



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 29, 2026 – 02:50 AM UTC

PDB ID : 2WSC / pdb_00002wsc
Title : Improved Model of Plant Photosystem I
Authors : Amunts, A.; Toporik, H.; Borovikov, A.; Nelson, N.
Deposited on : 2009-09-04
Resolution : 3.30 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

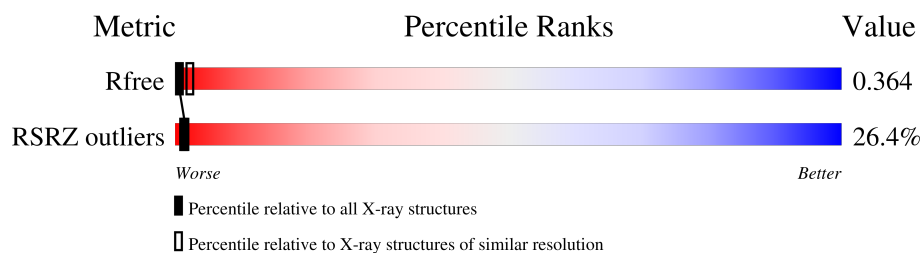
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.30 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R _{free}	180053	1169 (3.32-3.28)
RSRZ outliers	180081	1169 (3.32-3.28)

MolProbity failed to run properly - the sequence quality summary graphics cannot be shown.

2 Entry composition

There are 26 unique types of molecules in this entry. The entry contains 36379 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 AT3G54890.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	1	165	Total	C	N	O	S	0	0	0
			1264	822	208	230	4			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
1	-33	ILE	LYS	conflict	UNP Q9C5R7
1	-1	ARG	LYS	conflict	UNP Q9C5R7

- Molecule 2 is a protein called TYPE II CHLOROPHYLL A/B BINDING PROTEIN FROM PHOTOSYSTEM I.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	2	176	Total	C	N	O	S	0	0	0
			1374	899	226	245	4			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
2	195	ALA	-	insertion	UNP Q41038
2	?	-	GLY	deletion	UNP Q41038

- Molecule 3 is a protein called LHCA3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	3	162	Total	C	N	O	S	0	0	0
			1254	826	203	220	5			

- Molecule 4 is a protein called CHLOROPHYLL A-B BINDING PROTEIN P4, CHLOROPLASTIC.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	4	166	Total	C	N	O	S	0	0	0
			1319	861	219	236	3			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
4	?	-	ALA	deletion	UNP Q9SQL2

- Molecule 5 is a protein called PHOTOSYSTEM I P700 CHLOROPHYLL A APOPROTEIN A1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	A	730	Total	C	N	O	S	0	0	0
			5745	3766	974	987	18			

- Molecule 6 is a protein called PHOTOSYSTEM I P700 CHLOROPHYLL A APOPROTEIN A2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	B	733	Total	C	N	O	S	0	0	0
			5848	3843	997	995	13			

- Molecule 7 is a protein called PHOTOSYSTEM I IRON-SULFUR CENTER.

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

- Molecule 8 is a protein called PHOTOSYSTEM I REACTION CENTER SUBUNIT II, CHLOROPLASTIC.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	D	138	Total	C	N	O	S	0	0	0
			1095	704	189	198	4			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	-52	GLY	ALA	conflict	UNP P12353
D	-50	PRO	GLN	conflict	UNP P12353
D	-44	ARG	PRO	conflict	UNP P12353
D	-34	GLU	ASP	conflict	UNP P12353
D	-11	LEU	HIS	conflict	UNP P12353

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Chain	Residue	Modelled	Actual	Comment	Reference
D	-9	THR	SER	conflict	UNP P12353
D	12	THR	PRO	conflict	UNP P12353
D	14	ALA	GLY	conflict	UNP P12353

- Molecule 9 is a protein called PHOTOSYSTEM I REACTION CENTER SUBUNIT IV A, CHLOROPLASTIC.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
9	E	65	Total	C	N	O	0	0	0
			520	332	93	95			

- Molecule 10 is a protein called PHOTOSYSTEM I REACTION CENTER SUBUNIT III, CHLOROPLASTIC.

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

- Molecule 11 is a protein called PHOTOSYSTEM I REACTION CENTER SUBUNIT V, CHLOROPLASTIC.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	G	95	Total	C	N	O	S	0	0	0
			740	481	120	137	2			

- Molecule 12 is a protein called PHOTOSYSTEM I REACTION CENTER SUBUNIT VI, CHLOROPLASTIC.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
12	H	69	Total	C	N	O	0	0	0
			529	344	82	103			

- Molecule 13 is a protein called PHOTOSYSTEM I REACTION CENTER SUBUNIT VIII.

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

- Molecule 14 is a protein called PHOTOSYSTEM I REACTION CENTER SUBUNIT IX.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	J	42	Total	C	N	O	S	0	0	0
			338	230	51	56	1			

- Molecule 15 is a protein called PHOTOSYSTEM I REACTION CENTER SUBUNIT PSAK, CHLOROPLASTIC.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
15	K	84	Total	C	N	O	S	0	0	0
			593	374	102	113	4			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
K	47	ILE	LEU	conflict	UNP P36886

- Molecule 16 is a protein called PHOTOSYSTEM I REACTION CENTER SUBUNIT XI, CHLOROPLASTIC.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
16	L	161	Total	C	N	O	S	0	0	0
			1203	791	193	214	5			

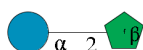
- Molecule 17 is a protein called PHOTOSYSTEM I-N SUBUNIT.

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

- Molecule 18 is a protein called PHOTOSYSTEM I-N SUBUNIT.

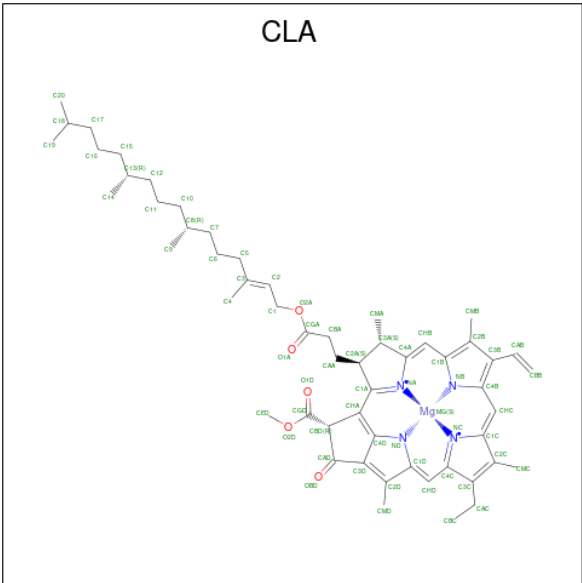
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
18	R	53	Total	C	N	O	0	0	0
			265	159	53	53			

- Molecule 19 is an oligosaccharide called beta-D-fructofuranose-(2-1)-alpha-D-glucopyranose.



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace
19	M	2	Total	C	O	0	0	0
			22	12	10			
19	O	2	Total	C	O	0	0	0
			23	12	11			
19	P	2	Total	C	O	0	0	0
			23	12	11			
19	Q	2	Total	C	O	0	0	0
			23	12	11			
19	S	2	Total	C	O	0	0	0
			23	12	11			
19	T	2	Total	C	O	0	0	0
			23	12	11			
19	U	2	Total	C	O	0	0	0
			23	12	11			
19	V	2	Total	C	O	0	0	0
			23	12	11			
19	W	2	Total	C	O	0	0	0
			23	12	11			
19	X	2	Total	C	O	0	0	0
			23	12	11			
19	Y	2	Total	C	O	0	0	0
			23	12	11			
19	Z	2	Total	C	O	0	0	0
			23	12	11			
19	a	2	Total	C	O	0	0	0
			23	12	11			

- Molecule 20 is CHLOROPHYLL A (CCD ID: CLA) (formula: C₅₅H₇₂MgN₄O₅).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
20	1	1	Total	C	Mg	N	O	0	0
			46	36	1	4	5		
20	1	1	Total	C	Mg	N	O	0	0
			47	37	1	4	5		
20	1	1	Total	C	Mg	N	O	0	0
			47	37	1	4	5		
20	1	1	Total	C	Mg	N	O	0	0
			46	36	1	4	5		
20	1	1	Total	C	Mg	N	O	0	0
			36	30	1	4	1		
20	1	1	Total	C	Mg	N	O	0	0
			61	51	1	4	5		
20	1	1	Total	C	Mg	N	O	0	0
			51	41	1	4	5		
20	1	1	Total	C	Mg	N		0	0
			25	20	1	4			
20	1	1	Total	C	Mg	N	O	0	0
			36	30	1	4	1		
20	1	1	Total	C	Mg	N	O	0	0
			36	30	1	4	1		
20	1	1	Total	C	Mg	N	O	0	0
			51	41	1	4	5		
20	1	1	Total	C	Mg	N	O	0	0
			61	51	1	4	5		
20	1	1	Total	C	Mg	N		0	0
			25	20	1	4			
20	1	1	Total	C	Mg	N	O	0	0
			51	41	1	4	5		
20	1	1	Total	C	Mg	N		0	0
			25	20	1	4			
20	2	1	Total	C	Mg	N	O	0	0
			51	41	1	4	5		
20	2	1	Total	C	Mg	N	O	0	0
			56	46	1	4	5		
20	2	1	Total	C	Mg	N		0	0
			25	20	1	4			
20	2	1	Total	C	Mg	N	O	0	0
			50	40	1	4	5		
20	2	1	Total	C	Mg	N		0	0
			25	20	1	4			
20	2	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
20	2	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
20	2	1	Total	C	Mg	N	0	0
			25	20	1	4		
20	2	1	Total	C	Mg	N	0	0
			25	20	1	4		
20	2	1	Total	C	Mg	N	O	0
			50	40	1	4	5	0
20	2	1	Total	C	Mg	N	O	0
			50	40	1	4	5	0
20	2	1	Total	C	Mg	N	O	0
			65	55	1	4	5	0
20	2	1	Total	C	Mg	N		0
			25	20	1	4		0
20	2	1	Total	C	Mg	N		0
			25	20	1	4		0
20	2	1	Total	C	Mg	N	O	0
			65	55	1	4	5	0
20	2	1	Total	C	Mg	N	O	0
			61	51	1	4	5	0
20	3	1	Total	C	Mg	N	O	0
			56	46	1	4	5	0
20	3	1	Total	C	Mg	N	O	0
			36	30	1	4	1	0
20	3	1	Total	C	Mg	N		0
			25	20	1	4		0
20	3	1	Total	C	Mg	N		0
			25	20	1	4		0
20	3	1	Total	C	Mg	N		0
			25	20	1	4		0
20	3	1	Total	C	Mg	N		0
			25	20	1	4		0
20	3	1	Total	C	Mg	N	O	0
			65	55	1	4	5	0
20	3	1	Total	C	Mg	N	O	0
			65	55	1	4	5	0
20	3	1	Total	C	Mg	N		0
			25	20	1	4		0
20	3	1	Total	C	Mg	N		0
			25	20	1	4		0
20	3	1	Total	C	Mg	N	O	0
			42	34	1	4	3	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
20	3	1	Total	C	Mg	N	O	0	0
			50	40	1	4	5		
20	3	1	Total	C	Mg	N		0	0
			25	20	1	4			
20	3	1	Total	C	Mg	N		0	0
			25	20	1	4			
20	3	1	Total	C	Mg	N	O	0	0
			36	30	1	4	1		
20	3	1	Total	C	Mg	N	O	0	0
			55	45	1	4	5		
20	4	1	Total	C	Mg	N	O	0	0
			55	45	1	4	5		
20	4	1	Total	C	Mg	N	O	0	0
			36	30	1	4	1		
20	4	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
20	4	1	Total	C	Mg	N	O	0	0
			55	45	1	4	5		
20	4	1	Total	C	Mg	N	O	0	0
			50	40	1	4	5		
20	4	1	Total	C	Mg	N	O	0	0
			52	42	1	4	5		
20	4	1	Total	C	Mg	N		0	0
			25	20	1	4			
20	4	1	Total	C	Mg	N		0	0
			25	20	1	4			
20	4	1	Total	C	Mg	N	O	0	0
			55	45	1	4	5		
20	4	1	Total	C	Mg	N		0	0
			25	20	1	4			
20	4	1	Total	C	Mg	N		0	0
			25	20	1	4			
20	4	1	Total	C	Mg	N	O	0	0
			36	30	1	4	1		
20	4	1	Total	C	Mg	N		0	0
			25	20	1	4			
20	4	1	Total	C	Mg	N	O	0	0
			46	36	1	4	5		
20	4	1	Total	C	Mg	N		0	0
			25	20	1	4			
20	4	1	Total	C	Mg	N	O	0	0
			52	42	1	4	5		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
20	4	1	Total 47	C 37	Mg 1	N 4	O 5	0	0
20	A	1	Total 50	C 40	Mg 1	N 4	O 5	0	0
20	A	1	Total 55	C 45	Mg 1	N 4	O 5	0	0
20	A	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
20	A	1	Total 57	C 47	Mg 1	N 4	O 5	0	0
20	A	1	Total 46	C 36	Mg 1	N 4	O 5	0	0
20	A	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
20	A	1	Total 55	C 45	Mg 1	N 4	O 5	0	0
20	A	1	Total 45	C 35	Mg 1	N 4	O 5	0	0
20	A	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
20	A	1	Total 54	C 44	Mg 1	N 4	O 5	0	0
20	A	1	Total 54	C 44	Mg 1	N 4	O 5	0	0
20	A	1	Total 45	C 35	Mg 1	N 4	O 5	0	0
20	A	1	Total 50	C 40	Mg 1	N 4	O 5	0	0
20	A	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
20	A	1	Total 52	C 42	Mg 1	N 4	O 5	0	0
20	A	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
20	A	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
20	A	1	Total 51	C 41	Mg 1	N 4	O 5	0	0
20	A	1	Total 42	C 34	Mg 1	N 4	O 3	0	0
20	A	1	Total 55	C 45	Mg 1	N 4	O 5	0	0

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

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
20	A	1	Total	C	Mg	N	O	0	0
			46	36	1	4	5		
20	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
20	A	1	Total	C	Mg	N		0	0
			25	20	1	4			
20	B	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
20	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
20	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
20	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
20	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
20	B	1	Total	C	Mg	N	O	0	0
			54	44	1	4	5		
20	B	1	Total	C	Mg	N	O	0	0
			55	45	1	4	5		
20	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
20	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
20	B	1	Total	C	Mg	N	O	0	0
			60	50	1	4	5		
20	B	1	Total	C	Mg	N	O	0	0
			46	36	1	4	5		
20	B	1	Total	C	Mg	N	O	0	0
			59	49	1	4	5		
20	B	1	Total	C	Mg	N	O	0	0
			60	50	1	4	5		
20	B	1	Total	C	Mg	N	O	0	0
			61	51	1	4	5		
20	B	1	Total	C	Mg	N	O	0	0
			50	40	1	4	5		
20	B	1	Total	C	Mg	N	O	0	0
			46	36	1	4	5		
20	B	1	Total	C	Mg	N	O	0	0
			55	45	1	4	5		
20	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
20	B	1	Total	C	Mg	N	O	0	0
			54	44	1	4	5		
20	B	1	Total	C	Mg	N	O	0	0
			58	48	1	4	5		
20	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
20	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
20	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
20	B	1	Total	C	Mg	N	O	0	0
			50	40	1	4	5		
20	B	1	Total	C	Mg	N	O	0	0
			50	40	1	4	5		
20	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
20	B	1	Total	C	Mg	N	O	0	0
			50	40	1	4	5		
20	B	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
20	B	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
20	B	1	Total	C	Mg	N	O	0	0
			51	41	1	4	5		
20	B	1	Total	C	Mg	N	O	0	0
			60	50	1	4	5		
20	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
20	B	1	Total	C	Mg	N	O	0	0
			47	37	1	4	5		
20	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
20	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
20	B	1	Total	C	Mg	N	O	0	0
			36	30	1	4	1		
20	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
20	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		

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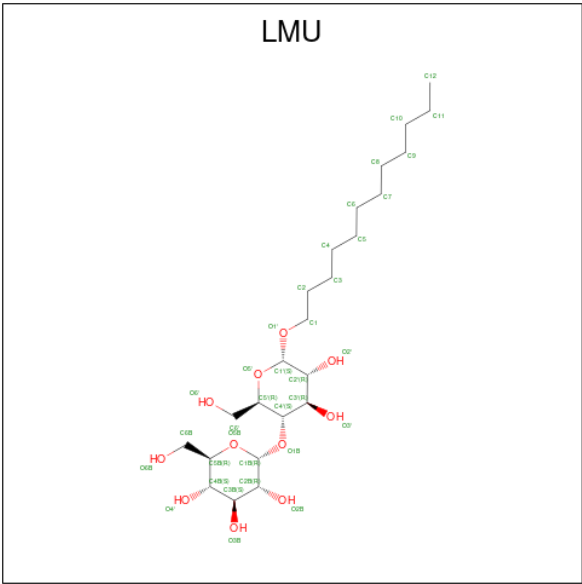
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
20	B	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
20	F	1	Total 36	C 30	Mg 1	N 4	O 1	0	0
20	F	1	Total 41	C 33	Mg 1	N 4	O 3	0	0
20	F	1	Total 53	C 43	Mg 1	N 4	O 5	0	0
20	G	1	Total 51	C 41	Mg 1	N 4	O 5	0	0
20	H	1	Total 55	C 45	Mg 1	N 4	O 5	0	0
20	H	1	Total 65	C 55	Mg 1	N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

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
20	L	1	Total	C	Mg	N	O	0	0
			47	37	1	4	5		
20	L	1	Total	C	Mg	N	O	0	0
			50	40	1	4	5		
20	R	1	Total	C	Mg	N	O	0	0
			57	47	1	4	5		
20	R	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		

- Molecule 21 is DODECYL-ALPHA-D-MALTOSIDE (CCD ID: LMU) (formula: C₂₄H₄₆O₁₁).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
21	1	1	Total	C	O	0	0
			35	24	11		
21	1	1	Total	C	O	0	0
			35	24	11		
21	1	1	Total	C	O	0	0
			35	24	11		
21	2	1	Total	C	O	0	0
			35	24	11		
21	2	1	Total	C	O	0	0
			35	24	11		
21	2	1	Total	C	O	0	0
			35	24	11		
21	2	1	Total	C	O	0	0
			35	24	11		

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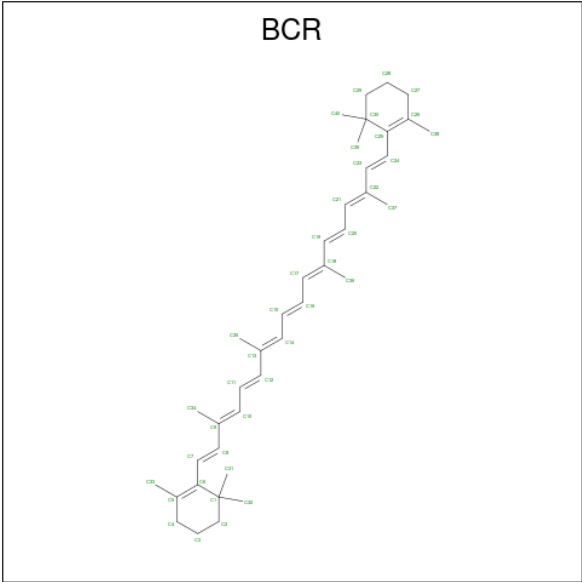
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
21	2	1	Total	C	O	0	0
			35	24	11		
21	3	1	Total	C	O	0	0
			35	24	11		
21	3	1	Total	C	O	0	0
			35	24	11		
21	4	1	Total	C	O	0	0
			35	24	11		
21	4	1	Total	C	O	0	0
			35	24	11		
21	4	1	Total	C	O	0	0
			34	23	11		
21	4	1	Total	C	O	0	0
			35	24	11		
21	4	1	Total	C	O	0	0
			35	24	11		
21	A	1	Total	C	O	0	0
			35	24	11		
21	A	1	Total	C	O	0	0
			35	24	11		
21	A	1	Total	C	O	0	0
			35	24	11		
21	A	1	Total	C	O	0	0
			35	24	11		
21	A	1	Total	C	O	0	0
			35	24	11		
21	A	1	Total	C	O	0	0
			35	24	11		
21	B	1	Total	C	O	0	0
			35	24	11		
21	B	1	Total	C	O	0	0
			35	24	11		
21	B	1	Total	C	O	0	0
			25	14	11		
21	C	1	Total	C	O	0	0
			35	24	11		
21	E	1	Total	C	O	0	0
			35	24	11		
21	F	1	Total	C	O	0	0
			34	23	11		
21	G	1	Total	C	O	0	0
			35	24	11		

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

- Molecule 22 is BETA-CAROTENE (CCD ID: BCR) (formula: $C_{40}H_{56}$).



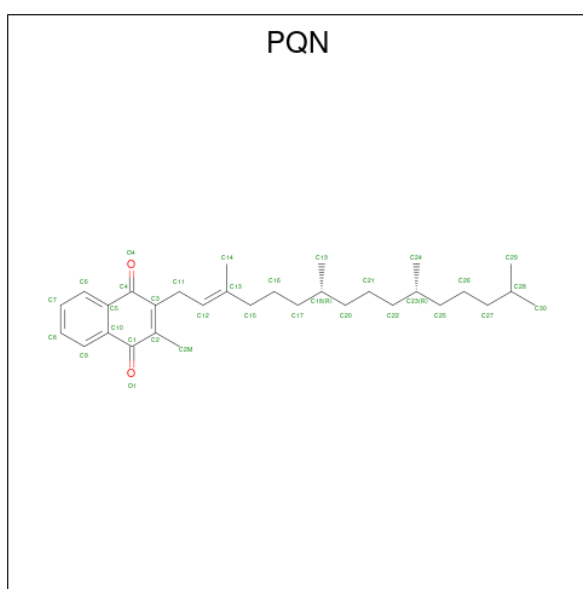
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
22	3	1	Total C 40 40	0	0
22	A	1	Total C 40 40	0	0
22	A	1	Total C 40 40	0	0
22	A	1	Total C 40 40	0	0
22	A	1	Total C 40 40	0	0
22	A	1	Total C 40 40	0	0
22	B	1	Total C 40 40	0	0
22	B	1	Total C 40 40	0	0
22	B	1	Total C 40 40	0	0
22	B	1	Total C 40 40	0	0
22	B	1	Total C 40 40	0	0
22	F	1	Total C 40 40	0	0
22	F	1	Total C 40 40	0	0
22	G	1	Total C 40 40	0	0

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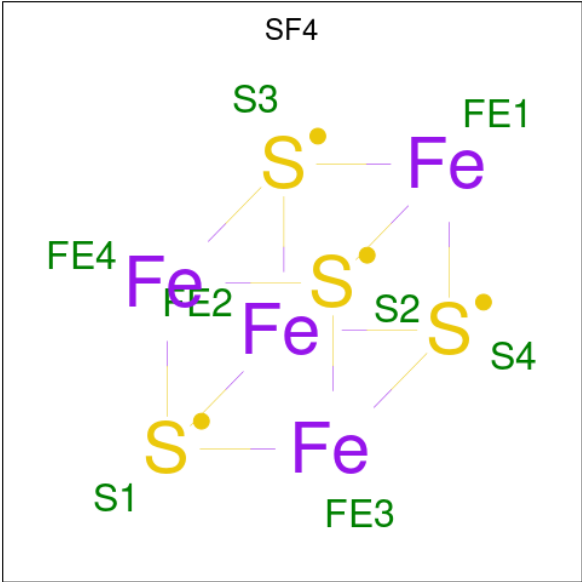
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
22	I	1	Total C 40 40	0	0
22	I	1	Total C 40 40	0	0
22	J	1	Total C 40 40	0	0
22	L	1	Total C 40 40	0	0

- Molecule 23 is PHYLLOQUINONE (CCD ID: PQN) (formula: $C_{31}H_{46}O_2$).



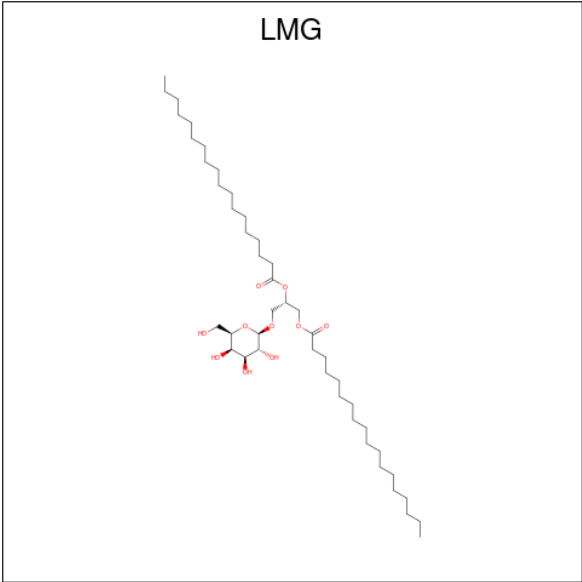
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
23	A	1	Total C O 33 31 2	0	0
23	B	1	Total C O 33 31 2	0	0

- Molecule 24 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe_4S_4).



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

- Molecule 25 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (CCD ID: LMG) (formula: C₄₅H₈₆O₁₀).



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

- Molecule 26 is UNKNOWN LIGAND (CCD ID: UNL) (formula:).

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
26	H	1	Total	C	O	0	0
			23	12	11		

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3 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	120.66Å 189.09Å 129.39Å 90.00° 91.24° 90.00°	Depositor
Resolution (Å)	30.00 – 3.30 30.00 – 3.30	Depositor EDS
% Data completeness (in resolution range)	99.5 (30.00-3.30) 99.3 (30.00-3.30)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.62 (at 3.19Å)	Xtriage
Refinement program	REFMAC 5.5.0072	Depositor
R, R_{free}	0.363 , 0.366 0.359 , 0.364	Depositor DCC
R_{free} test set	4685 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å ²)	78.5	Xtriage
Anisotropy	0.655	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.13 , 58.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.032 for h,-k,-l	Xtriage
F_o, F_c correlation	0.78	EDS
Total number of atoms	36379	wwPDB-VP
Average B, all atoms (Å ²)	25.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.11% 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.

4 Model quality [i](#)

4.1 Standard geometry [i](#)

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4.2 Too-close contacts [i](#)

MolProbity failed to run properly - this section is therefore empty.

4.3 Torsion angles [i](#)

4.3.1 Protein backbone [i](#)

MolProbity failed to run properly - this section is therefore empty.

4.3.2 Protein sidechains [i](#)

MolProbity failed to run properly - this section is therefore empty.

4.3.3 RNA [i](#)

MolProbity failed to run properly - this section is therefore empty.

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

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

4.5 Carbohydrates [i](#)

26 monosaccharides are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
19	GLC	M	1	19	10,10,12	1.47	3 (30%)	14,14,17	2.99	9 (64%)
19	FRU	M	2	19	11,12,12	1.03	1 (9%)	10,18,18	2.30	3 (30%)
19	GLC	O	1	19	11,11,12	0.90	0	15,15,17	3.29	8 (53%)
19	FRU	O	2	19	11,12,12	1.10	1 (9%)	10,18,18	1.70	2 (20%)
19	GLC	P	1	19	11,11,12	0.98	0	15,15,17	2.39	3 (20%)
19	FRU	P	2	19	11,12,12	1.04	1 (9%)	10,18,18	0.98	0
19	GLC	Q	1	19	11,11,12	1.16	1 (9%)	15,15,17	2.07	4 (26%)
19	FRU	Q	2	19	11,12,12	0.99	1 (9%)	10,18,18	1.76	4 (40%)
19	GLC	S	1	19	11,11,12	0.42	0	15,15,17	0.98	1 (6%)
19	FRU	S	2	19,21	11,12,12	0.65	0	10,18,18	1.11	0
19	GLC	T	1	19	11,11,12	1.05	1 (9%)	15,15,17	1.46	2 (13%)
19	FRU	T	2	19	11,12,12	1.94	4 (36%)	10,18,18	2.78	4 (40%)
19	GLC	U	1	19	11,11,12	1.02	1 (9%)	15,15,17	2.43	5 (33%)
19	FRU	U	2	19	11,12,12	0.95	0	10,18,18	1.53	2 (20%)
19	GLC	V	1	19	11,11,12	1.51	2 (18%)	15,15,17	1.79	4 (26%)
19	FRU	V	2	19	11,12,12	0.90	0	10,18,18	1.97	5 (50%)
19	GLC	W	1	19	11,11,12	1.27	2 (18%)	15,15,17	2.73	8 (53%)
19	FRU	W	2	19	11,12,12	1.18	2 (18%)	10,18,18	2.04	2 (20%)
19	GLC	X	1	19	11,11,12	1.17	1 (9%)	15,15,17	1.64	4 (26%)
19	FRU	X	2	19	11,12,12	1.54	2 (18%)	10,18,18	2.34	4 (40%)
19	GLC	Y	1	19	11,11,12	1.08	0	15,15,17	3.33	7 (46%)
19	FRU	Y	2	19	11,12,12	1.14	0	10,18,18	2.25	4 (40%)
19	GLC	Z	1	19	11,11,12	1.70	2 (18%)	15,15,17	4.23	8 (53%)
19	FRU	Z	2	19,21	11,12,12	1.05	1 (9%)	10,18,18	2.32	3 (30%)
19	GLC	a	1	19	11,11,12	1.02	0	15,15,17	1.34	3 (20%)
19	FRU	a	2	19	11,12,12	1.07	0	10,18,18	2.13	3 (30%)

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
19	GLC	M	1	19	-	-	0/1/1/1
19	FRU	M	2	19	1/1/4/4	0/5/24/24	0/1/1/1
19	GLC	O	1	19	-	1/2/19/22	0/1/1/1
19	FRU	O	2	19	1/1/4/4	4/5/24/24	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
19	GLC	P	1	19	-	2/2/19/22	0/1/1/1
19	FRU	P	2	19	1/1/4/4	2/5/24/24	0/1/1/1
19	GLC	Q	1	19	-	2/2/19/22	0/1/1/1
19	FRU	Q	2	19	1/1/4/4	3/5/24/24	0/1/1/1
19	GLC	S	1	19	-	1/2/19/22	0/1/1/1
19	FRU	S	2	19,21	1/1/4/4	0/5/24/24	0/1/1/1
19	GLC	T	1	19	-	2/2/19/22	0/1/1/1
19	FRU	T	2	19	1/1/4/4	3/5/24/24	0/1/1/1
19	GLC	U	1	19	-	2/2/19/22	0/1/1/1
19	FRU	U	2	19	1/1/4/4	3/5/24/24	0/1/1/1
19	GLC	V	1	19	-	0/2/19/22	0/1/1/1
19	FRU	V	2	19	1/1/4/4	3/5/24/24	0/1/1/1
19	GLC	W	1	19	-	1/2/19/22	0/1/1/1
19	FRU	W	2	19	1/1/4/4	2/5/24/24	0/1/1/1
19	GLC	X	1	19	-	2/2/19/22	0/1/1/1
19	FRU	X	2	19	1/1/4/4	3/5/24/24	0/1/1/1
19	GLC	Y	1	19	-	2/2/19/22	0/1/1/1
19	FRU	Y	2	19	1/1/4/4	1/5/24/24	0/1/1/1
19	GLC	Z	1	19	-	0/2/19/22	0/1/1/1
19	FRU	Z	2	19,21	1/1/4/4	3/5/24/24	0/1/1/1
19	GLC	a	1	19	-	2/2/19/22	0/1/1/1
19	FRU	a	2	19	1/1/4/4	2/5/24/24	0/1/1/1

The worst 5 of 26 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	Z	1	GLC	O5-C1	-3.89	1.37	1.43
19	T	2	FRU	O5-C2	-3.79	1.37	1.43
19	V	1	GLC	O5-C5	-2.74	1.38	1.43
19	M	1	GLC	O5-C5	-2.71	1.38	1.43
19	V	1	GLC	O5-C1	-2.68	1.39	1.43

The worst 5 of 102 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	Z	1	GLC	C1-O5-C5	-11.58	96.66	112.19
19	P	1	GLC	C1-O5-C5	7.80	122.64	112.19
19	Y	1	GLC	C1-O5-C5	7.58	122.35	112.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	T	2	FRU	O1-C1-C2	-6.73	96.79	111.67
19	M	1	GLC	C1-C2-C3	6.70	119.40	109.64

5 of 13 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
19	M	2	FRU	C2
19	O	2	FRU	C2
19	P	2	FRU	C2
19	Q	2	FRU	C2
19	S	2	FRU	C2

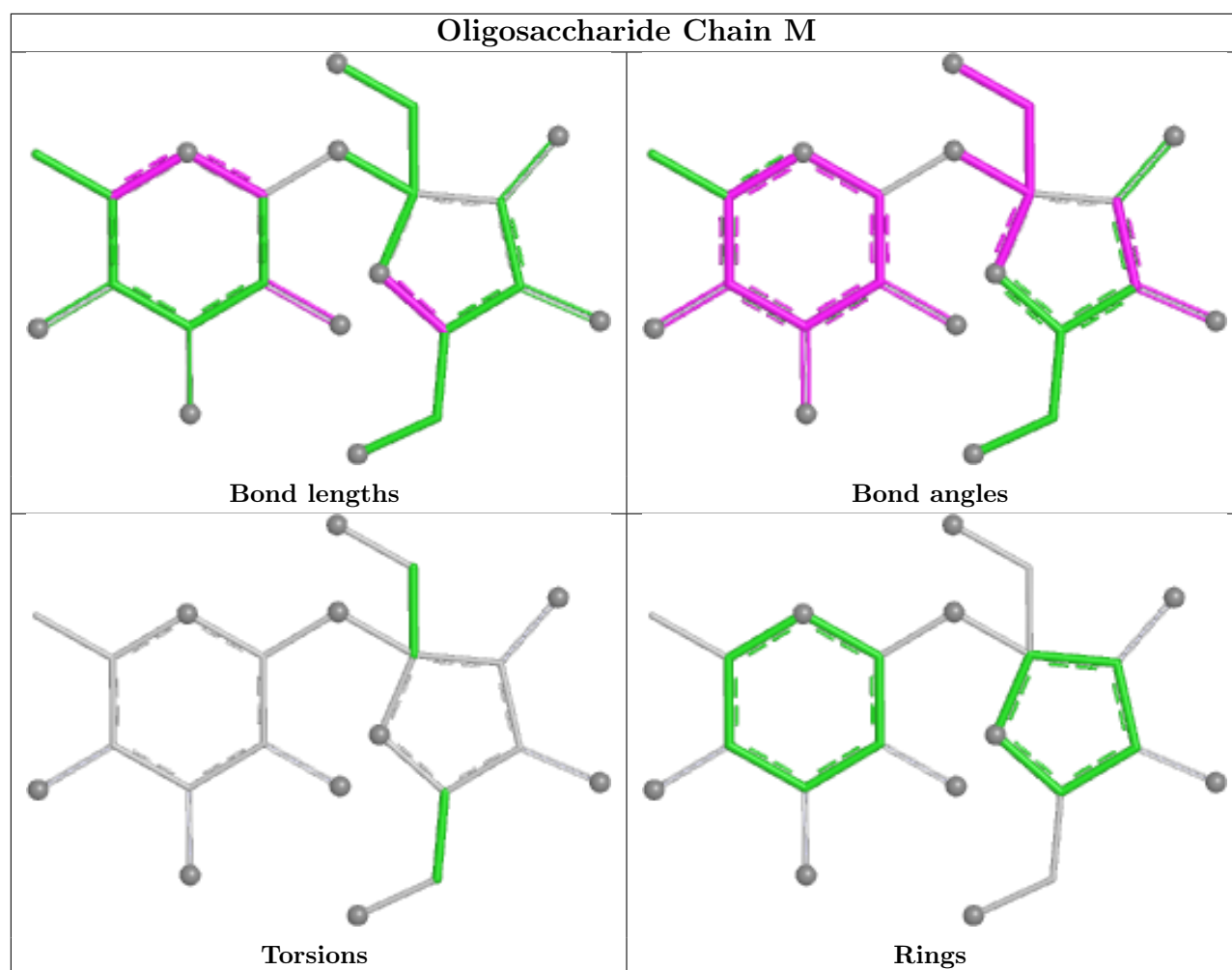
5 of 46 torsion outliers are listed below:

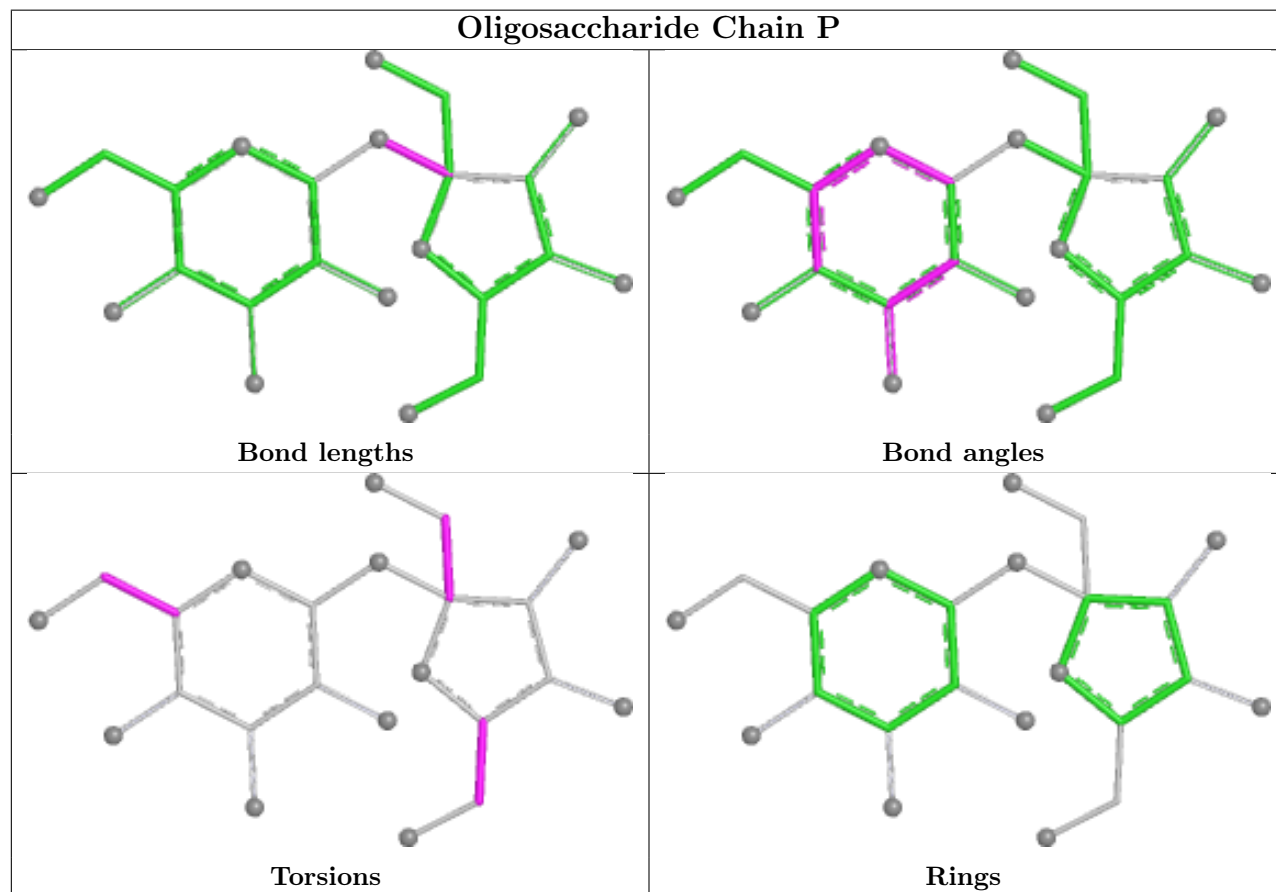
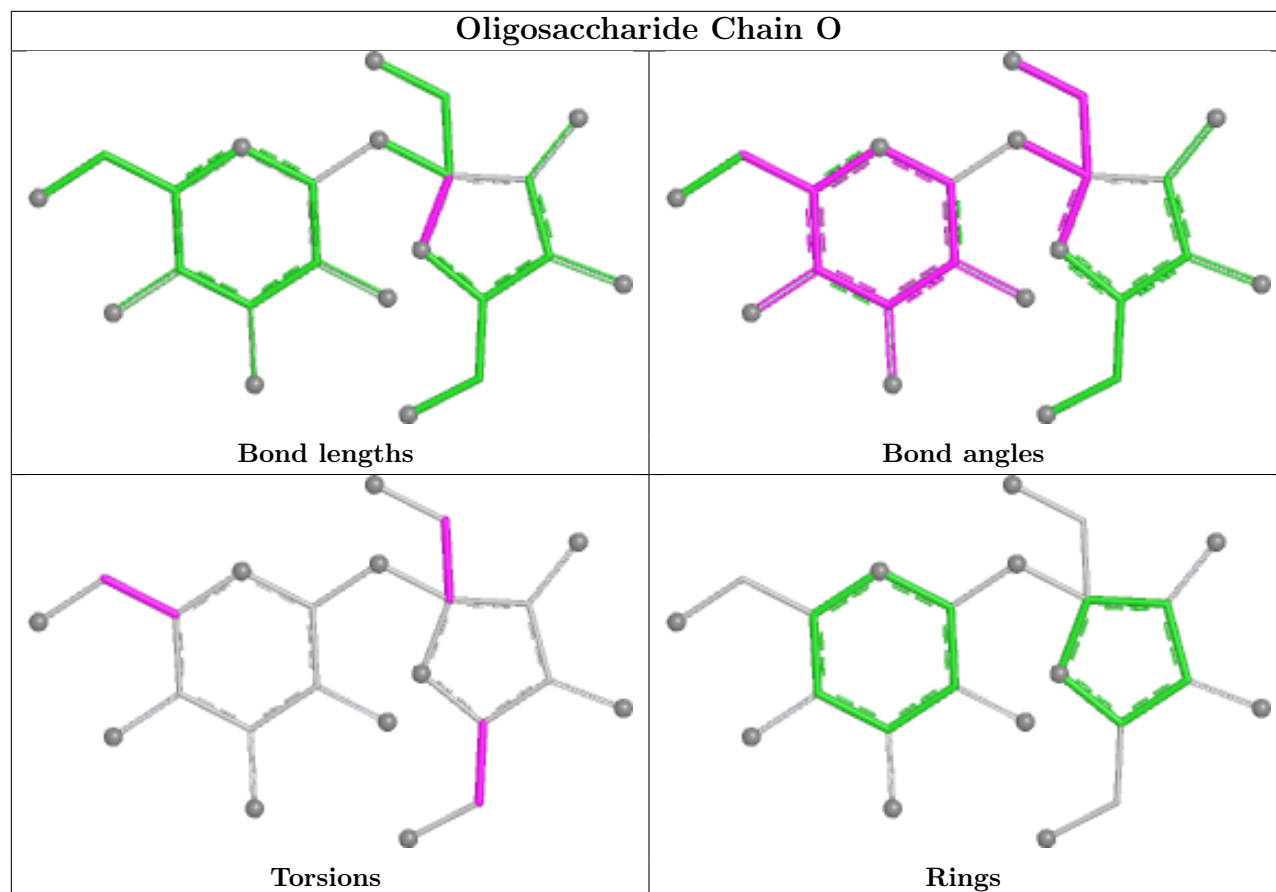
Mol	Chain	Res	Type	Atoms
19	O	2	FRU	O1-C1-C2-C3
19	O	2	FRU	O1-C1-C2-O2
19	Q	2	FRU	O1-C1-C2-C3
19	Q	2	FRU	O1-C1-C2-O2
19	Q	2	FRU	O1-C1-C2-O5

There are no ring outliers.

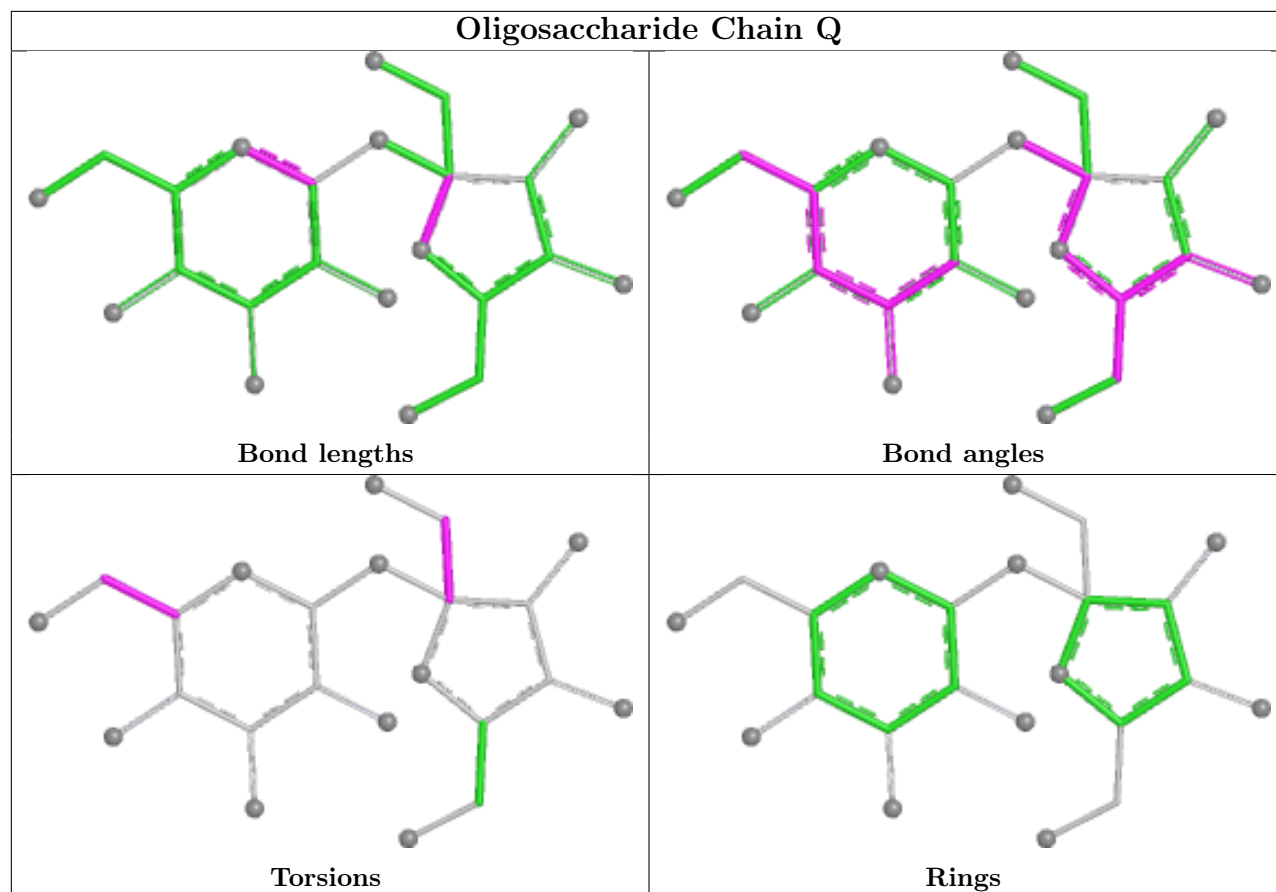
No monomer is involved in short contacts.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

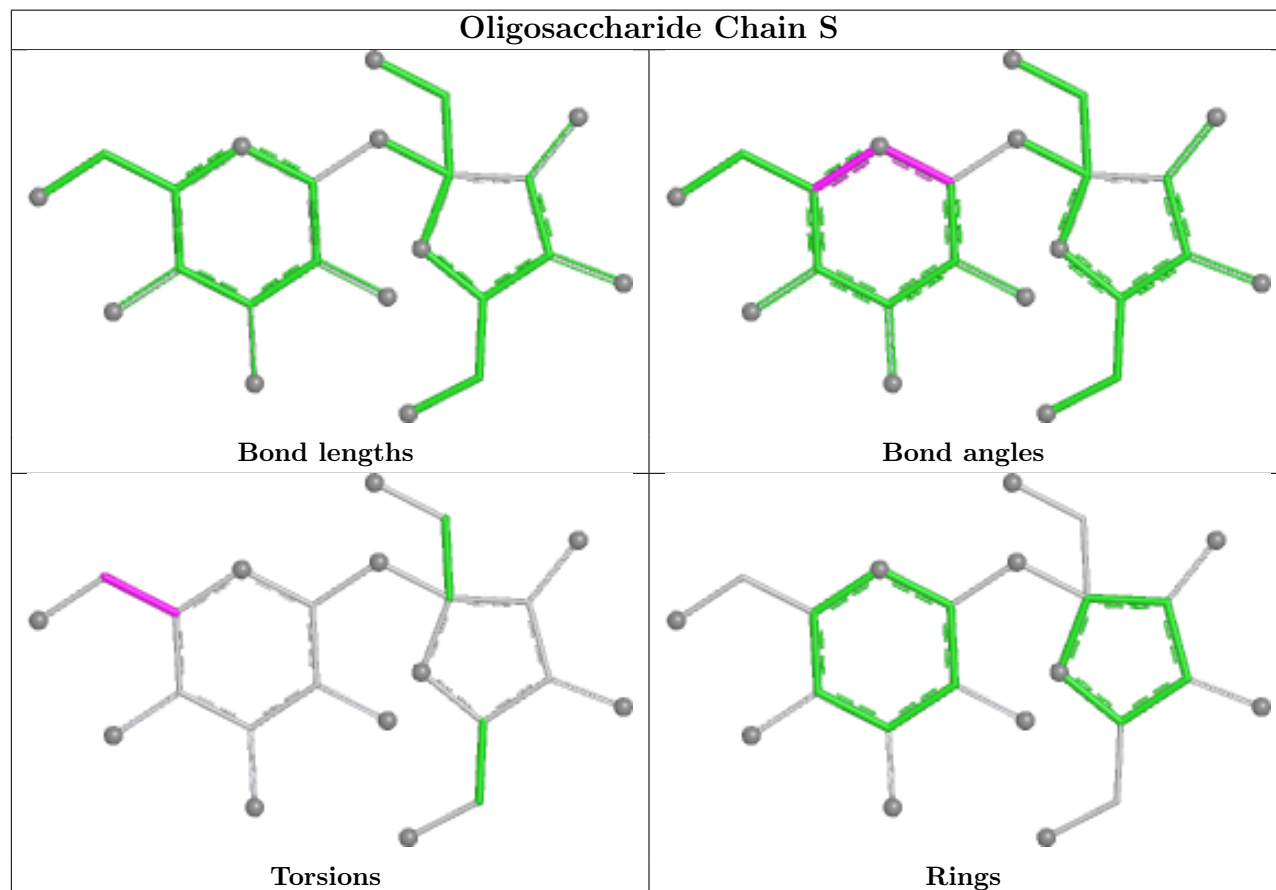


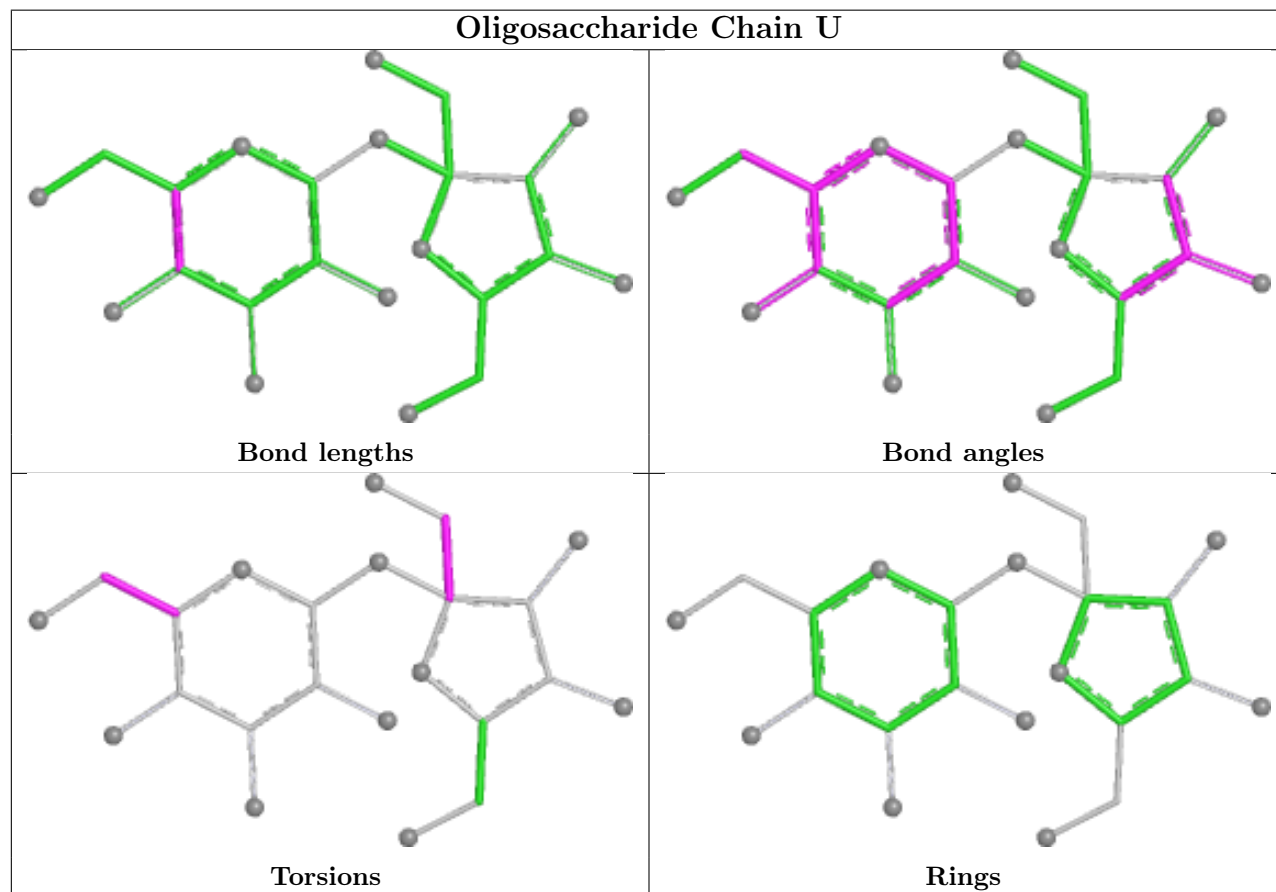
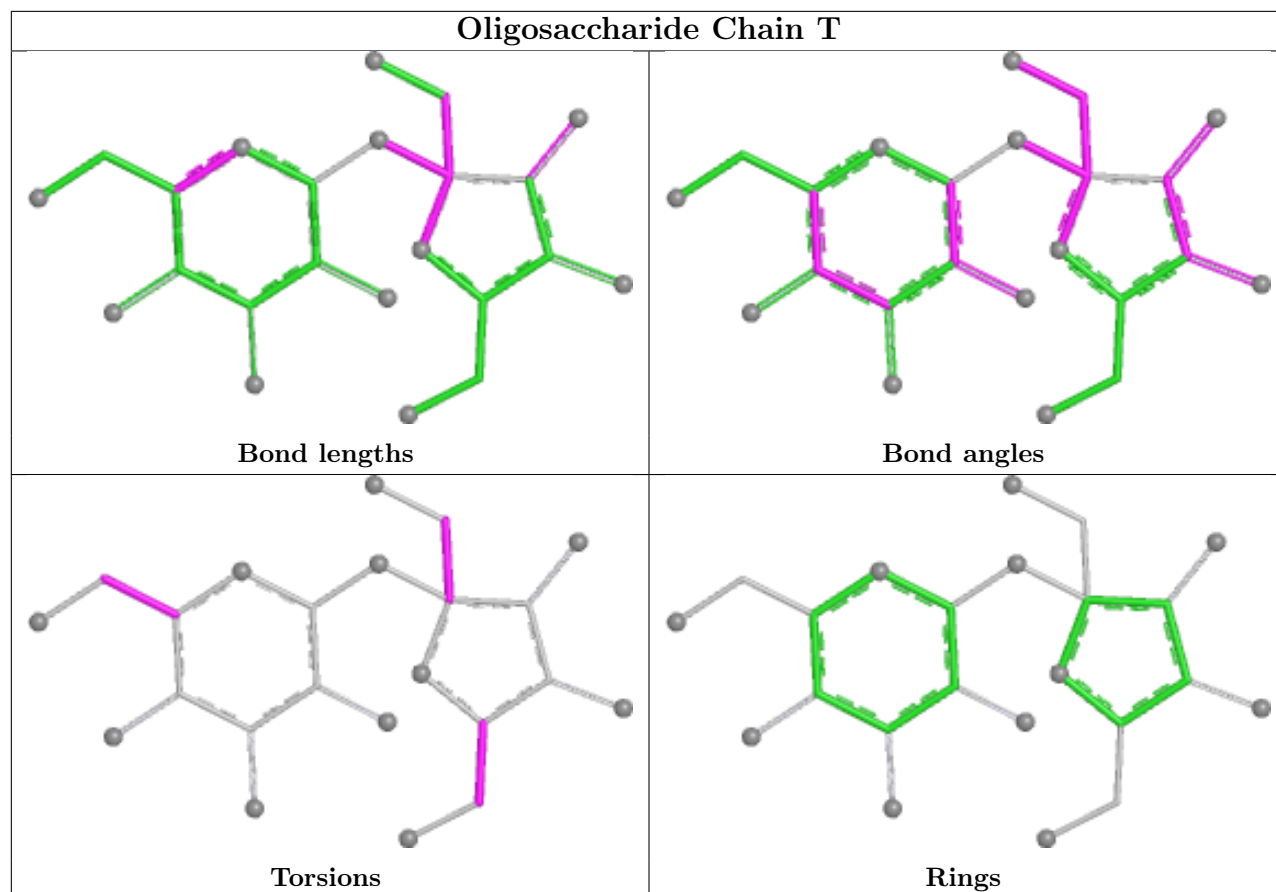


Oligosaccharide Chain Q

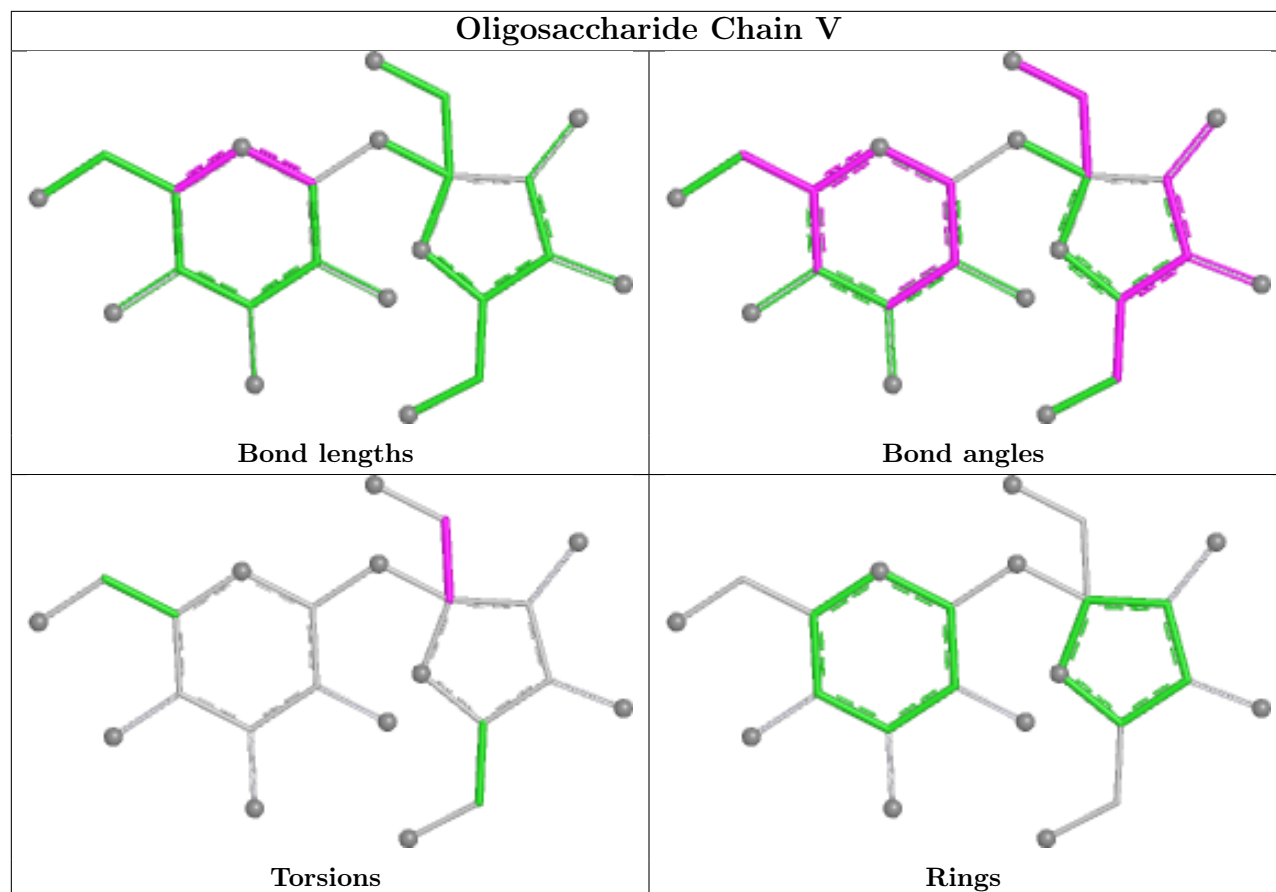


Oligosaccharide Chain S

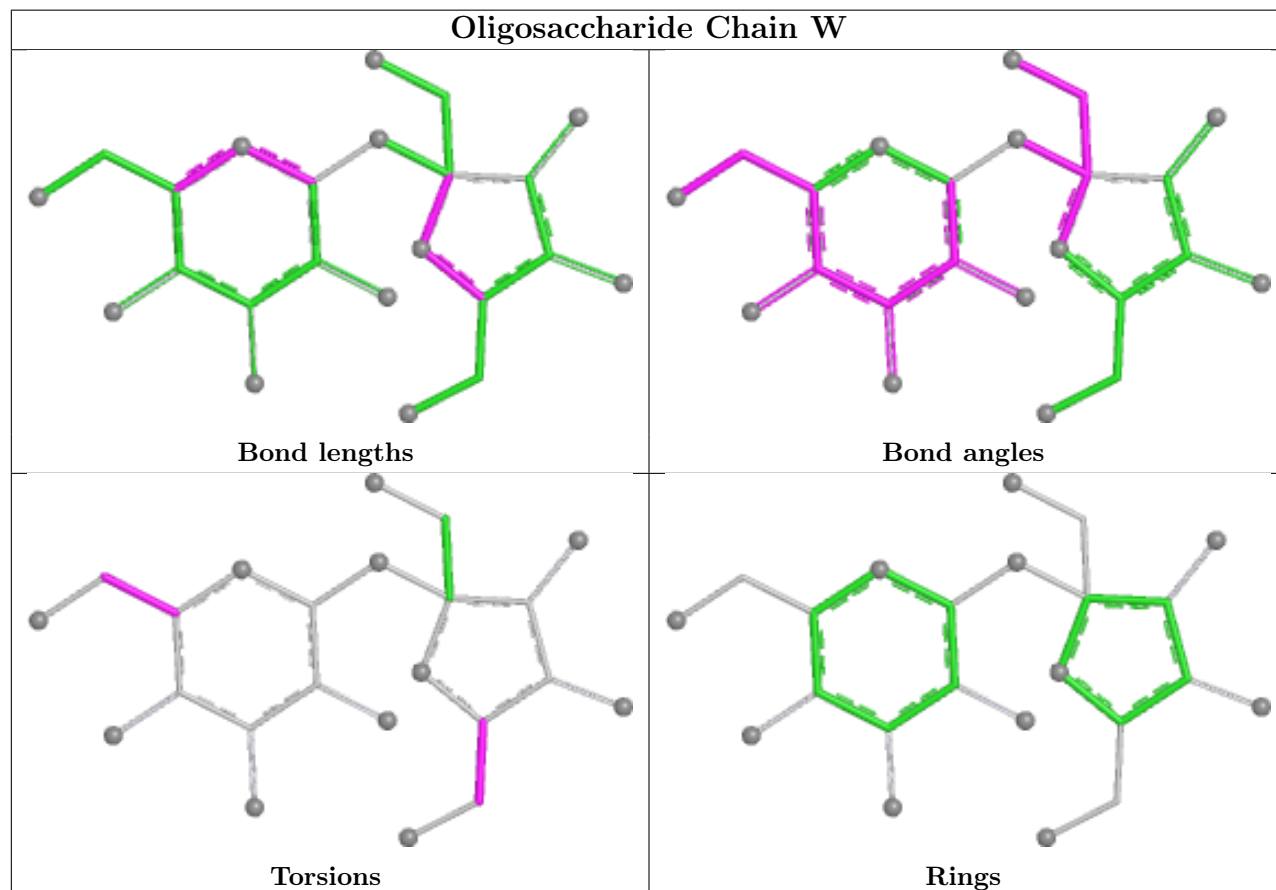


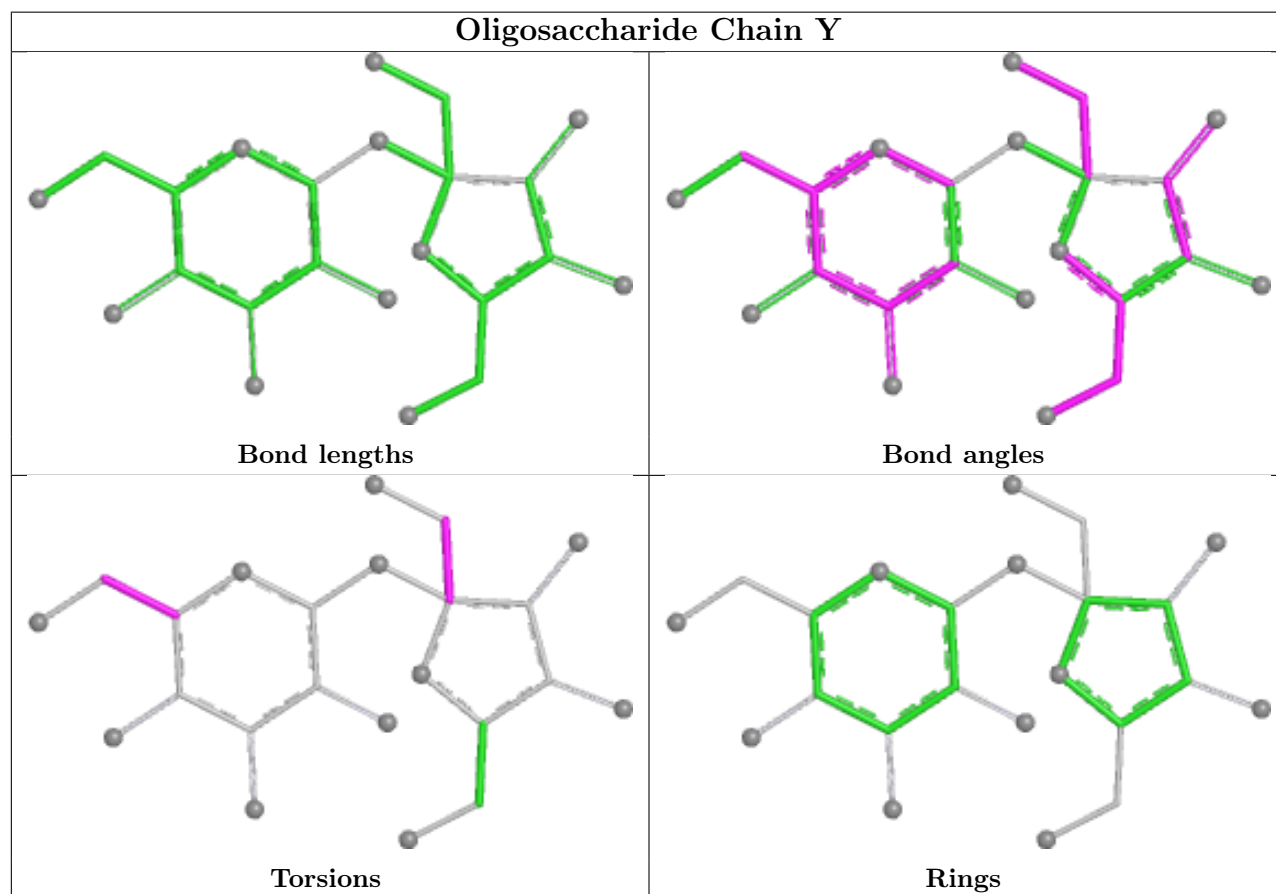
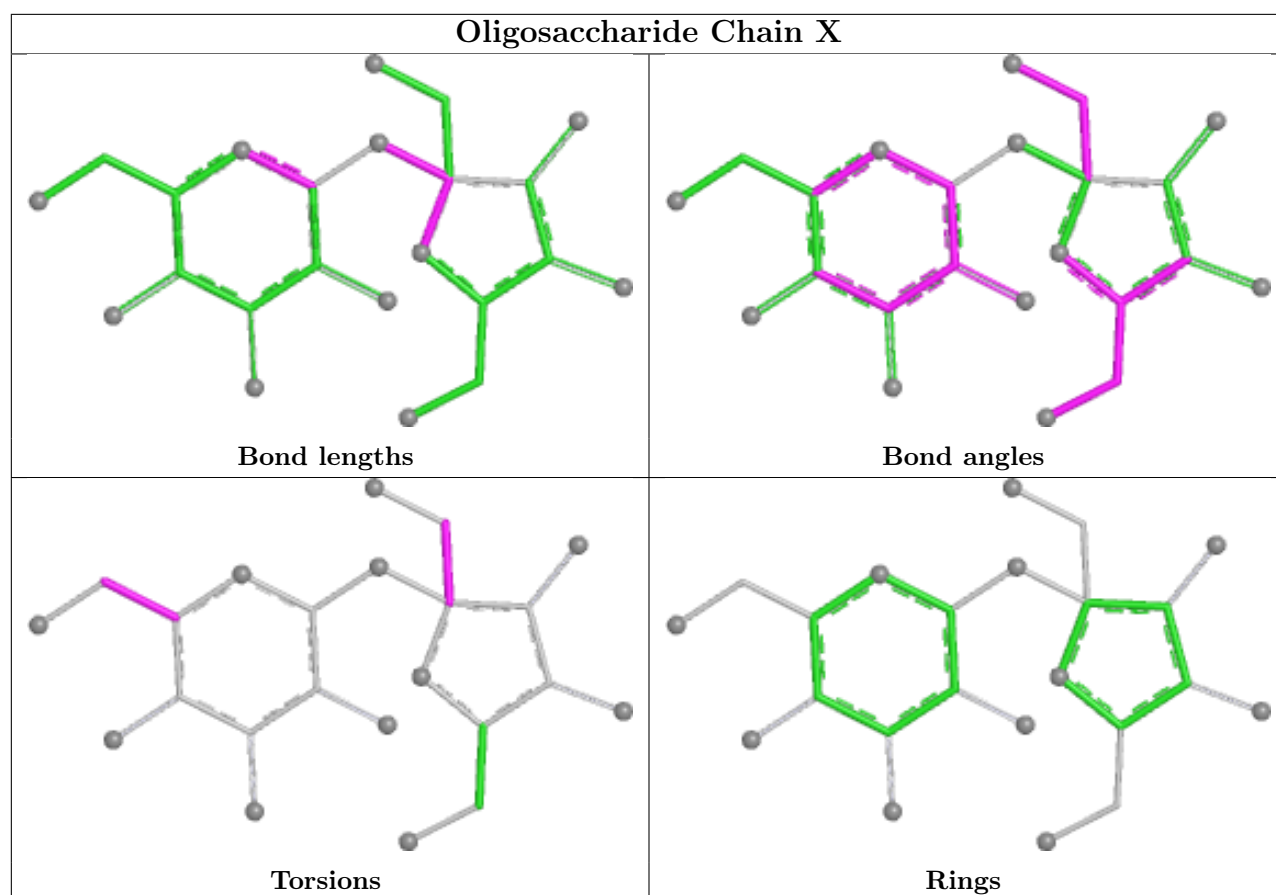


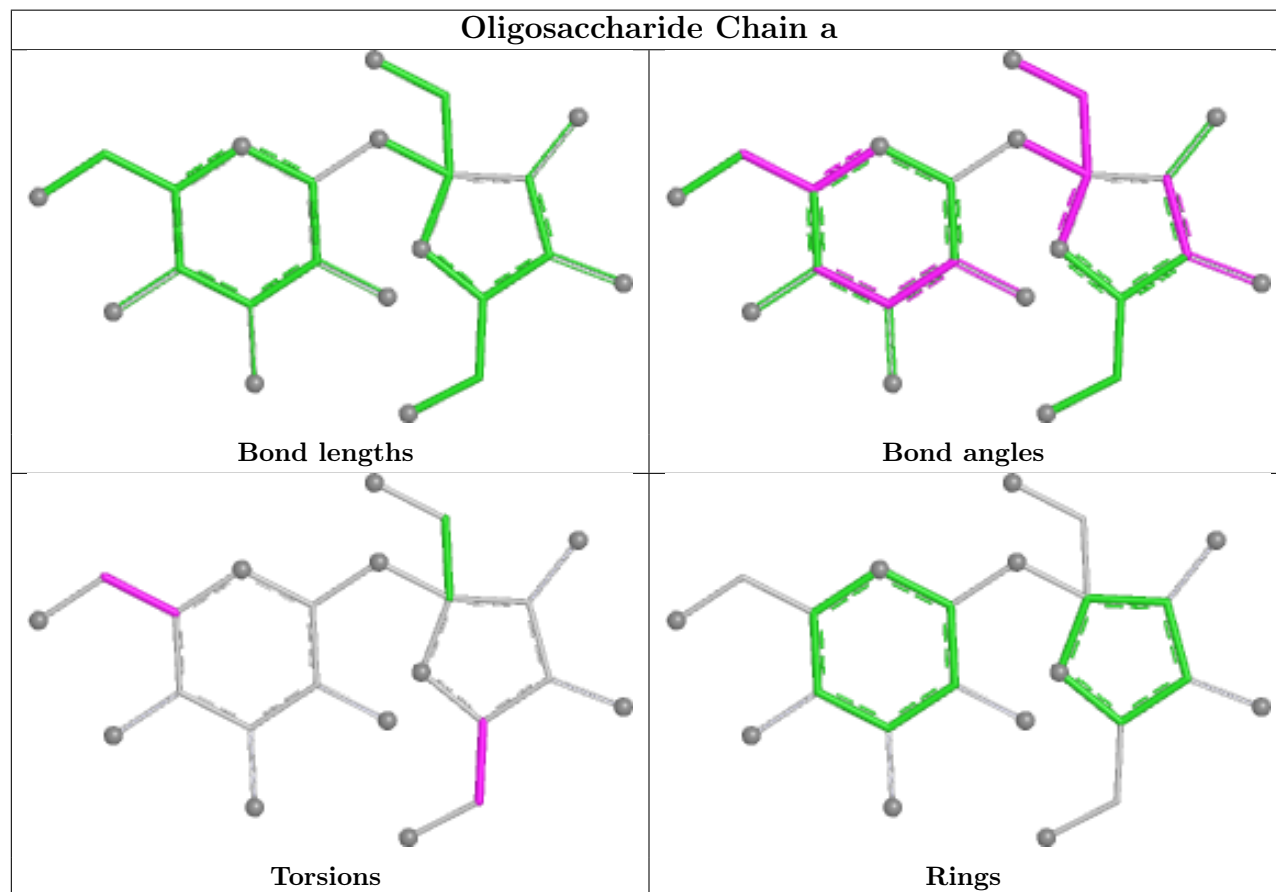
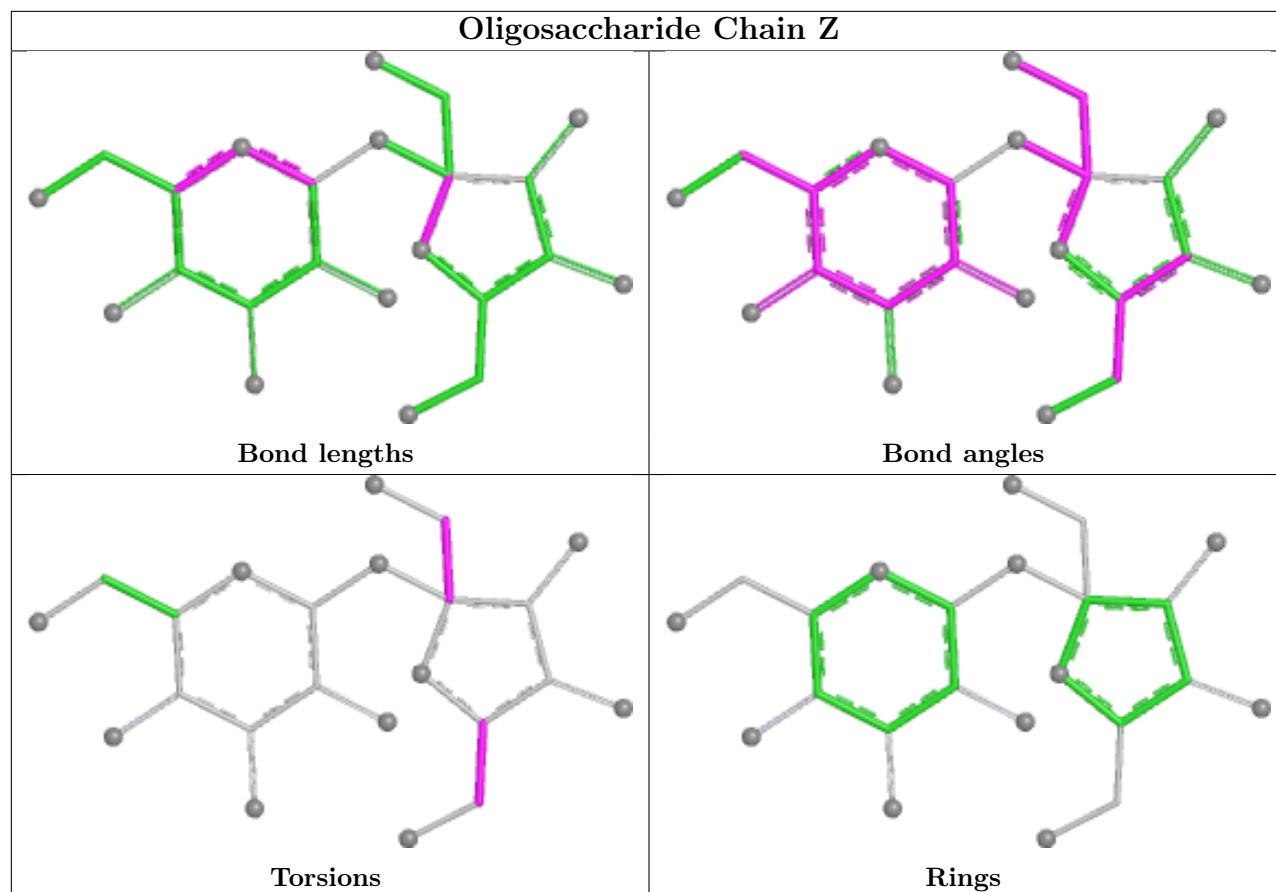
Oligosaccharide Chain V



Oligosaccharide Chain W







4.6 Ligand geometry

Of 243 ligands modelled in this entry, 1 is unknown - leaving 242 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
20	CLA	1	215	-	24,32,73	2.47	7 (29%)	31,54,113	3.38	19 (61%)
21	LMU	1	217	-	36,36,36	0.45	0	47,47,47	1.65	9 (19%)
20	CLA	4	315	-	50,54,73	2.72	20 (40%)	59,90,113	3.09	25 (42%)
22	BCR	F	203	-	41,41,41	2.48	12 (29%)	56,56,56	6.23	32 (57%)
20	CLA	4	317	-	24,32,73	2.35	8 (33%)	31,54,113	2.71	17 (54%)
20	CLA	4	310	-	59,63,73	2.41	12 (20%)	70,101,113	2.86	28 (40%)
21	LMU	R	109	-	36,36,36	1.15	2 (5%)	47,47,47	2.46	15 (31%)
20	CLA	R	106	-	61,65,73	2.38	13 (21%)	72,103,113	2.91	27 (37%)
20	CLA	A	811	-	58,62,73	2.25	14 (24%)	68,99,113	2.71	25 (36%)
20	CLA	A	815	-	56,60,73	2.46	13 (23%)	65,97,113	3.01	27 (41%)
20	CLA	A	820	-	59,63,73	2.40	14 (23%)	70,101,113	2.82	24 (34%)
20	CLA	3	314	-	46,50,73	2.51	11 (23%)	53,85,113	3.15	27 (50%)
20	CLA	A	813	-	54,58,73	2.57	13 (24%)	64,95,113	2.75	27 (42%)
21	LMU	4	321	-	36,36,36	1.03	1 (2%)	47,47,47	1.42	8 (17%)
20	CLA	A	837	-	69,73,73	2.17	15 (21%)	82,113,113	2.64	23 (28%)
20	CLA	B	822	-	62,66,73	2.29	15 (24%)	73,104,113	2.79	25 (34%)
20	CLA	1	213	-	24,32,73	2.46	8 (33%)	31,54,113	2.89	18 (58%)
20	CLA	B	831	20	49,53,73	2.71	16 (32%)	58,89,113	3.07	20 (34%)
21	LMU	2	318	-	36,36,36	1.12	1 (2%)	47,47,47	1.94	14 (29%)
20	CLA	A	857	-	24,32,73	2.34	10 (41%)	31,54,113	2.81	18 (58%)
20	CLA	L	201	-	69,73,73	2.22	14 (20%)	82,113,113	2.59	27 (32%)
22	BCR	B	843	-	41,41,41	1.68	5 (12%)	56,56,56	6.06	19 (33%)
20	CLA	3	319	-	38,44,73	2.83	11 (28%)	52,78,113	3.35	24 (46%)
20	CLA	A	827	-	54,58,73	2.47	12 (22%)	64,95,113	3.03	28 (43%)
22	BCR	I	103	-	41,41,41	2.45	8 (19%)	56,56,56	6.68	29 (51%)
20	CLA	A	850	-	50,54,73	2.79	15 (30%)	61,90,113	3.93	35 (57%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
20	CLA	3	320	-	59,63,73	2.34	12 (20%)	70,101,113	2.90	26 (37%)
21	LMU	A	852	-	36,36,36	0.62	1 (2%)	47,47,47	1.89	11 (23%)
20	CLA	B	829	-	69,73,73	2.27	16 (23%)	82,113,113	2.92	28 (34%)
22	BCR	I	101	-	41,41,41	2.38	16 (39%)	56,56,56	5.48	31 (55%)
20	CLA	K	103	21	54,58,73	2.46	15 (27%)	64,95,113	2.96	23 (35%)
20	CLA	A	817	-	69,73,73	2.20	16 (23%)	82,113,113	2.59	26 (31%)
20	CLA	L	207	22	51,55,73	2.46	12 (23%)	60,91,113	3.31	27 (45%)
21	LMU	L	205	-	36,36,36	0.70	2 (5%)	47,47,47	2.44	15 (31%)
20	CLA	A	808	-	49,53,73	2.71	13 (26%)	58,89,113	3.20	24 (41%)
22	BCR	B	842	-	41,41,41	1.70	5 (12%)	56,56,56	5.15	23 (41%)
20	CLA	A	821	-	69,73,73	2.11	13 (18%)	82,113,113	2.53	26 (31%)
20	CLA	3	307	-	24,32,73	2.38	9 (37%)	31,54,113	2.76	17 (54%)
20	CLA	B	847	-	69,73,73	2.16	15 (21%)	82,113,113	2.81	36 (43%)
20	CLA	B	815	-	64,68,73	2.19	14 (21%)	76,107,113	2.70	28 (36%)
20	CLA	H	109	16	54,58,73	2.49	12 (22%)	64,95,113	2.84	22 (34%)
20	CLA	A	801	-	54,58,73	2.37	14 (25%)	64,95,113	3.22	28 (43%)
20	CLA	3	315	-	54,58,73	2.50	18 (33%)	64,95,113	3.18	27 (42%)
20	CLA	4	311	-	24,32,73	2.38	9 (37%)	31,54,113	2.92	19 (61%)
21	LMU	A	851	-	36,36,36	0.41	0	47,47,47	0.71	1 (2%)
20	CLA	3	303	-	38,44,73	2.79	10 (26%)	52,78,113	3.04	21 (40%)
20	CLA	L	202	-	69,73,73	2.12	13 (18%)	82,113,113	2.79	29 (35%)
20	CLA	L	204	-	59,63,73	2.85	23 (38%)	70,101,113	3.59	32 (45%)
20	CLA	1	211	-	55,59,73	2.84	24 (43%)	64,96,113	4.11	31 (48%)
20	CLA	H	110	-	59,63,73	2.38	12 (20%)	70,101,113	2.95	25 (35%)
21	LMU	B	802	-	36,36,36	0.96	3 (8%)	47,47,47	2.48	13 (27%)
22	BCR	A	840	-	41,41,41	1.68	4 (9%)	56,56,56	6.06	18 (32%)
20	CLA	A	828	-	69,73,73	2.26	17 (24%)	82,113,113	2.67	23 (28%)
21	LMU	4	322	20	36,36,36	0.85	1 (2%)	47,47,47	1.25	4 (8%)
21	LMU	C	101	-	36,36,36	0.94	1 (2%)	47,47,47	1.36	7 (14%)
20	CLA	A	855	-	69,73,73	2.17	15 (21%)	82,113,113	2.64	23 (28%)
20	CLA	1	214	-	55,59,73	2.90	24 (43%)	64,96,113	3.50	32 (50%)
20	CLA	2	311	-	54,58,73	2.57	14 (25%)	64,95,113	3.01	24 (37%)
20	CLA	B	811	-	69,73,73	2.22	12 (17%)	82,113,113	2.51	28 (34%)
20	CLA	4	314	4	24,32,73	2.37	8 (33%)	31,54,113	2.63	17 (54%)
21	LMU	R	103	-	36,36,36	0.69	0	47,47,47	2.19	17 (36%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
20	CLA	B	818	-	50,54,73	2.50	13 (26%)	59,90,113	3.20	20 (33%)
21	LMU	B	845	-	26,26,36	1.04	1 (3%)	37,37,47	1.44	6 (16%)
22	BCR	G	102	-	41,41,41	1.69	5 (12%)	56,56,56	6.05	19 (33%)
20	CLA	A	812	-	49,53,73	2.63	12 (24%)	58,89,113	2.89	24 (41%)
20	CLA	4	319	21	51,55,73	2.53	15 (29%)	60,91,113	2.98	21 (35%)
20	CLA	3	301	20	60,64,73	2.44	20 (33%)	71,102,113	2.94	27 (38%)
21	LMU	2	313	-	36,36,36	0.90	1 (2%)	47,47,47	0.94	2 (4%)
21	LMU	F	201	-	35,35,36	1.20	4 (11%)	46,46,47	2.36	15 (32%)
20	CLA	R	107	-	69,73,73	2.28	12 (17%)	82,113,113	2.64	30 (36%)
20	CLA	2	303	-	24,32,73	2.35	9 (37%)	31,54,113	2.91	19 (61%)
20	CLA	A	848	-	69,73,73	2.24	18 (26%)	82,113,113	2.62	24 (29%)
20	CLA	B	821	-	58,62,73	2.43	19 (32%)	68,99,113	2.79	28 (41%)
22	BCR	A	843	-	41,41,41	1.68	5 (12%)	56,56,56	6.07	17 (30%)
22	BCR	B	844	-	41,41,41	1.67	5 (12%)	56,56,56	6.07	17 (30%)
20	CLA	2	307	20	69,73,73	2.18	12 (17%)	82,113,113	2.70	28 (34%)
22	BCR	F	202	-	41,41,41	1.68	5 (12%)	56,56,56	6.06	18 (32%)
20	CLA	3	306	-	24,32,73	2.40	9 (37%)	31,54,113	2.97	17 (54%)
20	CLA	B	816	-	65,69,73	2.19	15 (23%)	77,108,113	2.79	27 (35%)
20	CLA	A	819	5	46,50,73	2.59	12 (26%)	53,85,113	3.32	24 (45%)
20	CLA	B	817	-	54,58,73	2.41	13 (24%)	64,95,113	2.96	25 (39%)
20	CLA	A	838	-	54,58,73	2.53	15 (27%)	64,95,113	2.82	23 (35%)
22	BCR	A	842	-	41,41,41	1.68	5 (12%)	56,56,56	6.06	18 (32%)
20	CLA	B	832	20	49,53,73	2.63	13 (26%)	58,89,113	3.13	23 (39%)
22	BCR	A	844	-	41,41,41	1.68	5 (12%)	56,56,56	6.06	18 (32%)
20	CLA	H	107	-	69,73,73	2.26	13 (18%)	82,113,113	2.84	27 (32%)
20	CLA	4	318	-	56,60,73	2.45	13 (23%)	65,97,113	2.93	24 (36%)
20	CLA	4	309	-	24,32,73	2.45	8 (33%)	31,54,113	2.98	18 (58%)
20	CLA	B	849	-	69,73,73	2.26	15 (21%)	82,113,113	2.68	30 (36%)
20	CLA	3	313	-	24,32,73	2.47	9 (37%)	31,54,113	2.84	19 (61%)
20	CLA	A	814	-	69,73,73	2.26	19 (27%)	82,113,113	2.75	28 (34%)
20	CLA	A	847	-	69,73,73	2.20	15 (21%)	82,113,113	2.81	27 (32%)
20	CLA	1	206	-	65,69,73	2.28	15 (23%)	77,108,113	2.59	28 (36%)
21	LMU	H	102	19	36,36,36	1.21	3 (8%)	47,47,47	3.10	22 (46%)
20	CLA	1	207	-	55,59,73	2.53	16 (29%)	64,96,113	3.43	30 (46%)
21	LMU	1	218	-	36,36,36	1.02	3 (8%)	47,47,47	2.30	13 (27%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
20	CLA	3	304	-	24,32,73	2.42	11 (45%)	31,54,113	3.47	20 (64%)
20	CLA	1	204	-	50,54,73	2.64	14 (28%)	59,90,113	2.78	23 (38%)
20	CLA	3	316	-	24,32,73	2.45	9 (37%)	31,54,113	3.07	19 (61%)
20	CLA	B	839	-	38,44,73	2.88	12 (31%)	52,78,113	3.38	29 (55%)
25	LMG	B	846	-	49,49,55	0.96	2 (4%)	57,57,63	1.02	3 (5%)
21	LMU	E	101	-	36,36,36	0.89	2 (5%)	47,47,47	3.11	22 (46%)
21	LMU	4	320	-	35,35,36	0.41	0	46,46,47	0.71	1 (2%)
20	CLA	B	807	6	69,73,73	2.13	14 (20%)	82,113,113	2.69	24 (29%)
20	CLA	B	805	-	69,73,73	2.21	16 (23%)	82,113,113	3.02	34 (41%)
21	LMU	A	853	-	36,36,36	0.67	1 (2%)	47,47,47	1.96	17 (36%)
20	CLA	B	826	-	69,73,73	2.19	15 (21%)	82,113,113	2.98	27 (32%)
20	CLA	L	208	-	54,58,73	2.65	19 (35%)	64,95,113	3.23	25 (39%)
20	CLA	1	210	1	38,44,73	2.87	12 (31%)	52,78,113	3.10	23 (44%)
20	CLA	K	106	-	54,58,73	2.86	23 (42%)	64,95,113	3.24	30 (46%)
20	CLA	A	830	20	54,58,73	2.43	14 (25%)	64,95,113	2.85	26 (40%)
20	CLA	4	304	-	69,73,73	2.42	27 (39%)	82,113,113	3.52	38 (46%)
20	CLA	B	812	-	64,68,73	2.25	11 (17%)	76,107,113	2.60	26 (34%)
20	CLA	4	308	-	24,32,73	2.45	8 (33%)	31,54,113	2.90	18 (58%)
20	CLA	A	807	-	59,63,73	2.32	12 (20%)	70,101,113	2.98	30 (42%)
20	CLA	3	305	-	24,32,73	2.43	9 (37%)	31,54,113	2.97	17 (54%)
20	CLA	B	823	-	69,73,73	2.18	15 (21%)	82,113,113	2.64	23 (28%)
20	CLA	F	205	20	45,49,73	2.66	15 (33%)	54,84,113	3.14	20 (37%)
20	CLA	G	103	-	55,59,73	2.52	12 (21%)	64,96,113	2.88	26 (40%)
20	CLA	B	813	-	50,54,73	2.51	12 (24%)	59,90,113	2.96	24 (40%)
21	LMU	R	104	-	36,36,36	0.98	2 (5%)	47,47,47	1.64	11 (23%)
23	PQN	B	840	-	34,34,34	1.69	2 (5%)	43,45,45	1.59	6 (13%)
20	CLA	B	838	-	69,73,73	2.11	14 (20%)	82,113,113	2.76	30 (36%)
20	CLA	B	848	-	69,73,73	2.14	13 (18%)	82,113,113	2.76	31 (37%)
21	LMU	3	318	-	36,36,36	0.41	0	47,47,47	0.69	1 (2%)
20	CLA	2	321	20	65,69,73	2.44	25 (38%)	77,108,113	2.97	32 (41%)
20	CLA	A	804	-	61,65,73	2.33	14 (22%)	72,103,113	2.96	29 (40%)
21	LMU	R	108	-	36,36,36	0.40	0	47,47,47	0.70	1 (2%)
20	CLA	K	107	-	69,73,73	2.21	12 (17%)	82,113,113	2.53	27 (32%)
21	LMU	L	210	-	36,36,36	0.99	3 (8%)	47,47,47	1.49	9 (19%)
21	LMU	1	216	-	36,36,36	0.40	0	47,47,47	0.70	1 (2%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
20	CLA	2	302	-	60,64,73	2.38	15 (25%)	71,102,113	2.92	31 (43%)
20	CLA	B	827	-	54,58,73	2.67	16 (29%)	64,95,113	2.68	29 (45%)
20	CLA	1	205	-	38,44,73	3.00	12 (31%)	52,78,113	3.27	23 (44%)
20	CLA	A	834	-	51,55,73	2.52	15 (29%)	60,91,113	2.98	21 (35%)
20	CLA	B	810	-	69,73,73	2.24	15 (21%)	82,113,113	2.49	24 (29%)
20	CLA	B	834	-	64,68,73	2.21	13 (20%)	76,107,113	2.99	21 (27%)
21	LMU	2	320	-	36,36,36	1.12	1 (2%)	47,47,47	1.37	4 (8%)
20	CLA	B	835	-	69,73,73	2.13	13 (18%)	82,113,113	2.67	25 (30%)
20	CLA	B	808	-	58,62,73	2.65	14 (24%)	71,100,113	2.80	30 (42%)
21	LMU	R	101	-	36,36,36	0.40	0	47,47,47	1.75	12 (25%)
20	CLA	1	203	-	51,55,73	2.57	13 (25%)	60,91,113	3.26	24 (40%)
20	CLA	2	301	-	55,59,73	2.43	15 (27%)	64,96,113	2.96	23 (35%)
21	LMU	R	105	-	36,36,36	0.96	1 (2%)	47,47,47	1.59	10 (21%)
20	CLA	F	204	-	38,44,73	2.81	12 (31%)	52,78,113	3.20	27 (51%)
20	CLA	4	312	-	24,32,73	2.56	7 (29%)	31,54,113	2.94	20 (64%)
20	CLA	4	307	-	56,60,73	3.06	29 (51%)	65,97,113	3.78	38 (58%)
20	CLA	A	802	-	59,63,73	2.41	16 (27%)	70,101,113	2.81	26 (37%)
20	CLA	B	836	-	51,55,73	2.47	14 (27%)	60,91,113	2.92	26 (43%)
20	CLA	B	837	-	69,73,73	2.17	14 (20%)	82,113,113	2.84	30 (36%)
20	CLA	B	819	-	59,63,73	2.48	15 (25%)	70,101,113	2.76	22 (31%)
22	BCR	A	841	-	41,41,41	1.67	3 (7%)	56,56,56	6.06	17 (30%)
20	CLA	A	824	-	69,73,73	2.17	13 (18%)	82,113,113	2.72	30 (36%)
20	CLA	3	317	-	24,32,73	2.42	7 (29%)	31,54,113	2.82	18 (58%)
20	CLA	1	201	-	50,54,73	2.82	24 (48%)	59,90,113	4.11	36 (61%)
21	LMU	B	801	-	36,36,36	0.64	0	47,47,47	2.42	15 (31%)
20	CLA	3	308	-	24,32,73	2.40	9 (37%)	31,54,113	3.21	18 (58%)
21	LMU	A	854	-	36,36,36	0.83	1 (2%)	47,47,47	1.62	8 (17%)
20	CLA	1	202	-	51,55,73	2.55	14 (27%)	60,91,113	3.00	23 (38%)
20	CLA	4	303	-	38,44,73	3.08	15 (39%)	52,78,113	3.61	24 (46%)
20	CLA	4	305	-	59,63,73	2.31	12 (20%)	70,101,113	2.89	28 (40%)
20	CLA	2	315	-	24,32,73	2.46	8 (33%)	31,54,113	2.71	18 (58%)
20	CLA	B	833	-	55,59,73	2.53	12 (21%)	64,96,113	2.95	25 (39%)
20	CLA	L	203	-	59,63,73	2.43	12 (20%)	70,101,113	2.77	29 (41%)
20	CLA	A	805	-	50,54,73	2.51	12 (24%)	59,90,113	2.91	25 (42%)
20	CLA	2	309	-	24,32,73	2.38	8 (33%)	31,54,113	2.82	18 (58%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
21	LMU	3	302	-	36,36,36	0.40	0	47,47,47	0.70	1 (2%)
20	CLA	A	825	-	59,63,73	2.34	15 (25%)	70,101,113	2.78	27 (38%)
20	CLA	3	312	-	24,32,73	2.50	9 (37%)	31,54,113	2.91	20 (64%)
21	LMU	K	102	-	36,36,36	0.47	0	47,47,47	2.08	16 (34%)
20	CLA	A	803	-	69,73,73	2.13	12 (17%)	82,113,113	2.76	30 (36%)
21	LMU	4	301	-	36,36,36	0.40	0	47,47,47	0.70	1 (2%)
21	LMU	R	102	-	36,36,36	0.75	0	47,47,47	2.09	14 (29%)
22	BCR	L	209	-	41,41,41	2.17	10 (24%)	56,56,56	5.87	20 (35%)
20	CLA	A	818	-	55,59,73	2.50	14 (25%)	64,96,113	2.93	23 (35%)
20	CLA	4	302	-	59,63,73	2.35	15 (25%)	70,101,113	2.84	24 (34%)
20	CLA	B	809	-	59,63,73	2.28	15 (25%)	70,101,113	2.76	28 (40%)
20	CLA	K	105	-	49,53,73	2.56	16 (32%)	58,89,113	3.02	20 (34%)
21	LMU	A	845	-	36,36,36	0.94	0	47,47,47	1.40	6 (12%)
20	CLA	A	810	-	58,62,73	2.36	13 (22%)	68,99,113	2.57	23 (33%)
20	CLA	A	835	-	55,59,73	2.43	15 (27%)	64,96,113	2.96	23 (35%)
23	PQN	A	839	-	34,34,34	1.80	3 (8%)	43,45,45	1.49	9 (20%)
20	CLA	4	306	-	54,58,73	2.58	12 (22%)	64,95,113	2.75	21 (32%)
20	CLA	2	312	-	69,73,73	2.23	14 (20%)	82,113,113	2.70	25 (30%)
20	CLA	2	317	-	69,73,73	2.15	15 (21%)	82,113,113	2.50	22 (26%)
20	CLA	2	304	-	54,58,73	2.47	13 (24%)	64,95,113	2.67	24 (37%)
20	CLA	B	820	-	69,73,73	2.90	30 (43%)	82,113,113	2.92	28 (34%)
21	LMU	H	105	19	36,36,36	0.76	0	47,47,47	2.27	16 (34%)
20	CLA	2	308	-	24,32,73	2.40	8 (33%)	31,54,113	2.98	19 (61%)
20	CLA	H	108	-	59,63,73	2.42	12 (20%)	70,101,113	2.79	24 (34%)
20	CLA	A	822	-	69,73,73	2.17	15 (21%)	82,113,113	2.65	24 (29%)
20	CLA	4	313	-	38,44,73	2.71	11 (28%)	52,78,113	3.51	26 (50%)
20	CLA	J	102	-	65,69,73	2.23	15 (23%)	77,108,113	2.71	23 (29%)
22	BCR	B	841	-	41,41,41	1.69	5 (12%)	56,56,56	6.05	19 (33%)
20	CLA	A	831	5	49,53,73	2.57	15 (30%)	58,89,113	3.03	20 (34%)
20	CLA	A	806	5	69,73,73	2.21	15 (21%)	82,113,113	2.93	32 (39%)
20	CLA	A	849	-	69,73,73	2.34	16 (23%)	82,113,113	2.86	27 (32%)
20	CLA	B	824	-	69,73,73	2.34	14 (20%)	82,113,113	2.85	26 (31%)
20	CLA	2	306	-	69,73,73	2.21	13 (18%)	82,113,113	2.76	25 (30%)
20	CLA	3	310	-	69,73,73	2.16	15 (21%)	82,113,113	2.64	23 (28%)
20	CLA	F	206	20	57,61,73	2.73	24 (42%)	67,98,113	2.83	26 (38%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
20	CLA	B	825	-	69,73,73	2.15	14 (20%)	82,113,113	2.85	30 (36%)
21	LMU	2	316	-	36,36,36	0.39	0	47,47,47	0.70	1 (2%)
20	CLA	1	209	-	38,44,73	3.57	22 (57%)	52,78,113	4.04	26 (50%)
21	LMU	4	316	-	36,36,36	0.86	1 (2%)	47,47,47	1.19	3 (6%)
20	CLA	2	305	-	24,32,73	2.42	11 (45%)	31,54,113	3.11	20 (64%)
20	CLA	A	829	-	69,73,73	2.24	13 (18%)	82,113,113	2.93	32 (39%)
20	CLA	B	830	-	54,58,73	2.59	18 (33%)	64,95,113	3.14	27 (42%)
22	BCR	J	101	-	41,41,41	1.67	5 (12%)	56,56,56	6.06	18 (32%)
20	CLA	H	101	-	59,63,73	2.43	15 (25%)	70,101,113	2.96	29 (41%)
20	CLA	B	814	-	63,67,73	2.31	14 (22%)	74,105,113	2.41	24 (32%)
20	CLA	1	208	-	24,32,73	2.33	8 (33%)	31,54,113	2.76	19 (61%)
21	LMU	G	101	-	36,36,36	0.98	2 (5%)	47,47,47	2.60	13 (27%)
20	CLA	B	828	-	54,58,73	2.34	11 (20%)	64,95,113	3.02	29 (45%)
22	BCR	3	311	-	41,41,41	1.79	5 (12%)	56,56,56	6.05	22 (39%)
22	BCR	B	850	20	41,41,41	2.74	18 (43%)	56,56,56	6.57	27 (48%)
20	CLA	3	309	-	69,73,73	2.48	23 (33%)	82,113,113	3.15	29 (35%)
24	SF4	C	103	7	0,12,12	-	-	-	-	-
20	CLA	J	103	20	59,63,73	2.47	20 (33%)	70,101,113	2.99	27 (38%)
20	CLA	A	833	-	69,73,73	2.17	15 (21%)	82,113,113	2.65	23 (28%)
20	CLA	B	806	-	69,73,73	2.24	13 (18%)	82,113,113	2.78	29 (35%)
20	CLA	A	826	-	69,73,73	2.18	15 (21%)	82,113,113	2.65	30 (36%)
24	SF4	C	102	7	0,12,12	-	-	-	-	-
20	CLA	A	816	-	69,73,73	2.17	15 (21%)	82,113,113	2.61	30 (36%)
24	SF4	A	856	5,6	0,12,12	-	-	-	-	-
20	CLA	2	310	2	54,58,73	2.46	13 (24%)	64,95,113	2.98	25 (39%)
21	LMU	A	846	-	36,36,36	0.95	1 (2%)	47,47,47	1.66	11 (23%)
20	CLA	B	803	-	49,53,73	2.62	16 (32%)	58,89,113	3.13	22 (37%)
20	CLA	A	836	-	69,73,73	2.17	15 (21%)	82,113,113	2.64	23 (28%)
21	LMU	K	104	20	36,36,36	0.75	0	47,47,47	2.28	12 (25%)
20	CLA	1	212	-	65,69,73	2.33	21 (32%)	77,108,113	2.84	29 (37%)
20	CLA	B	804	-	69,73,73	2.16	14 (20%)	82,113,113	3.00	33 (40%)
20	CLA	A	832	-	55,59,73	2.44	15 (27%)	64,96,113	2.96	23 (35%)
21	LMU	2	319	-	36,36,36	1.09	1 (2%)	47,47,47	1.31	6 (12%)
20	CLA	I	102	-	64,68,73	2.31	15 (23%)	76,107,113	2.79	24 (31%)
21	LMU	H	104	-	36,36,36	0.98	3 (8%)	47,47,47	2.76	20 (42%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
20	CLA	A	823	20	69,73,73	2.17	16 (23%)	82,113,113	2.64	23 (28%)
20	CLA	2	314	-	24,32,73	2.44	11 (45%)	31,54,113	3.04	21 (67%)
21	LMU	H	103	-	36,36,36	0.89	1 (2%)	47,47,47	2.30	16 (34%)
21	LMU	K	101	-	36,36,36	0.61	0	47,47,47	1.91	14 (29%)
21	LMU	L	206	-	36,36,36	0.73	2 (5%)	47,47,47	1.91	17 (36%)
20	CLA	A	809	-	69,73,73	2.19	12 (17%)	82,113,113	3.02	31 (37%)

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
20	CLA	1	215	-	1/1/4/20	-	-
21	LMU	1	217	-	-	10/21/61/61	0/2/2/2
20	CLA	4	315	-	1/1/11/20	10/17/93/115	-
22	BCR	F	203	-	-	12/29/63/63	0/2/2/2
20	CLA	4	317	-	1/1/4/20	-	-
20	CLA	4	310	-	2/2/13/20	14/27/103/115	-
21	LMU	R	109	-	1/1/10/10	11/21/61/61	0/2/2/2
20	CLA	R	106	-	2/2/13/20	15/30/106/115	-
20	CLA	A	811	-	1/1/12/20	10/26/102/115	-
20	CLA	A	815	-	1/1/12/20	11/24/100/115	-
20	CLA	A	820	-	2/2/13/20	10/27/103/115	-
20	CLA	3	314	-	1/1/10/20	5/12/88/115	-
20	CLA	A	813	-	1/1/12/20	10/21/97/115	-
21	LMU	4	321	-	-	15/21/61/61	0/2/2/2
20	CLA	A	837	-	2/2/15/20	17/39/115/115	-
20	CLA	B	822	-	2/2/13/20	16/31/107/115	-
20	CLA	1	213	-	1/1/4/20	-	-
20	CLA	B	831	20	1/1/11/20	11/15/91/115	-
21	LMU	2	318	-	-	13/21/61/61	0/2/2/2
20	CLA	A	857	-	1/1/4/20	-	-
20	CLA	L	201	-	2/2/15/20	14/39/115/115	-
22	BCR	B	843	-	-	13/29/63/63	0/2/2/2
20	CLA	3	319	-	1/1/9/20	-	-
20	CLA	A	827	-	1/1/12/20	4/21/97/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	BCR	I	103	-	-	13/29/63/63	0/2/2/2
20	CLA	A	850	-	3/3/11/20	12/16/92/115	-
20	CLA	3	320	-	2/2/13/20	8/27/103/115	-
21	LMU	A	852	-	-	11/21/61/61	0/2/2/2
20	CLA	B	829	-	2/2/15/20	21/39/115/115	-
22	BCR	I	101	-	-	7/29/63/63	0/2/2/2
20	CLA	K	103	21	1/1/12/20	5/21/97/115	-
20	CLA	A	817	-	2/2/15/20	13/39/115/115	-
20	CLA	L	207	22	1/1/11/20	11/18/94/115	-
21	LMU	L	205	-	-	15/21/61/61	0/2/2/2
20	CLA	A	808	-	1/1/11/20	4/15/91/115	-
22	BCR	B	842	-	-	11/29/63/63	0/2/2/2
20	CLA	A	821	-	2/2/15/20	20/39/115/115	-
20	CLA	3	307	-	1/1/4/20	-	-
20	CLA	B	847	-	2/2/15/20	16/39/115/115	-
20	CLA	B	815	-	2/2/14/20	15/33/109/115	-
20	CLA	H	109	16	1/1/12/20	10/21/97/115	-
20	CLA	A	801	-	1/1/12/20	4/21/97/115	-
20	CLA	3	315	-	1/1/12/20	6/21/97/115	-
20	CLA	4	311	-	1/1/4/20	-	-
21	LMU	A	851	-	-	19/21/61/61	0/2/2/2
20	CLA	3	303	-	1/1/9/20	-	-
20	CLA	L	202	-	2/2/15/20	14/39/115/115	-
20	CLA	L	204	-	3/3/13/20	14/27/103/115	-
20	CLA	1	211	-	2/2/12/20	9/23/99/115	-
20	CLA	H	110	-	2/2/13/20	14/27/103/115	-
21	LMU	B	802	-	-	11/21/61/61	0/2/2/2
22	BCR	A	840	-	-	12/29/63/63	0/2/2/2
20	CLA	A	828	-	2/2/15/20	21/39/115/115	-
21	LMU	4	322	20	-	14/21/61/61	0/2/2/2
21	LMU	C	101	-	-	14/21/61/61	0/2/2/2
20	CLA	A	855	-	2/2/15/20	20/39/115/115	-
20	CLA	1	214	-	3/3/12/20	13/23/99/115	-
20	CLA	2	311	-	1/1/12/20	9/21/97/115	-
20	CLA	B	811	-	2/2/15/20	25/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
20	CLA	4	314	4	1/1/4/20	-	-
21	LMU	R	103	-	-	17/21/61/61	0/2/2/2
20	CLA	B	818	-	1/1/11/20	14/17/93/115	-
21	LMU	B	845	-	-	4/11/51/61	0/2/2/2
22	BCR	G	102	-	-	10/29/63/63	0/2/2/2
20	CLA	A	812	-	1/1/11/20	13/15/91/115	-
20	CLA	4	319	21	1/1/11/20	9/18/94/115	-
20	CLA	3	301	20	2/2/13/20	14/29/105/115	-
21	LMU	2	313	-	-	16/21/61/61	0/2/2/2
21	LMU	F	201	-	-	14/20/60/61	0/2/2/2
20	CLA	R	107	-	2/2/15/20	21/39/115/115	-
20	CLA	2	303	-	1/1/4/20	-	-
20	CLA	A	848	-	2/2/15/20	16/39/115/115	-
20	CLA	B	821	-	1/1/12/20	7/26/102/115	-
22	BCR	A	843	-	-	15/29/63/63	0/2/2/2
22	BCR	B	844	-	-	14/29/63/63	0/2/2/2
20	CLA	2	307	20	2/2/15/20	14/39/115/115	-
22	BCR	F	202	-	-	12/29/63/63	0/2/2/2
20	CLA	3	306	-	1/1/4/20	-	-
20	CLA	B	816	-	2/2/14/20	17/35/111/115	-
20	CLA	A	819	5	1/1/10/20	3/12/88/115	-
20	CLA	B	817	-	1/1/12/20	7/21/97/115	-
20	CLA	A	838	-	1/1/12/20	10/21/97/115	-
22	BCR	A	842	-	-	17/29/63/63	0/2/2/2
20	CLA	B	832	20	1/1/11/20	7/15/91/115	-
22	BCR	A	844	-	-	10/29/63/63	0/2/2/2
20	CLA	H	107	-	2/2/15/20	19/39/115/115	-
20	CLA	4	318	-	1/1/12/20	8/24/100/115	-
20	CLA	4	309	-	1/1/4/20	-	-
20	CLA	B	849	-	2/2/15/20	18/39/115/115	-
20	CLA	3	313	-	1/1/4/20	-	-
20	CLA	A	814	-	2/2/15/20	17/39/115/115	-
20	CLA	A	847	-	2/2/15/20	21/39/115/115	-
20	CLA	1	206	-	2/2/14/20	21/35/111/115	-
21	LMU	H	102	19	-	14/21/61/61	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
20	CLA	1	207	-	2/2/12/20	9/23/99/115	-
21	LMU	1	218	-	-	13/21/61/61	0/2/2/2
20	CLA	3	304	-	1/1/4/20	-	-
20	CLA	1	204	-	1/1/11/20	8/17/93/115	-
20	CLA	3	316	-	1/1/4/20	-	-
20	CLA	B	839	-	1/1/9/20	-	-
25	LMG	B	846	-	-	23/44/64/70	0/1/1/1
21	LMU	E	101	-	-	14/21/61/61	0/2/2/2
21	LMU	4	320	-	-	15/20/60/61	0/2/2/2
20	CLA	B	807	6	2/2/15/20	20/39/115/115	-
20	CLA	B	805	-	2/2/15/20	19/39/115/115	-
21	LMU	A	853	-	-	14/21/61/61	0/2/2/2
20	CLA	B	826	-	2/2/15/20	25/39/115/115	-
20	CLA	L	208	-	2/2/12/20	10/21/97/115	-
20	CLA	1	210	1	1/1/9/20	-	-
20	CLA	K	106	-	1/1/12/20	9/21/97/115	-
20	CLA	A	830	20	1/1/12/20	13/21/97/115	-
20	CLA	4	304	-	3/3/15/20	18/39/115/115	-
20	CLA	B	812	-	2/2/14/20	11/33/109/115	-
20	CLA	4	308	-	1/1/4/20	-	-
20	CLA	A	807	-	2/2/13/20	12/27/103/115	-
20	CLA	3	305	-	1/1/4/20	-	-
20	CLA	B	823	-	2/2/15/20	21/39/115/115	-
20	CLA	F	205	20	1/1/10/20	5/10/86/115	-
20	CLA	G	103	-	1/1/12/20	11/23/99/115	-
20	CLA	B	813	-	1/1/11/20	9/17/93/115	-
21	LMU	R	104	-	-	15/21/61/61	0/2/2/2
23	PQN	B	840	-	1/1/8/9	10/23/43/43	0/2/2/2
20	CLA	B	838	-	2/2/15/20	16/39/115/115	-
20	CLA	B	848	-	2/2/15/20	16/39/115/115	-
21	LMU	3	318	-	-	17/21/61/61	0/2/2/2
20	CLA	2	321	20	2/2/14/20	20/35/111/115	-
20	CLA	A	804	-	2/2/13/20	8/30/106/115	-
21	LMU	R	108	-	-	16/21/61/61	0/2/2/2
20	CLA	K	107	-	2/2/15/20	19/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
21	LMU	L	210	-	-	14/21/61/61	0/2/2/2
21	LMU	1	216	-	-	13/21/61/61	0/2/2/2
20	CLA	2	302	-	2/2/13/20	12/29/105/115	-
20	CLA	B	827	-	1/1/12/20	8/21/97/115	-
20	CLA	1	205	-	1/1/9/20	-	-
20	CLA	A	834	-	1/1/11/20	8/18/94/115	-
20	CLA	B	810	-	2/2/15/20	20/39/115/115	-
20	CLA	B	834	-	2/2/14/20	17/33/109/115	-
21	LMU	2	320	-	-	8/21/61/61	0/2/2/2
20	CLA	B	835	-	2/2/15/20	12/39/115/115	-
20	CLA	B	808	-	2/2/13/20	11/25/101/115	-
21	LMU	R	101	-	-	11/21/61/61	0/2/2/2
20	CLA	1	203	-	1/1/11/20	8/18/94/115	-
20	CLA	2	301	-	1/1/12/20	11/23/99/115	-
21	LMU	R	105	-	-	13/21/61/61	0/2/2/2
20	CLA	F	204	-	1/1/9/20	-	-
20	CLA	4	312	-	1/1/4/20	-	-
20	CLA	4	307	-	2/2/12/20	7/24/100/115	-
20	CLA	A	802	-	2/2/13/20	11/27/103/115	-
20	CLA	B	836	-	1/1/11/20	7/18/94/115	-
20	CLA	B	837	-	2/2/15/20	17/39/115/115	-
20	CLA	B	819	-	2/2/13/20	9/27/103/115	-
22	BCR	A	841	-	-	13/29/63/63	0/2/2/2
20	CLA	A	824	-	2/2/15/20	18/39/115/115	-
20	CLA	3	317	-	1/1/4/20	-	-
20	CLA	1	201	-	1/1/11/20	12/17/93/115	-
21	LMU	B	801	-	-	16/21/61/61	0/2/2/2
20	CLA	3	308	-	1/1/4/20	-	-
21	LMU	A	854	-	-	14/21/61/61	0/2/2/2
20	CLA	1	202	-	1/1/11/20	9/18/94/115	-
20	CLA	4	303	-	1/1/9/20	-	-
20	CLA	4	305	-	2/2/13/20	13/27/103/115	-
20	CLA	2	315	-	1/1/4/20	-	-
20	CLA	B	833	-	1/1/12/20	8/23/99/115	-
20	CLA	L	203	-	2/2/13/20	8/27/103/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
20	CLA	A	805	-	1/1/11/20	7/17/93/115	-
20	CLA	2	309	-	1/1/4/20	-	-
21	LMU	3	302	-	-	11/21/61/61	0/2/2/2
20	CLA	A	825	-	2/2/13/20	9/27/103/115	-
20	CLA	3	312	-	1/1/4/20	-	-
21	LMU	K	102	-	-	18/21/61/61	0/2/2/2
20	CLA	A	803	-	2/2/15/20	22/39/115/115	-
21	LMU	4	301	-	-	13/21/61/61	0/2/2/2
21	LMU	R	102	-	-	13/21/61/61	0/2/2/2
22	BCR	L	209	-	-	12/29/63/63	0/2/2/2
20	CLA	A	818	-	1/1/12/20	9/23/99/115	-
20	CLA	4	302	-	2/2/13/20	14/27/103/115	-
20	CLA	B	809	-	2/2/13/20	11/27/103/115	-
20	CLA	K	105	-	1/1/11/20	5/15/91/115	-
21	LMU	A	845	-	-	16/21/61/61	0/2/2/2
20	CLA	A	810	-	1/1/12/20	13/26/102/115	-
20	CLA	A	835	-	1/1/12/20	13/23/99/115	-
23	PQN	A	839	-	1/1/8/9	11/23/43/43	0/2/2/2
20	CLA	4	306	-	1/1/12/20	6/21/97/115	-
20	CLA	2	312	-	2/2/15/20	18/39/115/115	-
20	CLA	2	317	-	2/2/15/20	20/39/115/115	-
20	CLA	2	304	-	1/1/12/20	9/21/97/115	-
20	CLA	B	820	-	1/1/15/20	18/39/115/115	-
21	LMU	H	105	19	-	11/21/61/61	0/2/2/2
20	CLA	2	308	-	1/1/4/20	-	-
20	CLA	H	108	-	2/2/13/20	10/27/103/115	-
20	CLA	A	822	-	2/2/15/20	18/39/115/115	-
20	CLA	4	313	-	1/1/9/20	-	-
20	CLA	J	102	-	2/2/14/20	25/35/111/115	-
22	BCR	B	841	-	-	8/29/63/63	0/2/2/2
20	CLA	A	831	5	1/1/11/20	8/15/91/115	-
20	CLA	A	806	5	2/2/15/20	19/39/115/115	-
20	CLA	A	849	-	2/2/15/20	22/39/115/115	-
20	CLA	B	824	-	2/2/15/20	17/39/115/115	-
20	CLA	2	306	-	2/2/15/20	18/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
20	CLA	3	310	-	2/2/15/20	22/39/115/115	-
20	CLA	F	206	20	4/4/12/20	11/25/101/115	-
20	CLA	B	825	-	2/2/15/20	15/39/115/115	-
21	LMU	2	316	-	-	14/21/61/61	0/2/2/2
20	CLA	1	209	-	1/1/9/20	-	-
21	LMU	4	316	-	-	13/21/61/61	0/2/2/2
20	CLA	2	305	-	1/1/4/20	-	-
20	CLA	A	829	-	2/2/15/20	23/39/115/115	-
20	CLA	B	830	-	1/1/12/20	8/21/97/115	-
22	BCR	J	101	-	-	12/29/63/63	0/2/2/2
20	CLA	H	101	-	3/3/13/20	14/27/103/115	-
20	CLA	B	814	-	2/2/13/20	12/32/108/115	-
20	CLA	1	208	-	1/1/4/20	-	-
21	LMU	G	101	-	-	14/21/61/61	0/2/2/2
20	CLA	B	828	-	1/1/12/20	13/21/97/115	-
22	BCR	3	311	-	-	13/29/63/63	0/2/2/2
22	BCR	B	850	20	-	12/29/63/63	0/2/2/2
20	CLA	3	309	-	2/2/15/20	20/39/115/115	-
24	SF4	C	103	7	-	-	0/6/5/5
20	CLA	J	103	20	2/2/13/20	13/27/103/115	-
20	CLA	A	833	-	2/2/15/20	15/39/115/115	-
20	CLA	B	806	-	2/2/15/20	12/39/115/115	-
20	CLA	A	826	-	2/2/15/20	17/39/115/115	-
24	SF4	C	102	7	-	-	0/6/5/5
20	CLA	A	816	-	2/2/15/20	19/39/115/115	-
24	SF4	A	856	5,6	-	-	0/6/5/5
20	CLA	2	310	2	1/1/12/20	6/21/97/115	-
21	LMU	A	846	-	-	13/21/61/61	0/2/2/2
20	CLA	B	803	-	1/1/11/20	6/15/91/115	-
20	CLA	A	836	-	2/2/15/20	15/39/115/115	-
21	LMU	K	104	20	-	12/21/61/61	0/2/2/2
20	CLA	1	212	-	2/2/14/20	15/35/111/115	-
20	CLA	B	804	-	2/2/15/20	18/39/115/115	-
20	CLA	A	832	-	1/1/12/20	11/23/99/115	-
21	LMU	2	319	-	-	13/21/61/61	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
20	CLA	I	102	-	2/2/14/20	12/33/109/115	-
21	LMU	H	104	-	-	13/21/61/61	0/2/2/2
20	CLA	A	823	20	2/2/15/20	22/39/115/115	-
20	CLA	2	314	-	1/1/4/20	-	-
21	LMU	H	103	-	-	17/21/61/61	0/2/2/2
21	LMU	K	101	-	-	12/21/61/61	0/2/2/2
21	LMU	L	206	-	-	14/21/61/61	0/2/2/2
20	CLA	A	809	-	2/2/15/20	24/39/115/115	-

The worst 5 of 2618 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	1	209	CLA	CAB-C3B	-9.95	1.30	1.50
22	B	850	BCR	C20-C21	-9.80	1.12	1.43
22	L	209	BCR	C20-C21	-8.72	1.16	1.43
20	1	205	CLA	CAB-C3B	-8.54	1.33	1.50
22	F	203	BCR	C20-C21	-8.32	1.17	1.43

The worst 5 of 5222 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	B	844	BCR	C20-C21-C22	37.59	179.99	127.28
22	J	101	BCR	C20-C21-C22	37.57	179.97	127.28
22	A	842	BCR	C20-C21-C22	37.56	179.95	127.28
22	A	843	BCR	C20-C21-C22	37.56	179.95	127.28
22	A	841	BCR	C20-C21-C22	37.54	179.93	127.28

5 of 271 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
20	1	201	CLA	ND
20	1	202	CLA	ND
20	1	203	CLA	ND
20	1	204	CLA	ND
20	1	205	CLA	ND

5 of 2714 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
20	1	201	CLA	C1A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
20	1	201	CLA	C3A-C2A-CAA-CBA
20	1	201	CLA	CBA-CGA-O2A-C1
20	1	201	CLA	C4B-C3B-CAB-CBB
20	1	201	CLA	CHA-CBD-CGD-O1D

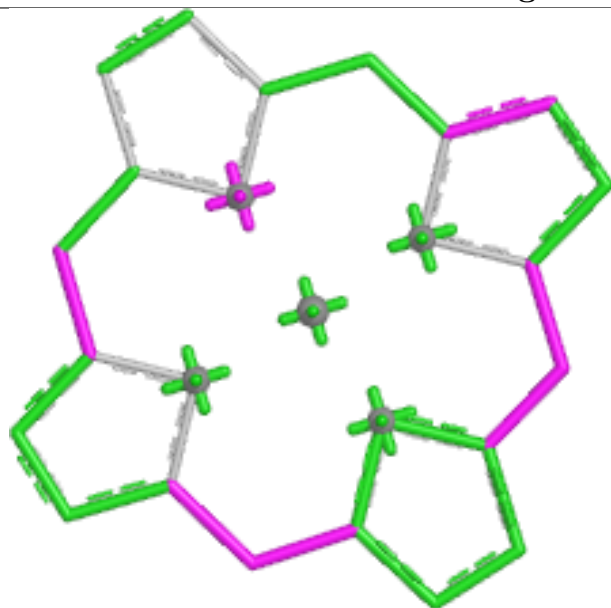
There are no ring outliers.

4 monomers are involved in 3 short contacts:

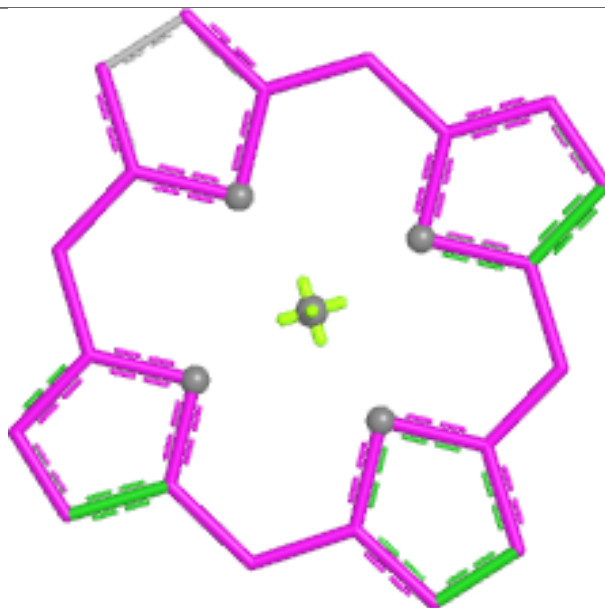
Mol	Chain	Res	Type	Clashes	Symm-Clashes
21	2	313	LMU	0	1
20	1	207	CLA	0	2
20	K	105	CLA	0	2
20	A	831	CLA	0	1

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.

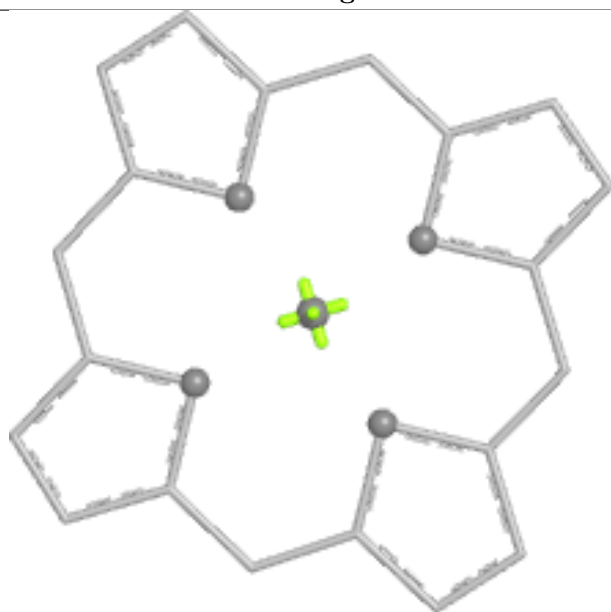
Ligand CLA 1 215



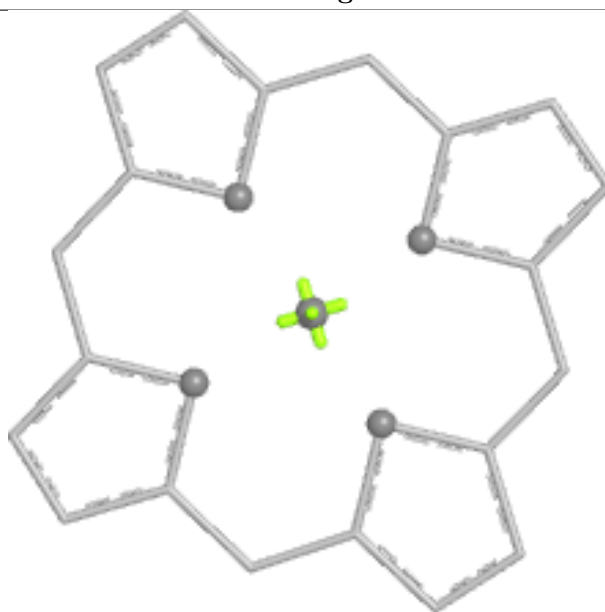
Bond lengths



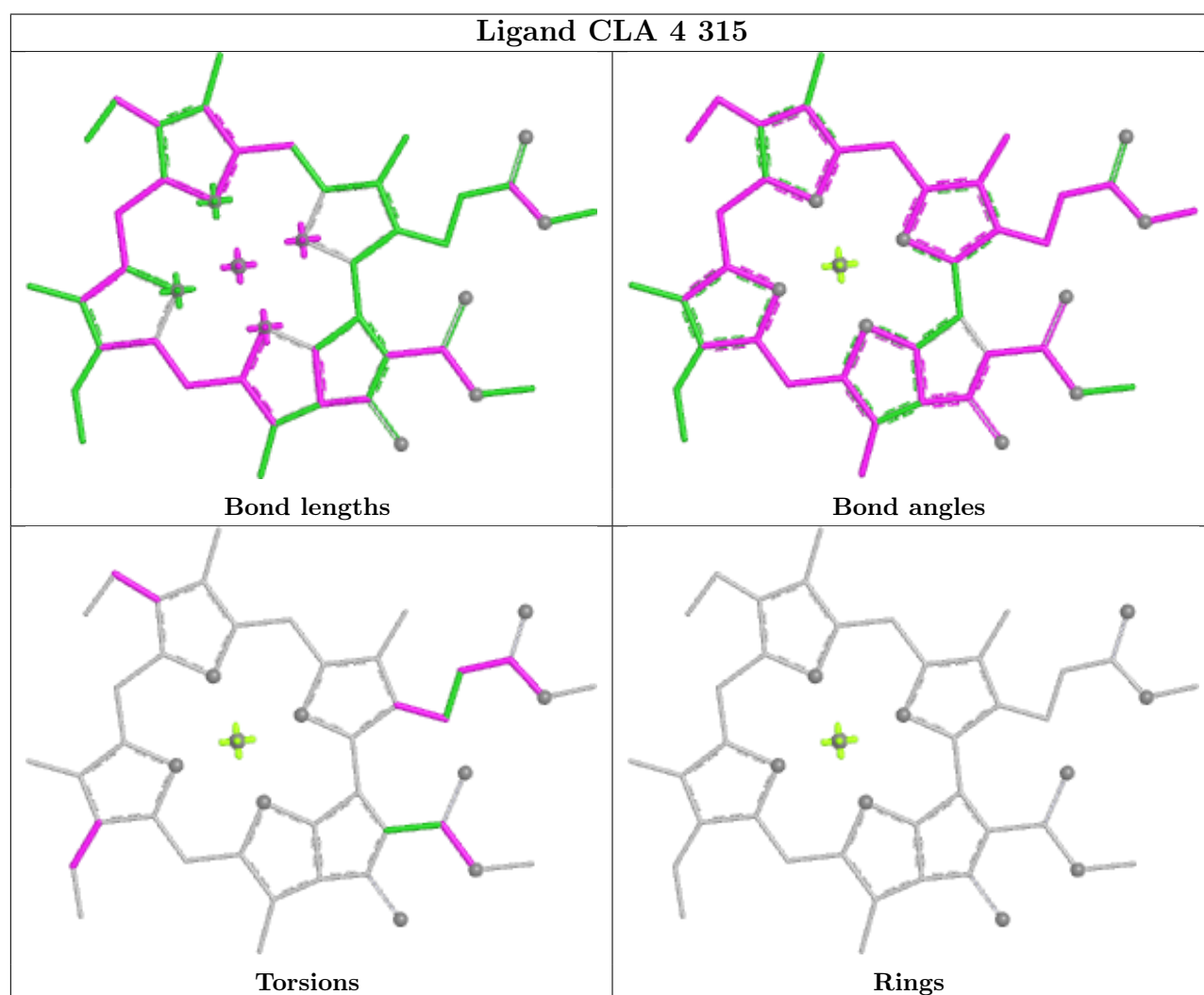
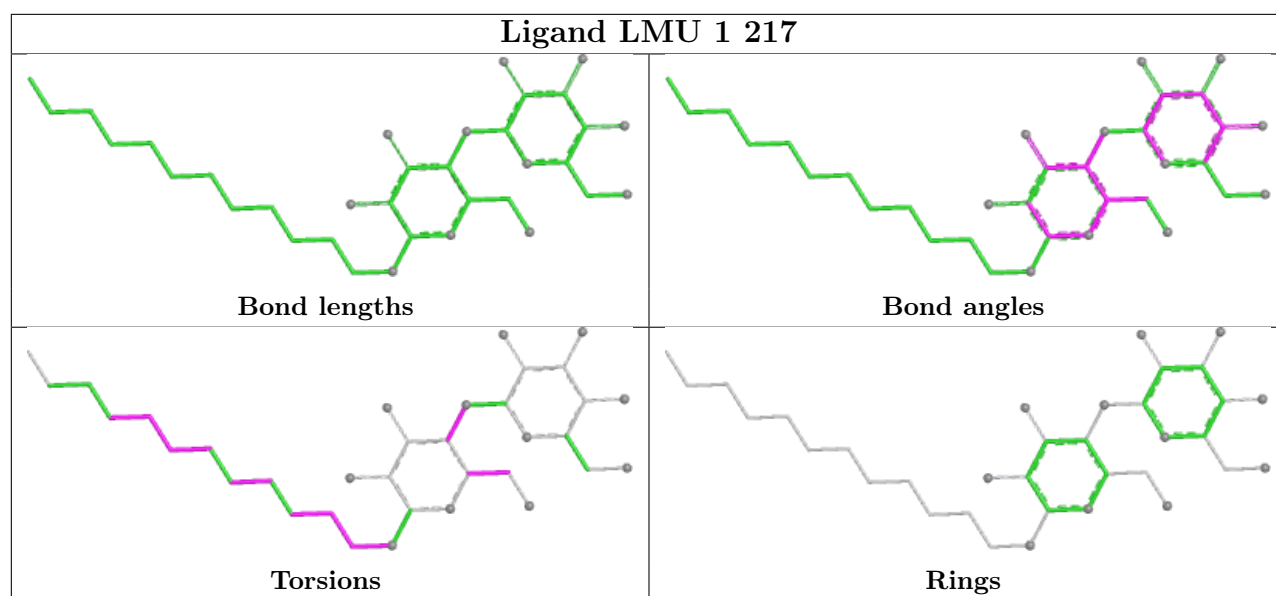
Bond angles

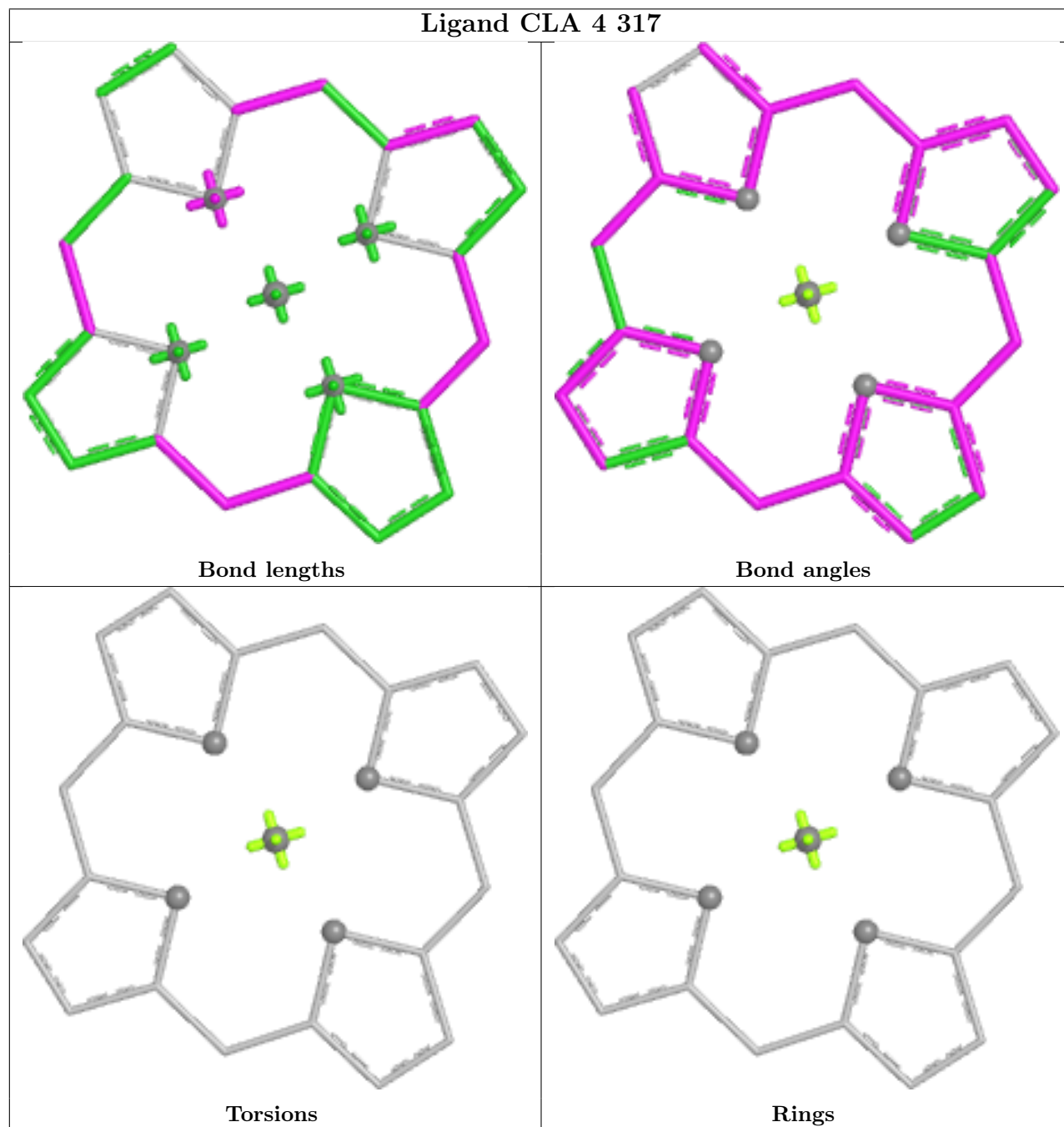
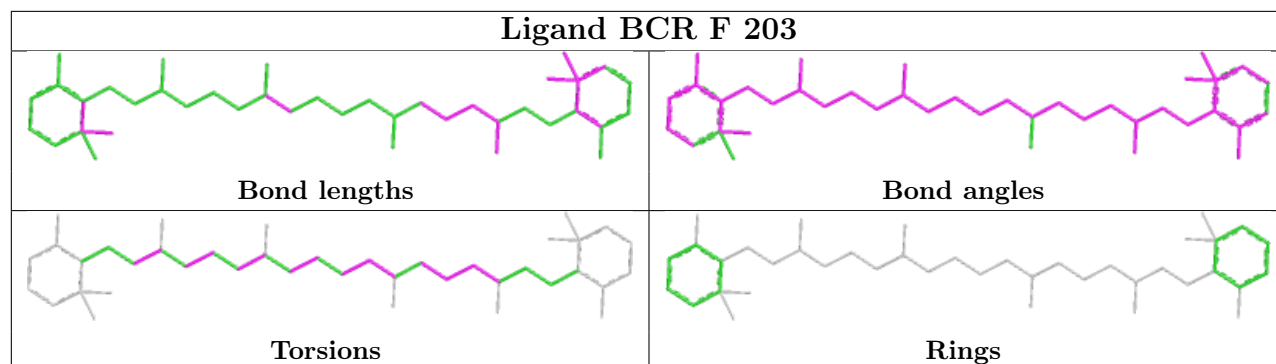


Torsions

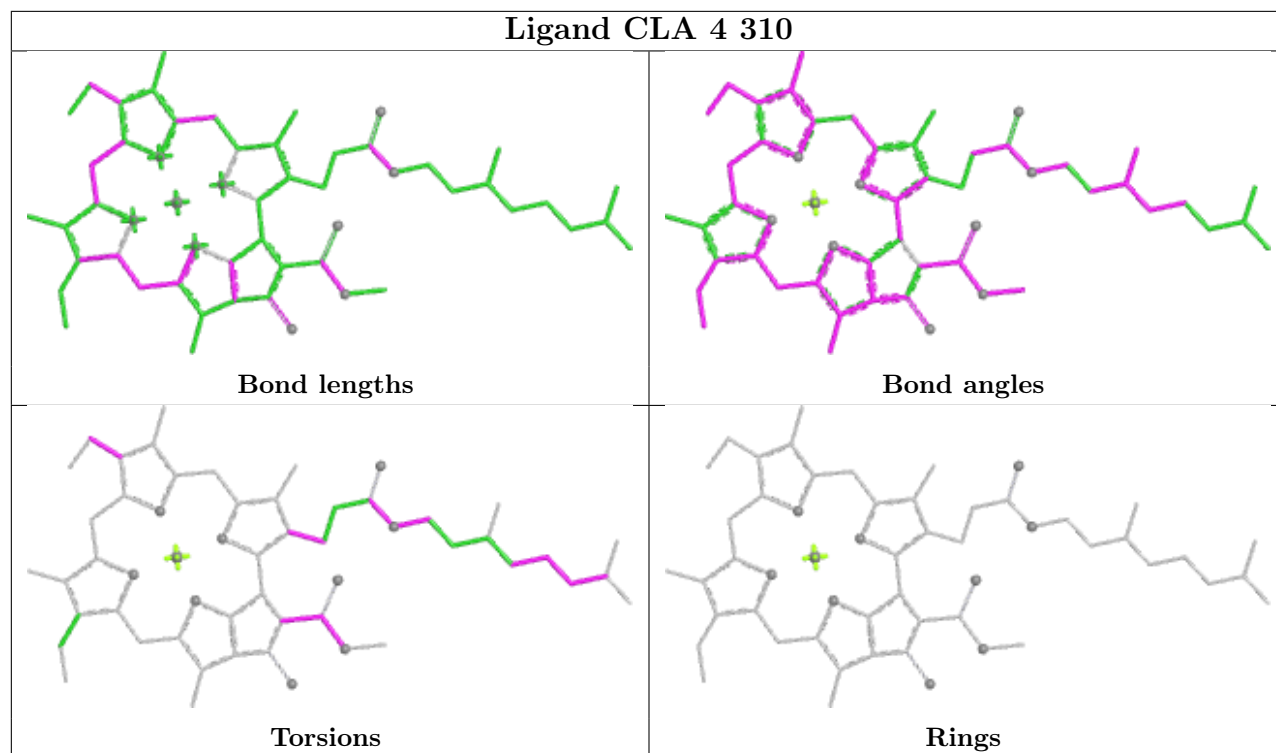


Rings

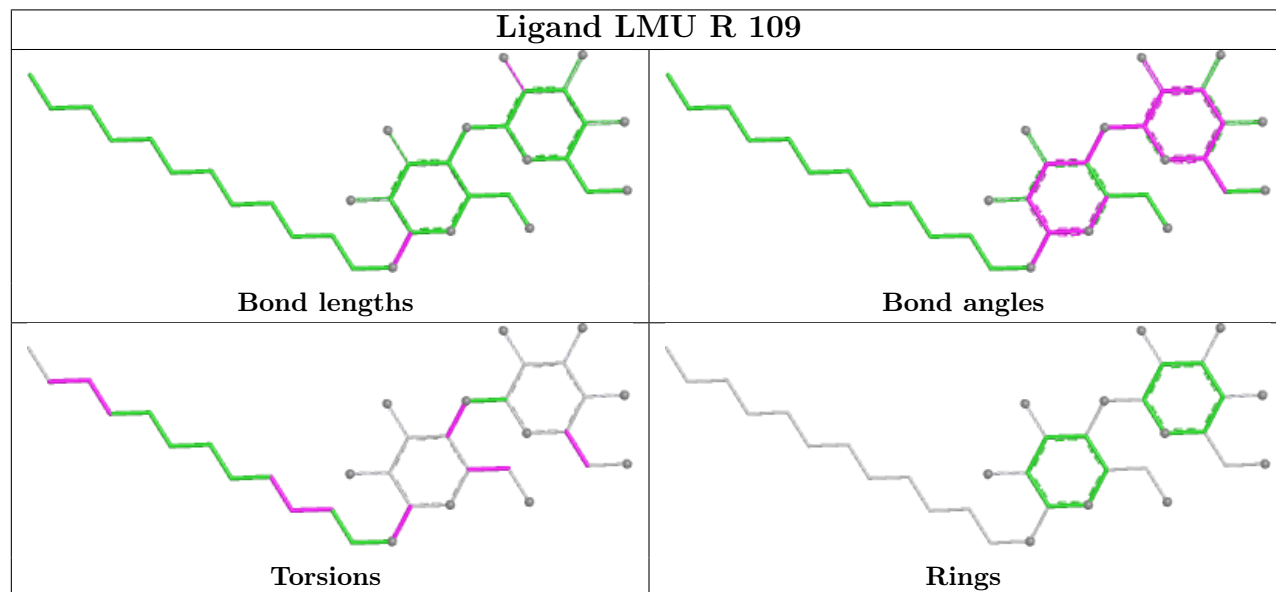




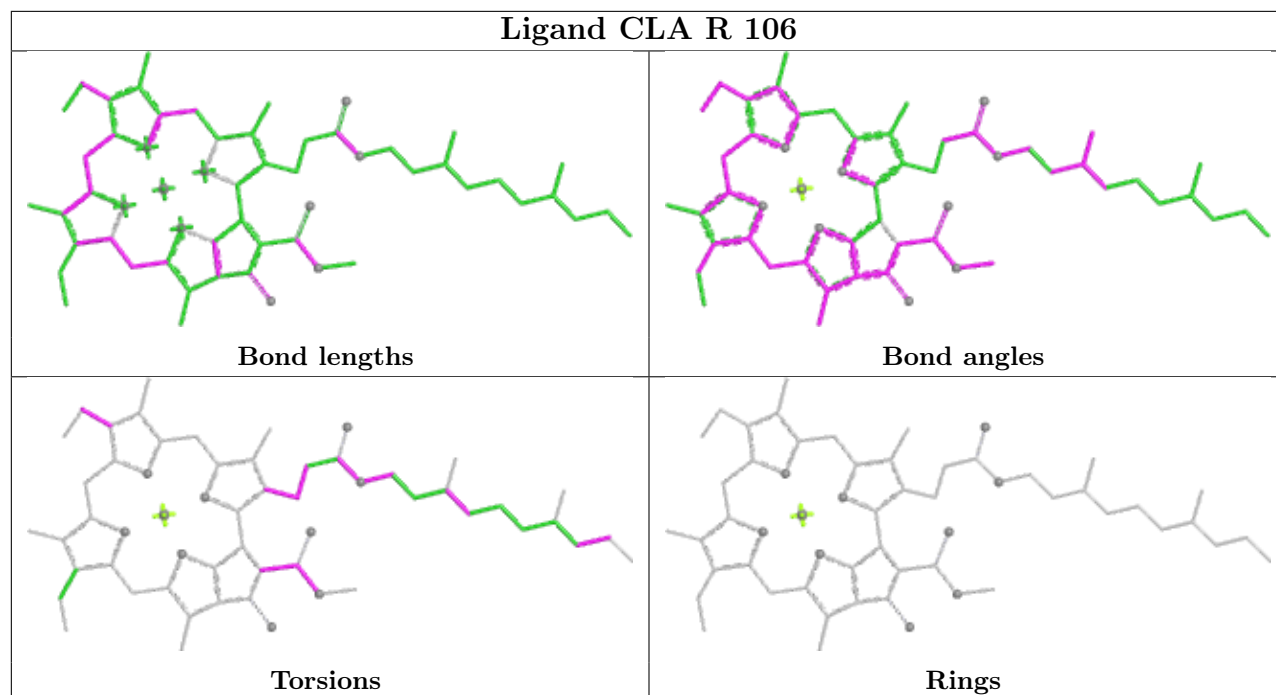
Ligand CLA 4 310



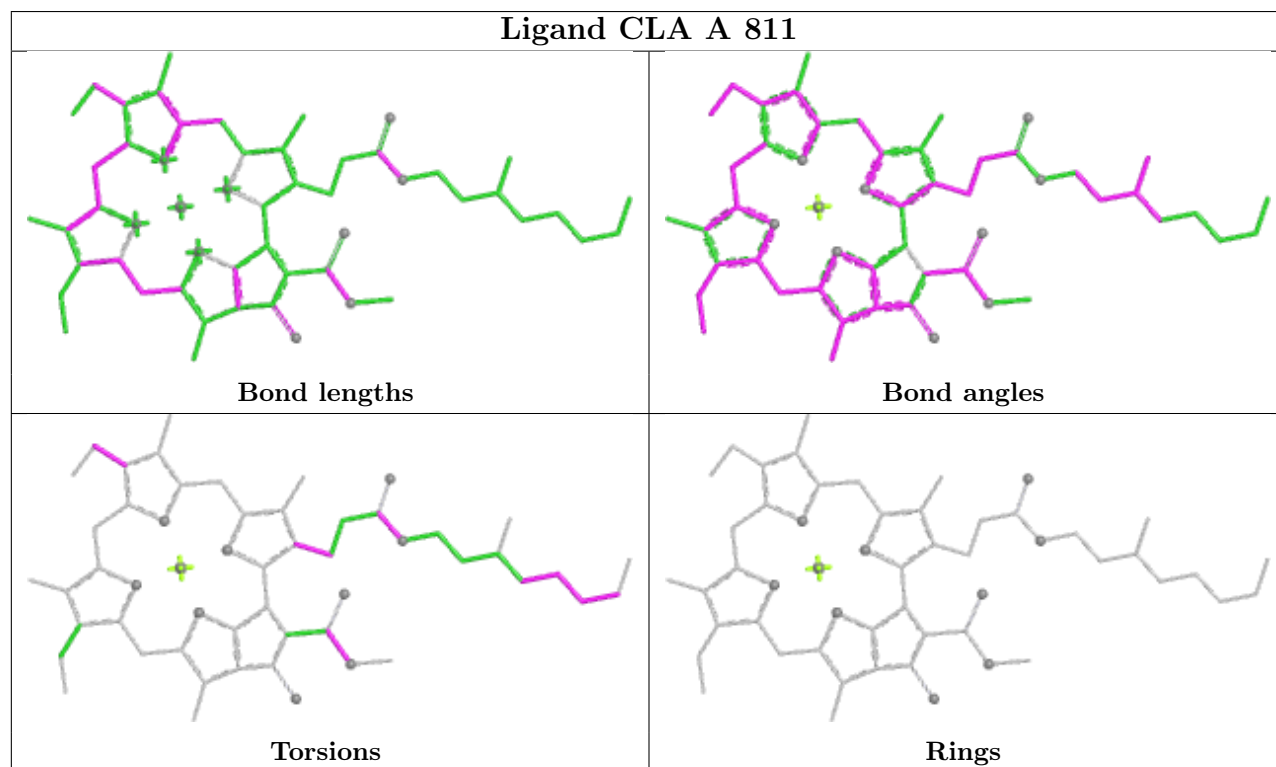
Ligand LMU R 109



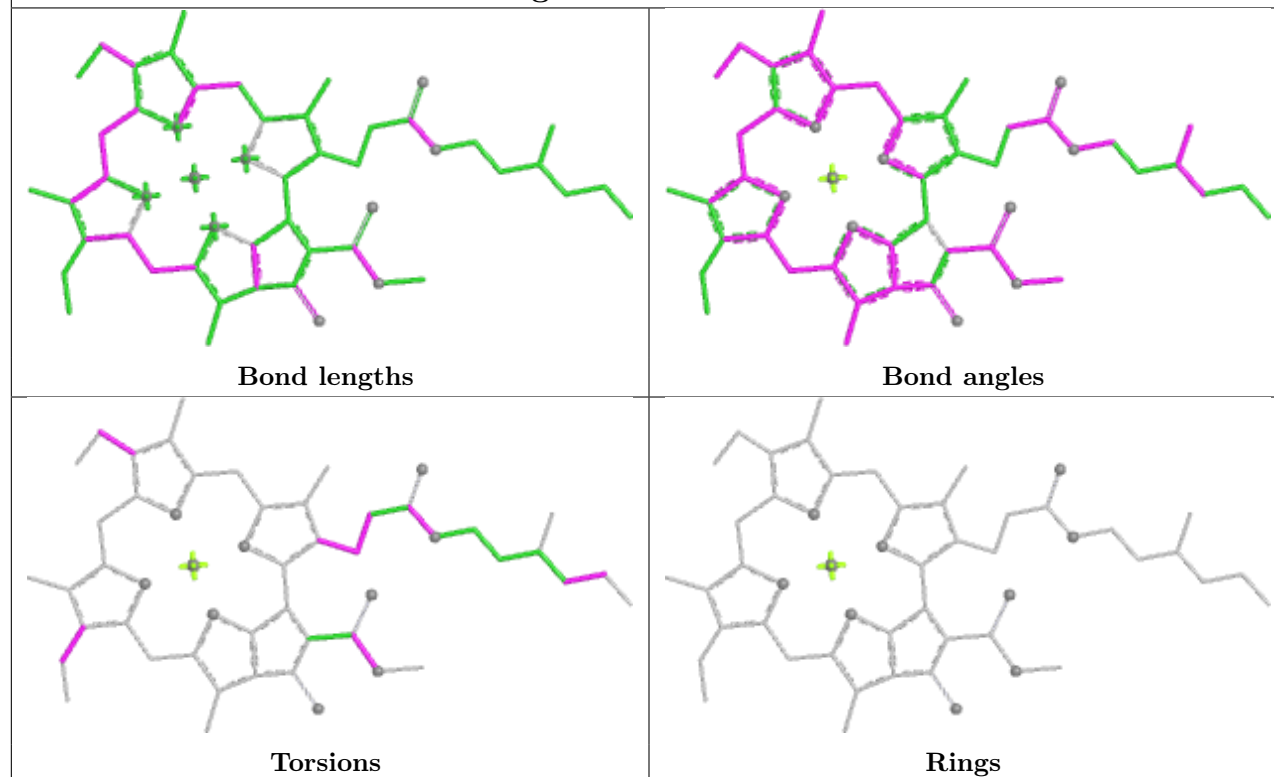
Ligand CLA R 106



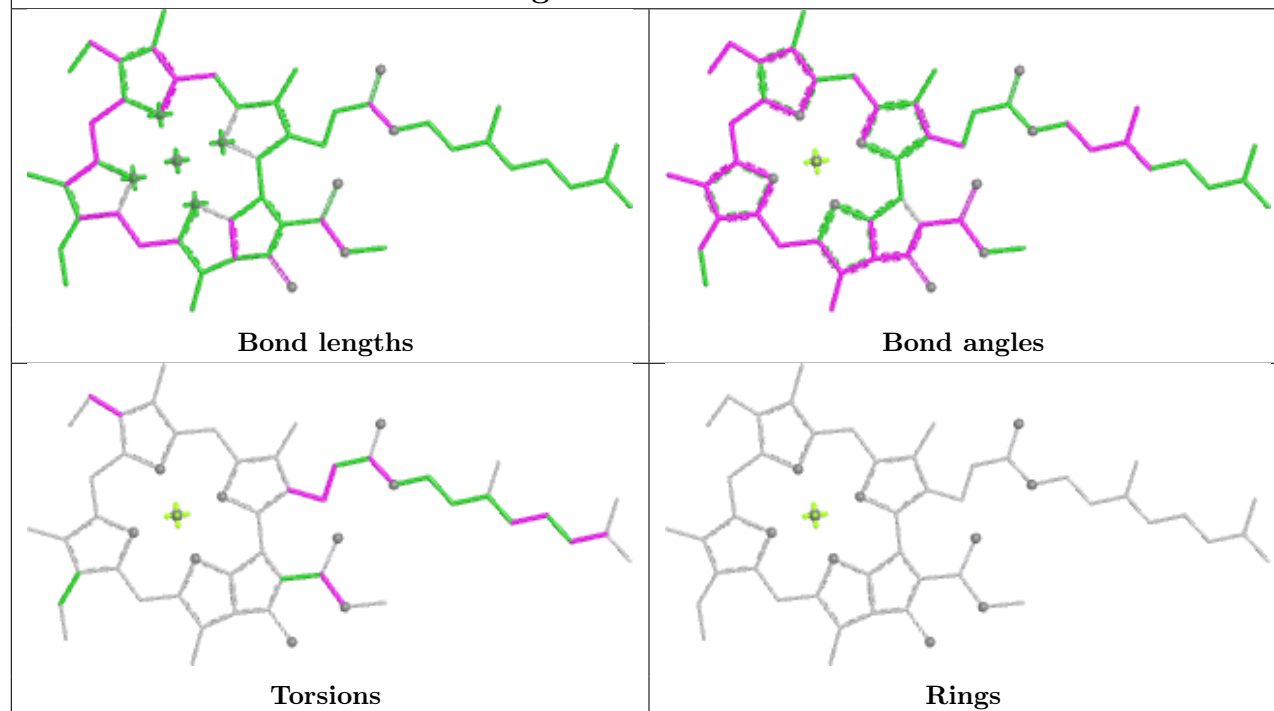
Ligand CLA A 811



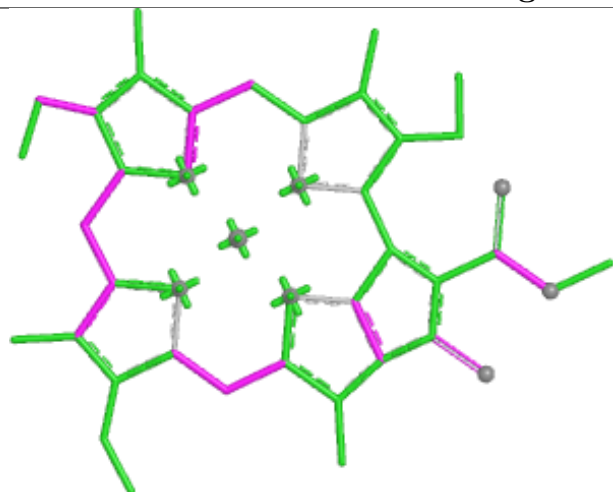
Ligand CLA A 815



Ligand CLA A 820



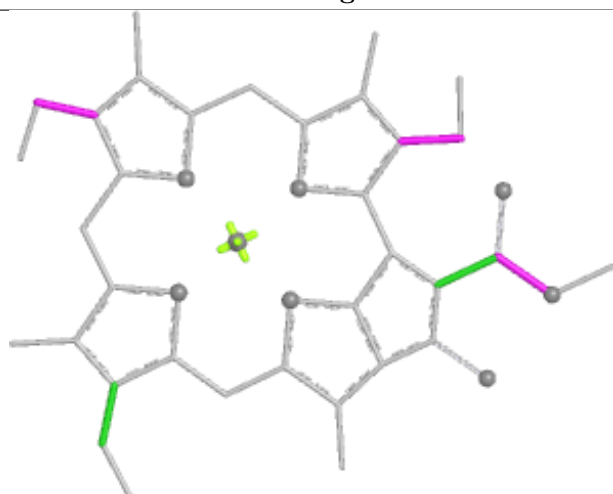
Ligand CLA 3 314



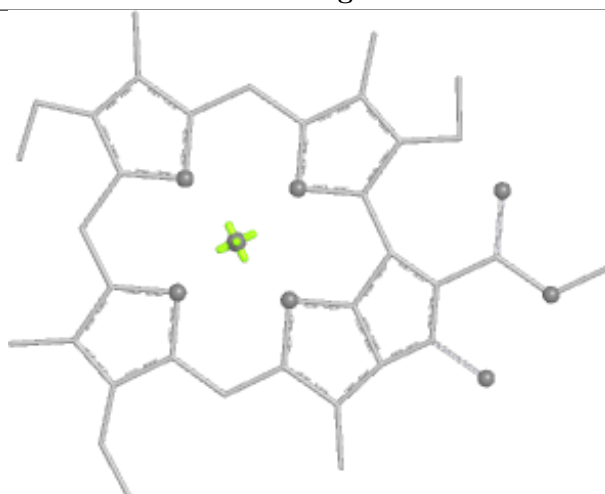
Bond lengths



Bond angles

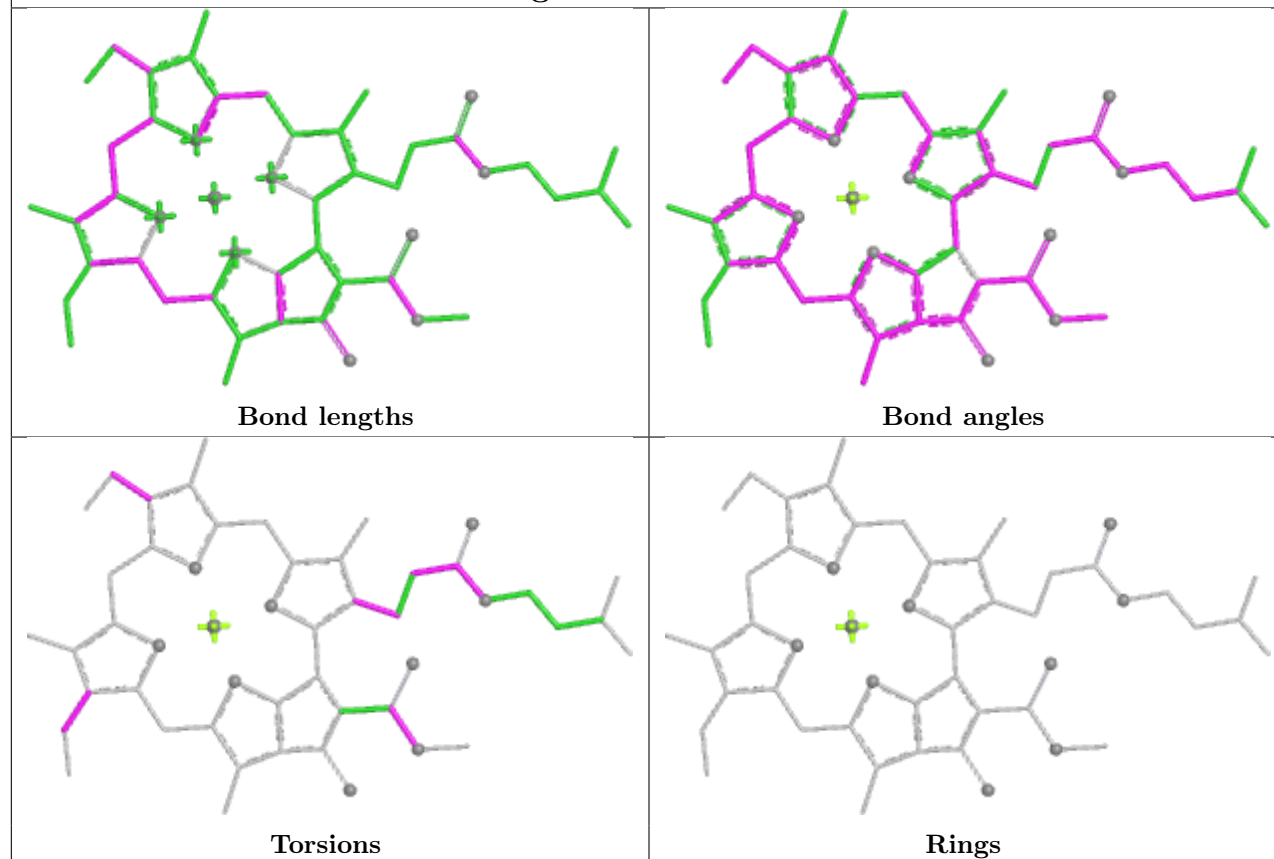


Torsions

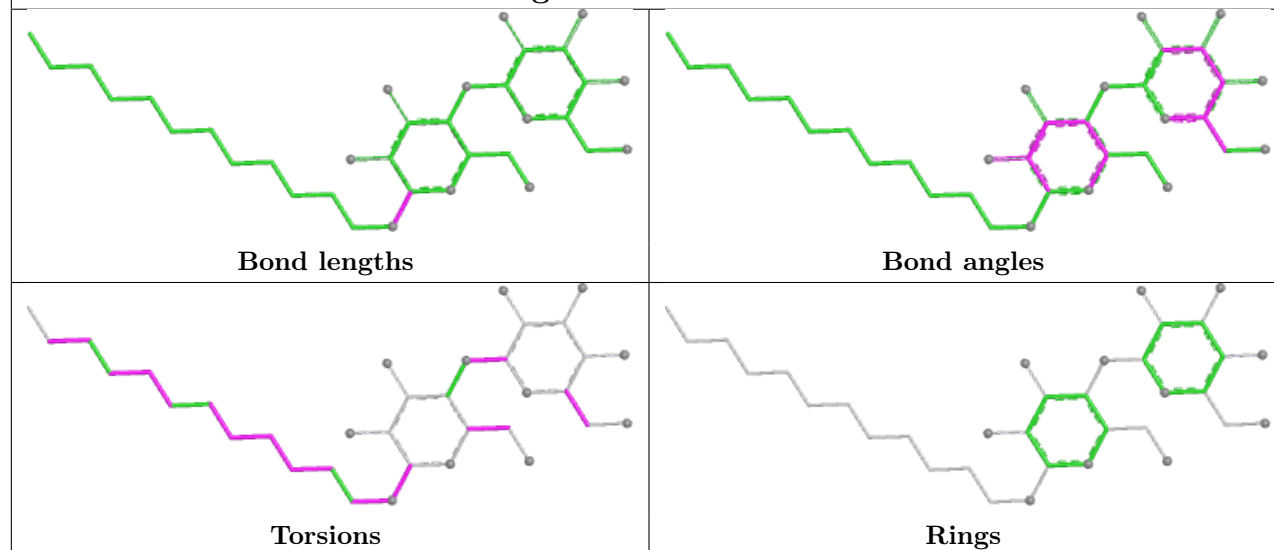


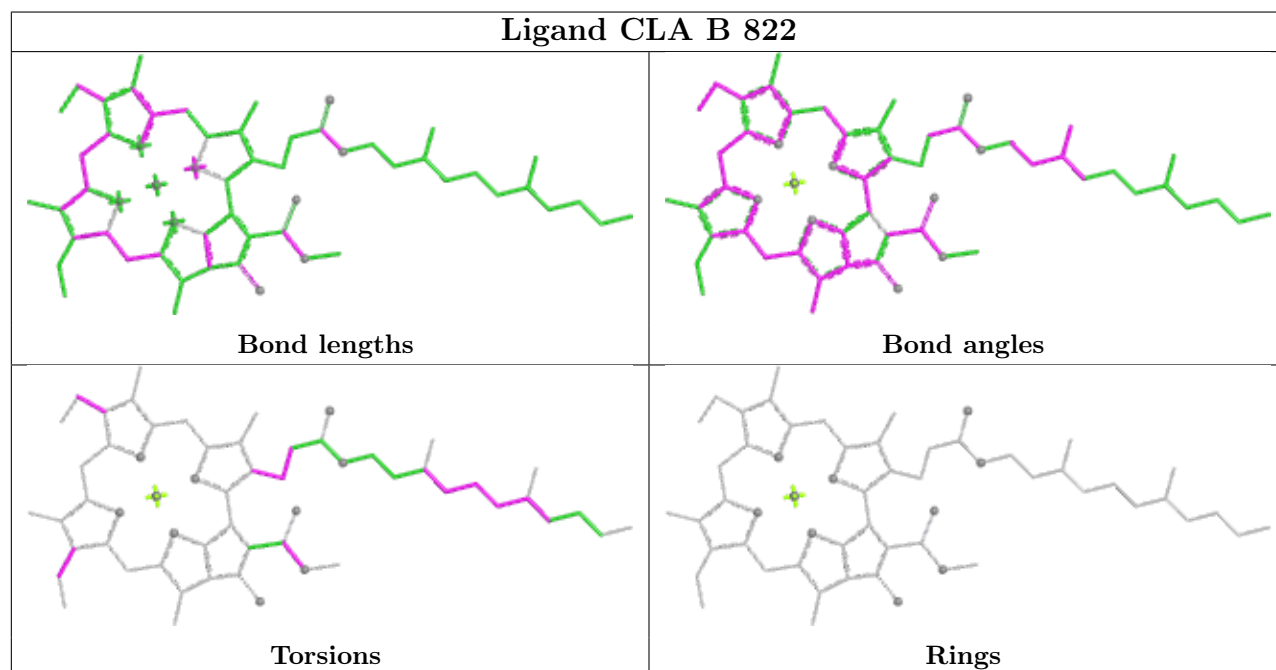
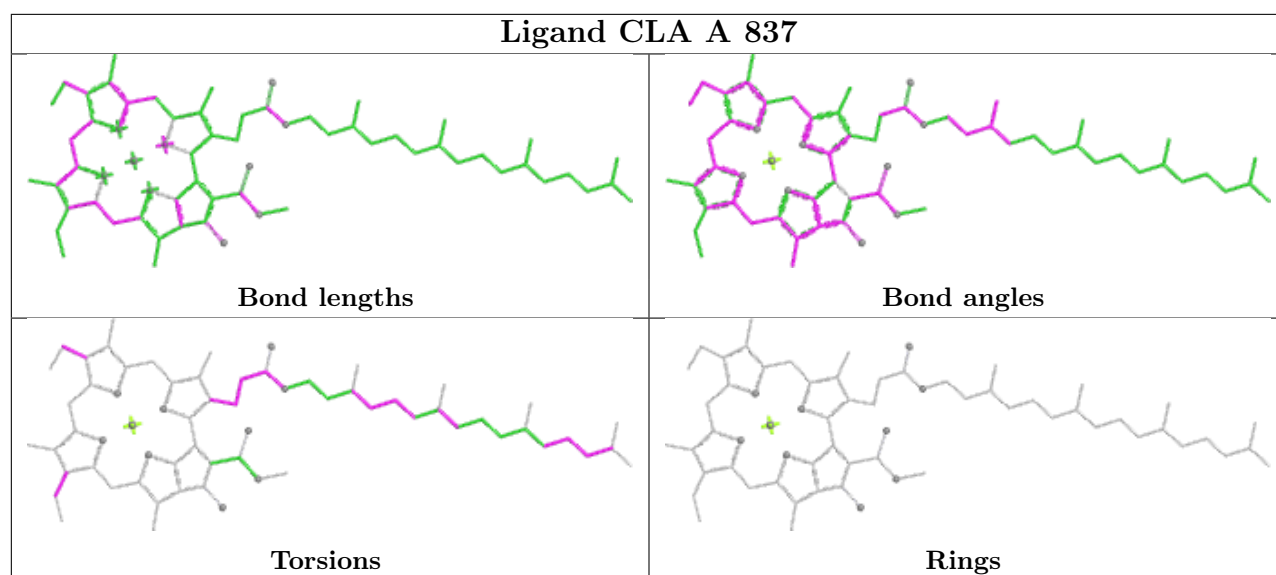
Rings

