



wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 20, 2020 – 10:19 PM BST

PDB ID : 4KT0
Title : Crystal structure of a virus like photosystem I from the cyanobacterium Synechocystis PCC 6803
Authors : Mazor, Y.; Nataf, D.; Toporik, H.; Nelson, N.
Deposited on : 2013-05-19
Resolution : 2.80 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The 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 : 2.13.1
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) : 2.13.1

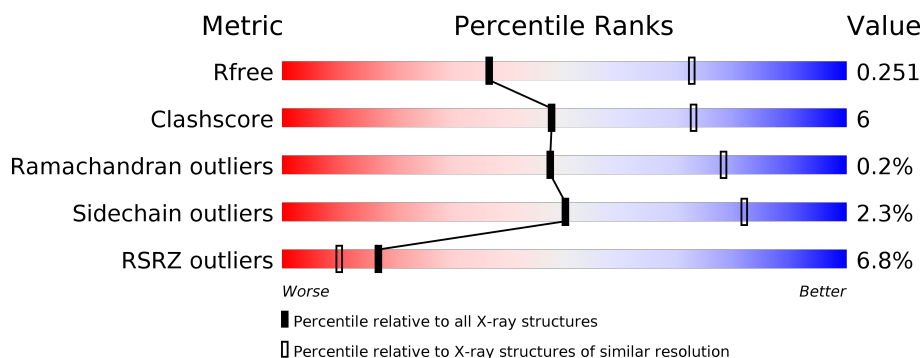
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	3140 (2.80-2.80)
Clashscore	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)
RSRZ outliers	127900	3078 (2.80-2.80)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on 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	751	<div> <div>8%</div> <div> <div></div> <div>90%</div> <div>9%</div> <div></div> </div> <div></div> </div>
2	B	731	<div> <div>3%</div> <div> <div></div> <div>91%</div> <div>8%</div> <div></div> </div> <div></div> </div>
3	C	81	<div> <div></div> <div> <div></div> <div>94%</div> <div></div> </div> <div></div> </div>
4	D	141	<div> <div>16%</div> <div> <div></div> <div>89%</div> <div>8%</div> <div></div> </div> <div></div> </div>
5	E	74	<div> <div>4%</div> <div> <div></div> <div>81%</div> <div>9%</div> <div></div> </div> <div></div> </div>
6	F	165	<div> <div>2%</div> <div> <div></div> <div>78%</div> <div>7%</div> <div></div> </div> <div></div> </div>

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Mol	Chain	Length	Quality of chain
7	J	40	
8	K	128	
9	M	31	

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
13	CL0	A	1011	X	-	-	-
13	CL0	A	1108	X	-	-	-
15	CLA	A	1012	X	-	-	-
15	CLA	A	1022	X	-	-	-
15	CLA	A	1101	X	-	-	-
15	CLA	A	1102	X	-	-	-
15	CLA	A	1103	X	-	-	-
15	CLA	A	1104	X	-	-	-
15	CLA	A	1105	X	-	-	-
15	CLA	A	1106	X	-	-	-
15	CLA	A	1107	X	-	-	-
15	CLA	A	1109	X	-	-	-
15	CLA	A	1110	X	-	-	-
15	CLA	A	1111	X	-	-	-
15	CLA	A	1112	X	-	-	-
15	CLA	A	1113	X	-	-	-
15	CLA	A	1114	X	-	-	-
15	CLA	A	1115	X	-	-	-
15	CLA	A	1116	X	-	-	-
15	CLA	A	1117	X	-	-	-
15	CLA	A	1118	X	-	-	-
15	CLA	A	1119	X	-	-	-
15	CLA	A	1120	X	-	-	-
15	CLA	A	1121	X	-	-	-
15	CLA	A	1122	X	-	-	-
15	CLA	A	1123	X	-	-	-
15	CLA	A	1124	X	-	-	-
15	CLA	A	1125	X	-	-	-
15	CLA	A	1126	X	-	-	-
15	CLA	A	1127	X	-	-	-
15	CLA	A	1128	X	-	-	-
15	CLA	A	1129	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
15	CLA	A	1130	X	-	-	-
15	CLA	A	1131	X	-	-	-
15	CLA	A	1132	X	-	-	-
15	CLA	A	1133	X	-	-	-
15	CLA	A	1134	X	-	-	-
15	CLA	A	1135	X	-	-	-
15	CLA	A	1136	X	-	-	-
15	CLA	A	1137	X	-	-	-
15	CLA	A	1138	X	-	-	-
15	CLA	A	1140	X	-	-	-
15	CLA	A	1801	X	-	-	-
15	CLA	B	1013	X	-	-	-
15	CLA	B	1021	X	-	-	-
15	CLA	B	1023	X	-	-	-
15	CLA	B	1201	X	-	-	-
15	CLA	B	1202	X	-	-	-
15	CLA	B	1203	X	-	-	-
15	CLA	B	1204	X	-	-	-
15	CLA	B	1205	X	-	-	-
15	CLA	B	1206	X	-	-	-
15	CLA	B	1207	X	-	-	-
15	CLA	B	1208	X	-	-	-
15	CLA	B	1209	X	-	-	-
15	CLA	B	1210	X	-	-	-
15	CLA	B	1211	X	-	-	-
15	CLA	B	1212	X	-	-	-
15	CLA	B	1213	X	-	-	-
15	CLA	B	1214	X	-	-	-
15	CLA	B	1215	X	-	-	-
15	CLA	B	1216	X	-	-	-
15	CLA	B	1217	X	-	-	-
15	CLA	B	1218	X	-	-	-
15	CLA	B	1219	X	-	-	-
15	CLA	B	1220	X	-	-	-
15	CLA	B	1221	X	-	-	-
15	CLA	B	1222	X	-	-	-
15	CLA	B	1223	X	-	-	-
15	CLA	B	1224	X	-	-	-
15	CLA	B	1225	X	-	-	-
15	CLA	B	1226	X	-	-	-
15	CLA	B	1227	X	-	-	-
15	CLA	B	1228	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
15	CLA	B	1229	X	-	-	-
15	CLA	B	1230	X	-	-	-
15	CLA	B	1231	X	-	-	-
15	CLA	B	1232	X	-	-	-
15	CLA	B	1234	X	-	-	-
15	CLA	B	1235	X	-	-	-
15	CLA	B	1236	X	-	-	-
15	CLA	B	1237	X	-	-	-
15	CLA	B	1238	X	-	-	-
15	CLA	B	1239	X	-	-	-
15	CLA	B	1240	X	-	-	-
15	CLA	F	1139	X	-	-	-
15	CLA	F	1301	X	-	-	-
15	CLA	F	1410	X	-	-	-
15	CLA	J	1302	X	-	-	-
15	CLA	J	1303	X	-	-	-
15	CLA	K	1401	X	-	-	-
15	CLA	K	1402	X	-	-	-

2 Entry composition

There are 19 unique types of molecules in this entry. The entry contains 22051 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	739	Total	C	N	O	S	0	0	0
			5787	3791	984	985	27			

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	138	Total	C	N	O	S	0	0	0
			1075	681	187	204	3			

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
5	E	68	Total	C	N	O	0	0	0
			533	335	94	104			

- Molecule 6 is a protein called Photosystem I subunit III.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	F	141	Total	C	N	O	S	0	0	0
			1099	711	183	200	5			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	J	40	Total	C	N	O	S	0	0	0
			319	215	47	54	3			

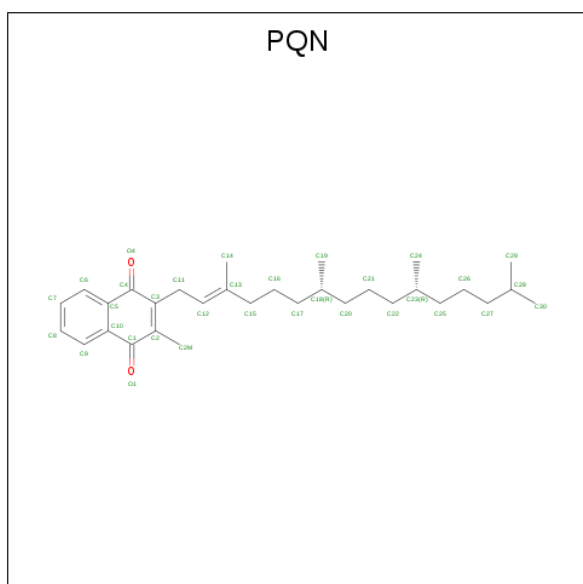
- Molecule 8 is a protein called Photosystem I reaction center subunit PsaK.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	K	53	Total	C	N	O	S	0	0	0
			366	242	56	63	5			

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
9	M	30	Total	C	N	O	0	0	0
			214	142	34	38			

- Molecule 10 is PHYLLOQUINONE (three-letter code: PQN) (formula: $C_{31}H_{46}O_2$).



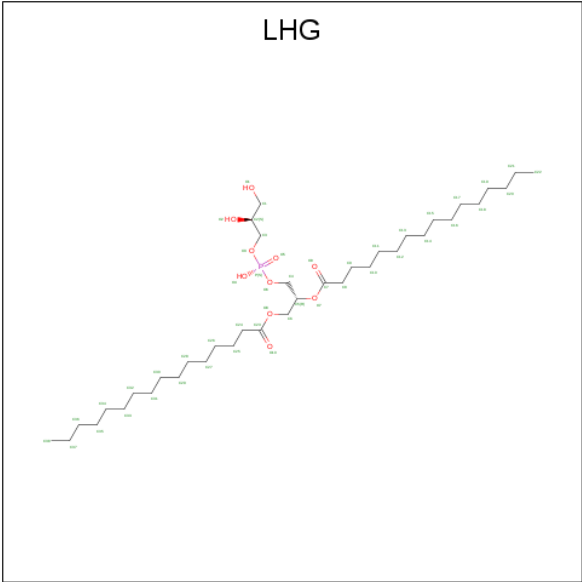
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
10	A	1	Total	C	O	0	0
			33	31	2		
10	B	1	Total	C	O	0	0
			33	31	2		

- Molecule 11 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe_4S_4).



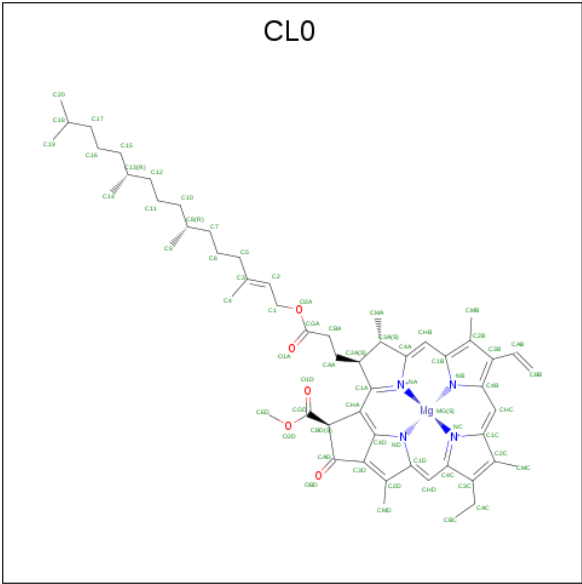
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
11	A	1	Total	Fe	S	0	0
			8	4	4		
11	C	1	Total	Fe	S	0	0
			8	4	4		
11	C	1	Total	Fe	S	0	0
			8	4	4		

- Molecule 12 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (three-letter code: LHG) (formula: C₃₈H₇₅O₁₀P).



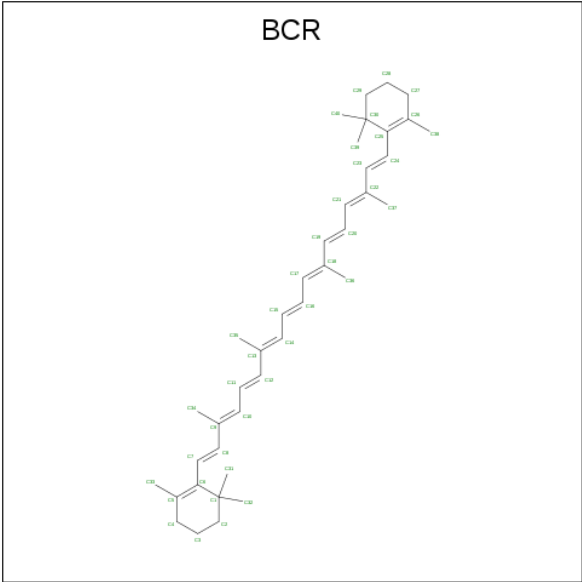
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
12	A	1	Total	C	O	P	0	0
			49	38	10	1		
12	A	1	Total	C	O	P	0	0
			49	38	10	1		
12	A	1	Total	C	O	P	0	0
			36	25	10	1		
12	B	1	Total	C	O	P	0	0
			49	38	10	1		

- Molecule 13 is CHLOROPHYLL A ISOMER (three-letter code: CL0) (formula: C₅₅H₇₂MgN₄O₅).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
13	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	A	1	Total	C	Mg	N	O	0
			45	35	1	4	5	

- Molecule 14 is BETA-CAROTENE (three-letter code: BCR) (formula: C₄₀H₅₆).



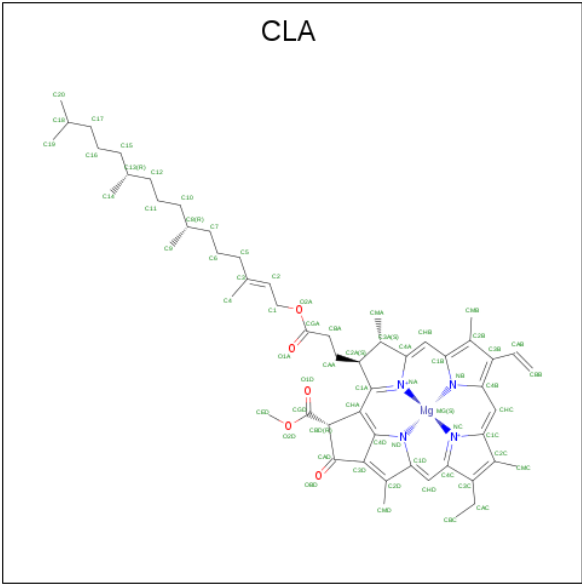
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
14	A	1	Total C 40 40	0	0
14	A	1	Total C 40 40	0	0
14	A	1	Total C 40 40	0	0
14	A	1	Total C 40 40	0	0
14	A	1	Total C 40 40	0	0
14	A	1	Total C 40 40	0	0
14	B	1	Total C 40 40	0	0
14	B	1	Total C 40 40	0	0
14	B	1	Total C 40 40	0	0
14	B	1	Total C 40 40	0	0
14	B	1	Total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

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
14	F	1	Total C 40 40	0	0
14	F	1	Total C 40 40	0	0
14	J	1	Total C 40 40	0	0

- Molecule 15 is CHLOROPHYLL A (three-letter code: CLA) (formula: C₅₅H₇₂MgN₄O₅).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
15	A	1	Total C Mg N O 52 42 1 4 5	0	0
15	A	1	Total C Mg N O 65 55 1 4 5	0	0
15	A	1	Total C Mg N O 65 55 1 4 5	0	0
15	A	1	Total C Mg N O 65 55 1 4 5	0	0
15	A	1	Total C Mg N O 65 55 1 4 5	0	0
15	A	1	Total C Mg N O 65 55 1 4 5	0	0
15	A	1	Total C Mg N O 65 55 1 4 5	0	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
15	A	1	Total	C	Mg	N	O	0	0
			50	40	1	4	5		
15	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
15	A	1	Total	C	Mg	N	O	0	0
			54	44	1	4	5		
15	A	1	Total	C	Mg	N	O	0	0
			60	50	1	4	5		
15	A	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
15	A	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
15	A	1	Total	C	Mg	N	O	0	0
			54	44	1	4	5		
15	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
15	A	1	Total	C	Mg	N	O	0	0
			46	36	1	4	5		
15	A	1	Total	C	Mg	N	O	0	0
			64	54	1	4	5		
15	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
15	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
15	A	1	Total	C	Mg	N	O	0	0
			55	45	1	4	5		
15	A	1	Total	C	Mg	N	O	0	0
			52	42	1	4	5		
15	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
15	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
15	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
15	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
15	A	1	Total	C	Mg	N	O	0	0
			50	40	1	4	5		
15	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
15	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
15	A	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
15	A	1	Total 49	C 39	Mg 1	N 4	O 5	0	0
15	A	1	Total 46	C 36	Mg 1	N 4	O 5	0	0
15	A	1	Total 49	C 39	Mg 1	N 4	O 5	0	0
15	A	1	Total 46	C 36	Mg 1	N 4	O 5	0	0
15	A	1	Total 46	C 36	Mg 1	N 4	O 5	0	0
15	A	1	Total 55	C 45	Mg 1	N 4	O 5	0	0
15	A	1	Total 55	C 45	Mg 1	N 4	O 5	0	0
15	A	1	Total 62	C 52	Mg 1	N 4	O 5	0	0
15	A	1	Total 46	C 36	Mg 1	N 4	O 5	0	0
15	A	1	Total 46	C 36	Mg 1	N 4	O 5	0	0
15	A	1	Total 55	C 45	Mg 1	N 4	O 5	0	0
15	B	1	Total 45	C 35	Mg 1	N 4	O 5	0	0
15	B	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
15	B	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
15	B	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
15	B	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
15	B	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
15	B	1	Total 55	C 45	Mg 1	N 4	O 5	0	0
15	B	1	Total 46	C 36	Mg 1	N 4	O 5	0	0
15	B	1	Total 45	C 35	Mg 1	N 4	O 5	0	0

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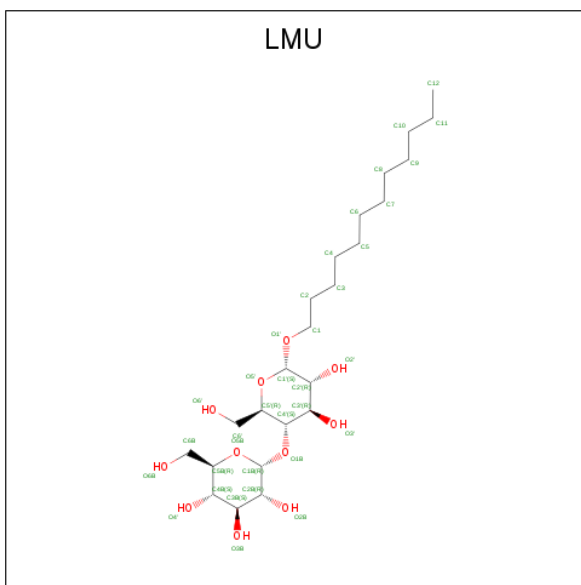
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
15	B	1	Total 45	C 35	Mg 1	N 4	O 5	0	0
15	B	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
15	B	1	Total 45	C 35	Mg 1	N 4	O 5	0	0
15	B	1	Total 50	C 40	Mg 1	N 4	O 5	0	0
15	B	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
15	B	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
15	B	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
15	B	1	Total 47	C 37	Mg 1	N 4	O 5	0	0
15	B	1	Total 51	C 41	Mg 1	N 4	O 5	0	0
15	B	1	Total 55	C 45	Mg 1	N 4	O 5	0	0
15	B	1	Total 56	C 46	Mg 1	N 4	O 5	0	0
15	B	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
15	B	1	Total 56	C 46	Mg 1	N 4	O 5	0	0
15	B	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
15	B	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
15	B	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
15	B	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
15	B	1	Total 45	C 35	Mg 1	N 4	O 5	0	0
15	B	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
15	B	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
15	B	1	Total 65	C 55	Mg 1	N 4	O 5	0	0

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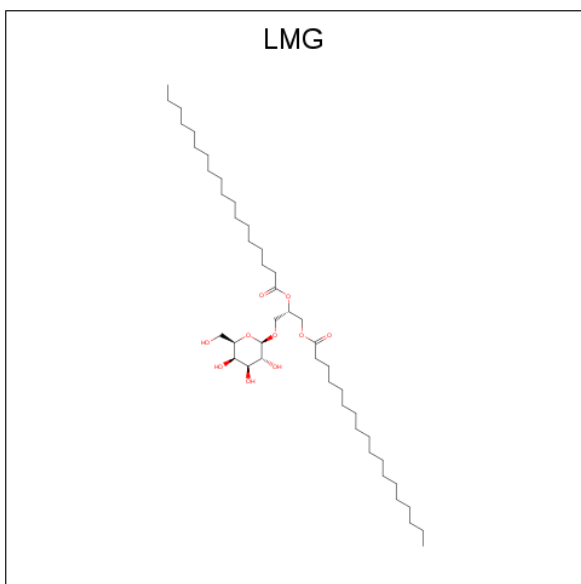
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
15	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
15	B	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
15	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
15	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
15	B	1	Total	C	Mg	N	O	0	0
			50	40	1	4	5		
15	B	1	Total	C	Mg	N	O	0	0
			46	36	1	4	5		
15	B	1	Total	C	Mg	N	O	0	0
			46	36	1	4	5		
15	B	1	Total	C	Mg	N	O	0	0
			46	36	1	4	5		
15	B	1	Total	C	Mg	N	O	0	0
			46	36	1	4	5		
15	B	1	Total	C	Mg	N	O	0	0
			55	45	1	4	5		
15	B	1	Total	C	Mg	N	O	0	0
			44	35	1	4	4		
15	B	1	Total	C	Mg	N	O	0	0
			46	36	1	4	5		
15	F	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
15	F	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
15	F	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
15	J	1	Total	C	Mg	N	O	0	0
			46	36	1	4	5		
15	J	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
15	K	1	Total	C	Mg	N	O	0	0
			46	36	1	4	5		
15	K	1	Total	C	Mg	N	O	0	0
			46	36	1	4	5		

- Molecule 16 is DODECYL-ALPHA-D-MALTOSIDE (three-letter code: LMU) (formula: $C_{24}H_{46}O_{11}$).



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

- Molecule 17 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (three-letter code: LMG) (formula: $C_{45}H_{86}O_{10}$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
17	B	1	Total	C	O	0	0
			55	45	10		

- Molecule 18 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
18	B	1	Total	Cl	0	0
			1	1		

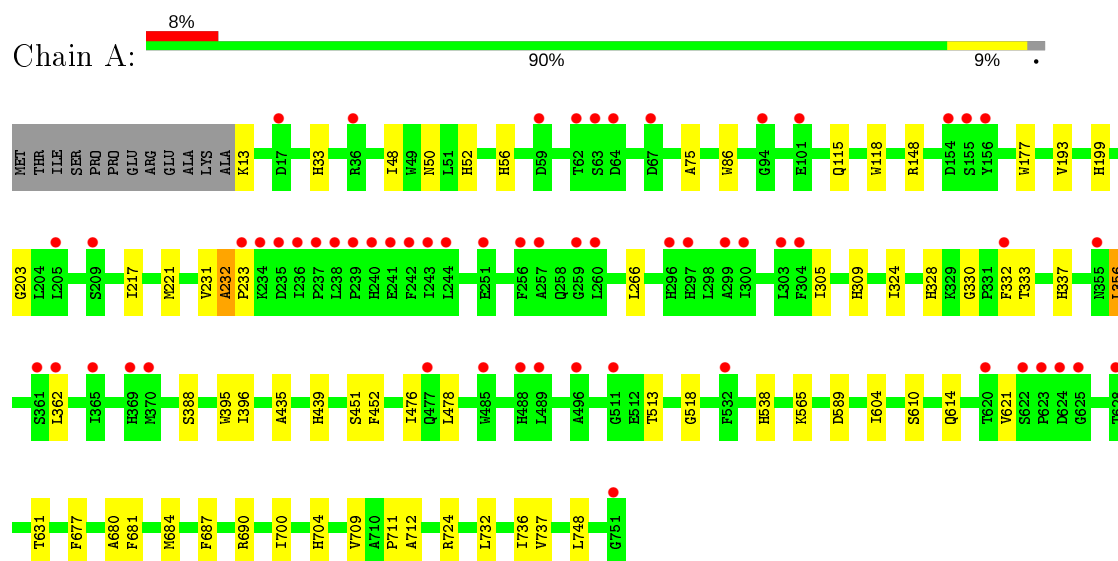
- Molecule 19 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
19	A	10	Total	O	0	0
			10	10		
19	B	15	Total	O	0	0
			15	15		
19	C	3	Total	O	0	0
			3	3		
19	F	1	Total	O	0	0
			1	1		

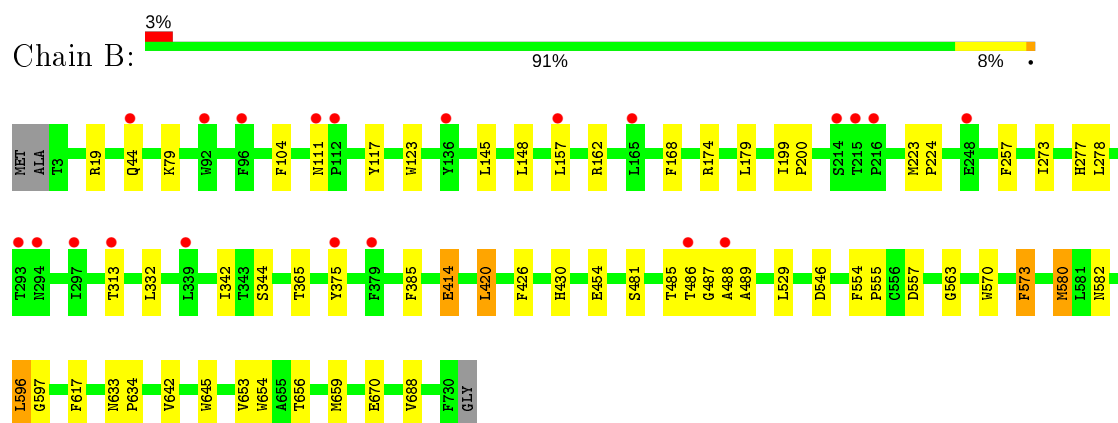
3 Residue-property plots [i](#)

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

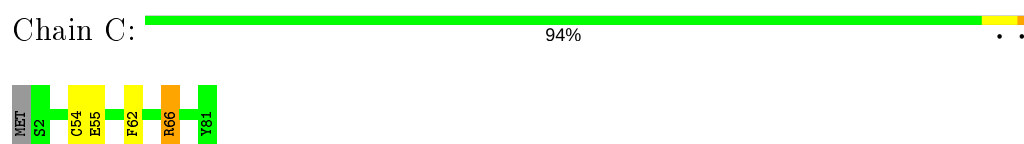
- Molecule 1: Photosystem I P700 chlorophyll a apoprotein A1



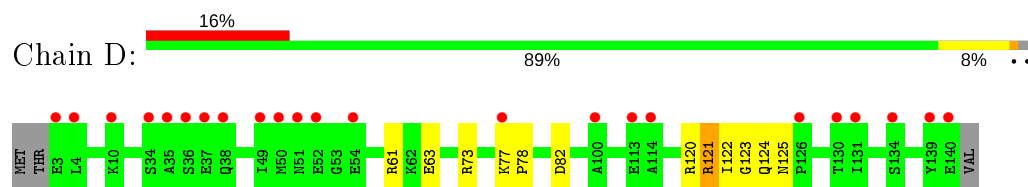
- Molecule 2: Photosystem I P700 chlorophyll a apoprotein A2



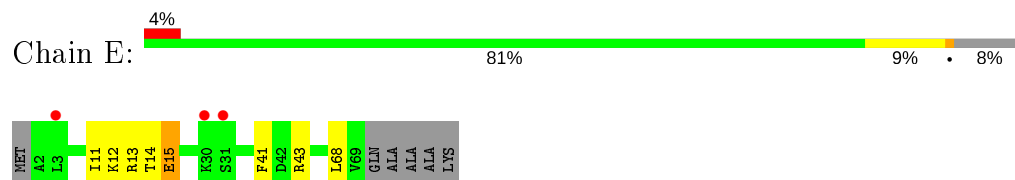
- Molecule 3: Photosystem I iron-sulfur center



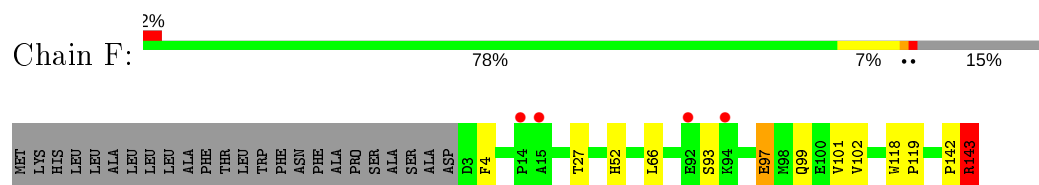
- Molecule 4: Photosystem I subunit II



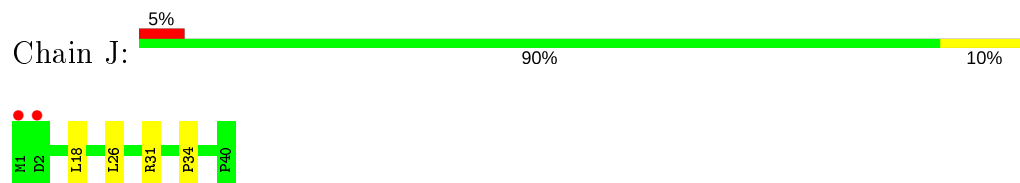
- Molecule 5: Photosystem I reaction center subunit IV



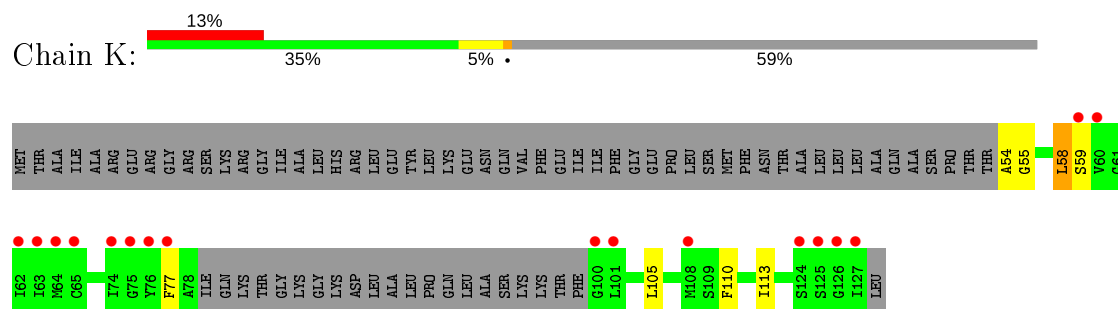
- Molecule 6: Photosystem I subunit III



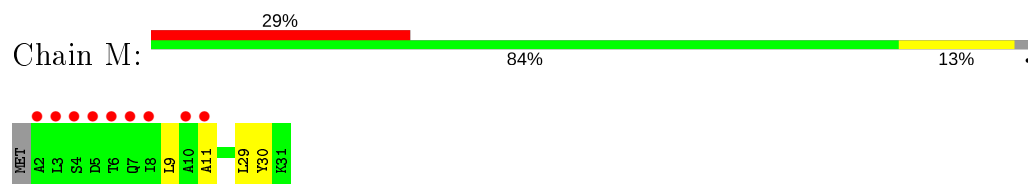
- Molecule 7: Photosystem I reaction center subunit IX



- Molecule 8: Photosystem I reaction center subunit PsaK



- Molecule 9: Photosystem I reaction center subunit XII



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	120.18Å 173.31Å 179.14Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.98 – 2.80 48.55 – 2.60	Depositor EDS
% Data completeness (in resolution range)	98.6 (29.98-2.80) 79.2 (48.55-2.60)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.32 (at 2.61Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.198 , 0.245 0.203 , 0.251	Depositor DCC
R_{free} test set	5715 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	57.1	Xtriage
Anisotropy	0.559	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 75.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.012 for -h,l,k	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	22051	wwPDB-VP
Average B, all atoms (Å ²)	92.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.71% 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: LHG, CL, SF4, LMU, PQN, CLA, CL0, BCR, LMG

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.22	0/5985	0.38	0/8158
2	B	0.23	0/5976	0.40	0/8173
3	C	0.24	0/610	0.45	0/826
4	D	0.23	0/1099	0.40	0/1482
5	E	0.24	0/542	0.45	0/733
6	F	0.23	0/1129	0.40	0/1535
7	J	0.26	0/328	0.38	0/443
8	K	0.25	0/371	0.39	0/499
9	M	0.22	0/217	0.35	0/295
All	All	0.23	0/16257	0.39	0/22144

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
4	D	0	1
6	F	0	1
All	All	0	2

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
4	D	121	ARG	Sidechain
6	F	143	ARG	Sidechain

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5787	0	5646	60	0
2	B	5765	0	5544	56	0
3	C	600	0	581	4	0
4	D	1075	0	1069	7	0
5	E	533	0	517	8	0
6	F	1099	0	1096	7	0
7	J	319	0	328	4	0
8	K	366	0	376	7	0
9	M	214	0	213	2	0
10	A	33	0	46	1	0
10	B	33	0	46	3	0
11	A	8	0	0	0	0
11	C	16	0	0	0	0
12	A	134	0	190	18	0
12	B	49	0	74	2	0
13	A	110	0	105	12	0
14	A	240	0	294	17	0
14	B	320	0	390	26	0
14	F	80	0	97	8	0
14	J	40	0	49	3	0
15	A	2352	0	2285	69	0
15	B	2365	0	2272	58	0
15	F	175	0	177	3	0
15	J	91	0	66	2	0
15	K	92	0	66	2	0
16	B	35	0	46	0	0
16	J	35	0	46	2	0
17	B	55	0	86	2	0
18	B	1	0	0	0	0
19	A	10	0	0	5	0
19	B	15	0	0	6	0
19	C	3	0	0	0	0
19	F	1	0	0	1	0
All	All	22051	0	21705	267	0

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

The worst 5 of 267 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)
13:A:1011:CL0:CMA	19:A:9109:HOH:O	1.91	1.19
13:A:1011:CL0:H6	19:A:9109:HOH:O	1.48	1.11
14:B:4004:BCR:H403	14:B:4004:BCR:H23C	1.51	0.92
13:A:1011:CL0:H71	19:A:9109:HOH:O	1.71	0.88
15:A:1110:CLA:HBD	15:A:1110:CLA:HBA1	1.57	0.86

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	737/751 (98%)	694 (94%)	40 (5%)	3 (0%)	34	66
2	B	726/731 (99%)	695 (96%)	31 (4%)	0	100	100
3	C	78/81 (96%)	74 (95%)	4 (5%)	0	100	100
4	D	136/141 (96%)	123 (90%)	13 (10%)	0	100	100
5	E	66/74 (89%)	57 (86%)	9 (14%)	0	100	100
6	F	139/165 (84%)	135 (97%)	4 (3%)	0	100	100
7	J	38/40 (95%)	38 (100%)	0	0	100	100
8	K	49/128 (38%)	46 (94%)	3 (6%)	0	100	100
9	M	28/31 (90%)	25 (89%)	3 (11%)	0	100	100
All	All	1997/2142 (93%)	1887 (94%)	107 (5%)	3 (0%)	47	78

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	115	GLN
1	A	232	ALA

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Mol	Chain	Res	Type
1	A	233	PRO

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	593/603 (98%)	584 (98%)	9 (2%)	65	89
2	B	582/583 (100%)	571 (98%)	11 (2%)	57	85
3	C	68/69 (99%)	67 (98%)	1 (2%)	65	89
4	D	112/116 (97%)	110 (98%)	2 (2%)	59	86
5	E	57/60 (95%)	54 (95%)	3 (5%)	22	54
6	F	118/137 (86%)	112 (95%)	6 (5%)	24	55
7	J	35/35 (100%)	35 (100%)	0	100	100
8	K	37/100 (37%)	33 (89%)	4 (11%)	6	19
9	M	19/25 (76%)	18 (95%)	1 (5%)	22	54
All	All	1621/1728 (94%)	1584 (98%)	37 (2%)	50	82

5 of 37 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	573	PHE
3	C	66	ARG
8	K	105	LEU
2	B	580	MET
2	B	596	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 8 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	614	GLN
4	D	95	GLN
2	B	114	ASN

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Mol	Chain	Res	Type
1	A	538	HIS
2	B	34	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 122 ligands modelled in this entry, 1 is monoatomic - leaving 121 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
15	CLA	B	1213	-	44,58,73	2.73	16 (36%)	49,95,113	2.38	13 (26%)
14	BCR	A	4008	-	41,41,41	2.74	7 (17%)	56,56,56	6.78	24 (42%)
14	BCR	B	4004	-	41,41,41	2.76	6 (14%)	56,56,56	6.37	26 (46%)
15	CLA	A	1118	-	40,54,73	2.87	14 (35%)	44,90,113	2.39	12 (27%)
15	CLA	B	1204	-	40,54,73	2.89	15 (37%)	44,90,113	2.38	13 (29%)
12	LHG	A	5005	-	35,35,48	1.08	2 (5%)	38,41,54	1.14	4 (10%)
15	CLA	B	1227	-	36,53,73	2.82	15 (41%)	39,89,113	2.48	11 (28%)
15	CLA	A	1022	19	59,73,73	2.35	16 (27%)	67,113,113	2.18	15 (22%)
15	CLA	J	1302	7	36,53,73	2.86	15 (41%)	39,89,113	2.39	10 (25%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
15	CLA	B	1207	-	40,54,73	2.89	15 (37%)	44,90,113	2.39	13 (29%)
15	CLA	F	1410	6	59,73,73	2.34	16 (27%)	67,113,113	2.17	15 (22%)
15	CLA	A	1134	1	40,54,73	2.91	16 (40%)	44,90,113	2.26	11 (25%)
15	CLA	A	1114	-	43,57,73	2.75	15 (34%)	46,93,113	2.46	14 (30%)
15	CLA	A	1110	-	48,62,73	2.55	15 (31%)	53,99,113	2.32	15 (28%)
15	CLA	B	1220	-	50,64,73	2.61	16 (32%)	56,102,113	2.23	16 (28%)
15	CLA	B	1240	12	36,53,73	2.90	15 (41%)	39,89,113	2.30	11 (28%)
15	CLA	B	1225	-	59,73,73	2.33	16 (27%)	67,113,113	2.20	16 (23%)
15	CLA	A	1128	-	59,73,73	2.30	15 (25%)	67,113,113	2.24	18 (26%)
10	PQN	B	2002	-	34,34,34	1.59	2 (5%)	42,45,45	1.13	4 (9%)
15	CLA	A	1105	-	59,73,73	2.35	16 (27%)	67,113,113	2.12	15 (22%)
14	BCR	B	4017	-	41,41,41	2.73	6 (14%)	56,56,56	6.59	25 (44%)
15	CLA	B	1209	-	36,53,73	2.87	14 (38%)	39,89,113	2.45	12 (30%)
15	CLA	B	1234	-	59,73,73	2.34	15 (25%)	67,113,113	2.13	16 (23%)
15	CLA	A	1124	-	49,63,73	2.58	16 (32%)	55,101,113	2.29	16 (29%)
15	CLA	A	1121	-	40,54,73	2.91	16 (40%)	44,90,113	2.37	12 (27%)
15	CLA	A	1104	-	59,73,73	2.30	15 (25%)	67,113,113	2.14	15 (22%)
15	CLA	B	1203	-	59,73,73	2.31	15 (25%)	67,113,113	2.16	13 (19%)
15	CLA	B	1217	-	41,55,73	2.77	16 (39%)	45,91,113	2.48	13 (28%)
15	CLA	B	1218	-	45,59,73	2.68	16 (35%)	50,96,113	2.63	17 (34%)
15	CLA	B	1201	-	40,54,73	2.89	16 (40%)	44,90,113	2.43	13 (29%)
12	LHG	A	5001	-	48,48,48	0.93	2 (4%)	51,54,54	1.06	3 (5%)
16	LMU	B	1301	-	36,36,36	0.44	0	47,47,47	0.88	4 (8%)
11	SF4	C	3002	3	0,12,12	0.00	-	-		
14	BCR	B	4009	-	41,41,41	2.75	7 (17%)	56,56,56	6.76	25 (44%)
15	CLA	A	1137	-	44,58,73	2.72	16 (36%)	49,95,113	2.47	13 (26%)
14	BCR	B	4005	-	41,41,41	2.75	6 (14%)	56,56,56	6.44	23 (41%)
15	CLA	B	1232	-	36,53,73	2.84	15 (41%)	39,89,113	2.37	10 (25%)
15	CLA	A	1138	-	59,73,73	2.39	15 (25%)	67,113,113	2.03	17 (25%)
15	CLA	B	1222	-	50,64,73	2.53	16 (32%)	56,102,113	2.39	16 (28%)
15	CLA	A	1101	-	59,73,73	2.34	15 (25%)	67,113,113	2.26	18 (26%)
15	CLA	A	1115	-	40,54,73	2.89	15 (37%)	44,90,113	2.34	13 (29%)
15	CLA	A	1123	-	59,73,73	2.35	15 (25%)	67,113,113	2.21	17 (25%)
15	CLA	F	1139	19	59,73,73	2.32	16 (27%)	67,113,113	2.11	12 (17%)
15	CLA	B	1224	-	59,73,73	2.34	15 (25%)	67,113,113	2.12	13 (19%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
15	CLA	B	1205	-	49,63,73	2.55	15 (30%)	55,101,113	2.48	15 (27%)
14	BCR	F	4015	-	41,41,41	2.76	7 (17%)	56,56,56	6.64	26 (46%)
15	CLA	A	1126	-	59,73,73	2.34	16 (27%)	67,113,113	2.15	20 (29%)
15	CLA	A	1801	12	46,60,73	2.68	16 (34%)	51,97,113	2.53	18 (35%)
15	CLA	B	1236	-	44,58,73	2.70	15 (34%)	49,95,113	2.39	15 (30%)
15	CLA	B	1212	-	36,53,73	2.88	15 (41%)	39,89,113	2.41	10 (25%)
15	CLA	B	1238	19	38,52,73	2.79	15 (39%)	40,87,113	2.24	10 (25%)
15	CLA	A	1120	-	43,57,73	2.75	15 (34%)	46,93,113	2.53	15 (32%)
14	BCR	F	4016	-	41,41,41	2.74	6 (14%)	56,56,56	6.73	23 (41%)
14	BCR	B	4011	-	41,41,41	2.77	6 (14%)	56,56,56	6.73	23 (41%)
15	CLA	B	1219	-	49,63,73	2.61	16 (32%)	55,101,113	2.39	15 (27%)
14	BCR	B	4014	-	41,41,41	2.75	6 (14%)	56,56,56	6.67	21 (37%)
15	CLA	A	1116	-	48,62,73	2.60	16 (33%)	53,99,113	2.38	17 (32%)
15	CLA	A	1122	-	59,73,73	2.34	16 (27%)	67,113,113	2.06	16 (23%)
17	LMG	B	5002	-	55,55,55	0.91	2 (3%)	63,63,63	0.98	2 (3%)
15	CLA	A	1127	-	59,73,73	2.34	16 (27%)	67,113,113	2.22	17 (25%)
15	CLA	A	1107	1	44,58,73	2.69	16 (36%)	49,95,113	2.42	18 (36%)
15	CLA	B	1023	-	59,73,73	2.31	15 (25%)	67,113,113	2.06	17 (25%)
14	BCR	B	4006	-	41,41,41	2.84	6 (14%)	56,56,56	6.69	24 (42%)
15	CLA	A	1135	-	49,63,73	2.58	15 (30%)	55,101,113	2.38	16 (29%)
14	BCR	J	4013	-	41,41,41	2.73	6 (14%)	56,56,56	6.62	28 (50%)
15	CLA	A	1119	-	58,72,73	2.37	16 (27%)	65,111,113	2.11	15 (23%)
15	CLA	B	1239	-	40,54,73	2.90	15 (37%)	44,90,113	2.49	12 (27%)
15	CLA	B	1230	-	59,73,73	2.32	15 (25%)	67,113,113	2.29	16 (23%)
15	CLA	K	1401	-	40,54,73	2.90	15 (37%)	44,90,113	2.38	14 (31%)
14	BCR	A	4012	-	41,41,41	2.81	6 (14%)	56,56,56	6.21	24 (42%)
15	CLA	B	1228	-	59,73,73	2.36	16 (27%)	67,113,113	1.98	13 (19%)
15	CLA	B	1214	-	59,73,73	2.34	16 (27%)	67,113,113	2.14	17 (25%)
15	CLA	A	1133	-	40,54,73	2.89	15 (37%)	44,90,113	2.38	12 (27%)
15	CLA	A	1117	-	59,73,73	2.36	16 (27%)	67,113,113	2.04	15 (22%)
15	CLA	J	1303	-	40,54,73	2.92	16 (40%)	44,90,113	2.38	12 (27%)
15	CLA	B	1208	-	36,53,73	2.89	14 (38%)	39,89,113	2.31	9 (23%)
15	CLA	A	1131	-	49,63,73	2.59	15 (30%)	55,101,113	2.39	16 (29%)
10	PQN	A	2001	-	34,34,34	1.60	2 (5%)	42,45,45	1.05	4 (9%)
15	CLA	A	1111	-	54,68,73	2.44	15 (27%)	61,107,113	2.16	15 (24%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
15	CLA	A	1136	-	59,73,73	2.33	15 (25%)	67,113,113	2.21	16 (23%)
15	CLA	B	1226	-	59,73,73	2.32	15 (25%)	67,113,113	2.22	14 (20%)
15	CLA	B	1221	-	59,73,73	2.34	16 (27%)	67,113,113	2.24	14 (20%)
15	CLA	B	1202	-	59,73,73	2.35	16 (27%)	67,113,113	2.14	14 (20%)
14	BCR	A	4003	-	41,41,41	2.74	6 (14%)	56,56,56	6.51	25 (44%)
14	BCR	B	4010	-	41,41,41	2.73	6 (14%)	56,56,56	6.65	23 (41%)
13	CL0	A	1108	-	36,53,73	2.86	15 (41%)	39,89,113	2.49	14 (35%)
15	CLA	A	1102	15	59,73,73	2.36	16 (27%)	67,113,113	2.12	15 (22%)
15	CLA	B	1211	-	40,54,73	2.89	16 (40%)	44,90,113	2.35	13 (29%)
15	CLA	B	1021	-	59,73,73	2.34	16 (27%)	67,113,113	2.27	21 (31%)
12	LHG	A	5003	15	48,48,48	0.95	2 (4%)	51,54,54	1.09	4 (7%)
15	CLA	B	1235	-	59,73,73	2.33	15 (25%)	67,113,113	2.12	15 (22%)
15	CLA	A	1112	-	36,53,73	2.87	15 (41%)	39,89,113	2.38	11 (28%)
15	CLA	B	1216	-	59,73,73	2.35	16 (27%)	67,113,113	2.00	15 (22%)
14	BCR	A	4002	-	41,41,41	2.76	6 (14%)	56,56,56	6.49	25 (44%)
11	SF4	C	3003	3	0,12,12	0.00	-	-	-	-
15	CLA	A	1132	-	56,70,73	2.39	16 (28%)	63,109,113	2.22	14 (22%)
15	CLA	A	1113	-	36,53,73	2.87	14 (38%)	39,89,113	2.32	12 (30%)
15	CLA	B	1206	2	40,54,73	2.91	16 (40%)	44,90,113	2.35	15 (34%)
15	CLA	A	1140	-	59,73,73	2.34	15 (25%)	67,113,113	2.06	14 (20%)
15	CLA	A	1012	19	59,73,73	2.37	16 (27%)	67,113,113	2.30	17 (25%)
15	CLA	A	1125	-	46,60,73	2.62	15 (32%)	51,97,113	2.51	18 (35%)
15	CLA	B	1237	19	49,63,73	2.57	16 (32%)	55,101,113	2.32	15 (27%)
14	BCR	A	4007	-	41,41,41	2.73	6 (14%)	56,56,56	6.72	25 (44%)
15	CLA	A	1129	-	40,54,73	2.87	15 (37%)	44,90,113	2.44	14 (31%)
12	LHG	B	5004	15	48,48,48	0.94	2 (4%)	51,54,54	1.14	4 (7%)
15	CLA	B	1013	-	59,73,73	2.32	14 (23%)	67,113,113	2.22	19 (28%)
15	CLA	B	1223	-	59,73,73	2.33	15 (25%)	67,113,113	2.17	15 (22%)
13	CL0	A	1011	-	59,73,73	2.30	14 (23%)	67,113,113	2.26	15 (22%)
16	LMU	J	1304	-	36,36,36	0.42	0	47,47,47	0.63	1 (2%)
15	CLA	A	1109	15	59,73,73	2.36	15 (25%)	67,113,113	2.20	18 (26%)
15	CLA	B	1229	-	59,73,73	2.33	15 (25%)	67,113,113	2.12	13 (19%)
15	CLA	B	1231	-	59,73,73	2.33	15 (25%)	67,113,113	2.16	15 (22%)
14	BCR	A	4001	-	41,41,41	2.77	6 (14%)	56,56,56	6.28	25 (44%)
15	CLA	F	1301	-	36,53,73	2.86	15 (41%)	39,89,113	2.32	10 (25%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
11	SF4	A	3001	1,2	0,12,12	0.00	-	-		
15	CLA	K	1402	-	40,54,73	2.90	16 (40%)	44,90,113	2.33	12 (27%)
15	CLA	A	1103	-	59,73,73	2.32	15 (25%)	67,113,113	2.10	16 (23%)
15	CLA	A	1106	1	59,73,73	2.35	16 (27%)	67,113,113	2.20	15 (22%)
15	CLA	A	1130	-	49,63,73	2.58	16 (32%)	55,101,113	2.22	14 (25%)
15	CLA	B	1215	-	59,73,73	2.36	15 (25%)	67,113,113	2.30	18 (26%)
15	CLA	B	1210	-	59,73,73	2.34	15 (25%)	67,113,113	2.09	14 (20%)

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
15	CLA	B	1213	-	2/2/17/25	7/19/117/135	-
14	BCR	A	4008	-	-	10/29/63/63	0/2/2/2
14	BCR	B	4004	-	-	12/29/63/63	0/2/2/2
15	CLA	A	1118	-	3/3/16/25	9/15/113/135	-
15	CLA	B	1204	-	3/3/16/25	5/15/113/135	-
12	LHG	A	5005	-	-	25/40/40/53	-
15	CLA	B	1227	-	2/2/16/25	2/11/111/135	-
15	CLA	A	1022	19	2/2/20/25	9/37/135/135	-
15	CLA	J	1302	7	3/3/16/25	4/11/111/135	-
15	CLA	B	1207	-	3/3/16/25	9/15/113/135	-
15	CLA	F	1410	6	2/2/20/25	17/37/135/135	-
15	CLA	A	1134	1	3/3/16/25	7/15/113/135	-
15	CLA	A	1114	-	3/3/16/25	9/18/116/135	-
15	CLA	A	1110	-	3/3/17/25	11/24/122/135	-
15	CLA	B	1220	-	3/3/18/25	9/27/125/135	-
15	CLA	B	1240	12	3/3/16/25	5/11/111/135	-
15	CLA	B	1225	-	3/3/20/25	16/37/135/135	-
15	CLA	A	1128	-	3/3/20/25	16/37/135/135	-
10	PQN	B	2002	-	-	4/23/43/43	0/2/2/2
15	CLA	A	1105	-	3/3/20/25	11/37/135/135	-
14	BCR	B	4017	-	-	8/29/63/63	0/2/2/2
15	CLA	B	1209	-	3/3/16/25	5/11/111/135	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
14	BCR	B	4011	-	-	15/29/63/63	0/2/2/2
15	CLA	B	1234	-	3/3/20/25	16/37/135/135	-
15	CLA	A	1124	-	3/3/18/25	7/25/123/135	-
15	CLA	A	1121	-	3/3/16/25	7/15/113/135	-
15	CLA	A	1104	-	3/3/20/25	14/37/135/135	-
15	CLA	B	1203	-	2/2/20/25	13/37/135/135	-
15	CLA	B	1217	-	3/3/16/25	7/16/114/135	-
15	CLA	B	1218	-	3/3/17/25	11/21/119/135	-
12	LHG	A	5001	-	-	29/53/53/53	-
16	LMU	B	1301	-	-	15/21/61/61	0/2/2/2
11	SF4	C	3002	3	-	-	0/6/5/5
14	BCR	B	4009	-	-	13/29/63/63	0/2/2/2
15	CLA	A	1137	-	3/3/17/25	9/19/117/135	-
14	BCR	B	4005	-	-	10/29/63/63	0/2/2/2
15	CLA	B	1232	-	3/3/16/25	4/11/111/135	-
15	CLA	A	1138	-	3/3/20/25	7/37/135/135	-
15	CLA	B	1222	-	2/2/18/25	10/27/125/135	-
15	CLA	A	1101	-	3/3/20/25	14/37/135/135	-
15	CLA	A	1115	-	3/3/16/25	7/15/113/135	-
15	CLA	A	1123	-	3/3/20/25	14/37/135/135	-
15	CLA	F	1139	19	3/3/20/25	12/37/135/135	-
15	CLA	B	1224	-	3/3/20/25	13/37/135/135	-
15	CLA	B	1205	-	3/3/18/25	10/25/123/135	-
14	BCR	F	4015	-	-	10/29/63/63	0/2/2/2
15	CLA	A	1126	-	1/1/20/25	9/37/135/135	-
15	CLA	A	1801	12	3/3/17/25	11/22/120/135	-
15	CLA	B	1236	-	2/2/17/25	5/19/117/135	-
15	CLA	B	1212	-	3/3/16/25	5/11/111/135	-
15	CLA	B	1238	19	3/3/15/25	4/11/110/135	-
15	CLA	A	1120	-	3/3/16/25	8/18/116/135	-
14	BCR	F	4016	-	-	15/29/63/63	0/2/2/2
15	CLA	B	1228	-	3/3/20/25	18/37/135/135	-
15	CLA	B	1219	-	3/3/18/25	9/25/123/135	-
14	BCR	B	4014	-	-	14/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
15	CLA	A	1116	-	3/3/17/25	7/24/122/135	-
15	CLA	A	1122	-	3/3/20/25	20/37/135/135	-
17	LMG	B	5002	-	-	30/50/70/70	0/1/1/1
15	CLA	A	1127	-	3/3/20/25	18/37/135/135	-
15	CLA	A	1107	1	2/2/17/25	6/19/117/135	-
15	CLA	B	1023	-	3/3/20/25	14/37/135/135	-
15	CLA	B	1237	19	3/3/18/25	10/25/123/135	-
15	CLA	A	1135	-	3/3/18/25	11/25/123/135	-
14	BCR	J	4013	-	-	13/29/63/63	0/2/2/2
15	CLA	A	1119	-	2/2/19/25	15/35/133/135	-
15	CLA	B	1239	-	3/3/16/25	8/15/113/135	-
15	CLA	B	1230	-	3/3/20/25	16/37/135/135	-
15	CLA	K	1401	-	3/3/16/25	12/15/113/135	-
14	BCR	A	4012	-	-	12/29/63/63	0/2/2/2
15	CLA	B	1201	-	3/3/16/25	5/15/113/135	-
15	CLA	B	1214	-	2/2/20/25	12/37/135/135	-
15	CLA	A	1133	-	3/3/16/25	6/15/113/135	-
15	CLA	A	1117	-	3/3/20/25	15/37/135/135	-
15	CLA	J	1303	-	3/3/16/25	5/15/113/135	-
15	CLA	B	1208	-	3/3/16/25	4/11/111/135	-
15	CLA	A	1131	-	3/3/18/25	12/25/123/135	-
10	PQN	A	2001	-	-	8/23/43/43	0/2/2/2
15	CLA	A	1111	-	3/3/19/25	13/31/129/135	-
15	CLA	A	1136	-	3/3/20/25	18/37/135/135	-
15	CLA	B	1226	-	3/3/20/25	14/37/135/135	-
15	CLA	B	1221	-	3/3/20/25	8/37/135/135	-
15	CLA	B	1202	-	3/3/20/25	21/37/135/135	-
14	BCR	A	4003	-	-	12/29/63/63	0/2/2/2
14	BCR	B	4010	-	-	8/29/63/63	0/2/2/2
13	CL0	A	1108	-	3/3/16/25	4/11/111/135	-
15	CLA	A	1102	15	3/3/20/25	14/37/135/135	-
15	CLA	B	1211	-	3/3/16/25	8/15/113/135	-
15	CLA	B	1021	-	3/3/20/25	23/37/135/135	-
12	LHG	A	5003	15	-	24/53/53/53	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
15	CLA	B	1235	-	3/3/20/25	14/37/135/135	-
15	CLA	A	1112	-	3/3/16/25	5/11/111/135	-
15	CLA	B	1216	-	2/2/20/25	12/37/135/135	-
14	BCR	A	4002	-	-	6/29/63/63	0/2/2/2
11	SF4	C	3003	3	-	-	0/6/5/5
15	CLA	A	1132	-	3/3/19/25	14/34/132/135	-
15	CLA	A	1113	-	3/3/16/25	4/11/111/135	-
15	CLA	B	1206	2	3/3/16/25	6/15/113/135	-
15	CLA	A	1140	-	3/3/20/25	15/37/135/135	-
15	CLA	A	1012	19	2/2/20/25	16/37/135/135	-
15	CLA	A	1125	-	2/2/17/25	4/22/120/135	-
14	BCR	B	4006	-	-	12/29/63/63	0/2/2/2
14	BCR	A	4007	-	-	6/29/63/63	0/2/2/2
15	CLA	A	1129	-	3/3/16/25	11/15/113/135	-
12	LHG	B	5004	15	-	21/53/53/53	-
15	CLA	B	1013	-	2/2/20/25	16/37/135/135	-
15	CLA	B	1223	-	3/3/20/25	19/37/135/135	-
13	CL0	A	1011	-	3/3/20/25	4/37/135/135	-
16	LMU	J	1304	-	-	10/21/61/61	0/2/2/2
15	CLA	A	1109	15	2/2/20/25	14/37/135/135	-
15	CLA	B	1229	-	3/3/20/25	20/37/135/135	-
15	CLA	B	1231	-	3/3/20/25	13/37/135/135	-
14	BCR	A	4001	-	-	13/29/63/63	0/2/2/2
15	CLA	F	1301	-	3/3/16/25	2/11/111/135	-
11	SF4	A	3001	1,2	-	-	0/6/5/5
15	CLA	K	1402	-	3/3/16/25	6/15/113/135	-
15	CLA	A	1103	-	3/3/20/25	17/37/135/135	-
15	CLA	A	1106	1	3/3/20/25	15/37/135/135	-
15	CLA	A	1130	-	3/3/18/25	10/25/123/135	-
15	CLA	B	1215	-	2/2/20/25	15/37/135/135	-
15	CLA	B	1210	-	3/3/20/25	17/37/135/135	-

The worst 5 of 1533 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	A	1123	CLA	MG-NA	9.66	2.29	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	A	1108	CL0	MG-NA	9.62	2.29	2.06
15	B	1220	CLA	MG-NA	9.61	2.29	2.06
15	A	1138	CLA	MG-NA	9.59	2.29	2.06
15	B	1221	CLA	MG-NA	9.58	2.29	2.06

The worst 5 of 1779 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	B	4009	BCR	C16-C17-C18	26.76	165.49	127.31
14	F	4016	BCR	C20-C21-C22	25.34	163.47	127.31
14	B	4006	BCR	C20-C21-C22	23.95	161.49	127.31
14	A	4008	BCR	C20-C21-C22	23.24	160.48	127.31
14	A	4007	BCR	C20-C21-C22	23.24	160.48	127.31

5 of 258 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
15	B	1213	CLA	NC
15	B	1213	CLA	NA
15	A	1118	CLA	NC
15	A	1118	CLA	ND
15	A	1118	CLA	NA

5 of 1338 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
14	A	4008	BCR	C11-C10-C9-C8
14	A	4008	BCR	C11-C10-C9-C34
14	A	4008	BCR	C10-C11-C12-C13
14	B	4004	BCR	C1-C6-C7-C8
14	B	4004	BCR	C5-C6-C7-C8

There are no ring outliers.

91 monomers are involved in 200 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
15	B	1213	CLA	1	0
14	A	4008	BCR	5	0
14	B	4004	BCR	3	0
15	A	1118	CLA	3	0
12	A	5005	LHG	10	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
15	B	1227	CLA	2	0
15	A	1022	CLA	3	0
15	J	1302	CLA	2	0
15	A	1114	CLA	2	0
15	A	1110	CLA	13	0
15	B	1220	CLA	1	0
15	A	1128	CLA	2	0
10	B	2002	PQN	3	0
15	A	1105	CLA	2	0
14	B	4017	BCR	6	0
15	A	1124	CLA	3	0
15	A	1121	CLA	2	0
15	A	1104	CLA	1	0
15	B	1203	CLA	2	0
15	B	1218	CLA	2	0
15	B	1201	CLA	1	0
12	A	5001	LHG	1	0
14	B	4009	BCR	1	0
15	A	1137	CLA	1	0
14	B	4005	BCR	1	0
15	B	1232	CLA	1	0
15	A	1138	CLA	1	0
15	B	1222	CLA	4	0
15	A	1101	CLA	3	0
15	A	1123	CLA	2	0
15	F	1139	CLA	3	0
15	B	1224	CLA	2	0
15	B	1205	CLA	1	0
14	F	4015	BCR	6	0
15	A	1126	CLA	8	0
15	A	1801	CLA	1	0
15	B	1236	CLA	3	0
15	B	1212	CLA	2	0
15	A	1120	CLA	1	0
14	F	4016	BCR	2	0
14	B	4011	BCR	7	0
14	B	4014	BCR	2	0
15	A	1122	CLA	4	0
17	B	5002	LMG	2	0
15	A	1127	CLA	4	0
15	A	1107	CLA	1	0
15	B	1023	CLA	3	0

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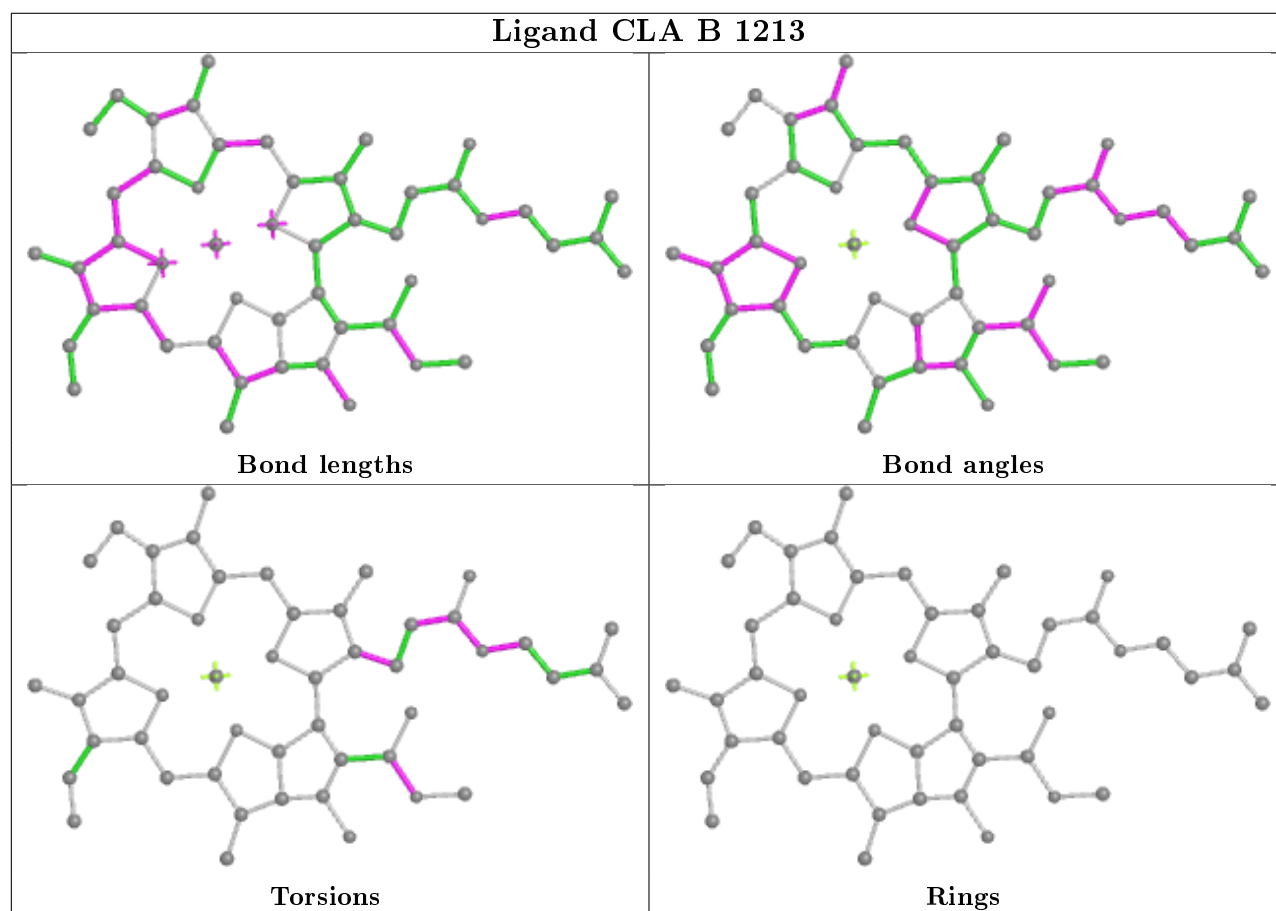
Mol	Chain	Res	Type	Clashes	Symm-Clashes
14	B	4006	BCR	1	0
15	A	1135	CLA	1	0
14	J	4013	BCR	3	0
15	A	1119	CLA	1	0
15	B	1239	CLA	2	0
15	B	1230	CLA	2	0
15	K	1401	CLA	1	0
14	A	4012	BCR	2	0
15	A	1133	CLA	2	0
15	A	1131	CLA	2	0
10	A	2001	PQN	1	0
15	A	1111	CLA	1	0
15	B	1226	CLA	3	0
15	B	1221	CLA	4	0
14	A	4003	BCR	3	0
14	B	4010	BCR	5	0
13	A	1108	CL0	3	0
15	A	1102	CLA	3	0
15	B	1211	CLA	2	0
15	B	1021	CLA	2	0
12	A	5003	LHG	7	0
15	B	1235	CLA	4	0
15	A	1112	CLA	1	0
15	B	1216	CLA	2	0
14	A	4002	BCR	3	0
15	A	1113	CLA	1	0
15	B	1206	CLA	1	0
15	A	1012	CLA	2	0
15	B	1237	CLA	1	0
14	A	4007	BCR	1	0
15	A	1129	CLA	2	0
12	B	5004	LHG	2	0
15	B	1013	CLA	8	0
13	A	1011	CL0	9	0
16	J	1304	LMU	2	0
15	A	1109	CLA	3	0
15	B	1229	CLA	4	0
15	B	1231	CLA	3	0
14	A	4001	BCR	3	0
15	K	1402	CLA	1	0
15	A	1103	CLA	5	0
15	A	1106	CLA	2	0

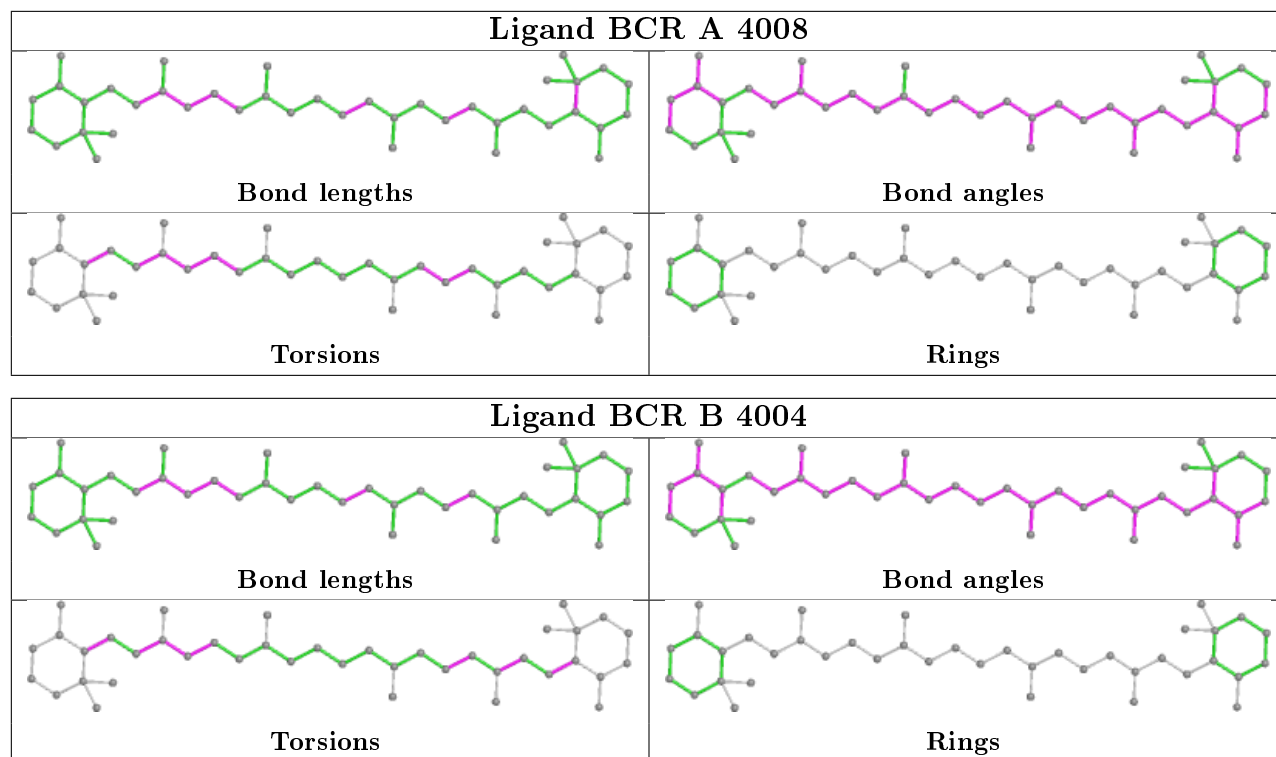
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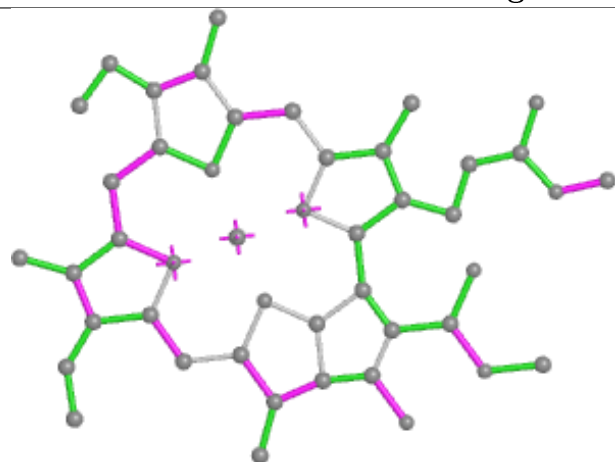
Mol	Chain	Res	Type	Clashes	Symm-Clashes
15	B	1215	CLA	4	0
15	B	1210	CLA	2	0

