



wwPDB X-ray Structure Validation Summary Report ⓘ

Jun 17, 2024 – 03:22 AM EDT

PDB ID : 2WSF
Title : Improved Model of Plant Photosystem I
Authors : Amunts, A.; Toporik, H.; Borovikov, A.; Nelson, N.
Deposited on : 2009-09-05
Resolution : 3.48 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	2.37.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

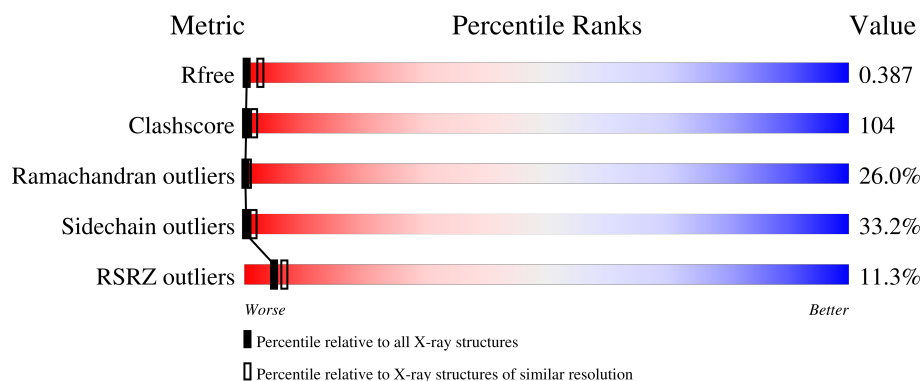
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.48 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1379 (3.56-3.40)
Clashscore	141614	1461 (3.56-3.40)
Ramachandran outliers	138981	1424 (3.56-3.40)
Sidechain outliers	138945	1425 (3.56-3.40)
RSRZ outliers	127900	1289 (3.56-3.40)

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

Mol	Chain	Length	Quality of chain
1	1	241	<div> <div>16%</div> <div>27%</div> <div>29%</div> <div>10%</div> <div>•</div> <div>32%</div> </div>
2	2	269	<div> <div>13%</div> <div>10%</div> <div>23%</div> <div>23%</div> <div>10%</div> <div>35%</div> </div>
3	3	276	<div> <div>11%</div> <div>15%</div> <div>21%</div> <div>13%</div> <div>5%</div> <div>45%</div> </div>
4	4	251	<div> <div>6%</div> <div>7%</div> <div>22%</div> <div>25%</div> <div>12%</div> <div>34%</div> </div>
5	A	758	<div> <div>7%</div> <div>10%</div> <div>50%</div> <div>30%</div> <div>7%</div> <div>•</div> </div>


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Mol	Chain	Length	Quality of chain
6	B	734	
7	C	81	
8	D	212	
9	E	143	
10	F	231	
11	G	167	
12	H	144	
13	I	40	
14	J	44	
15	K	131	
16	L	216	
17	N	170	
18	R	53	
19	M	2	
19	O	2	
19	P	2	
19	Q	2	
19	S	2	
19	T	2	
19	U	2	
19	V	2	
19	W	2	
19	X	2	
19	Y	2	
19	Z	2	

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Mol	Chain	Length	Quality of chain
19	a	2	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
19	FRU	M	2	X	-	-	-
19	GLC	O	1	-	-	X	-
19	FRU	O	2	X	-	-	X
19	GLC	P	1	-	-	X	-
19	FRU	P	2	X	-	X	-
19	FRU	Q	2	X	-	X	-
19	FRU	S	2	X	-	-	-
19	FRU	T	2	X	-	-	-
19	FRU	U	2	X	-	-	-
19	FRU	V	2	X	-	-	-
19	FRU	W	2	X	-	-	-
19	GLC	X	1	-	-	-	X
19	FRU	X	2	X	-	-	X
19	GLC	Y	1	-	-	X	-
19	FRU	Y	2	X	-	X	-
19	FRU	Z	2	X	-	X	-
19	FRU	a	2	X	-	-	-
20	CLA	1	201	X	-	-	-
20	CLA	1	202	X	-	-	-
20	CLA	1	203	X	-	-	-
20	CLA	1	204	X	-	-	-
20	CLA	1	205	X	-	-	-
20	CLA	1	206	X	-	-	-
20	CLA	1	207	X	-	-	-
20	CLA	1	208	X	-	-	-
20	CLA	1	209	X	-	-	-
20	CLA	1	210	X	-	-	-
20	CLA	1	211	X	-	-	X
20	CLA	1	212	X	-	-	-
20	CLA	1	213	X	-	-	-
20	CLA	1	214	X	-	-	-
20	CLA	1	215	X	-	-	-
20	CLA	2	301	X	-	-	X
20	CLA	2	302	X	-	-	-
20	CLA	2	303	X	-	X	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
20	CLA	2	304	X	-	-	X
20	CLA	2	305	X	-	-	-
20	CLA	2	306	X	-	-	-
20	CLA	2	307	X	-	X	-
20	CLA	2	308	X	-	-	-
20	CLA	2	309	X	-	-	-
20	CLA	2	310	X	-	X	-
20	CLA	2	311	X	-	-	-
20	CLA	2	312	X	-	-	-
20	CLA	2	315	X	-	-	-
20	CLA	2	316	X	-	-	-
20	CLA	2	317	X	-	-	-
20	CLA	3	301	X	-	-	-
20	CLA	3	302	X	-	-	X
20	CLA	3	303	X	-	-	-
20	CLA	3	304	X	-	-	-
20	CLA	3	305	X	-	-	-
20	CLA	3	306	X	-	-	-
20	CLA	3	307	X	-	-	-
20	CLA	3	308	X	-	-	-
20	CLA	3	309	X	-	-	-
20	CLA	3	310	X	-	-	-
20	CLA	3	311	X	-	-	X
20	CLA	3	313	X	-	-	X
20	CLA	3	314	X	-	-	X
20	CLA	3	315	X	-	-	-
20	CLA	3	316	X	-	-	X
20	CLA	3	317	X	-	-	-
20	CLA	3	318	X	-	-	-
20	CLA	4	301	X	-	X	-
20	CLA	4	302	X	-	-	-
20	CLA	4	303	X	-	-	-
20	CLA	4	304	X	-	X	-
20	CLA	4	305	X	-	-	X
20	CLA	4	306	X	-	-	-
20	CLA	4	307	X	-	-	-
20	CLA	4	308	X	-	-	-
20	CLA	4	309	X	-	-	-
20	CLA	4	310	X	-	X	-
20	CLA	4	311	X	-	-	-
20	CLA	4	312	X	-	-	-
20	CLA	4	313	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
20	CLA	4	314	X	-	-	-
20	CLA	4	315	X	-	-	-
20	CLA	4	317	X	-	-	X
20	CLA	4	318	X	-	-	-
20	CLA	A	801	X	-	-	-
20	CLA	A	802	X	-	-	X
20	CLA	A	803	X	-	-	-
20	CLA	A	804	X	-	X	-
20	CLA	A	805	X	-	-	-
20	CLA	A	806	X	-	-	-
20	CLA	A	807	X	-	X	-
20	CLA	A	808	X	-	X	-
20	CLA	A	809	X	-	X	-
20	CLA	A	810	X	-	-	-
20	CLA	A	811	X	-	X	X
20	CLA	A	812	X	-	-	-
20	CLA	A	813	X	-	X	-
20	CLA	A	814	X	-	-	-
20	CLA	A	815	X	-	-	-
20	CLA	A	816	X	-	X	-
20	CLA	A	817	X	-	-	-
20	CLA	A	818	X	-	X	-
20	CLA	A	819	X	-	X	-
20	CLA	A	820	X	-	-	-
20	CLA	A	821	X	-	-	-
20	CLA	A	822	X	-	-	-
20	CLA	A	823	X	-	-	-
20	CLA	A	824	X	-	X	-
20	CLA	A	825	X	-	X	-
20	CLA	A	826	X	-	X	-
20	CLA	A	827	X	-	-	-
20	CLA	A	828	X	-	-	-
20	CLA	A	829	X	-	-	-
20	CLA	A	830	X	-	X	-
20	CLA	A	831	X	-	X	-
20	CLA	A	832	X	-	-	-
20	CLA	A	833	X	-	-	-
20	CLA	A	834	X	-	-	-
20	CLA	A	835	X	-	-	-
20	CLA	A	836	X	-	-	-
20	CLA	A	837	X	-	-	-
20	CLA	A	838	X	-	X	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
20	CLA	A	839	X	-	X	-
20	CLA	A	840	X	-	-	-
20	CLA	A	841	X	-	-	-
20	CLA	A	849	X	-	X	-
20	CLA	A	850	X	-	X	-
20	CLA	A	851	X	-	X	-
20	CLA	B	802	X	-	-	-
20	CLA	B	803	X	-	X	-
20	CLA	B	806	X	-	X	-
20	CLA	B	807	X	-	-	-
20	CLA	B	808	X	-	X	-
20	CLA	B	809	X	-	X	-
20	CLA	B	810	X	-	-	-
20	CLA	B	811	X	-	-	-
20	CLA	B	812	X	-	-	-
20	CLA	B	813	X	-	-	-
20	CLA	B	814	X	-	X	-
20	CLA	B	815	X	-	-	-
20	CLA	B	816	X	-	-	-
20	CLA	B	817	X	-	-	X
20	CLA	B	818	X	-	-	-
20	CLA	B	819	X	-	-	-
20	CLA	B	820	X	-	-	-
20	CLA	B	821	X	-	-	-
20	CLA	B	822	X	-	-	-
20	CLA	B	823	X	-	-	-
20	CLA	B	824	X	-	X	-
20	CLA	B	825	X	-	X	-
20	CLA	B	826	X	-	X	-
20	CLA	B	827	X	-	X	-
20	CLA	B	828	X	-	-	-
20	CLA	B	829	X	-	X	-
20	CLA	B	830	X	-	X	-
20	CLA	B	831	X	-	-	-
20	CLA	B	832	X	-	X	-
20	CLA	B	833	X	-	-	-
20	CLA	B	834	X	-	X	-
20	CLA	B	835	X	-	X	-
20	CLA	B	836	X	-	-	-
20	CLA	B	837	X	-	-	-
20	CLA	B	838	X	-	X	-
20	CLA	B	839	X	-	X	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
20	CLA	B	840	X	-	-	-
20	CLA	B	841	X	-	-	-
20	CLA	B	842	X	-	-	-
20	CLA	B	850	X	-	-	-
20	CLA	F	201	X	-	X	-
20	CLA	F	205	X	-	-	-
20	CLA	F	206	X	-	-	-
20	CLA	F	207	X	-	-	-
20	CLA	G	105	X	-	-	X
20	CLA	H	101	X	-	-	X
20	CLA	H	102	X	-	-	-
20	CLA	H	111	X	-	X	-
20	CLA	H	112	X	-	-	-
20	CLA	I	102	X	-	-	-
20	CLA	J	101	X	-	-	-
20	CLA	J	103	X	-	-	-
20	CLA	K	101	X	-	-	-
20	CLA	K	102	X	-	X	-
20	CLA	K	103	X	-	-	-
20	CLA	K	104	X	-	-	-
20	CLA	L	201	X	-	X	-
20	CLA	L	202	X	-	-	X
20	CLA	L	203	X	-	X	-
20	CLA	L	204	X	-	-	X
20	CLA	L	208	X	-	-	-
20	CLA	L	209	X	-	X	-
20	CLA	L	210	X	-	-	-
20	CLA	R	107	X	-	-	-
20	CLA	R	108	X	-	-	-
21	LMU	2	313	-	-	X	-
21	LMU	A	852	-	-	-	X
21	LMU	A	853	-	-	X	-
21	LMU	G	101	-	-	X	-
21	LMU	K	107	-	-	X	-
22	BCR	2	318	-	-	-	X
22	BCR	A	843	-	-	X	X
22	BCR	A	844	-	-	X	-
22	BCR	A	845	-	-	X	-
22	BCR	B	801	-	-	X	-
22	BCR	B	846	-	-	X	-
22	BCR	B	847	-	-	X	-
22	BCR	F	203	-	-	X	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
22	BCR	F	204	-	-	X	-
22	BCR	G	104	-	-	-	X
22	BCR	I	103	-	-	X	X
22	BCR	J	102	-	-	X	-
22	BCR	L	211	-	-	X	X
23	PQN	A	842	X	-	-	-
23	PQN	B	843	X	-	X	-
24	SF4	A	856	-	-	X	-
24	SF4	C	102	-	-	X	-

2 Entry composition

There are 26 unique types of molecules in this entry. The entry contains 36033 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	153	Total	C	N	O	S	0	0	0
			1186	781	193	207	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			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
16	L	162	Total	C	N	O	S	0	0	0
			1215	800	194	216	5			

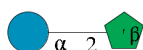
- Molecule 17 is a protein called PHOTOSYSTEM I-N SUBUNIT.

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.



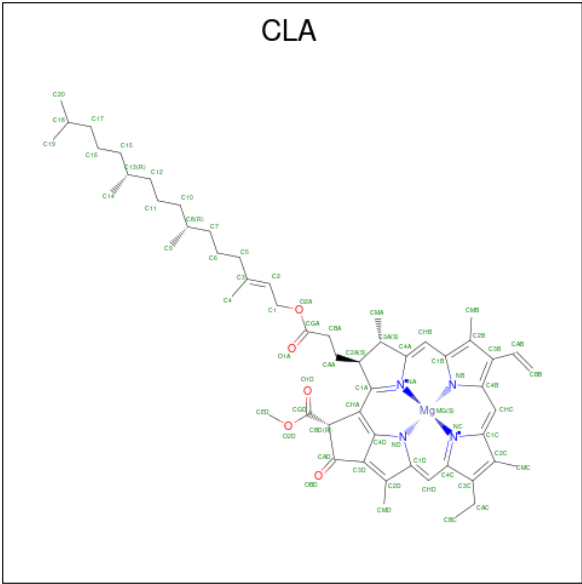
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace
19	M	2	Total	C	O	0	0	0
			23	12	11			
19	O	2	Total	C	O	0	0	0
			22	12	10			
19	P	2	Total	C	O	0	0	0
			23	12	11			

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace
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
			22	12	10			
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 (three-letter code: CLA) (formula: C₅₅H₇₂MgN₄O₅).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
20	1	1	Total	C	Mg	N	O	0	0
			46	36	1	4	5		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
20	1	1	Total	C	Mg	N	O	0	0
			41	33	1	4	3		
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		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
			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
			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
			51	41	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
			51	41	1	4	5		
20	2	1	Total	C	Mg	N	O	0	0
			58	48	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		

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

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
20	3	1	Total	C	Mg	N	O	0	0
			65	55	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	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		0	0
			25	20	1	4			
20	4	1	Total	C	Mg	N	O	0	0
			50	40	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	O	0	0
			52	42	1	4	5		
20	4	1	Total	C	Mg	N	O	0	0
			47	37	1	4	5		

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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		0	0
			25	20	1	4			
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
			55	45	1	4	5		
20	A	1	Total	C	Mg	N	O	0	0
			54	44	1	4	5		
20	A	1	Total	C	Mg	N	O	0	0
			56	46	1	4	5		
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
			60	50	1	4	5		
20	A	1	Total	C	Mg	N	O	0	0
			52	42	1	4	5		
20	A	1	Total	C	Mg	N	O	0	0
			45	35	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	O	0	0
			54	44	1	4	5		
20	A	1	Total	C	Mg	N	O	0	0
			50	40	1	4	5		
20	A	1	Total	C	Mg	N		0	0
			25	20	1	4			
20	A	1	Total	C	Mg	N	O	0	0
			50	40	1	4	5		
20	A	1	Total	C	Mg	N	O	0	0
			54	44	1	4	5		
20	A	1	Total	C	Mg	N	O	0	0
			52	42	1	4	5		
20	A	1	Total	C	Mg	N	O	0	0
			60	50	1	4	5		
20	A	1	Total	C	Mg	N	O	0	0
			58	48	1	4	5		
20	A	1	Total	C	Mg	N	O	0	0
			51	41	1	4	5		
20	A	1	Total	C	Mg	N	O	0	0
			42	34	1	4	3		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
20	A	1	Total	C	Mg	N	O	0	0
			50	40	1	4	5		
20	A	1	Total	C	Mg	N	O	0	0
			58	48	1	4	5		
20	A	1	Total	C	Mg	N	O	0	0
			59	49	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	O	0	0
			65	55	1	4	5		
20	A	1	Total	C	Mg	N	O	0	0
			55	45	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	O	0	0
			50	40	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	O	0	0
			65	55	1	4	5		
20	A	1	Total	C	Mg	N	O	0	0
			50	40	1	4	5		
20	A	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
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	O	0	0
			47	37	1	4	5		
20	A	1	Total	C	Mg	N	O	0	0
			51	41	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	O	0	0
			59	49	1	4	5		
20	A	1	Total	C	Mg	N	O	0	0
			55	45	1	4	5		
20	A	1	Total	C	Mg	N		0	0
			25	20	1	4			
20	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
20	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
20	A	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
			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
			45	35	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
			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		0	0
			25	20	1	4			
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
			60	50	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
			53	43	1	4	5		
20	B	1	Total	C	Mg	N	O	0	0
			41	33	1	4	3		
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		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
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
			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
			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
			59	49	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		

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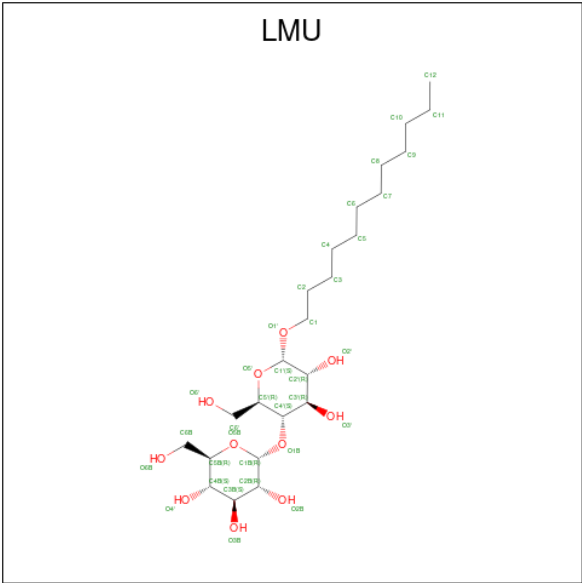
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
20	F	1	Total 50	C 40	Mg 1	N 4	O 5	0	0
20	F	1	Total 36	C 30	Mg 1	N 4	O 1	0	0
20	F	1	Total 41	C 33	Mg 1	N 4	O 3	0	0
20	F	1	Total 53	C 43	Mg 1	N 4	O 5	0	0
20	G	1	Total 51	C 41	Mg 1	N 4	O 5	0	0
20	H	1	Total 55	C 45	Mg 1	N 4	O 5	0	0
20	H	1	Total 55	C 45	Mg 1	N 4	O 5	0	0
20	H	1	Total 58	C 48	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 48	C 38	Mg 1	N 4	O 5	0	0
20	J	1	Total 61	C 51	Mg 1	N 4	O 5	0	0
20	K	1	Total 46	C 36	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 50	C 40	Mg 1	N 4	O 5	0	0
20	K	1	Total 56	C 46	Mg 1	N 4	O 5	0	0
20	L	1	Total 60	C 50	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 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 50	C 40	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 (three-letter code: 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		

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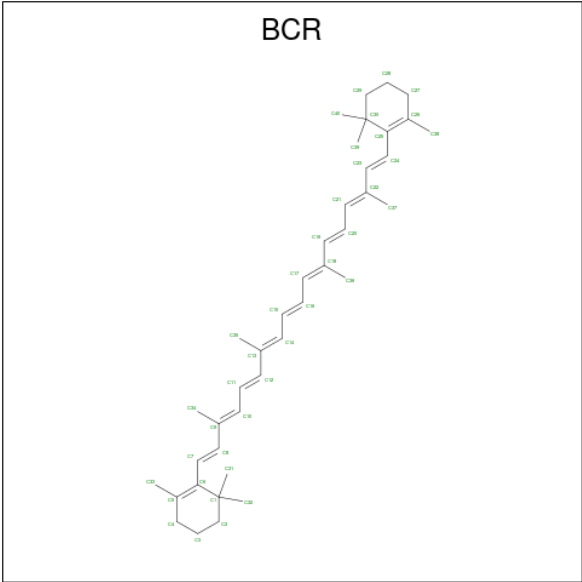
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
21	2	1	Total	C	O	0	0
			35	24	11		
21	3	1	Total	C	O	0	0
			35	24	11		
21	3	1	Total	C	O	0	0
			35	24	11		
21	4	1	Total	C	O	0	0
			35	24	11		
21	4	1	Total	C	O	0	0
			34	23	11		
21	4	1	Total	C	O	0	0
			35	24	11		
21	4	1	Total	C	O	0	0
			35	24	11		
21	A	1	Total	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	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	D	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		

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

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



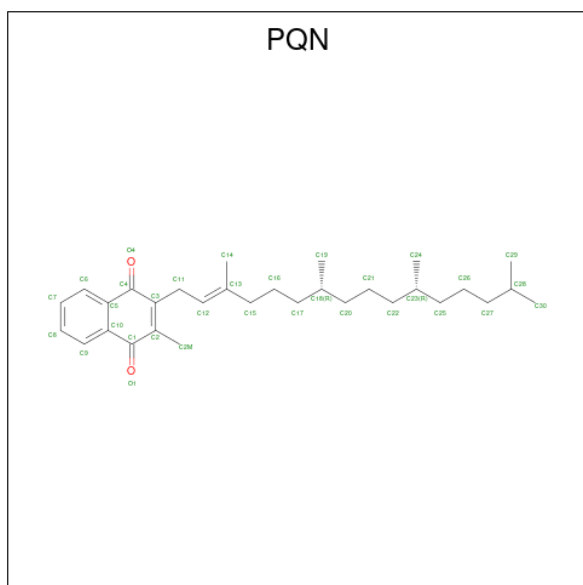
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
22	2	1	Total C 40 40	0	0
22	A	1	Total C 40 40	0	0
22	A	1	Total C 40 40	0	0
22	A	1	Total C 40 40	0	0
22	B	1	Total C 40 40	0	0
22	B	1	Total C 40 40	0	0
22	B	1	Total C 40 40	0	0
22	B	1	Total C 40 40	0	0
22	B	1	Total C 40 40	0	0
22	F	1	Total C 40 40	0	0
22	F	1	Total C 40 40	0	0
22	G	1	Total C 40 40	0	0
22	I	1	Total C 39 39	0	0
22	I	1	Total C 40 40	0	0

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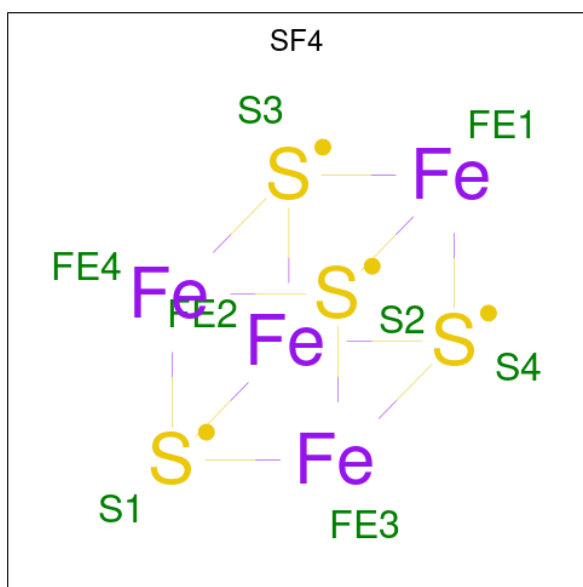
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
22	J	1	Total C 40 40	0	0
22	L	1	Total C 40 40	0	0

- Molecule 23 is PHYLLOQUINONE (three-letter code: PQN) (formula: $C_{31}H_{46}O_2$).