Ligand CLA A 813

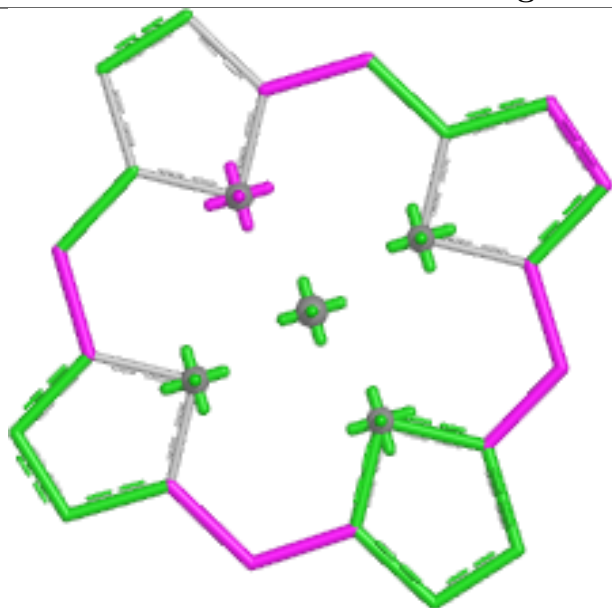


Ligand LMU 4 321

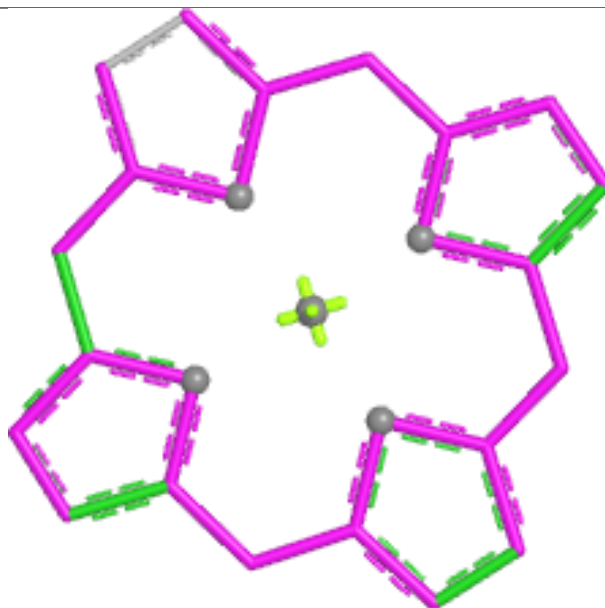




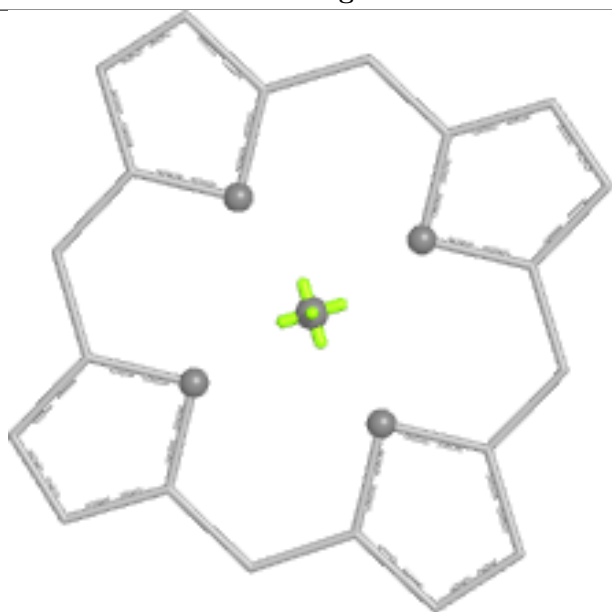
Ligand CLA 1 213



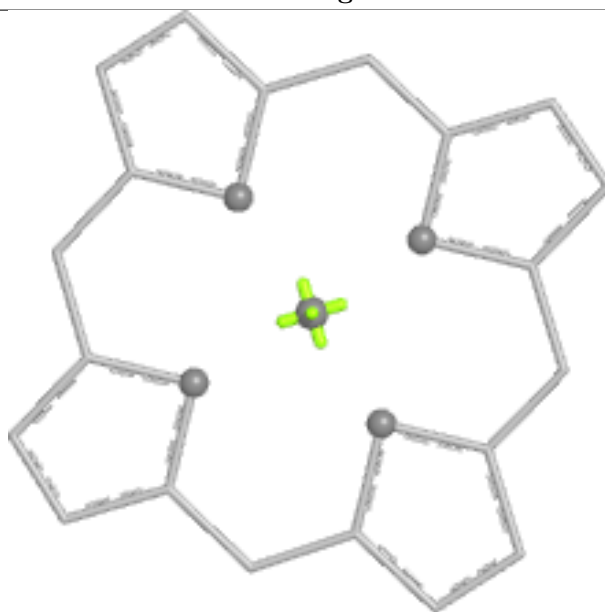
Bond lengths



Bond angles

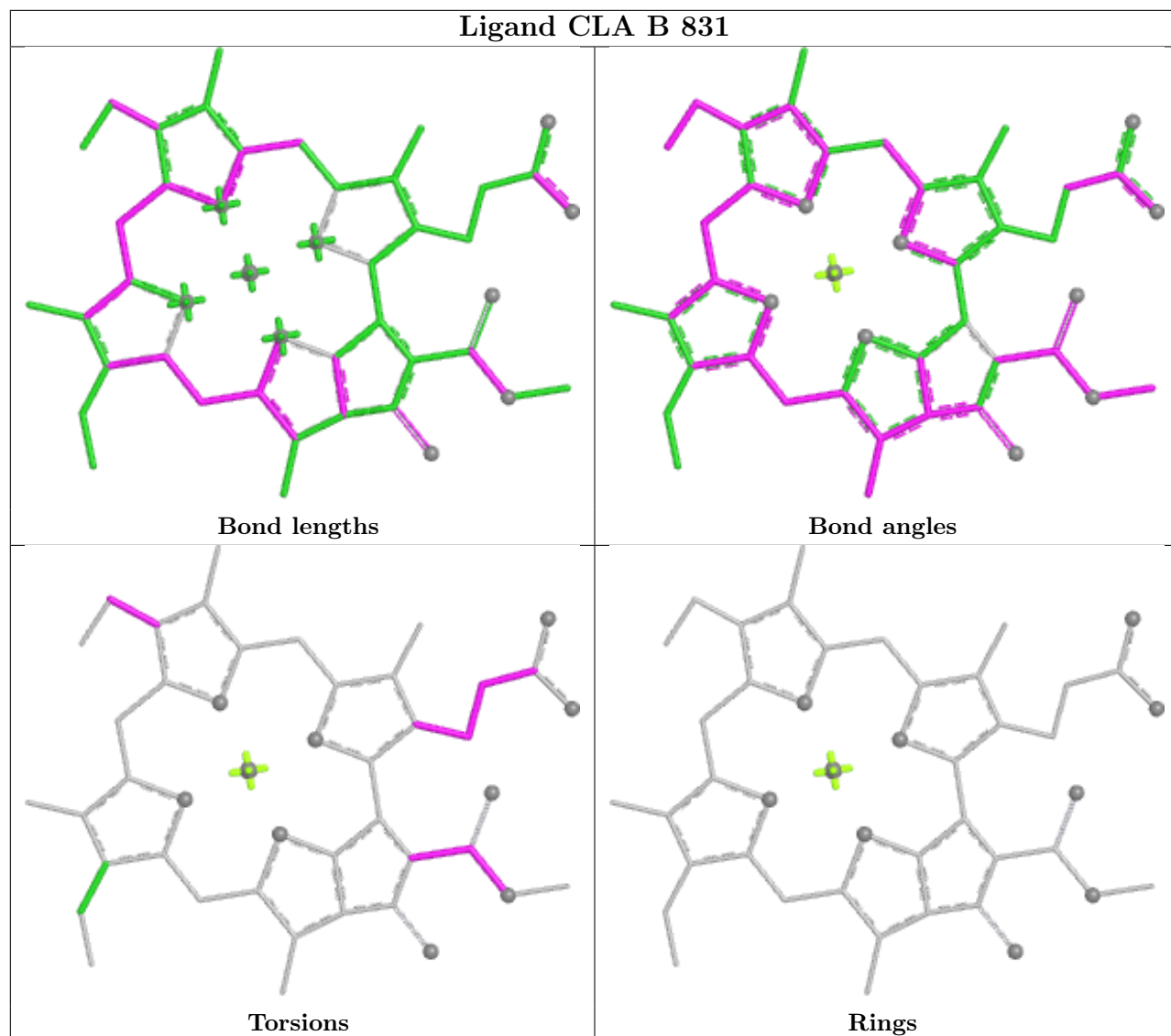


Torsions

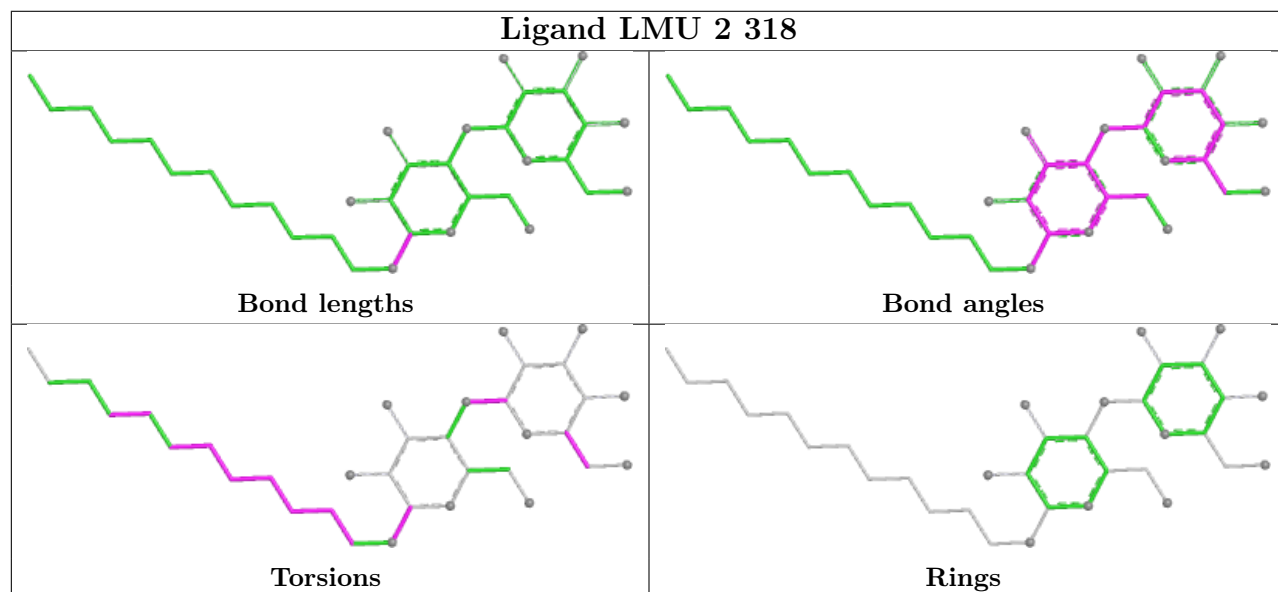


Rings

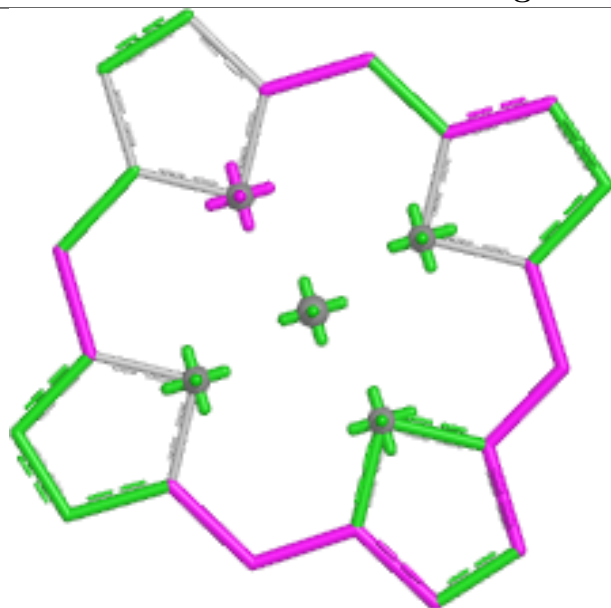
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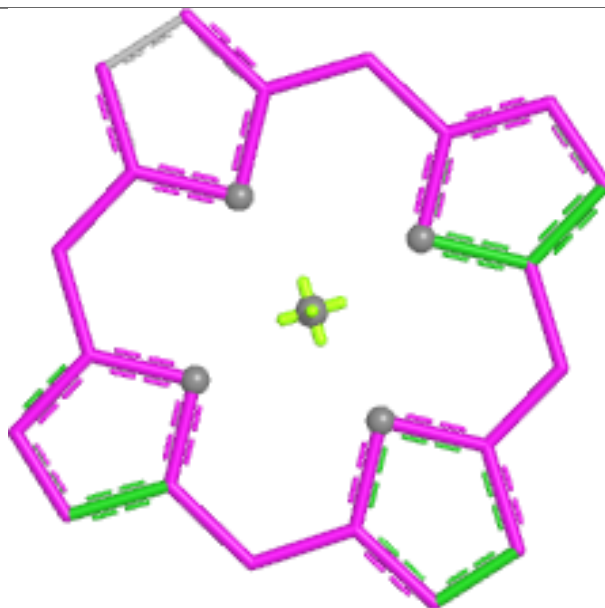
Ligand LMU 2 318



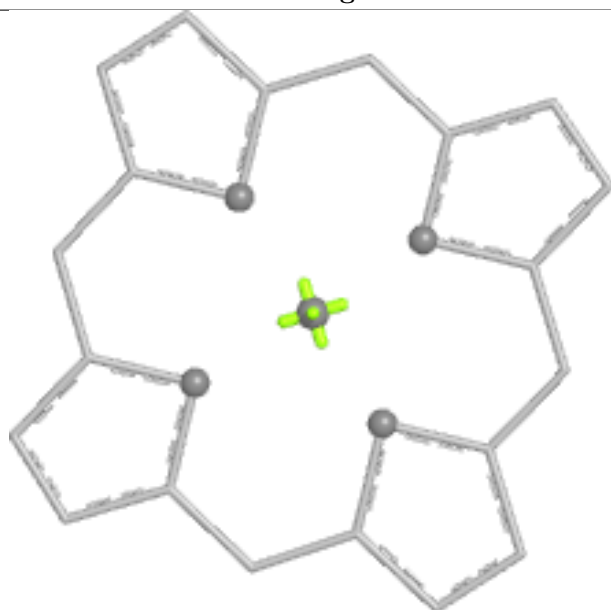
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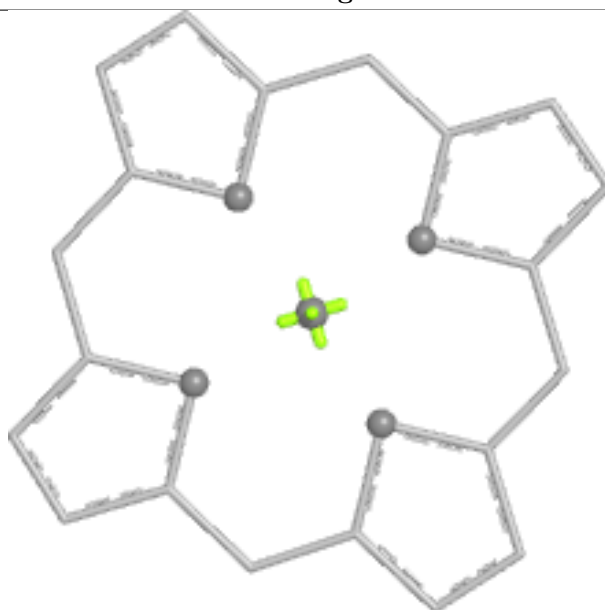
Bond lengths



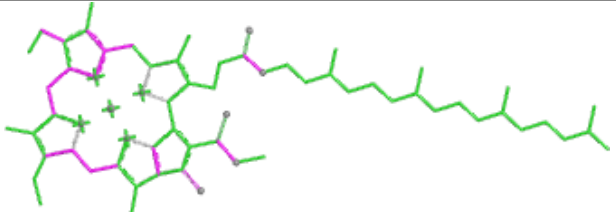
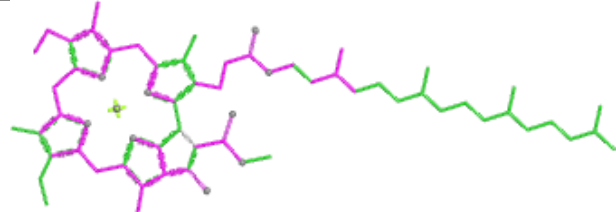
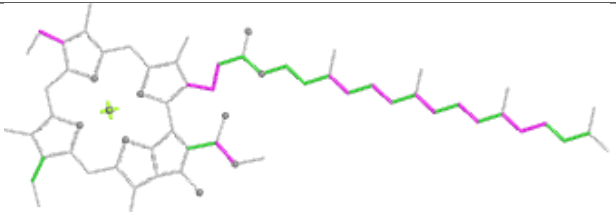
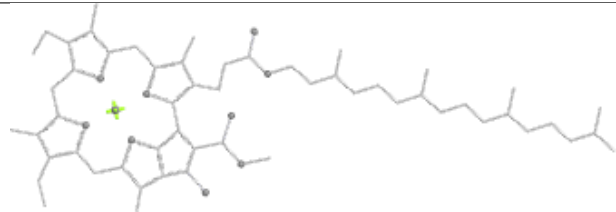
Bond angles

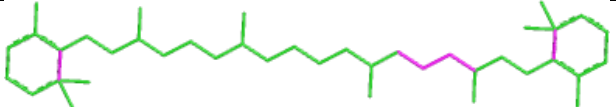
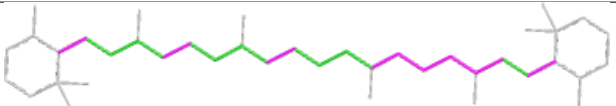
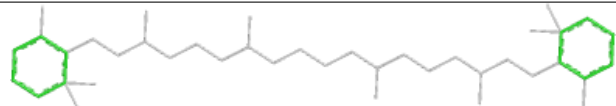


Torsions

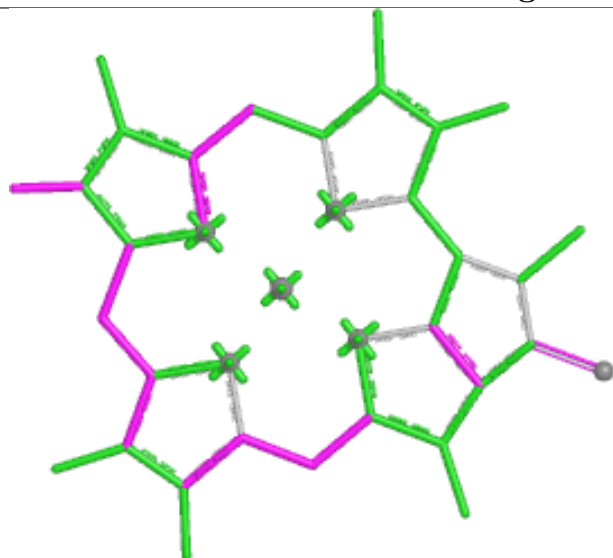


Rings

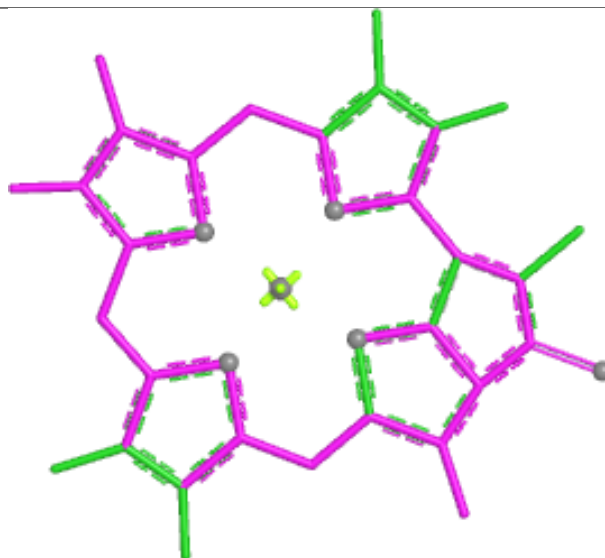
Ligand CLA L 201	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand BCR B 843	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA 3 319



Bond lengths



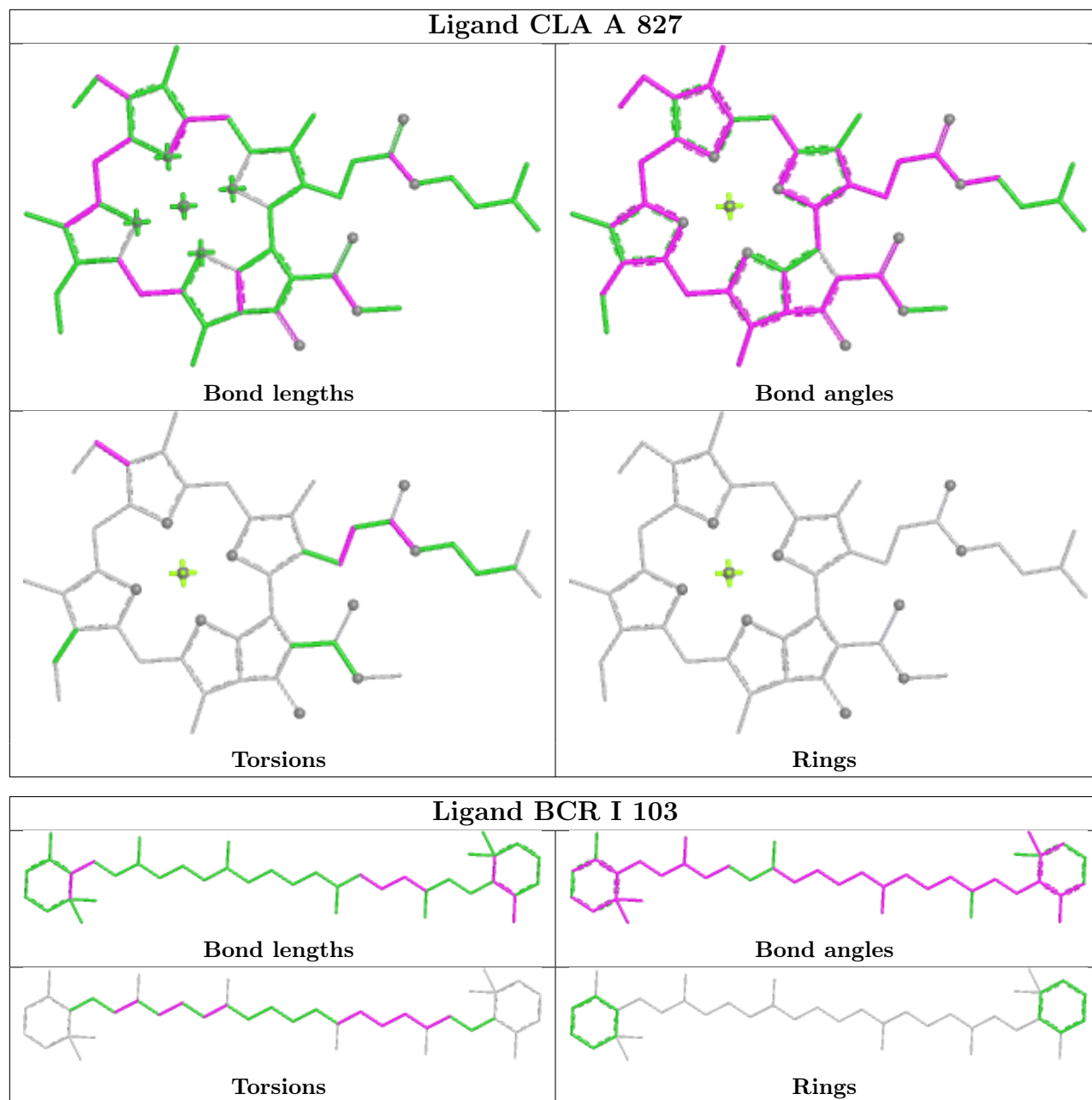
Bond angles



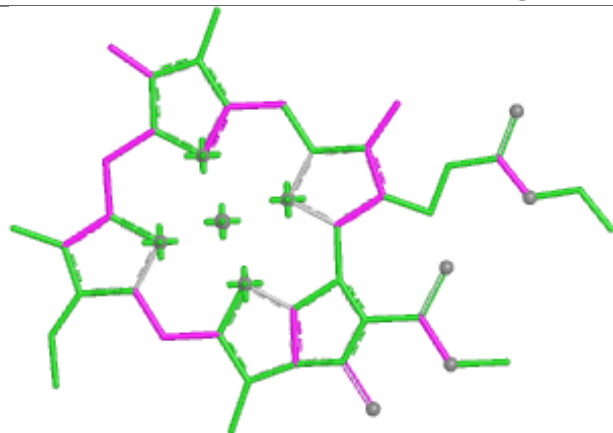
Torsions



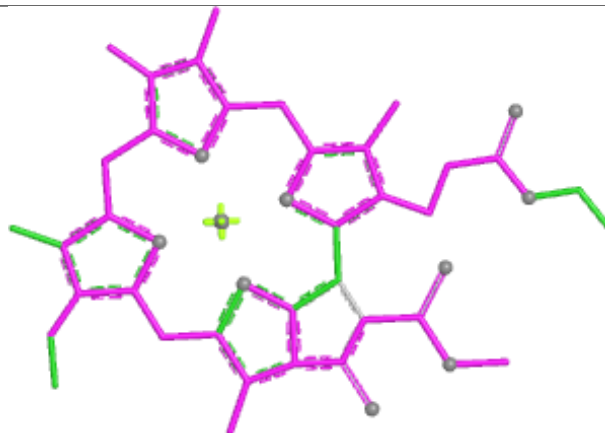
Rings



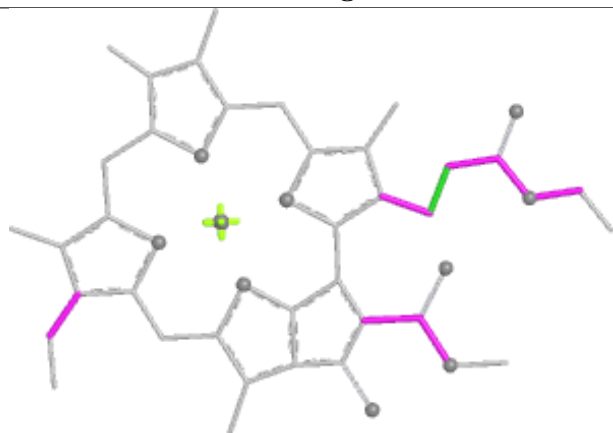
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Bond lengths



Bond angles

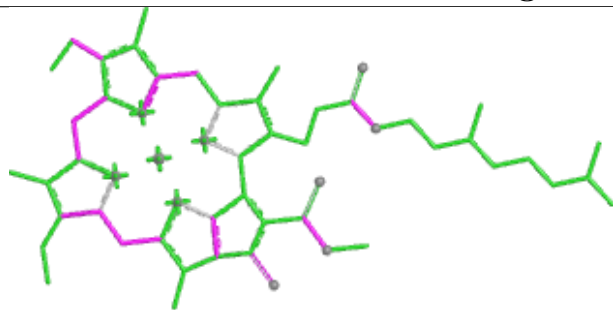


Torsions

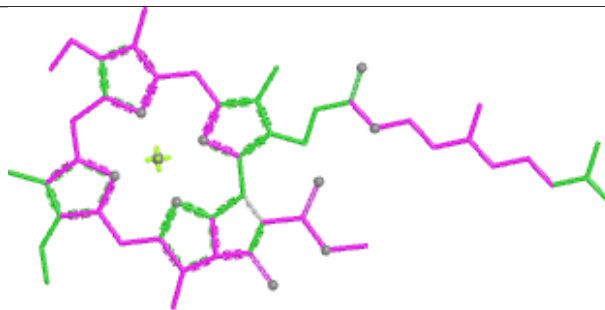


Rings

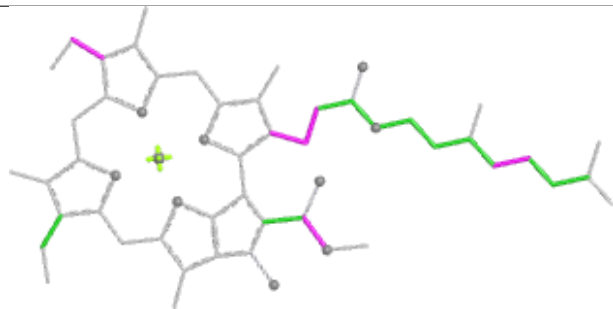
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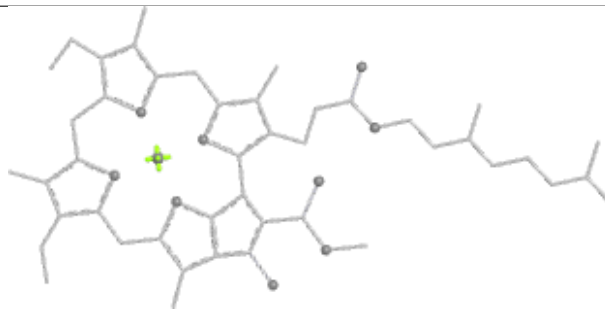
Bond lengths



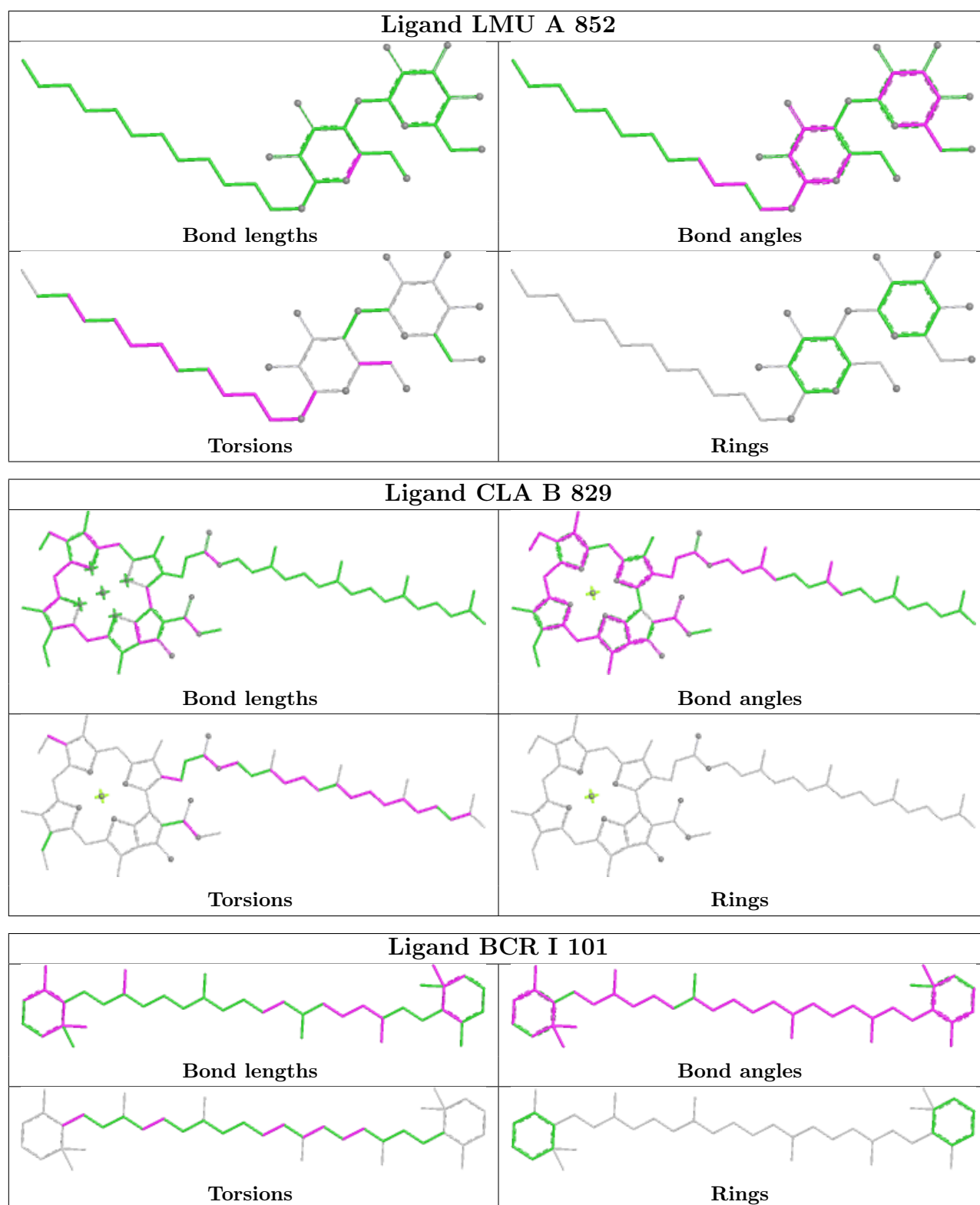
Bond angles



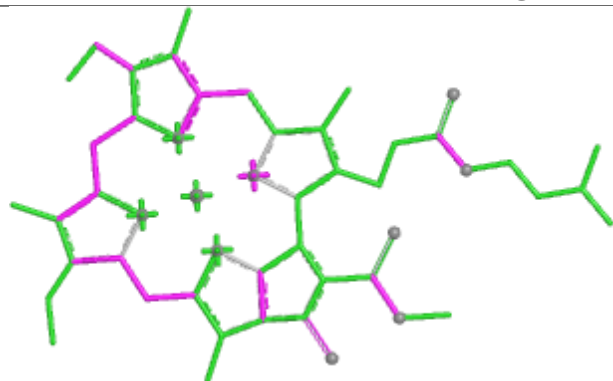
Torsions



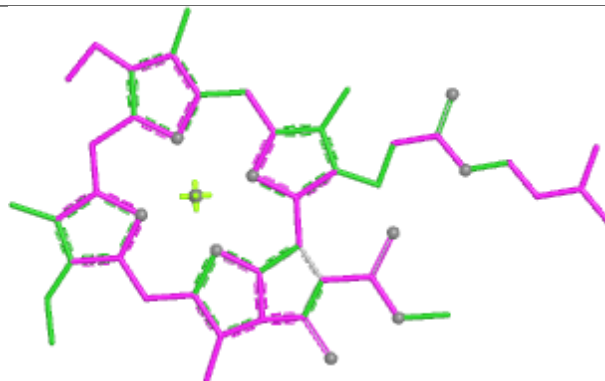
Rings



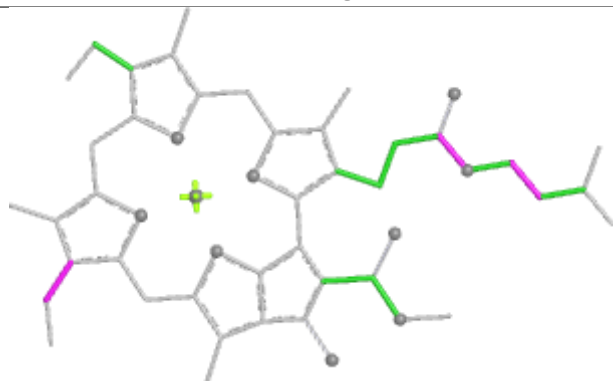
Ligand CLA K 103



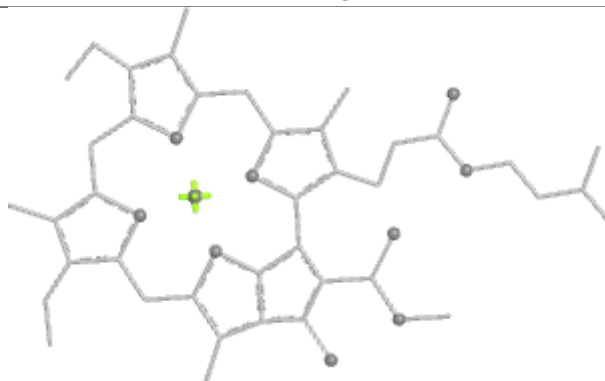
Bond lengths



Bond angles

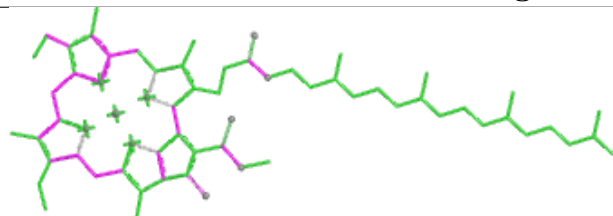


Torsions

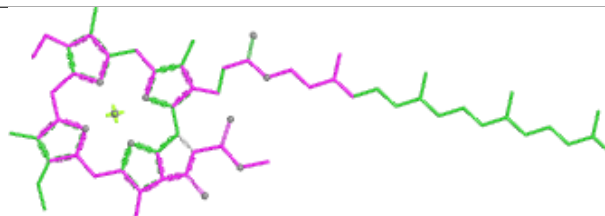


Rings

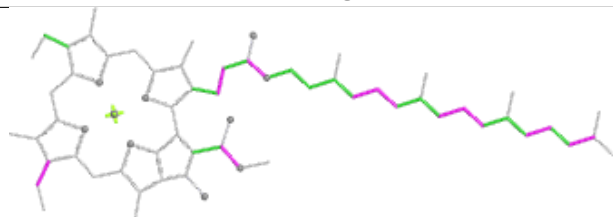
Ligand CLA A 817



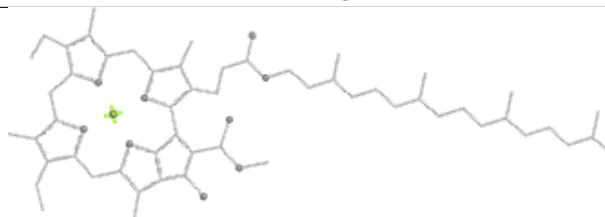
Bond lengths



Bond angles

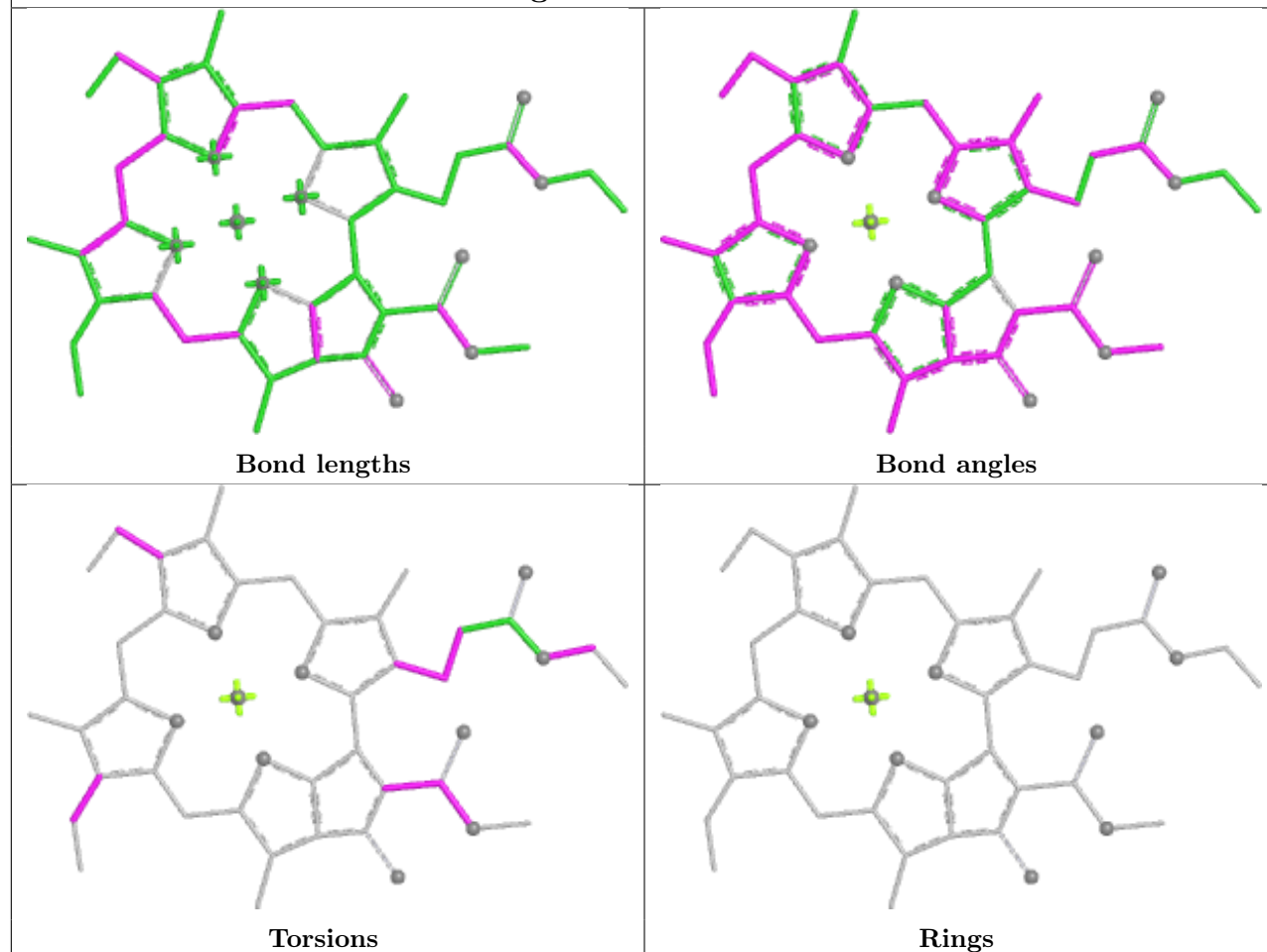


Torsions

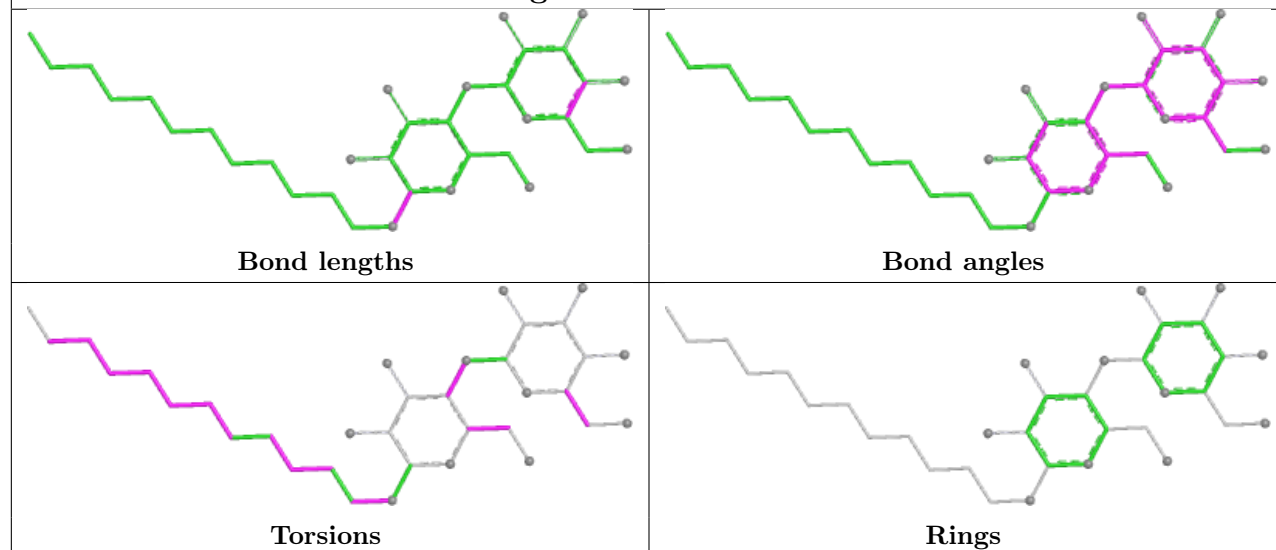


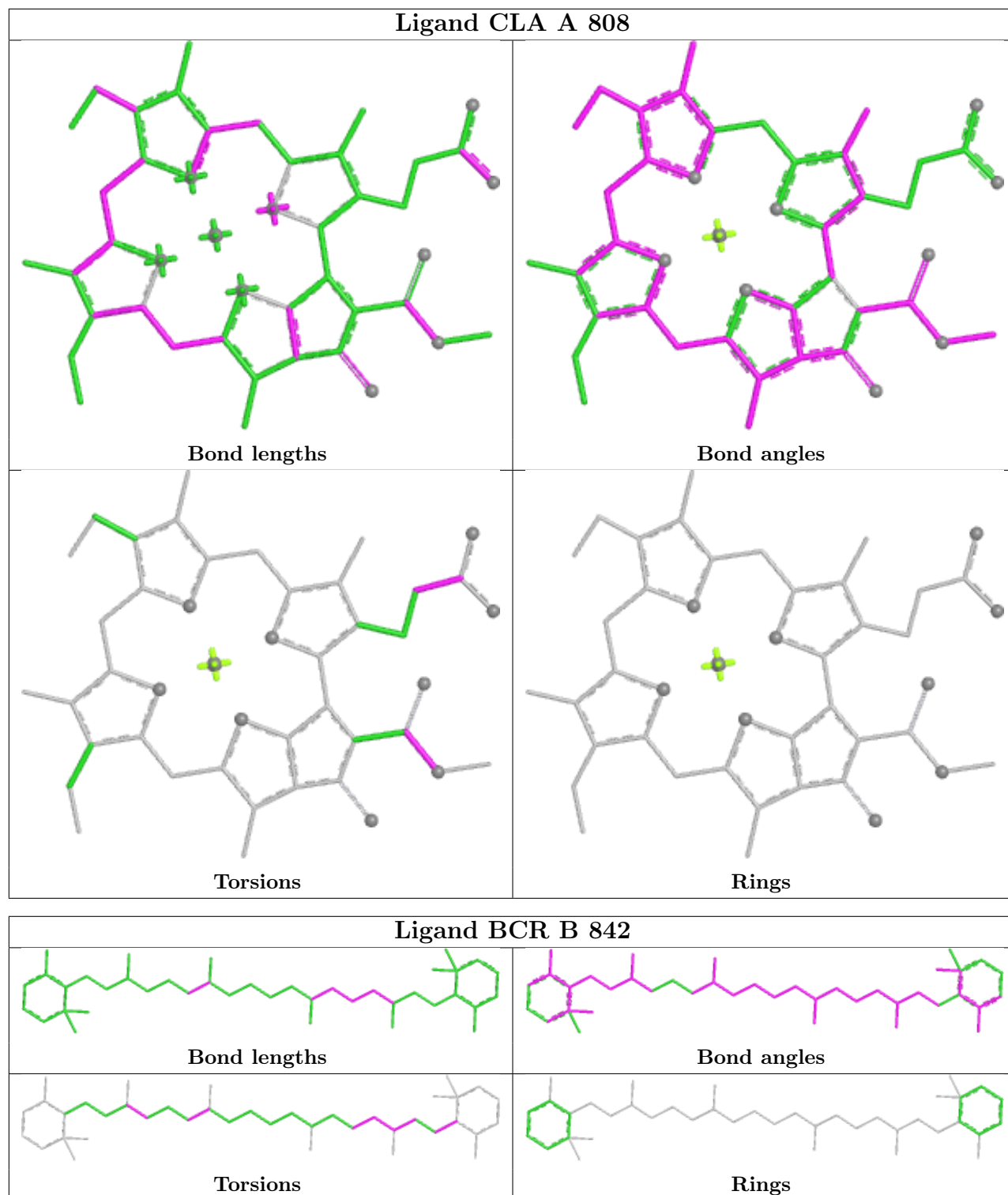
Rings

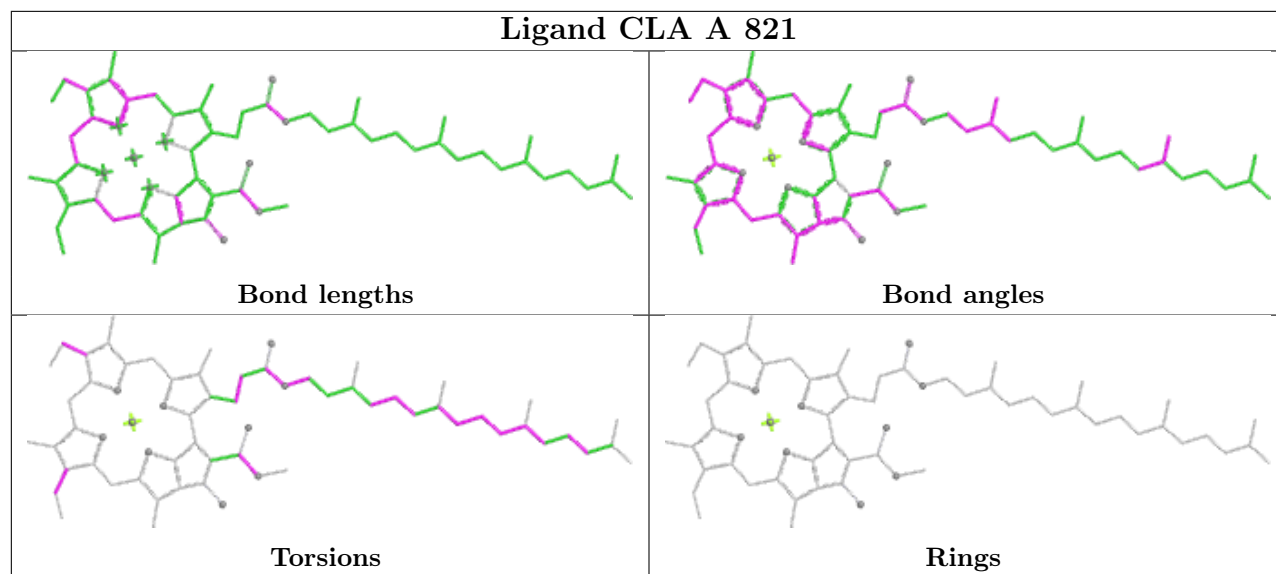
Ligand CLA L 207



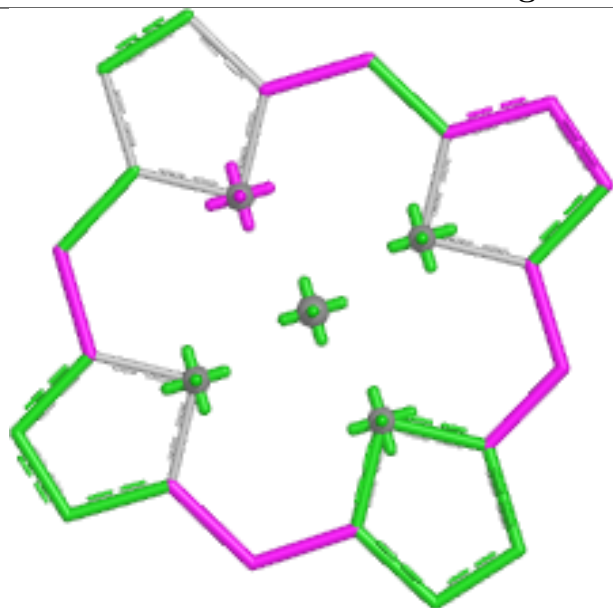
Ligand LMU L 205



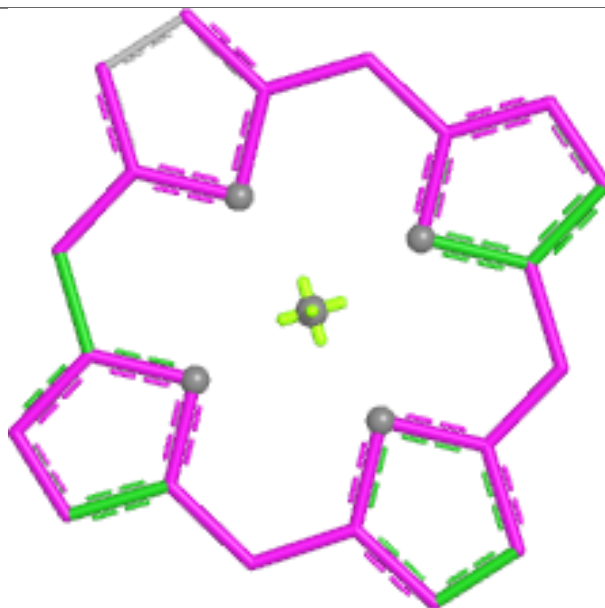




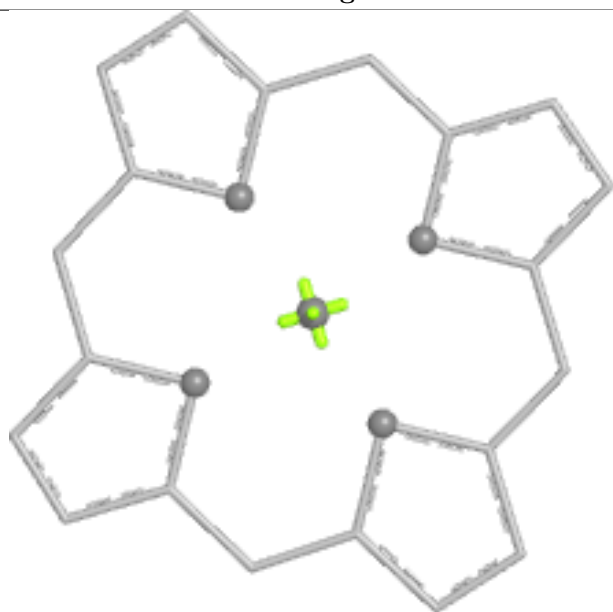
Ligand CLA 3 307



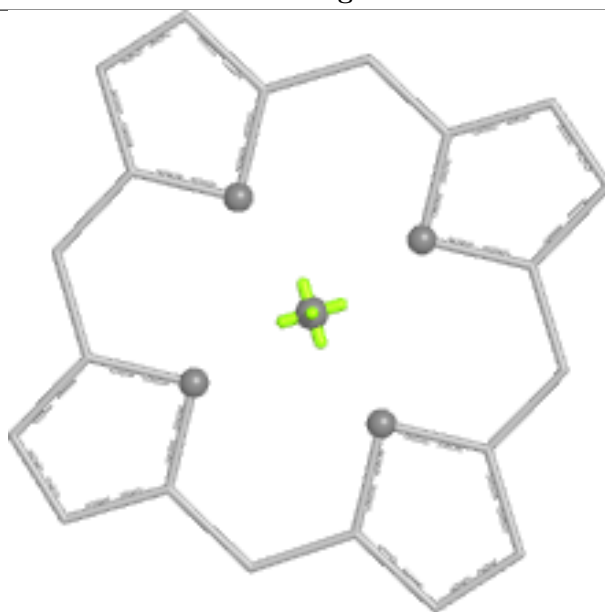
Bond lengths



Bond angles

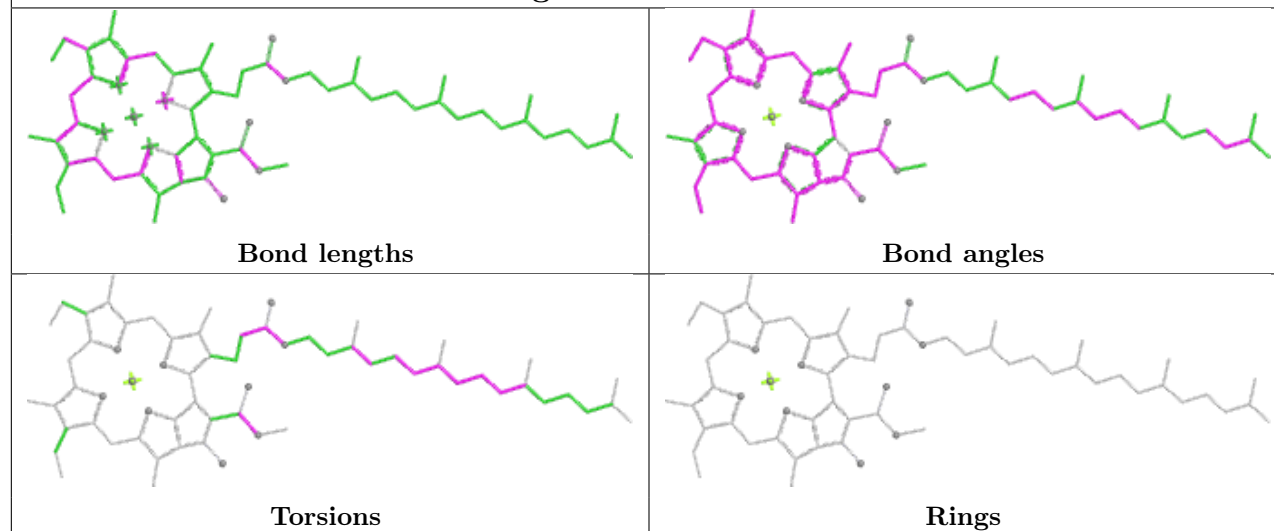


Torsions

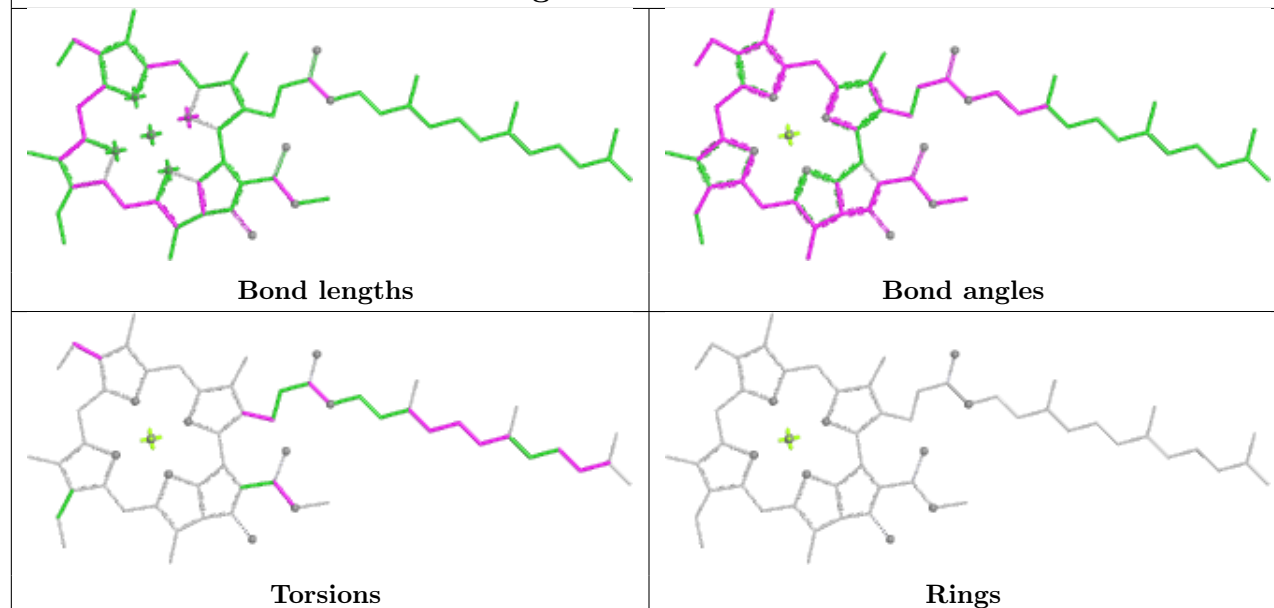


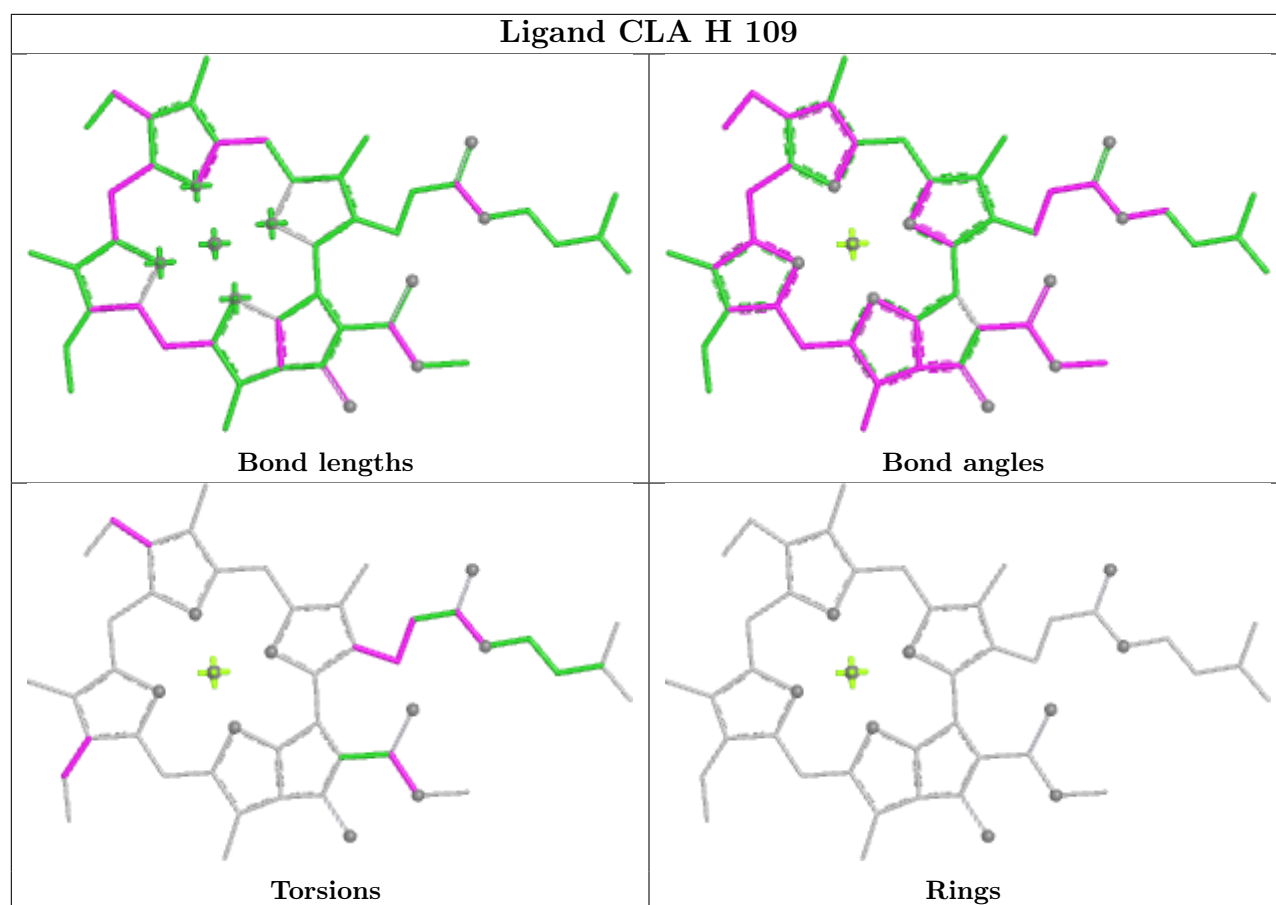
Rings

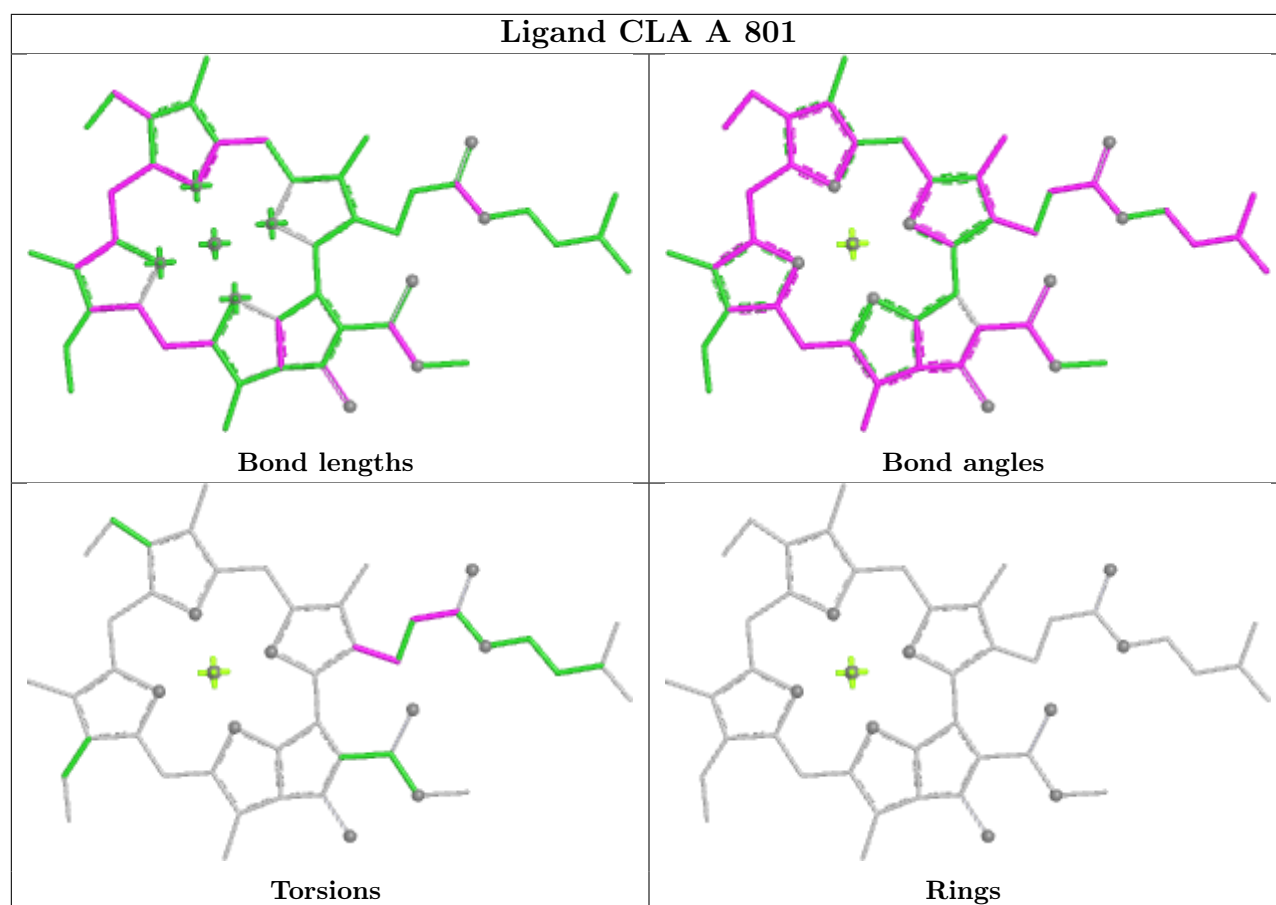
Ligand CLA B 847

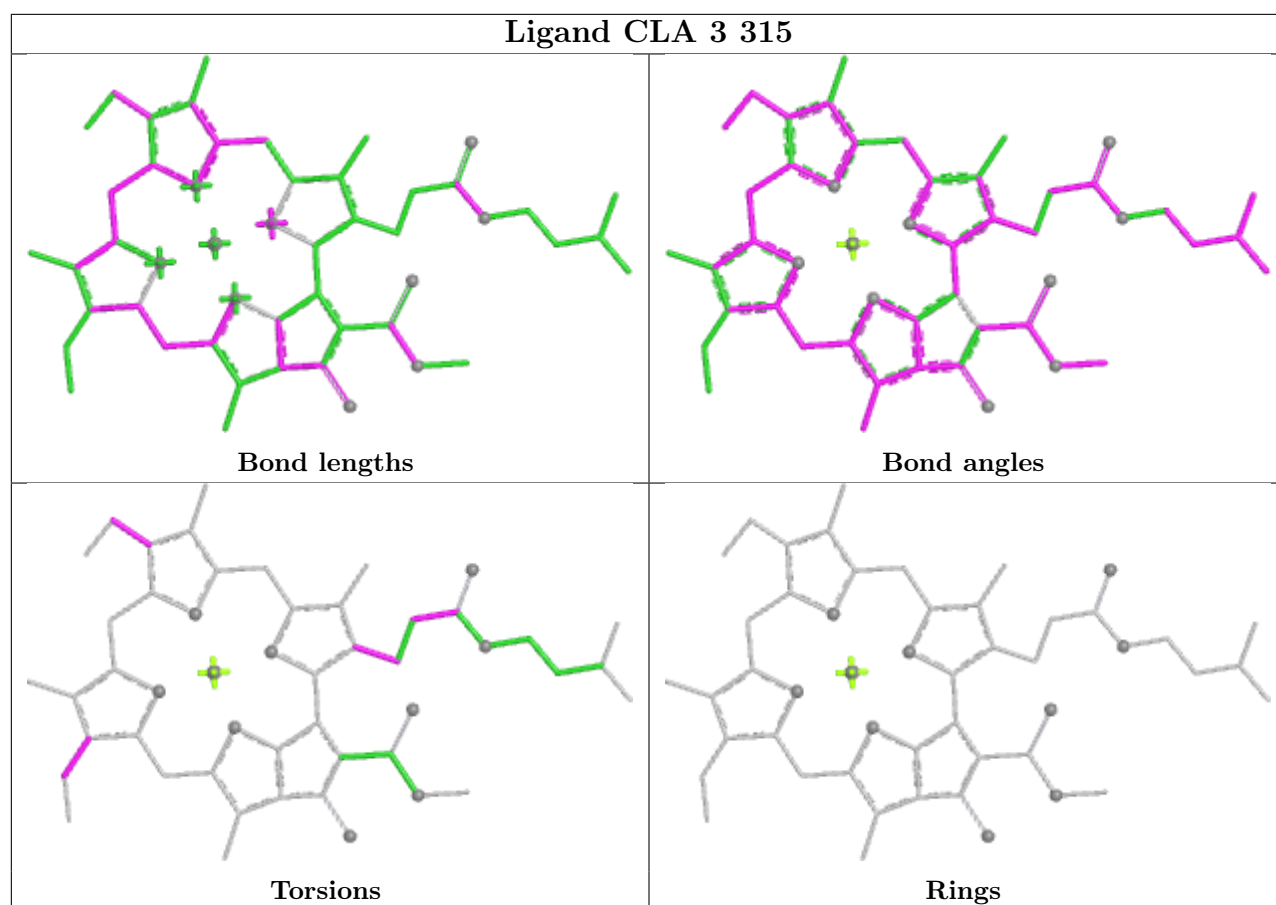


Ligand CLA B 815

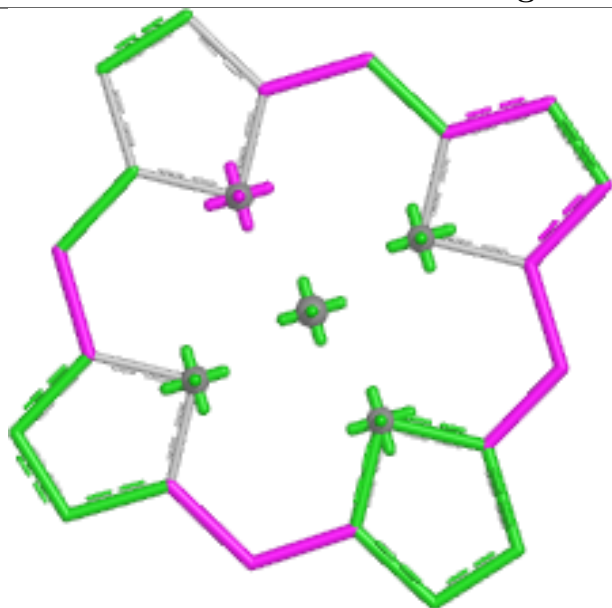




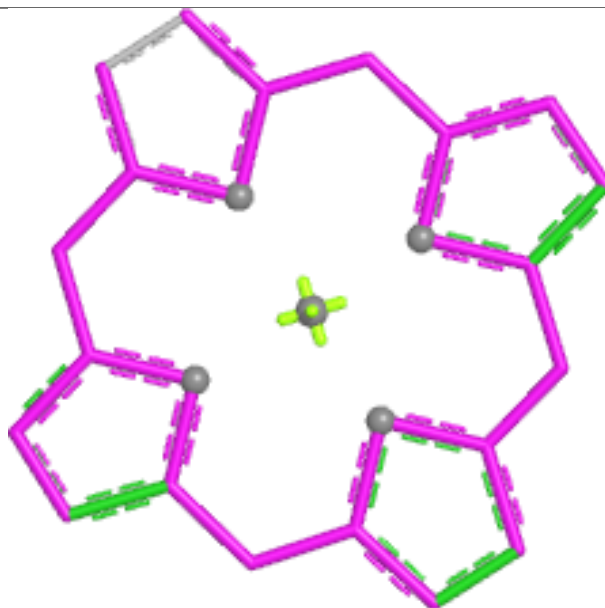




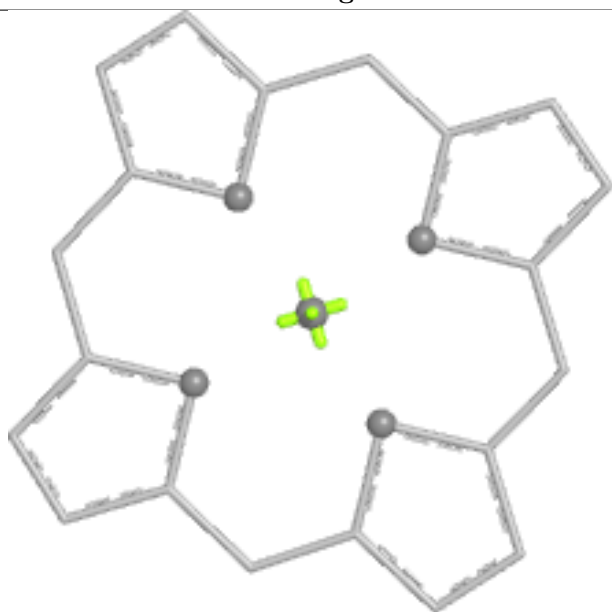
Ligand CLA 4 311



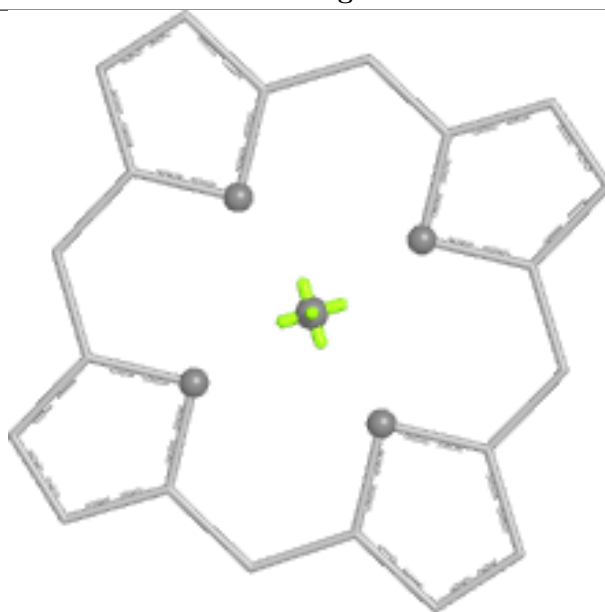
Bond lengths



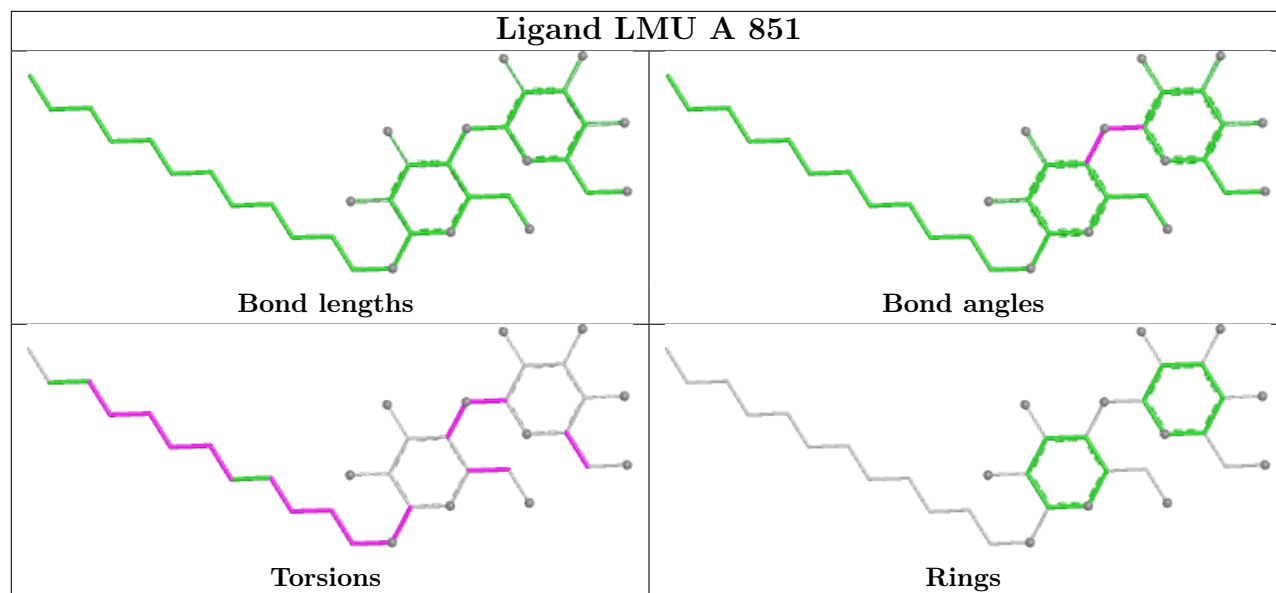
Bond angles



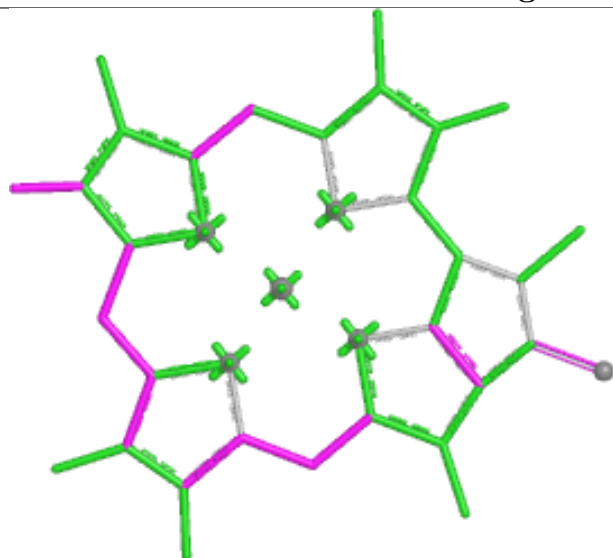
Torsions



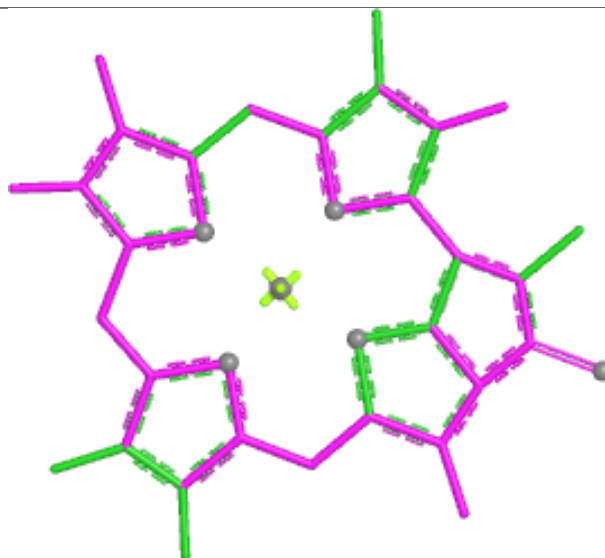
Rings



Ligand CLA 3 303



Bond lengths



Bond angles

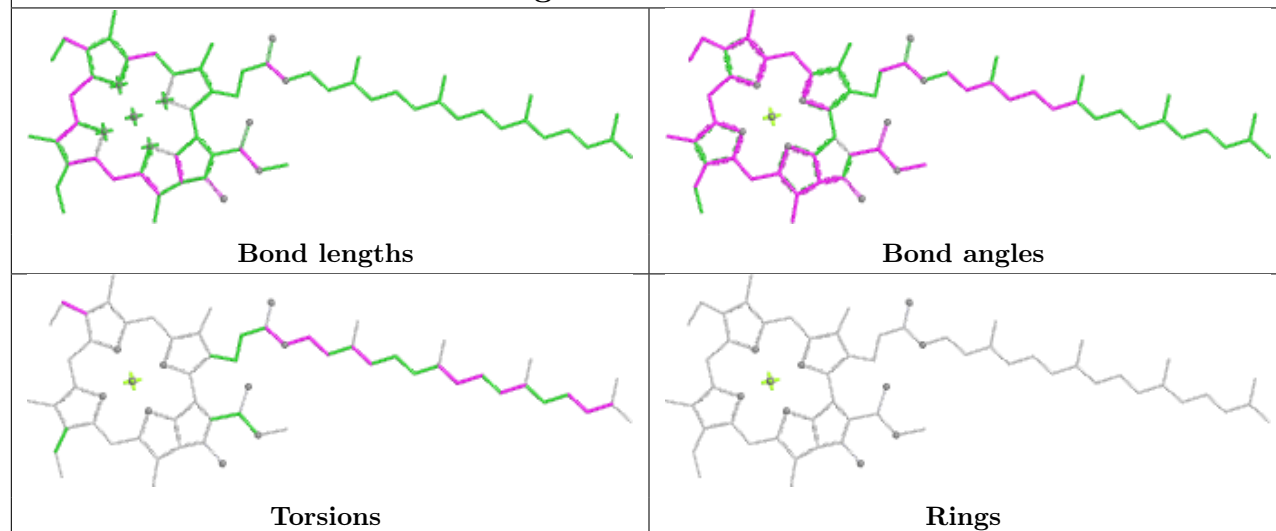


Torsions

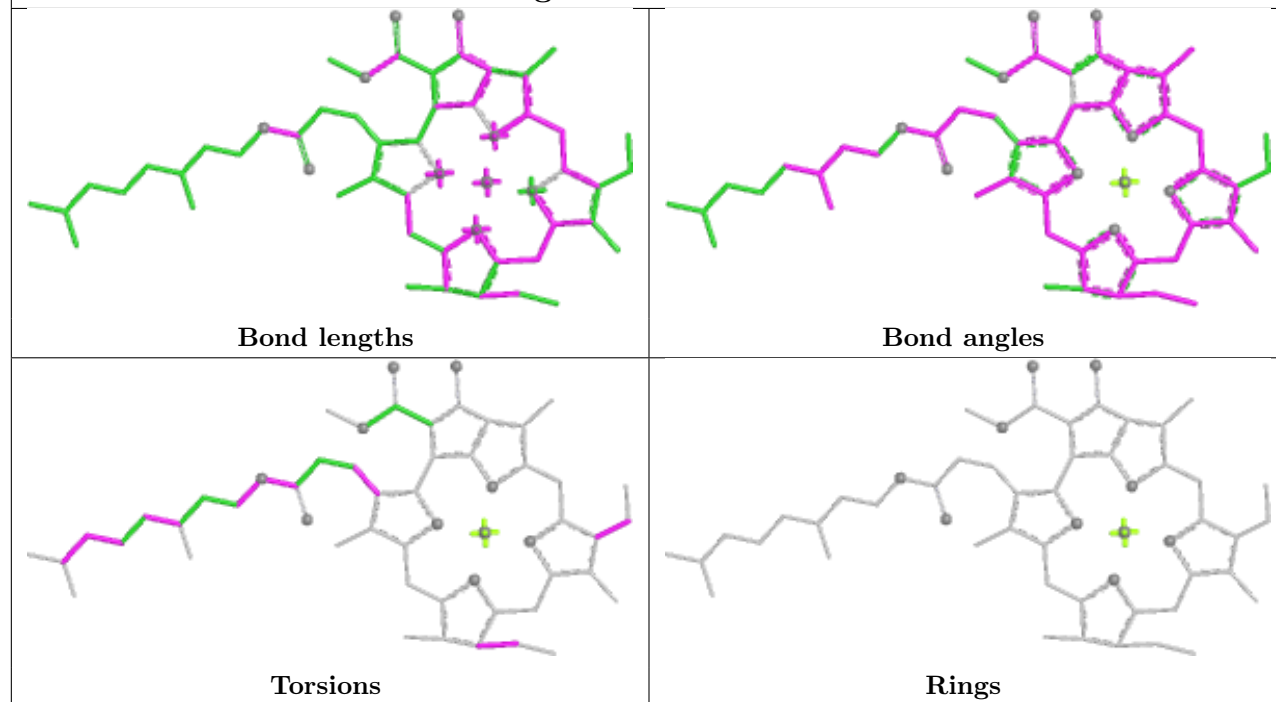


Rings

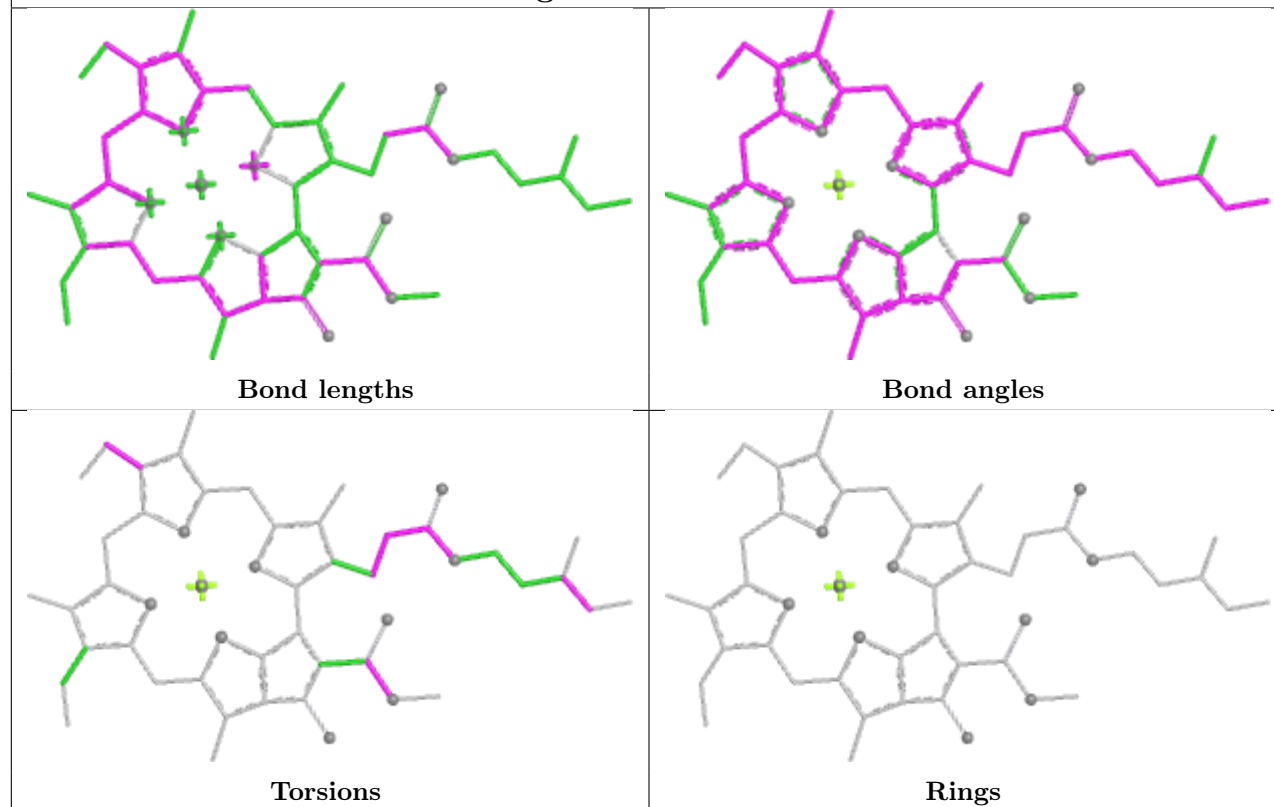
Ligand CLA L 202



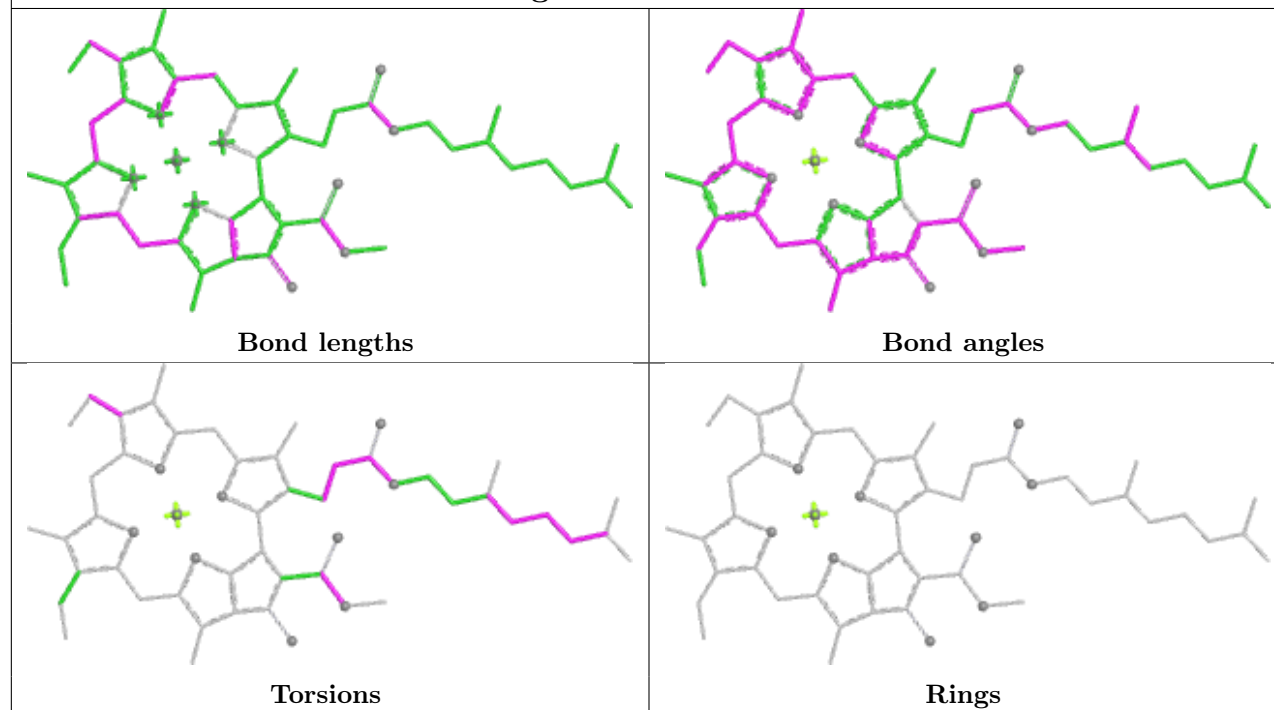
Ligand CLA L 204

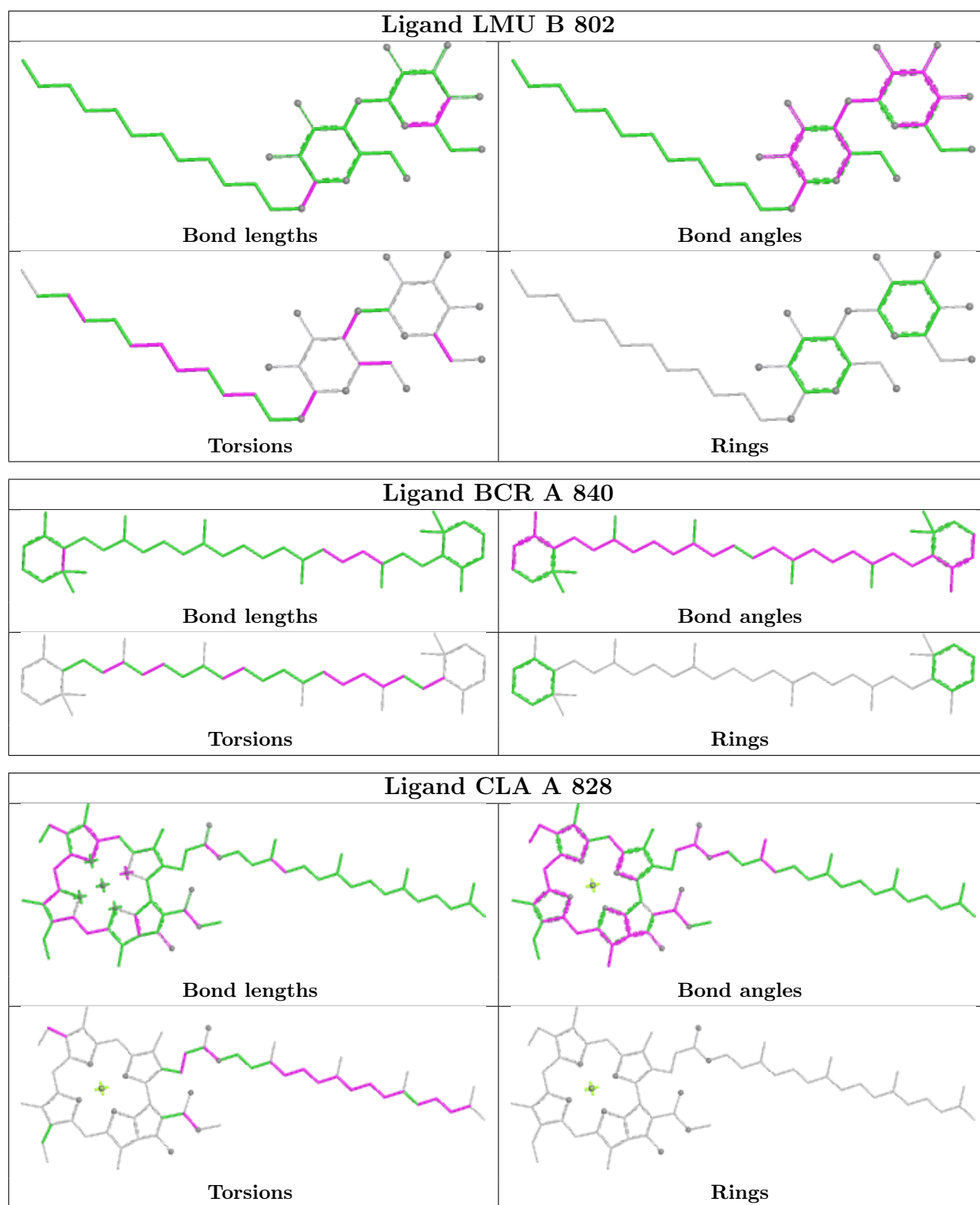


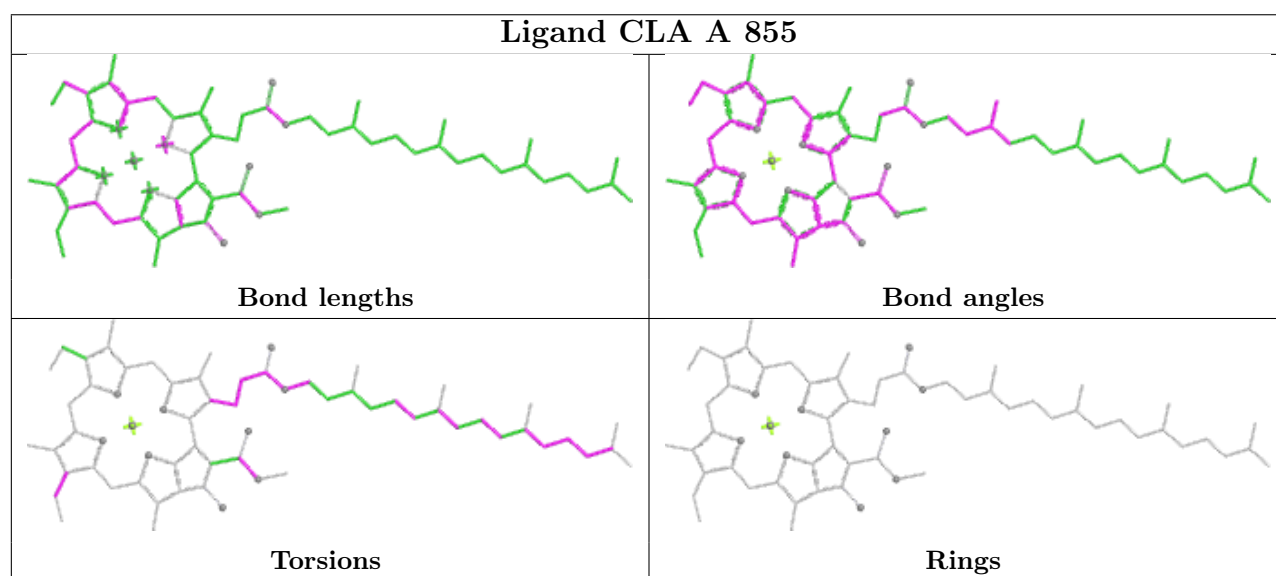
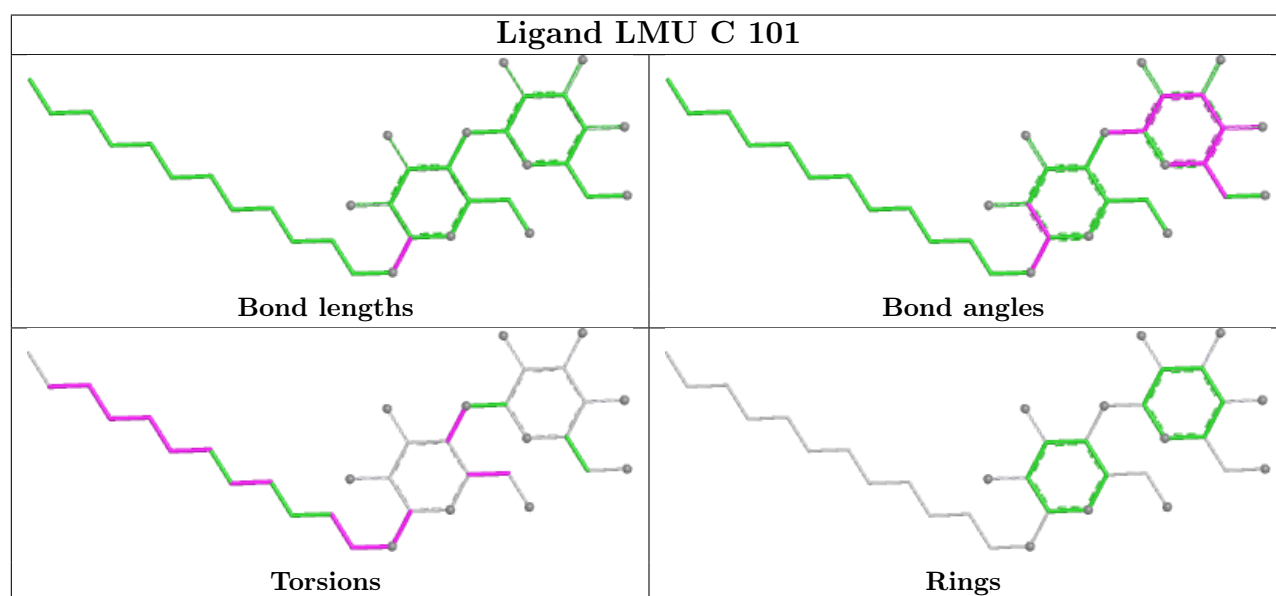
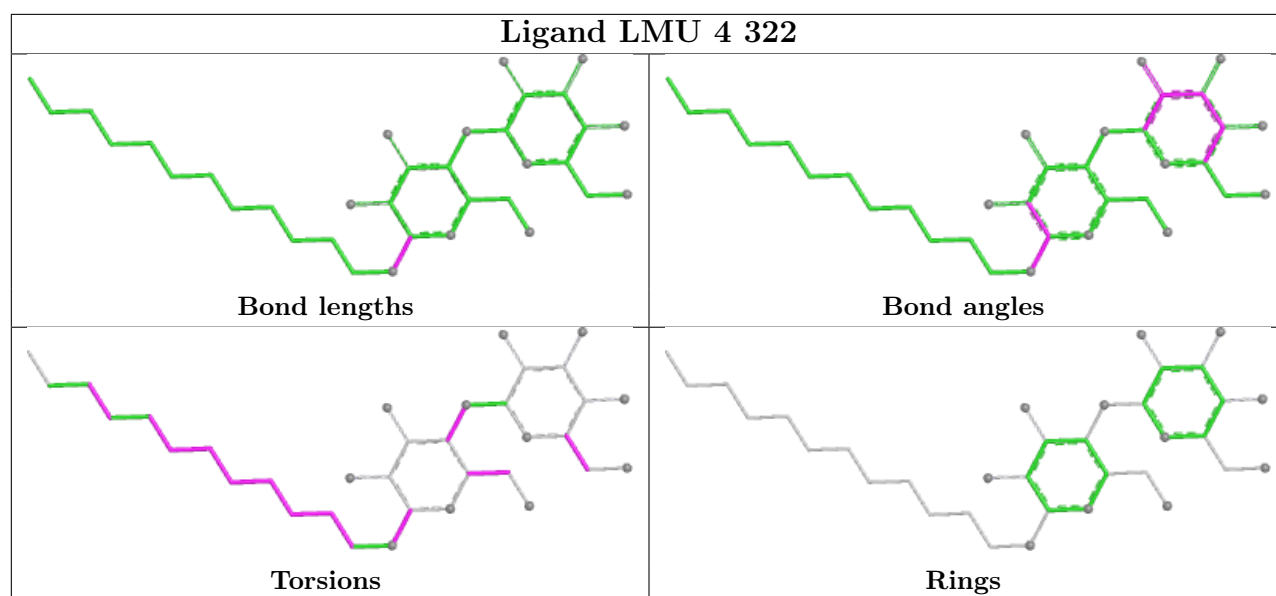
Ligand CLA 1 211



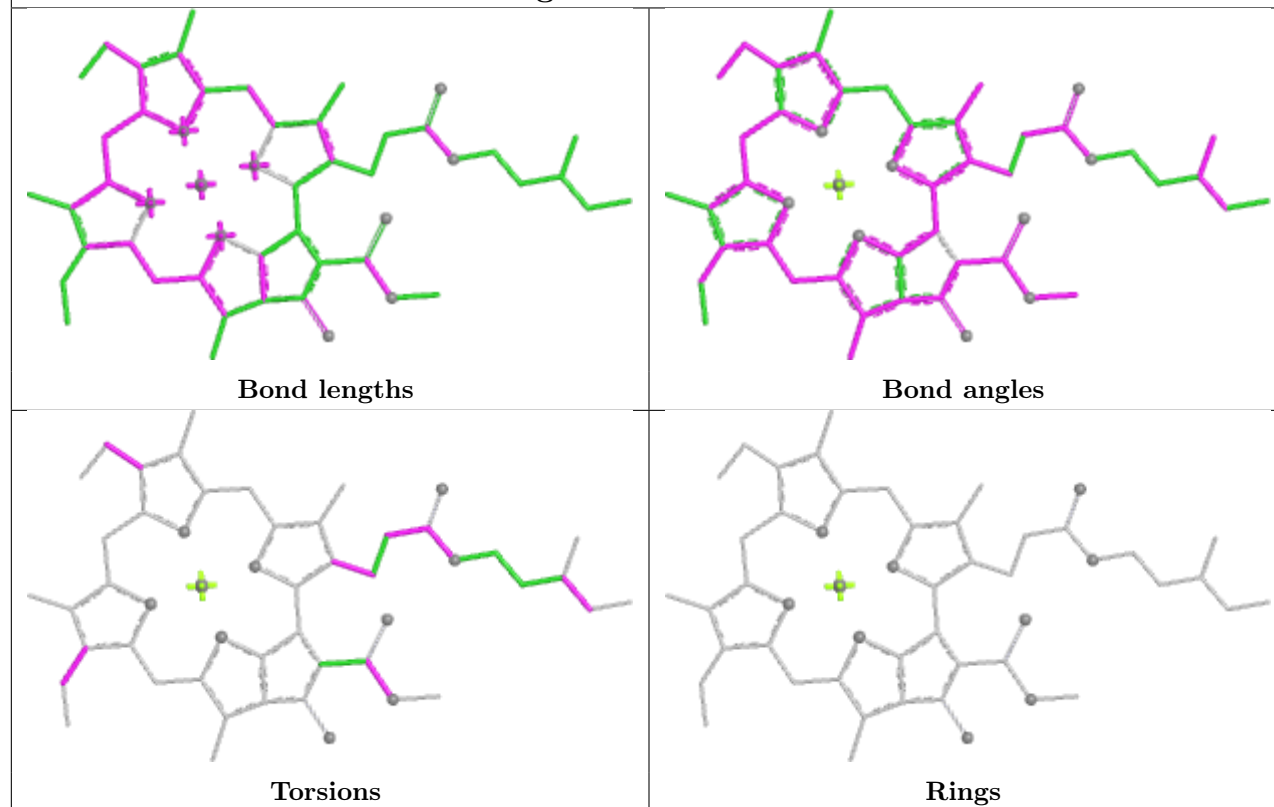
Ligand CLA H 110



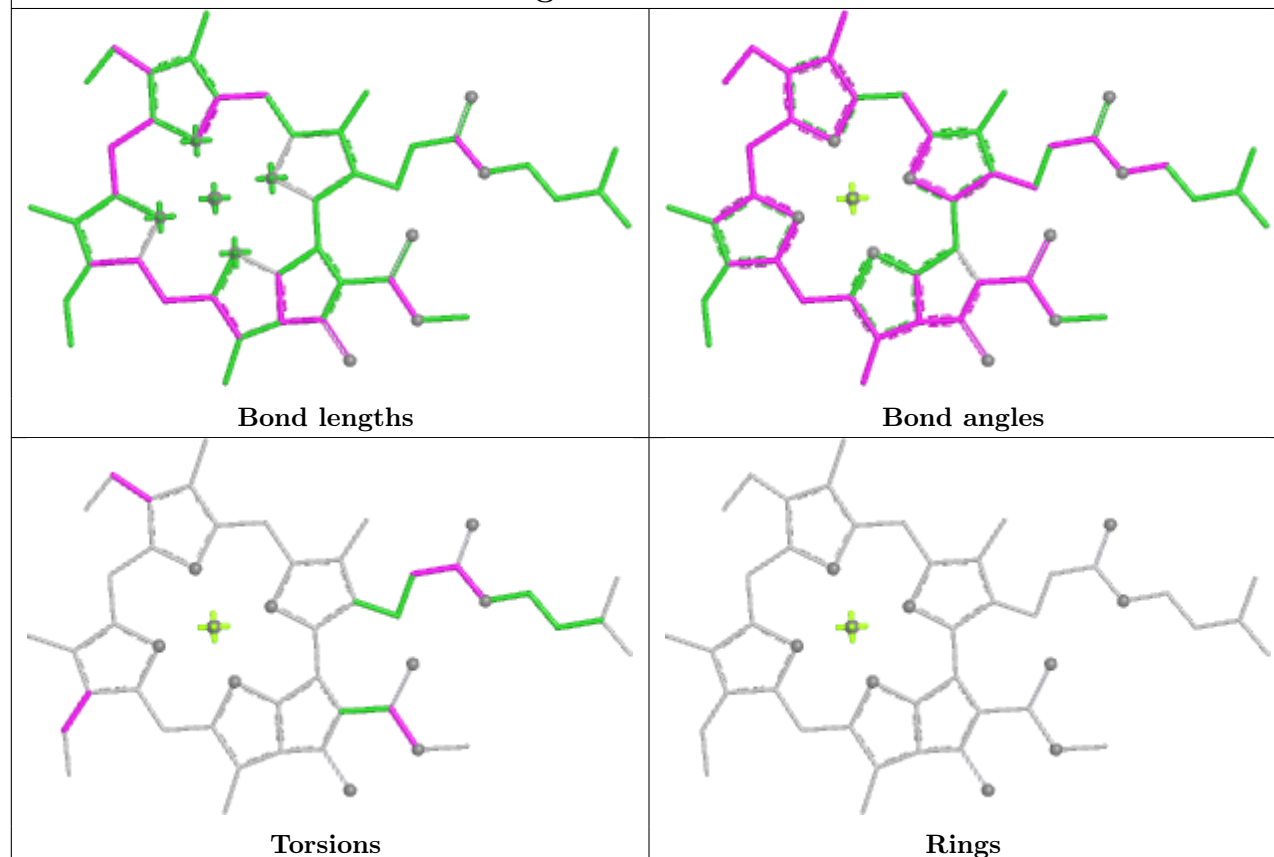


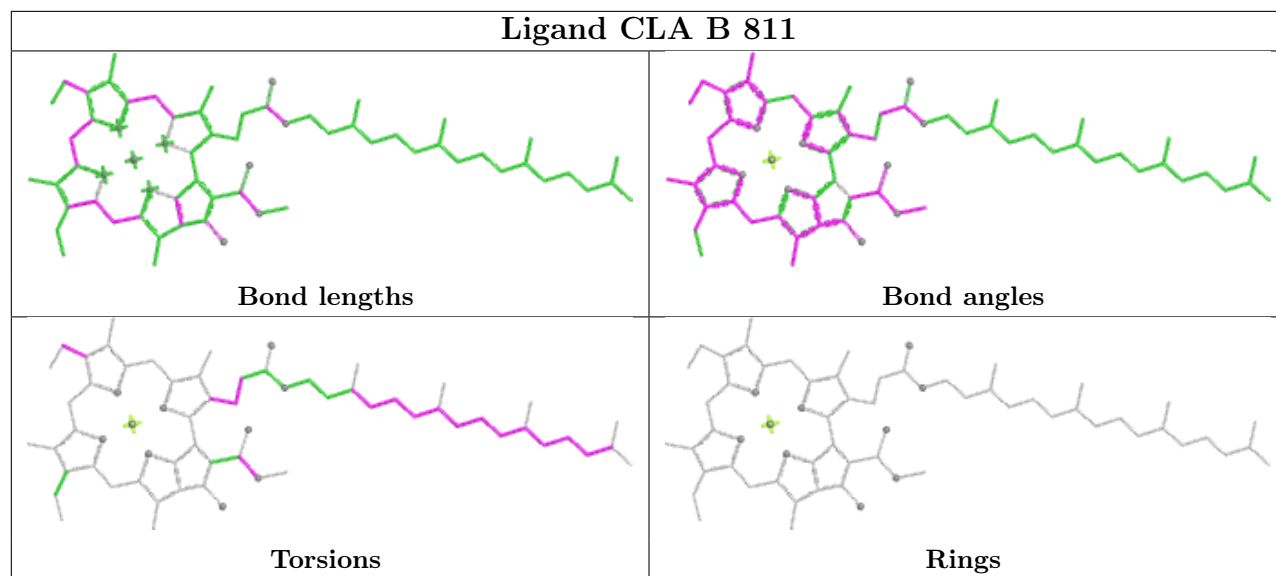


Ligand CLA 1 214

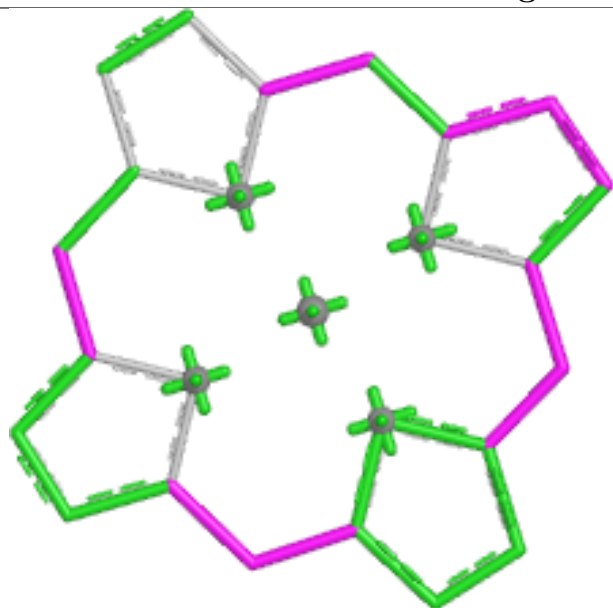


Ligand CLA 2 311

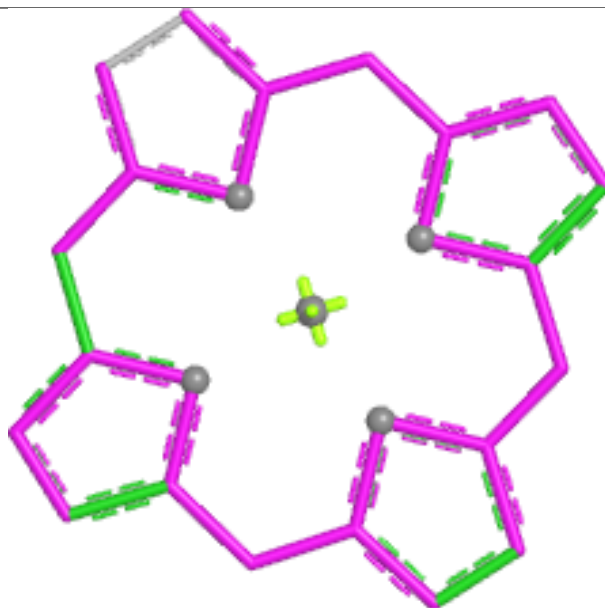




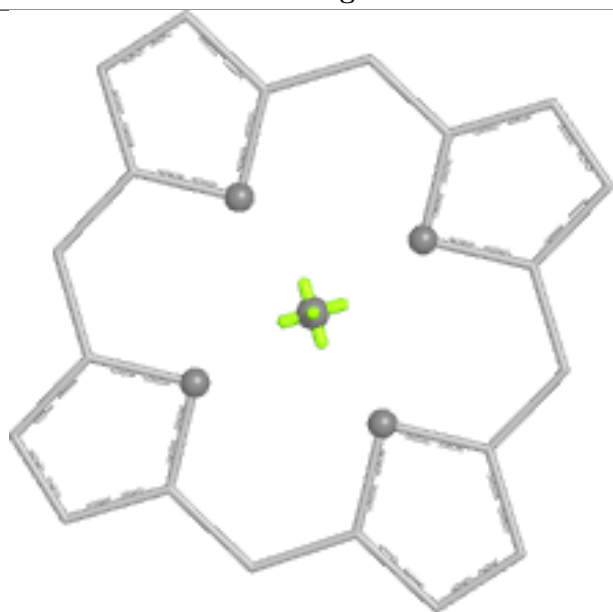
Ligand CLA 4 314



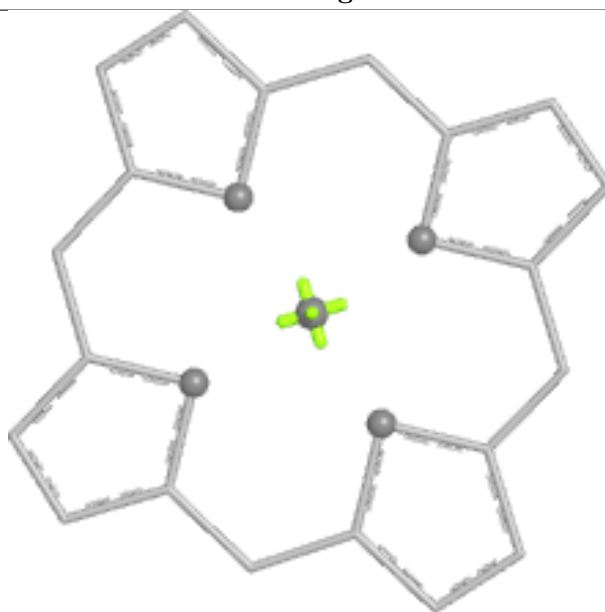
Bond lengths



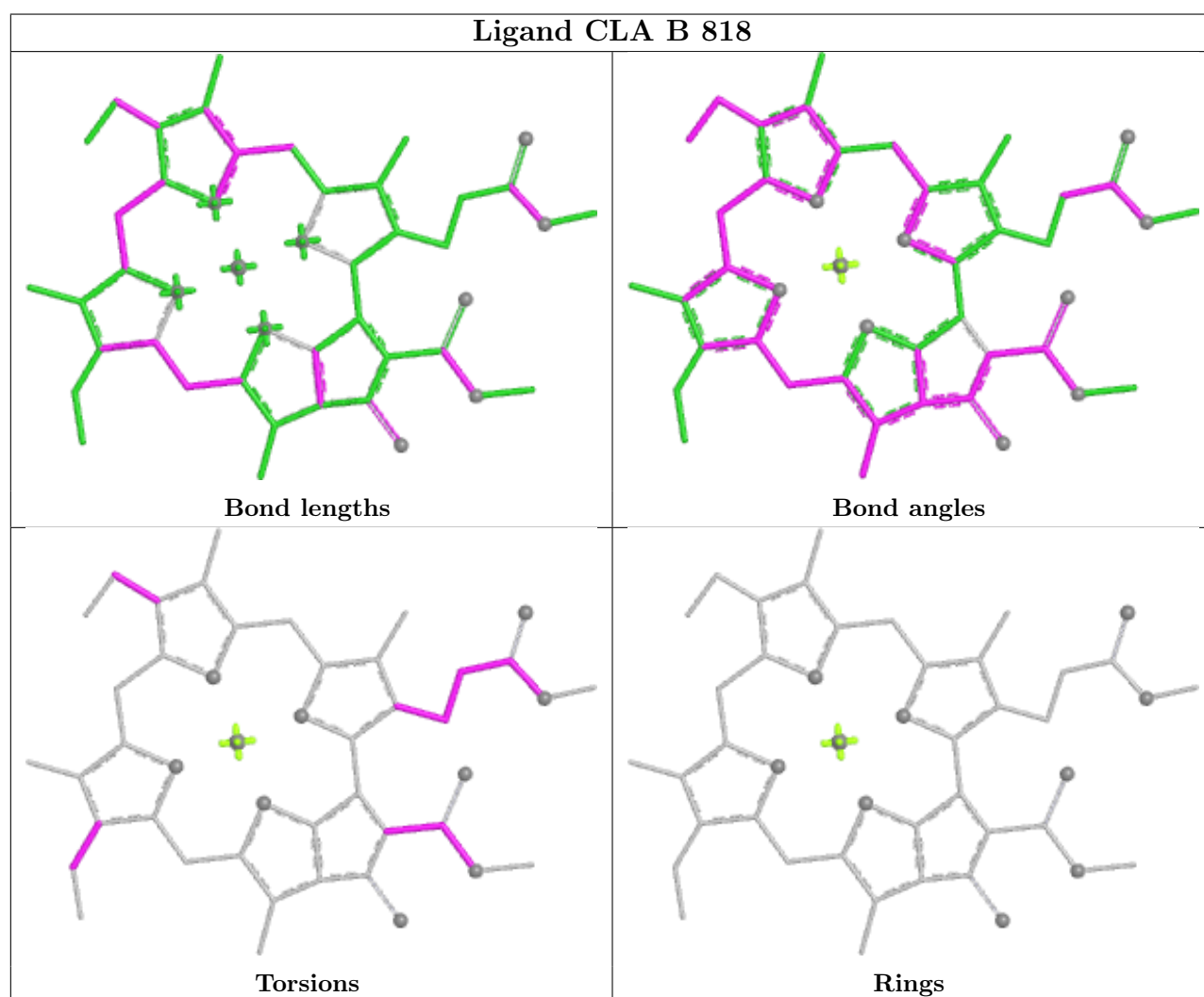
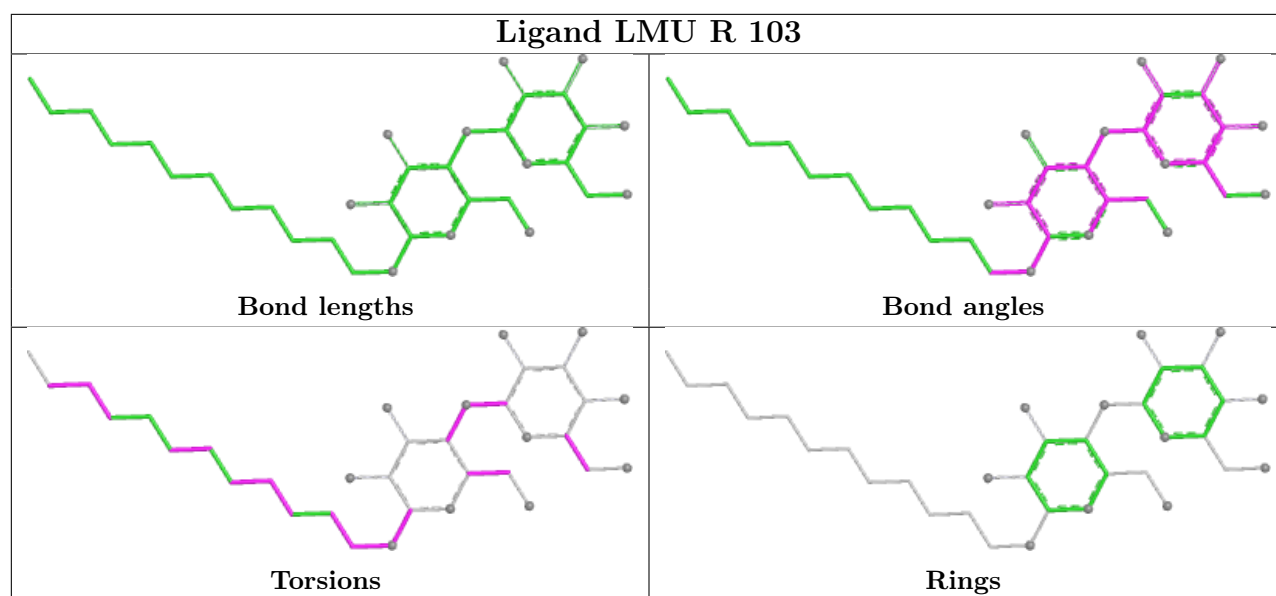
Bond angles

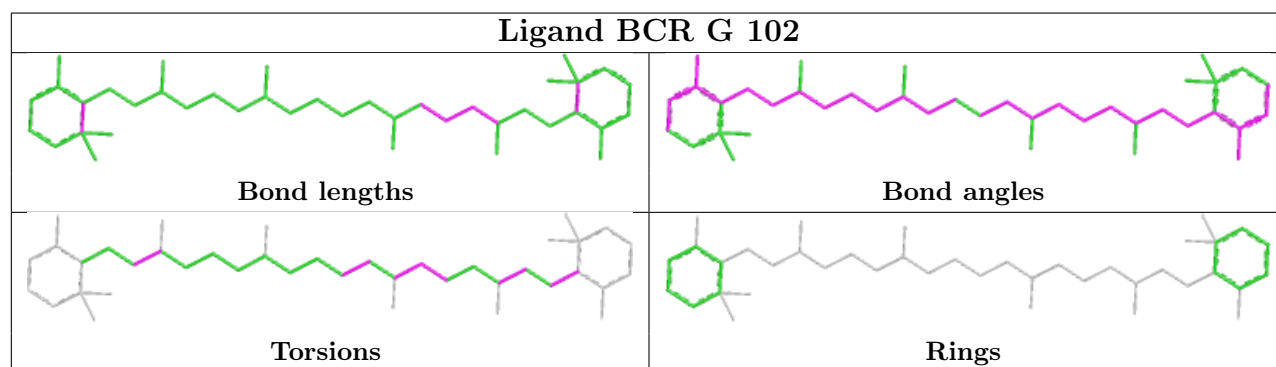
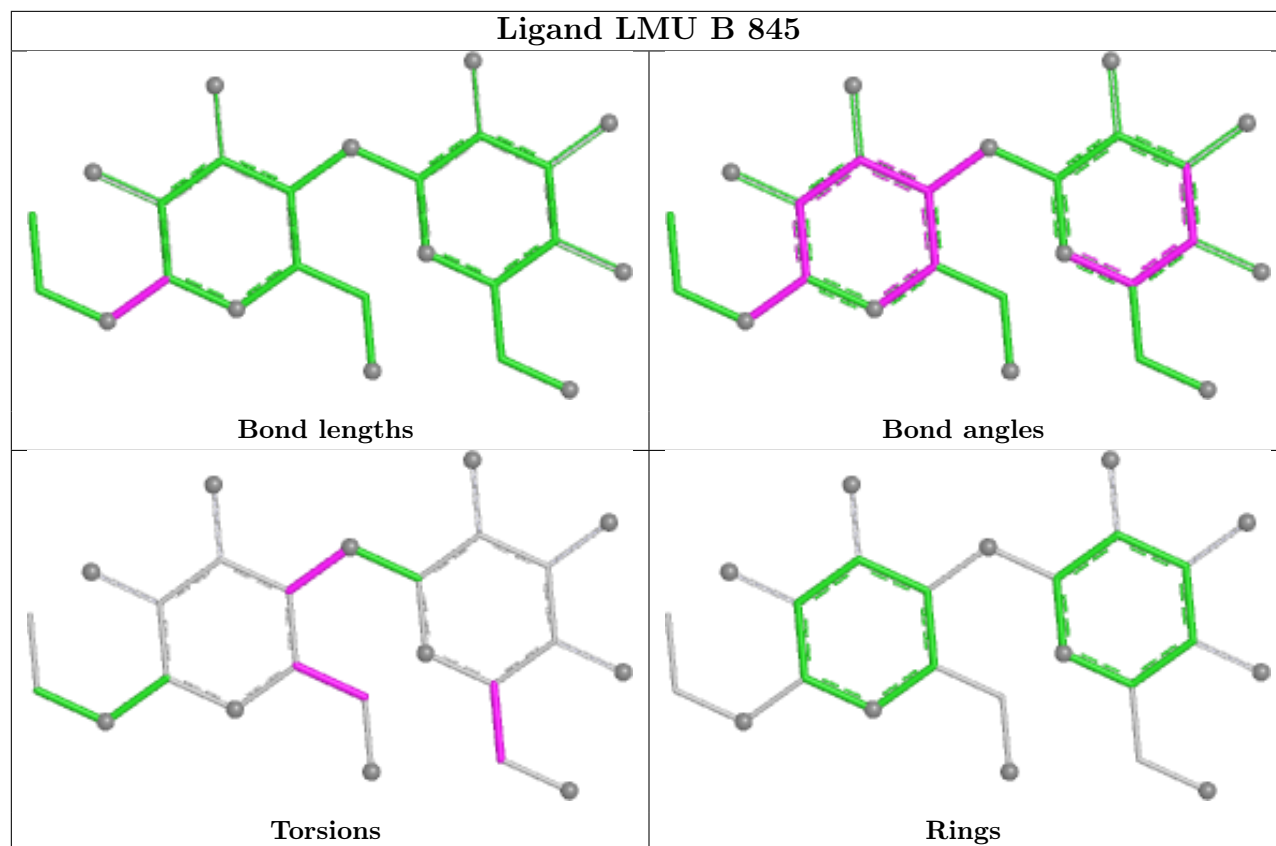


Torsions

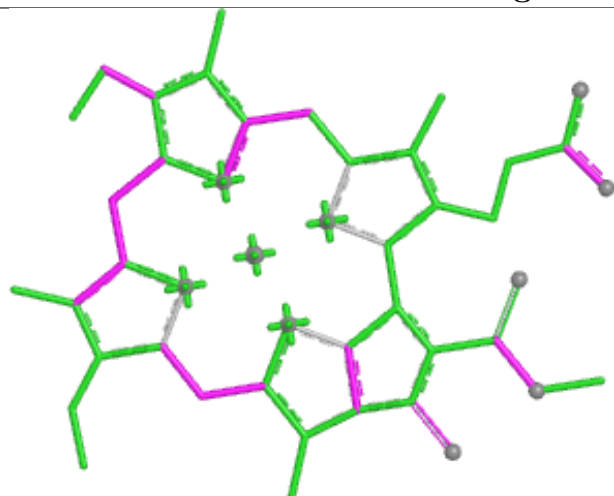


Rings

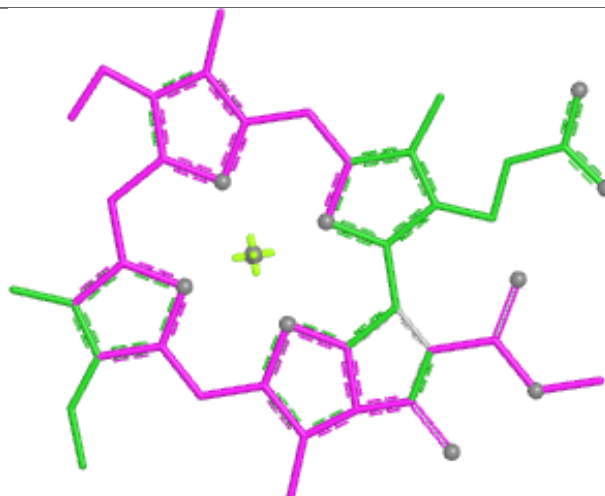




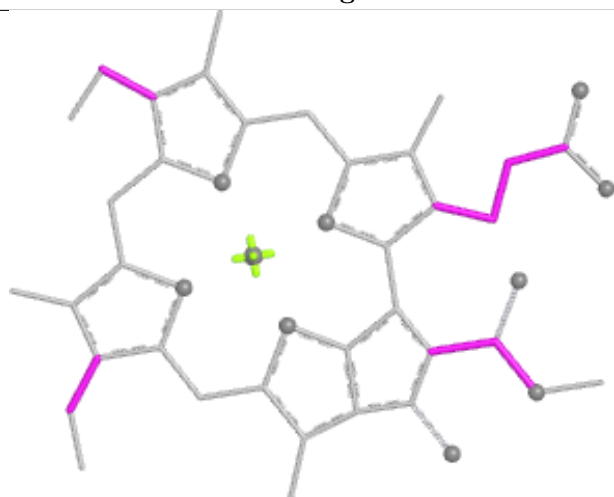
Ligand CLA A 812



Bond lengths



Bond angles

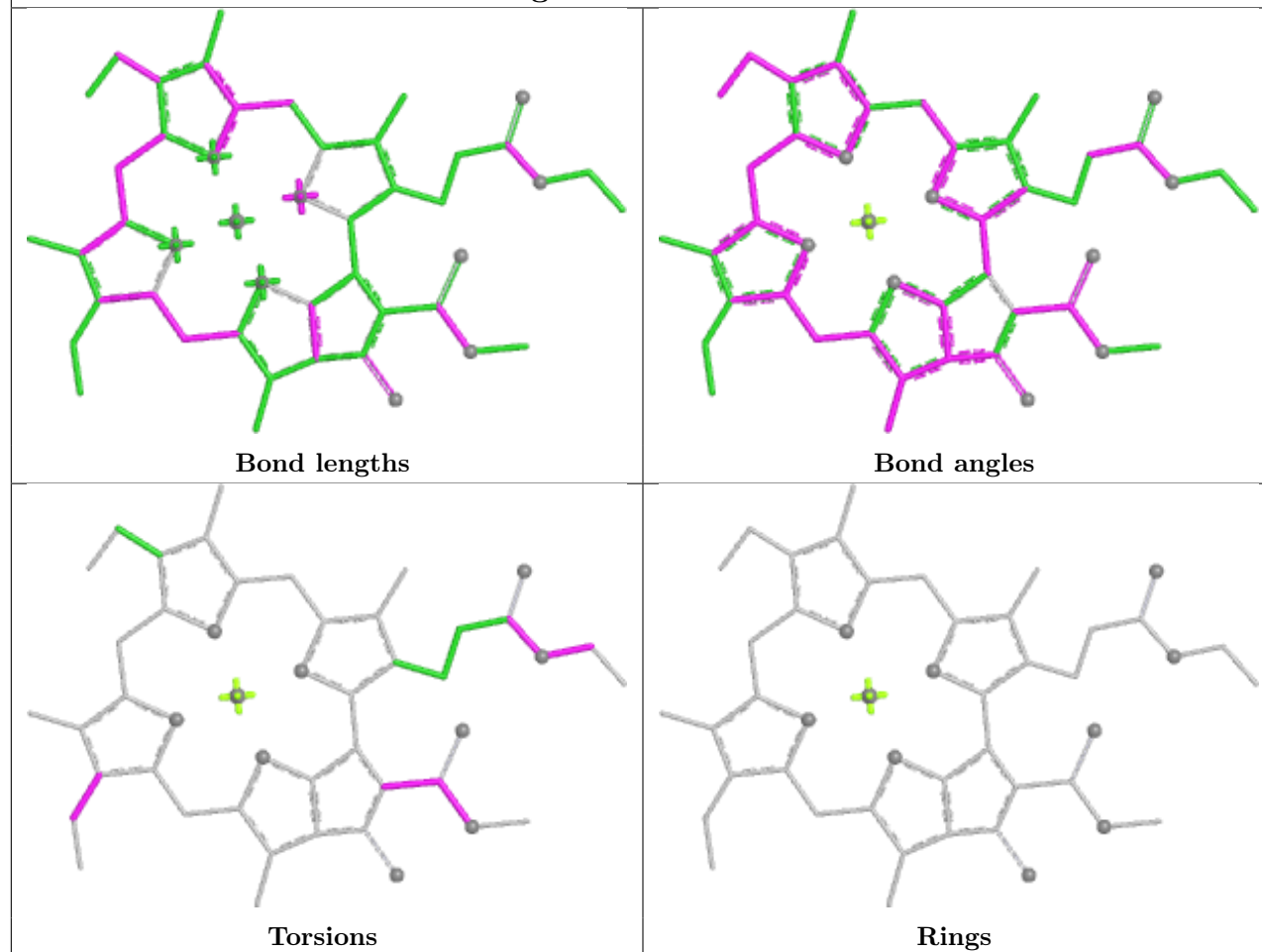


Torsions

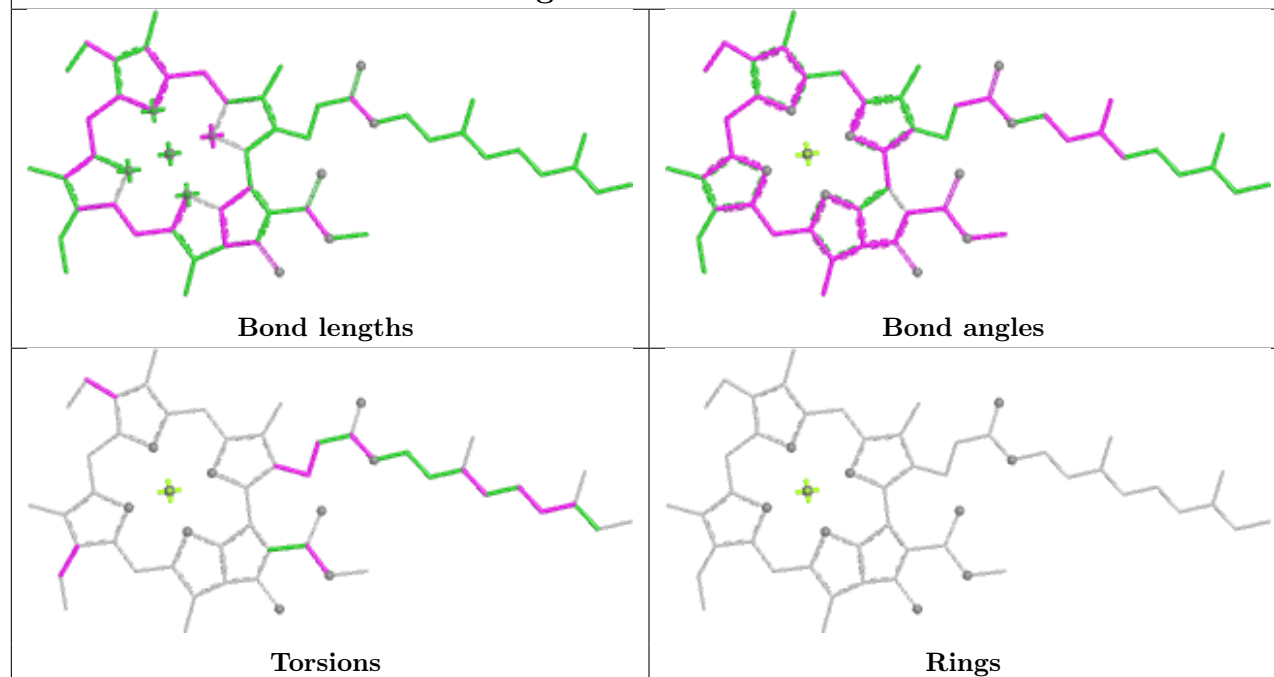


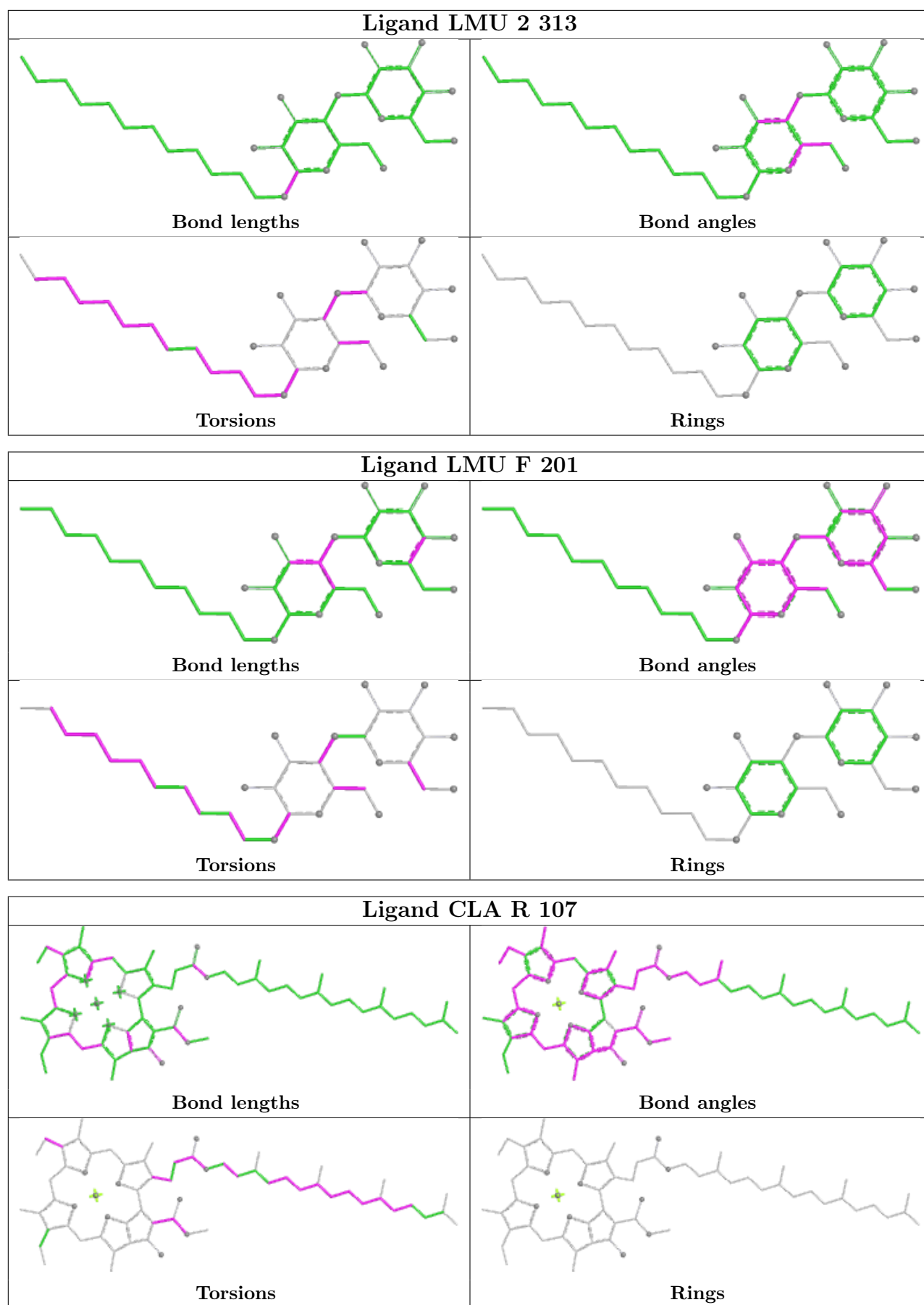
Rings

Ligand CLA 4 319

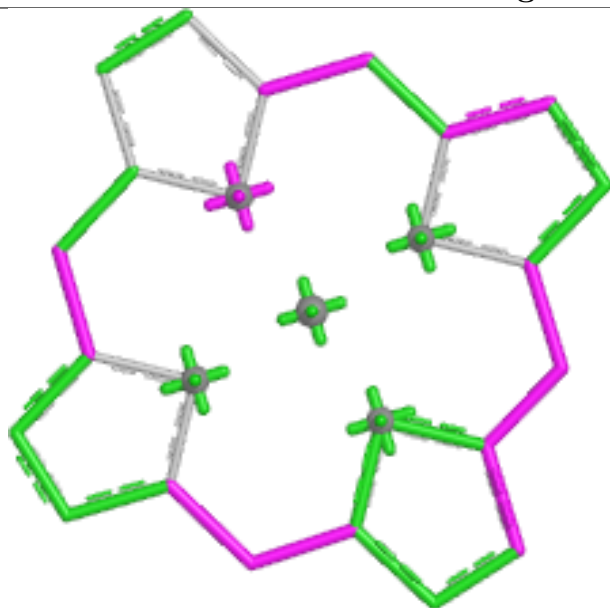


Ligand CLA 3 301

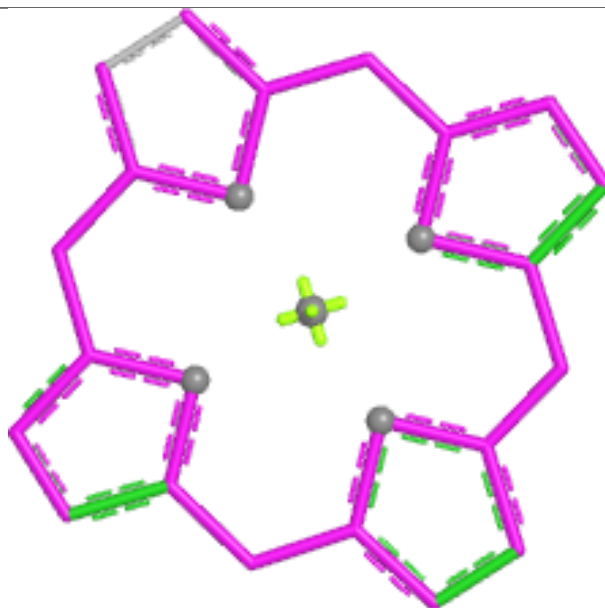




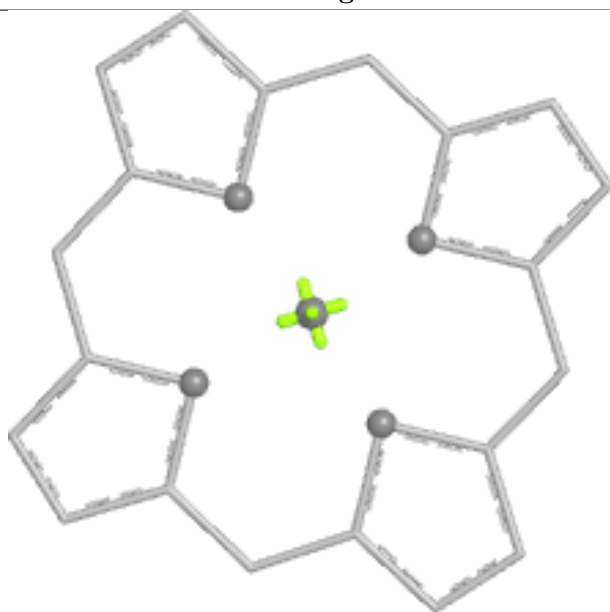
Ligand CLA 2 303



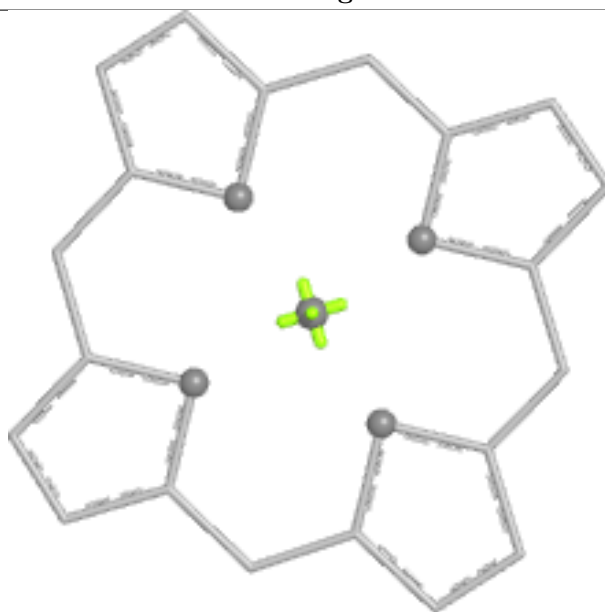
Bond lengths



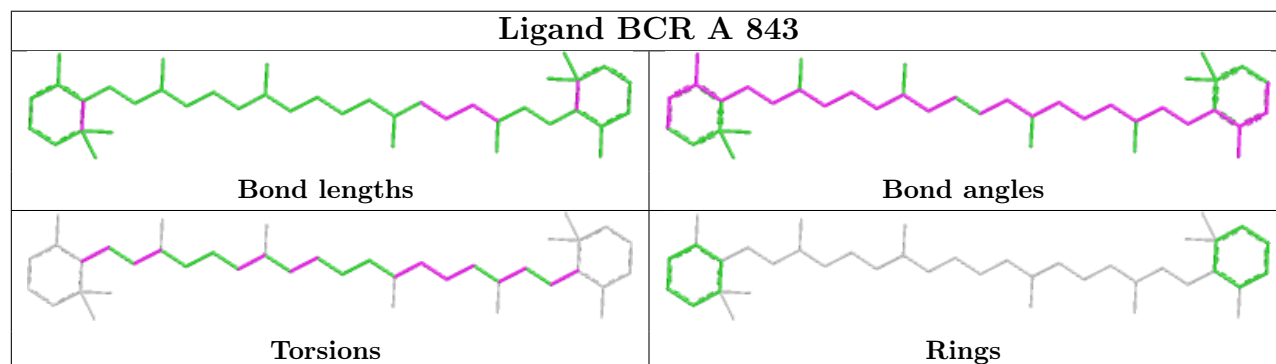
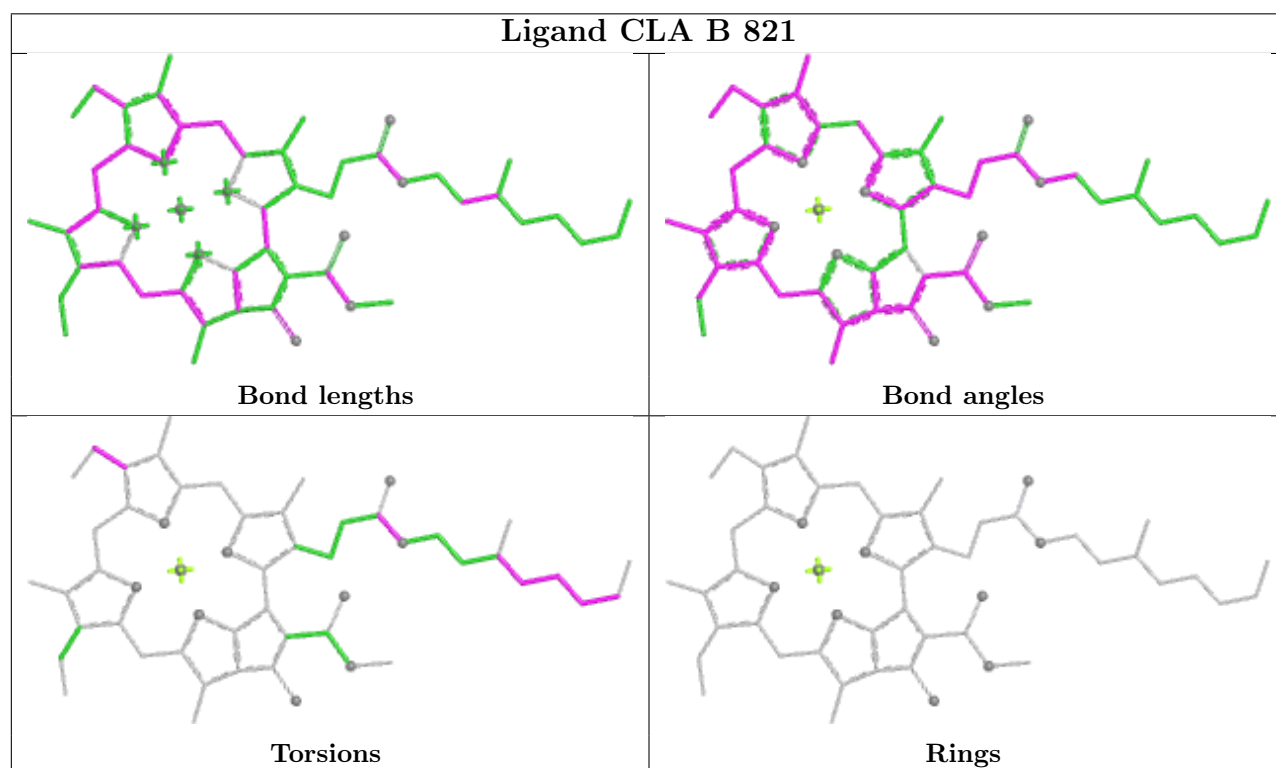
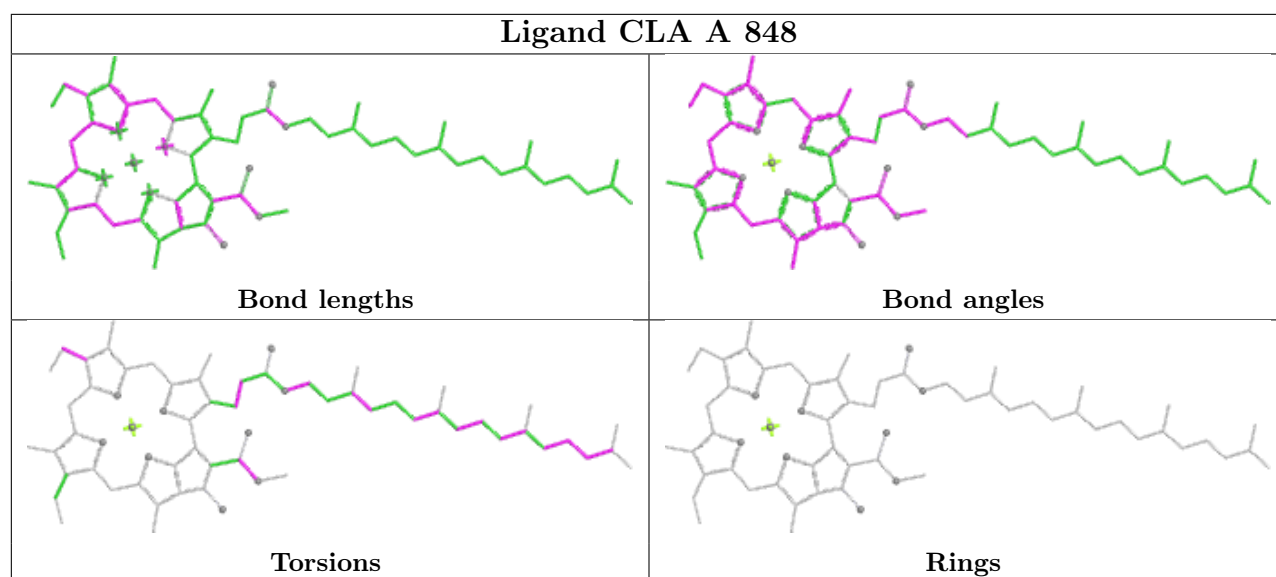
Bond angles

