



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 6, 2026 – 12:50 PM UTC

PDB ID : 4KT0 / pdb_00004kt0
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 types of validation reports are described at

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

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

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

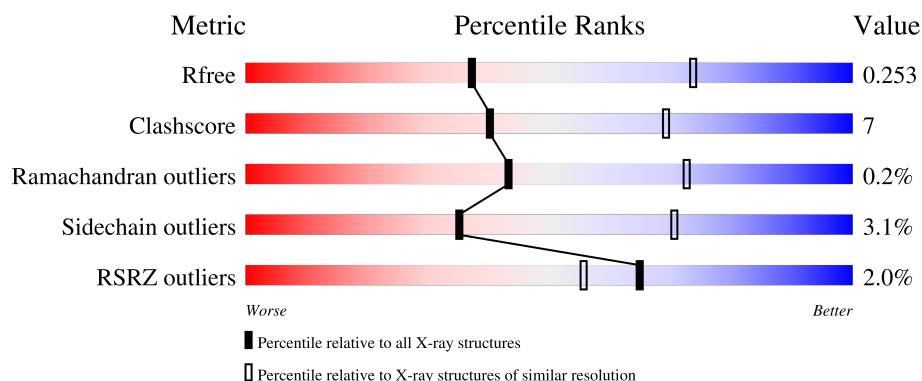
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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}	180053	3866 (2.80-2.80)
Clashscore	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)
RSRZ outliers	180081	3869 (2.80-2.80)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	751	% 89% 9% .
2	B	731	% 89% 10% .
3	C	81	4% 93% 5% ..
4	D	141	3% 89% 9% ..
5	E	74	% 78% 12% . 8%

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Mol	Chain	Length	Quality of chain
6	F	165	
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	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	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	1127	X	-	-	-
15	CLA	A	1128	X	-	-	-
15	CLA	A	1129	X	-	-	-
15	CLA	A	1130	X	-	-	-
15	CLA	A	1131	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
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	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	1215	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	1223	X	-	-	-
15	CLA	B	1224	X	-	-	-
15	CLA	B	1225	X	-	-	-
15	CLA	B	1226	X	-	-	-
15	CLA	B	1228	X	-	-	-
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	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
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			

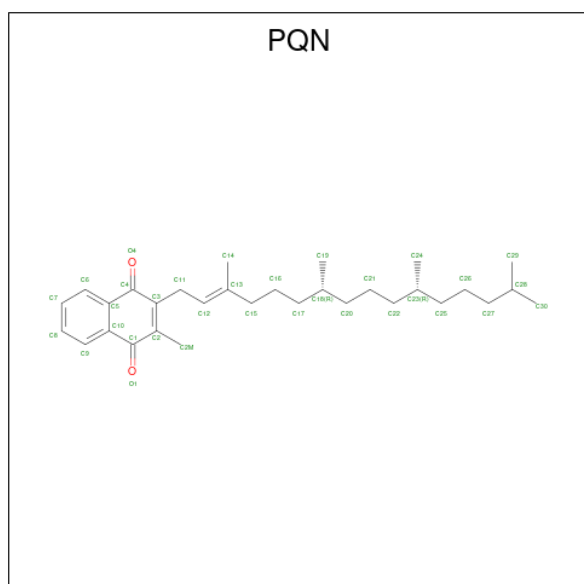
- Molecule 8 is a protein called Photosystem I reaction center subunit PsaK.

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.

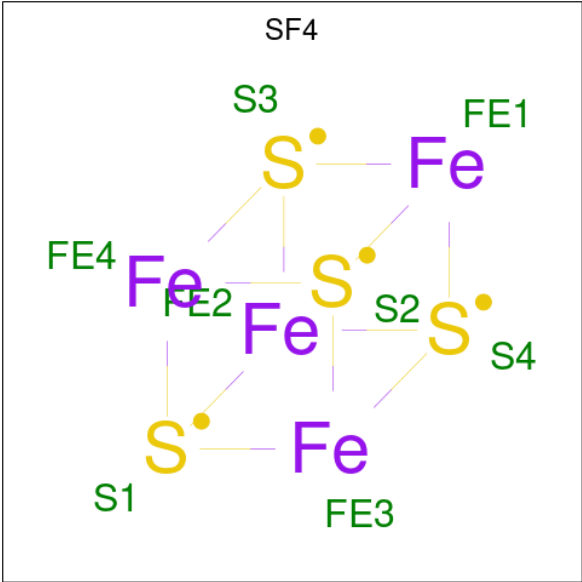
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
9	M	30	Total	C	N	O	0	0	0
			214	142	34	38			

- Molecule 10 is PHYLLOQUINONE (CCD ID: PQN) (formula: C₃₁H₄₆O₂).



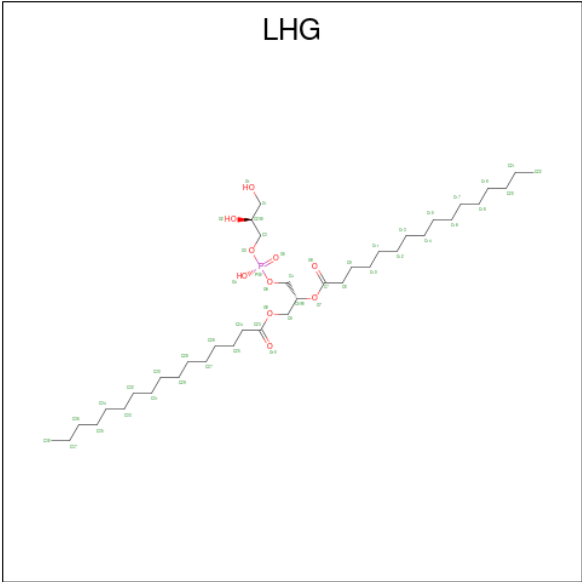
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
10	A	1	Total	C	O	0	0
			33	31	2		
10	B	1	Total	C	O	0	0
			33	31	2		

- Molecule 11 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe₄S₄).



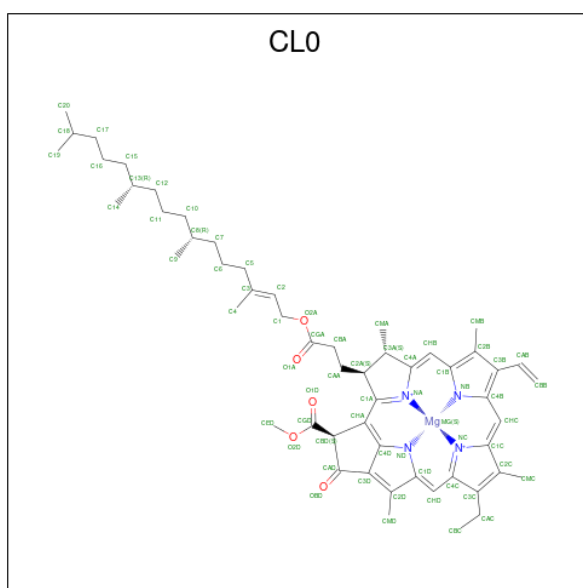
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
11	A	1	Total	Fe	S	0	0
			8	4	4		
11	C	1	Total	Fe	S	0	0
			8	4	4		
11	C	1	Total	Fe	S	0	0
			8	4	4		

- Molecule 12 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (CCD ID: LHG) (formula: C₃₈H₇₅O₁₀P).



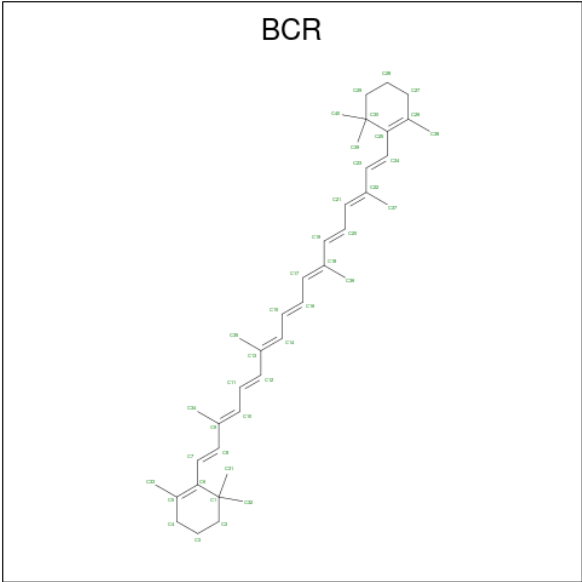
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
12	A	1	Total 49	C 38	O 10	P 1	0	0
12	A	1	Total 49	C 38	O 10	P 1	0	0
12	A	1	Total 36	C 25	O 10	P 1	0	0
12	B	1	Total 49	C 38	O 10	P 1	0	0

- Molecule 13 is CHLOROPHYLL A ISOMER (CCD ID: CL0) (formula: $C_{55}H_{72}MgN_4O_5$).



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

- Molecule 14 is BETA-CAROTENE (CCD ID: BCR) (formula: $C_{40}H_{56}$).



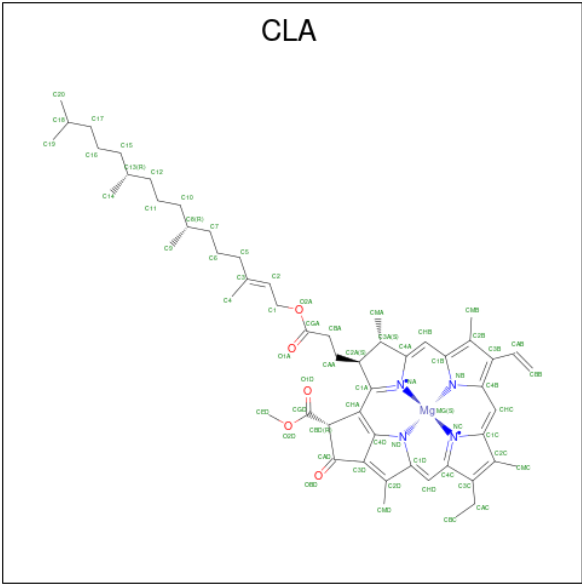
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
14	A	1	Total C 40 40	0	0
14	A	1	Total C 40 40	0	0
14	A	1	Total C 40 40	0	0
14	A	1	Total C 40 40	0	0
14	A	1	Total C 40 40	0	0
14	A	1	Total C 40 40	0	0
14	B	1	Total C 40 40	0	0
14	B	1	Total C 40 40	0	0
14	B	1	Total C 40 40	0	0
14	B	1	Total C 40 40	0	0
14	B	1	Total 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 (CCD ID: 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
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	C	Mg	N	O	0	0
			65	55	1	4	5		
15	A	1	Total	C	Mg	N	O	0	0
			49	39	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
			49	39	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
			46	36	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
			55	45	1	4	5		
15	A	1	Total	C	Mg	N	O	0	0
			62	52	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
			46	36	1	4	5		
15	A	1	Total	C	Mg	N	O	0	0
			55	45	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
			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
			55	45	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
			45	35	1	4	5		

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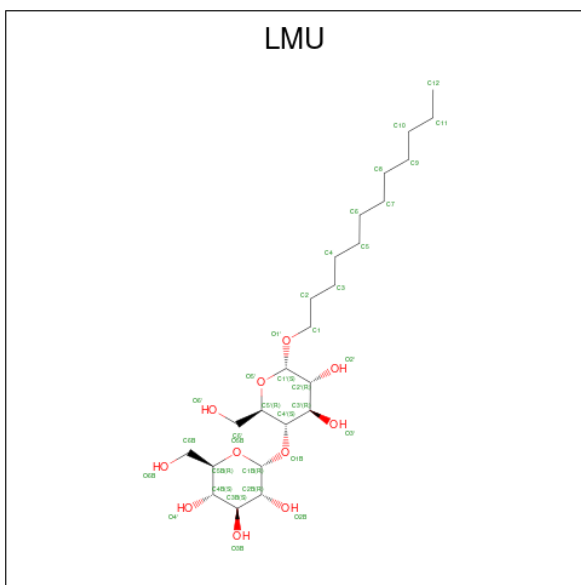
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
15	B	1	Total 45	C 35	Mg 1	N 4	O 5	0	0
15	B	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
15	B	1	Total 45	C 35	Mg 1	N 4	O 5	0	0
15	B	1	Total 50	C 40	Mg 1	N 4	O 5	0	0
15	B	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
15	B	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
15	B	1	Total 65	C 55	Mg 1	N 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 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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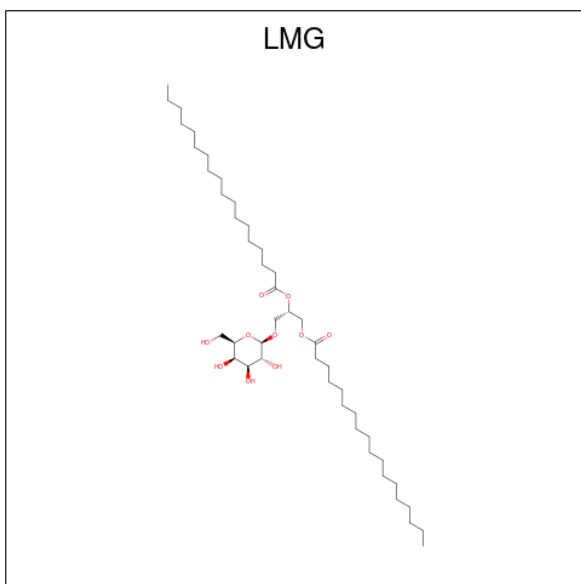
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
15	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
15	B	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
15	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
15	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
15	B	1	Total	C	Mg	N	O	0	0
			50	40	1	4	5		
15	B	1	Total	C	Mg	N	O	0	0
			46	36	1	4	5		
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 (CCD ID: LMU) (formula: C₂₄H₄₆O₁₁).



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 (CCD ID: 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 (CCD ID: CL) (formula: Cl).

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

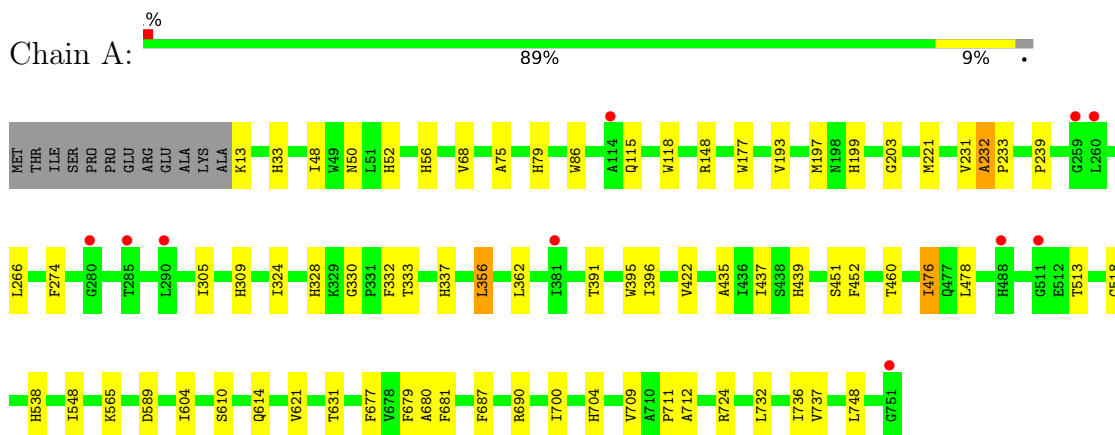
- Molecule 19 is water.

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		

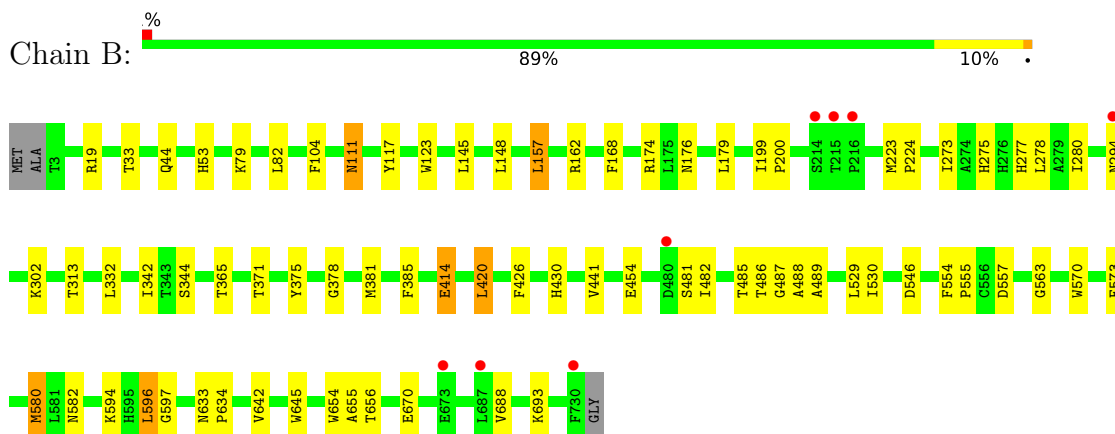
3 Residue-property plots

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.

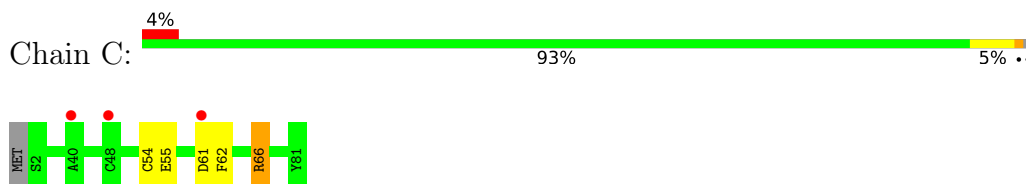
- Molecule 1: Photosystem I P700 chlorophyll a apoprotein A1



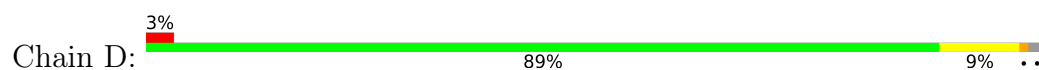
- Molecule 2: Photosystem I P700 chlorophyll a apoprotein A2



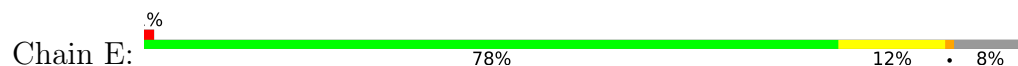
- Molecule 3: Photosystem I iron-sulfur center



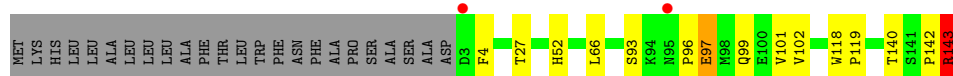
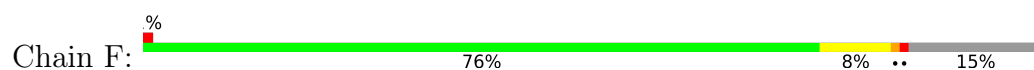
- Molecule 4: Photosystem I subunit II



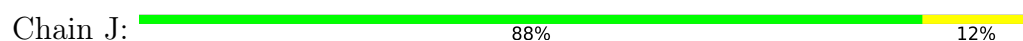
- Molecule 5: Photosystem I reaction center subunit IV



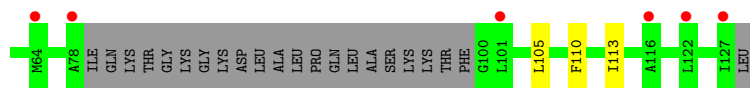
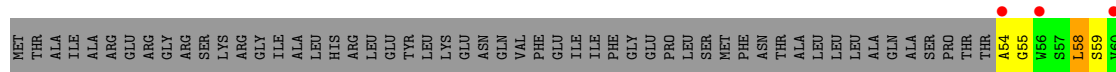
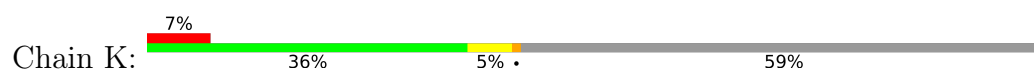
- Molecule 6: Photosystem I subunit III



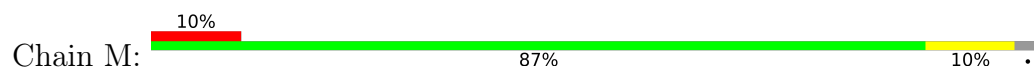
- Molecule 7: Photosystem I reaction center subunit IX



- 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 29.98 – 2.80	Depositor EDS
% Data completeness (in resolution range)	98.6 (29.98-2.80) 84.3 (29.98-2.80)	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 0.207 , 0.253	Depositor DCC
R_{free} test set	5715 reflections (4.85%)	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)	0.28 , 65.3	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	0.94	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: CLA, LMU, LMG, SF4, CL0, LHG, BCR, CL, PQN

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.30	0/5985	0.65	0/8158
2	B	0.31	0/5976	0.65	0/8173
3	C	0.33	0/610	0.65	0/826
4	D	0.29	0/1099	0.60	0/1482
5	E	0.29	0/542	0.69	0/733
6	F	0.33	0/1129	0.69	0/1535
7	J	0.31	0/328	0.65	0/443
8	K	0.36	0/371	0.75	0/499
9	M	0.30	0/217	0.68	0/295
All	All	0.31	0/16257	0.65	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	67	0
2	B	5765	0	5544	62	0
3	C	600	0	581	5	0
4	D	1075	0	1069	8	0
5	E	533	0	517	9	0
6	F	1099	0	1096	8	0
7	J	319	0	328	5	0
8	K	366	0	376	7	0
9	M	214	0	213	2	0
10	A	33	0	46	0	0
10	B	33	0	46	2	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	10	0
14	A	240	0	294	21	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	76	0
15	B	2365	0	2272	69	0
15	F	175	0	177	4	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	4	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	289	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 7.

The worst 5 of 289 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:H4	19:A:9109:HOH:O	1.32	1.23
13:A:1011:CL0:CMA	19:A:9109:HOH:O	1.91	1.06
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:HBA1	15:A:1110:CLA:HBD	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%)	30	60
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%)	43	72

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%)	580 (98%)	13 (2%)	45	78
2	B	582/583 (100%)	563 (97%)	19 (3%)	33	69
3	C	68/69 (99%)	67 (98%)	1 (2%)	57	84
4	D	112/116 (97%)	110 (98%)	2 (2%)	51	82
5	E	57/60 (95%)	53 (93%)	4 (7%)	14	40
6	F	118/137 (86%)	111 (94%)	7 (6%)	18	48
7	J	35/35 (100%)	34 (97%)	1 (3%)	37	73
8	K	37/100 (37%)	34 (92%)	3 (8%)	11	33
9	M	19/25 (76%)	19 (100%)	0	100	100
All	All	1621/1728 (94%)	1571 (97%)	50 (3%)	35	70

5 of 50 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	573	PHE
5	E	15	GLU
8	K	113	ILE
2	B	580	MET
3	C	66	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 22 such sidechains are listed below:

Mol	Chain	Res	Type
2	B	319	ASN
2	B	638	ASN
2	B	624	ASN

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Mol	Chain	Res	Type
4	D	51	ASN
1	A	614	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 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	A	1102	15	69,73,73	2.38	22 (31%)	82,113,113	2.43	24 (29%)
15	CLA	B	1204	-	50,54,73	2.83	22 (44%)	59,90,113	2.77	21 (35%)
15	CLA	A	1113	-	49,53,73	2.70	21 (42%)	58,89,113	2.74	23 (39%)
15	CLA	B	1225	-	69,73,73	2.36	23 (33%)	82,113,113	2.45	25 (30%)
15	CLA	A	1116	-	58,62,73	2.59	21 (36%)	68,99,113	2.69	26 (38%)
15	CLA	B	1021	-	69,73,73	2.37	23 (33%)	82,113,113	2.48	29 (35%)
15	CLA	B	1216	-	69,73,73	2.37	22 (31%)	82,113,113	2.35	24 (29%)
15	CLA	J	1302	7	49,53,73	2.69	21 (42%)	58,89,113	2.76	22 (37%)
12	LHG	B	5004	15	48,48,48	0.94	2 (4%)	51,54,54	1.15	4 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
15	CLA	B	1239	-	50,54,73	2.84	21 (42%)	59,90,113	2.79	23 (38%)
15	CLA	A	1126	-	69,73,73	2.38	23 (33%)	82,113,113	2.55	28 (34%)
15	CLA	B	1234	-	69,73,73	2.36	21 (30%)	82,113,113	2.46	25 (30%)
15	CLA	A	1135	-	59,63,73	2.57	21 (35%)	70,101,113	2.64	25 (35%)
14	BCR	A	4001	-	41,41,41	2.57	6 (14%)	56,56,56	6.41	25 (44%)
15	CLA	A	1109	15	69,73,73	2.38	22 (31%)	82,113,113	2.53	26 (31%)
15	CLA	A	1122	-	69,73,73	2.38	22 (31%)	82,113,113	2.46	26 (31%)
15	CLA	B	1222	-	60,64,73	2.52	21 (35%)	71,102,113	2.70	23 (32%)
14	BCR	B	4014	-	41,41,41	2.58	6 (14%)	56,56,56	6.83	19 (33%)
15	CLA	B	1240	12	49,53,73	2.72	22 (44%)	58,89,113	2.72	22 (37%)
15	CLA	A	1112	-	49,53,73	2.70	22 (44%)	58,89,113	2.78	22 (37%)
15	CLA	B	1205	-	59,63,73	2.54	21 (35%)	70,101,113	2.67	24 (34%)
15	CLA	A	1105	-	69,73,73	2.37	22 (31%)	82,113,113	2.47	25 (30%)
15	CLA	A	1127	-	69,73,73	2.37	23 (33%)	82,113,113	2.42	24 (29%)
15	CLA	A	1128	-	69,73,73	2.33	21 (30%)	82,113,113	2.44	27 (32%)
15	CLA	B	1202	-	69,73,73	2.36	22 (31%)	82,113,113	2.48	23 (28%)
15	CLA	B	1217	-	51,55,73	2.72	23 (45%)	60,91,113	2.78	22 (36%)
15	CLA	A	1117	-	69,73,73	2.39	22 (31%)	82,113,113	2.38	26 (31%)
15	CLA	B	1214	-	69,73,73	2.37	22 (31%)	82,113,113	2.45	25 (30%)
14	BCR	A	4003	-	41,41,41	2.57	6 (14%)	56,56,56	6.66	25 (44%)
15	CLA	B	1228	-	69,73,73	2.38	23 (33%)	82,113,113	2.38	23 (28%)
14	BCR	B	4011	-	41,41,41	2.59	6 (14%)	56,56,56	6.87	25 (44%)
15	CLA	A	1131	-	59,63,73	2.57	22 (37%)	70,101,113	2.69	26 (37%)
15	CLA	A	1124	-	59,63,73	2.57	22 (37%)	70,101,113	2.60	26 (37%)
14	BCR	B	4010	-	41,41,41	2.56	6 (14%)	56,56,56	6.80	23 (41%)
15	CLA	B	1231	-	69,73,73	2.36	22 (31%)	82,113,113	2.49	26 (31%)
15	CLA	B	1215	-	69,73,73	2.38	22 (31%)	82,113,113	2.53	26 (31%)
15	CLA	B	1223	-	69,73,73	2.36	22 (31%)	82,113,113	2.46	25 (30%)
15	CLA	B	1206	2	50,54,73	2.84	22 (44%)	59,90,113	2.71	23 (38%)
14	BCR	B	4004	-	41,41,41	2.58	6 (14%)	56,56,56	6.52	27 (48%)
10	PQN	B	2002	-	34,34,34	1.62	2 (5%)	43,45,45	1.15	4 (9%)
15	CLA	B	1210	-	69,73,73	2.35	22 (31%)	82,113,113	2.41	25 (30%)
15	CLA	B	1224	-	69,73,73	2.36	21 (30%)	82,113,113	2.46	23 (28%)
15	CLA	B	1218	-	55,59,73	2.65	22 (40%)	64,96,113	2.82	27 (42%)
15	CLA	A	1012	19	69,73,73	2.39	22 (31%)	82,113,113	2.42	24 (29%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
15	CLA	A	1132	-	66,70,73	2.40	21 (31%)	78,109,113	2.57	24 (30%)
15	CLA	B	1213	-	54,58,73	2.69	22 (40%)	64,95,113	2.70	22 (34%)
12	LHG	A	5001	-	48,48,48	0.93	2 (4%)	51,54,54	1.07	3 (5%)
14	BCR	B	4006	-	41,41,41	2.64	6 (14%)	56,56,56	6.84	24 (42%)
15	CLA	A	1136	-	69,73,73	2.35	21 (30%)	82,113,113	2.54	26 (31%)
14	BCR	B	4017	-	41,41,41	2.57	7 (17%)	56,56,56	6.74	25 (44%)
15	CLA	B	1211	-	50,54,73	2.83	22 (44%)	59,90,113	2.70	22 (37%)
15	CLA	B	1220	-	60,64,73	2.58	23 (38%)	71,102,113	2.52	25 (35%)
15	CLA	A	1138	-	69,73,73	2.41	22 (31%)	82,113,113	2.41	26 (31%)
15	CLA	B	1209	-	49,53,73	2.70	21 (42%)	58,89,113	2.79	24 (41%)
15	CLA	A	1101	-	69,73,73	2.36	23 (33%)	82,113,113	2.50	29 (35%)
15	CLA	B	1226	-	69,73,73	2.35	22 (31%)	82,113,113	2.48	23 (28%)
15	CLA	A	1110	-	58,62,73	2.55	21 (36%)	68,99,113	2.66	24 (35%)
15	CLA	B	1230	-	69,73,73	2.34	22 (31%)	82,113,113	2.57	26 (31%)
15	CLA	J	1303	-	50,54,73	2.85	23 (46%)	59,90,113	2.76	22 (37%)
15	CLA	A	1111	-	64,68,73	2.45	22 (34%)	76,107,113	2.51	24 (31%)
14	BCR	A	4002	-	41,41,41	2.58	7 (17%)	56,56,56	6.64	25 (44%)
16	LMU	J	1304	-	36,36,36	0.43	0	47,47,47	0.65	1 (2%)
11	SF4	C	3002	3	0,12,12	-	-	-	-	-
15	CLA	A	1125	-	56,60,73	2.61	22 (39%)	65,97,113	2.81	27 (41%)
15	CLA	B	1235	-	69,73,73	2.36	22 (31%)	82,113,113	2.49	25 (30%)
15	CLA	B	1219	-	59,63,73	2.57	23 (38%)	70,101,113	2.65	25 (35%)
12	LHG	A	5005	-	35,35,48	1.08	2 (5%)	38,41,54	1.16	4 (10%)
15	CLA	B	1229	-	69,73,73	2.34	22 (31%)	82,113,113	2.49	23 (28%)
15	CLA	B	1201	-	50,54,73	2.83	22 (44%)	59,90,113	2.74	22 (37%)
14	BCR	F	4016	-	41,41,41	2.57	6 (14%)	56,56,56	6.89	24 (42%)
15	CLA	A	1107	1	54,58,73	2.67	23 (42%)	64,95,113	2.77	29 (45%)
15	CLA	A	1022	19	69,73,73	2.37	23 (33%)	82,113,113	2.39	22 (26%)
15	CLA	A	1133	-	50,54,73	2.83	22 (44%)	59,90,113	2.71	21 (35%)
15	CLA	B	1227	-	49,53,73	2.68	21 (42%)	58,89,113	2.85	22 (37%)
16	LMU	B	1301	-	36,36,36	0.45	0	47,47,47	0.90	4 (8%)
14	BCR	A	4007	-	41,41,41	2.55	6 (14%)	56,56,56	6.87	24 (42%)
15	CLA	A	1130	-	59,63,73	2.58	23 (38%)	70,101,113	2.56	23 (32%)
14	BCR	B	4005	-	41,41,41	2.58	6 (14%)	56,56,56	6.60	24 (42%)
15	CLA	A	1140	-	69,73,73	2.36	22 (31%)	82,113,113	2.41	23 (28%)

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	-	-	-		
14	BCR	B	4009	-	41,41,41	2.59	7 (17%)	56,56,56	6.91	25 (44%)
10	PQN	A	2001	-	34,34,34	1.63	2 (5%)	43,45,45	1.08	4 (9%)
14	BCR	F	4015	-	41,41,41	2.59	7 (17%)	56,56,56	6.80	24 (42%)
15	CLA	B	1236	-	54,58,73	2.68	22 (40%)	64,95,113	2.75	25 (39%)
15	CLA	B	1212	-	49,53,73	2.70	22 (44%)	58,89,113	2.78	21 (36%)
15	CLA	F	1139	19	69,73,73	2.35	22 (31%)	82,113,113	2.42	24 (29%)
13	CL0	A	1011	-	58,73,73	3.17	17 (29%)	60,113,113	2.62	17 (28%)
14	BCR	A	4012	-	41,41,41	2.62	6 (14%)	56,56,56	6.35	23 (41%)
15	CLA	B	1221	-	69,73,73	2.36	23 (33%)	82,113,113	2.50	21 (25%)
11	SF4	C	3003	3	0,12,12	-	-	-		
15	CLA	A	1115	-	50,54,73	2.81	22 (44%)	59,90,113	2.71	21 (35%)
15	CLA	A	1129	-	50,54,73	2.83	22 (44%)	59,90,113	2.79	23 (38%)
15	CLA	B	1237	19	59,63,73	2.56	23 (38%)	70,101,113	2.64	24 (34%)
15	CLA	B	1238	19	47,52,73	2.75	21 (44%)	55,87,113	2.67	19 (34%)
14	BCR	A	4008	-	41,41,41	2.57	7 (17%)	56,56,56	6.95	24 (42%)
15	CLA	K	1402	-	50,54,73	2.83	21 (42%)	59,90,113	2.75	22 (37%)
15	CLA	A	1120	-	53,57,73	2.71	22 (41%)	61,93,113	2.81	24 (39%)
15	CLA	K	1401	-	50,54,73	2.83	22 (44%)	59,90,113	2.78	23 (38%)
15	CLA	A	1123	-	69,73,73	2.37	21 (30%)	82,113,113	2.47	25 (30%)
15	CLA	A	1801	12	56,60,73	2.65	23 (41%)	65,97,113	2.75	25 (38%)
15	CLA	A	1137	-	54,58,73	2.68	21 (38%)	64,95,113	2.73	22 (34%)
15	CLA	F	1410	6	69,73,73	2.37	23 (33%)	82,113,113	2.49	24 (29%)
15	CLA	A	1134	1	50,54,73	2.84	22 (44%)	59,90,113	2.70	20 (33%)
15	CLA	B	1208	-	49,53,73	2.71	21 (42%)	58,89,113	2.72	19 (32%)
15	CLA	B	1023	-	69,73,73	2.34	22 (31%)	82,113,113	2.41	26 (31%)
15	CLA	A	1118	-	50,54,73	2.80	20 (40%)	59,90,113	2.79	21 (35%)
17	LMG	B	5002	-	55,55,55	0.92	2 (3%)	63,63,63	0.98	2 (3%)
15	CLA	A	1106	1	69,73,73	2.38	22 (31%)	82,113,113	2.52	24 (29%)
15	CLA	A	1104	-	69,73,73	2.33	21 (30%)	82,113,113	2.50	25 (30%)
15	CLA	B	1232	-	49,53,73	2.69	20 (40%)	58,89,113	2.72	21 (36%)
15	CLA	B	1203	-	69,73,73	2.35	21 (30%)	82,113,113	2.46	23 (28%)
15	CLA	F	1301	-	49,53,73	2.69	22 (44%)	58,89,113	2.72	20 (34%)
15	CLA	B	1207	-	50,54,73	2.83	22 (44%)	59,90,113	2.76	22 (37%)
13	CL0	A	1108	-	38,53,73	3.87	15 (39%)	36,89,113	3.13	15 (41%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
15	CLA	A	1114	-	53,57,73	2.71	22 (41%)	61,93,113	2.80	24 (39%)
15	CLA	B	1013	-	69,73,73	2.35	21 (30%)	82,113,113	2.53	28 (34%)
15	CLA	A	1103	-	69,73,73	2.36	22 (31%)	82,113,113	2.42	24 (29%)
15	CLA	A	1119	-	68,72,73	2.40	23 (33%)	80,111,113	2.42	25 (31%)
12	LHG	A	5003	15	48,48,48	0.95	2 (4%)	51,54,54	1.11	4 (7%)
14	BCR	J	4013	-	41,41,41	2.57	7 (17%)	56,56,56	6.78	26 (46%)
15	CLA	A	1121	-	50,54,73	2.85	22 (44%)	59,90,113	2.72	21 (35%)

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	A	1102	15	1/1/15/20	13/39/115/115	-
15	CLA	B	1204	-	1/1/11/20	5/17/93/115	-
15	CLA	A	1113	-	1/1/11/20	4/15/91/115	-
15	CLA	B	1225	-	1/1/15/20	16/39/115/115	-
15	CLA	A	1116	-	1/1/12/20	9/26/102/115	-
15	CLA	B	1021	-	1/1/15/20	23/39/115/115	-
15	CLA	B	1216	-	-	13/39/115/115	-
15	CLA	J	1302	7	1/1/11/20	4/15/91/115	-
12	LHG	B	5004	15	-	21/53/53/53	-
15	CLA	B	1239	-	1/1/11/20	8/17/93/115	-
15	CLA	A	1126	-	-	11/39/115/115	-
15	CLA	B	1234	-	1/1/15/20	12/39/115/115	-
15	CLA	A	1135	-	1/1/13/20	10/27/103/115	-
15	CLA	A	1122	-	1/1/15/20	18/39/115/115	-
14	BCR	A	4001	-	-	13/29/63/63	0/2/2/2
15	CLA	A	1109	15	-	11/39/115/115	-
15	CLA	B	1222	-	-	11/29/105/115	-
14	BCR	B	4014	-	-	13/29/63/63	0/2/2/2
15	CLA	B	1240	12	1/1/11/20	6/15/91/115	-
15	CLA	A	1112	-	1/1/11/20	6/15/91/115	-
15	CLA	B	1205	-	1/1/13/20	13/27/103/115	-
15	CLA	A	1105	-	1/1/15/20	13/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
15	CLA	A	1127	-	1/1/15/20	17/39/115/115	-
15	CLA	A	1128	-	1/1/15/20	15/39/115/115	-
15	CLA	B	1202	-	1/1/15/20	21/39/115/115	-
15	CLA	B	1217	-	1/1/11/20	9/18/94/115	-
15	CLA	A	1117	-	1/1/15/20	17/39/115/115	-
15	CLA	B	1214	-	-	13/39/115/115	-
14	BCR	A	4003	-	-	12/29/63/63	0/2/2/2
15	CLA	B	1228	-	1/1/15/20	18/39/115/115	-
14	BCR	B	4011	-	-	15/29/63/63	0/2/2/2
15	CLA	A	1131	-	1/1/13/20	10/27/103/115	-
15	CLA	A	1124	-	1/1/13/20	9/27/103/115	-
15	CLA	B	1231	-	1/1/15/20	13/39/115/115	-
14	BCR	B	4010	-	-	8/29/63/63	0/2/2/2
15	CLA	B	1215	-	1/1/15/20	15/39/115/115	-
15	CLA	B	1223	-	1/1/15/20	18/39/115/115	-
15	CLA	B	1206	2	1/1/11/20	8/17/93/115	-
15	CLA	B	1210	-	1/1/15/20	17/39/115/115	-
10	PQN	B	2002	-	-	4/23/43/43	0/2/2/2
14	BCR	B	4004	-	-	12/29/63/63	0/2/2/2
15	CLA	B	1224	-	1/1/15/20	14/39/115/115	-
15	CLA	B	1218	-	1/1/12/20	10/23/99/115	-
15	CLA	A	1012	19	1/1/15/20	14/39/115/115	-
15	CLA	A	1132	-	1/1/14/20	16/36/112/115	-
15	CLA	B	1213	-	-	9/21/97/115	-
12	LHG	A	5001	-	-	28/53/53/53	-
14	BCR	B	4006	-	-	11/29/63/63	0/2/2/2
15	CLA	A	1136	-	1/1/15/20	16/39/115/115	-
14	BCR	B	4017	-	-	8/29/63/63	0/2/2/2
15	CLA	B	1211	-	1/1/11/20	9/17/93/115	-
15	CLA	B	1220	-	1/1/13/20	7/29/105/115	-
15	CLA	A	1138	-	1/1/15/20	5/39/115/115	-
15	CLA	B	1209	-	1/1/11/20	8/15/91/115	-
15	CLA	A	1101	-	1/1/15/20	13/39/115/115	-
15	CLA	B	1226	-	1/1/15/20	16/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
15	CLA	A	1110	-	1/1/12/20	10/26/102/115	-
15	CLA	B	1230	-	1/1/15/20	15/39/115/115	-
15	CLA	J	1303	-	1/1/11/20	5/17/93/115	-
15	CLA	A	1111	-	1/1/14/20	14/33/109/115	-
14	BCR	A	4002	-	-	6/29/63/63	0/2/2/2
16	LMU	J	1304	-	-	10/21/61/61	0/2/2/2
11	SF4	C	3002	3	-	-	0/6/5/5
15	CLA	A	1125	-	1/1/12/20	5/24/100/115	-
15	CLA	B	1235	-	1/1/15/20	13/39/115/115	-
15	CLA	B	1219	-	1/1/13/20	9/27/103/115	-
12	LHG	A	5005	-	-	24/40/40/53	-
15	CLA	B	1229	-	1/1/15/20	21/39/115/115	-
15	CLA	B	1201	-	1/1/11/20	4/17/93/115	-
14	BCR	F	4016	-	-	15/29/63/63	0/2/2/2
15	CLA	A	1107	1	-	6/21/97/115	-
15	CLA	A	1022	19	1/1/15/20	11/39/115/115	-
15	CLA	A	1133	-	1/1/11/20	6/17/93/115	-
15	CLA	B	1227	-	-	4/15/91/115	-
16	LMU	B	1301	-	-	15/21/61/61	0/2/2/2
14	BCR	A	4007	-	-	6/29/63/63	0/2/2/2
15	CLA	A	1130	-	1/1/13/20	11/27/103/115	-
15	CLA	A	1140	-	1/1/15/20	16/39/115/115	-
14	BCR	B	4005	-	-	10/29/63/63	0/2/2/2
11	SF4	A	3001	1,2	-	-	0/6/5/5
14	BCR	B	4009	-	-	13/29/63/63	0/2/2/2
10	PQN	A	2001	-	-	7/23/43/43	0/2/2/2
14	BCR	F	4015	-	-	10/29/63/63	0/2/2/2
15	CLA	B	1236	-	1/1/12/20	5/21/97/115	-
15	CLA	B	1212	-	1/1/11/20	8/15/91/115	-
15	CLA	F	1139	19	1/1/15/20	12/39/115/115	-
13	CL0	A	1011	-	3/3/20/25	6/37/135/135	-
15	CLA	B	1221	-	1/1/15/20	9/39/115/115	-
14	BCR	A	4012	-	-	11/29/63/63	0/2/2/2
15	CLA	A	1115	-	1/1/11/20	7/17/93/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
15	CLA	A	1129	-	1/1/11/20	12/17/93/115	-
11	SF4	C	3003	3	-	-	0/6/5/5
15	CLA	B	1237	19	1/1/13/20	10/27/103/115	-
15	CLA	B	1238	19	1/1/10/20	4/14/90/115	-
14	BCR	A	4008	-	-	10/29/63/63	0/2/2/2
15	CLA	K	1402	-	1/1/11/20	7/17/93/115	-
15	CLA	A	1120	-	1/1/11/20	10/20/96/115	-
15	CLA	K	1401	-	1/1/11/20	10/17/93/115	-
15	CLA	A	1123	-	1/1/15/20	18/39/115/115	-
15	CLA	A	1801	12	1/1/12/20	11/24/100/115	-
15	CLA	A	1137	-	1/1/12/20	7/21/97/115	-
15	CLA	F	1410	6	1/1/15/20	19/39/115/115	-
15	CLA	A	1134	1	1/1/11/20	7/17/93/115	-
15	CLA	B	1208	-	1/1/11/20	3/15/91/115	-
15	CLA	B	1023	-	1/1/15/20	13/39/115/115	-
15	CLA	A	1118	-	1/1/11/20	9/17/93/115	-
17	LMG	B	5002	-	-	30/50/70/70	0/1/1/1
15	CLA	A	1106	1	1/1/15/20	16/39/115/115	-
15	CLA	A	1104	-	1/1/15/20	12/39/115/115	-
15	CLA	B	1232	-	1/1/11/20	8/15/91/115	-
15	CLA	B	1203	-	1/1/15/20	11/39/115/115	-
15	CLA	F	1301	-	1/1/11/20	6/15/91/115	-
15	CLA	B	1207	-	1/1/11/20	8/17/93/115	-
13	CL0	A	1108	-	3/3/16/25	5/13/111/135	-
15	CLA	A	1114	-	1/1/11/20	7/20/96/115	-
15	CLA	B	1013	-	-	17/39/115/115	-
15	CLA	A	1103	-	1/1/15/20	17/39/115/115	-
15	CLA	A	1119	-	-	13/37/113/115	-
12	LHG	A	5003	15	-	24/53/53/53	-
14	BCR	J	4013	-	-	13/29/63/63	0/2/2/2
15	CLA	A	1121	-	1/1/11/20	7/17/93/115	-

The worst 5 of 2125 bond length outliers are listed below:

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	A	1123	CLA	MG-NA	9.66	2.29	2.06
15	B	1220	CLA	MG-NA	9.61	2.29	2.06
13	A	1011	CL0	C1A-CHA	9.60	1.50	1.40
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 2623 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	B	4009	BCR	C16-C17-C18	27.25	165.49	127.28
14	F	4016	BCR	C20-C21-C22	25.81	163.47	127.28
14	B	4006	BCR	C20-C21-C22	24.39	161.49	127.28
14	A	4008	BCR	C20-C21-C22	23.67	160.48	127.28
14	A	4007	BCR	C20-C21-C22	23.67	160.48	127.28

5 of 86 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
13	A	1011	CL0	ND
13	A	1011	CL0	NC
13	A	1011	CL0	NA
13	A	1108	CL0	ND
13	A	1108	CL0	NC

5 of 1356 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
12	A	5001	LHG	C1-C2-C3-O3
12	A	5003	LHG	C1-C2-C3-O3
12	A	5003	LHG	C3-O3-P-O6
12	A	5003	LHG	C4-O6-P-O3
12	A	5005	LHG	O1-C1-C2-C3

There are no ring outliers.

98 monomers are involved in 218 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
15	A	1102	CLA	2	0
15	A	1113	CLA	1	0
15	B	1021	CLA	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
15	B	1216	CLA	2	0
15	J	1302	CLA	2	0
12	B	5004	LHG	2	0
15	B	1239	CLA	1	0
15	A	1126	CLA	7	0
15	A	1135	CLA	1	0
14	A	4001	BCR	3	0
15	A	1109	CLA	2	0
15	A	1122	CLA	6	0
15	B	1222	CLA	3	0
14	B	4014	BCR	2	0
15	B	1240	CLA	1	0
15	A	1112	CLA	2	0
15	B	1205	CLA	1	0
15	A	1105	CLA	2	0
15	A	1127	CLA	4	0
15	A	1128	CLA	3	0
15	B	1202	CLA	1	0
15	B	1217	CLA	1	0
15	B	1214	CLA	1	0
14	A	4003	BCR	3	0
15	B	1228	CLA	1	0
14	B	4011	BCR	7	0
15	A	1131	CLA	2	0
15	A	1124	CLA	3	0
14	B	4010	BCR	5	0
15	B	1231	CLA	4	0
15	B	1215	CLA	4	0
15	B	1206	CLA	2	0
14	B	4004	BCR	3	0
10	B	2002	PQN	2	0
15	B	1210	CLA	2	0
15	B	1224	CLA	3	0
15	B	1218	CLA	2	0
15	A	1012	CLA	1	0
15	A	1132	CLA	1	0
15	B	1213	CLA	1	0
12	A	5001	LHG	1	0
14	B	4006	BCR	1	0
14	B	4017	BCR	6	0
15	B	1211	CLA	2	0
15	B	1220	CLA	2	0

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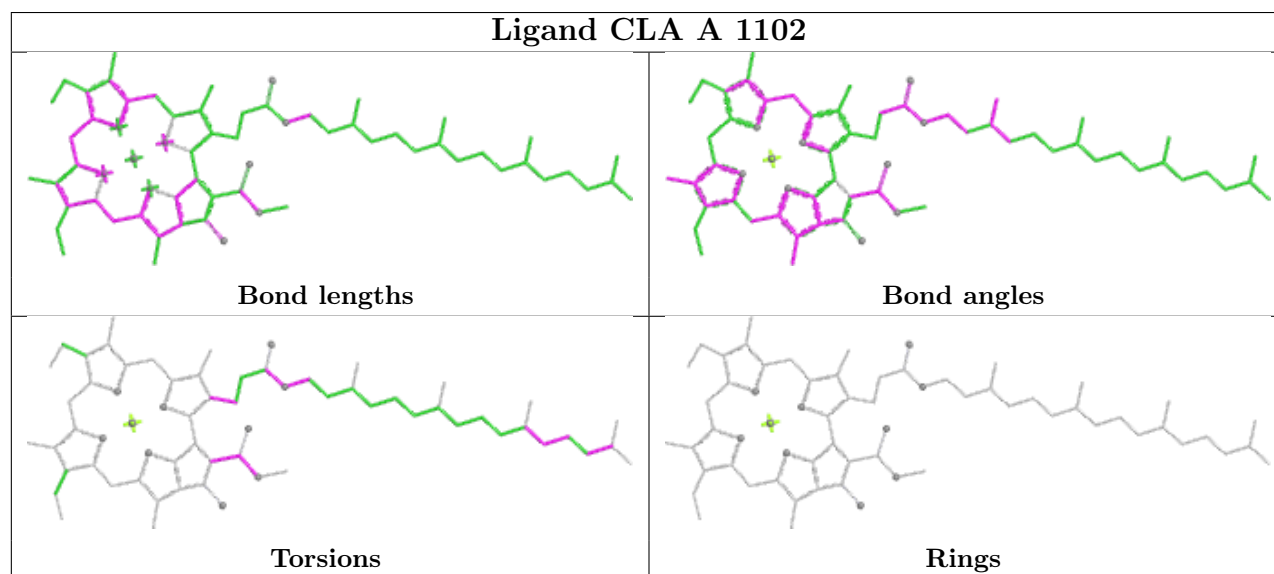
Mol	Chain	Res	Type	Clashes	Symm-Clashes
15	A	1138	CLA	2	0
15	A	1101	CLA	3	0
15	B	1226	CLA	2	0
15	A	1110	CLA	11	0
15	B	1230	CLA	2	0
15	A	1111	CLA	1	0
14	A	4002	BCR	3	0
16	J	1304	LMU	2	0
15	A	1125	CLA	1	0
15	B	1235	CLA	5	0
12	A	5005	LHG	10	0
15	B	1229	CLA	4	0
15	B	1201	CLA	1	0
14	F	4016	BCR	2	0
15	A	1107	CLA	4	0
15	A	1022	CLA	2	0
15	A	1133	CLA	3	0
15	B	1227	CLA	2	0
14	A	4007	BCR	2	0
14	B	4005	BCR	1	0
14	B	4009	BCR	1	0
14	F	4015	BCR	6	0
15	B	1236	CLA	5	0
15	B	1212	CLA	2	0
15	F	1139	CLA	3	0
13	A	1011	CL0	8	0
14	A	4012	BCR	5	0
15	B	1221	CLA	5	0
15	A	1129	CLA	1	0
15	B	1237	CLA	1	0
14	A	4008	BCR	5	0
15	K	1402	CLA	1	0
15	A	1120	CLA	1	0
15	K	1401	CLA	1	0
15	A	1123	CLA	4	0
15	A	1801	CLA	2	0
15	A	1137	CLA	1	0
15	B	1023	CLA	6	0
15	A	1118	CLA	2	0
17	B	5002	LMG	2	0
15	A	1106	CLA	1	0
15	A	1104	CLA	2	0

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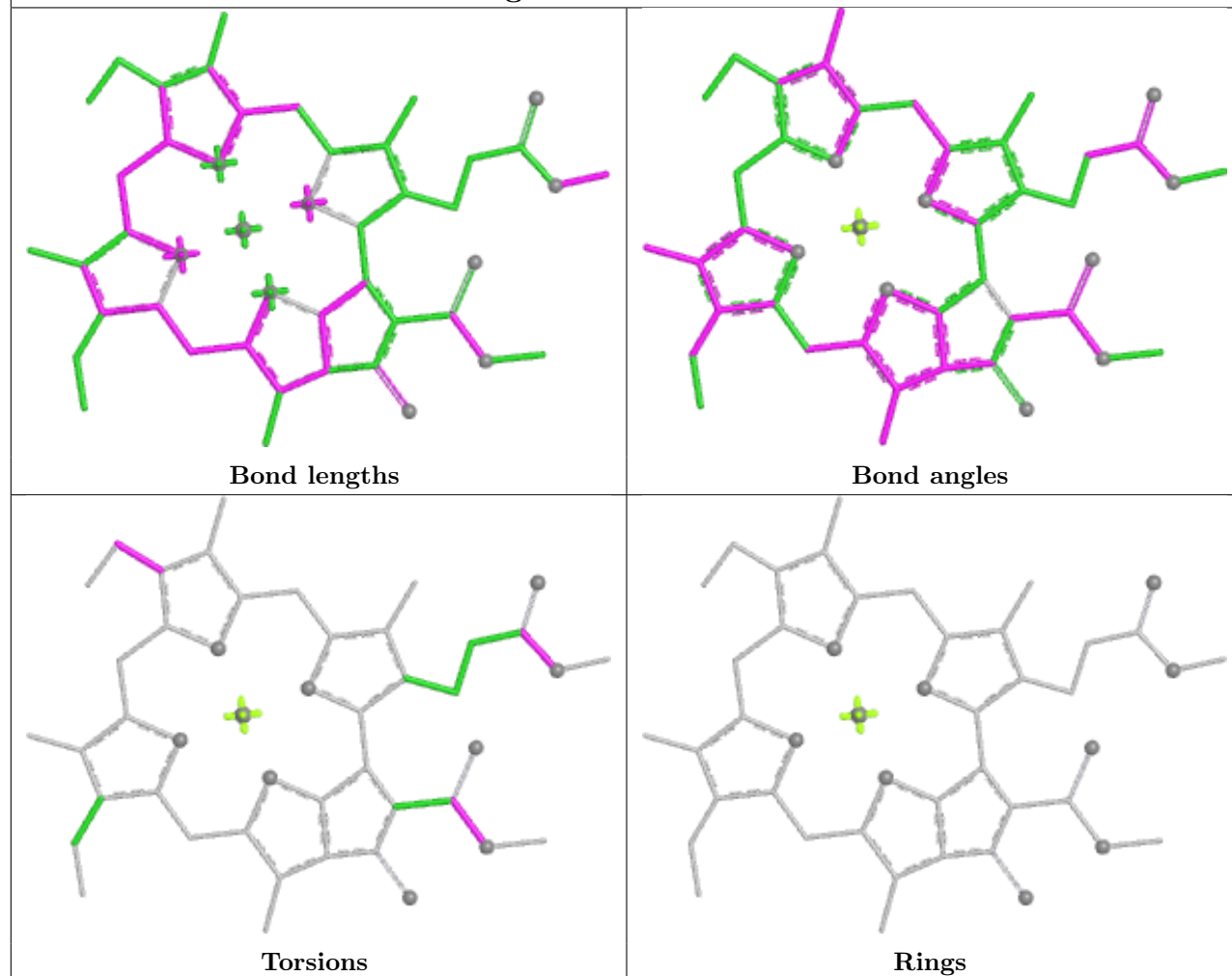
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
15	B	1232	CLA	2	0
15	B	1203	CLA	2	0
15	F	1301	CLA	1	0
13	A	1108	CL0	2	0
15	A	1114	CLA	2	0
15	B	1013	CLA	10	0
15	A	1103	CLA	6	0
15	A	1119	CLA	2	0
12	A	5003	LHG	7	0
14	J	4013	BCR	3	0
15	A	1121	CLA	2	0

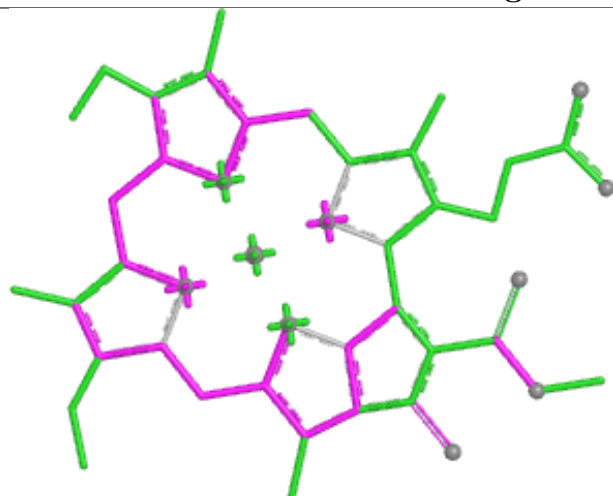
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



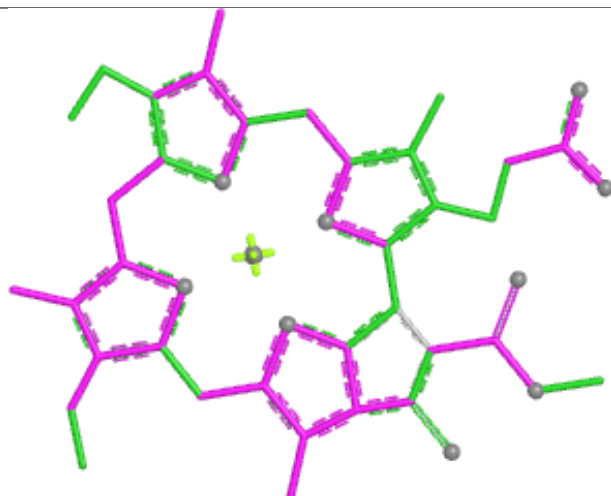
Ligand CLA B 1204



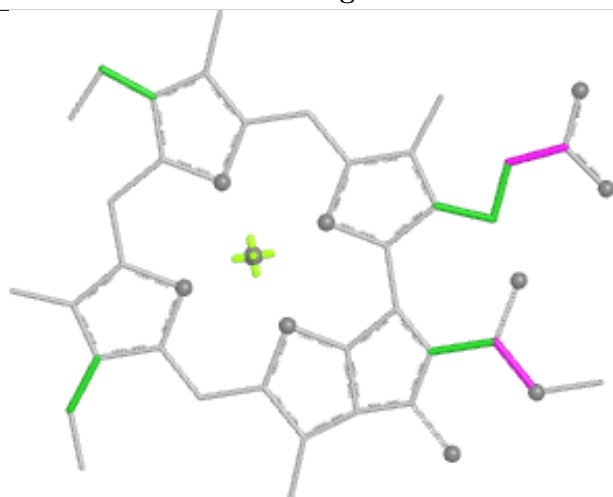
Ligand CLA A 1113



Bond lengths



Bond angles

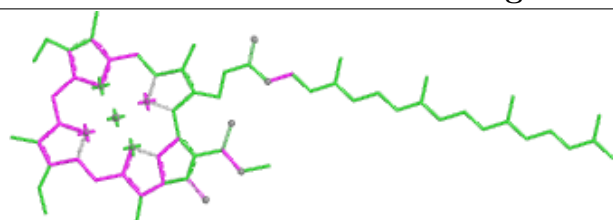


Torsions

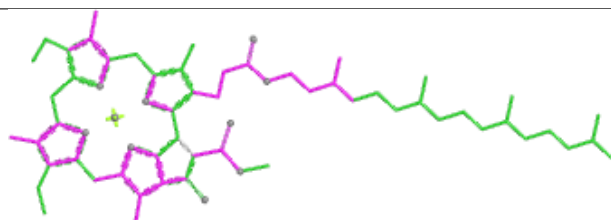


Rings

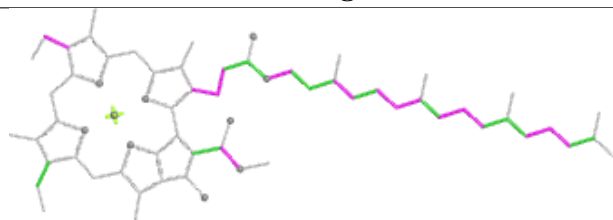
Ligand CLA B 1225



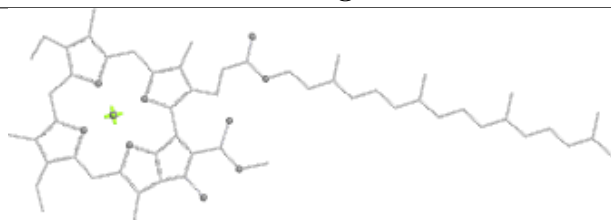
Bond lengths



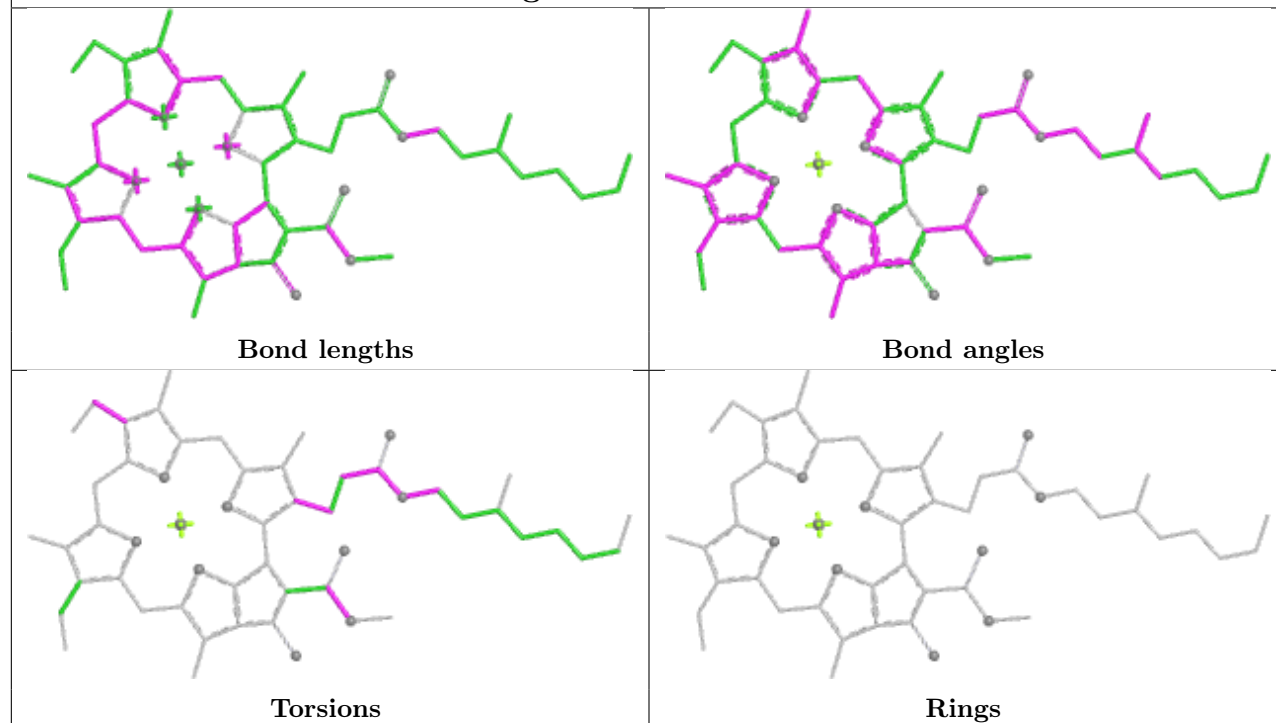
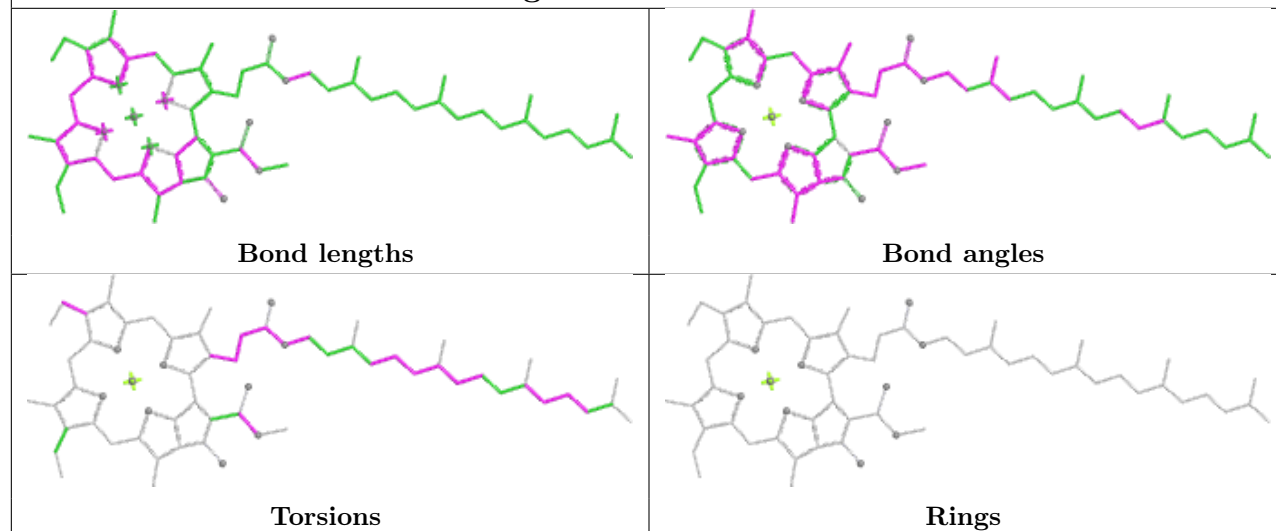
Bond angles

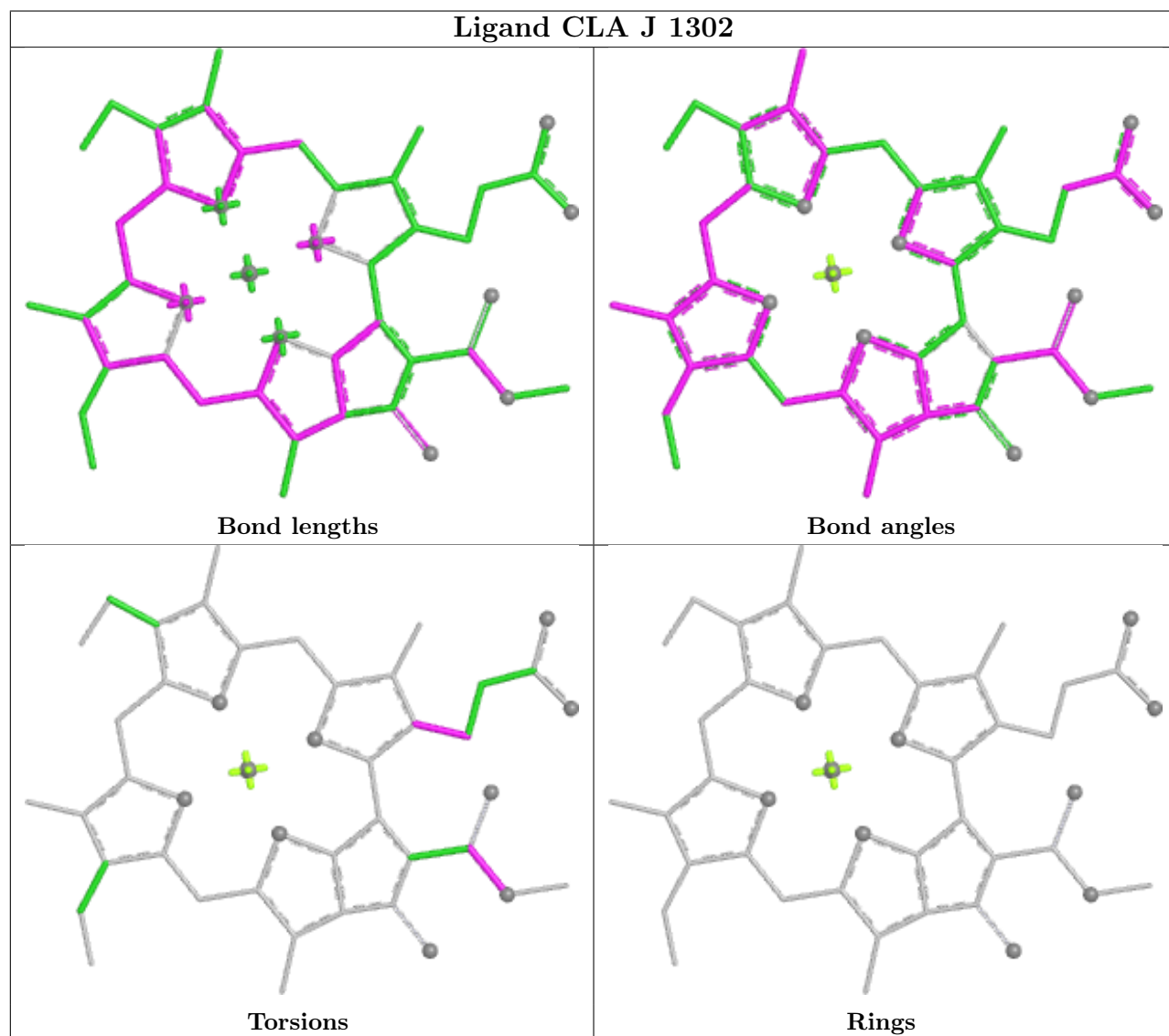
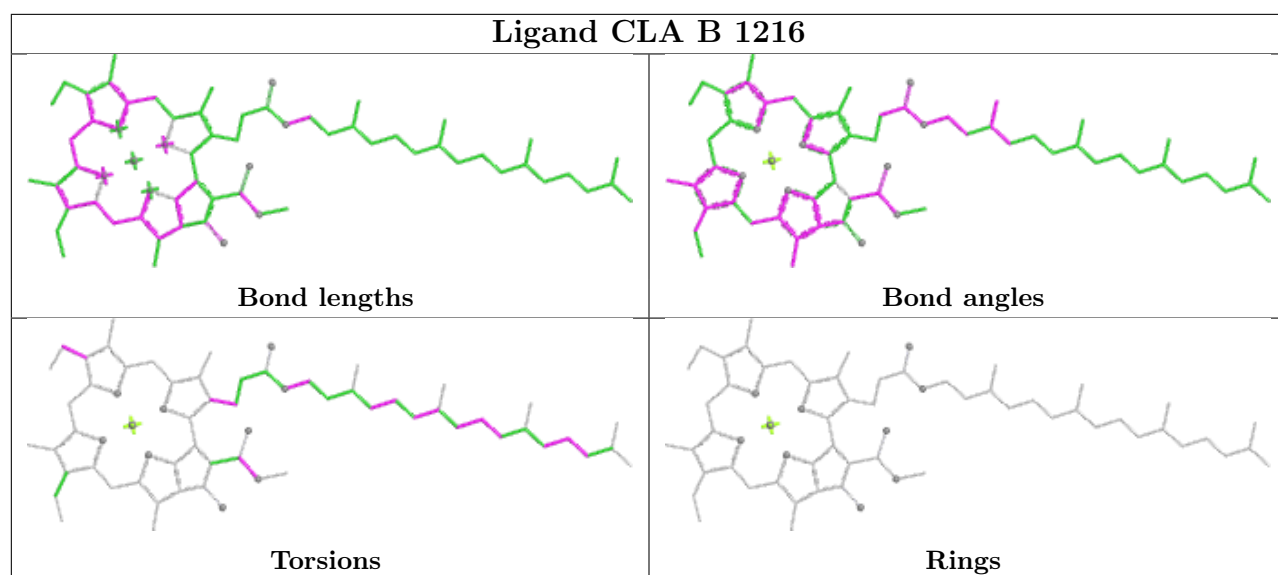