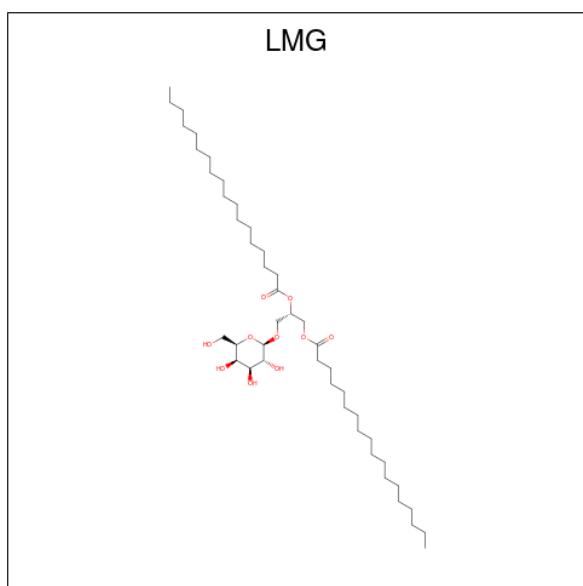
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
23	A	1	Total C O 33 31 2	0	0
23	B	1	Total C O 33 31 2	0	0

- Molecule 24 is IRON/SULFUR CLUSTER (three-letter code: 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		

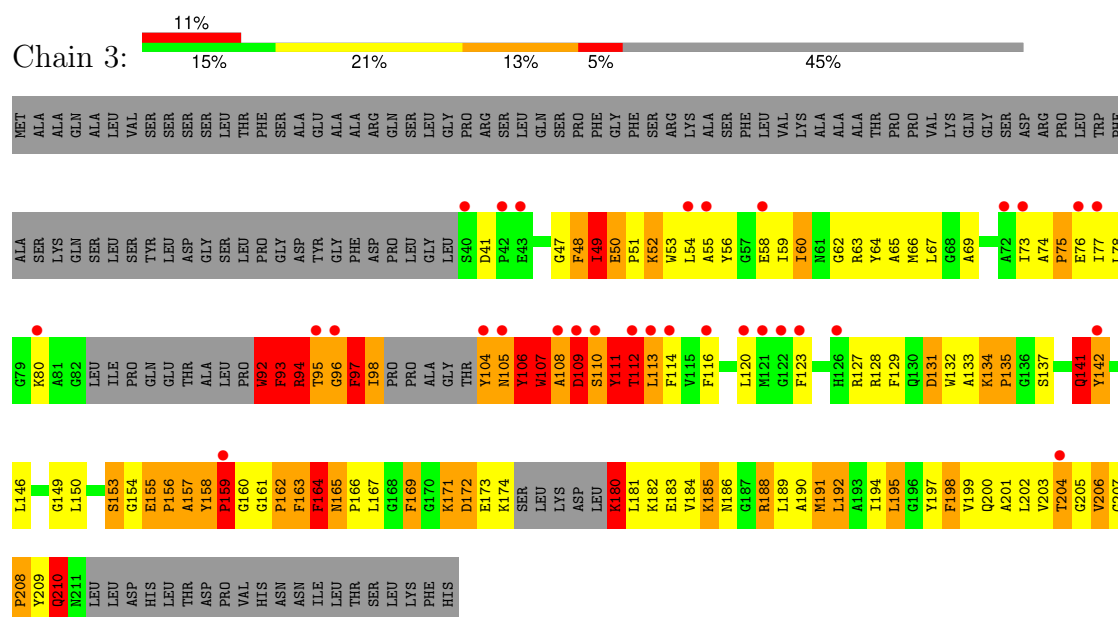
- Molecule 25 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (three-letter code: LMG) (formula: $C_{45}H_{86}O_{10}$).



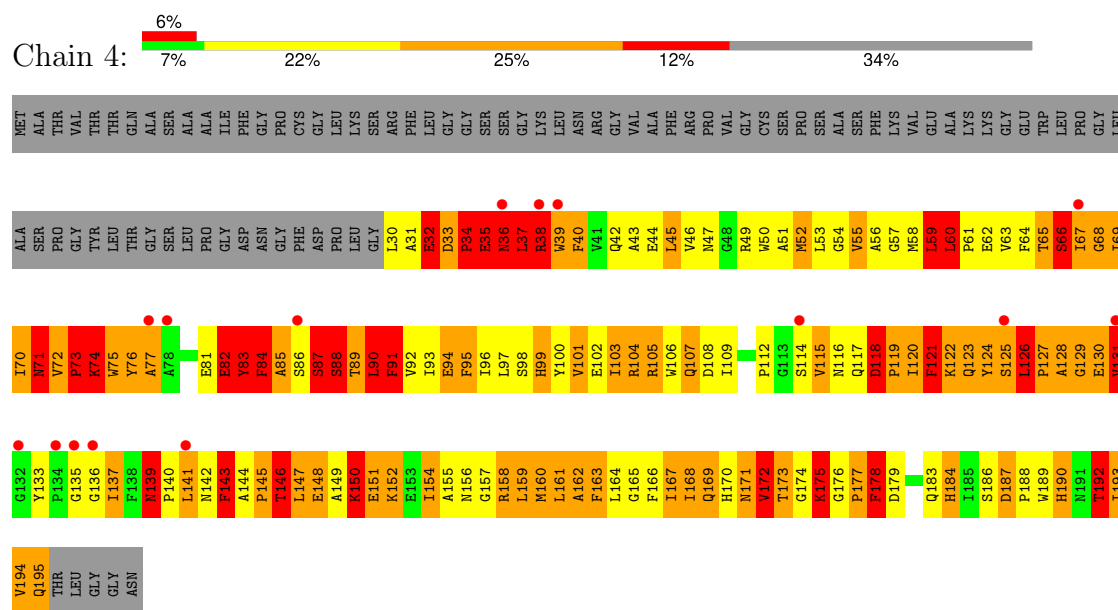
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
25	B	1	Total	C	O	0	0
			49	39	10		

- Molecule 26 is UNKNOWN LIGAND (three-letter code: UNL) (formula:).

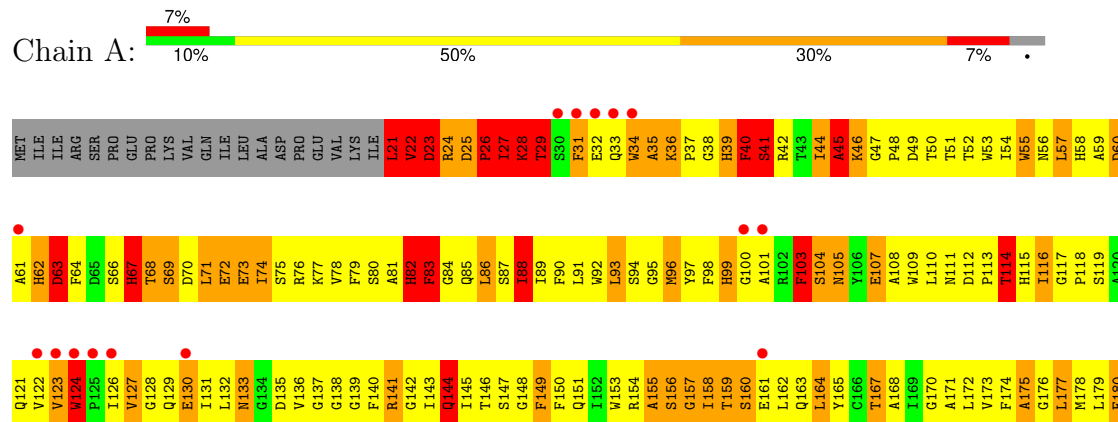
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
26	H	1	Total	C	O	0	0
			23	12	11		

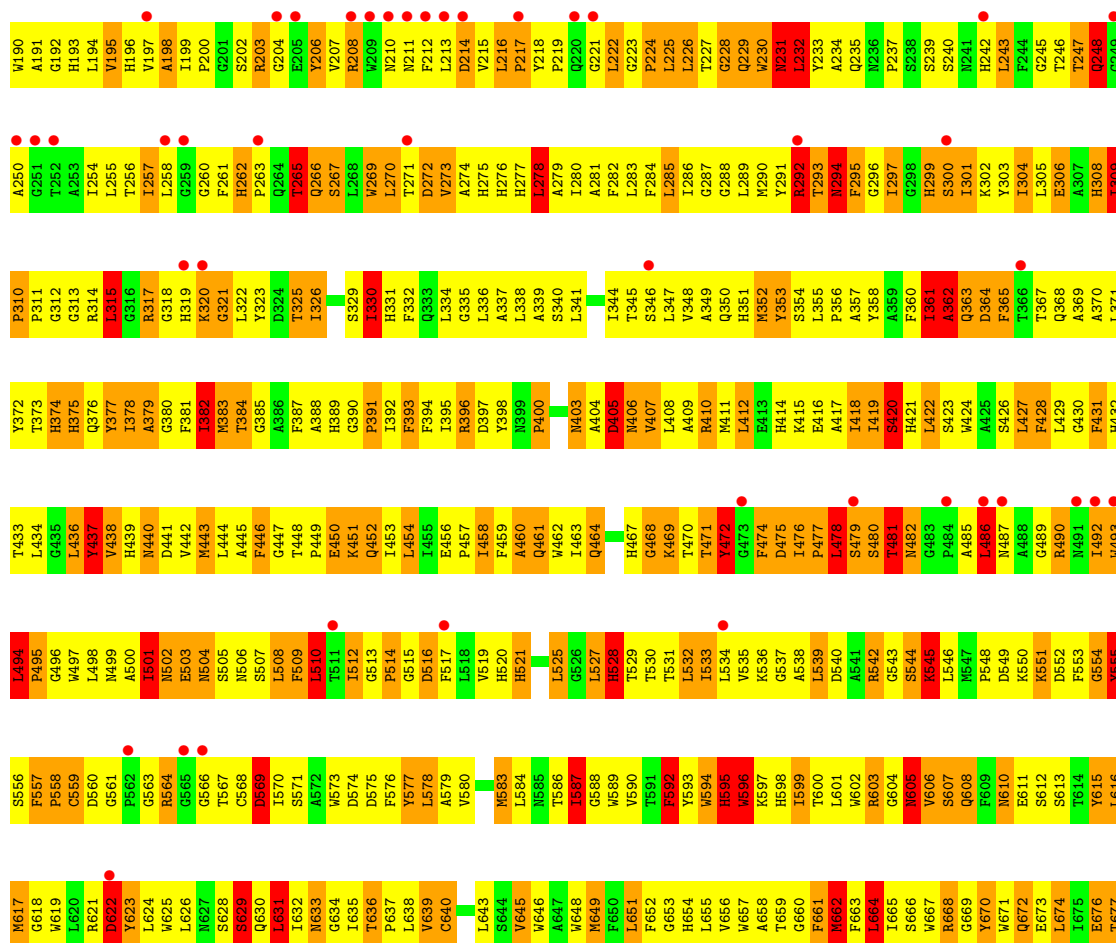


- Molecule 4: CHLOROPHYLL A-B BINDING PROTEIN P4, CHLOROPLASTIC

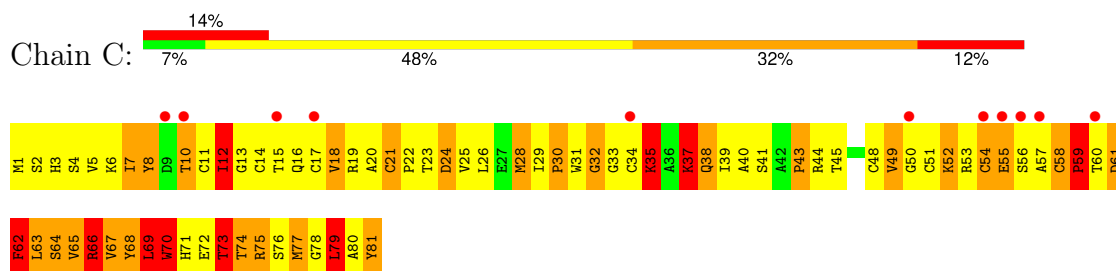


- Molecule 5: PHOTOSYSTEM I P700 CHLOROPHYLL A APOPROTEIN A1

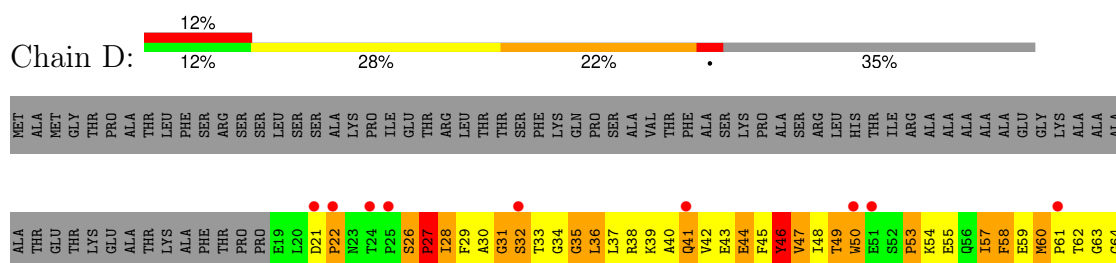


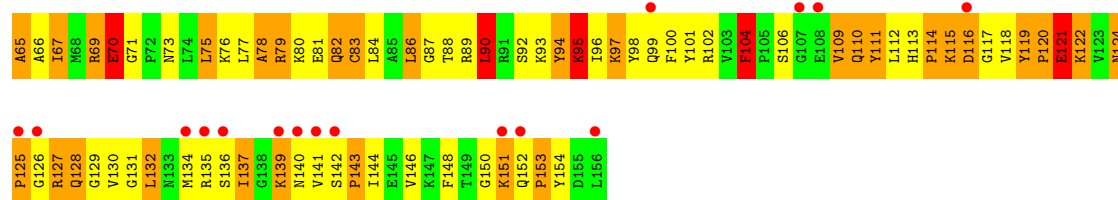


• Molecule 7: PHOTOSYSTEM I IRON-SULFUR CENTER

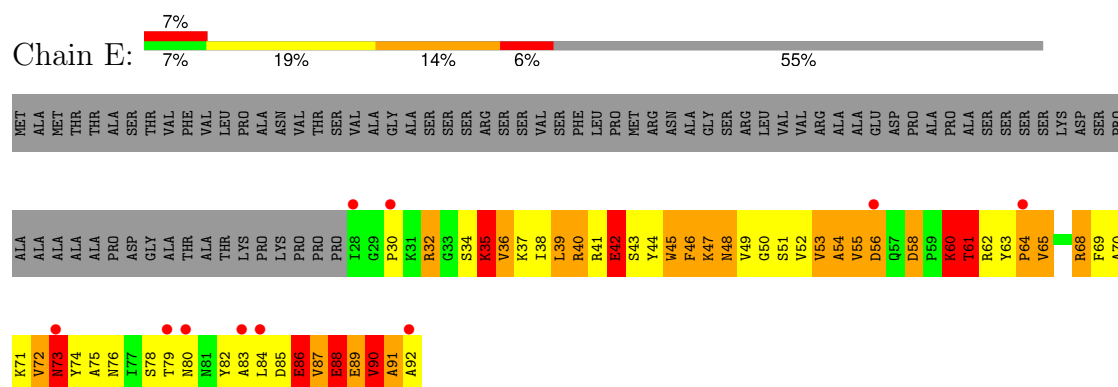


• Molecule 8: PHOTOSYSTEM I REACTION CENTER SUBUNIT II, CHLOROPLASTIC

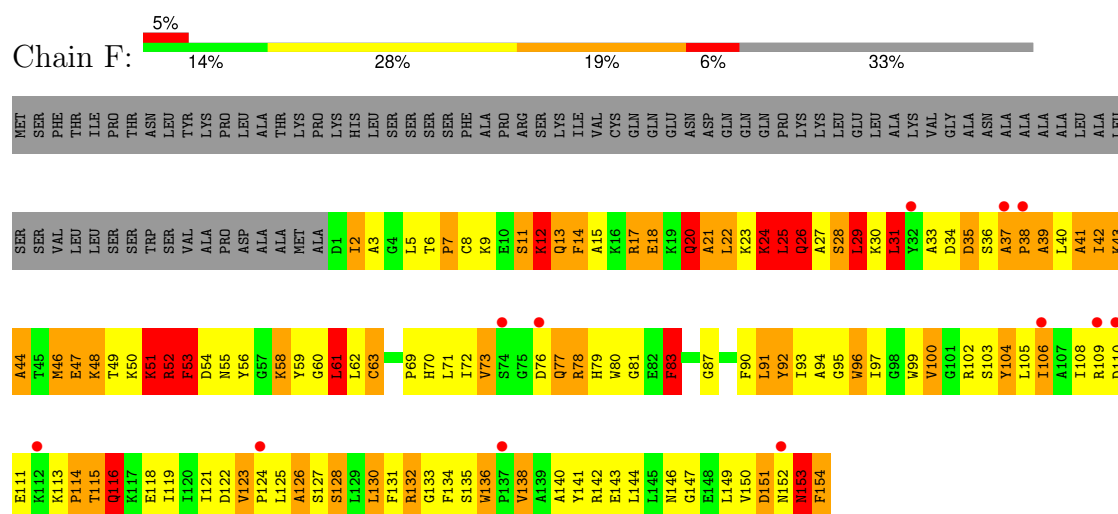




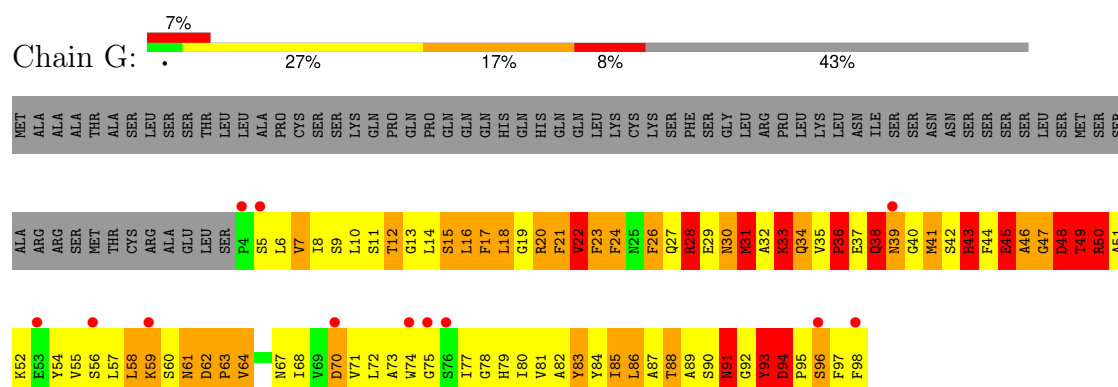
• Molecule 9: PHOTOSYSTEM I REACTION CENTER SUBUNIT IV A, CHLOROPLASTIC



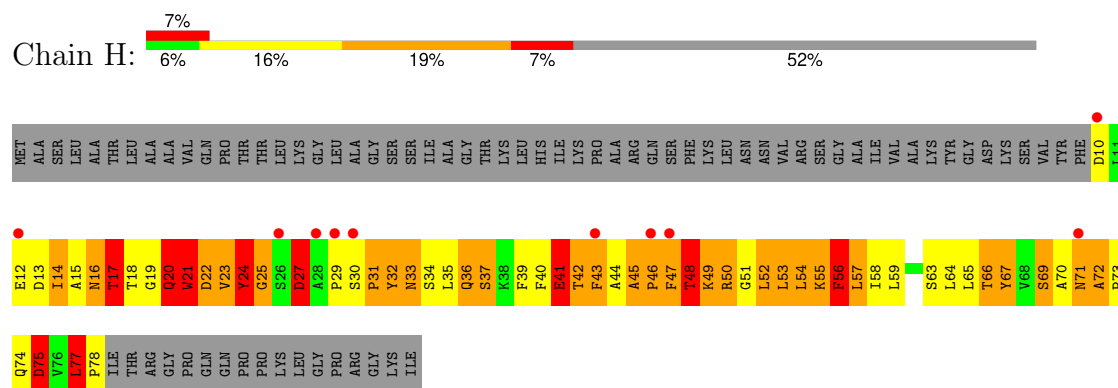
• Molecule 10: PHOTOSYSTEM I REACTION CENTER SUBUNIT III, CHLOROPLASTIC



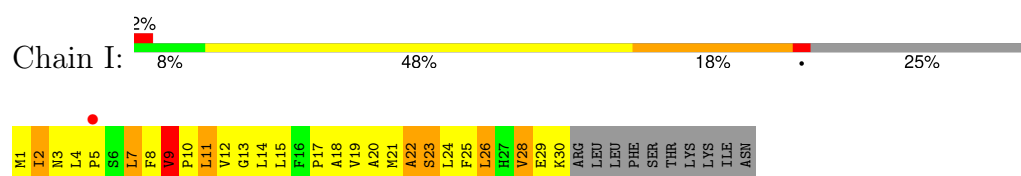
• Molecule 11: PHOTOSYSTEM I REACTION CENTER SUBUNIT V, CHLOROPLASTIC



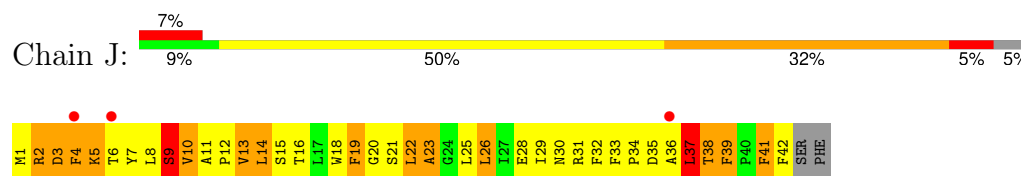
● Molecule 12: PHOTOSYSTEM I REACTION CENTER SUBUNIT VI, CHLOROPLASTIC



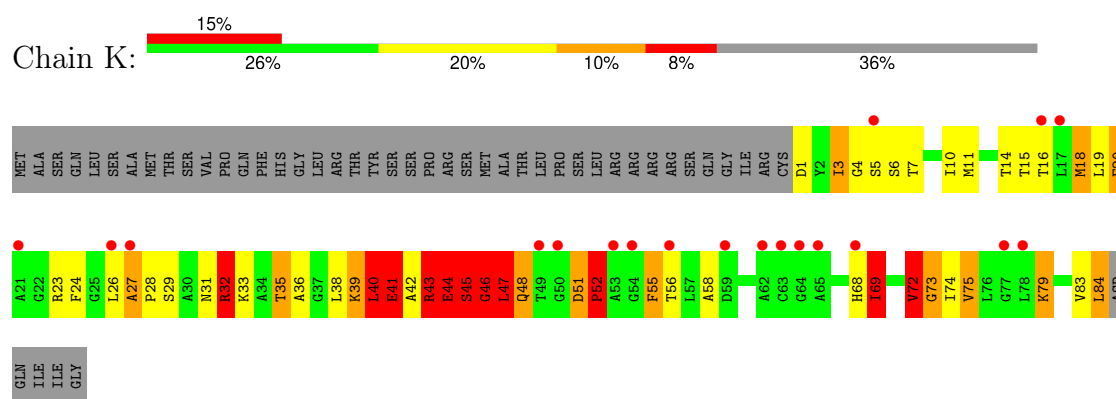
● Molecule 13: PHOTOSYSTEM I REACTION CENTER SUBUNIT VIII



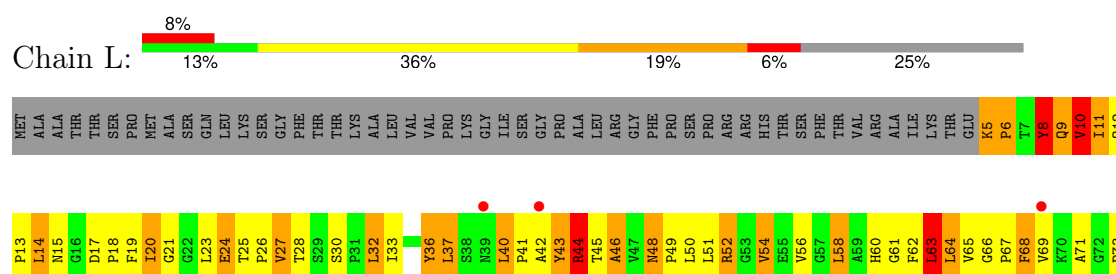
● Molecule 14: PHOTOSYSTEM I REACTION CENTER SUBUNIT IX

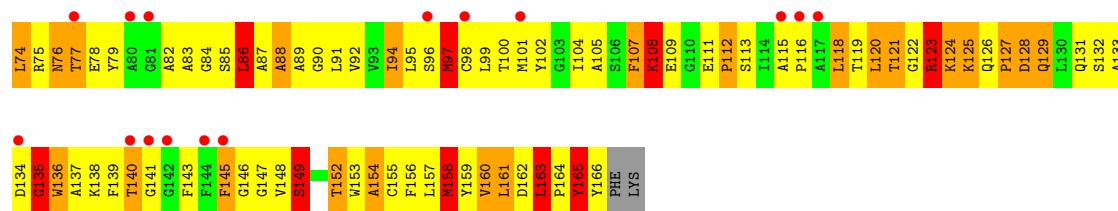


● Molecule 15: PHOTOSYSTEM I REACTION CENTER SUBUNIT PSAK, CHLOROPLASTIC

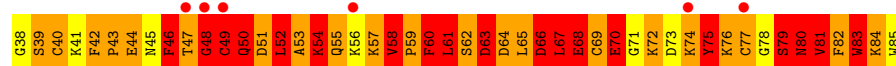
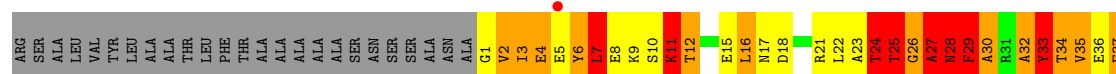
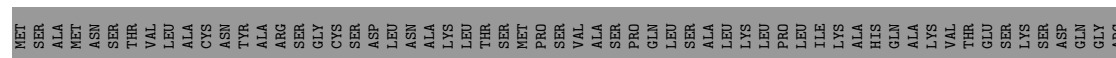
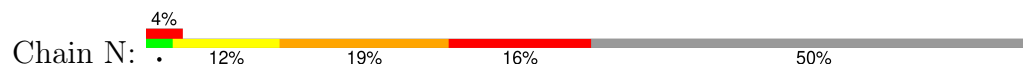