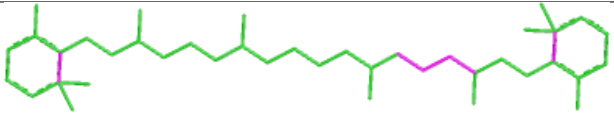
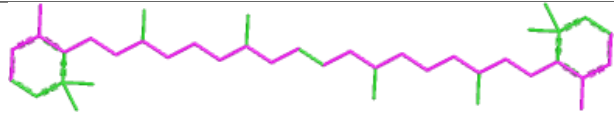
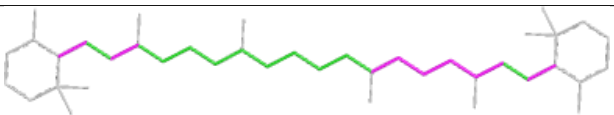
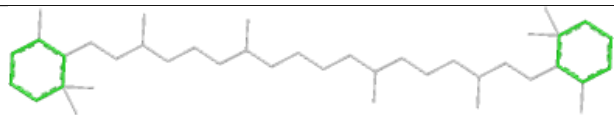


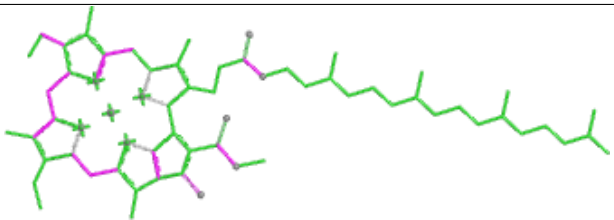
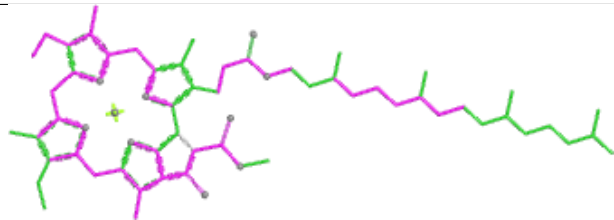
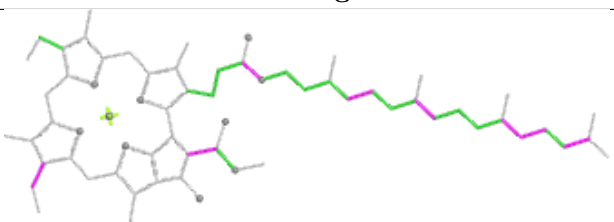
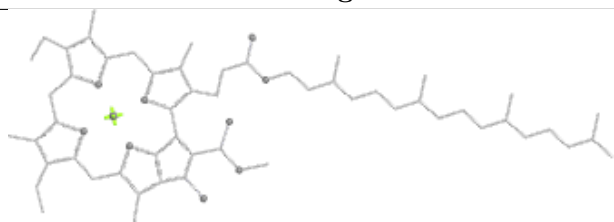
Torsions

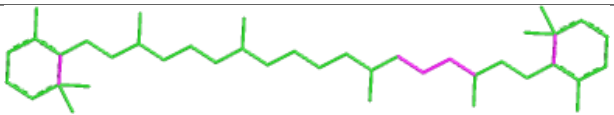
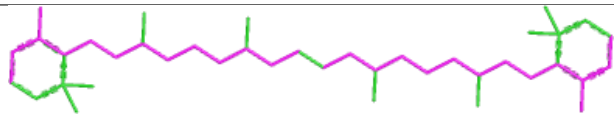
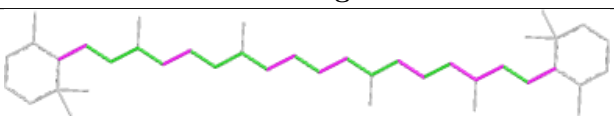
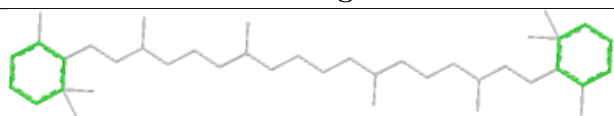


Rings

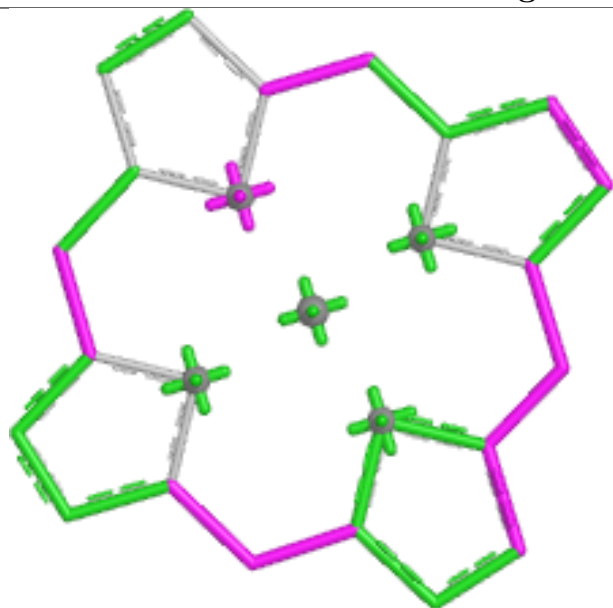


Ligand BCR B 844	
	
Bond lengths	Bond angles
	
Torsions	Rings

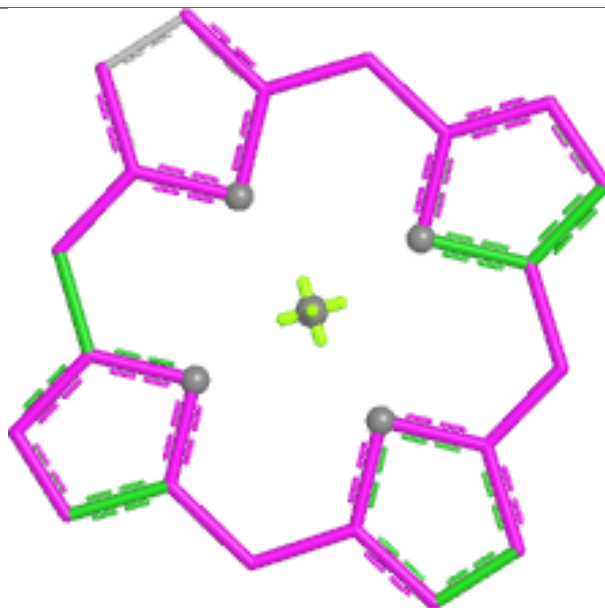
Ligand CLA 2 307	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand BCR F 202	
	
Bond lengths	Bond angles
	
Torsions	Rings

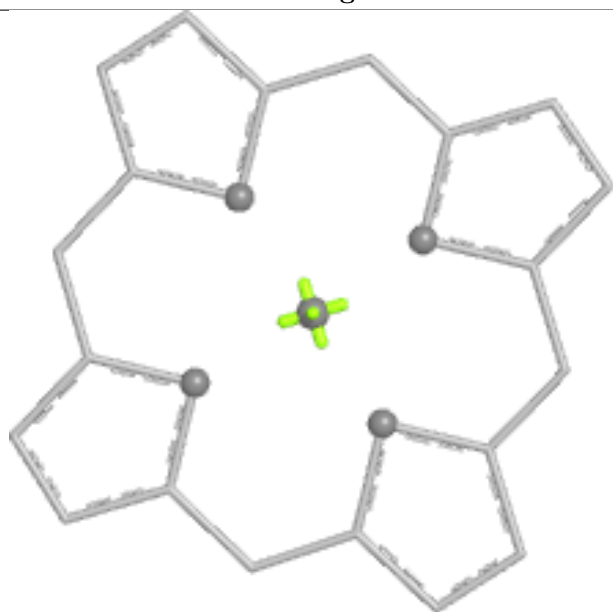
Ligand CLA 3 306



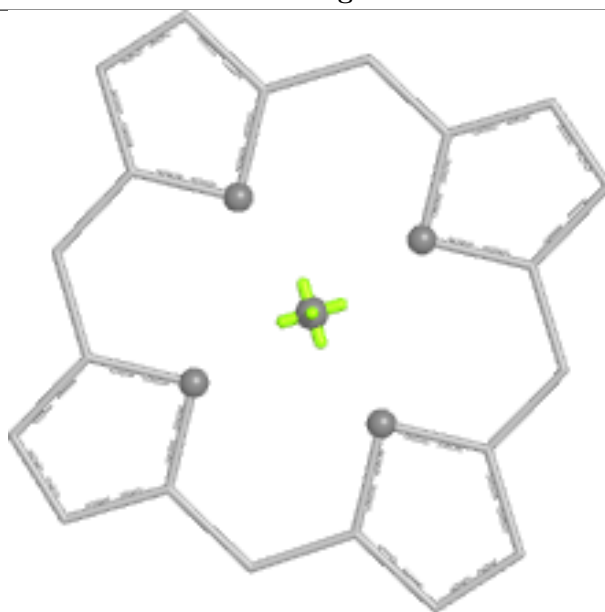
Bond lengths



Bond angles

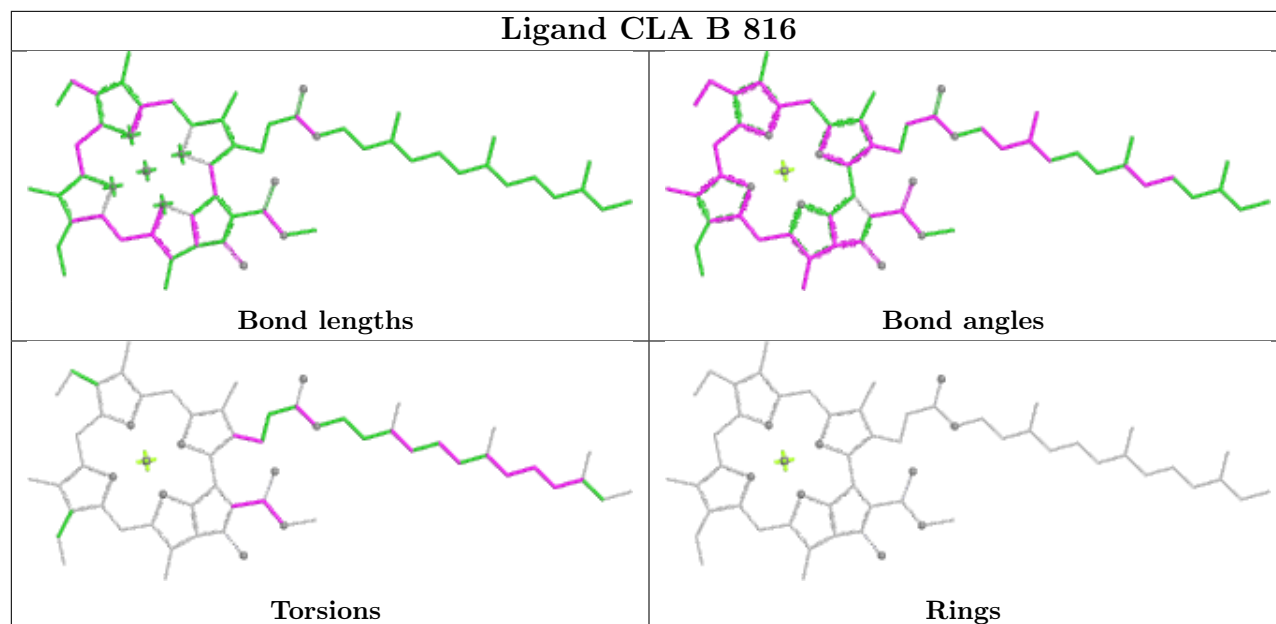


Torsions

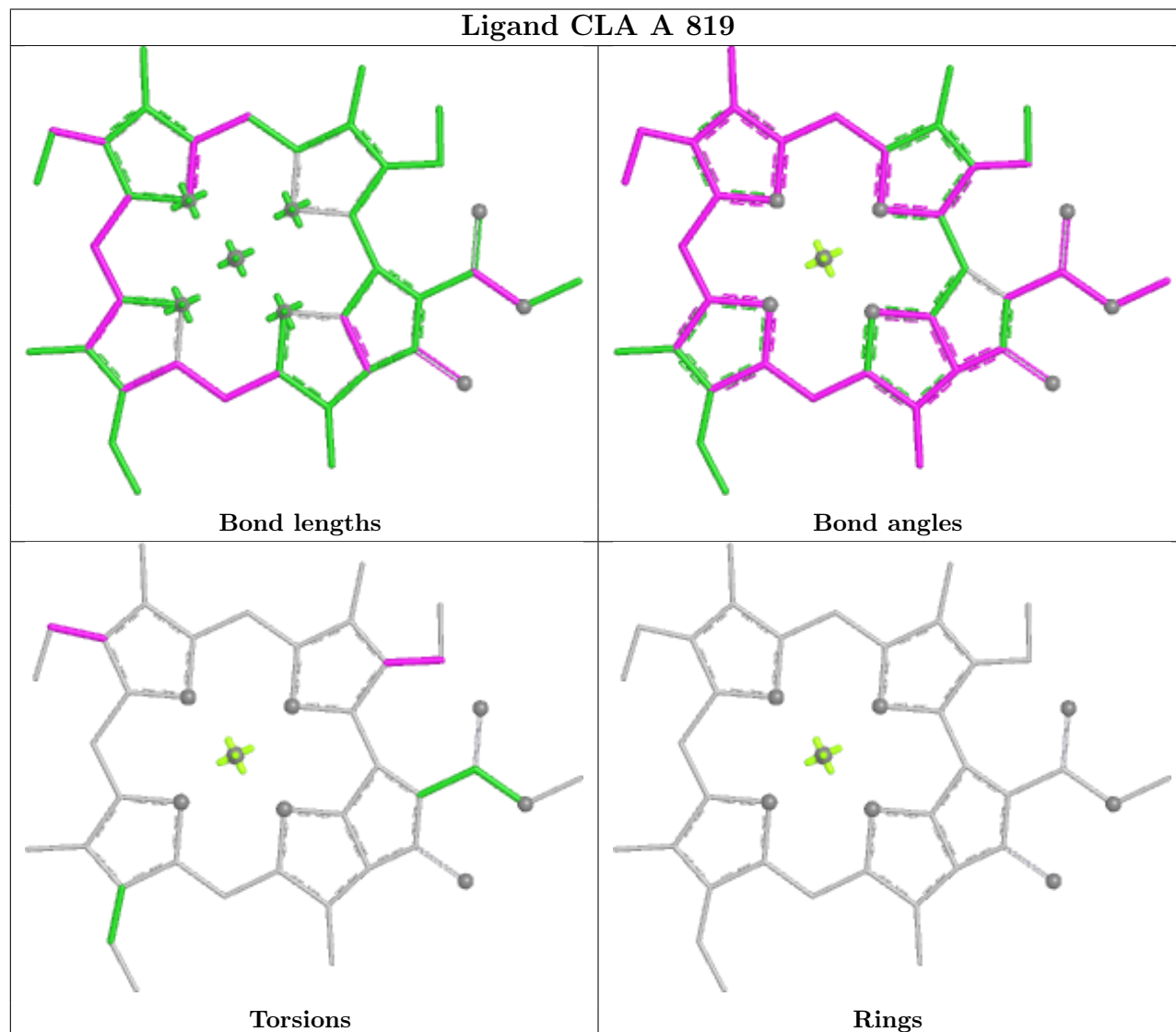


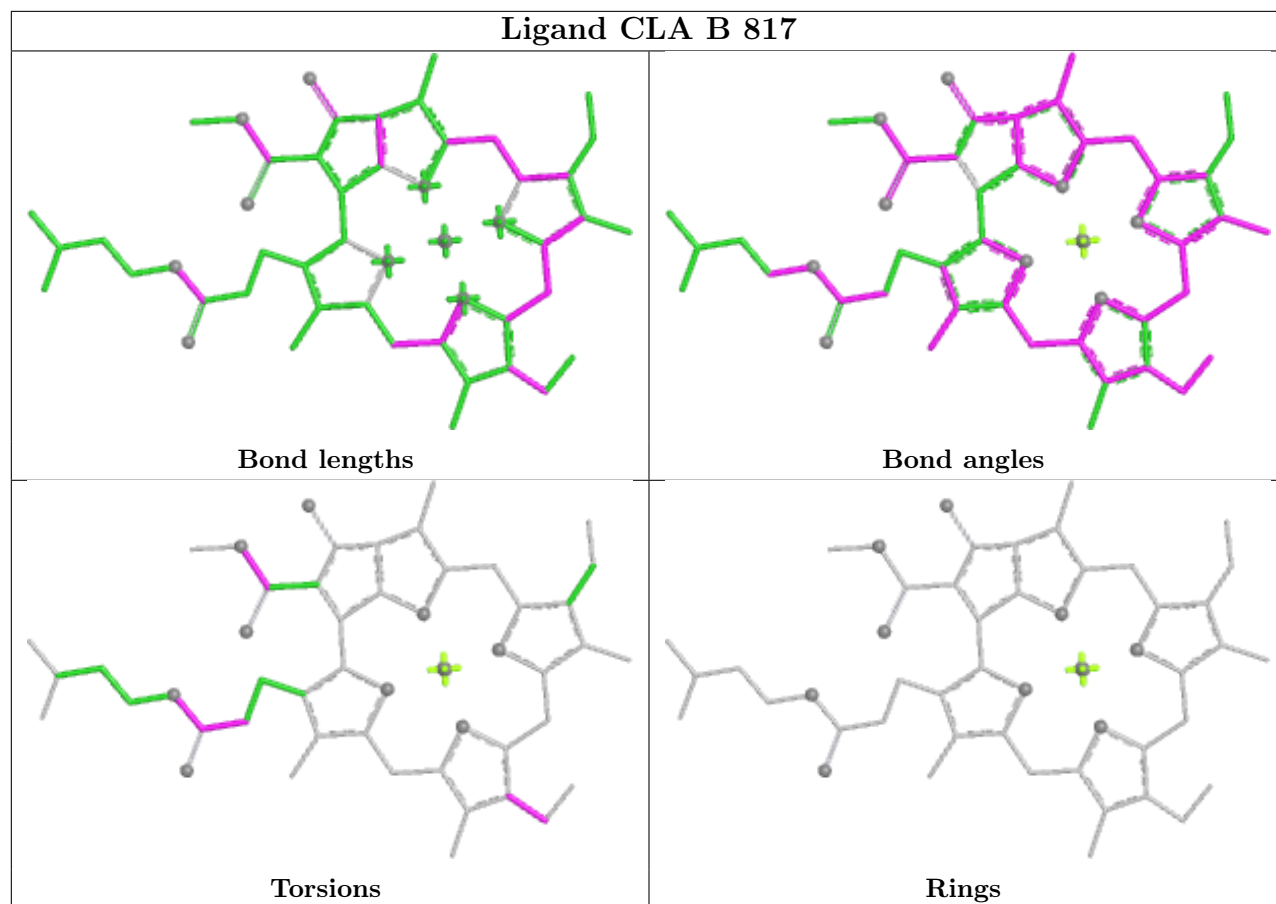
Rings

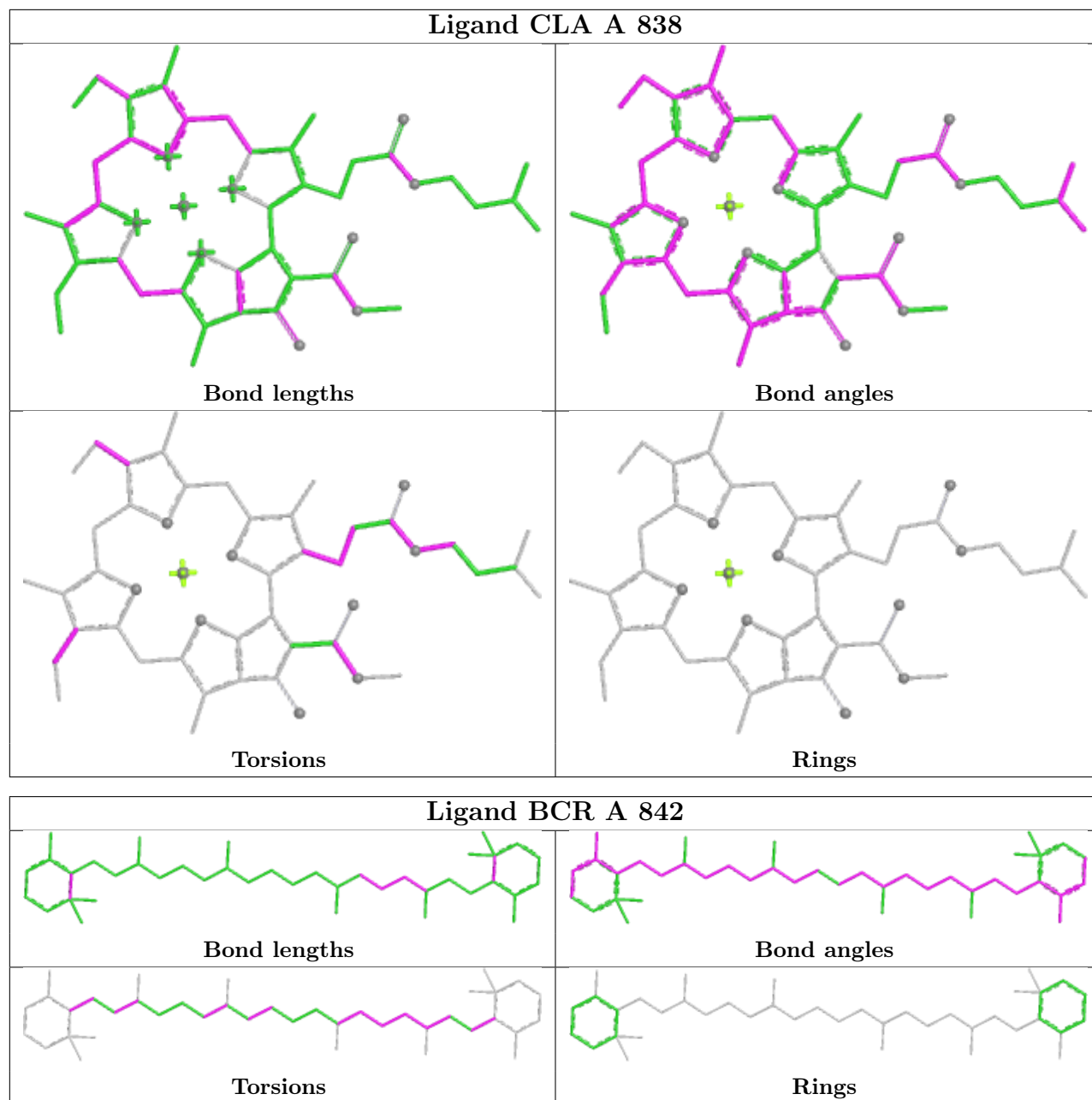
Ligand CLA B 816



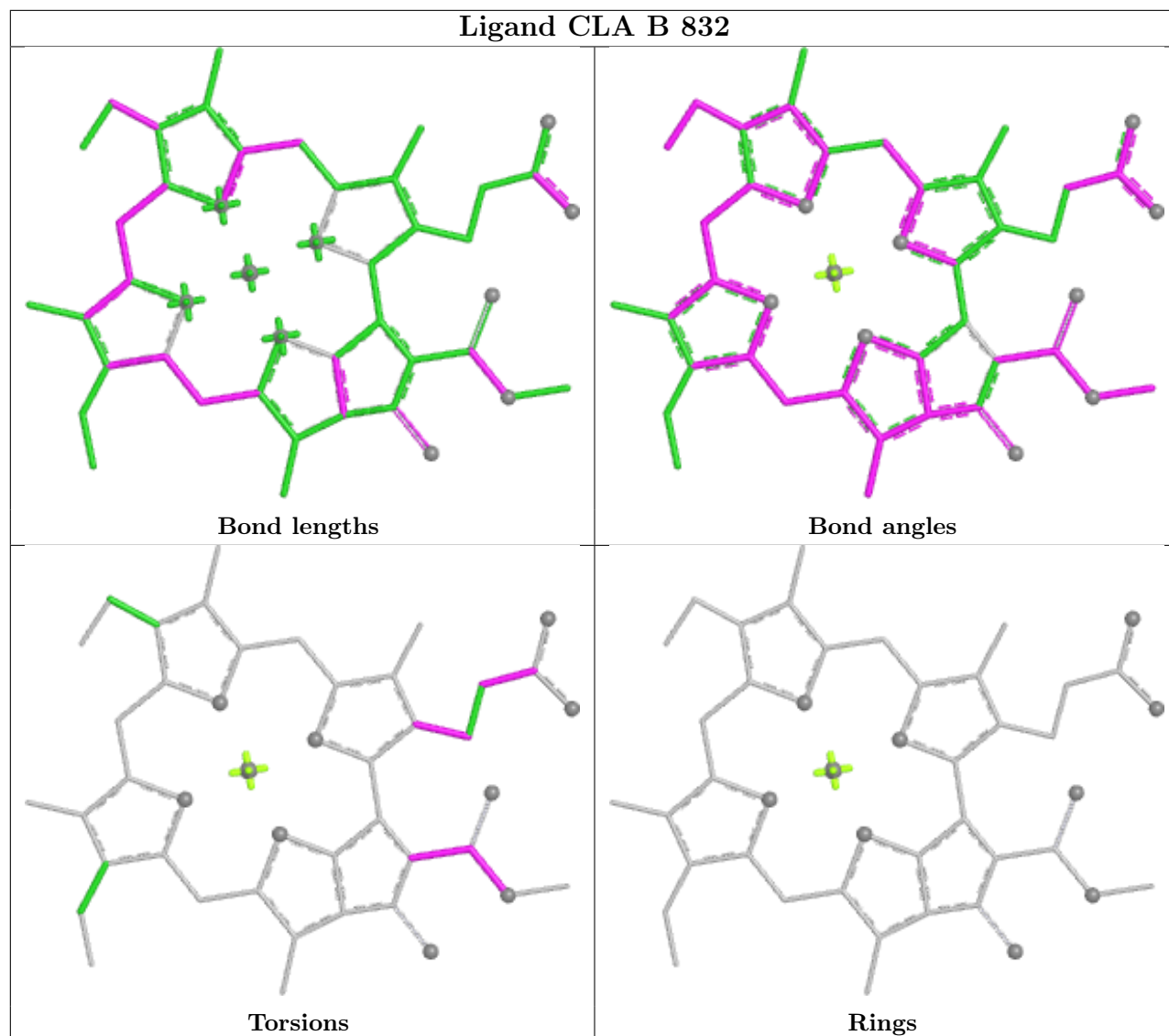
Ligand CLA A 819



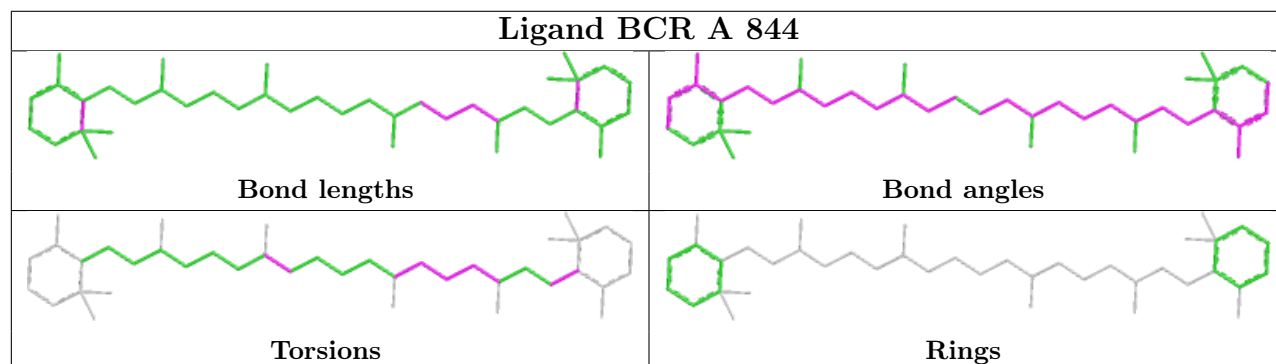


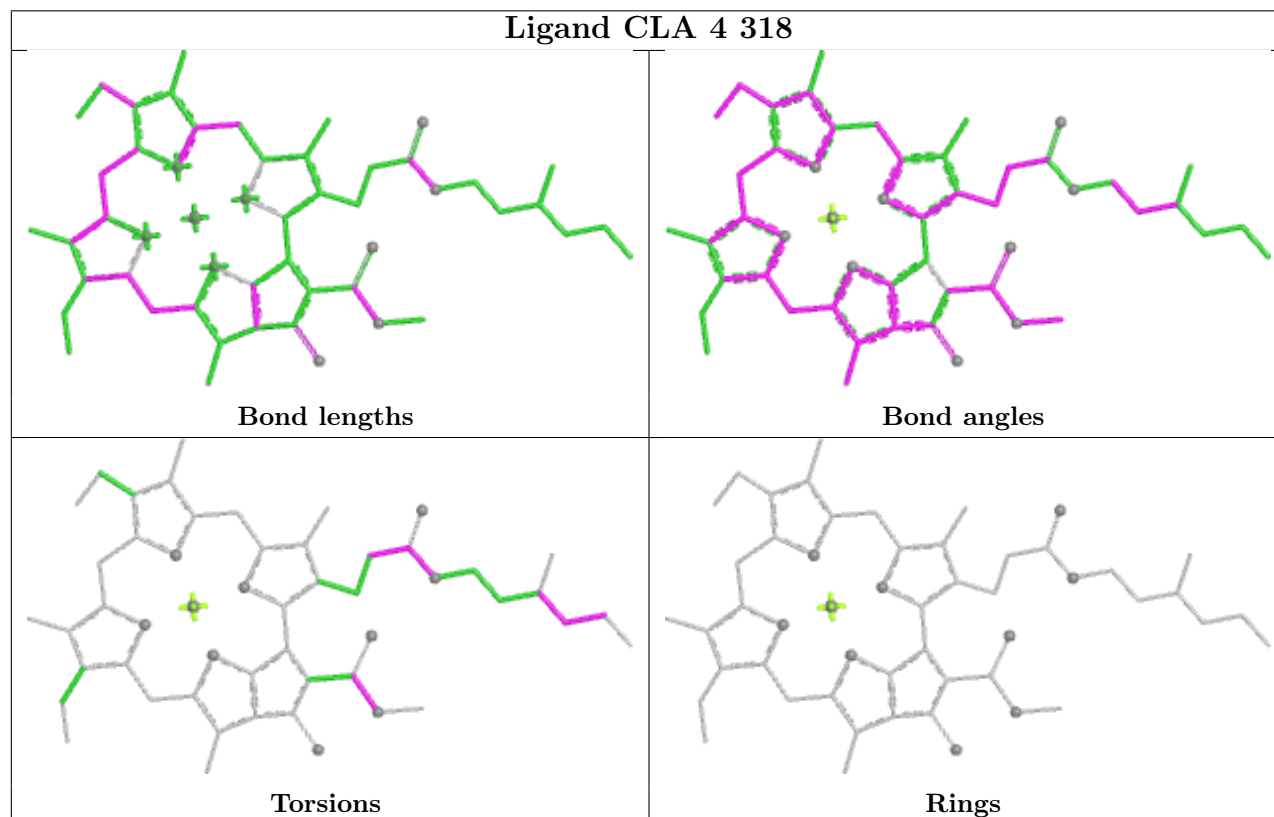
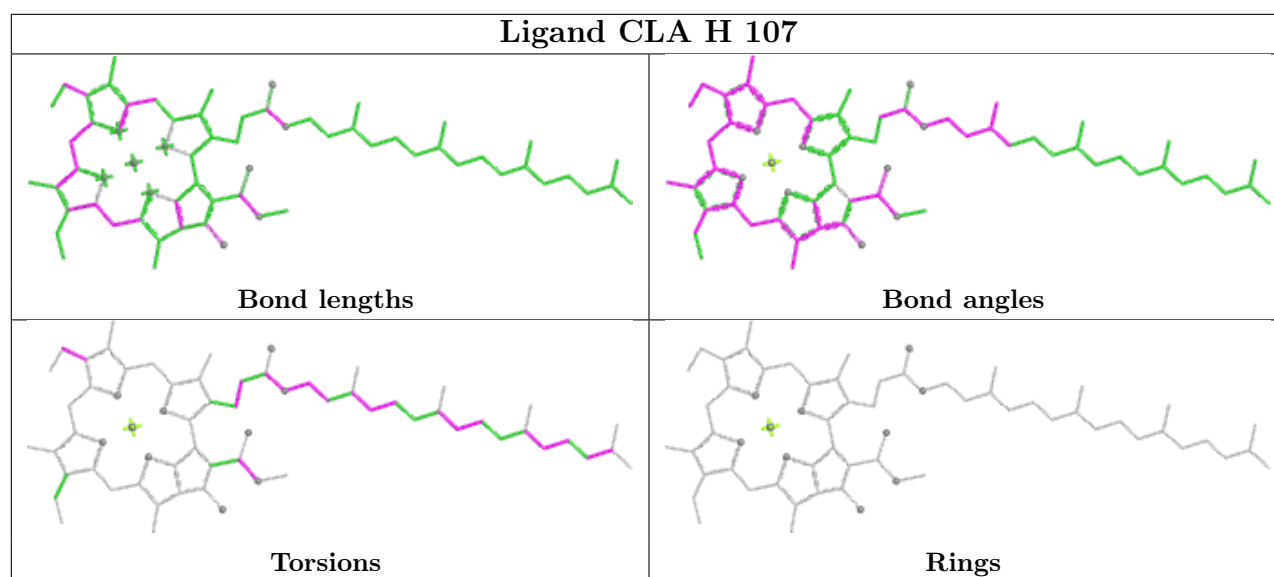


Ligand CLA B 832

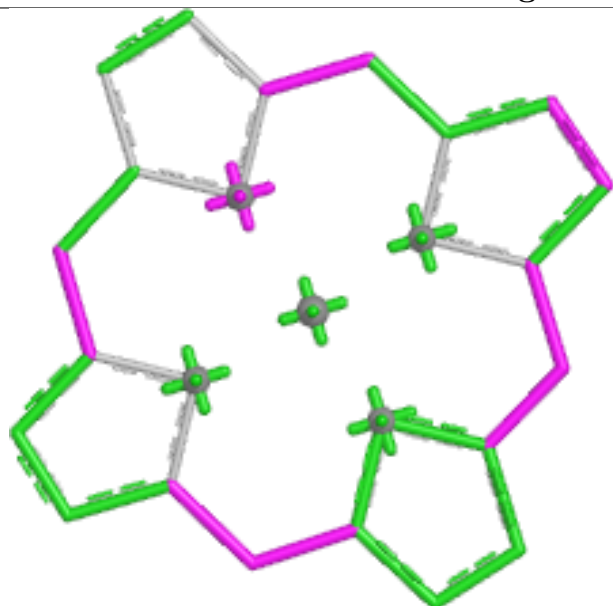


Ligand BCR A 844

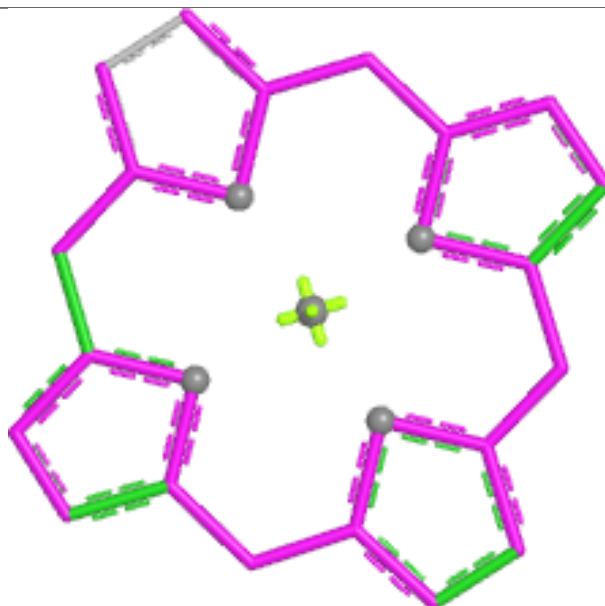




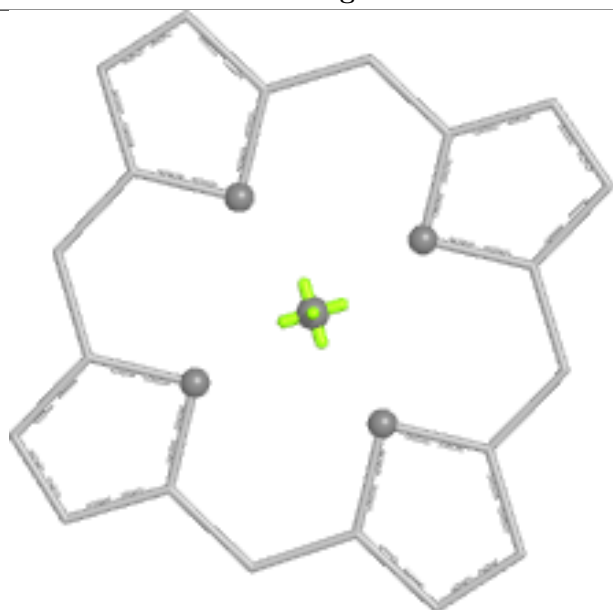
Ligand CLA 4 309



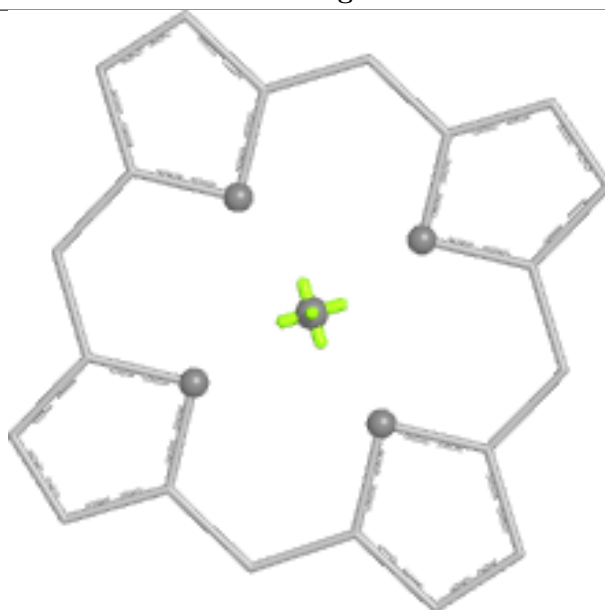
Bond lengths



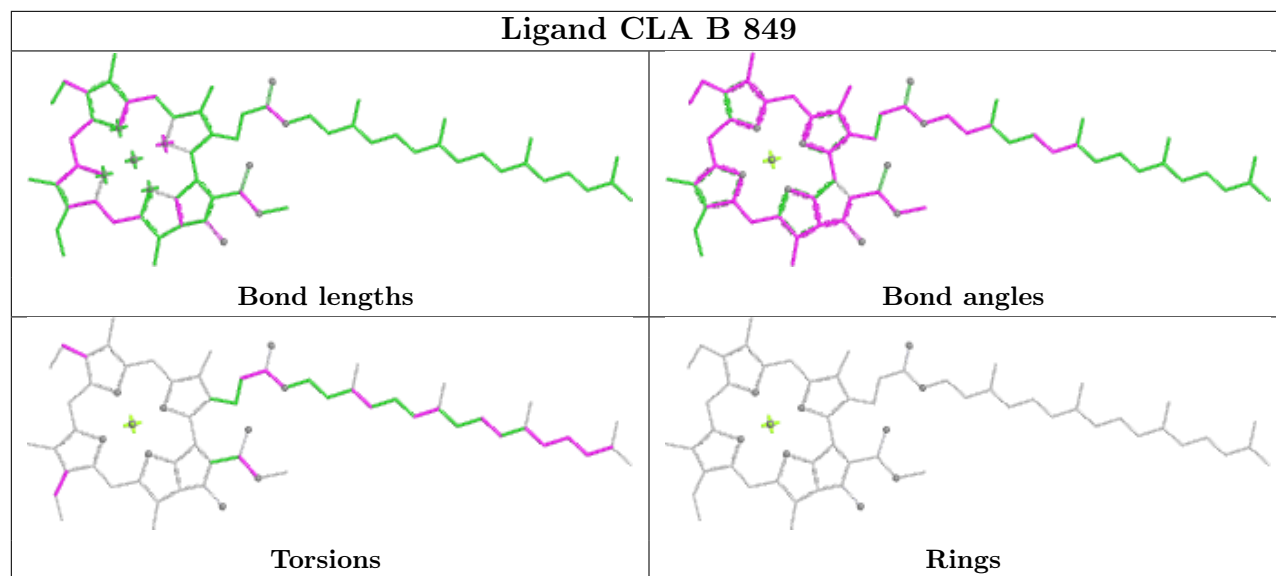
Bond angles



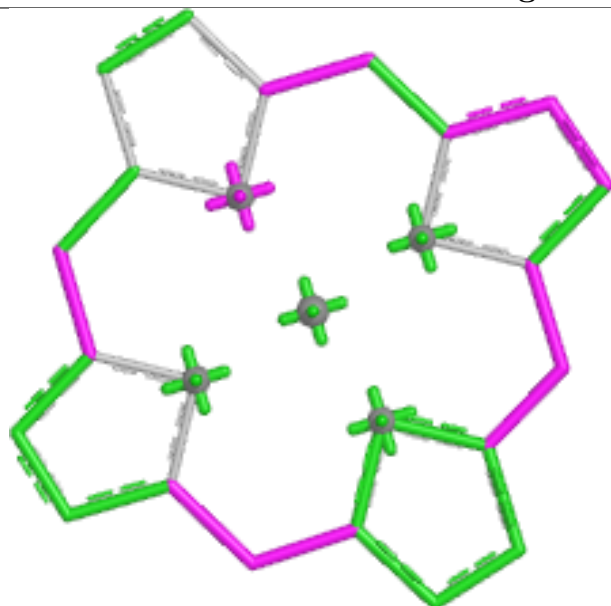
Torsions



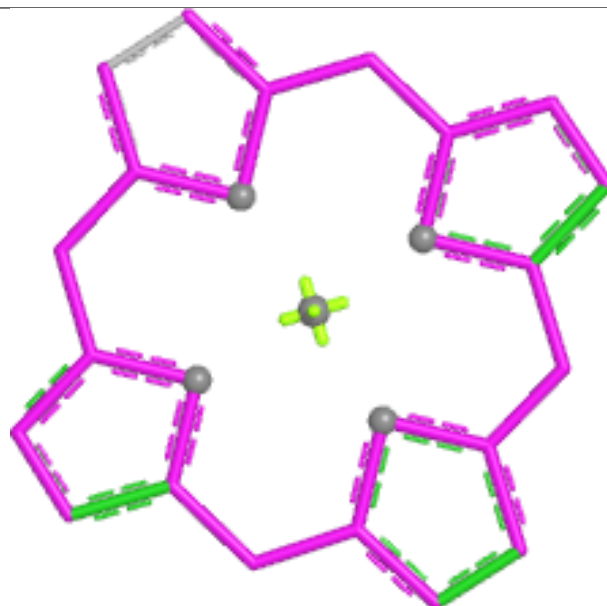
Rings



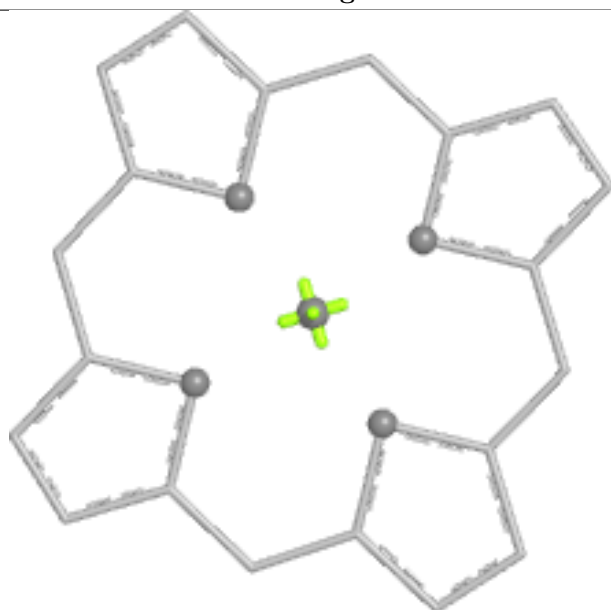
Ligand CLA 3 313



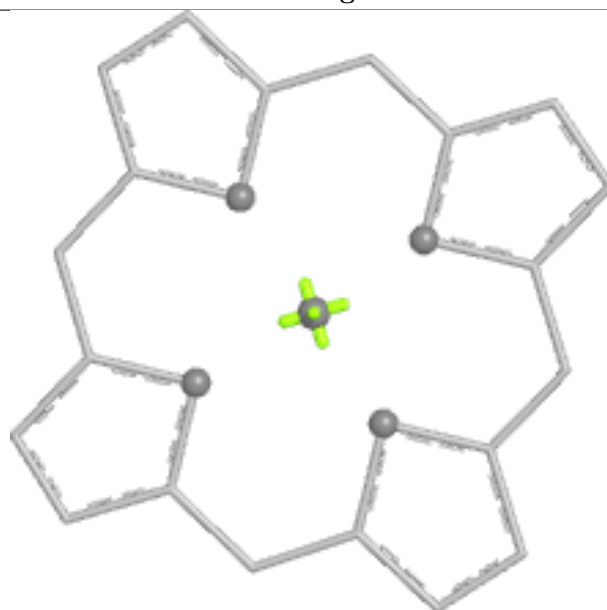
Bond lengths



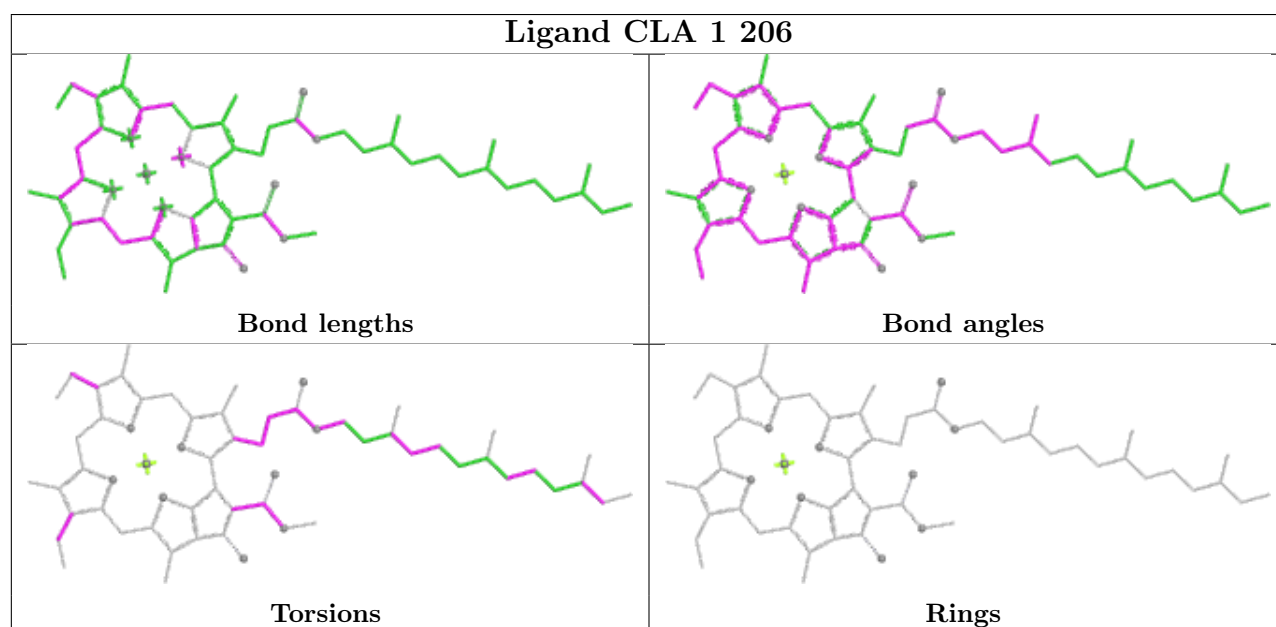
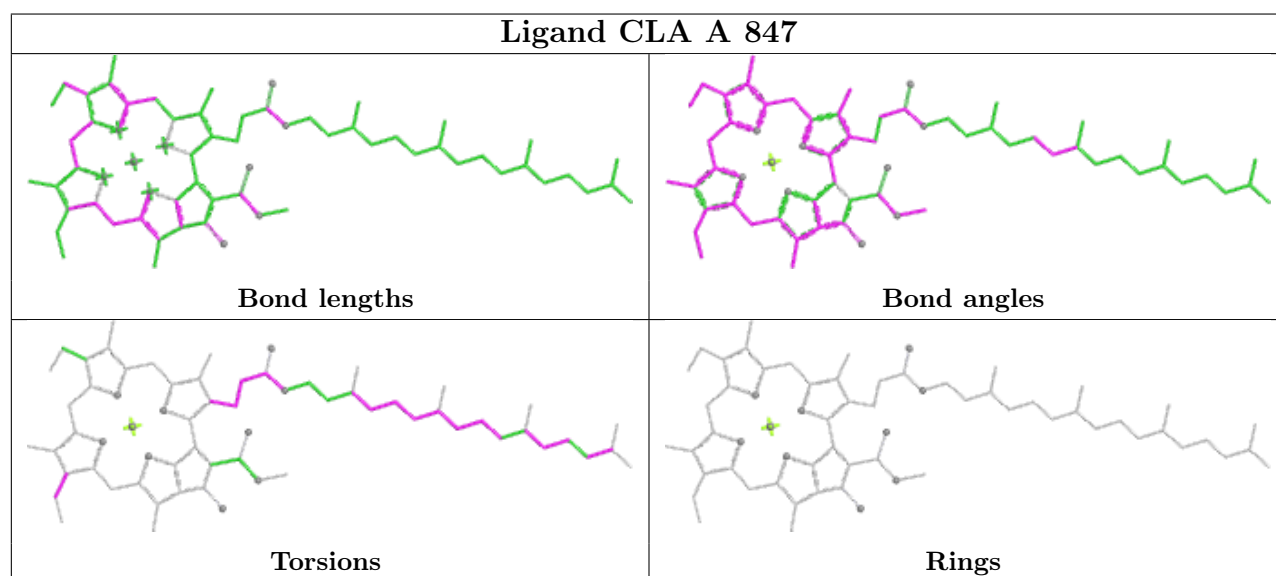
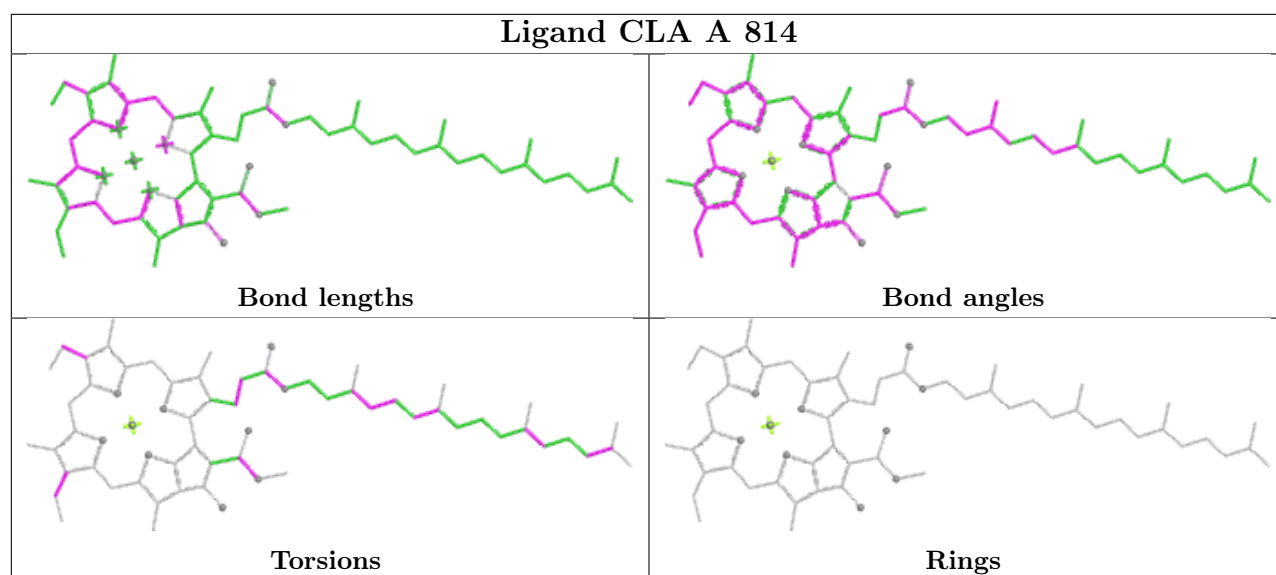
Bond angles

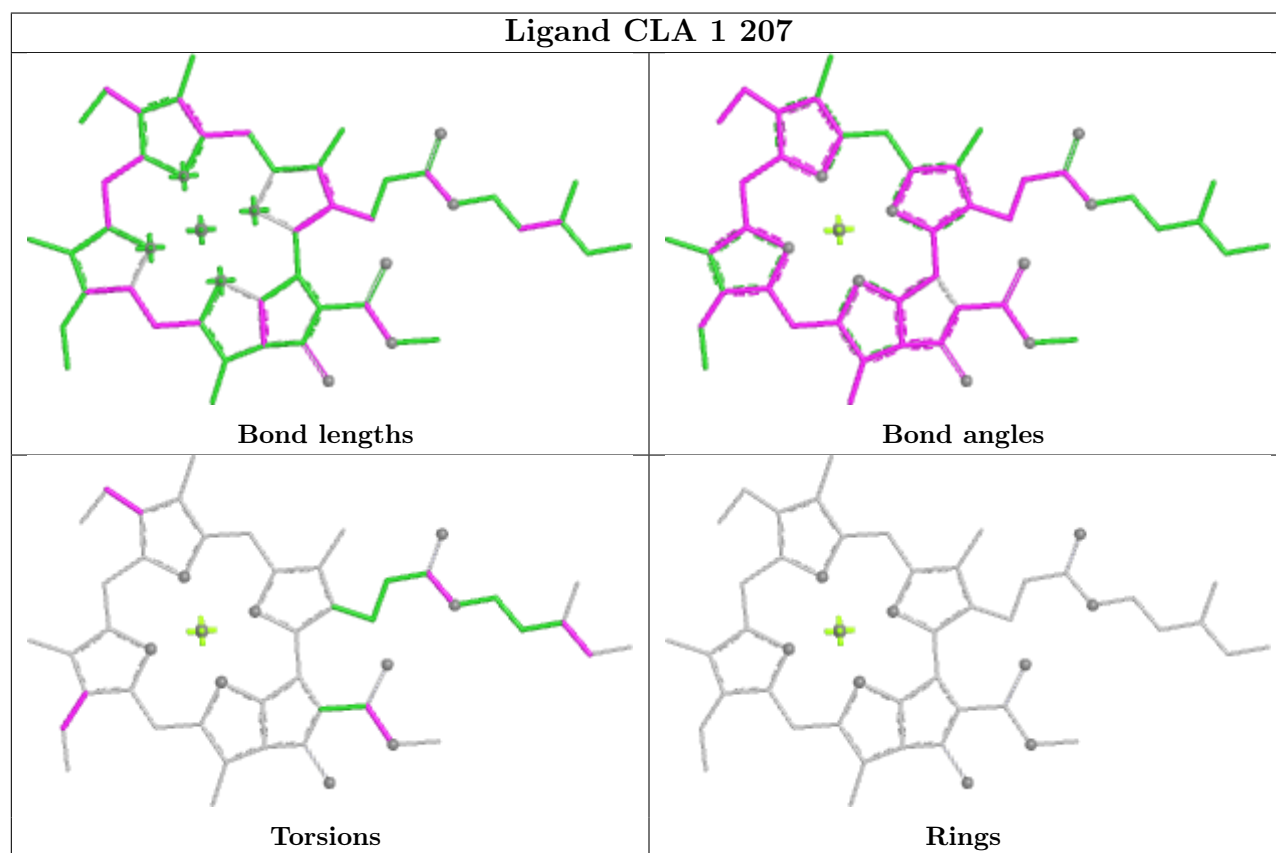
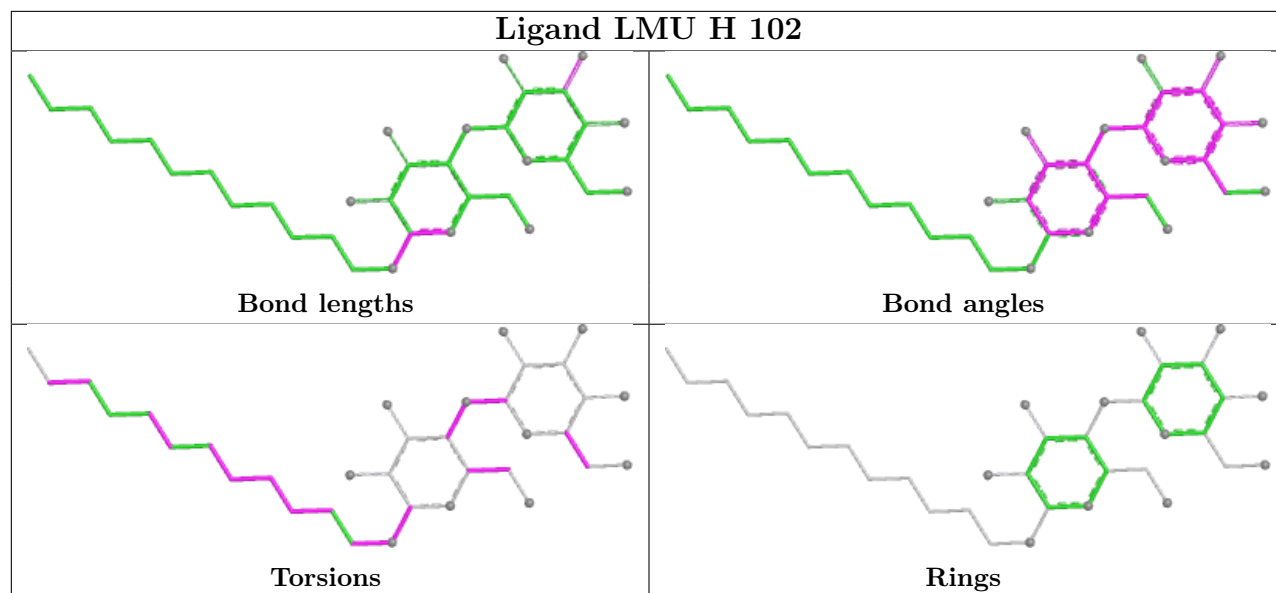


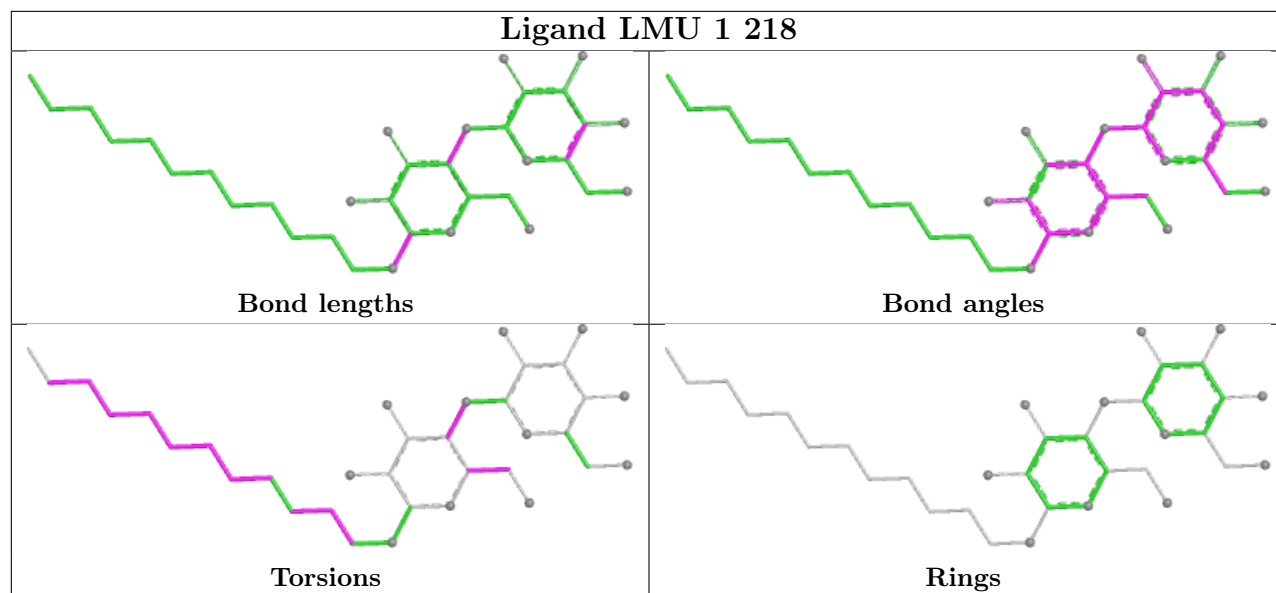
Torsions



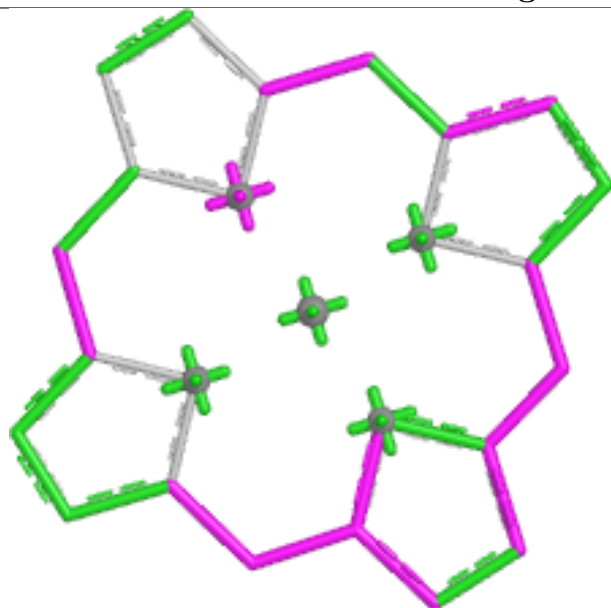
Rings



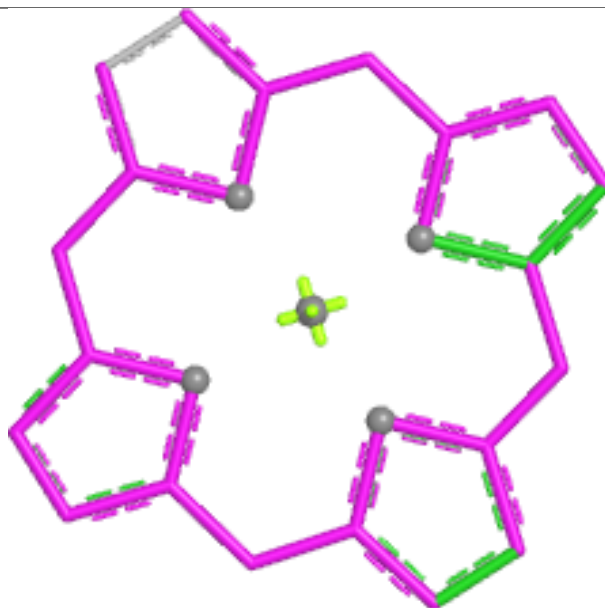




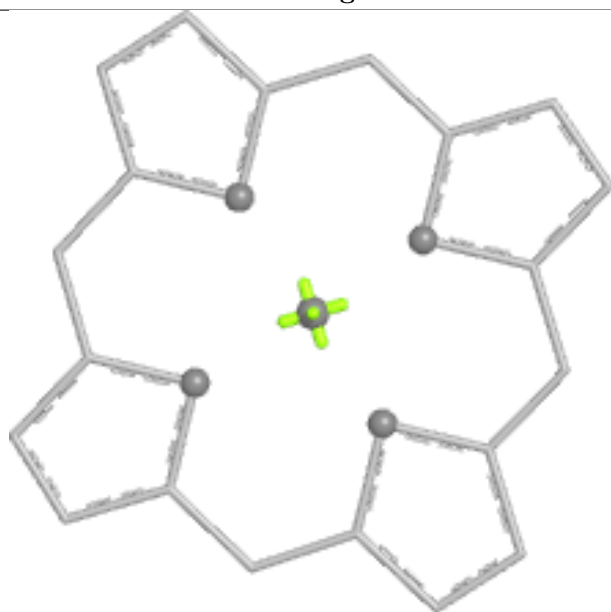
Ligand CLA 3 304



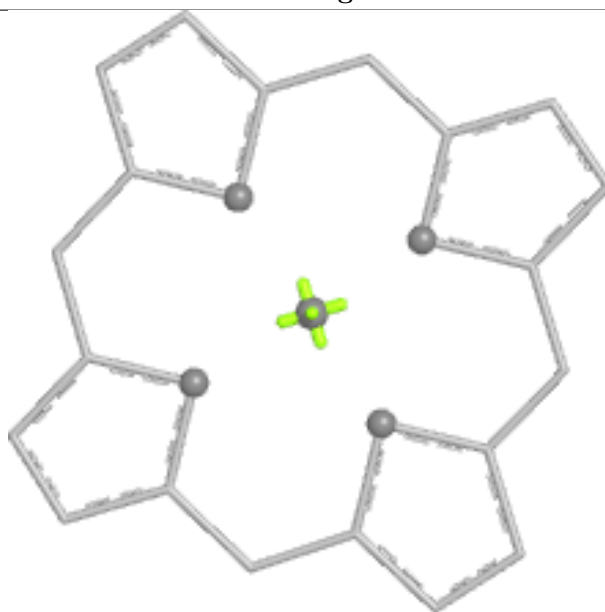
Bond lengths



Bond angles

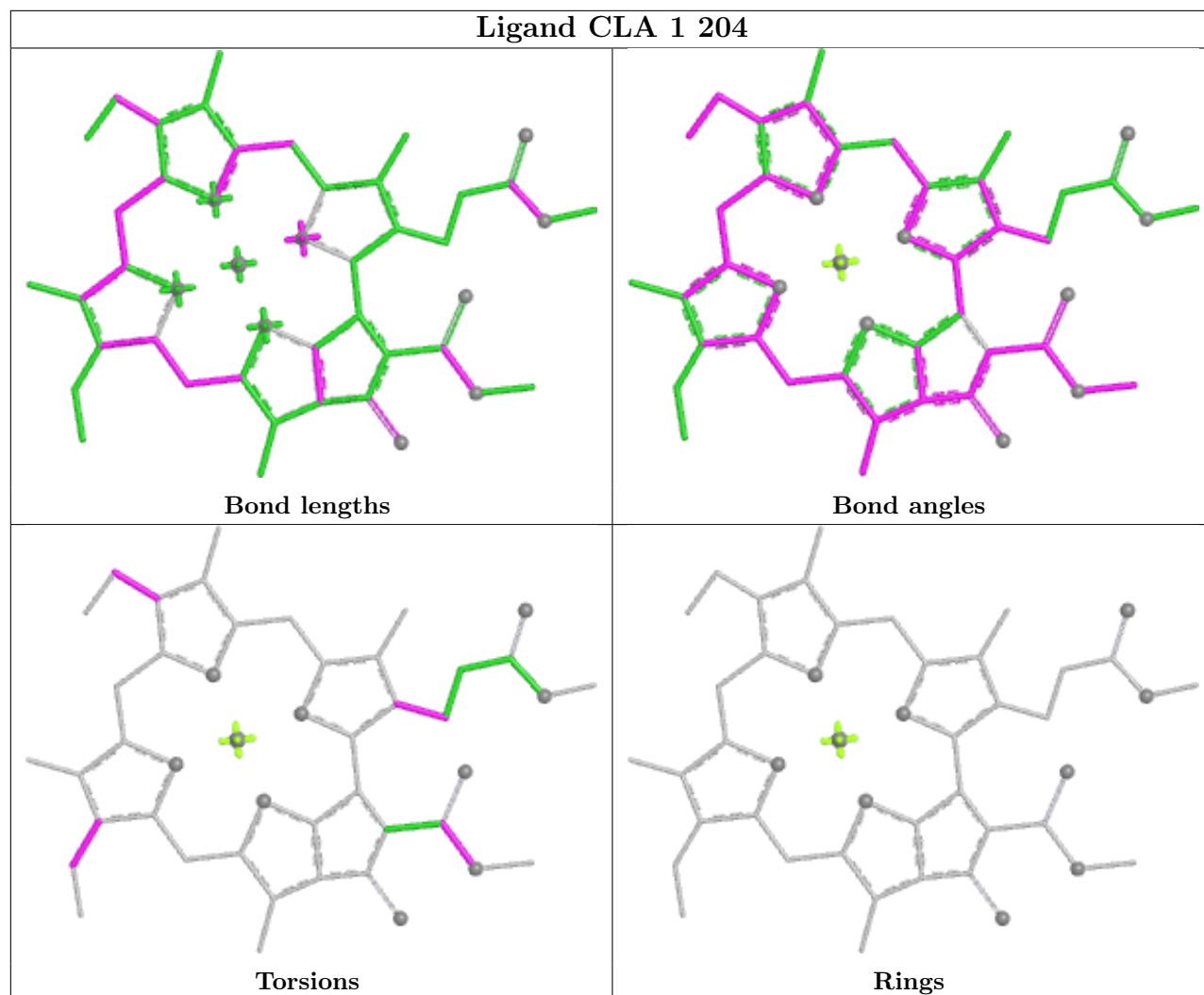


Torsions

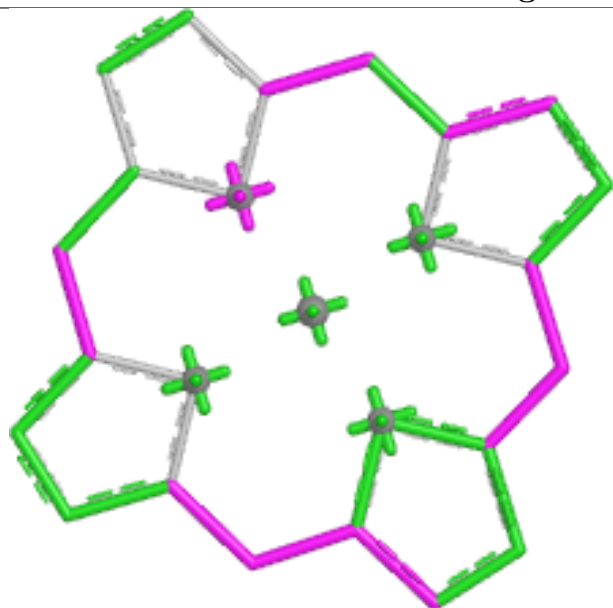


Rings

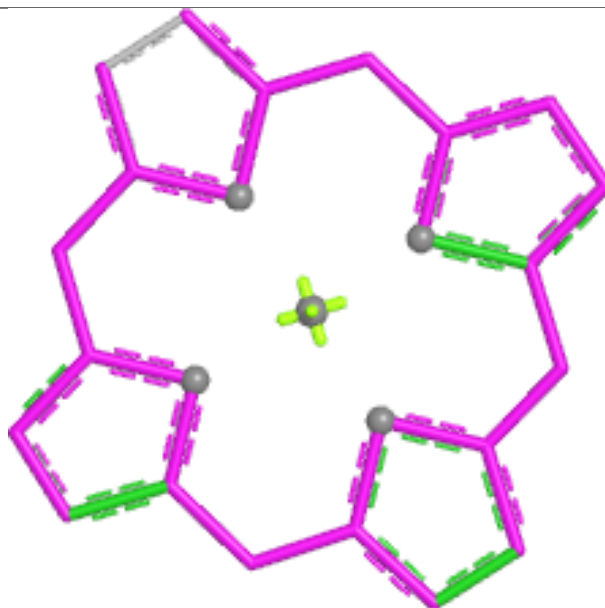
Ligand CLA 1 204



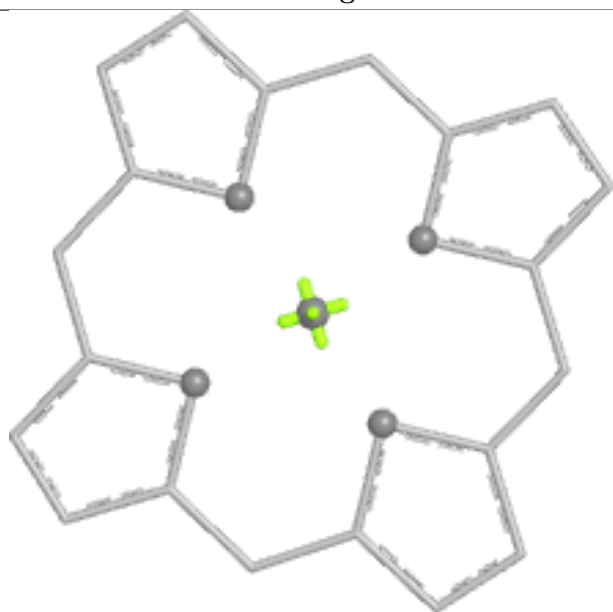
Ligand CLA 3 316



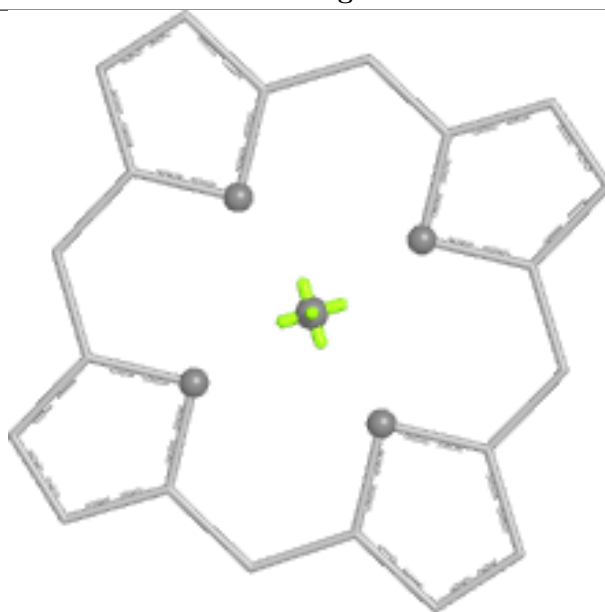
Bond lengths



Bond angles

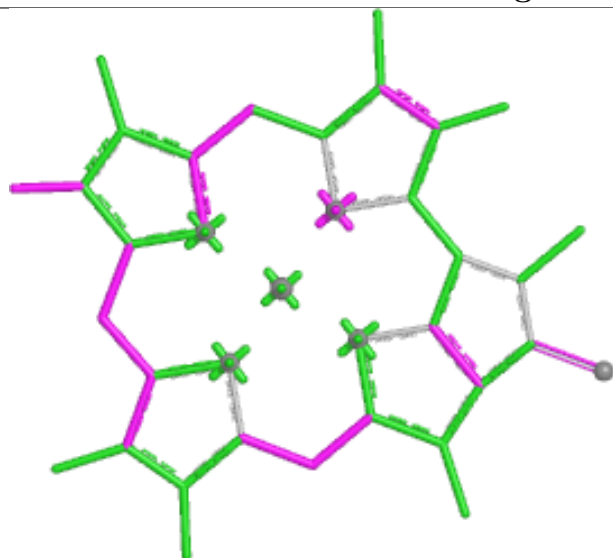


Torsions

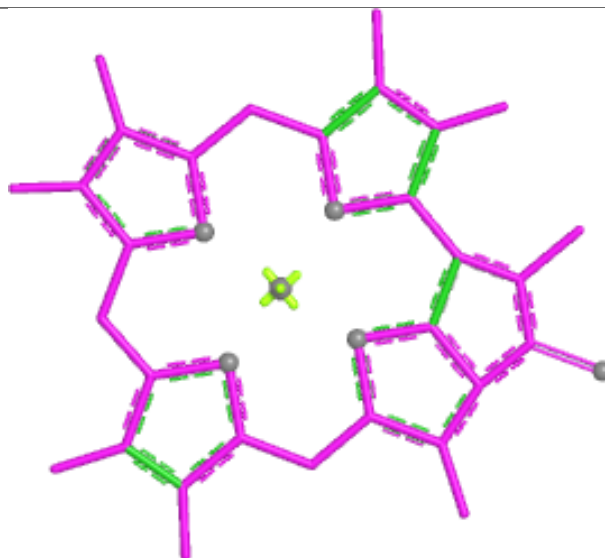


Rings

Ligand CLA B 839



Bond lengths



Bond angles

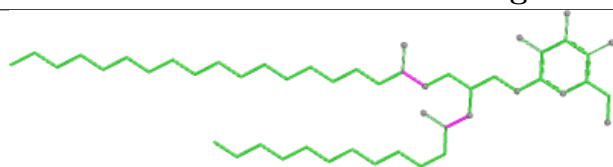


Torsions

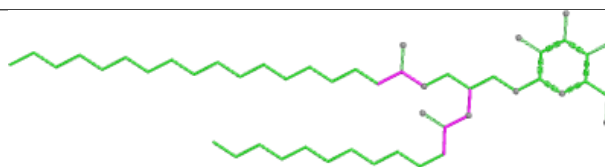


Rings

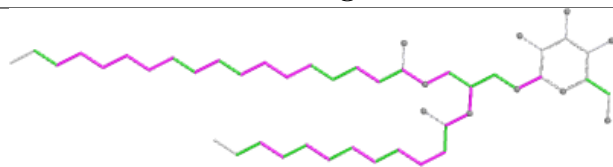
Ligand LMG B 846



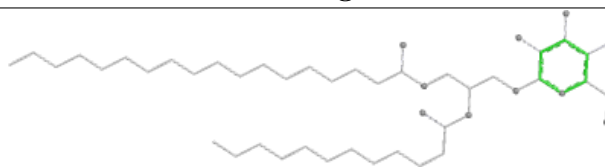
Bond lengths



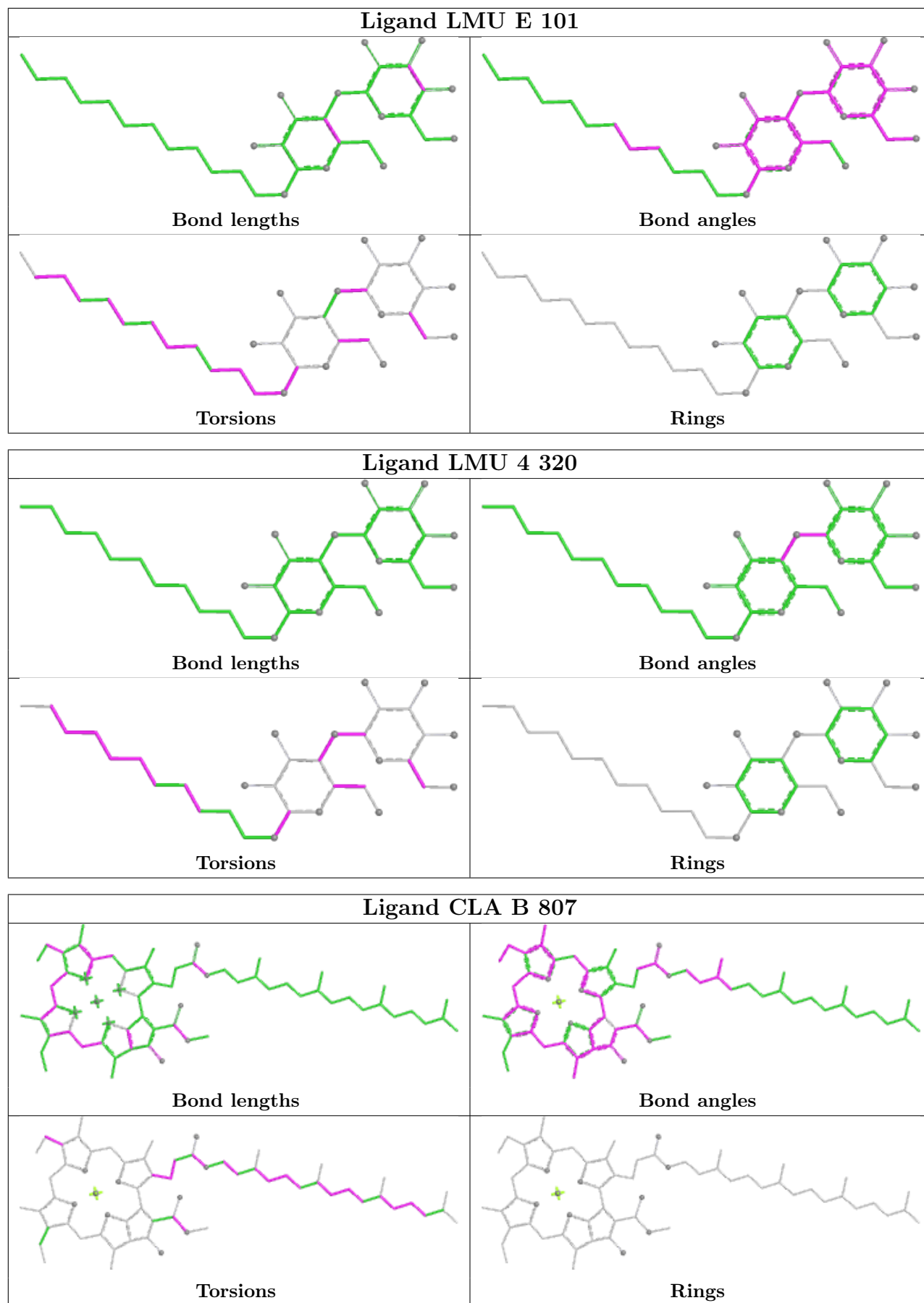
Bond angles

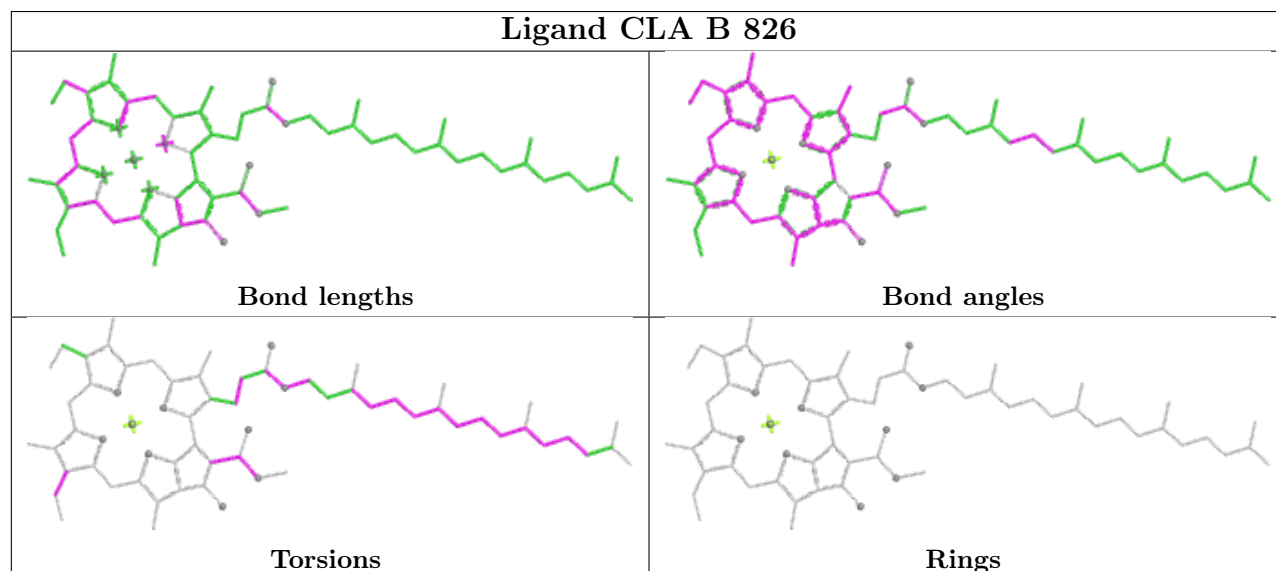
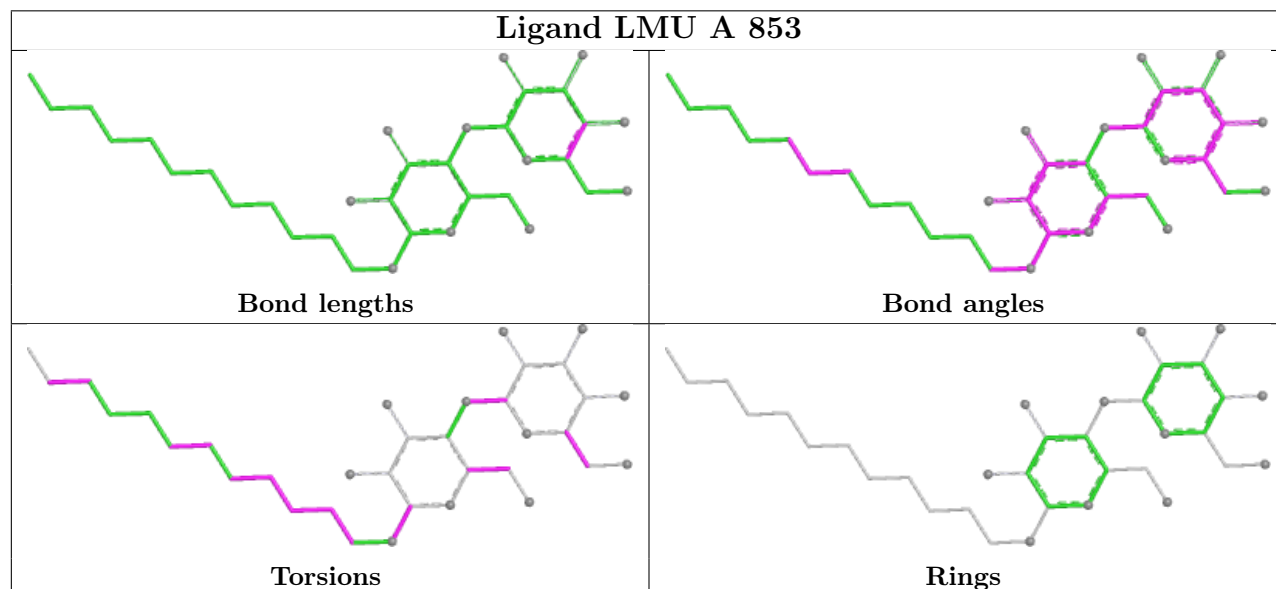
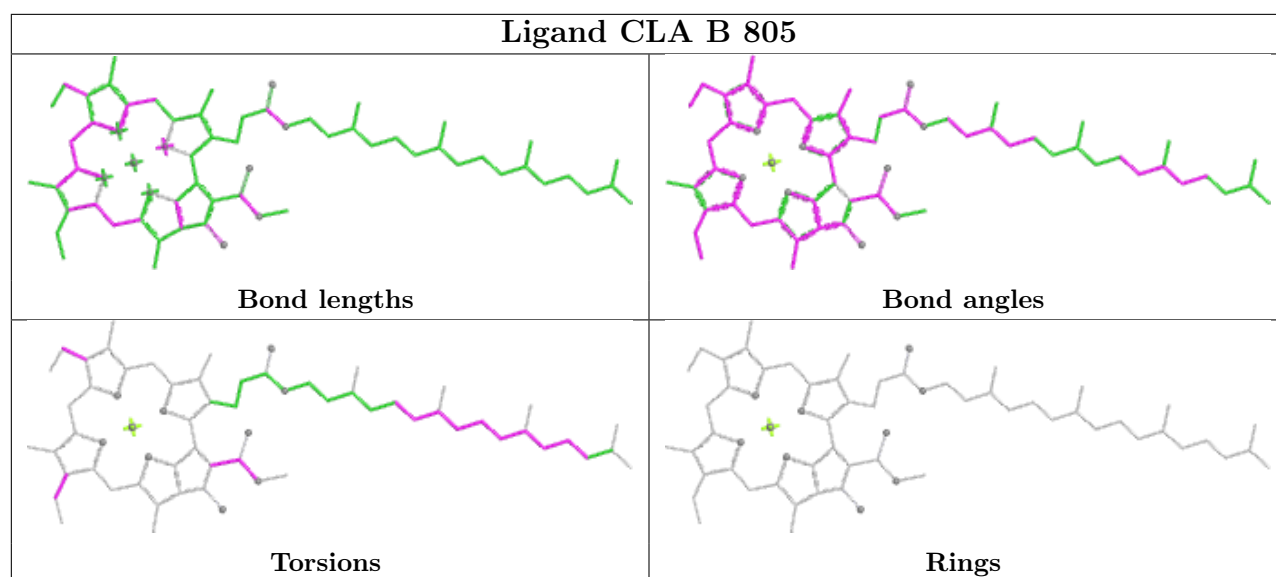


Torsions

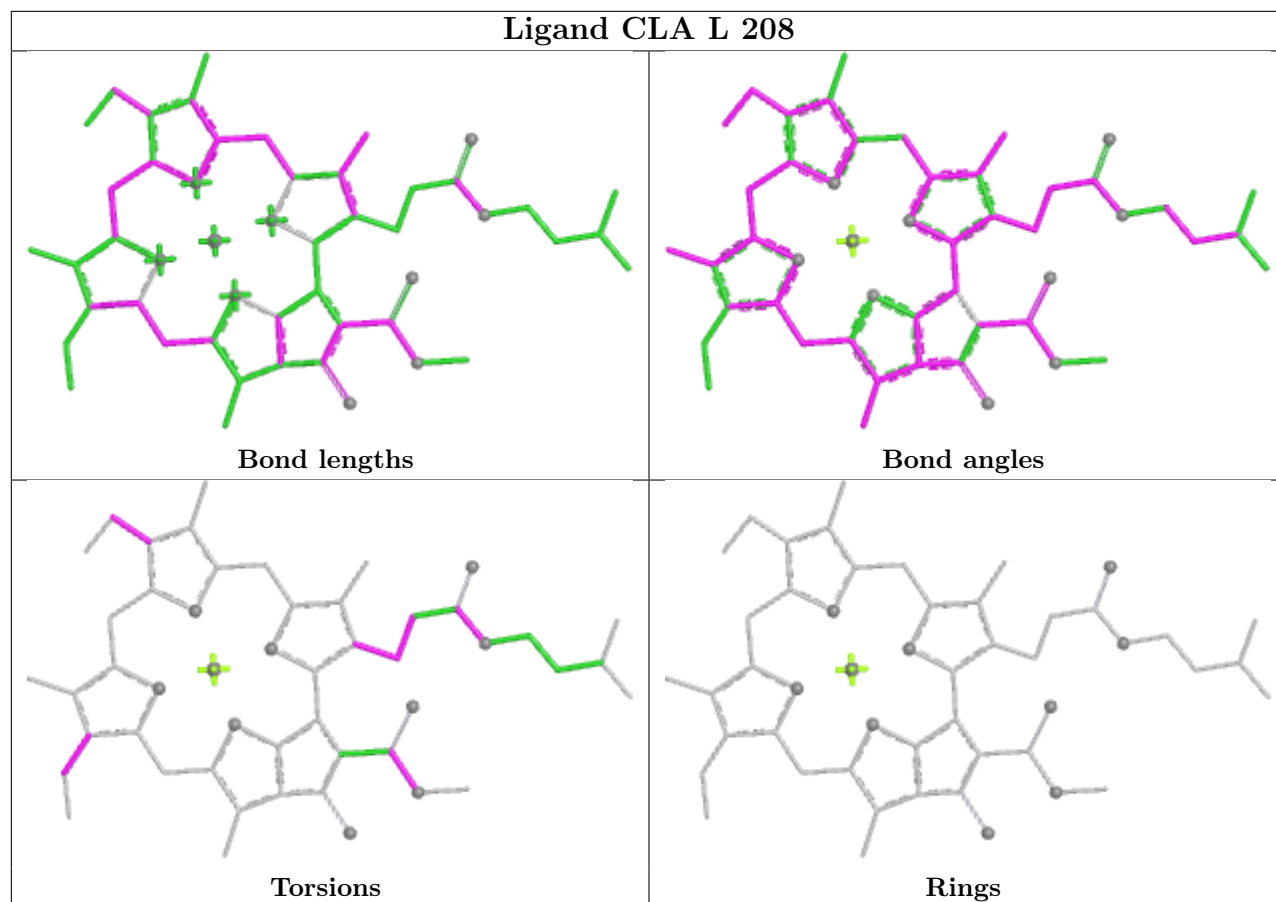


Rings

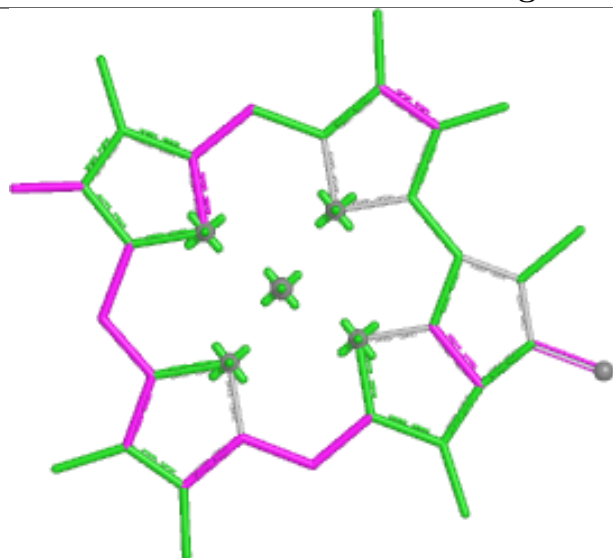




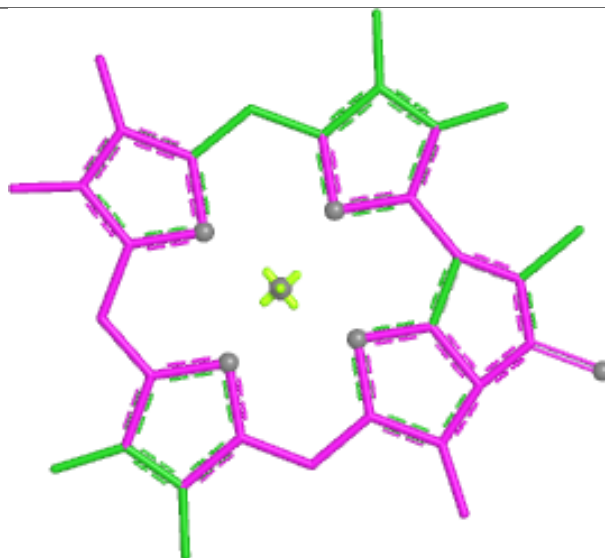
Ligand CLA L 208



Ligand CLA 1 210



Bond lengths



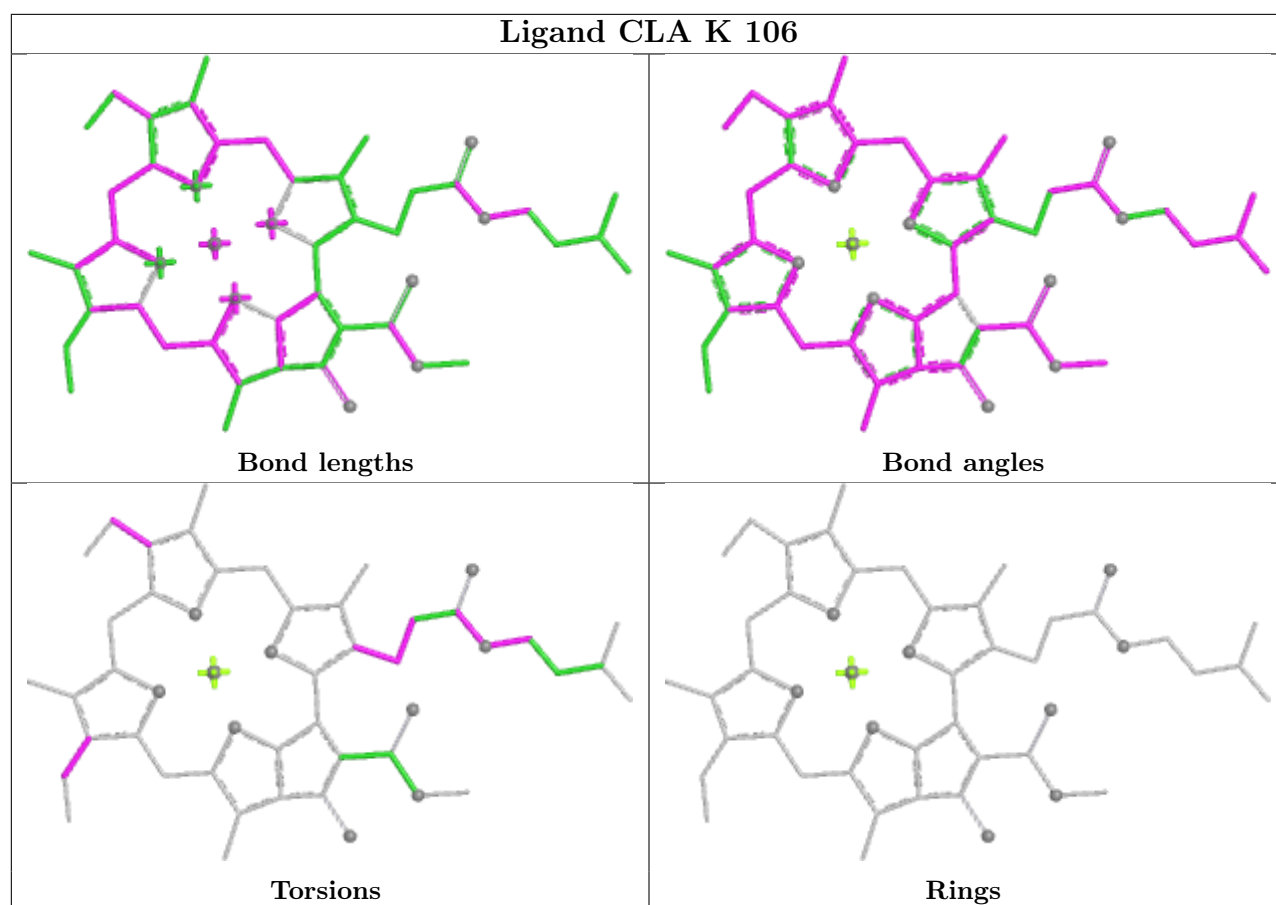
Bond angles



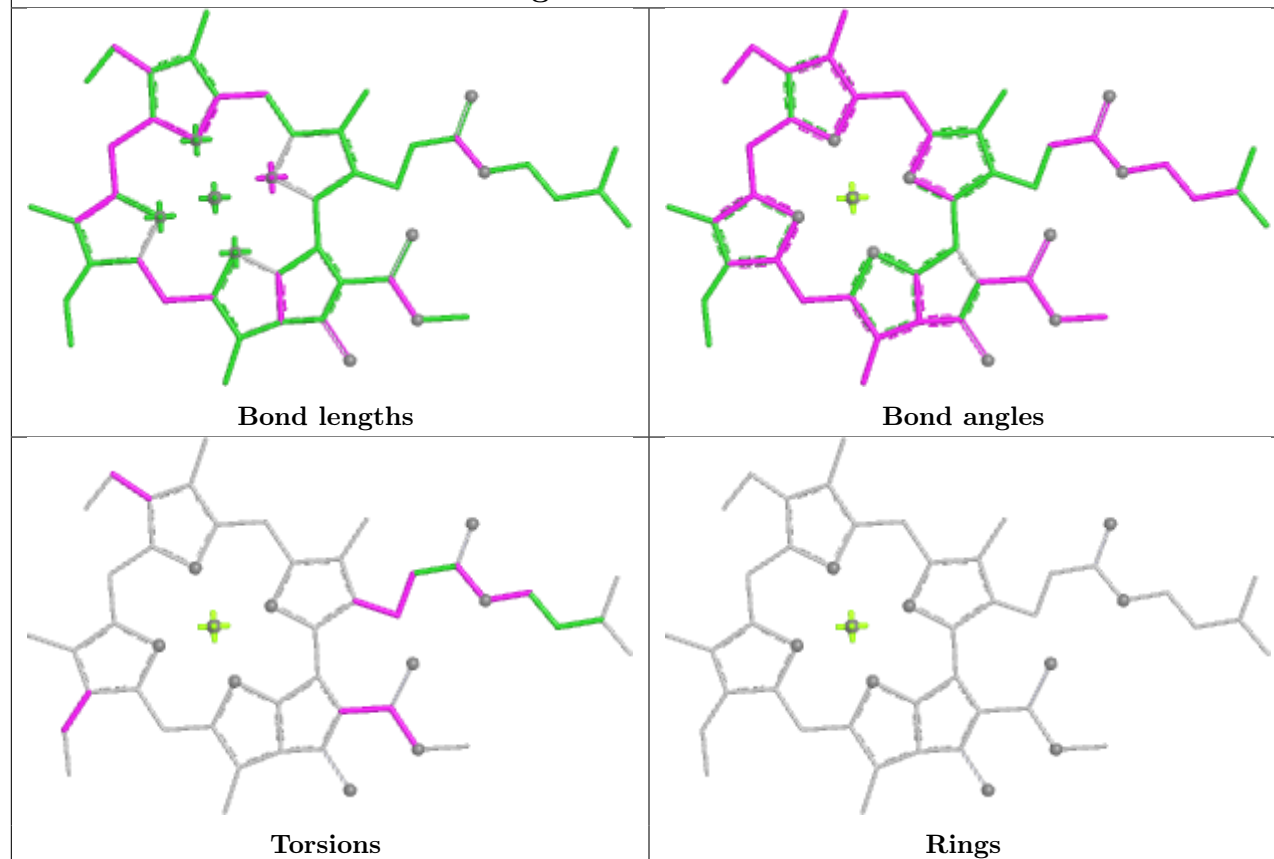
Torsions



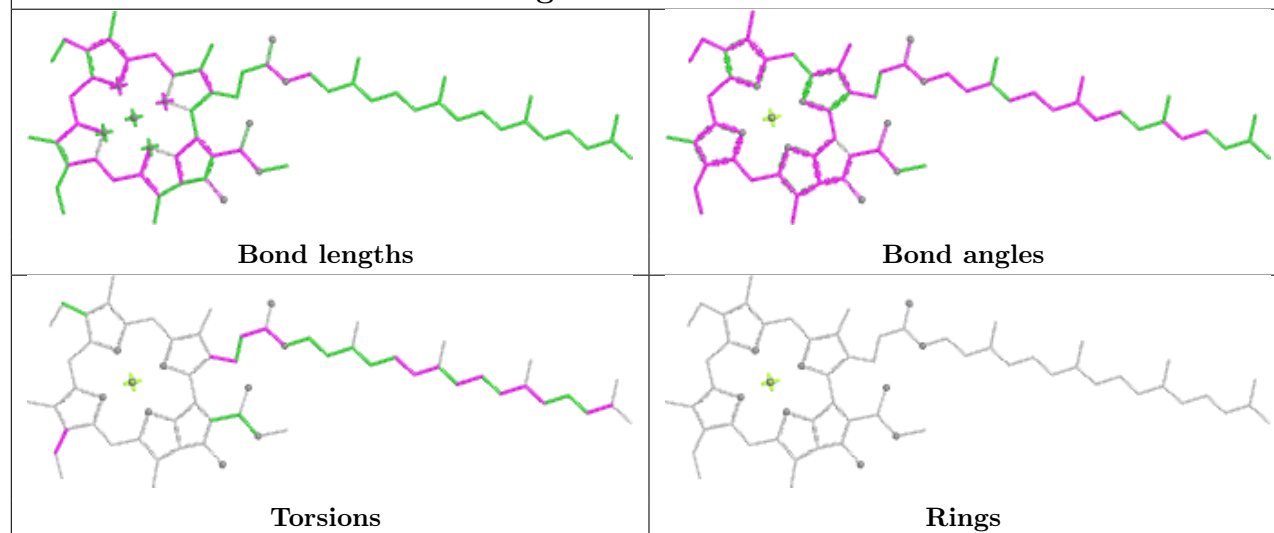
Rings

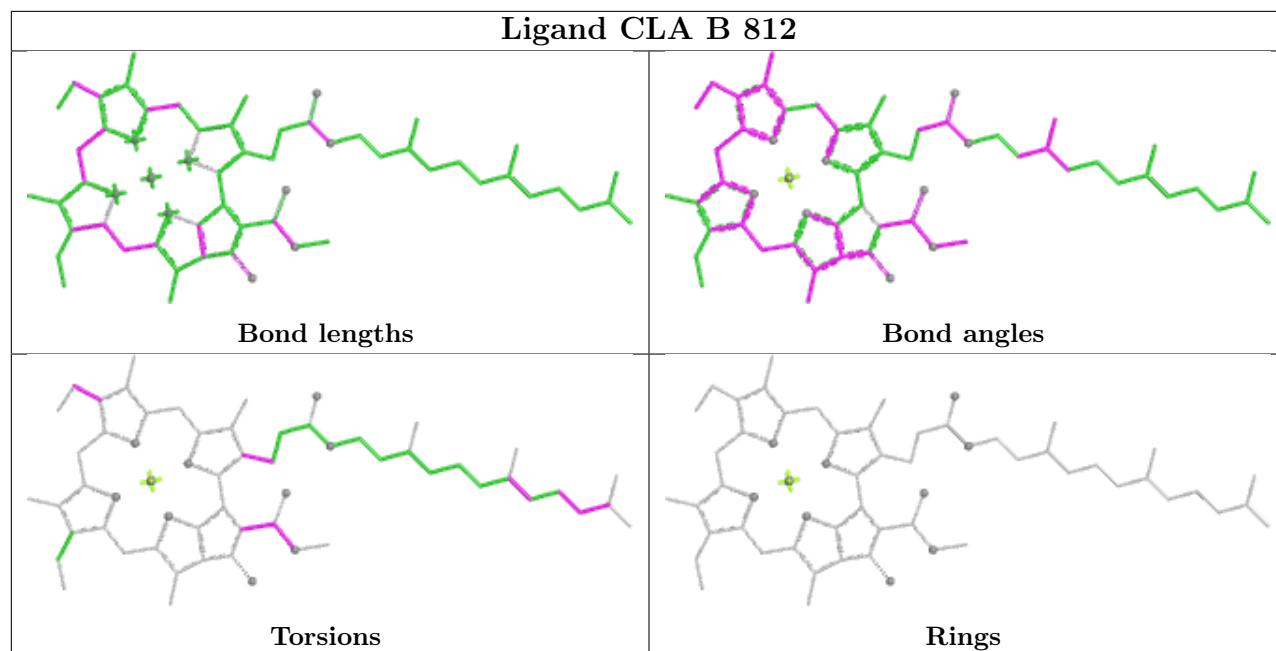


Ligand CLA A 830

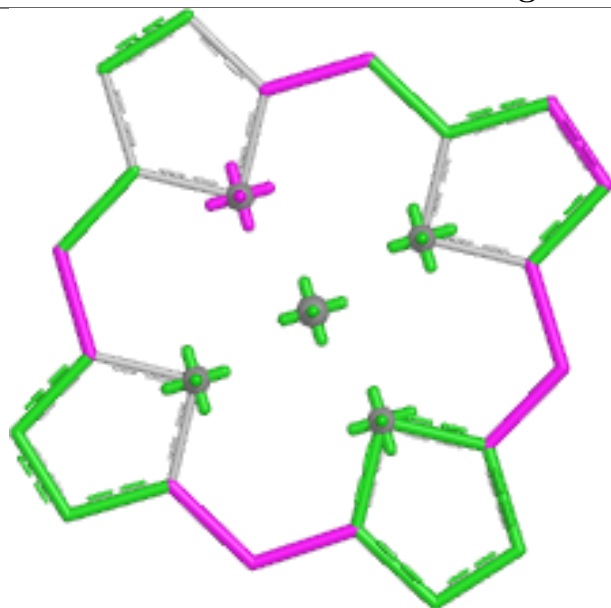


Ligand CLA 4 304

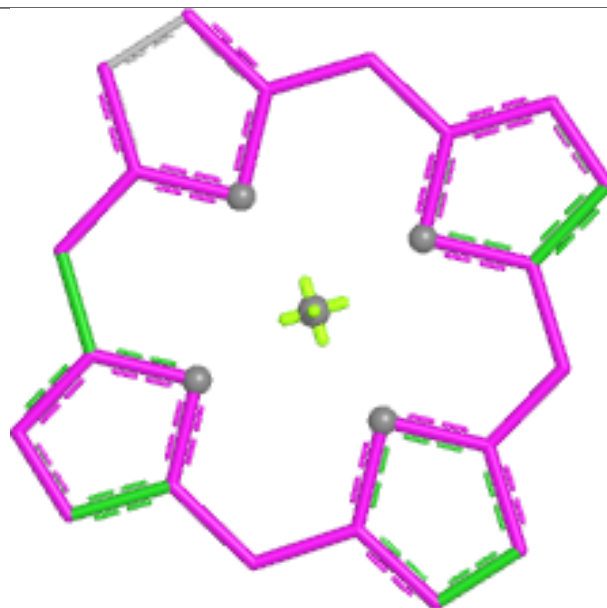




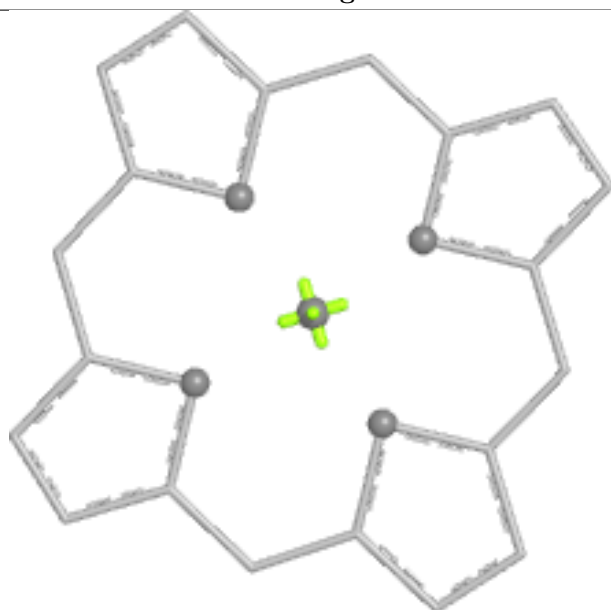
Ligand CLA 4 308



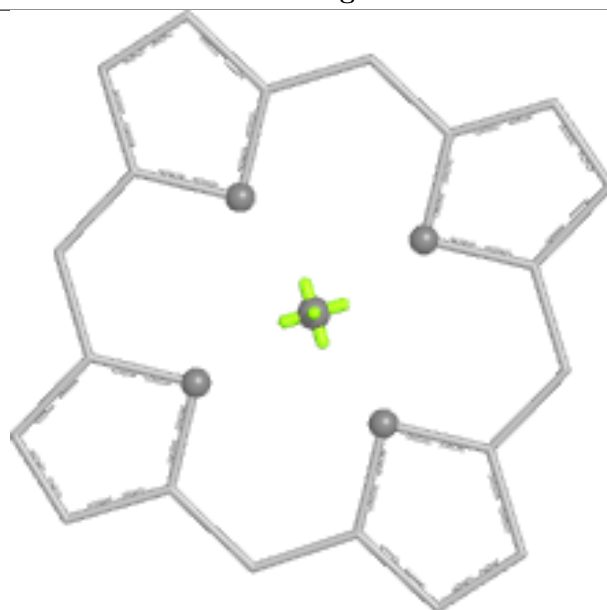
Bond lengths



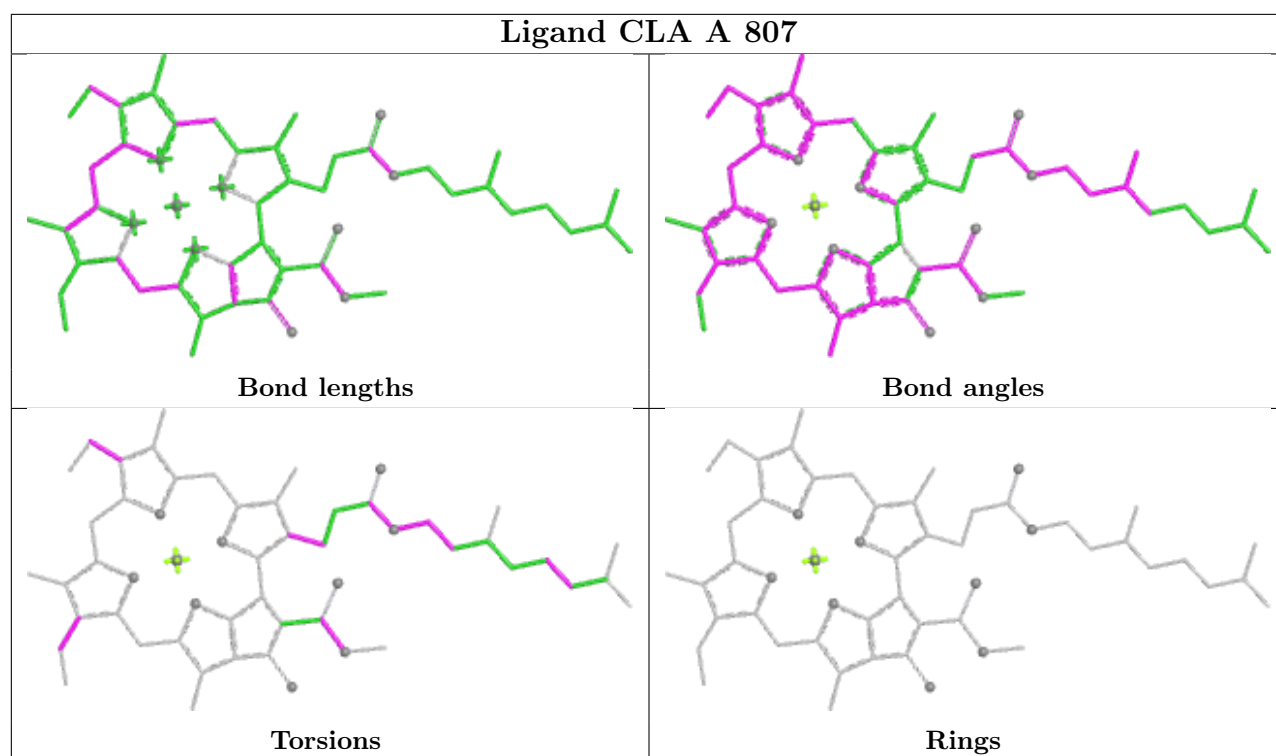
Bond angles



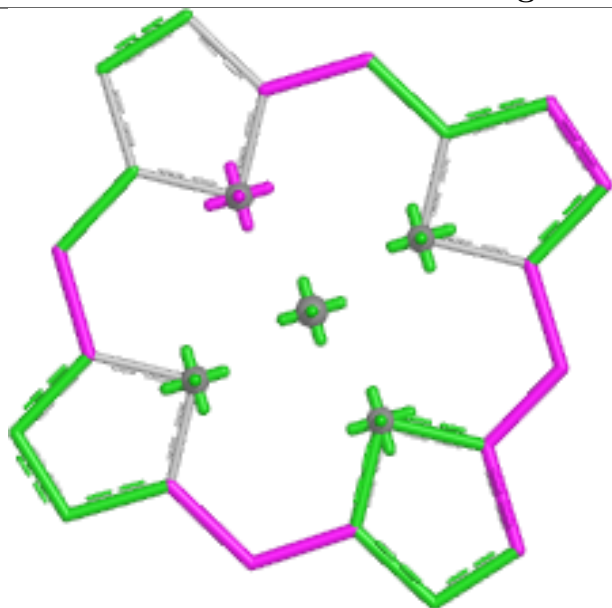
Torsions



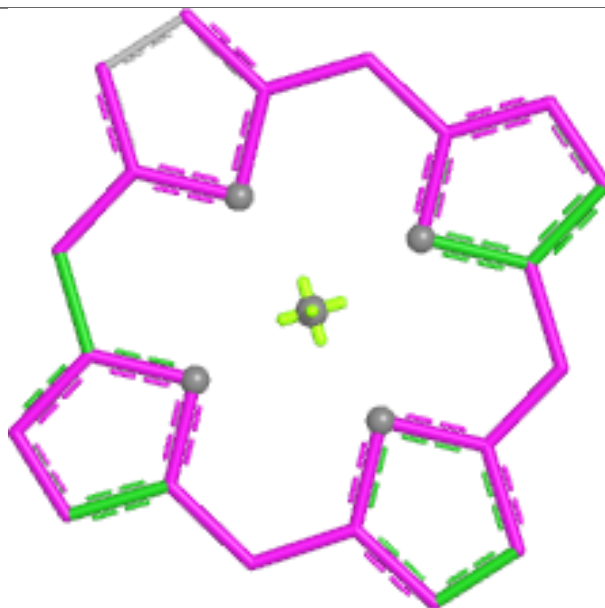
Rings



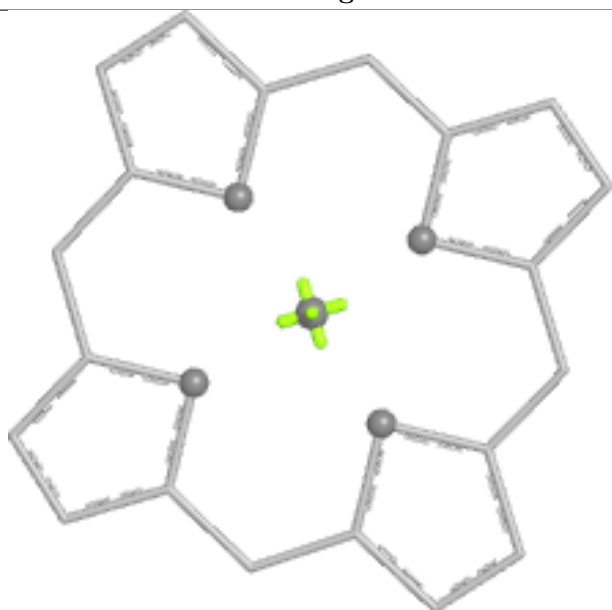
Ligand CLA 3 305



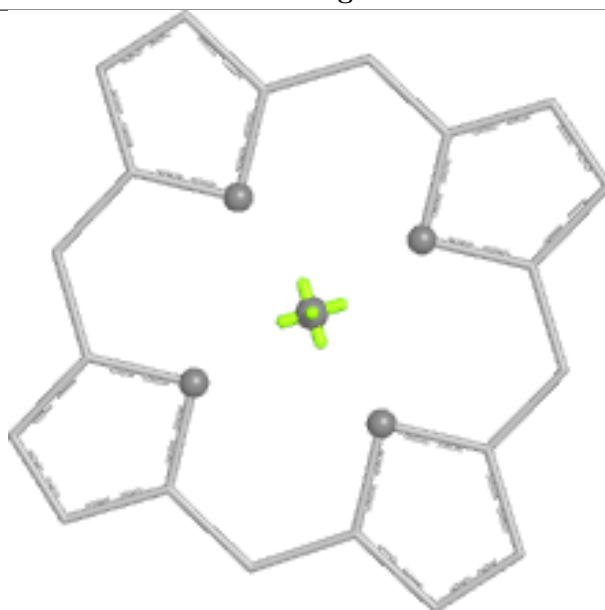
Bond lengths



Bond angles

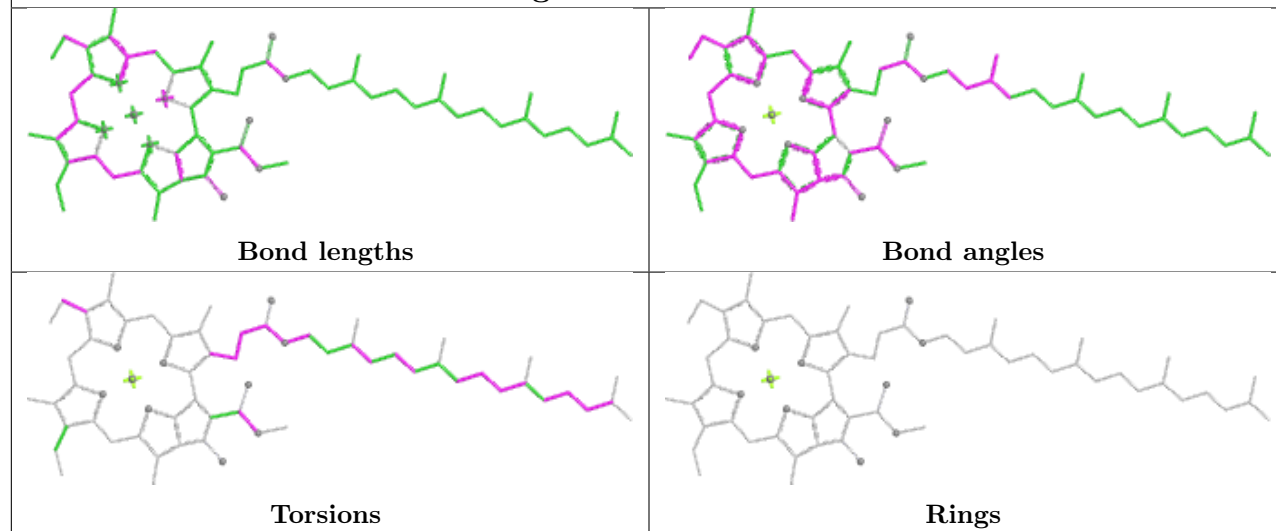


Torsions

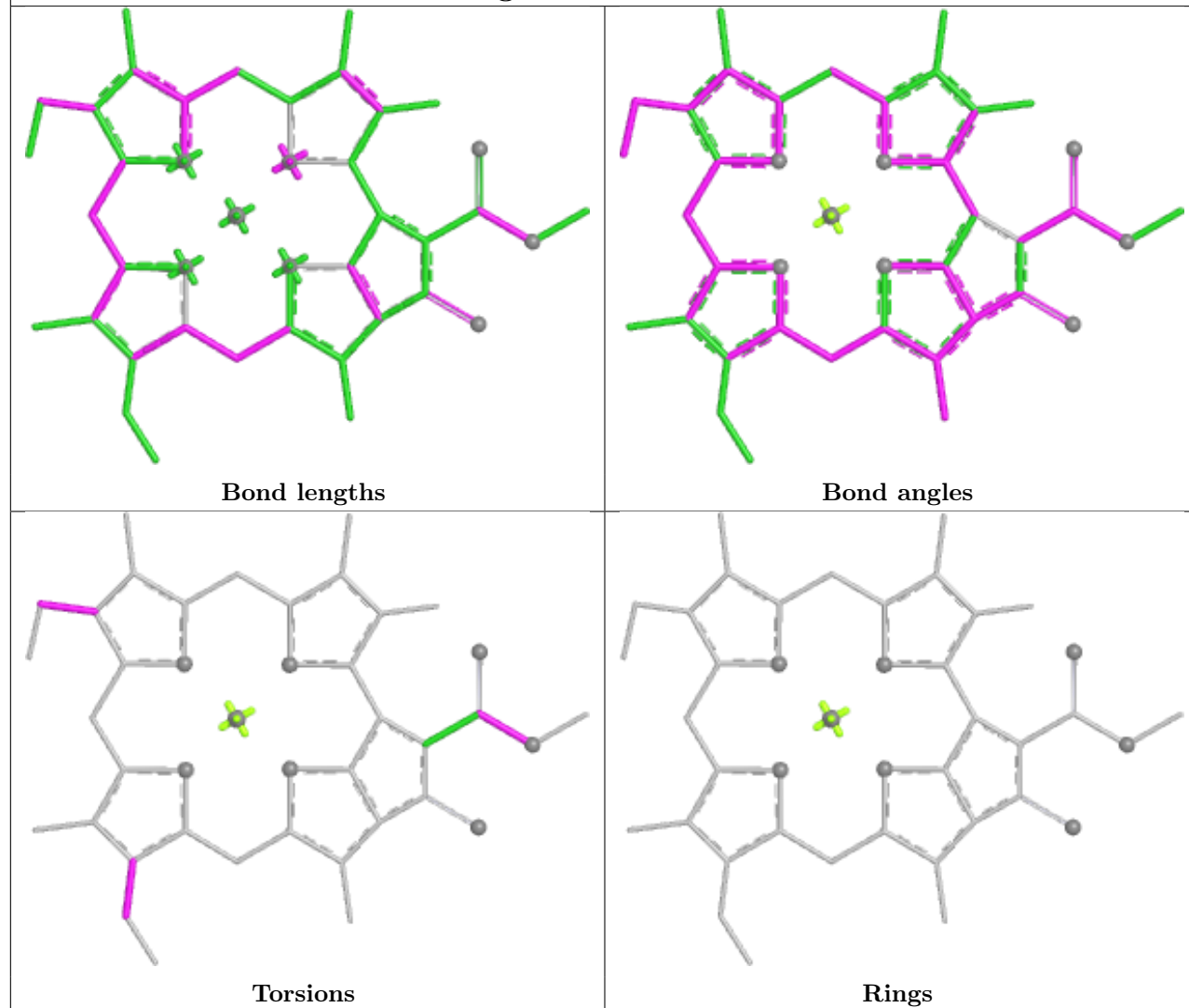


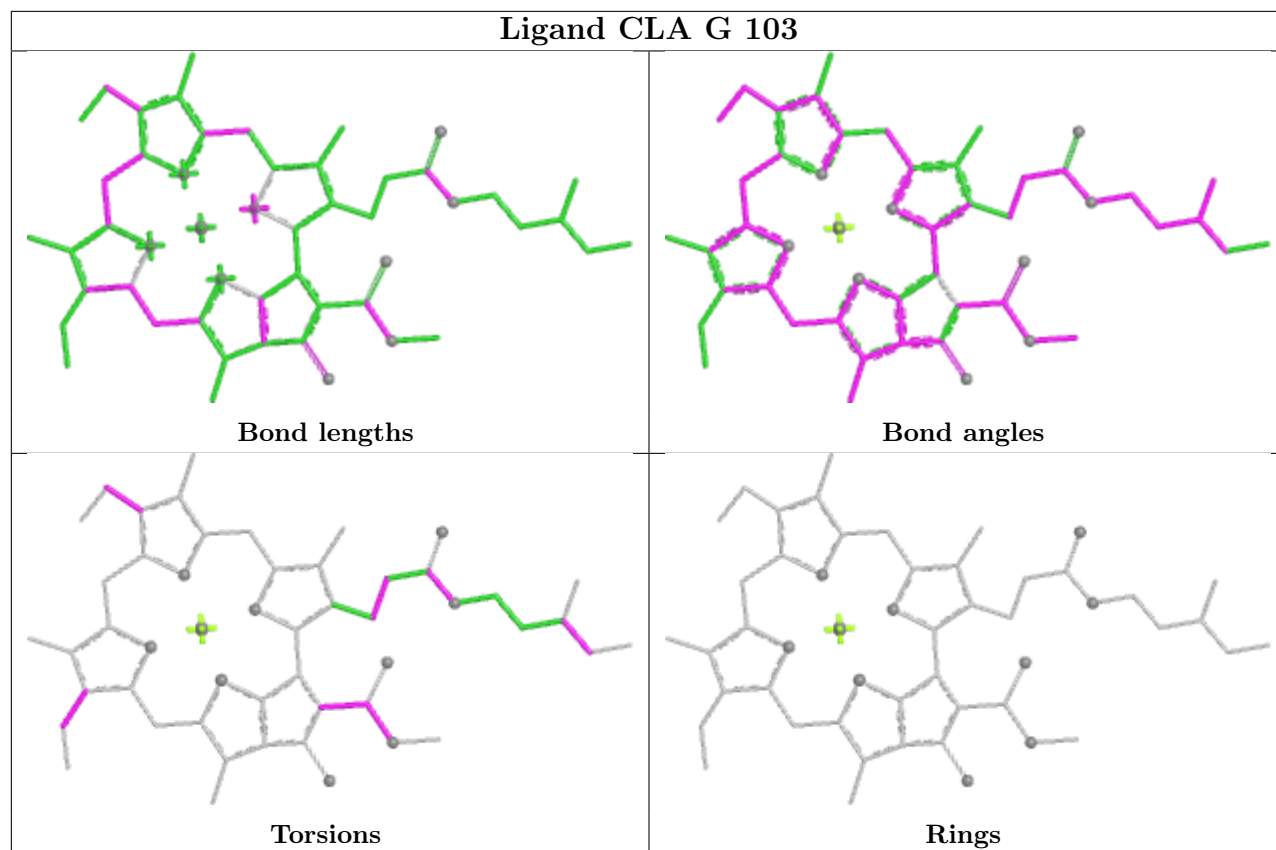
Rings

Ligand CLA B 823

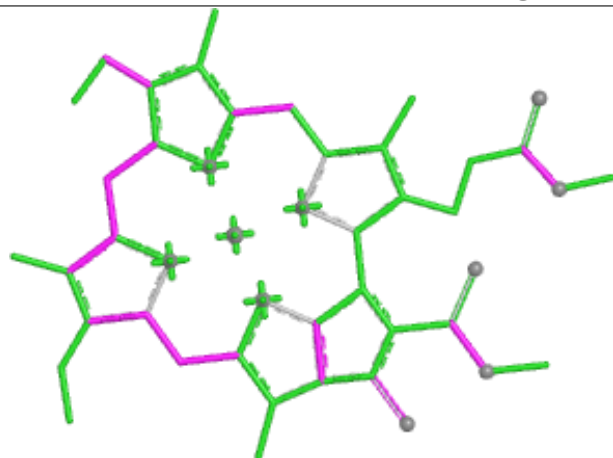


Ligand CLA F 205

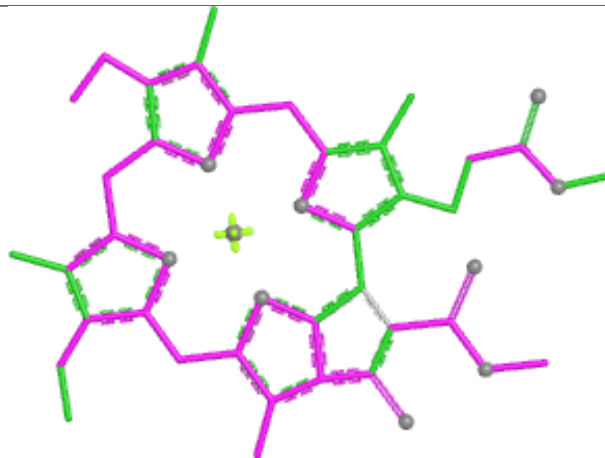




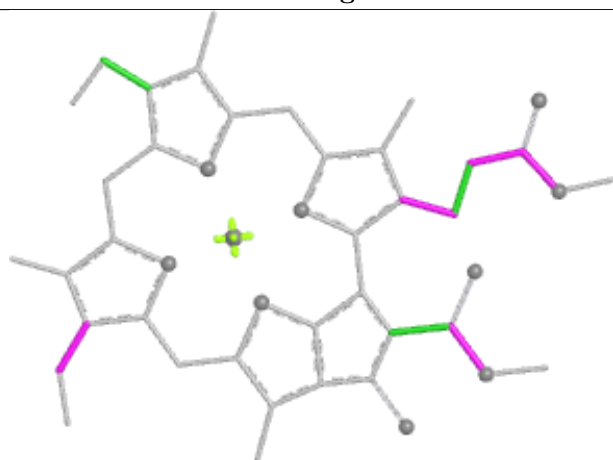
Ligand CLA B 813



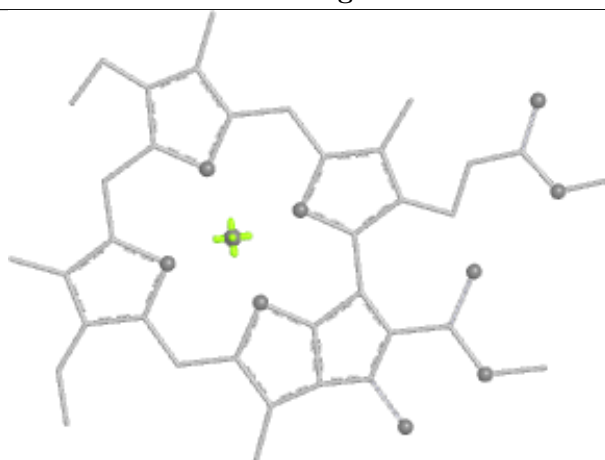
Bond lengths



Bond angles

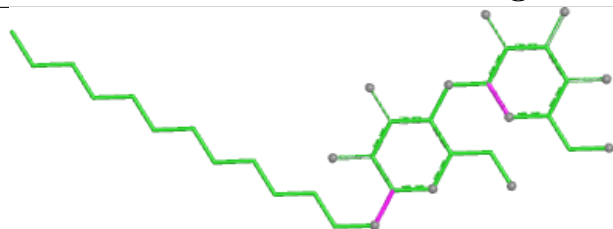


Torsions

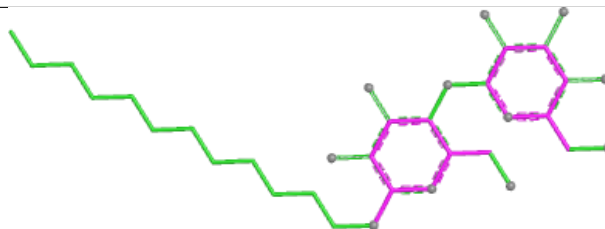


Rings

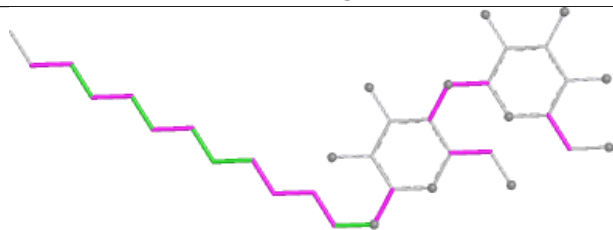
Ligand LMU R 104



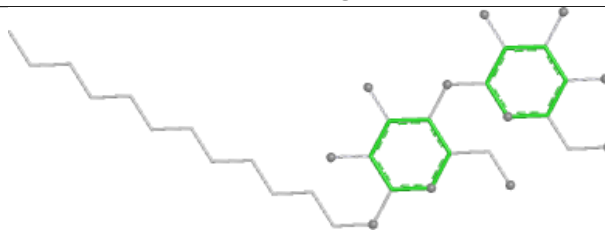
Bond lengths



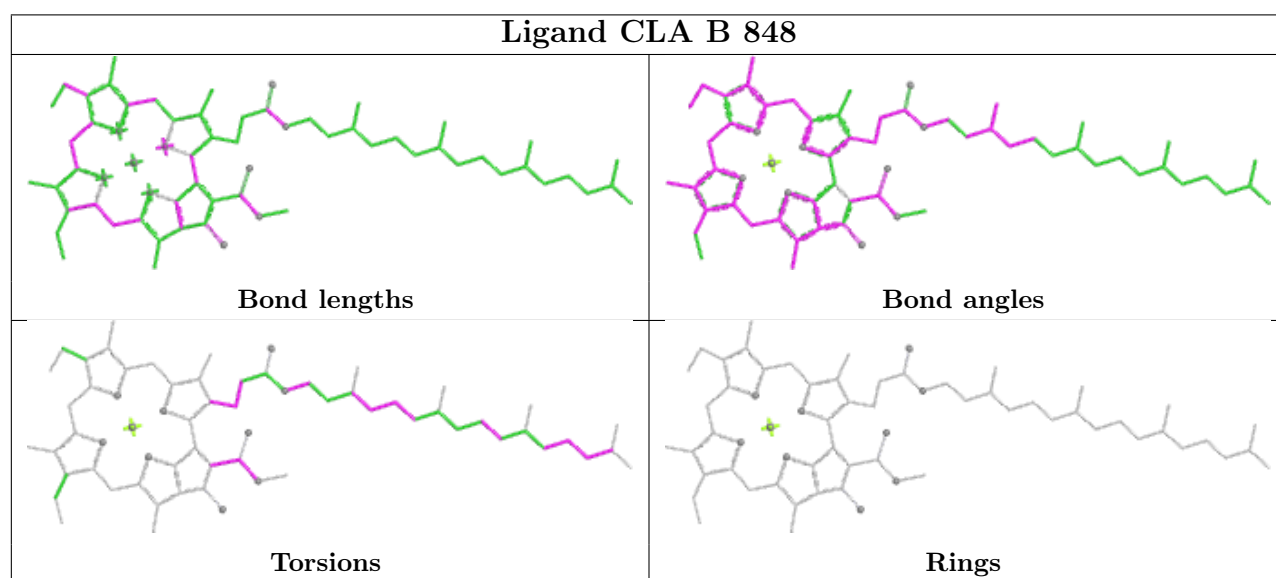
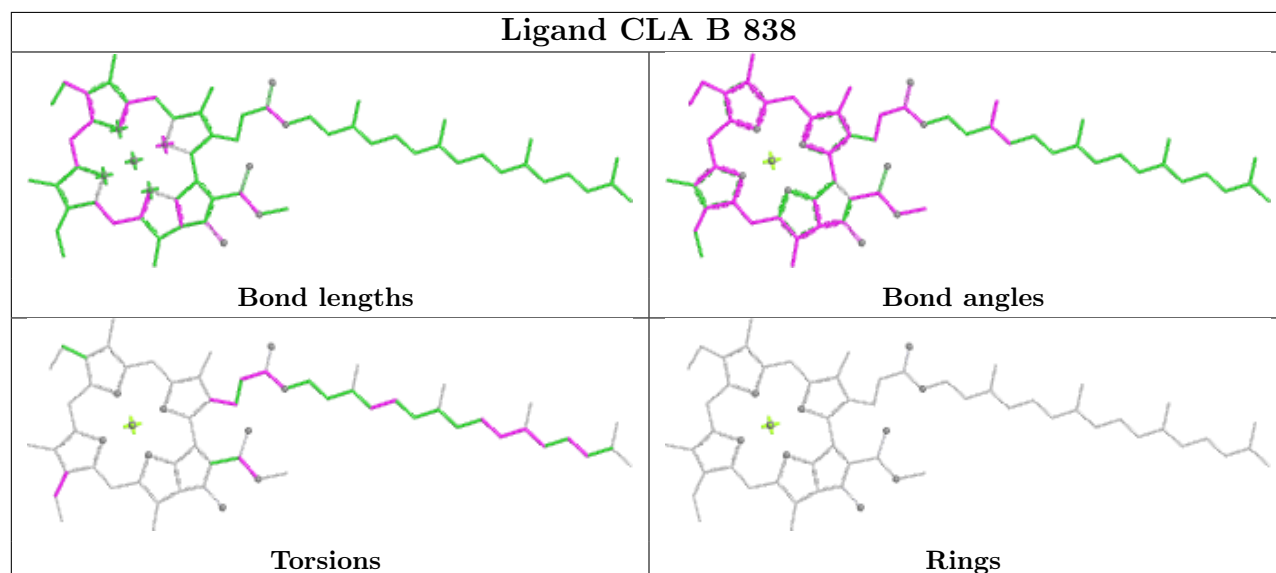
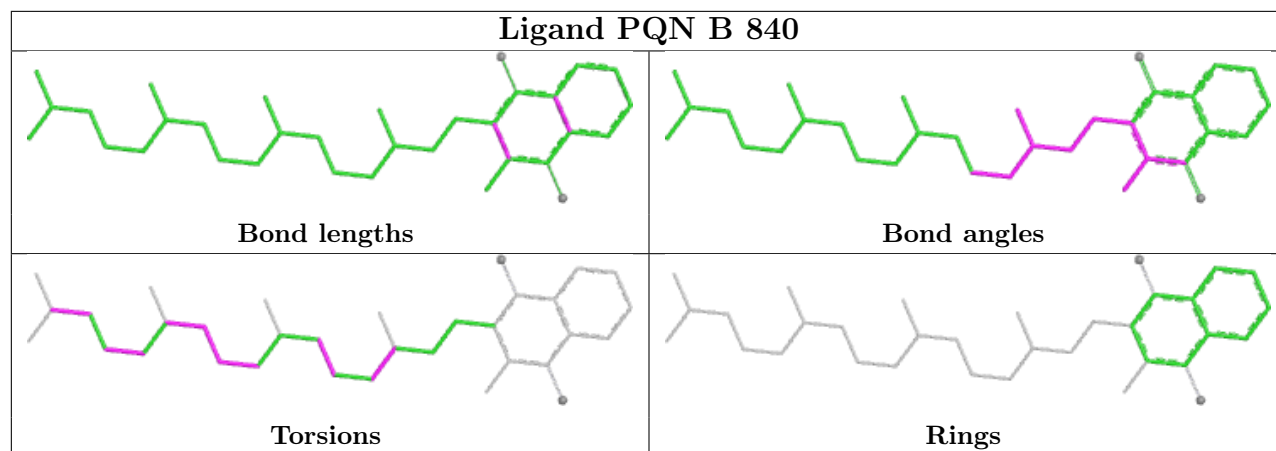
Bond angles

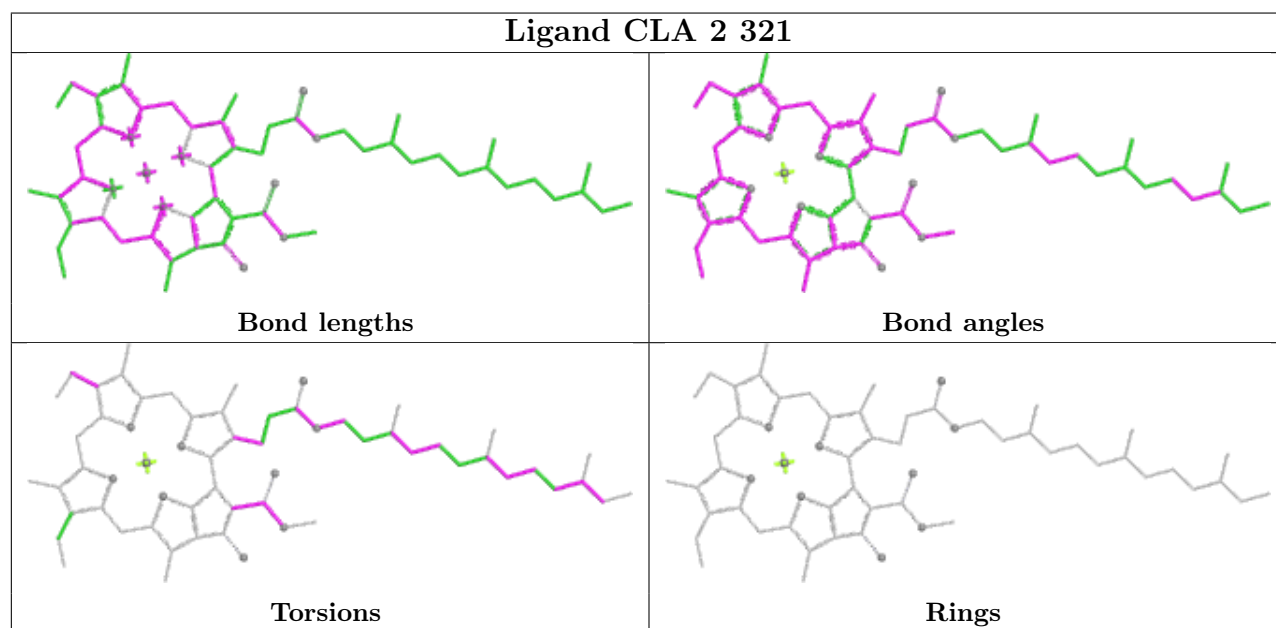
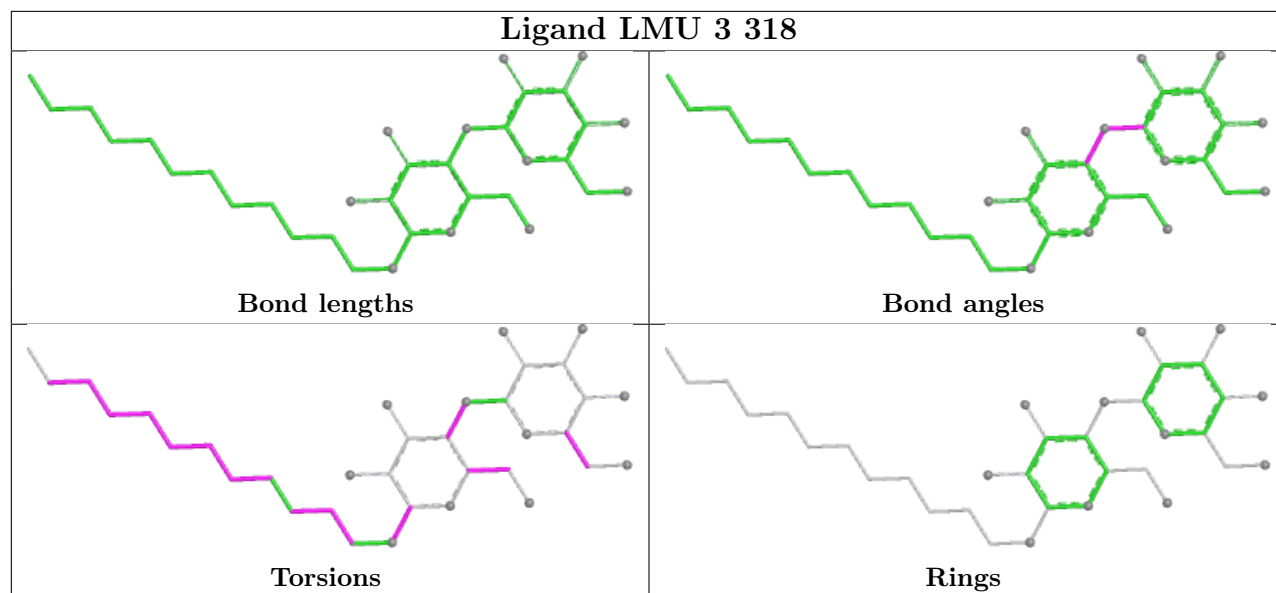