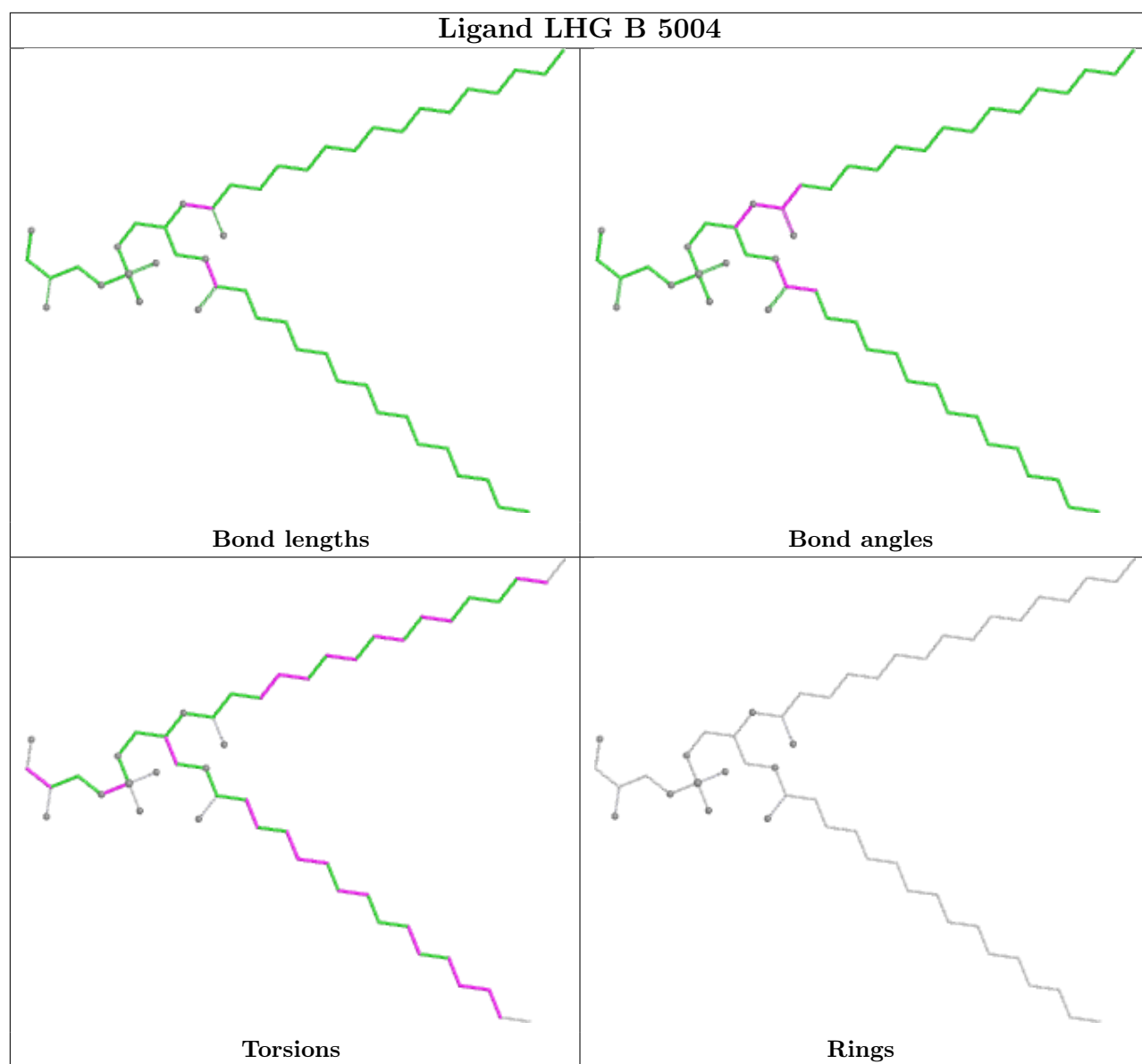
Torsions



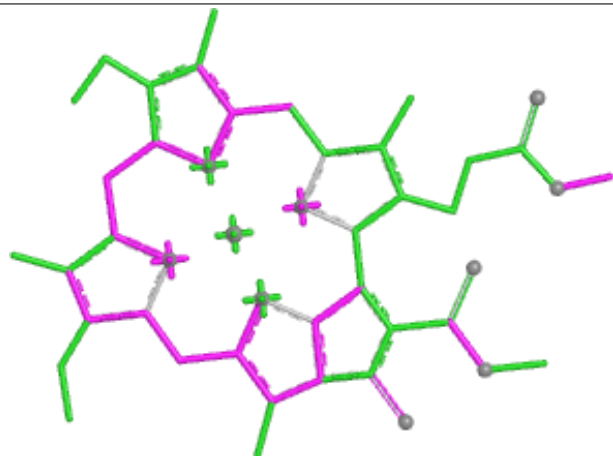
Rings

Ligand CLA A 1116**Ligand CLA B 1021**

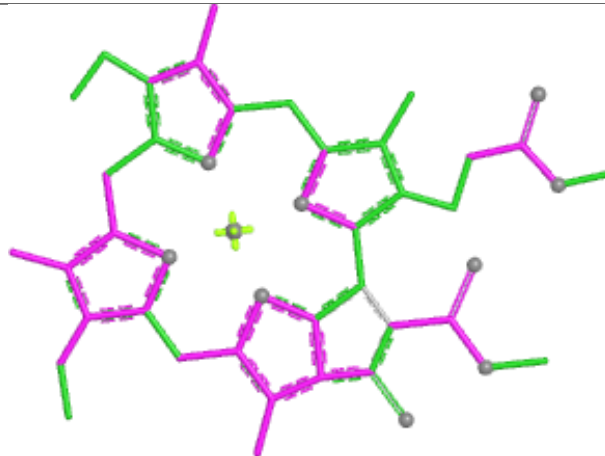




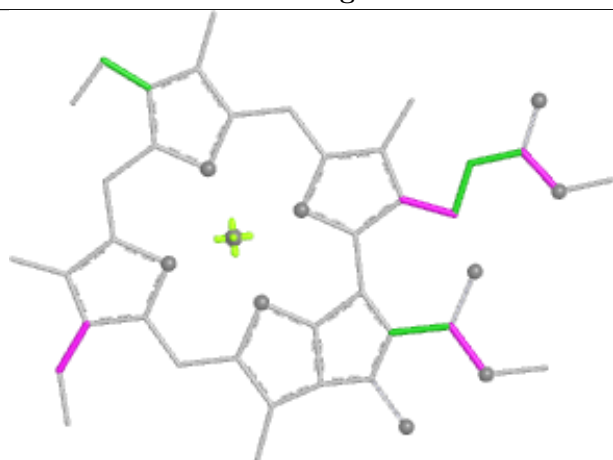
Ligand CLA B 1239



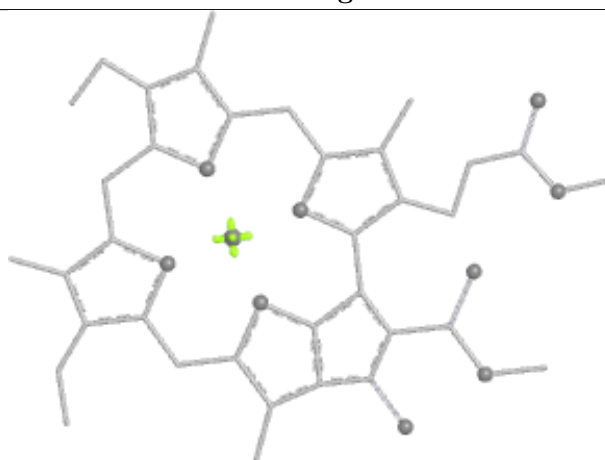
Bond lengths



Bond angles

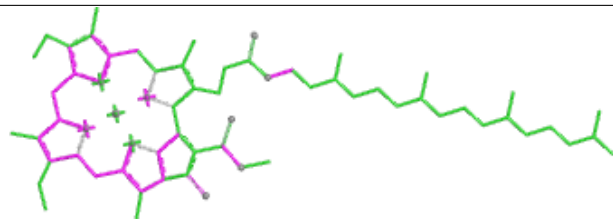


Torsions

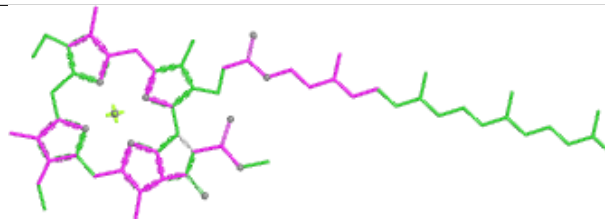


Rings

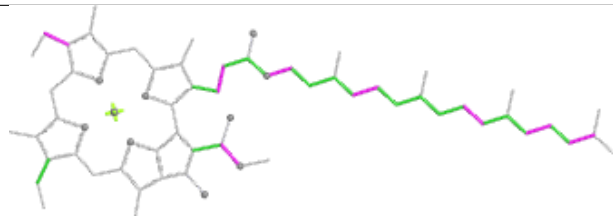
Ligand CLA A 1126



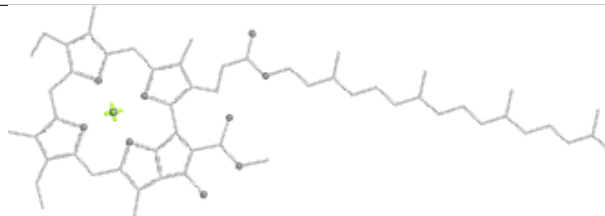
Bond lengths



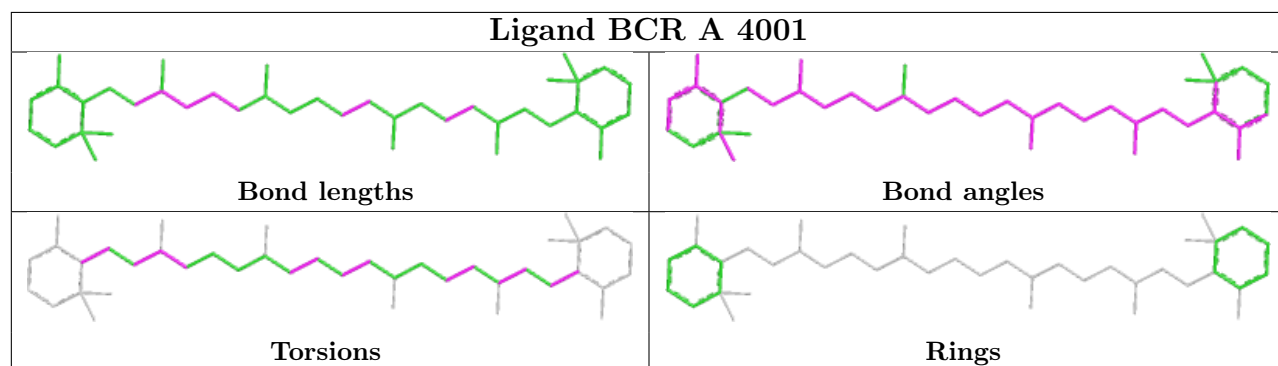
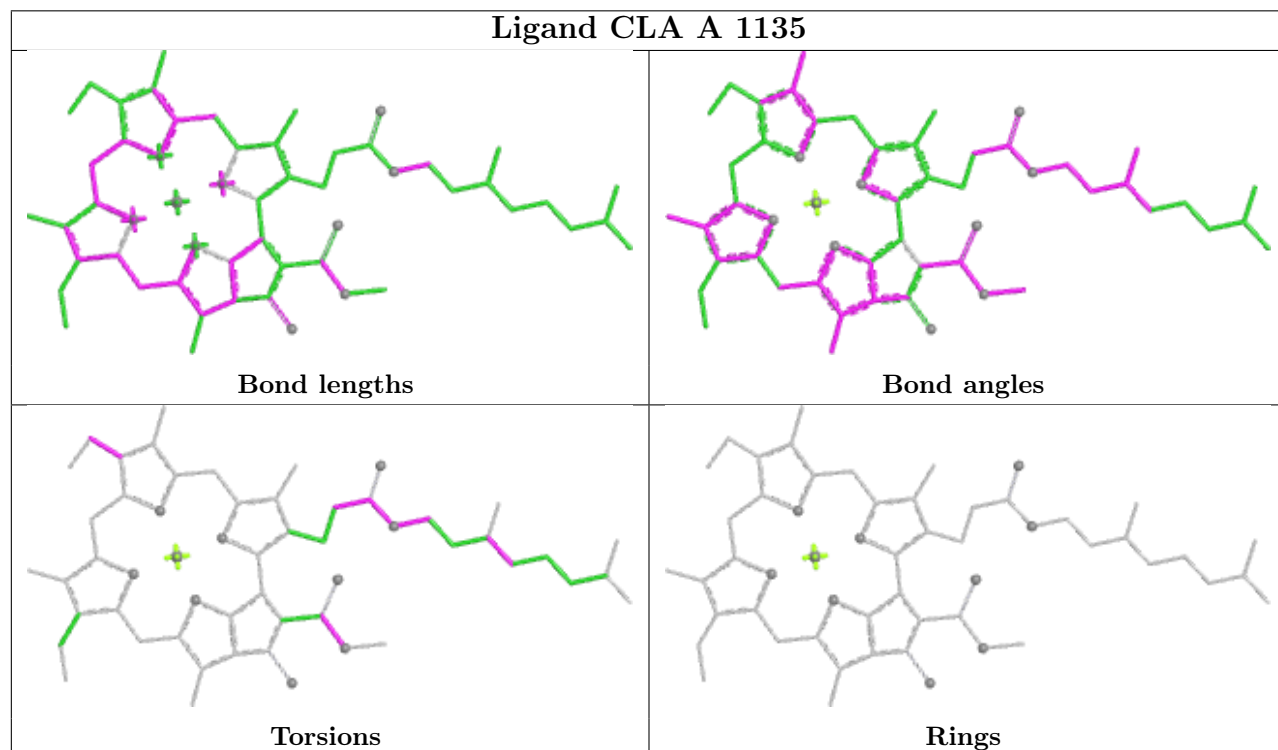
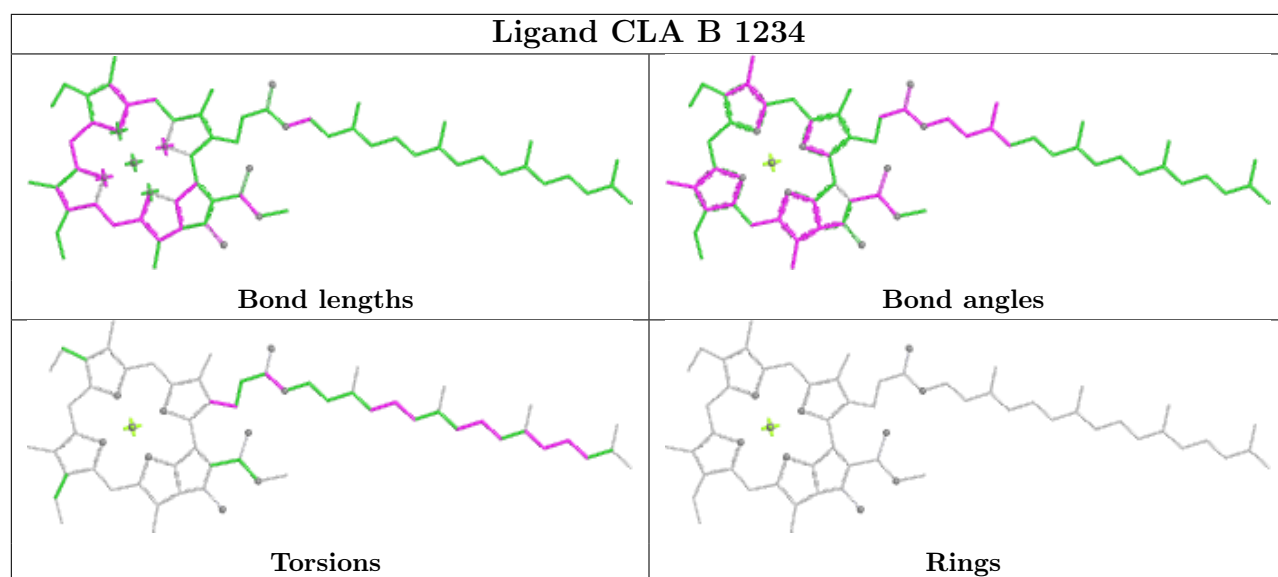
Bond angles

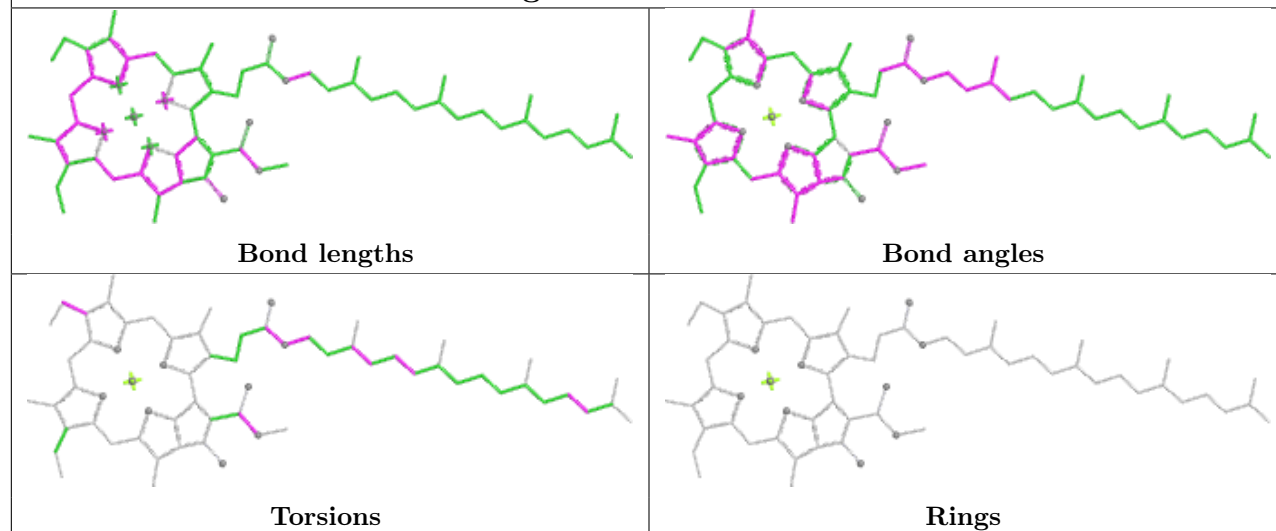
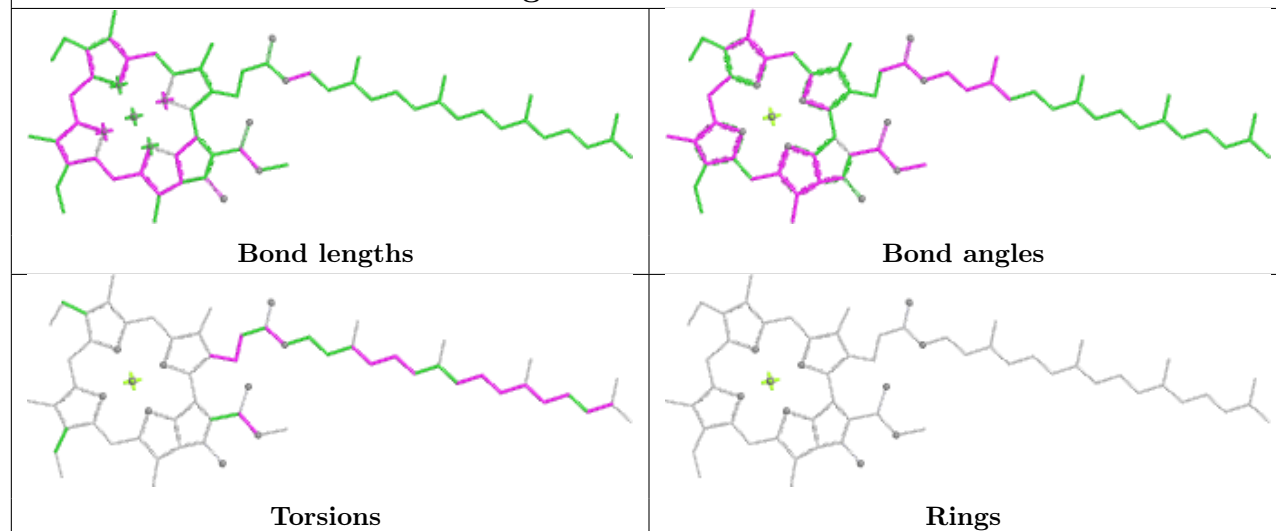


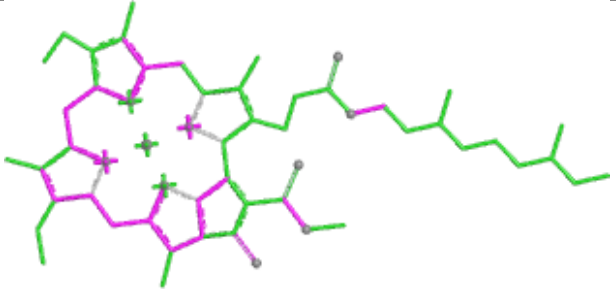
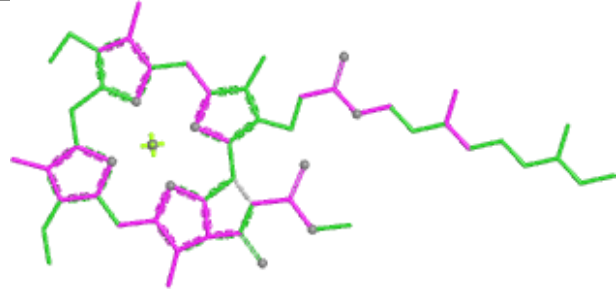
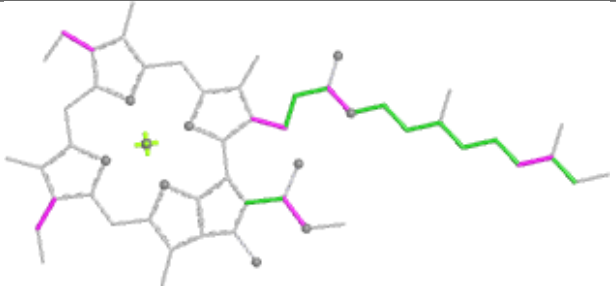
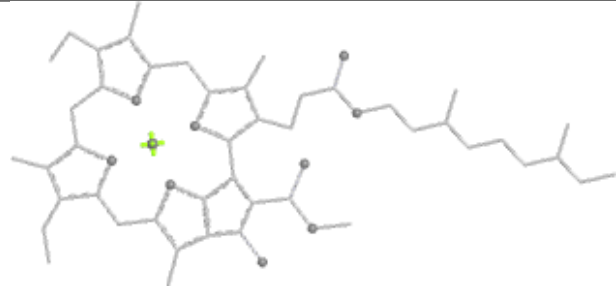
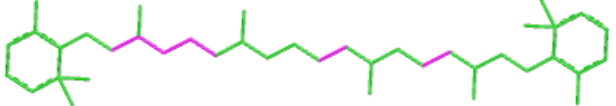
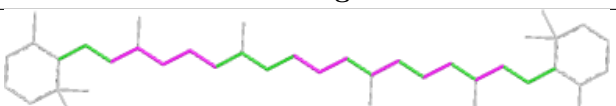
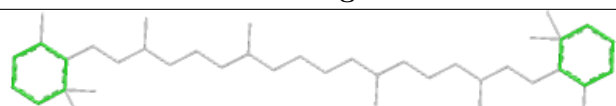
Torsions



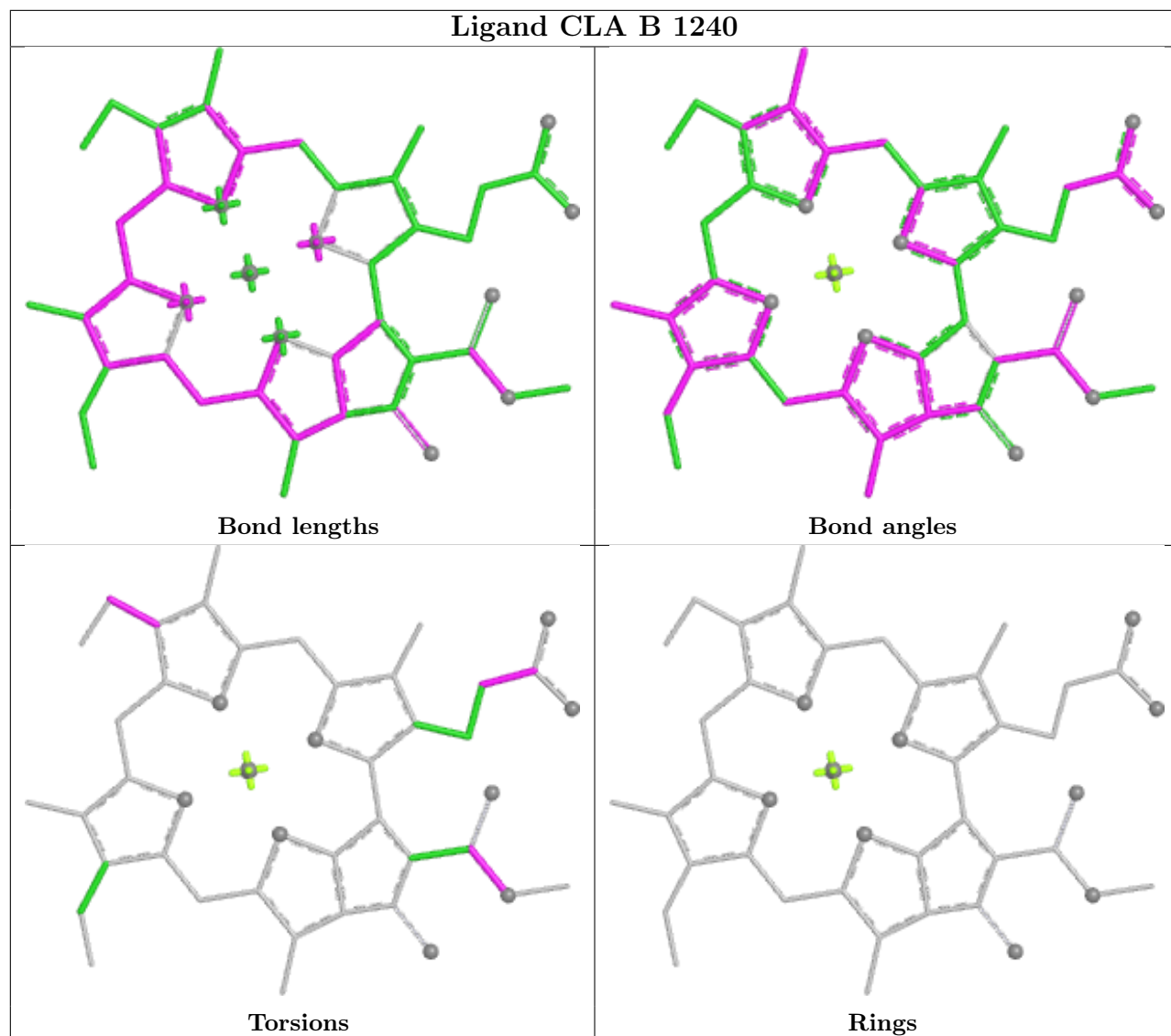
Rings



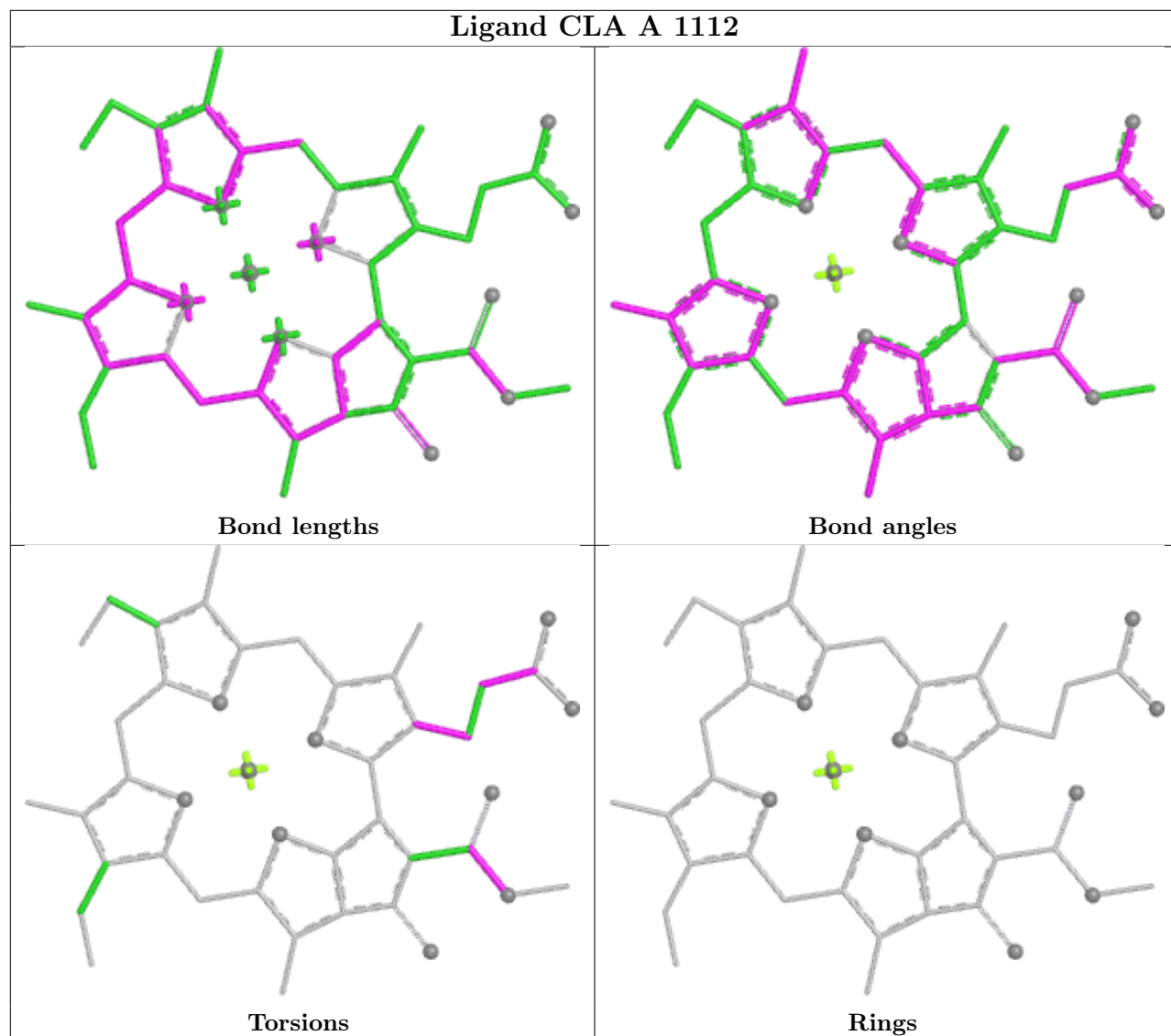
Ligand CLA A 1109**Ligand CLA A 1122**

Ligand CLA B 1222	
	
Bond lengths	Bond angles
	
Torsions	Rings
Ligand BCR B 4014	
	
Bond lengths	Bond angles
	
Torsions	Rings

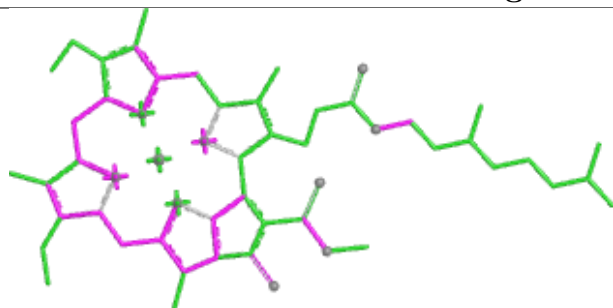
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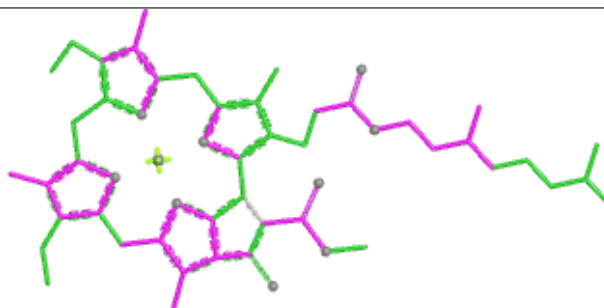
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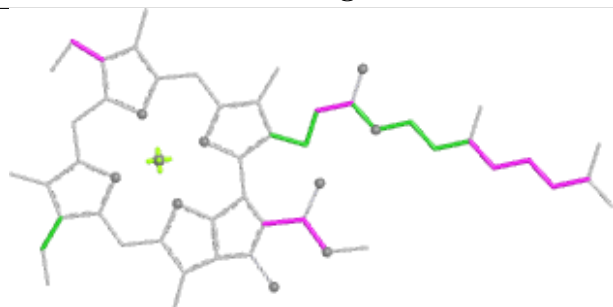
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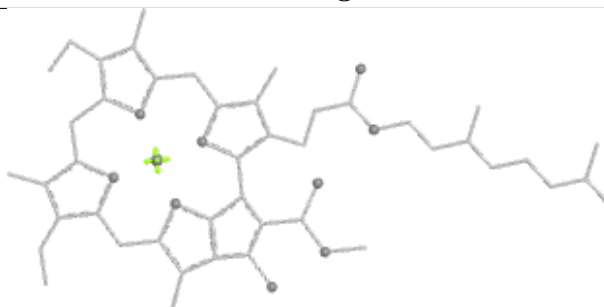
Bond lengths



Bond angles

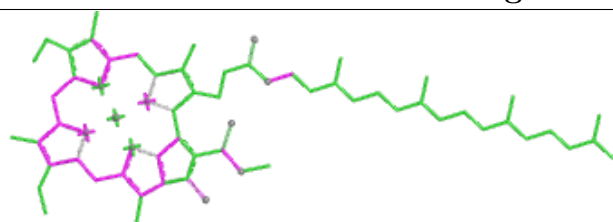


Torsions

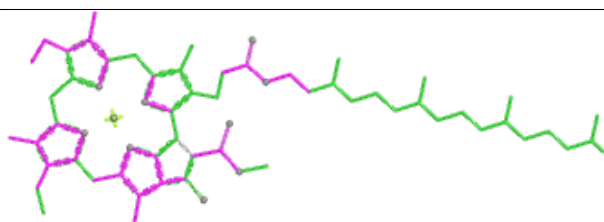


Rings

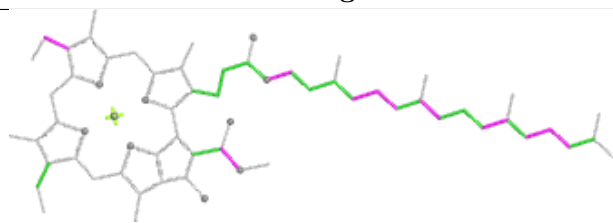
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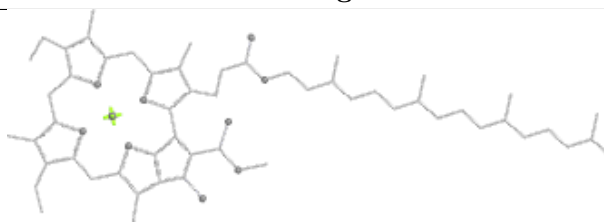
Bond lengths



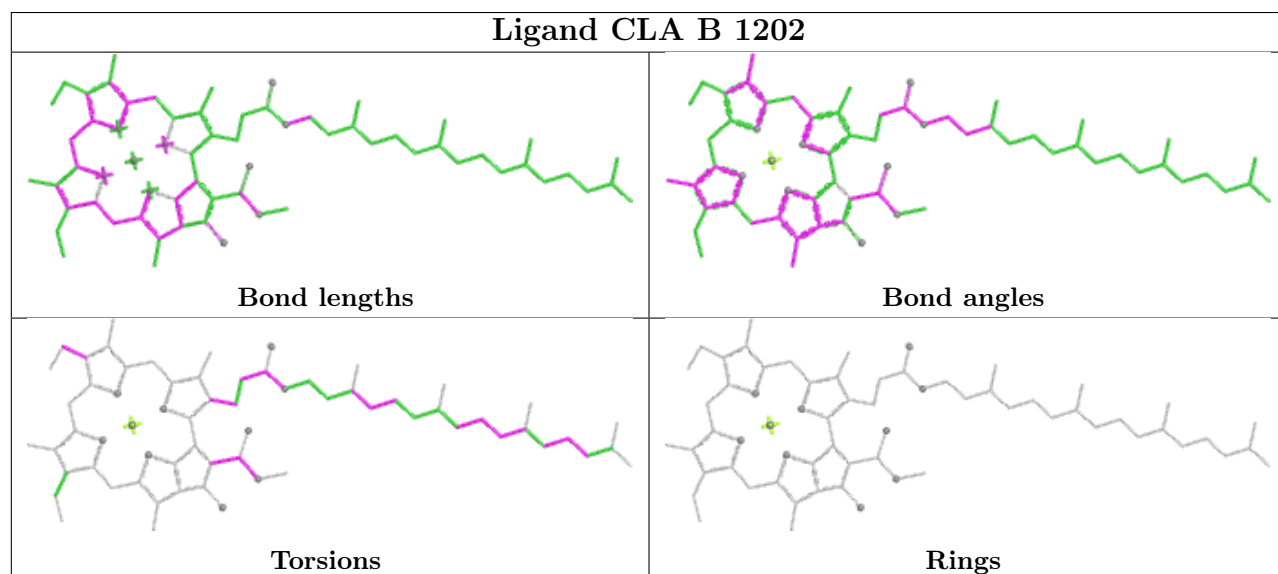
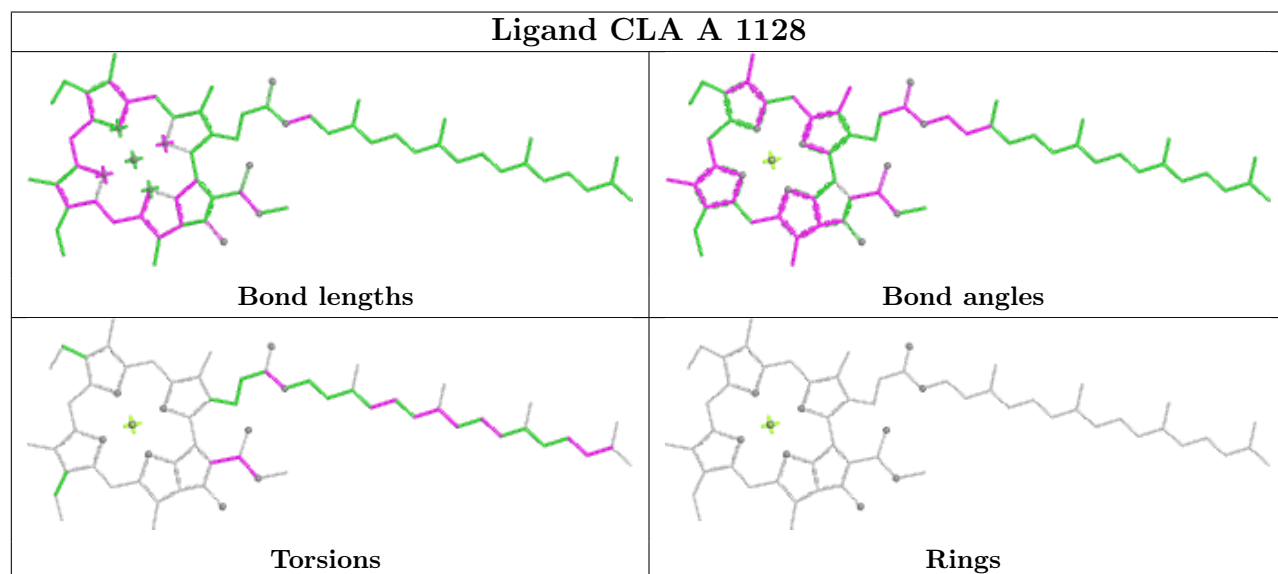
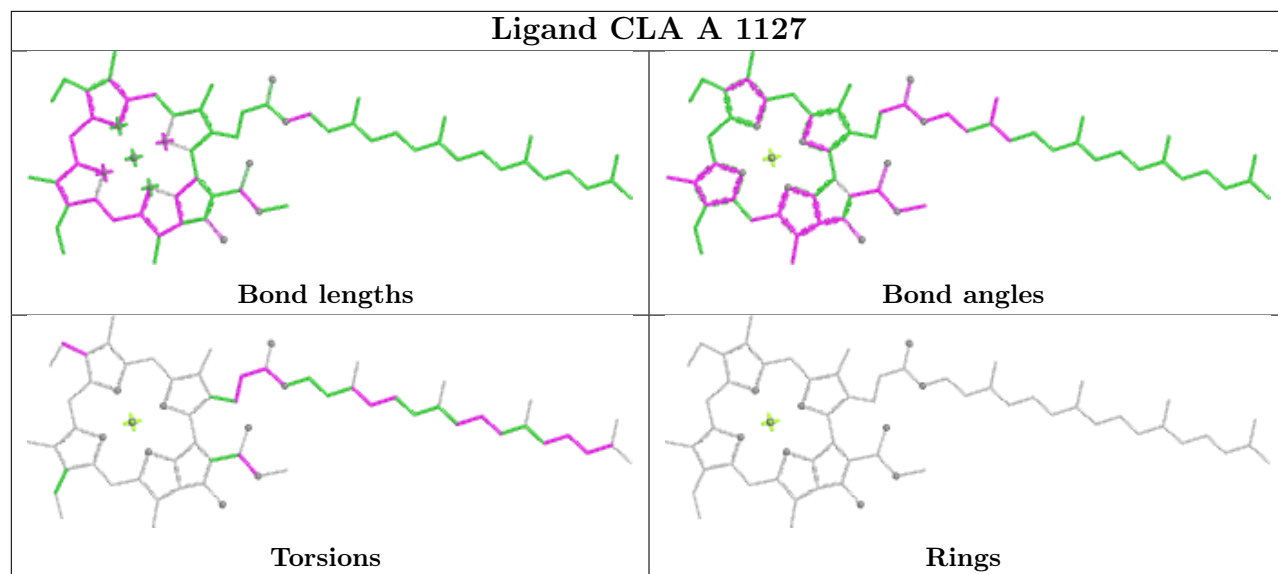
Bond angles



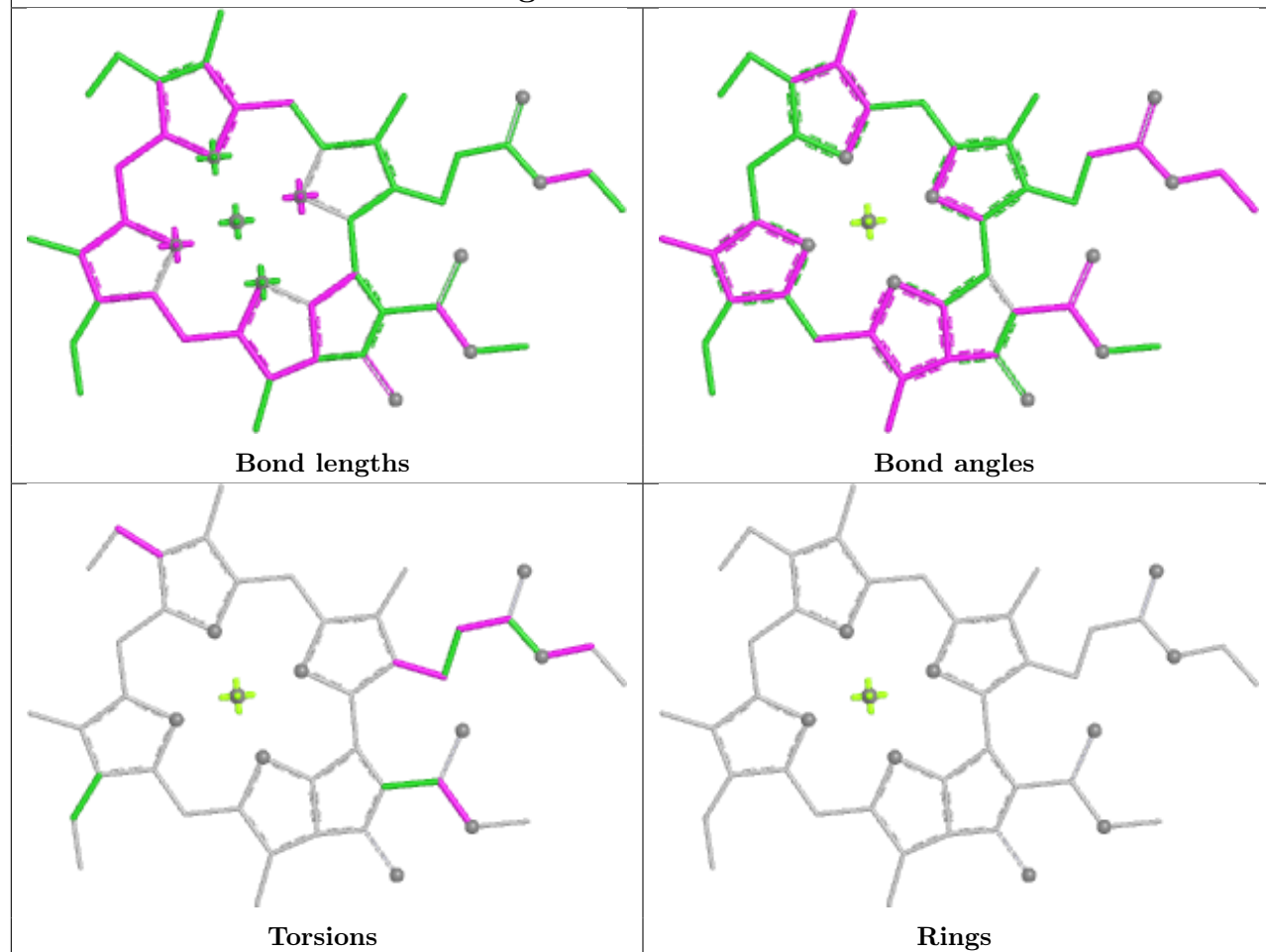
Torsions



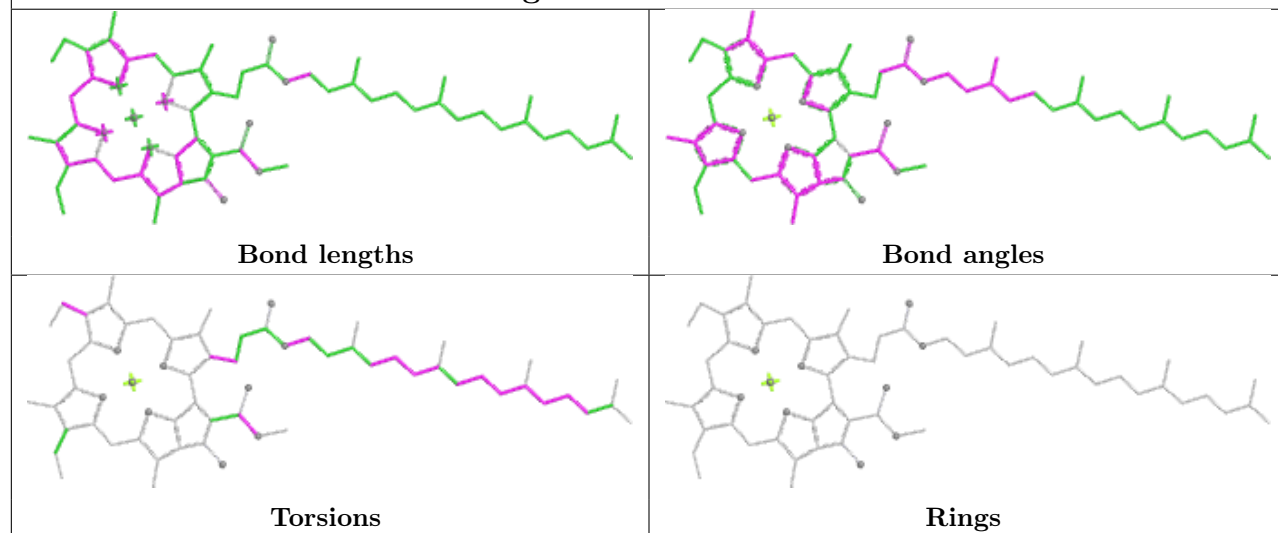
Rings

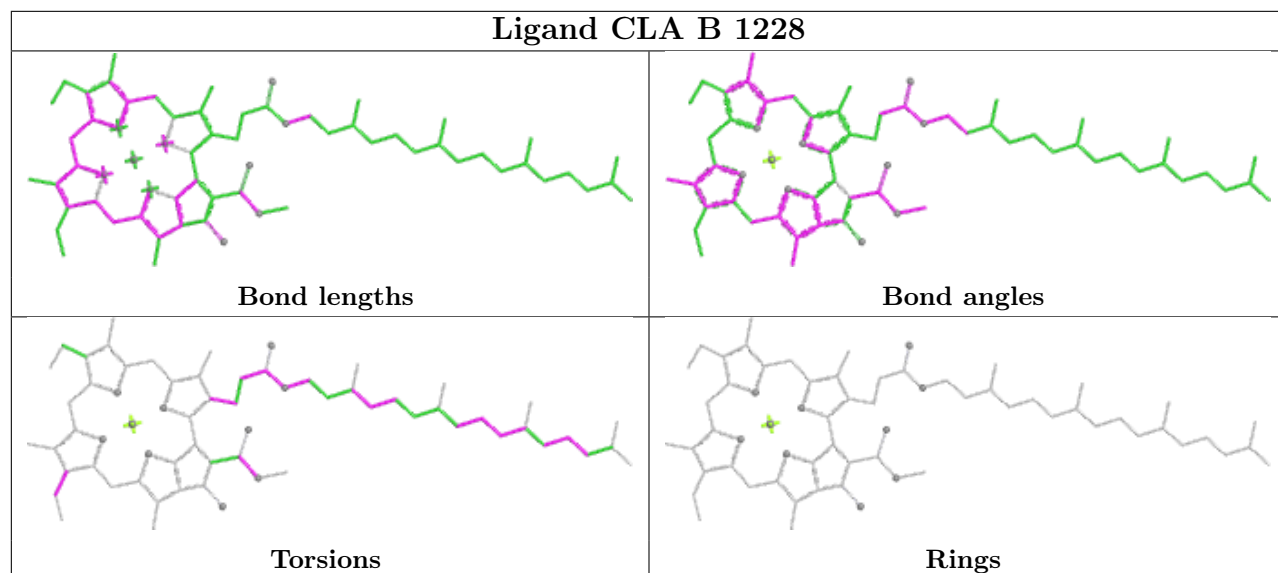
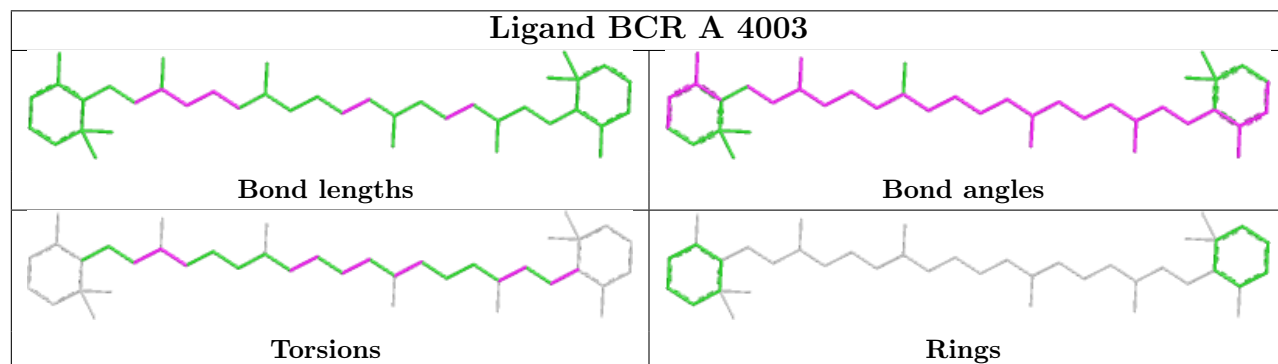
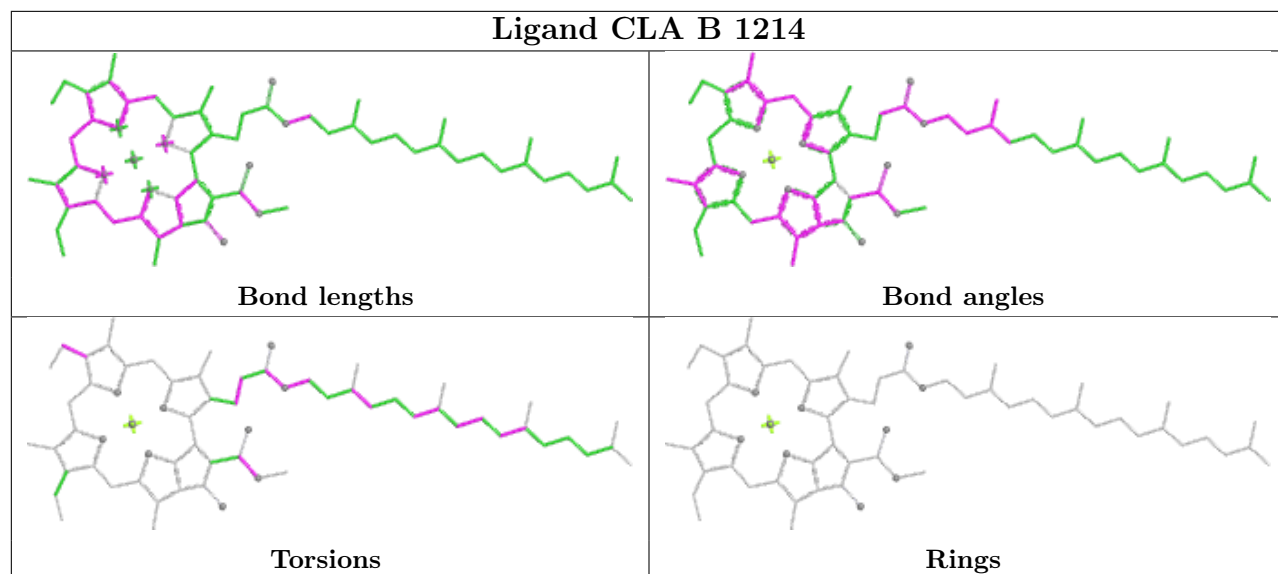


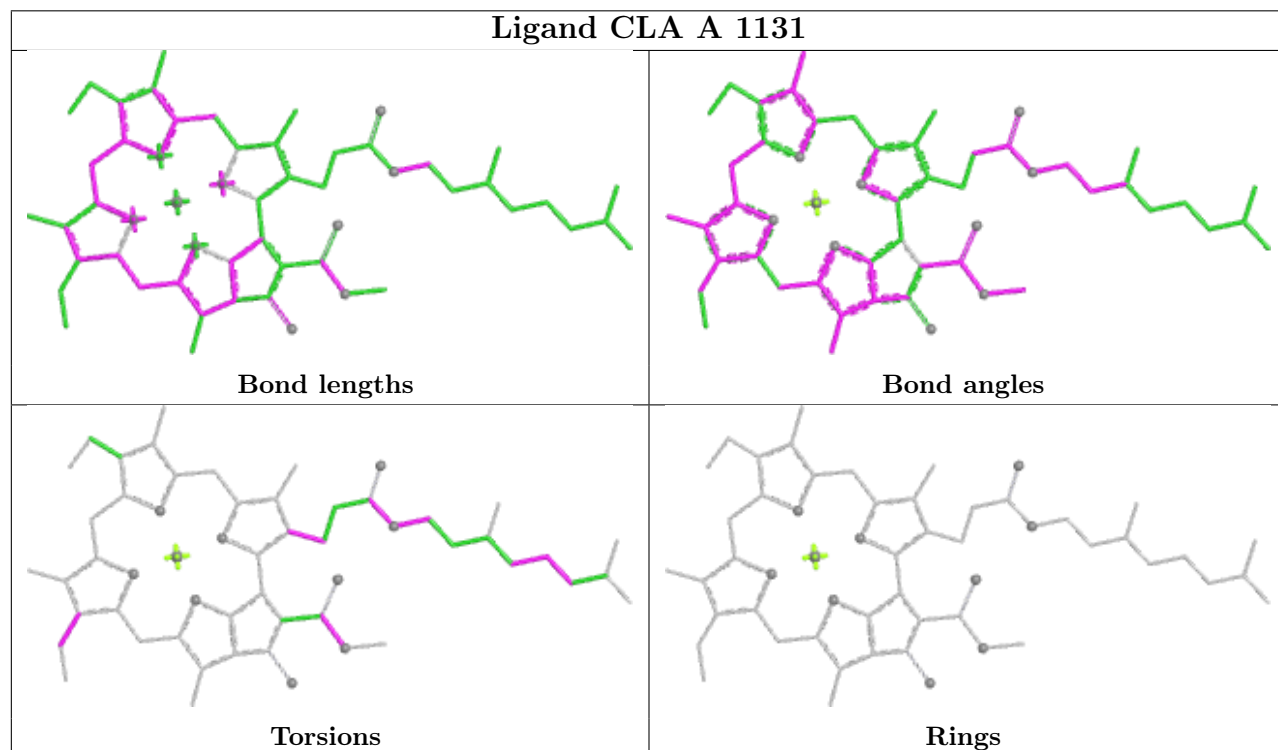
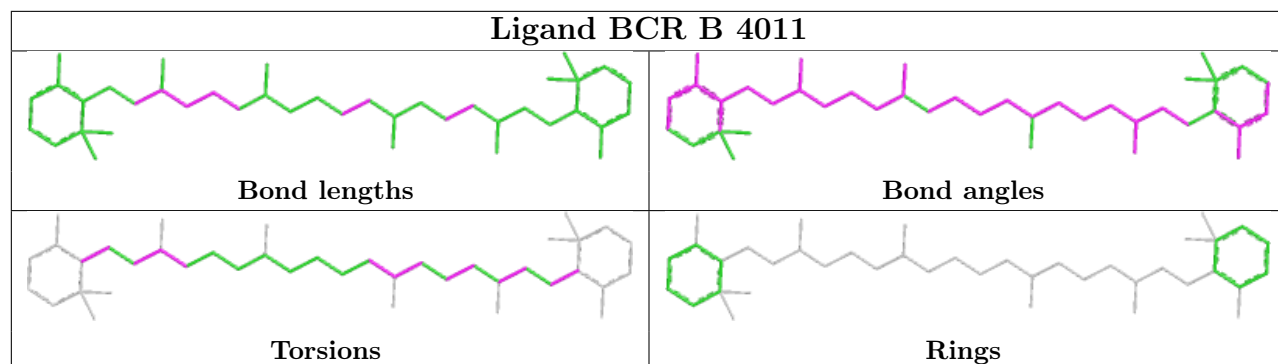
Ligand CLA B 1217

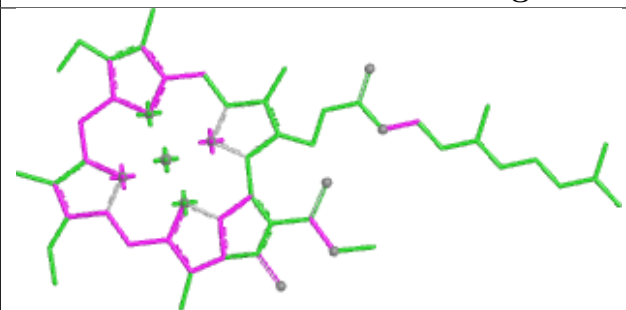
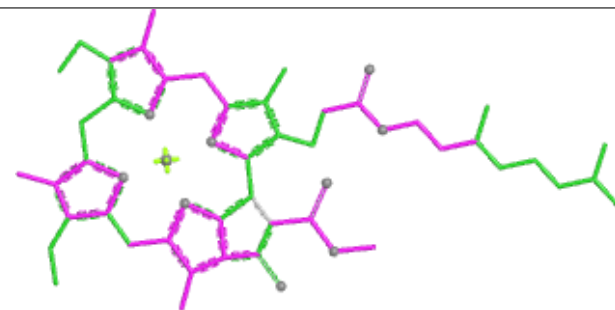
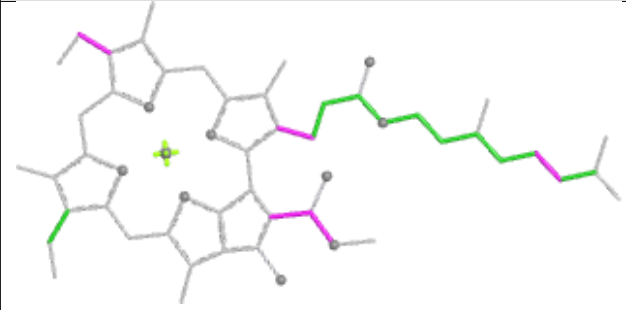
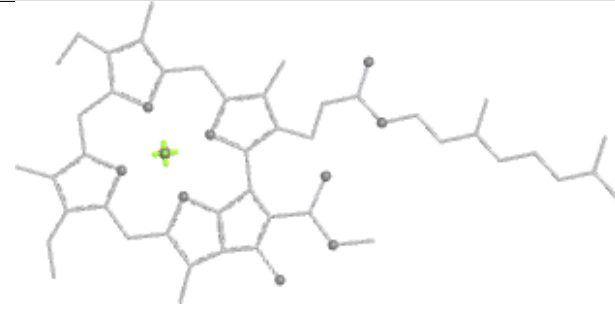


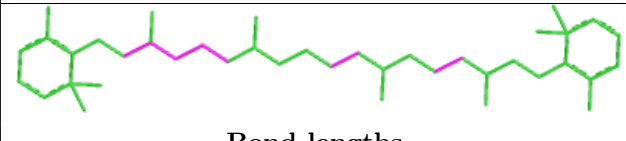
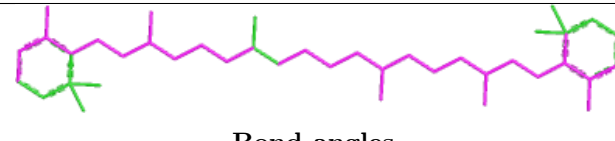
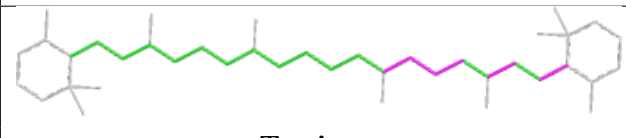
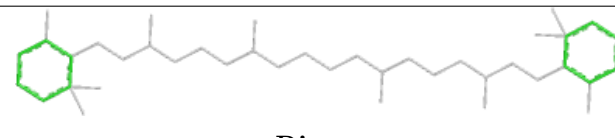
Ligand CLA A 1117

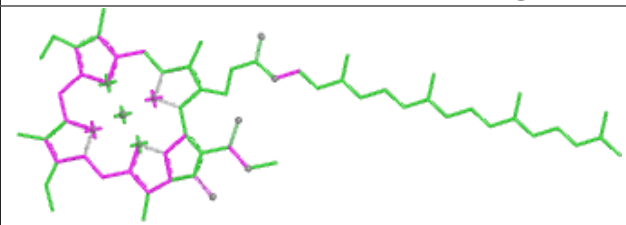
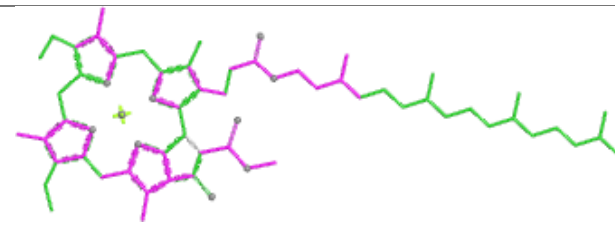
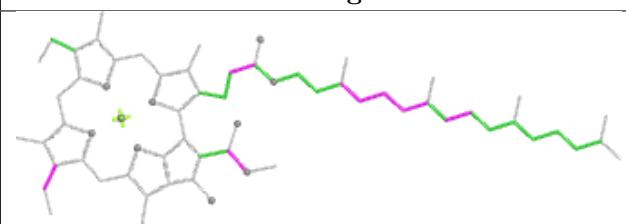
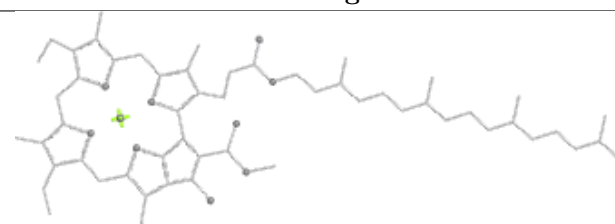


