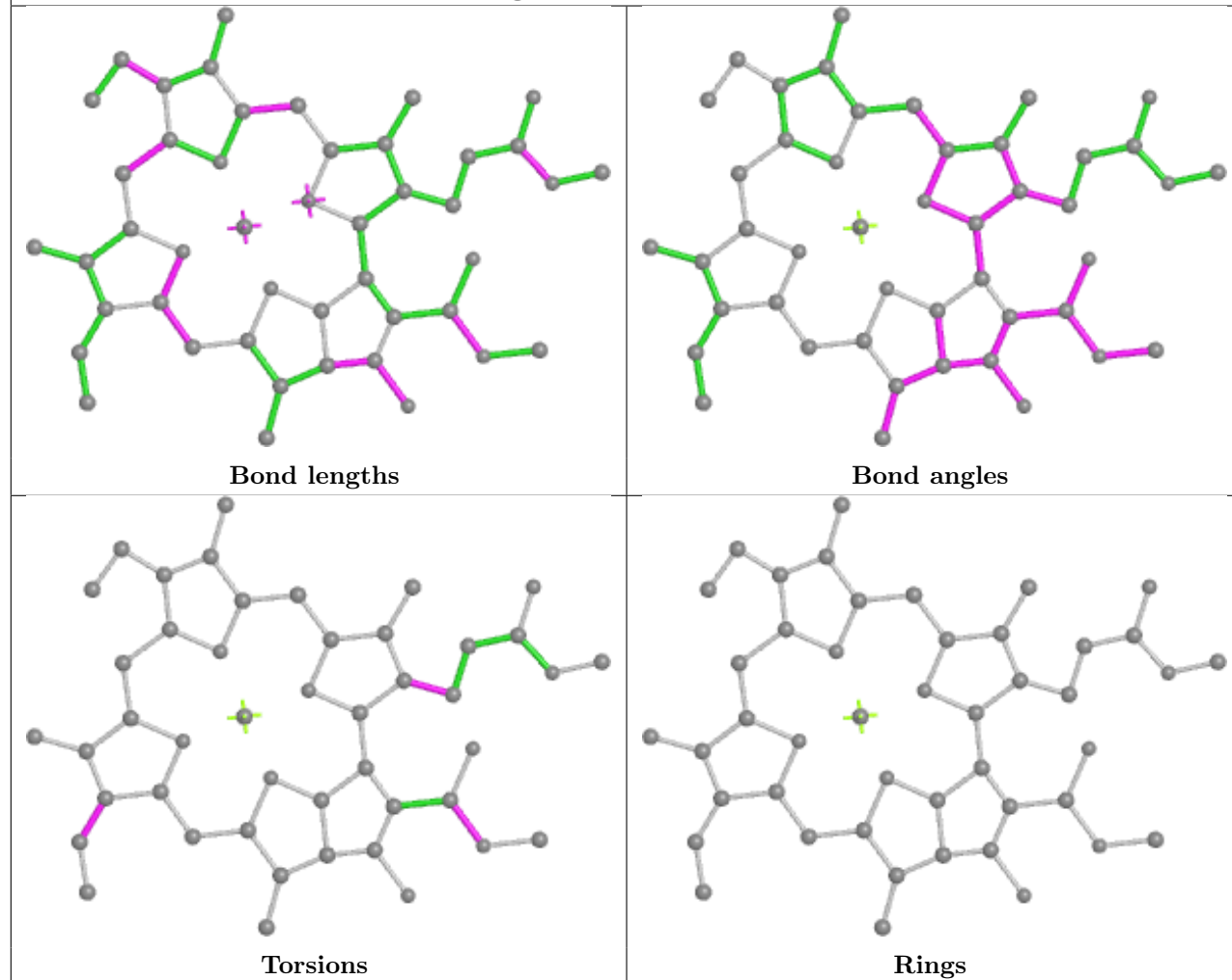
Ligand CLA 3 1147

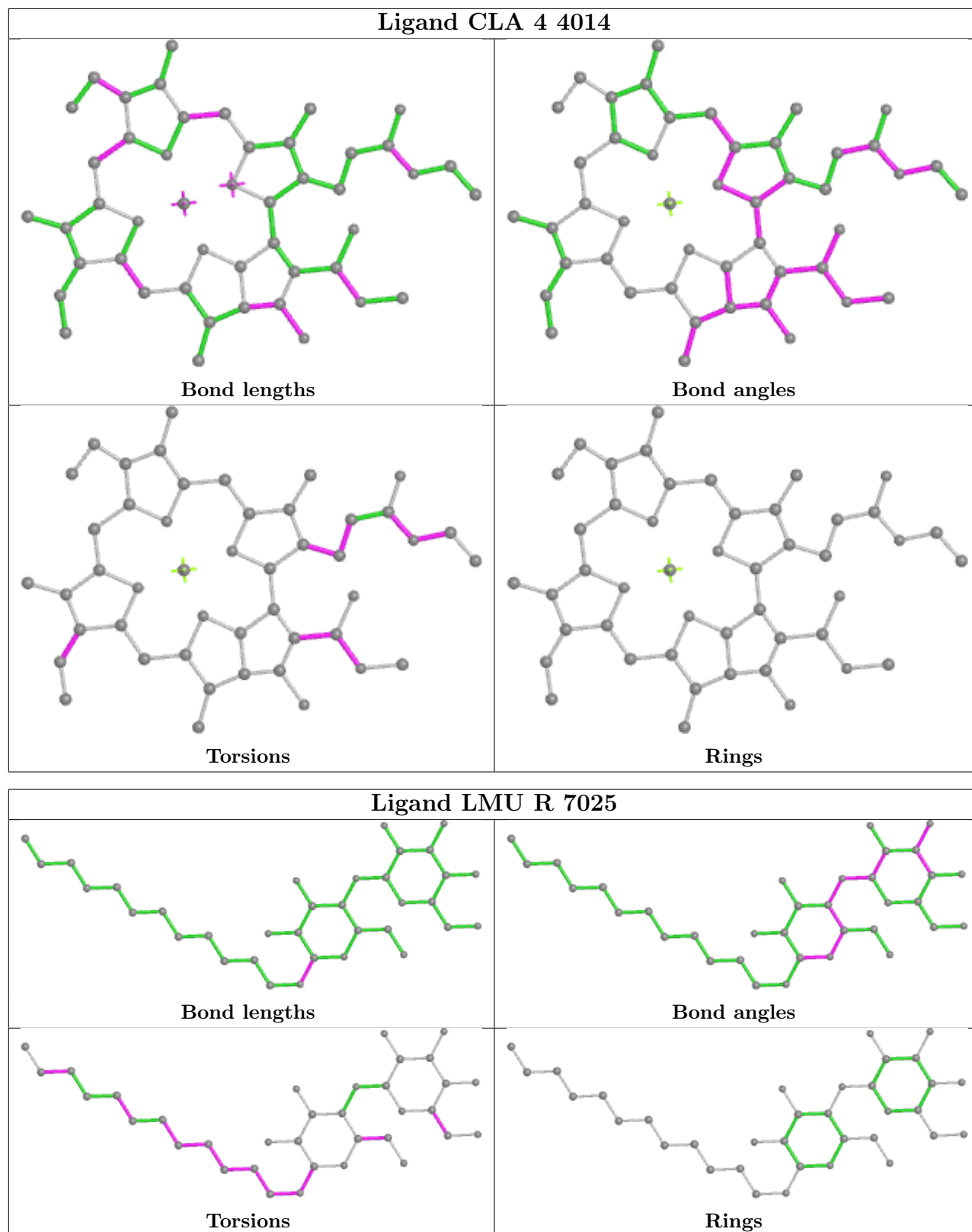


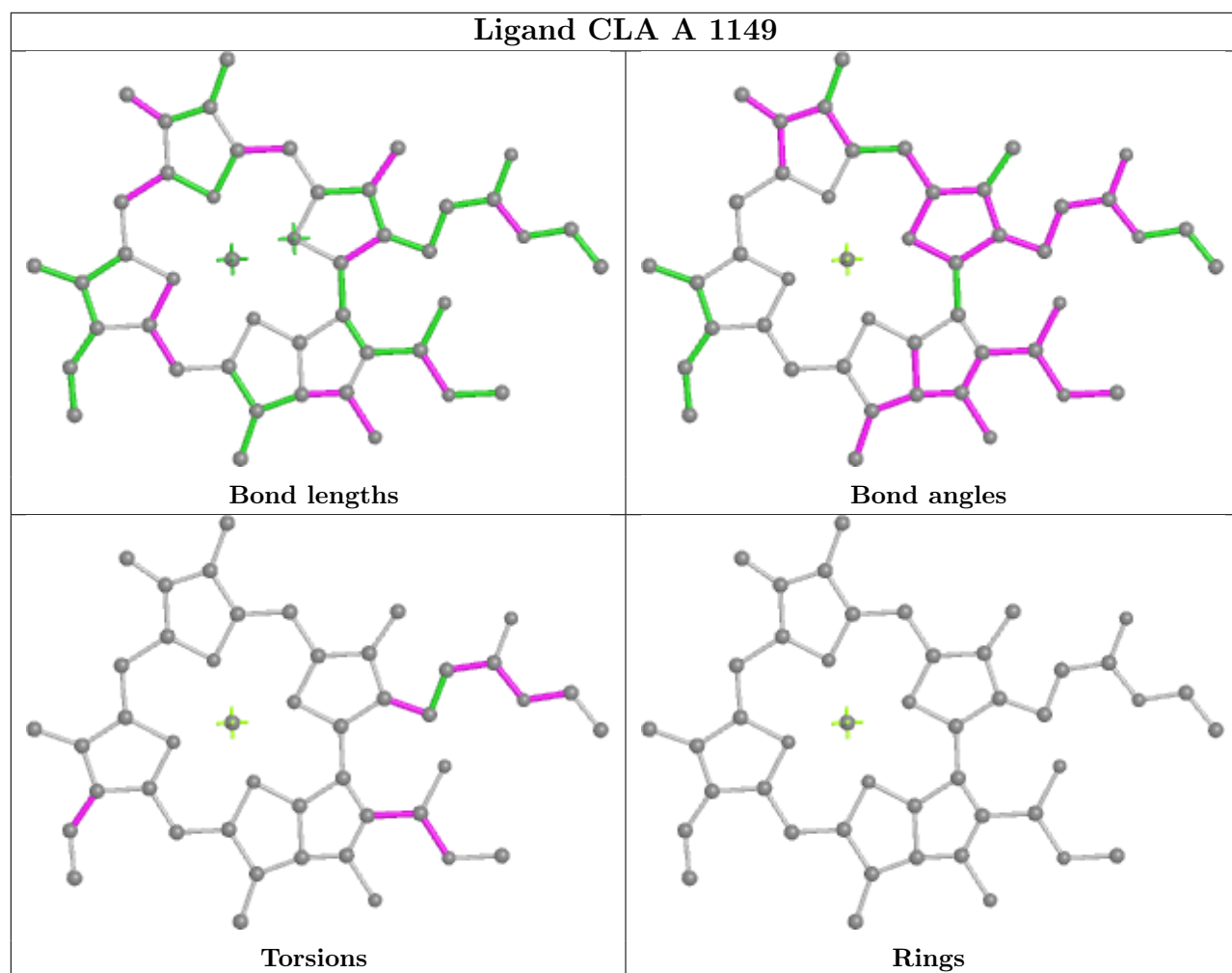
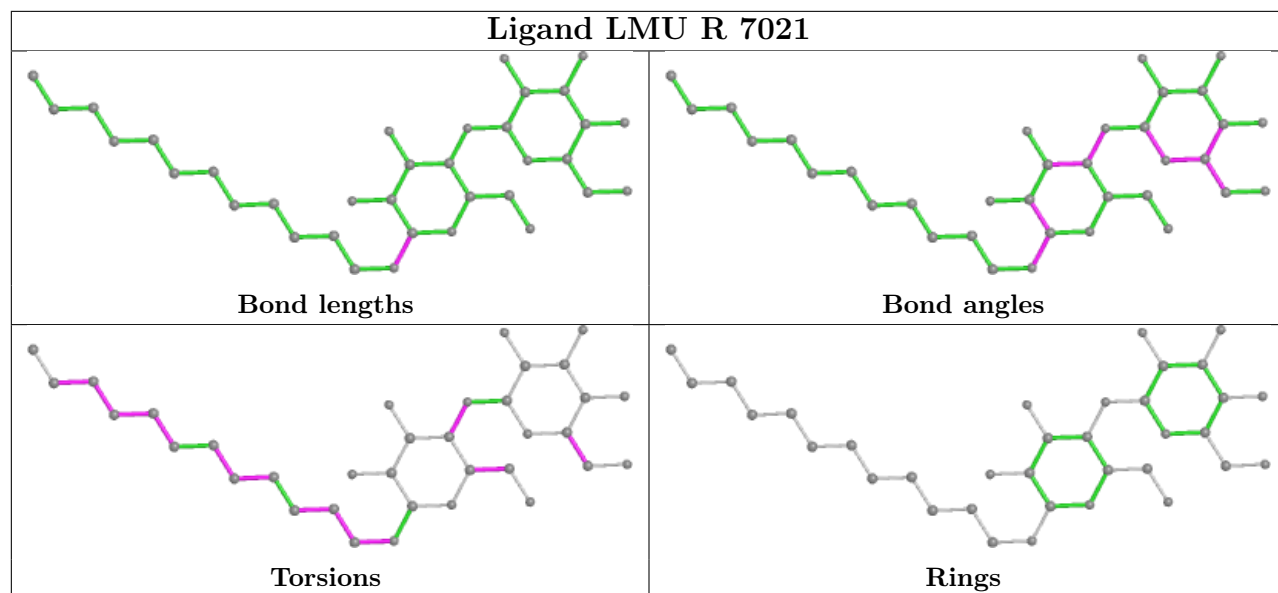
Ligand CLA B 9010

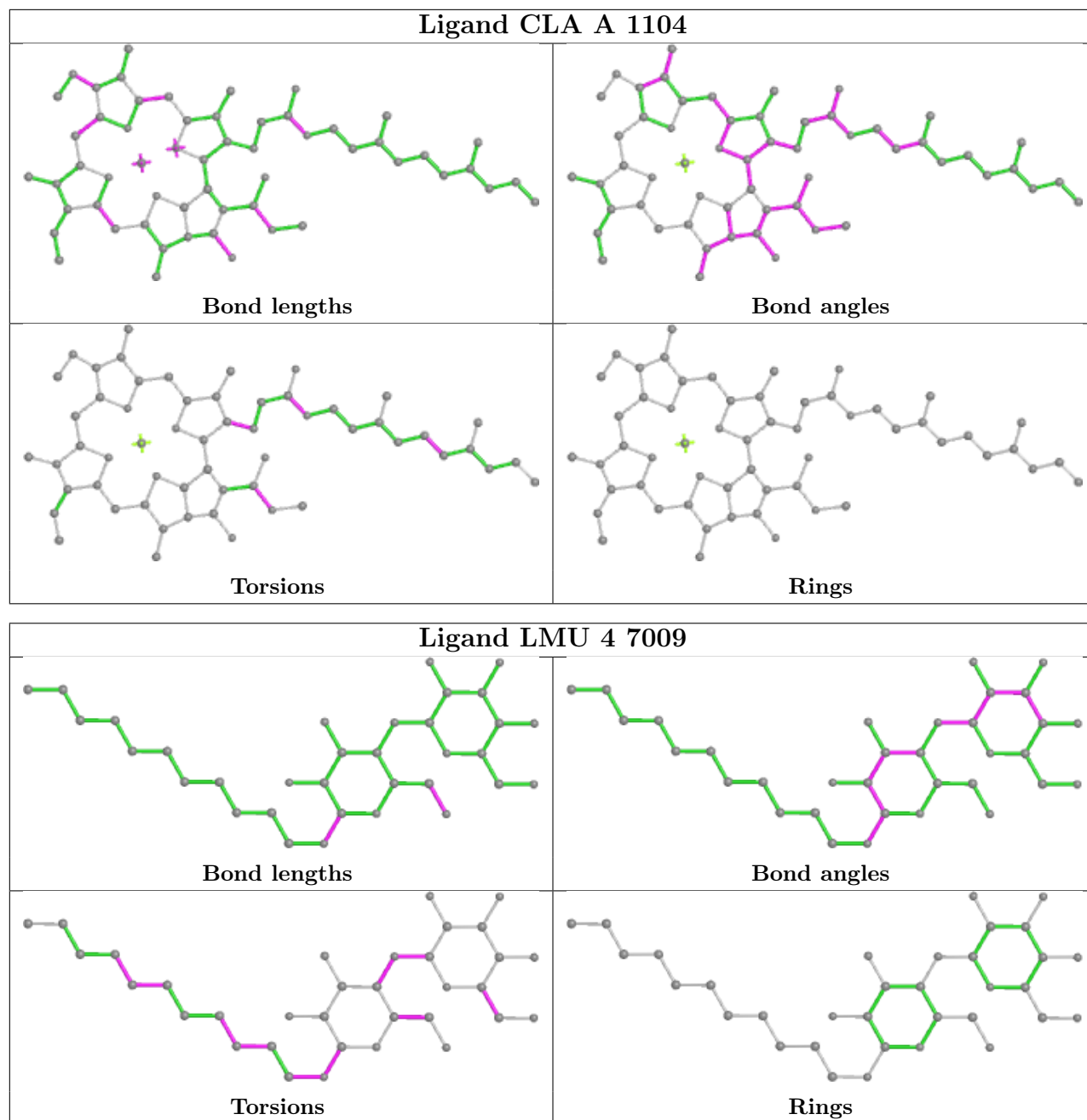


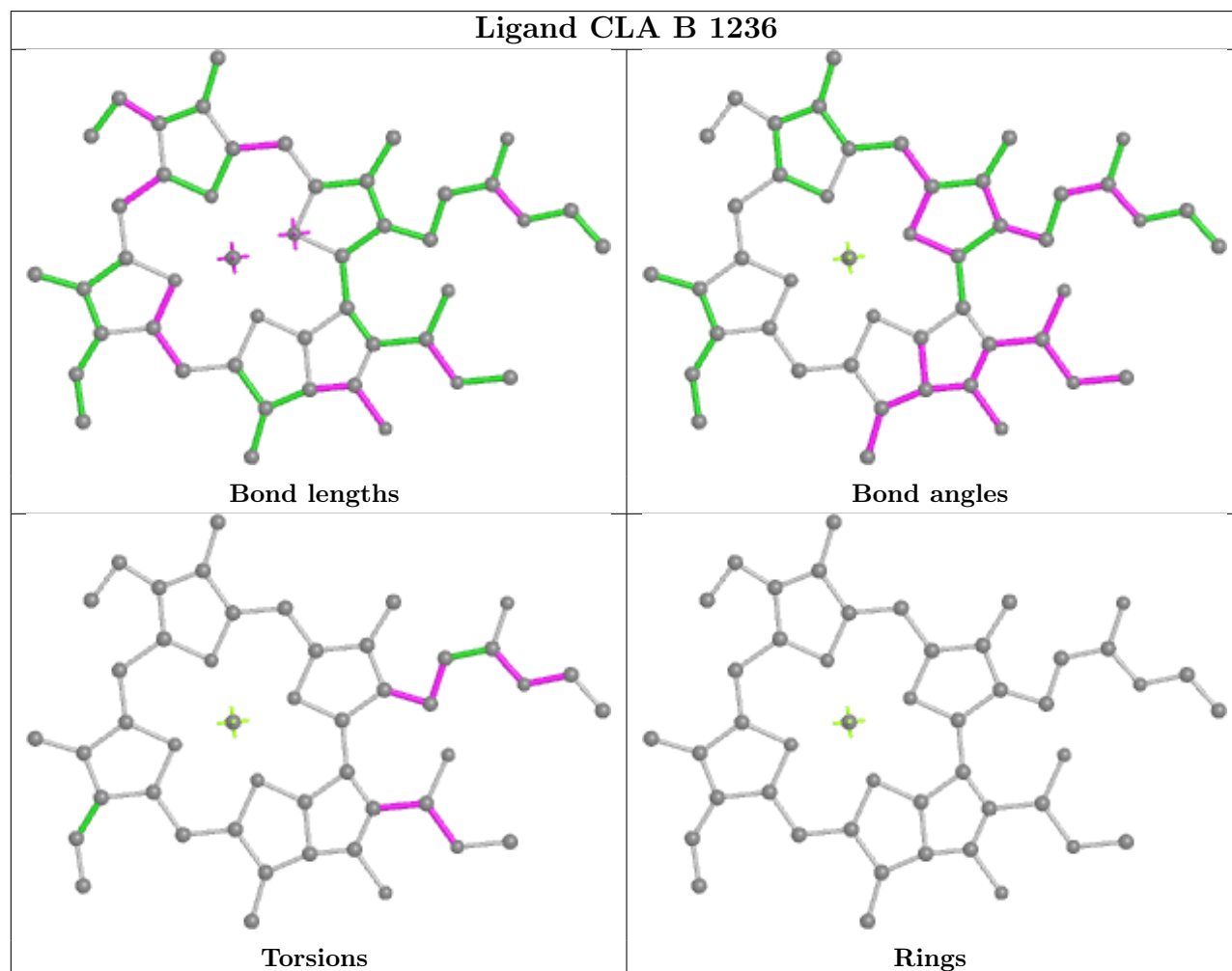
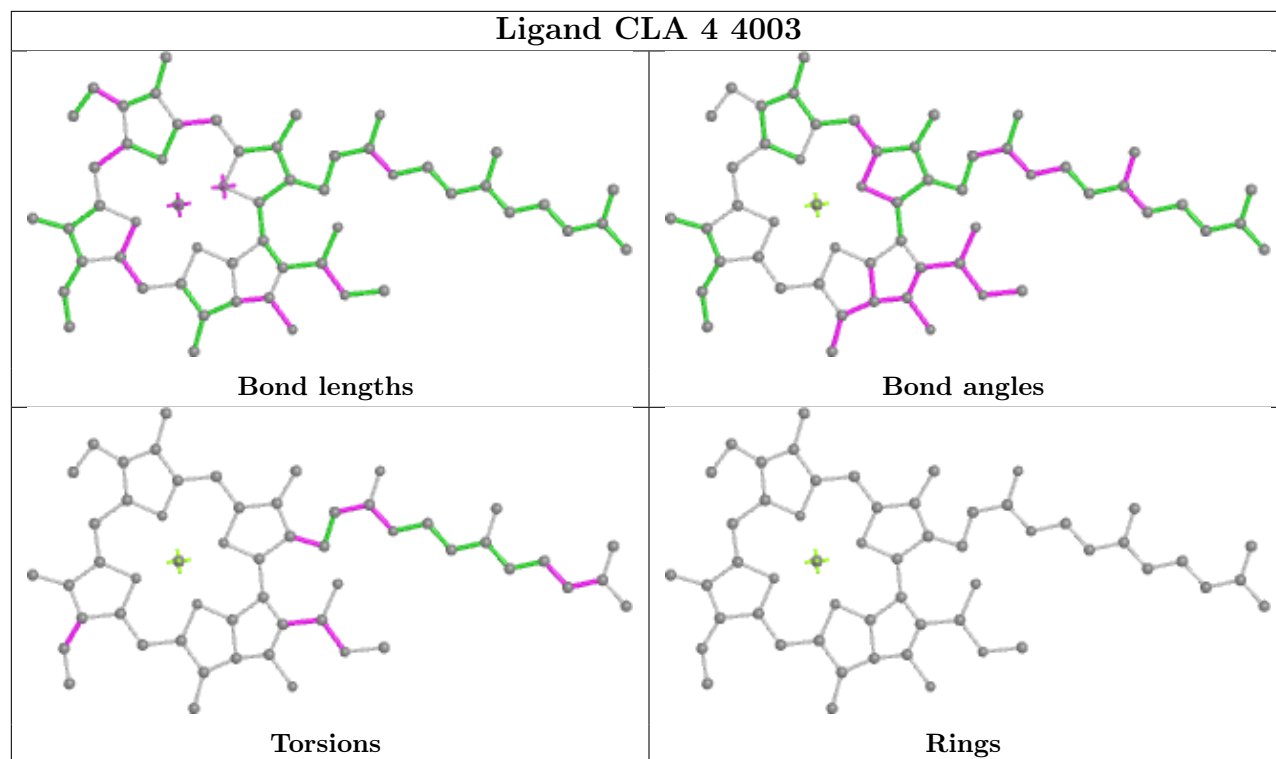
Ligand CLA 1 1005

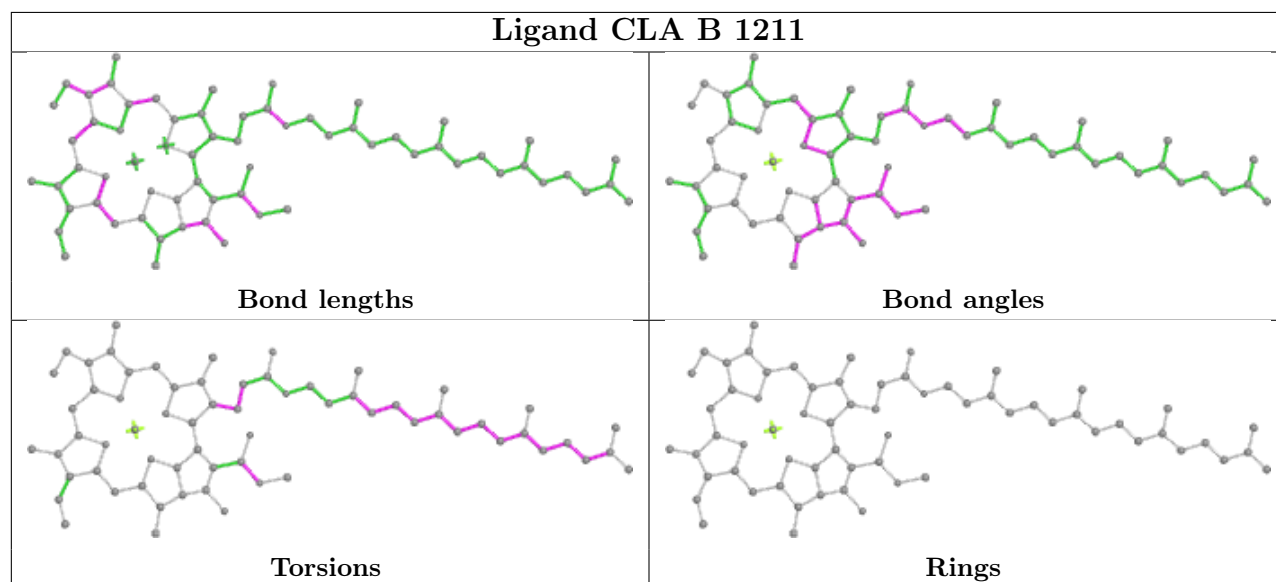
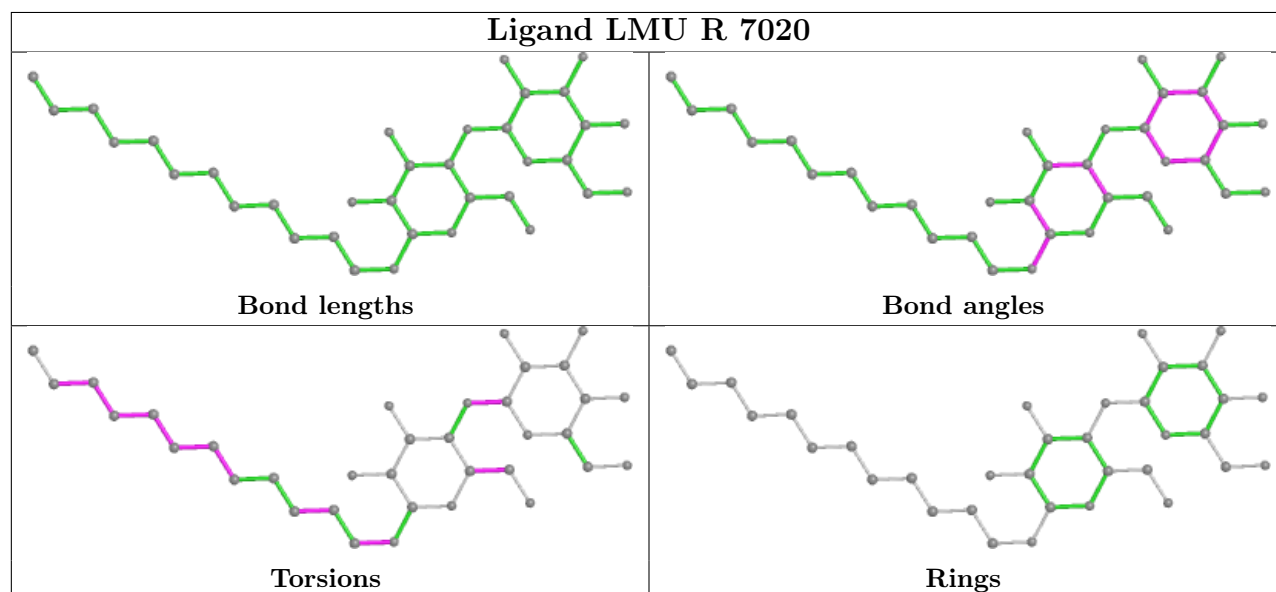
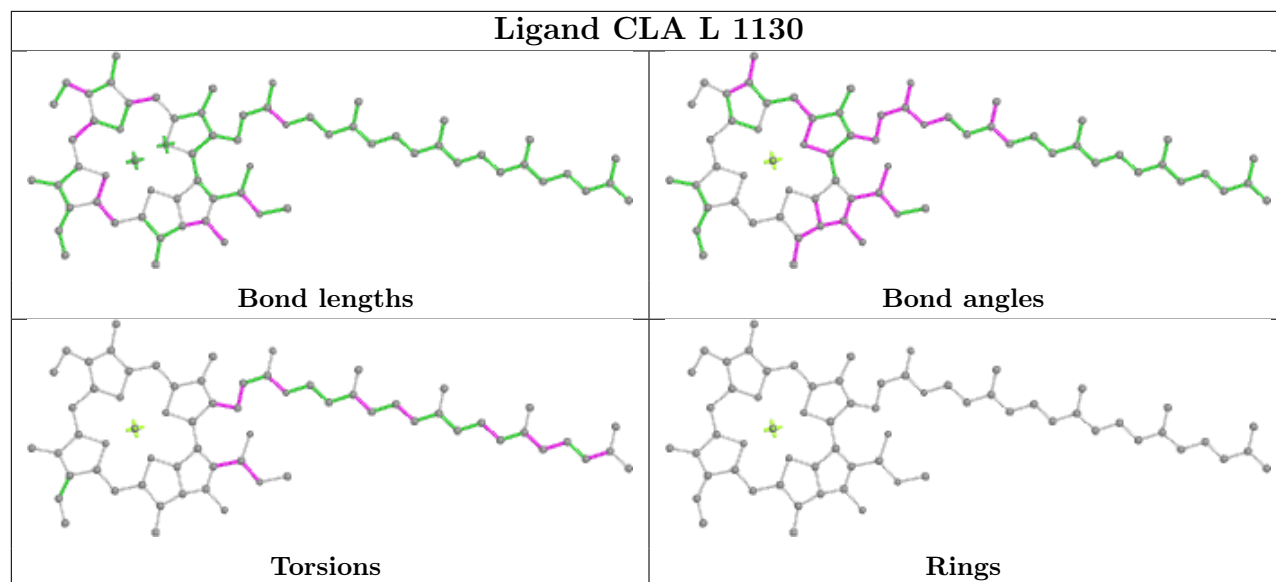


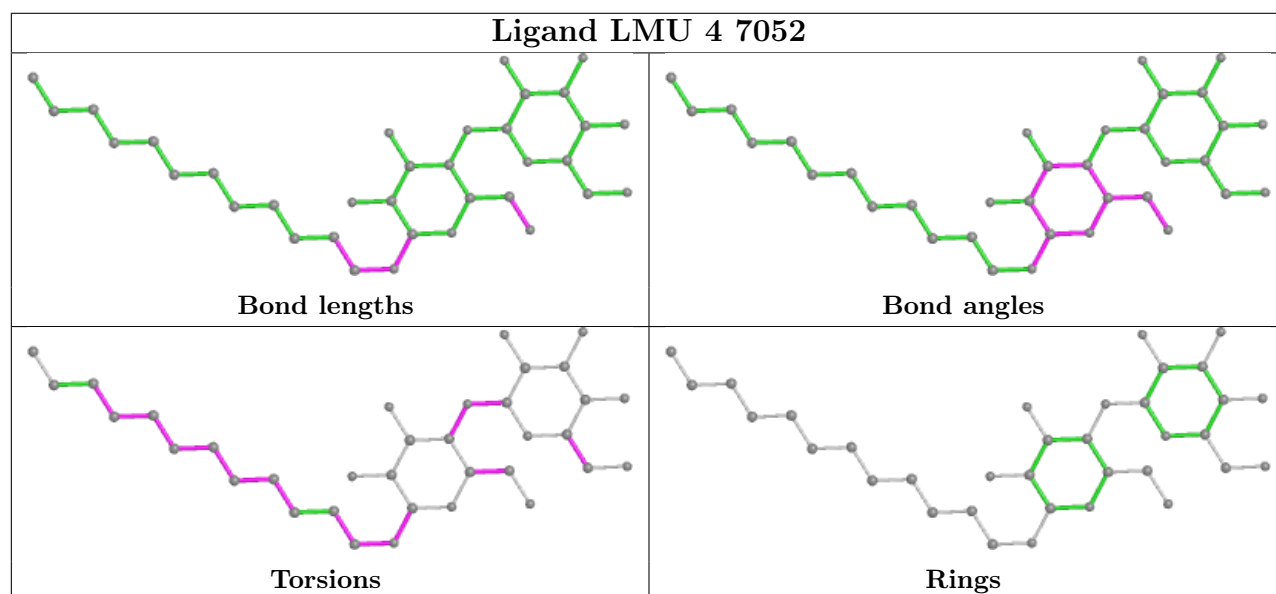
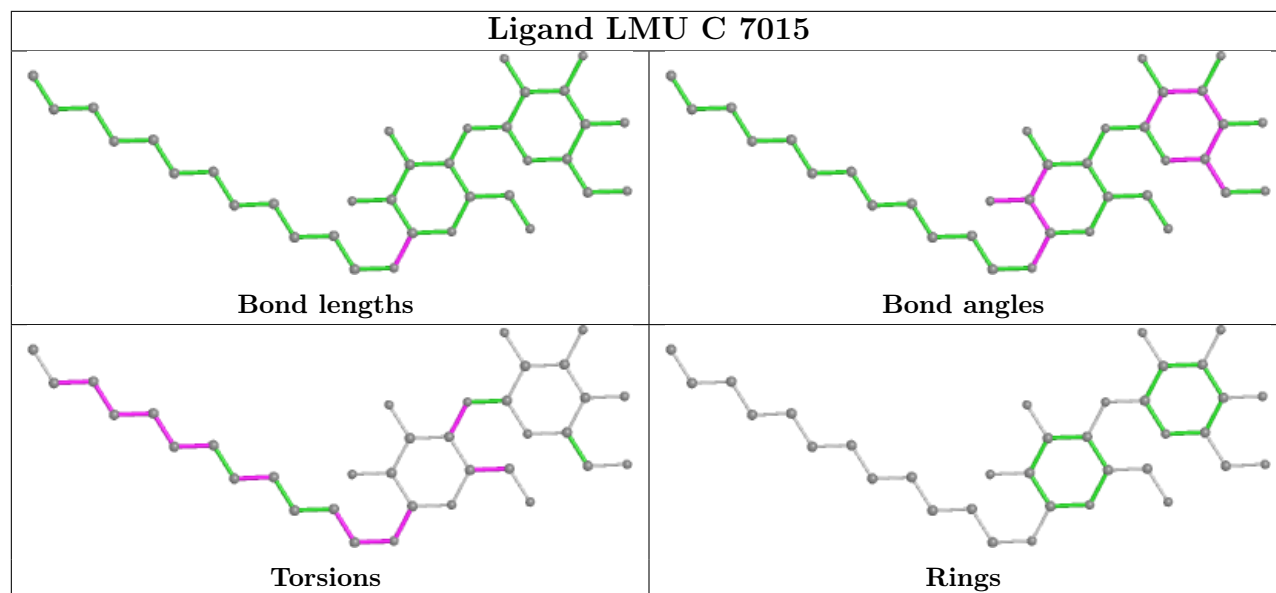




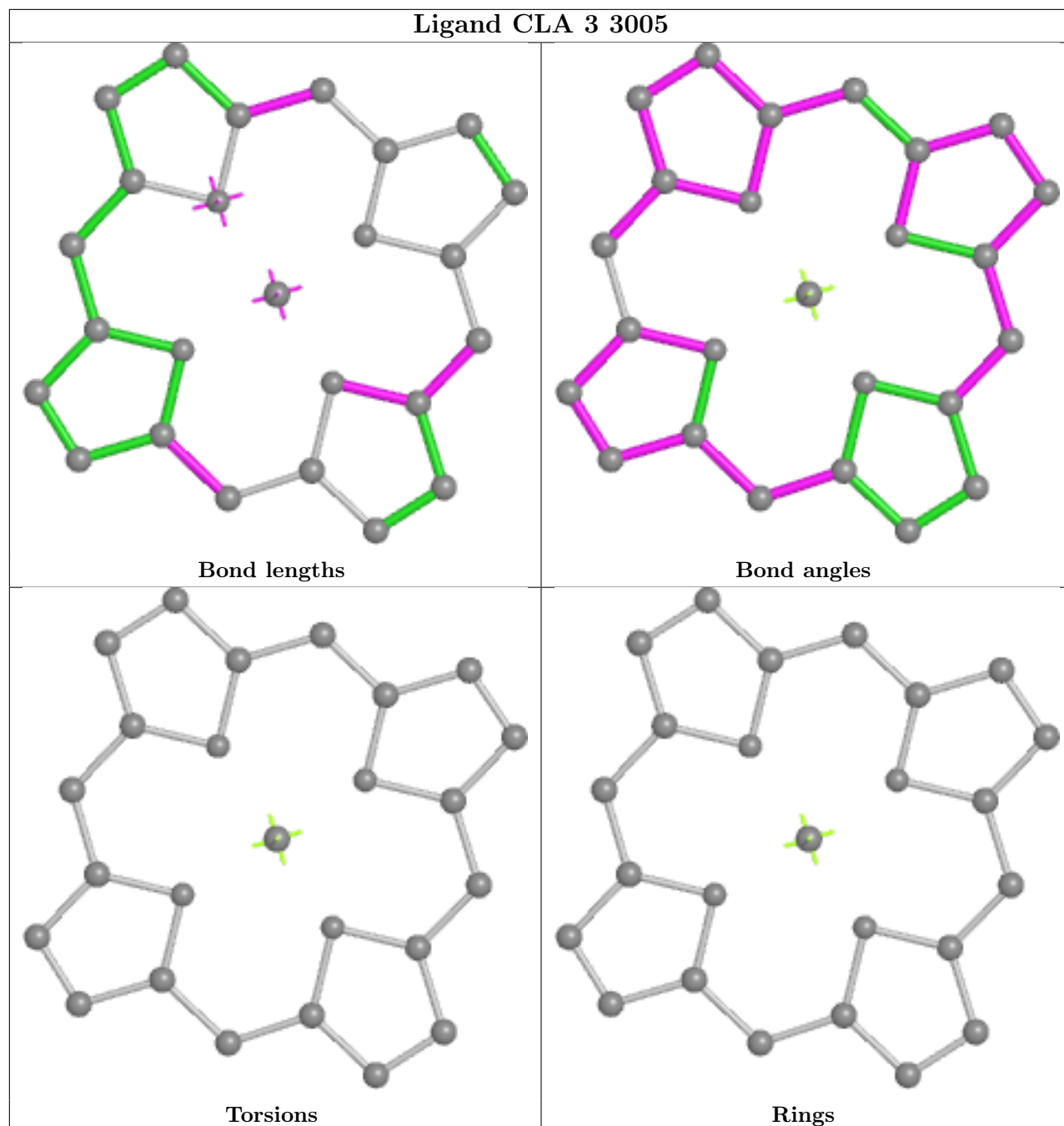


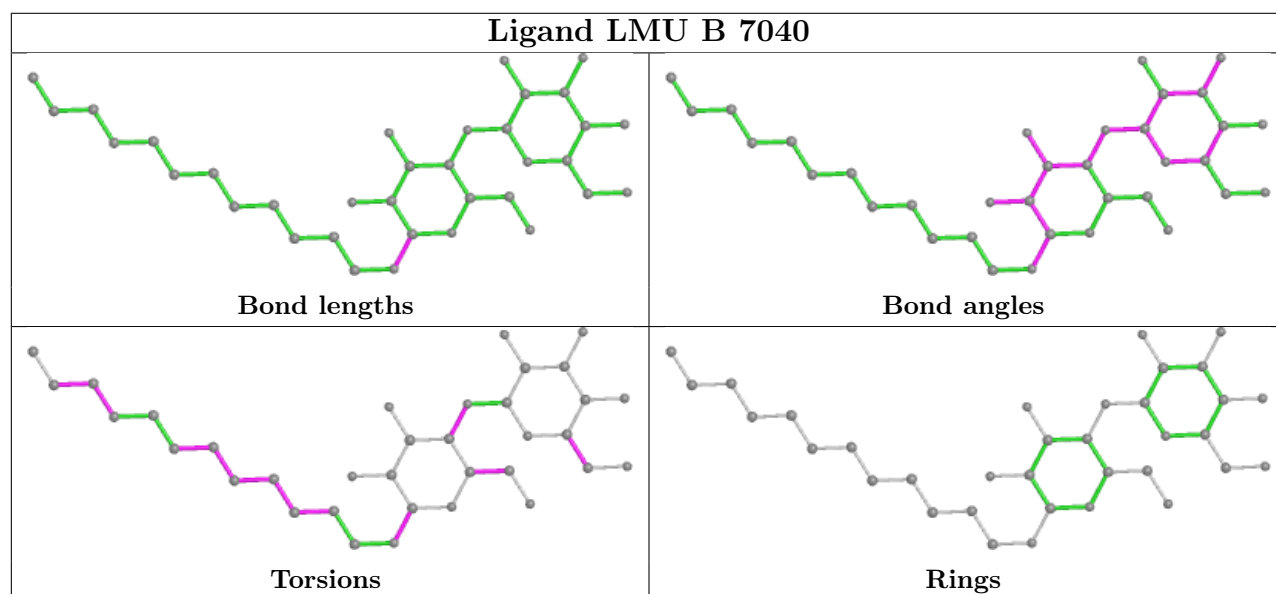
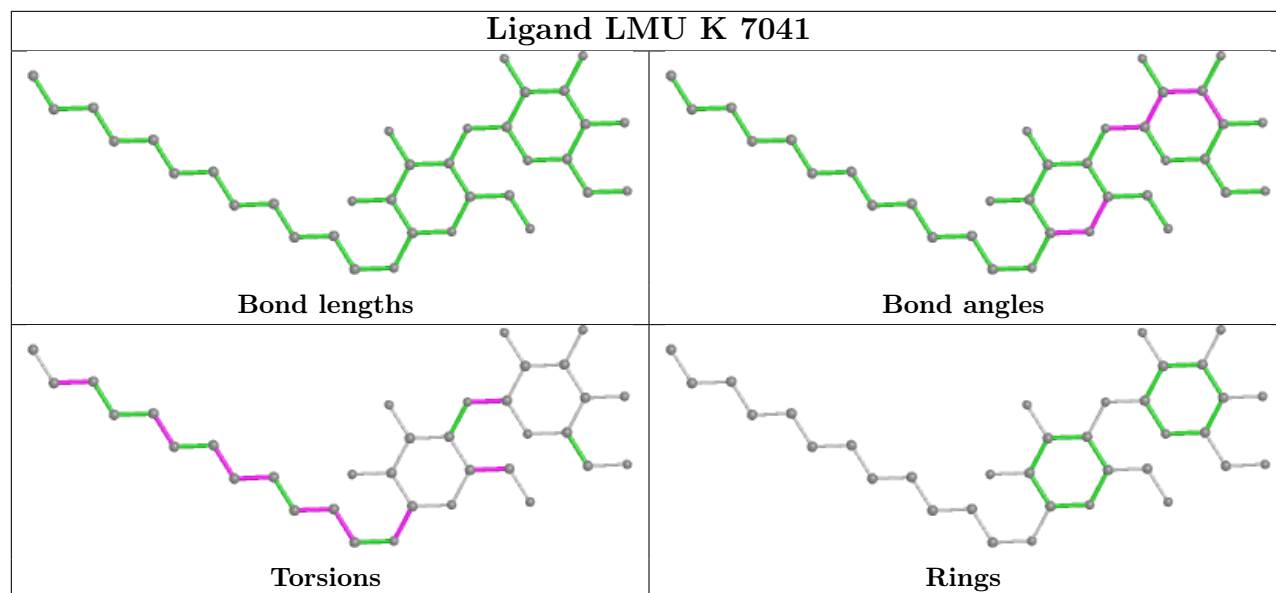


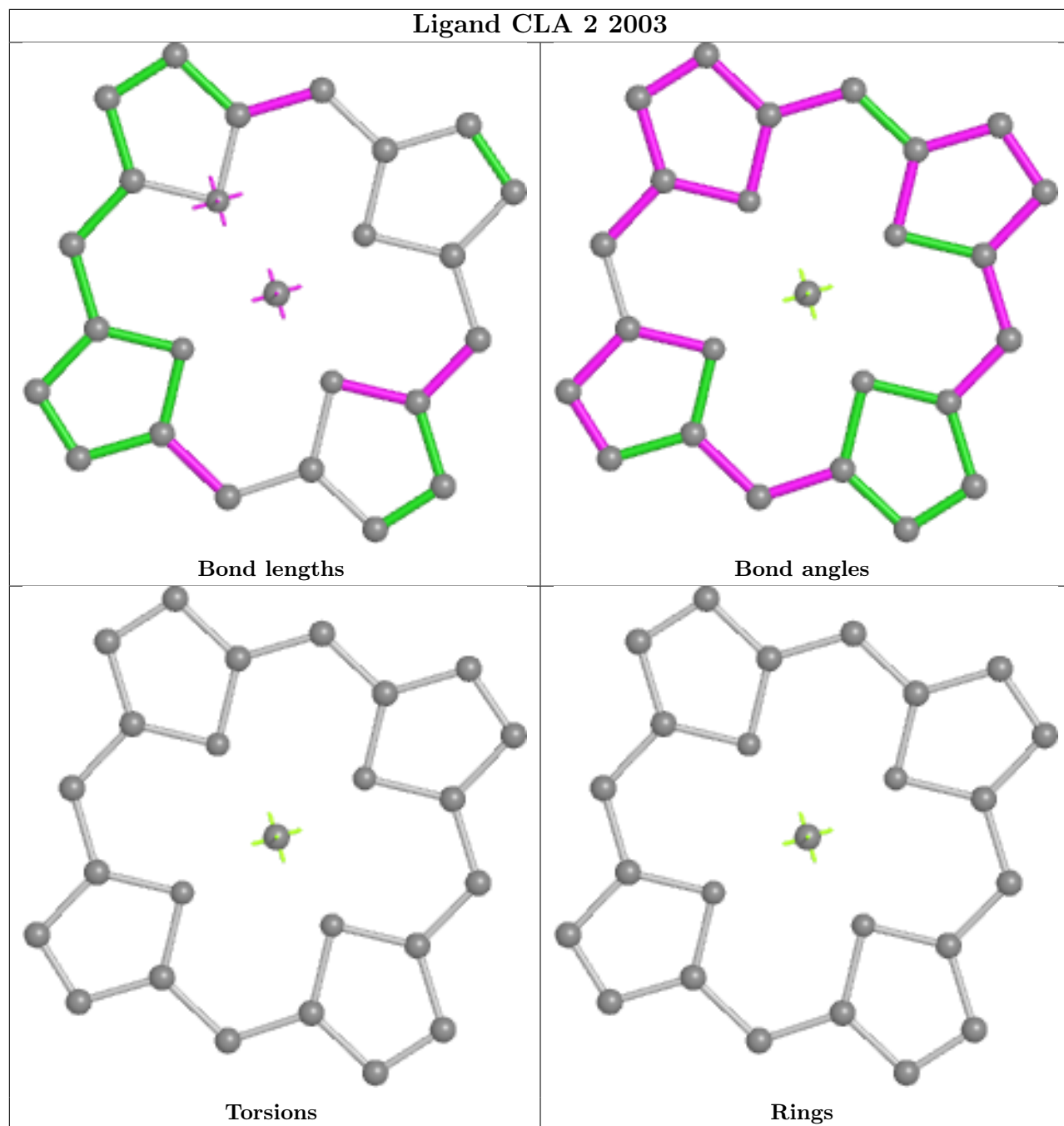


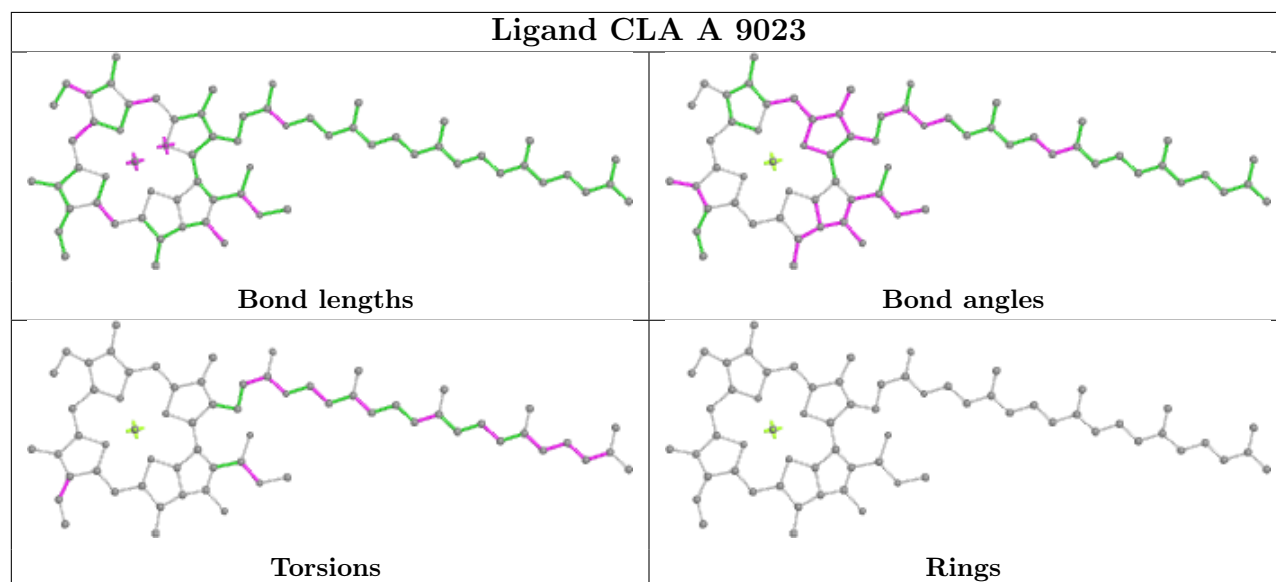
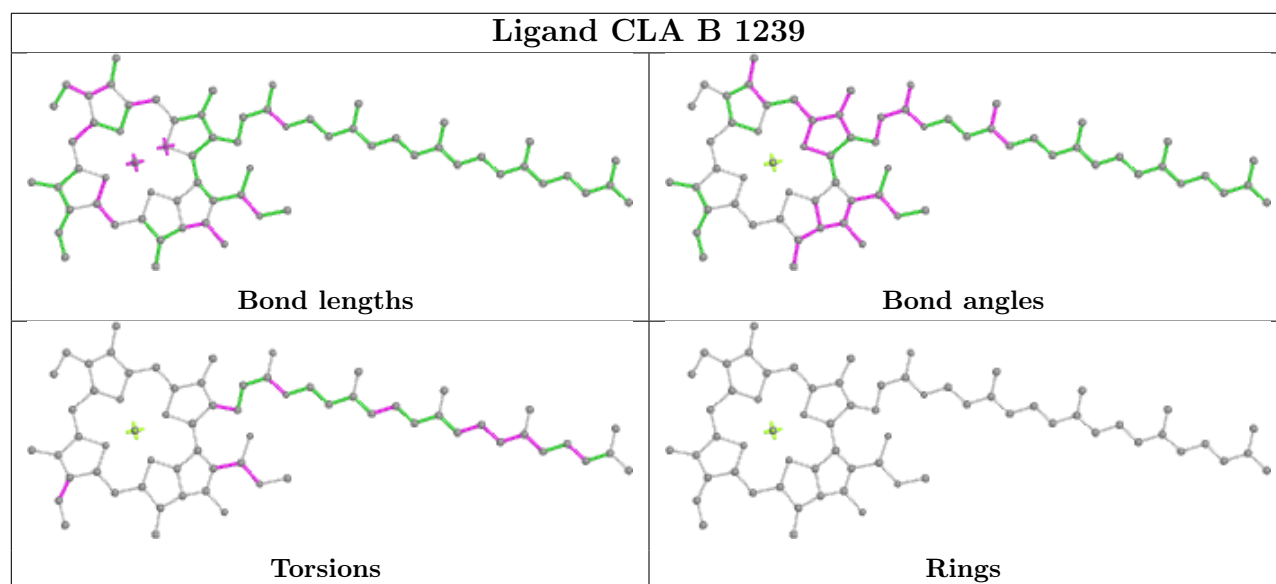
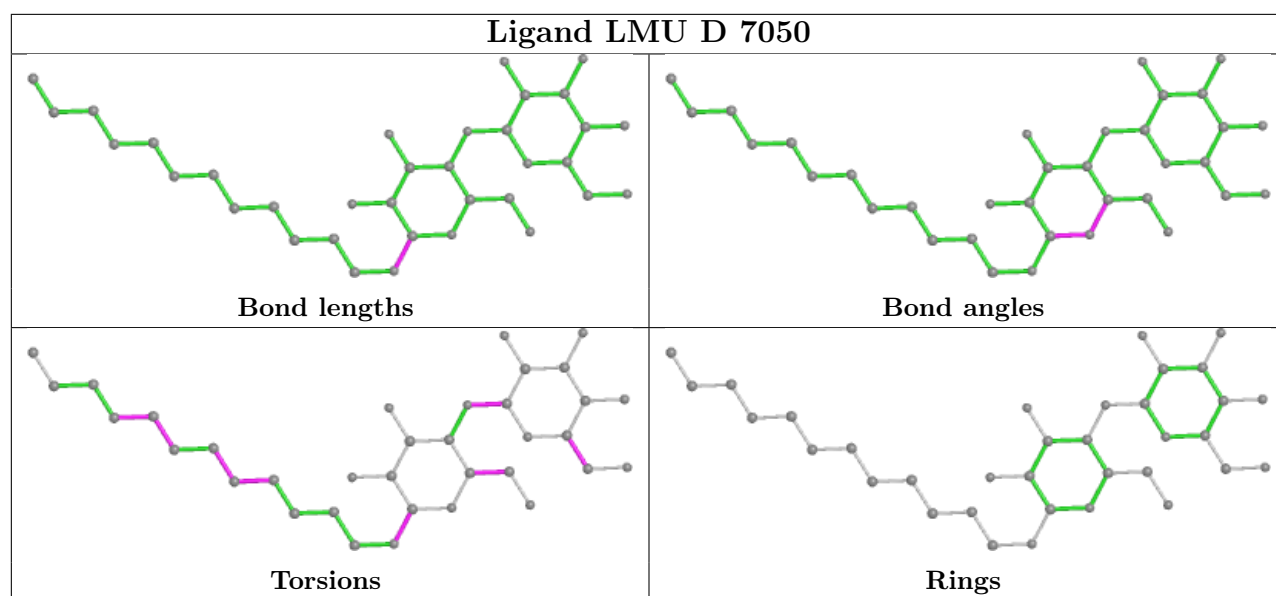


Ligand CLA 3 3005

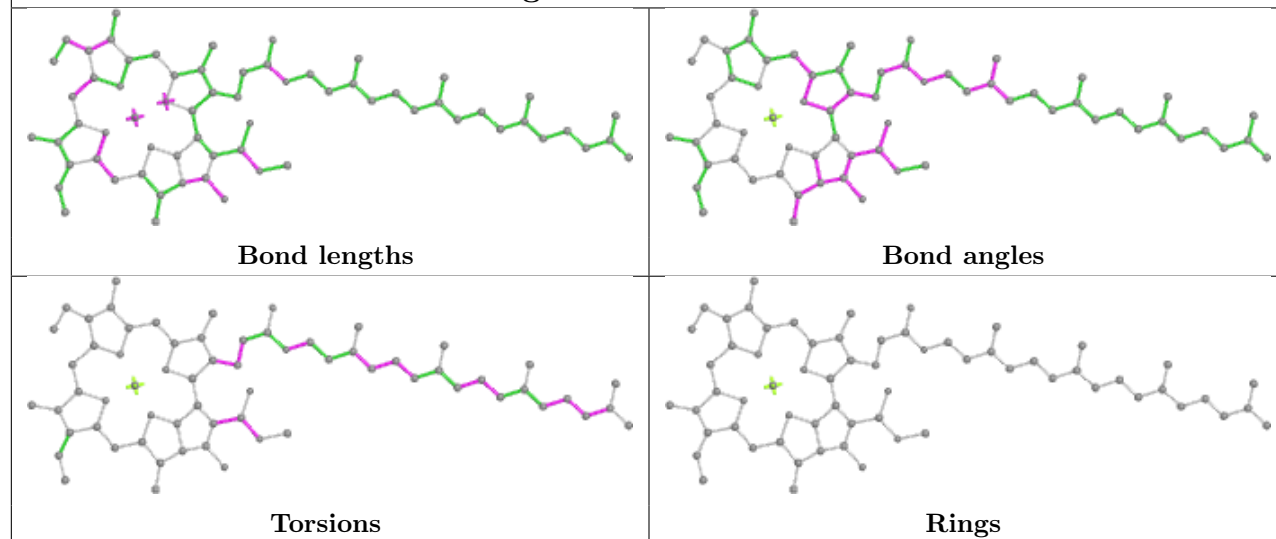




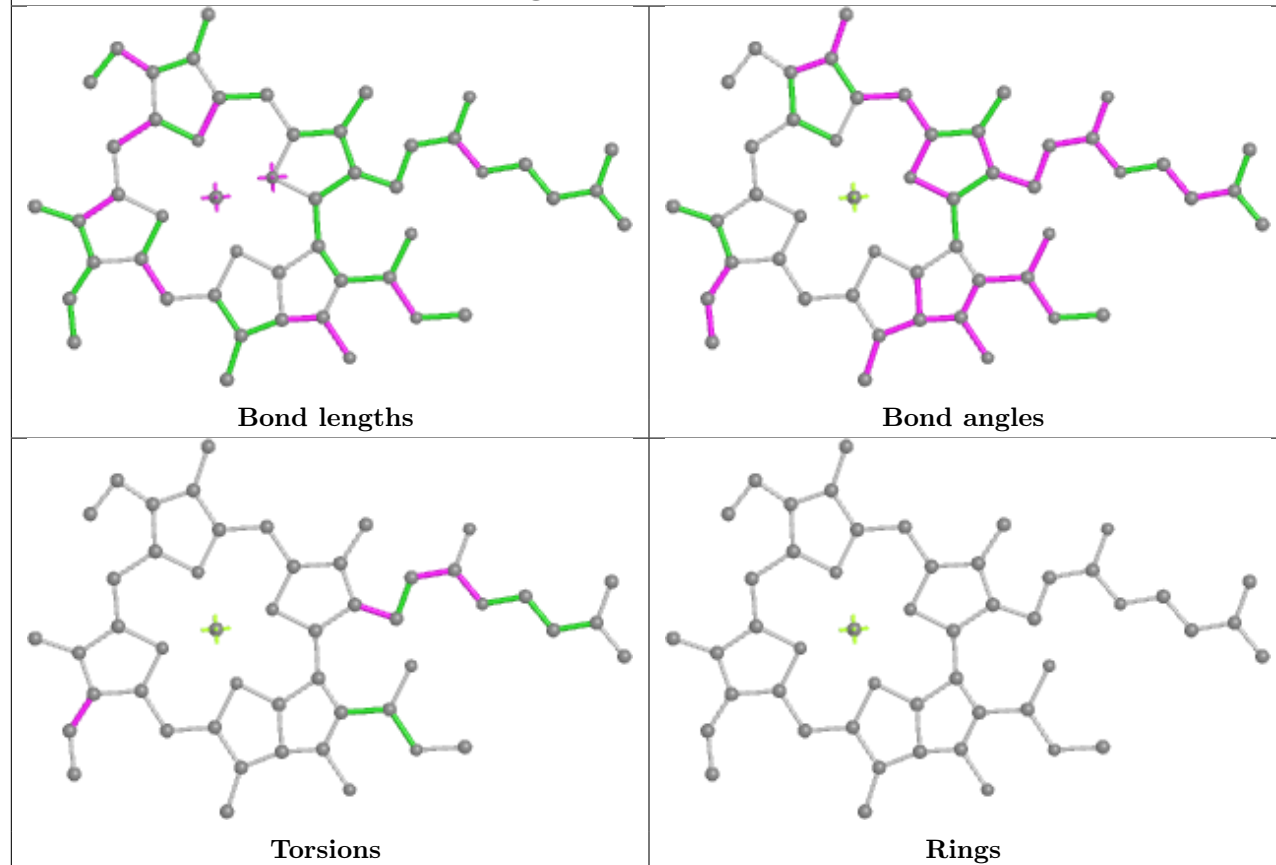




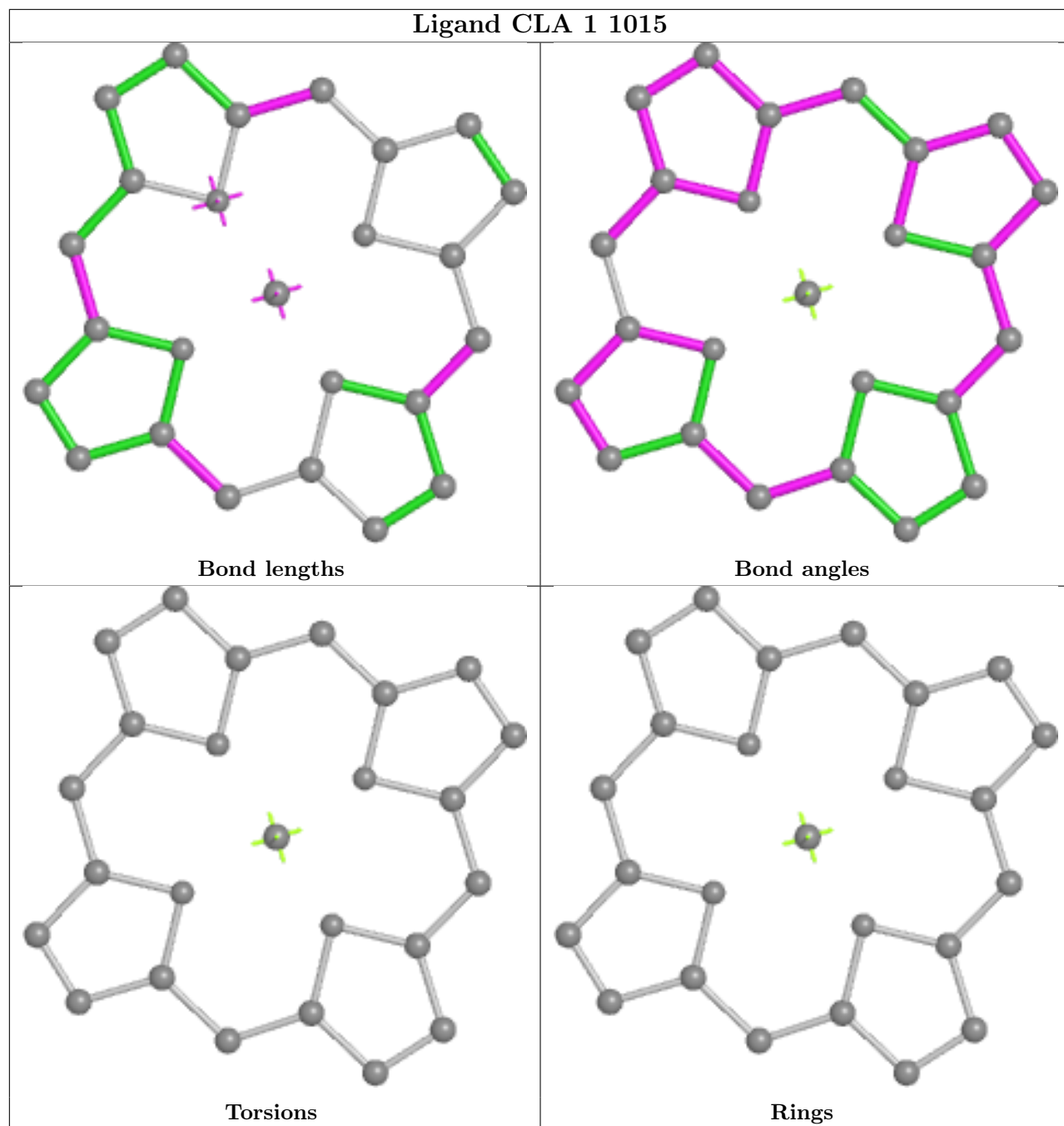
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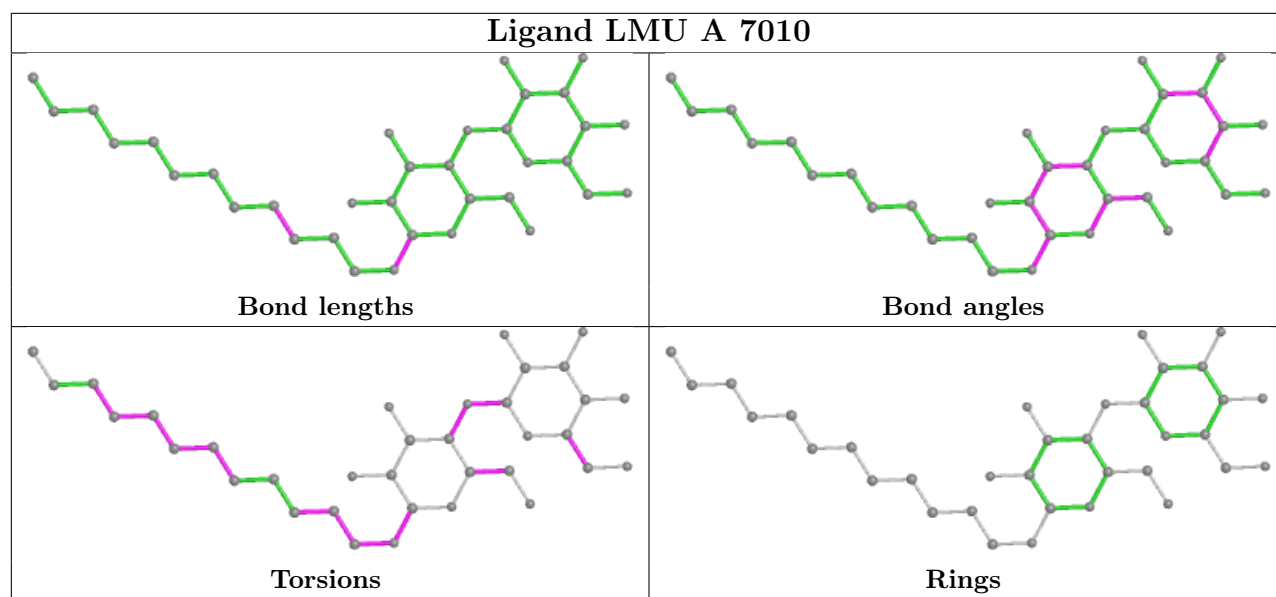
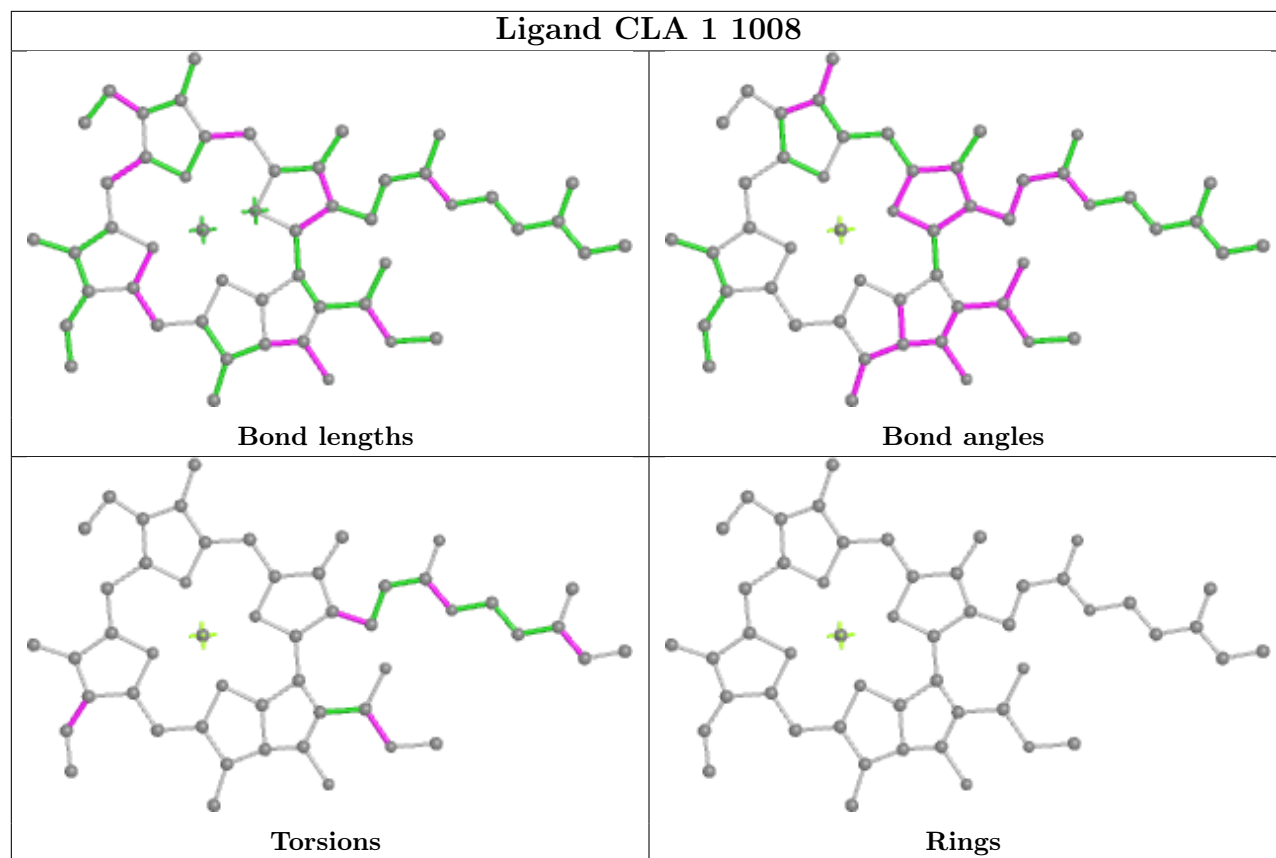


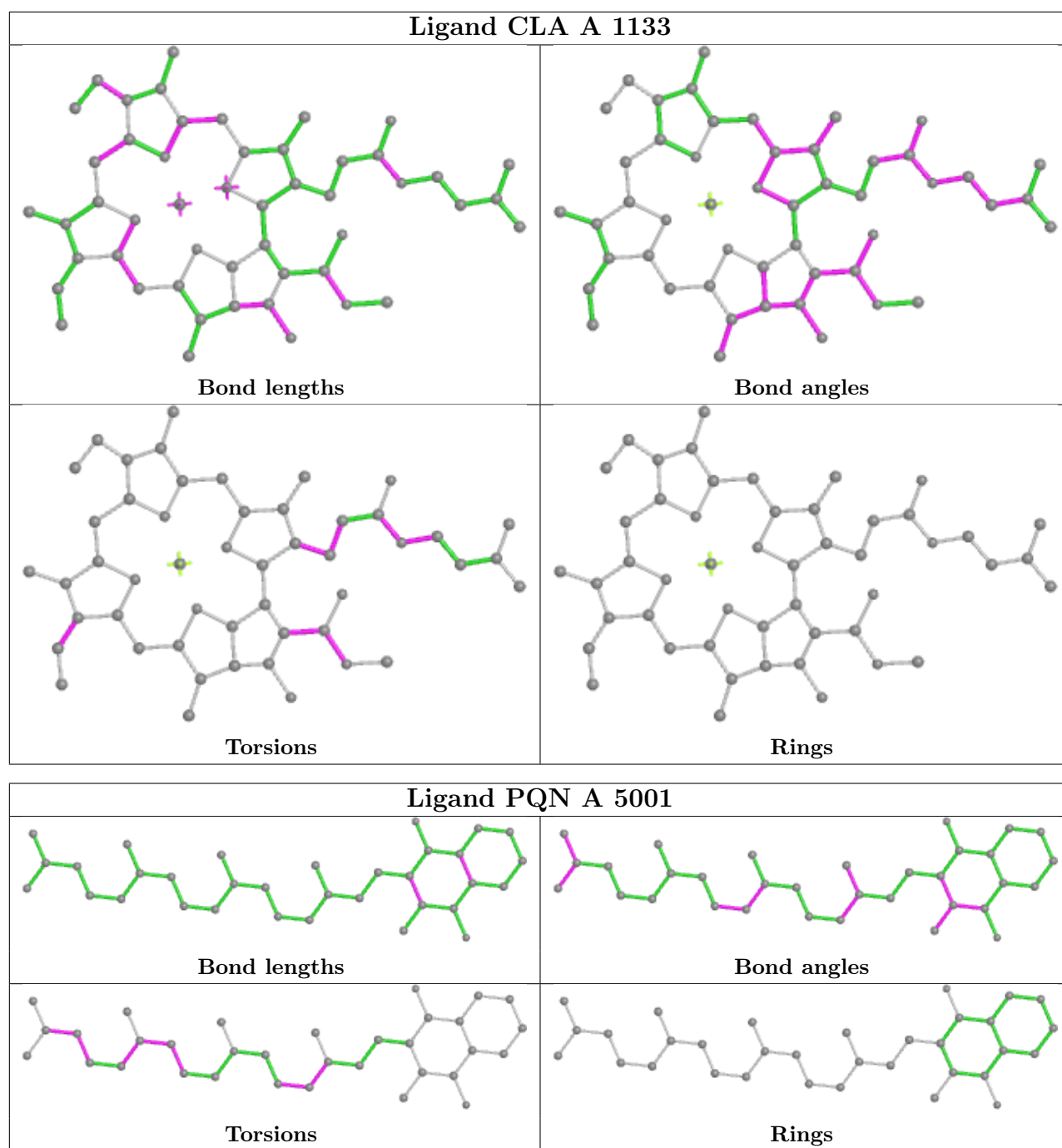
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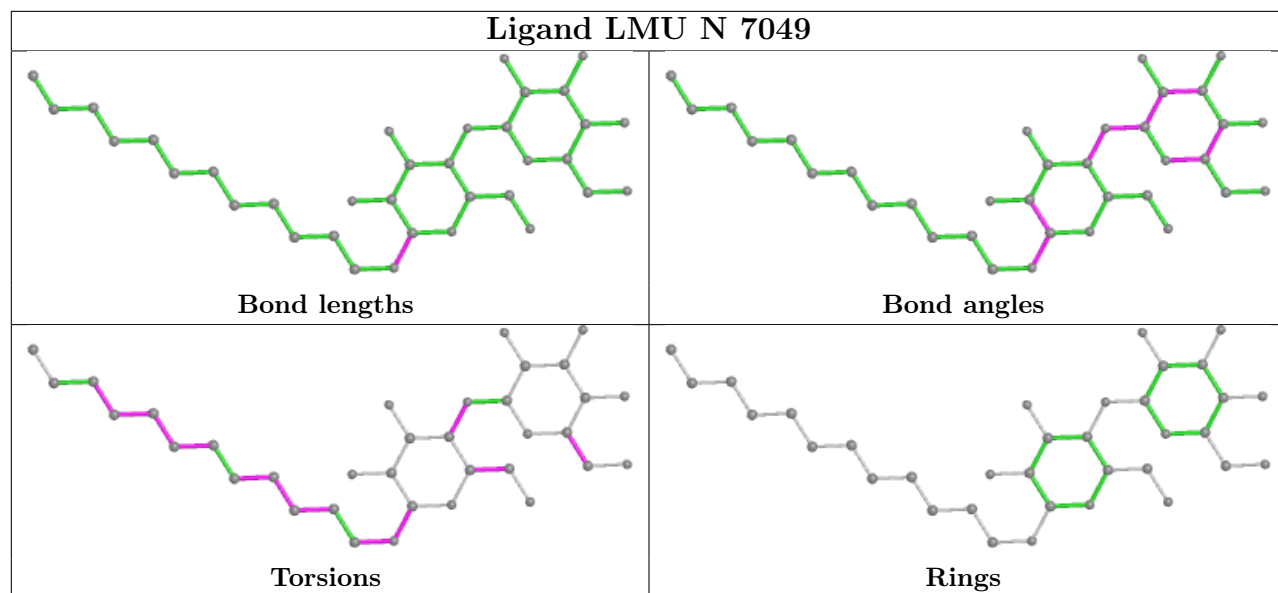
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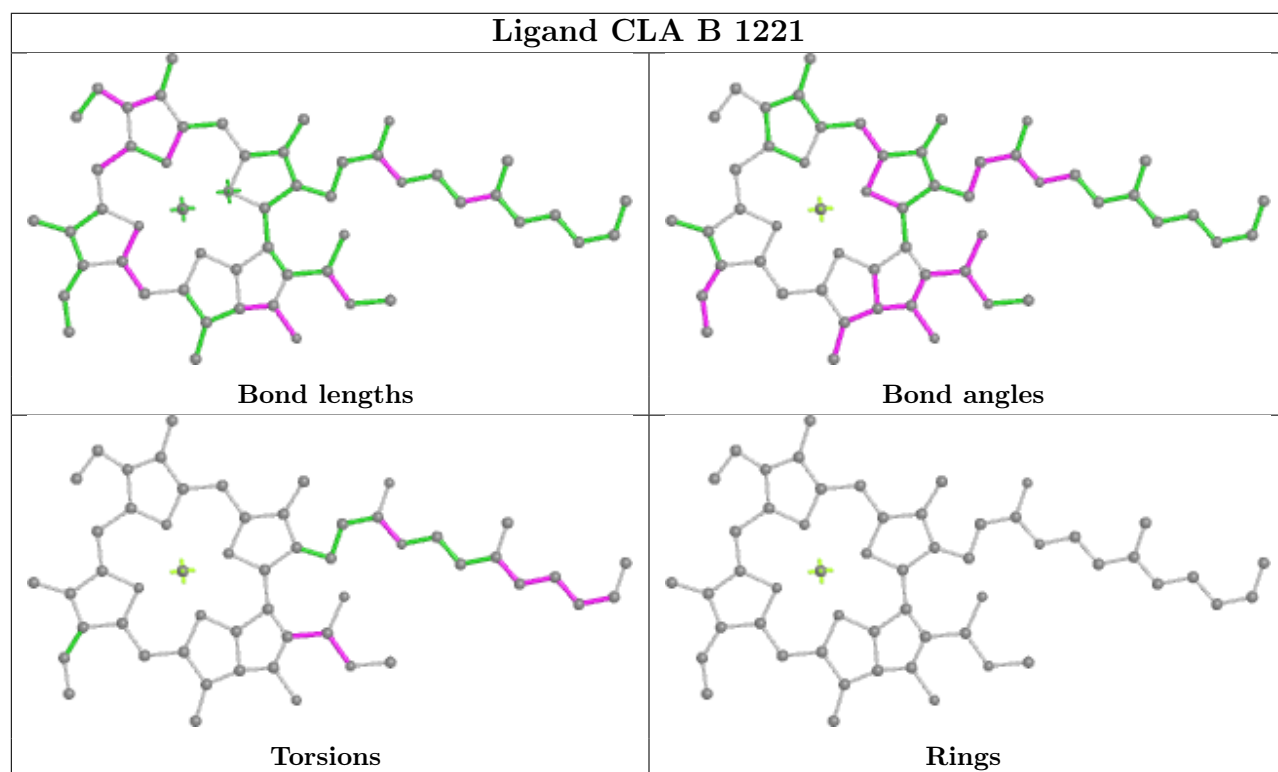


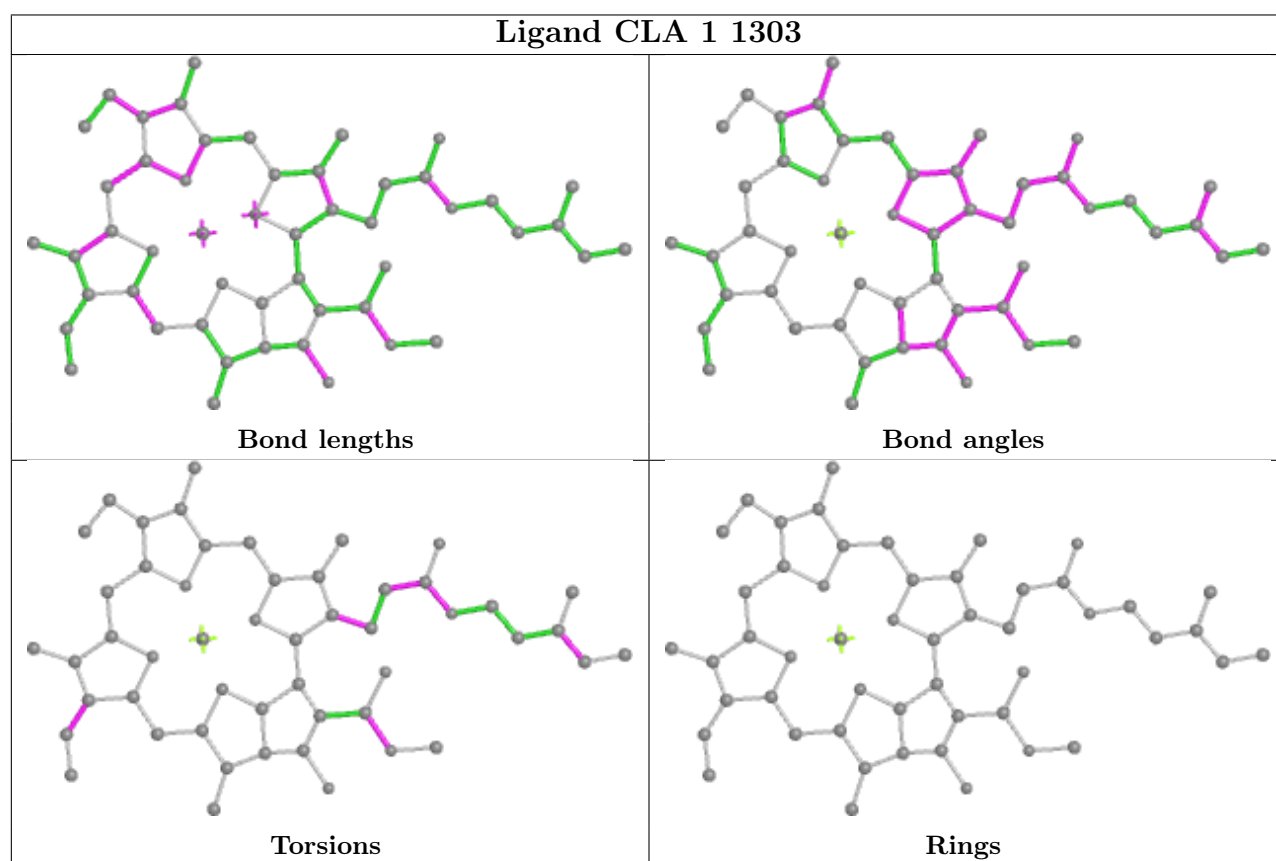
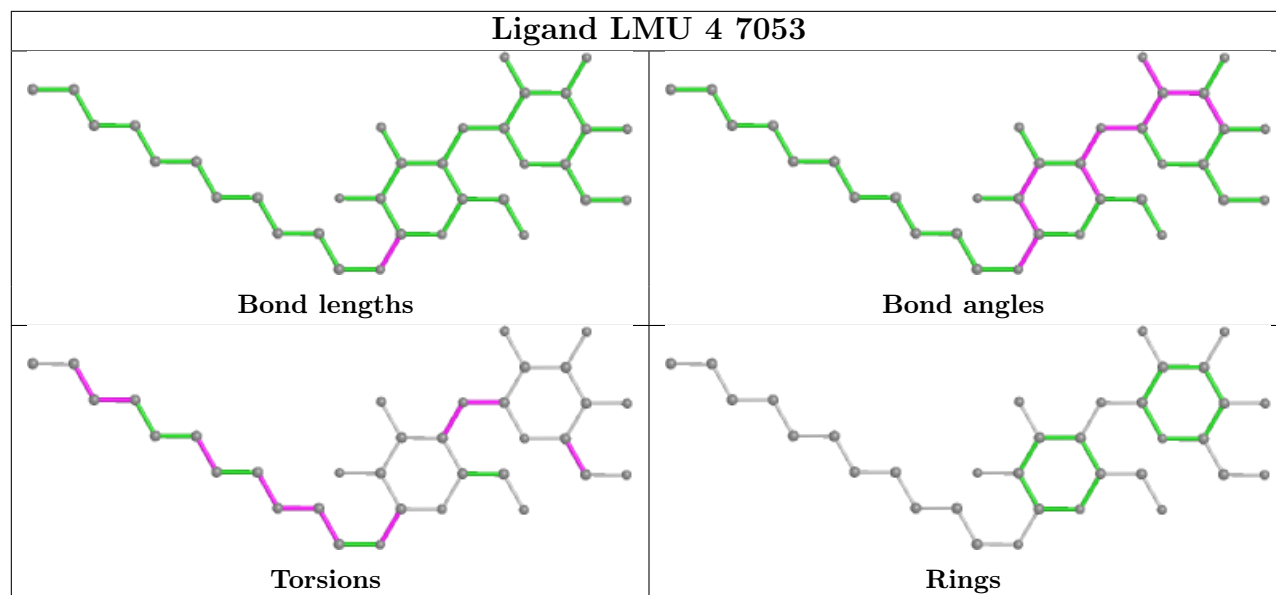


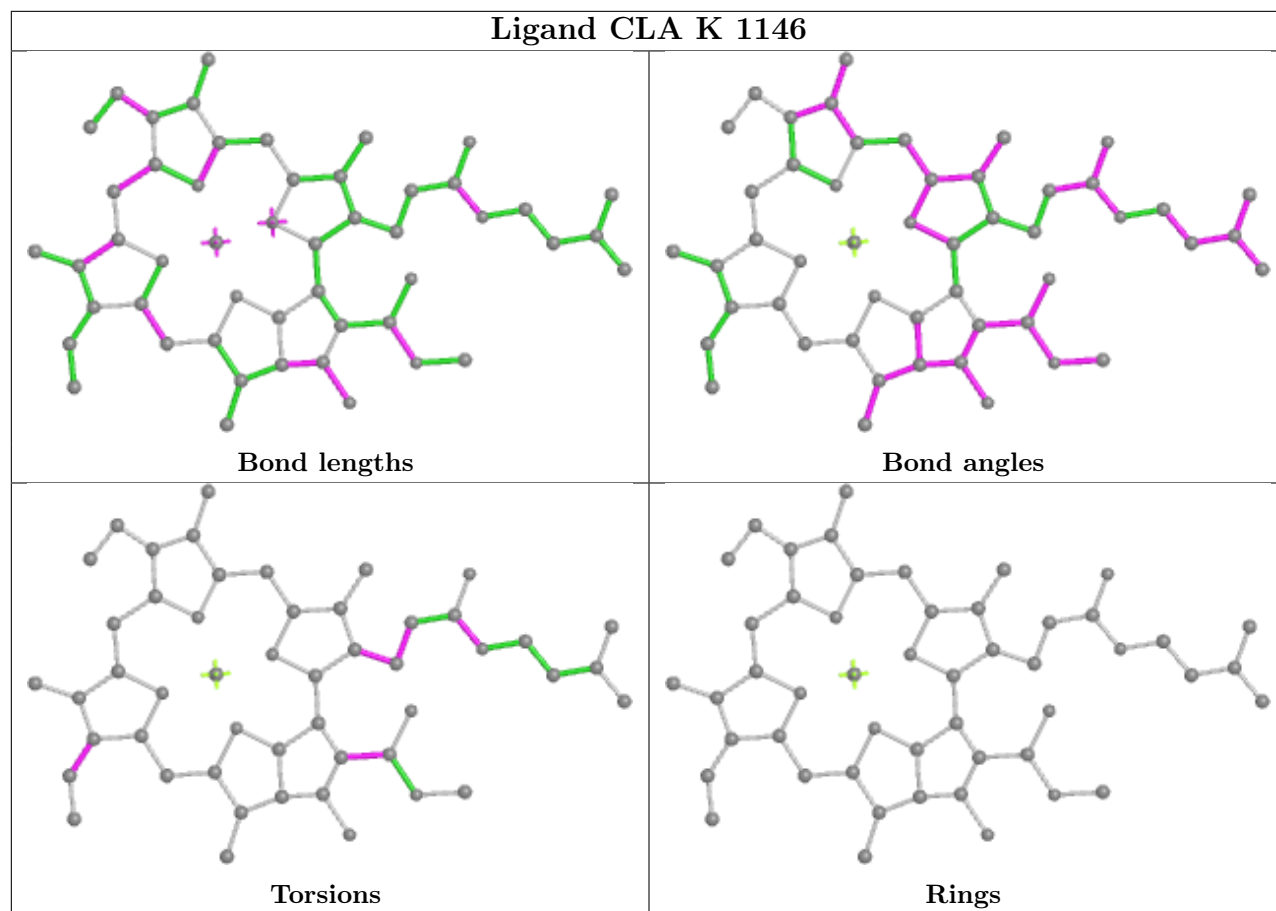
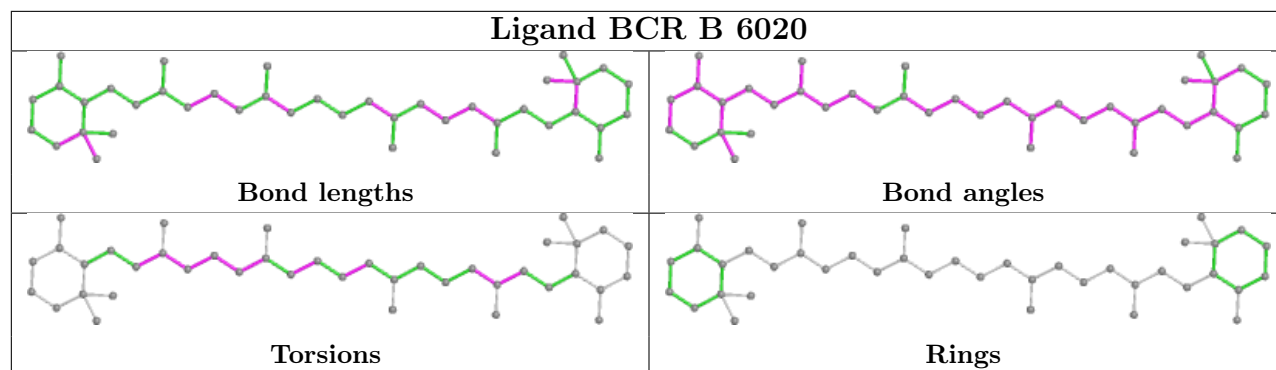
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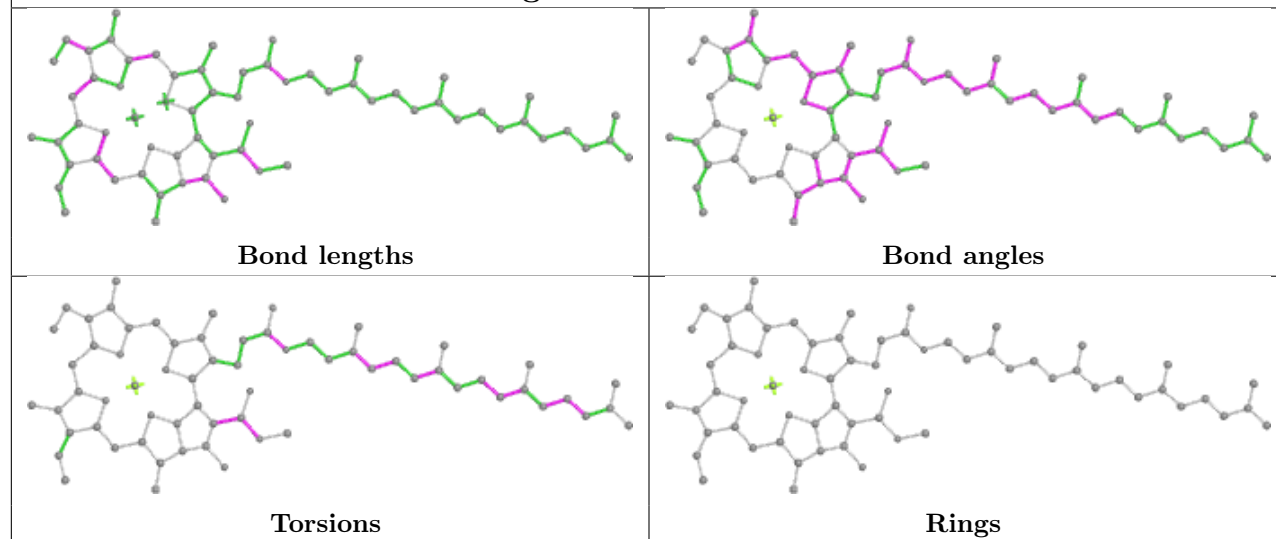
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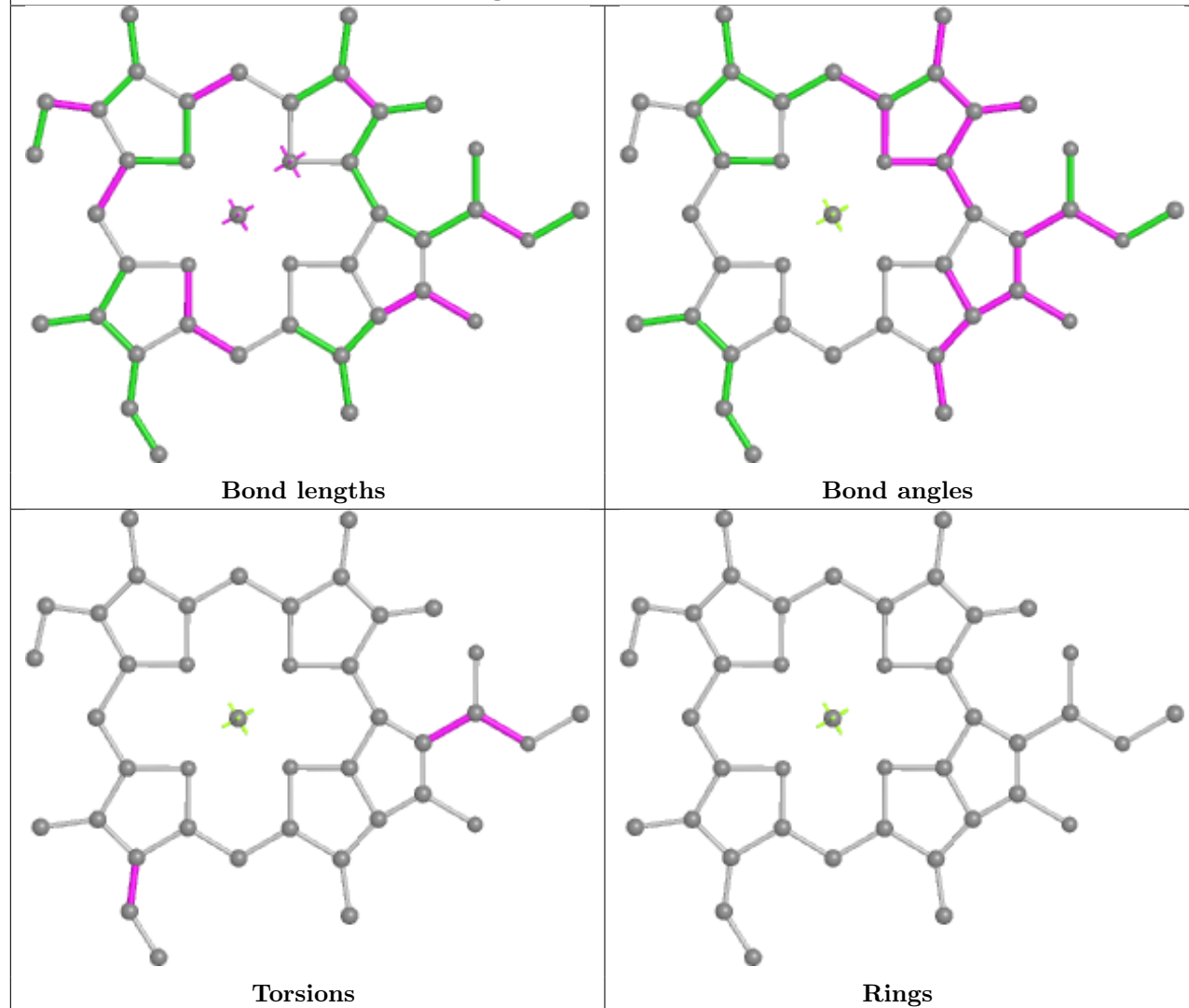


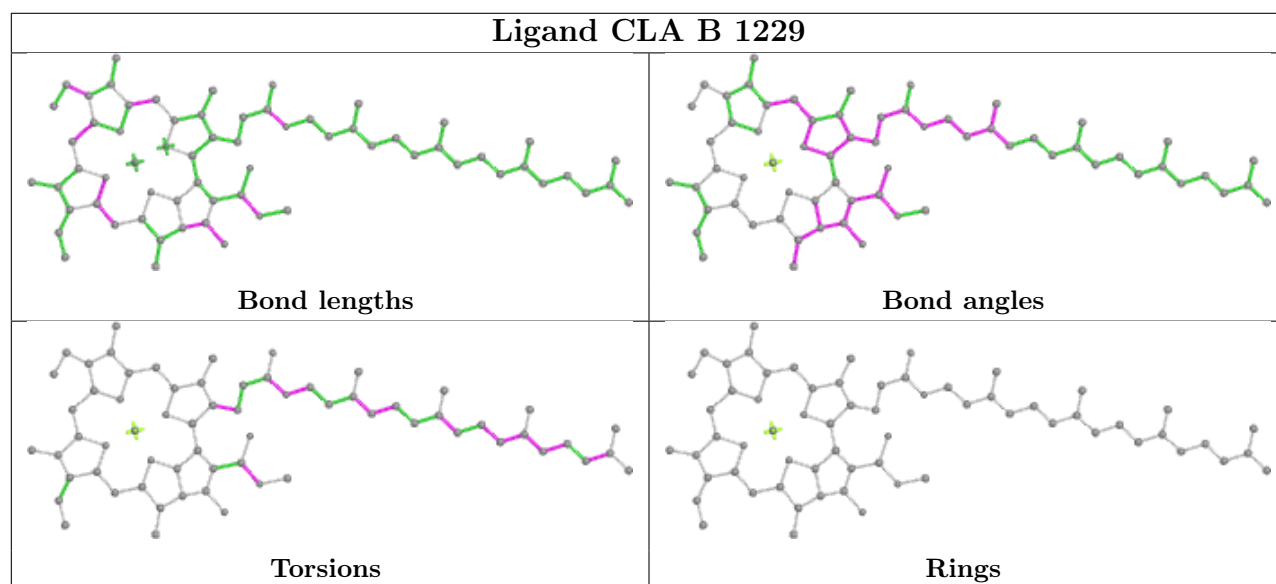
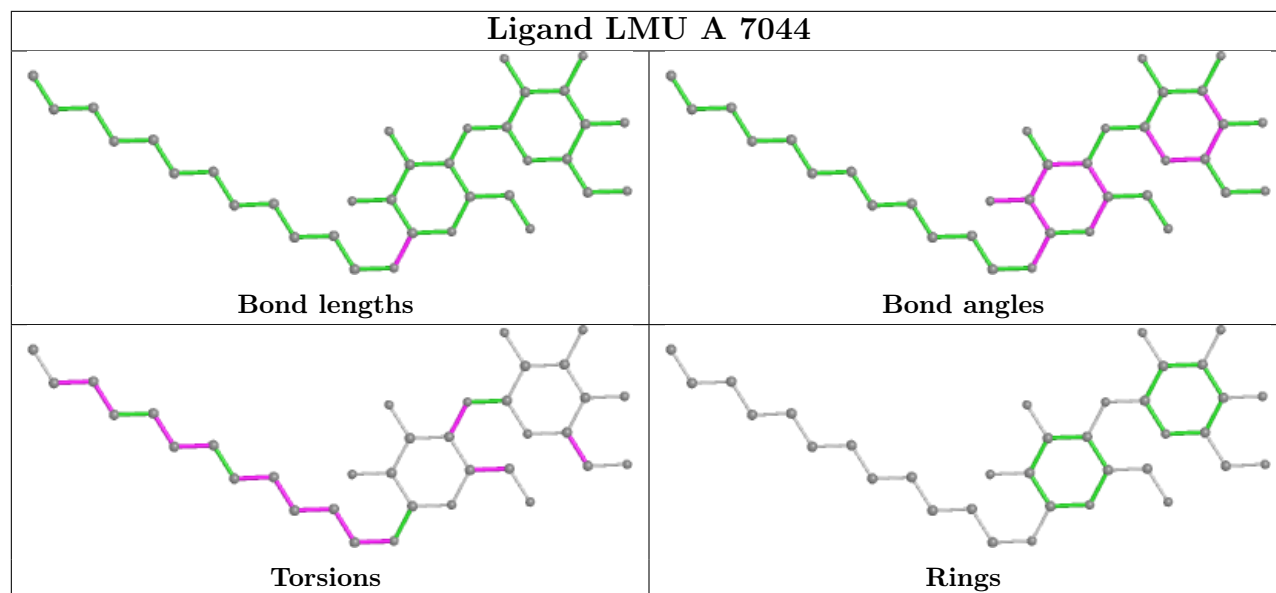


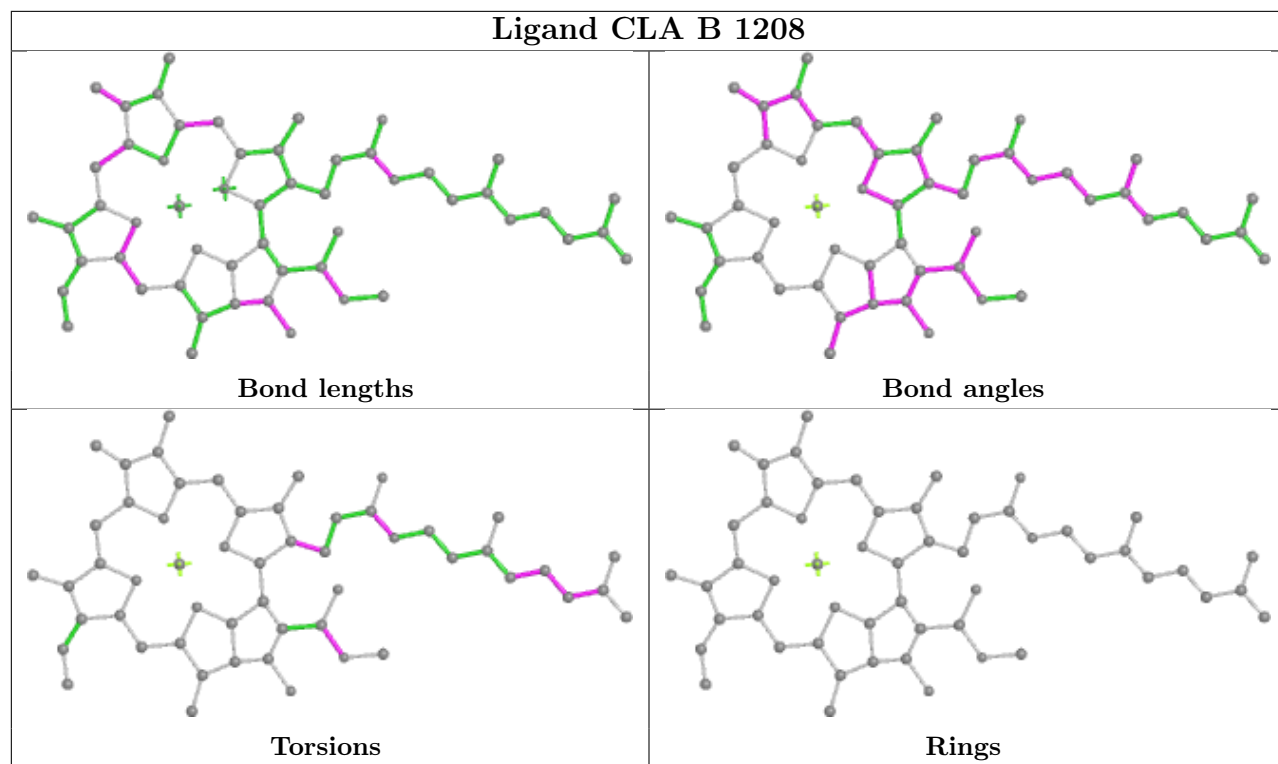
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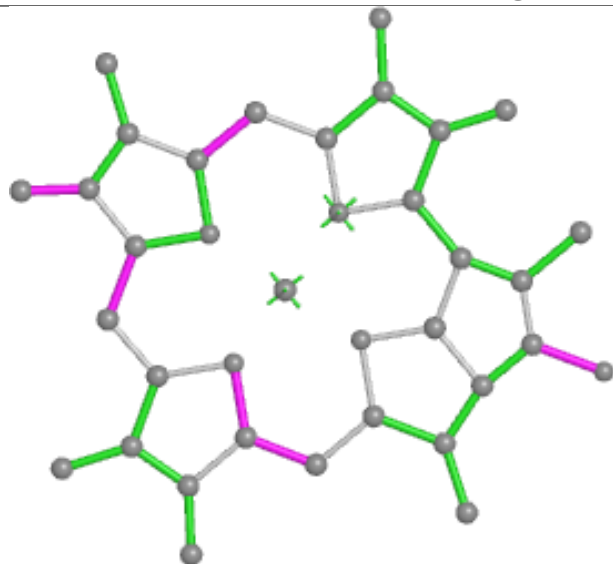
Ligand CLA F 1302



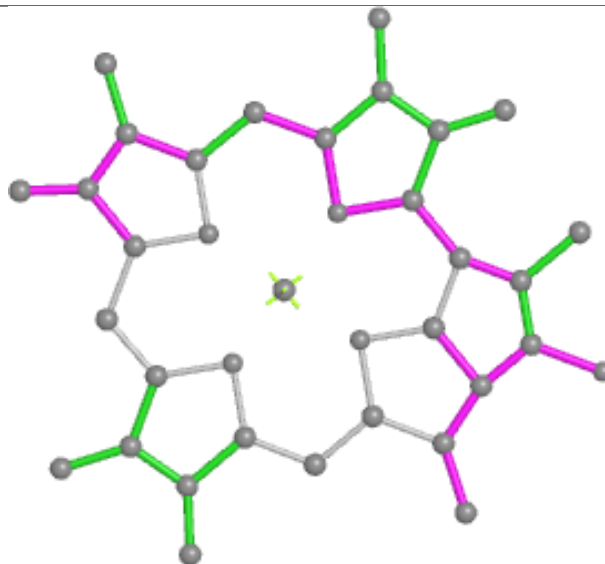




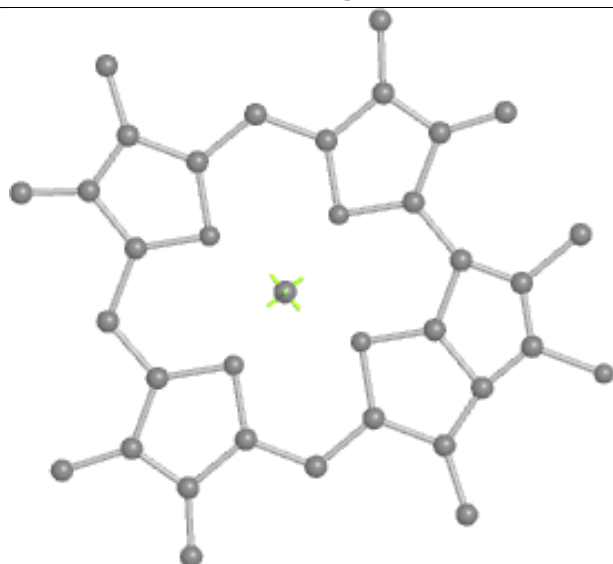
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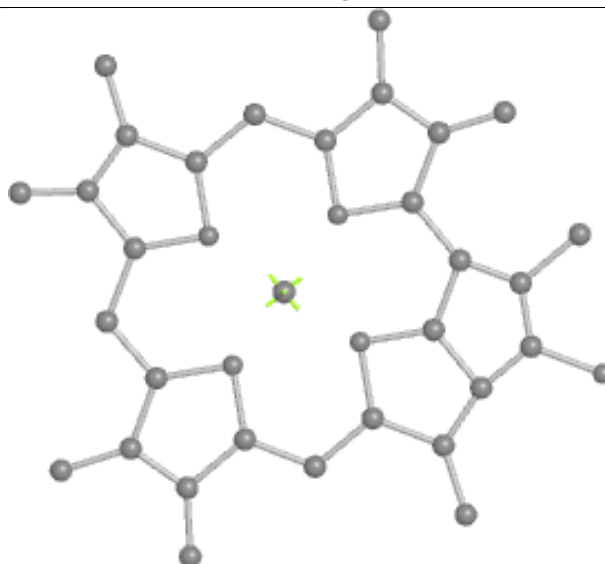
Bond lengths