● Molecule 16: PHOTOSYSTEM I REACTION CENTER SUBUNIT XI, CHLOROPLASTIC





• Molecule 17: PHOTOSYSTEM I-N SUBUNIT



• Molecule 18: PHOTOSYSTEM I-N SUBUNIT



• Molecule 19: beta-D-fructofuranose-(2-1)-alpha-D-glucopyranose



• Molecule 19: beta-D-fructofuranose-(2-1)-alpha-D-glucopyranose



• Molecule 19: beta-D-fructofuranose-(2-1)-alpha-D-glucopyranose



• Molecule 19: beta-D-fructofuranose-(2-1)-alpha-D-glucopyranose



GLC1
FRU2

- Molecule 19: beta-D-fructofuranose-(2-1)-alpha-D-glucopyranose

Chain S:  50% 50%GLC1
FRU2

- Molecule 19: beta-D-fructofuranose-(2-1)-alpha-D-glucopyranose

Chain T:  100%GLC1
FRU2

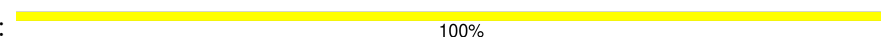
- Molecule 19: beta-D-fructofuranose-(2-1)-alpha-D-glucopyranose

Chain U:  100%GLC1
FRU2

- Molecule 19: beta-D-fructofuranose-(2-1)-alpha-D-glucopyranose

Chain V:  100%GLC1
FRU2

- Molecule 19: beta-D-fructofuranose-(2-1)-alpha-D-glucopyranose

Chain W:  100%GLC1
FRU2

- Molecule 19: beta-D-fructofuranose-(2-1)-alpha-D-glucopyranose

Chain X:  50% 50%GLC1
FRU2

- Molecule 19: beta-D-fructofuranose-(2-1)-alpha-D-glucopyranose

Chain Y:  100%GLC1
FRU2

- Molecule 19: beta-D-fructofuranose-(2-1)-alpha-D-glucopyranose

Chain Z:  50% 50%



- Molecule 19: beta-D-fructofuranose-(2-1)-alpha-D-glucopyranose

Chain a:  50% 50%



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	120.20Å 190.20Å 130.30Å 90.00° 91.53° 90.00°	Depositor
Resolution (Å)	50.00 – 3.48 49.46 – 3.47	Depositor EDS
% Data completeness (in resolution range)	96.4 (50.00-3.48) 96.2 (49.46-3.47)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.61 (at 3.48Å)	Xtriage
Refinement program	REFMAC 5.5.0072	Depositor
R, R_{free}	0.391 , 0.425 0.383 , 0.387	Depositor DCC
R_{free} test set	1456 reflections (2.01%)	wwPDB-VP
Wilson B-factor (Å ²)	81.0	Xtriage
Anisotropy	0.408	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.09 , 30.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.016 for h,-k,-l	Xtriage
F_o, F_c correlation	0.74	EDS
Total number of atoms	36033	wwPDB-VP
Average B, all atoms (Å ²)	26.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.96% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: UNL, LMG, SF4, PQN, LMU, GLC, CLA, BCR, FRU

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	1	0.55	1/1303 (0.1%)	0.73	1/1774 (0.1%)
2	2	0.67	0/1420	1.10	7/1943 (0.4%)
3	3	0.60	0/1221	0.91	2/1642 (0.1%)
4	4	0.77	0/1359	1.12	10/1851 (0.5%)
5	A	0.61	1/5938 (0.0%)	0.88	9/8104 (0.1%)
6	B	0.58	0/6058	0.86	8/8278 (0.1%)
7	C	0.78	0/632	1.05	1/856 (0.1%)
8	D	0.71	0/1122	0.91	0/1514
9	E	0.70	0/530	0.95	1/718 (0.1%)
10	F	0.67	0/1250	0.88	0/1687
11	G	0.84	1/760 (0.1%)	1.20	7/1031 (0.7%)
12	H	0.70	0/543	1.02	0/741
13	I	0.62	0/235	0.80	0/320
14	J	0.65	0/349	0.91	0/475
15	K	0.65	1/599 (0.2%)	0.88	1/810 (0.1%)
16	L	0.69	1/1251 (0.1%)	0.94	2/1709 (0.1%)
17	N	0.89	0/699	1.22	5/936 (0.5%)
All	All	0.65	5/25269 (0.0%)	0.93	54/34389 (0.2%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	1	0	3
2	2	0	17
3	3	0	17
4	4	0	20
5	A	0	20
6	B	0	12

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Mol	Chain	#Chirality outliers	#Planarity outliers
7	C	0	1
8	D	0	1
9	E	0	3
10	F	0	7
11	G	1	13
12	H	0	9
15	K	0	6
16	L	0	2
17	N	0	22
18	R	0	16
All	All	1	169

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	L	165	TYR	CE2-CZ	-6.04	1.30	1.38
11	G	15	SER	CB-OG	5.83	1.49	1.42
1	1	185	TRP	CB-CG	-5.34	1.40	1.50
15	K	41	GLU	CG-CD	5.15	1.59	1.51
5	A	22	VAL	CA-CB	-5.05	1.44	1.54

The worst 5 of 54 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	3	180	LYS	C-N-CA	-10.34	95.85	121.70
11	G	46	ALA	N-CA-C	-10.20	83.47	111.00
6	B	731	GLY	N-CA-C	-7.75	93.73	113.10
11	G	16	LEU	CA-CB-CG	7.25	131.98	115.30
6	B	315	LEU	CA-CB-CG	7.00	131.41	115.30

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
11	G	21	PHE	CA

5 of 169 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	1	184	PRO	Peptide
1	1	185	TRP	Peptide
1	1	72	GLN	Peptide

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Mol	Chain	Res	Type	Group
2	2	42	ARG	Peptide
2	2	73	ILE	Peptide

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	1	1264	0	1229	137	3
2	2	1374	0	1331	301	2
3	3	1186	0	1147	293	16
4	4	1319	0	1282	610	5
5	A	5745	0	5597	1351	0
6	B	5848	0	5655	1211	15
7	C	619	0	608	204	0
8	D	1095	0	1112	189	0
9	E	520	0	528	129	0
10	F	1221	0	1249	201	0
11	G	740	0	708	191	1
12	H	529	0	514	106	0
13	I	229	0	252	55	0
14	J	338	0	340	64	0
15	K	593	0	619	110	0
16	L	1215	0	1222	311	5
17	N	685	0	668	321	1
18	R	265	0	68	78	0
19	M	23	0	21	0	0
19	O	22	0	18	10	0
19	P	23	0	21	10	0
19	Q	23	0	21	6	0
19	S	23	0	21	1	0
19	T	23	0	21	3	0
19	U	23	0	21	1	0
19	V	23	0	21	4	0
19	W	23	0	21	3	0
19	X	22	0	18	3	0
19	Y	23	0	21	1	41
19	Z	23	0	21	14	0
19	a	23	0	21	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
20	1	617	0	388	89	1
20	2	650	0	465	147	0
20	3	620	0	362	75	0
20	4	694	0	443	167	0
20	A	2346	0	2062	726	0
20	B	2226	0	2061	684	0
20	F	180	0	123	46	0
20	G	51	0	40	4	0
20	H	223	0	197	57	0
20	I	60	0	58	12	0
20	J	109	0	95	26	0
20	K	202	0	158	54	1
20	L	382	0	335	103	0
20	R	122	0	123	14	0
21	1	105	0	137	32	0
21	2	175	0	230	45	0
21	3	70	0	92	16	0
21	4	139	0	179	24	3
21	A	245	0	322	53	0
21	B	95	0	115	11	0
21	C	35	0	46	0	0
21	D	35	0	46	3	0
21	E	35	0	46	11	0
21	F	34	0	41	8	0
21	G	105	0	138	27	41
21	H	140	0	184	42	0
21	K	105	0	138	41	0
21	L	105	0	138	2	0
21	R	245	0	322	43	3
22	2	40	0	54	9	0
22	A	120	0	162	103	0
22	B	200	0	270	114	0
22	F	80	0	108	60	0
22	G	40	0	54	5	0
22	I	79	0	105	46	0
22	J	40	0	54	36	0
22	L	40	0	54	36	0
23	A	33	0	46	7	0
23	B	33	0	46	28	0
24	A	8	0	0	18	0
24	C	16	0	0	5	0
25	B	49	0	71	17	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
26	H	23	0	0	1	0
All	All	36033	0	34504	7353	69

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 104.

The worst 5 of 7353 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:4:160:MET:CE	20:4:306:CLA:HBB2	1.18	1.65
4:4:69:ILE:HD11	4:4:175:LYS:CB	1.26	1.65
3:3:97:PHE:CD2	3:3:98:ILE:HG23	1.33	1.62
1:1:185:TRP:CH2	20:1:213:CLA:H12	1.38	1.59
3:3:97:PHE:CE2	3:3:98:ILE:HD13	1.42	1.55

The worst 5 of 69 symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:Y:2:FRU:O2	21:G:101:LMU:C5B[1_456]	0.08	2.12
3:3:180:LYS:CD	6:B:490:ARG:CZ[1_556]	0.31	1.89
3:3:180:LYS:NZ	6:B:490:ARG:CD[1_556]	0.56	1.64
19:Y:1:GLC:O2	21:G:101:LMU:O4'[1_456]	1.01	1.19
3:3:180:LYS:CG	6:B:490:ARG:NE[1_556]	1.05	1.15

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	1	161/241 (67%)	84 (52%)	39 (24%)	38 (24%)	0 1
2	2	174/269 (65%)	67 (38%)	51 (29%)	56 (32%)	0 0

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	3	145/276 (52%)	76 (52%)	36 (25%)	33 (23%)	0	1
4	4	164/251 (65%)	57 (35%)	44 (27%)	63 (38%)	0	0
5	A	726/758 (96%)	366 (50%)	187 (26%)	173 (24%)	0	0
6	B	731/734 (100%)	379 (52%)	204 (28%)	148 (20%)	0	1
7	C	79/81 (98%)	23 (29%)	31 (39%)	25 (32%)	0	0
8	D	136/212 (64%)	47 (35%)	48 (35%)	41 (30%)	0	0
9	E	63/143 (44%)	30 (48%)	15 (24%)	18 (29%)	0	0
10	F	152/231 (66%)	71 (47%)	40 (26%)	41 (27%)	0	0
11	G	93/167 (56%)	38 (41%)	27 (29%)	28 (30%)	0	0
12	H	67/144 (46%)	30 (45%)	16 (24%)	21 (31%)	0	0
13	I	28/40 (70%)	11 (39%)	10 (36%)	7 (25%)	0	0
14	J	40/44 (91%)	19 (48%)	11 (28%)	10 (25%)	0	0
15	K	82/131 (63%)	50 (61%)	13 (16%)	19 (23%)	0	0
16	L	160/216 (74%)	72 (45%)	49 (31%)	39 (24%)	0	0
17	N	83/170 (49%)	21 (25%)	19 (23%)	43 (52%)	0	0
All	All	3084/4108 (75%)	1441 (47%)	840 (27%)	803 (26%)	0	0

5 of 803 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	1	25	ASP
1	1	30	GLY
1	1	35	ASN
1	1	58	LEU
1	1	73	GLU

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	1	127/190 (67%)	100 (79%)	27 (21%)	1 4

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	2	140/216 (65%)	81 (58%)	59 (42%)	0	0
3	3	112/215 (52%)	76 (68%)	36 (32%)	0	1
4	4	138/201 (69%)	85 (62%)	53 (38%)	0	1
5	A	592/618 (96%)	410 (69%)	182 (31%)	0	2
6	B	598/600 (100%)	397 (66%)	201 (34%)	0	1
7	C	70/70 (100%)	41 (59%)	29 (41%)	0	0
8	D	118/173 (68%)	82 (70%)	36 (30%)	0	2
9	E	56/114 (49%)	38 (68%)	18 (32%)	0	1
10	F	127/190 (67%)	80 (63%)	47 (37%)	0	1
11	G	79/144 (55%)	53 (67%)	26 (33%)	0	1
12	H	57/115 (50%)	30 (53%)	27 (47%)	0	0
13	I	26/36 (72%)	22 (85%)	4 (15%)	2	14
14	J	36/39 (92%)	25 (69%)	11 (31%)	0	2
15	K	61/102 (60%)	43 (70%)	18 (30%)	0	2
16	L	125/169 (74%)	88 (70%)	37 (30%)	0	2
17	N	74/139 (53%)	43 (58%)	31 (42%)	0	0
All	All	2536/3331 (76%)	1694 (67%)	842 (33%)	0	1

5 of 842 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
6	B	420	SER
7	C	54	CYS
16	L	120	LEU
6	B	452	GLN
6	B	419	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 103 such sidechains are listed below:

Mol	Chain	Res	Type
6	B	333	GLN
6	B	630	GLN
16	L	48	ASN
6	B	403	ASN
6	B	521	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

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	11,11,12	0.53	0	15,15,17	2.21	2 (13%)
19	FRU	M	2	19	11,12,12	0.66	0	10,18,18	0.75	0
19	GLC	O	1	19	10,10,12	0.91	0	14,14,17	2.18	3 (21%)
19	FRU	O	2	19	11,12,12	0.60	0	10,18,18	1.14	1 (10%)
19	GLC	P	1	19	11,11,12	0.51	0	15,15,17	1.67	4 (26%)
19	FRU	P	2	19	11,12,12	0.71	0	10,18,18	1.21	2 (20%)
19	GLC	Q	1	19	11,11,12	0.58	0	15,15,17	2.28	5 (33%)
19	FRU	Q	2	19	11,12,12	0.72	0	10,18,18	1.21	1 (10%)
19	GLC	S	1	19	11,11,12	0.61	0	15,15,17	0.96	0
19	FRU	S	2	19	11,12,12	0.81	0	10,18,18	1.49	2 (20%)
19	GLC	T	1	19	11,11,12	0.50	0	15,15,17	0.76	1 (6%)
19	FRU	T	2	19	11,12,12	0.64	0	10,18,18	1.25	1 (10%)
19	GLC	U	1	19	11,11,12	0.64	0	15,15,17	2.54	4 (26%)
19	FRU	U	2	19	11,12,12	0.67	0	10,18,18	1.37	2 (20%)
19	GLC	V	1	19	11,11,12	0.55	0	15,15,17	1.80	4 (26%)
19	FRU	V	2	19	11,12,12	0.70	0	10,18,18	1.23	1 (10%)
19	GLC	W	1	19	11,11,12	0.57	0	15,15,17	0.91	0
19	FRU	W	2	19	11,12,12	0.49	0	10,18,18	1.18	0
19	GLC	X	1	19	10,10,12	0.90	0	14,14,17	1.88	5 (35%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
19	FRU	X	2	19	11,12,12	0.54	0	10,18,18	0.61	0
19	GLC	Y	1	19	11,11,12	1.64	3 (27%)	15,15,17	2.37	6 (40%)
19	FRU	Y	2	19	11,12,12	1.38	1 (9%)	10,18,18	1.45	2 (20%)
19	GLC	Z	1	19	11,11,12	0.41	0	15,15,17	0.98	1 (6%)
19	FRU	Z	2	19	11,12,12	0.66	0	10,18,18	1.11	0
19	GLC	a	1	19	11,11,12	0.76	0	15,15,17	1.32	1 (6%)
19	FRU	a	2	19	11,12,12	0.44	0	10,18,18	1.09	0

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	-	2/2/19/22	0/1/1/1
19	FRU	M	2	19	1/1/4/4	1/5/24/24	0/1/1/1
19	GLC	O	1	19	-	-	0/1/1/1
19	FRU	O	2	19	1/1/4/4	0/5/24/24	0/1/1/1
19	GLC	P	1	19	-	0/2/19/22	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	5/5/24/24	0/1/1/1
19	GLC	S	1	19	-	2/2/19/22	0/1/1/1
19	FRU	S	2	19	1/1/4/4	1/5/24/24	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	1/5/24/24	0/1/1/1
19	GLC	U	1	19	-	1/2/19/22	0/1/1/1
19	FRU	U	2	19	1/1/4/4	0/5/24/24	0/1/1/1
19	GLC	V	1	19	-	2/2/19/22	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	-	2/2/19/22	0/1/1/1
19	FRU	W	2	19	1/1/4/4	3/5/24/24	0/1/1/1
19	GLC	X	1	19	-	-	0/1/1/1
19	FRU	X	2	19	1/1/4/4	5/5/24/24	0/1/1/1
19	GLC	Y	1	19	-	0/2/19/22	0/1/1/1
19	FRU	Y	2	19	1/1/4/4	3/5/24/24	0/1/1/1
19	GLC	Z	1	19	-	1/2/19/22	0/1/1/1
19	FRU	Z	2	19	1/1/4/4	0/5/24/24	0/1/1/1
19	GLC	a	1	19	-	0/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
19	FRU	a	2	19	1/1/4/4	4/5/24/24	0/1/1/1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	Y	2	FRU	O2-C2	4.23	1.48	1.40
19	Y	1	GLC	C1-C2	3.20	1.59	1.52
19	Y	1	GLC	C2-C3	2.89	1.56	1.52
19	Y	1	GLC	O2-C2	2.28	1.48	1.43

The worst 5 of 48 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	M	1	GLC	C1-O5-C5	7.93	122.82	112.19
19	U	1	GLC	C1-O5-C5	7.81	122.65	112.19
19	O	1	GLC	C1-C2-C3	6.00	118.38	109.64
19	Y	1	GLC	C6-C5-C4	5.70	127.01	113.02
19	V	1	GLC	C1-O5-C5	4.79	118.61	112.19

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 42 torsion outliers are listed below:

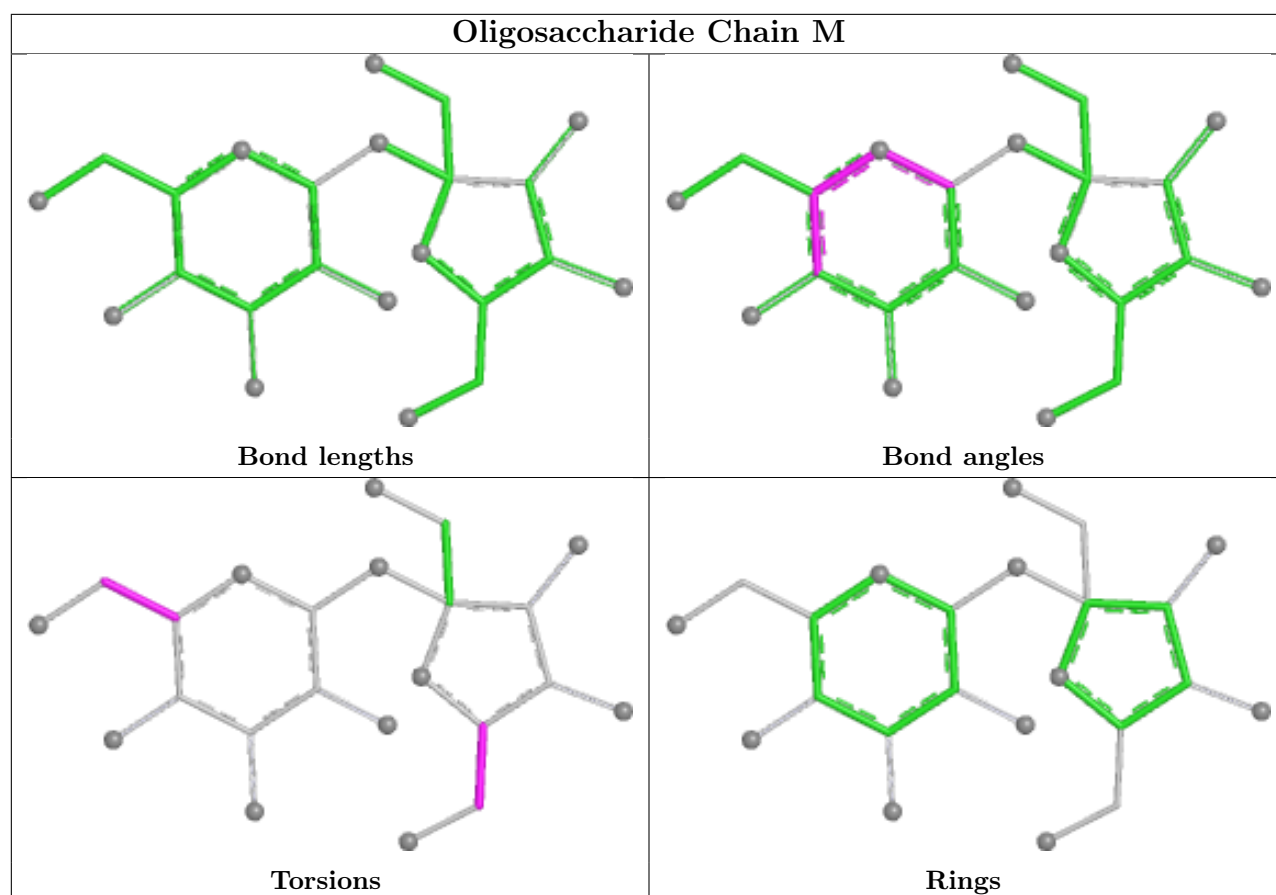
Mol	Chain	Res	Type	Atoms
19	P	2	FRU	C4-C5-C6-O6
19	P	2	FRU	O5-C5-C6-O6
19	Q	2	FRU	O1-C1-C2-C3
19	Q	2	FRU	O1-C1-C2-O2
19	V	2	FRU	O1-C1-C2-C3

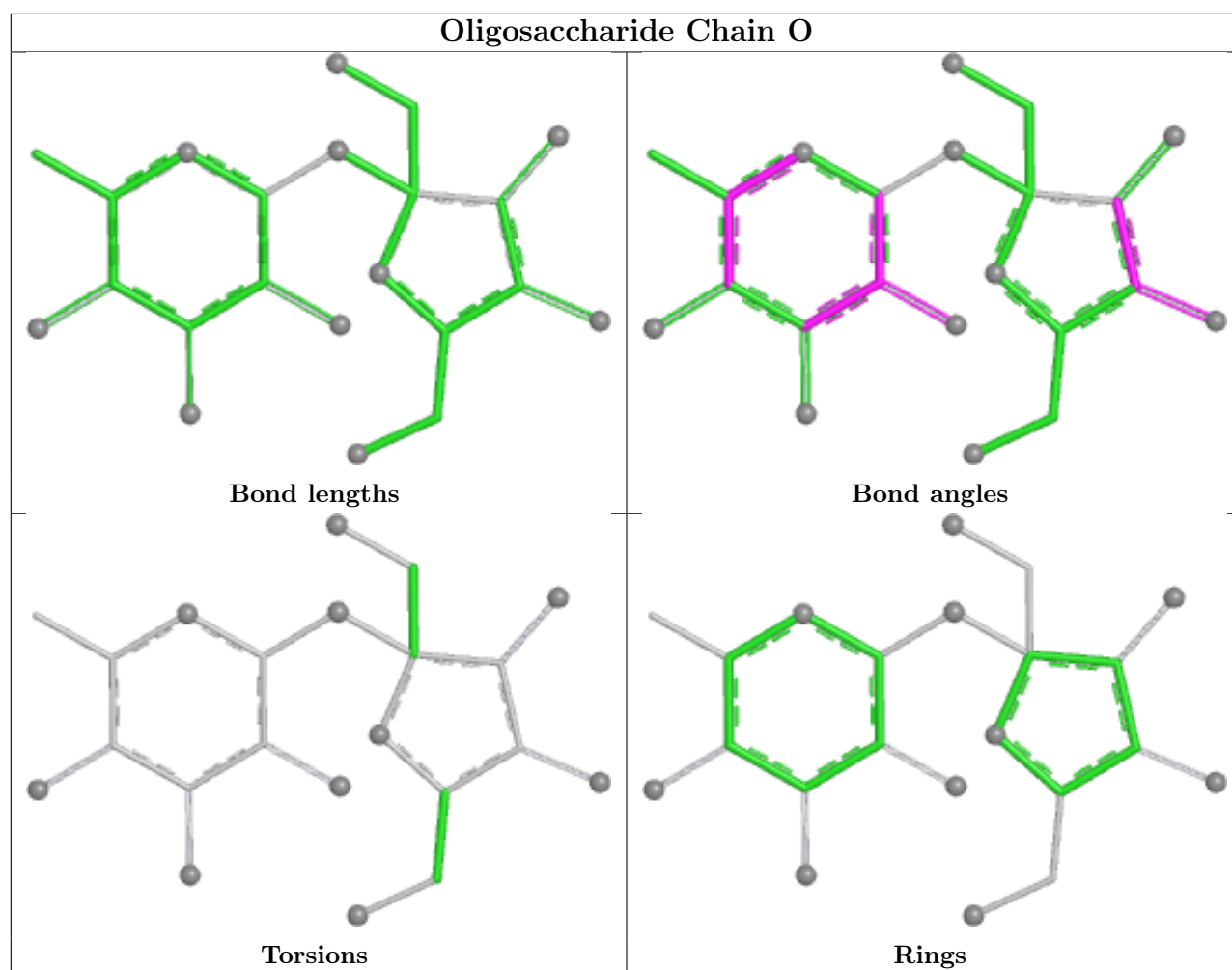
There are no ring outliers.