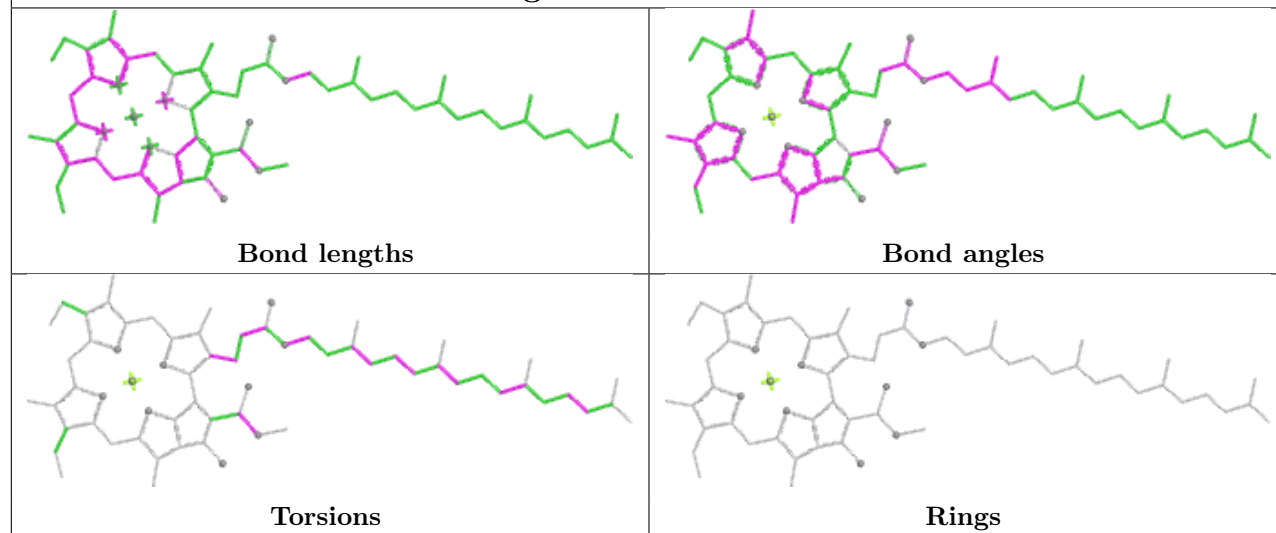
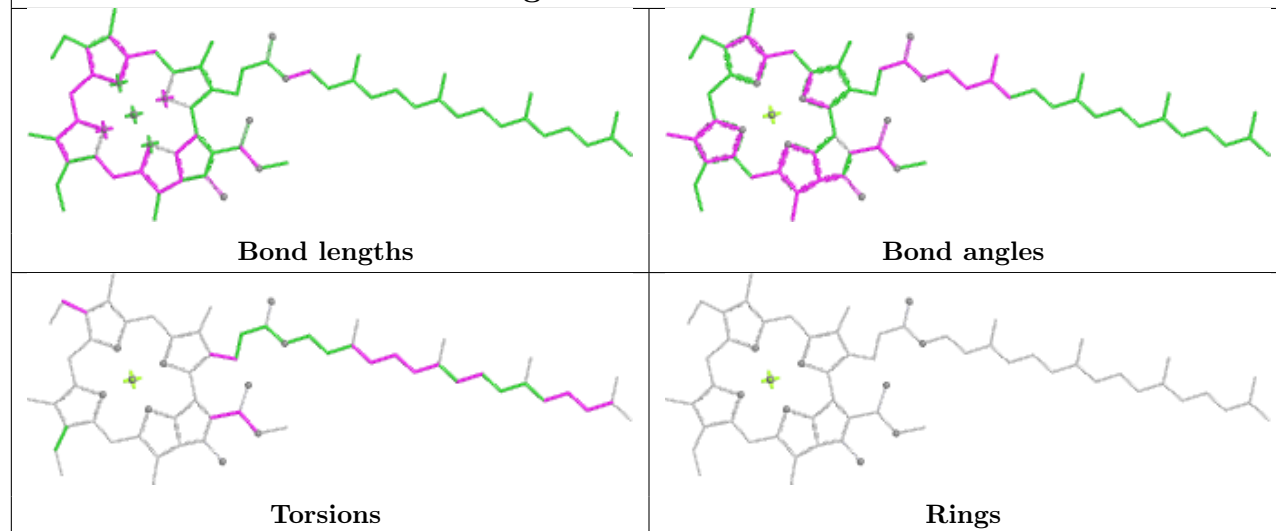


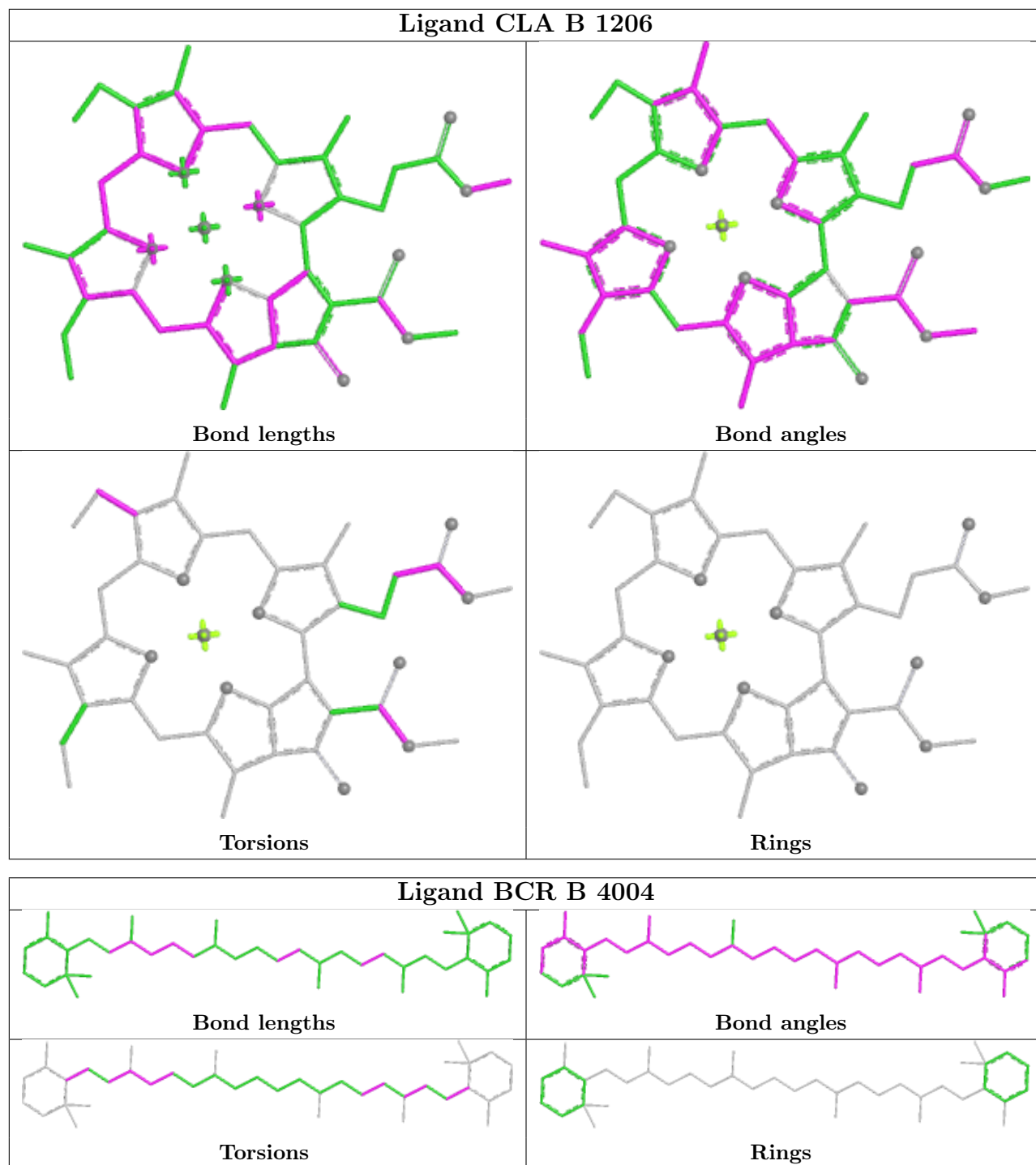


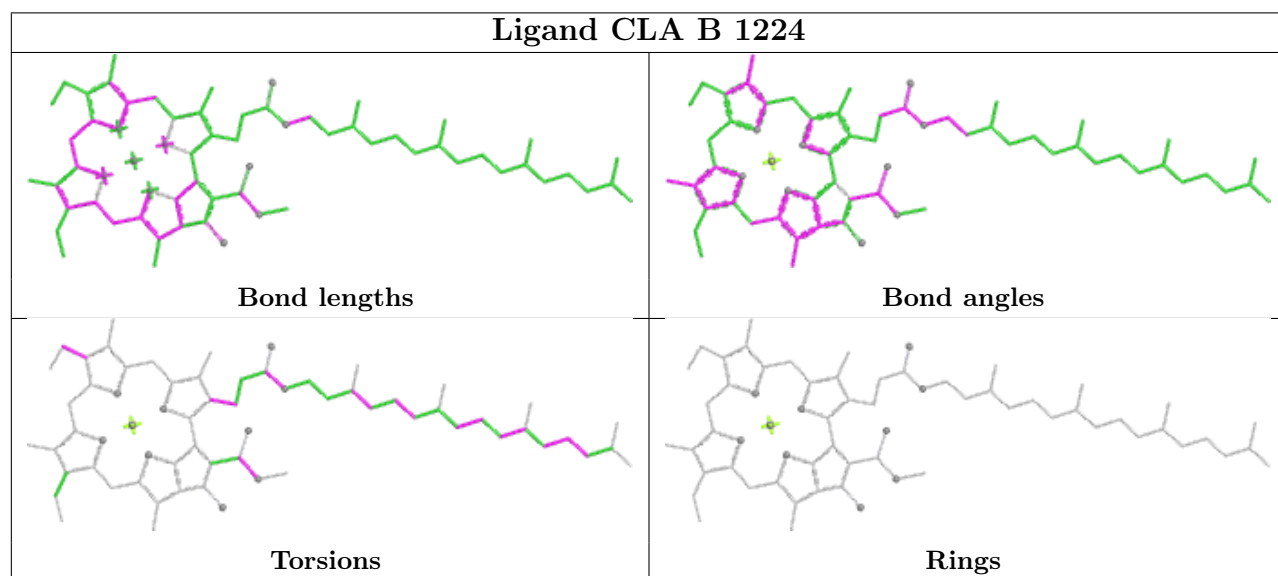
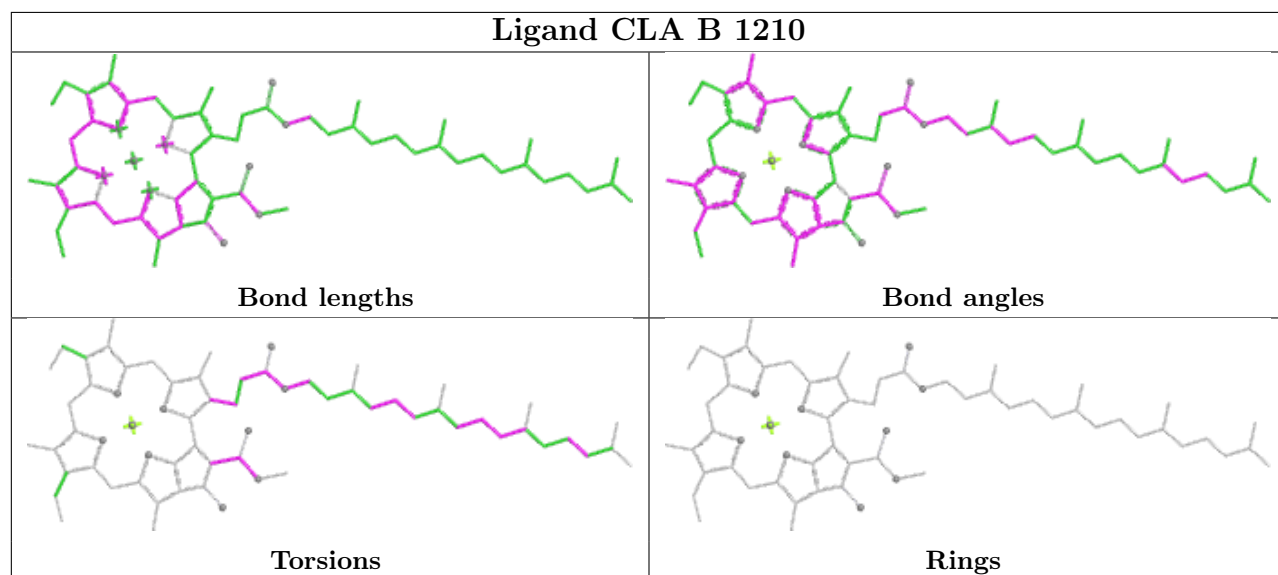
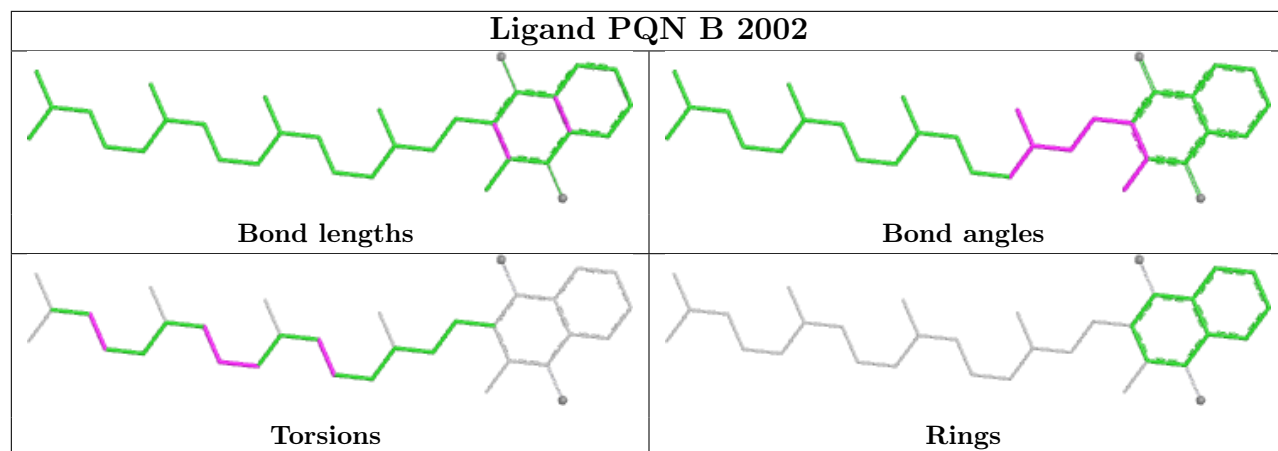
Ligand CLA A 1124	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand BCR B 4010	
	
Bond lengths	Bond angles
	
Torsions	Rings

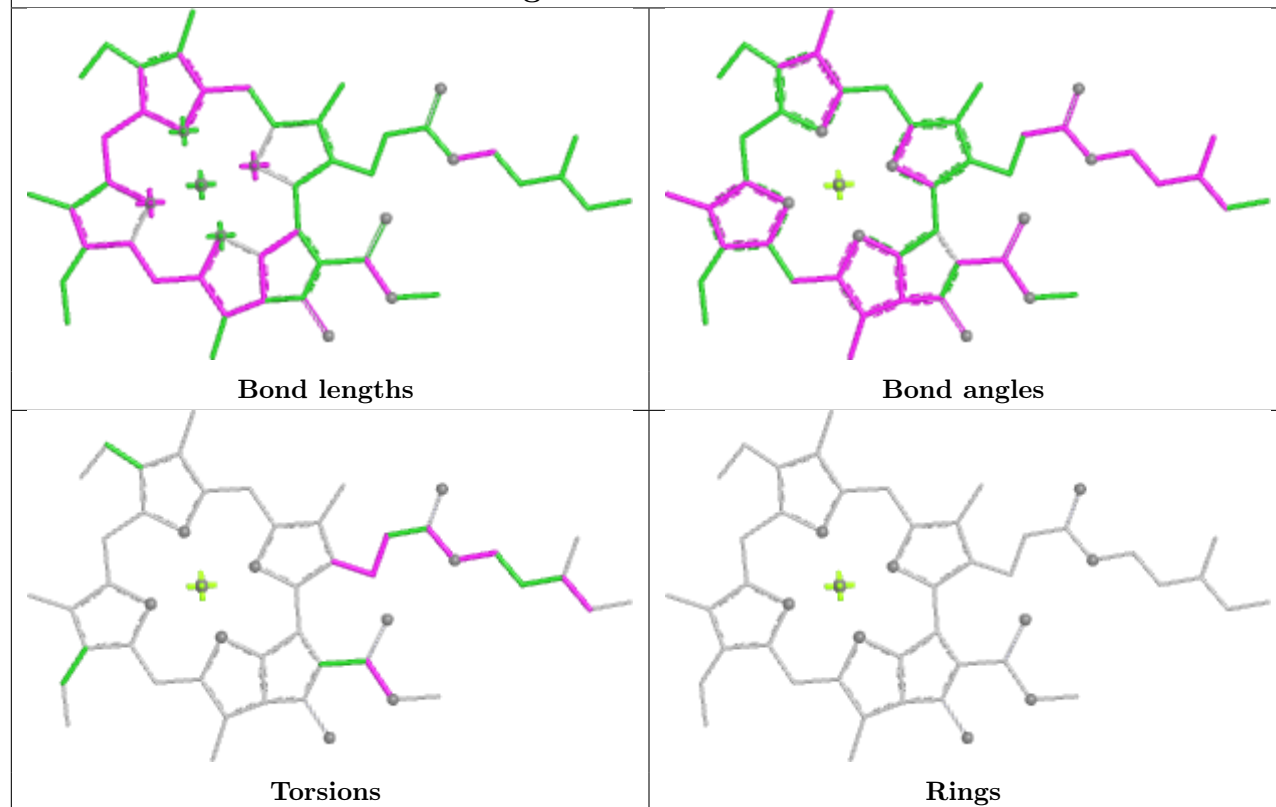
Ligand CLA B 1231	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA B 1215**Ligand CLA B 1223**

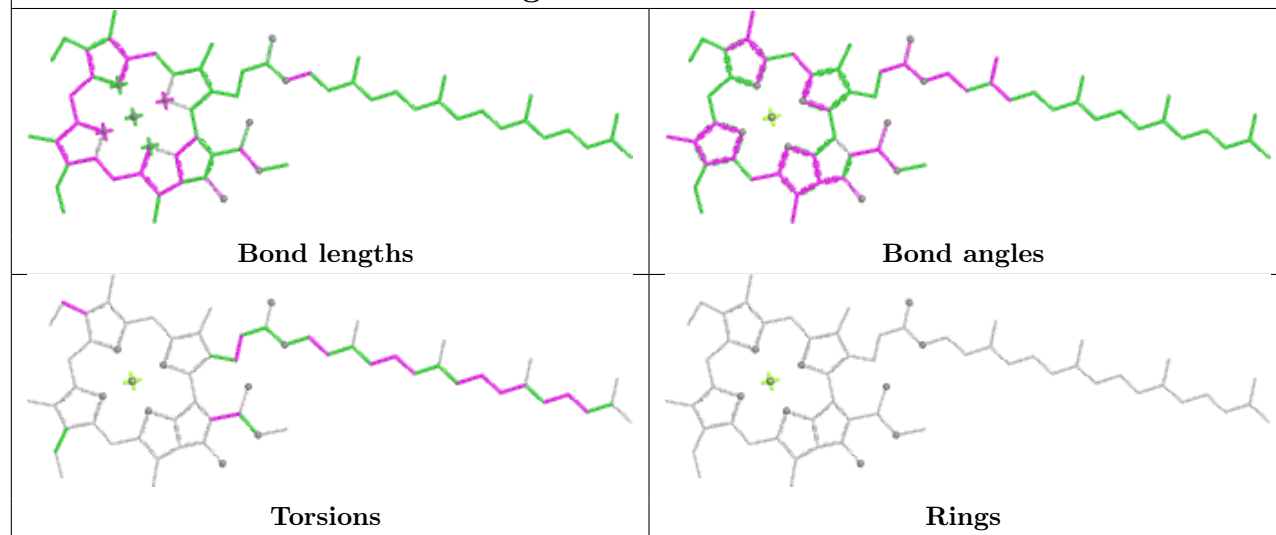




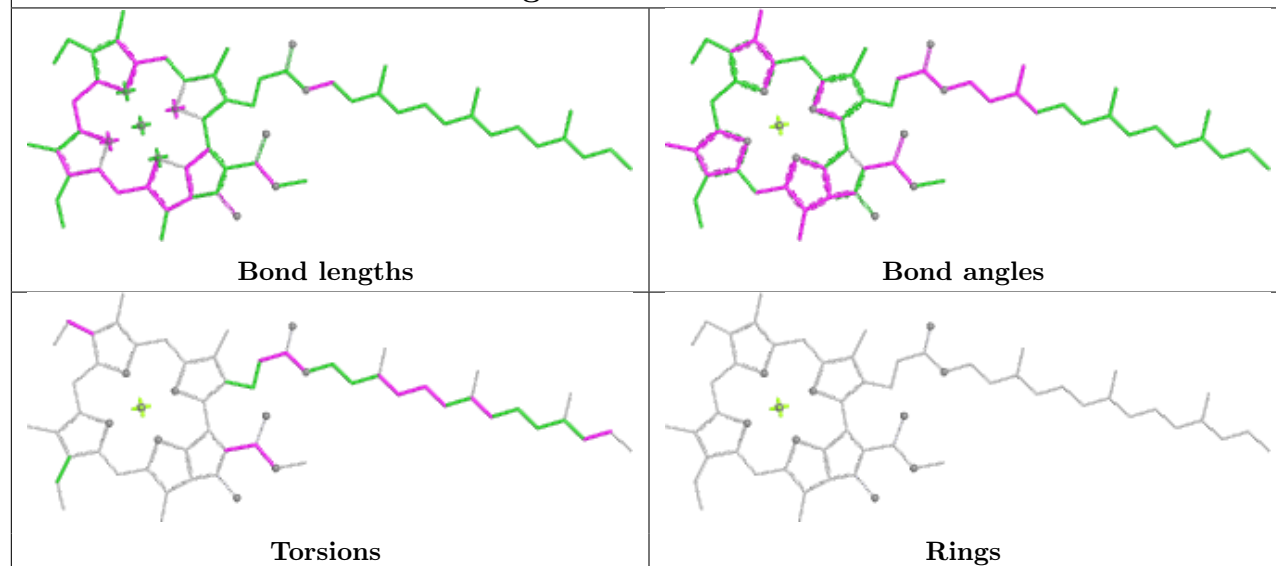
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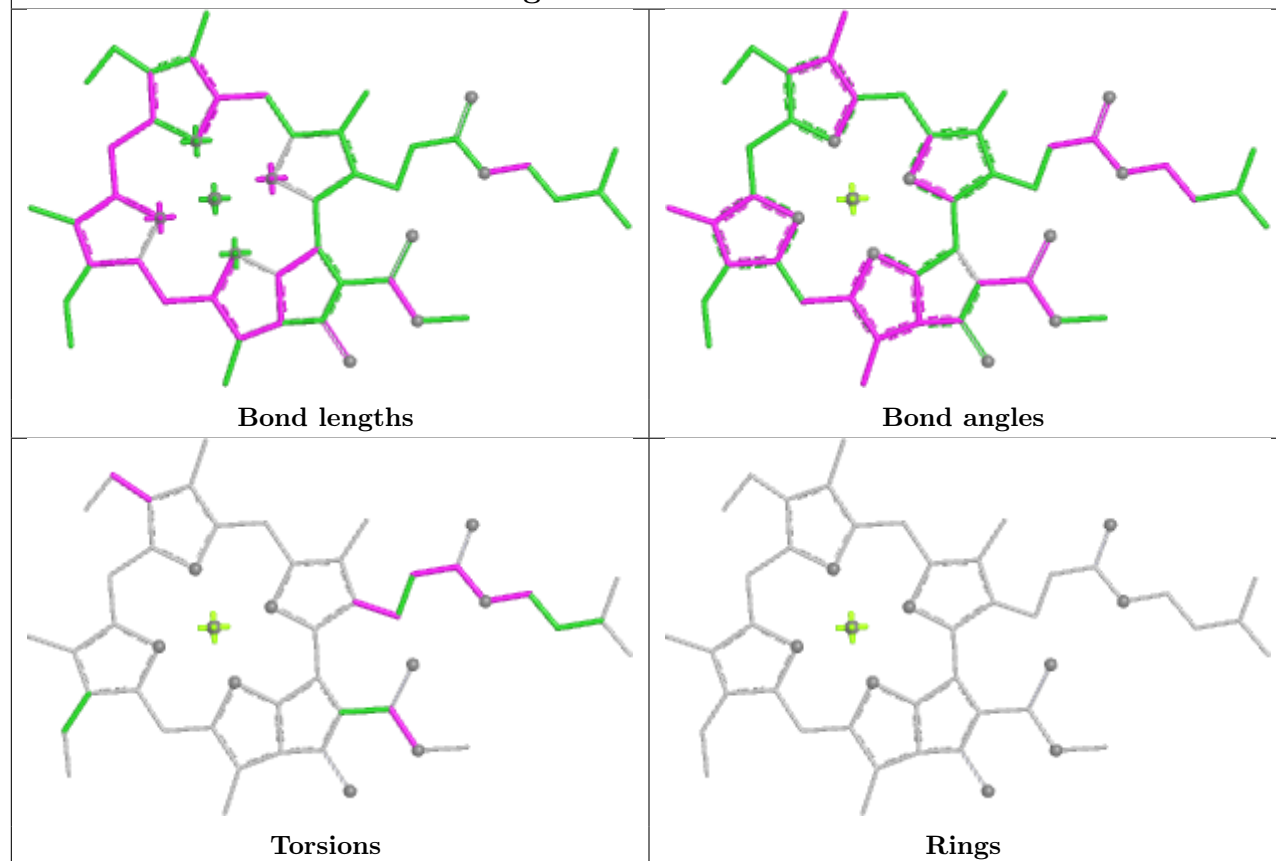
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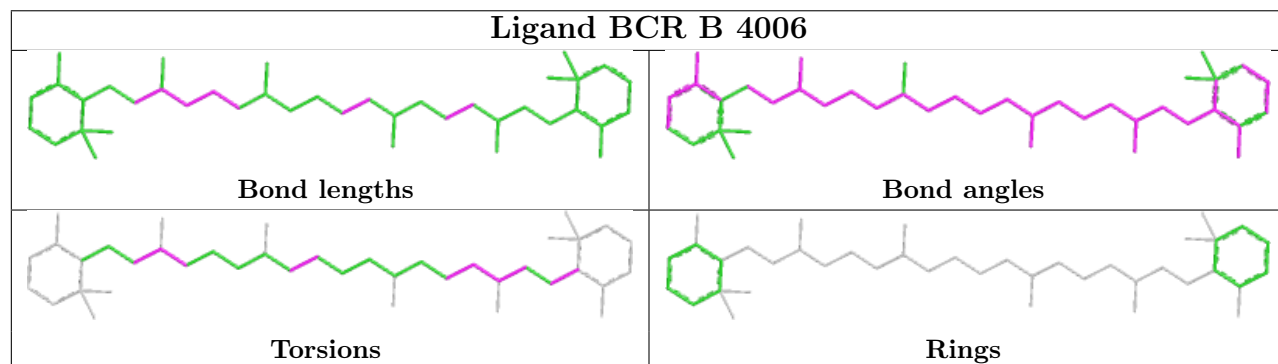
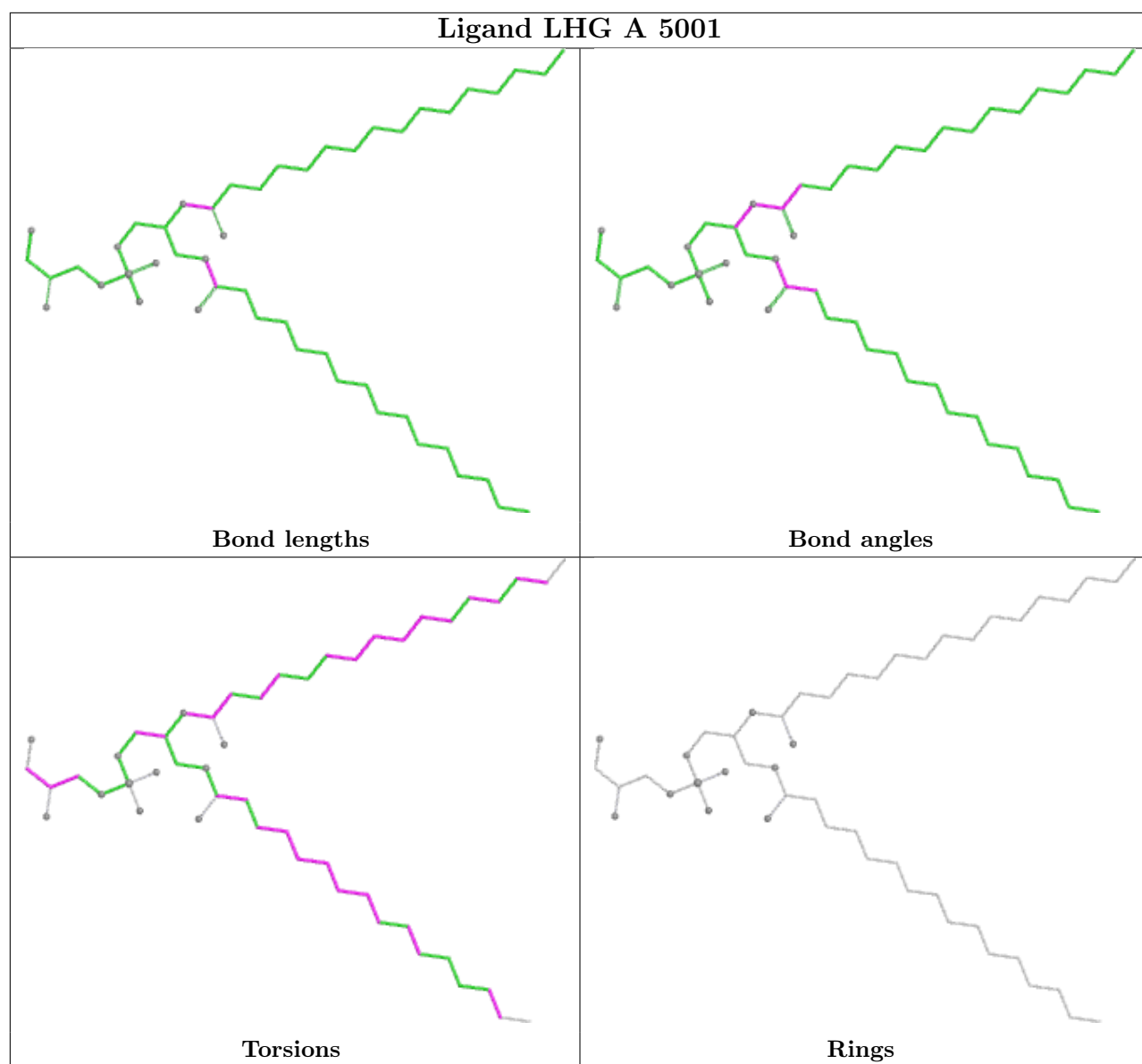


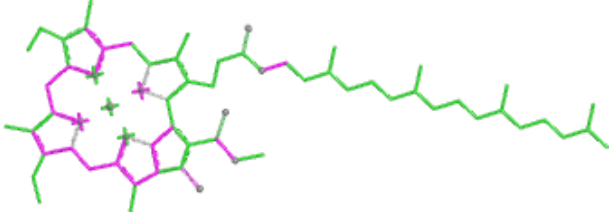
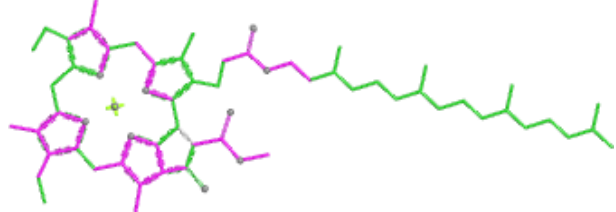
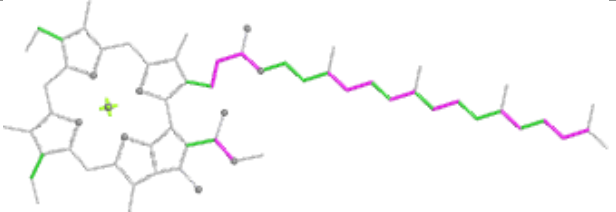
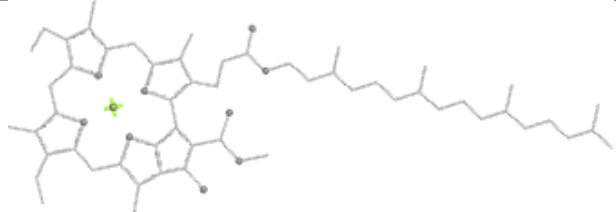
Ligand CLA A 1132

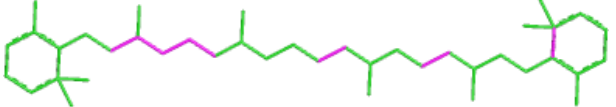
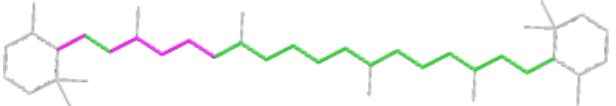
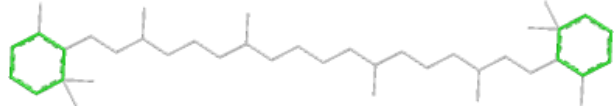


Ligand CLA B 1213

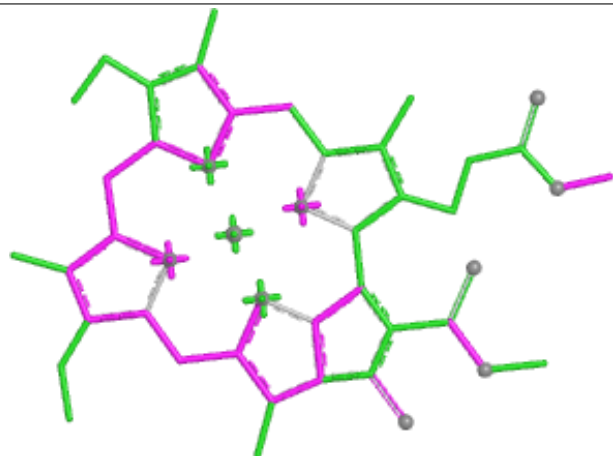




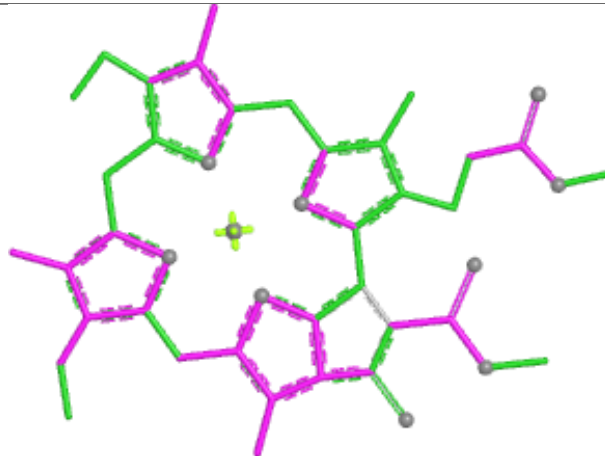
Ligand CLA A 1136			
			
Bond lengths	Bond angles		
			
Torsions	Rings		

Ligand BCR B 4017			
			
Bond lengths	Bond angles		
			
Torsions	Rings		

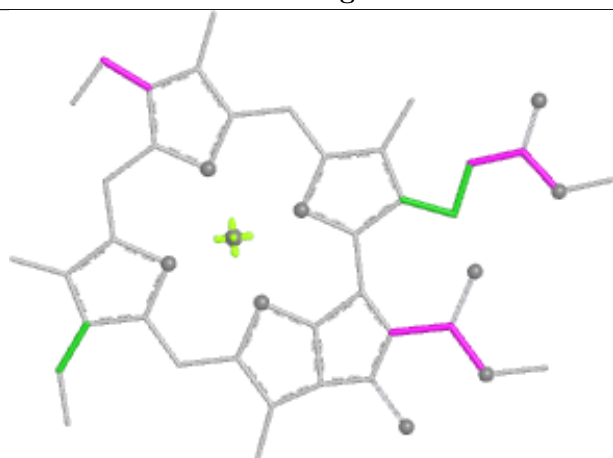
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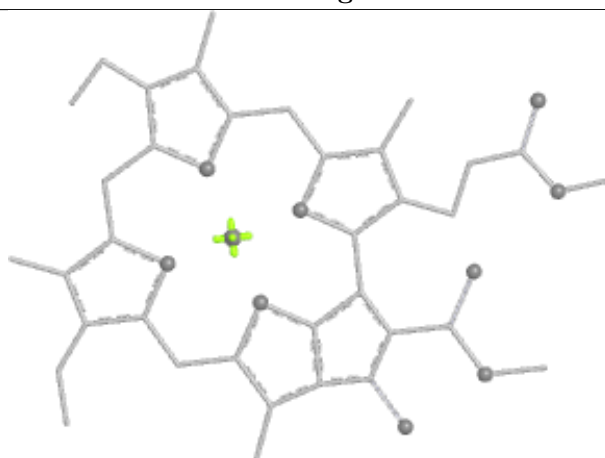
Bond lengths



Bond angles

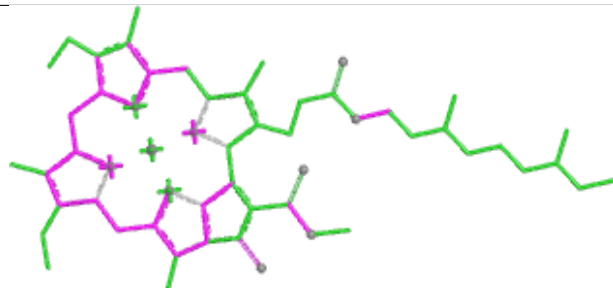


Torsions

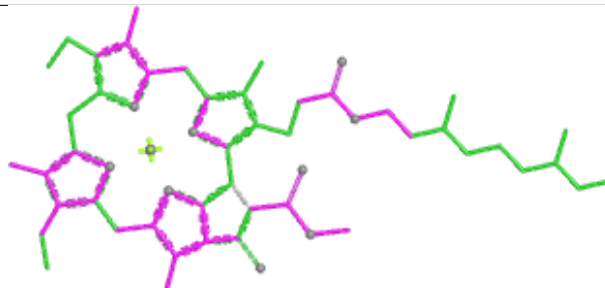


Rings

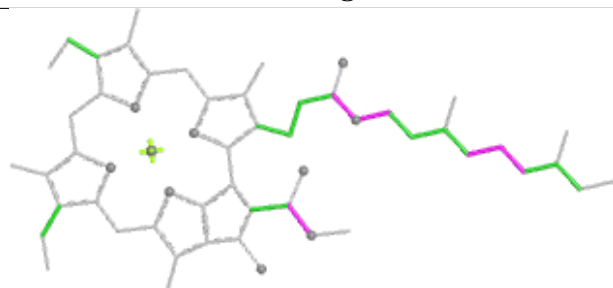
Ligand CLA B 1220



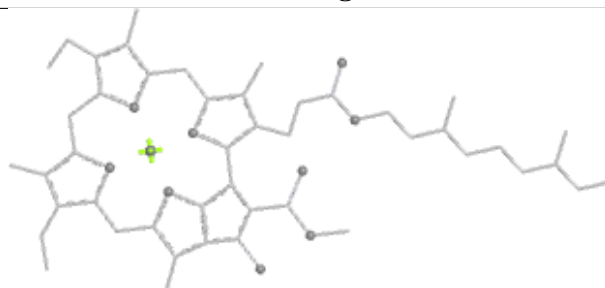
Bond lengths



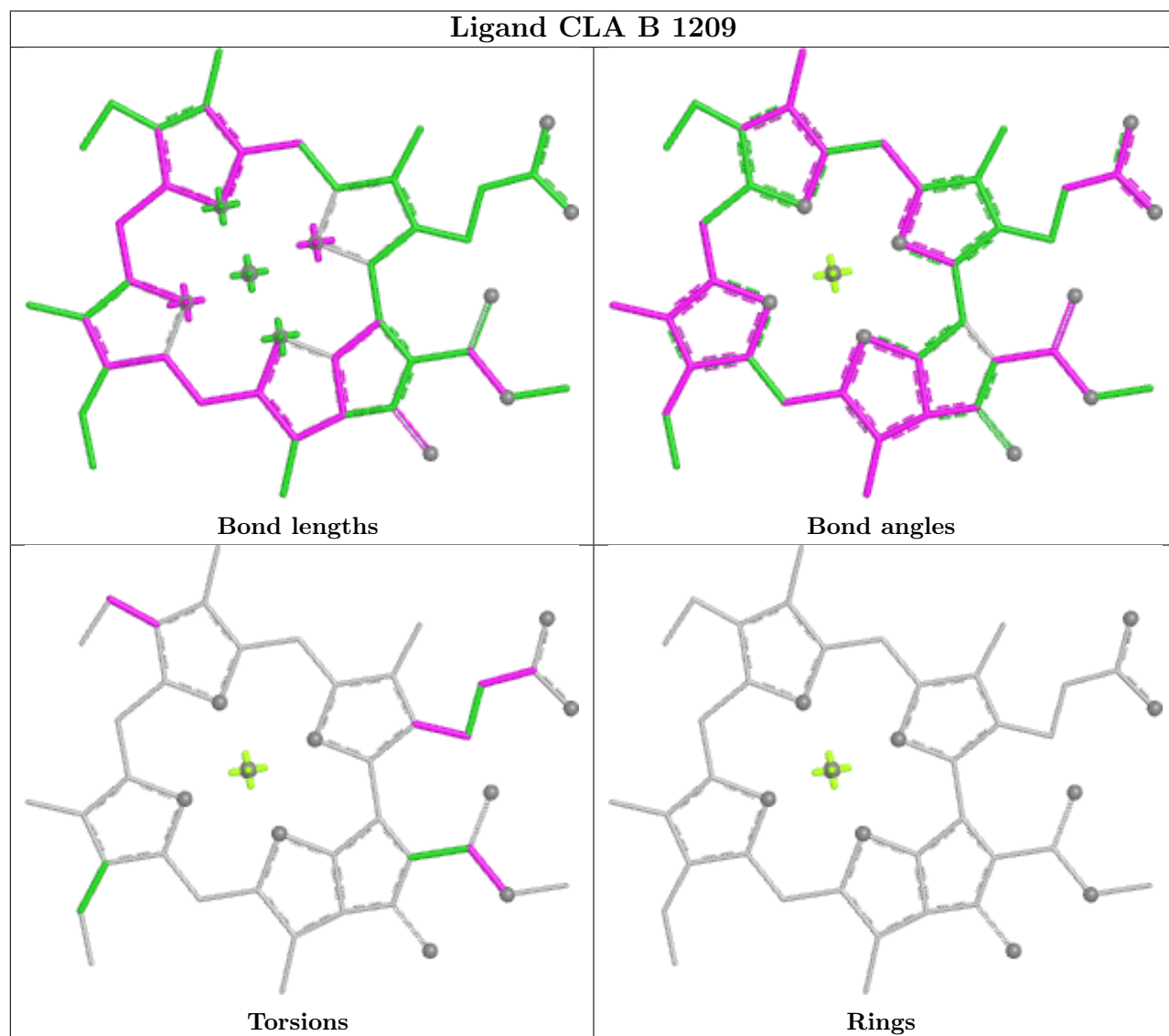
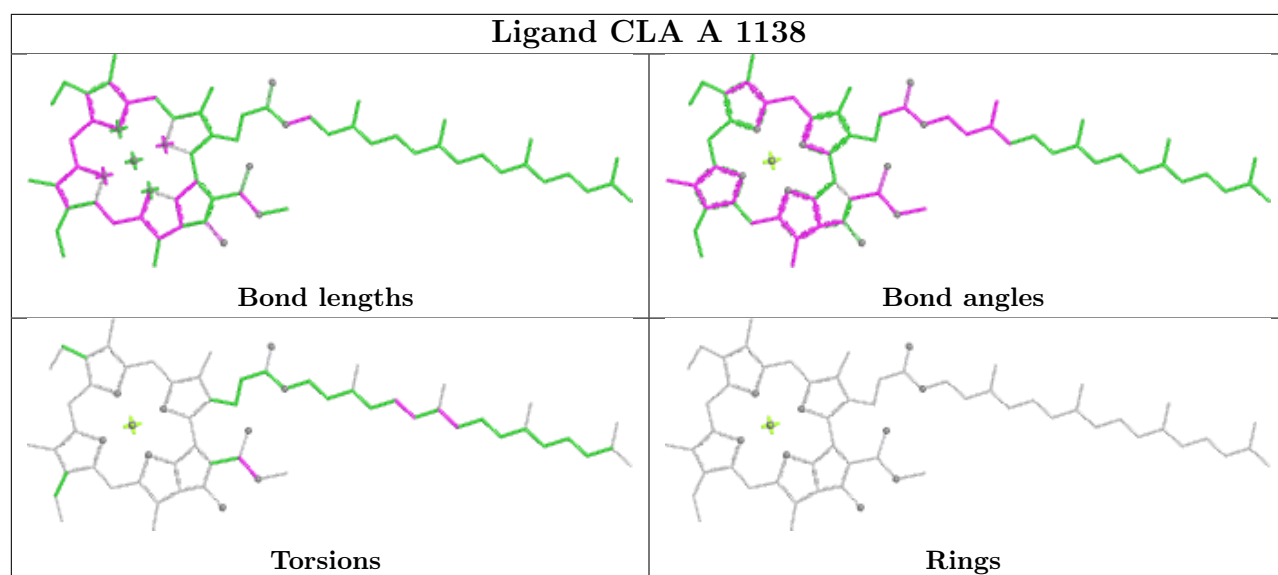
Bond angles

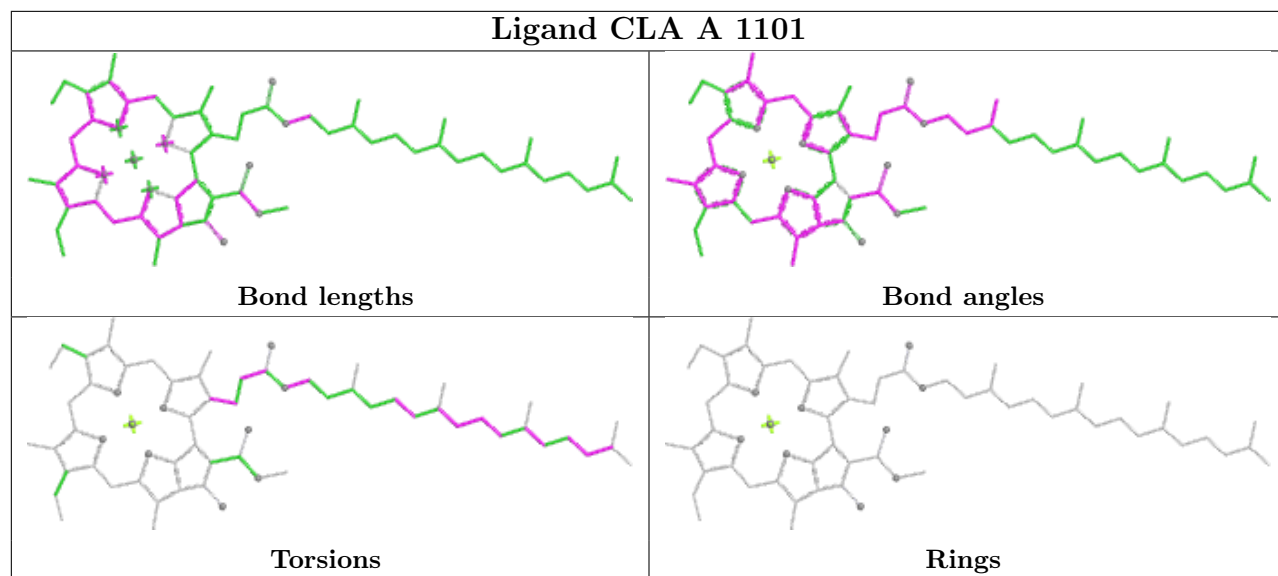
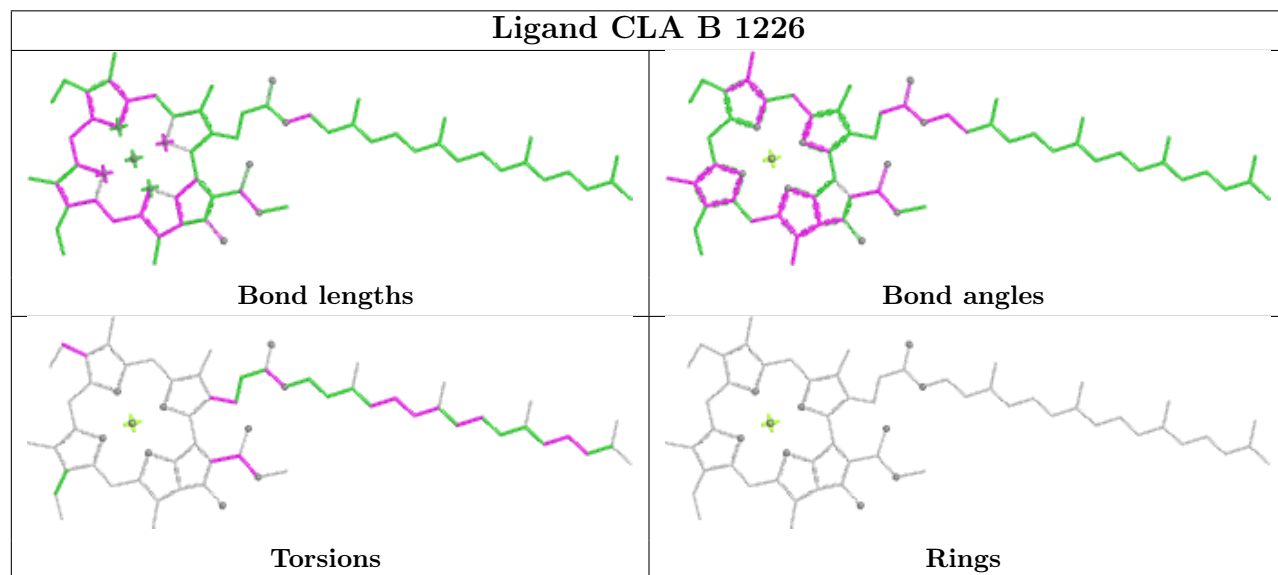


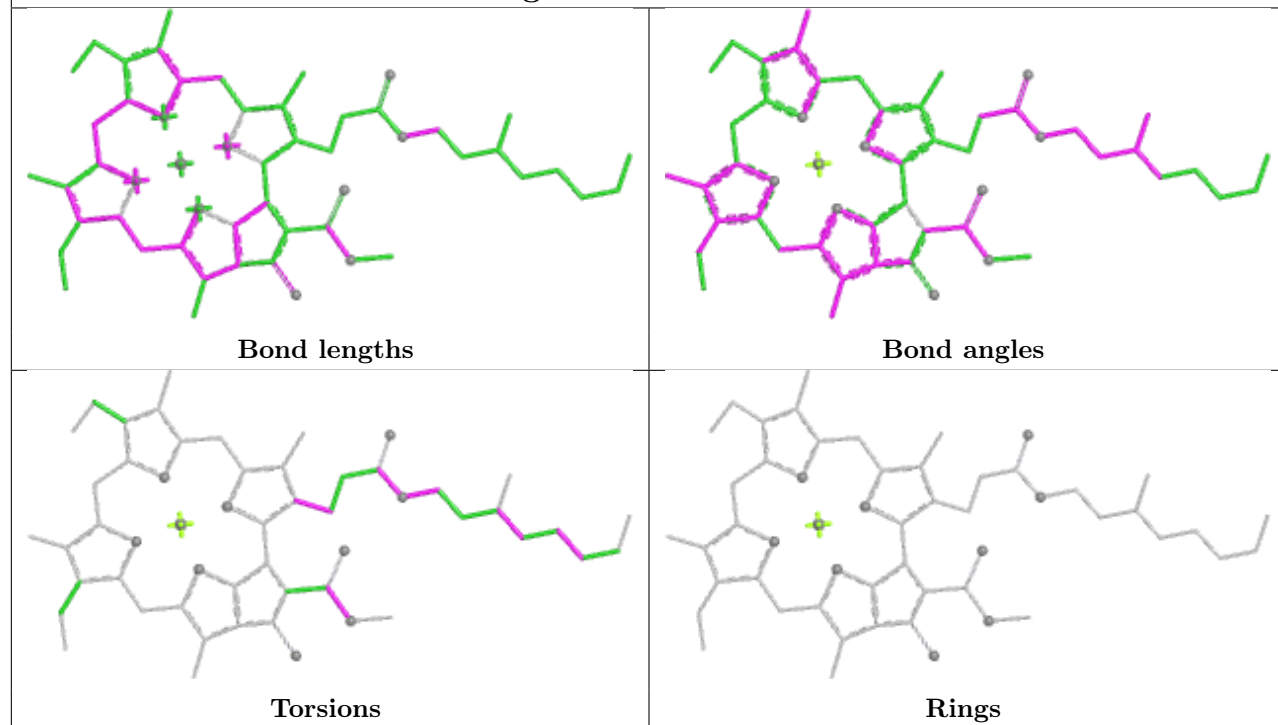
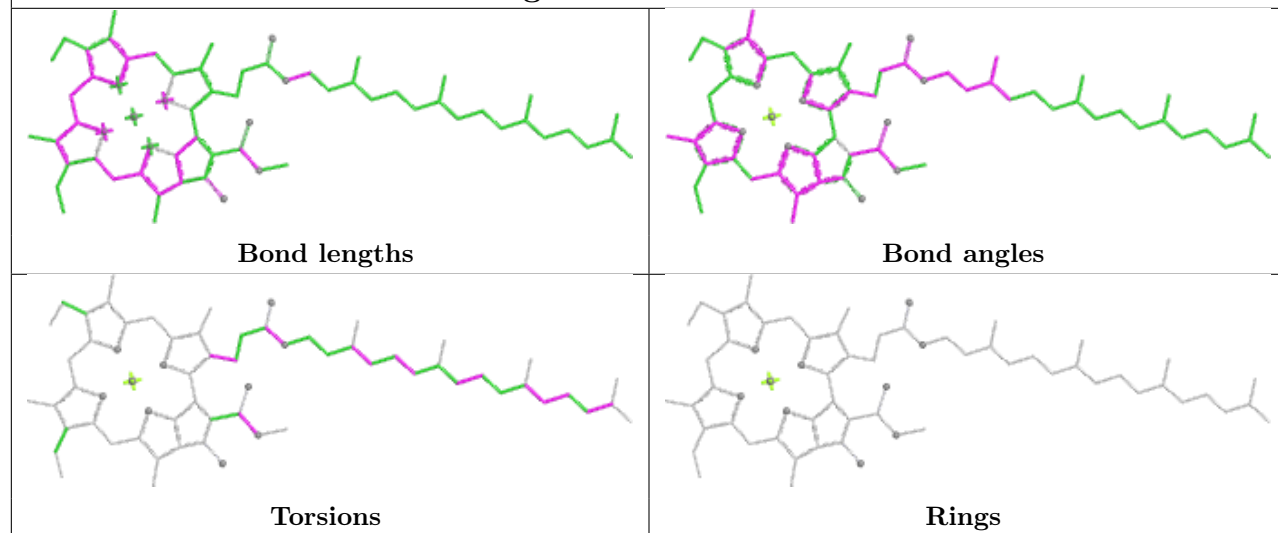
Torsions

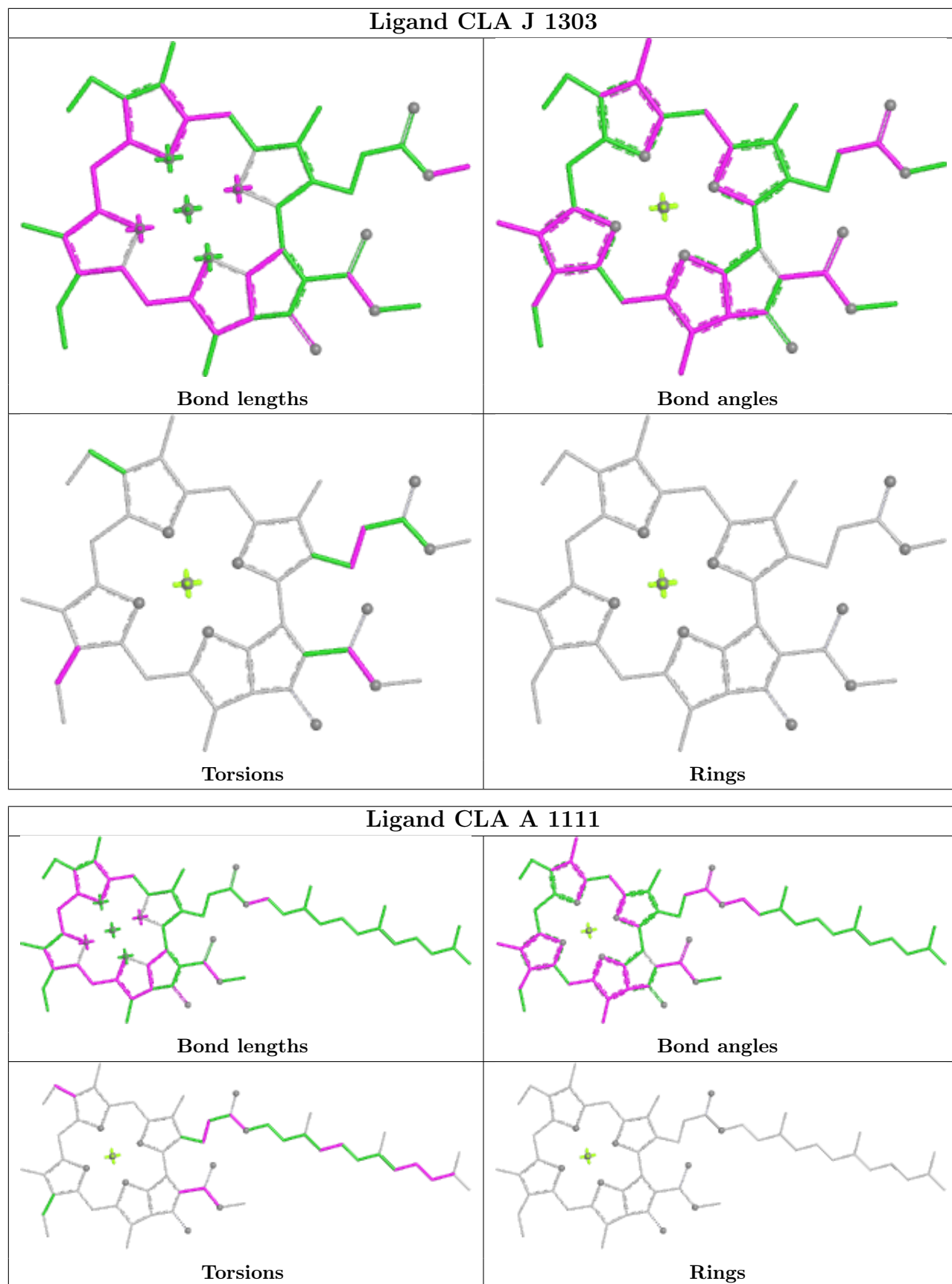


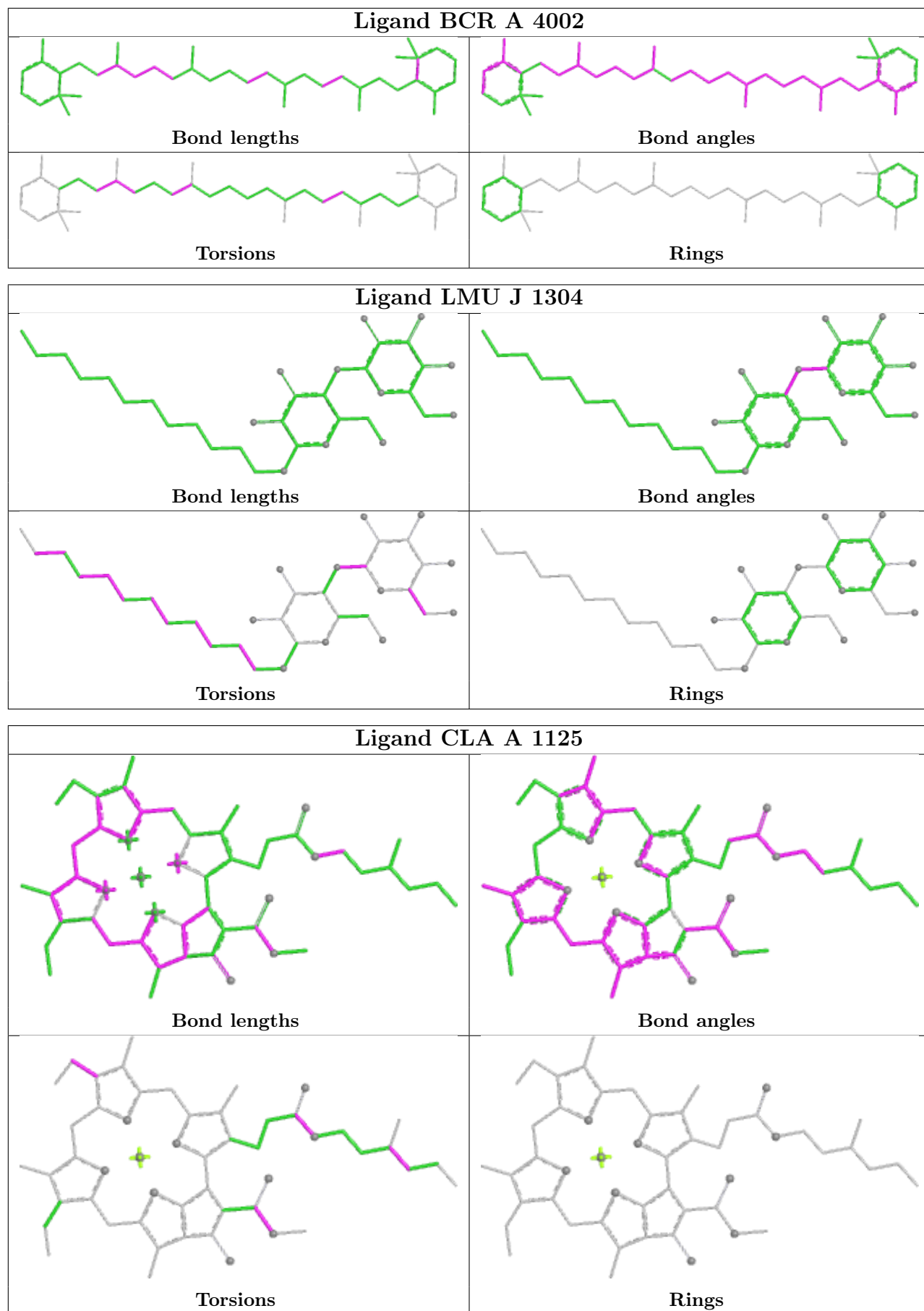
Rings

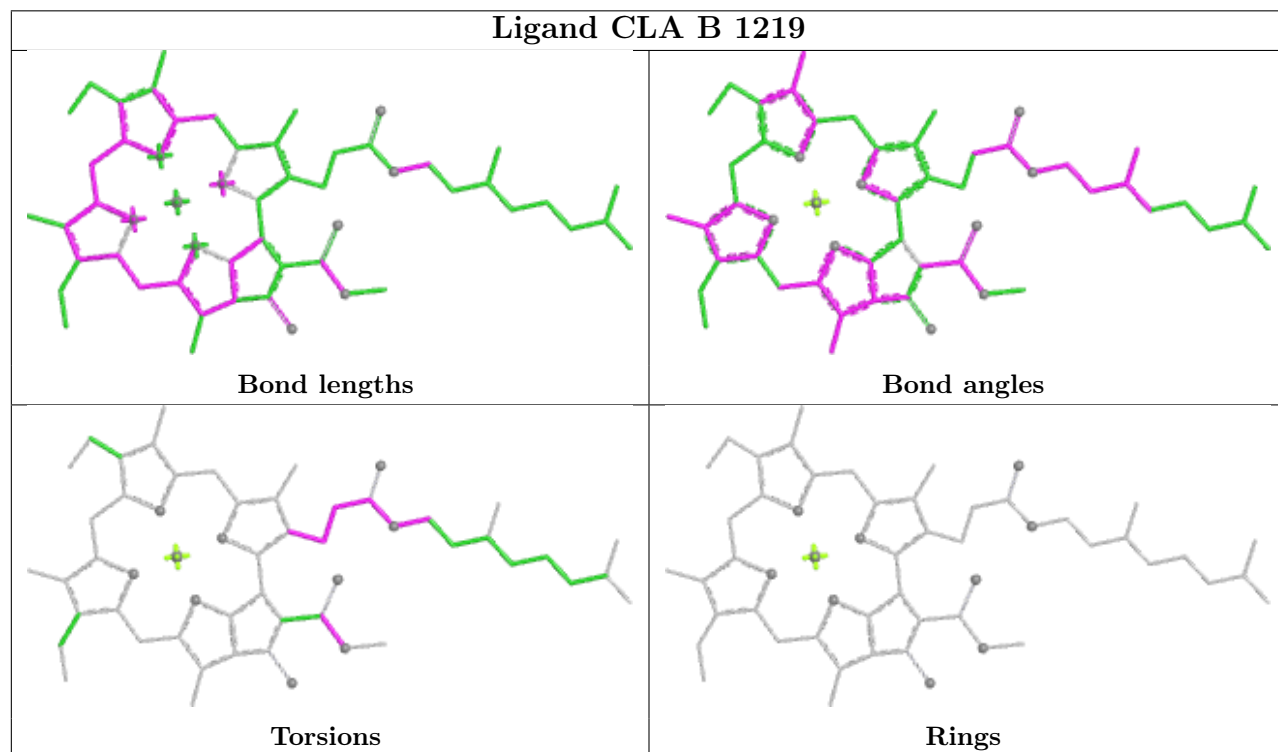
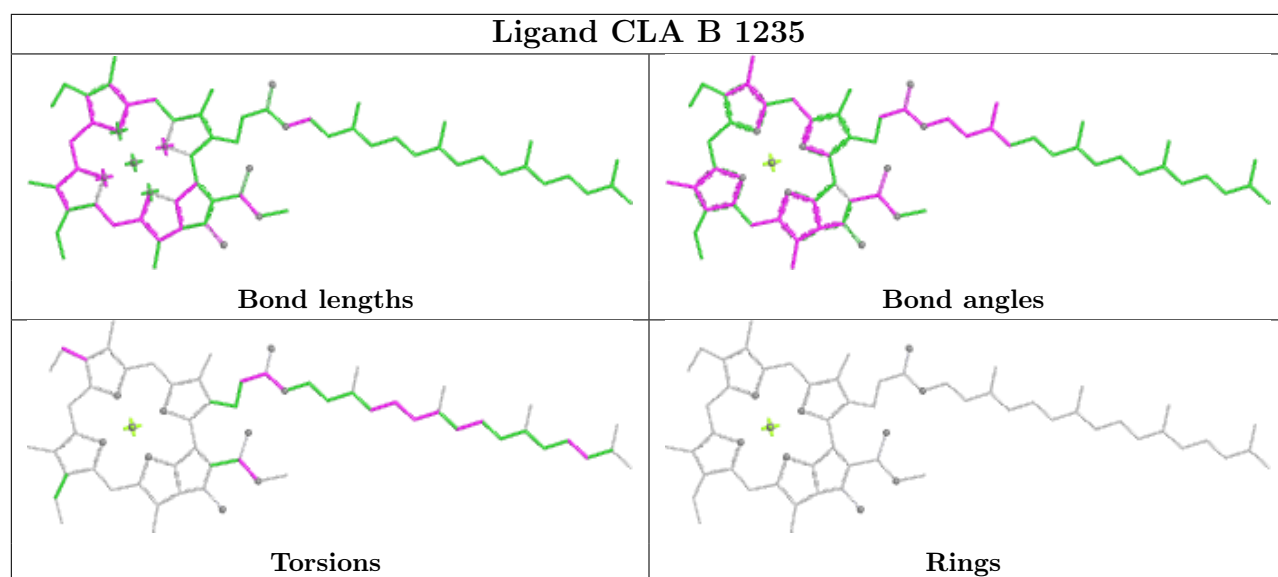