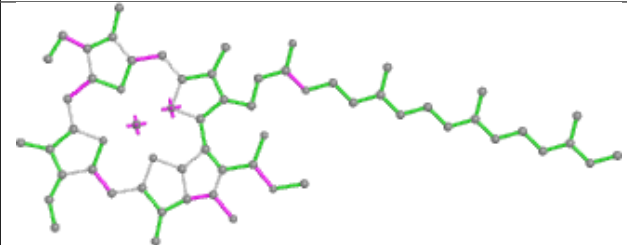
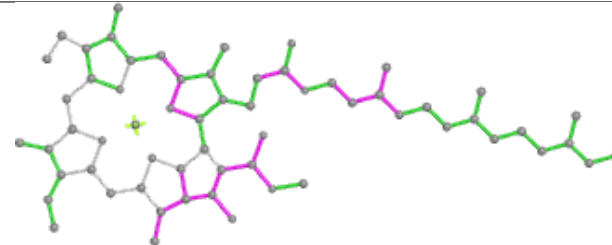
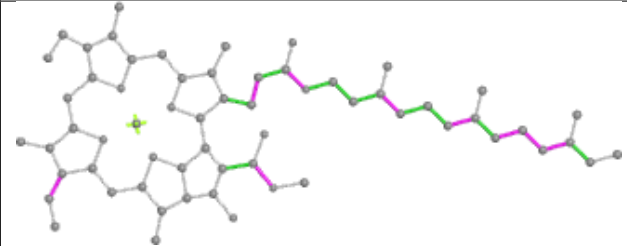
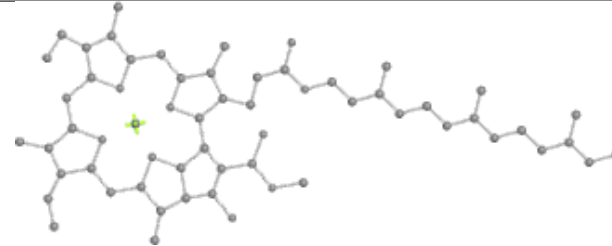
Bond angles

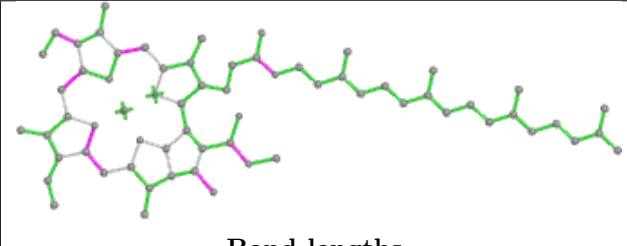
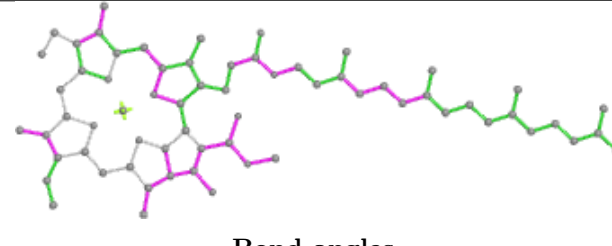
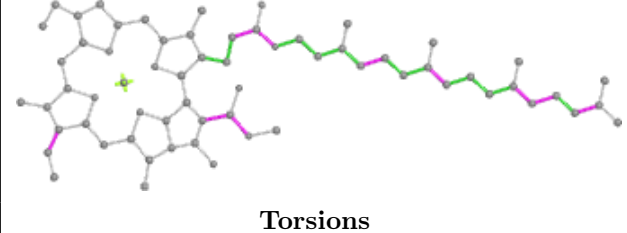
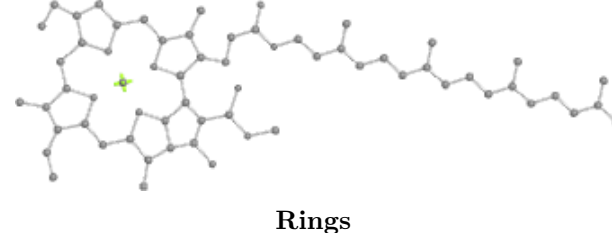


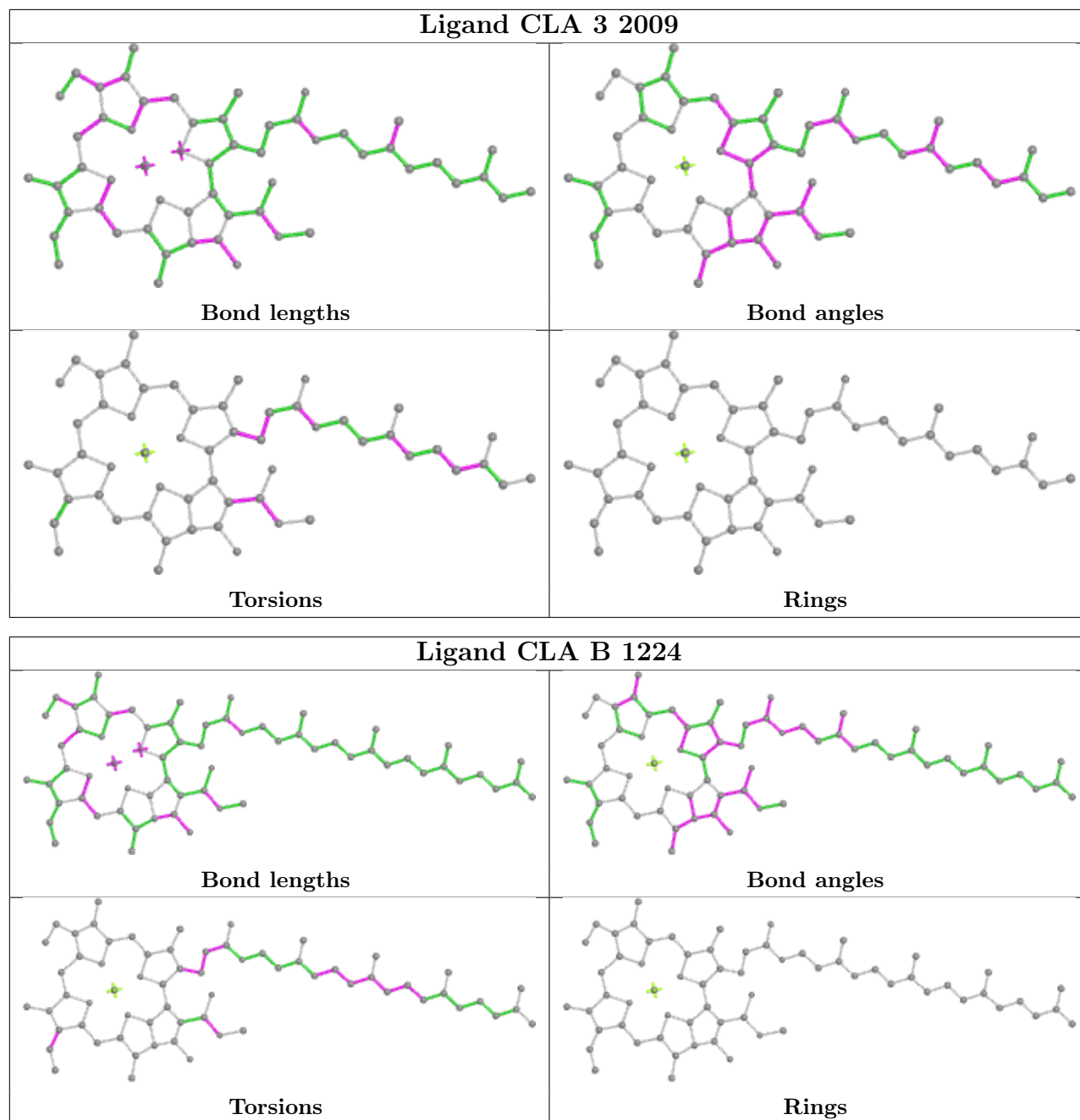
Torsions



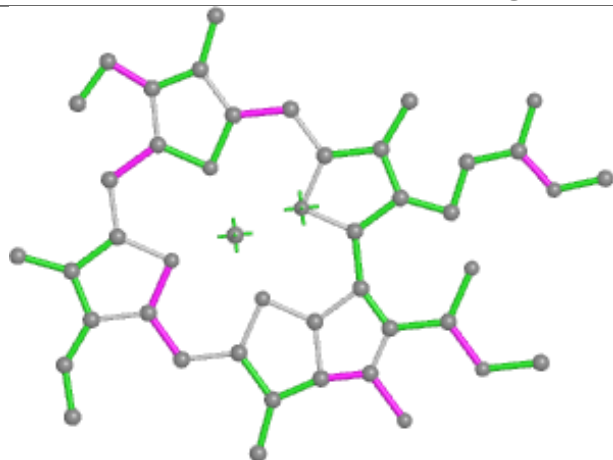
Rings

Ligand CLA 1 1014	
	
Bond lengths	Bond angles
	
Torsions	Rings

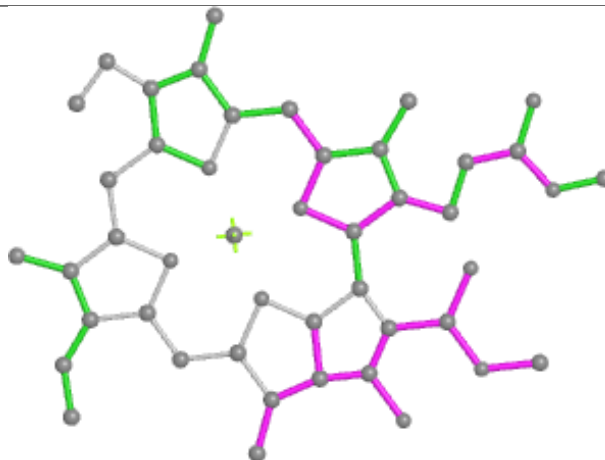
Ligand CLA 2 2007	
	
Bond lengths	Bond angles
	
Torsions	Rings



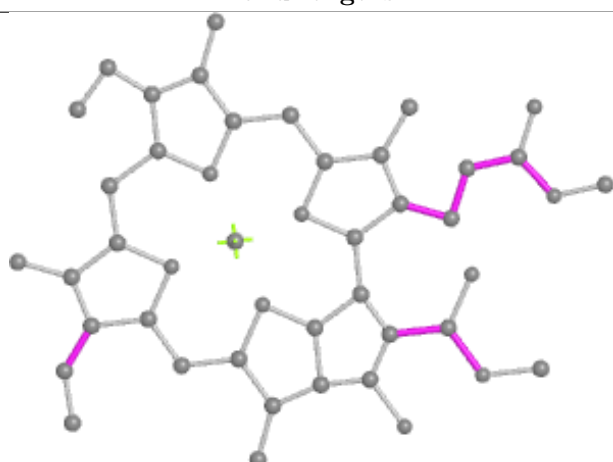
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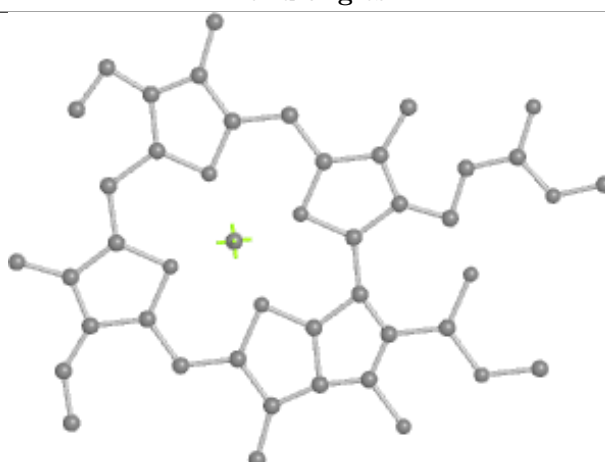
Bond lengths



Bond angles

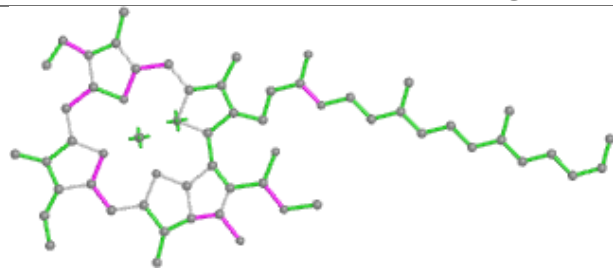


Torsions

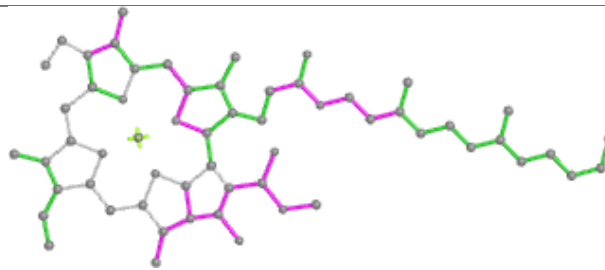


Rings

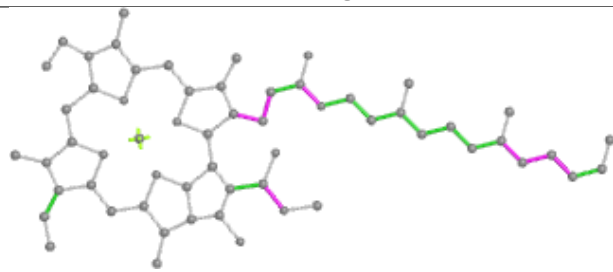
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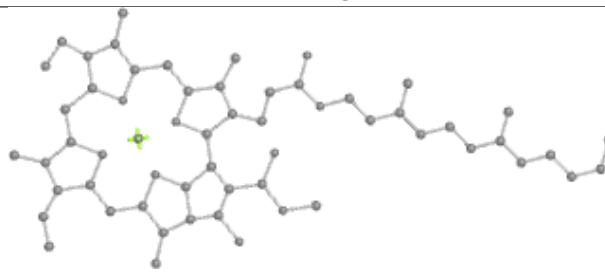
Bond lengths



Bond angles

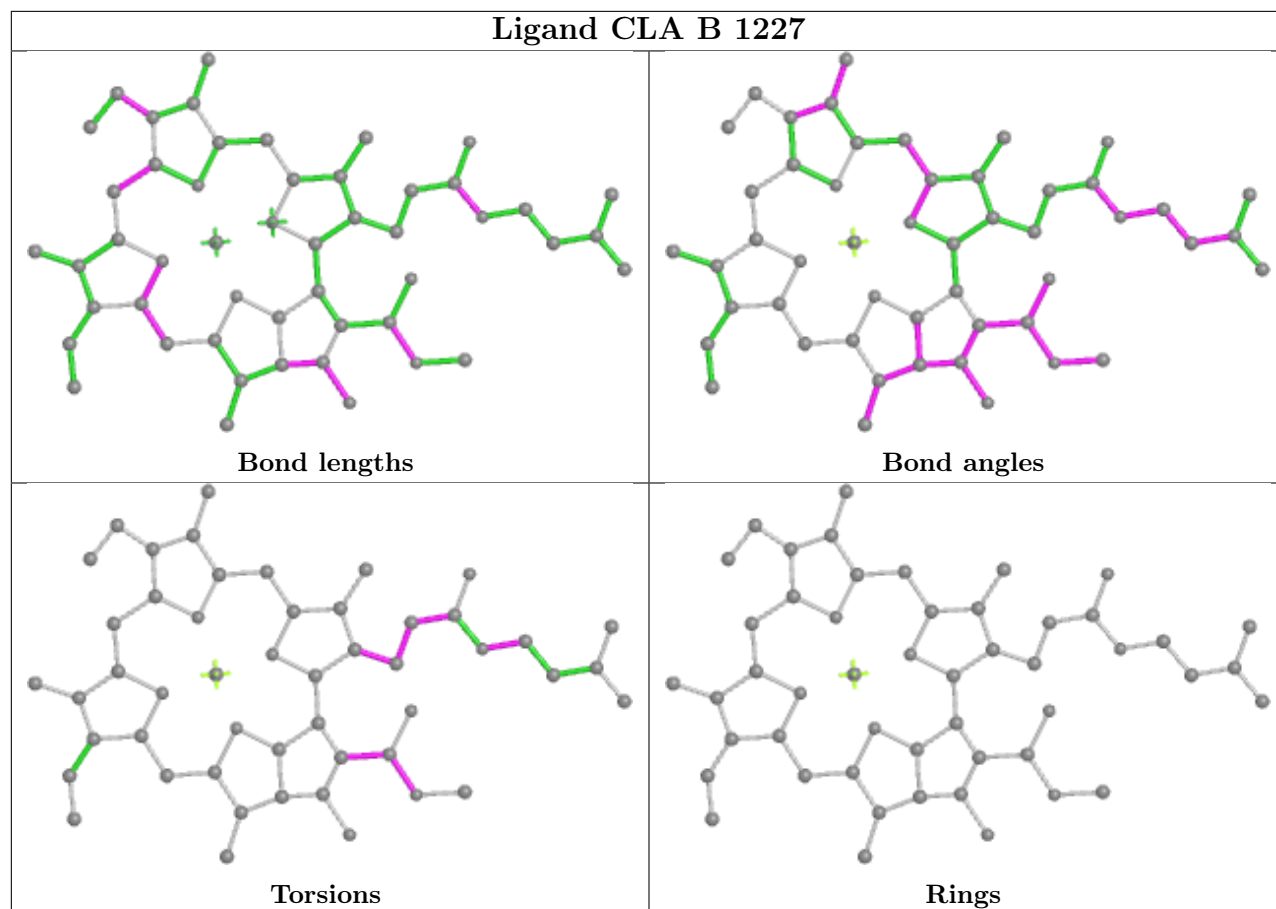


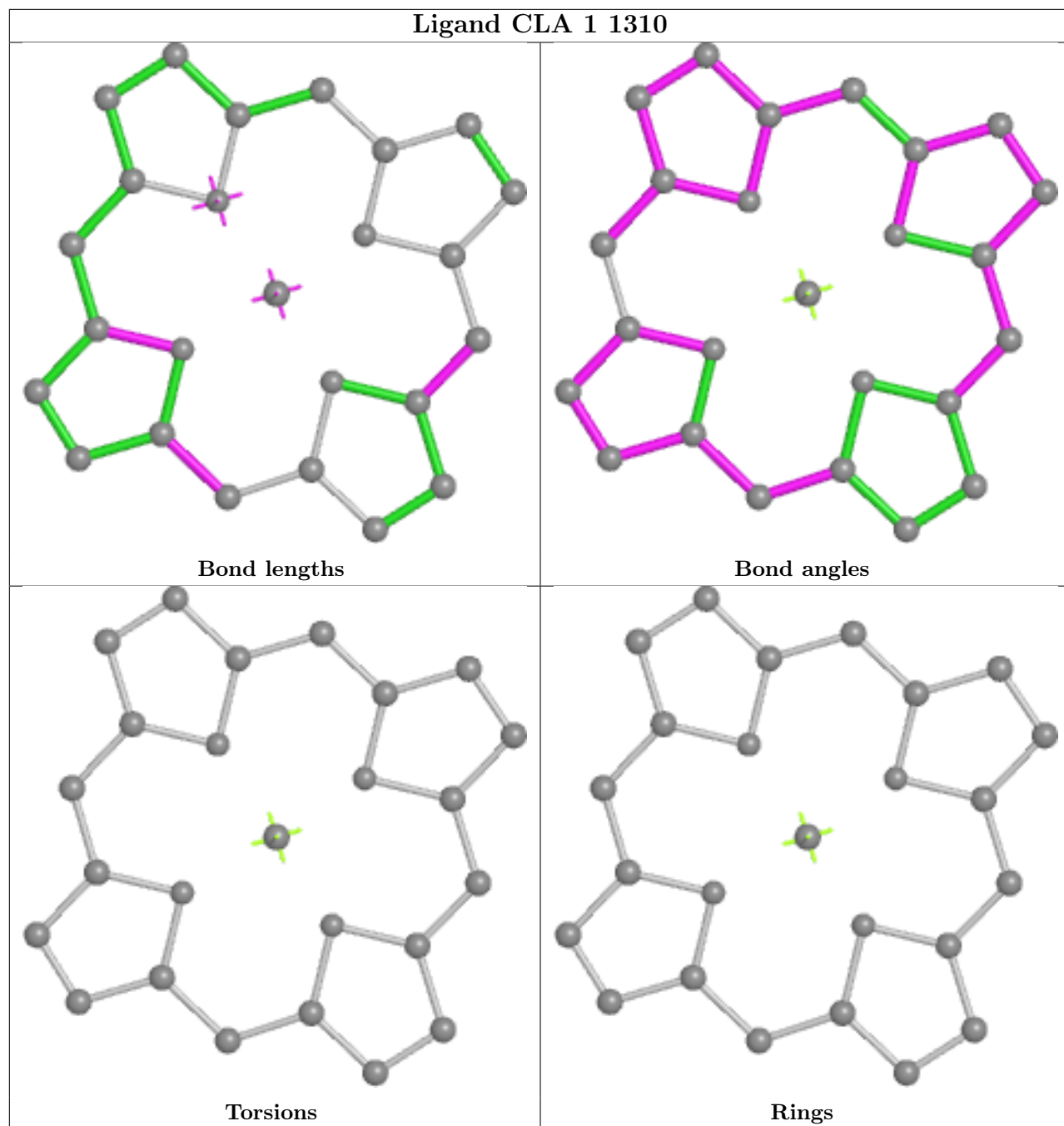
Torsions

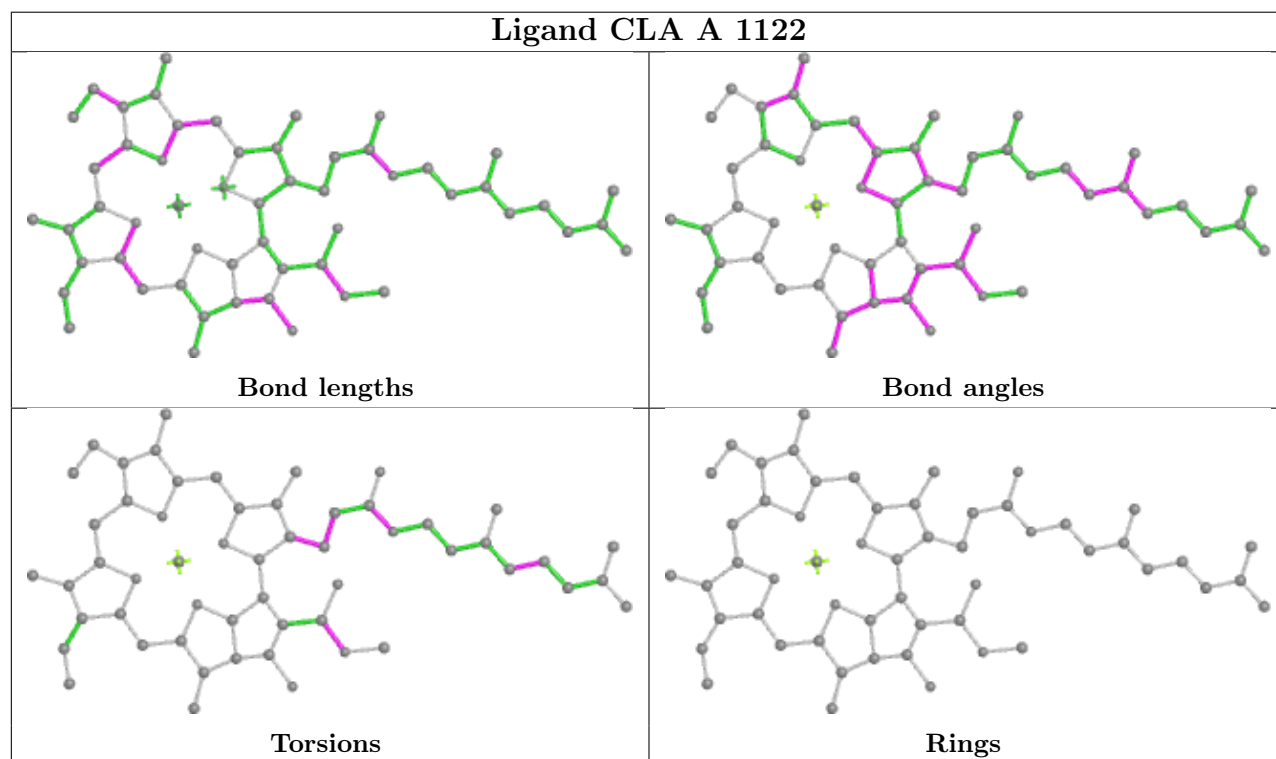
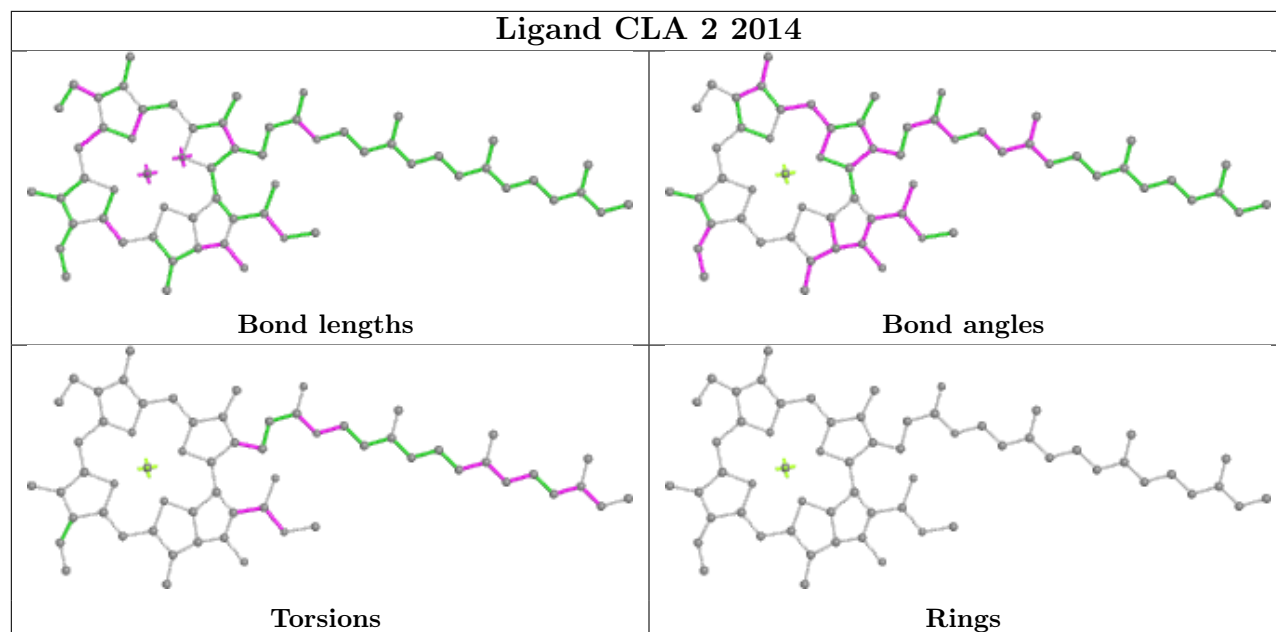


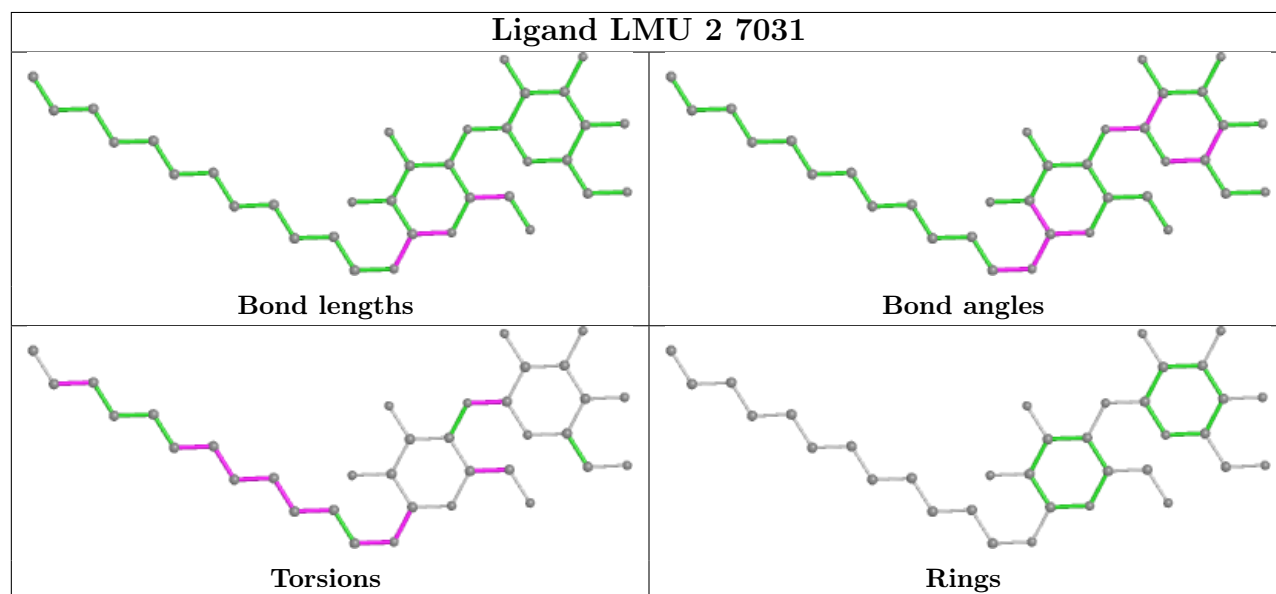
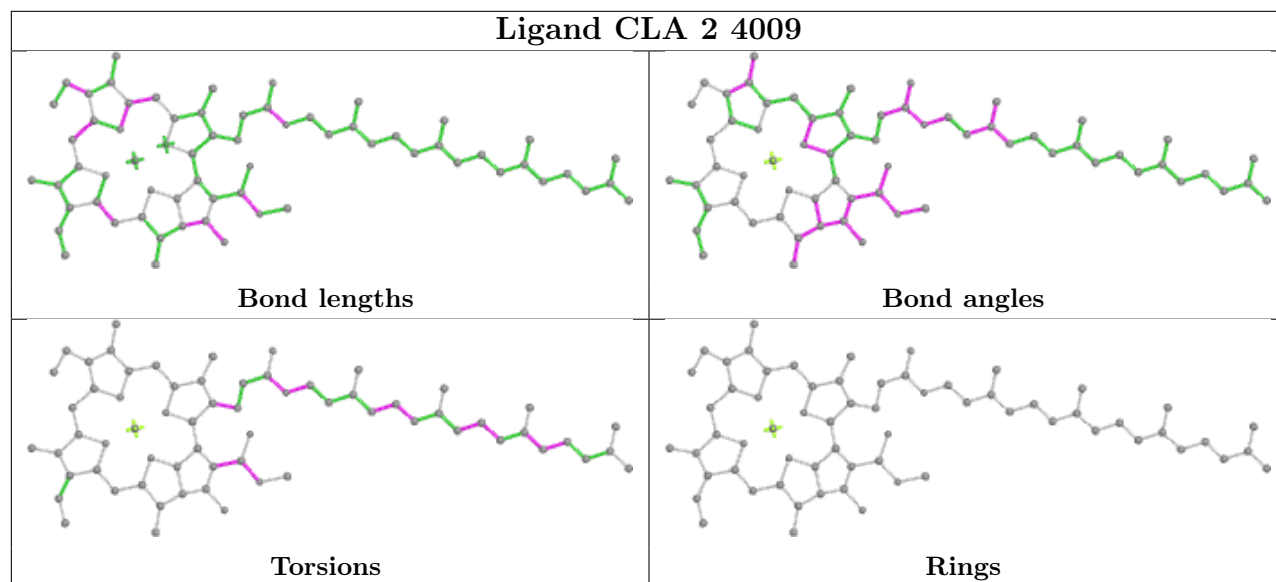
Rings

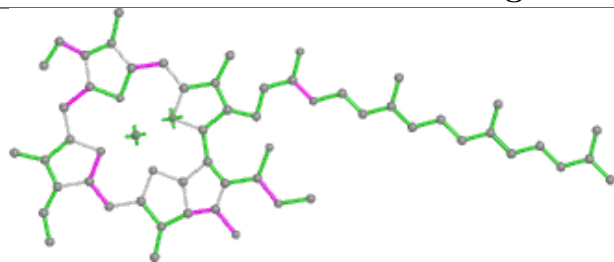
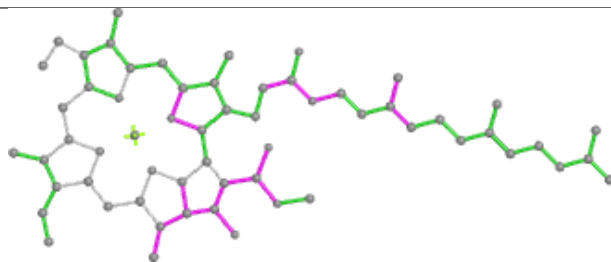
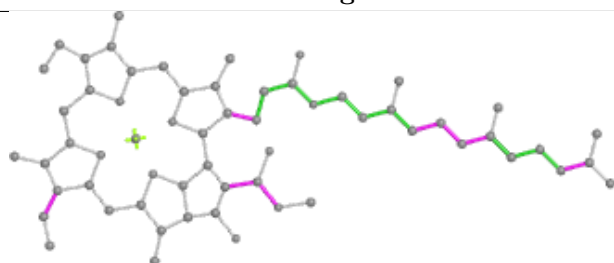
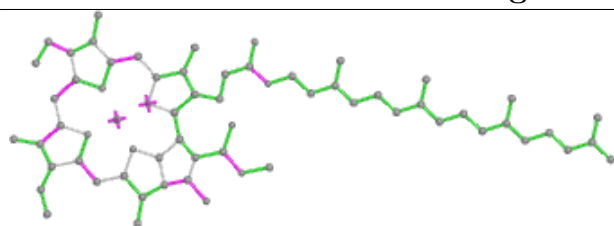
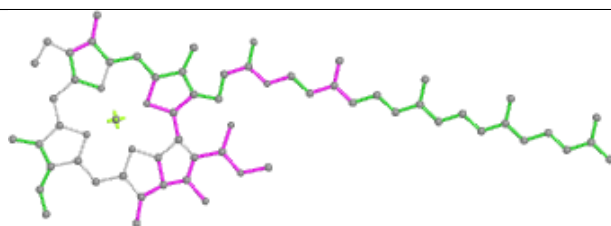
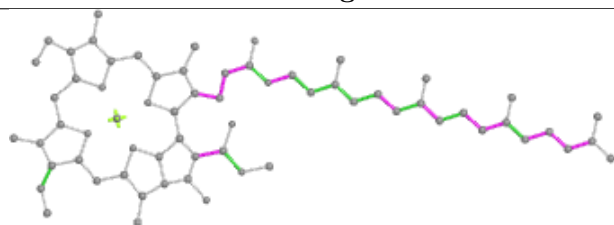
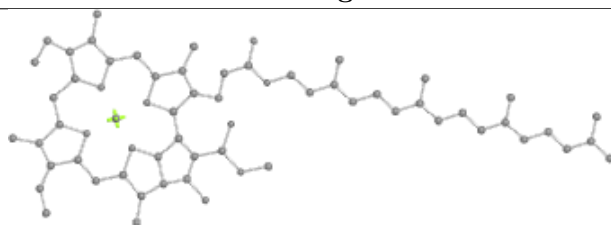
Ligand CLA B 1227

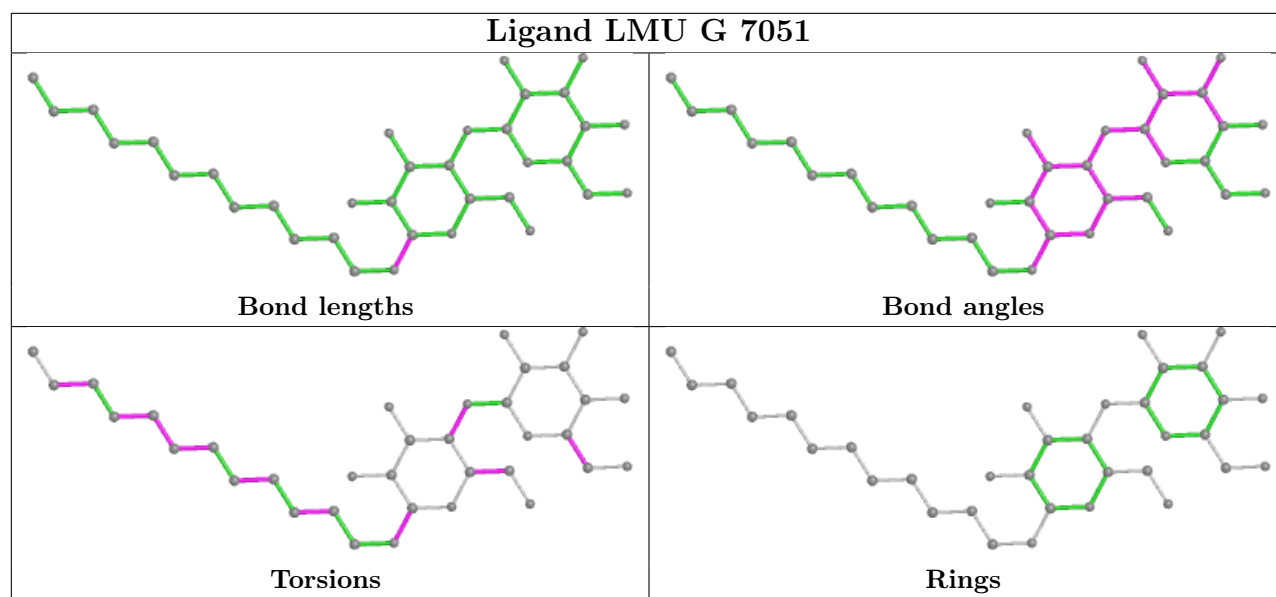
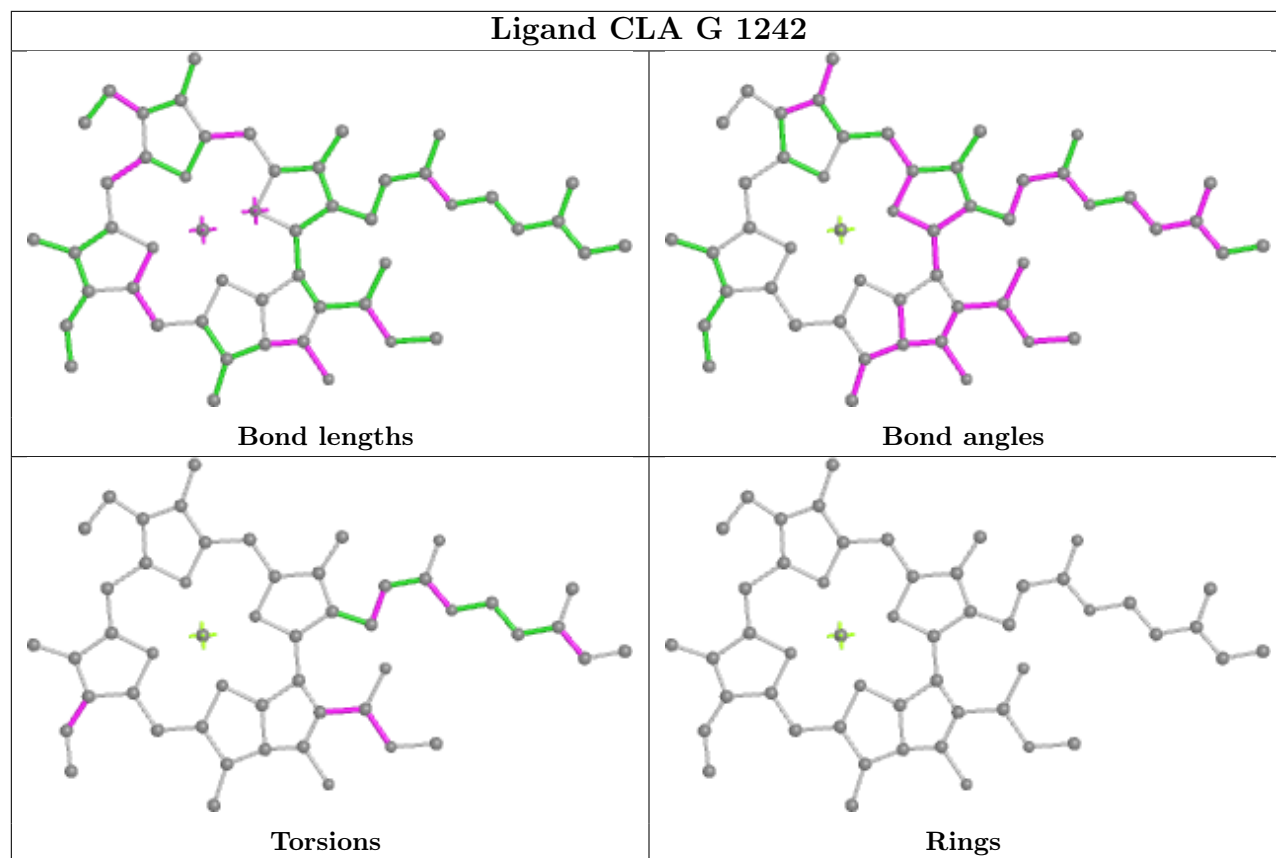


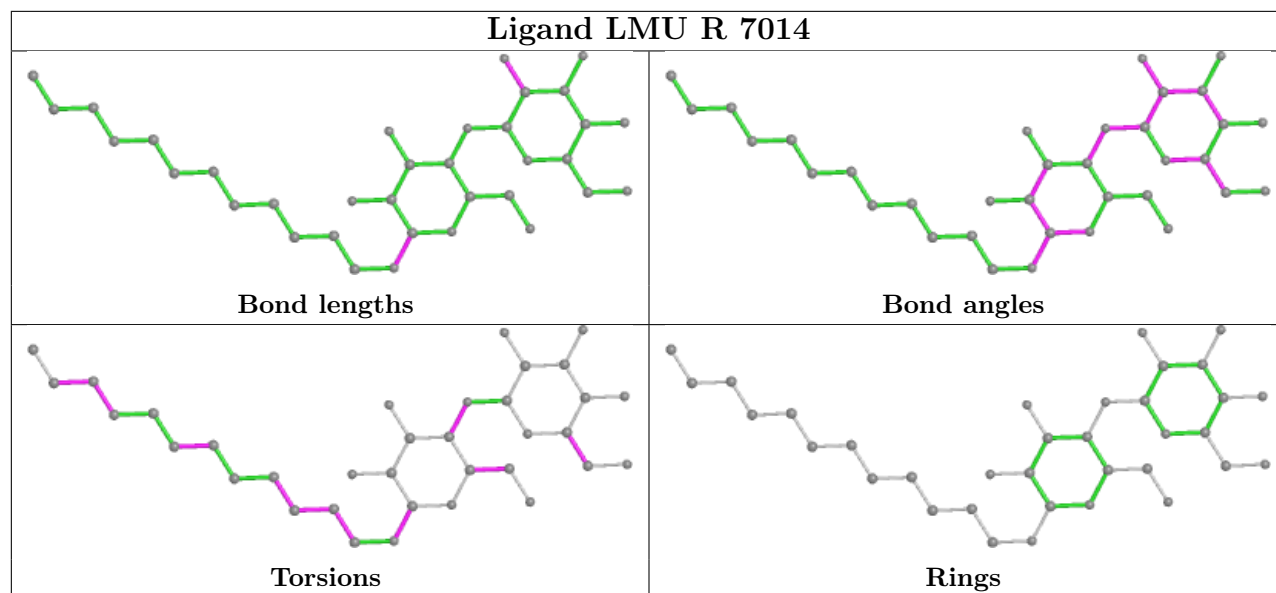




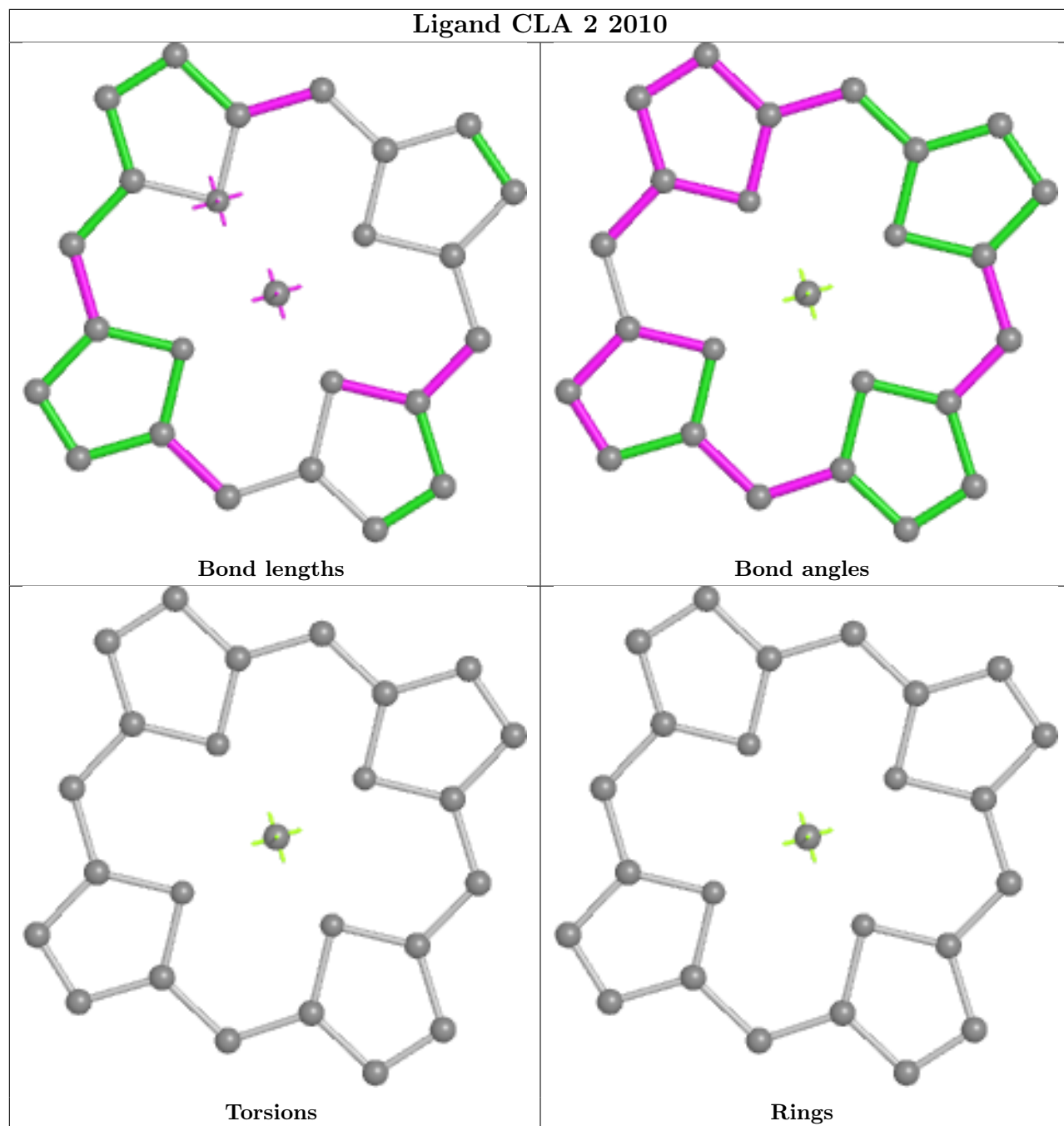


Ligand CLA B 1234**Bond lengths****Bond angles****Torsions****Rings****Ligand CLA 3 3013****Bond lengths****Bond angles****Torsions****Rings**

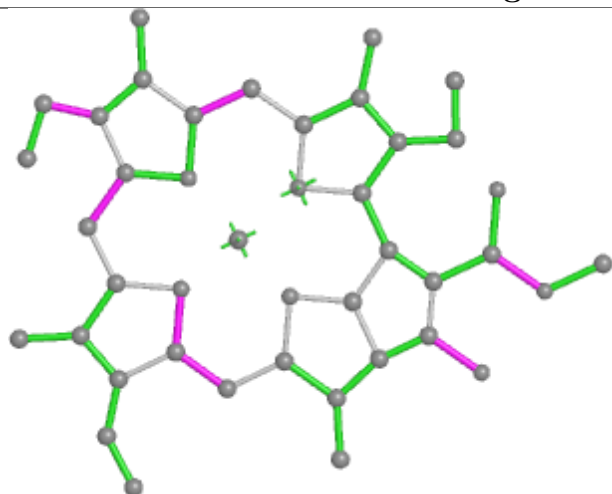




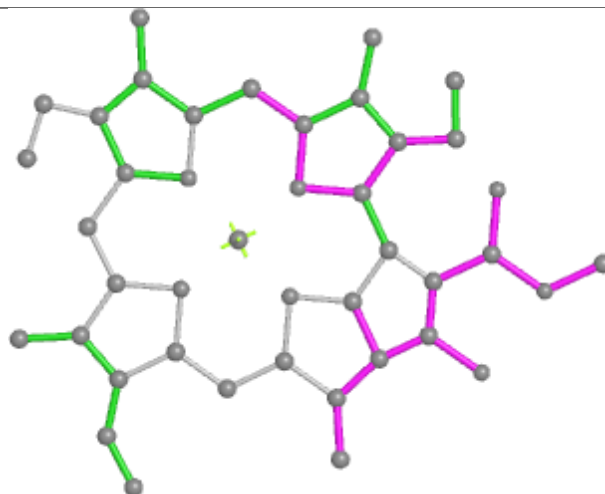
Ligand CLA 2 2010



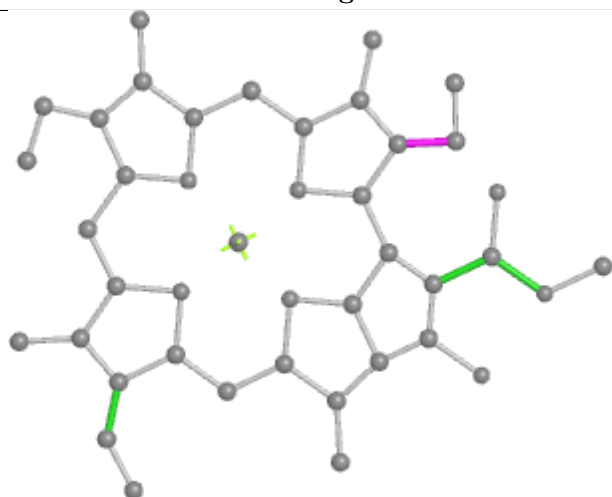
Ligand CLA A 1121



Bond lengths



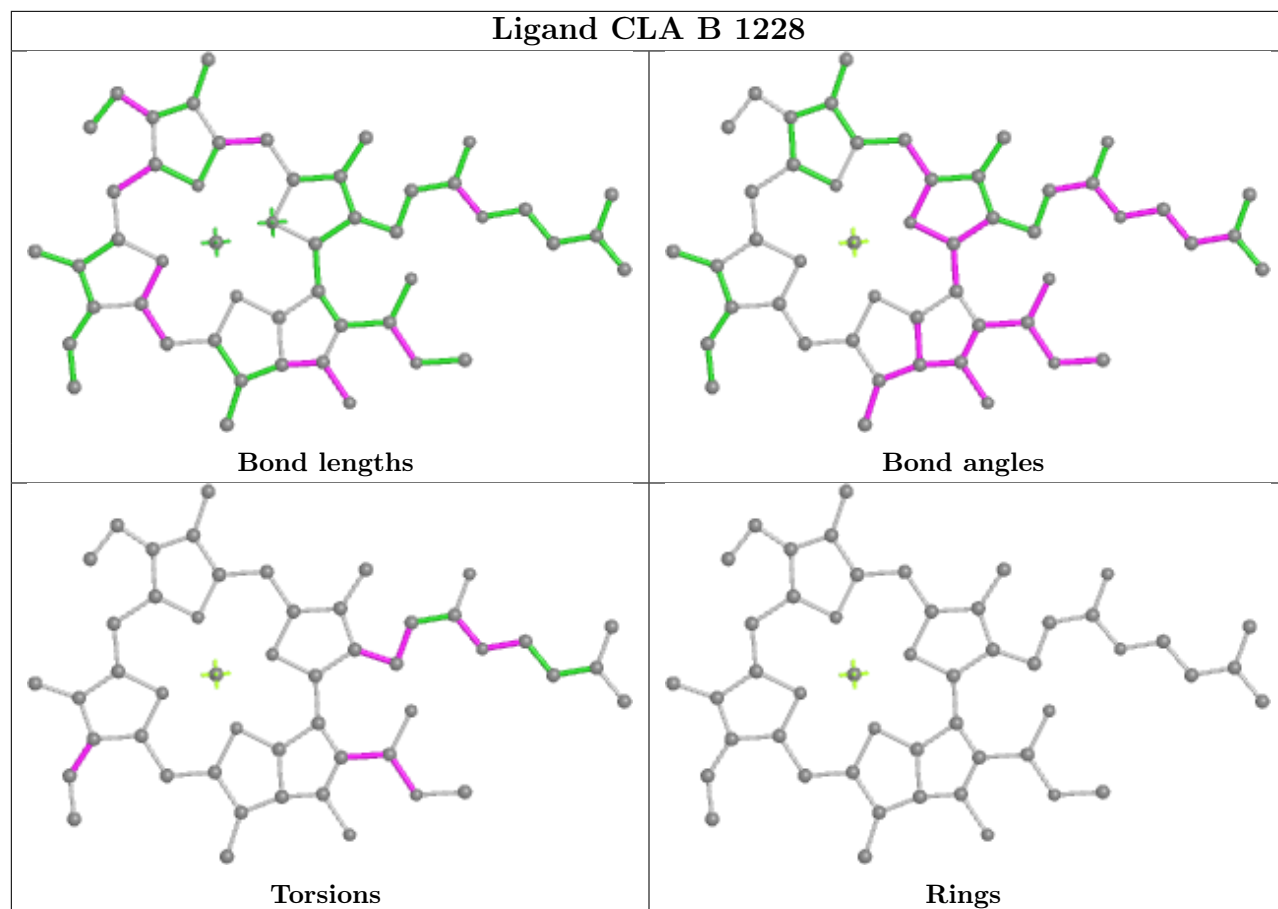
Bond angles

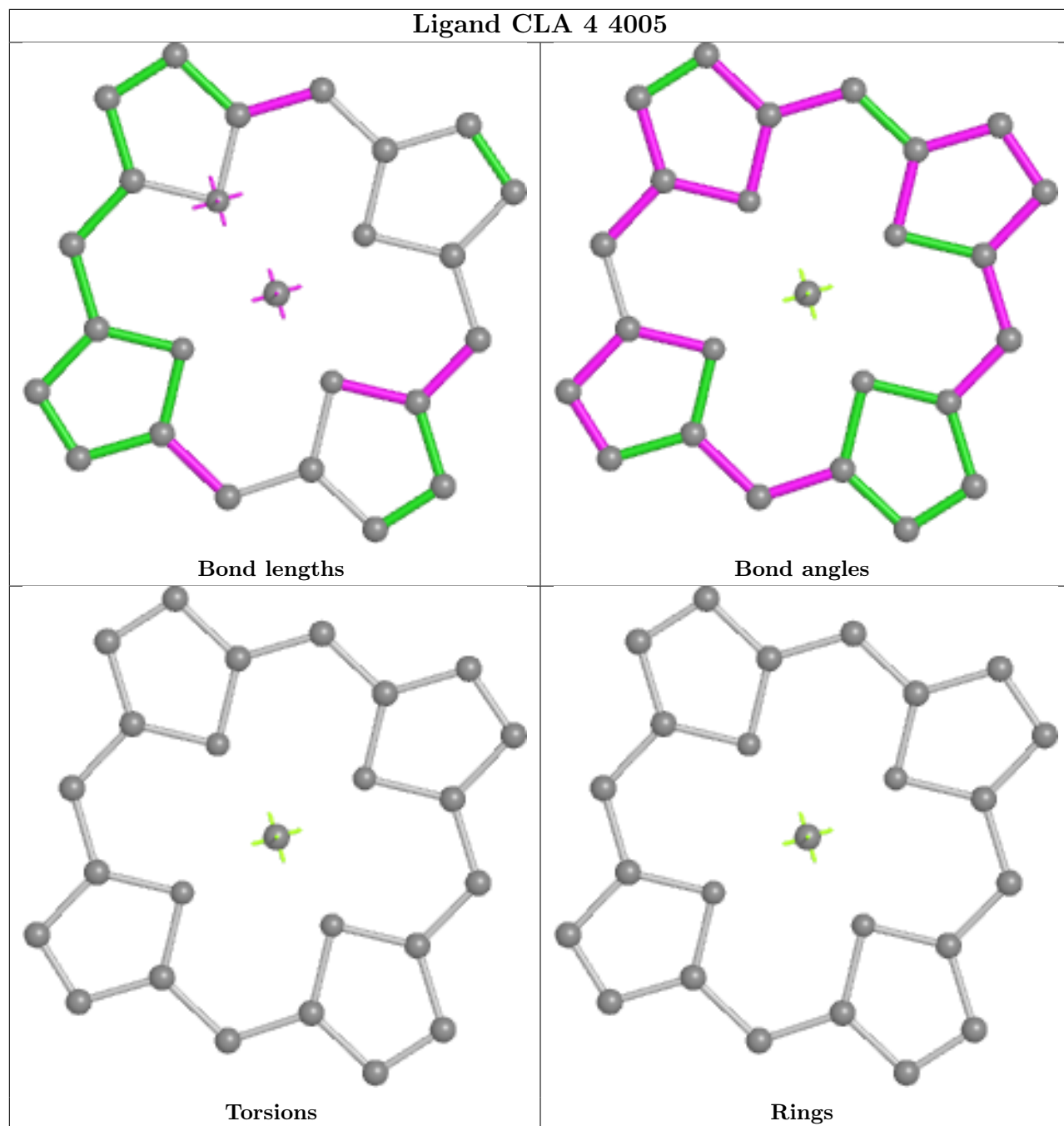


Torsions

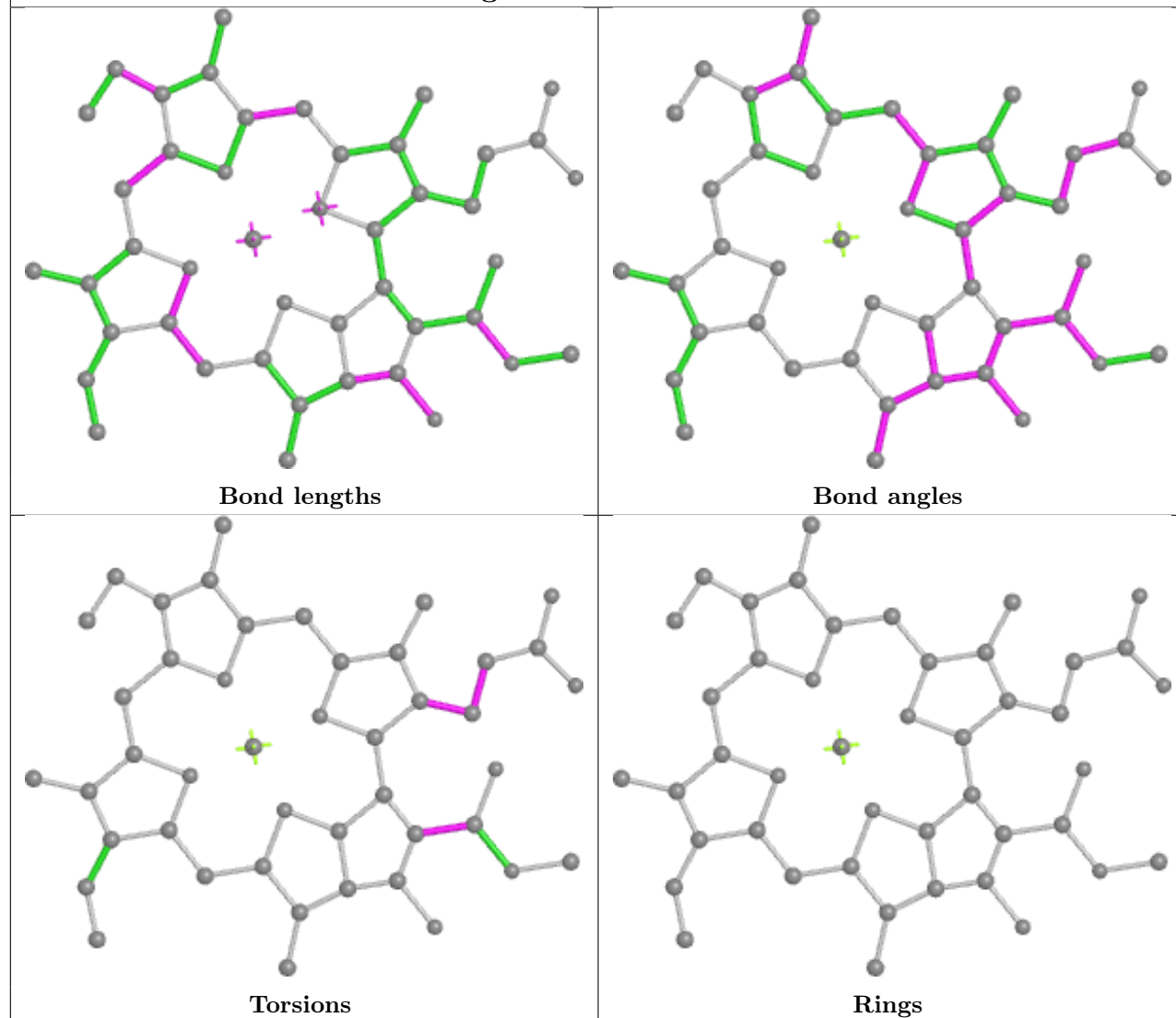


Rings

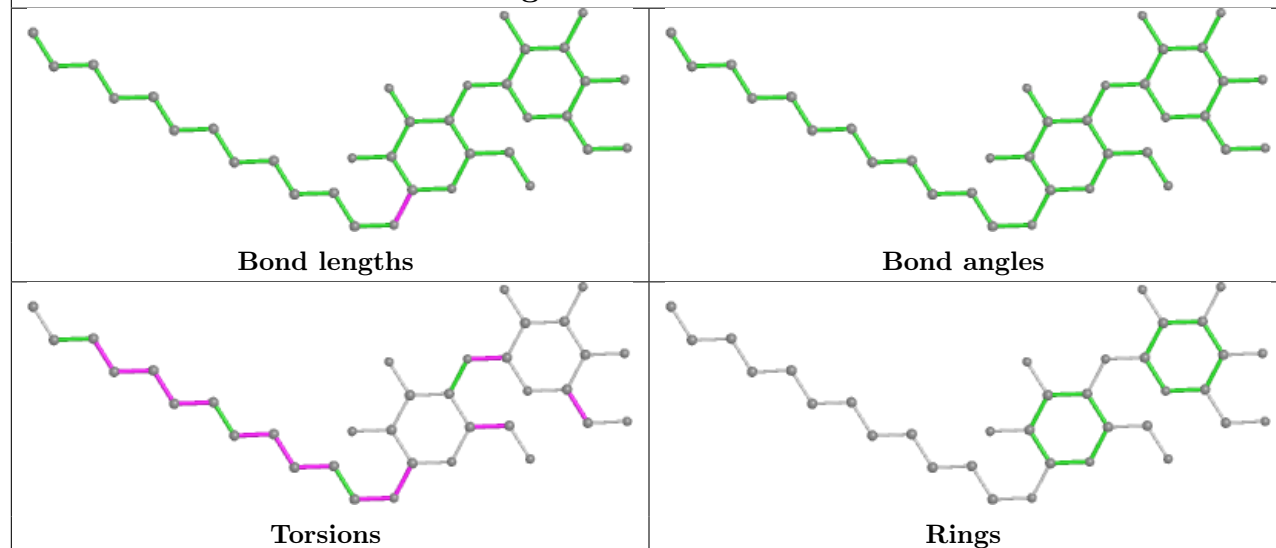




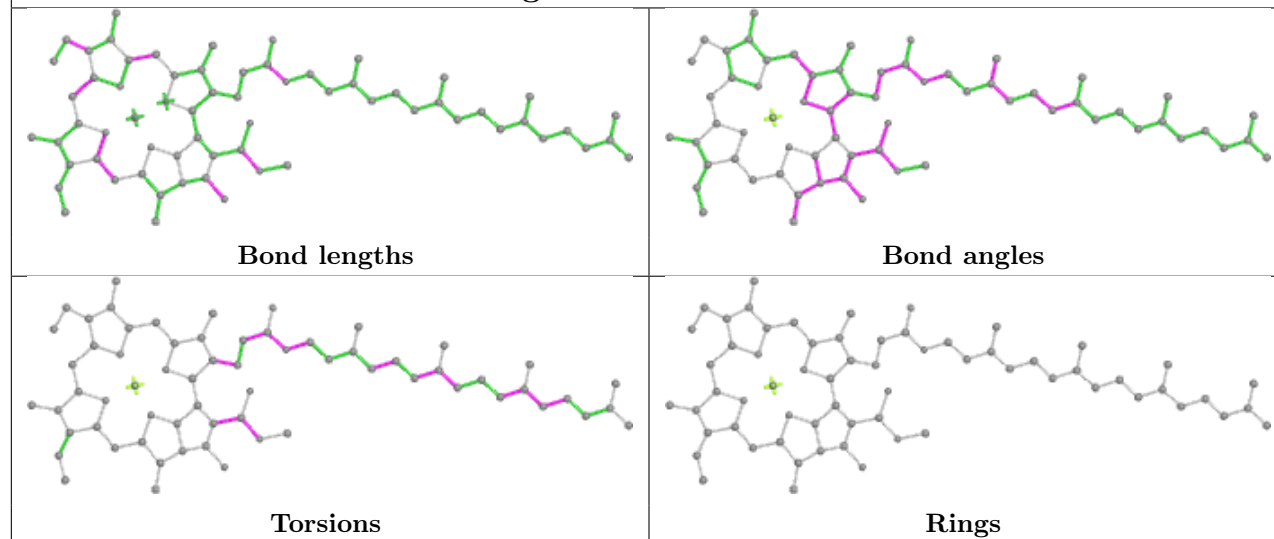
Ligand CLA K 1142



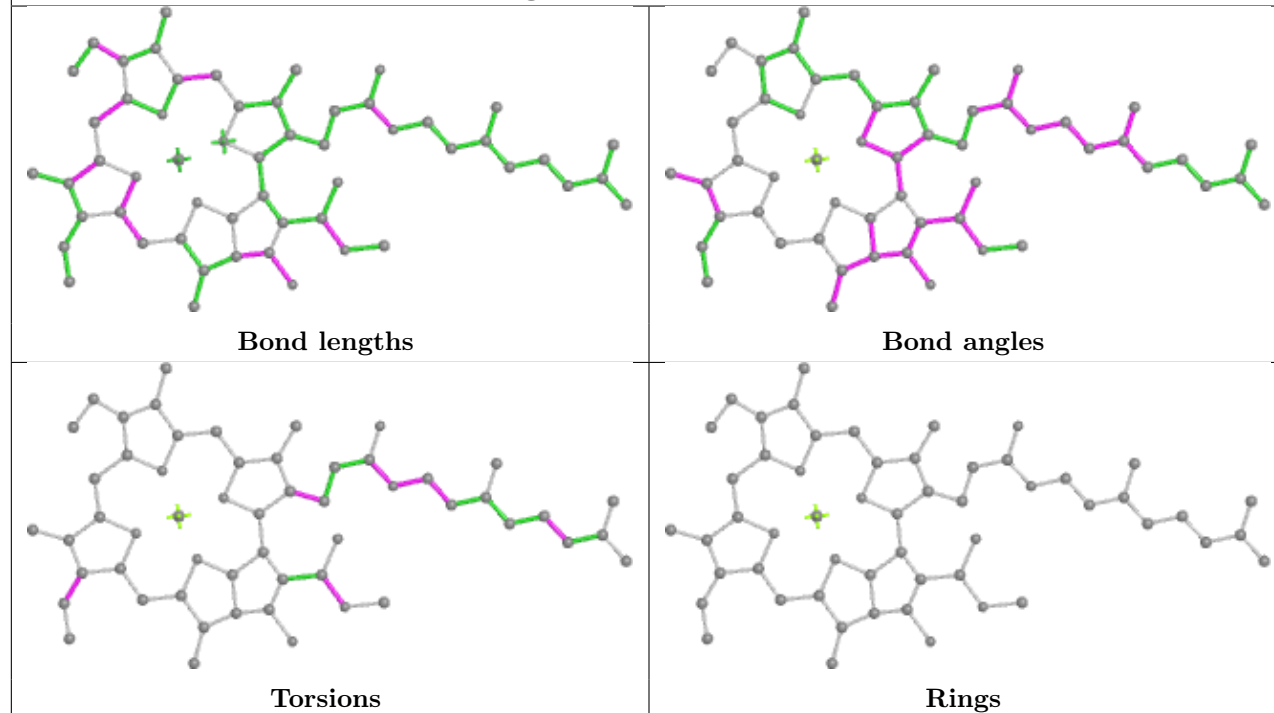
Ligand LMU L 7029



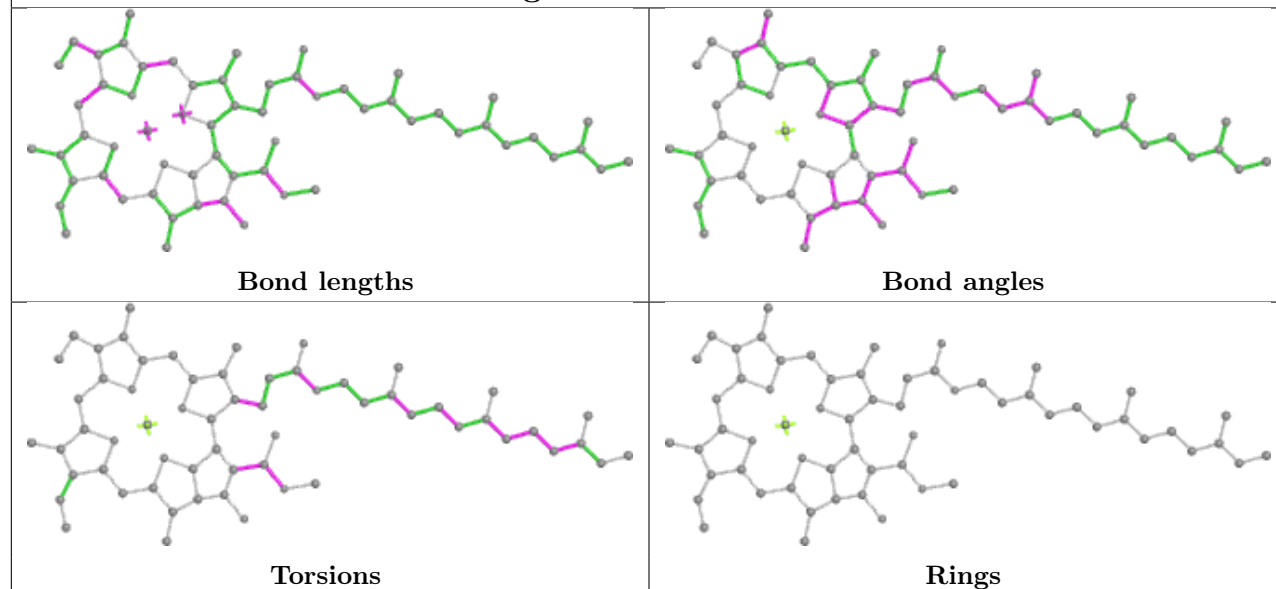
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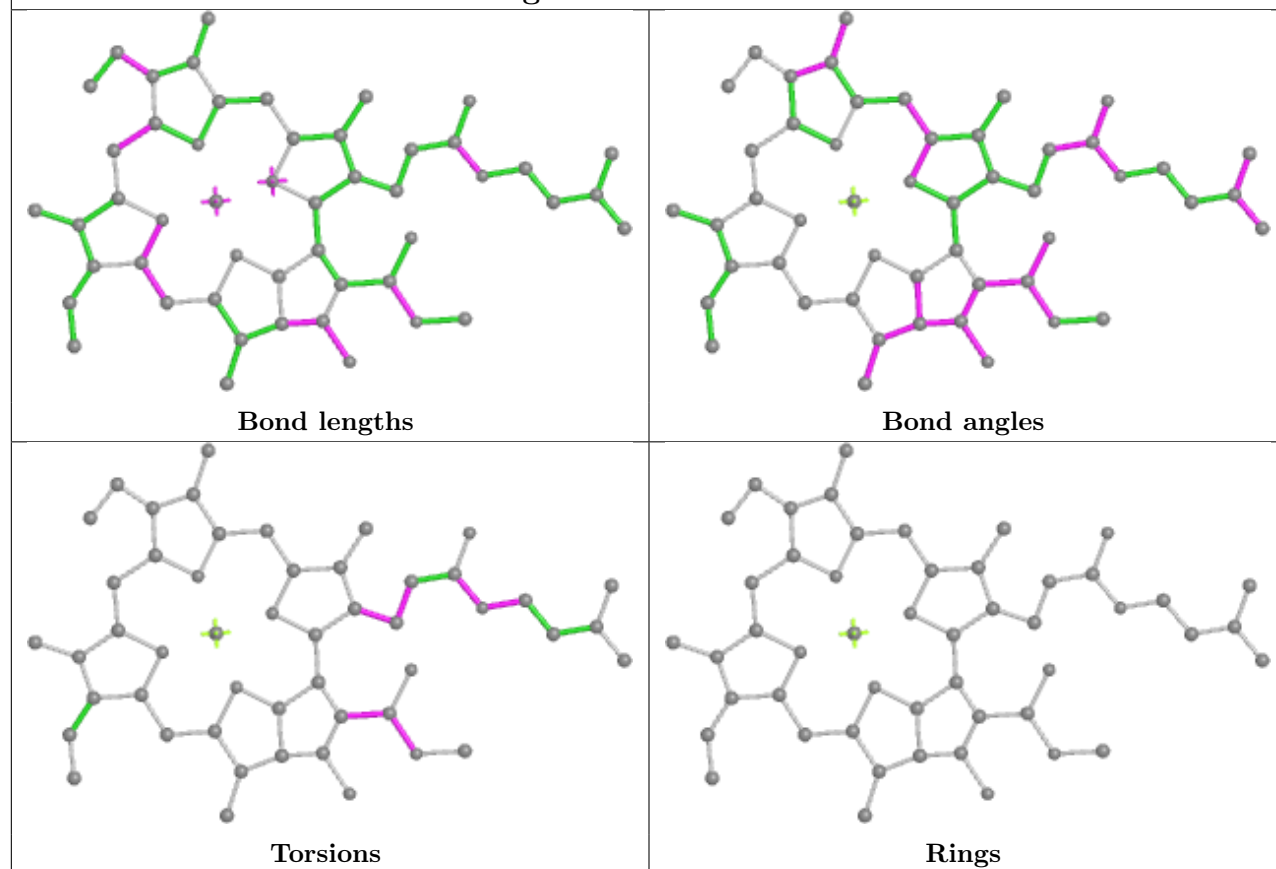
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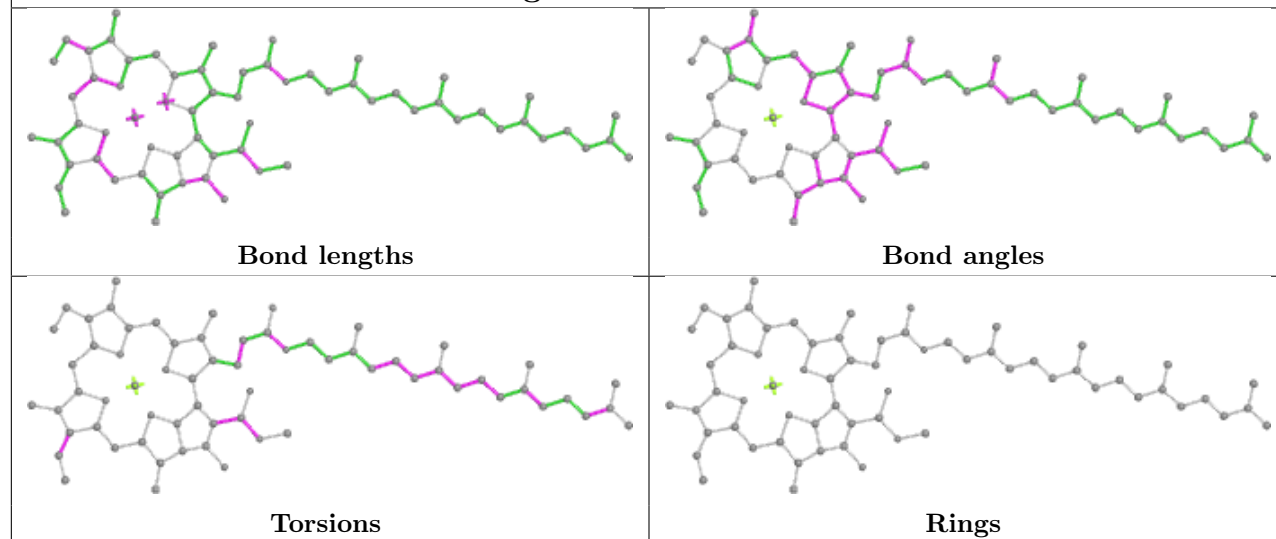
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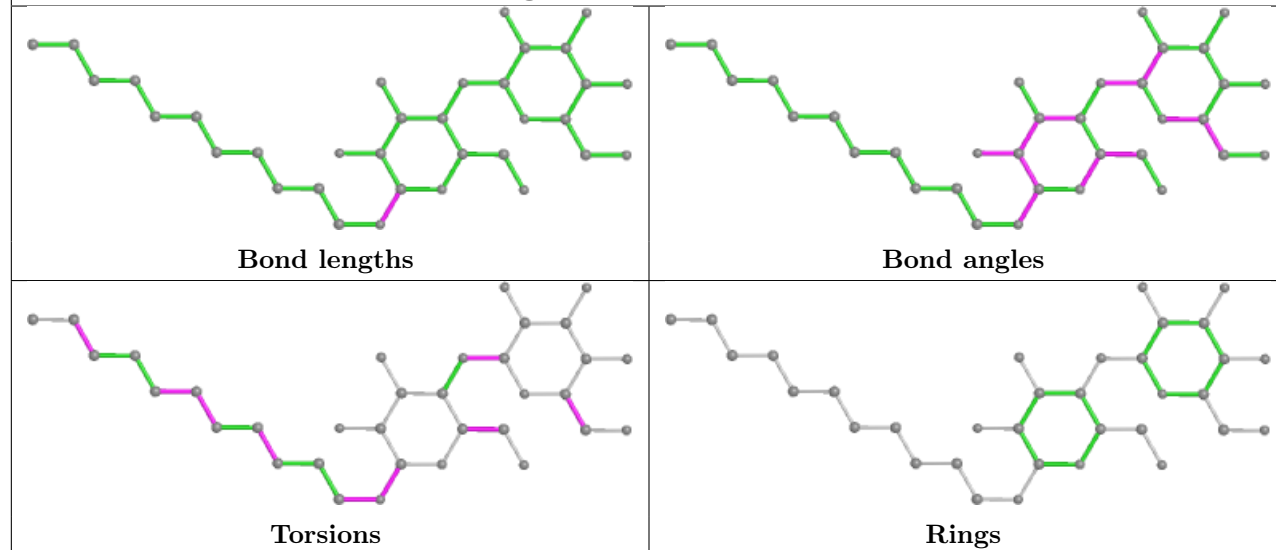
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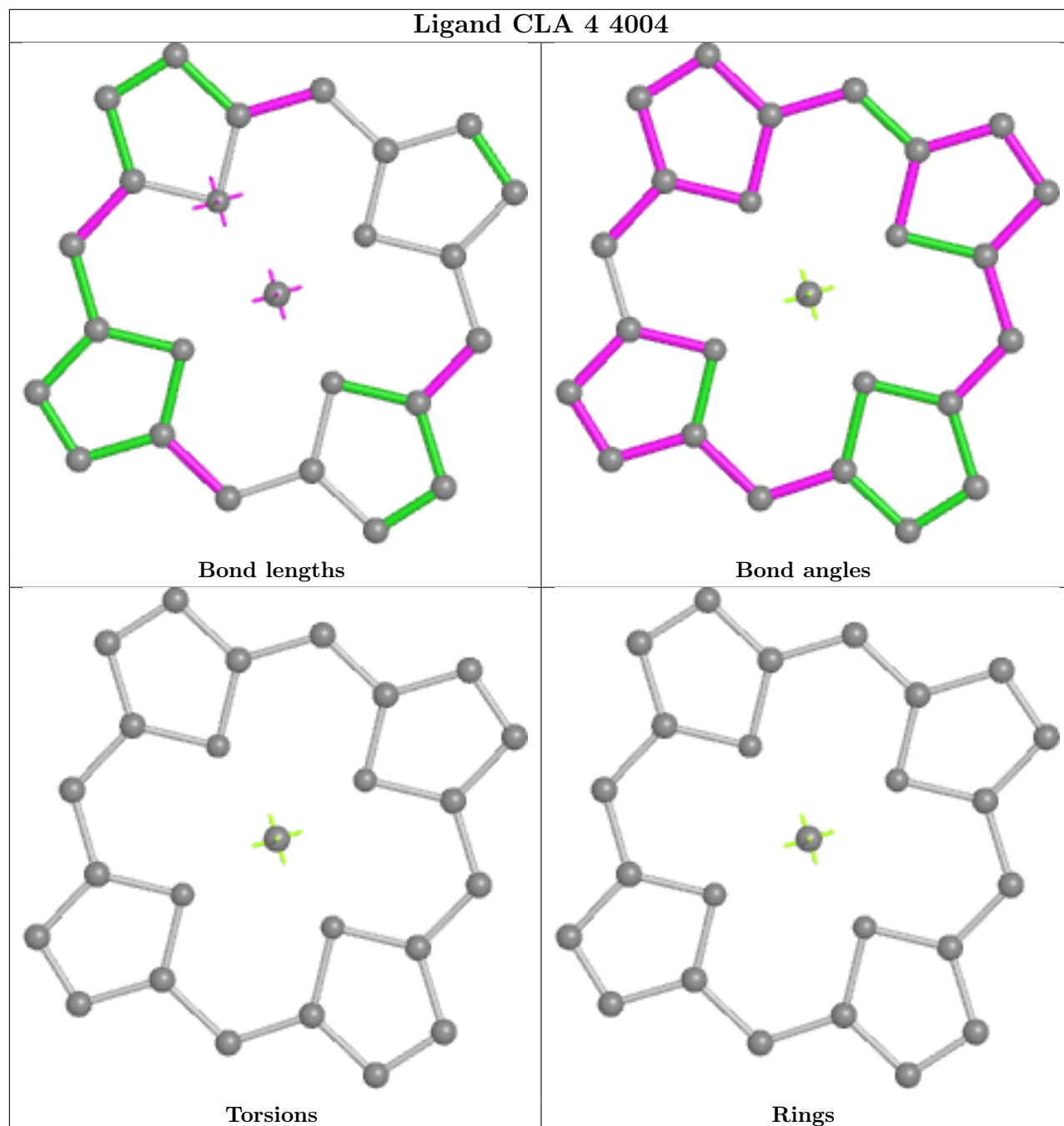
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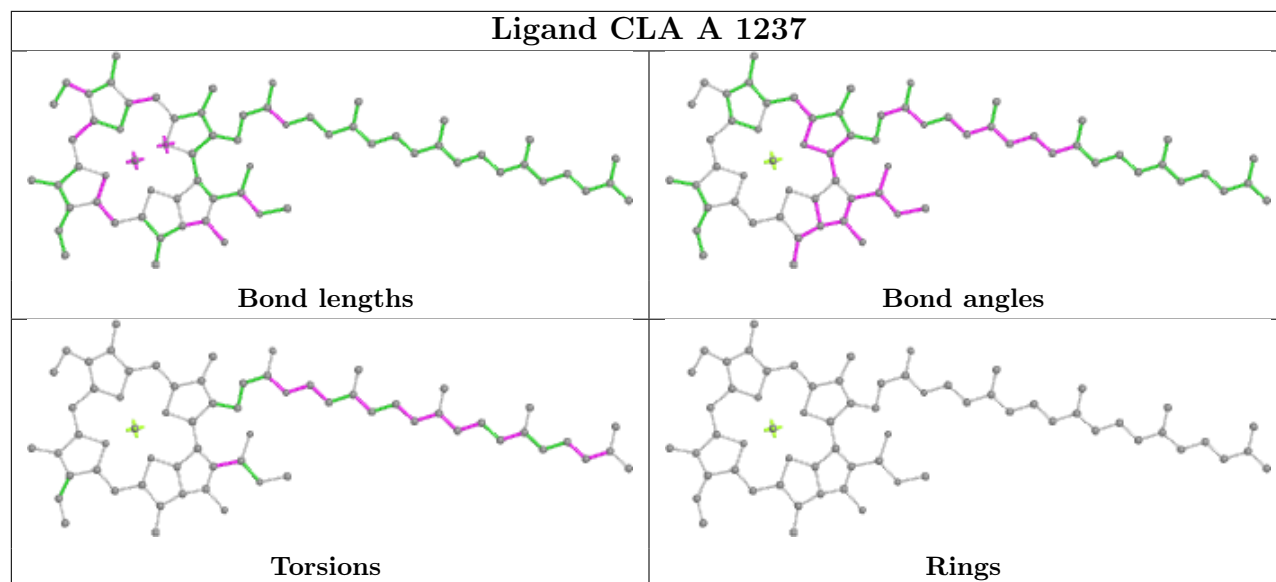
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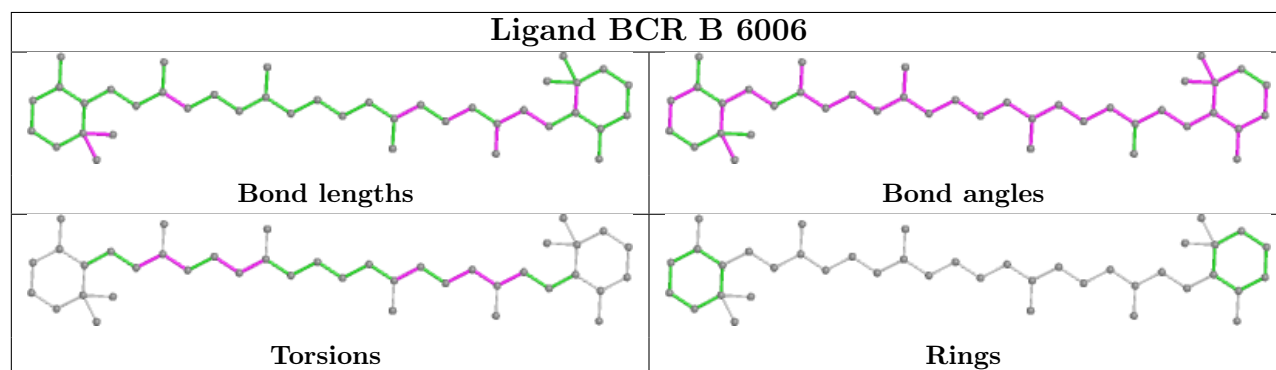
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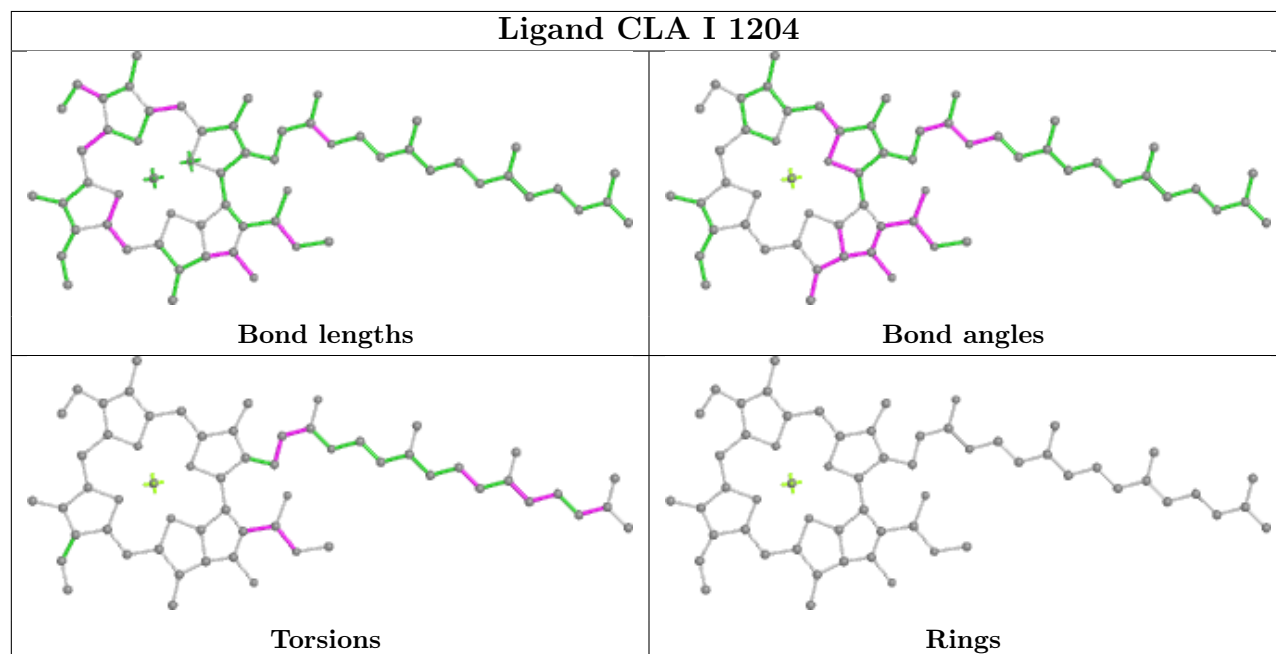
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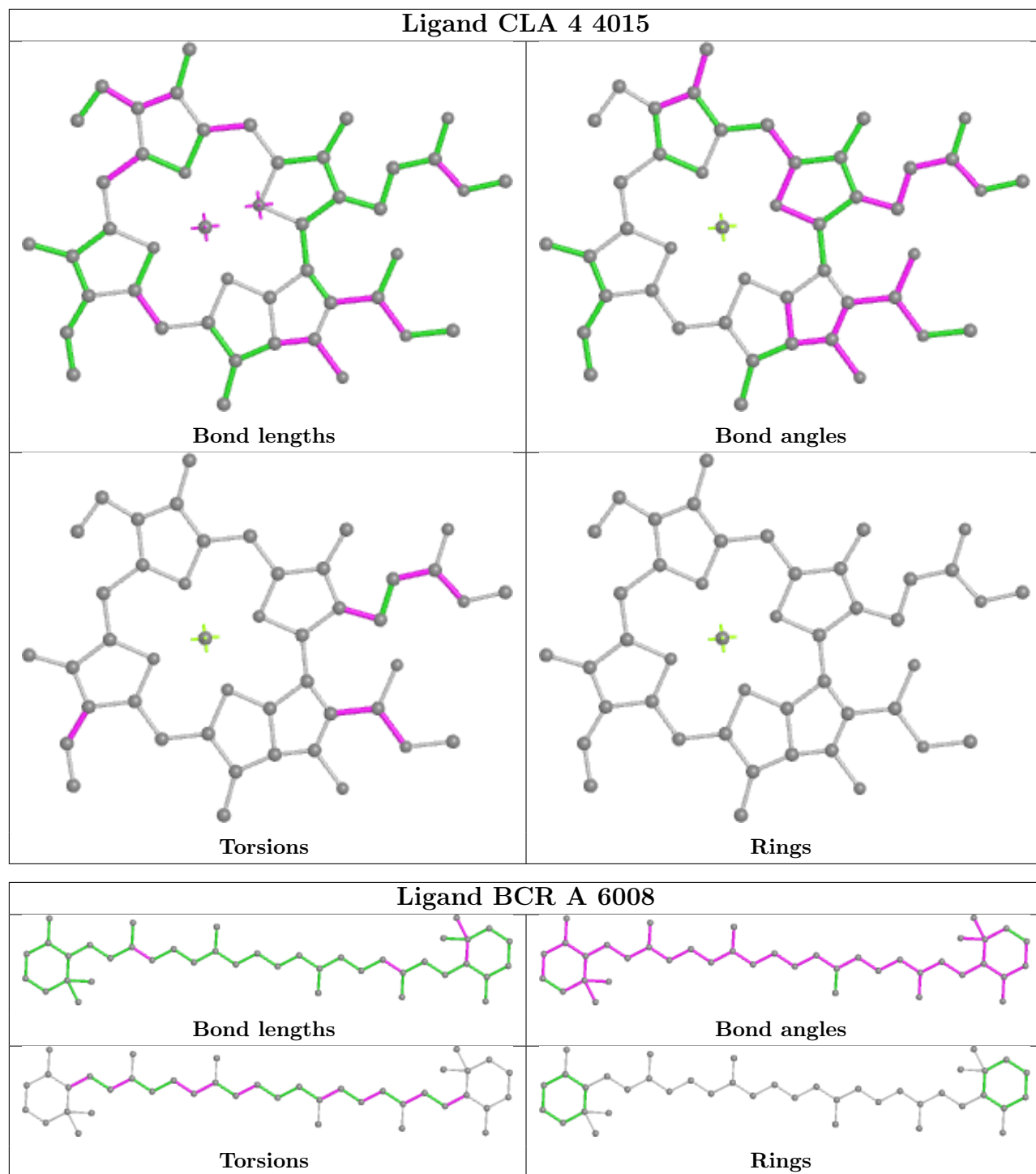


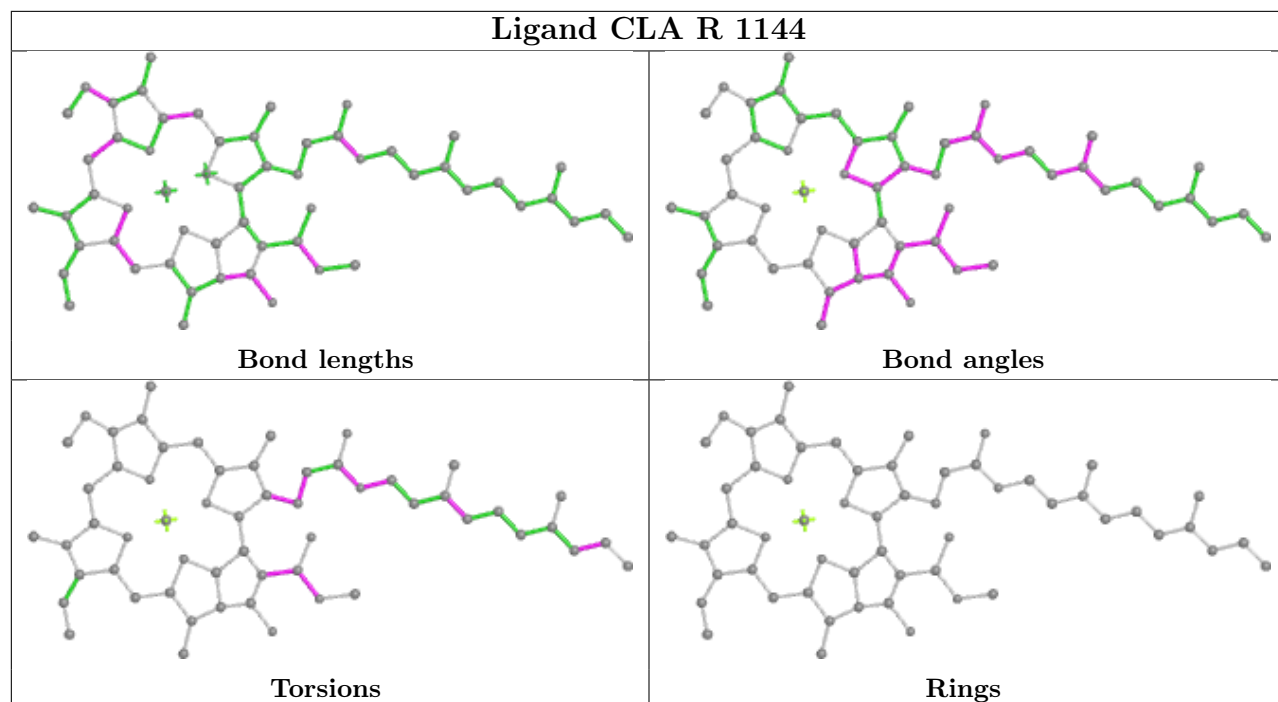
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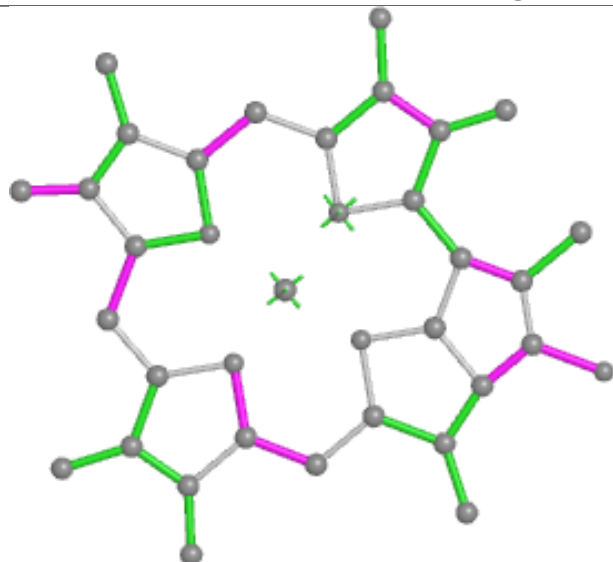
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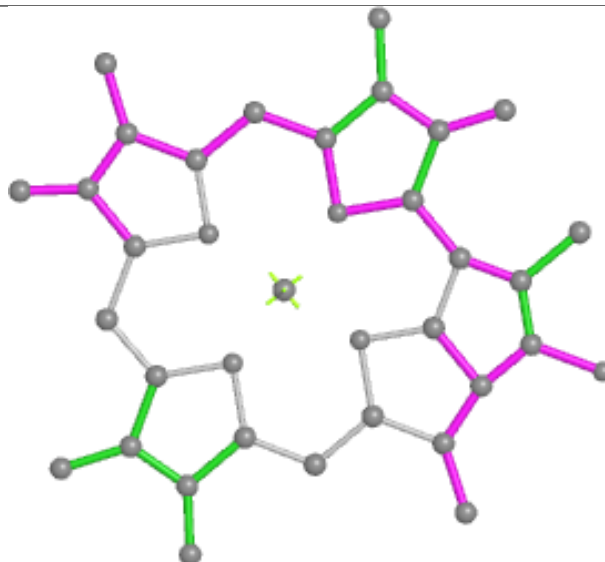




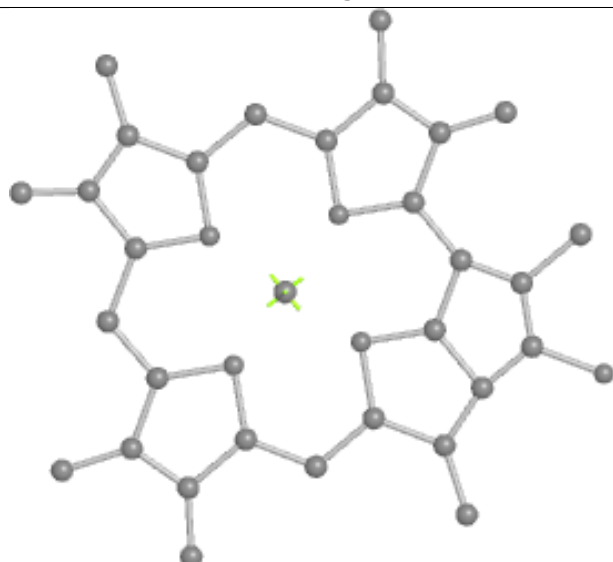
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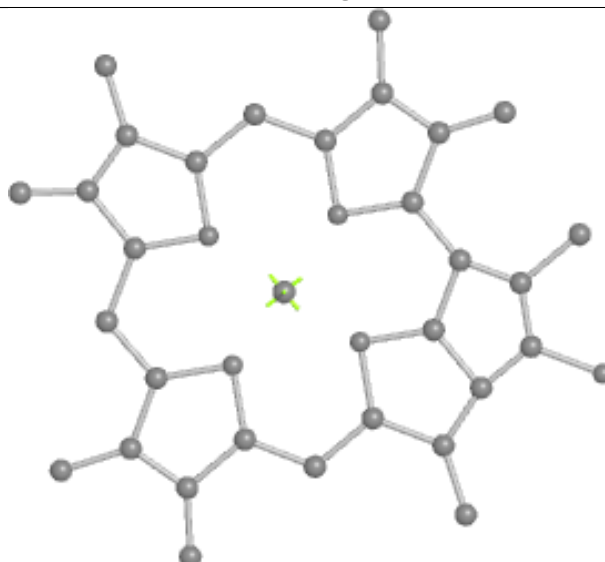
Bond lengths



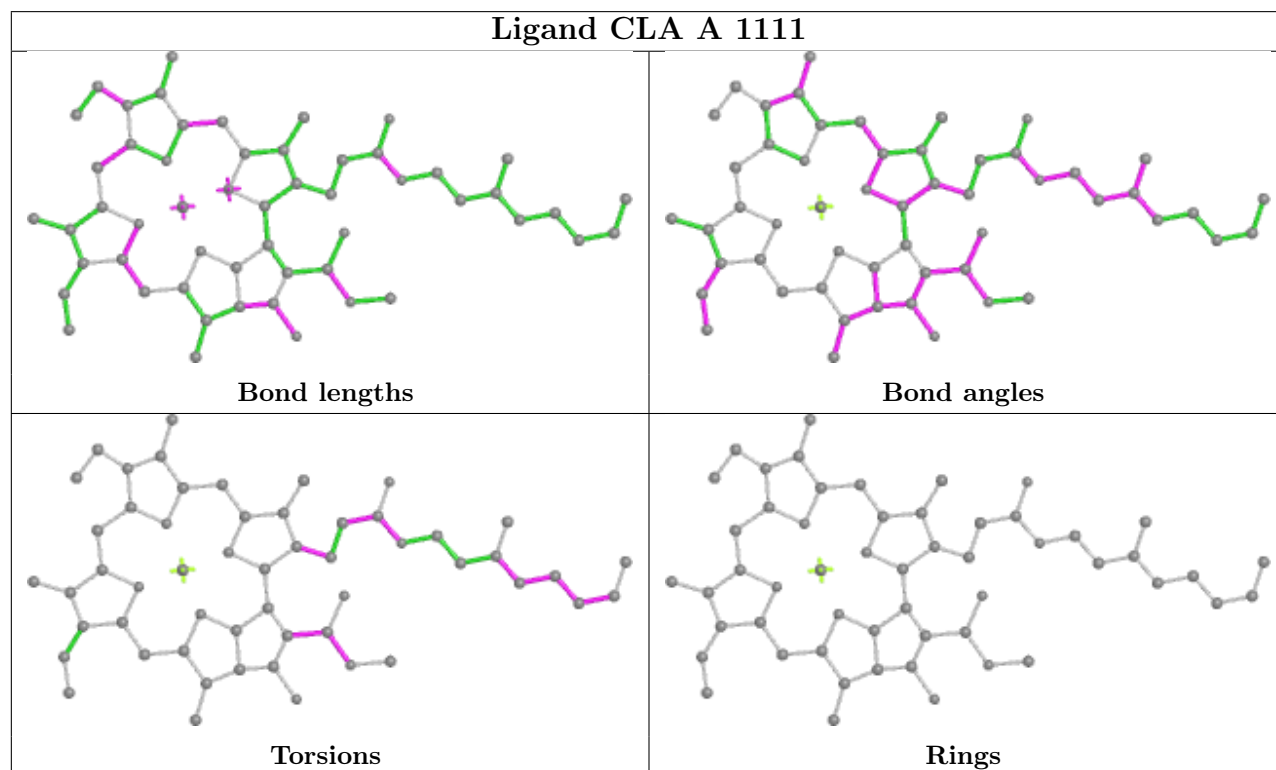
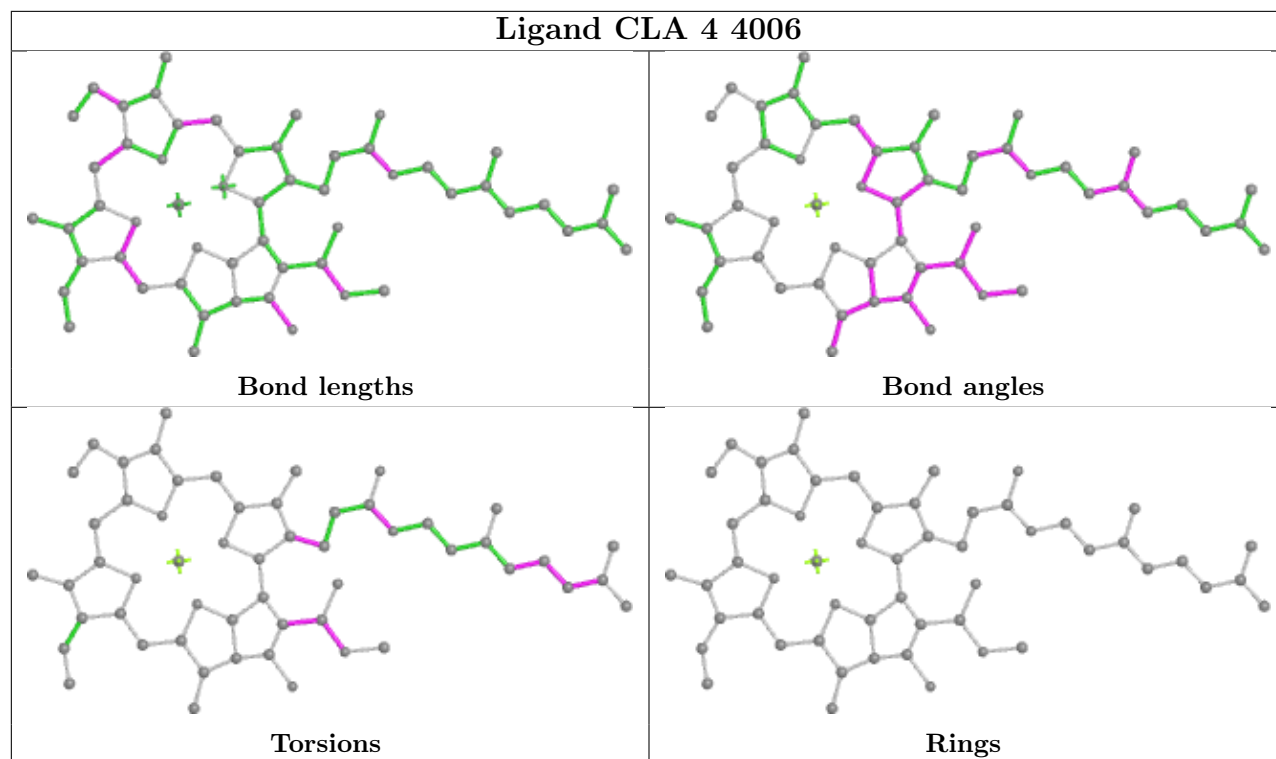
Bond angles