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

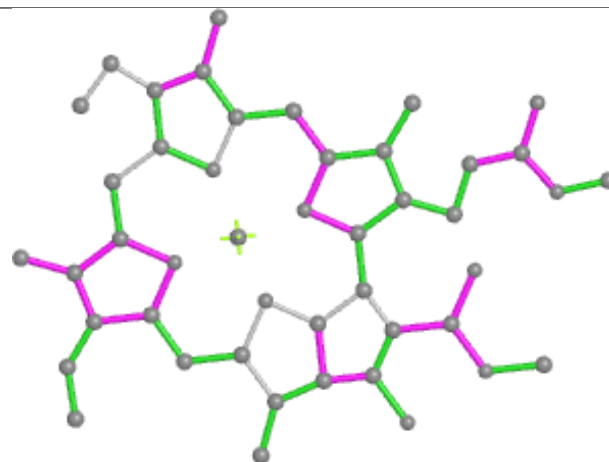




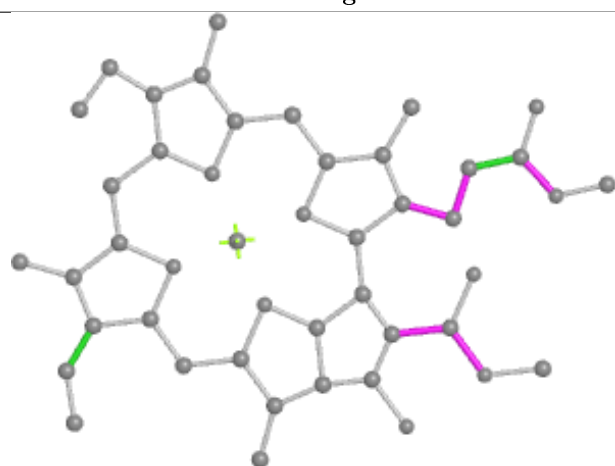
Ligand CLA A 1118



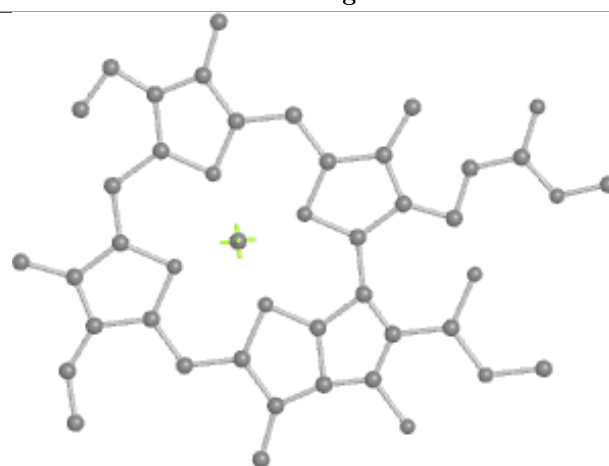
Bond lengths



Bond angles

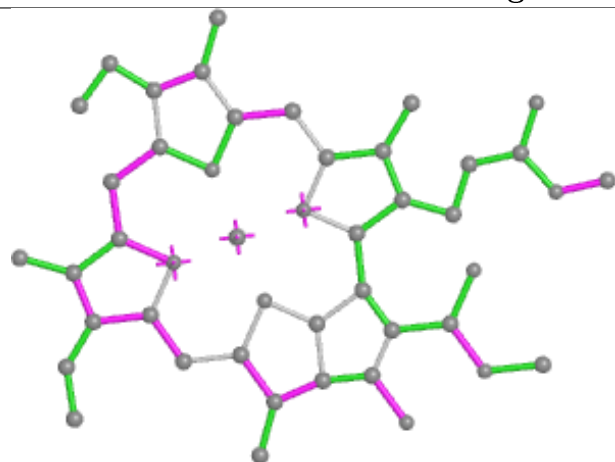


Torsions

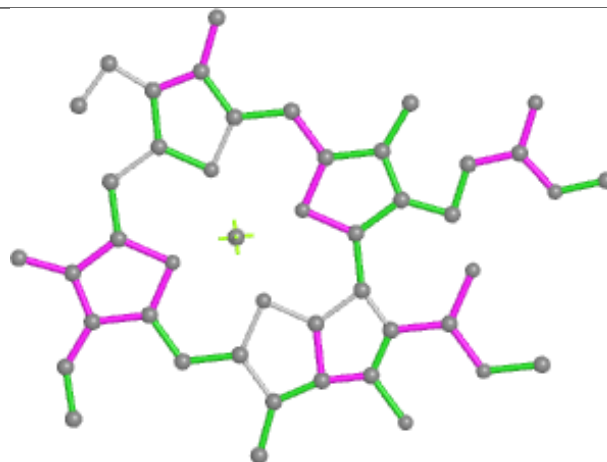


Rings

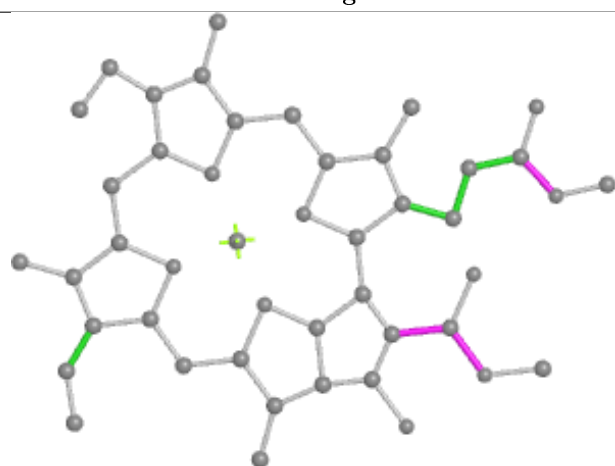
Ligand CLA B 1204



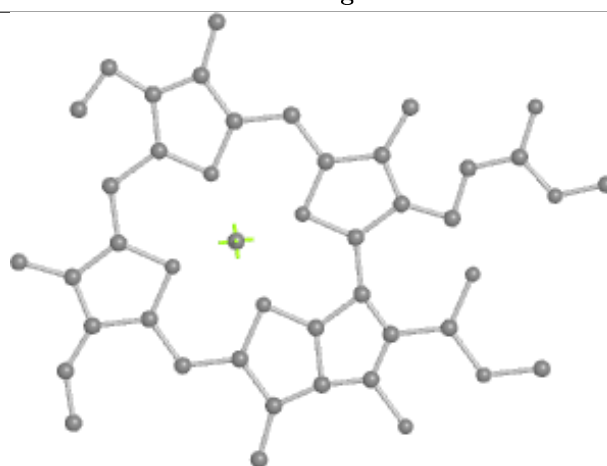
Bond lengths



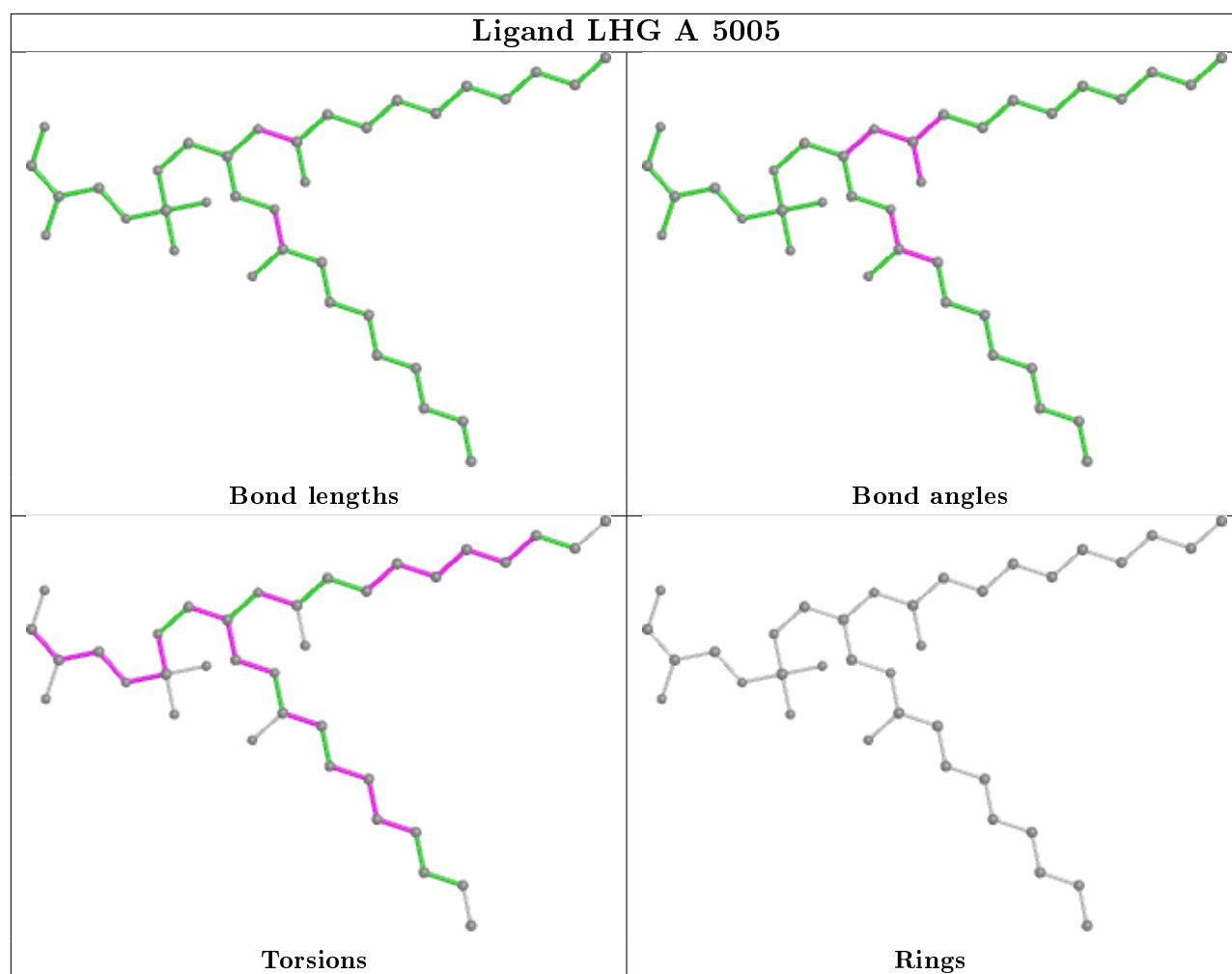
Bond angles



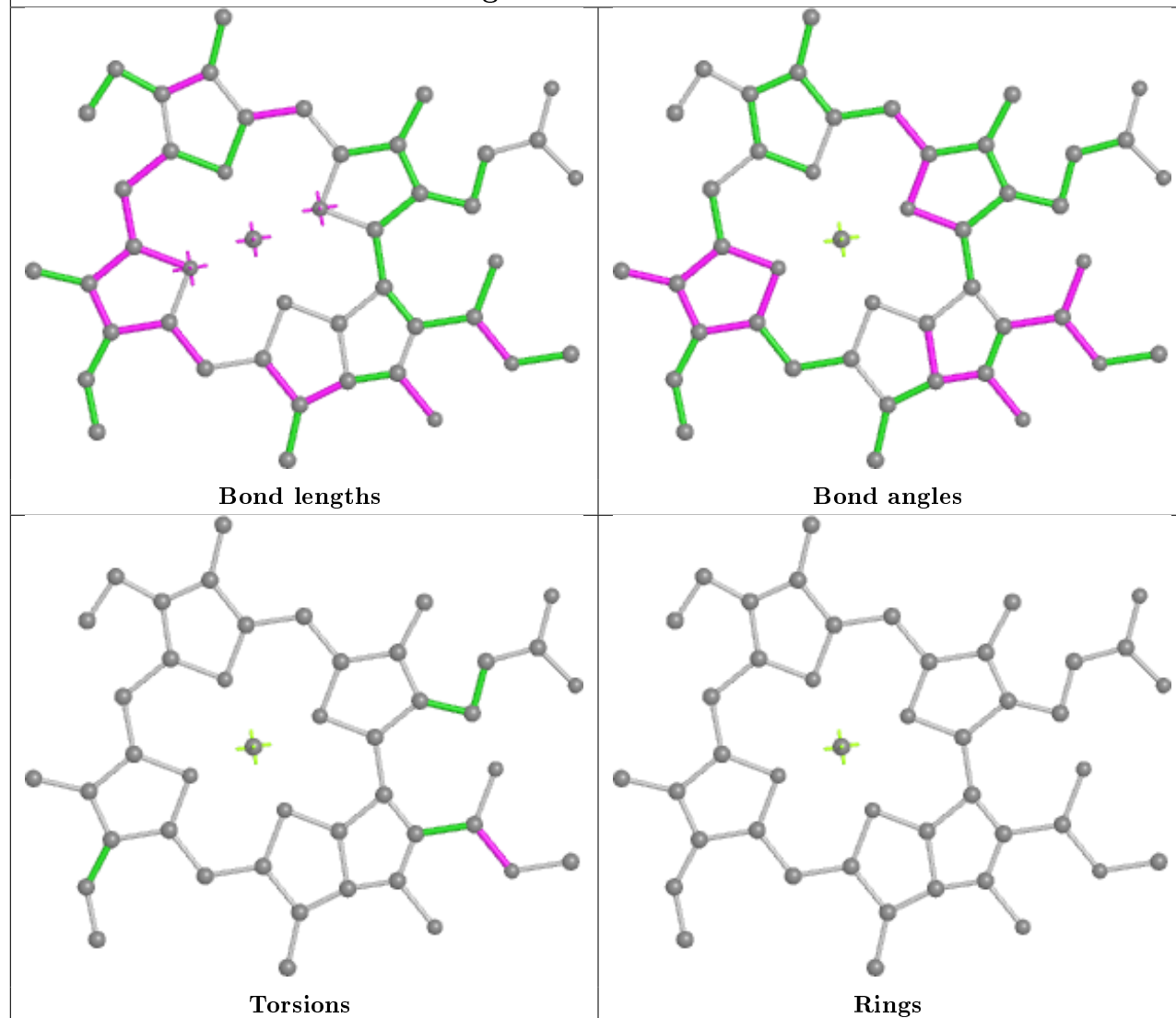
Torsions



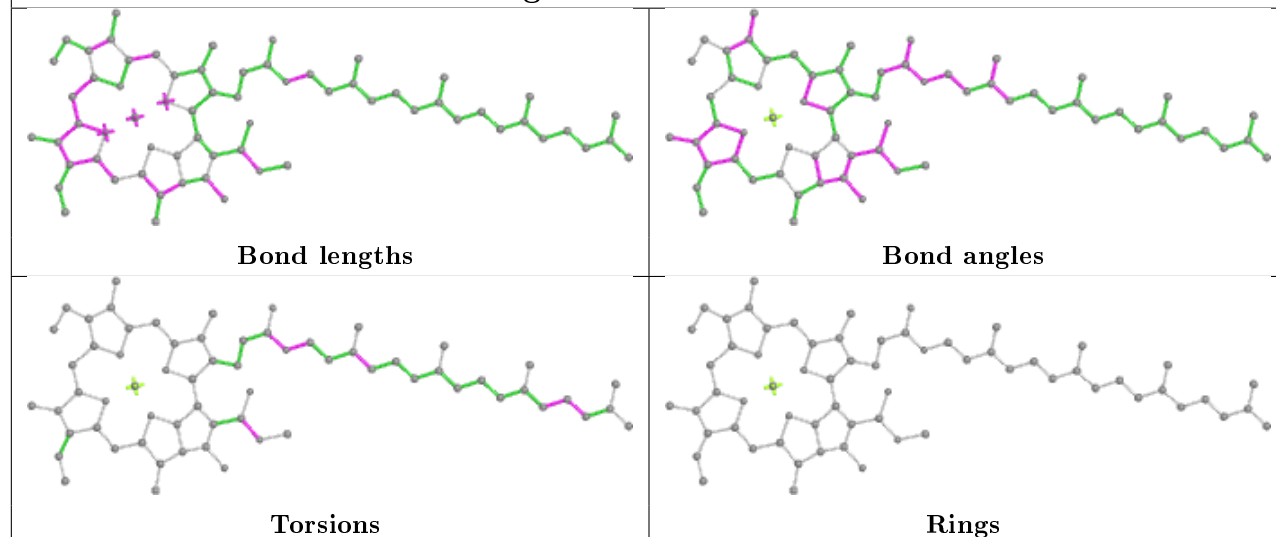
Rings

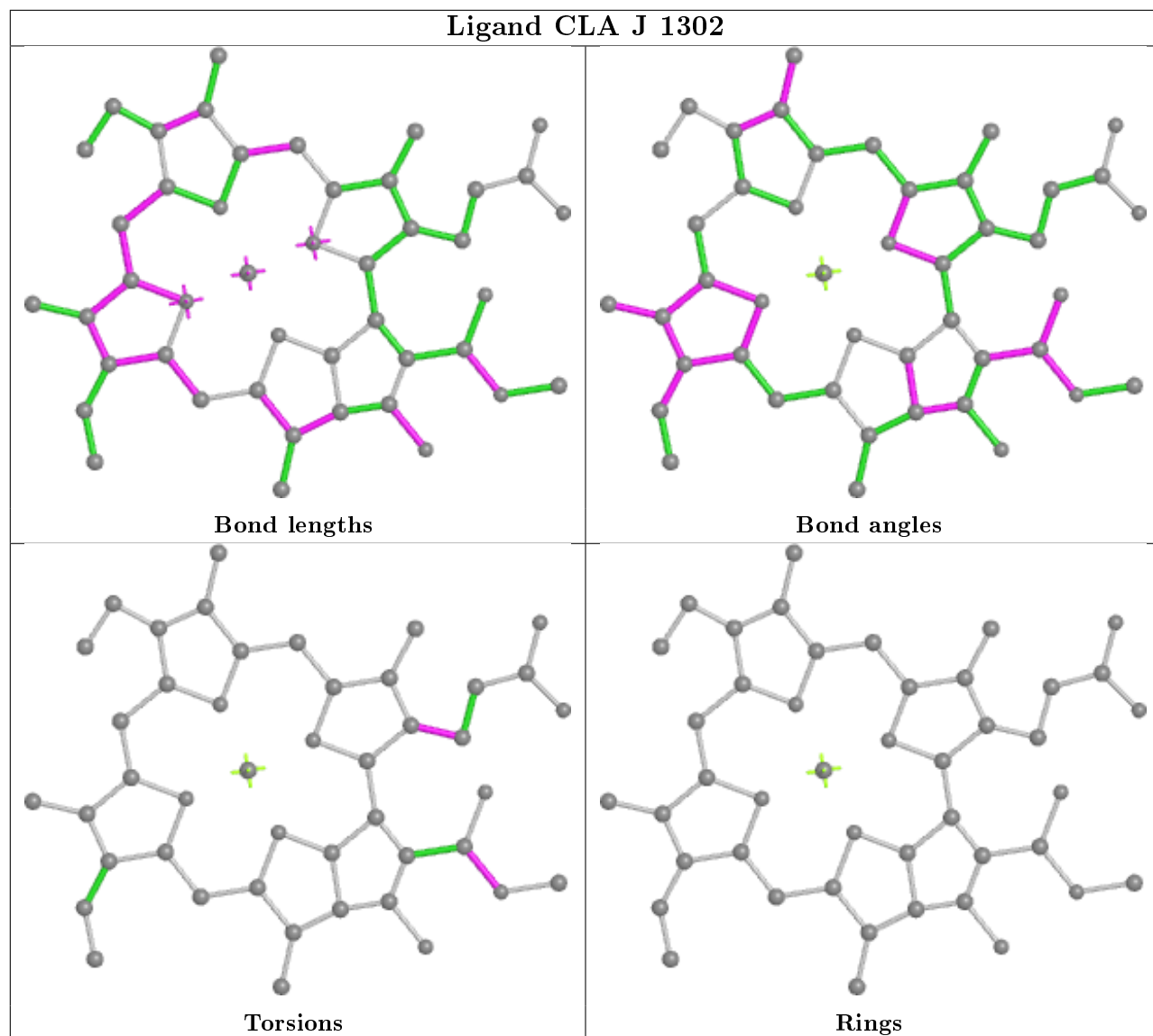


Ligand CLA B 1227

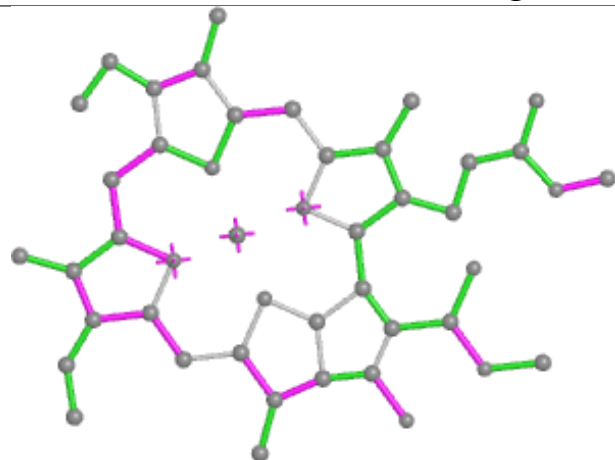


Ligand CLA A 1022

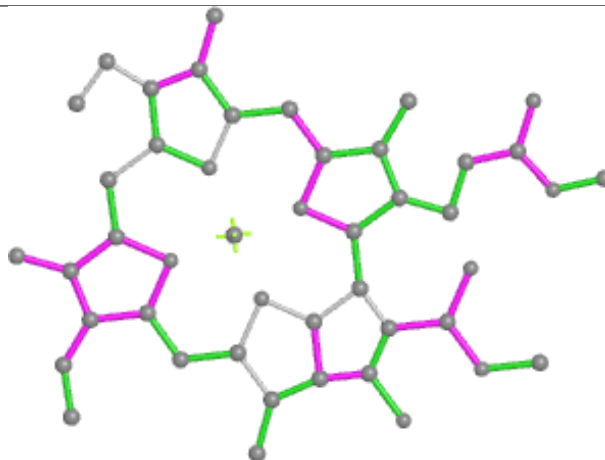




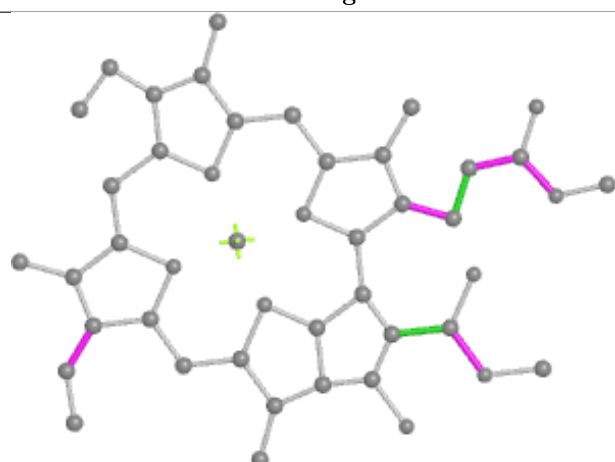
Ligand CLA B 1207



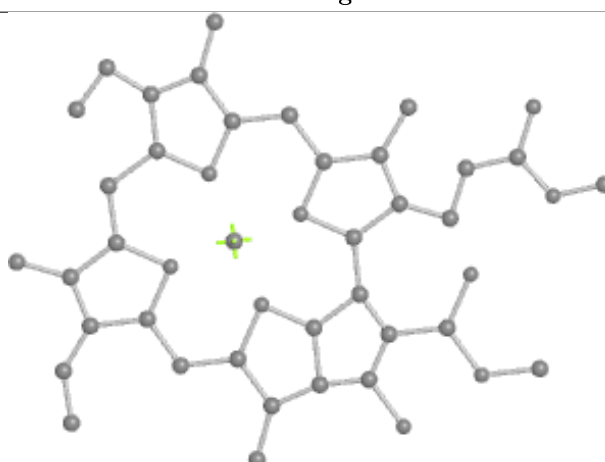
Bond lengths



Bond angles

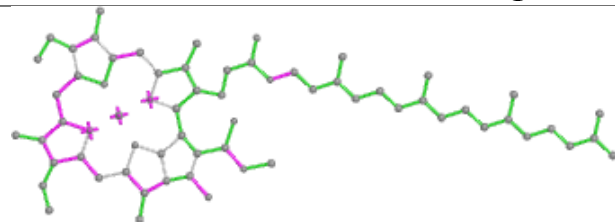


Torsions

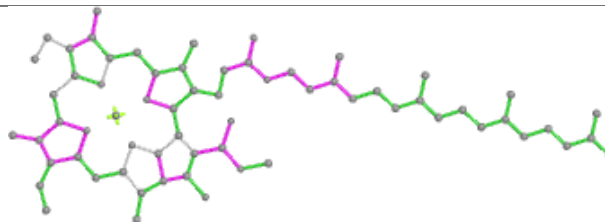


Rings

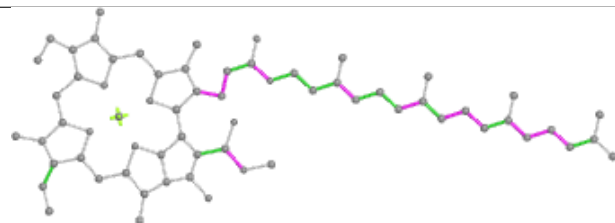
Ligand CLA F 1410



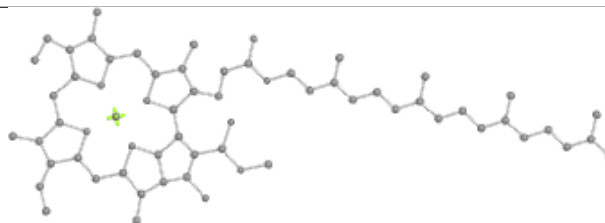
Bond lengths



Bond angles

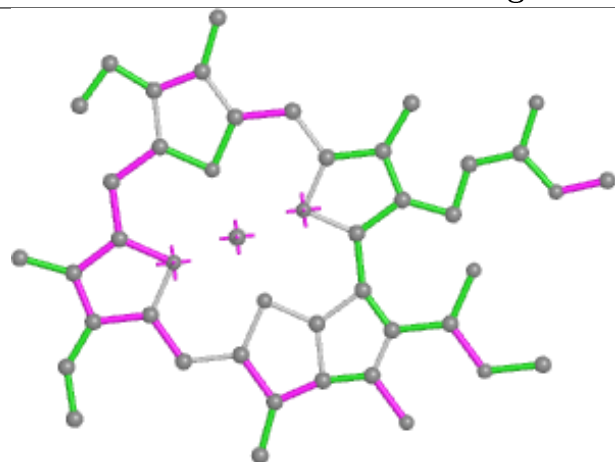


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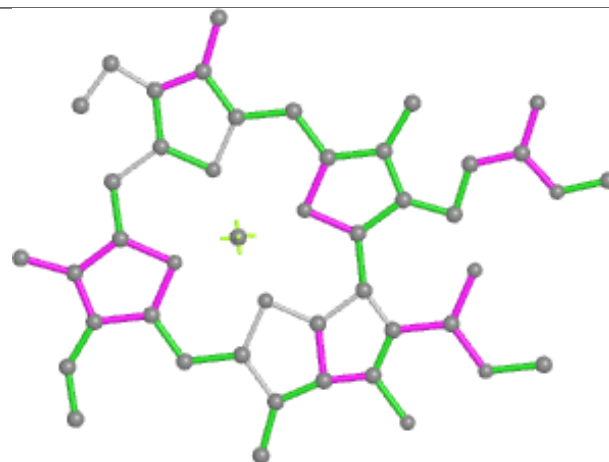


Rings

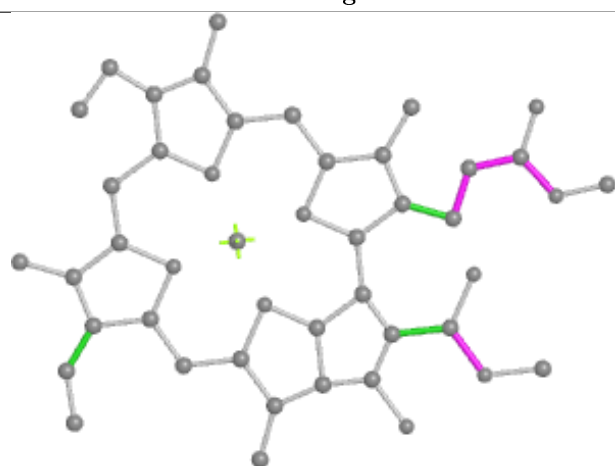
Ligand CLA A 1134



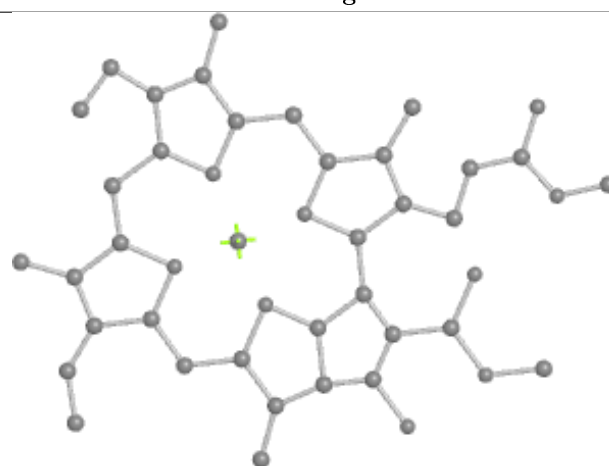
Bond lengths



Bond angles

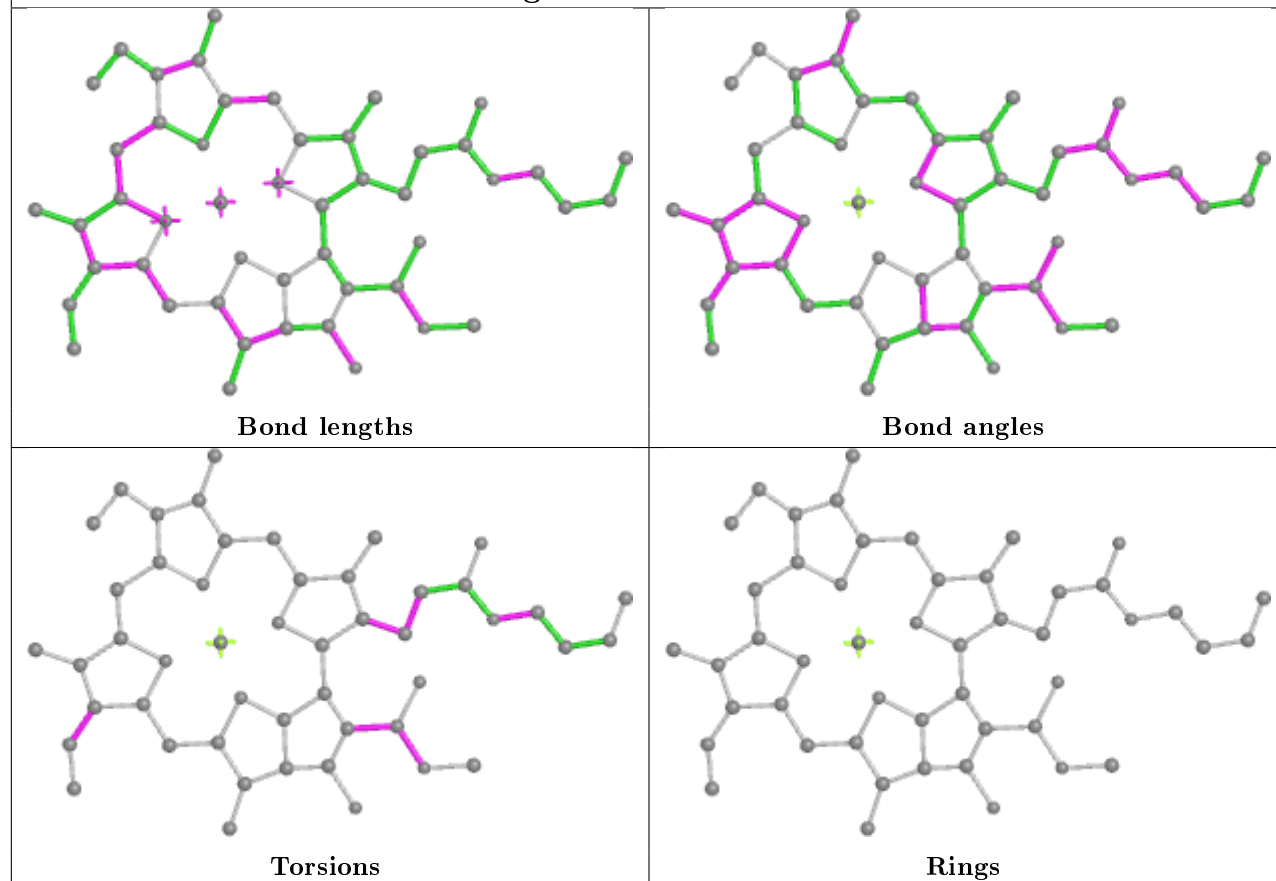


Torsions

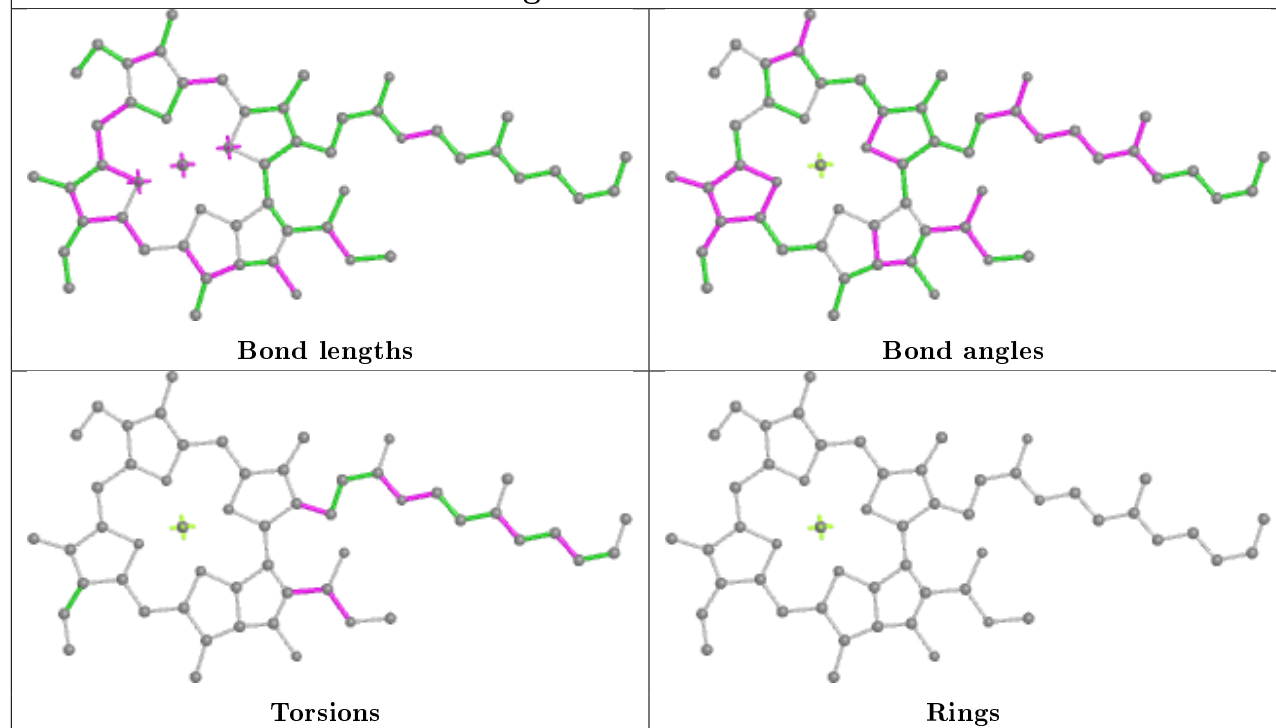


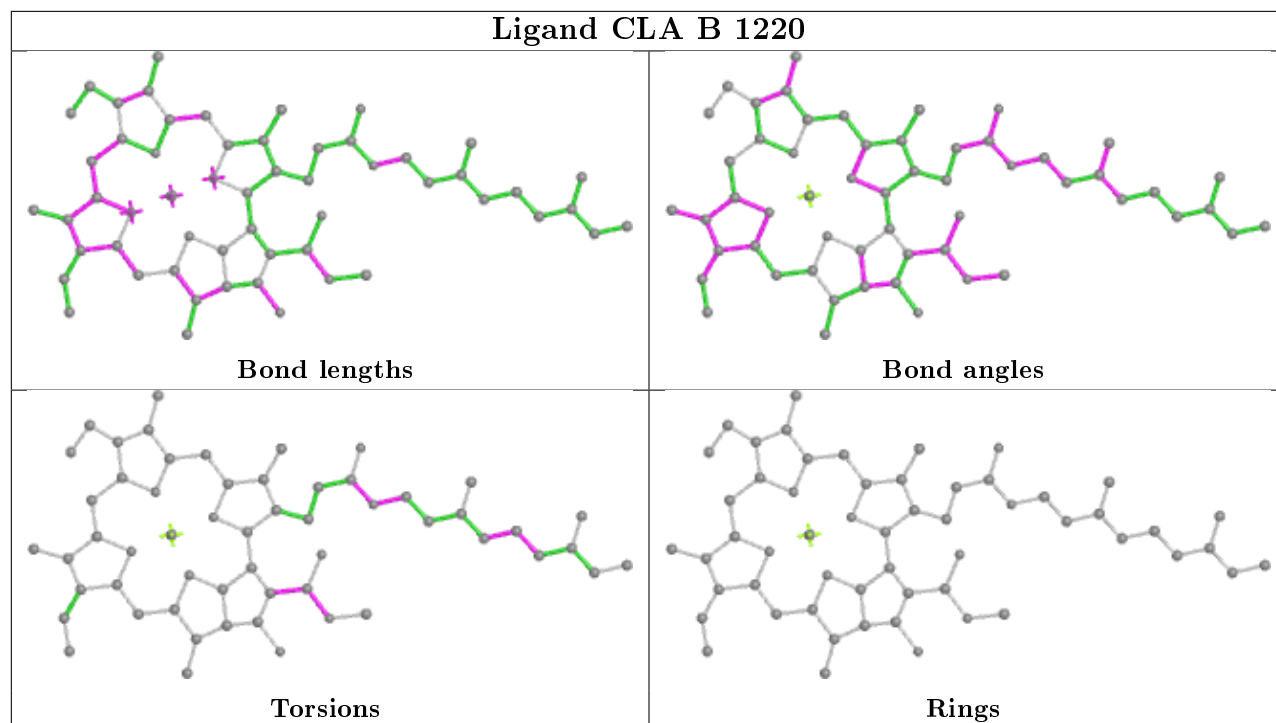
Rings

Ligand CLA A 1114

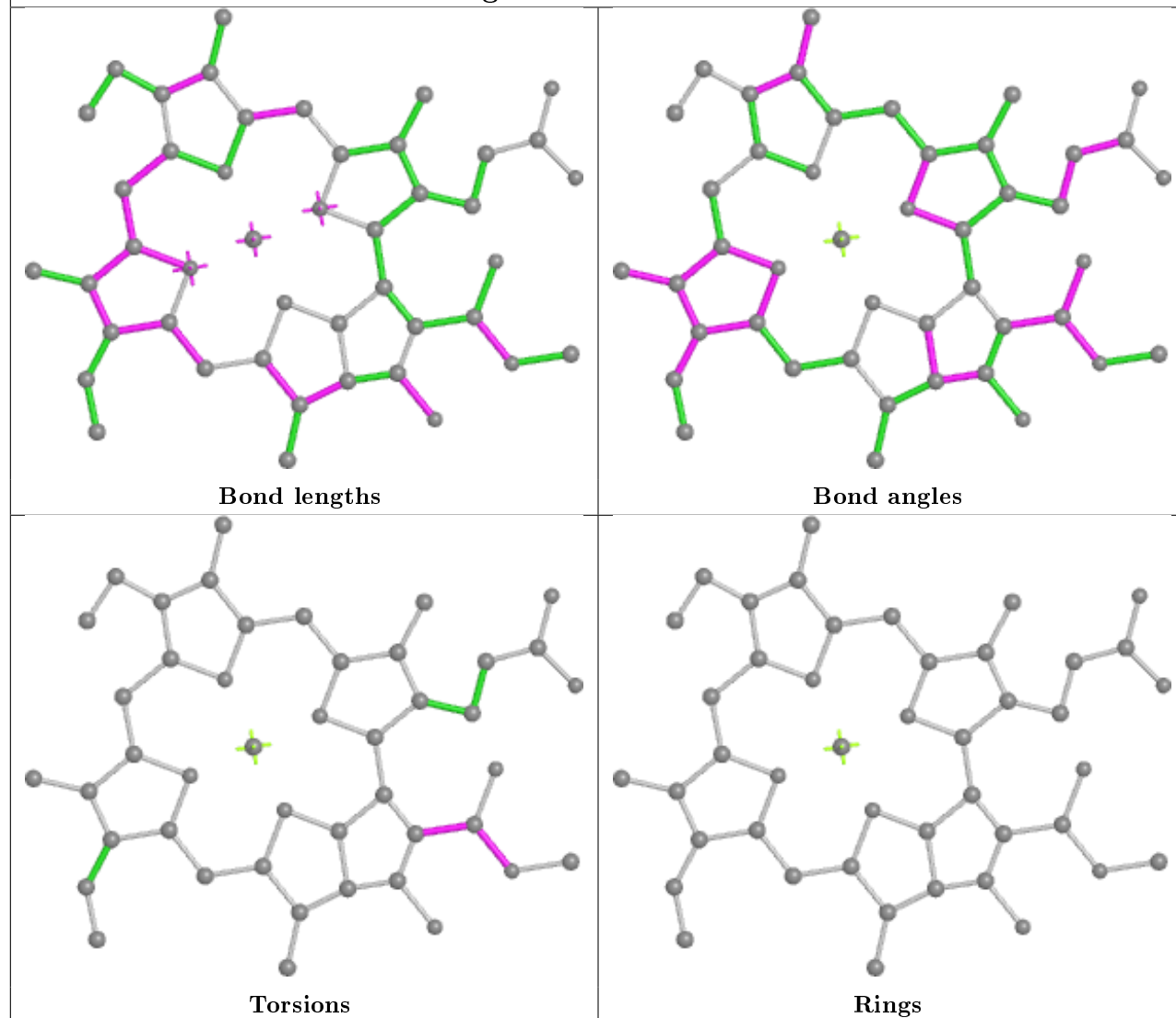


Ligand CLA A 1110

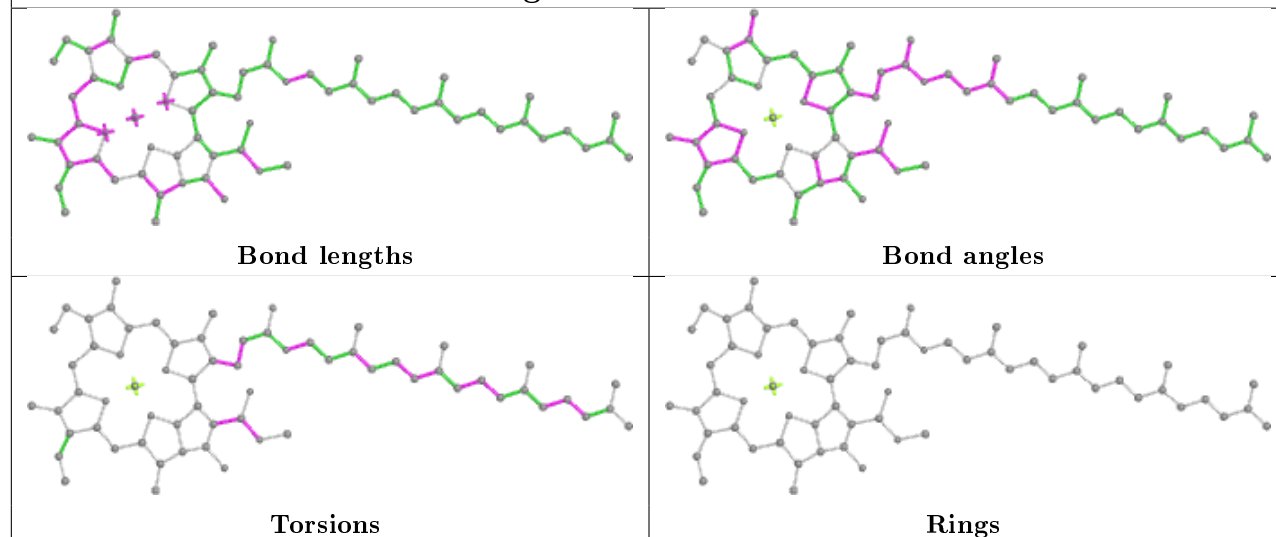


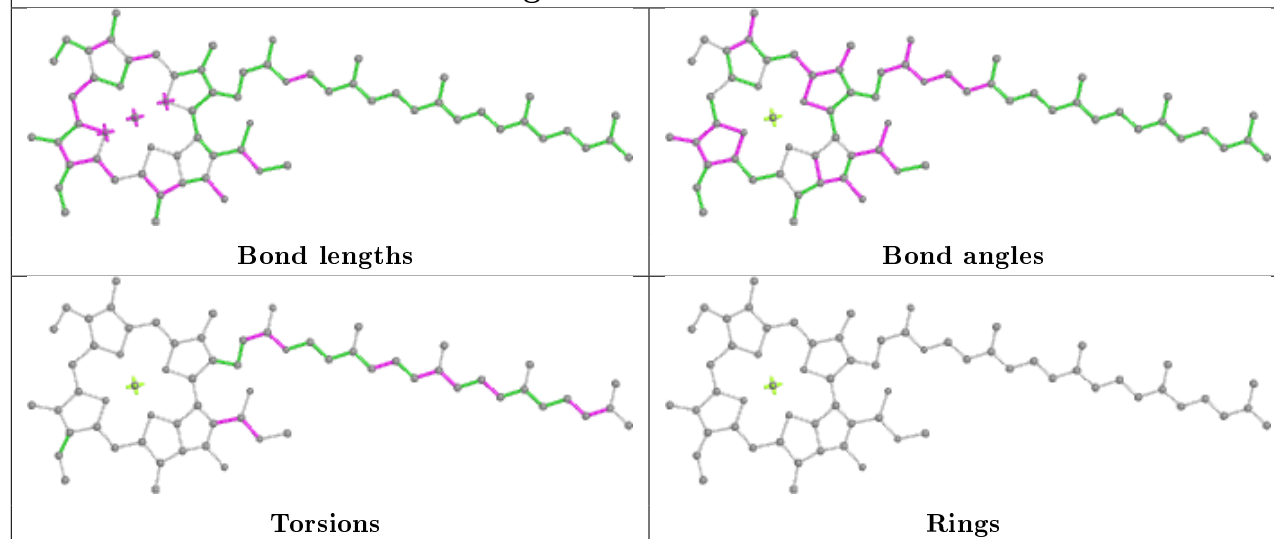
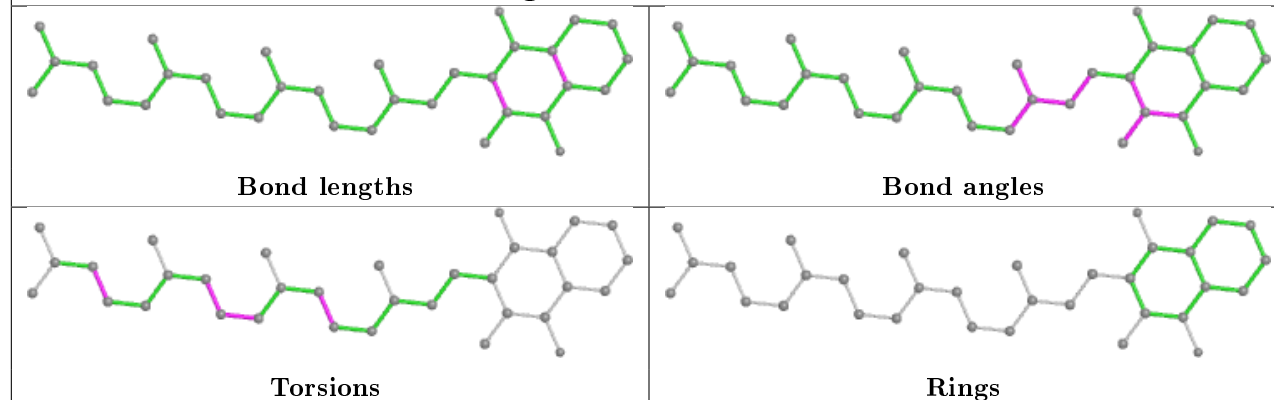
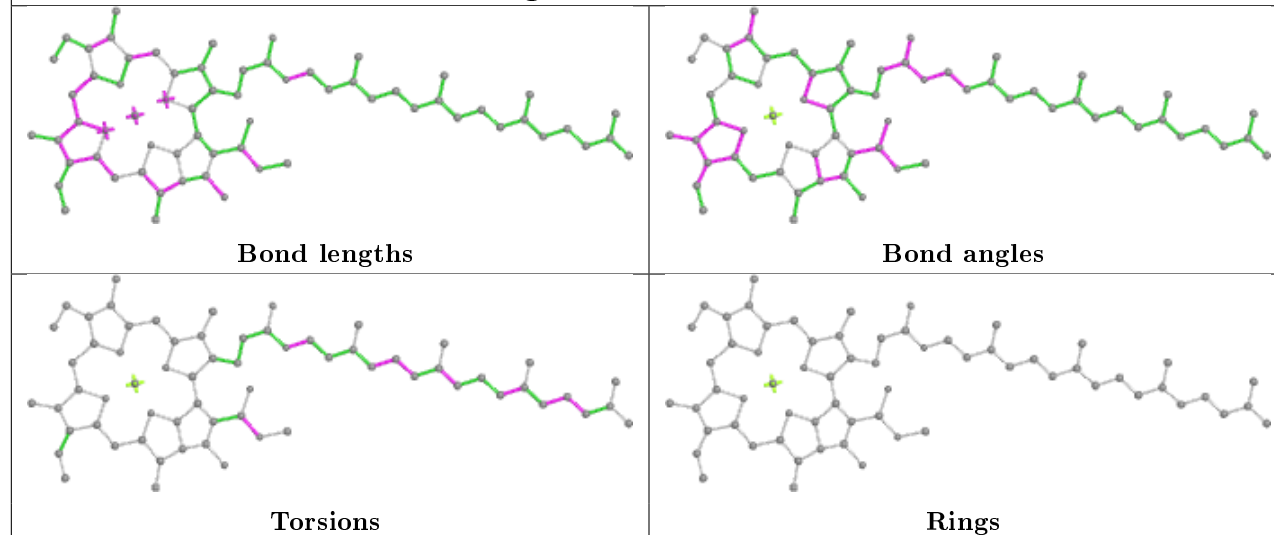


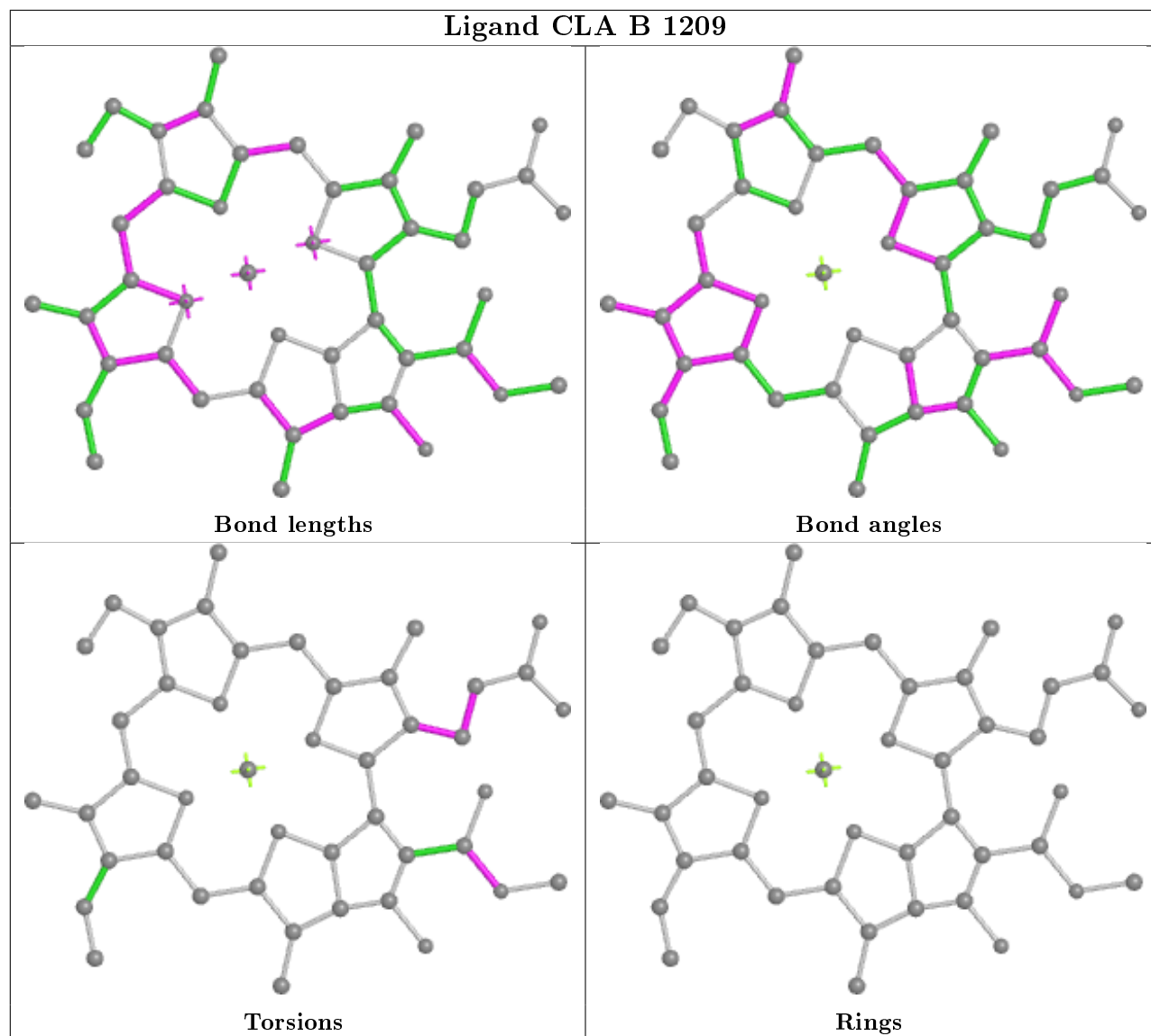
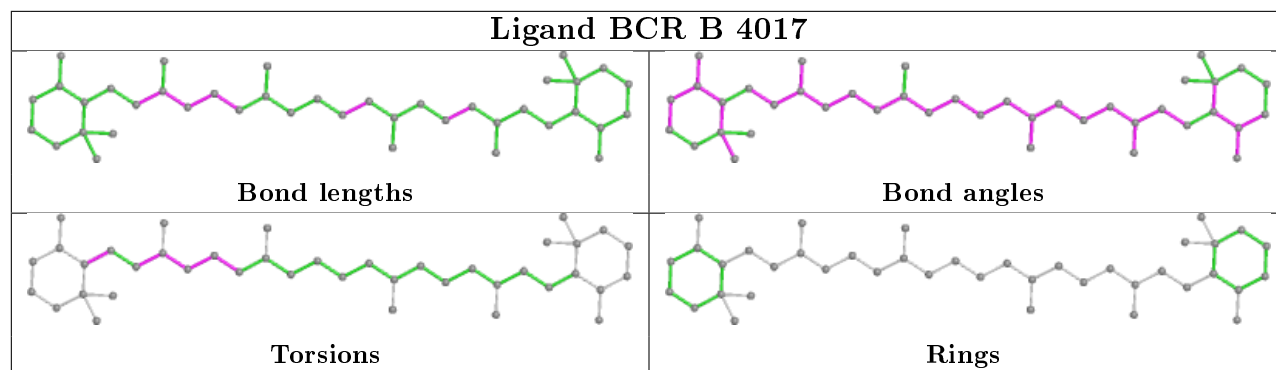
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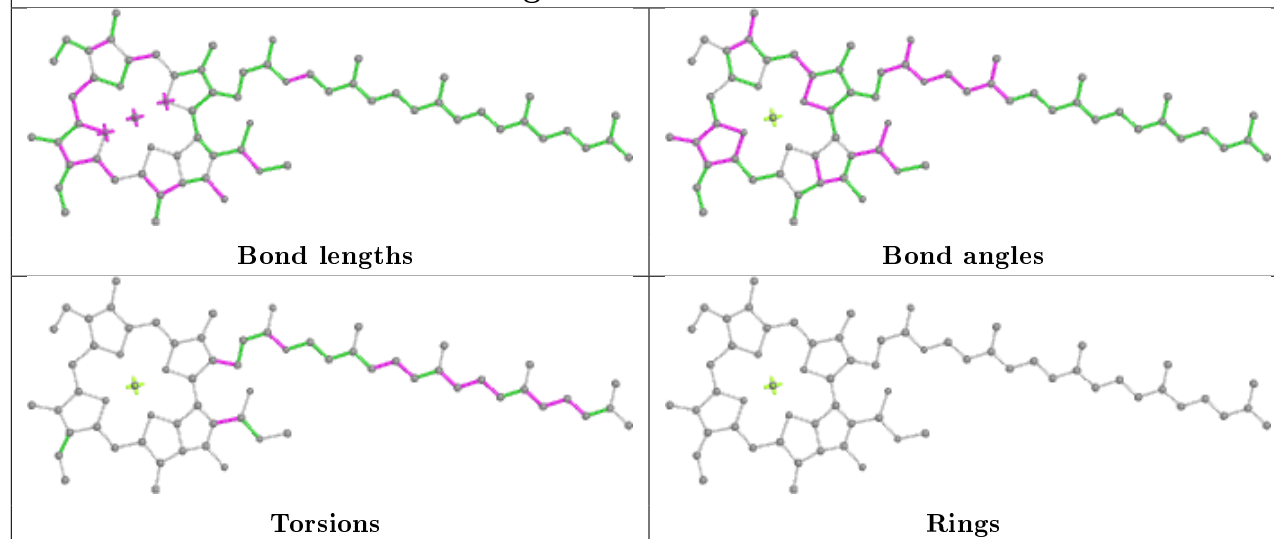
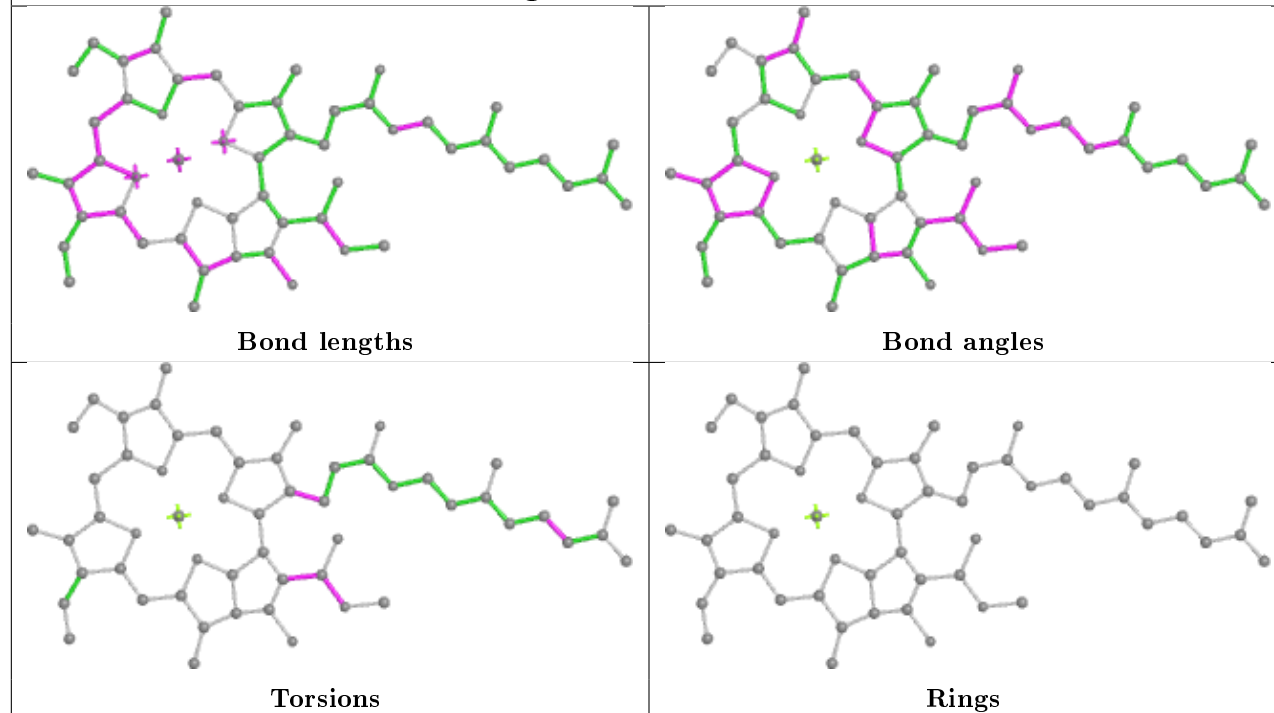


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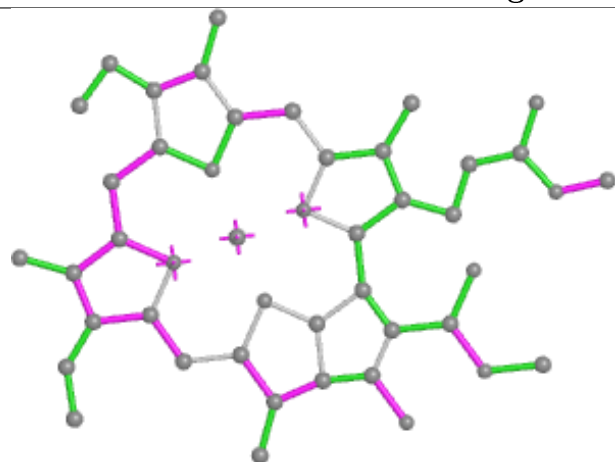


Ligand CLA A 1128**Ligand PQN B 2002****Ligand CLA A 1105**

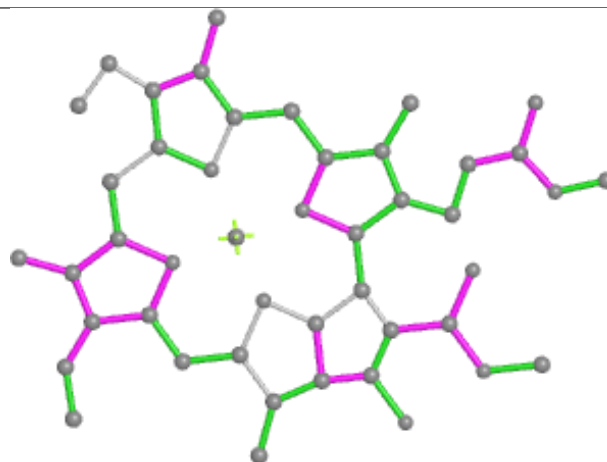


Ligand CLA B 1234**Ligand CLA A 1124**

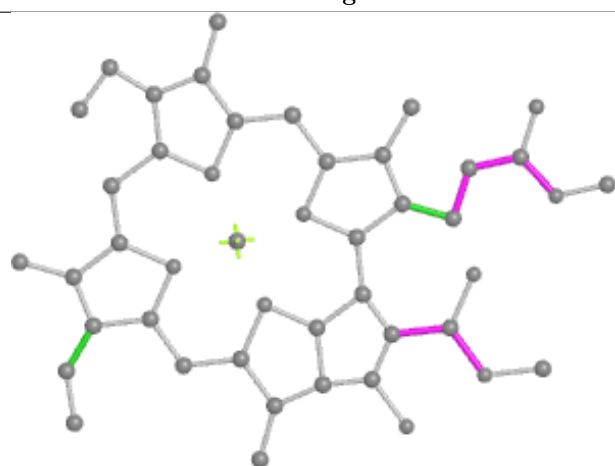
Ligand CLA A 1121



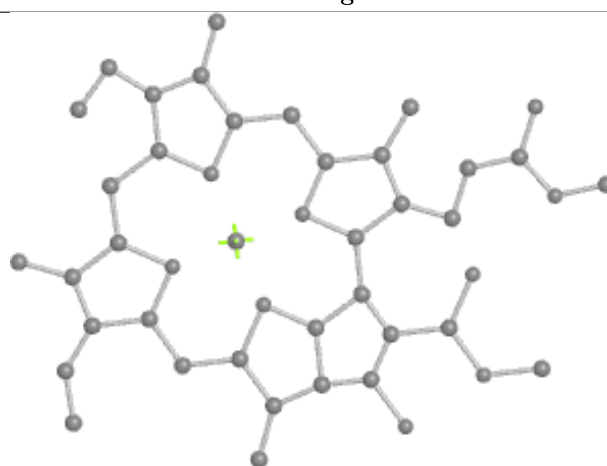
Bond lengths



Bond angles

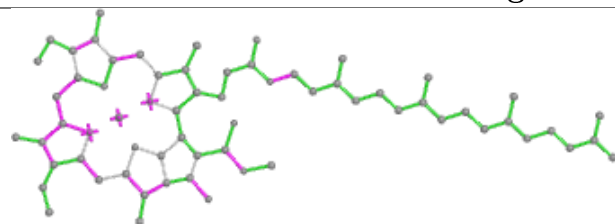


Torsions

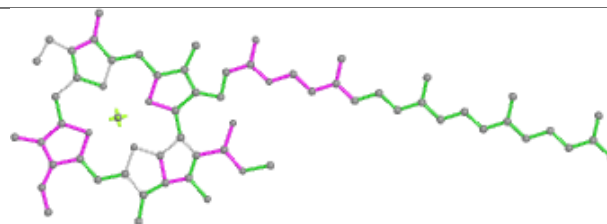


Rings

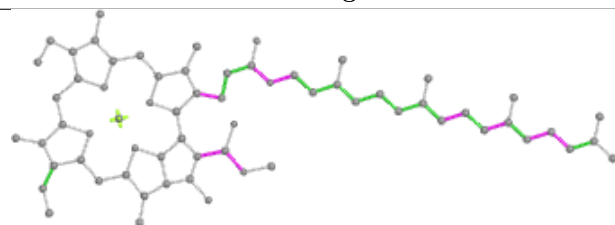
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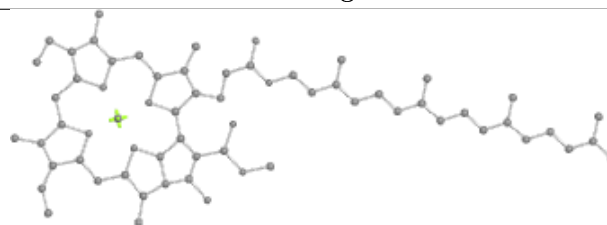
Bond lengths



Bond angles

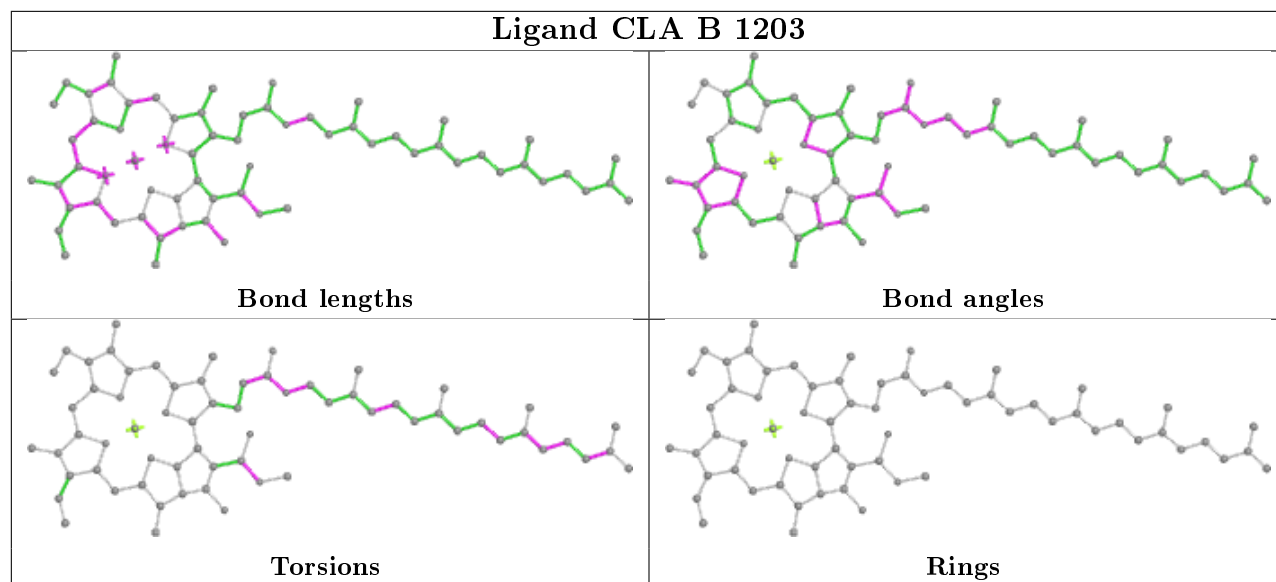


Torsions

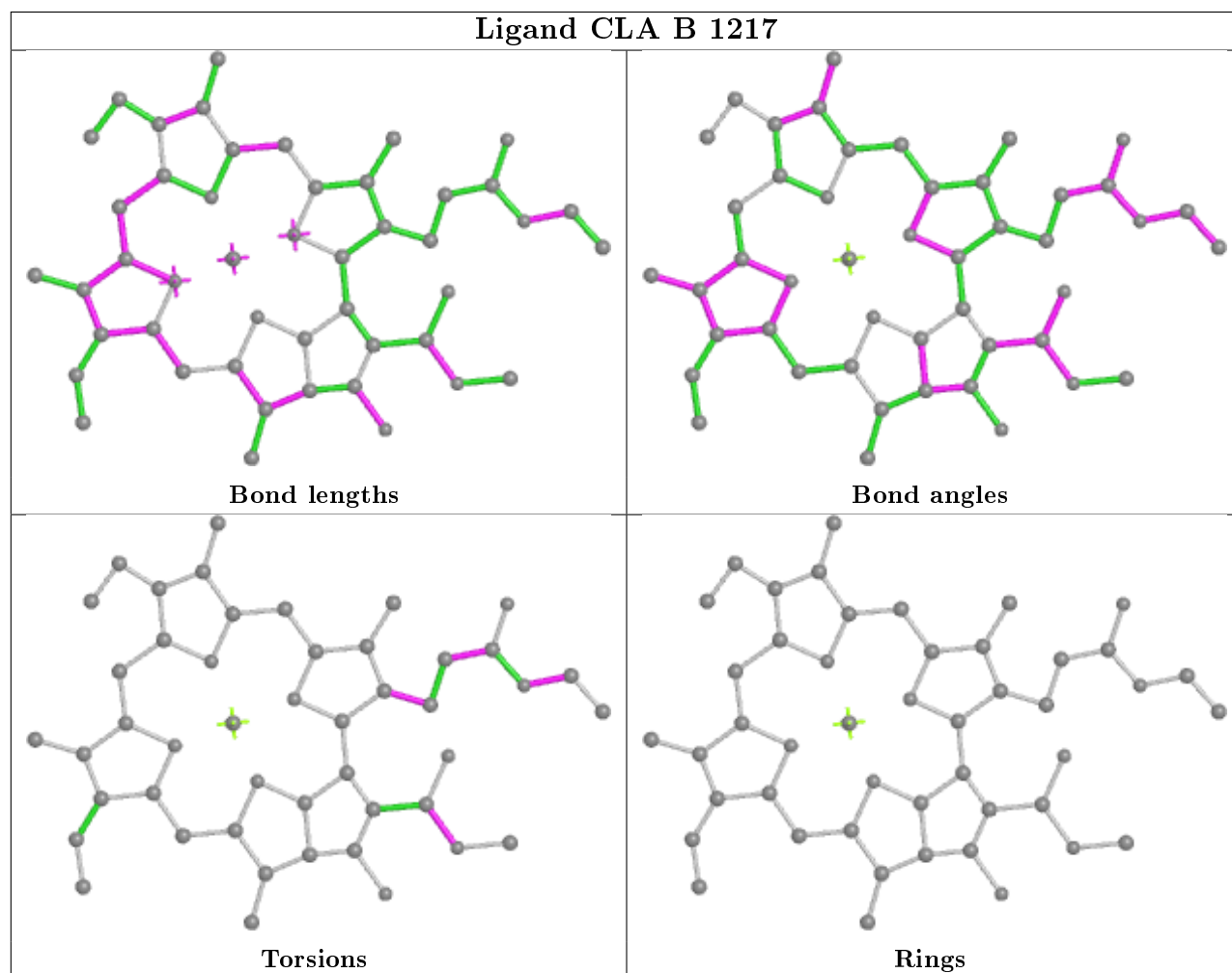


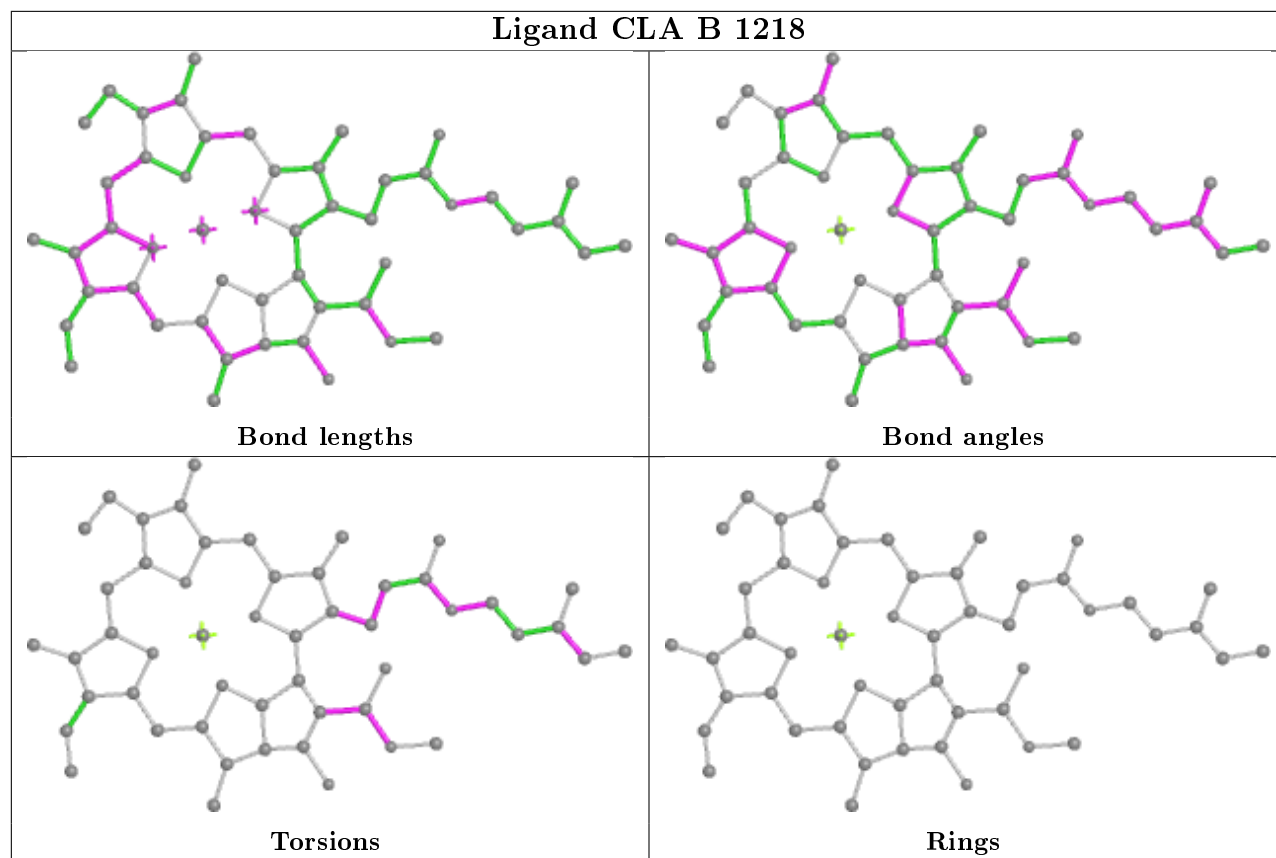
Rings

Ligand CLA B 1203

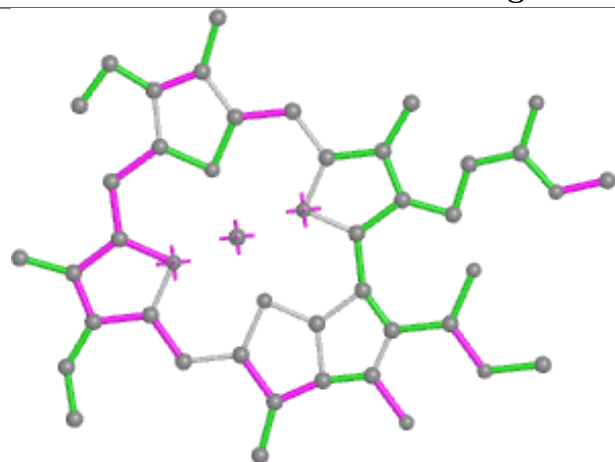


Ligand CLA B 1217

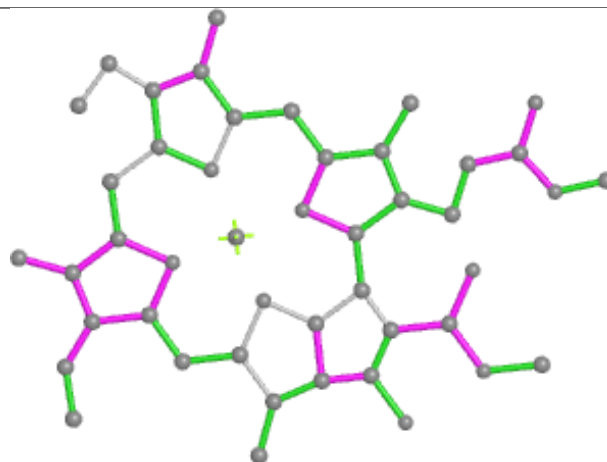




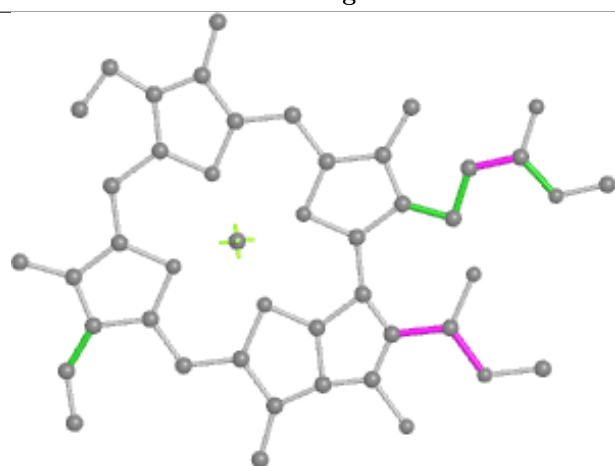
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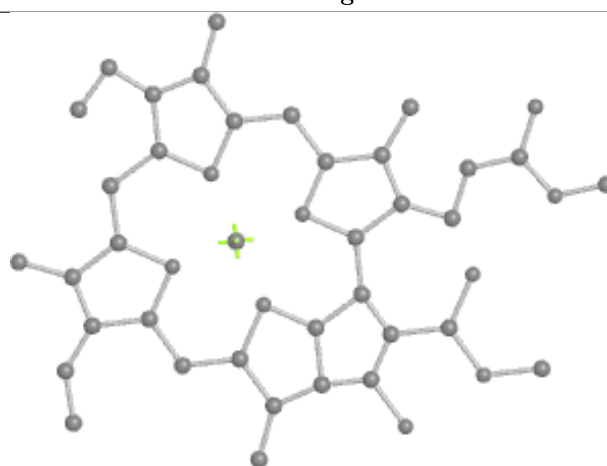
Bond lengths