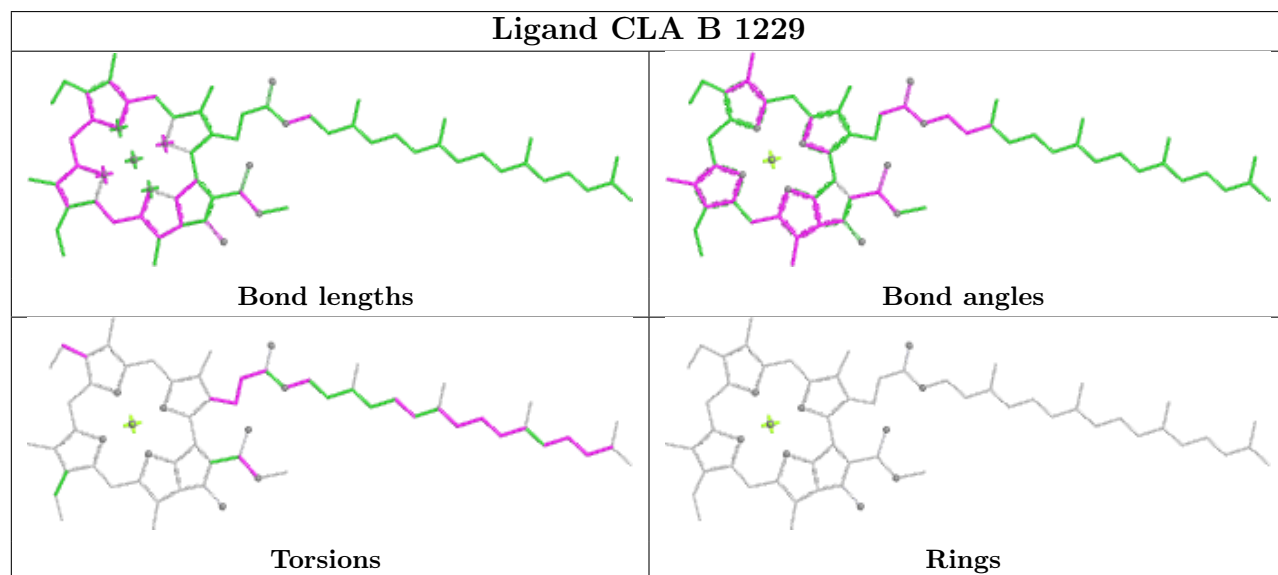
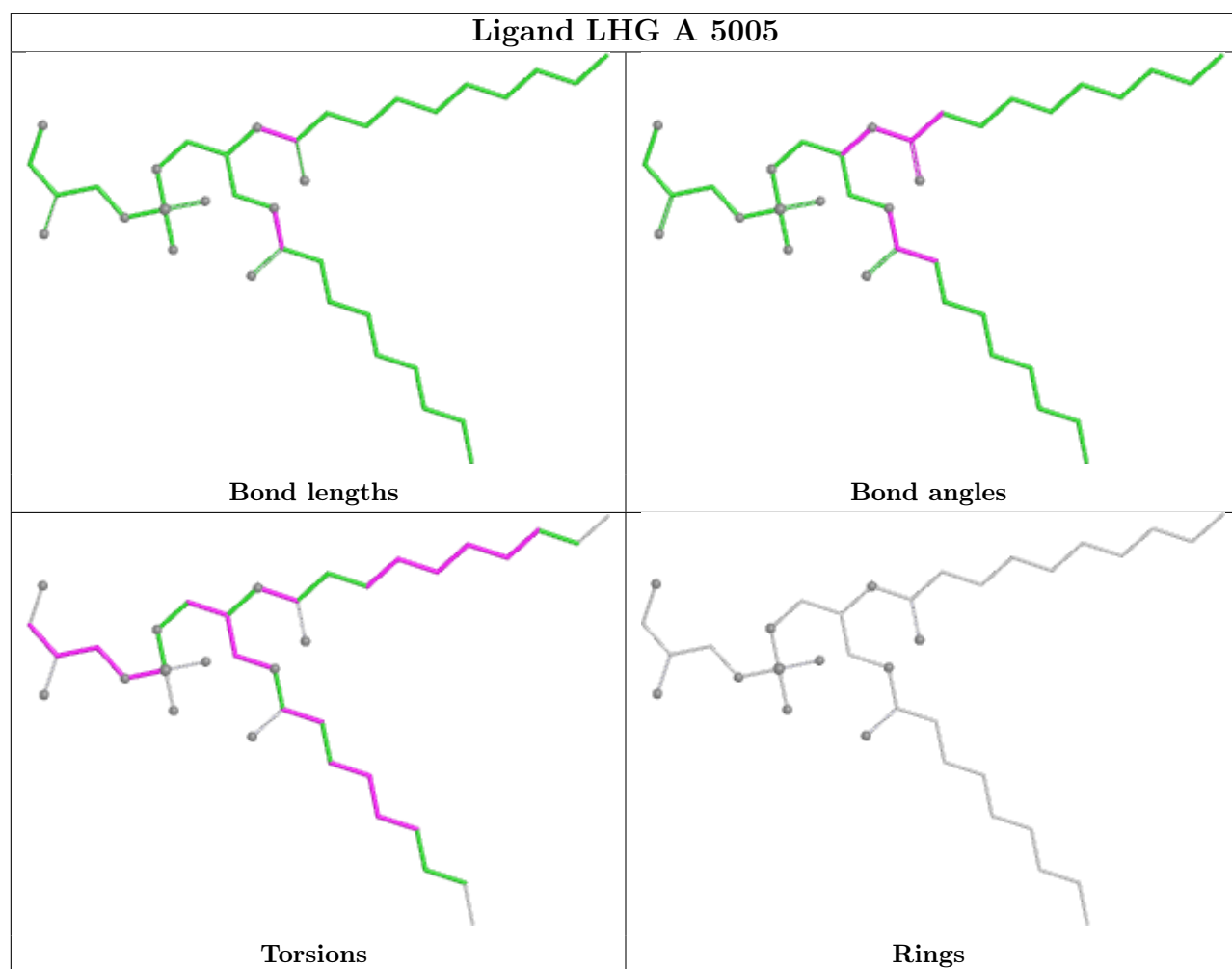
Ligand CLA A 1101**Ligand CLA B 1226**

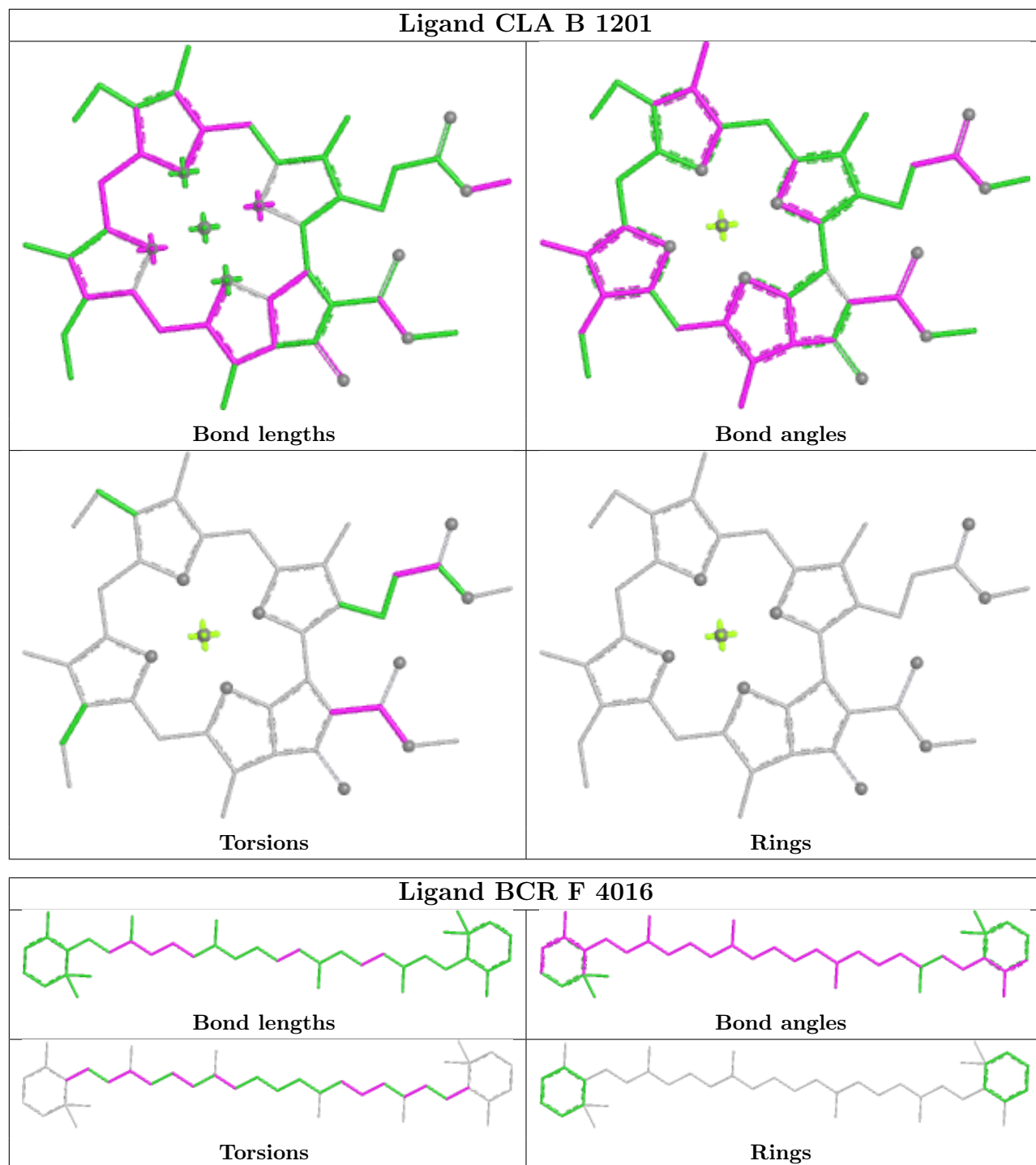
Ligand CLA A 1110**Ligand CLA B 1230**



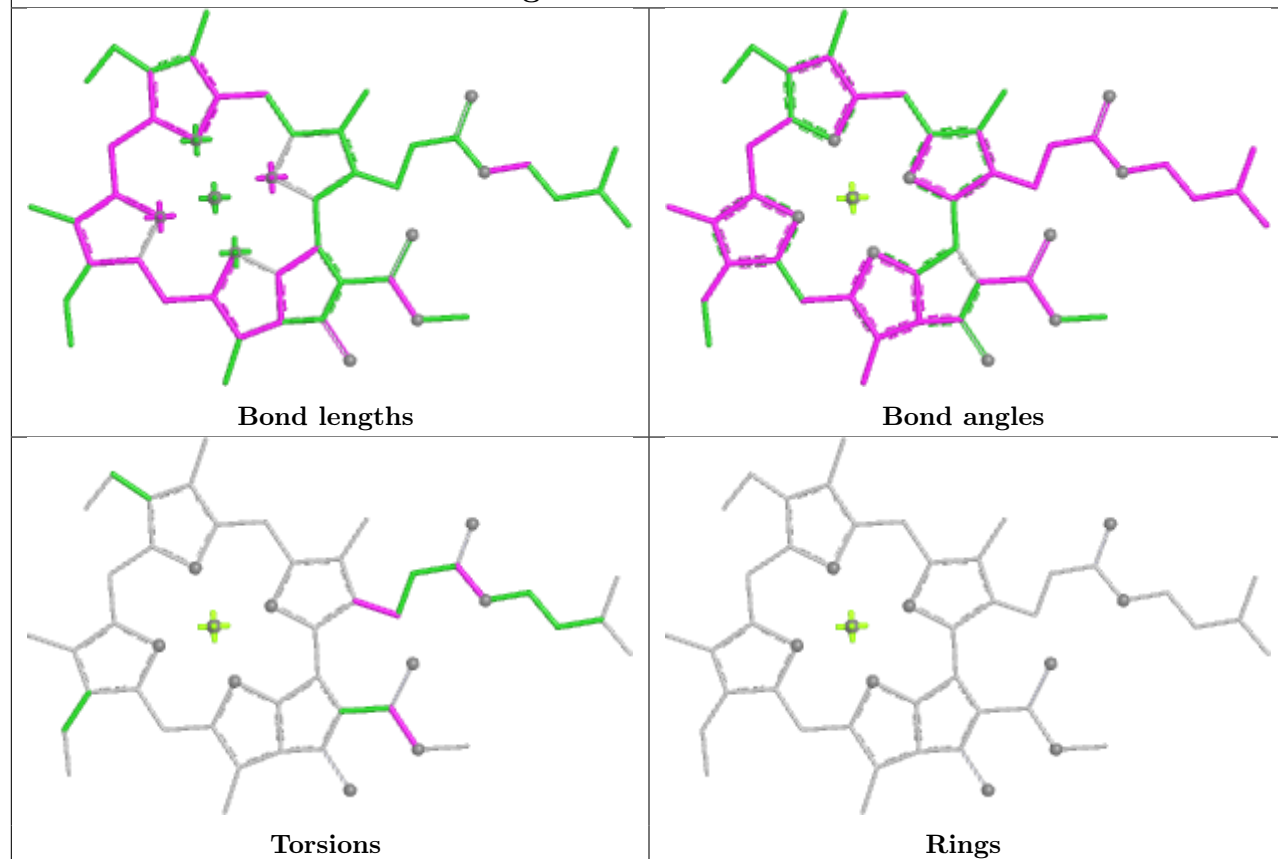




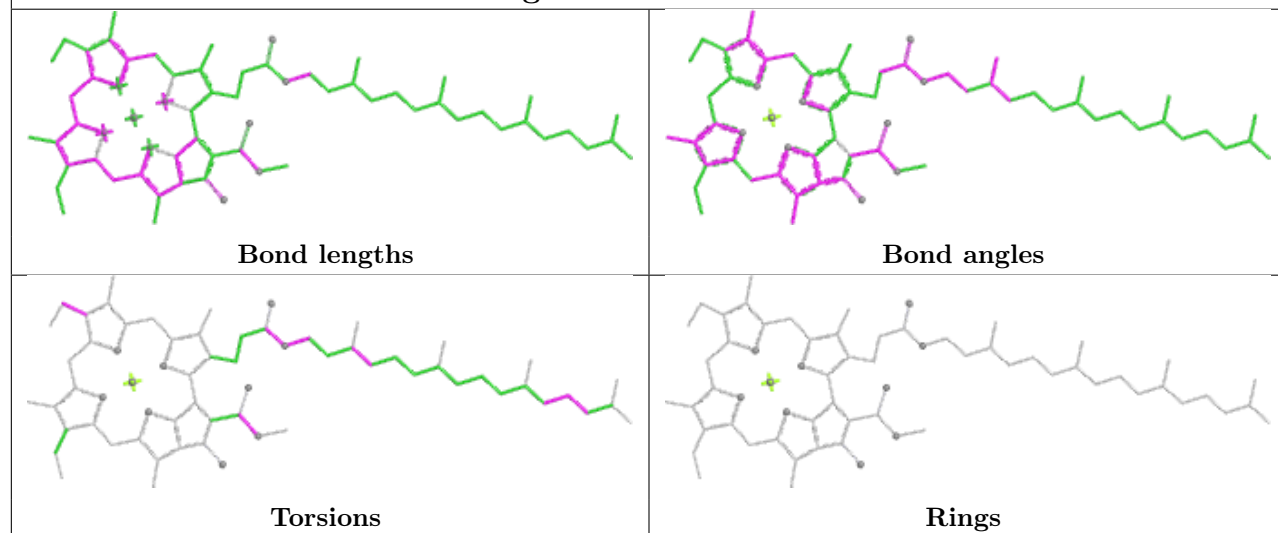




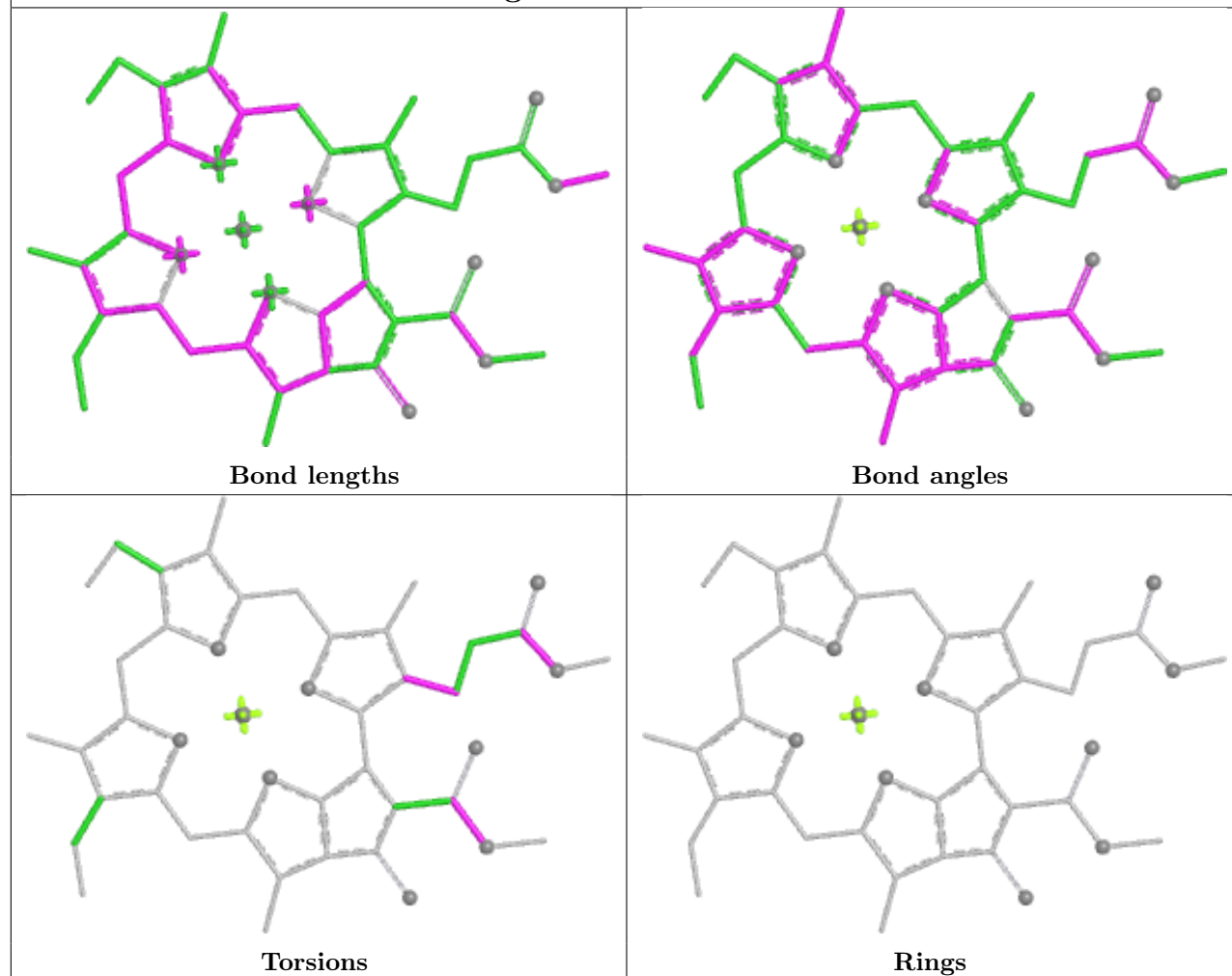
Ligand CLA A 1107



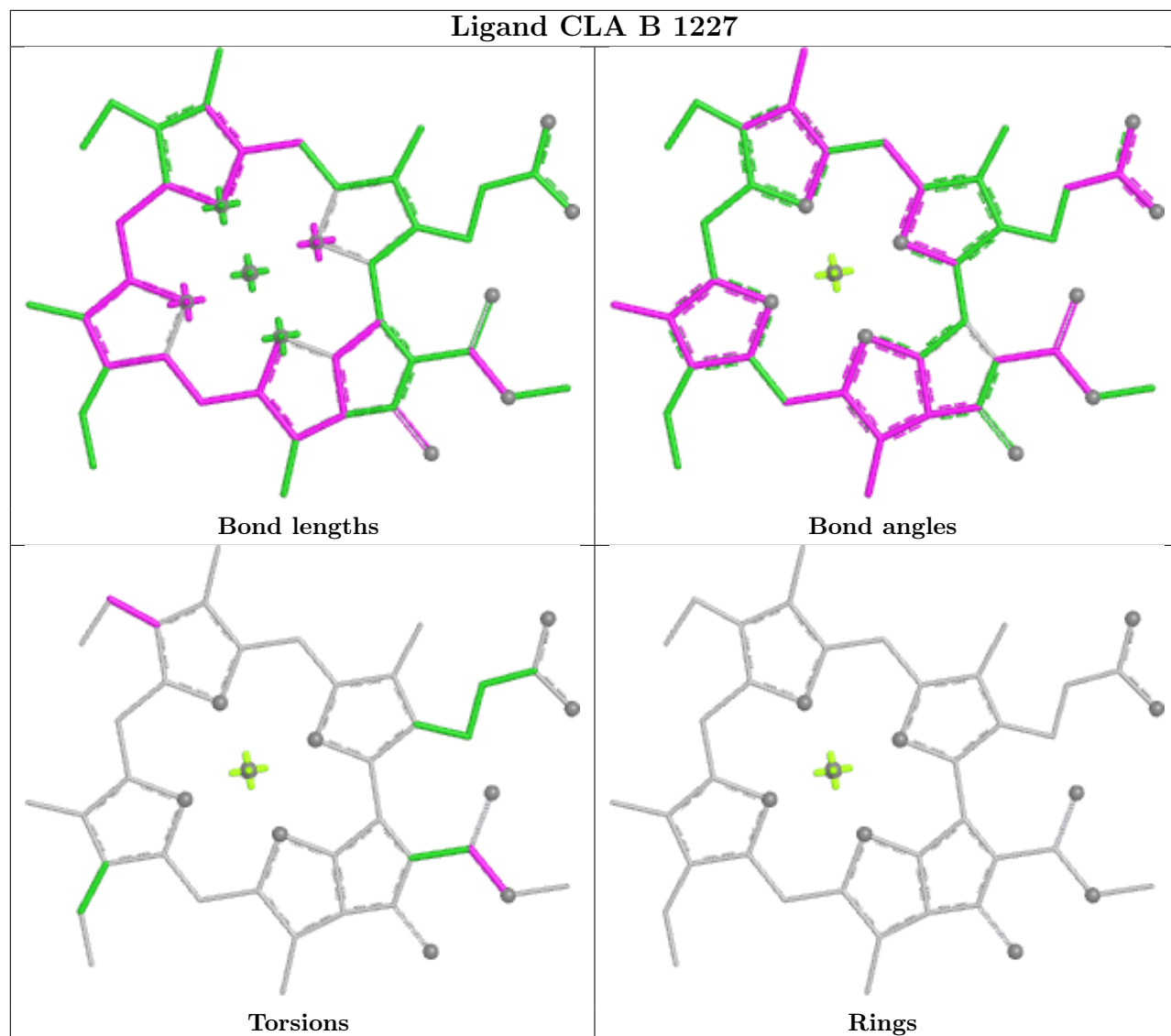
Ligand CLA A 1022



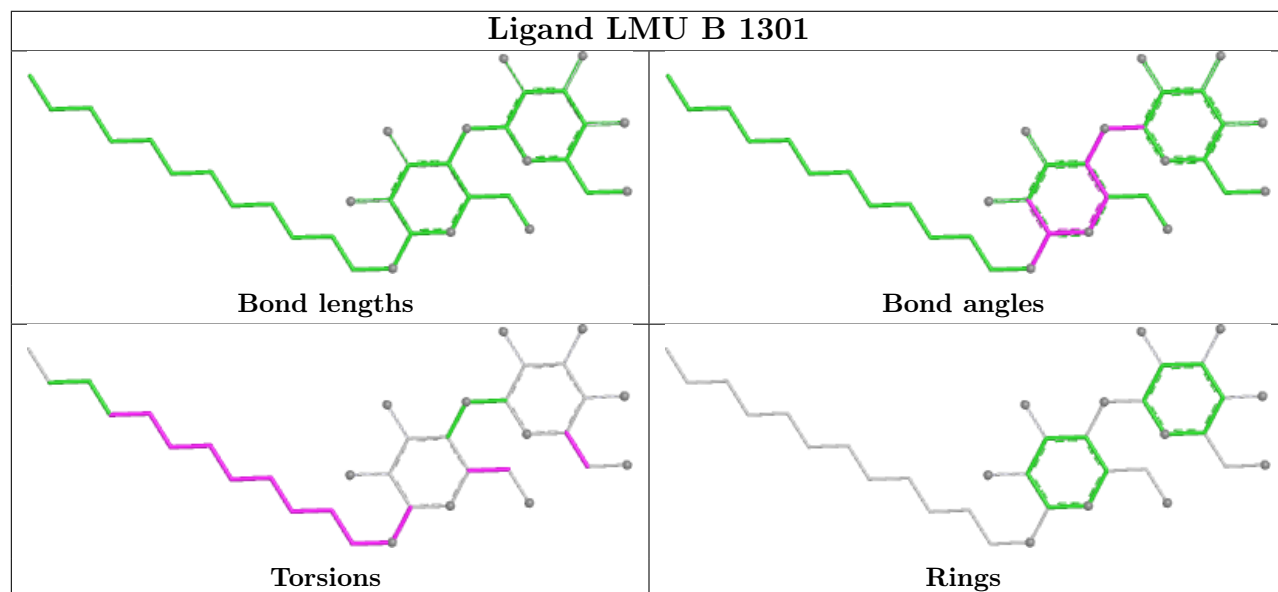
Ligand CLA A 1133

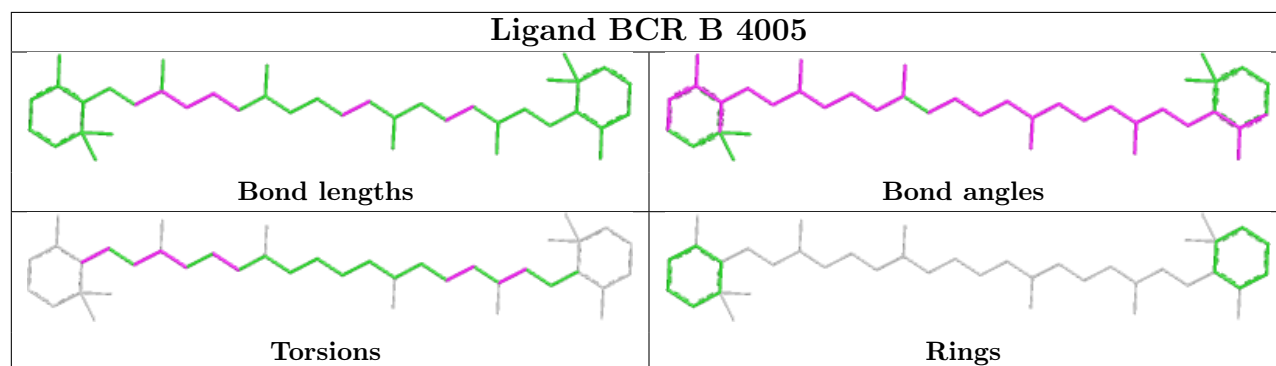
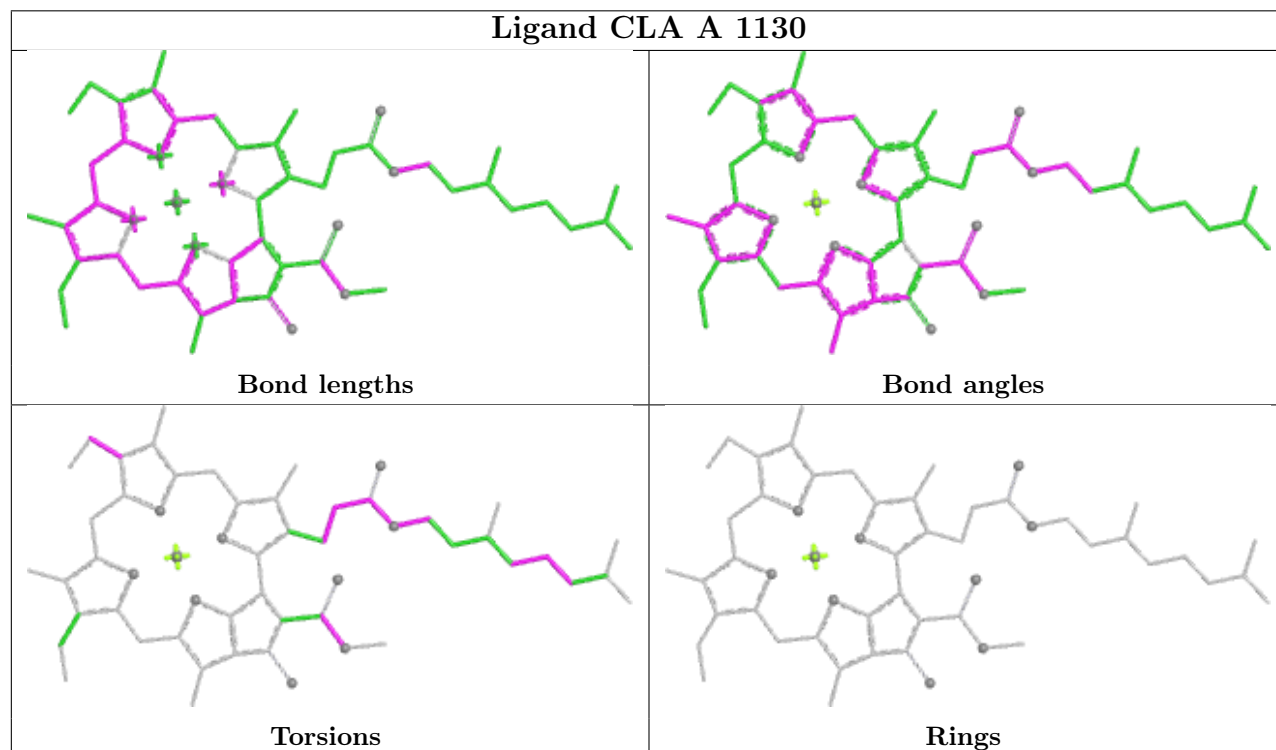
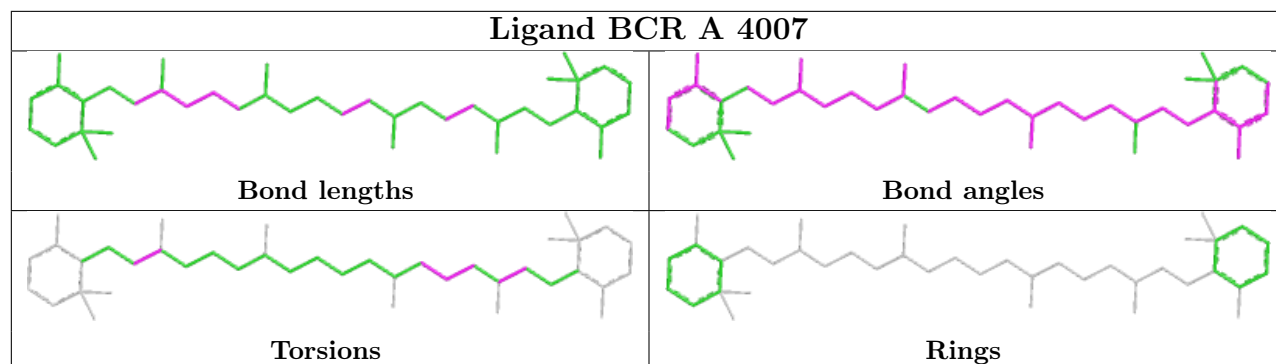


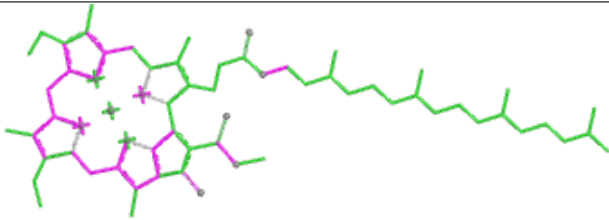
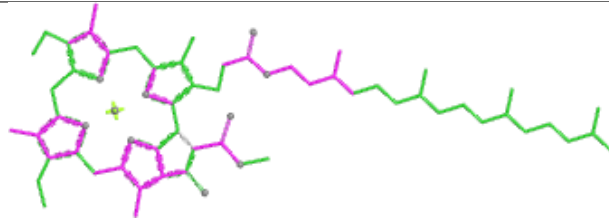
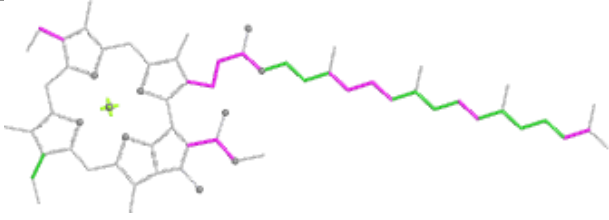
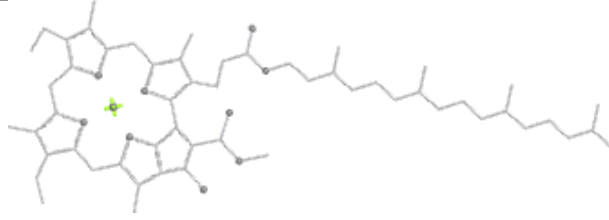
Ligand CLA B 1227

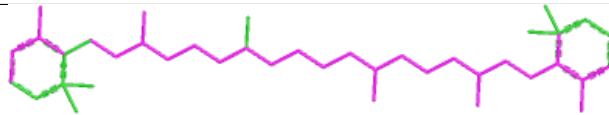
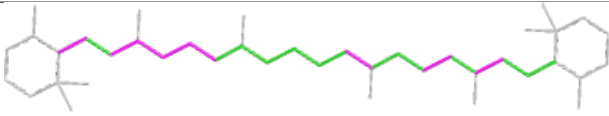
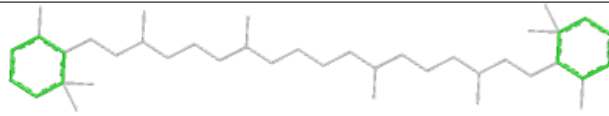


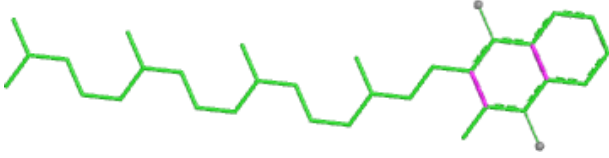
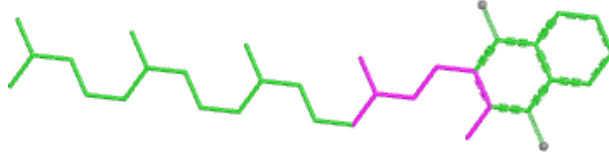
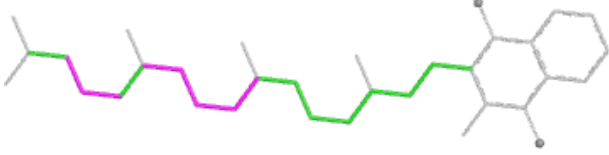
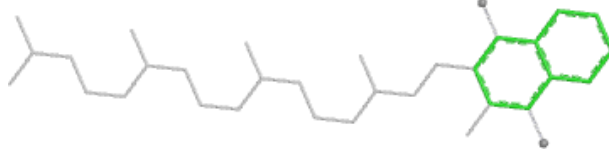
Ligand LMU B 1301

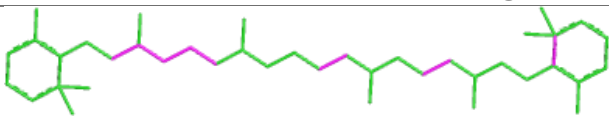
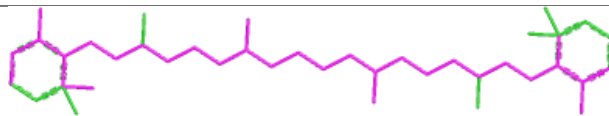
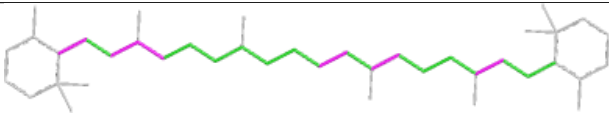
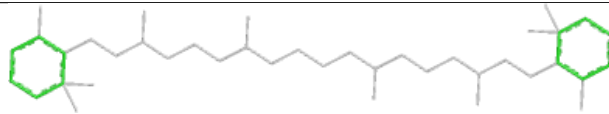


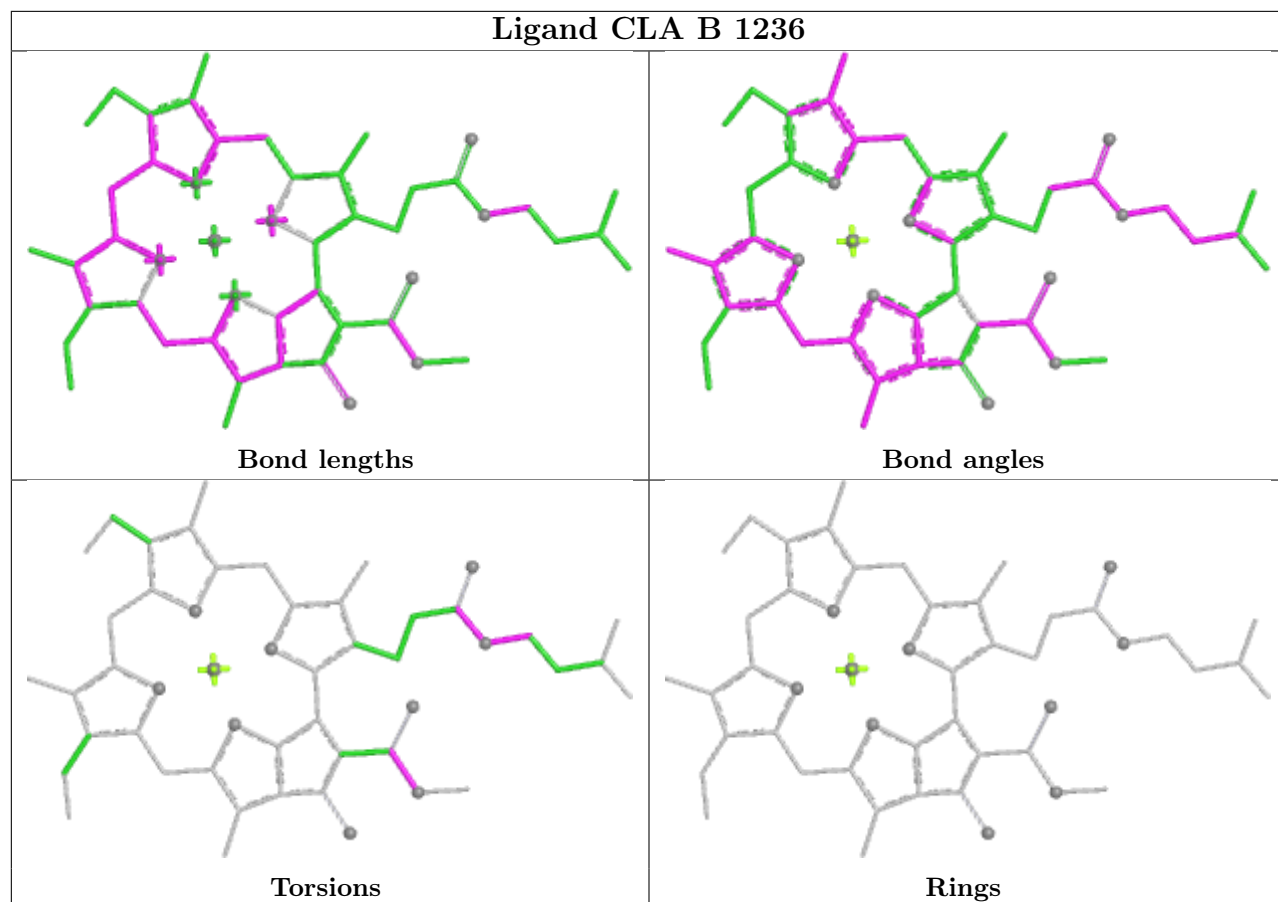


Ligand CLA A 1140	
	
Bond lengths	Bond angles
	
Torsions	Rings

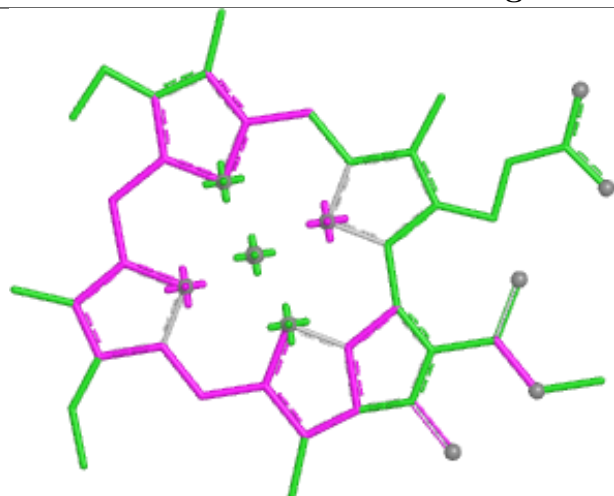
Ligand BCR B 4009	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand PQN A 2001	
	
Bond lengths	Bond angles
	
Torsions	Rings

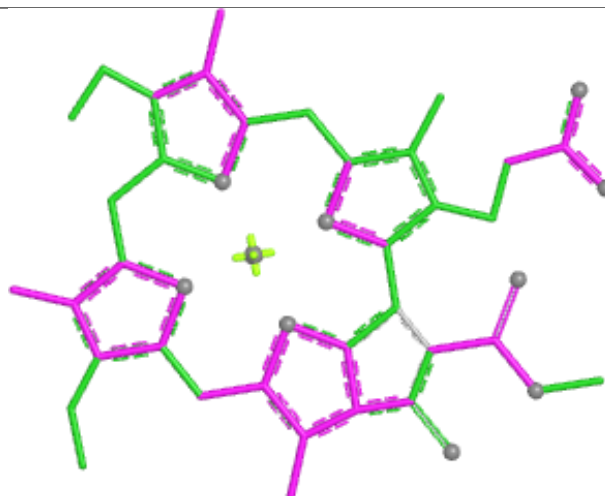
Ligand BCR F 4015	
	
Bond lengths	Bond angles
	
Torsions	Rings



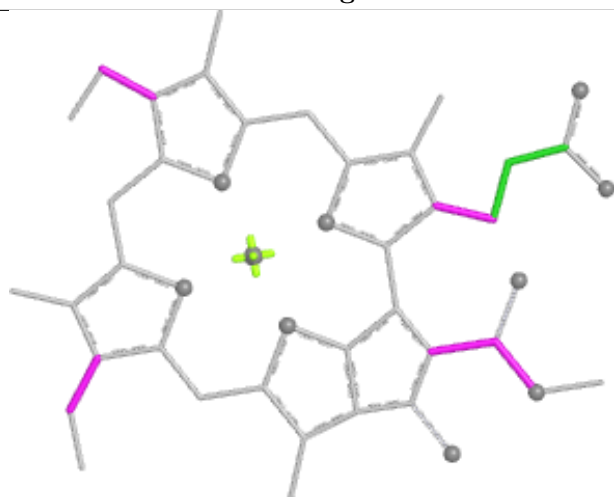
Ligand CLA B 1212



Bond lengths



Bond angles

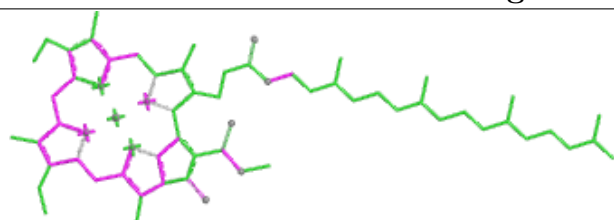


Torsions

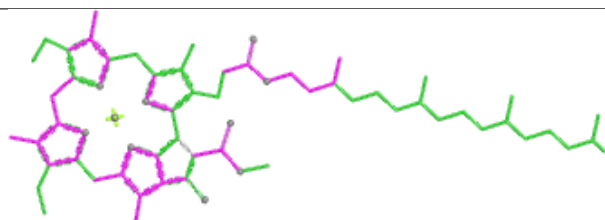


Rings

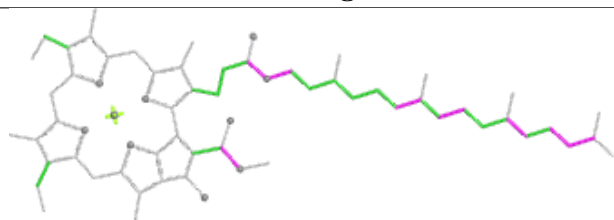
Ligand CLA F 1139



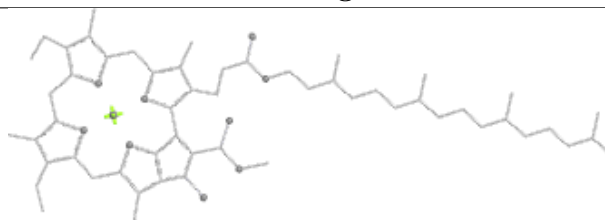
Bond lengths



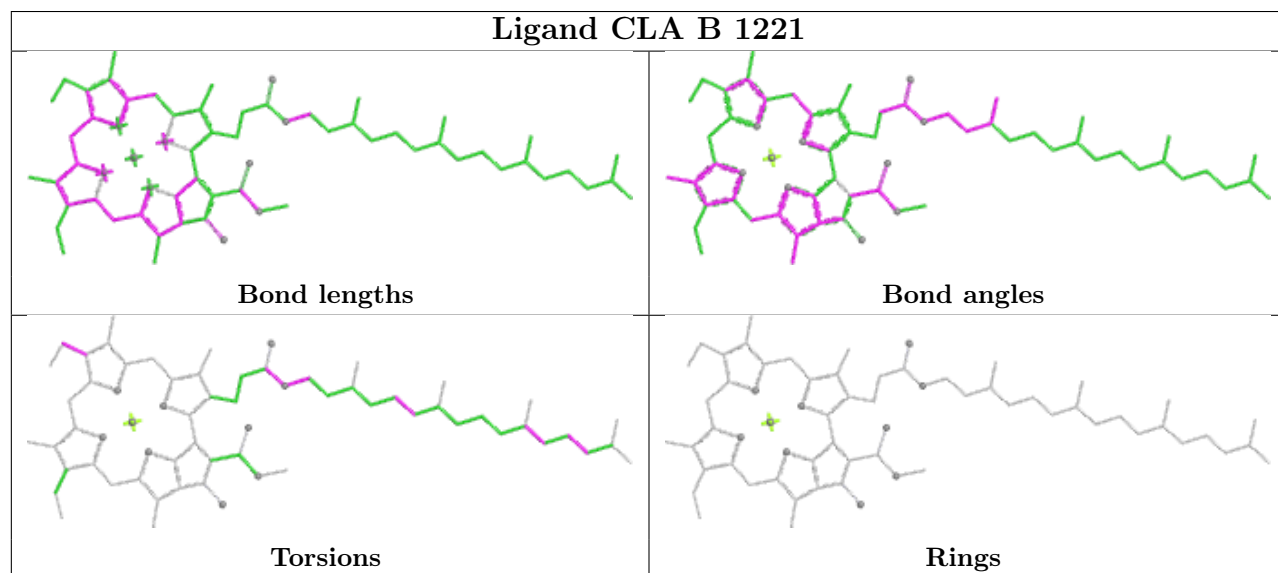
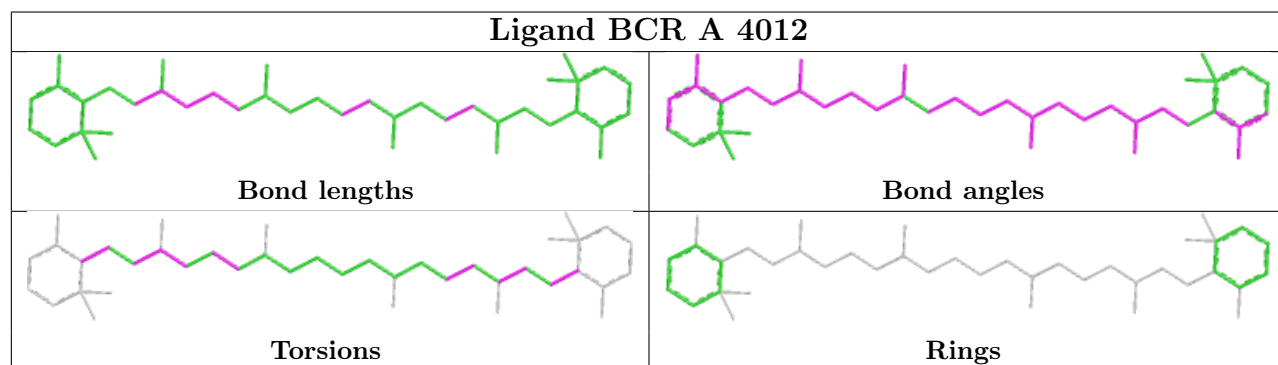
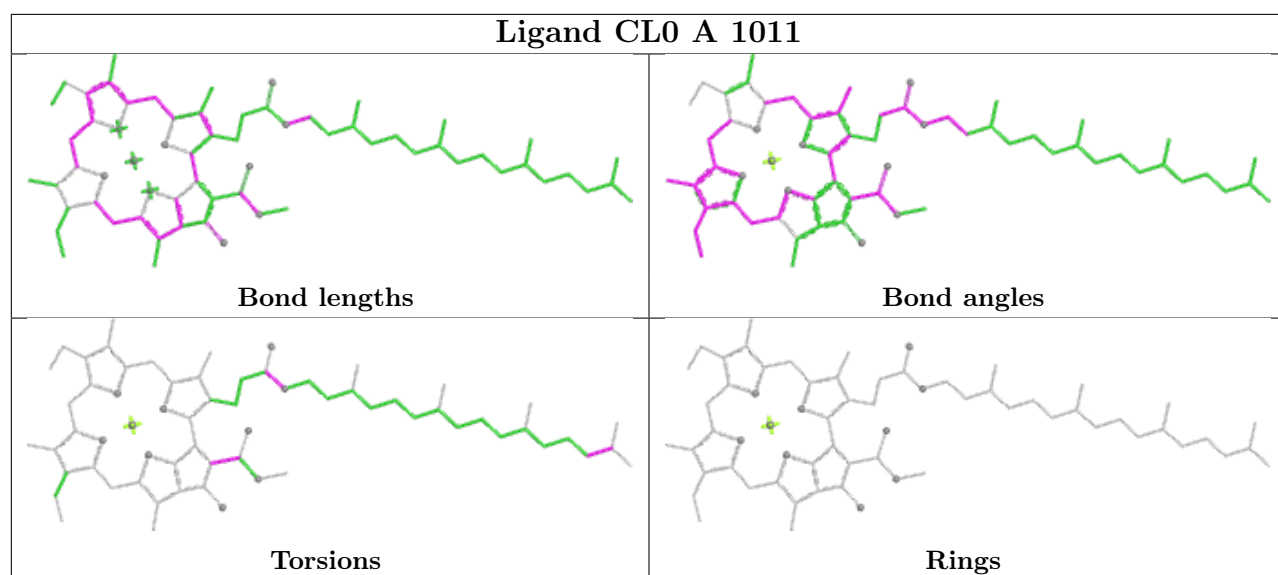
Bond angles