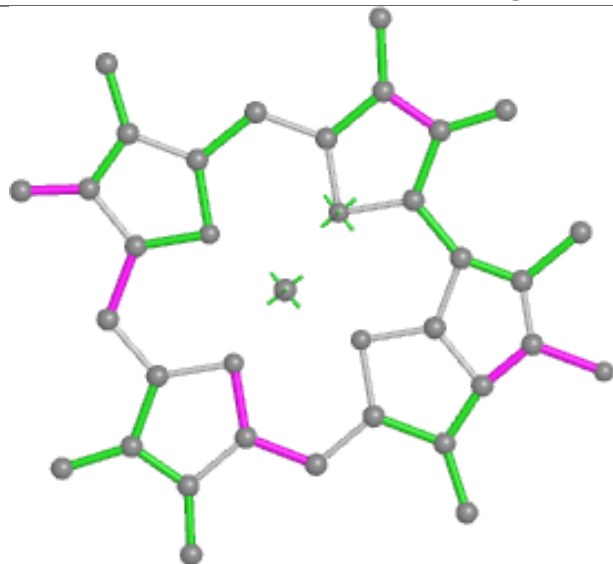
Torsions



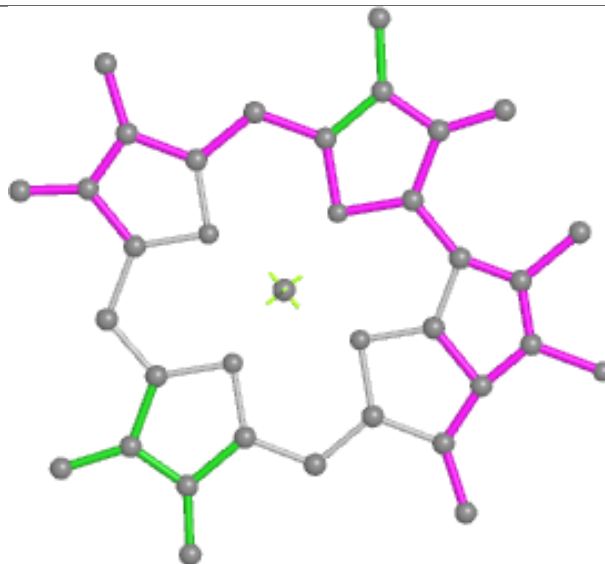
Rings



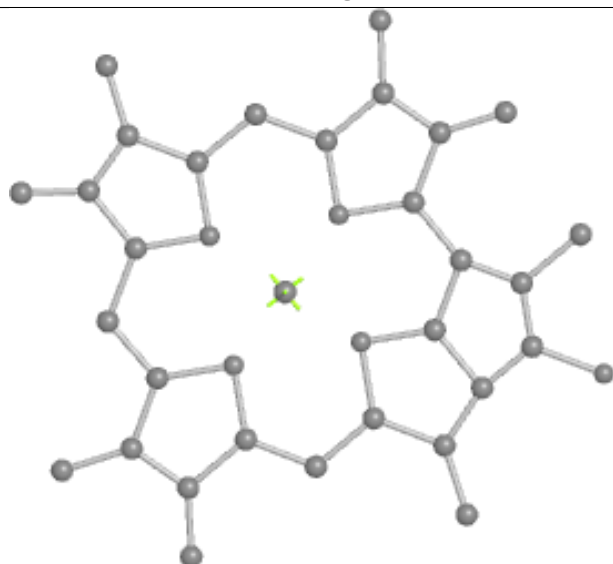
Ligand CLA F 1240



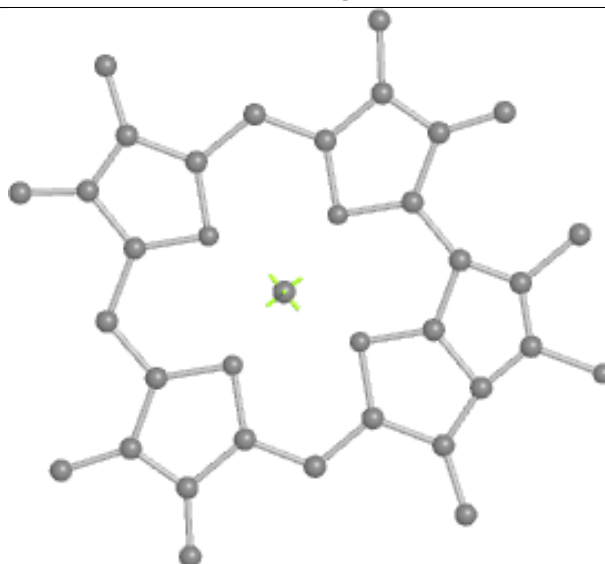
Bond lengths



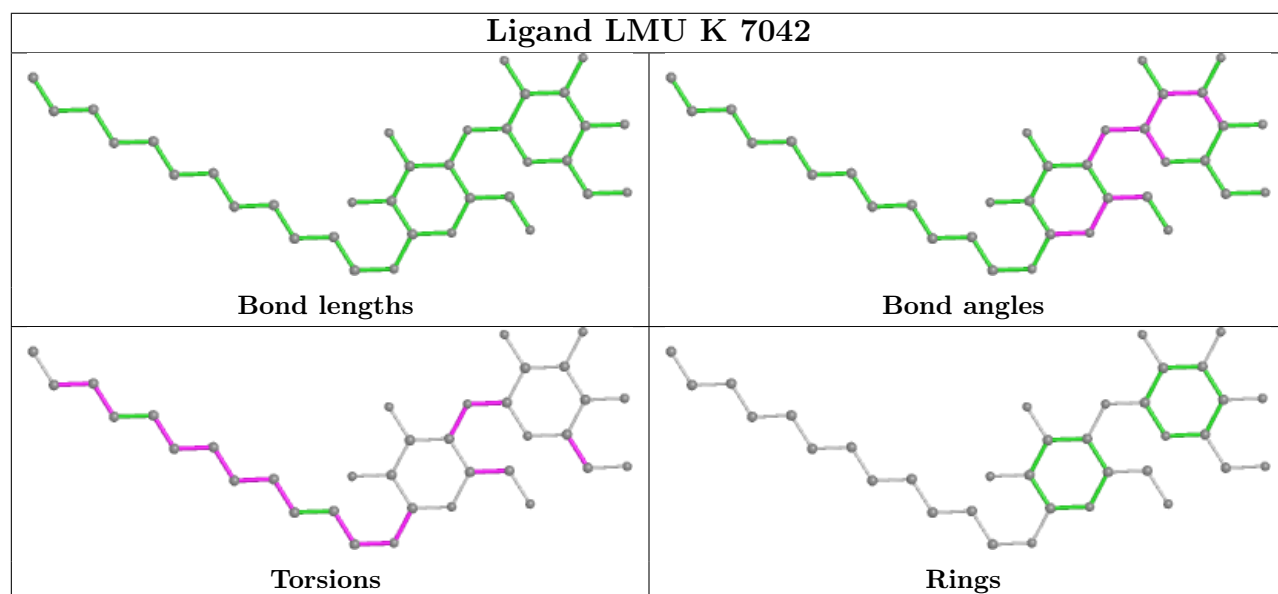
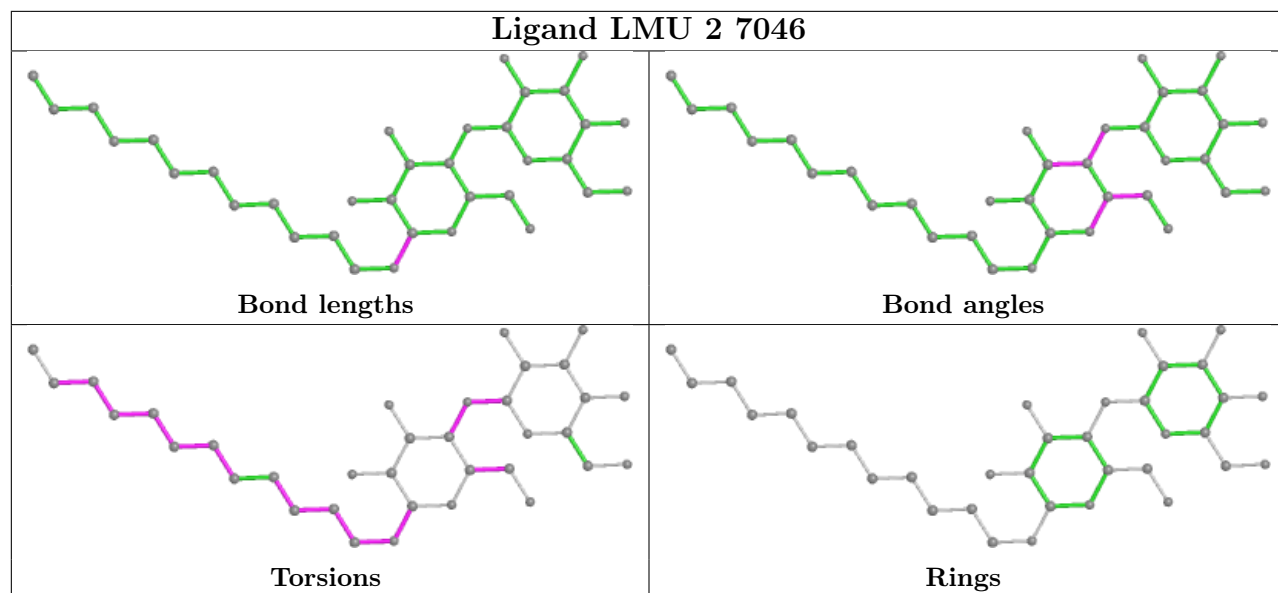
Bond angles

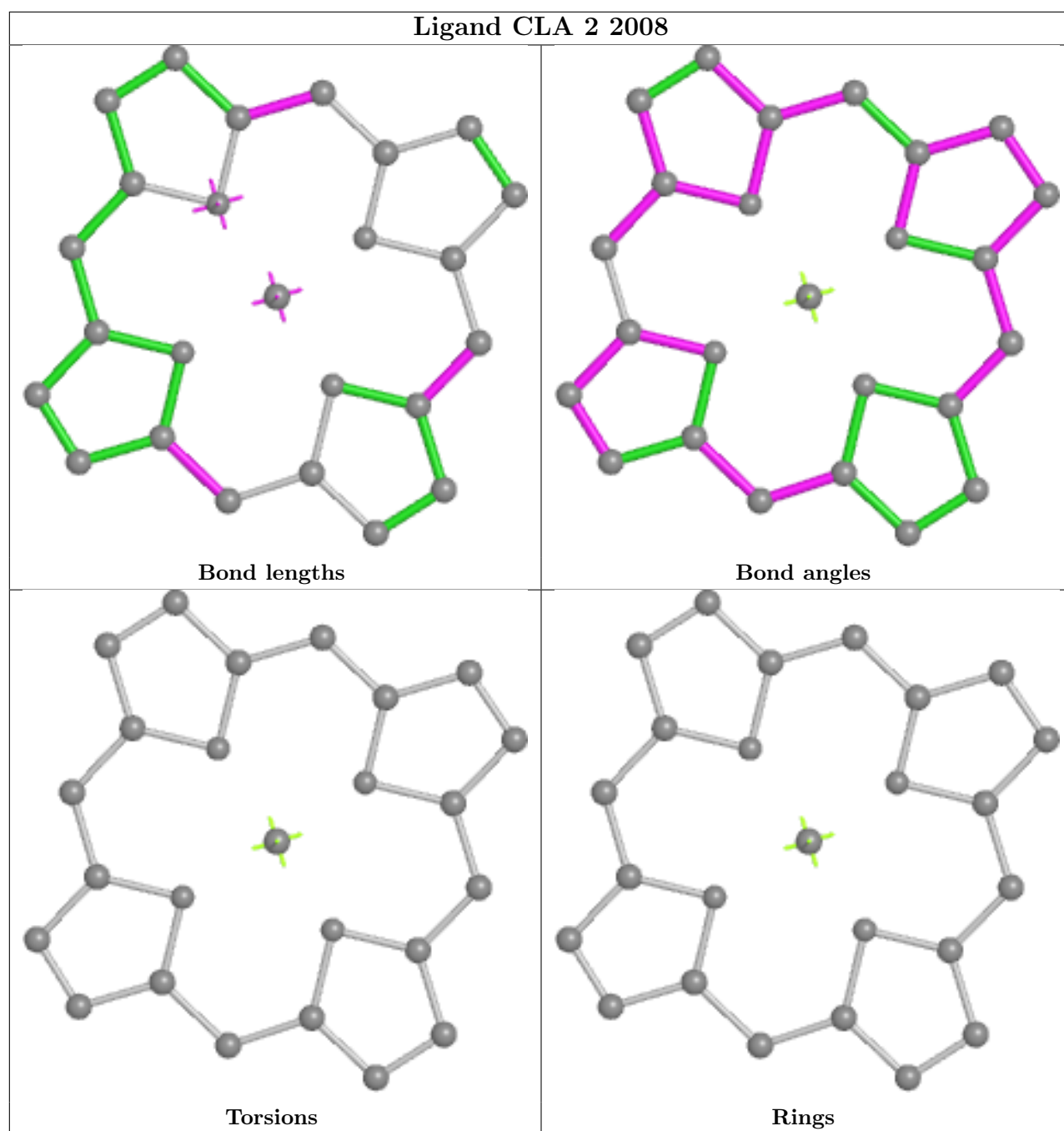


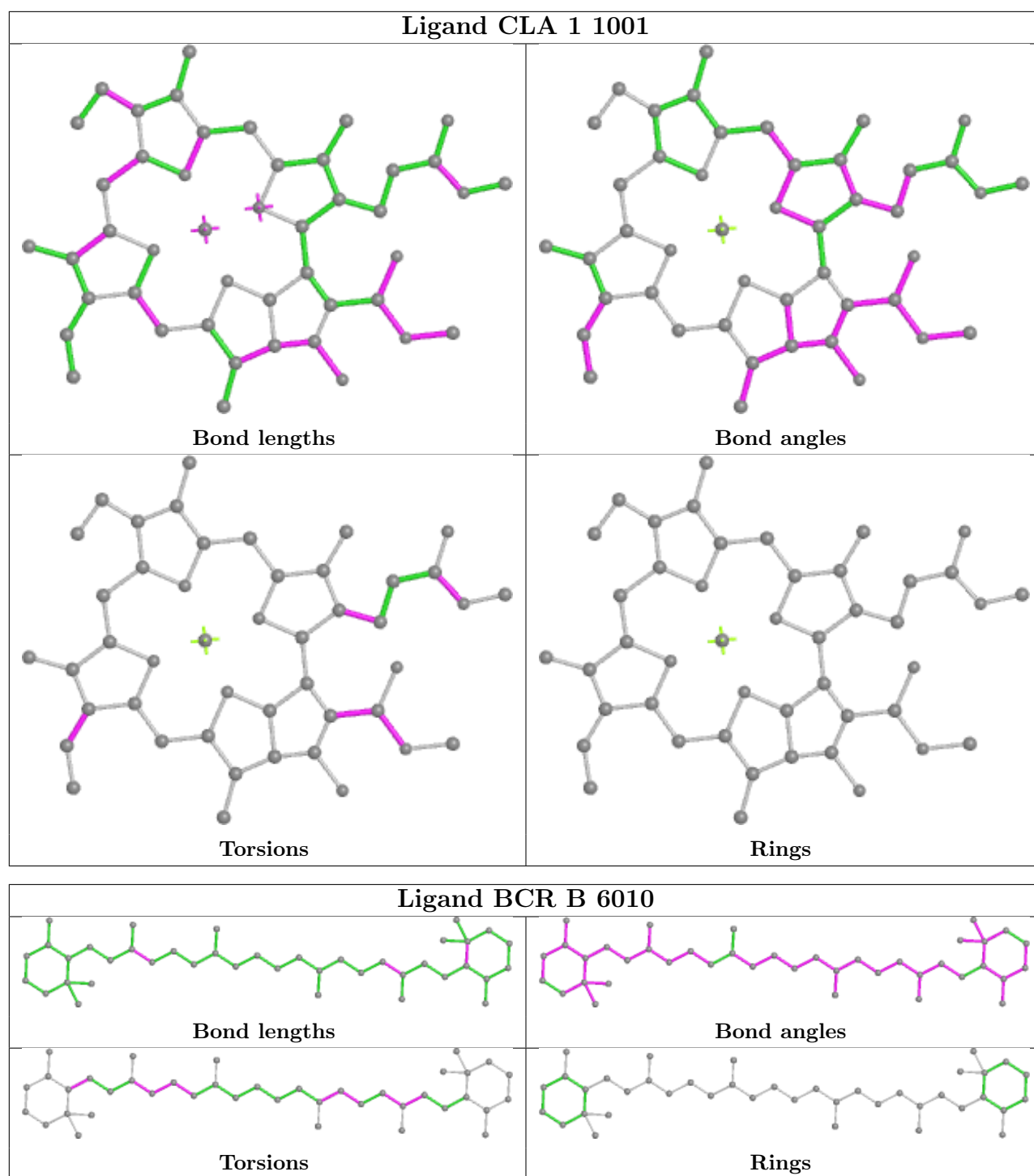
Torsions

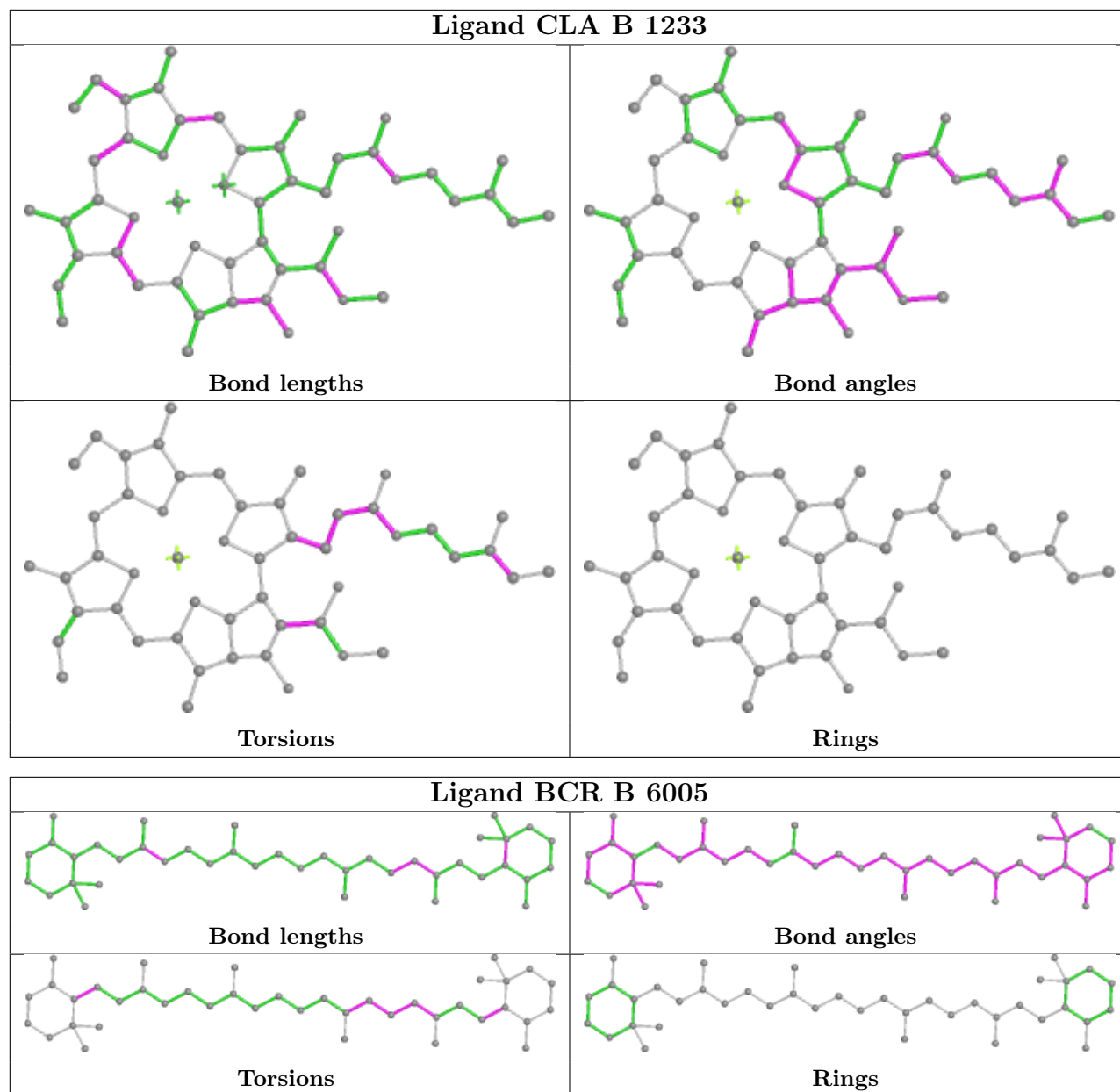


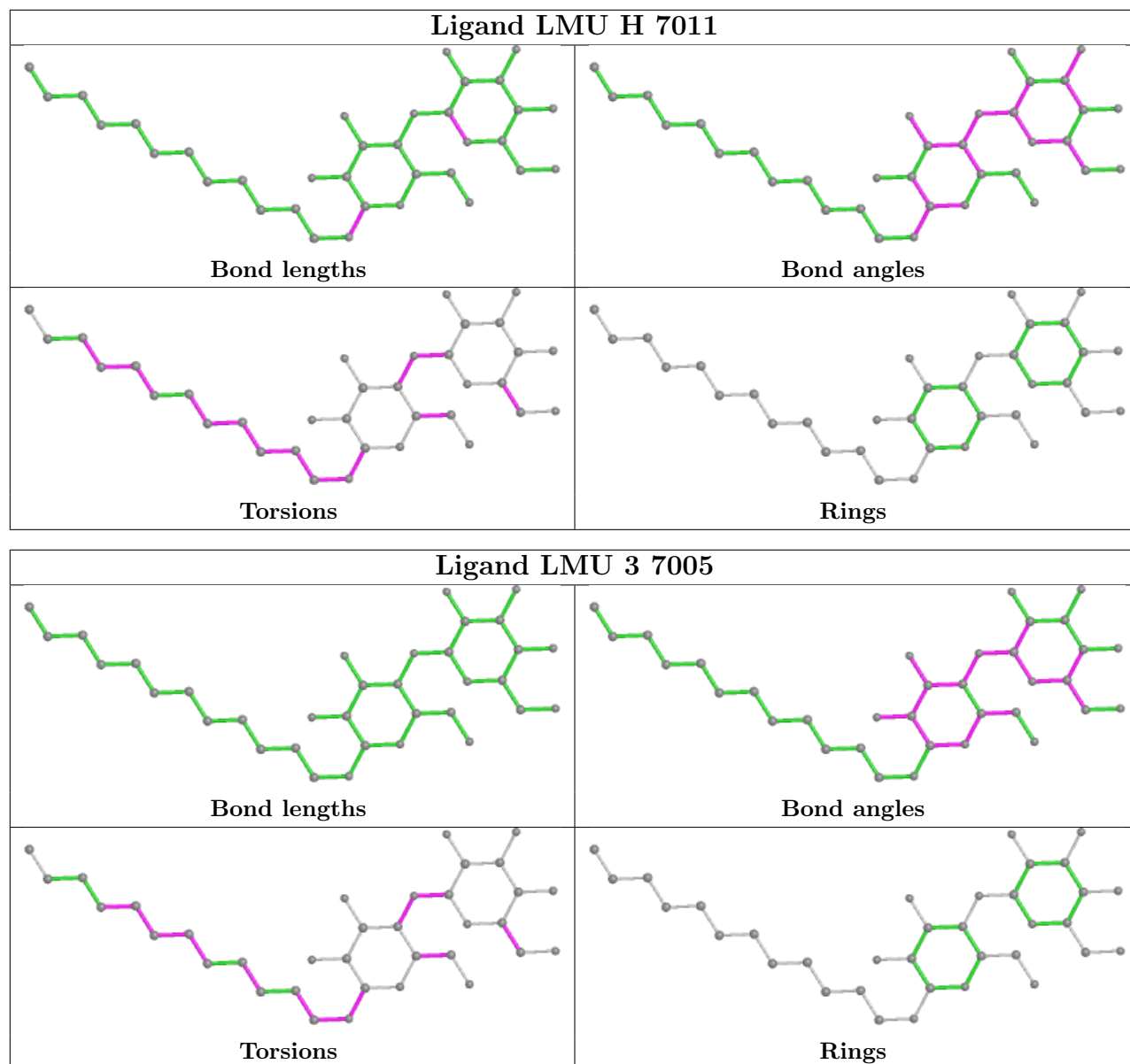
Rings



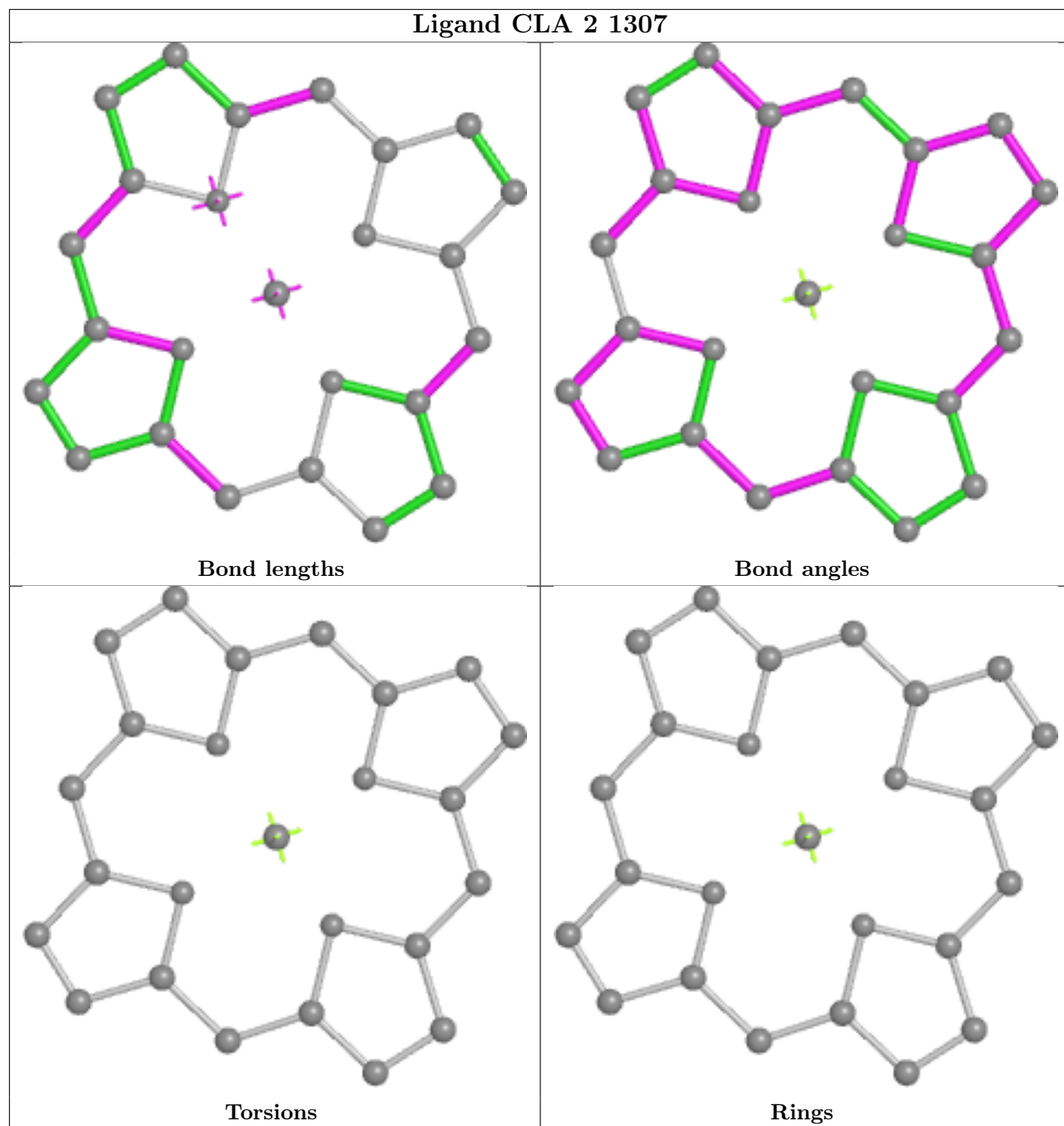




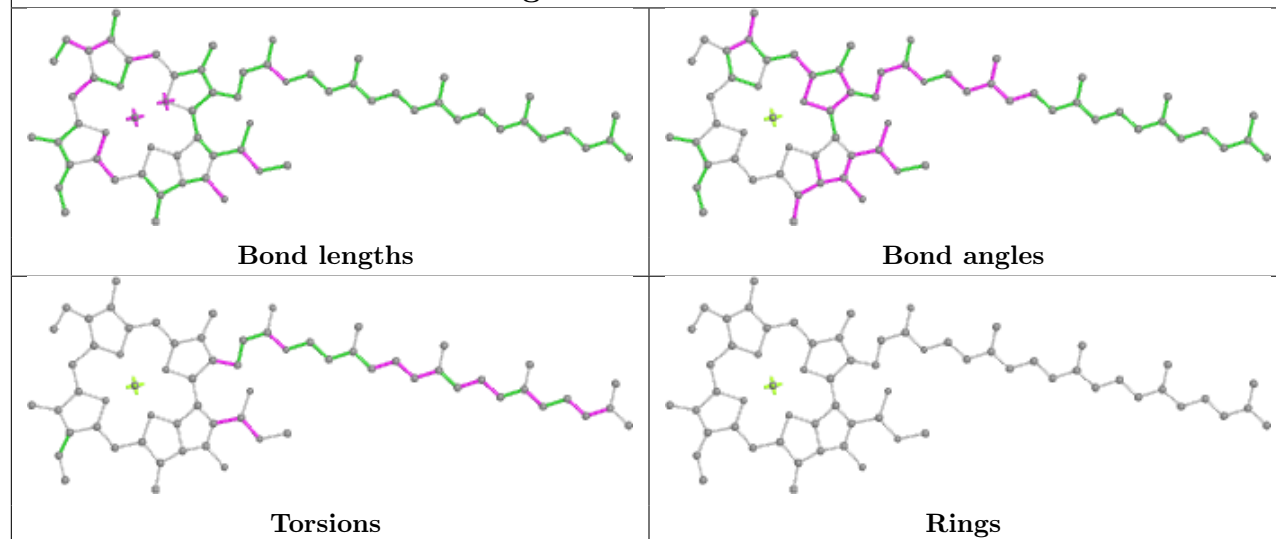




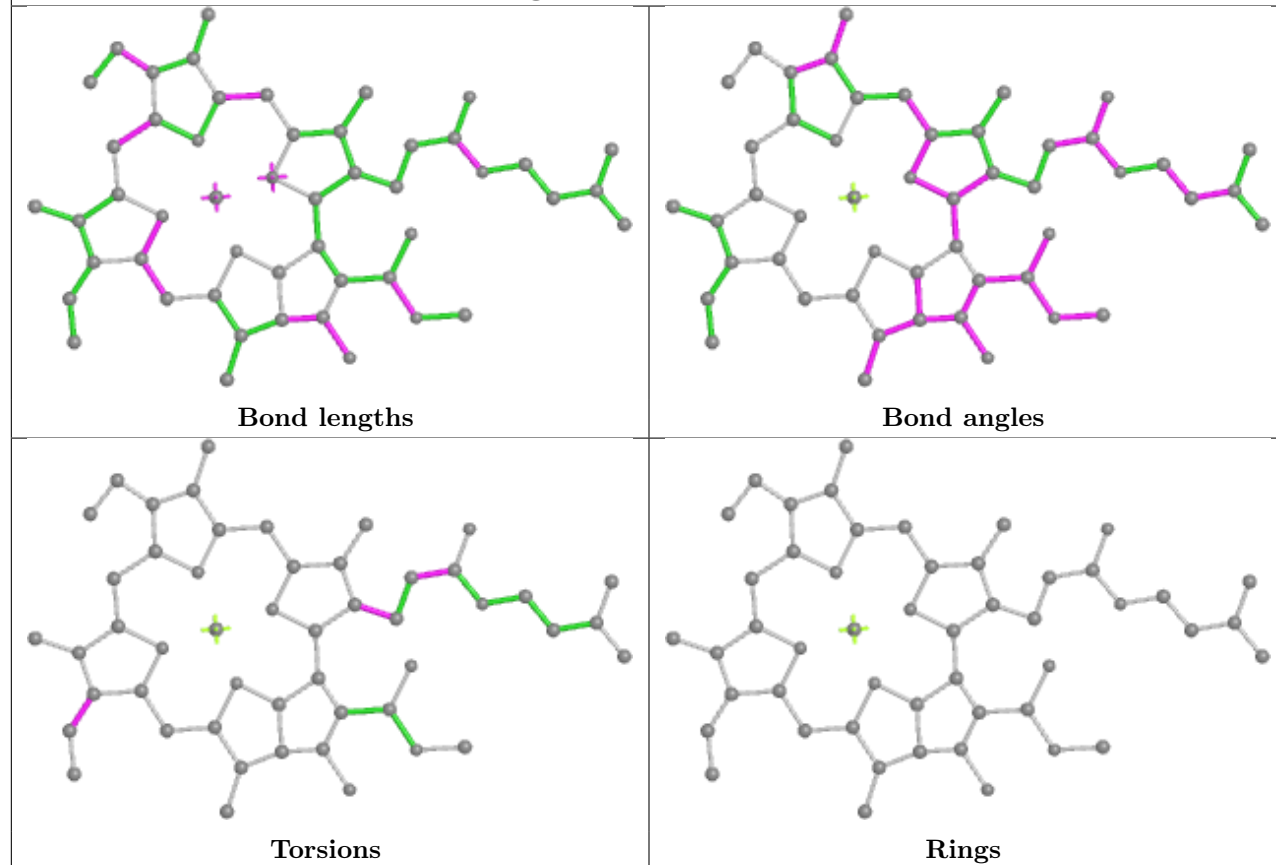
Ligand CLA 2 1307

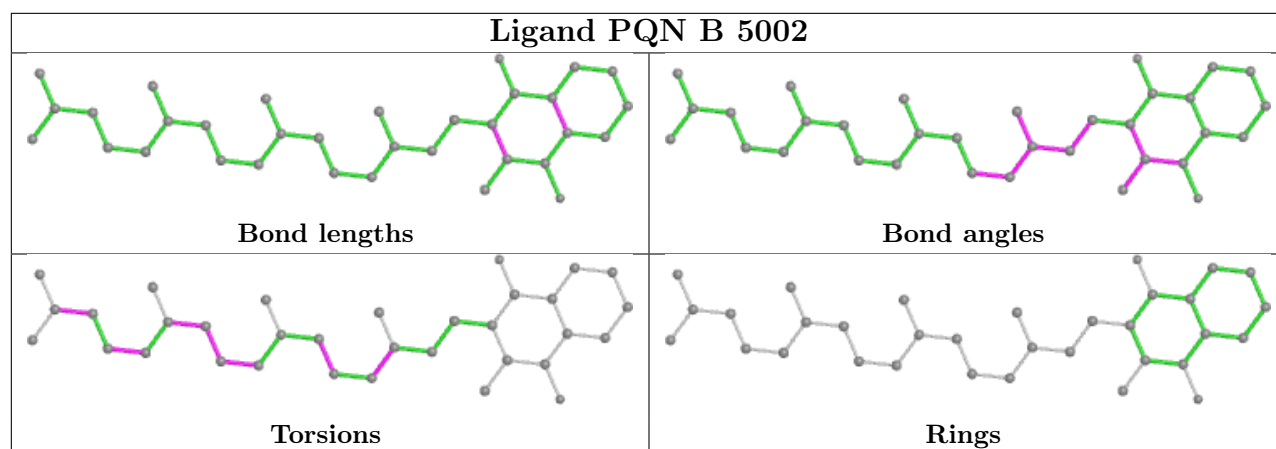
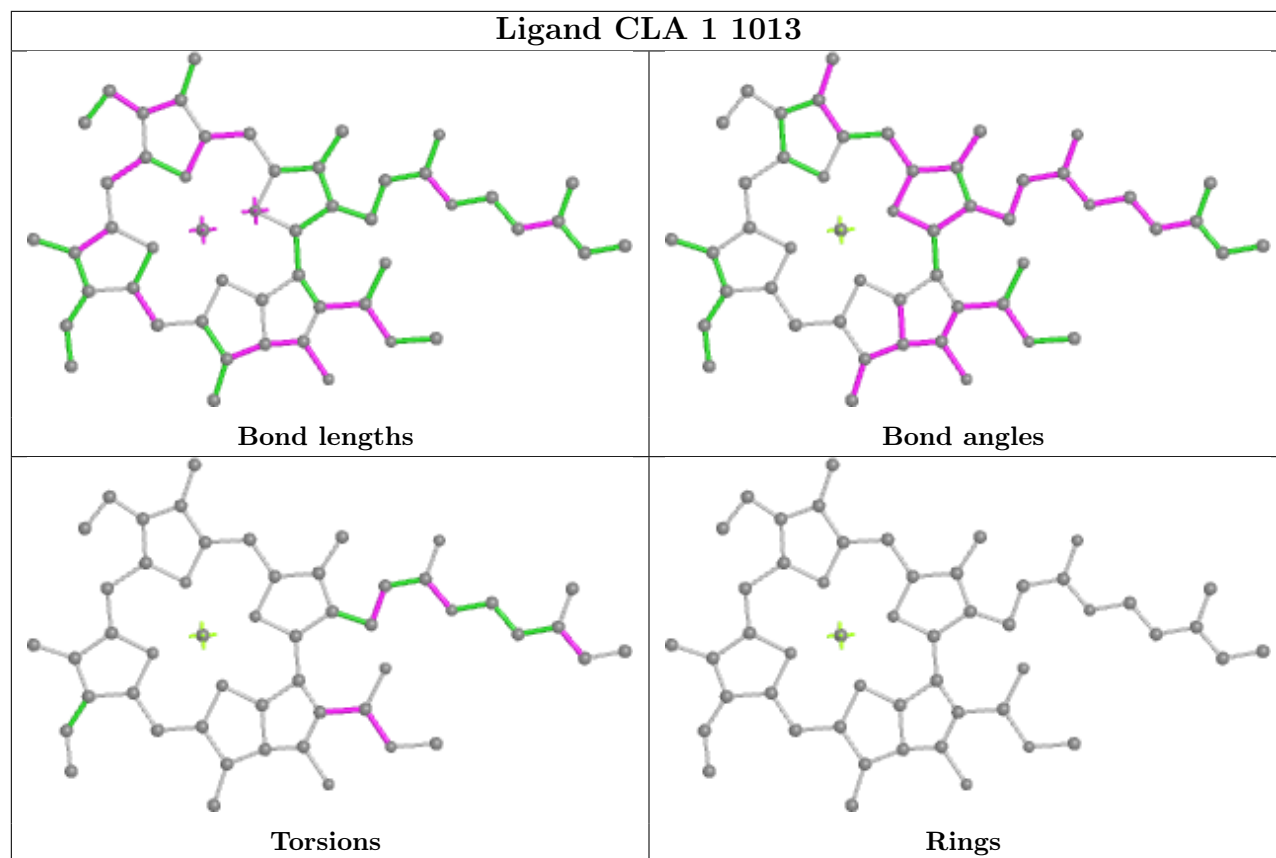


Ligand CLA A 1117

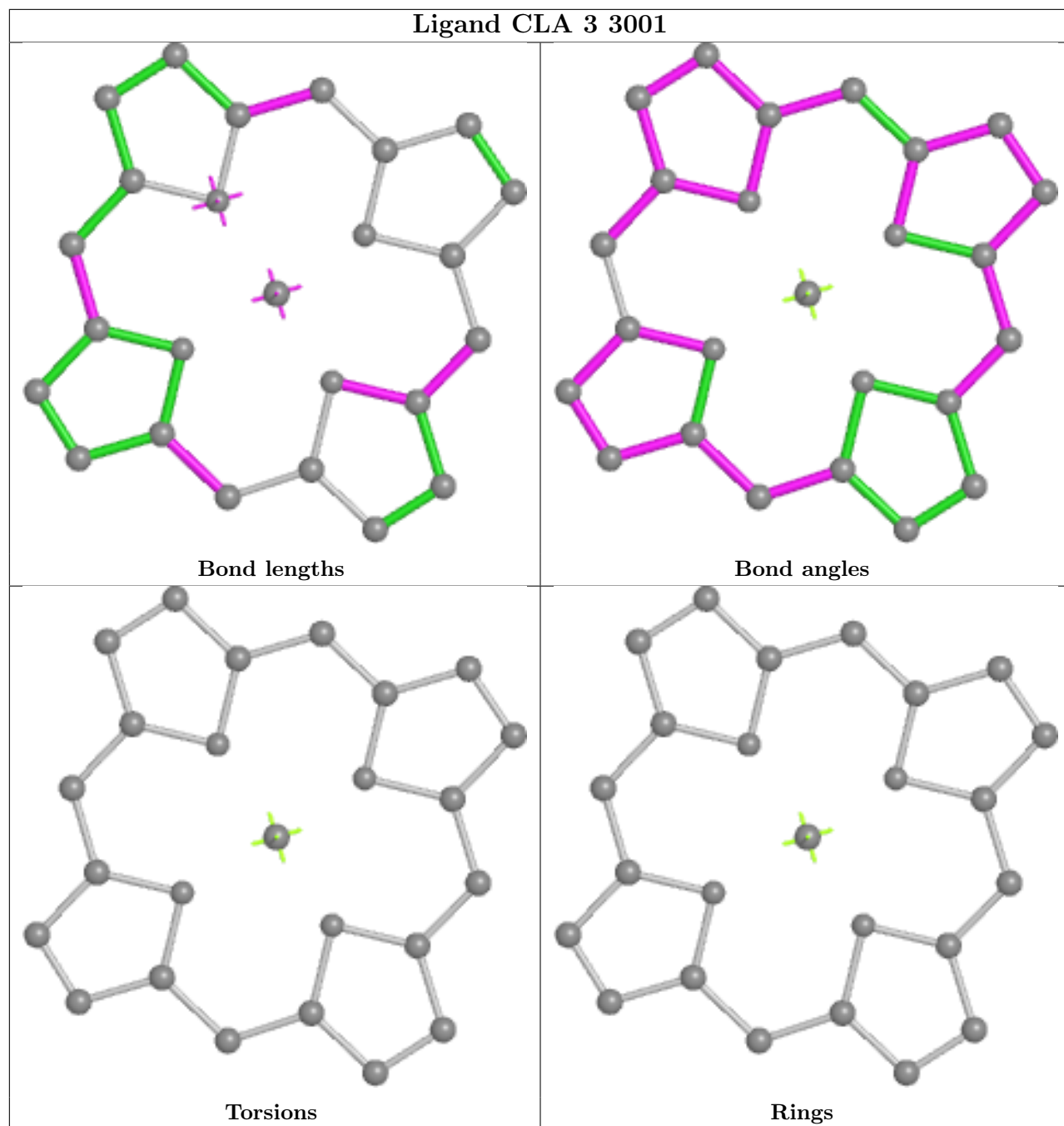


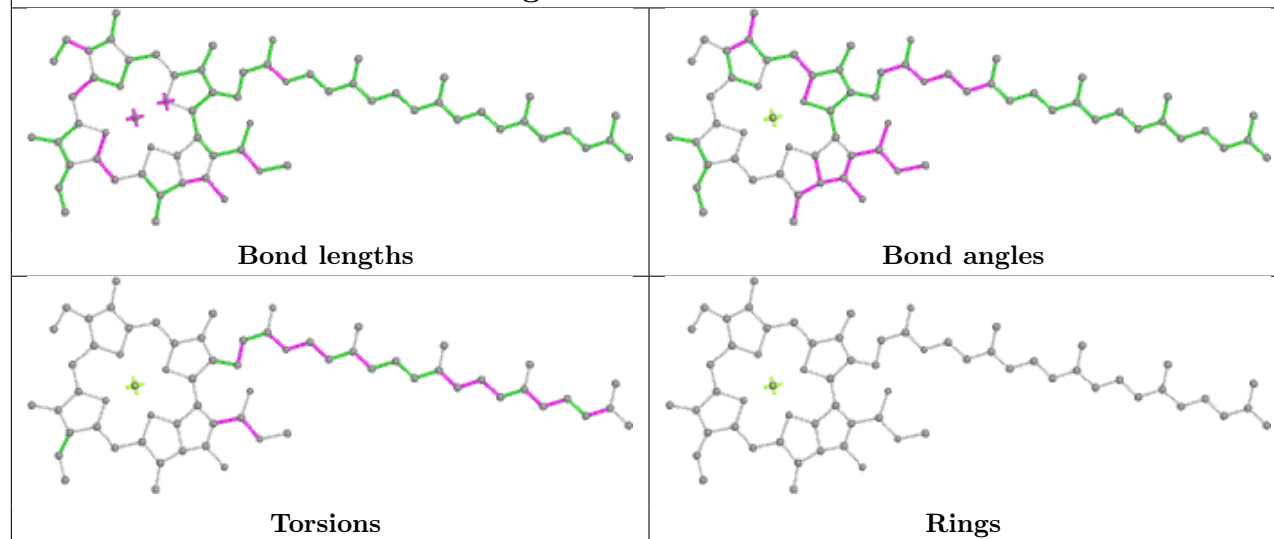
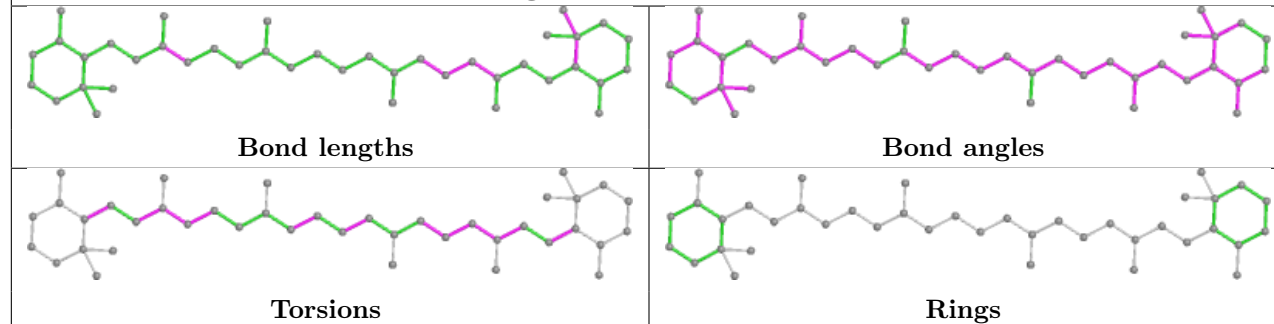
Ligand CLA 3 3008



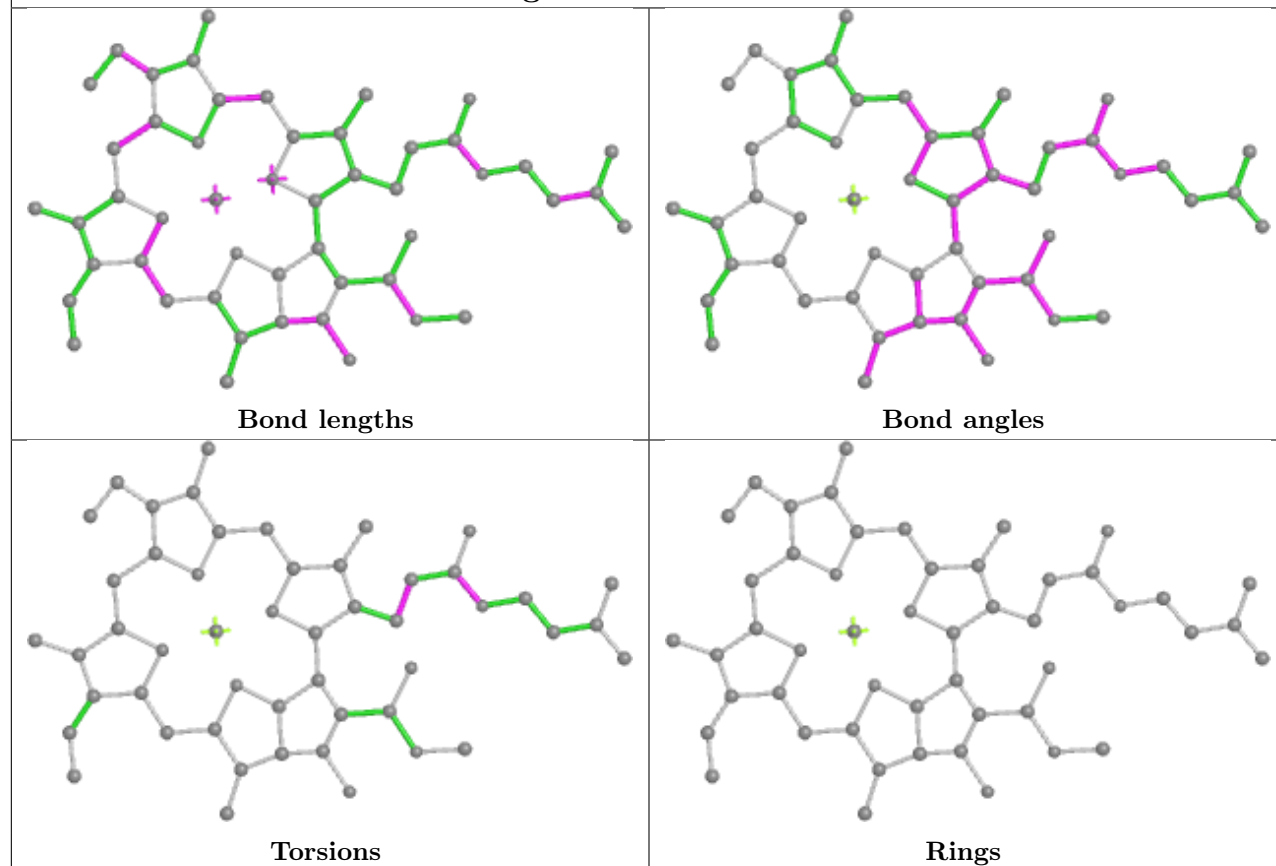


Ligand CLA 3 3001

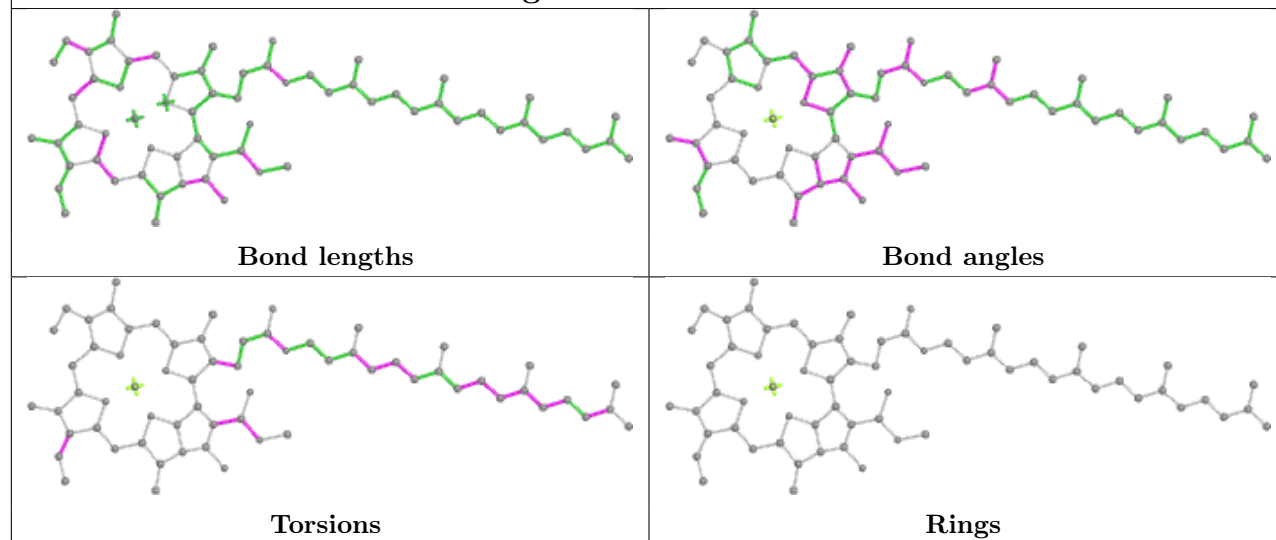


Ligand CLA H 1207**Ligand BCR F 6014**

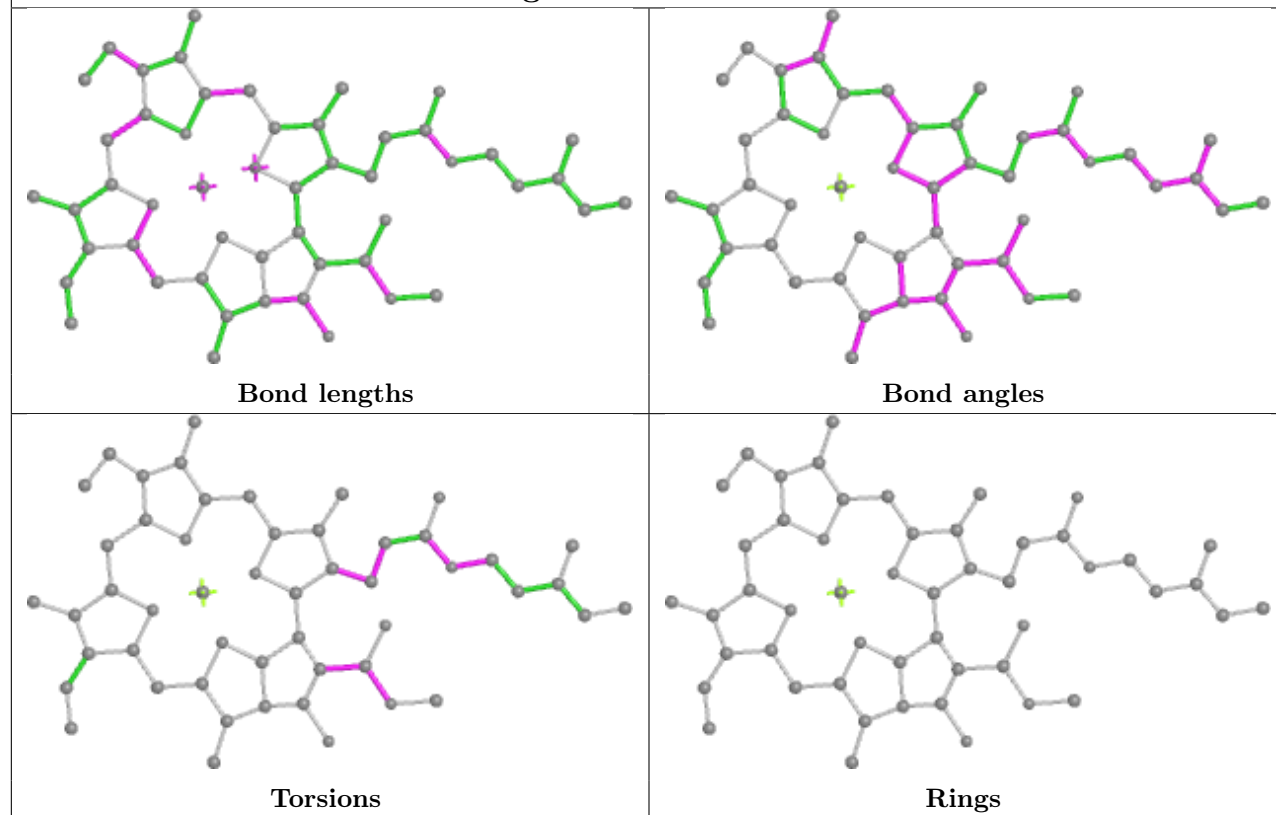
Ligand CLA A 1129



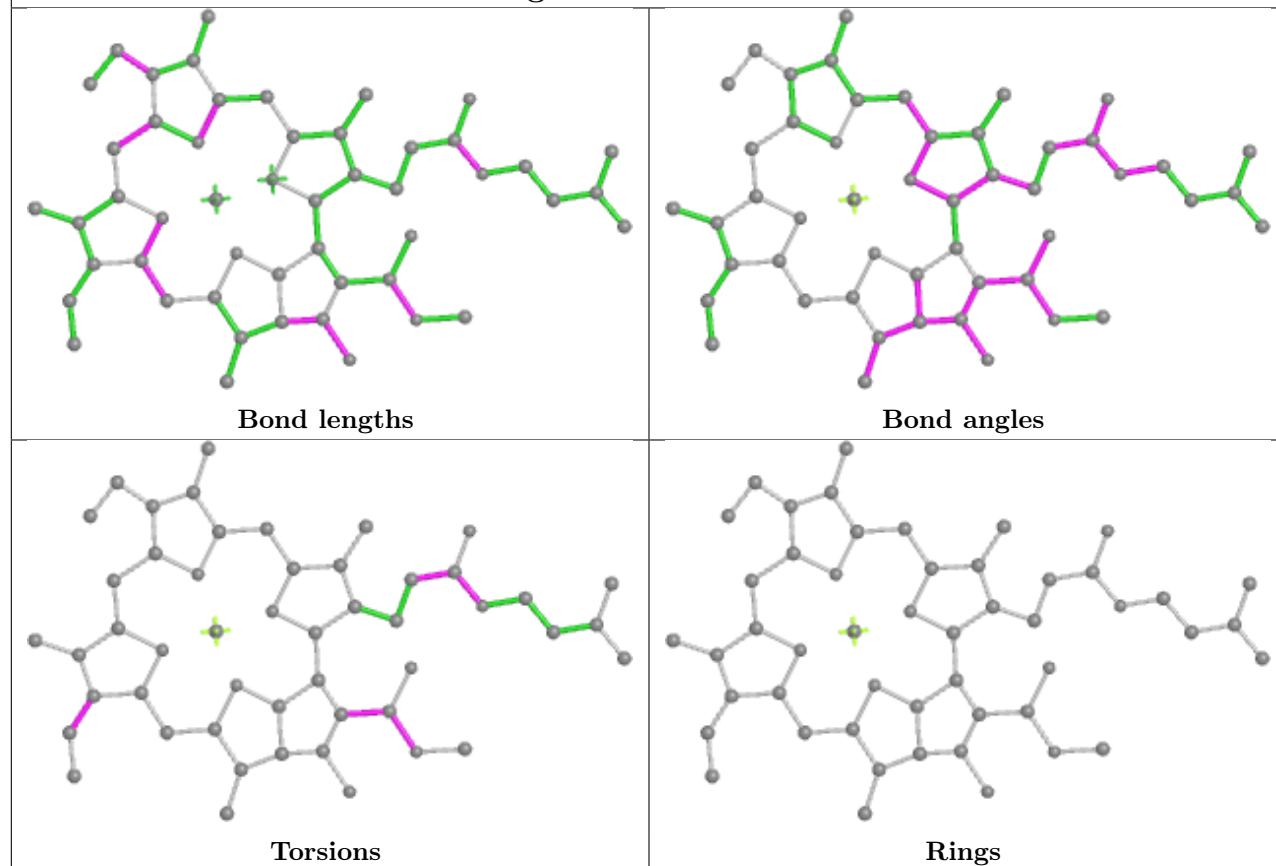
Ligand CLA A 1132

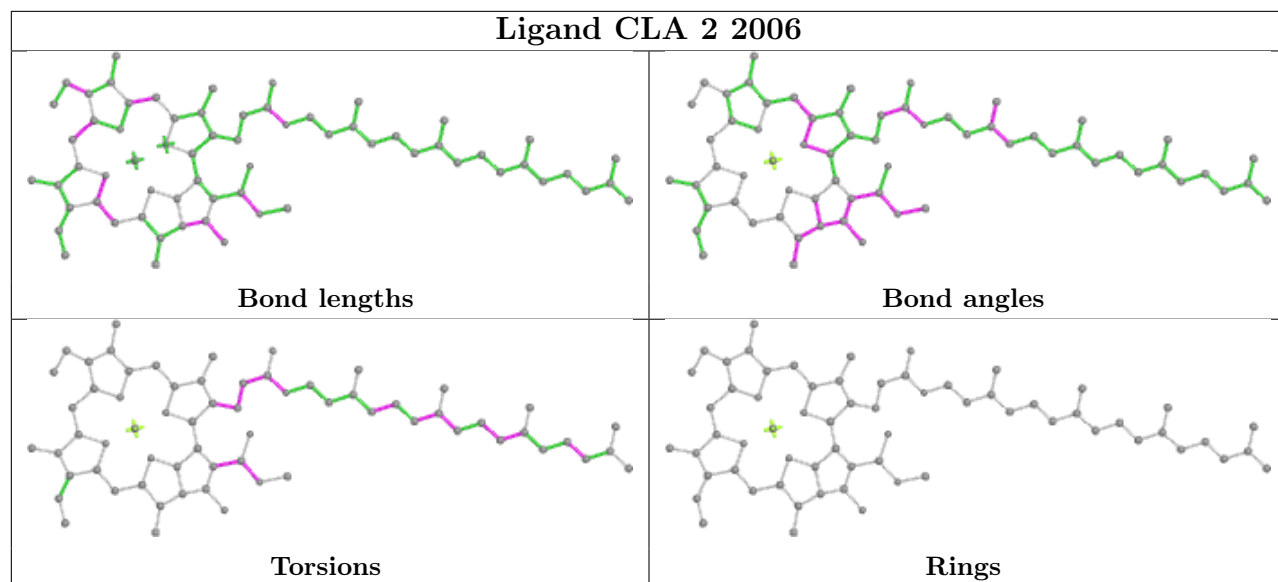


Ligand CLA A 1135

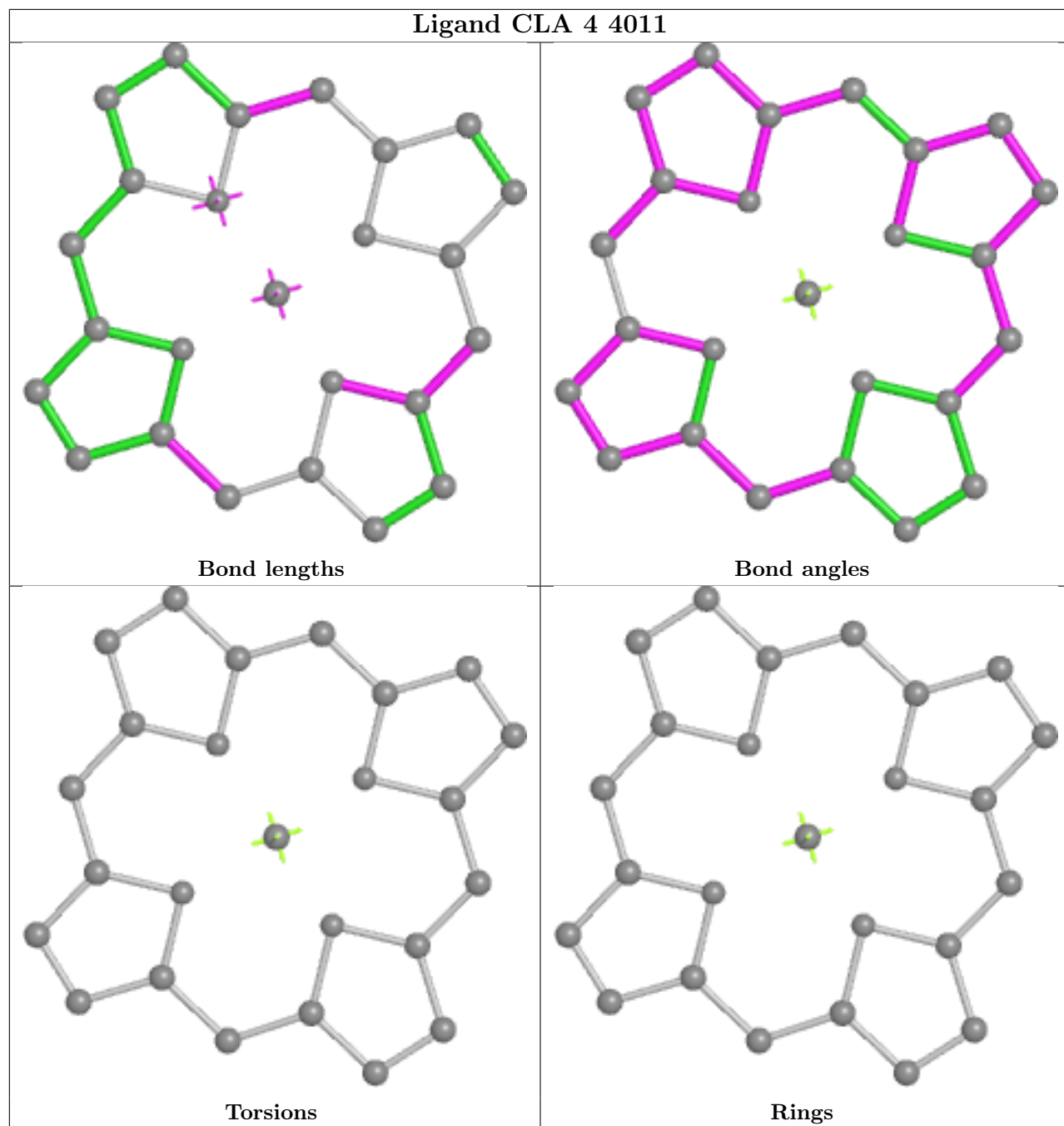


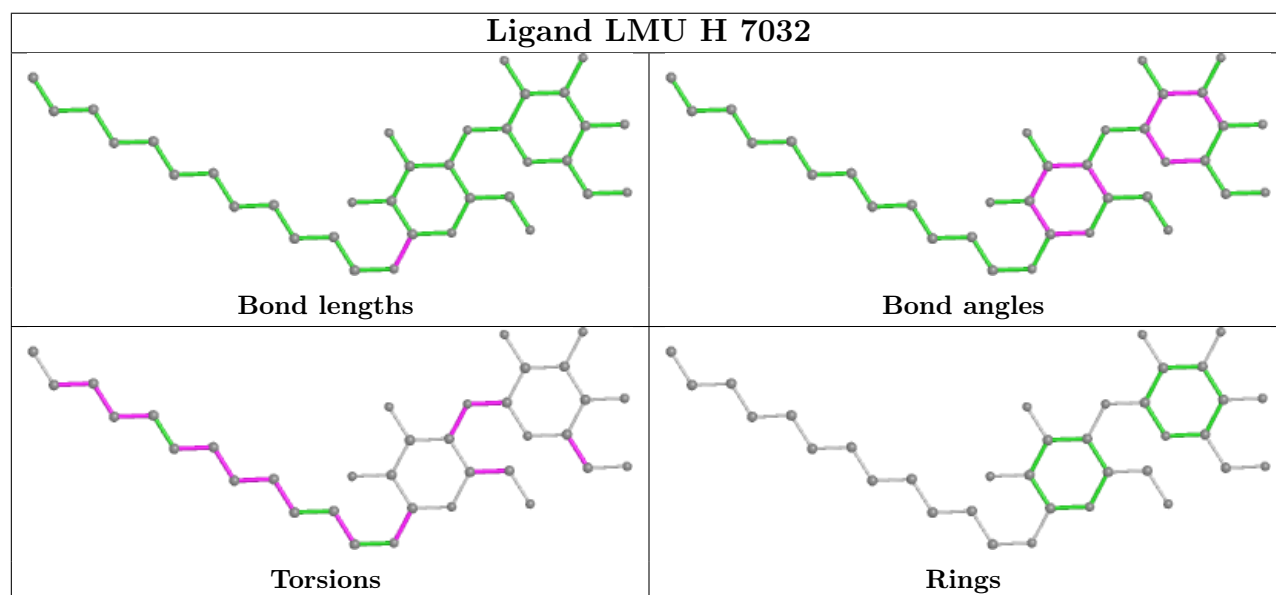
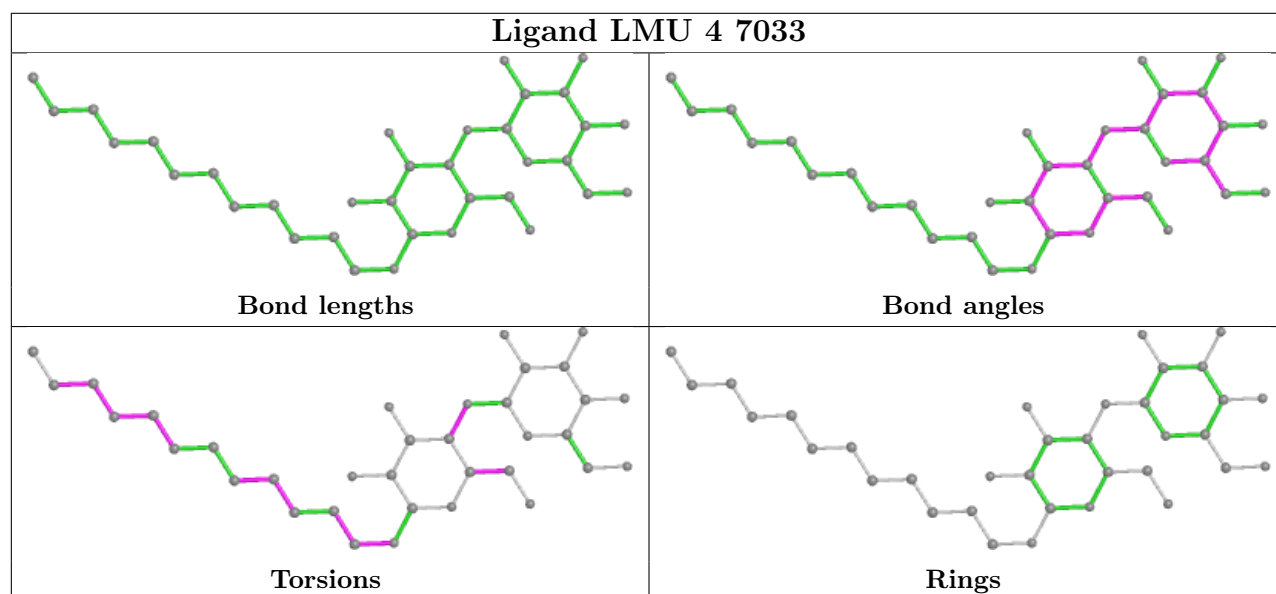
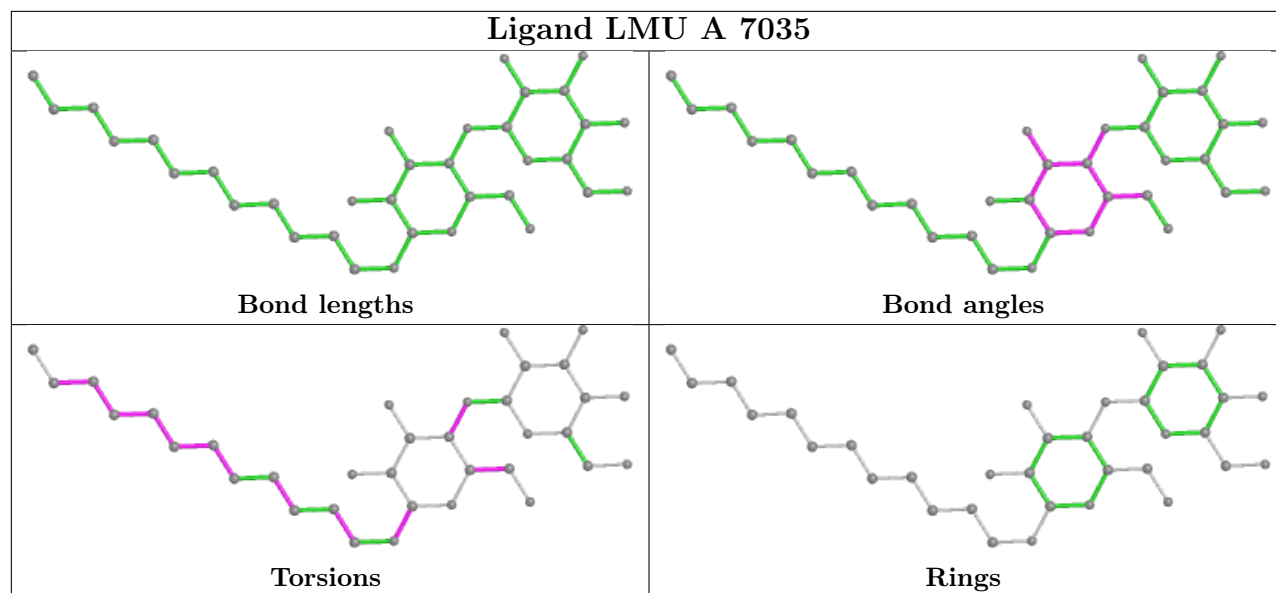
Ligand CLA 2 2013



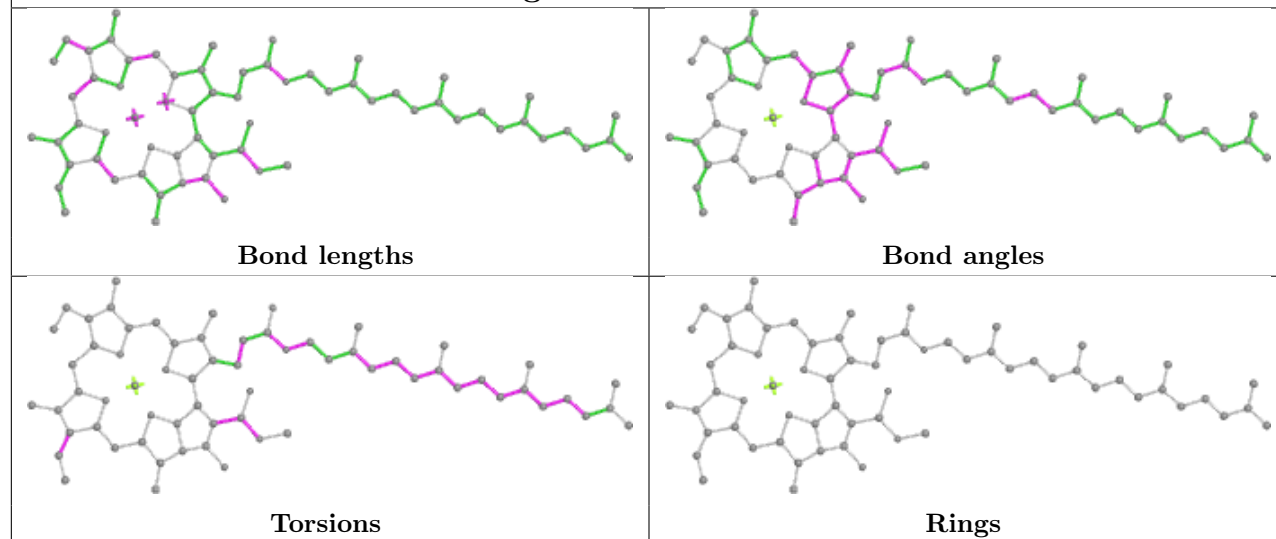


Ligand CLA 4 4011

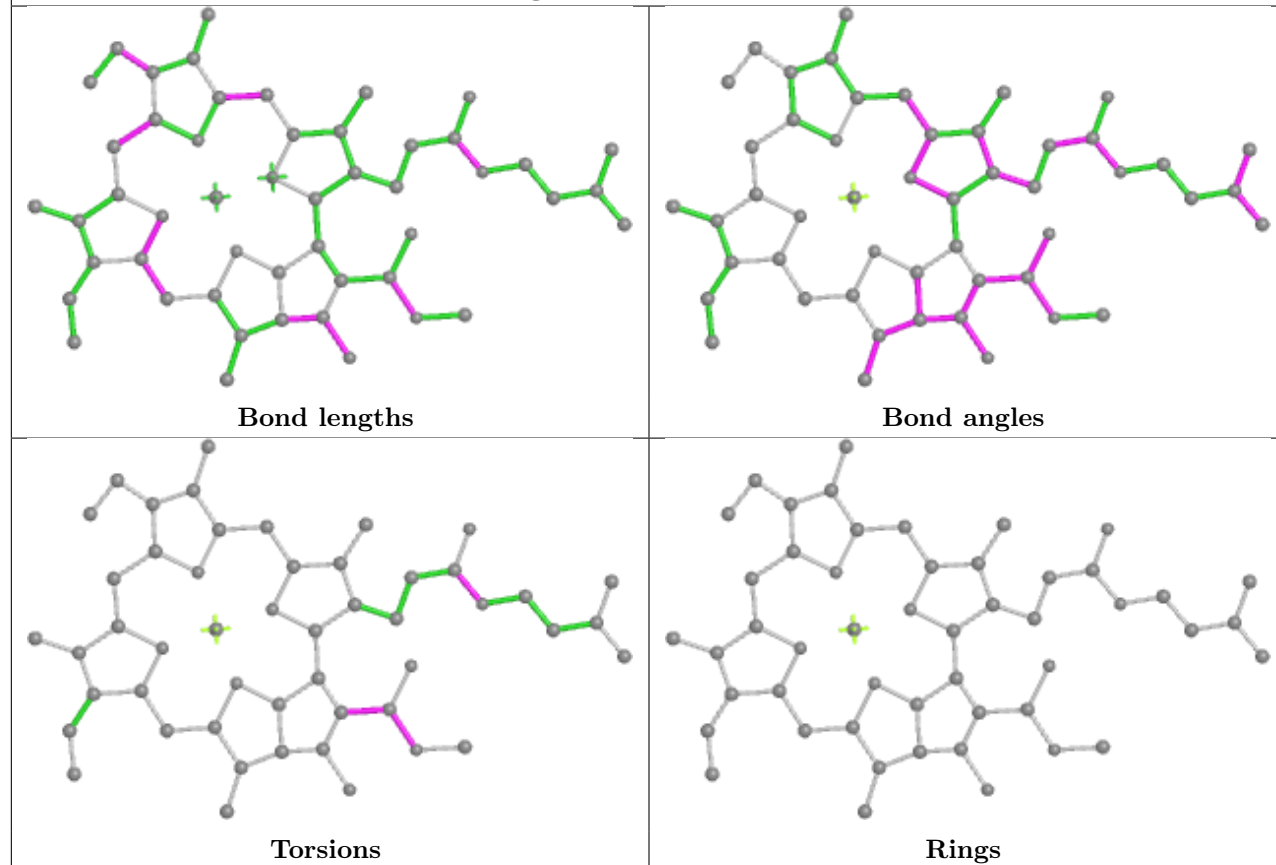




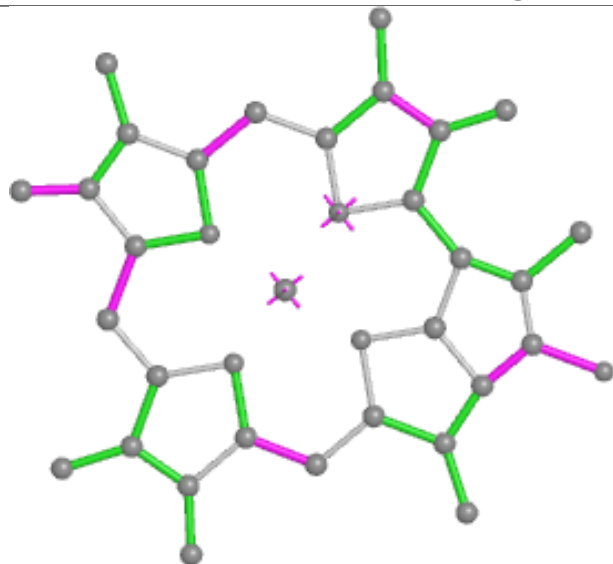
Ligand CLA B 1226



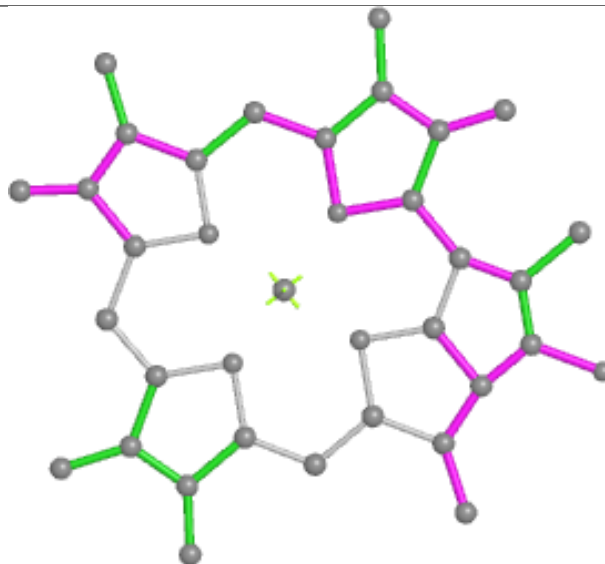
Ligand CLA 2 2012



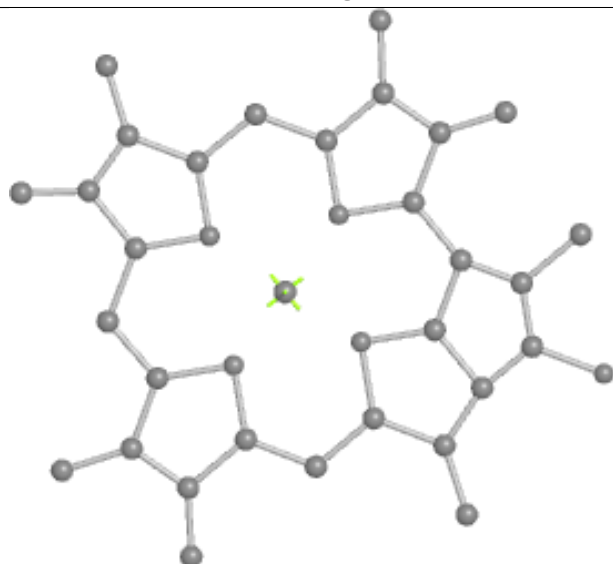
Ligand CLA 4 4012



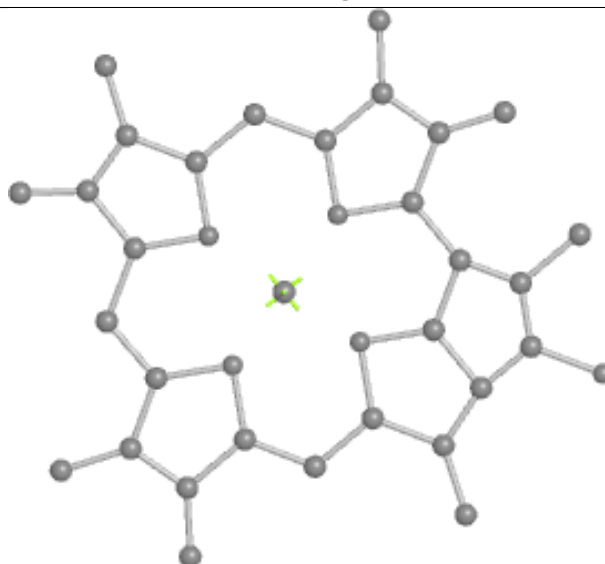
Bond lengths



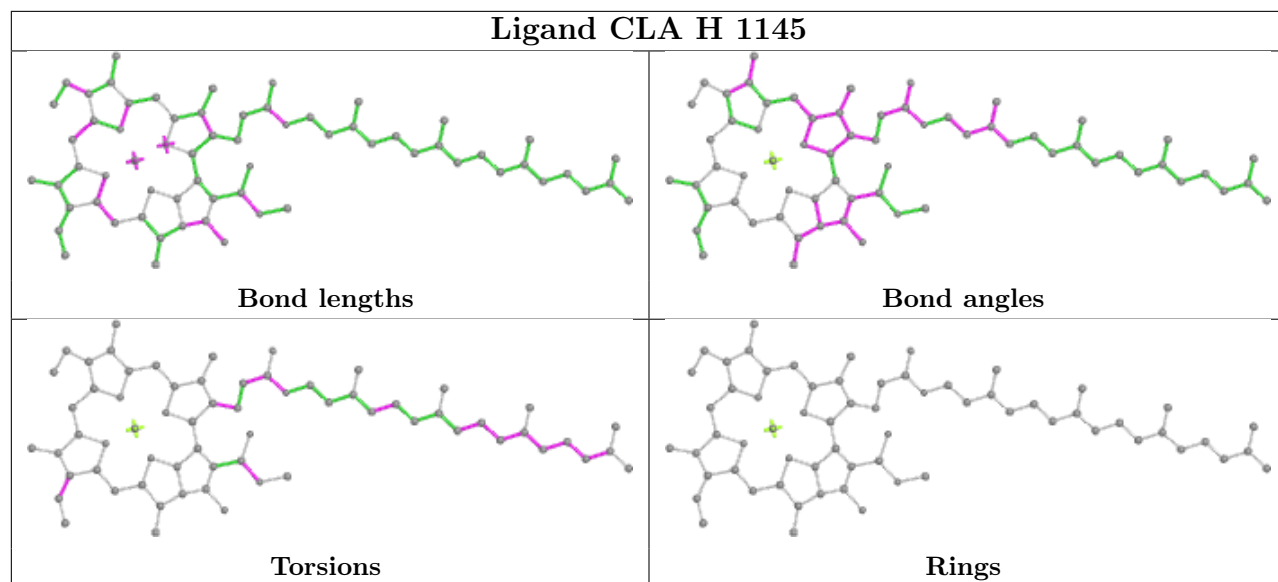
Bond angles



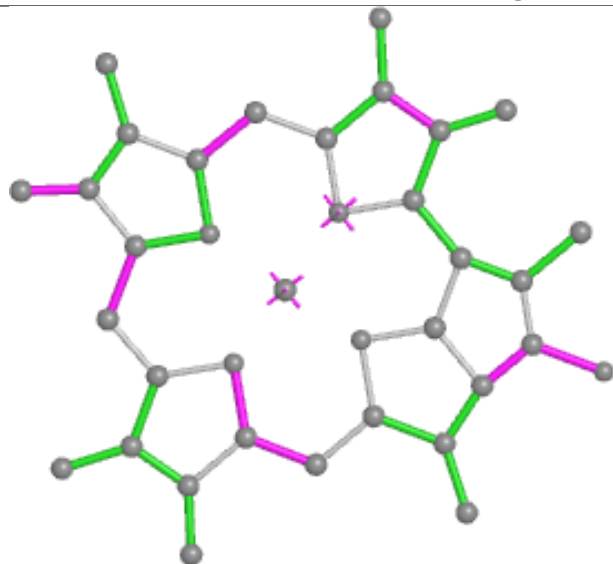
Torsions



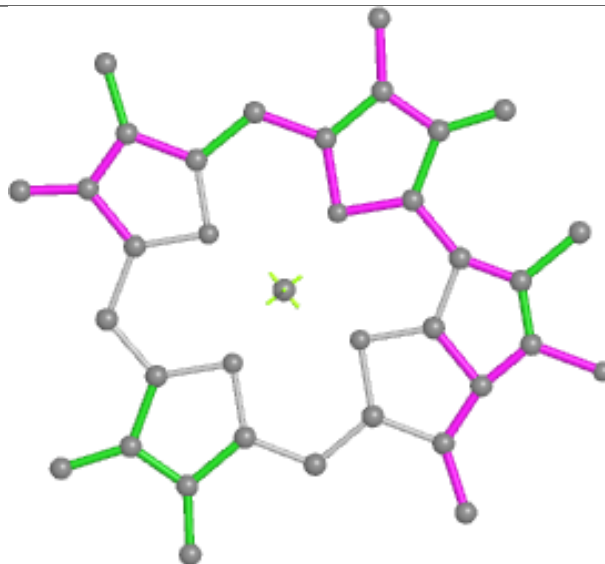
Rings



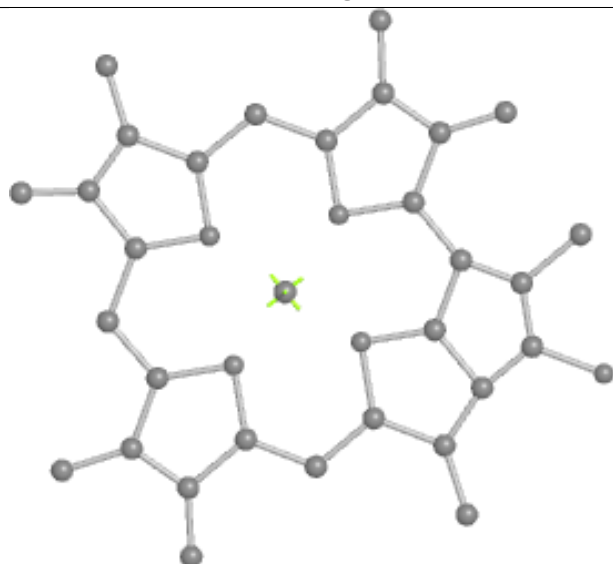
Ligand CLA 1 1006



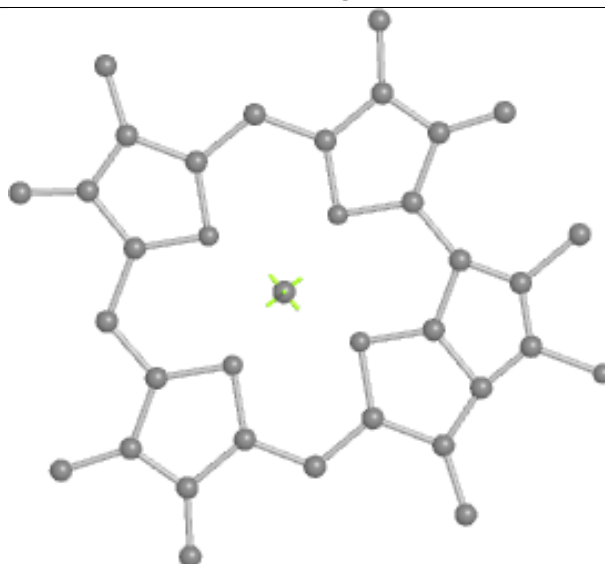
Bond lengths



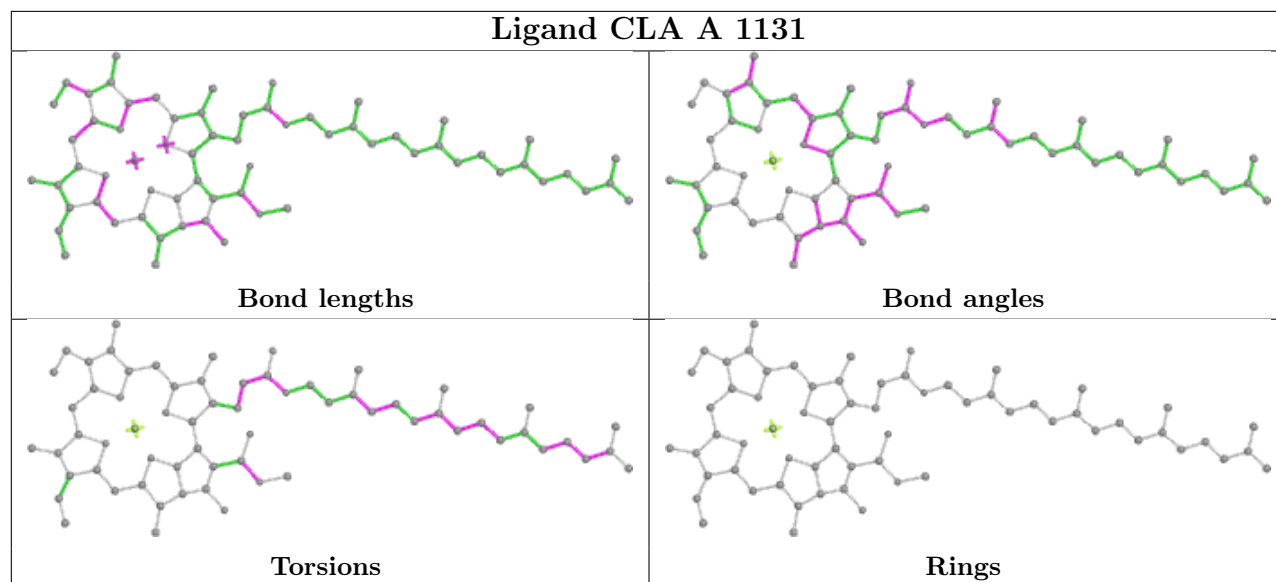
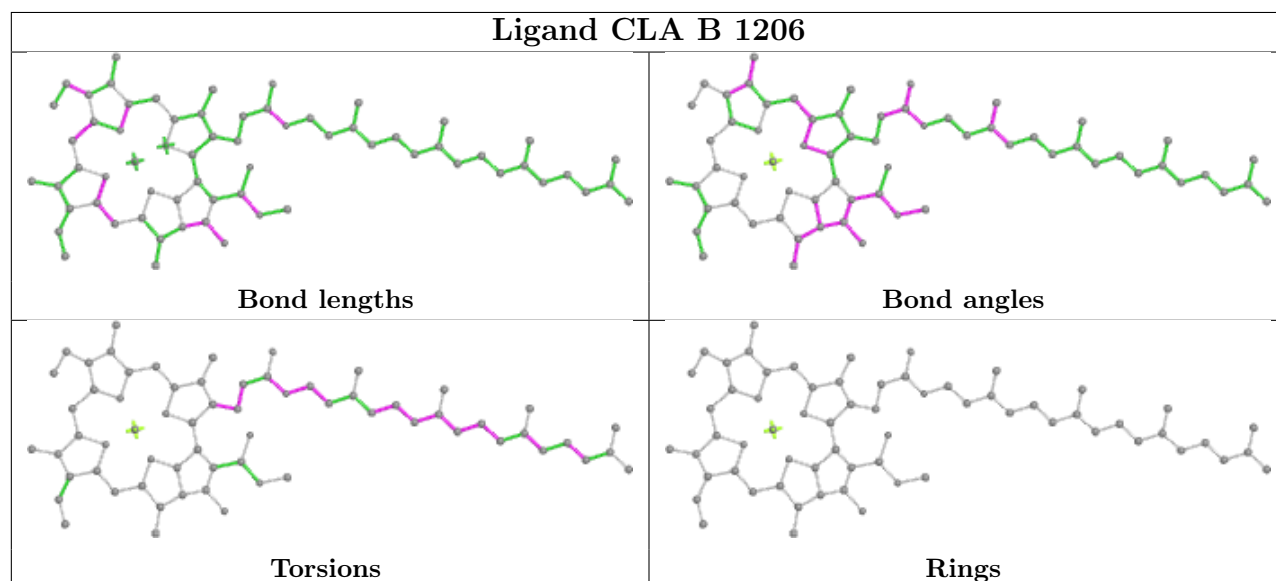
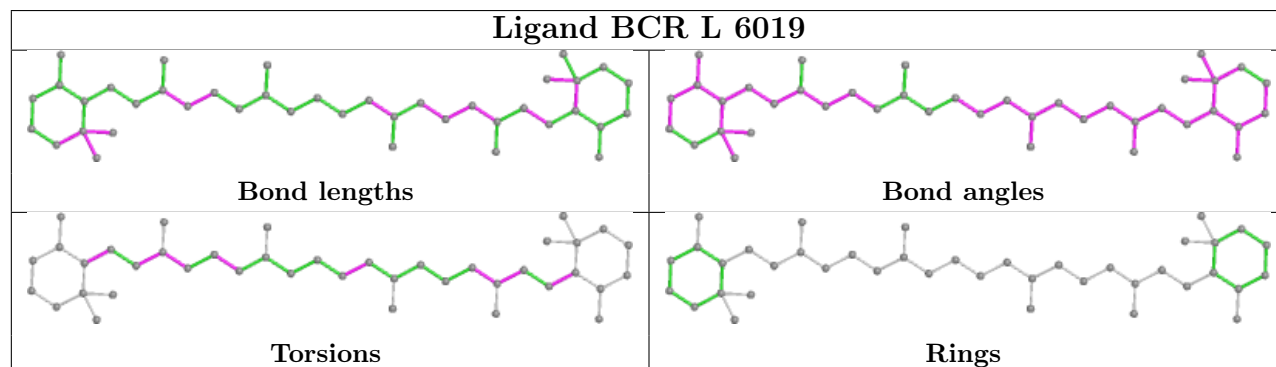
Bond angles

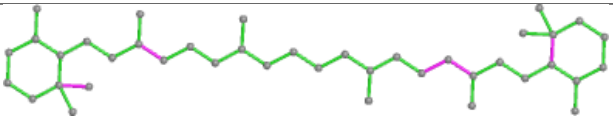
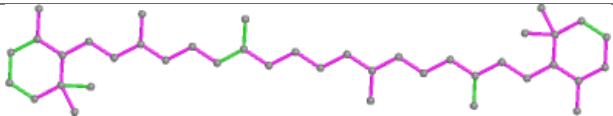
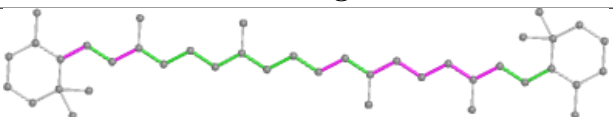
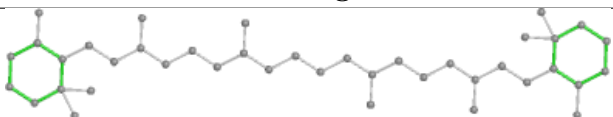
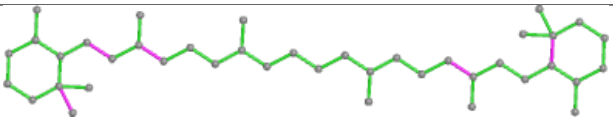
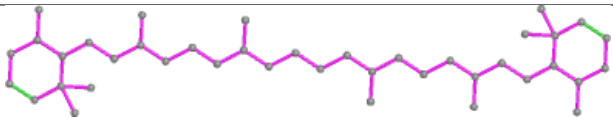
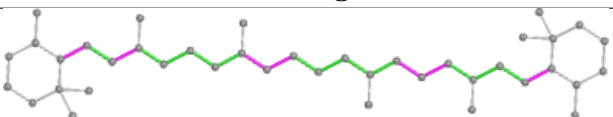
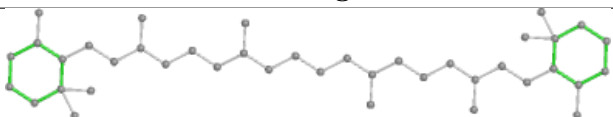
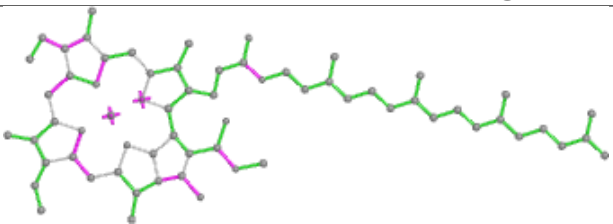
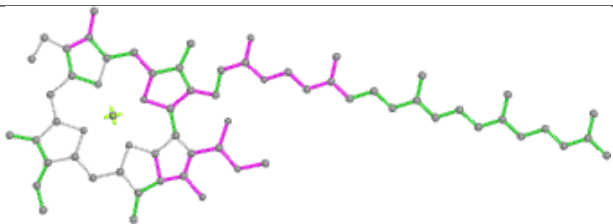
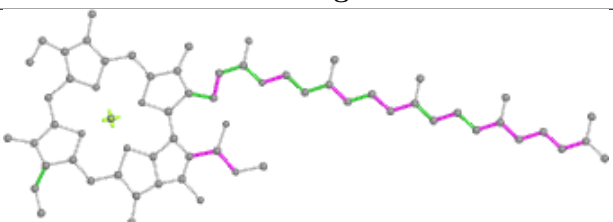
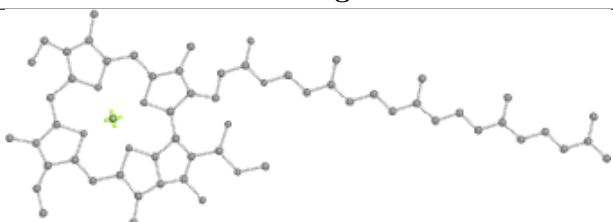


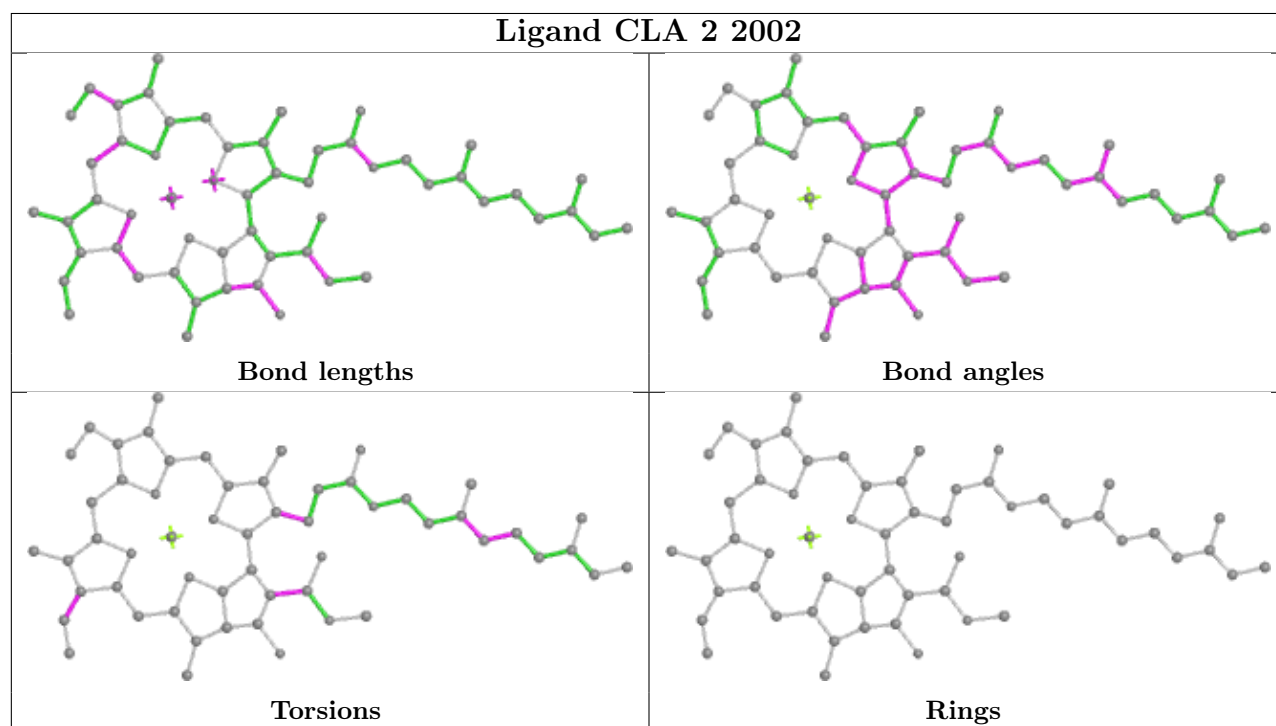
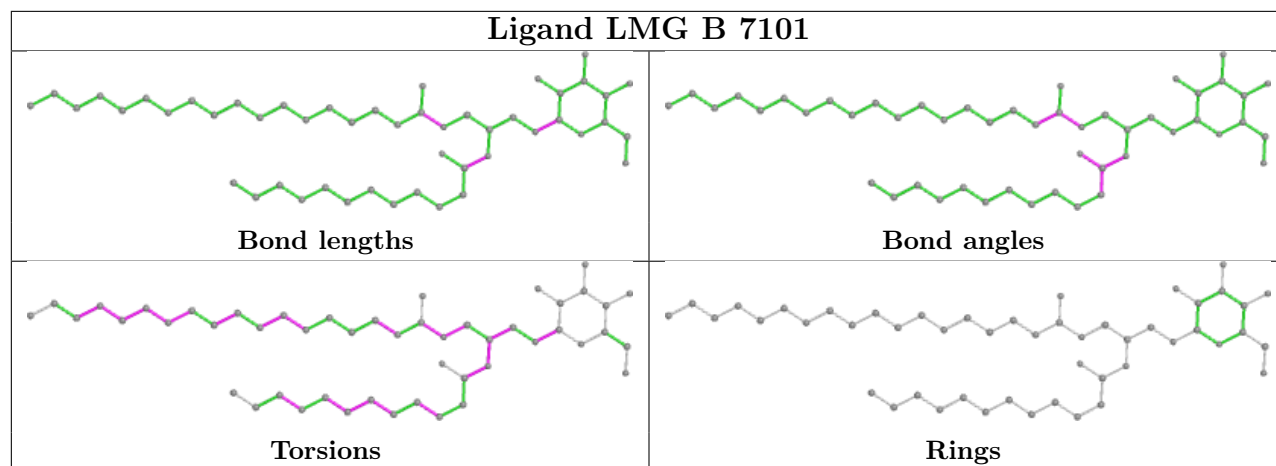
Torsions



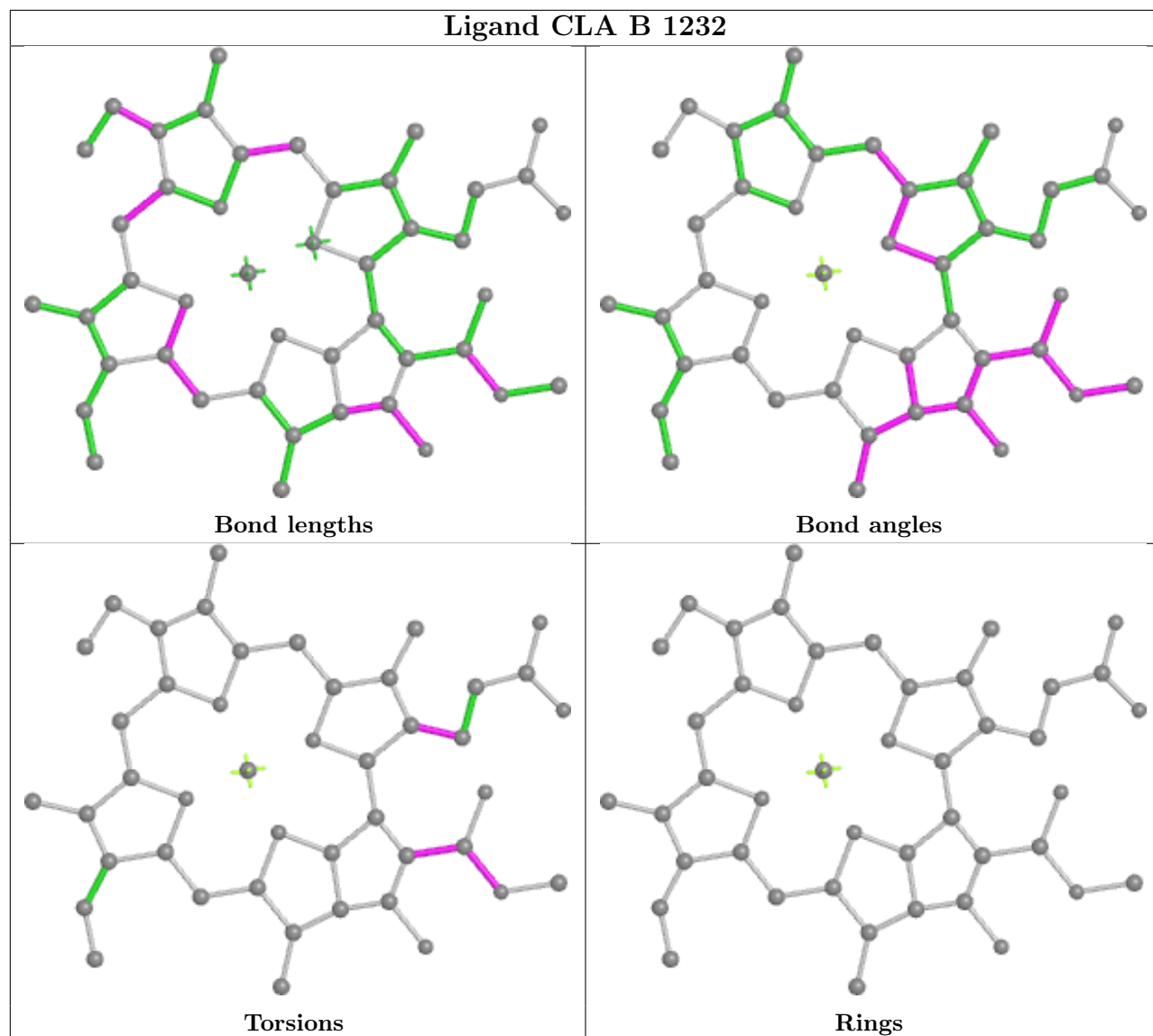
Rings

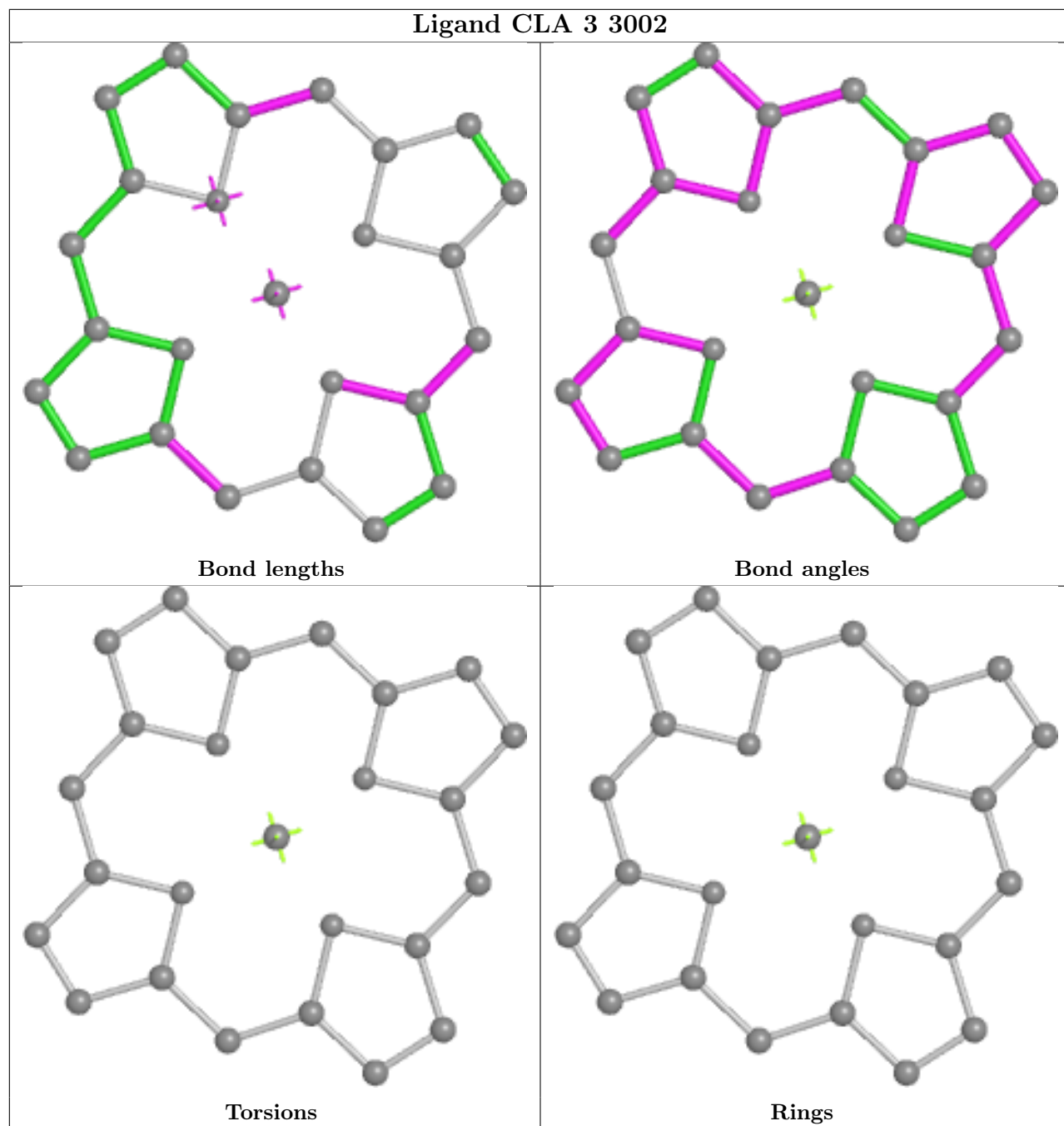
Ligand CLA A 1131**Ligand CLA B 1206****Ligand BCR L 6019**