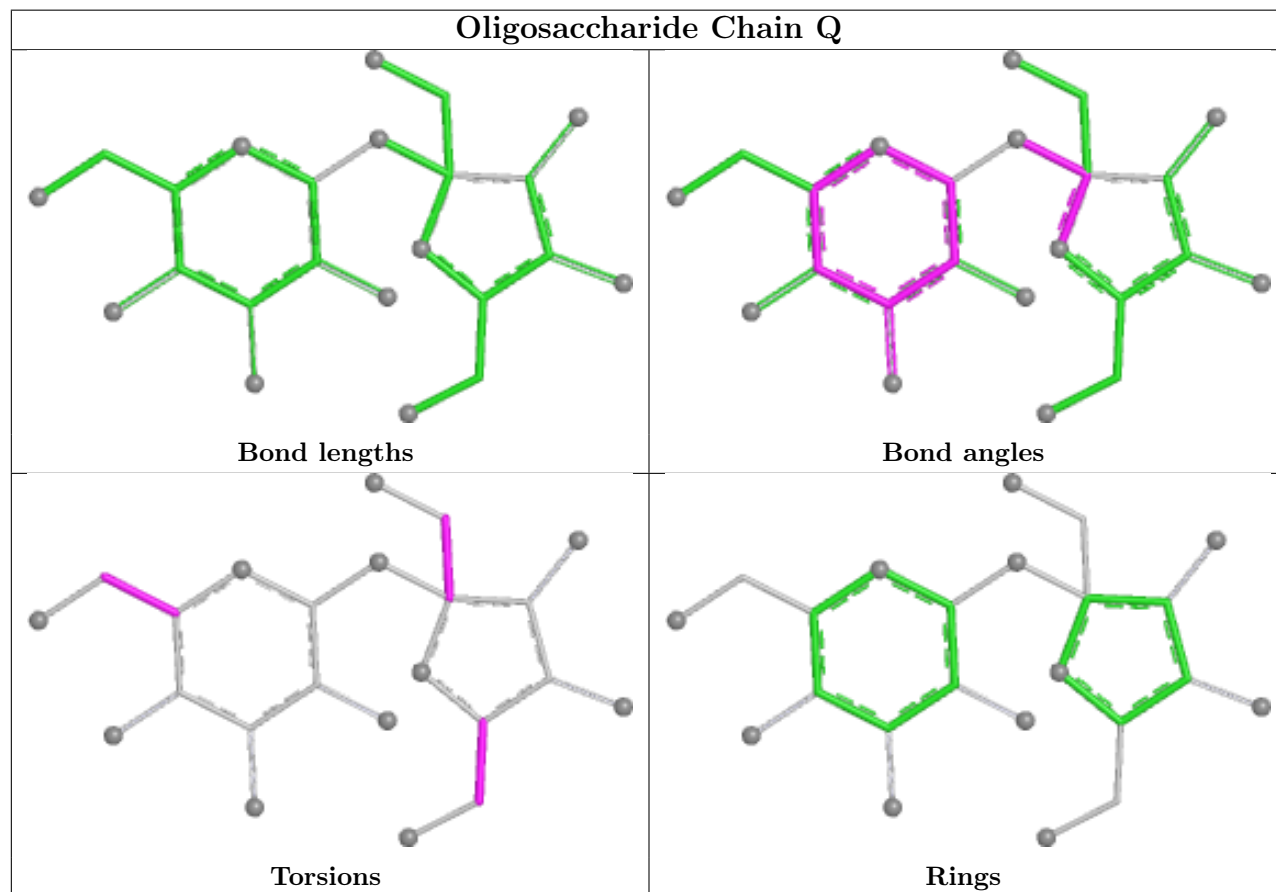
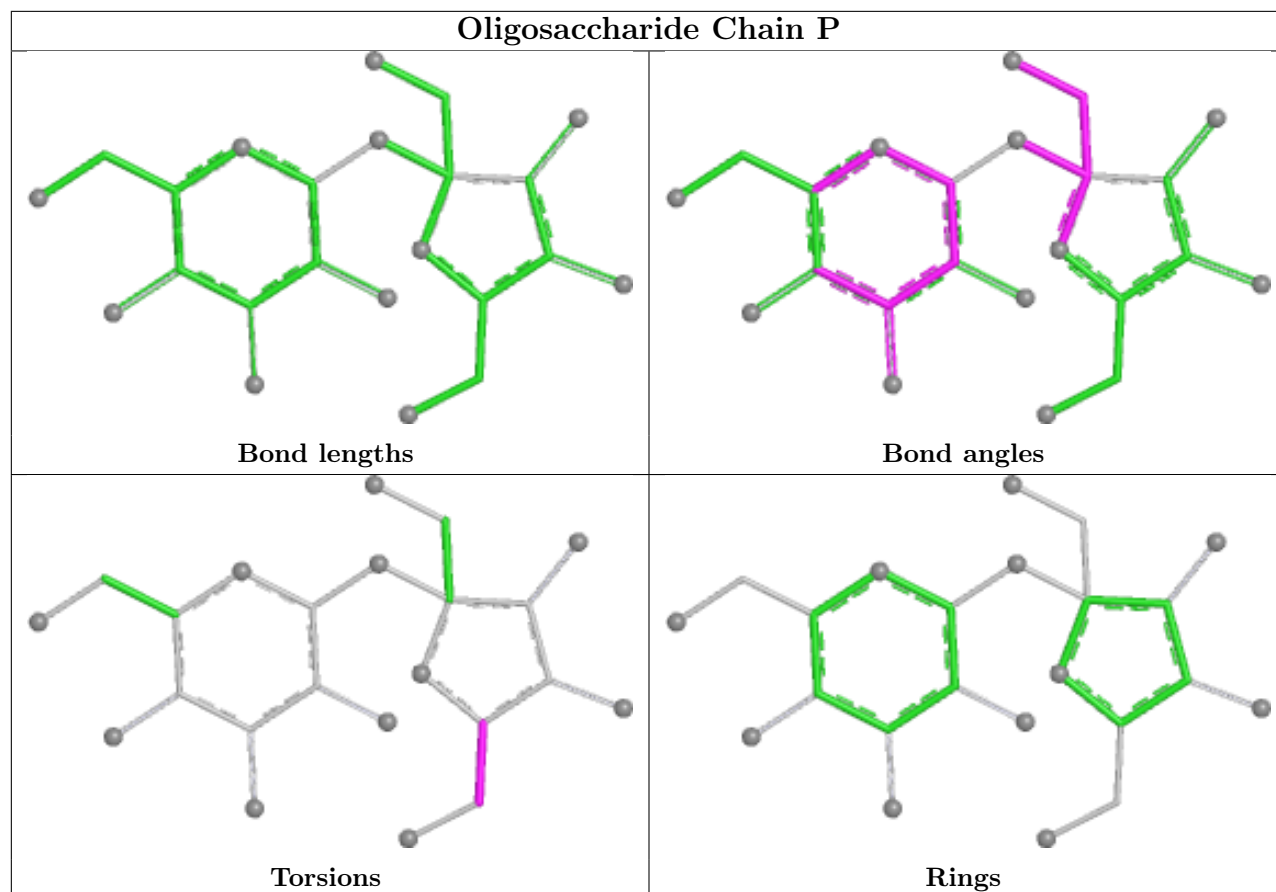
21 monomers are involved in 97 short contacts:

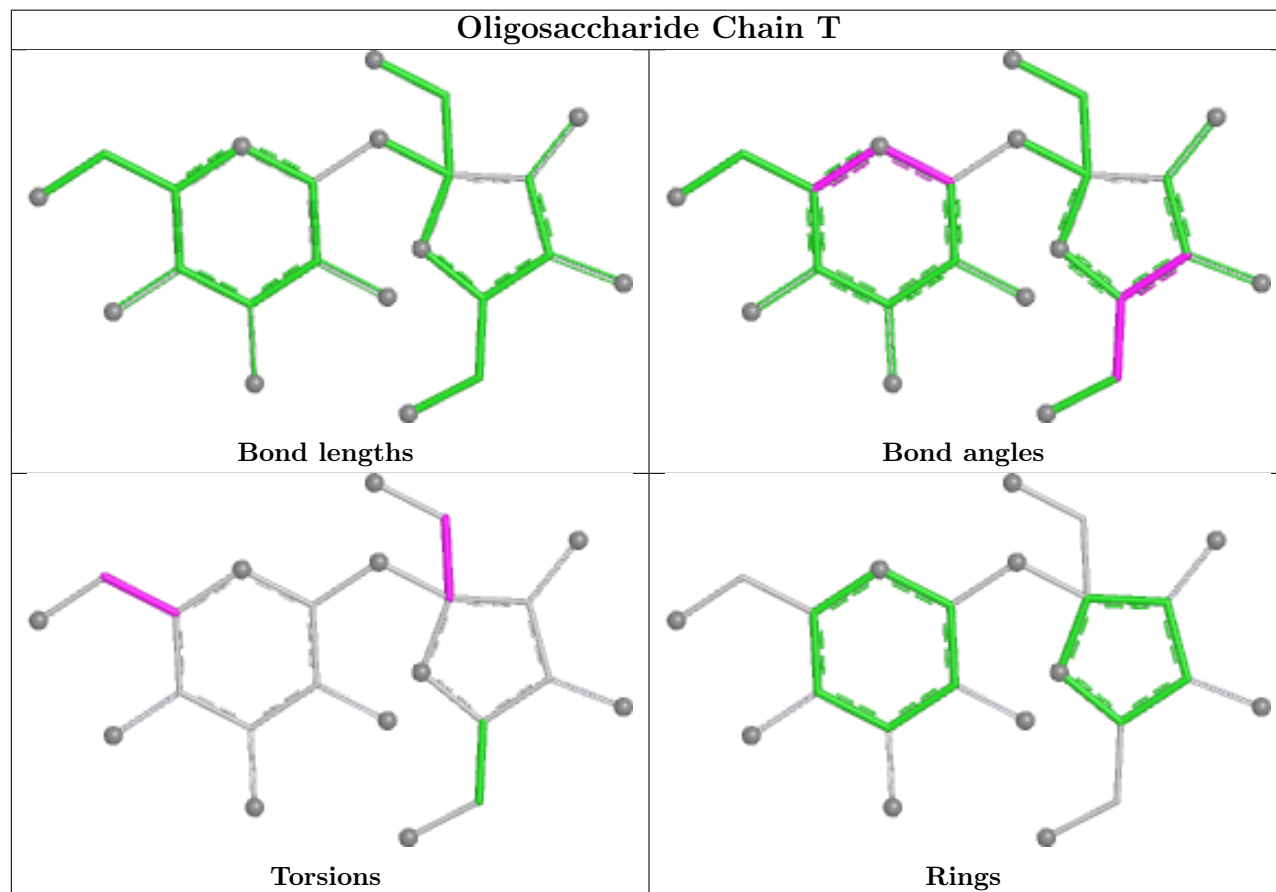
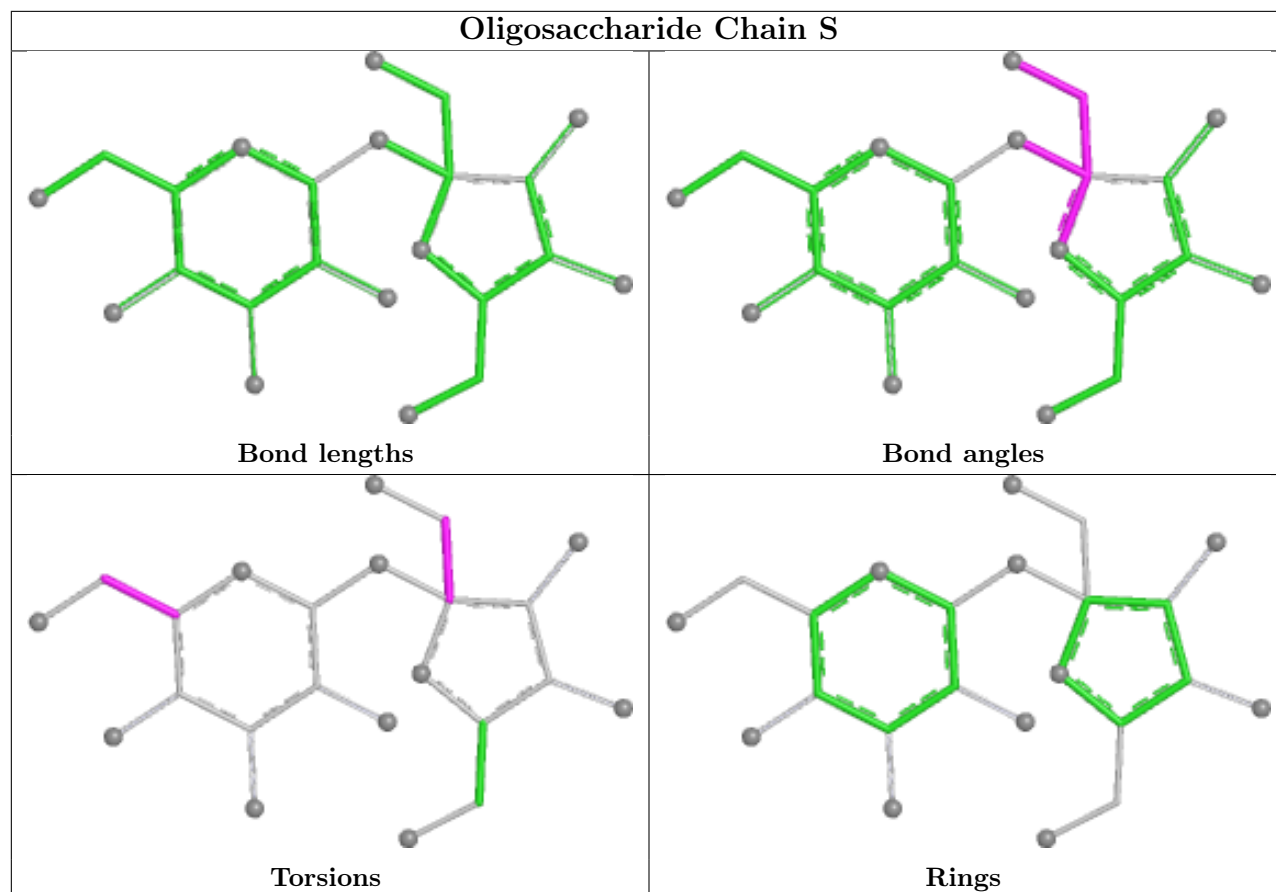
Mol	Chain	Res	Type	Clashes	Symm-Clashes
19	V	2	FRU	4	0
19	P	1	GLC	8	0
19	S	2	FRU	1	0
19	Z	1	GLC	1	0
19	Z	2	FRU	13	0
19	Q	2	FRU	6	0
19	X	1	GLC	3	0
19	O	1	GLC	10	0
19	O	2	FRU	3	0
19	X	2	FRU	3	0
19	T	2	FRU	3	0
19	Y	1	GLC	0	22
19	Y	2	FRU	1	19
19	Q	1	GLC	3	0
19	W	1	GLC	3	0
19	W	2	FRU	3	0
19	U	1	GLC	1	0
19	P	2	FRU	9	0
19	U	2	FRU	1	0
19	T	1	GLC	3	0
19	V	1	GLC	3	0

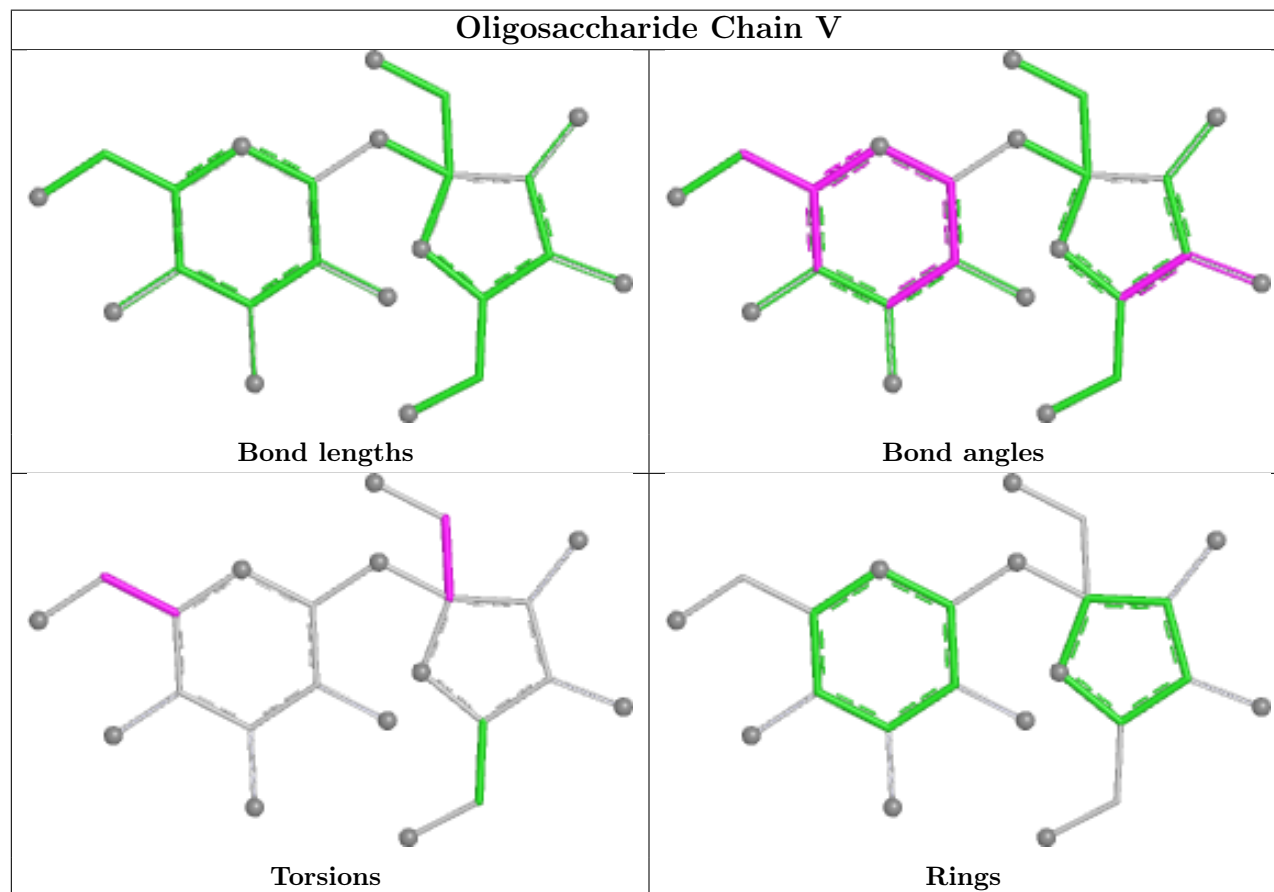
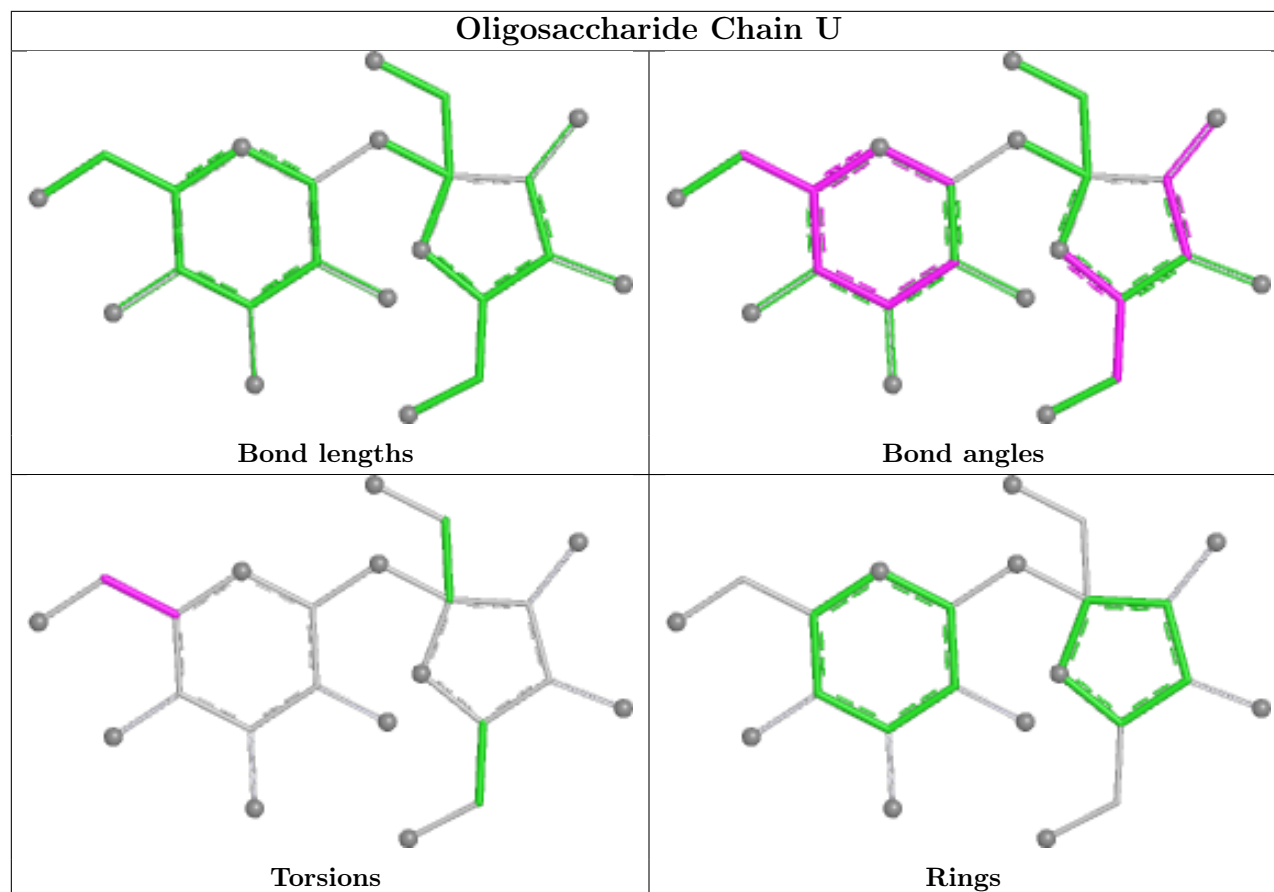
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