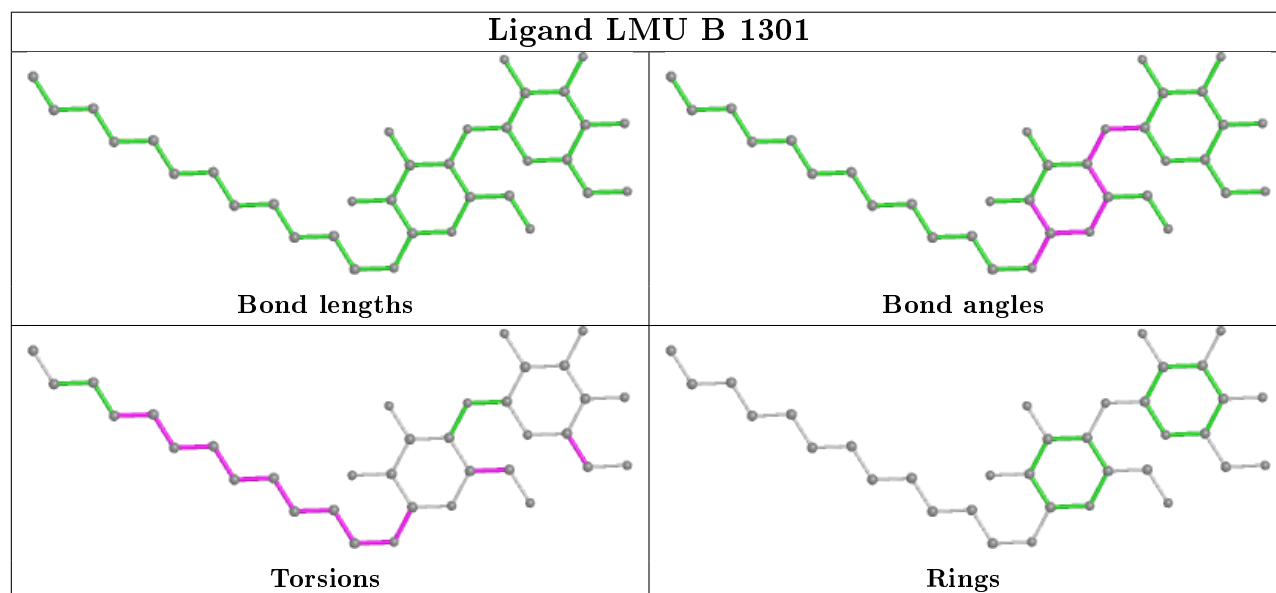
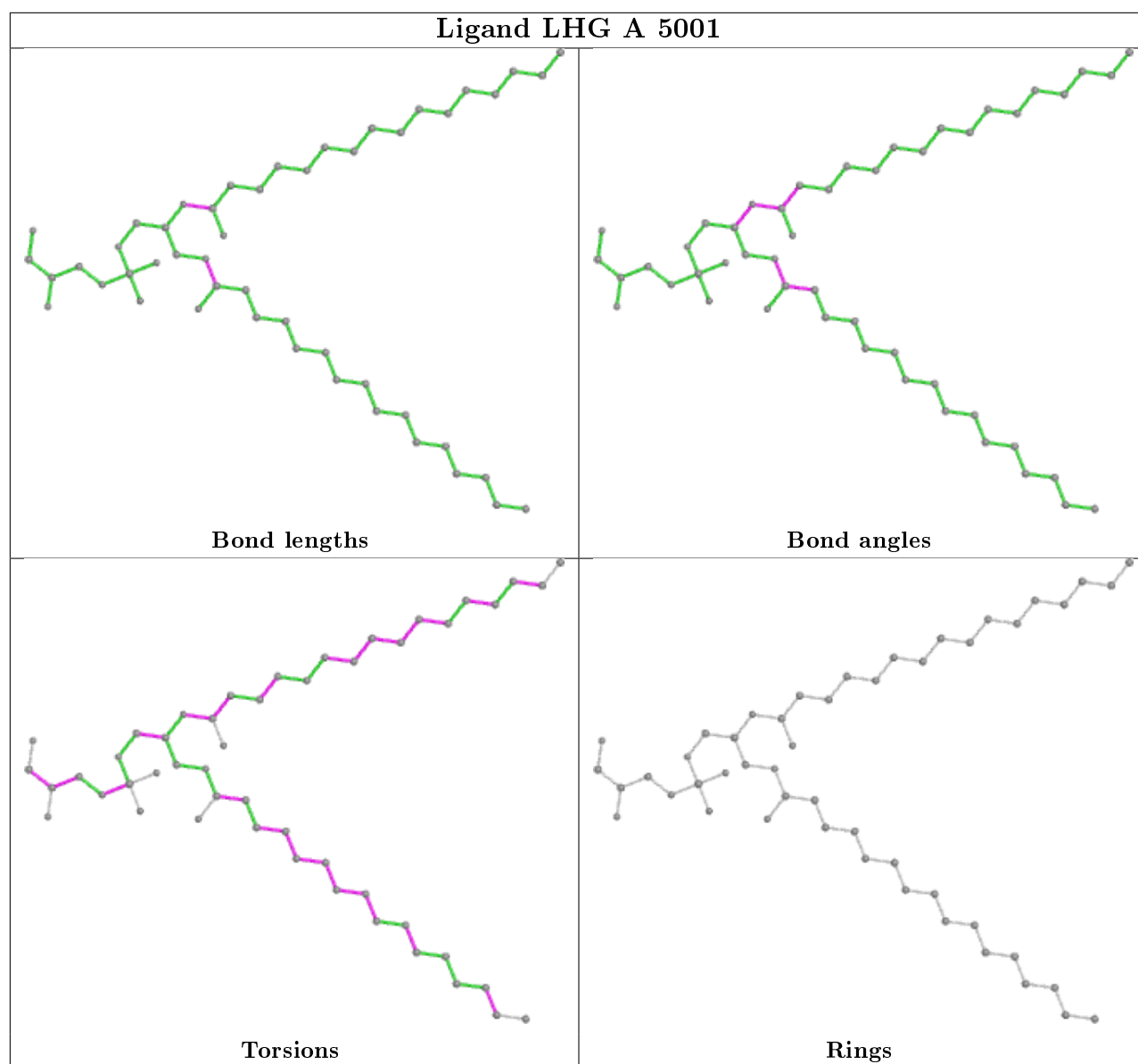
Bond angles

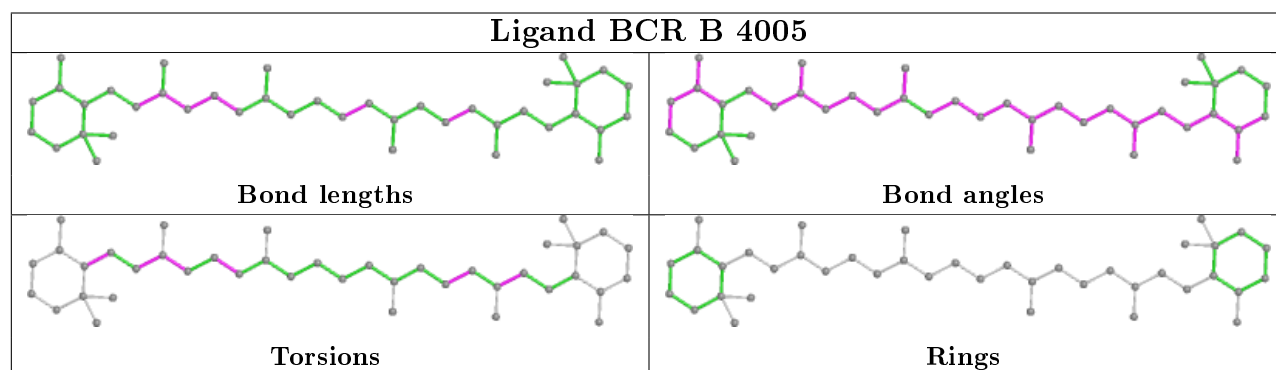
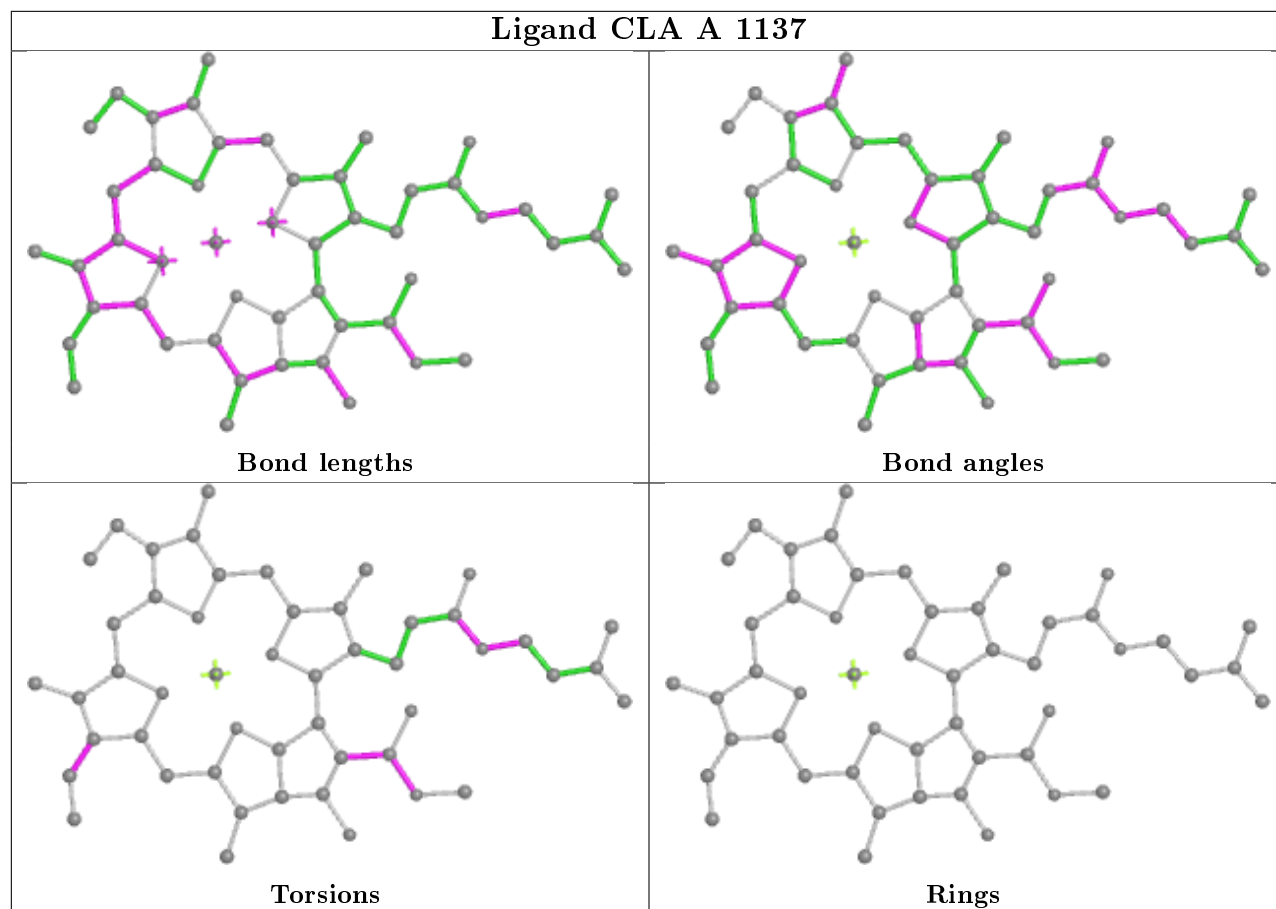
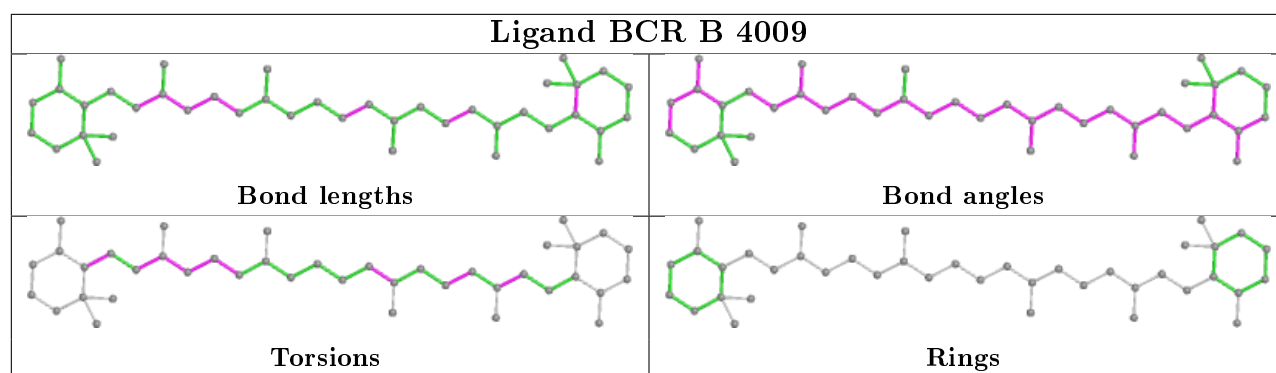


Torsions

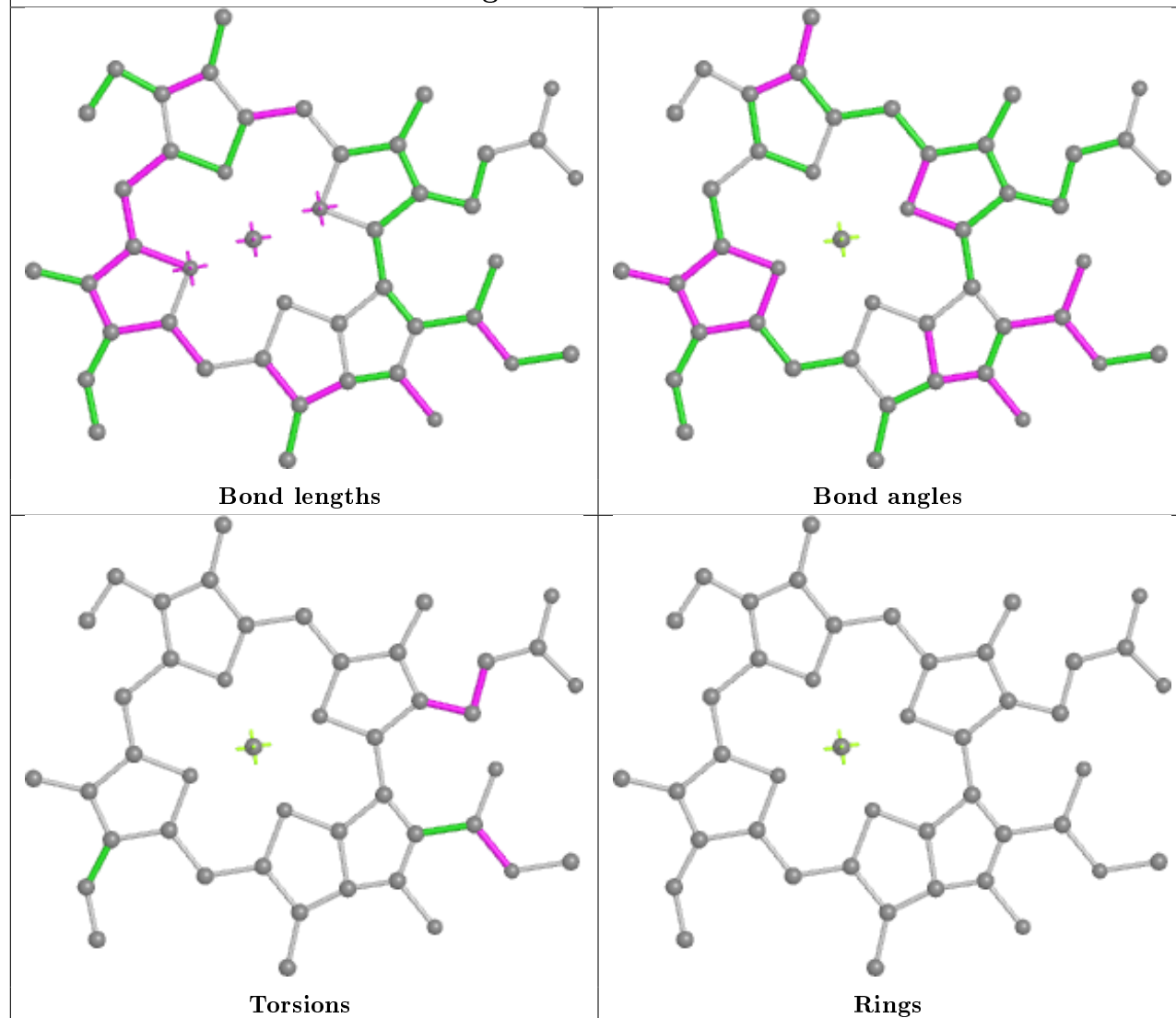


Rings

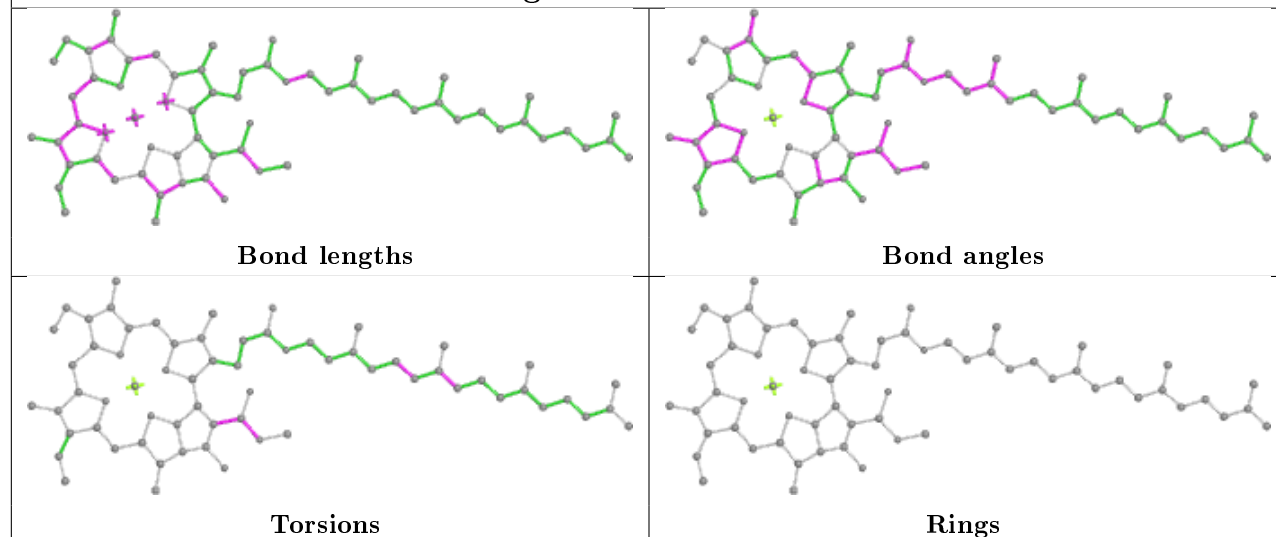


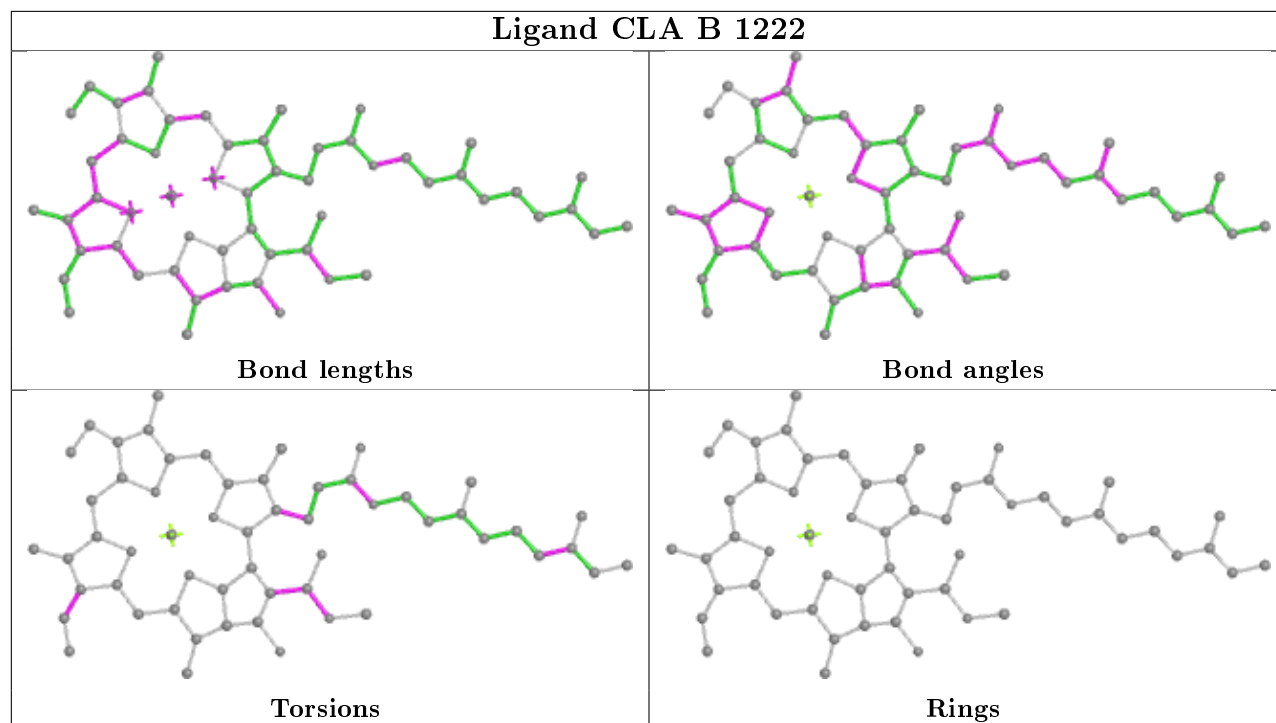
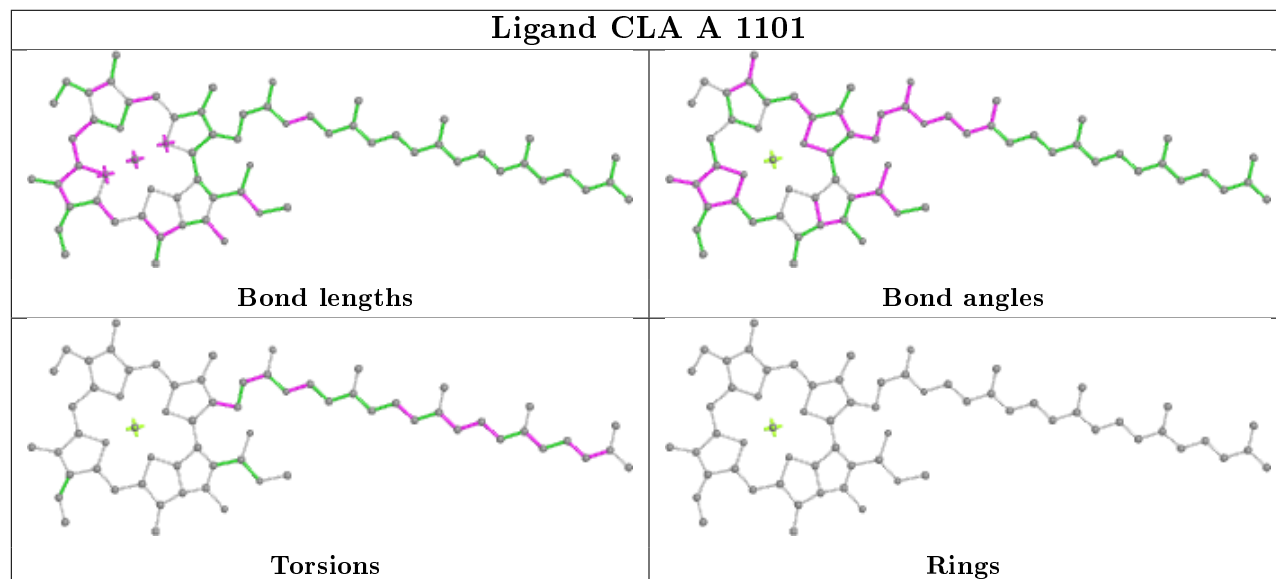


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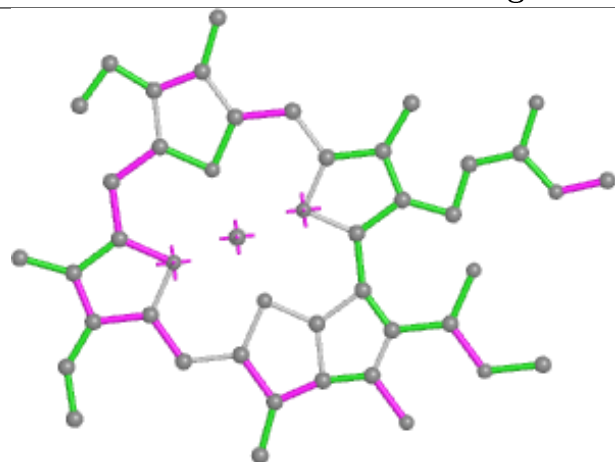


Ligand CLA A 1138

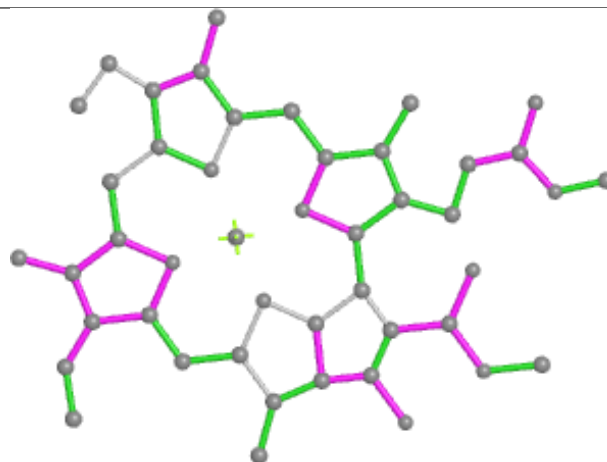


Ligand CLA B 1222**Ligand CLA A 1101**

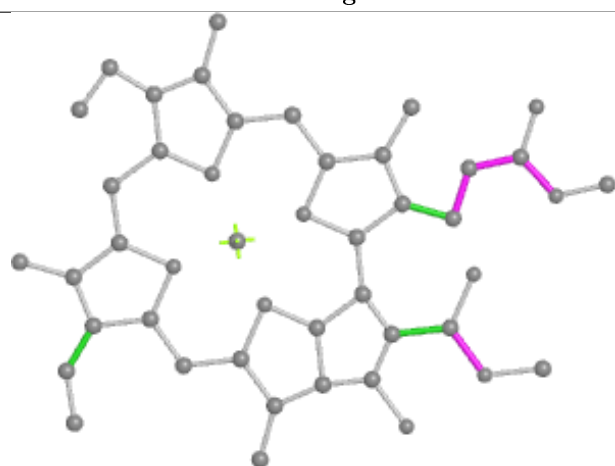
Ligand CLA A 1115



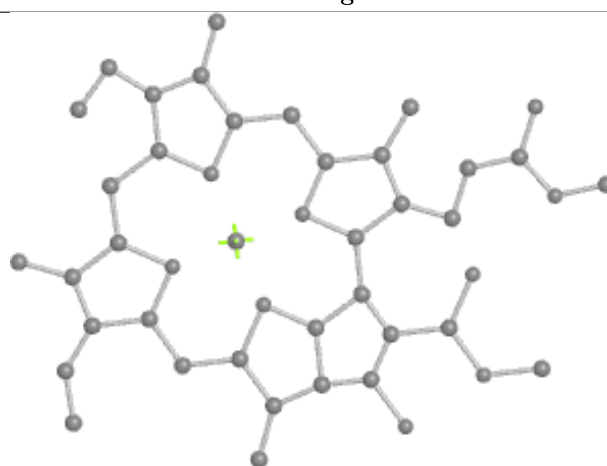
Bond lengths



Bond angles

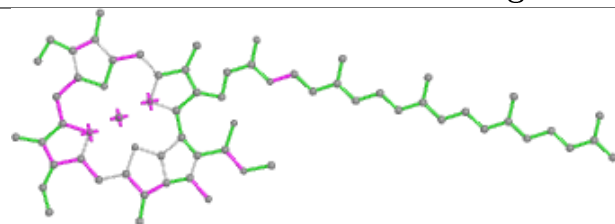


Torsions

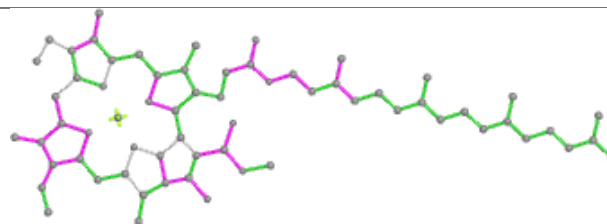


Rings

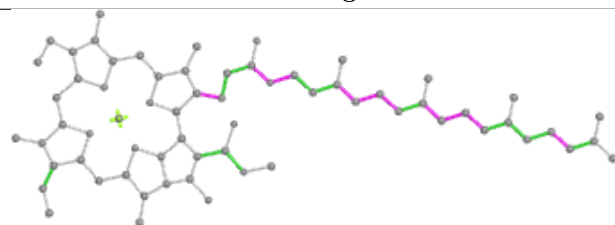
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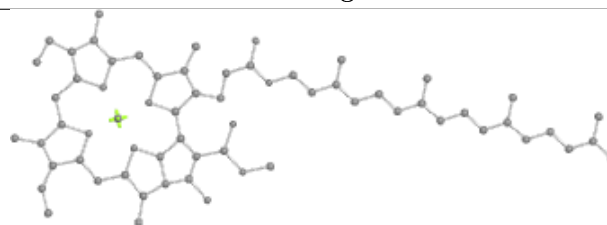
Bond lengths



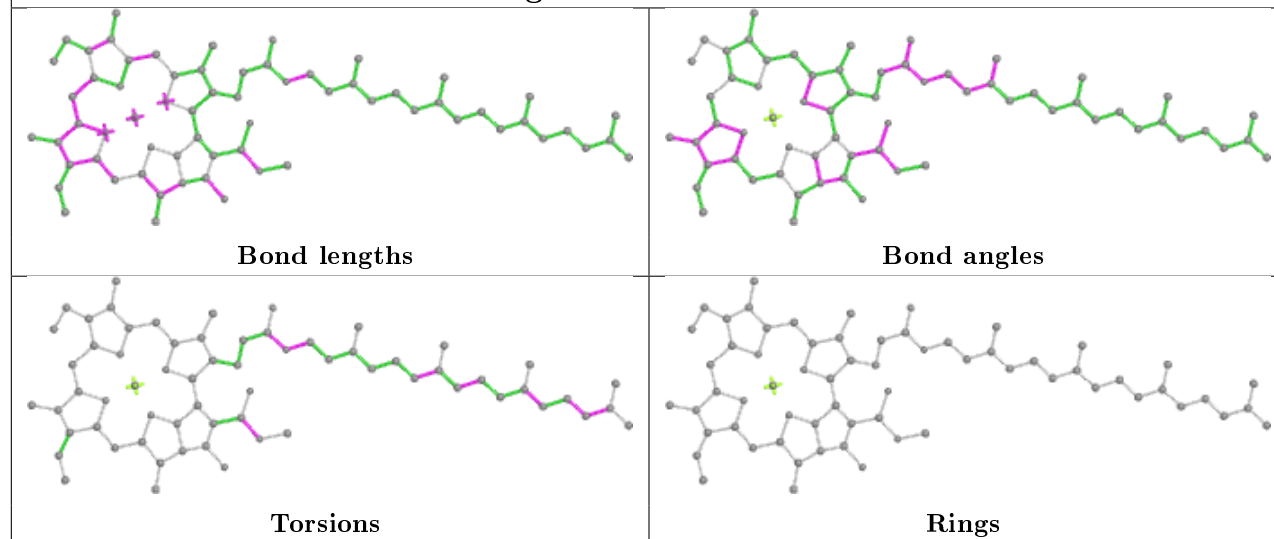
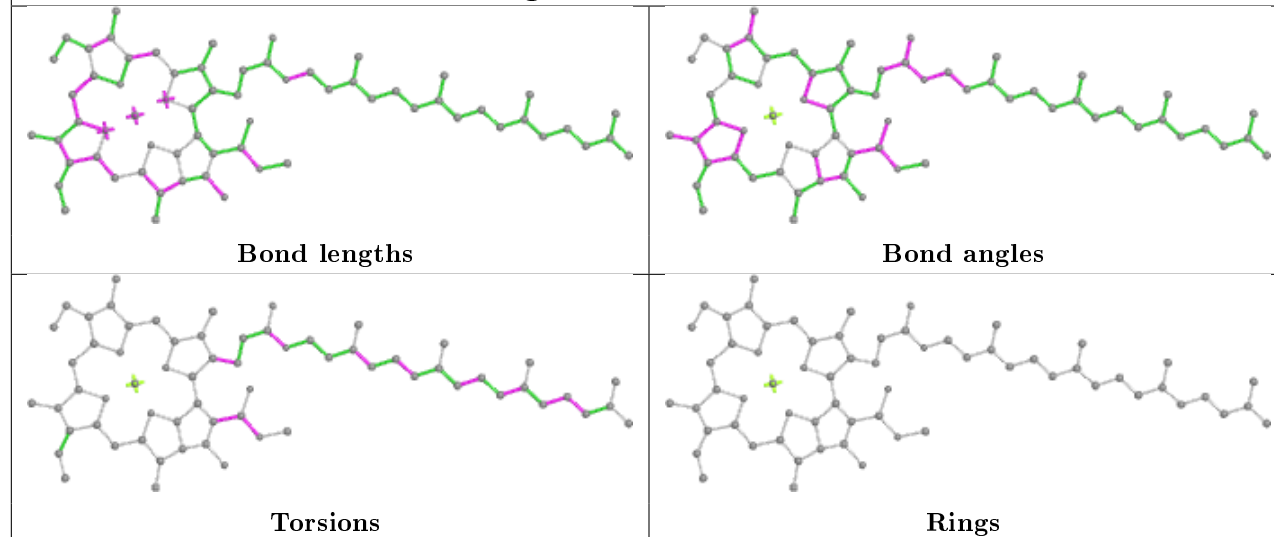
Bond angles

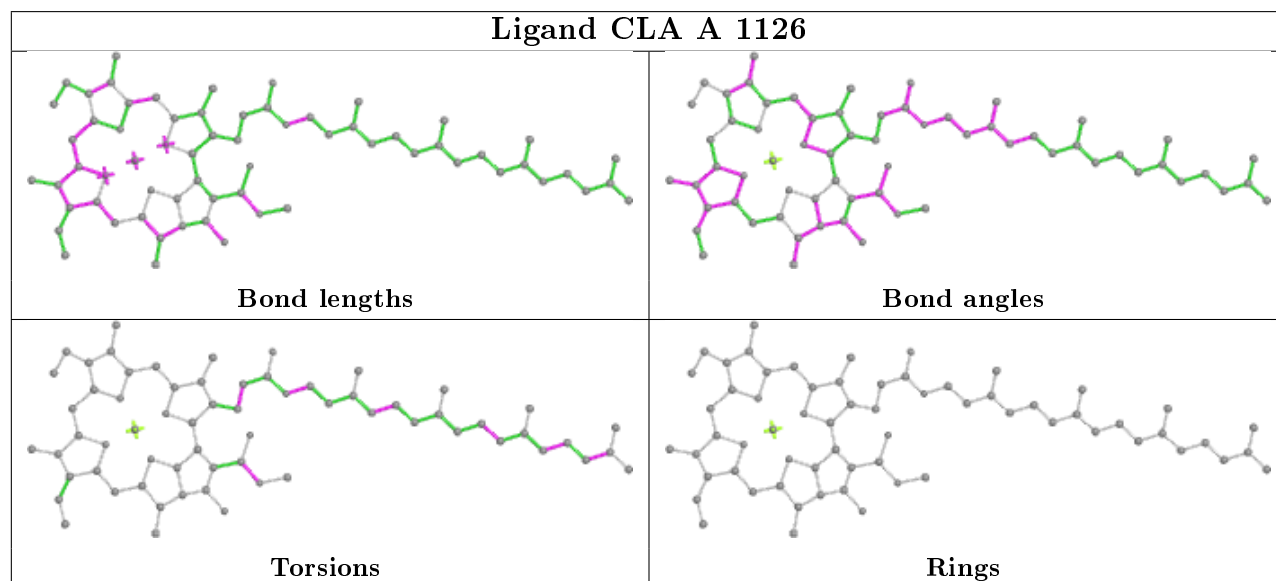
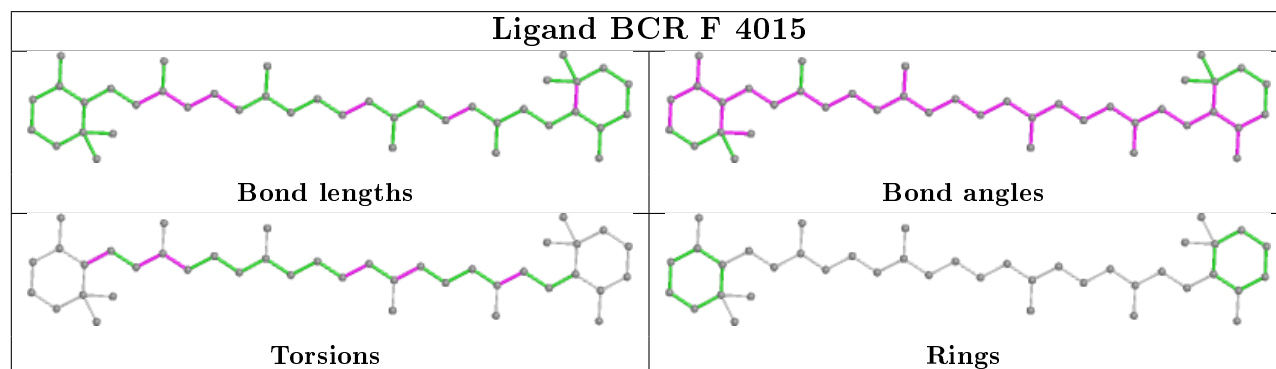
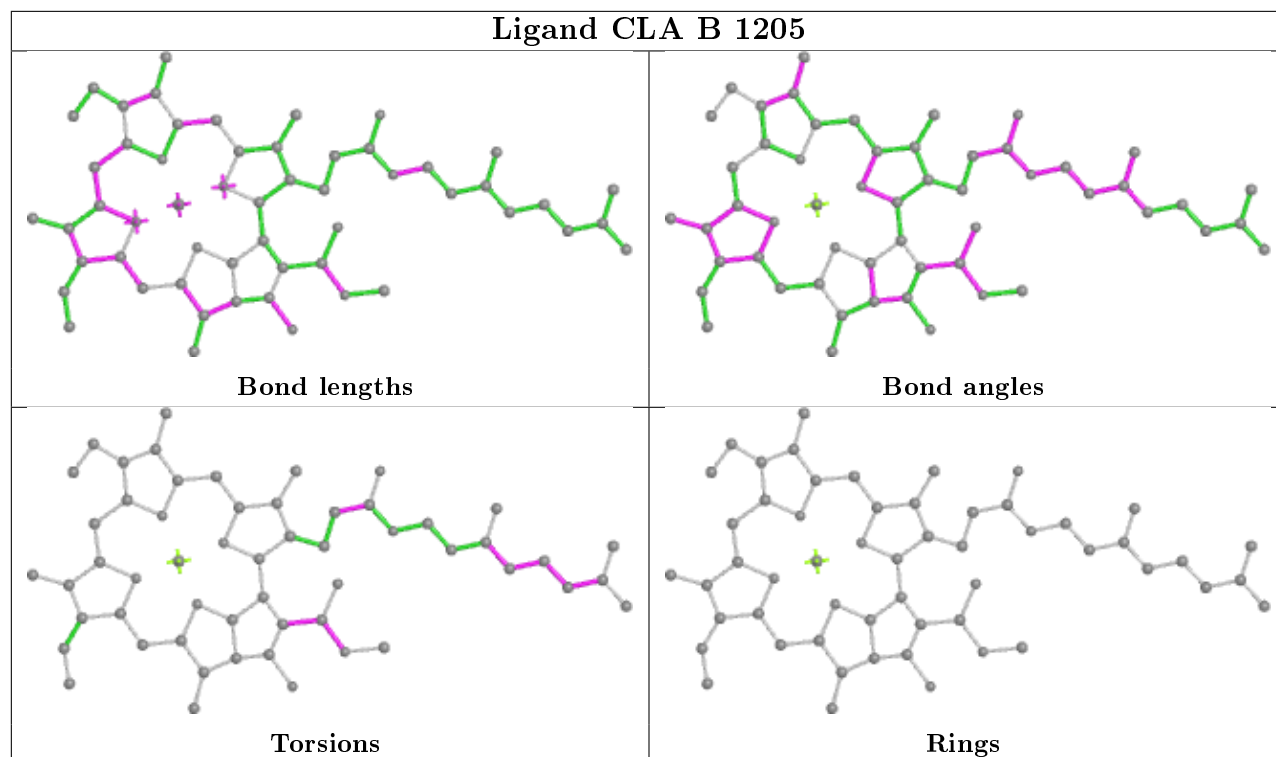


Torsions

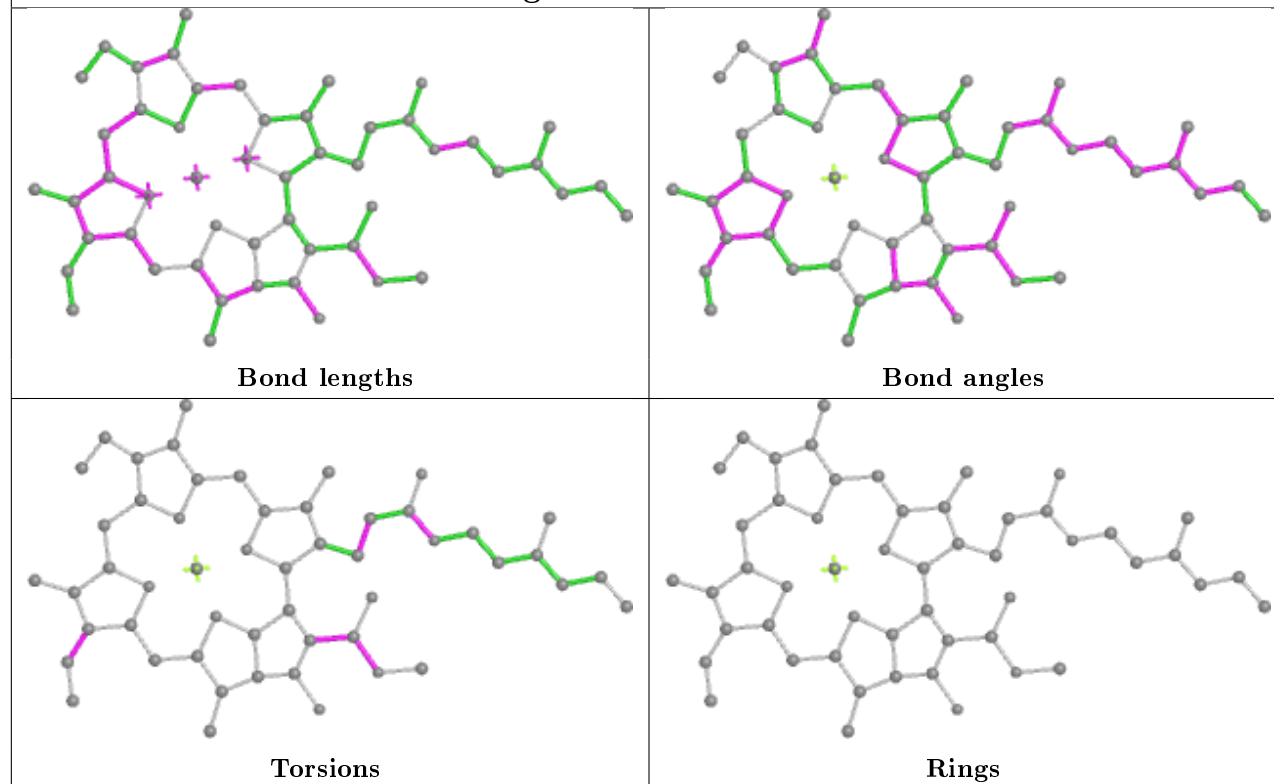


Rings

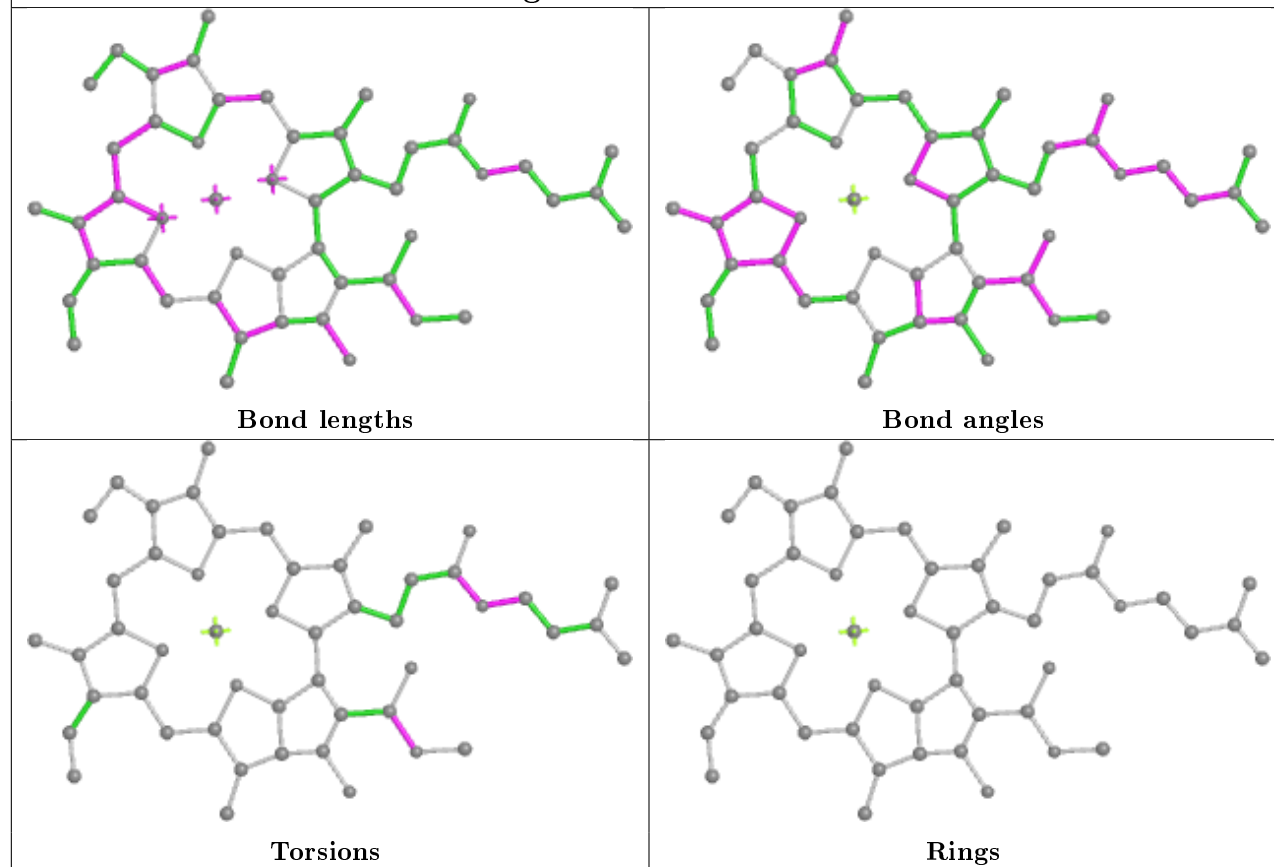
Ligand CLA F 1139**Ligand CLA B 1224**



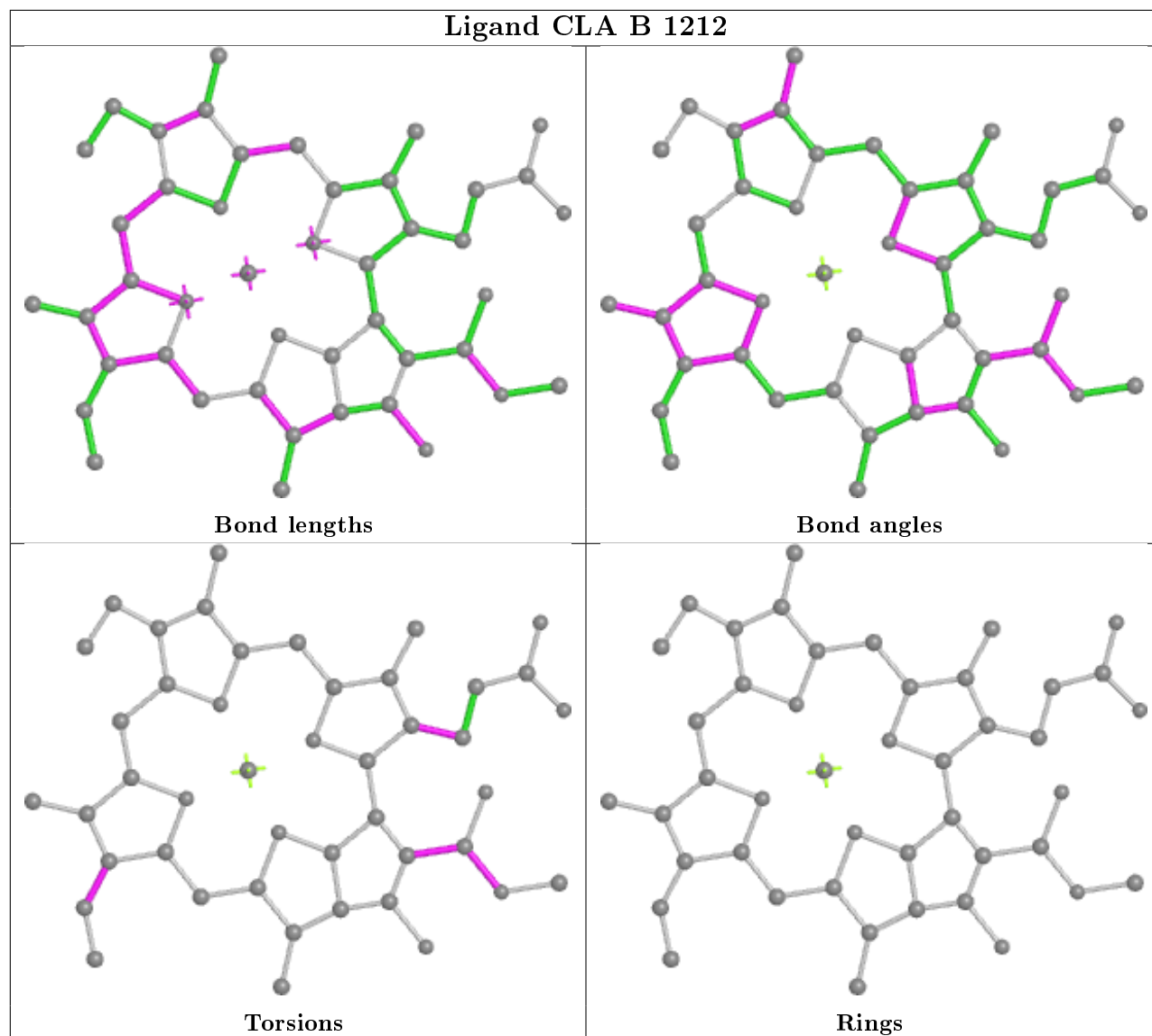
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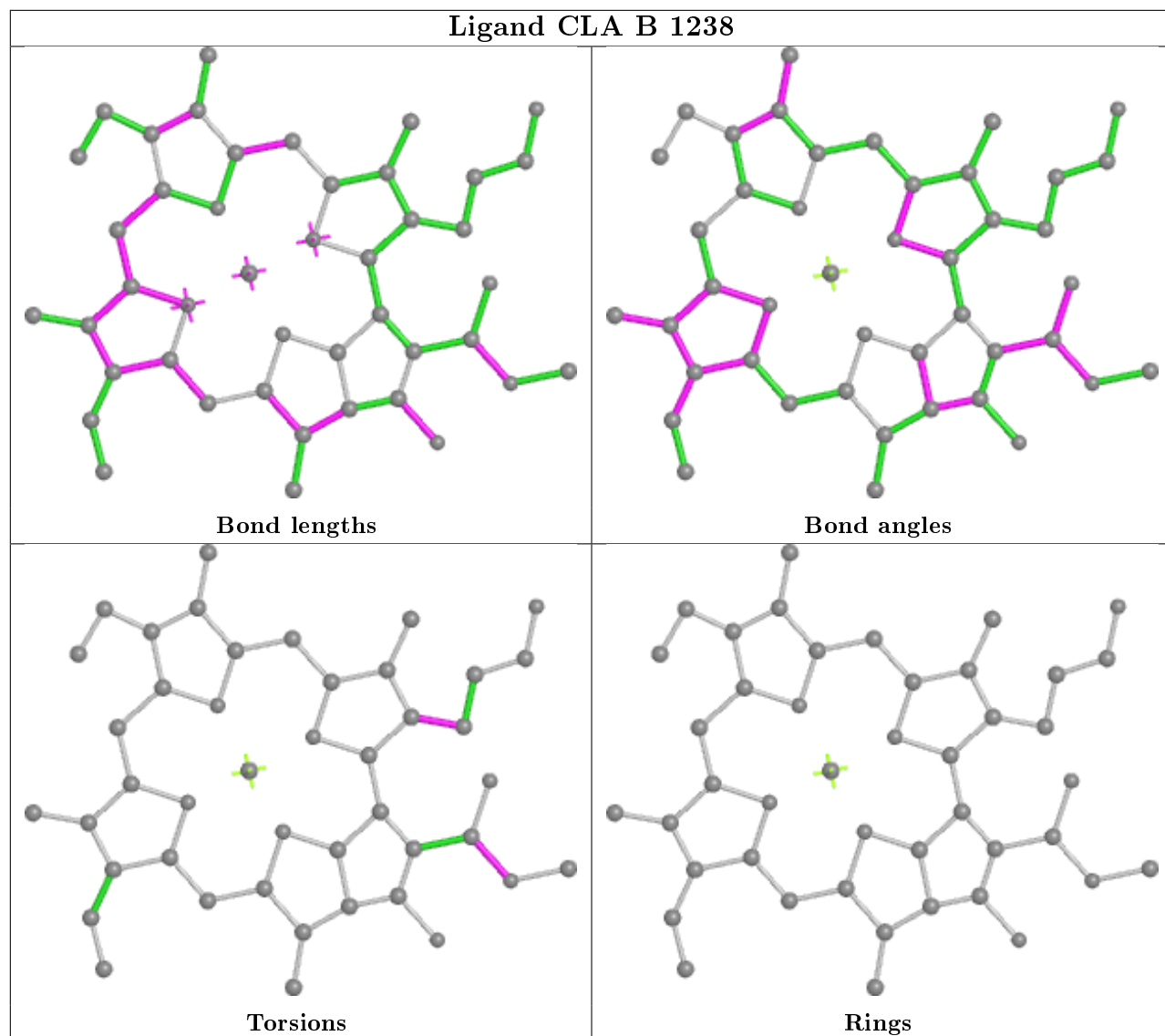
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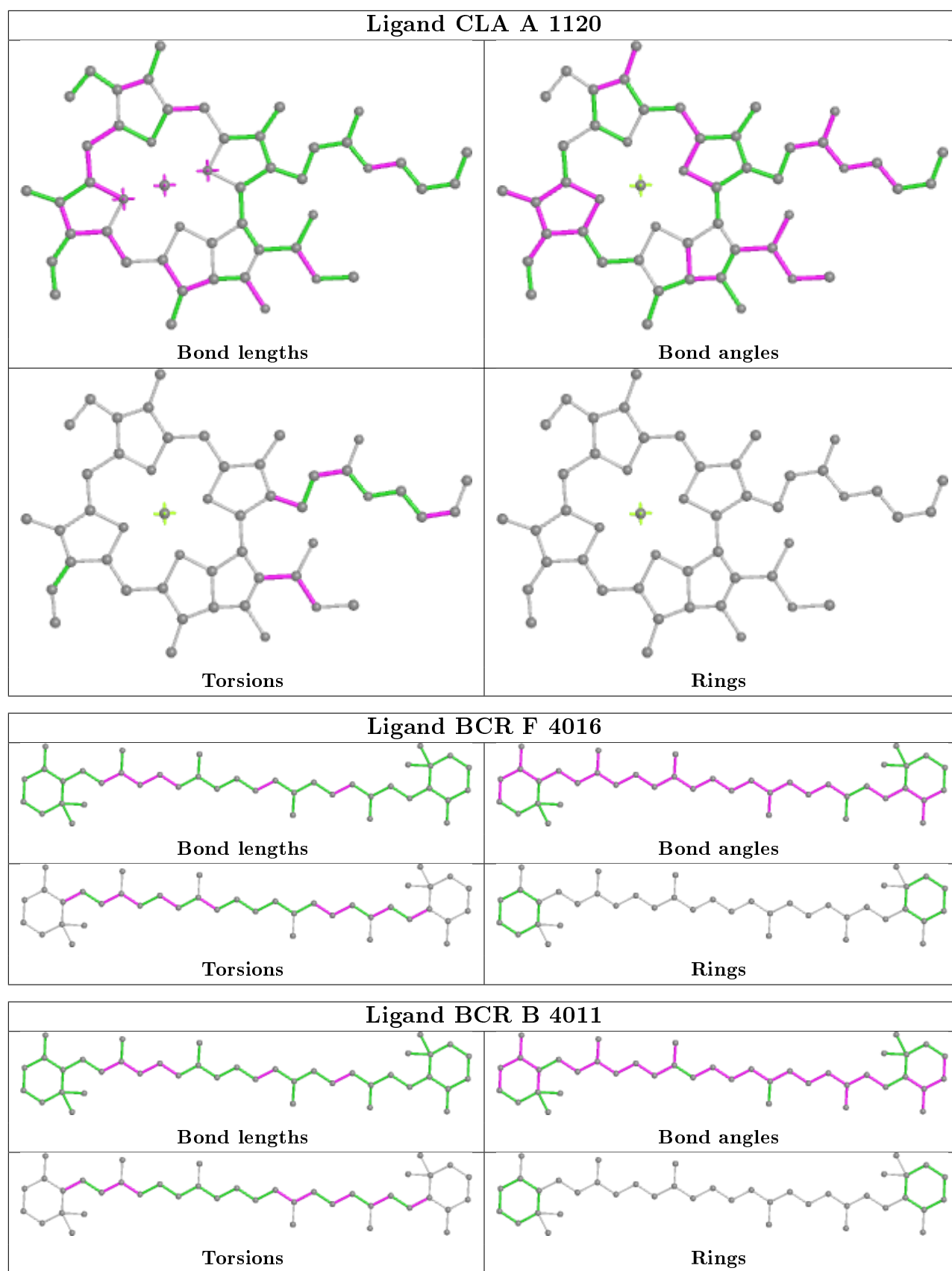


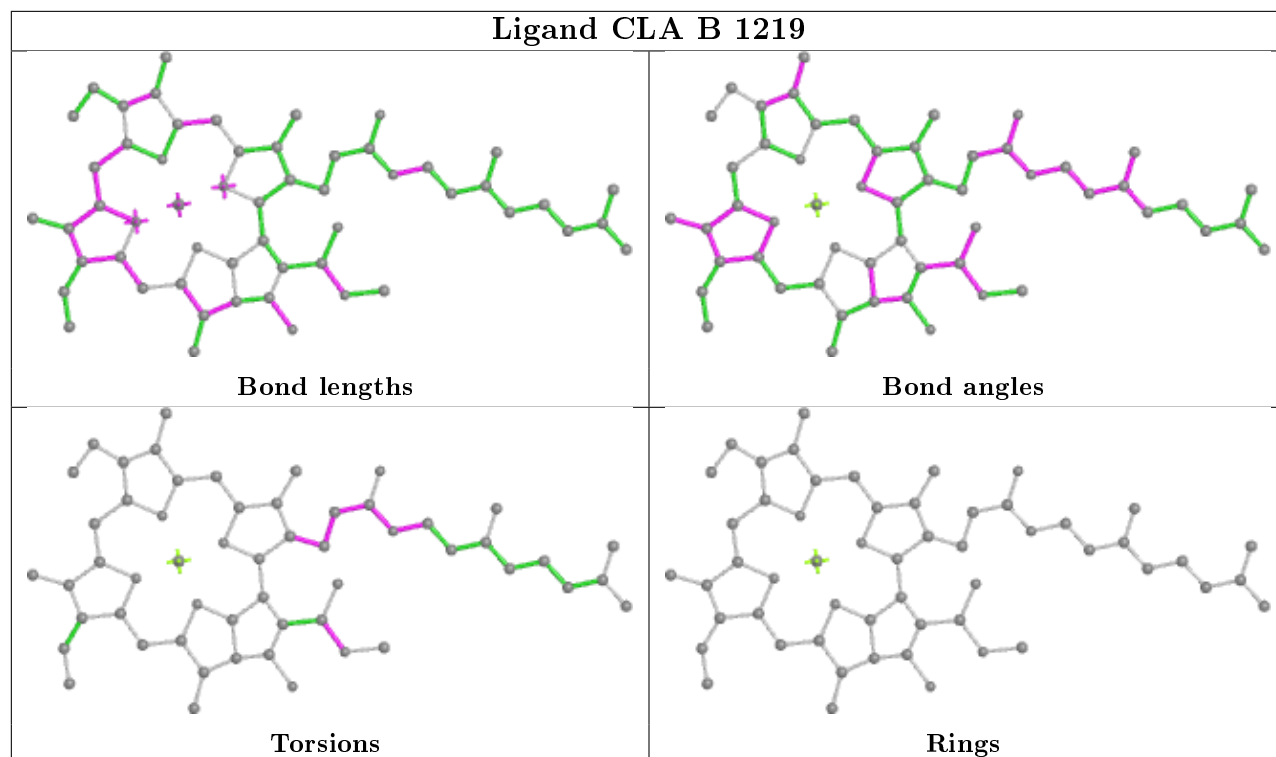
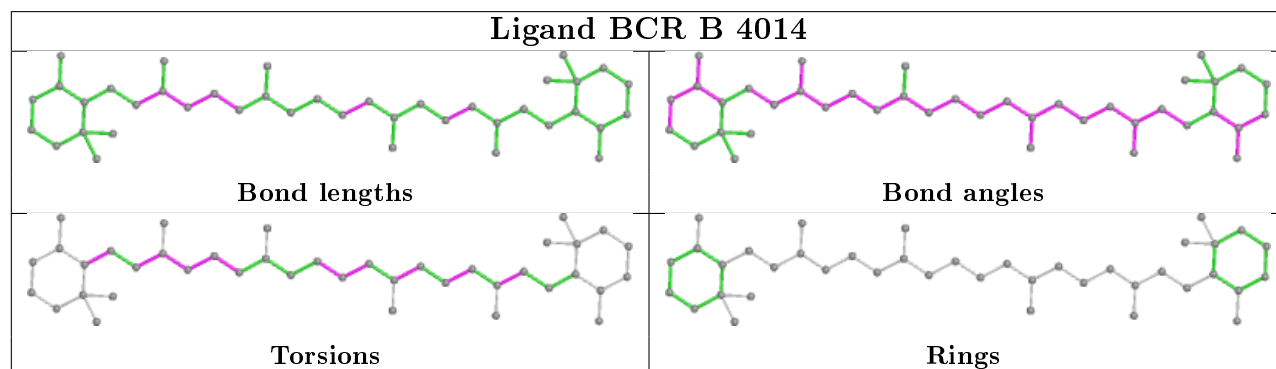
Ligand CLA B 1212

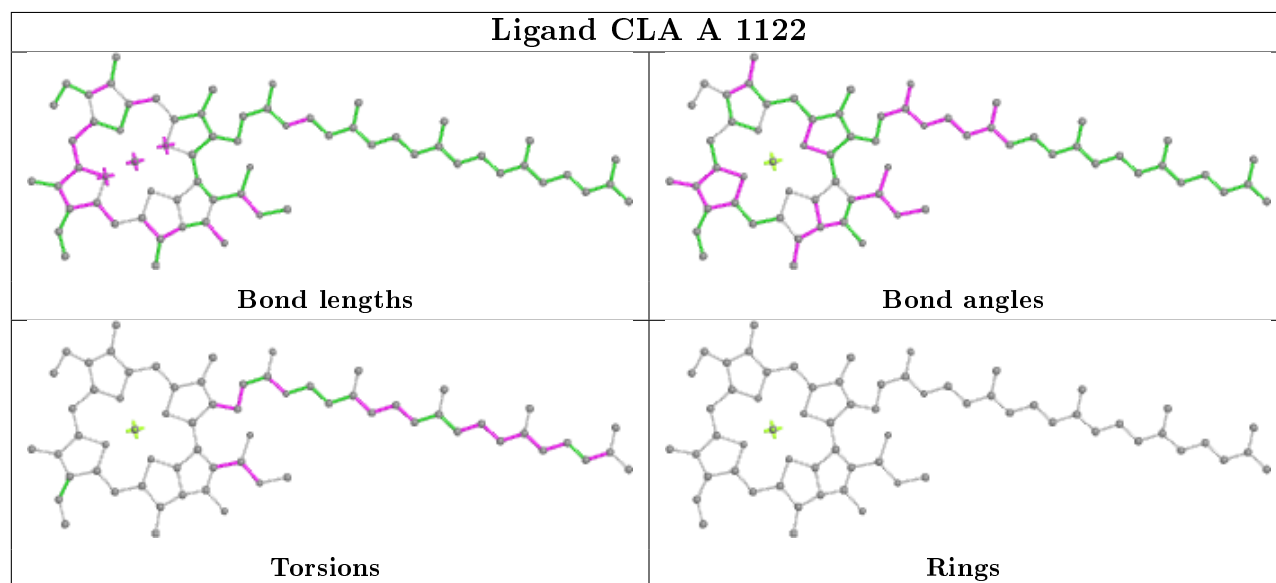
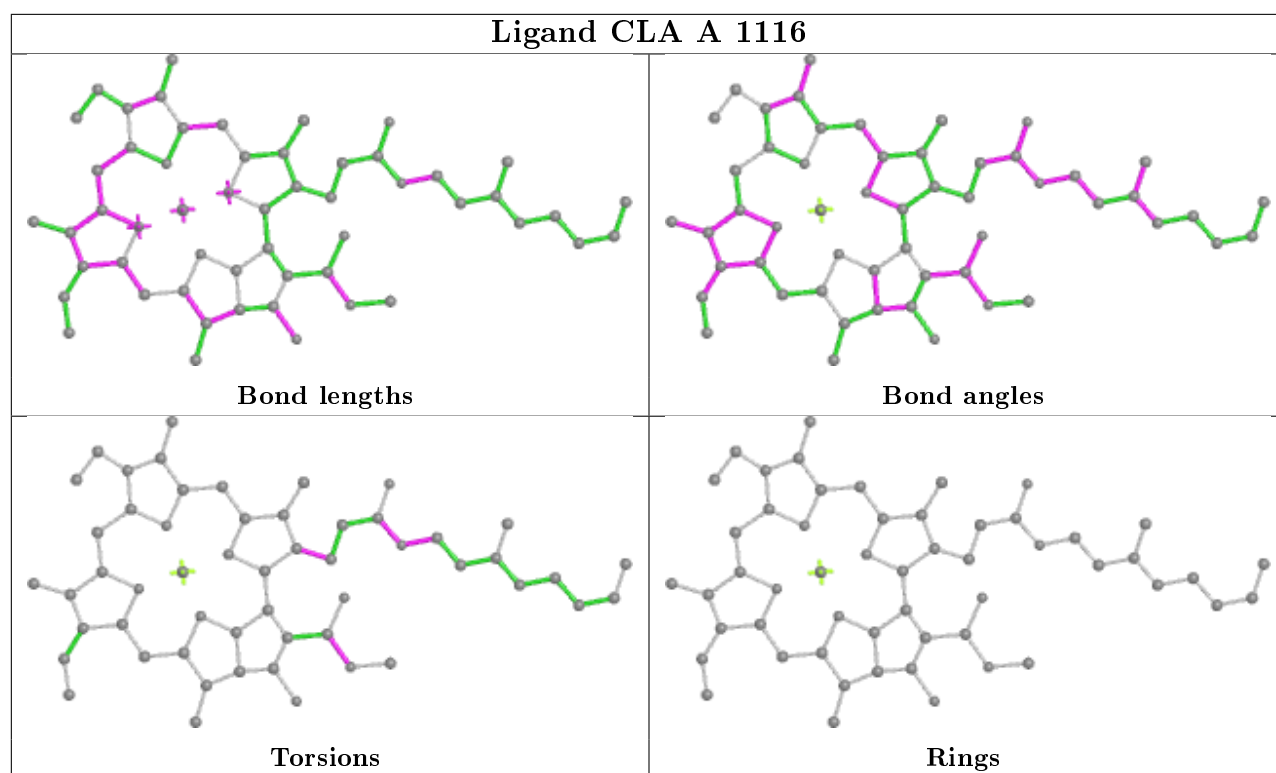


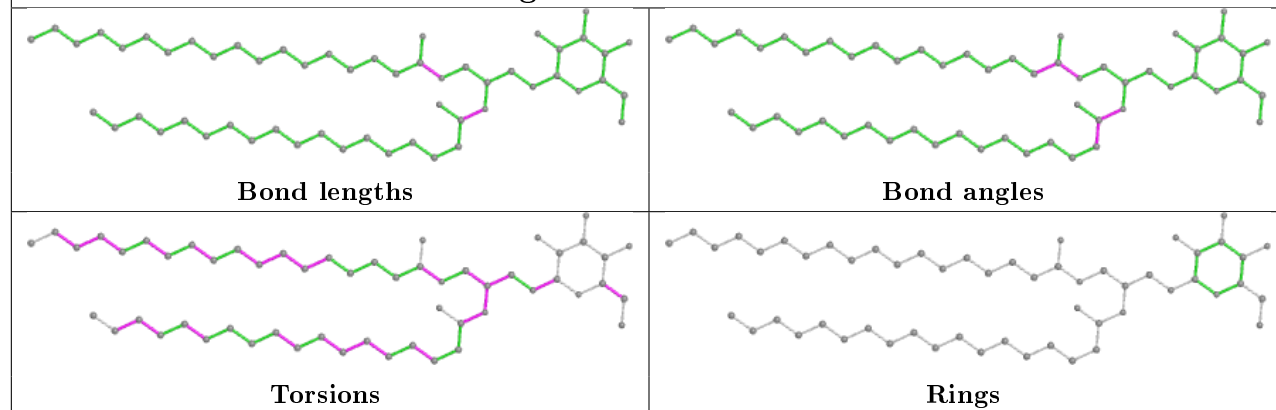
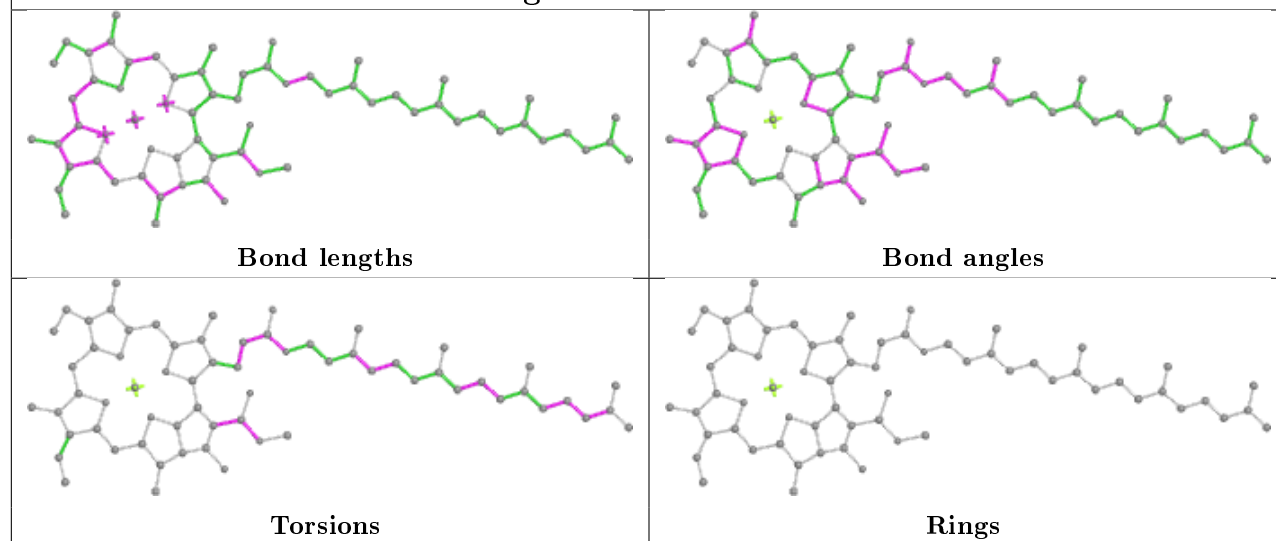
Ligand CLA B 1238



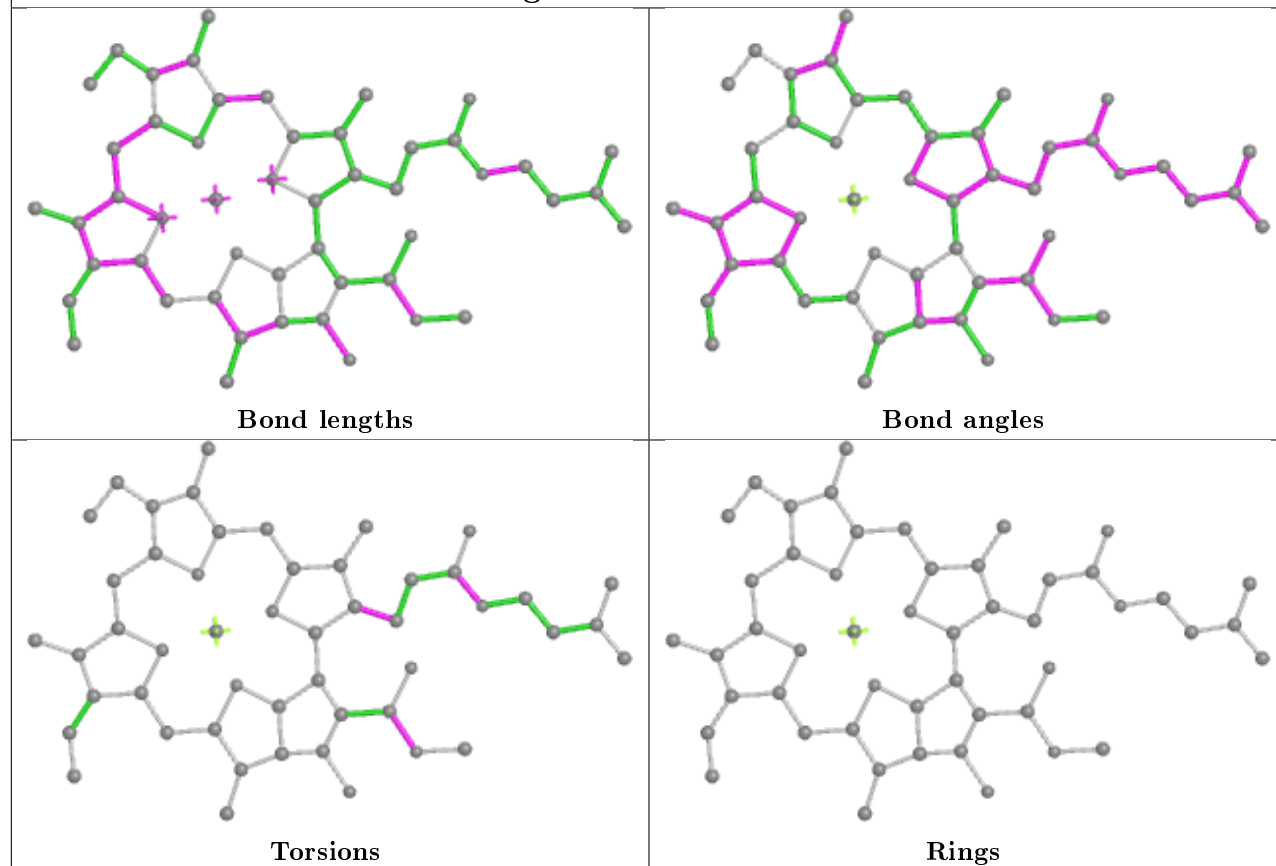


Ligand CLA B 1219**Ligand BCR B 4014**

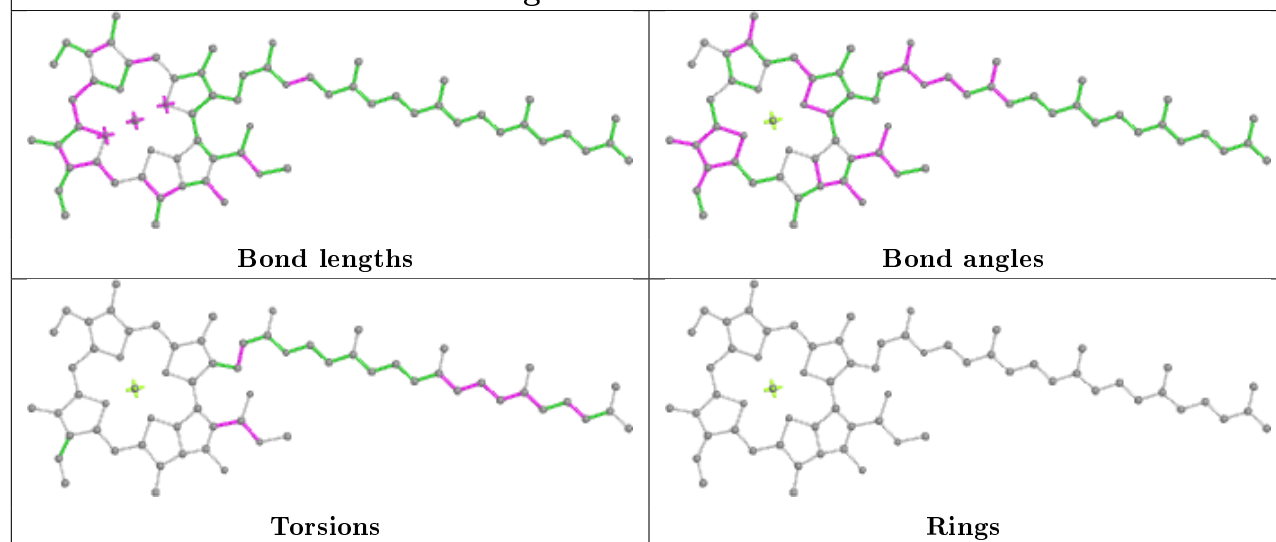


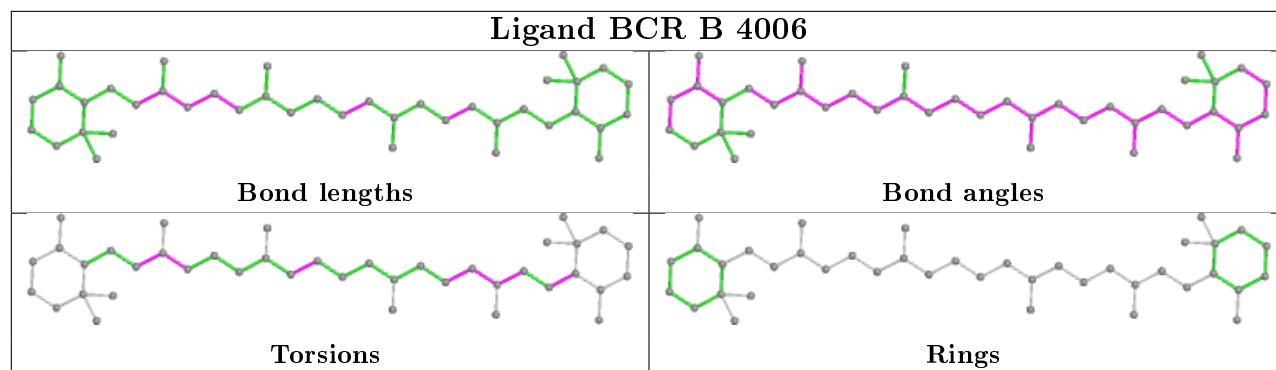
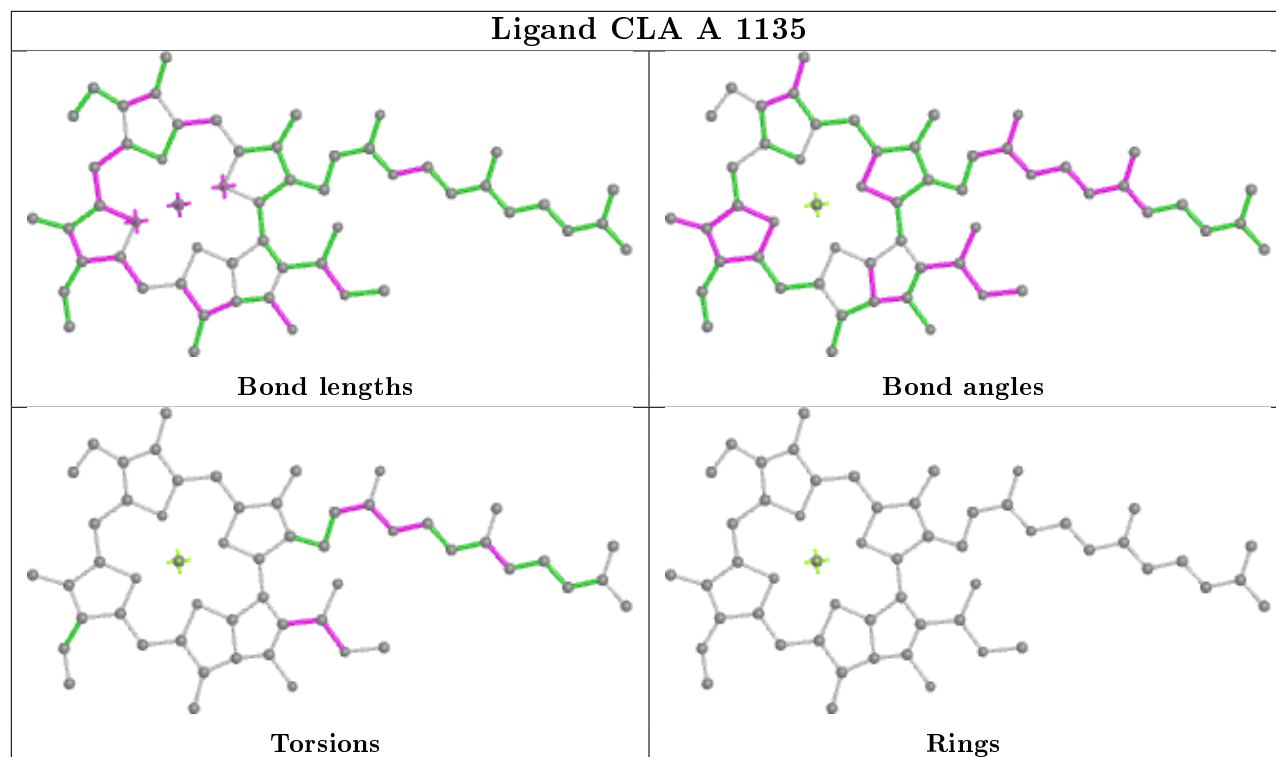
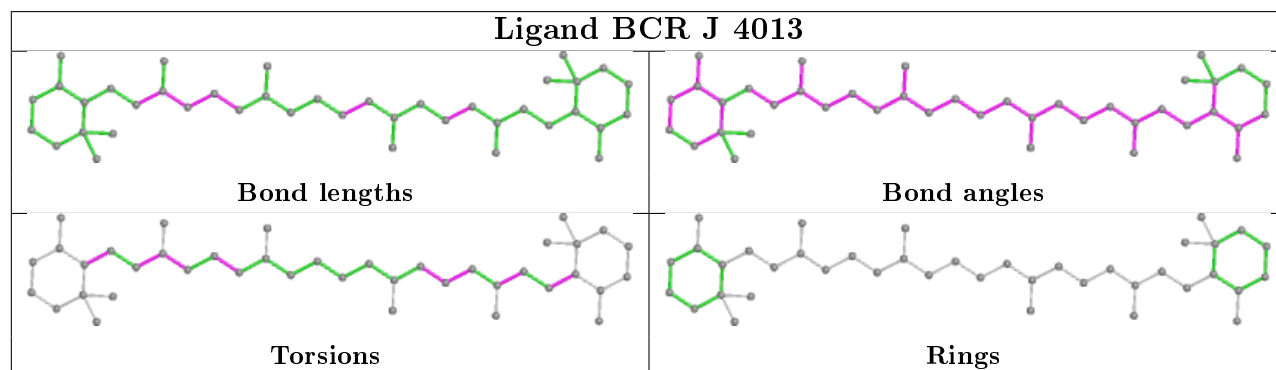
Ligand LMG B 5002**Ligand CLA A 1127**