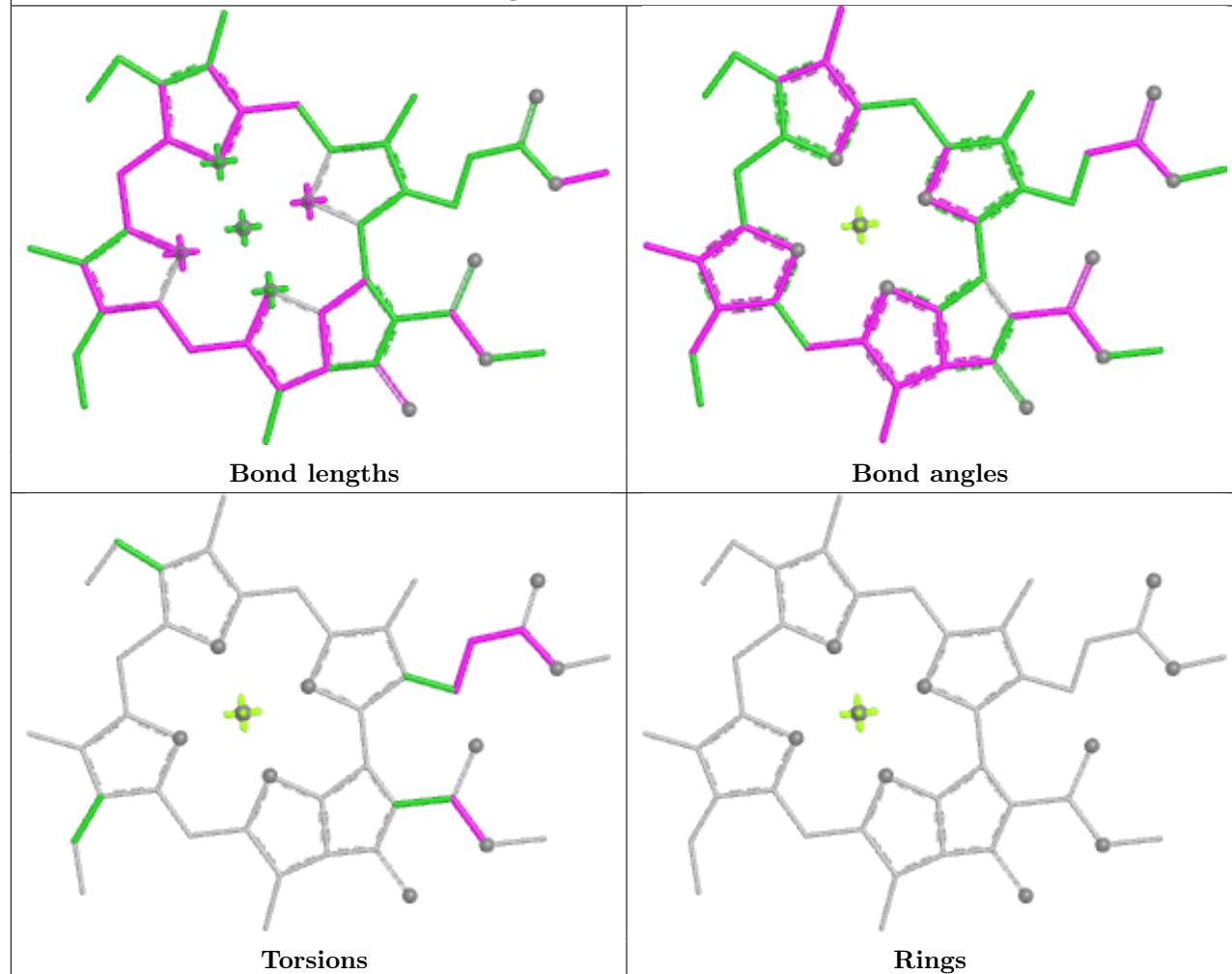
Torsions



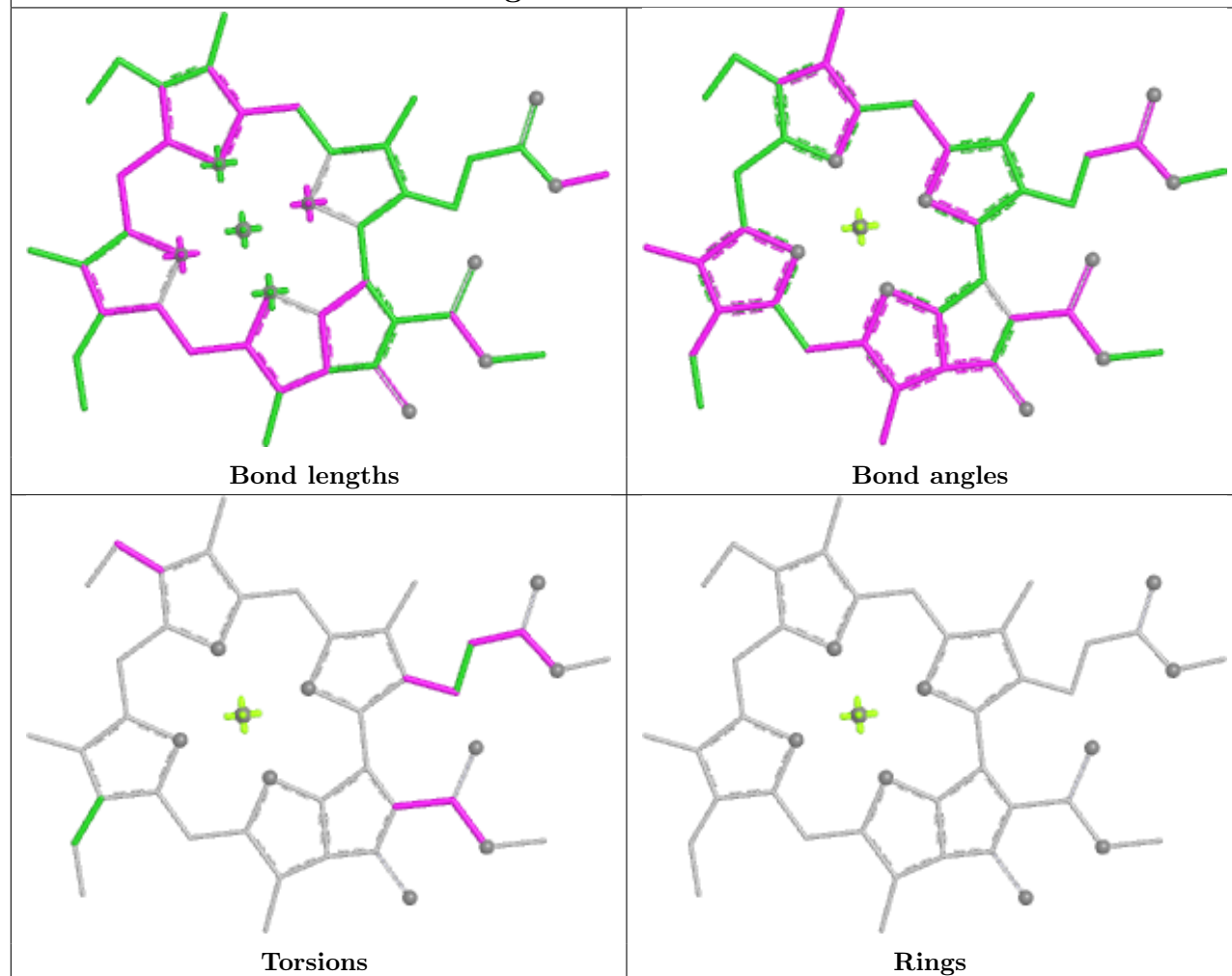
Rings

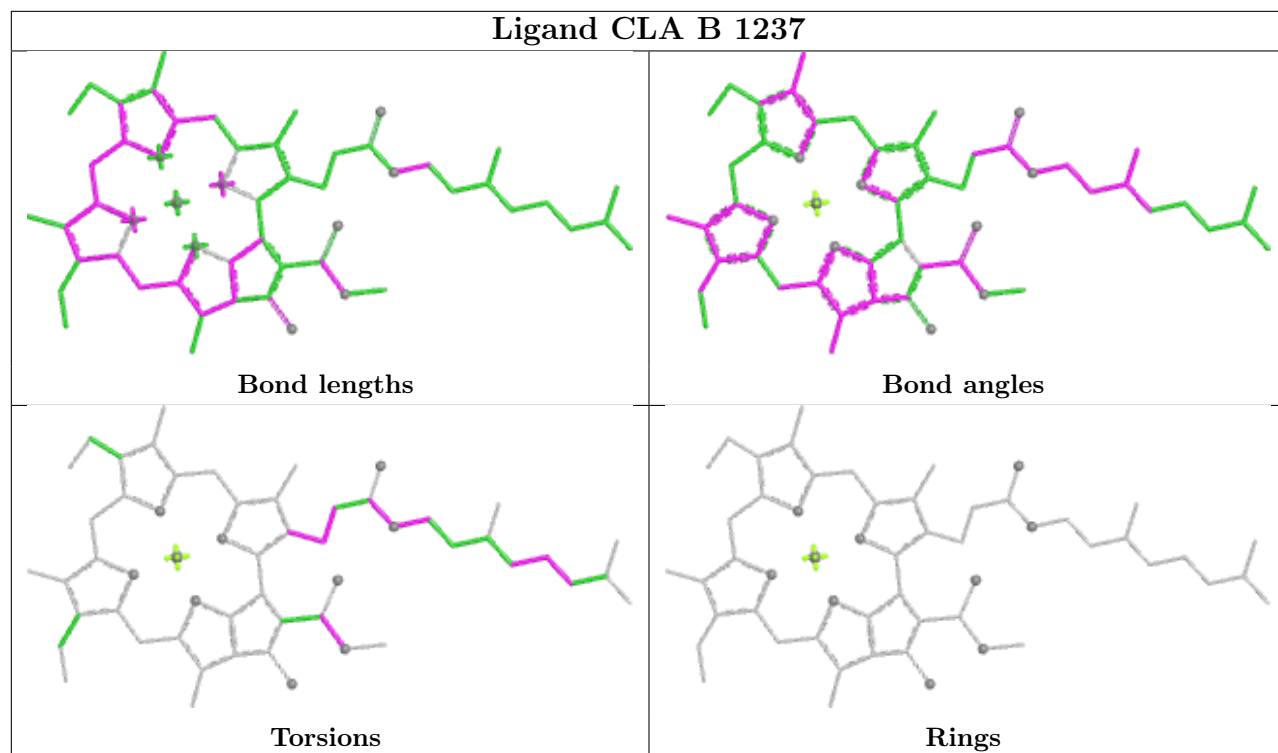


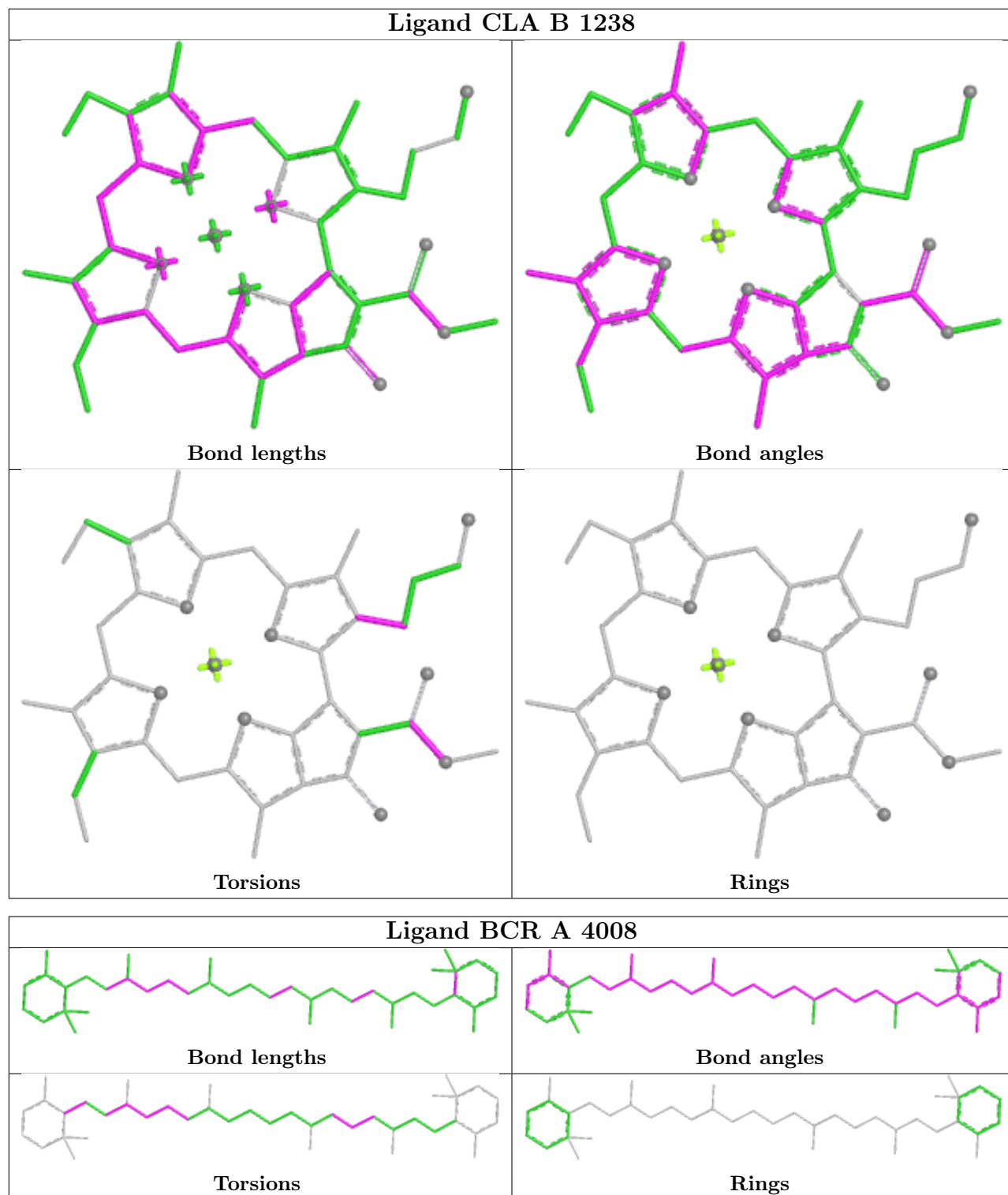
Ligand CLA A 1115



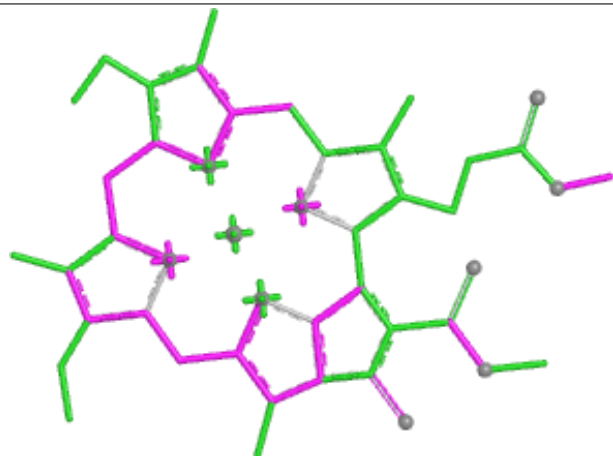
Ligand CLA A 1129



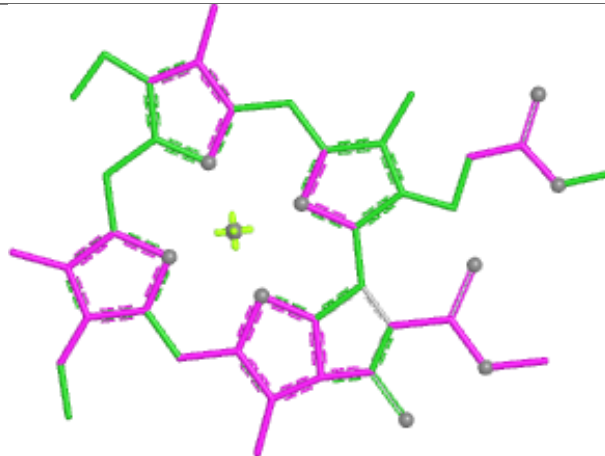




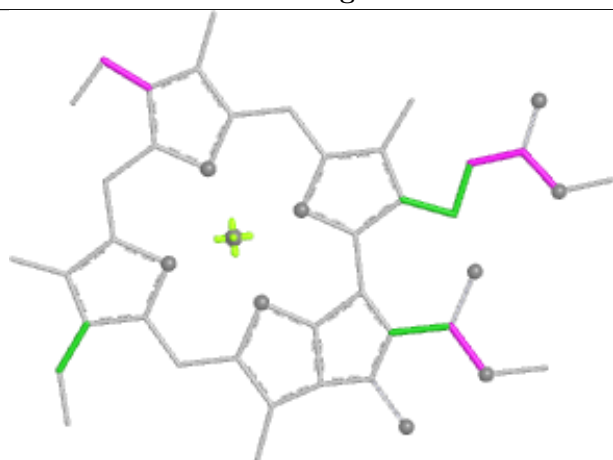
Ligand CLA K 1402



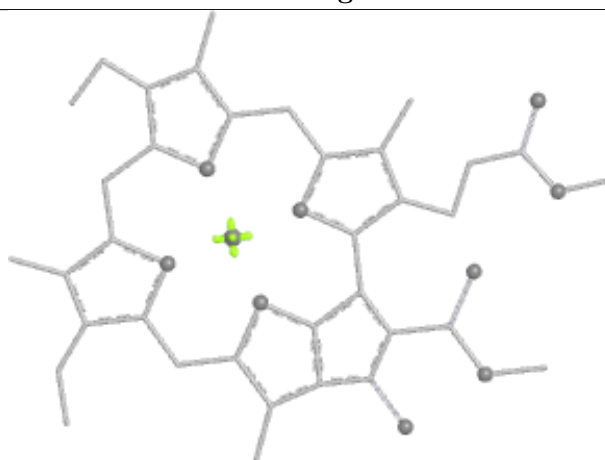
Bond lengths



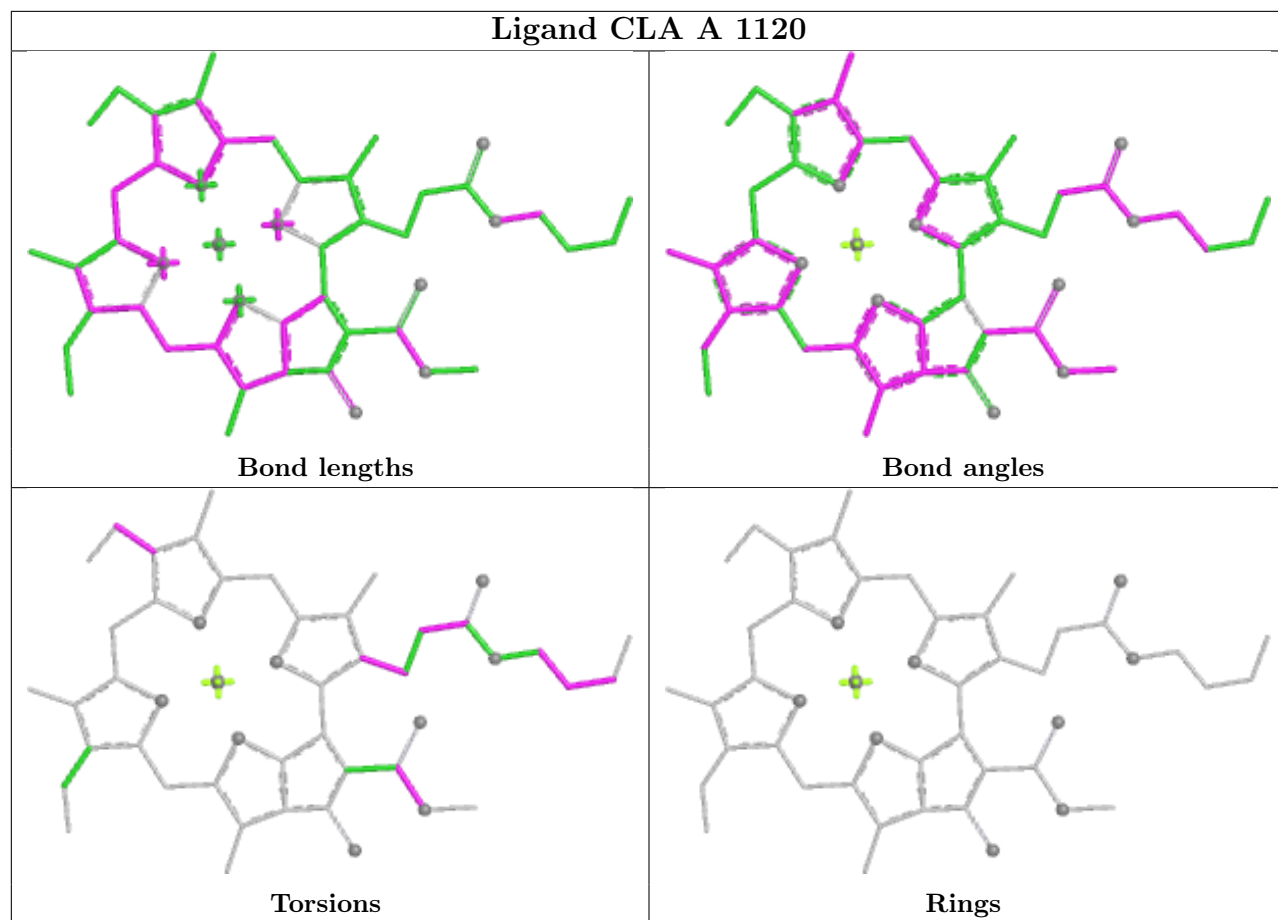
Bond angles



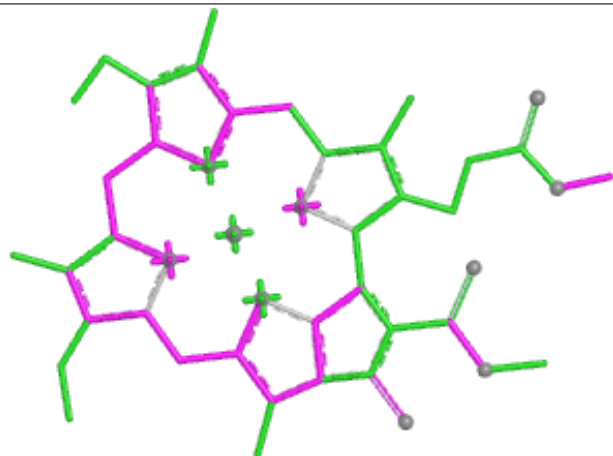
Torsions



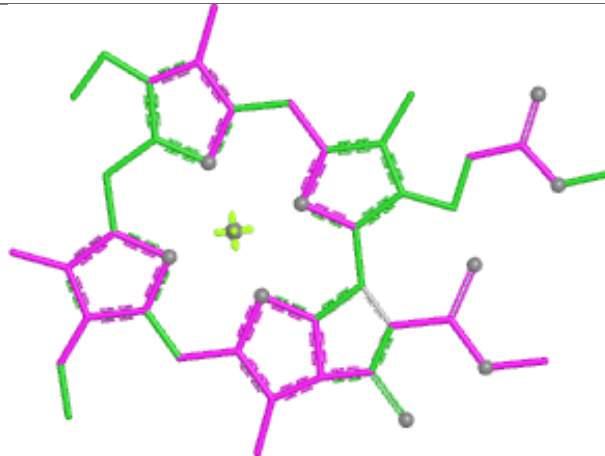
Rings



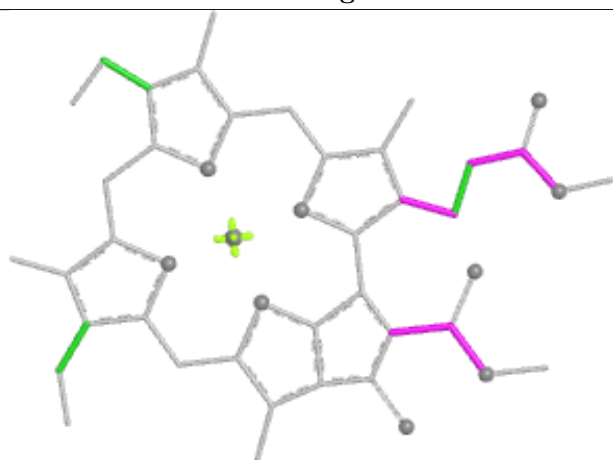
Ligand CLA K 1401



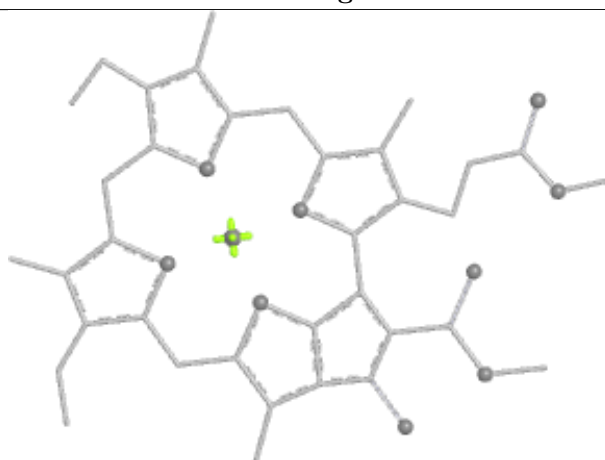
Bond lengths



Bond angles

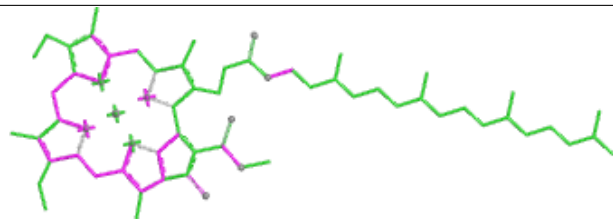


Torsions

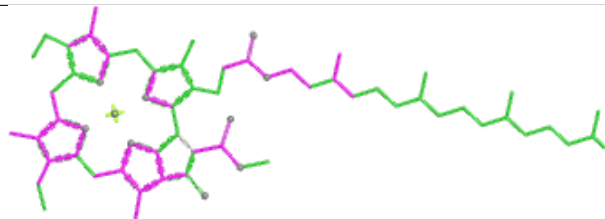


Rings

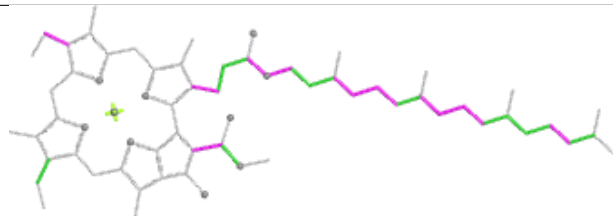
Ligand CLA A 1123



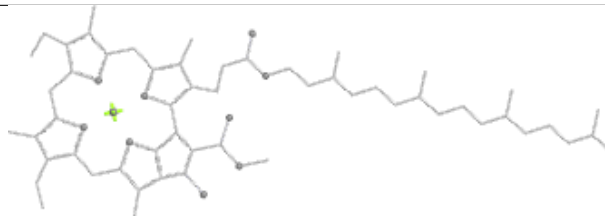
Bond lengths



Bond angles

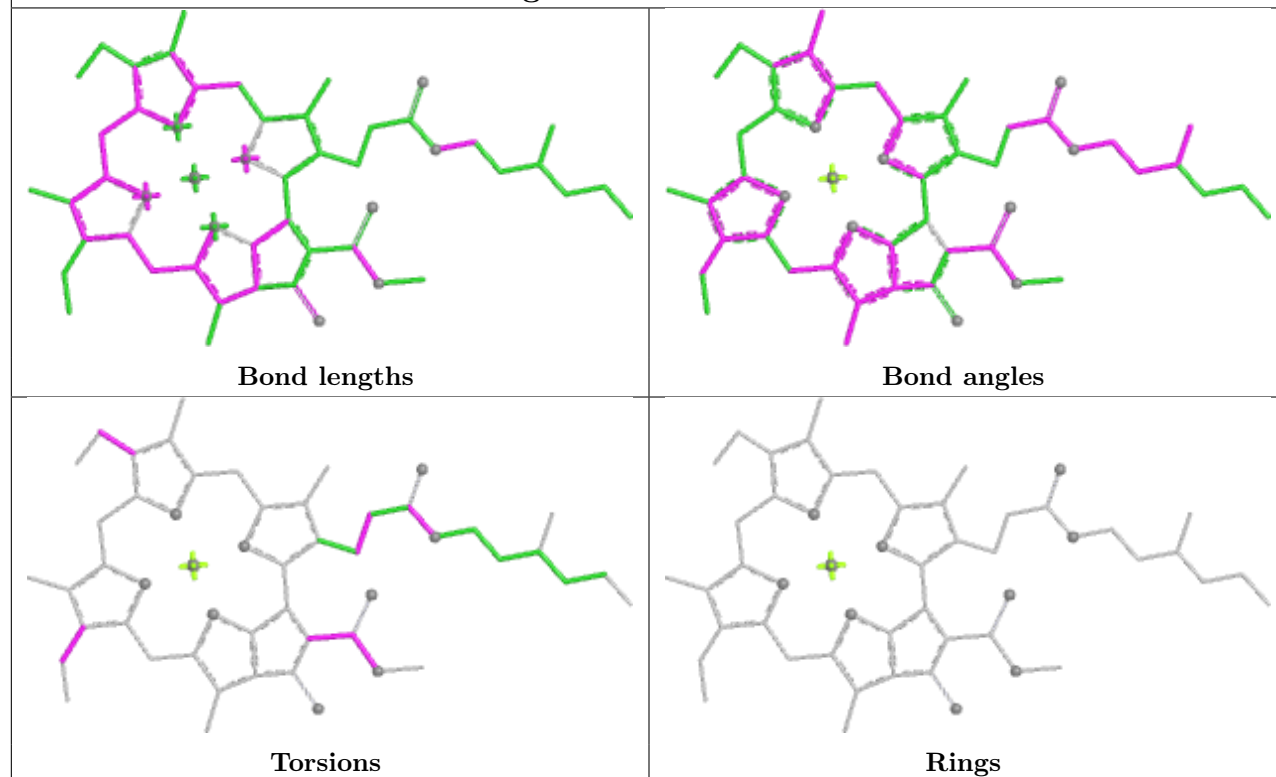


Torsions

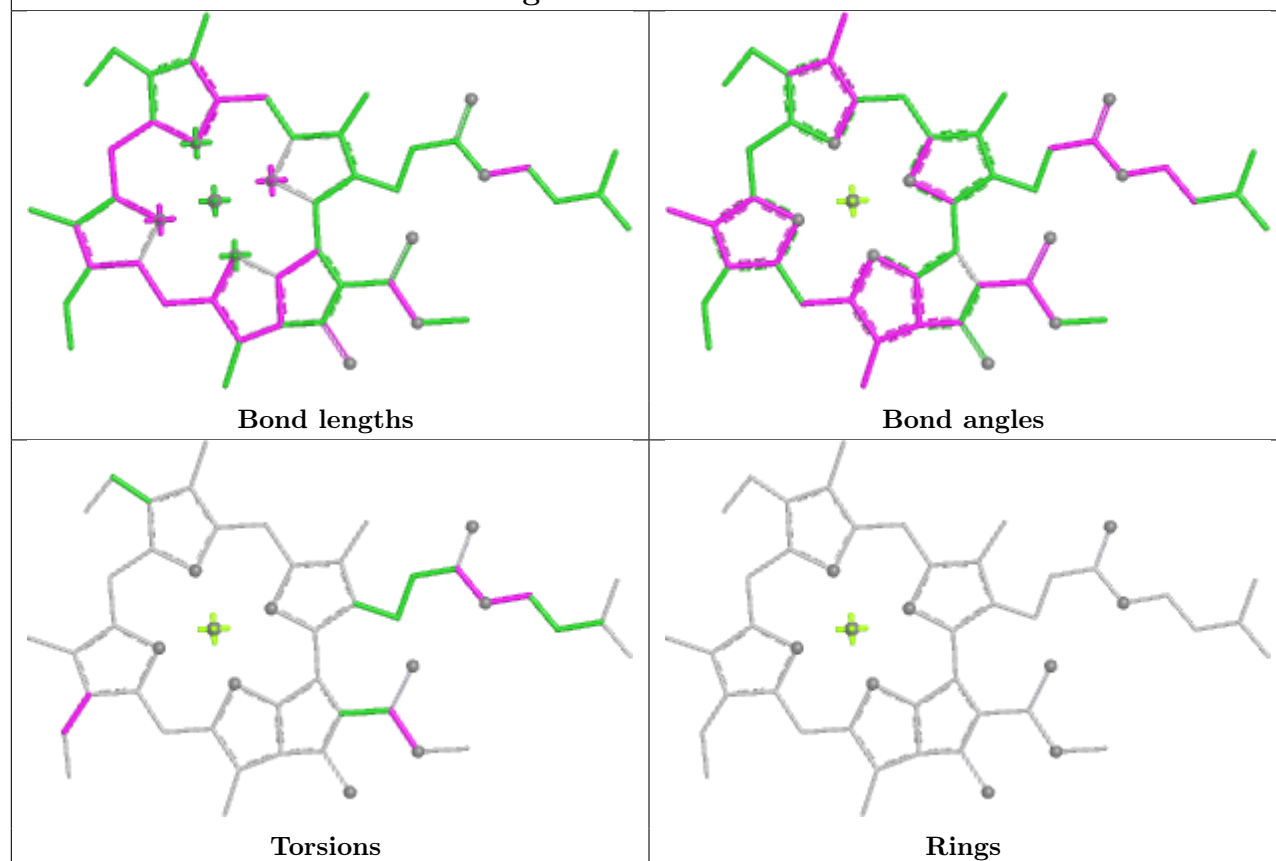


Rings

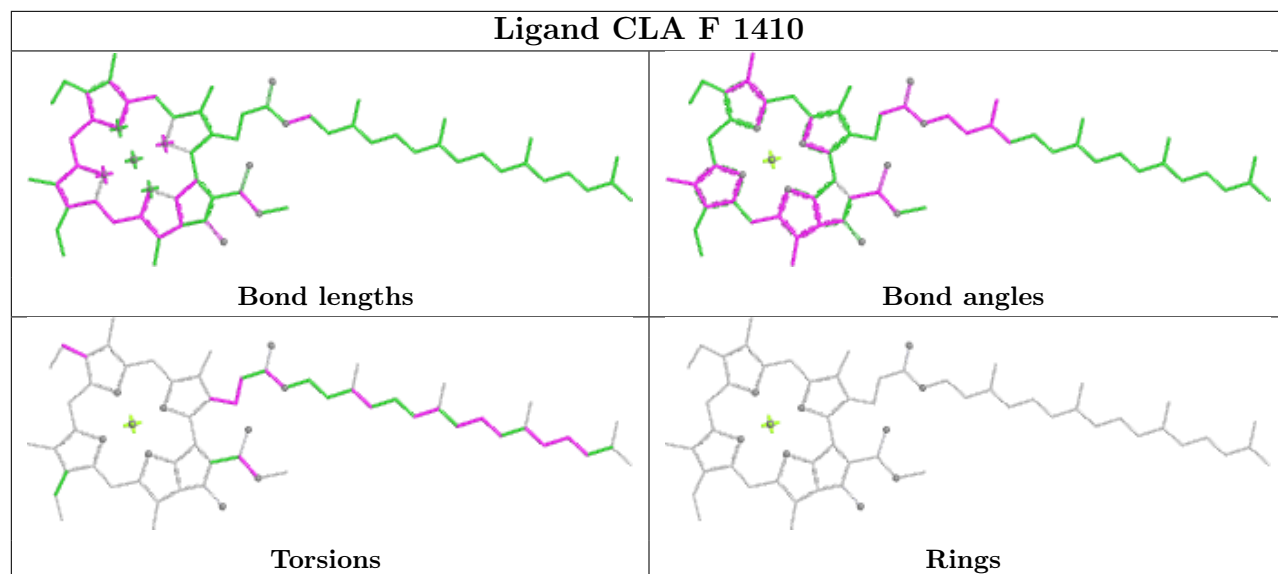
Ligand CLA A 1801



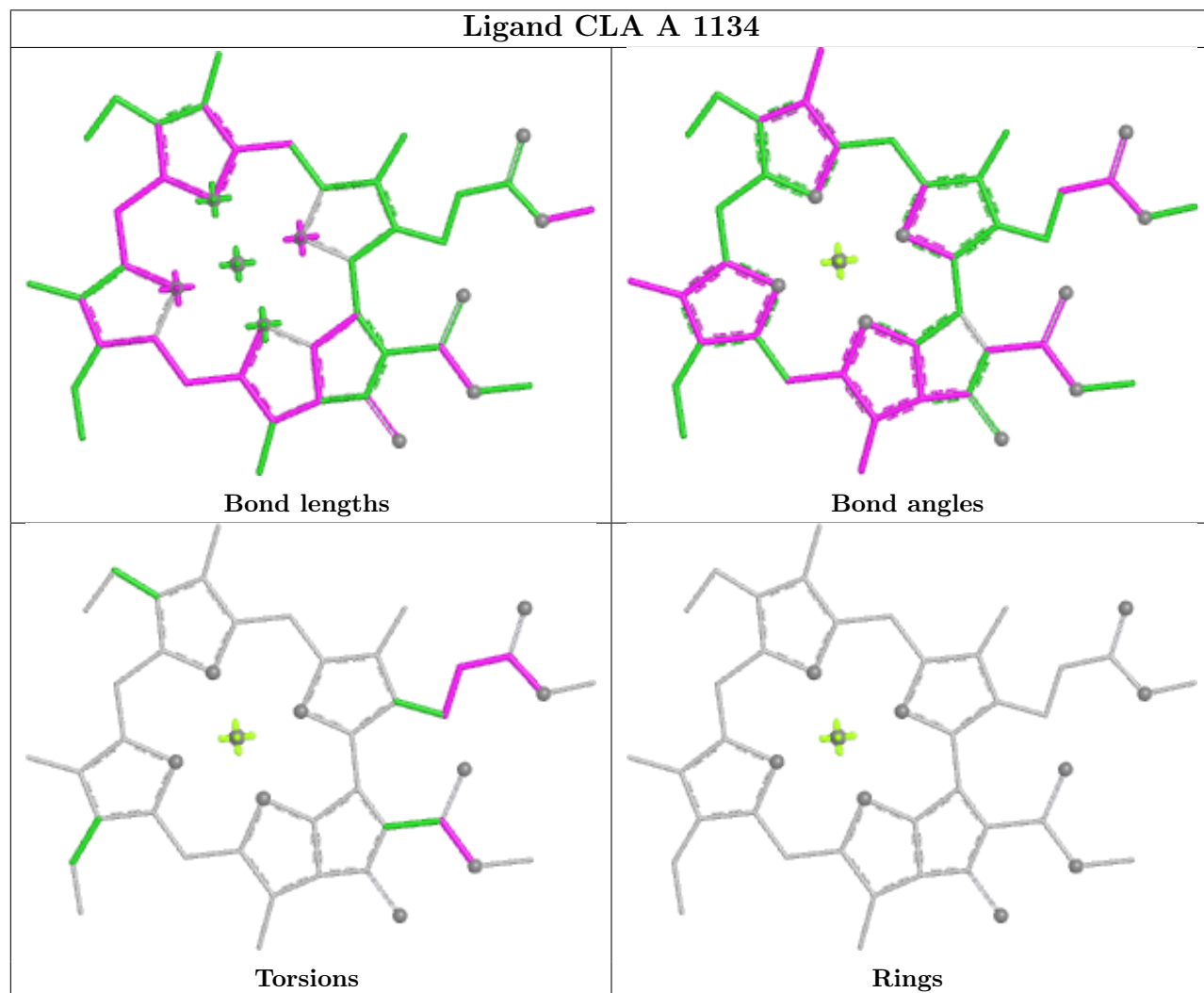
Ligand CLA A 1137



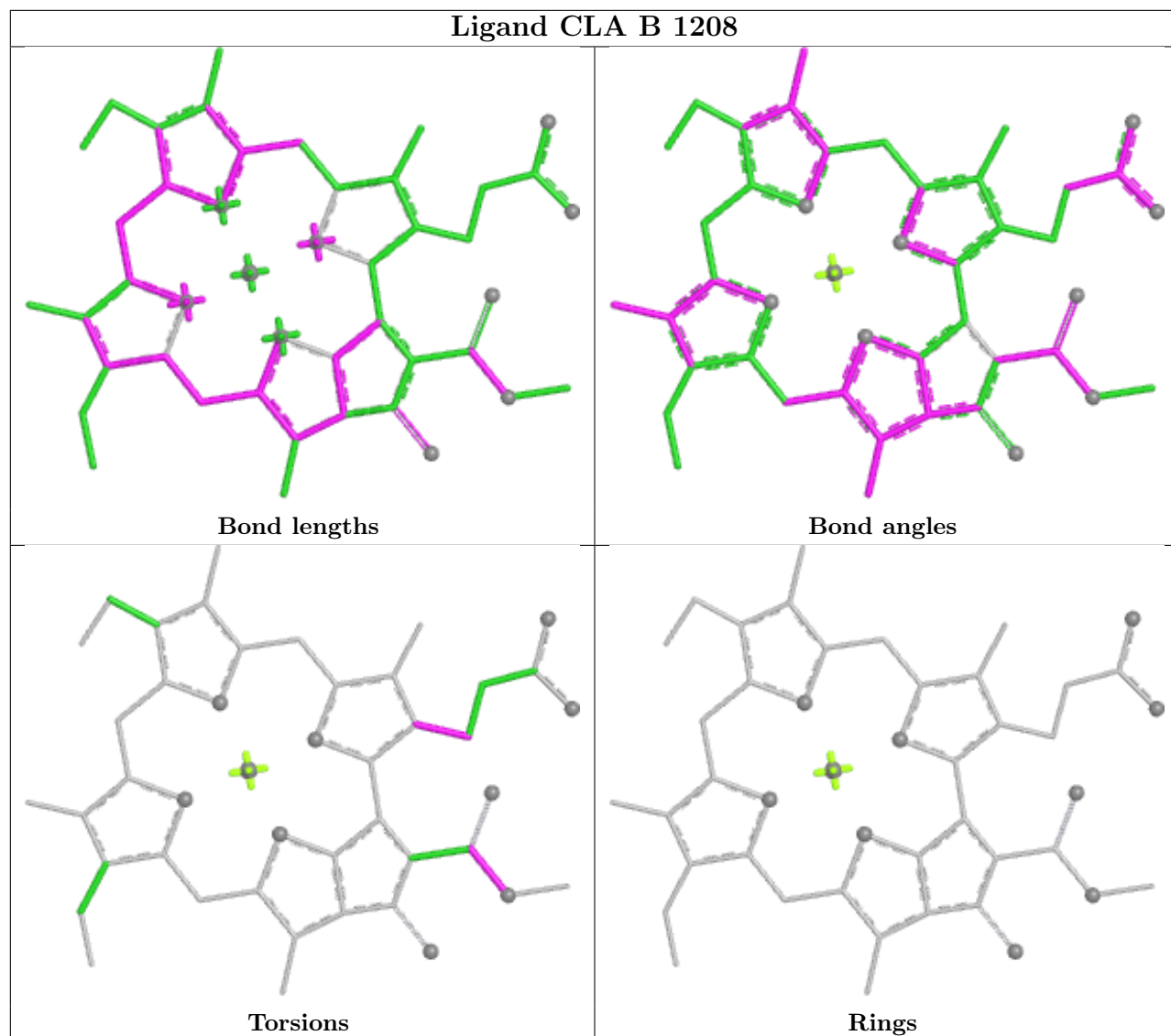
Ligand CLA F 1410



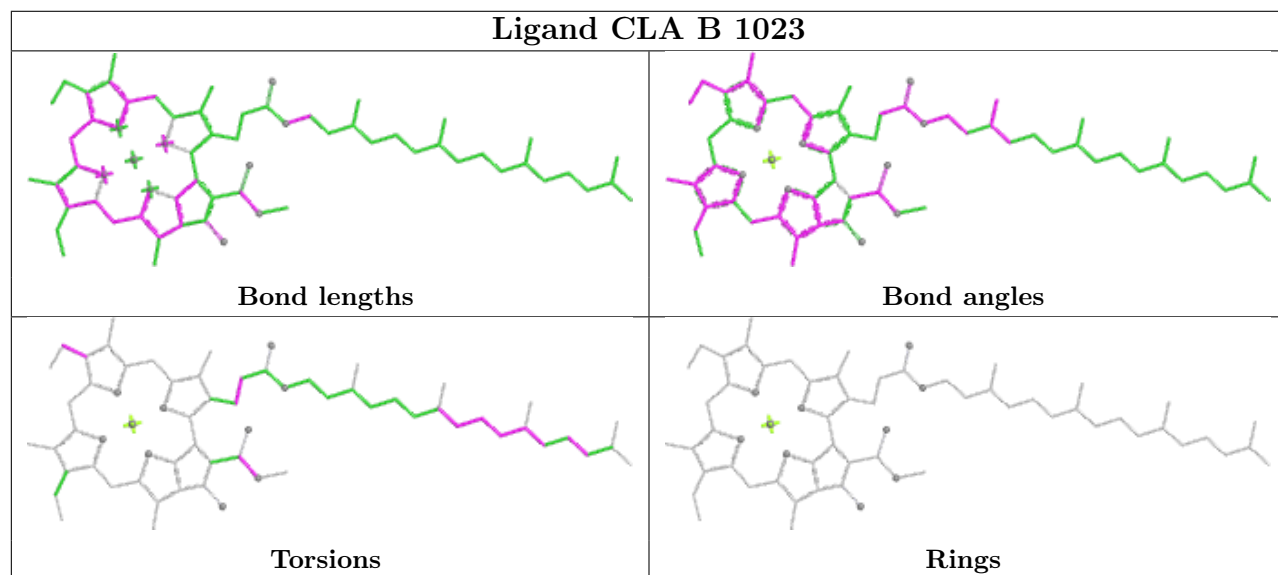
Ligand CLA A 1134

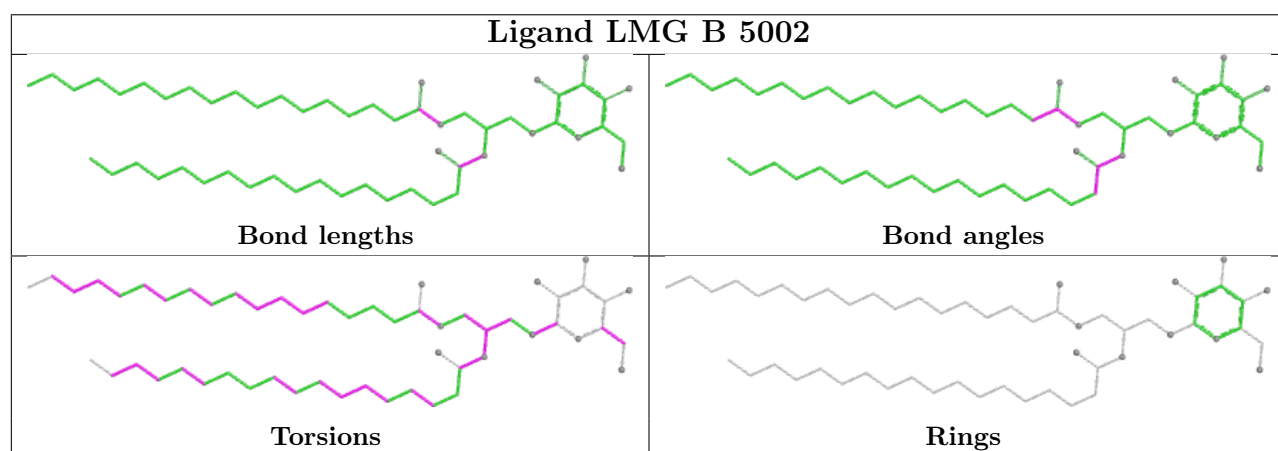
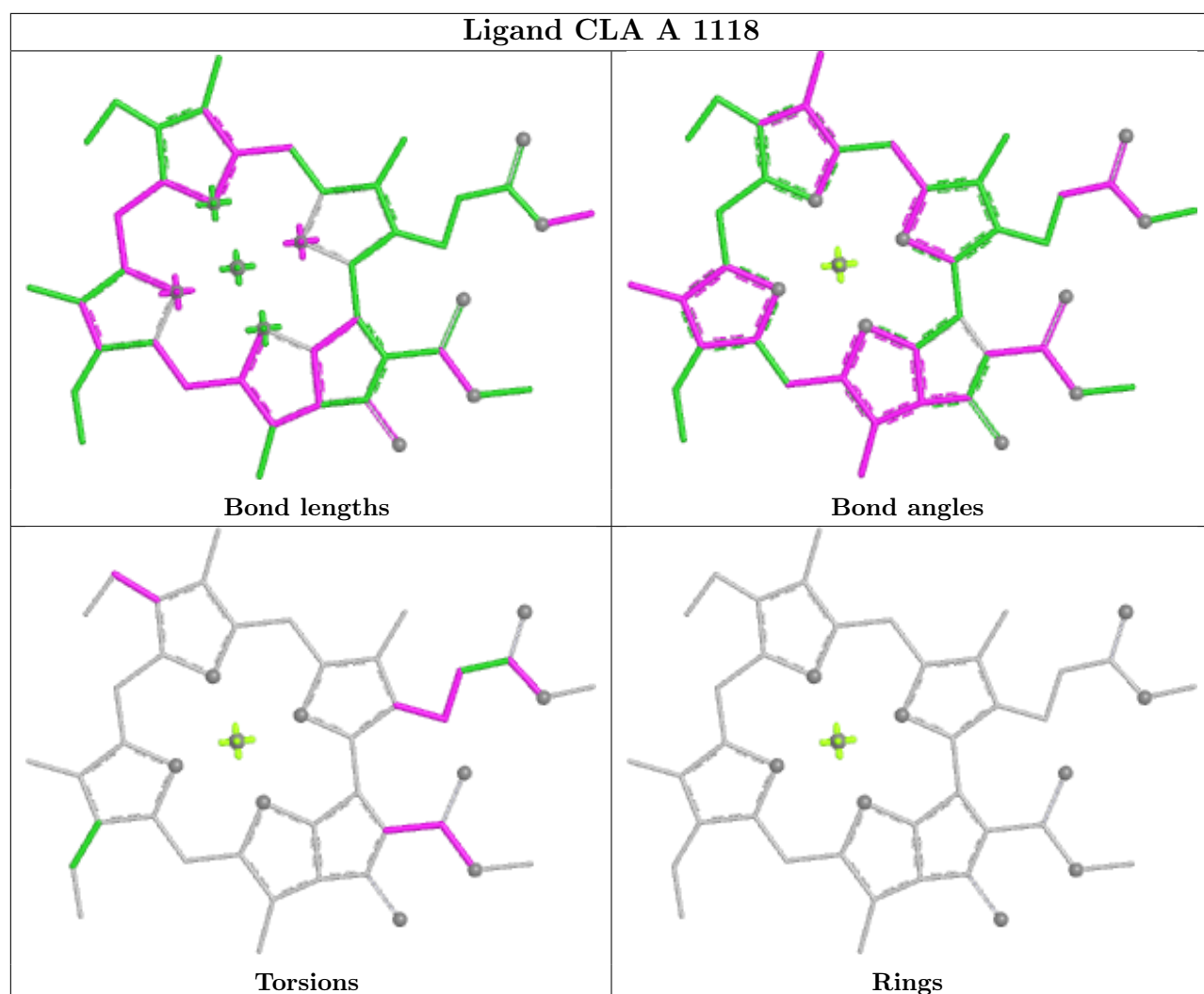


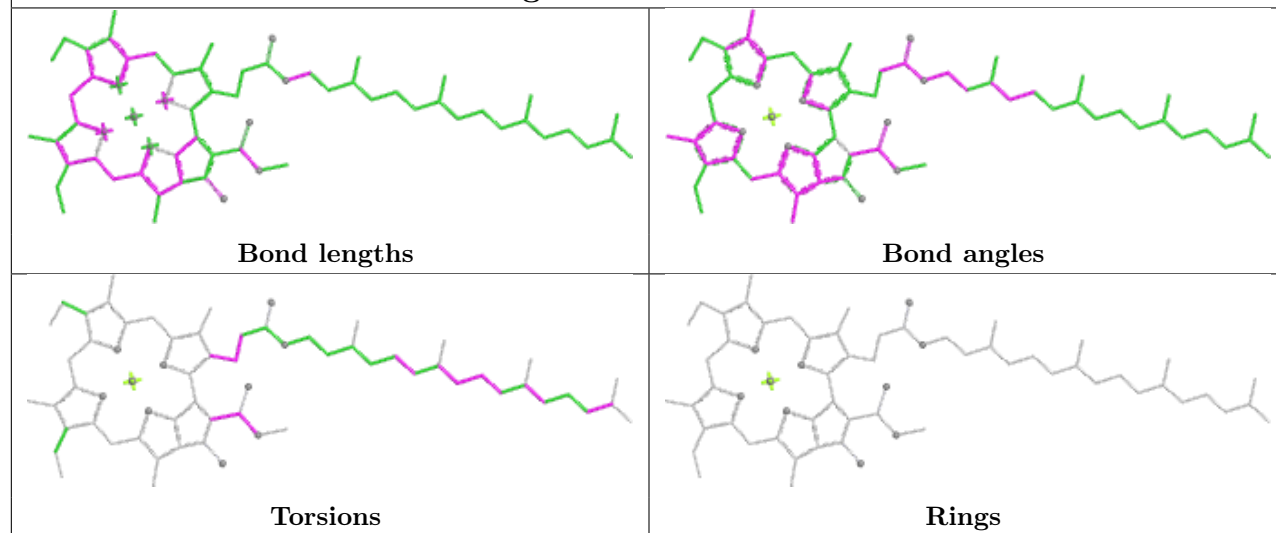
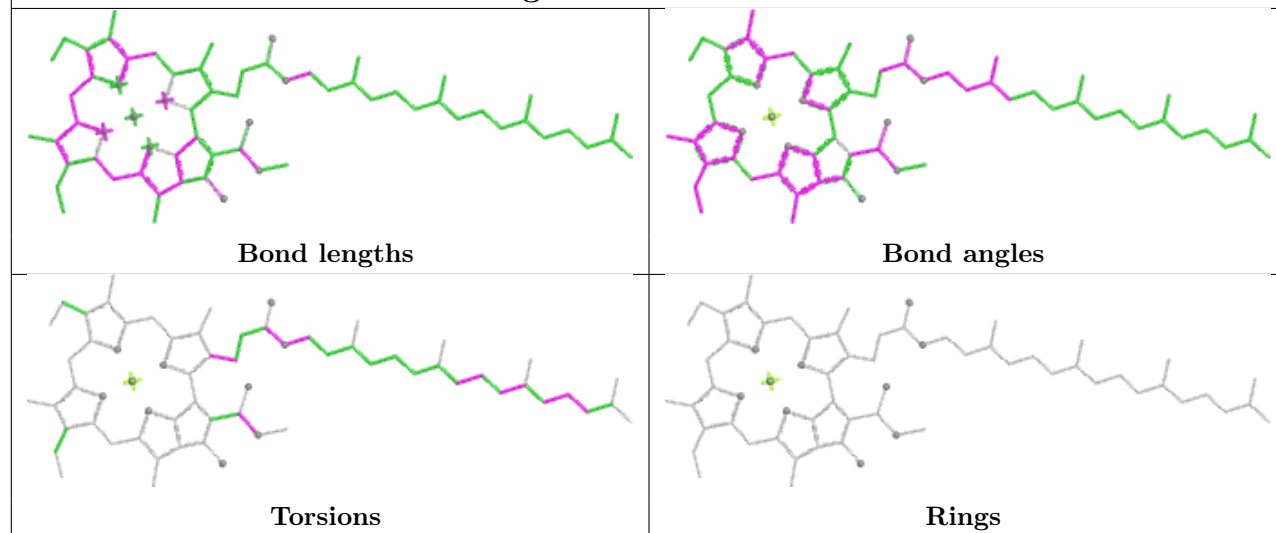
Ligand CLA B 1208



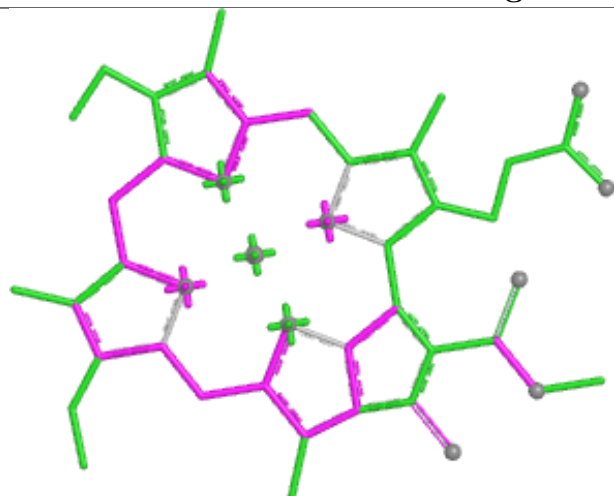
Ligand CLA B 1023



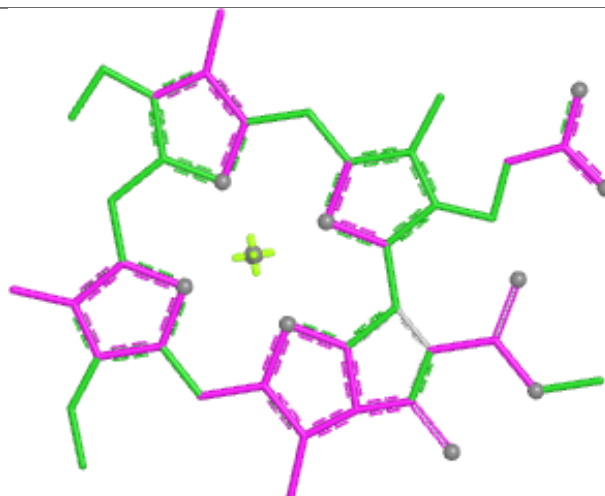


Ligand CLA A 1106**Ligand CLA A 1104**

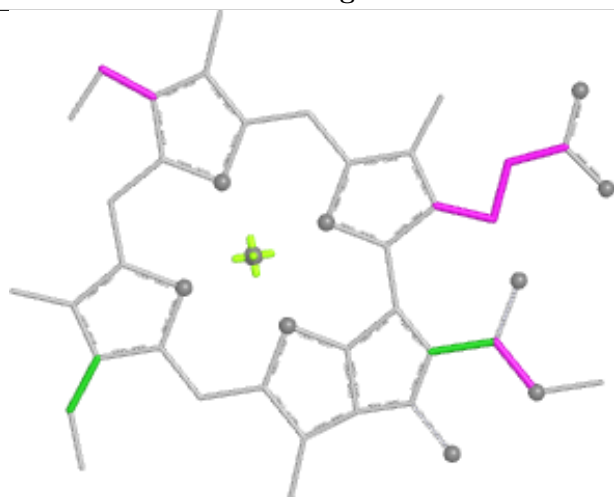
Ligand CLA B 1232



Bond lengths



Bond angles

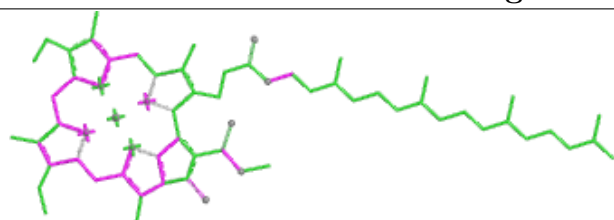


Torsions

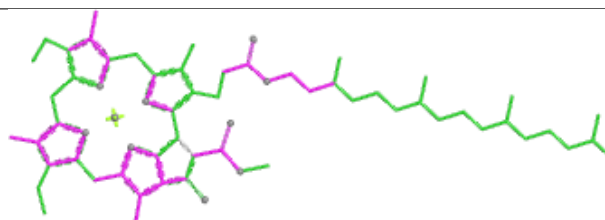


Rings

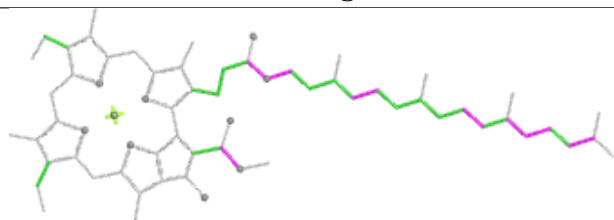
Ligand CLA B 1203



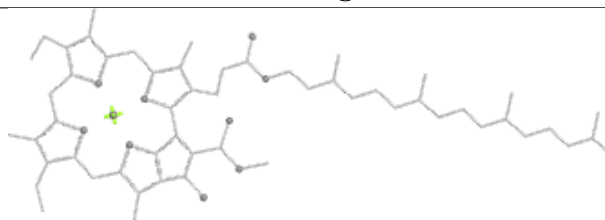
Bond lengths



Bond angles

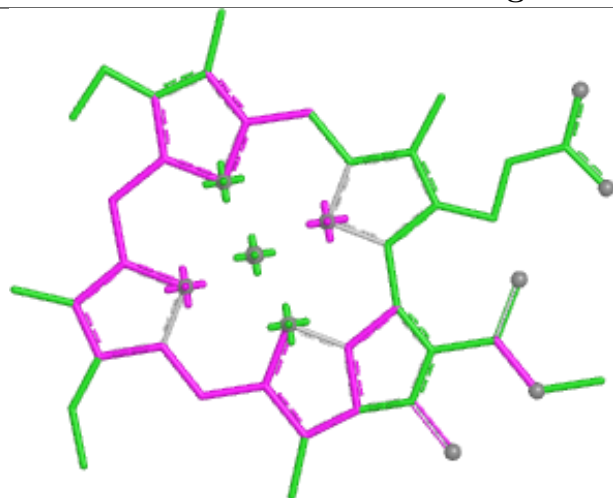


Torsions

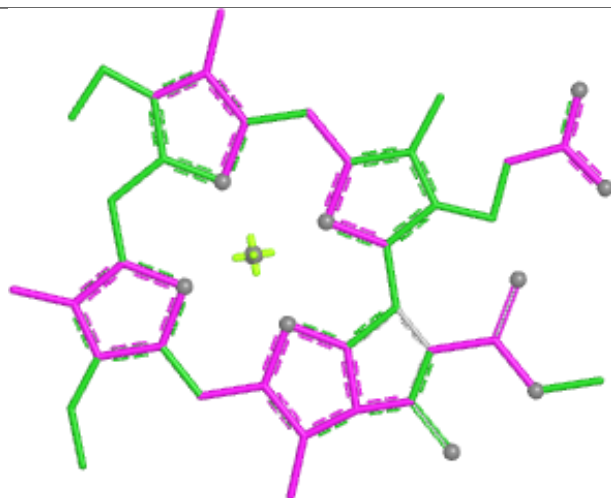


Rings

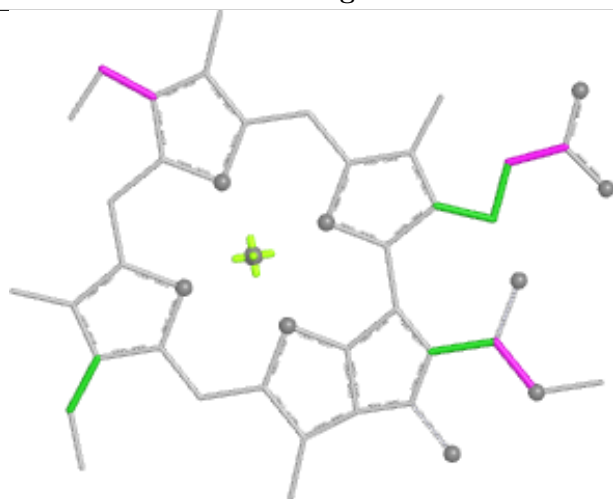
Ligand CLA F 1301



Bond lengths



Bond angles

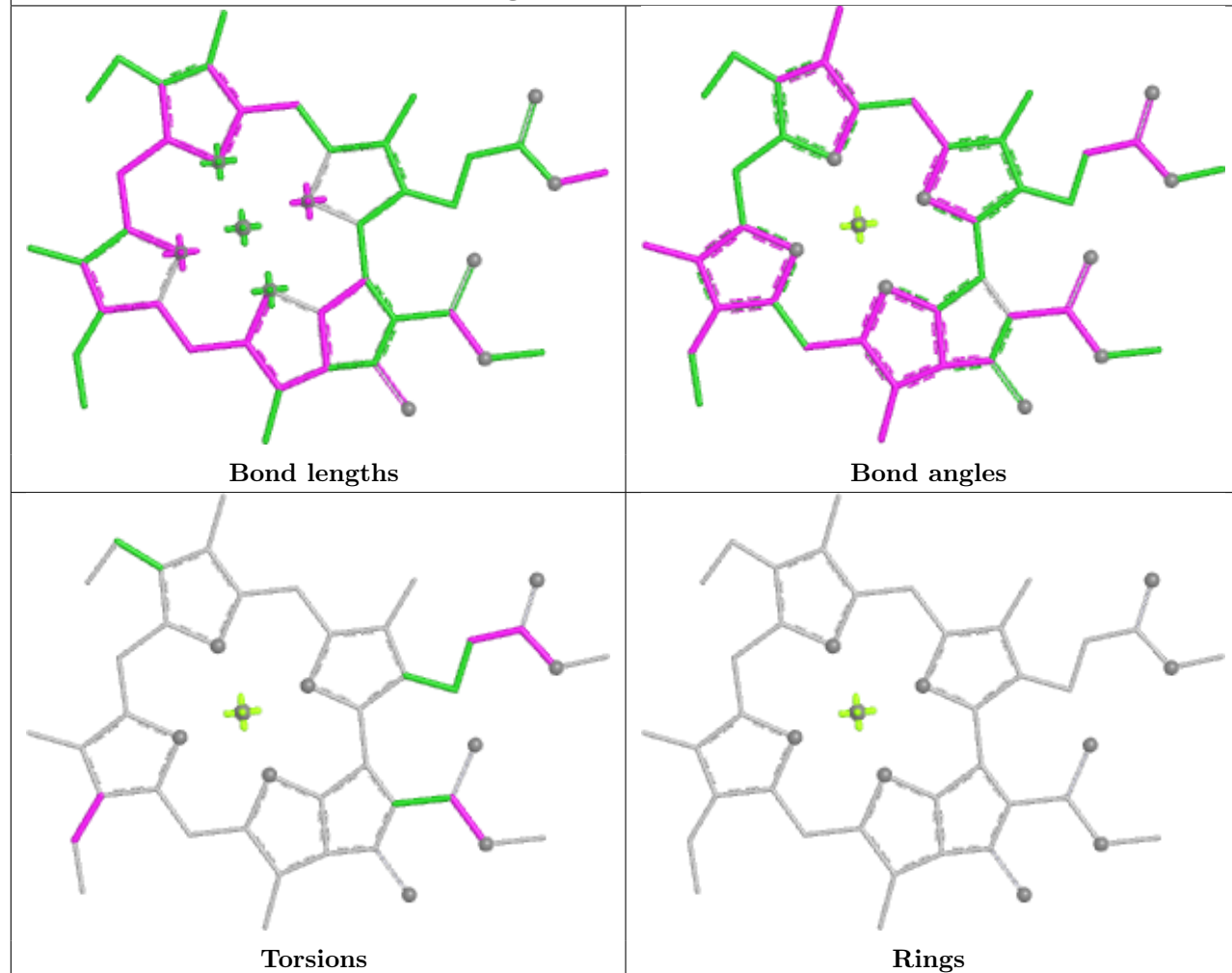


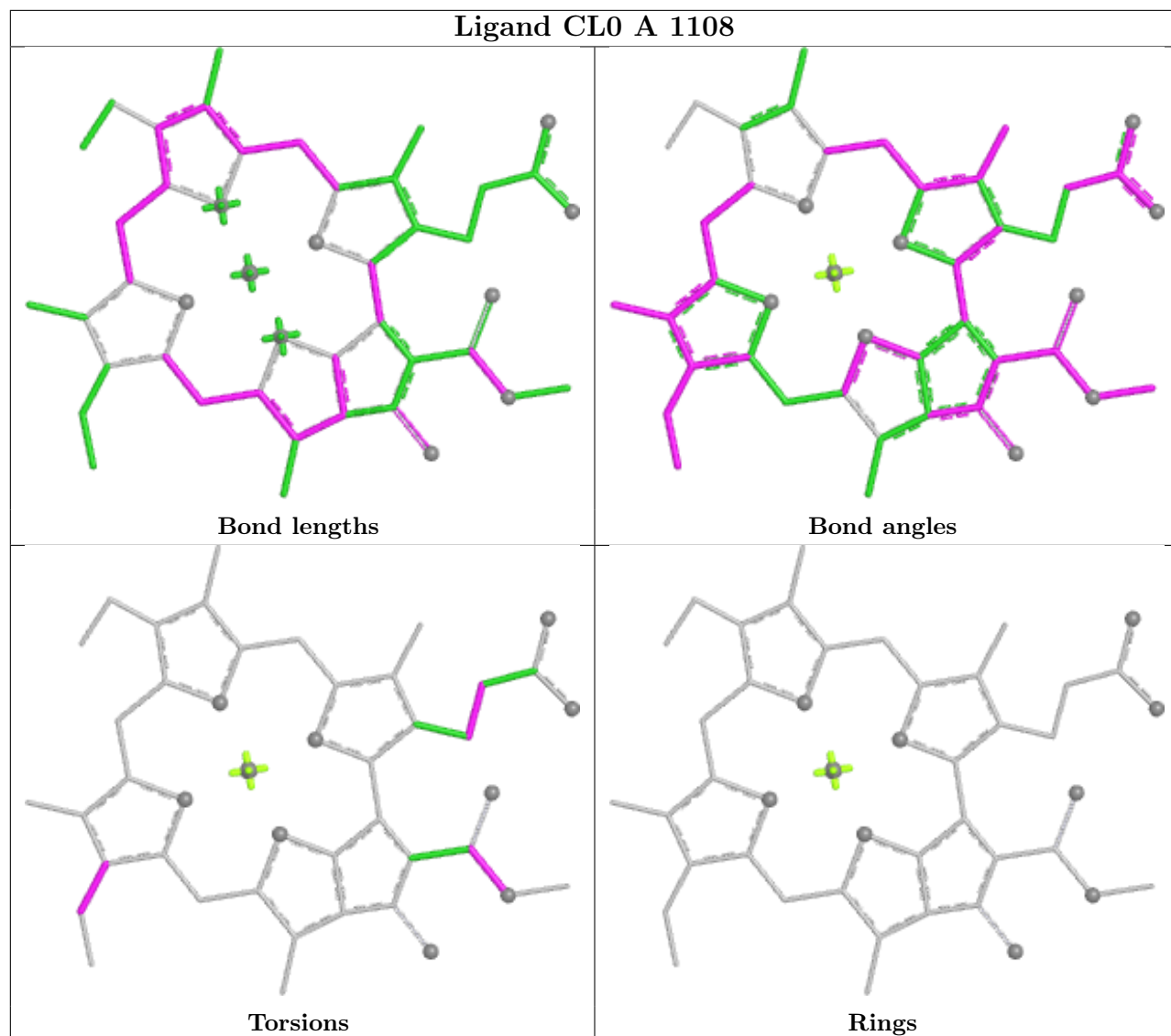
Torsions



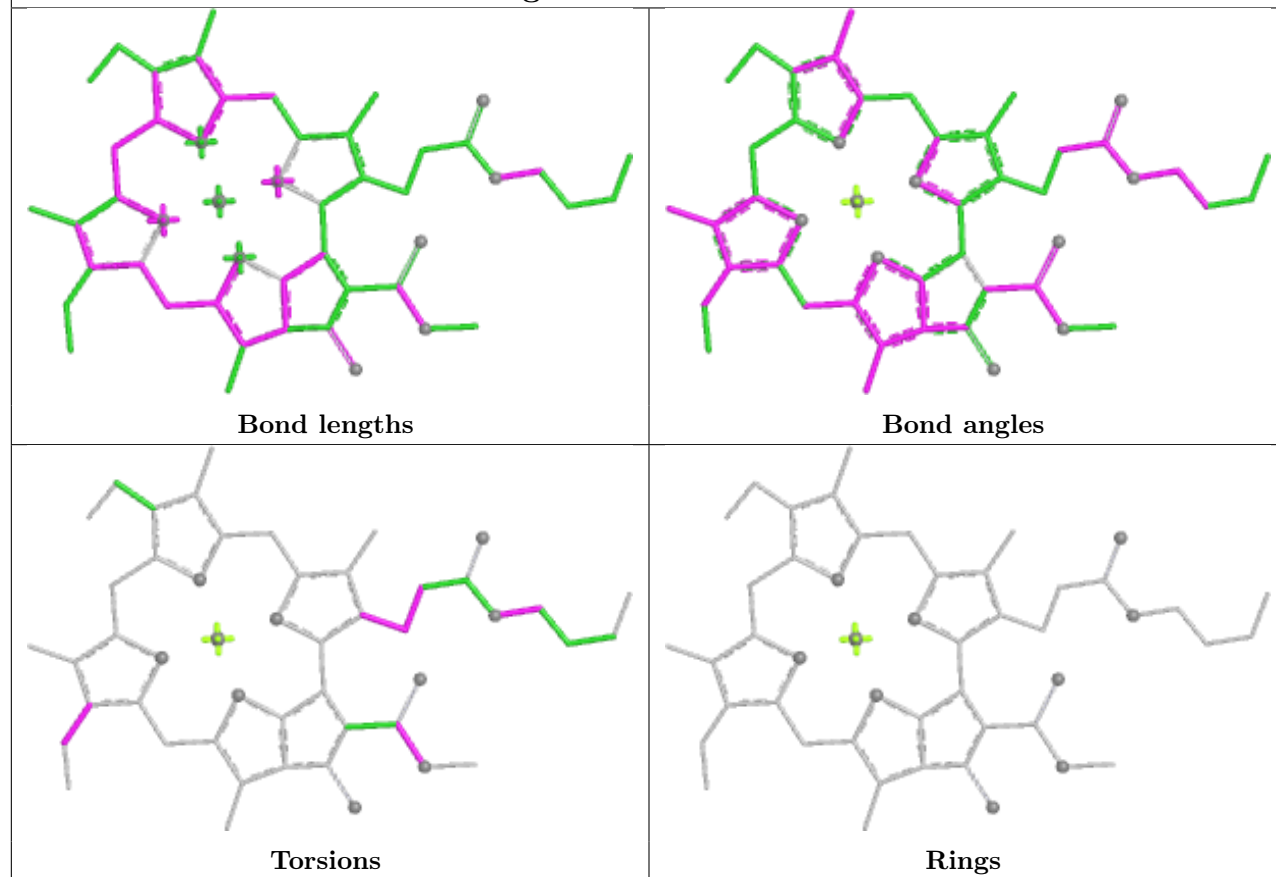
Rings

Ligand CLA B 1207

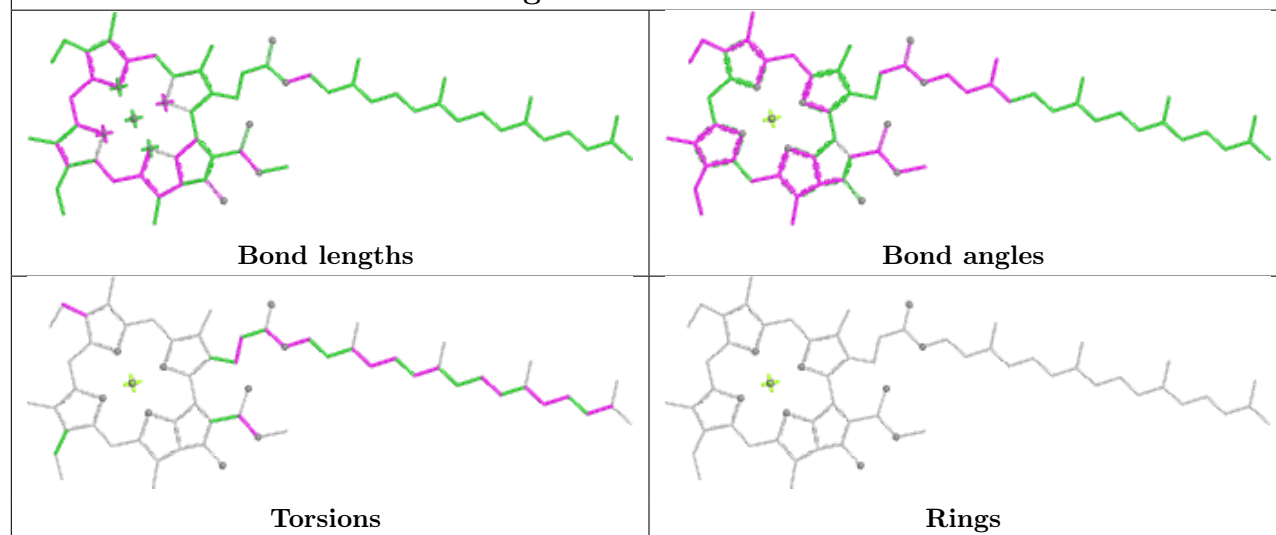


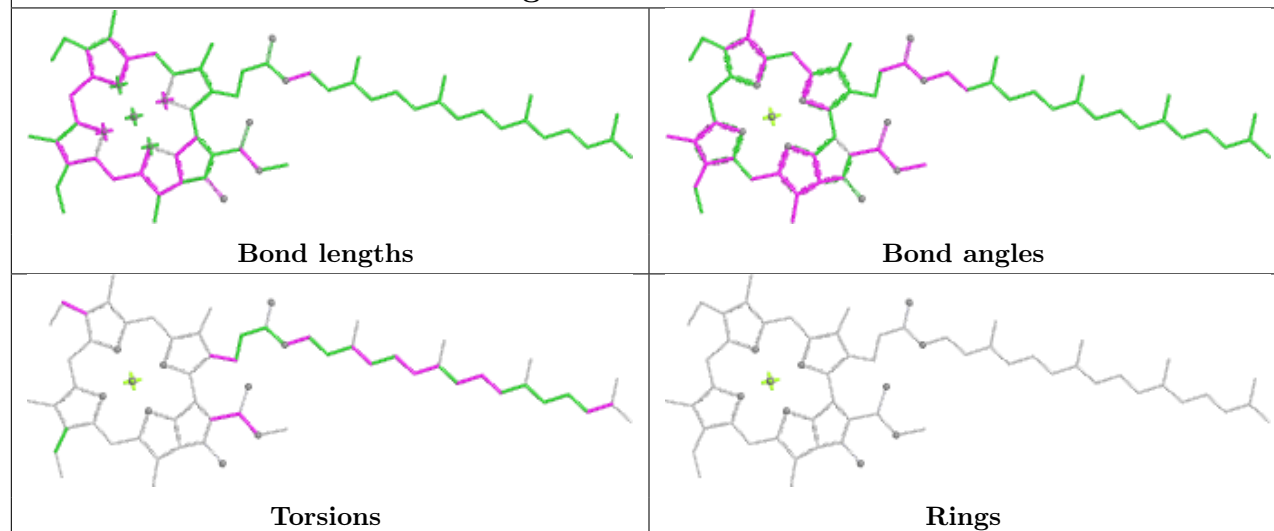
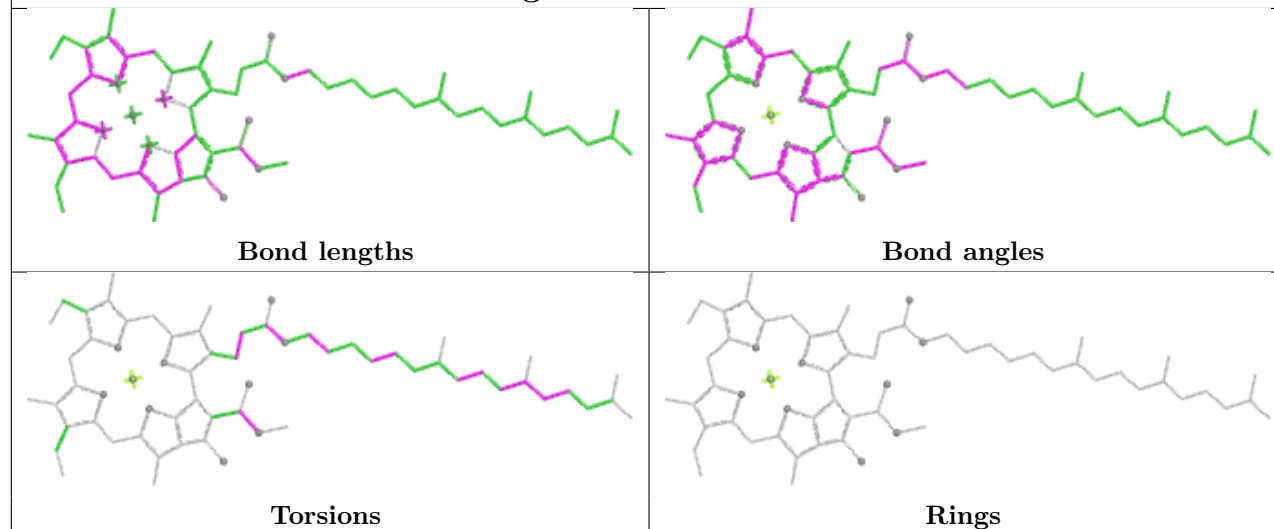


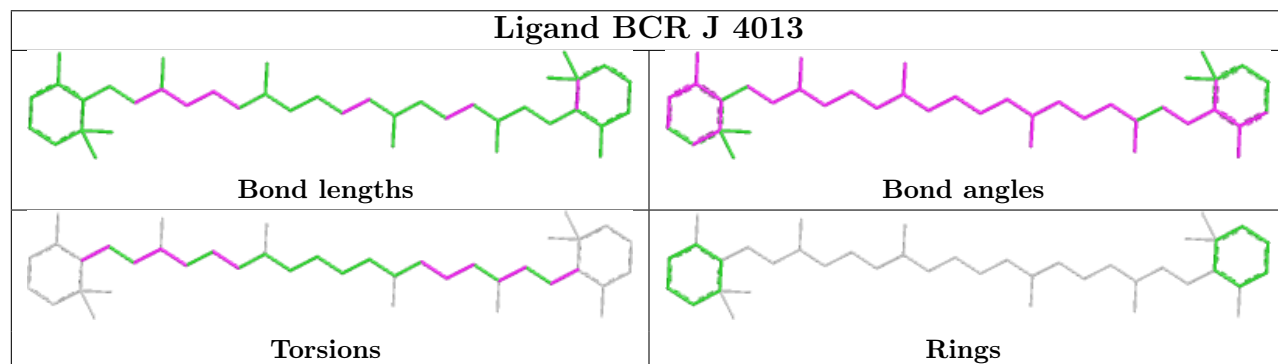
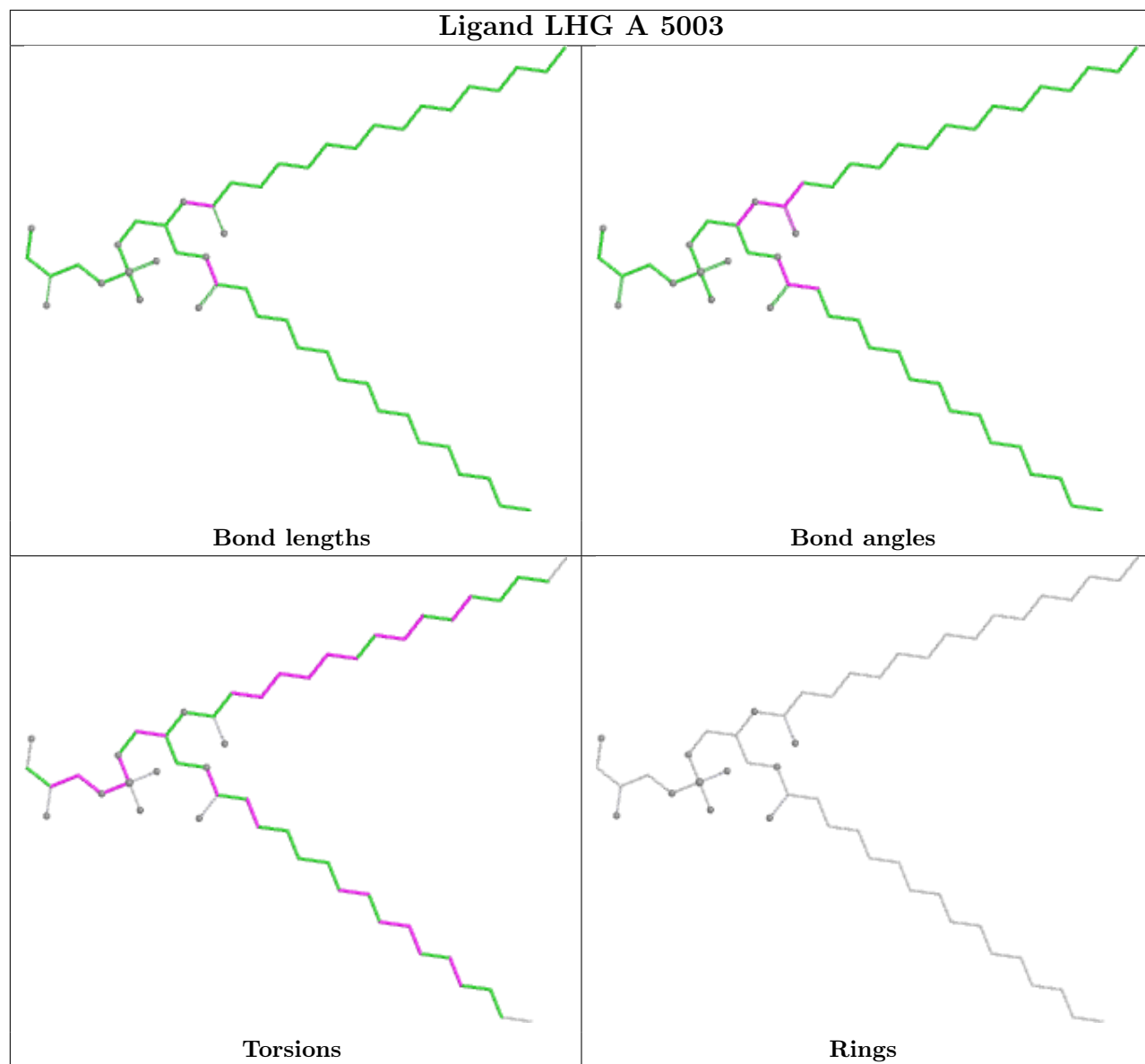
Ligand CLA A 1114

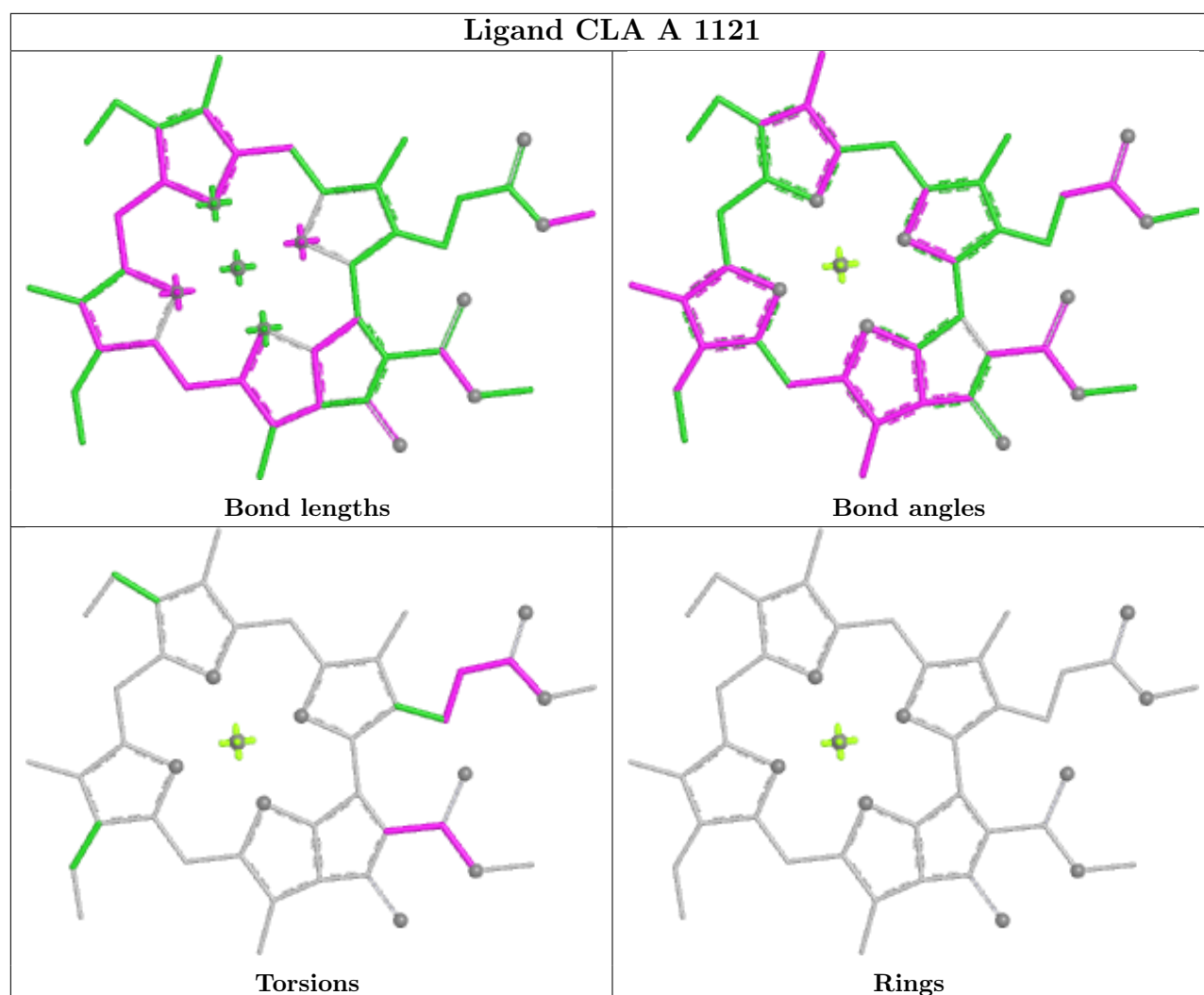


Ligand CLA B 1013



Ligand CLA A 1103**Ligand CLA A 1119**





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%)	-0.01	10 (1%) 73 64	43, 90, 141, 226	0
2	B	728/731 (99%)	-0.06	8 (1%) 78 70	53, 83, 126, 179	0
3	C	80/81 (98%)	0.09	3 (3%) 44 35	60, 72, 95, 105	0
4	D	138/141 (97%)	0.24	4 (2%) 53 43	72, 90, 125, 161	0
5	E	68/74 (91%)	0.13	1 (1%) 72 63	59, 75, 109, 138	0
6	F	141/165 (85%)	-0.10	2 (1%) 73 64	64, 82, 111, 169	0
7	J	40/40 (100%)	-0.28	0 100 100	66, 76, 124, 148	0
8	K	53/128 (41%)	1.14	9 (16%) 4 3	134, 160, 207, 253	0
9	M	30/31 (96%)	0.55	3 (10%) 12 9	109, 132, 158, 172	0
All	All	2017/2142 (94%)	0.02	40 (1%) 65 56	43, 86, 145, 253	0

The worst 5 of 40 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	216	PRO	5.5
5	E	14	THR	4.5
9	M	2	ALA	4.2
8	K	127	ILE	4.1
1	A	751	GLY	3.6

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 oligosaccharides in this entry.