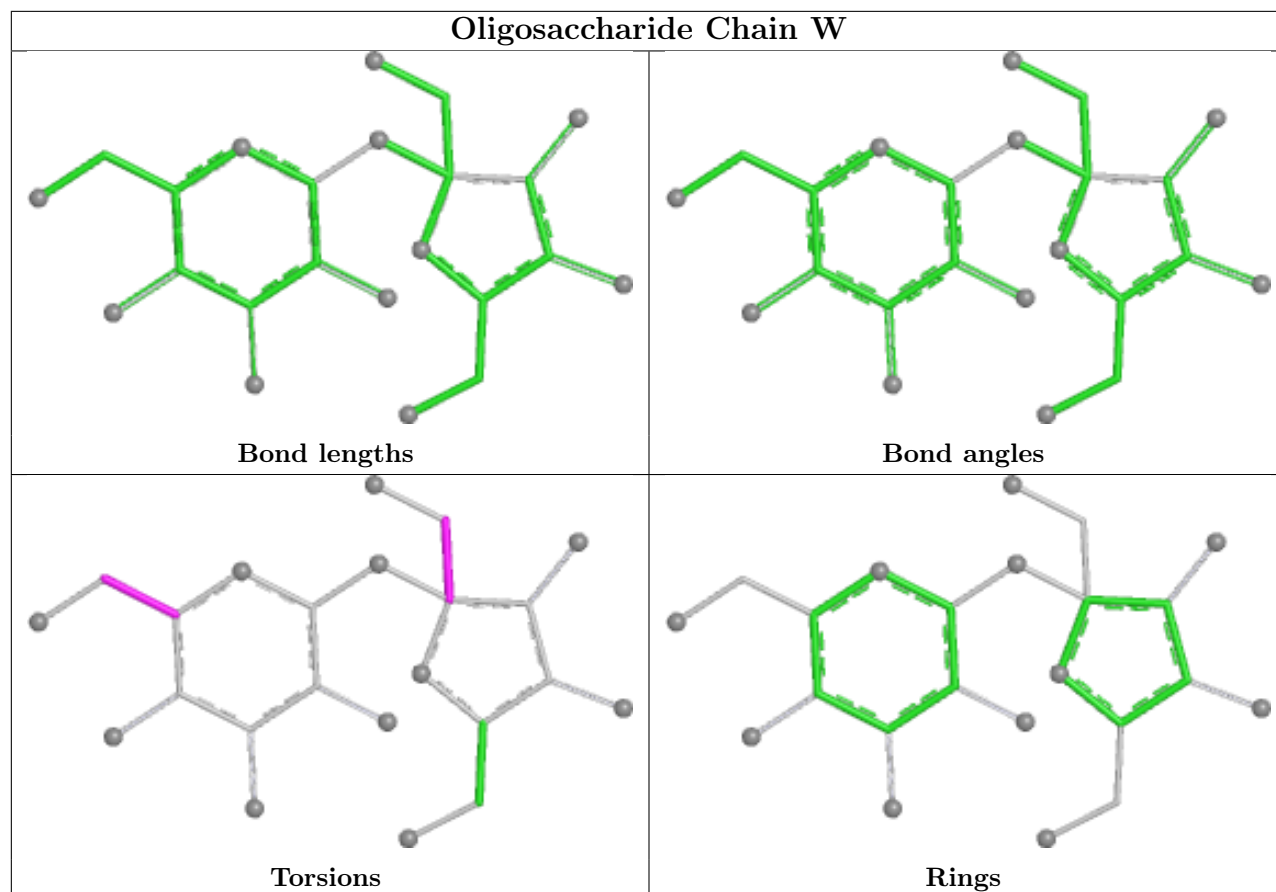


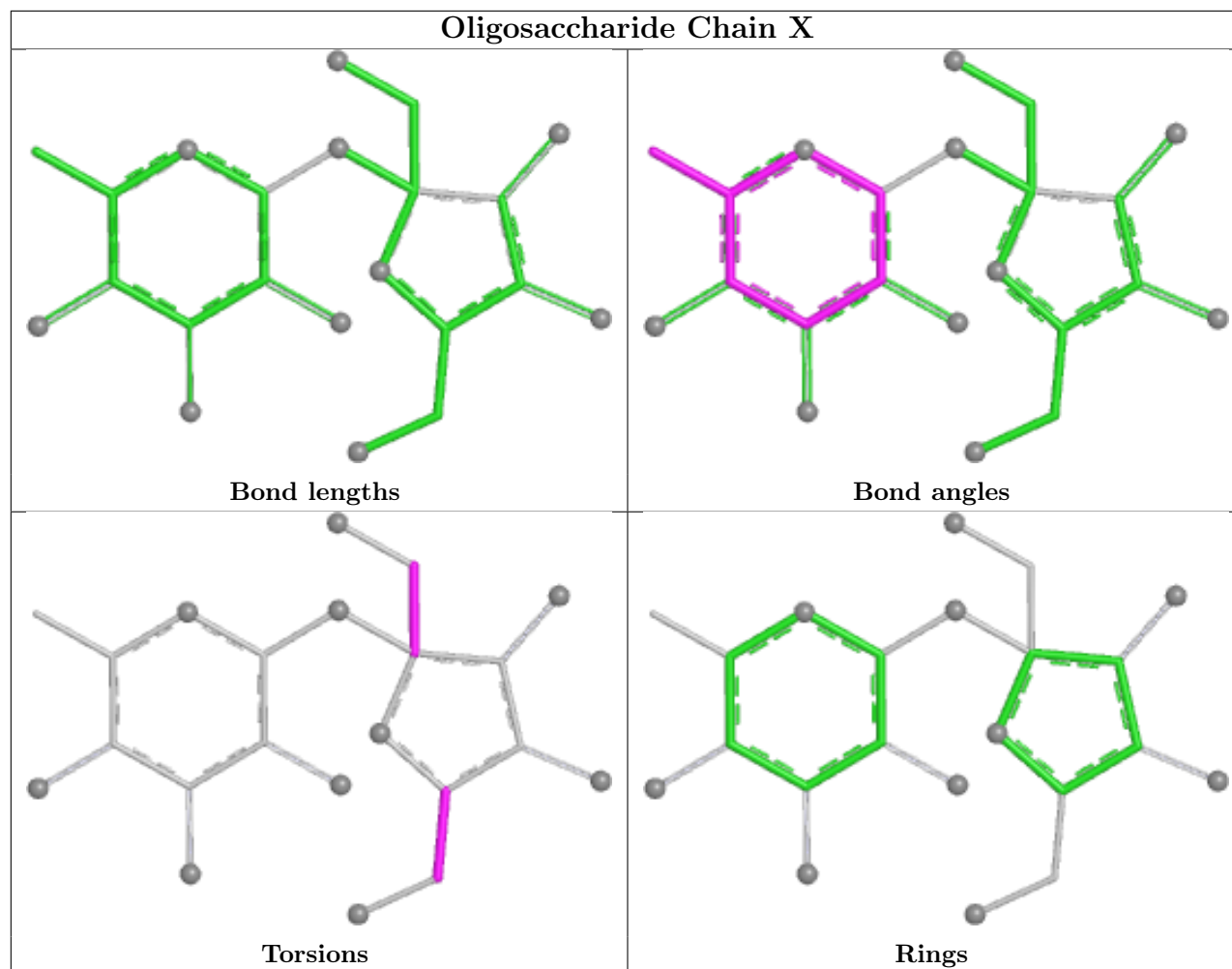


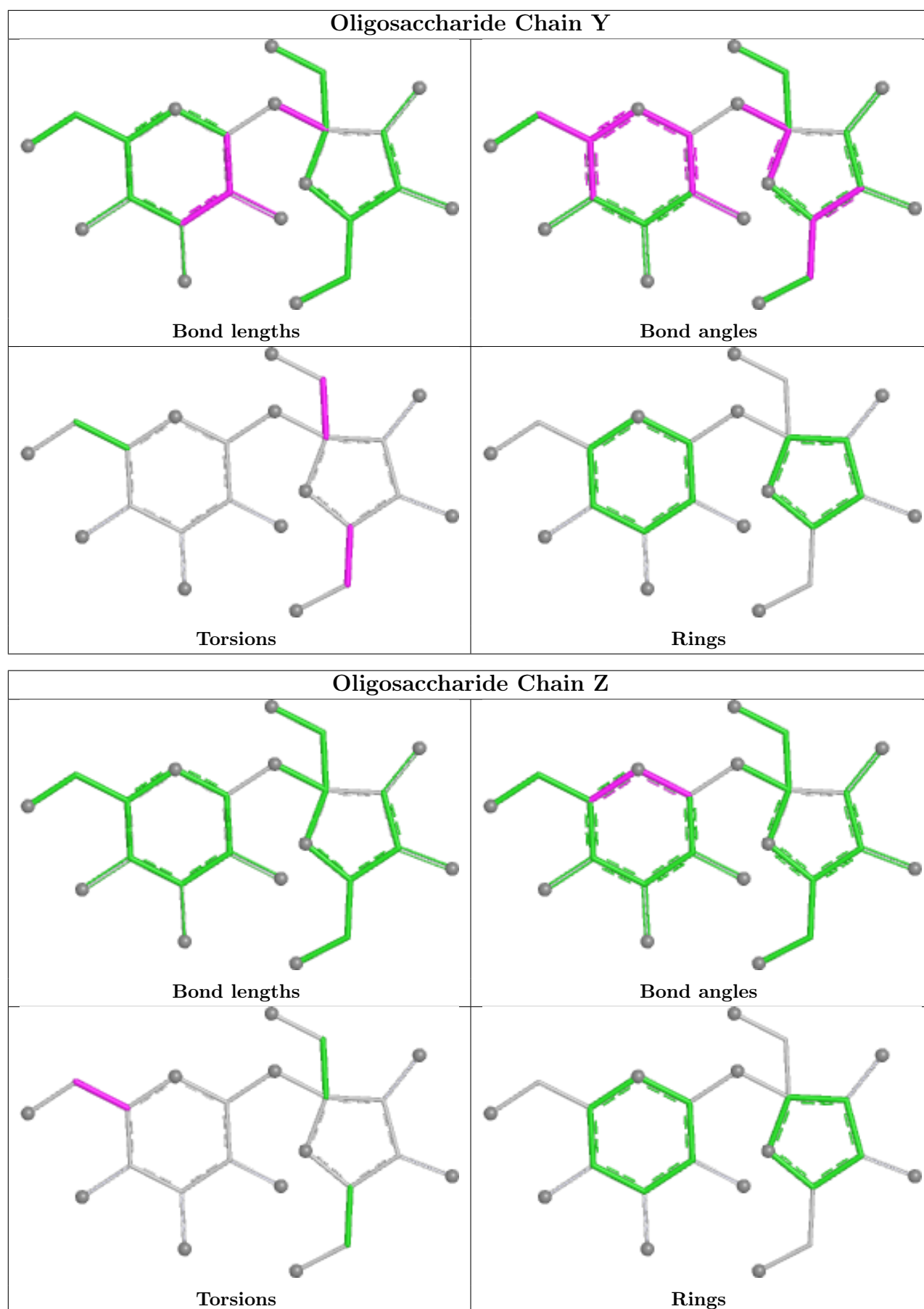


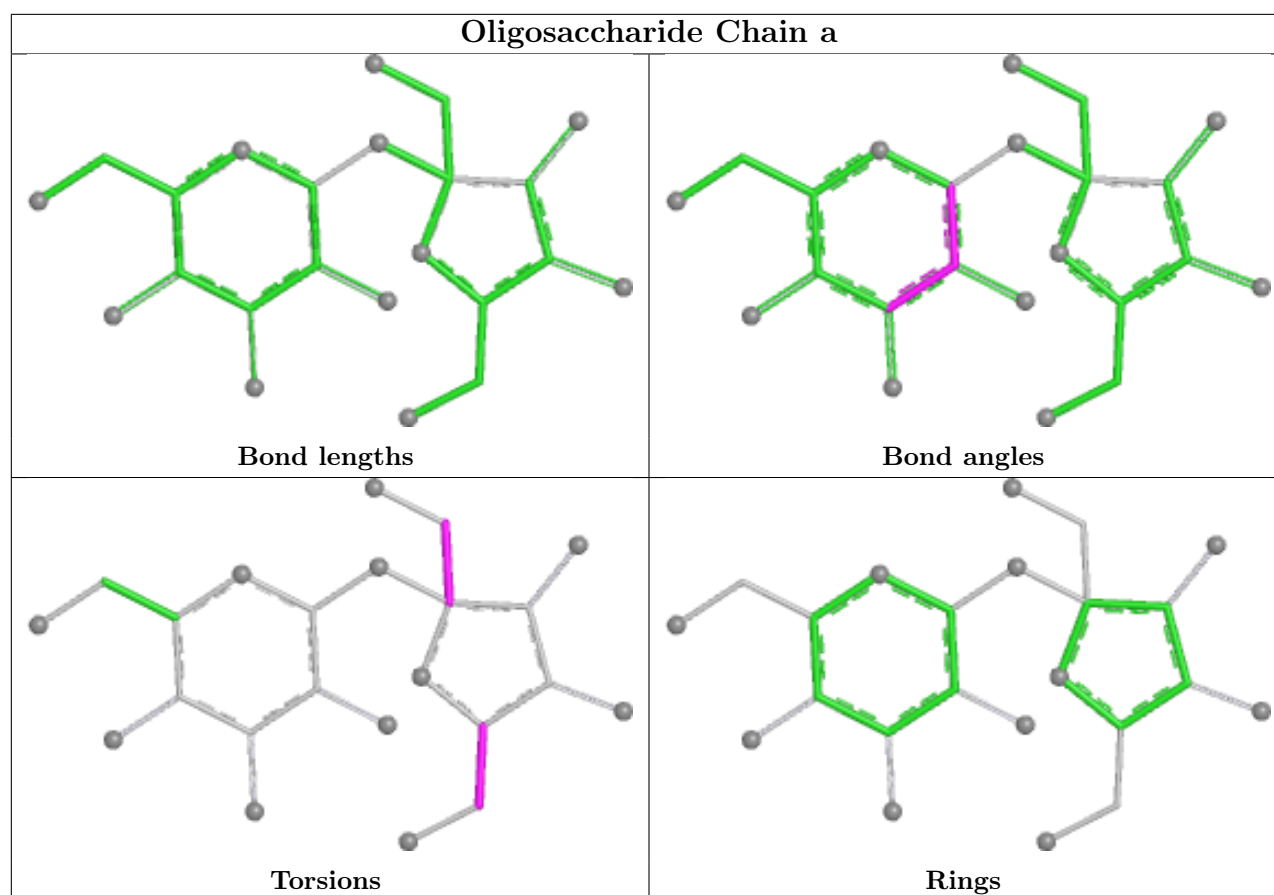












5.6 Ligand geometry [i](#)

Of 244 ligands modelled in this entry, 1 is unknown - leaving 243 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	B	828	-	63,73,73	2.12	12 (19%)	74,113,113	2.47	22 (29%)
22	BCR	F	204	-	41,41,41	1.85	5 (12%)	56,56,56	5.90	23 (41%)
20	CLA	3	303	-	33,44,73	2.98	10 (30%)	46,78,113	3.44	20 (43%)
20	CLA	4	308	-	25,32,73	2.19	10 (40%)	27,54,113	3.17	16 (59%)
20	CLA	4	313	-	33,44,73	2.90	11 (33%)	46,78,113	3.69	20 (43%)
20	CLA	A	812	-	52,62,73	2.25	12 (23%)	60,99,113	2.36	17 (28%)
24	SF4	A	856	6,5	0,12,12	-	-	-	-	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
20	CLA	2	303	-	56,66,73	2.29	16 (28%)	65,104,113	2.91	25 (38%)
22	BCR	B	844	-	41,41,41	1.65	5 (12%)	56,56,56	5.31	24 (42%)
22	BCR	F	203	-	41,41,41	1.72	3 (7%)	56,56,56	5.62	19 (33%)
20	CLA	L	203	-	63,73,73	2.03	12 (19%)	74,113,113	2.41	21 (28%)
20	CLA	A	810	-	43,53,73	2.59	13 (30%)	50,89,113	2.80	18 (36%)
20	CLA	2	316	-	25,32,73	2.09	7 (28%)	27,54,113	2.81	15 (55%)
20	CLA	A	801	-	45,54,73	2.77	15 (33%)	55,90,113	3.92	25 (45%)
24	SF4	C	103	7	0,12,12	-	-	-		
20	CLA	L	208	16	48,58,73	2.38	11 (22%)	56,95,113	2.56	20 (35%)
20	CLA	3	313	-	25,32,73	2.11	7 (28%)	27,54,113	3.02	16 (59%)
20	CLA	A	815	-	48,58,73	2.41	11 (22%)	56,95,113	2.54	21 (37%)
21	LMU	K	107	-	36,36,36	0.53	0	47,47,47	1.32	7 (14%)
21	LMU	R	102	-	36,36,36	0.57	0	47,47,47	1.51	9 (19%)
20	CLA	2	304	-	25,32,73	2.13	10 (40%)	27,54,113	3.08	16 (59%)
21	LMU	R	103	-	36,36,36	0.71	1 (2%)	47,47,47	1.48	6 (12%)
20	CLA	2	317	-	63,73,73	2.12	16 (25%)	74,113,113	2.57	22 (29%)
20	CLA	4	310	-	48,58,73	2.43	16 (33%)	56,95,113	3.02	18 (32%)
20	CLA	B	816	-	58,68,73	2.13	11 (18%)	68,107,113	2.23	20 (29%)
20	CLA	A	838	-	63,73,73	2.09	13 (20%)	74,113,113	2.33	24 (32%)
21	LMU	B	804	-	36,36,36	0.69	0	47,47,47	1.77	12 (25%)
20	CLA	1	213	-	49,59,73	2.58	19 (38%)	56,96,113	3.03	25 (44%)
20	CLA	3	308	-	25,32,73	2.08	7 (28%)	27,54,113	3.20	16 (59%)
20	CLA	A	820	-	49,59,73	2.37	12 (24%)	56,96,113	2.74	18 (32%)
22	BCR	A	845	-	41,41,41	1.73	4 (9%)	56,56,56	5.85	25 (44%)
21	LMU	2	313	-	36,36,36	0.52	0	47,47,47	1.61	6 (12%)
21	LMU	4	316	-	36,36,36	0.73	1 (2%)	47,47,47	1.09	3 (6%)
22	BCR	B	845	-	41,41,41	1.56	3 (7%)	56,56,56	4.89	19 (33%)
20	CLA	B	803	-	63,73,73	2.07	11 (17%)	74,113,113	2.34	21 (28%)
20	CLA	2	311	-	48,58,73	2.37	12 (25%)	56,95,113	2.72	21 (37%)
20	CLA	B	824	-	63,73,73	2.22	18 (28%)	74,113,113	2.43	21 (28%)
20	CLA	1	207	-	49,59,73	2.43	15 (30%)	56,96,113	3.20	22 (39%)
20	CLA	A	804	20	53,63,73	2.30	12 (22%)	62,101,113	2.49	22 (35%)
20	CLA	B	809	-	63,73,73	2.06	12 (19%)	74,113,113	2.58	23 (31%)
20	CLA	1	208	-	25,32,73	2.02	7 (28%)	27,54,113	2.94	16 (59%)
20	CLA	B	830	-	63,73,73	2.10	15 (23%)	74,113,113	2.44	21 (28%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
20	CLA	4	312	-	25,32,73	2.15	7 (28%)	27,54,113	3.03	18 (66%)
21	LMU	R	109	-	36,36,36	0.49	0	47,47,47	0.83	1 (2%)
20	CLA	3	310	-	63,73,73	2.05	15 (23%)	74,113,113	2.62	26 (35%)
20	CLA	2	309	-	25,32,73	2.19	10 (40%)	27,54,113	2.88	16 (59%)
21	LMU	R	101	-	36,36,36	0.85	2 (5%)	47,47,47	2.10	11 (23%)
20	CLA	B	825	-	52,62,73	2.26	12 (23%)	60,99,113	2.46	19 (31%)
20	CLA	B	808	-	59,69,73	2.12	17 (28%)	69,108,113	2.39	20 (28%)
20	CLA	A	822	-	48,58,73	2.36	12 (25%)	56,95,113	2.54	18 (32%)
20	CLA	H	102	-	53,63,73	2.24	11 (20%)	62,101,113	2.57	19 (30%)
20	CLA	B	819	-	39,49,73	2.89	17 (43%)	46,84,113	3.13	17 (36%)
20	CLA	L	204	-	53,63,73	2.28	12 (22%)	62,101,113	2.49	22 (35%)
20	CLA	A	830	-	63,73,73	2.06	12 (19%)	74,113,113	2.26	17 (22%)
22	BCR	I	101	-	39,40,41	1.38	3 (7%)	51,53,56	4.37	19 (37%)
20	CLA	A	806	-	54,64,73	2.22	12 (22%)	63,102,113	2.51	20 (31%)
20	CLA	A	817	-	50,60,73	2.31	12 (24%)	57,97,113	2.65	17 (29%)
20	CLA	2	312	-	59,69,73	2.15	13 (22%)	69,108,113	2.63	26 (37%)
20	CLA	A	833	5	43,53,73	2.56	12 (27%)	50,89,113	2.93	20 (40%)
20	CLA	B	822	-	44,54,73	2.41	11 (25%)	51,90,113	2.84	16 (31%)
20	CLA	B	835	-	43,53,73	2.46	12 (27%)	50,89,113	2.70	19 (38%)
20	CLA	A	808	5	58,68,73	2.19	13 (22%)	68,107,113	2.47	23 (33%)
20	CLA	1	201	-	44,54,73	2.41	14 (31%)	51,90,113	3.16	21 (41%)
20	CLA	B	840	-	63,73,73	2.07	12 (19%)	74,113,113	2.33	21 (28%)
21	LMU	2	320	-	36,36,36	0.82	1 (2%)	47,47,47	1.58	11 (23%)
20	CLA	2	306	-	25,32,73	2.03	8 (32%)	27,54,113	2.73	14 (51%)
20	CLA	A	814	-	25,32,73	2.14	10 (40%)	27,54,113	3.14	16 (59%)
20	CLA	J	101	-	46,56,73	2.38	12 (26%)	53,92,113	2.65	16 (30%)
21	LMU	D	201	-	36,36,36	0.47	0	47,47,47	1.45	6 (12%)
20	CLA	B	839	-	45,55,73	2.63	17 (37%)	52,91,113	3.37	20 (38%)
20	CLA	B	820	-	59,69,73	2.05	13 (22%)	69,108,113	2.45	19 (27%)
20	CLA	H	111	-	56,66,73	2.35	19 (33%)	65,104,113	2.60	22 (33%)
20	CLA	A	850	-	63,73,73	2.05	11 (17%)	74,113,113	2.31	20 (27%)
20	CLA	H	101	-	53,63,73	2.32	12 (22%)	62,101,113	2.58	21 (33%)
20	CLA	B	829	-	63,73,73	2.06	15 (23%)	74,113,113	2.44	21 (28%)
21	LMU	R	106	-	36,36,36	0.52	0	47,47,47	1.23	4 (8%)
22	BCR	B	846	-	41,41,41	1.69	4 (9%)	56,56,56	5.71	23 (41%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
20	CLA	B	815	-	58,68,73	2.16	12 (20%)	68,107,113	2.21	17 (25%)
20	CLA	A	805	-	52,62,73	2.25	12 (23%)	60,99,113	2.58	18 (30%)
21	LMU	R	105	-	36,36,36	0.75	1 (2%)	47,47,47	1.40	8 (17%)
20	CLA	4	301	-	53,63,73	2.24	12 (22%)	62,101,113	2.55	19 (30%)
20	CLA	A	839	-	57,67,73	2.31	16 (28%)	66,105,113	2.75	25 (37%)
20	CLA	B	842	-	33,44,73	2.97	12 (36%)	46,78,113	3.68	22 (47%)
20	CLA	1	205	-	33,44,73	3.05	11 (33%)	46,78,113	3.39	18 (39%)
20	CLA	B	802	-	52,62,73	2.23	12 (23%)	60,99,113	2.66	20 (33%)
21	LMU	B	805	-	36,36,36	0.68	1 (2%)	47,47,47	1.69	12 (25%)
20	CLA	4	304	-	53,63,73	2.23	12 (22%)	62,101,113	2.56	19 (30%)
20	CLA	F	207	-	51,61,73	2.60	19 (37%)	59,98,113	2.93	25 (42%)
22	BCR	J	102	-	41,41,41	1.64	3 (7%)	56,56,56	5.69	19 (33%)
20	CLA	A	825	-	63,73,73	2.05	12 (19%)	74,113,113	2.21	16 (21%)
21	LMU	1	216	-	36,36,36	0.46	0	47,47,47	1.40	6 (12%)
20	CLA	4	317	-	50,60,73	2.34	14 (28%)	57,97,113	2.89	23 (40%)
20	CLA	H	112	-	53,63,73	2.27	11 (20%)	62,101,113	2.42	19 (30%)
20	CLA	A	829	-	48,58,73	2.40	12 (25%)	56,95,113	2.62	17 (30%)
20	CLA	K	104	-	54,64,73	2.26	14 (25%)	63,102,113	2.80	20 (31%)
20	CLA	1	214	-	25,32,73	2.12	8 (32%)	27,54,113	3.23	16 (59%)
21	LMU	2	322	-	36,36,36	0.82	1 (2%)	47,47,47	1.20	4 (8%)
20	CLA	4	315	-	44,54,73	2.41	15 (34%)	51,90,113	2.64	18 (35%)
20	CLA	F	201	-	48,58,73	2.37	17 (35%)	56,95,113	2.82	19 (33%)
20	CLA	G	105	-	49,59,73	2.37	13 (26%)	56,96,113	2.86	19 (33%)
21	LMU	B	849	-	26,26,36	0.78	1 (3%)	37,37,47	1.30	6 (16%)
20	CLA	A	831	-	63,73,73	2.22	18 (28%)	74,113,113	2.78	24 (32%)
20	CLA	B	837	-	58,68,73	2.10	11 (18%)	68,107,113	2.46	15 (22%)
20	CLA	1	215	-	49,59,73	2.40	17 (34%)	56,96,113	3.01	21 (37%)
20	CLA	3	301	-	33,44,73	2.92	12 (36%)	46,78,113	3.67	18 (39%)
21	LMU	A	847	-	36,36,36	0.68	1 (2%)	47,47,47	1.43	7 (14%)
20	CLA	2	301	-	25,32,73	2.11	8 (32%)	27,54,113	3.03	18 (66%)
20	CLA	B	833	-	48,58,73	2.34	14 (29%)	56,95,113	2.77	20 (35%)
21	LMU	2	321	-	36,36,36	0.46	0	47,47,47	1.28	3 (6%)
21	LMU	4	319	-	35,35,36	0.80	2 (5%)	46,46,47	1.83	11 (23%)
21	LMU	K	105	-	36,36,36	0.67	1 (2%)	47,47,47	1.56	8 (17%)
21	LMU	A	853	-	36,36,36	0.50	0	47,47,47	1.43	7 (14%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
22	BCR	L	211	-	41,41,41	1.71	3 (7%)	56,56,56	5.79	17 (30%)
20	CLA	B	832	-	57,67,73	2.18	12 (21%)	66,105,113	2.68	21 (31%)
21	LMU	A	848	-	36,36,36	0.49	0	47,47,47	0.86	3 (6%)
20	CLA	3	317	-	25,32,73	2.13	7 (28%)	27,54,113	3.15	15 (55%)
20	CLA	L	202	-	53,63,73	2.24	12 (22%)	62,101,113	2.57	20 (32%)
20	CLA	B	806	-	63,73,73	2.07	14 (22%)	74,113,113	2.22	20 (27%)
22	BCR	A	844	-	41,41,41	1.71	3 (7%)	56,56,56	5.71	21 (37%)
20	CLA	B	834	-	43,53,73	2.51	12 (27%)	50,89,113	2.66	16 (32%)
20	CLA	3	318	-	33,44,73	2.94	12 (36%)	46,78,113	3.56	20 (43%)
20	CLA	J	103	-	59,69,73	2.09	14 (23%)	69,108,113	2.22	18 (26%)
21	LMU	1	217	-	36,36,36	0.57	0	47,47,47	1.01	1 (2%)
20	CLA	B	831	-	48,58,73	2.42	11 (22%)	56,95,113	2.43	20 (35%)
20	CLA	2	305	-	48,58,73	2.37	11 (22%)	56,95,113	2.39	20 (35%)
20	CLA	B	818	-	51,61,73	2.28	11 (21%)	59,98,113	2.44	18 (30%)
20	CLA	1	212	-	25,32,73	2.11	8 (32%)	27,54,113	2.98	16 (59%)
20	CLA	4	311	-	25,32,73	2.06	8 (32%)	27,54,113	3.08	16 (59%)
20	CLA	I	102	-	58,68,73	2.14	11 (18%)	68,107,113	2.36	16 (23%)
21	LMU	H	104	-	36,36,36	0.60	0	47,47,47	1.65	7 (14%)
21	LMU	L	206	-	36,36,36	0.51	0	47,47,47	1.02	3 (6%)
20	CLA	A	841	-	25,32,73	2.21	8 (32%)	27,54,113	3.10	15 (55%)
20	CLA	4	303	-	63,73,73	2.11	13 (20%)	74,113,113	2.81	26 (35%)
20	CLA	A	813	-	48,58,73	2.32	12 (25%)	56,95,113	2.59	20 (35%)
21	LMU	H	106	-	36,36,36	0.61	1 (2%)	47,47,47	1.59	11 (23%)
20	CLA	2	302	-	49,59,73	2.44	15 (30%)	56,96,113	2.90	22 (39%)
20	CLA	1	203	-	45,55,73	2.54	16 (35%)	52,91,113	3.16	22 (42%)
22	BCR	B	801	-	41,41,41	2.05	4 (9%)	56,56,56	6.23	22 (39%)
20	CLA	4	314	4	25,32,73	2.07	7 (28%)	27,54,113	2.84	18 (66%)
20	CLA	A	811	20	63,73,73	2.10	12 (19%)	74,113,113	2.31	21 (28%)
20	CLA	A	818	-	58,68,73	2.23	16 (27%)	68,107,113	2.78	25 (36%)
20	CLA	K	102	-	48,58,73	2.35	12 (25%)	56,95,113	2.69	19 (33%)
20	CLA	2	310	2	48,58,73	2.43	13 (27%)	56,95,113	2.82	21 (37%)
21	LMU	4	320	-	36,36,36	0.78	1 (2%)	47,47,47	1.29	6 (12%)
20	CLA	4	306	-	50,60,73	2.48	15 (30%)	57,97,113	3.15	31 (54%)
22	BCR	2	318	-	41,41,41	1.68	3 (7%)	56,56,56	5.84	18 (32%)
20	CLA	A	803	-	44,54,73	2.48	17 (38%)	51,90,113	3.18	17 (33%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
20	CLA	A	851	-	63,73,73	2.11	12 (19%)	74,113,113	2.39	20 (27%)
20	CLA	A	840	-	53,63,73	2.21	13 (24%)	62,101,113	2.55	17 (27%)
20	CLA	K	103	-	48,58,73	2.44	13 (27%)	56,95,113	2.76	23 (41%)
20	CLA	3	311	-	63,73,73	2.07	11 (17%)	74,113,113	2.38	20 (27%)
20	CLA	A	809	-	50,60,73	2.28	11 (22%)	57,97,113	2.58	22 (38%)
22	BCR	B	847	-	41,41,41	1.67	3 (7%)	56,56,56	5.60	18 (32%)
21	LMU	A	855	-	36,36,36	0.66	1 (2%)	47,47,47	1.42	7 (14%)
20	CLA	B	821	-	48,58,73	2.31	12 (25%)	56,95,113	2.66	22 (39%)
20	CLA	3	307	-	40,50,73	2.59	13 (32%)	45,85,113	3.04	20 (44%)
20	CLA	B	817	-	44,54,73	2.41	11 (25%)	51,90,113	2.73	20 (39%)
20	CLA	2	307	-	63,73,73	2.07	14 (22%)	74,113,113	2.51	22 (29%)
20	CLA	B	838	-	63,73,73	1.99	11 (17%)	74,113,113	2.31	19 (25%)
21	LMU	R	104	-	36,36,36	0.57	1 (2%)	47,47,47	1.32	6 (12%)
21	LMU	K	106	-	36,36,36	0.37	0	47,47,47	1.07	3 (6%)
20	CLA	A	828	-	63,73,73	2.08	12 (19%)	74,113,113	2.40	21 (28%)
21	LMU	3	319	-	36,36,36	0.49	1 (2%)	47,47,47	0.73	1 (2%)
20	CLA	B	810	-	58,68,73	2.18	13 (22%)	68,107,113	2.47	19 (27%)
21	LMU	G	102	-	36,36,36	0.61	0	47,47,47	1.61	8 (17%)
20	CLA	1	202	-	39,49,73	2.57	11 (28%)	46,84,113	2.74	16 (34%)
20	CLA	A	819	-	56,66,73	2.20	11 (19%)	65,104,113	2.53	22 (33%)
20	CLA	3	314	-	48,58,73	2.40	10 (20%)	56,95,113	2.39	19 (33%)
22	BCR	I	103	-	41,41,41	1.88	5 (12%)	56,56,56	6.31	27 (48%)
20	CLA	B	823	-	53,63,73	2.26	13 (24%)	62,101,113	2.35	18 (29%)
20	CLA	K	101	-	44,54,73	2.50	14 (31%)	51,90,113	2.64	16 (31%)
21	LMU	F	202	-	35,35,36	0.58	0	46,46,47	1.38	5 (10%)
20	CLA	4	318	-	45,55,73	2.43	14 (31%)	52,91,113	2.96	23 (44%)
21	LMU	L	212	-	36,36,36	0.71	1 (2%)	47,47,47	1.30	4 (8%)
23	PQN	B	843	-	34,34,34	1.69	2 (5%)	43,45,45	1.35	6 (13%)
22	BCR	A	843	-	41,41,41	1.66	3 (7%)	56,56,56	5.62	21 (37%)
20	CLA	3	305	-	25,32,73	2.02	7 (28%)	27,54,113	2.93	14 (51%)
20	CLA	B	841	-	63,73,73	2.00	14 (22%)	74,113,113	2.19	18 (24%)
20	CLA	L	209	-	45,55,73	2.43	10 (22%)	52,91,113	2.88	20 (38%)
20	CLA	A	835	-	63,73,73	2.10	12 (19%)	74,113,113	2.45	24 (32%)
20	CLA	A	836	-	45,55,73	2.43	12 (26%)	52,91,113	2.35	15 (28%)
20	CLA	3	304	-	25,32,73	2.13	9 (36%)	27,54,113	3.16	15 (55%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
20	CLA	L	210	-	48,58,73	2.39	13 (27%)	56,95,113	2.89	19 (33%)
20	CLA	B	807	-	43,53,73	2.54	12 (27%)	50,89,113	2.78	16 (32%)
21	LMU	C	101	-	36,36,36	0.70	1 (2%)	47,47,47	1.26	4 (8%)
20	CLA	R	107	-	55,65,73	2.22	11 (20%)	64,103,113	2.55	22 (34%)
20	CLA	1	206	-	59,69,73	2.13	13 (22%)	69,108,113	2.44	23 (33%)
21	LMU	A	846	-	36,36,36	0.70	0	47,47,47	1.29	7 (14%)
20	CLA	A	832	-	48,58,73	2.36	12 (25%)	56,95,113	2.50	19 (33%)
20	CLA	B	827	-	63,73,73	2.01	12 (19%)	74,113,113	2.31	20 (27%)
21	LMU	A	852	-	36,36,36	0.56	1 (2%)	47,47,47	0.86	1 (2%)
21	LMU	L	205	-	36,36,36	0.64	1 (2%)	47,47,47	1.96	13 (27%)
20	CLA	A	823	-	56,66,73	2.14	11 (19%)	65,104,113	2.31	19 (29%)
20	CLA	3	302	-	25,32,73	2.08	7 (28%)	27,54,113	2.94	15 (55%)