Ligand CLA A 1107

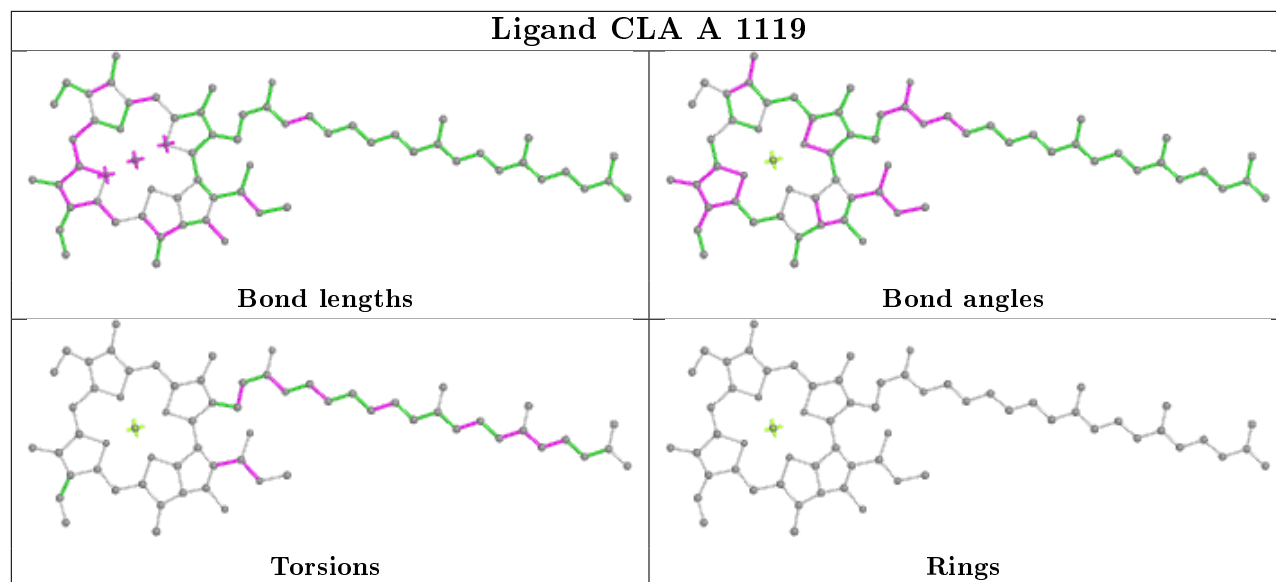


Ligand CLA B 1023

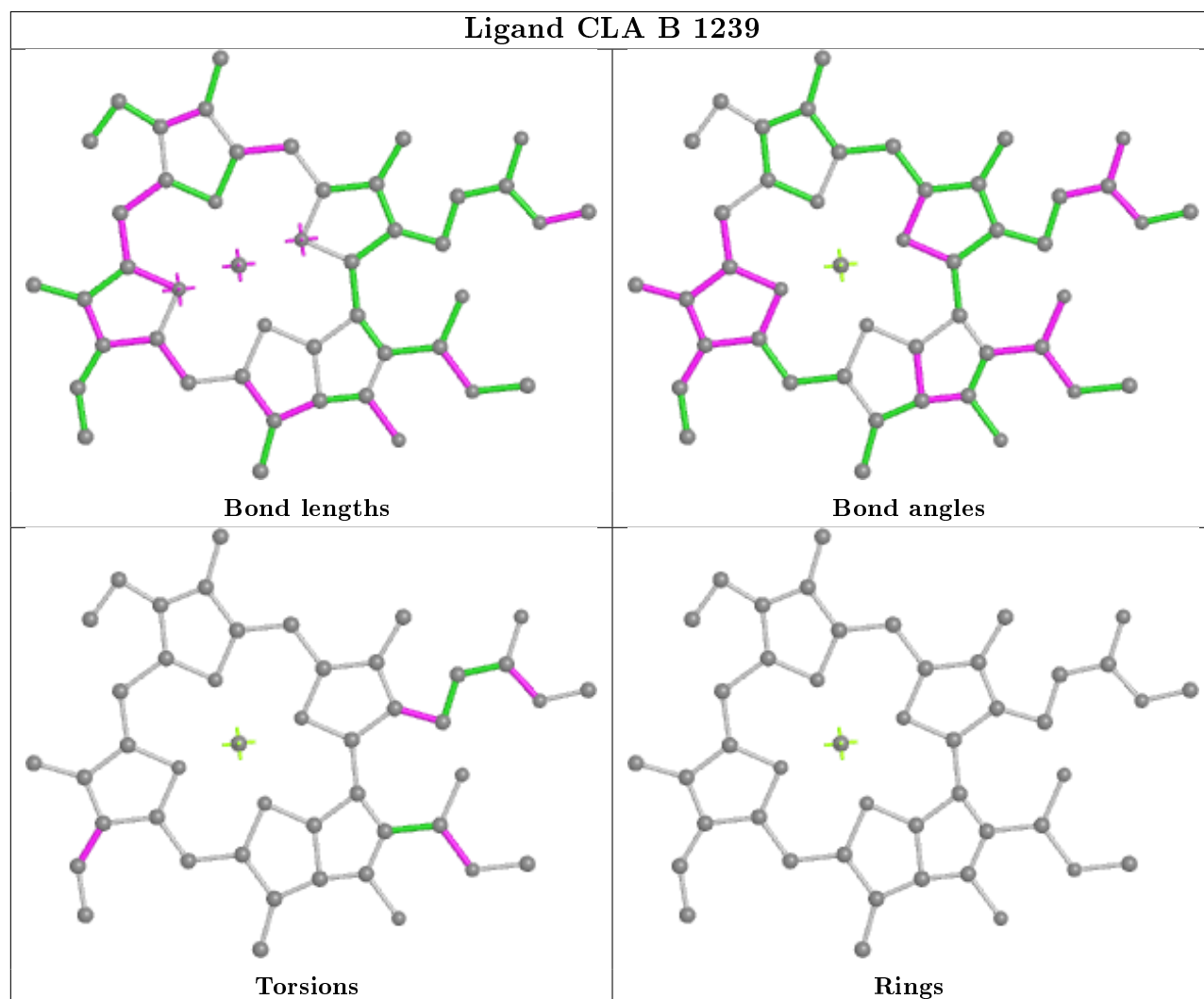


Ligand BCR B 4006**Ligand CLA A 1135****Ligand BCR J 4013**

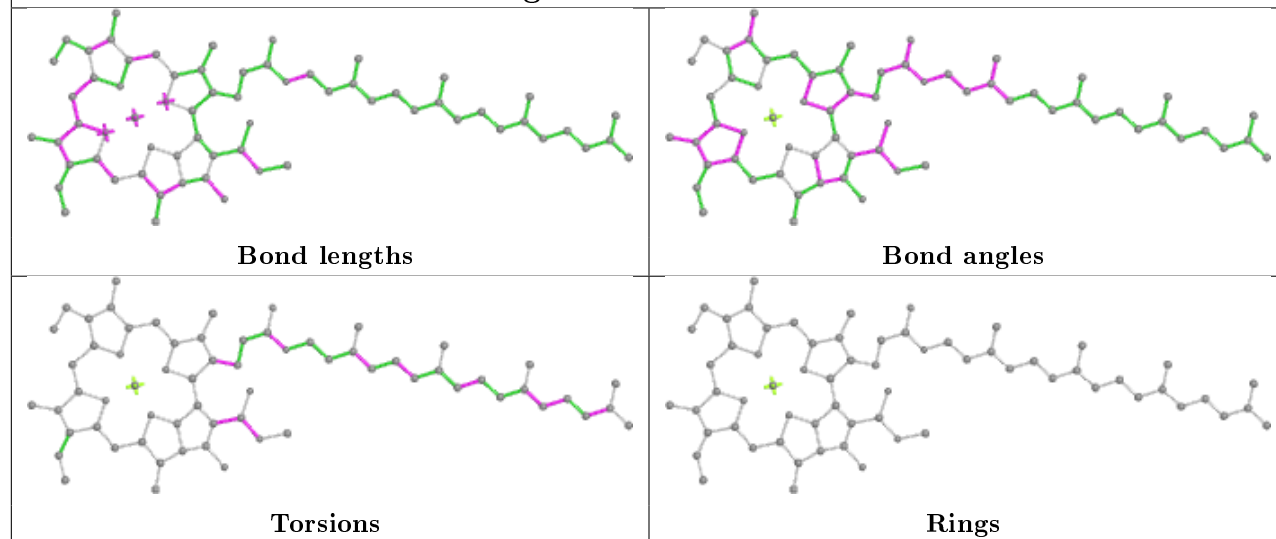
Ligand CLA A 1119



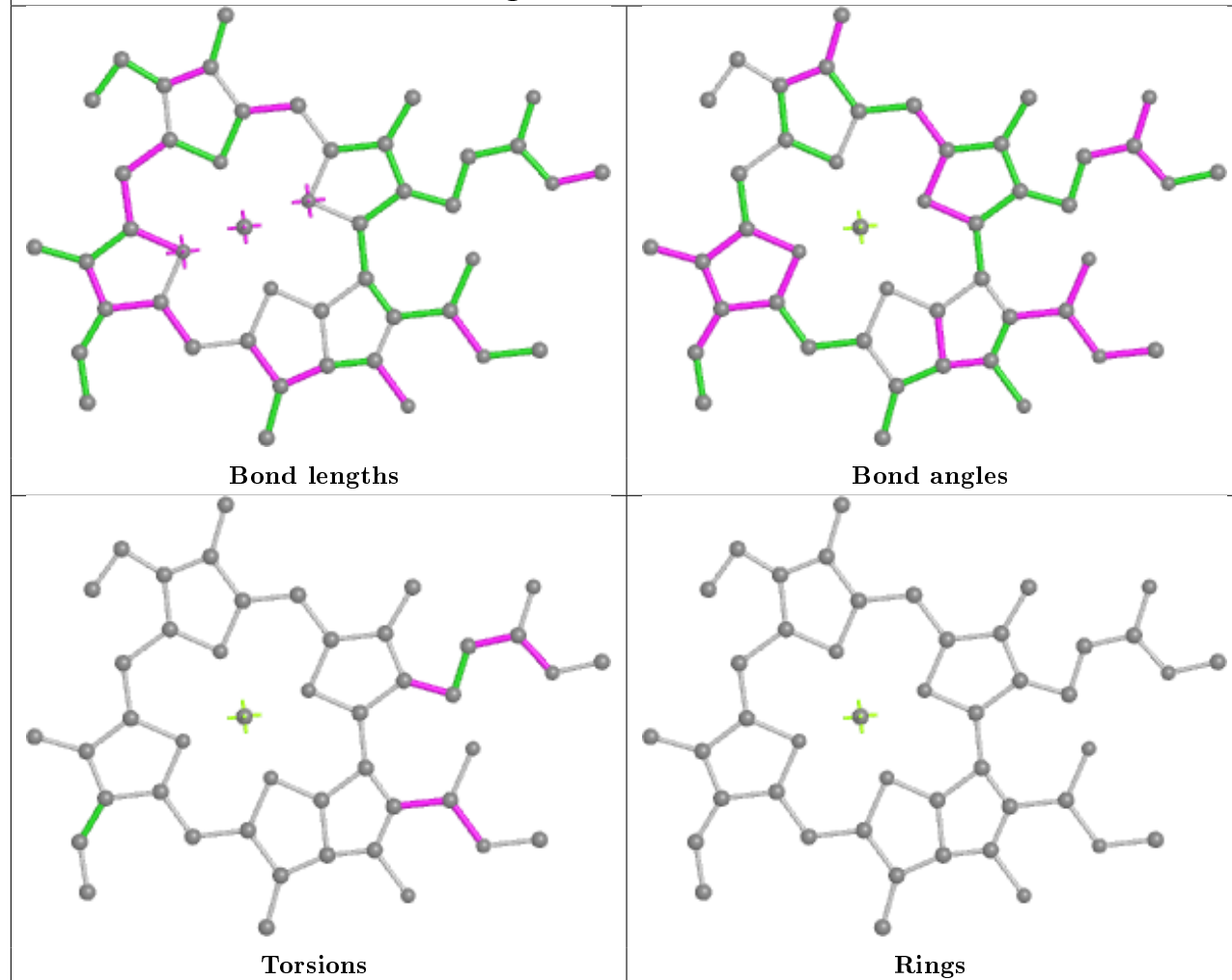
Ligand CLA B 1239

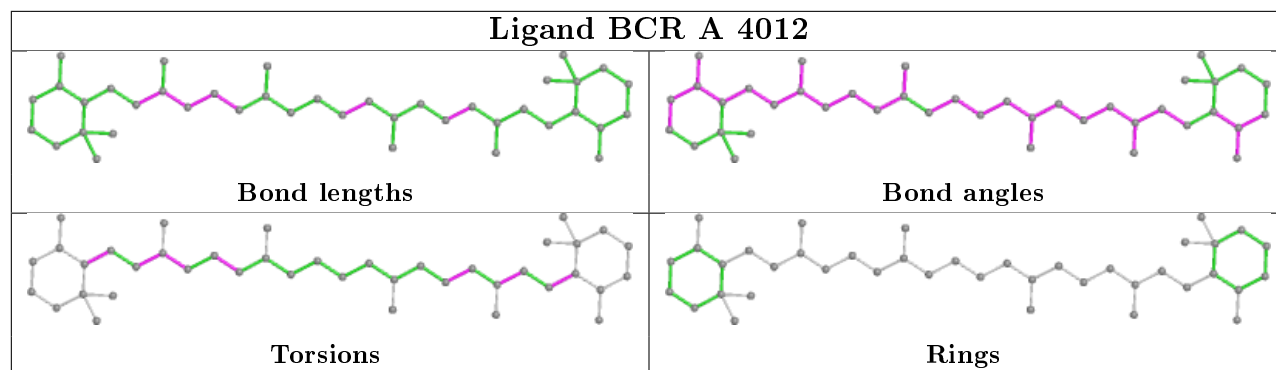
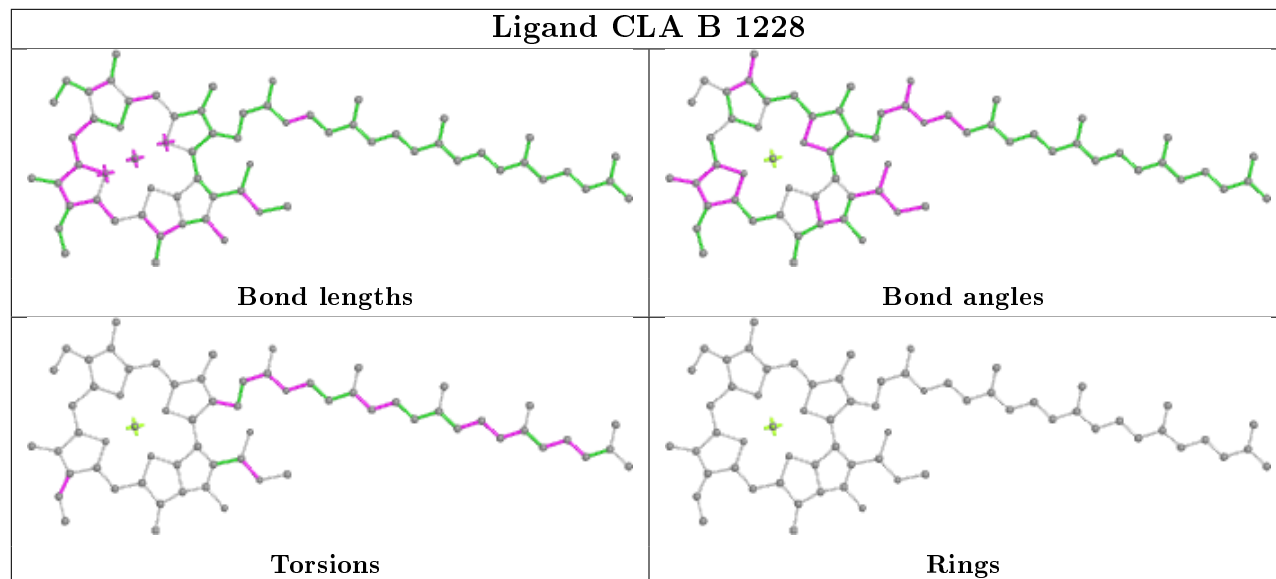
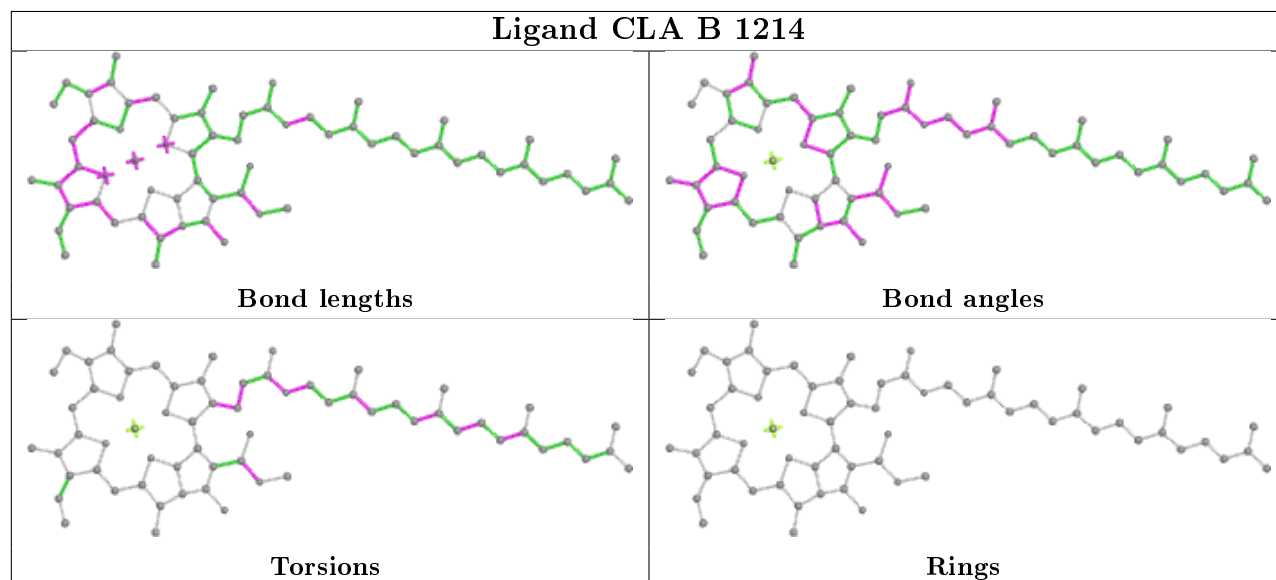


Ligand CLA B 1230

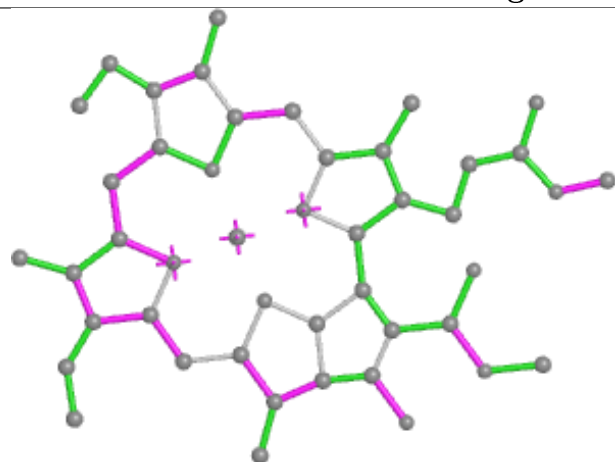


Ligand CLA K 1401

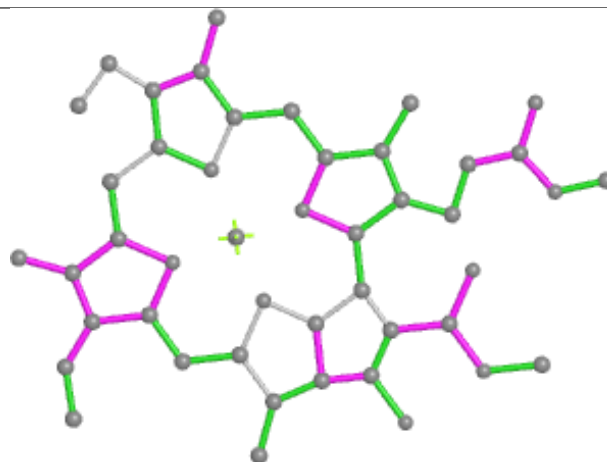


Ligand BCR A 4012**Ligand CLA B 1228****Ligand CLA B 1214**

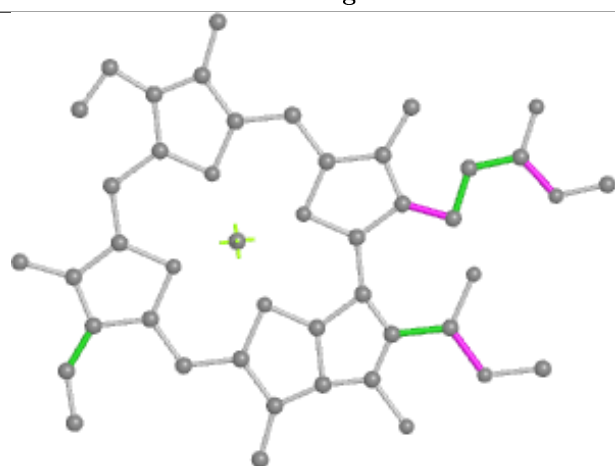
Ligand CLA A 1133



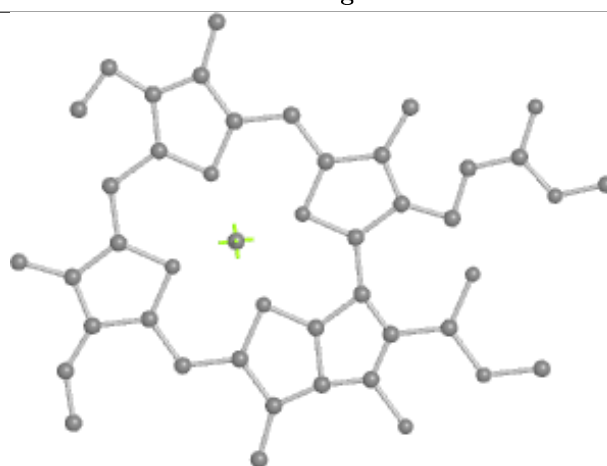
Bond lengths



Bond angles

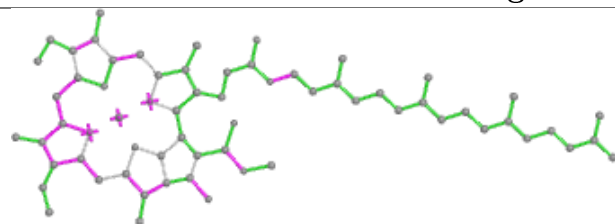


Torsions

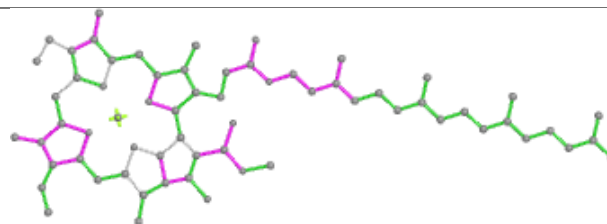


Rings

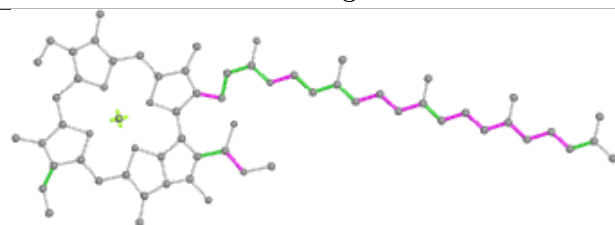
Ligand CLA A 1117



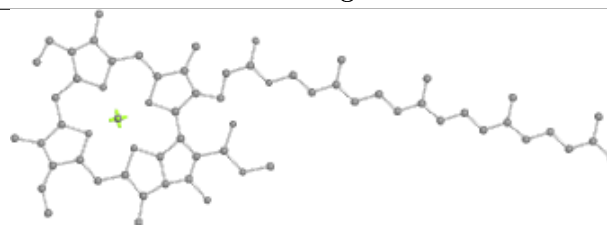
Bond lengths



Bond angles

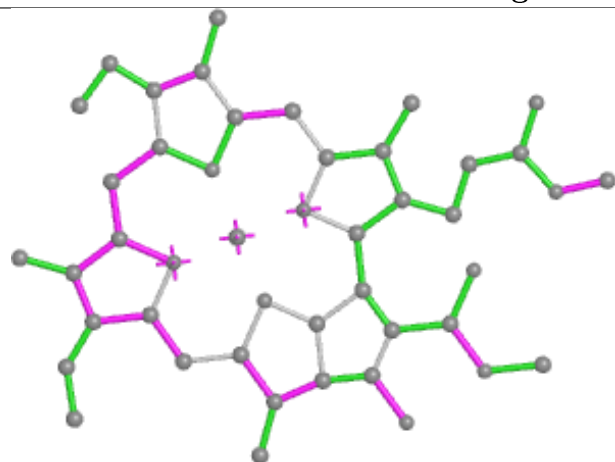


Torsions

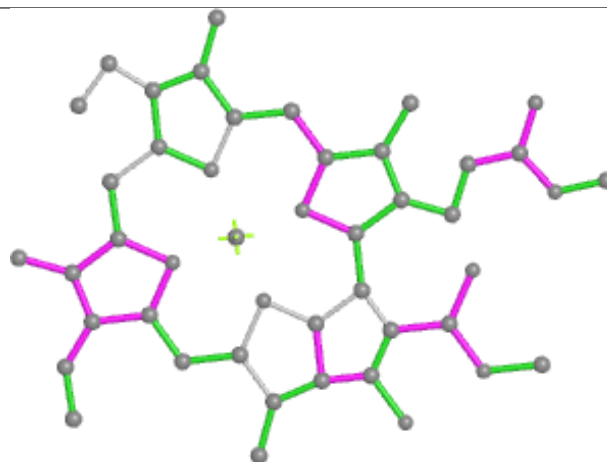


Rings

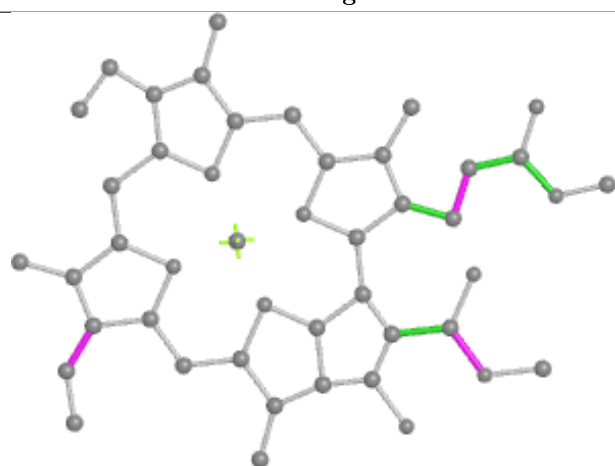
Ligand CLA J 1303



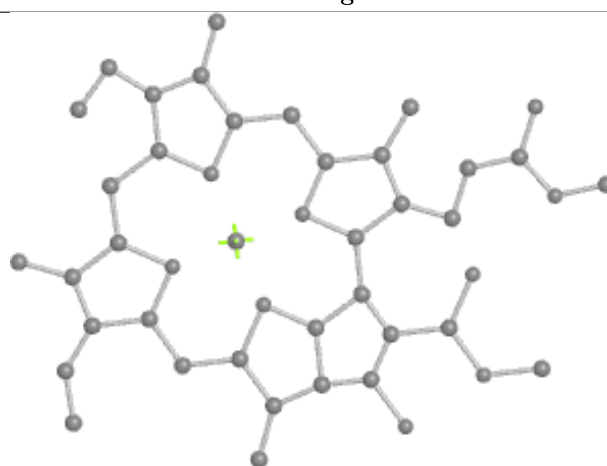
Bond lengths



Bond angles

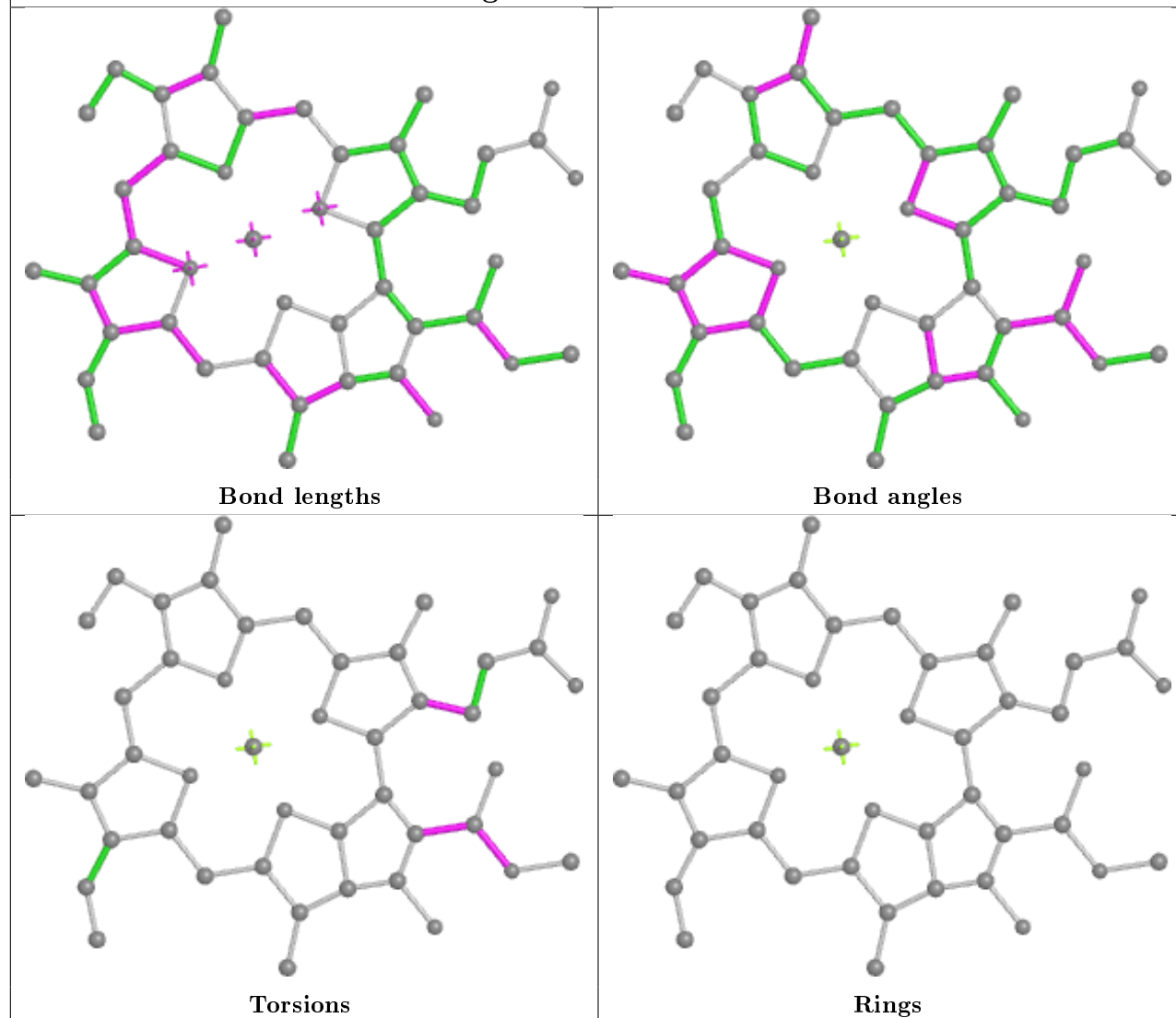


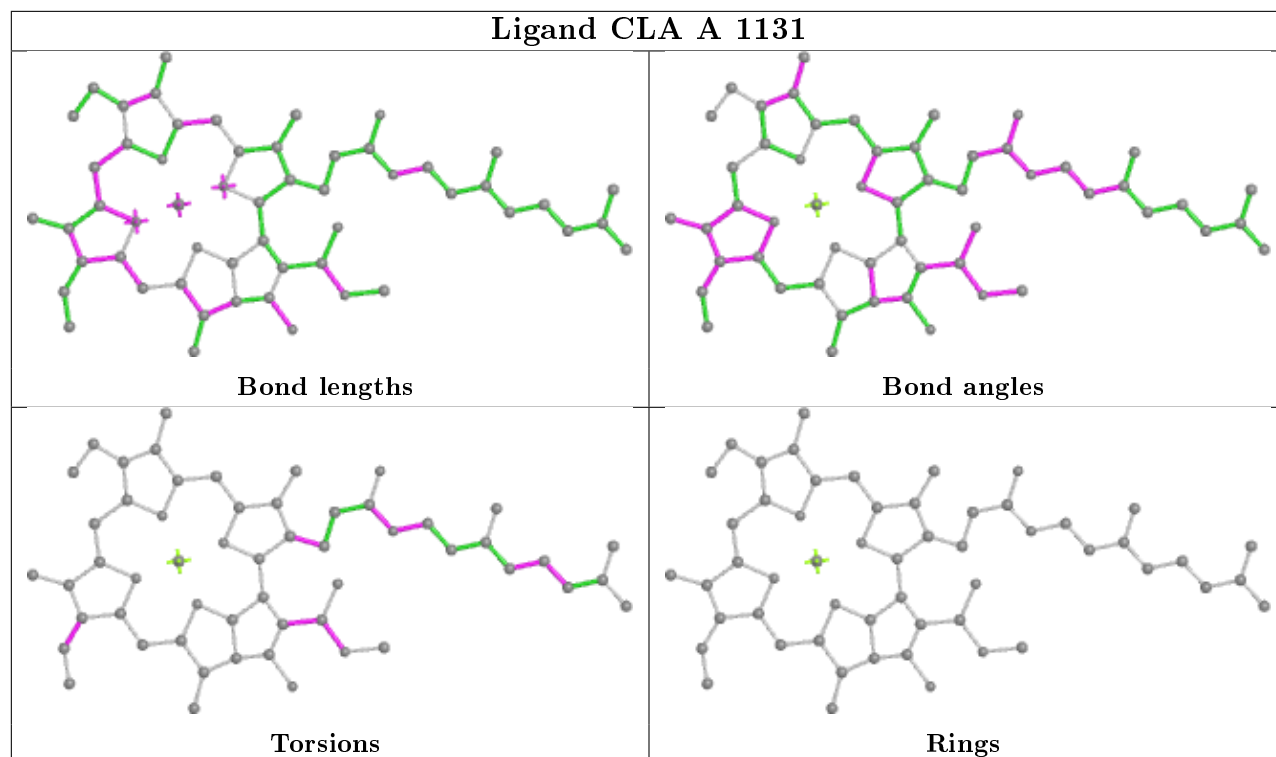
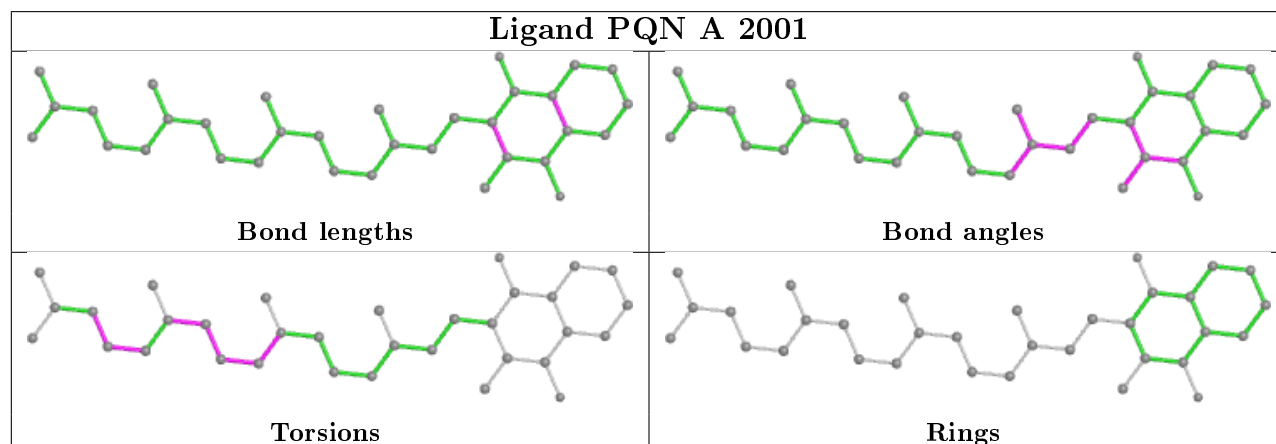
Torsions

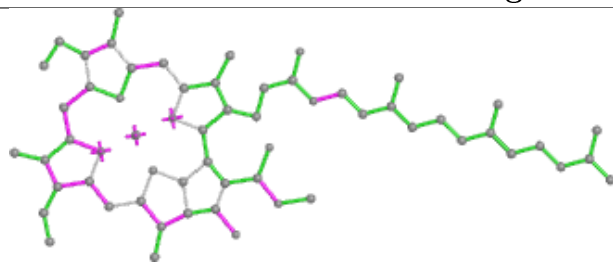
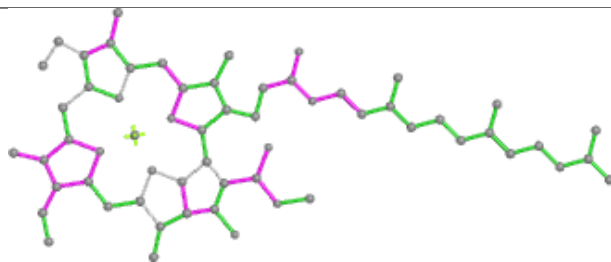
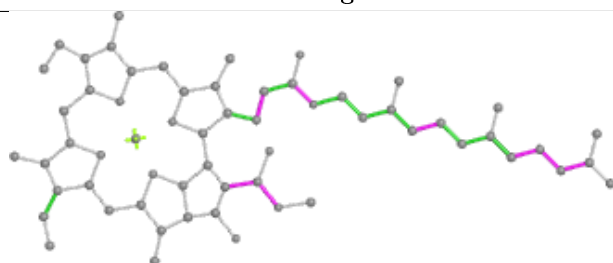
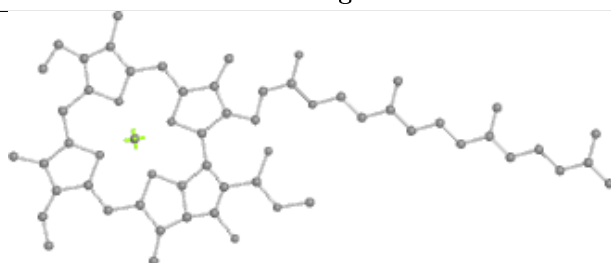
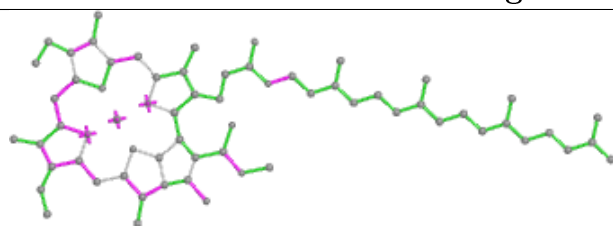
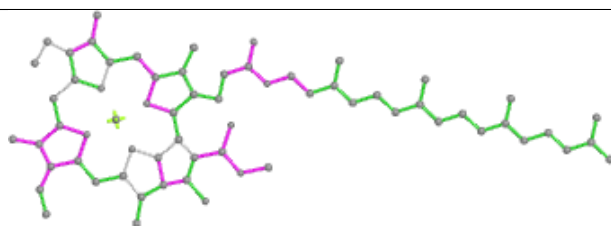
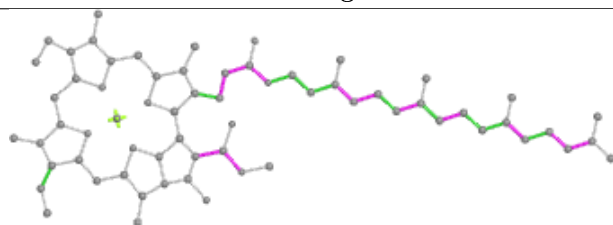
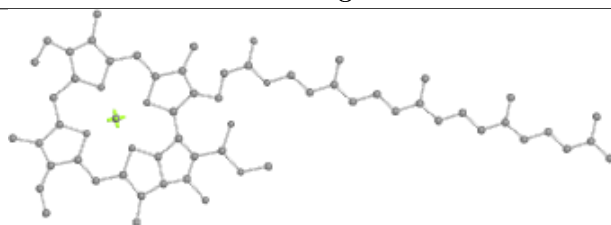


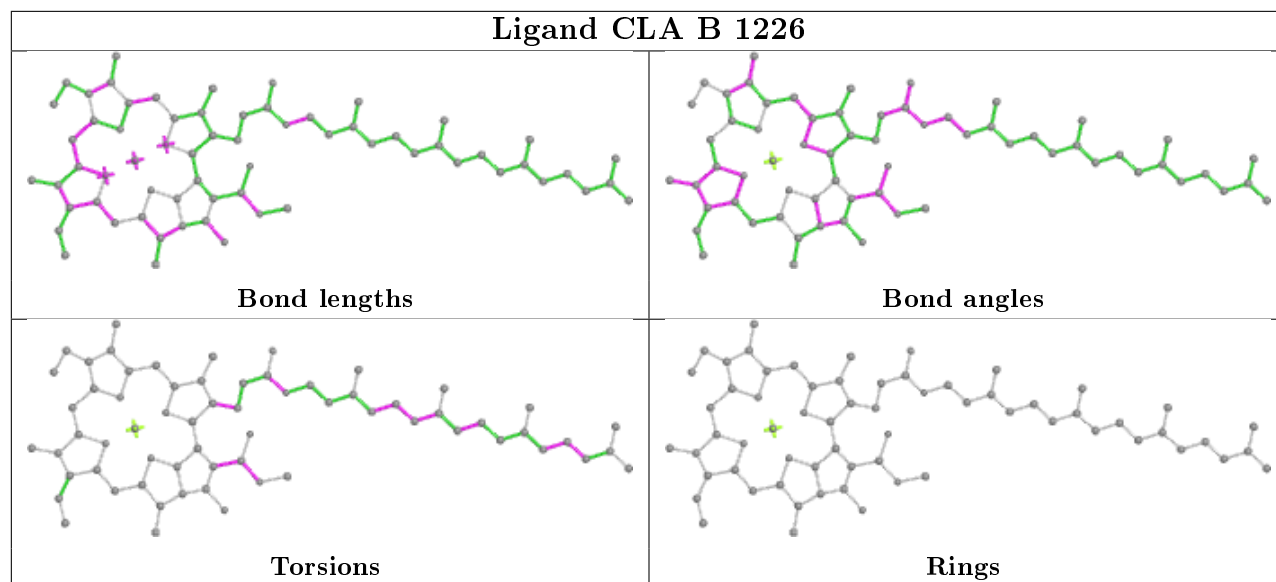
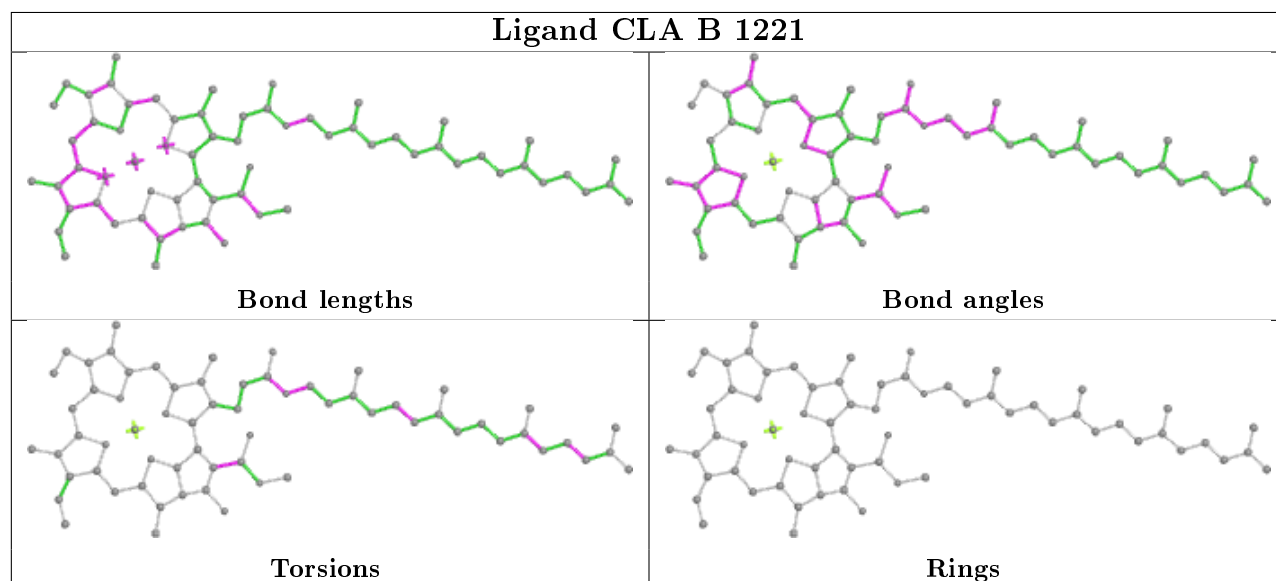
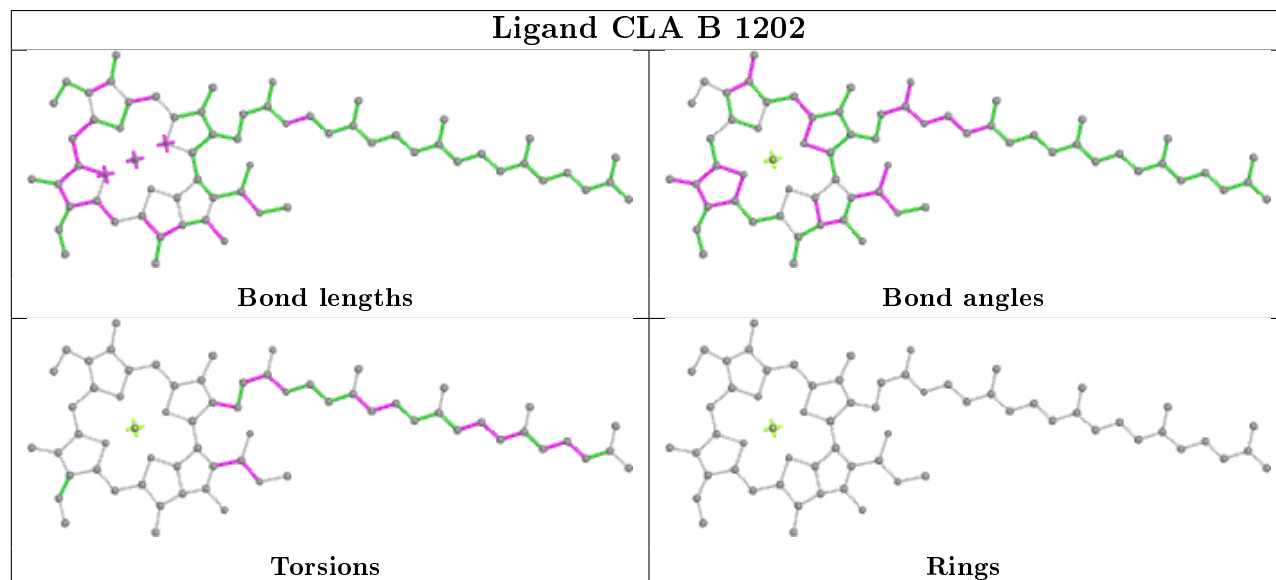
Rings

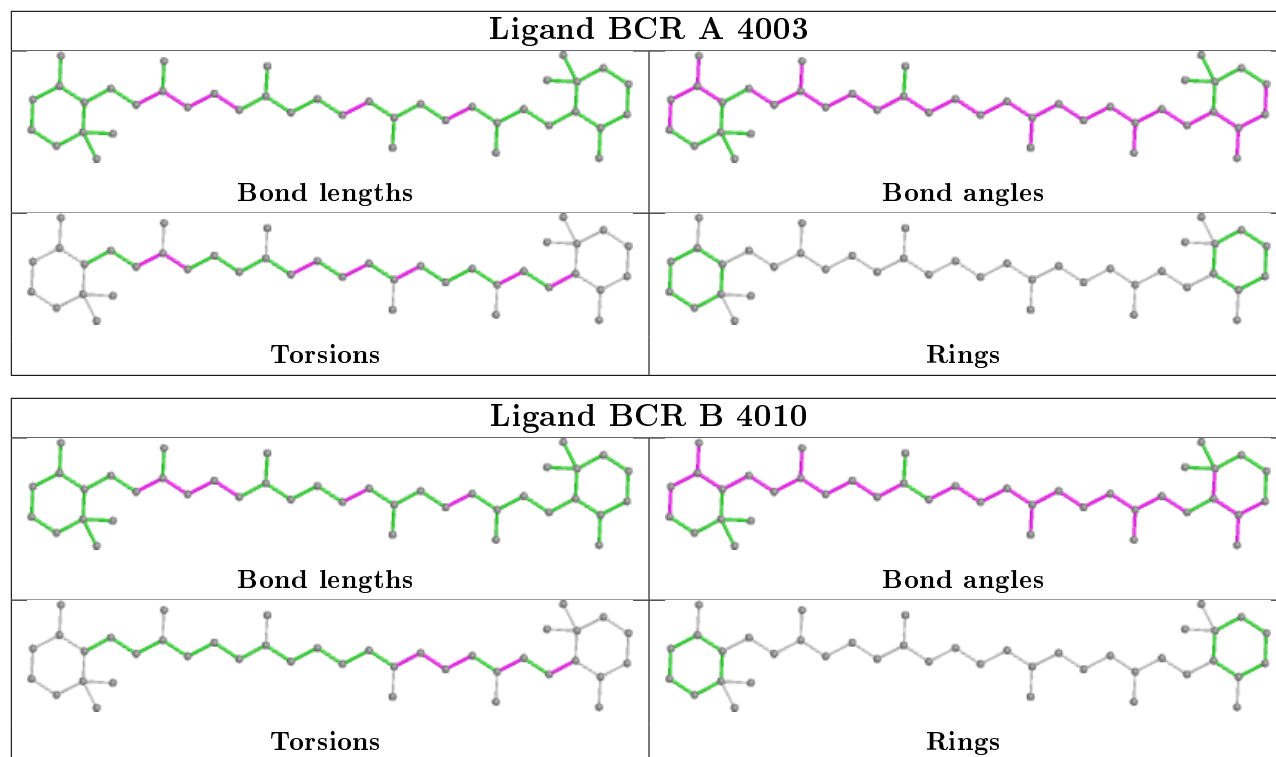
Ligand CLA B 1208

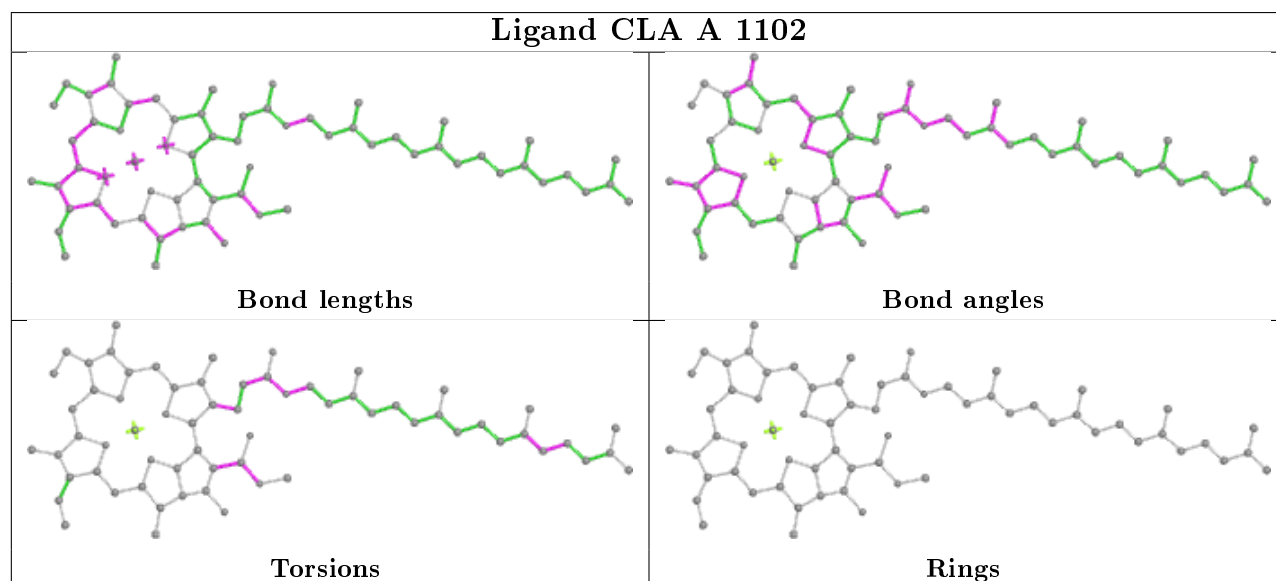
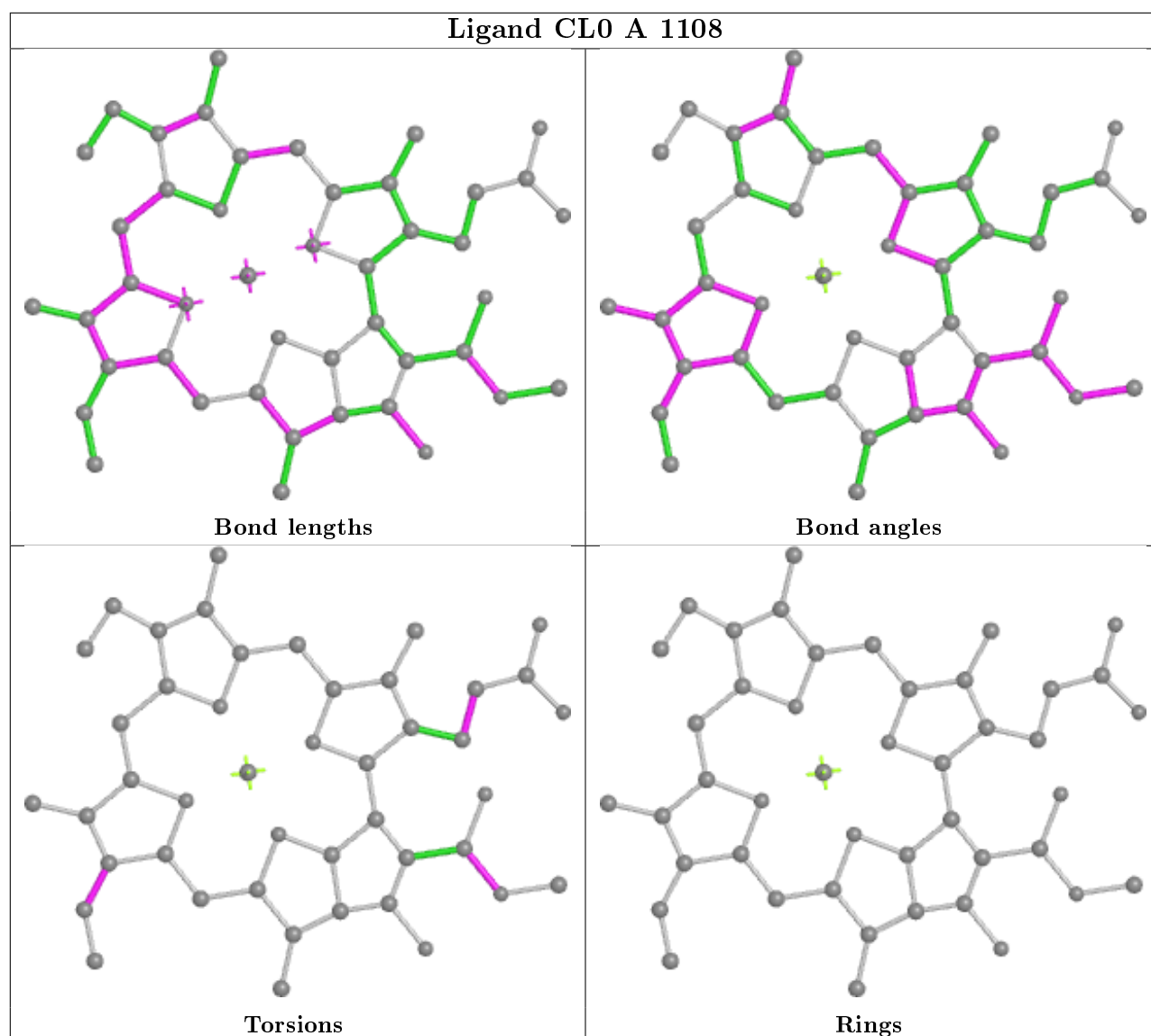


Ligand CLA A 1131**Ligand PQN A 2001**

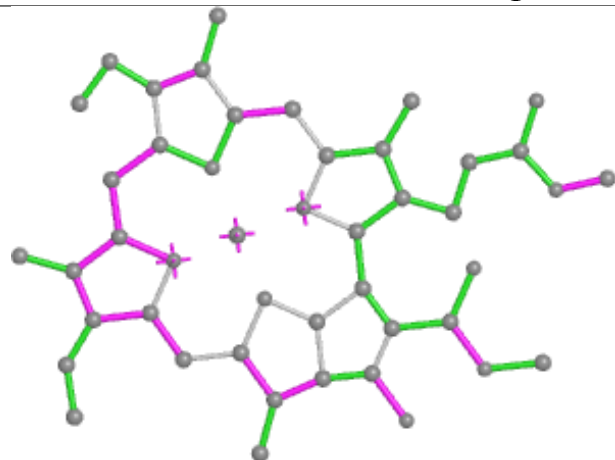
Ligand CLA A 1111**Bond lengths****Bond angles****Torsions****Rings****Ligand CLA A 1136****Bond lengths****Bond angles****Torsions****Rings**

Ligand CLA B 1226**Ligand CLA B 1221****Ligand CLA B 1202**

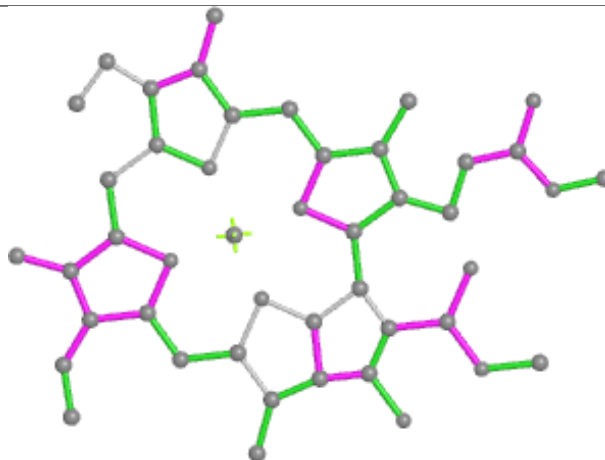




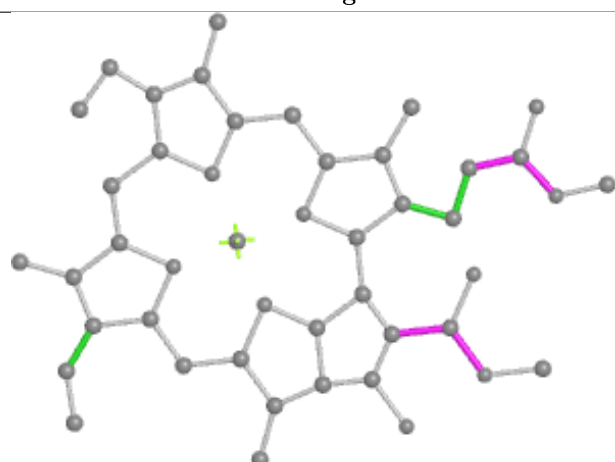
Ligand CLA B 1211



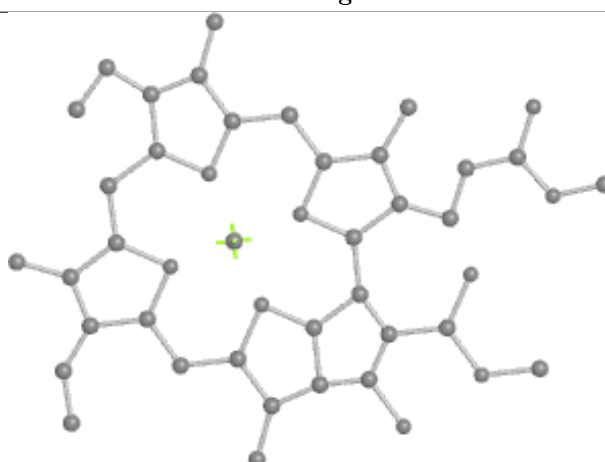
Bond lengths



Bond angles

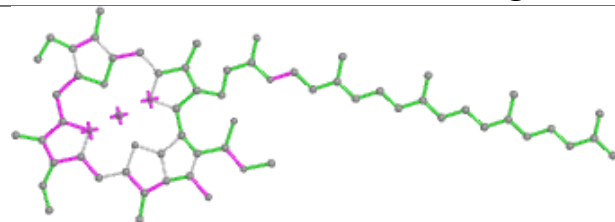


Torsions

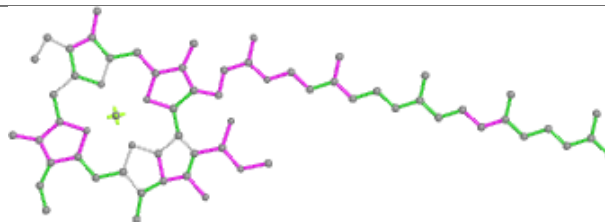


Rings

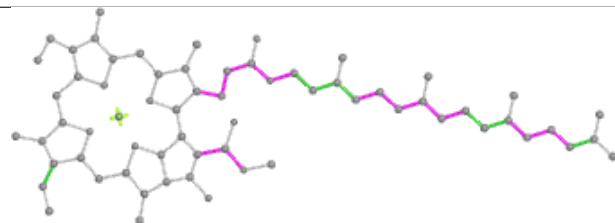
Ligand CLA B 1021



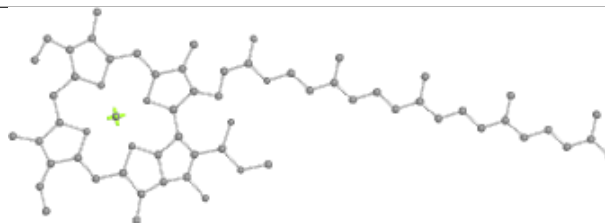
Bond lengths



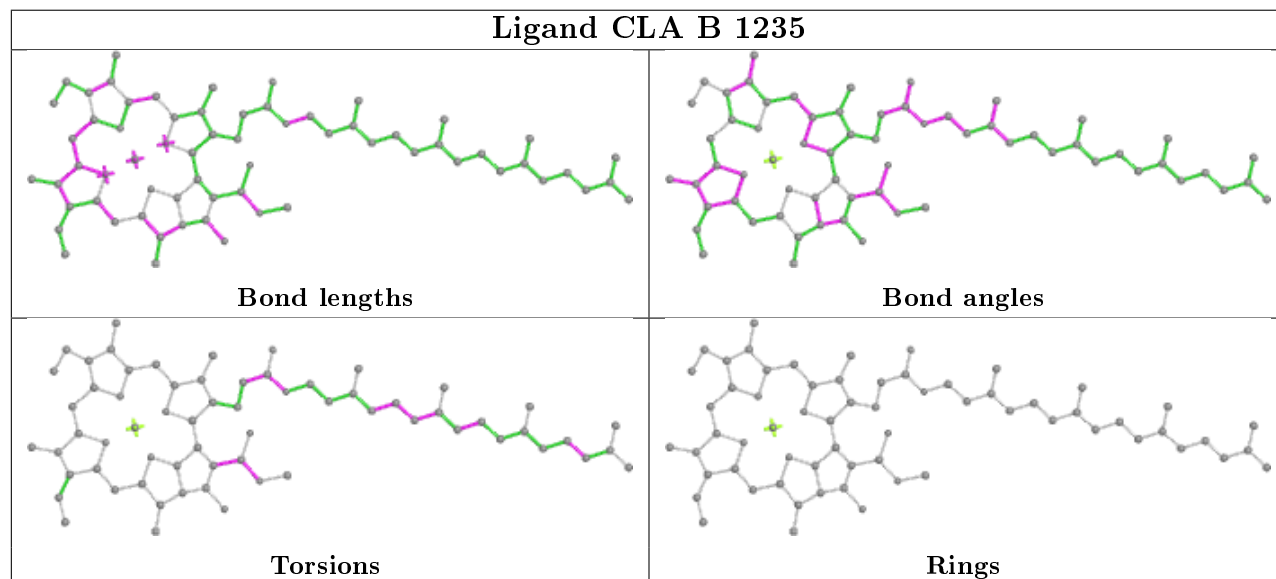
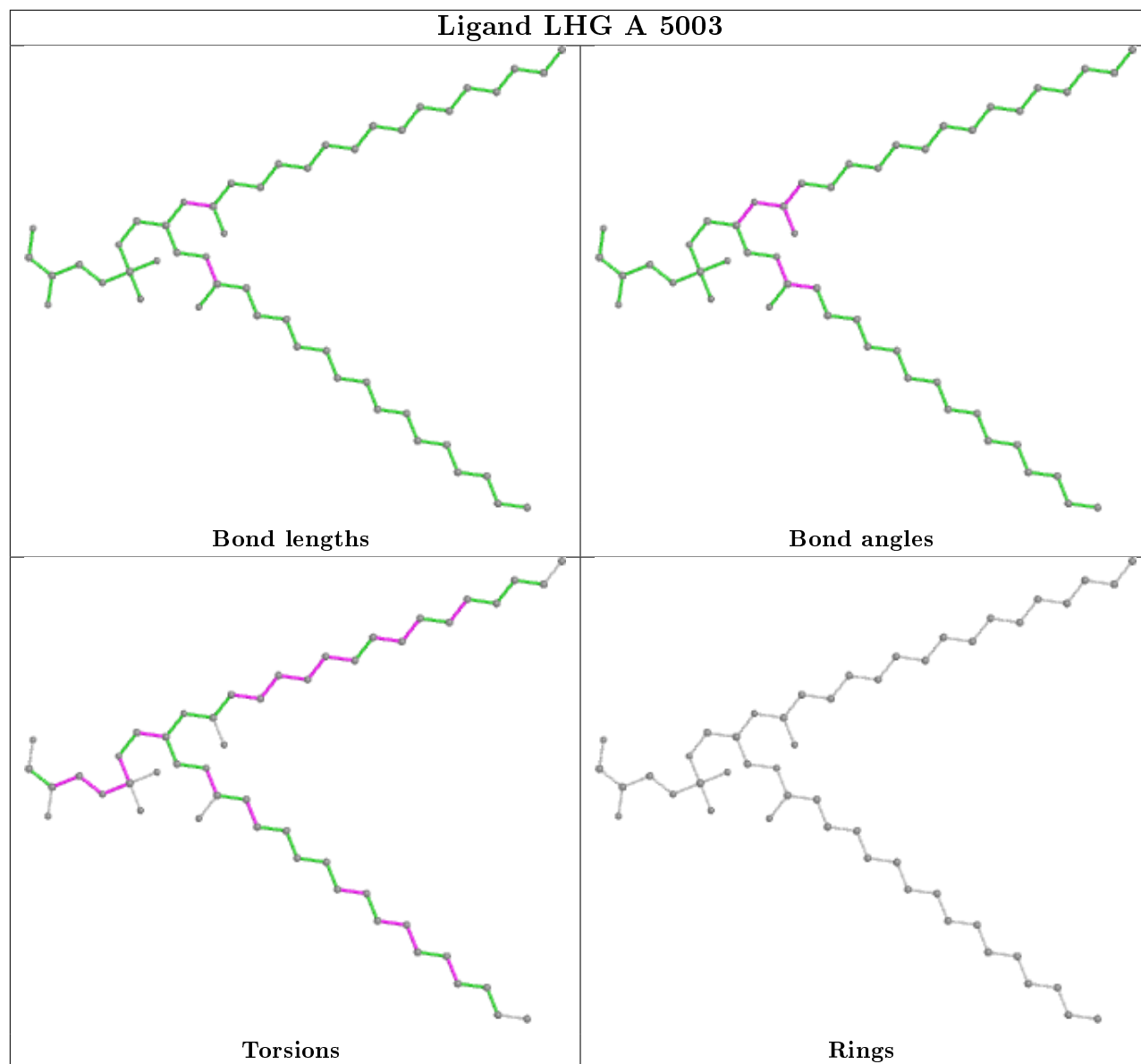
Bond angles