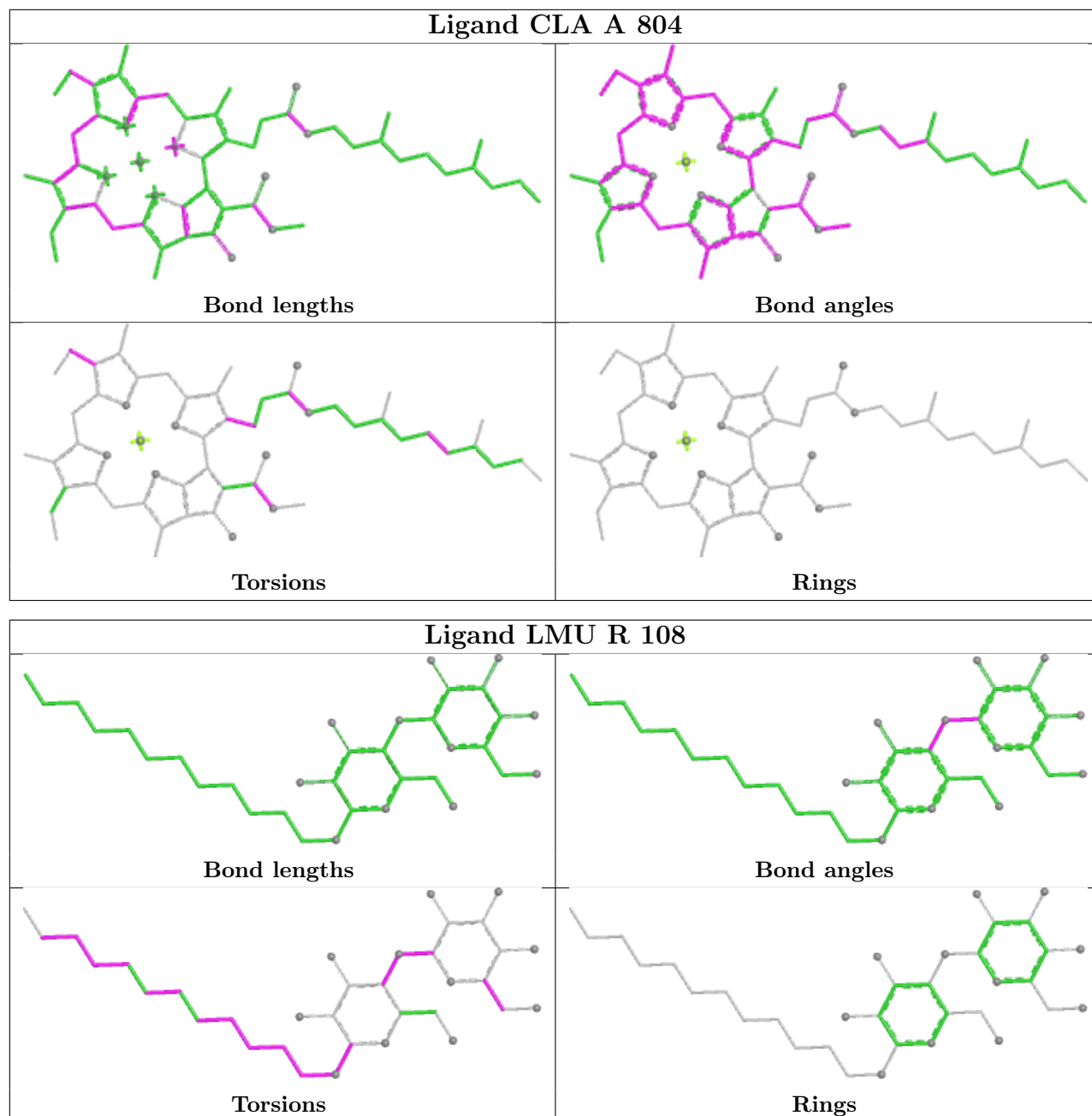
Torsions

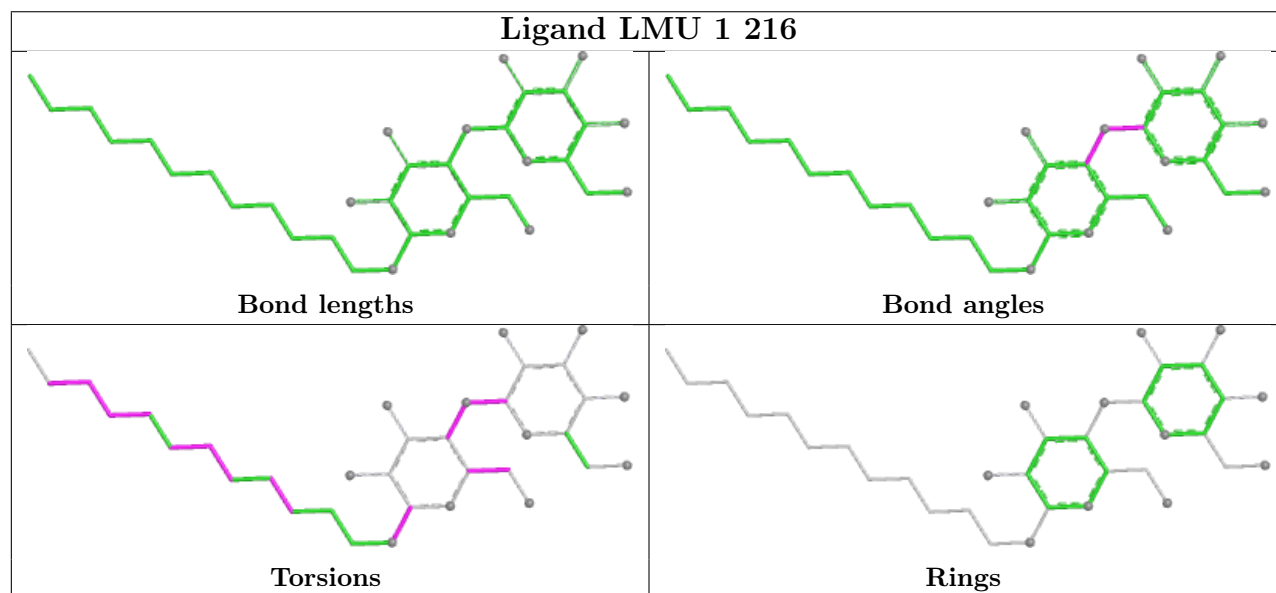
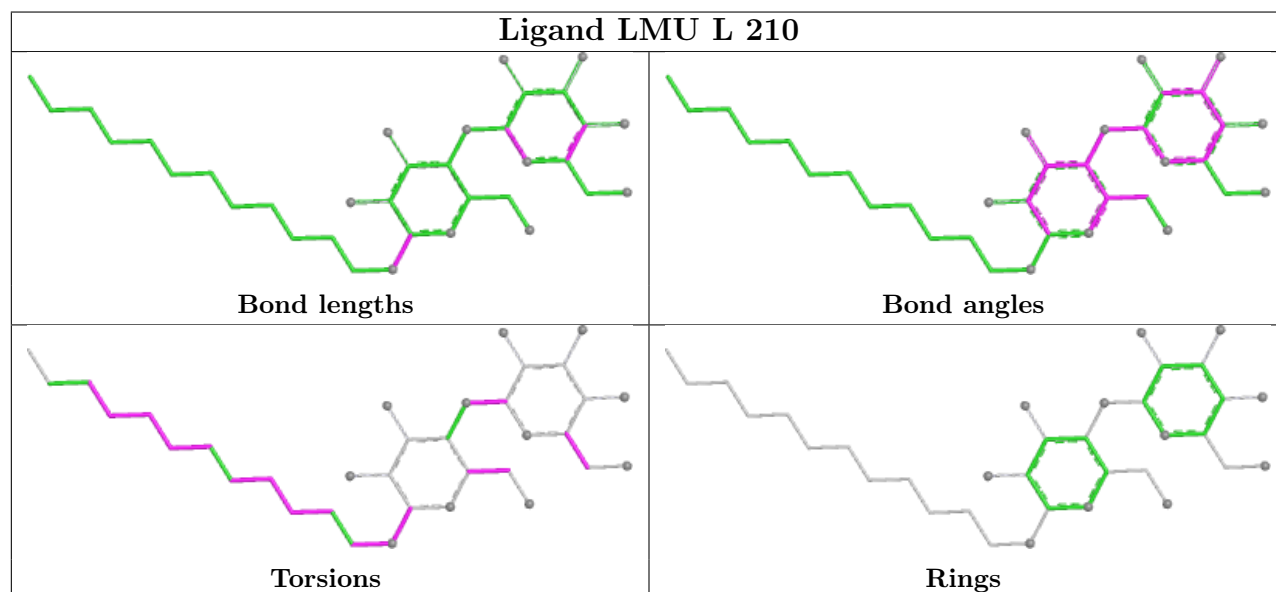
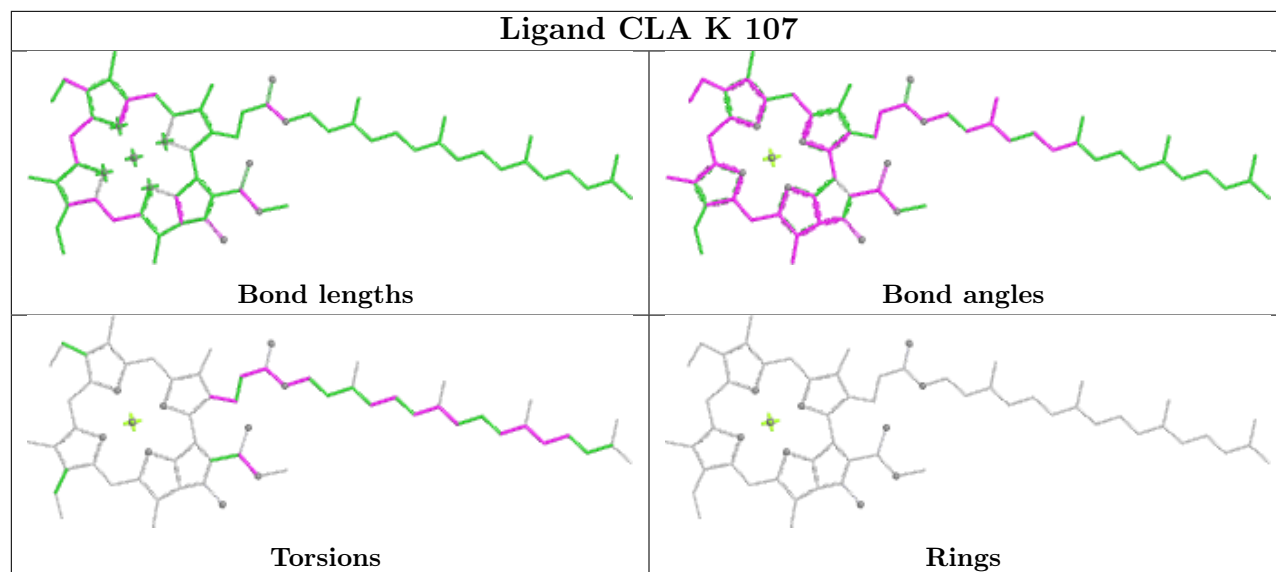


Rings

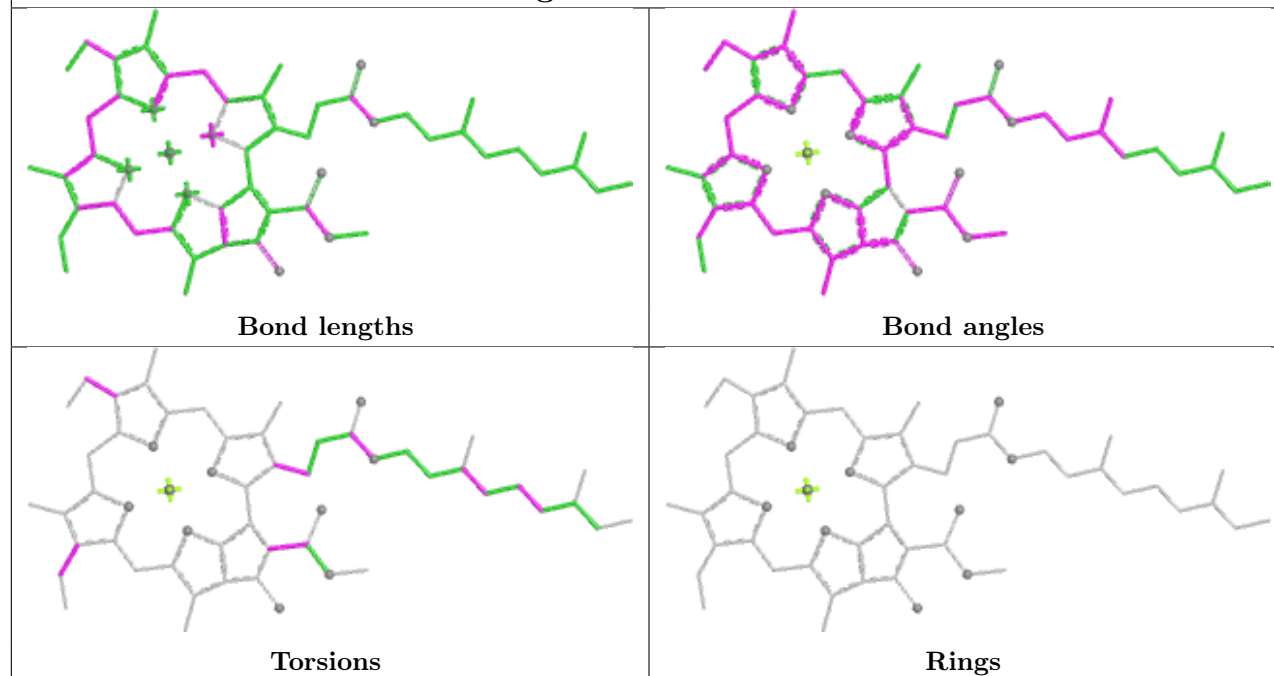




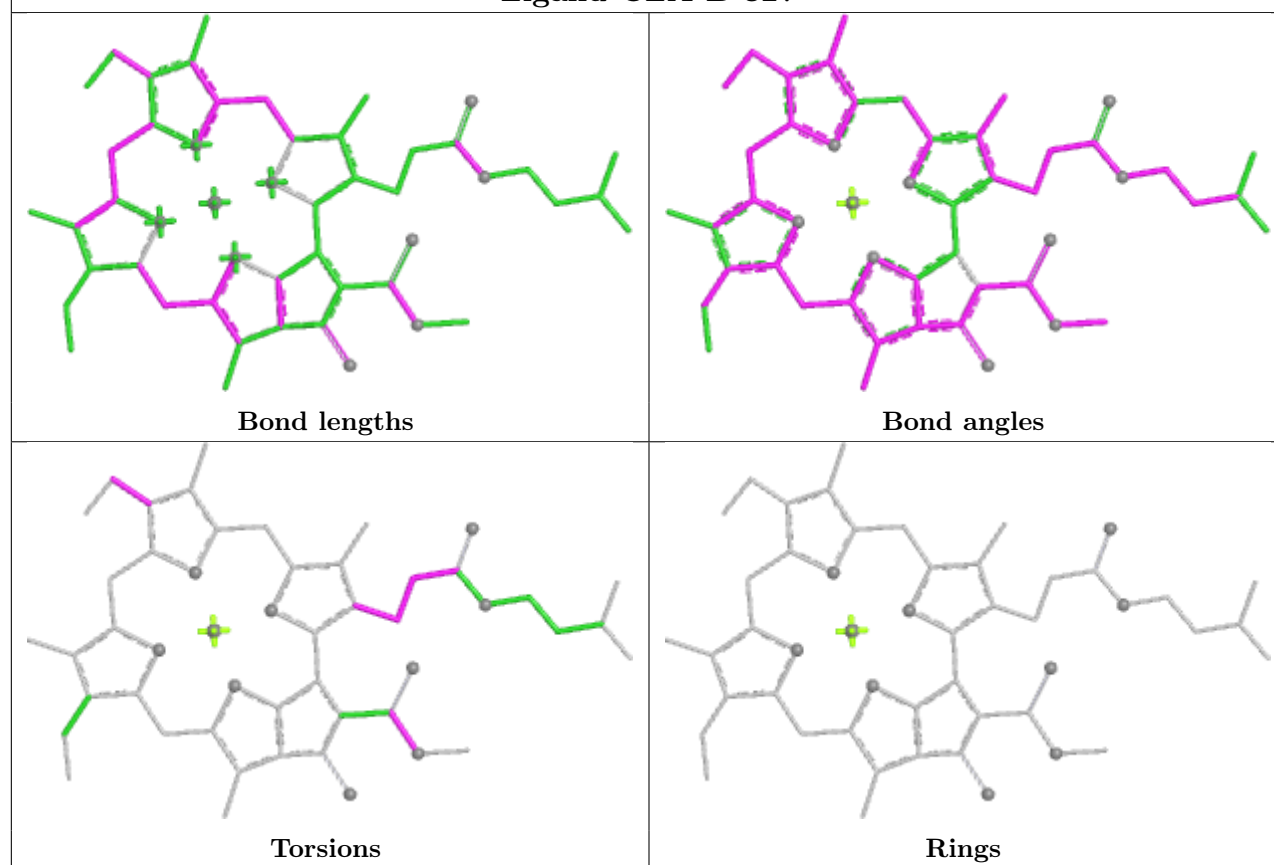




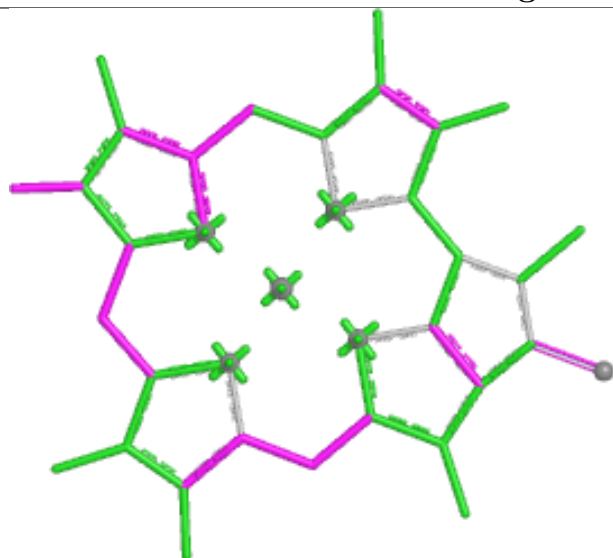
Ligand CLA 2 302



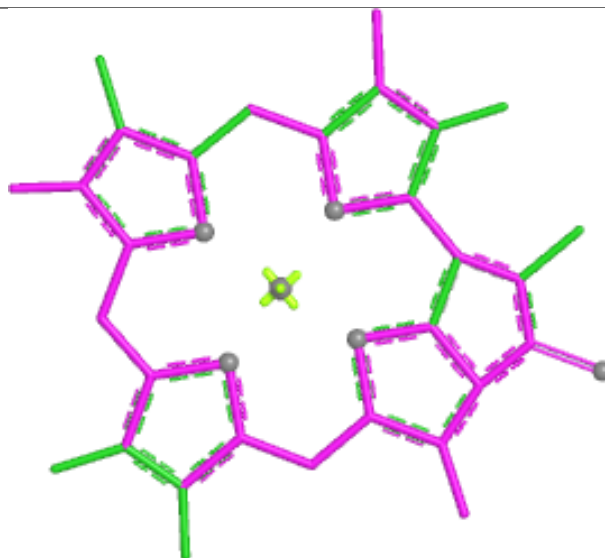
Ligand CLA B 827



Ligand CLA 1 205



Bond lengths



Bond angles

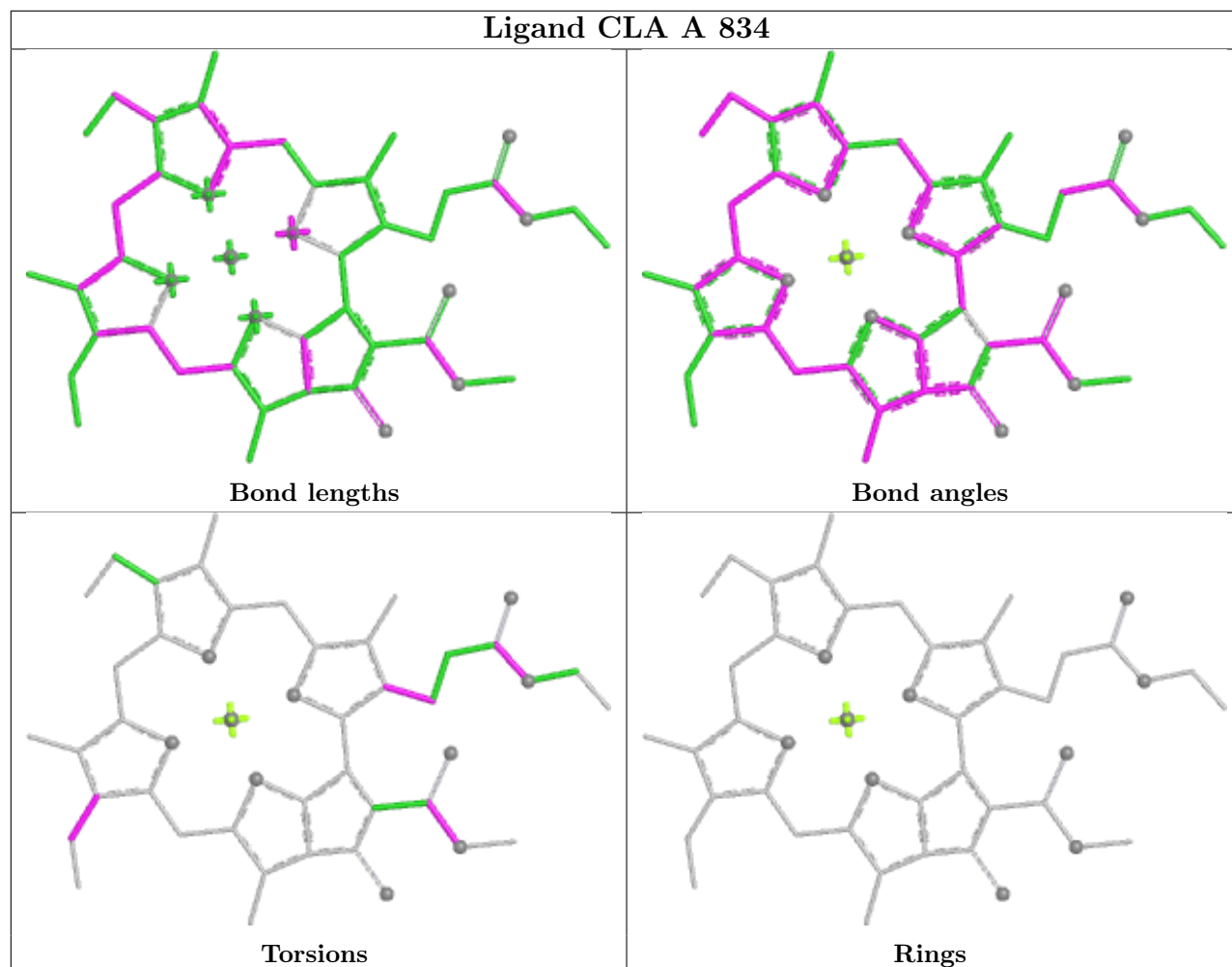


Torsions

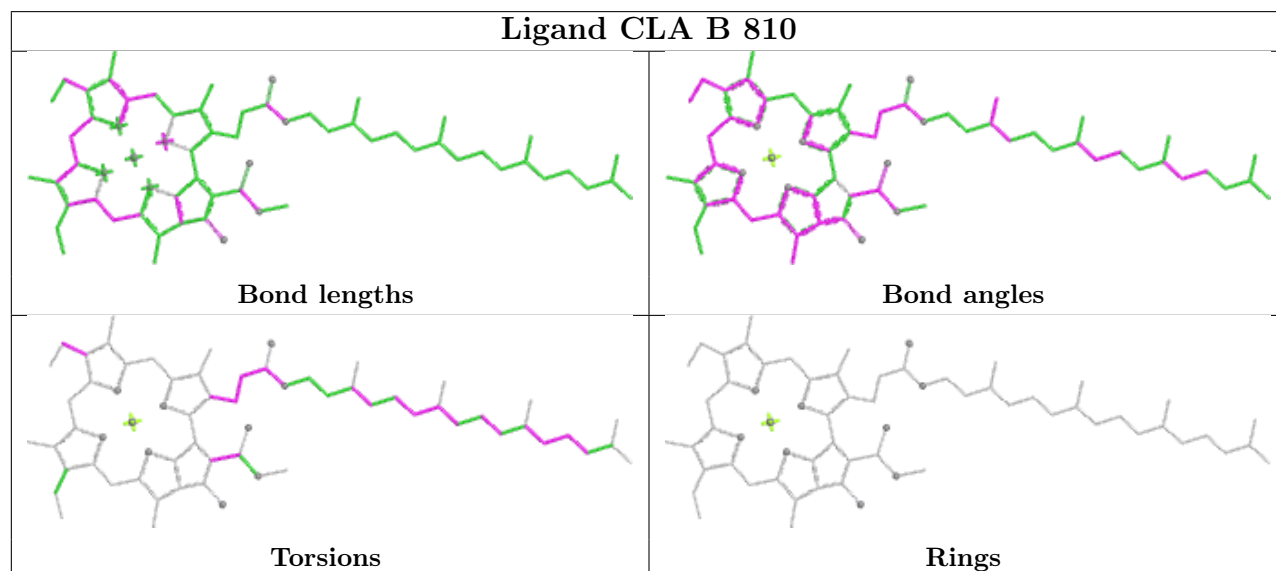


Rings

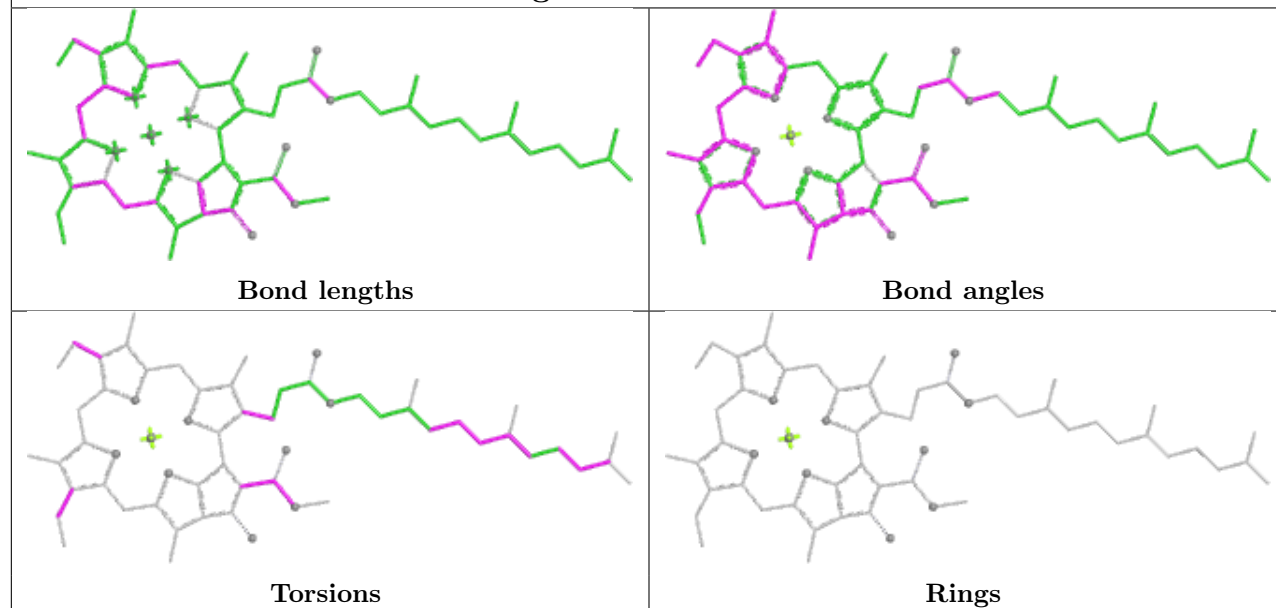
Ligand CLA A 834



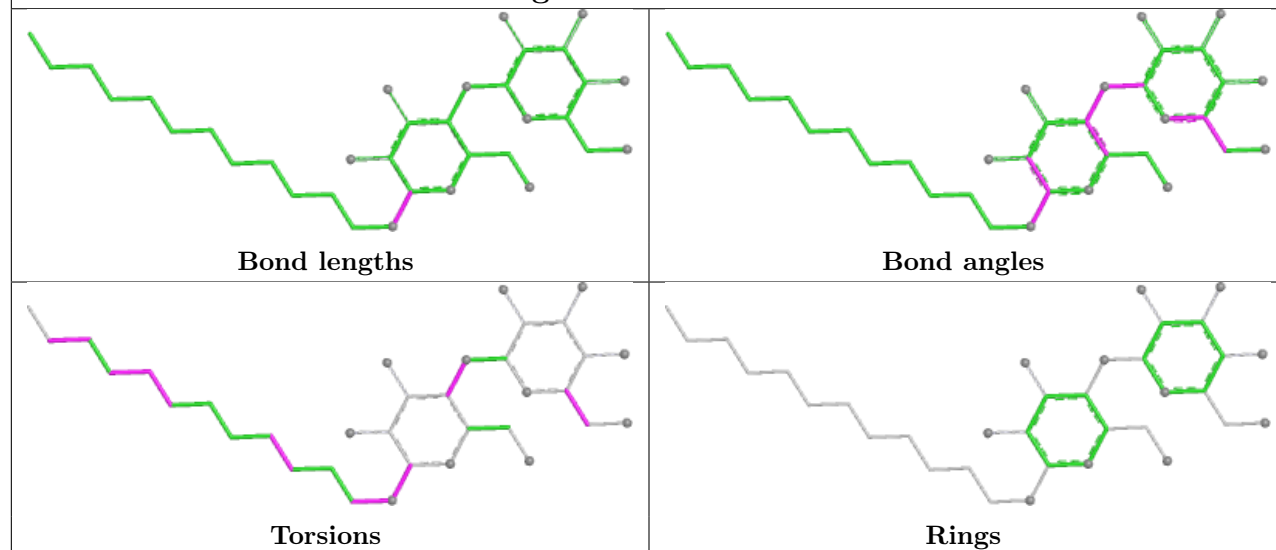
Ligand CLA B 810

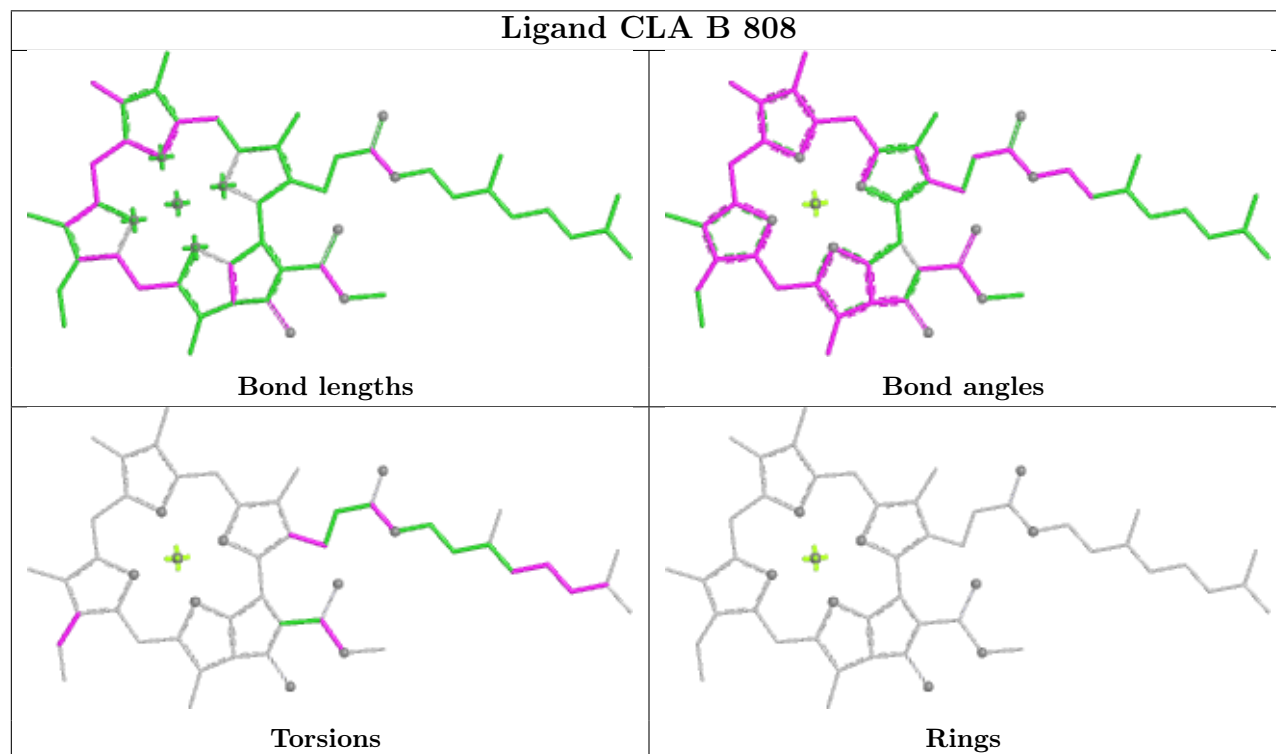
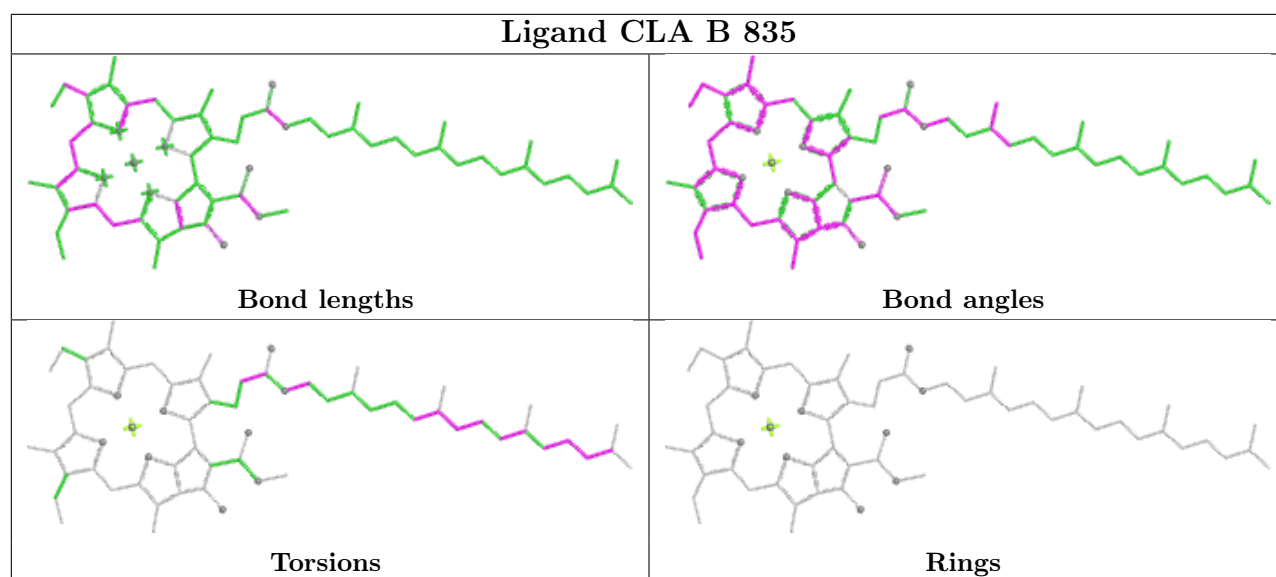


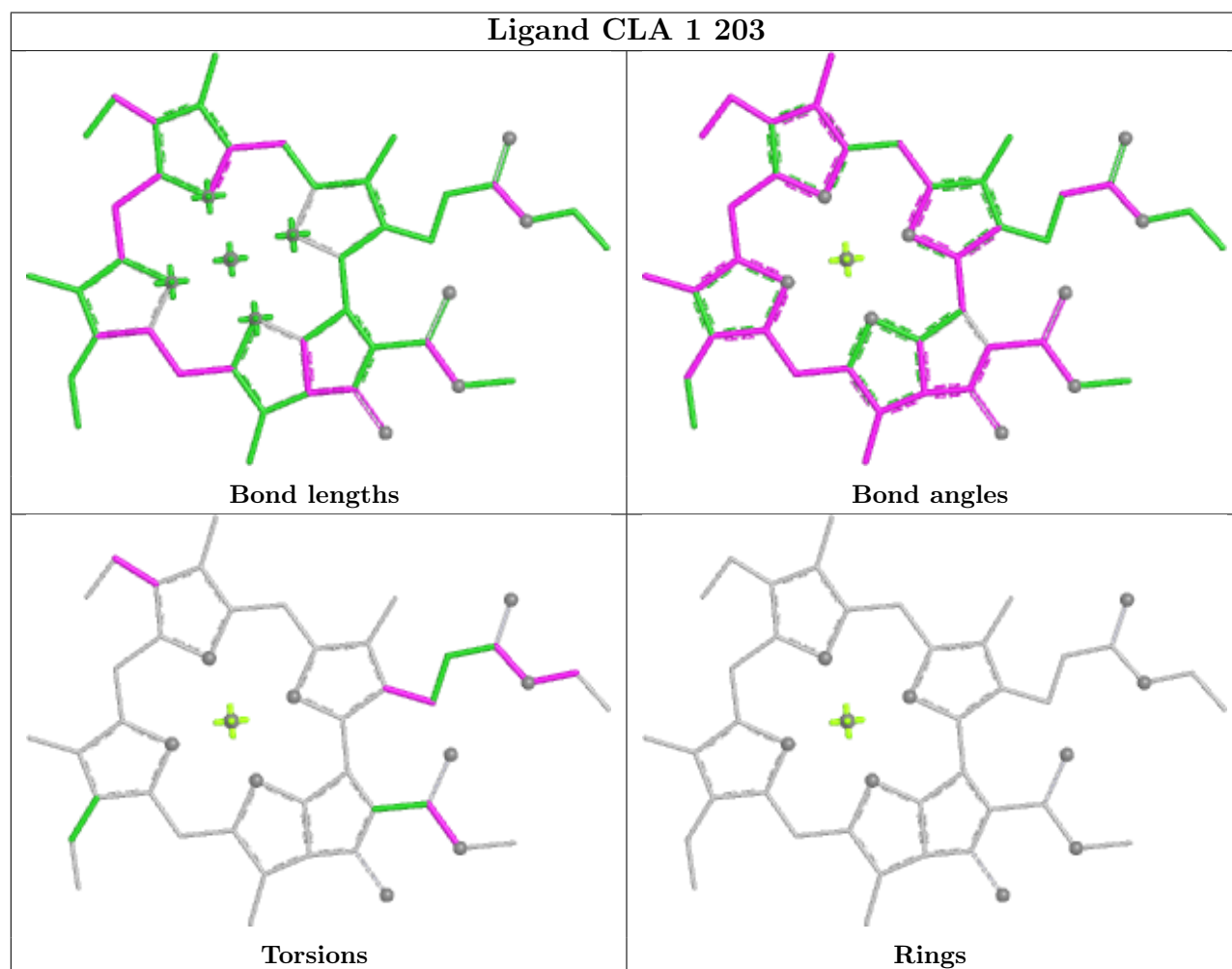
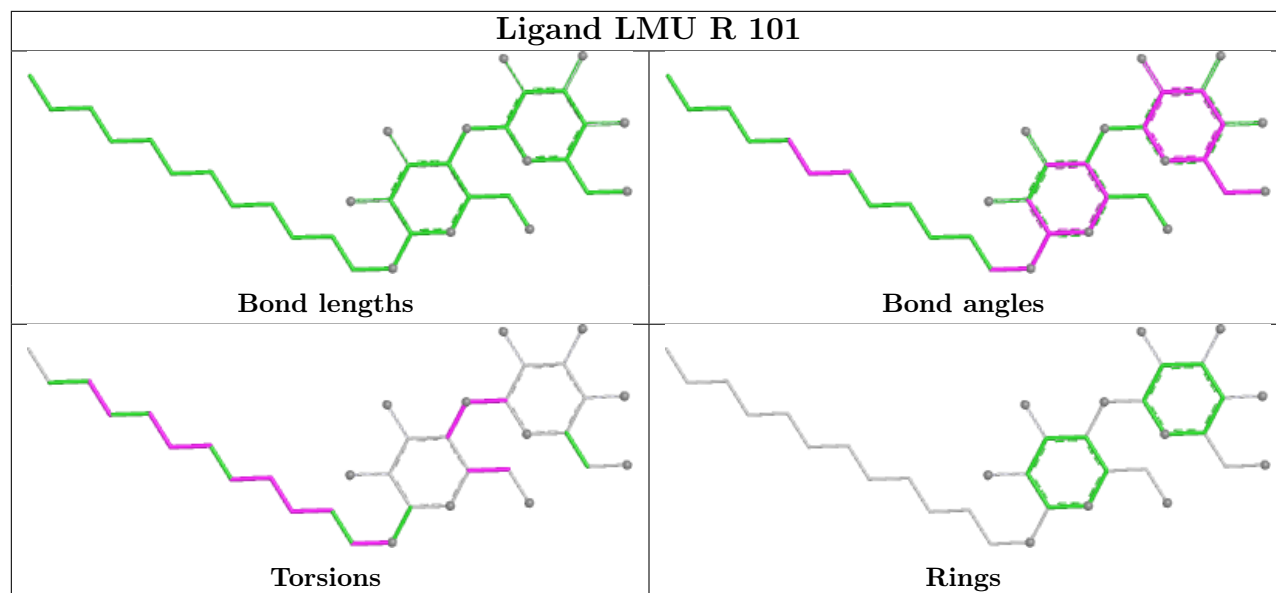
Ligand CLA B 834



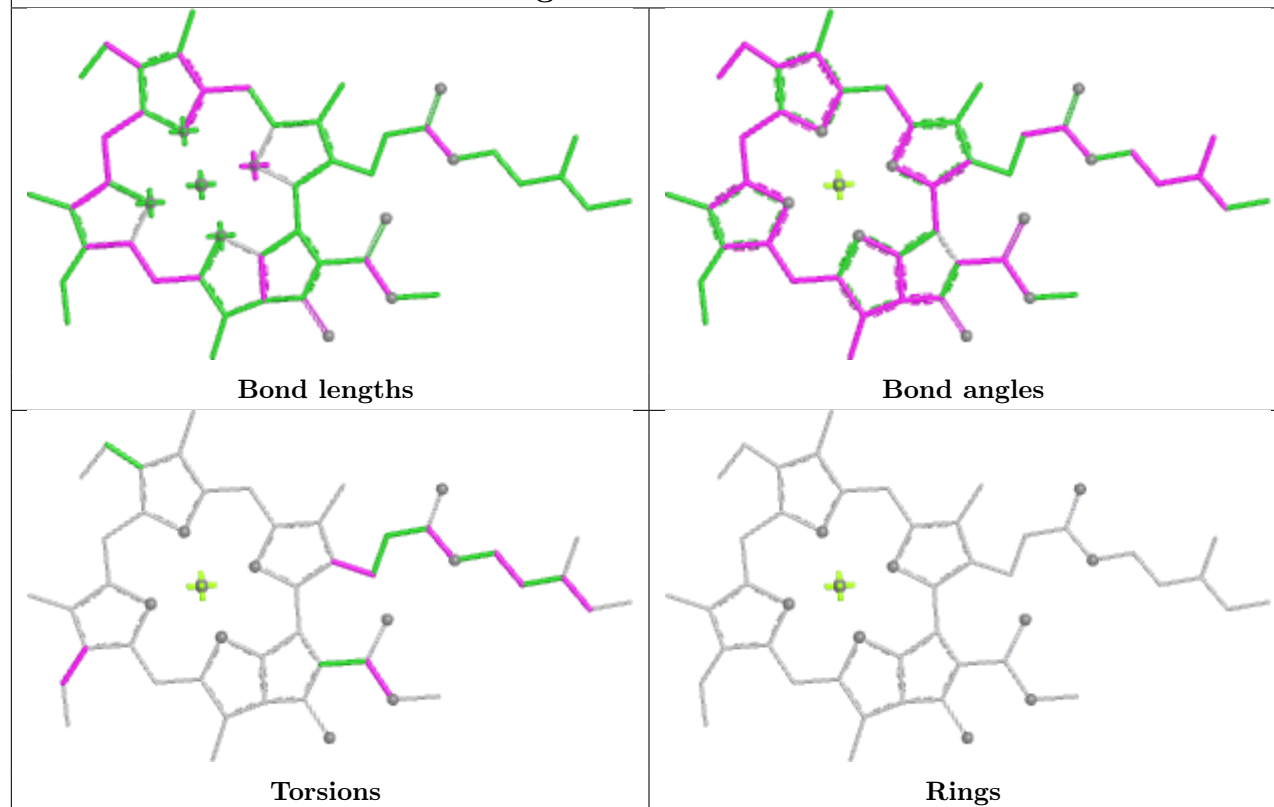
Ligand LMU 2 320



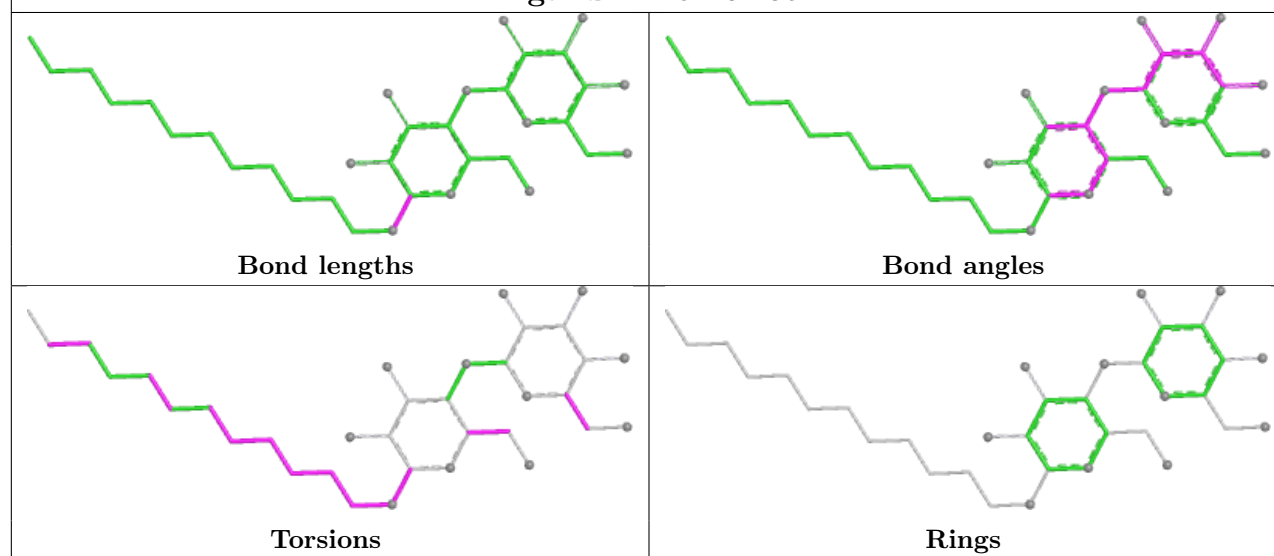




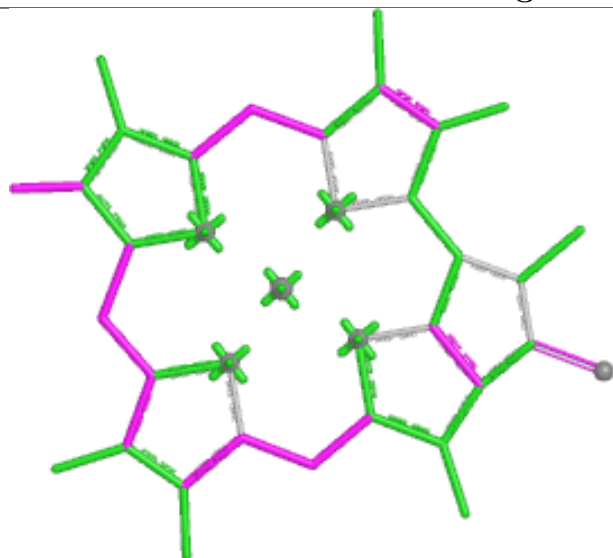
Ligand CLA 2 301



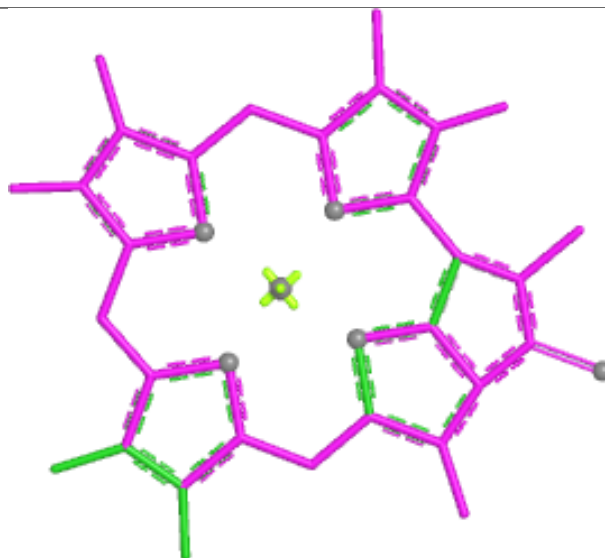
Ligand LMU R 105



Ligand CLA F 204



Bond lengths



Bond angles

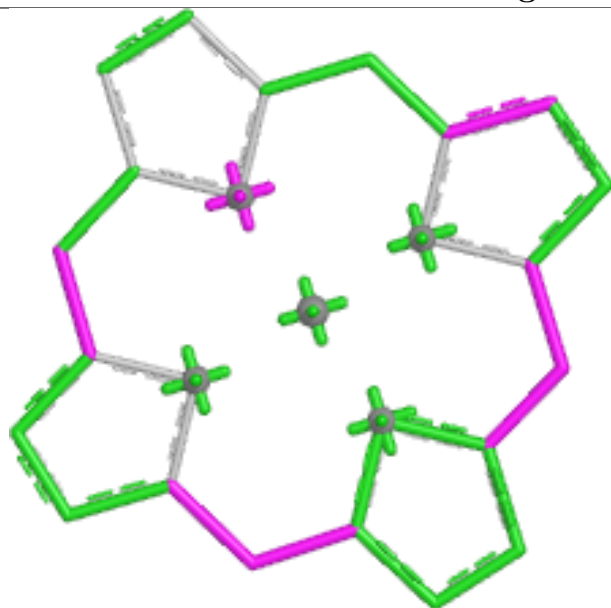


Torsions

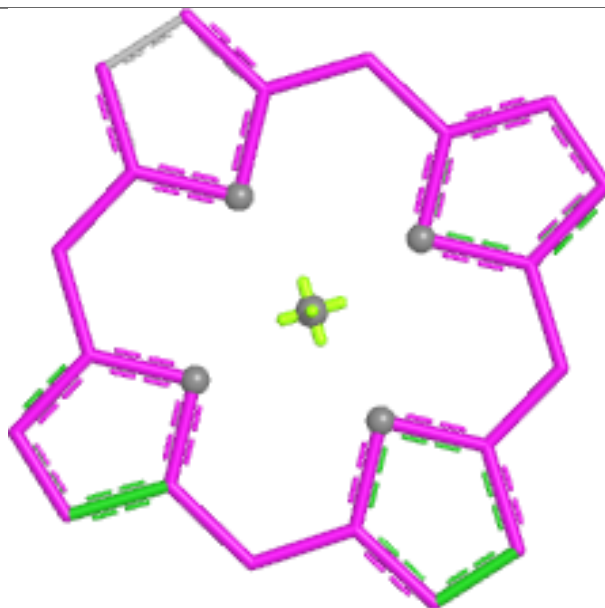


Rings

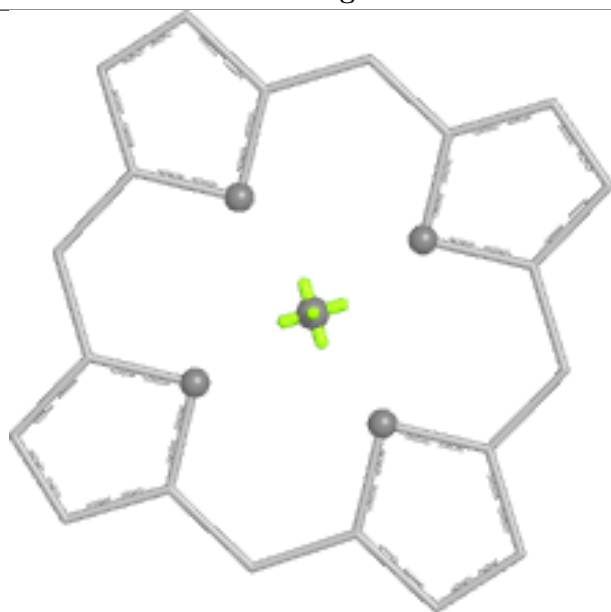
Ligand CLA 4 312



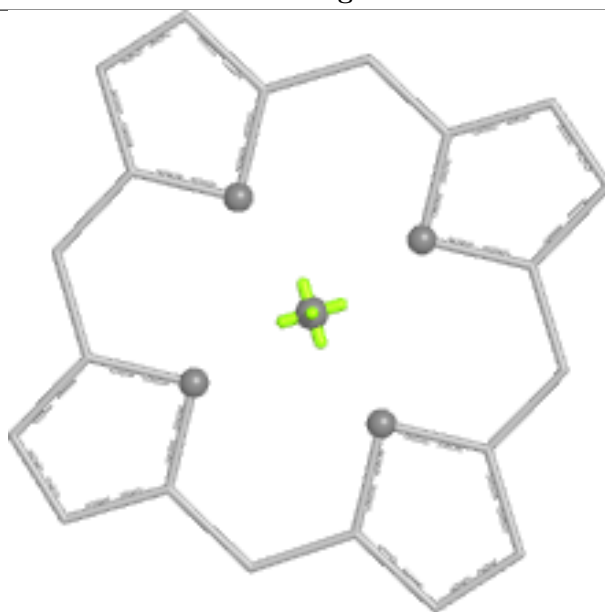
Bond lengths



Bond angles

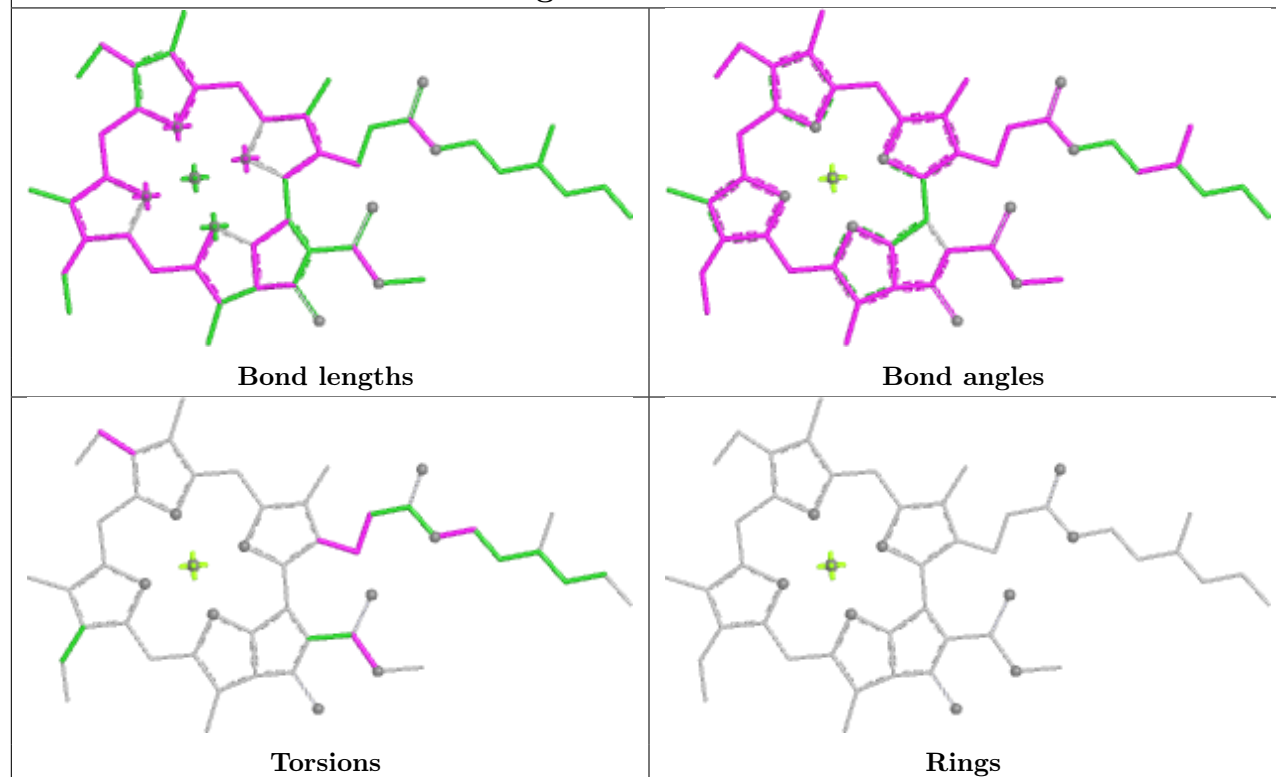


Torsions

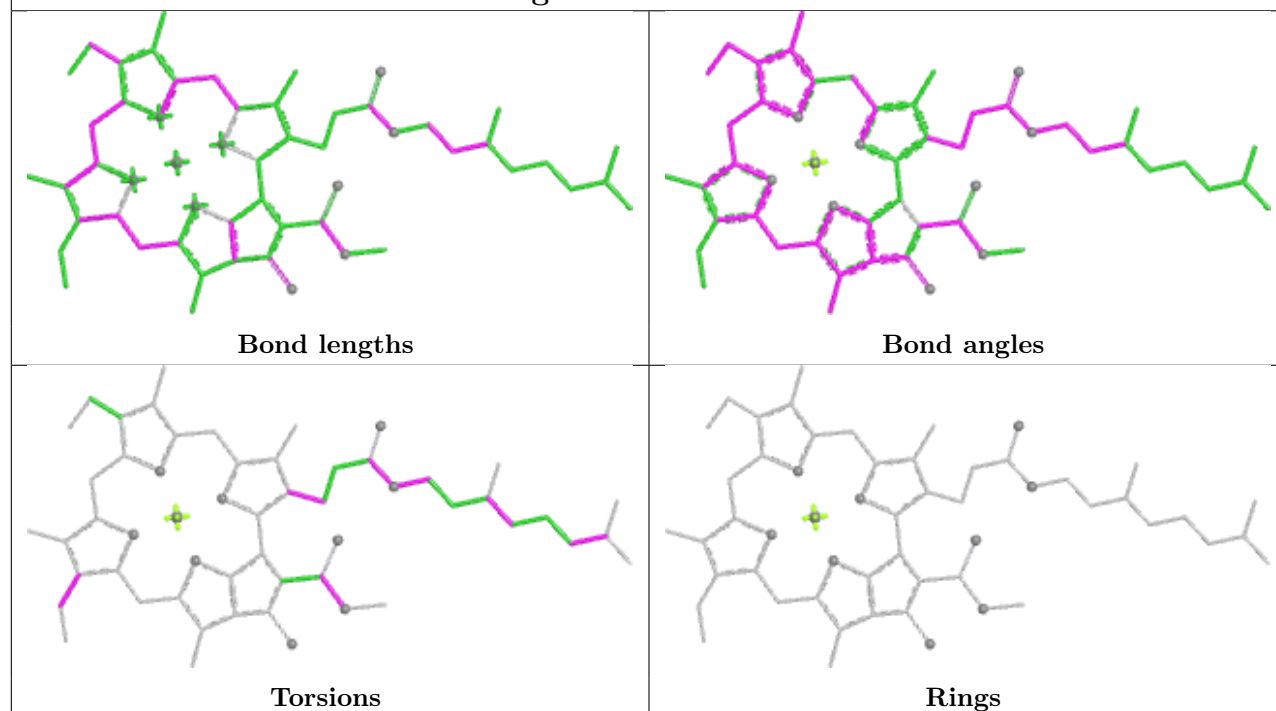


Rings

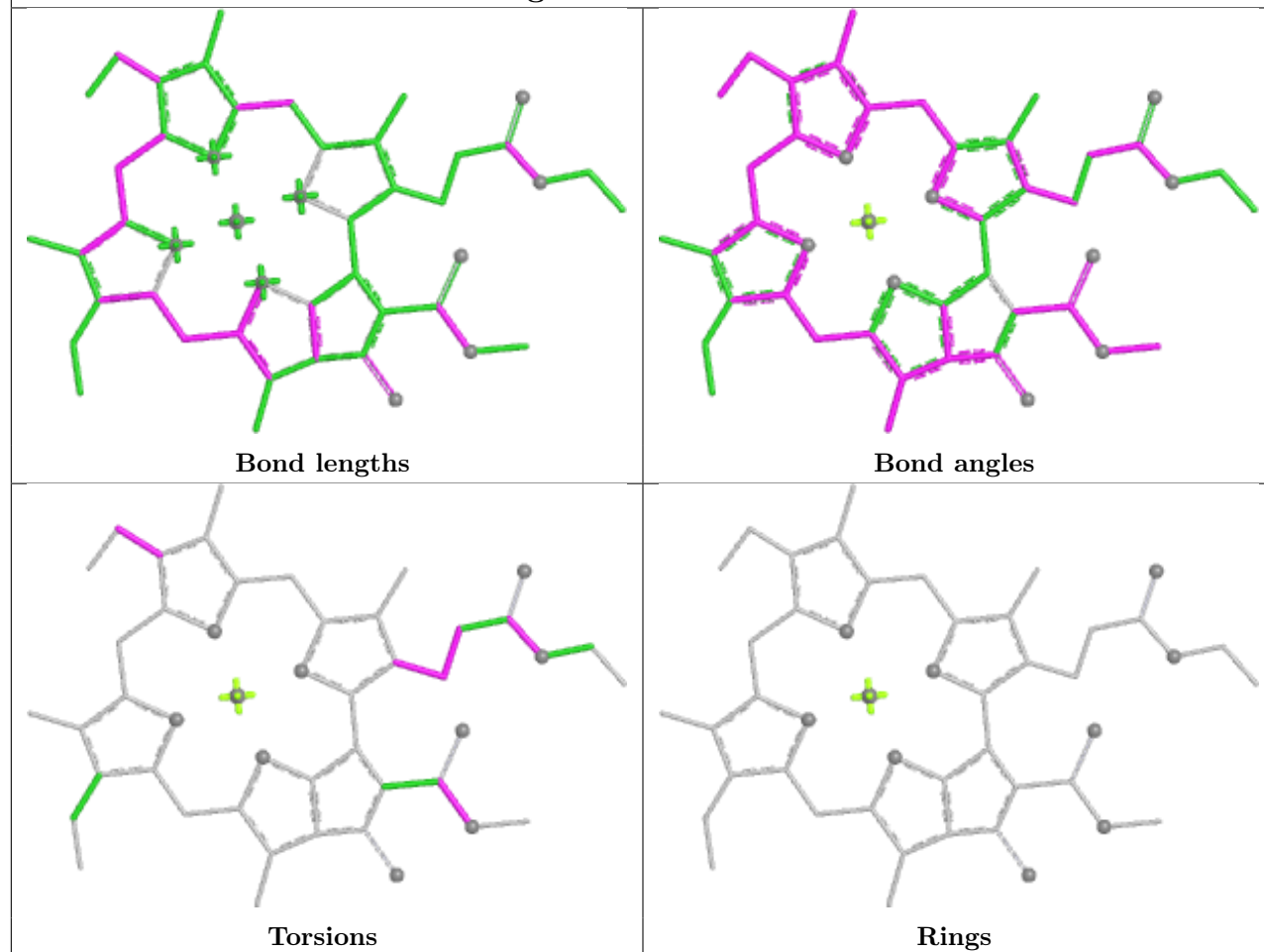
Ligand CLA 4 307



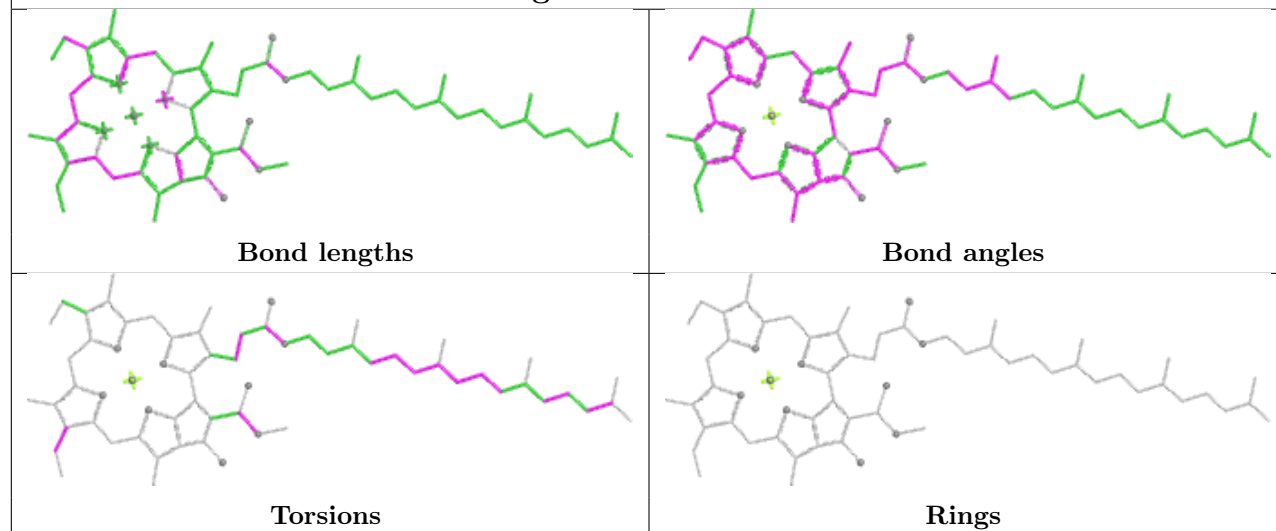
Ligand CLA A 802

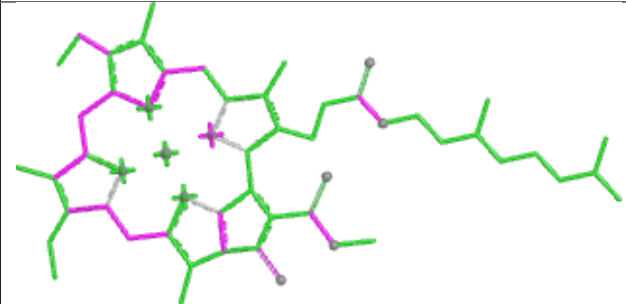
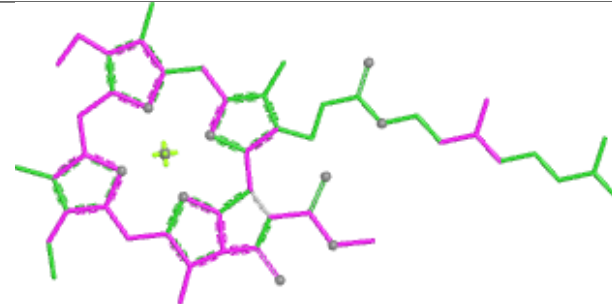
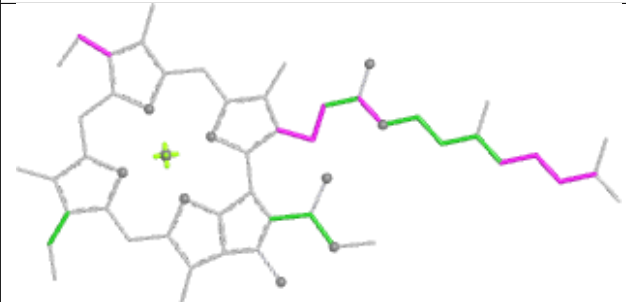
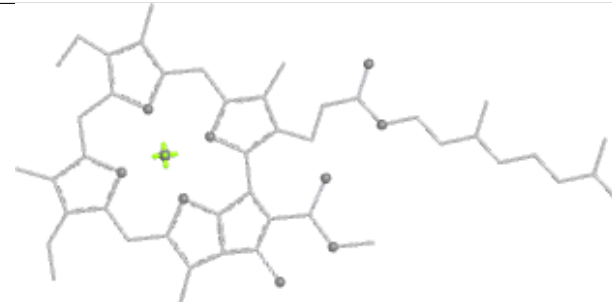


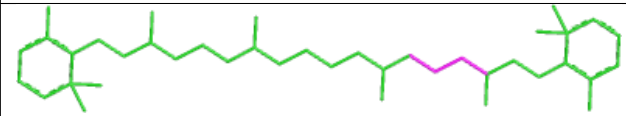
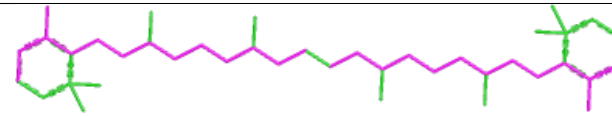
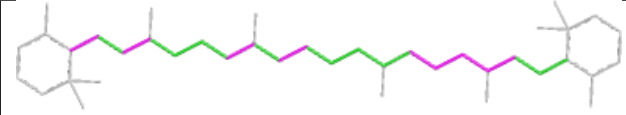
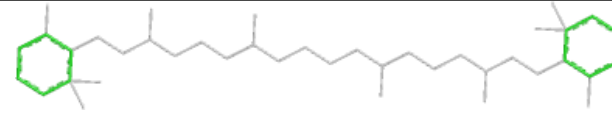
Ligand CLA B 836

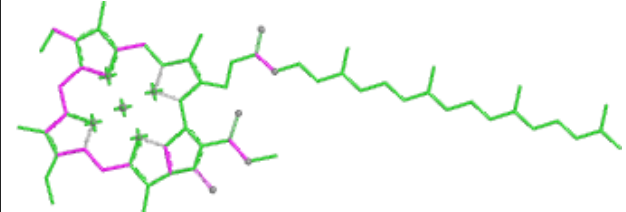
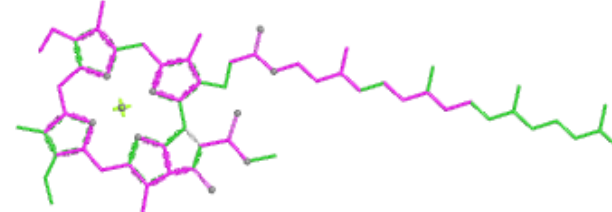
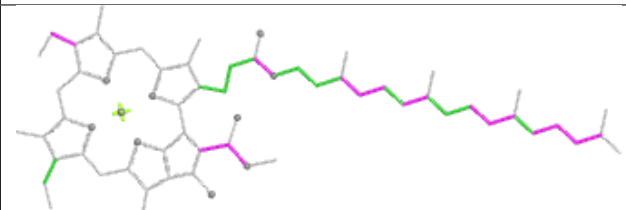
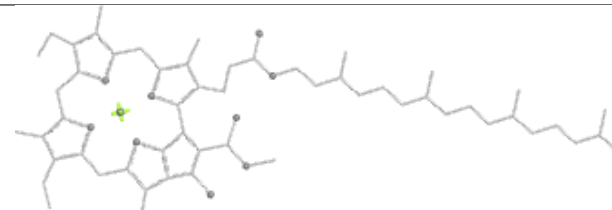


Ligand CLA B 837

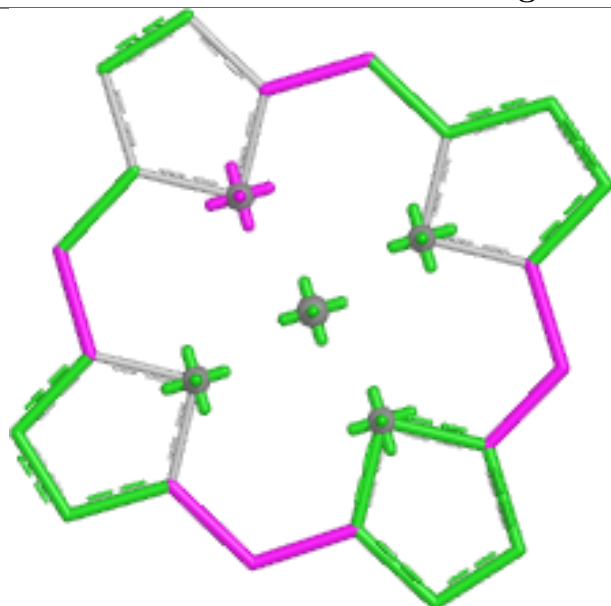


Ligand CLA B 819	
	
Bond lengths	Bond angles
	
Torsions	Rings

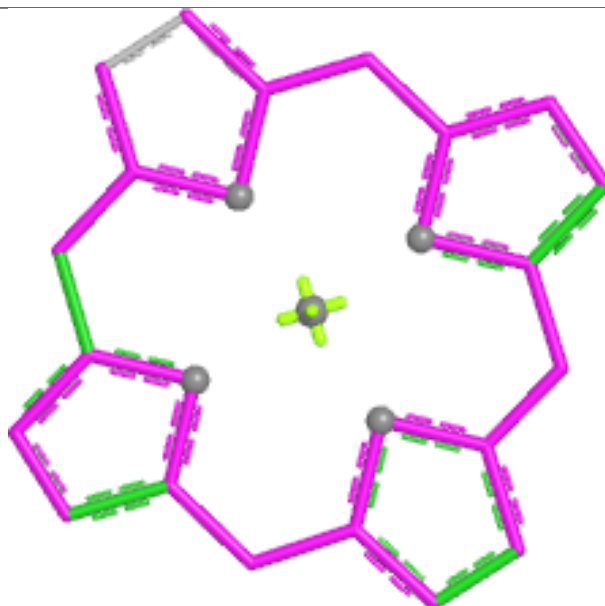
Ligand BCR A 841	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA A 824	
	
Bond lengths	Bond angles
	
Torsions	Rings

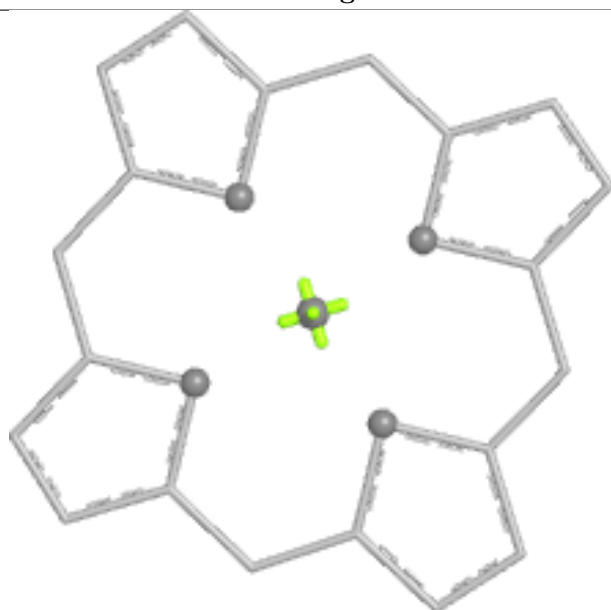
Ligand CLA 3 317



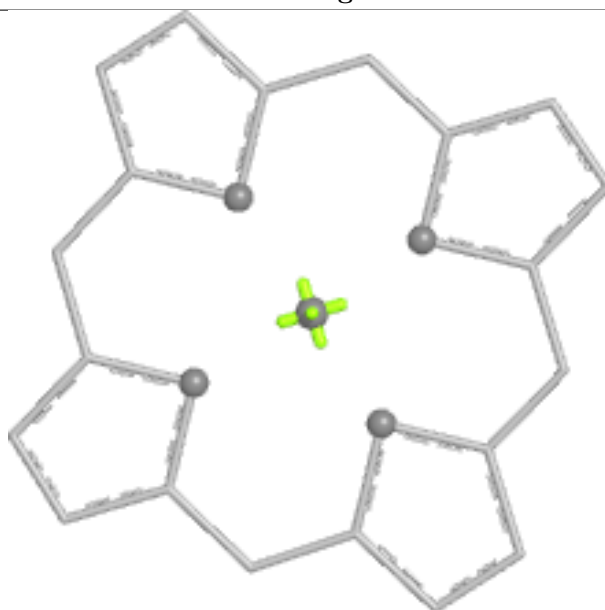
Bond lengths



Bond angles

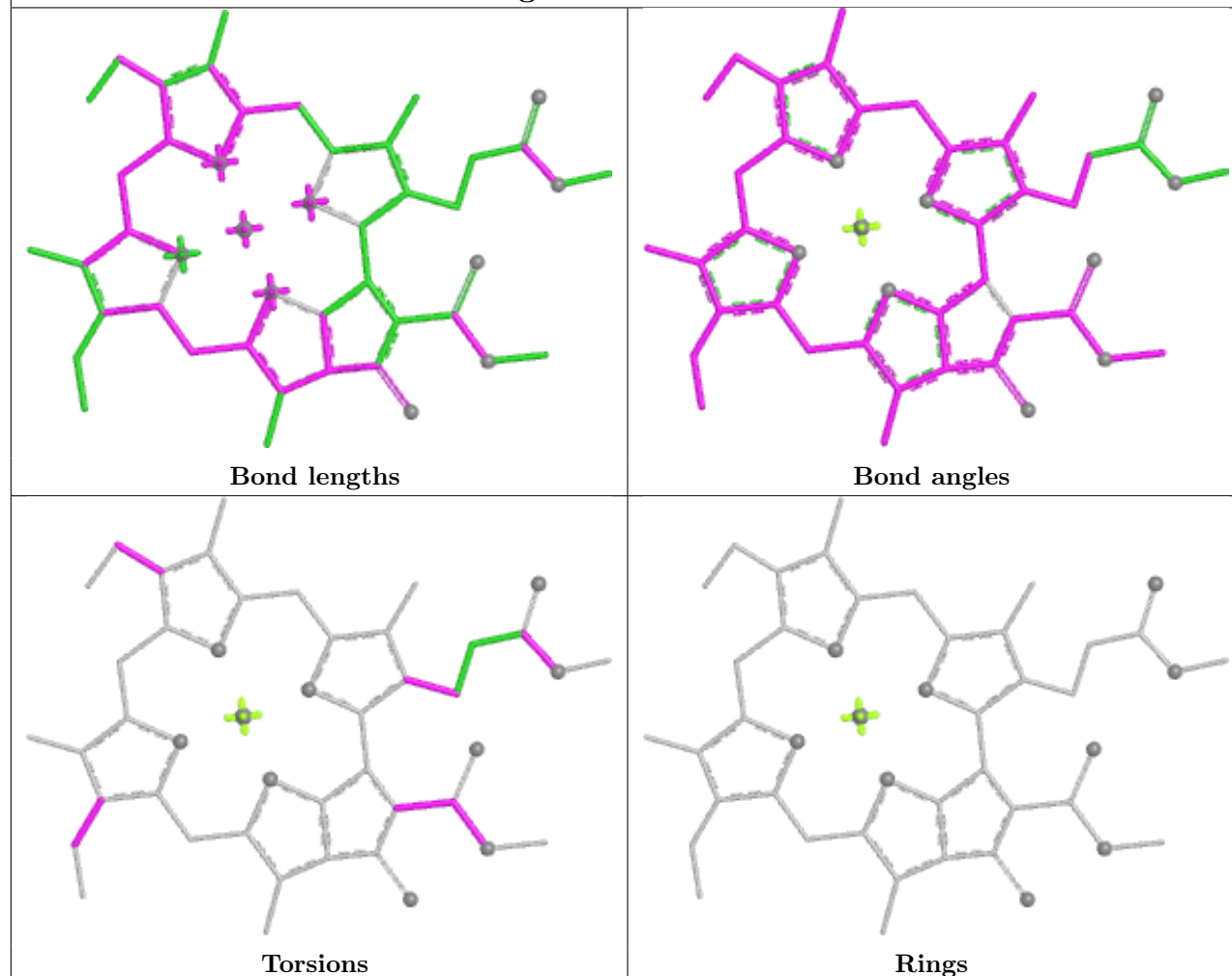


Torsions

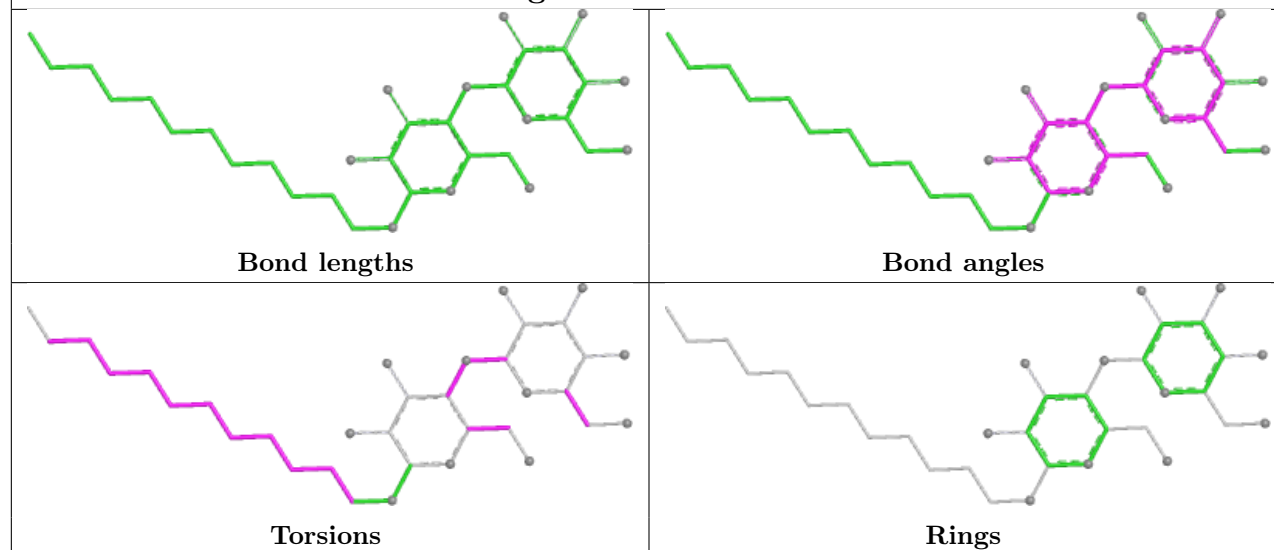


Rings

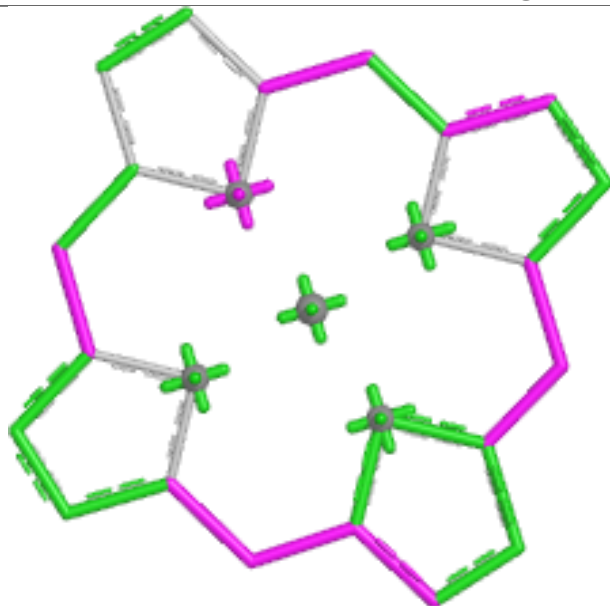
Ligand CLA 1 201



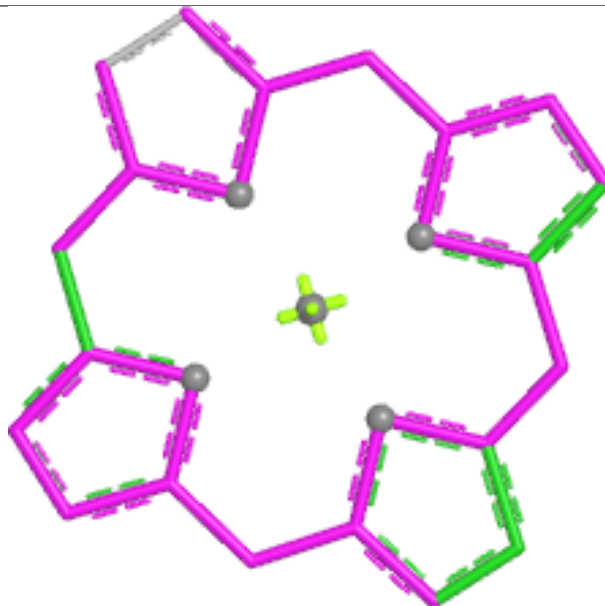
Ligand LMU B 801



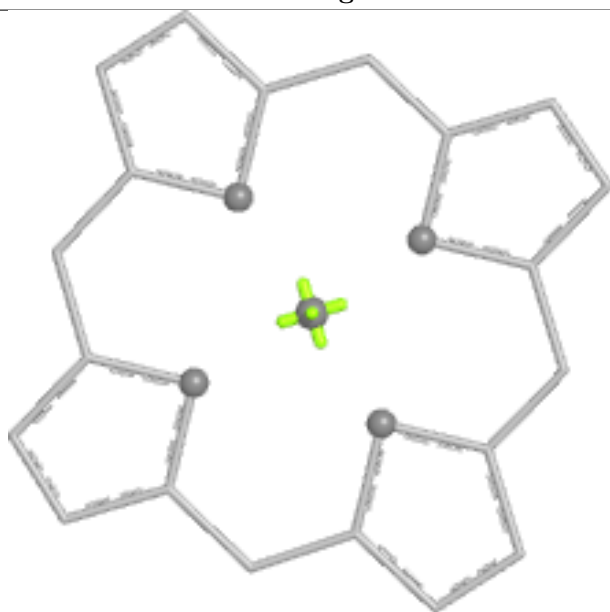
Ligand CLA 3 308



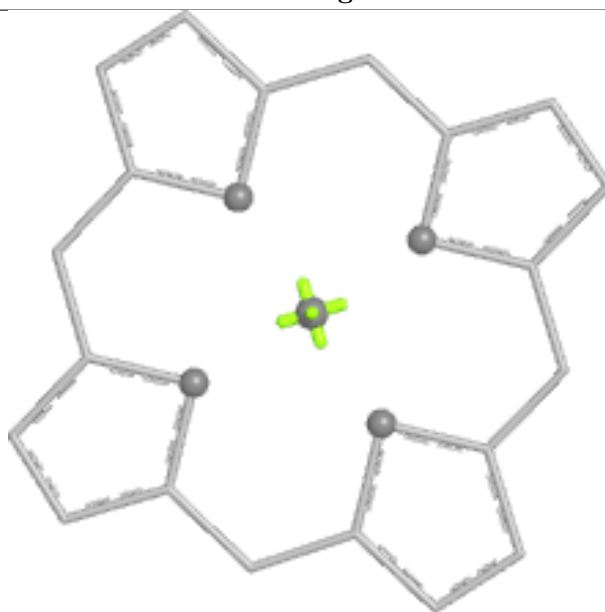
Bond lengths



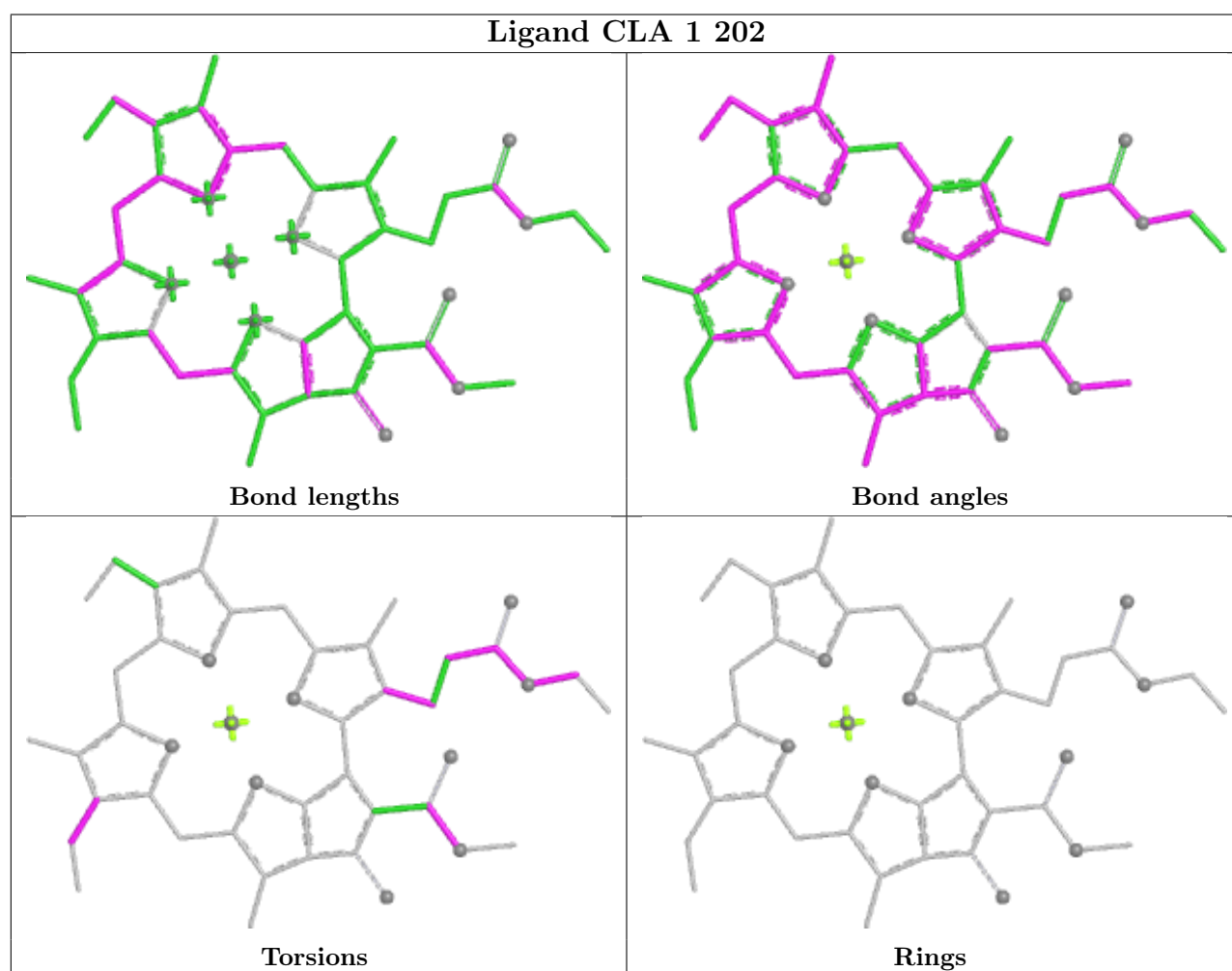
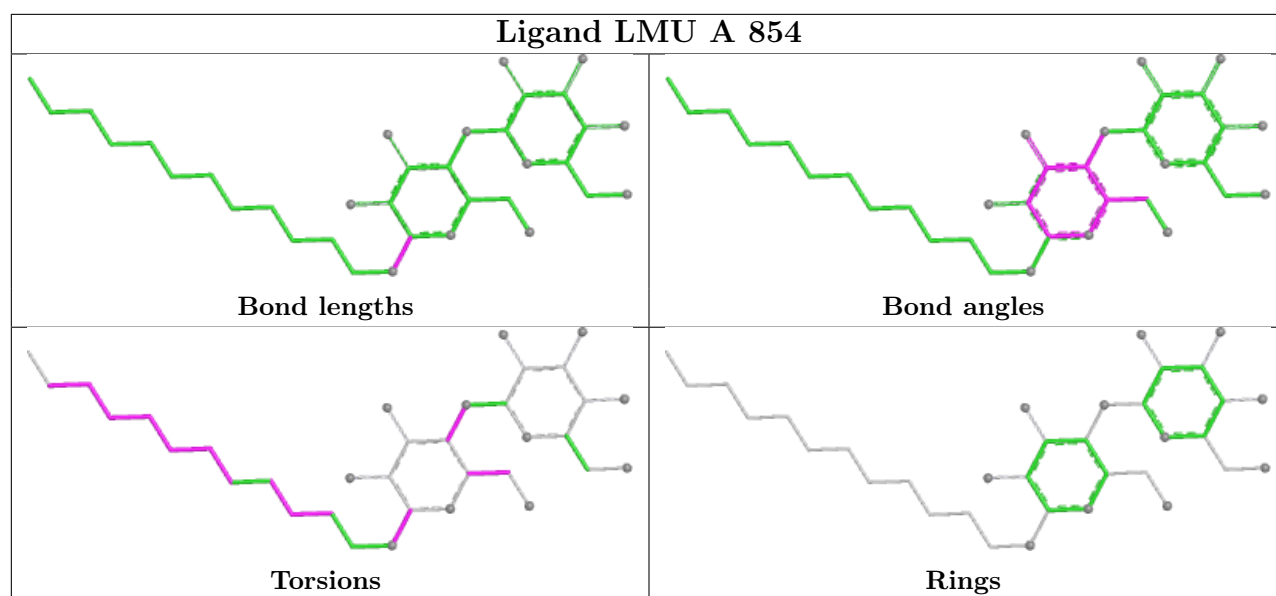
Bond angles



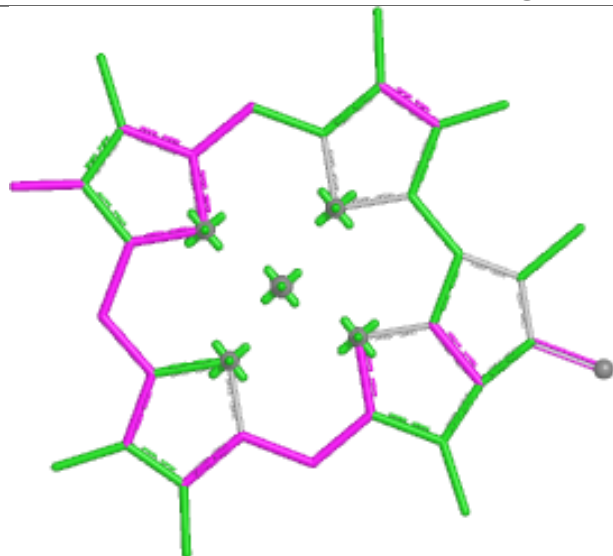
Torsions



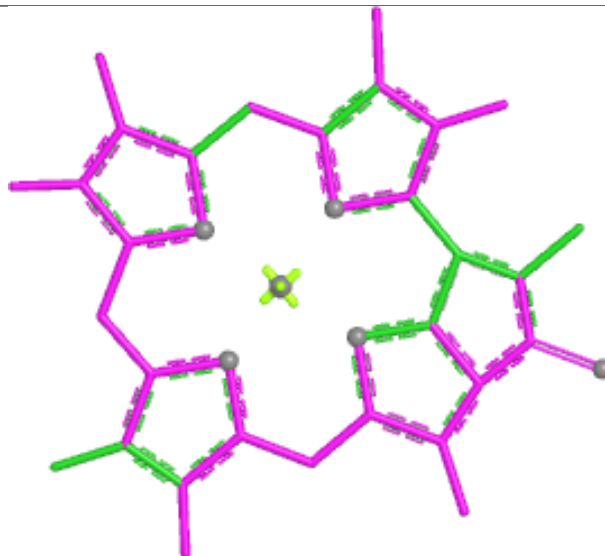
Rings



Ligand CLA 4 303



Bond lengths



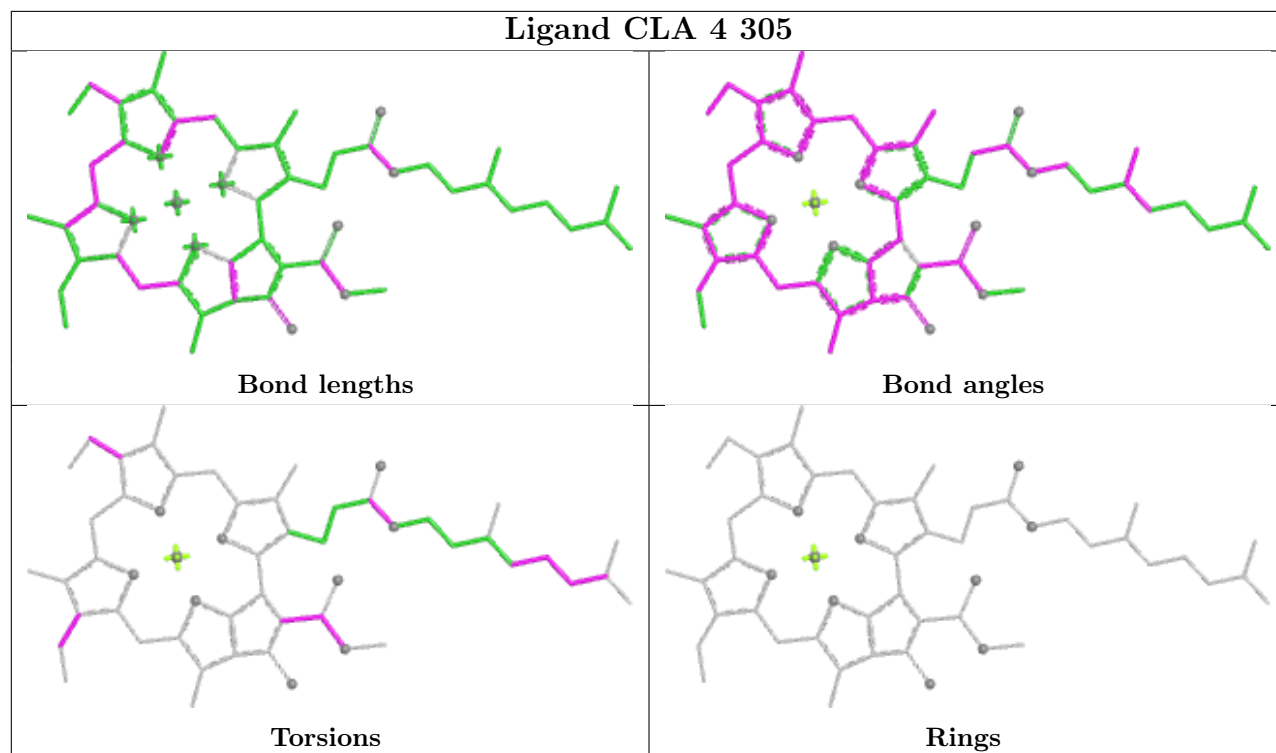
Bond angles



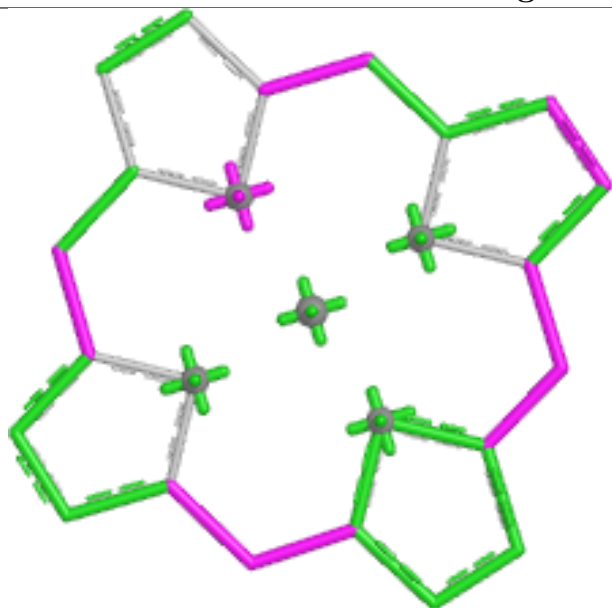
Torsions



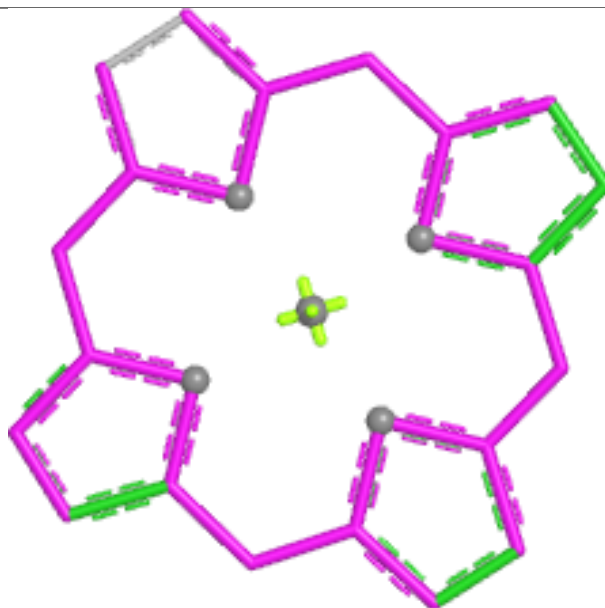
Rings



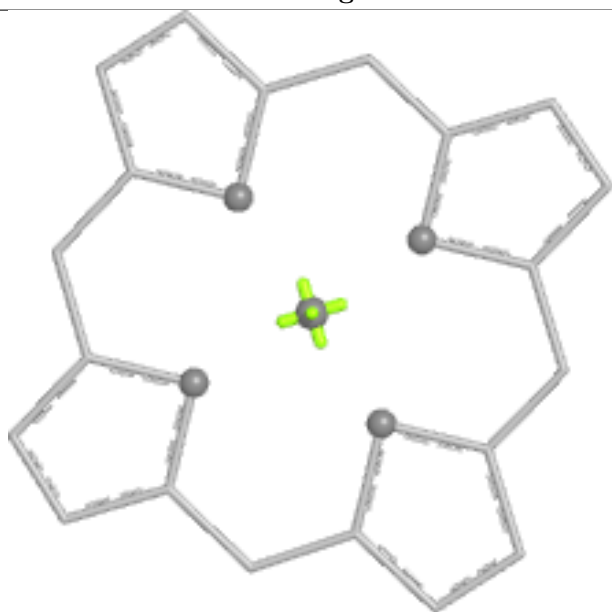
Ligand CLA 2 315



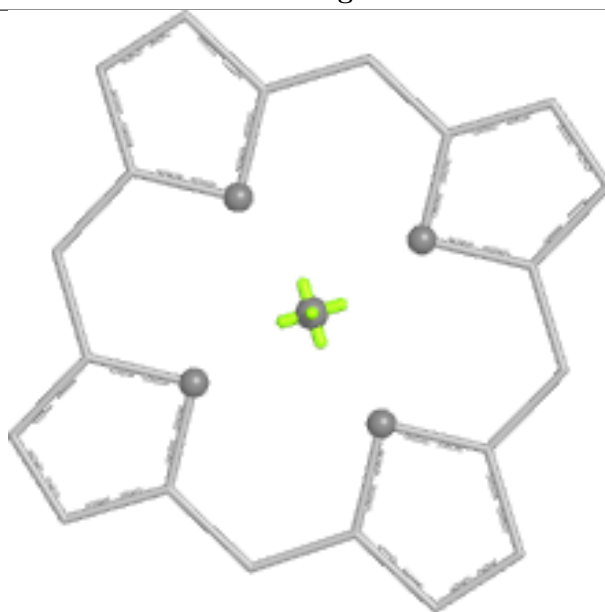
Bond lengths



Bond angles

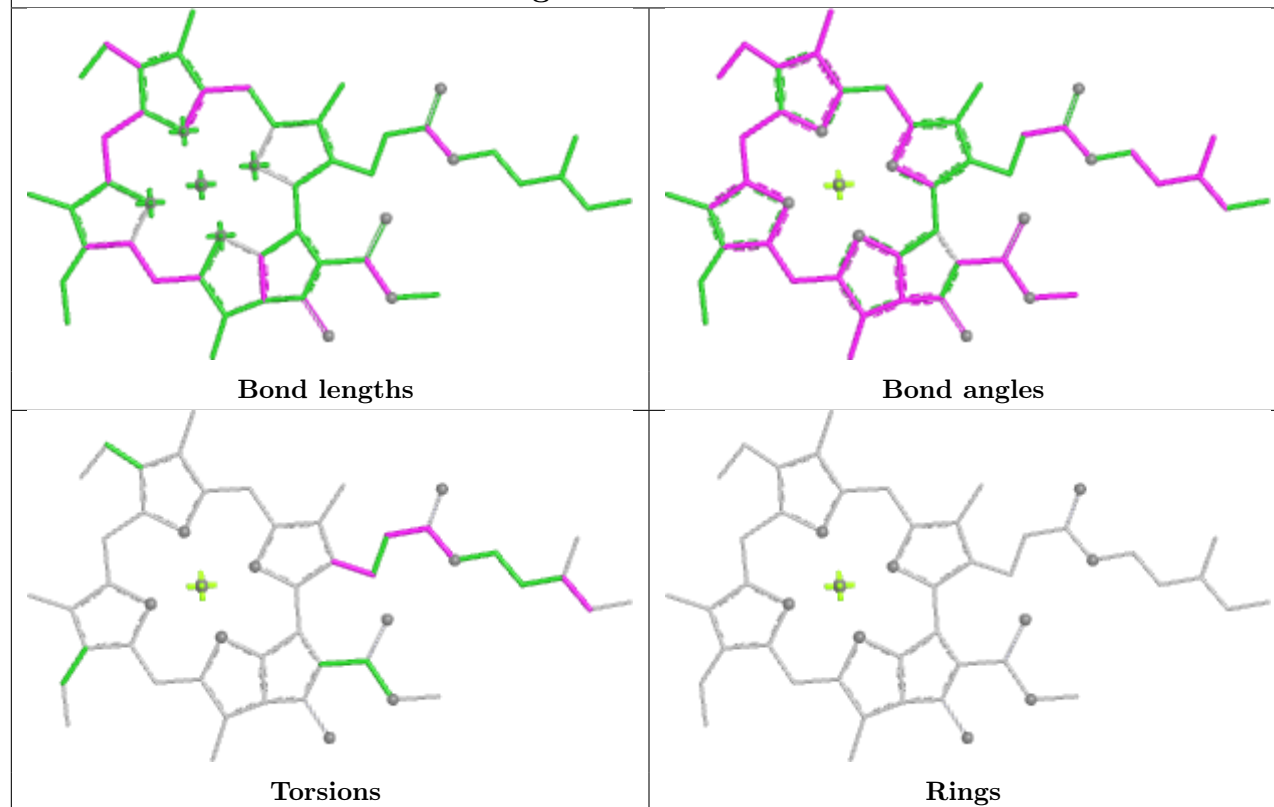


Torsions

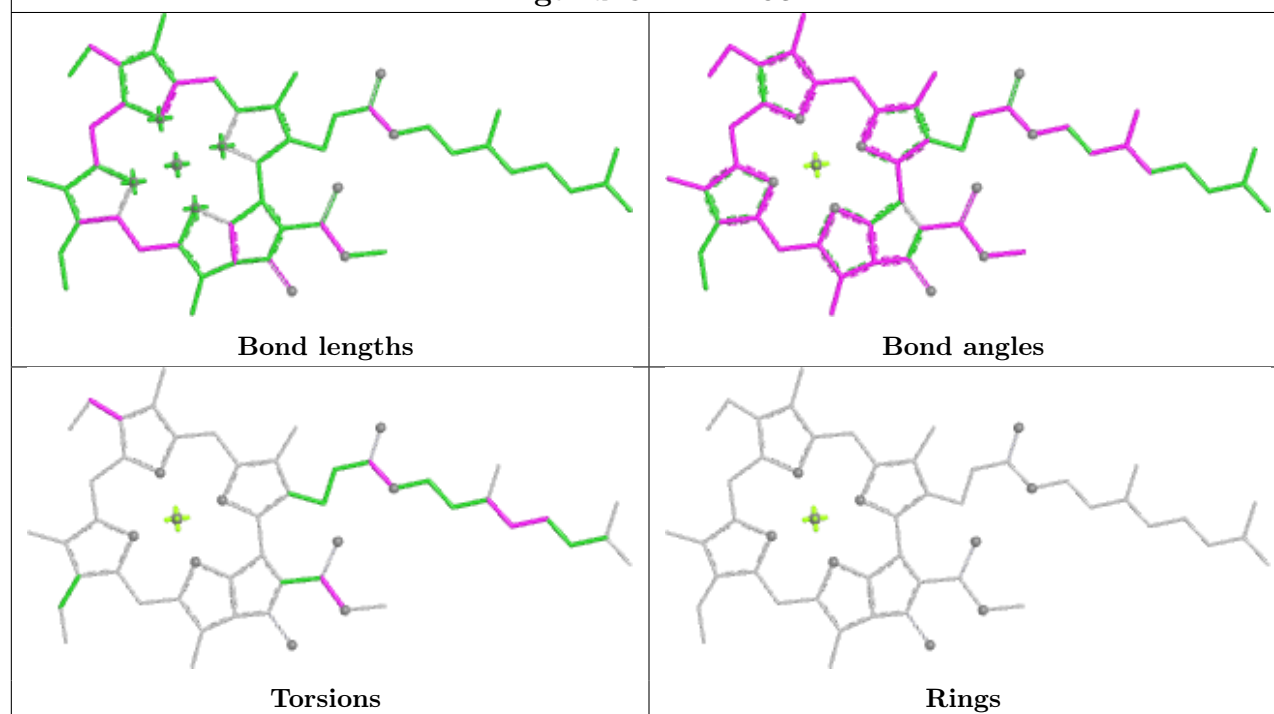


Rings

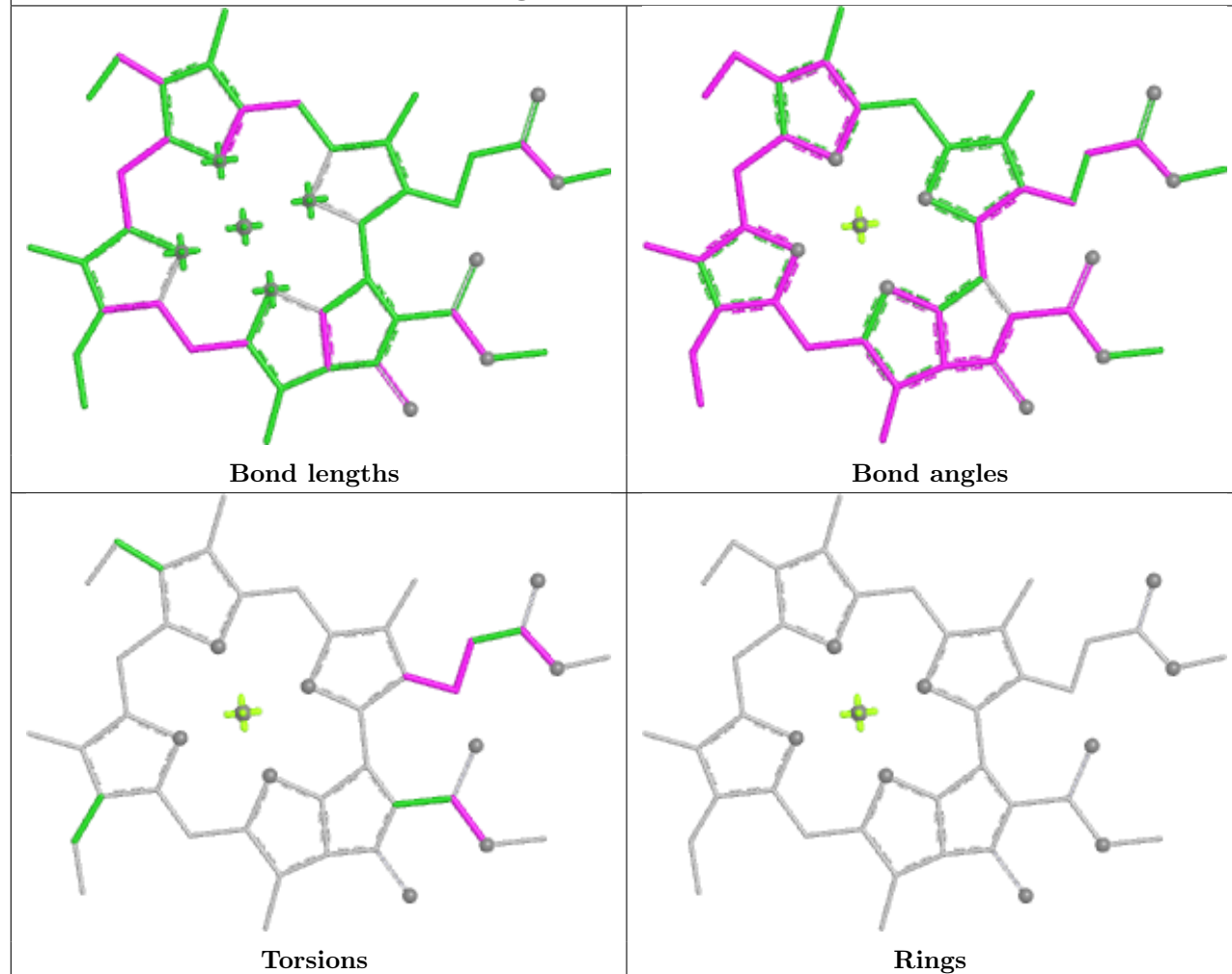
Ligand CLA B 833



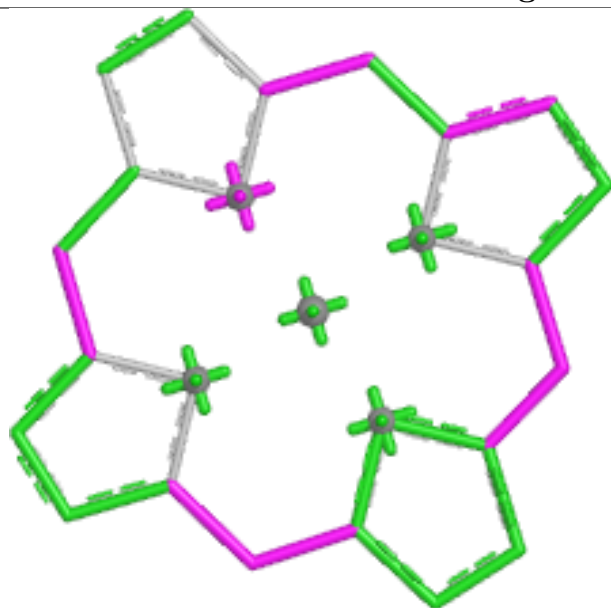
Ligand CLA L 203



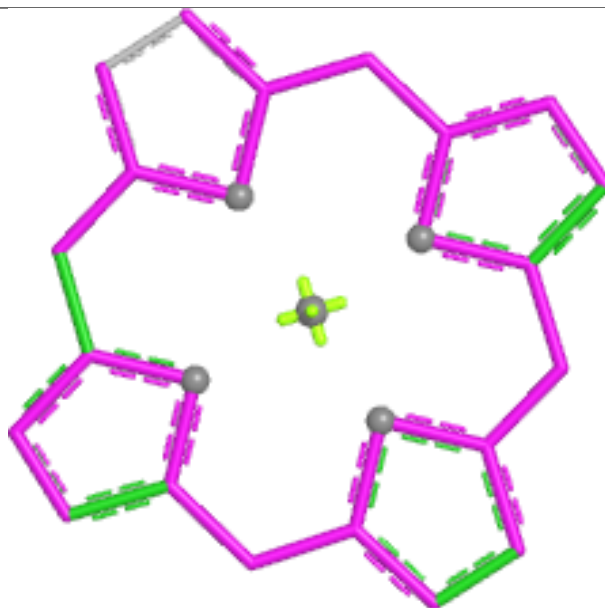
Ligand CLA A 805



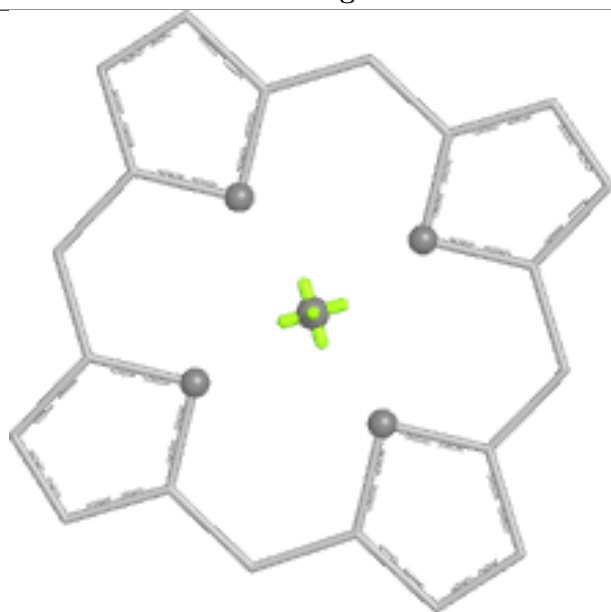
Ligand CLA 2 309



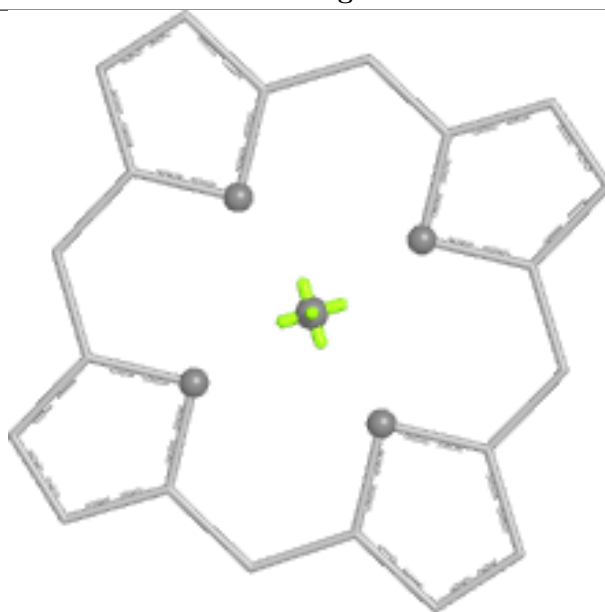
Bond lengths



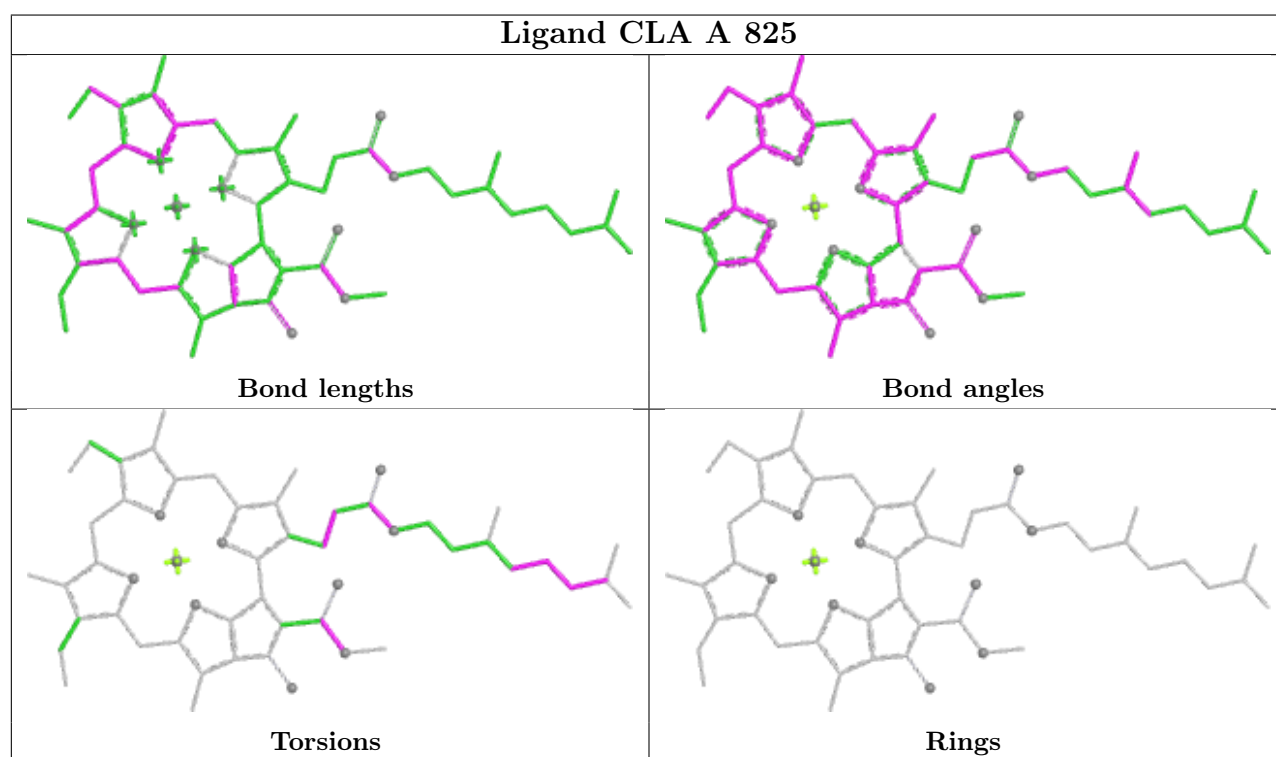
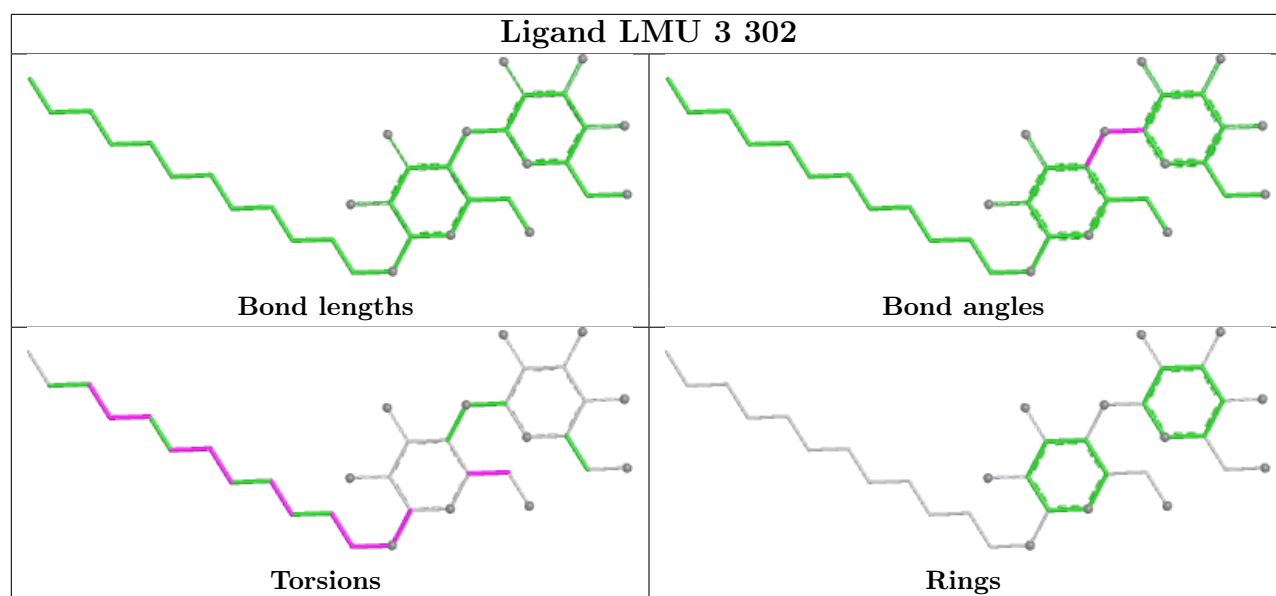
Bond angles



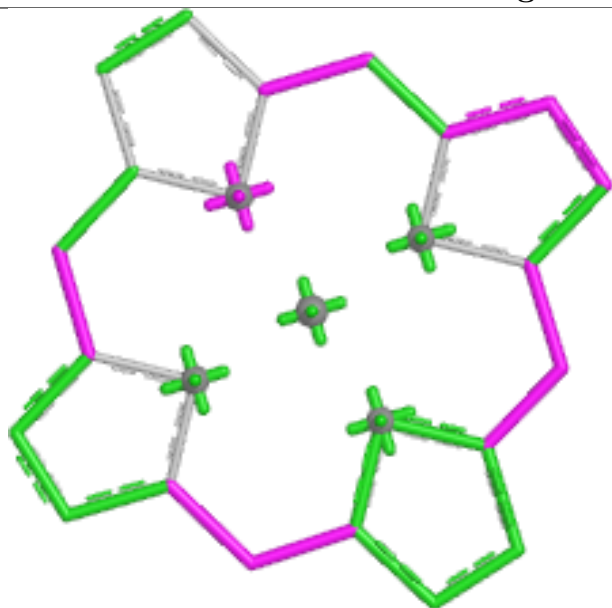
Torsions



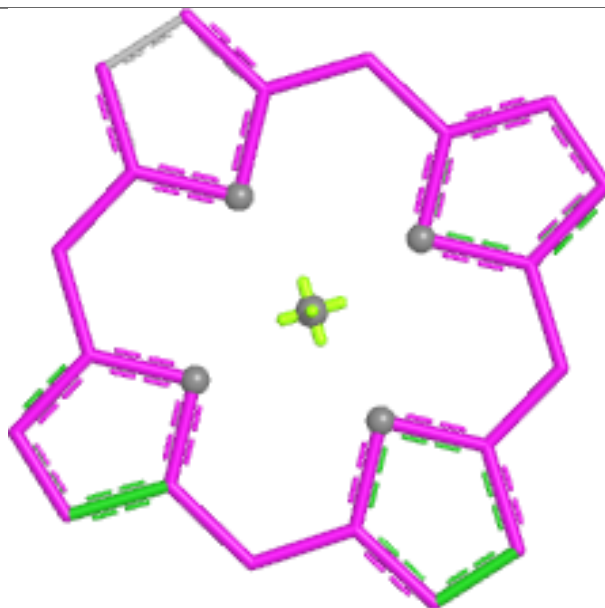
Rings



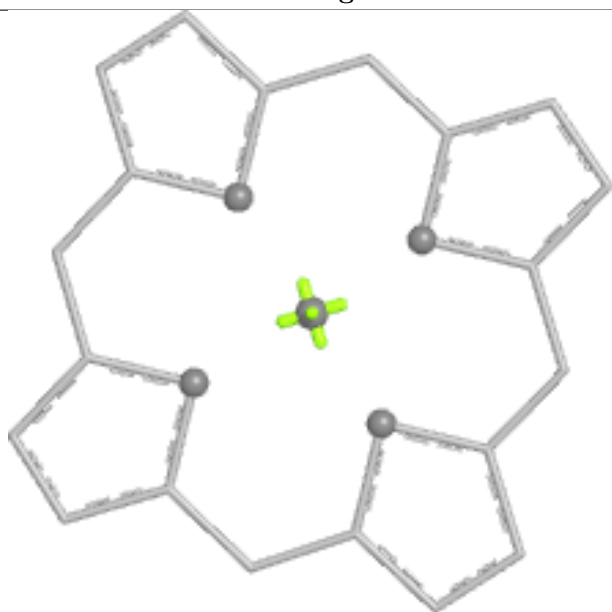
Ligand CLA 3 312



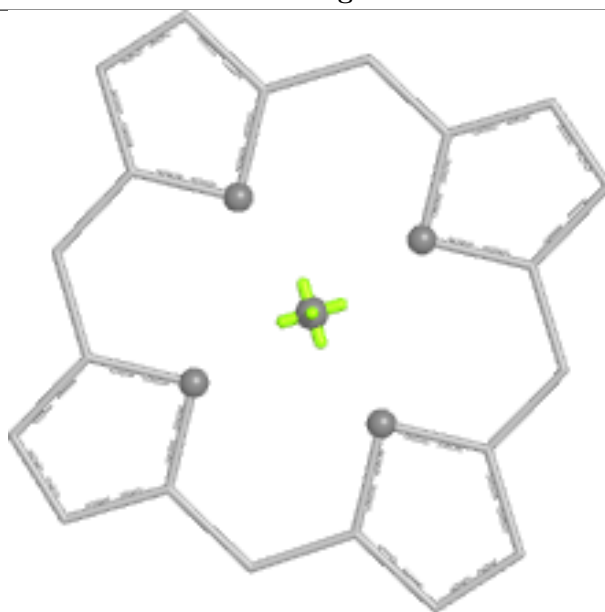
Bond lengths



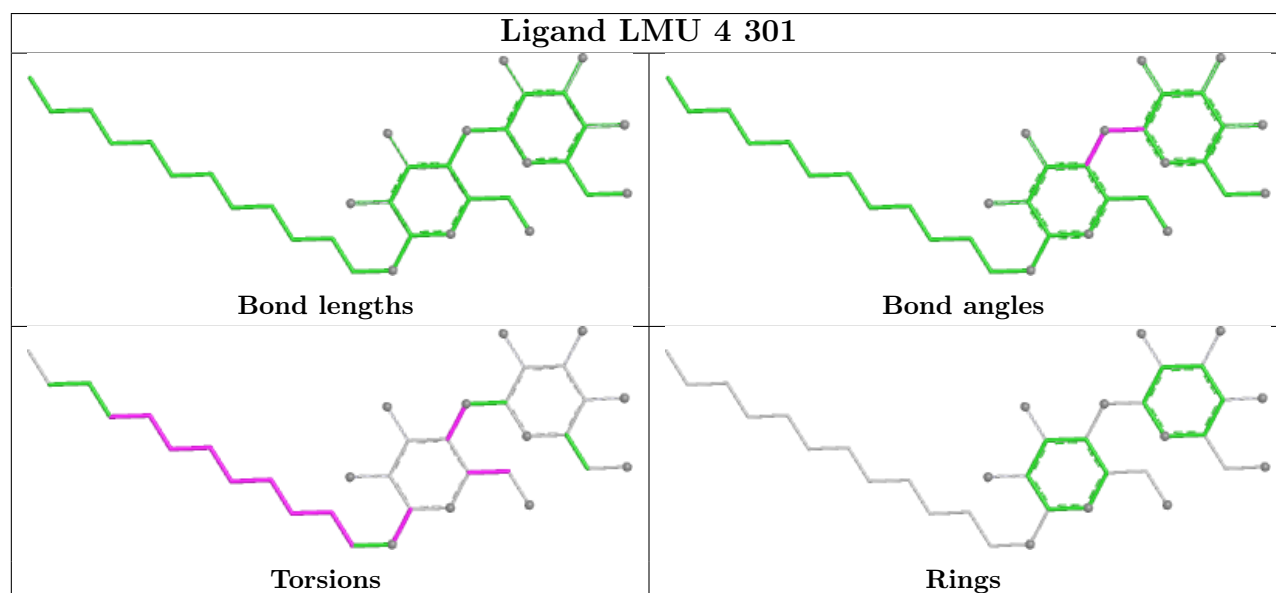
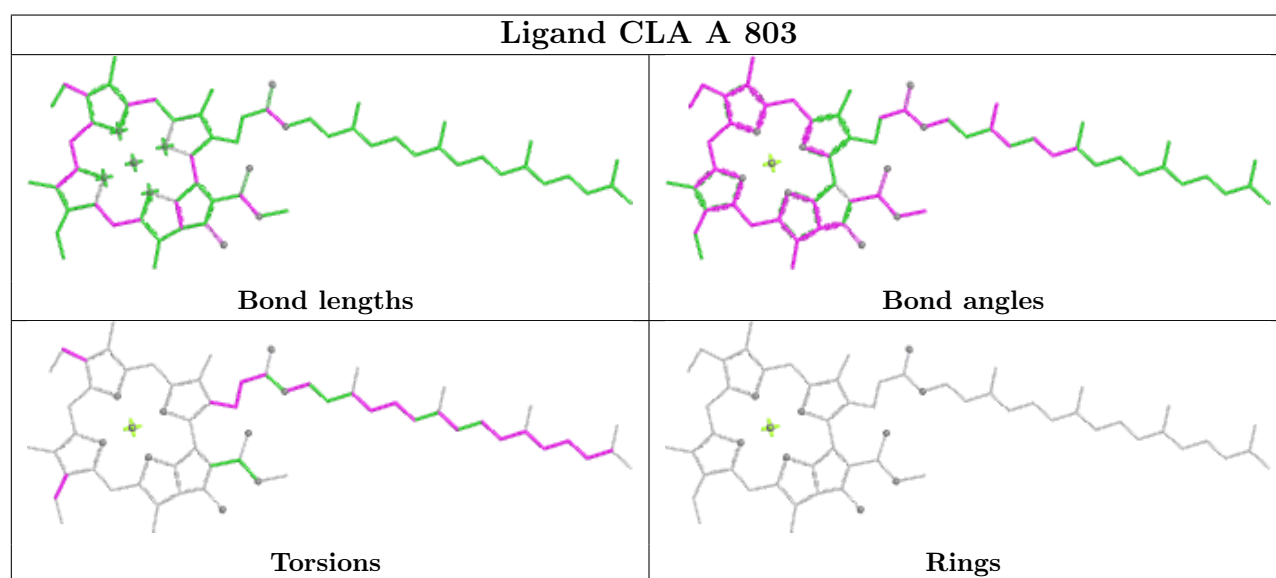
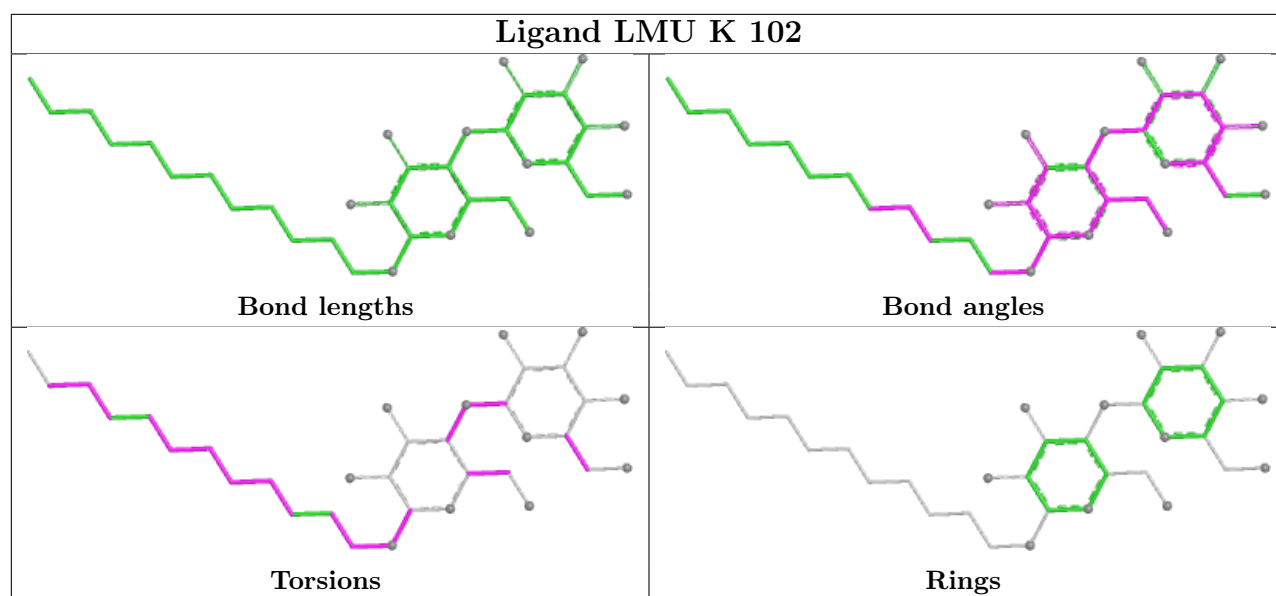
Bond angles

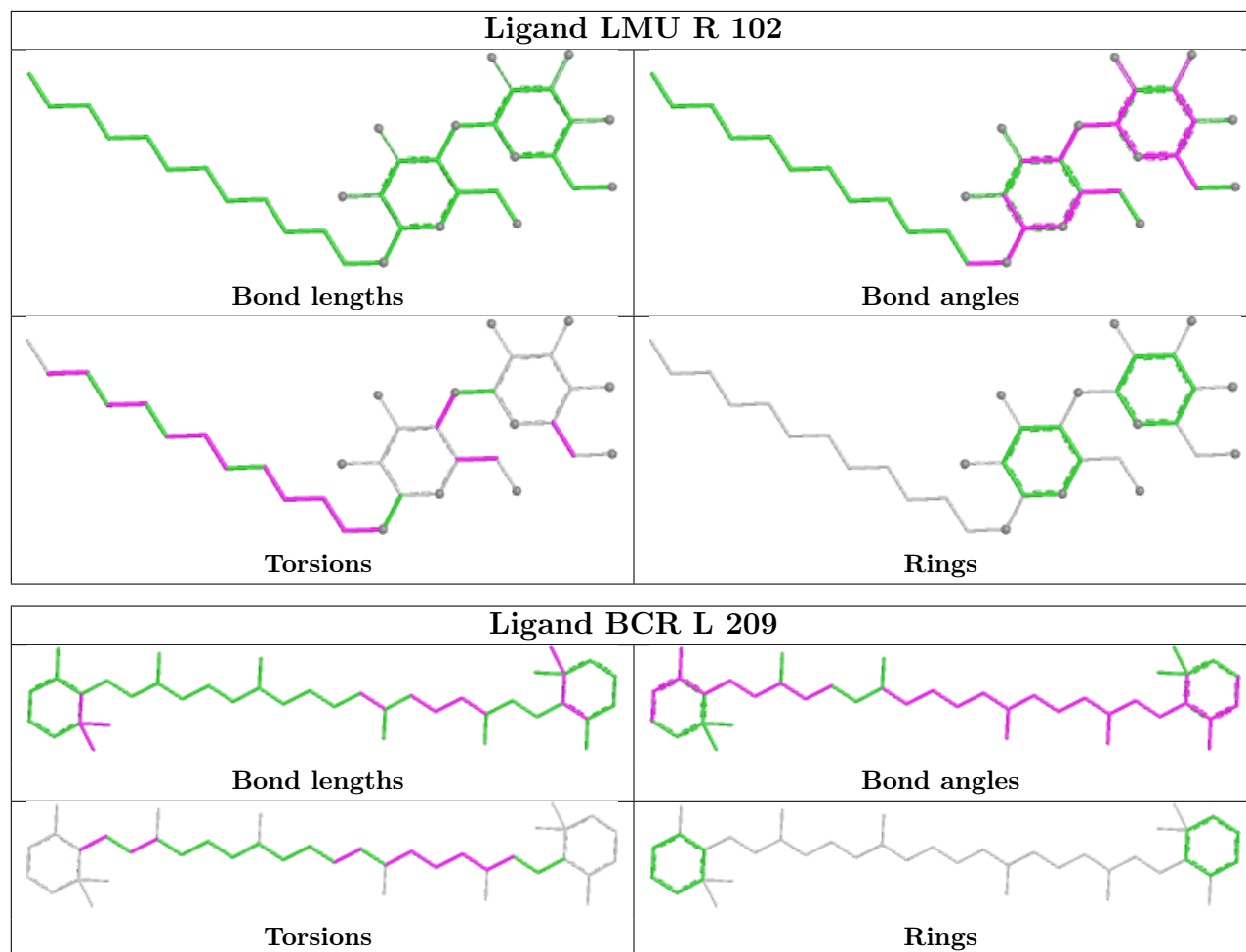


Torsions

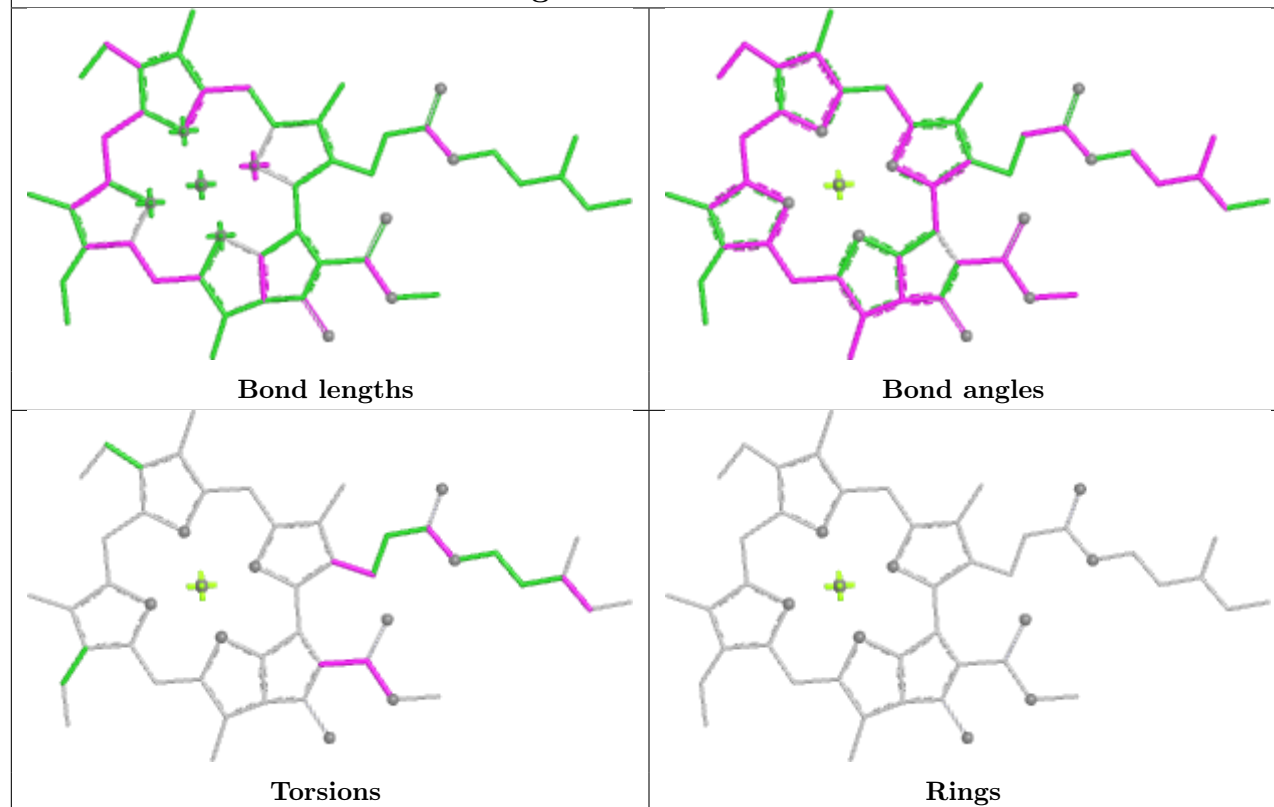


Rings

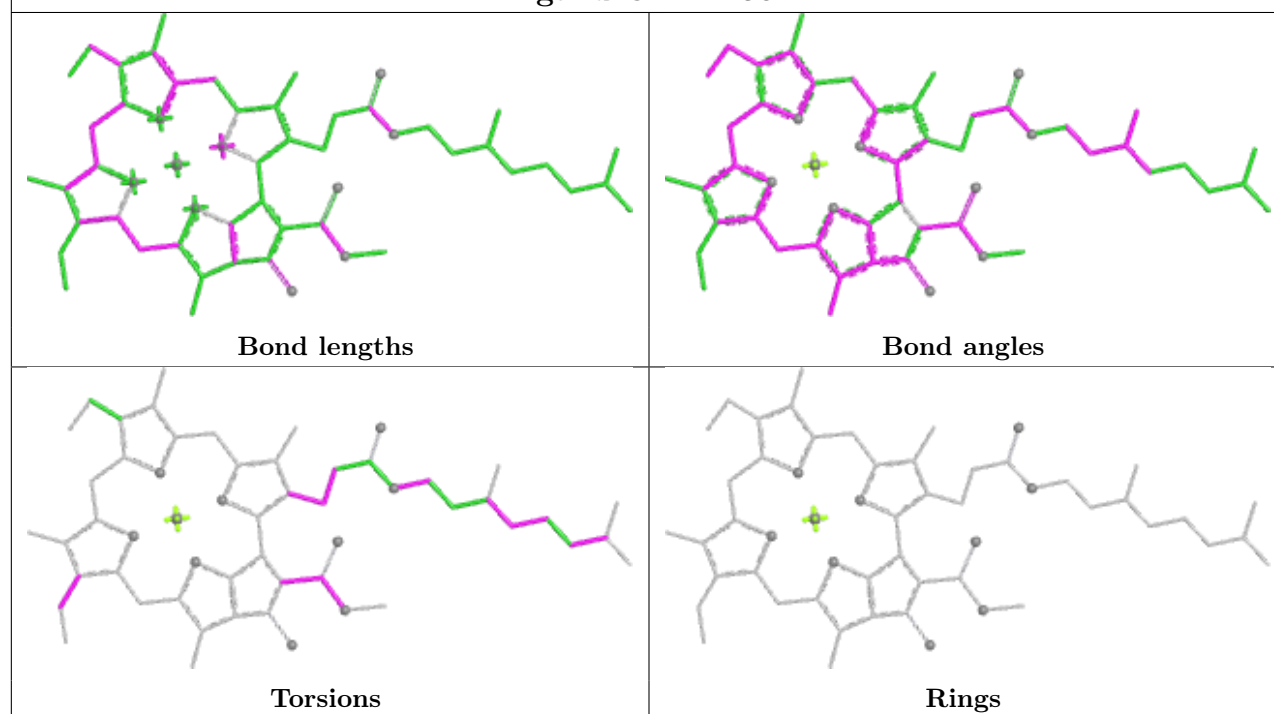


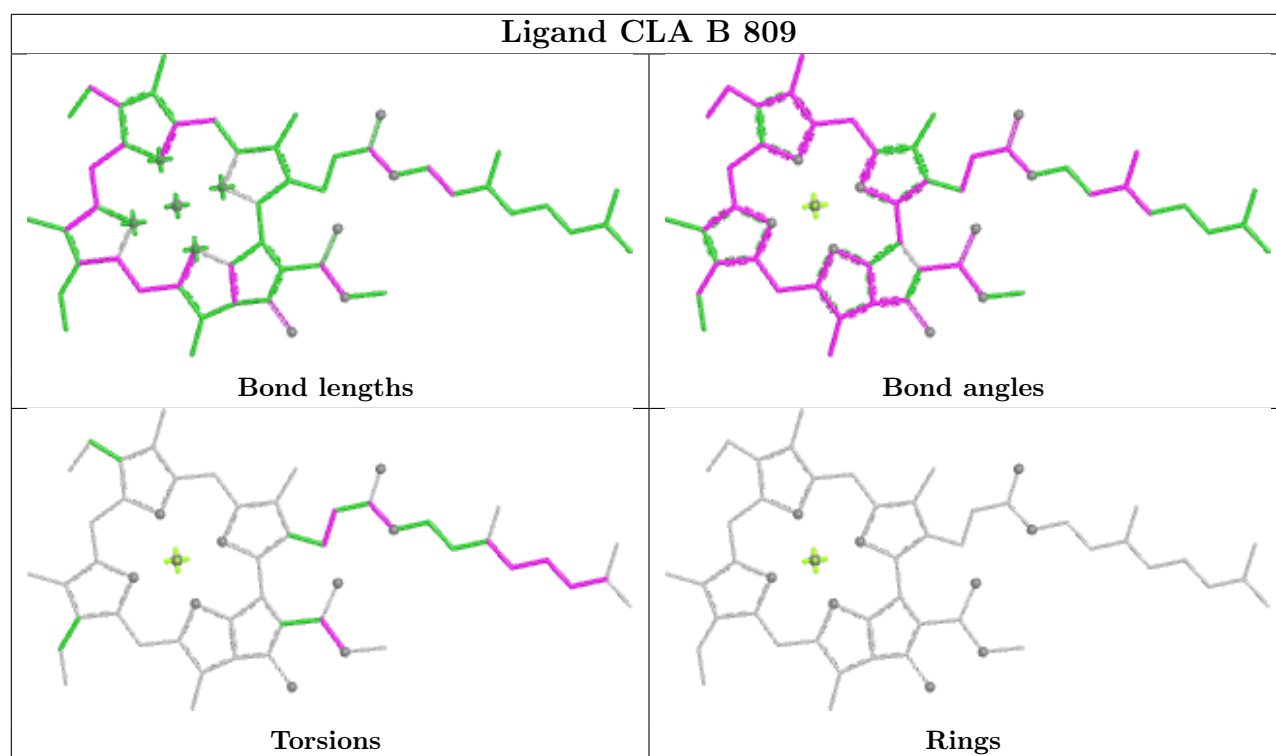


Ligand CLA A 818

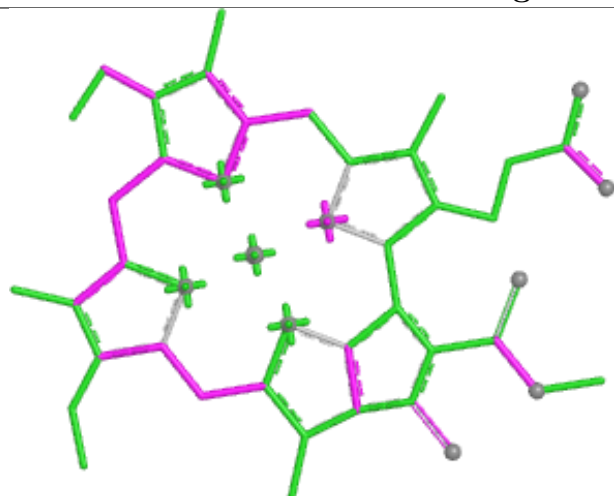


Ligand CLA 4 302

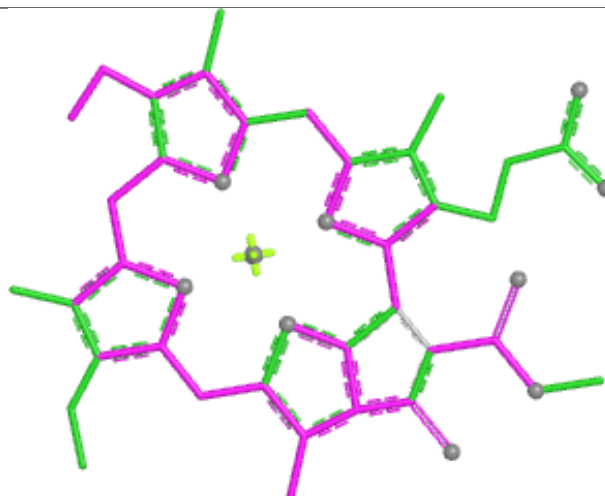




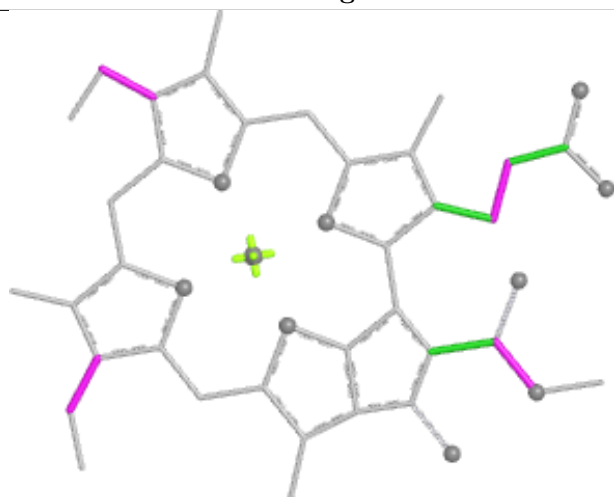
Ligand CLA K 105



Bond lengths



Bond angles

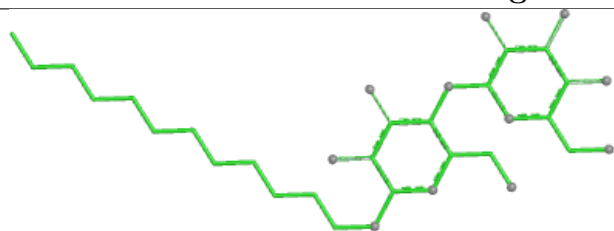


Torsions

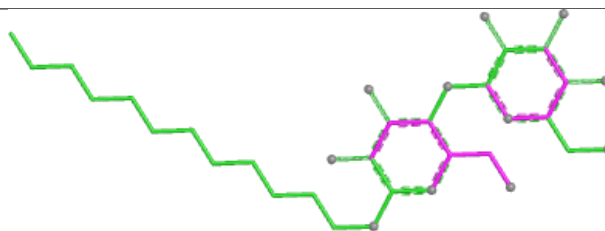


Rings

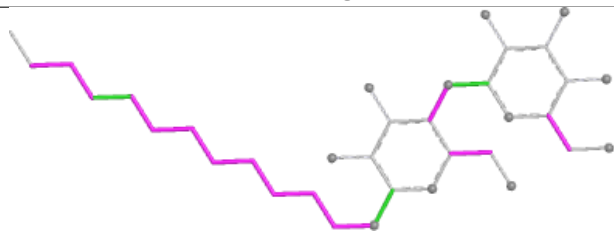
Ligand LMU A 845



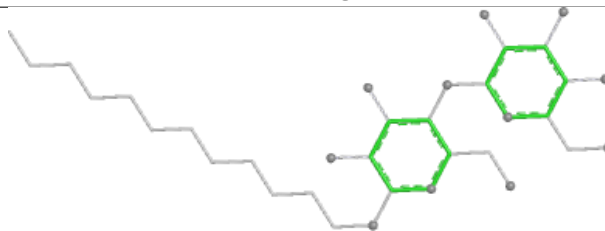
Bond lengths



Bond angles

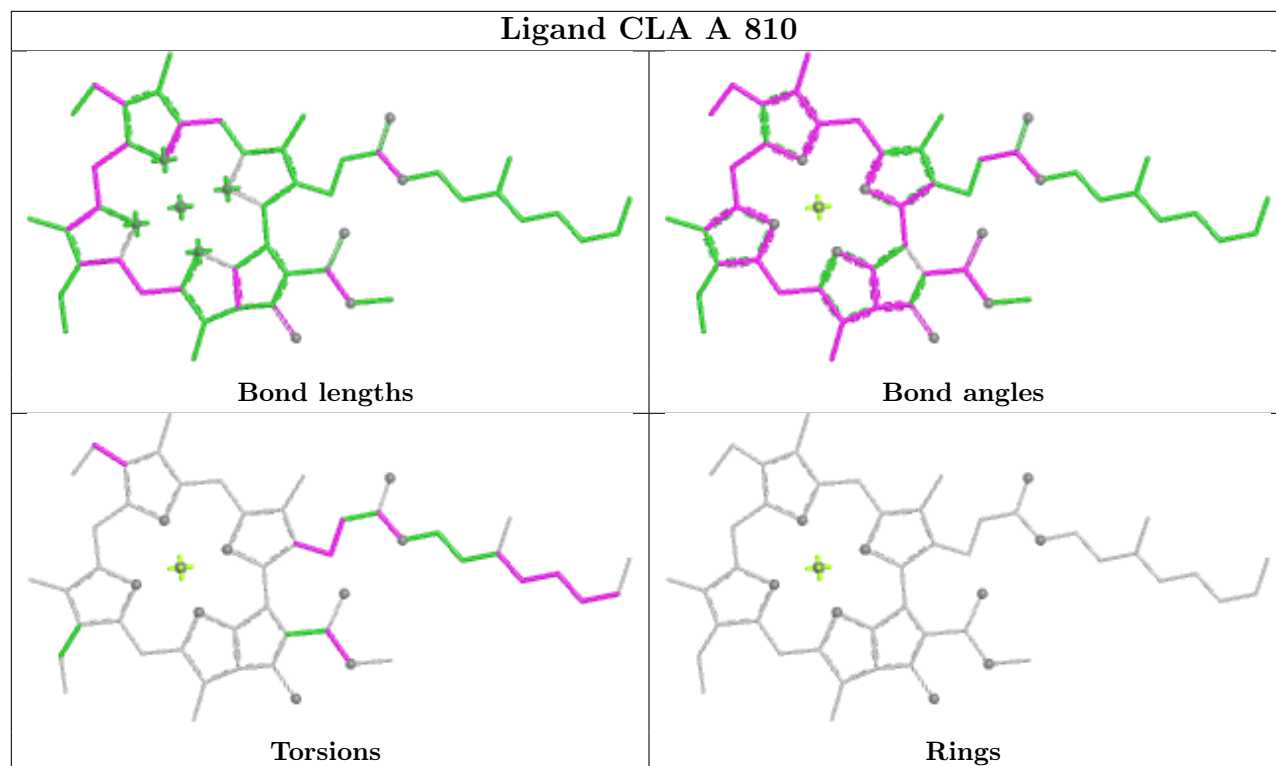


Torsions

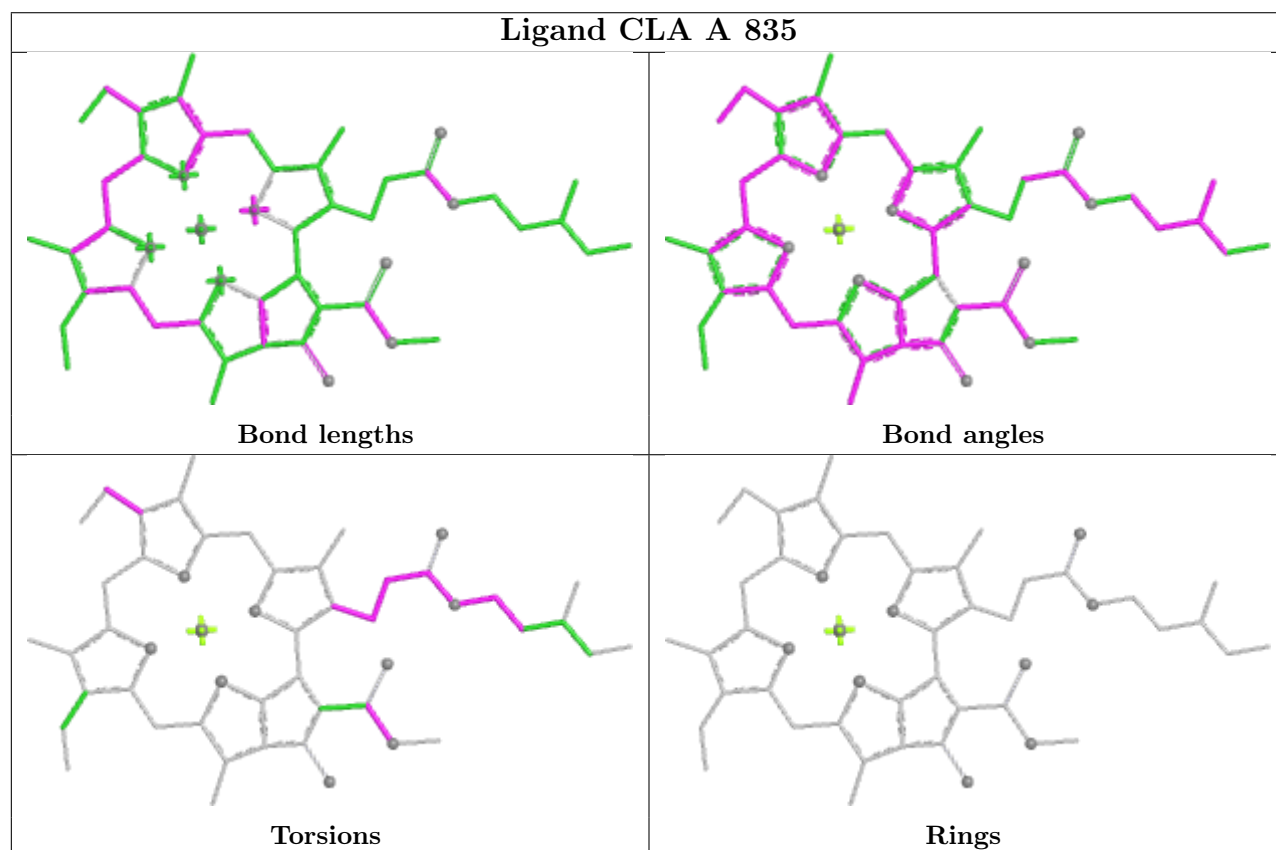


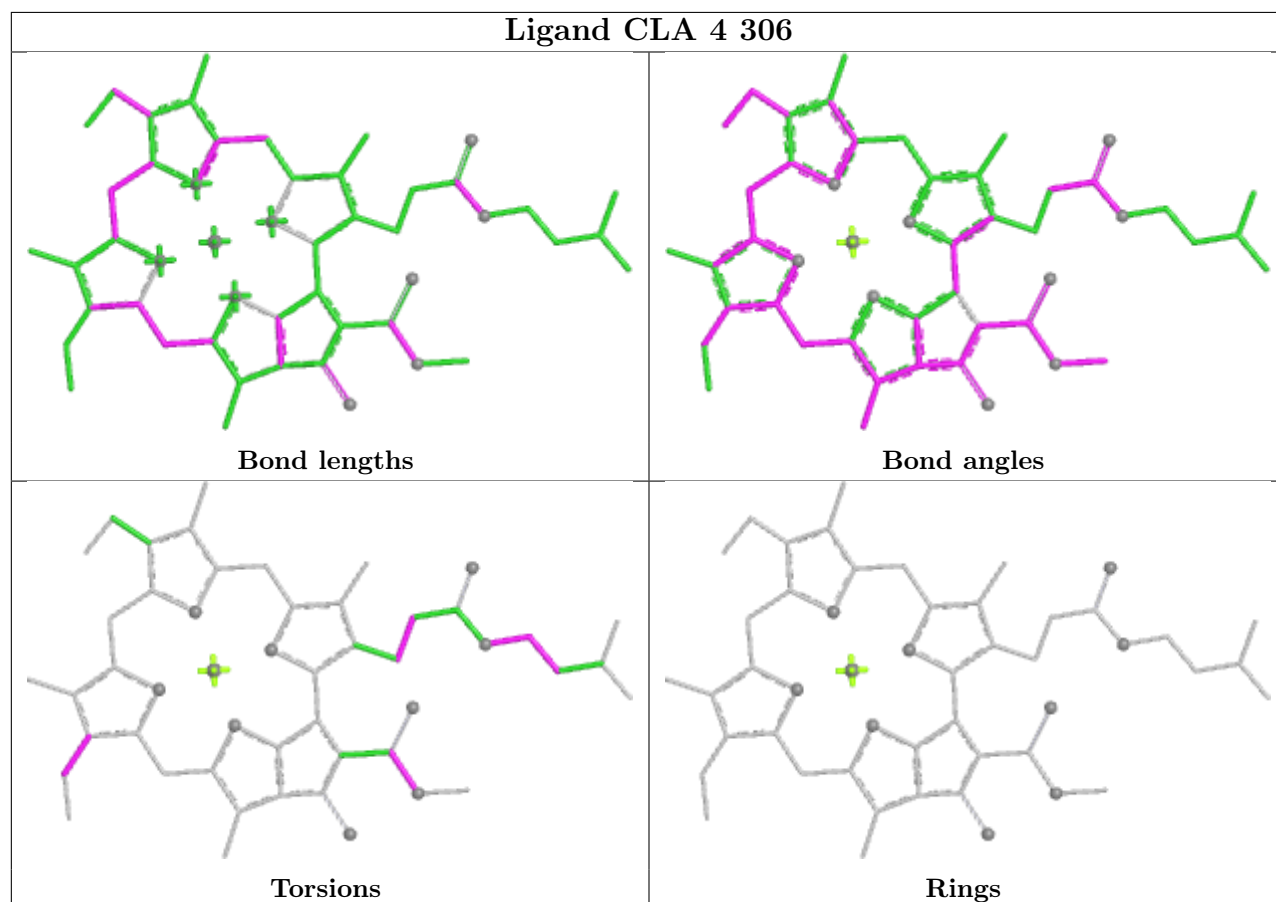
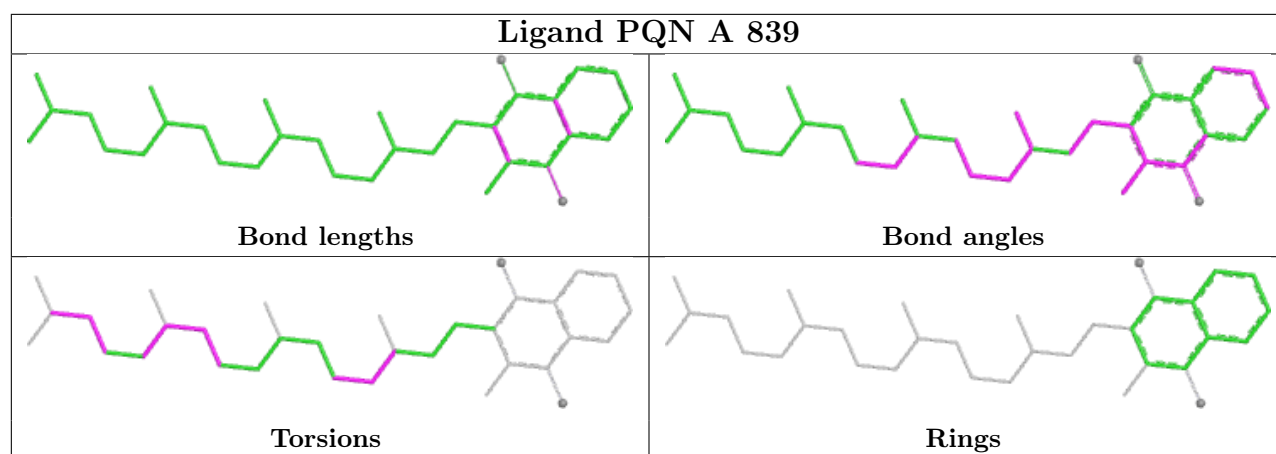
Rings