20	CLA	B	811	6	25,32,73	2.20	10 (40%)	27,54,113	2.77	14 (51%)
20	CLA	F	205	-	33,44,73	2.86	11 (33%)	46,78,113	3.28	22 (47%)
21	LMU	G	101	-	36,36,36	1.09	3 (8%)	47,47,47	2.05	11 (23%)
20	CLA	4	302	-	33,44,73	3.10	12 (36%)	46,78,113	3.74	21 (45%)
20	CLA	A	837	-	49,59,73	2.31	12 (24%)	56,96,113	2.77	20 (35%)
20	CLA	A	802	-	25,32,73	2.16	7 (28%)	27,54,113	3.15	17 (62%)
20	CLA	A	816	-	52,62,73	2.29	14 (26%)	60,99,113	2.74	22 (36%)
20	CLA	A	824	-	57,67,73	2.12	12 (21%)	66,105,113	2.51	22 (33%)
20	CLA	3	306	-	25,32,73	2.06	7 (28%)	27,54,113	3.03	17 (62%)
20	CLA	R	108	-	63,73,73	2.10	12 (19%)	74,113,113	2.26	21 (28%)
20	CLA	1	204	-	44,54,73	2.54	14 (31%)	51,90,113	3.13	23 (45%)
20	CLA	1	210	1	33,44,73	2.92	11 (33%)	46,78,113	3.54	18 (39%)
21	LMU	4	321	-	36,36,36	0.46	0	47,47,47	1.46	7 (14%)
20	CLA	1	211	-	49,59,73	2.47	18 (36%)	56,96,113	3.26	22 (39%)
20	CLA	A	821	5	40,50,73	2.49	12 (30%)	45,85,113	3.00	16 (35%)
20	CLA	1	209	-	25,32,73	2.23	8 (32%)	27,54,113	3.11	18 (66%)
20	CLA	2	308	-	25,32,73	2.24	11 (44%)	27,54,113	3.30	16 (59%)
20	CLA	B	850	-	63,73,73	2.06	15 (23%)	74,113,113	2.36	26 (35%)
20	CLA	A	834	-	44,54,73	2.45	13 (29%)	51,90,113	2.63	18 (35%)
20	CLA	B	813	-	53,63,73	2.21	13 (24%)	62,101,113	2.51	20 (32%)
20	CLA	4	307	-	25,32,73	2.13	8 (32%)	27,54,113	2.97	14 (51%)
20	CLA	A	807	-	44,54,73	2.43	12 (27%)	51,90,113	2.63	20 (39%)
23	PQN	A	842	-	34,34,34	1.73	2 (5%)	43,45,45	1.22	4 (9%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
24	SF4	C	102	7	0,12,12	-	-	-		
21	LMU	A	854	-	36,36,36	0.52	0	47,47,47	1.28	7 (14%)
20	CLA	3	315	-	63,73,73	2.11	16 (25%)	74,113,113	2.62	21 (28%)
20	CLA	A	827	-	53,63,73	2.21	13 (24%)	62,101,113	2.49	20 (32%)
20	CLA	4	309	-	25,32,73	2.08	7 (28%)	27,54,113	3.04	16 (59%)
21	LMU	1	218	-	36,36,36	0.70	0	47,47,47	1.69	9 (19%)
20	CLA	3	309	-	25,32,73	2.15	9 (36%)	27,54,113	3.30	16 (59%)
25	LMG	B	848	-	49,49,55	0.99	2 (4%)	57,57,63	1.09	3 (5%)
20	CLA	4	305	-	48,58,73	2.42	16 (33%)	56,95,113	2.70	20 (35%)
20	CLA	2	315	-	48,58,73	2.40	15 (31%)	56,95,113	2.92	18 (32%)
21	LMU	E	101	-	36,36,36	0.62	0	47,47,47	1.91	13 (27%)
20	CLA	A	826	-	63,73,73	2.02	11 (17%)	74,113,113	2.38	23 (31%)
21	LMU	3	320	-	36,36,36	0.44	0	47,47,47	1.14	4 (8%)
20	CLA	F	206	-	39,49,73	2.60	12 (30%)	46,84,113	2.82	17 (36%)
20	CLA	B	836	-	49,59,73	2.32	14 (28%)	56,96,113	2.89	20 (35%)
20	CLA	B	812	-	53,62,73	2.66	18 (33%)	65,100,113	3.43	25 (38%)
20	CLA	L	201	-	58,68,73	2.17	12 (20%)	68,107,113	2.30	22 (32%)
21	LMU	2	319	-	36,36,36	0.57	0	47,47,47	0.69	0
22	BCR	G	104	-	41,41,41	1.63	3 (7%)	56,56,56	5.88	19 (33%)
21	LMU	G	103	-	36,36,36	0.50	0	47,47,47	0.95	2 (4%)
21	LMU	H	105	-	36,36,36	0.73	1 (2%)	47,47,47	1.67	9 (19%)
20	CLA	B	826	-	56,66,73	2.16	12 (21%)	65,104,113	2.42	17 (26%)
20	CLA	B	814	-	63,73,73	2.03	12 (19%)	74,113,113	2.26	22 (29%)
20	CLA	3	316	-	25,32,73	2.25	9 (36%)	27,54,113	3.15	17 (62%)
21	LMU	H	103	-	36,36,36	0.85	1 (2%)	47,47,47	2.15	13 (27%)
20	CLA	A	849	-	63,73,73	2.02	15 (23%)	74,113,113	2.28	20 (27%)

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	B	828	-	2/2/15/20	16/37/115/115	-
22	BCR	F	204	-	-	9/29/63/63	0/2/2/2
20	CLA	3	303	-	1/1/9/20	-	-
20	CLA	4	308	-	1/1/4/20	-	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
20	CLA	4	313	-	1/1/9/20	-	-
20	CLA	A	812	-	1/1/12/20	11/24/102/115	-
24	SF4	A	856	6,5	-	-	0/6/5/5
20	CLA	2	303	-	2/2/13/20	14/29/107/115	-
22	BCR	B	844	-	-	5/29/63/63	0/2/2/2
22	BCR	F	203	-	-	13/29/63/63	0/2/2/2
20	CLA	L	203	-	2/2/15/20	14/37/115/115	-
20	CLA	A	810	-	1/1/11/20	4/13/91/115	-
20	CLA	2	316	-	1/1/4/20	-	-
20	CLA	A	801	-	3/3/11/20	11/16/92/115	-
24	SF4	C	103	7	-	-	0/6/5/5
20	CLA	L	208	16	1/1/12/20	8/19/97/115	-
20	CLA	3	313	-	1/1/4/20	-	-
20	CLA	A	815	-	1/1/12/20	8/19/97/115	-
21	LMU	K	107	-	-	17/21/61/61	0/2/2/2
21	LMU	R	102	-	-	11/21/61/61	0/2/2/2
20	CLA	2	304	-	1/1/4/20	-	-
21	LMU	R	103	-	-	11/21/61/61	0/2/2/2
20	CLA	2	317	-	2/2/15/20	15/37/115/115	-
20	CLA	4	310	-	1/1/12/20	12/19/97/115	-
20	CLA	B	816	-	2/2/14/20	11/31/109/115	-
20	CLA	A	838	-	2/2/15/20	17/37/115/115	-
21	LMU	B	804	-	-	16/21/61/61	0/2/2/2
20	CLA	1	213	-	3/3/12/20	10/21/99/115	-
20	CLA	3	308	-	1/1/4/20	-	-
20	CLA	A	820	-	1/1/12/20	8/21/99/115	-
22	BCR	A	845	-	-	10/29/63/63	0/2/2/2
21	LMU	2	313	-	-	16/21/61/61	0/2/2/2
21	LMU	4	316	-	-	13/21/61/61	0/2/2/2
22	BCR	B	845	-	-	9/29/63/63	0/2/2/2
20	CLA	B	803	-	2/2/15/20	16/37/115/115	-
20	CLA	2	311	-	1/1/12/20	8/19/97/115	-
20	CLA	B	824	-	2/2/15/20	17/37/115/115	-
20	CLA	1	207	-	2/2/12/20	9/21/99/115	-
20	CLA	A	804	20	2/2/13/20	11/25/103/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
20	CLA	B	809	-	2/2/15/20	17/37/115/115	-
20	CLA	1	208	-	1/1/4/20	-	-
20	CLA	B	830	-	2/2/15/20	24/37/115/115	-
20	CLA	4	312	-	1/1/4/20	-	-
21	LMU	R	109	-	-	14/21/61/61	0/2/2/2
20	CLA	3	310	-	2/2/15/20	17/37/115/115	-
20	CLA	2	309	-	1/1/4/20	-	-
21	LMU	R	101	-	-	13/21/61/61	0/2/2/2
20	CLA	B	825	-	1/1/12/20	8/24/102/115	-
20	CLA	B	808	-	2/2/14/20	18/33/111/115	-
20	CLA	A	822	-	1/1/12/20	7/19/97/115	-
20	CLA	H	102	-	2/2/13/20	13/25/103/115	-
20	CLA	B	819	-	1/1/10/20	2/8/86/115	-
20	CLA	L	204	-	2/2/13/20	7/25/103/115	-
20	CLA	A	830	-	2/2/15/20	17/37/115/115	-
22	BCR	I	101	-	-	10/29/60/63	0/2/2/2
20	CLA	A	806	-	2/2/13/20	7/27/105/115	-
20	CLA	A	817	-	1/1/12/20	11/22/100/115	-
20	CLA	2	312	-	2/2/14/20	19/33/111/115	-
20	CLA	A	833	5	1/1/11/20	6/13/91/115	-
20	CLA	B	822	-	1/1/11/20	11/15/93/115	-
20	CLA	B	835	-	1/1/11/20	6/13/91/115	-
20	CLA	A	808	5	2/2/14/20	13/31/109/115	-
20	CLA	1	201	-	1/1/11/20	10/15/93/115	-
20	CLA	B	840	-	2/2/15/20	15/37/115/115	-
21	LMU	2	320	-	-	12/21/61/61	0/2/2/2
20	CLA	2	306	-	1/1/4/20	-	-
20	CLA	A	814	-	1/1/4/20	-	-
20	CLA	J	101	-	1/1/11/20	9/17/95/115	-
21	LMU	D	201	-	-	9/21/61/61	0/2/2/2
20	CLA	B	839	-	1/1/11/20	12/16/94/115	-
20	CLA	B	820	-	2/2/14/20	17/33/111/115	-
20	CLA	H	111	-	2/2/13/20	15/29/107/115	-
20	CLA	A	850	-	2/2/15/20	17/37/115/115	-
20	CLA	H	101	-	3/3/13/20	12/25/103/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
20	CLA	B	829	-	2/2/15/20	16/37/115/115	-
21	LMU	R	106	-	-	12/21/61/61	0/2/2/2
22	BCR	B	846	-	-	14/29/63/63	0/2/2/2
20	CLA	B	815	-	2/2/14/20	17/31/109/115	-
20	CLA	A	805	-	1/1/12/20	12/24/102/115	-
21	LMU	R	105	-	-	14/21/61/61	0/2/2/2
20	CLA	4	301	-	2/2/13/20	14/25/103/115	-
20	CLA	A	839	-	2/2/13/20	13/29/107/115	-
20	CLA	B	842	-	1/1/9/20	-	-
20	CLA	1	205	-	1/1/9/20	-	-
20	CLA	B	802	-	1/1/12/20	11/24/102/115	-
21	LMU	B	805	-	-	14/21/61/61	0/2/2/2
20	CLA	4	304	-	2/2/13/20	12/25/103/115	-
20	CLA	F	207	-	4/4/12/20	11/23/101/115	-
22	BCR	J	102	-	-	11/29/63/63	0/2/2/2
20	CLA	A	825	-	2/2/15/20	22/37/115/115	-
21	LMU	1	216	-	-	9/21/61/61	0/2/2/2
20	CLA	4	317	-	1/1/12/20	10/22/100/115	-
20	CLA	H	112	-	2/2/13/20	7/25/103/115	-
20	CLA	A	829	-	1/1/12/20	5/19/97/115	-
20	CLA	K	104	-	2/2/13/20	11/27/105/115	-
20	CLA	1	214	-	1/1/4/20	-	-
21	LMU	2	322	-	-	8/21/61/61	0/2/2/2
20	CLA	4	315	-	1/1/11/20	9/15/93/115	-
20	CLA	F	201	-	1/1/12/20	9/19/97/115	-
20	CLA	G	105	-	1/1/12/20	6/21/99/115	-
21	LMU	B	849	-	-	5/11/51/61	0/2/2/2
20	CLA	A	831	-	2/2/15/20	19/37/115/115	-
20	CLA	B	837	-	2/2/14/20	15/31/109/115	-
20	CLA	1	215	-	2/2/12/20	8/21/99/115	-
20	CLA	3	301	-	1/1/9/20	-	-
21	LMU	A	847	-	-	13/21/61/61	0/2/2/2
20	CLA	2	301	-	1/1/4/20	-	-
20	CLA	B	833	-	1/1/12/20	5/19/97/115	-
21	LMU	2	321	-	-	18/21/61/61	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
21	LMU	4	319	-	-	13/20/60/61	0/2/2/2
21	LMU	K	105	-	-	12/21/61/61	0/2/2/2
21	LMU	A	853	-	-	11/21/61/61	0/2/2/2
22	BCR	L	211	-	-	10/29/63/63	0/2/2/2
20	CLA	B	832	-	2/2/13/20	16/30/108/115	-
21	LMU	A	848	-	-	11/21/61/61	0/2/2/2
20	CLA	3	317	-	1/1/4/20	-	-
20	CLA	L	202	-	2/2/13/20	14/25/103/115	-
20	CLA	B	806	-	2/2/15/20	18/37/115/115	-
22	BCR	A	844	-	-	14/29/63/63	0/2/2/2
20	CLA	B	834	-	1/1/11/20	9/13/91/115	-
20	CLA	3	318	-	1/1/9/20	-	-
20	CLA	J	103	-	2/2/14/20	20/33/111/115	-
21	LMU	1	217	-	-	9/21/61/61	0/2/2/2
20	CLA	B	831	-	1/1/12/20	7/19/97/115	-
20	CLA	2	305	-	1/1/12/20	7/19/97/115	-
20	CLA	B	818	-	1/1/12/20	9/23/101/115	-
20	CLA	1	212	-	1/1/4/20	-	-
20	CLA	4	311	-	1/1/4/20	-	-
20	CLA	I	102	-	2/2/14/20	11/31/109/115	-
21	LMU	H	104	-	-	12/21/61/61	0/2/2/2
21	LMU	L	206	-	-	14/21/61/61	0/2/2/2
20	CLA	A	841	-	1/1/4/20	-	-
20	CLA	4	303	-	3/3/15/20	19/37/115/115	-
20	CLA	A	813	-	1/1/12/20	8/19/97/115	-
21	LMU	H	106	-	-	9/21/61/61	0/2/2/2
20	CLA	2	302	-	1/1/12/20	12/21/99/115	-
20	CLA	1	203	-	1/1/11/20	7/16/94/115	-
22	BCR	B	801	-	-	13/29/63/63	0/2/2/2
20	CLA	4	314	4	1/1/4/20	-	-
20	CLA	A	811	20	2/2/15/20	20/37/115/115	-
20	CLA	A	818	-	2/2/14/20	13/31/109/115	-
20	CLA	K	102	-	1/1/12/20	4/19/97/115	-
20	CLA	2	310	2	1/1/12/20	5/19/97/115	-
21	LMU	4	320	-	-	16/21/61/61	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
20	CLA	4	306	-	2/2/12/20	7/22/100/115	-
22	BCR	2	318	-	-	15/29/63/63	0/2/2/2
20	CLA	A	803	-	1/1/11/20	2/15/93/115	-
20	CLA	A	851	-	2/2/15/20	22/37/115/115	-
20	CLA	A	840	-	2/2/13/20	8/25/103/115	-
20	CLA	K	103	-	1/1/12/20	9/19/97/115	-
20	CLA	3	311	-	2/2/15/20	21/37/115/115	-
20	CLA	A	809	-	1/1/12/20	10/22/100/115	-
22	BCR	B	847	-	-	11/29/63/63	0/2/2/2
21	LMU	A	855	-	-	13/21/61/61	0/2/2/2
20	CLA	B	821	-	1/1/12/20	6/19/97/115	-
20	CLA	3	307	-	1/1/10/20	7/10/88/115	-
20	CLA	B	817	-	1/1/11/20	10/15/93/115	-
20	CLA	2	307	-	2/2/15/20	20/37/115/115	-
20	CLA	B	838	-	2/2/15/20	11/37/115/115	-
21	LMU	R	104	-	-	14/21/61/61	0/2/2/2
21	LMU	K	106	-	-	13/21/61/61	0/2/2/2
20	CLA	A	828	-	2/2/15/20	18/37/115/115	-
21	LMU	3	319	-	-	12/21/61/61	0/2/2/2
20	CLA	B	810	-	2/2/14/20	10/31/109/115	-
21	LMU	G	102	-	-	13/21/61/61	0/2/2/2
20	CLA	1	202	-	1/1/10/20	4/8/86/115	-
20	CLA	A	819	-	2/2/13/20	10/29/107/115	-
20	CLA	3	314	-	1/1/12/20	7/19/97/115	-
22	BCR	I	103	-	-	15/29/63/63	0/2/2/2
20	CLA	B	823	-	2/2/13/20	10/25/103/115	-
20	CLA	K	101	-	1/1/11/20	5/15/93/115	-
21	LMU	F	202	-	-	13/20/60/61	0/2/2/2
20	CLA	4	318	-	1/1/11/20	12/16/94/115	-
21	LMU	L	212	-	-	16/21/61/61	0/2/2/2
23	PQN	B	843	-	1/1/8/9	10/23/43/43	0/2/2/2
22	BCR	A	843	-	-	14/29/63/63	0/2/2/2
20	CLA	3	305	-	1/1/4/20	-	-
20	CLA	B	841	-	2/2/15/20	16/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
20	CLA	L	209	-	1/1/11/20	9/16/94/115	-
20	CLA	A	835	-	2/2/15/20	13/37/115/115	-
20	CLA	A	836	-	1/1/11/20	7/16/94/115	-
20	CLA	3	304	-	1/1/4/20	-	-
20	CLA	L	210	-	2/2/12/20	9/19/97/115	-
20	CLA	B	807	-	1/1/11/20	5/13/91/115	-
21	LMU	C	101	-	-	14/21/61/61	0/2/2/2
20	CLA	R	107	-	2/2/13/20	14/28/106/115	-
20	CLA	1	206	-	2/2/14/20	20/33/111/115	-
21	LMU	A	846	-	-	16/21/61/61	0/2/2/2
20	CLA	A	832	-	1/1/12/20	12/19/97/115	-
20	CLA	B	827	-	2/2/15/20	20/37/115/115	-
21	LMU	A	852	-	-	20/21/61/61	0/2/2/2
21	LMU	L	205	-	-	13/21/61/61	0/2/2/2
20	CLA	A	823	-	2/2/13/20	12/29/107/115	-
20	CLA	3	302	-	1/1/4/20	-	-
20	CLA	B	811	6	1/1/4/20	-	-
20	CLA	F	205	-	1/1/9/20	-	-
21	LMU	G	101	-	-	13/21/61/61	0/2/2/2
20	CLA	4	302	-	1/1/9/20	-	-
20	CLA	A	837	-	1/1/12/20	13/21/99/115	-
20	CLA	A	802	-	1/1/4/20	-	-
20	CLA	A	816	-	1/1/12/20	10/24/102/115	-
20	CLA	A	824	-	2/2/13/20	14/30/108/115	-
20	CLA	3	306	-	1/1/4/20	-	-
20	CLA	R	108	-	2/2/15/20	21/37/115/115	-
20	CLA	1	204	-	1/1/11/20	8/15/93/115	-
20	CLA	1	210	1	1/1/9/20	-	-
21	LMU	4	321	-	-	15/21/61/61	0/2/2/2
20	CLA	1	211	-	2/2/12/20	8/21/99/115	-
20	CLA	A	821	5	1/1/10/20	2/10/88/115	-
20	CLA	1	209	-	1/1/4/20	-	-
20	CLA	2	308	-	1/1/4/20	-	-
20	CLA	B	850	-	2/2/15/20	18/37/115/115	-
20	CLA	A	834	-	1/1/11/20	6/15/93/115	-
20	CLA	B	813	-	2/2/13/20	10/25/103/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
20	CLA	4	307	-	1/1/4/20	-	-
20	CLA	A	807	-	1/1/11/20	7/15/93/115	-
23	PQN	A	842	-	1/1/8/9	11/23/43/43	0/2/2/2
24	SF4	C	102	7	-	-	0/6/5/5
21	LMU	A	854	-	-	16/21/61/61	0/2/2/2
20	CLA	3	315	-	2/2/15/20	16/37/115/115	-
20	CLA	A	827	-	2/2/13/20	9/25/103/115	-
20	CLA	4	309	-	1/1/4/20	-	-
21	LMU	1	218	-	-	13/21/61/61	0/2/2/2
20	CLA	3	309	-	1/1/4/20	-	-
25	LMG	B	848	-	-	27/44/64/70	0/1/1/1
20	CLA	4	305	-	1/1/12/20	8/19/97/115	-
20	CLA	2	315	-	1/1/12/20	7/19/97/115	-
21	LMU	E	101	-	-	14/21/61/61	0/2/2/2
20	CLA	A	826	-	2/2/15/20	14/37/115/115	-
21	LMU	3	320	-	-	11/21/61/61	0/2/2/2
20	CLA	F	206	-	1/1/10/20	4/8/86/115	-
20	CLA	B	836	-	1/1/12/20	11/21/99/115	-
20	CLA	B	812	-	2/2/13/20	7/25/101/115	-
20	CLA	L	201	-	2/2/14/20	12/31/109/115	-
21	LMU	2	319	-	-	13/21/61/61	0/2/2/2
22	BCR	G	104	-	-	14/29/63/63	0/2/2/2
21	LMU	G	103	-	-	14/21/61/61	0/2/2/2
21	LMU	H	105	-	-	17/21/61/61	0/2/2/2
20	CLA	B	826	-	2/2/13/20	18/29/107/115	-
20	CLA	B	814	-	2/2/15/20	18/37/115/115	-
20	CLA	3	316	-	1/1/4/20	-	-
21	LMU	H	103	-	-	14/21/61/61	0/2/2/2
20	CLA	A	849	-	2/2/15/20	21/37/115/115	-