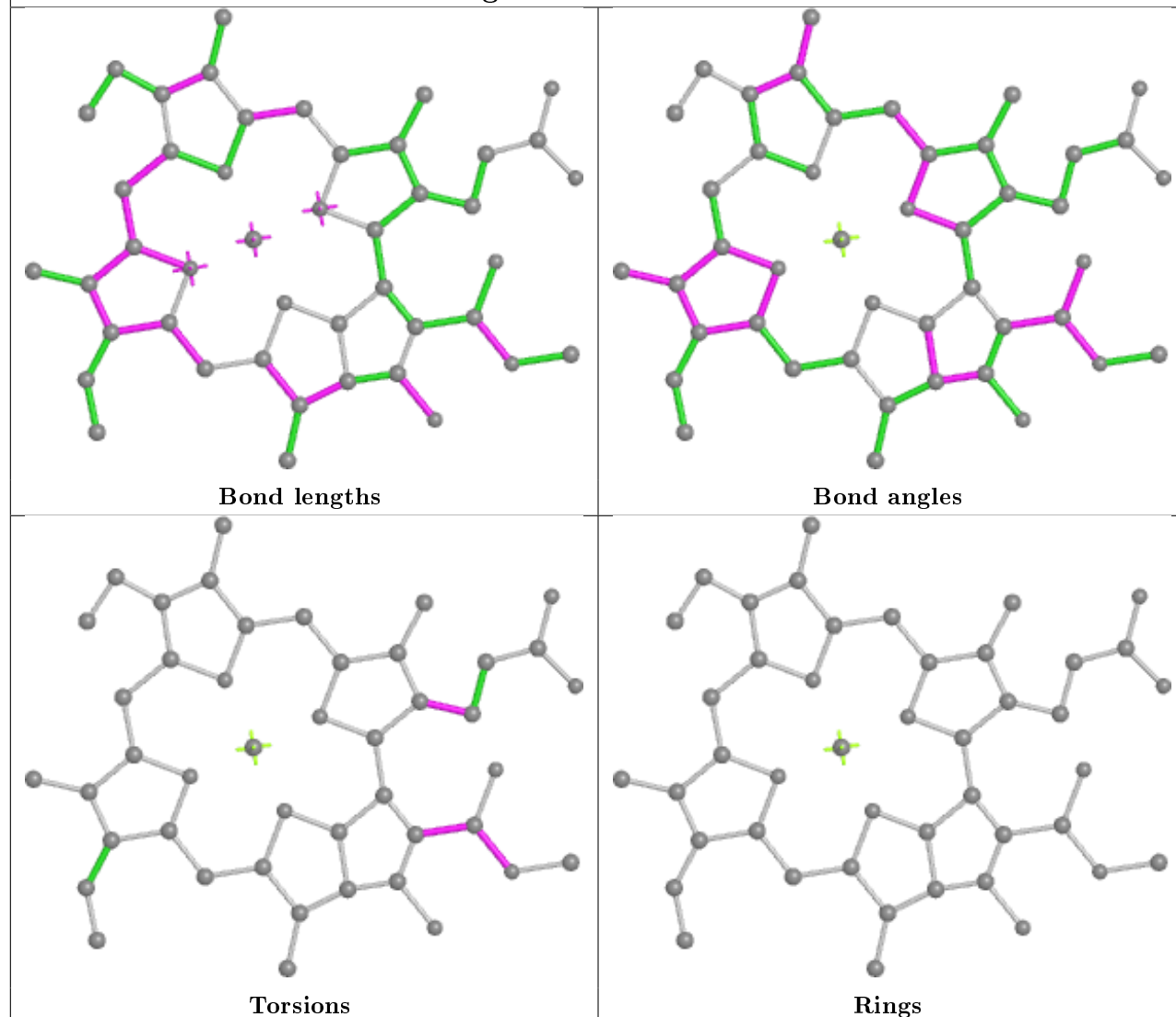
Torsions



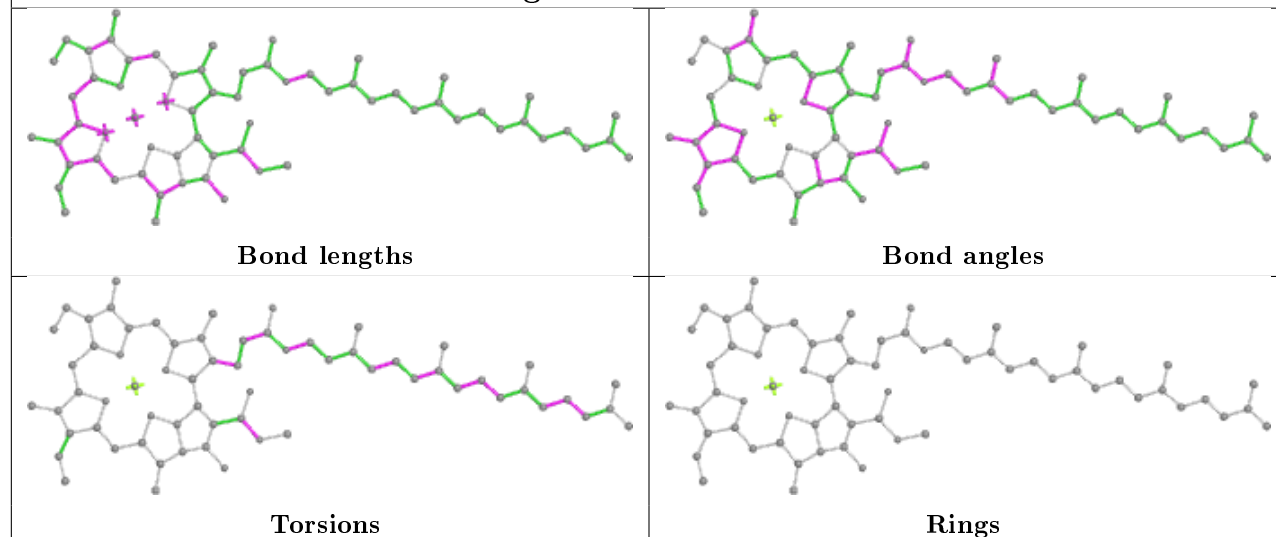
Rings

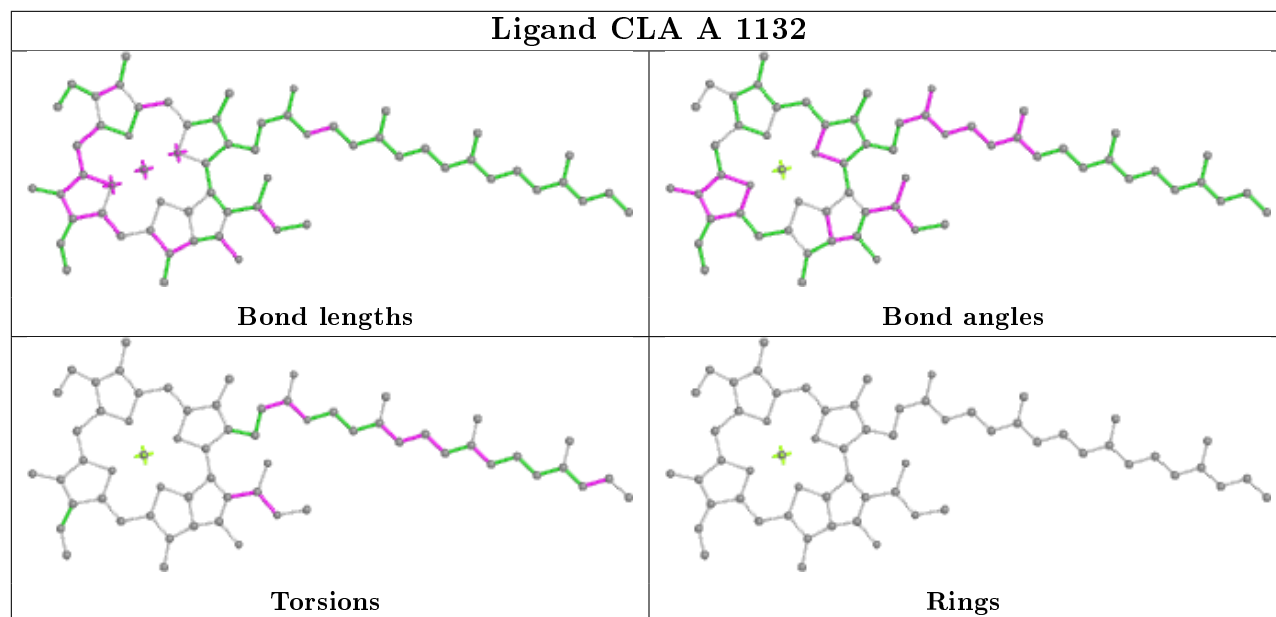
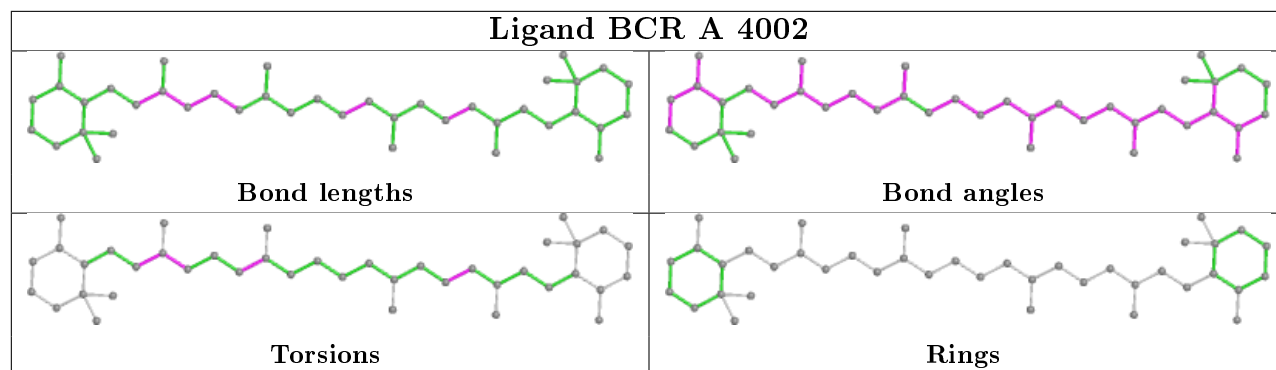


Ligand CLA A 1112

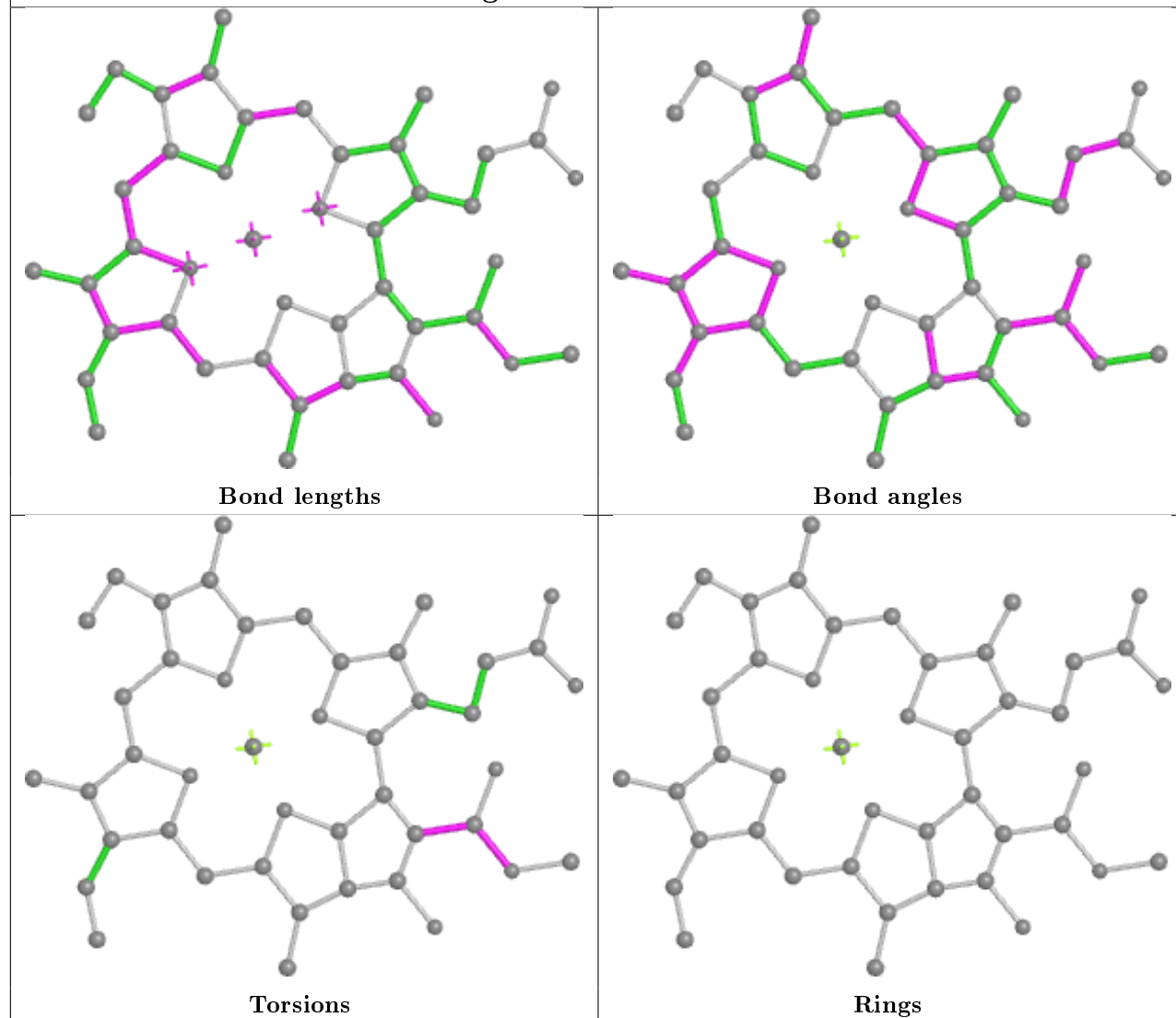


Ligand CLA B 1216

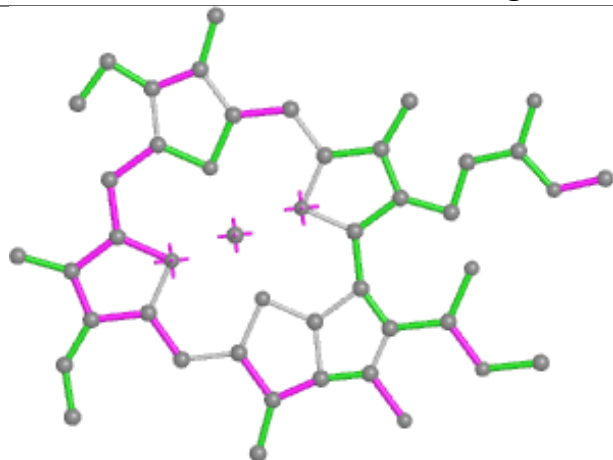




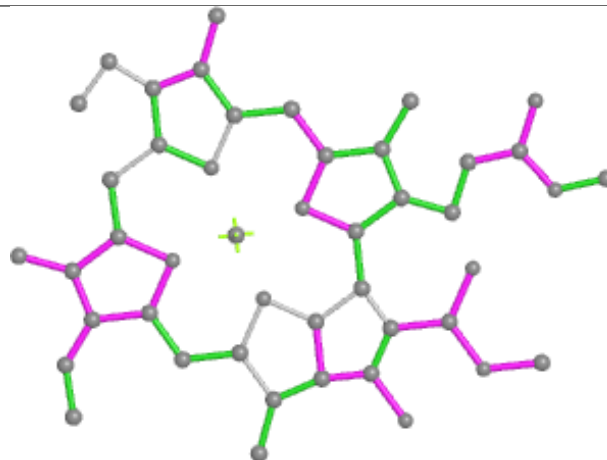
Ligand CLA A 1113



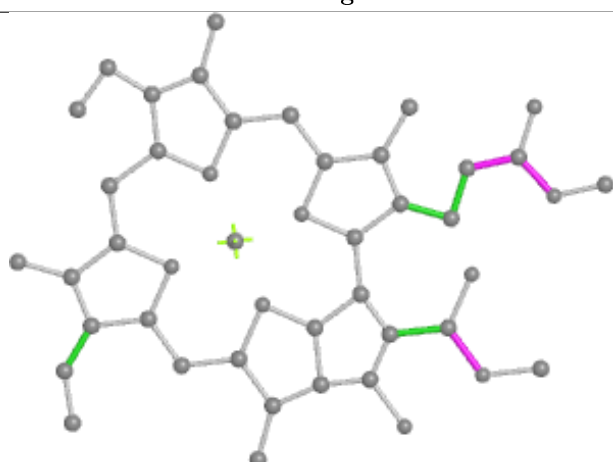
Ligand CLA B 1206



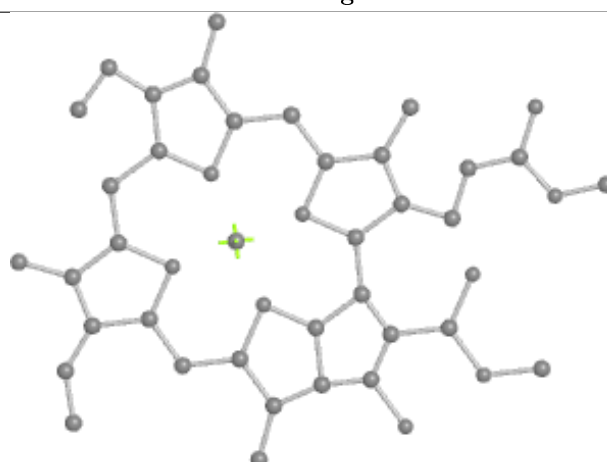
Bond lengths



Bond angles

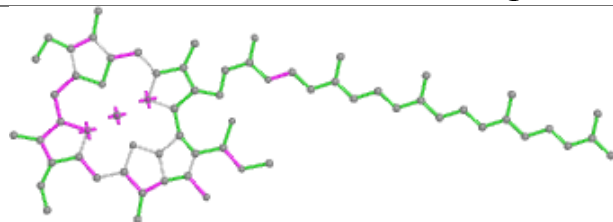


Torsions

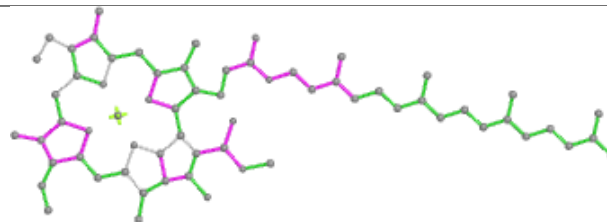


Rings

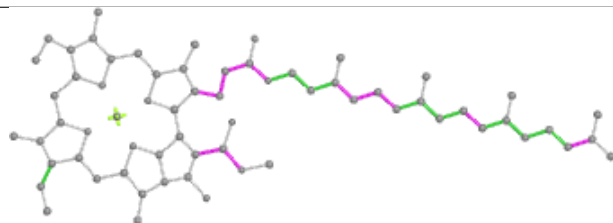
Ligand CLA A 1140



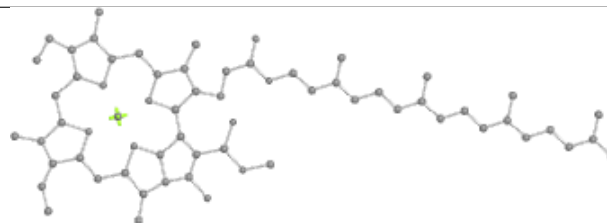
Bond lengths



Bond angles

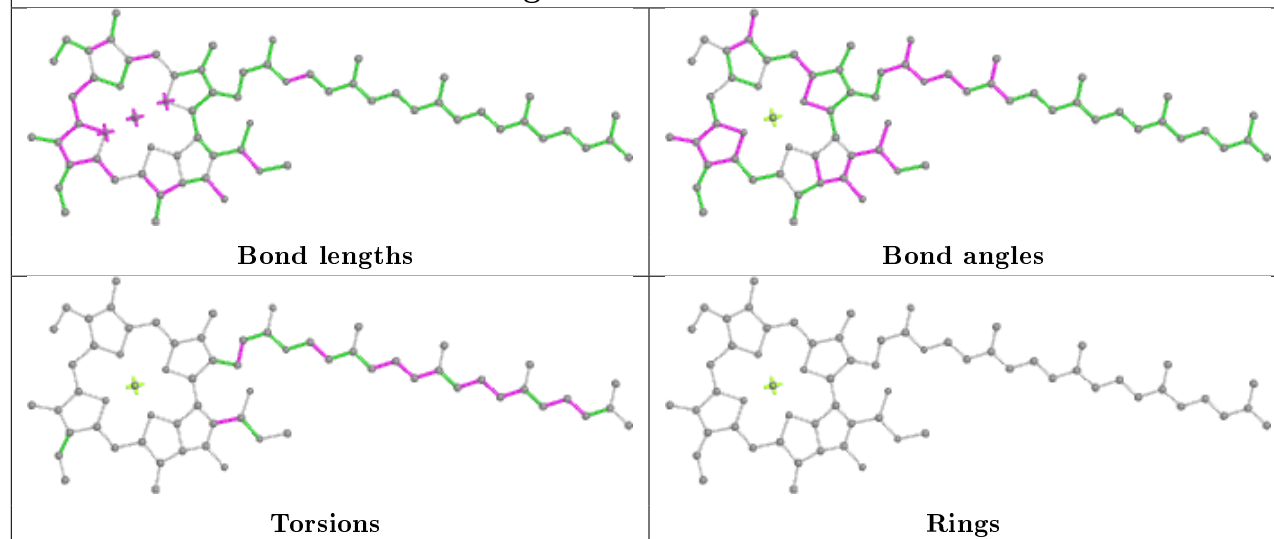


Torsions

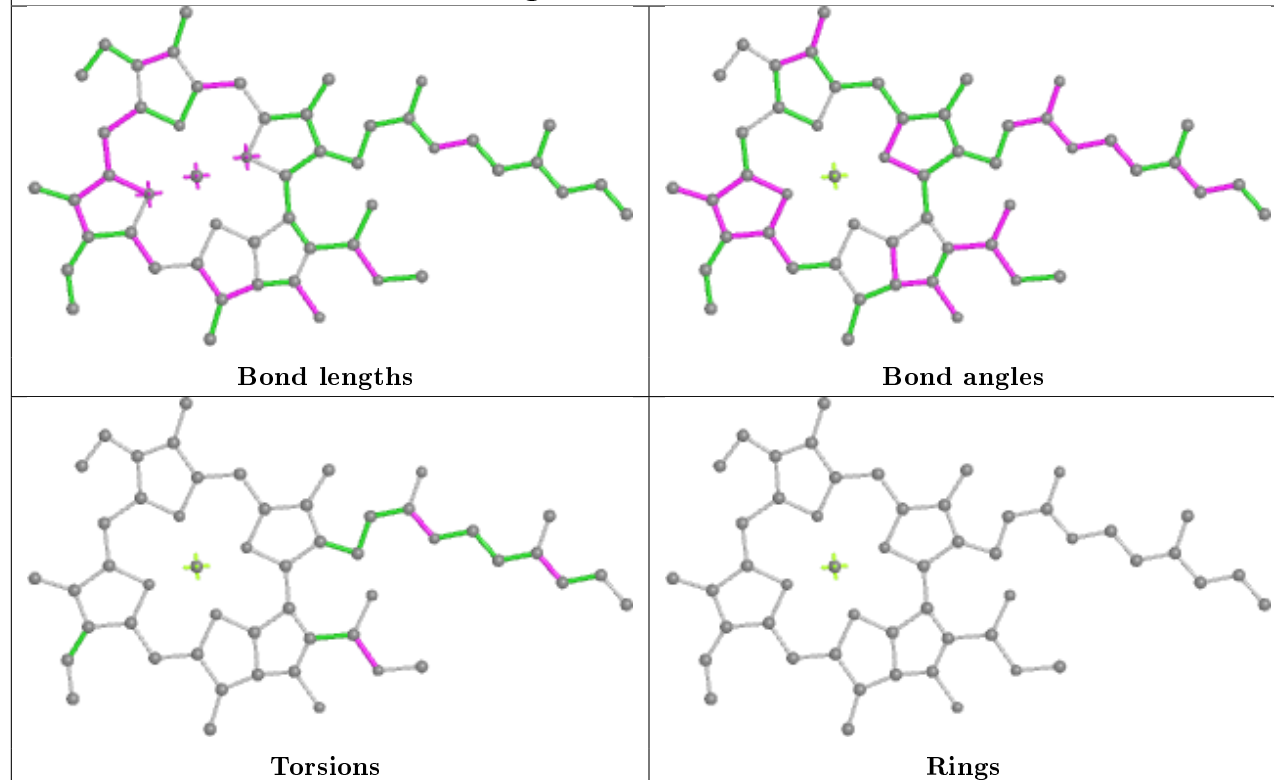


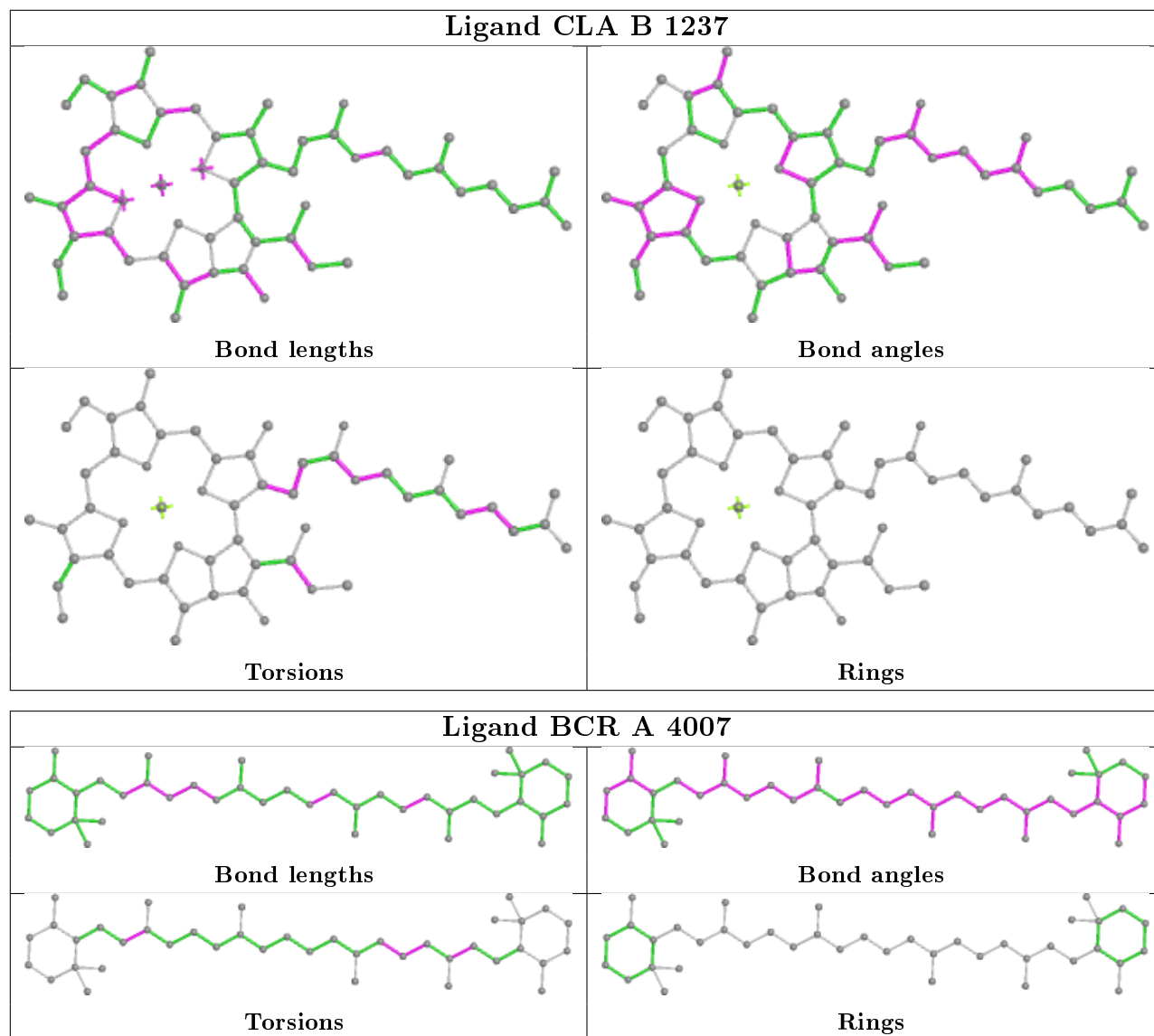
Rings

Ligand CLA A 1012

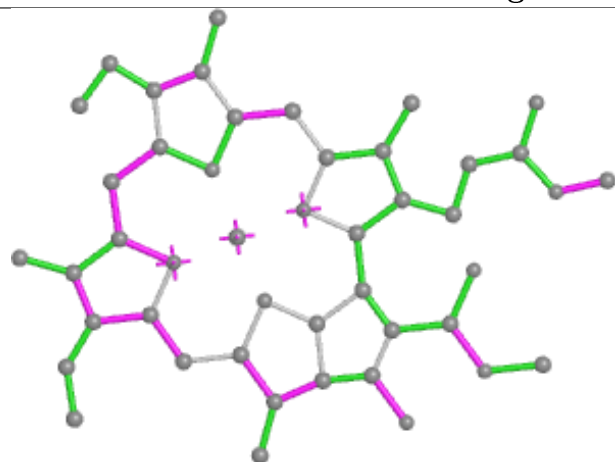


Ligand CLA A 1125

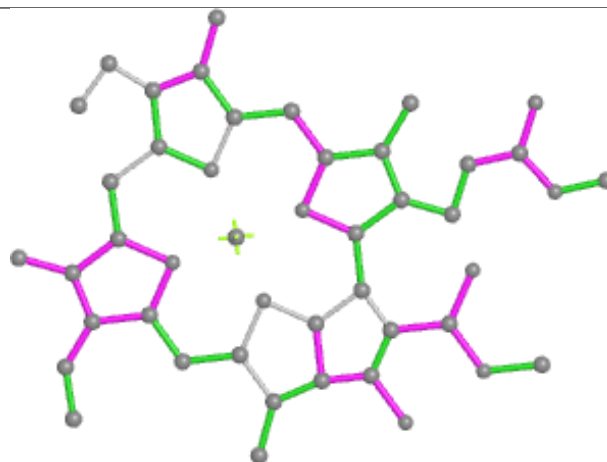




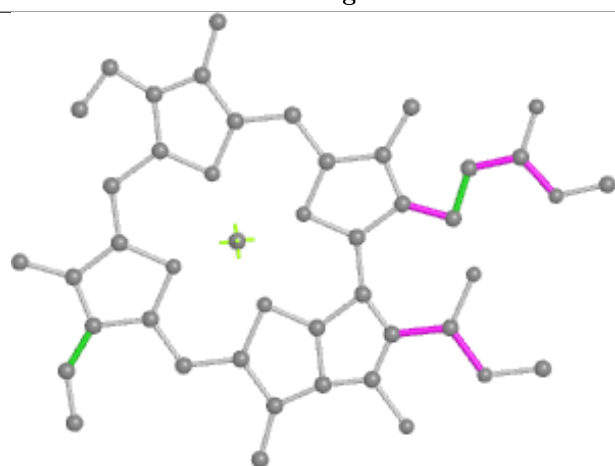
Ligand CLA A 1129



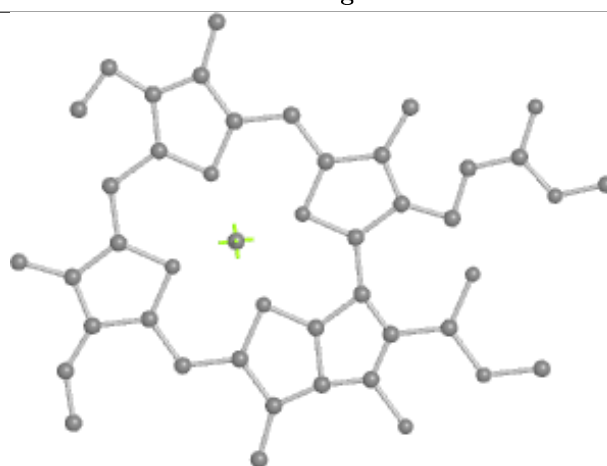
Bond lengths



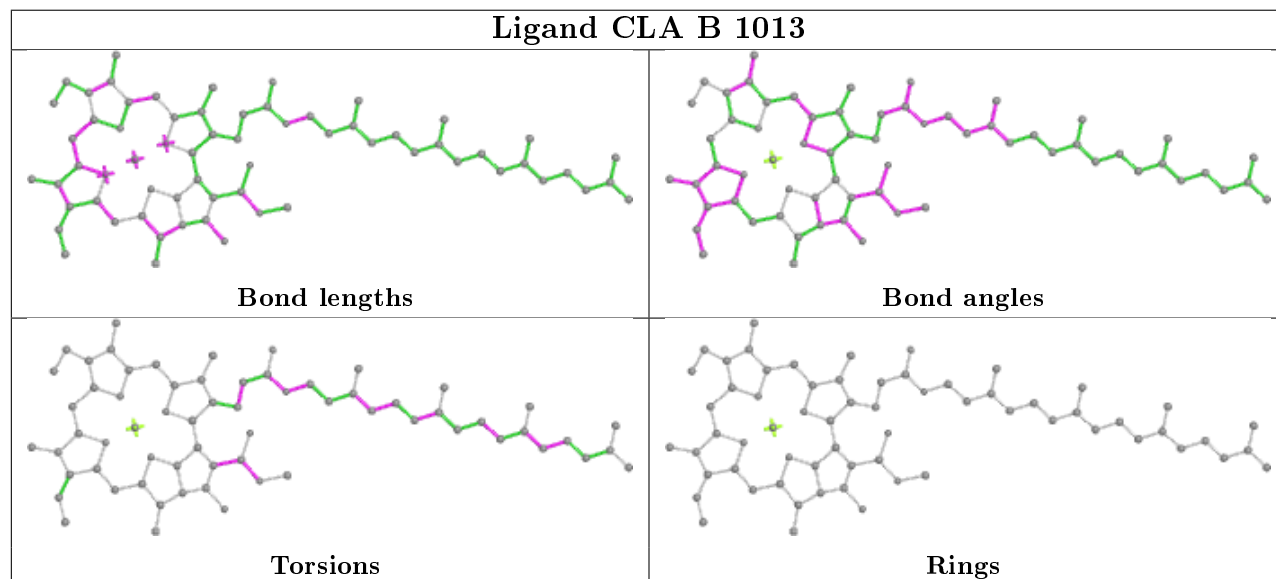
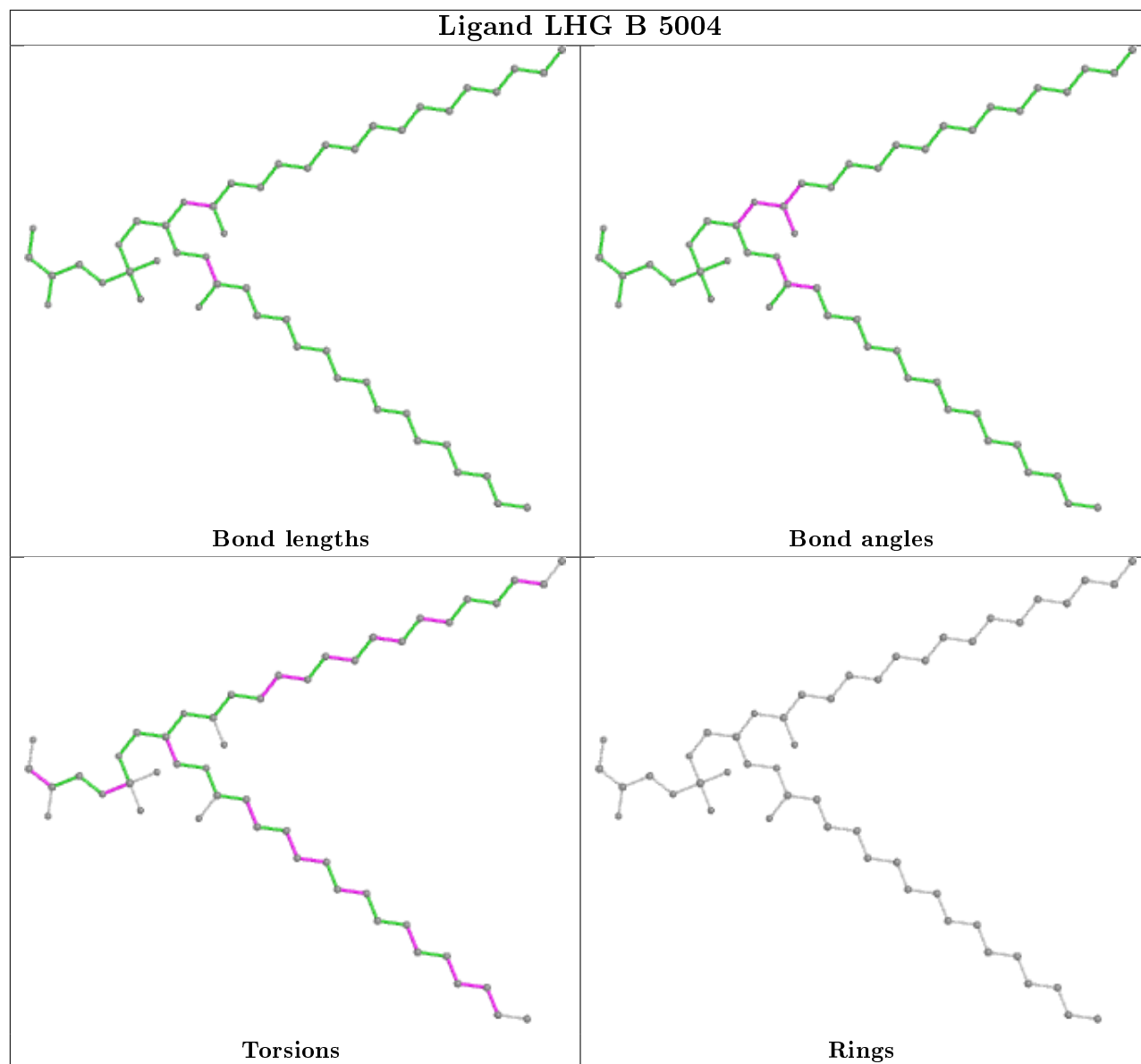
Bond angles

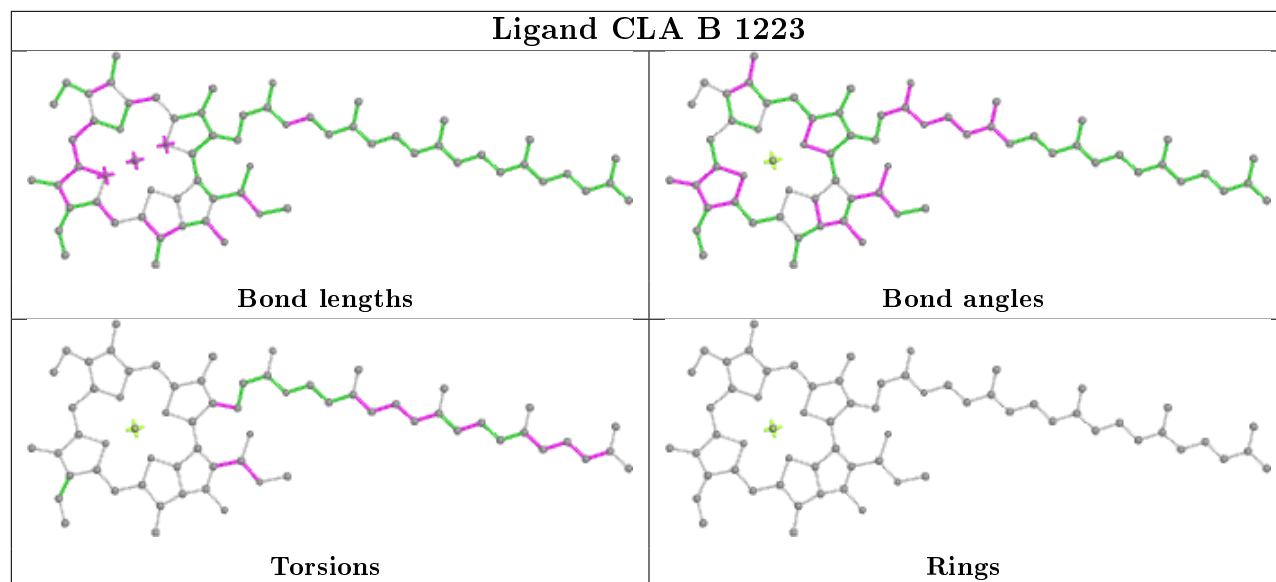
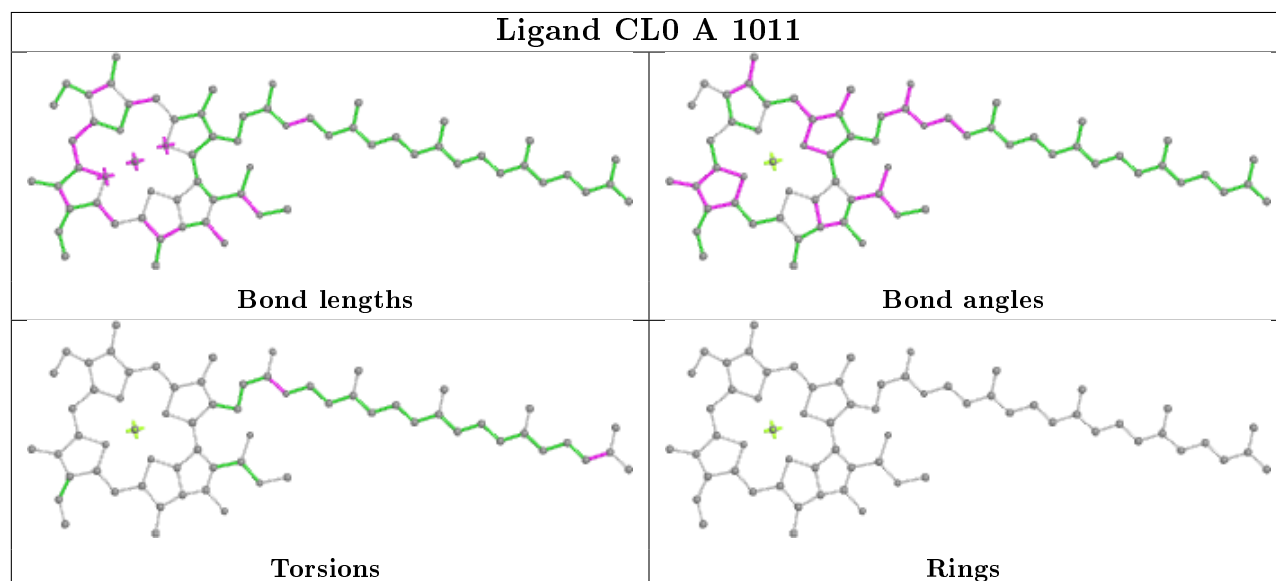
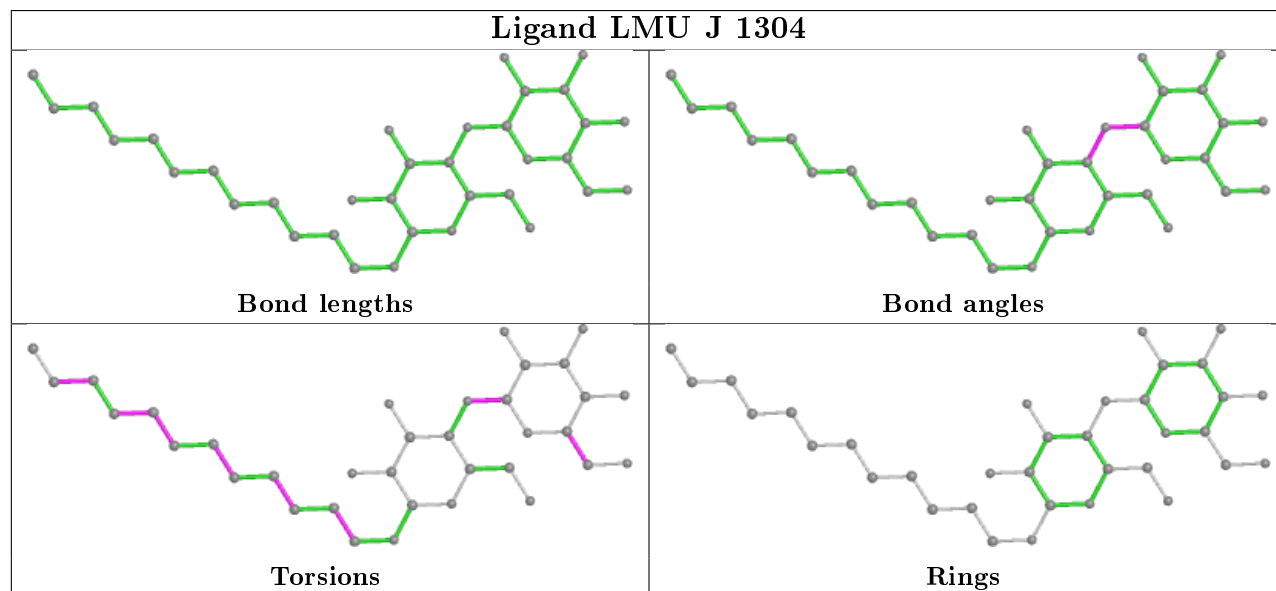


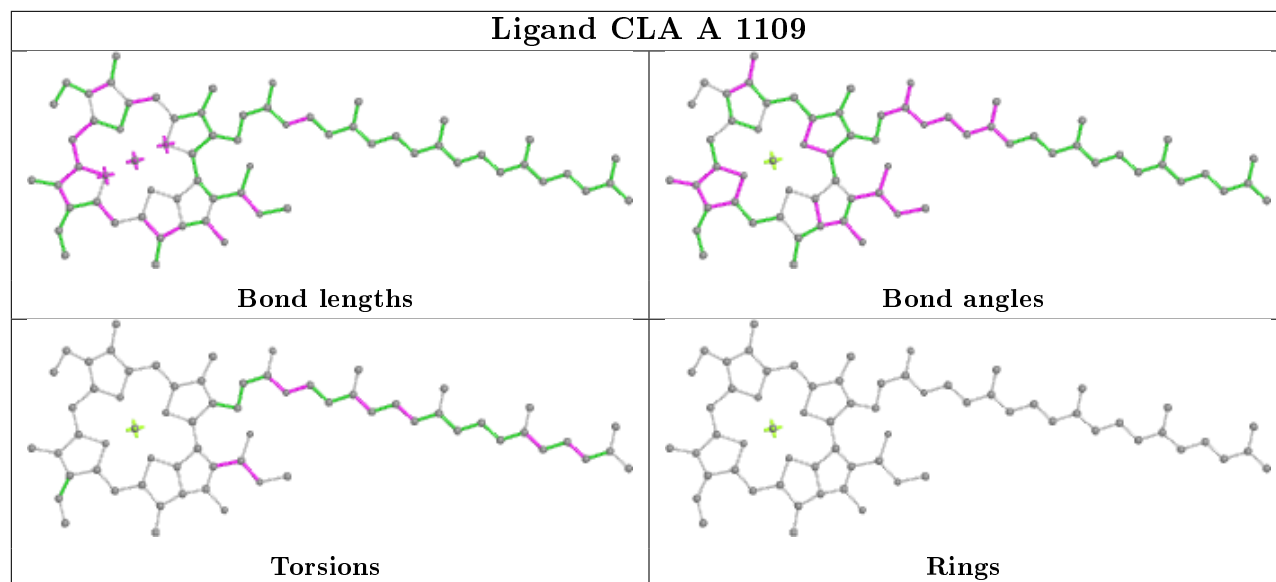
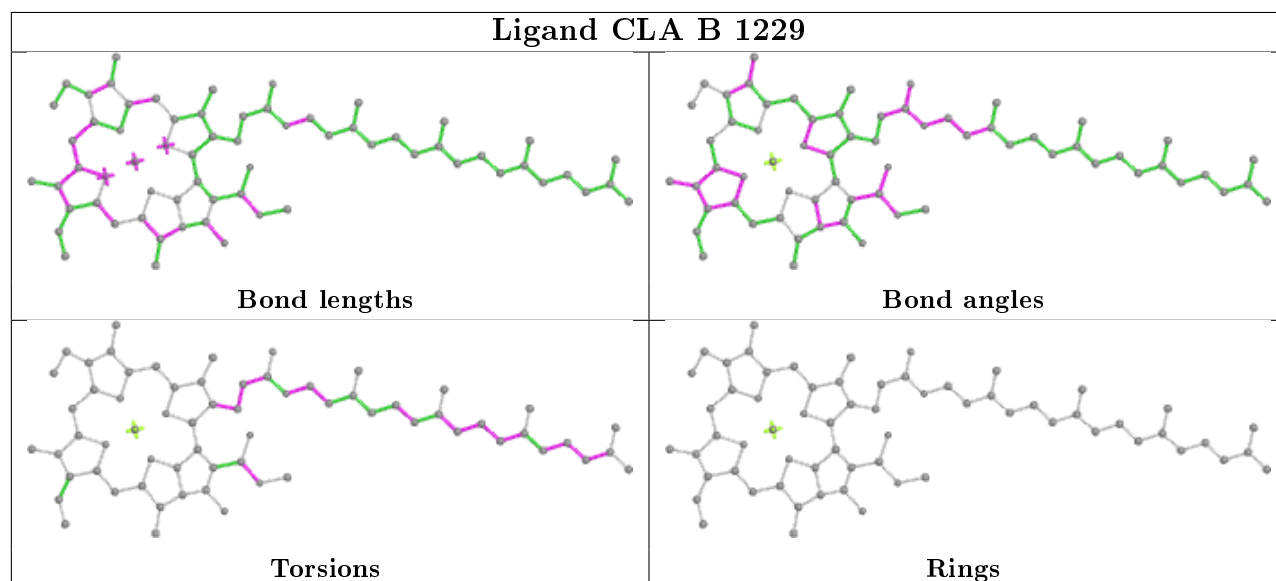
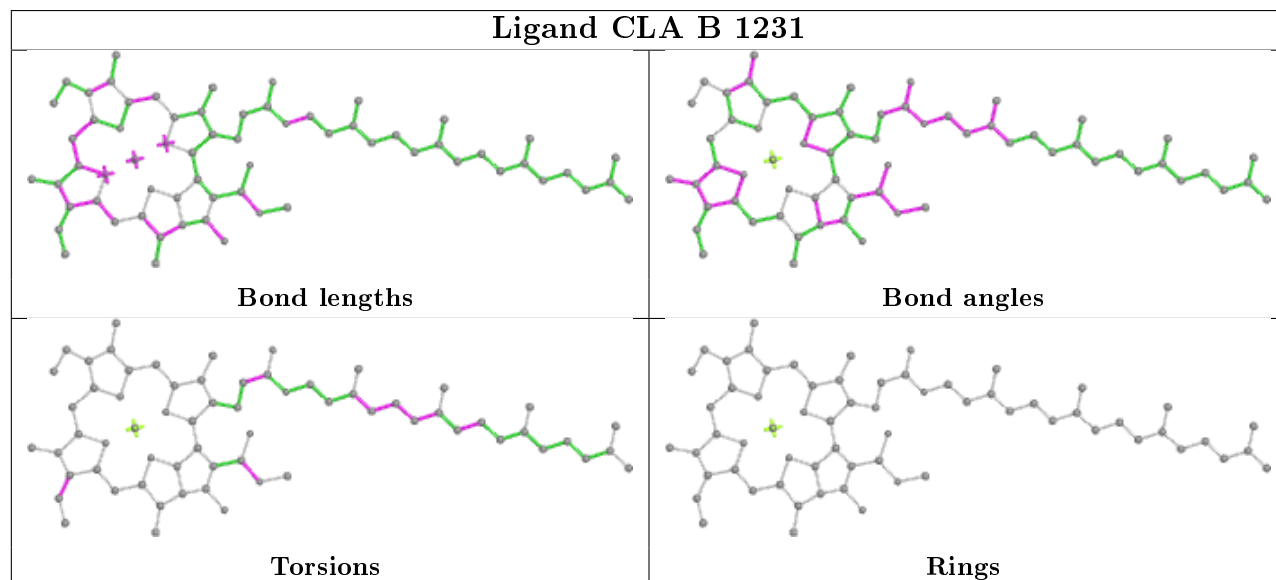
Torsions

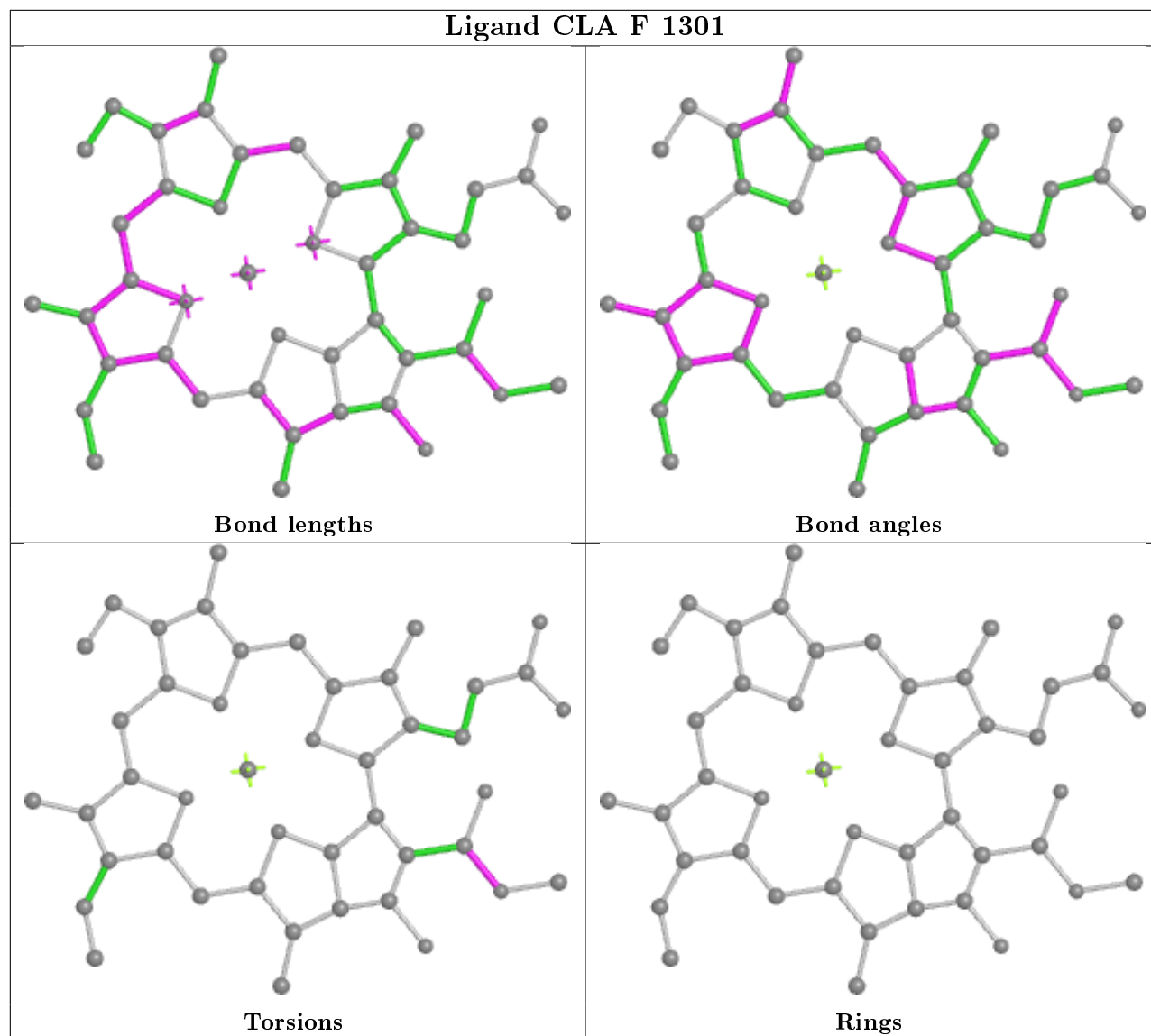
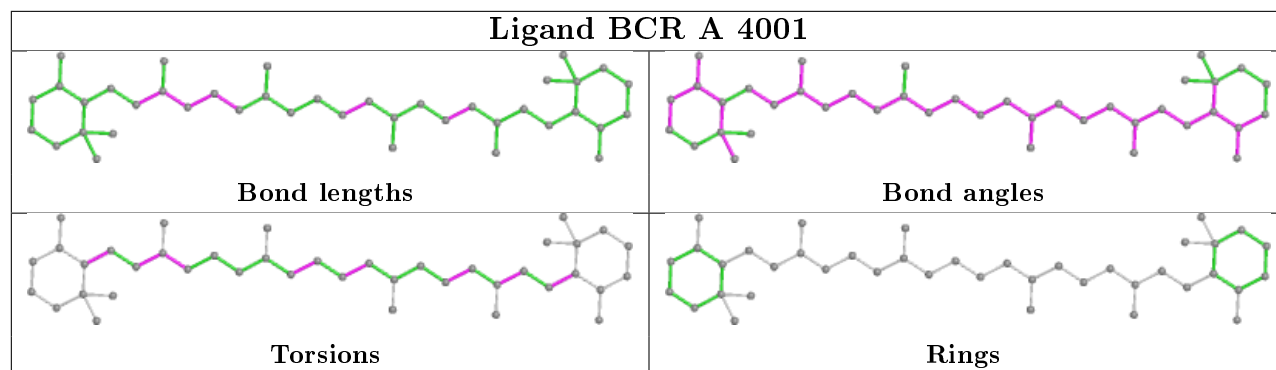


Rings

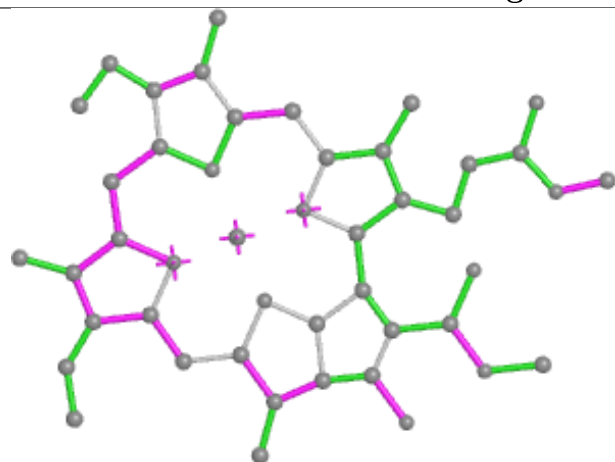


Ligand CLA B 1223**Ligand CL0 A 1011****Ligand LMU J 1304**

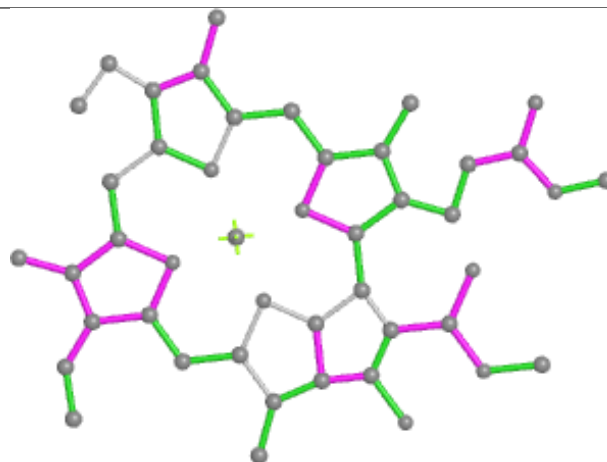
Ligand CLA A 1109**Ligand CLA B 1229****Ligand CLA B 1231**



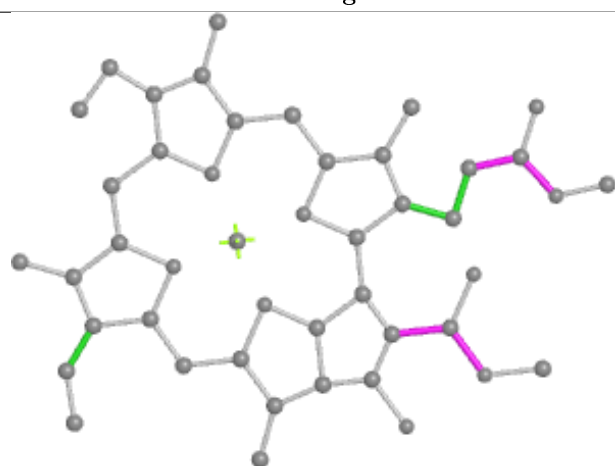
Ligand CLA K 1402



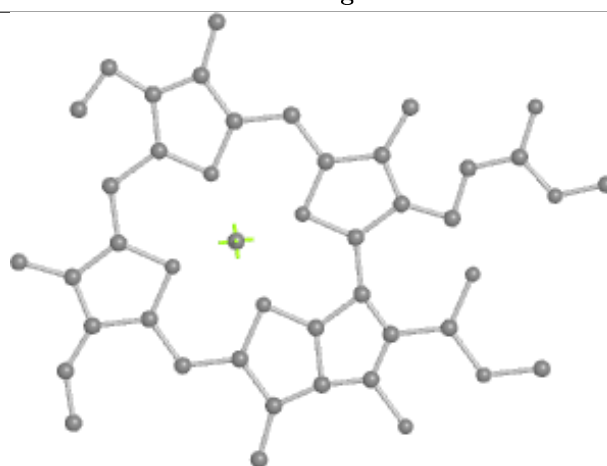
Bond lengths



Bond angles

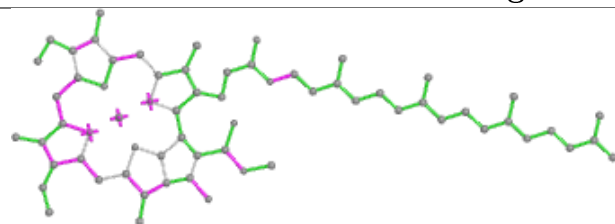


Torsions

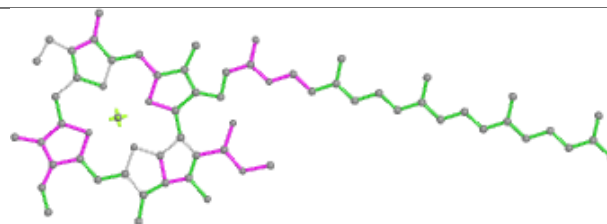


Rings

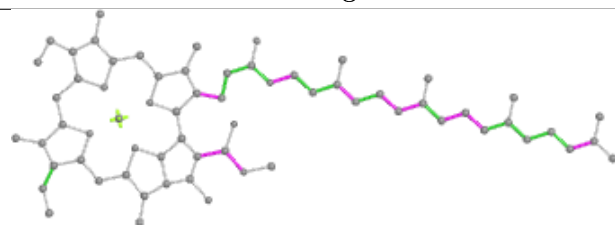
Ligand CLA A 1103



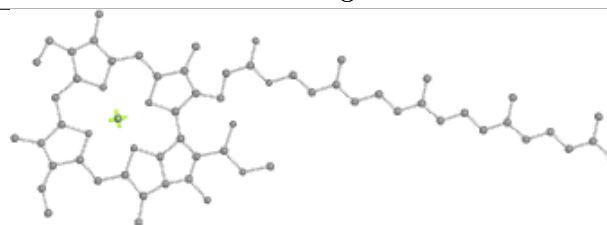
Bond lengths



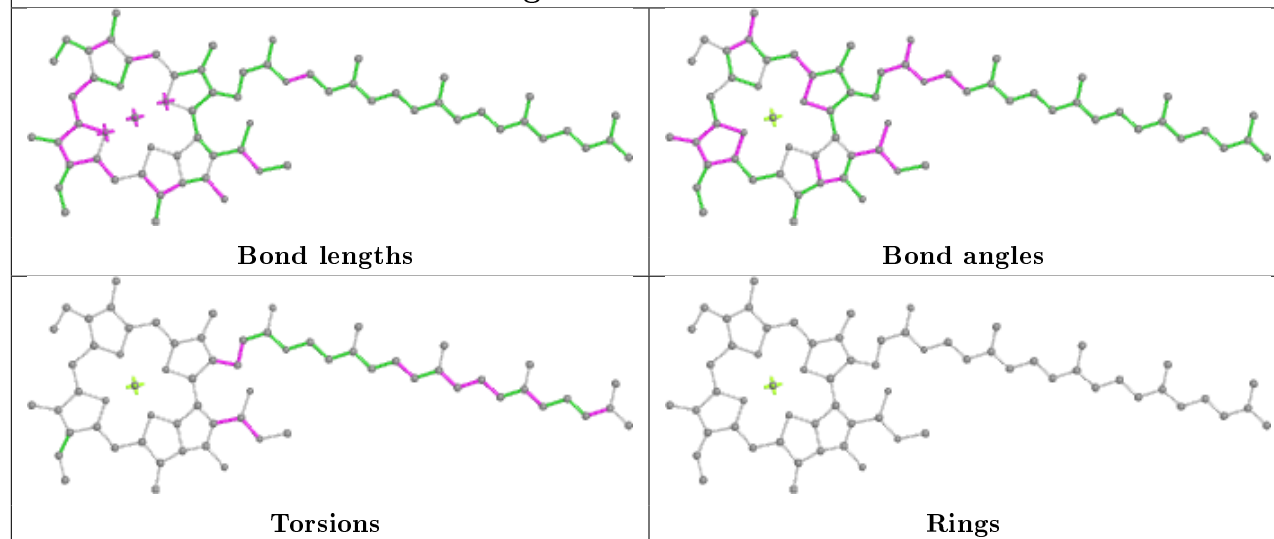
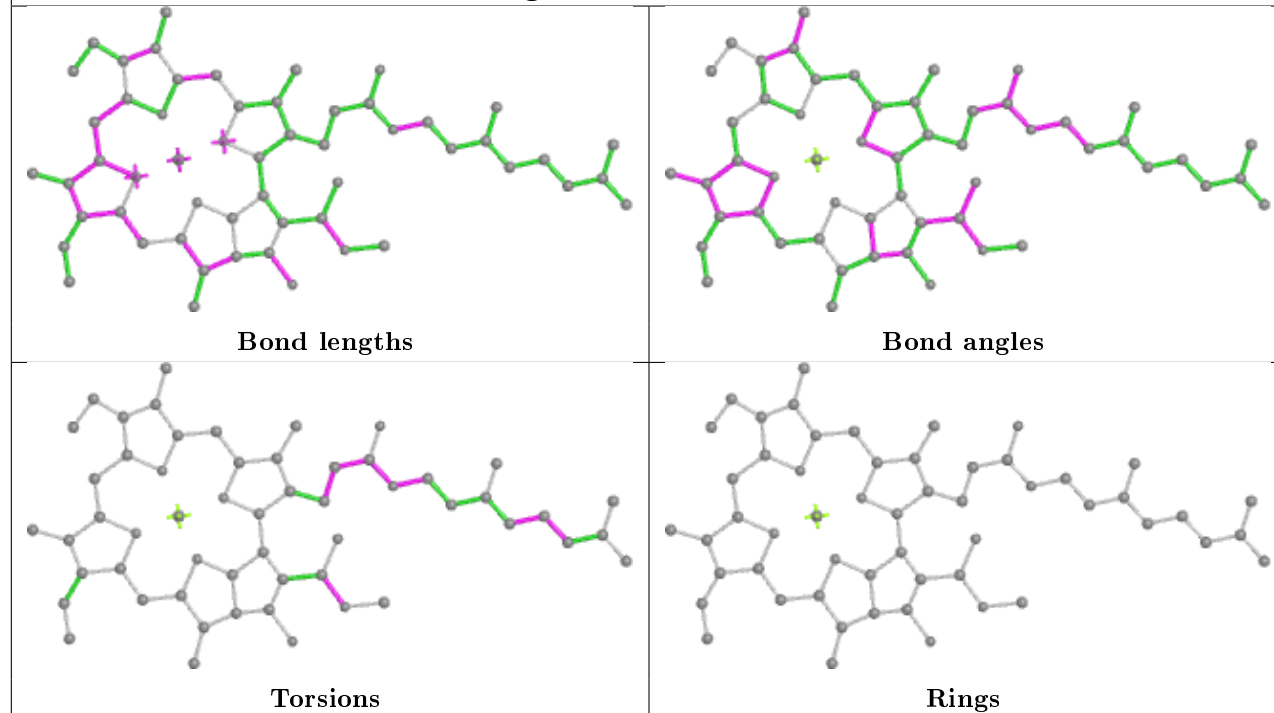
Bond angles

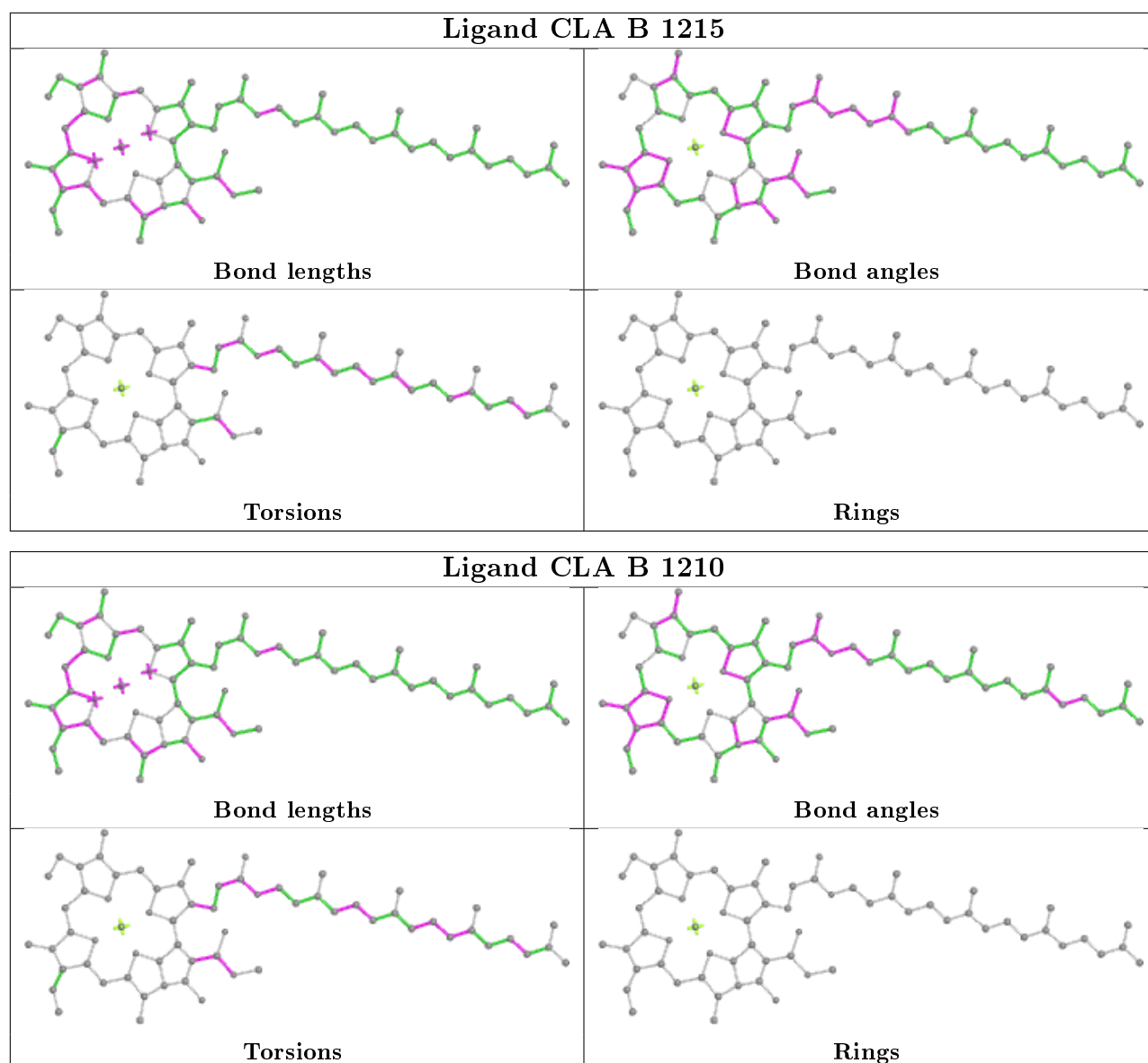


Torsions



Rings

Ligand CLA A 1106**Ligand CLA A 1130**



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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	739/751 (98%)	0.20	58 (7%) 13 7	43, 90, 141, 226	0
2	B	728/731 (99%)	-0.09	21 (2%) 51 41	53, 83, 126, 179	0
3	C	80/81 (98%)	-0.30	0 100 100	60, 72, 95, 105	0
4	D	138/141 (97%)	0.46	23 (16%) 1 1	72, 90, 125, 161	0
5	E	68/74 (91%)	-0.00	3 (4%) 34 24	59, 75, 109, 138	0
6	F	141/165 (85%)	-0.26	4 (2%) 53 43	64, 82, 111, 169	0
7	J	40/40 (100%)	-0.45	2 (5%) 28 19	66, 76, 124, 149	0
8	K	53/128 (41%)	1.48	17 (32%) 0 0	134, 160, 207, 253	0
9	M	30/31 (96%)	1.98	9 (30%) 0 0	109, 132, 158, 172	0
All	All	2017/2142 (94%)	0.10	137 (6%) 17 10	43, 86, 145, 253	0

The worst 5 of 137 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
9	M	2	ALA	21.6
9	M	3	LEU	12.4
8	K	127	ILE	10.2
1	A	751	GLY	8.3
1	A	257	ALA	5.8

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 ⓘ

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
14	BCR	B	4004	40/40	0.66	0.31	101,115,147,151	0
15	CLA	K	1401	46/65	0.67	0.34	120,155,169,173	0
14	BCR	A	4007	40/40	0.69	0.39	69,86,137,139	0
16	LMU	J	1304	35/35	0.69	0.26	91,159,172,173	0
14	BCR	A	4003	40/40	0.75	0.39	69,111,146,146	0
14	BCR	B	4009	40/40	0.77	0.27	72,103,147,151	0
15	CLA	K	1402	46/65	0.79	0.30	163,187,214,221	0
16	LMU	B	1301	35/35	0.82	0.21	120,136,148,154	0
14	BCR	A	4008	40/40	0.82	0.29	67,93,105,115	0
14	BCR	J	4013	40/40	0.82	0.29	78,97,112,121	0
15	CLA	B	1207	46/65	0.82	0.40	118,164,185,189	0
14	BCR	B	4005	40/40	0.83	0.27	73,93,125,128	0
15	CLA	A	1135	55/65	0.83	0.26	70,98,132,135	0
14	BCR	B	4006	40/40	0.84	0.22	86,109,141,142	0
12	LHG	A	5005	36/49	0.84	0.35	103,143,182,188	0
15	CLA	B	1212	45/65	0.84	0.19	101,117,128,143	0
17	LMG	B	5002	55/55	0.84	0.29	71,101,130,137	0
12	LHG	B	5004	49/49	0.85	0.24	59,88,99,106	0
15	CLA	A	1114	49/65	0.85	0.36	98,124,137,150	0
15	CLA	A	1133	46/65	0.85	0.29	86,103,118,128	0
14	BCR	A	4001	40/40	0.86	0.23	111,127,138,140	0
15	CLA	B	1210	65/65	0.86	0.26	75,95,108,120	0
13	CL0	A	1108	45/65	0.87	0.23	86,113,154,170	0
12	LHG	A	5003	49/49	0.87	0.30	91,121,142,143	0
15	CLA	J	1303	46/65	0.87	0.35	94,114,141,159	0
15	CLA	A	1110	54/65	0.87	0.22	96,121,150,154	0
15	CLA	A	1113	45/65	0.88	0.23	112,129,158,162	0
15	CLA	A	1118	46/65	0.88	0.22	99,113,135,154	0
15	CLA	A	1134	46/65	0.88	0.24	109,127,151,186	0
15	CLA	A	1111	60/65	0.88	0.24	78,96,107,112	0
15	CLA	A	1119	64/65	0.88	0.27	78,97,115,137	0
15	CLA	A	1124	55/65	0.88	0.27	61,92,120,129	0
15	CLA	B	1214	65/65	0.88	0.24	72,89,119,133	0
15	CLA	A	1116	54/65	0.89	0.37	84,113,130,141	0
15	CLA	B	1213	50/65	0.89	0.16	89,104,128,136	0
15	CLA	J	1302	45/65	0.89	0.30	82,93,138,150	0
15	CLA	B	1224	65/65	0.89	0.26	60,78,98,108	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
15	CLA	B	1216	65/65	0.89	0.18	67,91,106,118	0
11	SF4	C	3002	8/8	0.89	0.20	60,88,151,152	0
15	CLA	B	1221	65/65	0.90	0.19	68,79,105,125	0
15	CLA	A	1123	65/65	0.90	0.27	75,88,98,104	0
15	CLA	A	1105	65/65	0.90	0.21	70,96,111,120	0
15	CLA	B	1208	45/65	0.90	0.19	88,114,130,140	0
15	CLA	A	1112	45/65	0.90	0.18	89,115,127,130	0
15	CLA	A	1801	52/65	0.90	0.43	100,122,154,158	0
15	CLA	A	1103	65/65	0.90	0.24	61,80,108,118	0
15	CLA	A	1132	62/65	0.90	0.24	74,105,153,156	0
15	CLA	A	1129	46/65	0.91	0.21	76,92,115,151	0
15	CLA	B	1217	47/65	0.91	0.25	96,114,132,157	0
14	BCR	F	4015	40/40	0.91	0.22	52,73,107,111	0
15	CLA	B	1231	65/65	0.91	0.22	66,89,115,138	0
15	CLA	A	1128	65/65	0.91	0.20	54,74,90,101	0
10	PQN	B	2002	33/33	0.91	0.25	59,79,99,105	0
15	CLA	A	1120	49/65	0.91	0.19	101,116,140,156	0
15	CLA	B	1211	46/65	0.91	0.17	90,106,116,133	0
14	BCR	A	4002	40/40	0.92	0.21	88,109,128,130	0
15	CLA	B	1203	65/65	0.92	0.22	62,83,99,104	0
15	CLA	F	1410	65/65	0.92	0.23	69,96,135,147	0
15	CLA	B	1218	51/65	0.92	0.21	86,98,125,159	0
15	CLA	B	1232	45/65	0.92	0.17	72,89,109,115	0
14	BCR	B	4010	40/40	0.92	0.21	55,74,102,113	0
14	BCR	F	4016	40/40	0.92	0.16	59,72,89,94	0
15	CLA	A	1102	65/65	0.92	0.17	55,81,107,112	0
15	CLA	B	1228	65/65	0.92	0.18	54,74,105,114	0
15	CLA	B	1201	46/65	0.92	0.21	72,83,107,123	0
15	CLA	A	1022	65/65	0.92	0.25	53,78,96,103	0
15	CLA	B	1023	65/65	0.92	0.24	55,79,111,119	0
15	CLA	B	1222	56/65	0.93	0.21	52,66,101,108	0
15	CLA	A	1101	65/65	0.93	0.17	55,73,89,96	0
15	CLA	A	1136	65/65	0.93	0.26	78,105,139,142	0
15	CLA	B	1226	65/65	0.93	0.20	54,79,133,144	0
15	CLA	A	1125	52/65	0.93	0.29	76,98,124,133	0
15	CLA	B	1227	45/65	0.93	0.16	54,72,94,98	0
15	CLA	B	1202	65/65	0.93	0.20	67,82,99,106	0
15	CLA	F	1139	65/65	0.93	0.22	47,58,90,98	0
15	CLA	B	1223	65/65	0.93	0.22	59,77,94,98	0
15	CLA	B	1219	55/65	0.93	0.19	74,86,119,142	0
15	CLA	A	1109	65/65	0.93	0.18	66,81,105,112	0
14	BCR	B	4014	40/40	0.93	0.19	46,62,88,89	0

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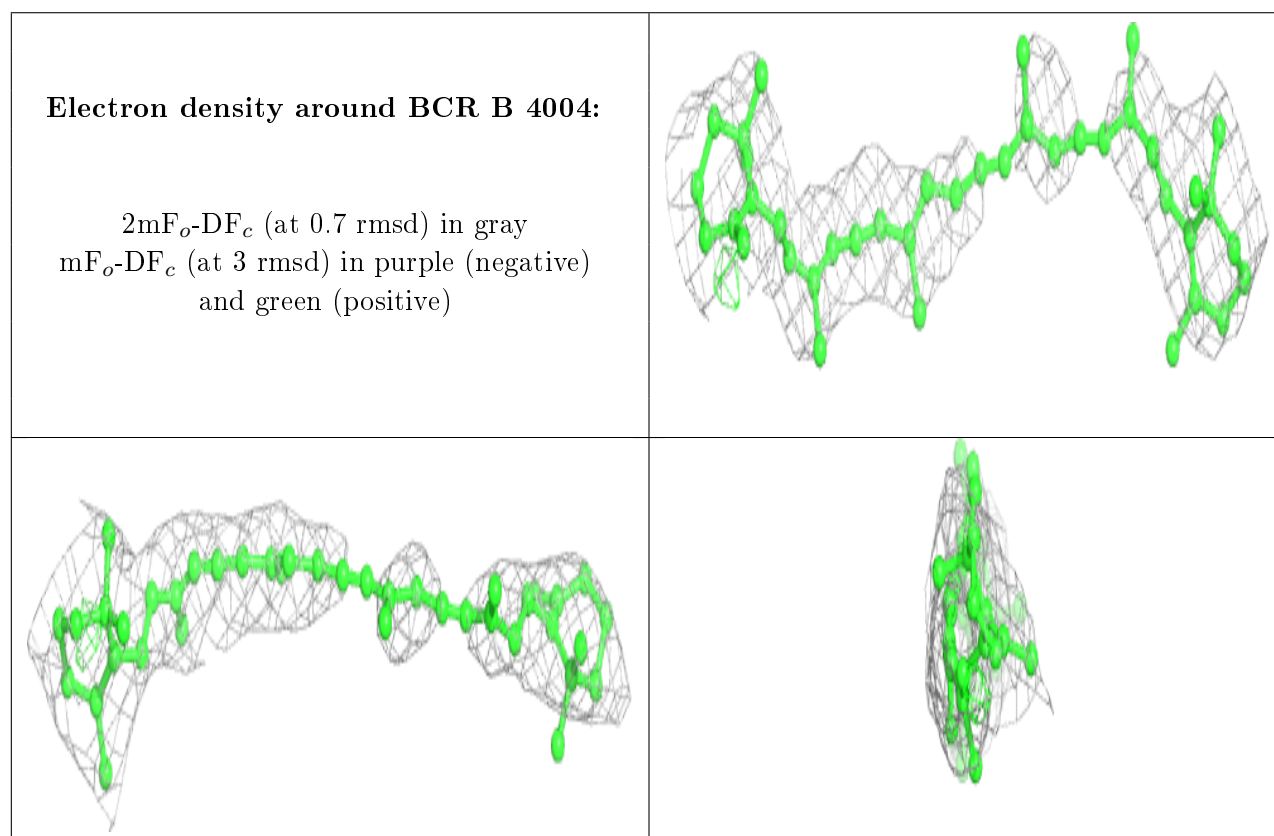
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
15	CLA	B	1234	65/65	0.93	0.21	56,73,108,120	0
11	SF4	A	3001	8/8	0.93	0.23	50,62,210,290	0
15	CLA	A	1122	65/65	0.93	0.19	74,91,119,129	0
15	CLA	B	1240	45/65	0.93	0.30	71,83,124,151	0
15	CLA	A	1127	65/65	0.93	0.42	67,79,100,106	0
15	CLA	A	1131	55/65	0.94	0.26	78,107,126,140	0
10	PQN	A	2001	33/33	0.94	0.20	45,57,68,74	0
15	CLA	A	1138	65/65	0.94	0.22	47,55,69,77	0
15	CLA	B	1236	50/65	0.94	0.20	52,72,106,114	0
15	CLA	B	1237	55/65	0.94	0.19	71,82,117,132	0
15	CLA	B	1204	46/65	0.94	0.17	79,96,115,137	0
15	CLA	B	1238	44/65	0.94	0.13	68,80,92,111	0
15	CLA	B	1220	56/65	0.94	0.15	61,77,111,119	0
15	CLA	B	1013	65/65	0.94	0.22	46,53,77,89	0
15	CLA	A	1115	46/65	0.94	0.21	109,129,140,151	0
13	CL0	A	1011	65/65	0.94	0.20	51,69,81,99	0
14	BCR	B	4011	40/40	0.94	0.26	49,67,84,91	0
14	BCR	A	4012	40/40	0.94	0.18	55,77,87,91	0
15	CLA	A	1121	46/65	0.94	0.25	91,114,141,163	0
15	CLA	A	1137	50/65	0.94	0.18	72,94,128,134	0
15	CLA	F	1301	45/65	0.94	0.16	54,75,97,131	0
15	CLA	A	1104	65/65	0.94	0.23	58,72,83,96	0
15	CLA	B	1235	65/65	0.94	0.16	55,66,85,92	0
12	LHG	A	5001	49/49	0.94	0.20	49,70,91,100	0
15	CLA	A	1106	65/65	0.94	0.20	59,79,98,109	0
15	CLA	B	1215	65/65	0.94	0.31	72,85,104,106	0
15	CLA	A	1126	65/65	0.94	0.23	63,80,101,116	0
14	BCR	B	4017	40/40	0.95	0.18	70,87,101,104	0
15	CLA	A	1117	65/65	0.95	0.43	80,100,111,113	0
15	CLA	B	1206	46/65	0.95	0.18	78,100,119,149	0
18	CL	B	6000	1/1	0.95	0.12	82,82,82,82	0
15	CLA	A	1012	65/65	0.95	0.27	47,60,86,93	0
15	CLA	B	1230	65/65	0.95	0.17	53,68,118,125	0
15	CLA	B	1225	65/65	0.95	0.29	66,80,100,104	0
15	CLA	B	1021	65/65	0.95	0.26	49,69,80,84	0
15	CLA	A	1140	65/65	0.96	0.22	52,73,103,116	0
15	CLA	B	1239	46/65	0.96	0.21	62,78,107,141	0
15	CLA	B	1229	65/65	0.96	0.17	50,62,86,107	0
15	CLA	A	1107	50/65	0.96	0.15	56,64,98,112	0
15	CLA	A	1130	55/65	0.96	0.20	82,106,133,139	0
15	CLA	B	1205	55/65	0.96	0.17	68,87,100,112	0
15	CLA	B	1209	45/65	0.96	0.19	102,113,134,148	0

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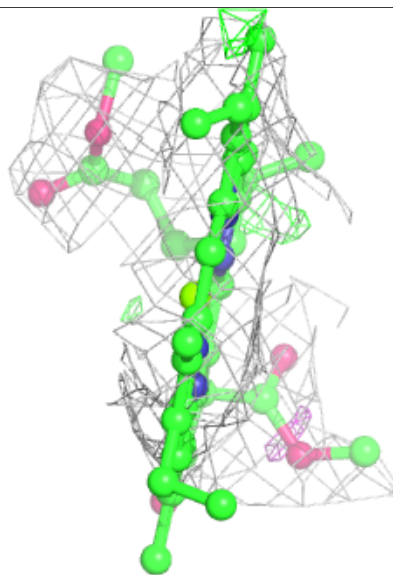
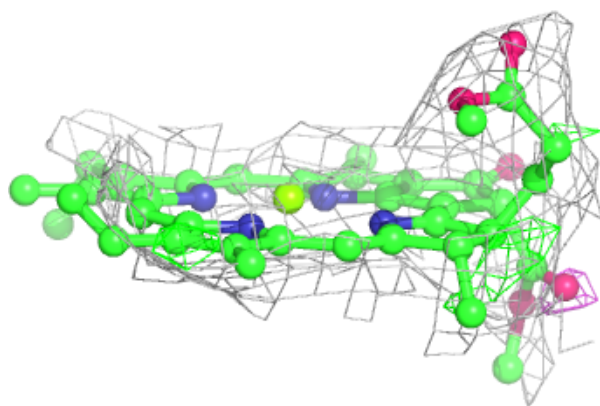
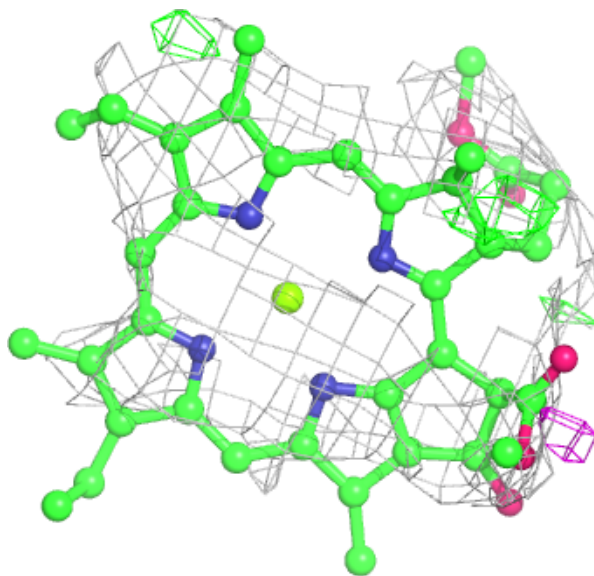
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
11	SF4	C	3003	8/8	0.97	0.19	60,67,100,115	0

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.