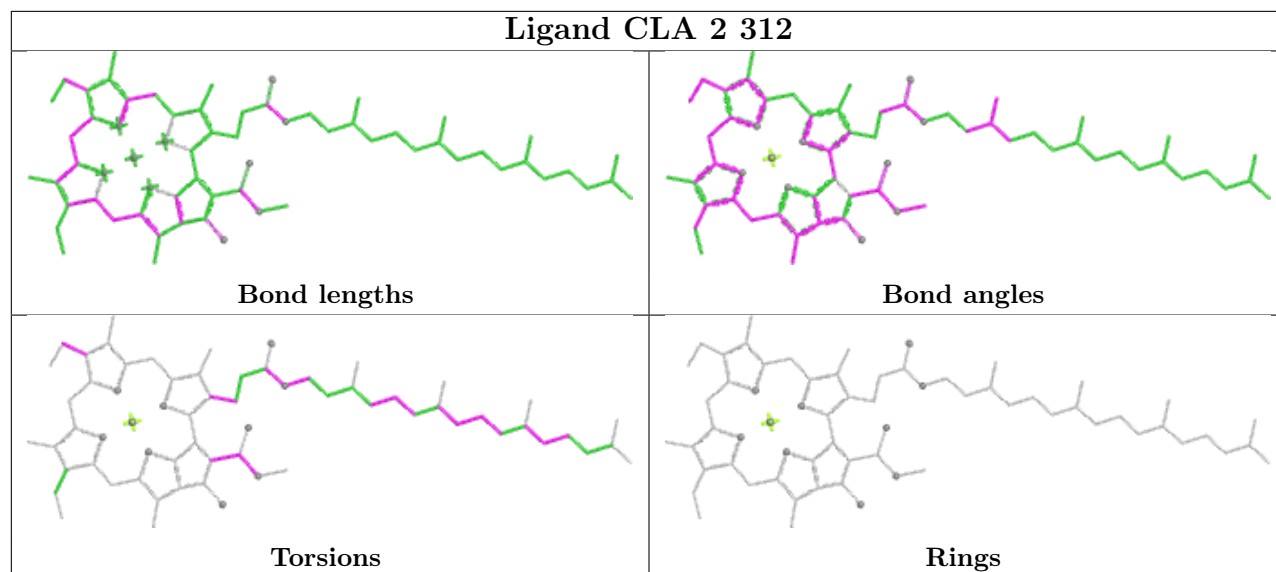
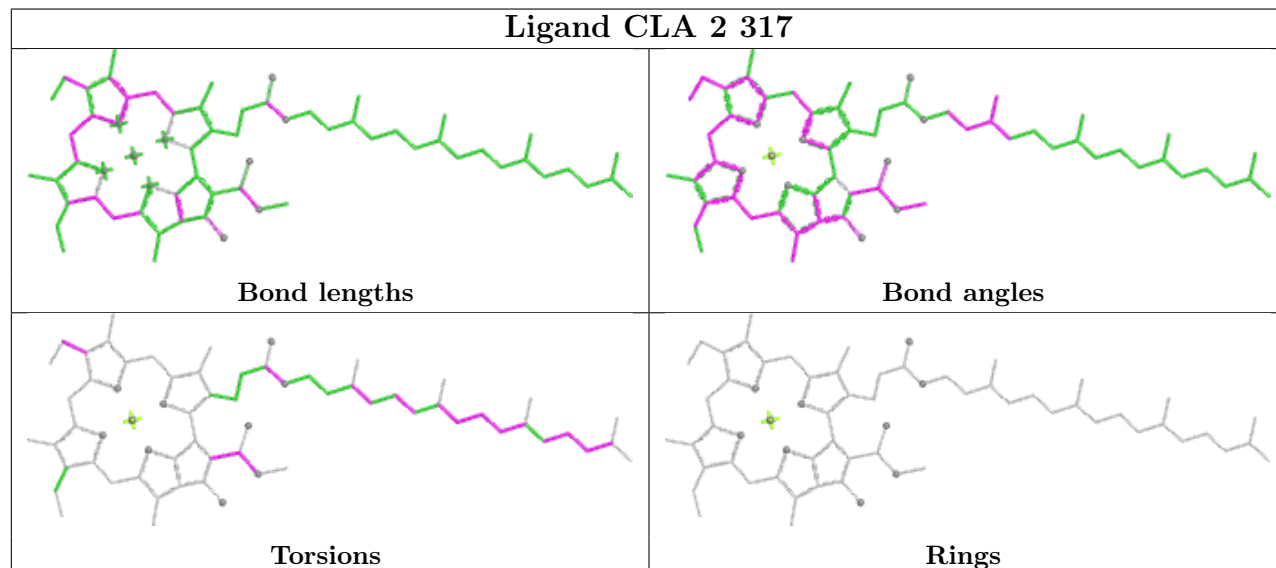
Ligand CLA A 810



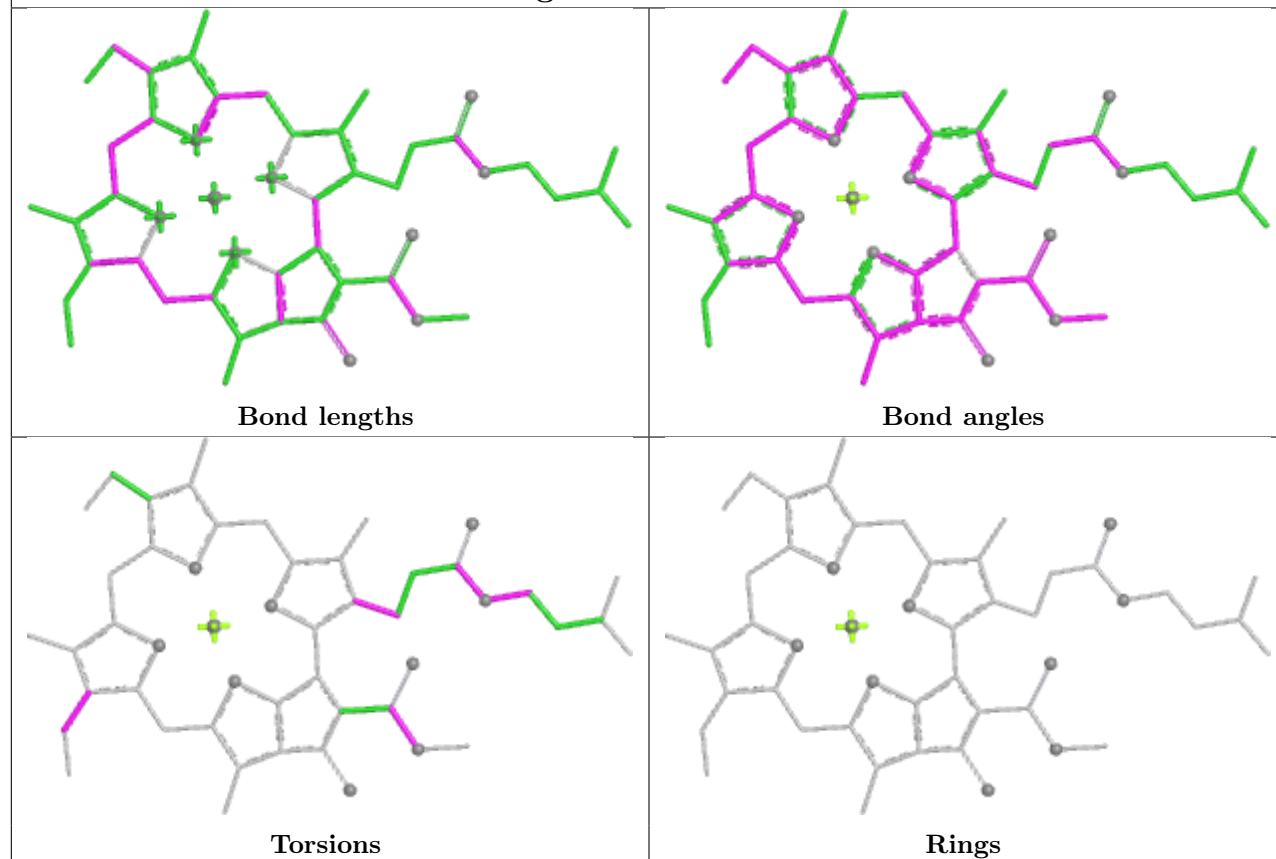
Ligand CLA A 835



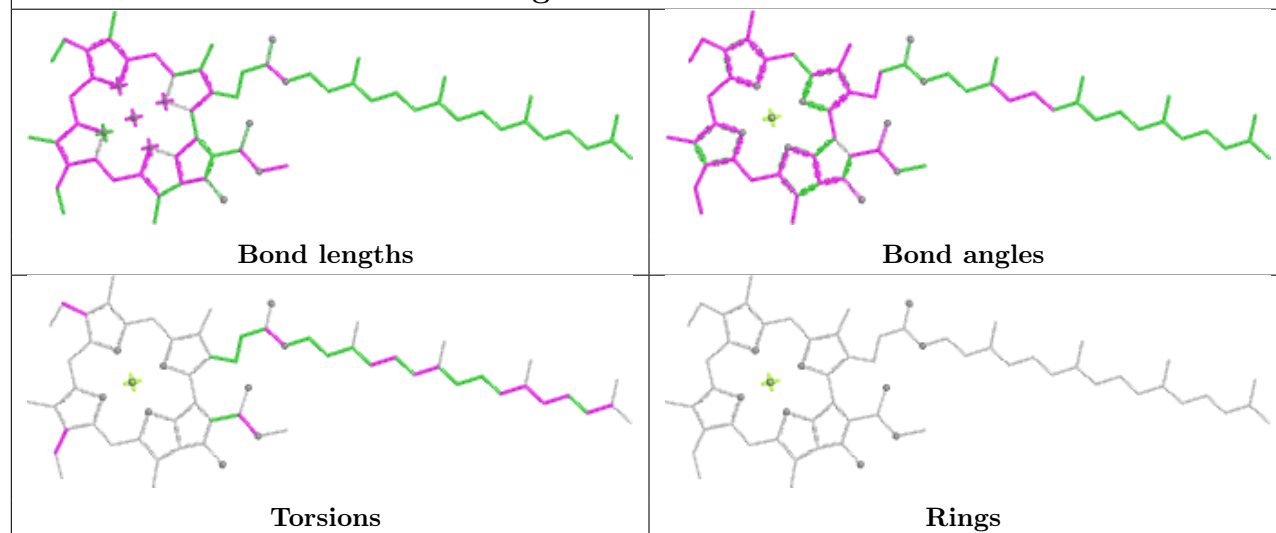


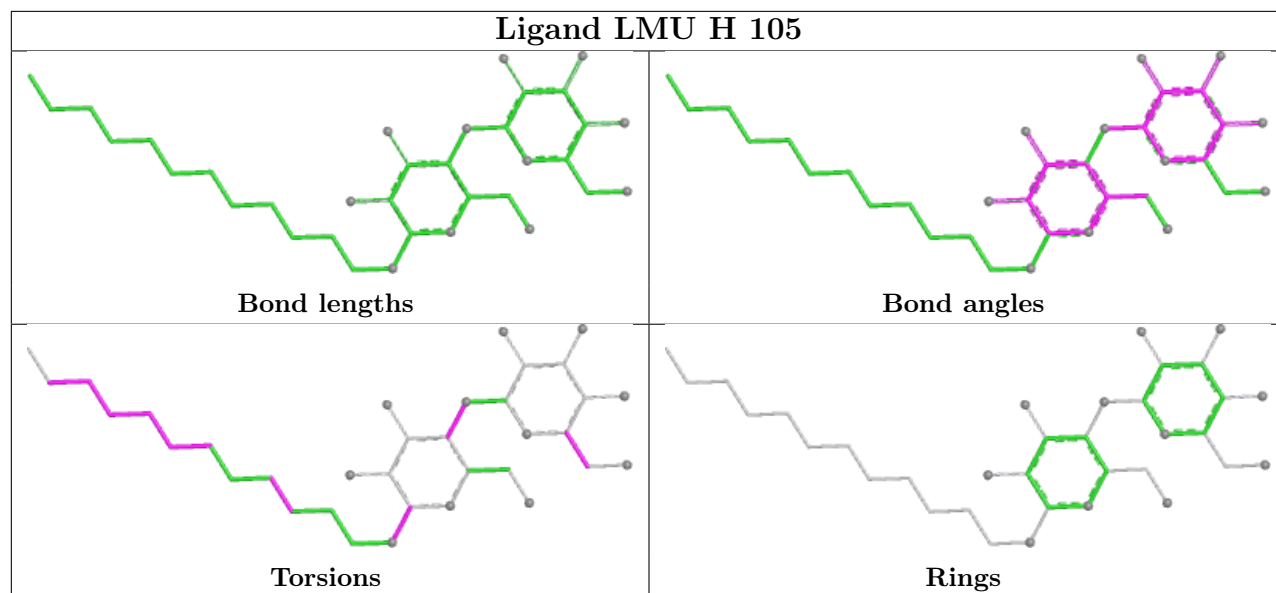
Ligand CLA 2 312**Ligand CLA 2 317**

Ligand CLA 2 304

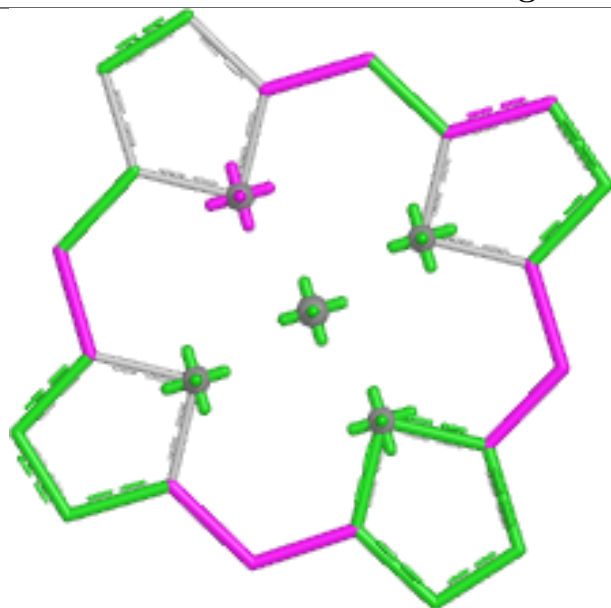


Ligand CLA B 820

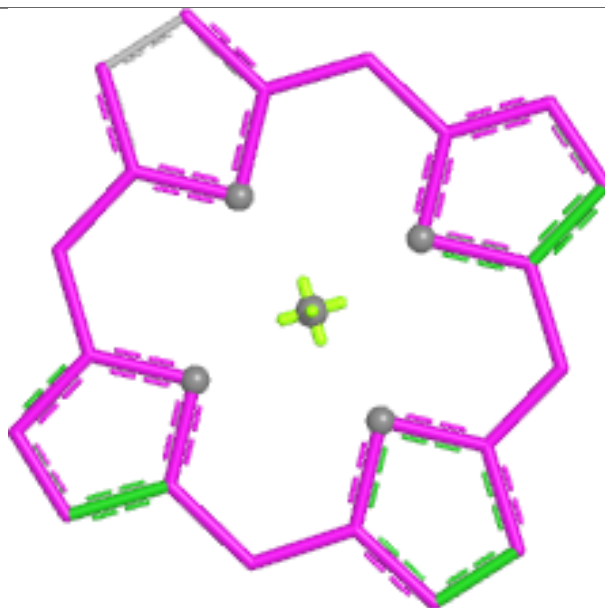




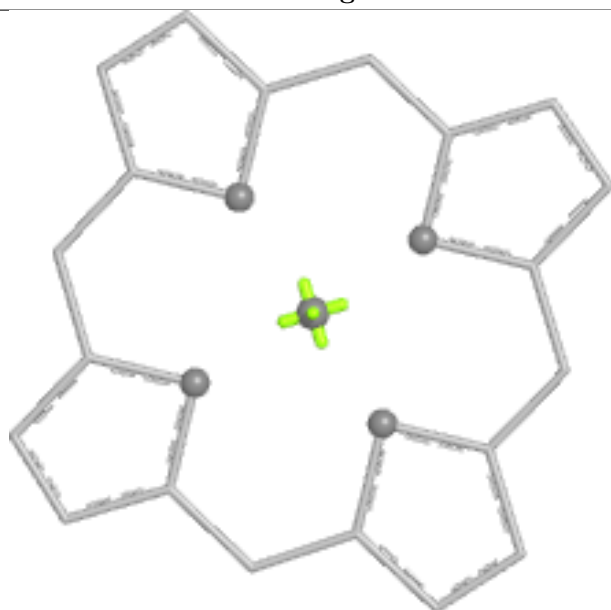
Ligand CLA 2 308



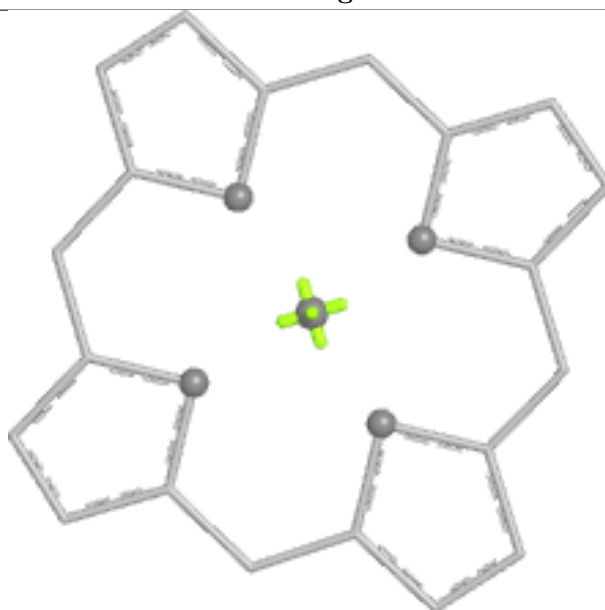
Bond lengths



Bond angles

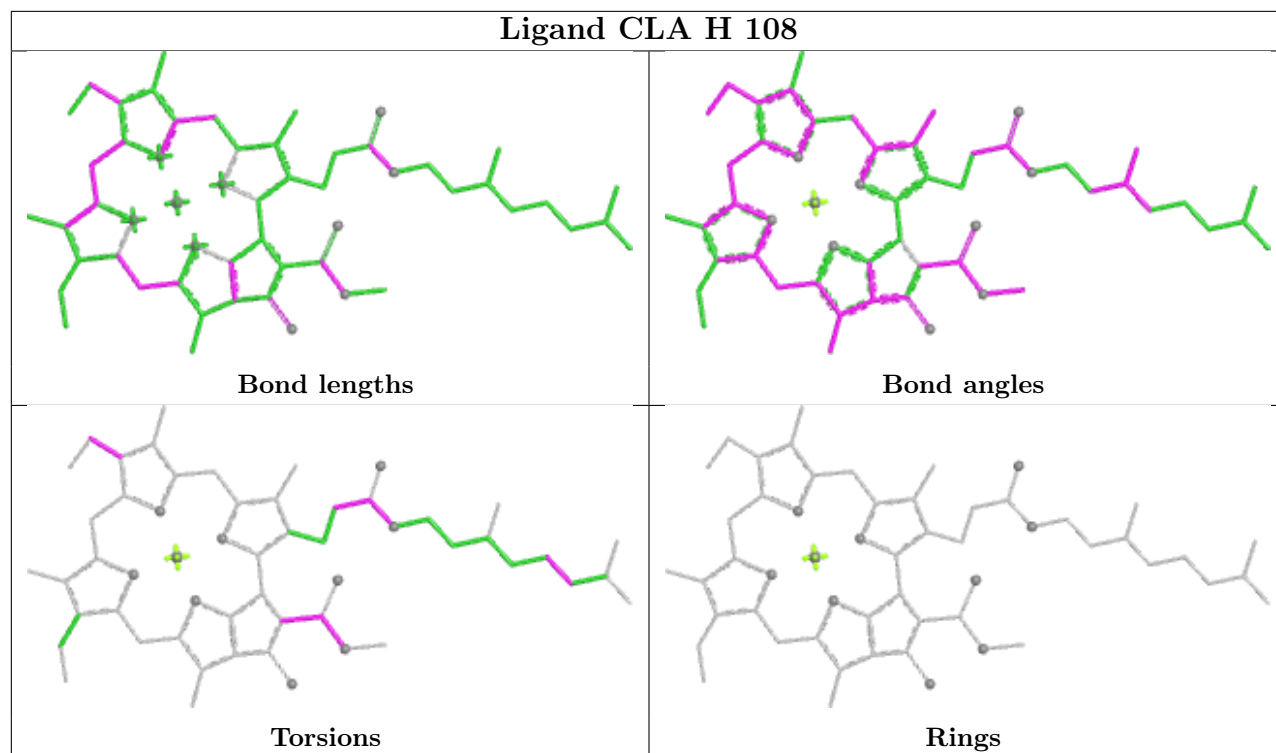


Torsions

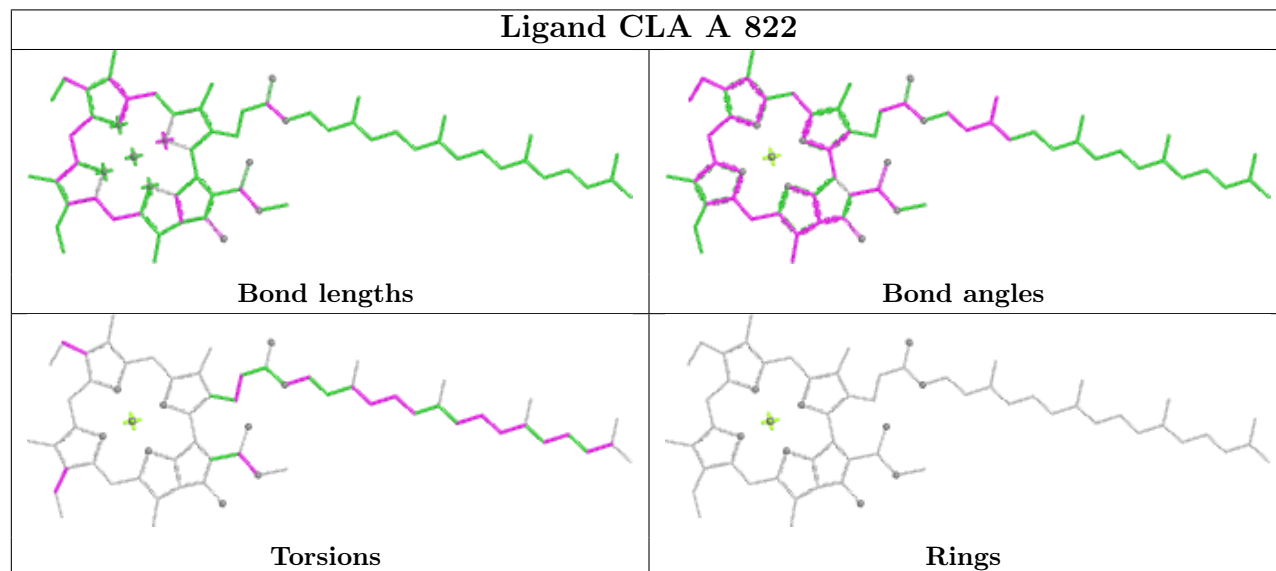


Rings

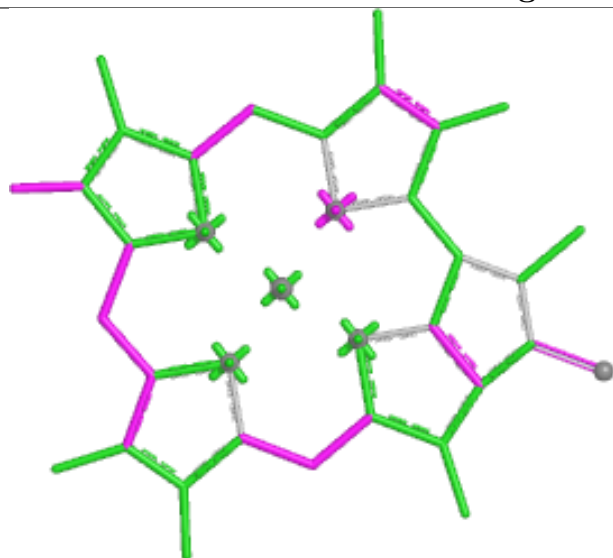
Ligand CLA H 108



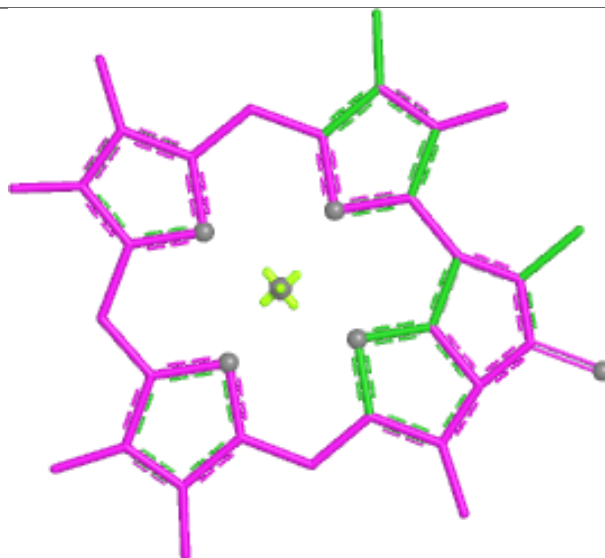
Ligand CLA A 822



Ligand CLA 4 313



Bond lengths



Bond angles

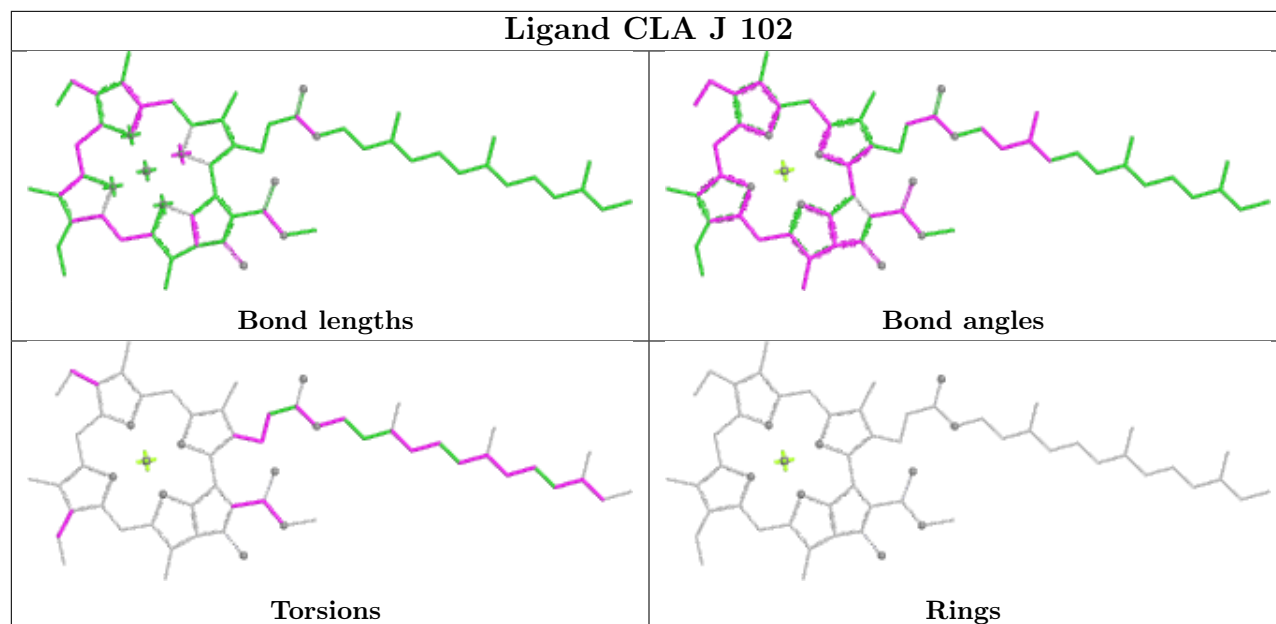


Torsions

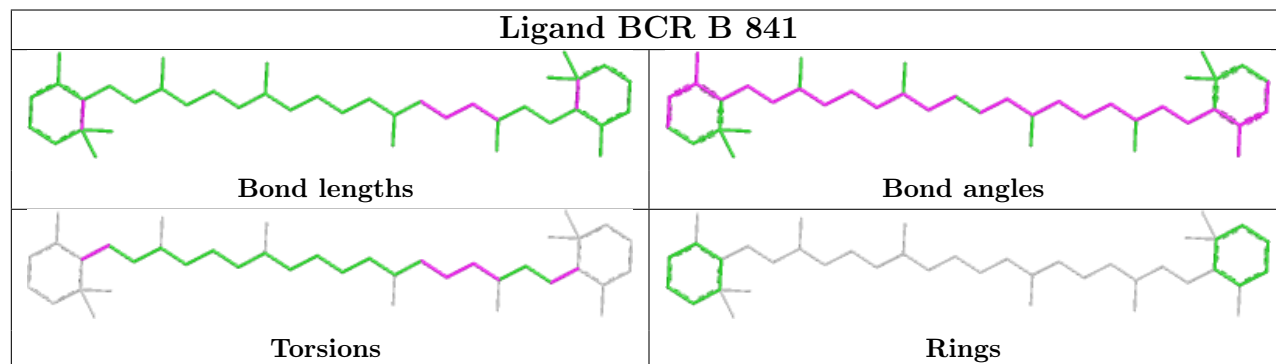


Rings

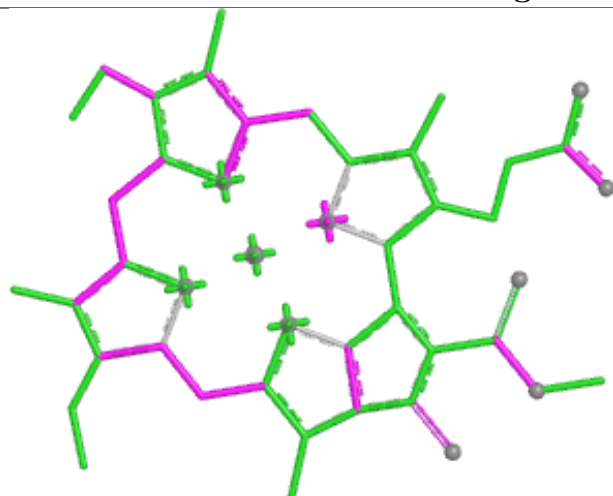
Ligand CLA J 102



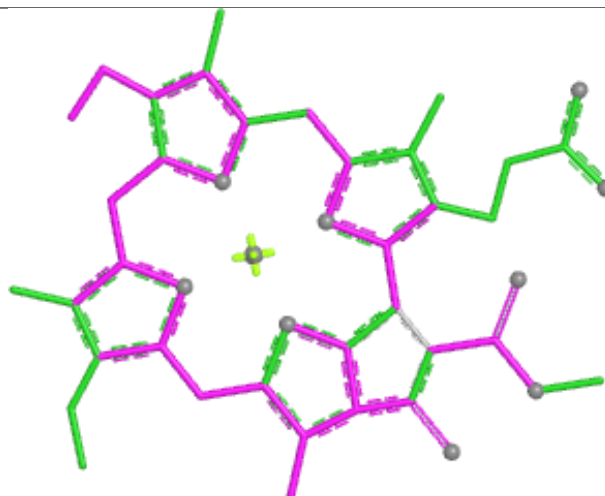
Ligand BCR B 841



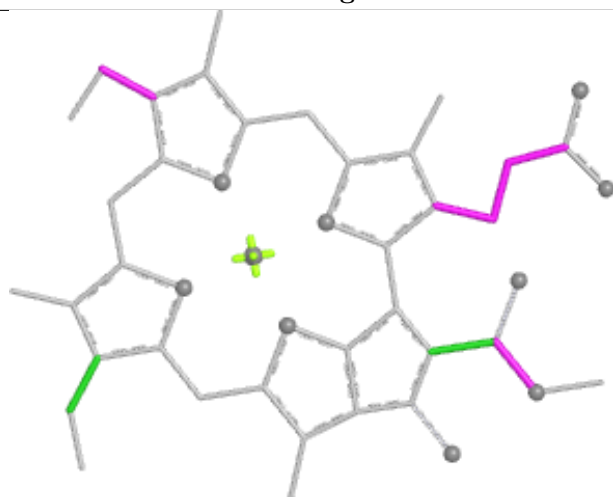
Ligand CLA A 831



Bond lengths



Bond angles

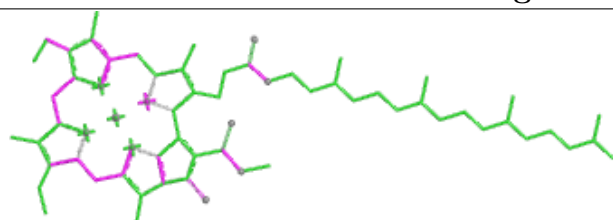


Torsions

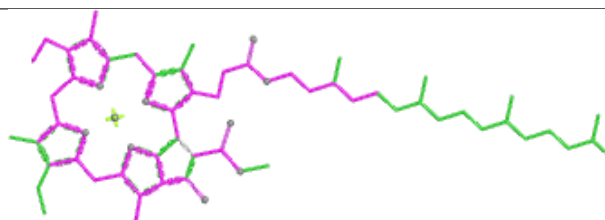


Rings

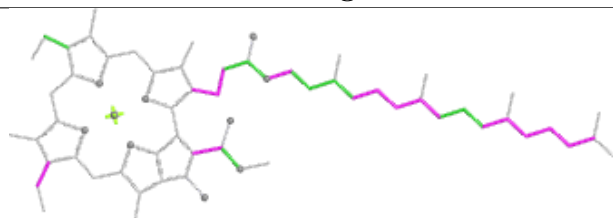
Ligand CLA A 806



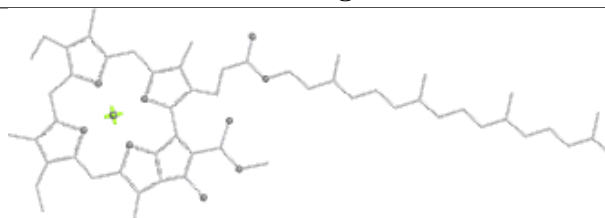
Bond lengths



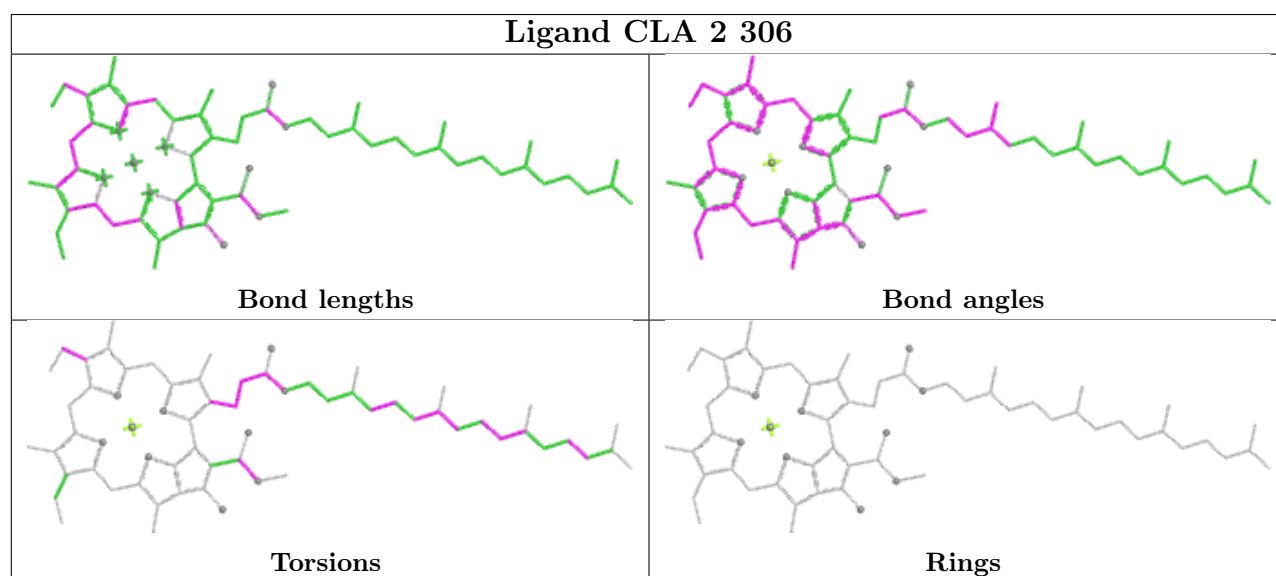
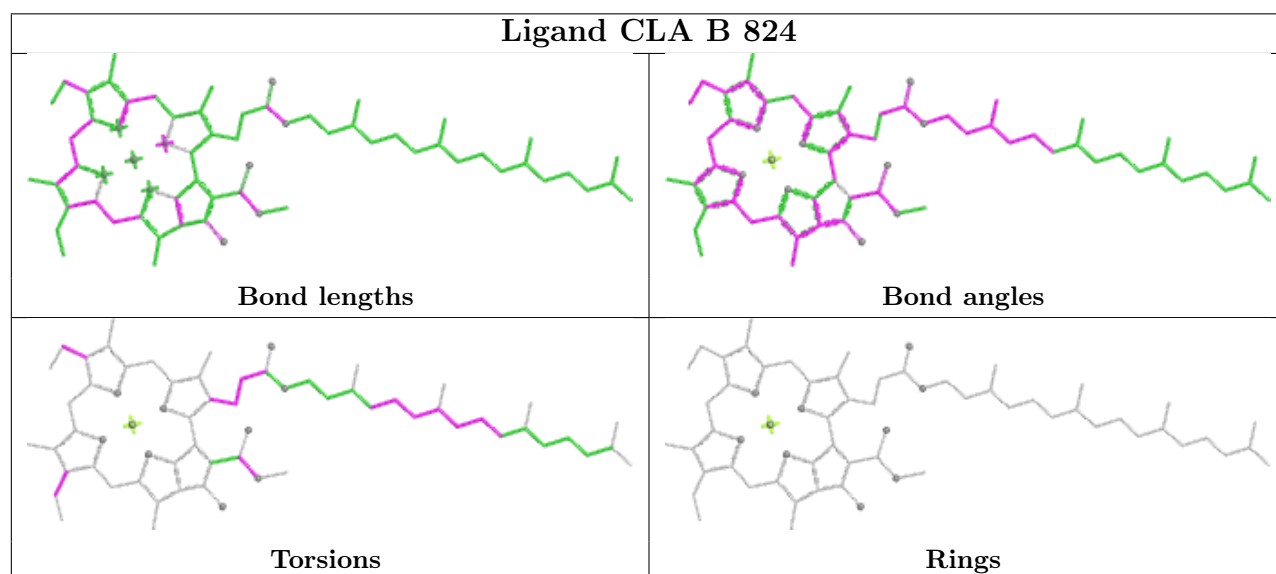
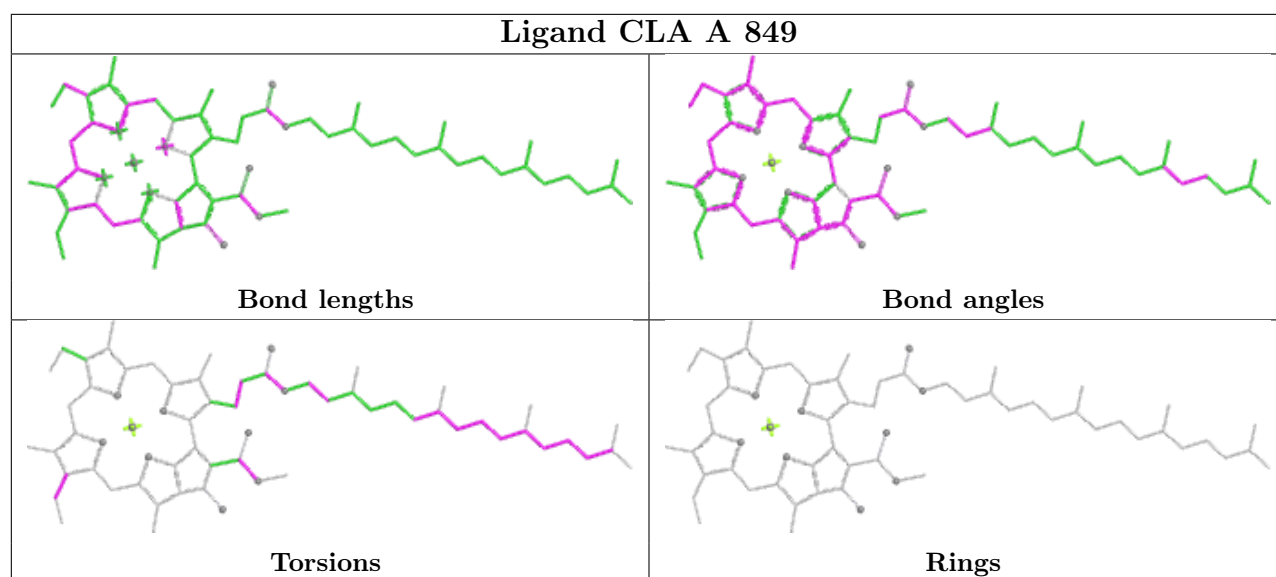
Bond angles

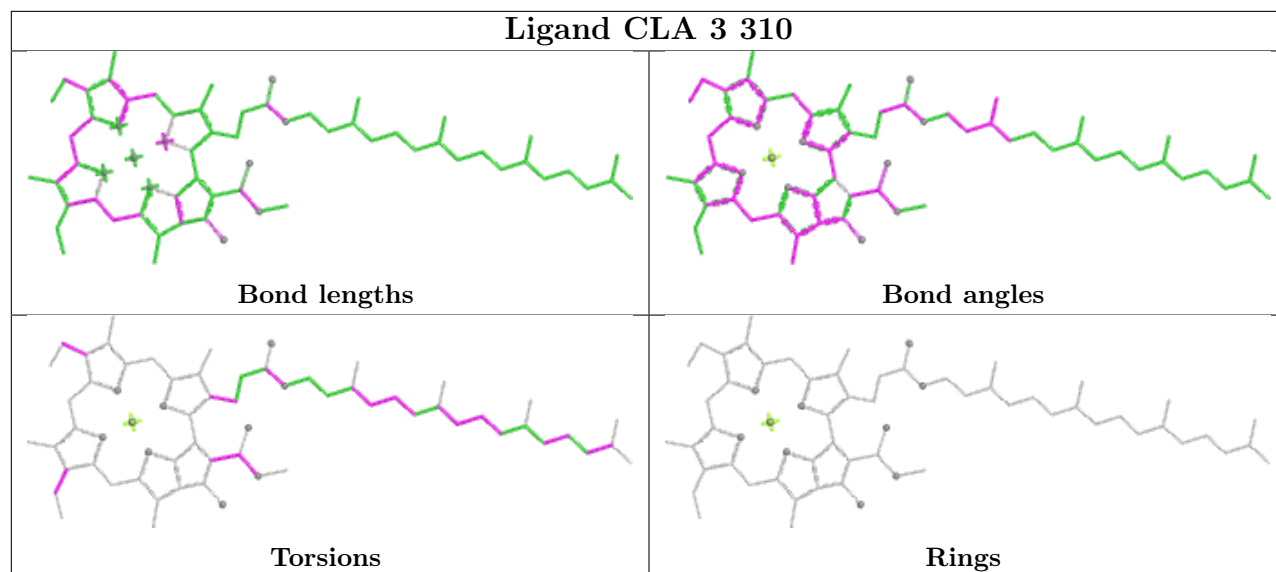
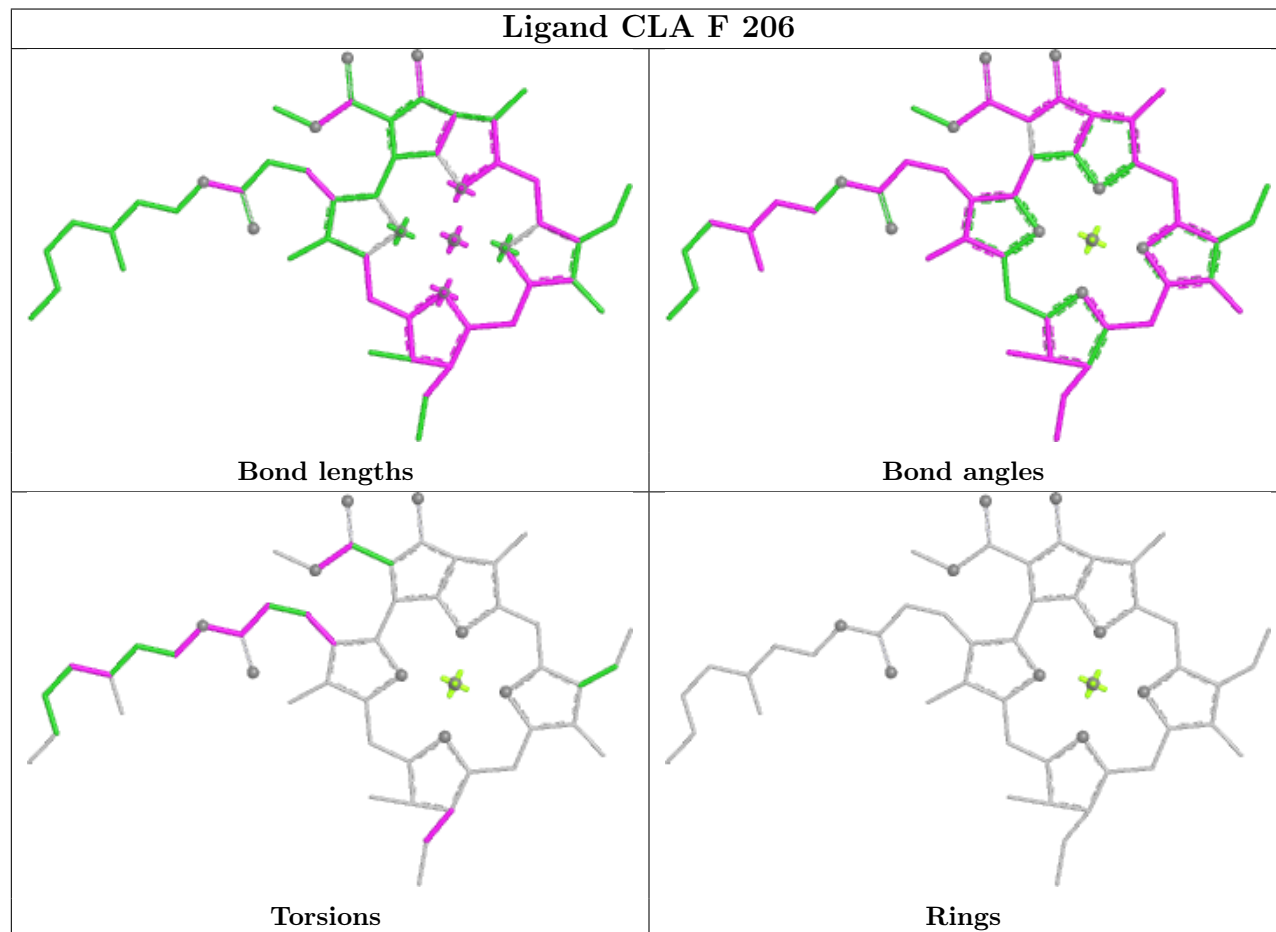


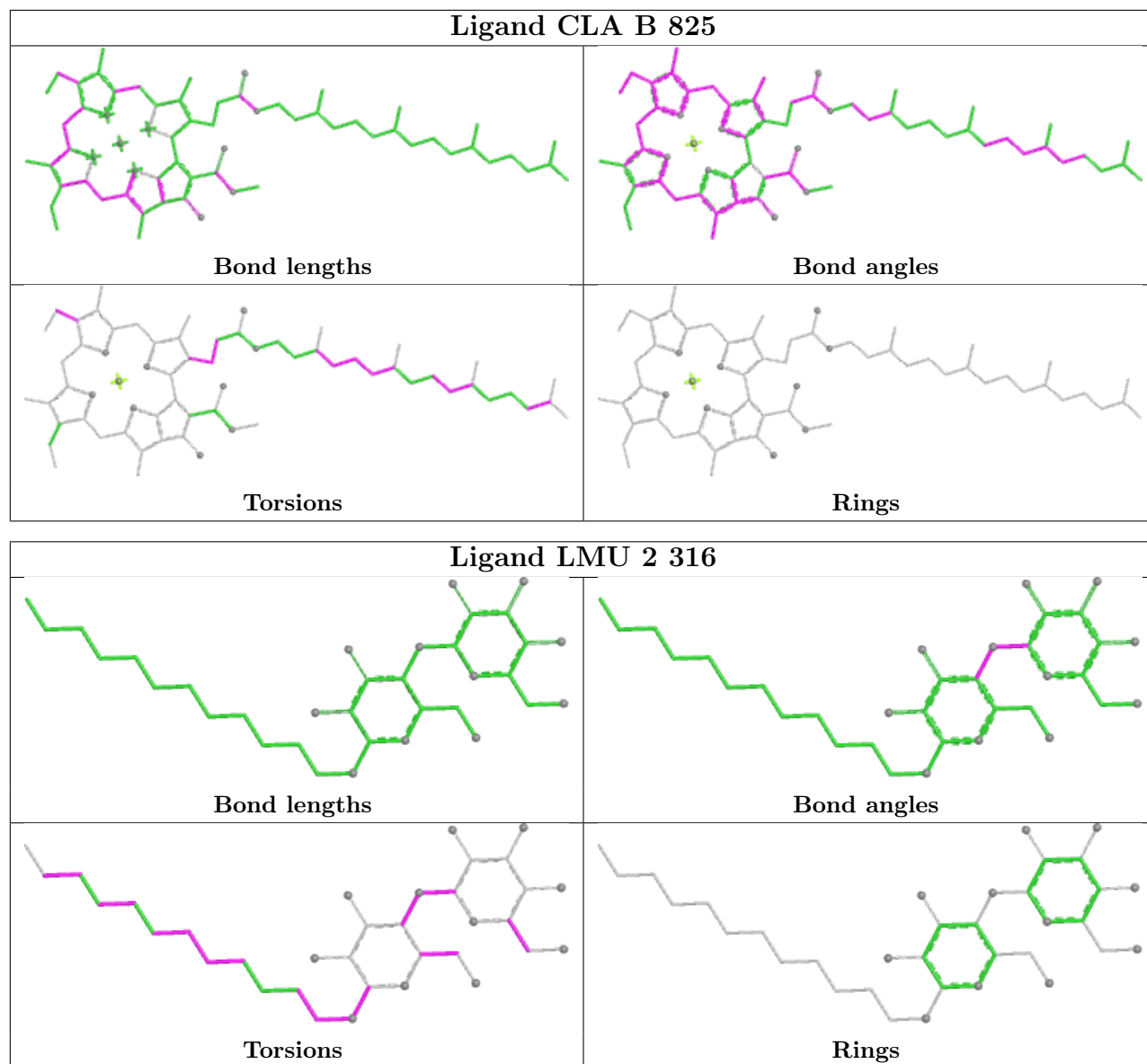
Torsions



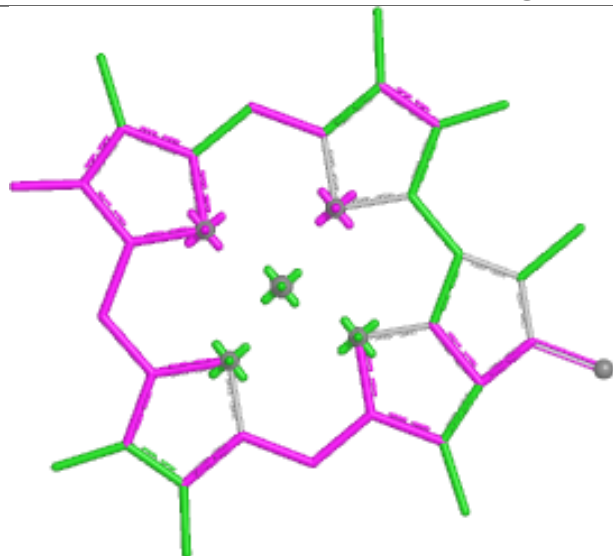
Rings



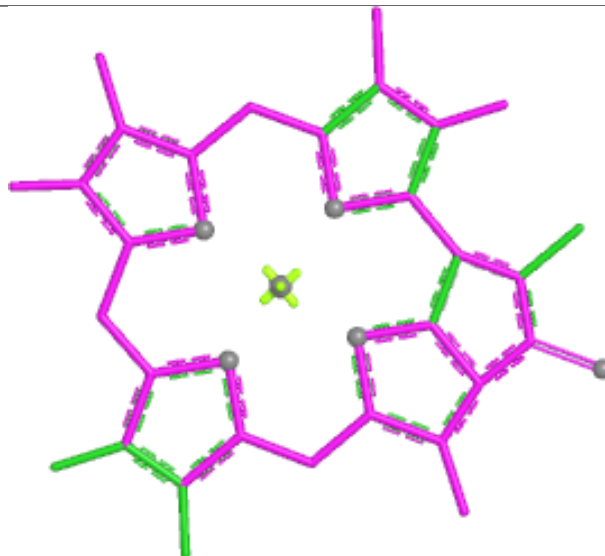
Ligand CLA 3 310**Ligand CLA F 206**



Ligand CLA 1 209



Bond lengths



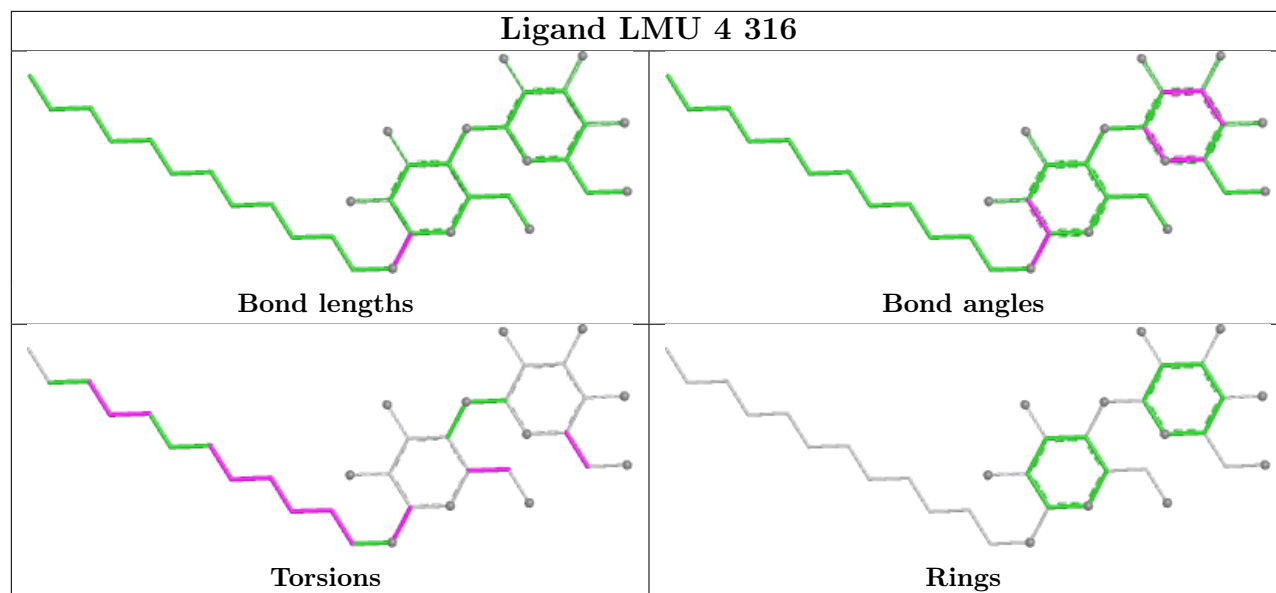
Bond angles



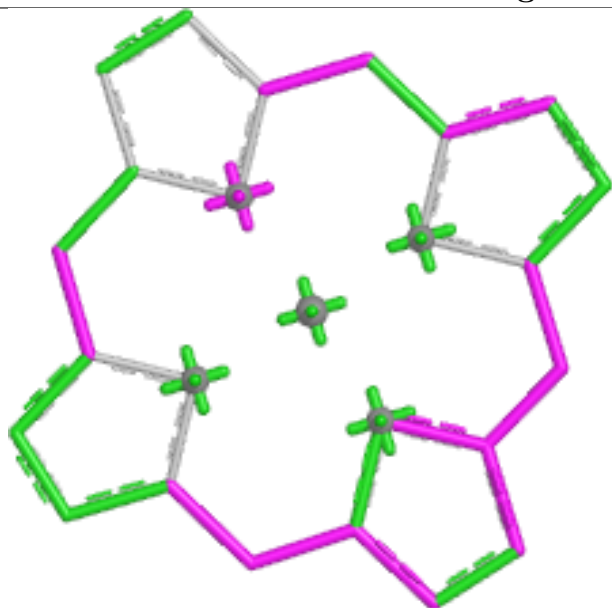
Torsions



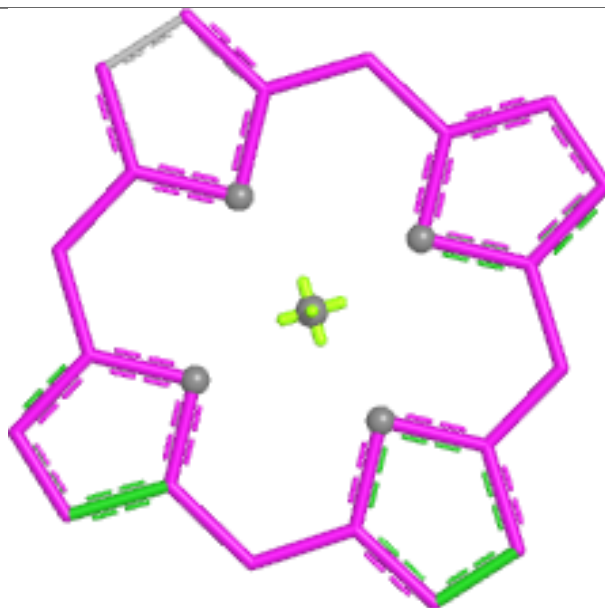
Rings



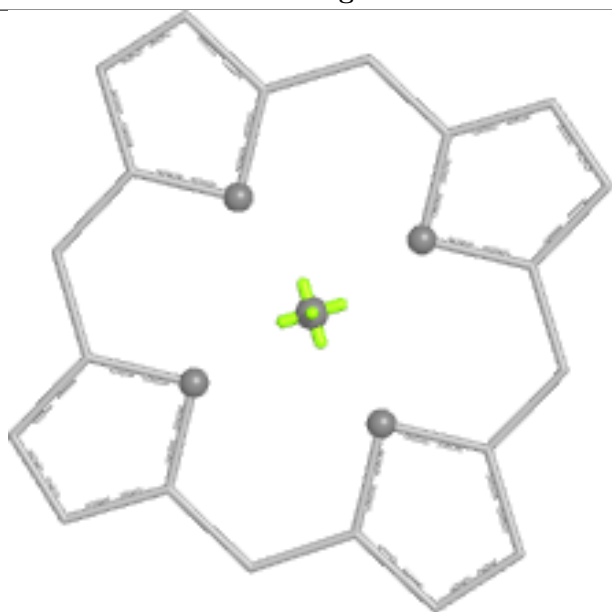
Ligand CLA 2 305



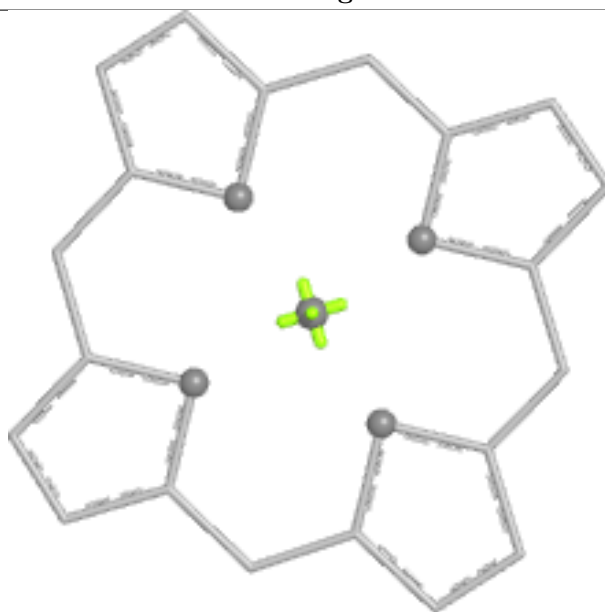
Bond lengths



Bond angles

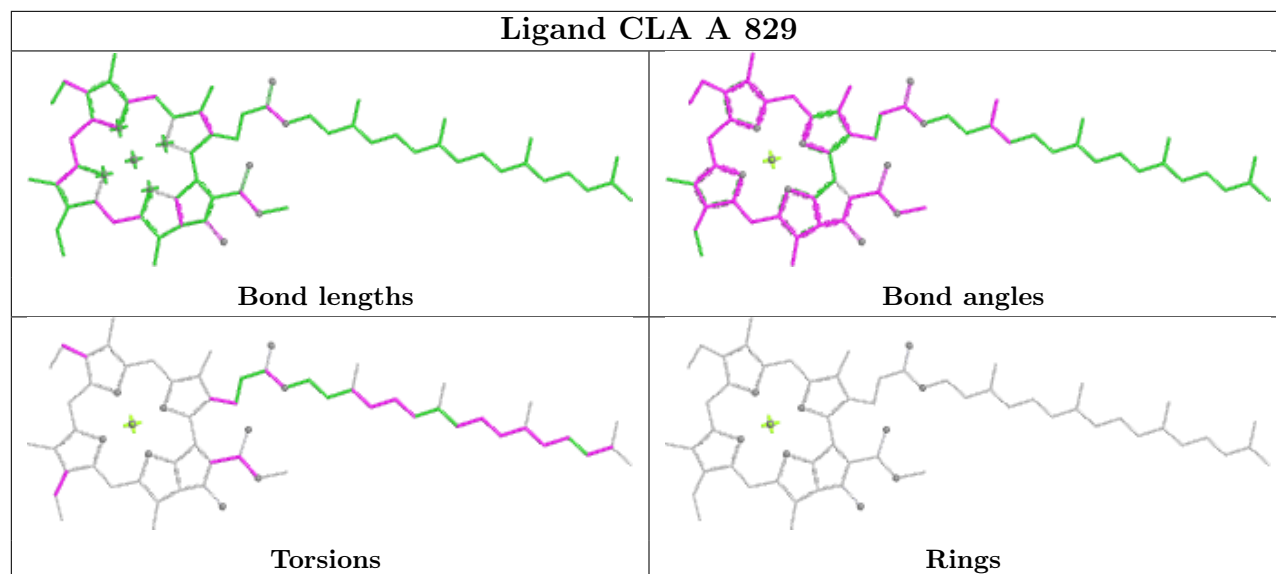


Torsions

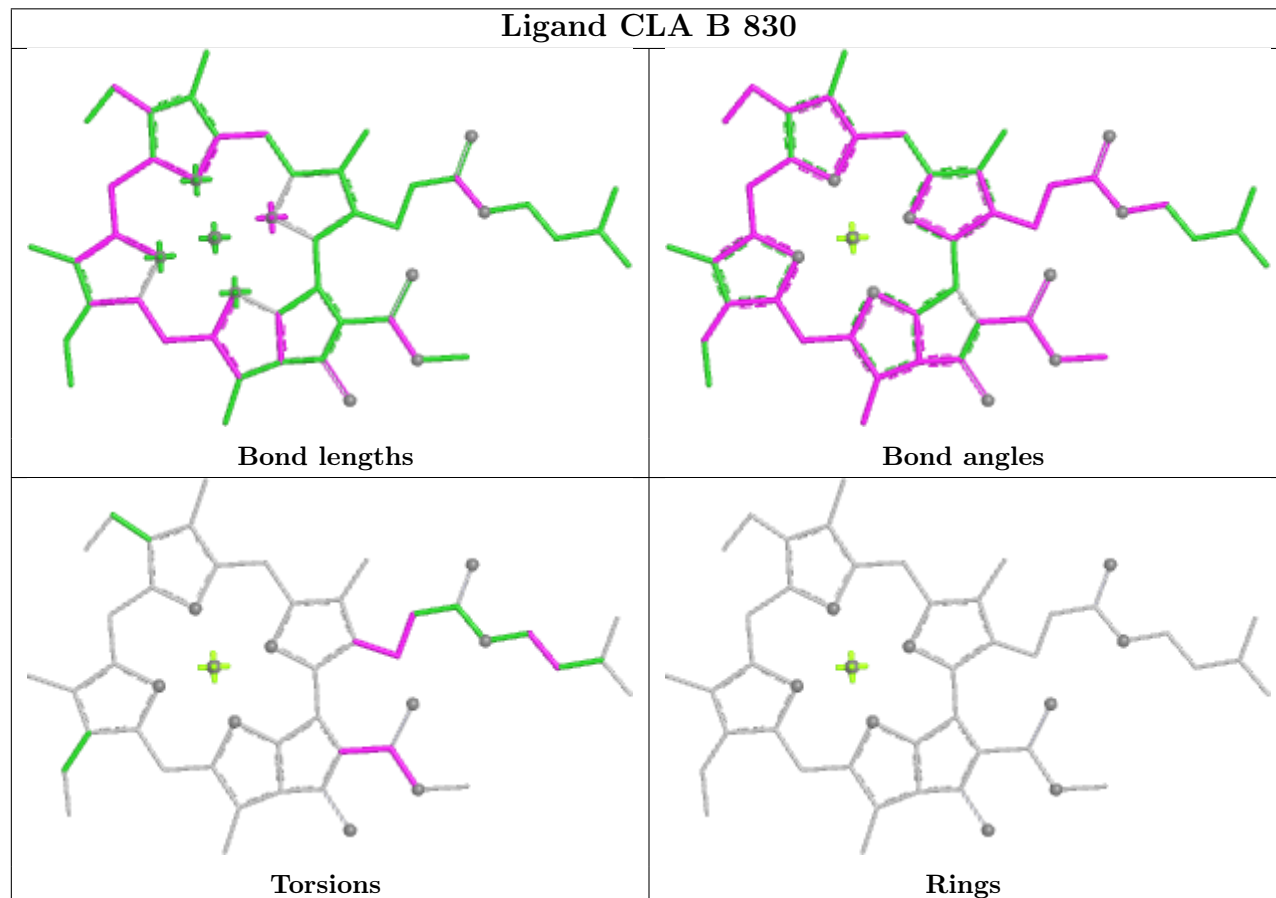


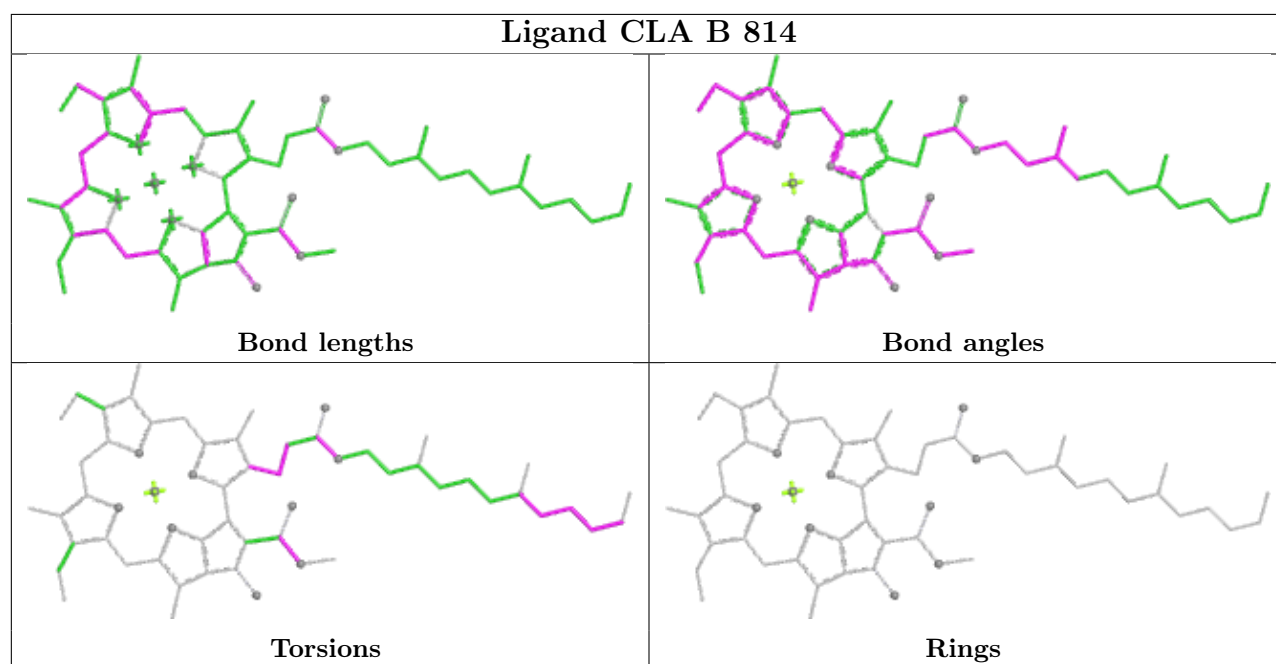
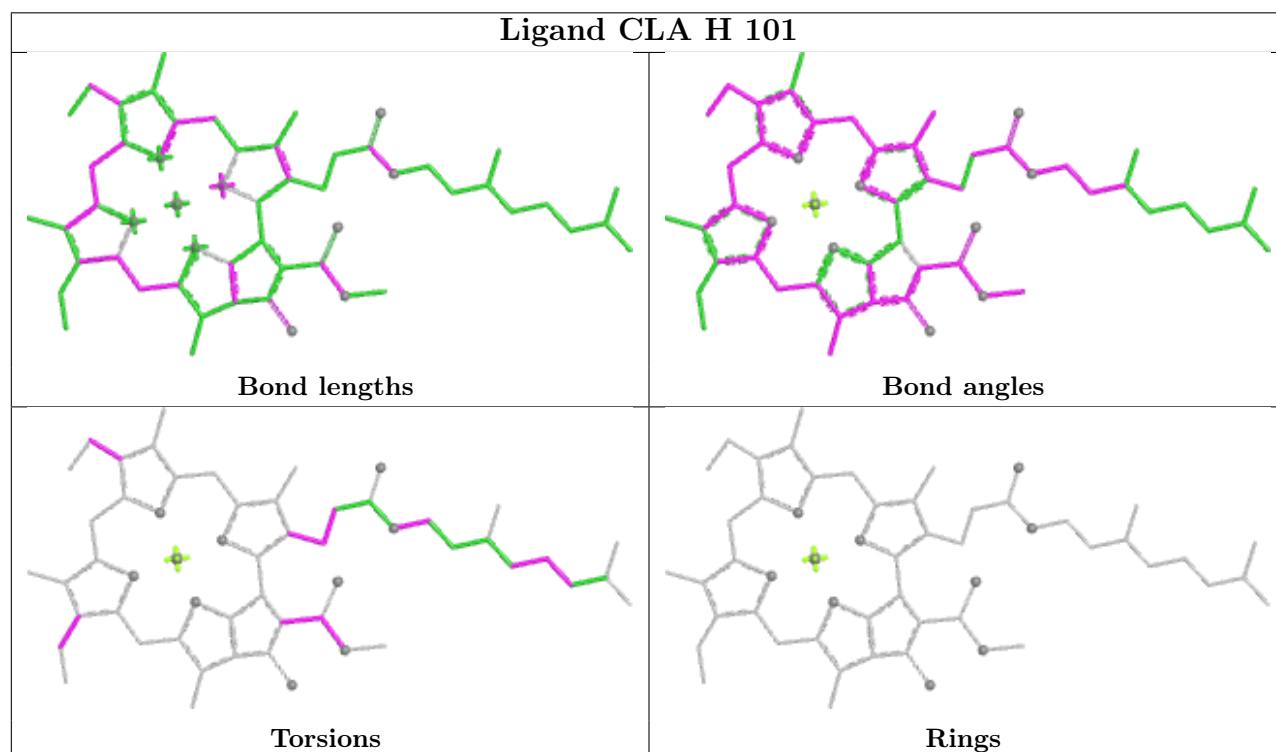
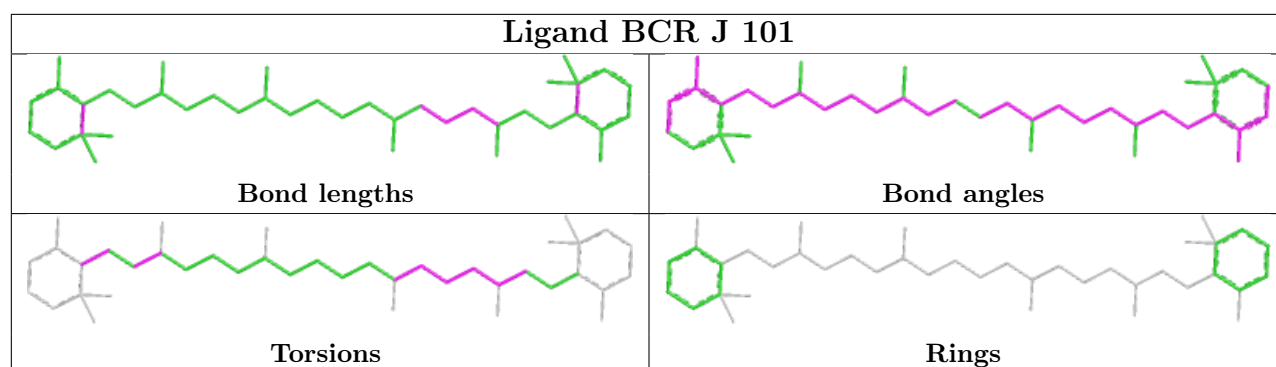
Rings

Ligand CLA A 829

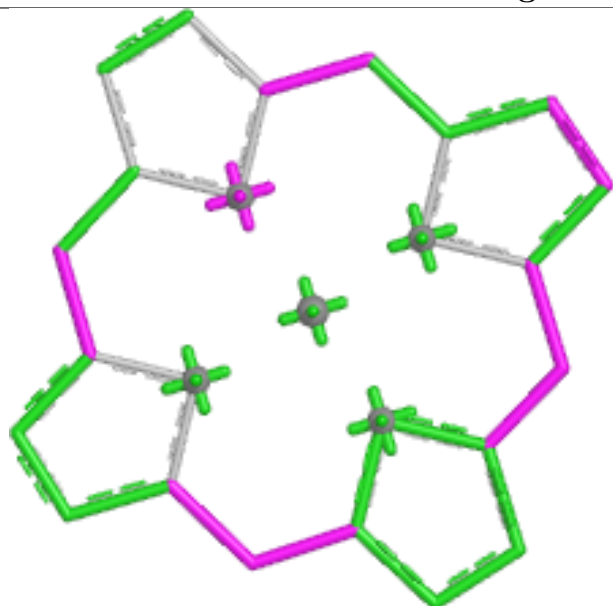


Ligand CLA B 830

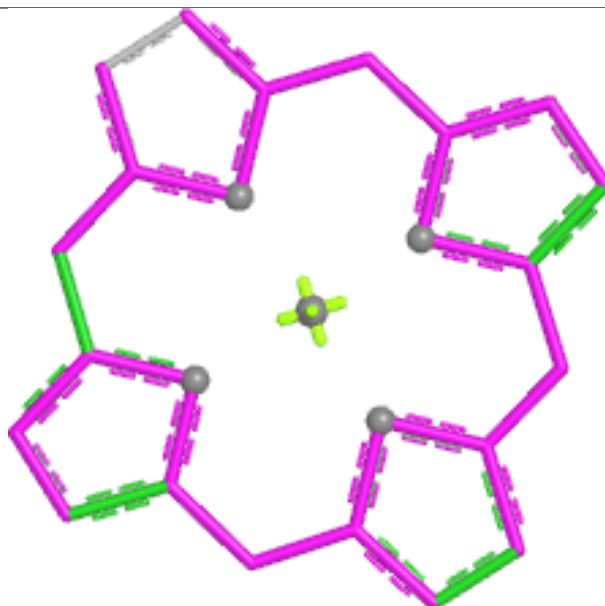




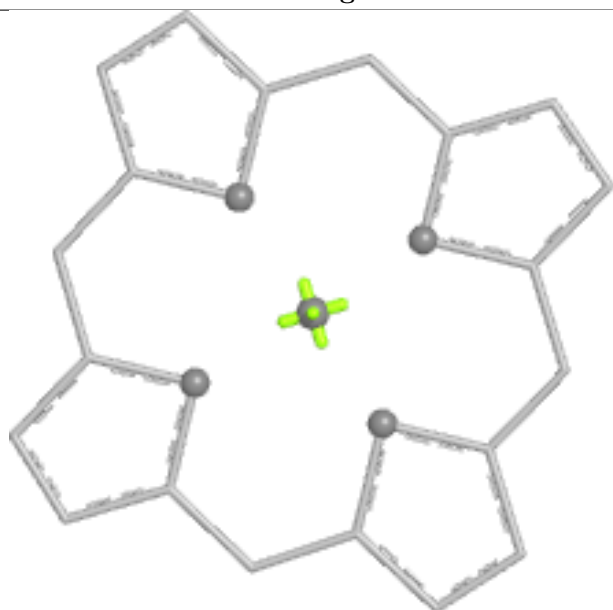
Ligand CLA 1 208



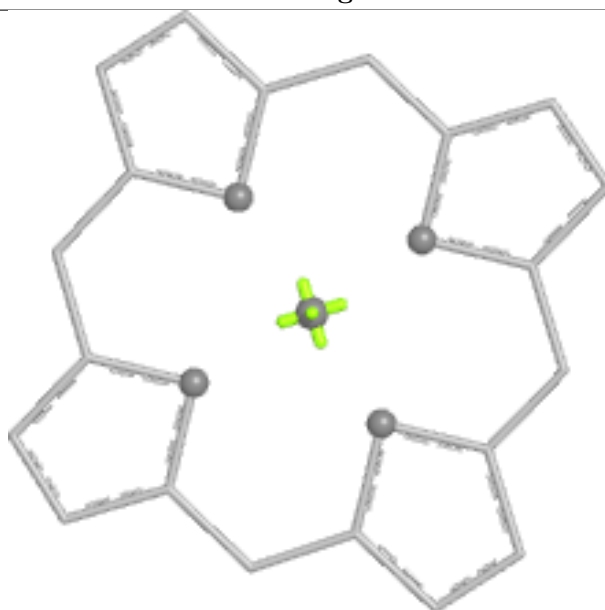
Bond lengths



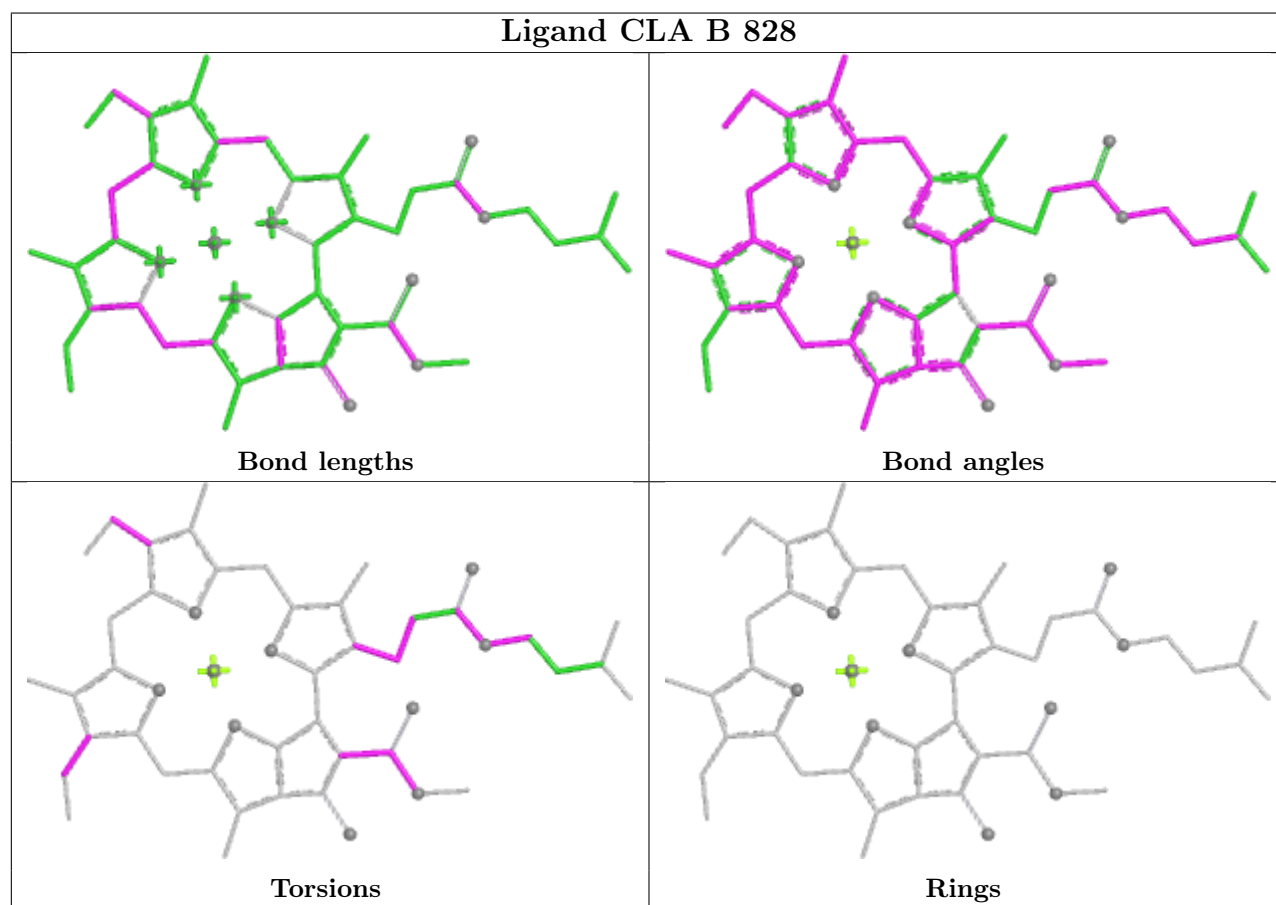
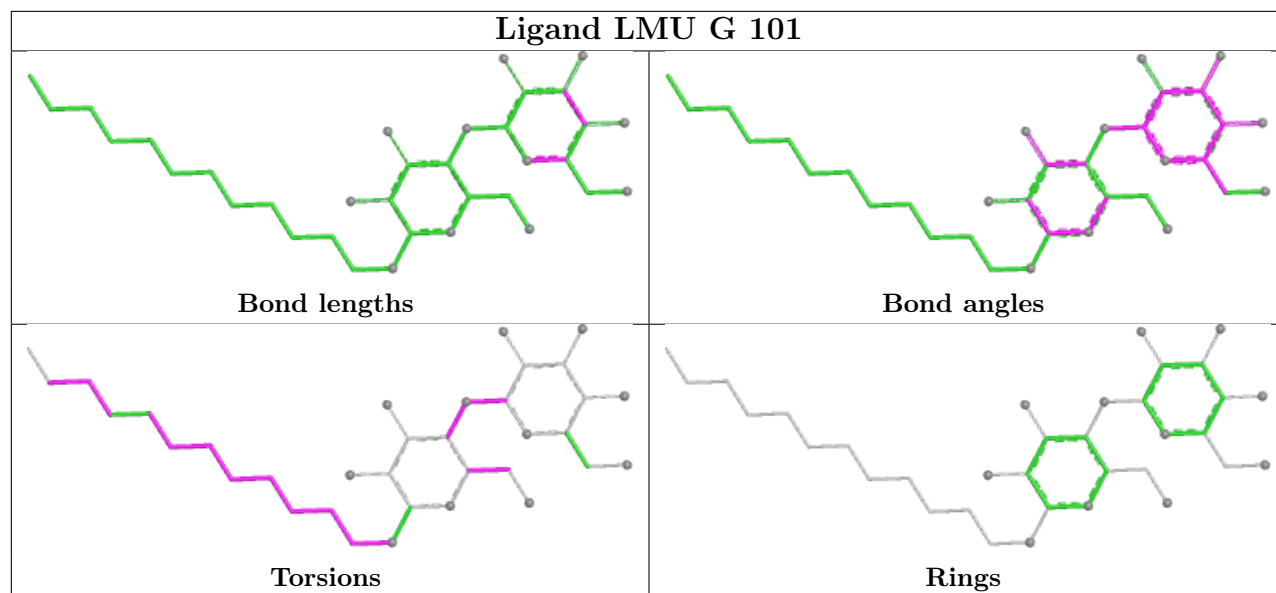
Bond angles

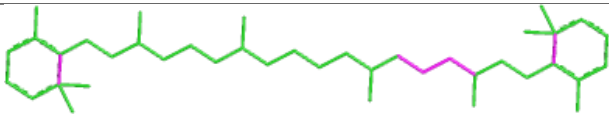
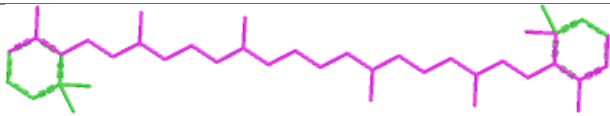
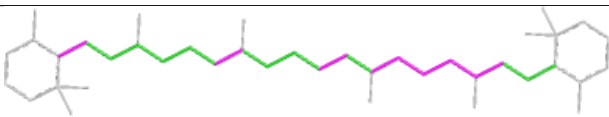
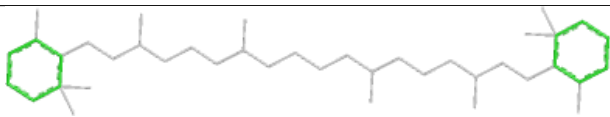


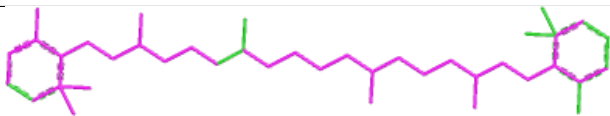
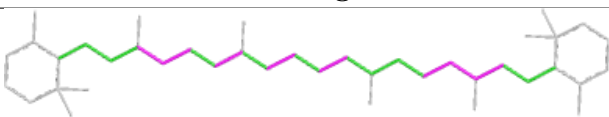
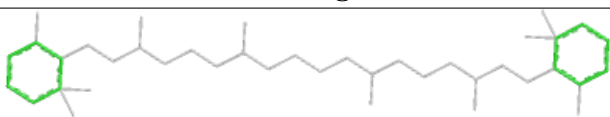
Torsions

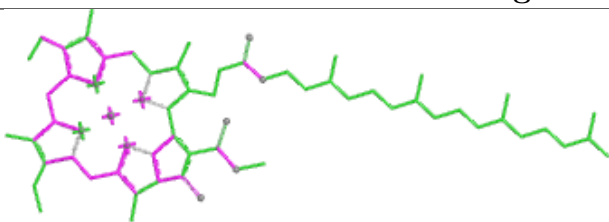
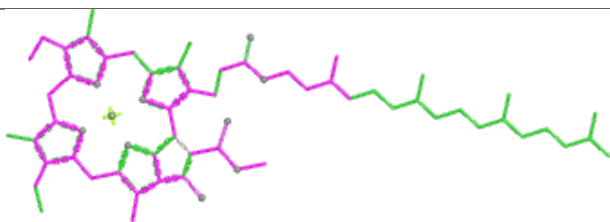
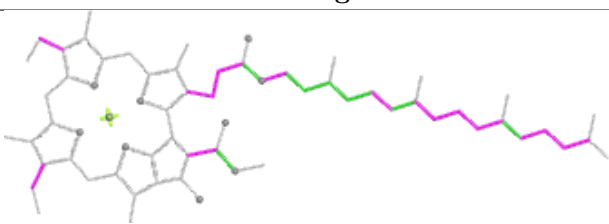
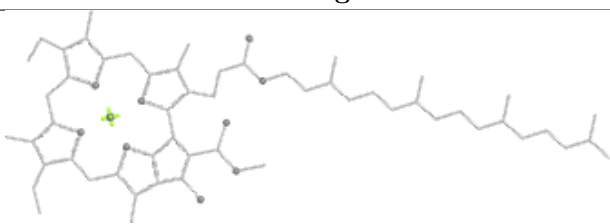


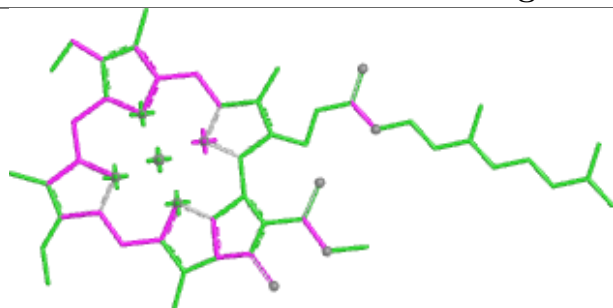
Rings



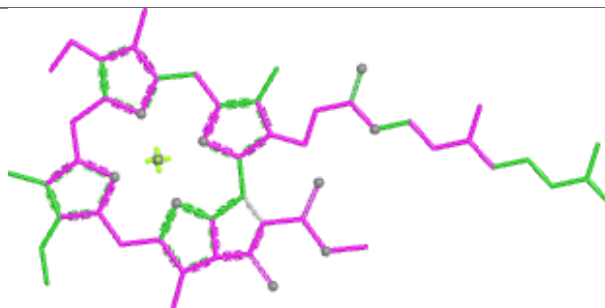
Ligand BCR 3 311	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand BCR B 850	
	
Bond lengths	Bond angles
	
Torsions	Rings

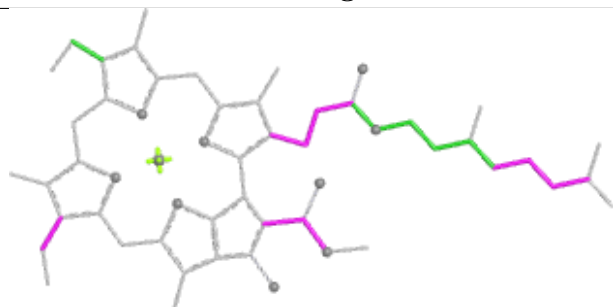
Ligand CLA 3 309	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA J 103

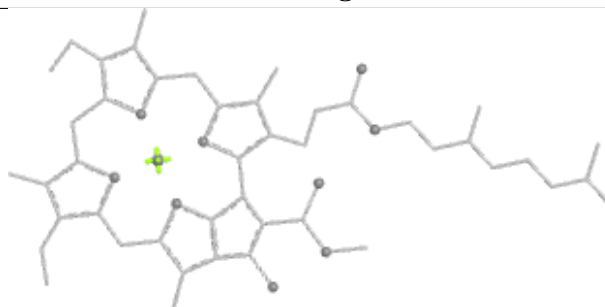
Bond lengths



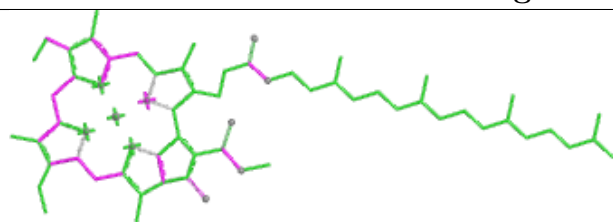
Bond angles



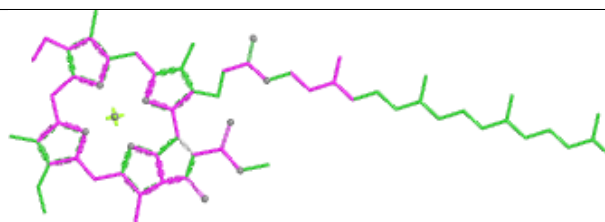
Torsions



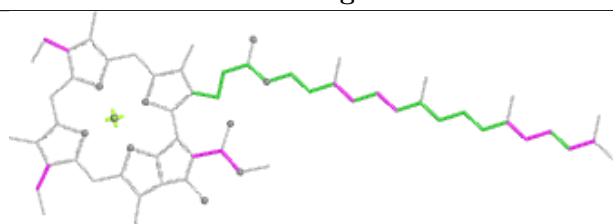
Rings

Ligand CLA A 833

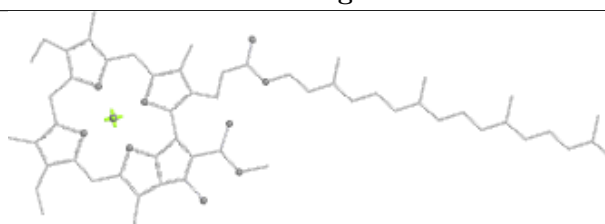
Bond lengths



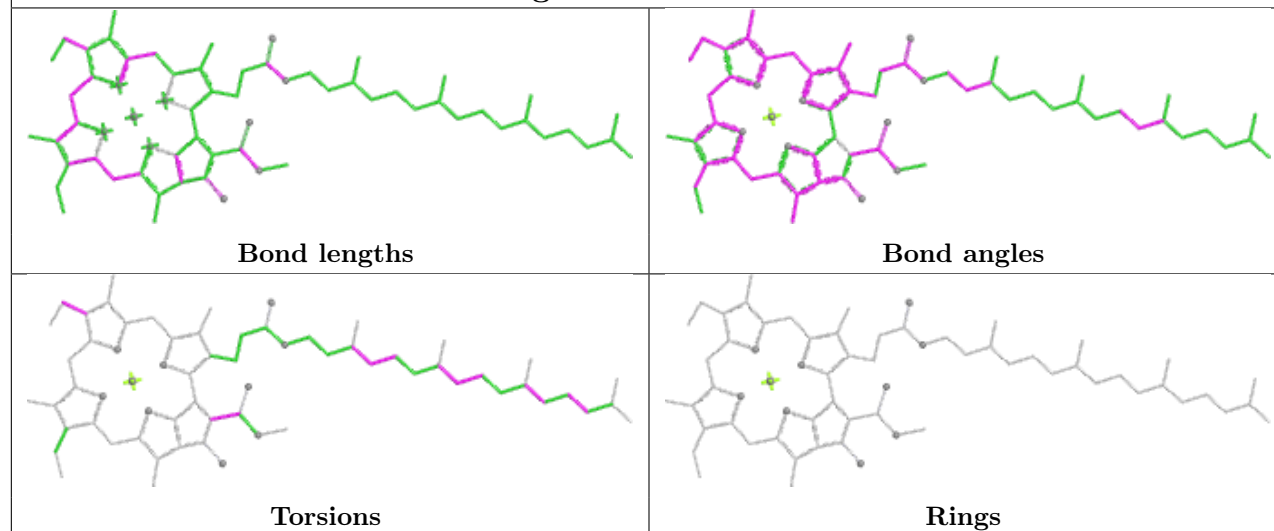
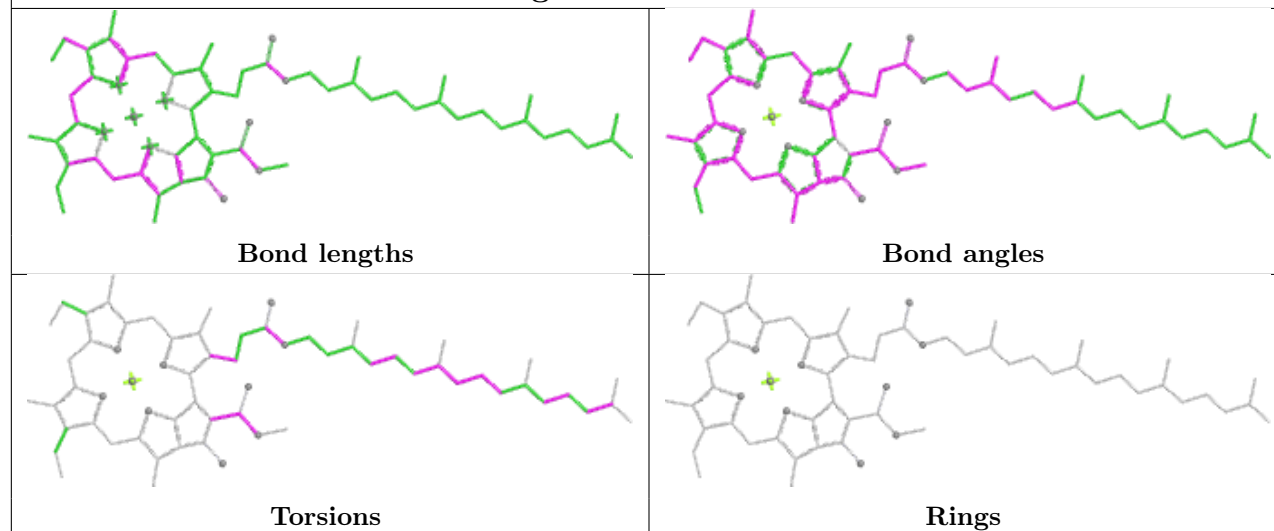
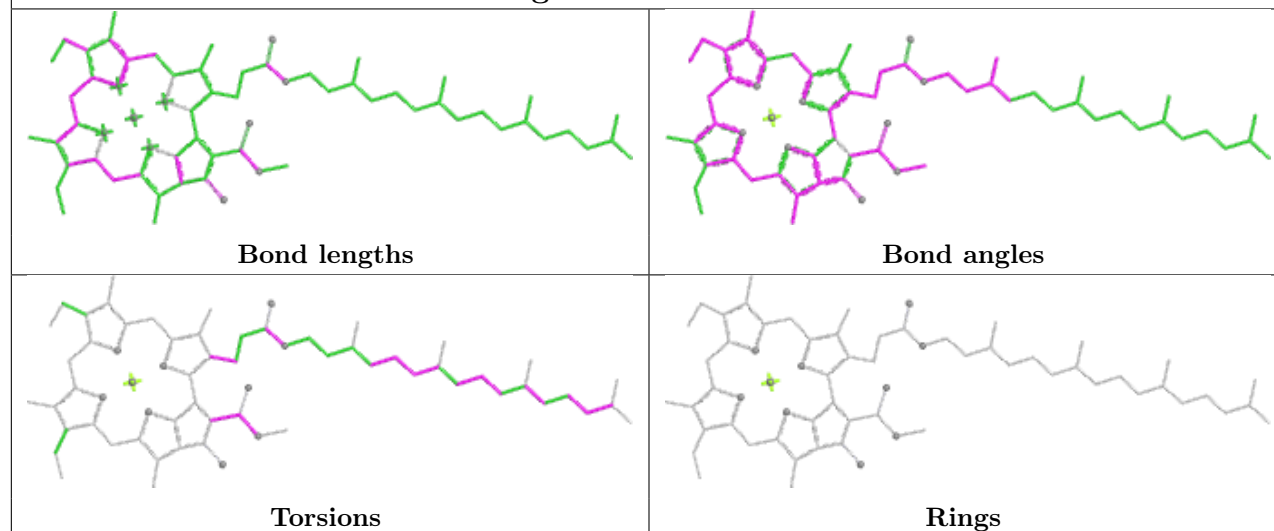
Bond angles



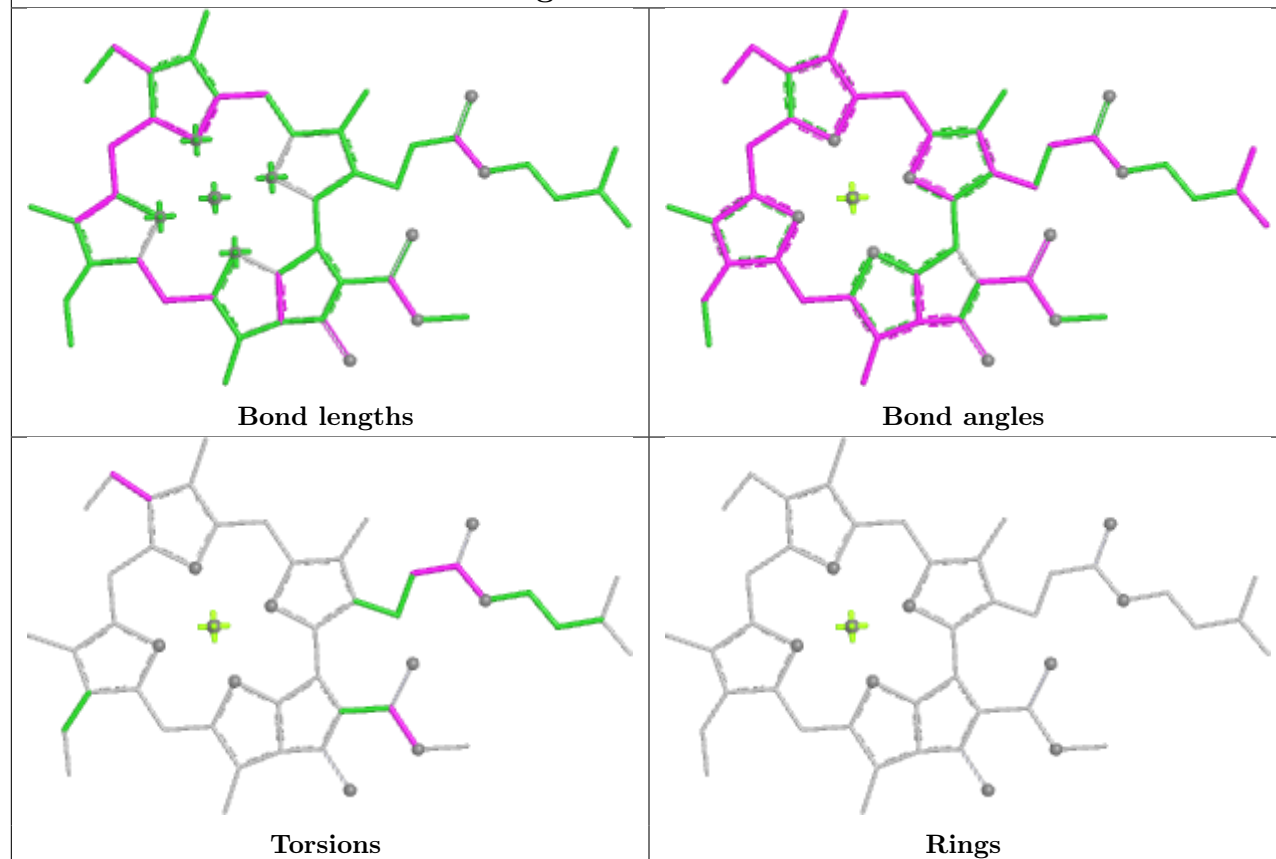
Torsions



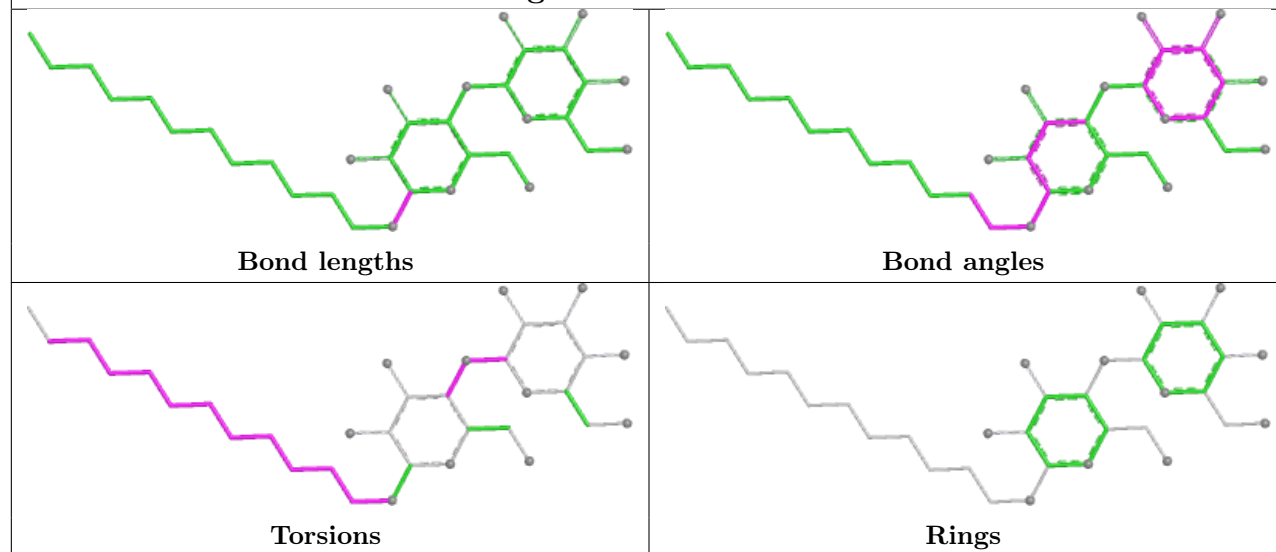
Rings

Ligand CLA B 806**Ligand CLA A 826****Ligand CLA A 816**

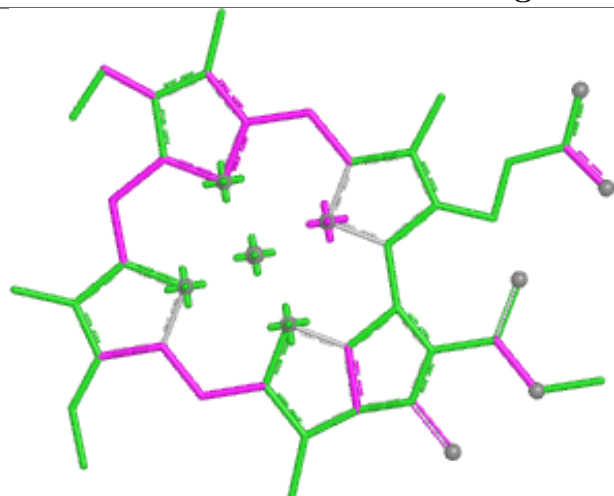
Ligand CLA 2 310



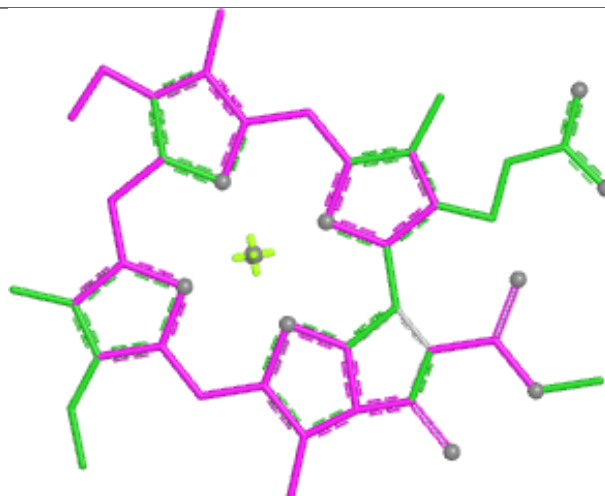
Ligand LMU A 846



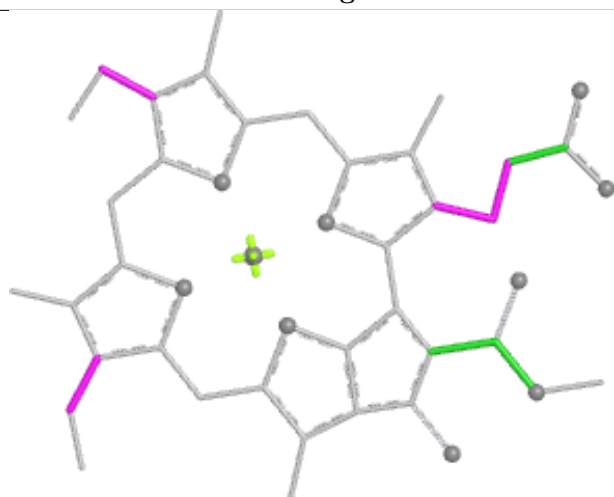
Ligand CLA B 803



Bond lengths



Bond angles

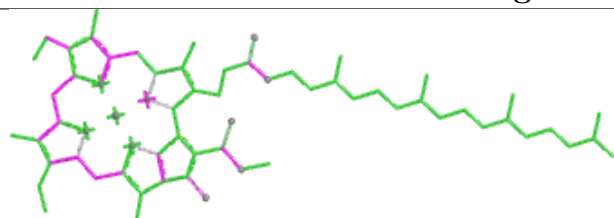


Torsions

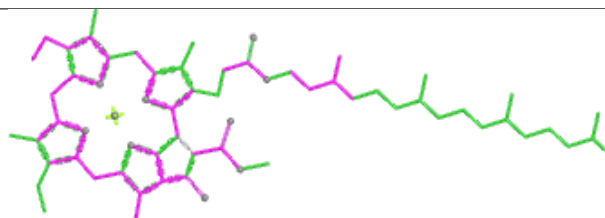


Rings

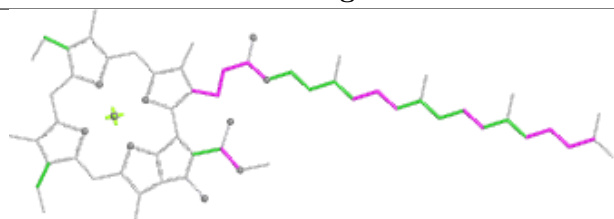
Ligand CLA A 836



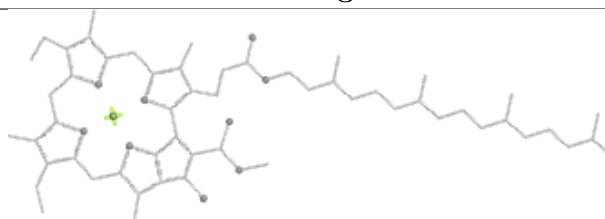
Bond lengths



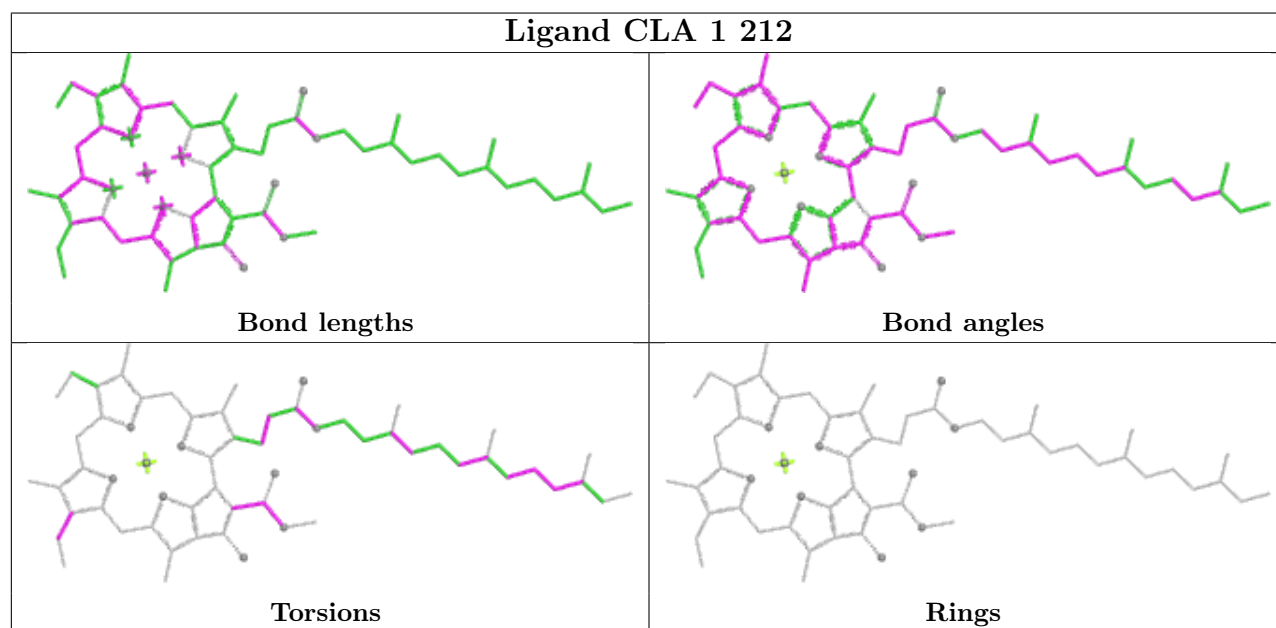
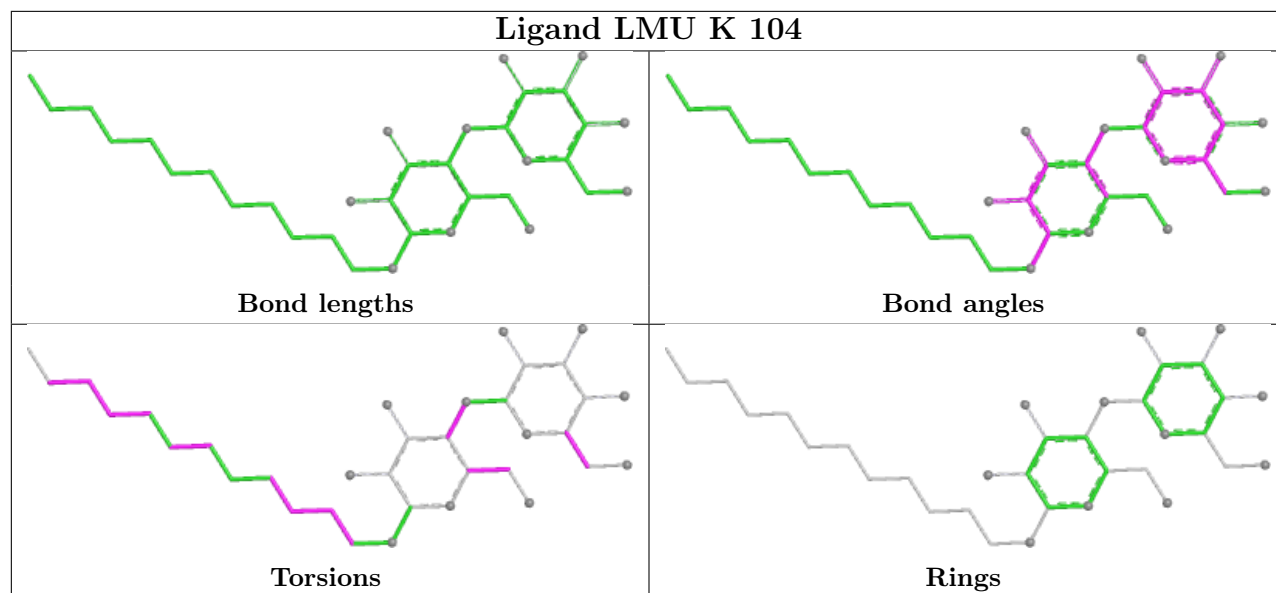
Bond angles



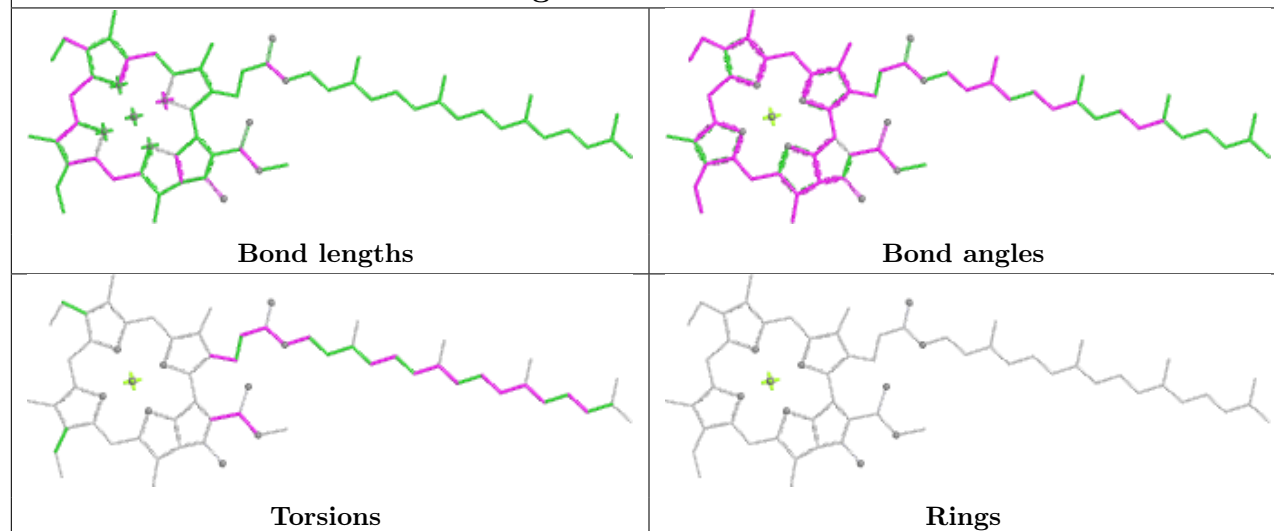
Torsions



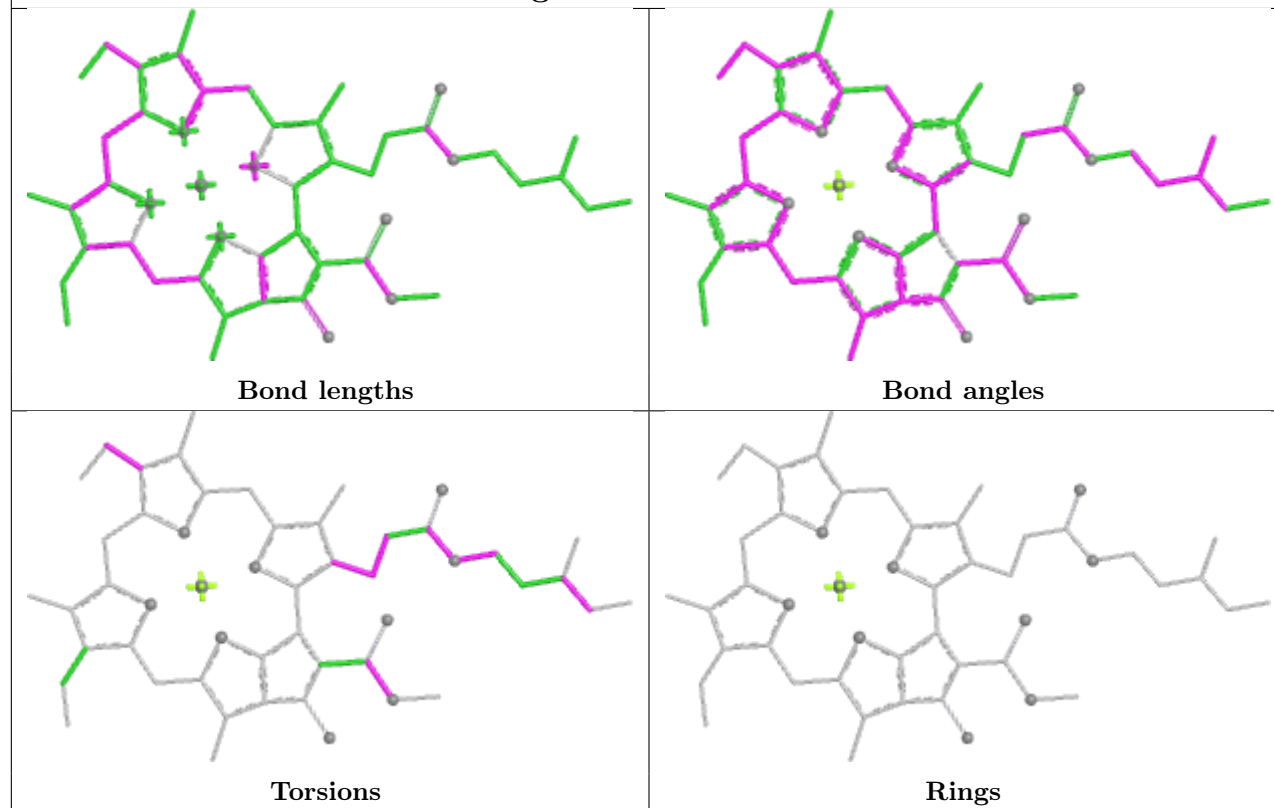
Rings

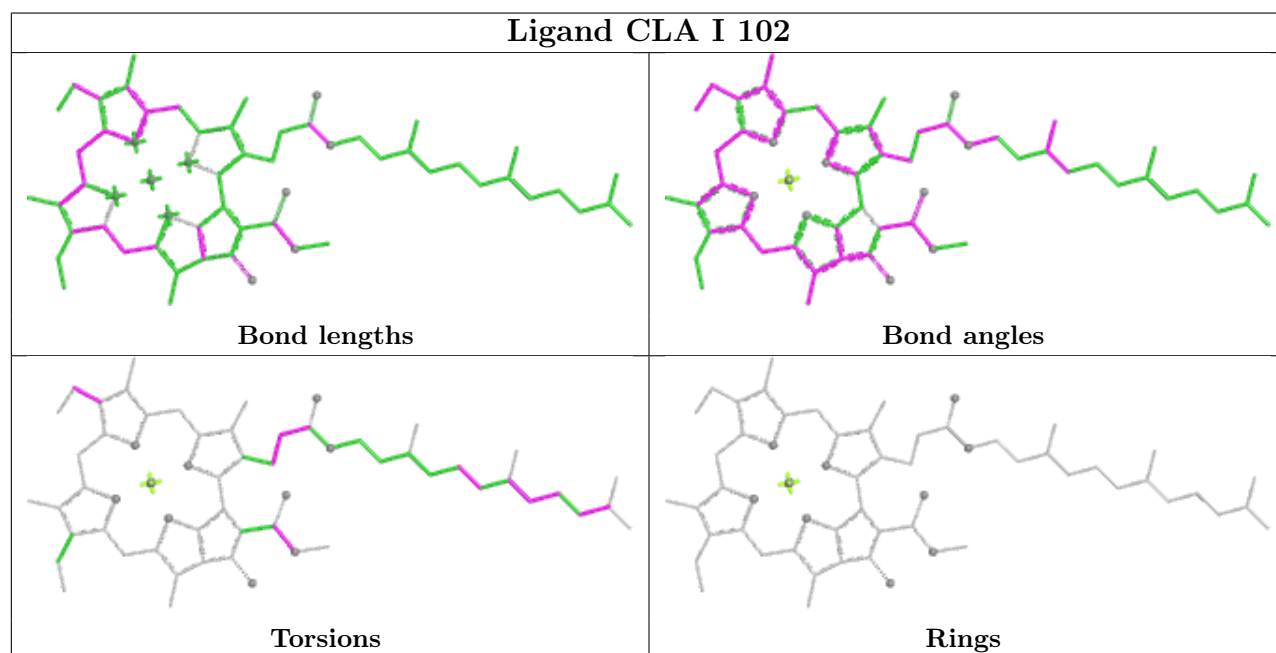
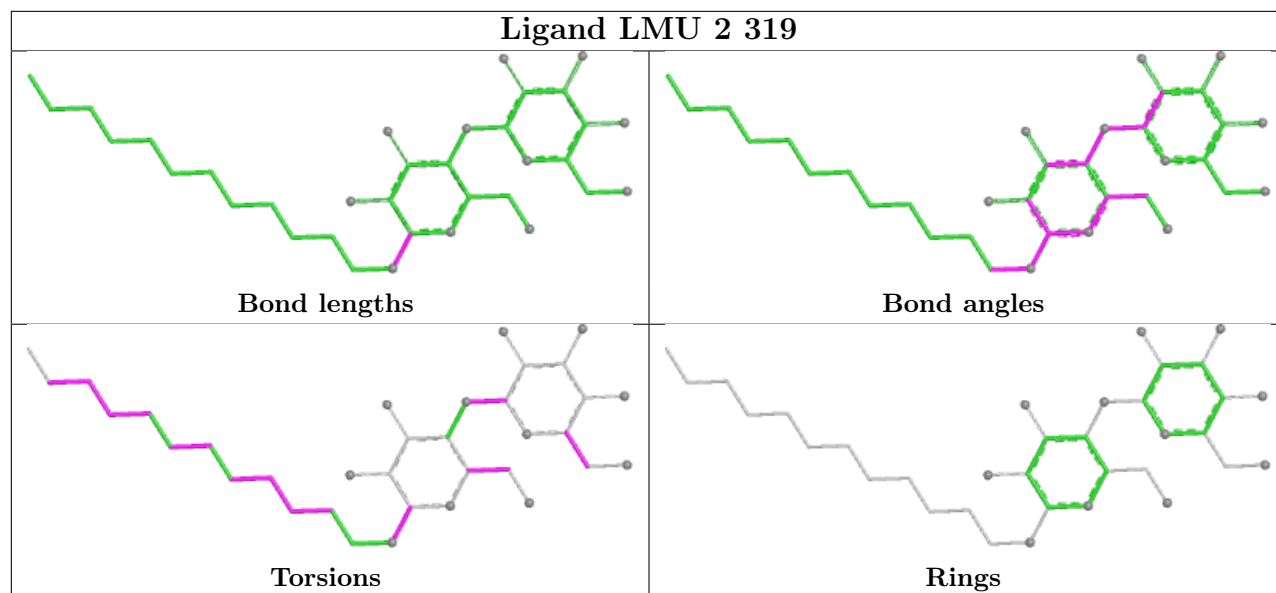


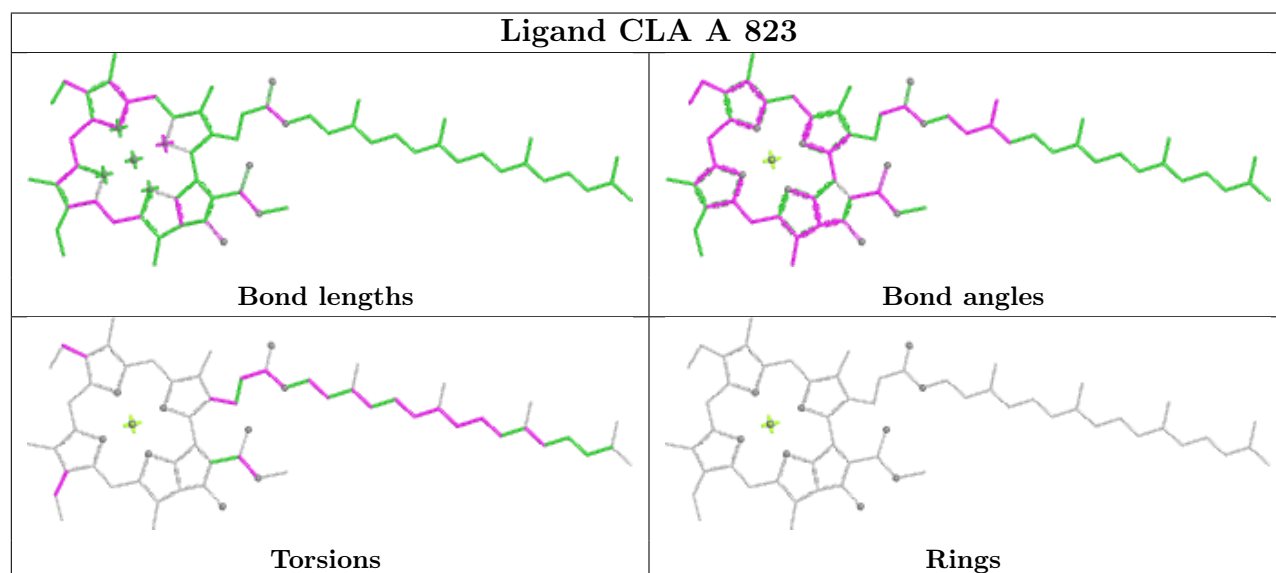
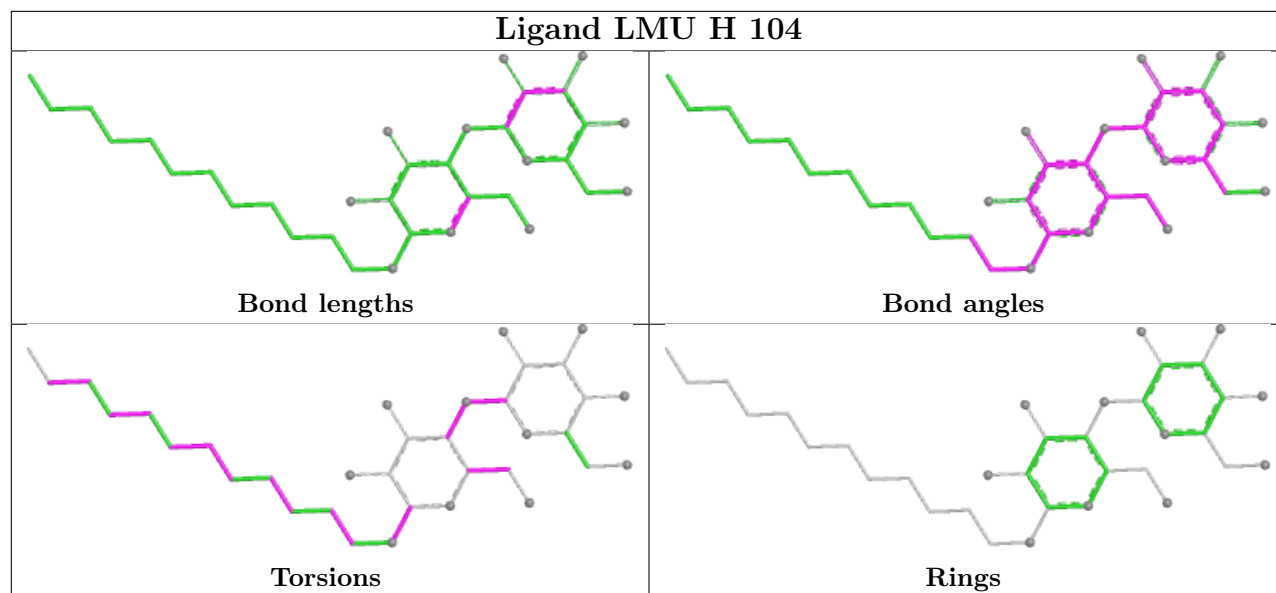
Ligand CLA B 804



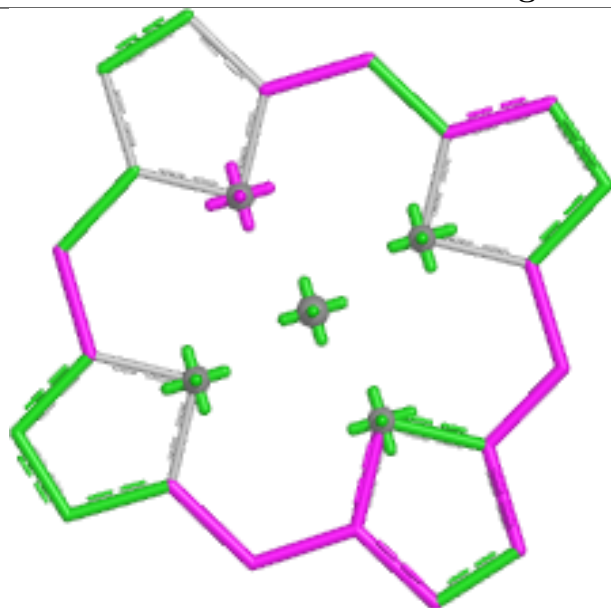
Ligand CLA A 832



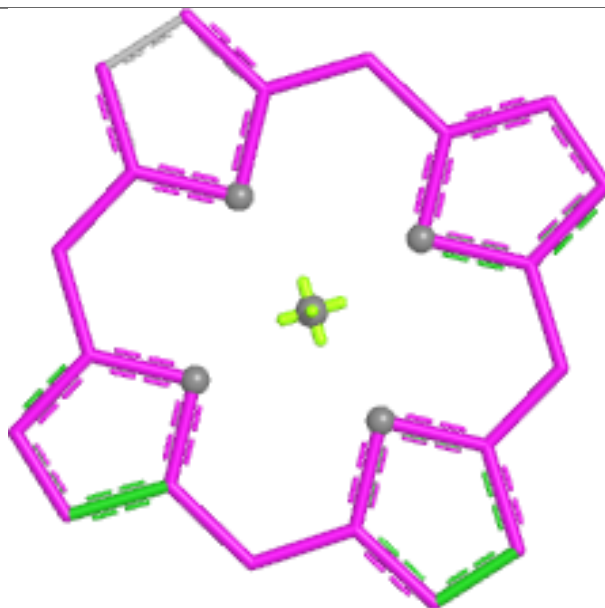




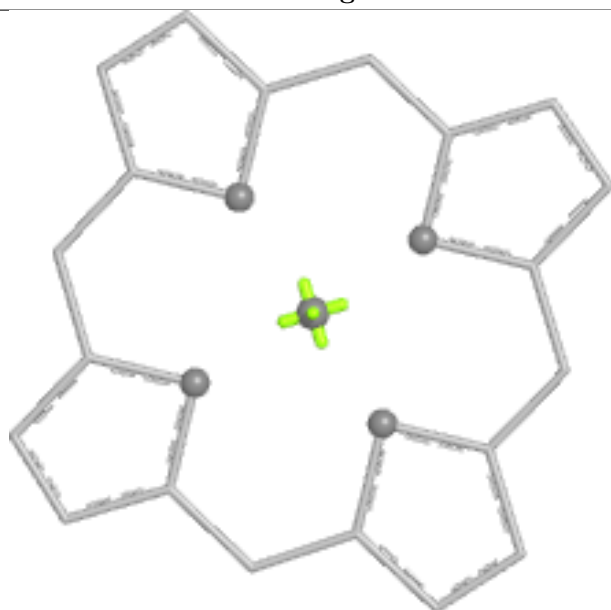
Ligand CLA 2 314



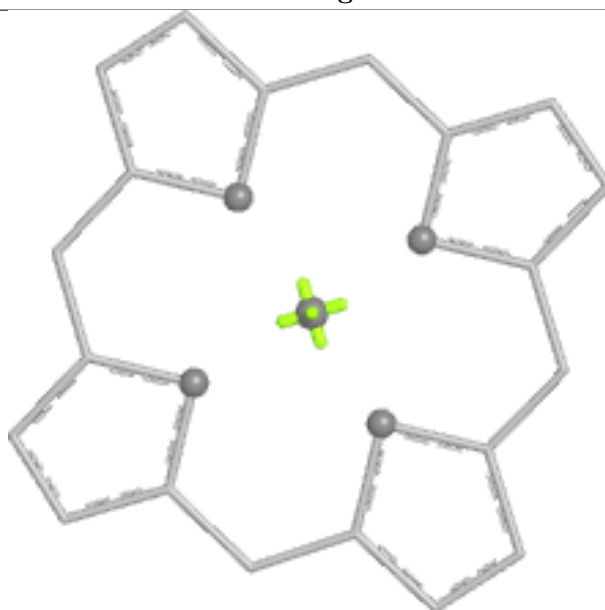
Bond lengths



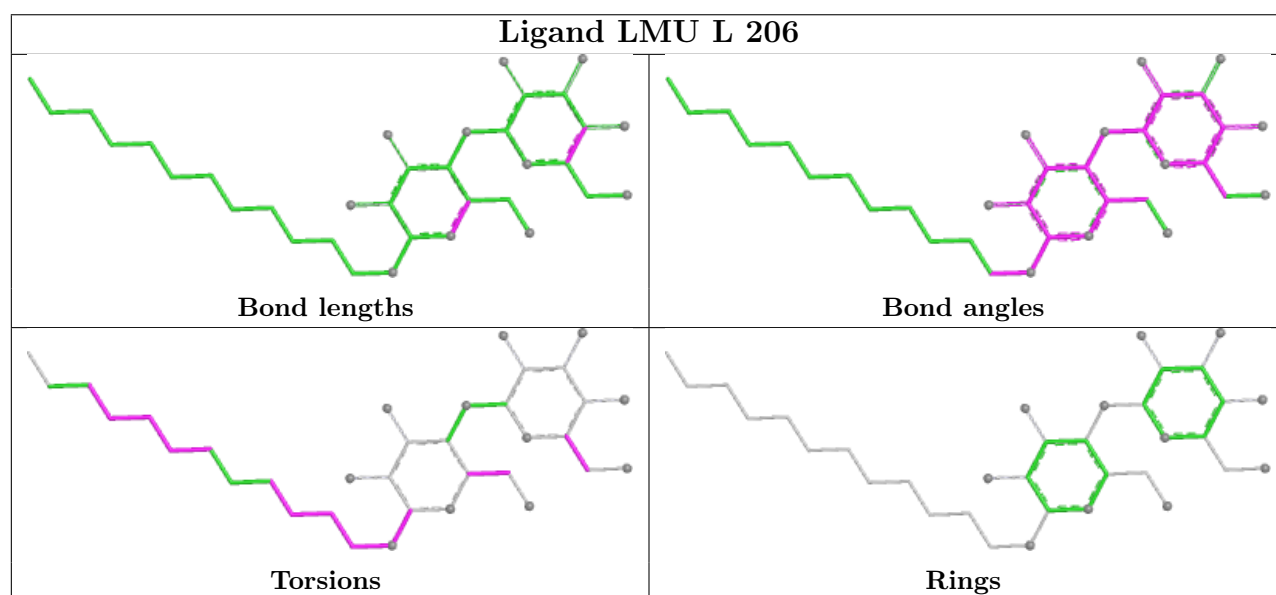
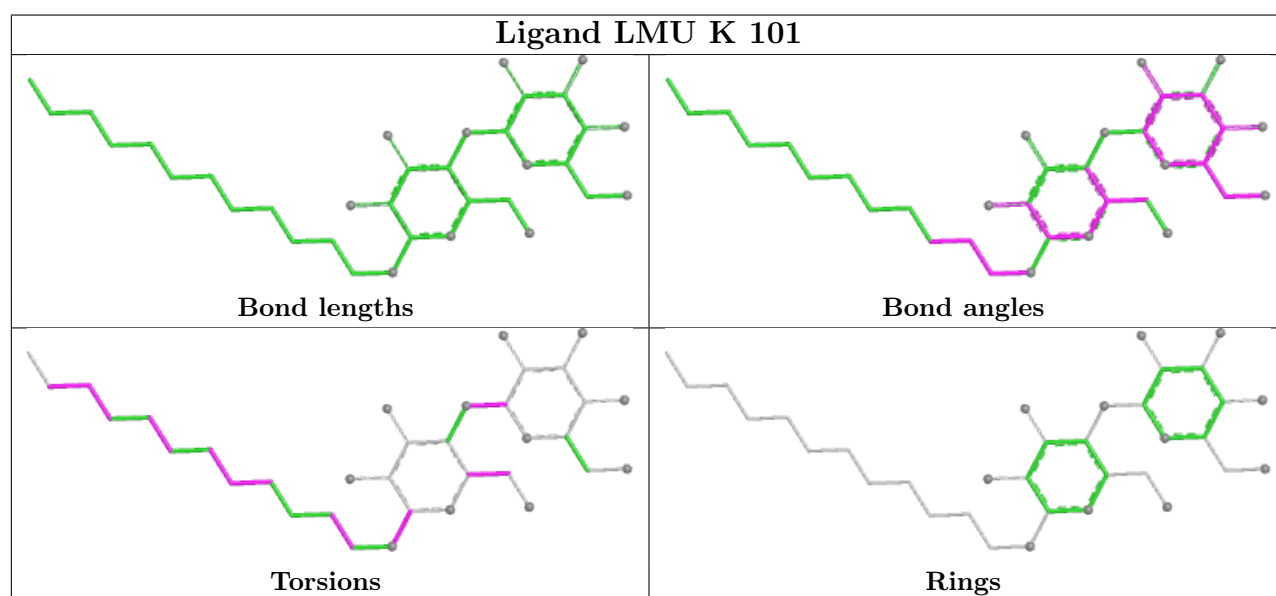
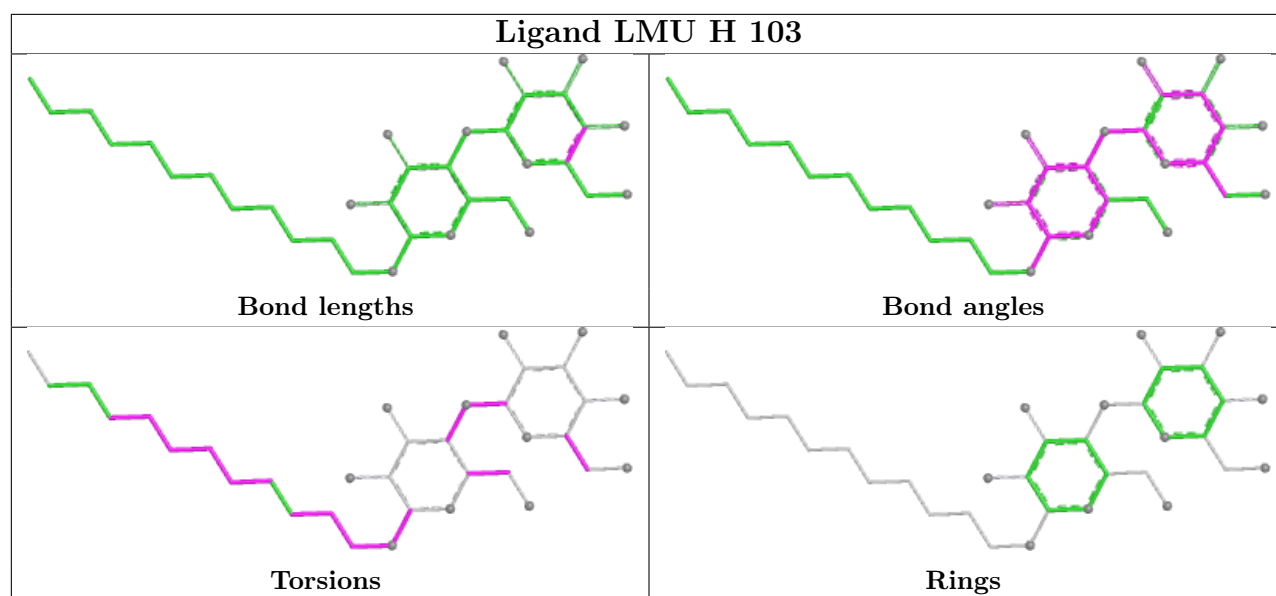
Bond angles

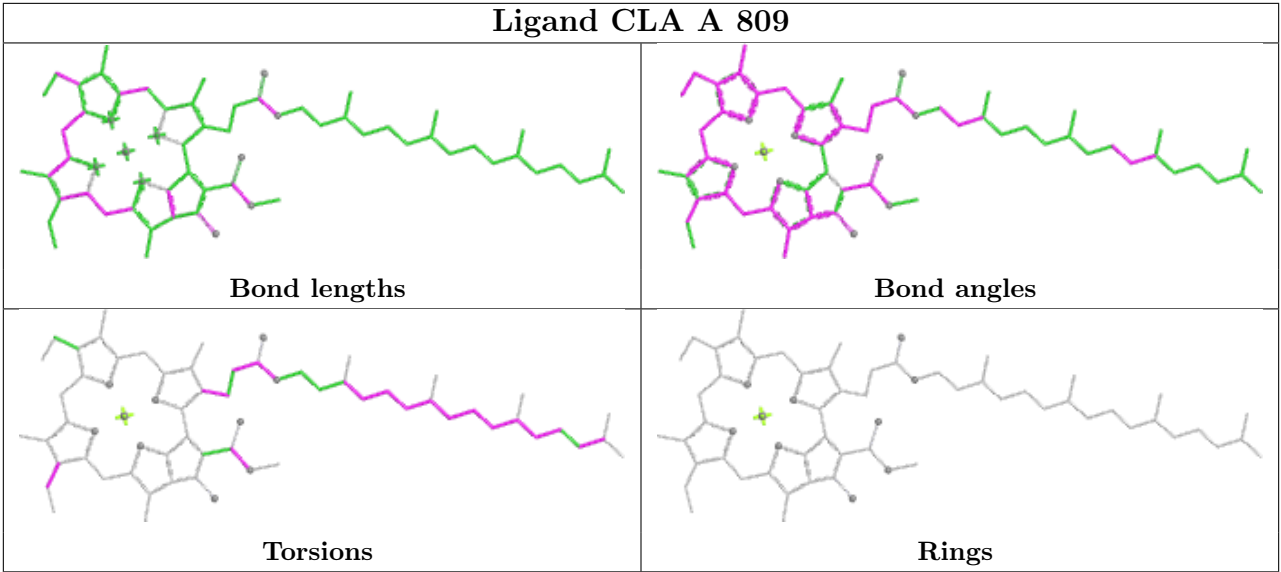


Torsions



Rings





4.7 Other polymers ⓘ

There are no such residues in this entry.

4.8 Polymer linkage issues ⓘ

The following chains have linkage breaks:

Mol	Chain	Number of breaks
5	A	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	317:TYR	C	318:ARG	N	1.17

5 Fit of model and data

5.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	1	165/241 (68%)	2.47	91 (55%) 0 0	31, 61, 71, 72	0
2	2	176/269 (65%)	1.97	66 (37%) 1 1	33, 52, 64, 68	0
3	3	162/276 (58%)	2.41	90 (55%) 0 0	49, 79, 110, 112	0
4	4	166/251 (66%)	1.96	68 (40%) 0 0	21, 44, 57, 58	0
5	A	730/758 (96%)	1.44	170 (23%) 2 2	20, 20, 20, 20	0
6	B	733/734 (99%)	1.51	186 (25%) 1 1	20, 20, 20, 20	0
7	C	81/81 (100%)	1.87	31 (38%) 1 1	20, 20, 20, 20	0
8	D	138/212 (65%)	1.15	19 (13%) 6 5	20, 20, 20, 20	0
9	E	65/143 (45%)	1.13	10 (15%) 5 4	20, 20, 20, 20	0
10	F	154/231 (66%)	1.16	31 (20%) 3 2	20, 20, 20, 20	0
11	G	95/167 (56%)	0.91	8 (8%) 17 13	20, 20, 20, 20	0
12	H	69/144 (47%)	1.03	9 (13%) 7 6	20, 20, 20, 20	0
13	I	30/40 (75%)	0.57	0 100 100	20, 20, 20, 20	0
14	J	42/44 (95%)	0.95	4 (9%) 14 11	20, 20, 20, 20	0
15	K	84/131 (64%)	1.08	12 (14%) 6 5	20, 20, 20, 20	0
16	L	161/216 (74%)	1.16	29 (18%) 3 3	20, 20, 20, 20	0
17	N	85/170 (50%)	0.50	3 (3%) 47 31	20, 20, 20, 20	0
18	R	0/53	-	-	-	-
All	All	3136/4161 (75%)	1.51	827 (26%) 1 1	20, 20, 65, 112	0

The worst 5 of 827 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
6	B	491	ASN	11.2
2	2	123	PRO	10.9
1	1	92	GLY	9.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	1	113	SER	8.7
1	1	75	ALA	8.7

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

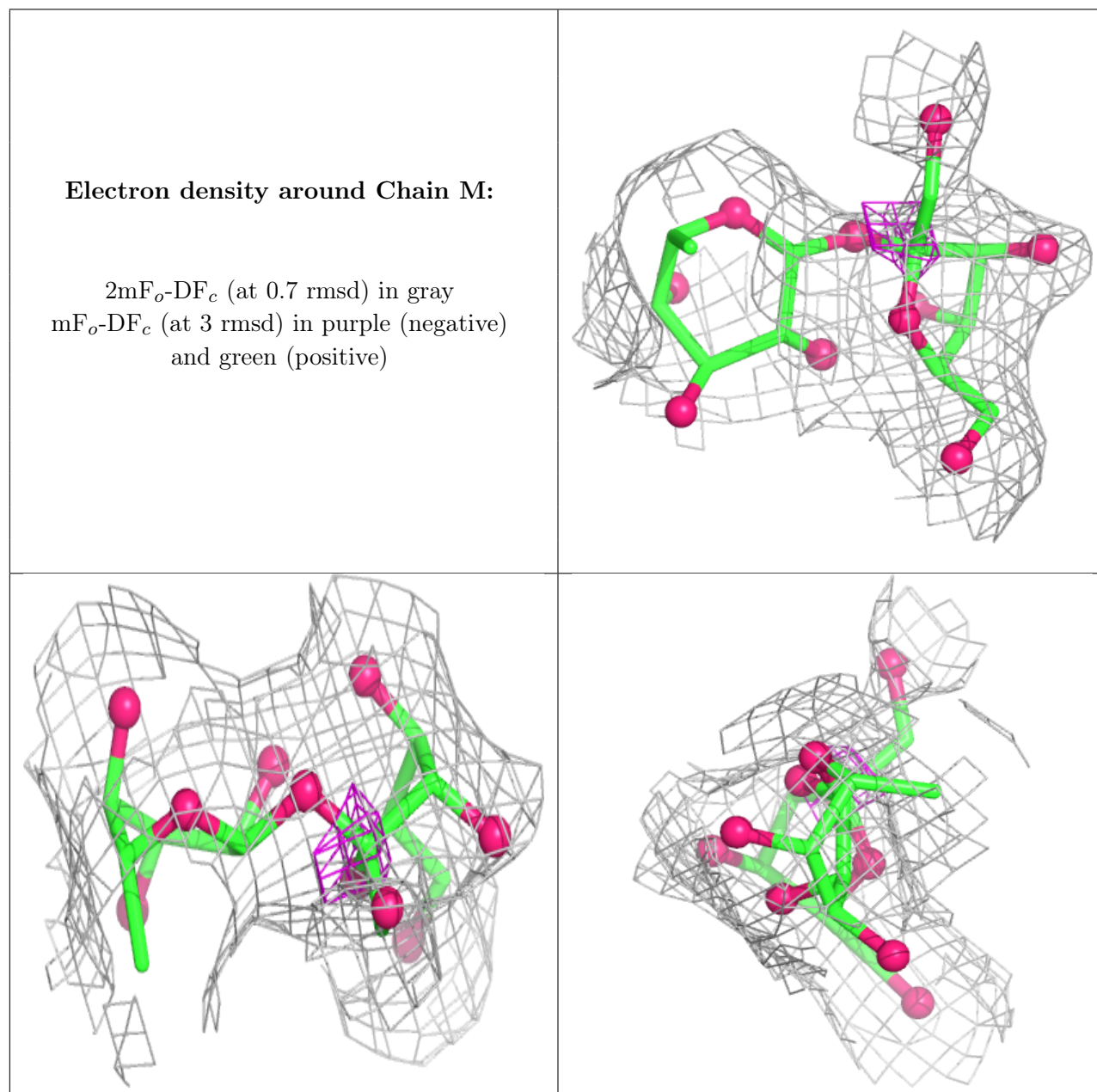
There are no non-standard protein/DNA/RNA residues in this entry.

5.3 Carbohydrates [i](#)

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

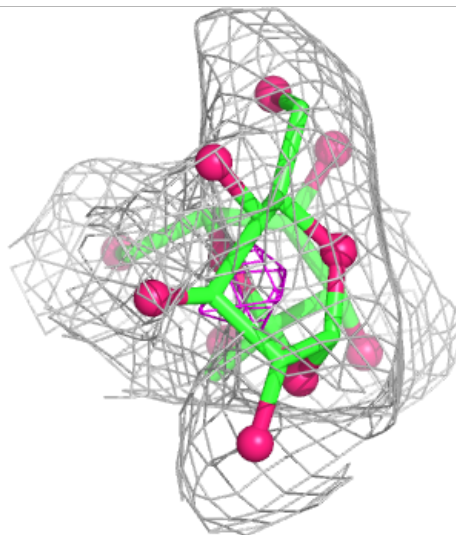
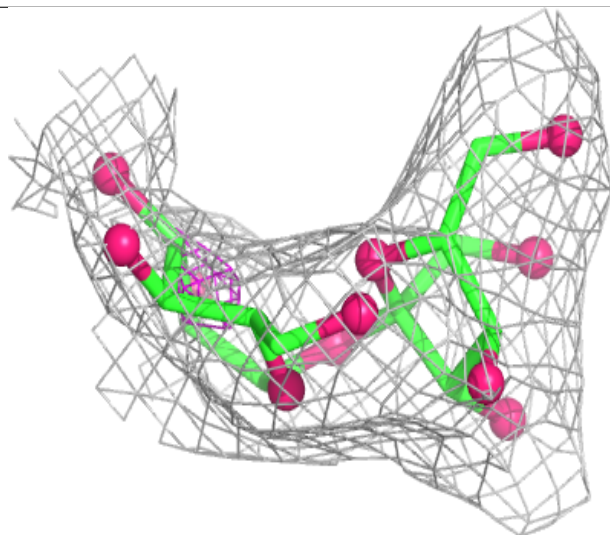
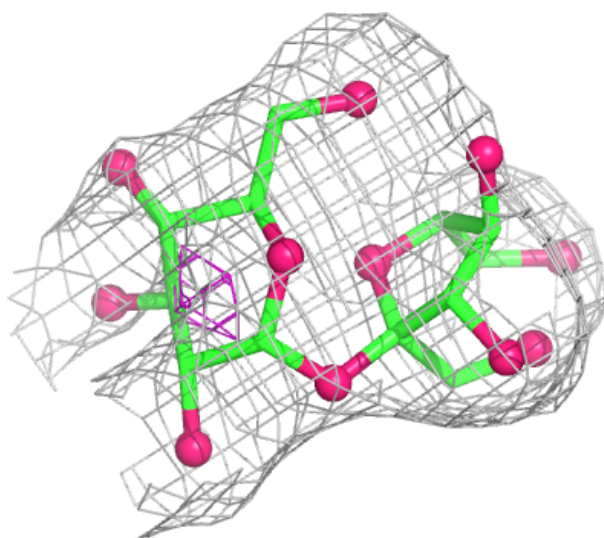
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
19	GLC	M	1	10/12	-	-	20,20,20,20	0
19	FRU	M	2	12/12	-	-	20,20,20,20	0
19	GLC	O	1	11/12	-	-	20,20,20,20	0
19	FRU	O	2	12/12	-	-	20,20,20,20	0
19	GLC	P	1	11/12	-	-	20,20,20,20	0
19	FRU	P	2	12/12	-	-	20,20,20,20	0
19	GLC	Q	1	11/12	-	-	20,20,20,20	0
19	FRU	Q	2	12/12	-	-	20,20,20,20	0
19	FRU	W	2	12/12	0.58	0.16	20,20,20,20	0
19	GLC	T	1	11/12	0.65	0.15	20,20,20,20	0
19	GLC	W	1	11/12	0.66	0.12	20,20,20,20	0
19	GLC	X	1	11/12	0.72	0.17	20,20,20,20	0
19	GLC	S	1	11/12	0.73	0.14	4,31,60,60	0
19	GLC	U	1	11/12	0.74	0.12	20,20,20,20	0
19	FRU	S	2	12/12	0.75	0.20	3,43,60,60	0
19	FRU	V	2	12/12	0.76	0.13	20,20,20,20	0
19	GLC	Z	1	11/12	0.76	0.12	20,20,20,20	0
19	GLC	V	1	11/12	0.78	0.11	20,20,20,20	0
19	FRU	Y	2	12/12	0.81	0.11	20,20,20,20	0
19	FRU	X	2	12/12	0.83	0.10	20,20,20,20	0
19	FRU	Z	2	12/12	0.84	0.10	20,20,20,20	0
19	FRU	U	2	12/12	0.86	0.10	20,20,20,20	0
19	FRU	T	2	12/12	0.88	0.09	20,20,20,20	0
19	GLC	Y	1	11/12	0.89	0.08	20,20,20,20	0
19	GLC	a	1	11/12	-	-	20,20,20,20	0
19	FRU	a	2	12/12	-	-	20,20,20,20	0

The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.