The worst 5 of 2206 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	1	205	CLA	CAB-C3B	-9.18	1.33	1.51
22	B	801	BCR	C20-C21	-9.11	1.14	1.43
20	B	812	CLA	CAB-C3B	-9.08	1.33	1.51
20	4	302	CLA	CAB-C3B	-8.83	1.34	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	B	842	CLA	CAB-C3B	-8.58	1.34	1.51

The worst 5 of 4044 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	G	104	BCR	C20-C21-C22	36.93	179.07	127.28
22	L	211	BCR	C20-C21-C22	36.44	178.38	127.28
22	A	845	BCR	C20-C21-C22	36.19	178.03	127.28
22	J	102	BCR	C20-C21-C22	36.12	177.93	127.28
22	B	846	BCR	C20-C21-C22	36.04	177.82	127.28

5 of 258 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 2433 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
20	1	201	CLA	C1A-C2A-CAA-CBA
20	1	201	CLA	C3A-C2A-CAA-CBA
20	1	201	CLA	CBA-CGA-O2A-C1
20	1	201	CLA	CHA-CBD-CGD-O1D
20	1	201	CLA	CHA-CBD-CGD-O2D

There are no ring outliers.

224 monomers are involved in 2729 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
20	B	828	CLA	13	0
22	F	204	BCR	34	0
20	3	303	CLA	4	0
20	4	313	CLA	5	0
20	A	812	CLA	4	0
24	A	856	SF4	18	0
20	2	303	CLA	25	0
22	B	844	BCR	8	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
22	F	203	BCR	26	0
20	L	203	CLA	29	0
20	A	810	CLA	4	0
20	A	801	CLA	9	0
24	C	103	SF4	1	0
20	L	208	CLA	3	0
20	A	815	CLA	4	0
21	K	107	LMU	21	0
21	R	102	LMU	8	0
20	2	304	CLA	2	0
21	R	103	LMU	9	0
20	2	317	CLA	11	0
20	4	310	CLA	25	0
20	B	816	CLA	8	0
20	A	838	CLA	33	0
21	B	804	LMU	7	0
20	1	213	CLA	16	0
20	3	308	CLA	2	0
20	A	820	CLA	8	0
22	A	845	BCR	48	0
21	2	313	LMU	29	0
21	4	316	LMU	1	0
22	B	845	BCR	18	0
20	B	803	CLA	44	0
20	2	311	CLA	6	0
20	B	824	CLA	30	0
20	1	207	CLA	6	1
20	A	804	CLA	36	0
20	B	809	CLA	22	0
20	1	208	CLA	3	0
20	B	830	CLA	24	0
20	4	312	CLA	4	0
21	R	109	LMU	9	3
20	3	310	CLA	17	0
21	R	101	LMU	3	0
20	B	825	CLA	24	0
20	B	808	CLA	31	0
20	A	822	CLA	20	0
20	H	102	CLA	2	0
20	B	819	CLA	7	0
20	L	204	CLA	13	0
20	A	830	CLA	31	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
22	I	101	BCR	9	0
20	A	806	CLA	13	0
20	A	817	CLA	8	0
20	2	312	CLA	19	0
20	A	833	CLA	13	0
20	B	822	CLA	16	0
20	B	835	CLA	30	0
20	A	808	CLA	21	0
20	1	201	CLA	13	0
20	B	840	CLA	18	0
21	2	320	LMU	5	0
20	A	814	CLA	14	0
20	J	101	CLA	12	0
21	D	201	LMU	3	0
20	B	839	CLA	47	0
20	B	820	CLA	17	0
20	H	111	CLA	27	0
20	A	850	CLA	30	0
20	H	101	CLA	15	0
20	B	829	CLA	25	0
21	R	106	LMU	9	0
22	B	846	BCR	32	0
20	B	815	CLA	17	0
20	A	805	CLA	16	0
20	4	301	CLA	34	0
20	A	839	CLA	27	0
20	B	842	CLA	2	0
20	1	205	CLA	6	0
20	B	802	CLA	17	0
21	B	805	LMU	3	0
20	4	304	CLA	21	0
20	F	207	CLA	13	0
22	J	102	BCR	36	0
20	A	825	CLA	51	0
21	1	216	LMU	3	0
20	4	317	CLA	3	0
20	H	112	CLA	13	0
20	A	829	CLA	7	0
20	K	104	CLA	17	0
20	4	315	CLA	5	0
20	F	201	CLA	29	0
20	G	105	CLA	4	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
21	B	849	LMU	1	0
20	A	831	CLA	37	0
20	B	837	CLA	12	0
20	1	215	CLA	1	0
20	3	301	CLA	1	0
21	A	847	LMU	4	0
20	B	833	CLA	18	0
21	2	321	LMU	5	0
21	4	319	LMU	8	3
21	K	105	LMU	13	0
21	A	853	LMU	21	0
22	L	211	BCR	36	0
20	B	832	CLA	24	0
21	A	848	LMU	4	0
20	L	202	CLA	10	0
20	B	806	CLA	25	0
22	A	844	BCR	23	0
20	B	834	CLA	23	0
20	J	103	CLA	14	0
21	1	217	LMU	20	0
20	B	831	CLA	11	0
20	2	305	CLA	16	0
20	B	818	CLA	17	0
20	1	212	CLA	2	0
20	4	311	CLA	3	0
20	I	102	CLA	12	0
21	H	104	LMU	9	0
20	A	841	CLA	1	0
20	4	303	CLA	18	0
20	A	813	CLA	21	0
21	H	106	LMU	9	0
20	2	302	CLA	13	0
20	1	203	CLA	8	0
22	B	801	BCR	24	0
20	4	314	CLA	10	0
20	A	811	CLA	22	0
20	A	818	CLA	46	0
20	K	102	CLA	27	0
20	2	310	CLA	21	0
21	4	320	LMU	2	0
20	4	306	CLA	18	0
22	2	318	BCR	9	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
20	A	803	CLA	20	0
20	A	851	CLA	26	0
20	A	840	CLA	6	0
20	K	103	CLA	9	0
20	3	311	CLA	10	0
20	A	809	CLA	32	0
22	B	847	BCR	32	0
20	B	821	CLA	7	0
20	3	307	CLA	14	0
20	B	817	CLA	19	0
20	2	307	CLA	22	0
20	B	838	CLA	42	0
21	R	104	LMU	5	0
21	K	106	LMU	8	0
20	A	828	CLA	18	0
21	3	319	LMU	2	0
20	B	810	CLA	18	0
21	G	102	LMU	7	0
20	1	202	CLA	1	0
20	A	819	CLA	33	0
20	3	314	CLA	1	0
22	I	103	BCR	38	0
20	B	823	CLA	15	0
20	K	101	CLA	16	1
21	F	202	LMU	8	0
20	4	318	CLA	14	0
21	L	212	LMU	1	0
23	B	843	PQN	28	0
22	A	843	BCR	32	0
20	3	305	CLA	3	0
20	B	841	CLA	17	0
20	L	209	CLA	27	0
20	A	835	CLA	15	0
20	A	836	CLA	6	0
20	3	304	CLA	2	0
20	L	210	CLA	9	0
20	B	807	CLA	9	0
20	R	107	CLA	10	0
20	1	206	CLA	9	0
21	A	846	LMU	5	0
20	A	832	CLA	19	0
20	B	827	CLA	36	0

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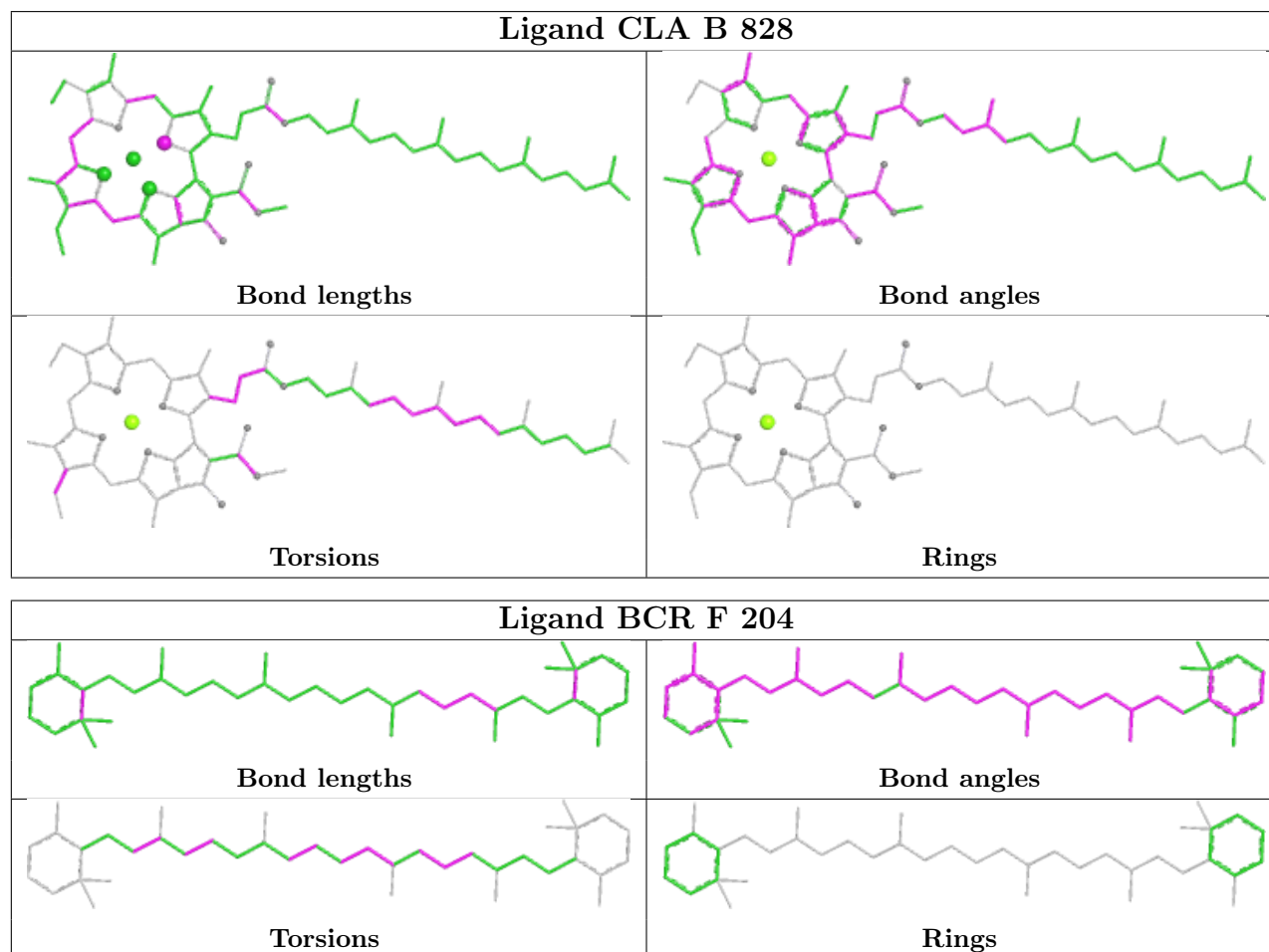
Mol	Chain	Res	Type	Clashes	Symm-Clashes
21	A	852	LMU	5	0
21	L	205	LMU	1	0
20	A	823	CLA	10	0
20	B	811	CLA	4	0
20	F	205	CLA	1	0
21	G	101	LMU	4	41
20	4	302	CLA	3	0
20	A	837	CLA	17	0
20	A	816	CLA	21	0
20	A	824	CLA	43	0
20	3	306	CLA	7	0
20	R	108	CLA	4	0
20	1	204	CLA	15	0
20	1	210	CLA	8	0
21	4	321	LMU	13	0
20	1	211	CLA	7	0
20	A	821	CLA	8	0
20	1	209	CLA	1	0
20	2	308	CLA	1	0
20	B	850	CLA	18	0
20	A	834	CLA	7	0
20	B	813	CLA	8	0
20	A	807	CLA	33	0
23	A	842	PQN	7	0
24	C	102	SF4	4	0
21	A	854	LMU	15	0
20	3	315	CLA	13	0
20	A	827	CLA	19	0
21	1	218	LMU	9	0
20	3	309	CLA	1	0
25	B	848	LMG	17	0
20	4	305	CLA	5	0
20	2	315	CLA	17	0
21	E	101	LMU	11	0
20	A	826	CLA	49	0
21	3	320	LMU	14	0
20	F	206	CLA	5	0
20	B	836	CLA	9	0
20	B	812	CLA	9	0
20	L	201	CLA	23	0
21	2	319	LMU	6	0
22	G	104	BCR	5	0

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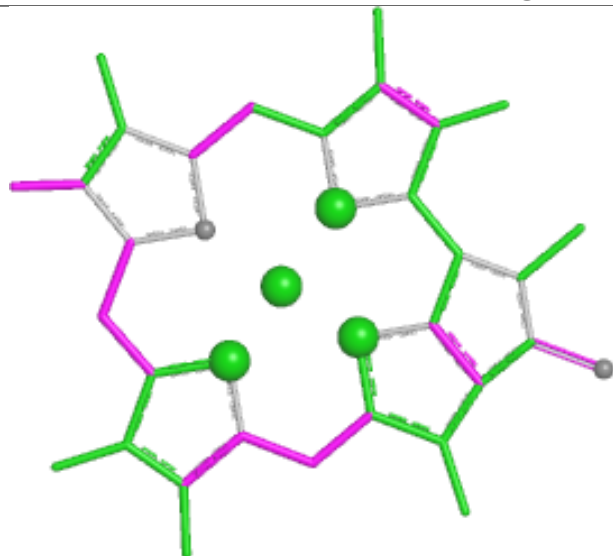
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
21	G	103	LMU	16	0
21	H	105	LMU	18	0
20	B	826	CLA	39	0
20	B	814	CLA	30	0
21	H	103	LMU	6	0
20	A	849	CLA	21	0

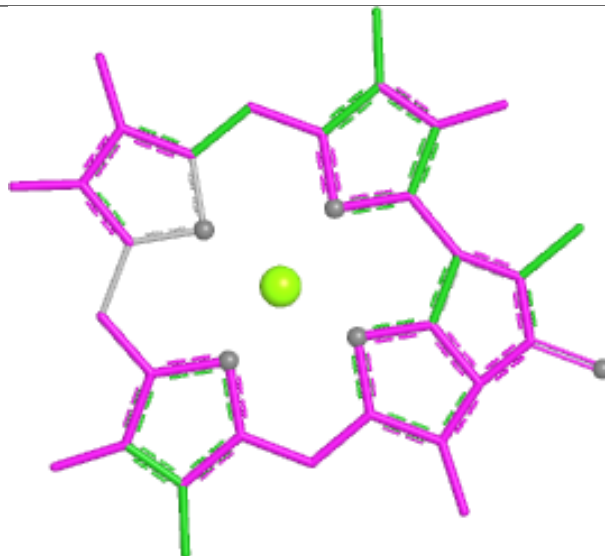
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