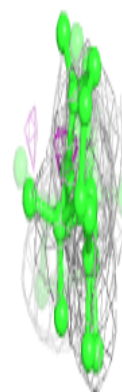
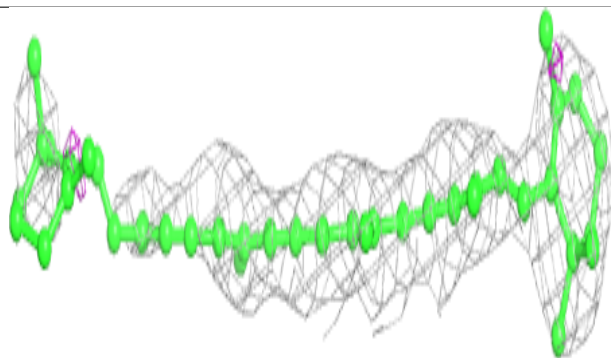
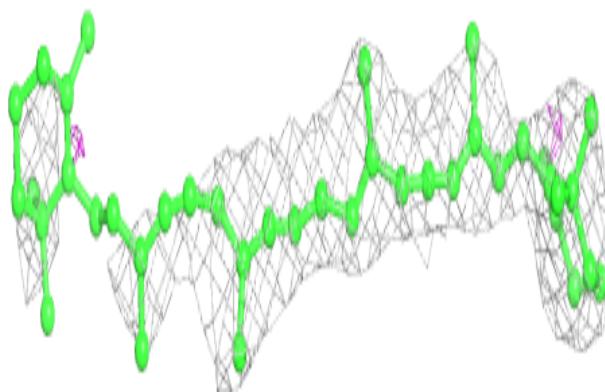
Electron density around CLA K 1401:

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

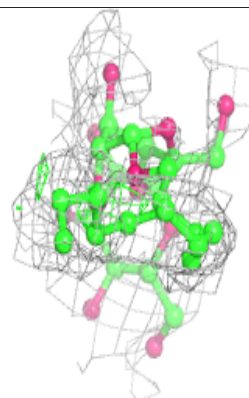
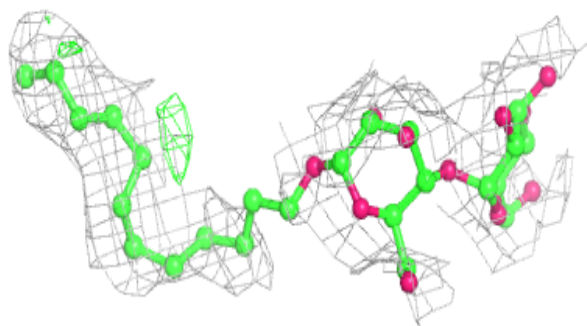
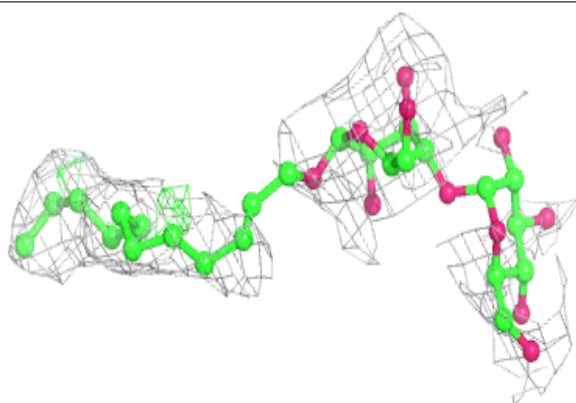


Electron density around BCR A 4007:

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

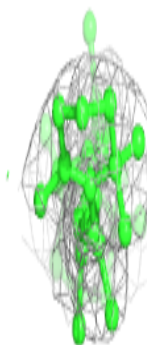
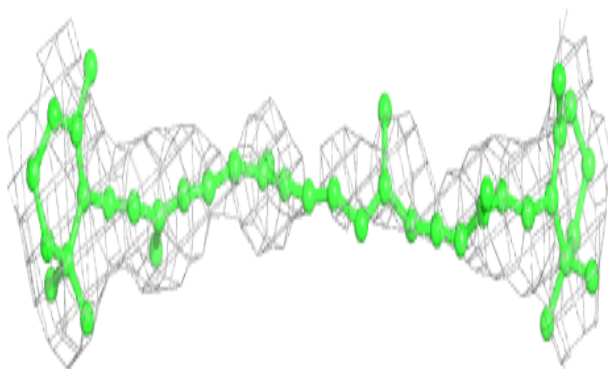
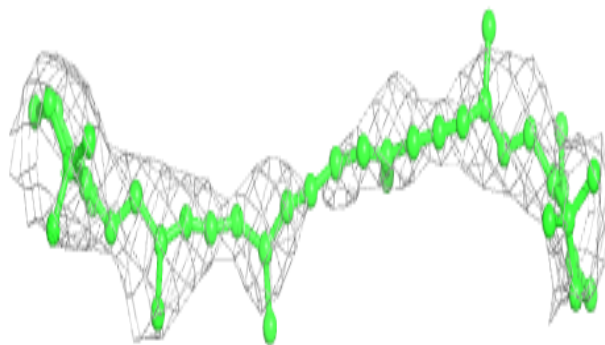
**Electron density around LMU J 1304:**

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

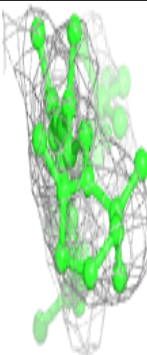
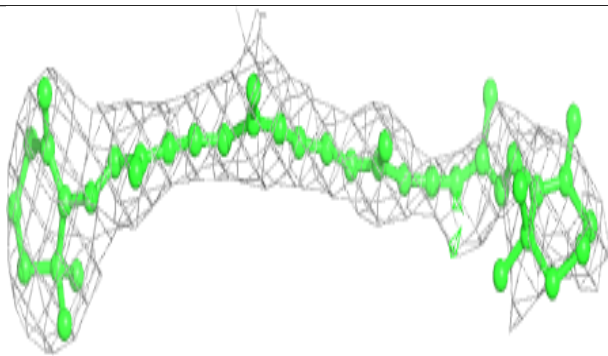
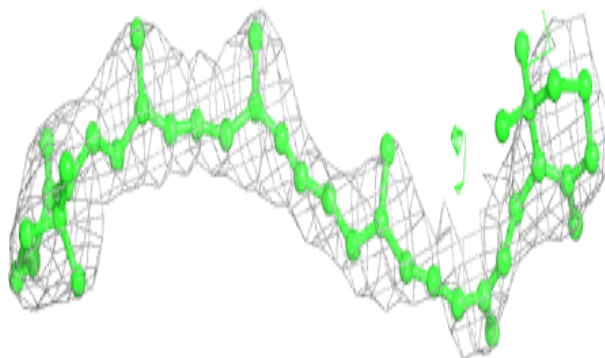


Electron density around BCR A 4003:

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

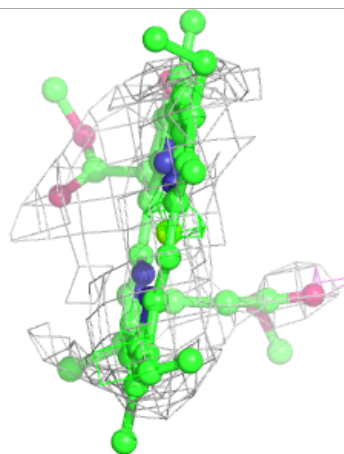
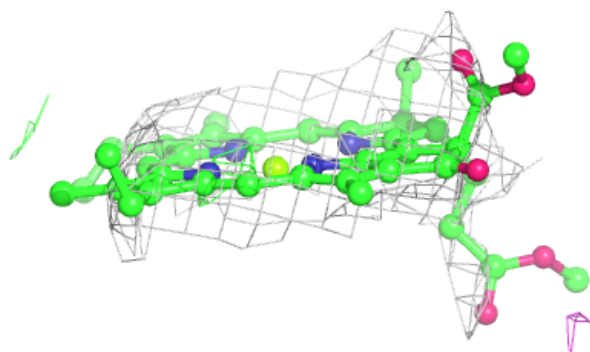
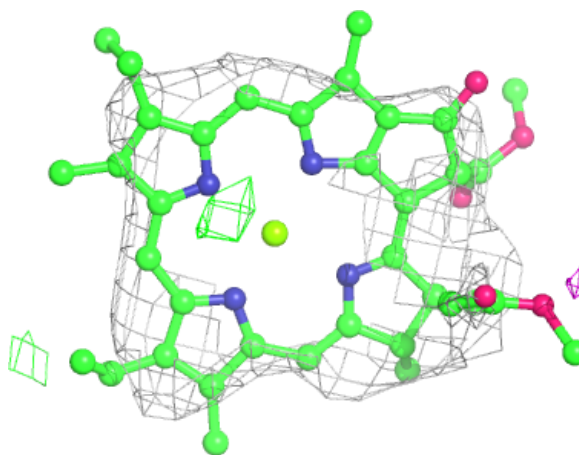
**Electron density around BCR B 4009:**

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



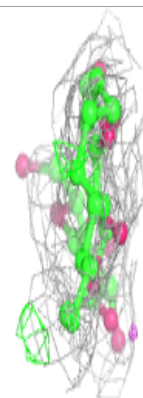
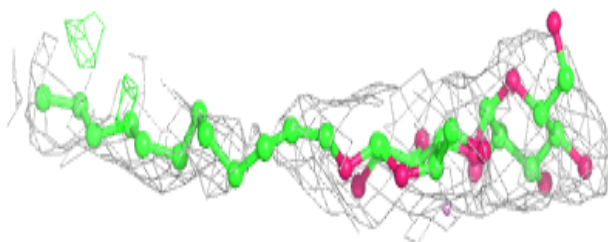
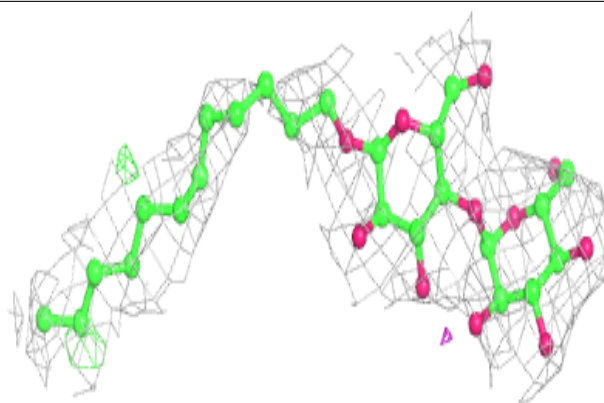
Electron density around CLA K 1402:

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

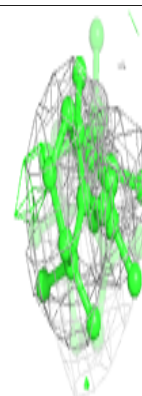
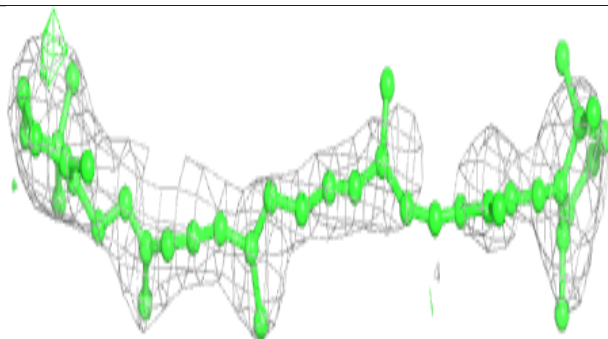
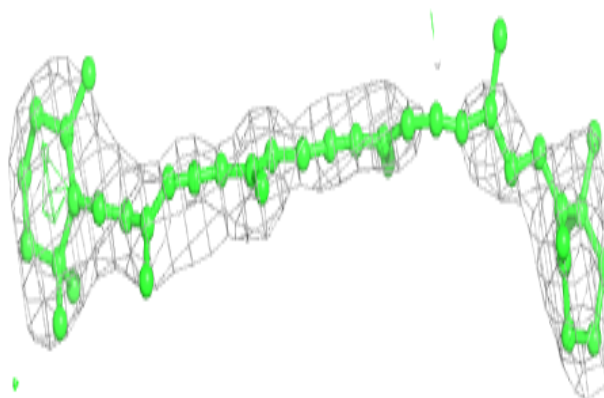


Electron density around LMU B 1301:

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

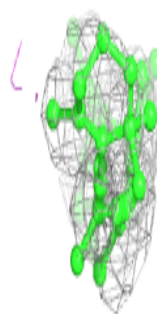
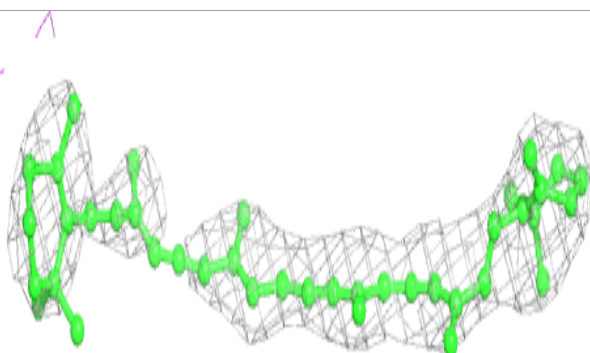
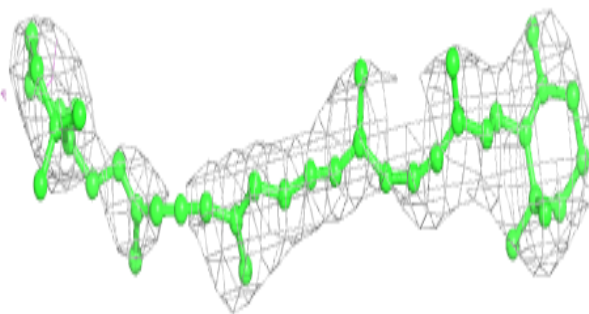
**Electron density around BCR A 4008:**

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



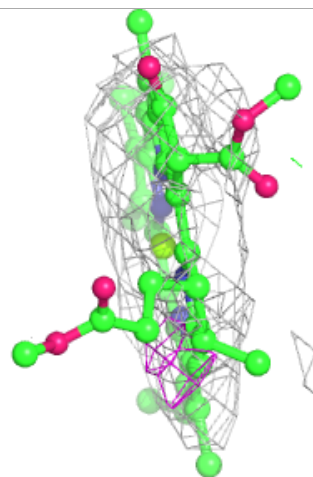
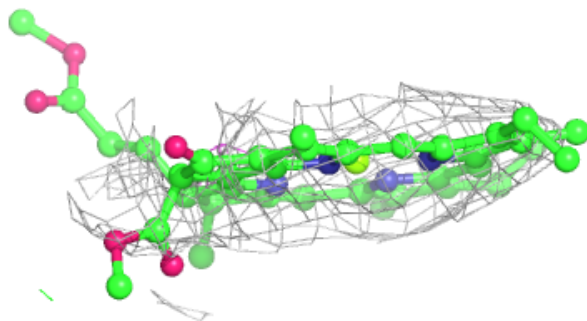
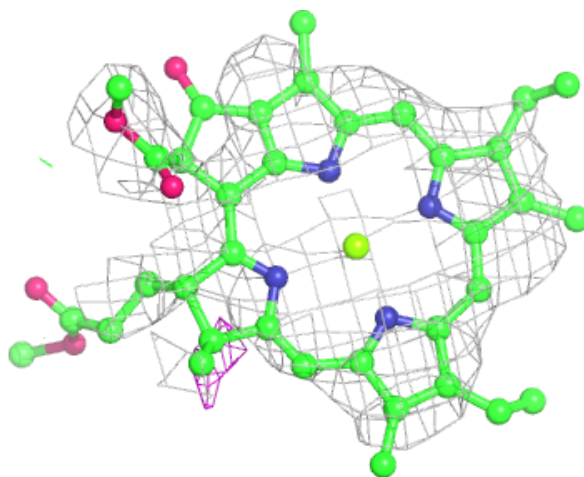
Electron density around BCR J 4013:

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



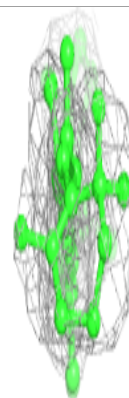
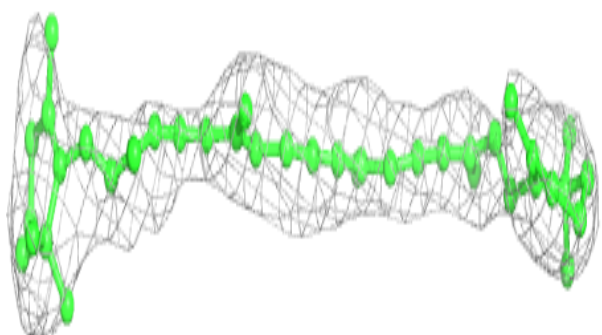
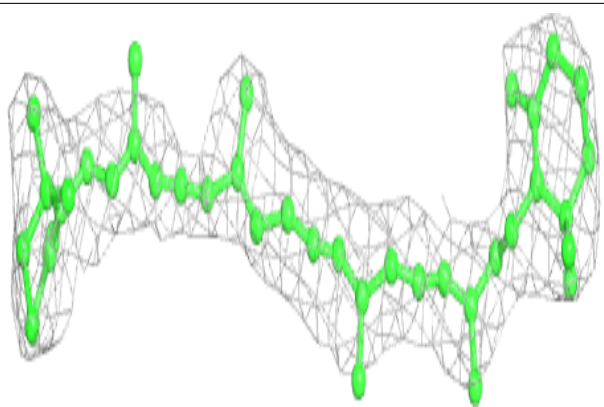
Electron density around CLA B 1207:

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

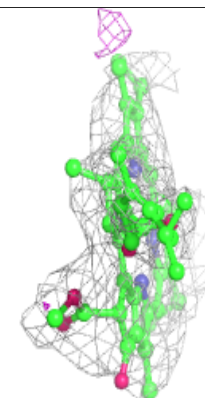
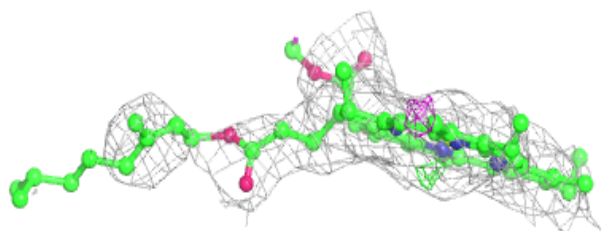
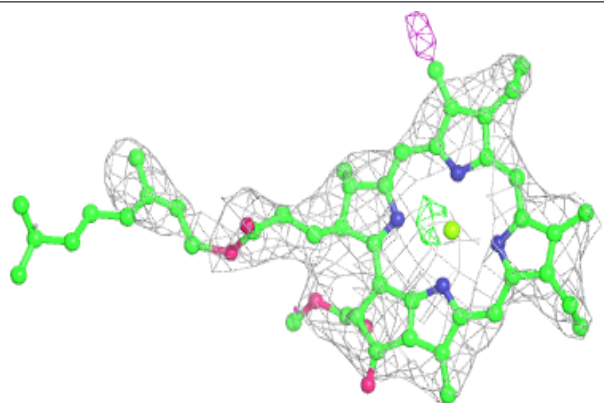


Electron density around BCR B 4005:

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

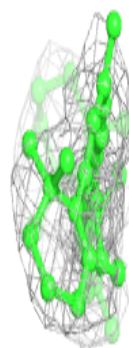
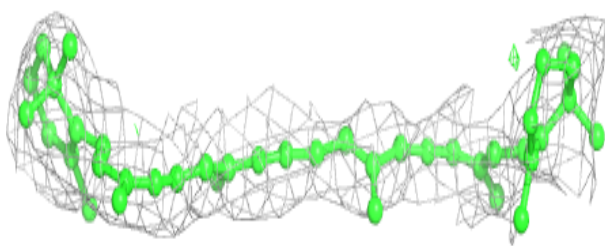
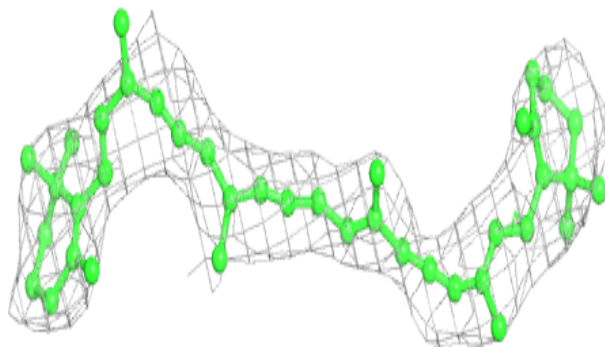
**Electron density around CLA A 1135:**

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

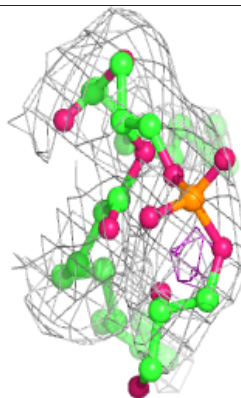
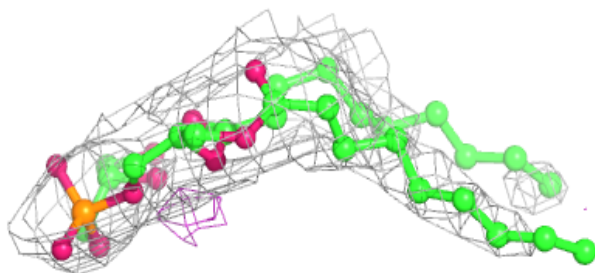
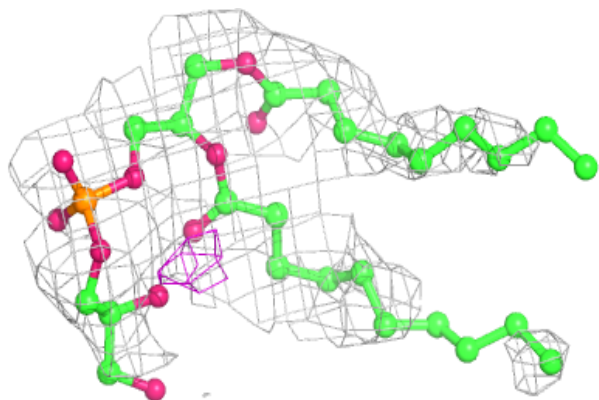


Electron density around BCR B 4006:

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

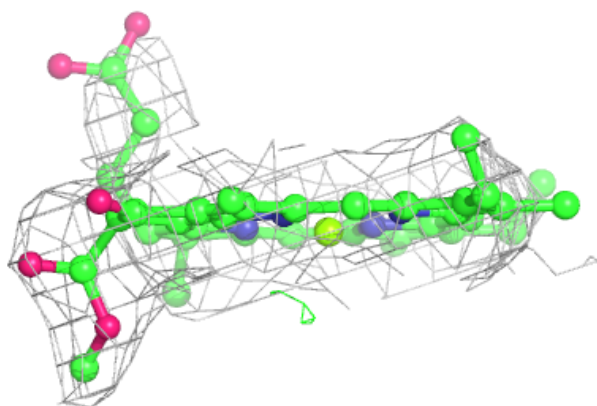
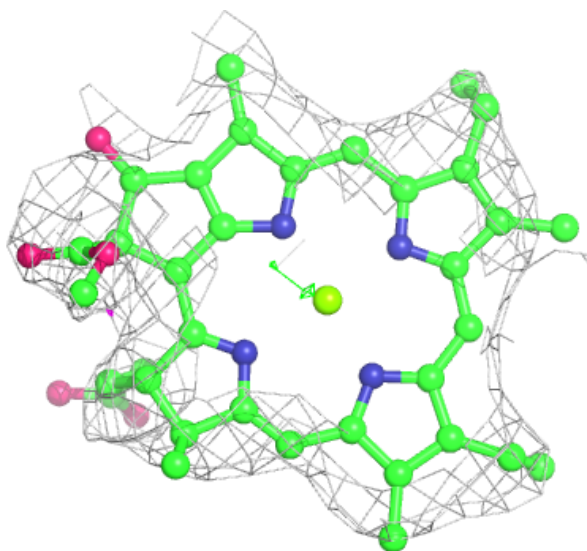
**Electron density around LHG A 5005:**

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



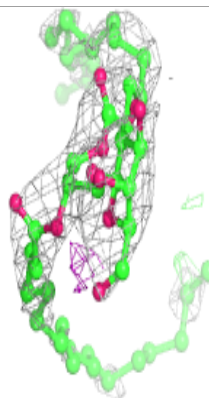
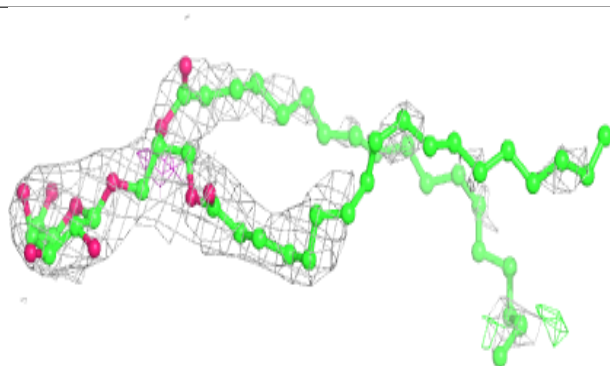
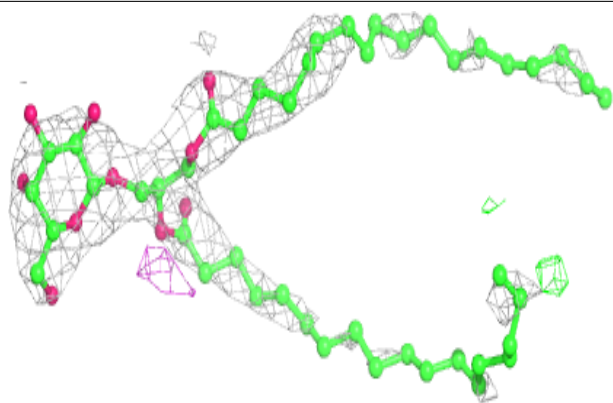
Electron density around CLA B 1212:

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



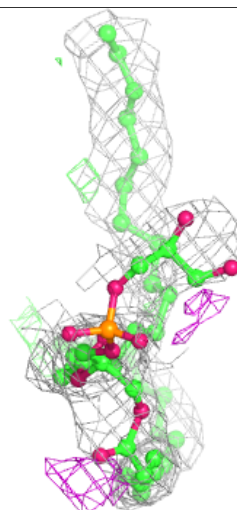
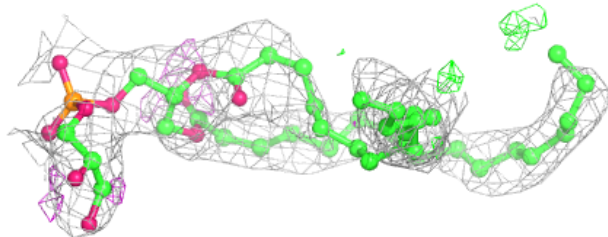
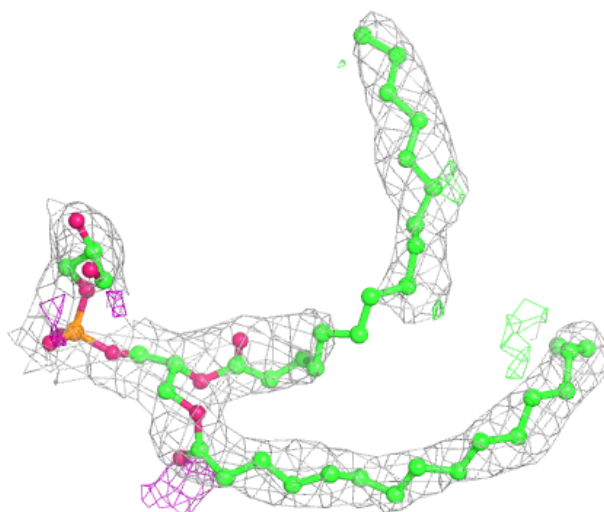
Electron density around LMG B 5002:

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



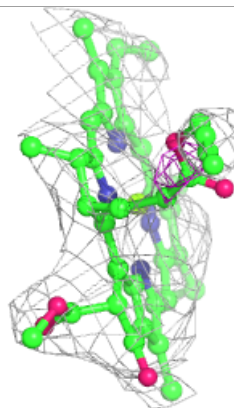
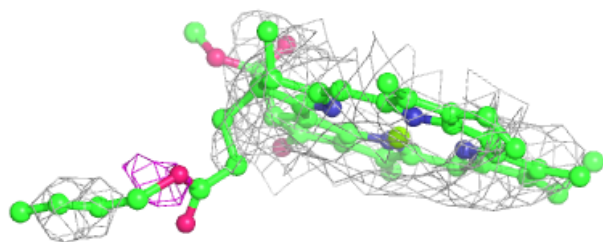
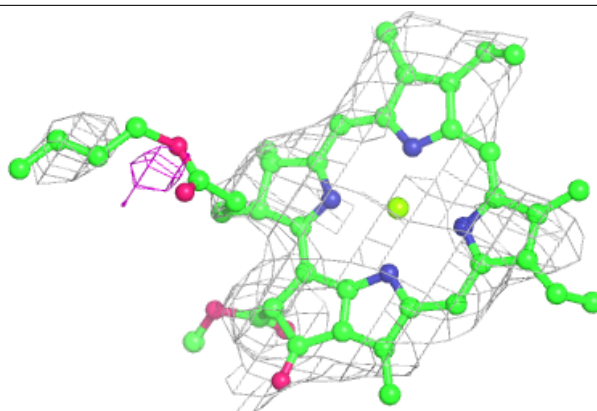
Electron density around LHG B 5004:

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



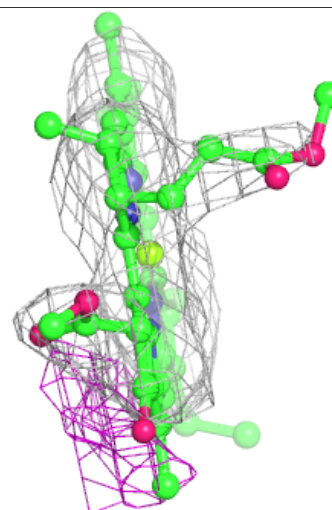
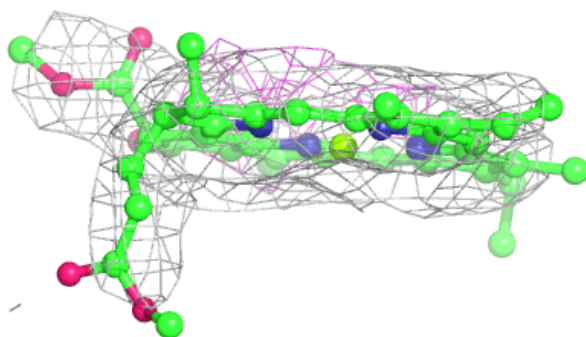
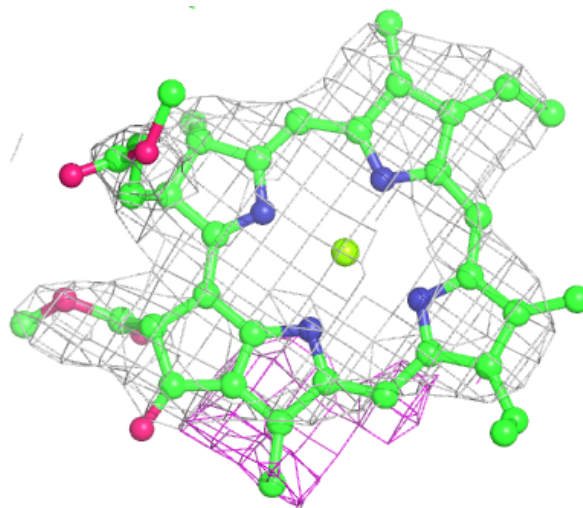
Electron density around CLA A 1114:

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



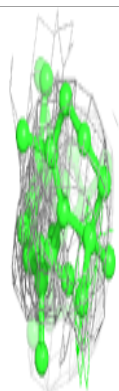
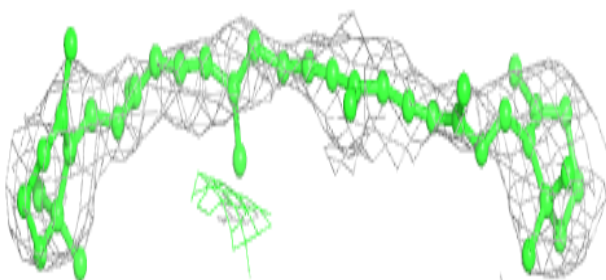
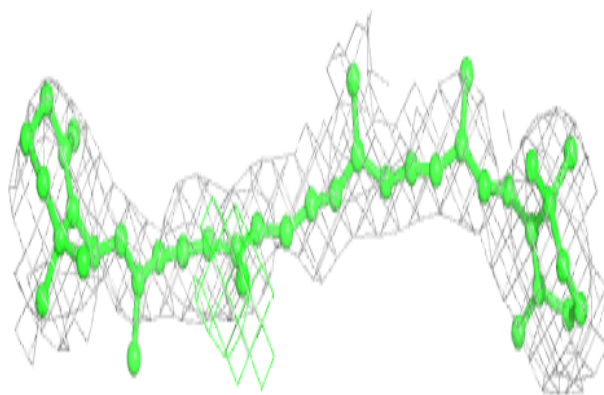
Electron density around CLA A 1133:

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

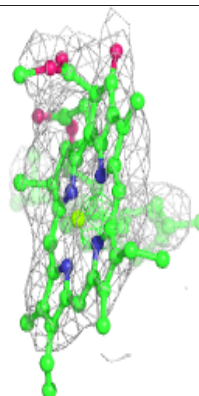
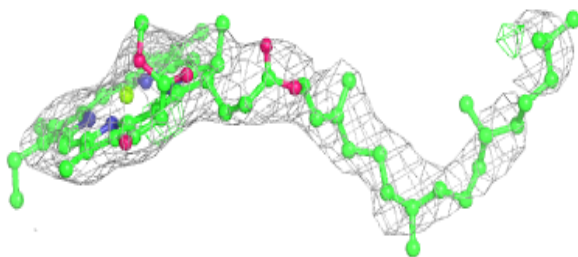
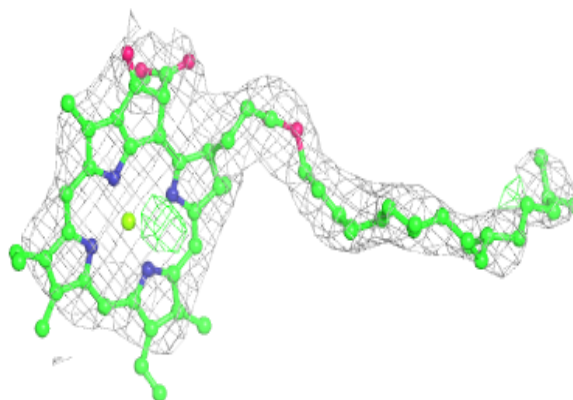


Electron density around BCR A 4001:

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

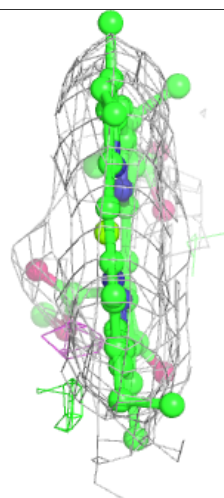
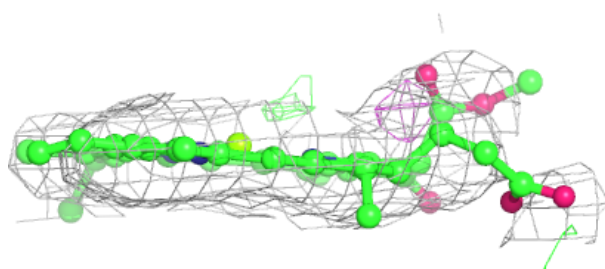
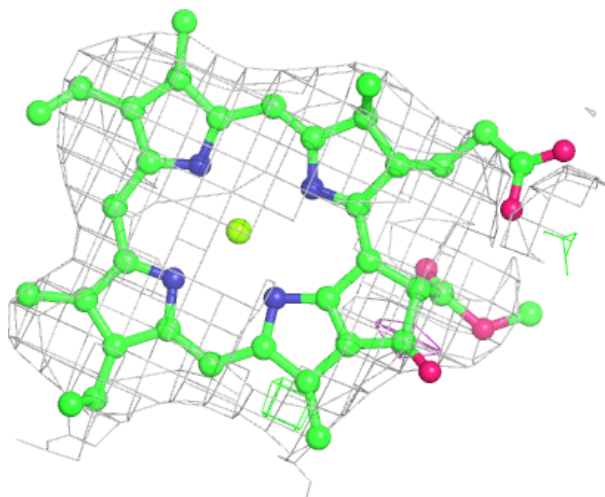
**Electron density around CLA B 1210:**

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



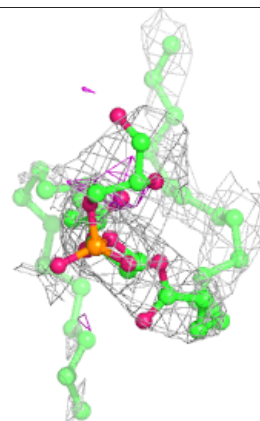
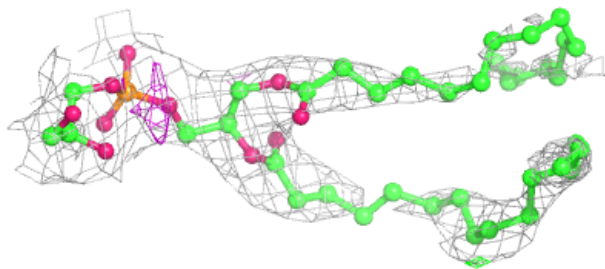
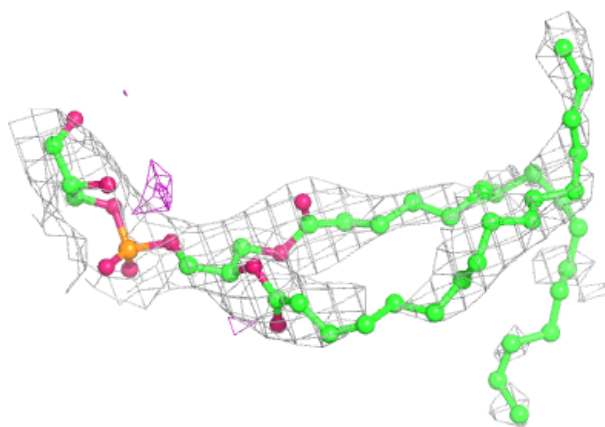
Electron density around CL0 A 1108:

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



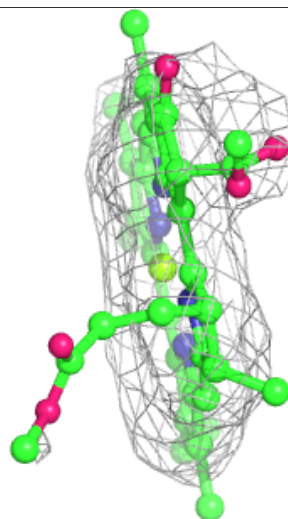
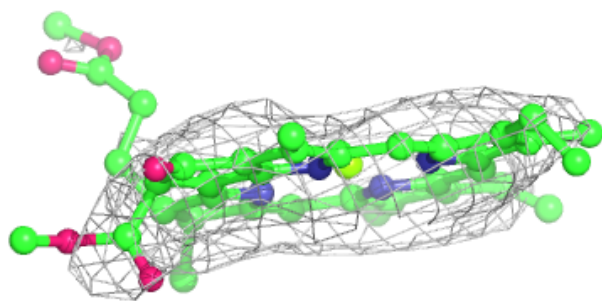
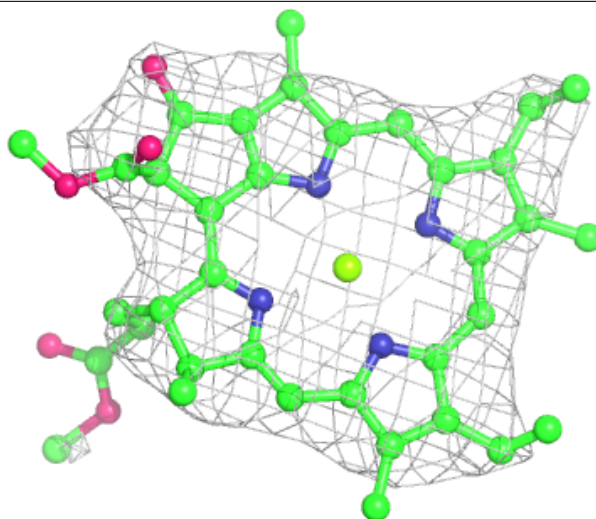
Electron density around LHG A 5003:

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



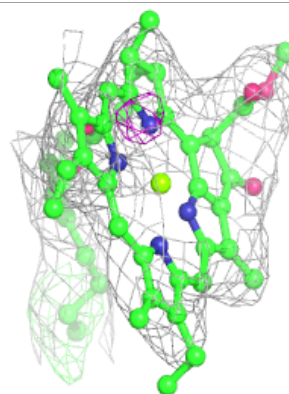
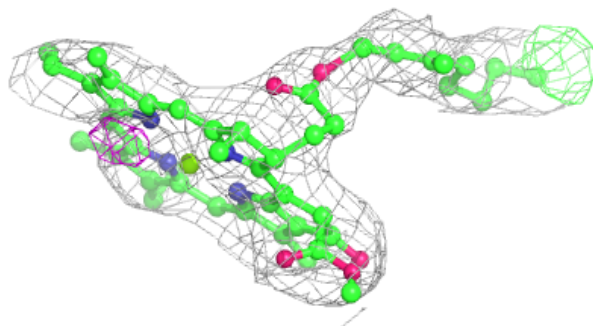
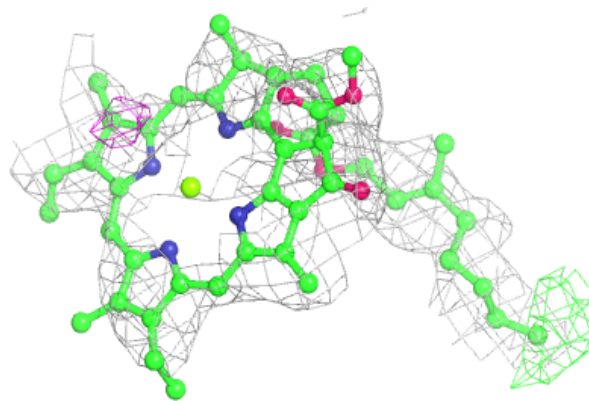
Electron density around CLA J 1303:

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



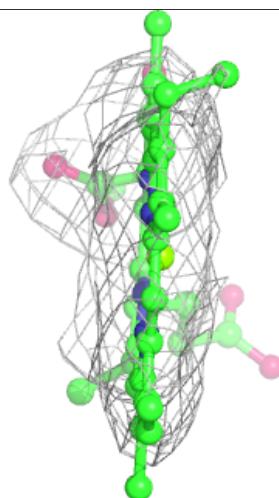
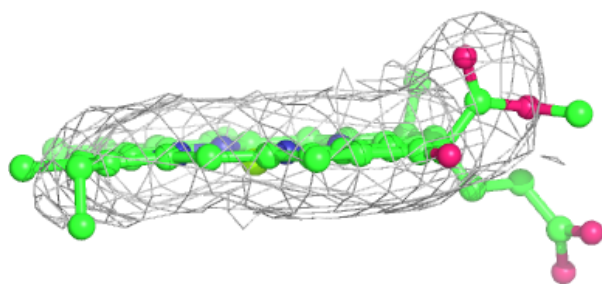
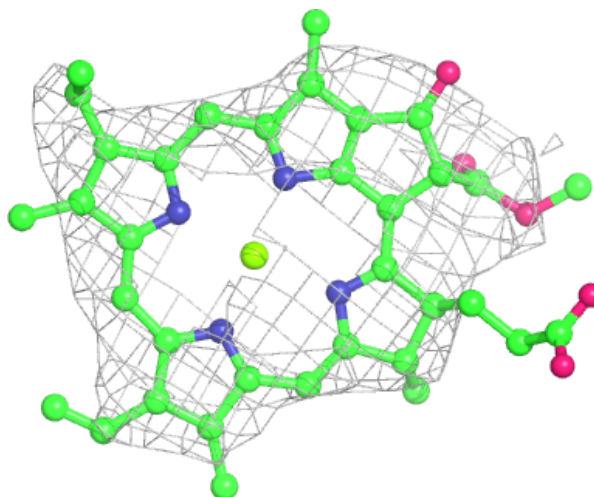
Electron density around CLA A 1110:

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



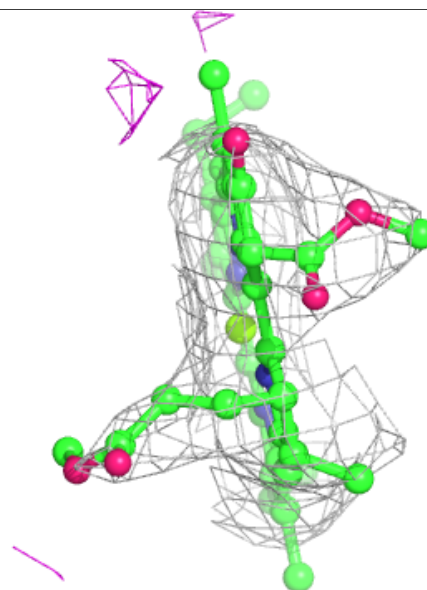
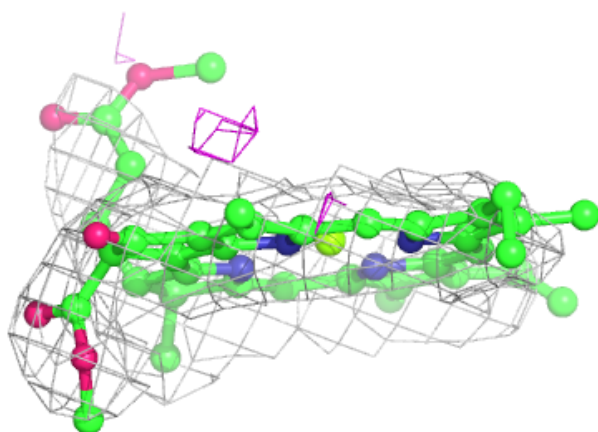
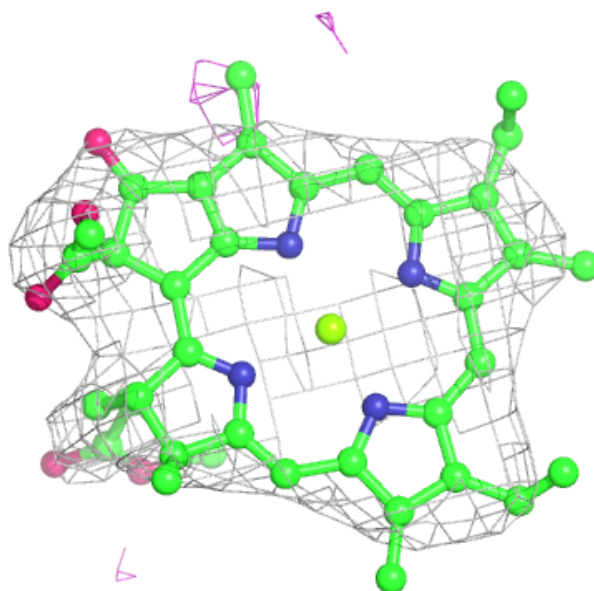
Electron density around CLA A 1113:

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



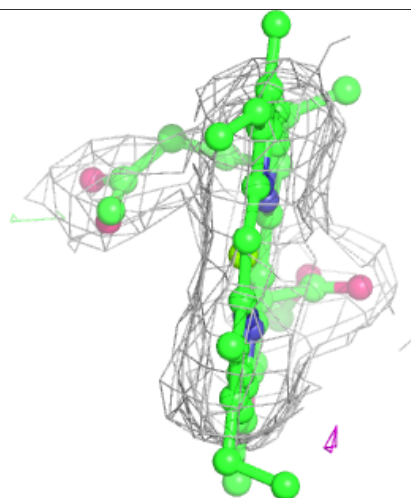
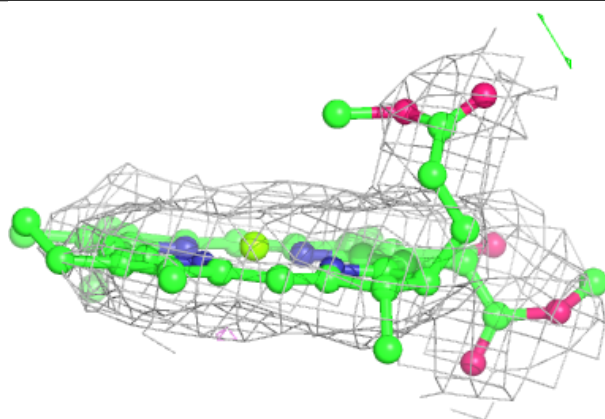
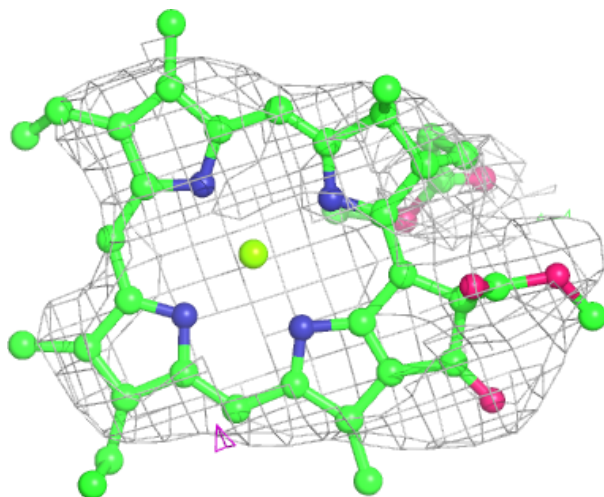
Electron density around CLA A 1118:

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



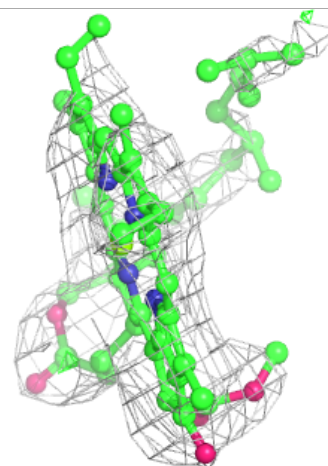
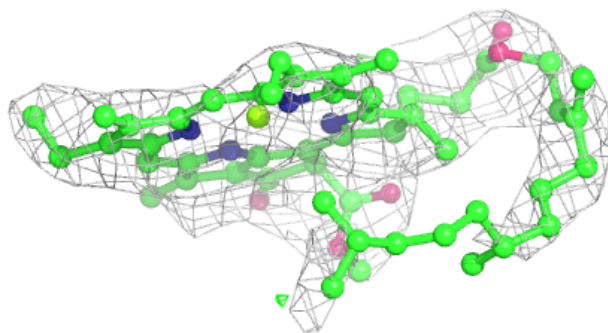
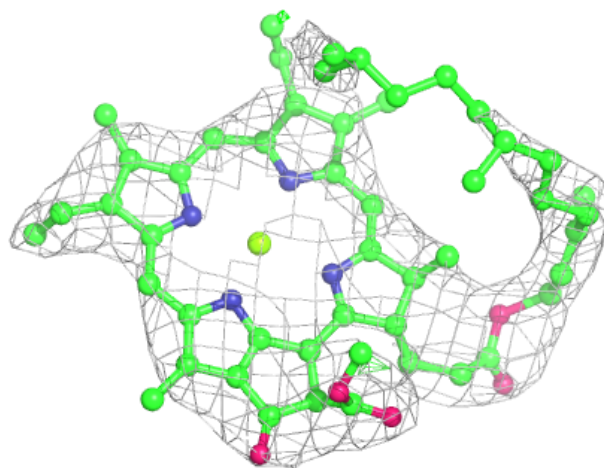
Electron density around CLA A 1134:

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



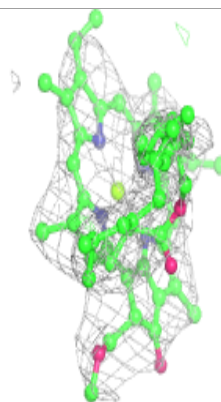
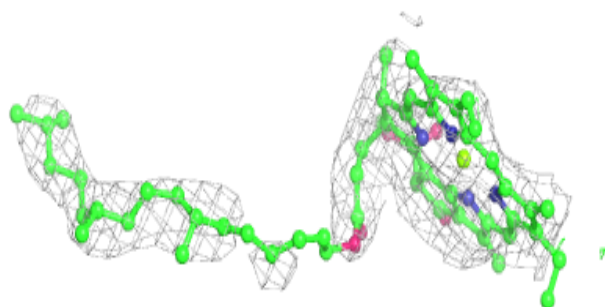
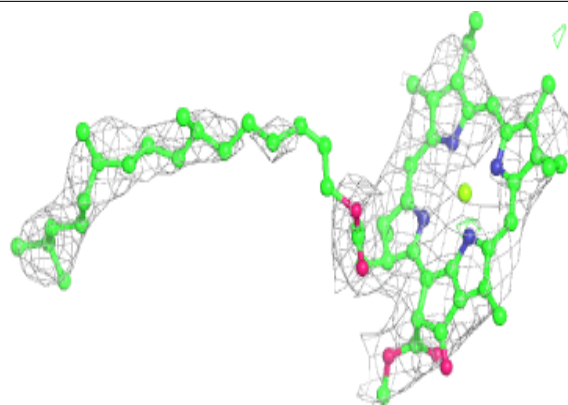
Electron density around CLA A 1111:

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

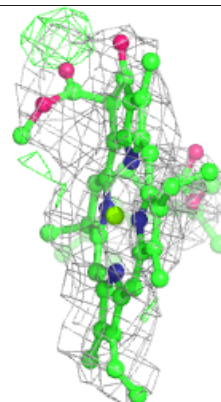
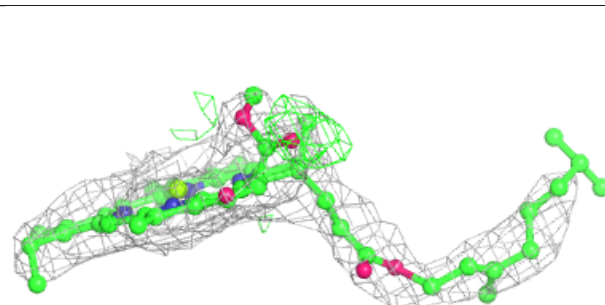
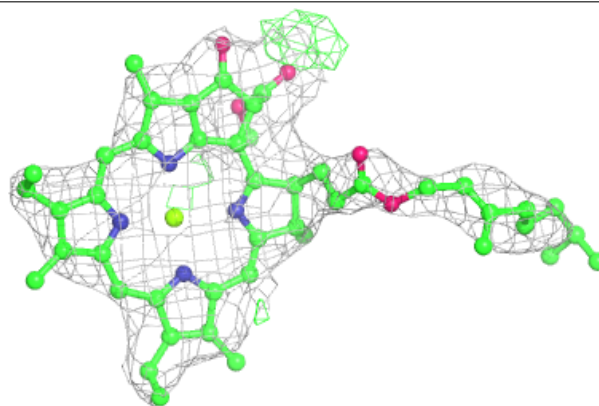


Electron density around CLA A 1119:

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

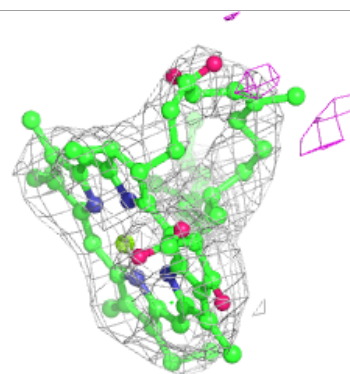
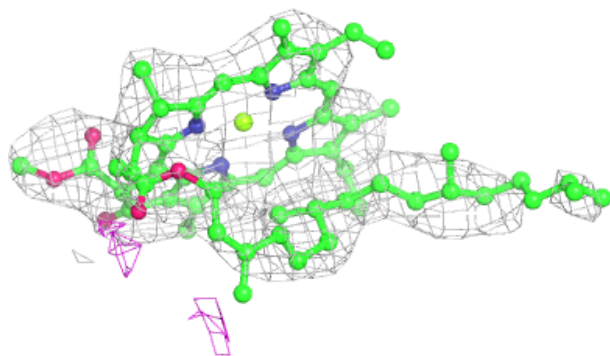
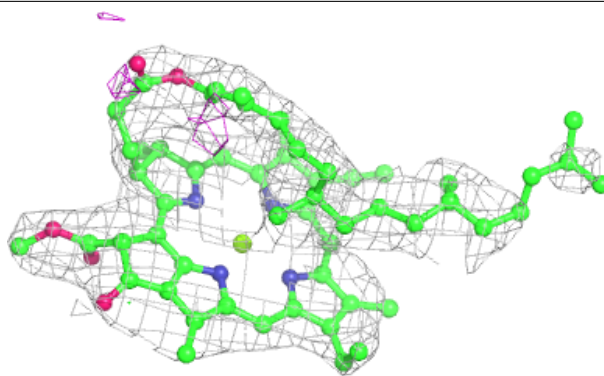
**Electron density around CLA A 1124:**

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

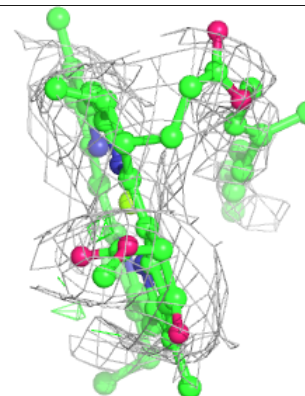
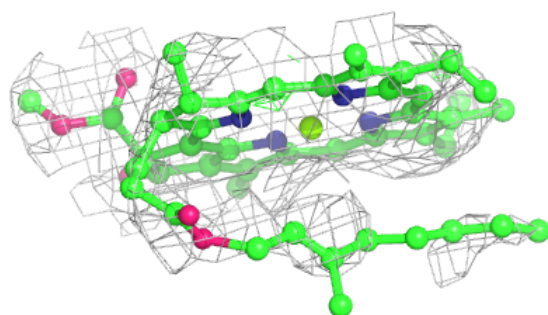
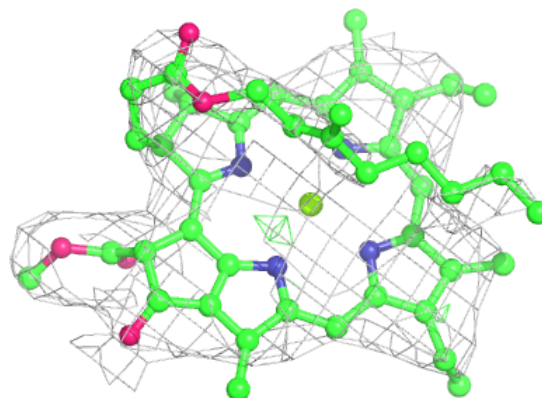


Electron density around CLA B 1214:

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

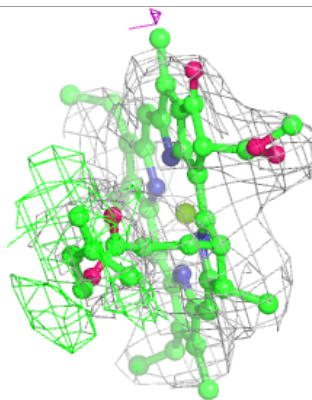
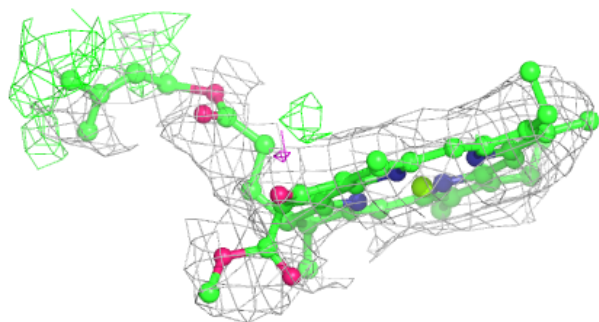
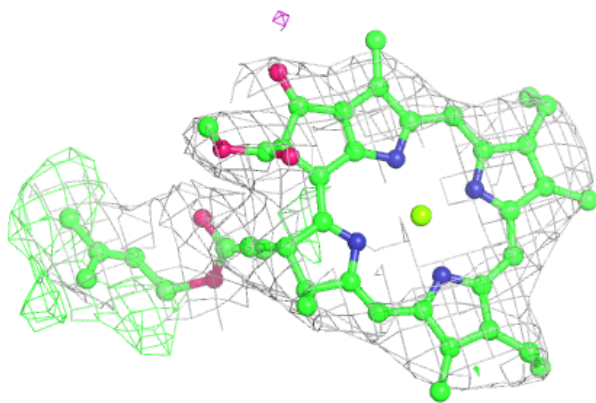
**Electron density around CLA A 1116:**

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



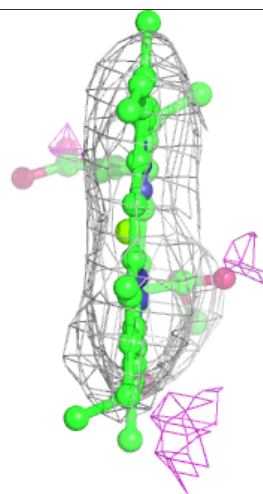
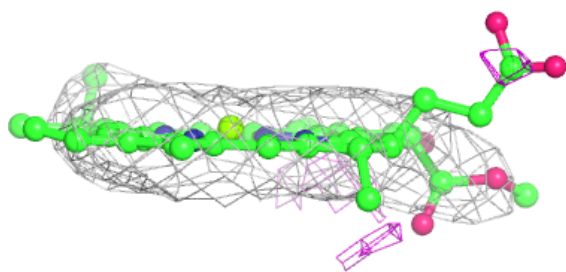
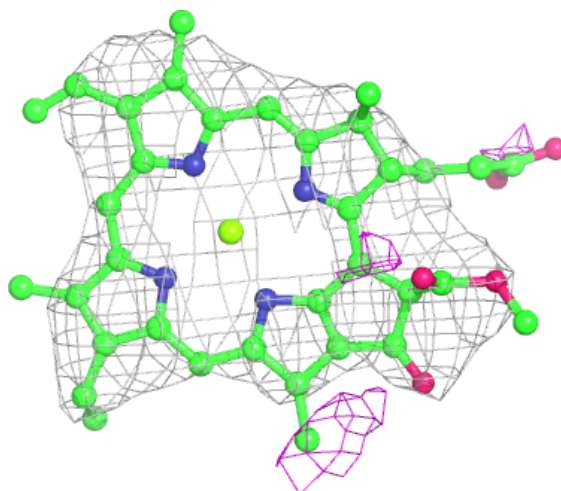
Electron density around CLA B 1213:

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



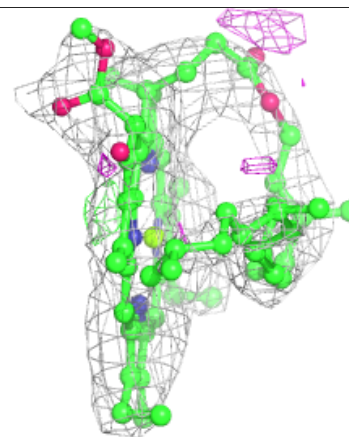
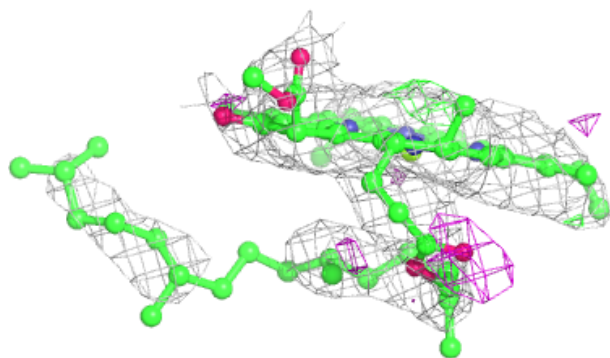
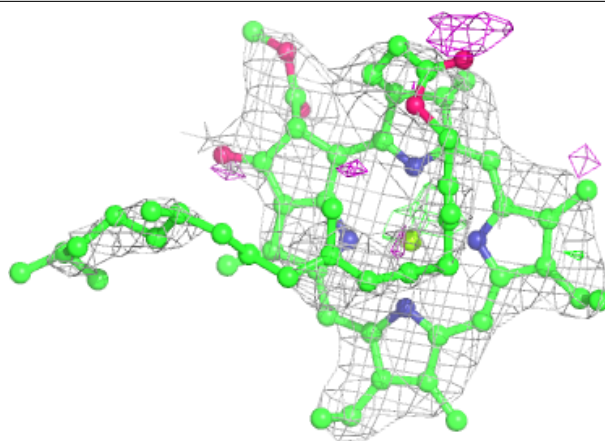
Electron density around CLA J 1302:

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



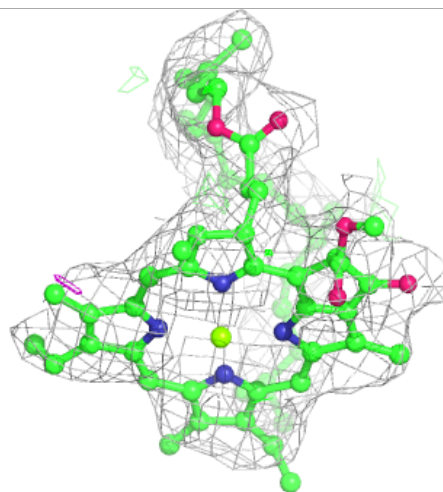
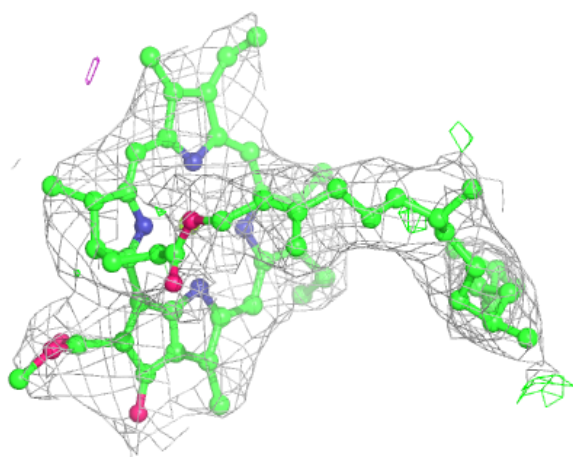
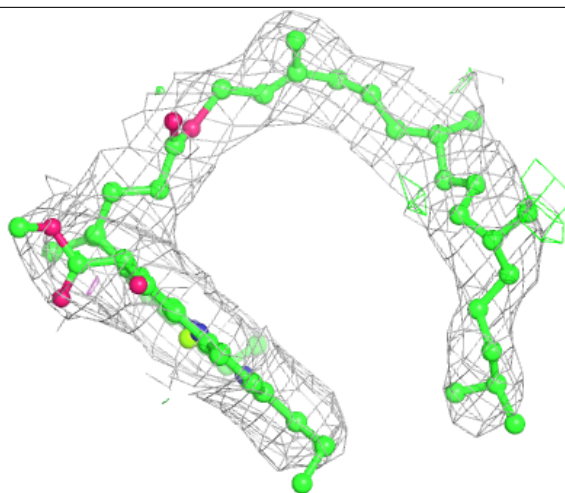
Electron density around CLA B 1224:

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



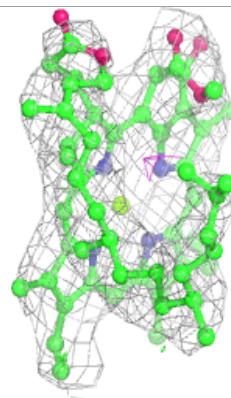
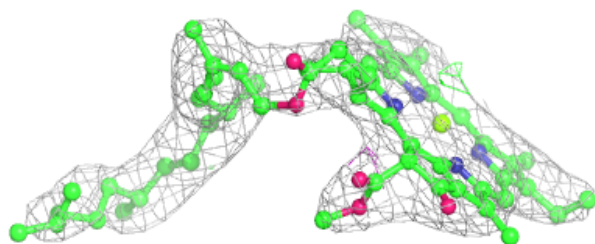
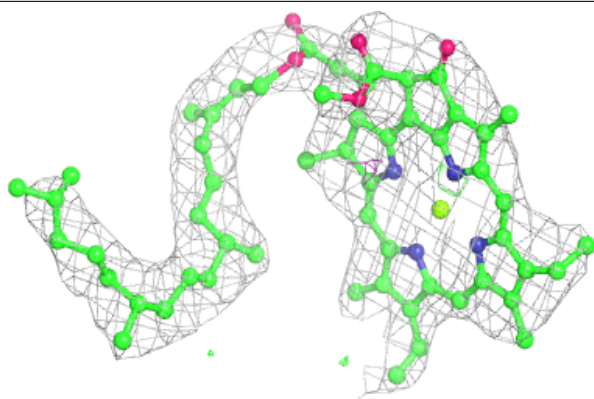
Electron density around CLA B 1216:

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



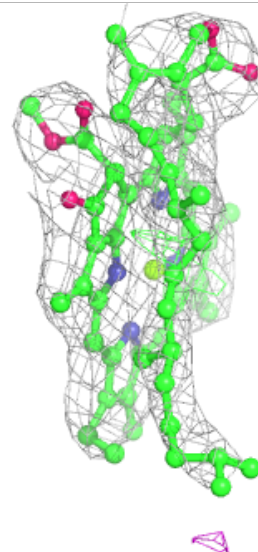
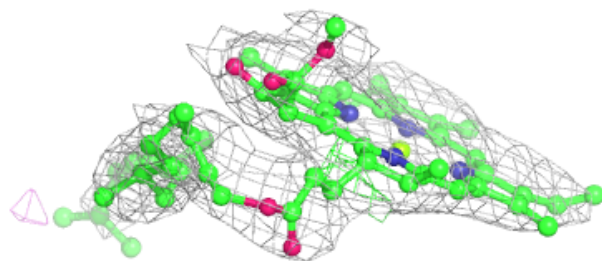
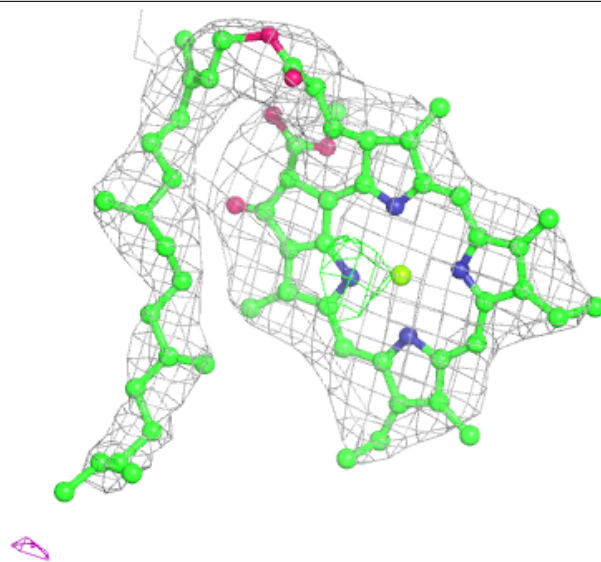
Electron density around CLA B 1221:

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



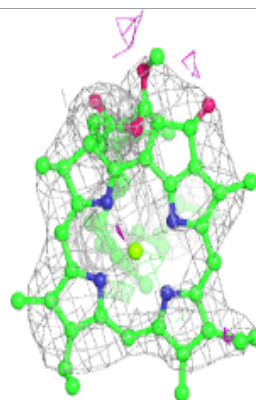
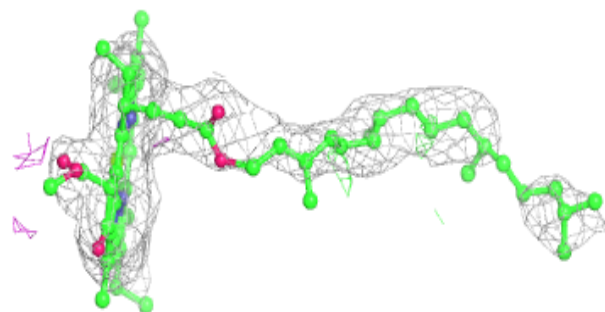
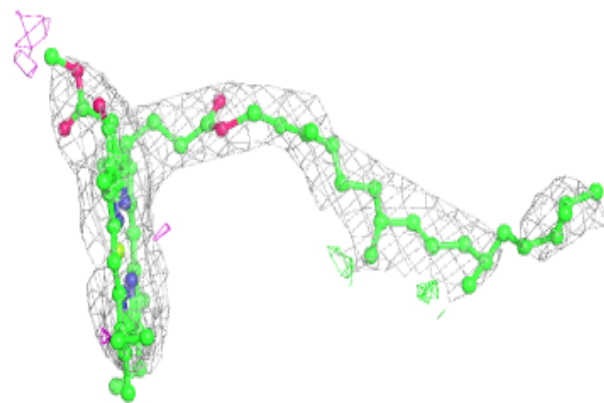
Electron density around CLA A 1123:

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

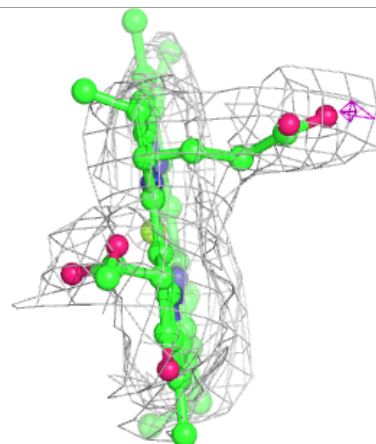
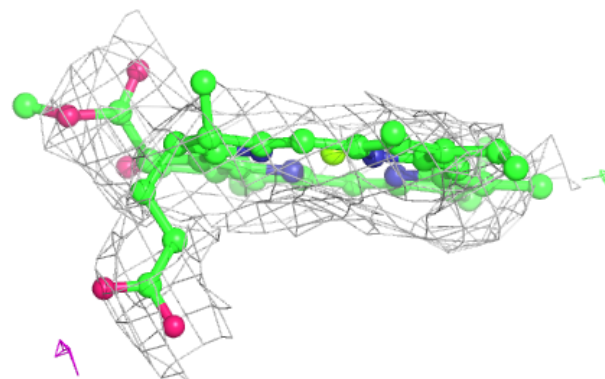
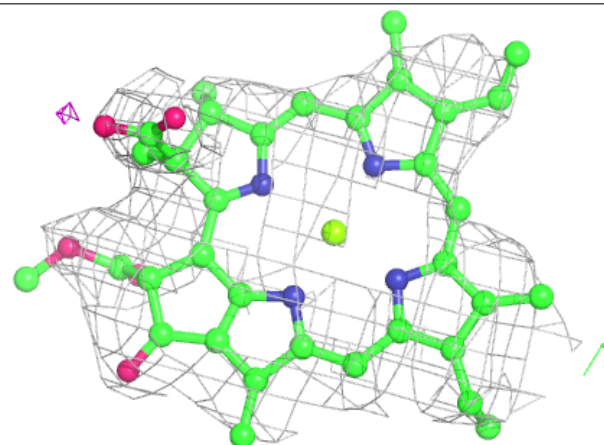


Electron density around CLA A 1105:

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

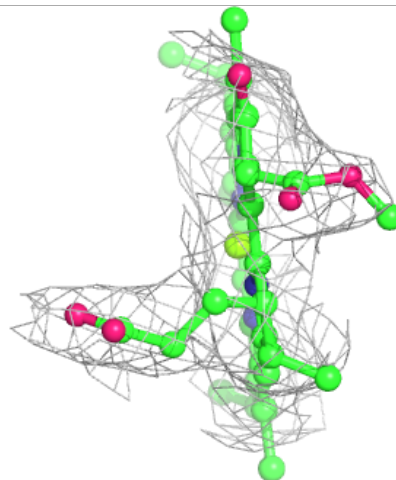
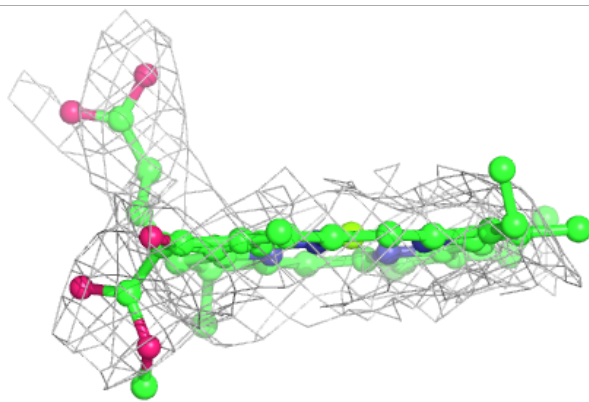
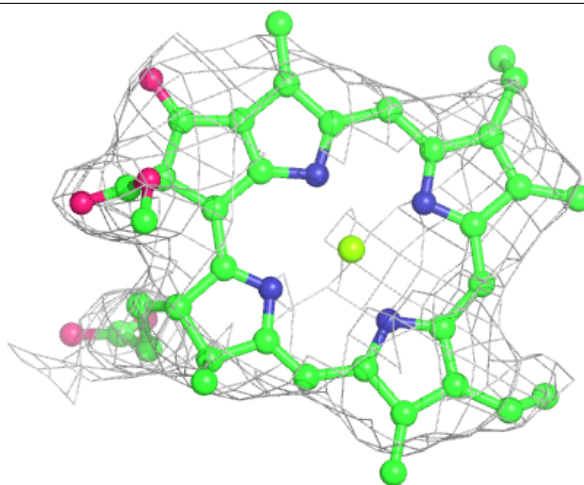
**Electron density around CLA B 1208:**

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



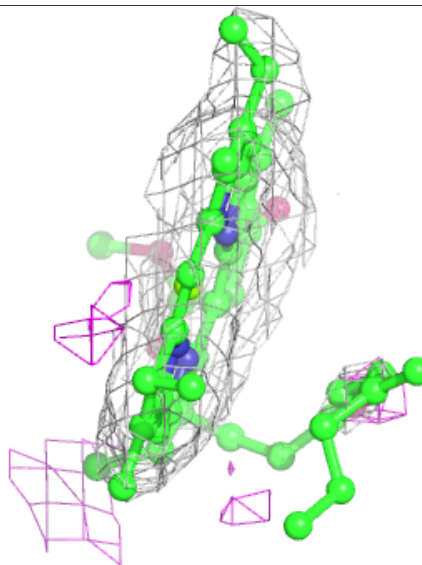
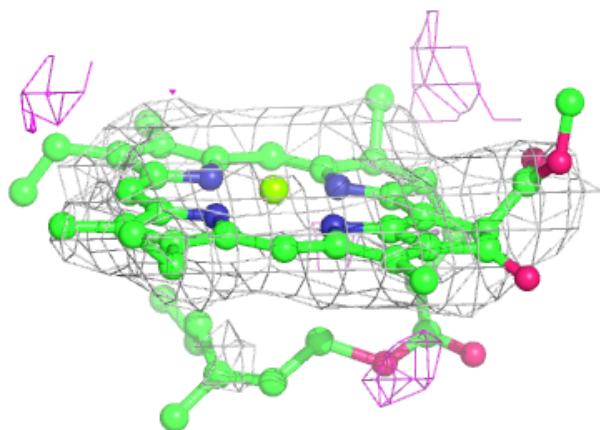
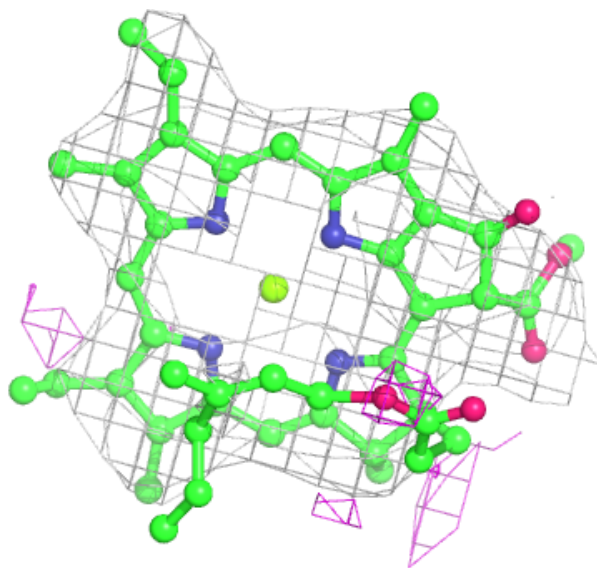
Electron density around CLA A 1112:

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



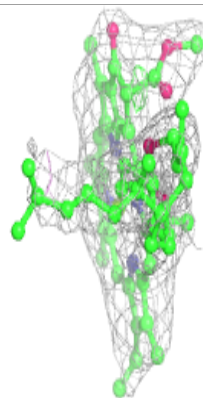
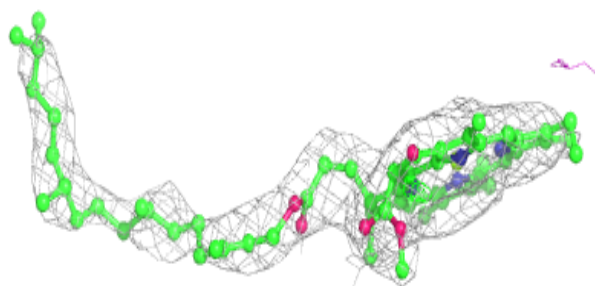
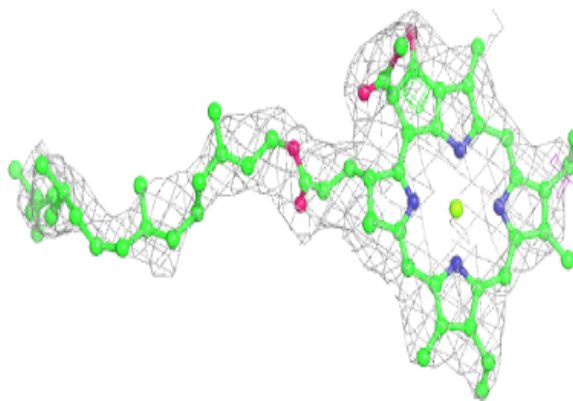
Electron density around CLA A 1801:

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

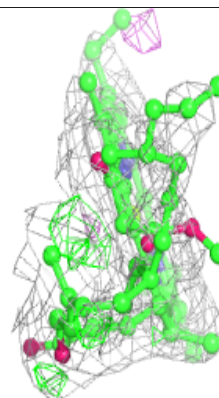
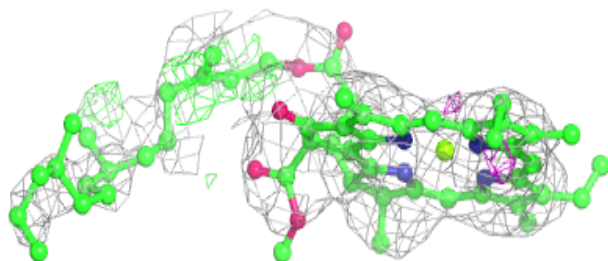
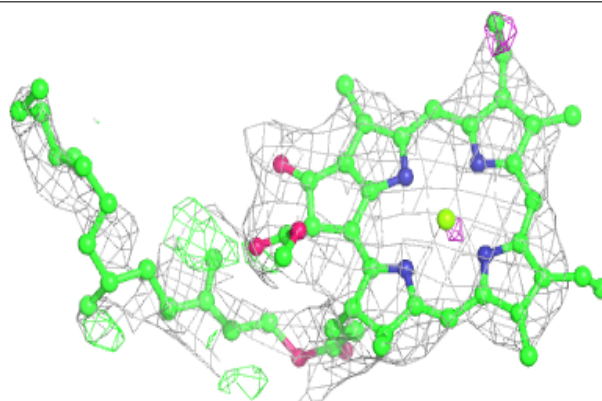


Electron density around CLA A 1103:

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

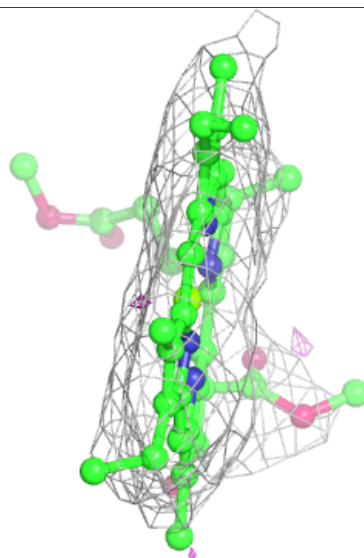
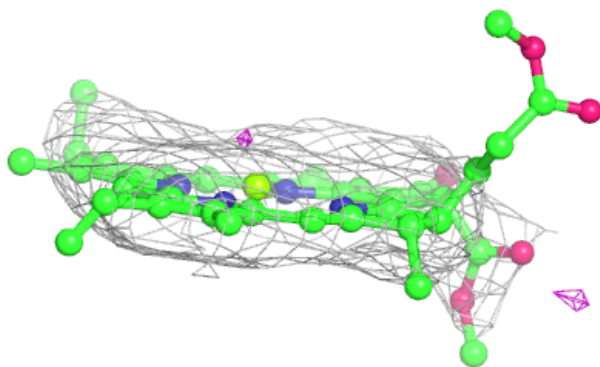
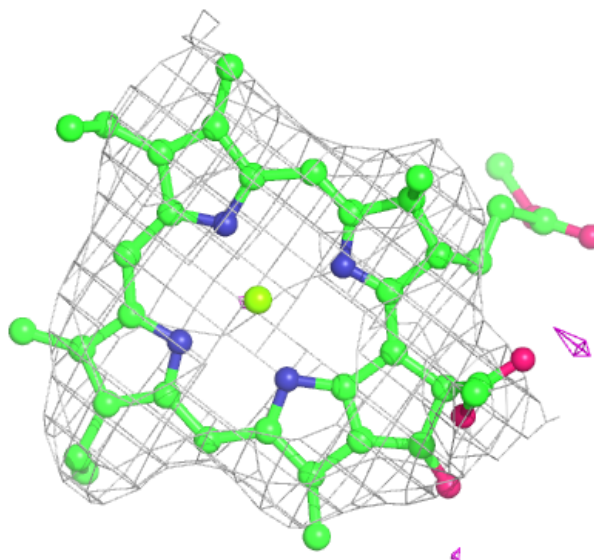
**Electron density around CLA A 1132:**

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



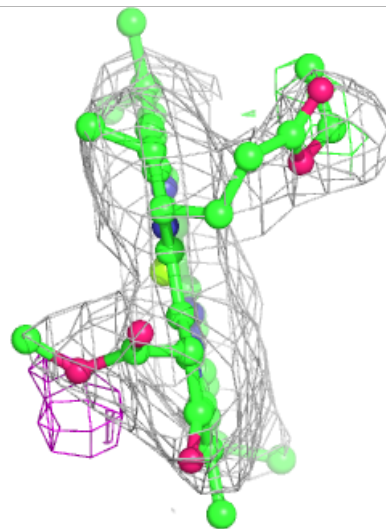
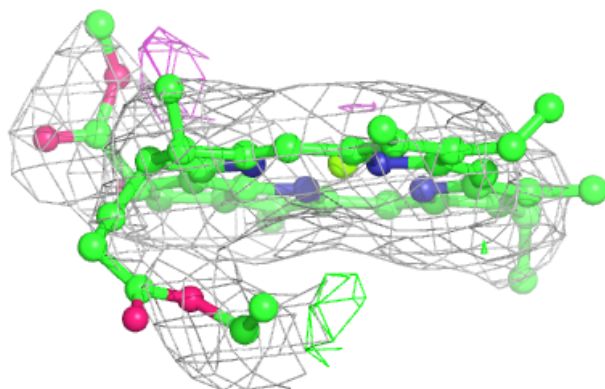
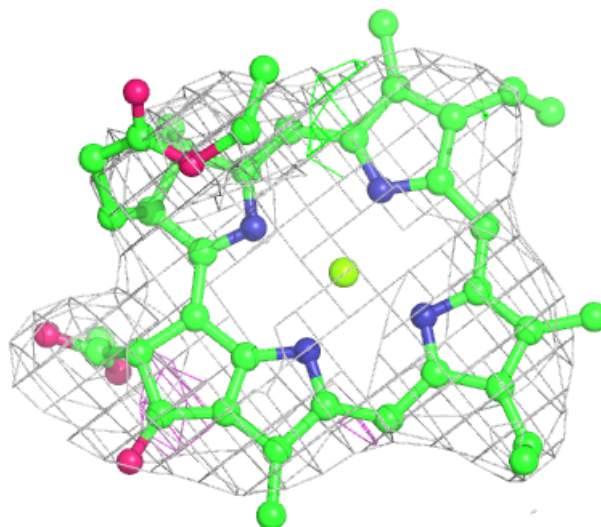
Electron density around CLA A 1129:

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



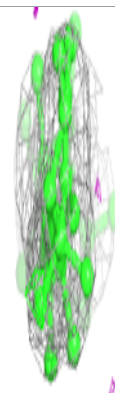
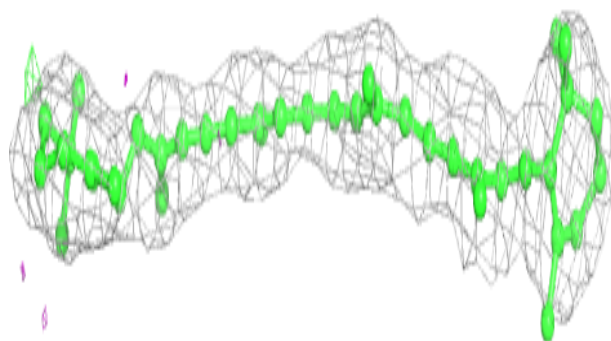
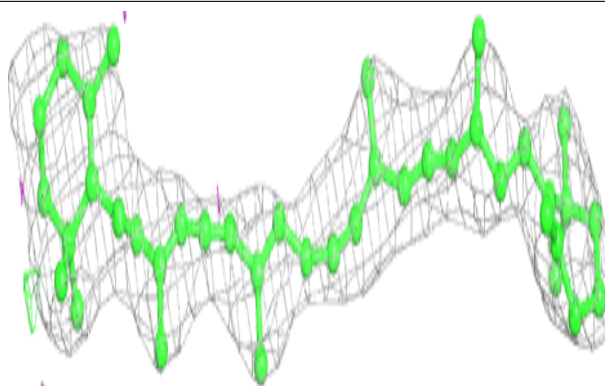
Electron density around CLA B 1217:

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

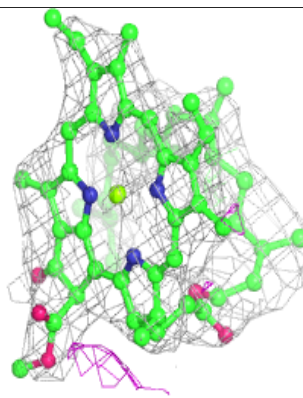
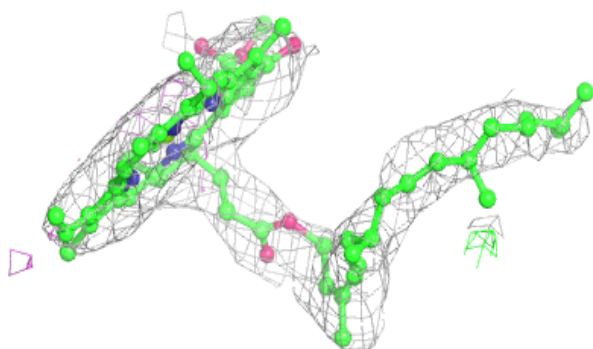
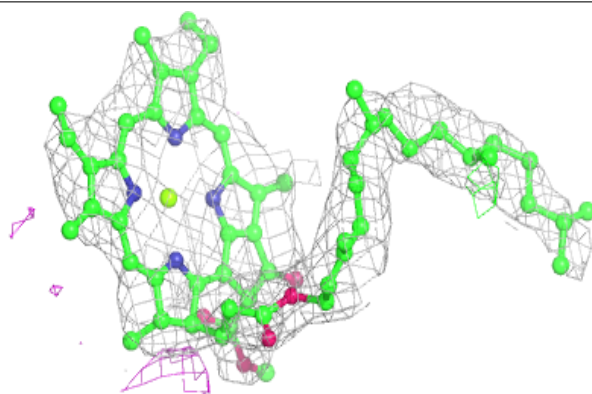


Electron density around BCR F 4015:

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

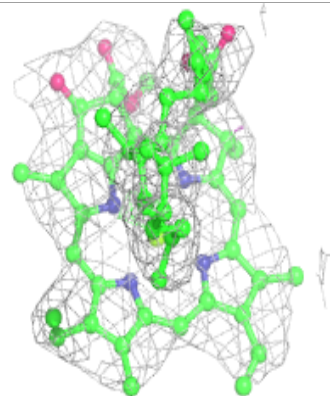
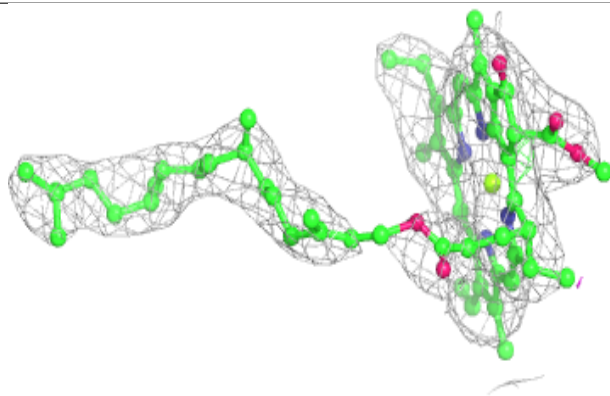
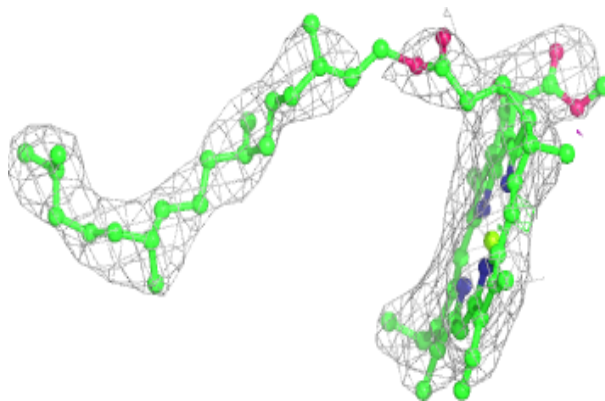
**Electron density around CLA B 1231:**

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

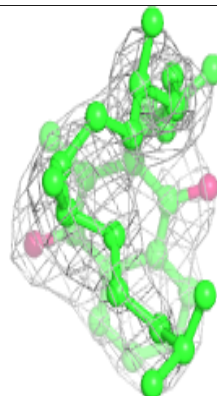
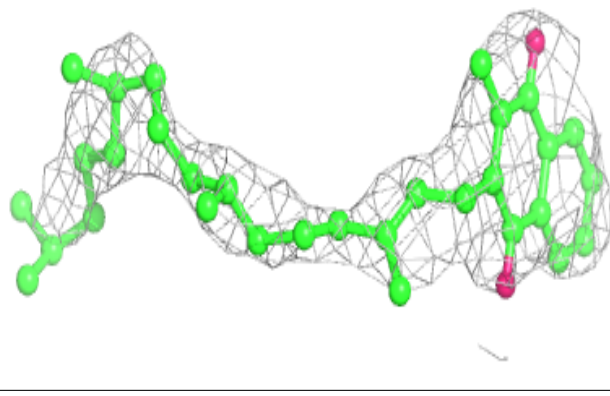
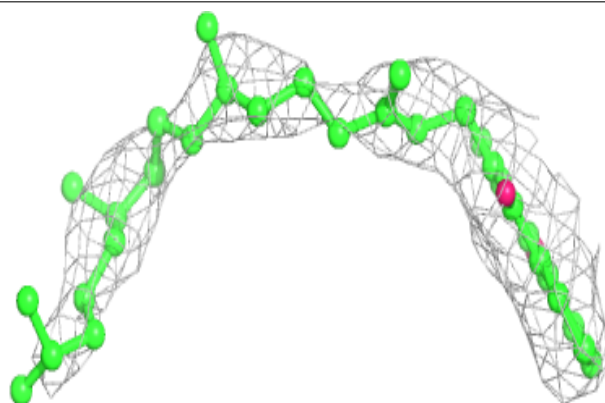


Electron density around CLA A 1128:

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

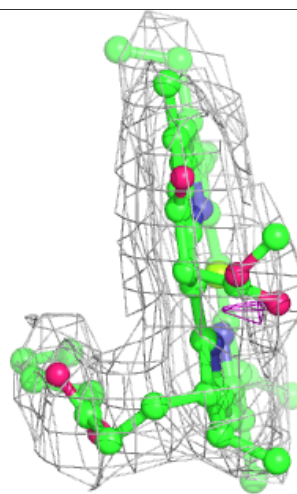
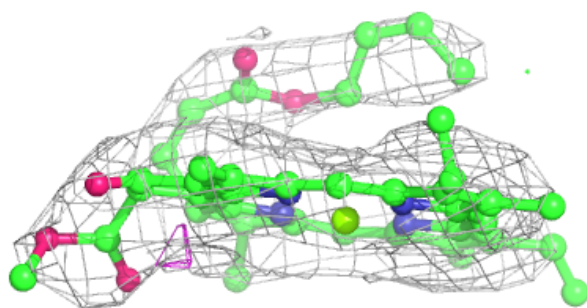
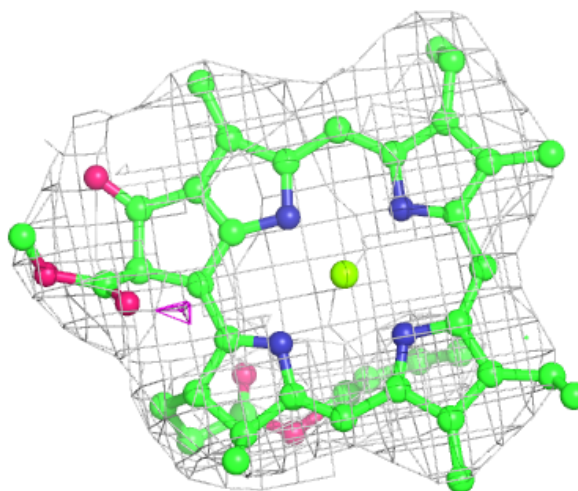
**Electron density around PQN B 2002:**

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



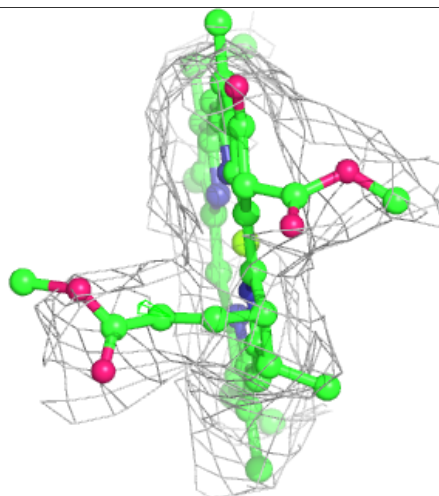
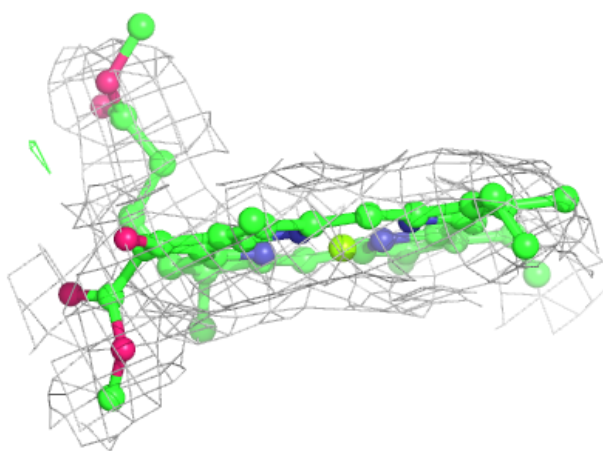
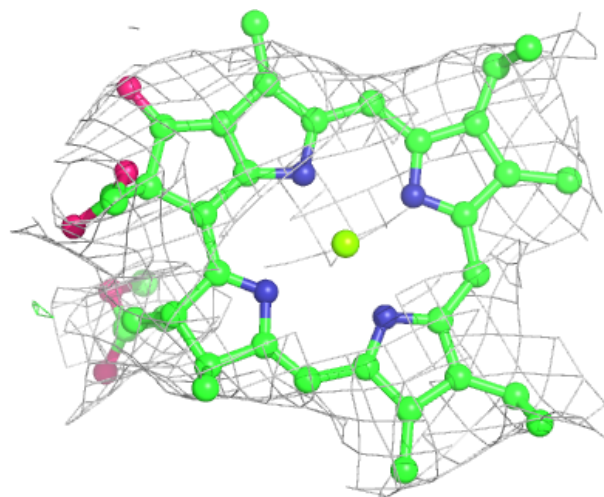
Electron density around CLA A 1120:

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



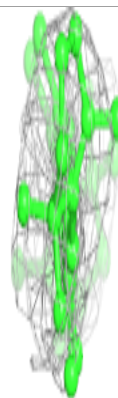
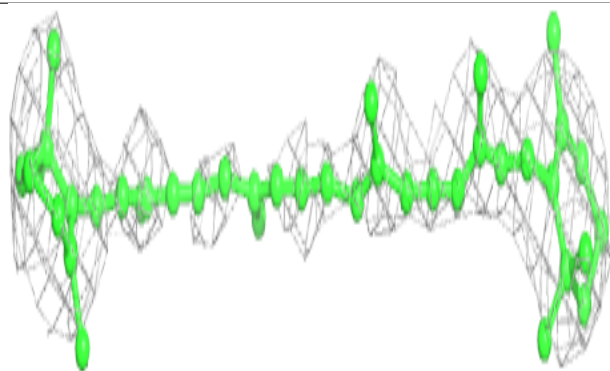
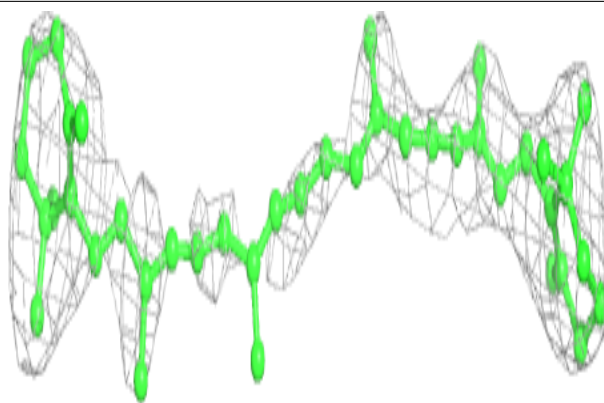
Electron density around CLA B 1211:

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



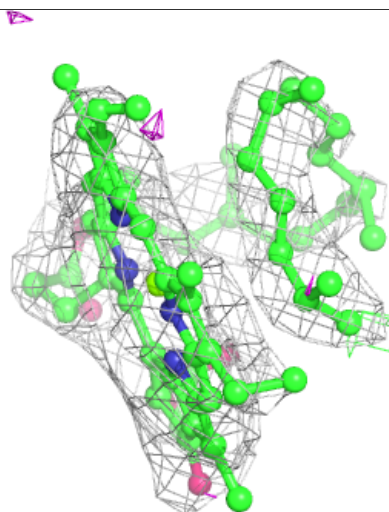
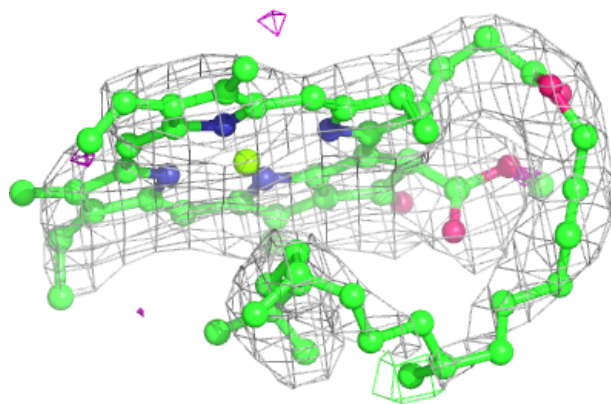
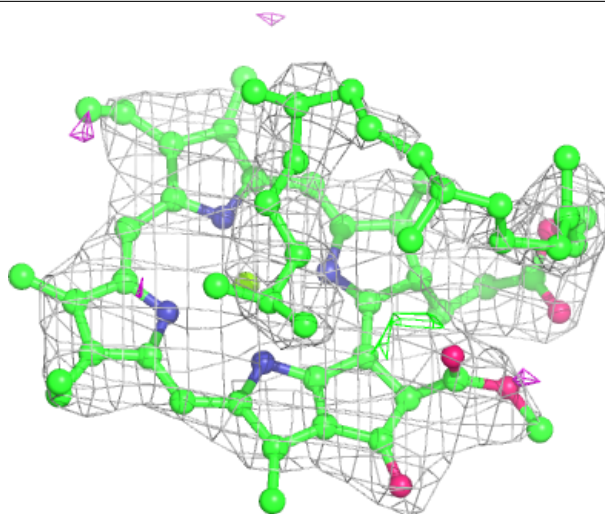
Electron density around BCR A 4002:

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



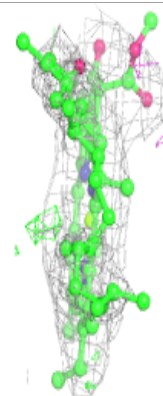
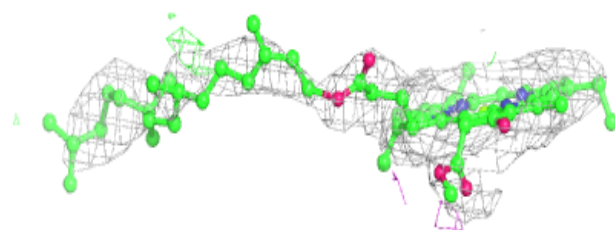
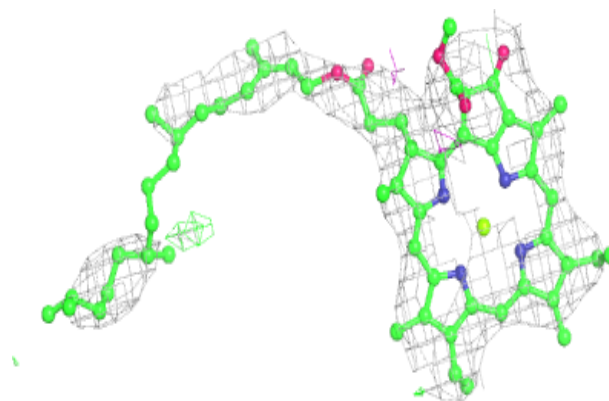
Electron density around CLA B 1203:

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



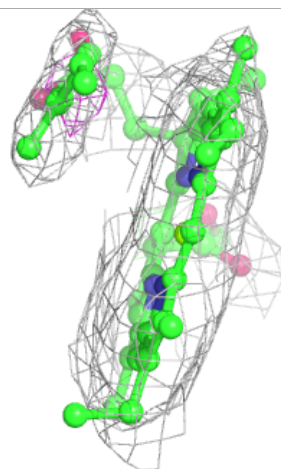
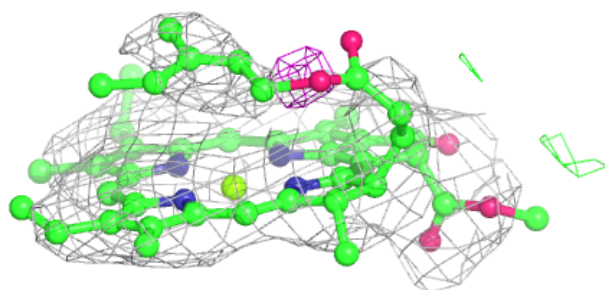
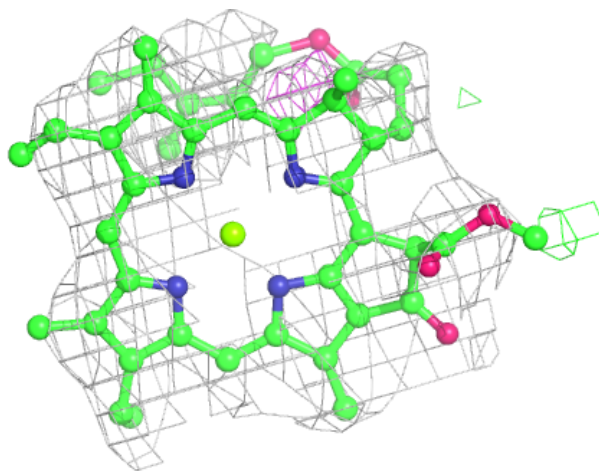
Electron density around CLA F 1410:

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



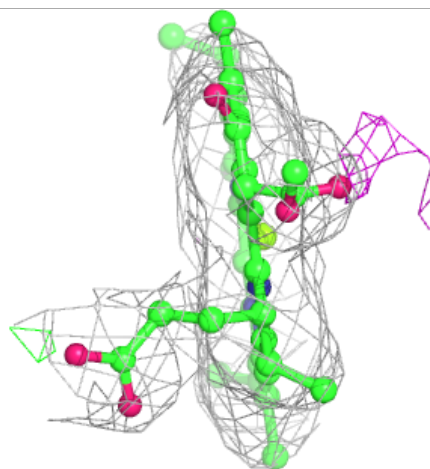
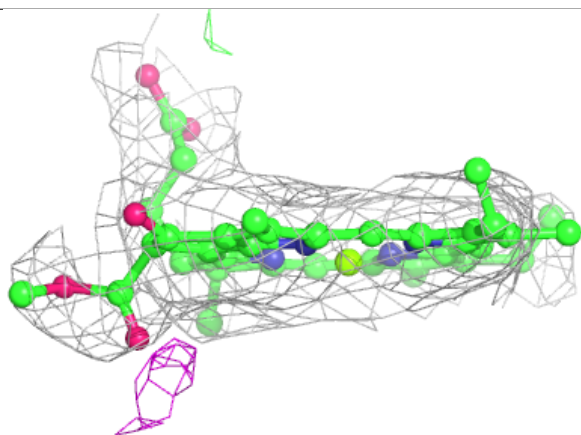
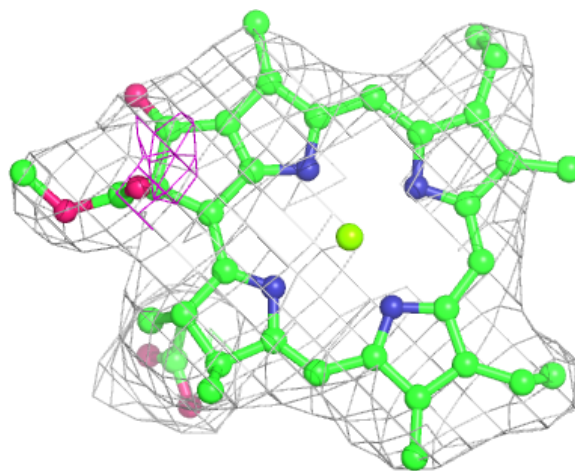
Electron density around CLA B 1218:

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



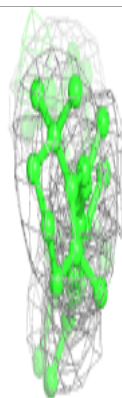
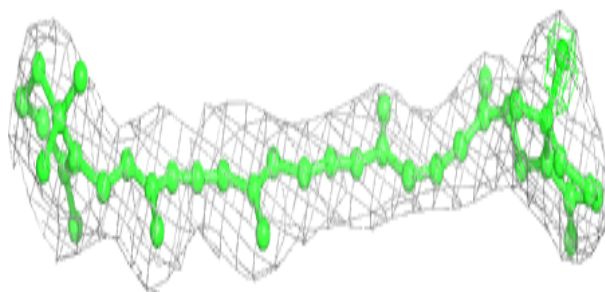
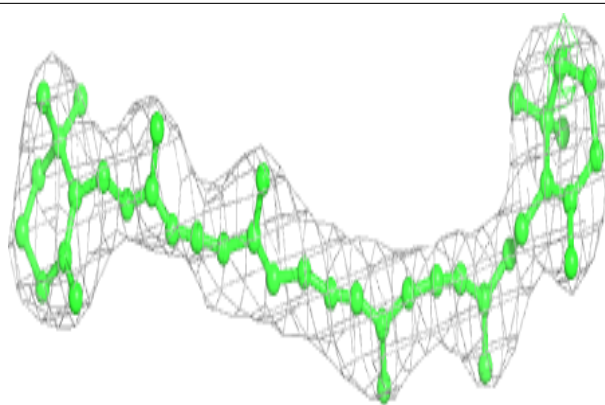
Electron density around CLA B 1232:

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

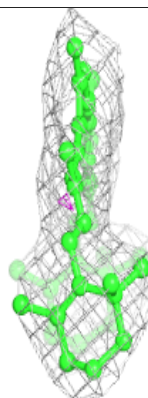
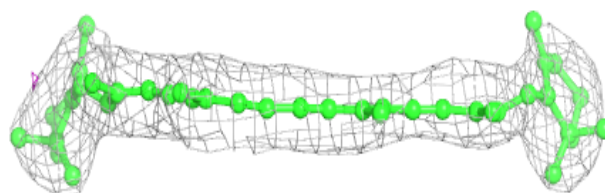
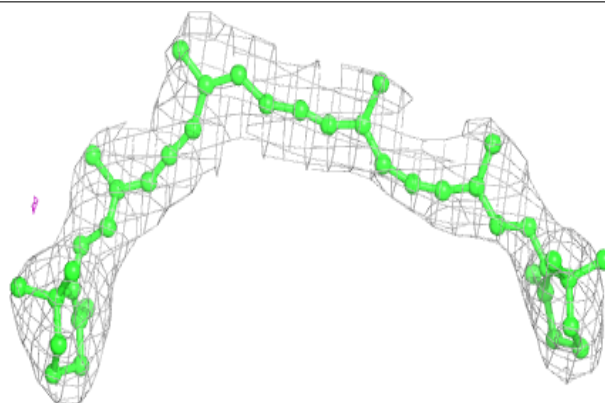


Electron density around BCR B 4010:

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

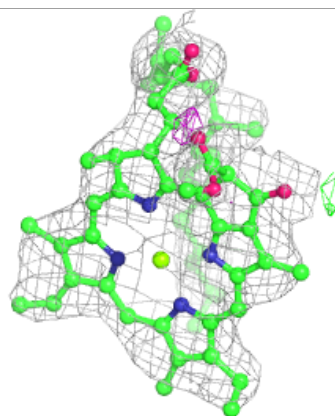
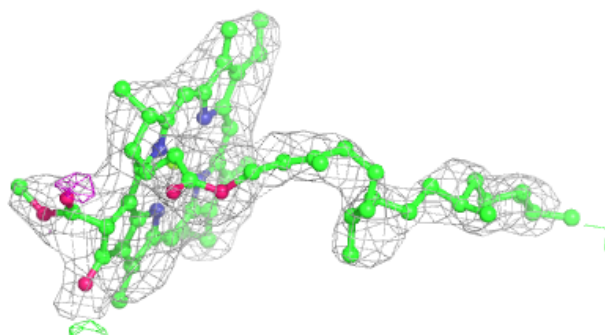
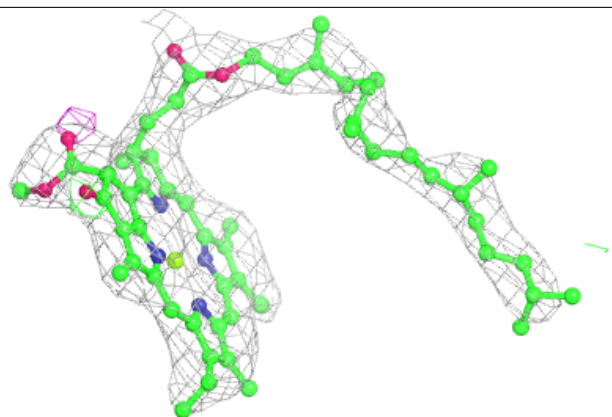
**Electron density around BCR F 4016:**

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



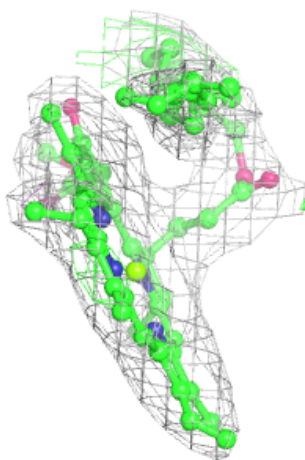
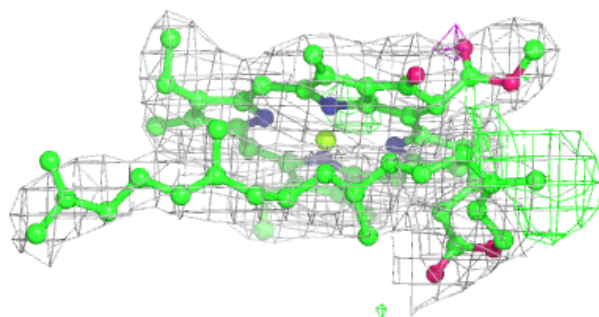
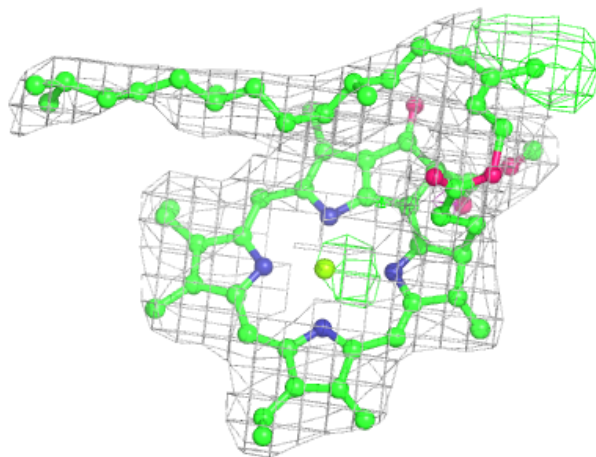
Electron density around CLA A 1102:

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



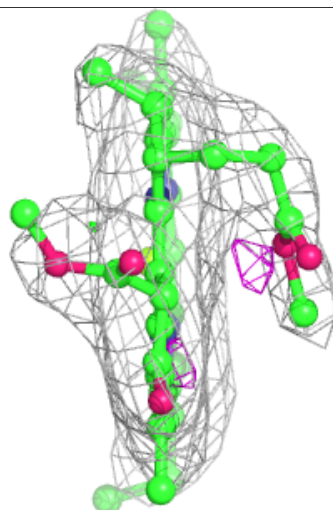
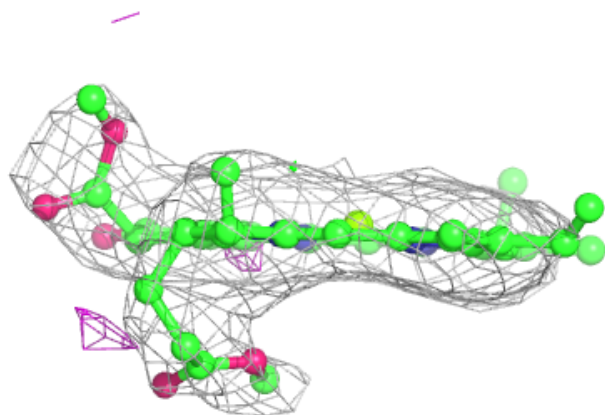
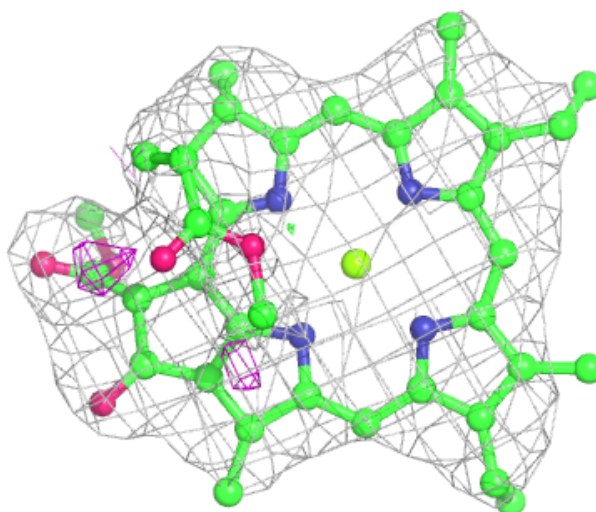
Electron density around CLA B 1228:

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



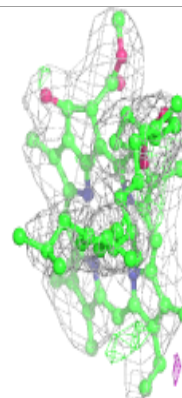
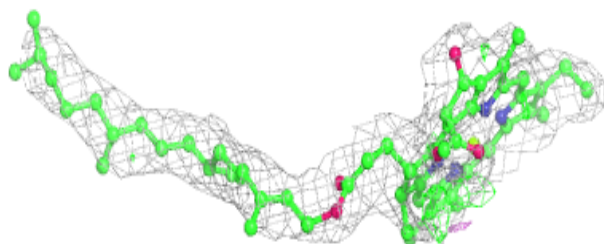
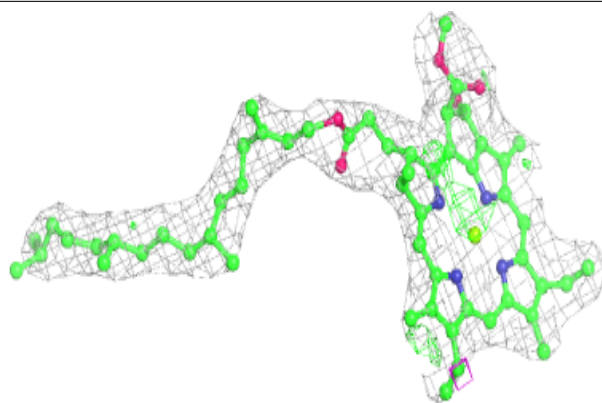
Electron density around CLA B 1201:

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

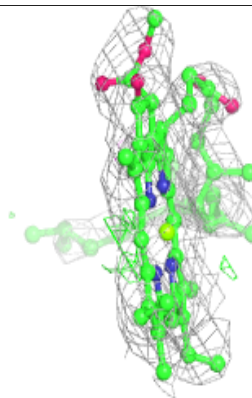
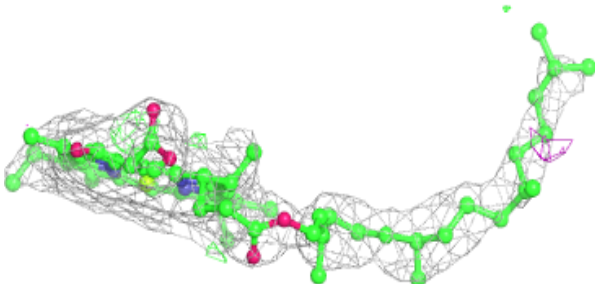
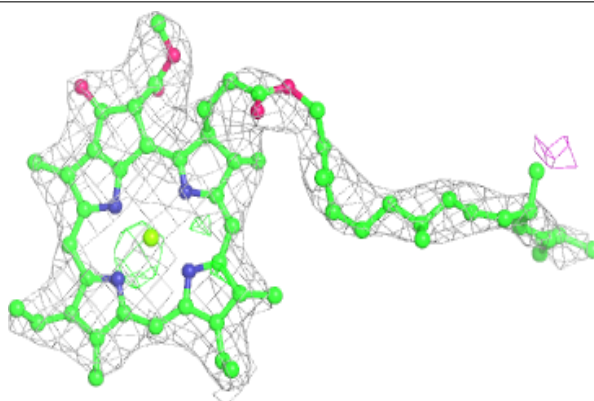


Electron density around CLA A 1022:

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

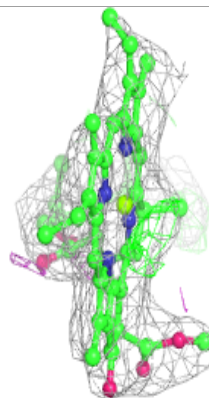
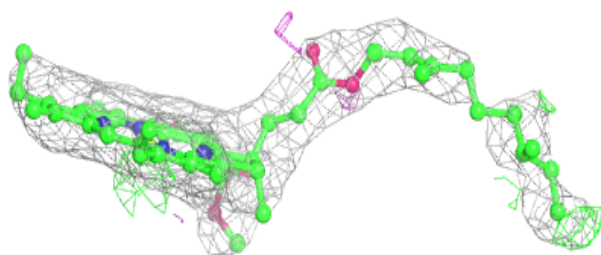
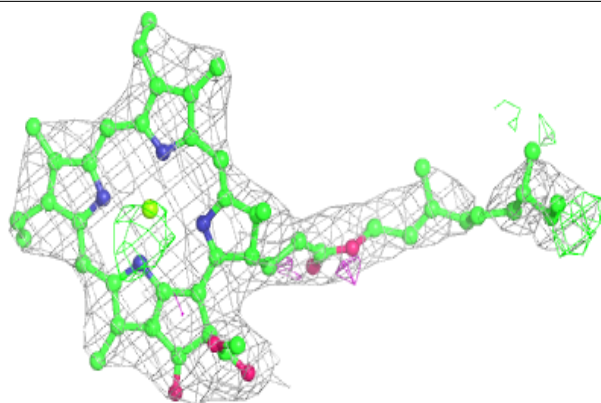
**Electron density around CLA B 1023:**

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

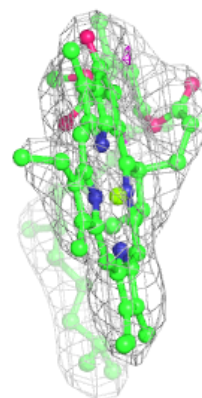
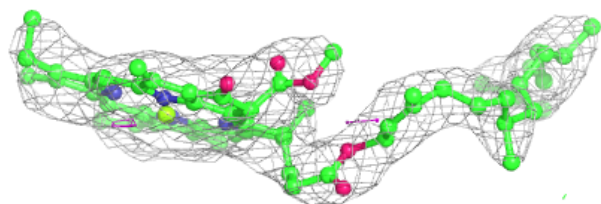
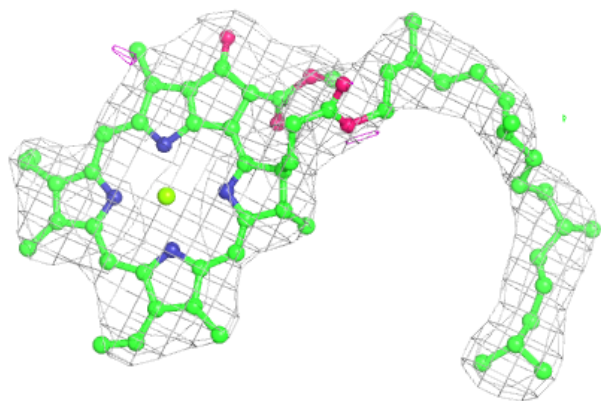


Electron density around CLA B 1222:

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

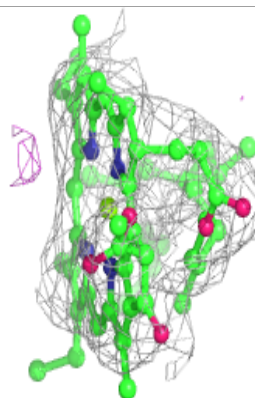
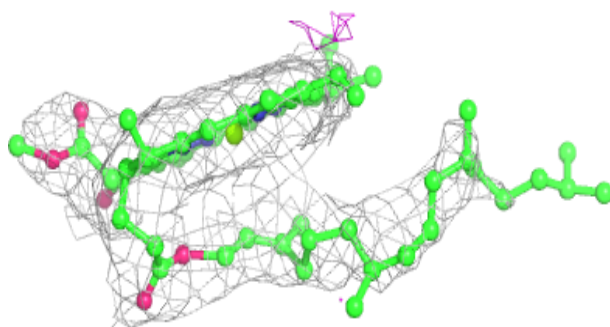
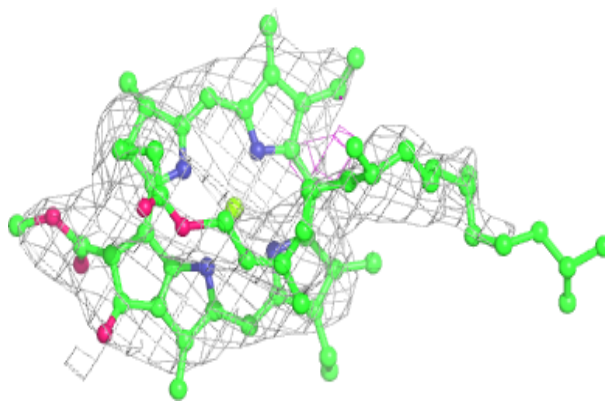
**Electron density around CLA A 1101:**

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

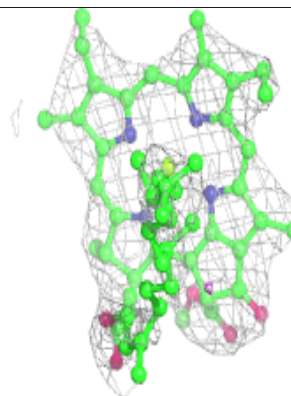
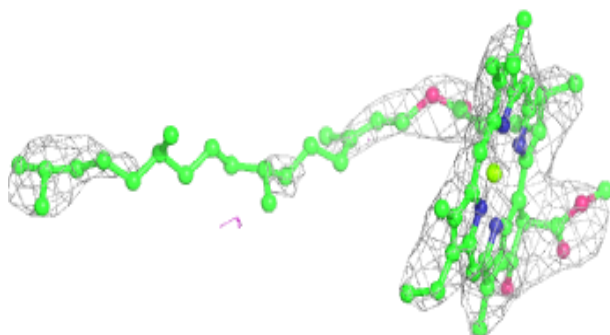
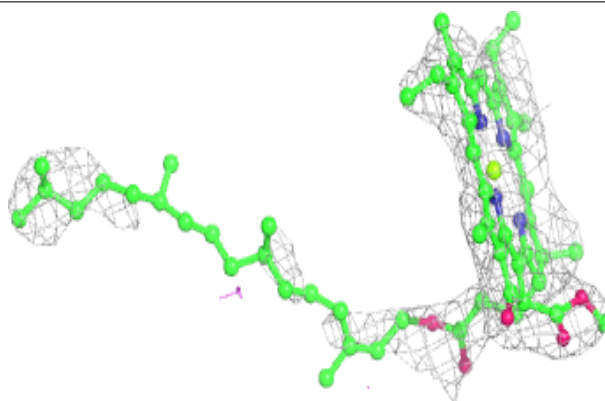


Electron density around CLA A 1136:

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

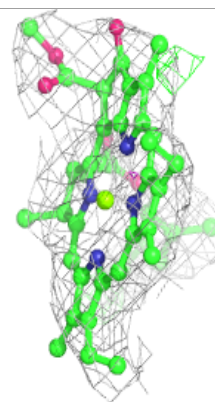
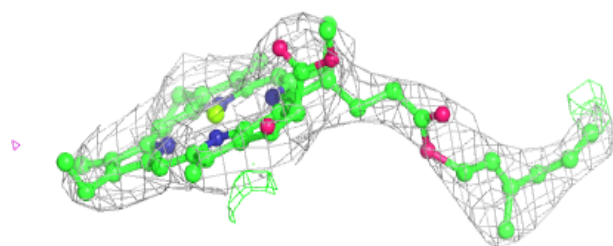
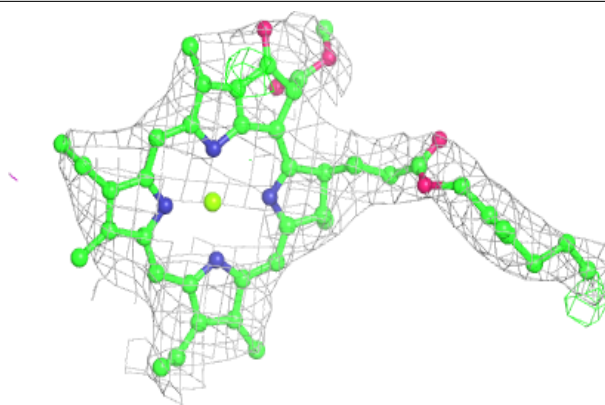
**Electron density around CLA B 1226:**

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



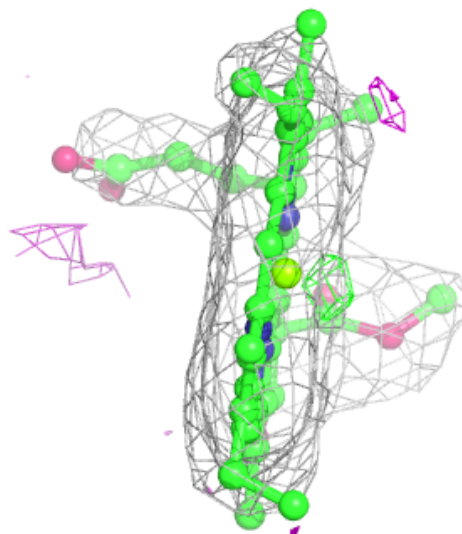
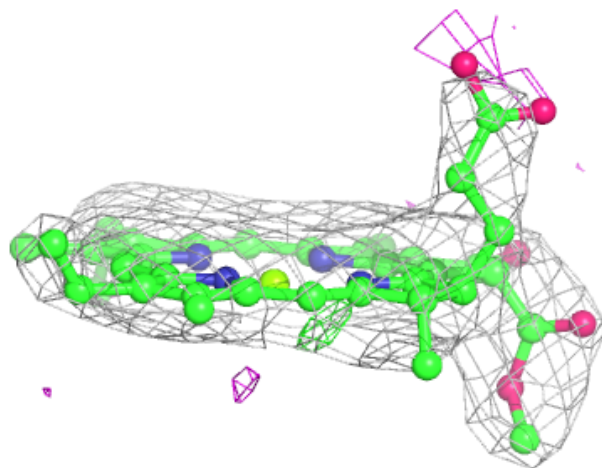
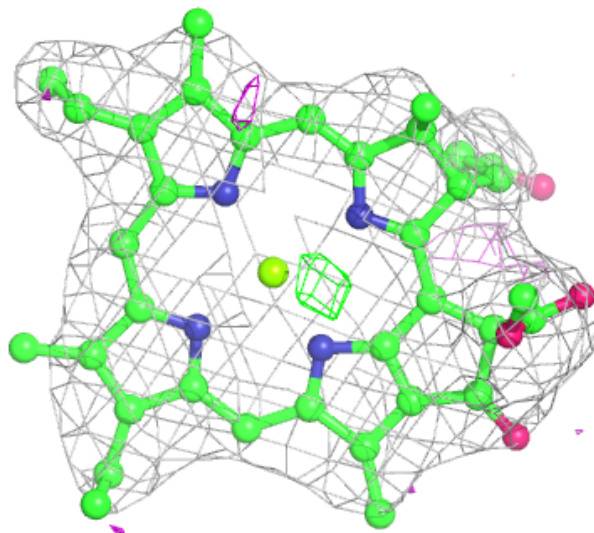
Electron density around CLA A 1125:

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



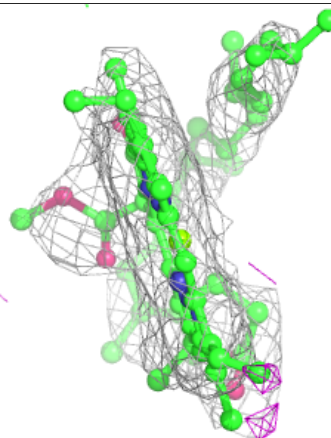
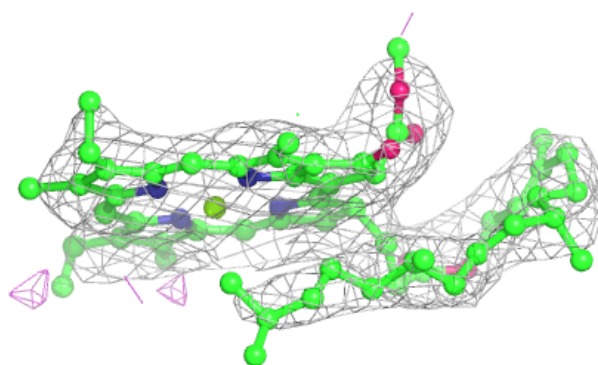
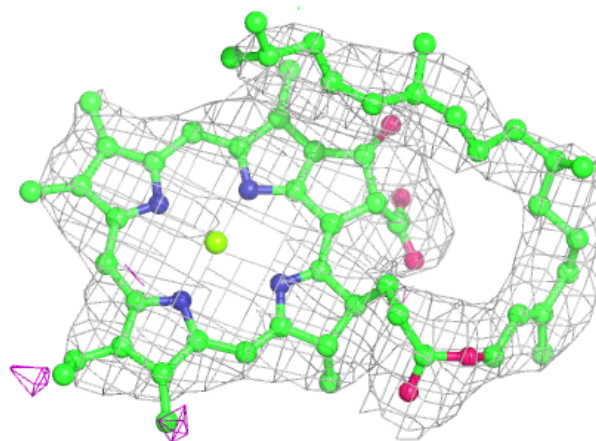
Electron density around CLA B 1227:

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

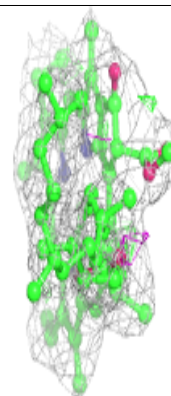
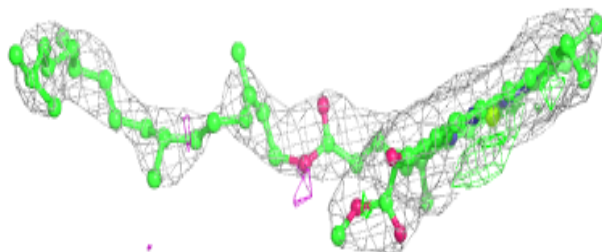
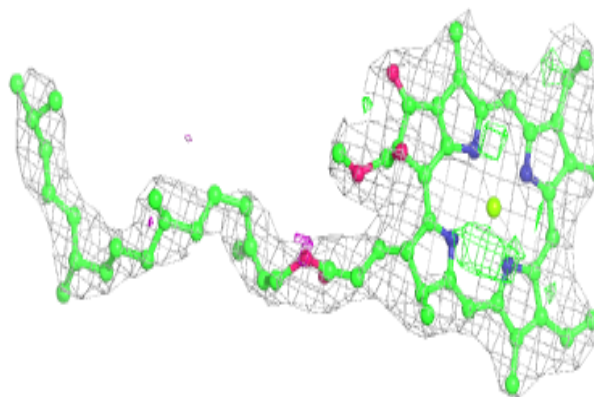


Electron density around CLA B 1202:

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

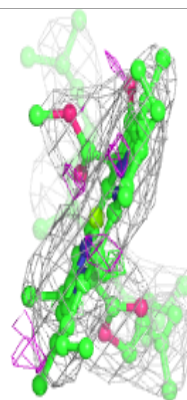
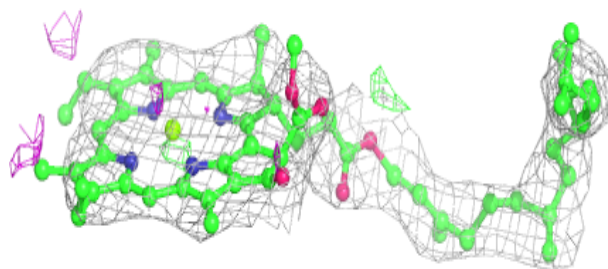
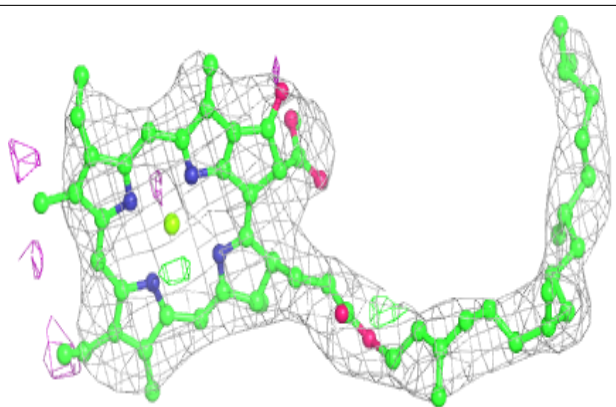
**Electron density around CLA F 1139:**

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



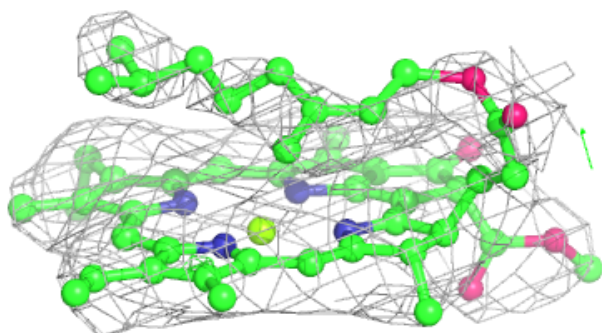
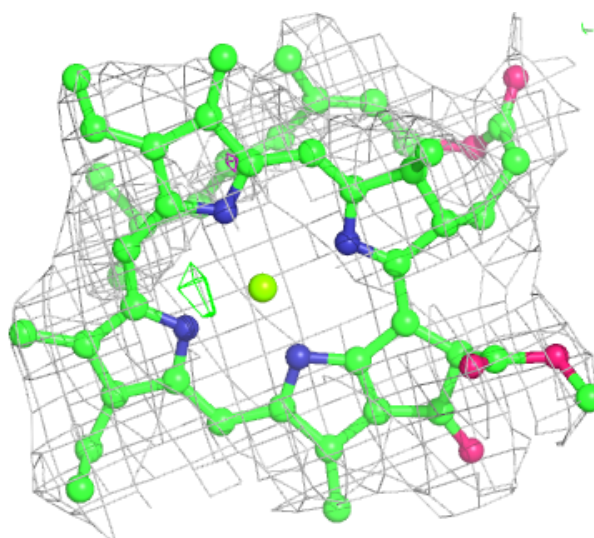
Electron density around CLA B 1223:

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



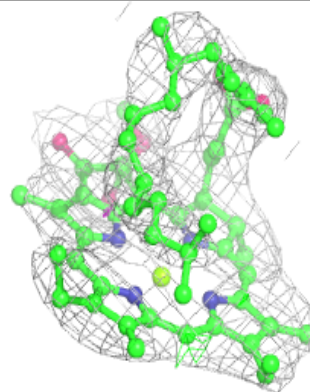
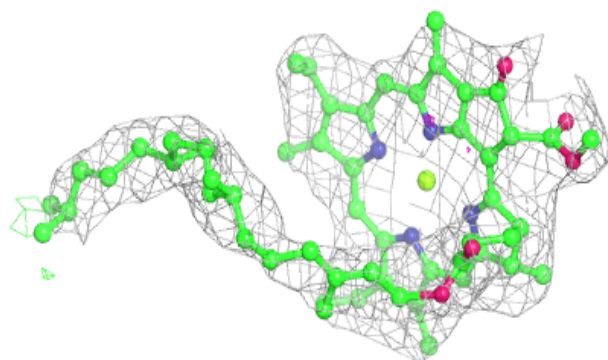
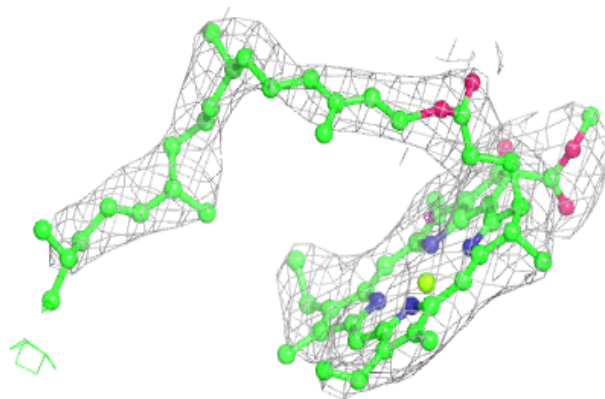
Electron density around CLA B 1219:

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

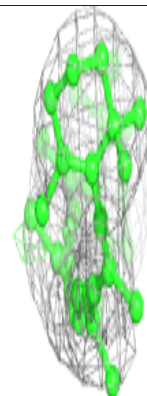
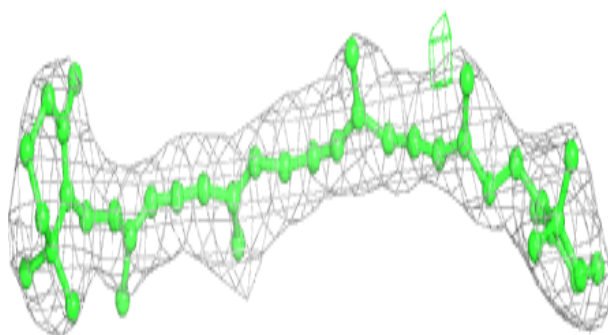
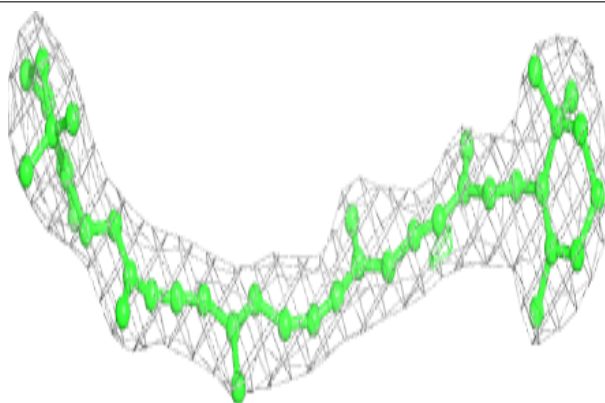


Electron density around CLA A 1109:

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

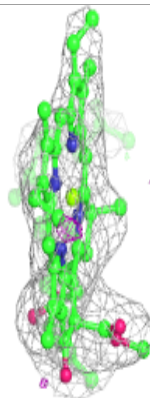
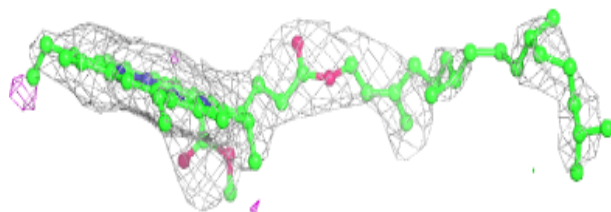
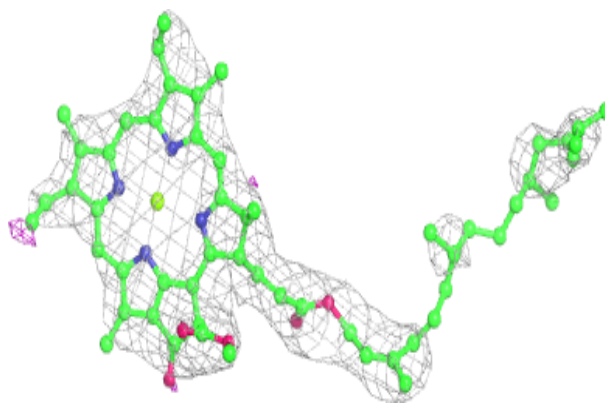
**Electron density around BCR B 4014:**

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

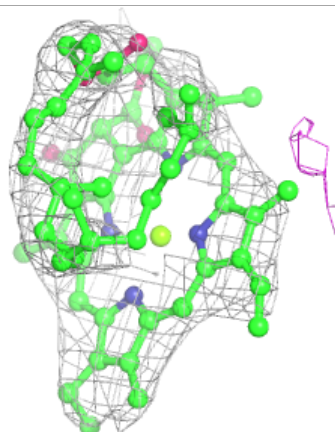
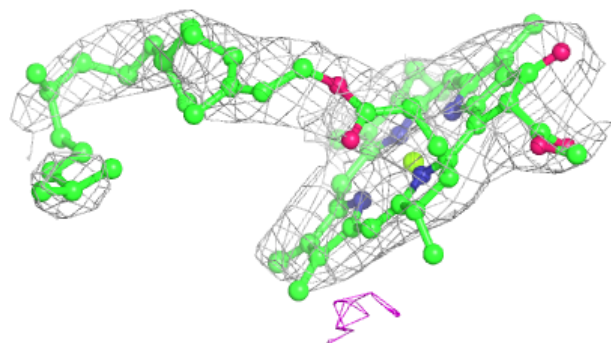
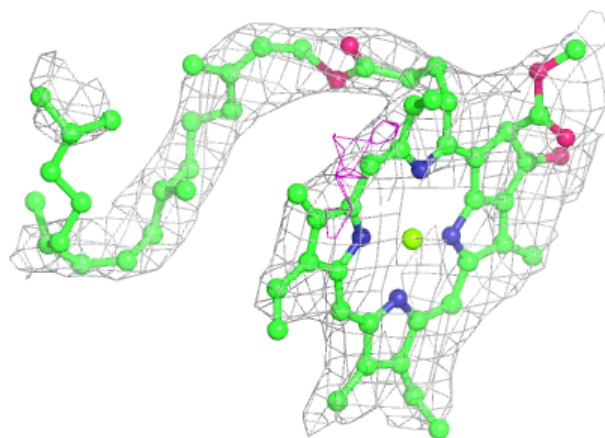


Electron density around CLA B 1234:

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

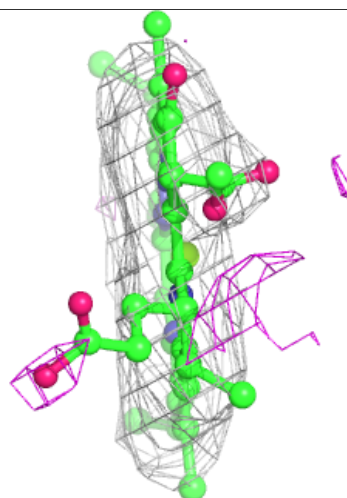
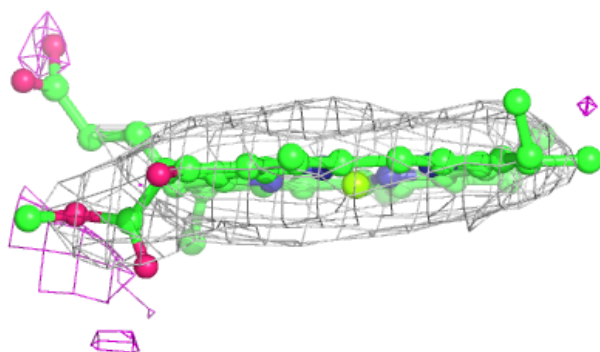
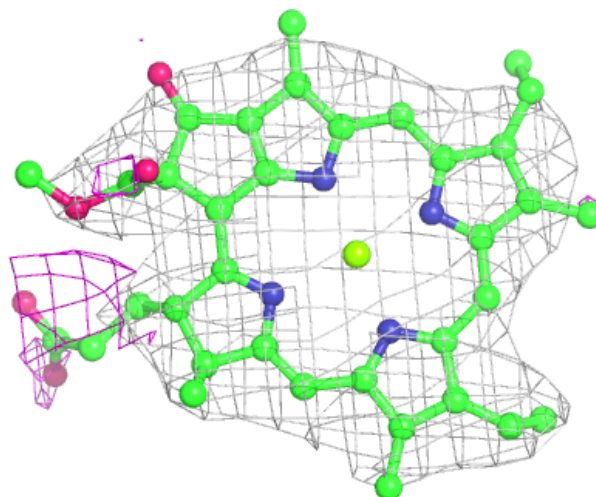
**Electron density around CLA A 1122:**

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



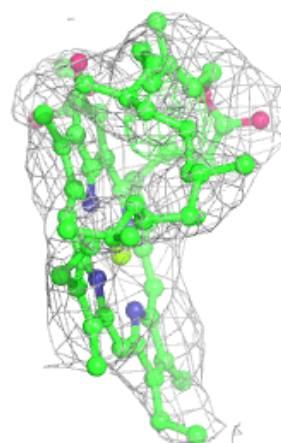
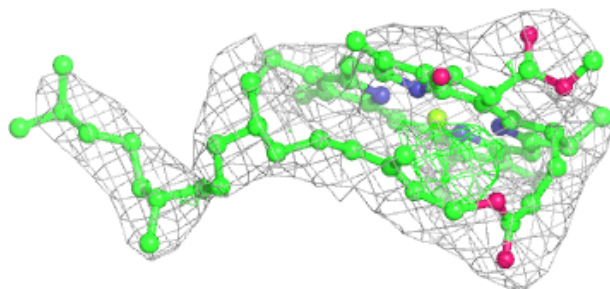
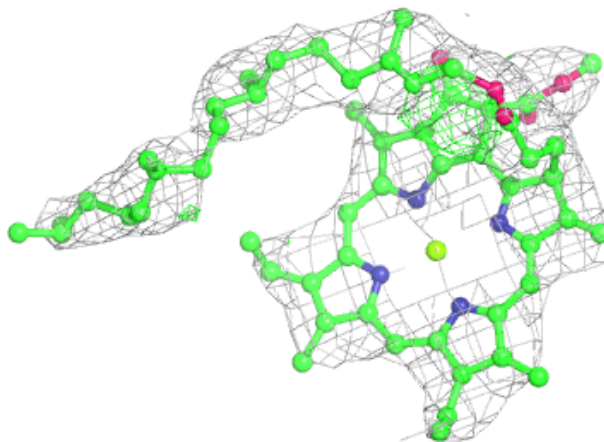
Electron density around CLA B 1240:

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



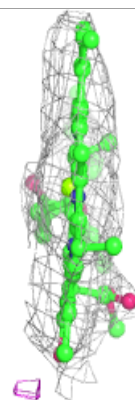
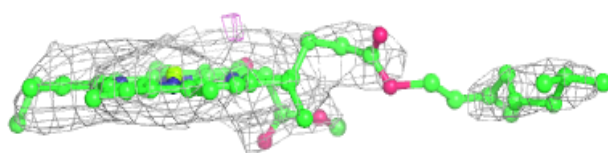
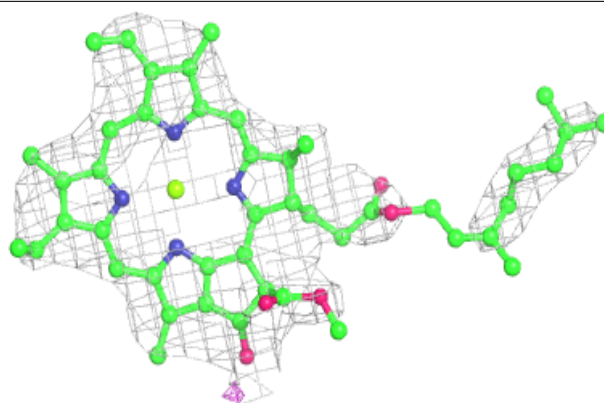
Electron density around CLA A 1127:

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

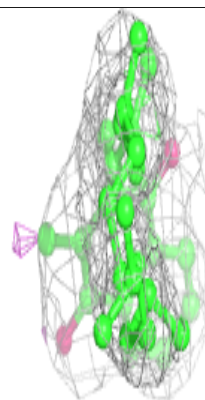
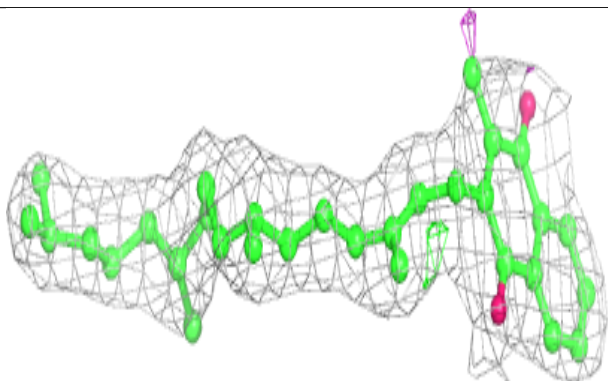
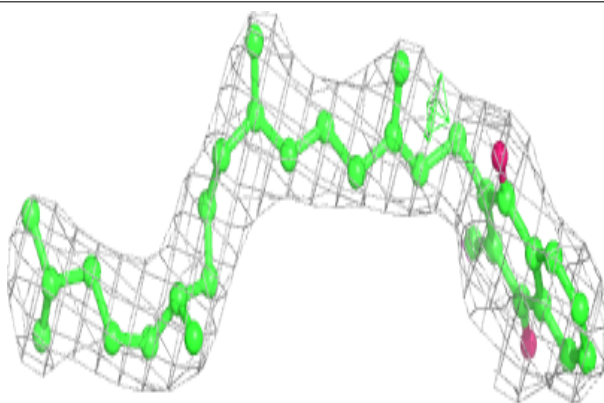


Electron density around CLA A 1131:

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

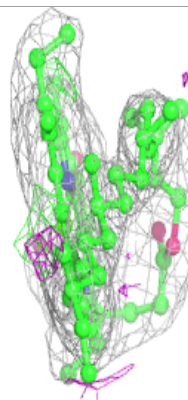
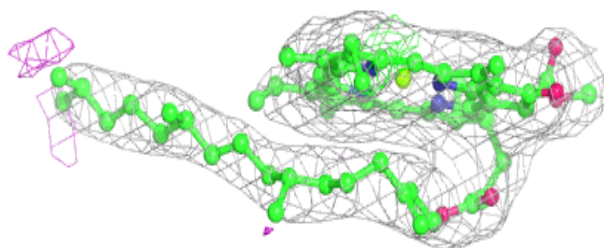
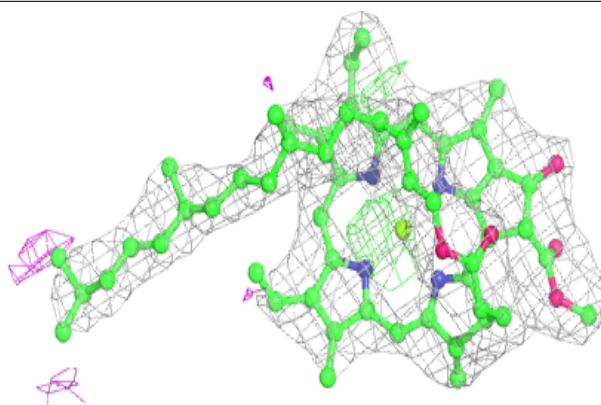
**Electron density around PQN A 2001:**

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



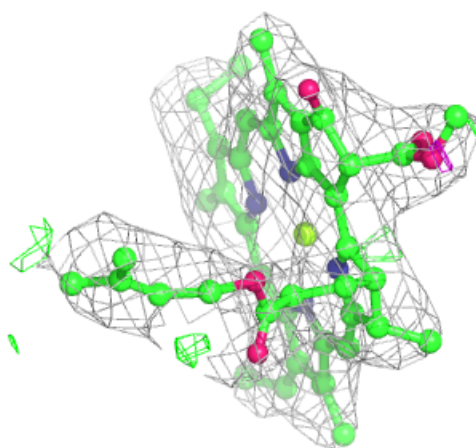
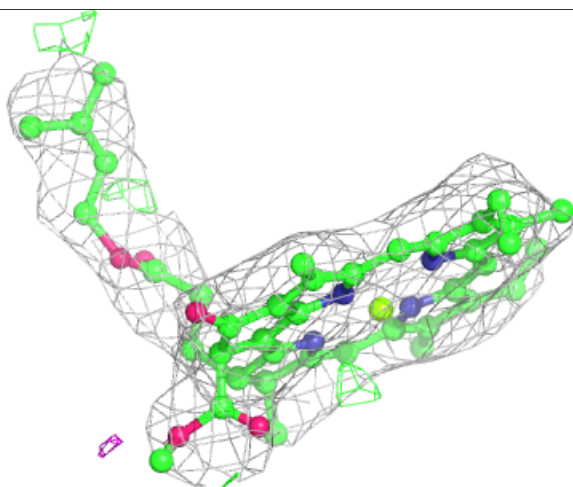
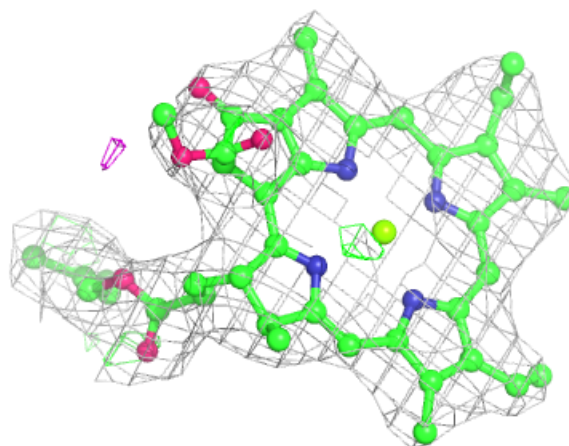
Electron density around CLA A 1138:

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



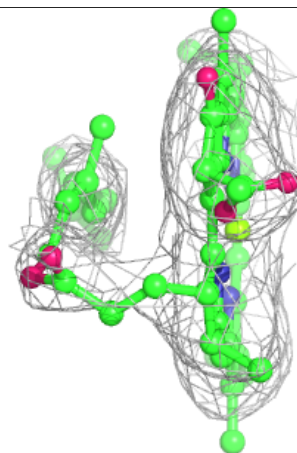
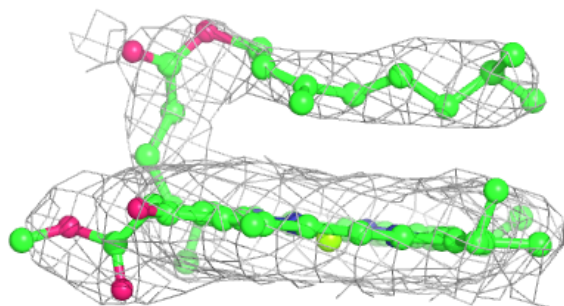
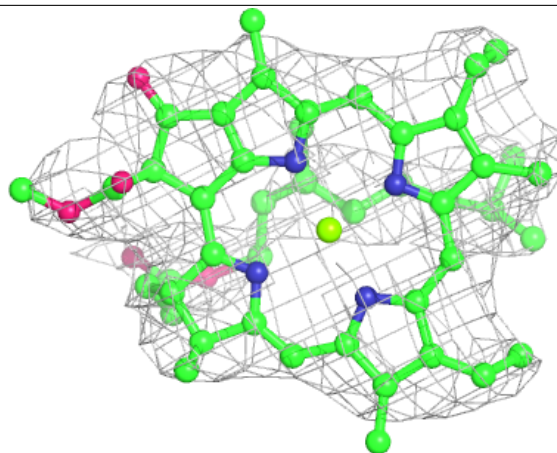
Electron density around CLA B 1236:

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



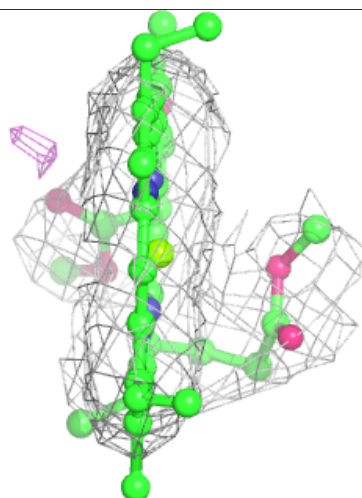
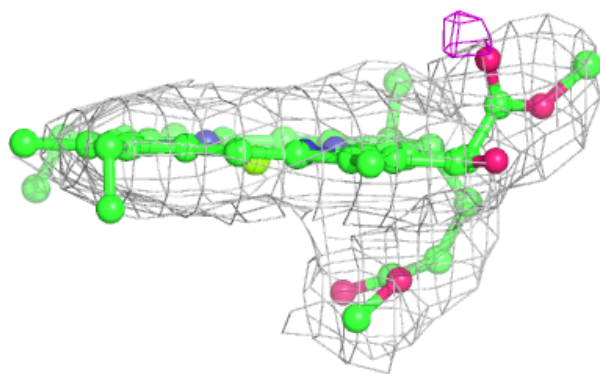
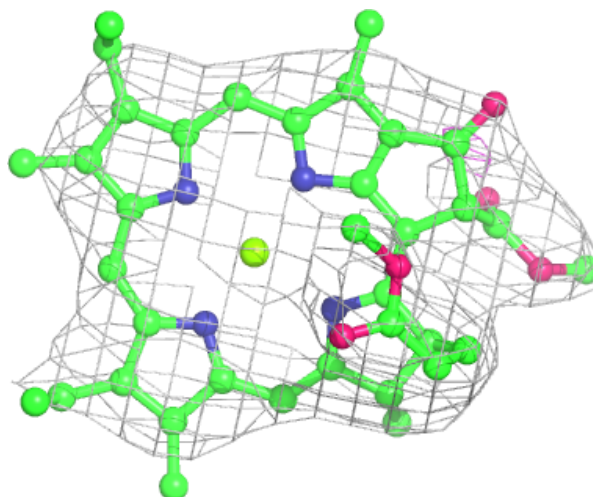
Electron density around CLA B 1237:

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



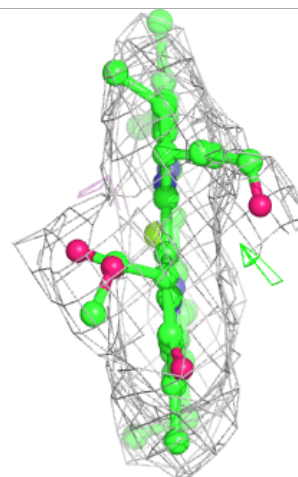
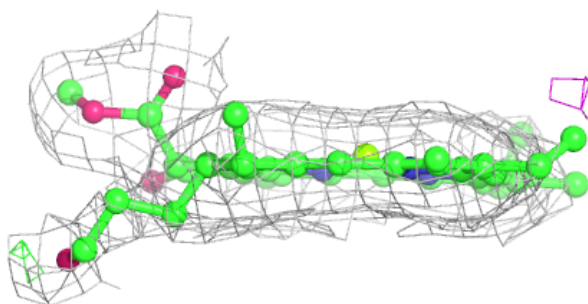
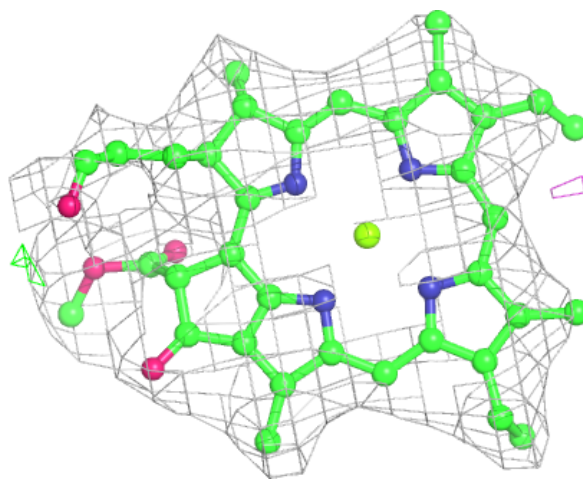
Electron density around CLA B 1204:

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



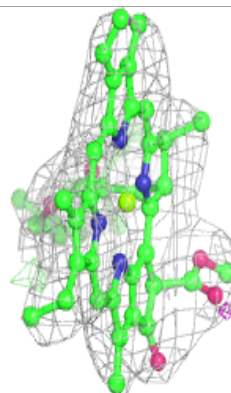
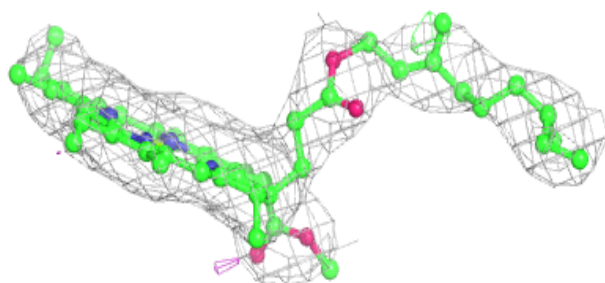
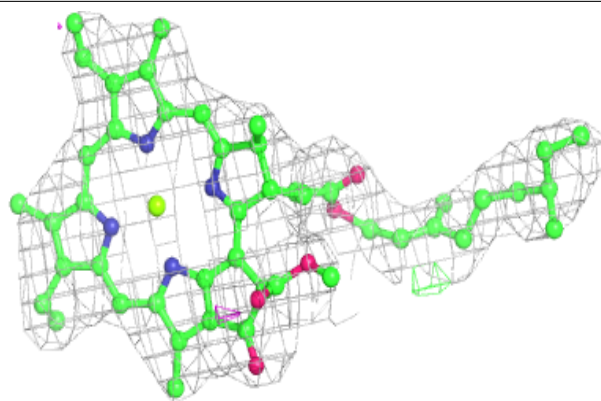
Electron density around CLA B 1238:

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

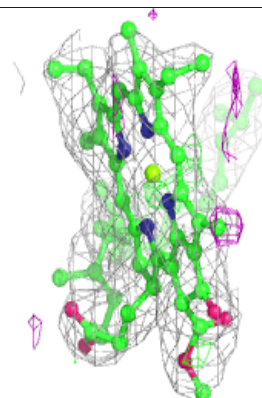
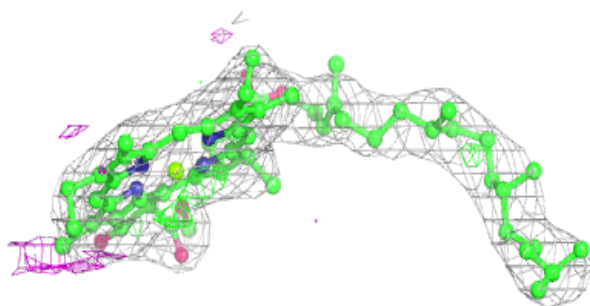
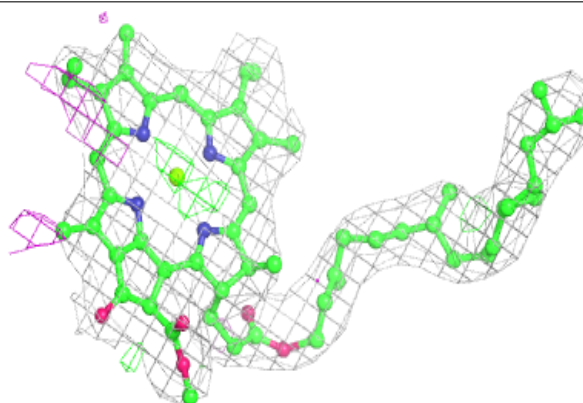


Electron density around CLA B 1220:

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

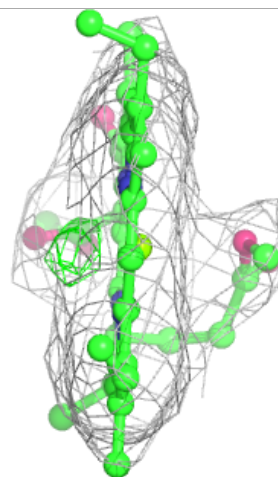
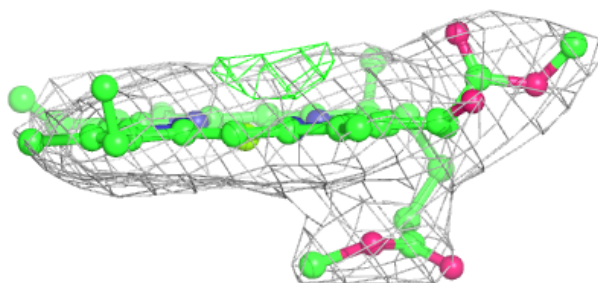
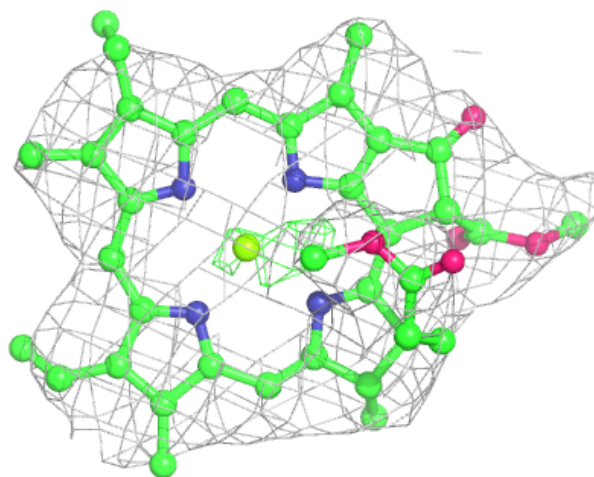
**Electron density around CLA B 1013:**

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



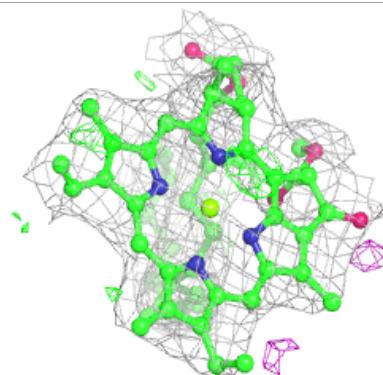
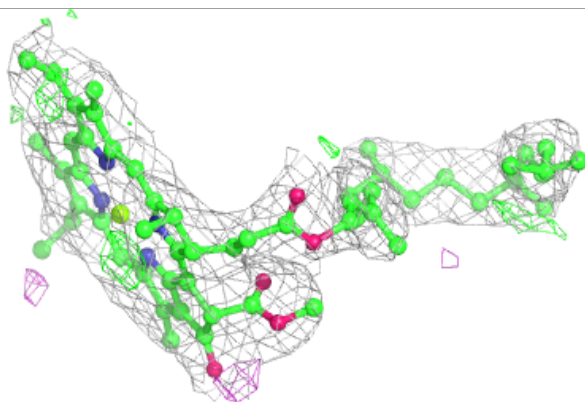
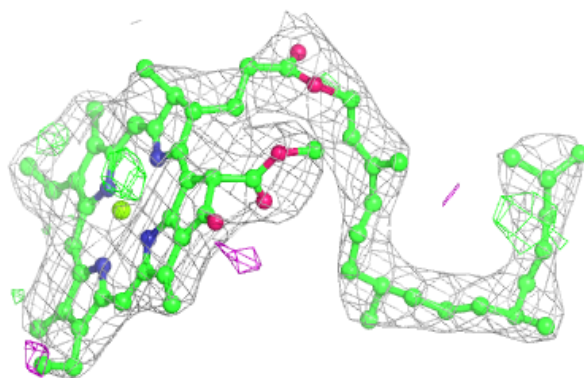
Electron density around CLA A 1115:

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

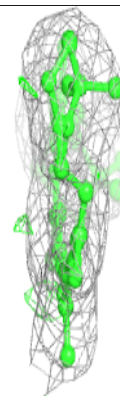
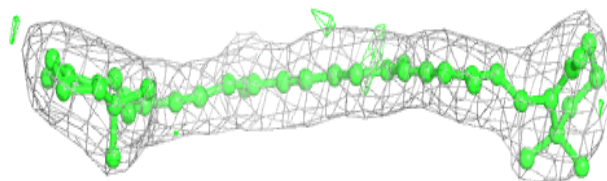
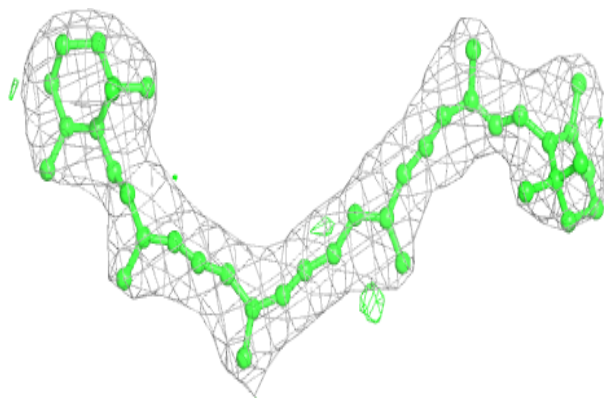


Electron density around CL0 A 1011:

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

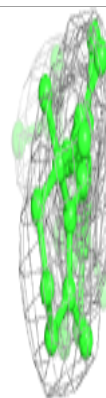
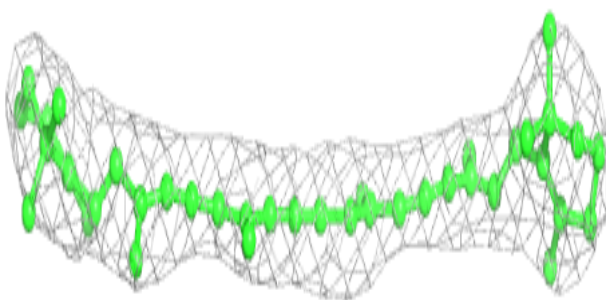
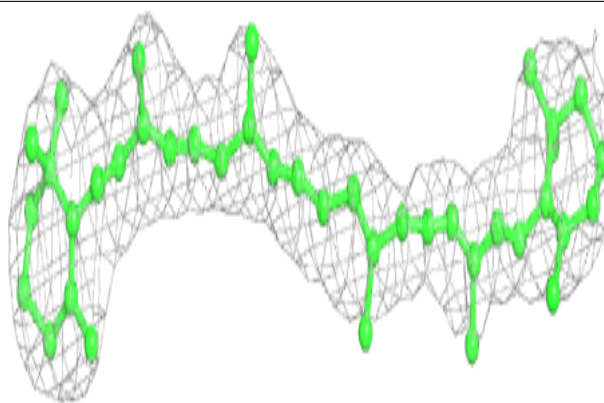
**Electron density around BCR B 4011:**

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



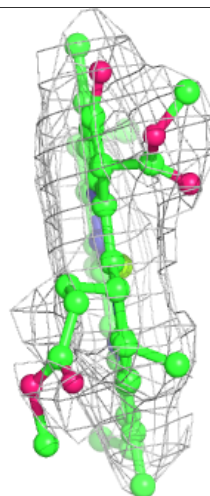
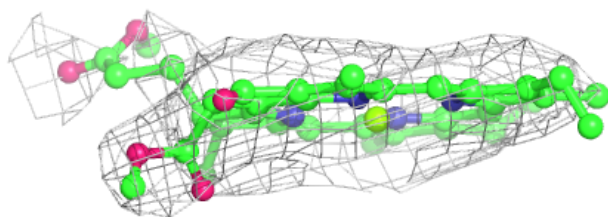
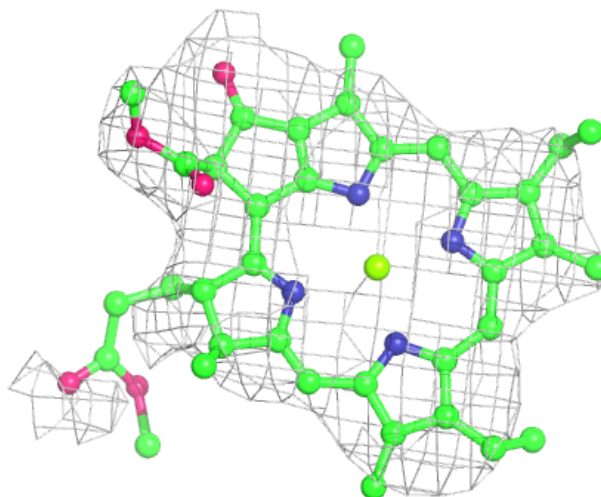
Electron density around BCR A 4012:

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



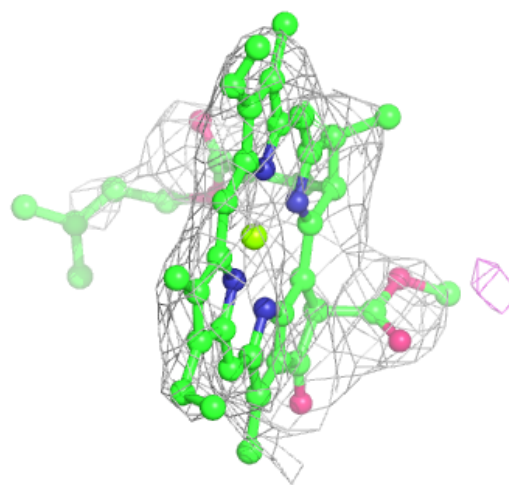
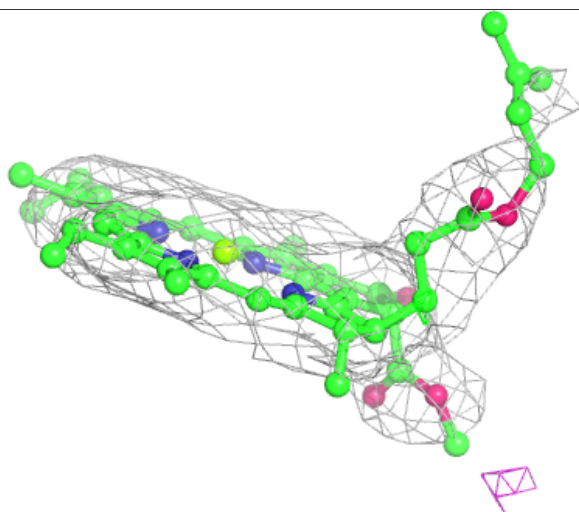
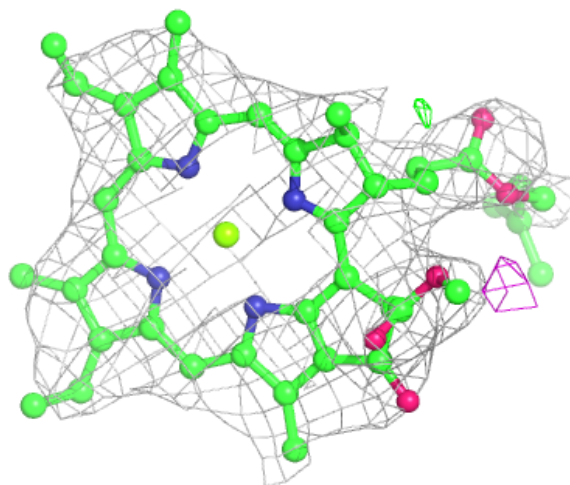
Electron density around CLA A 1121:

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



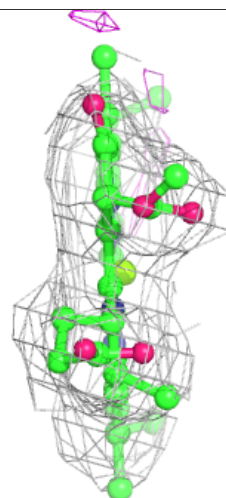
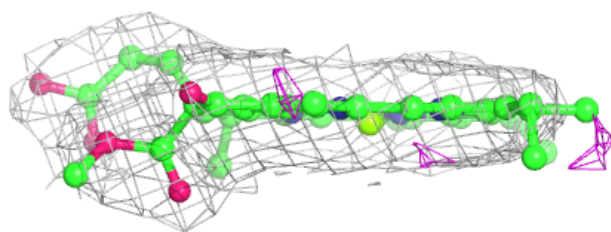
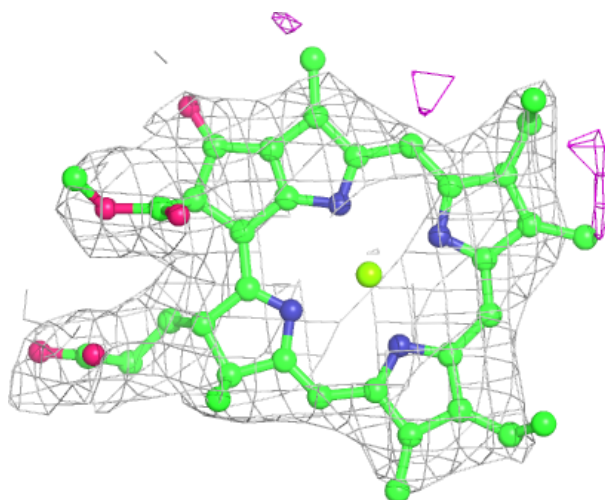
Electron density around CLA A 1137:

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



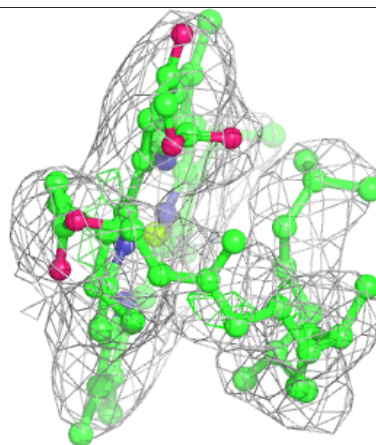
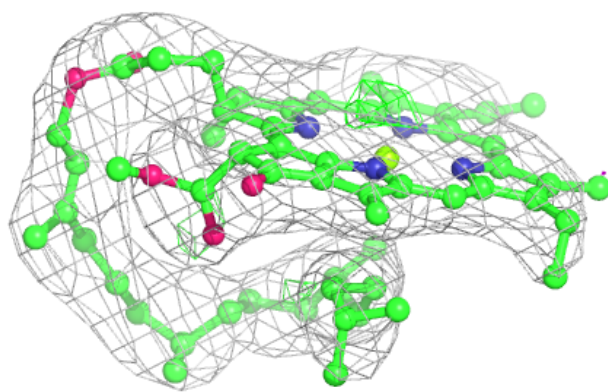
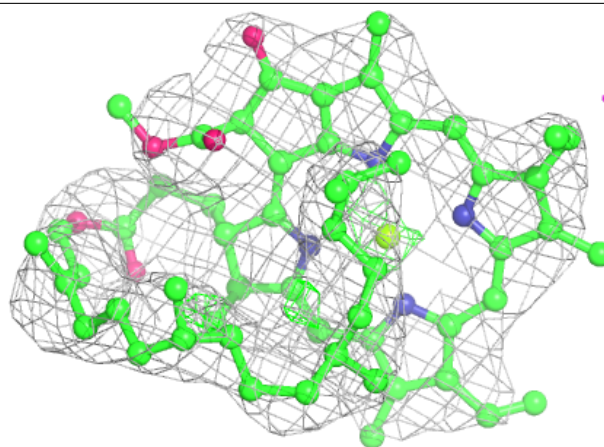
Electron density around CLA F 1301:

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

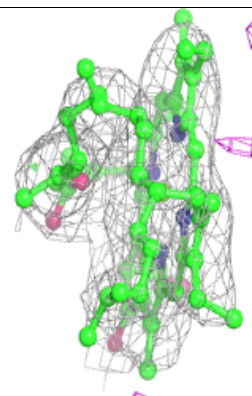
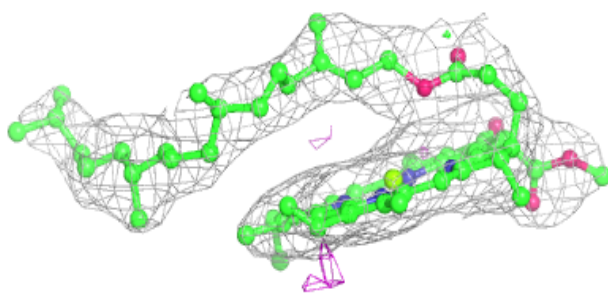
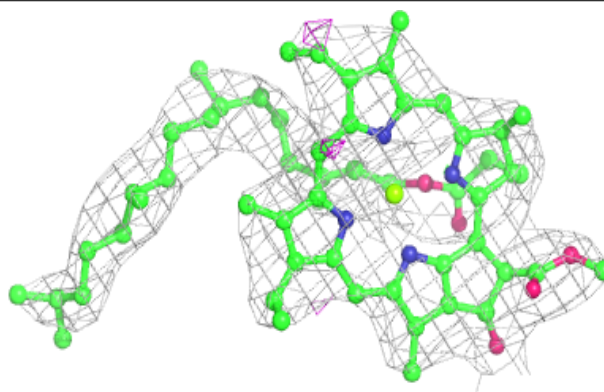


Electron density around CLA A 1104:

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

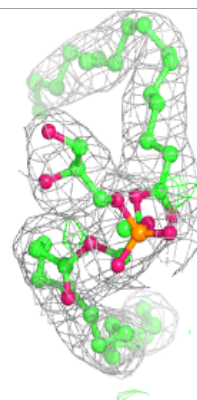
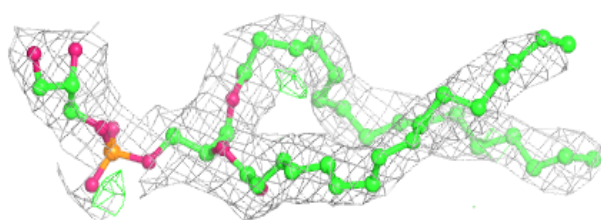
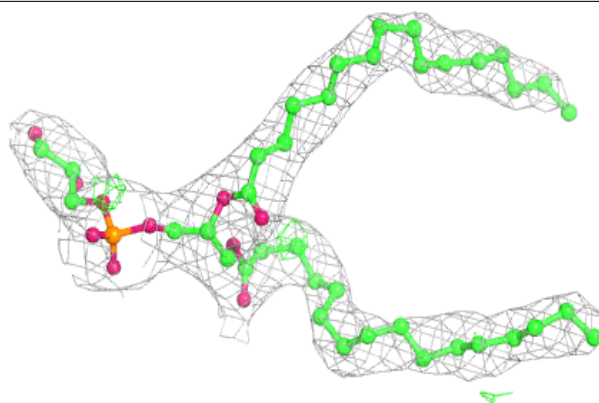
**Electron density around CLA B 1235:**

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

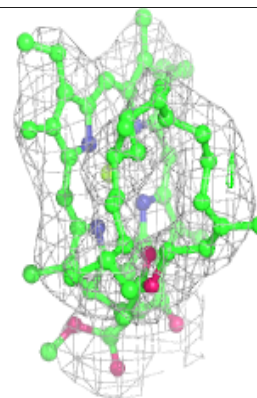
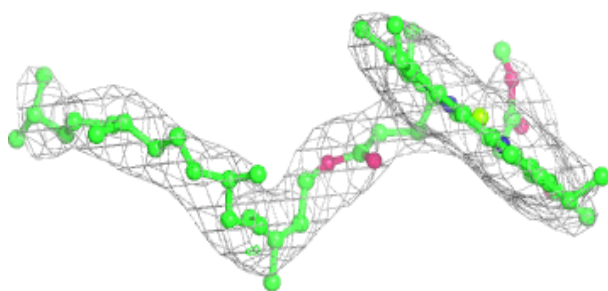
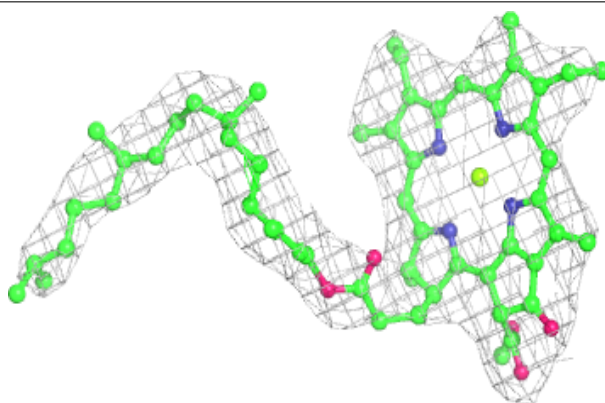


Electron density around LHG A 5001:

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

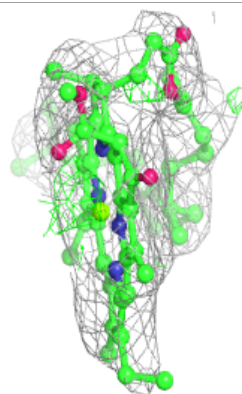
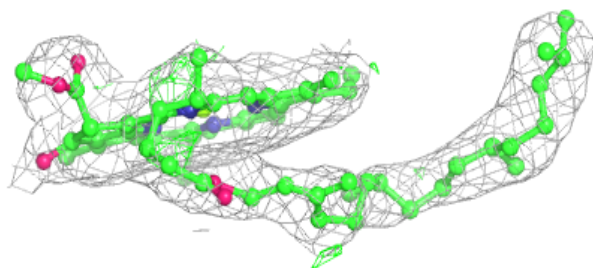
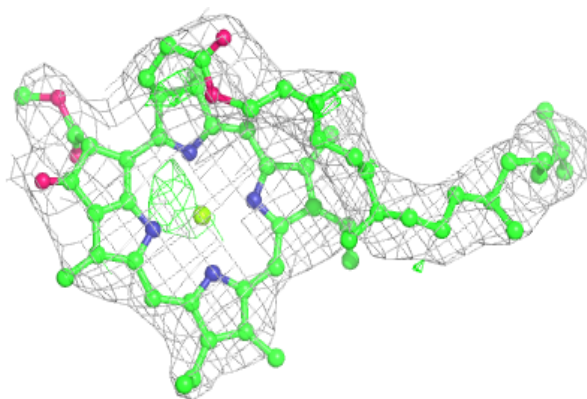
**Electron density around CLA A 1106:**

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

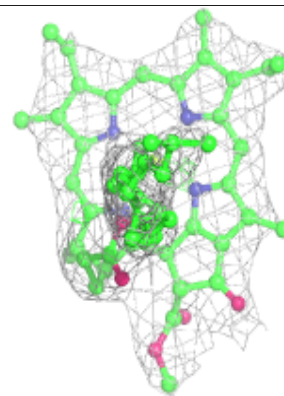
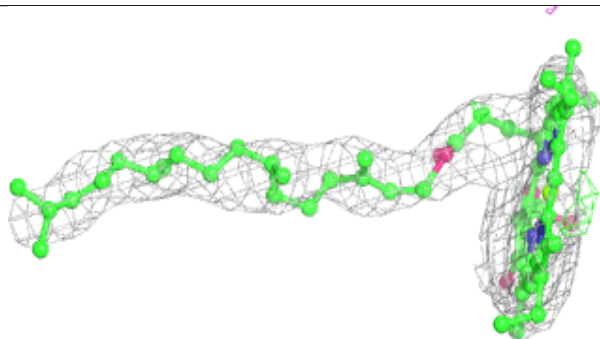
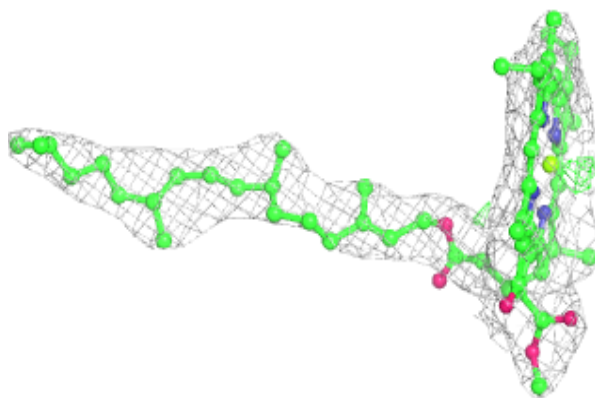


Electron density around CLA B 1215:

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

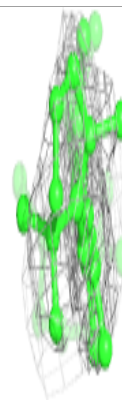
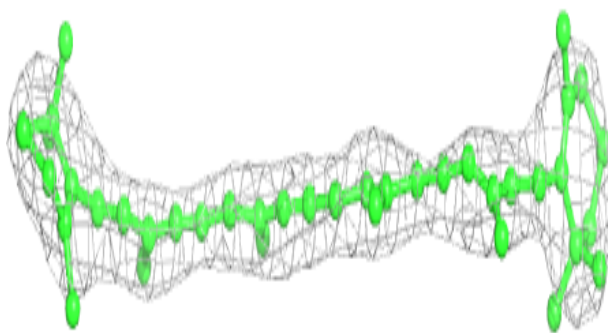
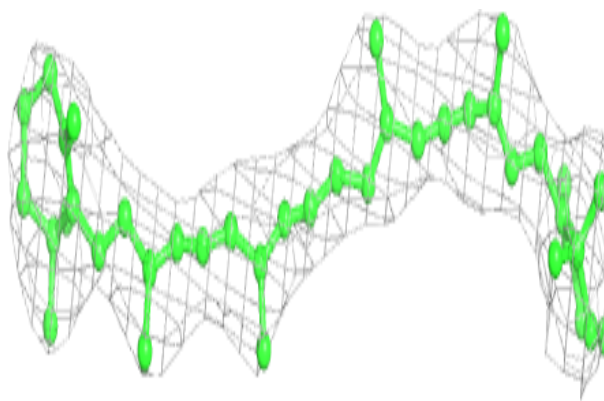
**Electron density around CLA A 1126:**

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

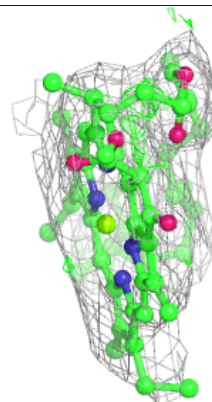
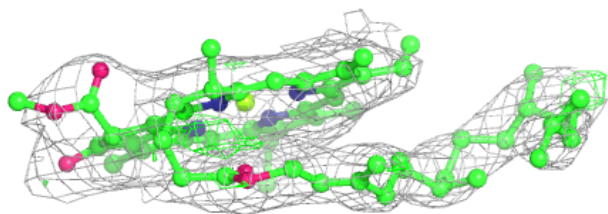
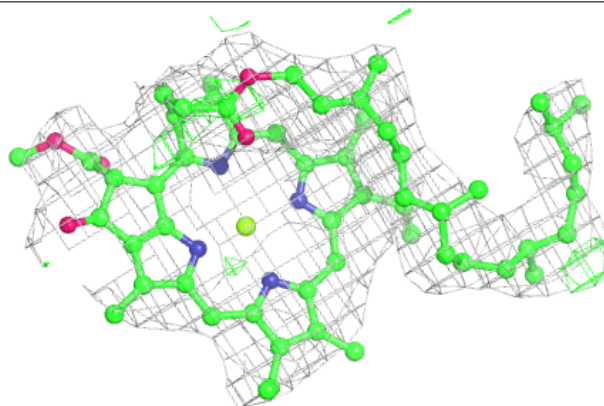


Electron density around BCR B 4017:

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

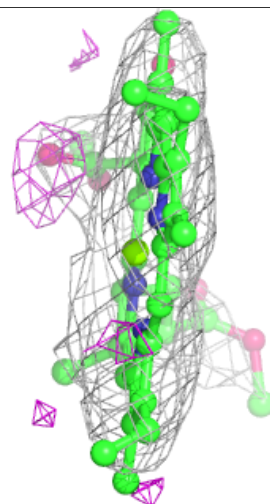
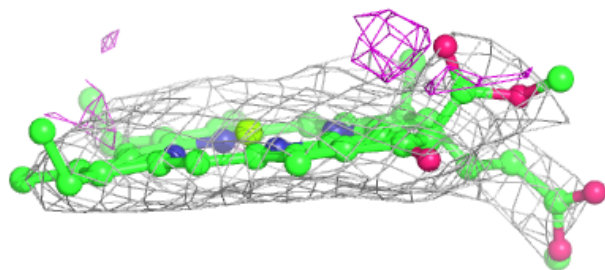
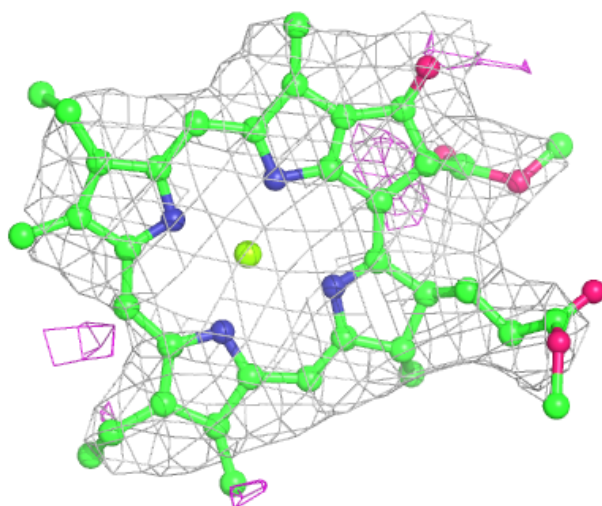
**Electron density around CLA A 1117:**

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



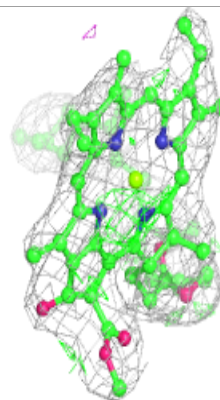
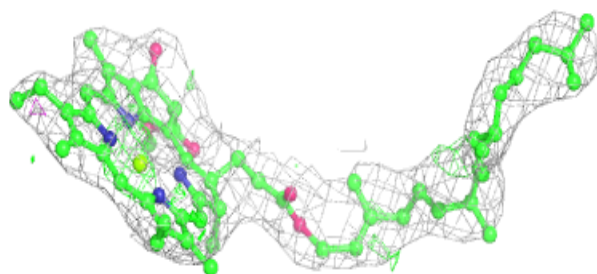
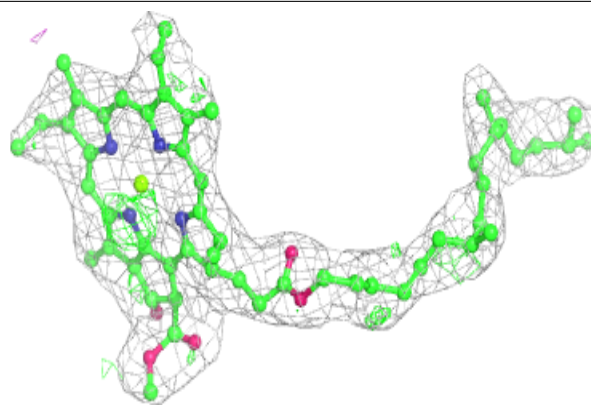
Electron density around CLA B 1206:

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

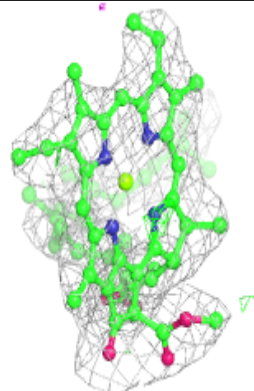
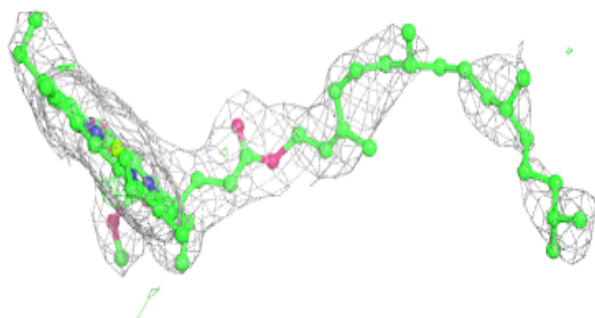
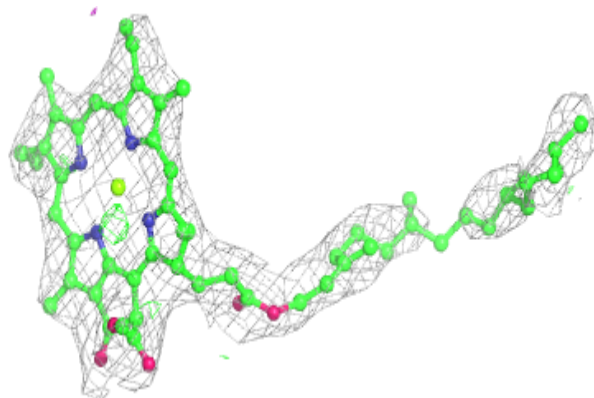


Electron density around CLA A 1012:

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

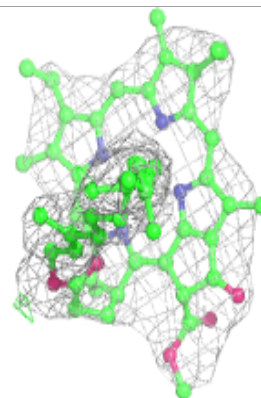
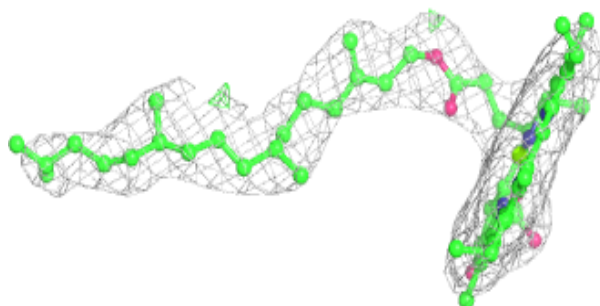
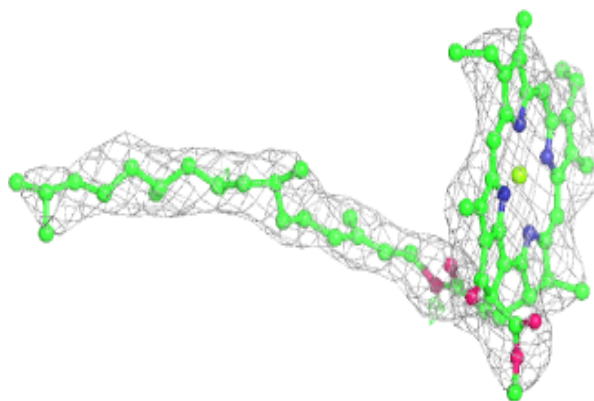
**Electron density around CLA B 1230:**

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

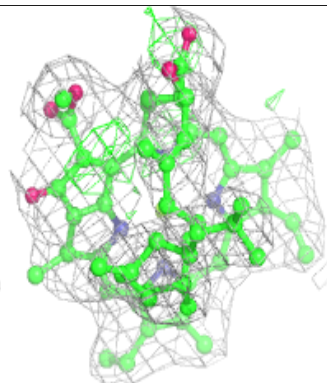
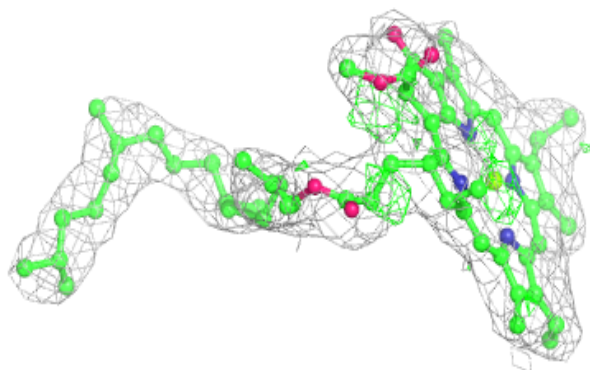
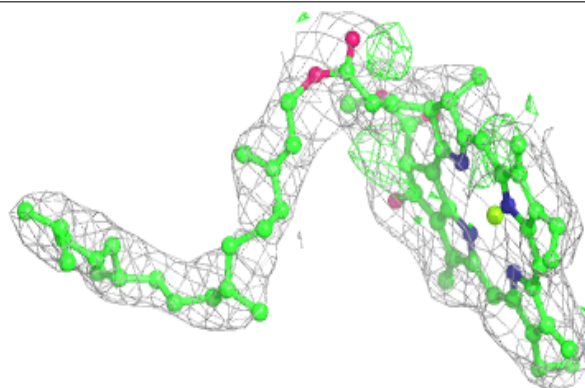


Electron density around CLA B 1225:

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

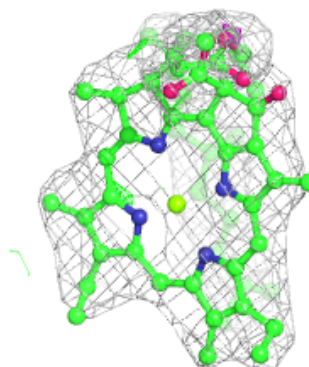
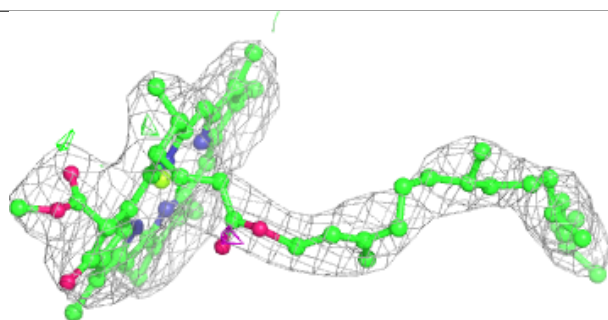
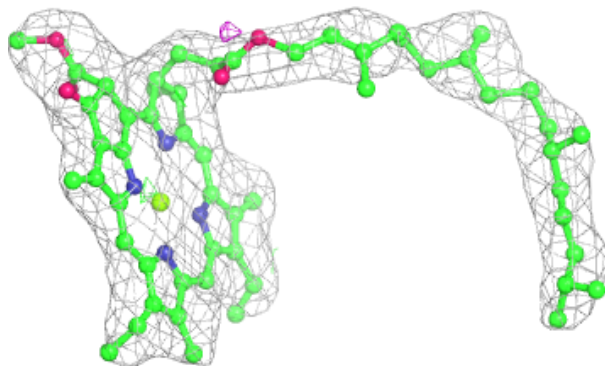
**Electron density around CLA B 1021:**

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



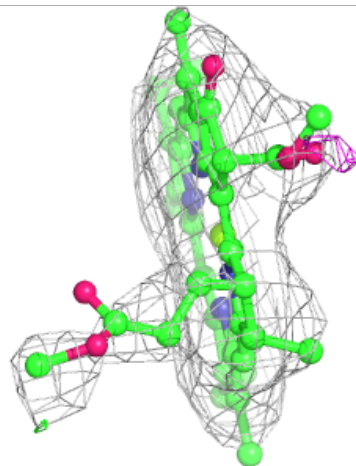
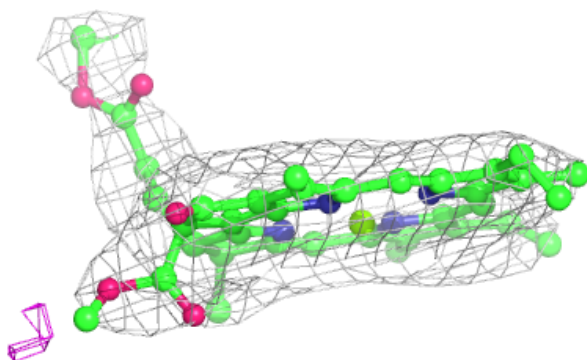
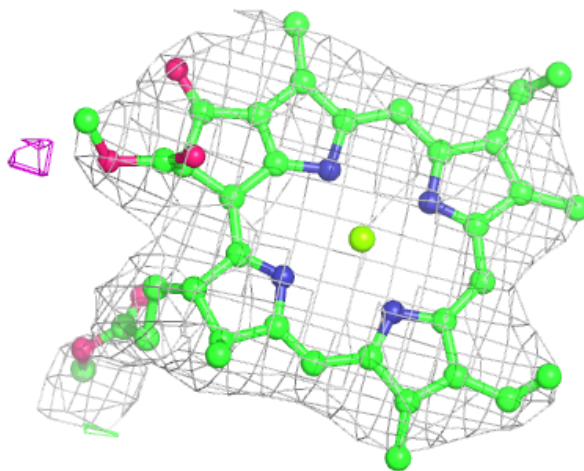
Electron density around CLA A 1140:

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



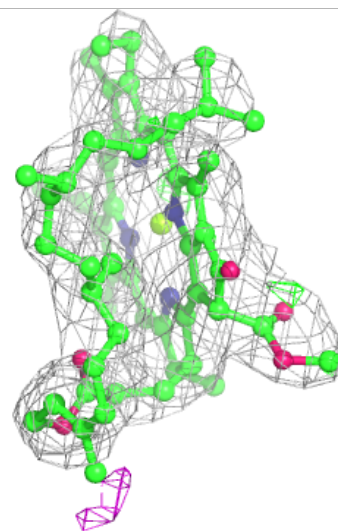
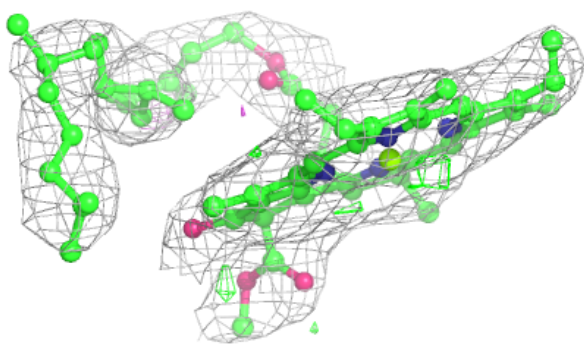
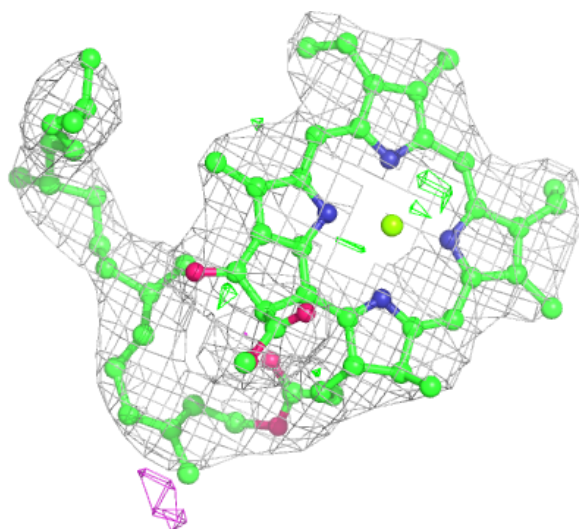
Electron density around CLA B 1239:

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



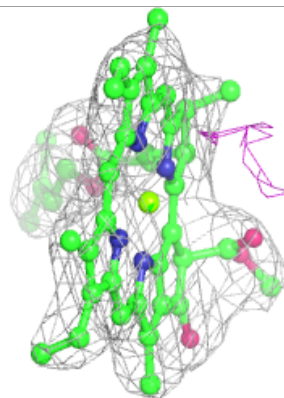
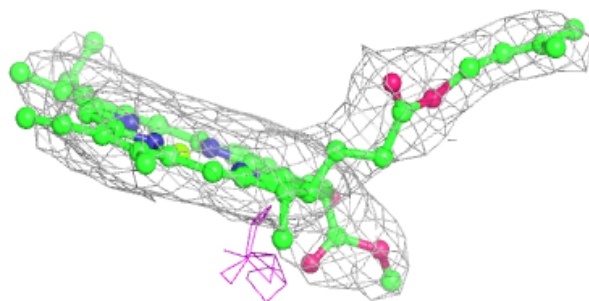
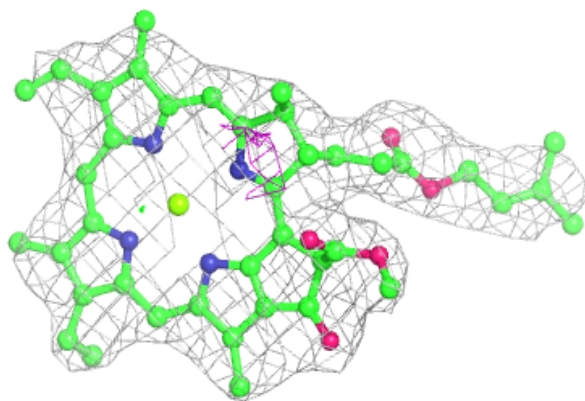
Electron density around CLA B 1229:

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



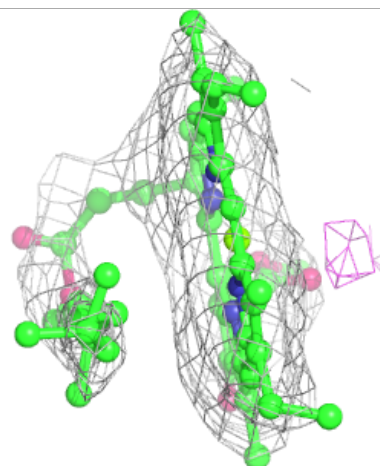
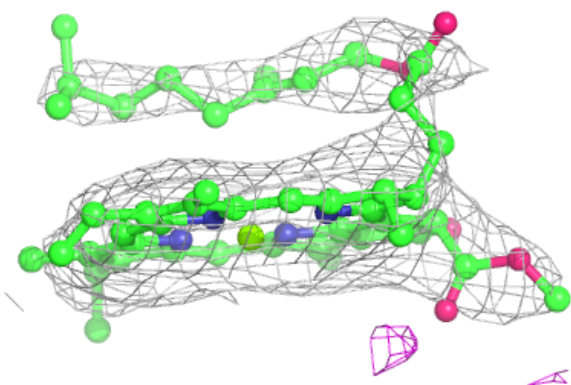
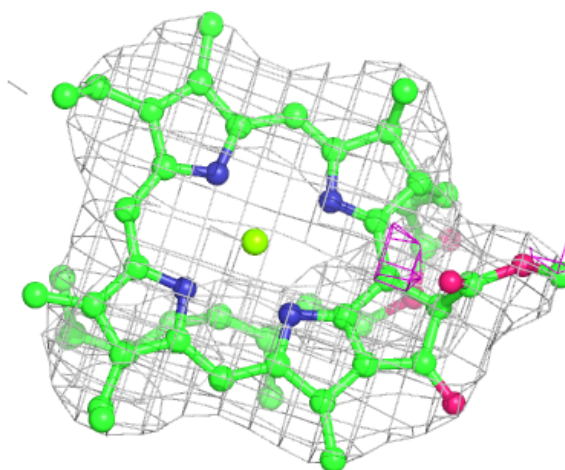
Electron density around CLA A 1107:

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



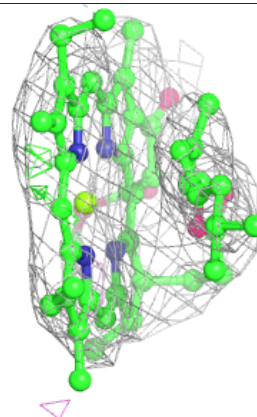
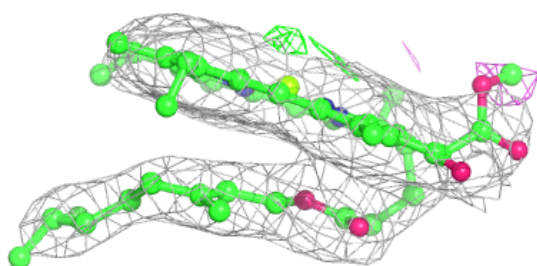
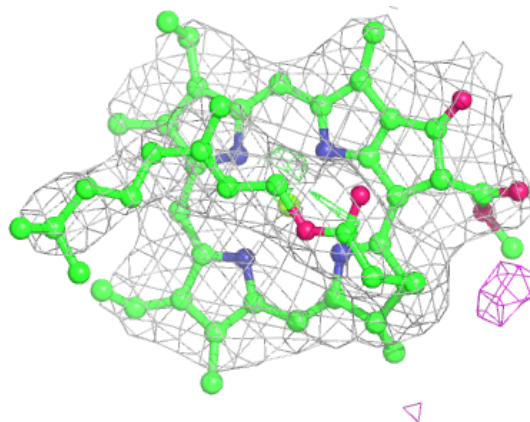
Electron density around CLA A 1130:

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



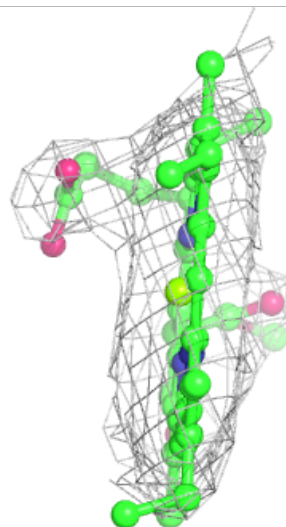
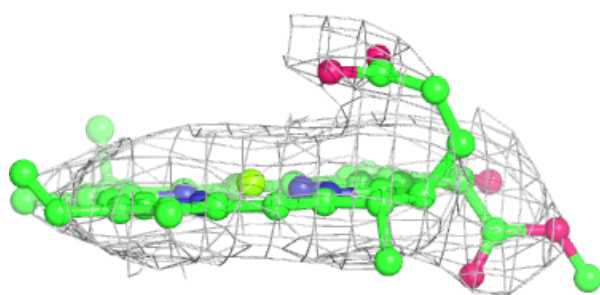
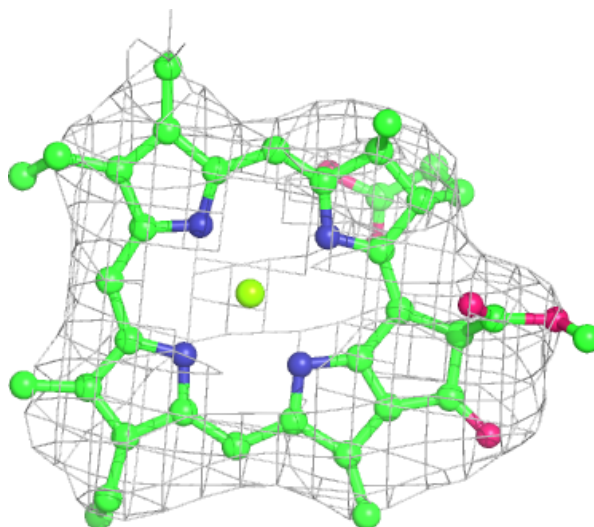
Electron density around CLA B 1205:

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



Electron density around CLA B 1209:

$2mF_o-DF_c$ (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.