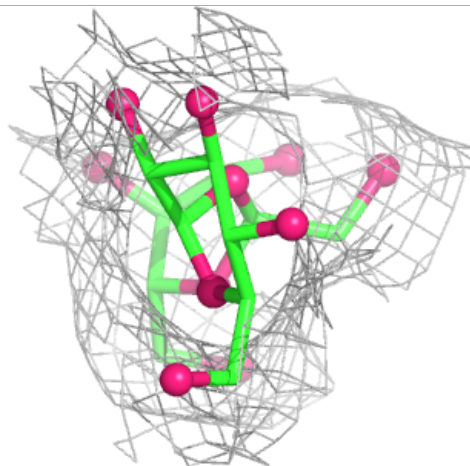
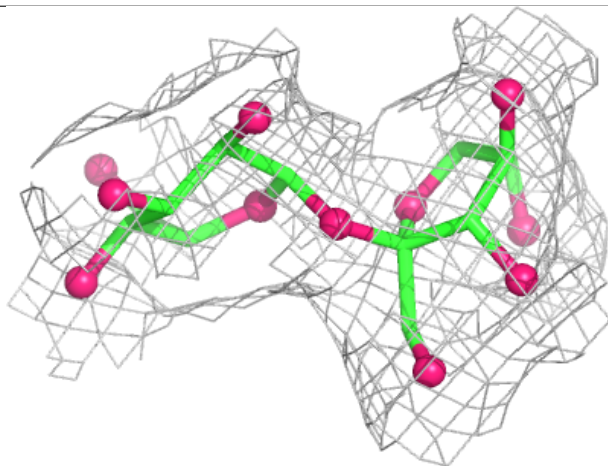
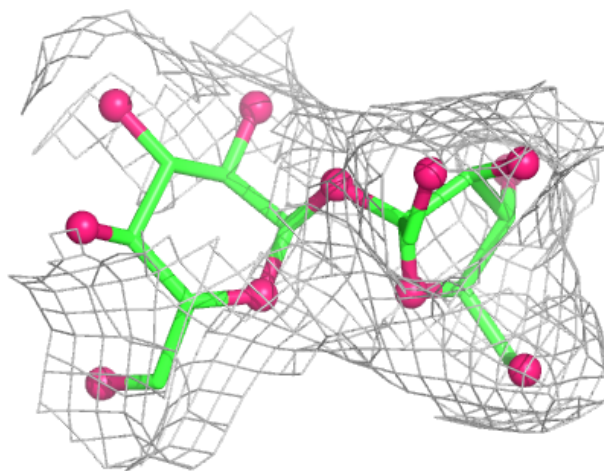
Electron density around Chain O:

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



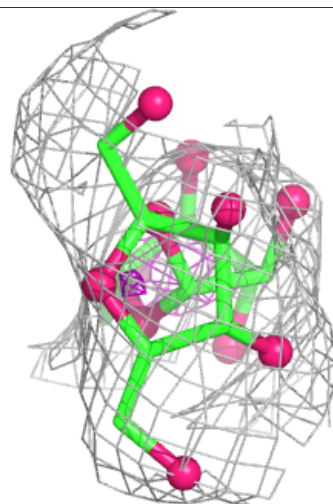
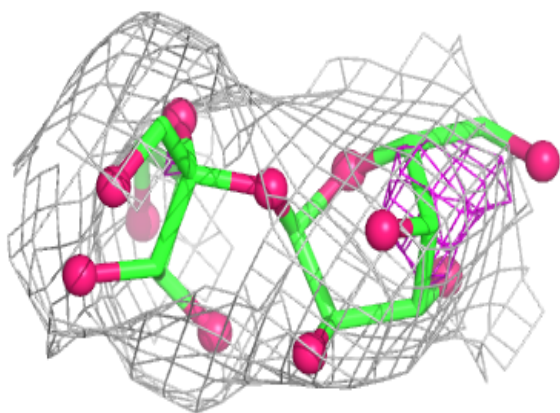
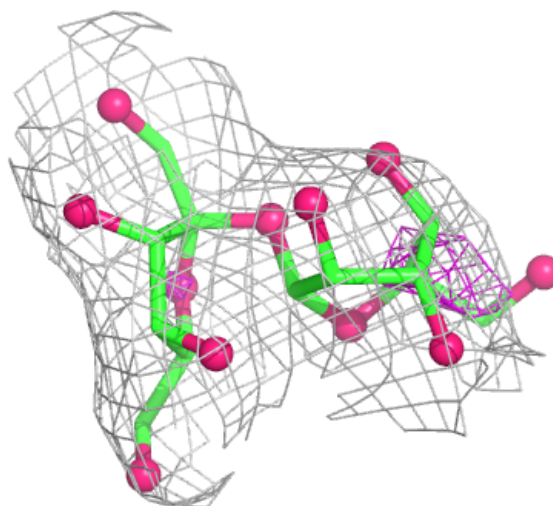
Electron density around Chain P:

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



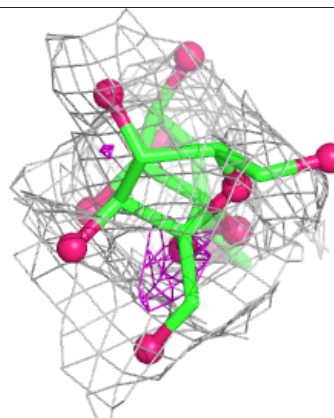
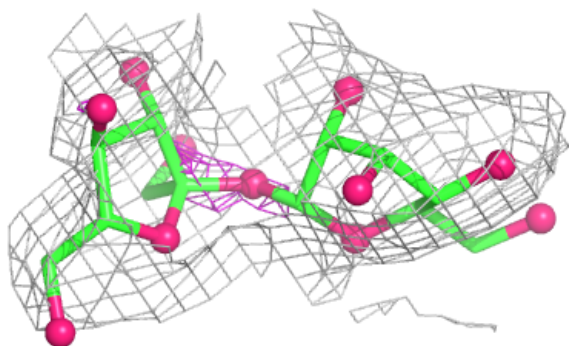
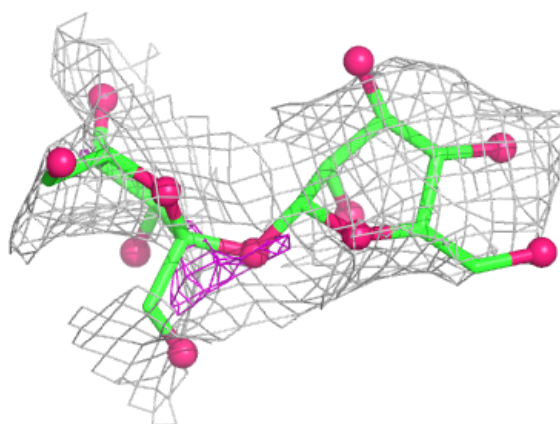
Electron density around Chain Q:

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

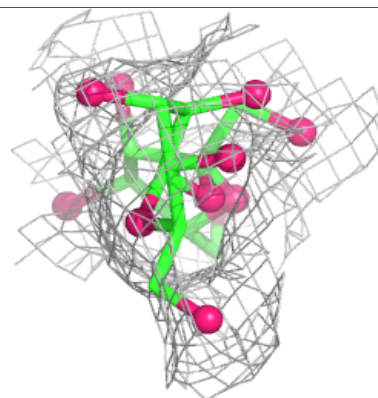
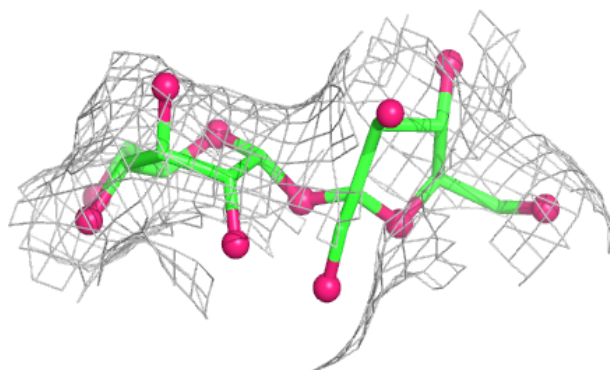
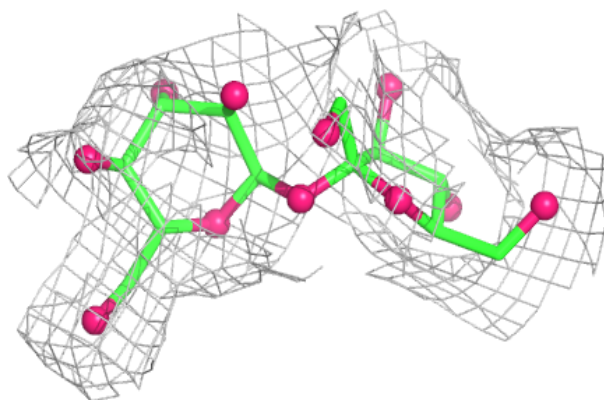


Electron density around Chain S:

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

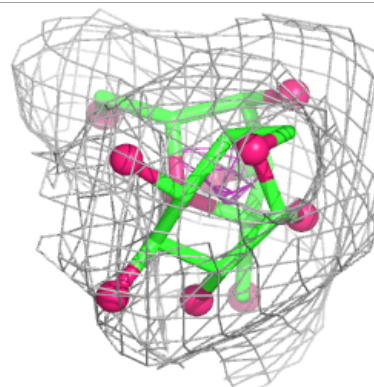
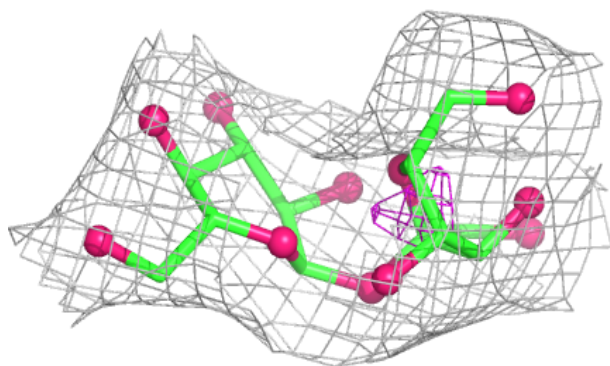
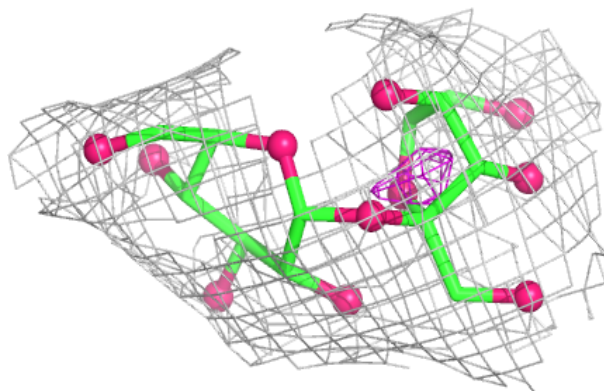
**Electron density around Chain T:**

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

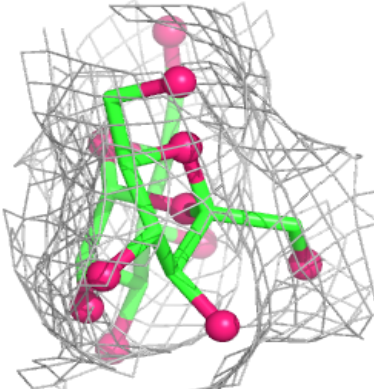
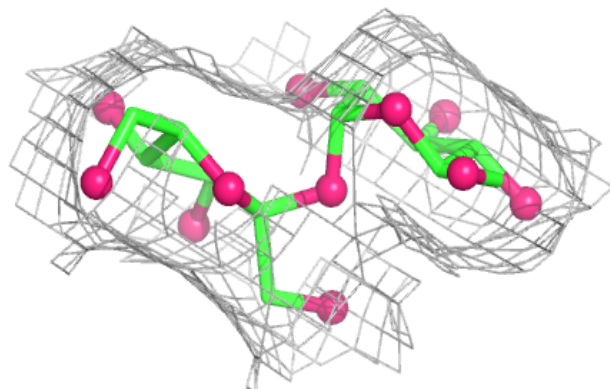
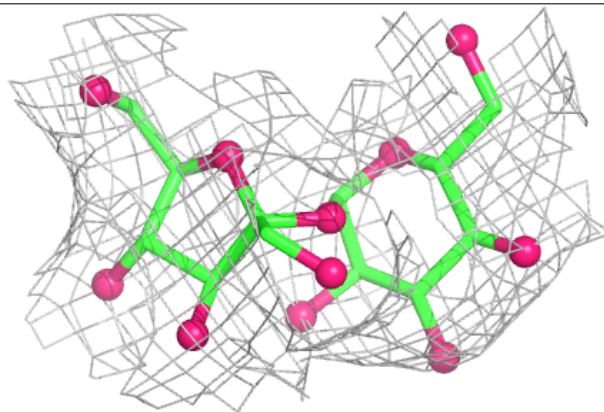


Electron density around Chain U:

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

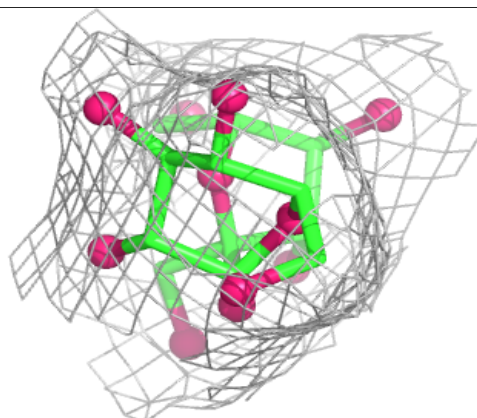
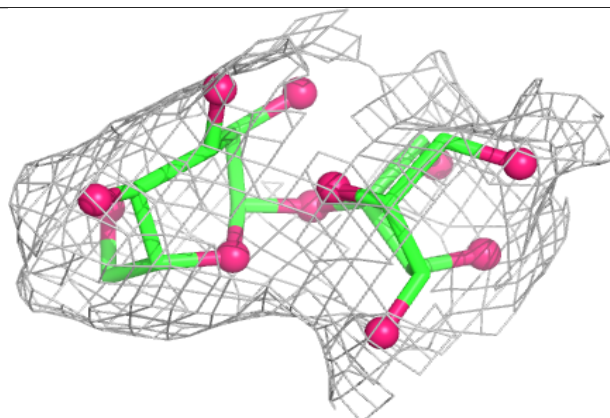
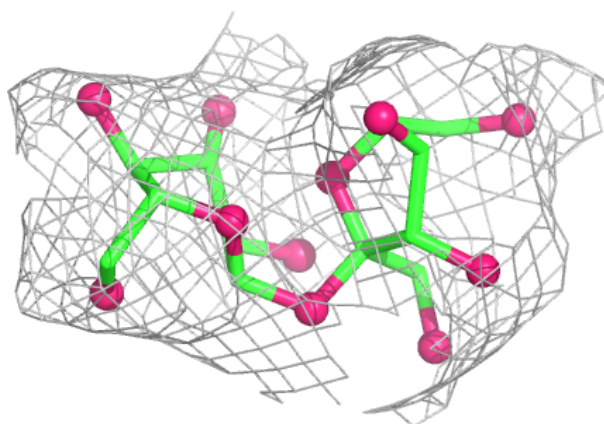
**Electron density around Chain V:**

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

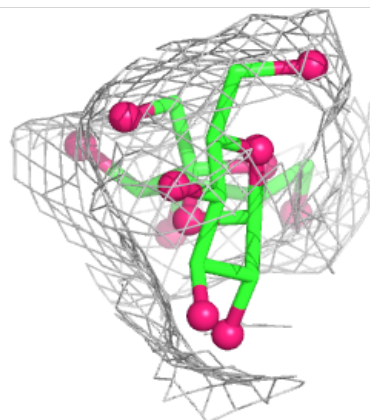
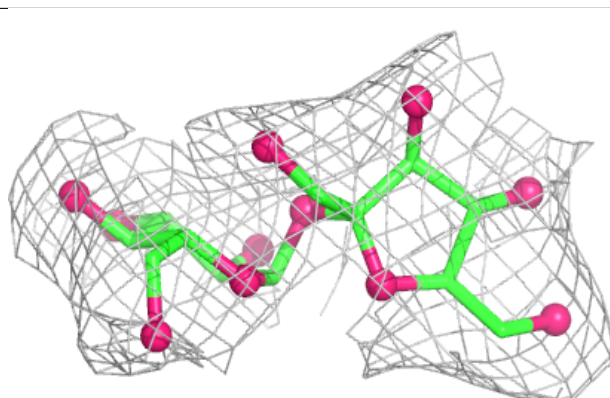
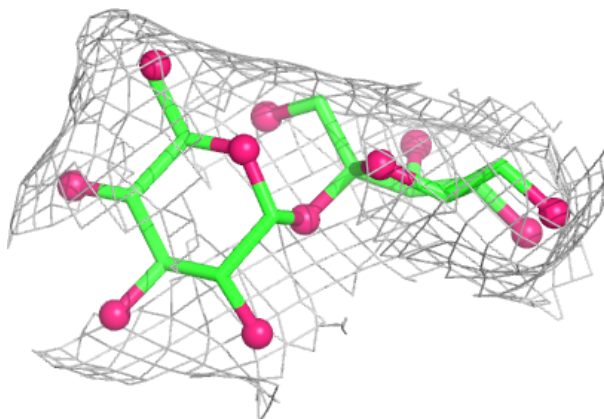


Electron density around Chain W:

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

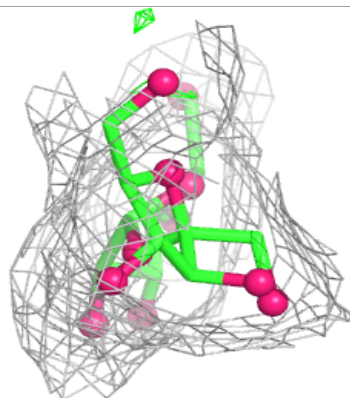
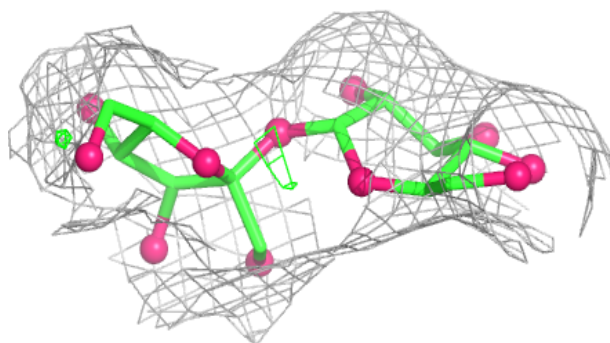
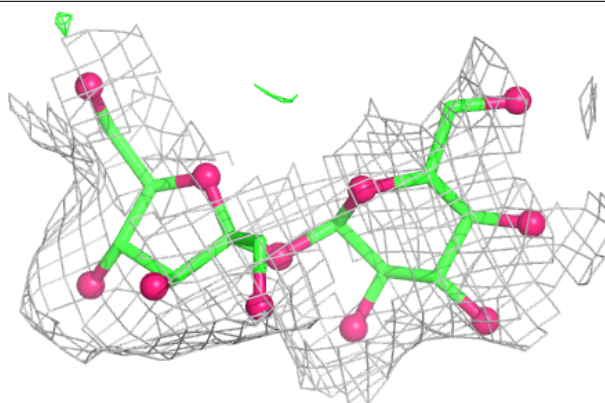
**Electron density around Chain X:**

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

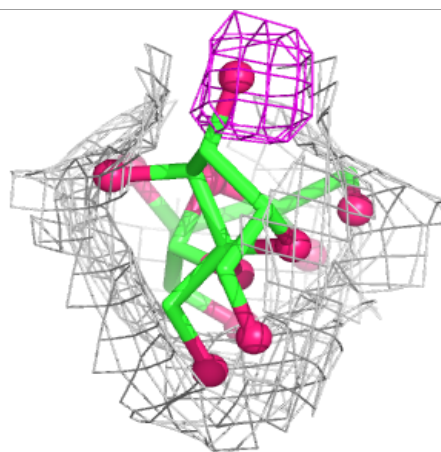
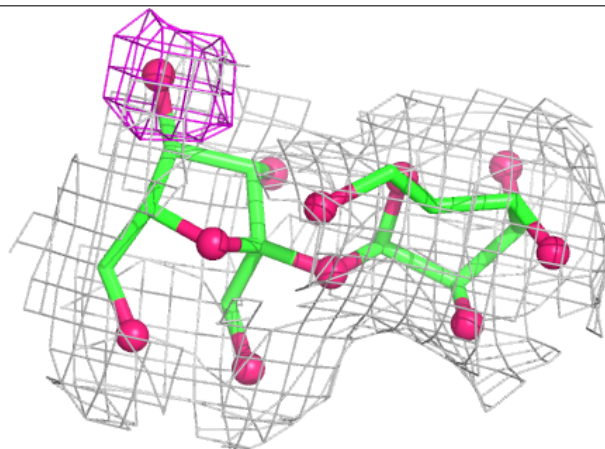


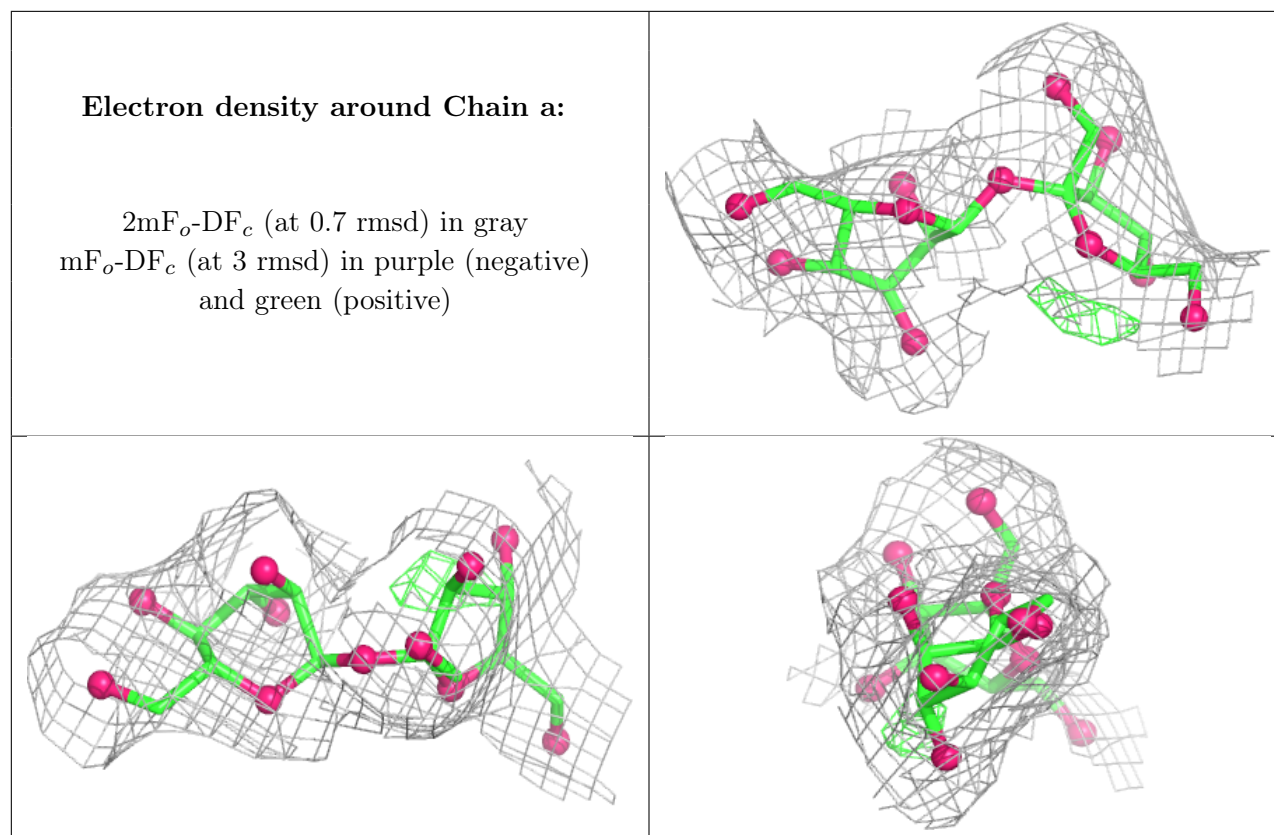
Electron density around Chain Y:

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

**Electron density around Chain Z:**

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





5.4 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
20	CLA	A	857	25/65	0.43	0.17	5,42,60,60	0
22	BCR	A	840	40/40	0.50	0.24	20,20,20,20	0
21	LMU	1	217	35/35	0.57	0.16	20,20,20,20	0
20	CLA	H	110	55/65	0.58	0.17	20,20,20,20	0
20	CLA	3	308	25/65	0.58	0.19	20,20,20,20	0
20	CLA	1	213	25/65	0.58	0.22	20,20,20,20	0
20	CLA	2	307	65/65	0.59	0.18	20,20,20,20	0
22	BCR	J	101	40/40	0.59	0.22	20,20,20,20	0
21	LMU	E	101	35/35	0.60	0.18	20,20,20,20	0
20	CLA	H	108	55/65	0.61	0.16	20,20,20,20	0
22	BCR	3	311	40/40	0.61	0.19	20,20,20,20	0
20	CLA	4	317	25/65	0.61	0.17	20,20,20,20	0
20	CLA	2	301	51/65	0.61	0.20	20,20,20,20	0
20	CLA	A	837	65/65	0.62	0.17	20,20,20,20	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
21	LMU	2	313	35/35	0.62	0.16	20,20,20,20	0
20	CLA	B	813	46/65	0.63	0.21	20,20,20,20	0
20	CLA	B	833	51/65	0.63	0.17	20,20,20,20	0
20	CLA	3	310	65/65	0.63	0.17	20,20,20,20	0
21	LMU	K	101	35/35	0.63	0.16	20,20,20,20	0
20	CLA	3	305	25/65	0.63	0.19	20,20,20,20	0
20	CLA	K	105	45/65	0.63	0.16	20,20,20,20	0
20	CLA	L	203	55/65	0.63	0.19	20,20,20,20	0
20	CLA	B	812	60/65	0.64	0.18	20,20,20,20	0
21	LMU	1	216	35/35	0.65	0.15	20,20,20,20	0
20	CLA	2	321	61/65	0.65	0.17	20,20,20,20	0
20	CLA	4	306	50/65	0.65	0.19	20,20,20,20	0
20	CLA	3	301	56/65	0.65	0.16	2,36,60,60	0
20	CLA	4	318	52/65	0.65	0.16	20,20,20,20	0
20	CLA	2	305	25/65	0.65	0.17	20,20,20,20	0
20	CLA	A	838	50/65	0.65	0.15	20,20,20,20	0
20	CLA	1	205	36/65	0.65	0.15	20,20,20,20	0
20	CLA	3	314	42/65	0.66	0.16	20,20,20,20	0
20	CLA	K	107	65/65	0.67	0.17	20,20,20,20	0
20	CLA	4	319	47/65	0.67	0.17	20,20,20,20	0
21	LMU	A	851	35/35	0.67	0.15	20,20,20,20	0
20	CLA	3	309	65/65	0.67	0.17	20,20,20,20	0
20	CLA	4	302	55/65	0.68	0.17	20,20,20,20	0
20	CLA	1	212	61/65	0.68	0.15	2,35,60,60	0
21	LMU	L	205	35/35	0.68	0.13	20,20,20,20	0
20	CLA	B	822	58/65	0.68	0.23	20,20,20,20	0
21	LMU	4	320	34/35	0.68	0.15	20,20,20,20	0
22	BCR	A	842	40/40	0.68	0.21	20,20,20,20	0
20	CLA	L	204	55/65	0.68	0.14	20,20,20,20	0
20	CLA	R	106	57/65	0.69	0.16	20,20,20,20	0
20	CLA	1	211	51/65	0.69	0.15	20,20,20,20	0
21	LMU	C	101	35/35	0.69	0.14	20,20,20,20	0
20	CLA	F	205	41/65	0.69	0.17	20,20,20,20	0
20	CLA	H	101	55/65	0.69	0.14	20,20,20,20	0
21	LMU	H	105	35/35	0.70	0.13	20,20,20,20	0
20	CLA	4	304	65/65	0.70	0.17	20,20,20,20	0
20	CLA	4	305	55/65	0.70	0.16	20,20,20,20	0
21	LMU	4	322	35/35	0.70	0.15	20,20,20,20	0
20	CLA	J	102	61/65	0.70	0.15	20,20,20,20	0
20	CLA	G	103	51/65	0.70	0.14	20,20,20,20	0
20	CLA	B	832	45/65	0.70	0.15	20,20,20,20	0
20	CLA	1	207	51/65	0.71	0.14	20,20,20,20	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
21	LMU	H	103	35/35	0.71	0.12	20,20,20,20	0
20	CLA	A	808	45/65	0.71	0.16	20,20,20,20	0
20	CLA	A	812	45/65	0.71	0.19	20,20,20,20	0
21	LMU	A	845	35/35	0.71	0.14	20,20,20,20	0
21	LMU	A	846	35/35	0.71	0.14	20,20,20,20	0
20	CLA	A	831	45/65	0.71	0.16	20,20,20,20	0
21	LMU	B	801	35/35	0.71	0.13	20,20,20,20	0
20	CLA	1	214	51/65	0.71	0.15	20,20,20,20	0
20	CLA	K	103	50/65	0.72	0.15	20,20,20,20	0
20	CLA	3	304	25/65	0.72	0.15	20,20,20,20	0
20	CLA	K	106	50/65	0.72	0.14	20,20,20,20	0
20	CLA	2	304	50/65	0.72	0.17	20,20,20,20	0
20	CLA	3	312	25/65	0.72	0.15	20,20,20,20	0
20	CLA	2	311	50/65	0.72	0.20	20,20,20,20	0
20	CLA	F	206	53/65	0.72	0.14	20,20,20,20	0
20	CLA	3	316	25/65	0.72	0.15	20,20,20,20	0
20	CLA	3	319	36/65	0.72	0.15	20,20,20,20	0
20	CLA	3	320	55/65	0.72	0.17	20,20,20,20	0
21	LMU	R	105	35/35	0.72	0.15	20,20,20,20	0
21	LMU	2	318	35/35	0.72	0.13	20,20,20,20	0
21	LMU	2	319	35/35	0.72	0.13	20,20,20,20	0
20	CLA	A	805	46/65	0.72	0.17	20,20,20,20	0
22	BCR	I	103	40/40	0.72	0.15	20,20,20,20	0
20	CLA	B	818	46/65	0.72	0.19	20,20,20,20	0
20	CLA	2	302	56/65	0.73	0.16	20,20,20,20	0
20	CLA	2	314	25/65	0.73	0.13	20,20,20,20	0
21	LMU	L	206	35/35	0.73	0.13	20,20,20,20	0
21	LMU	R	101	35/35	0.73	0.13	20,20,20,20	0
20	CLA	1	201	46/65	0.73	0.14	20,20,20,20	0
20	CLA	3	306	25/65	0.73	0.15	20,20,20,20	0
21	LMU	2	320	35/35	0.73	0.13	20,20,20,20	0
21	LMU	3	318	35/35	0.73	0.14	20,20,20,20	0
22	BCR	B	842	40/40	0.73	0.18	20,20,20,20	0
22	BCR	B	844	40/40	0.73	0.27	20,20,20,20	0
20	CLA	A	821	65/65	0.73	0.24	20,20,20,20	0
20	CLA	3	313	25/65	0.73	0.14	20,20,20,20	0
21	LMU	4	301	35/35	0.74	0.12	20,20,20,20	0
20	CLA	4	314	25/65	0.74	0.14	20,20,20,20	0
20	CLA	2	306	65/65	0.74	0.15	20,20,20,20	0
20	CLA	1	208	25/65	0.74	0.15	20,20,20,20	0
20	CLA	A	819	42/65	0.74	0.14	20,20,20,20	0
21	LMU	K	102	35/35	0.74	0.14	20,20,20,20	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
21	LMU	K	104	35/35	0.74	0.12	20,20,20,20	0
20	CLA	R	107	65/65	0.74	0.14	20,20,20,20	0
20	CLA	4	310	55/65	0.74	0.17	20,20,20,20	0
20	CLA	1	206	61/65	0.75	0.14	20,20,20,20	0
21	LMU	3	302	35/35	0.75	0.13	20,20,20,20	0
21	LMU	F	201	34/35	0.75	0.13	20,20,20,20	0
22	BCR	A	843	40/40	0.75	0.20	20,20,20,20	0
21	LMU	2	316	35/35	0.75	0.13	20,20,20,20	0
20	CLA	L	208	50/65	0.75	0.18	20,20,20,20	0
20	CLA	H	107	65/65	0.75	0.20	20,20,20,20	0
21	LMU	R	109	35/35	0.75	0.12	20,20,20,20	0
21	LMU	4	321	35/35	0.76	0.12	20,20,20,20	0
20	CLA	A	850	46/65	0.76	0.13	20,20,20,20	0
20	CLA	3	303	36/65	0.76	0.13	20,20,20,20	0
20	CLA	1	202	47/65	0.76	0.15	20,20,20,20	0
21	LMU	4	316	35/35	0.76	0.12	20,20,20,20	0
20	CLA	1	203	47/65	0.76	0.14	20,20,20,20	0
21	LMU	B	845	25/35	0.76	0.12	20,20,20,20	0
25	LMG	B	846	49/55	0.76	0.22	20,20,20,20	0
20	CLA	4	315	46/65	0.77	0.13	20,20,20,20	0
20	CLA	A	809	65/65	0.77	0.18	20,20,20,20	0
20	CLA	B	831	45/65	0.77	0.17	20,20,20,20	0
20	CLA	4	308	25/65	0.77	0.15	20,20,20,20	0
22	BCR	A	841	40/40	0.77	0.18	20,20,20,20	0
20	CLA	H	109	50/65	0.77	0.16	20,20,20,20	0
20	CLA	4	309	25/65	0.77	0.15	20,20,20,20	0
22	BCR	A	844	40/40	0.77	0.22	20,20,20,20	0
22	BCR	B	841	40/40	0.77	0.20	20,20,20,20	0
21	LMU	A	853	35/35	0.77	0.12	20,20,20,20	0
20	CLA	B	839	36/65	0.77	0.13	20,20,20,20	0
22	BCR	G	102	40/40	0.77	0.20	20,20,20,20	0
20	CLA	3	315	50/65	0.77	0.13	20,20,20,20	0
20	CLA	2	312	65/65	0.77	0.15	20,20,20,20	0
21	LMU	R	102	35/35	0.77	0.12	20,20,20,20	0
20	CLA	1	209	36/65	0.78	0.14	20,20,20,20	0
20	CLA	L	201	65/65	0.78	0.18	20,20,20,20	0
21	LMU	1	218	35/35	0.78	0.12	20,20,20,20	0
20	CLA	A	813	50/65	0.78	0.15	20,20,20,20	0
22	BCR	F	203	40/40	0.78	0.18	20,20,20,20	0
20	CLA	J	103	55/65	0.78	0.13	2,33,60,60	0
20	CLA	A	814	65/65	0.78	0.17	2,35,60,60	0
20	CLA	B	829	65/65	0.78	0.20	20,20,20,20	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
22	BCR	L	209	40/40	0.78	0.18	20,20,20,20	0
20	CLA	A	817	65/65	0.78	0.18	20,20,20,20	0
20	CLA	3	317	25/65	0.79	0.13	20,20,20,20	0
20	CLA	1	204	46/65	0.79	0.14	20,20,20,20	0
20	CLA	1	210	36/65	0.79	0.16	20,20,20,20	0
20	CLA	1	215	25/65	0.79	0.13	20,20,20,20	0
20	CLA	2	315	25/65	0.79	0.15	20,20,20,20	0
20	CLA	B	808	54/65	0.79	0.17	20,20,20,20	0
21	LMU	B	802	35/35	0.79	0.12	20,20,20,20	0
20	CLA	B	809	55/65	0.79	0.18	20,20,20,20	0
20	CLA	2	317	65/65	0.79	0.13	20,20,20,20	0
21	LMU	R	103	35/35	0.79	0.13	20,20,20,20	0
20	CLA	3	307	25/65	0.79	0.12	20,20,20,20	0
21	LMU	R	108	35/35	0.79	0.12	20,20,20,20	0
20	CLA	2	308	25/65	0.79	0.14	20,20,20,20	0
21	LMU	H	102	35/35	0.79	0.12	20,20,20,20	0
20	CLA	B	823	65/65	0.80	0.18	20,20,20,20	0
20	CLA	A	855	65/65	0.80	0.22	20,20,20,20	0
20	CLA	A	803	65/65	0.80	0.21	20,20,20,20	0
20	CLA	A	822	65/65	0.80	0.17	20,20,20,20	0
20	CLA	A	823	65/65	0.80	0.16	20,20,20,20	0
20	CLA	B	811	65/65	0.80	0.17	20,20,20,20	0
20	CLA	4	311	25/65	0.80	0.18	20,20,20,20	0
20	CLA	2	309	25/65	0.80	0.15	20,20,20,20	0
20	CLA	4	303	36/65	0.80	0.17	20,20,20,20	0
20	CLA	A	811	54/65	0.80	0.17	20,20,20,20	0
20	CLA	A	818	51/65	0.81	0.14	20,20,20,20	0
20	CLA	B	803	45/65	0.81	0.17	20,20,20,20	0
21	LMU	L	210	35/35	0.81	0.11	20,20,20,20	0
20	CLA	B	807	65/65	0.81	0.19	20,20,20,20	0
20	CLA	B	828	50/65	0.81	0.16	20,20,20,20	0
22	BCR	B	843	40/40	0.81	0.22	20,20,20,20	0
20	CLA	A	810	54/65	0.81	0.13	20,20,20,20	0
22	BCR	F	202	40/40	0.81	0.22	20,20,20,20	0
20	CLA	B	830	50/65	0.81	0.20	20,20,20,20	0
20	CLA	4	313	36/65	0.81	0.17	20,20,20,20	0
20	CLA	A	849	65/65	0.81	0.19	20,20,20,20	0
20	CLA	A	816	65/65	0.81	0.21	20,20,20,20	0
21	LMU	A	854	35/35	0.81	0.13	20,20,20,20	0
20	CLA	A	802	55/65	0.81	0.17	20,20,20,20	0
20	CLA	2	303	25/65	0.82	0.12	20,20,20,20	0
20	CLA	I	102	60/65	0.82	0.17	20,20,20,20	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
20	CLA	2	310	50/65	0.82	0.15	20,20,20,20	0
20	CLA	4	307	52/65	0.82	0.12	20,20,20,20	0
20	CLA	B	820	65/65	0.82	0.16	20,20,20,20	0
20	CLA	A	827	50/65	0.82	0.15	20,20,20,20	0
20	CLA	A	807	55/65	0.83	0.18	20,20,20,20	0
20	CLA	F	204	36/65	0.83	0.15	20,20,20,20	0
20	CLA	B	814	59/65	0.83	0.16	20,20,20,20	0
20	CLA	A	832	51/65	0.83	0.17	20,20,20,20	0
21	LMU	A	852	35/35	0.83	0.10	20,20,20,20	0
20	CLA	A	815	52/65	0.83	0.17	20,20,20,20	0
20	CLA	A	829	65/65	0.83	0.18	20,20,20,20	0
20	CLA	L	207	47/65	0.83	0.16	20,20,20,20	0
23	PQN	A	839	33/33	0.83	0.23	20,20,20,20	0
20	CLA	A	848	65/65	0.83	0.20	20,20,20,20	0
20	CLA	4	312	25/65	0.84	0.15	20,20,20,20	0
20	CLA	A	833	65/65	0.84	0.18	20,20,20,20	0
20	CLA	A	835	51/65	0.84	0.20	20,20,20,20	0
21	LMU	G	101	35/35	0.84	0.10	20,20,20,20	0
21	LMU	R	104	35/35	0.84	0.10	20,20,20,20	0
20	CLA	B	810	65/65	0.84	0.17	20,20,20,20	0
20	CLA	B	834	60/65	0.84	0.19	20,20,20,20	0
20	CLA	B	836	47/65	0.84	0.20	20,20,20,20	0
20	CLA	B	837	65/65	0.84	0.18	20,20,20,20	0
20	CLA	A	836	65/65	0.84	0.16	20,20,20,20	0
20	CLA	B	826	65/65	0.84	0.19	20,20,20,20	0
20	CLA	A	825	55/65	0.84	0.18	20,20,20,20	0
20	CLA	A	826	65/65	0.84	0.18	20,20,20,20	0
21	LMU	H	104	35/35	0.85	0.10	20,20,20,20	0
20	CLA	B	819	55/65	0.85	0.14	20,20,20,20	0
20	CLA	A	828	65/65	0.85	0.15	20,20,20,20	0
20	CLA	A	801	50/65	0.85	0.14	20,20,20,20	0
20	CLA	A	830	50/65	0.85	0.15	20,20,20,20	0
20	CLA	A	806	65/65	0.85	0.22	20,20,20,20	0
22	BCR	I	101	40/40	0.85	0.16	20,20,20,20	0
20	CLA	B	815	60/65	0.85	0.21	20,20,20,20	0
20	CLA	B	849	65/65	0.85	0.20	20,20,20,20	0
20	CLA	B	816	61/65	0.85	0.17	20,20,20,20	0
20	CLA	B	817	50/65	0.85	0.16	20,20,20,20	0
20	CLA	A	804	57/65	0.85	0.16	20,20,20,20	0
20	CLA	L	202	65/65	0.86	0.15	20,20,20,20	0
20	CLA	B	825	65/65	0.86	0.21	20,20,20,20	0
22	BCR	B	850	40/40	0.86	0.18	20,20,20,20	0

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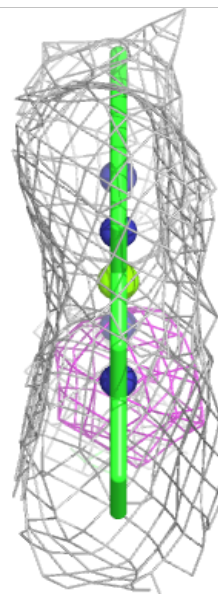
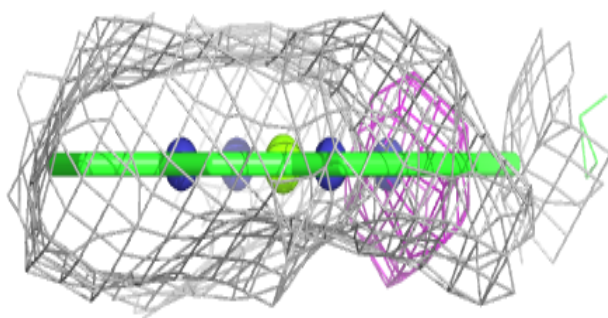
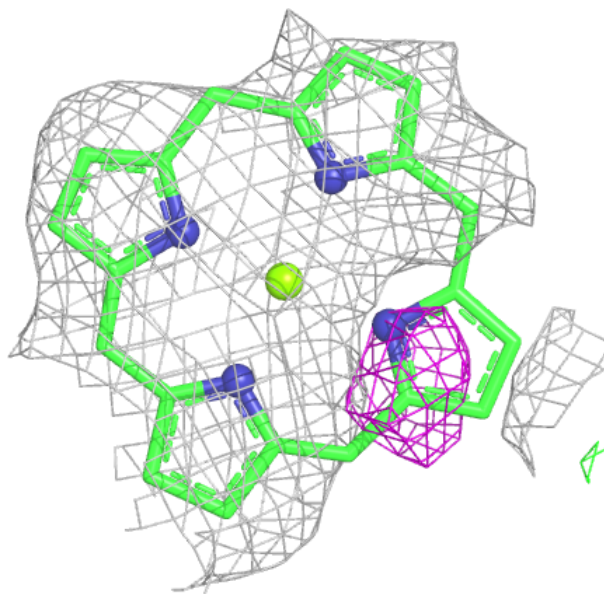
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
26	UNL	H	106	23/-	0.86	0.09	20,20,20,20	0
20	CLA	B	824	65/65	0.87	0.18	20,20,20,20	0
20	CLA	A	834	47/65	0.87	0.17	20,20,20,20	0
20	CLA	B	838	65/65	0.87	0.17	20,20,20,20	0
20	CLA	B	821	54/65	0.87	0.18	20,20,20,20	0
20	CLA	B	847	65/65	0.87	0.20	20,20,20,20	0
20	CLA	B	804	65/65	0.87	0.18	20,20,20,20	0
20	CLA	A	820	55/65	0.87	0.16	20,20,20,20	0
20	CLA	B	835	65/65	0.87	0.18	20,20,20,20	0
23	PQN	B	840	33/33	0.88	0.18	20,20,20,20	0
20	CLA	B	848	65/65	0.88	0.18	20,20,20,20	0
20	CLA	B	805	65/65	0.88	0.17	20,20,20,20	0
20	CLA	A	847	65/65	0.89	0.23	20,20,20,20	0
20	CLA	B	827	50/65	0.89	0.14	20,20,20,20	0
20	CLA	B	806	65/65	0.89	0.20	20,20,20,20	0
20	CLA	A	824	65/65	0.89	0.18	20,20,20,20	0
24	SF4	C	102	8/8	0.98	0.06	20,20,20,20	0
24	SF4	A	856	8/8	0.99	0.05	20,20,20,20	0
24	SF4	C	103	8/8	0.99	0.05	20,20,20,20	0

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

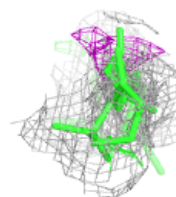
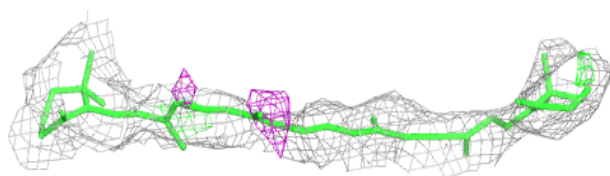
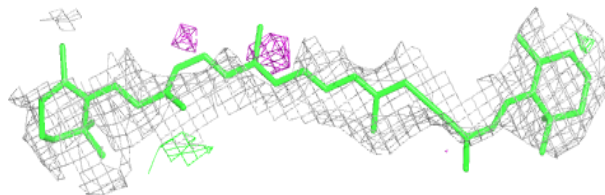
Electron density around CLA A 857:

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



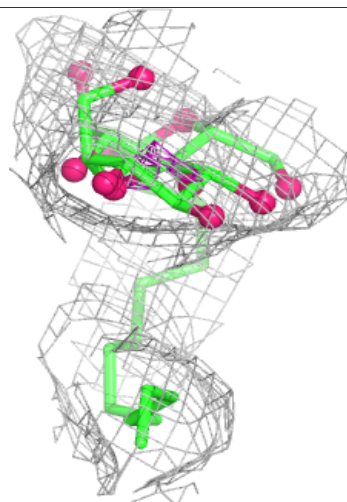
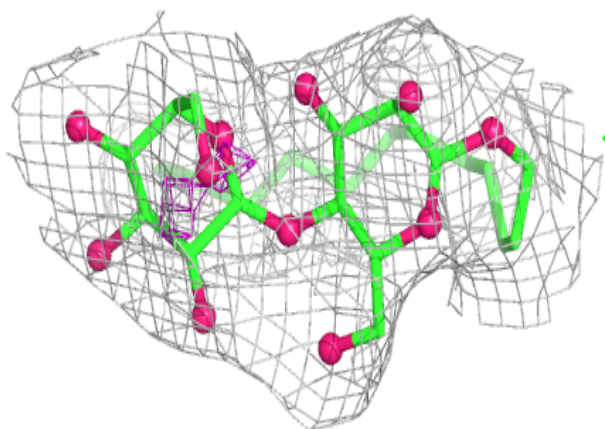
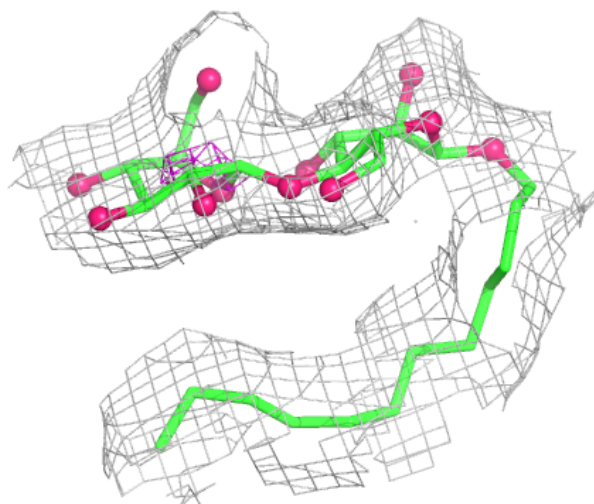
Electron density around BCR A 840:

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



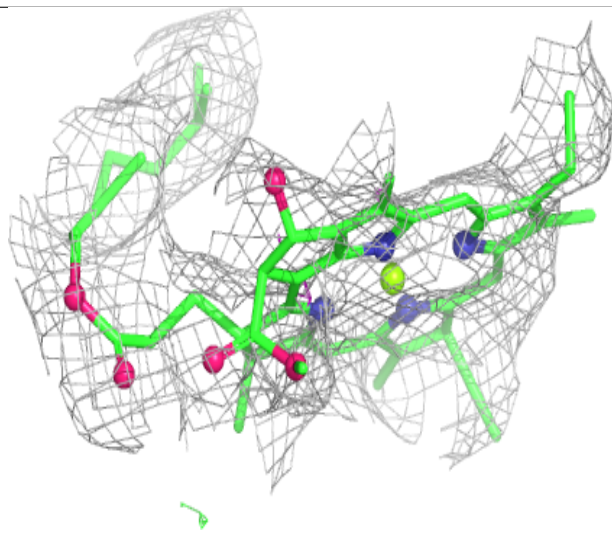
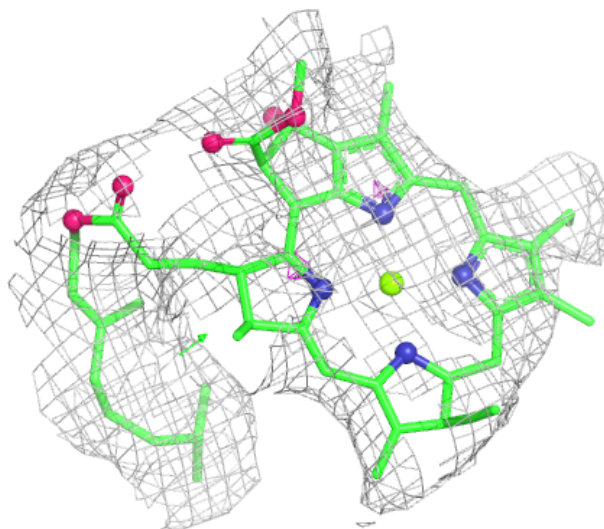
Electron density around LMU 1 217:

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



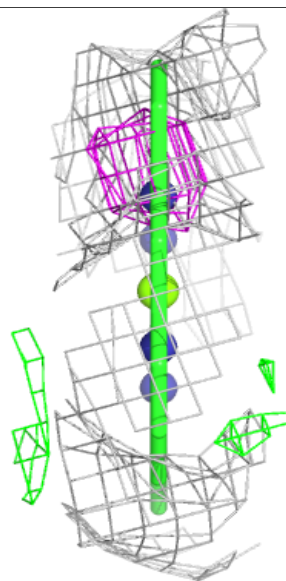
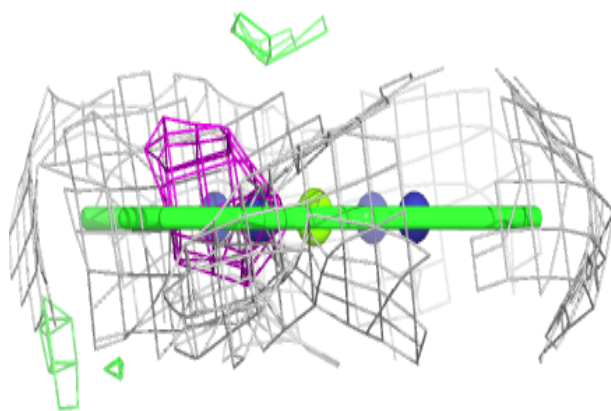
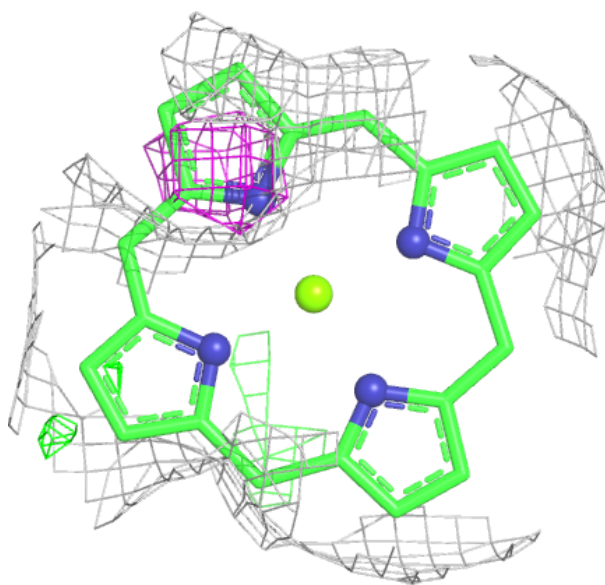
Electron density around CLA H 110:

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



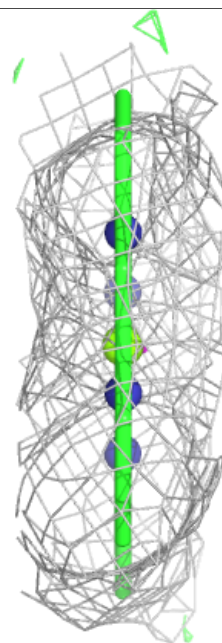
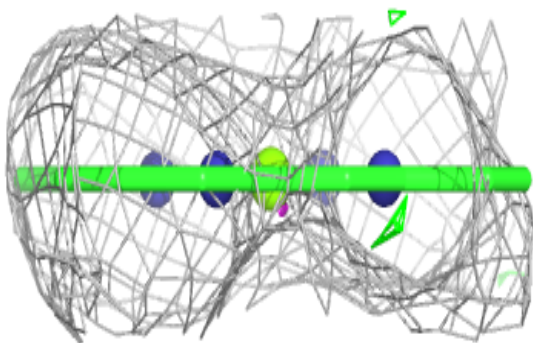
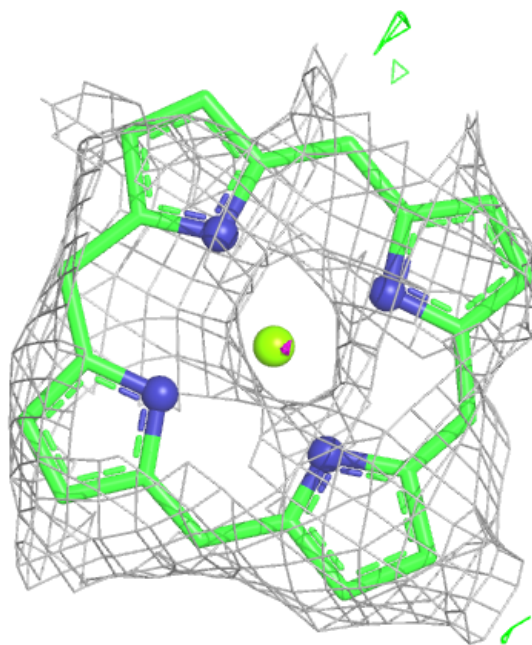
Electron density around CLA 3 308:

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



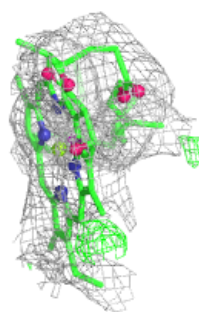
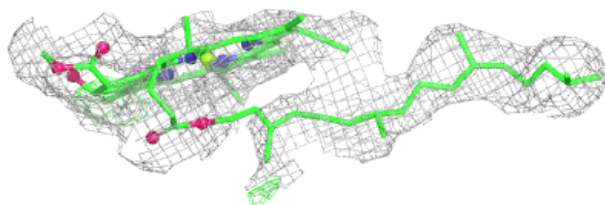
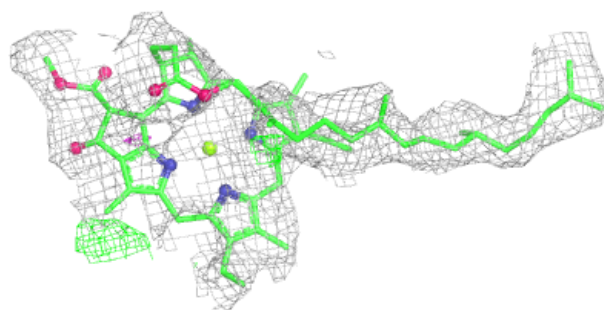
Electron density around CLA 1 213:

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

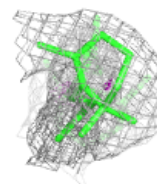
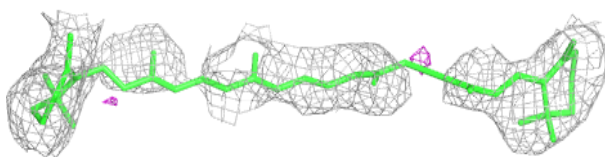
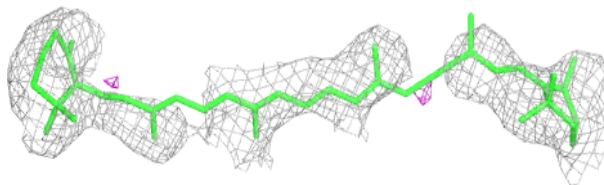


Electron density around CLA 2 307:

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

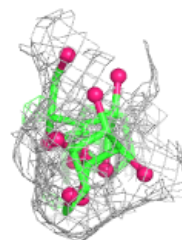
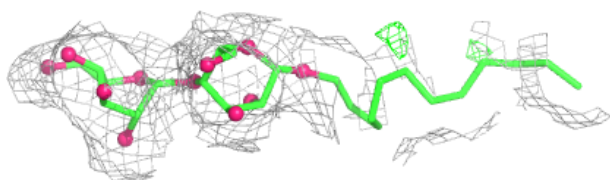
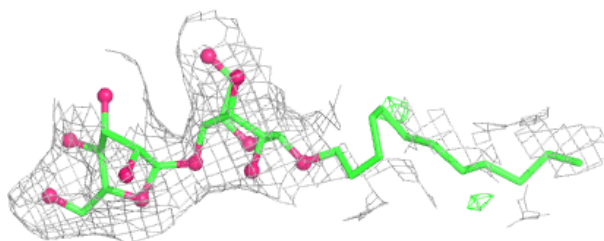
**Electron density around BCR J 101:**

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

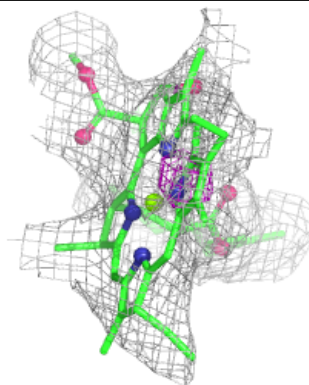
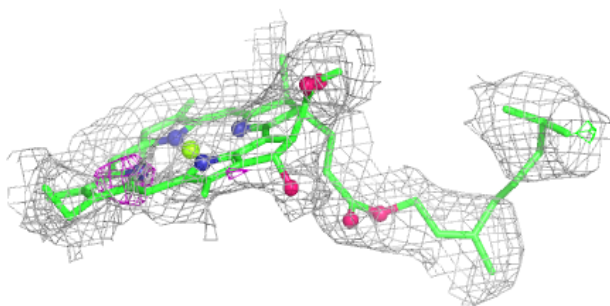
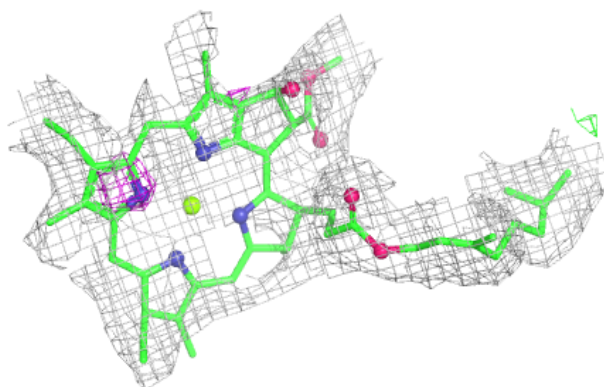


Electron density around LMU E 101:

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

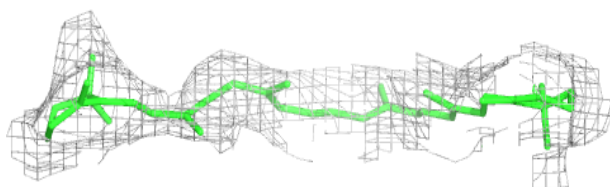
**Electron density around CLA H 108:**

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



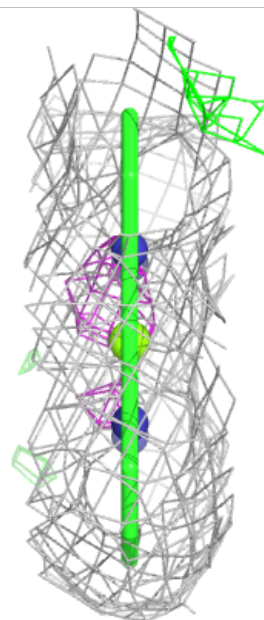
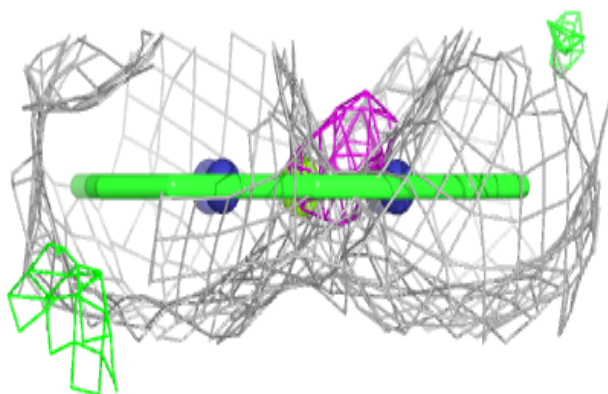
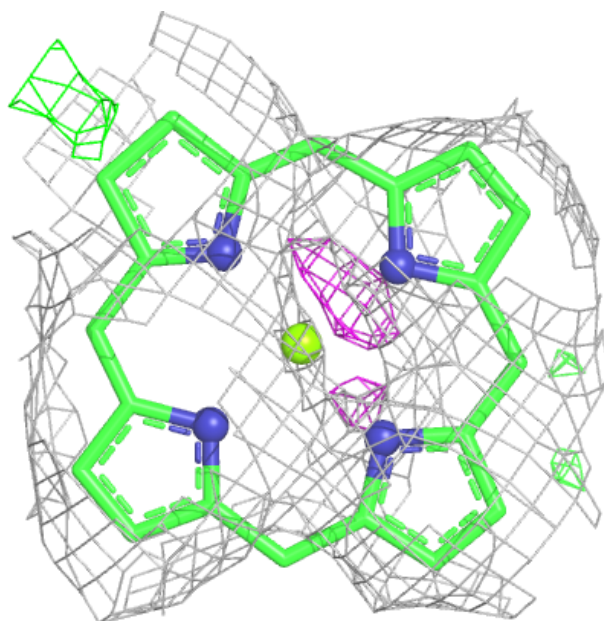
Electron density around BCR 3 311:

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



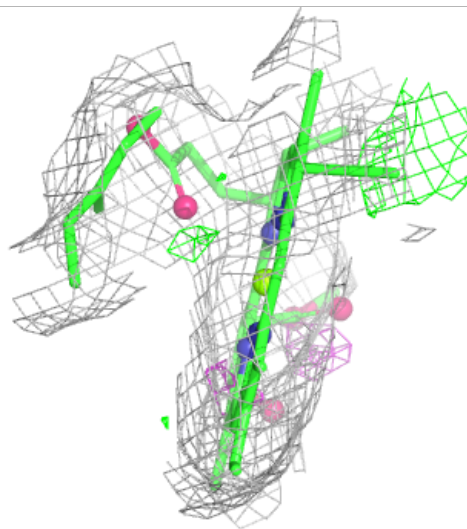
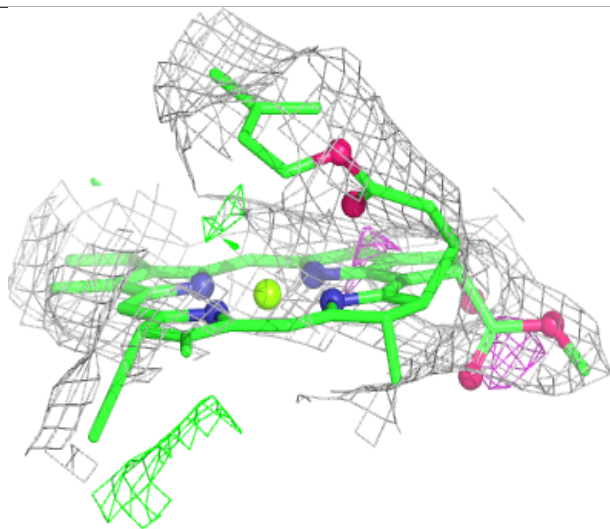
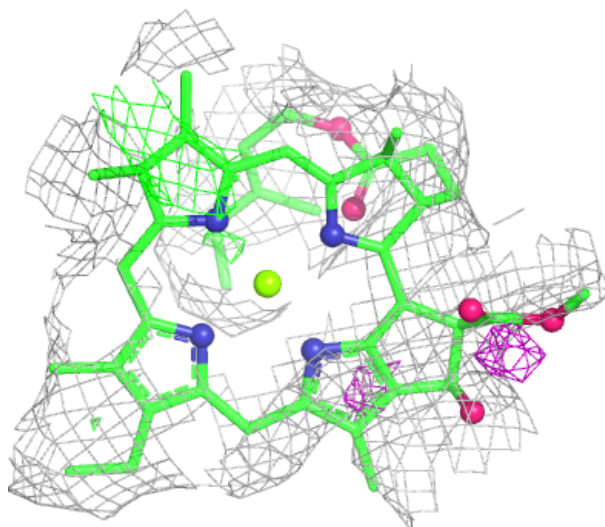
Electron density around CLA 4 317:

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



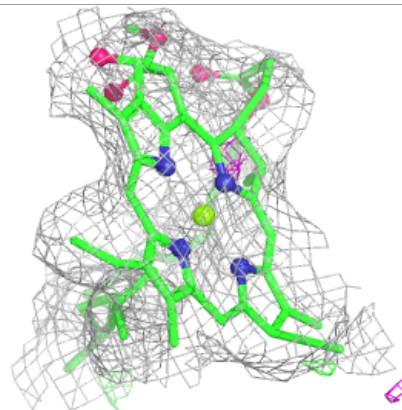
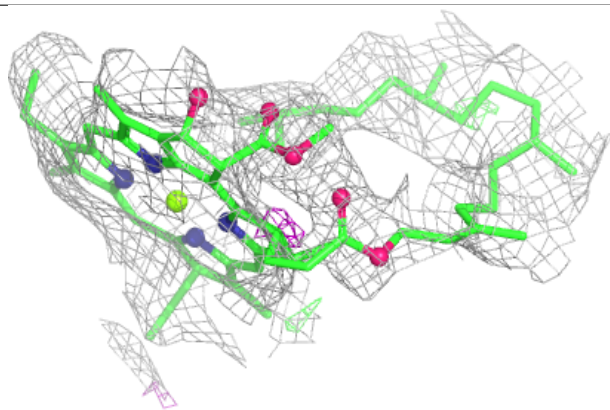
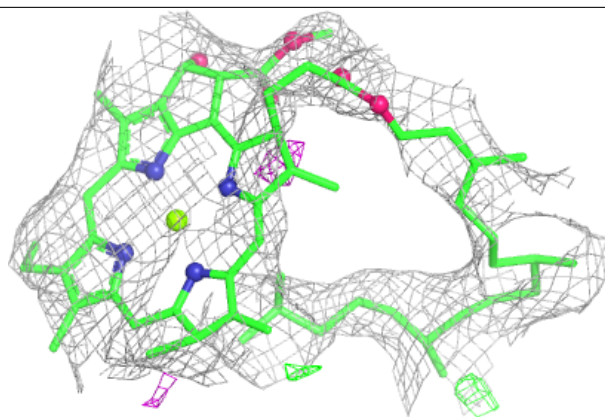
Electron density around CLA 2 301:

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

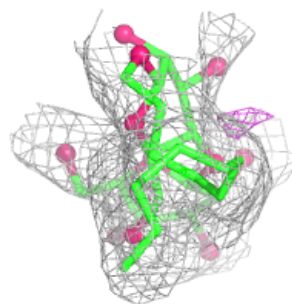
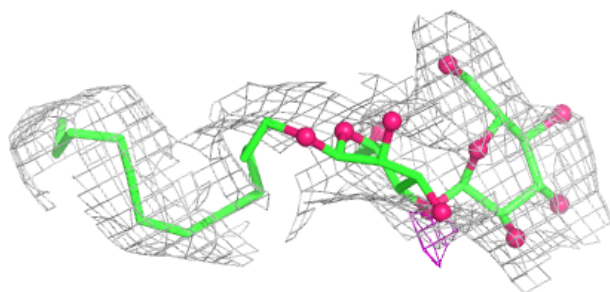


Electron density around CLA A 837:

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

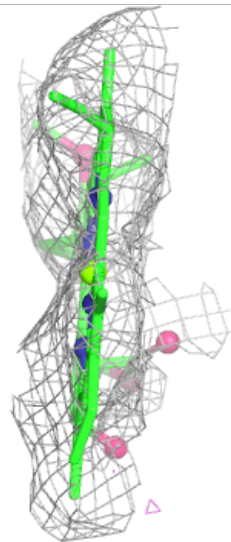
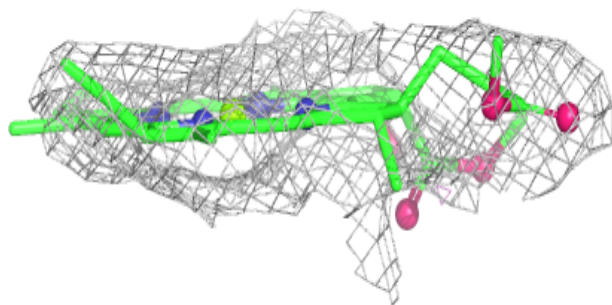
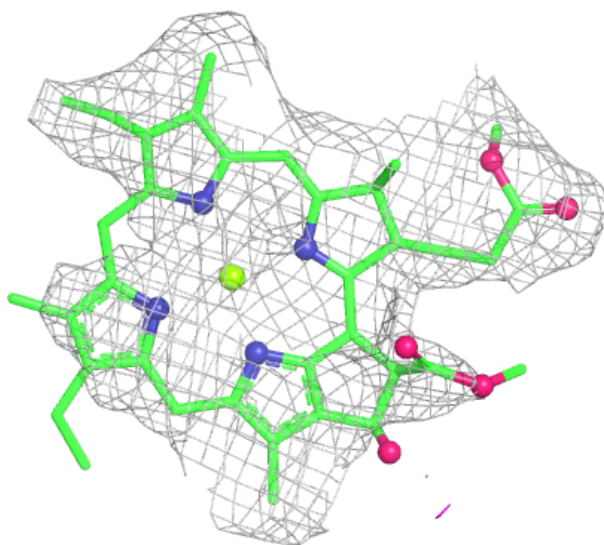
**Electron density around LMU 2 313:**

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



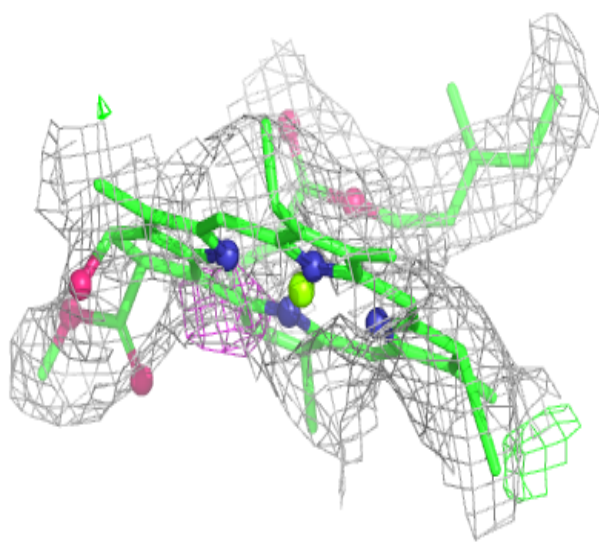
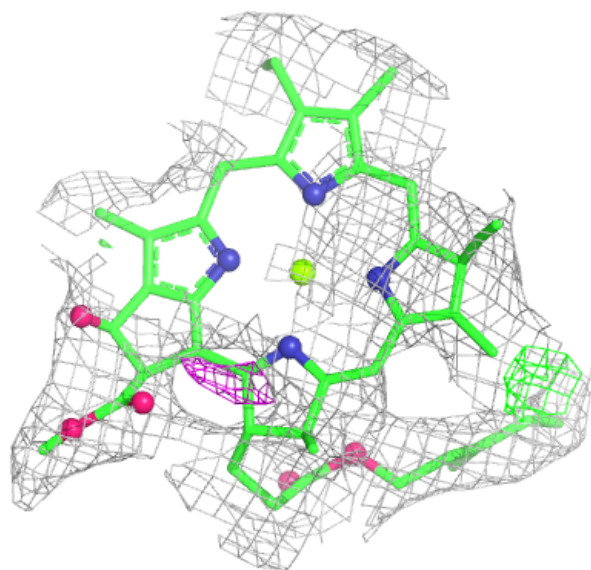
Electron density around CLA B 813:

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



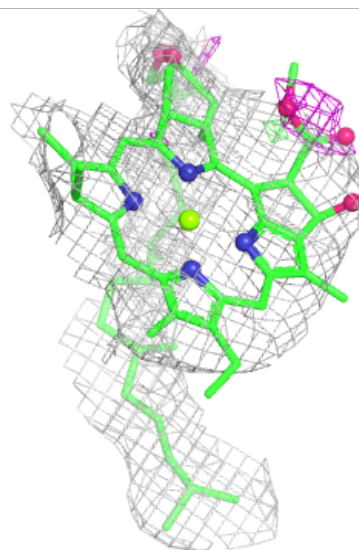
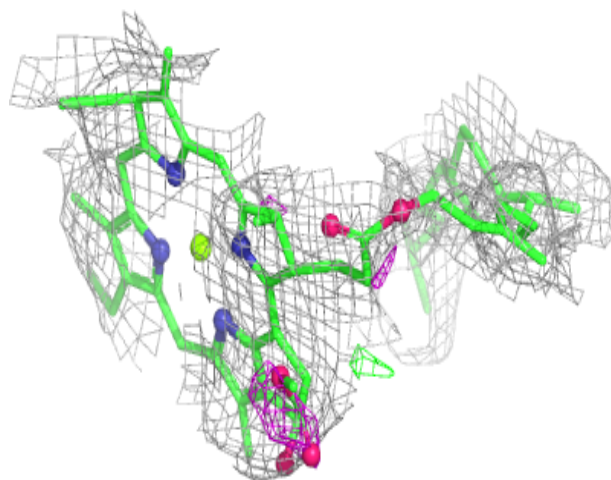
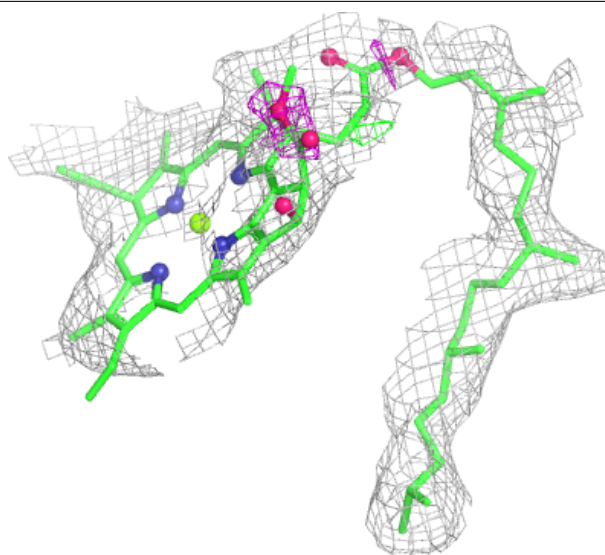
Electron density around CLA B 833:

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



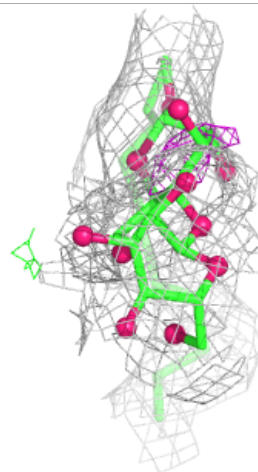
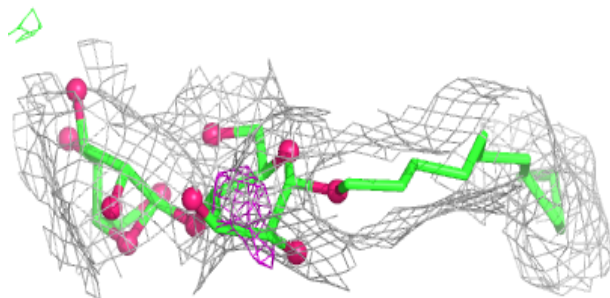
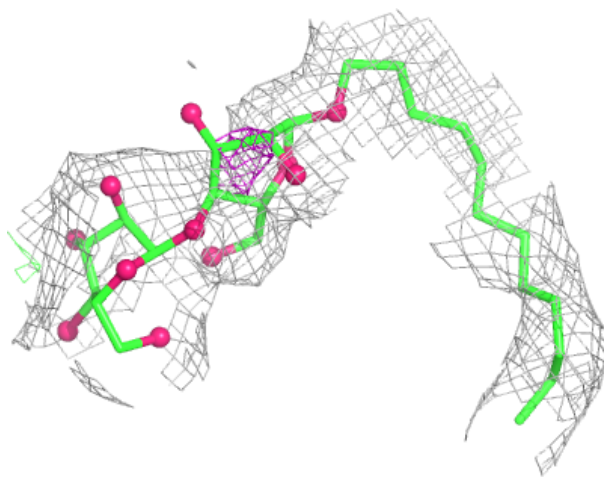
Electron density around CLA 3 310:

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



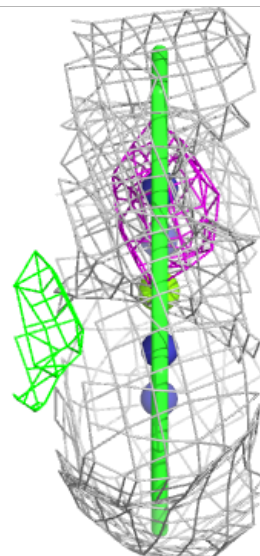
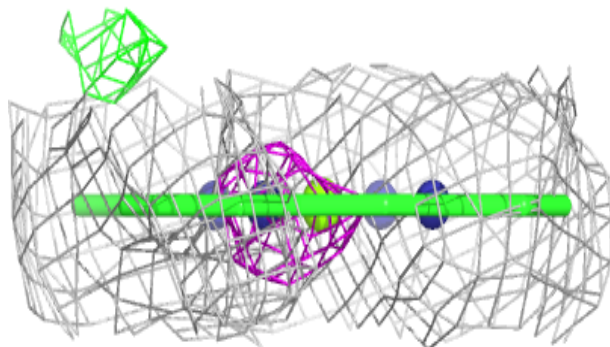
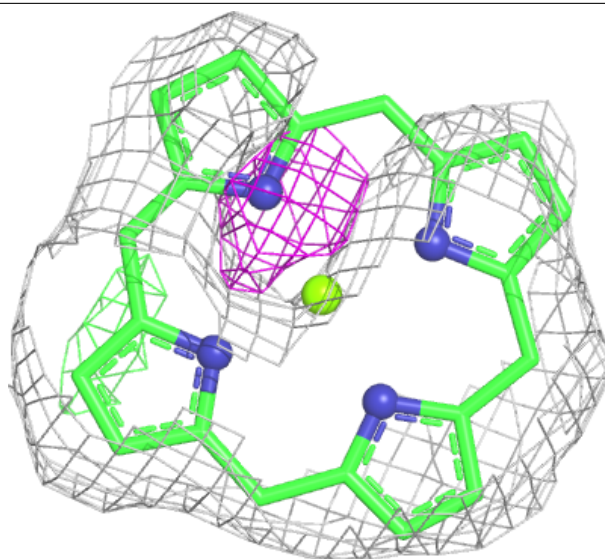
Electron density around LMU K 101:

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



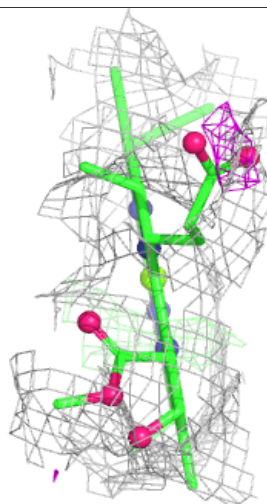
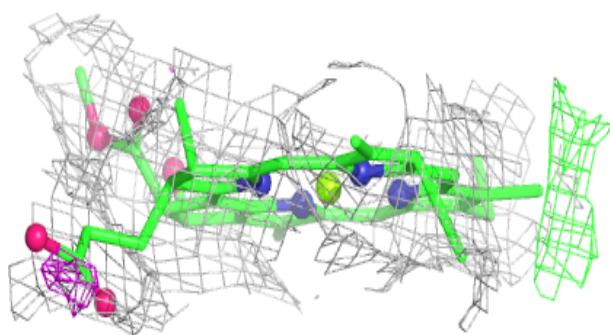
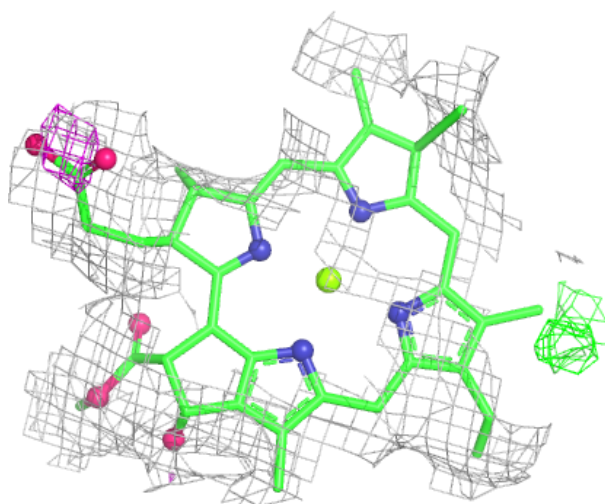
Electron density around CLA 3 305:

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



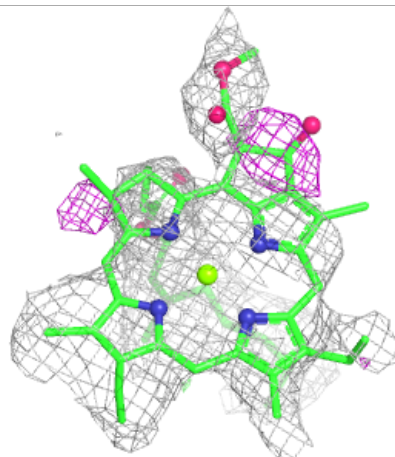
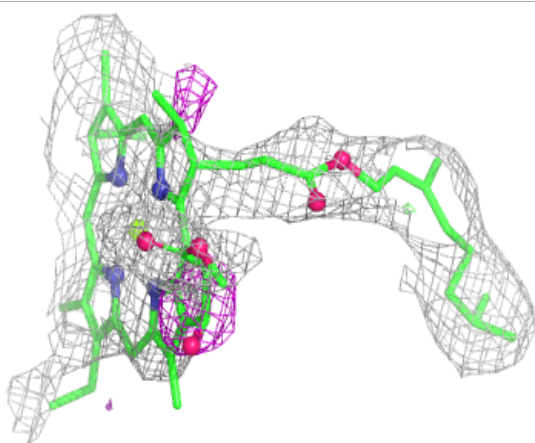
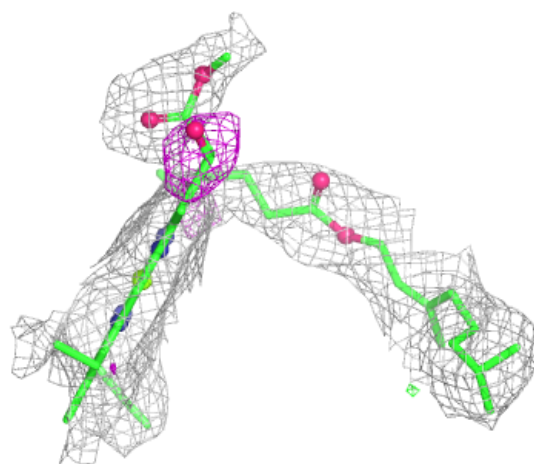
Electron density around CLA K 105:

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



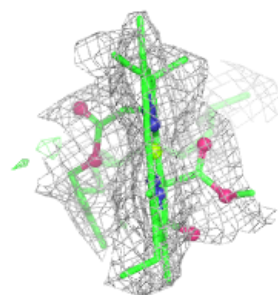
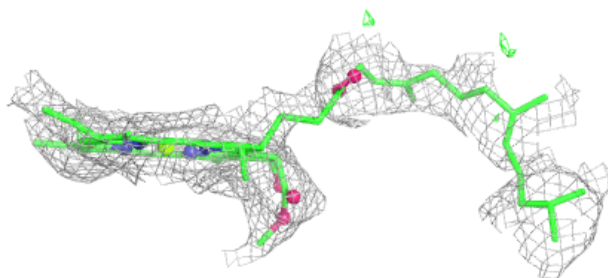
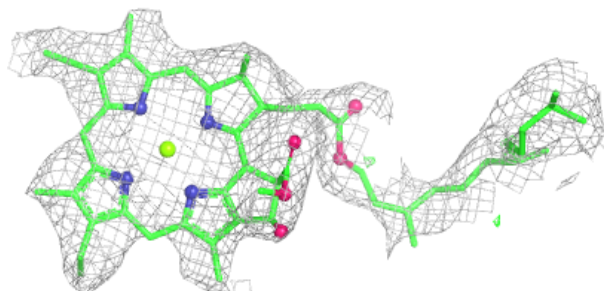
Electron density around CLA L 203:

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

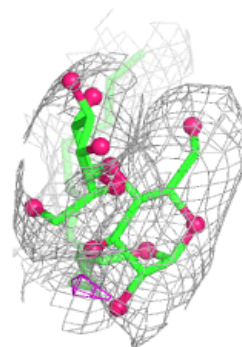
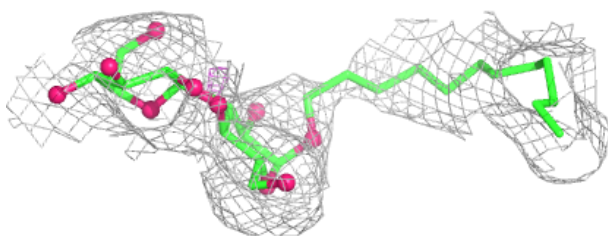


Electron density around CLA B 812:

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

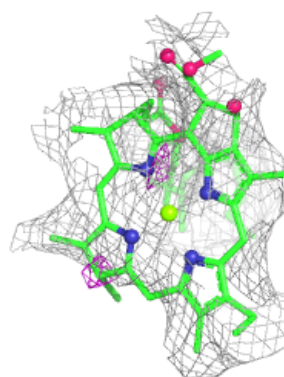
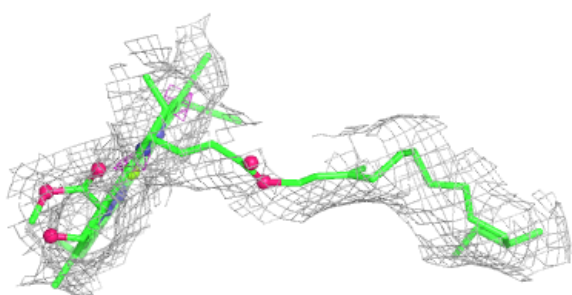
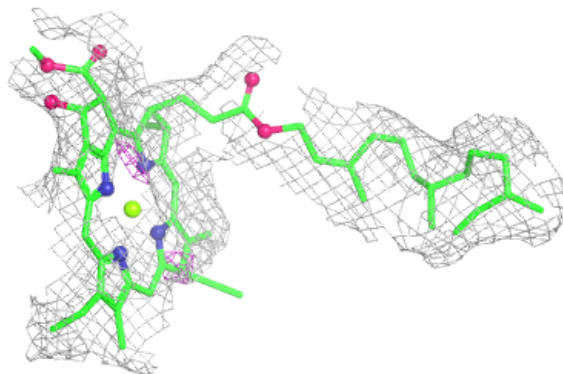
**Electron density around LMU 1 216:**

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

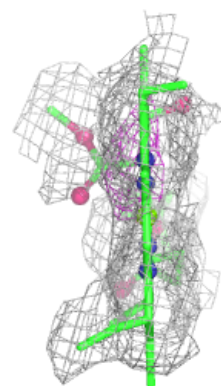
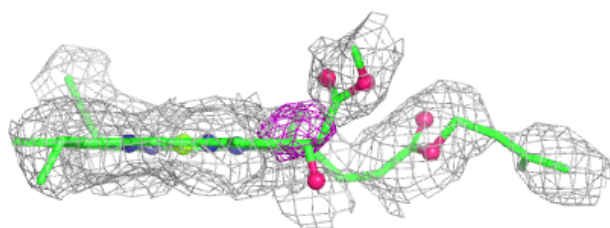
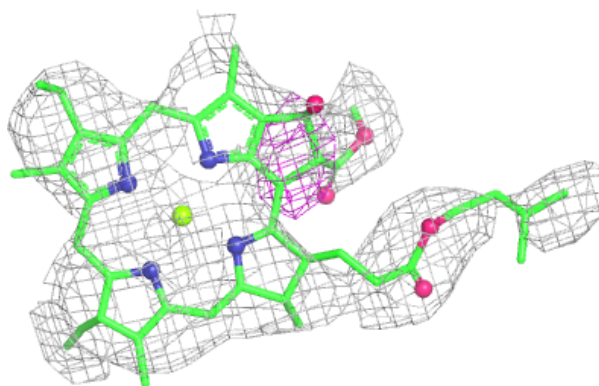


Electron density around CLA 2 321:

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

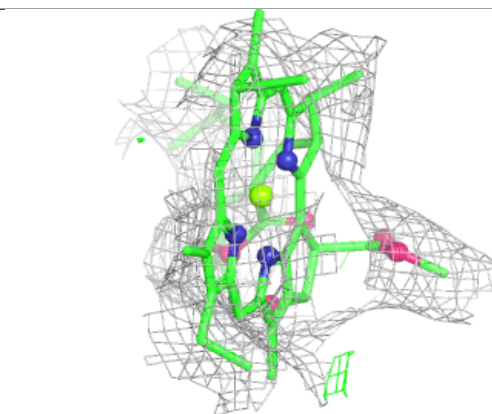
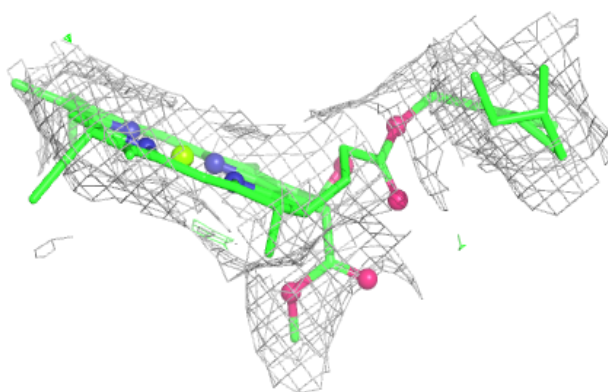
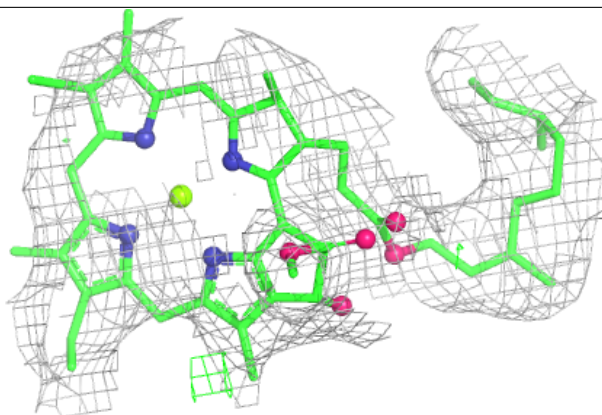
**Electron density around CLA 4 306:**

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

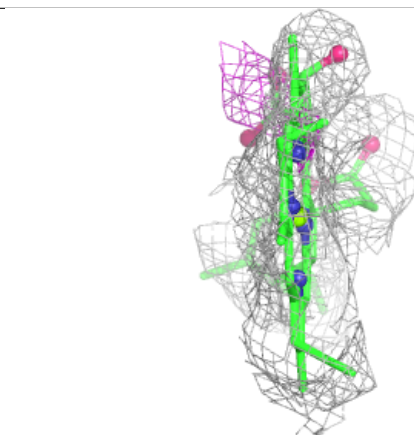
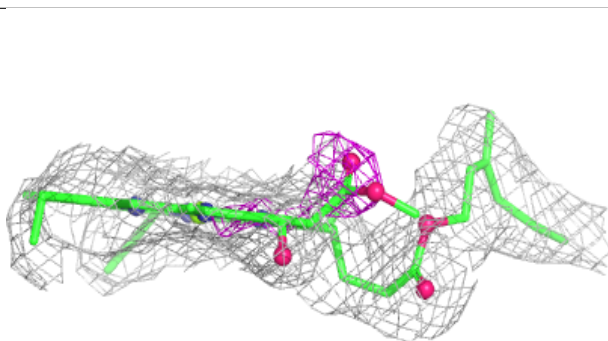
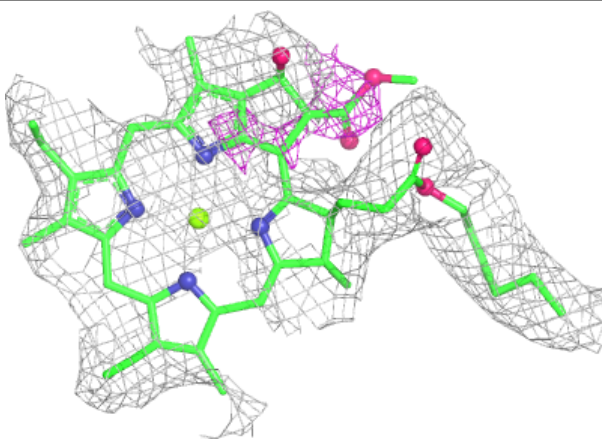


Electron density around CLA 3 301:

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

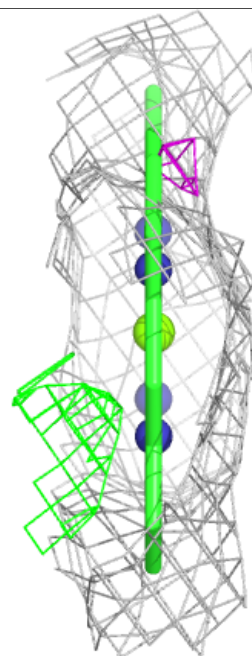
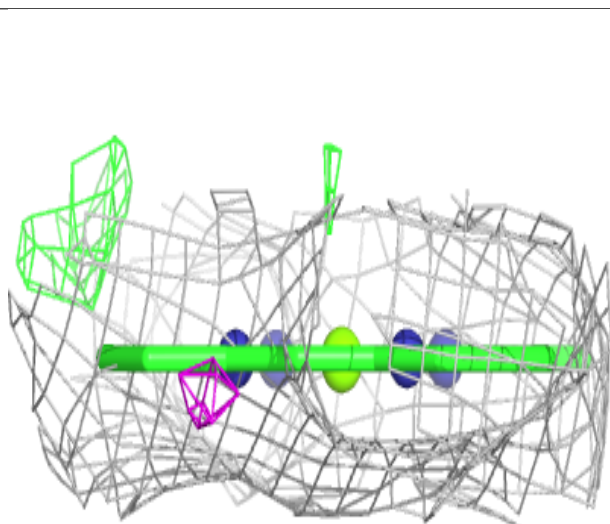
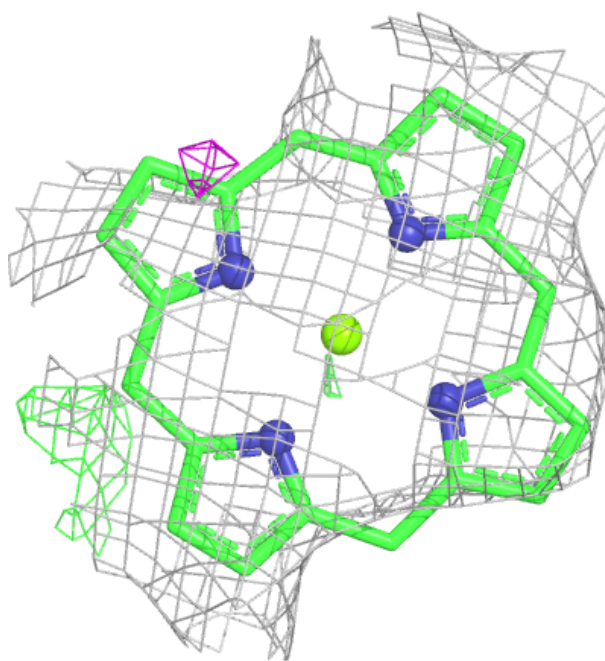
**Electron density around CLA 4 318:**

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



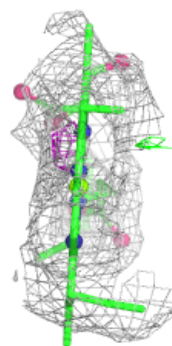
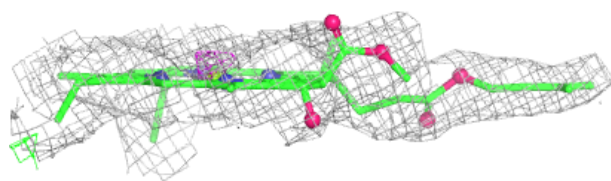
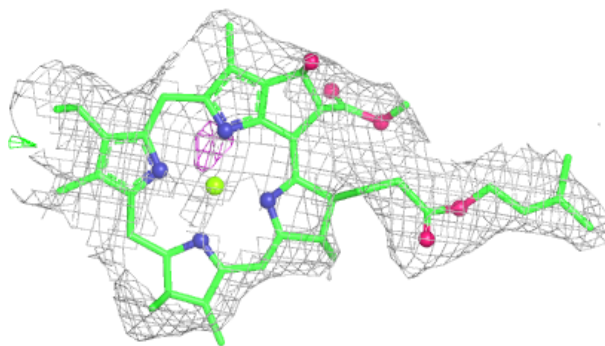
Electron density around CLA 2 305:

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



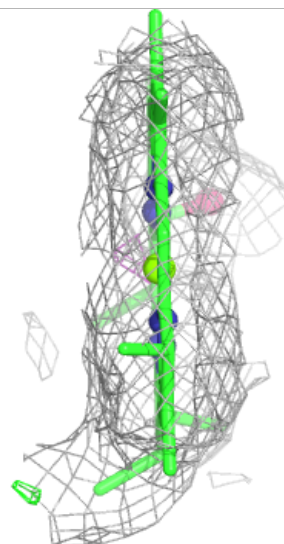
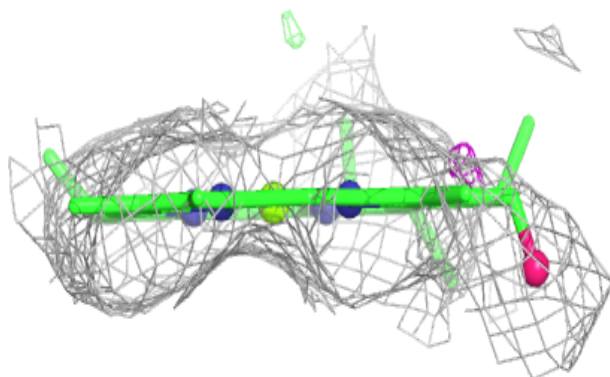
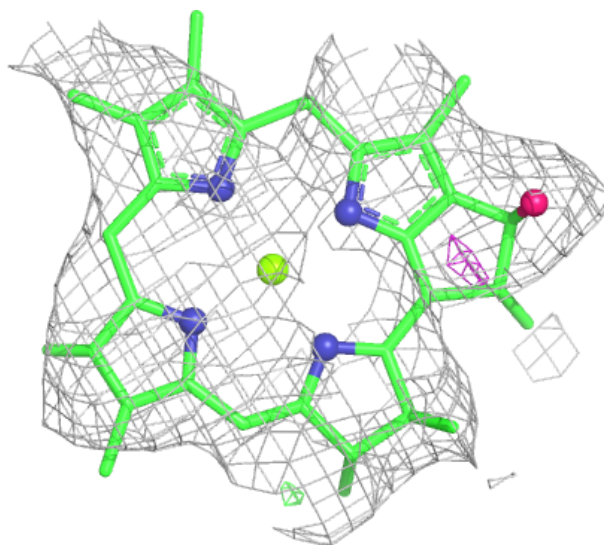
Electron density around CLA A 838:

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



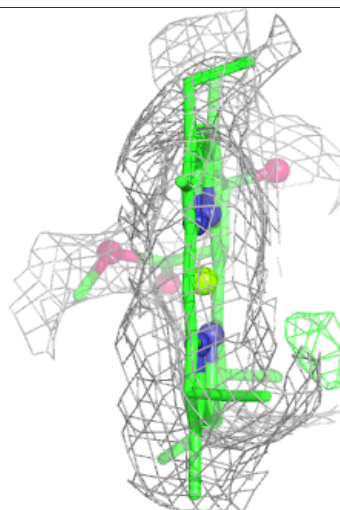
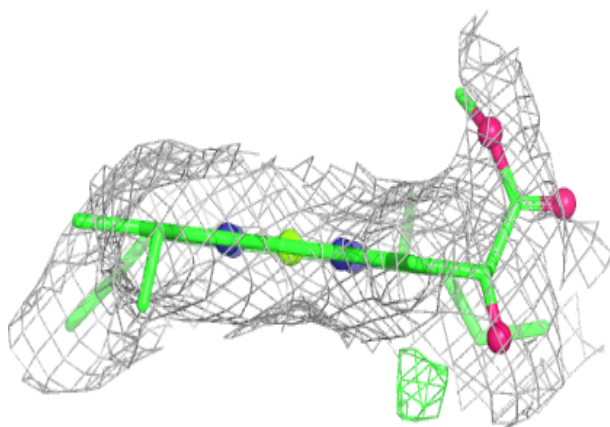
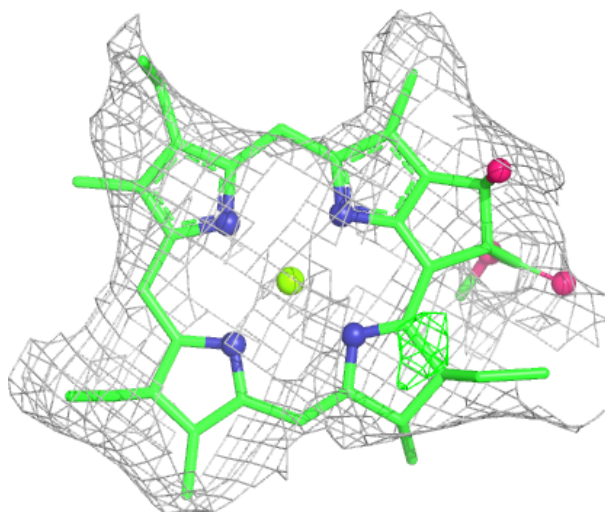
Electron density around CLA 1 205:

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



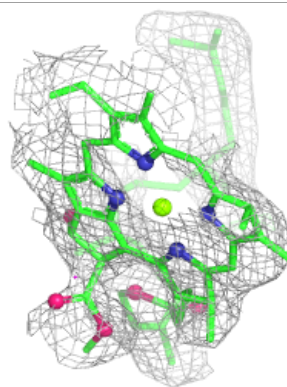
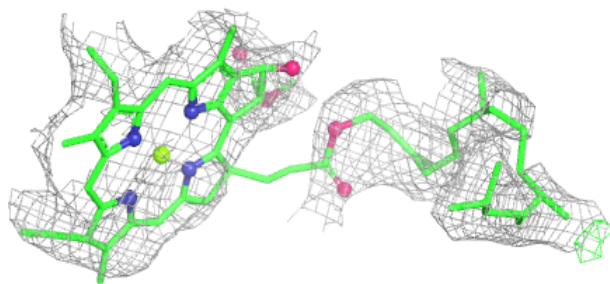
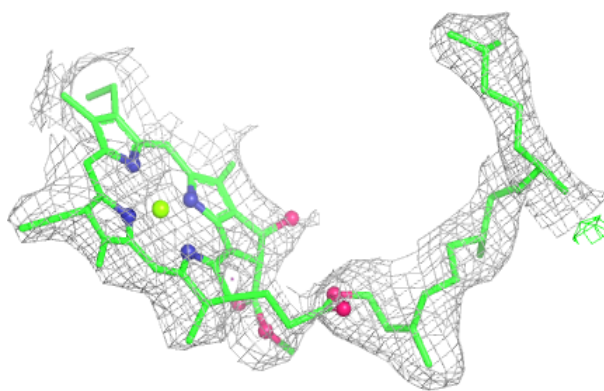
Electron density around CLA 3 314:

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



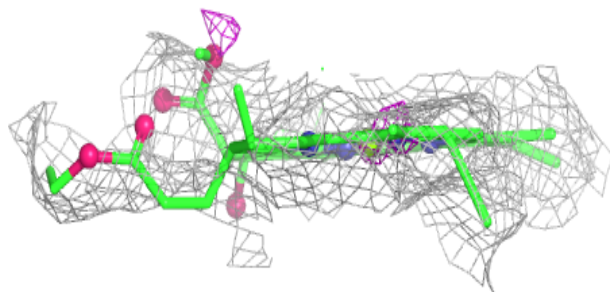
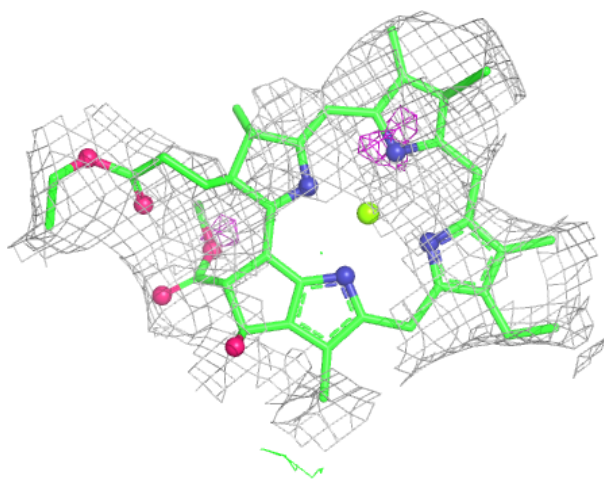
Electron density around CLA K 107:

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



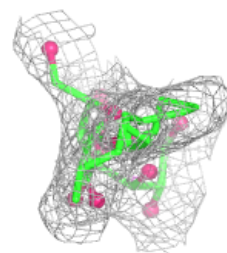
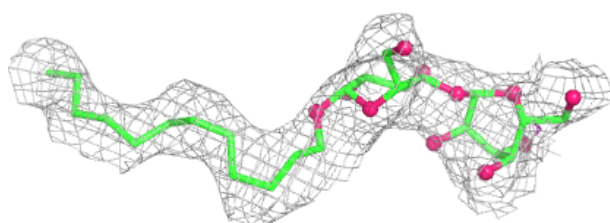
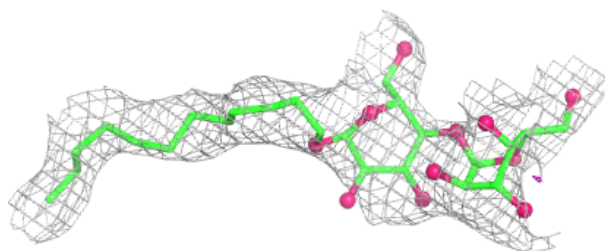
Electron density around CLA 4 319:

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



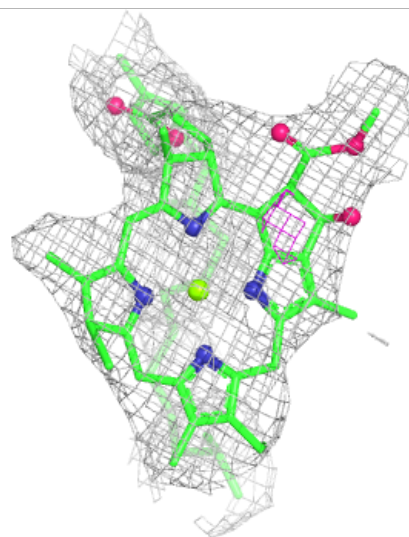
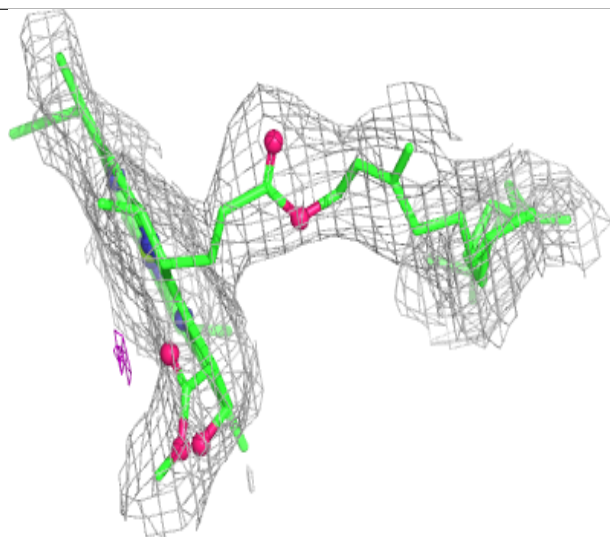
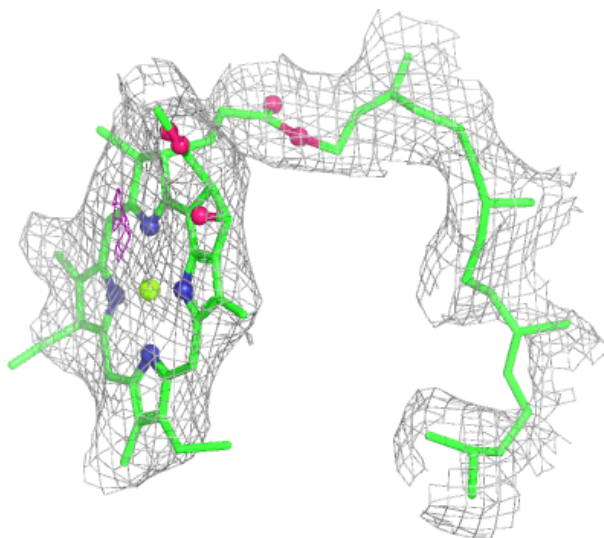
Electron density around LMU A 851:

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



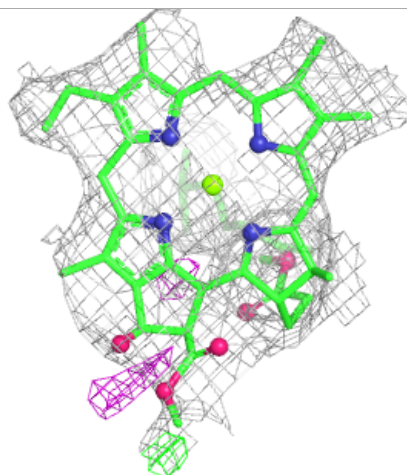
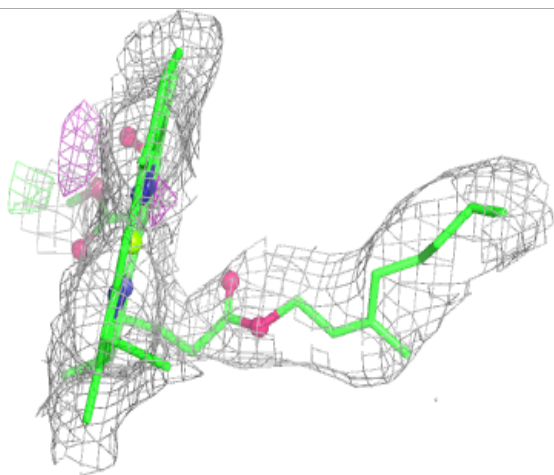
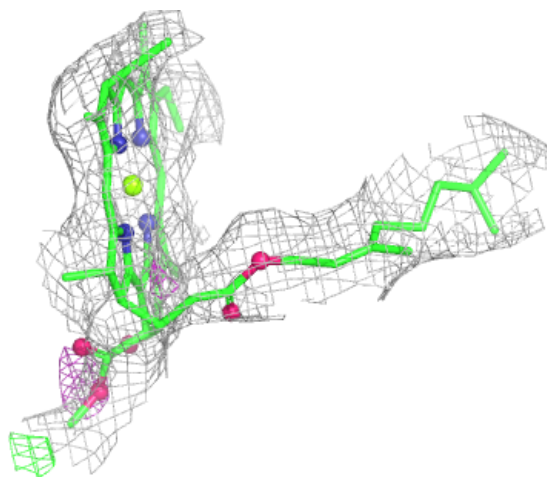
Electron density around CLA 3 309:

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



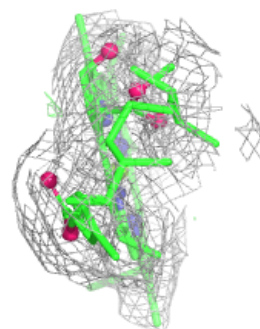
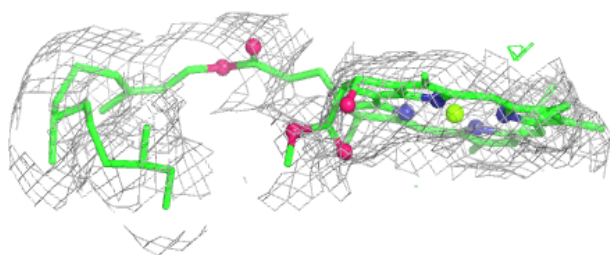
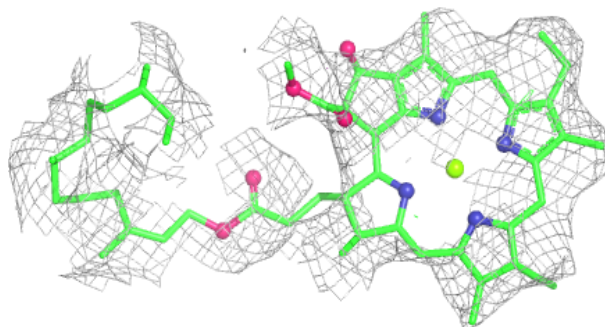
Electron density around CLA 4 302:

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

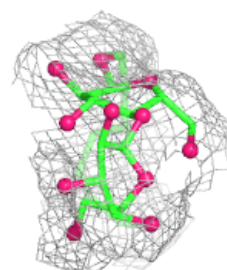
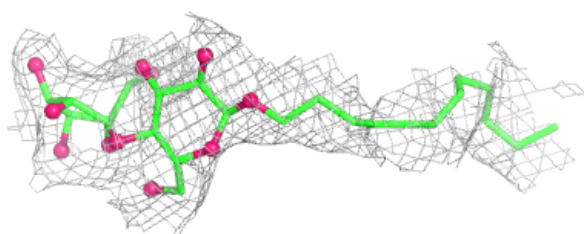
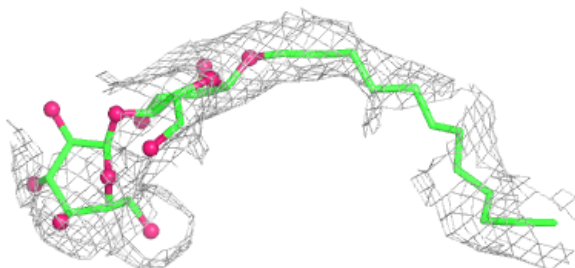


Electron density around CLA 1 212:

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

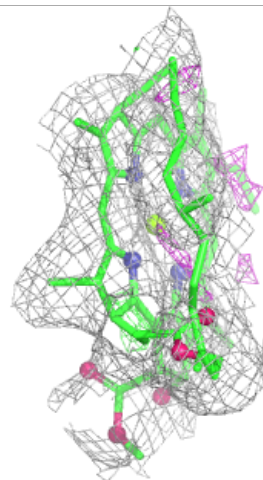
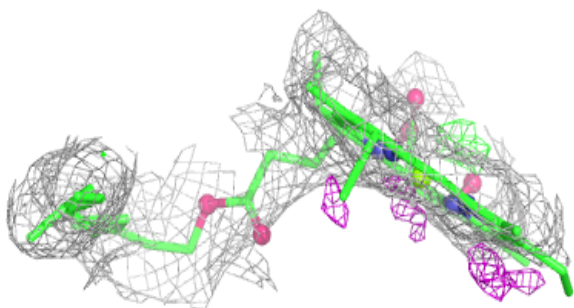
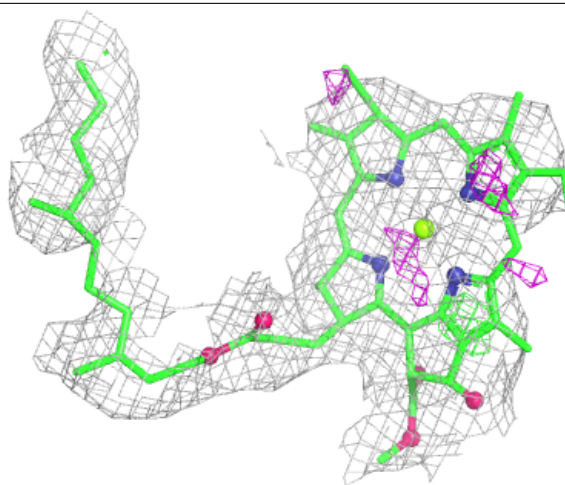
**Electron density around LMU L 205:**

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



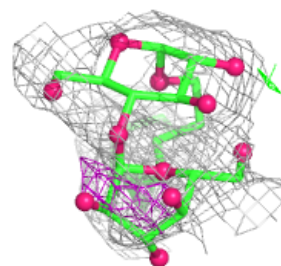
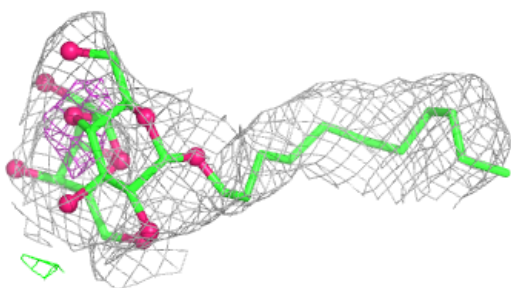
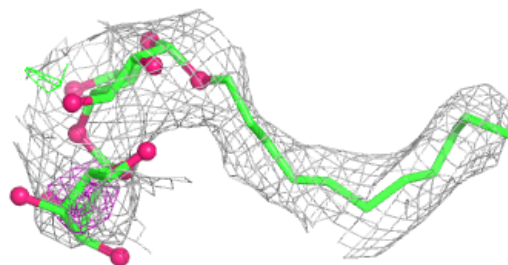
Electron density around CLA B 822:

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

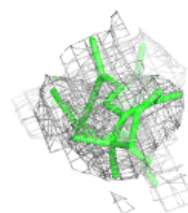
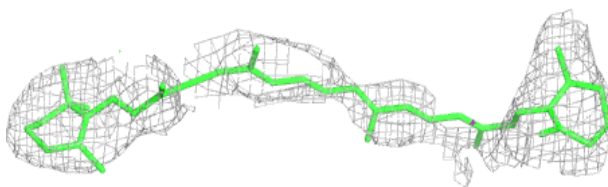
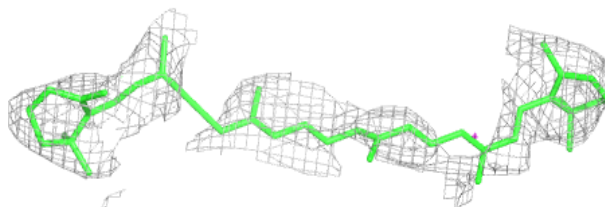


Electron density around LMU 4 320:

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

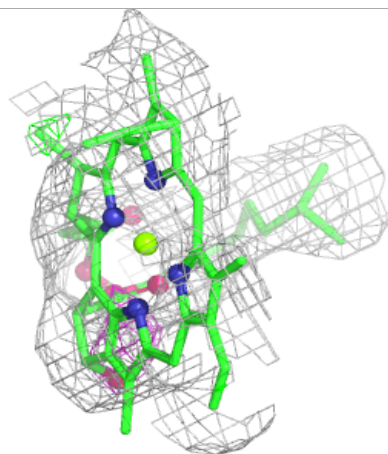
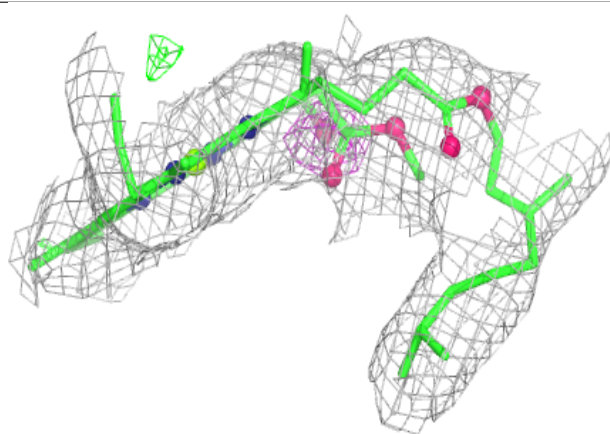
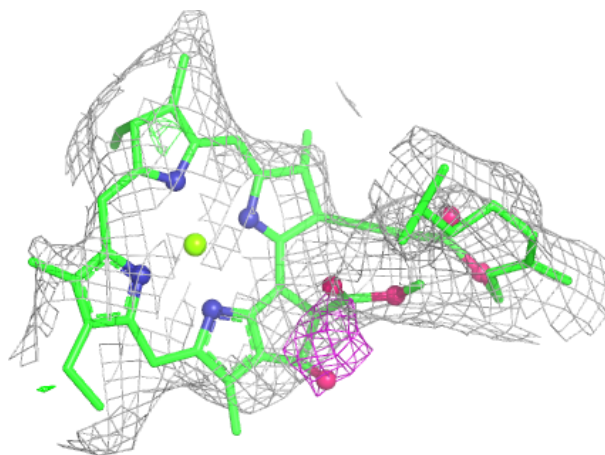
**Electron density around BCR A 842:**

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



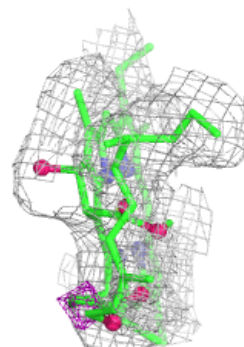
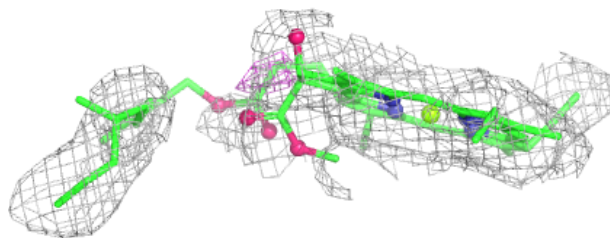
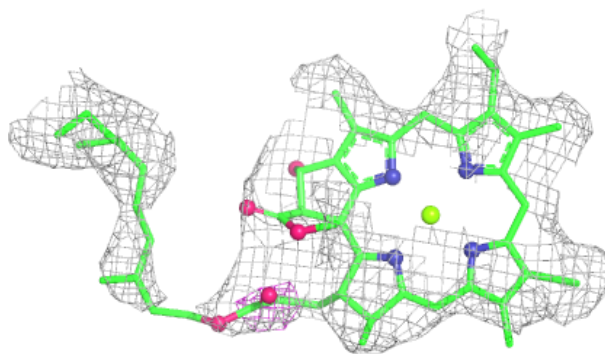
Electron density around CLA L 204:

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

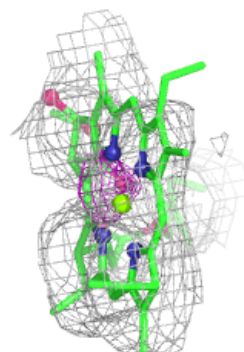
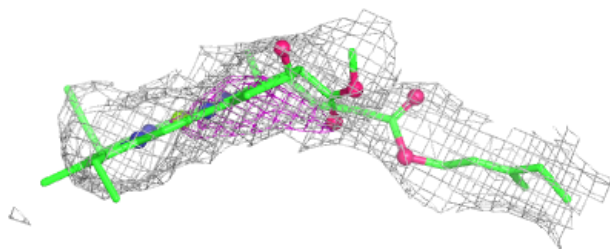
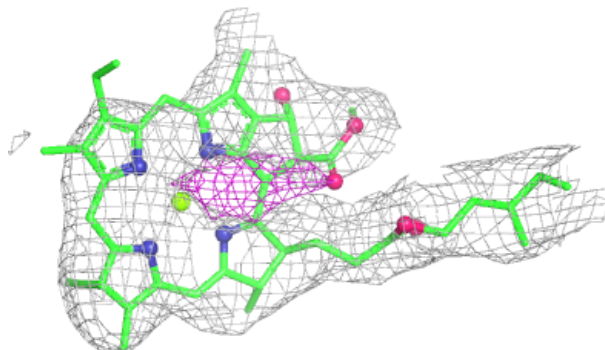


Electron density around CLA R 106:

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

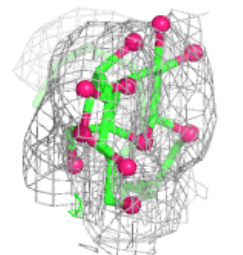
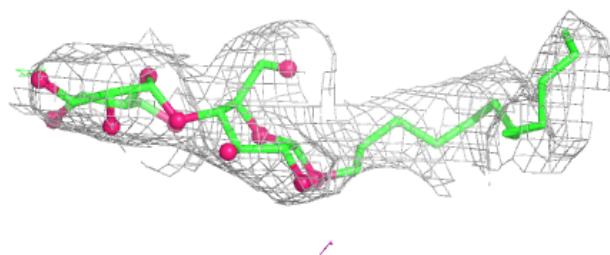
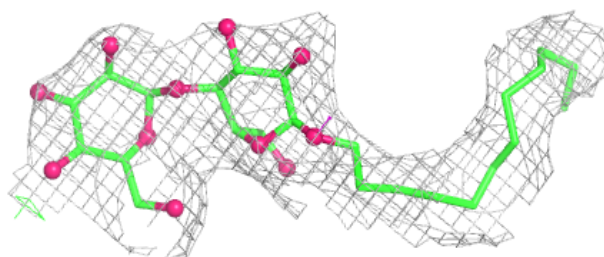
**Electron density around CLA 1 211:**

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



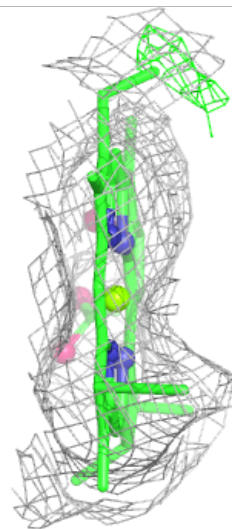
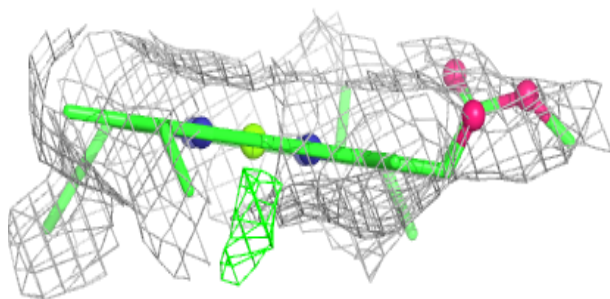
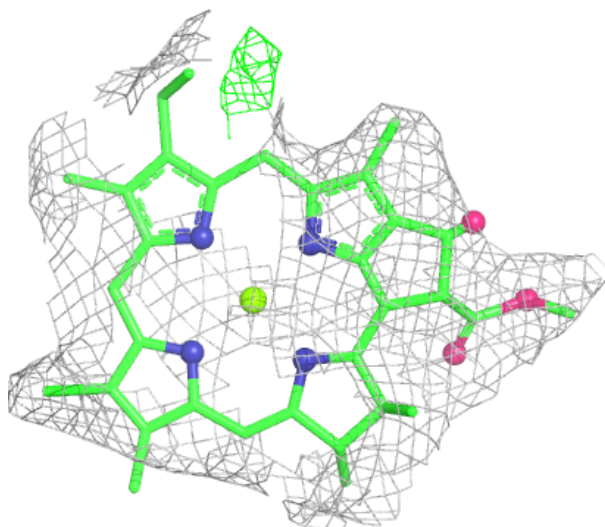
Electron density around LMU C 101:

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



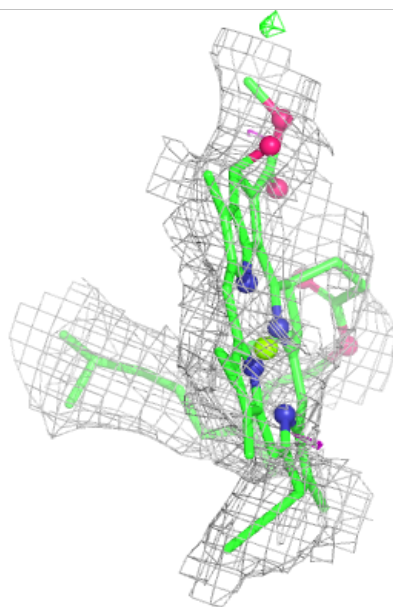
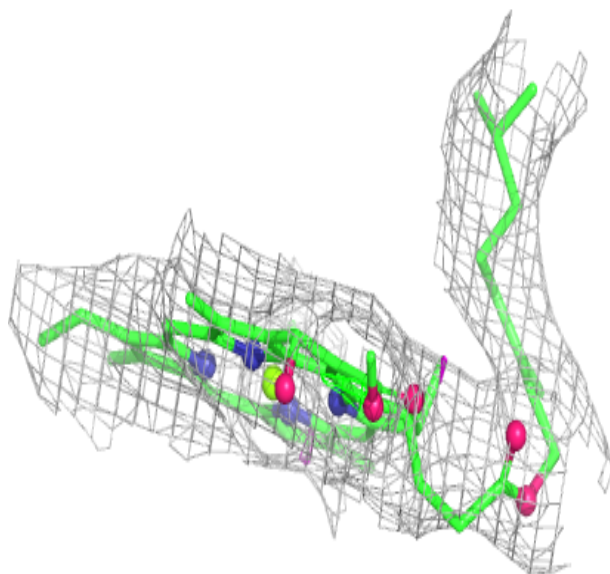
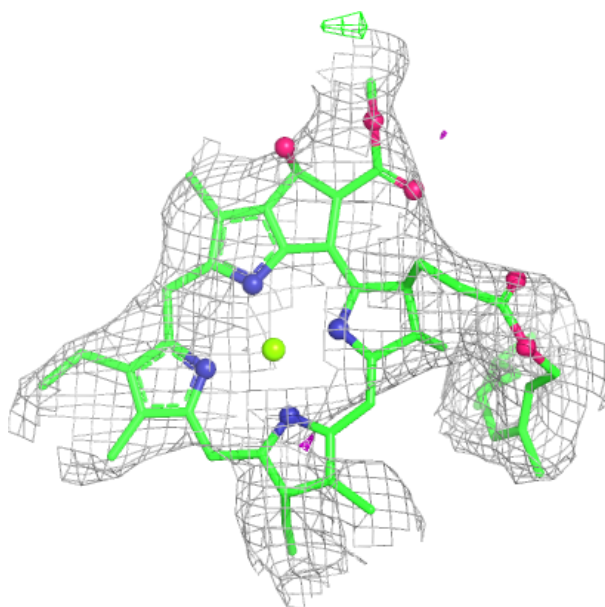
Electron density around CLA F 205:

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



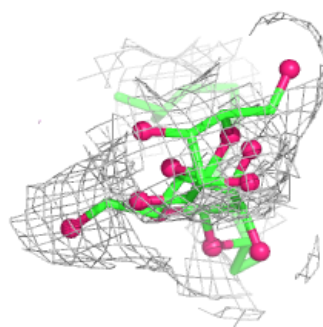
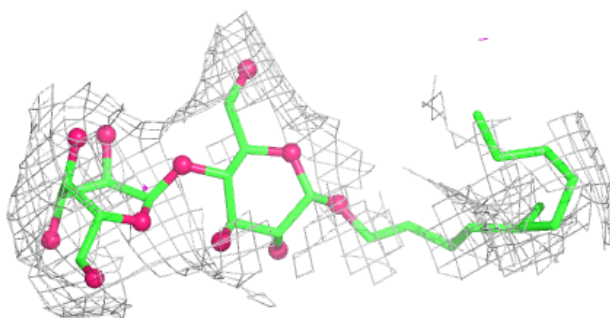
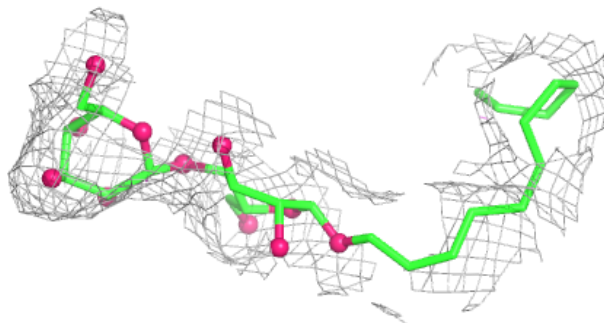
Electron density around CLA H 101:

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

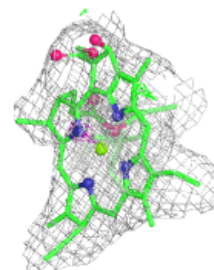
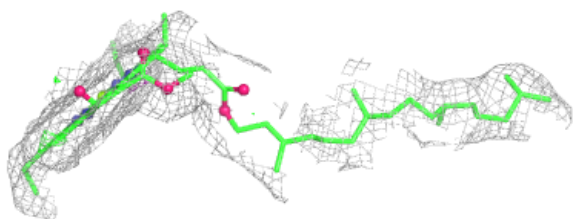
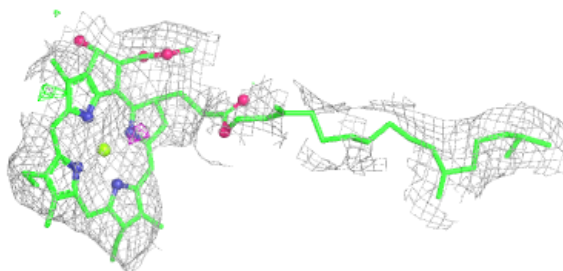


Electron density around LMU H 105:

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

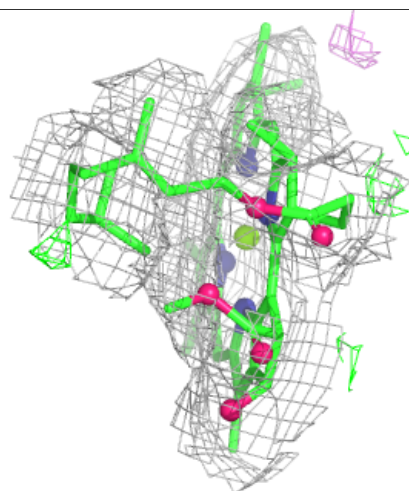
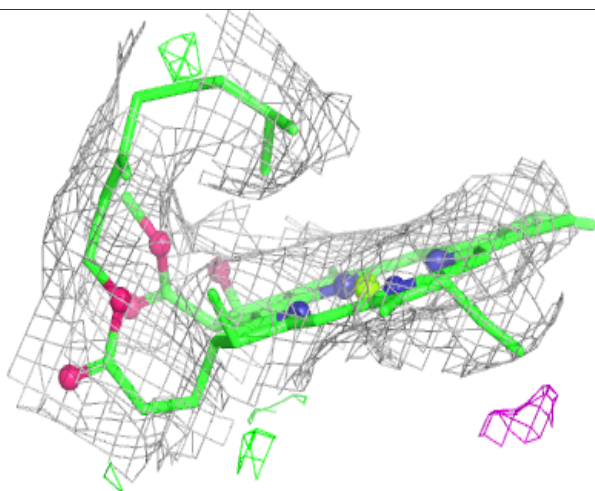
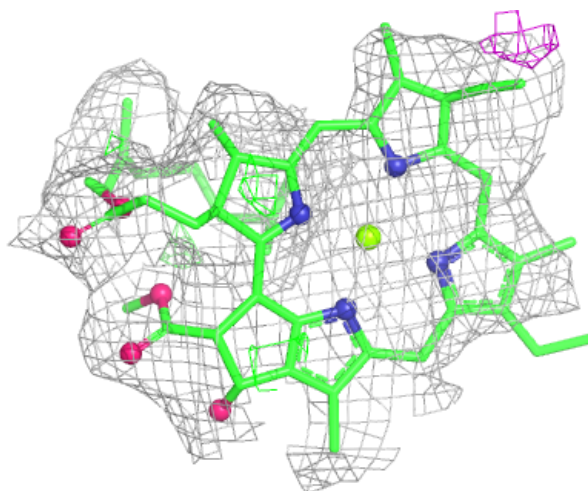
**Electron density around CLA 4 304:**

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



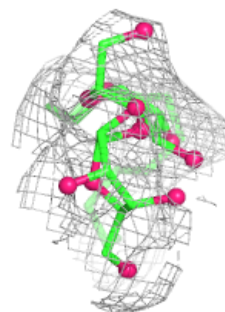
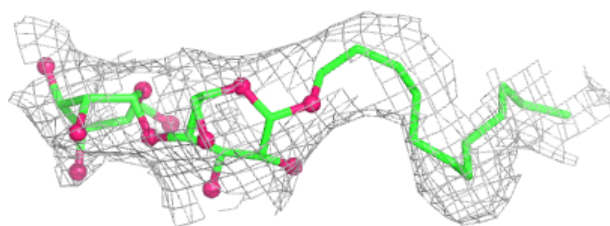
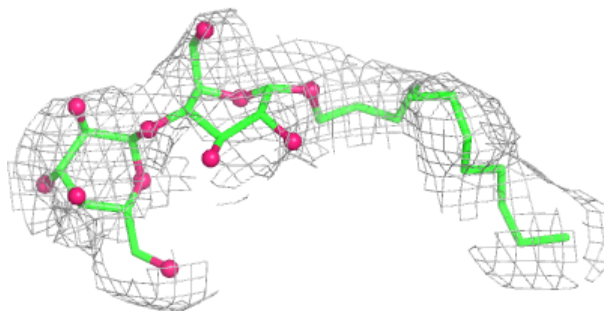
Electron density around CLA 4 305:

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



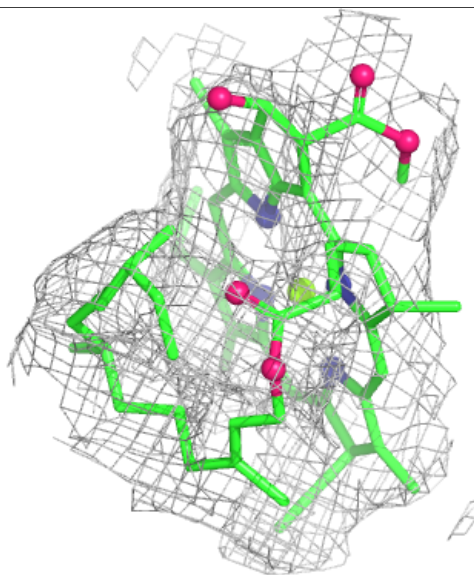
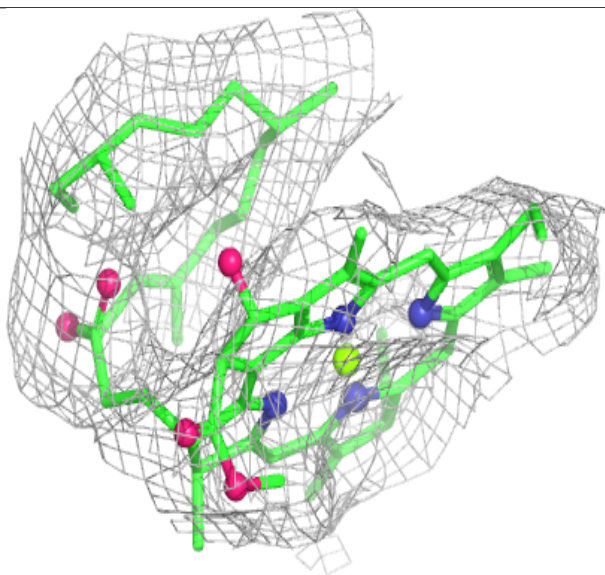
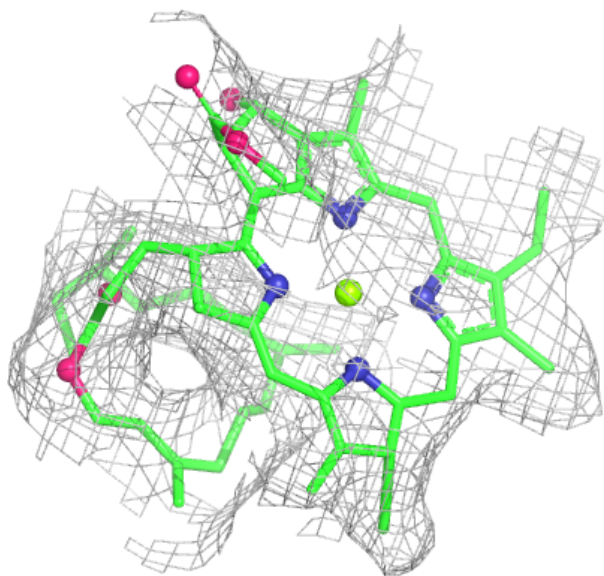
Electron density around LMU 4 322:

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



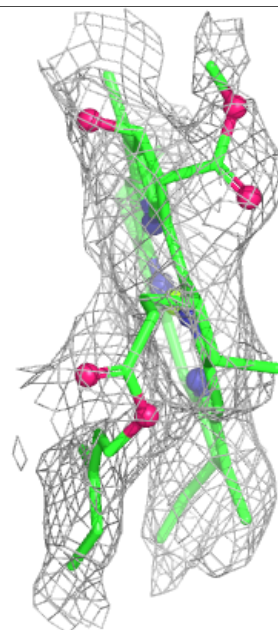
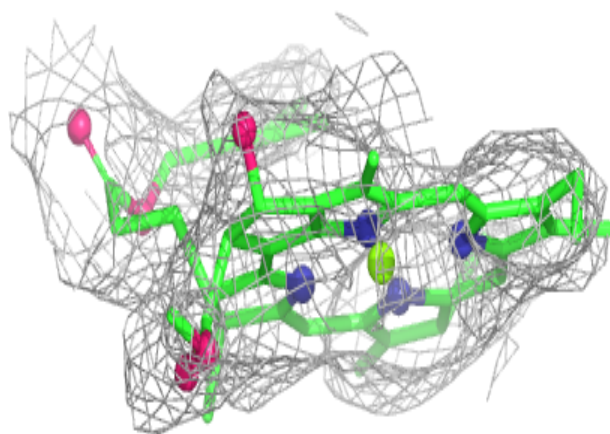
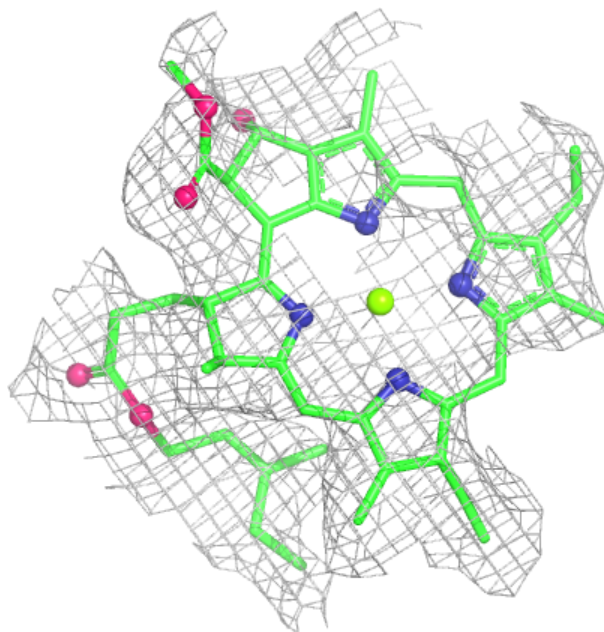
Electron density around CLA J 102:

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



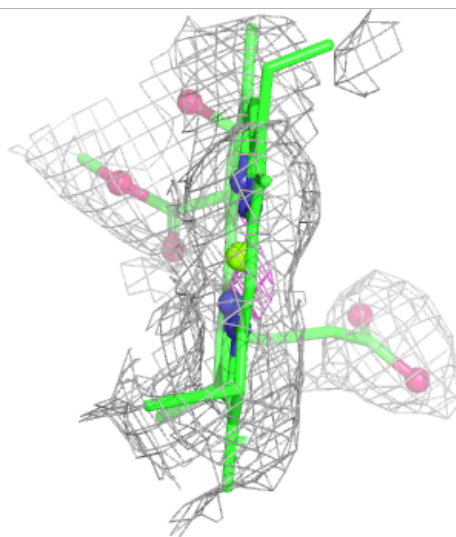
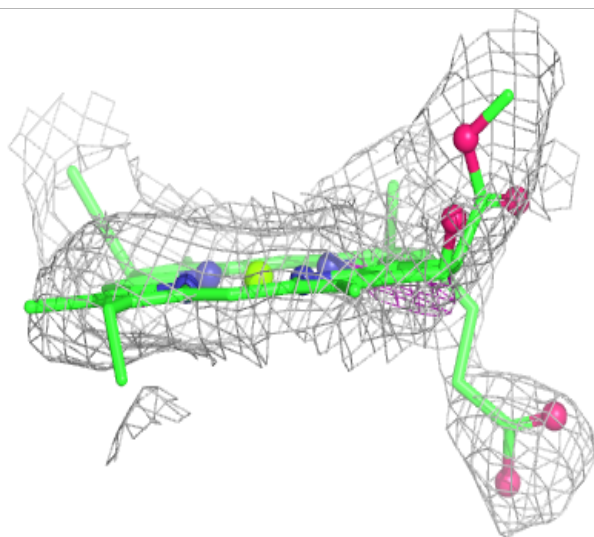
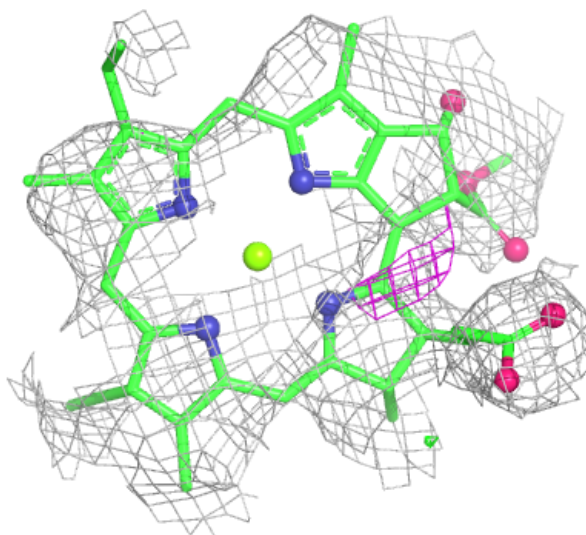
Electron density around CLA G 103:

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



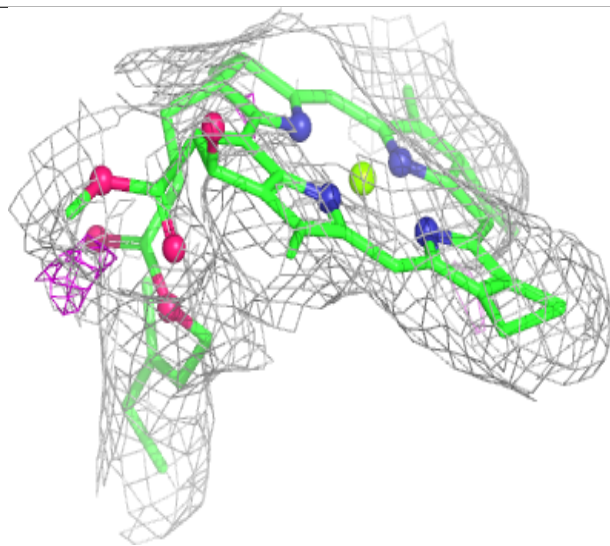
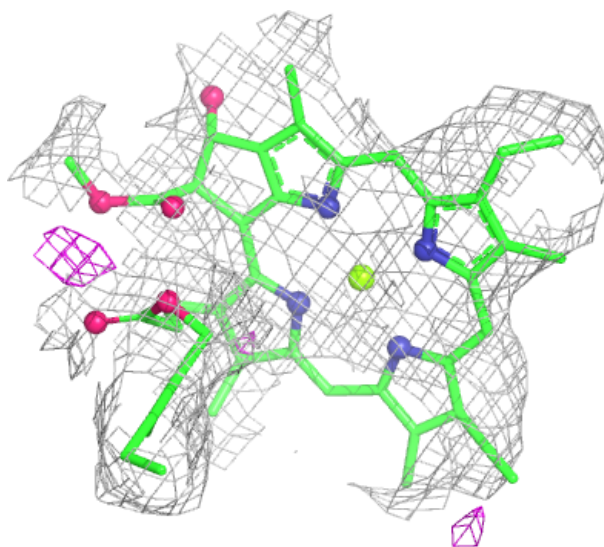
Electron density around CLA B 832:

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



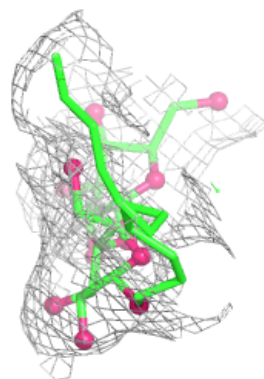
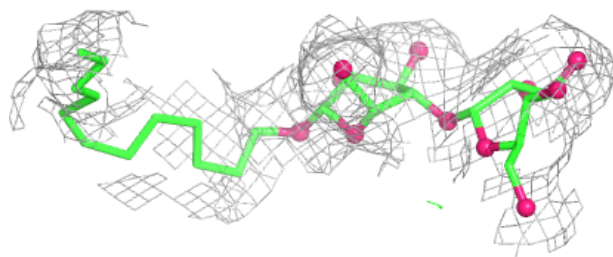
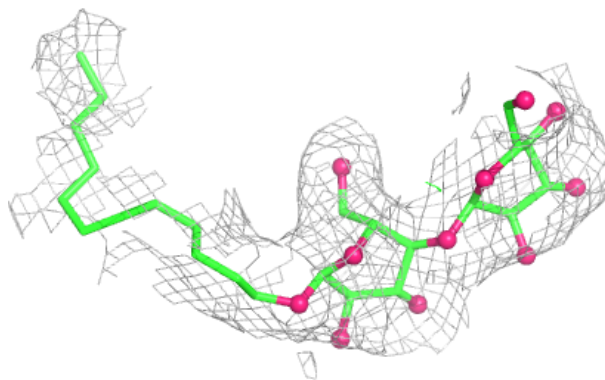
Electron density around CLA 1 207:

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



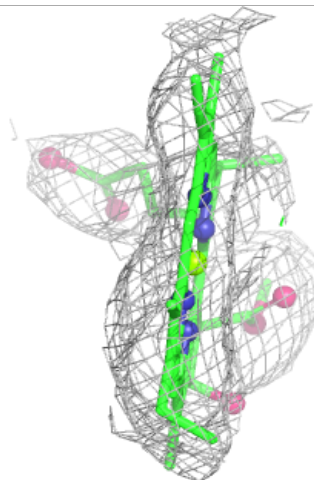
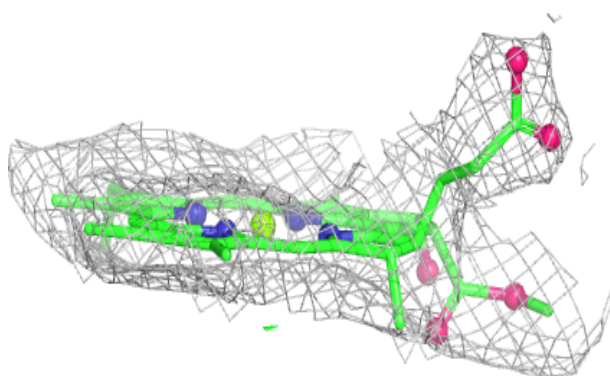
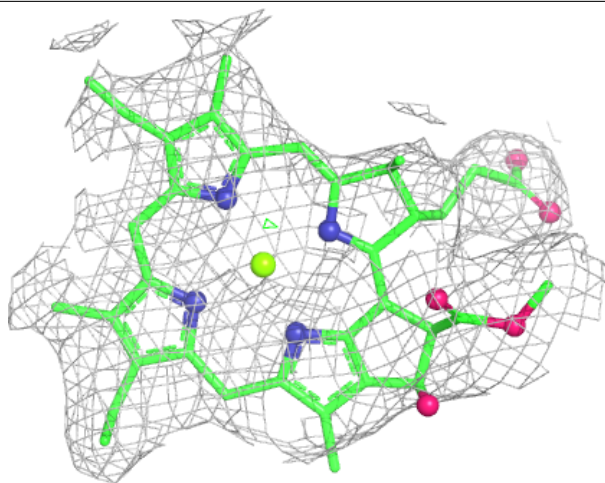
Electron density around LMU H 103:

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



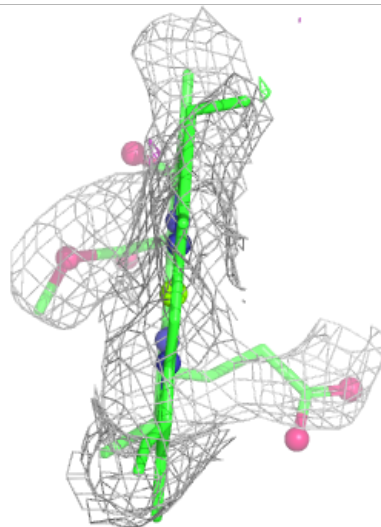
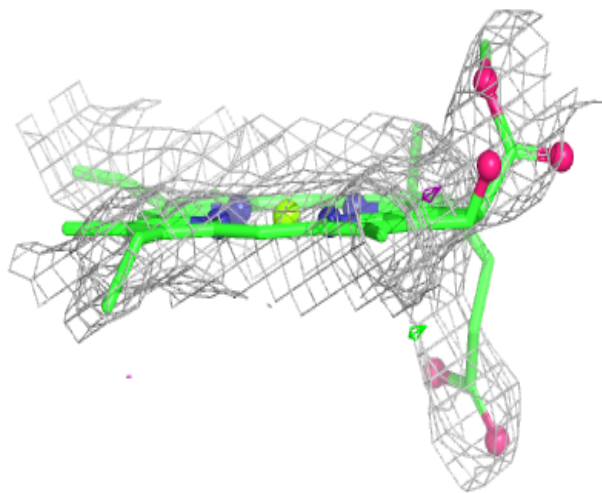
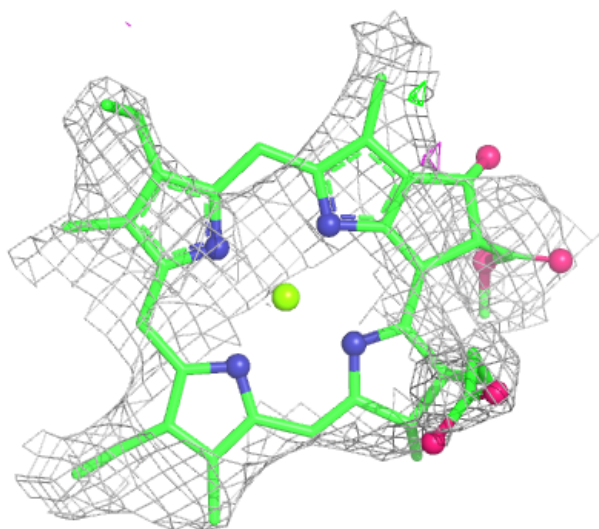
Electron density around CLA A 808:

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



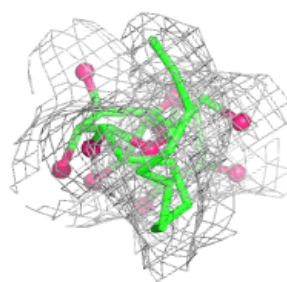
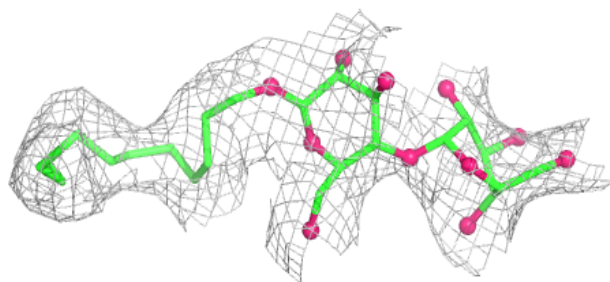
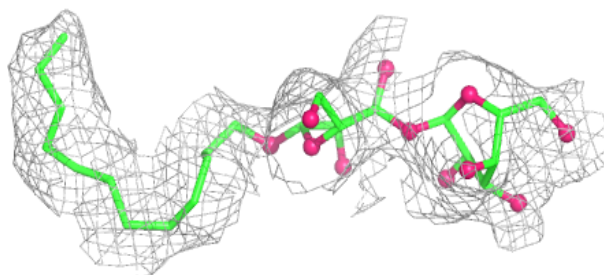
Electron density around CLA A 812:

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

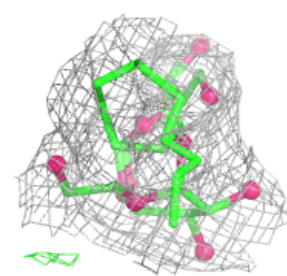
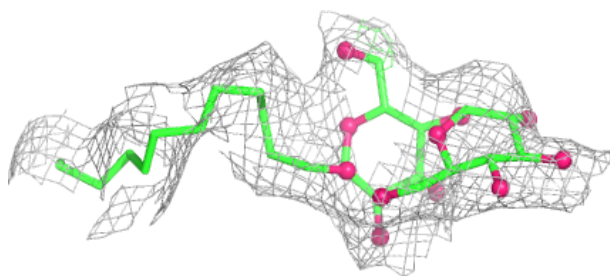
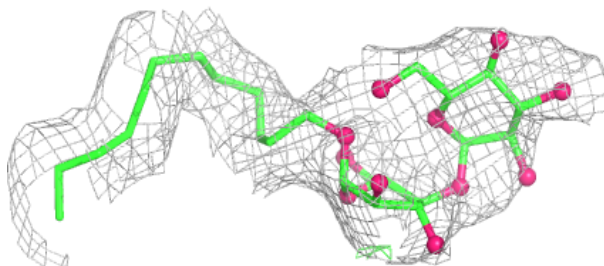


Electron density around LMU A 845:

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

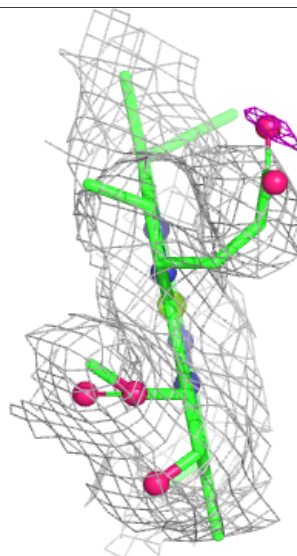
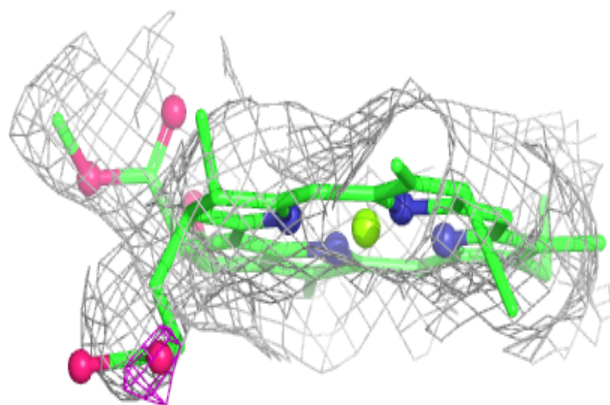
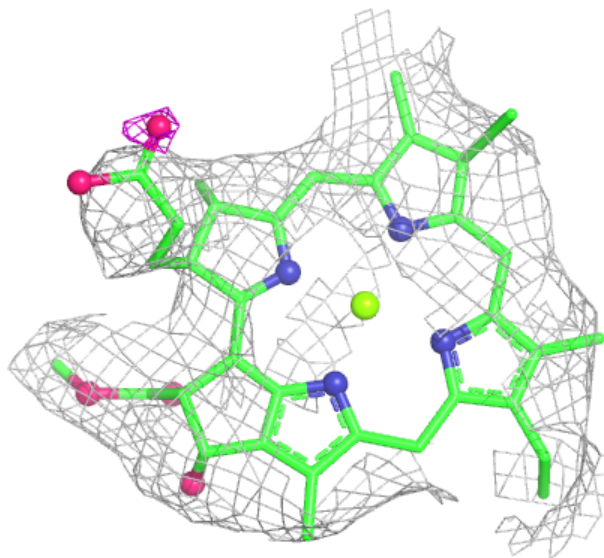
**Electron density around LMU A 846:**

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



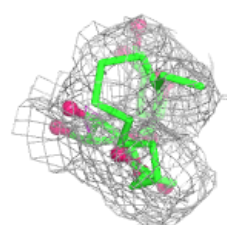
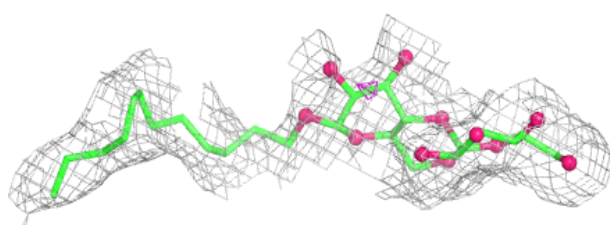
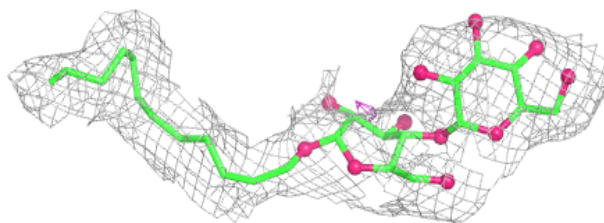
Electron density around CLA A 831:

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

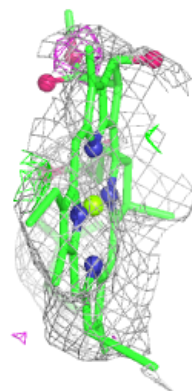
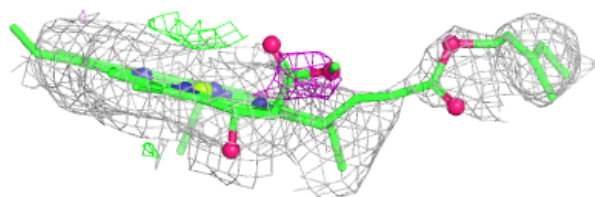
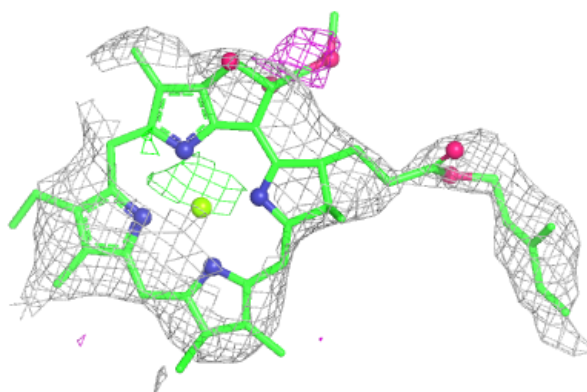


Electron density around LMU B 801:

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

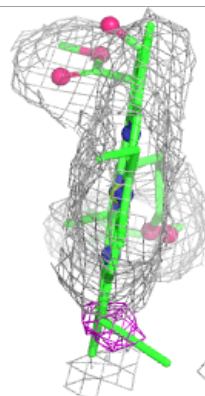
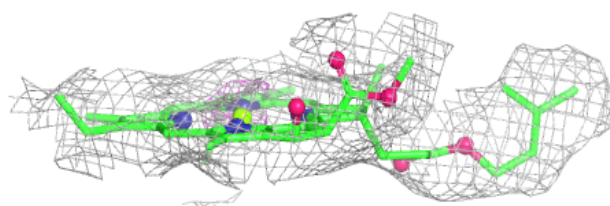
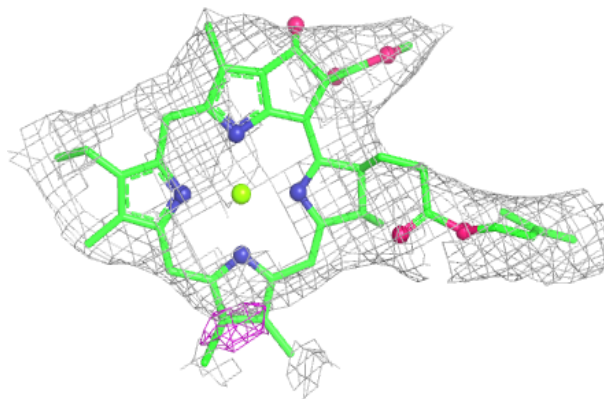
**Electron density around CLA 1 214:**

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



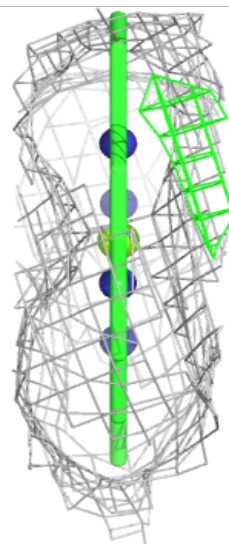
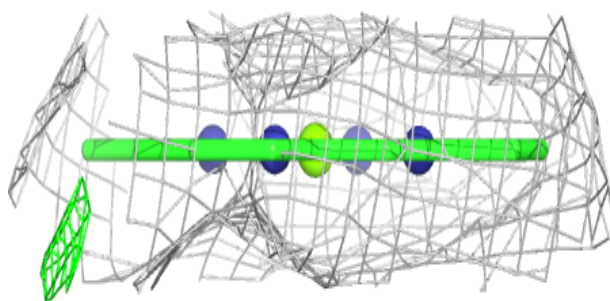
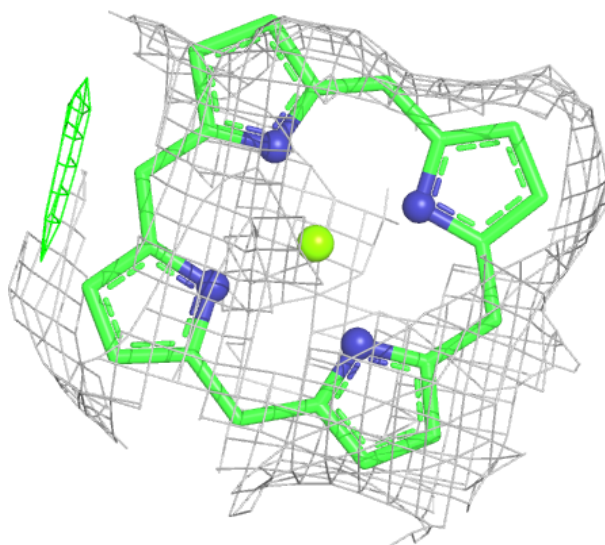
Electron density around CLA K 103:

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



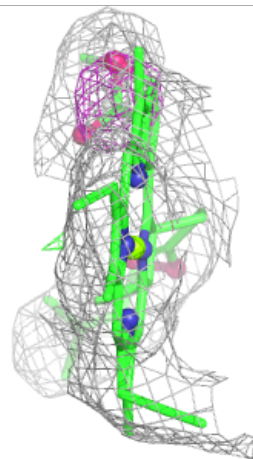
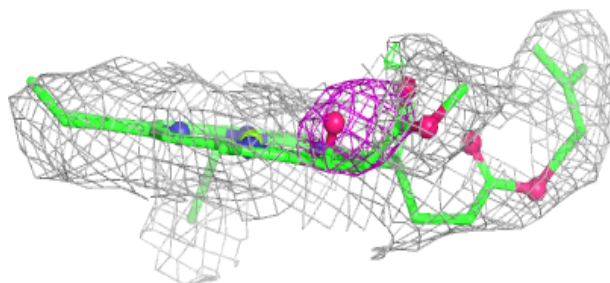
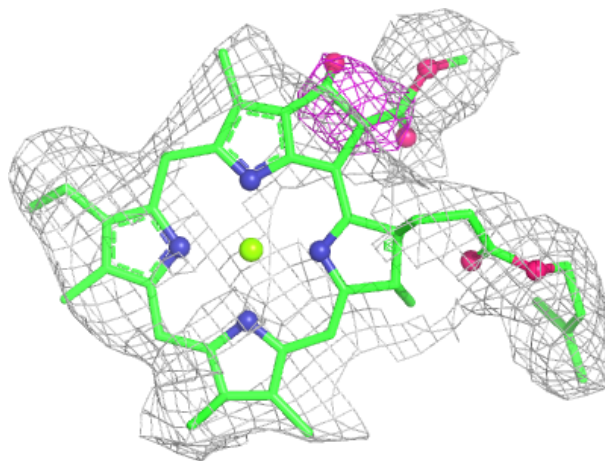
Electron density around CLA 3 304:

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



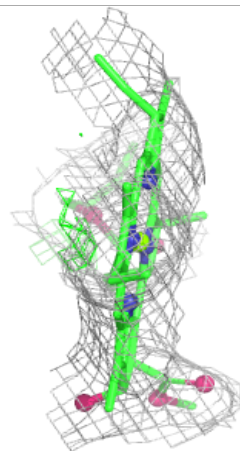
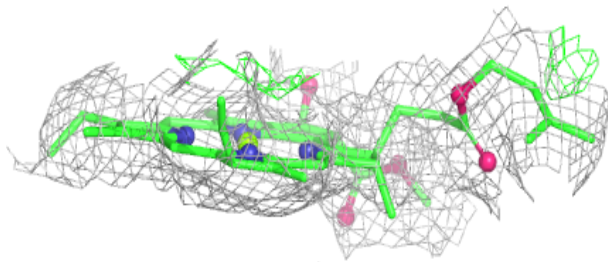
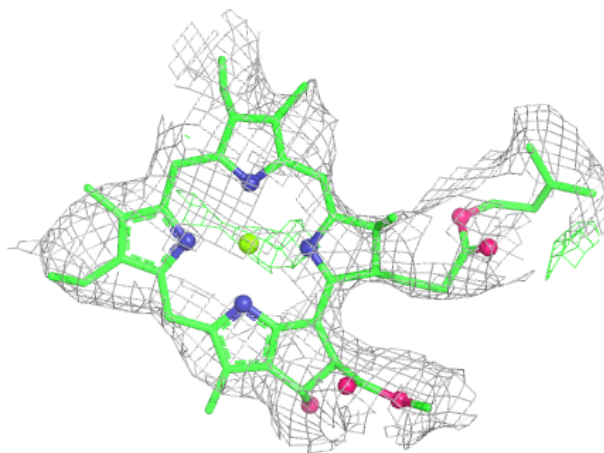
Electron density around CLA K 106:

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



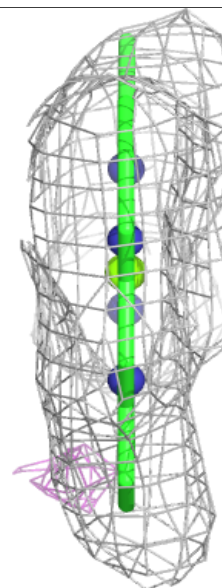
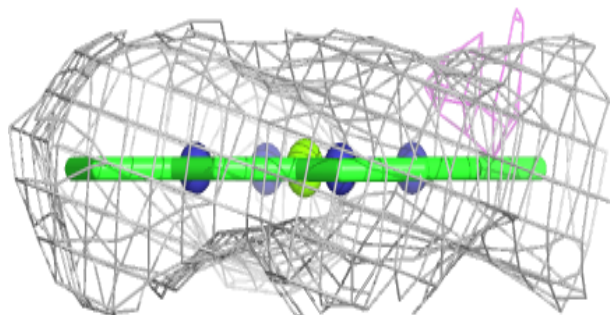
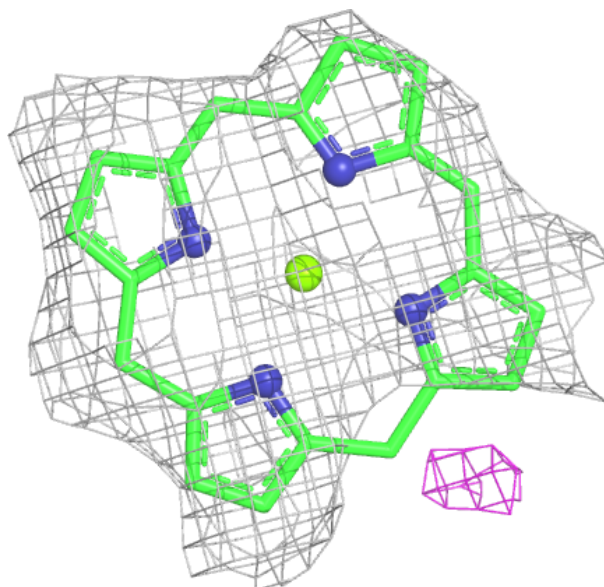
Electron density around CLA 2 304:

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



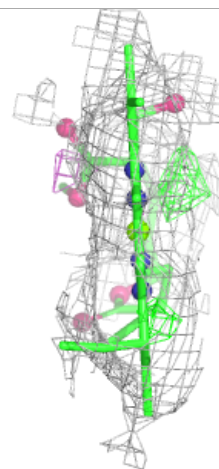
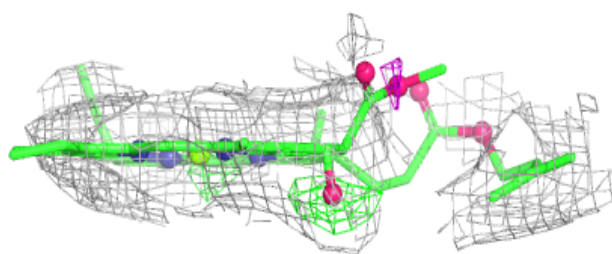
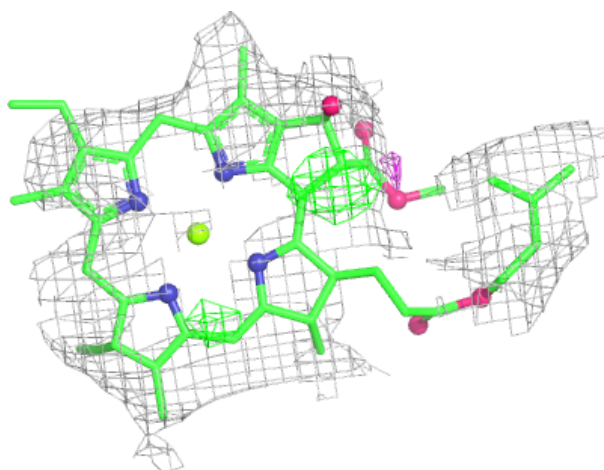
Electron density around CLA 3 312:

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



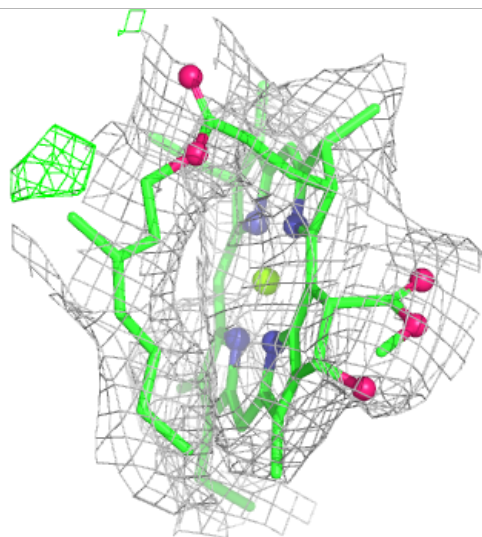
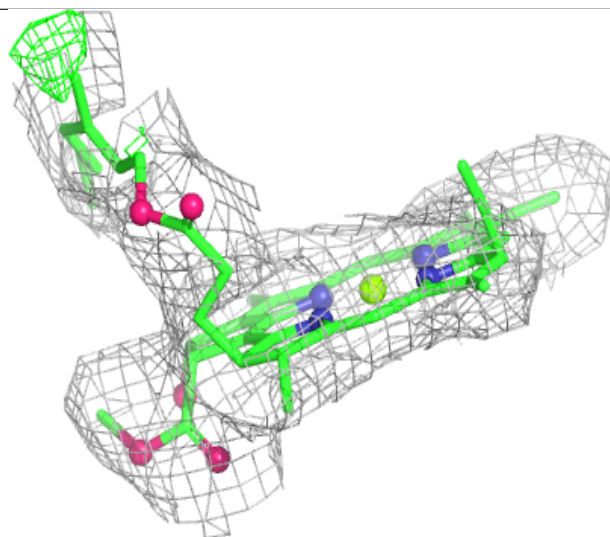
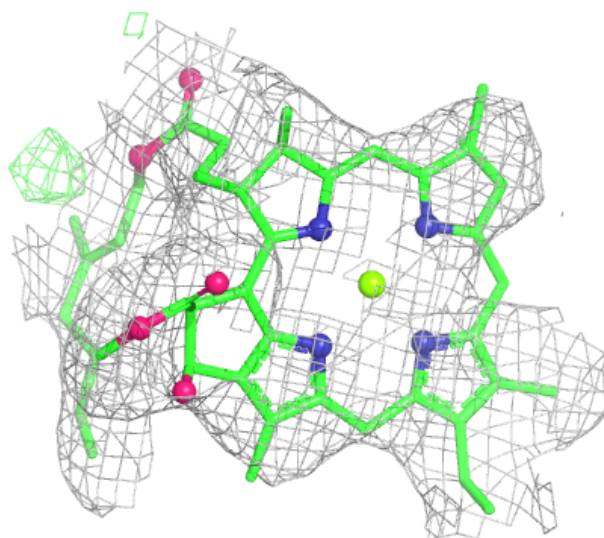
Electron density around CLA 2 311:

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



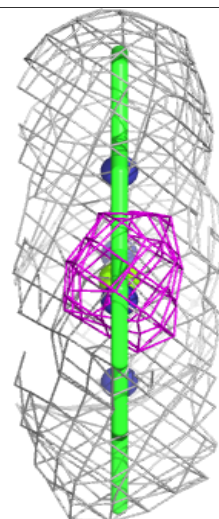
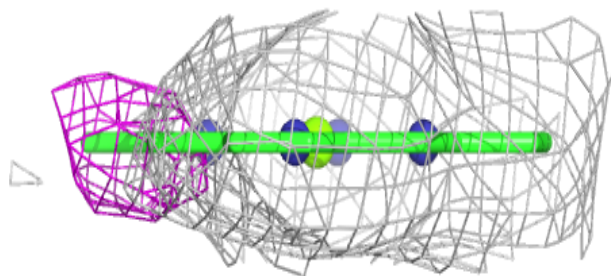
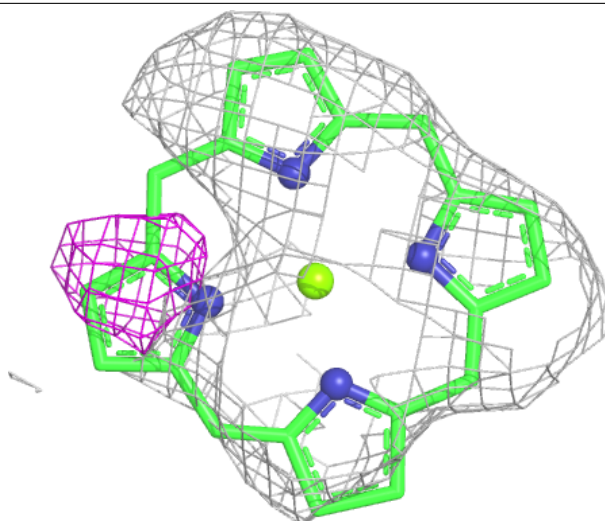
Electron density around CLA F 206:

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



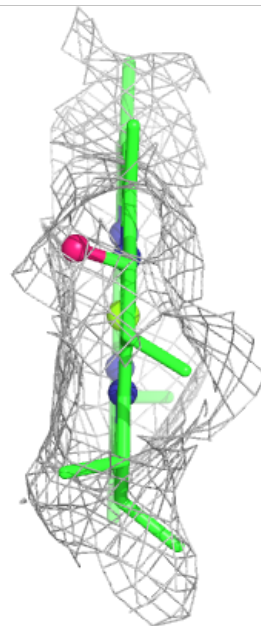
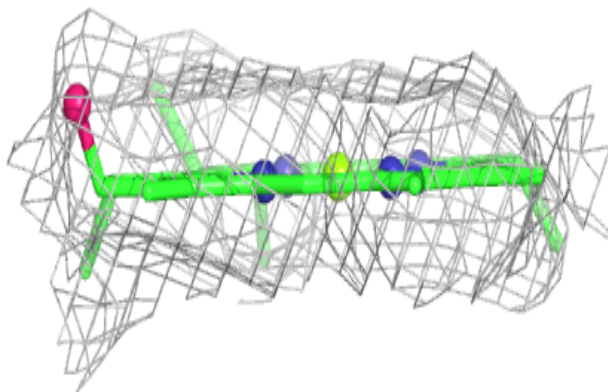
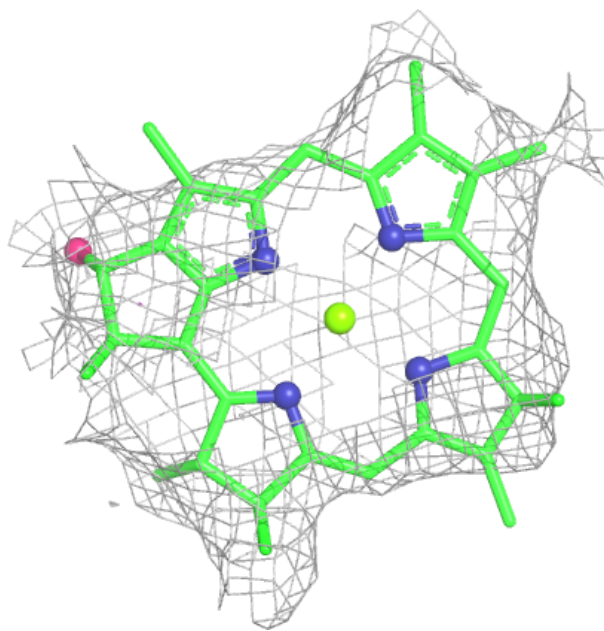
Electron density around CLA 3 316:

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



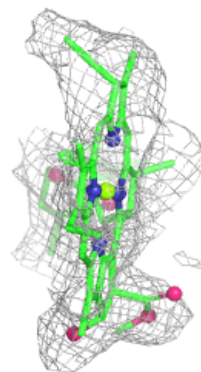
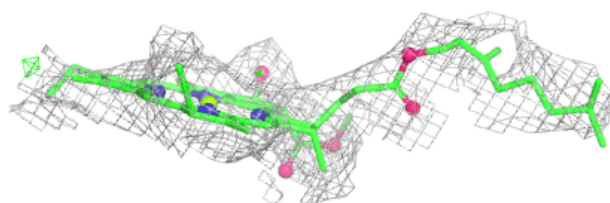
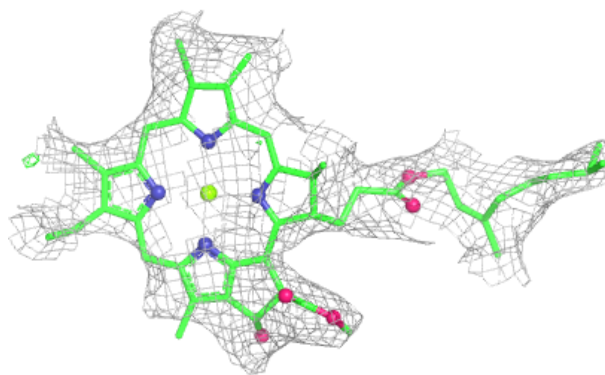
Electron density around CLA 3 319:

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

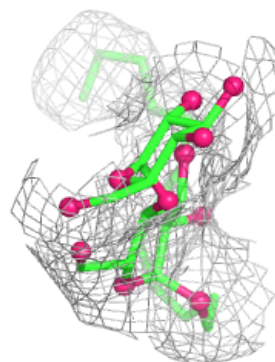
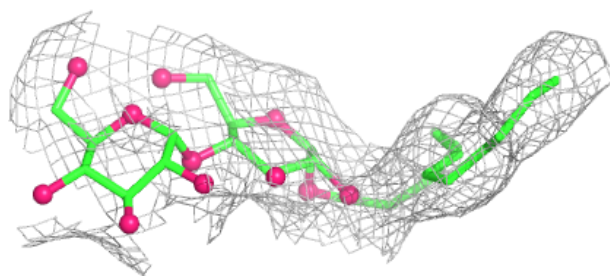
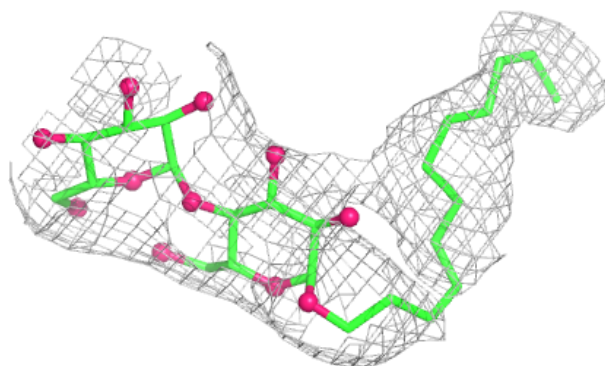


Electron density around CLA 3 320:

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

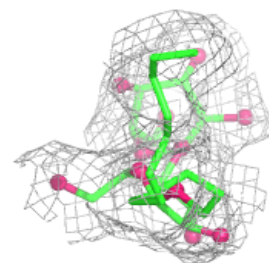
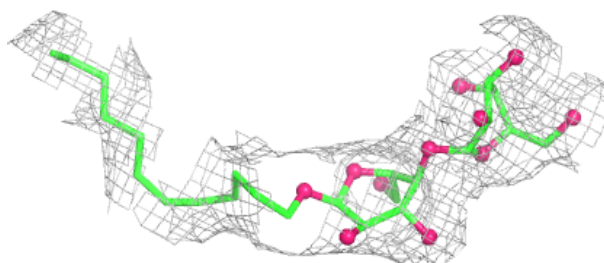
**Electron density around LMU R 105:**

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

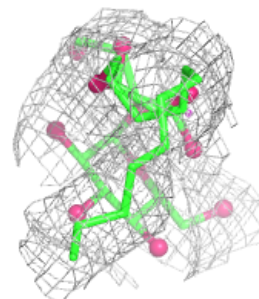
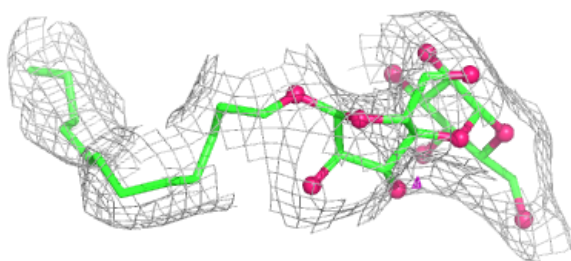
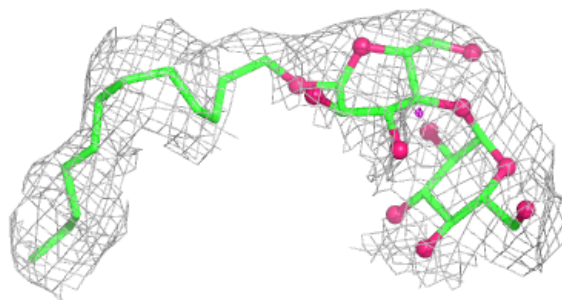


Electron density around LMU 2 318:

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

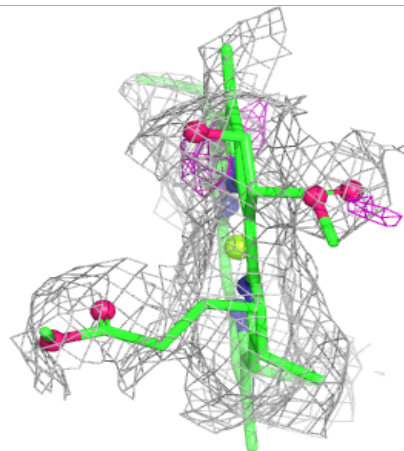
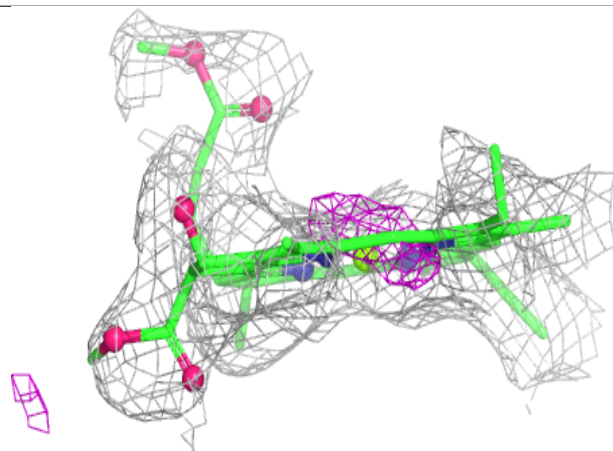
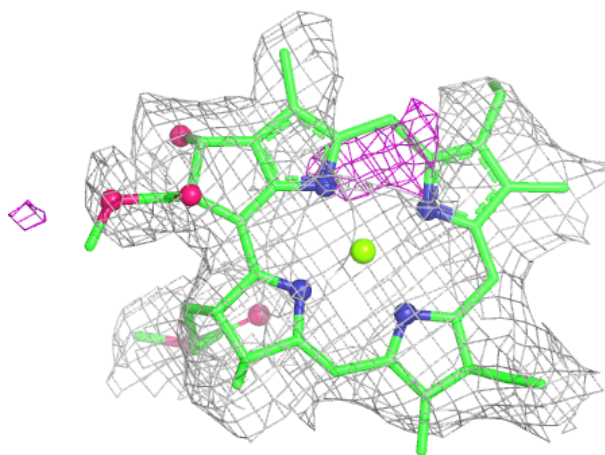
**Electron density around LMU 2 319:**

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



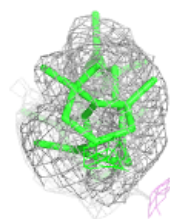
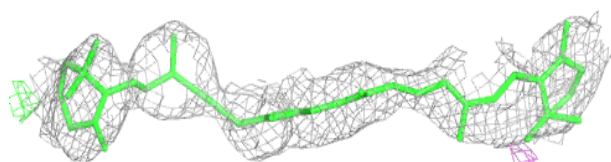
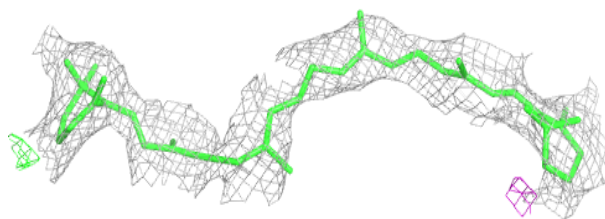
Electron density around CLA A 805:

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



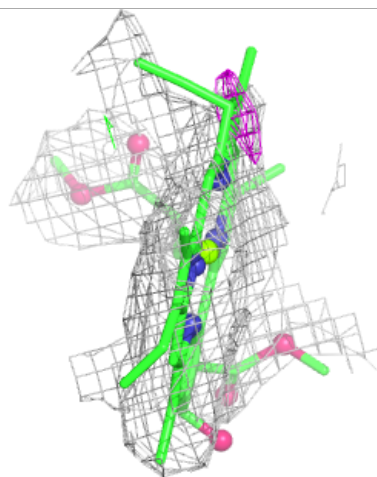
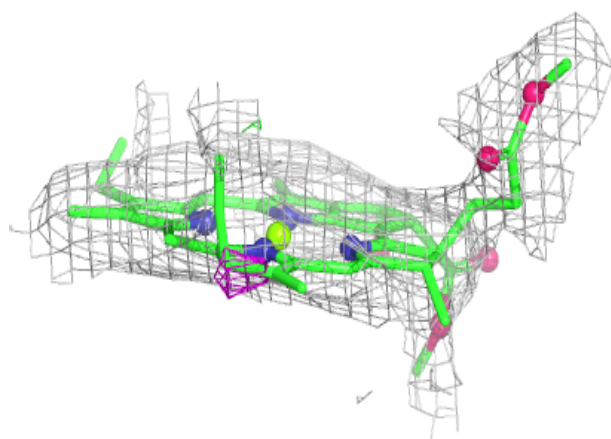
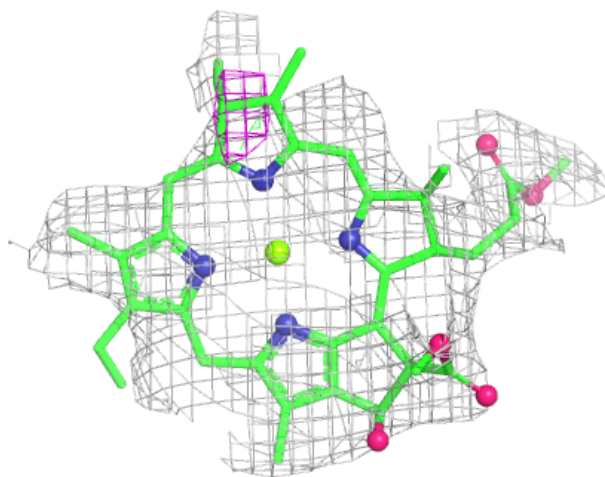
Electron density around BCR I 103:

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



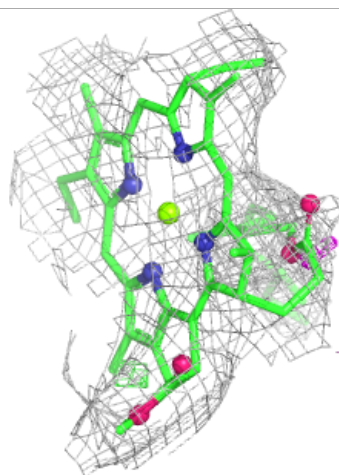
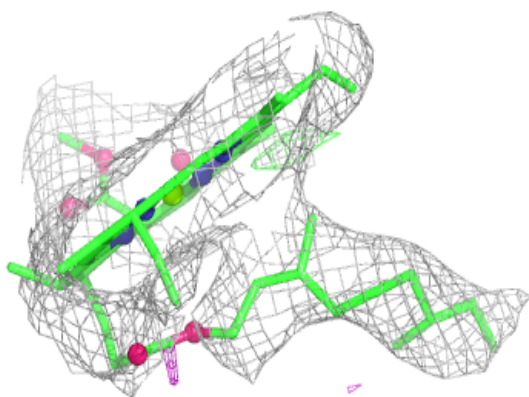
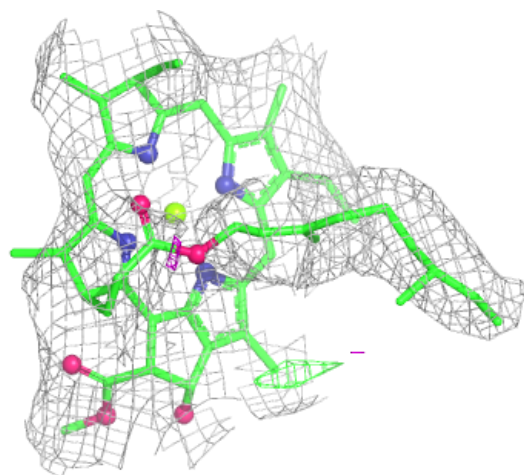
Electron density around CLA B 818:

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



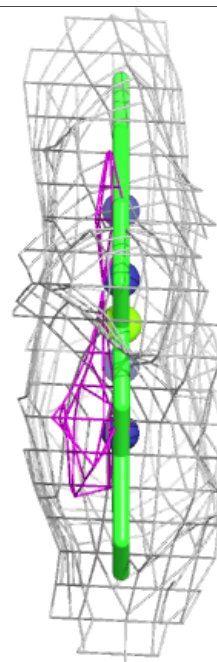
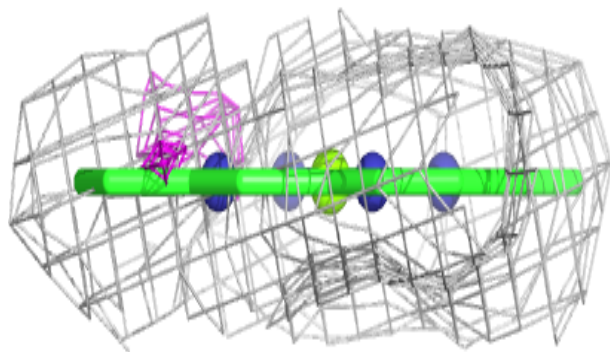
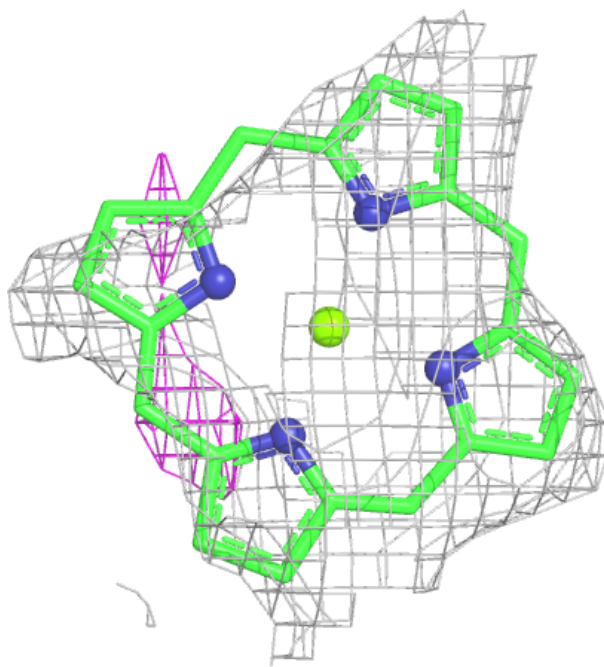
Electron density around CLA 2 302:

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



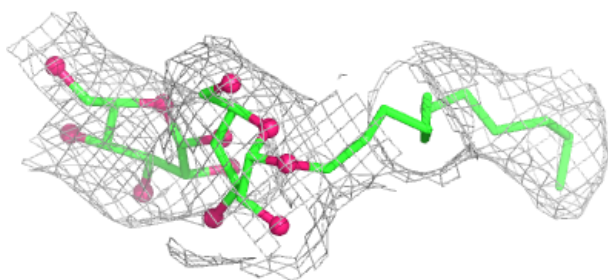
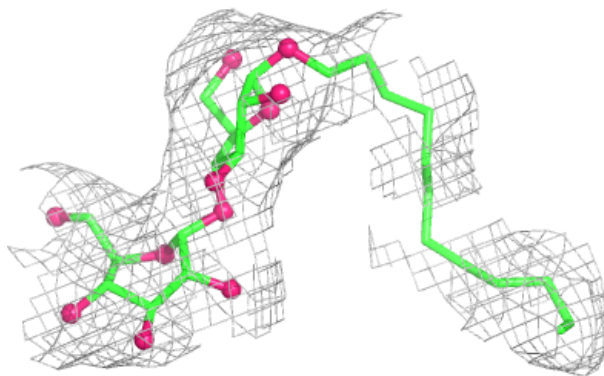
Electron density around CLA 2 314:

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

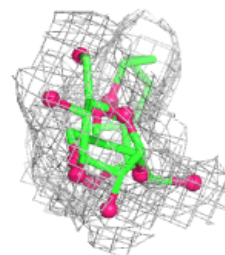
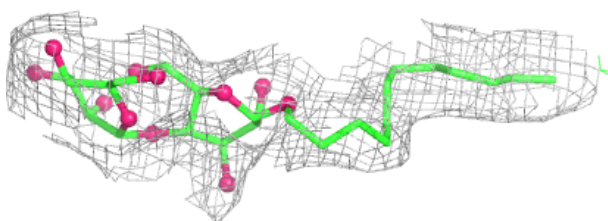
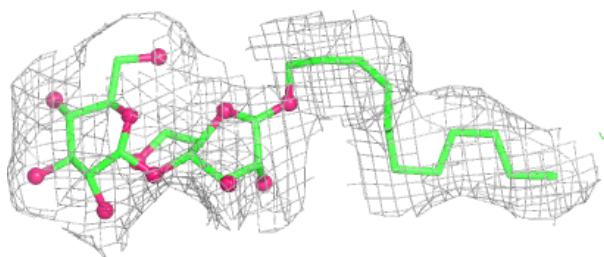


Electron density around LMU L 206:

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

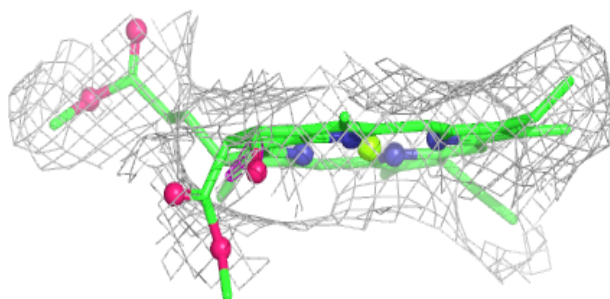
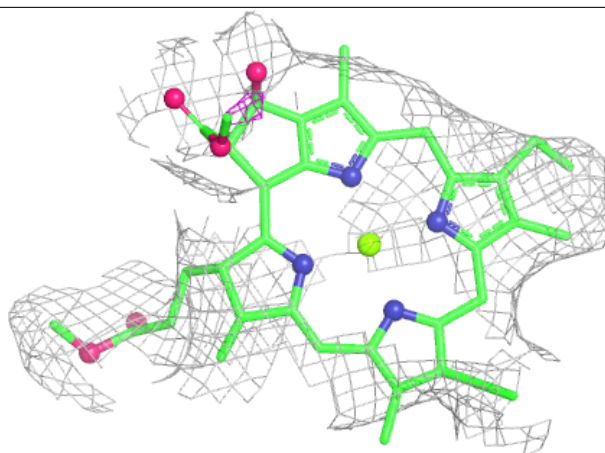
**Electron density around LMU R 101:**

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



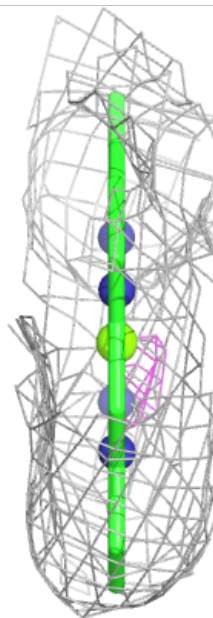
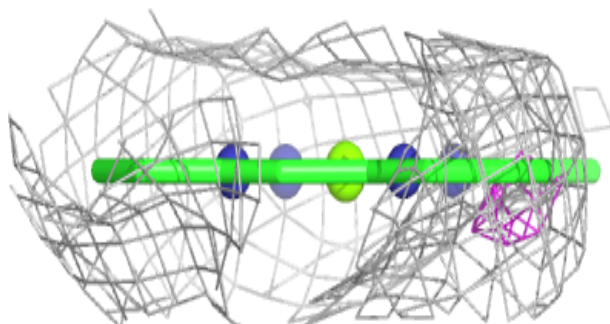
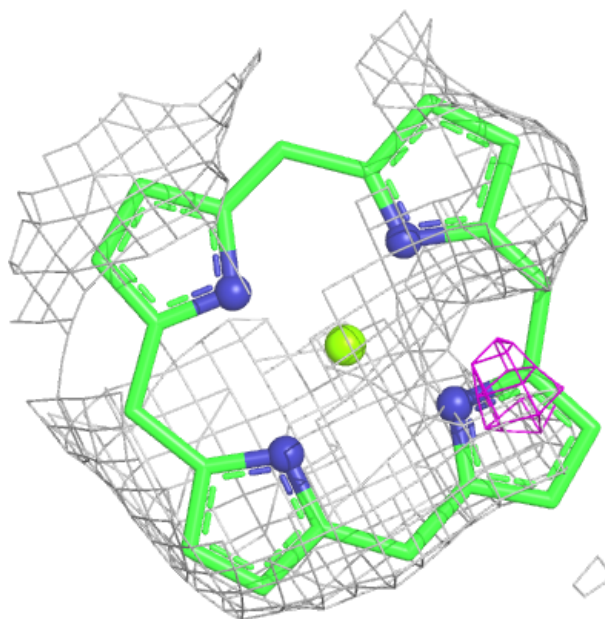
Electron density around CLA 1 201:

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



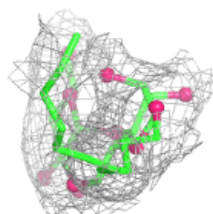
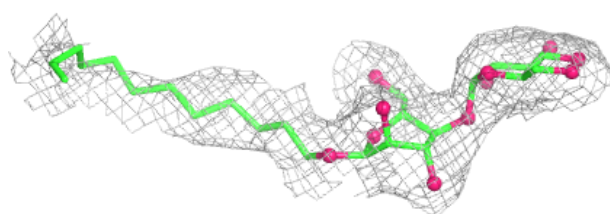
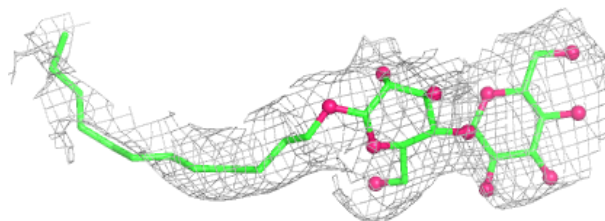
Electron density around CLA 3 306:

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

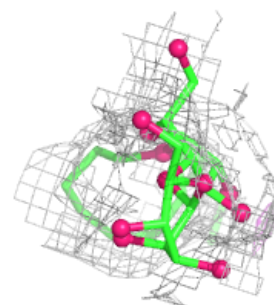
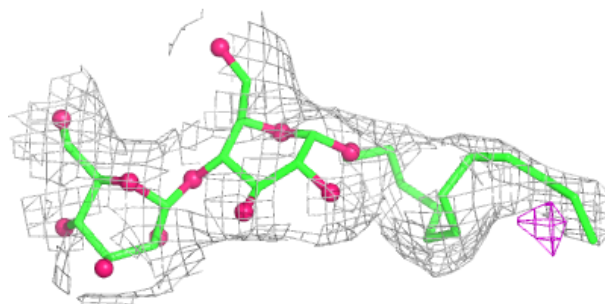


Electron density around LMU 2 320:

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

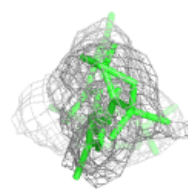
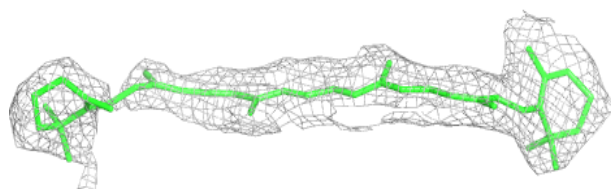
**Electron density around LMU 3 318:**

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

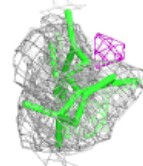
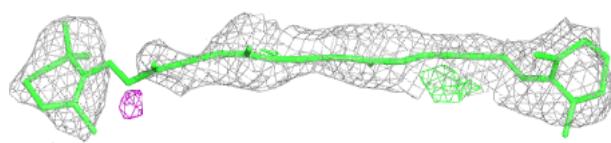
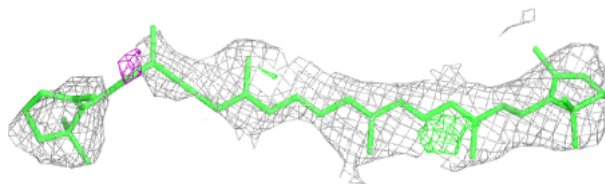


Electron density around BCR B 842:

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

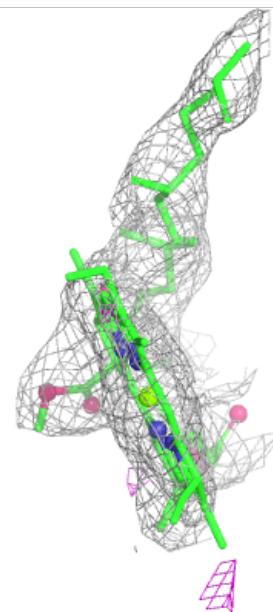
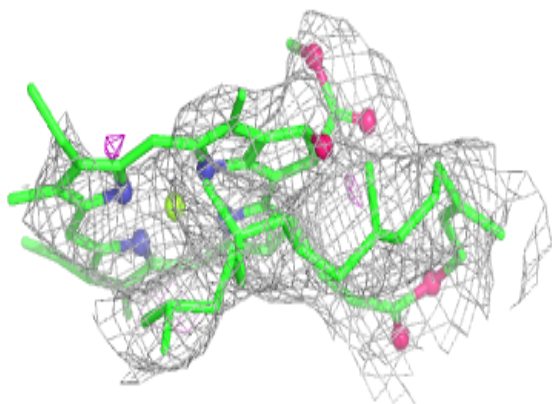
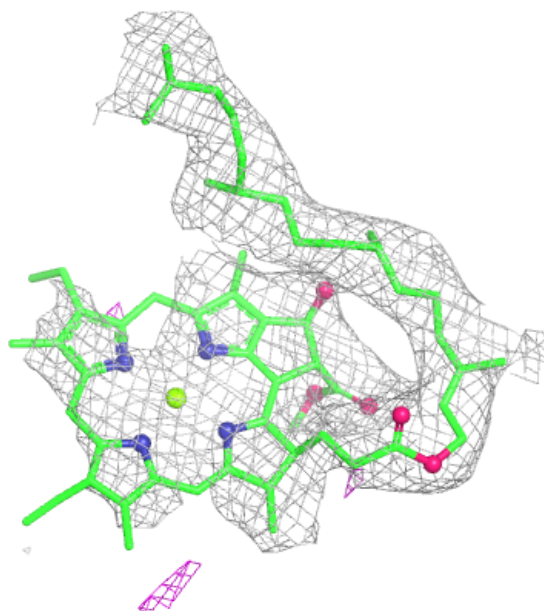
**Electron density around BCR B 844:**

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



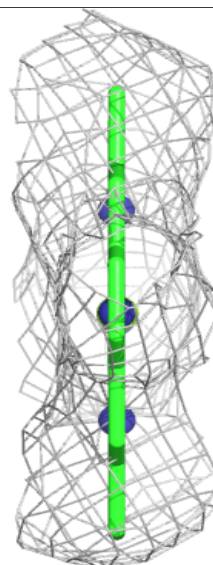
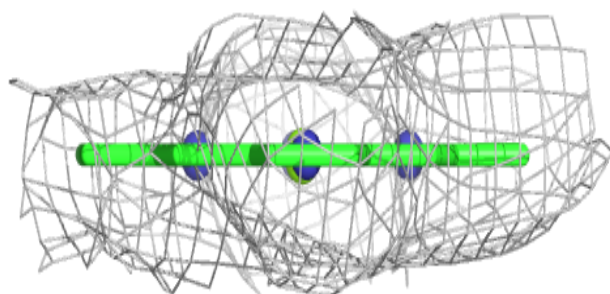
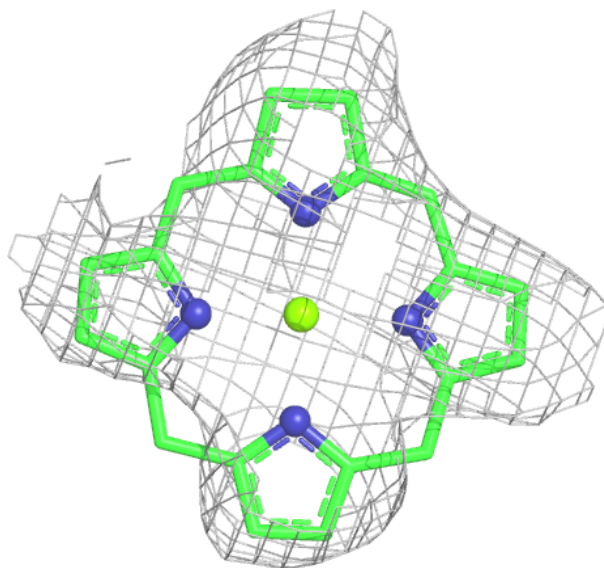
Electron density around CLA A 821:

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



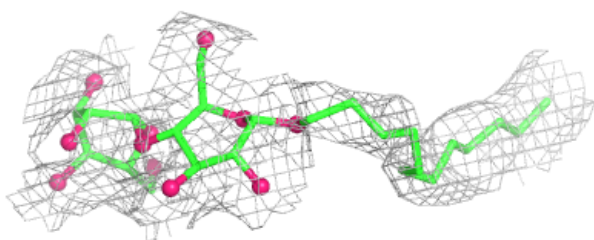
Electron density around CLA 3 313:

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



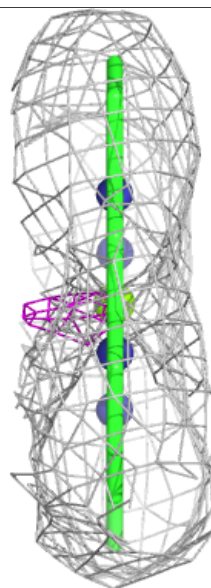
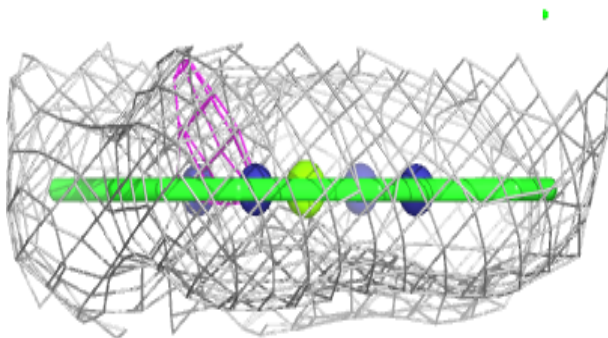
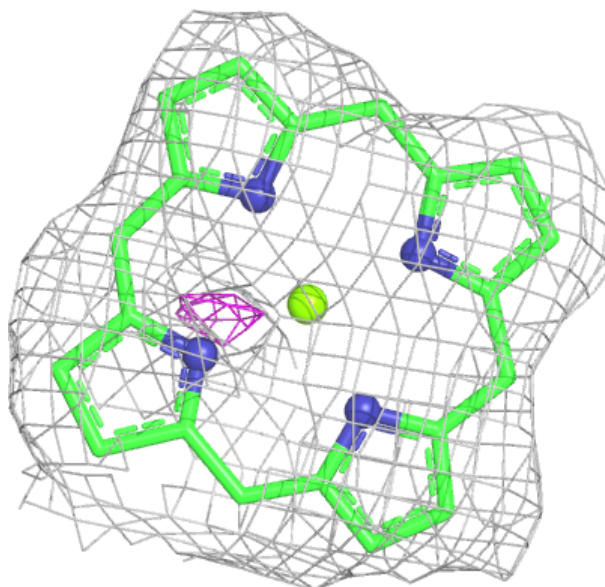
Electron density around LMU 4 301:

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



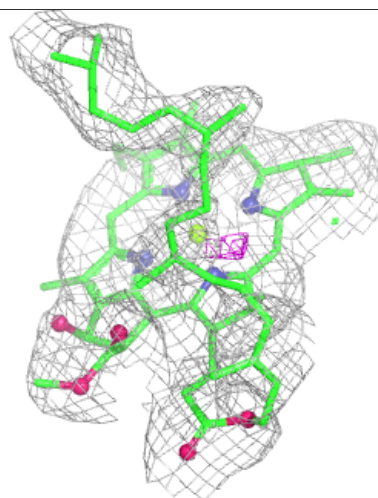
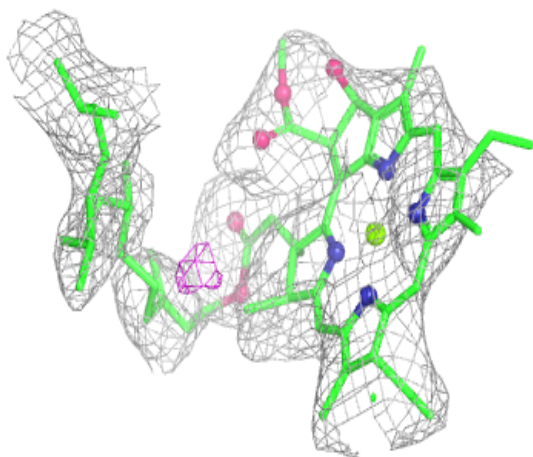
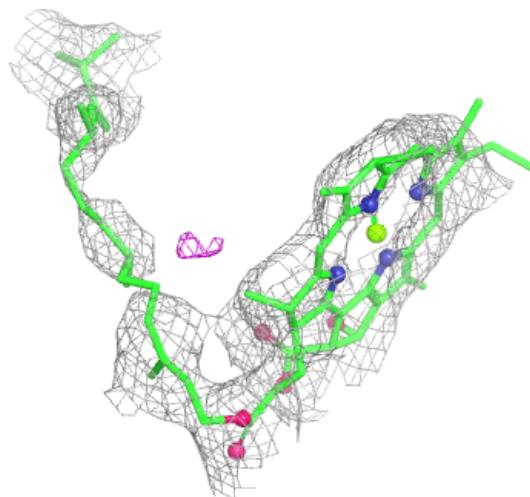
Electron density around CLA 4 314:

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



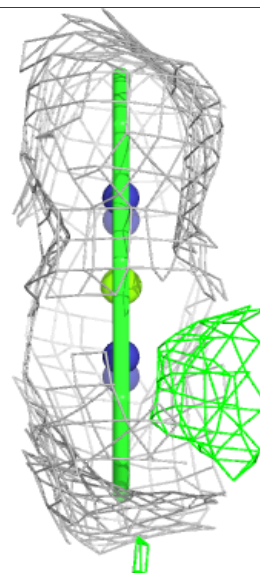
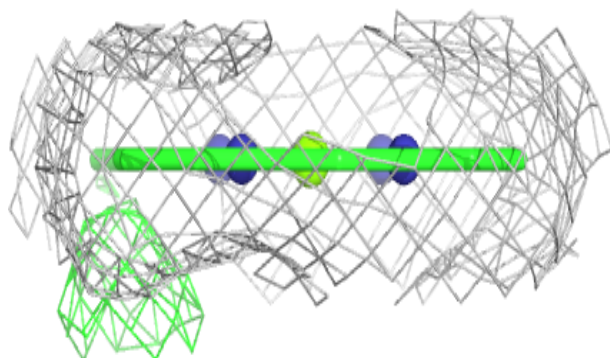
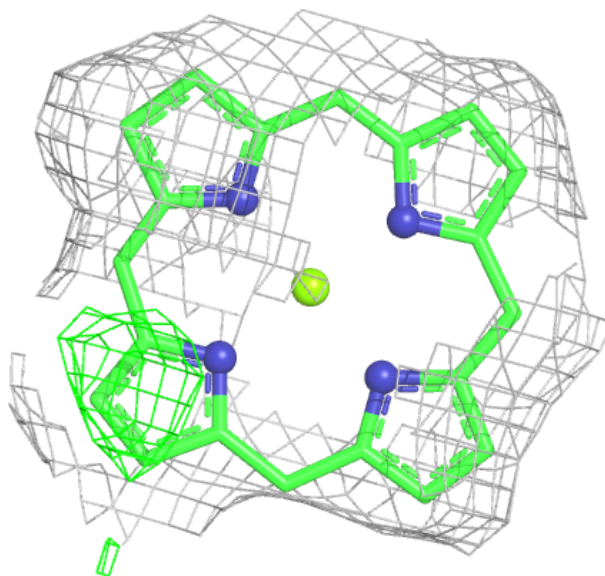
Electron density around CLA 2 306:

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



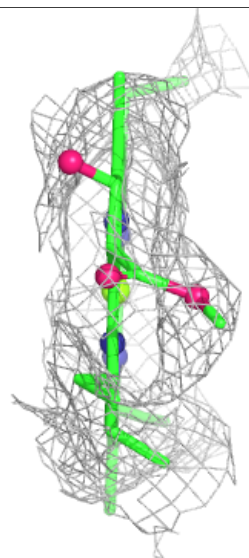
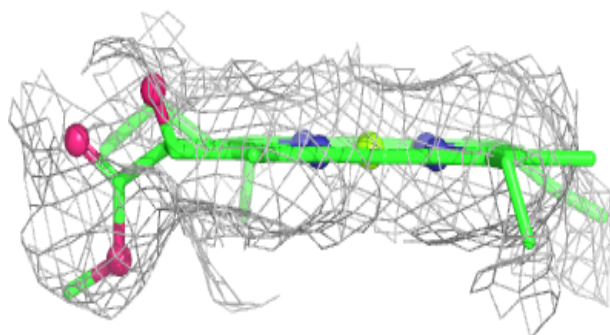
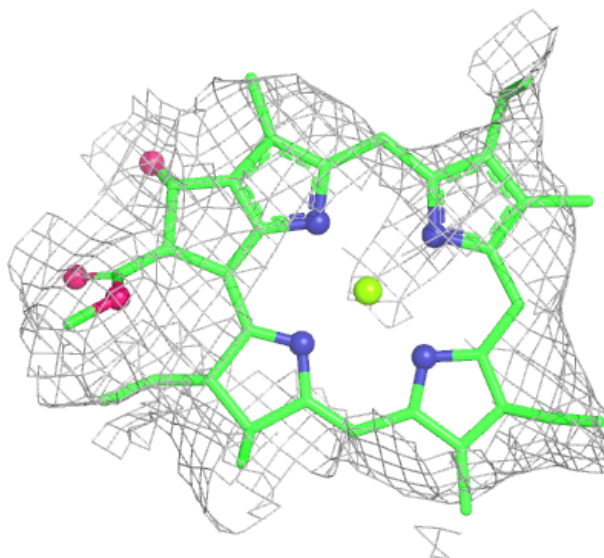
Electron density around CLA 1 208:

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



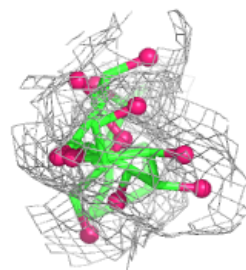
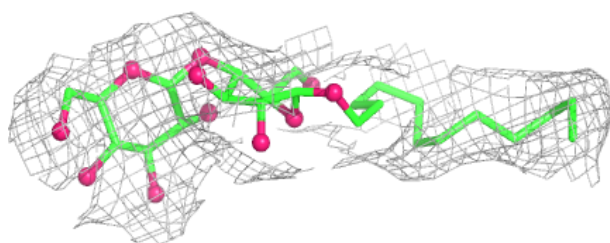
Electron density around CLA A 819:

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

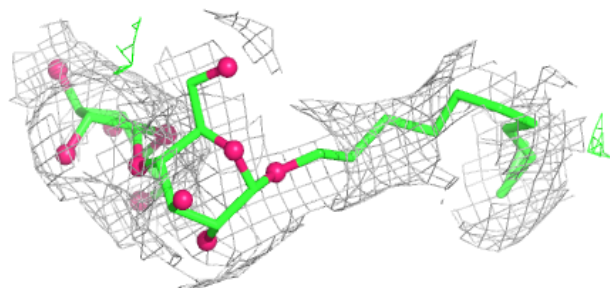
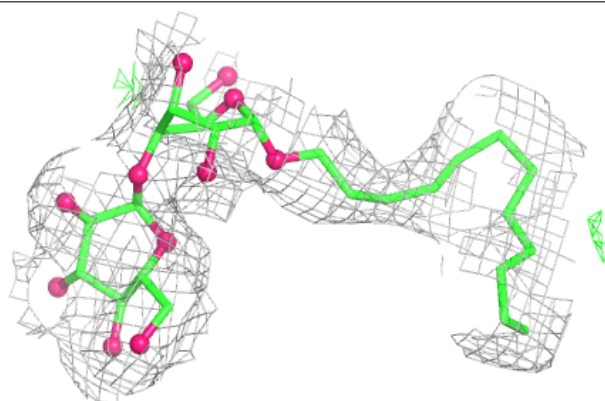


Electron density around LMU K 102:

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

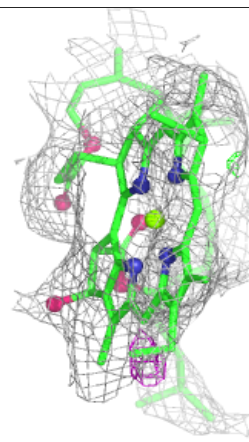
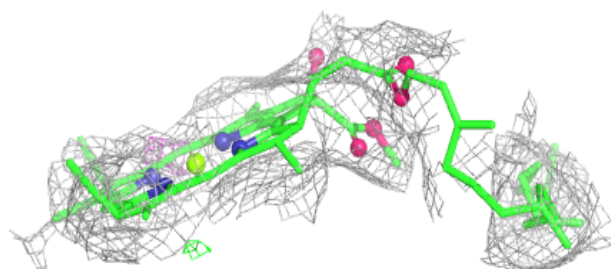
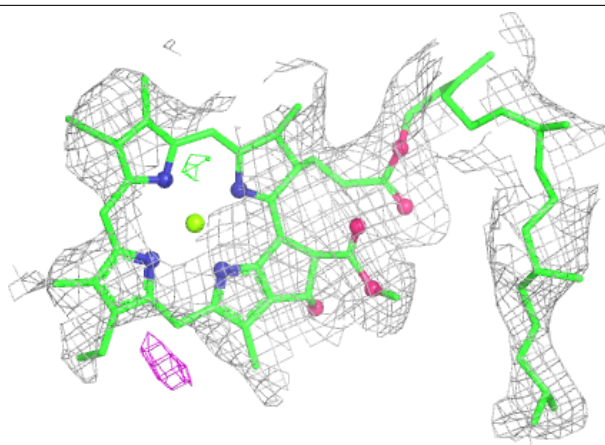
**Electron density around LMU K 104:**

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



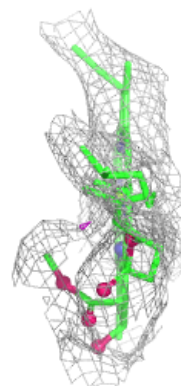
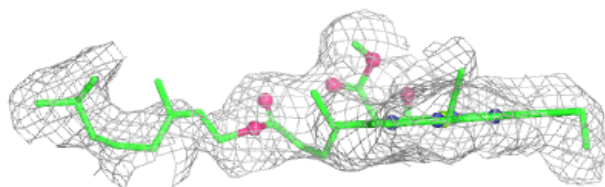
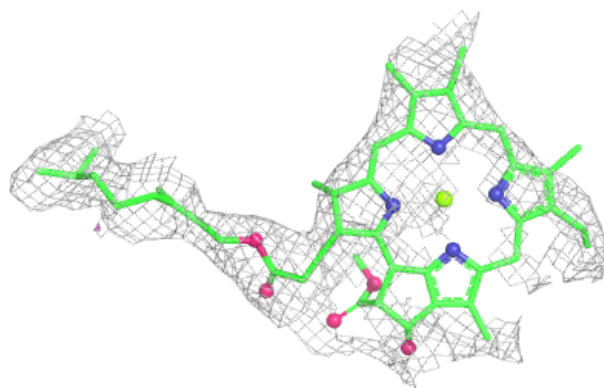
Electron density around CLA R 107:

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



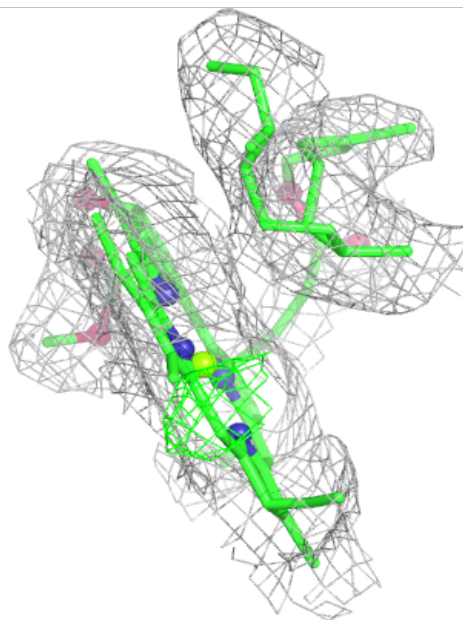
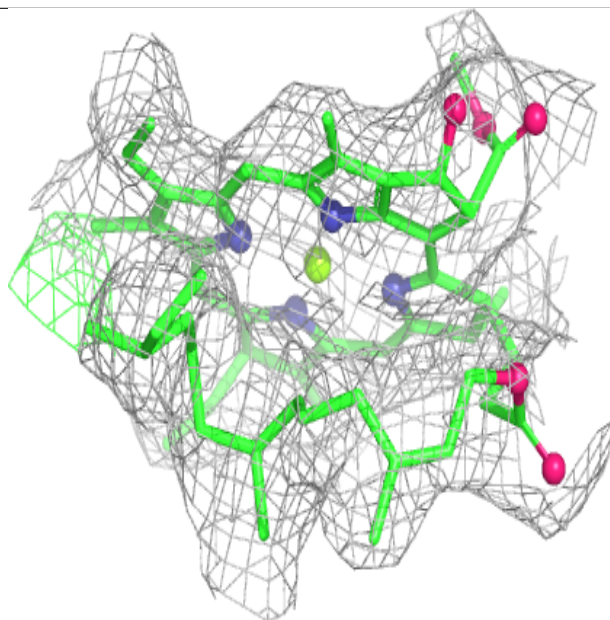
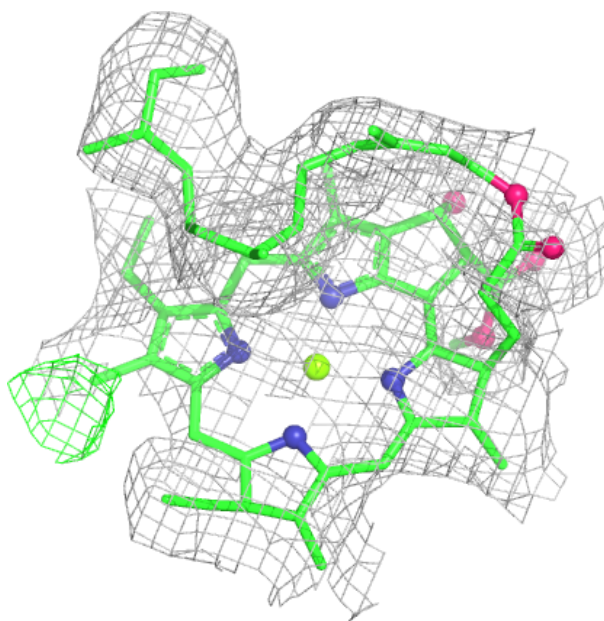
Electron density around CLA 4 310:

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



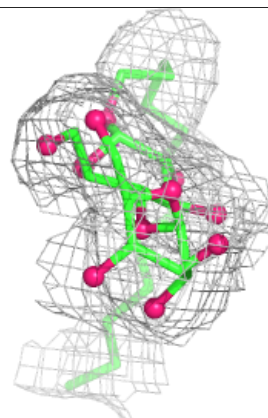
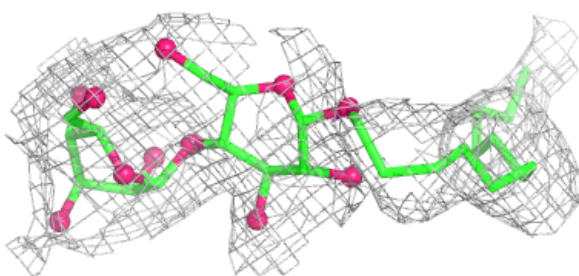
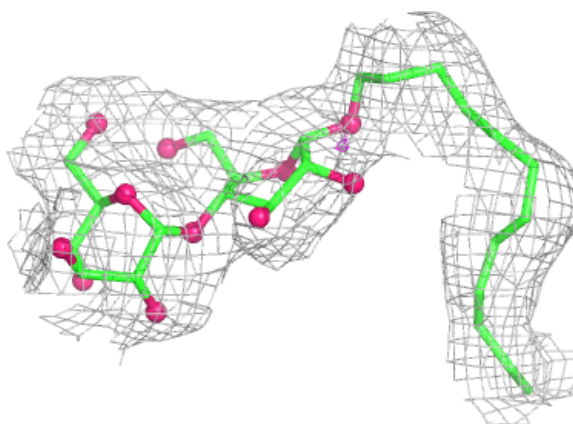
Electron density around CLA 1 206:

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

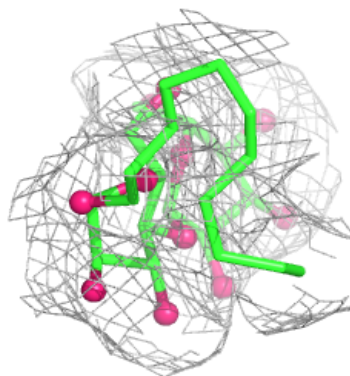
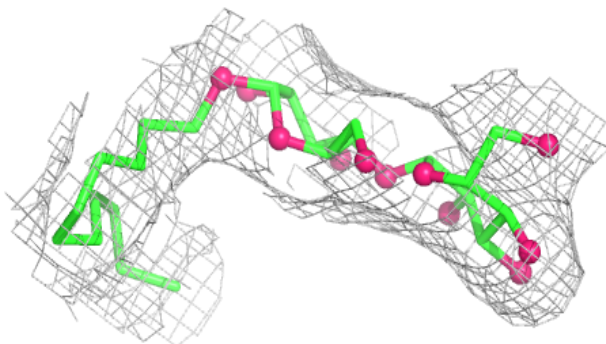
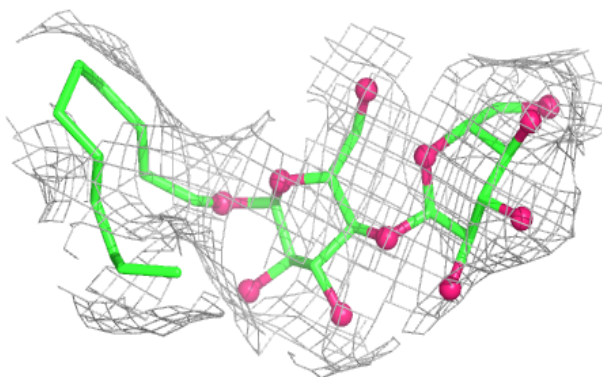


Electron density around LMU 3 302:

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

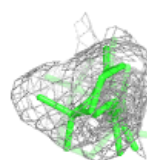
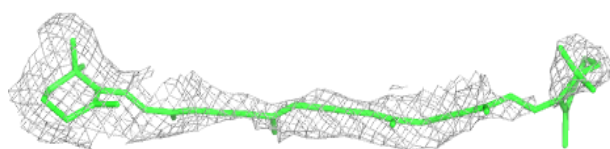
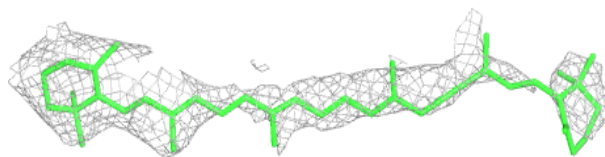
**Electron density around LMU F 201:**

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

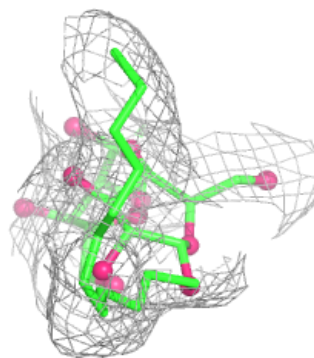
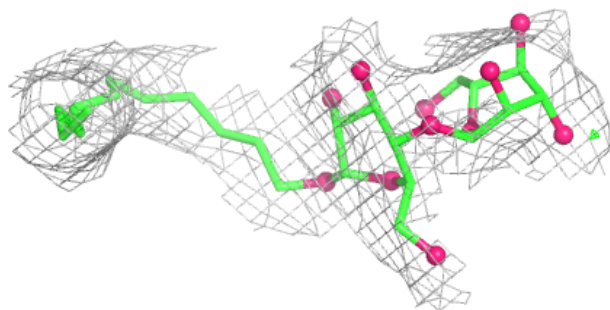


Electron density around BCR A 843:

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

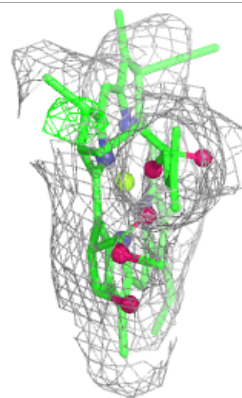
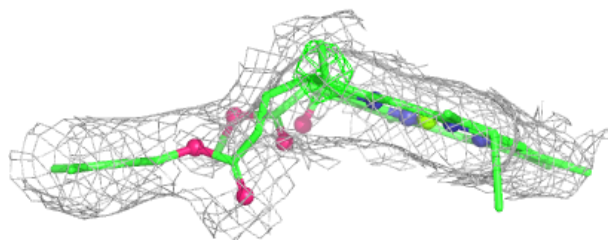
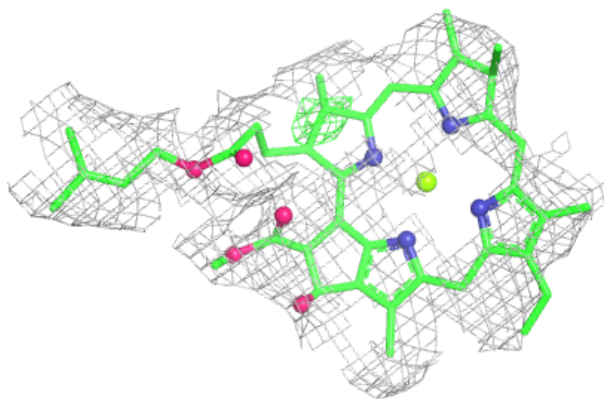
**Electron density around LMU 2 316:**

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

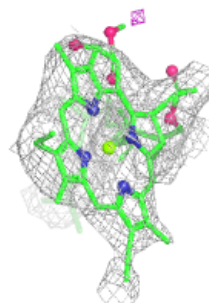
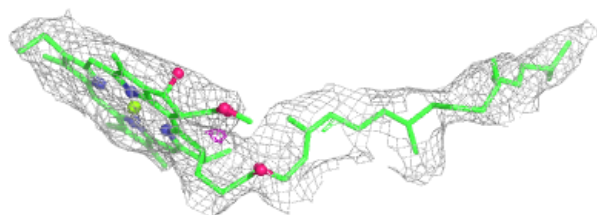
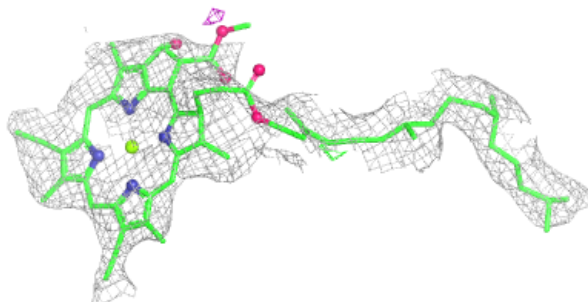


Electron density around CLA L 208:

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

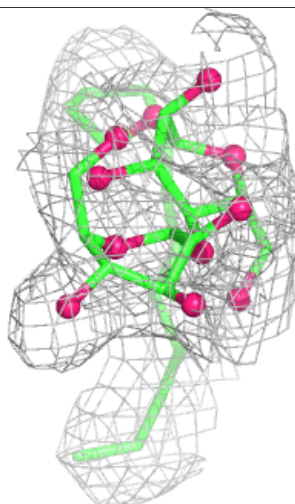
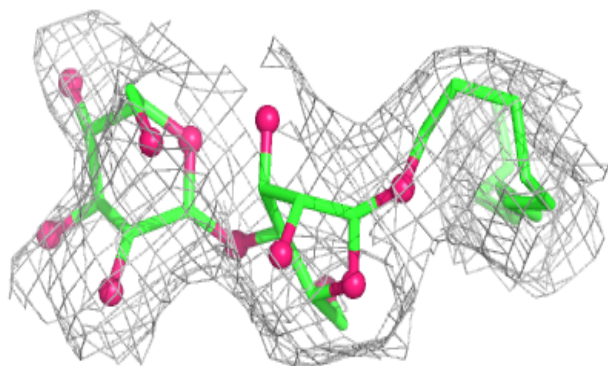
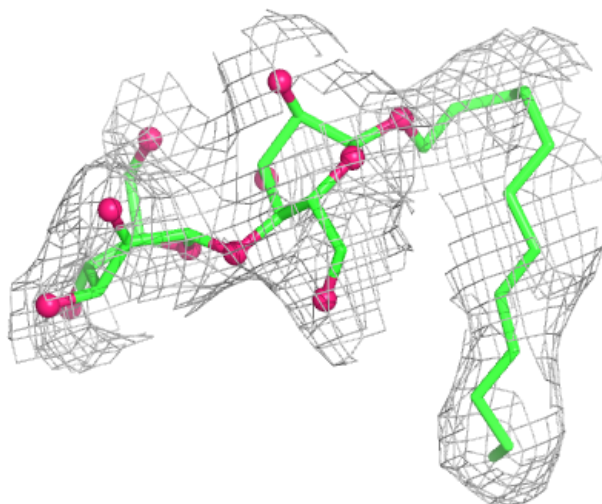
**Electron density around CLA H 107:**

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



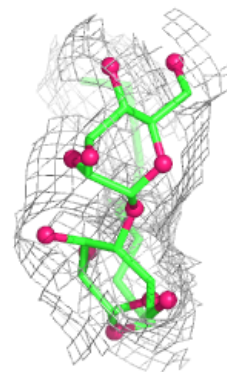
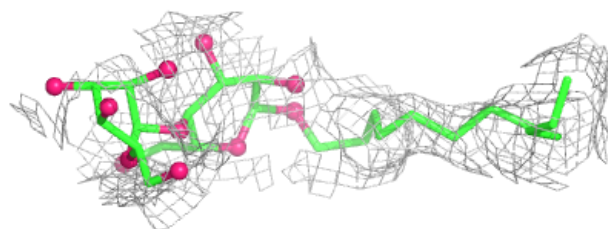
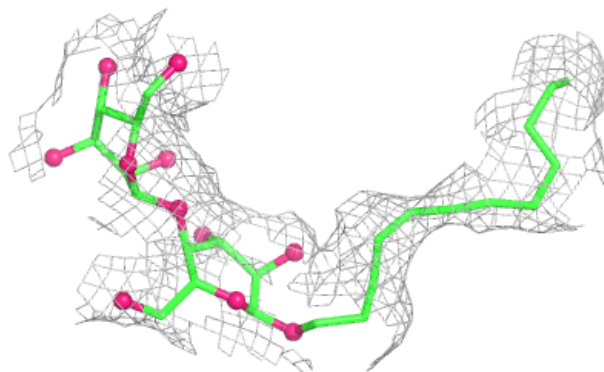
Electron density around LMU R 109:

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



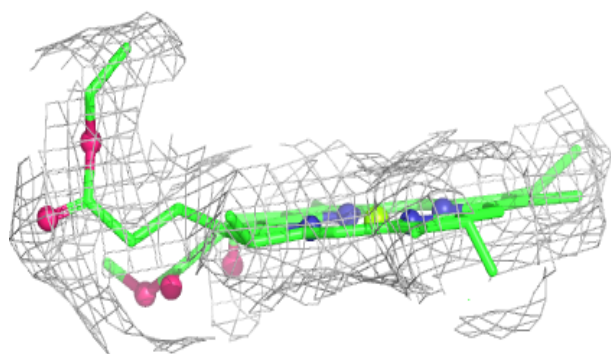
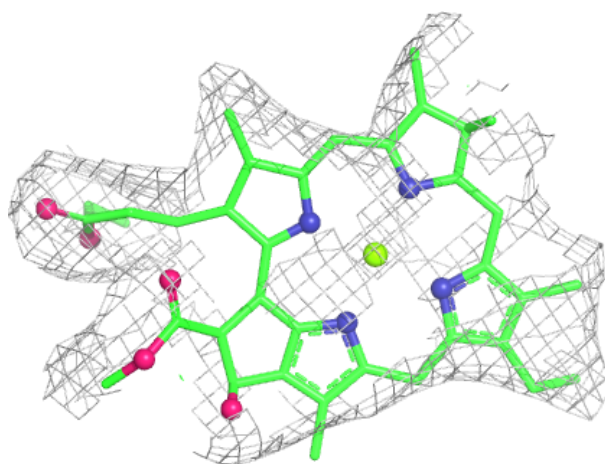
Electron density around LMU 4 321:

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



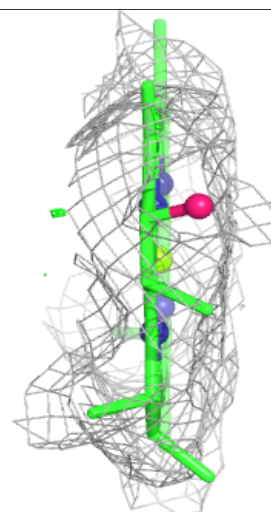
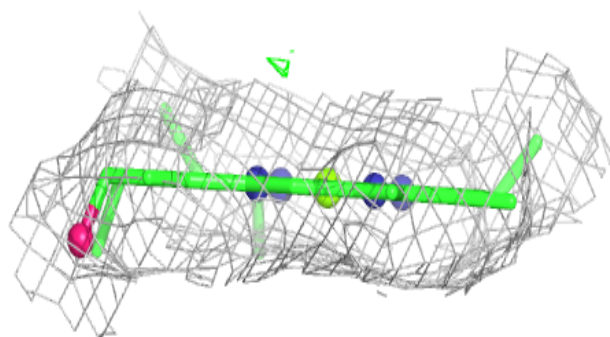
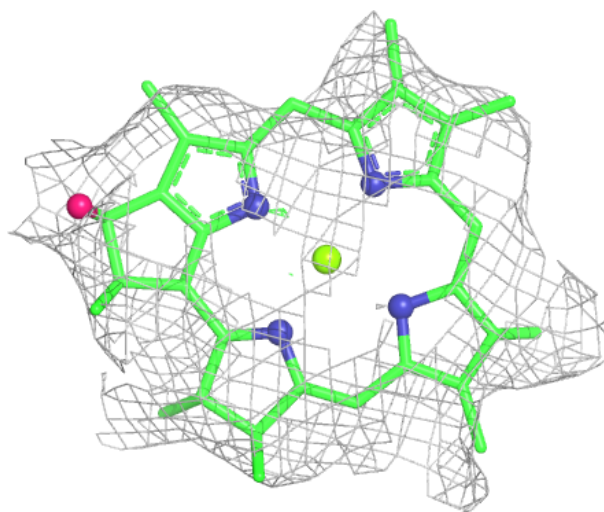
Electron density around CLA A 850:

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



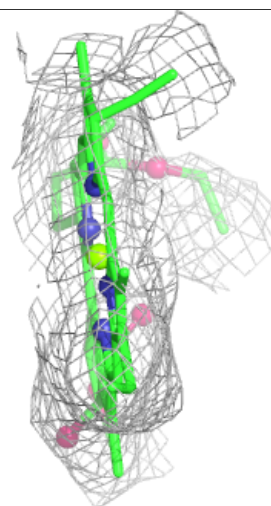
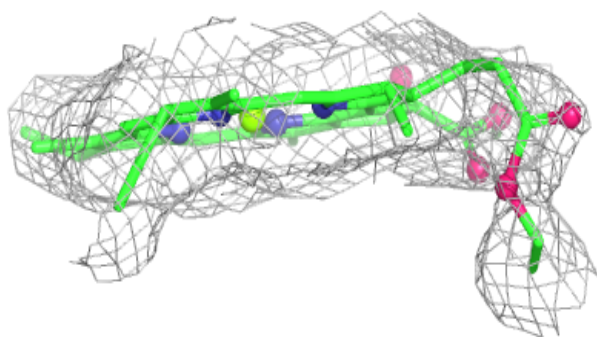
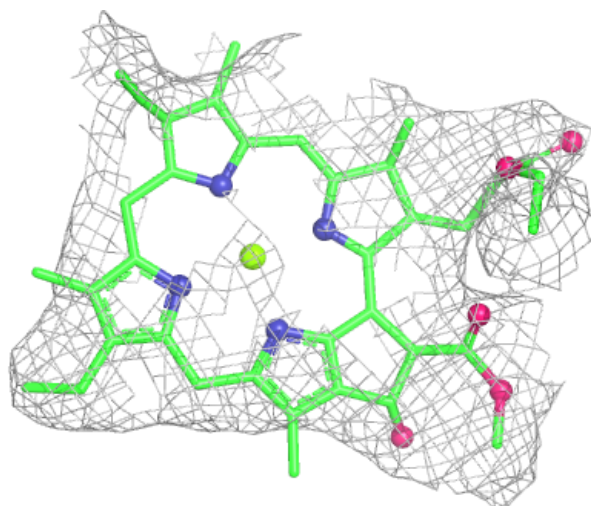
Electron density around CLA 3 303:

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



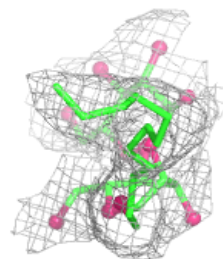
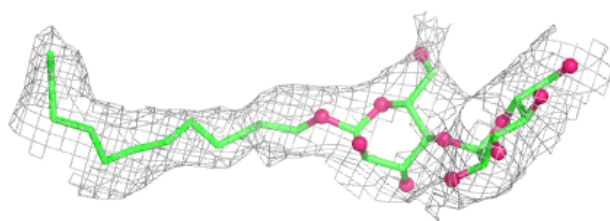
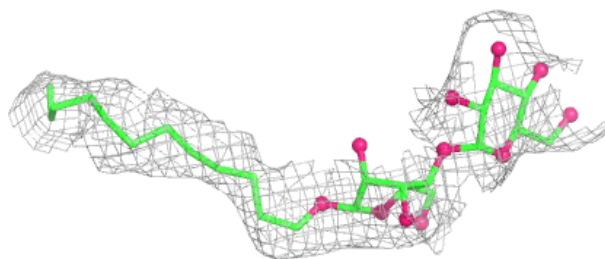
Electron density around CLA 1 202:

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

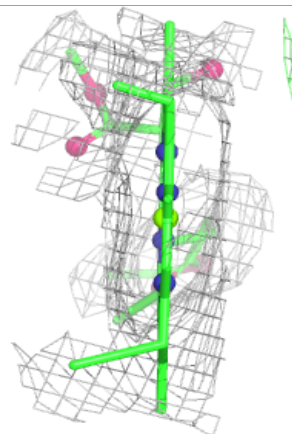
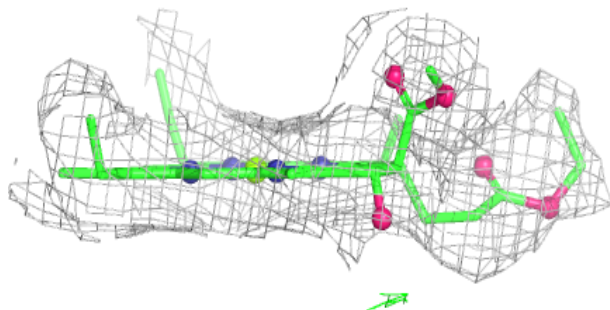
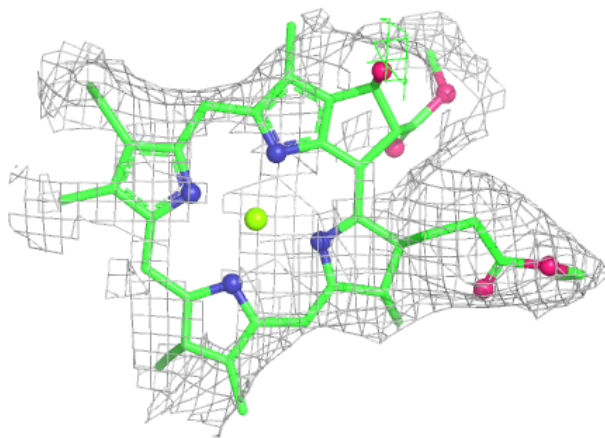


Electron density around LMU 4 316:

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

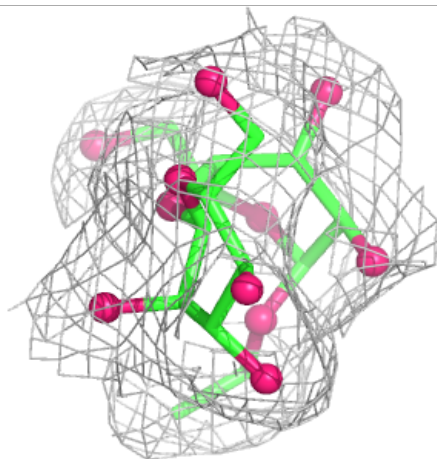
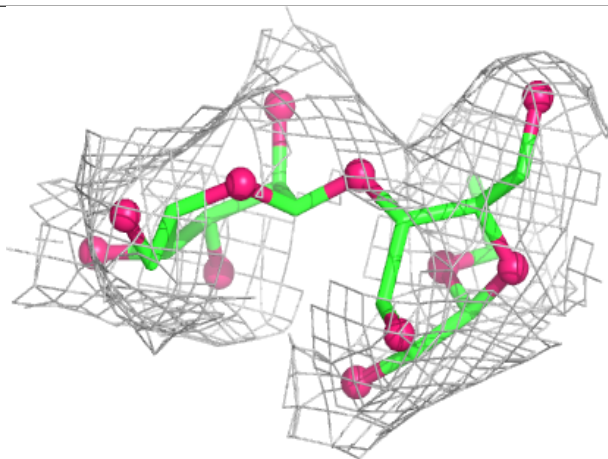
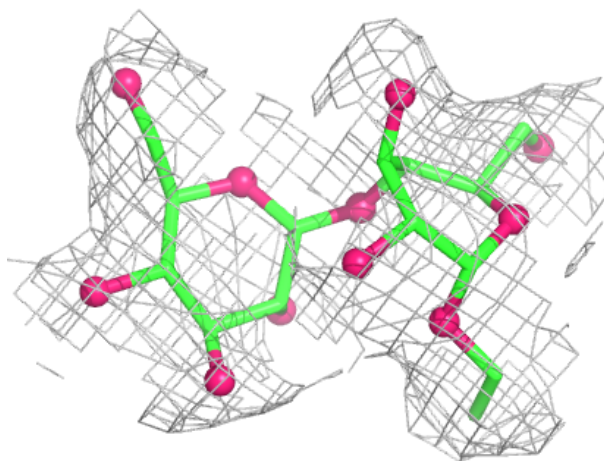
**Electron density around CLA 1 203:**

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



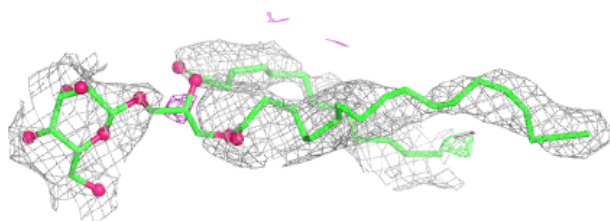
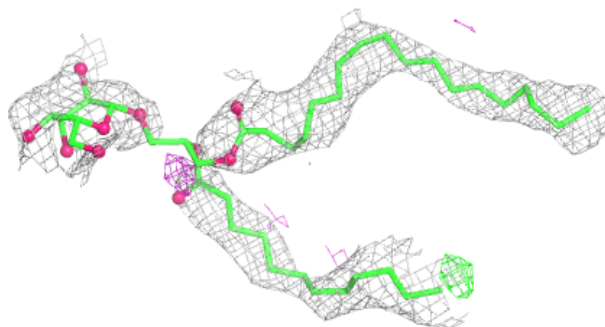
Electron density around LMU B 845:

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



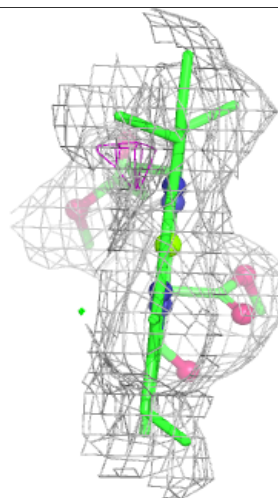
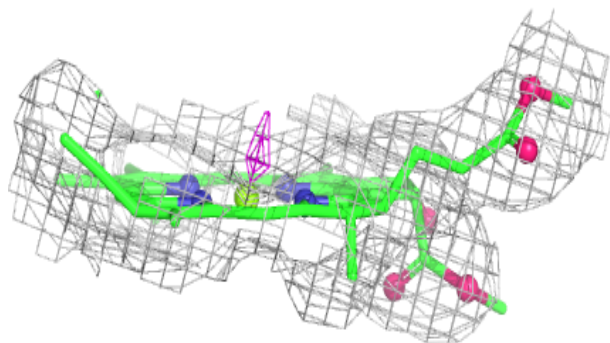
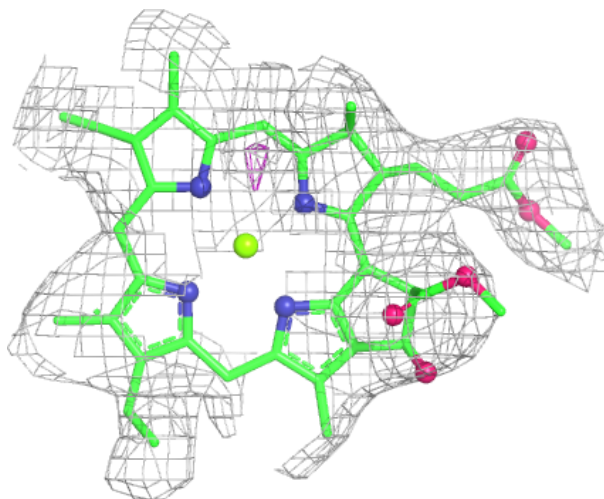
Electron density around LMG B 846:

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



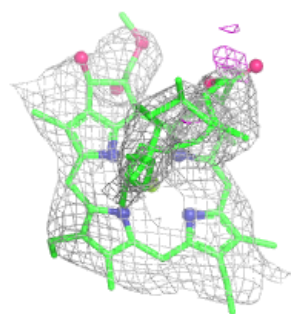
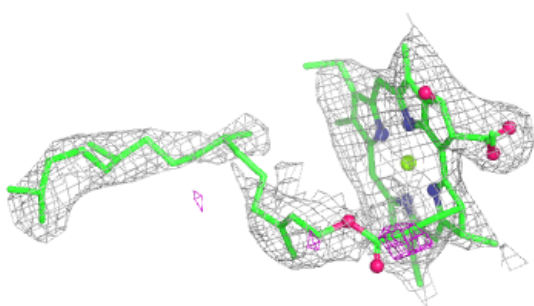
Electron density around CLA 4 315:

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



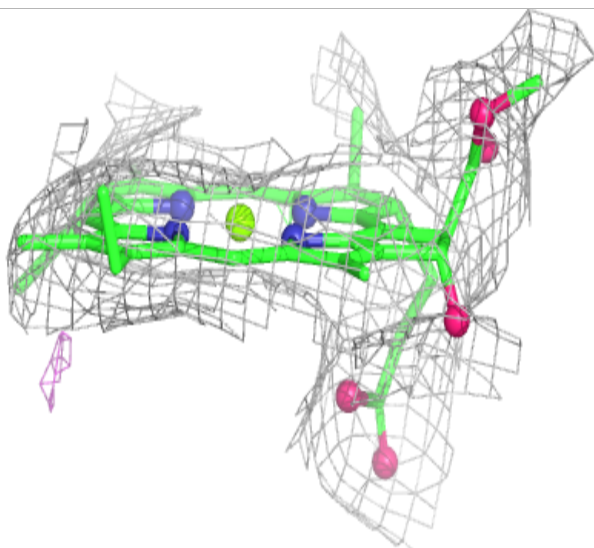
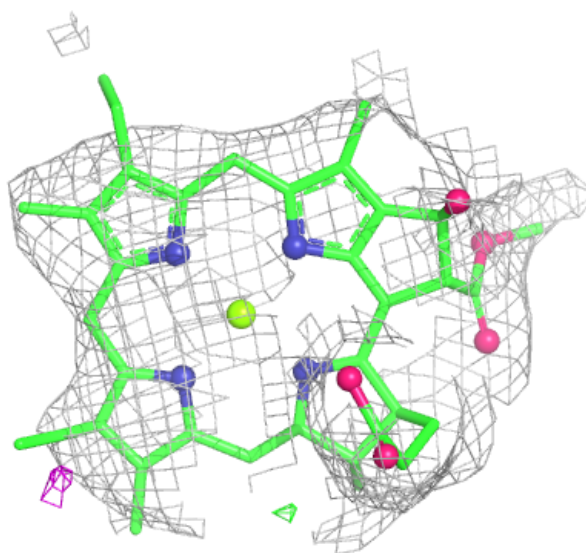
Electron density around CLA A 809:

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



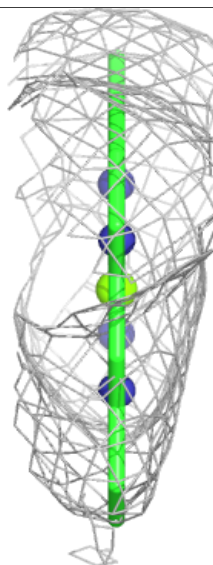
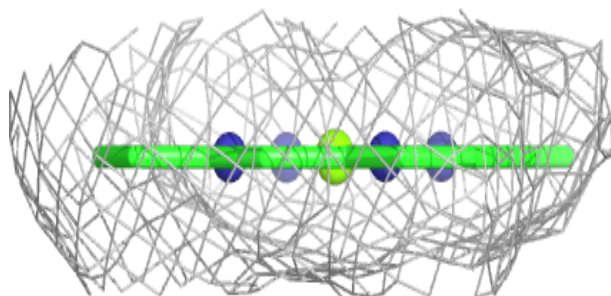
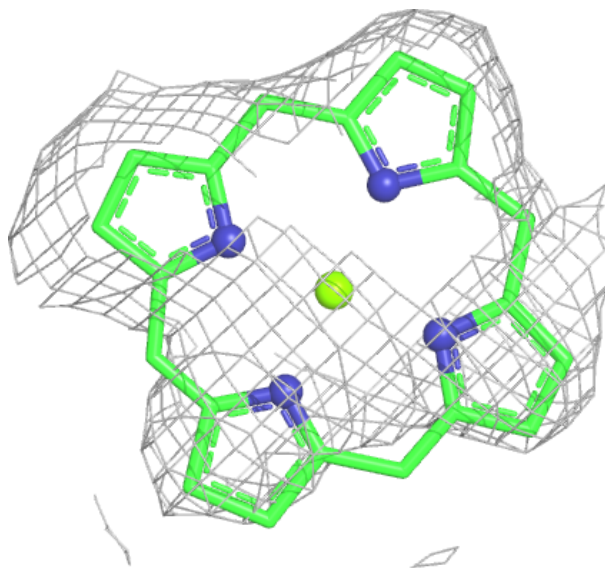
Electron density around CLA B 831:

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



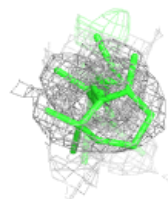
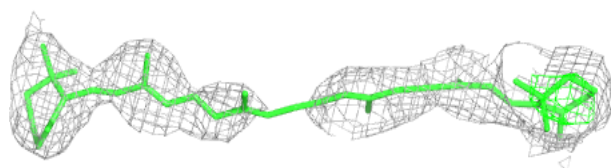
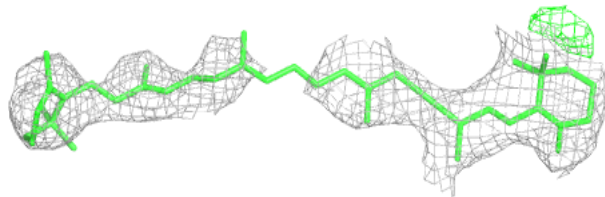
Electron density around CLA 4 308:

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



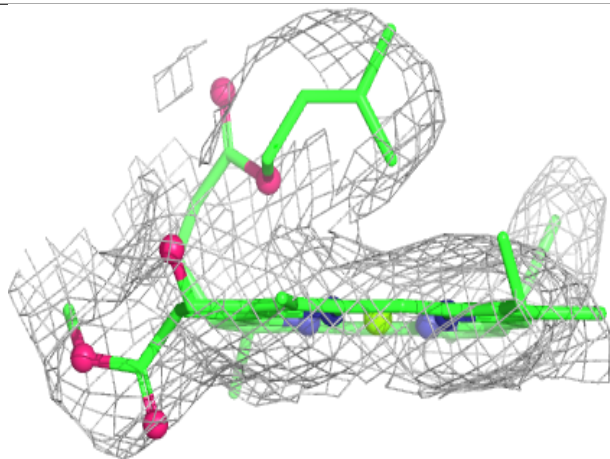
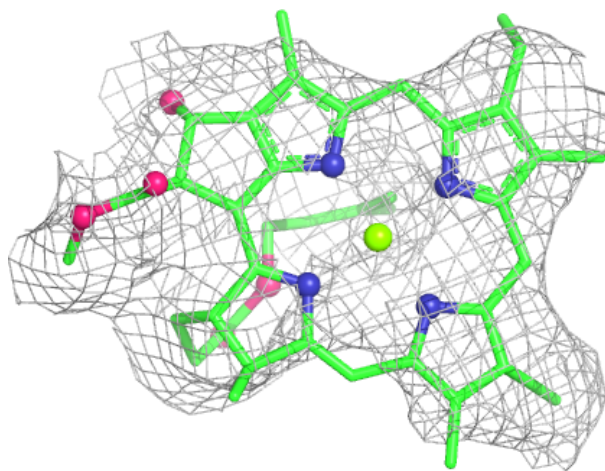
Electron density around BCR A 841:

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



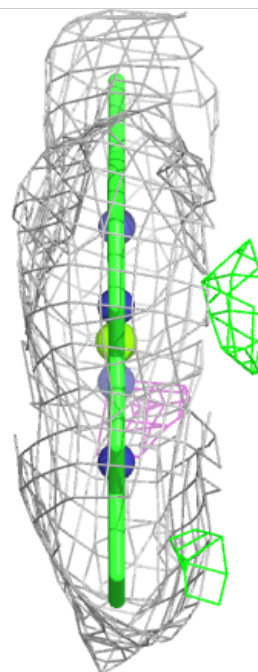
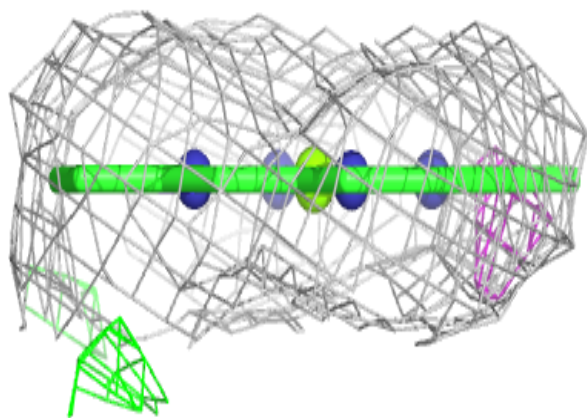
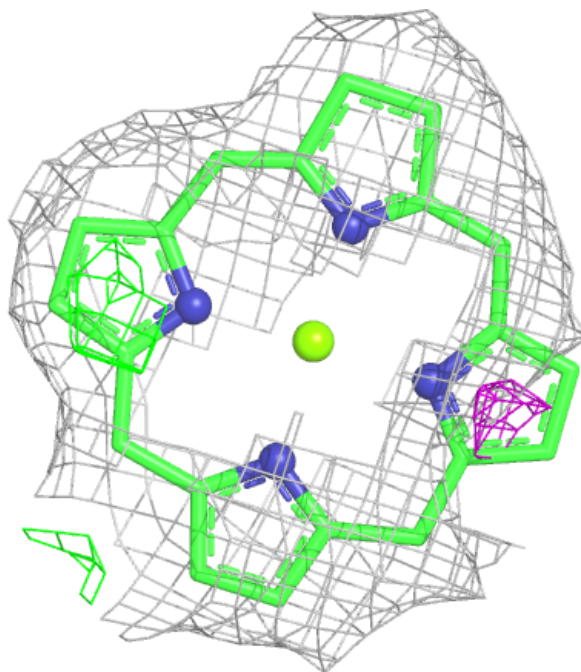
Electron density around CLA H 109:

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



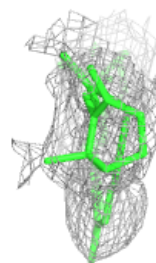
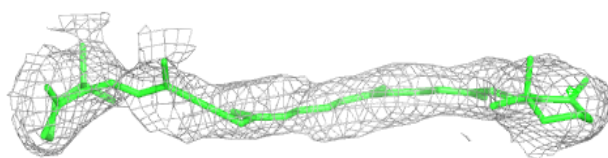
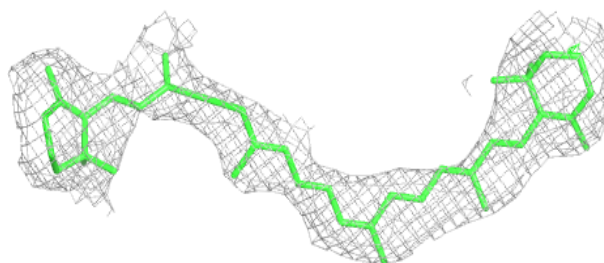
Electron density around CLA 4 309:

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

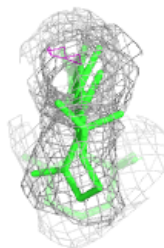
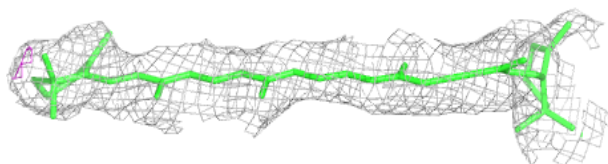
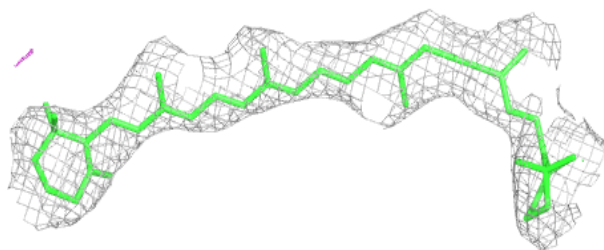


Electron density around BCR A 844:

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

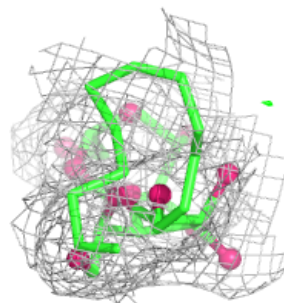
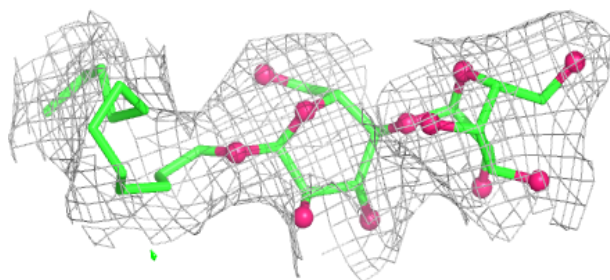
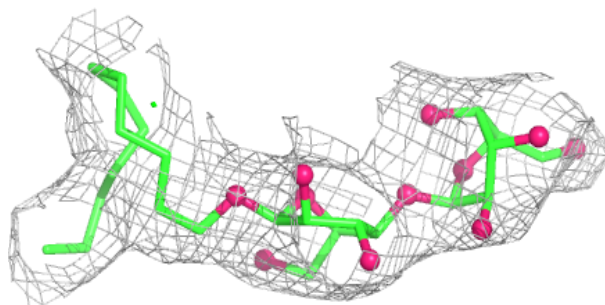
**Electron density around BCR B 841:**

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



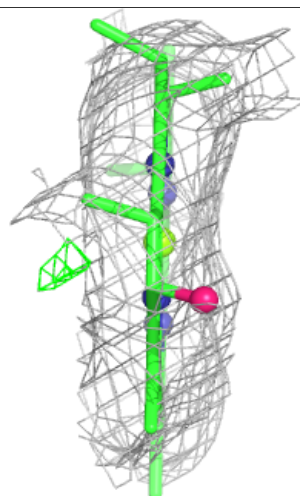
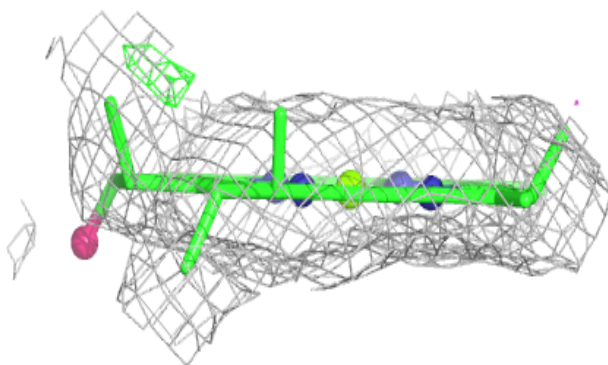
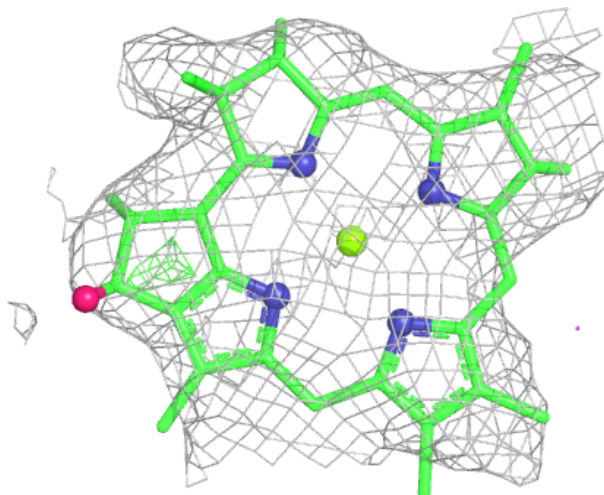
Electron density around LMU A 853:

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



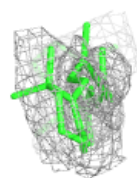
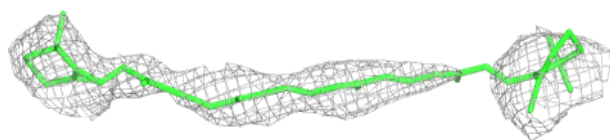
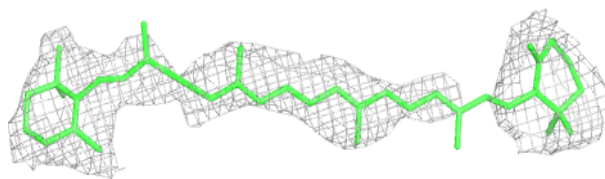
Electron density around CLA B 839:

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



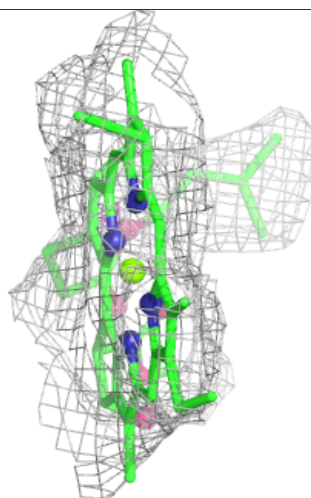
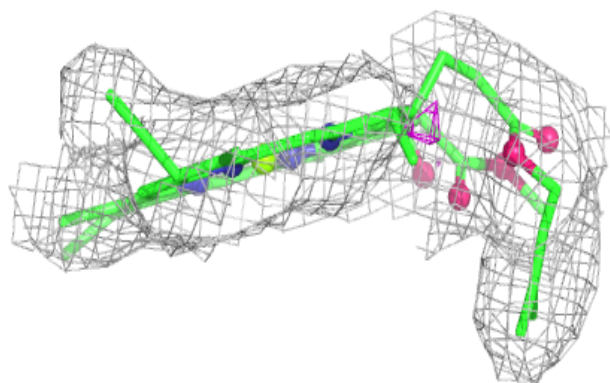
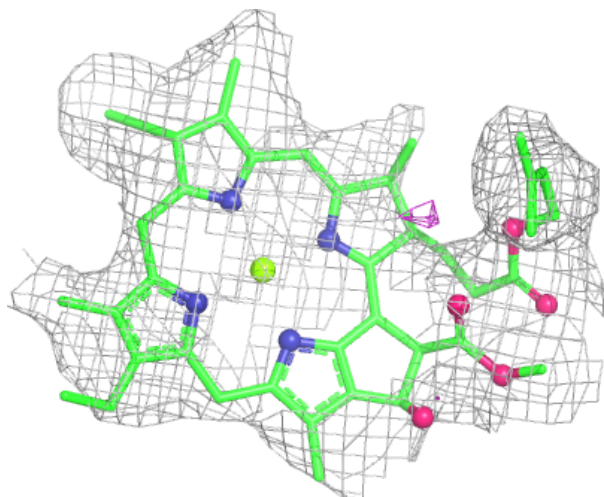
Electron density around BCR G 102:

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



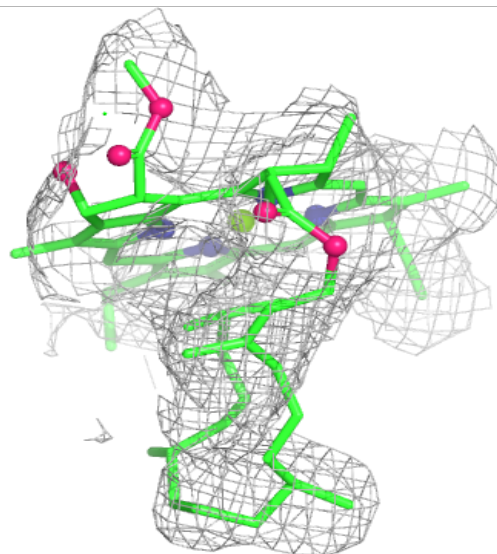
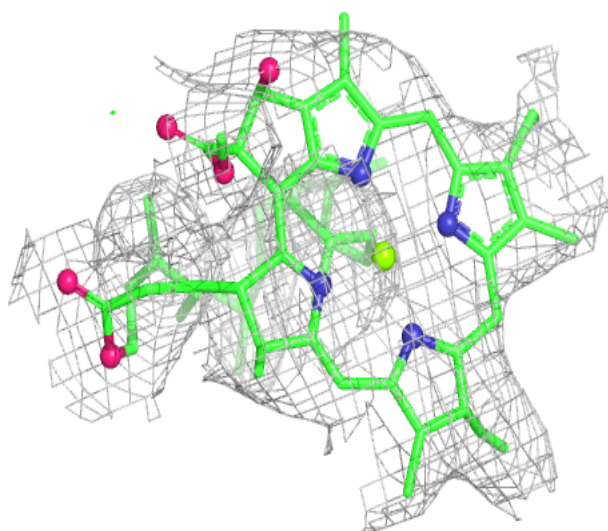
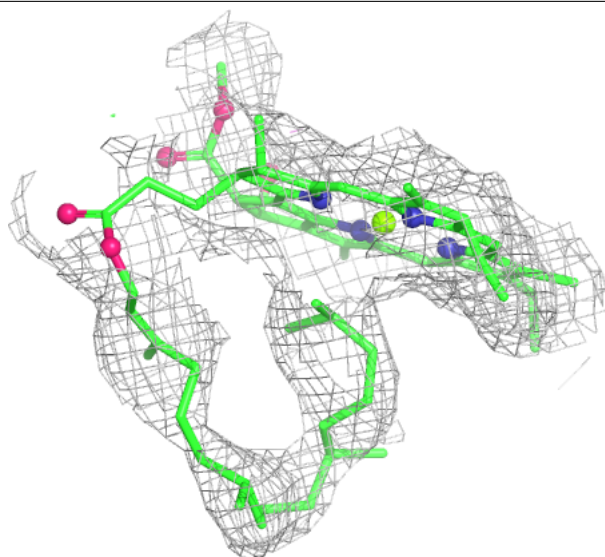
Electron density around CLA 3 315:

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



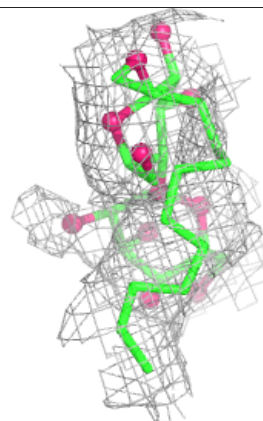
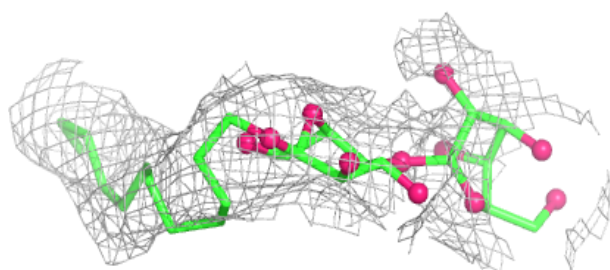
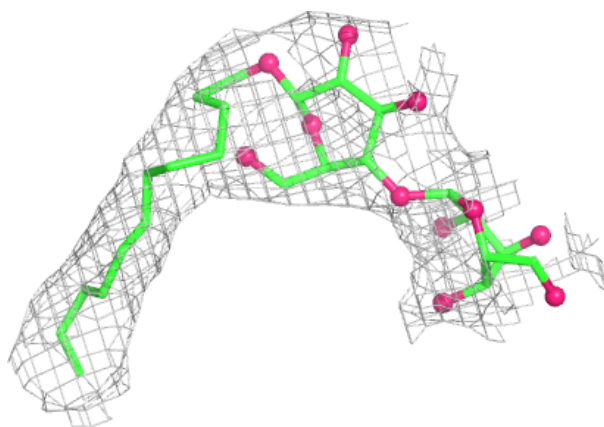
Electron density around CLA 2 312:

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



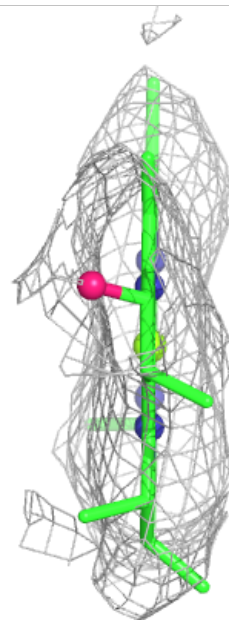
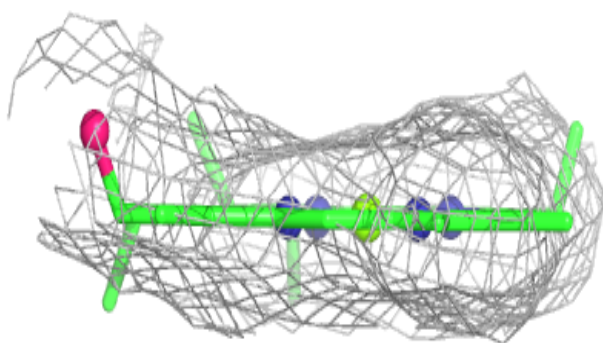
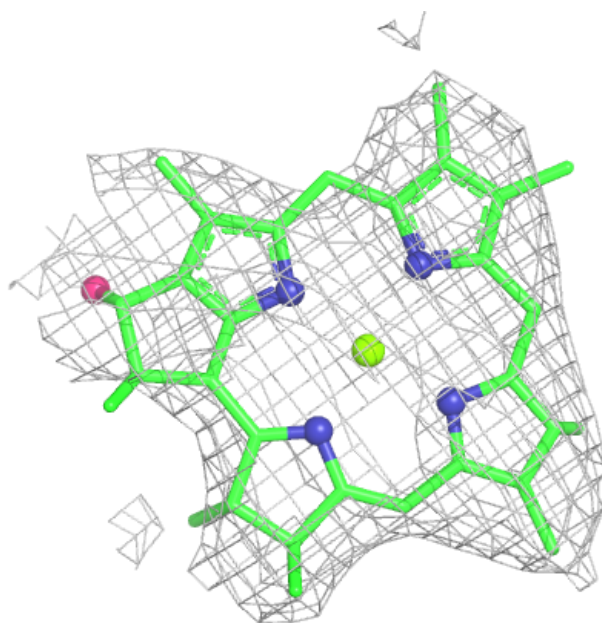
Electron density around LMU R 102:

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



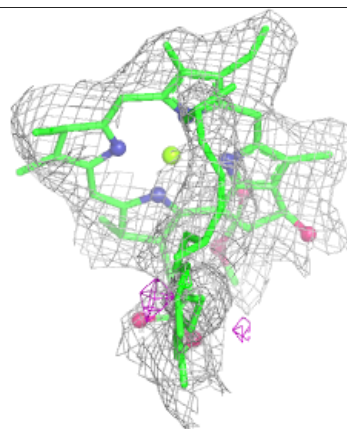
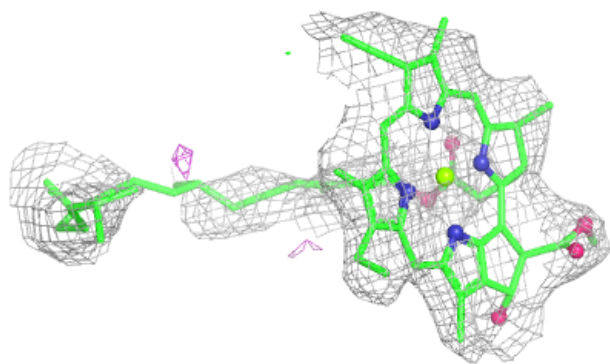
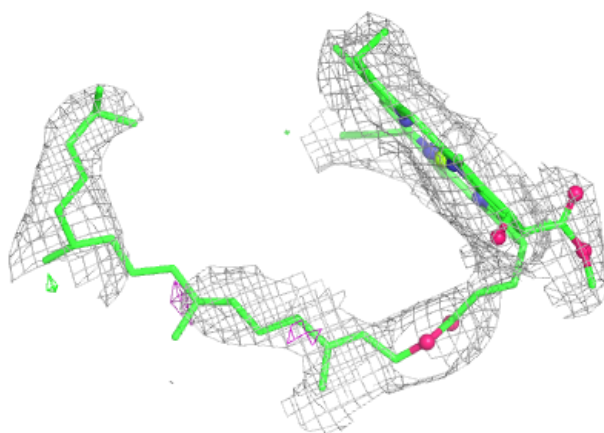
Electron density around CLA 1 209:

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

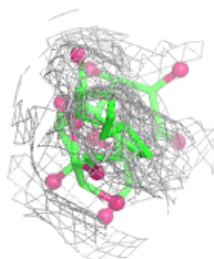
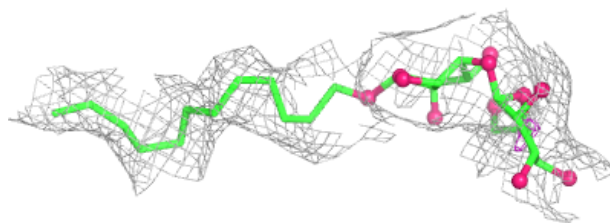
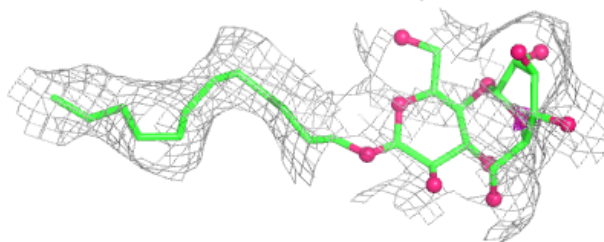


Electron density around CLA L 201:

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

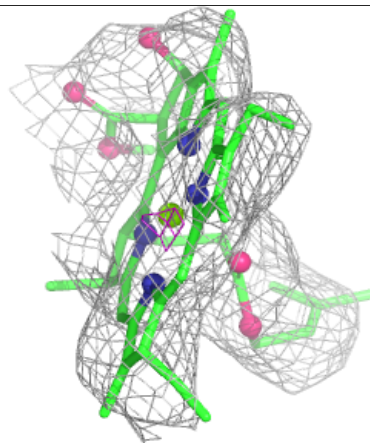
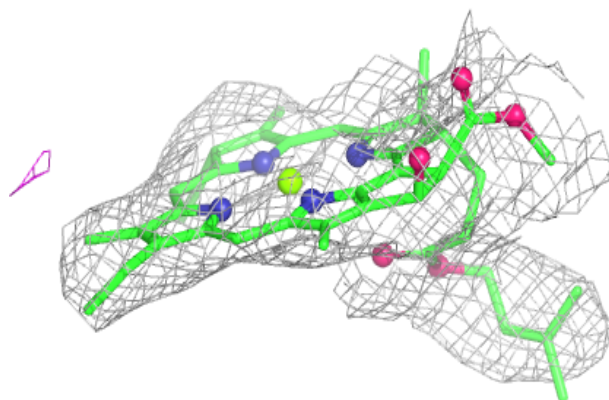
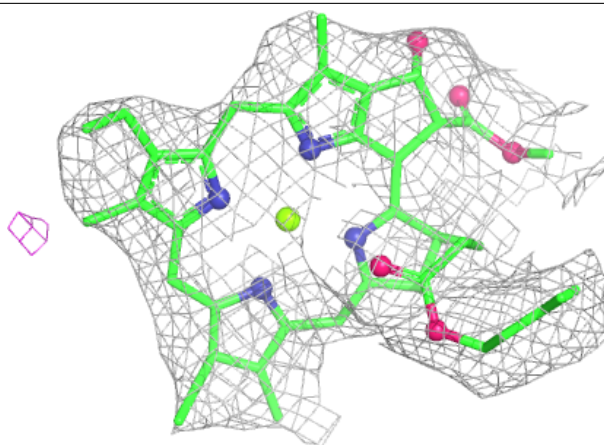
**Electron density around LMU 1 218:**

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

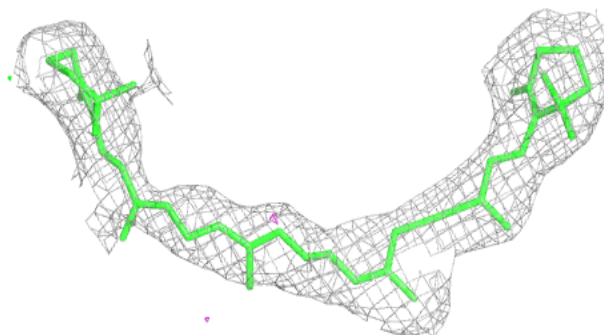


Electron density around CLA A 813:

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

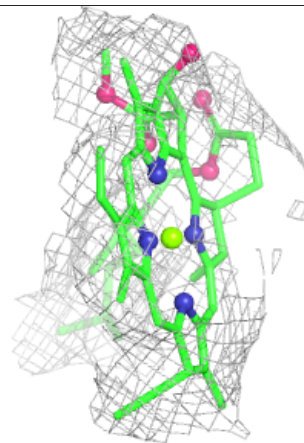
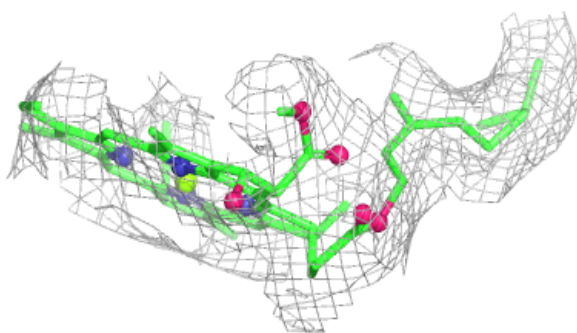
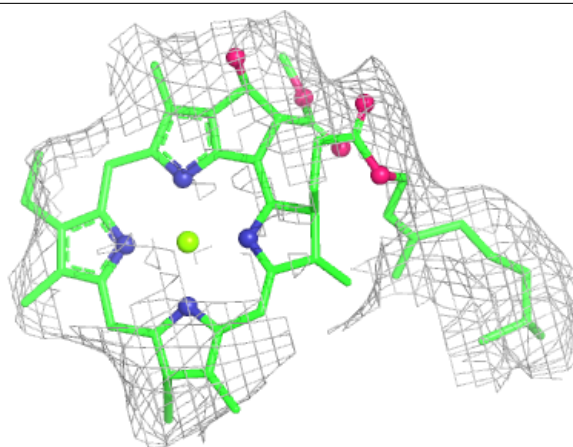
**Electron density around BCR F 203:**

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



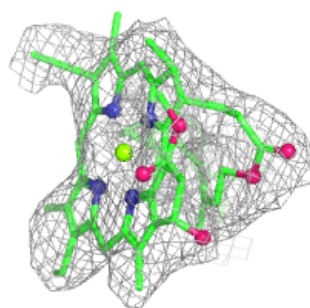
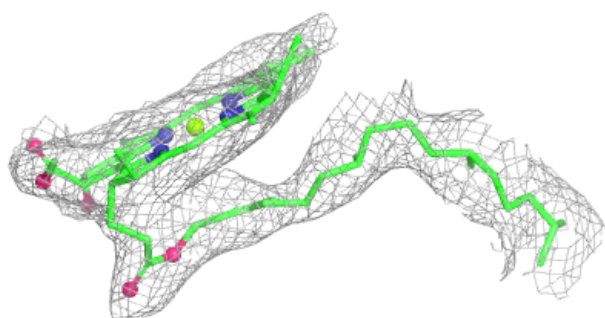
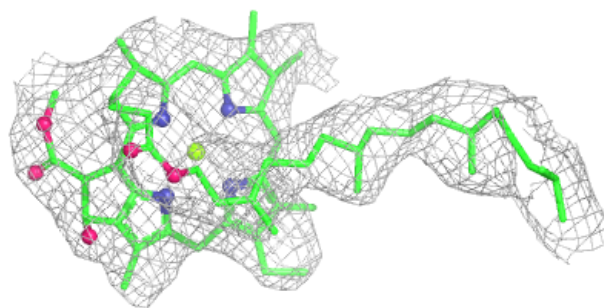
Electron density around CLA J 103:

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



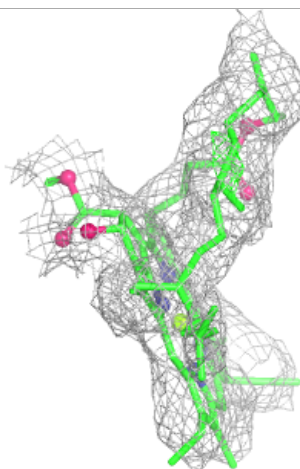
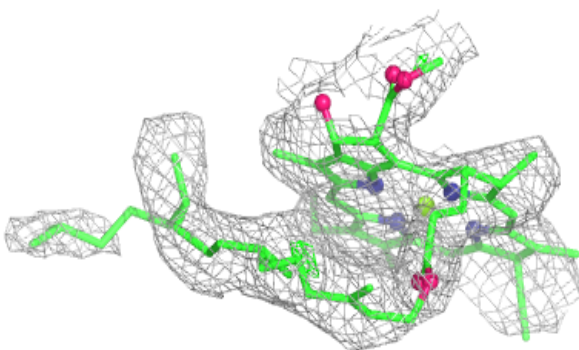
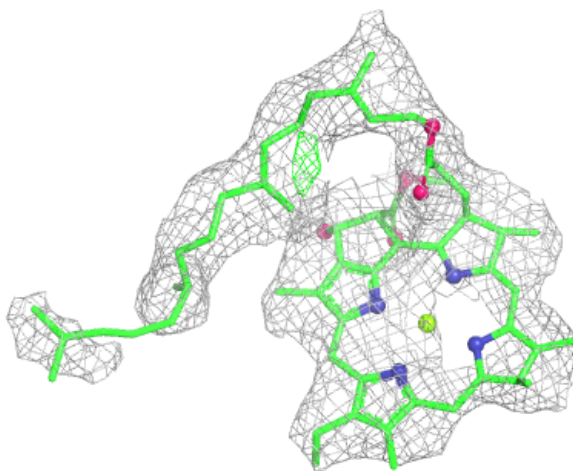
Electron density around CLA A 814:

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



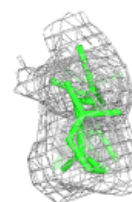
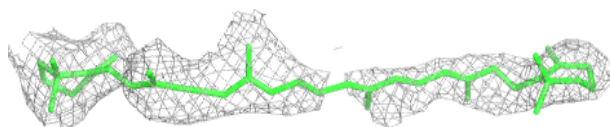
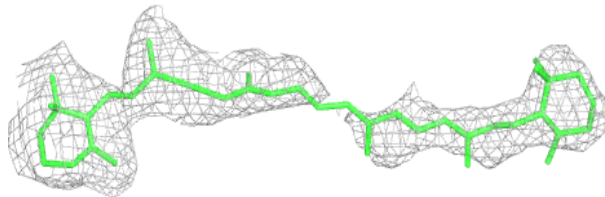
Electron density around CLA B 829:

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

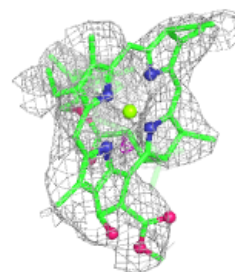
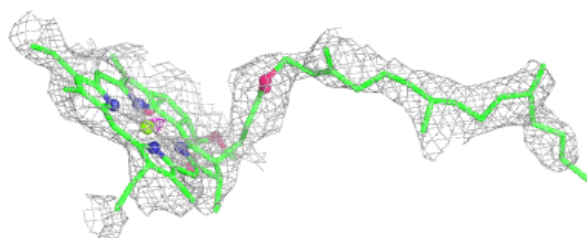
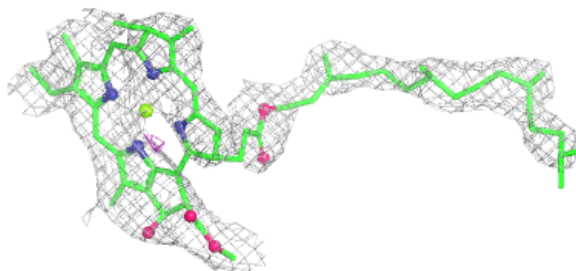


Electron density around BCR L 209:

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

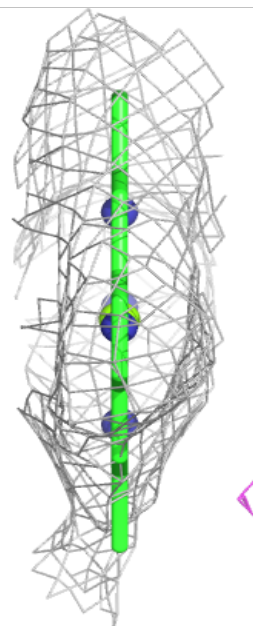
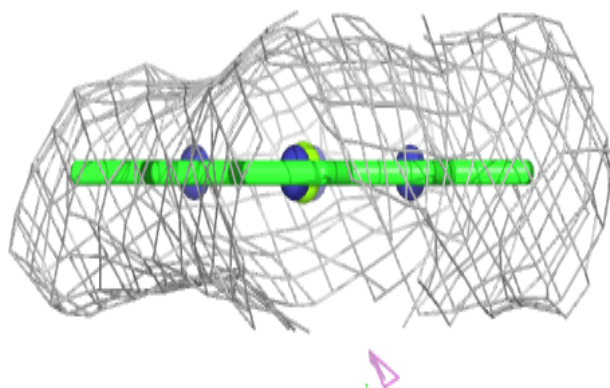
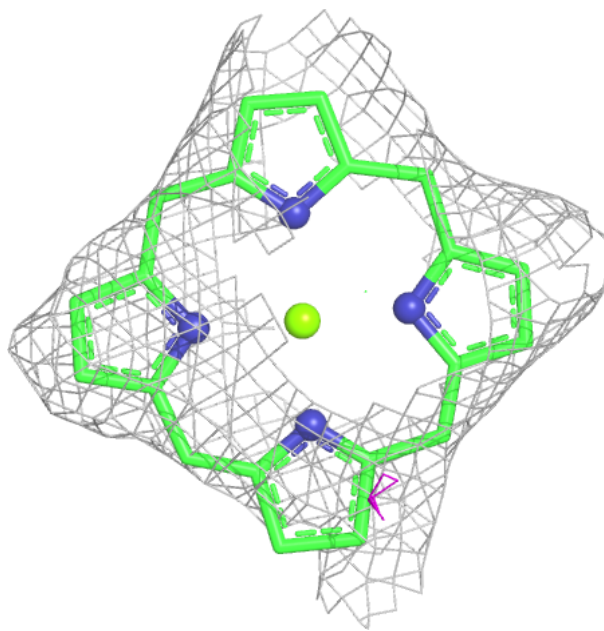
**Electron density around CLA A 817:**

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



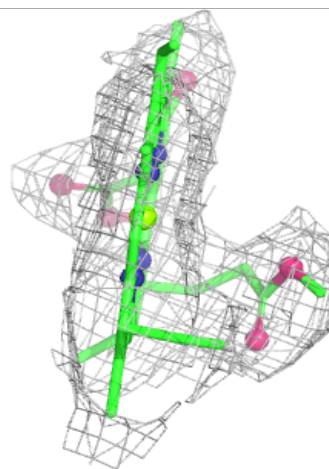
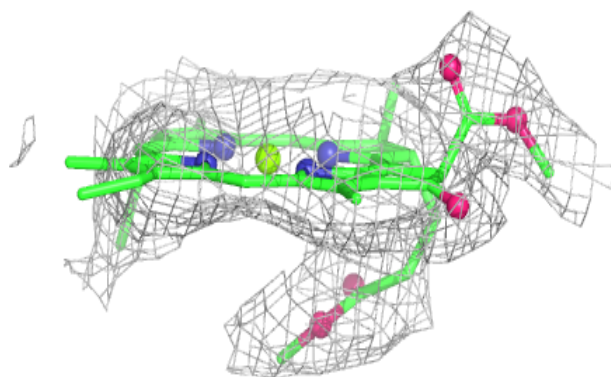
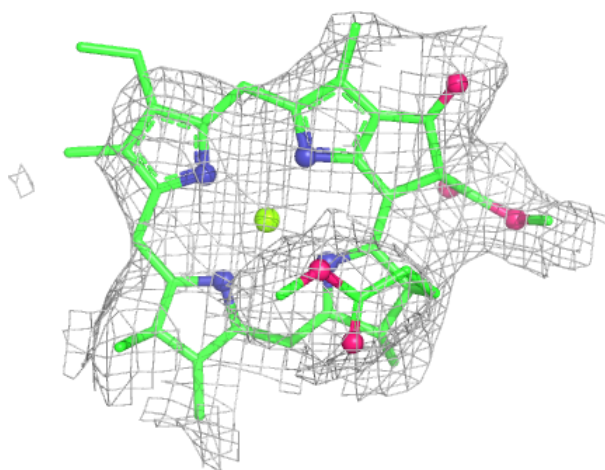
Electron density around CLA 3 317:

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



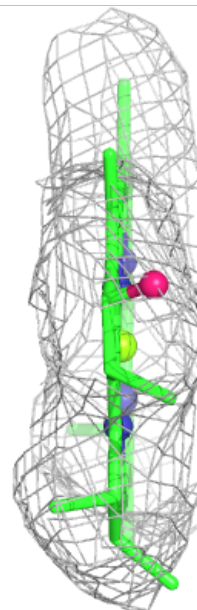
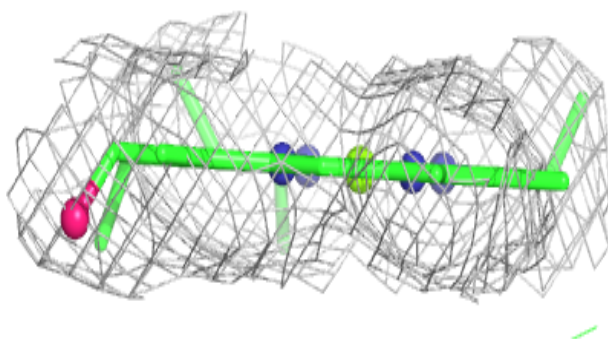
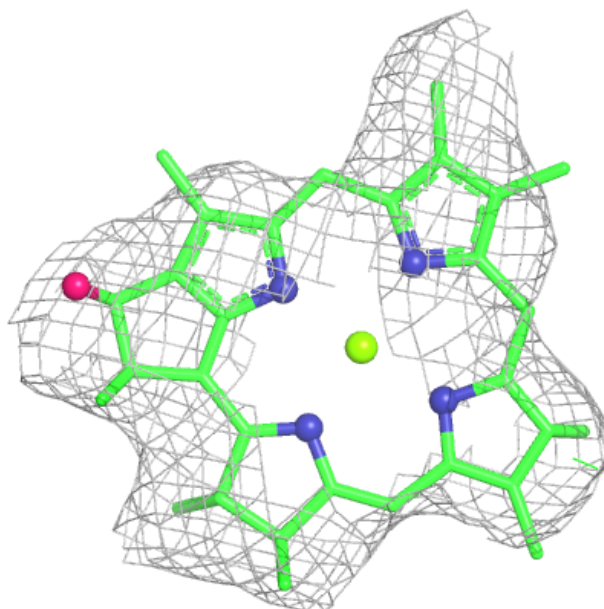
Electron density around CLA 1 204:

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



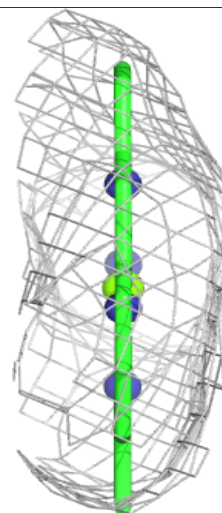
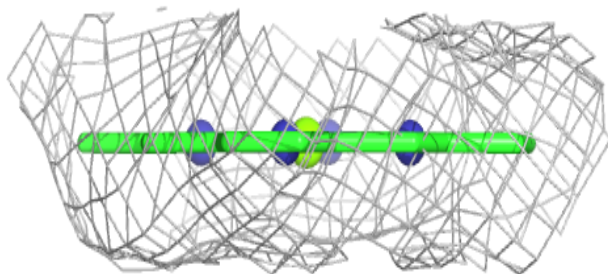
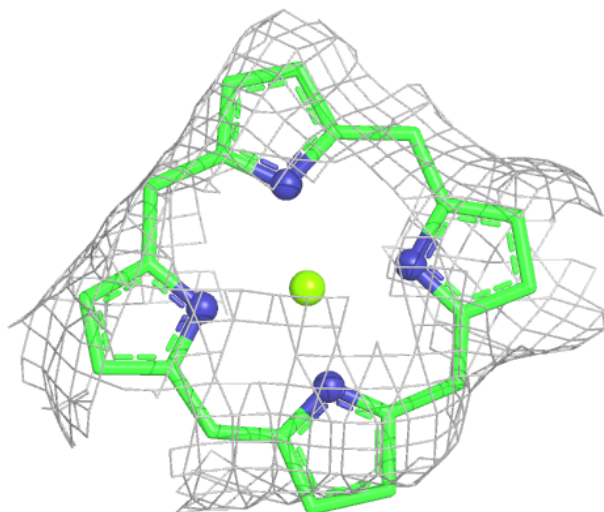
Electron density around CLA 1 210:

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



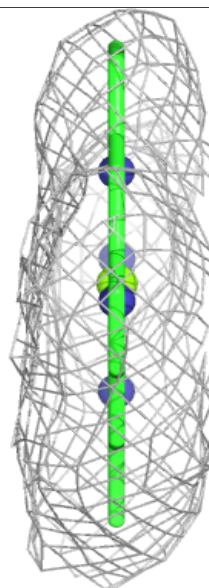
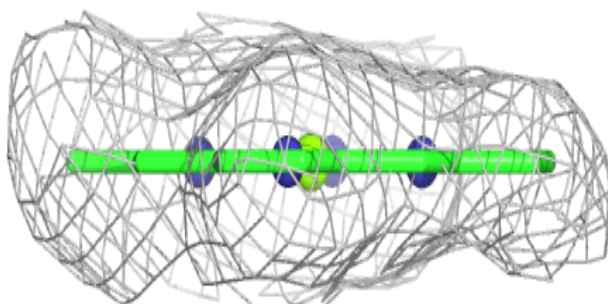
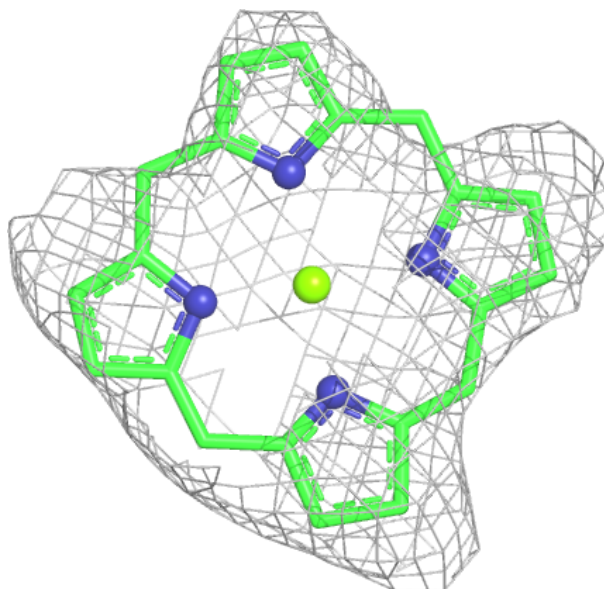
Electron density around CLA 1 215:

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



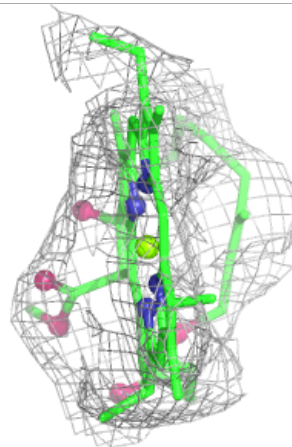
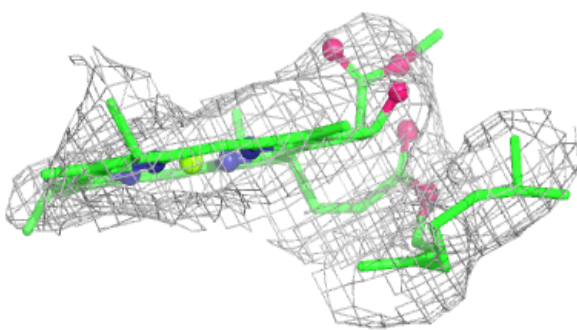
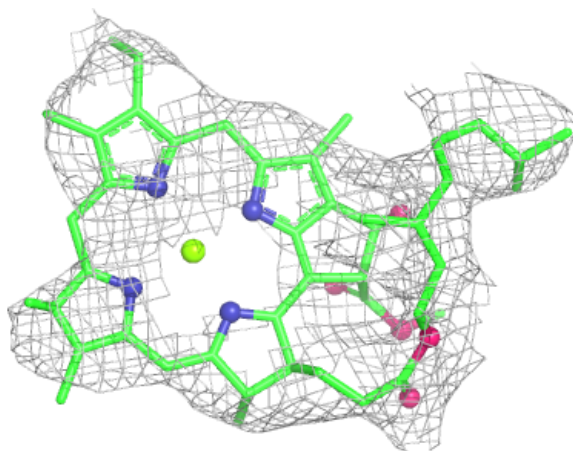
Electron density around CLA 2 315:

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



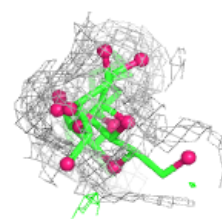
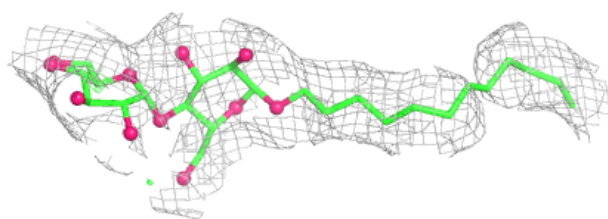
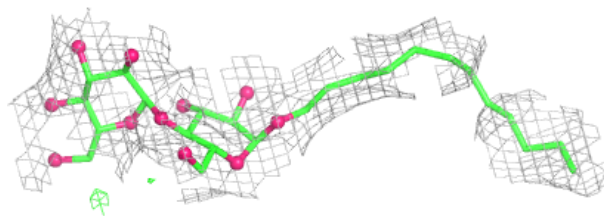
Electron density around CLA B 808:

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



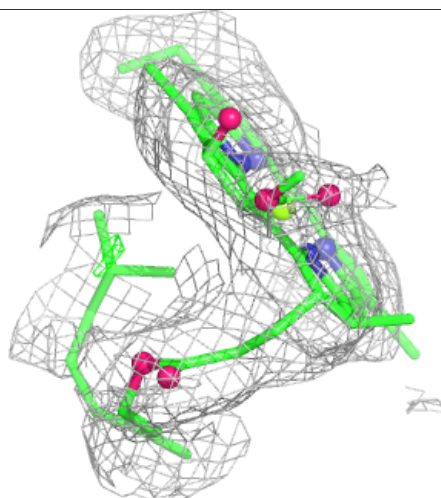
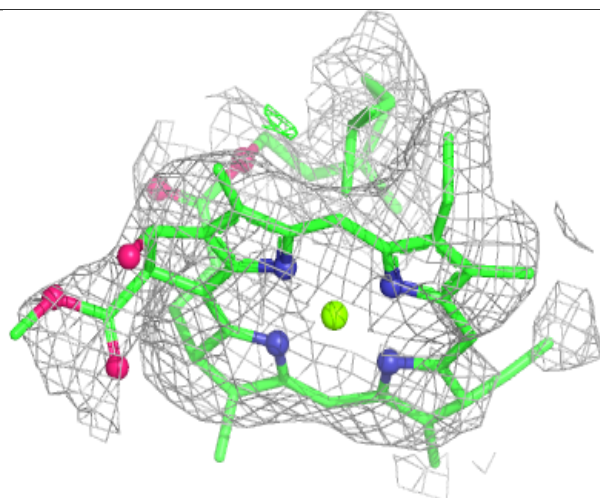
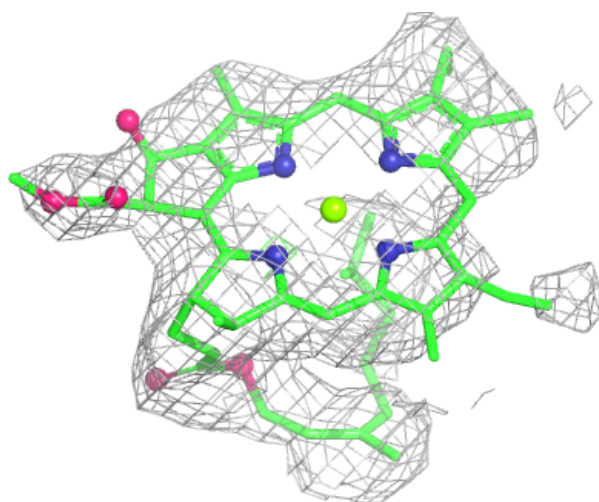
Electron density around LMU B 802:

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



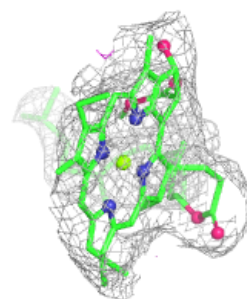
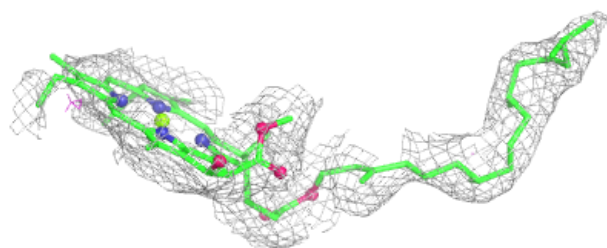
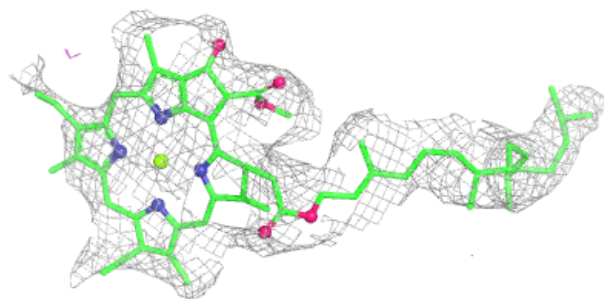
Electron density around CLA B 809:

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

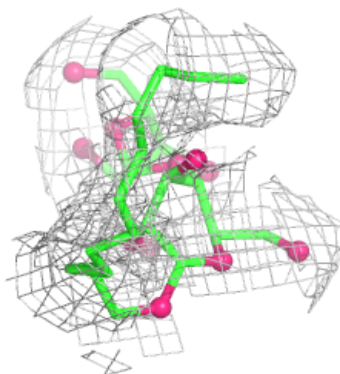
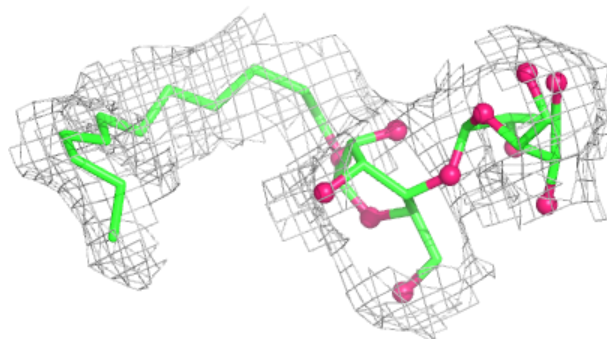
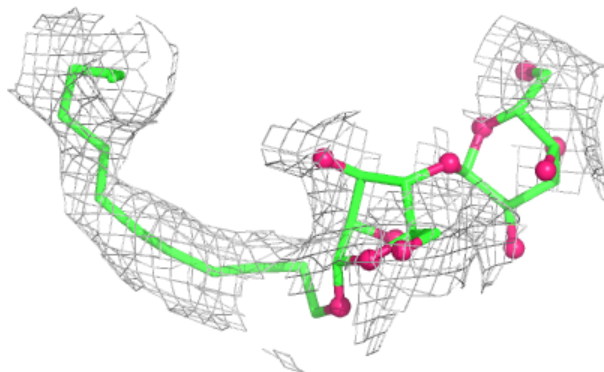


Electron density around CLA 2 317:

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

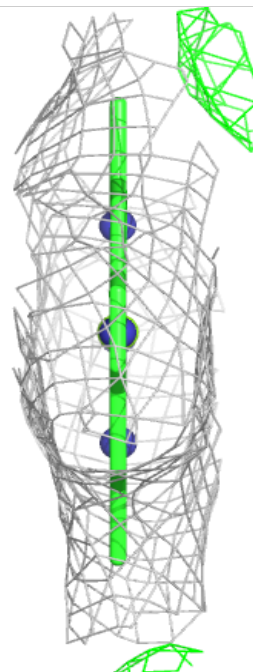
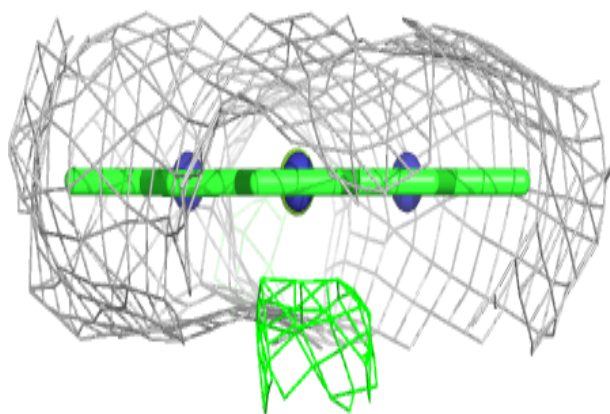
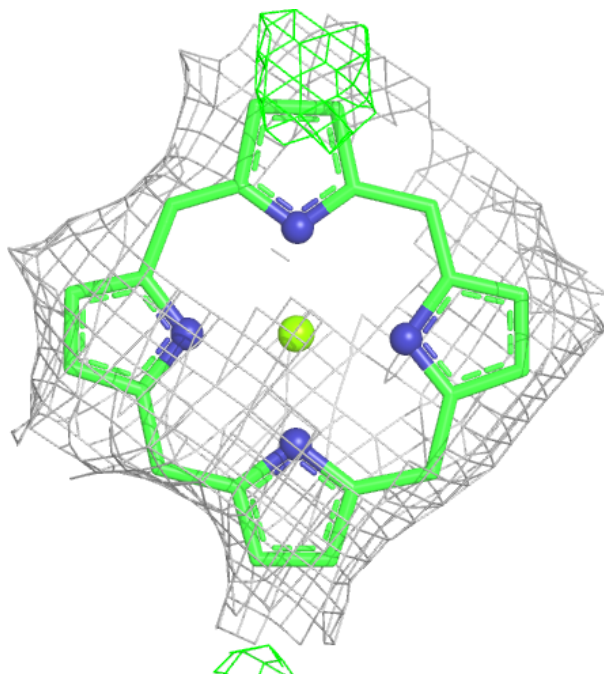
**Electron density around LMU R 103:**

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



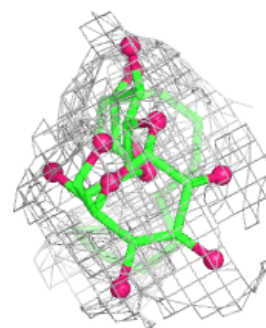
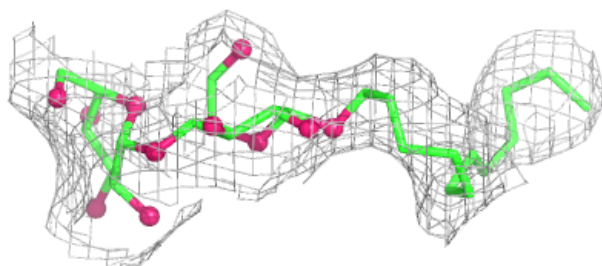
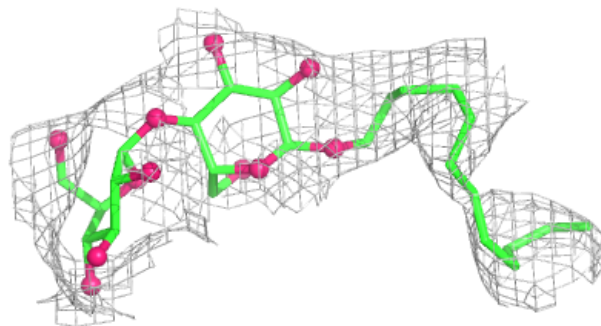
Electron density around CLA 3 307:

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



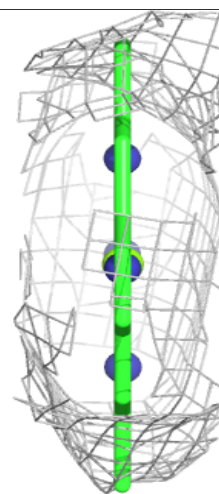
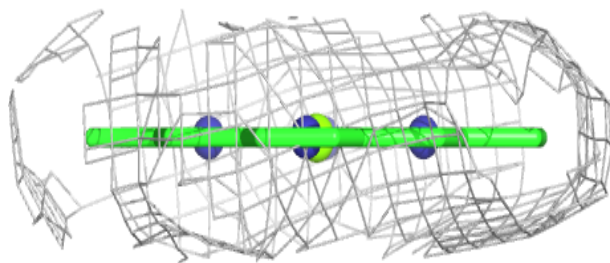
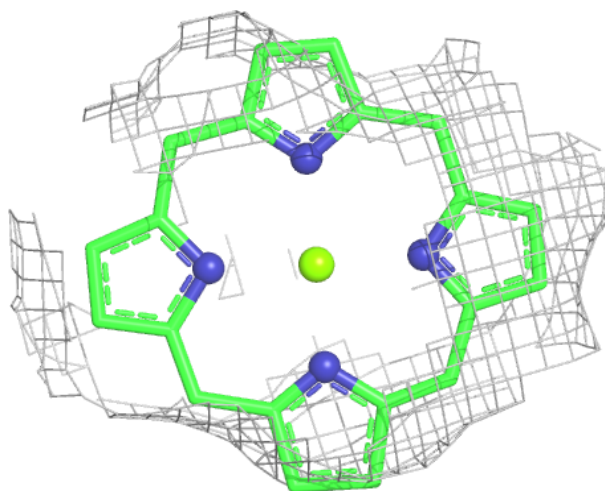
Electron density around LMU R 108:

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



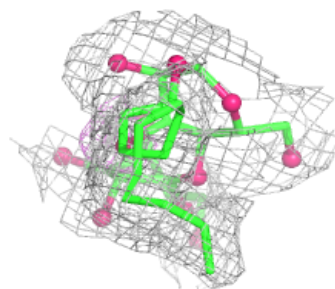
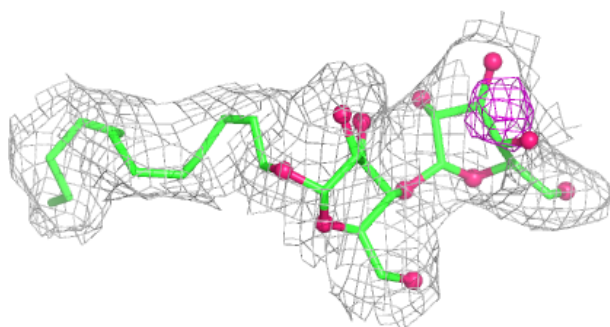
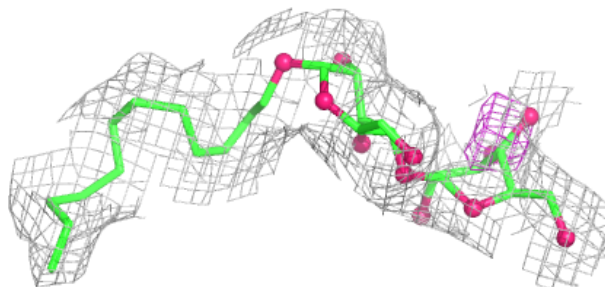
Electron density around CLA 2 308:

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

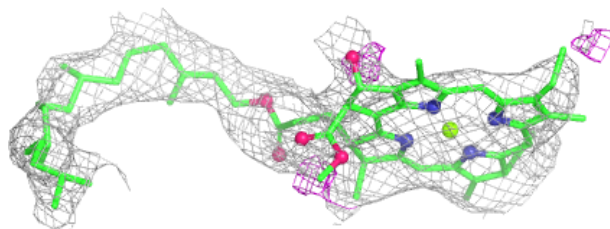
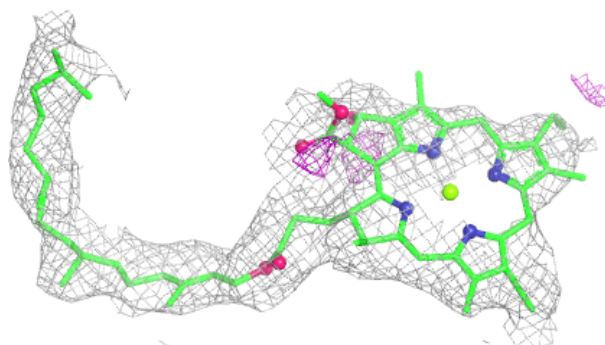


Electron density around LMU H 102:

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

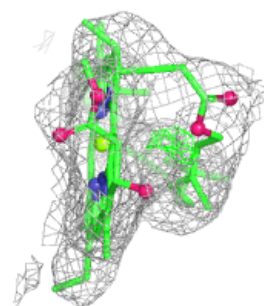
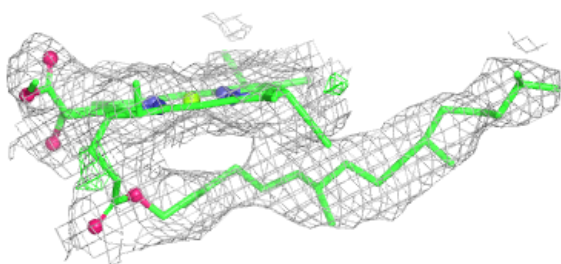
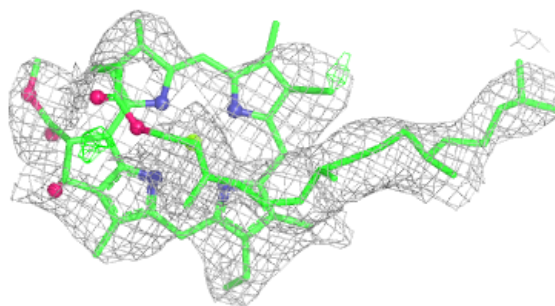
**Electron density around CLA B 823:**

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

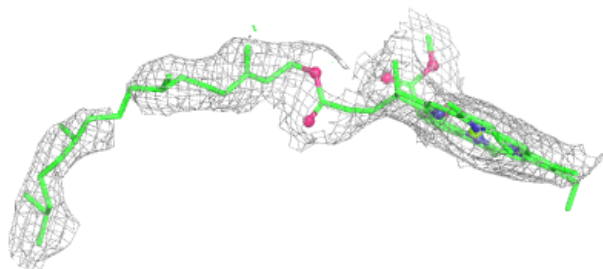
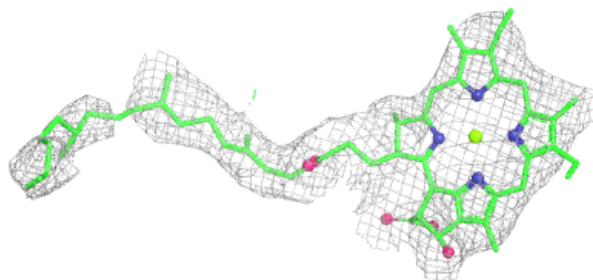


Electron density around CLA A 855:

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

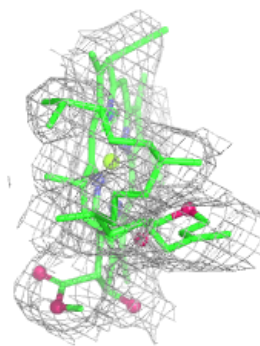
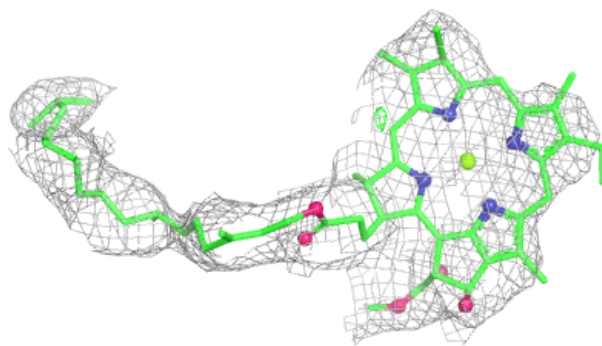
**Electron density around CLA A 803:**

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

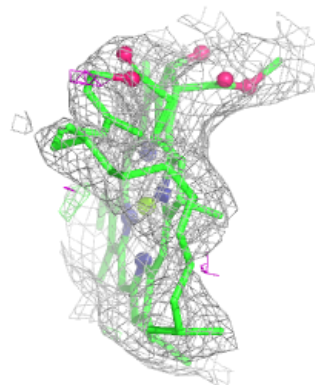
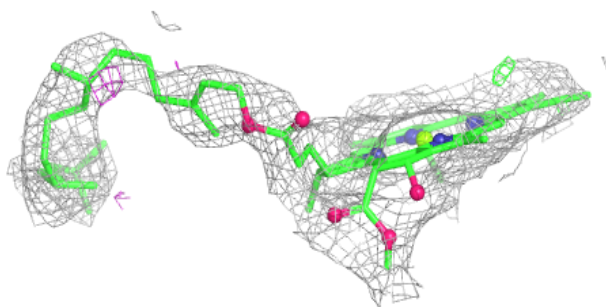
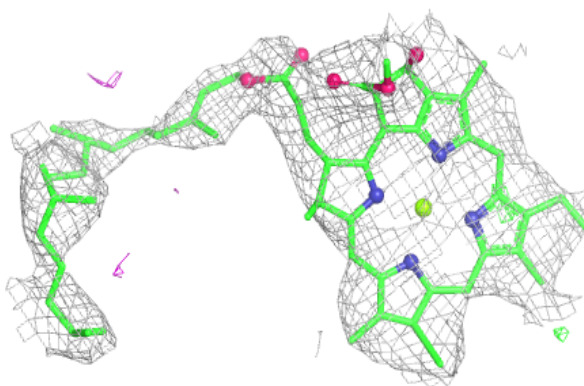


Electron density around CLA A 822:

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

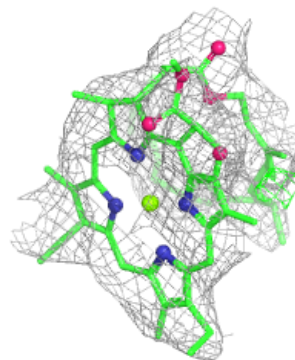
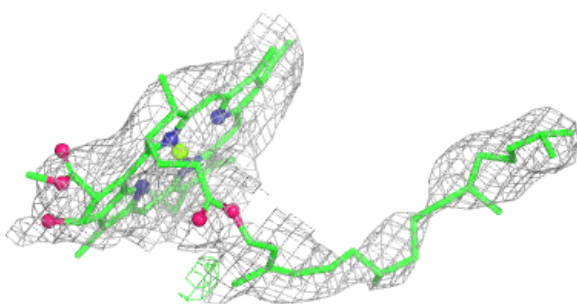
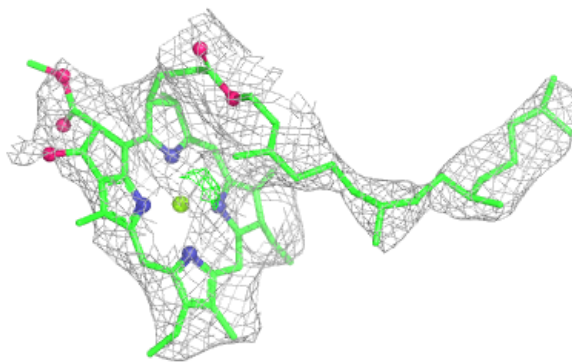
**Electron density around CLA A 823:**

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



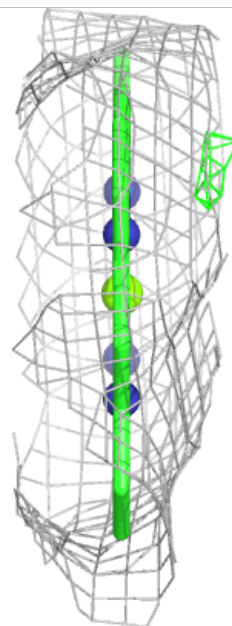
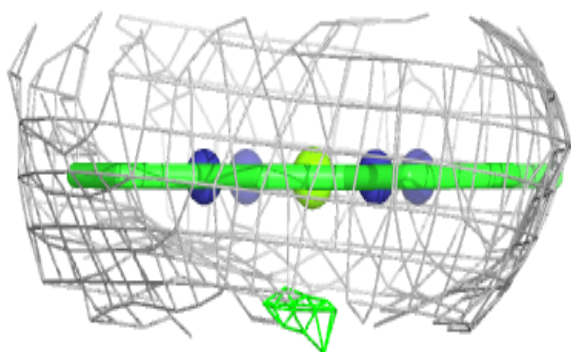
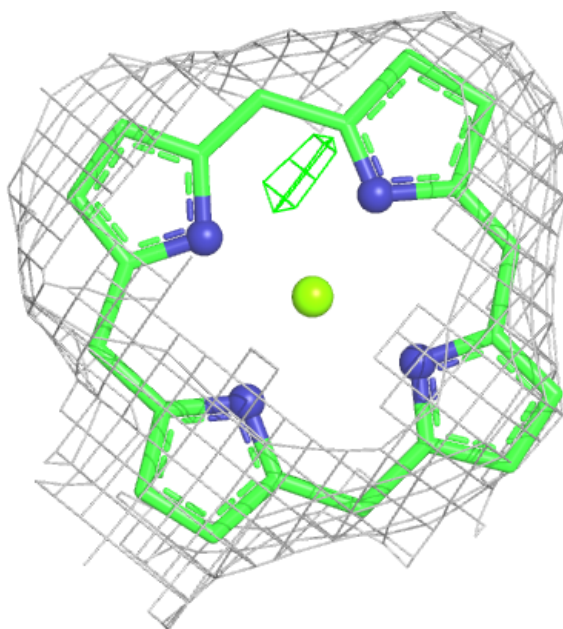
Electron density around CLA B 811:

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



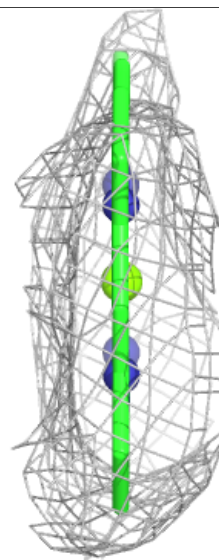
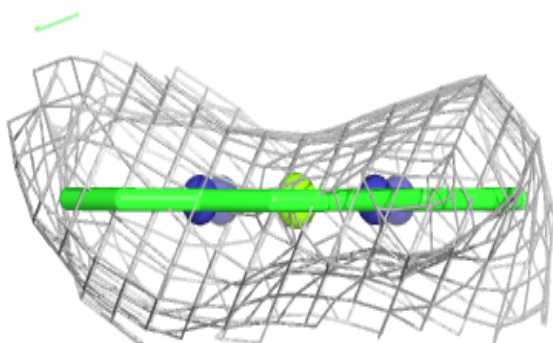
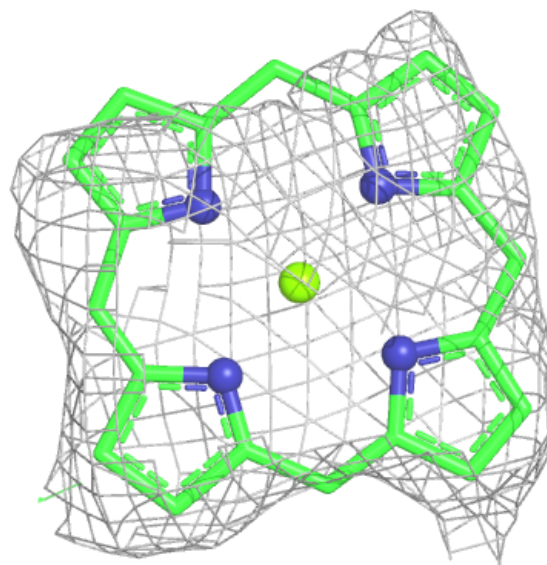
Electron density around CLA 4 311:

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



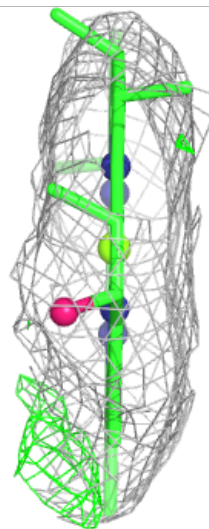
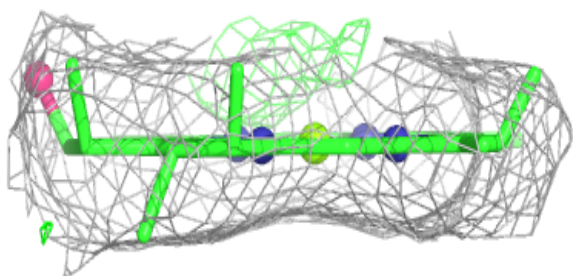
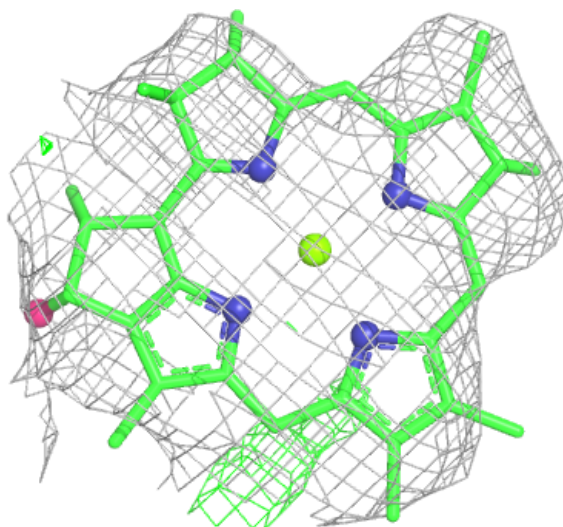
Electron density around CLA 2 309:

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



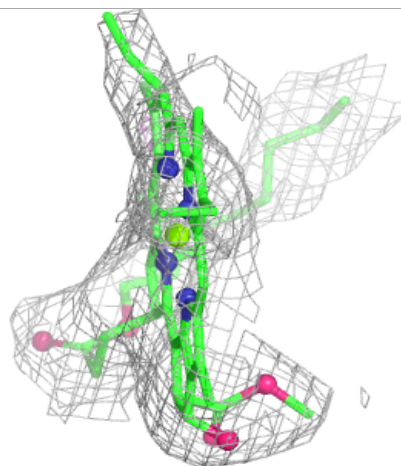
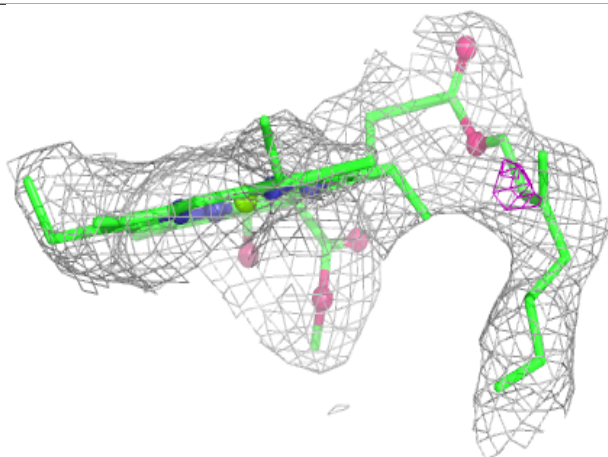
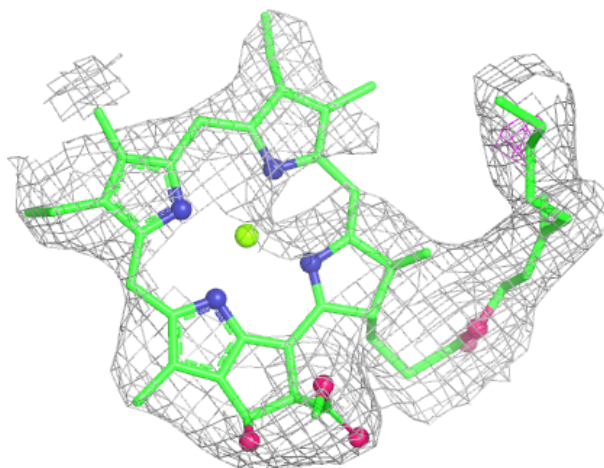
Electron density around CLA 4 303:

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



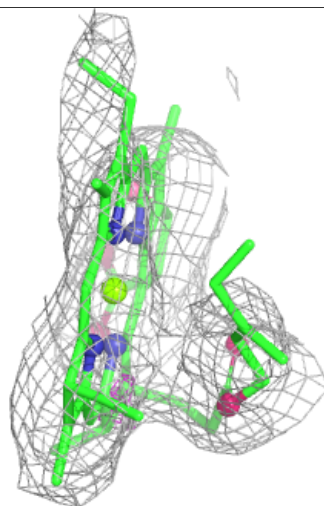
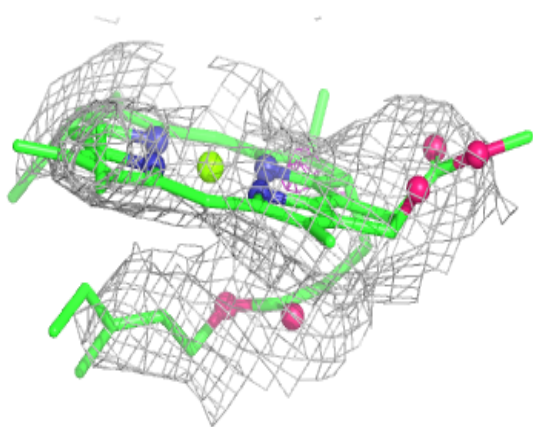
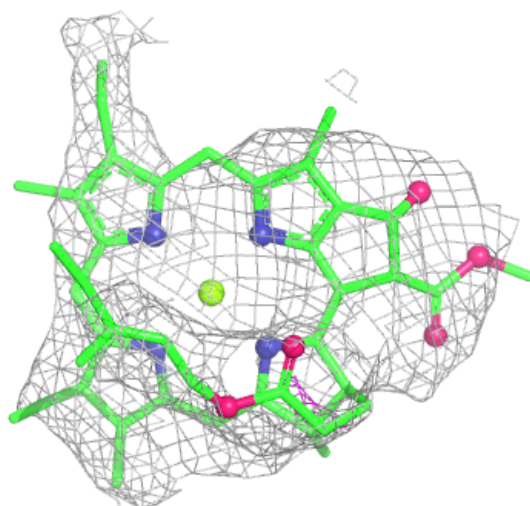
Electron density around CLA A 811:

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



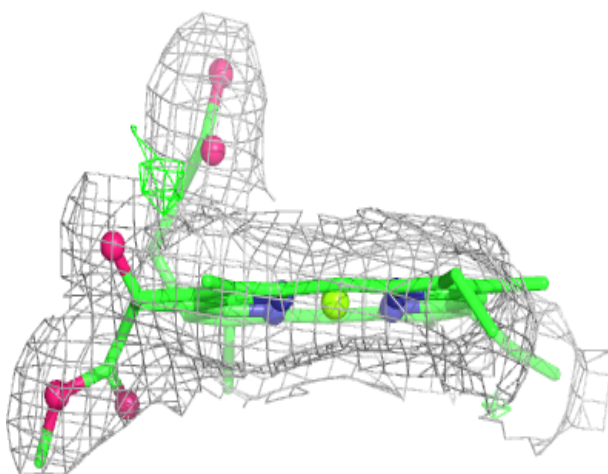
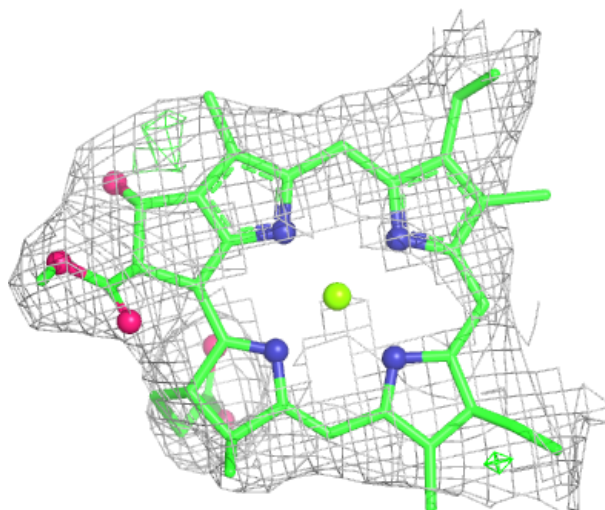
Electron density around CLA A 818:

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



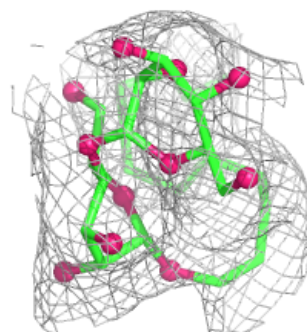
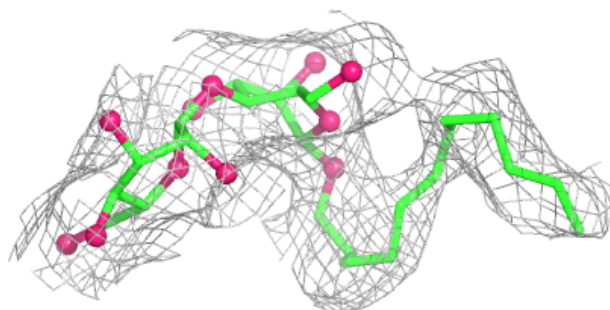
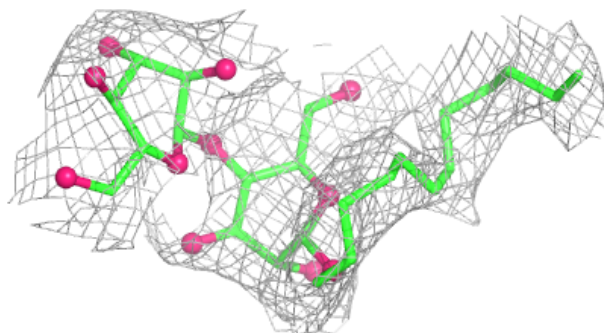
Electron density around CLA B 803:

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

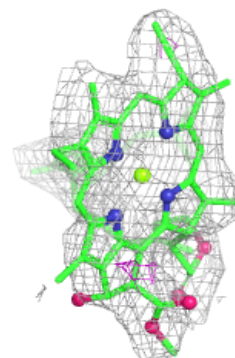
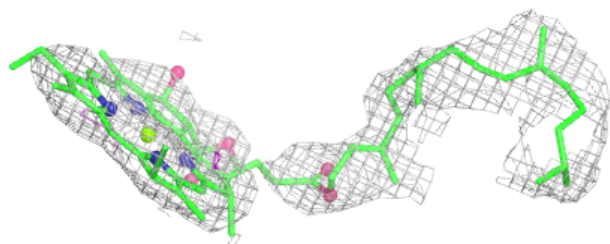
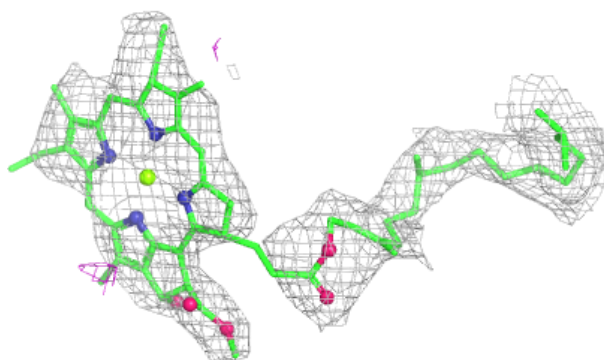


Electron density around LMU L 210:

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

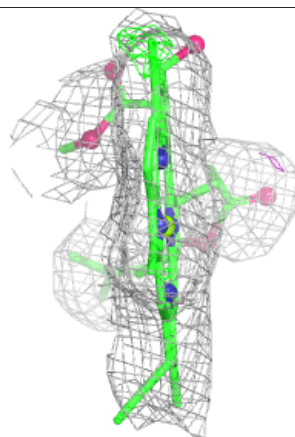
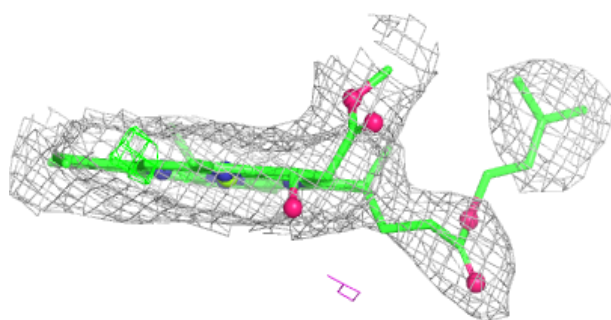
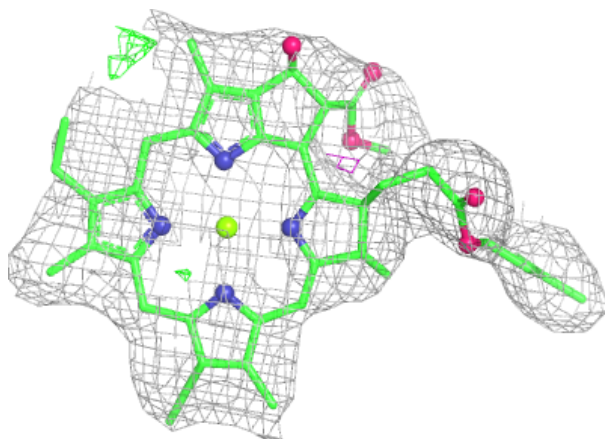
**Electron density around CLA B 807:**

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

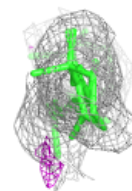
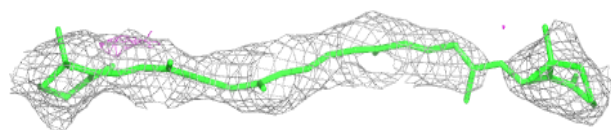
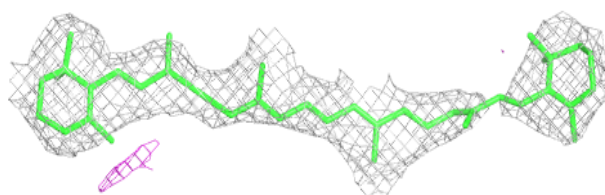


Electron density around CLA B 828:

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

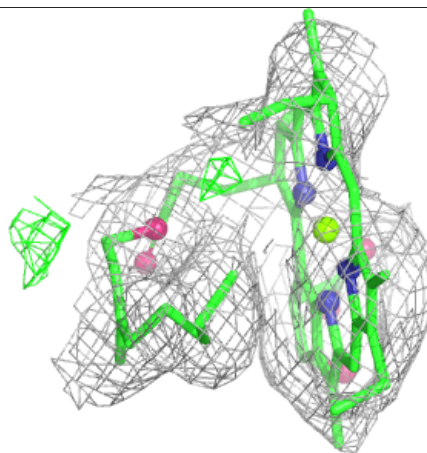
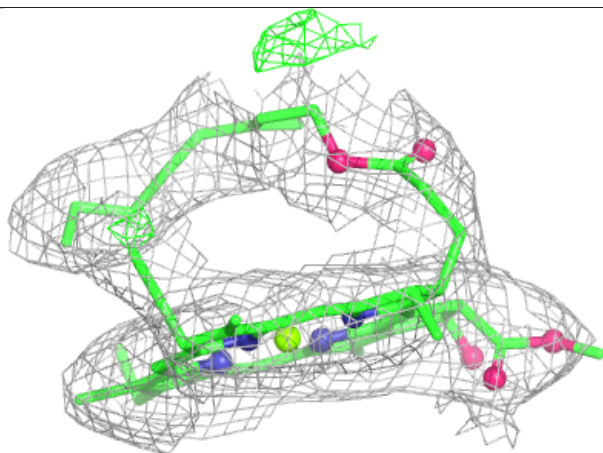
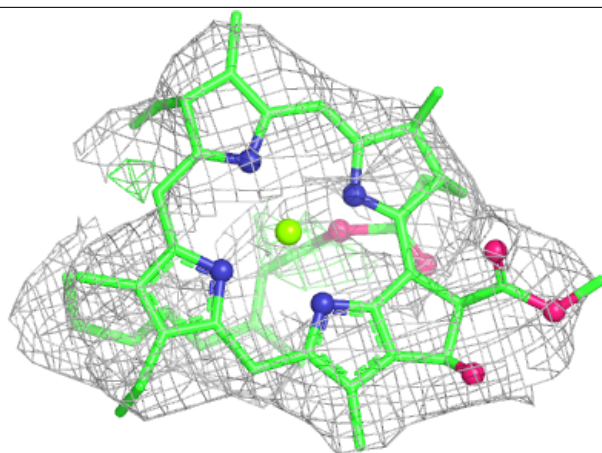
**Electron density around BCR B 843:**

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

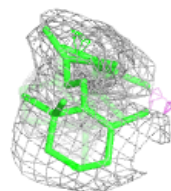
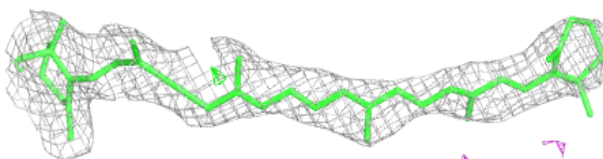
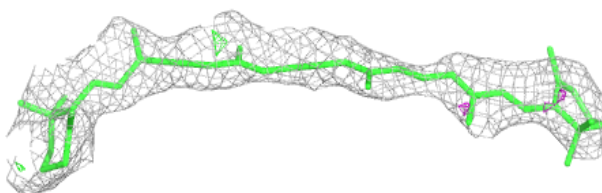


Electron density around CLA A 810:

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

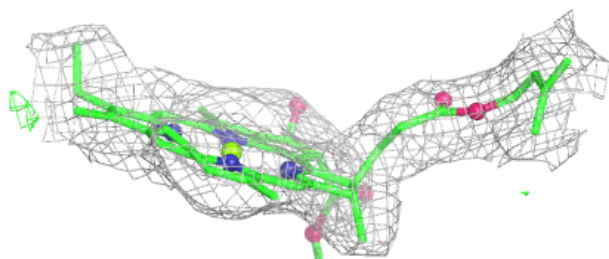
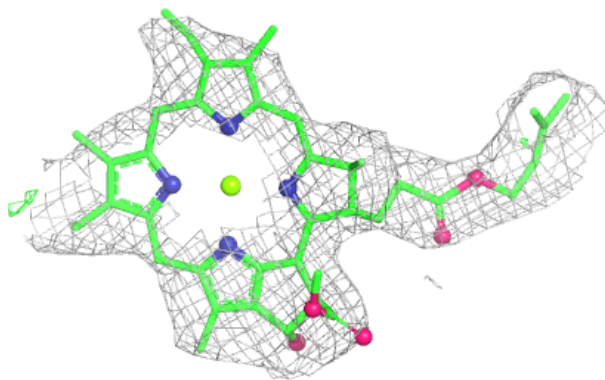
**Electron density around BCR F 202:**

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



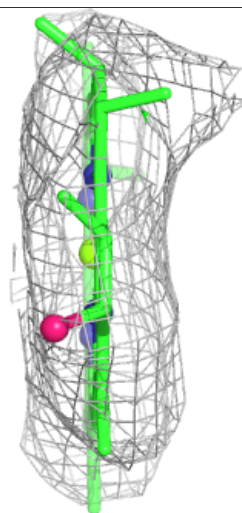
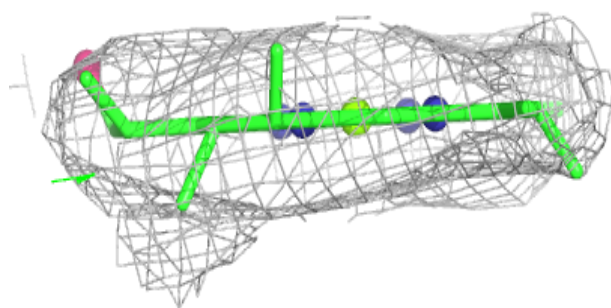
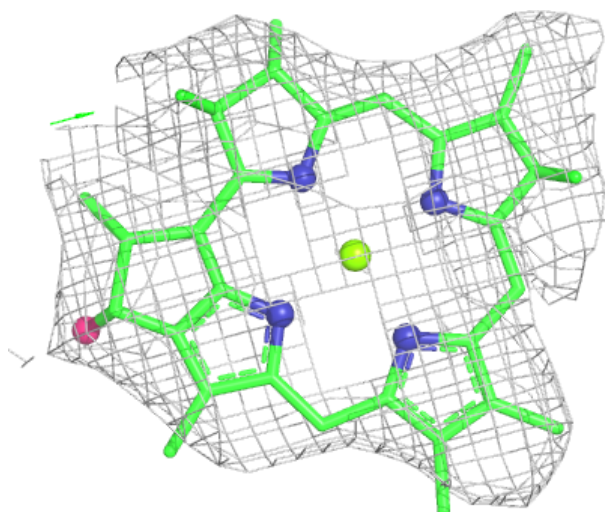
Electron density around CLA B 830:

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



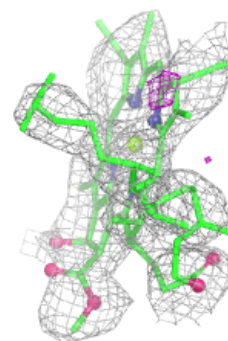
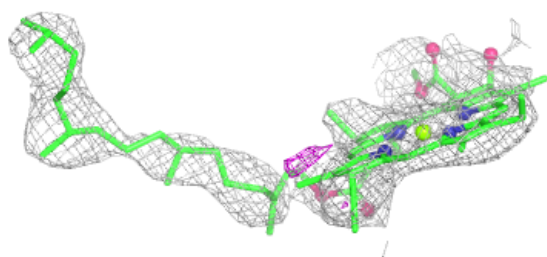
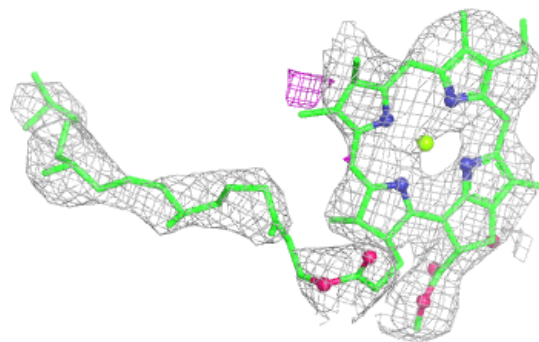
Electron density around CLA 4 313:

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

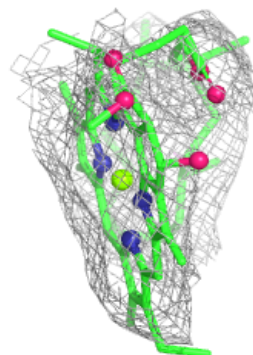
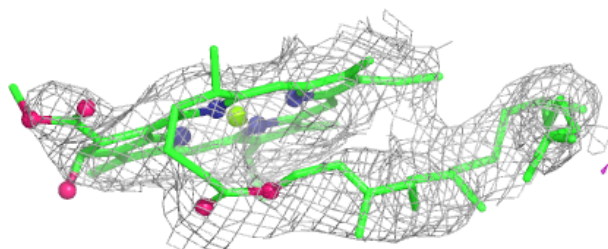
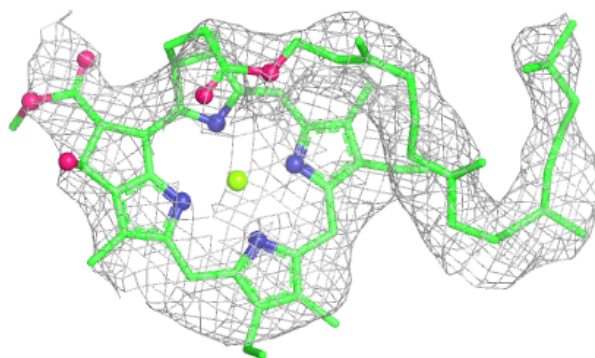


Electron density around CLA A 849:

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

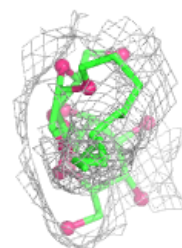
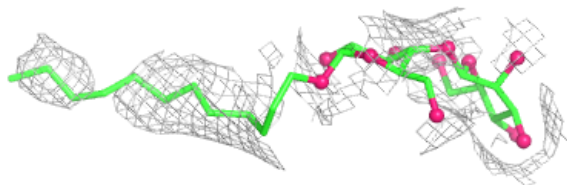
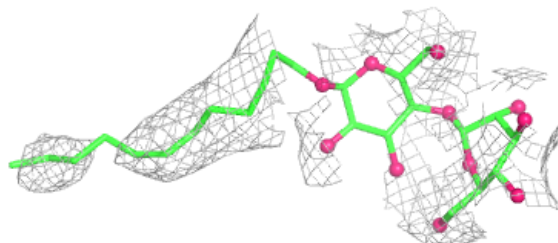
**Electron density around CLA A 816:**

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



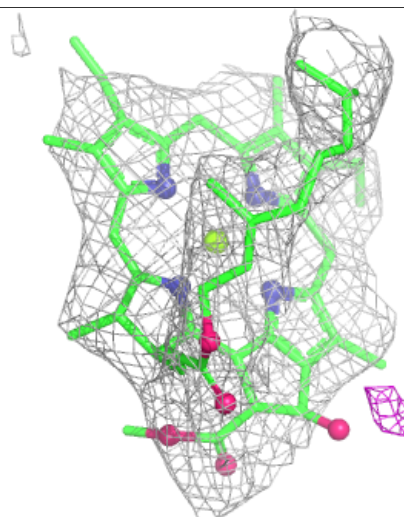
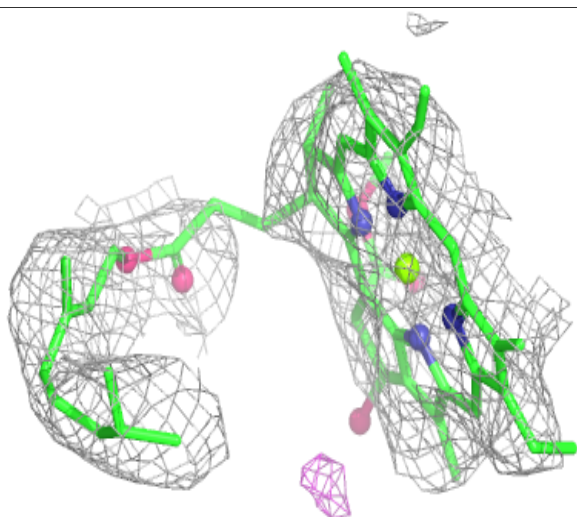
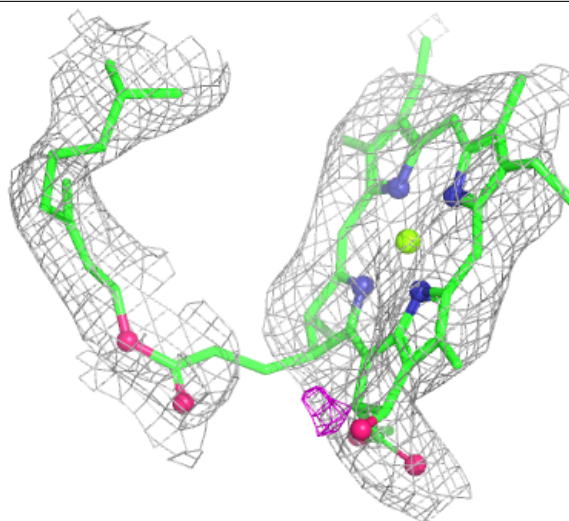
Electron density around LMU A 854:

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



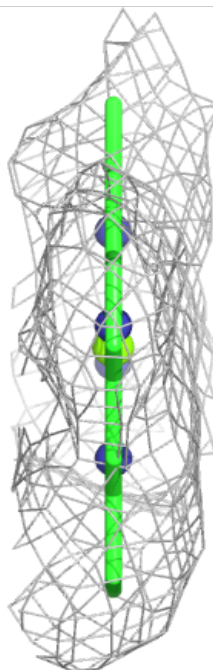
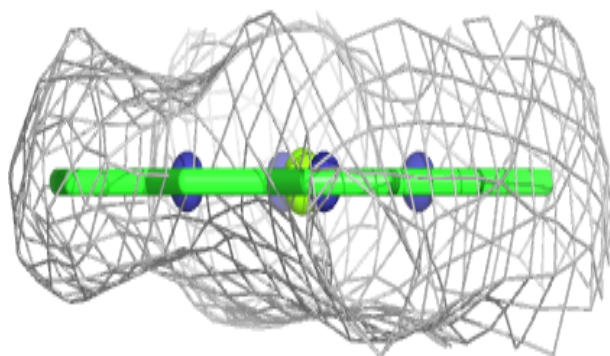
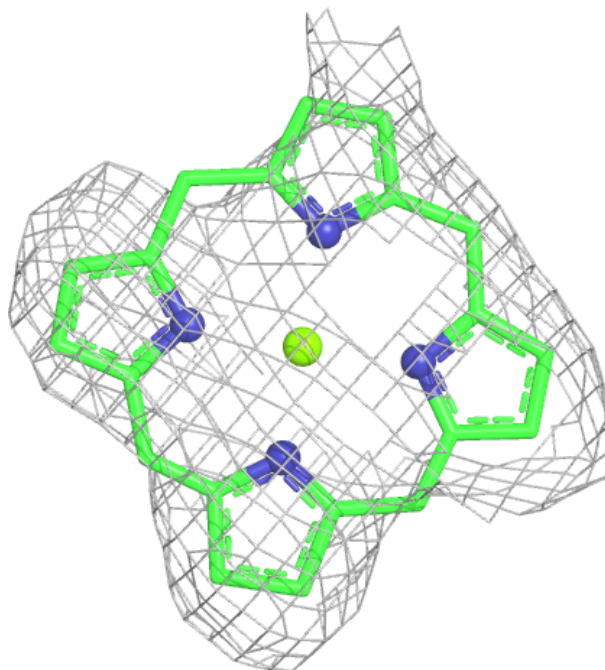
Electron density around CLA A 802:

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



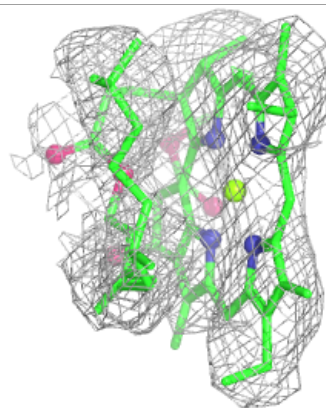
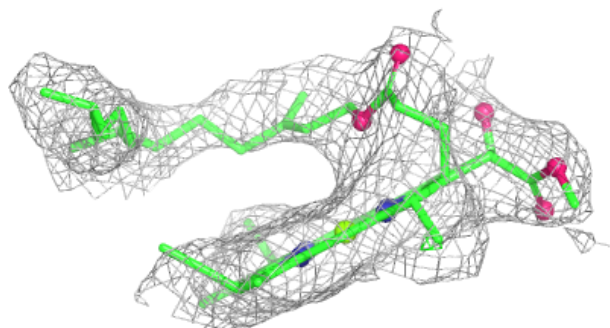
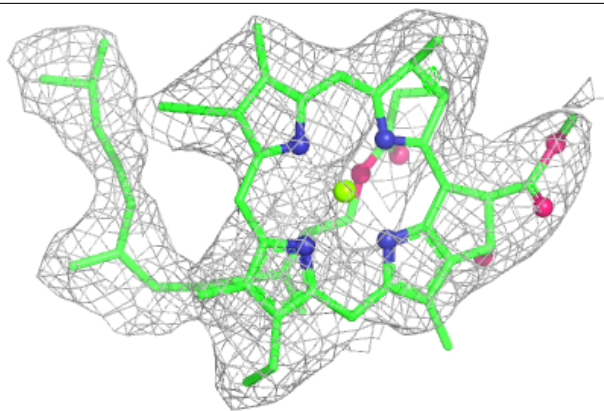
Electron density around CLA 2 303:

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

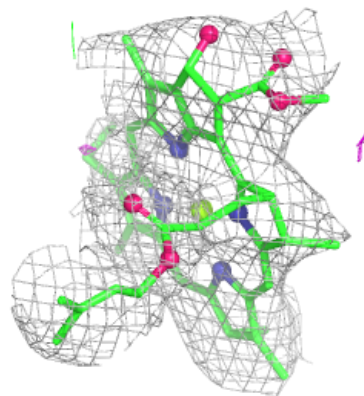
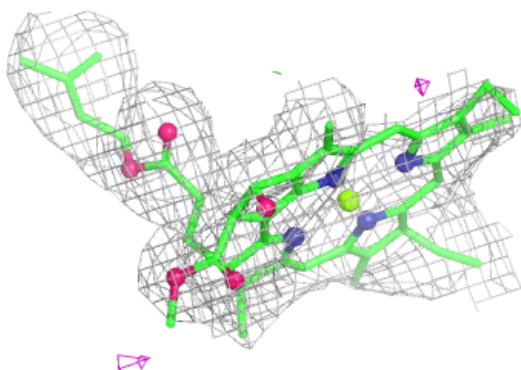
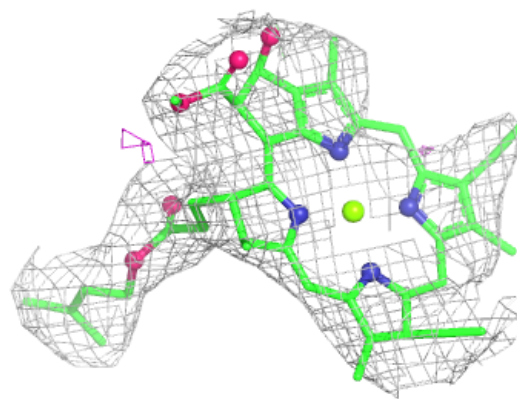


Electron density around CLA I 102:

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

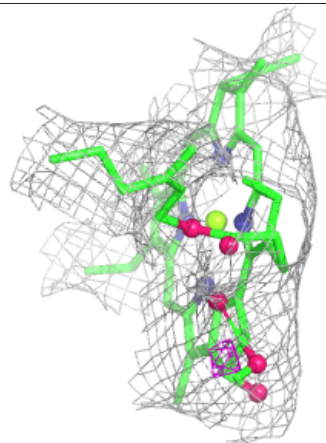
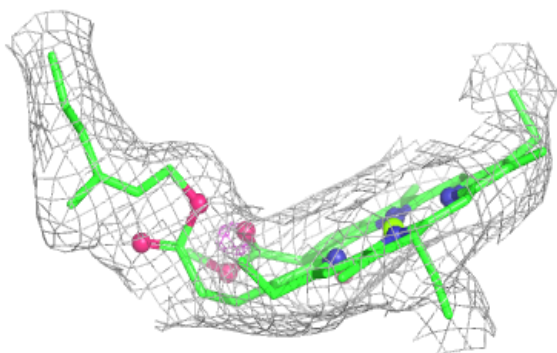
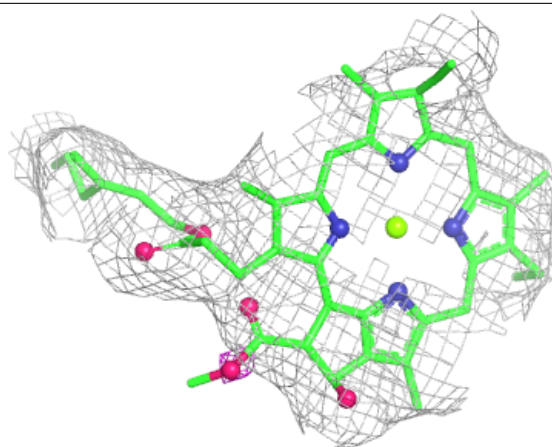
**Electron density around CLA 2 310:**

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



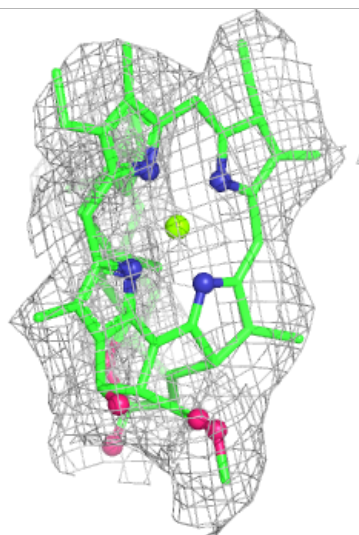
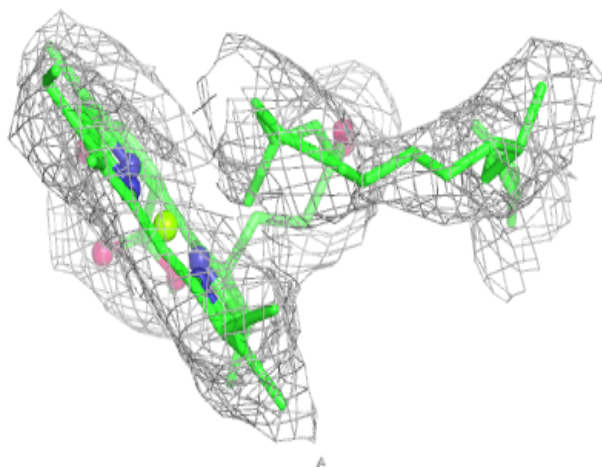
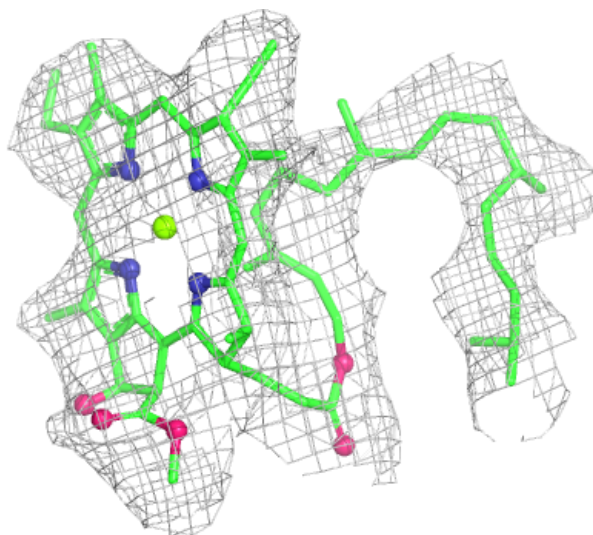
Electron density around CLA 4 307:

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



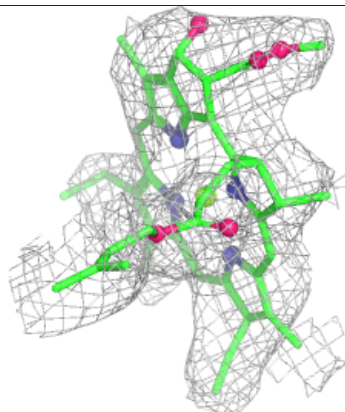
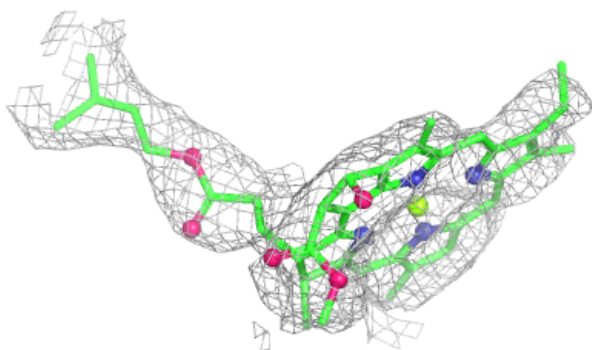
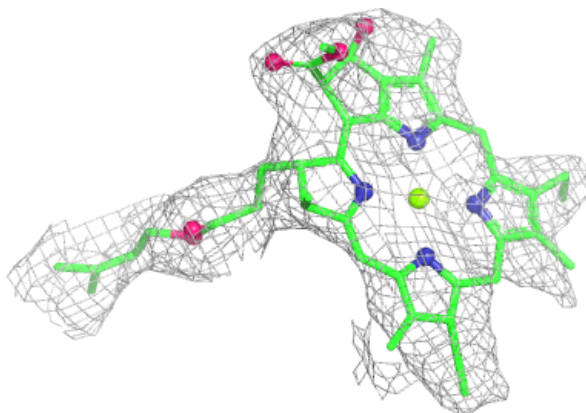
Electron density around CLA B 820:

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

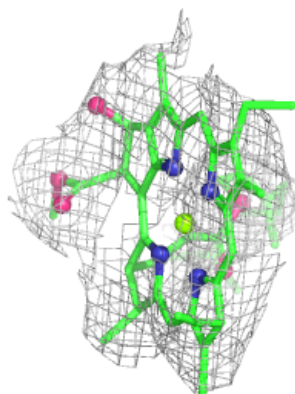
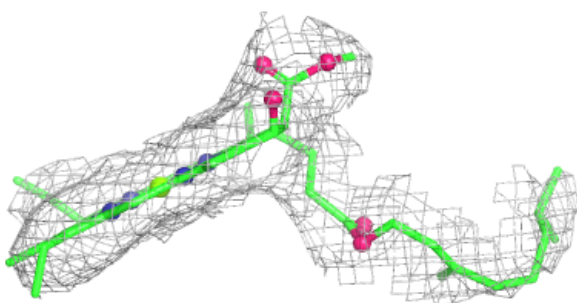
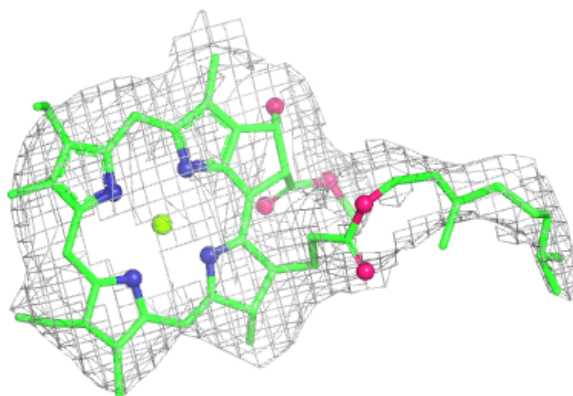


Electron density around CLA A 827:

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

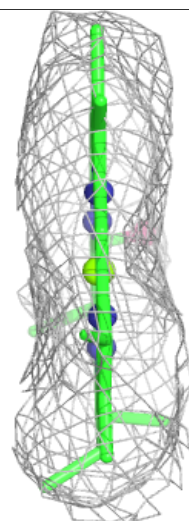
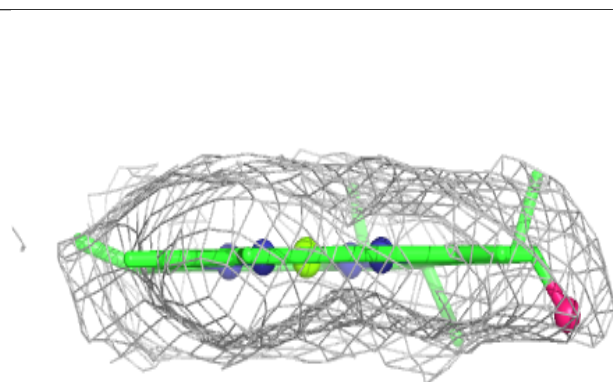
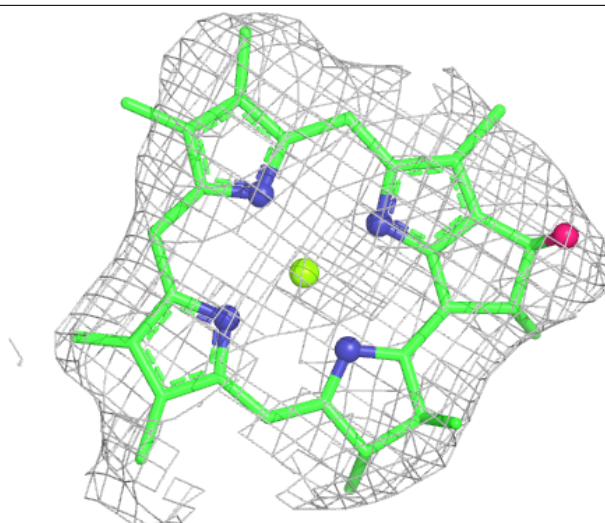
**Electron density around CLA A 807:**

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



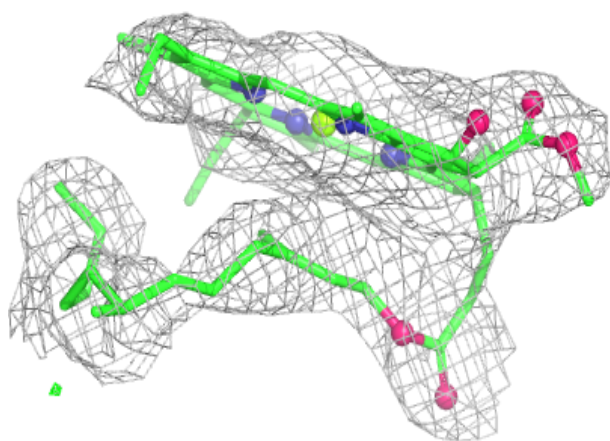
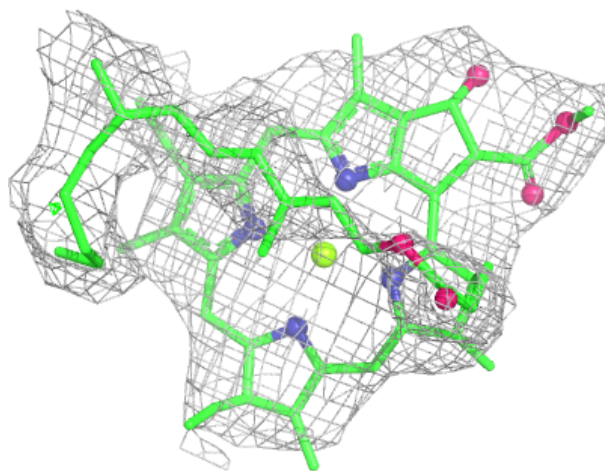
Electron density around CLA F 204:

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



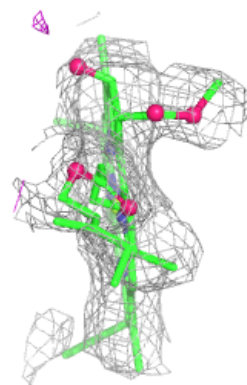
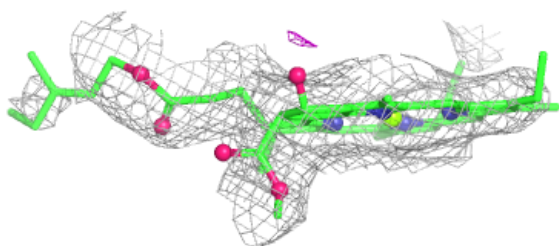
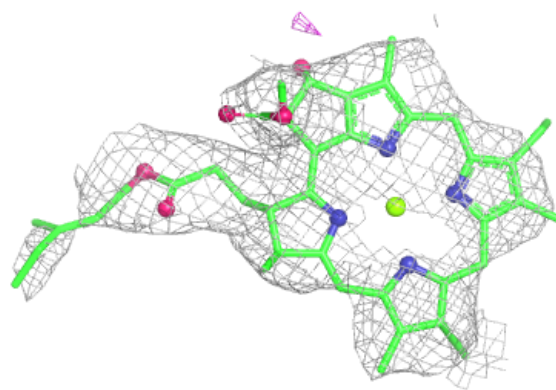
Electron density around CLA B 814:

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

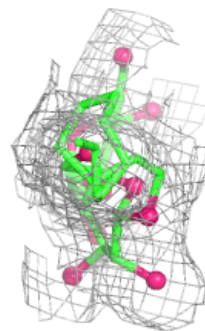
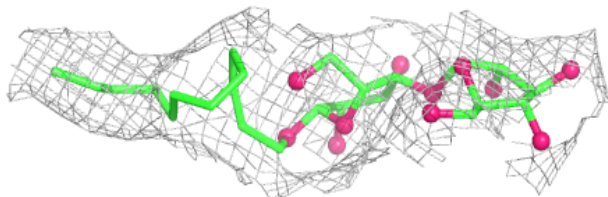
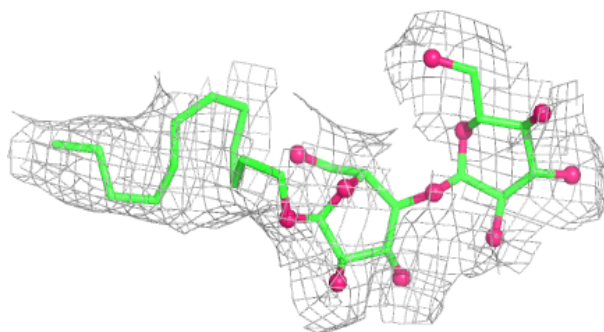


Electron density around CLA A 832:

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

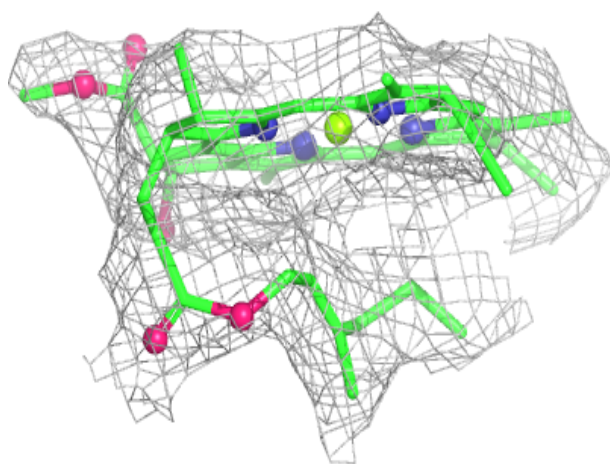
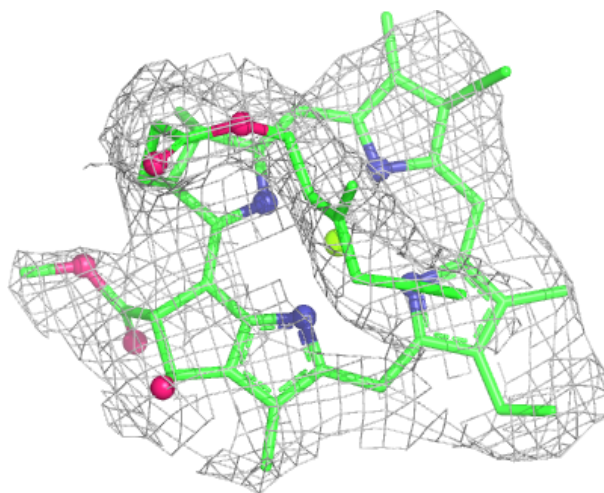
**Electron density around LMU A 852:**

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



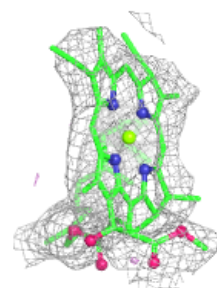
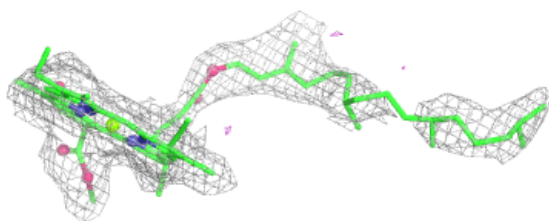
Electron density around CLA A 815:

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



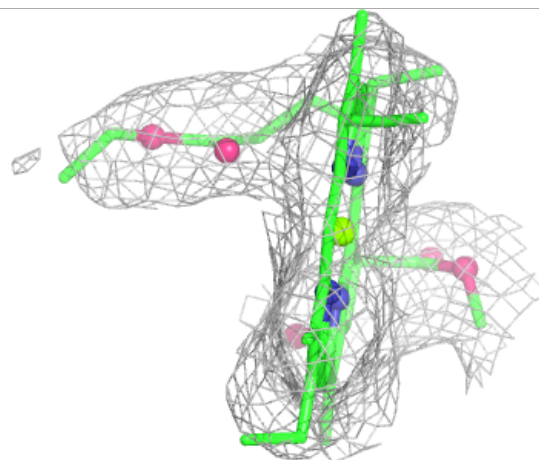
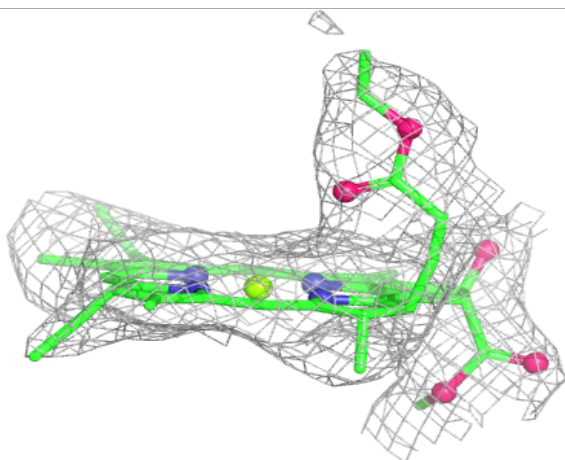
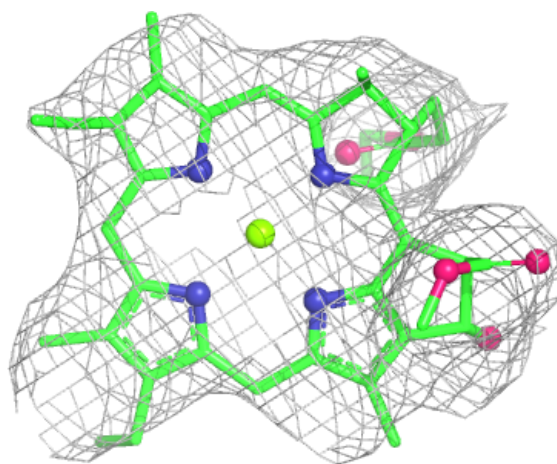
Electron density around CLA A 829:

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



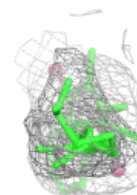
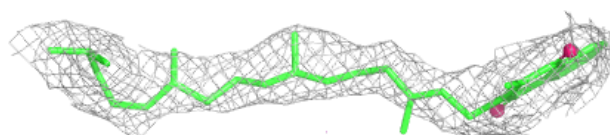
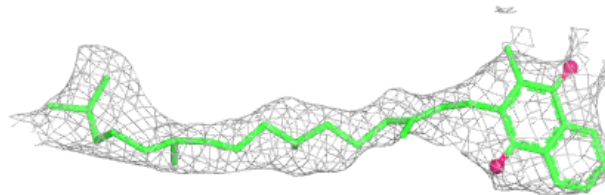
Electron density around CLA L 207:

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

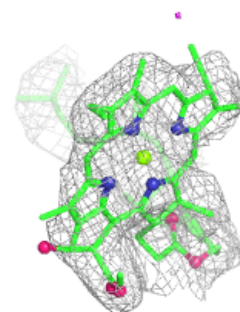
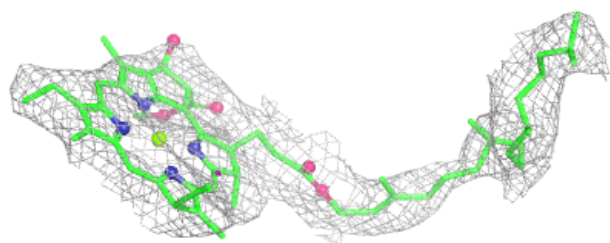
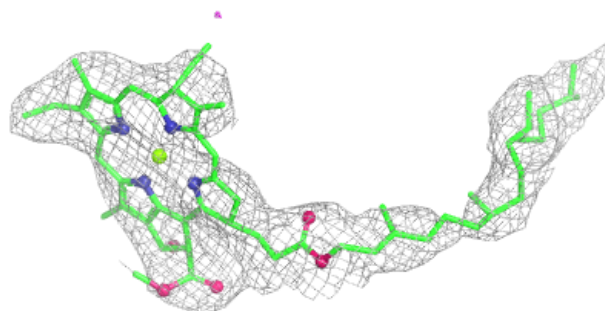


Electron density around PQN A 839:

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

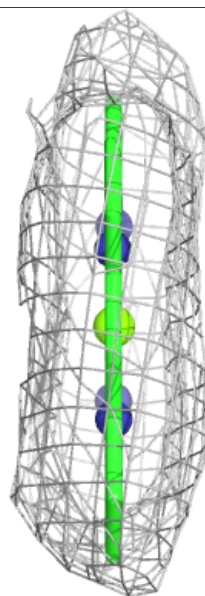
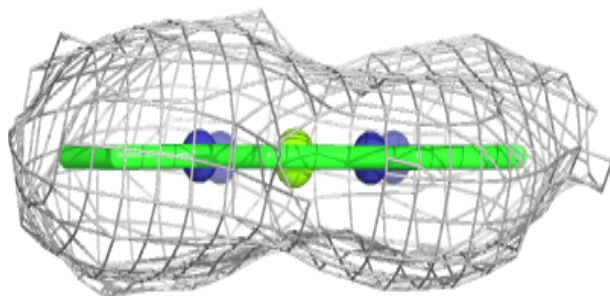
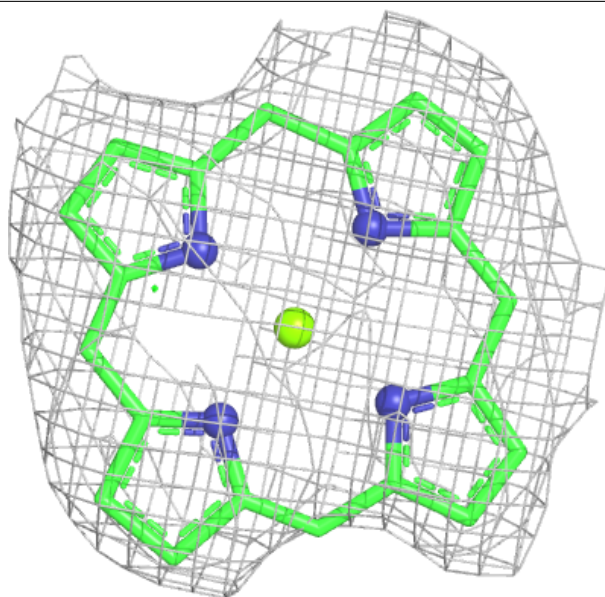
**Electron density around CLA A 848:**

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



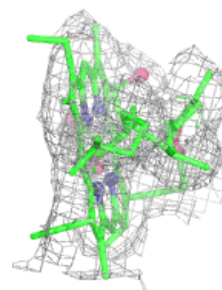
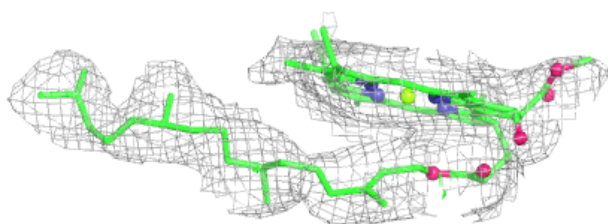
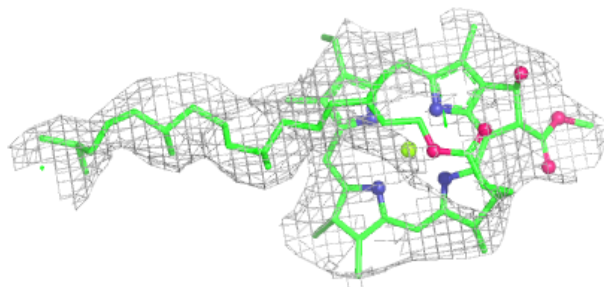
Electron density around CLA 4 312:

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

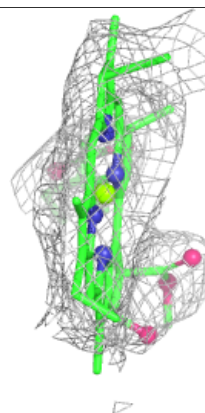
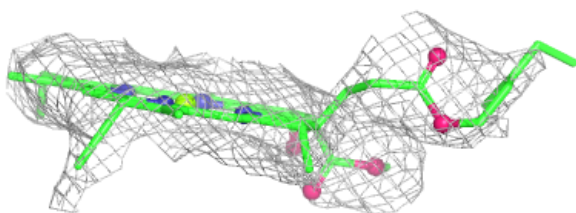
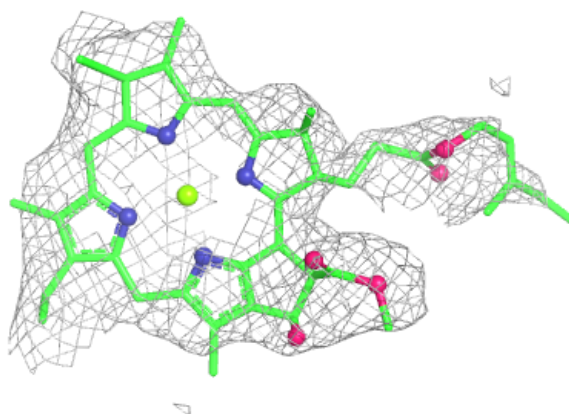


Electron density around CLA A 833:

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

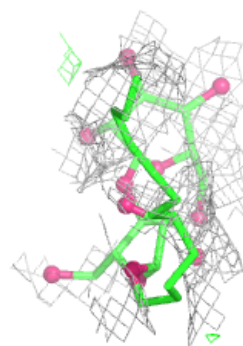
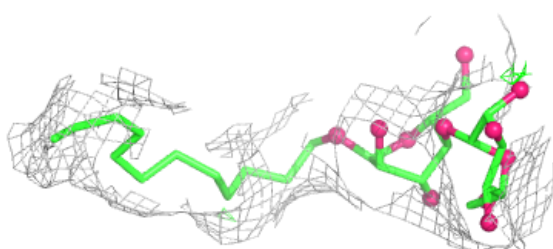
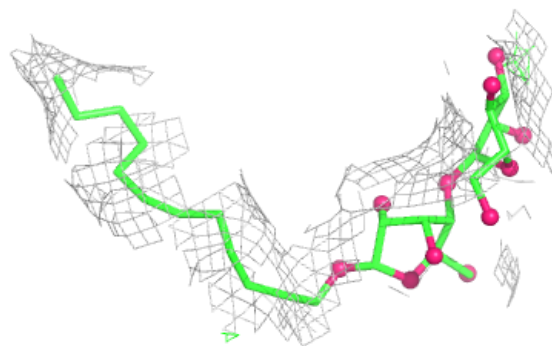
**Electron density around CLA A 835:**

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

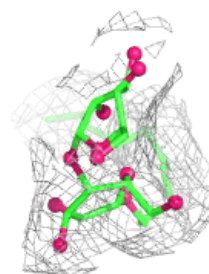
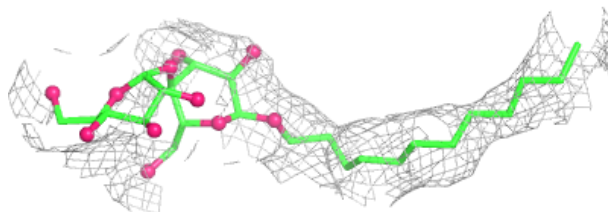
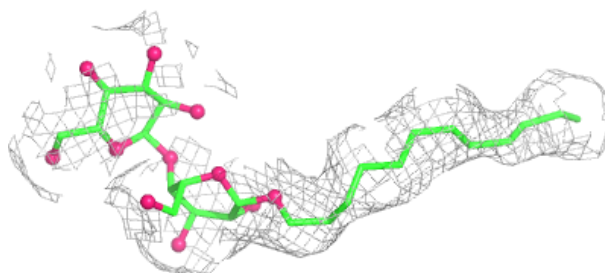


Electron density around LMU G 101:

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

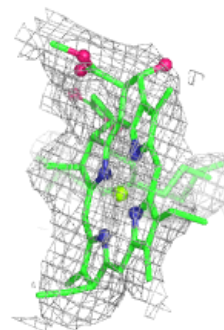
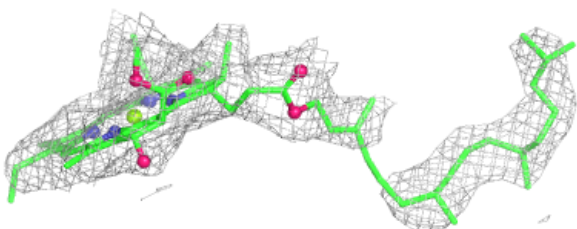
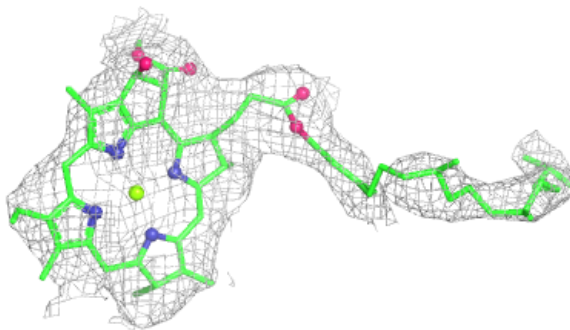
**Electron density around LMU R 104:**

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

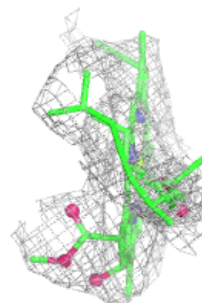
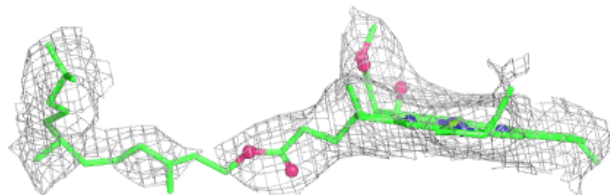
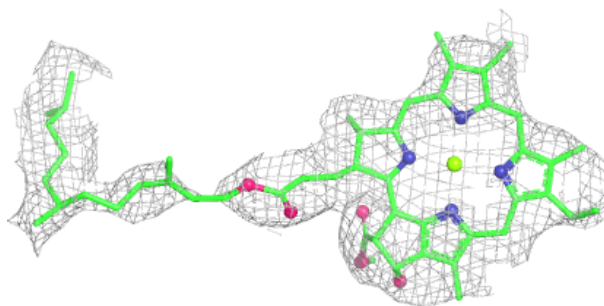


Electron density around CLA B 810:

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

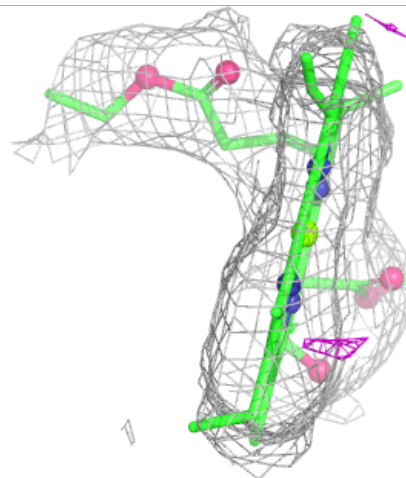
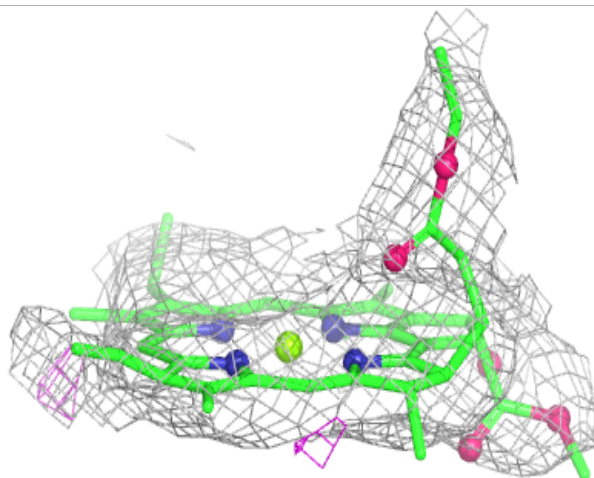
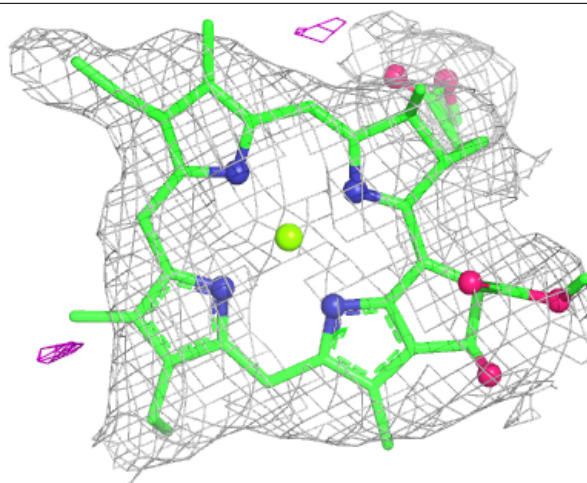
**Electron density around CLA B 834:**

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



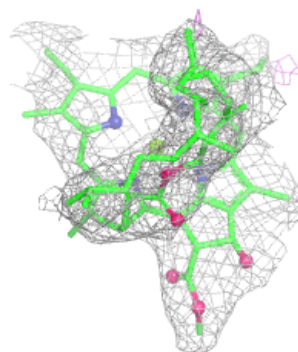
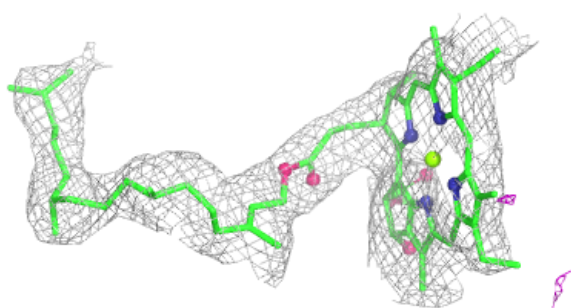
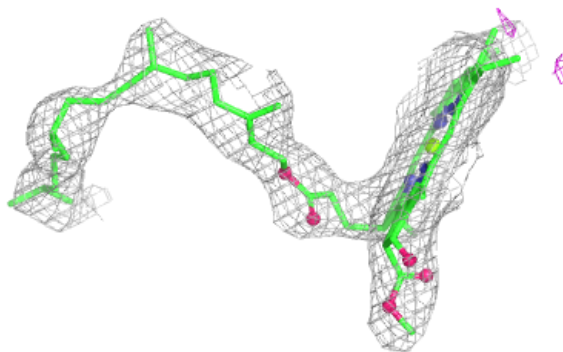
Electron density around CLA B 836:

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

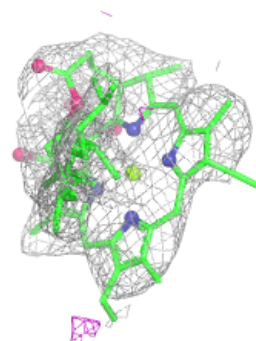
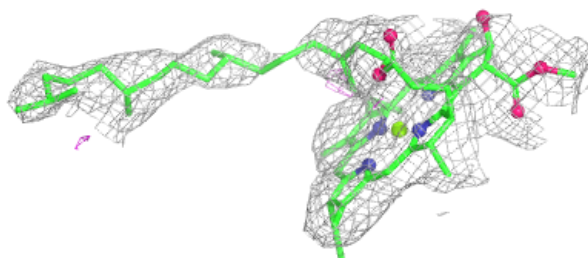
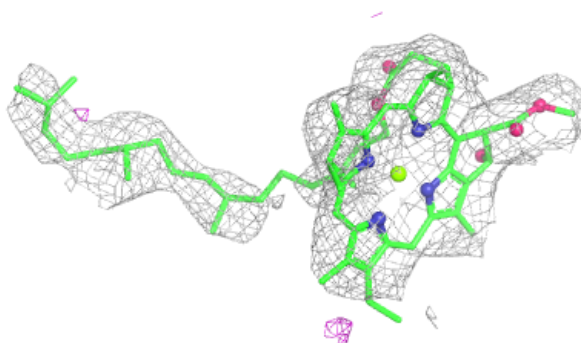


Electron density around CLA B 837:

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

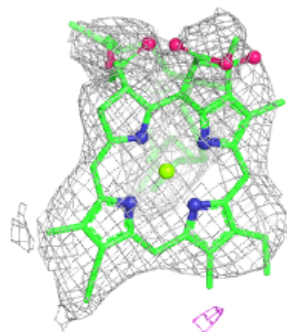
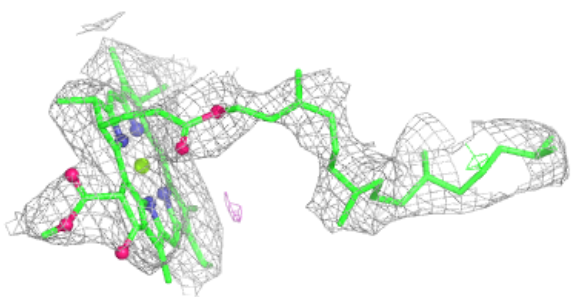
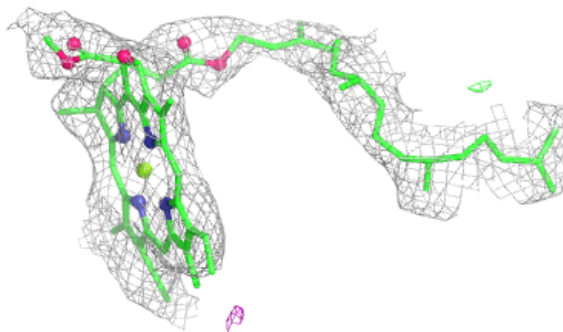
**Electron density around CLA A 836:**

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



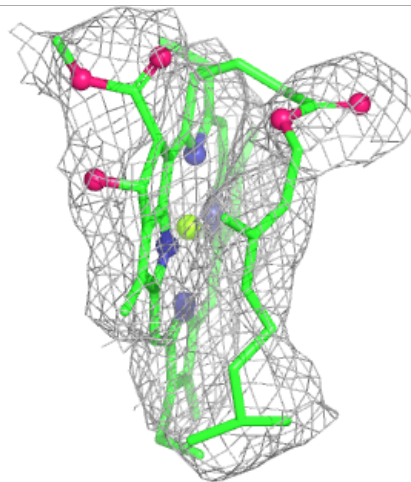
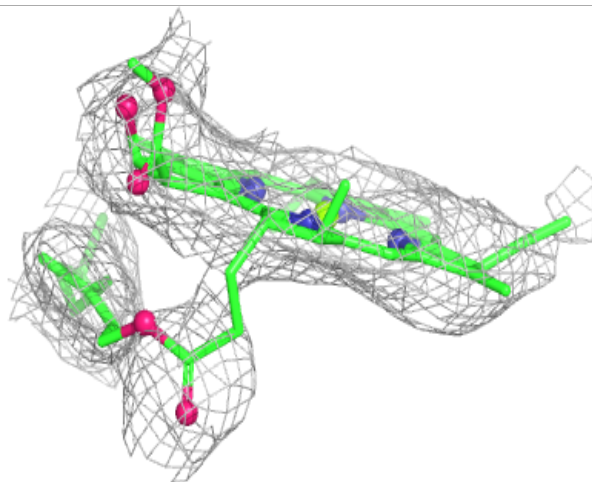
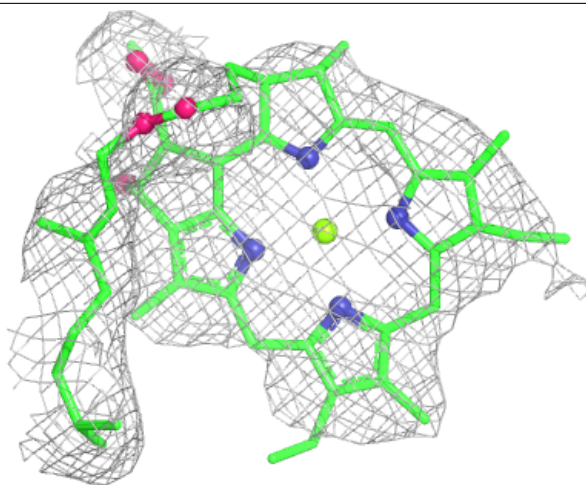
Electron density around CLA B 826:

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



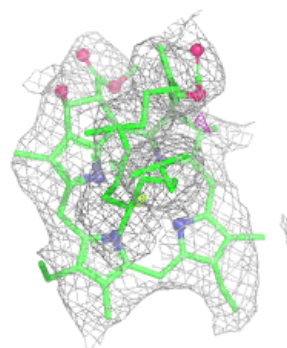
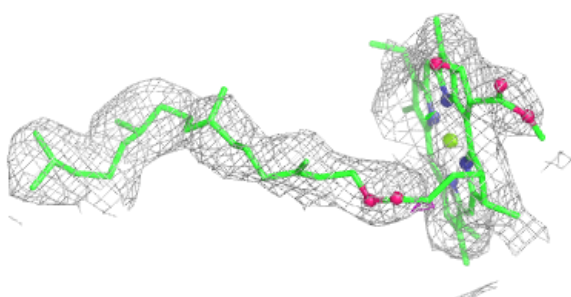
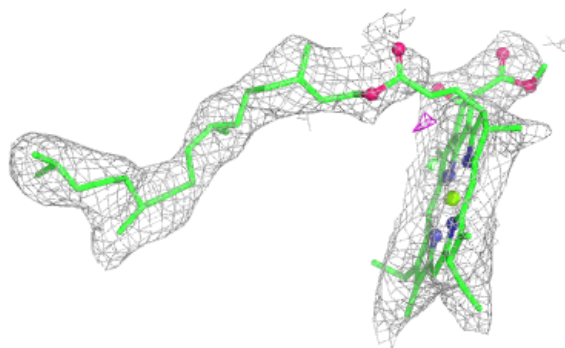
Electron density around CLA A 825:

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

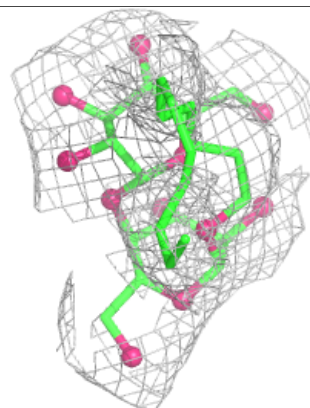
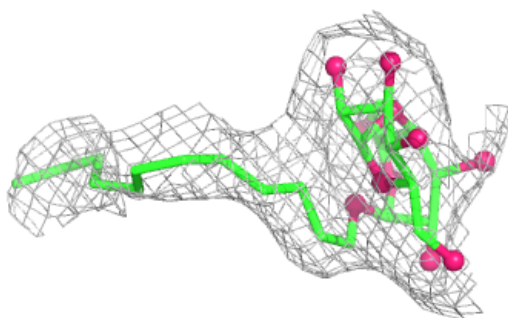
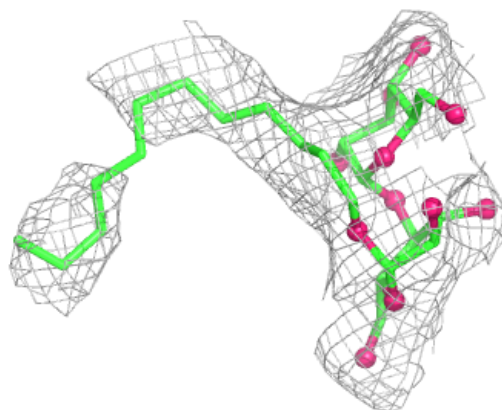


Electron density around CLA A 826:

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

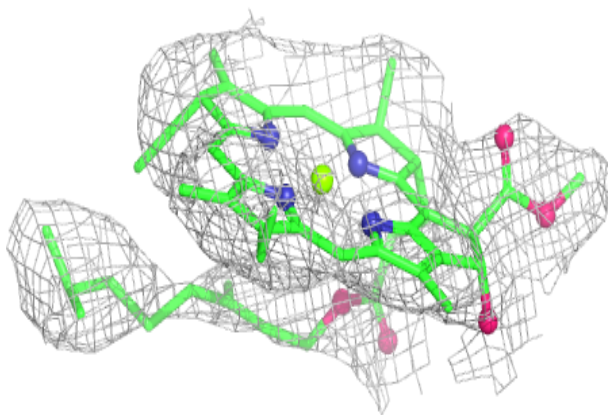
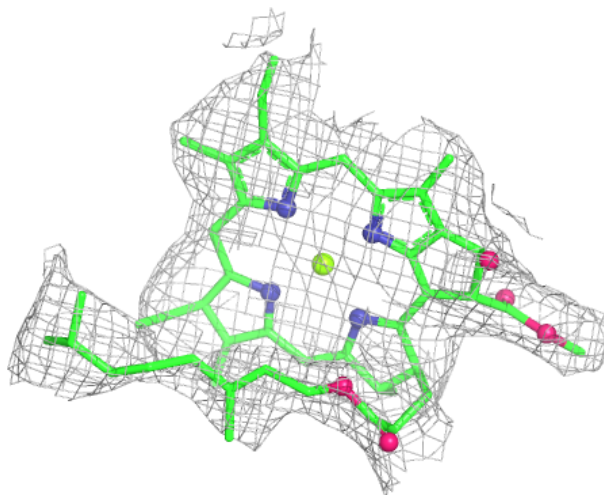
**Electron density around LMU H 104:**

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



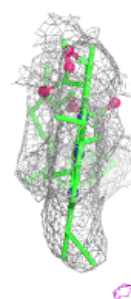
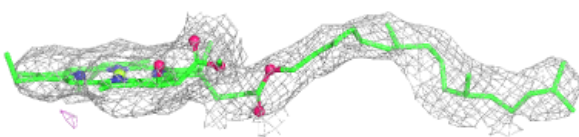
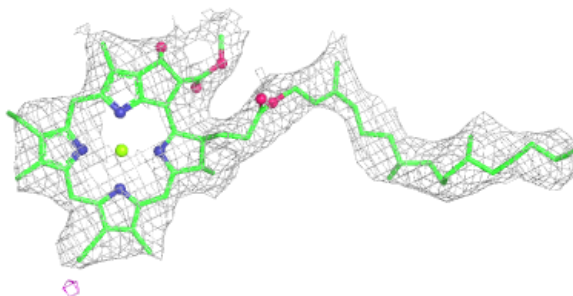
Electron density around CLA B 819:

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

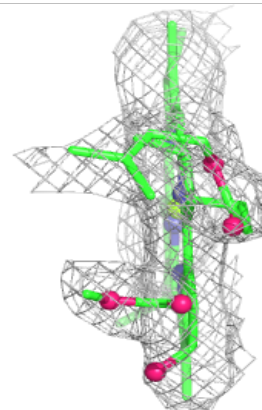
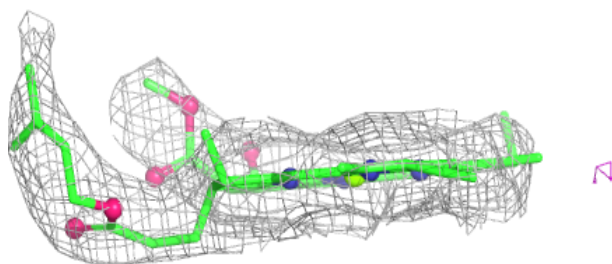
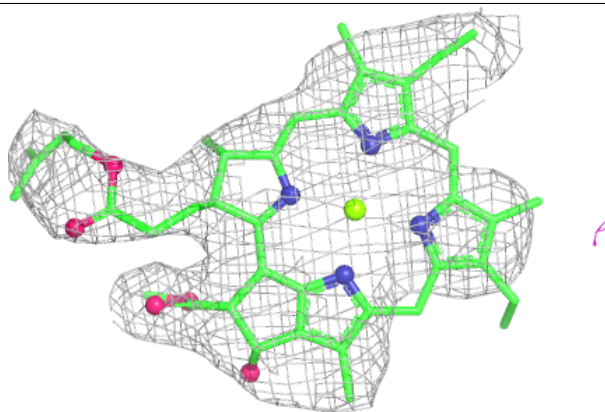


Electron density around CLA A 828:

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

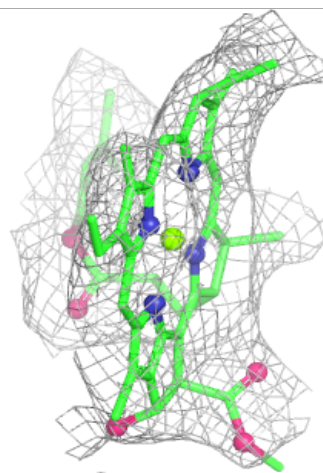
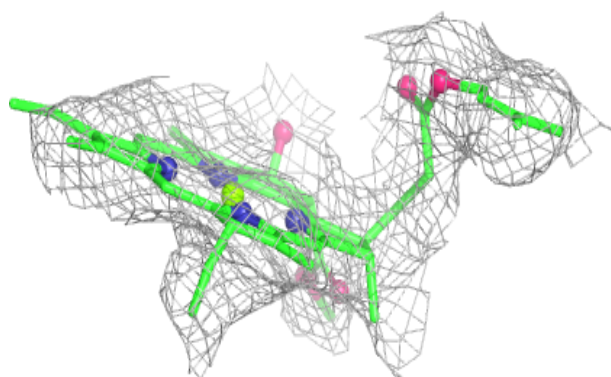
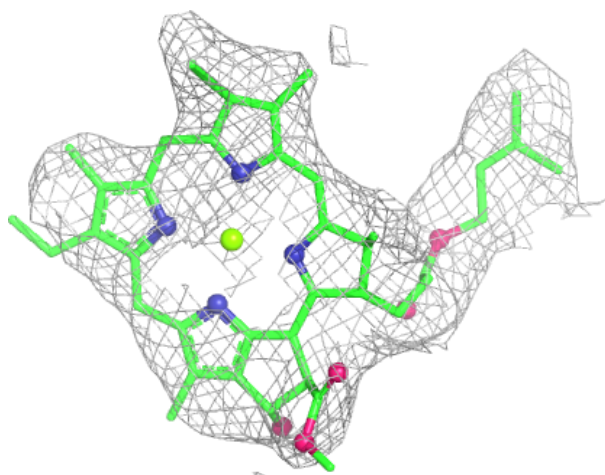
**Electron density around CLA A 801:**

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



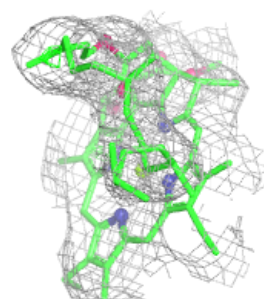
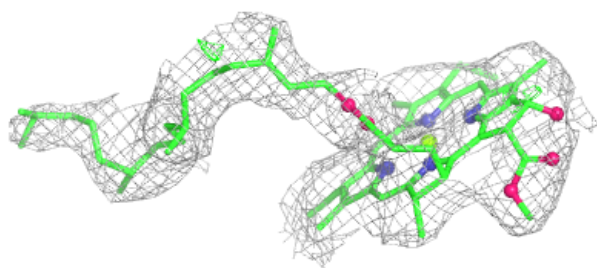
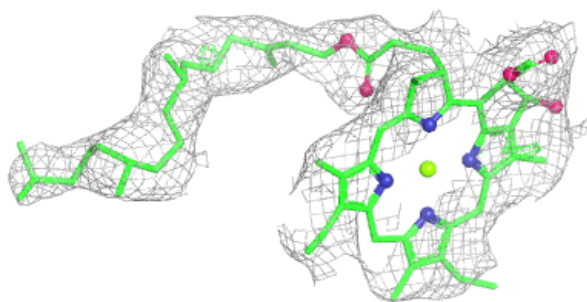
Electron density around CLA A 830:

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

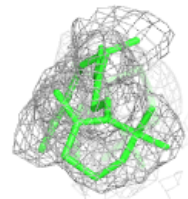
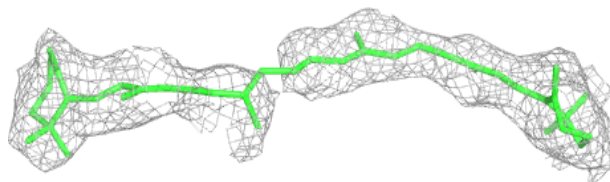
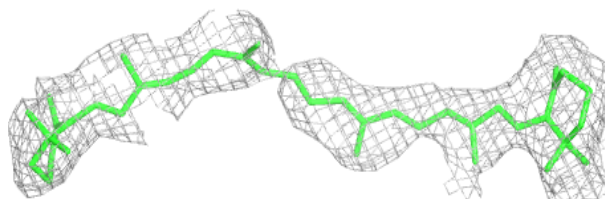


Electron density around CLA A 806:

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

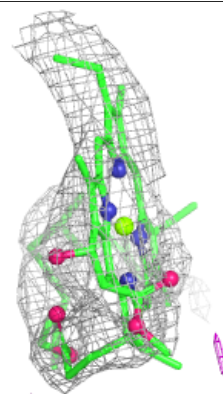
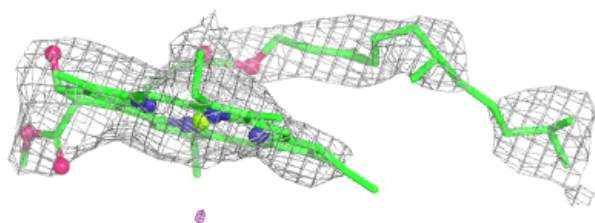
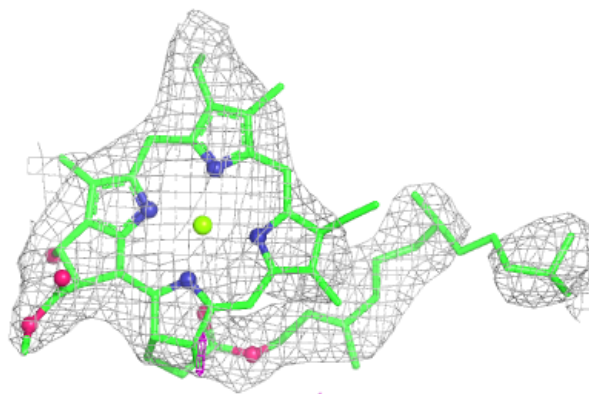
**Electron density around BCR I 101:**

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

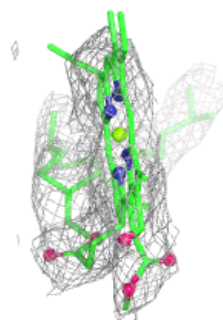
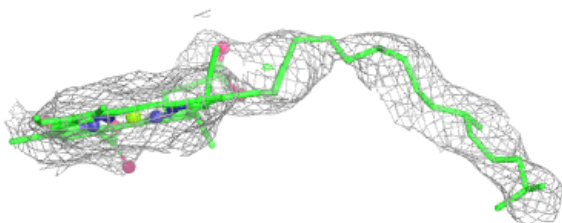
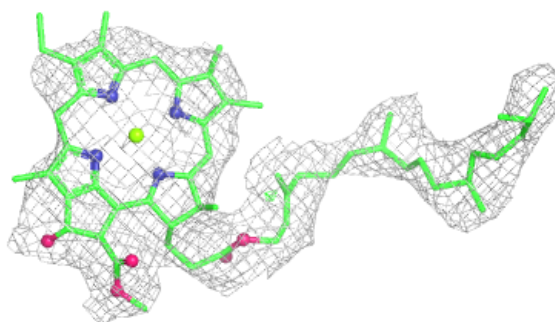


Electron density around CLA B 815:

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

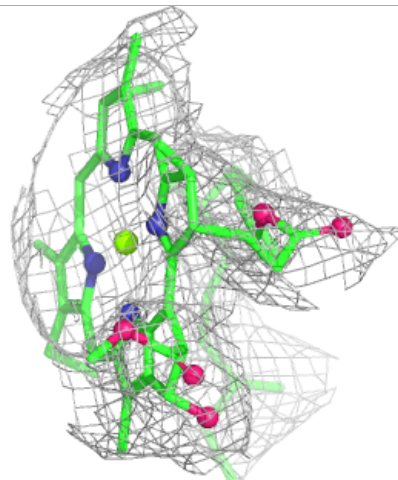
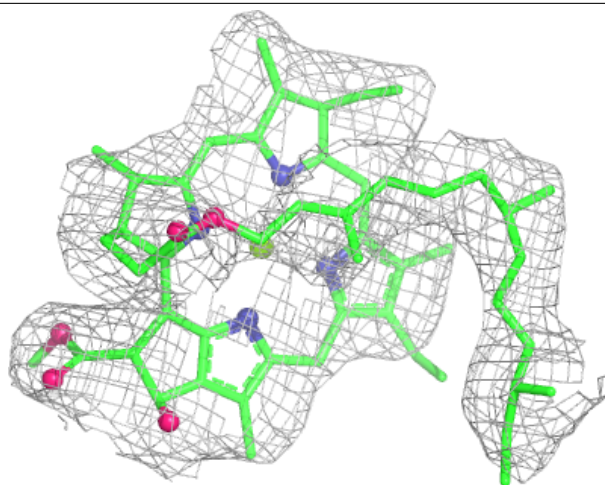
**Electron density around CLA B 849:**

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



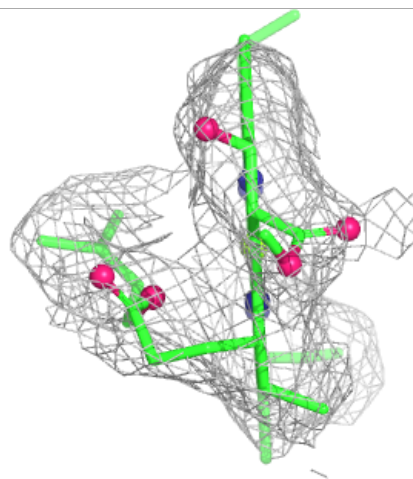
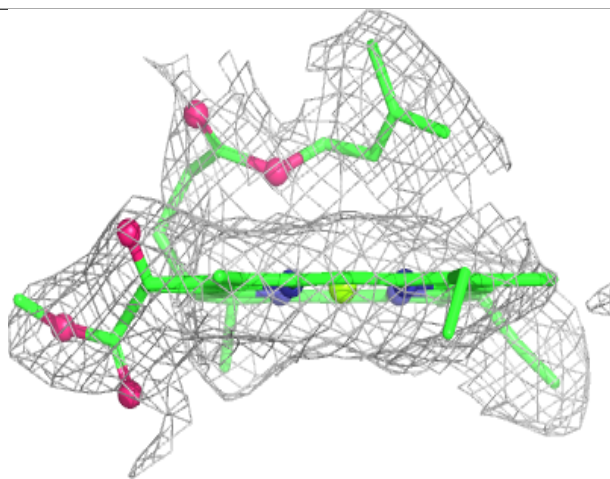
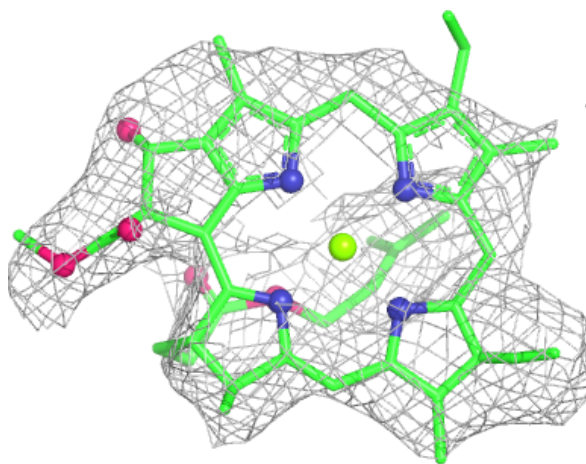
Electron density around CLA B 816:

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



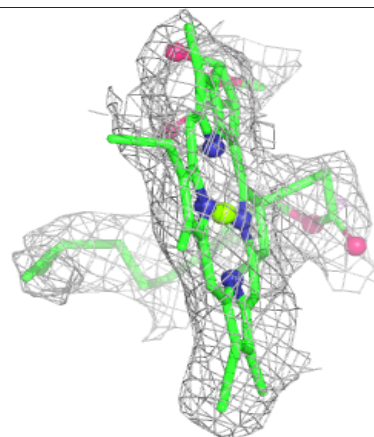
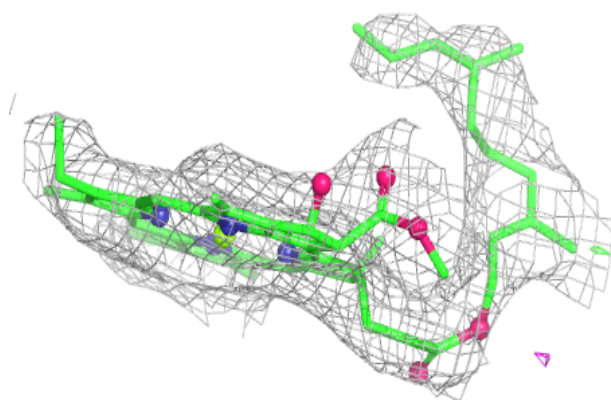
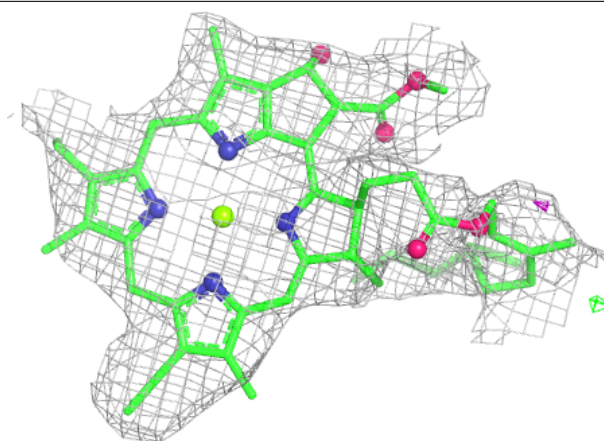
Electron density around CLA B 817:

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



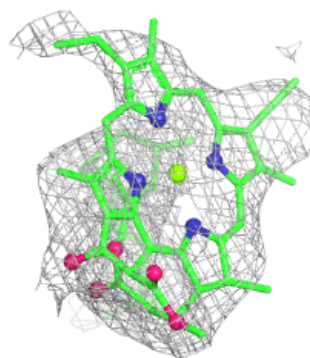
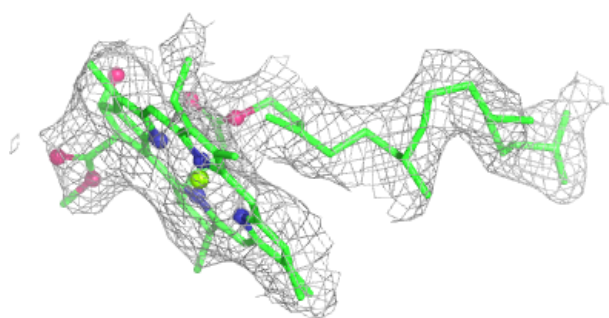
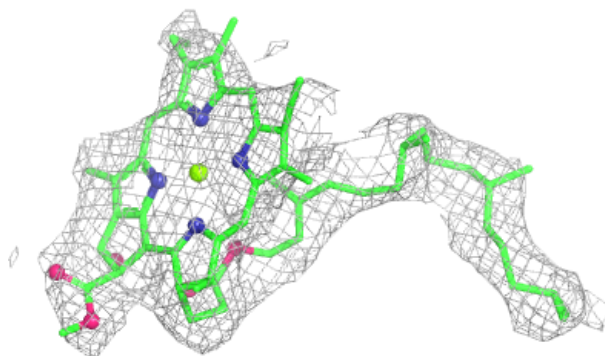
Electron density around CLA A 804:

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

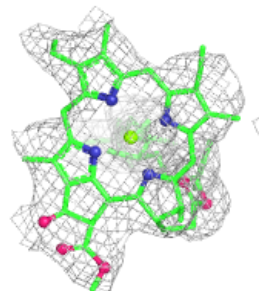
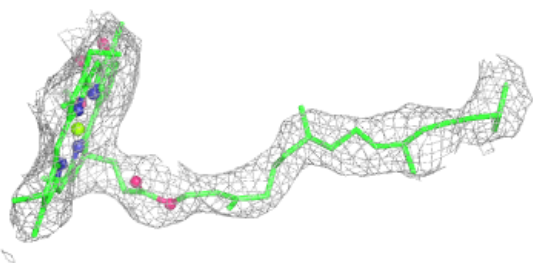
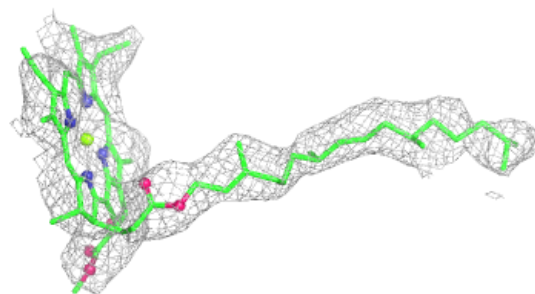


Electron density around CLA L 202:

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

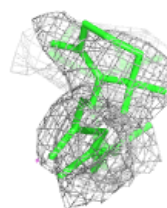
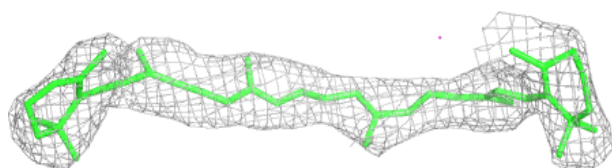
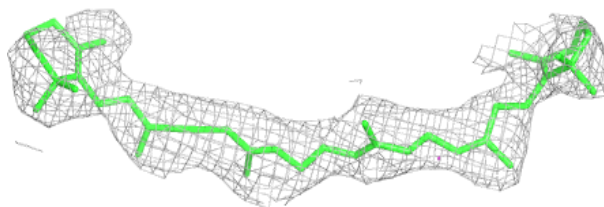
**Electron density around CLA B 825:**

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

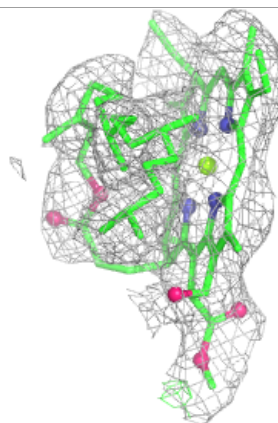
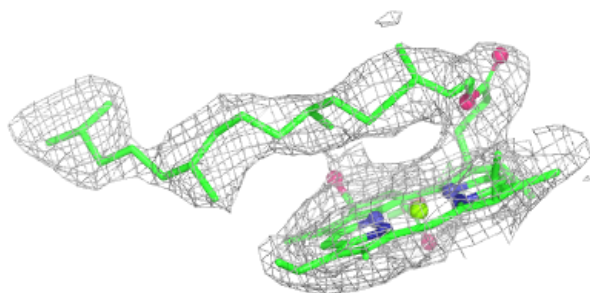
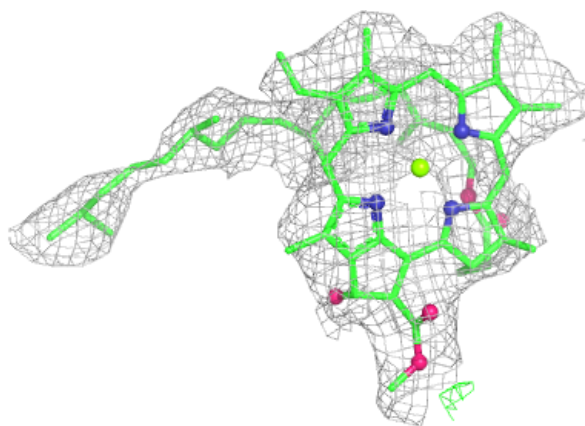


Electron density around BCR B 850:

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

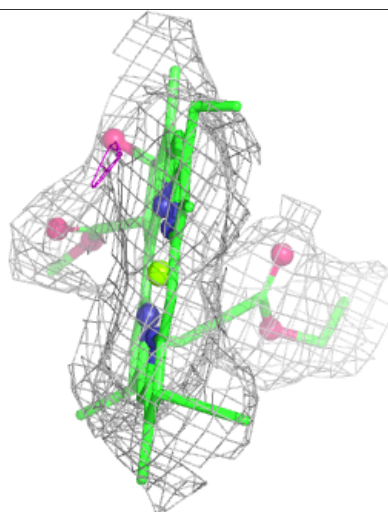
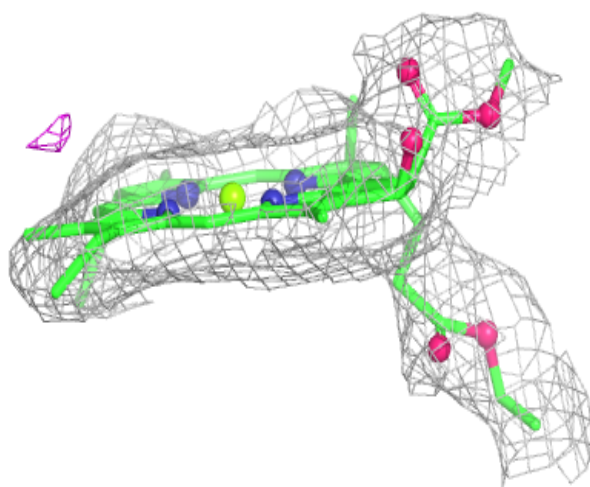
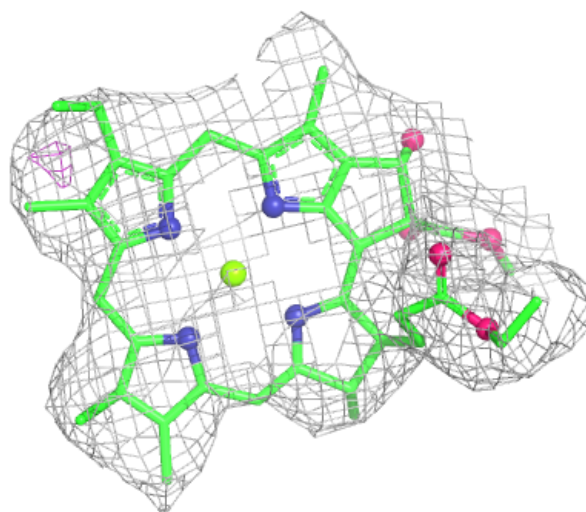
**Electron density around CLA B 824:**

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



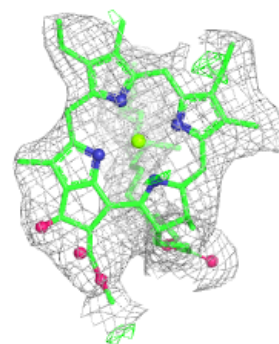
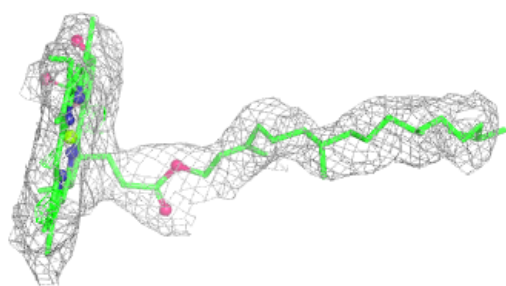
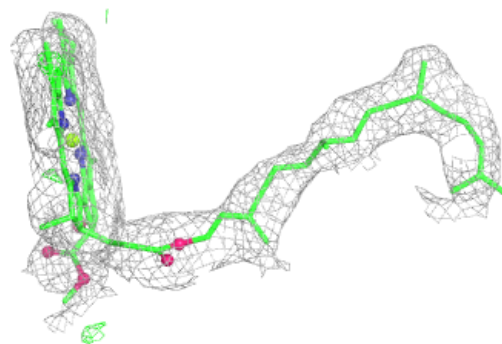
Electron density around CLA A 834:

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



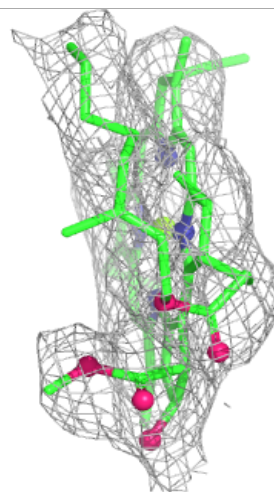
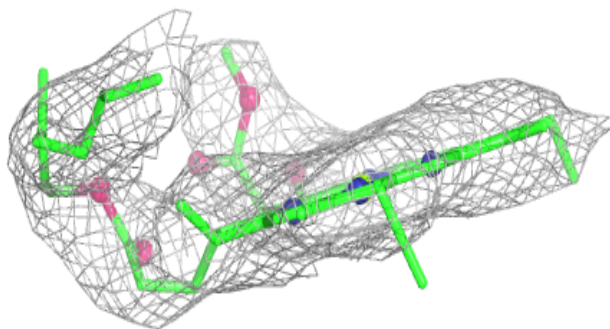
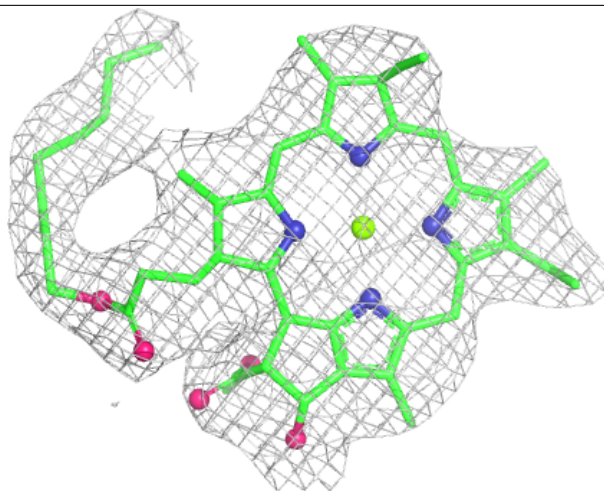
Electron density around CLA B 838:

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



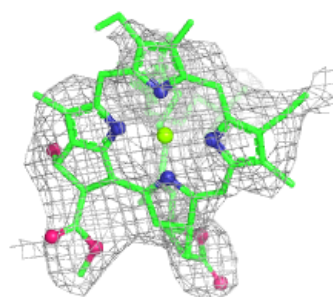
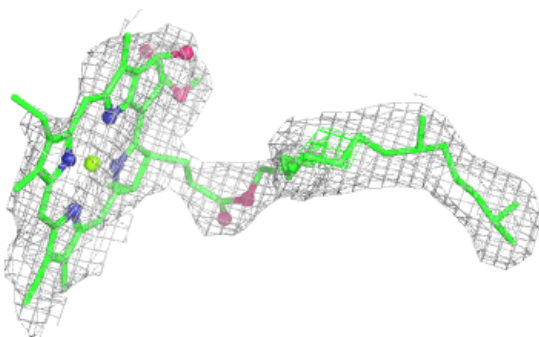
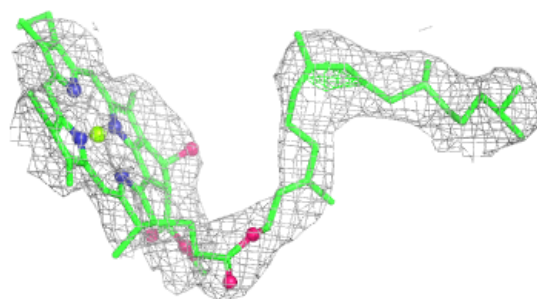
Electron density around CLA B 821:

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



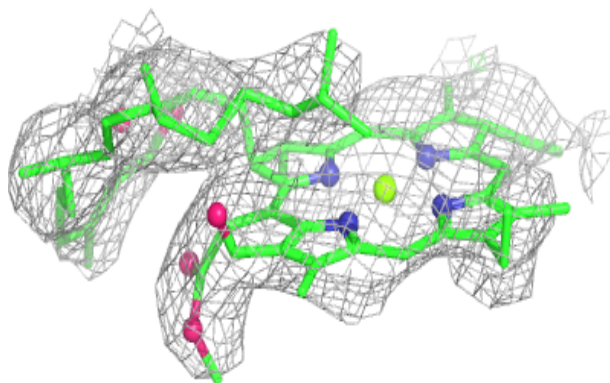
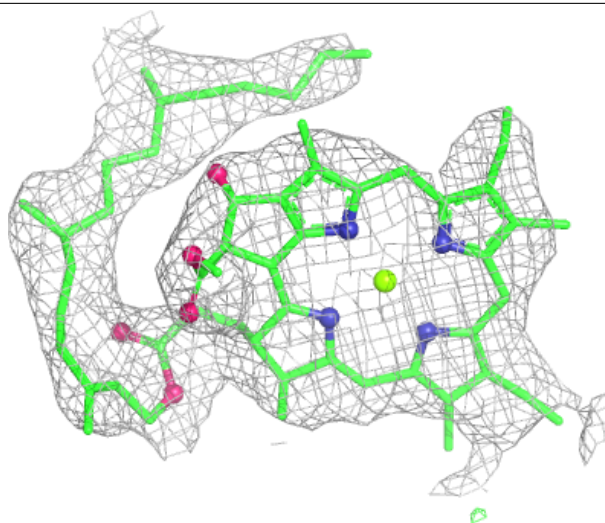
Electron density around CLA B 847:

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



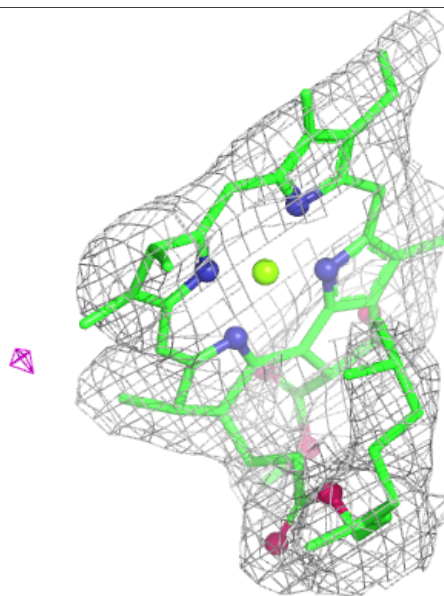
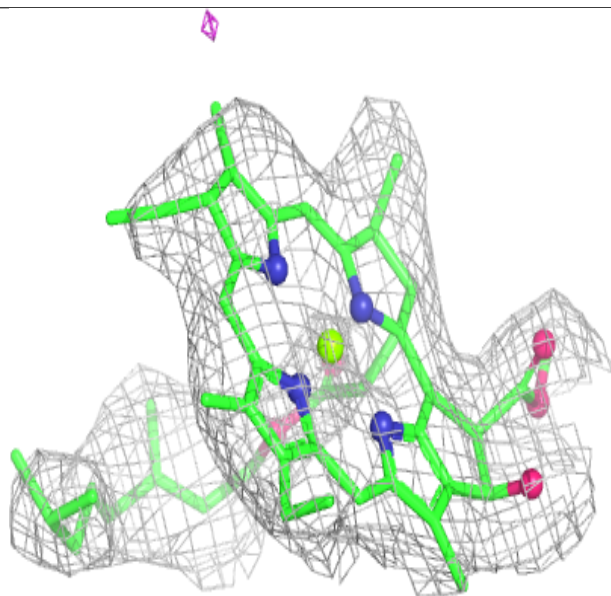
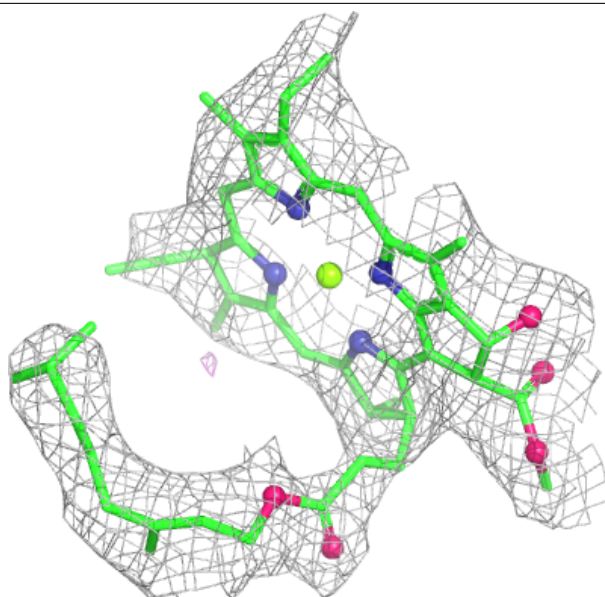
Electron density around CLA B 804:

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



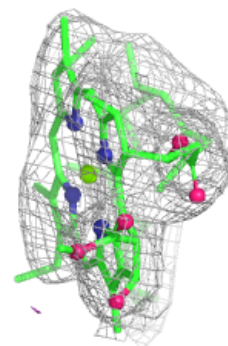
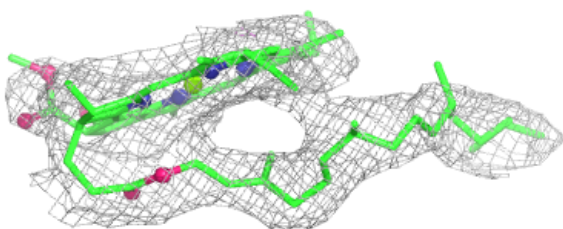
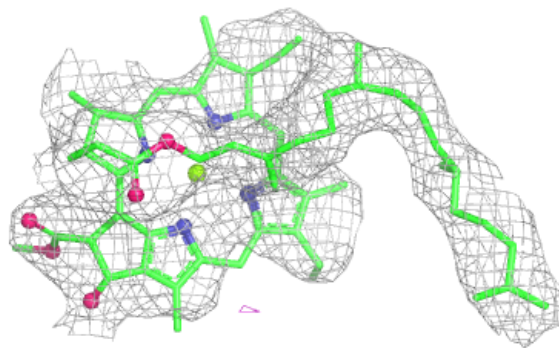
Electron density around CLA A 820:

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

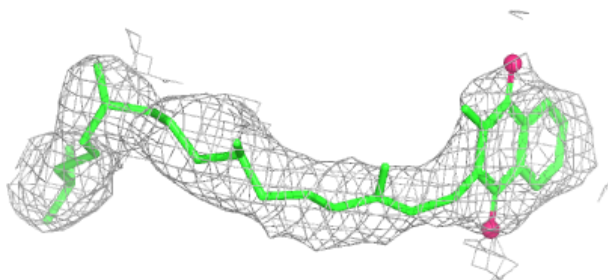
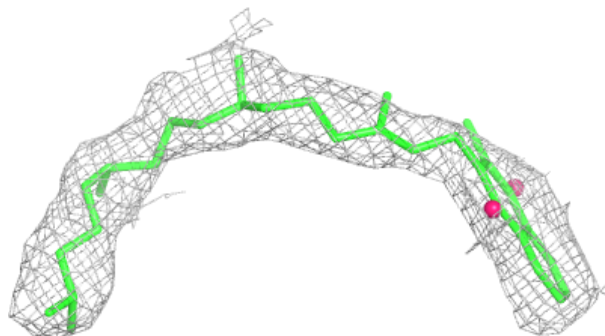


Electron density around CLA B 835:

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

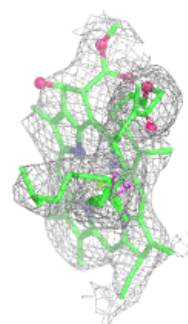
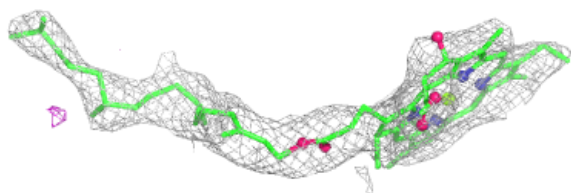
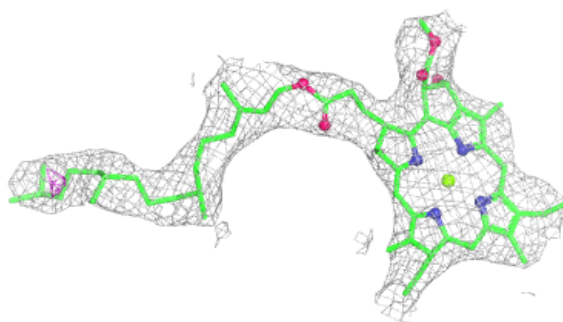
**Electron density around PQN B 840:**

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

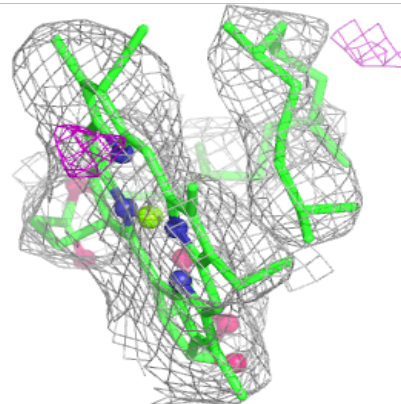
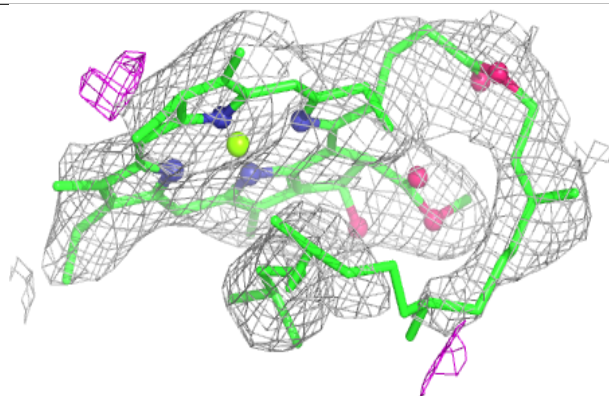
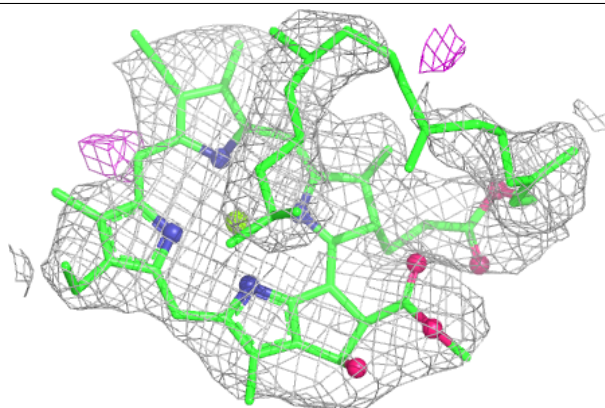


Electron density around CLA B 848:

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

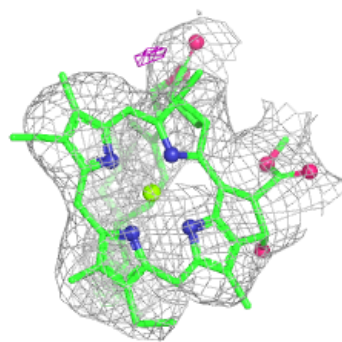
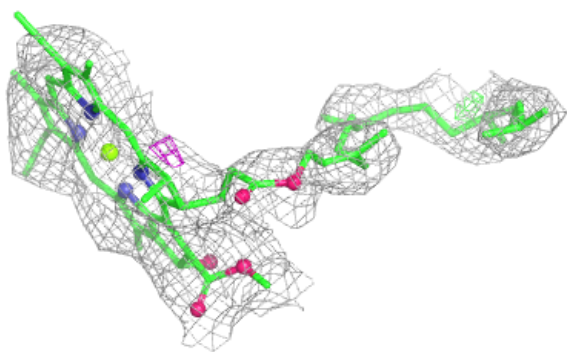
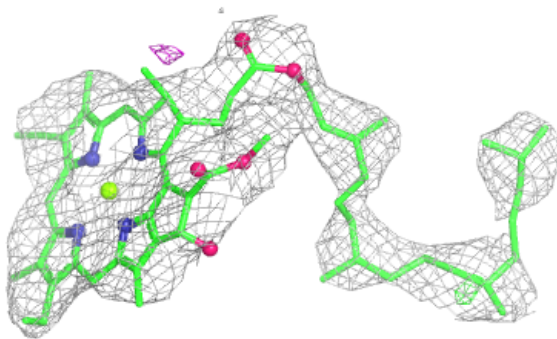
**Electron density around CLA B 805:**

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



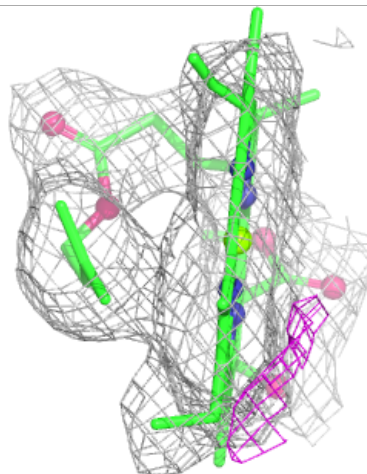
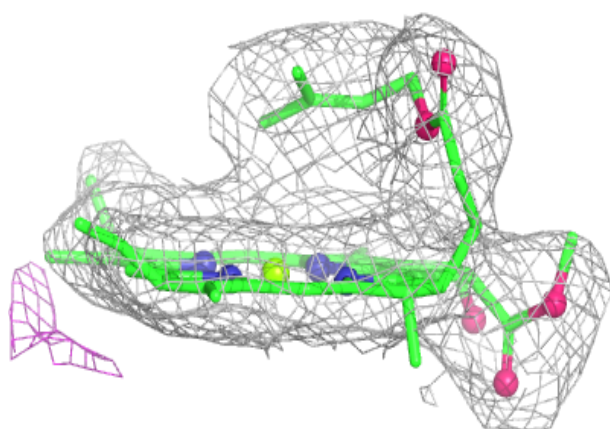
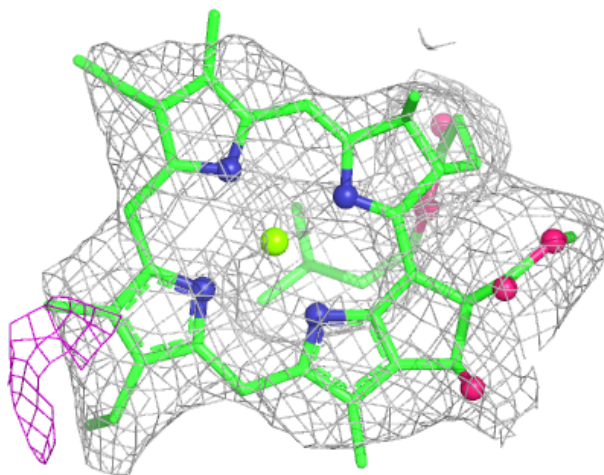
Electron density around CLA A 847:

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



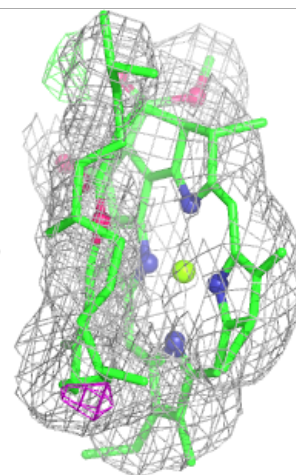
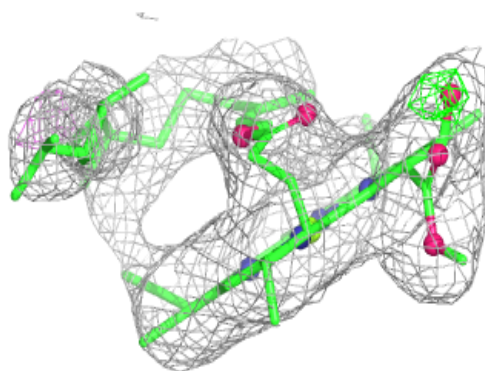
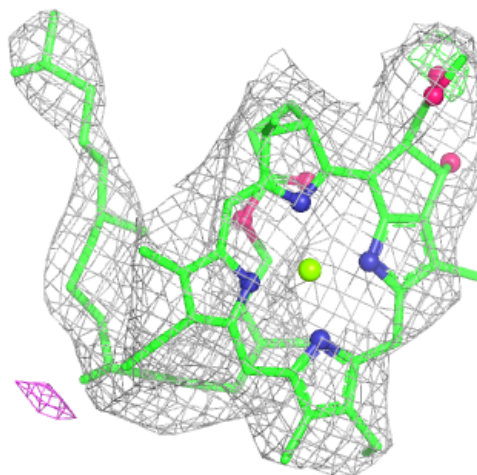
Electron density around CLA B 827:

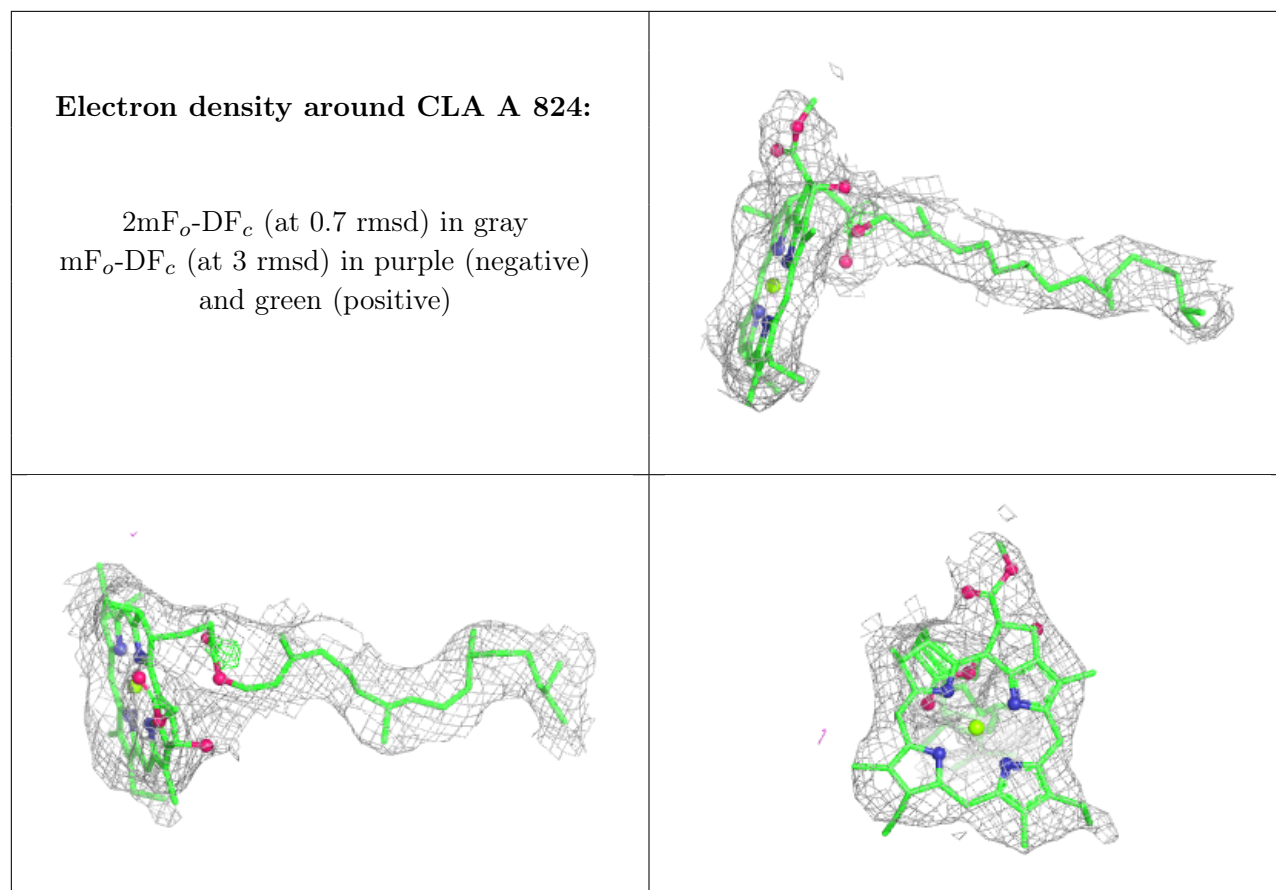
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around CLA B 806:

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





5.5 Other polymers ⓘ

There are no such residues in this entry.