6.4 Ligands ⓘ

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
16	LMU	J	1304	35/35	0.55	0.15	91,159,172,173	0
16	LMU	B	1301	35/35	0.59	0.17	120,136,148,154	0
15	CLA	B	1207	46/65	0.69	0.16	118,164,185,189	0
12	LHG	A	5005	36/49	0.78	0.16	103,143,182,188	0
15	CLA	B	1213	50/65	0.78	0.16	89,104,128,136	0
15	CLA	K	1402	46/65	0.80	0.18	163,187,214,221	0
15	CLA	K	1401	46/65	0.81	0.17	120,155,169,173	0
15	CLA	A	1110	54/65	0.81	0.15	96,121,150,154	0
14	BCR	A	4001	40/40	0.83	0.17	111,127,138,140	0
15	CLA	A	1132	62/65	0.83	0.16	74,105,153,156	0
12	LHG	A	5003	49/49	0.84	0.15	91,121,142,143	0
15	CLA	A	1801	52/65	0.84	0.14	100,122,154,158	0
14	BCR	A	4007	40/40	0.86	0.14	69,86,137,139	0
15	CLA	J	1303	46/65	0.86	0.11	94,114,141,159	0
14	BCR	A	4008	40/40	0.86	0.13	67,93,105,115	0
14	BCR	B	4009	40/40	0.87	0.14	72,103,147,151	0
15	CLA	J	1302	45/65	0.87	0.10	82,93,138,150	0
15	CLA	A	1114	49/65	0.88	0.13	98,124,137,150	0
13	CL0	A	1108	45/65	0.88	0.15	86,113,154,170	0
14	BCR	A	4003	40/40	0.88	0.15	69,111,146,146	0
15	CLA	B	1208	45/65	0.88	0.11	88,114,130,140	0
14	BCR	B	4004	40/40	0.88	0.14	101,115,147,151	0
15	CLA	F	1410	65/65	0.88	0.13	69,96,135,147	0
15	CLA	A	1120	49/65	0.89	0.12	101,116,140,156	0
15	CLA	B	1230	65/65	0.89	0.15	53,68,118,125	0
15	CLA	B	1231	65/65	0.89	0.12	66,89,115,138	0
12	LHG	B	5004	49/49	0.89	0.12	59,88,99,106	0
15	CLA	B	1212	45/65	0.89	0.12	101,117,128,143	0
17	LMG	B	5002	55/55	0.89	0.14	71,101,130,137	0
15	CLA	B	1218	51/65	0.90	0.11	86,98,125,159	0
15	CLA	B	1228	65/65	0.90	0.12	54,74,105,114	0
15	CLA	A	1105	65/65	0.90	0.13	70,96,111,120	0
14	BCR	J	4013	40/40	0.90	0.15	78,97,112,121	0
15	CLA	A	1134	46/65	0.90	0.10	109,127,151,186	0
15	CLA	A	1135	55/65	0.90	0.14	70,98,132,135	0
15	CLA	B	1240	45/65	0.90	0.10	71,83,124,151	0
15	CLA	A	1111	60/65	0.90	0.13	78,96,107,112	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
15	CLA	A	1113	45/65	0.90	0.10	112,129,158,162	0
15	CLA	A	1124	55/65	0.90	0.12	61,92,120,129	0
14	BCR	B	4005	40/40	0.90	0.13	73,93,125,128	0
15	CLA	B	1217	47/65	0.90	0.11	96,114,132,157	0
15	CLA	B	1224	65/65	0.91	0.12	60,78,98,108	0
14	BCR	B	4006	40/40	0.91	0.13	86,109,141,142	0
15	CLA	A	1118	46/65	0.91	0.12	99,113,135,154	0
15	CLA	A	1102	65/65	0.91	0.12	55,81,107,112	0
15	CLA	B	1203	65/65	0.91	0.10	62,83,99,104	0
15	CLA	F	1301	45/65	0.91	0.10	54,75,97,131	0
15	CLA	A	1125	52/65	0.91	0.12	76,98,124,133	0
14	BCR	A	4002	40/40	0.91	0.12	88,109,128,130	0
14	BCR	F	4015	40/40	0.91	0.13	52,73,107,111	0
15	CLA	A	1121	46/65	0.91	0.11	91,114,141,163	0
15	CLA	B	1214	65/65	0.91	0.14	72,89,119,133	0
15	CLA	A	1131	55/65	0.91	0.10	78,107,126,140	0
10	PQN	B	2002	33/33	0.91	0.10	59,79,99,105	0
15	CLA	B	1232	45/65	0.92	0.10	72,89,109,115	0
15	CLA	B	1234	65/65	0.92	0.12	56,73,108,120	0
15	CLA	B	1236	50/65	0.92	0.11	52,72,106,114	0
15	CLA	B	1201	46/65	0.92	0.10	72,83,107,123	0
15	CLA	A	1133	46/65	0.92	0.09	86,103,118,128	0
15	CLA	A	1122	65/65	0.92	0.11	74,91,119,129	0
15	CLA	B	1219	55/65	0.92	0.10	74,86,119,142	0
15	CLA	B	1221	65/65	0.92	0.12	68,79,105,125	0
15	CLA	B	1222	56/65	0.92	0.10	52,66,101,108	0
14	BCR	B	4010	40/40	0.92	0.12	55,74,102,113	0
12	LHG	A	5001	49/49	0.92	0.12	49,70,91,100	0
15	CLA	A	1119	64/65	0.92	0.13	78,97,115,137	0
15	CLA	B	1216	65/65	0.92	0.10	67,91,106,118	0
15	CLA	B	1225	65/65	0.93	0.11	66,80,100,104	0
15	CLA	B	1226	65/65	0.93	0.12	54,79,133,144	0
15	CLA	B	1227	45/65	0.93	0.10	54,72,94,98	0
15	CLA	A	1109	65/65	0.93	0.12	66,81,105,112	0
15	CLA	B	1023	65/65	0.93	0.11	55,79,111,119	0
15	CLA	A	1126	65/65	0.93	0.11	63,80,101,116	0
15	CLA	A	1136	65/65	0.93	0.12	78,105,139,142	0
14	BCR	F	4016	40/40	0.93	0.10	59,72,89,94	0
15	CLA	B	1210	65/65	0.93	0.12	75,95,108,120	0
15	CLA	A	1115	46/65	0.93	0.11	109,129,140,151	0
15	CLA	B	1204	46/65	0.93	0.09	79,96,115,137	0
14	BCR	B	4011	40/40	0.93	0.10	49,67,84,91	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
14	BCR	B	4014	40/40	0.93	0.11	46,62,88,89	0
15	CLA	A	1129	46/65	0.93	0.11	76,92,115,151	0
15	CLA	A	1130	55/65	0.93	0.10	82,106,133,139	0
15	CLA	A	1116	54/65	0.93	0.13	84,113,130,141	0
15	CLA	A	1101	65/65	0.93	0.10	55,73,89,96	0
14	BCR	B	4017	40/40	0.93	0.10	70,87,101,104	0
15	CLA	A	1103	65/65	0.93	0.13	61,80,108,118	0
10	PQN	A	2001	33/33	0.93	0.10	45,57,68,74	0
15	CLA	A	1127	65/65	0.94	0.12	67,79,100,106	0
15	CLA	A	1106	65/65	0.94	0.11	59,79,98,109	0
15	CLA	B	1215	65/65	0.94	0.11	72,85,104,106	0
15	CLA	A	1137	50/65	0.94	0.09	72,94,128,134	0
15	CLA	B	1235	65/65	0.94	0.09	55,66,85,92	0
15	CLA	A	1012	65/65	0.94	0.12	47,60,86,93	0
15	CLA	A	1117	65/65	0.94	0.10	80,100,111,113	0
15	CLA	B	1013	65/65	0.94	0.10	46,53,77,89	0
15	CLA	B	1211	46/65	0.94	0.09	90,106,116,133	0
15	CLA	B	1237	55/65	0.94	0.09	71,82,117,132	0
15	CLA	B	1238	44/65	0.94	0.09	68,80,92,111	0
15	CLA	B	1239	46/65	0.94	0.09	62,78,107,141	0
15	CLA	B	1220	56/65	0.94	0.10	61,77,111,119	0
15	CLA	A	1107	50/65	0.94	0.09	56,64,98,112	0
14	BCR	A	4012	40/40	0.94	0.09	55,77,87,91	0
15	CLA	B	1223	65/65	0.94	0.11	59,77,94,98	0
15	CLA	A	1022	65/65	0.94	0.11	53,78,96,103	0
15	CLA	A	1104	65/65	0.94	0.10	58,72,83,96	0
15	CLA	B	1209	45/65	0.94	0.10	102,113,134,148	0
15	CLA	A	1112	45/65	0.94	0.11	89,115,127,130	0
11	SF4	C	3002	8/8	0.94	0.11	60,88,151,152	0
15	CLA	F	1139	65/65	0.95	0.11	47,58,90,98	0
15	CLA	B	1229	65/65	0.95	0.09	50,62,86,107	0
15	CLA	A	1140	65/65	0.95	0.09	52,73,103,116	0
15	CLA	B	1206	46/65	0.95	0.10	78,100,119,149	0
13	CL0	A	1011	65/65	0.95	0.11	51,69,81,99	0
15	CLA	B	1205	55/65	0.95	0.10	68,87,100,112	0
15	CLA	A	1128	65/65	0.95	0.10	54,74,90,101	0
11	SF4	A	3001	8/8	0.95	0.16	50,62,210,290	0
15	CLA	A	1123	65/65	0.95	0.11	75,88,98,104	0
15	CLA	B	1202	65/65	0.96	0.11	67,82,99,106	0
15	CLA	B	1021	65/65	0.96	0.10	49,69,80,84	0
15	CLA	A	1138	65/65	0.96	0.09	47,55,69,77	0
11	SF4	C	3003	8/8	0.98	0.12	60,67,100,115	0

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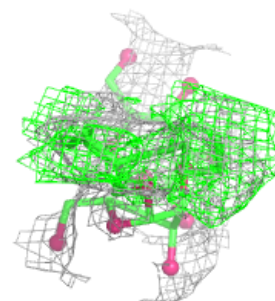
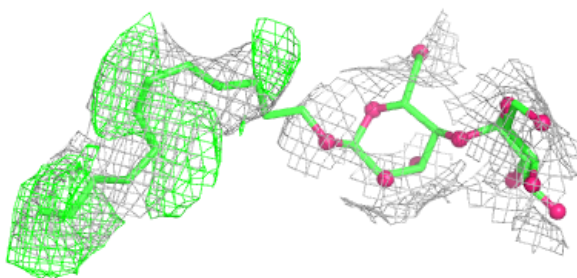
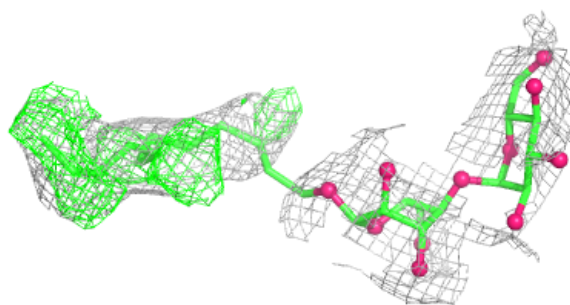
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
18	CL	B	6000	1/1	0.98	0.08	82,82,82,82	0

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.

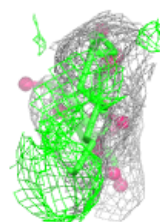
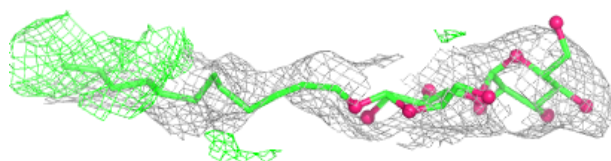
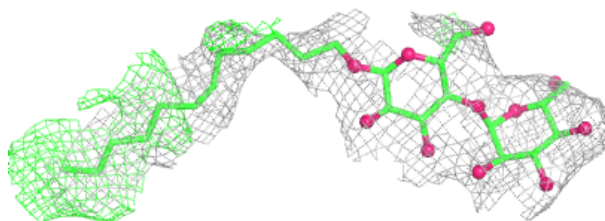
Electron density around LMU J 1304:

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

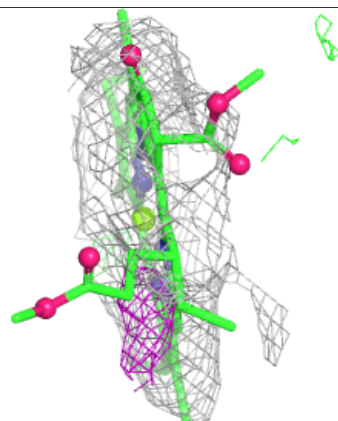
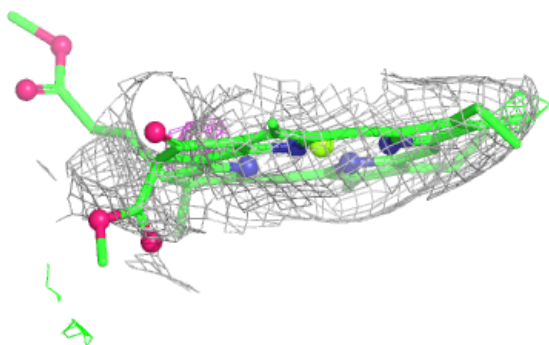
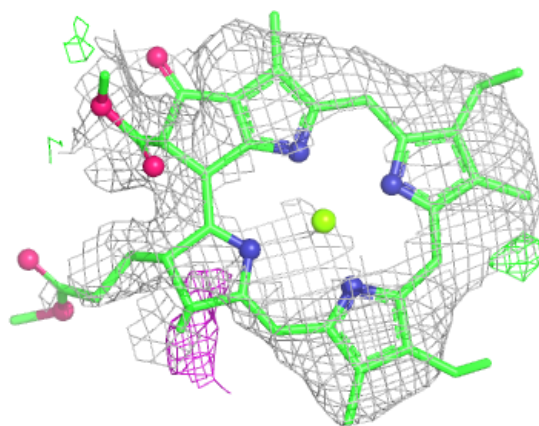


Electron density around LMU B 1301:

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

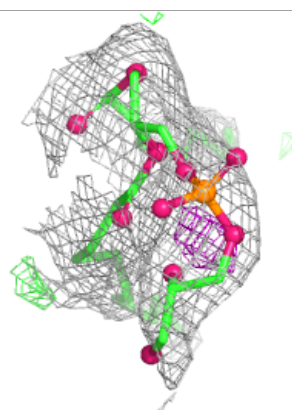
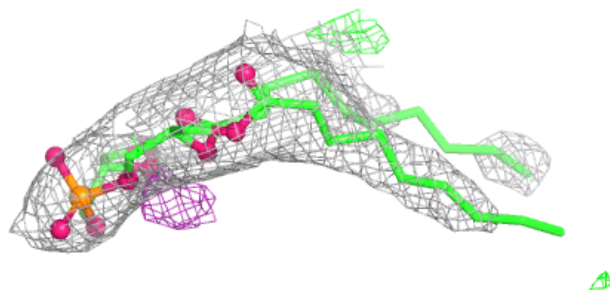
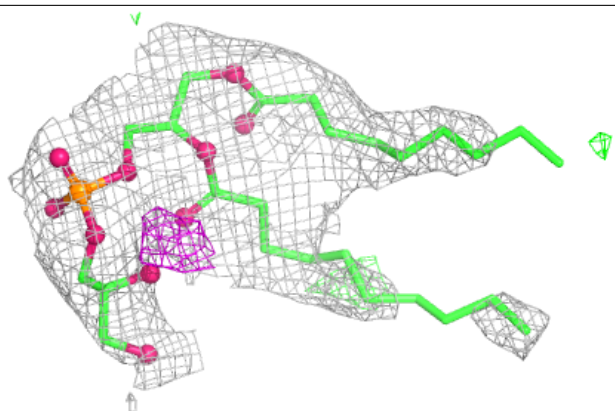
**Electron density around CLA B 1207:**

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

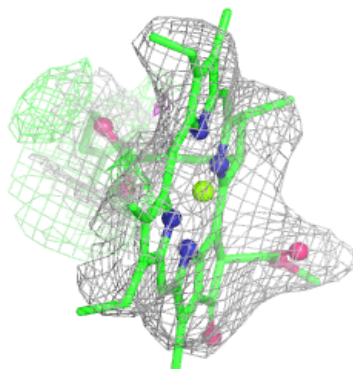
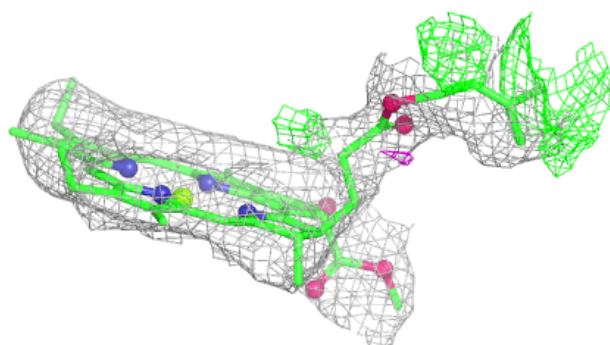
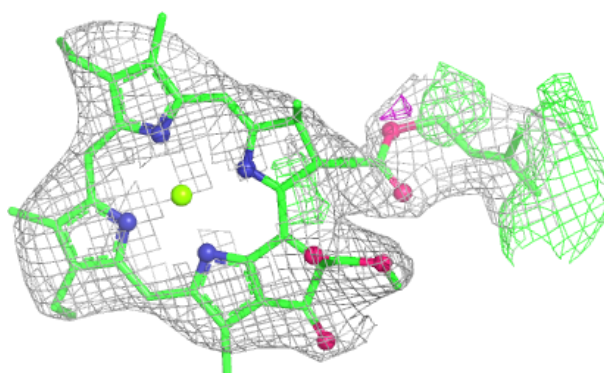


Electron density around LHG A 5005:

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

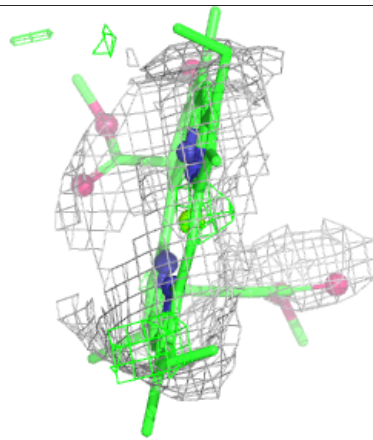
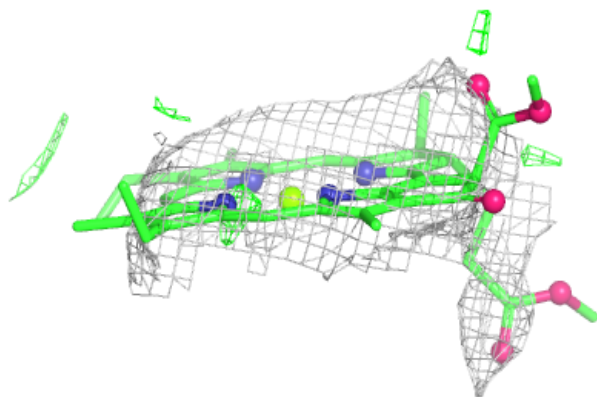
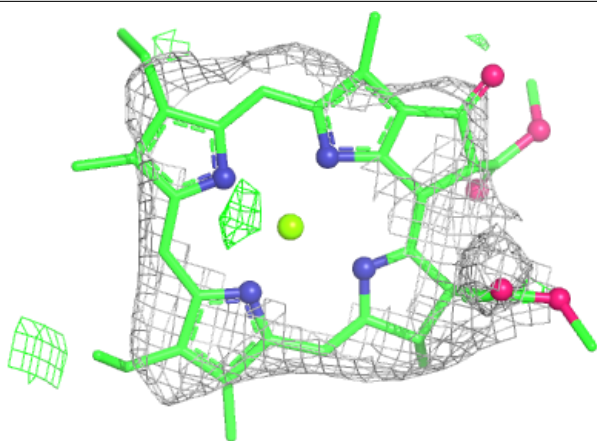
**Electron density around CLA B 1213:**

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



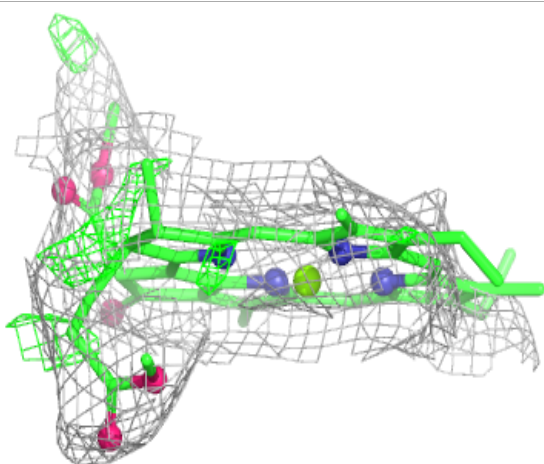
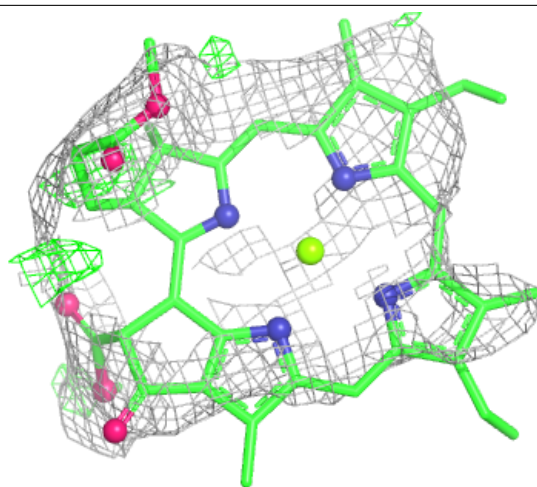
Electron density around CLA K 1402:

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



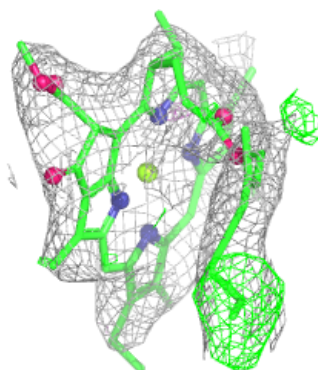
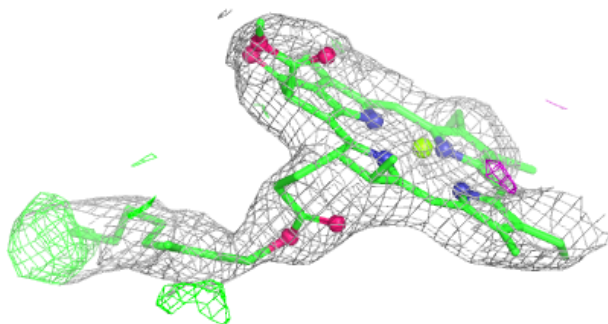
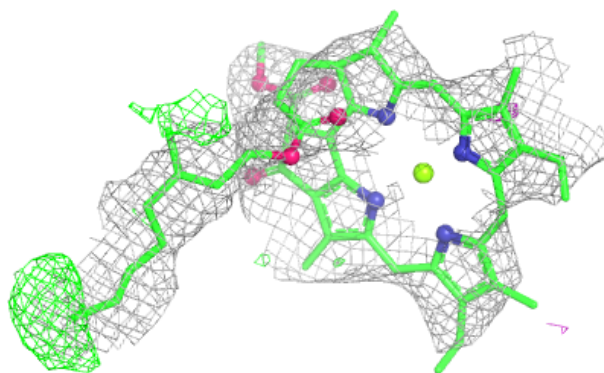
Electron density around CLA K 1401:

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

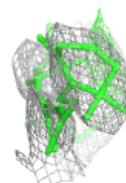
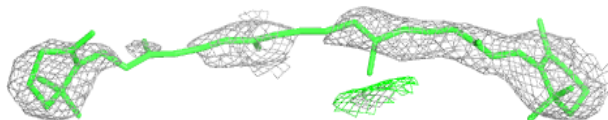
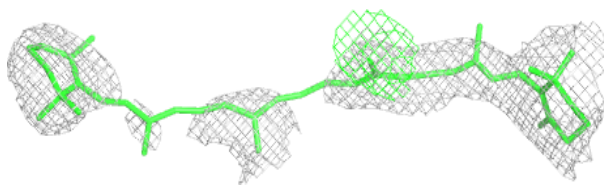


Electron density around CLA A 1110:

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

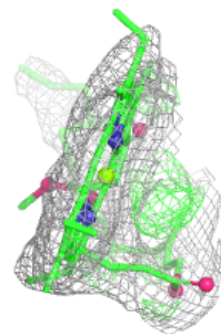
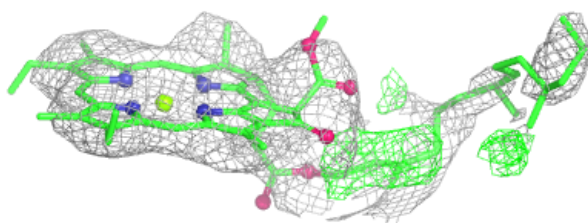
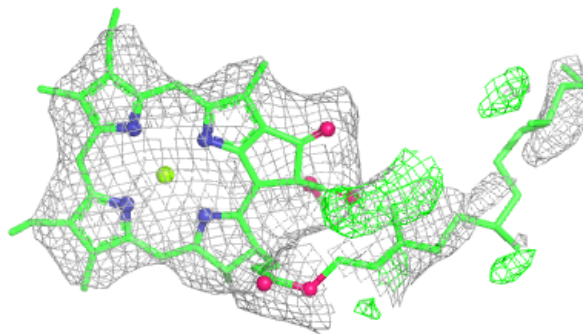
**Electron density around BCR A 4001:**

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

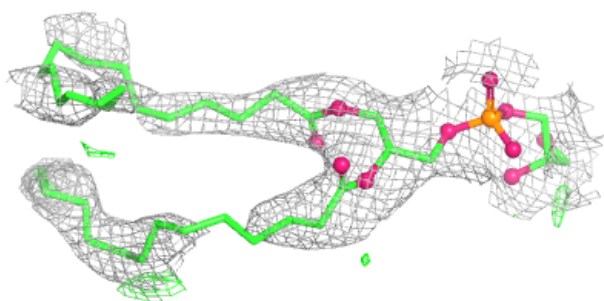
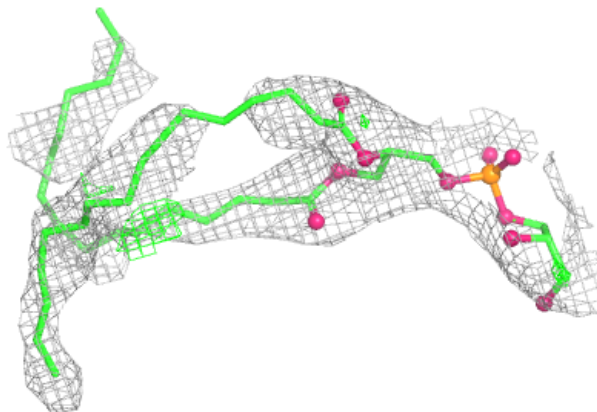


Electron density around CLA A 1132:

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

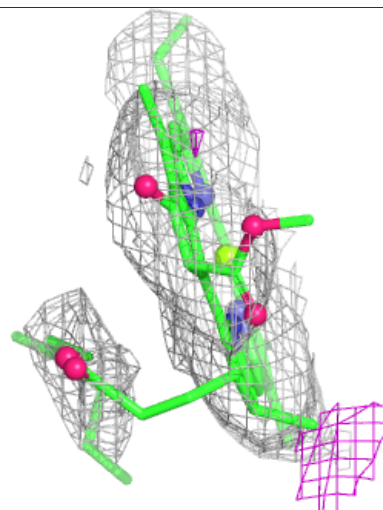
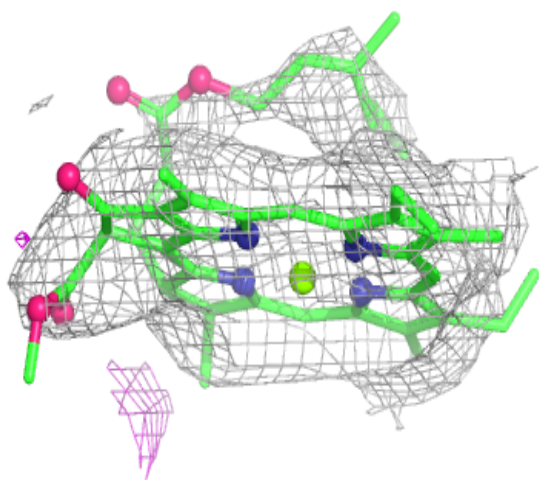
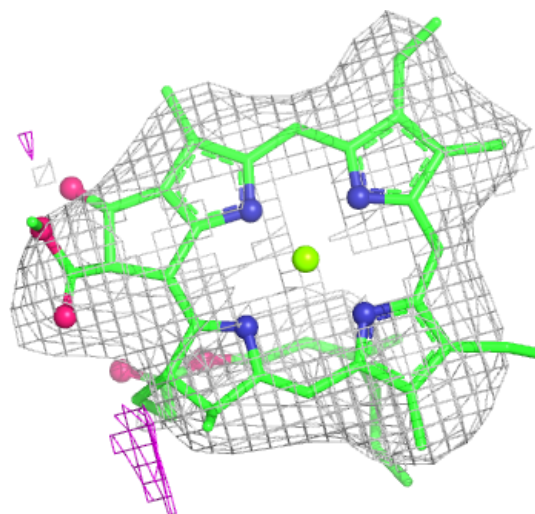
**Electron density around LHG A 5003:**

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



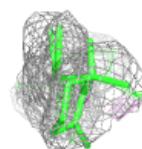
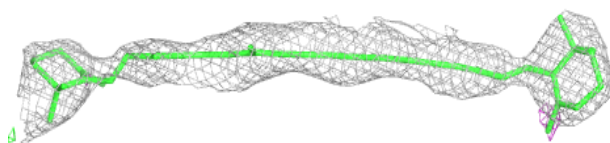
Electron density around CLA A 1801:

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



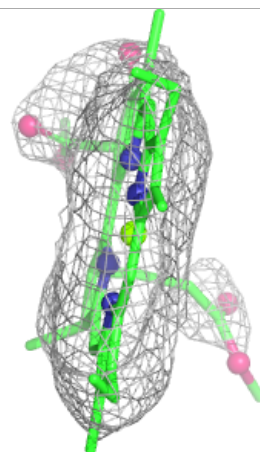
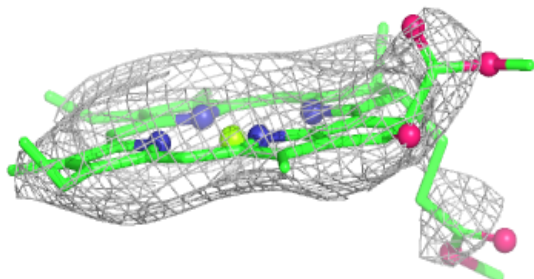
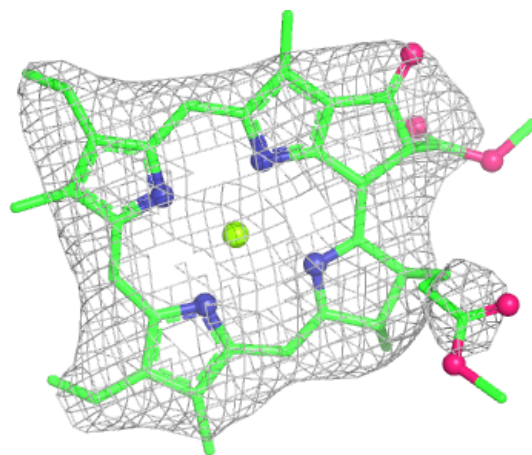
Electron density around BCR A 4007:

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



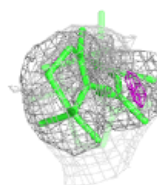
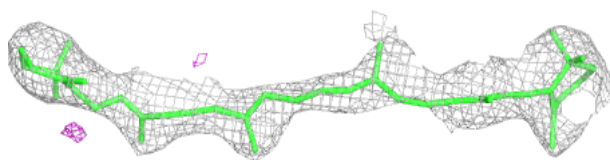
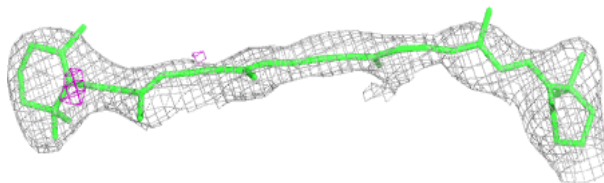
Electron density around CLA J 1303:

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

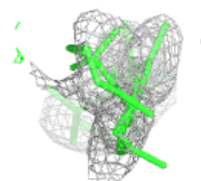
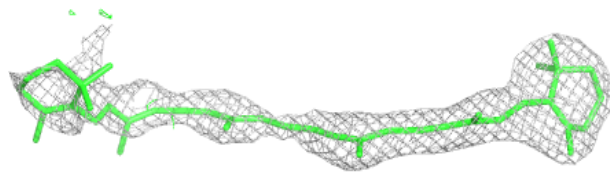
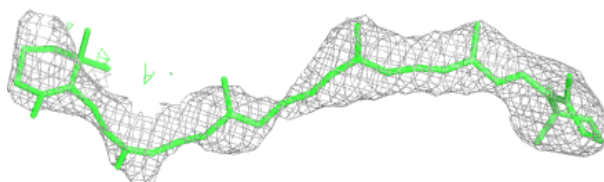


Electron density around BCR A 4008:

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

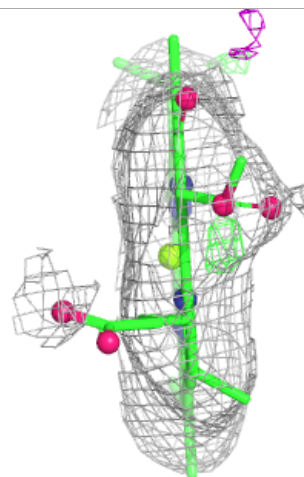
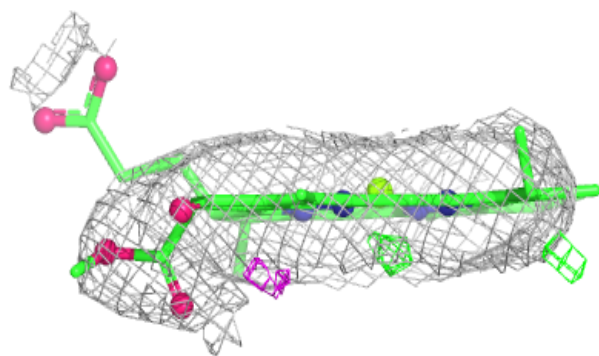
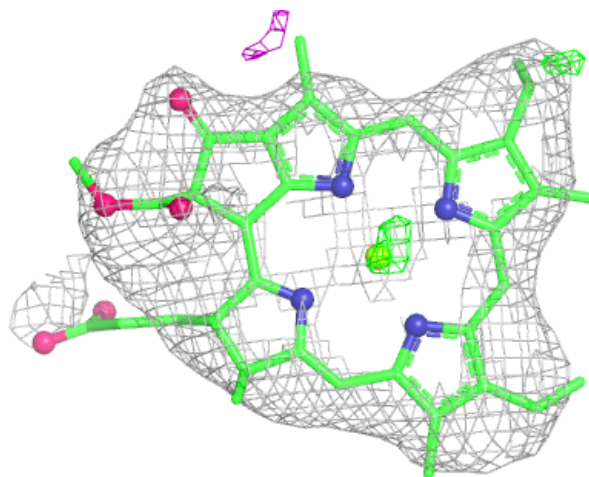
**Electron density around BCR B 4009:**

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



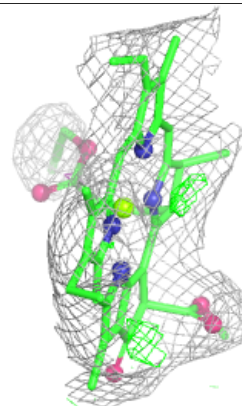
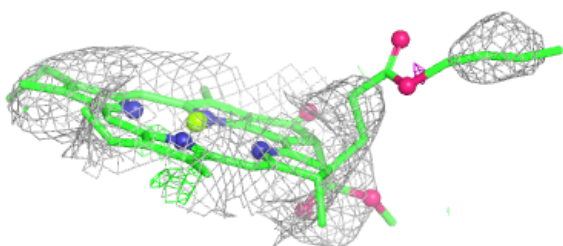
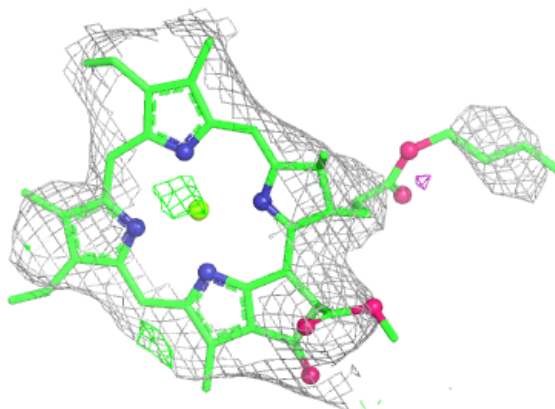
Electron density around CLA J 1302:

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



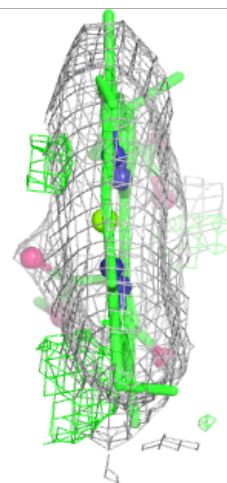
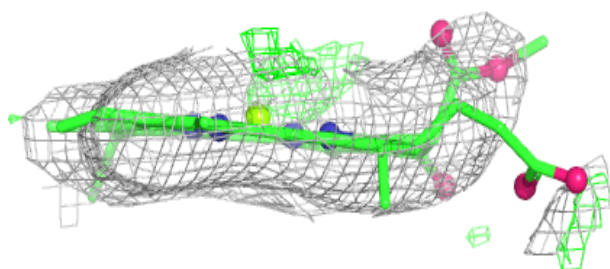
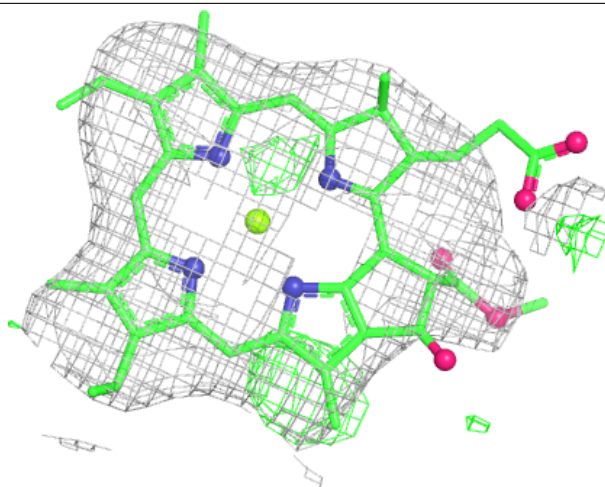
Electron density around CLA A 1114:

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



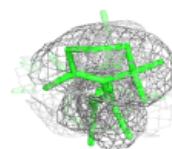
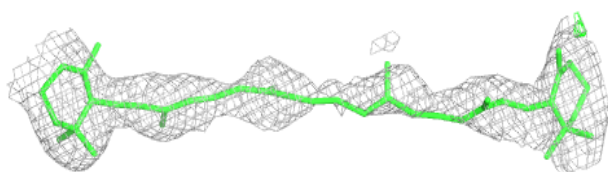
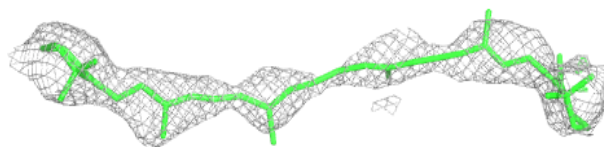
Electron density around CL0 A 1108:

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

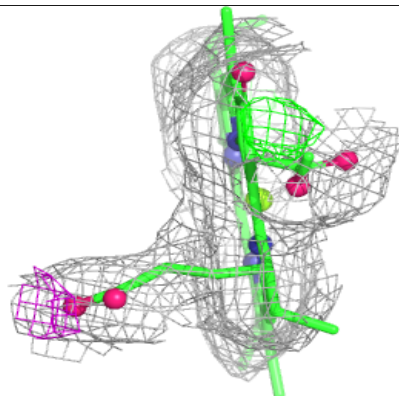
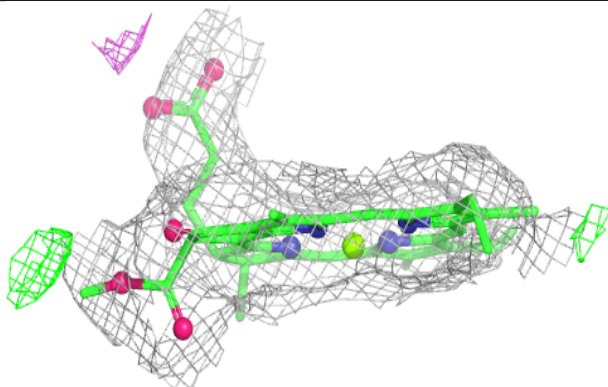
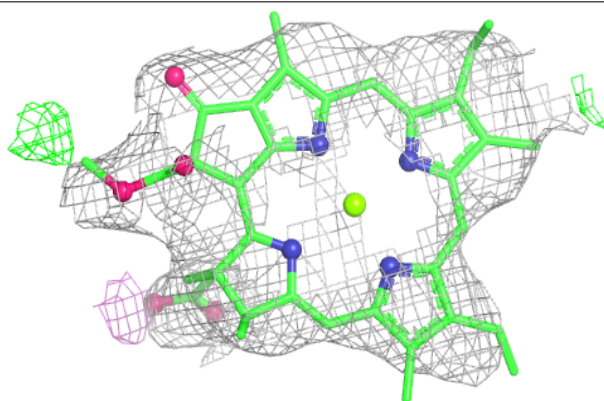


Electron density around BCR A 4003:

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

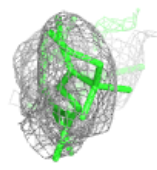
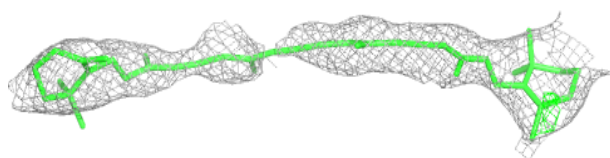
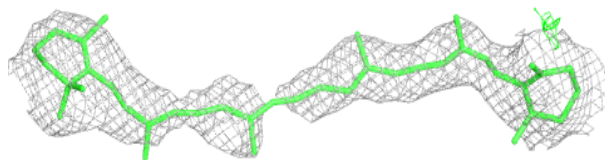
**Electron density around CLA B 1208:**

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

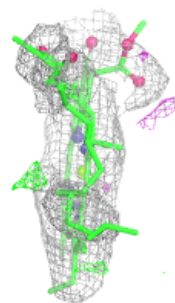
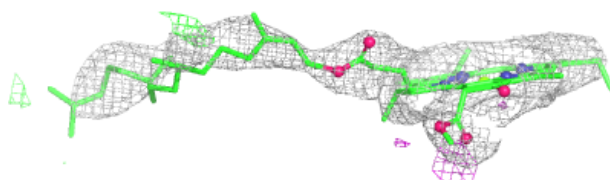
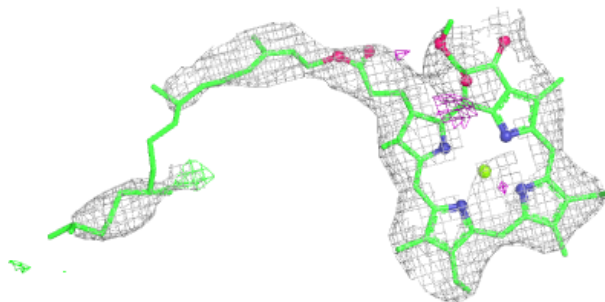


Electron density around BCR B 4004:

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

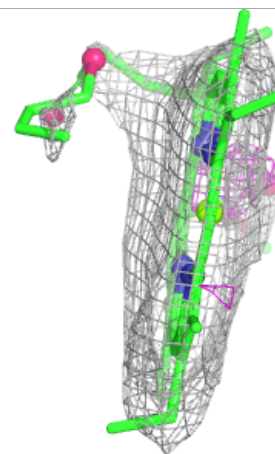
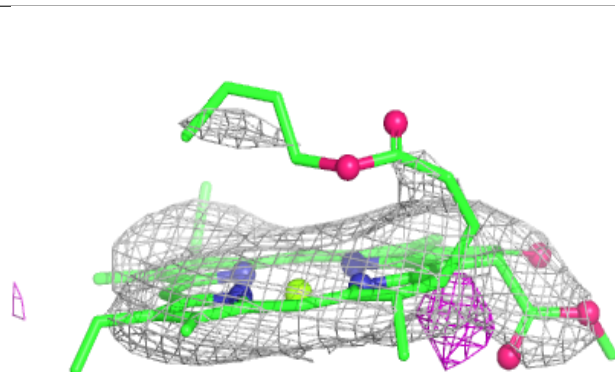
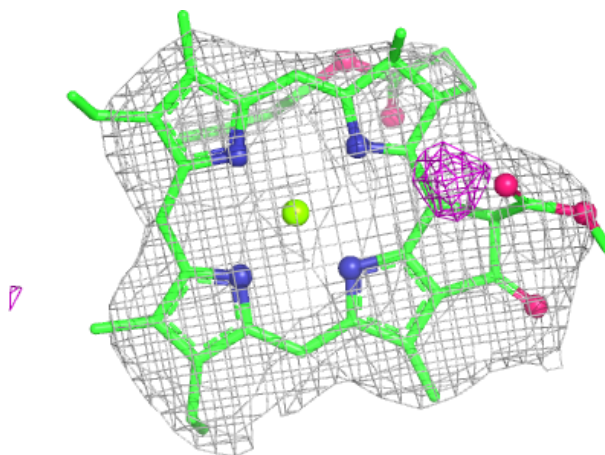
**Electron density around CLA F 1410:**

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



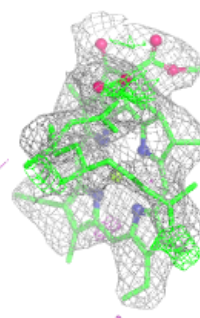
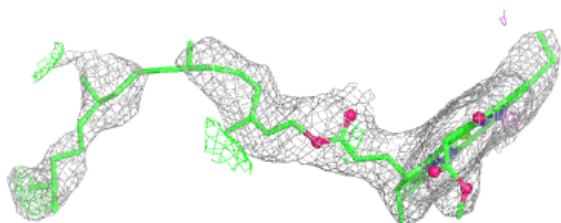
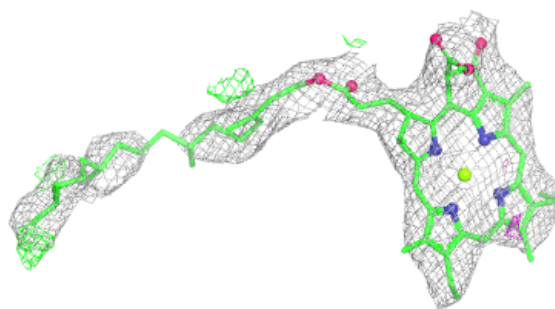
Electron density around CLA A 1120:

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

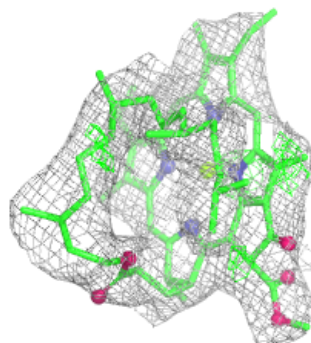
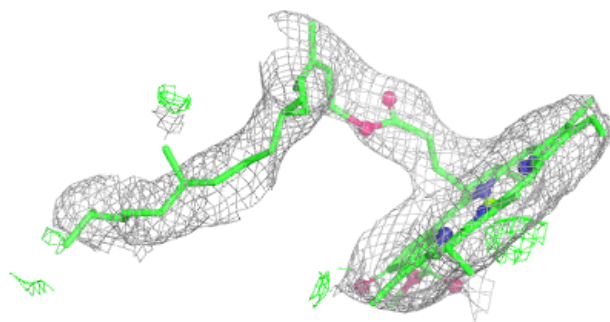
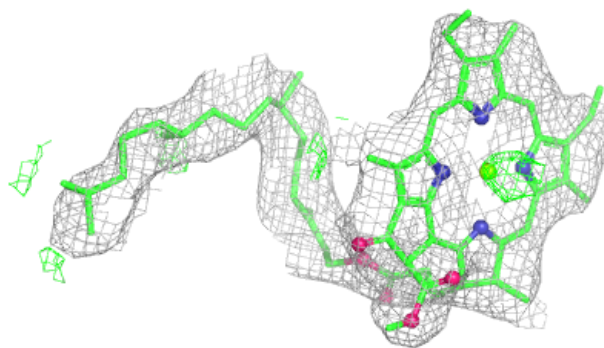


Electron density around CLA B 1230:

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

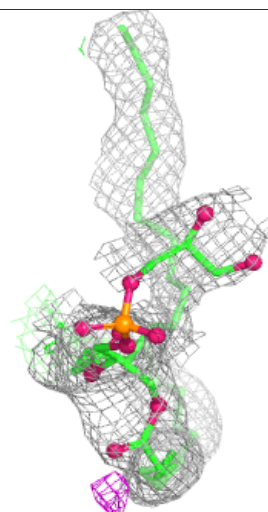
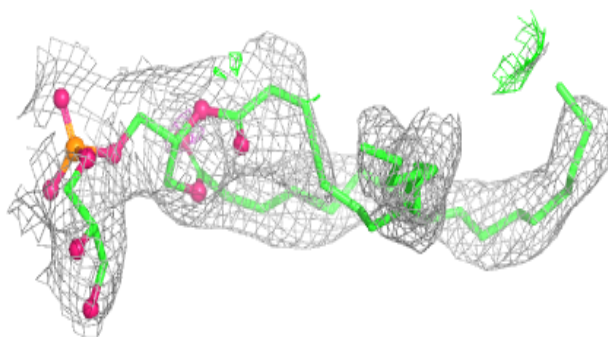
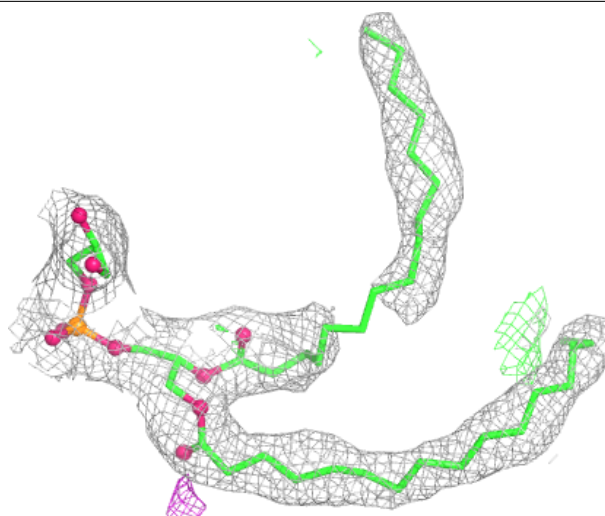
**Electron density around CLA B 1231:**

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



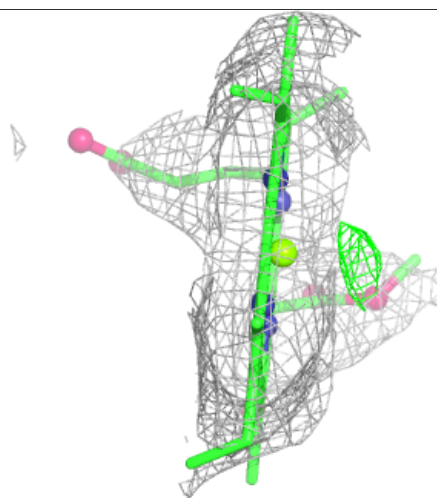
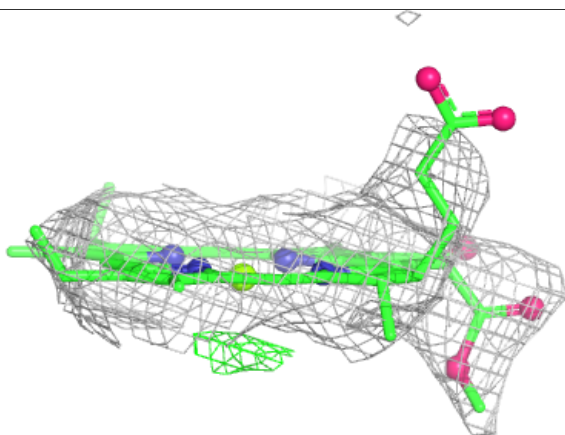
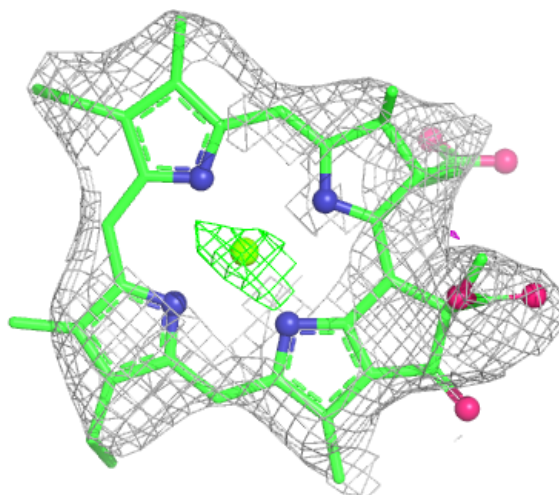
Electron density around LHG B 5004:

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



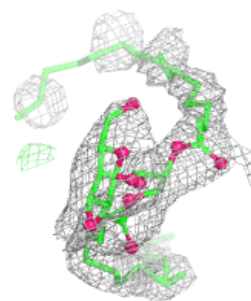
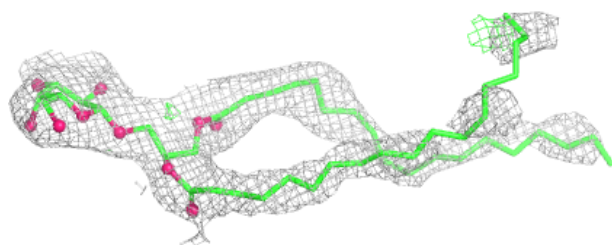
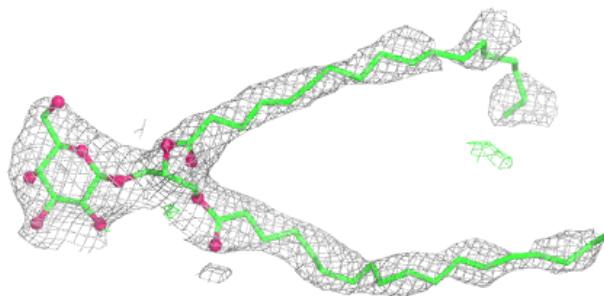
Electron density around CLA B 1212:

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



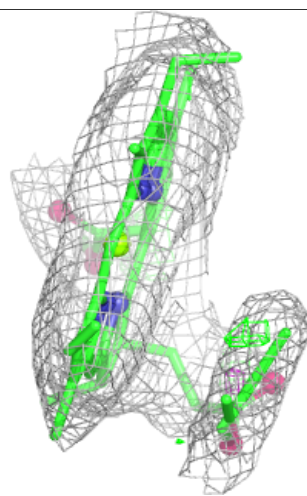
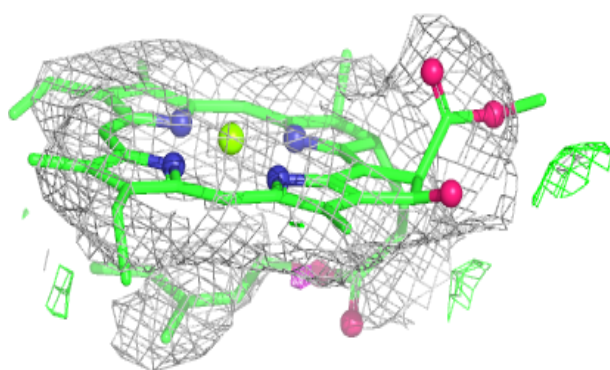
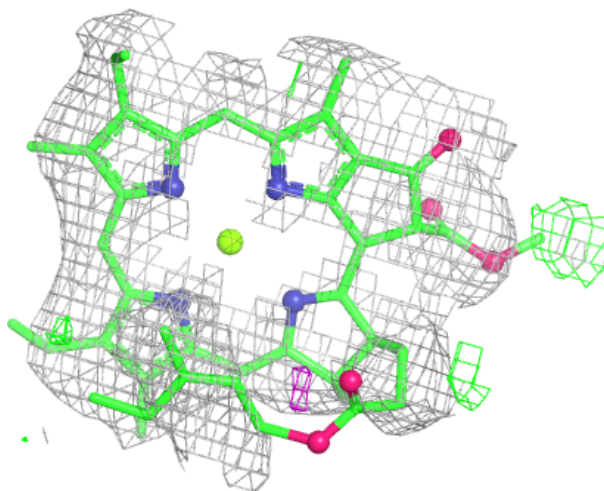
Electron density around LMG B 5002:

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



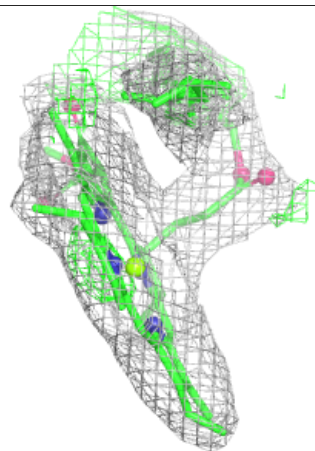
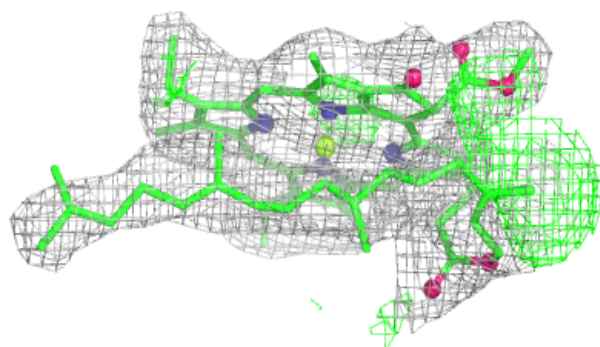
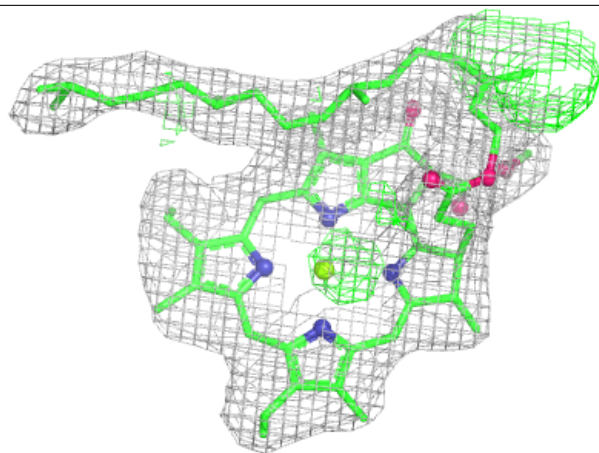
Electron density around CLA B 1218:

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



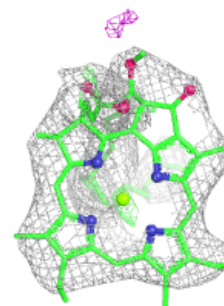
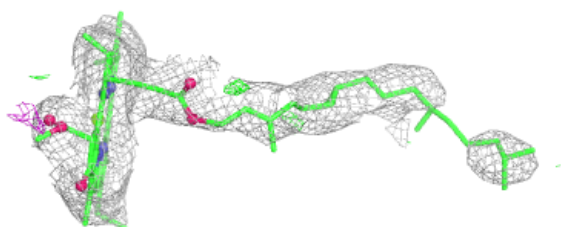
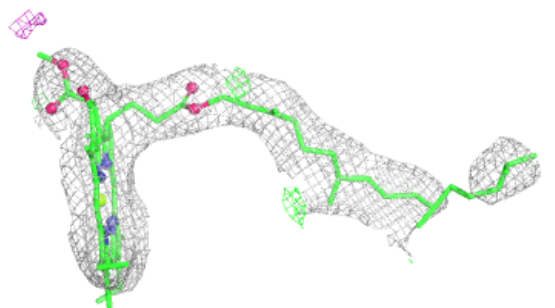
Electron density around CLA B 1228:

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

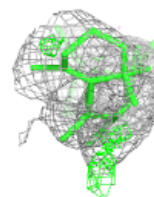
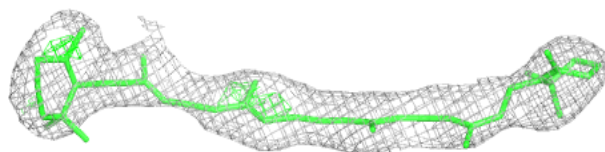
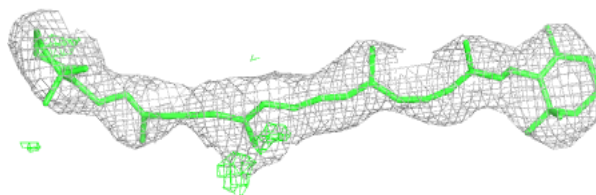


Electron density around CLA A 1105:

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

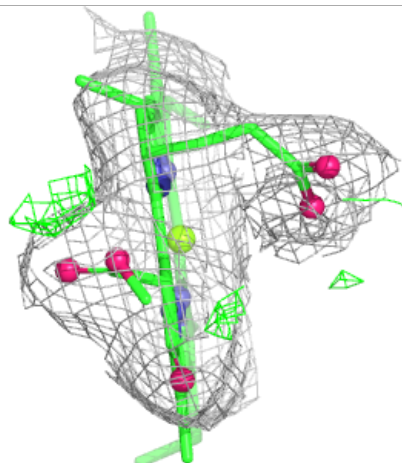
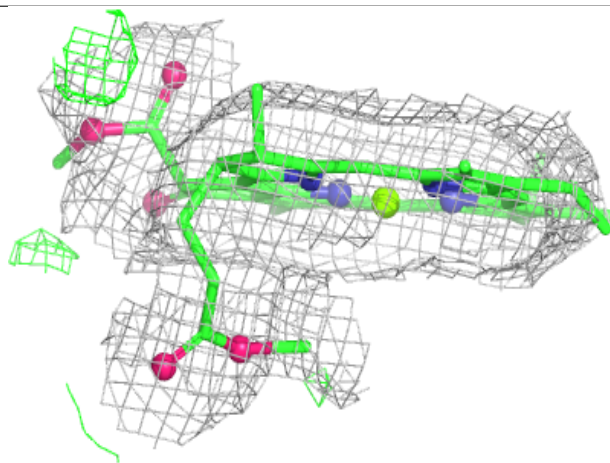
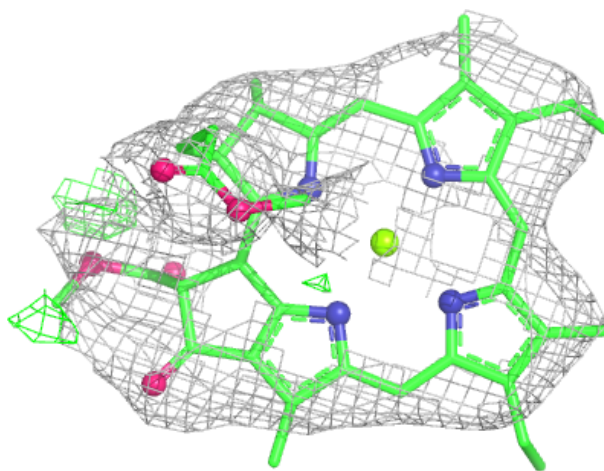
**Electron density around BCR J 4013:**

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



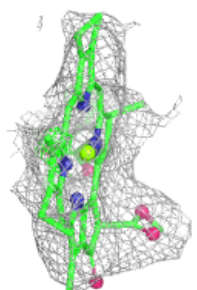
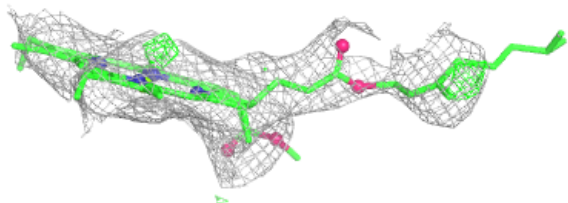
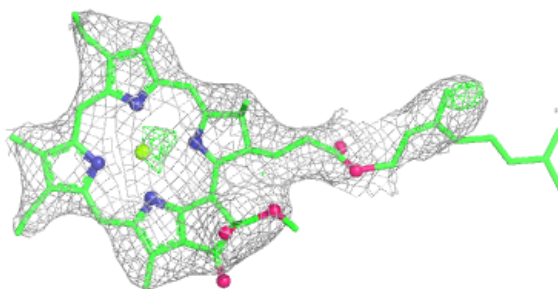
Electron density around CLA A 1134:

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



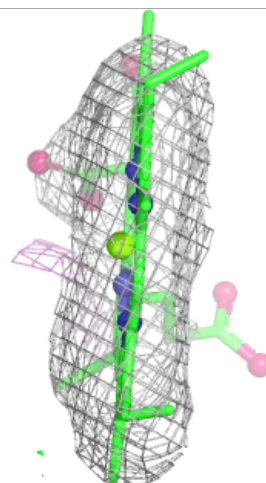
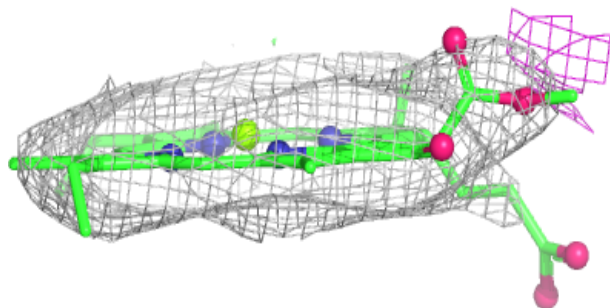
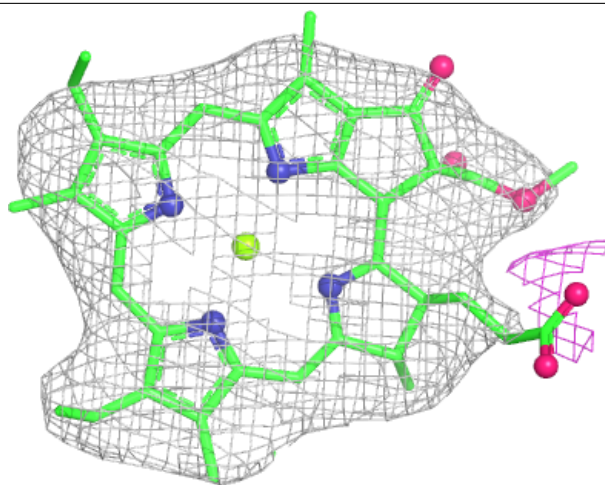
Electron density around CLA A 1135:

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



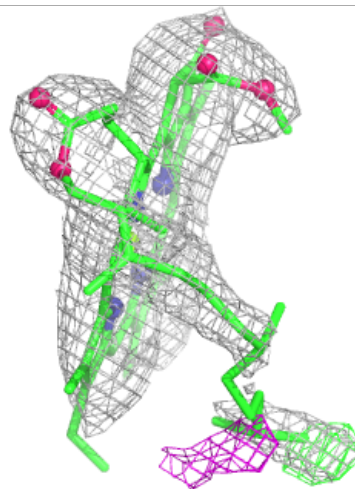
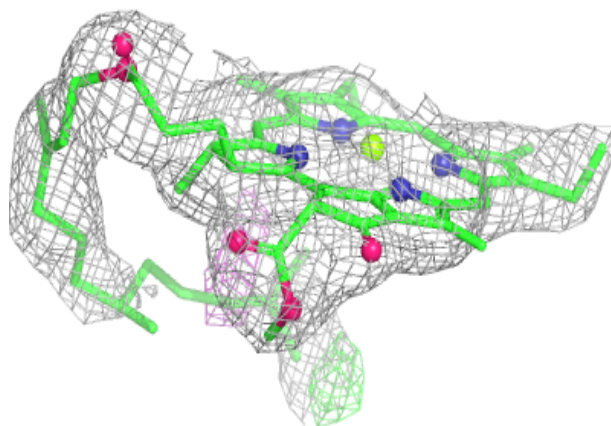
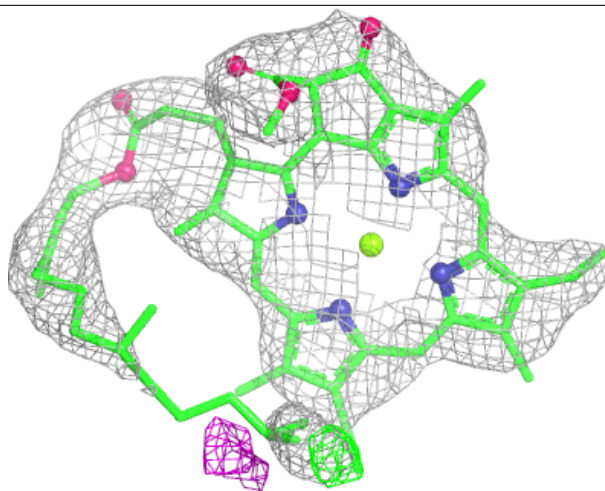
Electron density around CLA B 1240:

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



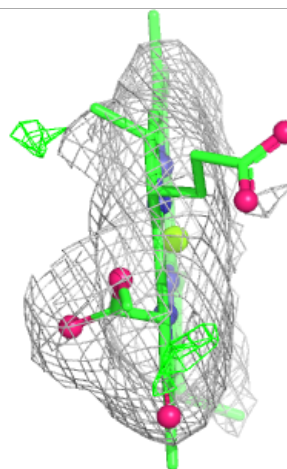
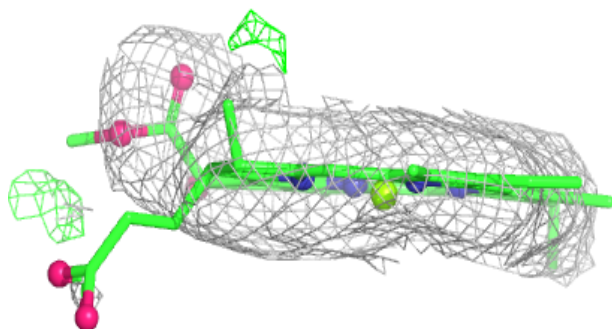
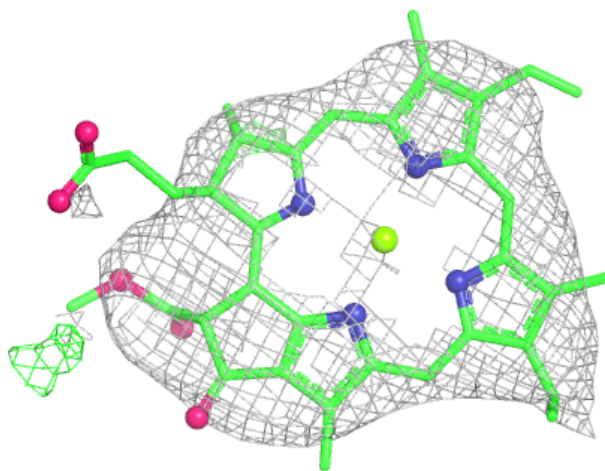
Electron density around CLA A 1111:

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



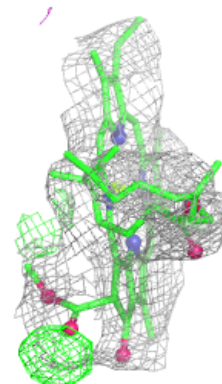
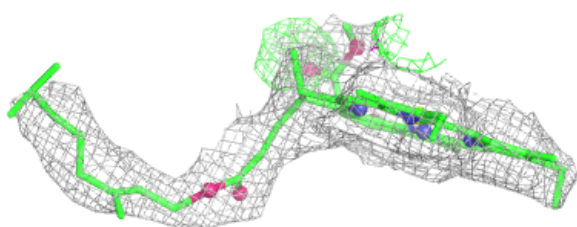
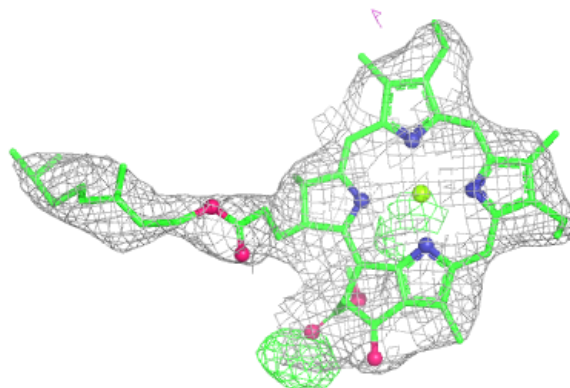
Electron density around CLA A 1113:

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

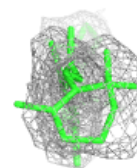
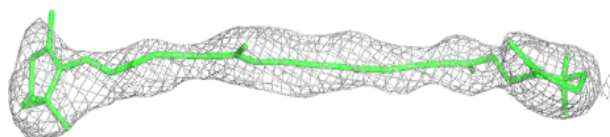
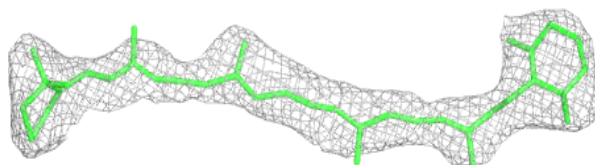


Electron density around CLA A 1124:

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

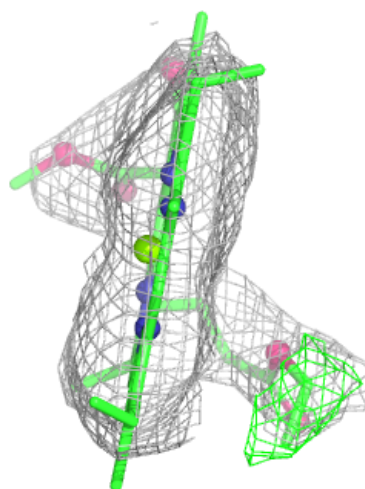
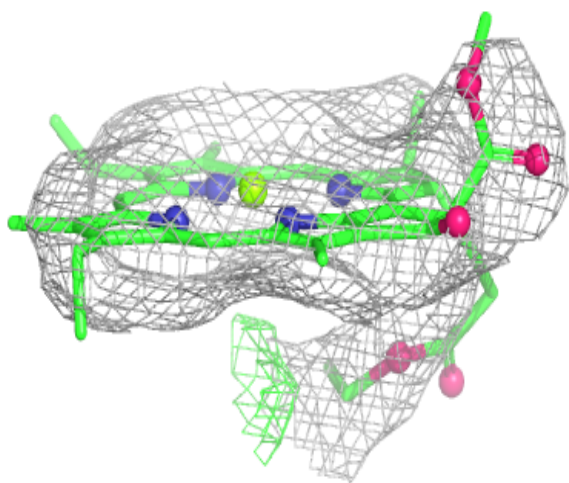
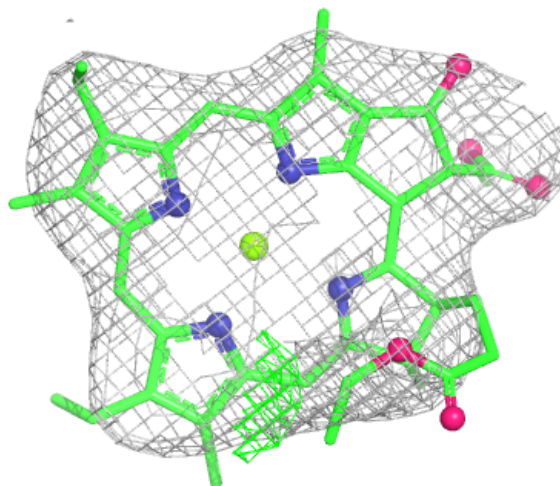
**Electron density around BCR B 4005:**

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



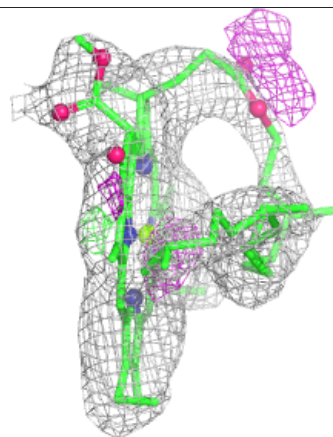
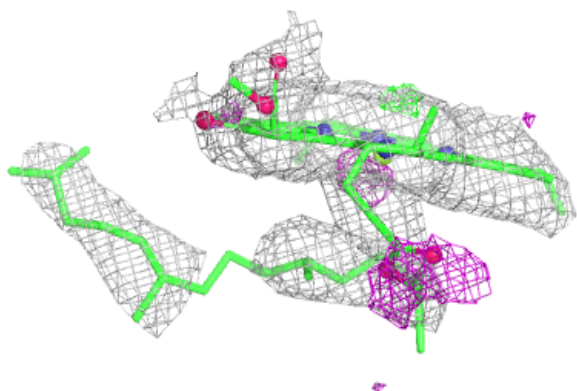
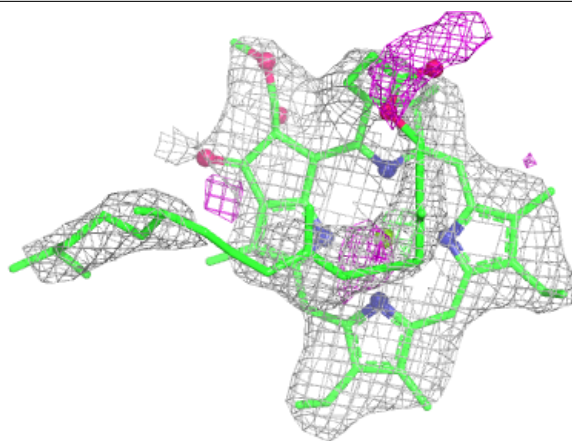
Electron density around CLA B 1217:

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

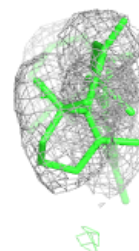
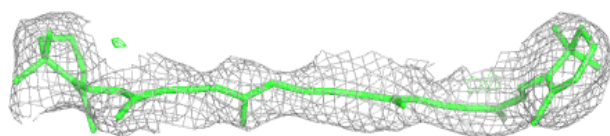
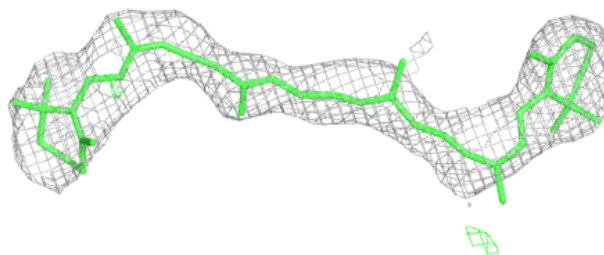


Electron density around CLA B 1224:

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

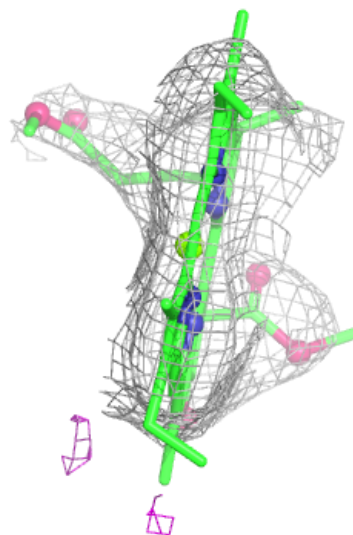
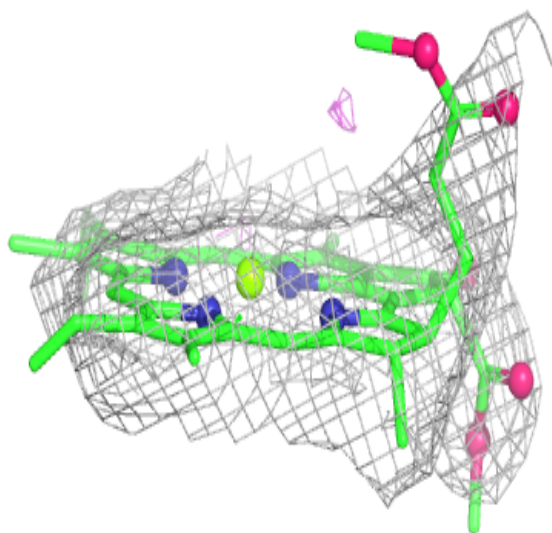
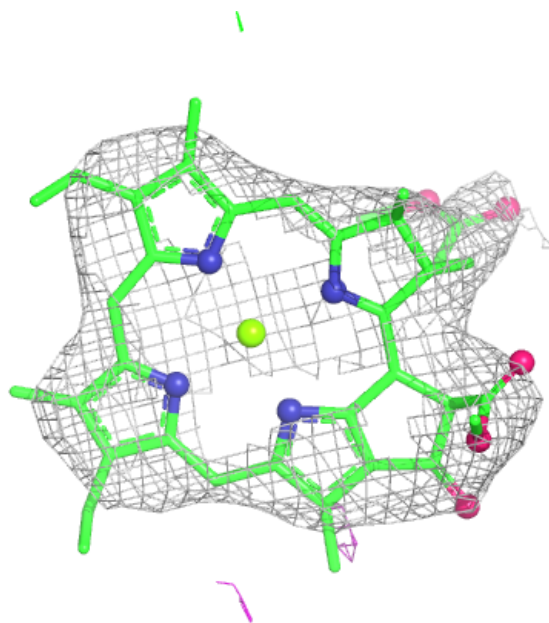
**Electron density around BCR B 4006:**

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



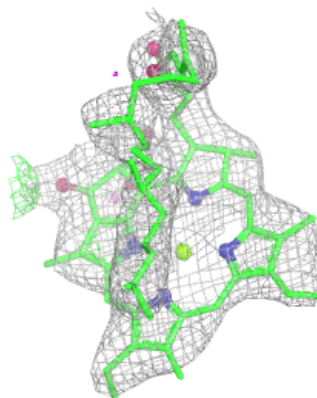
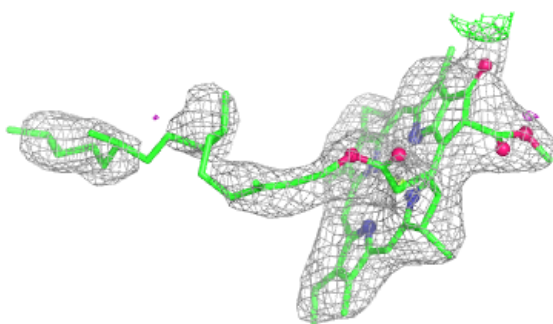
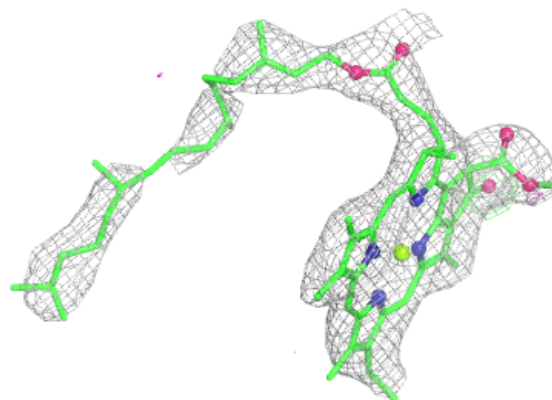
Electron density around CLA A 1118:

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



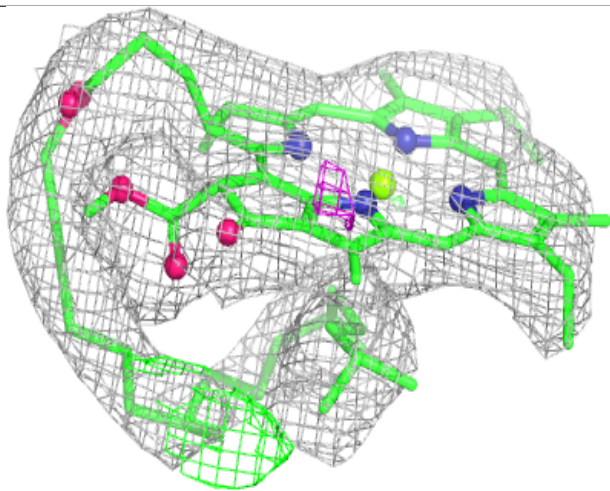
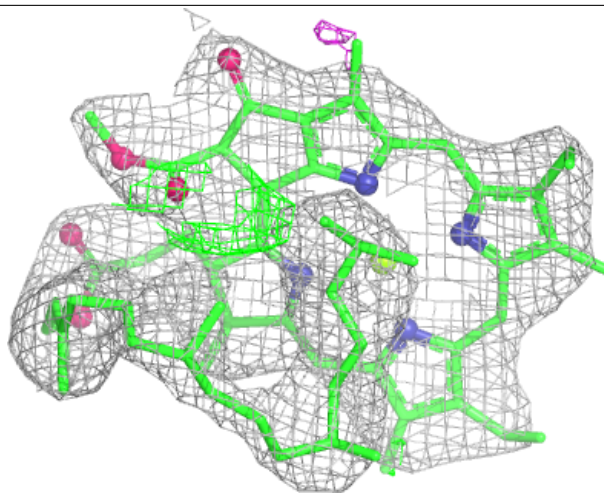
Electron density around CLA A 1102:

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



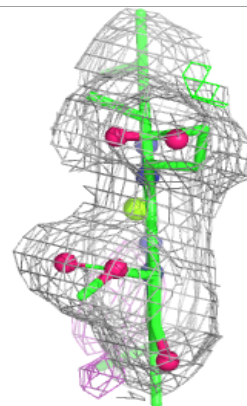
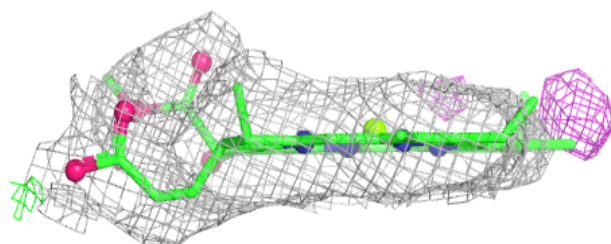
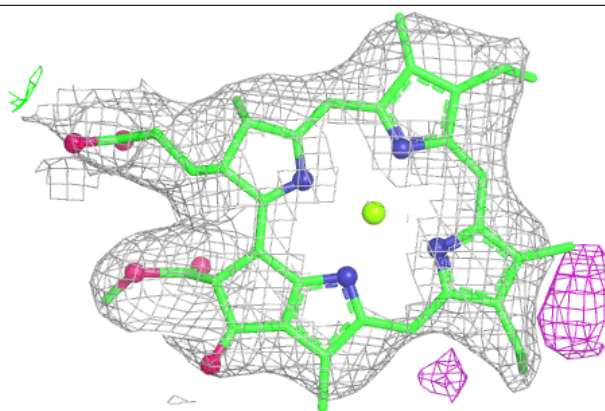
Electron density around CLA B 1203:

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

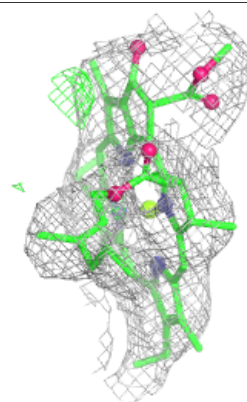
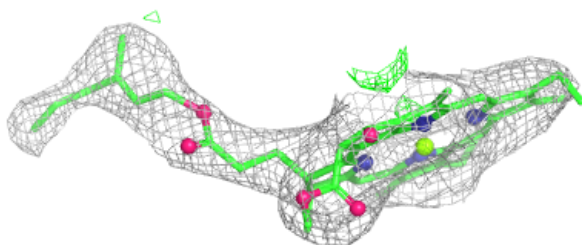
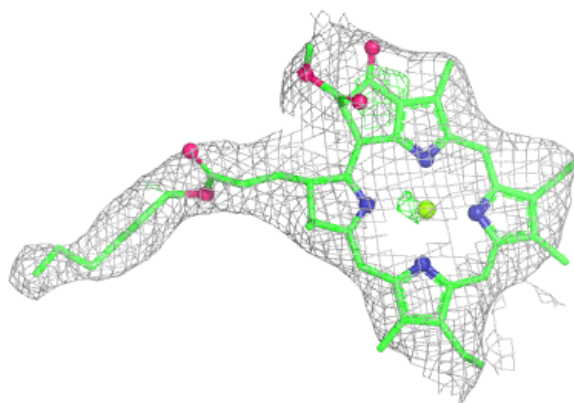


Electron density around CLA F 1301:

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

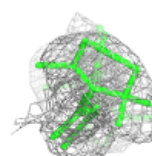
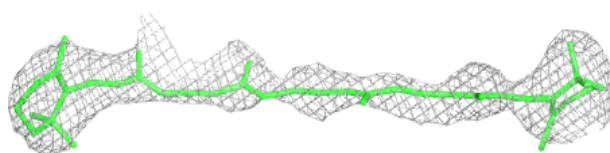
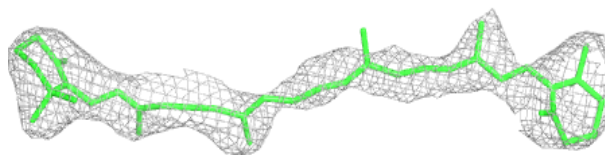
**Electron density around CLA A 1125:**

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

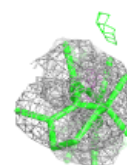
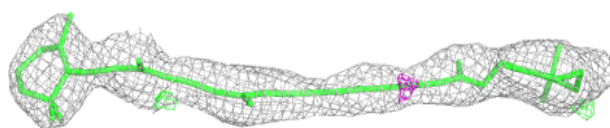
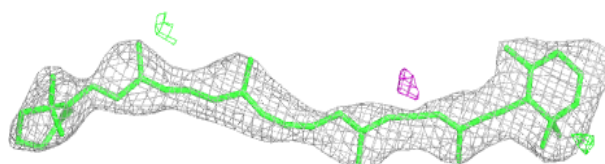


Electron density around BCR A 4002:

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

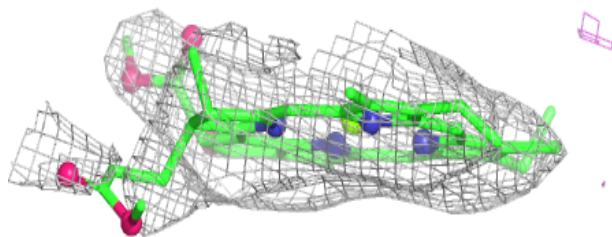
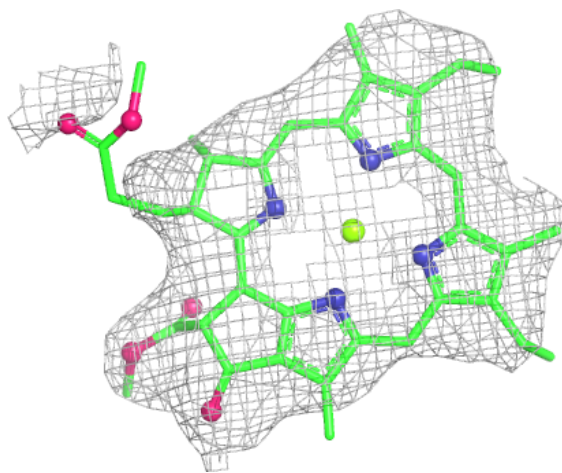
**Electron density around BCR F 4015:**

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



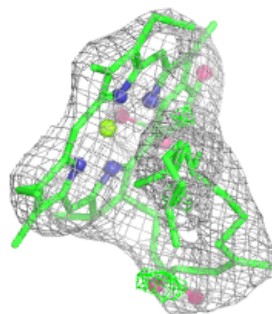
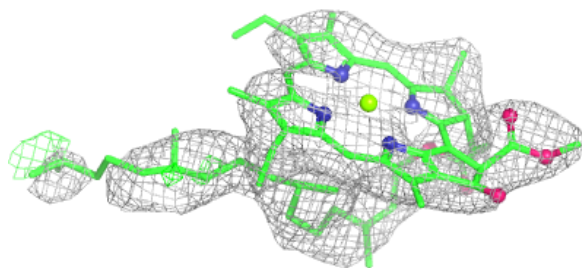
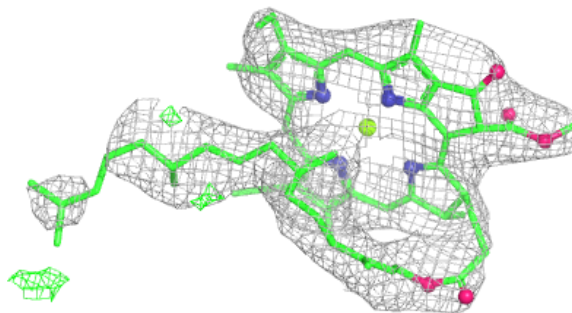
Electron density around CLA A 1121:

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

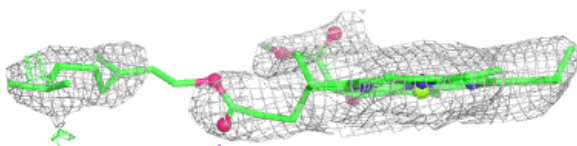
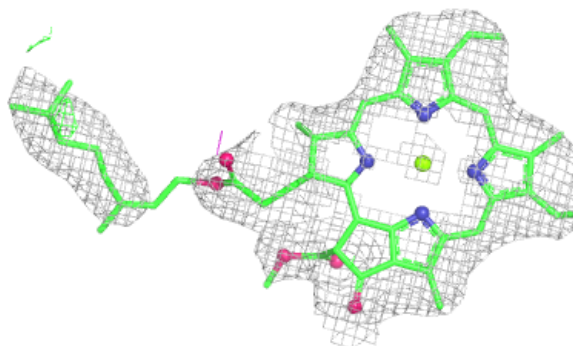


Electron density around CLA B 1214:

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

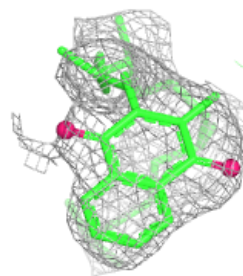
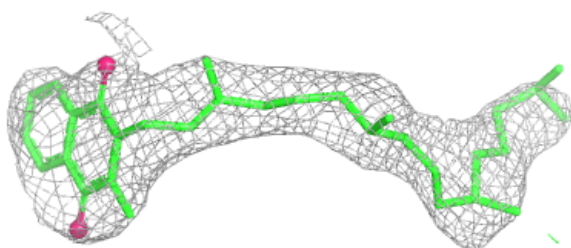
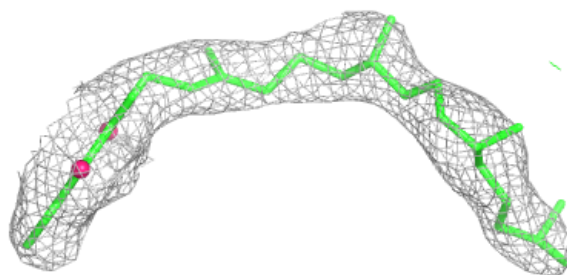
**Electron density around CLA A 1131:**

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



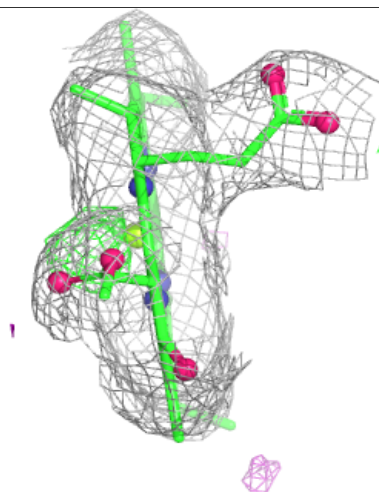
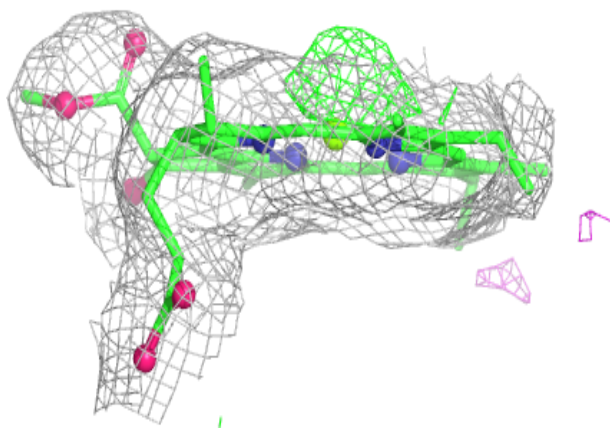
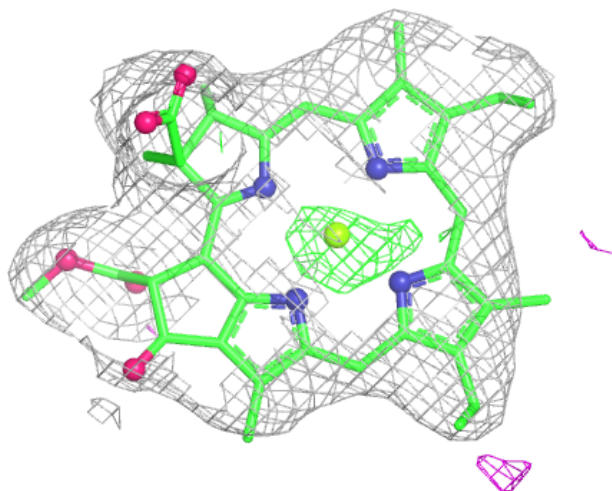
Electron density around PQN B 2002:

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



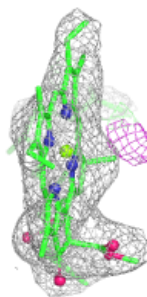
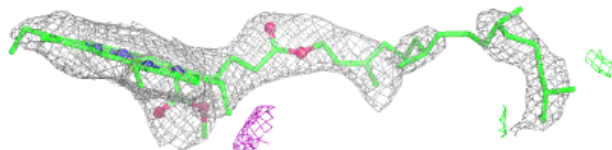
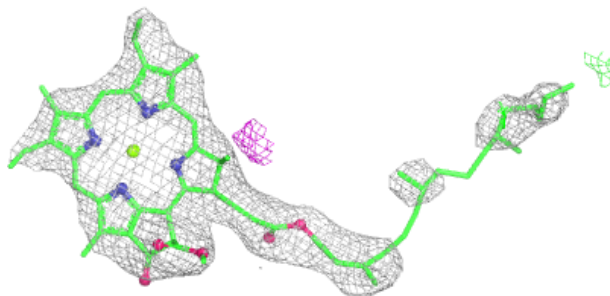
Electron density around CLA B 1232:

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

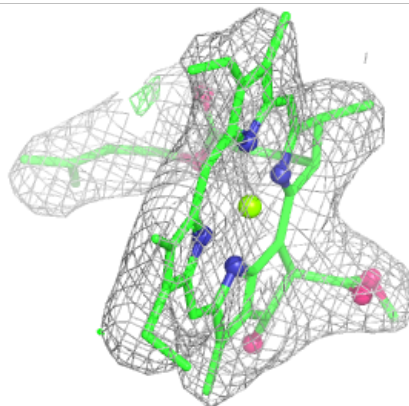
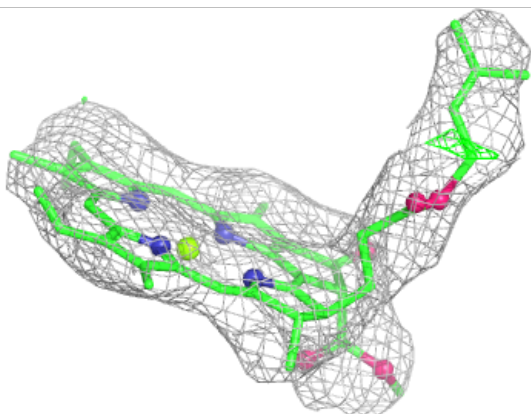
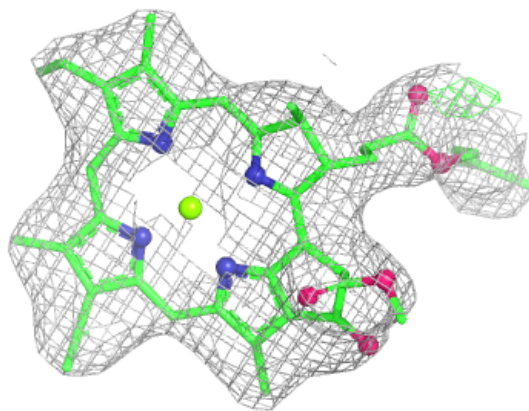


Electron density around CLA B 1234:

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

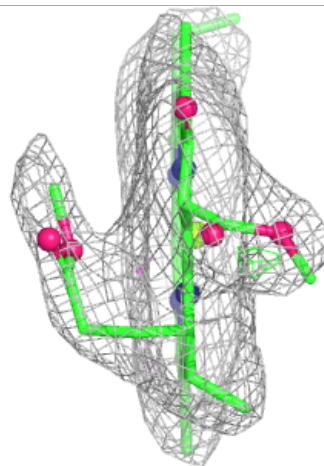
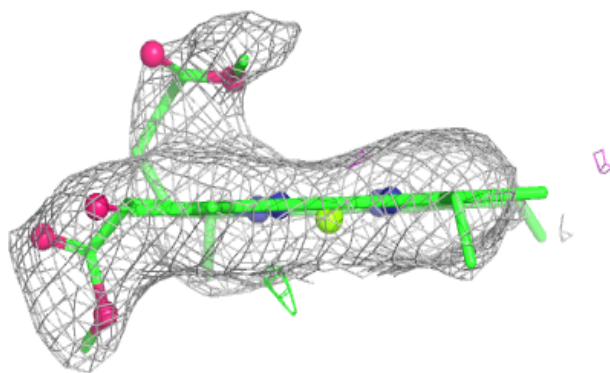
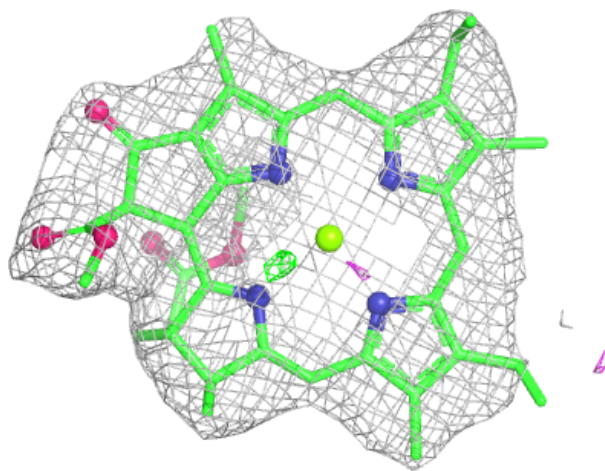
**Electron density around CLA B 1236:**

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



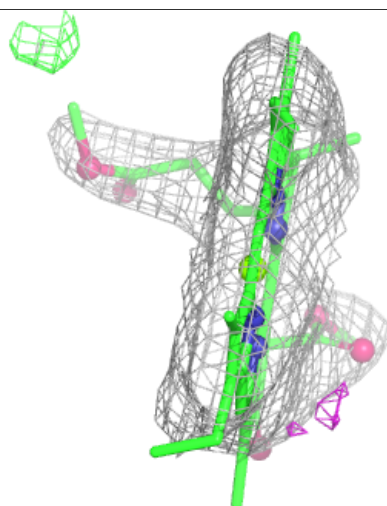
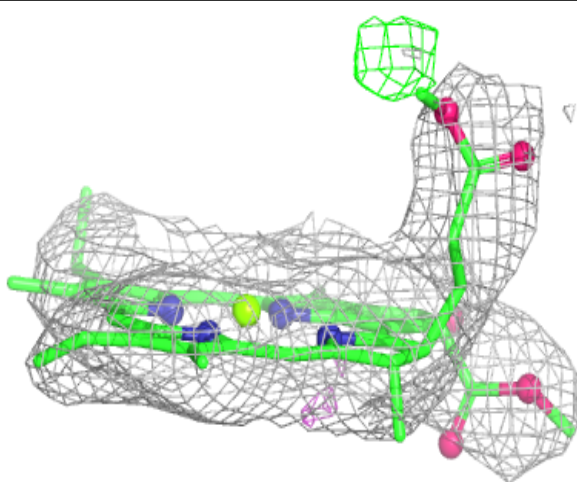
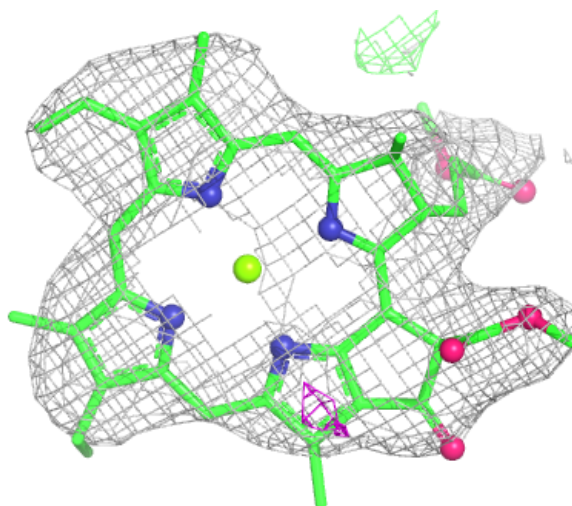
Electron density around CLA B 1201:

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



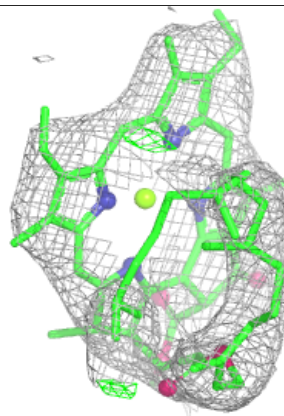
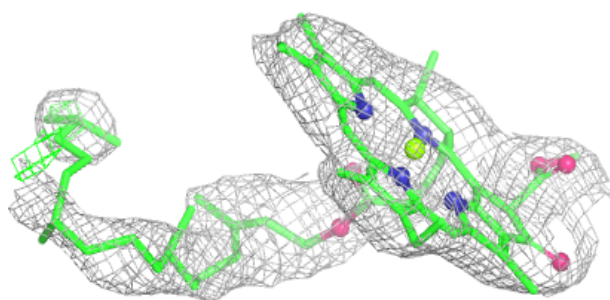
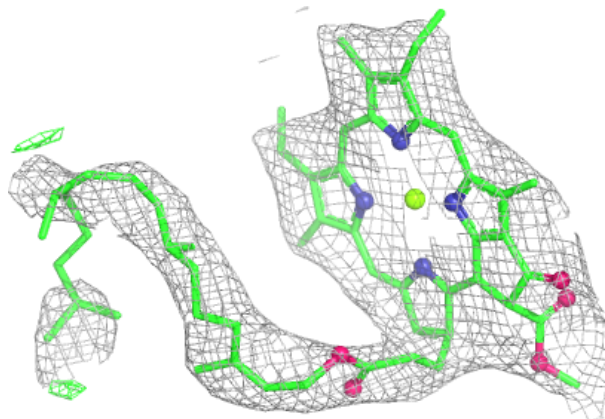
Electron density around CLA A 1133:

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



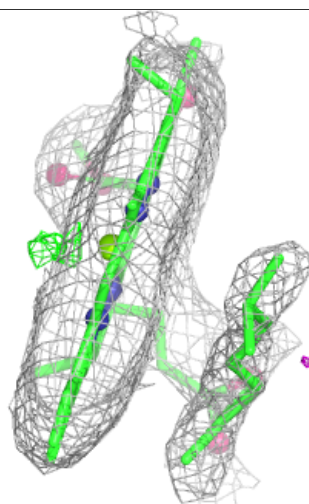
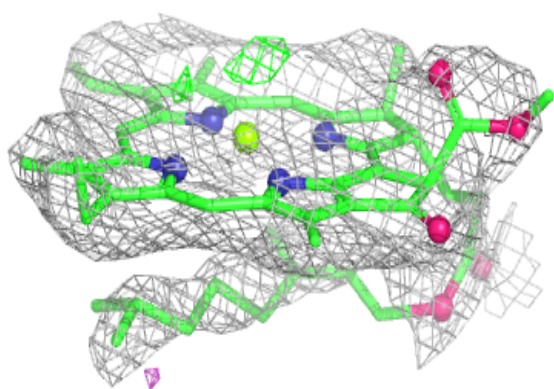
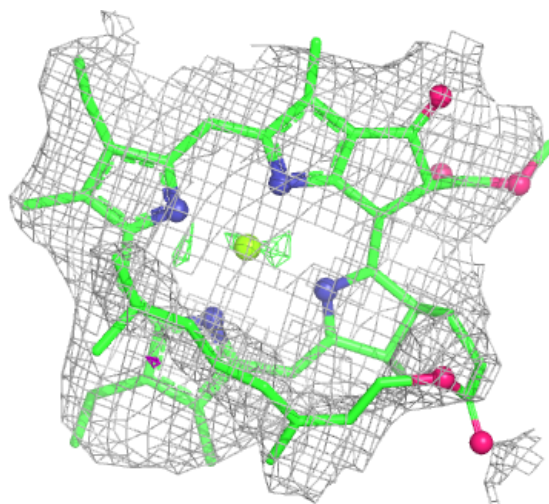
Electron density around CLA A 1122:

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



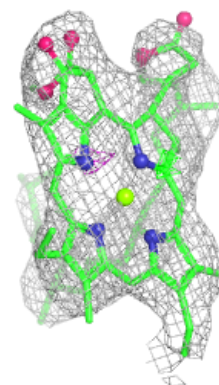
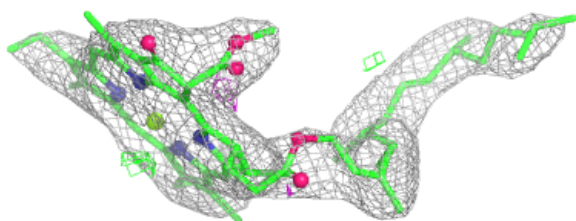
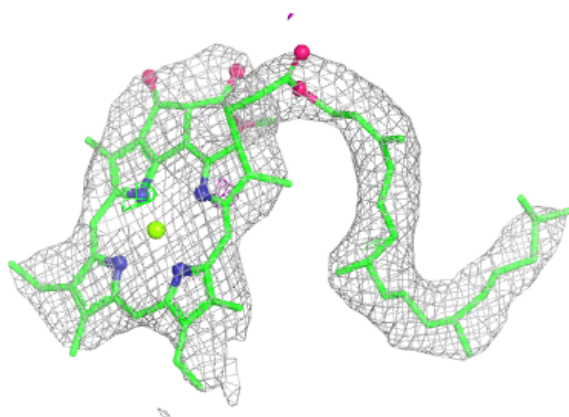
Electron density around CLA B 1219:

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

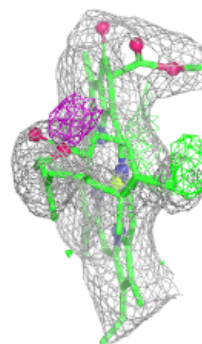
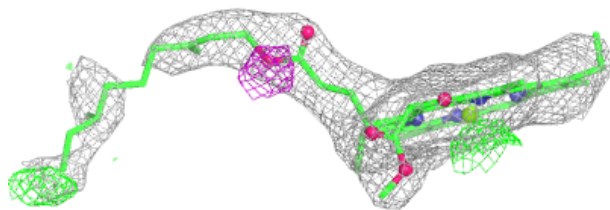
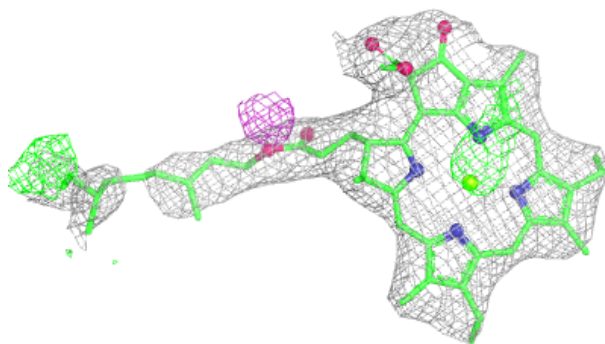


Electron density around CLA B 1221:

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

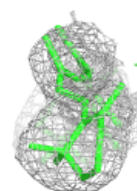
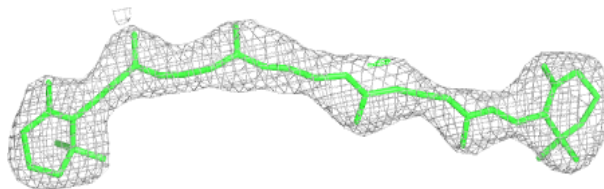
**Electron density around CLA B 1222:**

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

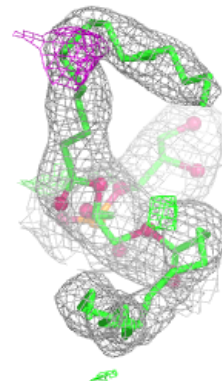
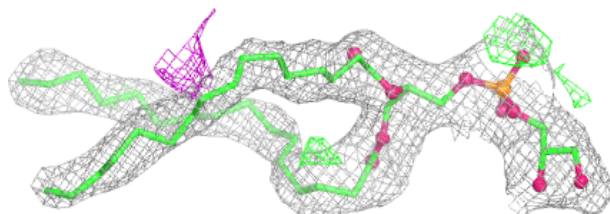
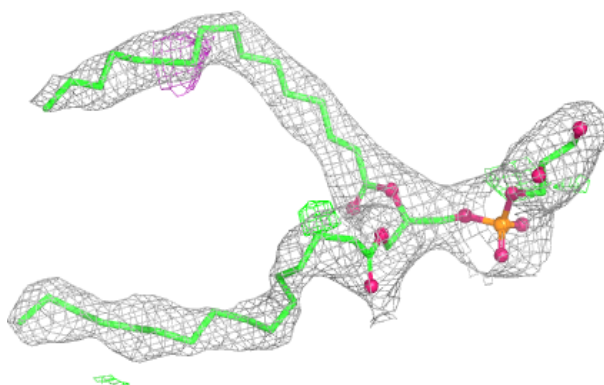


Electron density around BCR B 4010:

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

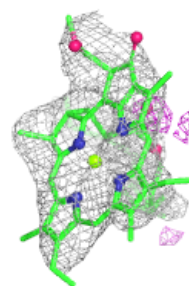
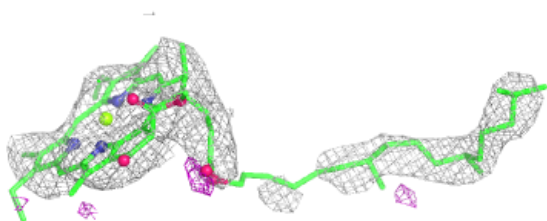
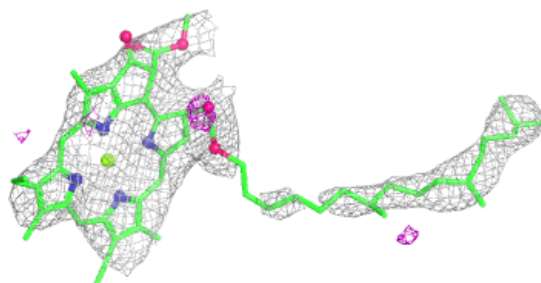
**Electron density around LHG A 5001:**

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



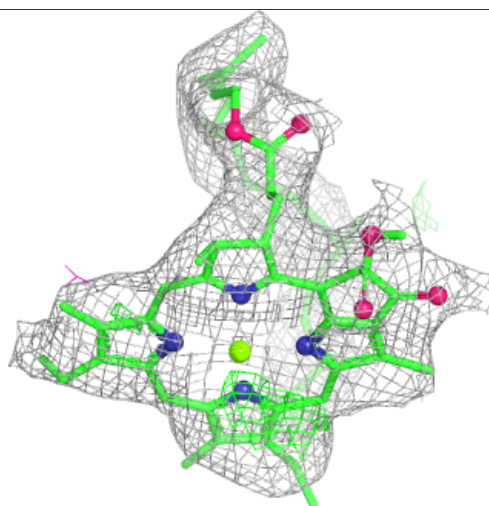
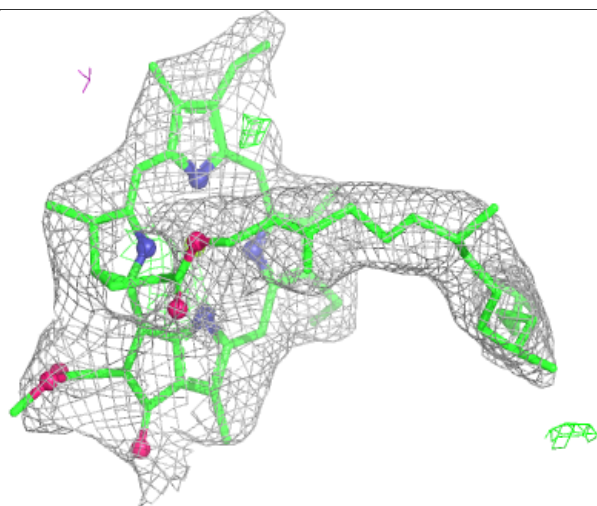
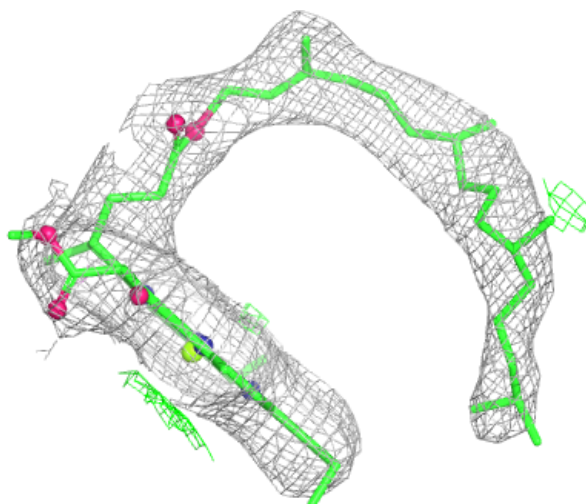
Electron density around CLA A 1119:

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



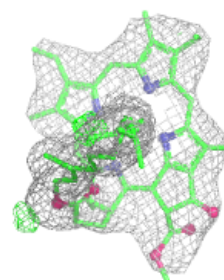
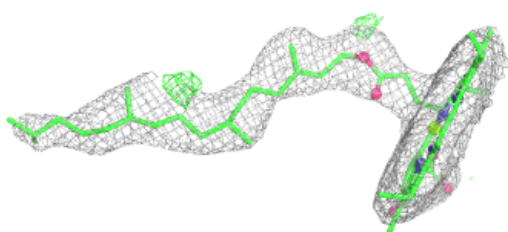
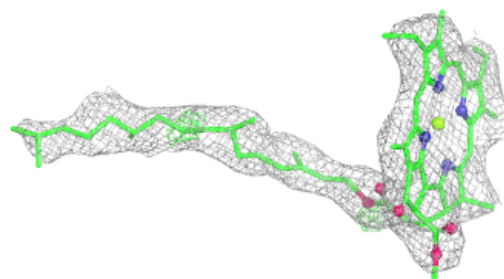
Electron density around CLA B 1216:

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

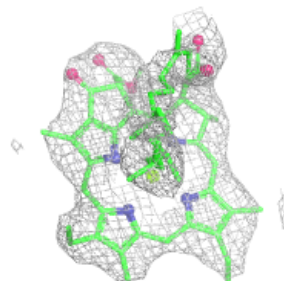
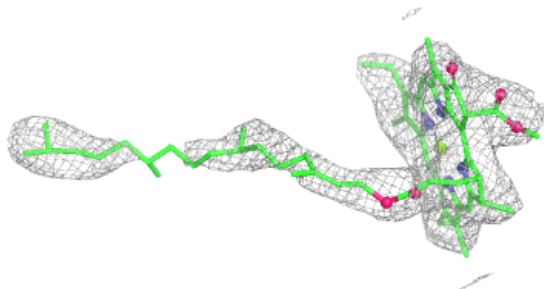
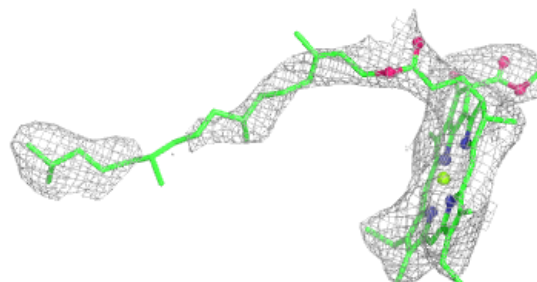


Electron density around CLA B 1225:

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

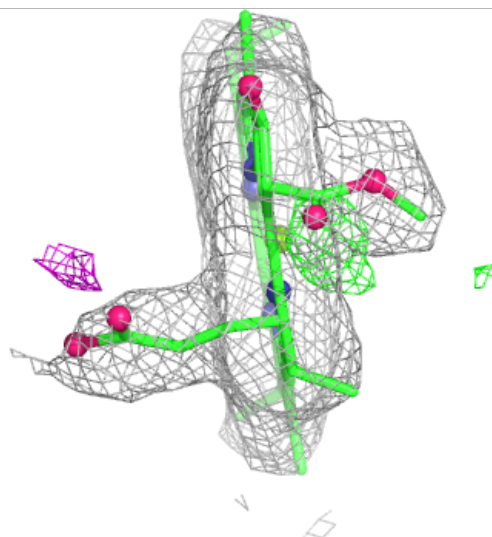
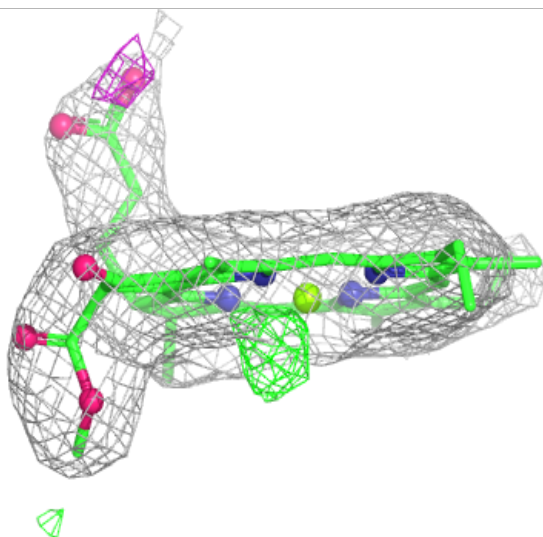
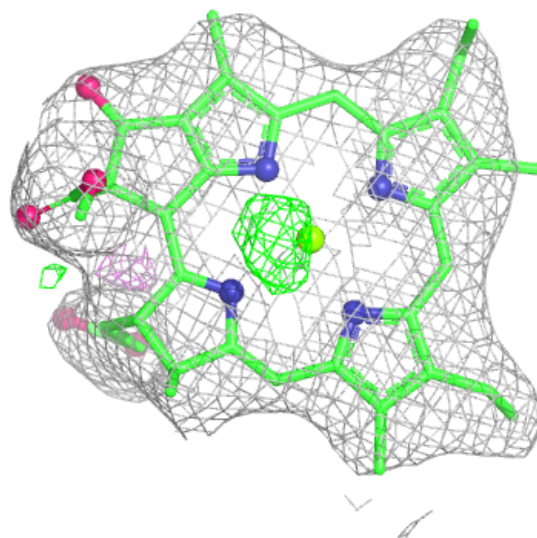
**Electron density around CLA B 1226:**

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



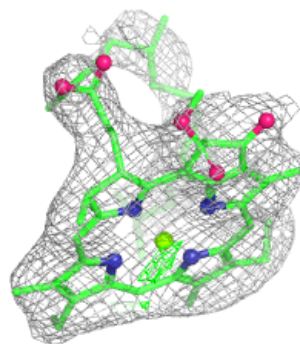
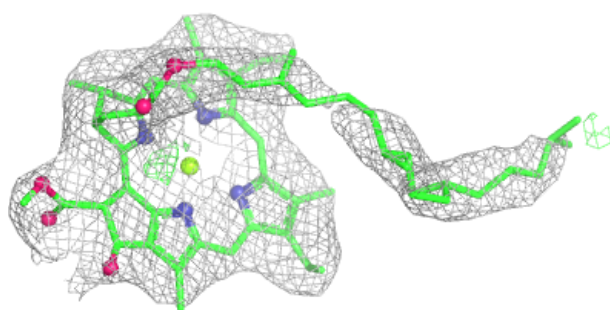
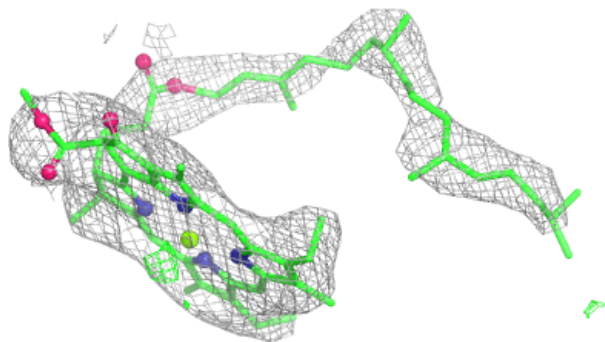
Electron density around CLA B 1227:

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

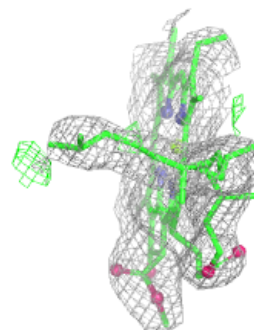
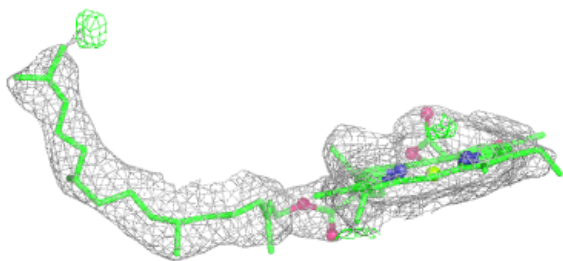
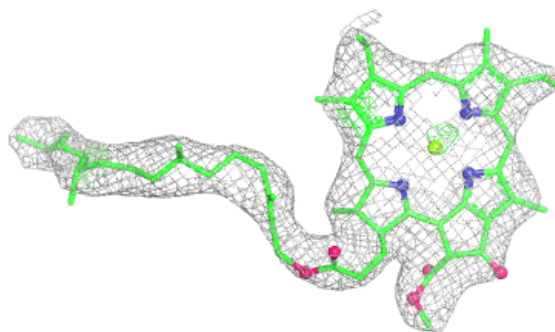


Electron density around CLA A 1109:

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

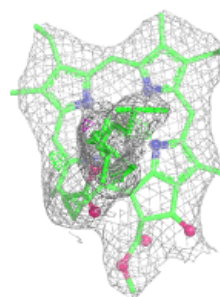
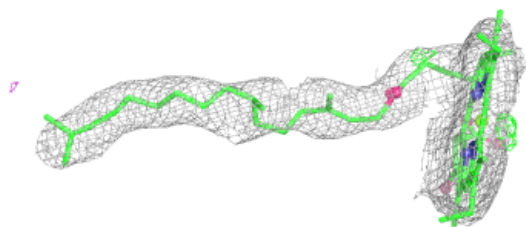
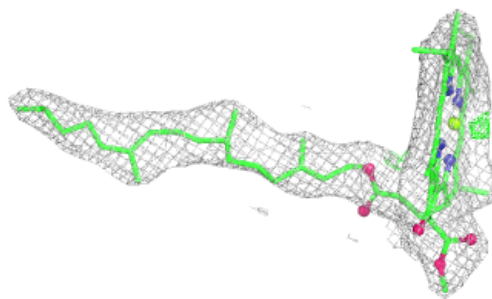
**Electron density around CLA B 1023:**

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

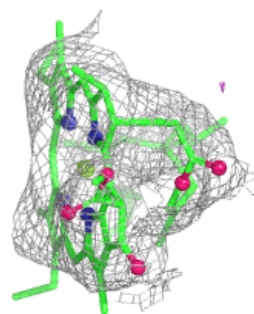
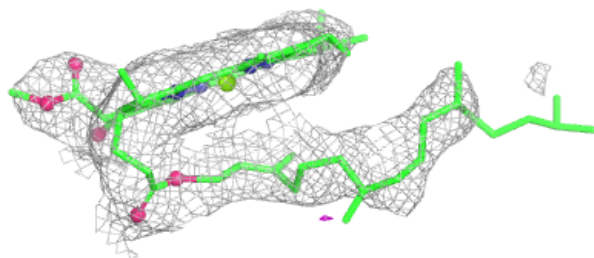
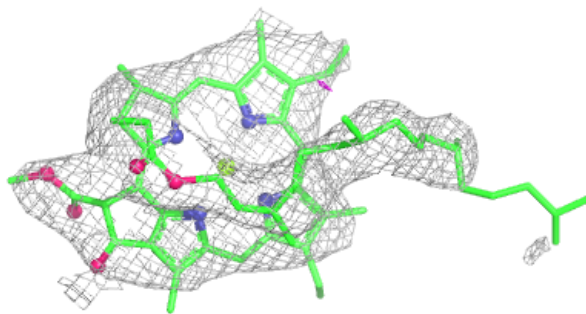


Electron density around CLA A 1126:

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

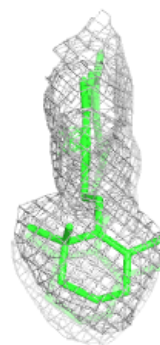
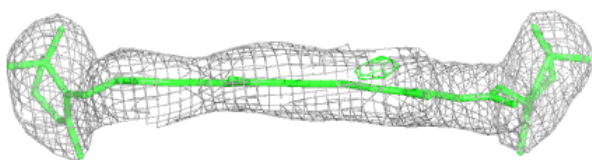
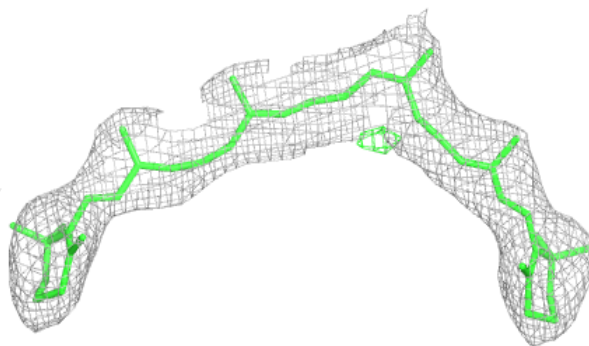
**Electron density around CLA A 1136:**

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

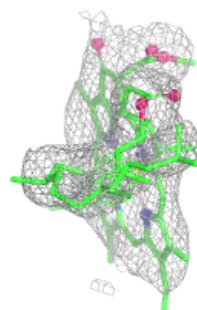
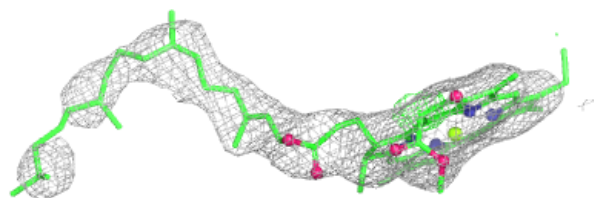
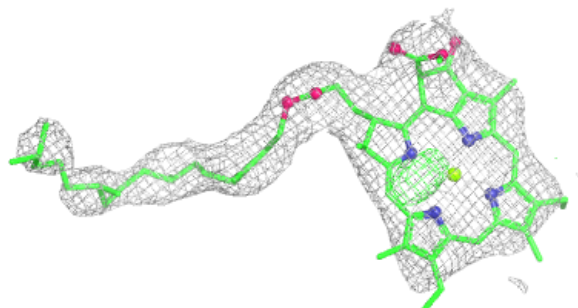


Electron density around BCR F 4016:

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

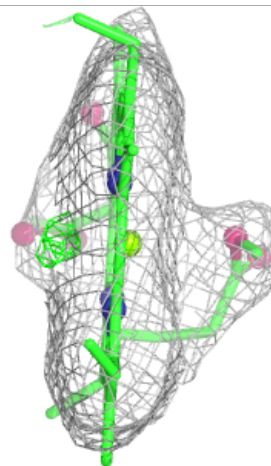
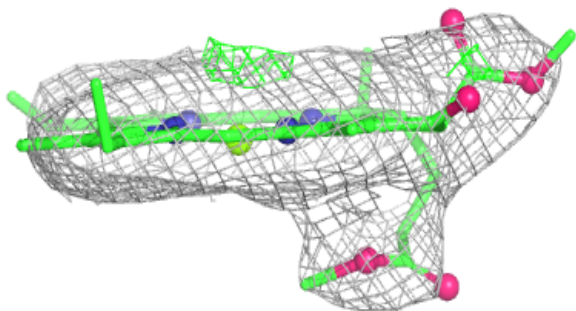
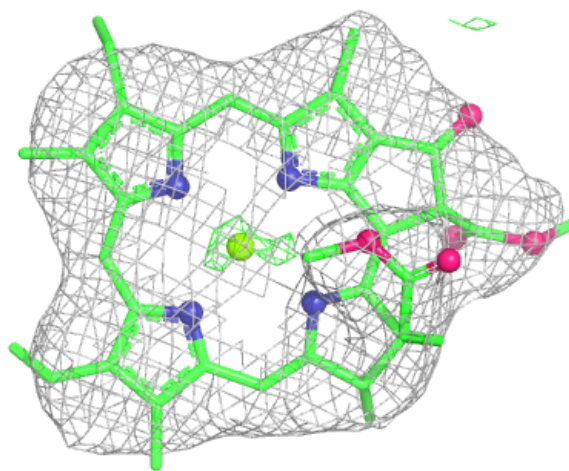
**Electron density around CLA B 1210:**