Ligand BCR J 6012	
	
Bond lengths	Bond angles
	
Torsions	Rings
Ligand BCR A 6011	
	
Bond lengths	Bond angles
	
Torsions	Rings
Ligand CLA A 9012	
	
Bond lengths	Bond angles
	
Torsions	Rings

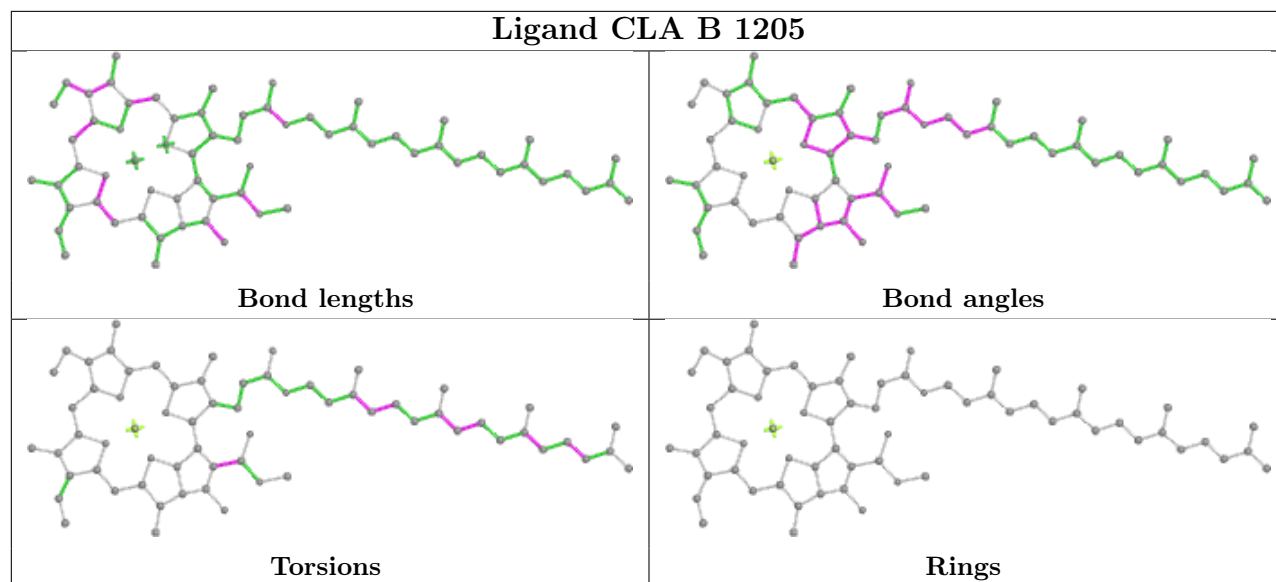


Ligand CLA B 1232

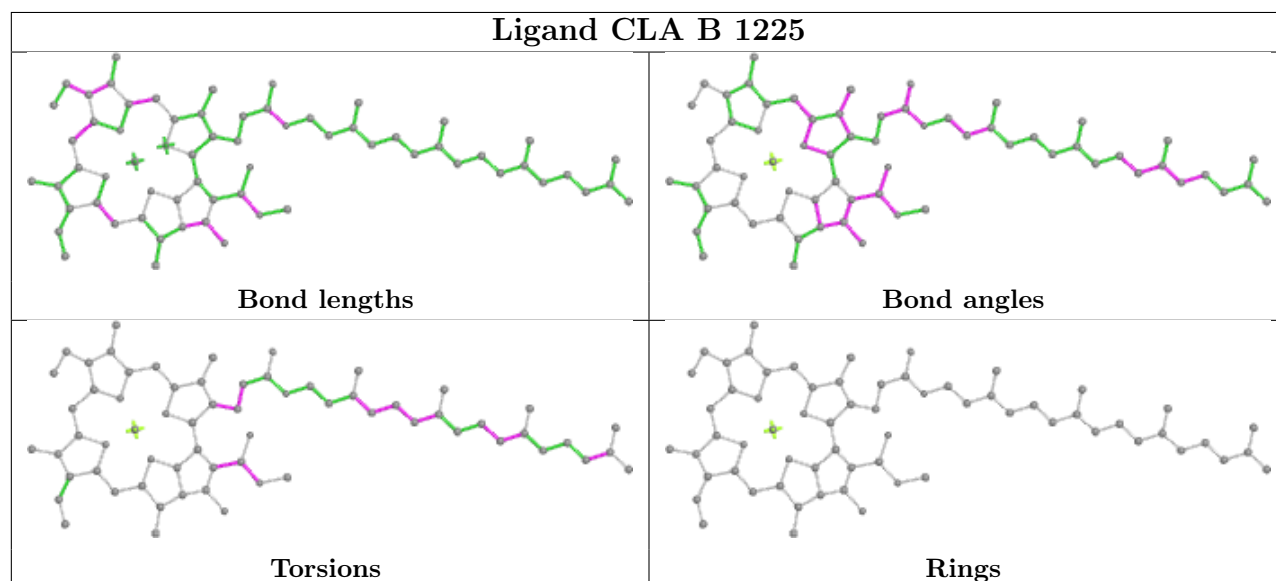




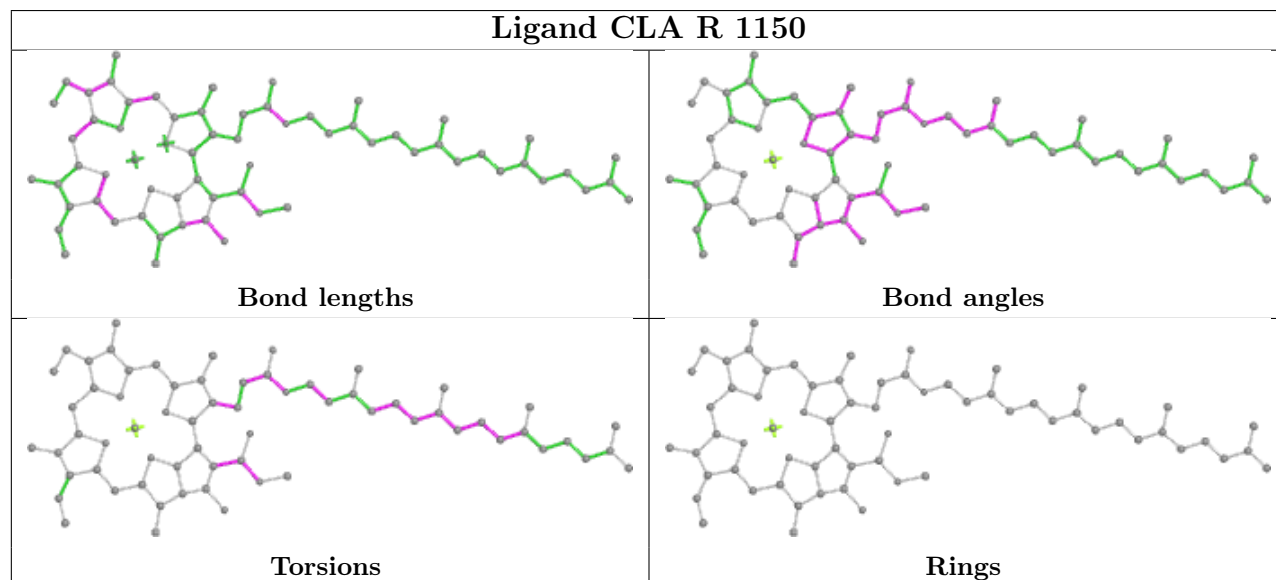
Ligand CLA B 1205

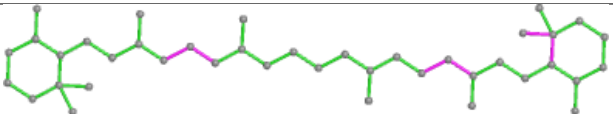
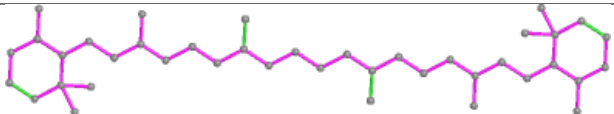
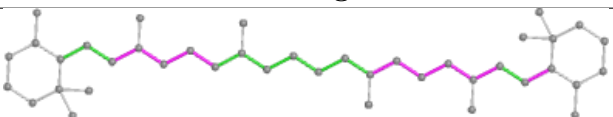
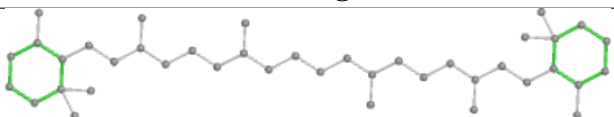


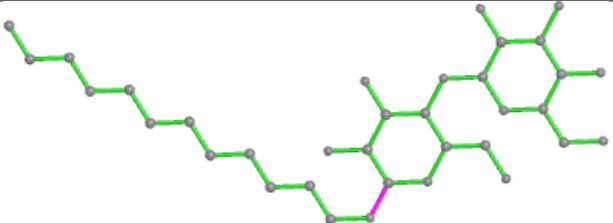
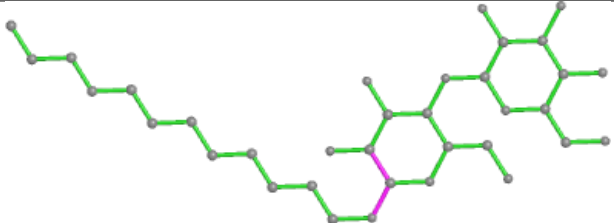
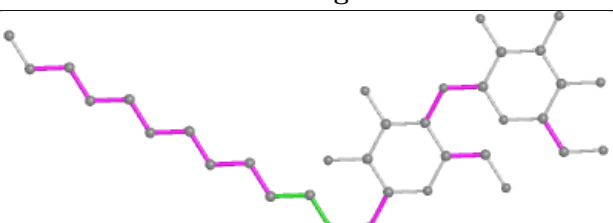
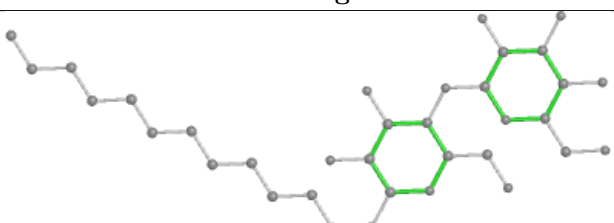
Ligand CLA B 1225

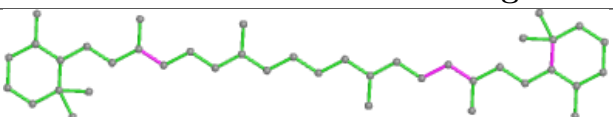
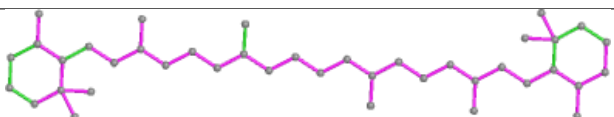
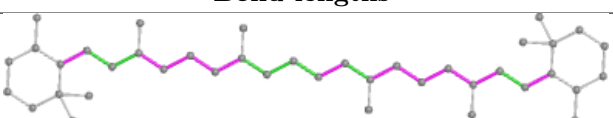
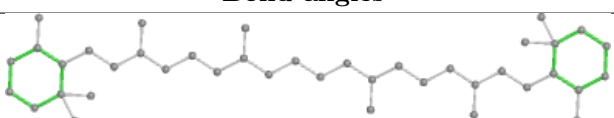


Ligand CLA R 1150

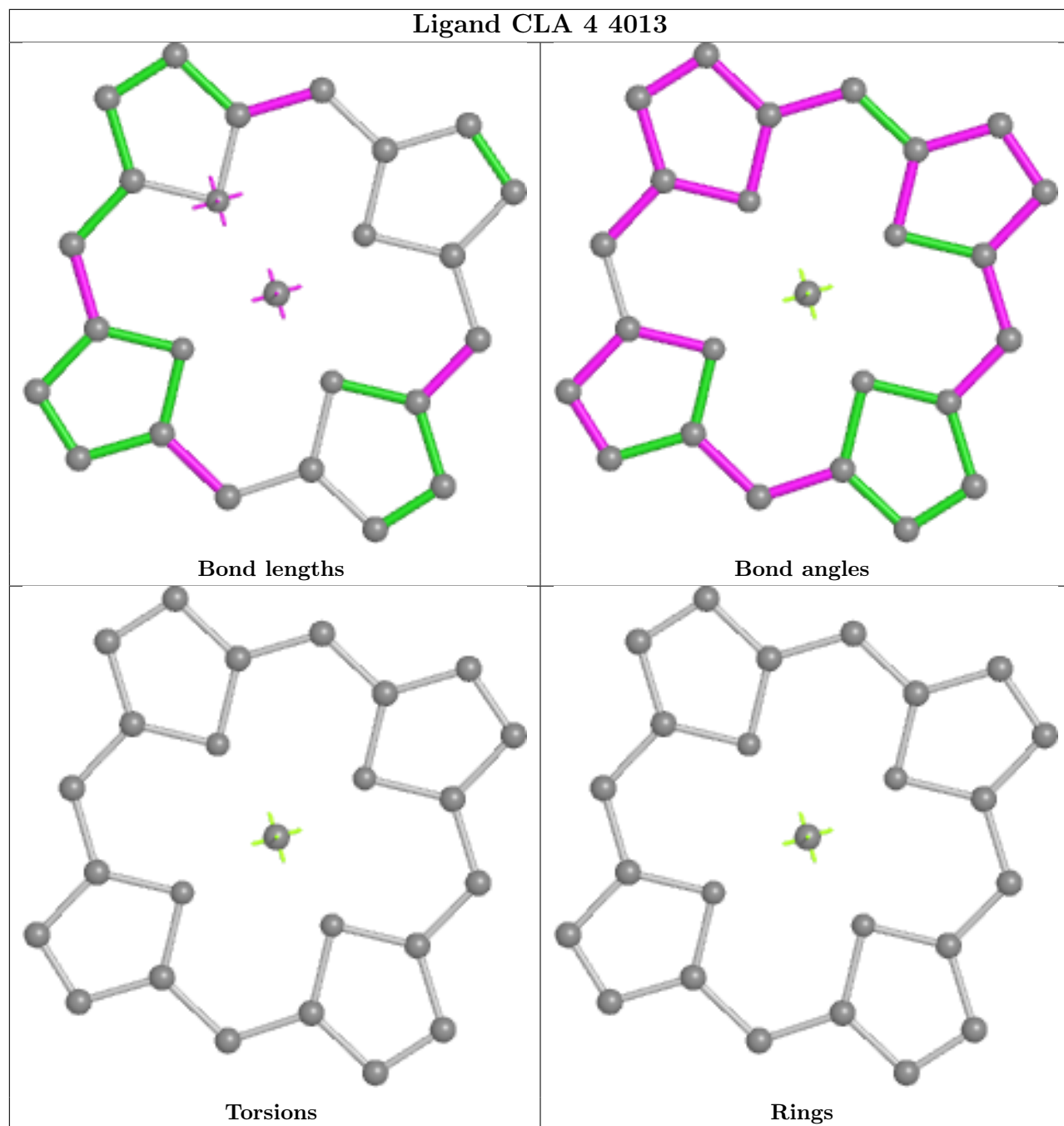


Ligand BCR A 6002	
	Bond lengths
	Bond angles
	Torsions
	Rings

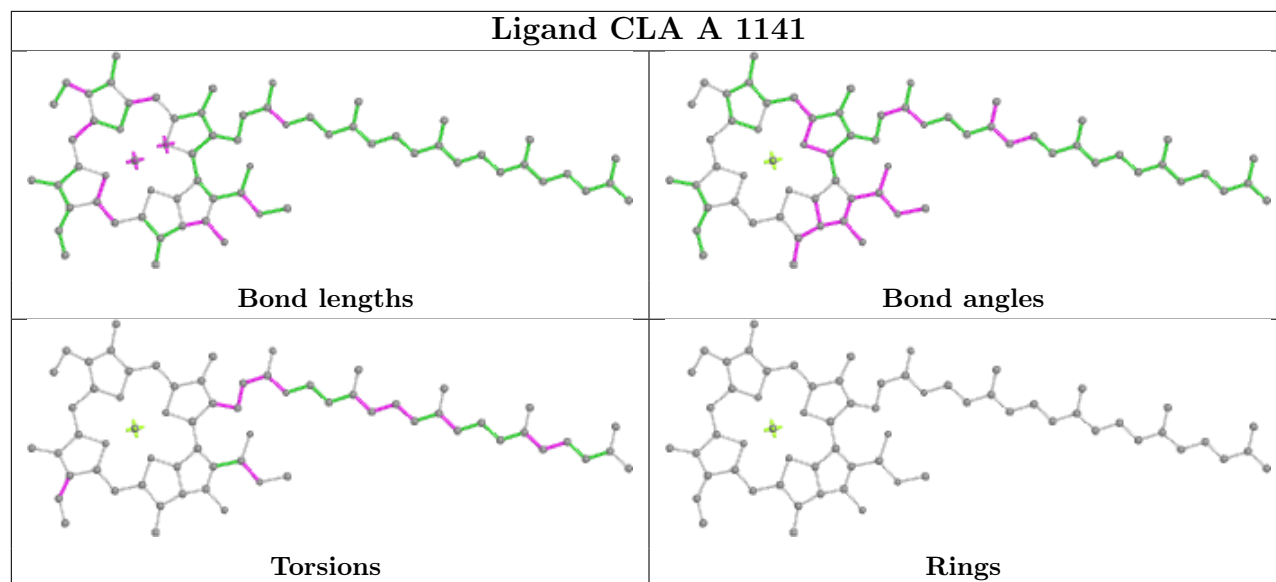
Ligand LMU 1 7004	
	Bond lengths
	Bond angles
	Torsions
	Rings

Ligand BCR 3 6022	
	Bond lengths
	Bond angles
	Torsions
	Rings

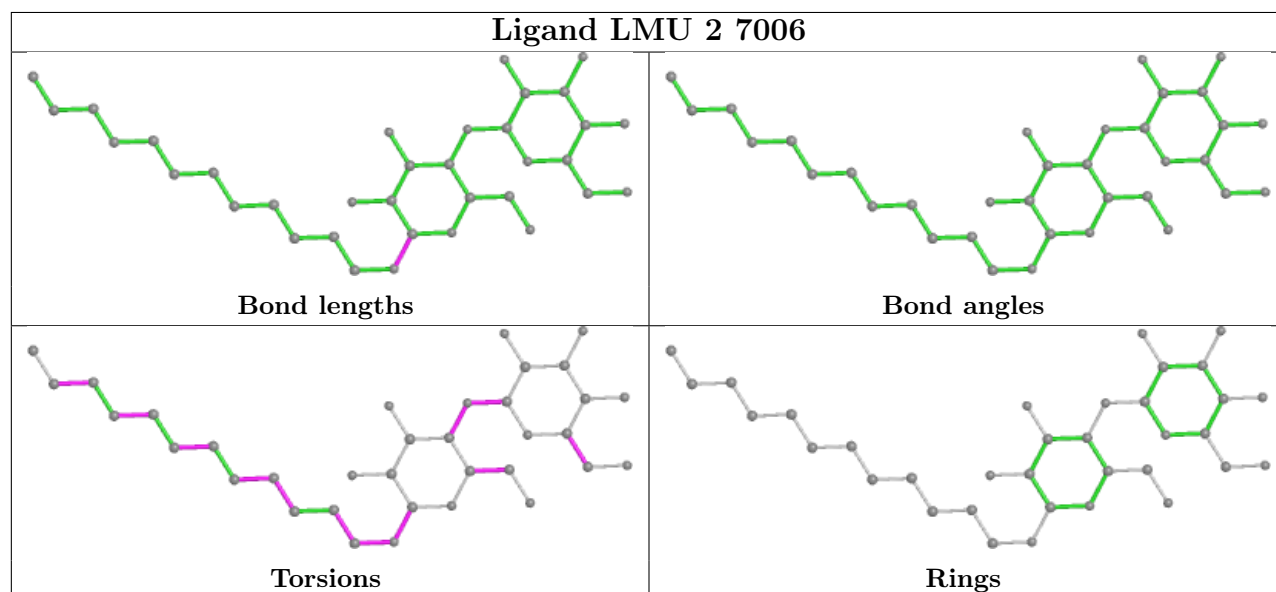
Ligand CLA 4 4013



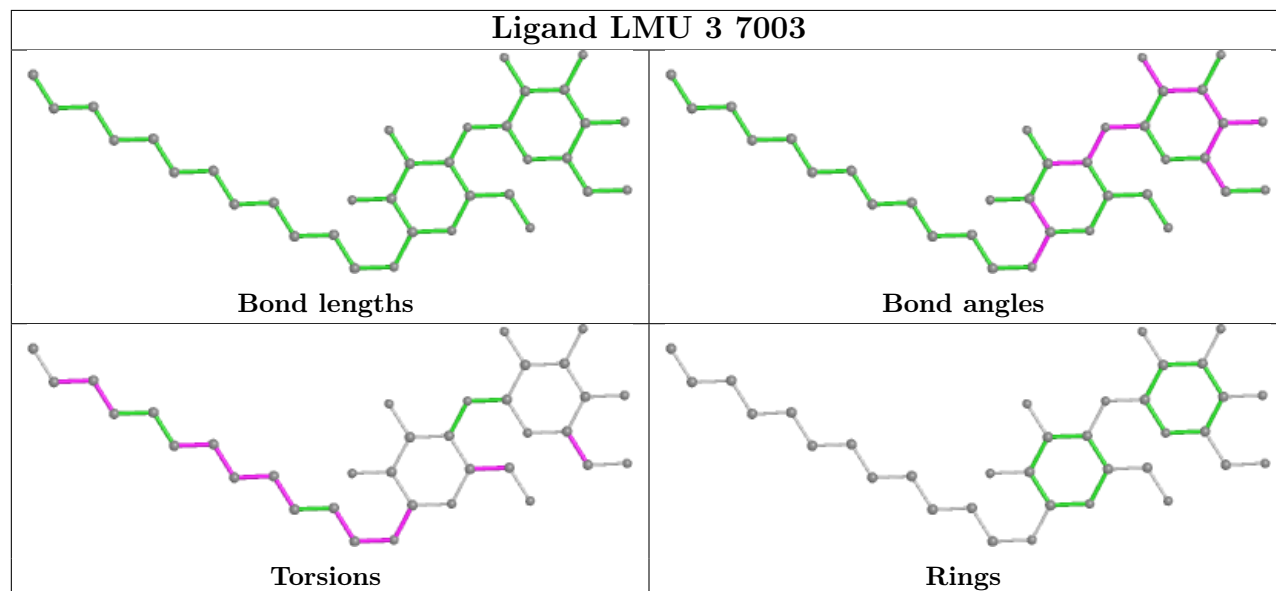
Ligand CLA A 1141



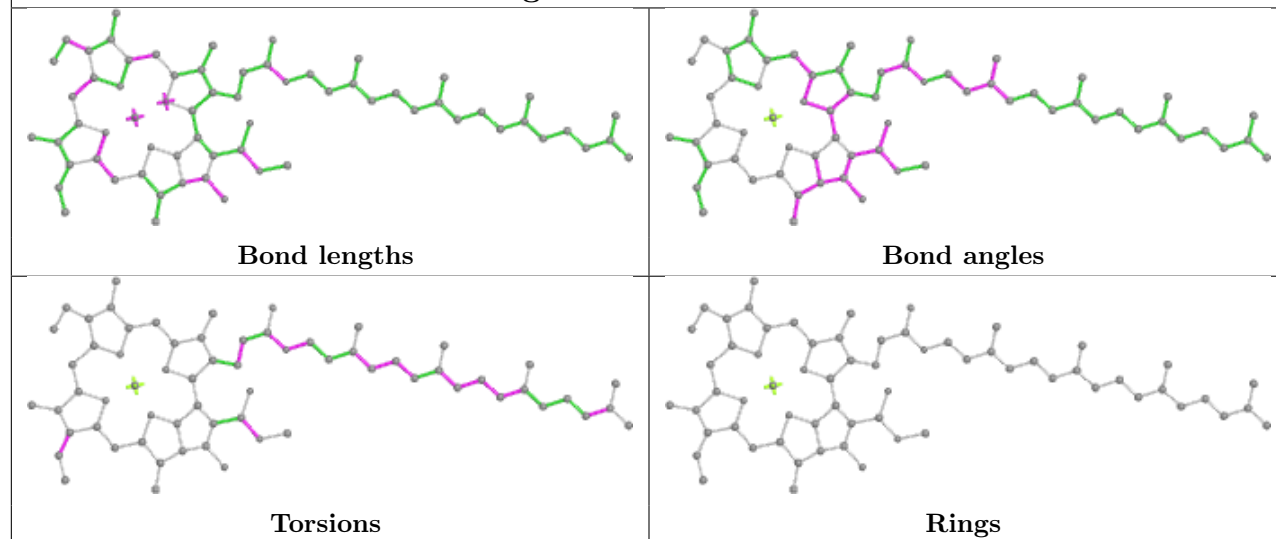
Ligand LMU 2 7006



Ligand LMU 3 7003



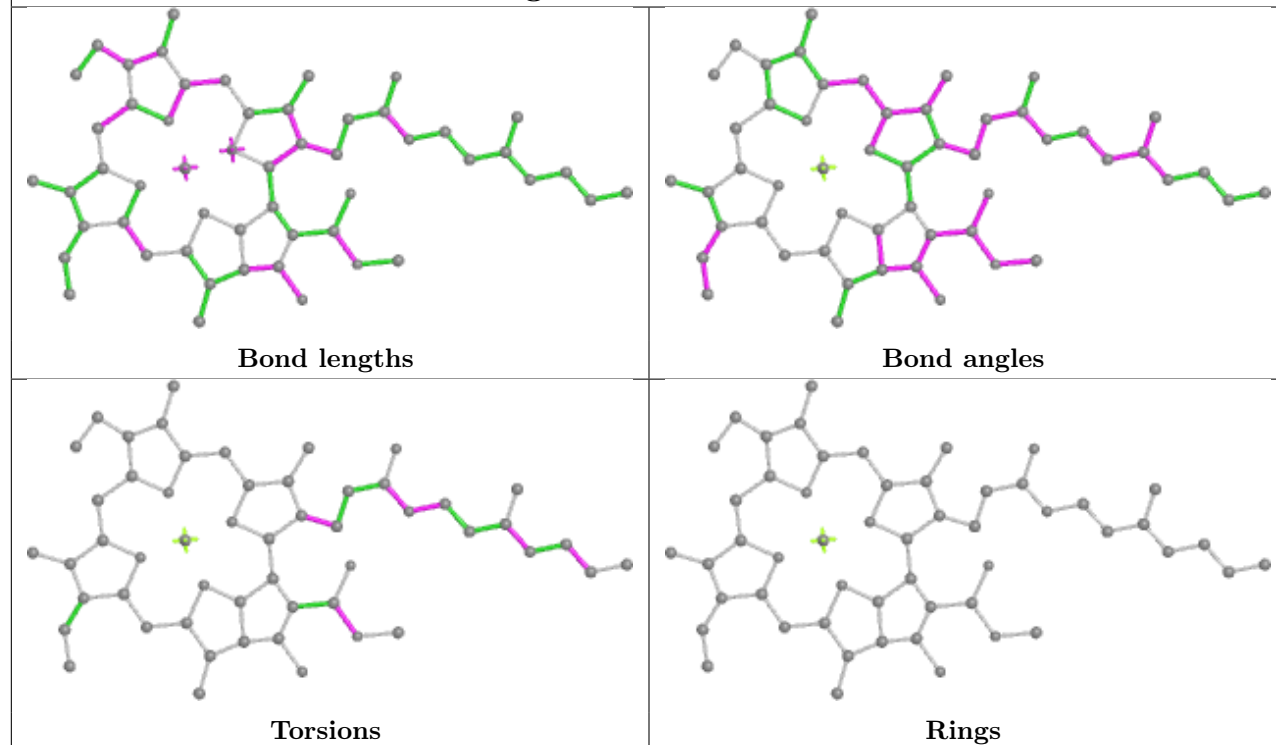
Ligand CLA A 1124

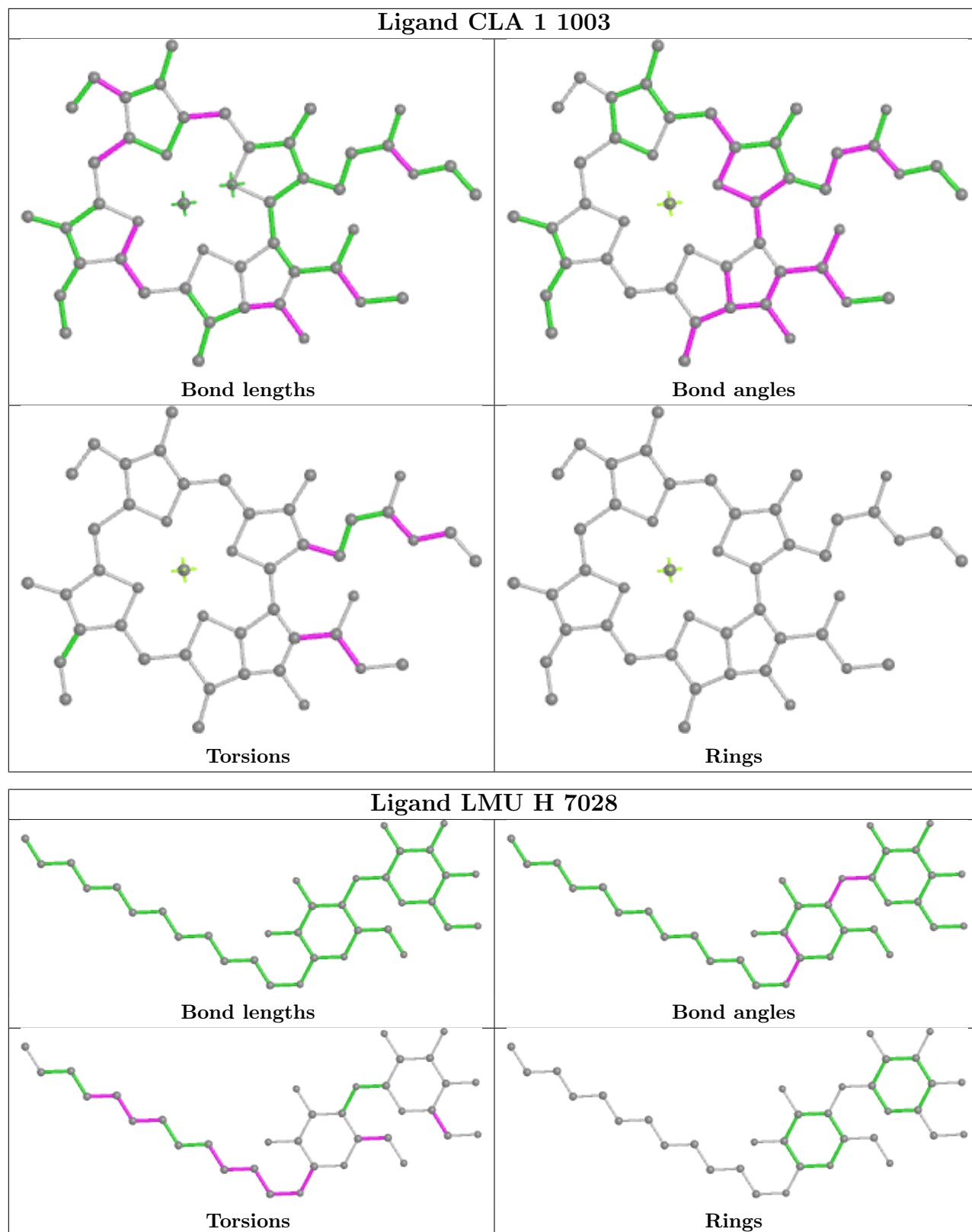


Ligand BCR I 6021

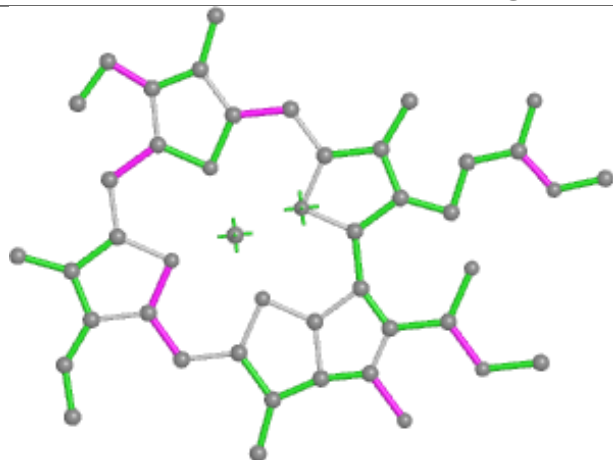


Ligand CLA F 1305

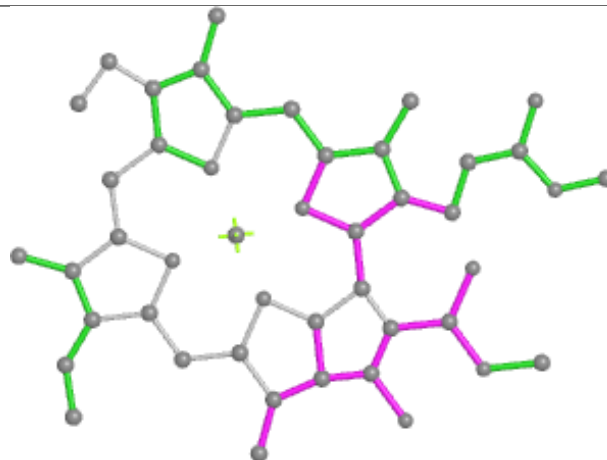




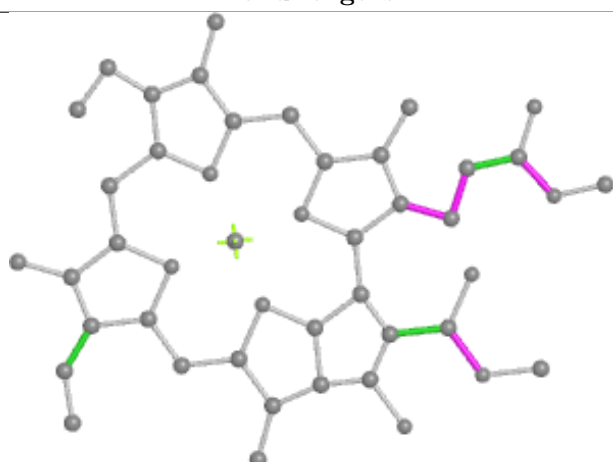
Ligand CLA A 1105



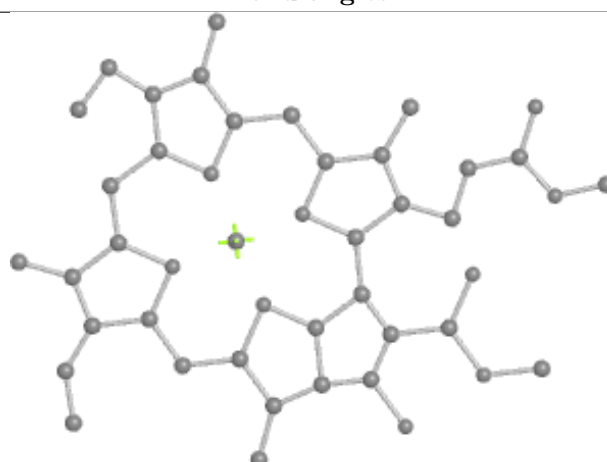
Bond lengths



Bond angles

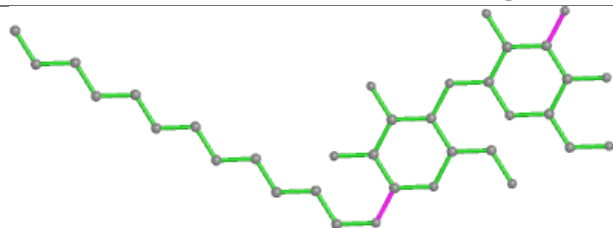


Torsions

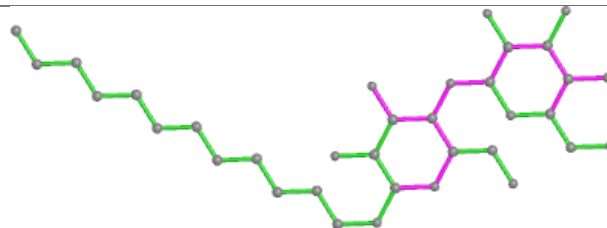


Rings

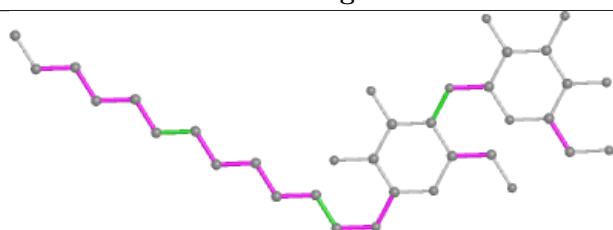
Ligand LMU G 7026



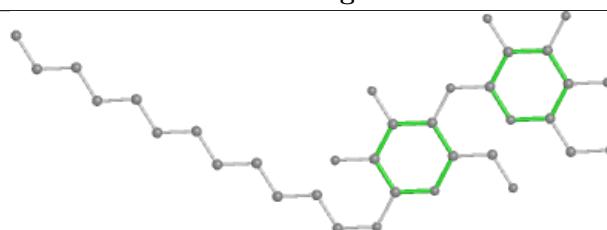
Bond lengths



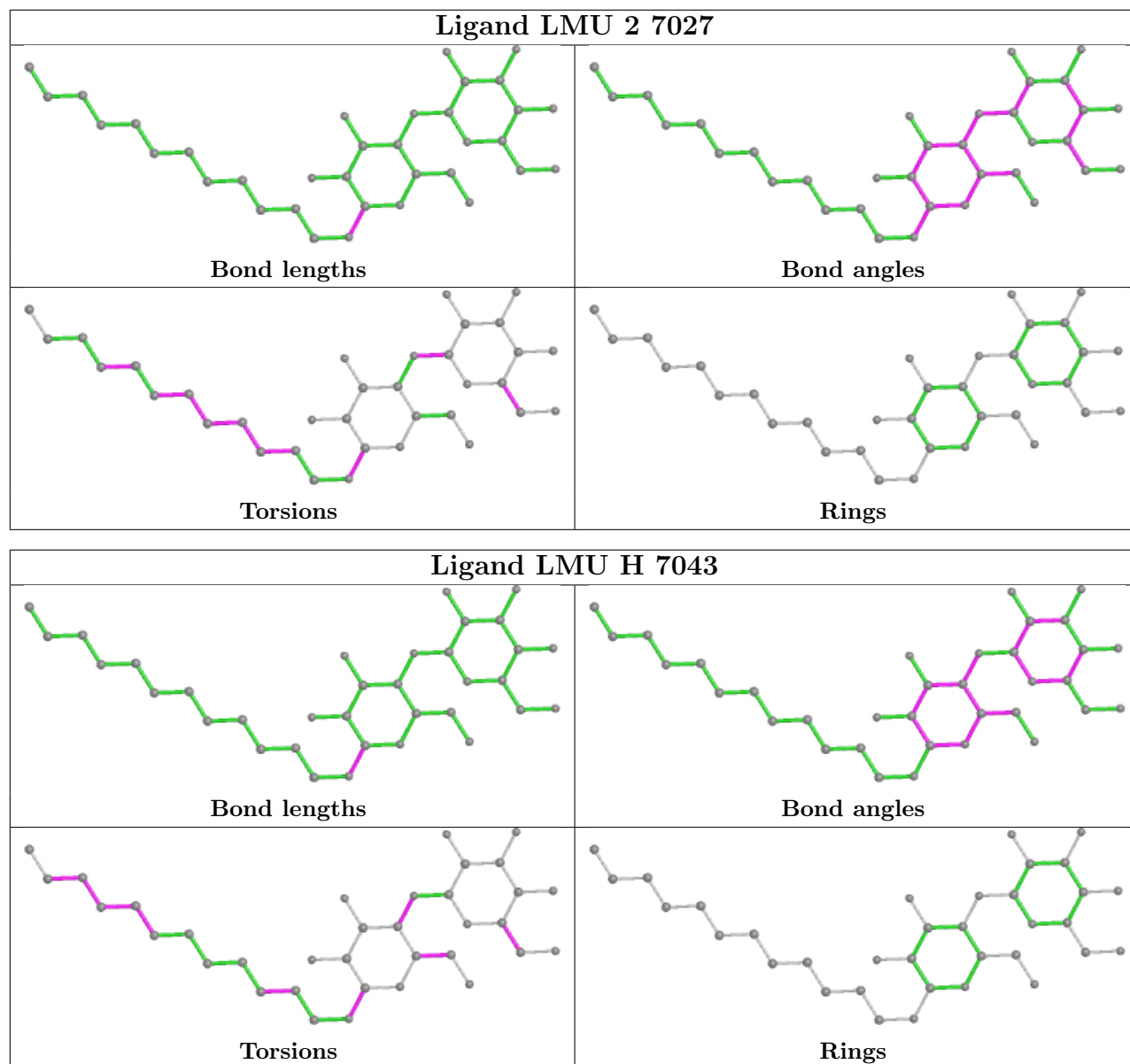
Bond angles



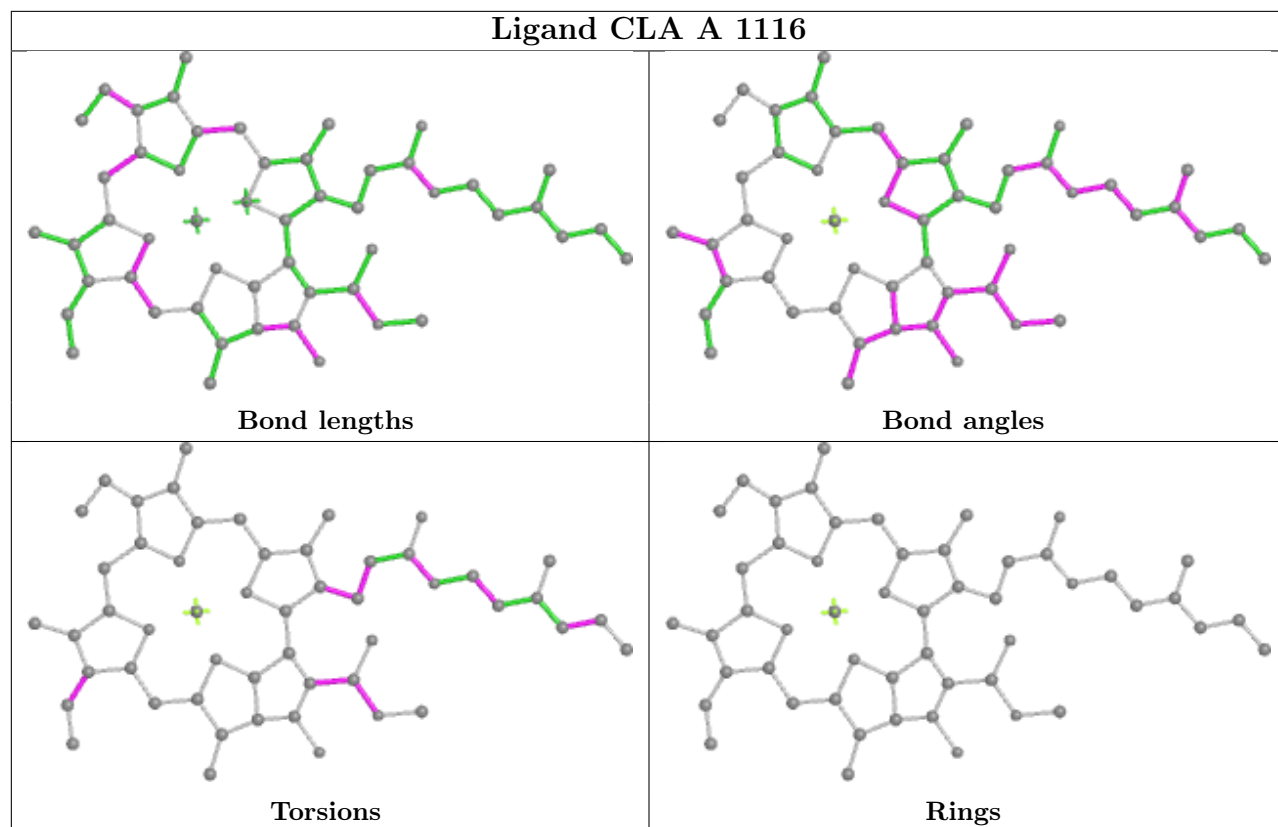
Torsions



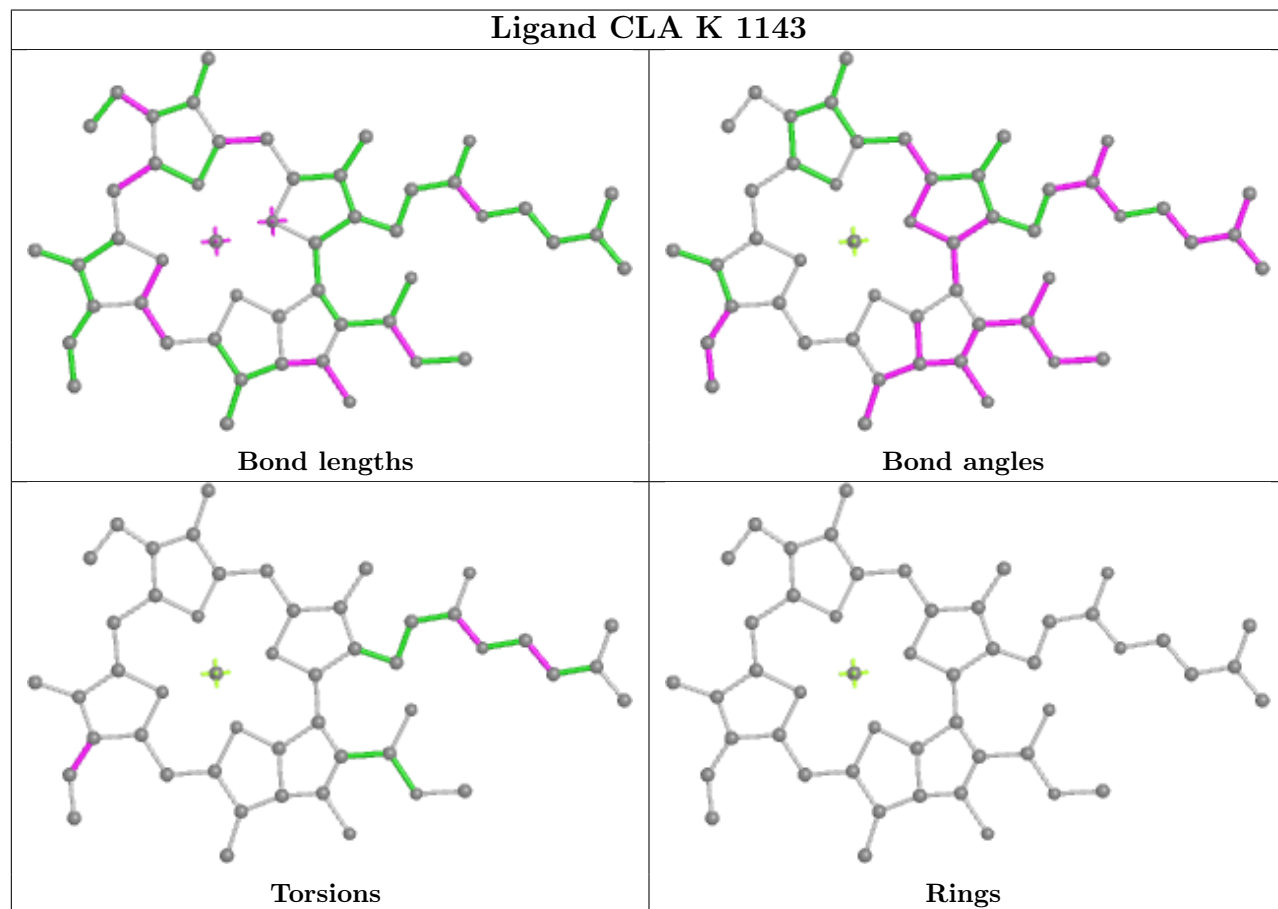
Rings



Ligand CLA A 1116



Ligand CLA K 1143



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	730/738 (98%)	0.15	17 (2%) 60 59	12, 19, 25, 27	0
2	B	733/733 (100%)	0.09	12 (1%) 72 70	8, 18, 26, 28	0
3	C	81/81 (100%)	0.69	10 (12%) 4 3	17, 21, 23, 24	0
4	D	138/138 (100%)	0.24	8 (5%) 23 22	18, 22, 25, 27	0
5	E	64/64 (100%)	0.15	4 (6%) 20 20	17, 21, 24, 25	0
6	F	154/154 (100%)	0.11	7 (4%) 33 32	17, 22, 25, 26	0
7	G	95/95 (100%)	0.41	5 (5%) 26 24	20, 25, 28, 29	0
8	H	69/69 (100%)	0.25	2 (2%) 51 50	22, 24, 29, 30	0
9	I	30/30 (100%)	0.02	2 (6%) 17 17	17, 19, 22, 22	0
10	J	42/42 (100%)	0.24	3 (7%) 16 16	17, 20, 25, 26	0
11	K	84/84 (100%)	1.02	17 (20%) 1 1	24, 27, 29, 30	0
12	L	161/161 (100%)	0.18	7 (4%) 35 34	16, 20, 26, 27	0
13	N	85/85 (100%)	0.13	3 (3%) 44 42	22, 25, 28, 29	0
14	R	0/53	-	-	-	-
15	1	165/170 (97%)	0.36	12 (7%) 15 15	32, 59, 69, 70	0
16	2	176/176 (100%)	0.20	9 (5%) 28 26	32, 52, 63, 66	0
17	3	156/172 (90%)	0.27	8 (5%) 28 26	25, 28, 32, 33	0
18	4	166/166 (100%)	0.27	11 (6%) 18 18	20, 44, 56, 57	0
All	All	3129/3211 (97%)	0.21	137 (4%) 34 33	8, 22, 57, 70	0

The worst 5 of 137 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
11	K	62	SER	8.6
16	2	181	PRO	8.3
15	1	132	GLY	8.2

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Mol	Chain	Res	Type	RSRZ
2	B	491	ASN	6.5
6	F	229	ASN	5.2

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
19	CLA	3	3014	25/65	0.53	0.52	31,31,32,32	0
22	LMU	1	7013	35/35	0.56	0.33	15,34,47,48	0
19	CLA	L	1504	55/65	0.57	0.42	18,25,27,27	0
19	CLA	3	3012	25/65	0.57	0.28	30,31,31,31	0
19	CLA	A	1309	25/65	0.58	0.56	25,46,54,54	0
22	LMU	E	7048	35/35	0.59	0.30	19,30,44,46	0
19	CLA	3	3005	25/65	0.59	0.28	31,31,31,31	0
22	LMU	4	7053	34/35	0.59	0.30	21,41,47,48	0
21	BCR	1	6023	40/40	0.61	0.40	21,28,29,30	0
22	LMU	1	7004	35/35	0.61	0.49	17,44,50,52	0
19	CLA	3	1118	36/65	0.62	0.33	28,29,30,30	0
19	CLA	1	1006	36/65	0.63	0.42	29,30,30,31	0
19	CLA	4	4003	55/65	0.63	0.29	15,34,47,50	0
22	LMU	L	7029	35/35	0.63	0.31	30,44,53,55	0
19	CLA	H	1505	55/65	0.64	0.39	18,27,28,29	0
19	CLA	2	2014	61/65	0.64	0.33	24,26,28,28	0
22	LMU	A	7010	35/35	0.64	0.32	16,38,45,48	0
19	CLA	3	3016	65/65	0.64	0.47	23,26,29,31	0
22	LMU	2	7046	35/35	0.65	0.30	4,27,42,42	0
22	LMU	4	7052	35/35	0.65	0.26	18,30,48,75	0
19	CLA	4	4014	47/65	0.65	0.28	21,35,46,48	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
22	LMU	B	7038	35/35	0.66	0.42	13,35,48,48	0
21	BCR	A	6002	40/40	0.66	0.39	23,27,32,33	0
19	CLA	B	1233	51/65	0.66	0.40	24,27,27,28	0
19	CLA	2	2001	51/65	0.66	0.26	27,28,29,29	0
19	CLA	K	1142	45/65	0.67	0.25	27,29,30,31	0
19	CLA	2	2005	25/65	0.67	0.25	30,31,32,32	0
22	LMU	N	7049	35/35	0.67	0.28	15,28,40,41	0
19	CLA	2	2007	65/65	0.67	0.30	17,25,26,26	0
19	CLA	4	4004	25/65	0.68	0.36	29,30,30,30	0
19	CLA	F	1305	53/65	0.68	0.36	22,23,25,25	0
19	CLA	4	4001	50/65	0.68	0.43	21,23,25,25	0
22	LMU	H	7011	35/35	0.68	0.27	17,32,38,43	0
22	LMU	H	7030	35/35	0.68	0.36	16,29,46,50	0
19	CLA	G	1242	51/65	0.68	0.34	26,28,29,29	0
19	CLA	B	1213	46/65	0.69	0.37	19,21,24,25	0
19	CLA	B	1232	45/65	0.69	0.42	23,26,27,27	0
22	LMU	B	7040	35/35	0.69	0.22	12,26,40,43	0
19	CLA	A	1112	45/65	0.69	0.41	23,26,26,27	0
19	CLA	1	1010	46/65	0.69	0.26	24,25,26,27	0
19	CLA	1	1310	25/65	0.69	0.31	27,28,28,28	0
22	LMU	H	7043	35/35	0.69	0.19	12,31,46,47	0
22	LMU	E	7037	35/35	0.70	0.22	8,21,40,40	0
22	LMU	4	7008	35/35	0.70	0.34	11,29,41,42	0
19	CLA	3	3010	25/65	0.70	0.23	32,32,33,33	0
19	CLA	4	4007	52/65	0.70	0.29	22,26,27,28	0
19	CLA	4	1306	55/65	0.71	0.32	20,26,27,27	0
19	CLA	2	2011	25/65	0.71	0.31	24,25,25,25	0
19	CLA	A	1141	65/65	0.71	0.26	28,30,31,32	0
22	LMU	G	7051	35/35	0.71	0.28	20,32,43,44	0
21	BCR	3	6022	40/40	0.71	0.25	21,22,23,23	0
19	CLA	1	1015	25/65	0.71	0.24	27,28,28,28	0
19	CLA	K	3009	65/65	0.71	0.37	22,25,27,28	0
22	LMU	K	7047	35/35	0.71	0.27	14,33,46,49	0
22	LMU	K	7041	35/35	0.72	0.24	15,31,45,45	0
19	CLA	1	1001	46/65	0.72	0.27	28,29,30,30	0
19	CLA	2	2008	25/65	0.72	0.22	24,24,25,25	0
22	LMU	C	7015	35/35	0.72	0.35	9,22,37,39	0
19	CLA	A	1151	50/65	0.72	0.37	24,27,29,29	0
19	CLA	3	3015	25/65	0.72	0.42	28,28,29,29	0
19	CLA	2	1307	25/65	0.72	0.50	29,30,31,31	0
19	CLA	4	1304	65/65	0.72	0.26	21,23,25,25	0
19	CLA	H	1241	55/65	0.72	0.26	23,25,26,26	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
19	CLA	1	1014	61/65	0.72	0.27	3,31,46,46	0
19	CLA	3	1147	46/65	0.73	0.28	25,27,28,28	0
19	CLA	J	1311	61/65	0.73	0.27	19,26,27,28	0
19	CLA	3	3007	42/65	0.73	0.32	27,30,30,30	0
19	CLA	4	1004	55/65	0.73	0.26	22,25,26,27	0
19	CLA	A	1134	45/65	0.73	0.26	22,26,27,28	0
19	CLA	4	4015	46/65	0.73	0.36	24,25,26,27	0
22	LMU	4	7009	34/35	0.73	0.26	22,44,50,50	0
22	LMU	4	7018	35/35	0.73	0.29	9,23,41,42	0
22	LMU	4	7034	35/35	0.73	0.28	14,30,42,47	0
22	LMU	K	7042	35/35	0.73	0.23	13,23,42,43	0
19	CLA	F	1302	41/65	0.73	0.25	24,26,26,26	0
19	CLA	3	3003	36/65	0.74	0.34	29,30,31,31	0
22	LMU	H	7017	35/35	0.74	0.21	8,23,39,41	0
19	CLA	2	2013	50/65	0.74	0.27	20,22,24,26	0
22	LMU	3	7005	35/35	0.74	0.25	20,32,42,43	0
19	CLA	1	1003	47/65	0.74	0.24	17,19,19,20	0
19	CLA	3	3008	50/65	0.74	0.35	20,26,27,27	0
19	CLA	B	1212	60/65	0.74	0.32	20,23,25,26	0
19	CLA	3	3011	65/65	0.74	0.30	23,25,26,26	0
21	BCR	A	6007	40/40	0.74	0.38	19,23,28,28	0
19	CLA	L	1148	55/65	0.74	0.32	21,25,26,27	0
19	CLA	R	1150	65/65	0.75	0.28	22,24,25,25	0
19	CLA	1	1013	51/65	0.75	0.42	26,27,29,29	0
22	LMU	2	7031	35/35	0.75	0.23	17,37,45,48	0
19	CLA	3	3002	25/65	0.75	0.27	28,28,28,28	0
22	LMU	3	7003	35/35	0.75	0.20	8,25,41,41	0
22	LMU	K	7001	35/35	0.75	0.20	17,34,48,50	0
19	CLA	A	1113	50/65	0.75	0.31	19,22,23,24	0
19	CLA	2	2004	50/65	0.75	0.26	23,25,25,25	0
22	LMU	G	7026	35/35	0.75	0.30	12,35,46,51	0
22	LMU	4	7019	35/35	0.75	0.22	11,25,40,43	0
19	CLA	3	3006	25/65	0.75	0.21	26,27,28,28	0
19	CLA	1	1008	51/65	0.75	0.35	24,26,27,27	0
22	LMU	R	7021	35/35	0.75	0.25	17,28,45,46	0
24	LMG	B	7101	49/55	0.75	0.36	14,18,26,27	0
22	LMU	2	7006	35/35	0.76	0.22	22,25,26,27	0
22	LMU	2	7027	35/35	0.76	0.21	6,17,40,40	0
19	CLA	H	1145	65/65	0.76	0.24	12,24,33,39	0
19	CLA	A	1121	42/65	0.76	0.24	26,28,28,28	0
21	BCR	A	6003	40/40	0.76	0.35	21,24,26,26	0
22	LMU	D	7050	35/35	0.76	0.23	14,31,46,46	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
19	CLA	A	1149	46/65	0.76	0.32	22,25,25,25	0
21	BCR	J	6012	40/40	0.76	0.33	19,24,26,26	0
22	LMU	F	7036	34/35	0.76	0.30	19,32,42,45	0
19	CLA	3	3017	50/65	0.76	0.23	26,37,49,52	0
19	CLA	B	1301	36/65	0.76	0.30	27,28,29,29	0
22	LMU	R	7024	35/35	0.76	0.21	6,19,32,40	0
19	CLA	R	1144	57/65	0.76	0.25	24,27,28,28	0
22	LMU	A	7016	35/35	0.76	0.26	10,30,46,46	0
22	LMU	H	7002	35/35	0.77	0.17	16,29,41,43	0
19	CLA	3	3013	65/65	0.77	0.26	20,21,24,25	0
19	CLA	A	1105	46/65	0.77	0.37	22,23,24,24	0
22	LMU	H	7028	35/35	0.77	0.17	7,21,40,40	0
22	LMU	A	7045	35/35	0.77	0.19	11,23,41,43	0
19	CLA	3	3004	25/65	0.77	0.20	27,28,28,28	0
19	CLA	2	2010	25/65	0.77	0.28	23,23,24,24	0
19	CLA	2	2002	56/65	0.77	0.23	21,22,25,25	0
19	CLA	2	2003	25/65	0.77	0.38	23,24,25,25	0
19	CLA	1	1303	51/65	0.77	0.32	23,28,28,29	0
21	BCR	I	6021	40/40	0.77	0.30	16,20,22,22	0
19	CLA	K	1143	50/65	0.77	0.26	24,27,28,28	0
22	LMU	R	7014	35/35	0.77	0.35	9,26,40,44	0
19	CLA	2	2006	65/65	0.77	0.38	18,23,24,25	0
19	CLA	K	1146	50/65	0.77	0.27	25,28,30,30	0
22	LMU	R	7025	35/35	0.77	0.25	5,22,39,42	0
22	LMU	R	7020	35/35	0.78	0.23	7,26,40,44	0
19	CLA	A	1108	45/65	0.78	0.29	19,22,23,24	0
19	CLA	A	1116	52/65	0.78	0.28	24,25,26,26	0
19	CLA	3	2009	56/65	0.78	0.23	13,35,50,50	0
22	LMU	A	7044	35/35	0.78	0.18	8,20,39,40	0
19	CLA	B	1218	46/65	0.78	0.30	20,20,22,23	0
19	CLA	4	4005	25/65	0.78	0.27	20,21,22,22	0
19	CLA	4	4006	55/65	0.78	0.23	16,23,24,24	0
19	CLA	1	1007	61/65	0.78	0.26	14,20,21,22	0
19	CLA	4	4010	25/65	0.78	0.23	26,27,27,27	0
19	CLA	B	1222	58/65	0.79	0.35	18,21,23,24	0
19	CLA	A	1102	55/65	0.79	0.30	13,19,20,20	0
21	BCR	L	6019	40/40	0.79	0.34	15,17,19,19	0
22	LMU	A	7023	35/35	0.79	0.25	6,20,39,41	0
19	CLA	3	3001	25/65	0.79	0.28	24,25,25,25	0
22	LMU	R	7022	35/35	0.79	0.18	5,21,33,35	0
21	BCR	B	6006	40/40	0.80	0.38	15,19,20,21	0
19	CLA	B	1201	45/65	0.80	0.28	19,21,22,22	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
22	LMU	4	7033	35/35	0.80	0.20	12,26,40,41	0
19	CLA	2	4009	65/65	0.80	0.23	18,23,24,24	0
19	CLA	J	1308	55/65	0.80	0.23	12,30,44,45	0
21	BCR	A	6008	40/40	0.80	0.35	21,24,27,27	0
21	BCR	B	6004	40/40	0.80	0.33	18,20,22,22	0
19	CLA	A	1119	65/65	0.81	0.35	13,18,19,20	0
19	CLA	A	1115	65/65	0.81	0.24	10,28,41,42	0
19	CLA	1	1002	47/65	0.81	0.23	22,23,24,24	0
19	CLA	L	1130	65/65	0.81	0.28	13,18,19,20	0
19	CLA	A	1110	54/65	0.81	0.25	19,22,23,23	0
19	CLA	L	1503	50/65	0.81	0.25	19,21,23,24	0
19	CLA	H	1207	65/65	0.81	0.28	15,17,19,20	0
19	CLA	B	1231	45/65	0.81	0.28	19,20,21,21	0
21	BCR	B	6017	40/40	0.81	0.34	15,18,20,20	0
21	BCR	I	6018	40/40	0.81	0.31	14,15,18,18	0
22	LMU	B	7012	25/35	0.81	0.18	22,32,44,49	0
21	BCR	B	6010	40/40	0.82	0.34	13,15,16,16	0
19	CLA	B	1229	65/65	0.82	0.27	8,12,14,15	0
19	CLA	1	1005	46/65	0.82	0.23	19,21,22,22	0
19	CLA	B	1223	65/65	0.82	0.32	13,18,19,20	0
22	LMU	H	7032	35/35	0.82	0.31	8,25,36,45	0
19	CLA	1	1011	36/65	0.82	0.22	27,27,28,28	0
19	CLA	2	2012	50/65	0.82	0.26	20,22,23,23	0
19	CLA	4	4002	52/65	0.83	0.21	21,22,24,25	0
19	CLA	A	1123	65/65	0.83	0.30	12,18,19,20	0
19	CLA	B	1209	55/65	0.83	0.25	18,19,20,21	0
19	CLA	B	1211	65/65	0.83	0.31	17,20,21,21	0
19	CLA	L	1502	47/65	0.83	0.25	17,19,20,20	0
21	BCR	F	6014	40/40	0.83	0.31	9,11,15,15	0
19	CLA	B	1230	50/65	0.83	0.28	17,18,19,20	0
19	CLA	A	1117	65/65	0.84	0.31	10,20,21,22	0
19	CLA	A	1124	65/65	0.84	0.28	18,21,23,24	0
21	BCR	F	6016	40/40	0.84	0.28	13,16,17,17	0
19	CLA	A	1109	65/65	0.84	0.28	13,20,22,23	0
19	CLA	B	1216	61/65	0.84	0.28	12,18,19,20	0
19	CLA	B	1217	50/65	0.84	0.26	19,21,22,23	0
19	CLA	A	1135	51/65	0.84	0.27	16,19,19,21	0
19	CLA	A	1111	54/65	0.84	0.26	20,24,24,24	0
19	CLA	I	1204	60/65	0.84	0.24	13,17,18,18	0
19	CLA	4	4013	25/65	0.84	0.19	20,21,21,21	0
19	CLA	A	1138	65/65	0.85	0.29	15,18,19,20	0
19	CLA	B	1219	55/65	0.85	0.24	18,18,21,21	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
19	CLA	A	1140	65/65	0.85	0.28	15,18,19,21	0
22	LMU	A	7035	35/35	0.85	0.27	6,18,32,40	0
19	CLA	B	1234	60/65	0.85	0.28	13,14,21,21	0
19	CLA	A	1120	51/65	0.85	0.37	22,24,24,26	0
19	CLA	B	1208	54/65	0.85	0.26	18,18,21,22	0
19	CLA	4	1009	36/65	0.85	0.20	20,22,22,23	0
19	CLA	A	1103	65/65	0.85	0.29	13,14,21,22	0
22	LMU	R	7007	35/35	0.85	0.24	8,21,40,41	0
19	CLA	L	1501	50/65	0.85	0.24	20,20,21,21	0
19	CLA	A	1237	65/65	0.86	0.28	8,17,18,18	0
19	CLA	1	1012	36/65	0.86	0.22	23,24,25,25	0
19	CLA	A	1132	65/65	0.86	0.27	13,17,18,19	0
19	CLA	B	1228	50/65	0.86	0.23	12,14,14,15	0
21	BCR	A	6011	40/40	0.86	0.30	10,15,16,16	0
19	CLA	4	4011	25/65	0.86	0.18	10,11,12,12	0
19	CLA	4	4012	36/65	0.86	0.21	14,15,16,16	0
19	CLA	A	1133	50/65	0.86	0.23	17,19,19,20	0
19	CLA	B	1238	65/65	0.86	0.27	10,14,15,16	0
19	CLA	A	1128	65/65	0.86	0.27	14,16,17,18	0
19	CLA	B	1239	65/65	0.87	0.30	8,11,13,14	0
22	LMU	G	7039	35/35	0.87	0.15	15,30,47,47	0
21	BCR	B	6005	40/40	0.87	0.29	14,16,17,17	0
19	CLA	A	1107	55/65	0.87	0.26	15,16,24,24	0
19	CLA	F	1240	36/65	0.87	0.23	15,16,17,17	0
19	CLA	B	1220	65/65	0.87	0.24	13,15,20,21	0
19	CLA	B	1214	59/65	0.87	0.24	18,20,22,23	0
19	CLA	A	1125	65/65	0.87	0.24	15,17,19,20	0
19	CLA	A	1101	50/65	0.87	0.23	17,18,18,19	0
19	CLA	B	1206	65/65	0.87	0.27	10,12,17,18	0
19	CLA	B	1235	65/65	0.88	0.26	14,15,16,17	0
19	CLA	B	1236	47/65	0.88	0.28	14,15,17,17	0
19	CLA	B	1226	65/65	0.88	0.31	11,12,19,19	0
19	CLA	A	1129	50/65	0.88	0.20	17,19,20,20	0
20	PQN	A	5001	33/33	0.88	0.29	12,13,14,15	0
19	CLA	A	1131	65/65	0.88	0.25	12,14,16,16	0
19	CLA	A	1126	65/65	0.88	0.29	12,14,15,15	0
19	CLA	A	1139	51/65	0.88	0.23	16,16,17,18	0
19	CLA	A	1122	55/65	0.88	0.22	13,14,18,18	0
19	CLA	B	1224	65/65	0.88	0.27	9,13,14,15	0
19	CLA	B	1225	65/65	0.88	0.29	9,12,13,14	0
19	CLA	A	1136	65/65	0.89	0.27	14,15,16,17	0
19	CLA	B	1202	65/65	0.89	0.25	7,16,16,18	0

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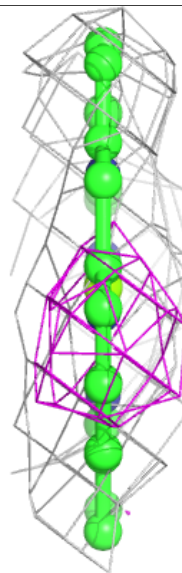
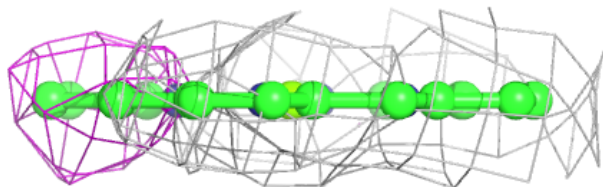
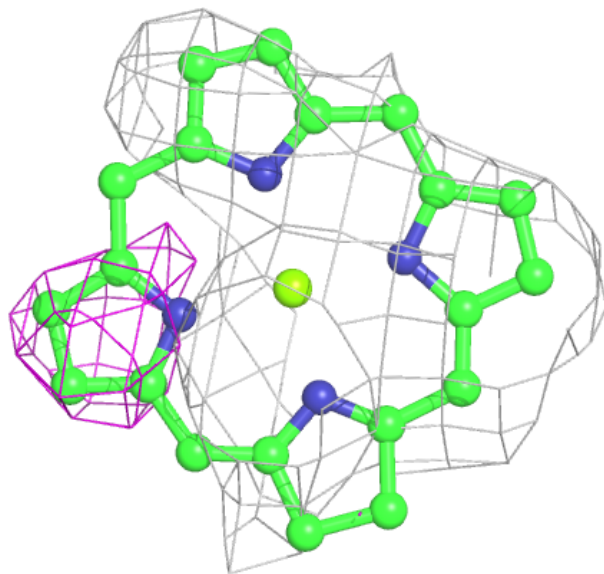
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
19	CLA	B	1215	60/65	0.89	0.27	11,13,15,16	0
19	CLA	B	1205	65/65	0.89	0.26	9,13,14,14	0
19	CLA	B	1227	50/65	0.89	0.23	13,15,16,17	0
19	CLA	A	1127	55/65	0.89	0.25	13,16,17,18	0
19	CLA	A	1104	57/65	0.89	0.27	13,15,18,18	0
19	CLA	B	9010	65/65	0.89	0.25	2,12,34,40	0
19	CLA	A	9012	65/65	0.89	0.25	2,14,28,36	0
21	BCR	B	6020	40/40	0.89	0.25	8,11,12,13	0
19	CLA	A	9013	65/65	0.89	0.25	2,10,29,32	0
19	CLA	A	9023	65/65	0.89	0.27	2,14,29,38	0
19	CLA	A	9022	65/65	0.90	0.28	2,12,26,31	0
19	CLA	A	1137	47/65	0.90	0.24	13,14,15,17	0
19	CLA	B	1210	65/65	0.90	0.23	16,20,21,22	0
19	CLA	A	1106	65/65	0.91	0.29	10,12,13,14	0
20	PQN	B	5002	33/33	0.91	0.26	7,8,14,14	0
19	CLA	A	9011	65/65	0.91	0.26	2,11,30,40	0
19	CLA	B	1203	65/65	0.91	0.24	10,13,14,15	0
19	CLA	B	1221	54/65	0.91	0.22	13,13,16,16	0
23	SF4	C	8002	8/8	0.97	0.08	14,16,24,28	0
23	SF4	C	8003	8/8	0.98	0.07	14,19,21,22	0
23	SF4	A	8001	8/8	0.99	0.09	12,17,19,21	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.

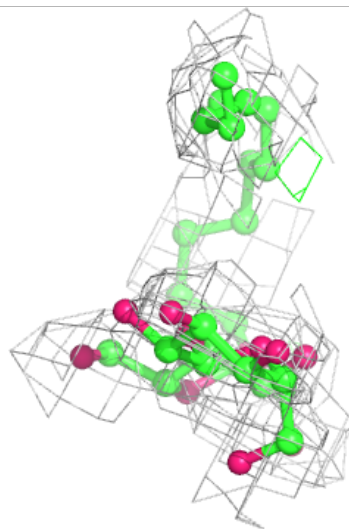
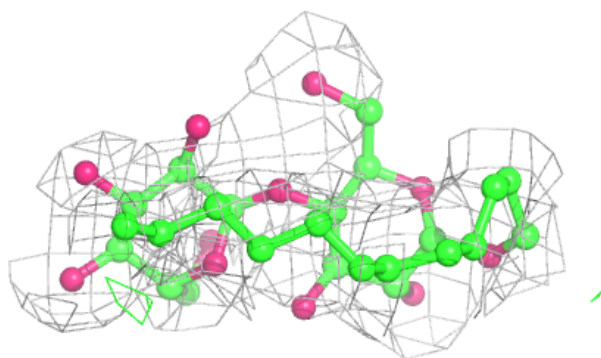
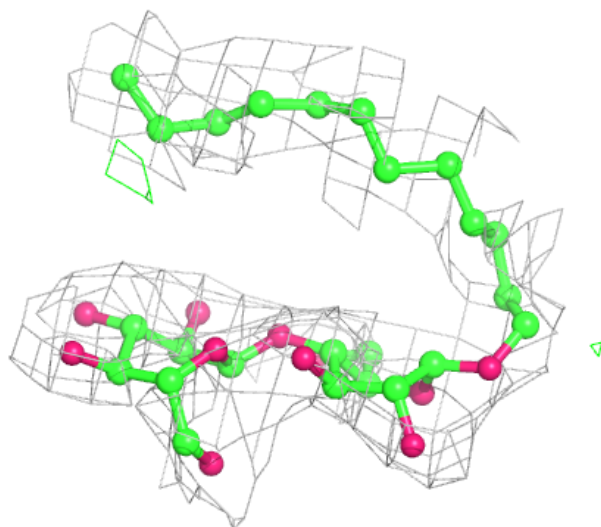
Electron density around CLA 3 3014:

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



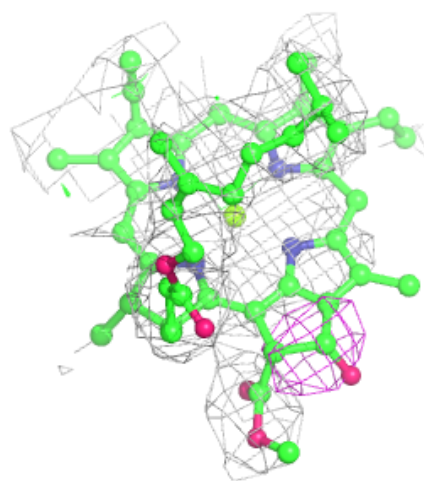
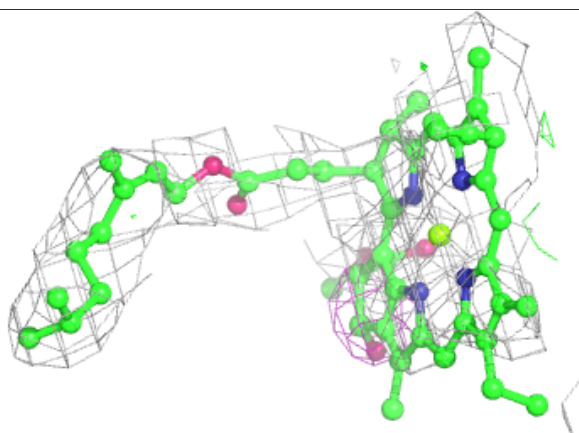
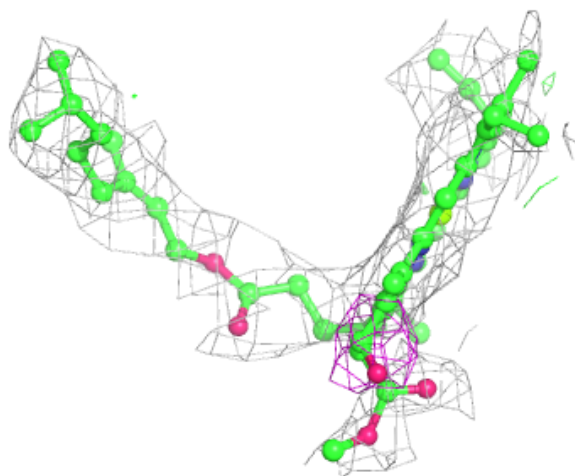
Electron density around LMU 1 7013:

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



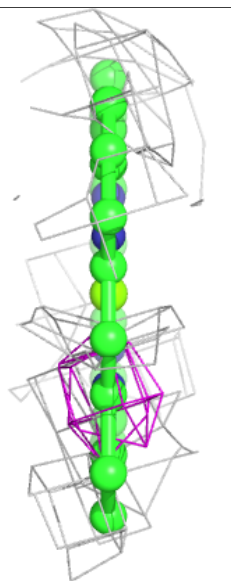
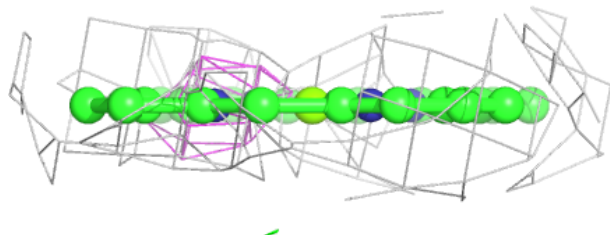
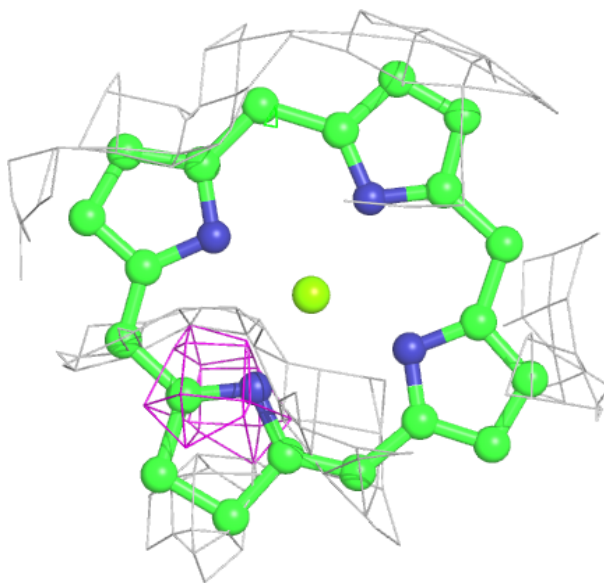
Electron density around CLA L 1504:

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



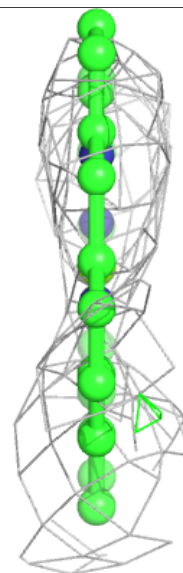
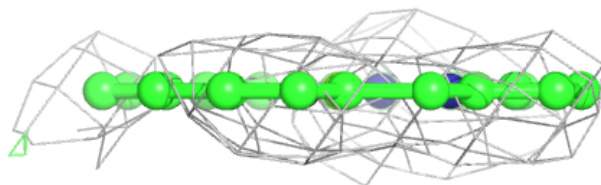
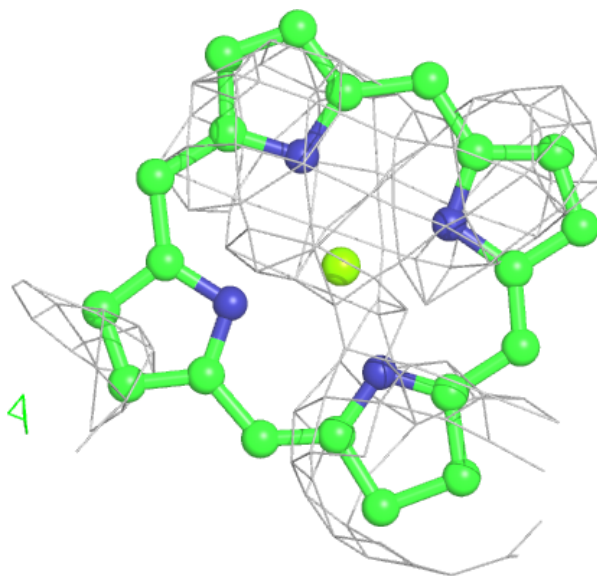
Electron density around CLA 3 3012:

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



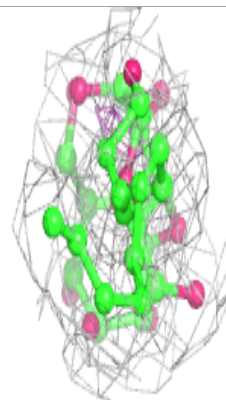
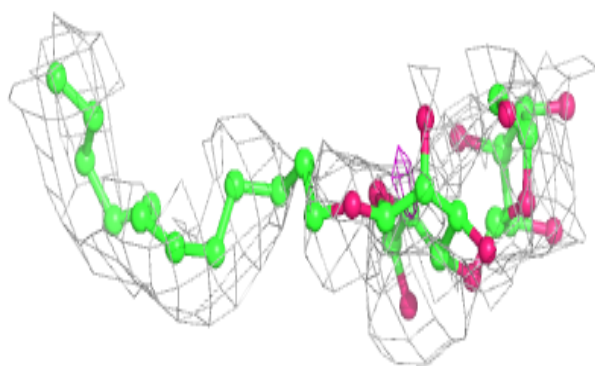
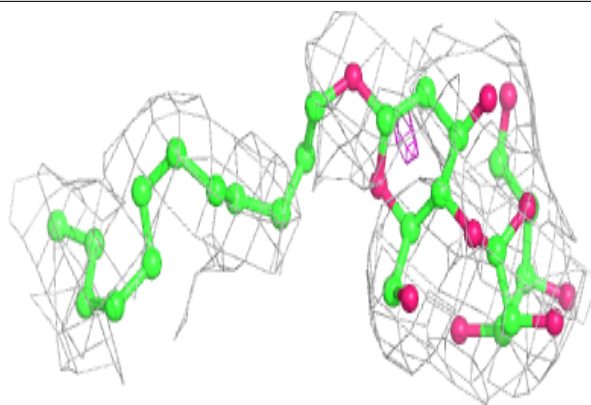
Electron density around CLA A 1309:

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



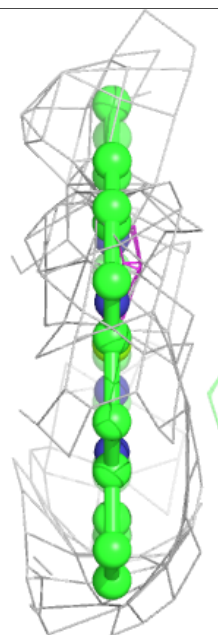
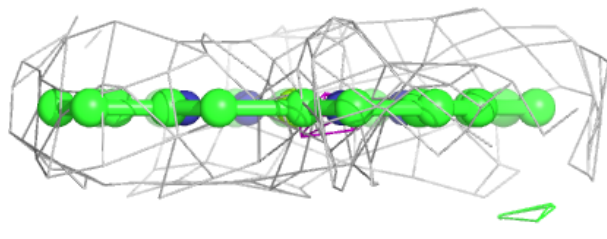
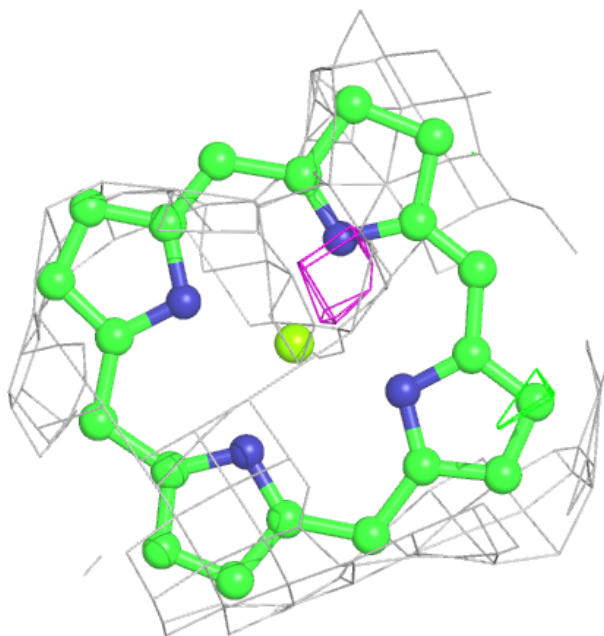
Electron density around LMU E 7048:

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



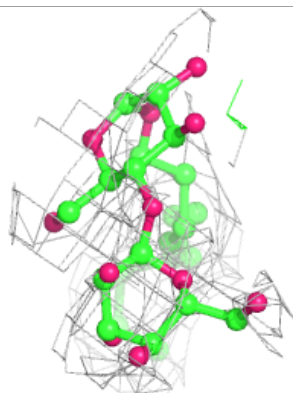
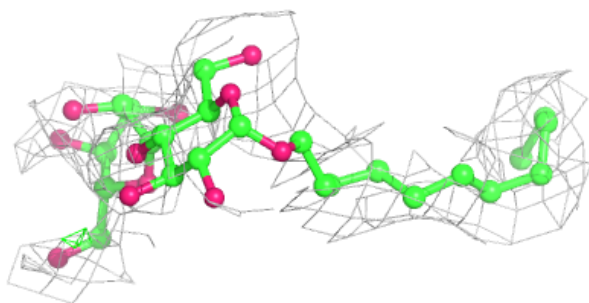
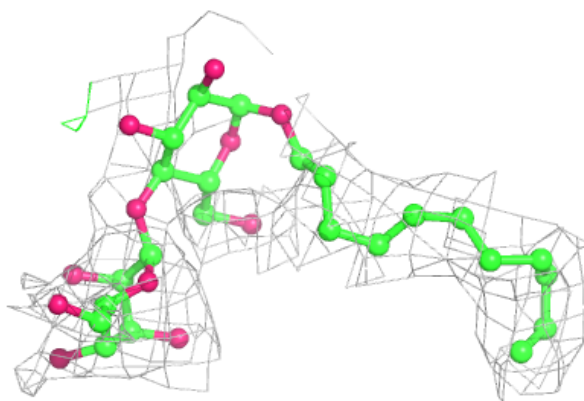
Electron density around CLA 3 3005:

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

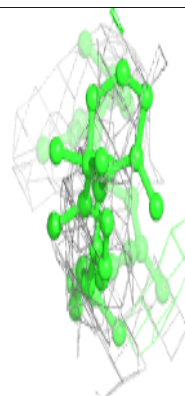
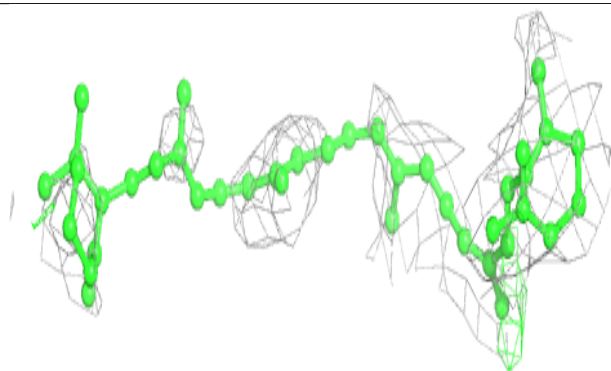
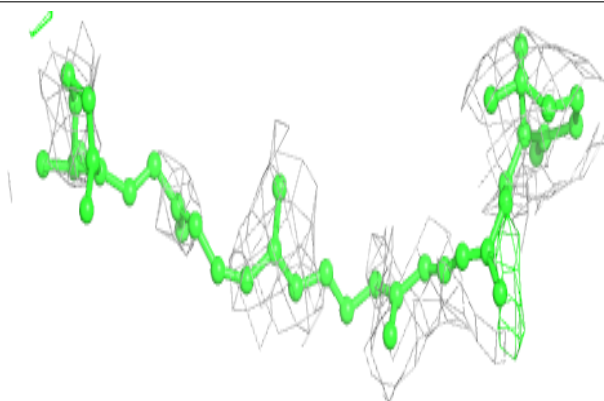


Electron density around LMU 4 7053:

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

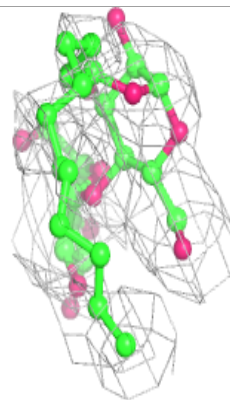
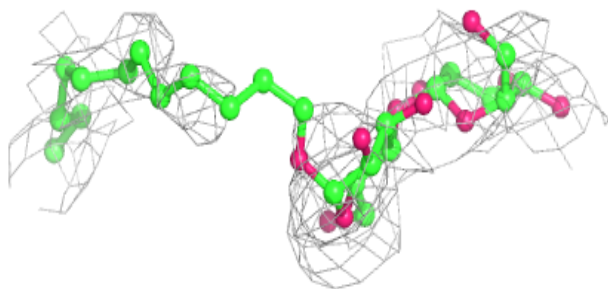
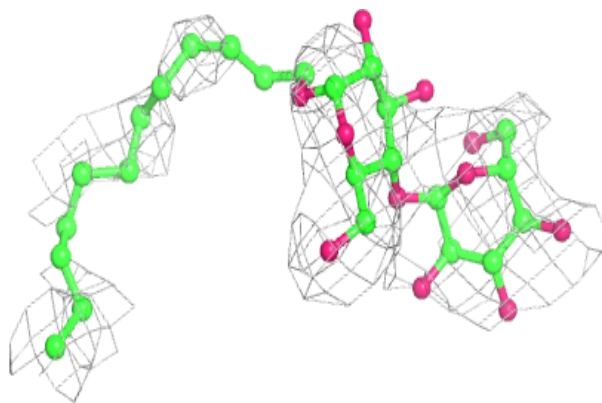
**Electron density around BCR 1 6023:**

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



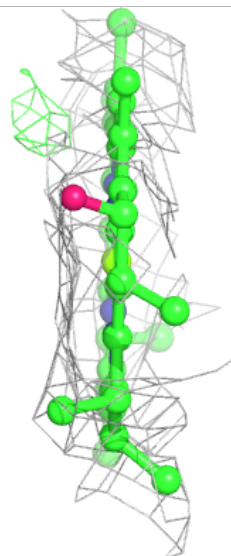
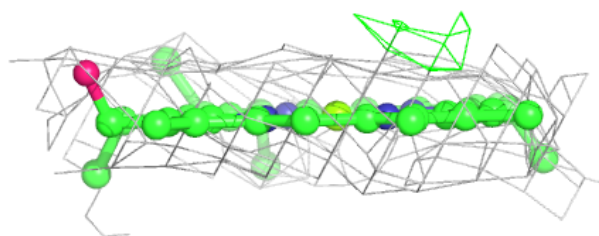
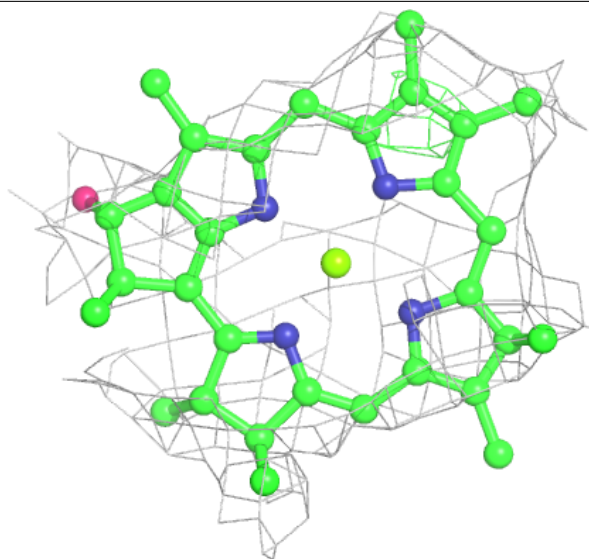
Electron density around LMU 1 7004:

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



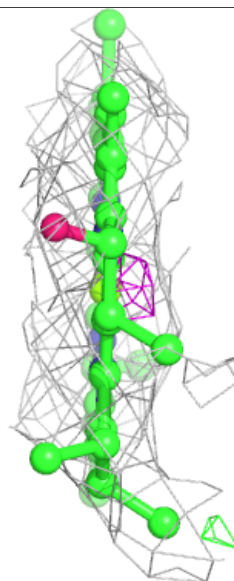
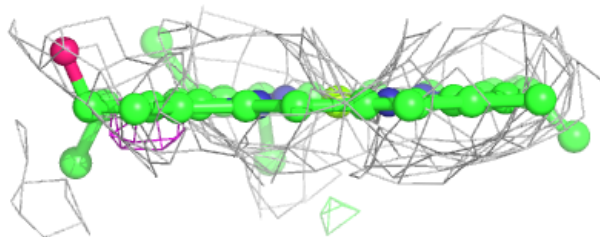
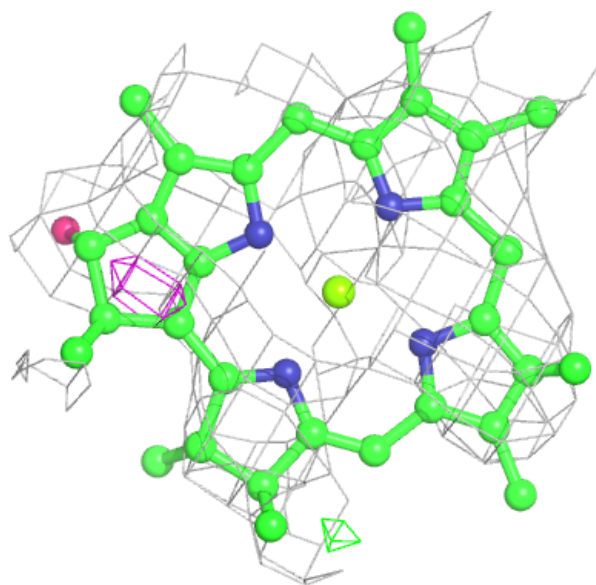
Electron density around CLA 3 1118:

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



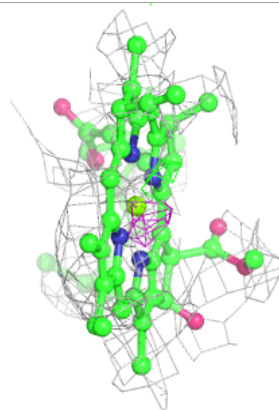
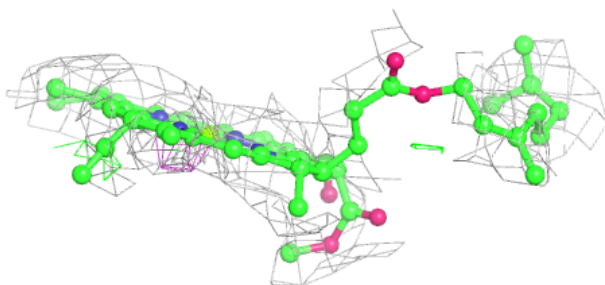
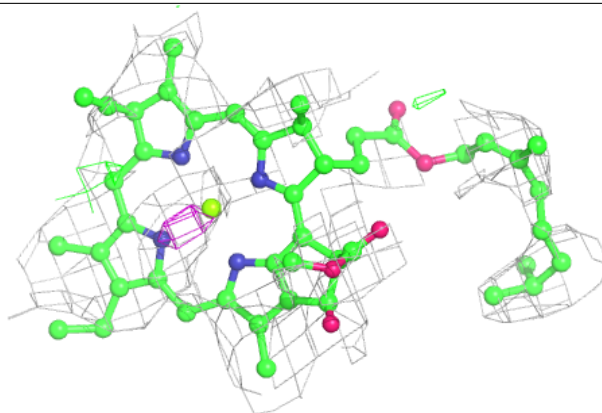
Electron density around CLA 1 1006:

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

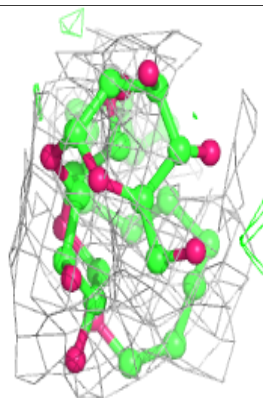
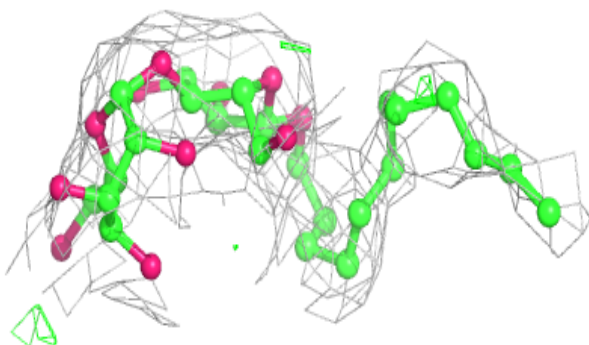
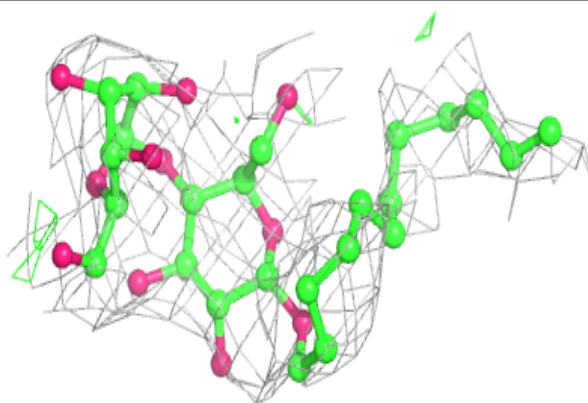


Electron density around CLA 4 4003:

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

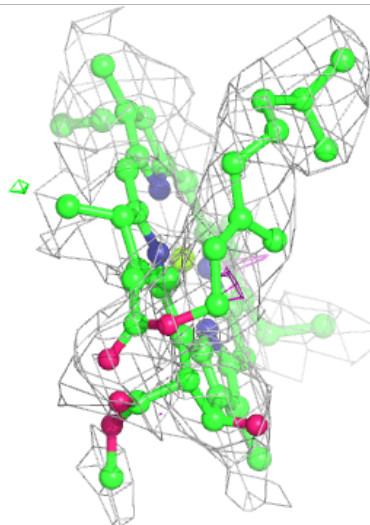
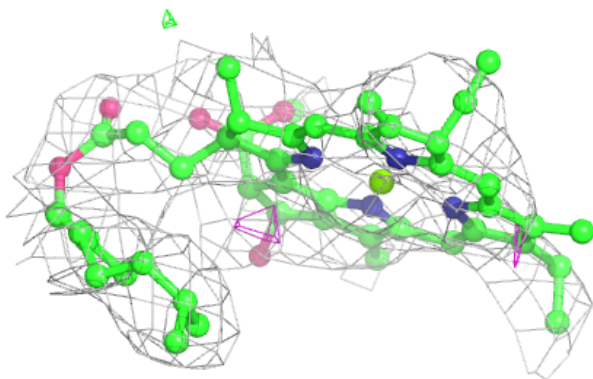
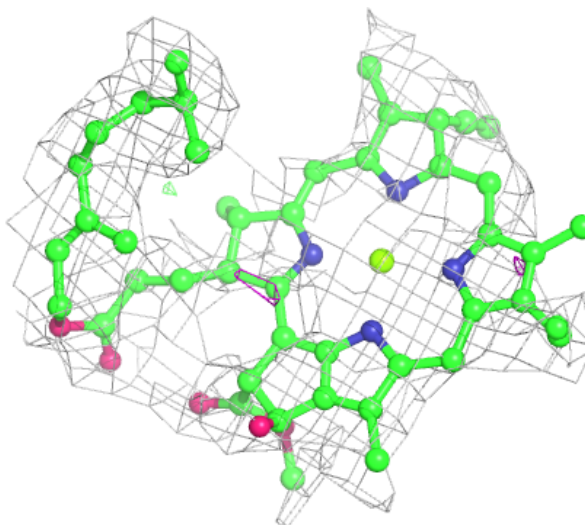
**Electron density around LMU L 7029:**

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



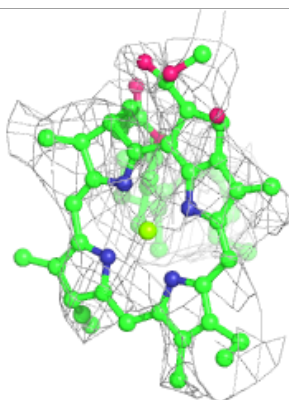
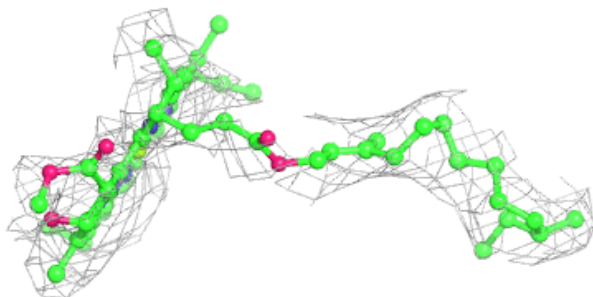
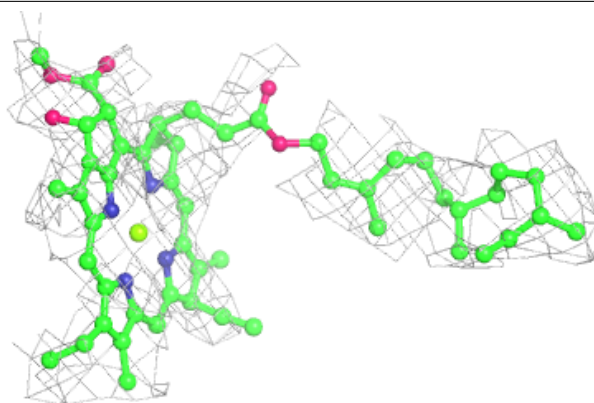
Electron density around CLA H 1505:

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

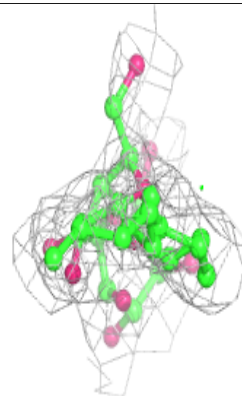
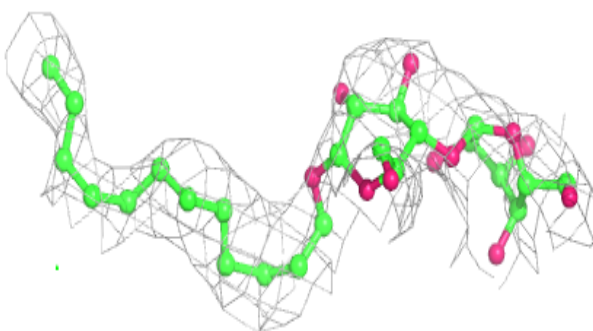
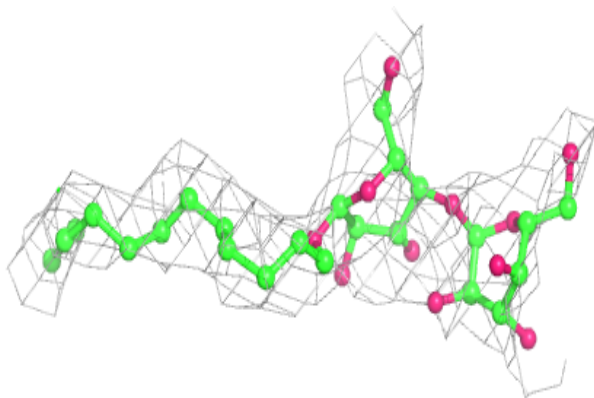


Electron density around CLA 2 2014:

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

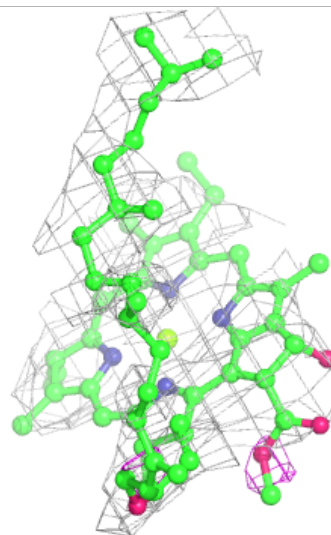
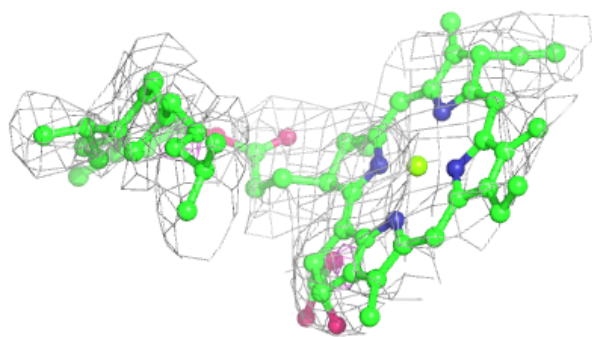
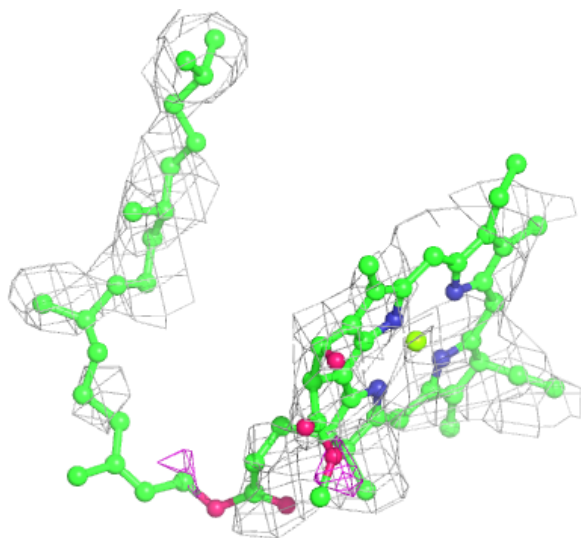
**Electron density around LMU A 7010:**

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



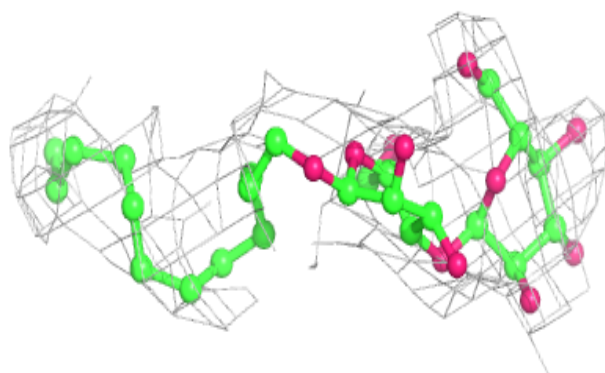
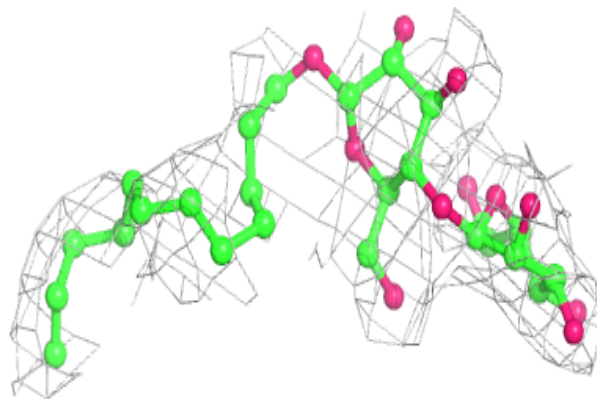
Electron density around CLA 3 3016:

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

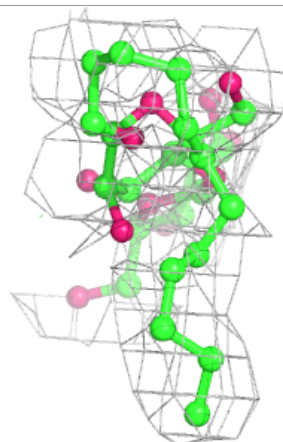
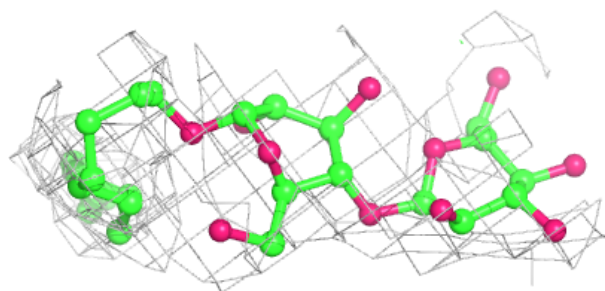
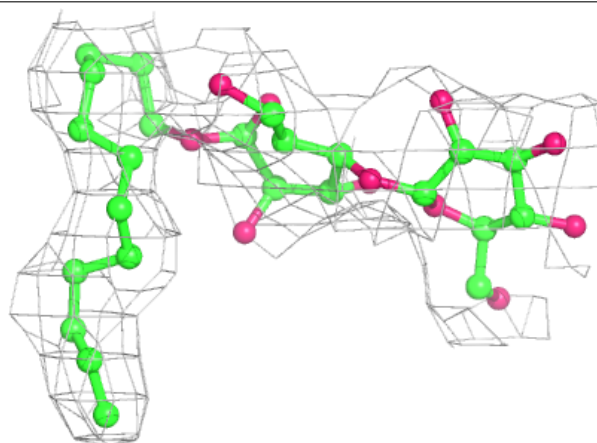


Electron density around LMU 2 7046:

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

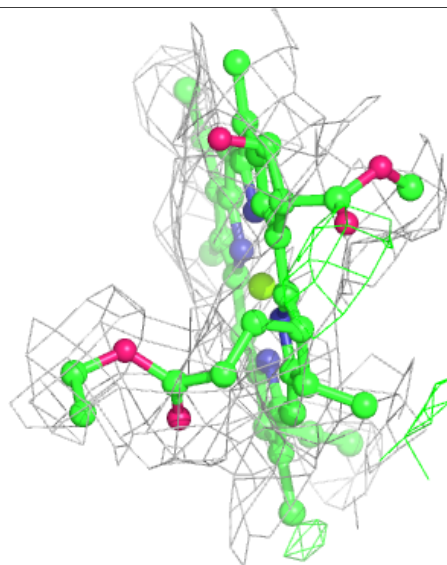
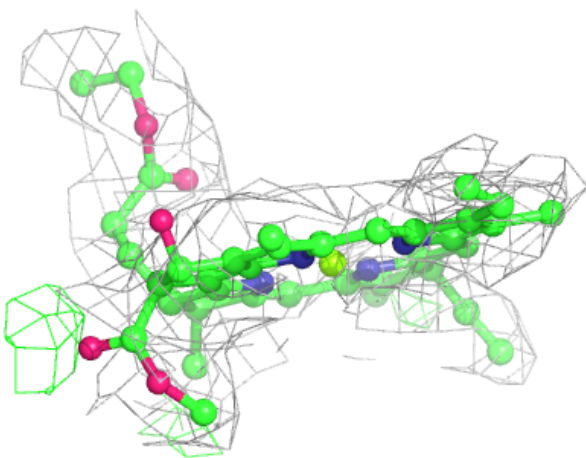
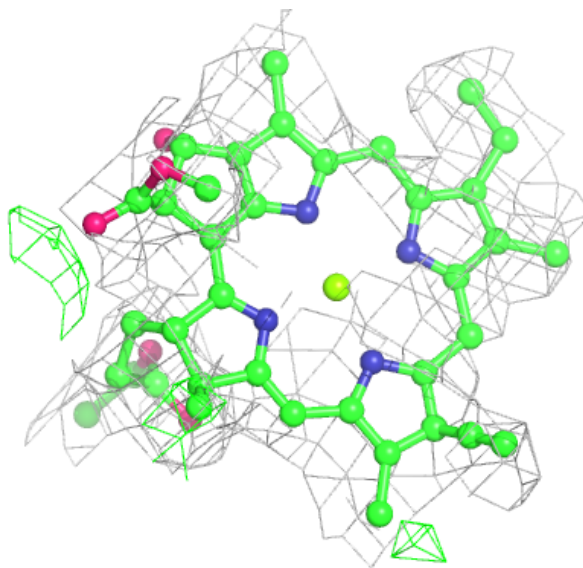
**Electron density around LMU 4 7052:**

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



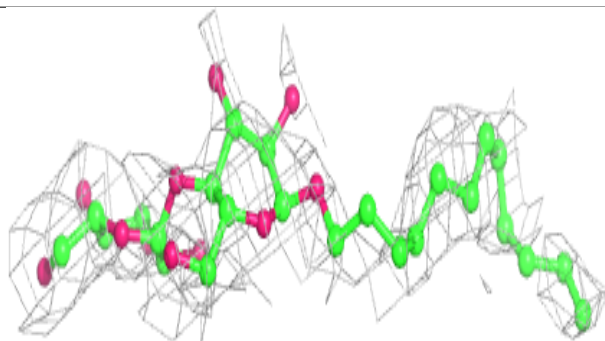
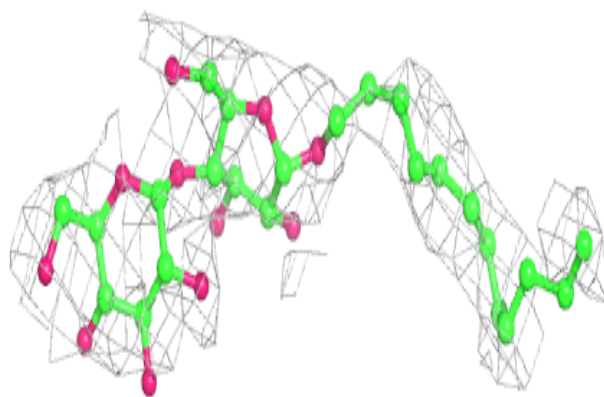
Electron density around CLA 4 4014:

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

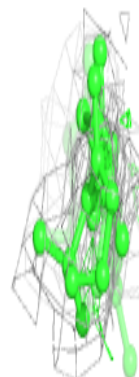
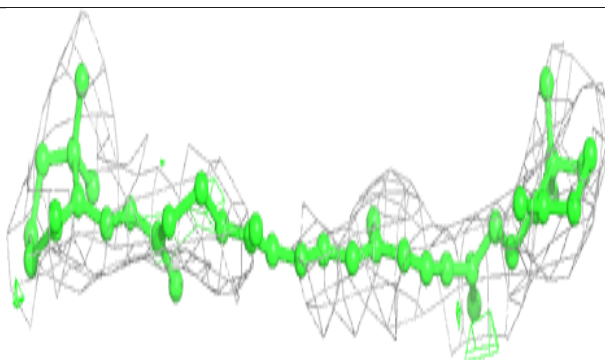
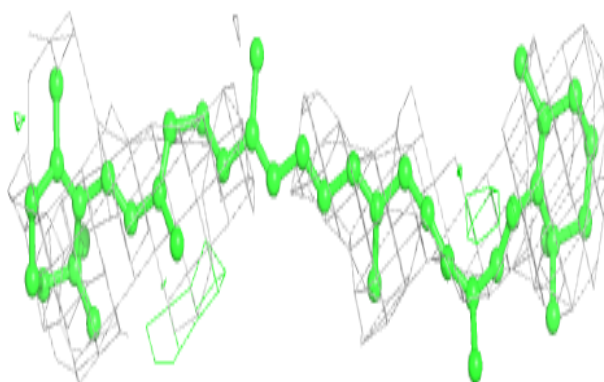


Electron density around LMU B 7038:

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

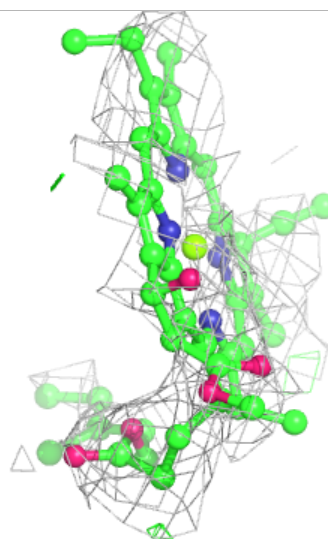
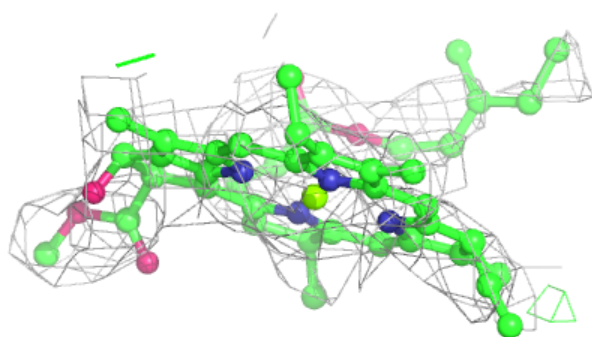
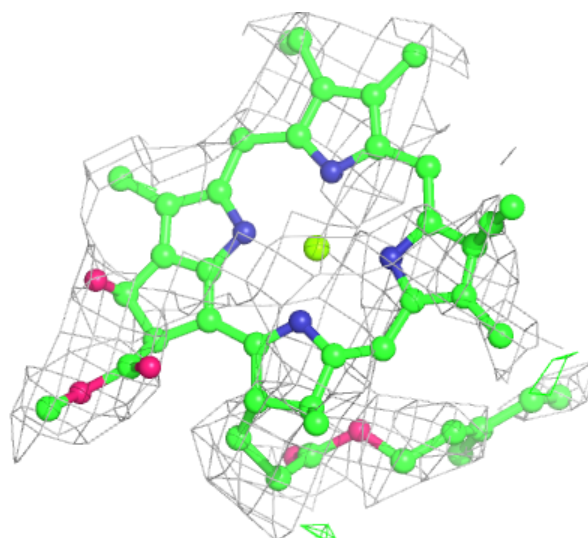
**Electron density around BCR A 6002:**

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



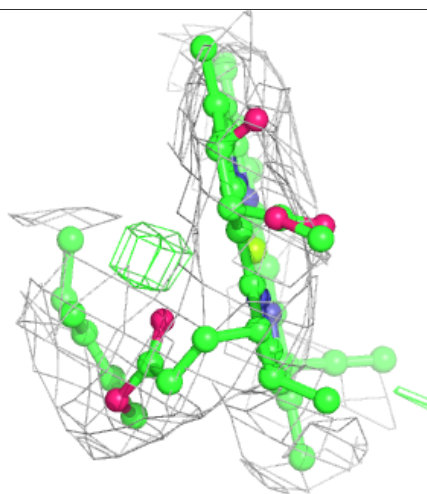
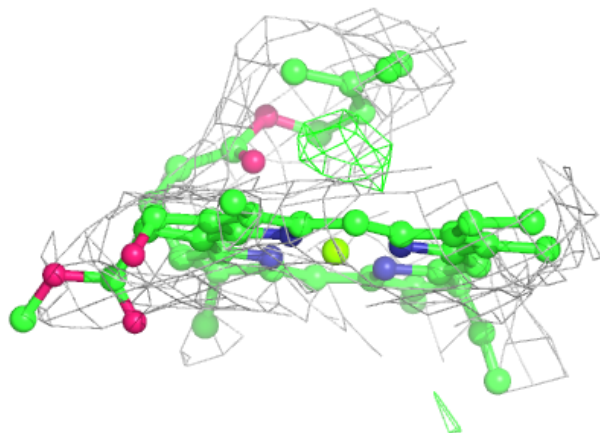
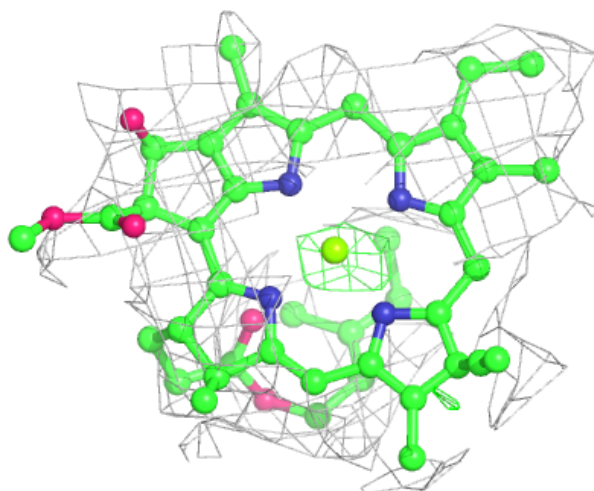
Electron density around CLA B 1233:

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



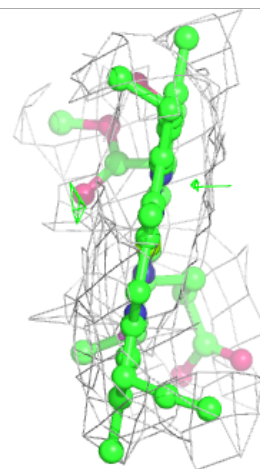
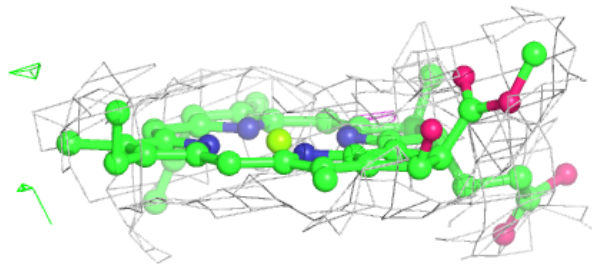
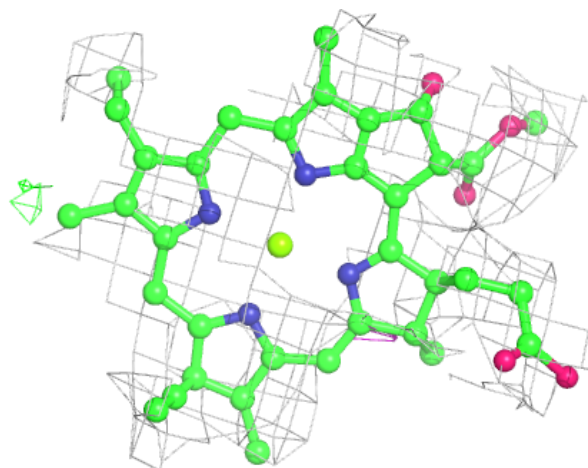
Electron density around CLA 2 2001:

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



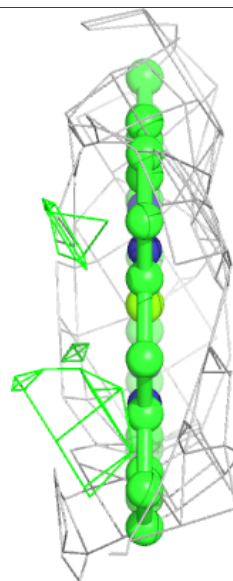
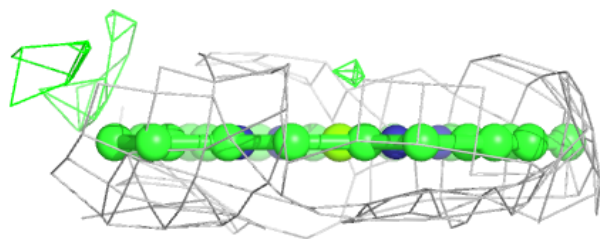
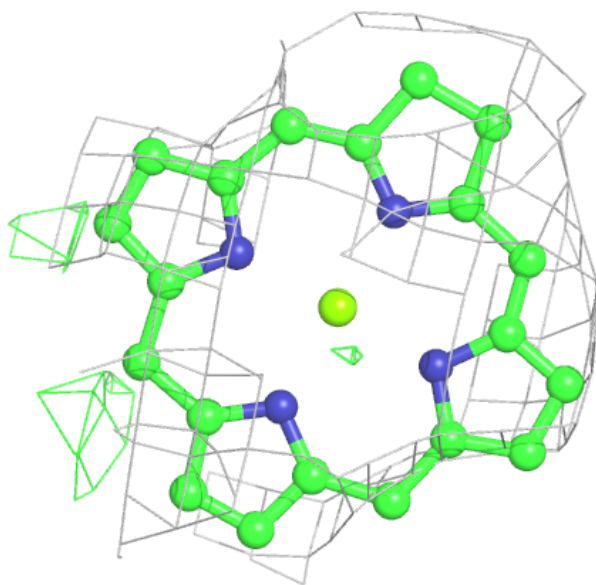
Electron density around CLA K 1142:

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



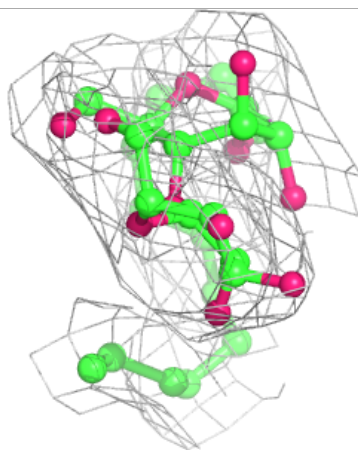
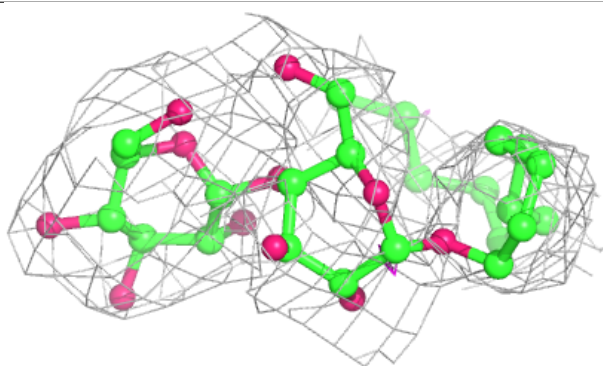
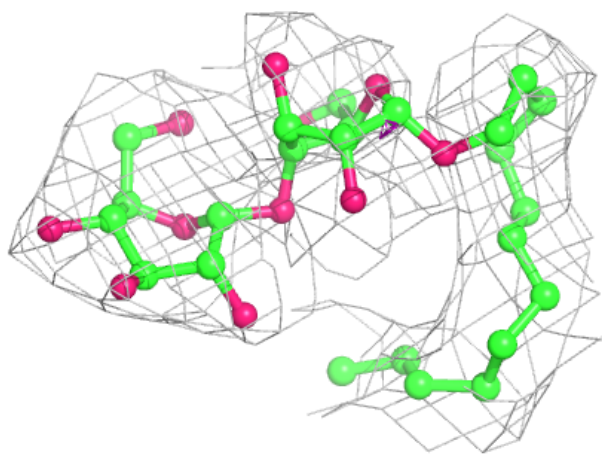
Electron density around CLA 2 2005:

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



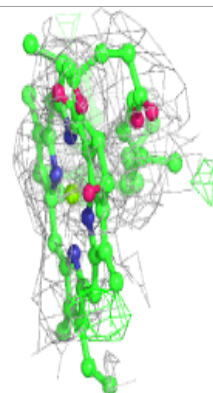
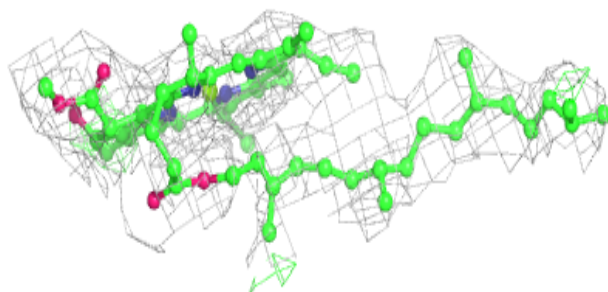
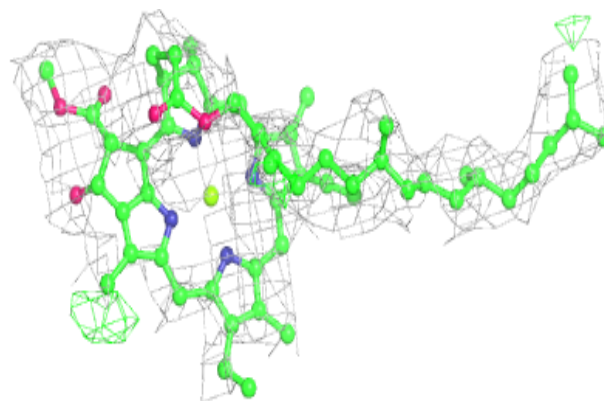
Electron density around LMU N 7049:

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



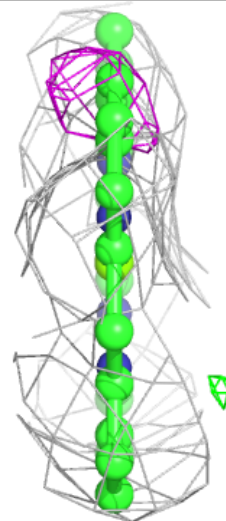
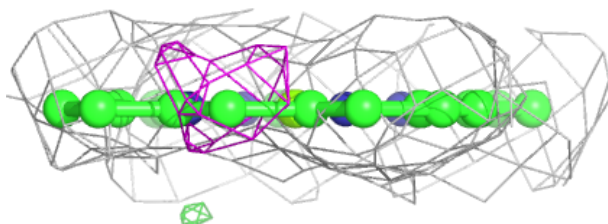
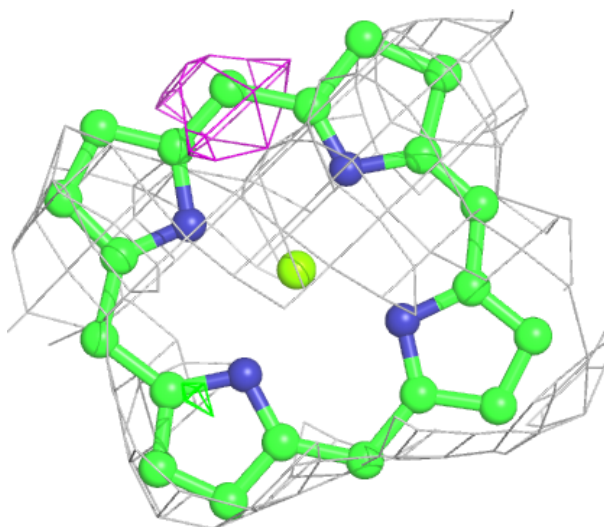
Electron density around CLA 2 2007:

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



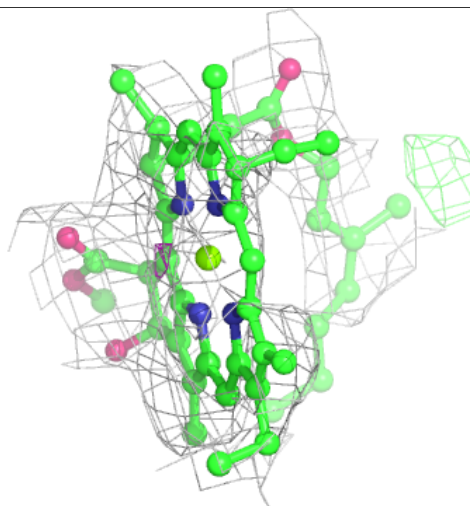
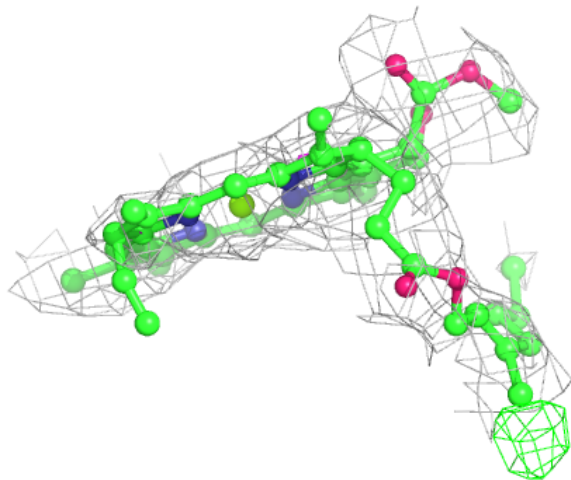
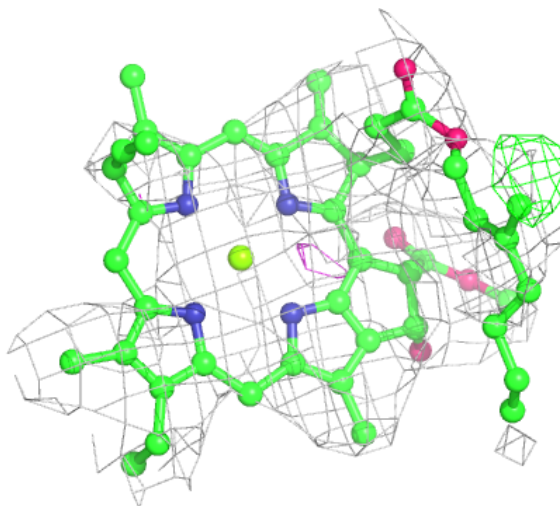
Electron density around CLA 4 4004:

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



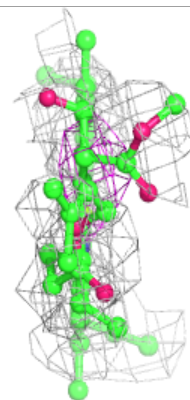
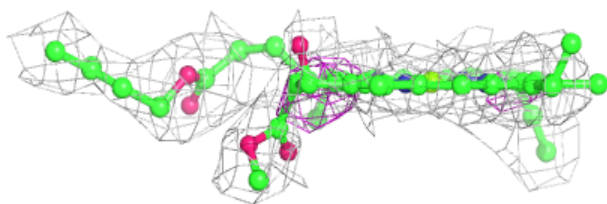
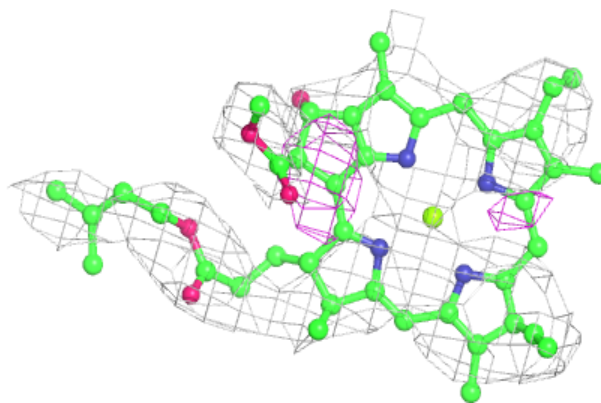
Electron density around CLA F 1305:

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

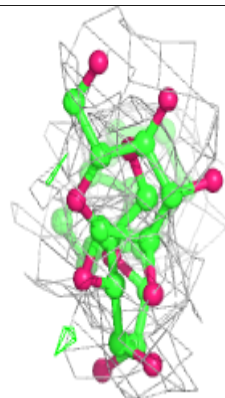
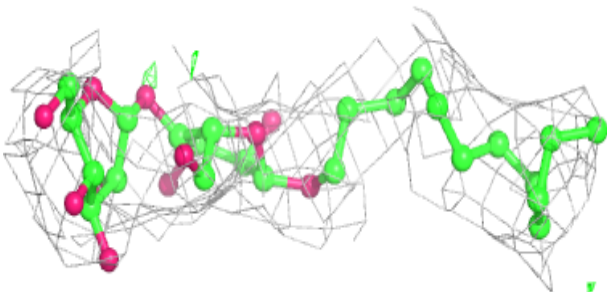
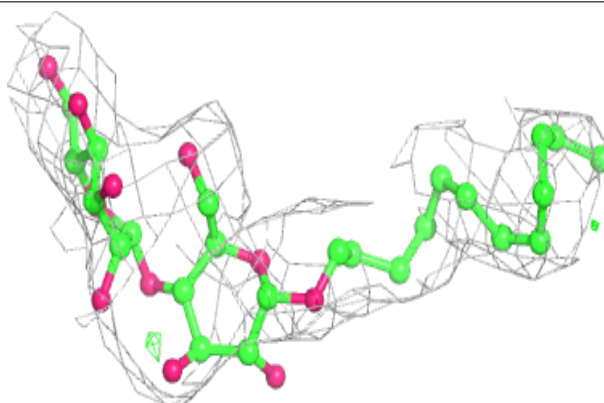


Electron density around CLA 4 4001:

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

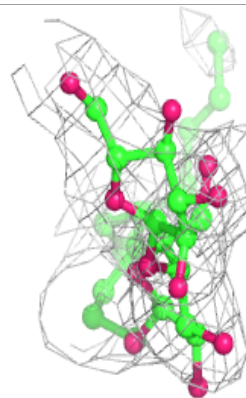
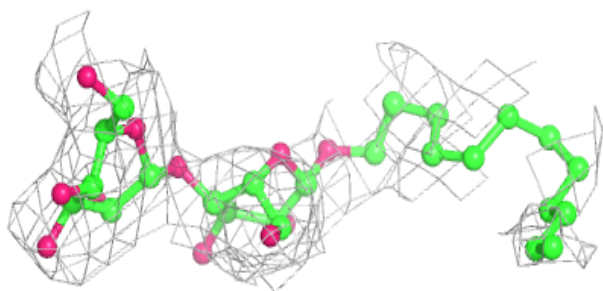
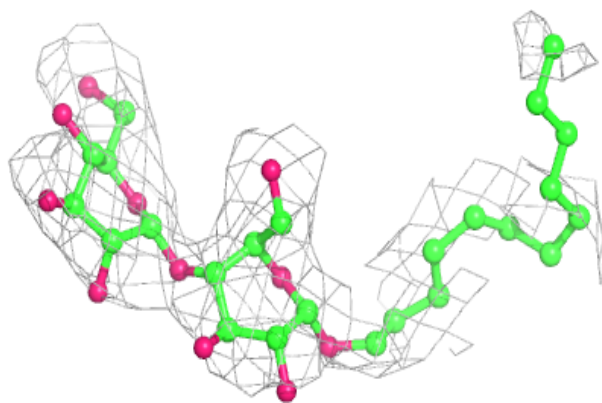
**Electron density around LMU H 7011:**

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



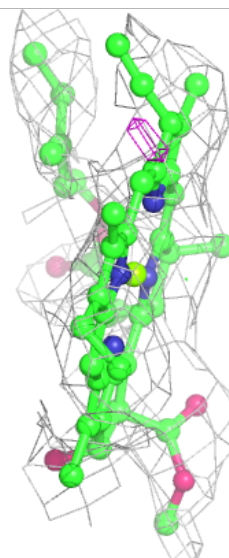
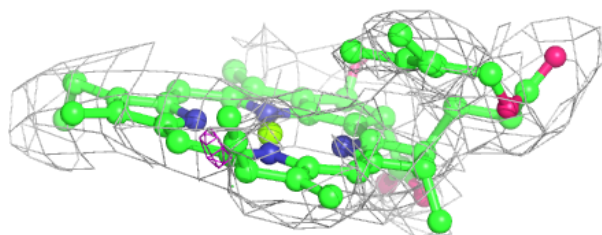
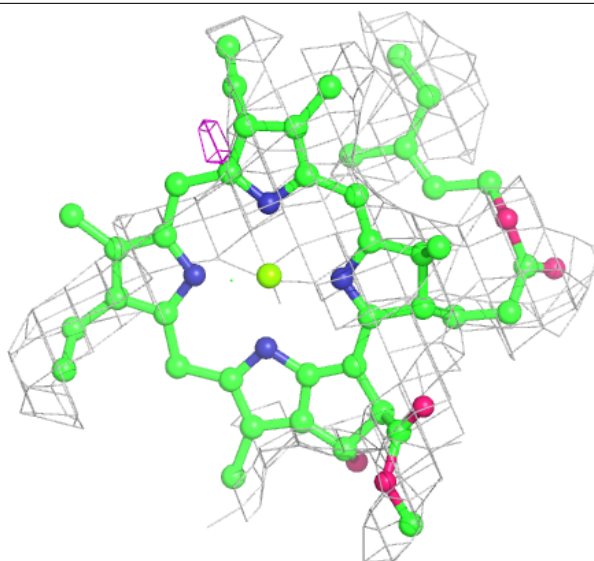
Electron density around LMU H 7030:

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



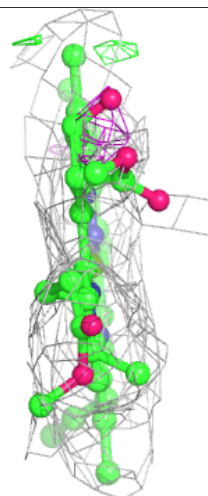
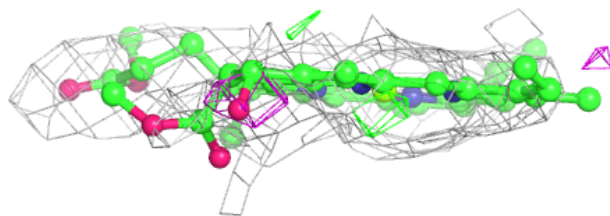
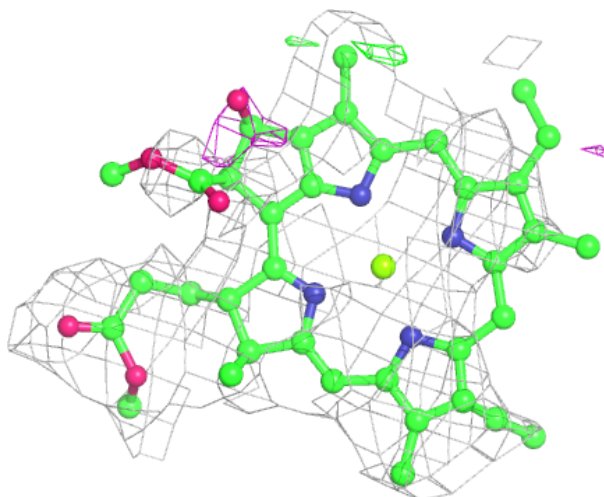
Electron density around CLA G 1242:

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



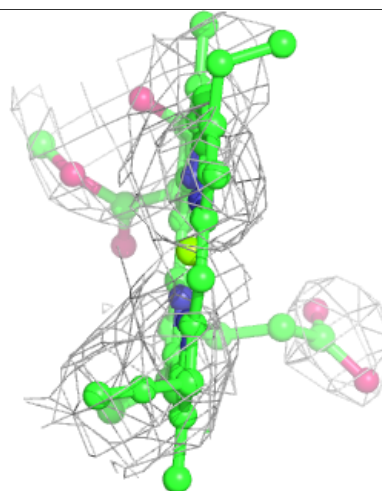
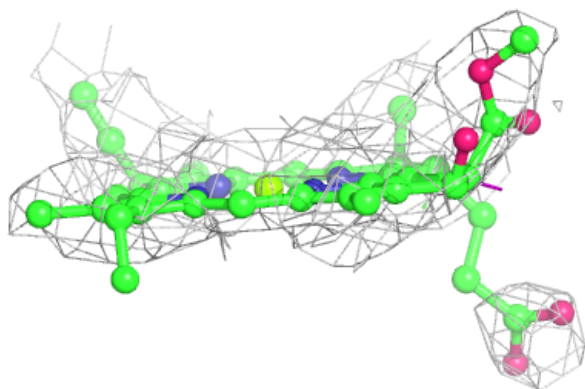
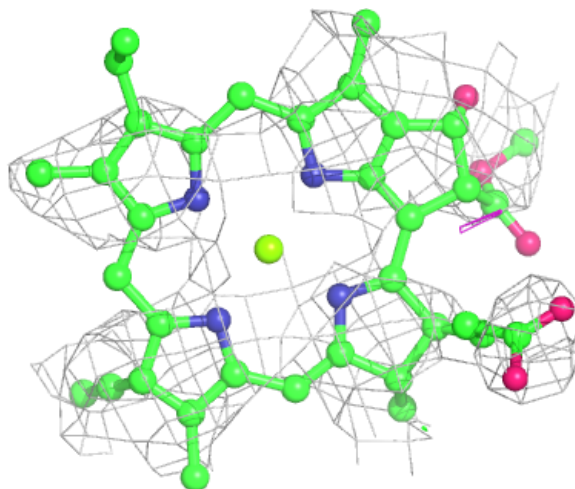
Electron density around CLA B 1213:

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



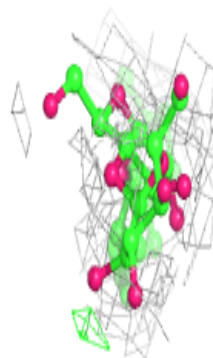
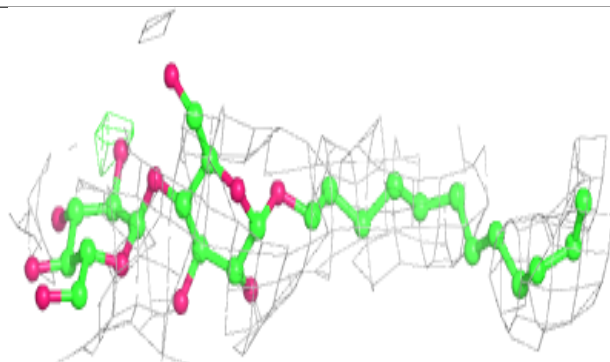
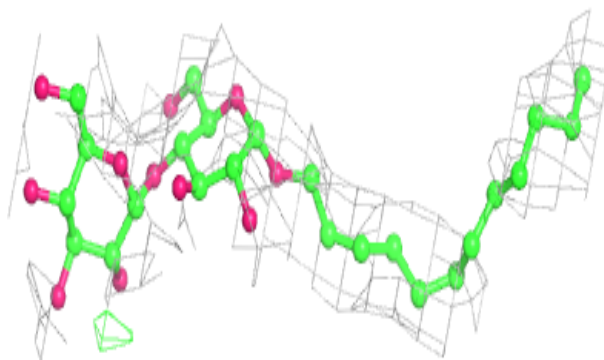
Electron density around CLA B 1232:

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



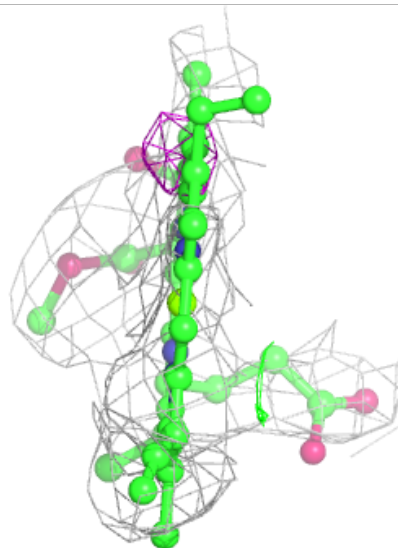
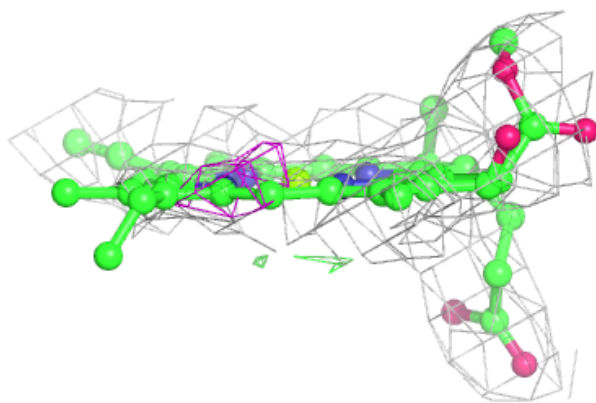
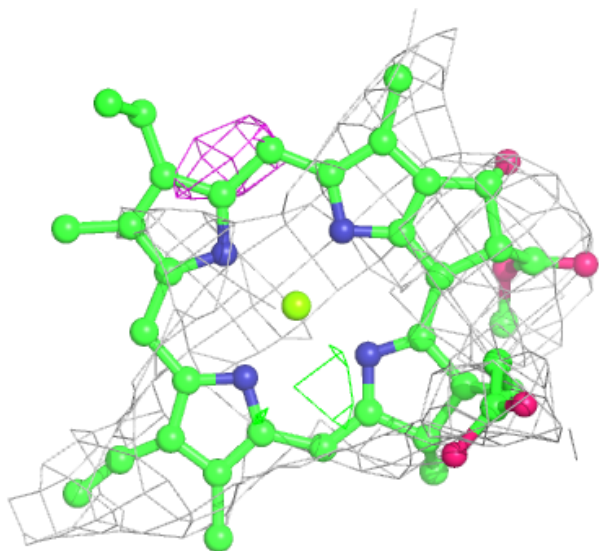
Electron density around LMU B 7040:

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



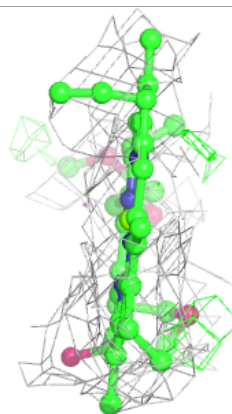
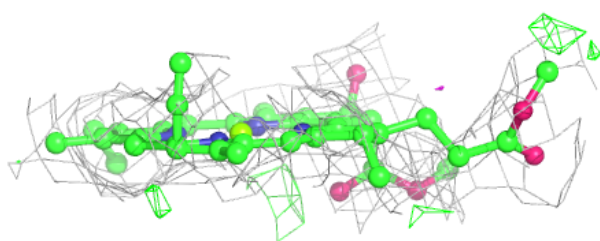
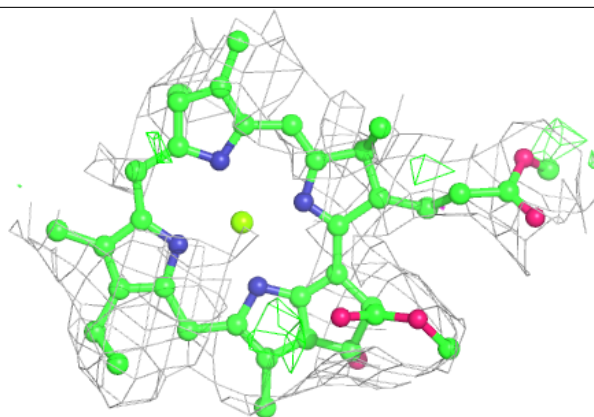
Electron density around CLA A 1112:

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



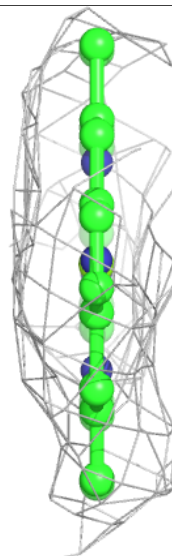
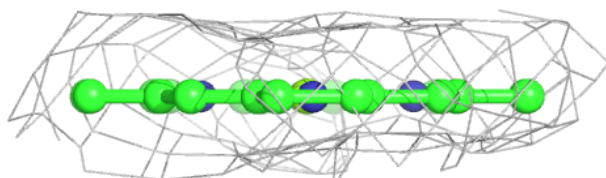
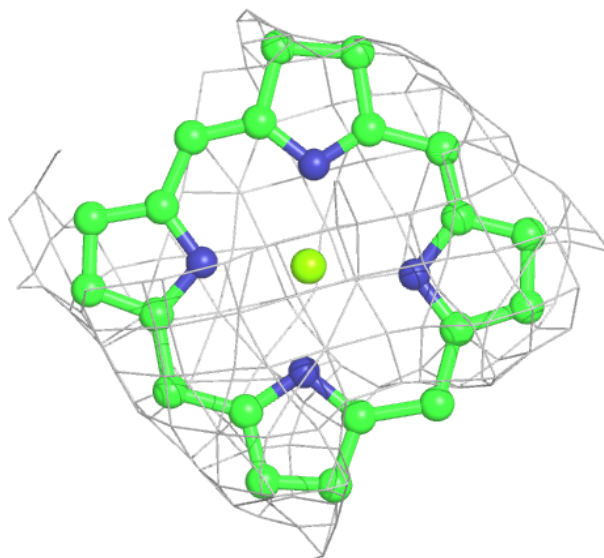
Electron density around CLA 1 1010:

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



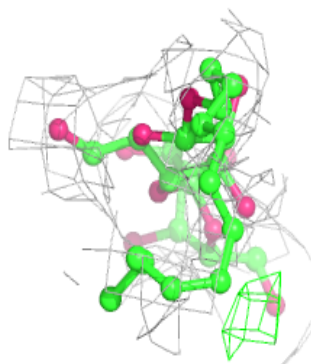
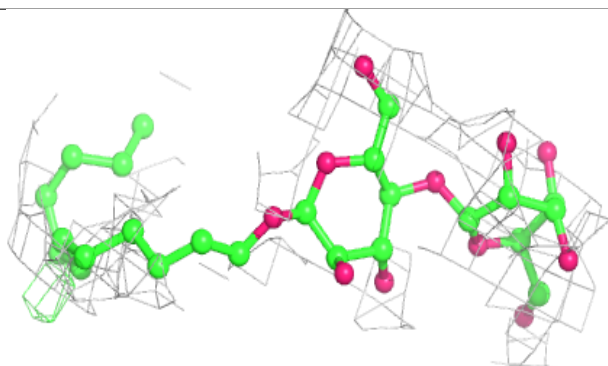
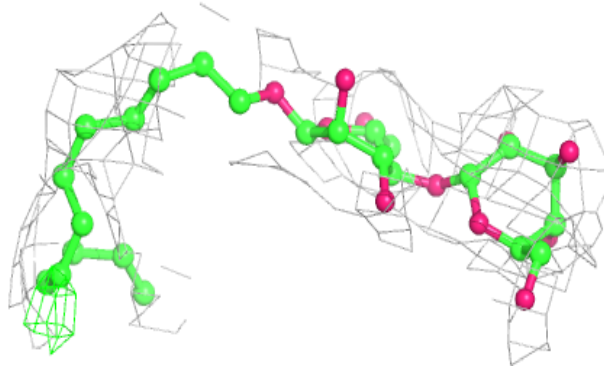
Electron density around CLA 1 1310:

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

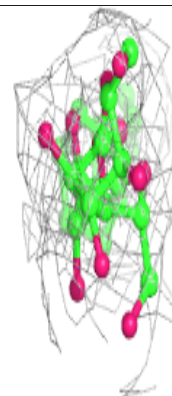
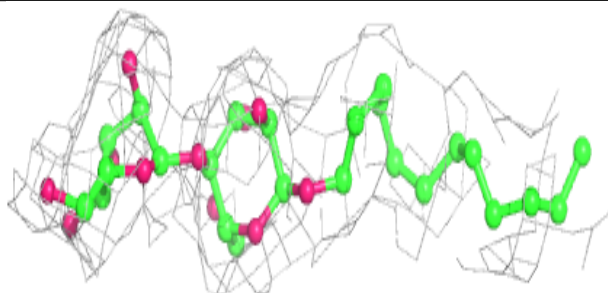
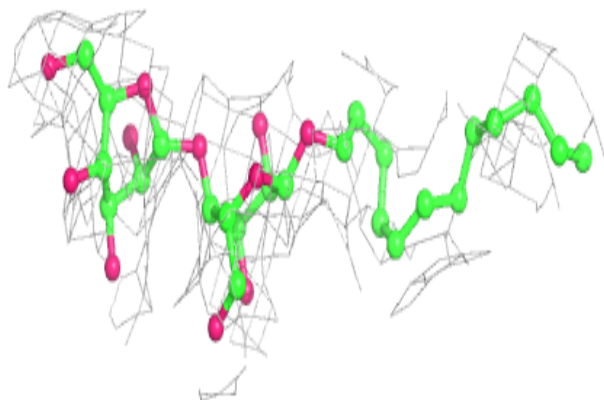


Electron density around LMU H 7043:

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

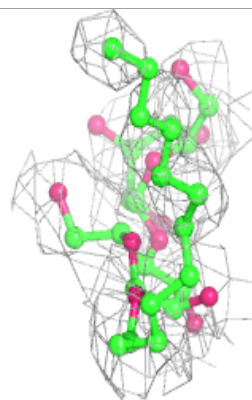
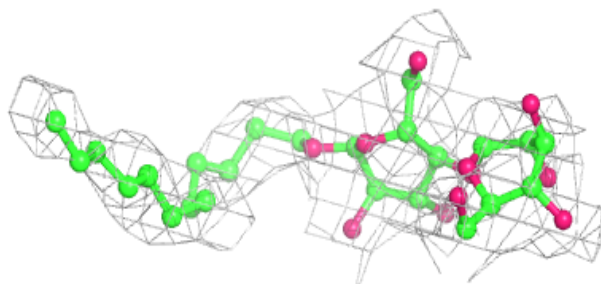
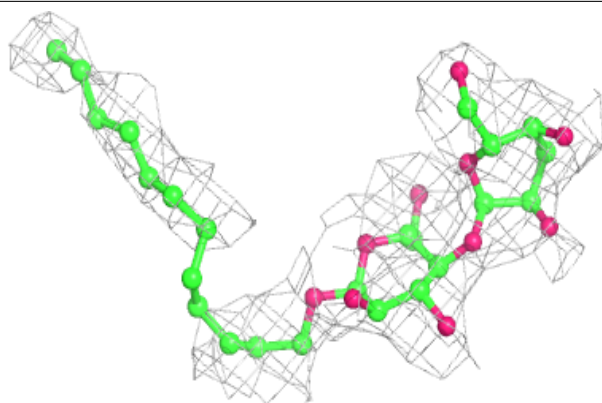
**Electron density around LMU E 7037:**

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



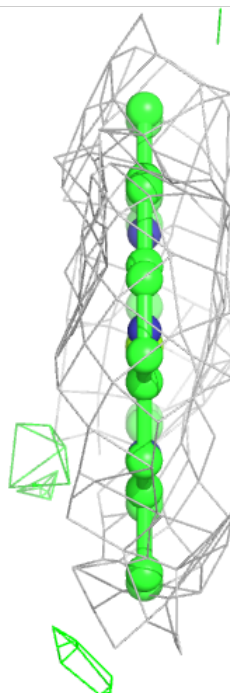
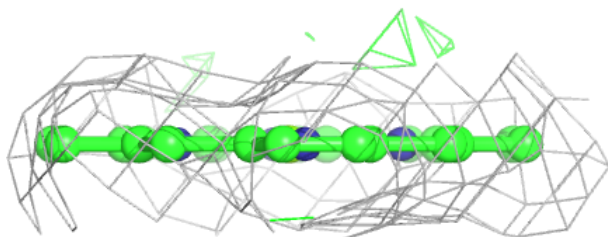
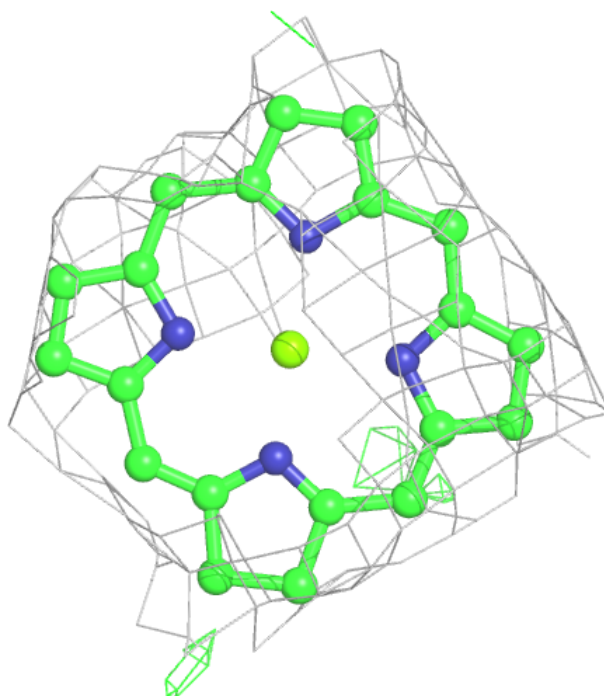
Electron density around LMU 4 7008:

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



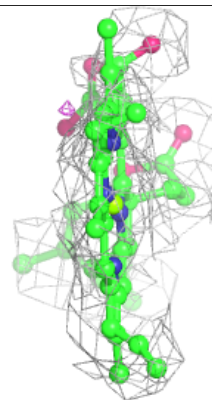
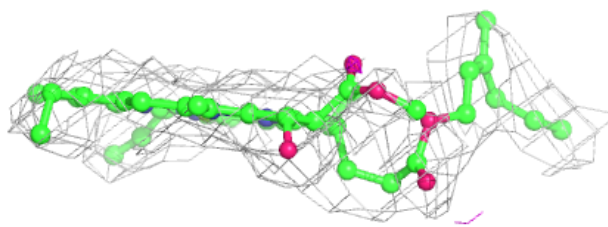
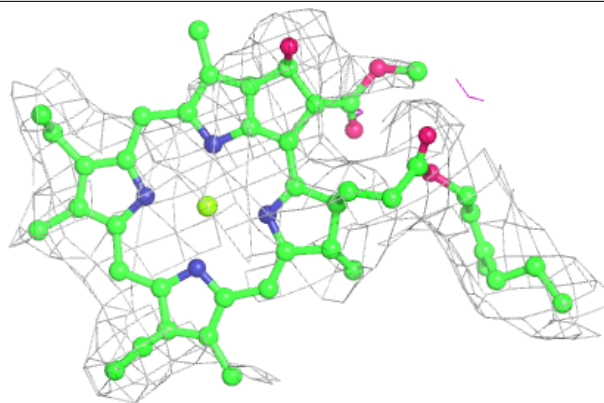
Electron density around CLA 3 3010:

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



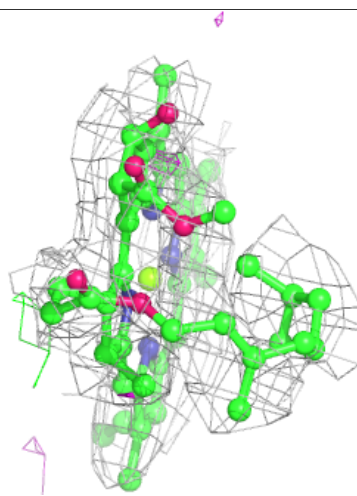
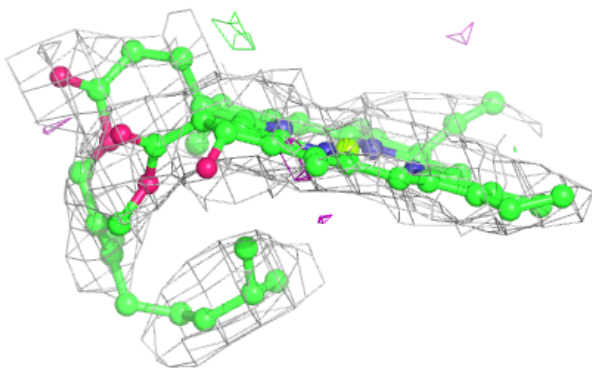
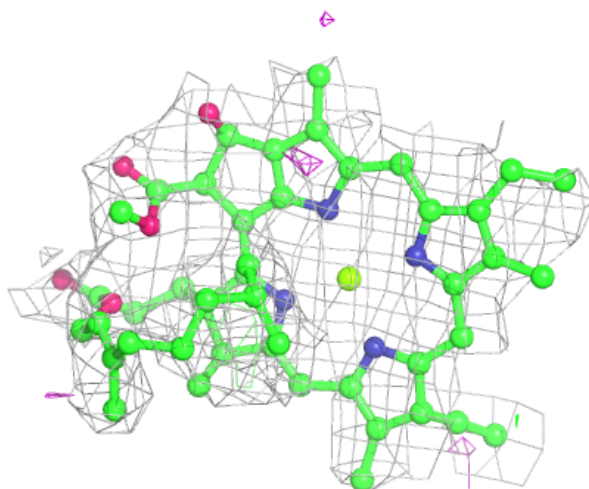
Electron density around CLA 4 4007:

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



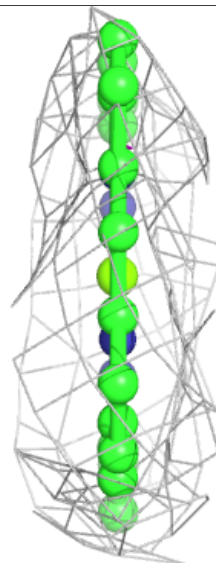
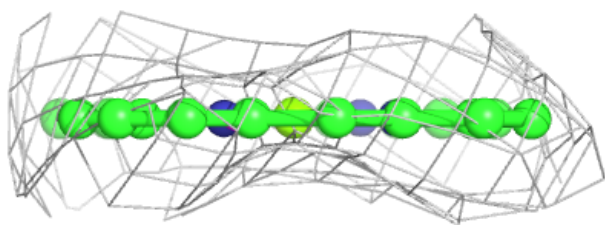
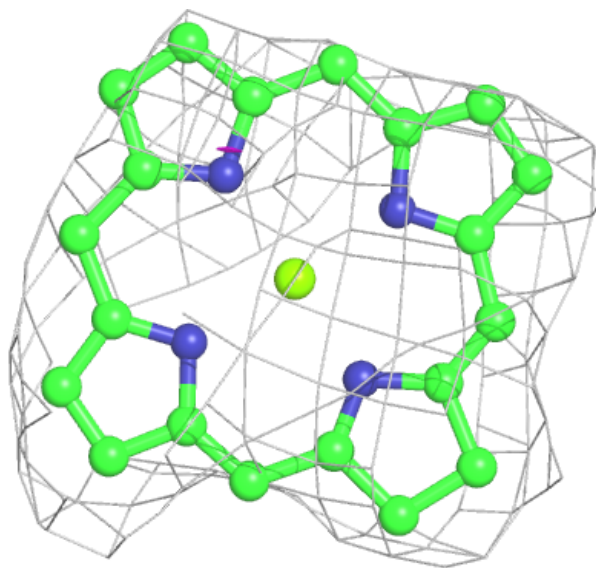
Electron density around CLA 4 1306:

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



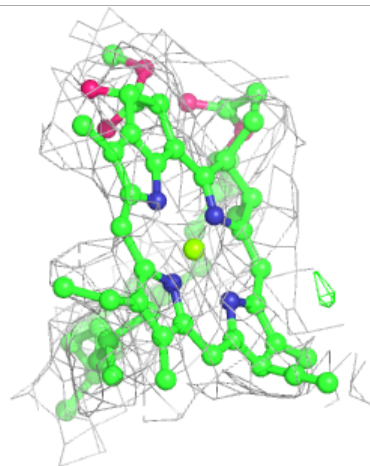
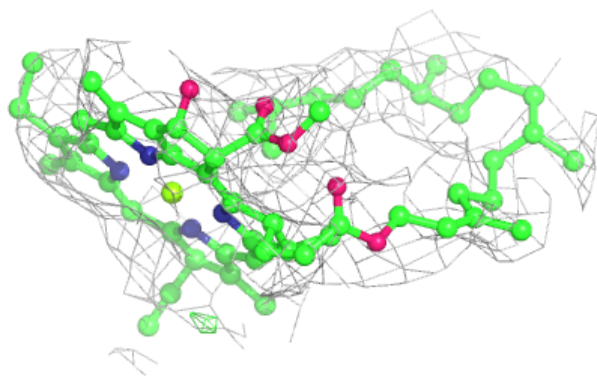
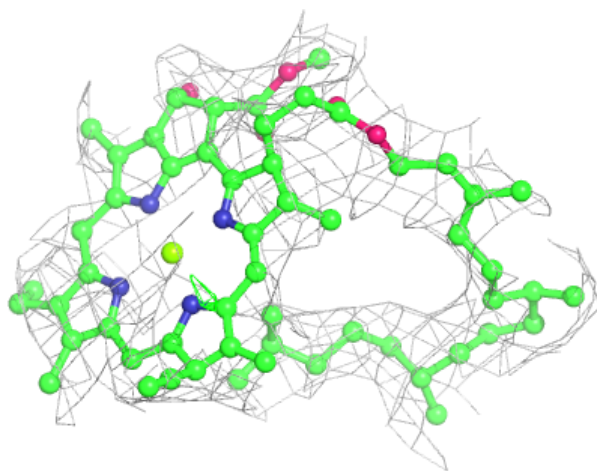
Electron density around CLA 2 2011:

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



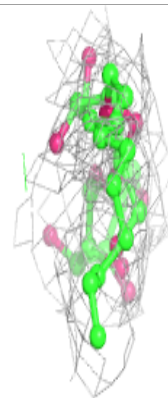
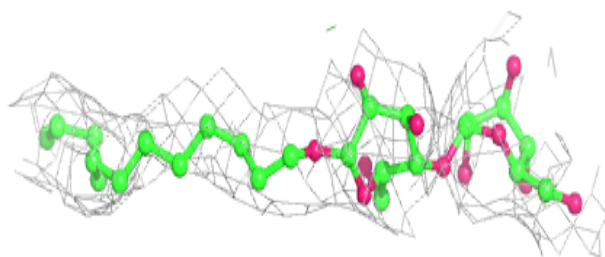
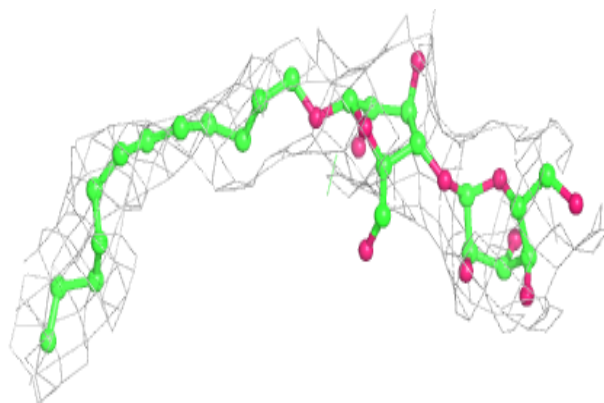
Electron density around CLA A 1141:

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

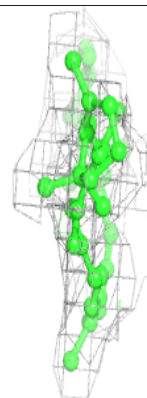
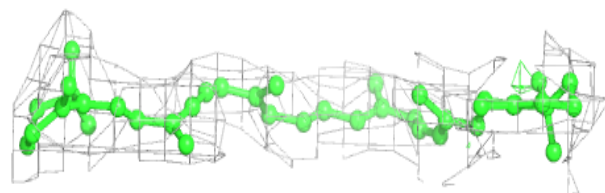
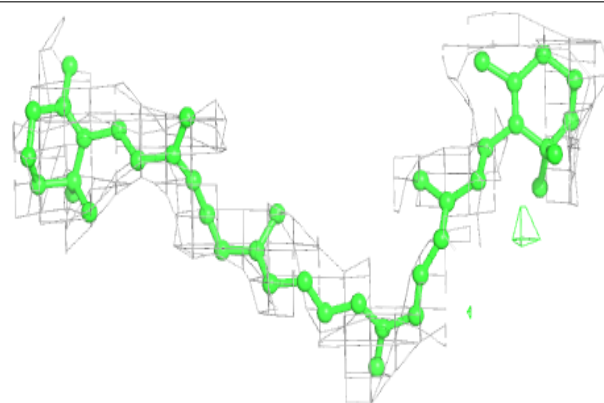


Electron density around LMU G 7051:

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

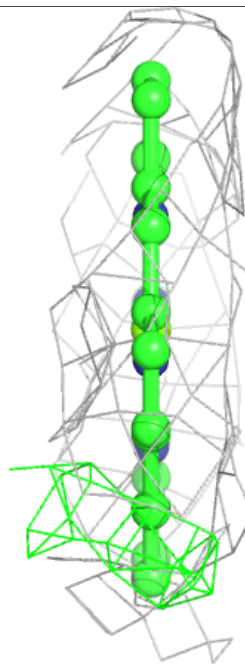
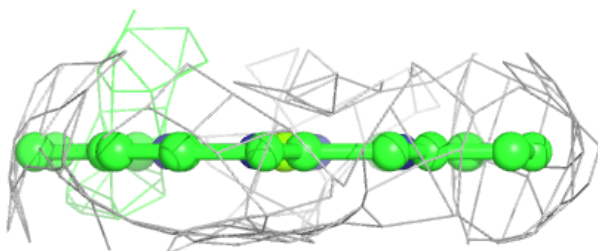
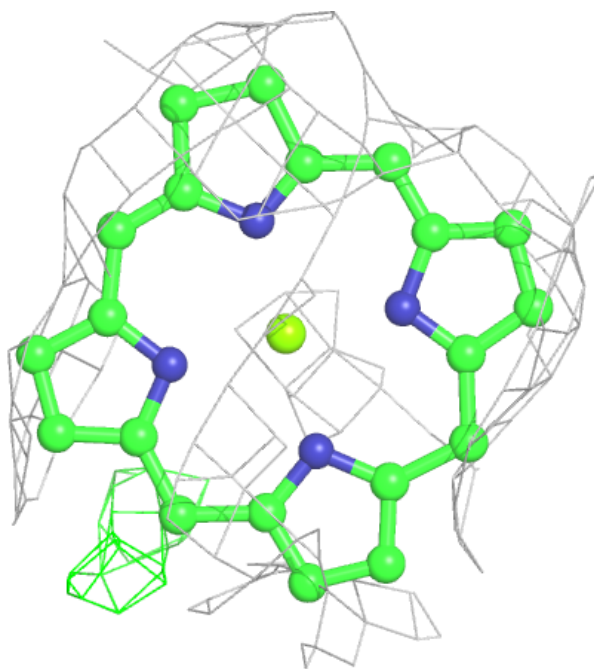
**Electron density around BCR 3 6022:**

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



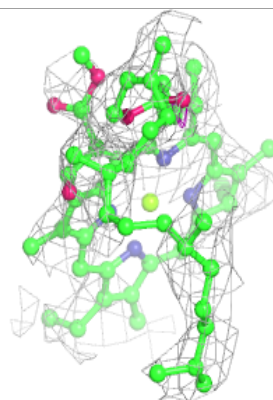
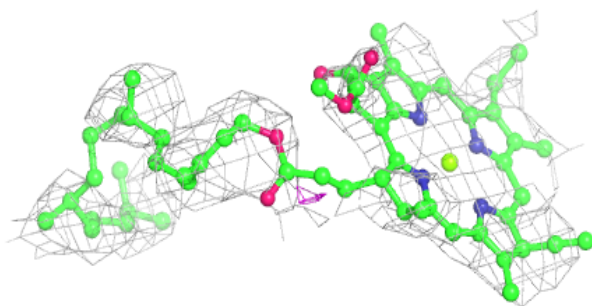
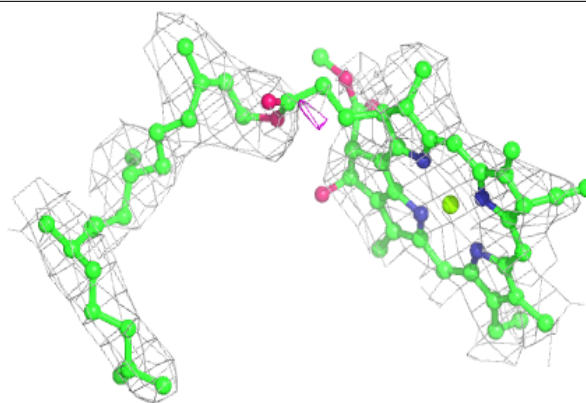
Electron density around CLA 1 1015:

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

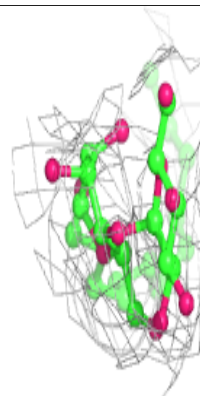
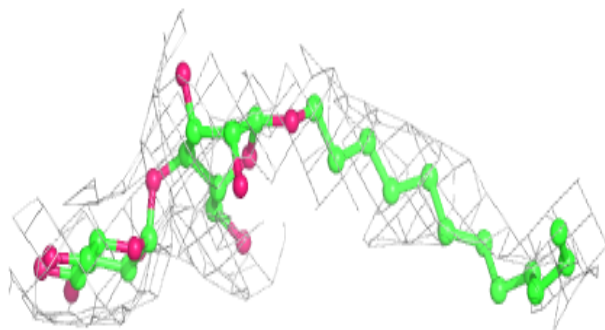
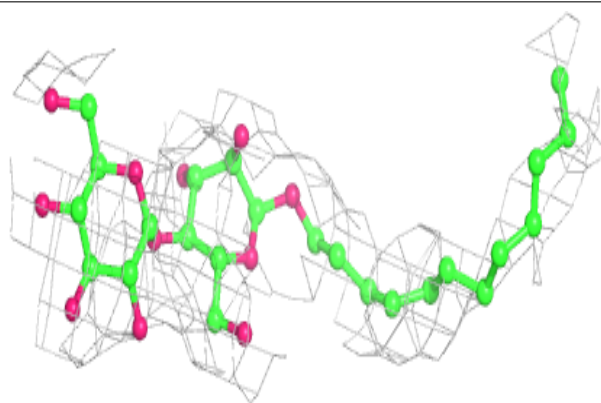


Electron density around CLA K 3009:

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

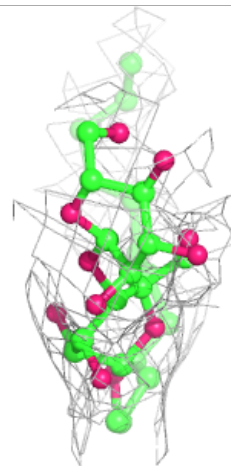
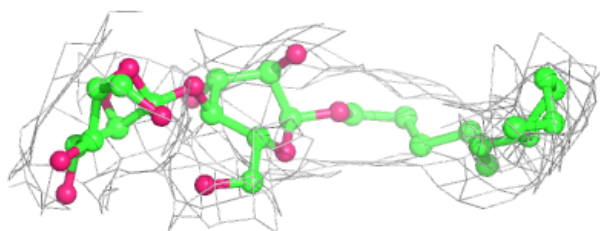
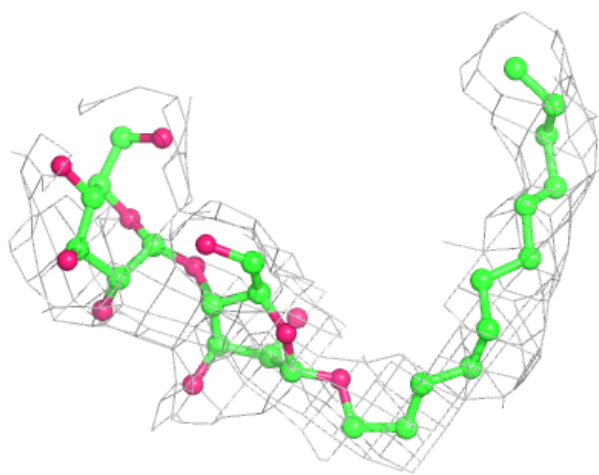
**Electron density around LMU K 7047:**

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



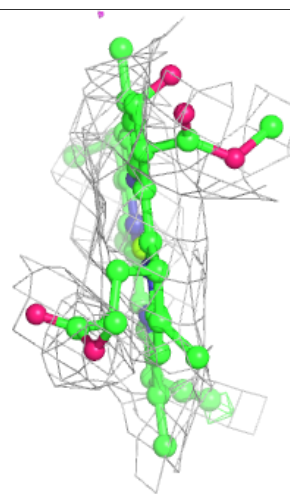
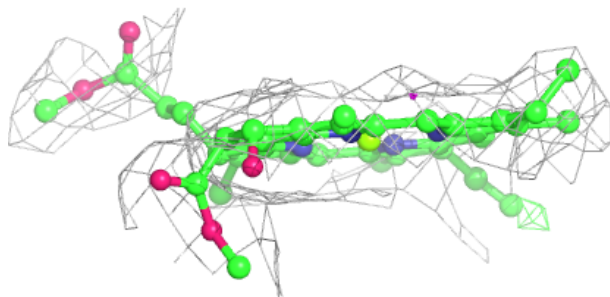
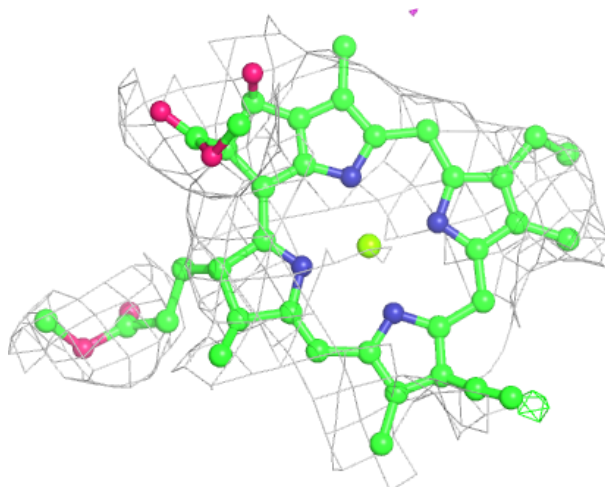
Electron density around LMU K 7041:

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



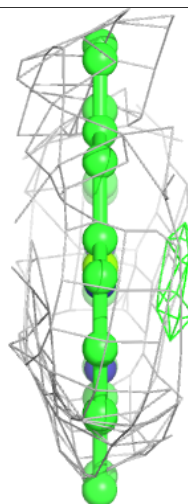
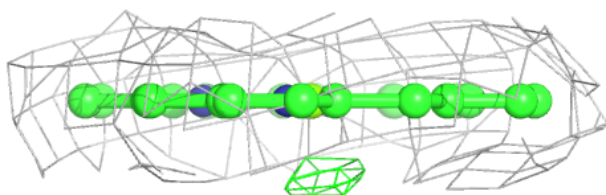
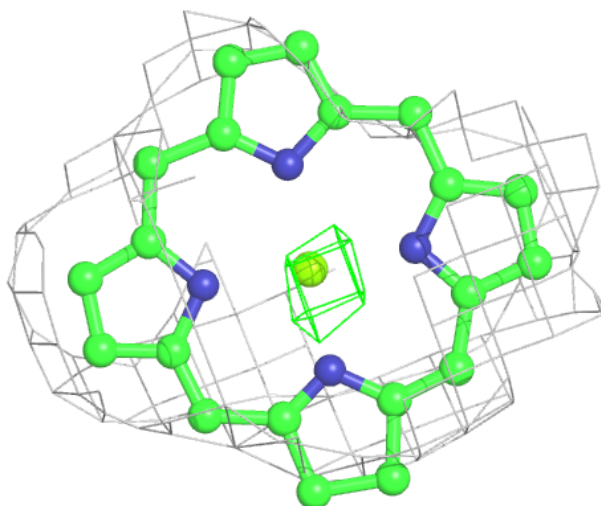
Electron density around CLA 1 1001:

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



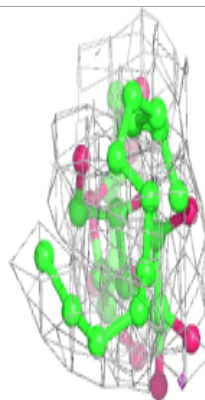
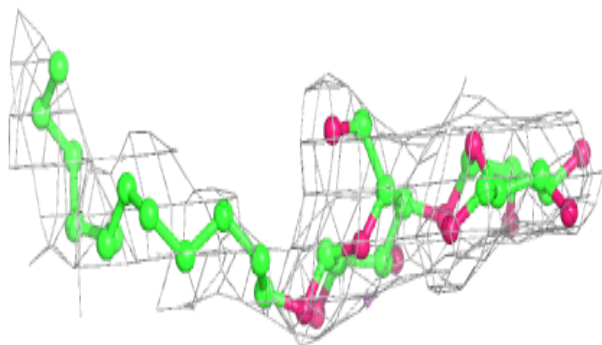
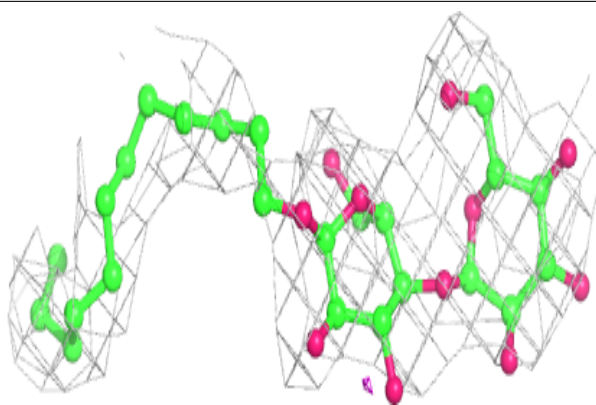
Electron density around CLA 2 2008:

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

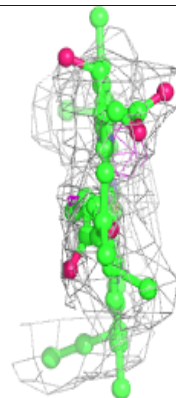
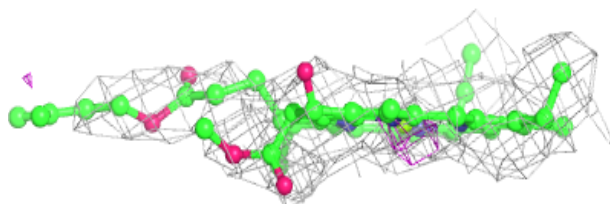
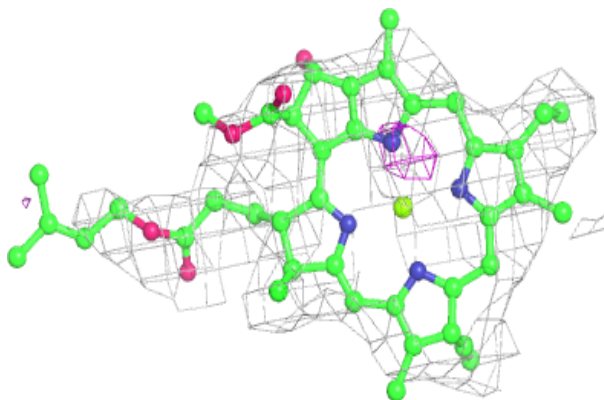


Electron density around LMU C 7015:

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

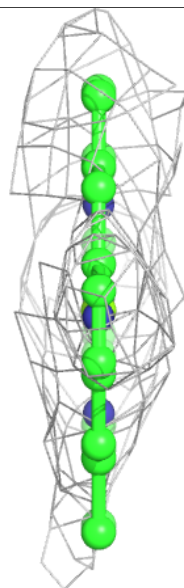
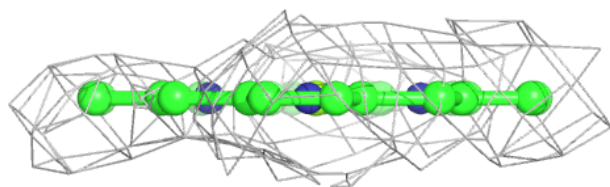
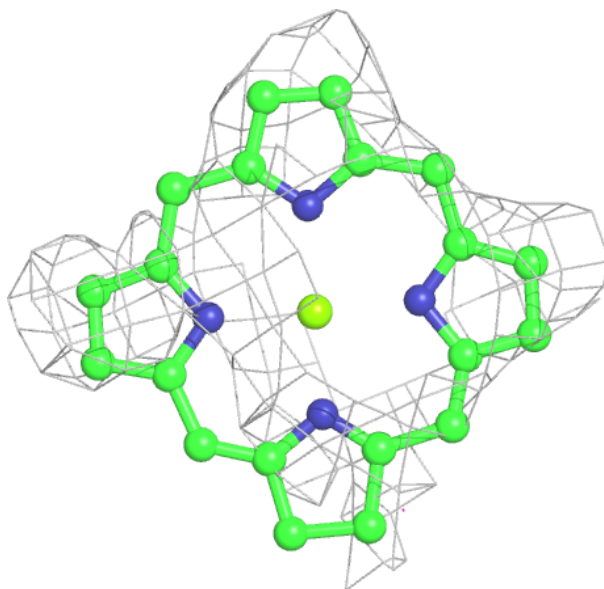
**Electron density around CLA A 1151:**

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



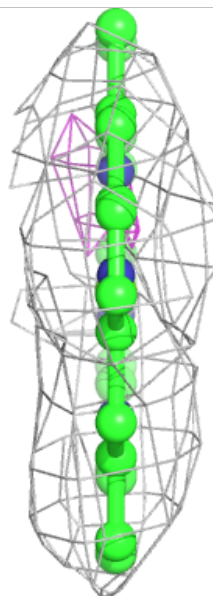
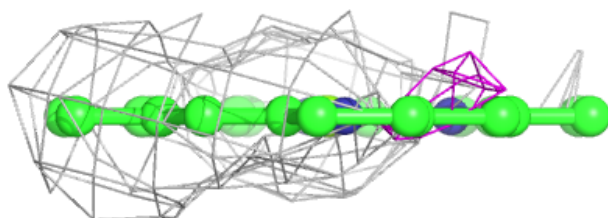
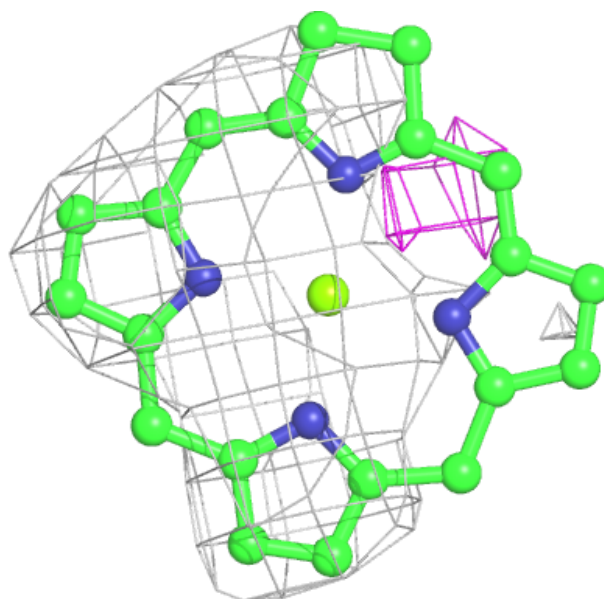
Electron density around CLA 3 3015:

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



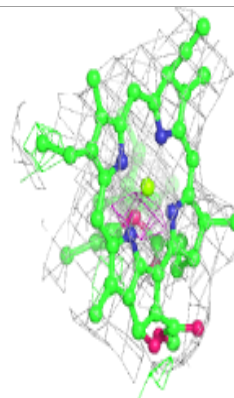
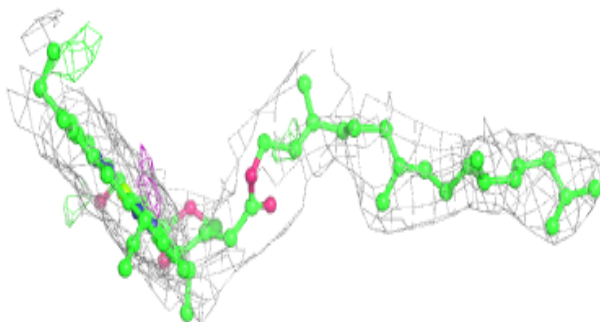
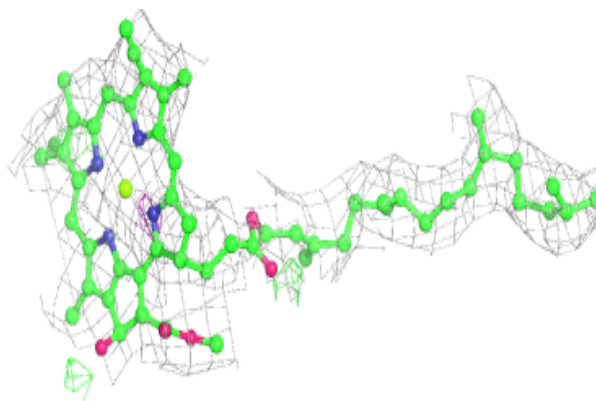
Electron density around CLA 2 1307:

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

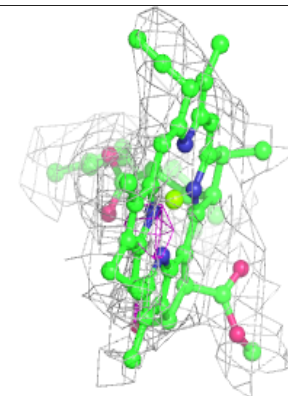
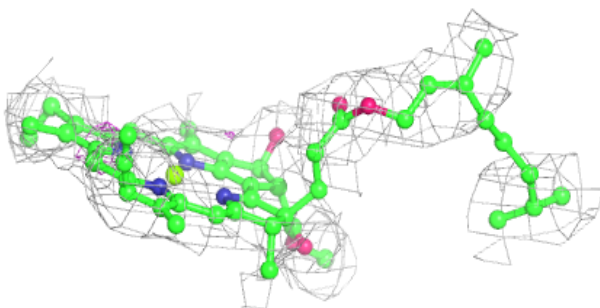
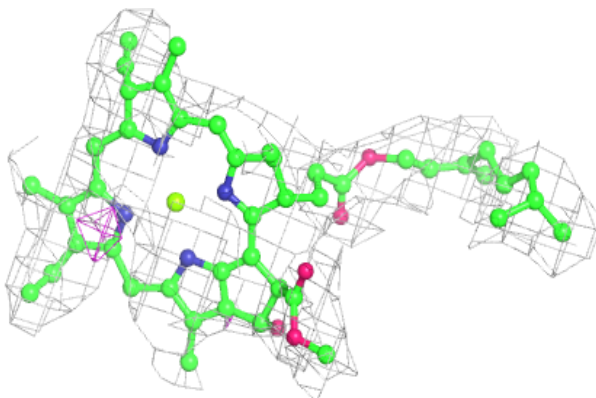


Electron density around CLA 4 1304:

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

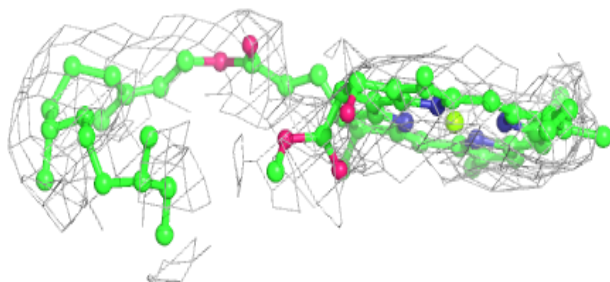
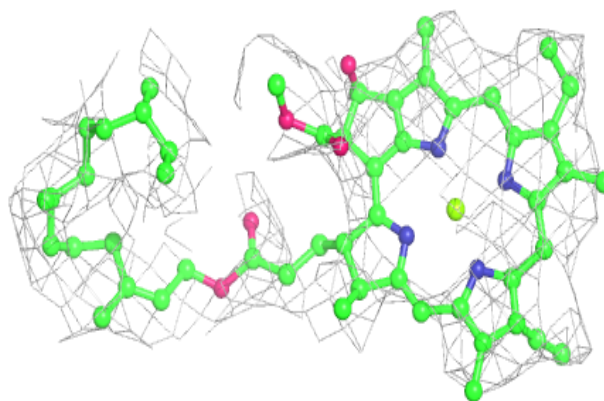
**Electron density around CLA H 1241:**

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

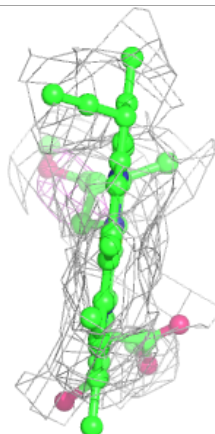
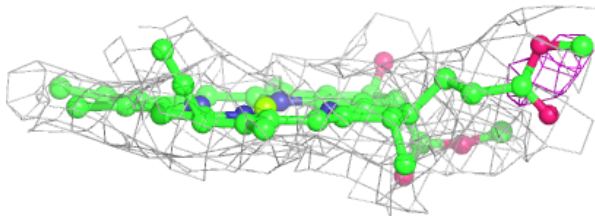
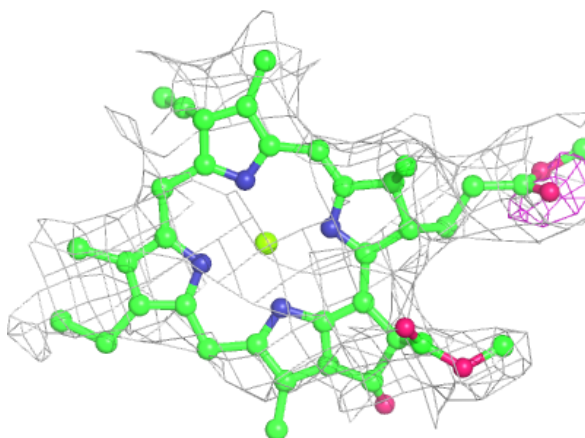


Electron density around CLA 1 1014:

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

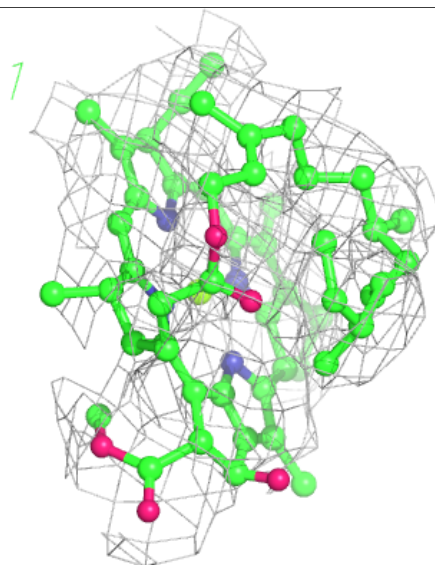
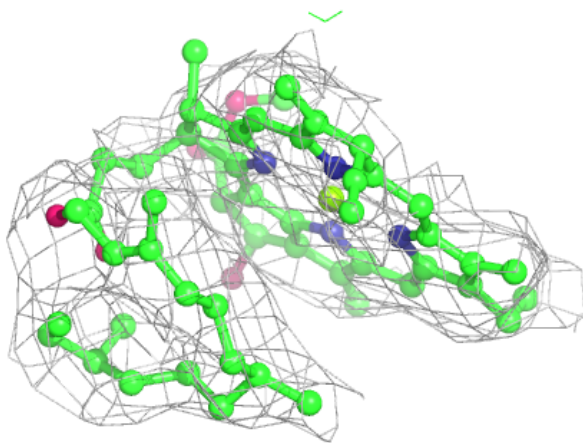
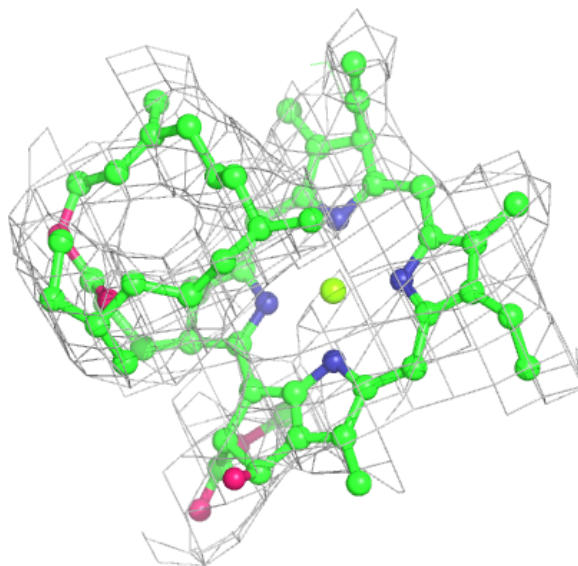
**Electron density around CLA 3 1147:**

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



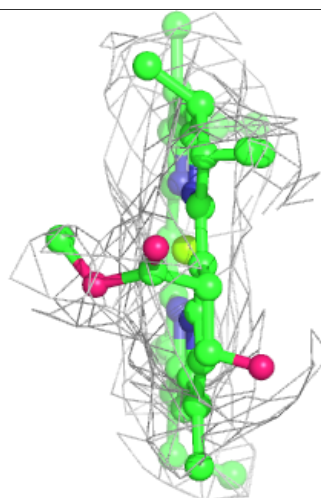
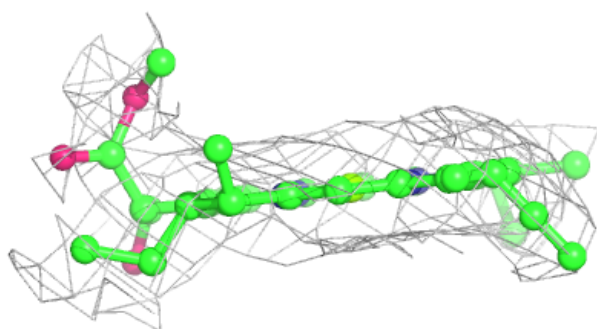
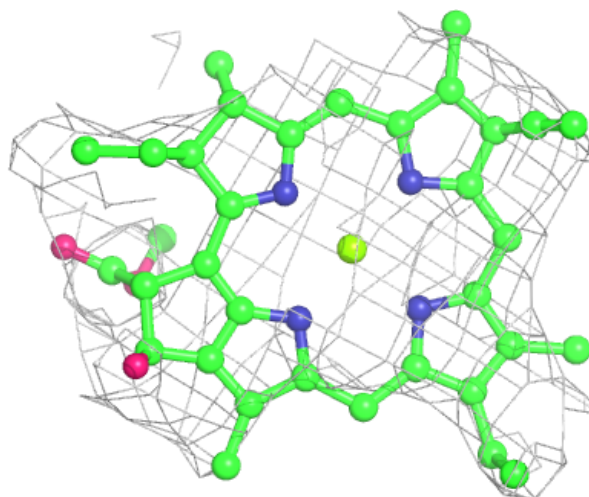
Electron density around CLA J 1311:

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



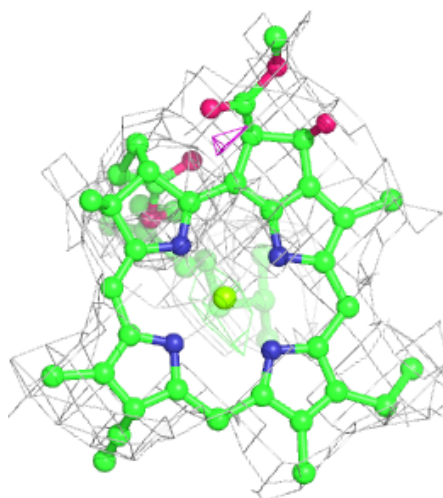
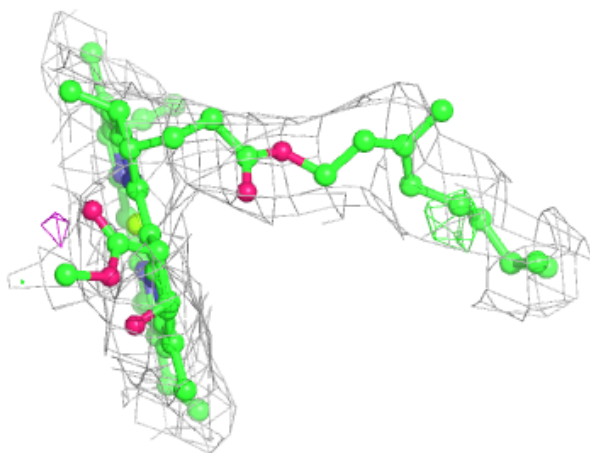
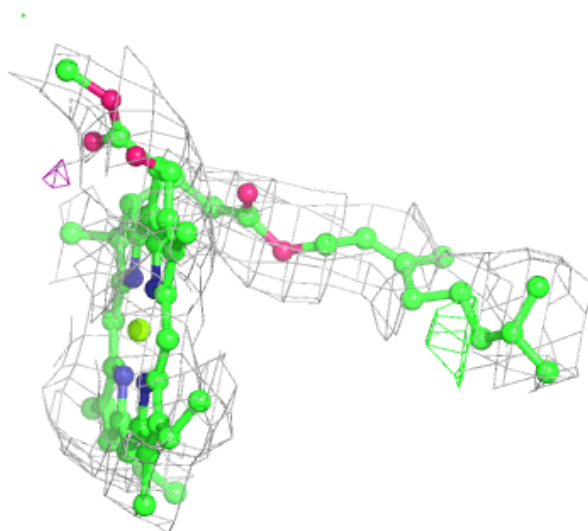
Electron density around CLA 3 3007:

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



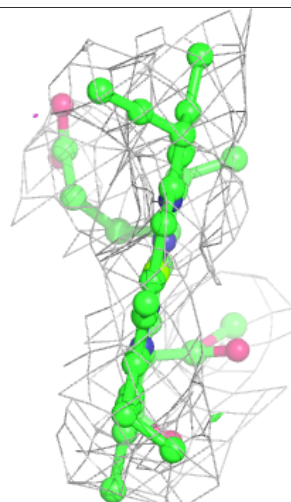
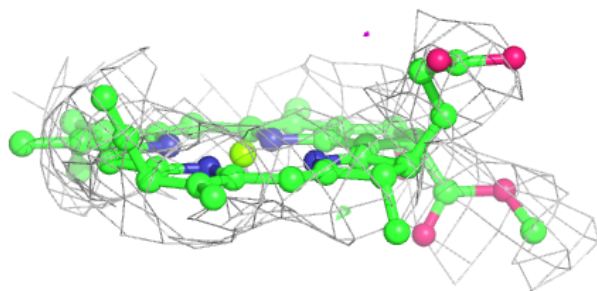
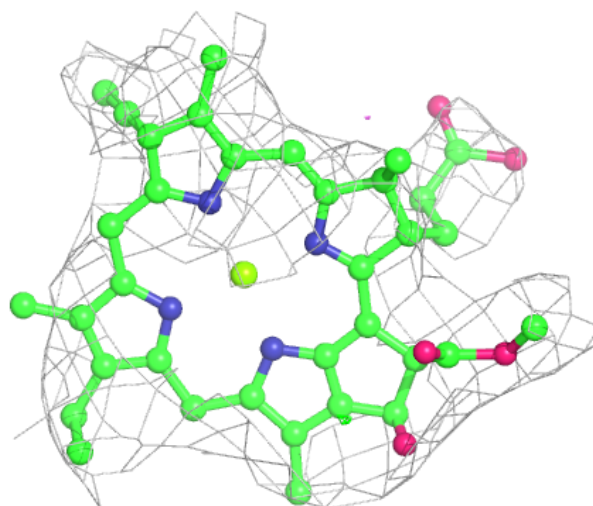
Electron density around CLA 4 1004:

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



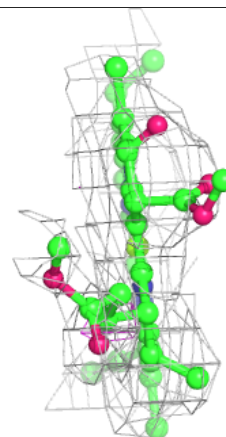
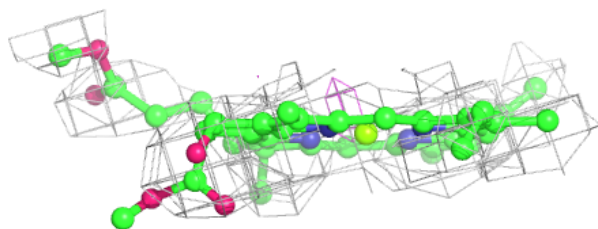
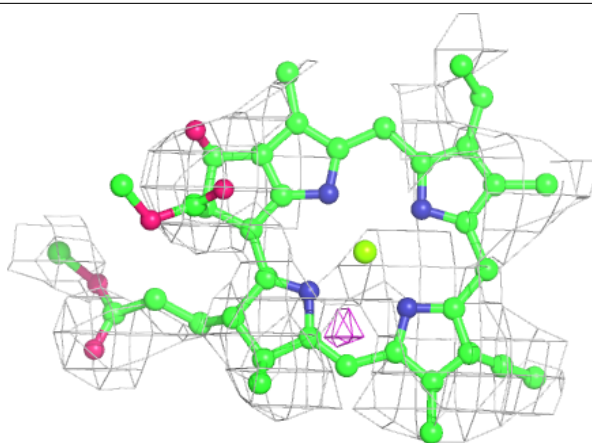
Electron density around CLA A 1134:

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

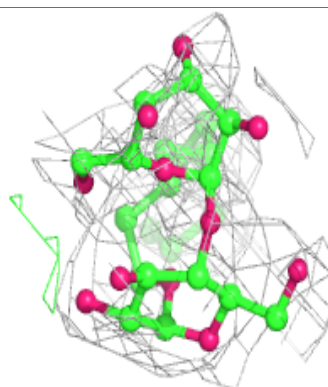
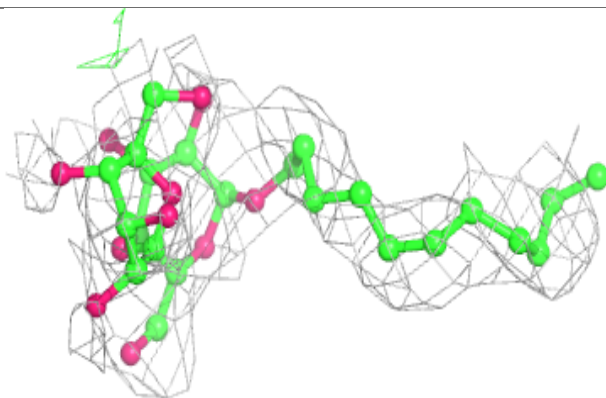
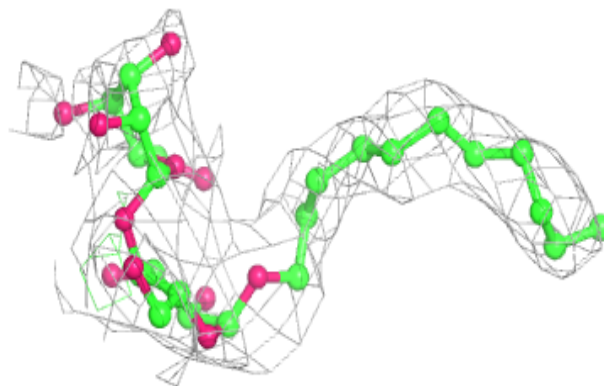


Electron density around CLA 4 4015:

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

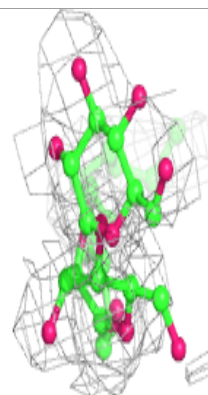
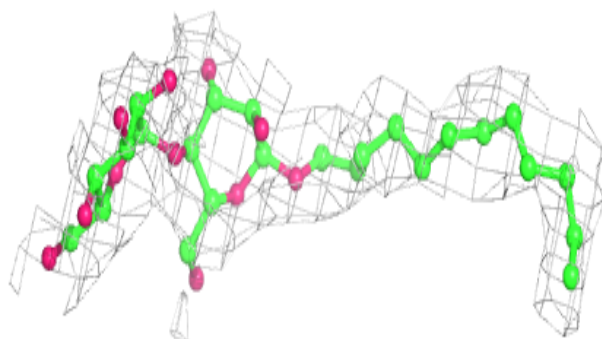
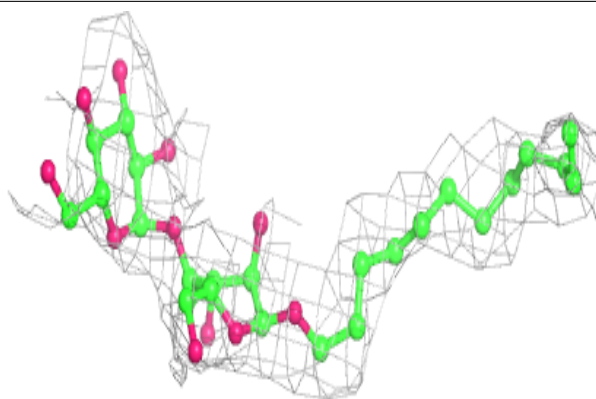
**Electron density around LMU 4 7009:**

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

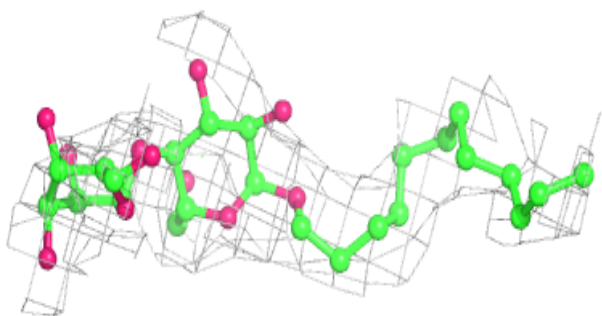
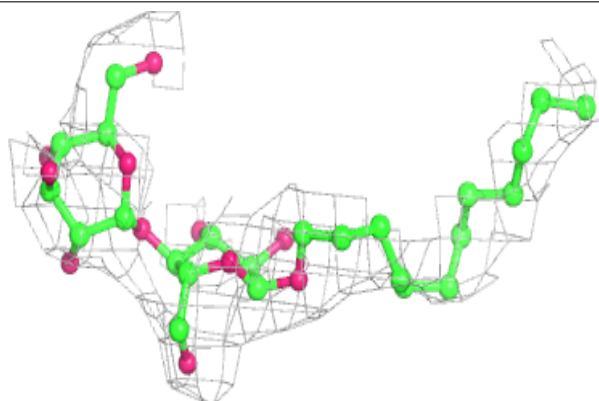


Electron density around LMU 4 7018:

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

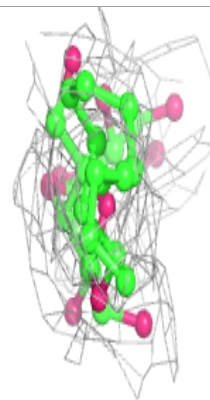
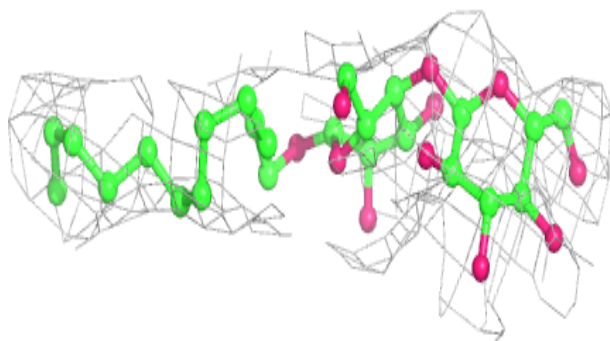
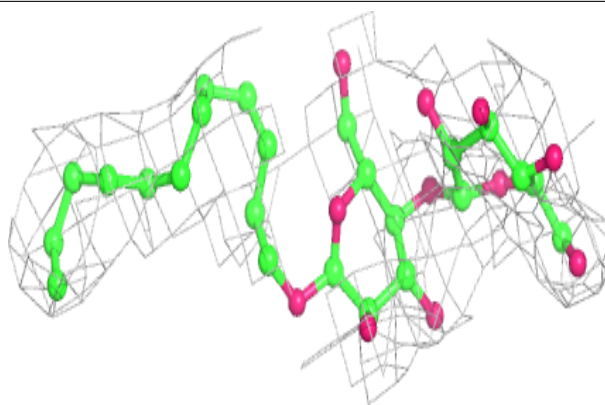
**Electron density around LMU 4 7034:**

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



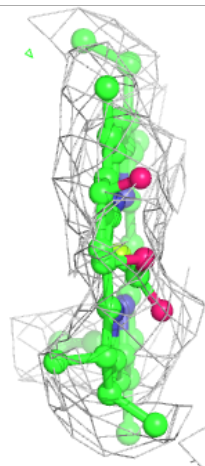
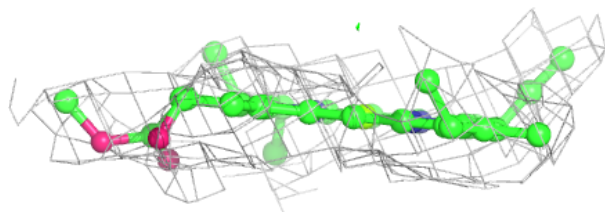
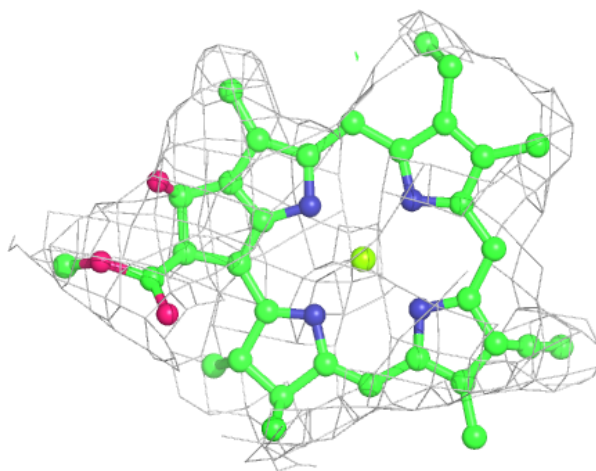
Electron density around LMU K 7042:

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



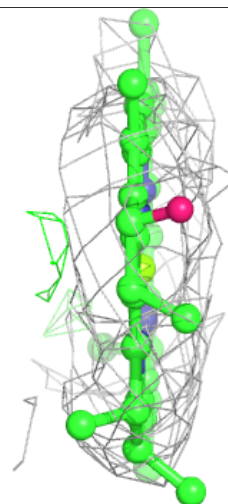
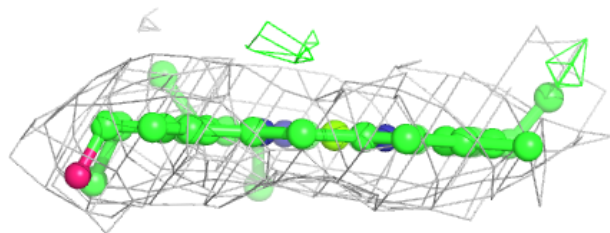
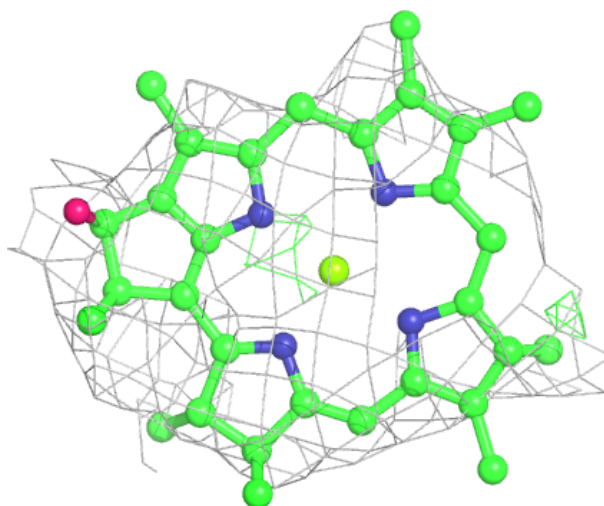
Electron density around CLA F 1302:

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



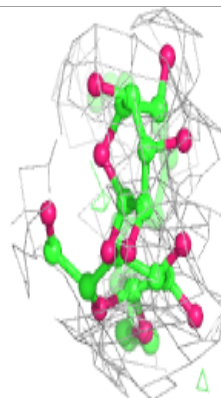
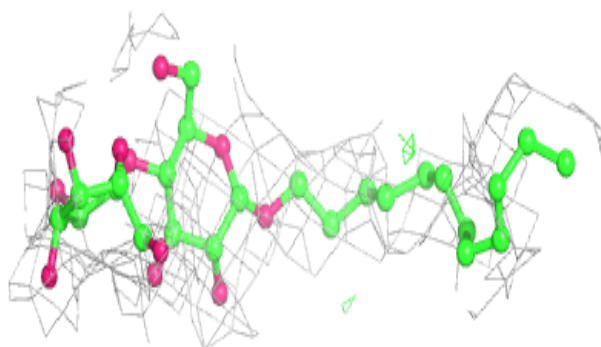
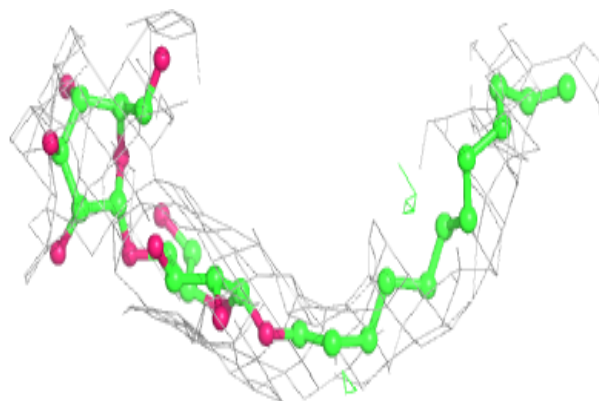
Electron density around CLA 3 3003:

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



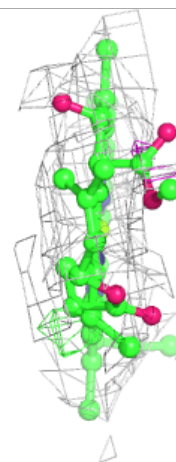
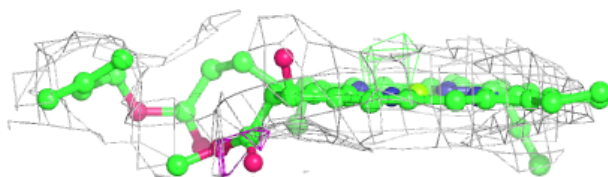
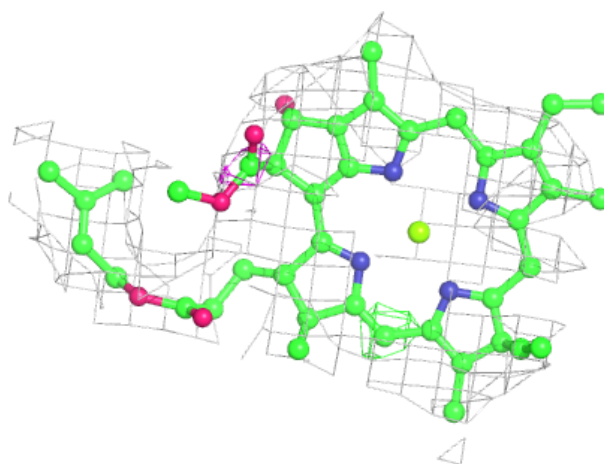
Electron density around LMU H 7017:

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



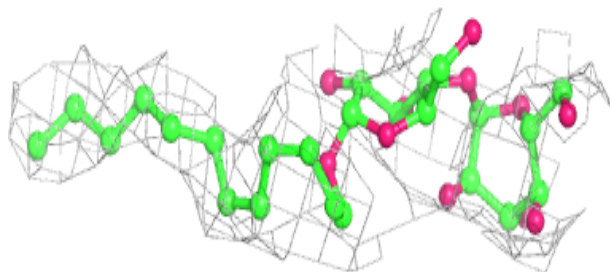
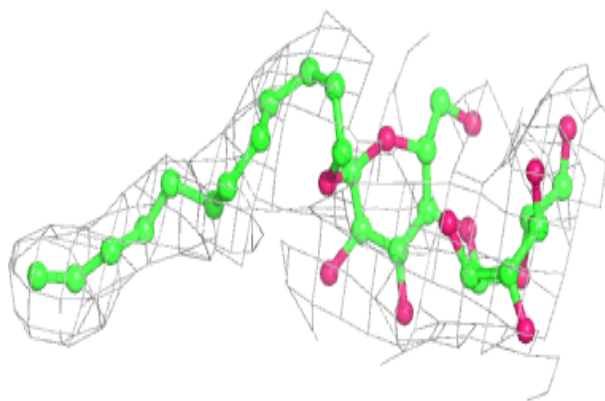
Electron density around CLA 2 2013:

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

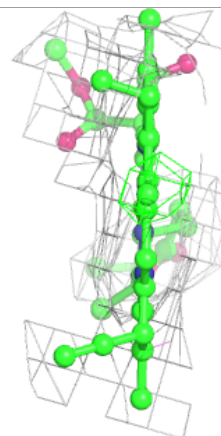
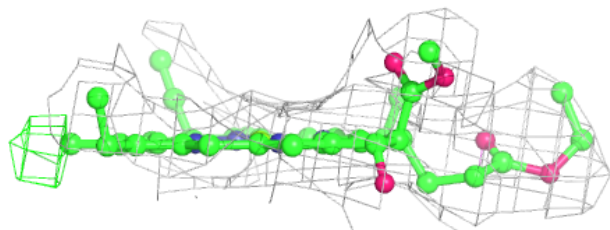
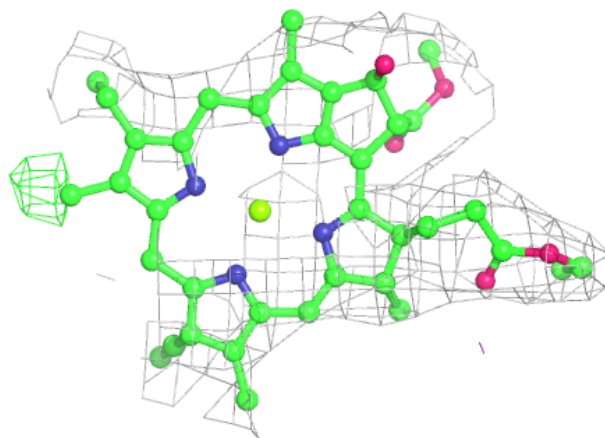


Electron density around LMU 3 7005:

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

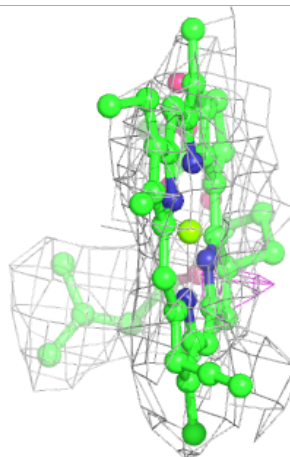
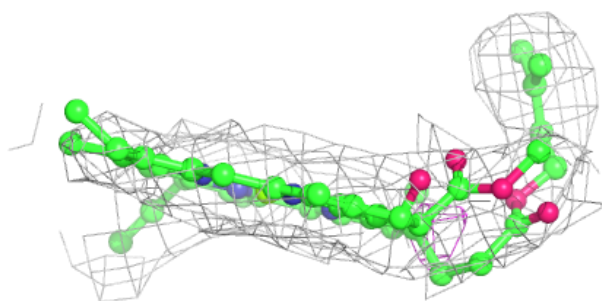
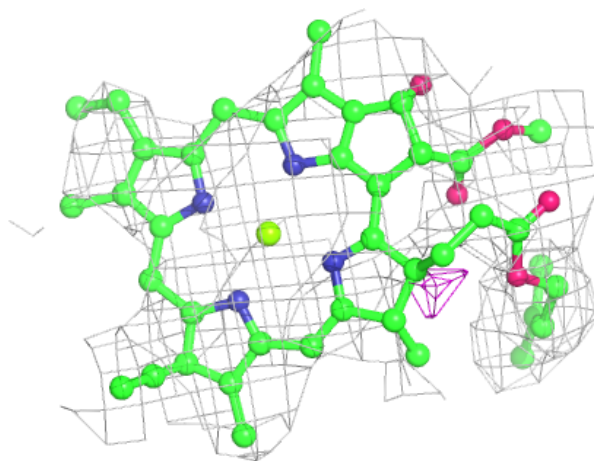
**Electron density around CLA 1 1003:**

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



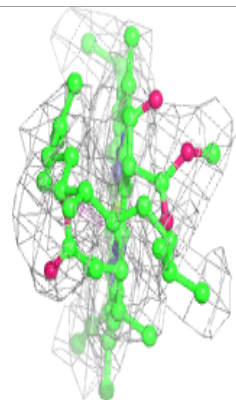
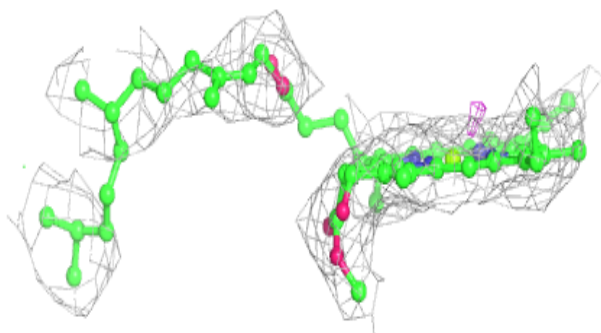
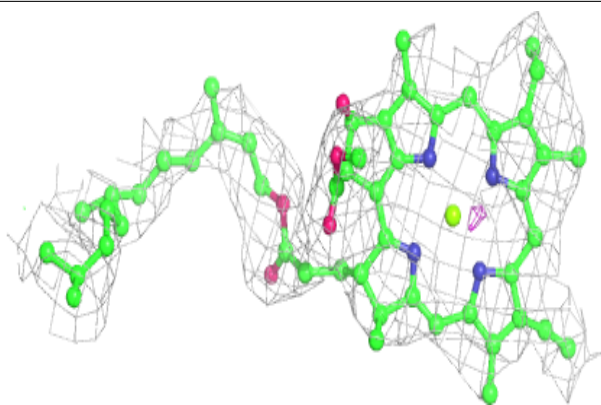
Electron density around CLA 3 3008:

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

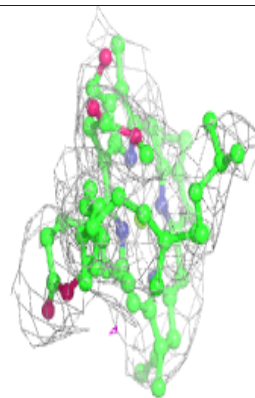
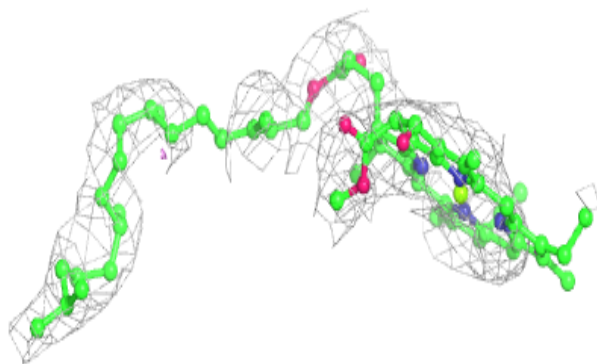
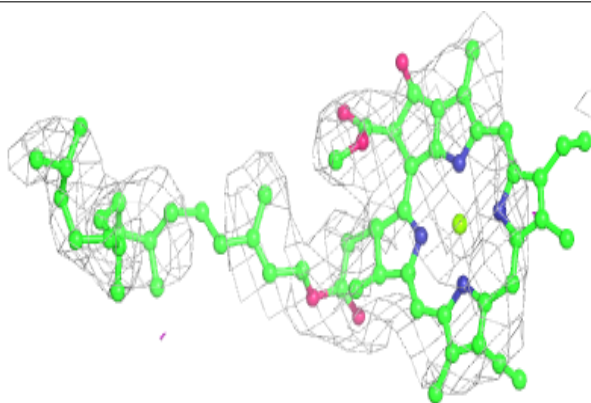


Electron density around CLA B 1212:

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

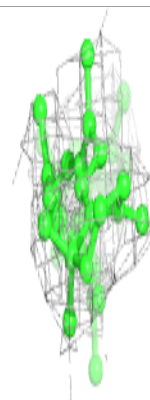
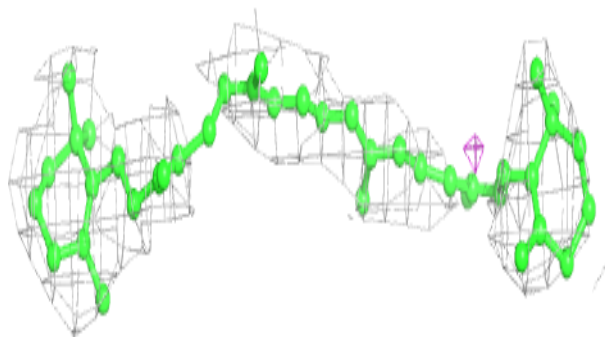
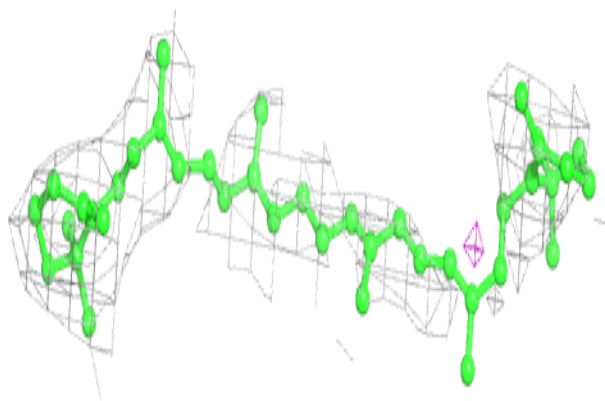
**Electron density around CLA 3 3011:**

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



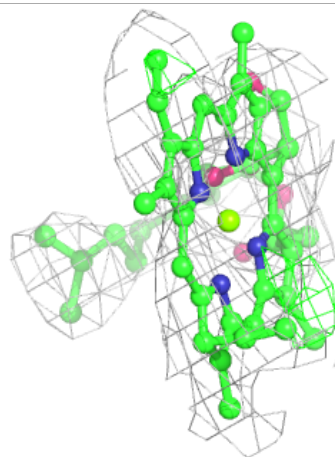
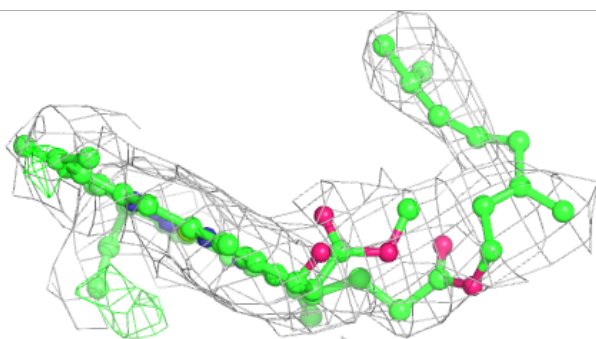
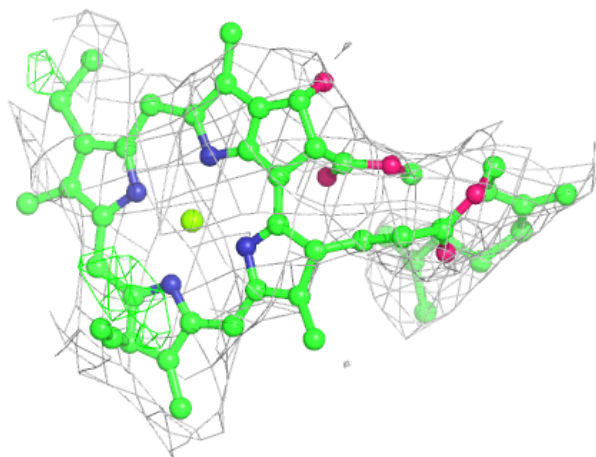
Electron density around BCR A 6007:

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



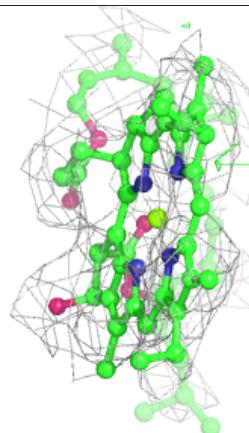
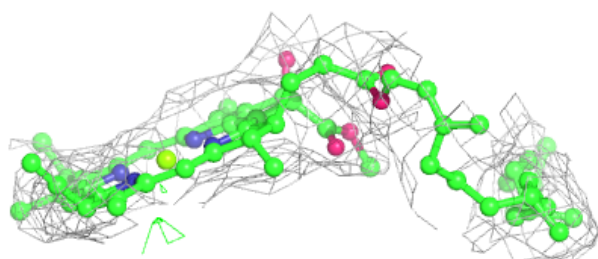
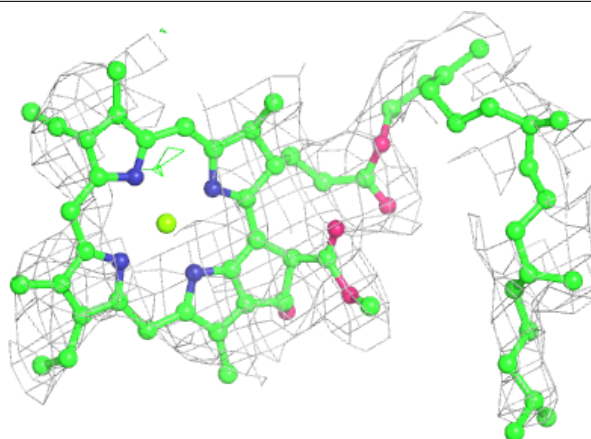
Electron density around CLA L 1148:

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

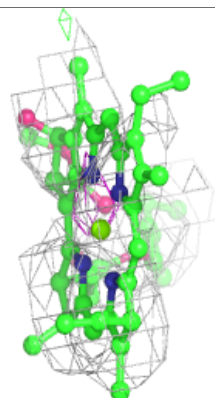
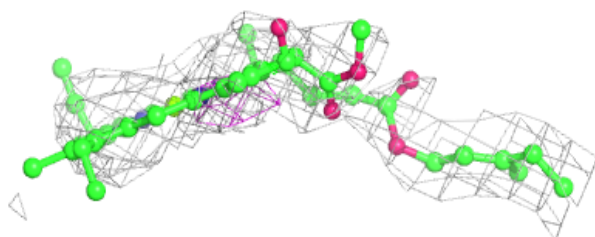
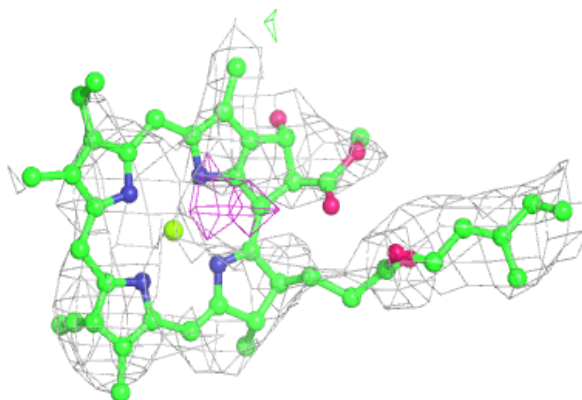


Electron density around CLA R 1150:

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

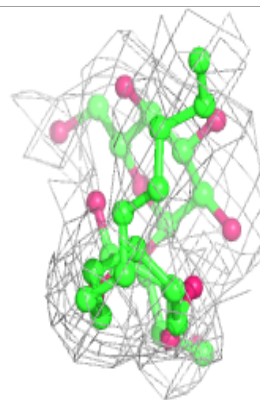
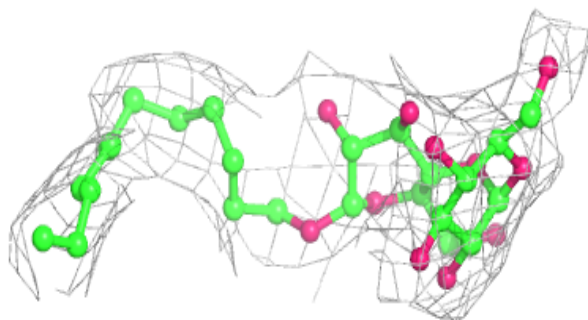
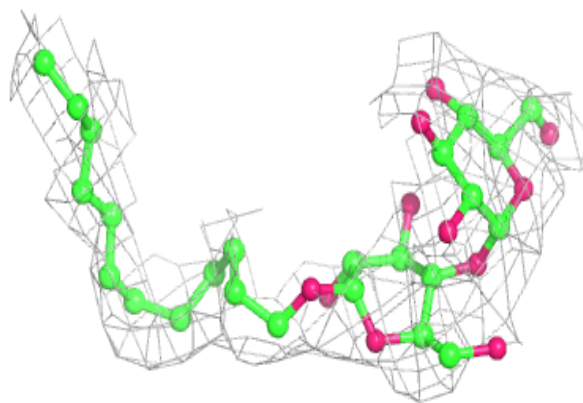
**Electron density around CLA 1 1013:**

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



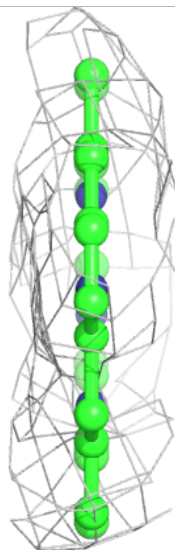
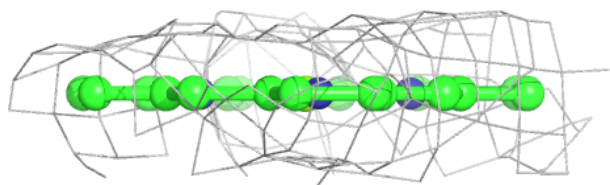
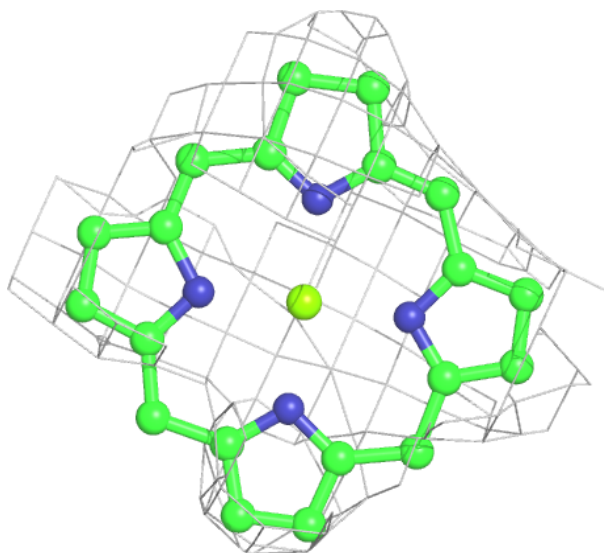
Electron density around LMU 2 7031:

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



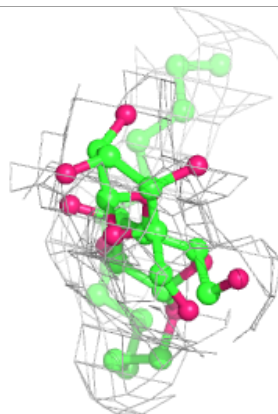
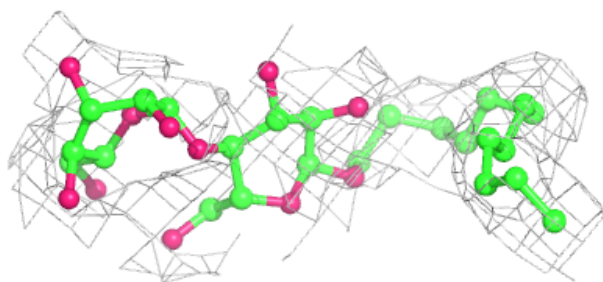
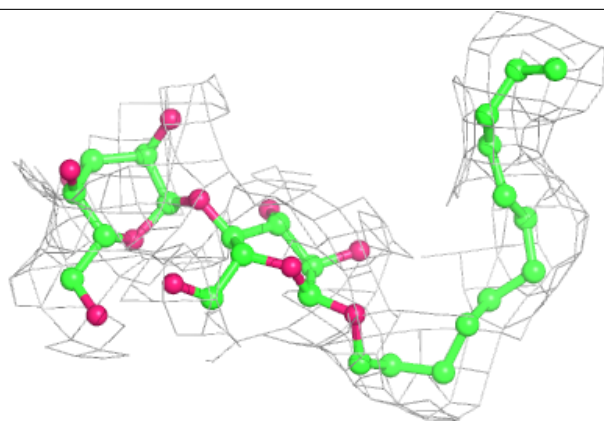
Electron density around CLA 3 3002:

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

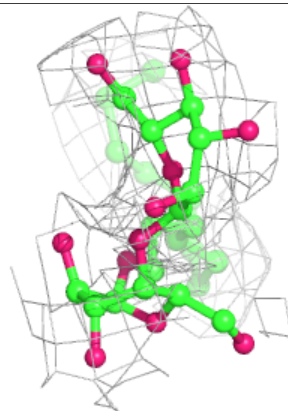
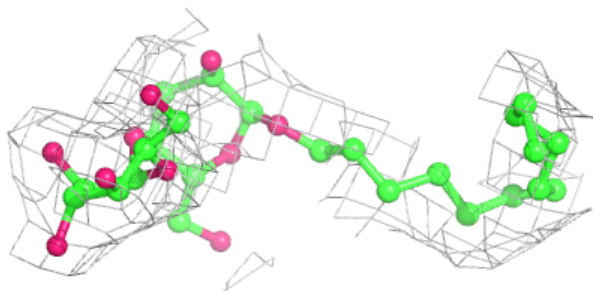
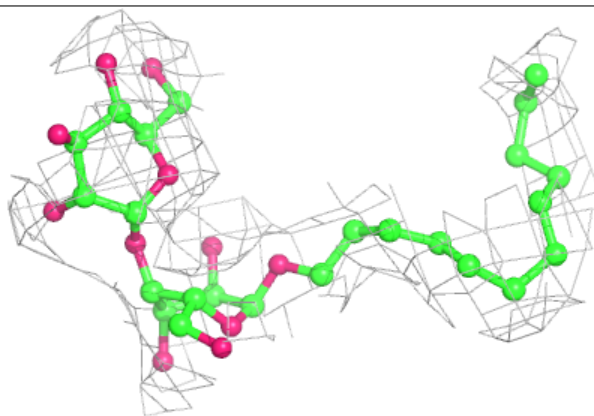


Electron density around LMU 3 7003:

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

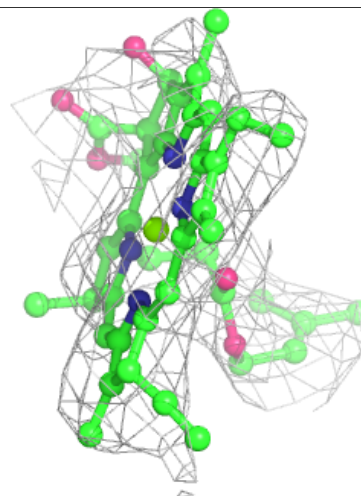
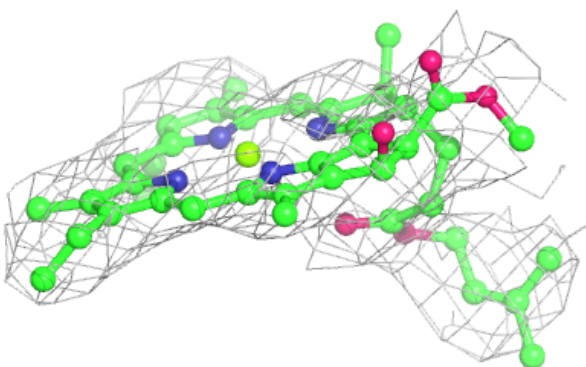
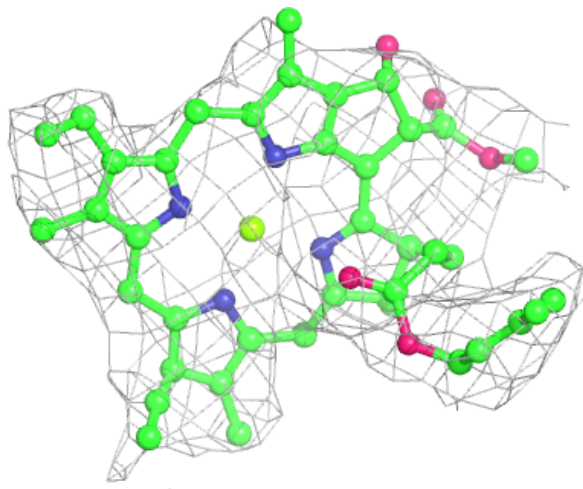
**Electron density around LMU K 7001:**

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



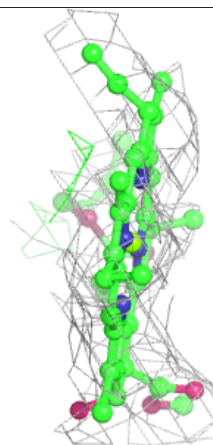
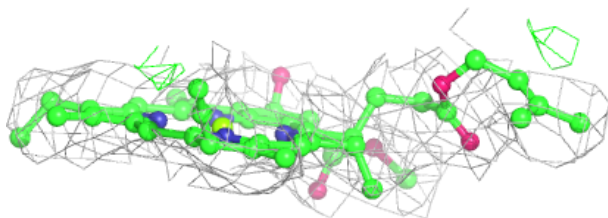
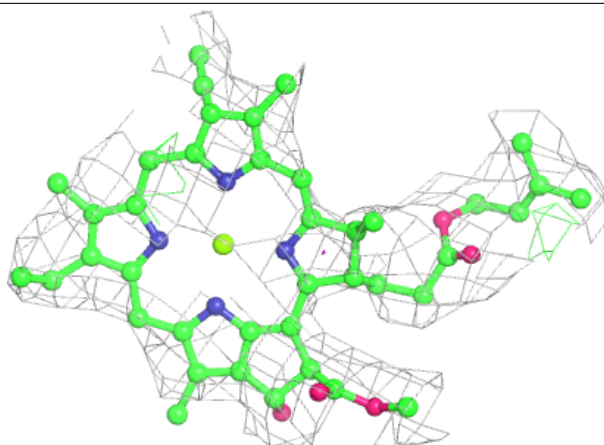
Electron density around CLA A 1113:

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

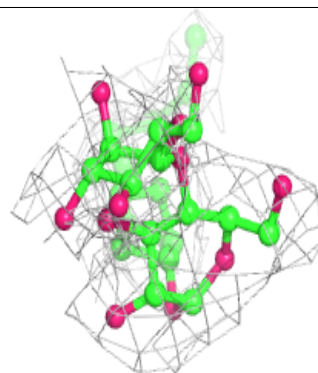
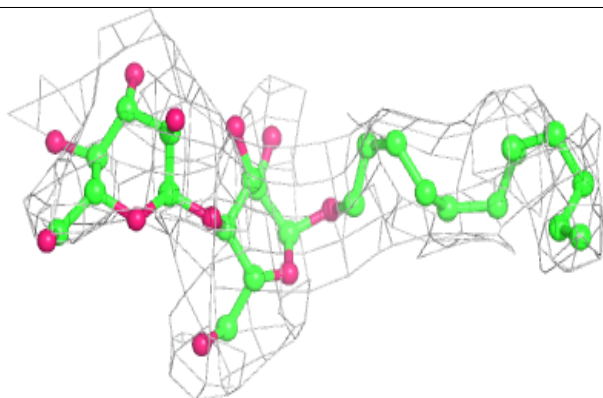
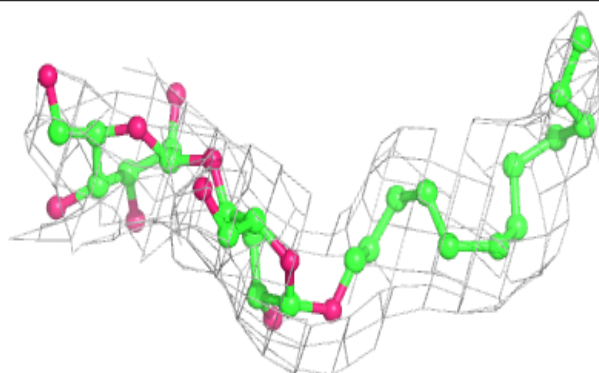


Electron density around CLA 2 2004:

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

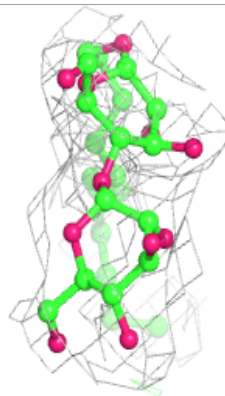
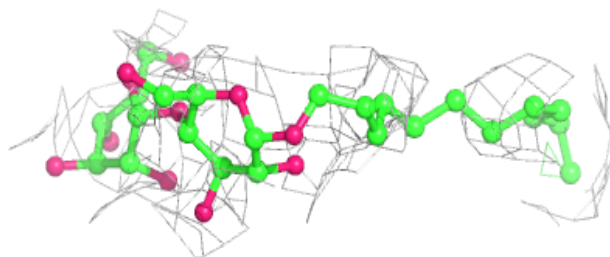
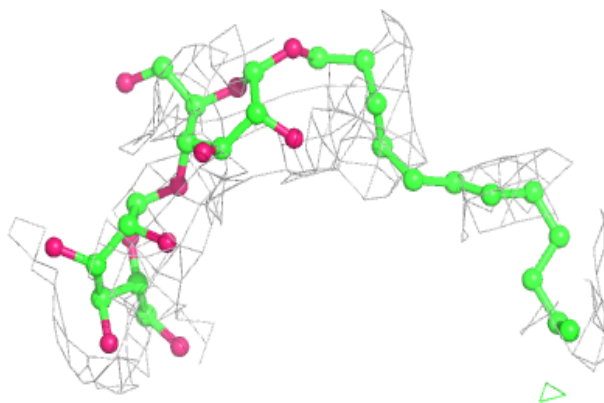
**Electron density around LMU G 7026:**

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



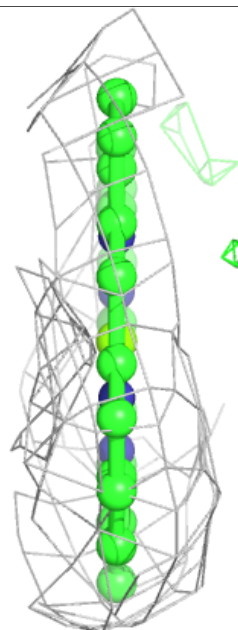
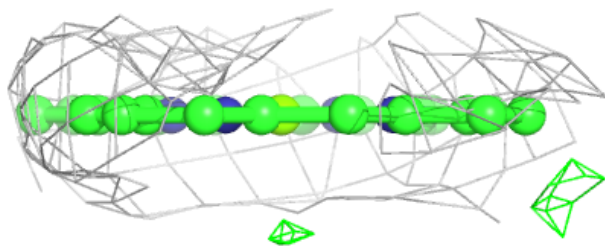
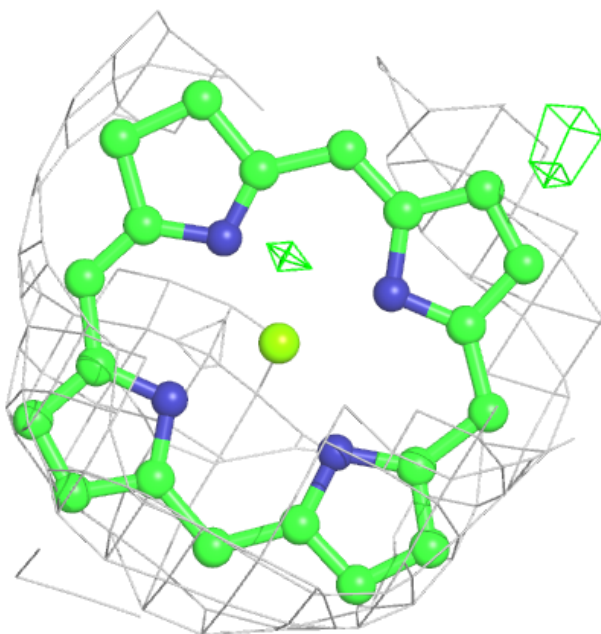
Electron density around LMU 4 7019:

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



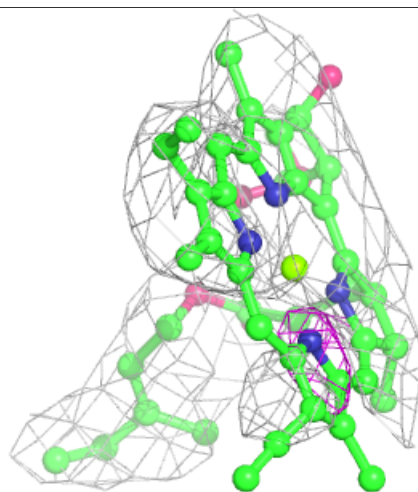
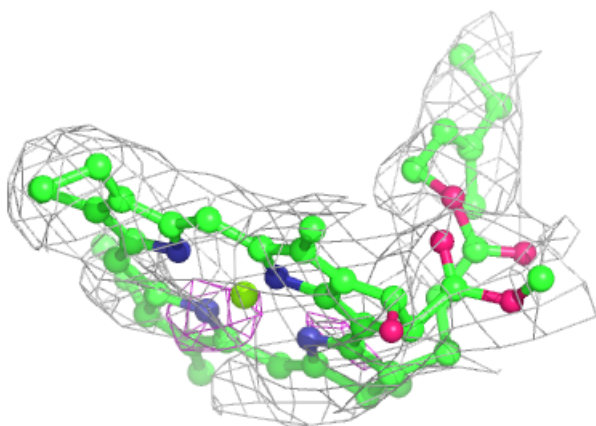
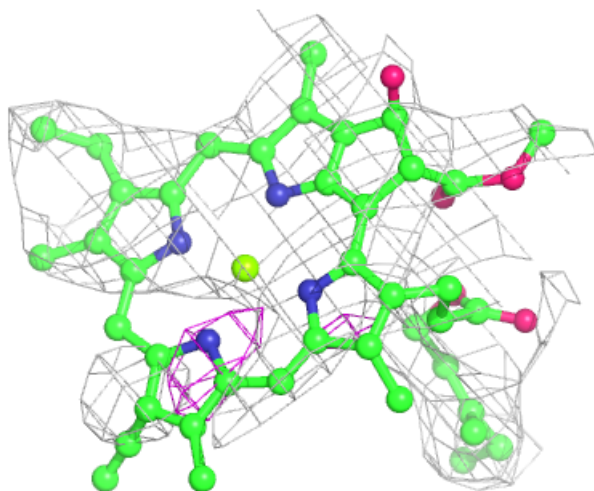
Electron density around CLA 3 3006:

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



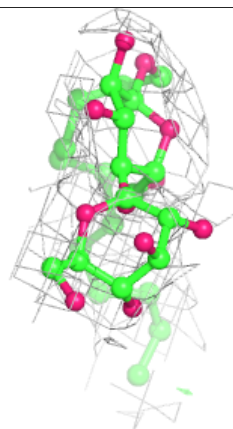
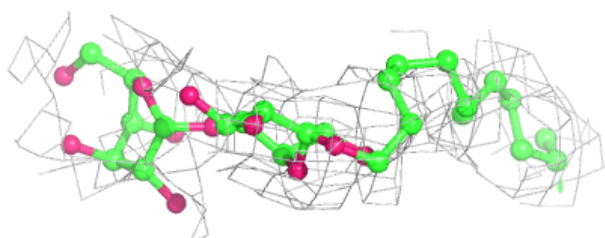
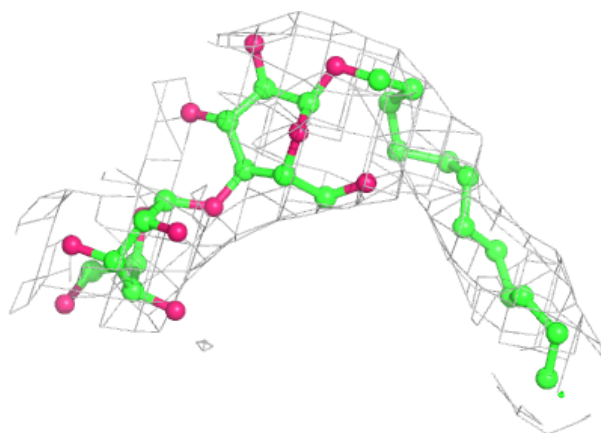
Electron density around CLA 1 1008:

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

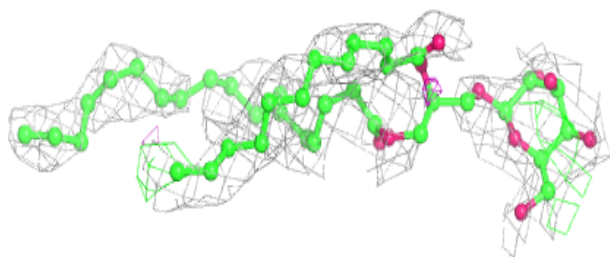
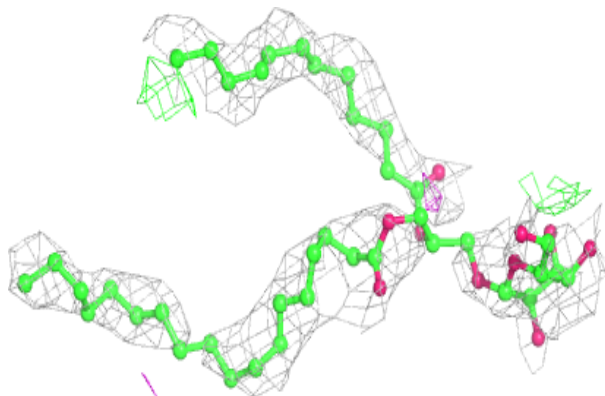


Electron density around LMU R 7021:

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

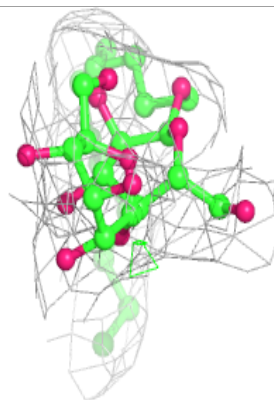
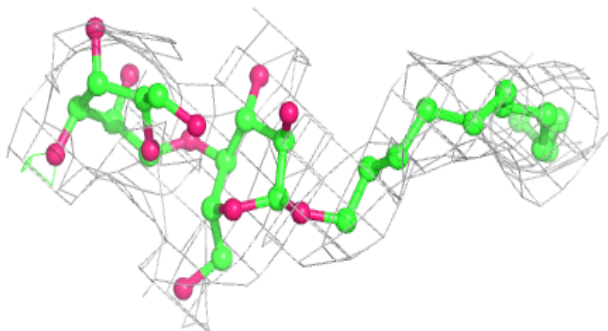
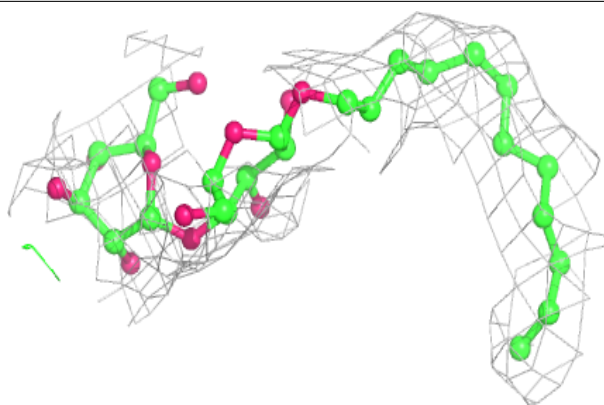
**Electron density around LMG B 7101:**

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

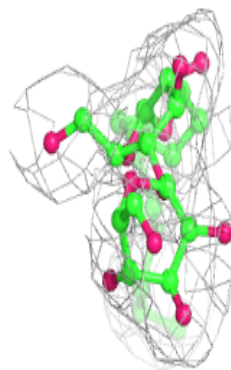
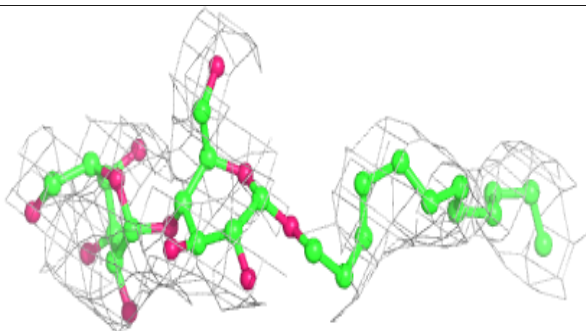
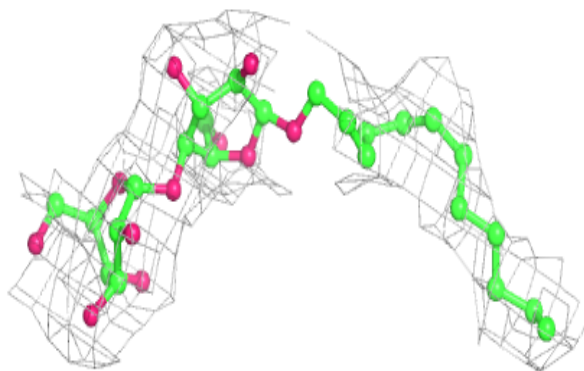


Electron density around LMU 2 7006:

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

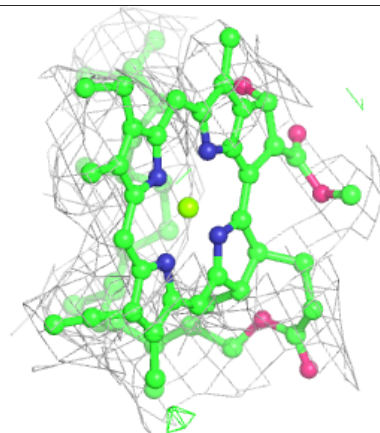
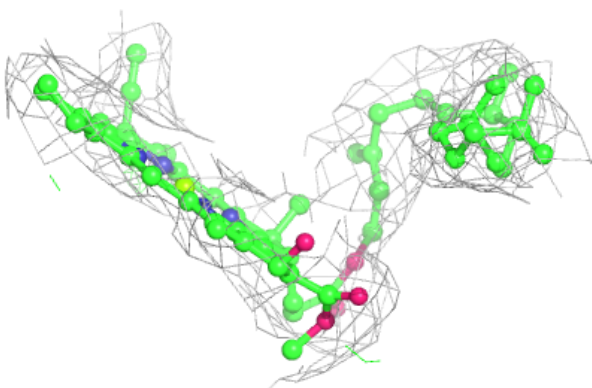
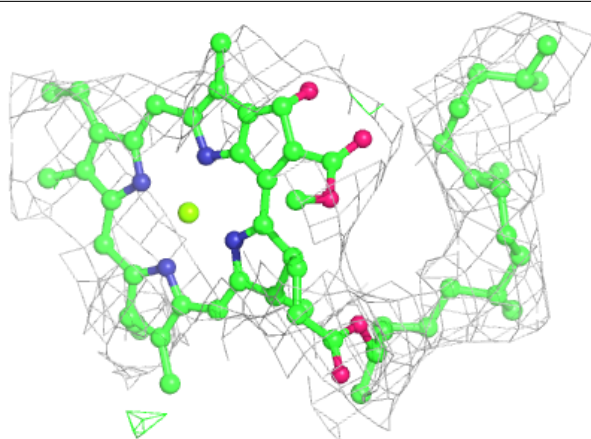
**Electron density around LMU 2 7027:**

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



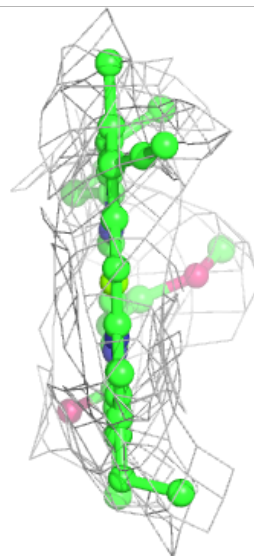
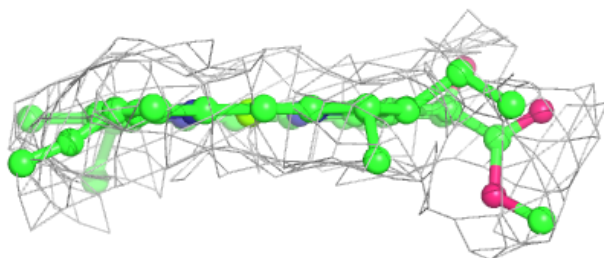
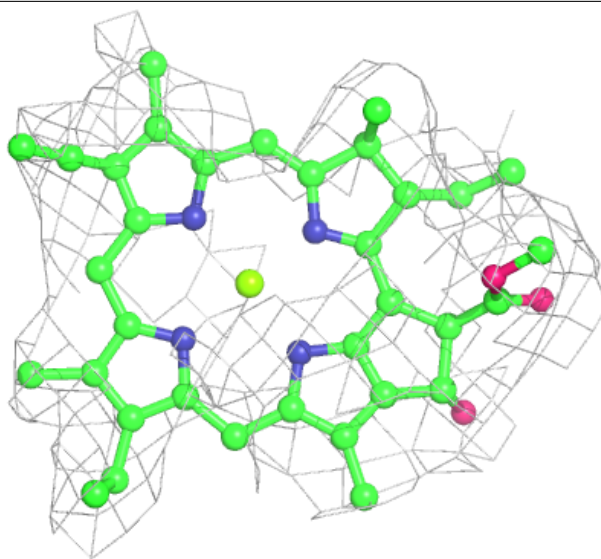
Electron density around CLA H 1145:

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



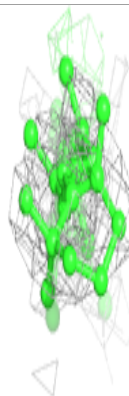
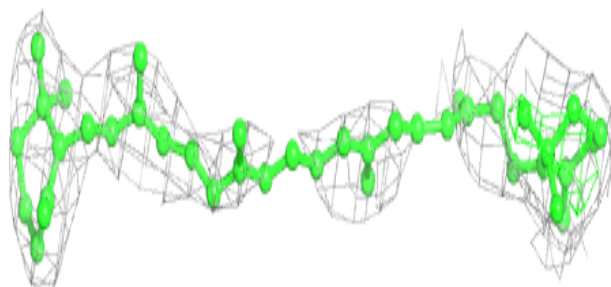
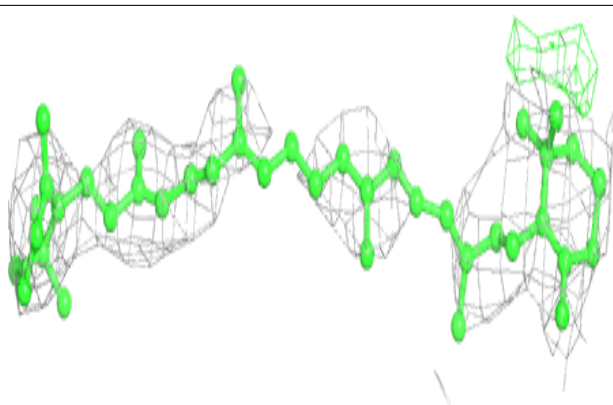
Electron density around CLA A 1121:

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

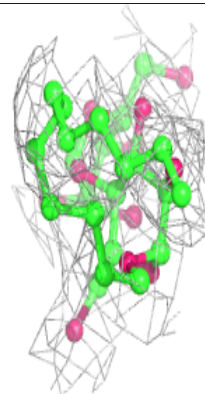
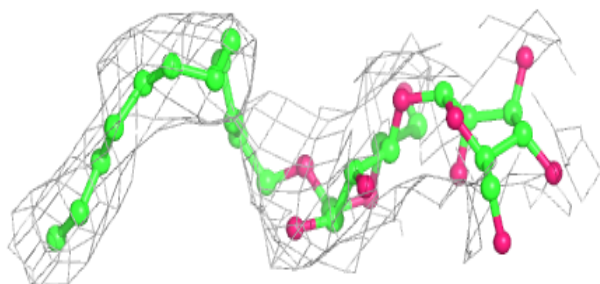
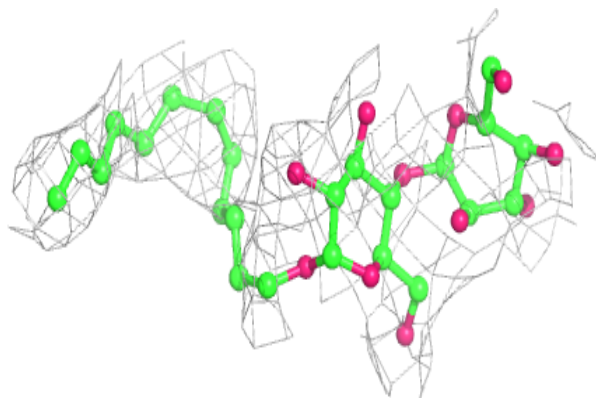


Electron density around BCR A 6003:

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

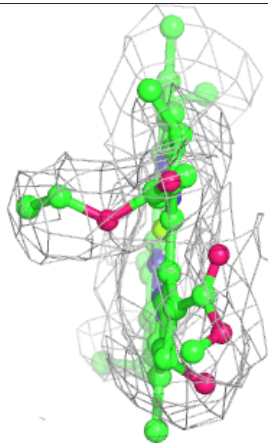
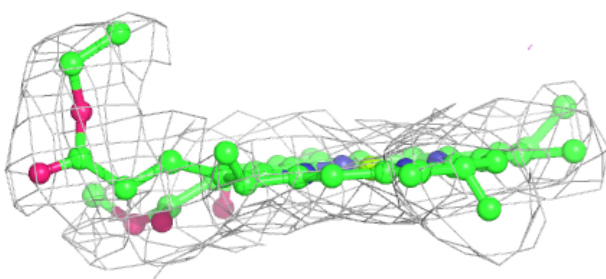
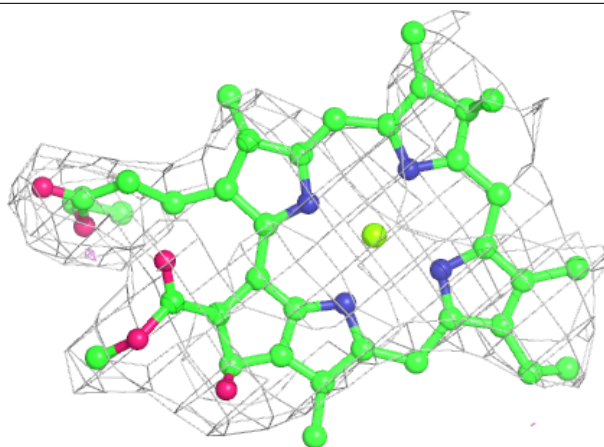
**Electron density around LMU D 7050:**

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

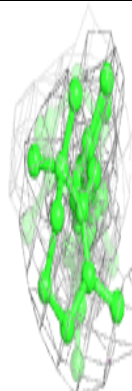
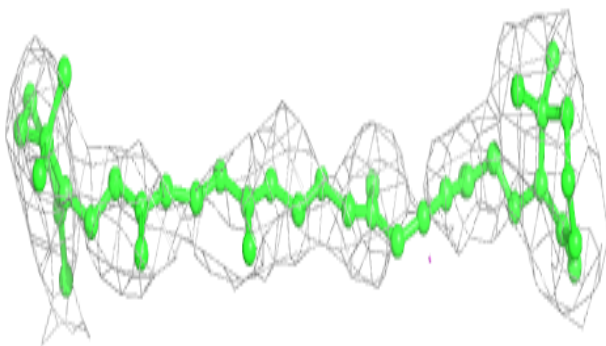
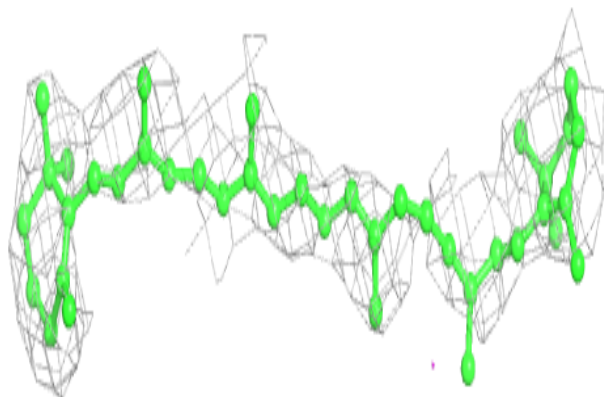


Electron density around CLA A 1149:

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

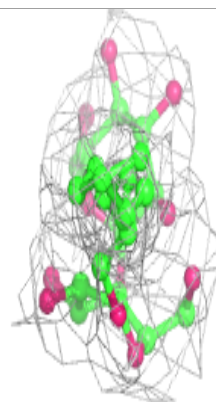
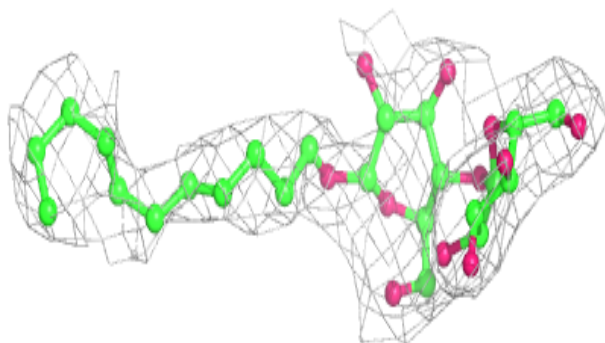
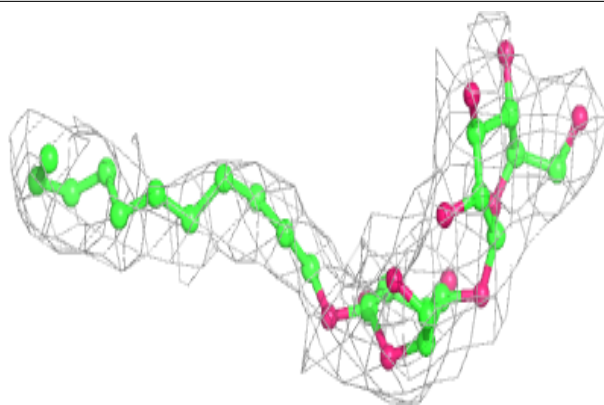
**Electron density around BCR J 6012:**

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



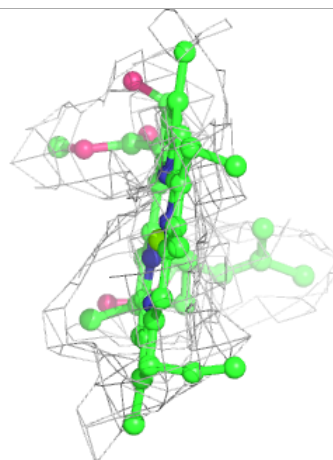
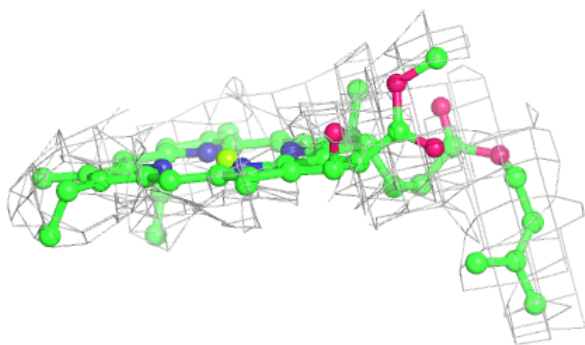
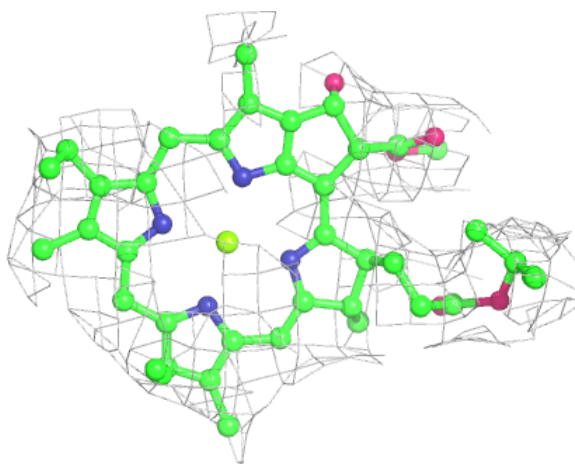
Electron density around LMU F 7036:

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



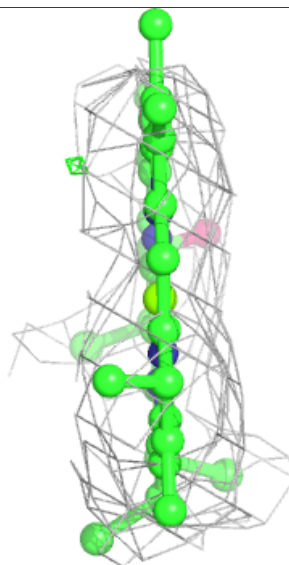
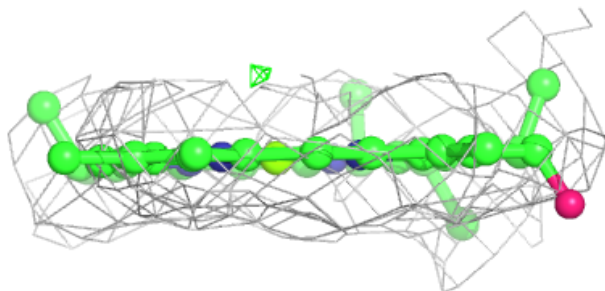
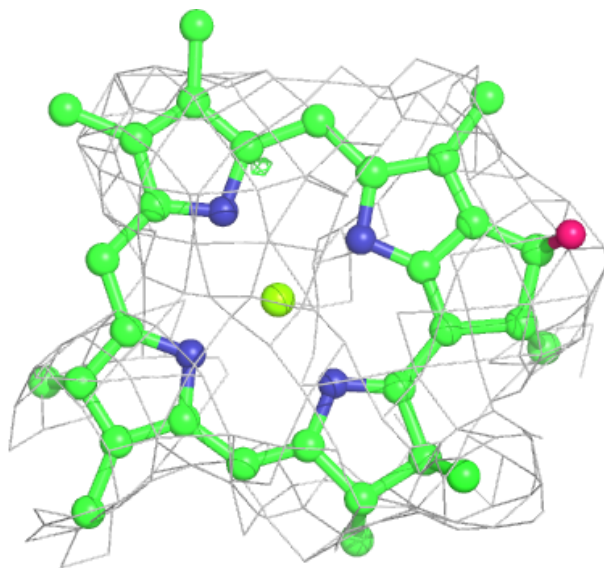
Electron density around CLA 3 3017:

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



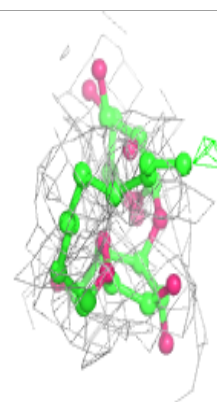
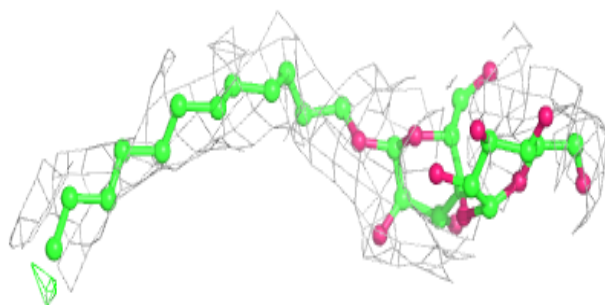
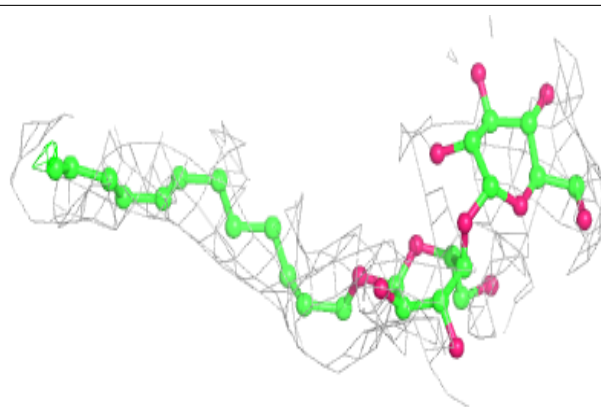
Electron density around CLA B 1301:

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

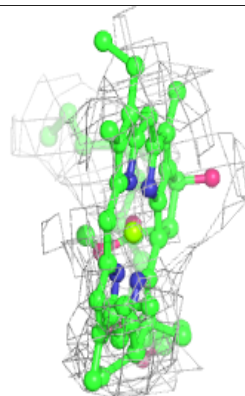
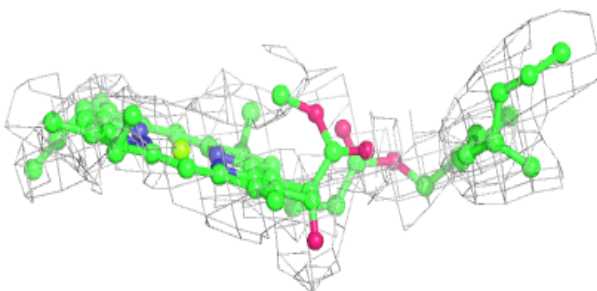
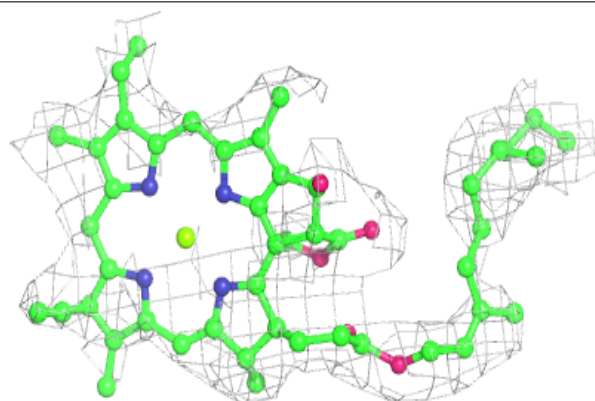


Electron density around LMU R 7024:

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

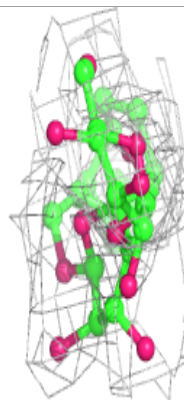
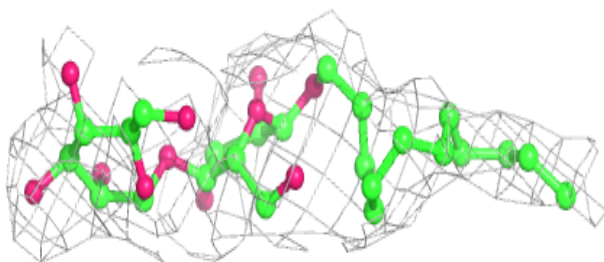
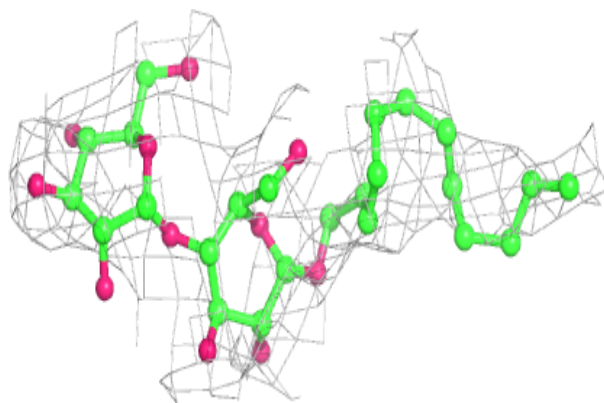
**Electron density around CLA R 1144:**

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

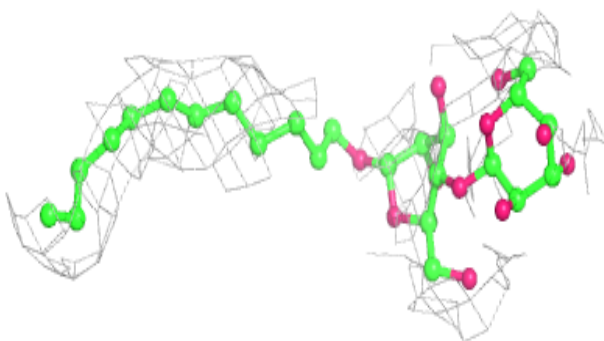
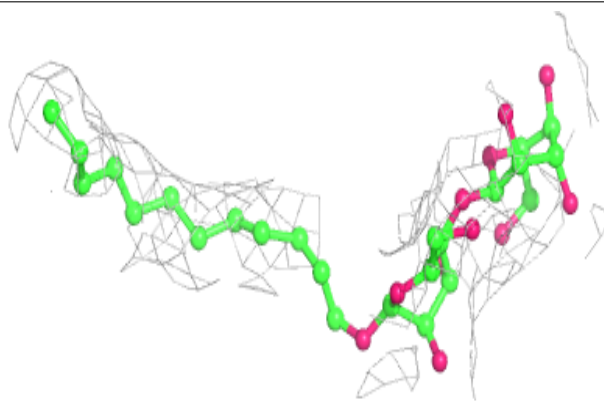


Electron density around LMU A 7016:

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

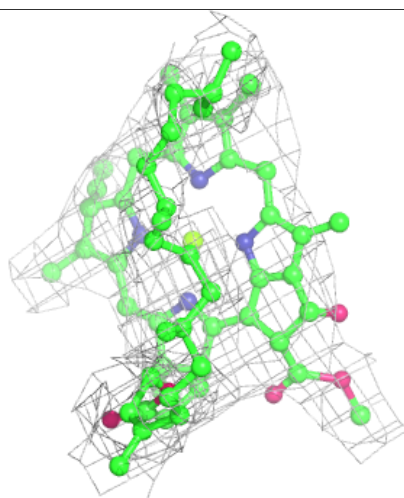
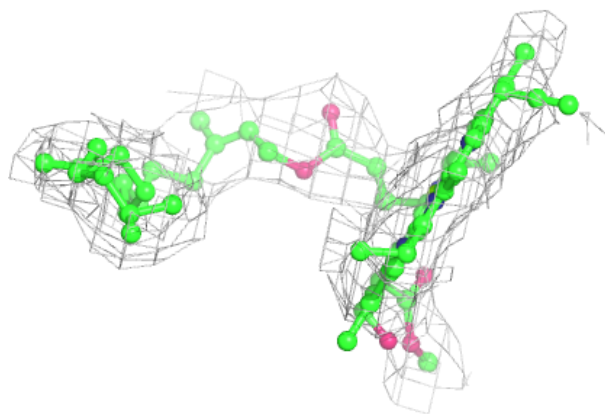
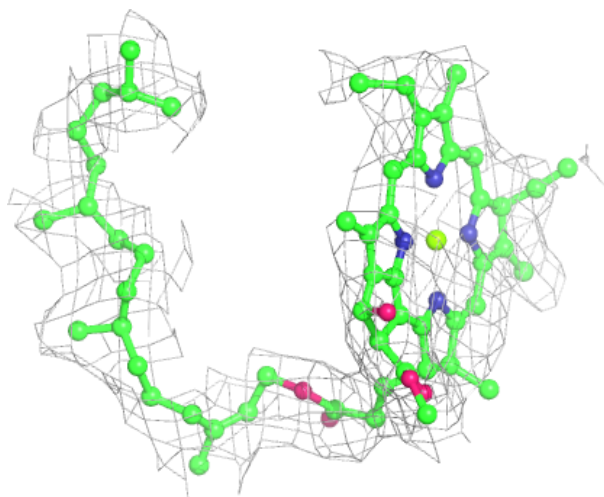
**Electron density around LMU H 7002:**

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



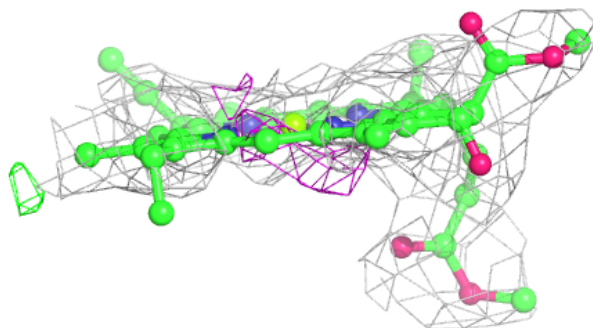
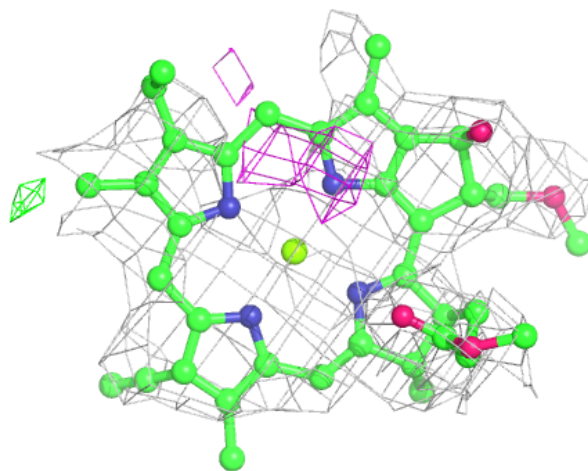
Electron density around CLA 3 3013:

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



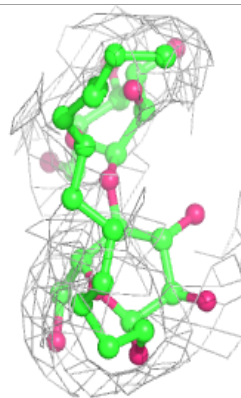
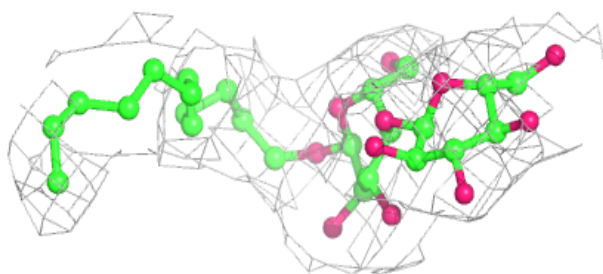
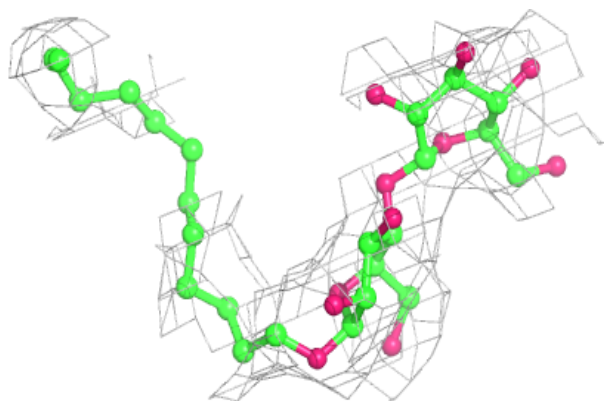
Electron density around CLA A 1105:

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

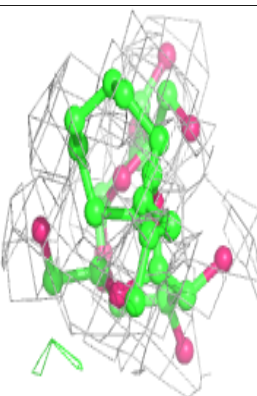
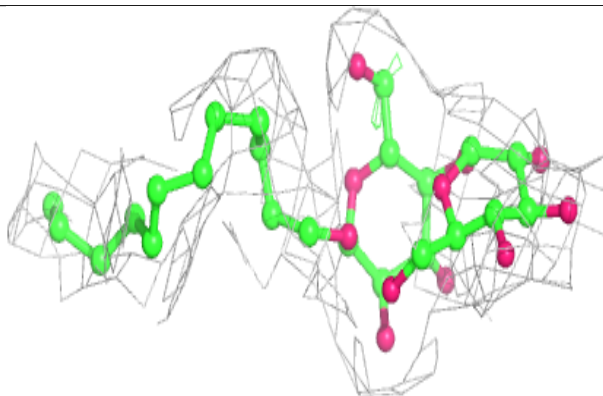
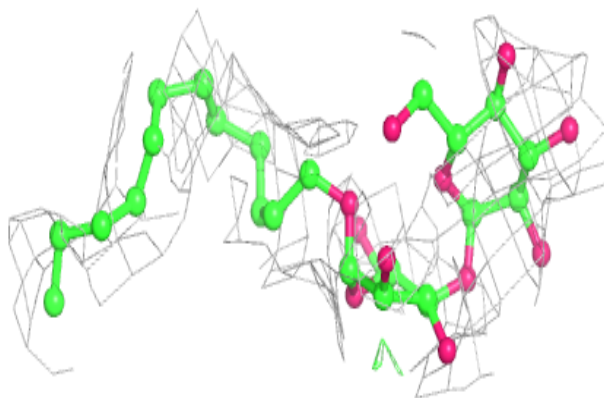


Electron density around LMU H 7028:

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

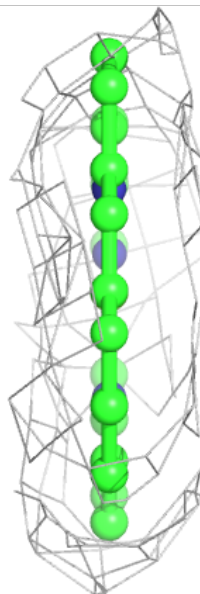
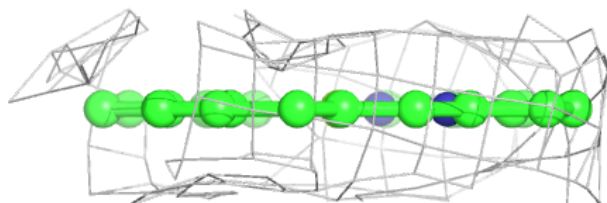
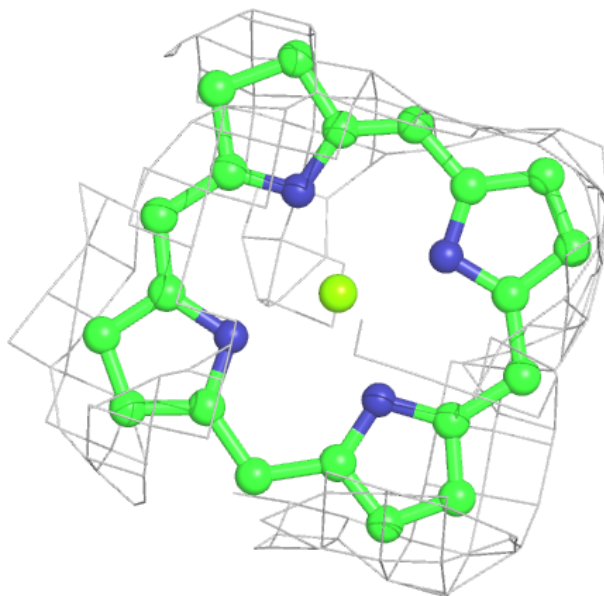
**Electron density around LMU A 7045:**

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



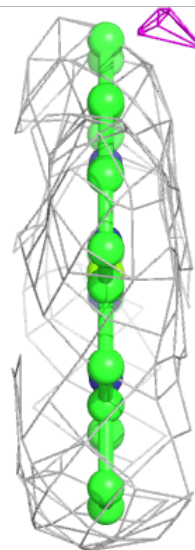
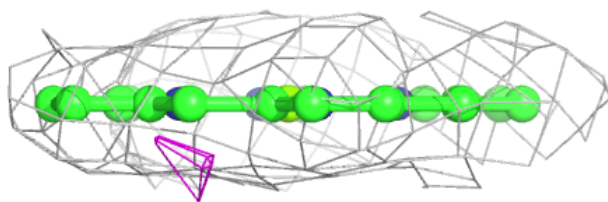
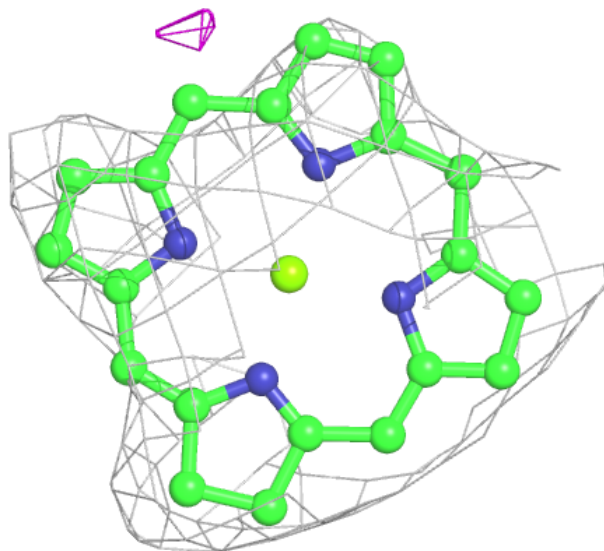
Electron density around CLA 3 3004:

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



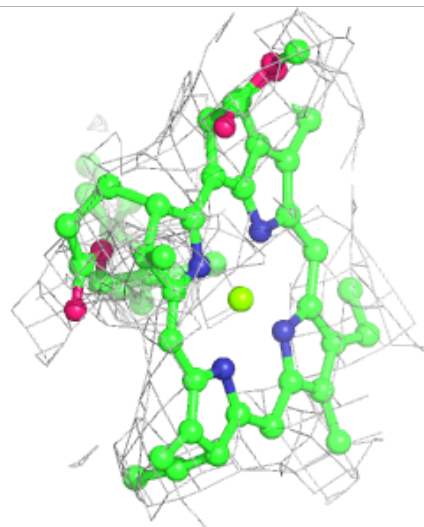
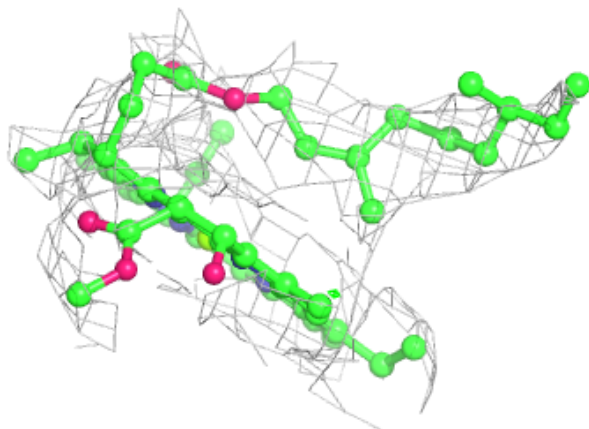
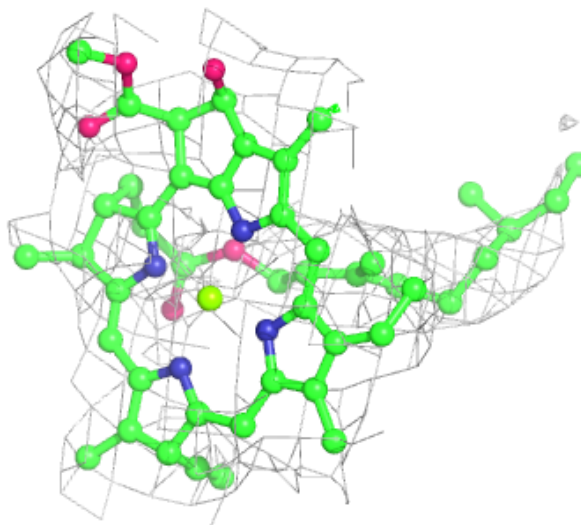
Electron density around CLA 2 2010:

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



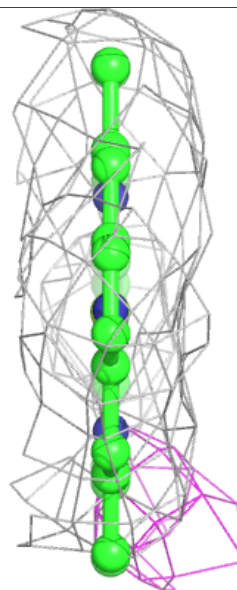
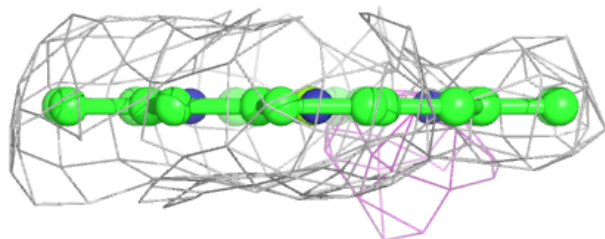
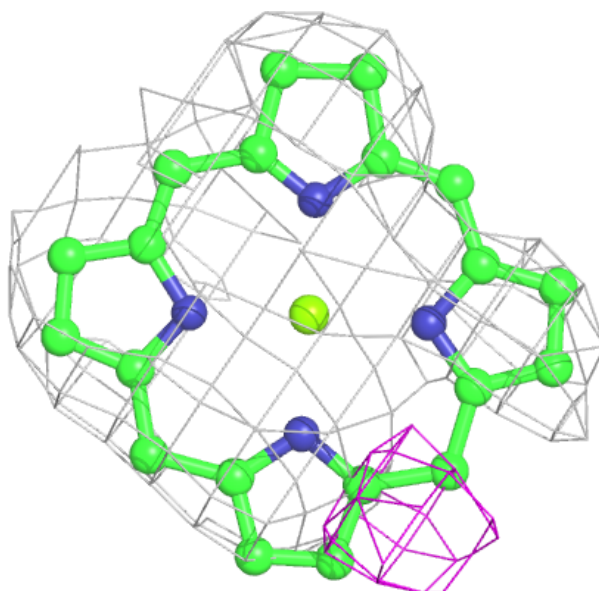
Electron density around CLA 2 2002:

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



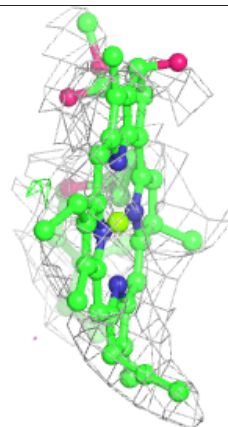
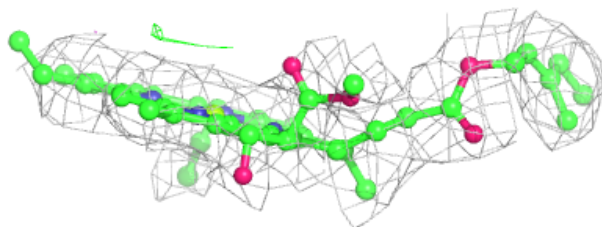
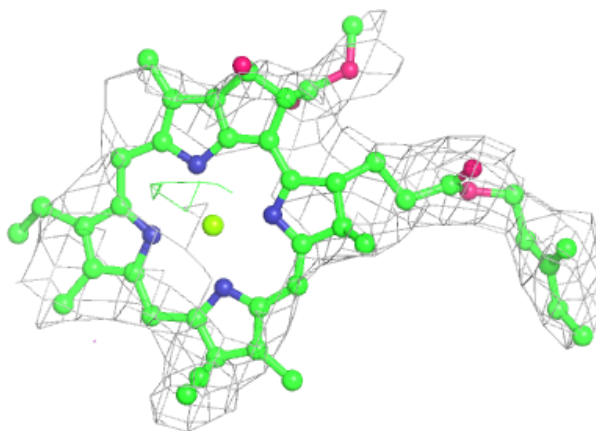
Electron density around CLA 2 2003:

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

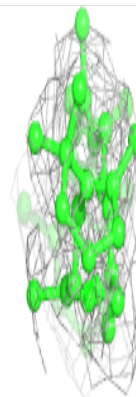
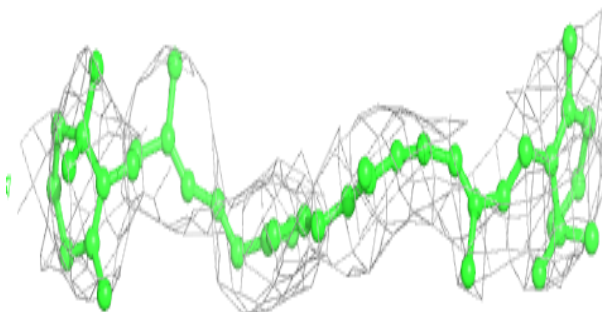
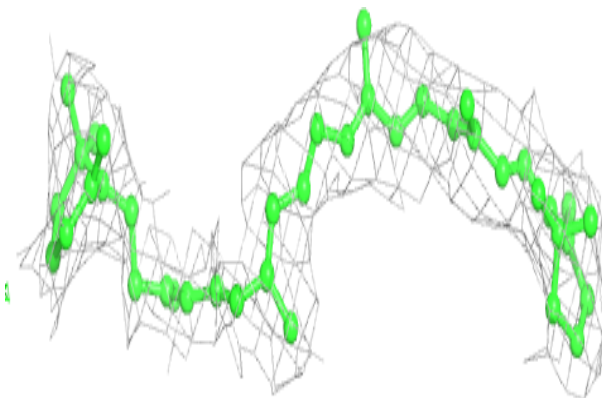


Electron density around CLA 1 1303:

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

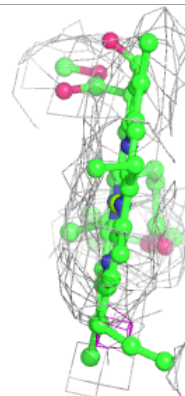
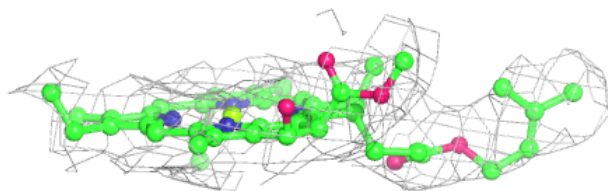
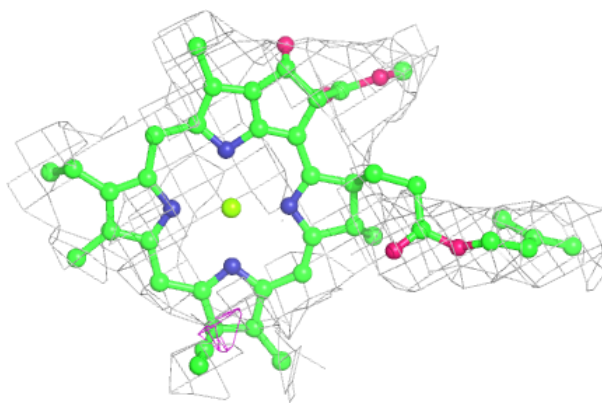
**Electron density around BCR I 6021:**

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



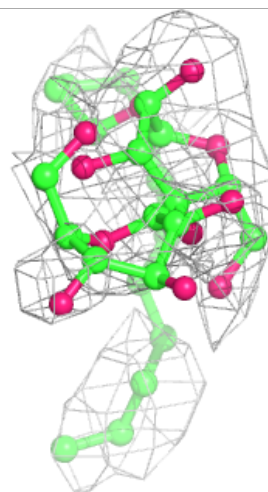
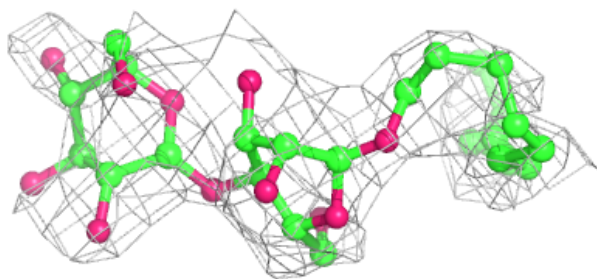
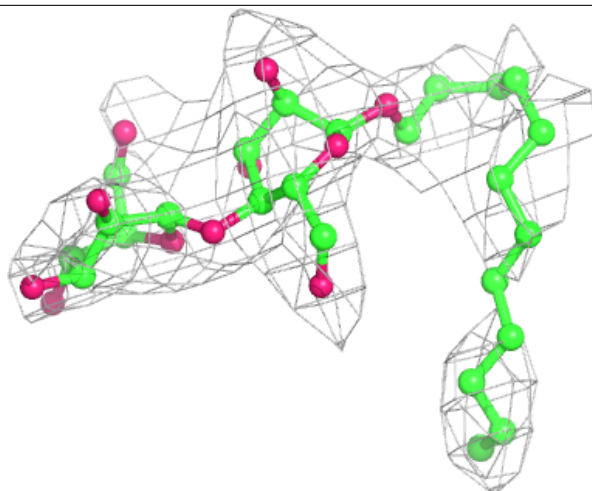
Electron density around CLA K 1143:

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



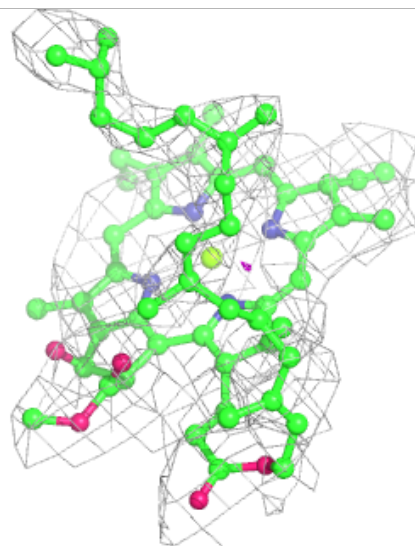
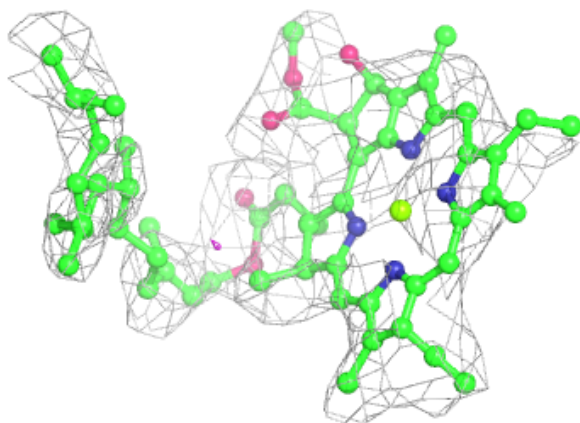
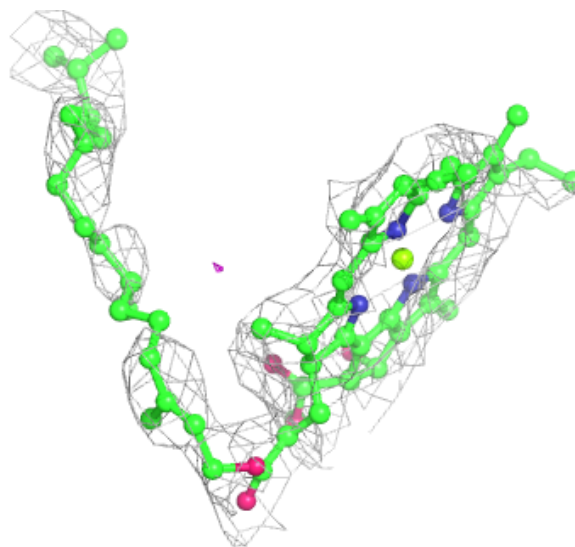
Electron density around LMU R 7014:

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



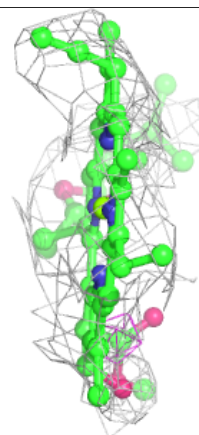
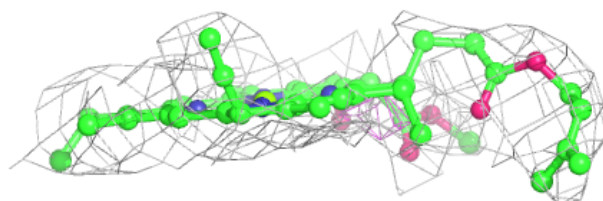
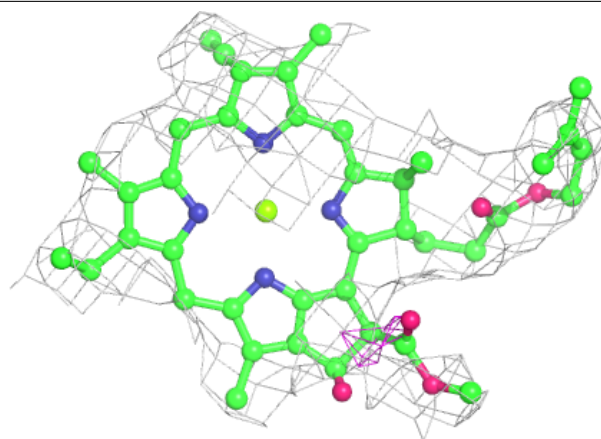
Electron density around CLA 2 2006:

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

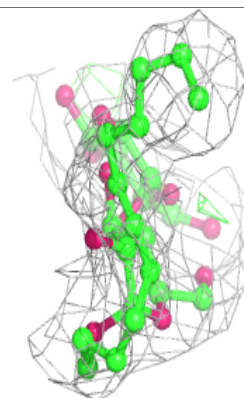
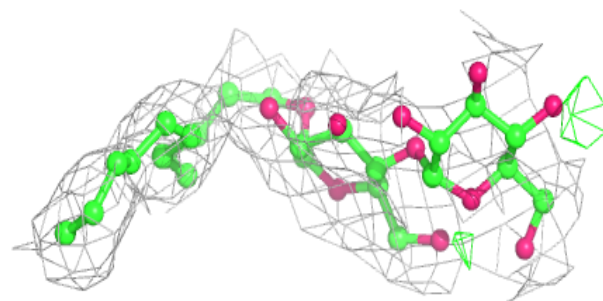
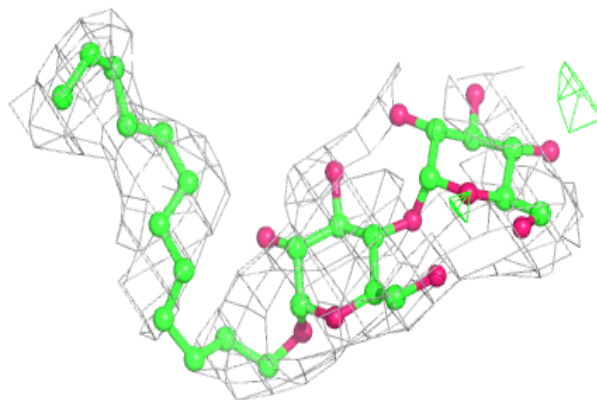


Electron density around CLA K 1146:

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

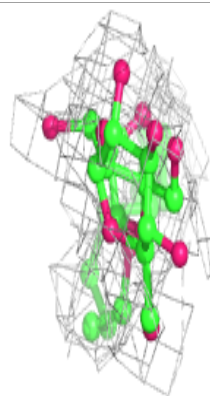
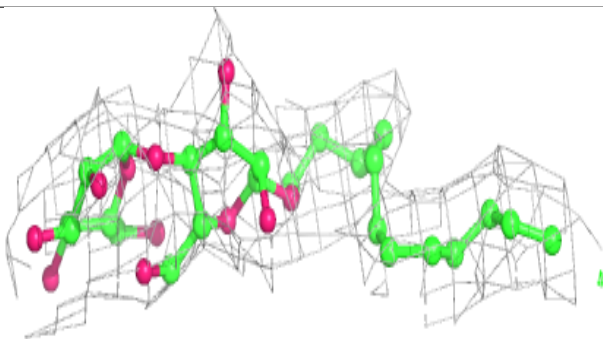
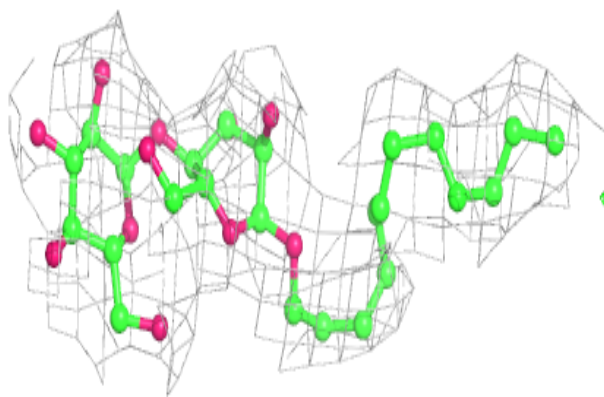
**Electron density around LMU R 7025:**

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



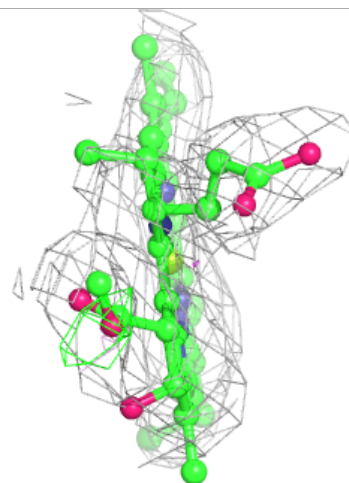
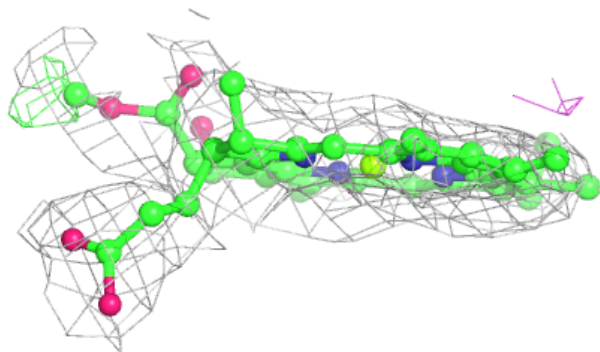
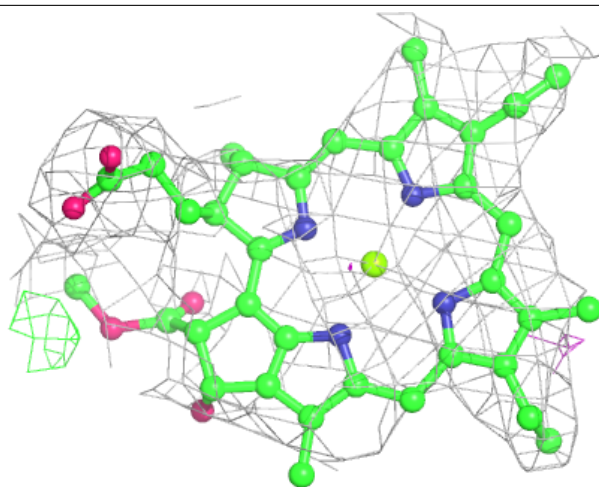
Electron density around LMU R 7020:

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



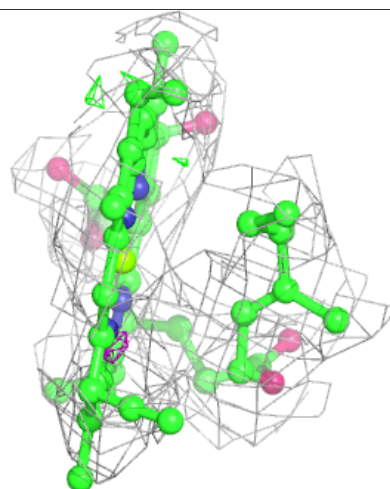
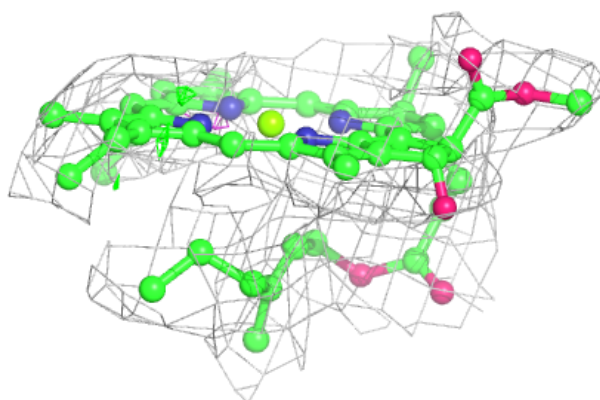
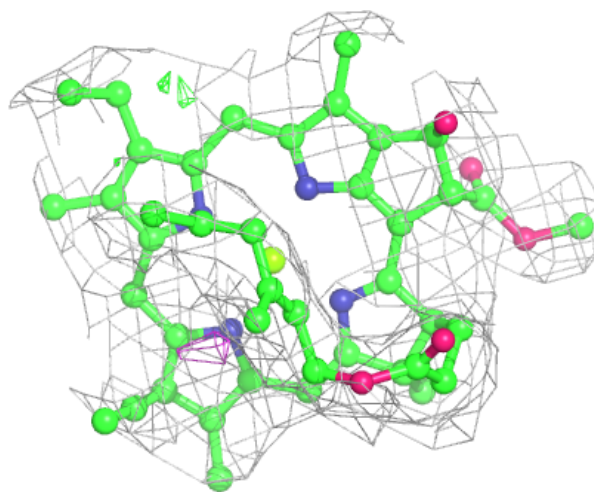
Electron density around CLA A 1108:

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



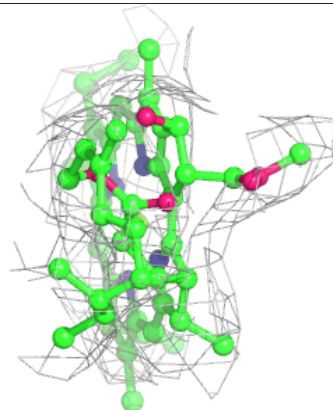
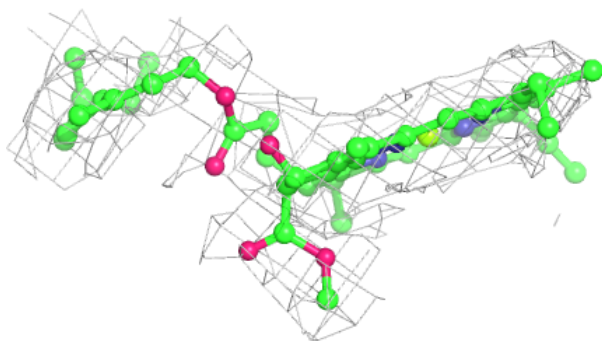
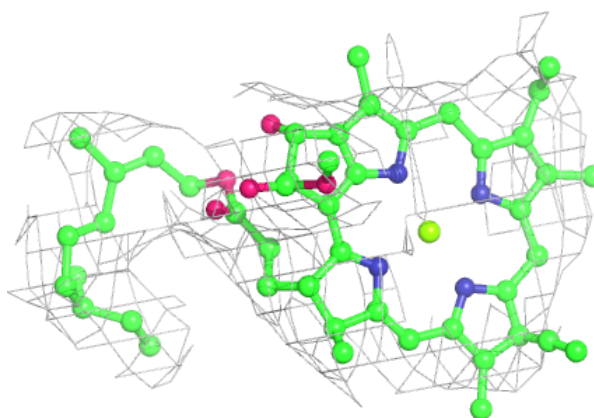
Electron density around CLA A 1116:

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

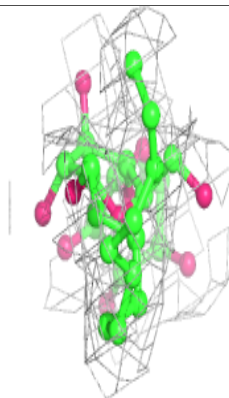
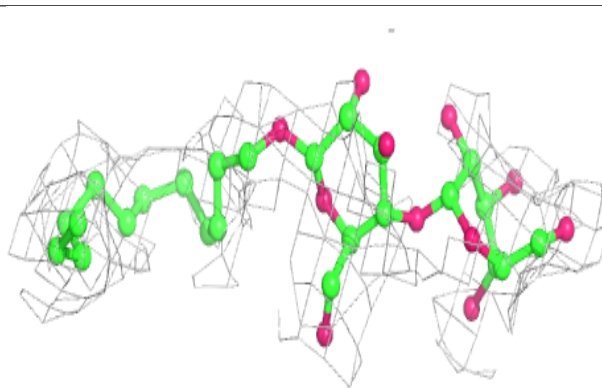
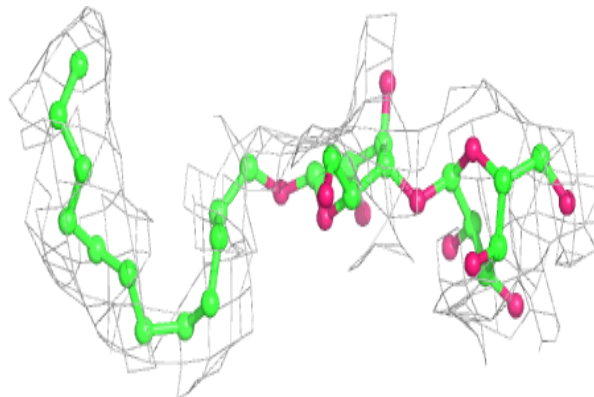


Electron density around CLA 3 2009:

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

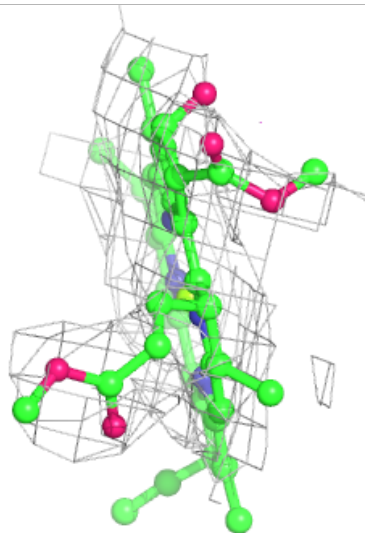
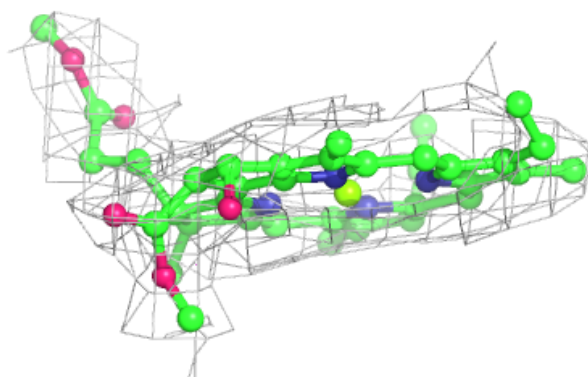
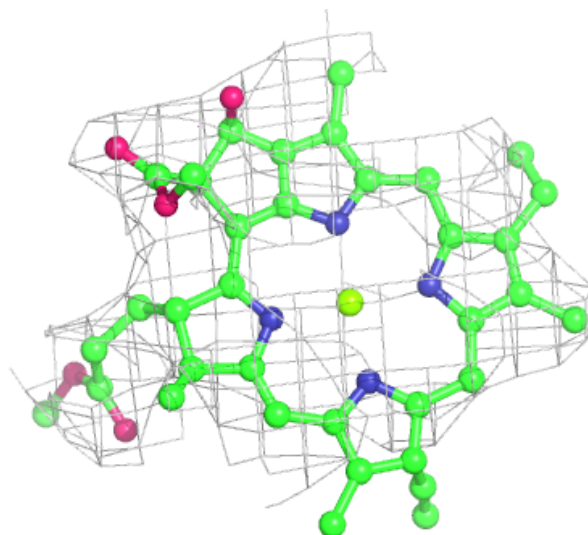
**Electron density around LMU A 7044:**

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



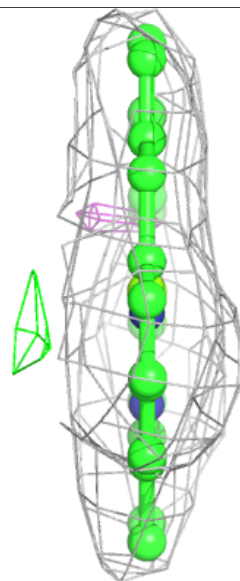
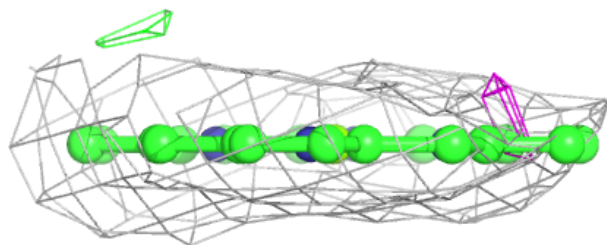
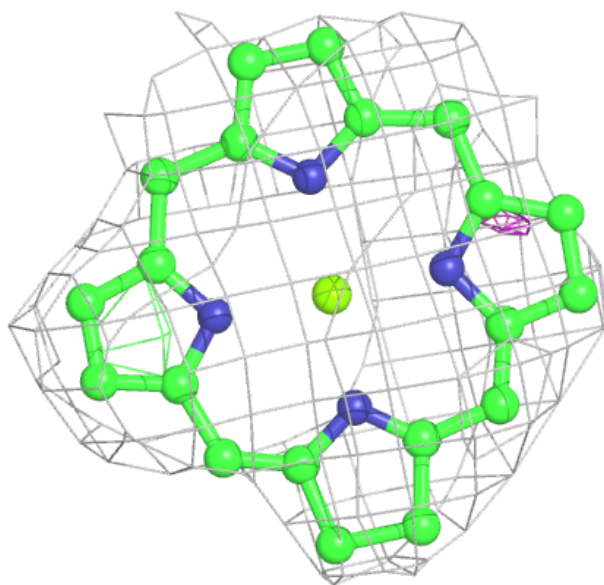
Electron density around CLA B 1218:

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



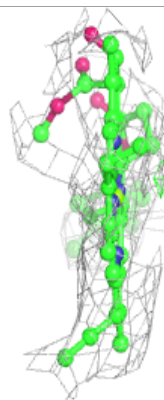
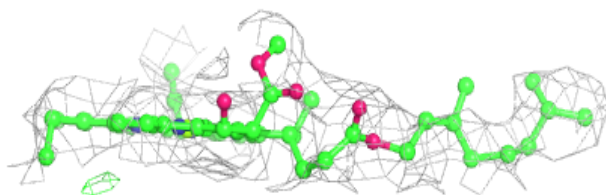
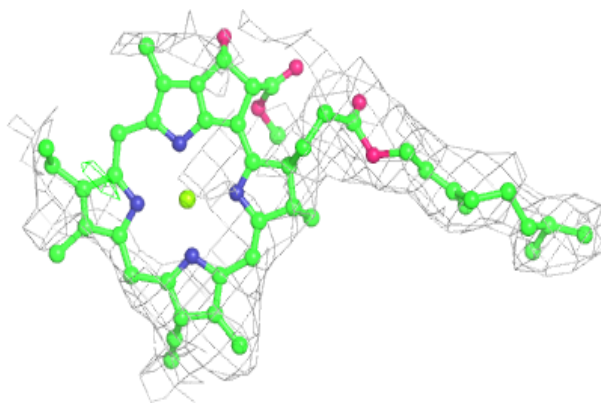
Electron density around CLA 4 4005:

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



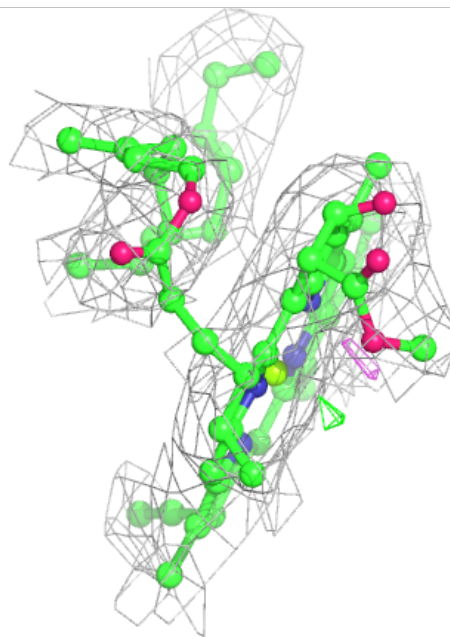
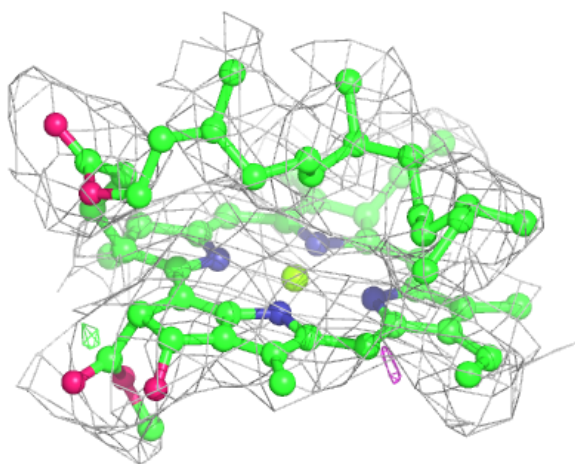
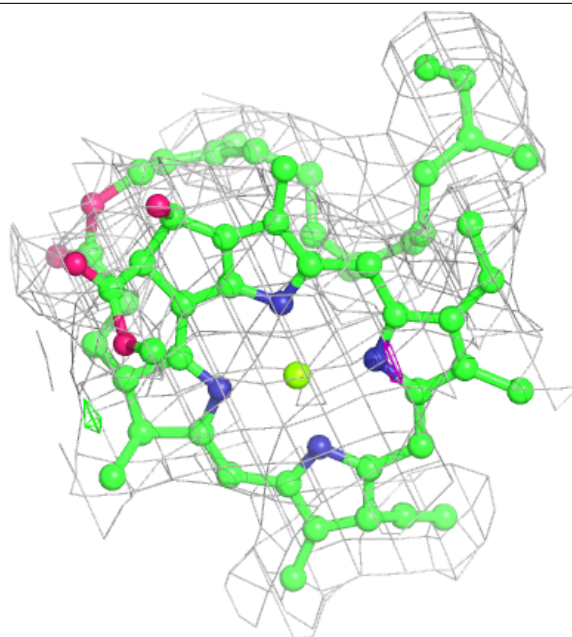
Electron density around CLA 4 4006:

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



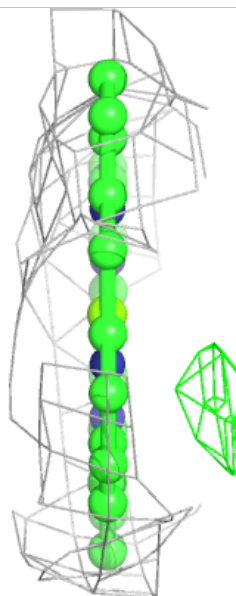
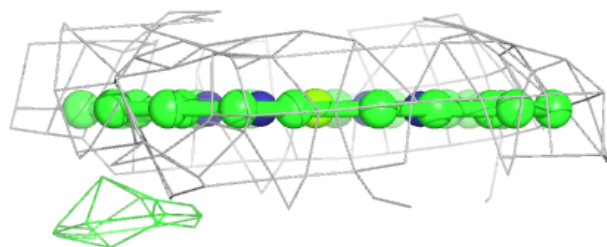
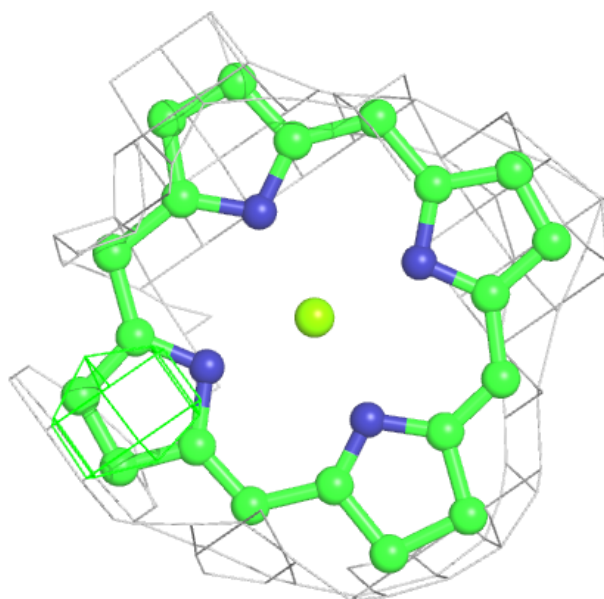
Electron density around CLA 1 1007:

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



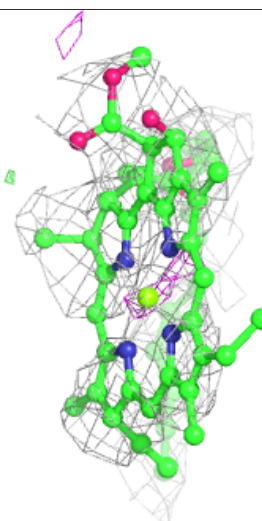
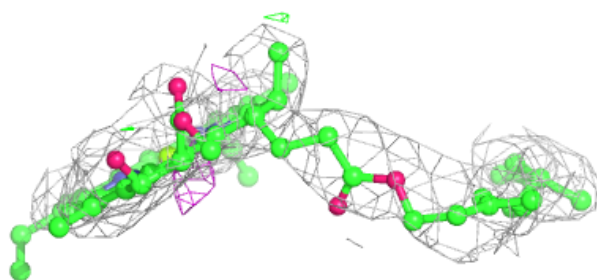
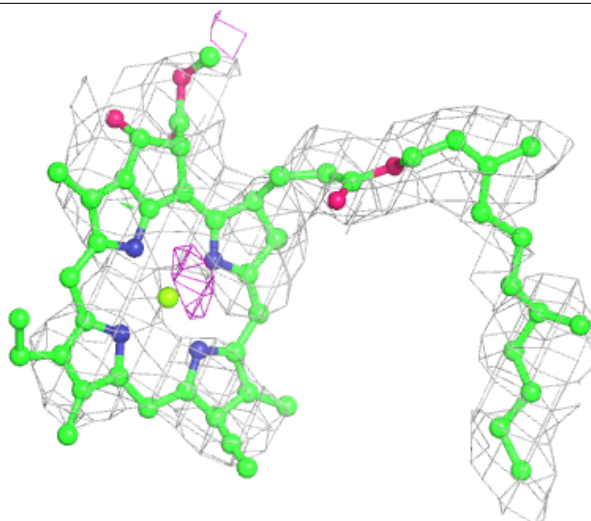
Electron density around CLA 4 4010:

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



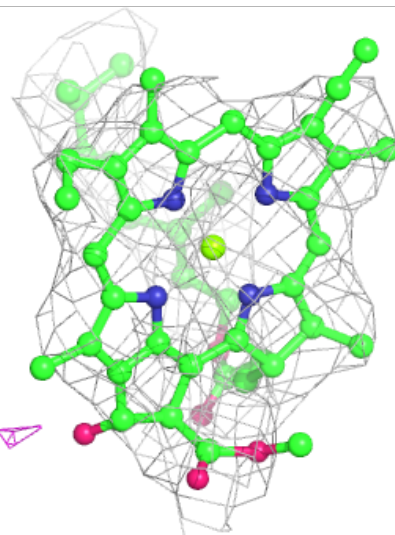
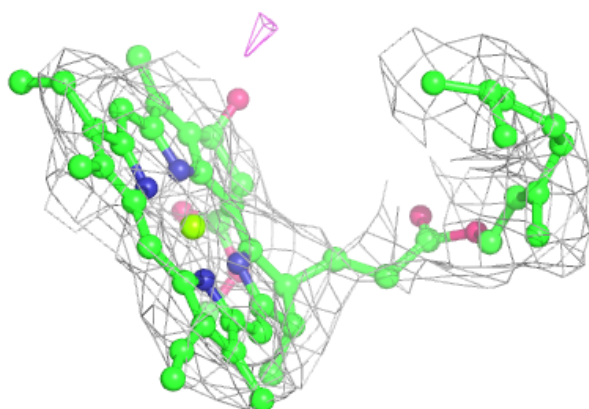
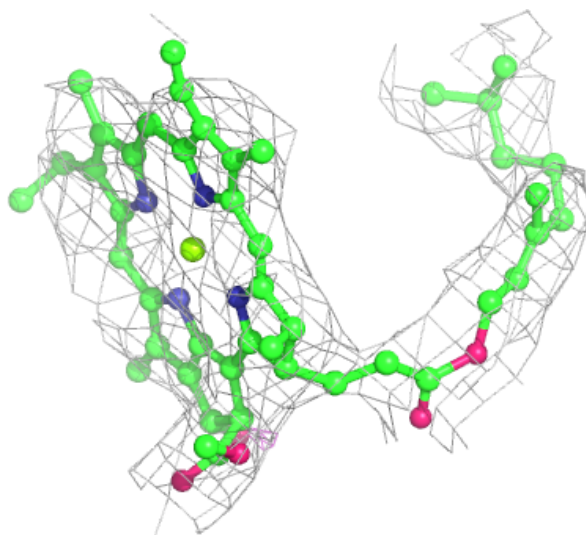
Electron density around CLA B 1222:

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



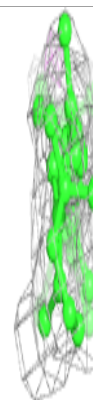
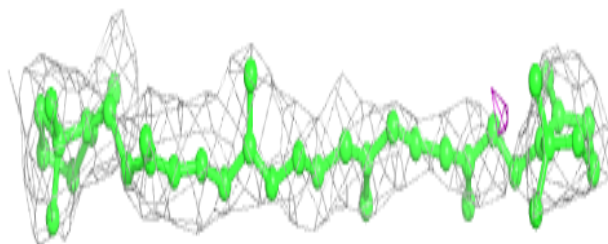
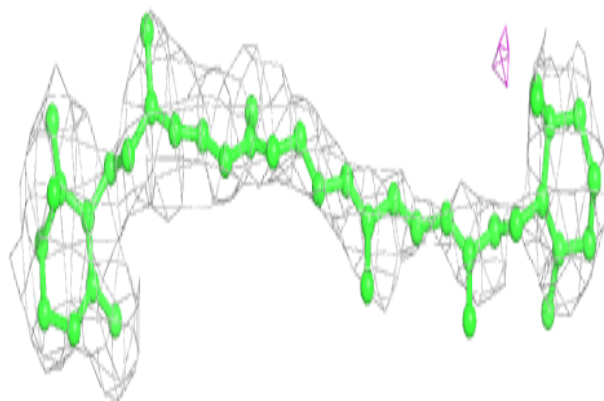
Electron density around CLA A 1102:

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

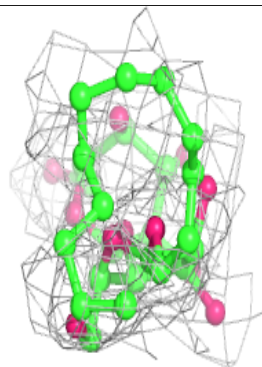
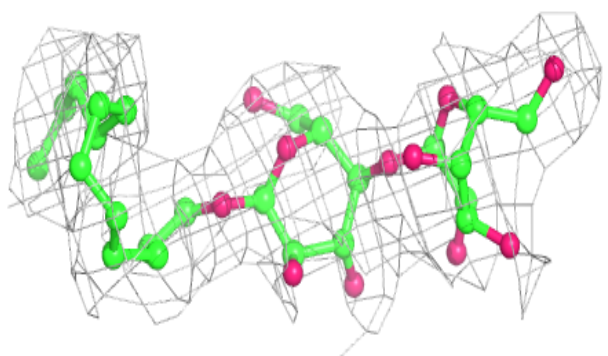
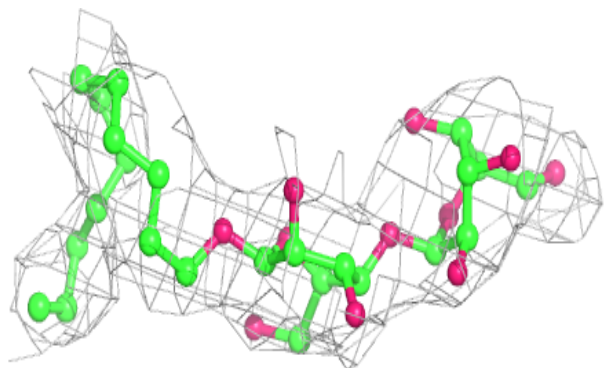


Electron density around BCR L 6019:

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

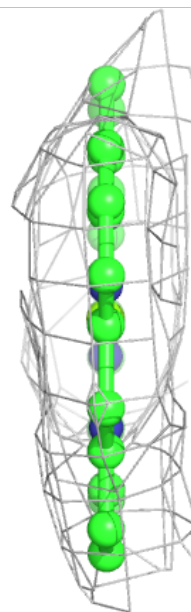
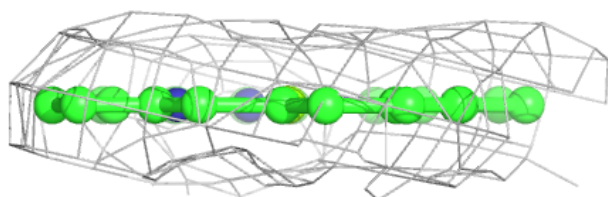
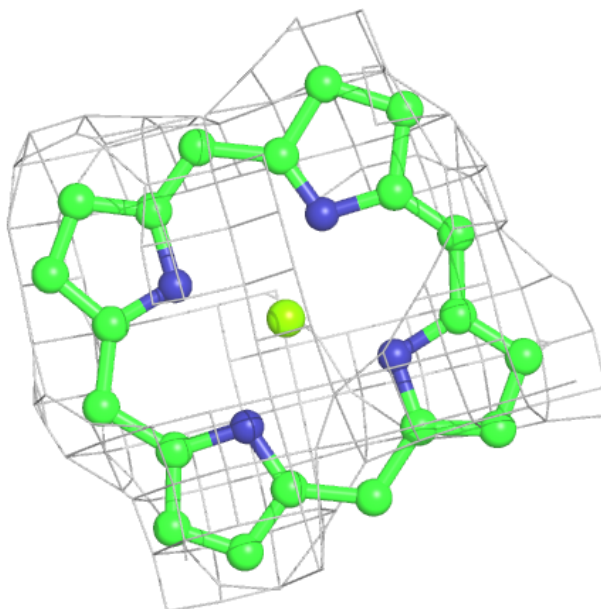
**Electron density around LMU A 7023:**

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



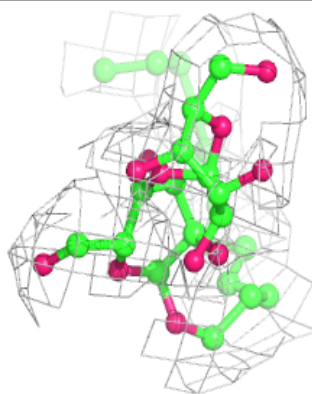
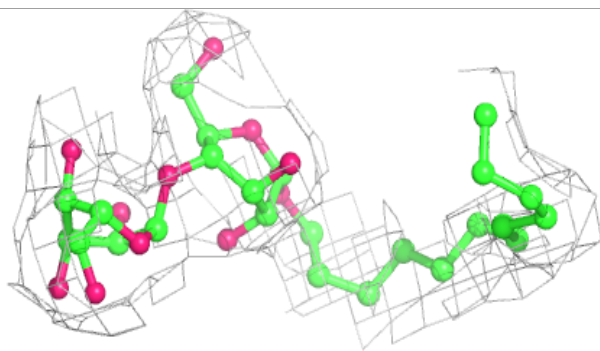
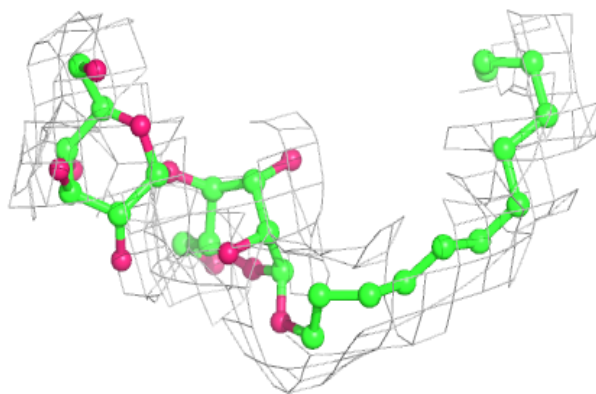
Electron density around CLA 3 3001:

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

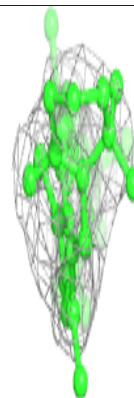
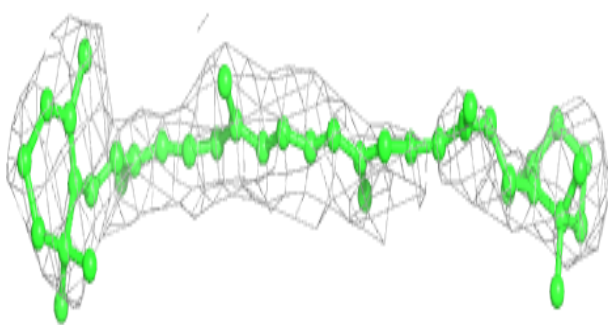
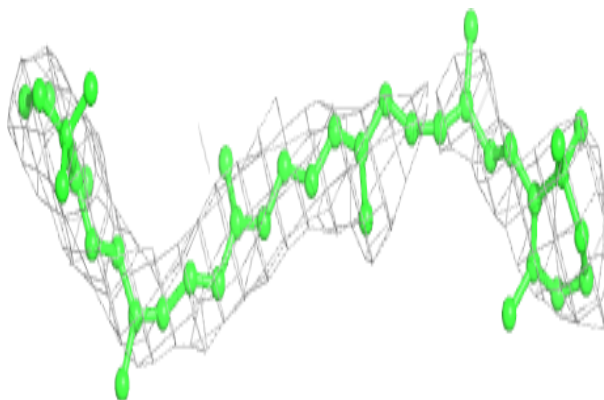


Electron density around LMU R 7022:

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

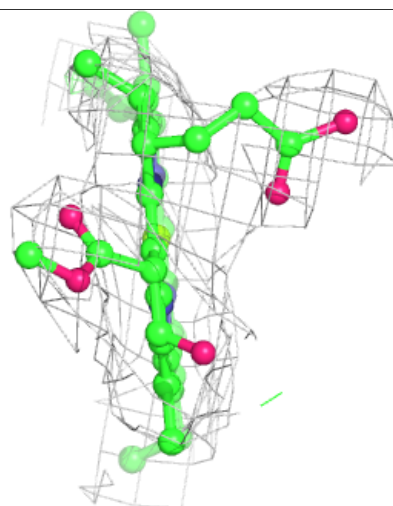
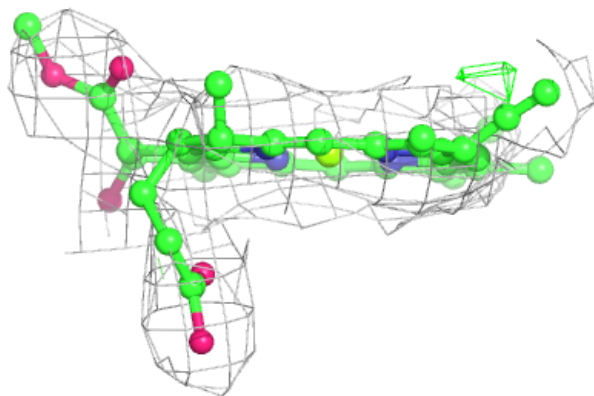
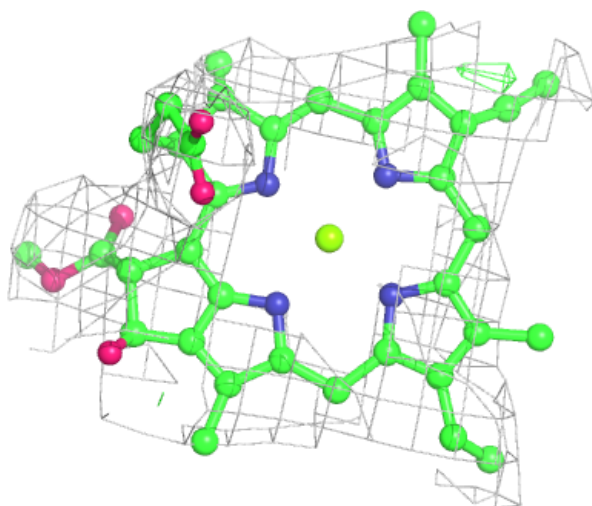
**Electron density around BCR B 6006:**

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



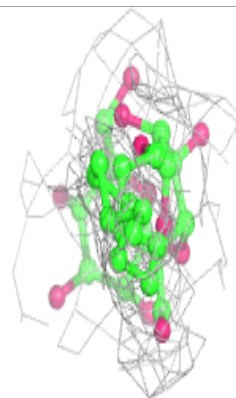
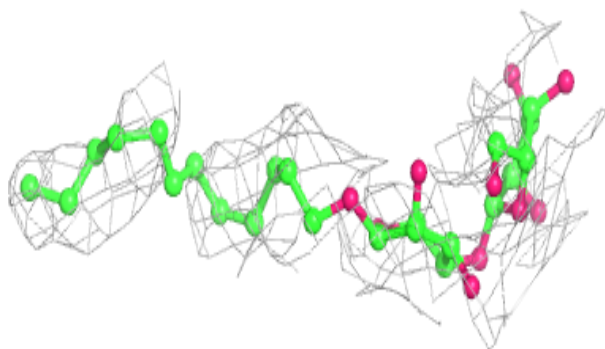
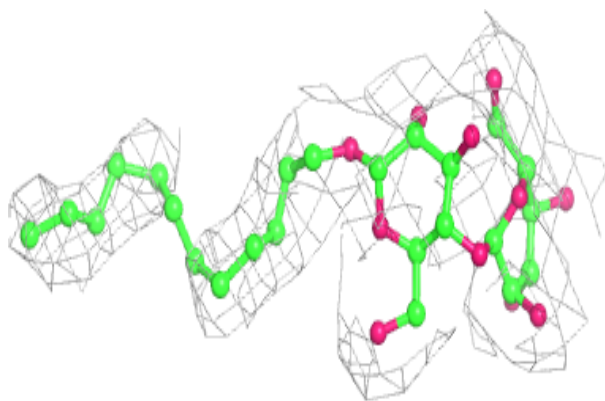
Electron density around CLA B 1201:

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



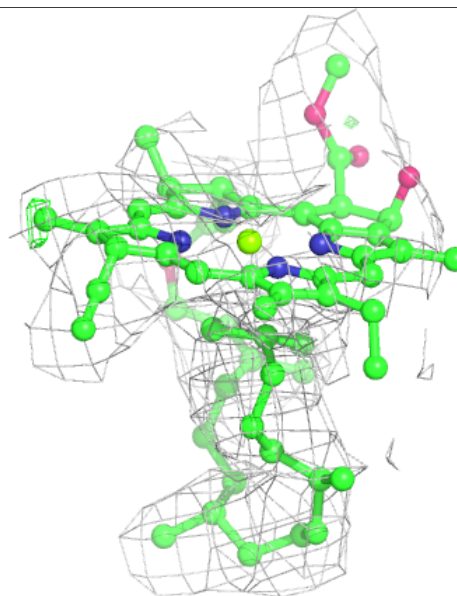
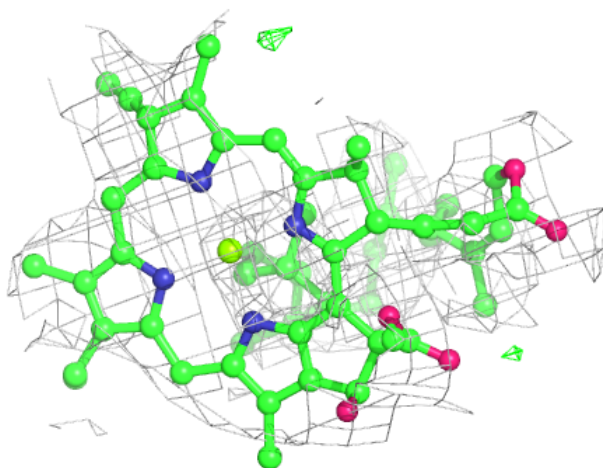
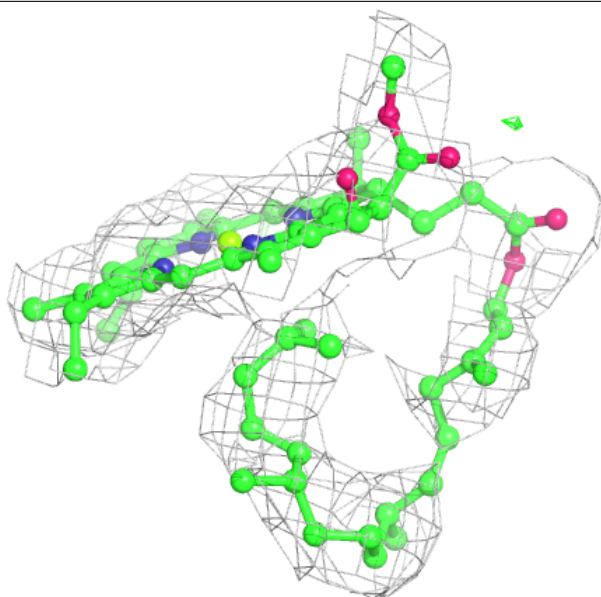
Electron density around LMU 4 7033:

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



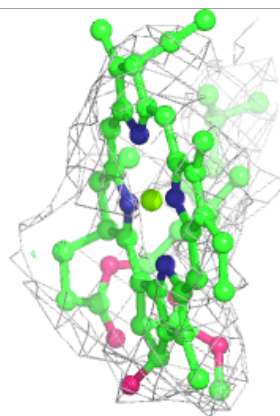
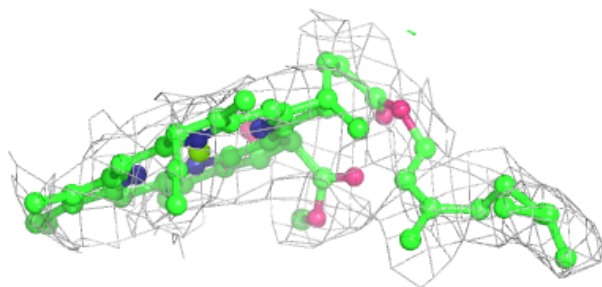
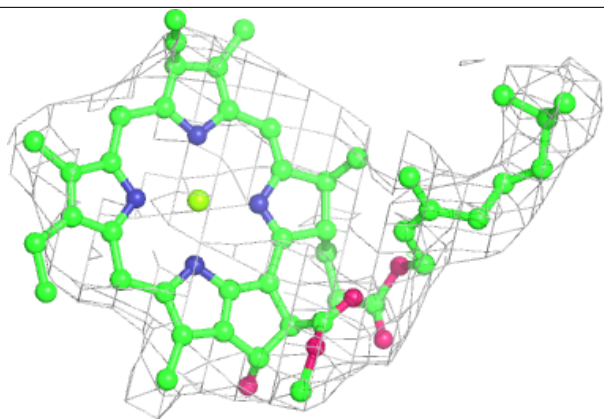
Electron density around CLA 2 4009:

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

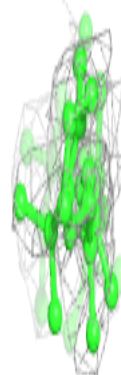
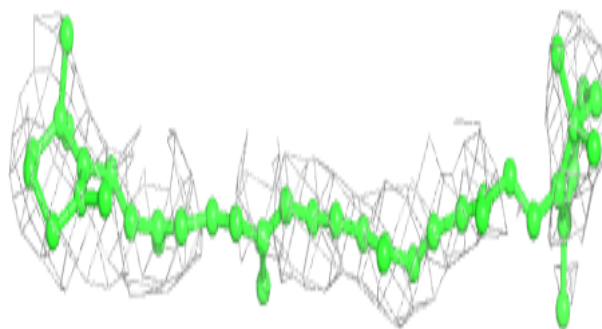
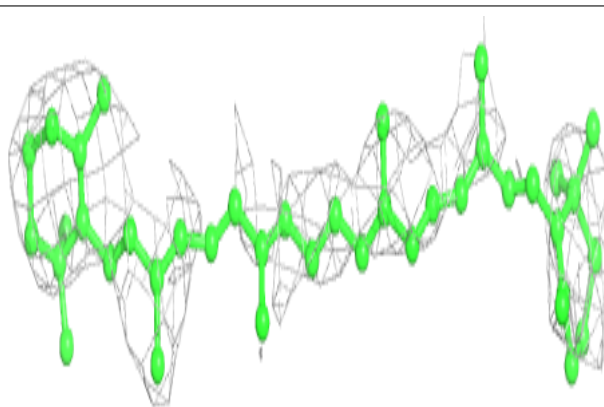


Electron density around CLA J 1308:

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

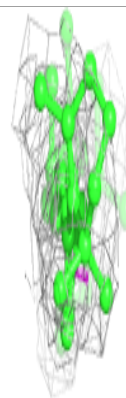
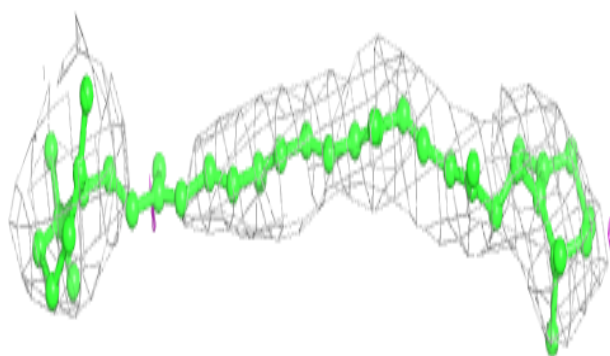
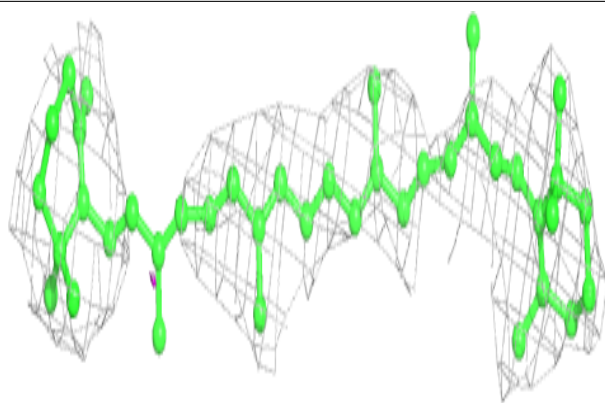
**Electron density around BCR A 6008:**

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

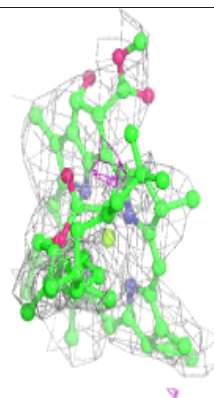
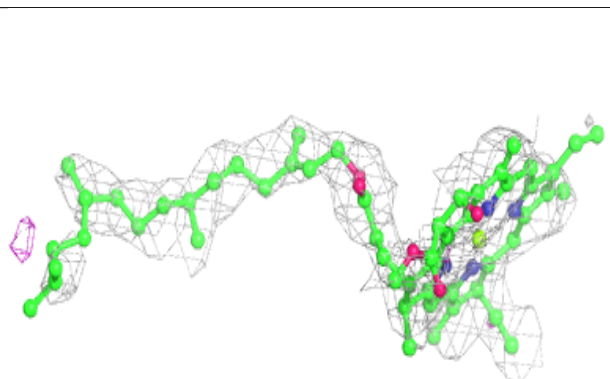
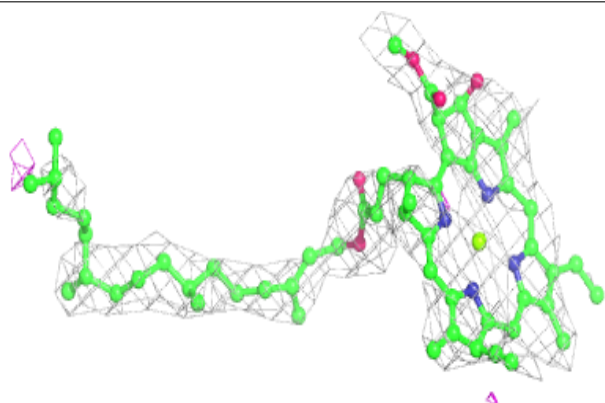


Electron density around BCR B 6004:

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

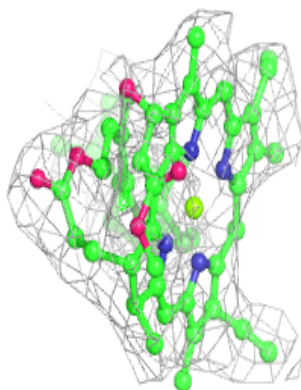
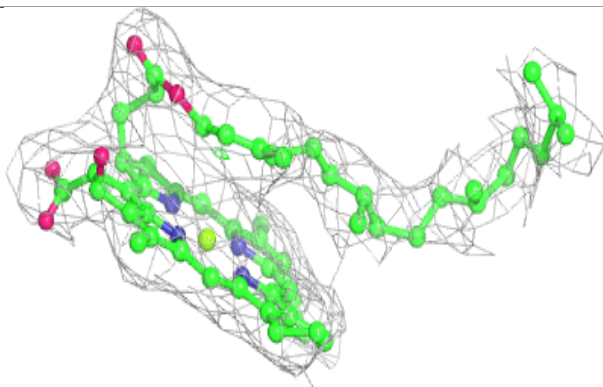
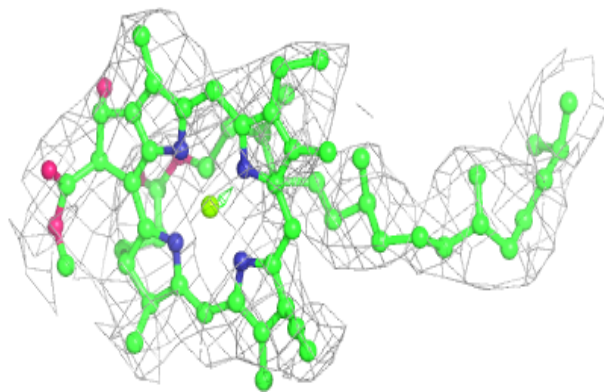
**Electron density around CLA A 1119:**

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



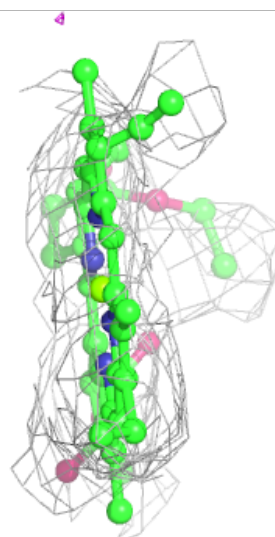
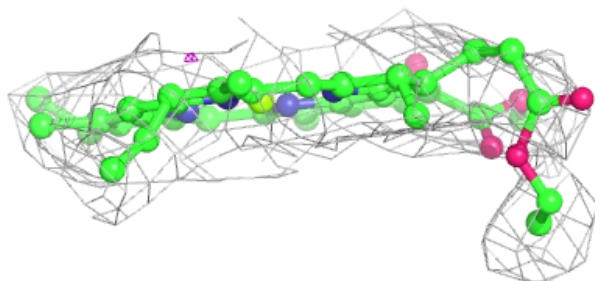
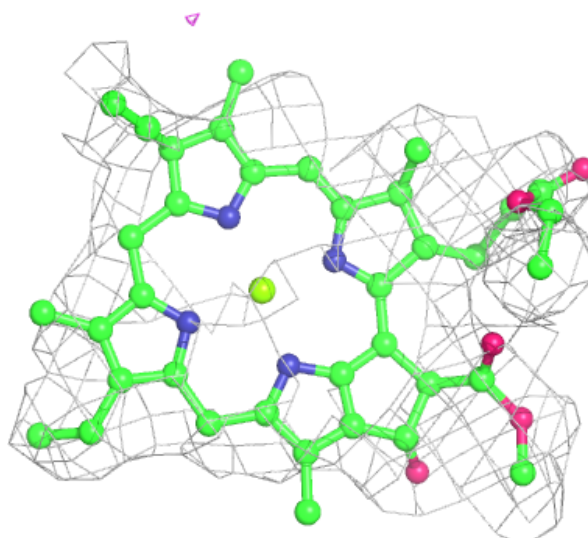
Electron density around CLA A 1115:

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



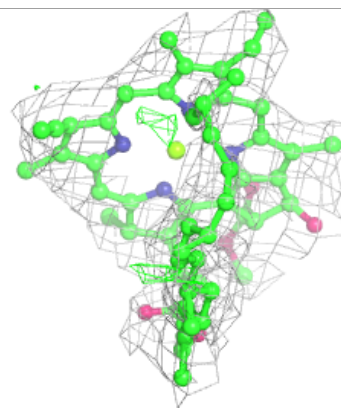
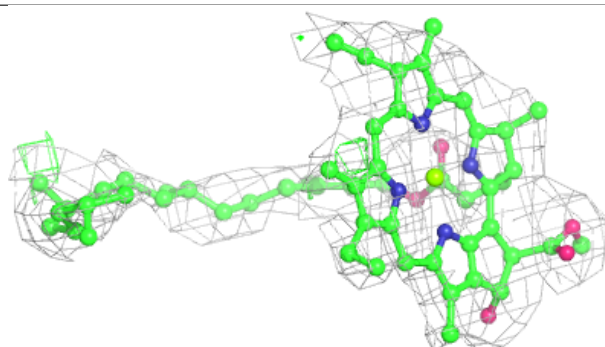
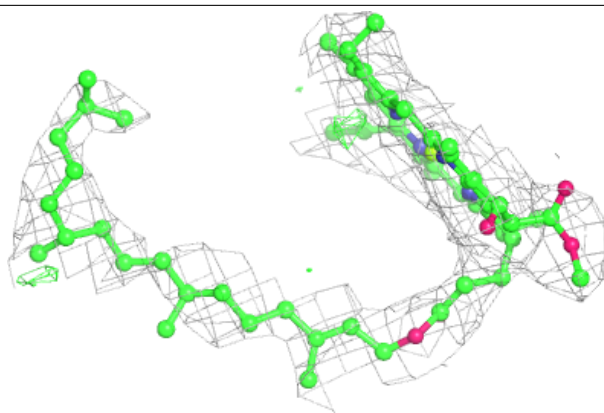
Electron density around CLA 1 1002:

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



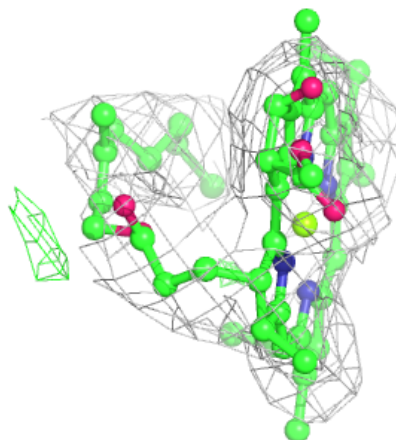
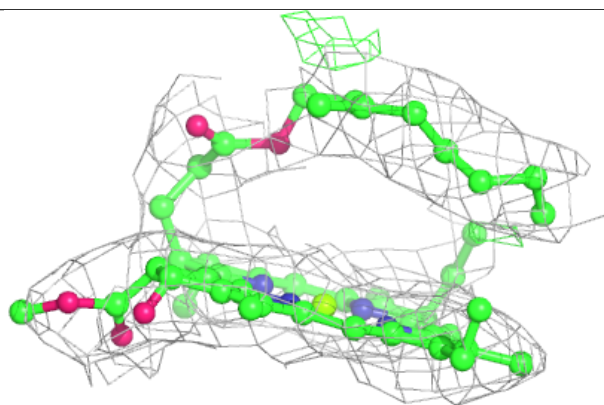
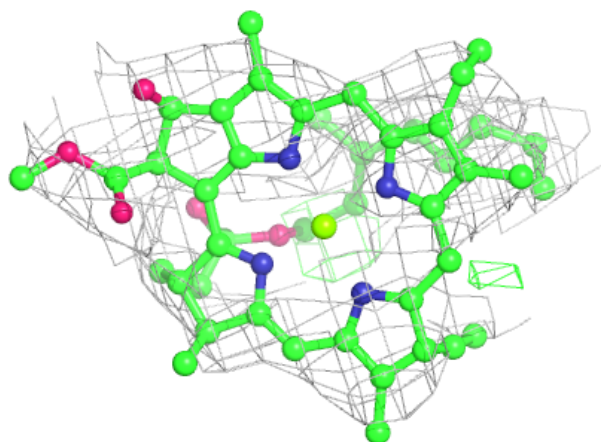
Electron density around CLA L 1130:

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



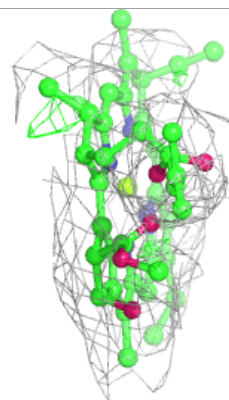
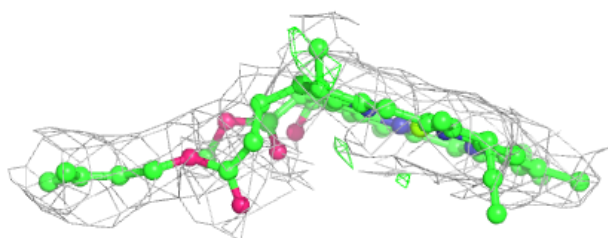
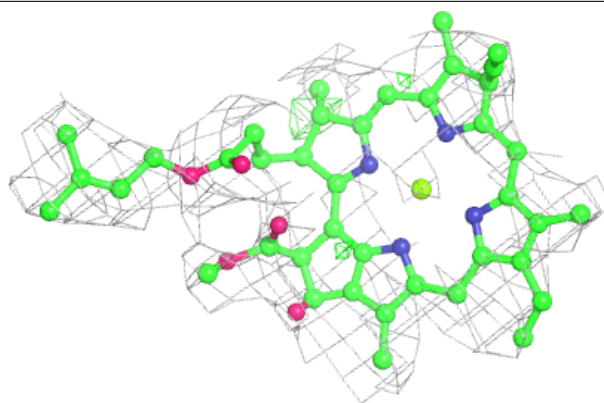
Electron density around CLA A 1110:

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

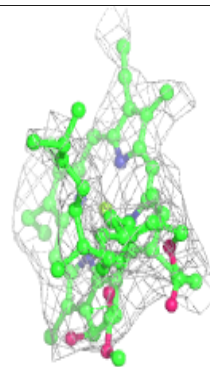
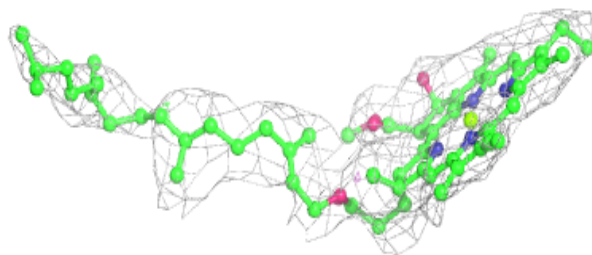
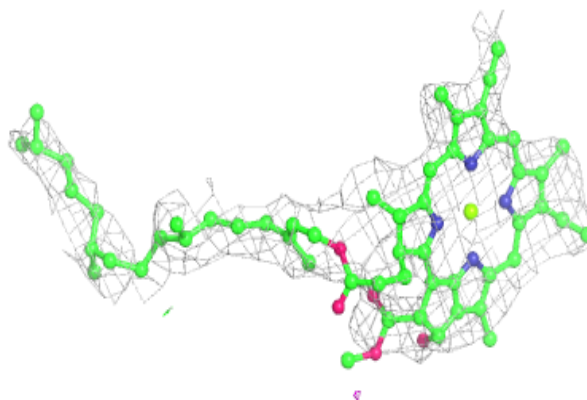


Electron density around CLA L 1503:

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

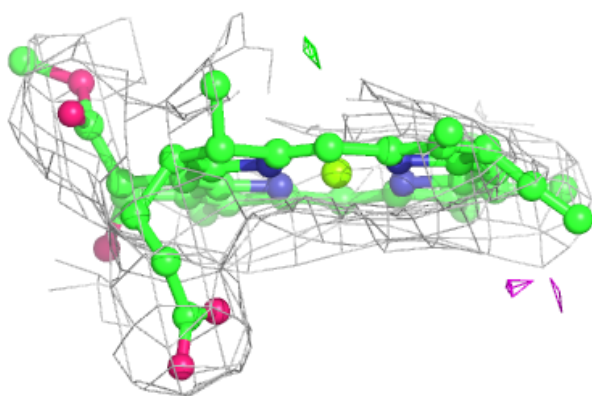
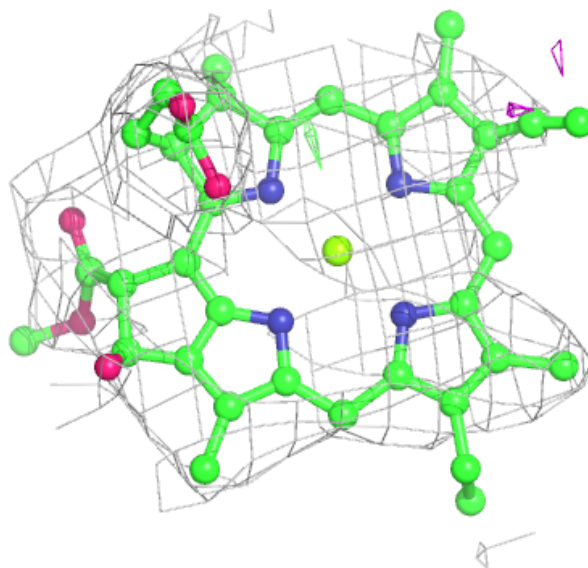
**Electron density around CLA H 1207:**

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



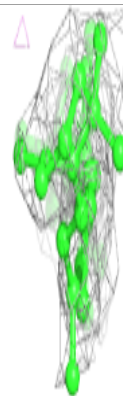
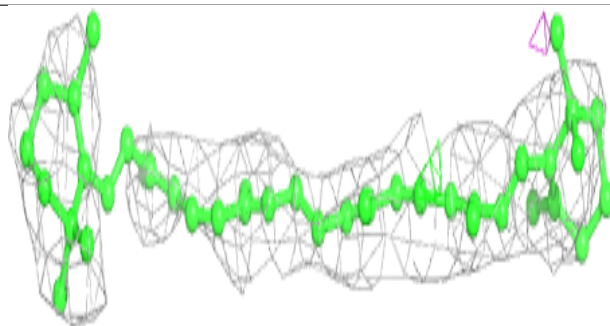
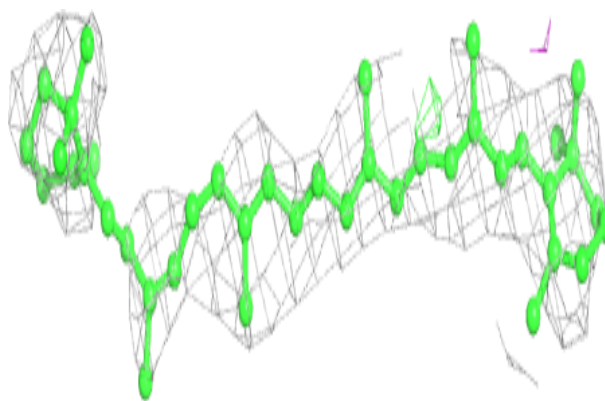
Electron density around CLA B 1231:

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

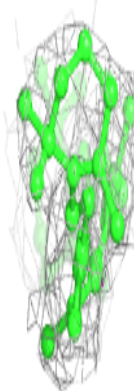
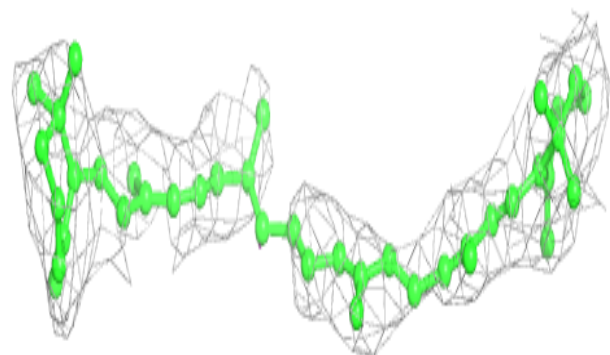
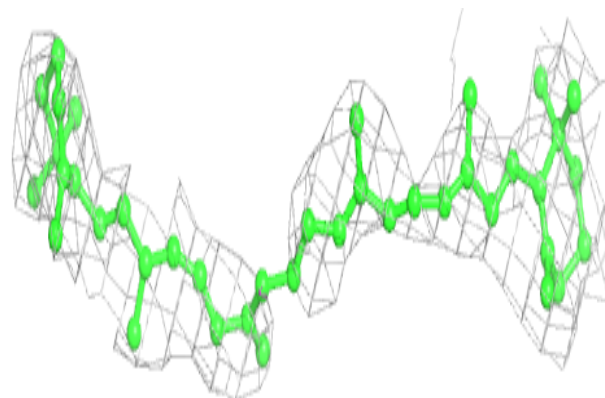


Electron density around BCR B 6017:

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

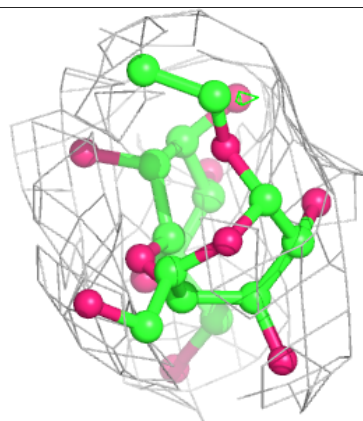
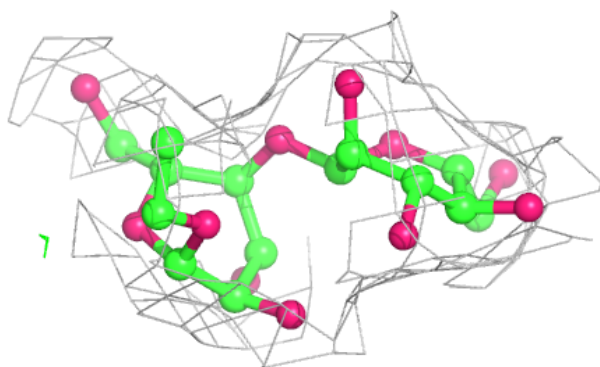
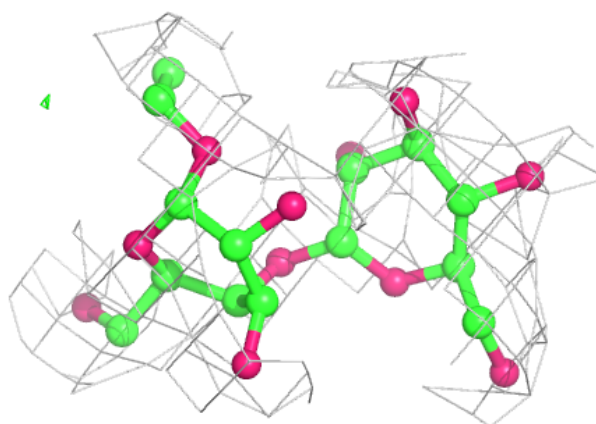
**Electron density around BCR I 6018:**

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

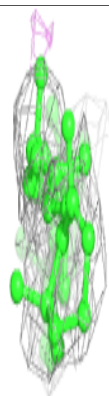
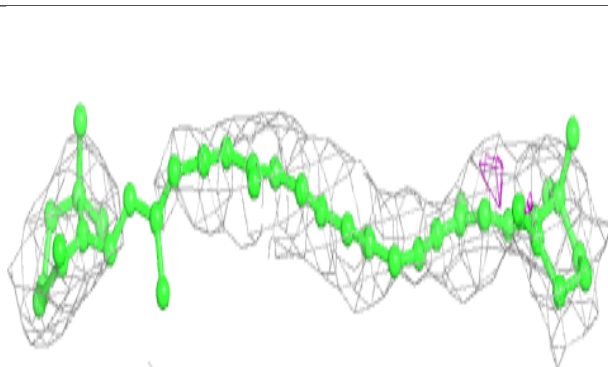
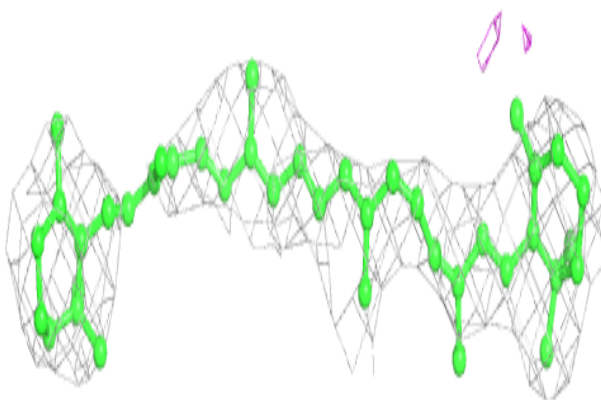


Electron density around LMU B 7012:

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

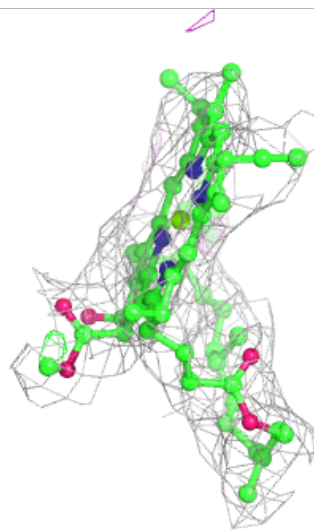
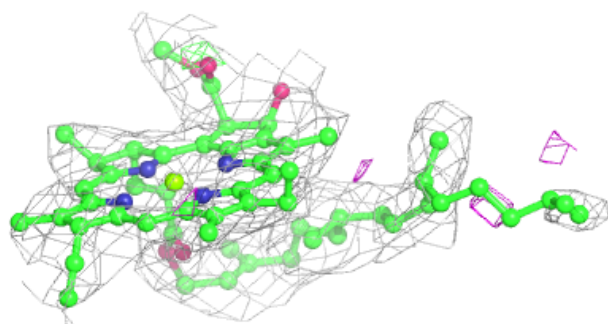
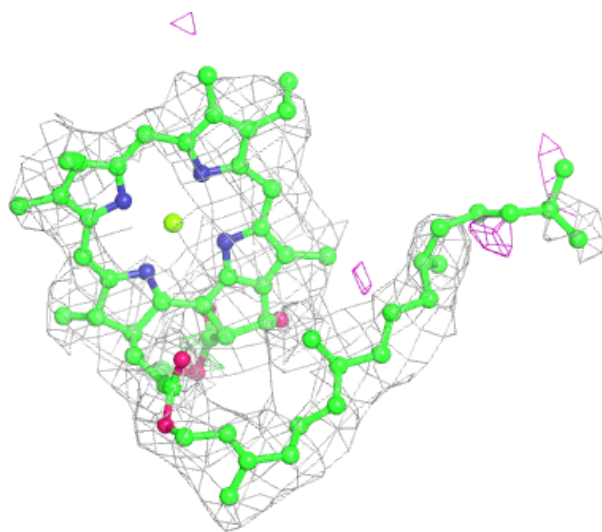
**Electron density around BCR B 6010:**

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



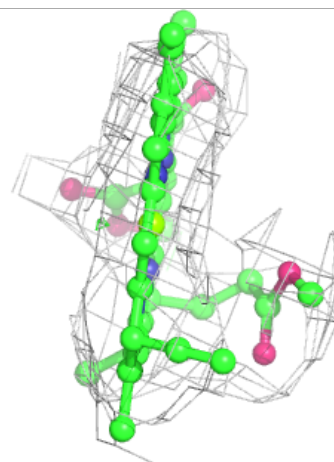
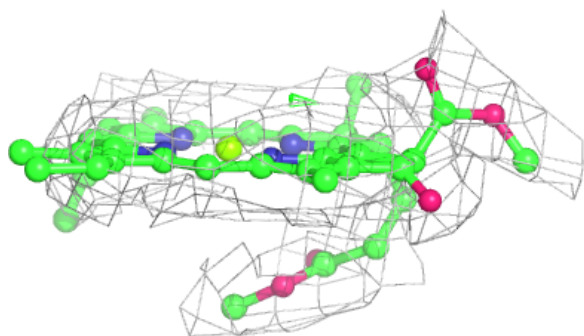
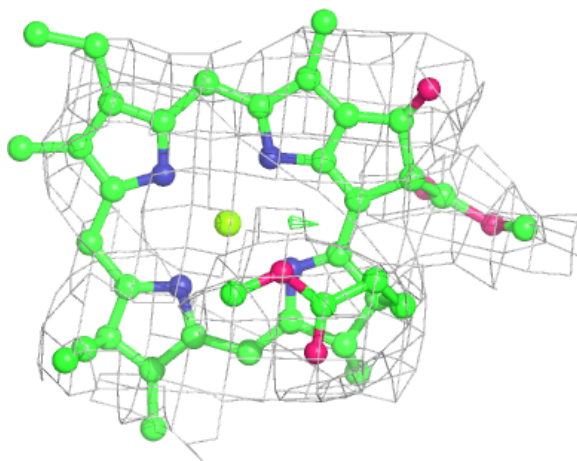
Electron density around CLA B 1229:

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



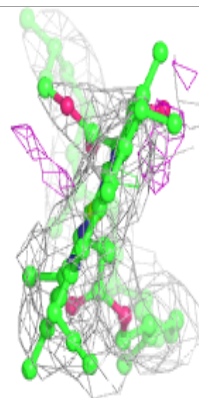
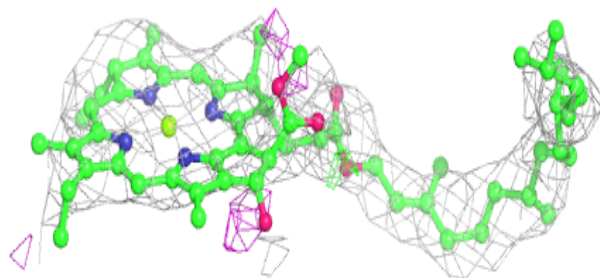
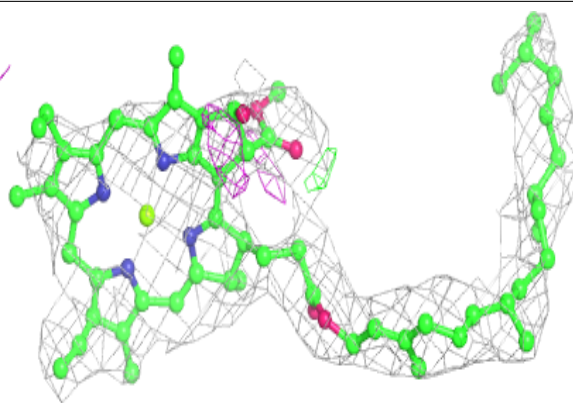
Electron density around CLA 1 1005:

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



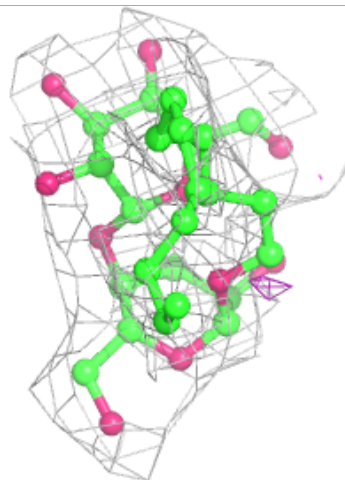
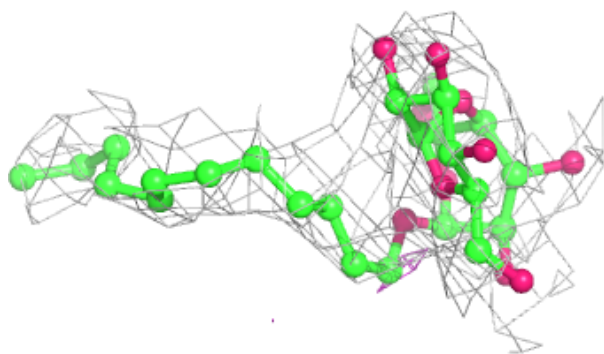
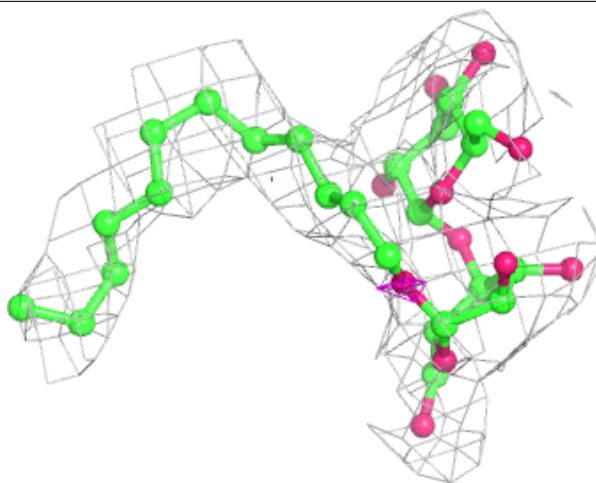
Electron density around CLA B 1223:

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



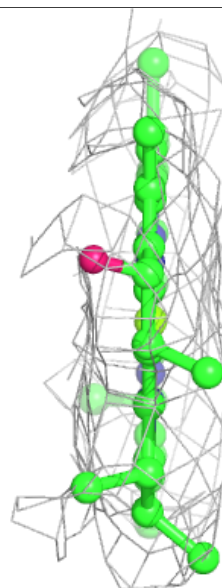
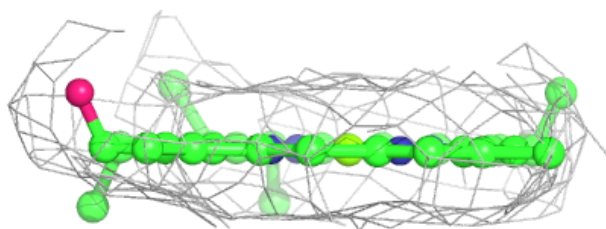
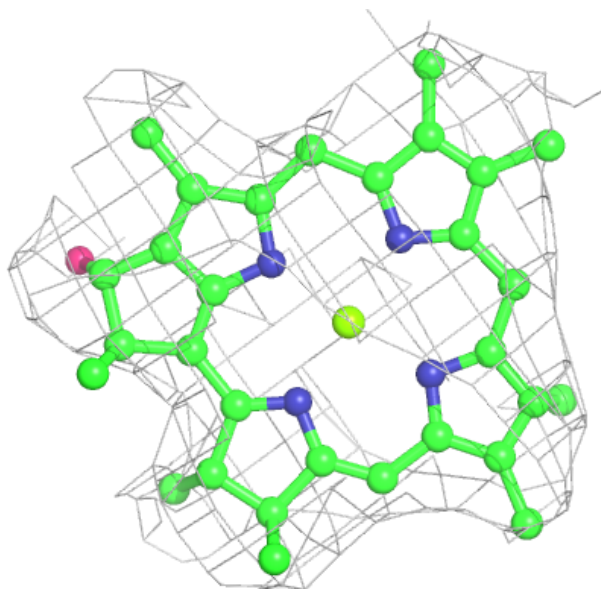
Electron density around LMU H 7032:

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



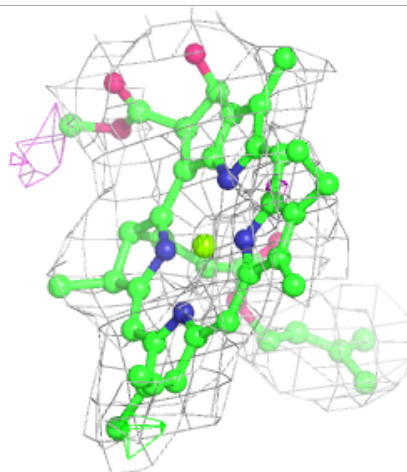
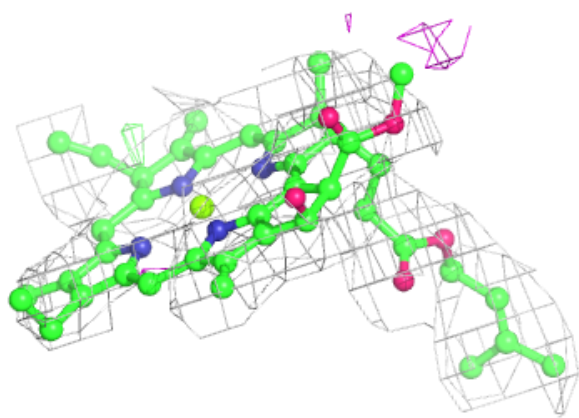
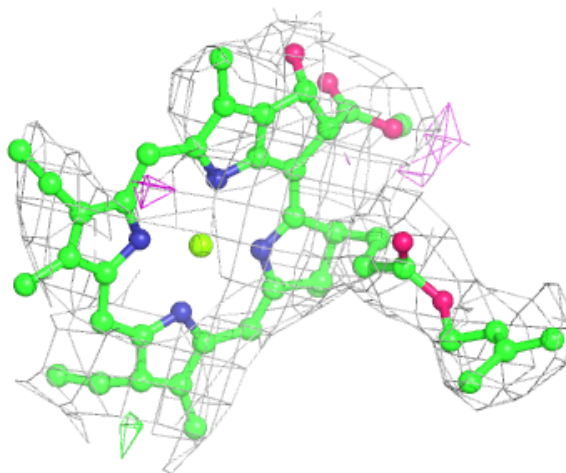
Electron density around CLA 1 1011:

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



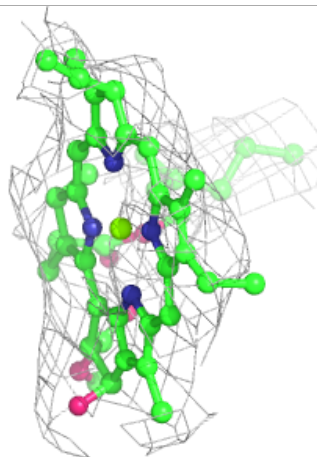
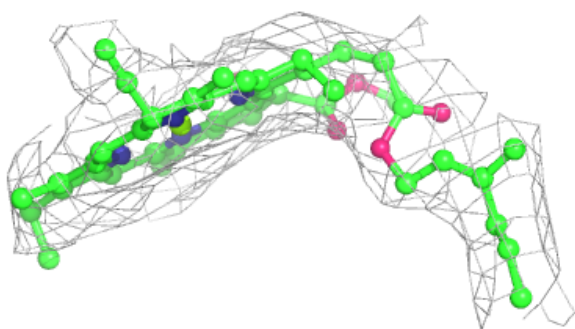
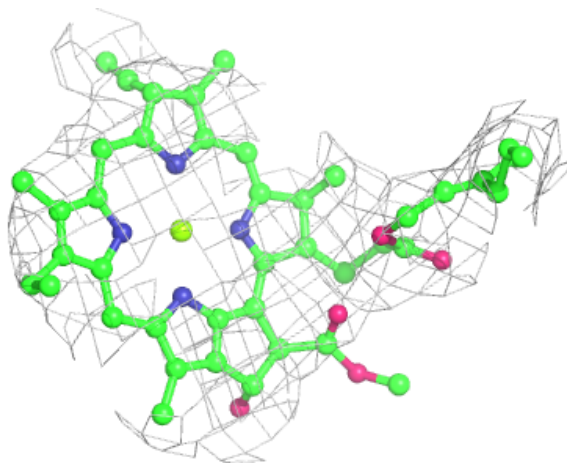
Electron density around CLA 2 2012:

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



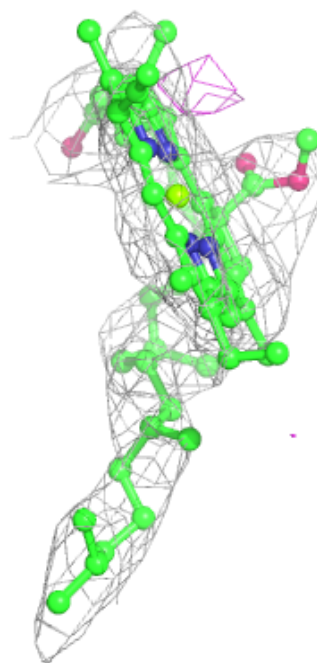
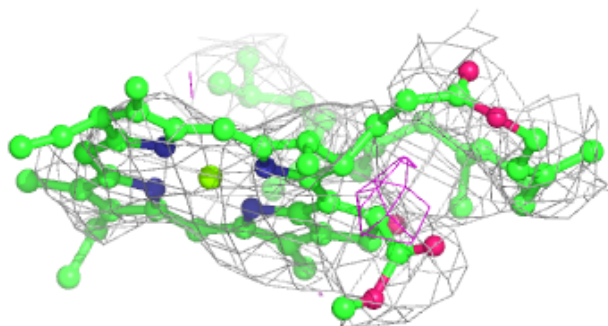
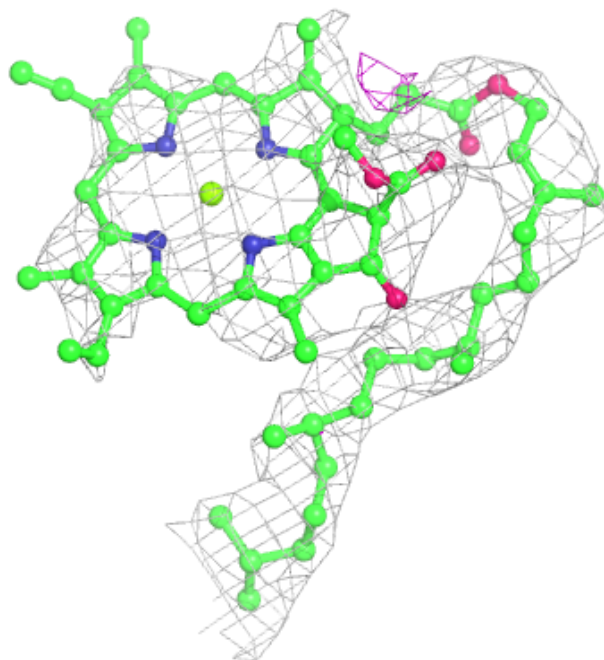
Electron density around CLA 4 4002:

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



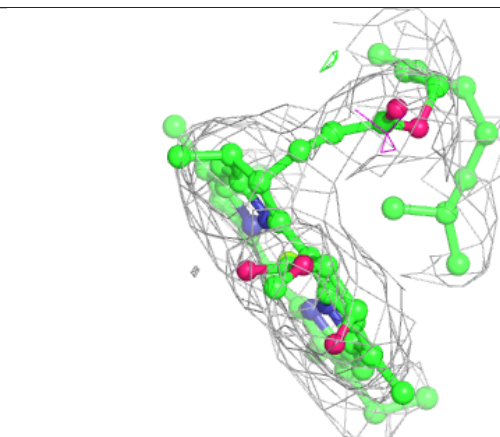
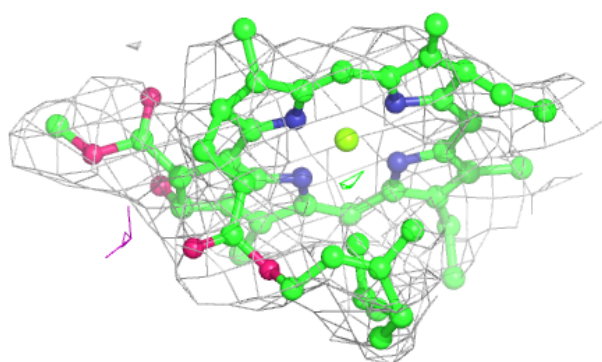
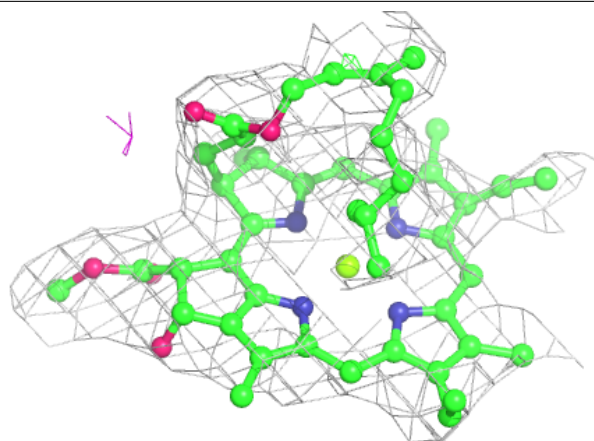
Electron density around CLA A 1123:

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

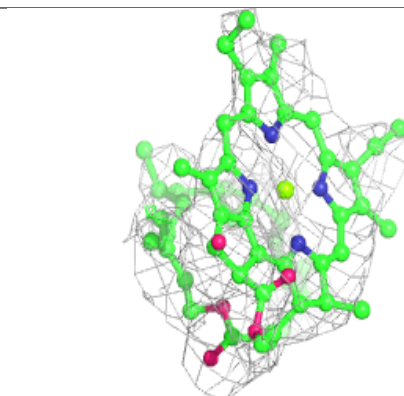
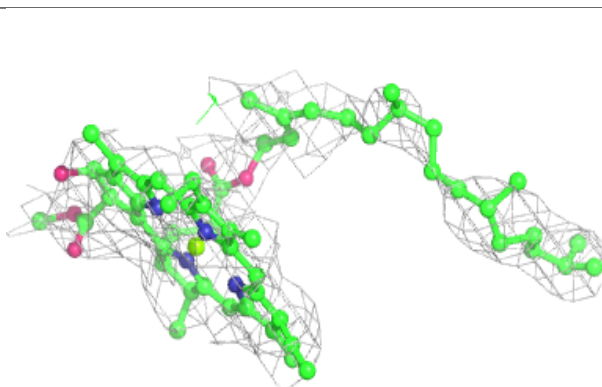
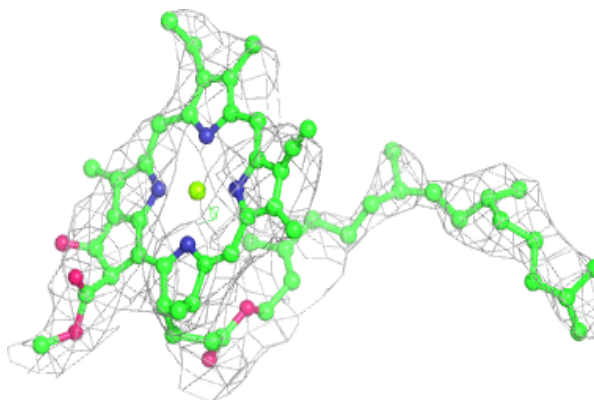


Electron density around CLA B 1209:

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

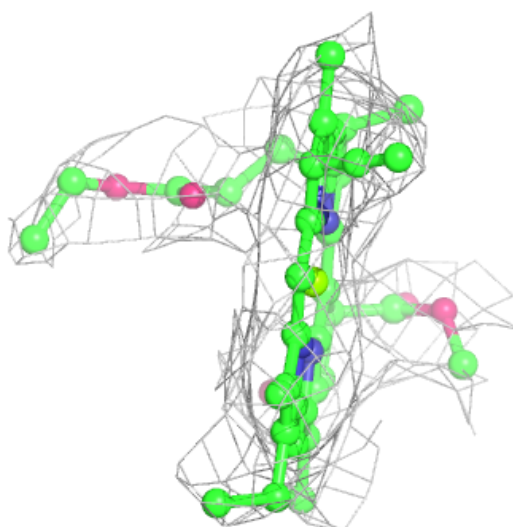
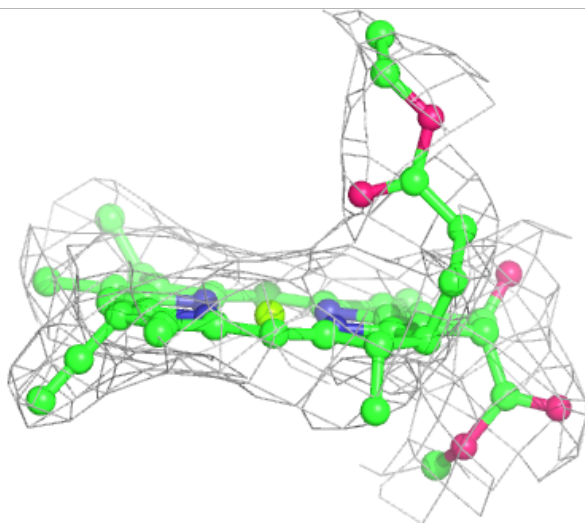
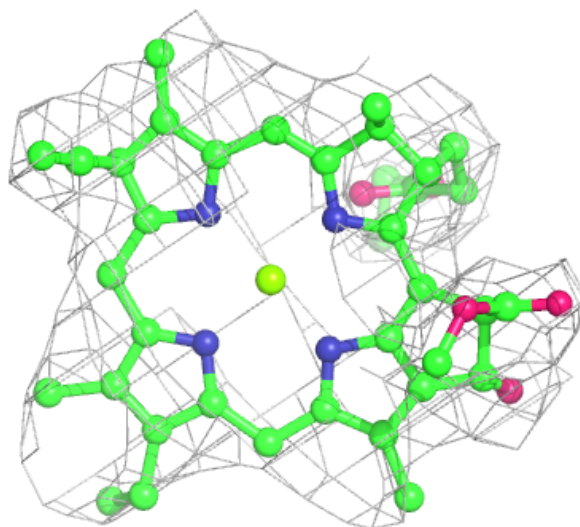
**Electron density around CLA B 1211:**

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



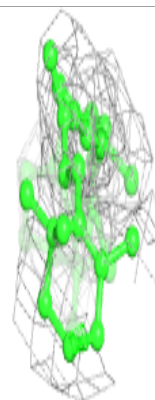
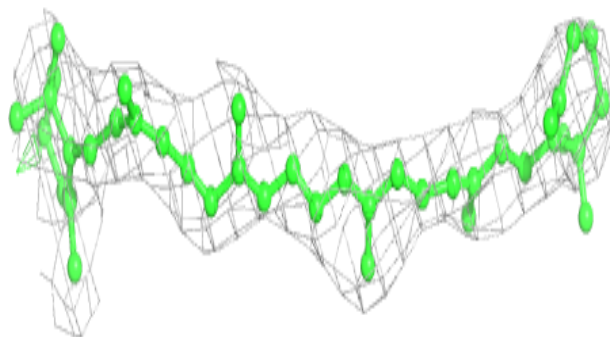
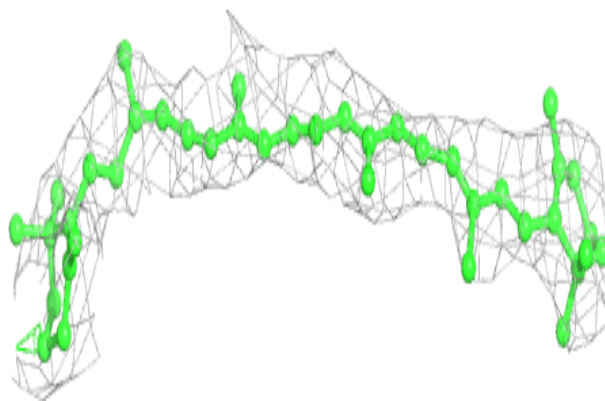
Electron density around CLA L 1502:

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

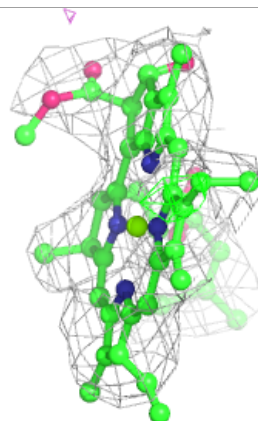
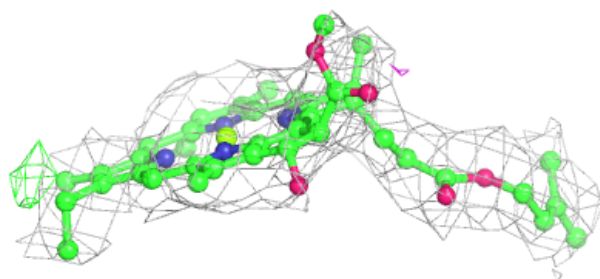
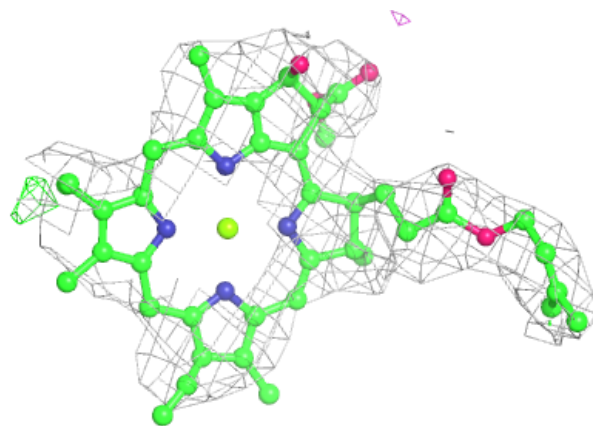


Electron density around BCR F 6014:

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

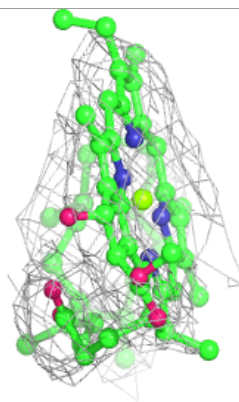
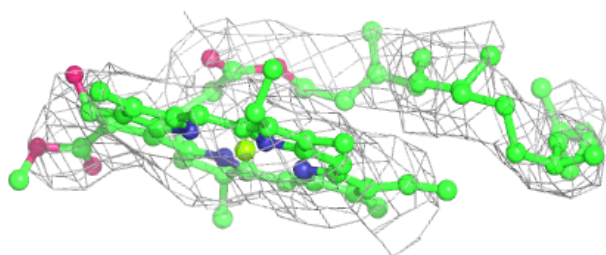
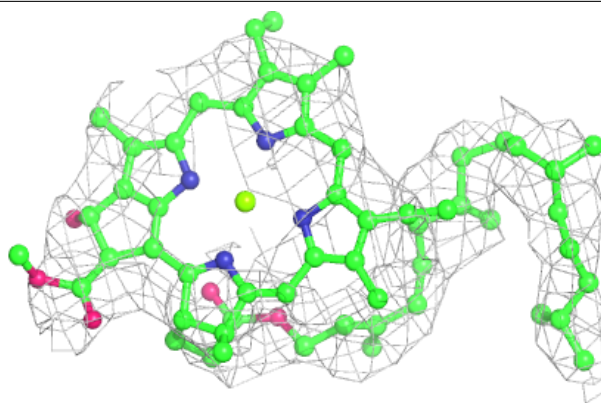
**Electron density around CLA B 1230:**

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

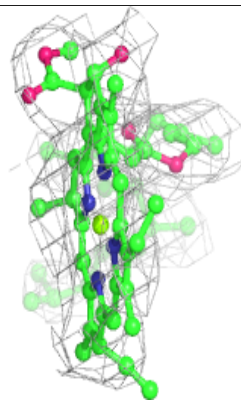
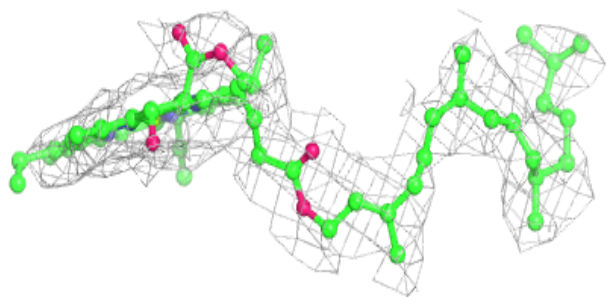
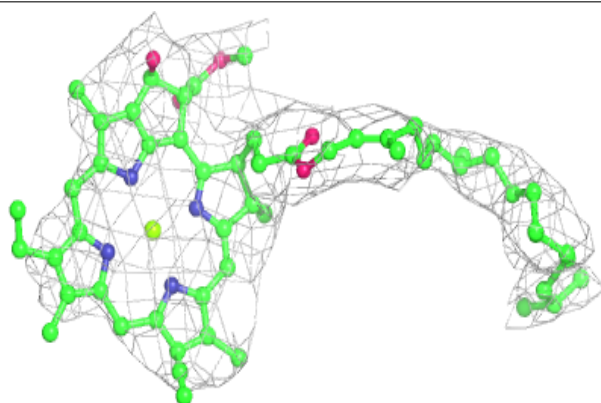


Electron density around CLA A 1117:

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

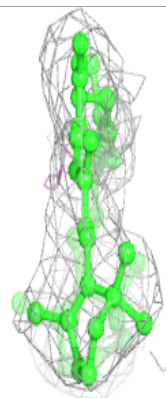
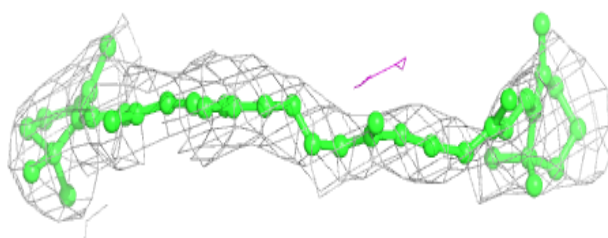
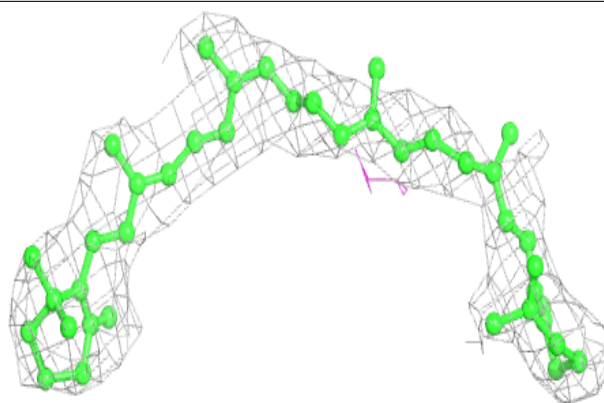
**Electron density around CLA A 1124:**

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

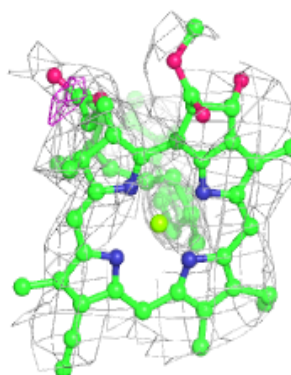
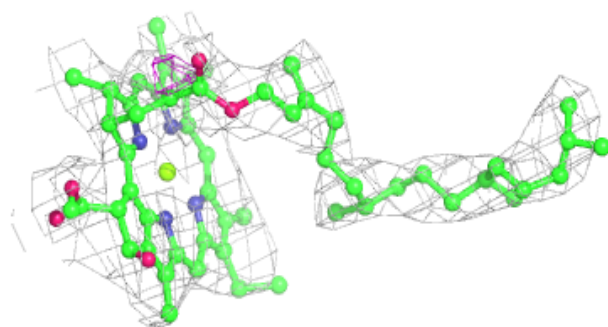
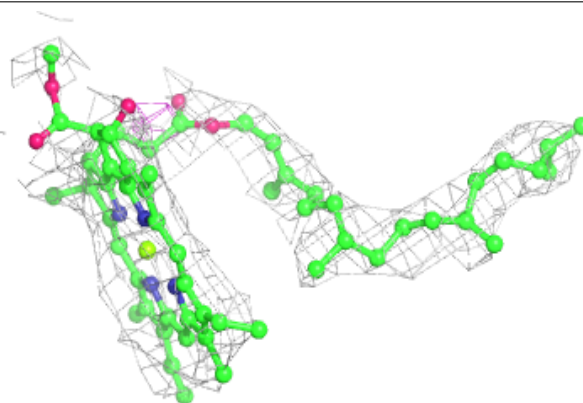


Electron density around BCR F 6016:

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

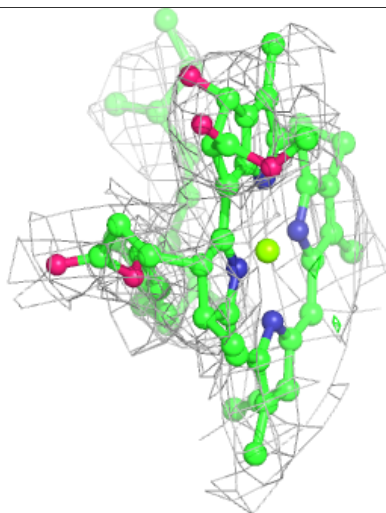
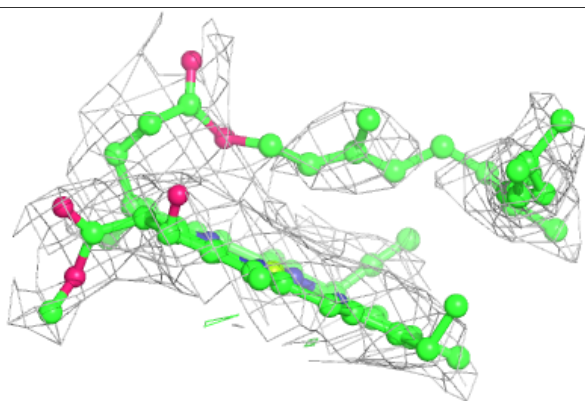
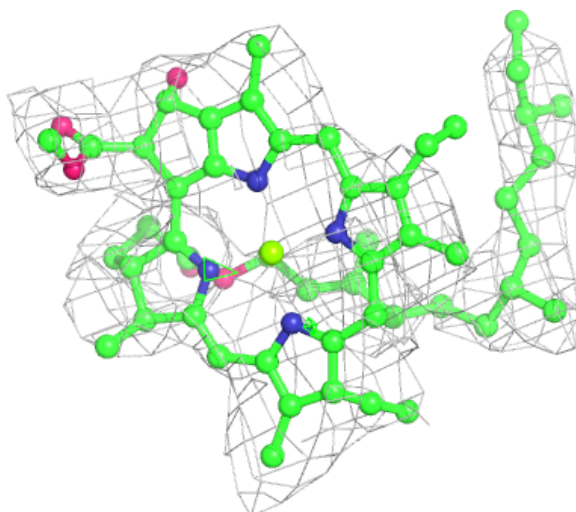
**Electron density around CLA A 1109:**

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



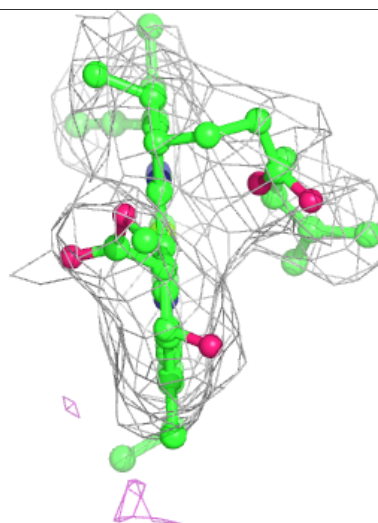
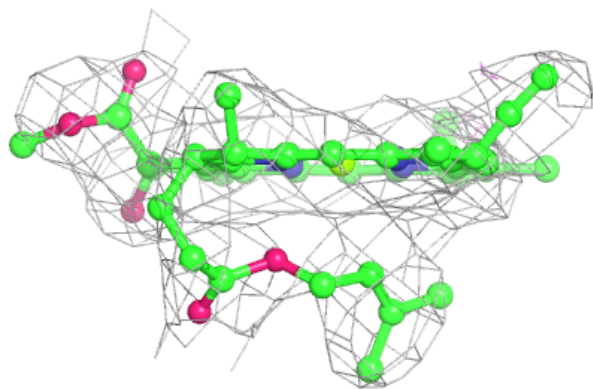
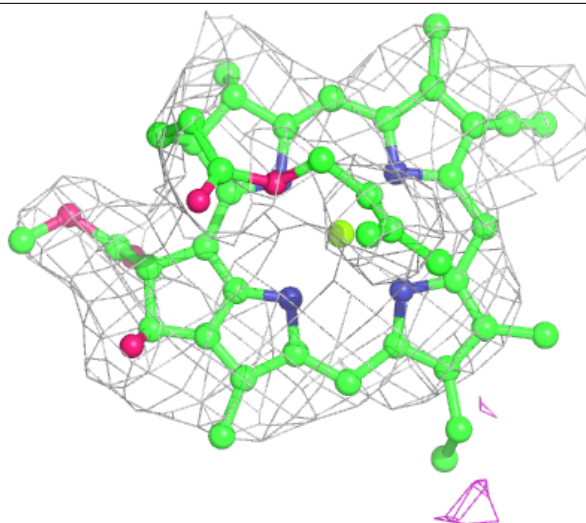
Electron density around CLA B 1216:

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



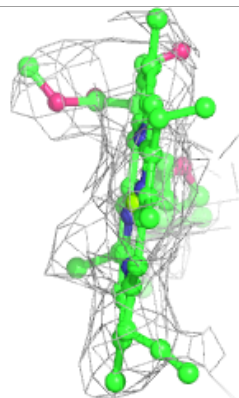
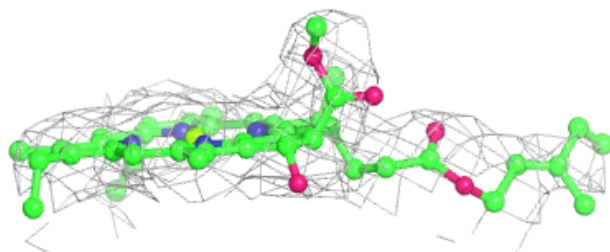
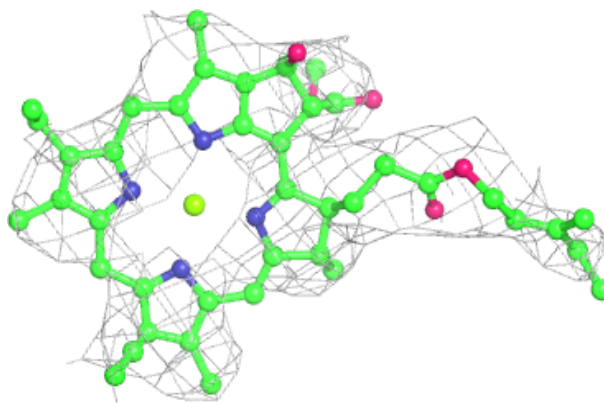
Electron density around CLA B 1217:

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



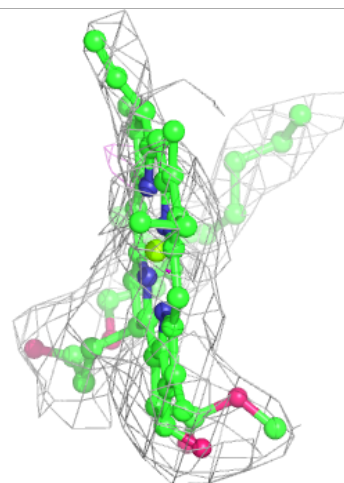
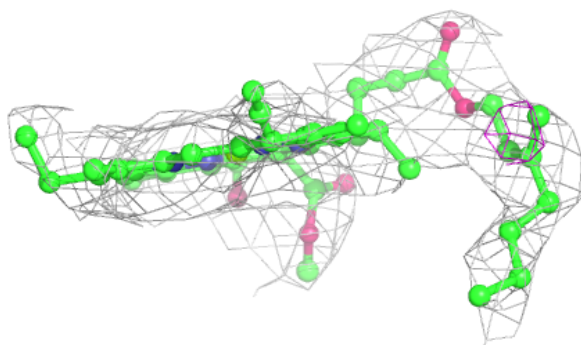
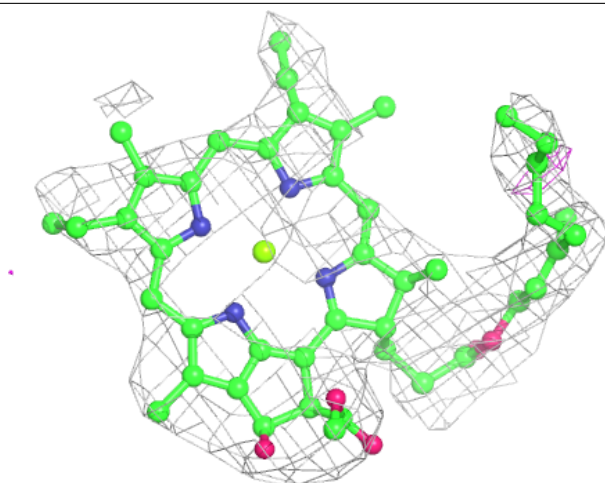
Electron density around CLA A 1135:

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



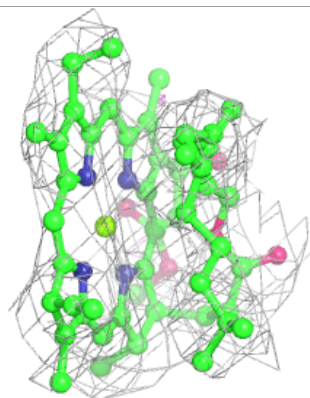
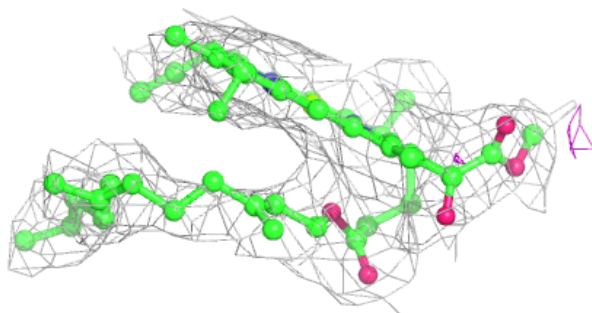
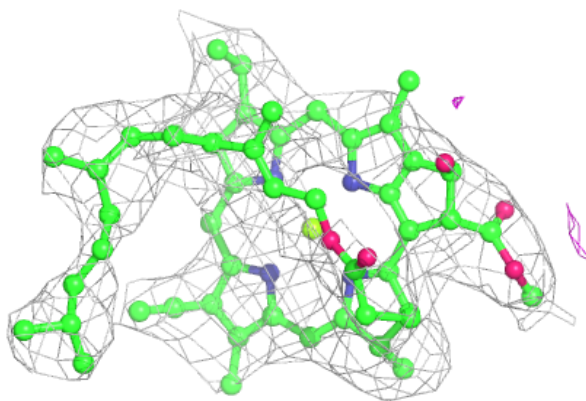
Electron density around CLA A 1111:

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



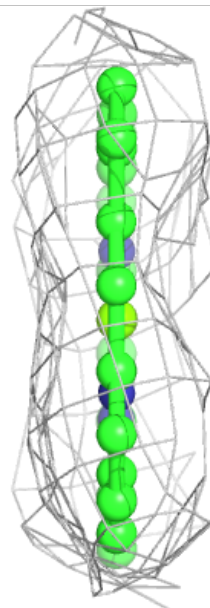
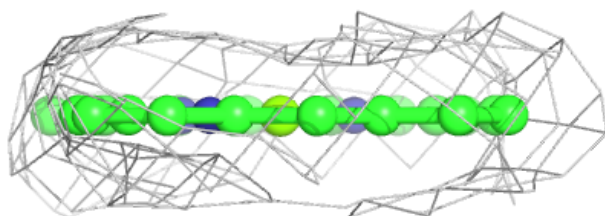
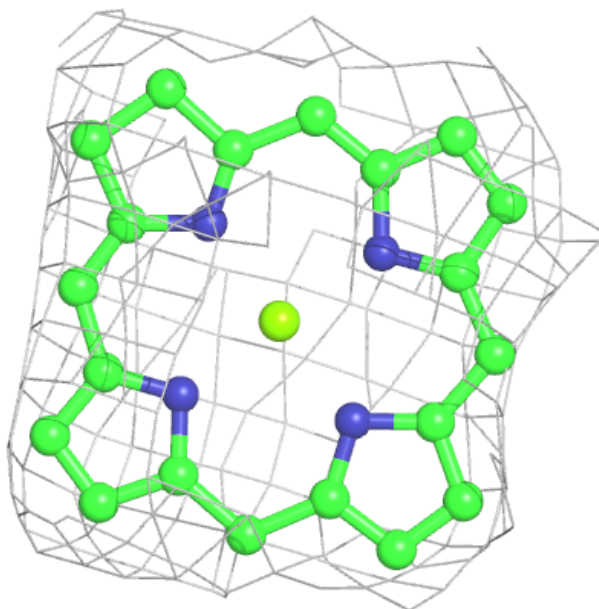
Electron density around CLA I 1204:

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



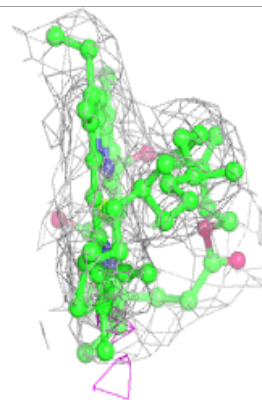
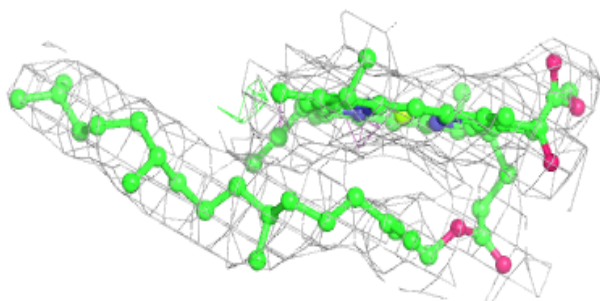
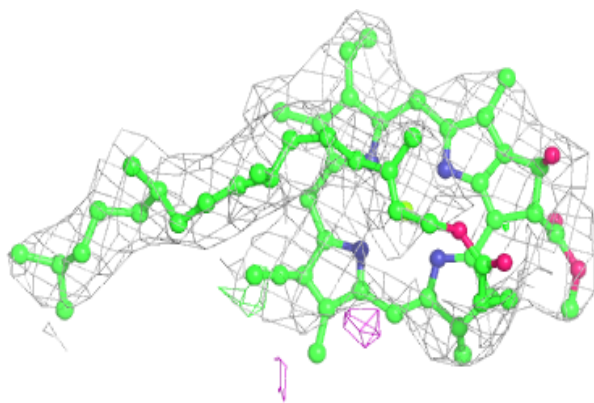
Electron density around CLA 4 4013:

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

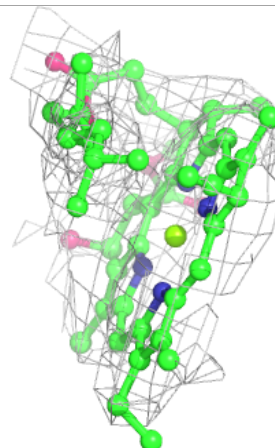
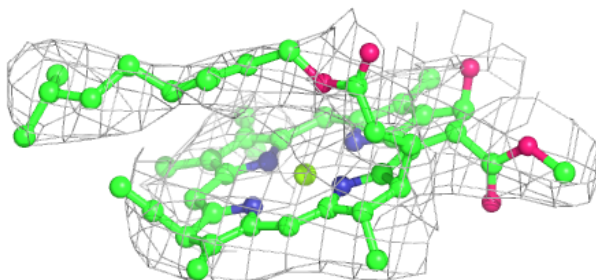
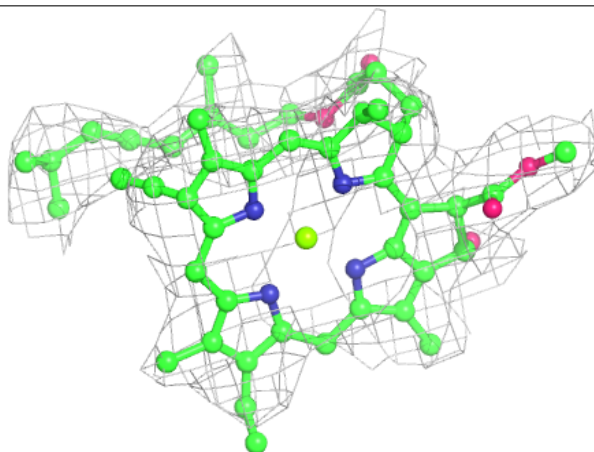


Electron density around CLA A 1138:

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

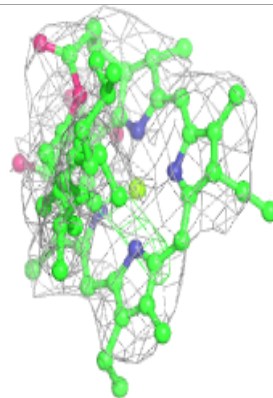
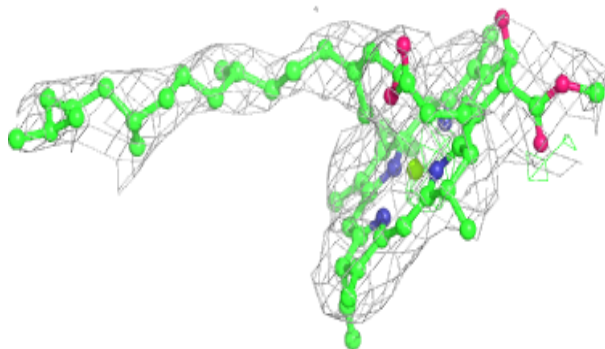
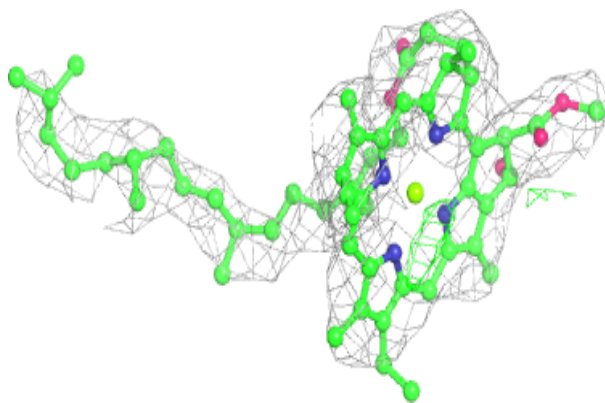
**Electron density around CLA B 1219:**

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

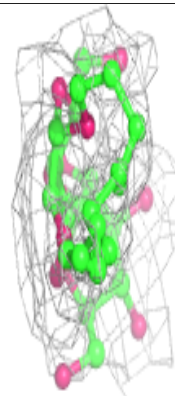
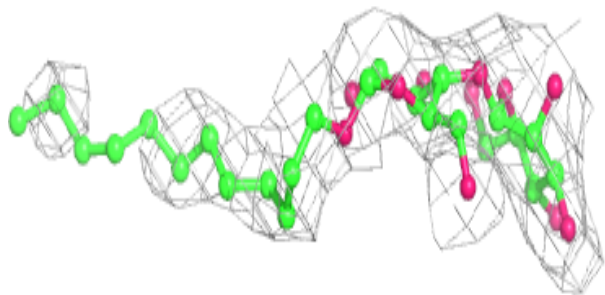
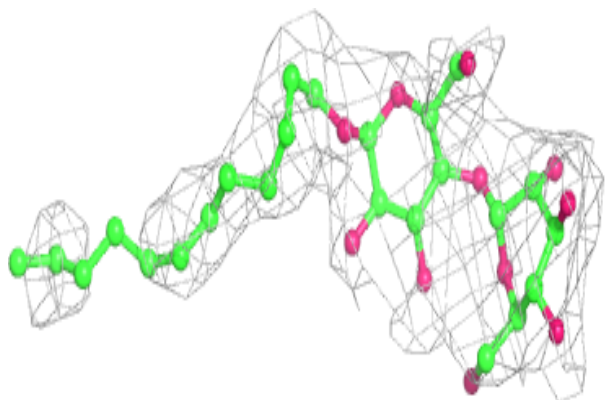


Electron density around CLA A 1140:

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

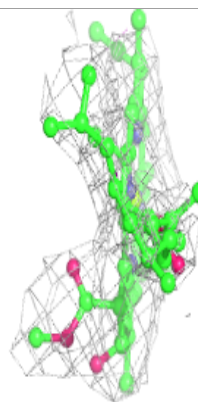
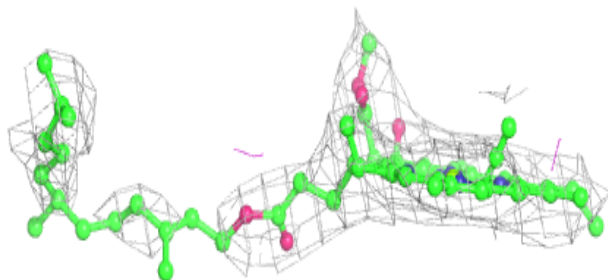
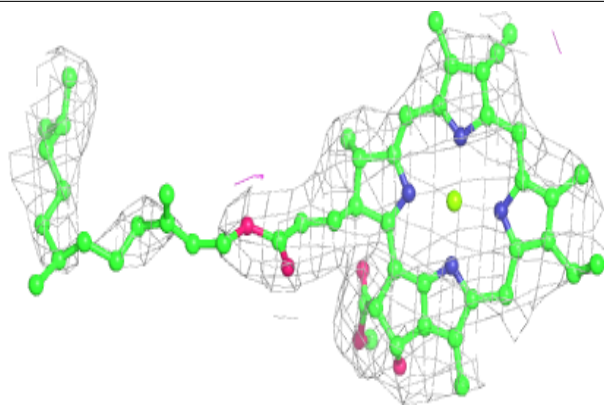
**Electron density around LMU A 7035:**

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



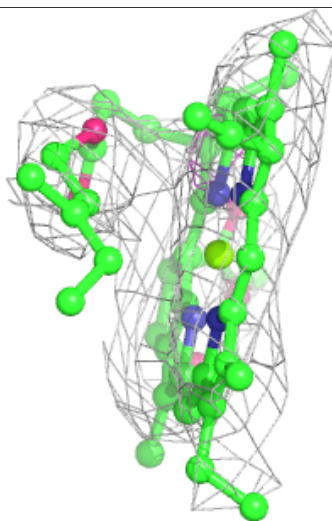
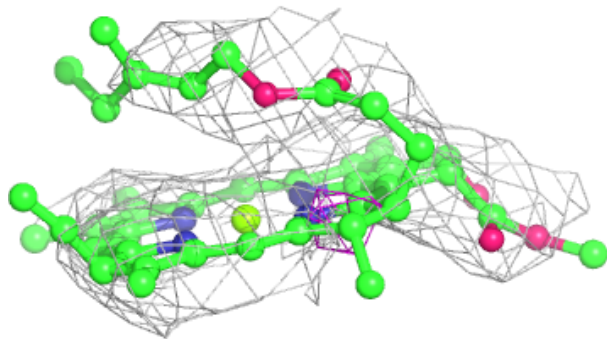
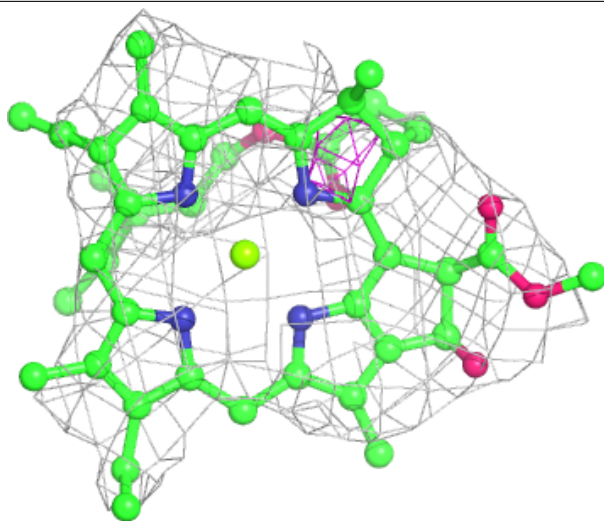
Electron density around CLA B 1234:

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



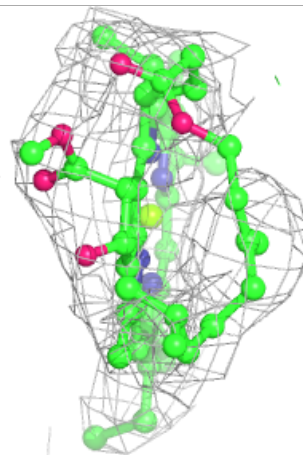
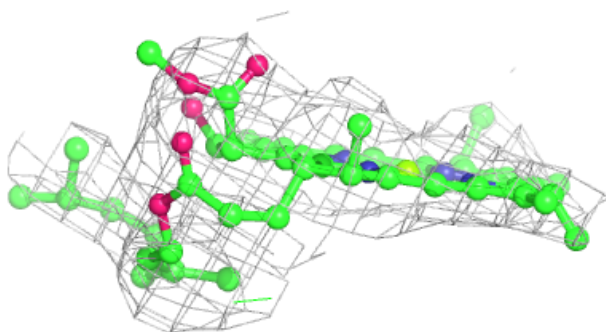
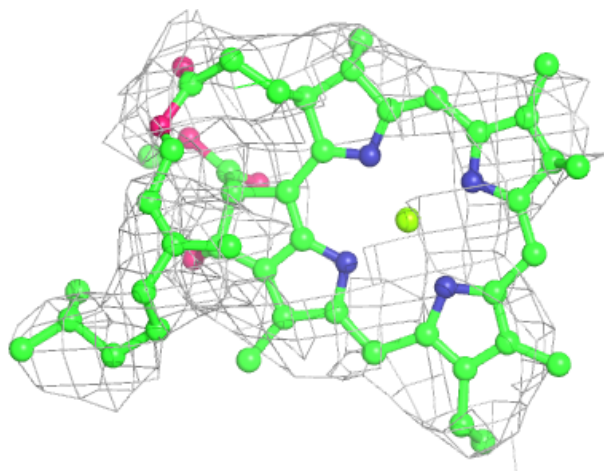
Electron density around CLA A 1120:

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



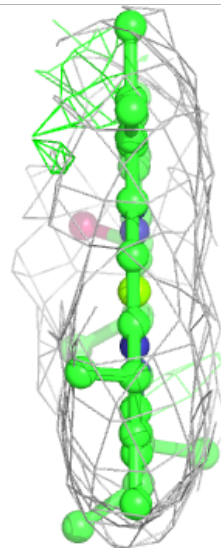
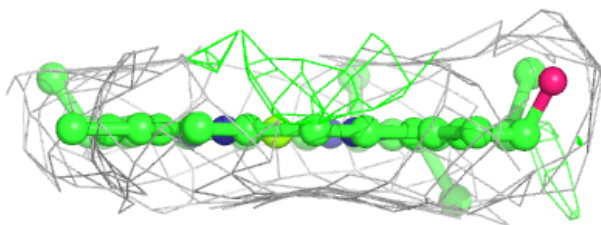
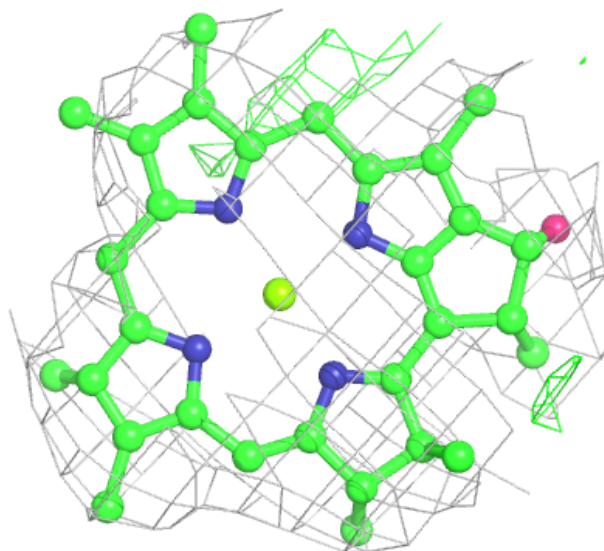
Electron density around CLA B 1208:

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



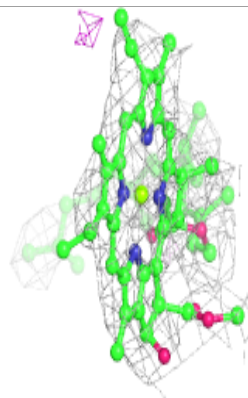
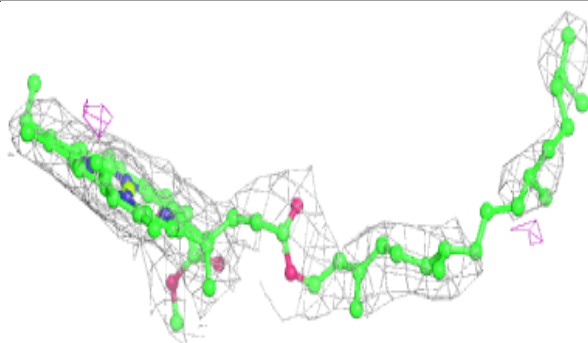
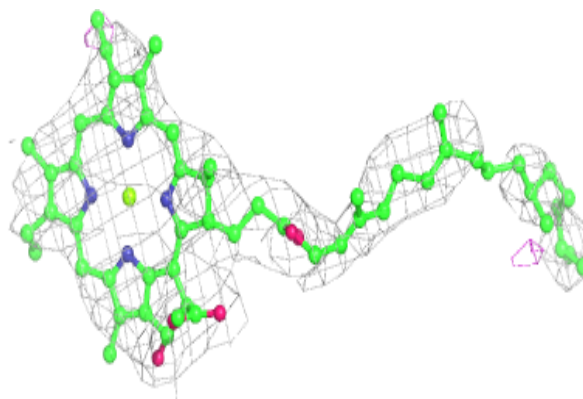
Electron density around CLA 4 1009:

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

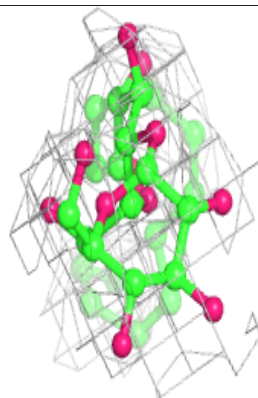
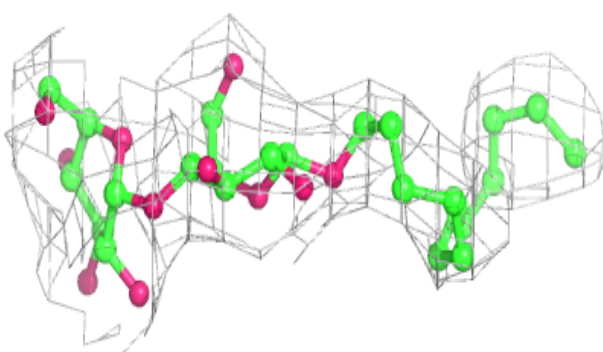
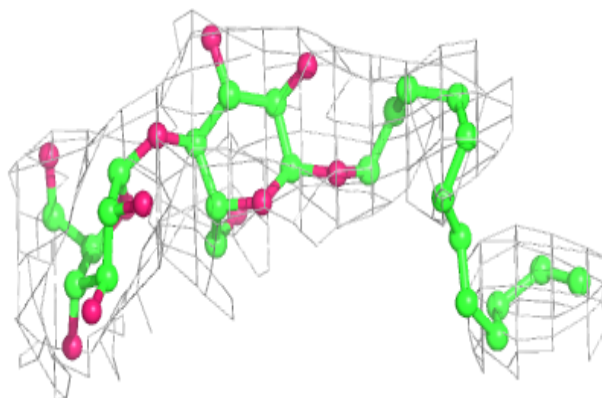


Electron density around CLA A 1103:

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

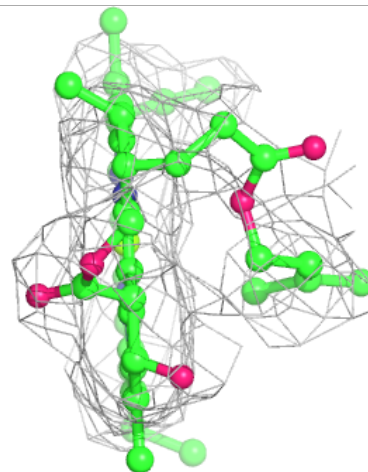
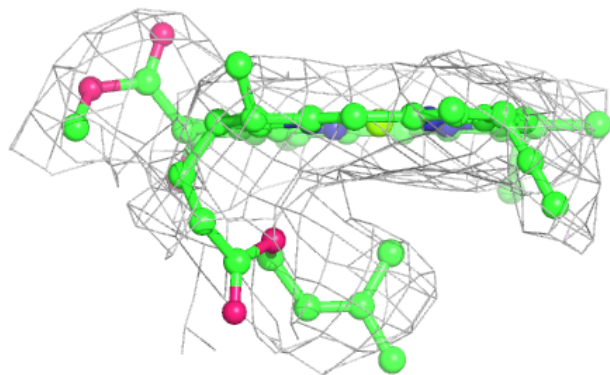
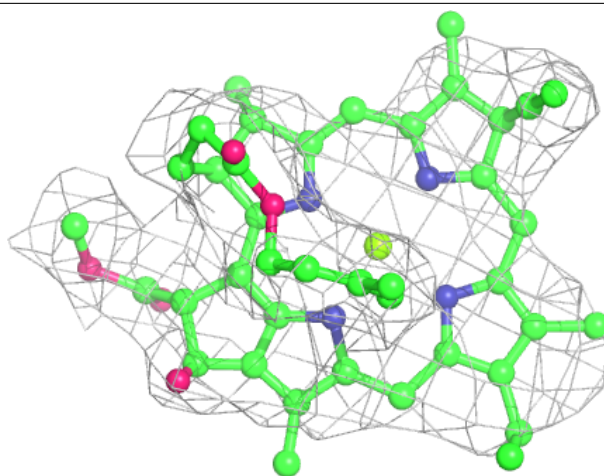
**Electron density around LMU R 7007:**

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



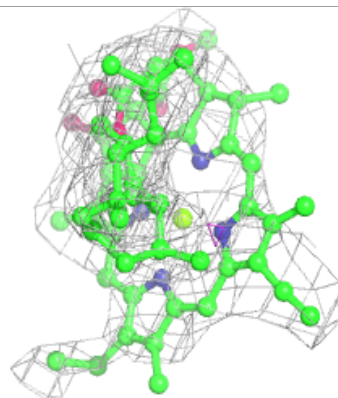
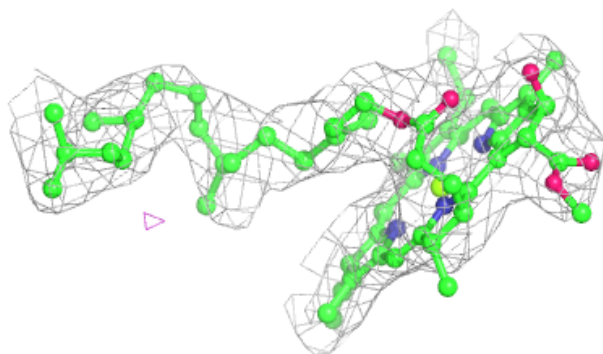
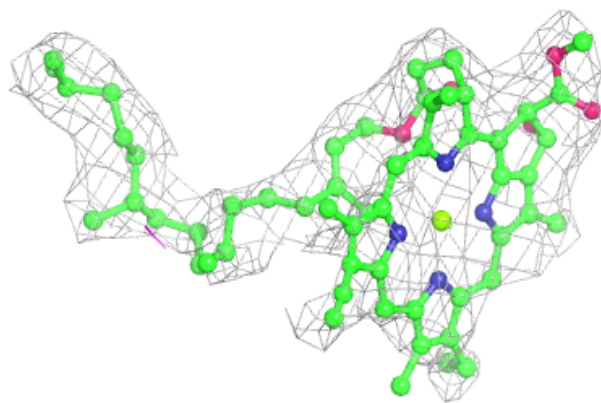
Electron density around CLA L 1501:

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



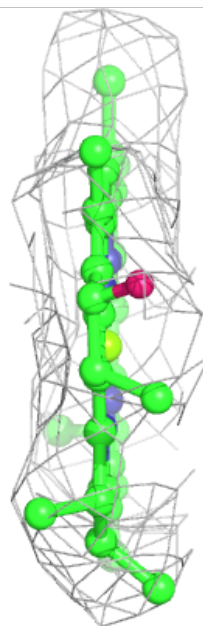
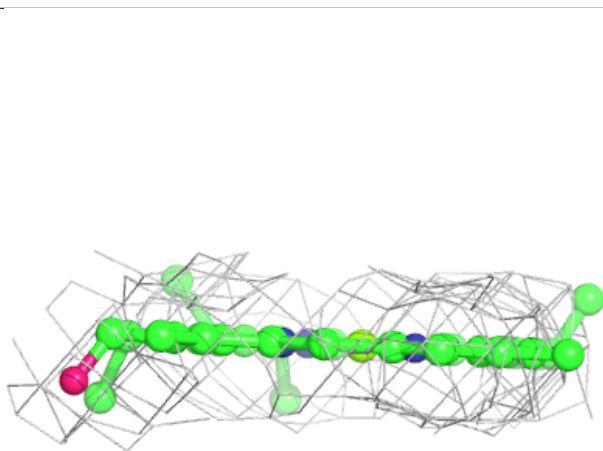
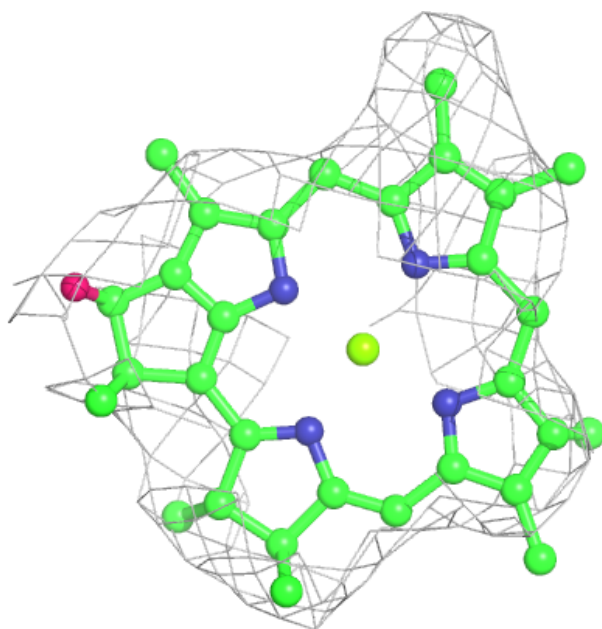
Electron density around CLA A 1237:

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



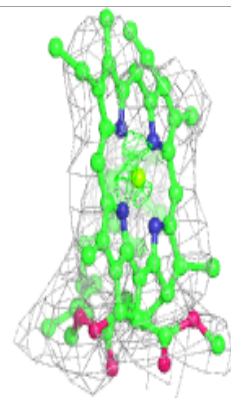
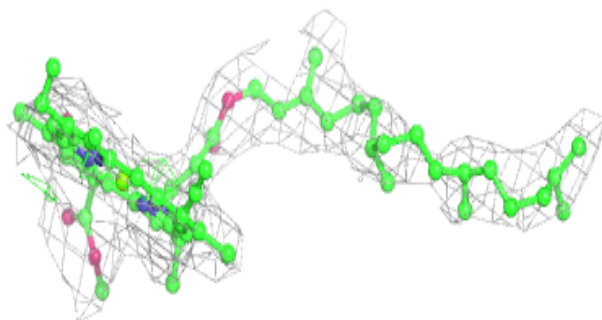
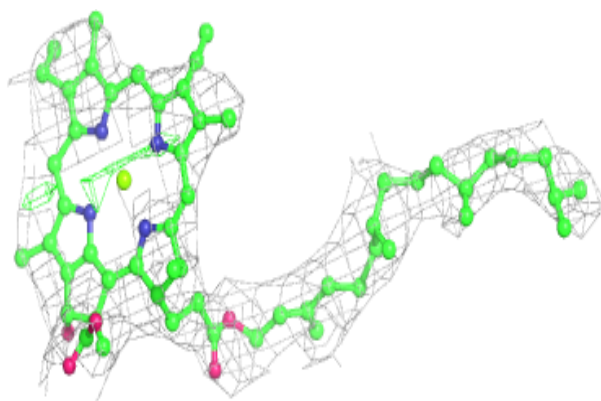
Electron density around CLA 1 1012:

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

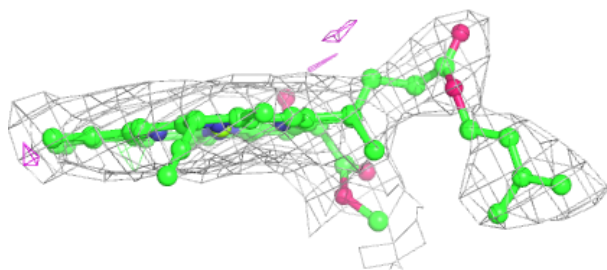
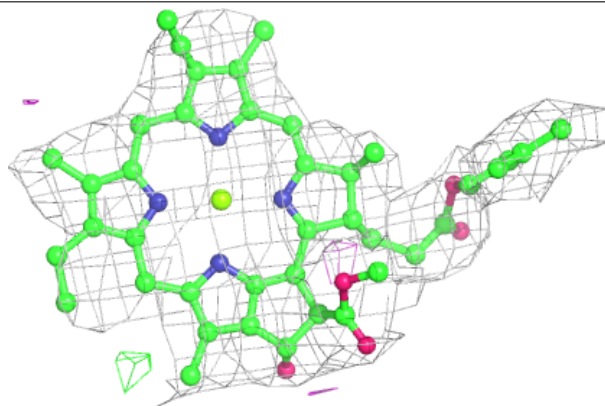


Electron density around CLA A 1132:

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

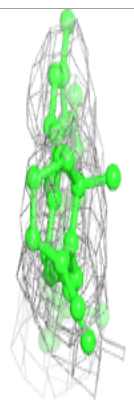
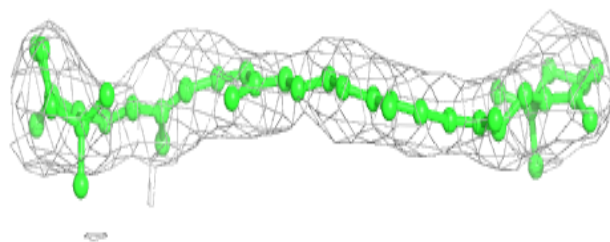
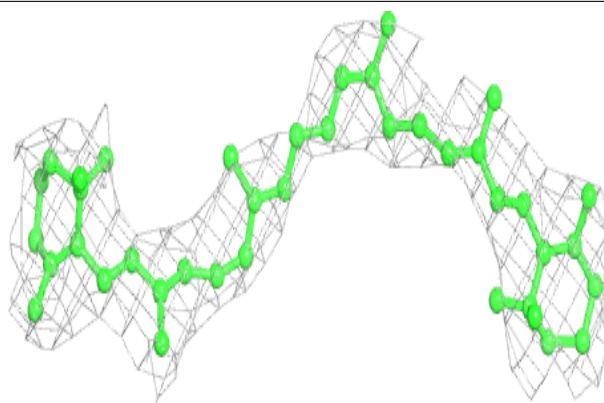
**Electron density around CLA B 1228:**

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



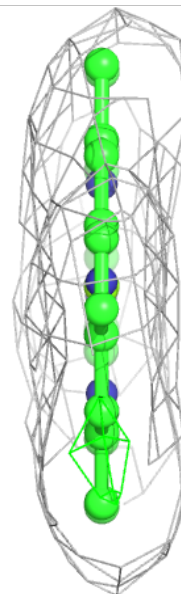
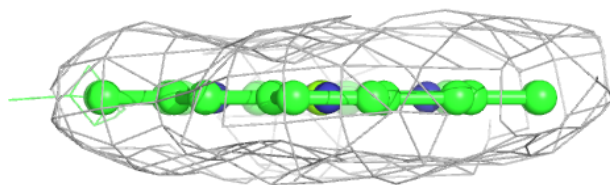
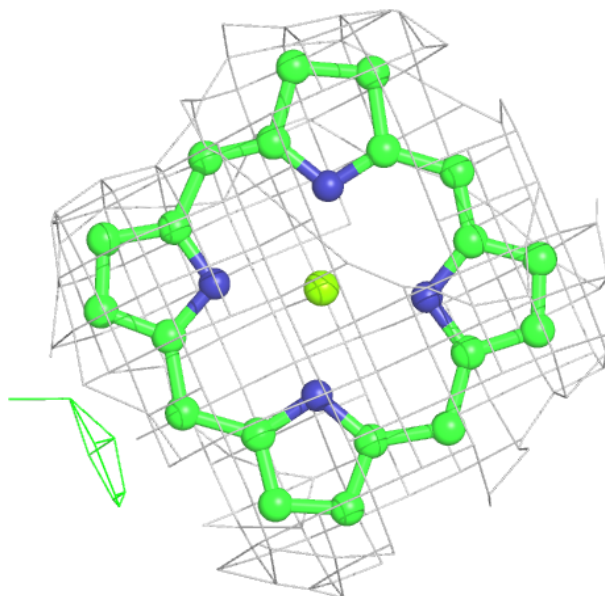
Electron density around BCR A 6011:

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



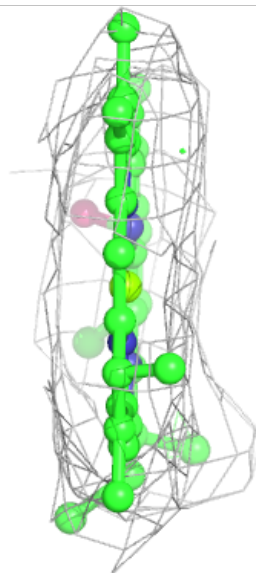
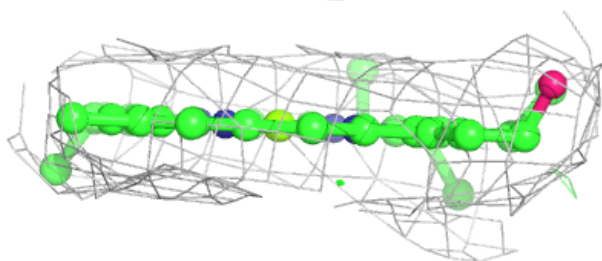
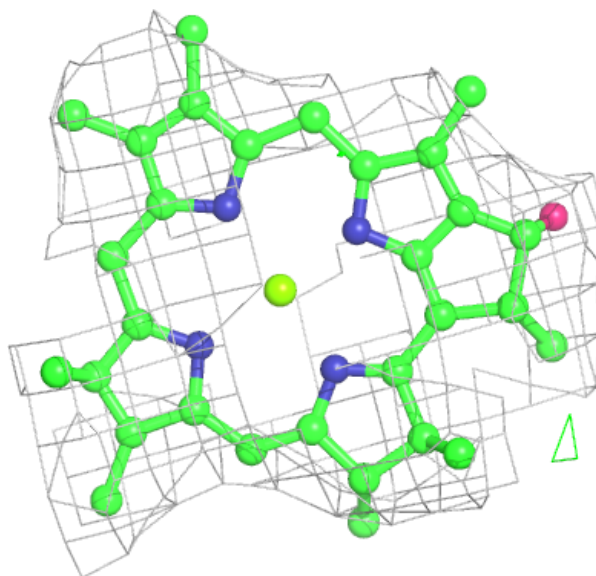
Electron density around CLA 4 4011:

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



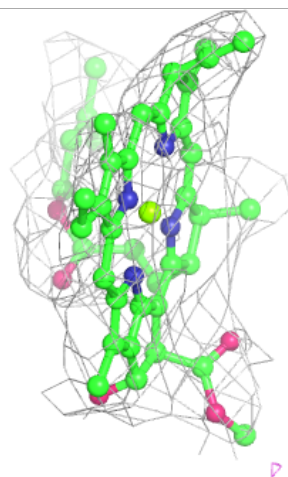
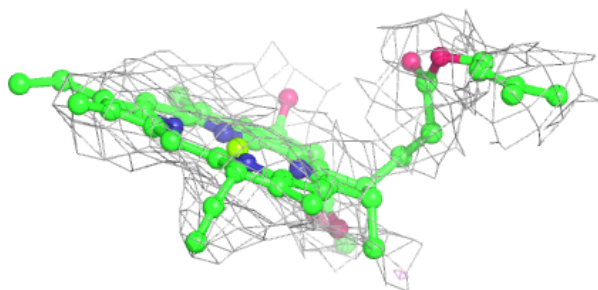
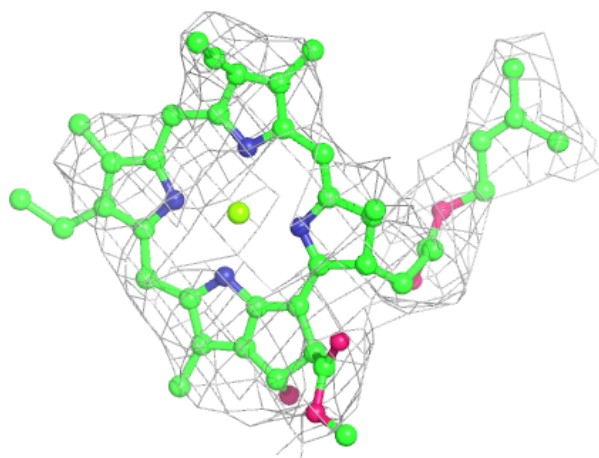
Electron density around CLA 4 4012:

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



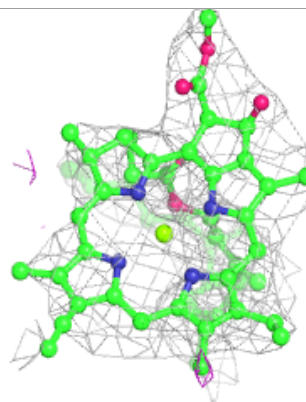
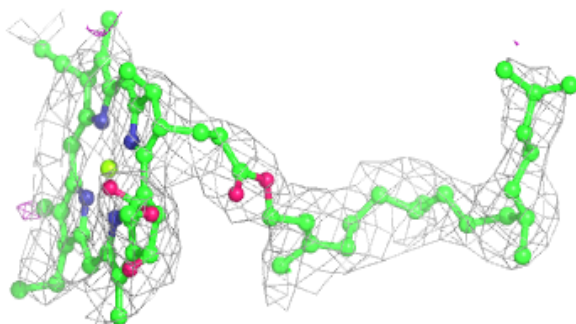
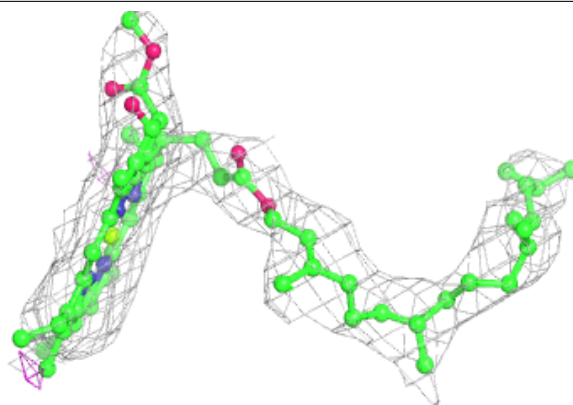
Electron density around CLA A 1133:

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

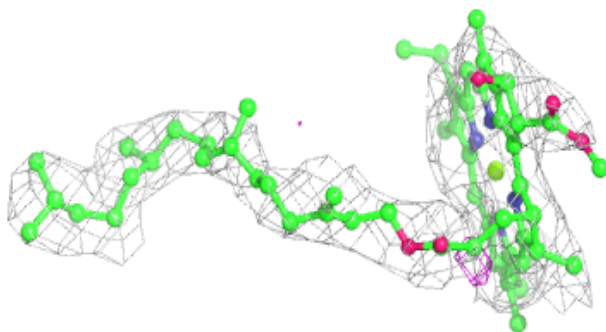
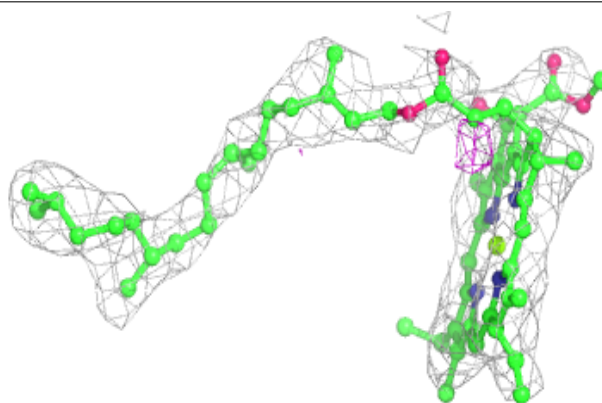


Electron density around CLA B 1238:

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

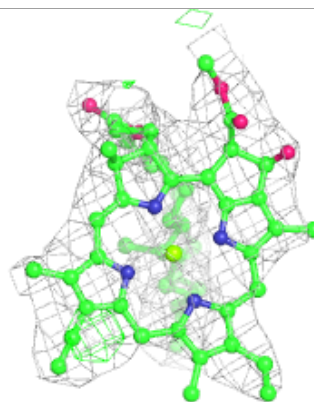
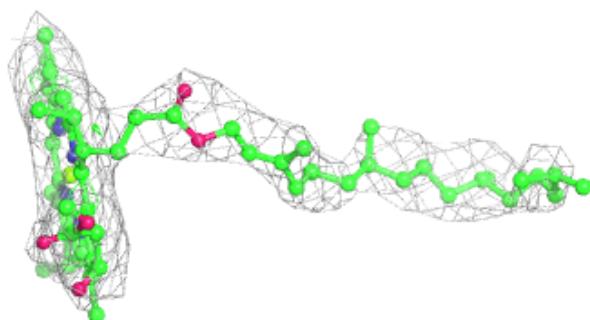
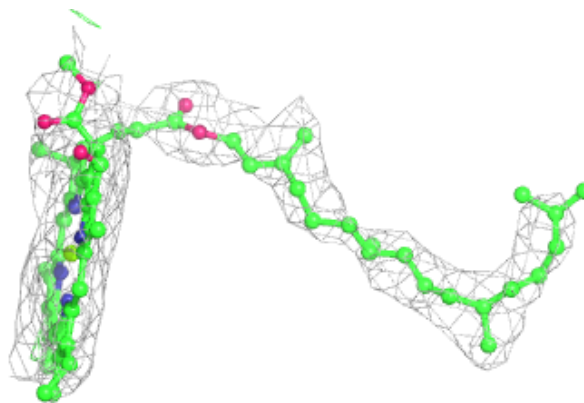
**Electron density around CLA A 1128:**

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

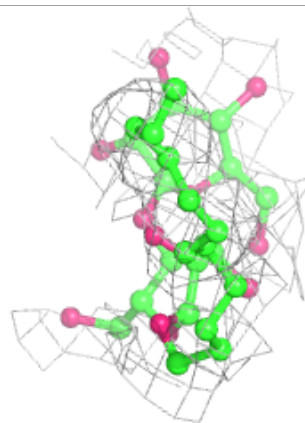
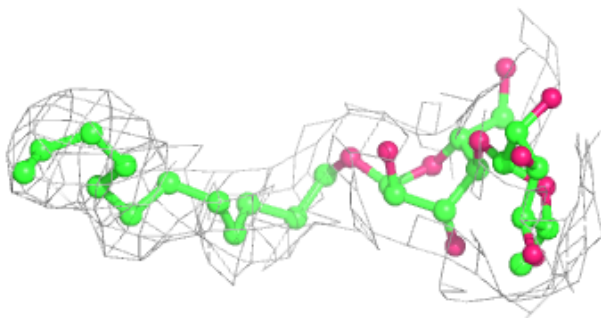
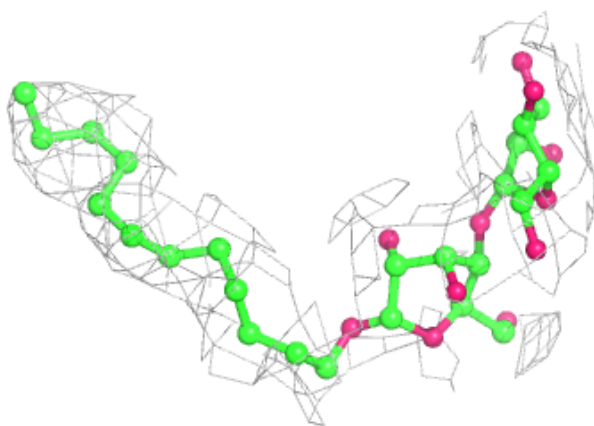


Electron density around CLA B 1239:

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

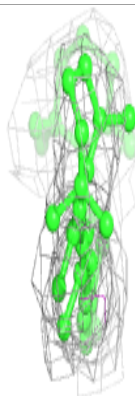
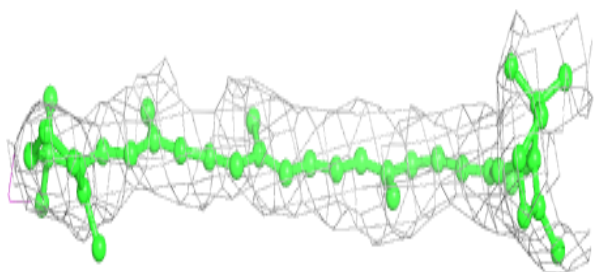
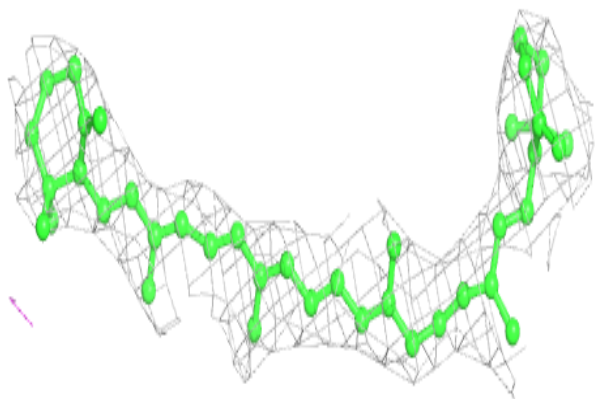
**Electron density around LMU G 7039:**

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

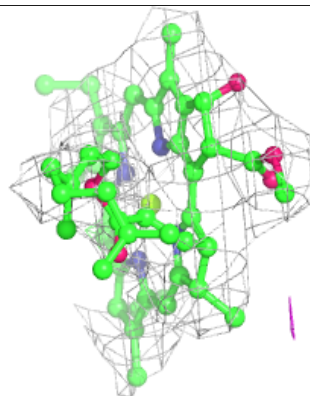
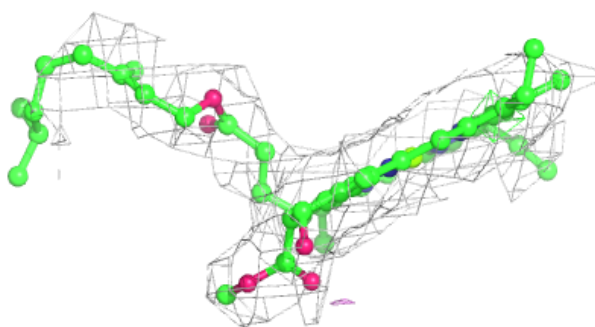
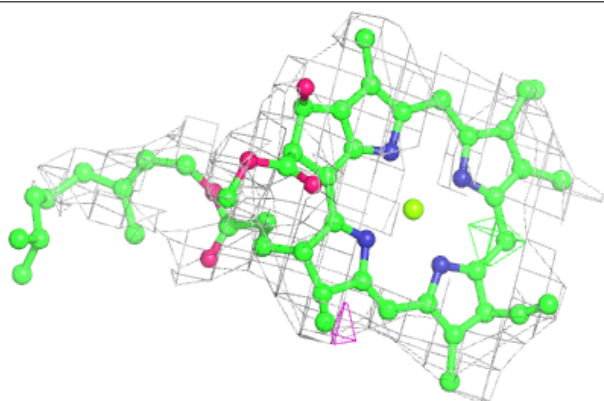


Electron density around BCR B 6005:

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

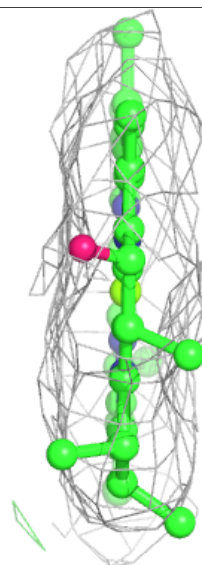
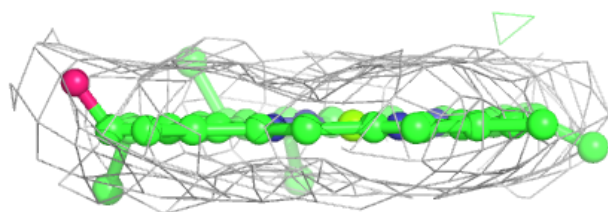
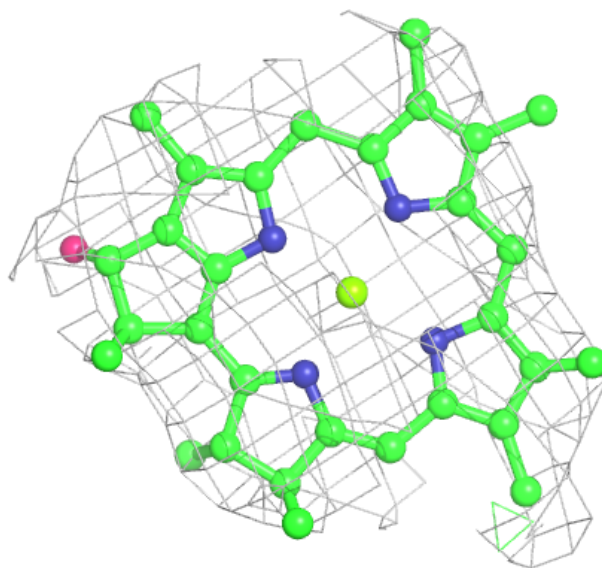
**Electron density around CLA A 1107:**

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



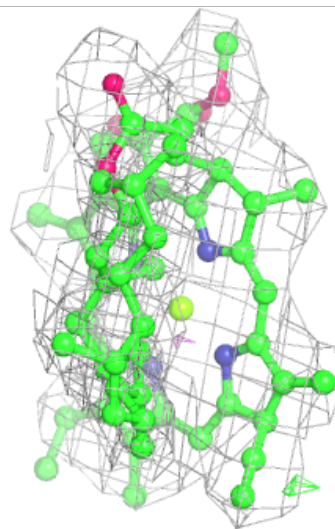
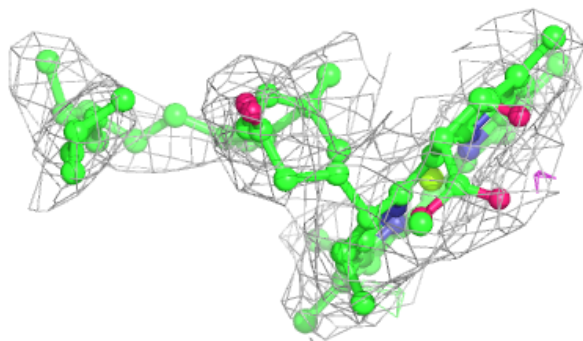
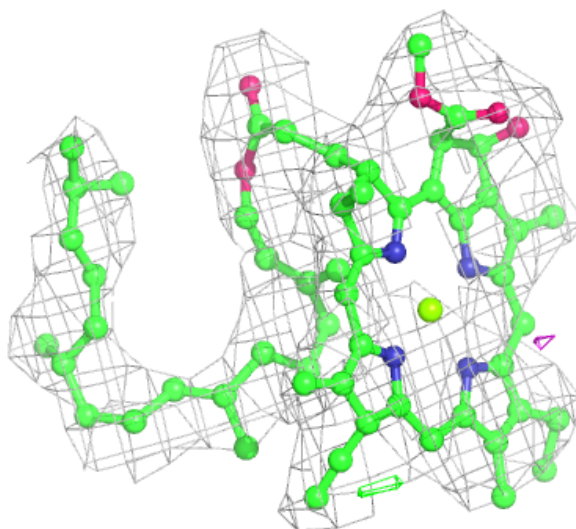
Electron density around CLA F 1240:

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



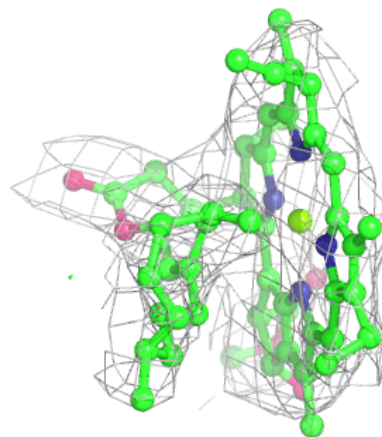
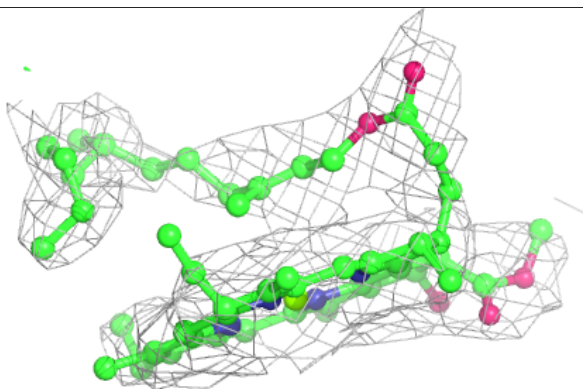
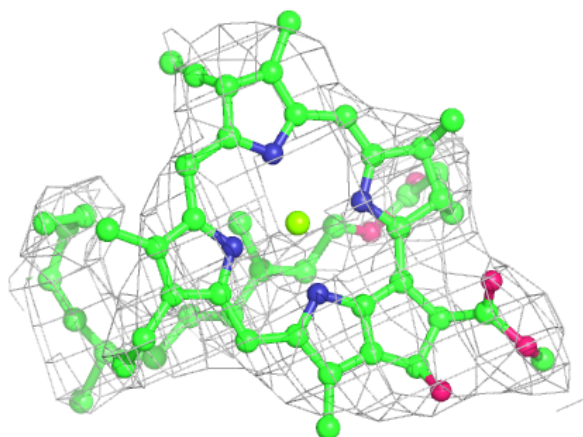
Electron density around CLA B 1220:

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

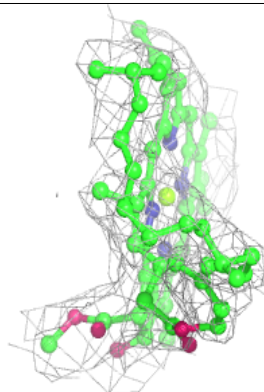
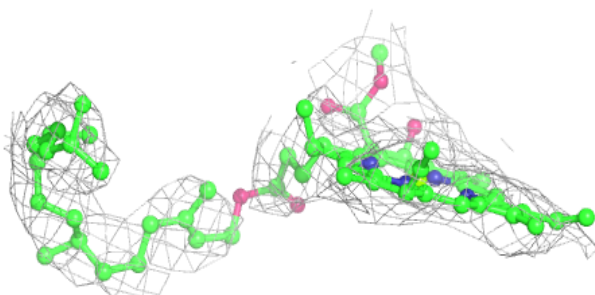
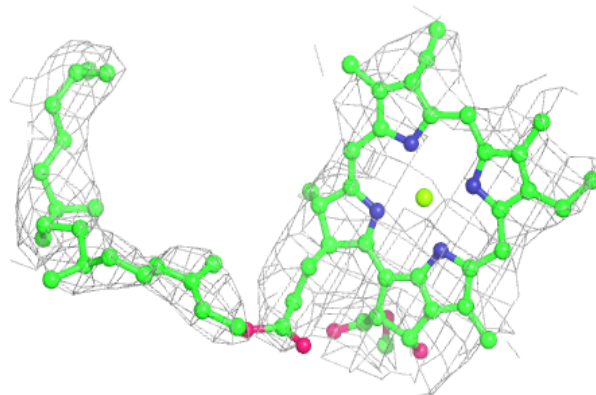


Electron density around CLA B 1214:

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

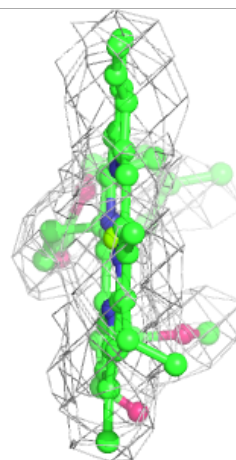
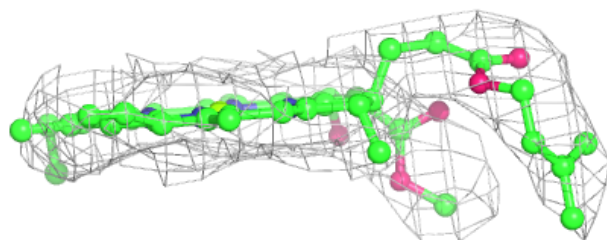
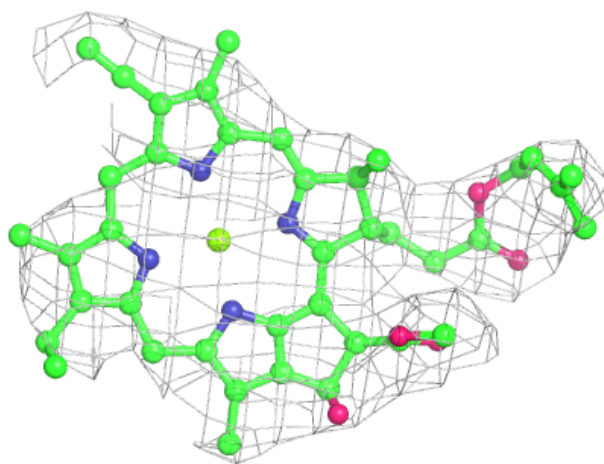
**Electron density around CLA A 1125:**

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



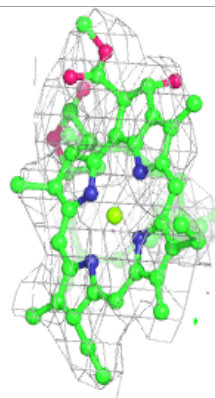
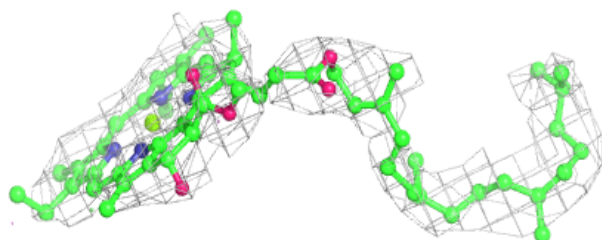
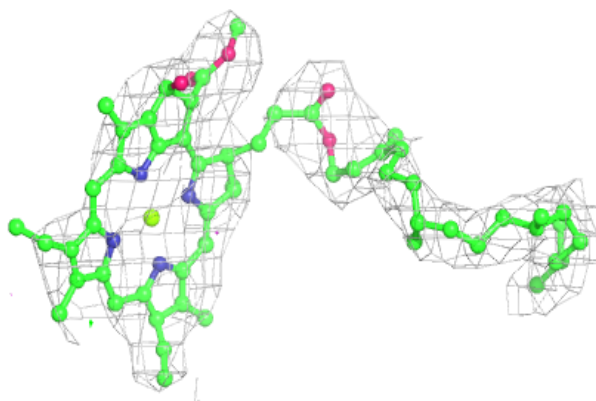
Electron density around CLA A 1101:

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

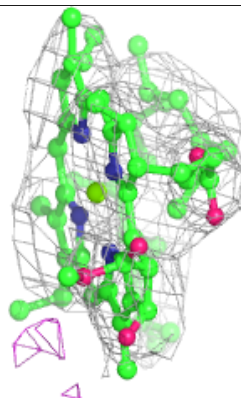
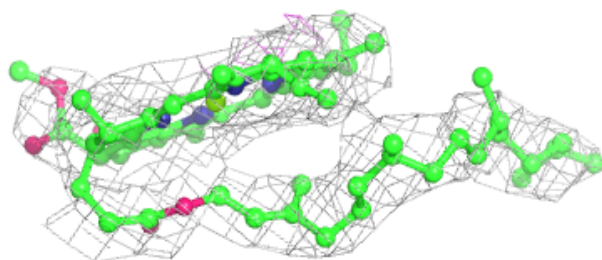
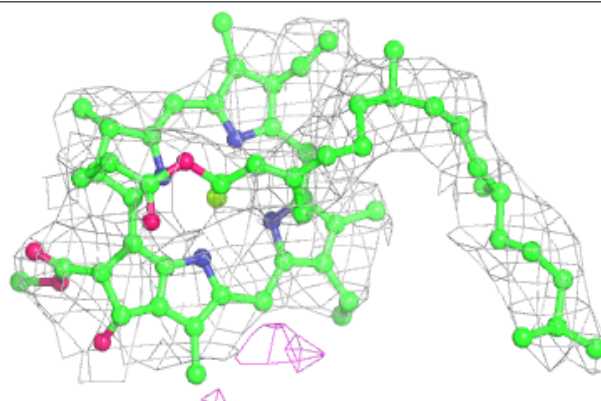


Electron density around CLA B 1206:

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

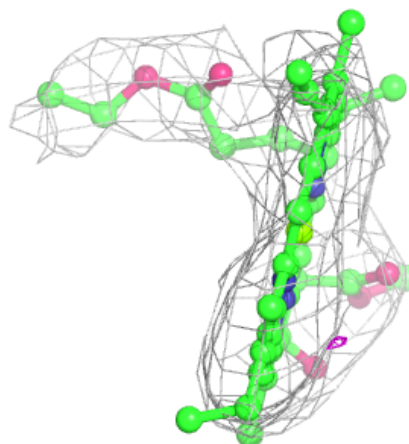
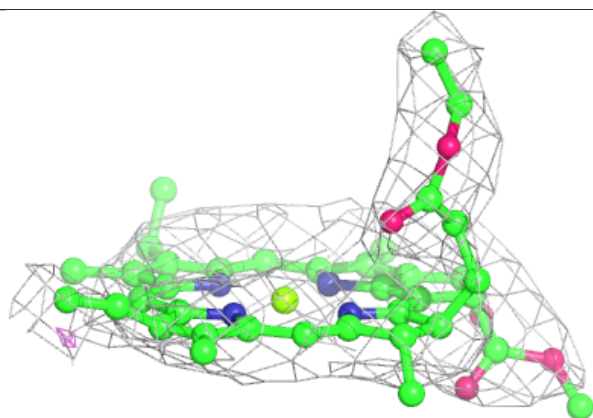
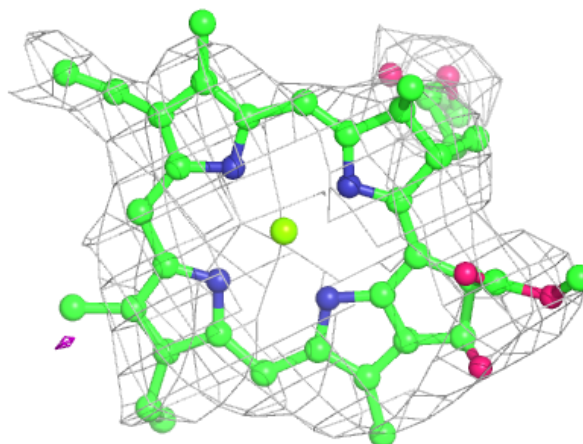
**Electron density around CLA B 1235:**

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



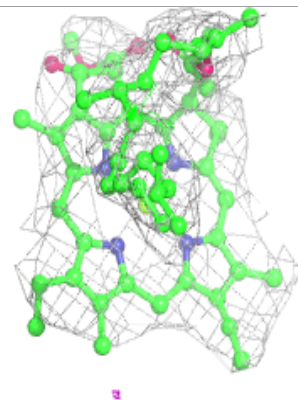
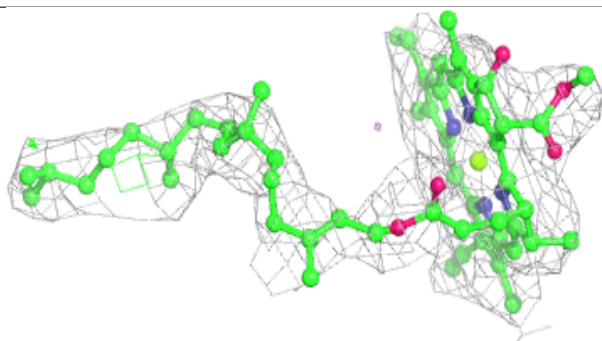
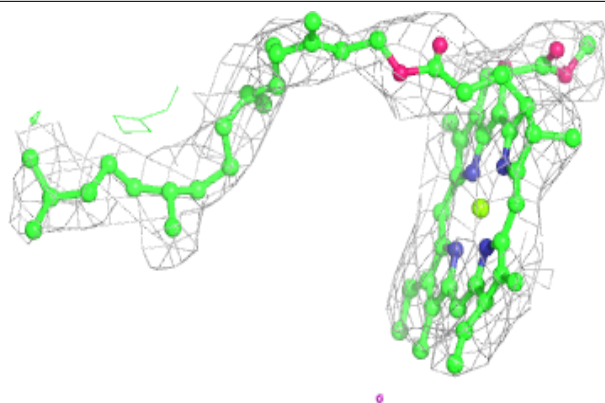
Electron density around CLA B 1236:

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

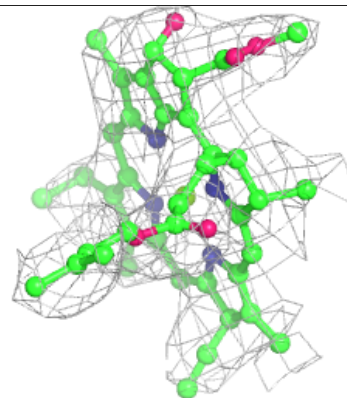
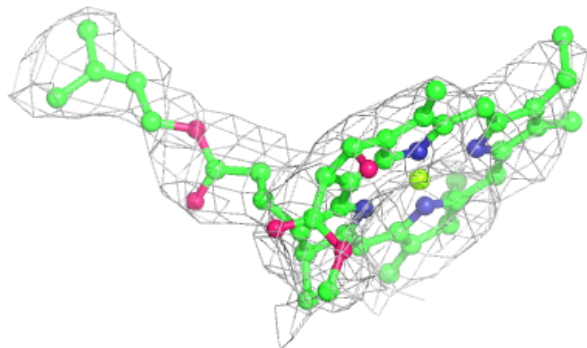
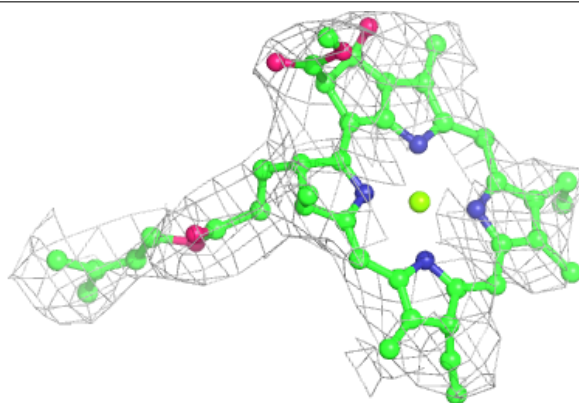


Electron density around CLA B 1226:

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

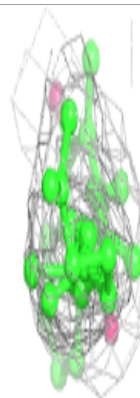
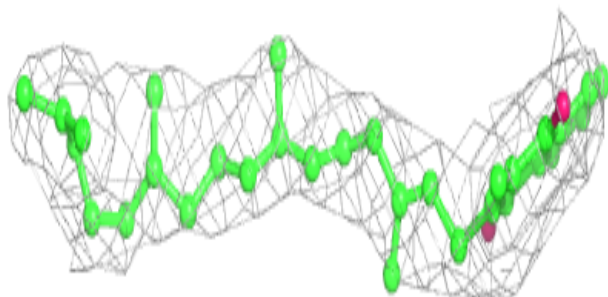
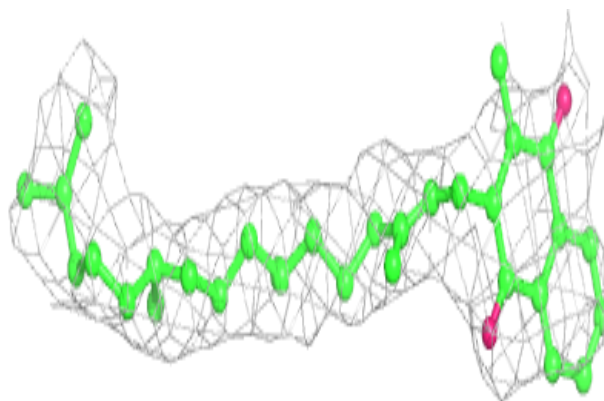
**Electron density around CLA A 1129:**

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

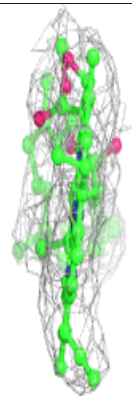
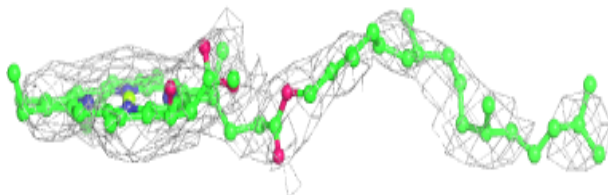
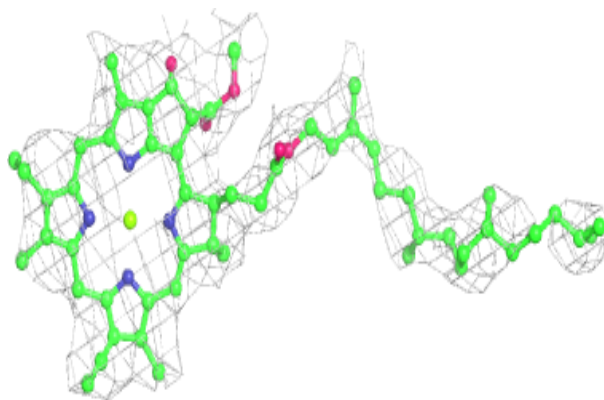


Electron density around PQN A 5001:

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

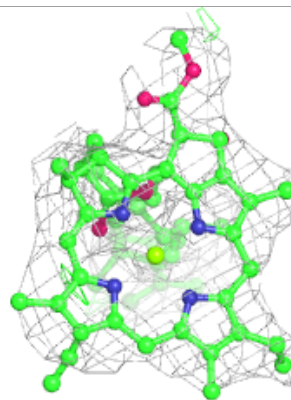
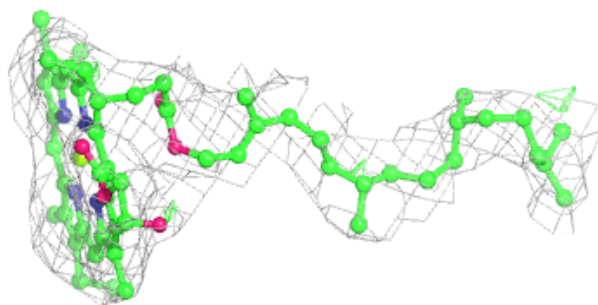
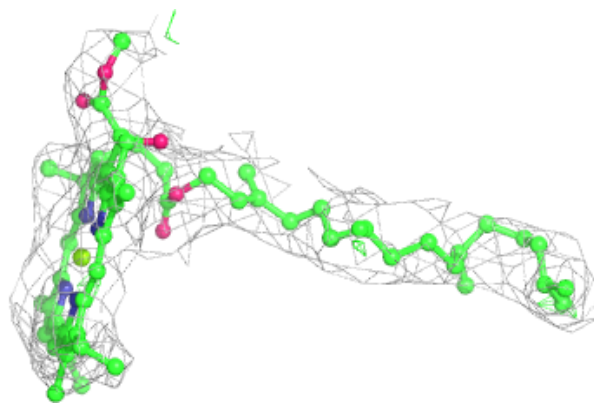
**Electron density around CLA A 1131:**

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

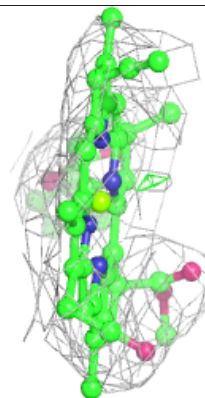
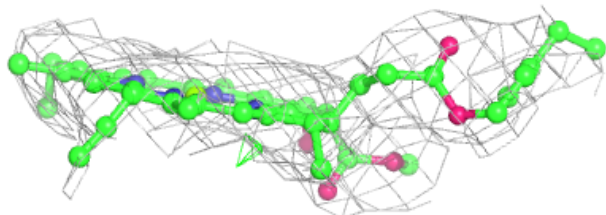
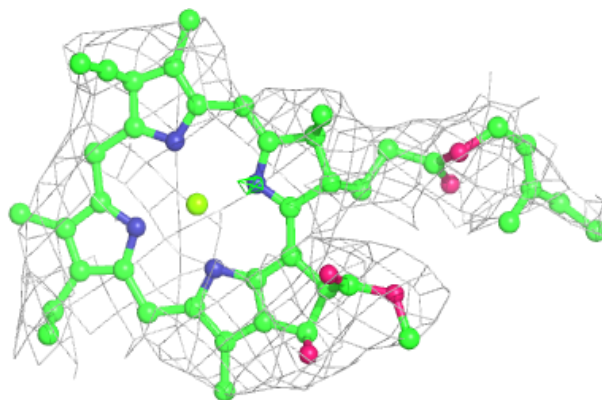


Electron density around CLA A 1126:

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

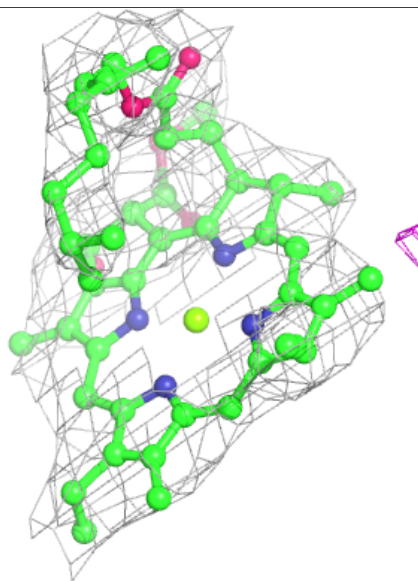
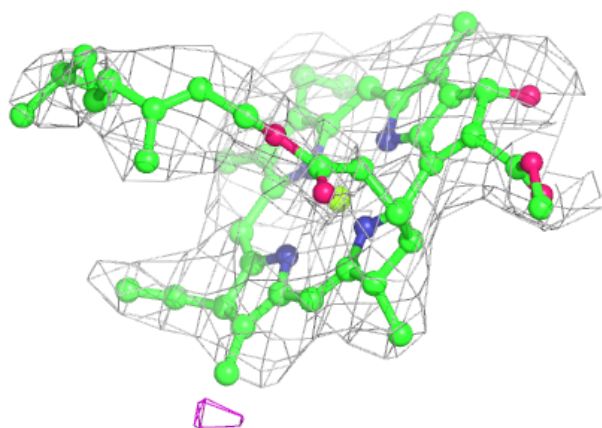
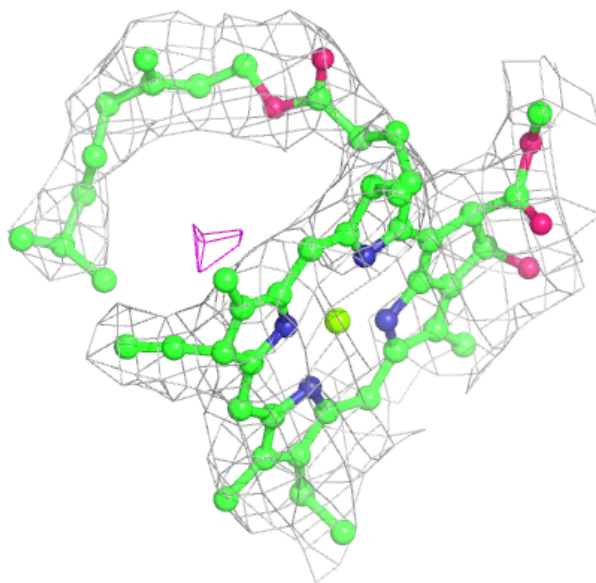
**Electron density around CLA A 1139:**

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



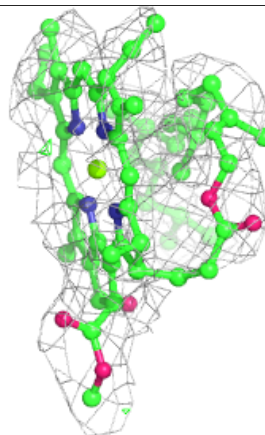
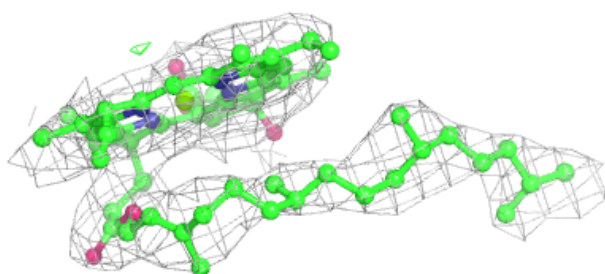
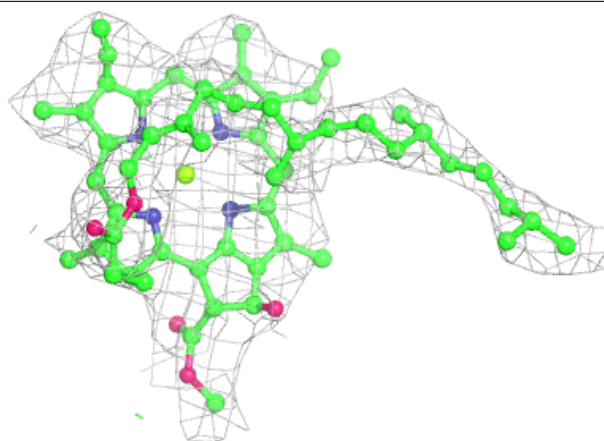
Electron density around CLA A 1122:

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

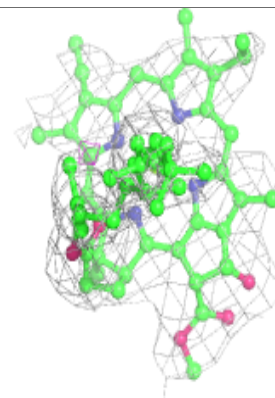
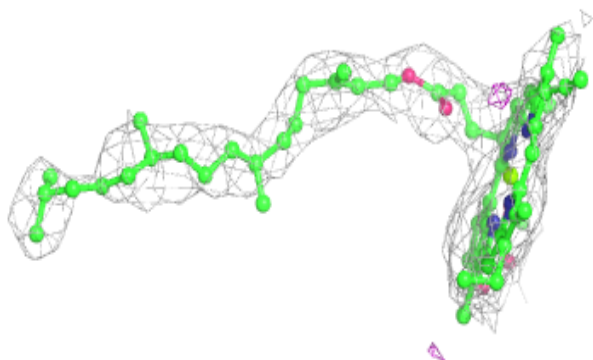
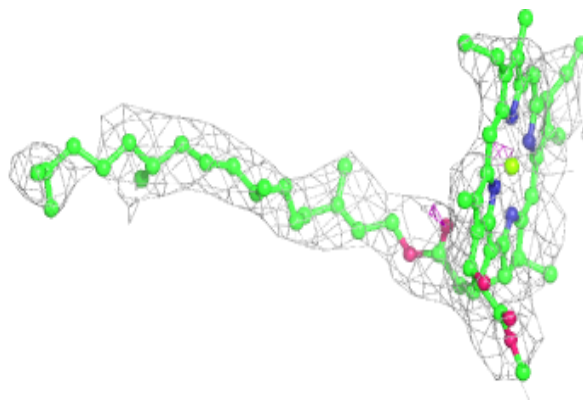


Electron density around CLA B 1224:

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

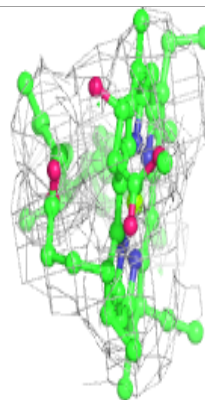
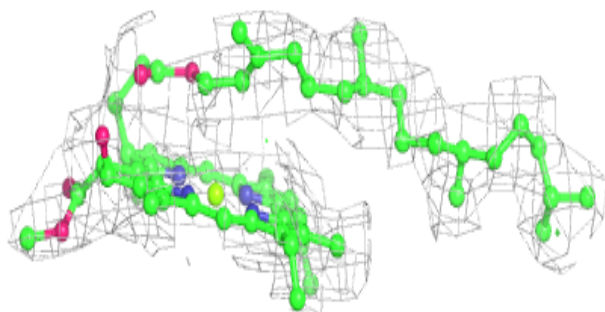
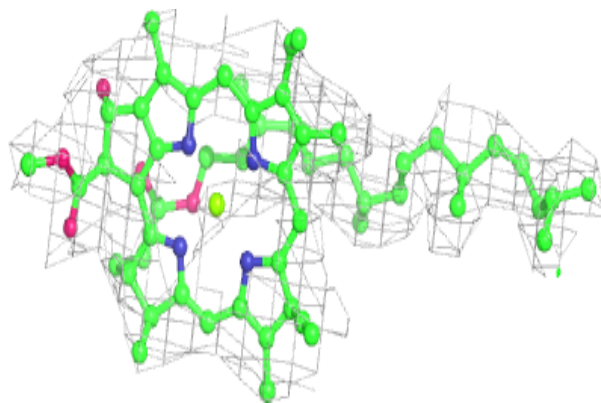
**Electron density around CLA B 1225:**

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



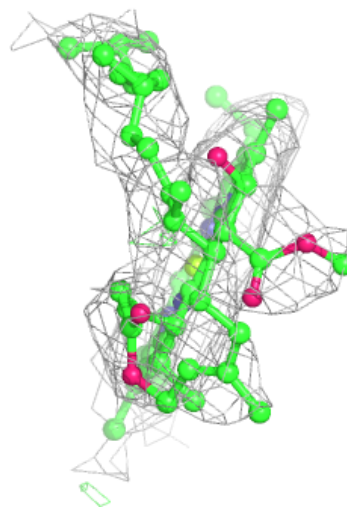
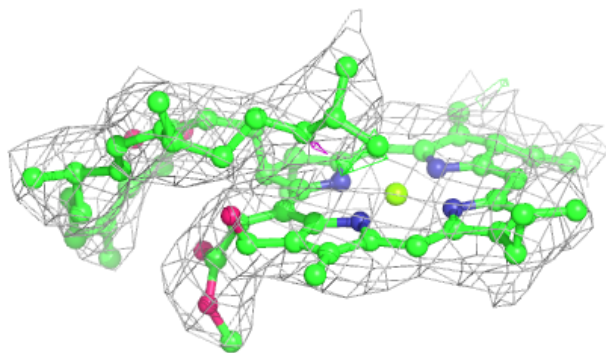
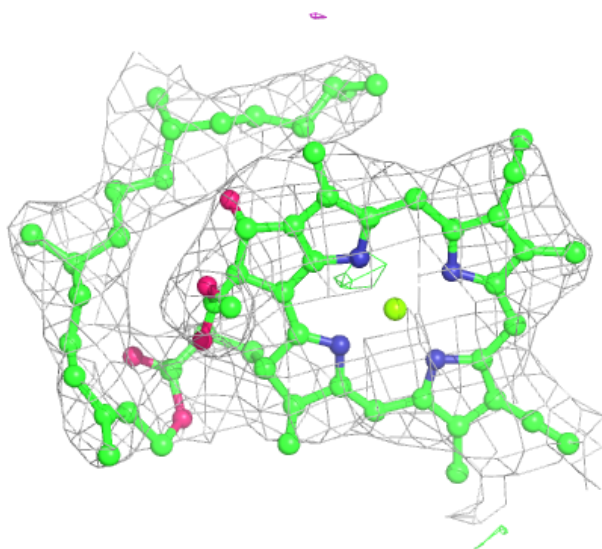
Electron density around CLA A 1136:

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



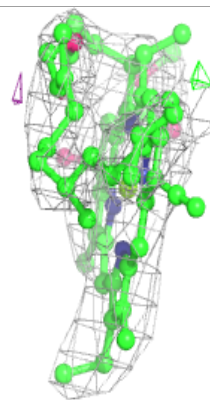
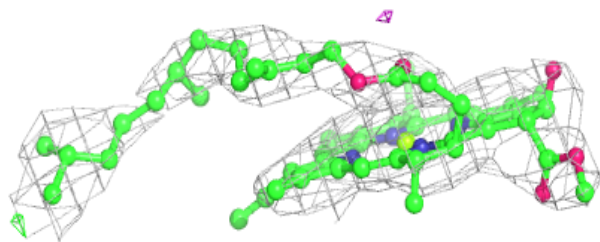
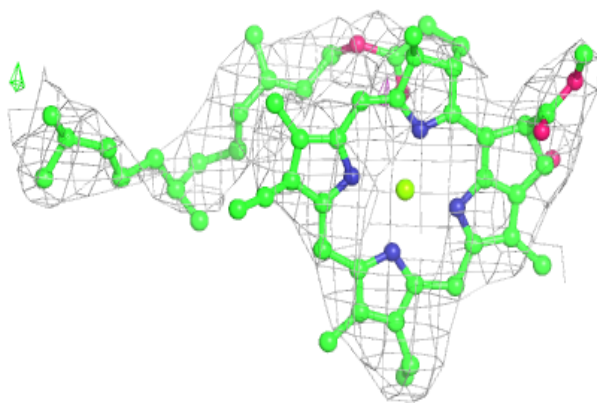
Electron density around CLA B 1202:

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



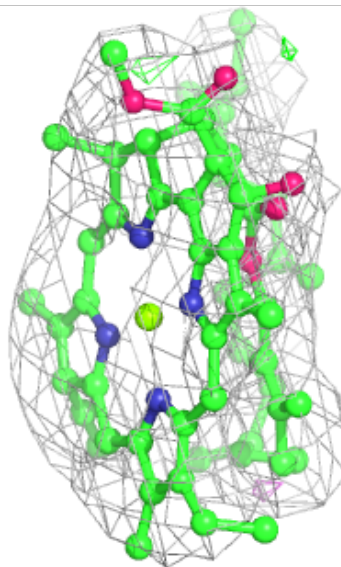
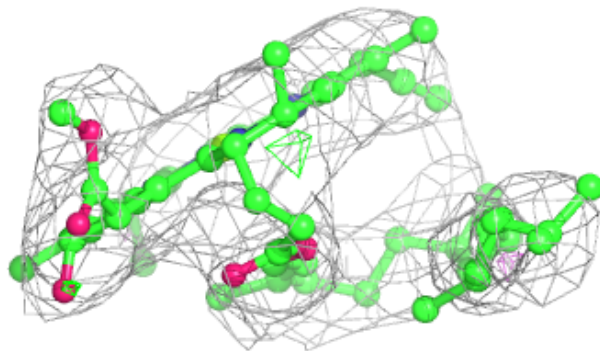
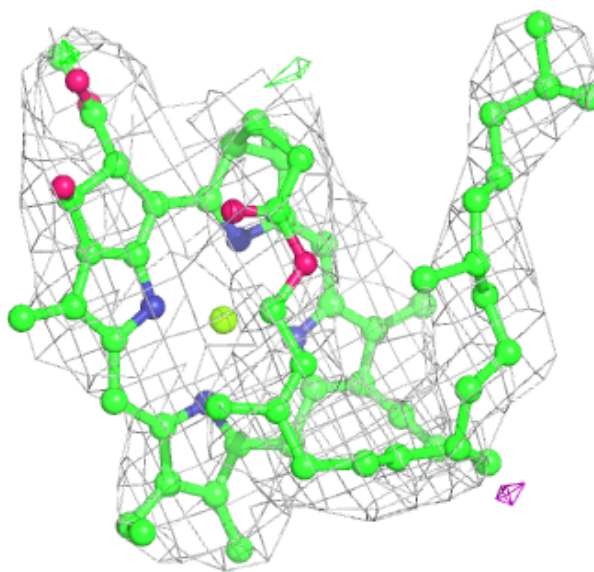
Electron density around CLA B 1215:

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



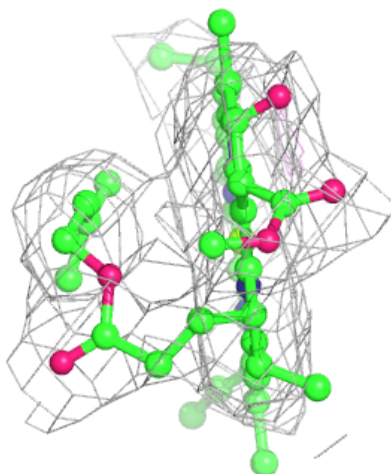
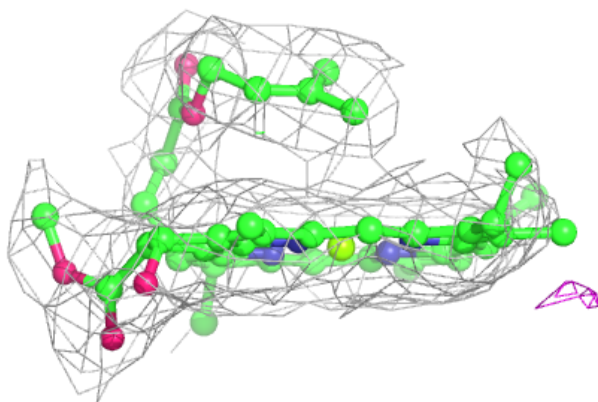
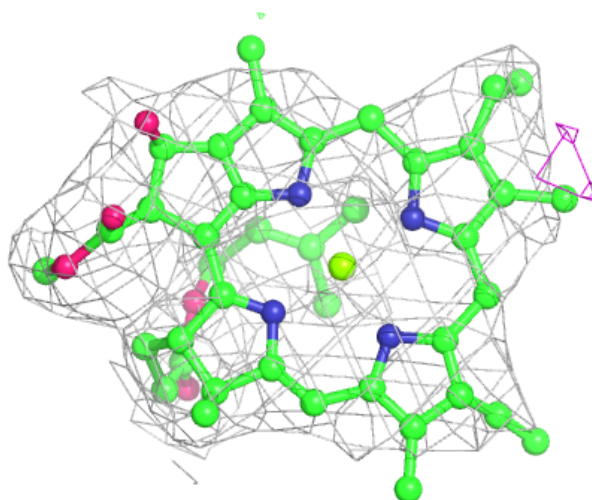
Electron density around CLA B 1205:

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



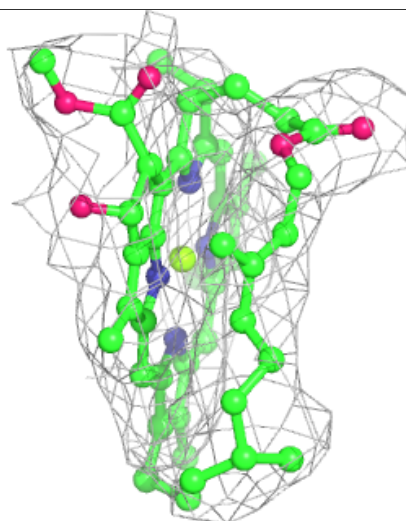
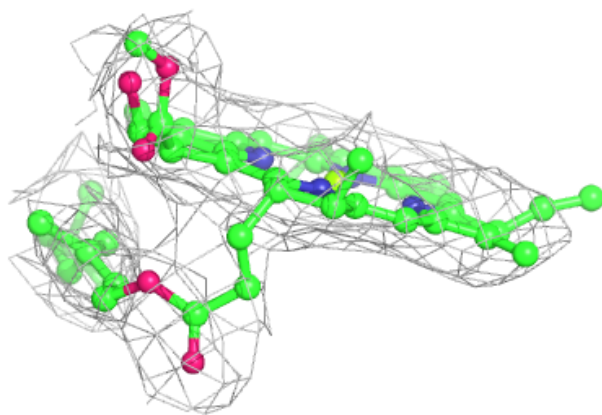
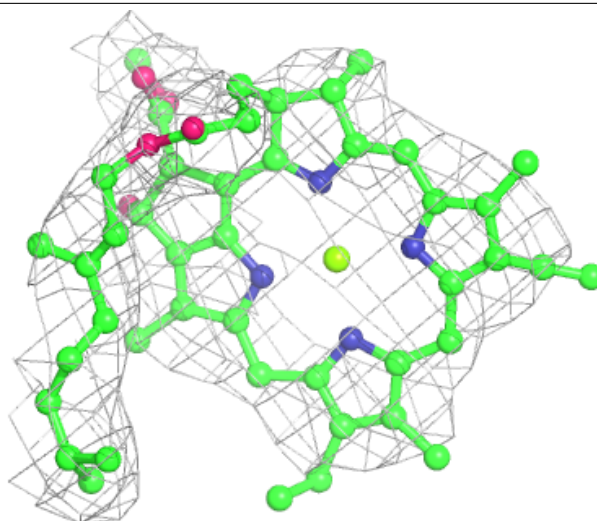
Electron density around CLA B 1227:

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



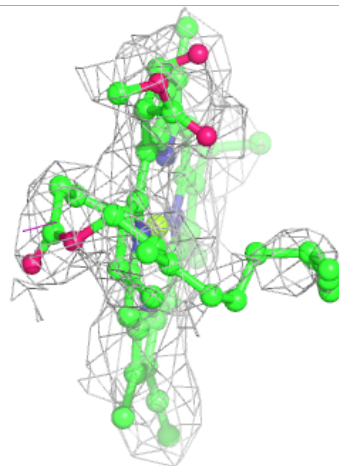
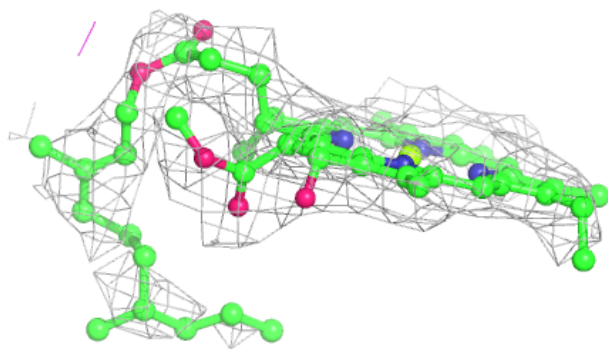
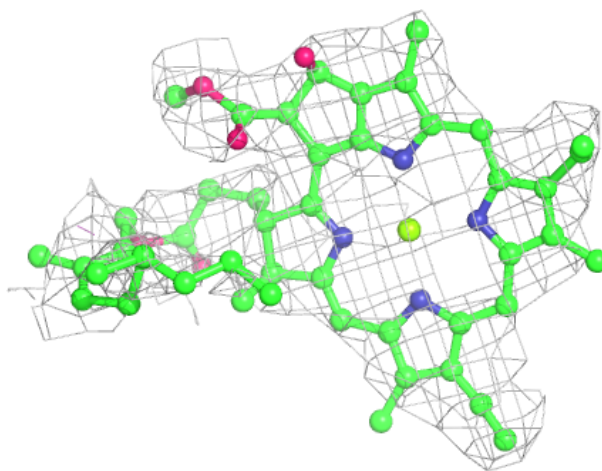
Electron density around CLA A 1127:

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



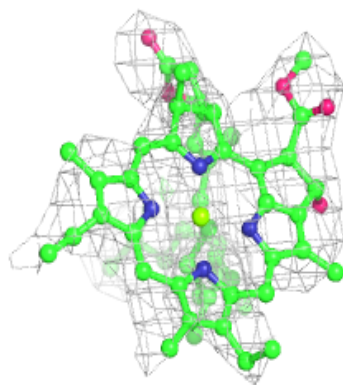
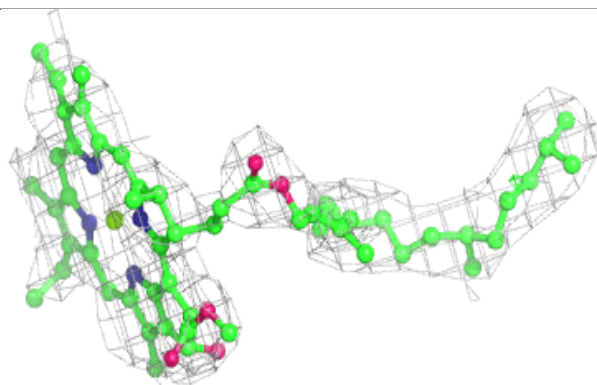
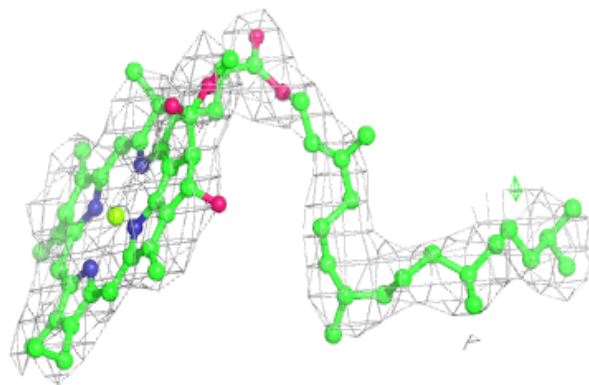
Electron density around CLA A 1104:

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

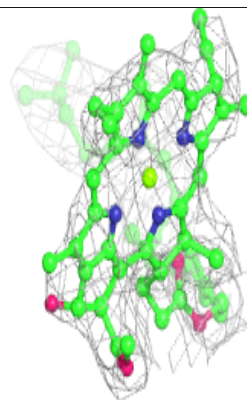
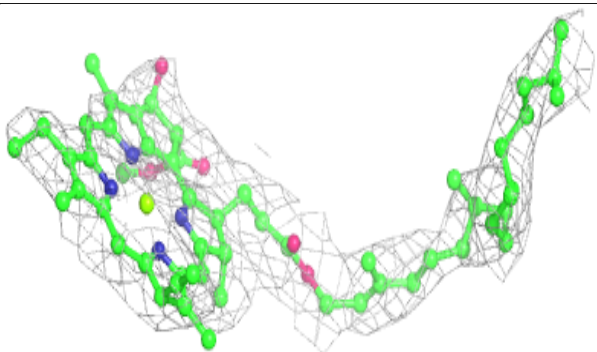
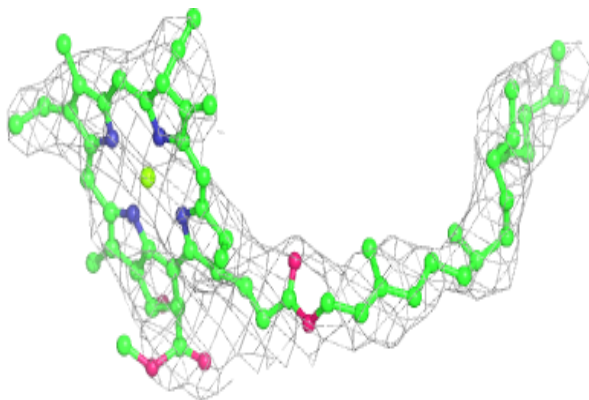


Electron density around CLA B 9010:

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

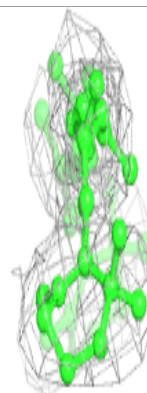
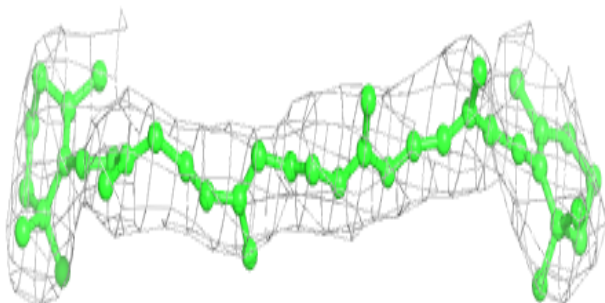
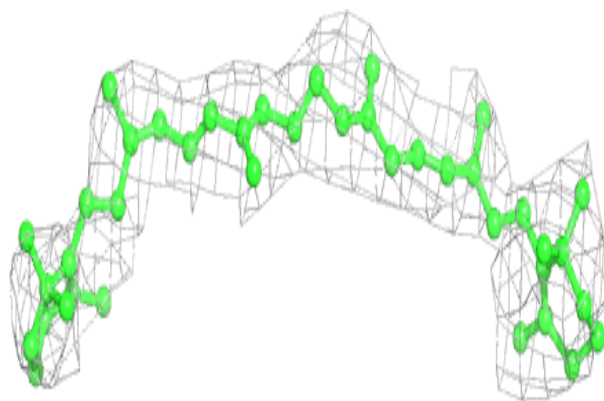
**Electron density around CLA A 9012:**

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

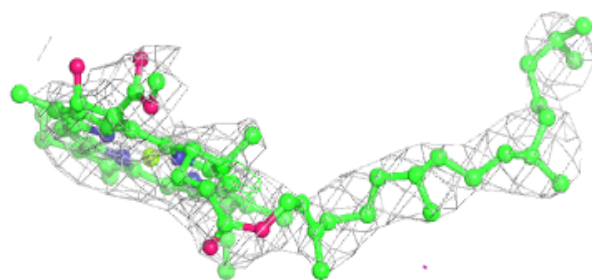
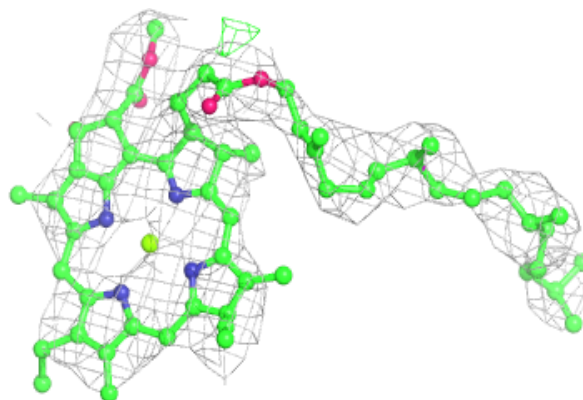


Electron density around BCR B 6020:

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

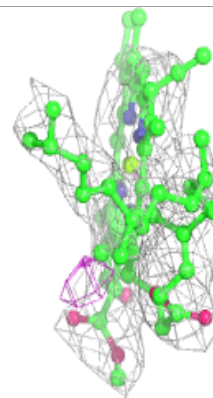
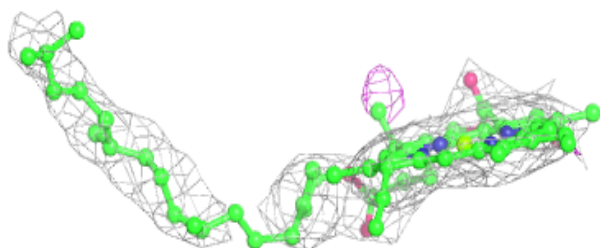
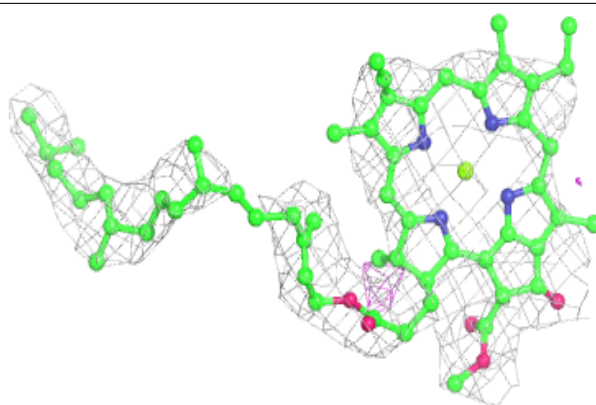
**Electron density around CLA A 9013:**

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

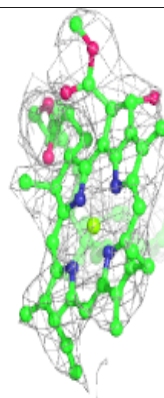
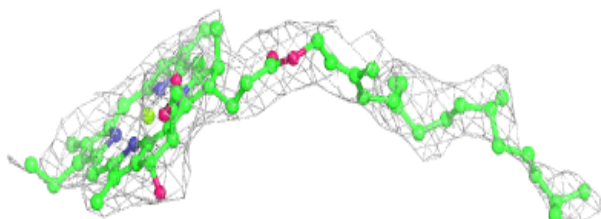
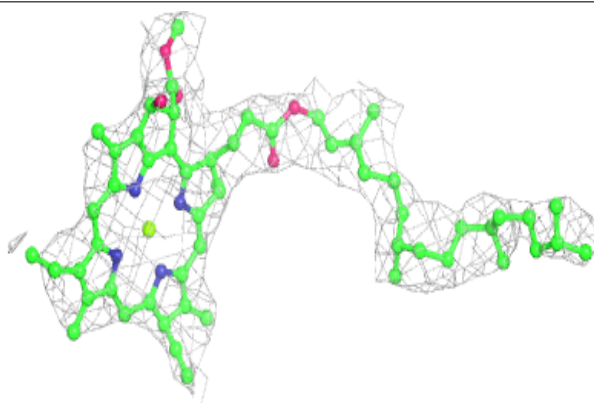


Electron density around CLA A 9023:

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

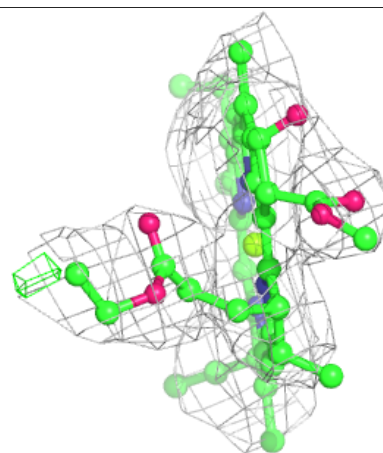
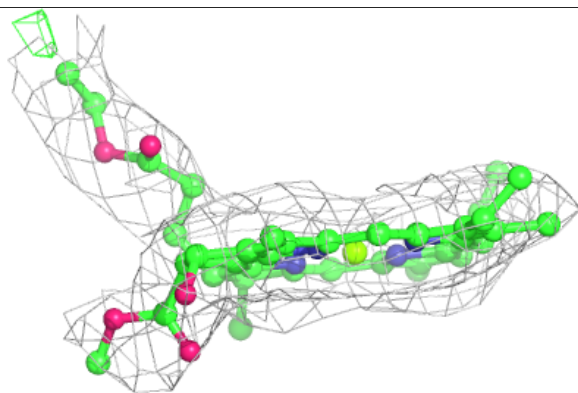
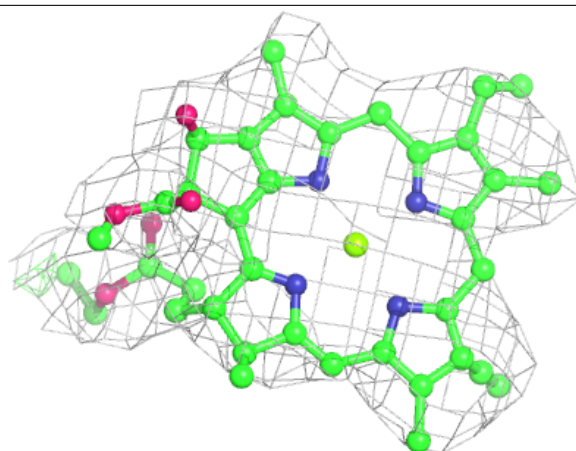
**Electron density around CLA A 9022:**

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

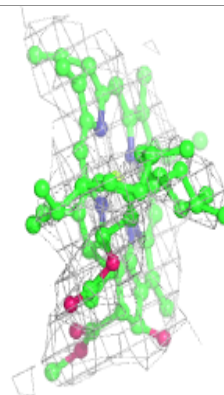
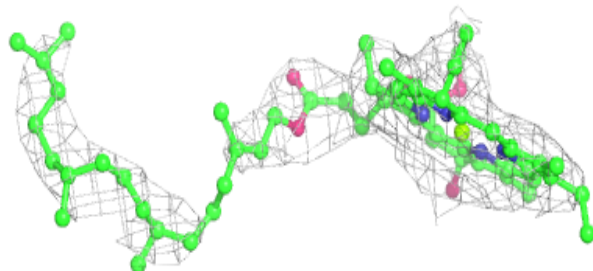
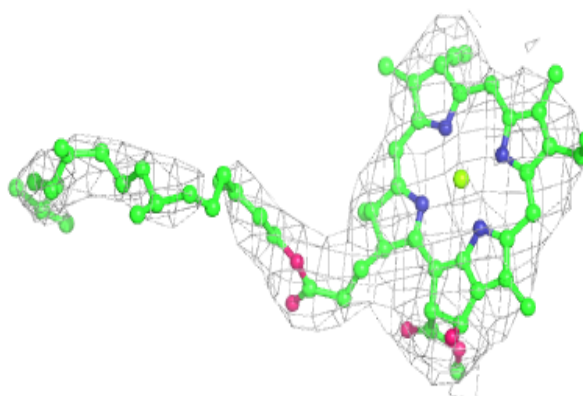


Electron density around CLA A 1137:

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

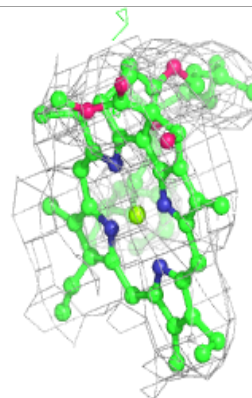
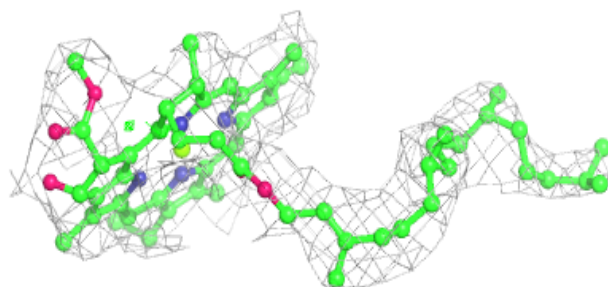
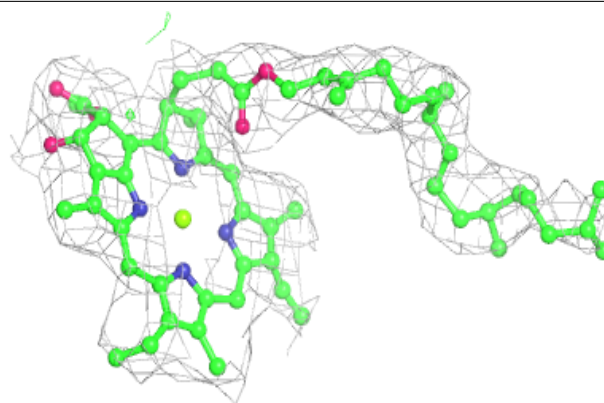
**Electron density around CLA B 1210:**

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

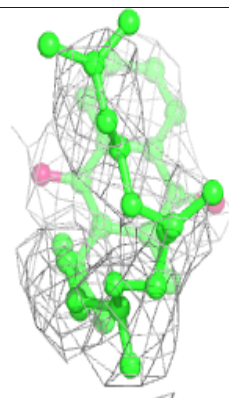
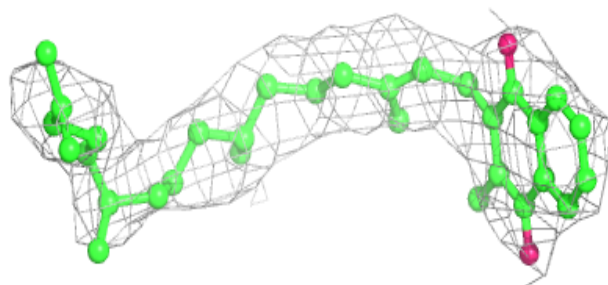
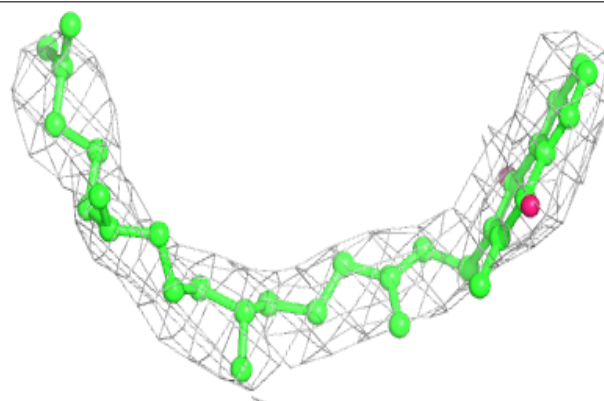


Electron density around CLA A 1106:

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

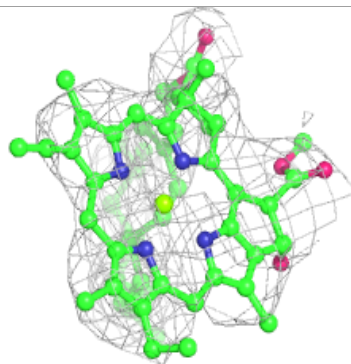
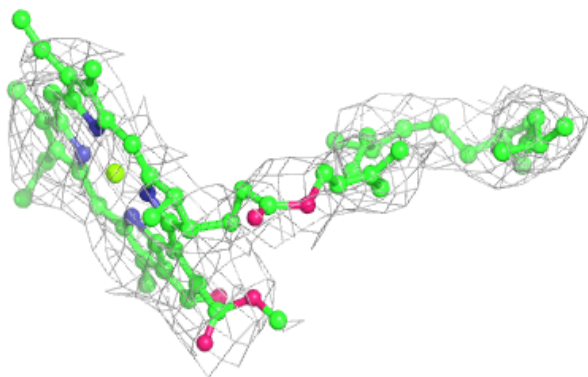
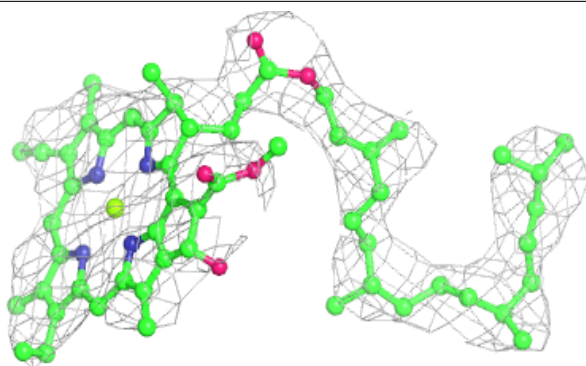
**Electron density around PQN B 5002:**

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

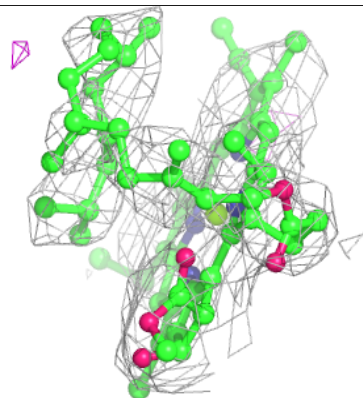
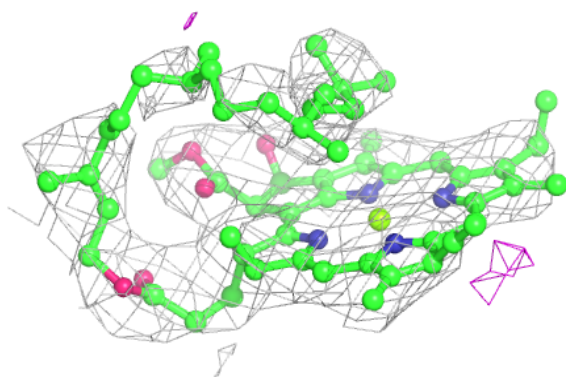
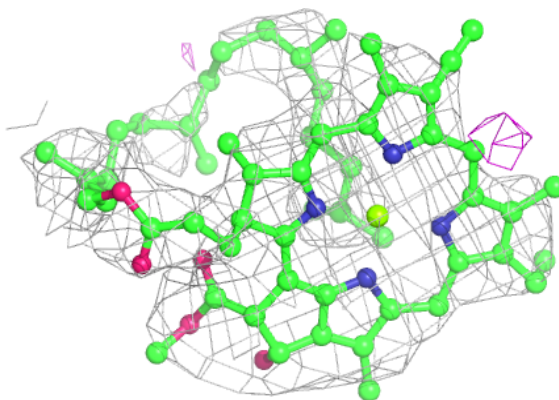


Electron density around CLA A 9011:

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

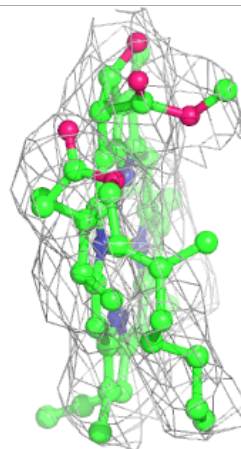
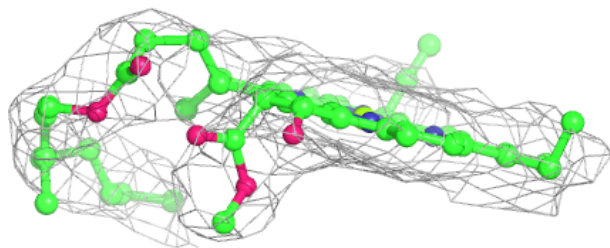
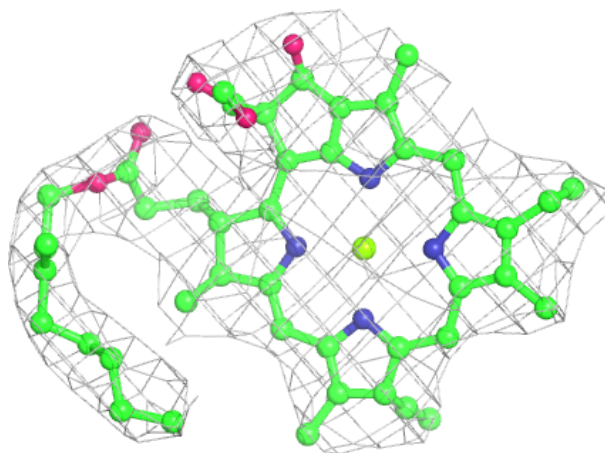
**Electron density around CLA B 1203:**

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



Electron density around CLA B 1221:

$2mF_o-DF_c$ (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.