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



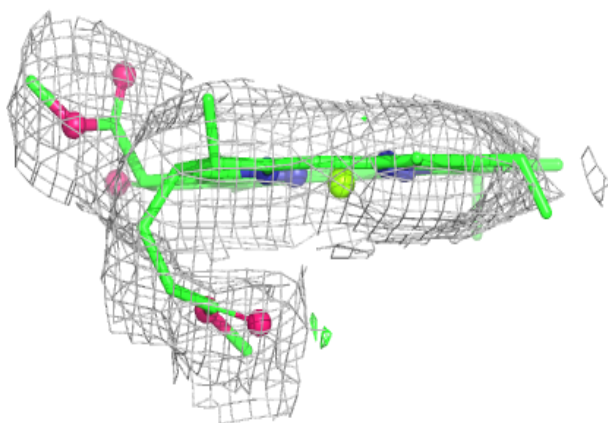
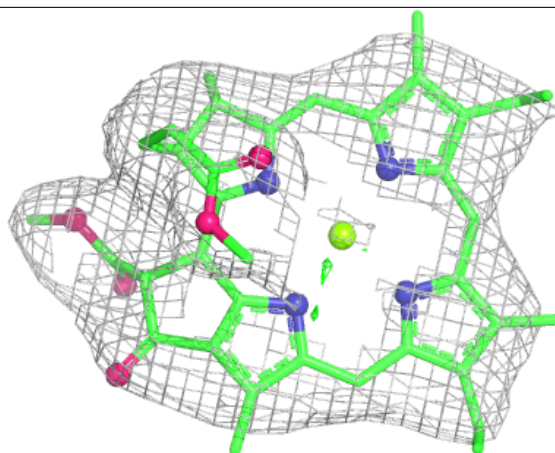
Electron density around CLA A 1115:

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

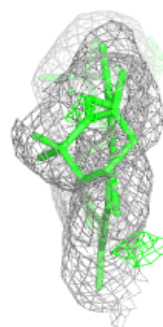
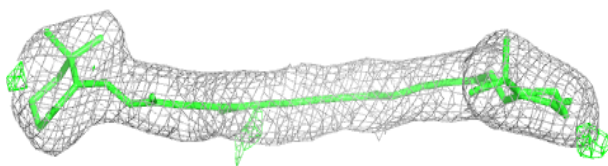
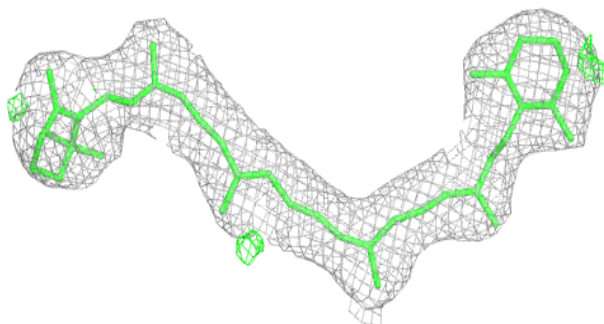


Electron density around CLA B 1204:

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

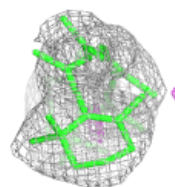
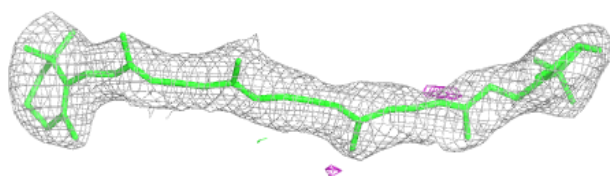
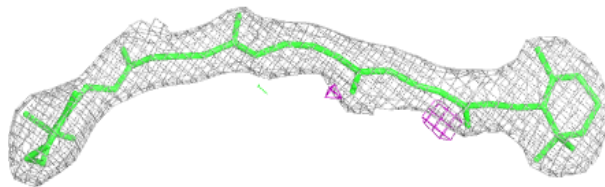
**Electron density around BCR B 4011:**

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



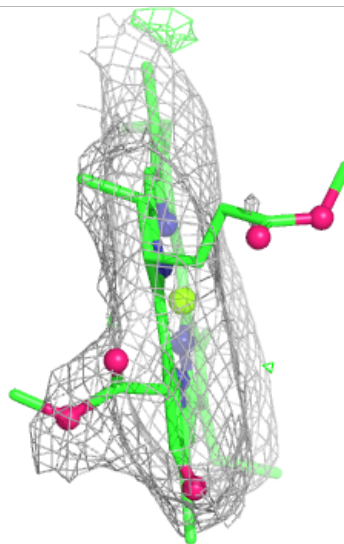
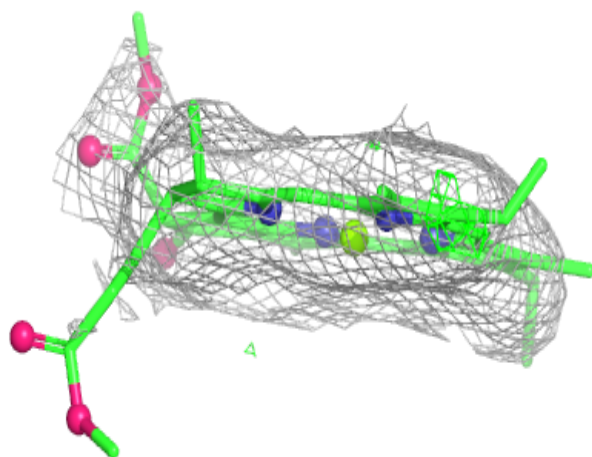
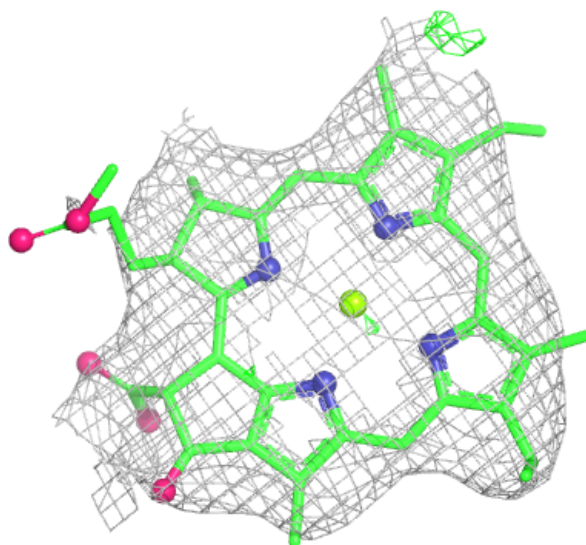
Electron density around BCR B 4014:

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



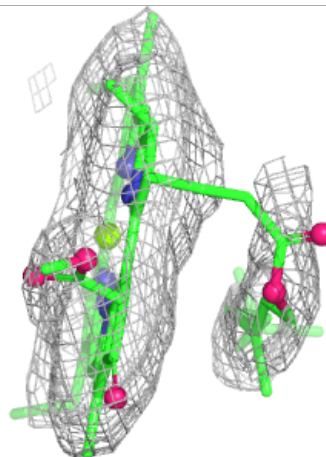
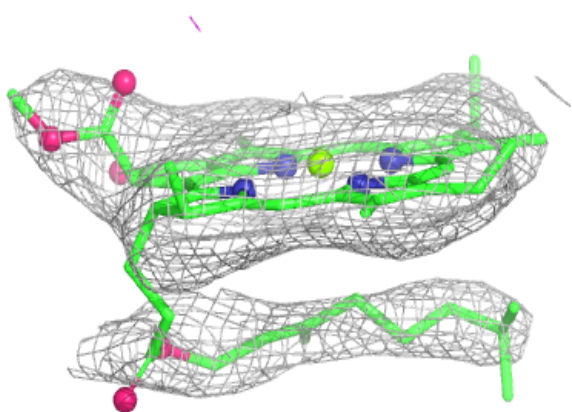
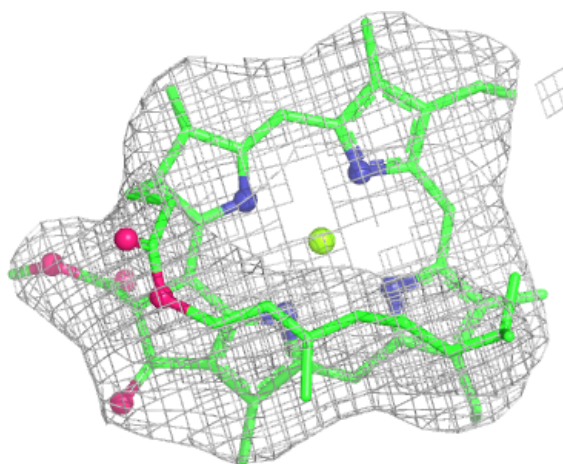
Electron density around CLA A 1129:

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



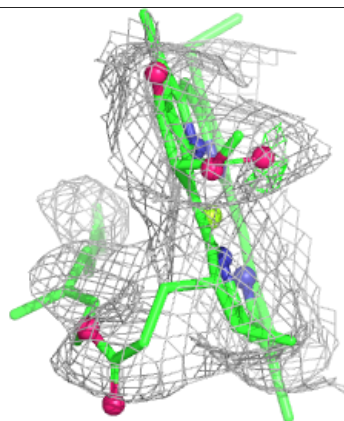
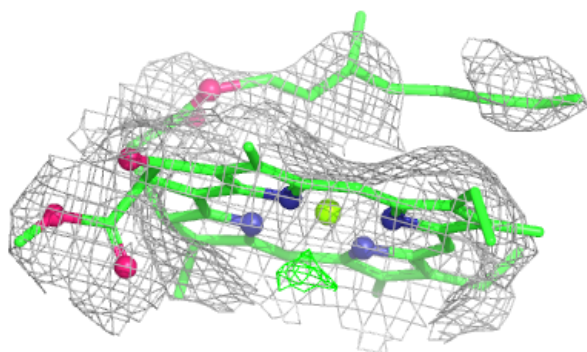
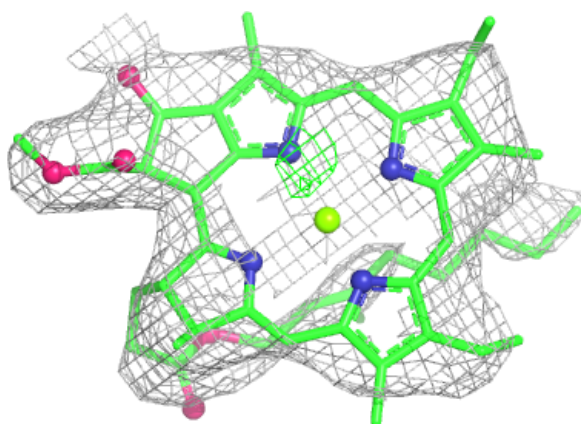
Electron density around CLA A 1130:

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

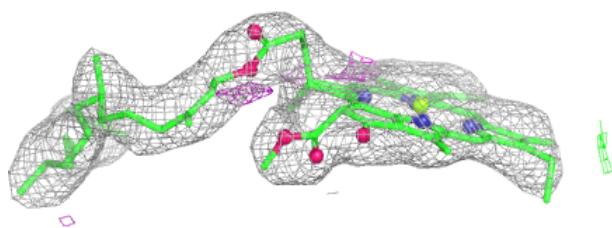
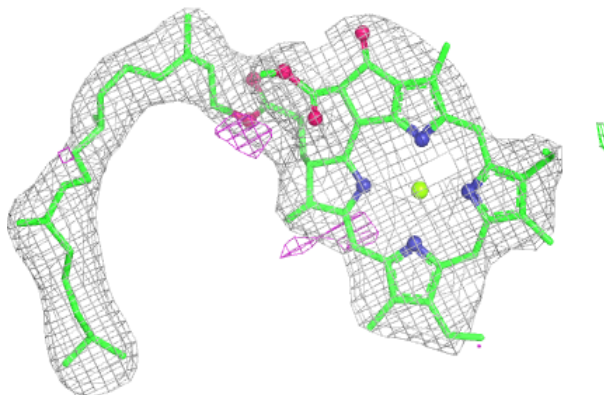


Electron density around CLA A 1116:

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

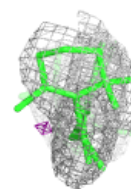
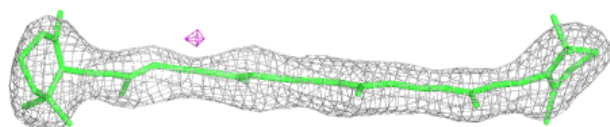
**Electron density around CLA A 1101:**

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

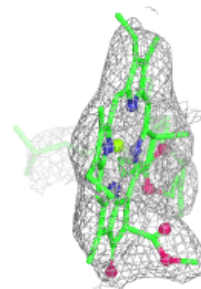
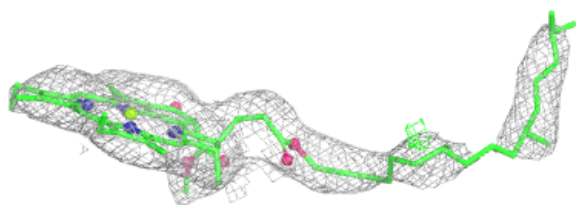
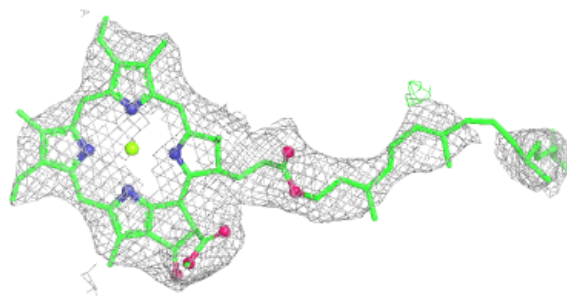


Electron density around BCR B 4017:

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

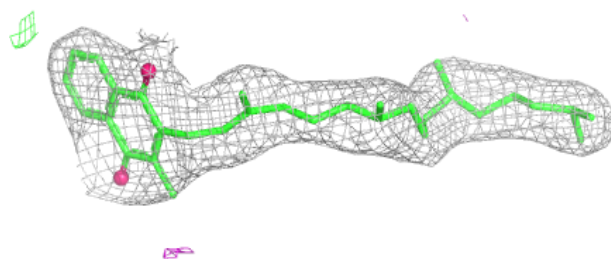
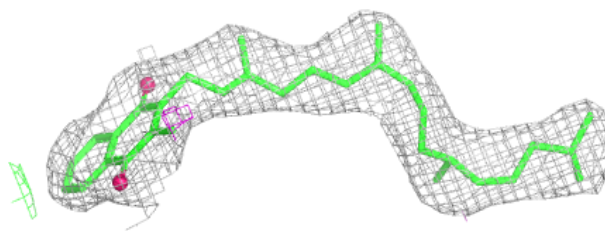
**Electron density around CLA A 1103:**

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

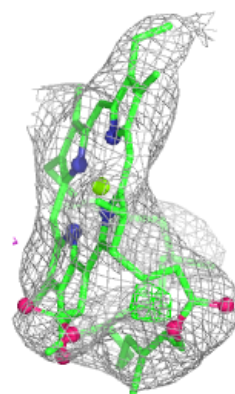
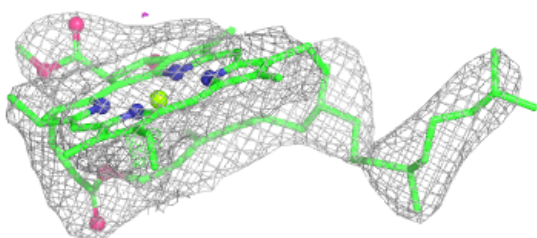
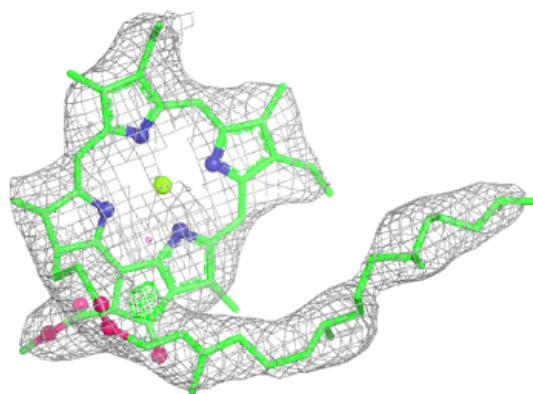


Electron density around PQN A 2001:

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

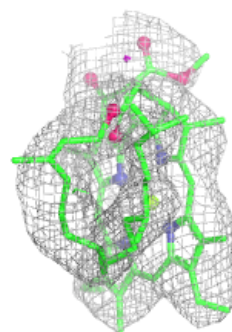
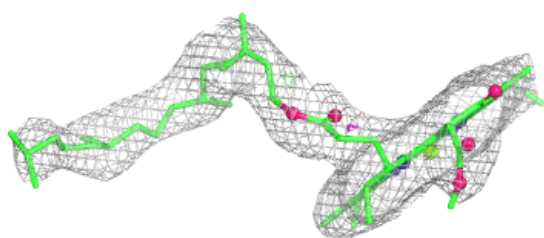
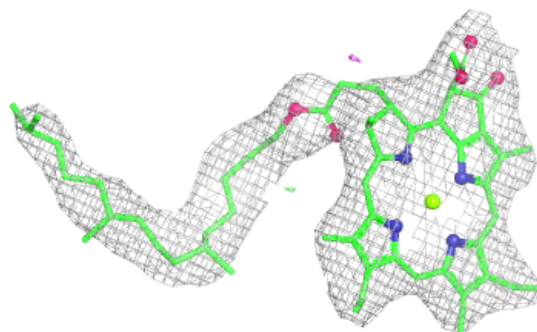
**Electron density around CLA A 1127:**

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

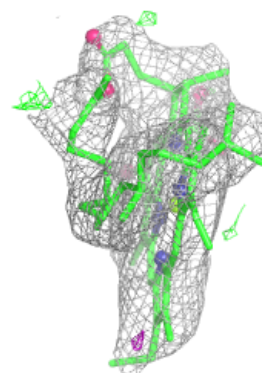
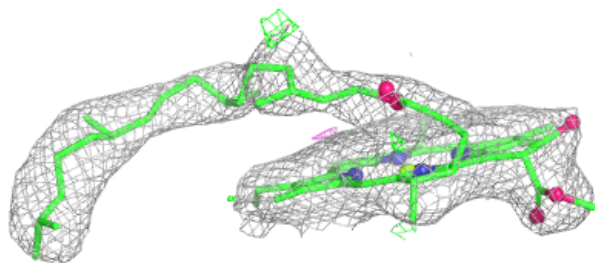
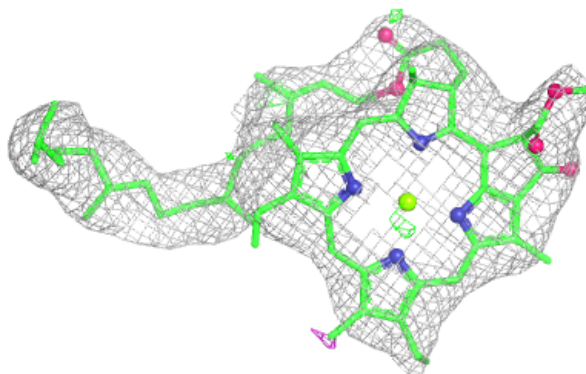


Electron density around CLA A 1106:

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

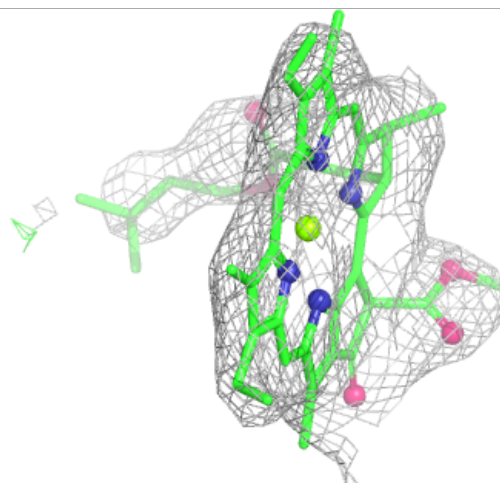
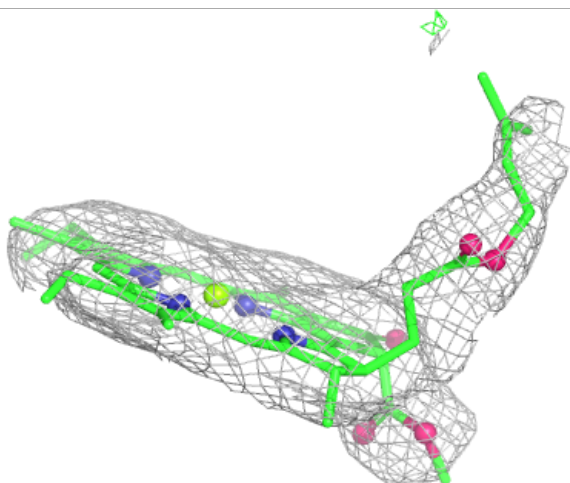
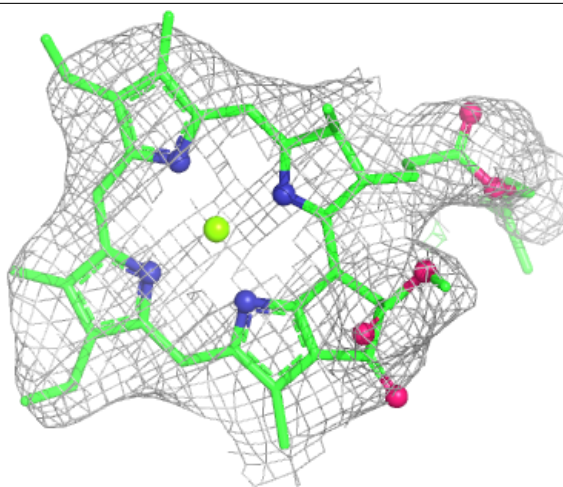
**Electron density around CLA B 1215:**

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



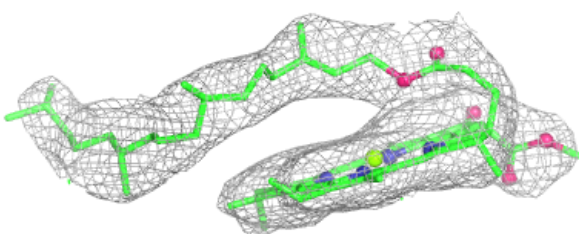
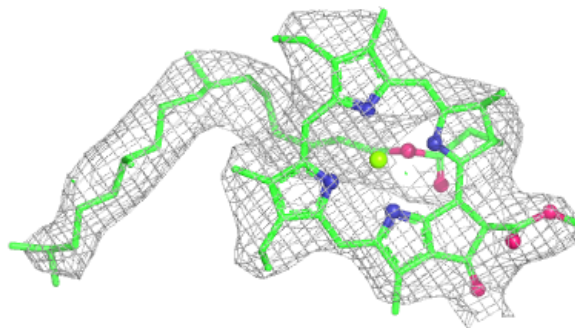
Electron density around CLA A 1137:

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

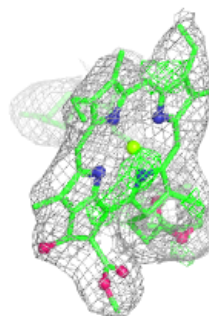
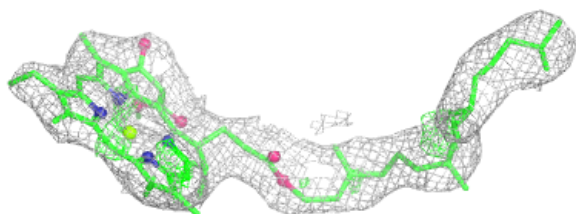
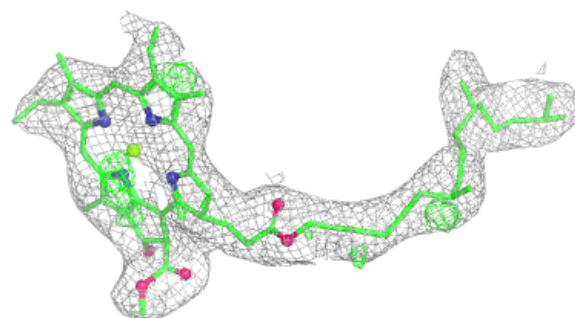


Electron density around CLA B 1235:

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

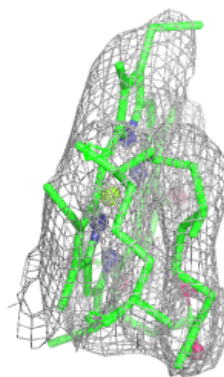
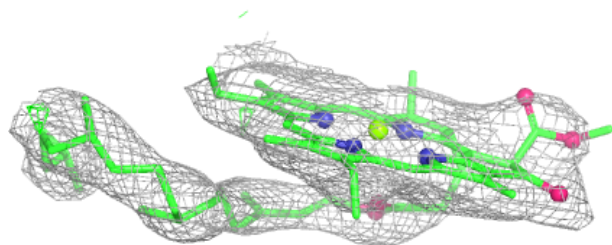
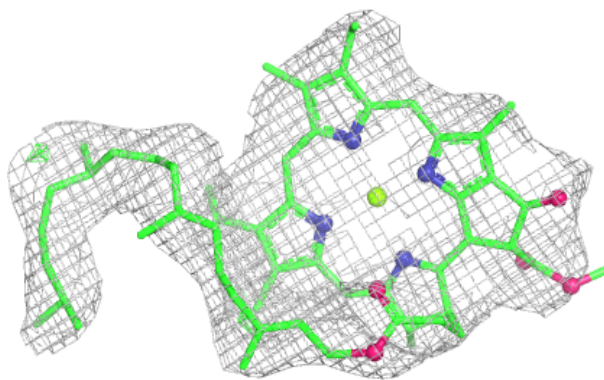
**Electron density around CLA A 1012:**

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

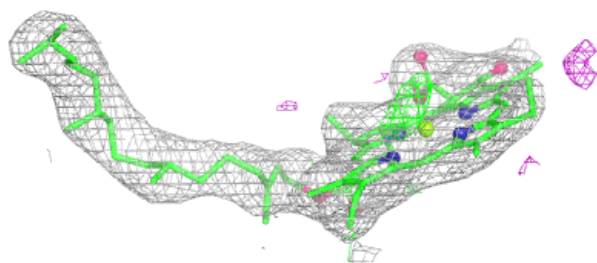
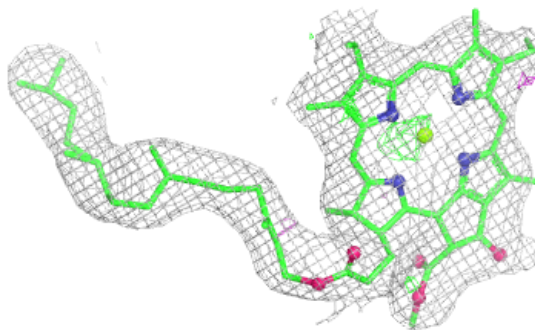


Electron density around CLA A 1117:

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

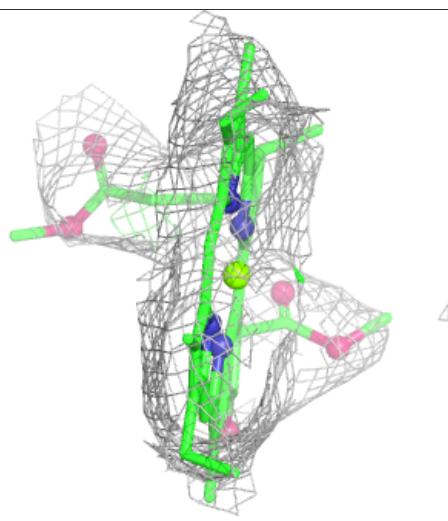
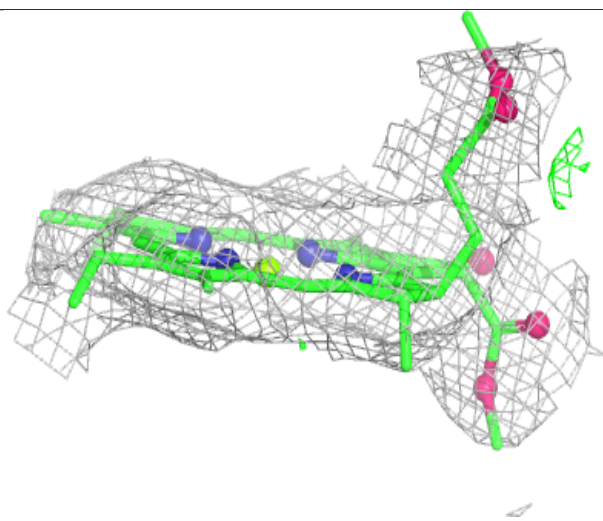
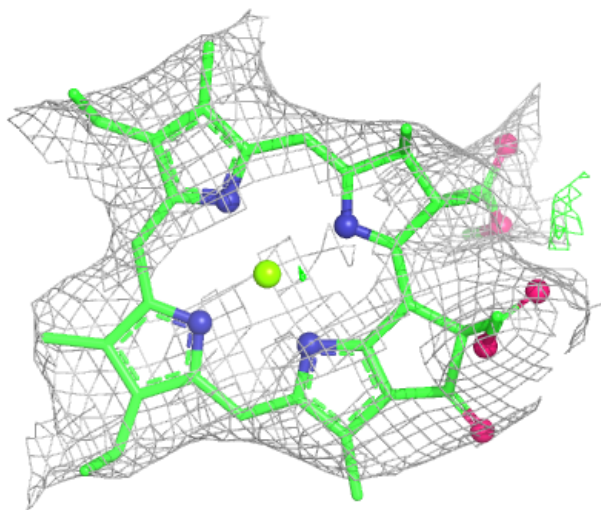
**Electron density around CLA B 1013:**

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



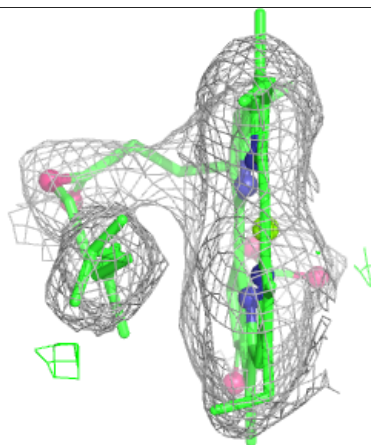
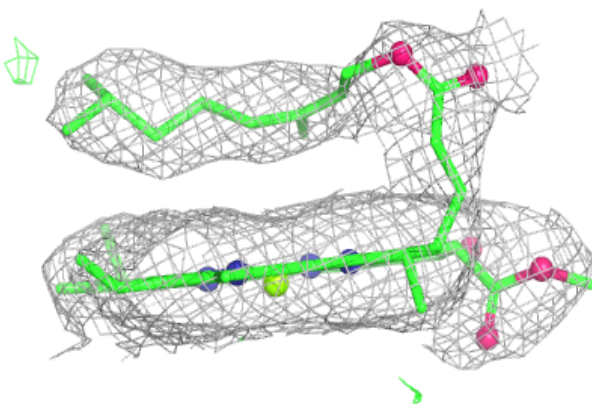
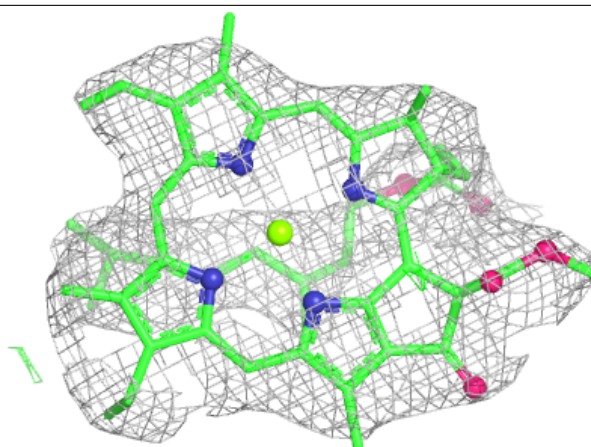
Electron density around CLA B 1211:

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



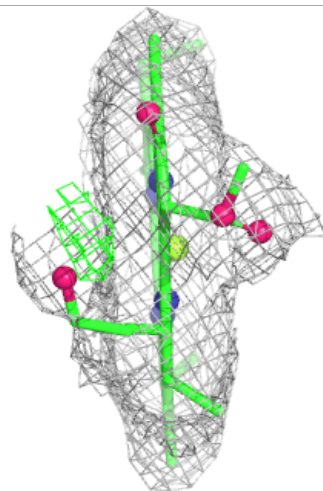
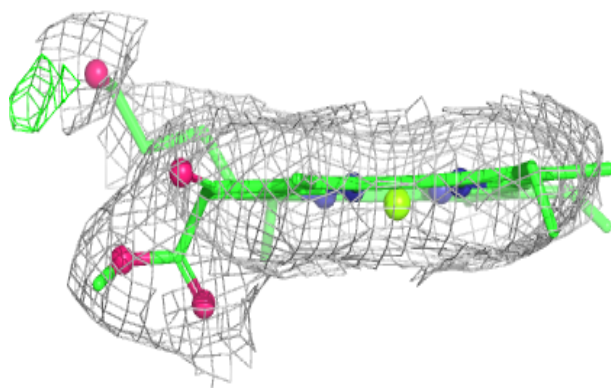
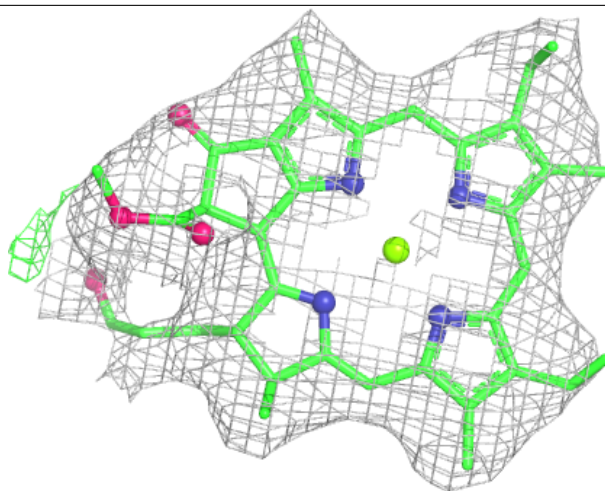
Electron density around CLA B 1237:

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



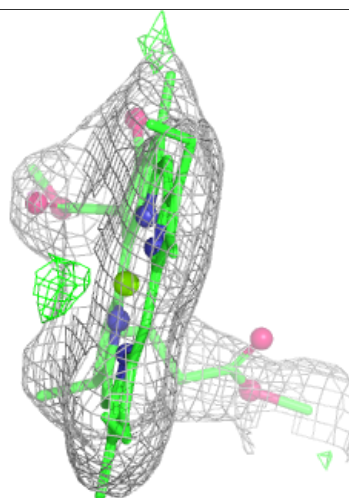
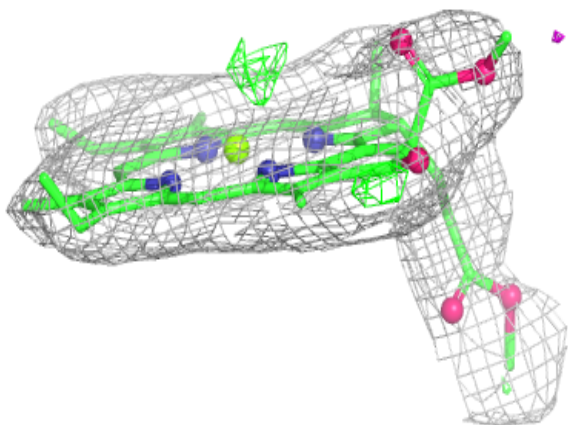
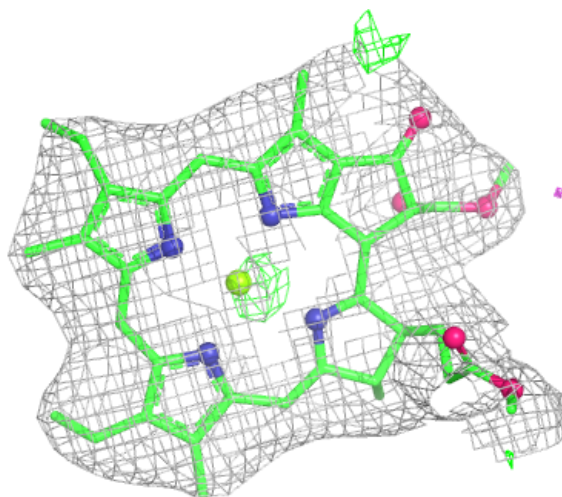
Electron density around CLA B 1238:

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



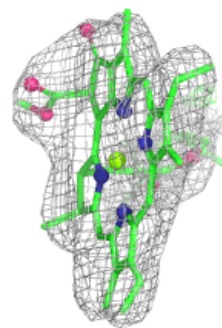
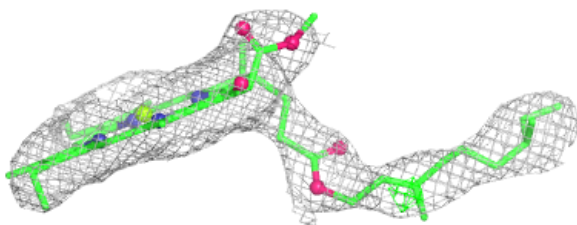
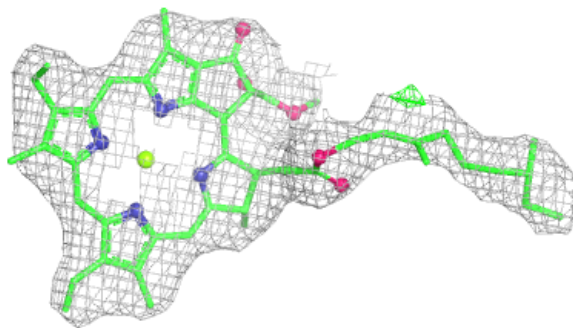
Electron density around CLA B 1239:

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

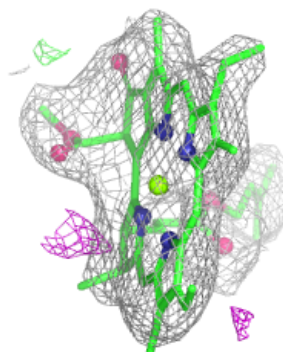
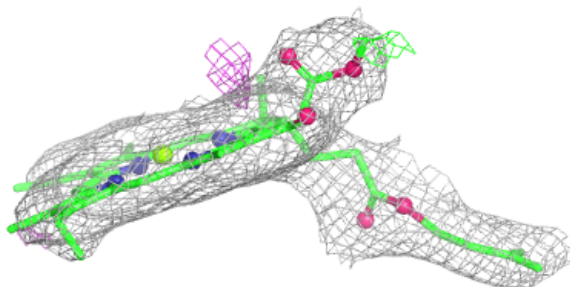
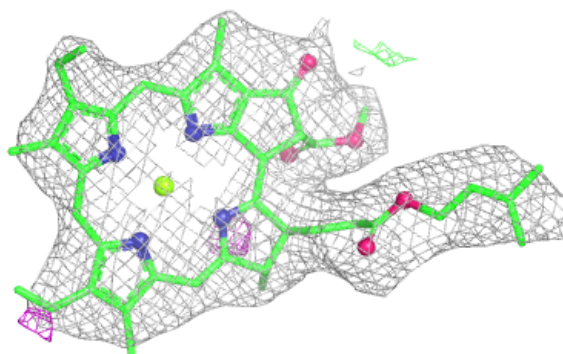


Electron density around CLA B 1220:

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

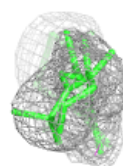
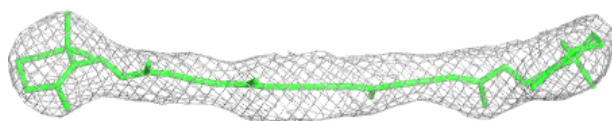
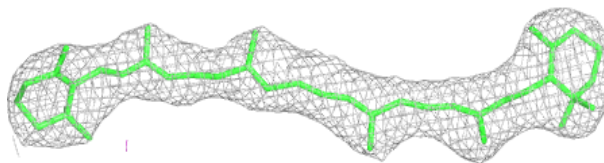
**Electron density around CLA A 1107:**

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

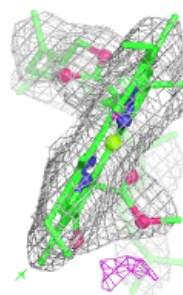
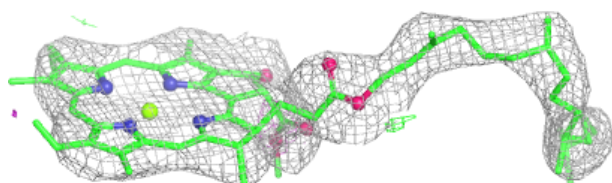
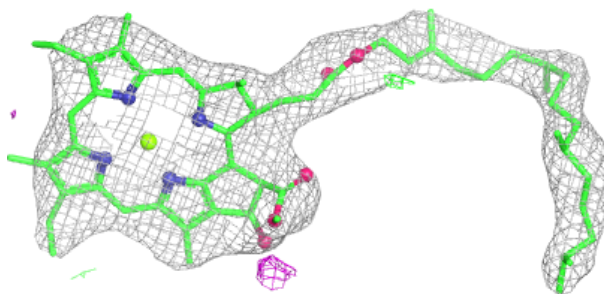


Electron density around BCR A 4012:

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

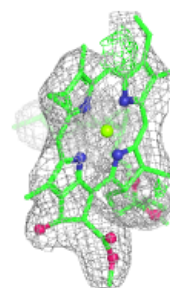
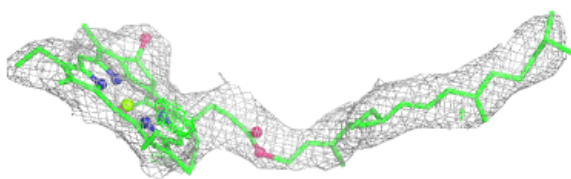
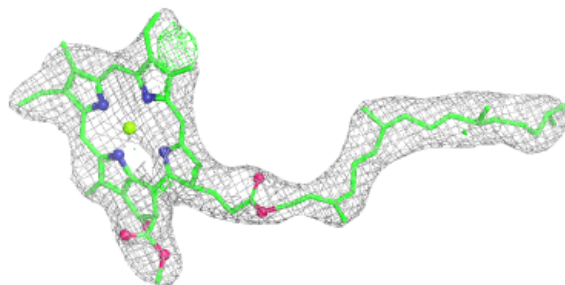
**Electron density around CLA B 1223:**

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



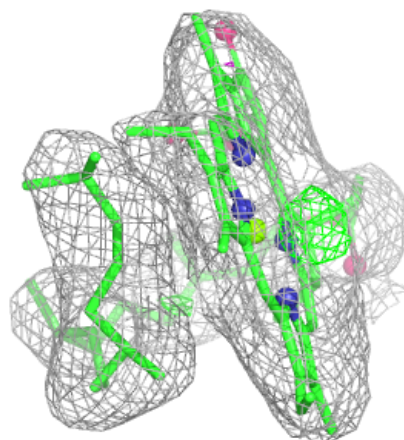
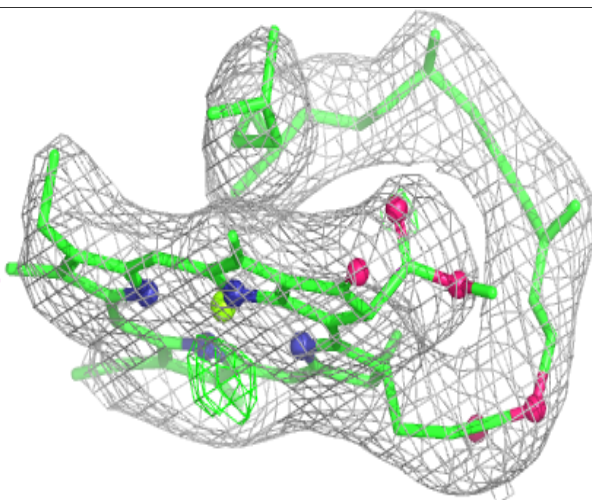
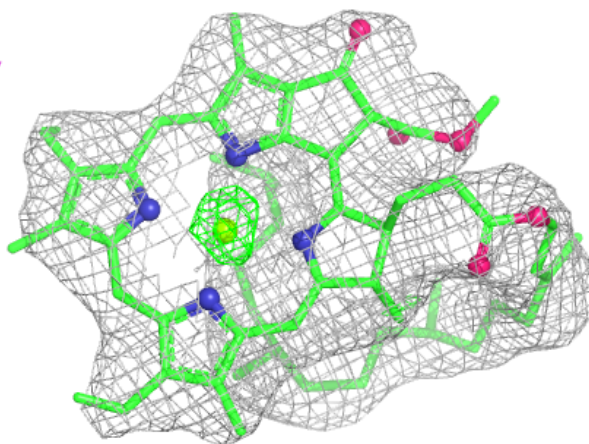
Electron density around CLA A 1022:

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



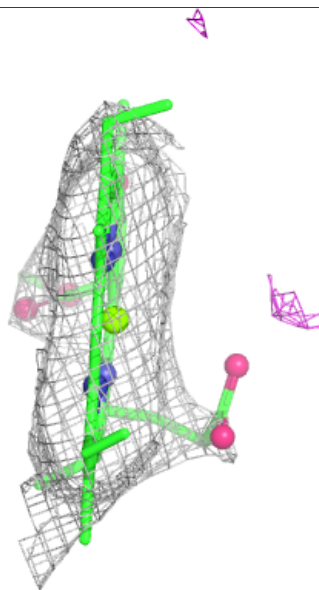
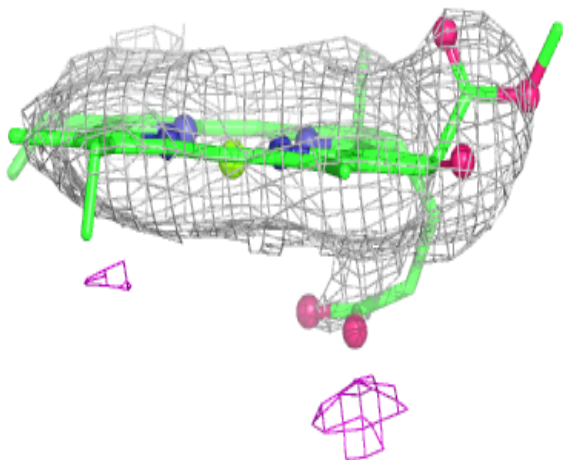
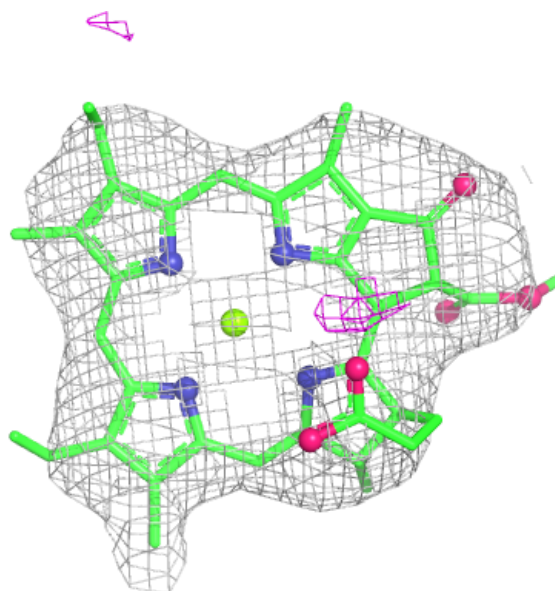
Electron density around CLA A 1104:

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



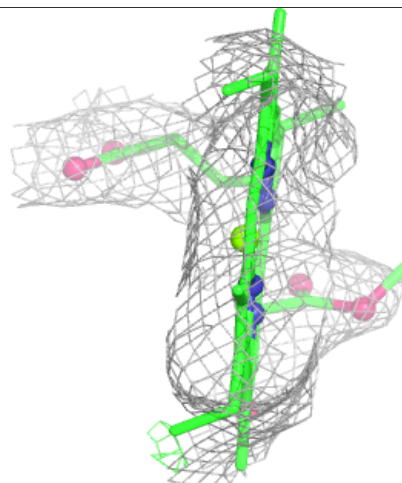
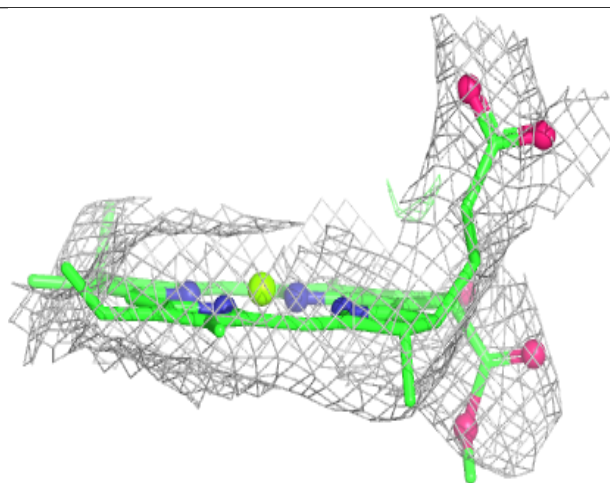
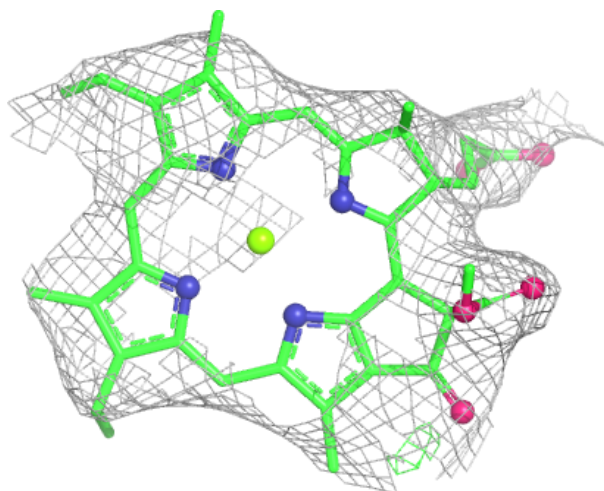
Electron density around CLA B 1209:

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



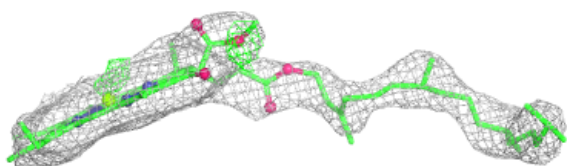
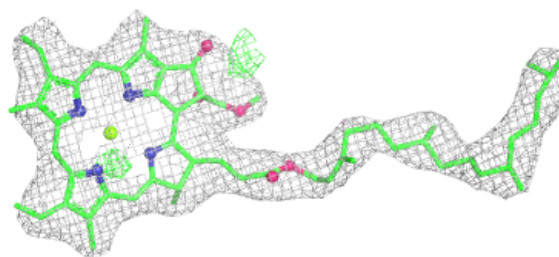
Electron density around CLA A 1112:

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



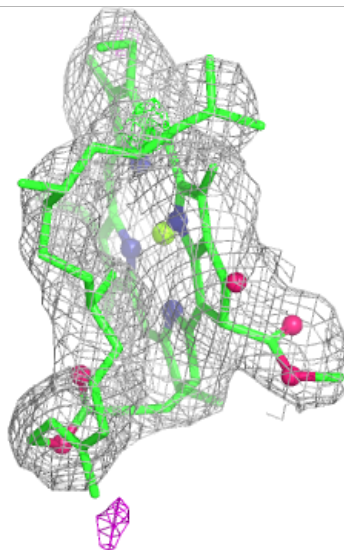
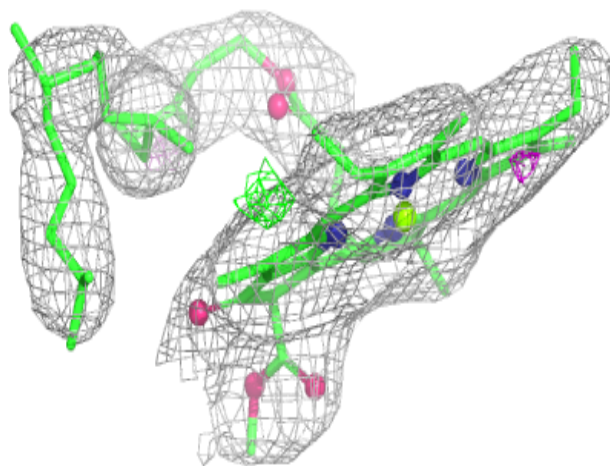
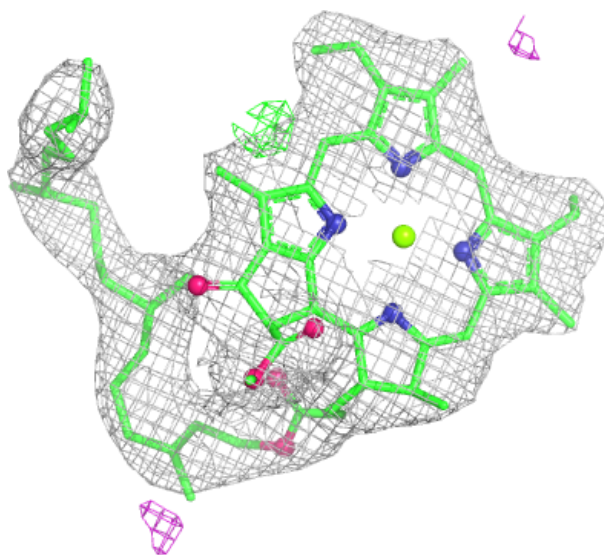
Electron density around CLA F 1139:

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



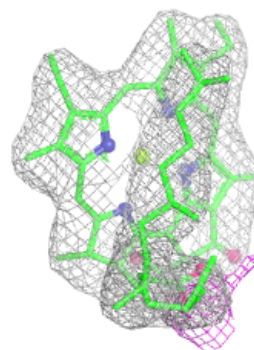
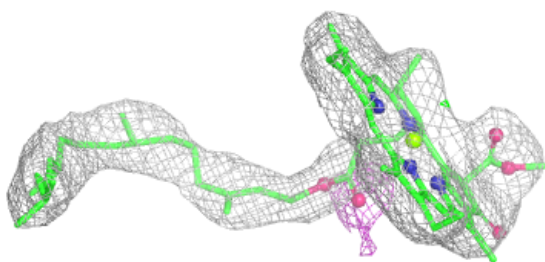
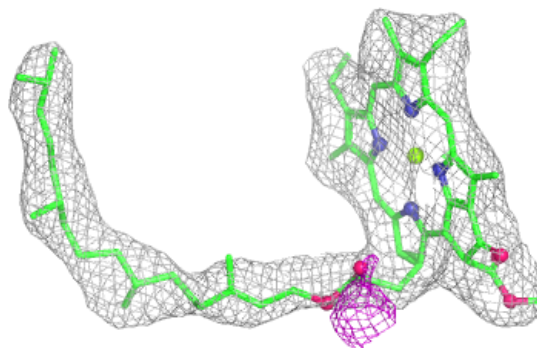
Electron density around CLA B 1229:

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



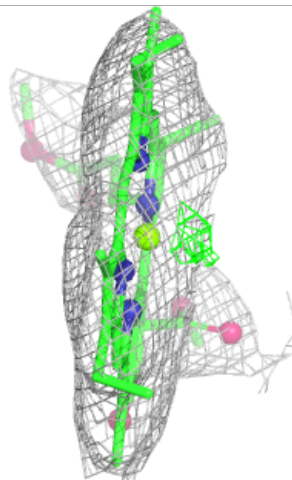
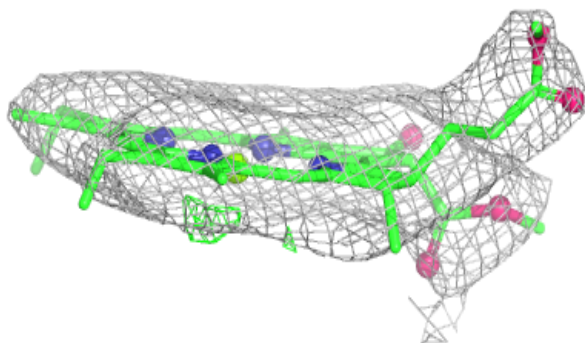
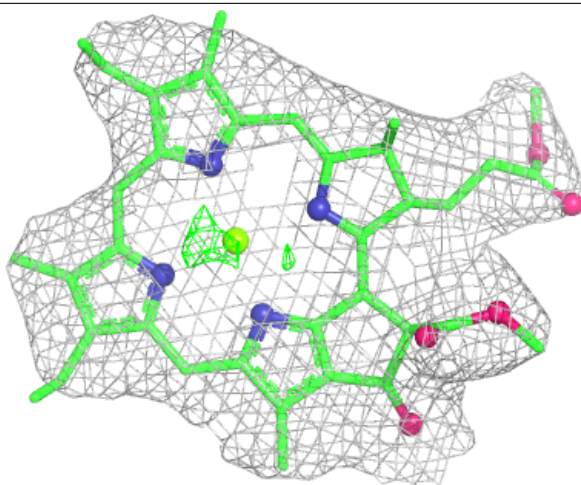
Electron density around CLA A 1140:

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



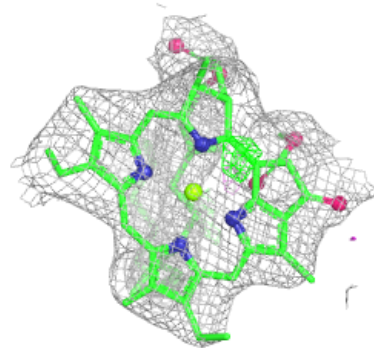
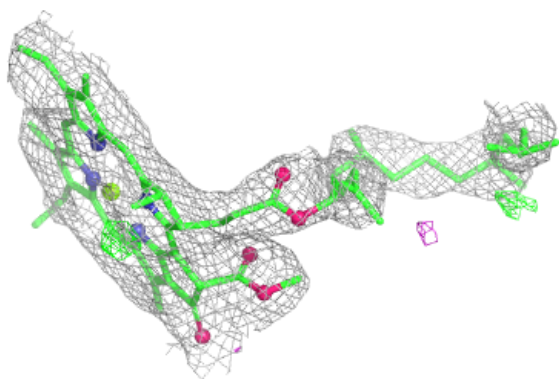
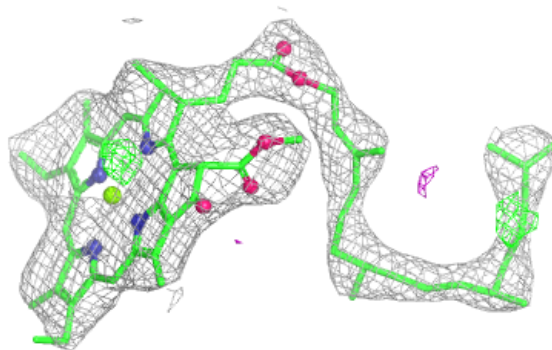
Electron density around CLA B 1206:

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

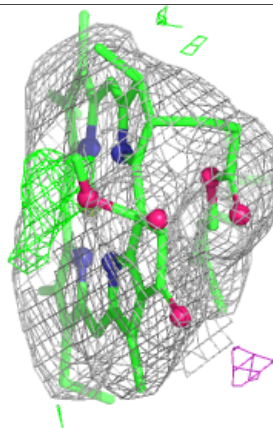
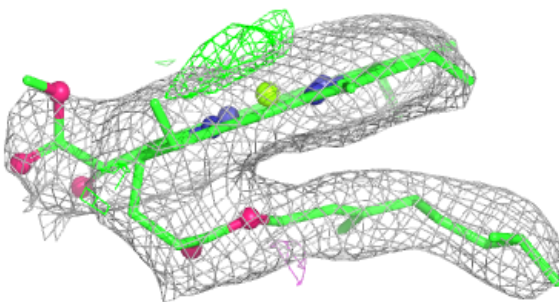
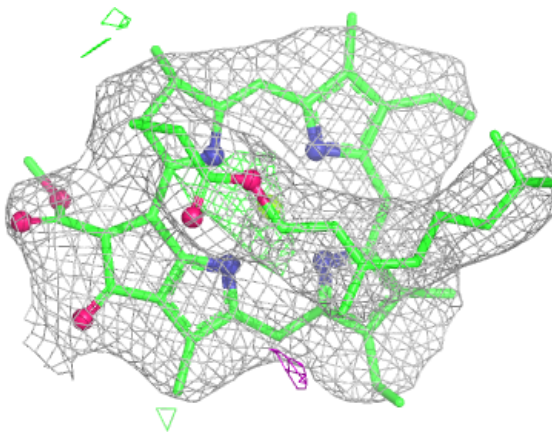


Electron density around CL0 A 1011:

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

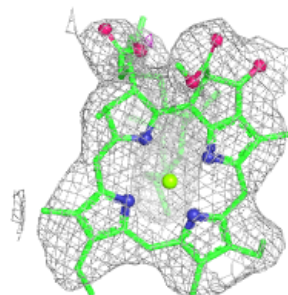
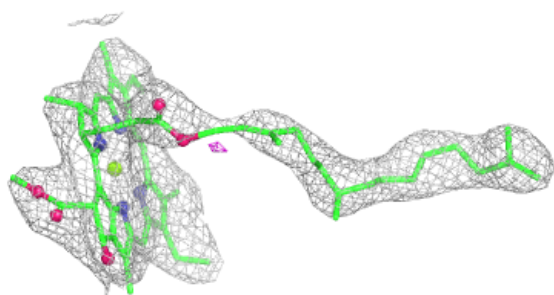
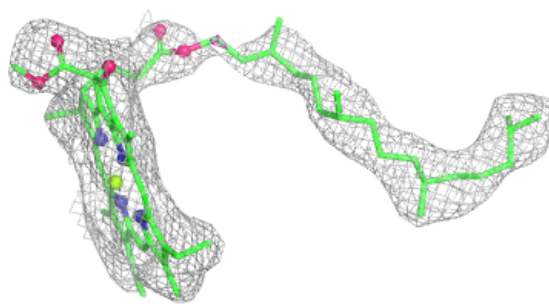
**Electron density around CLA B 1205:**

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



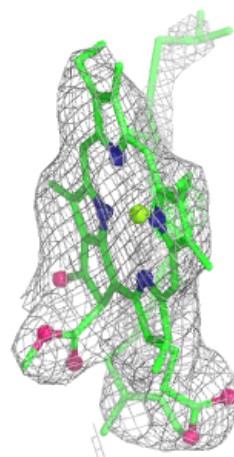
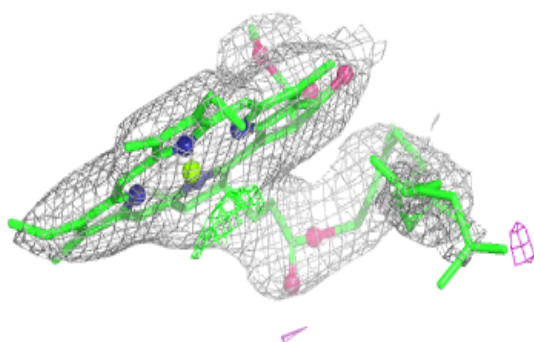
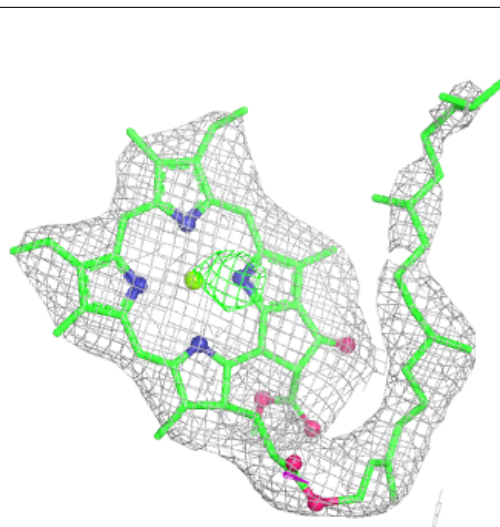
Electron density around CLA A 1128:

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



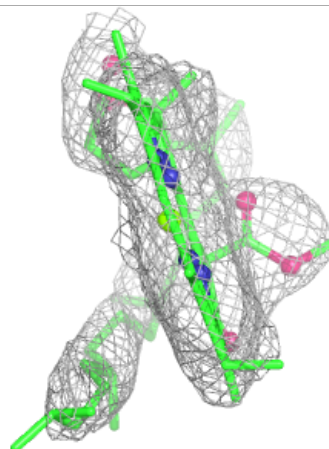
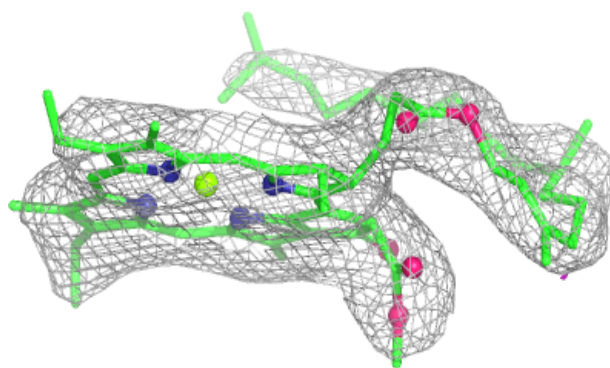
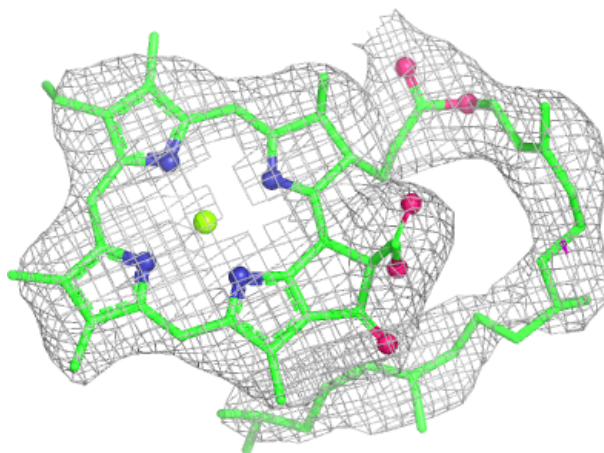
Electron density around CLA A 1123:

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



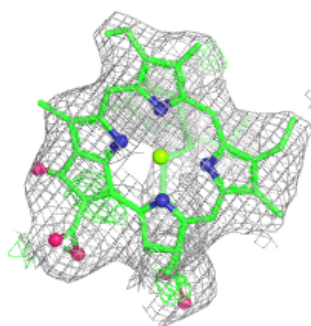
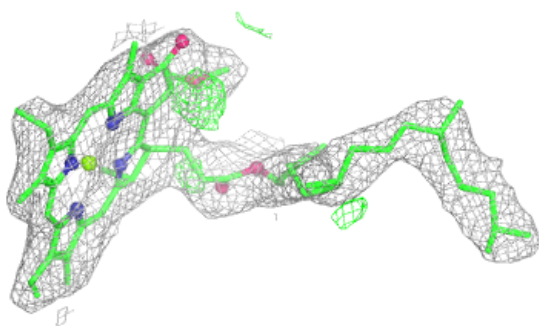
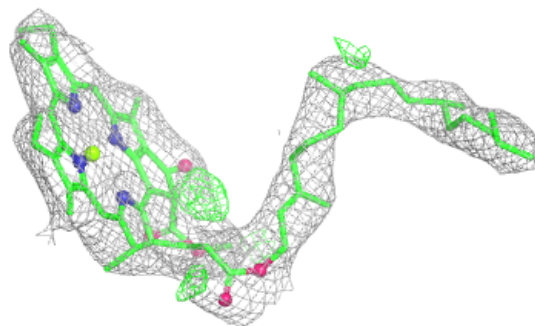
Electron density around CLA B 1202:

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

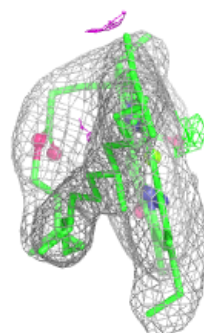
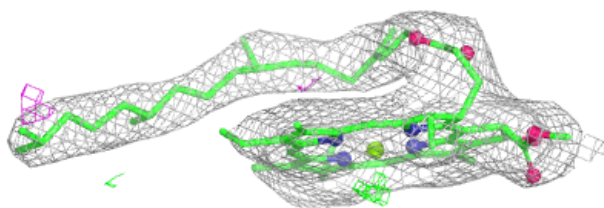
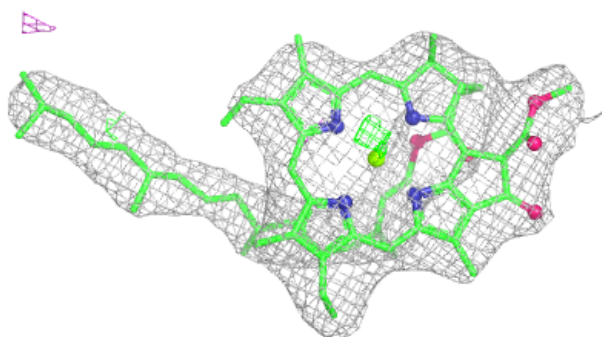


Electron density around CLA B 1021:

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

**Electron density around CLA A 1138:**

$2mF_o-DF_c$ (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.