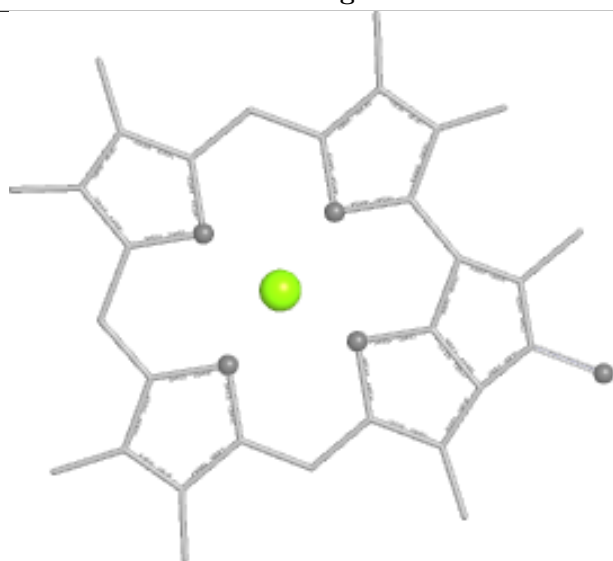
Ligand CLA 3 303



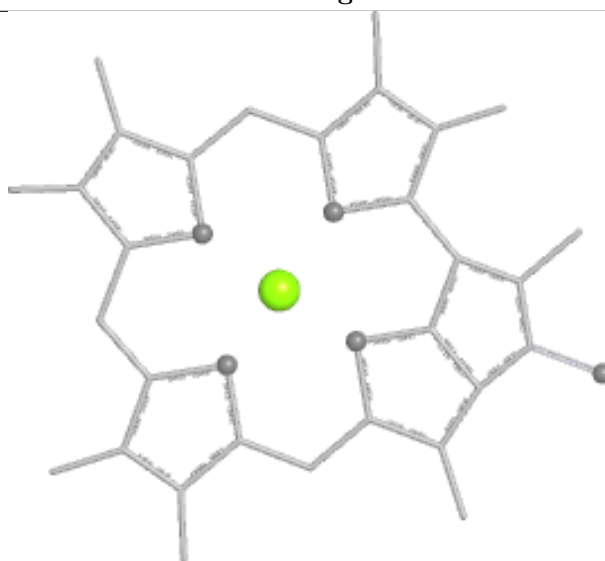
Bond lengths



Bond angles

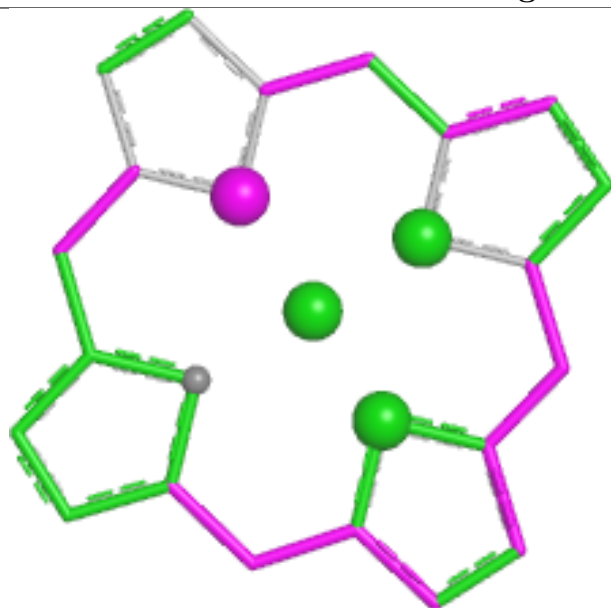


Torsions

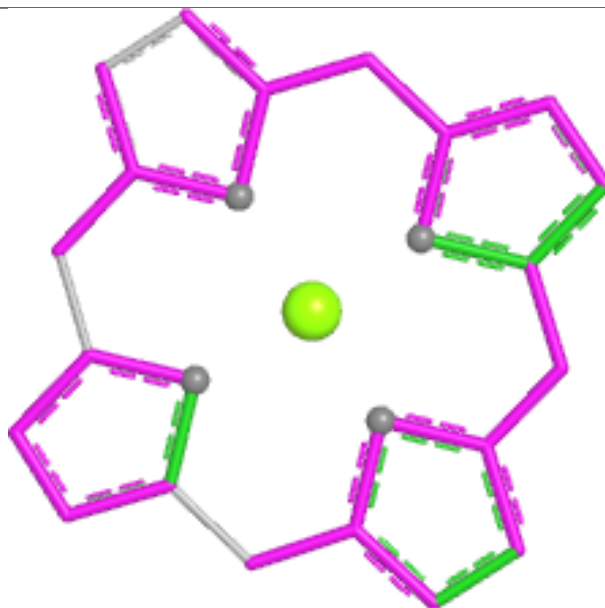


Rings

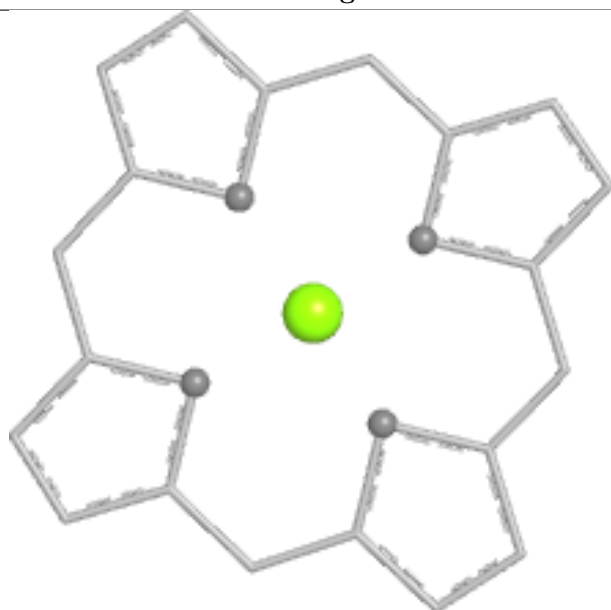
Ligand CLA 4 308



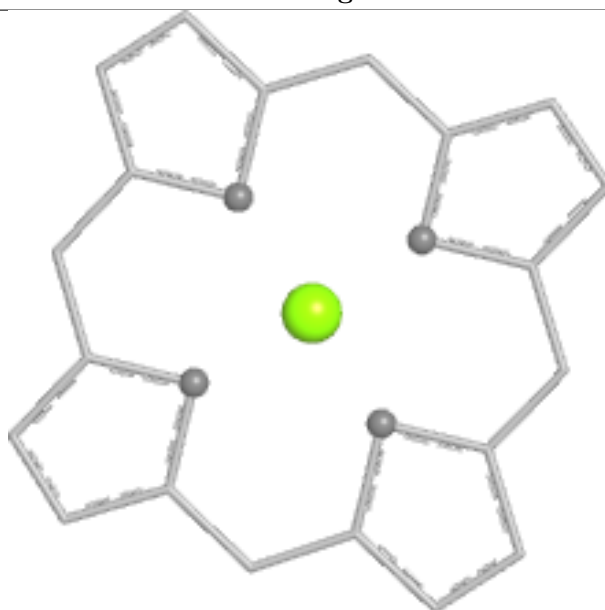
Bond lengths



Bond angles

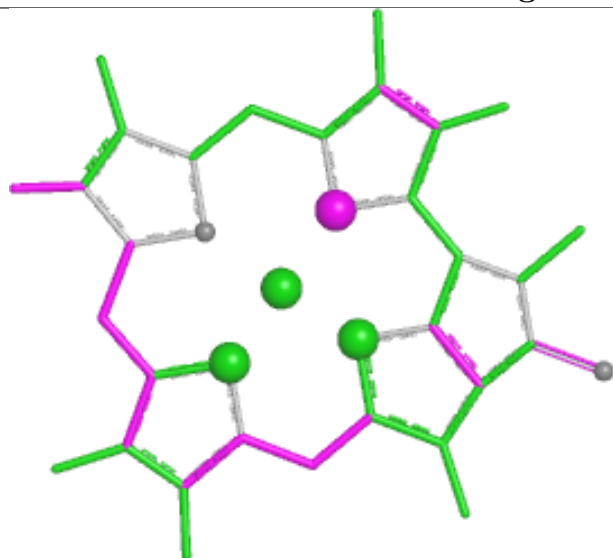


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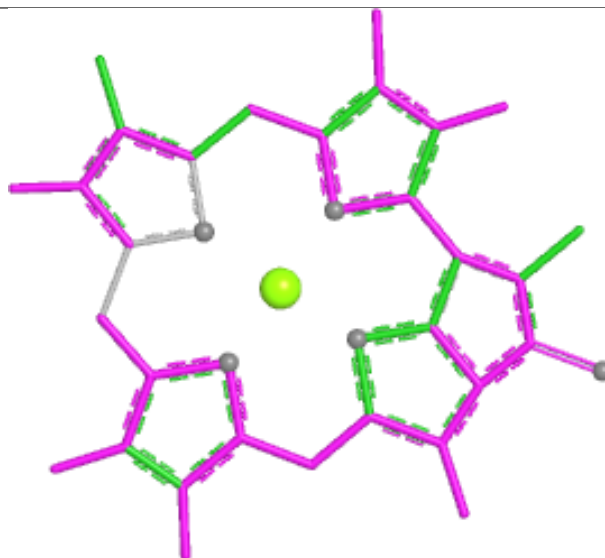


Rings

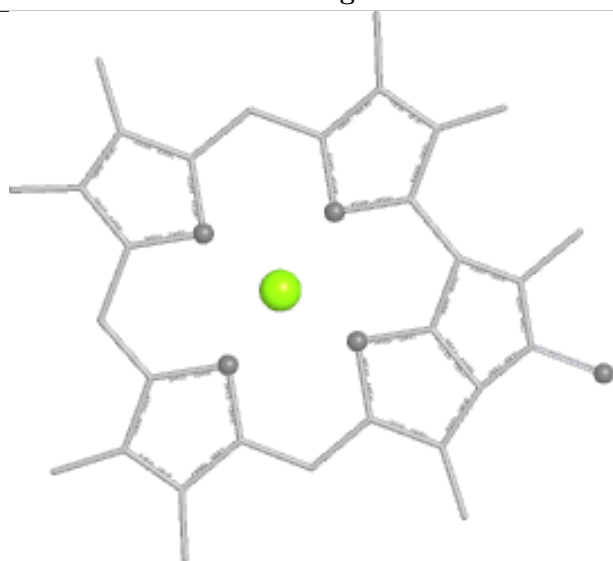
Ligand CLA 4 313



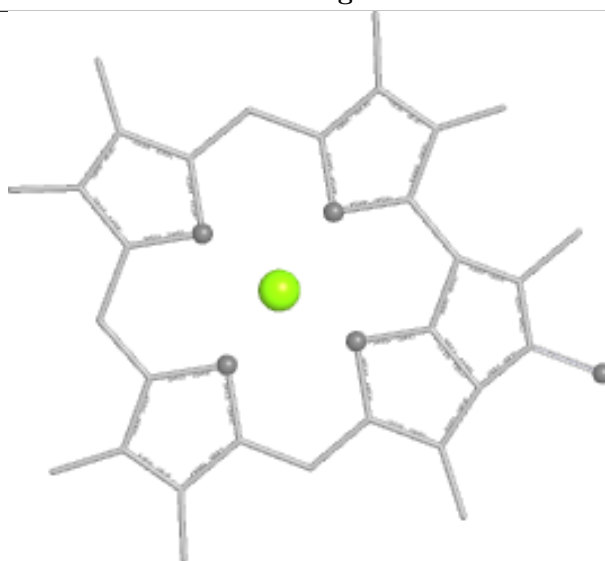
Bond lengths



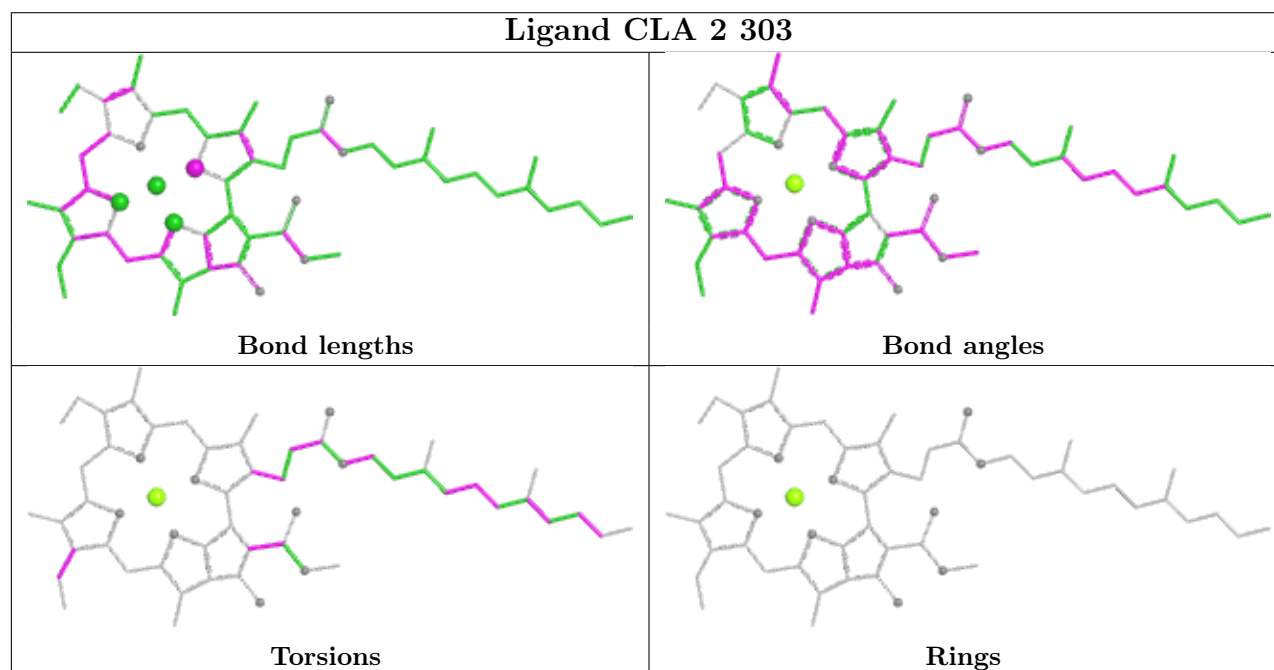
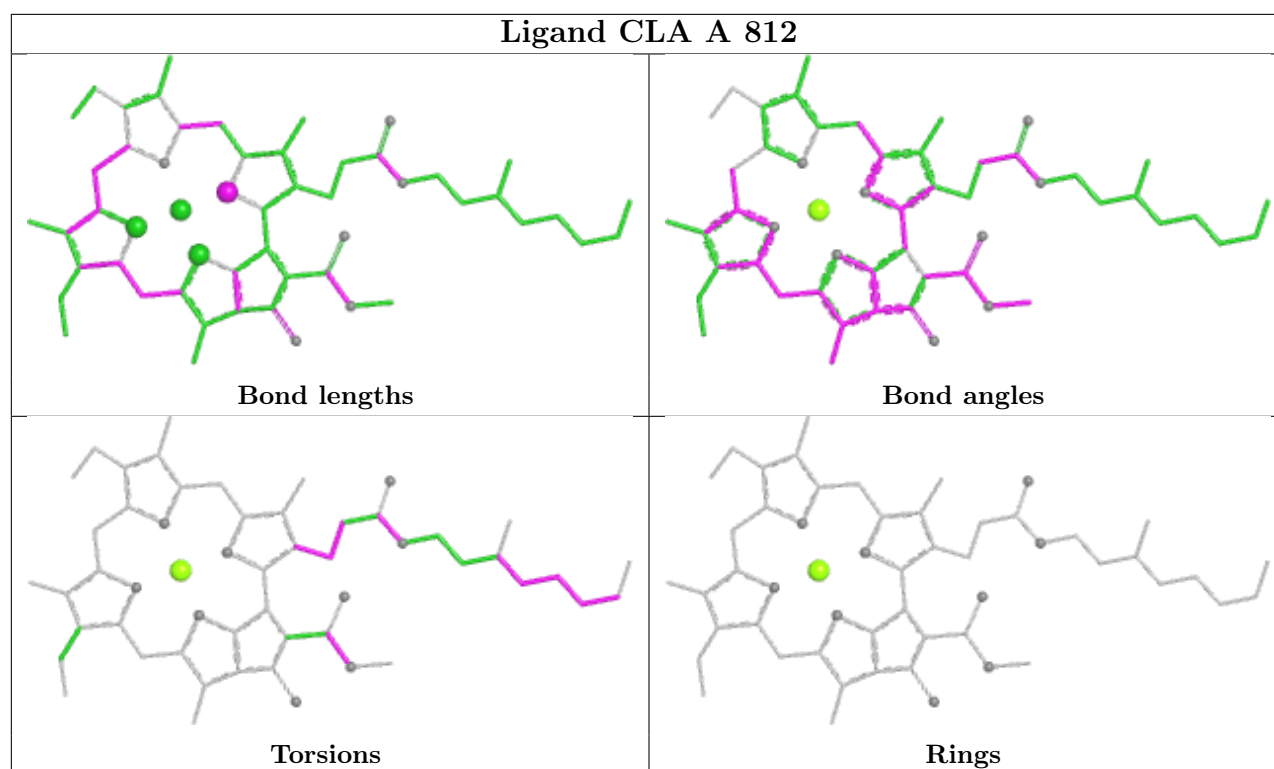
Bond angles

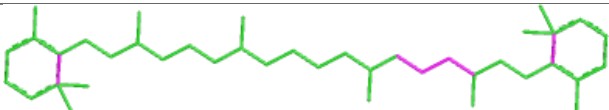
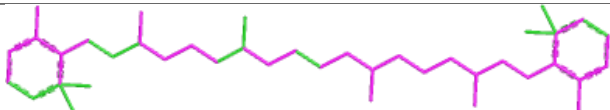
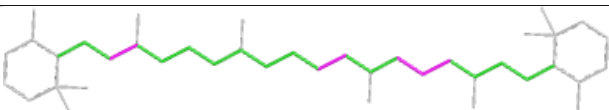
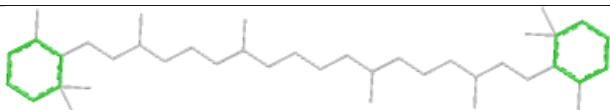




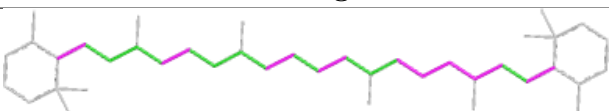
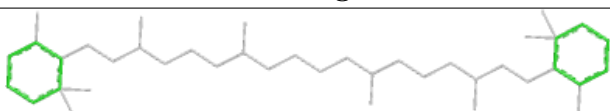
Torsions

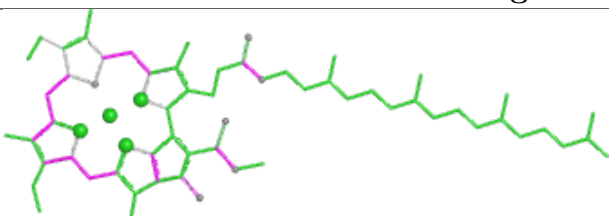
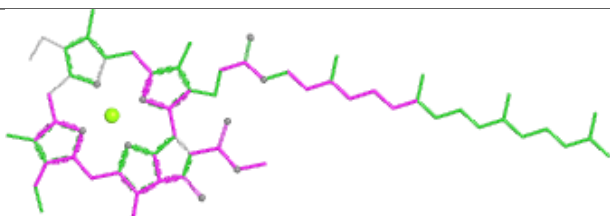
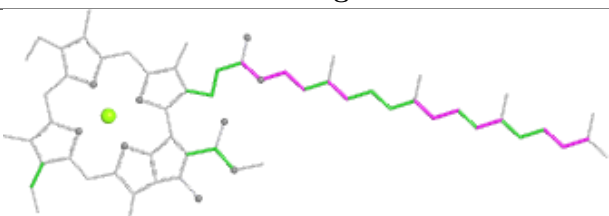
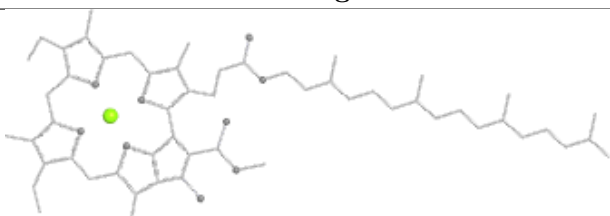


Rings

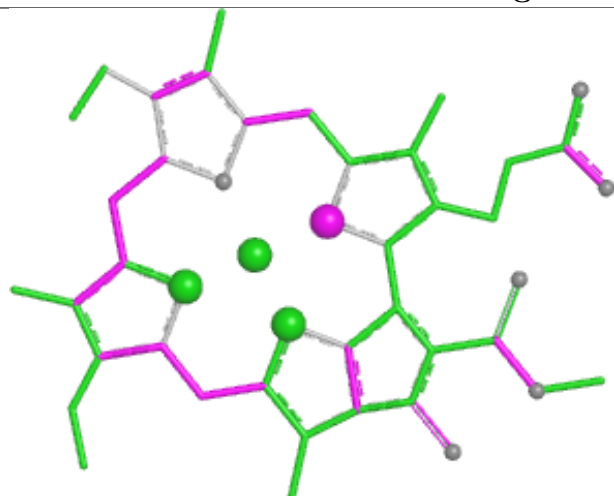


Ligand BCR B 844	
	
Bond lengths	Bond angles
	
Torsions	Rings

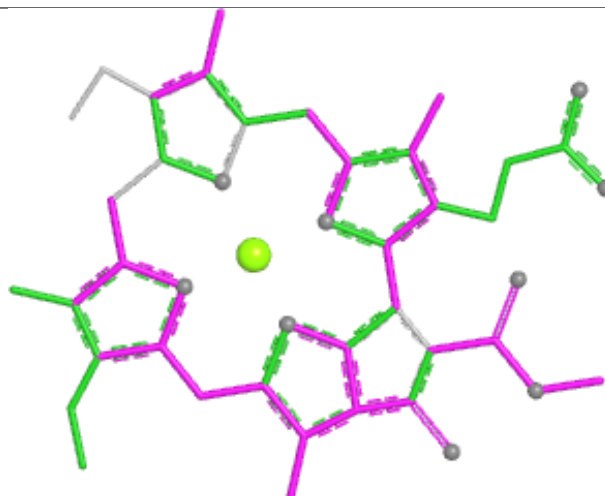
Ligand BCR F 203	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA L 203	
	
Bond lengths	Bond angles
	
Torsions	Rings

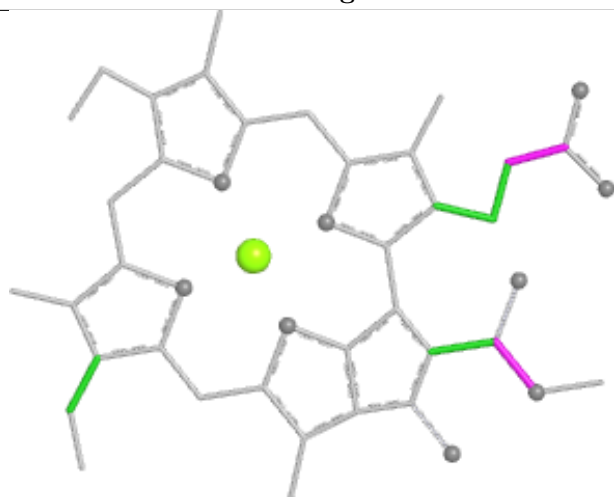
Ligand CLA A 810



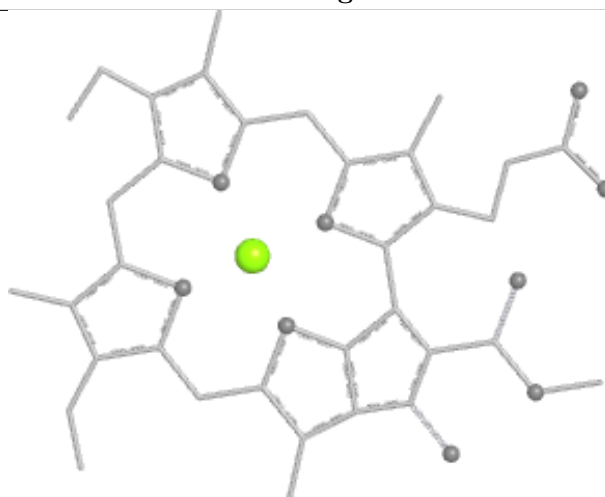
Bond lengths



Bond angles

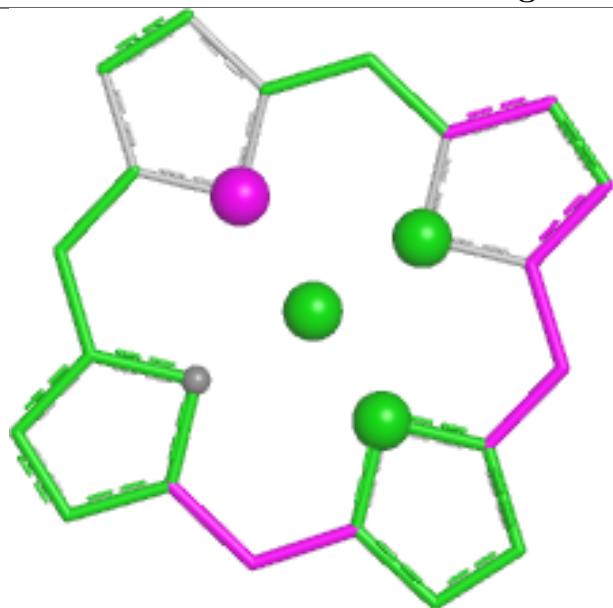


Torsions

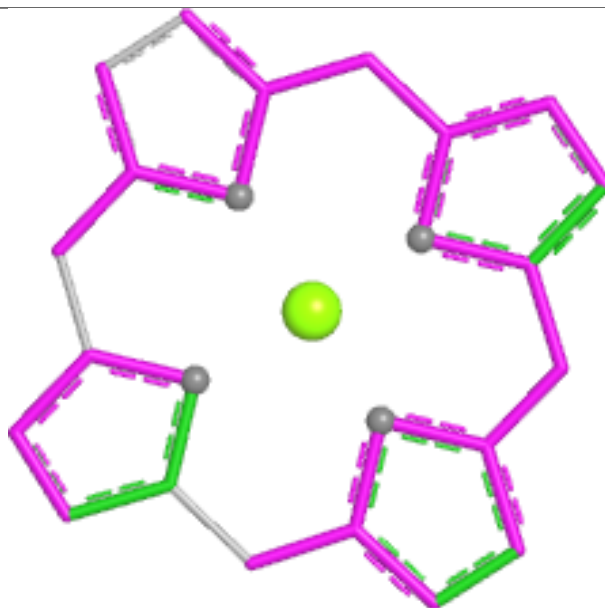


Rings

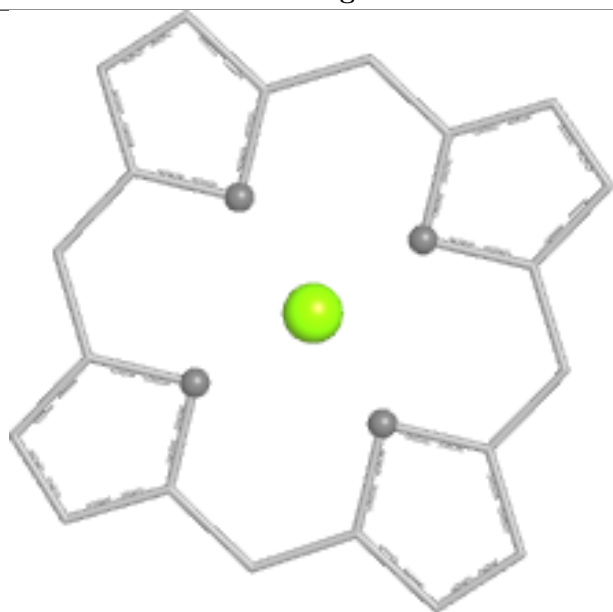
Ligand CLA 2 316



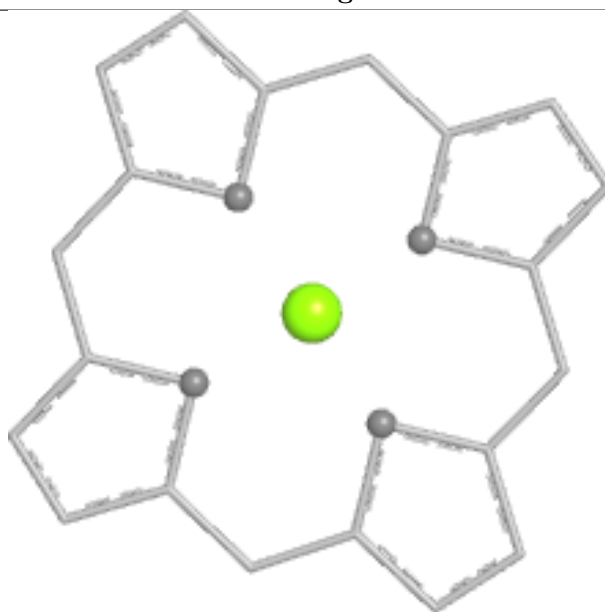
Bond lengths



Bond angles

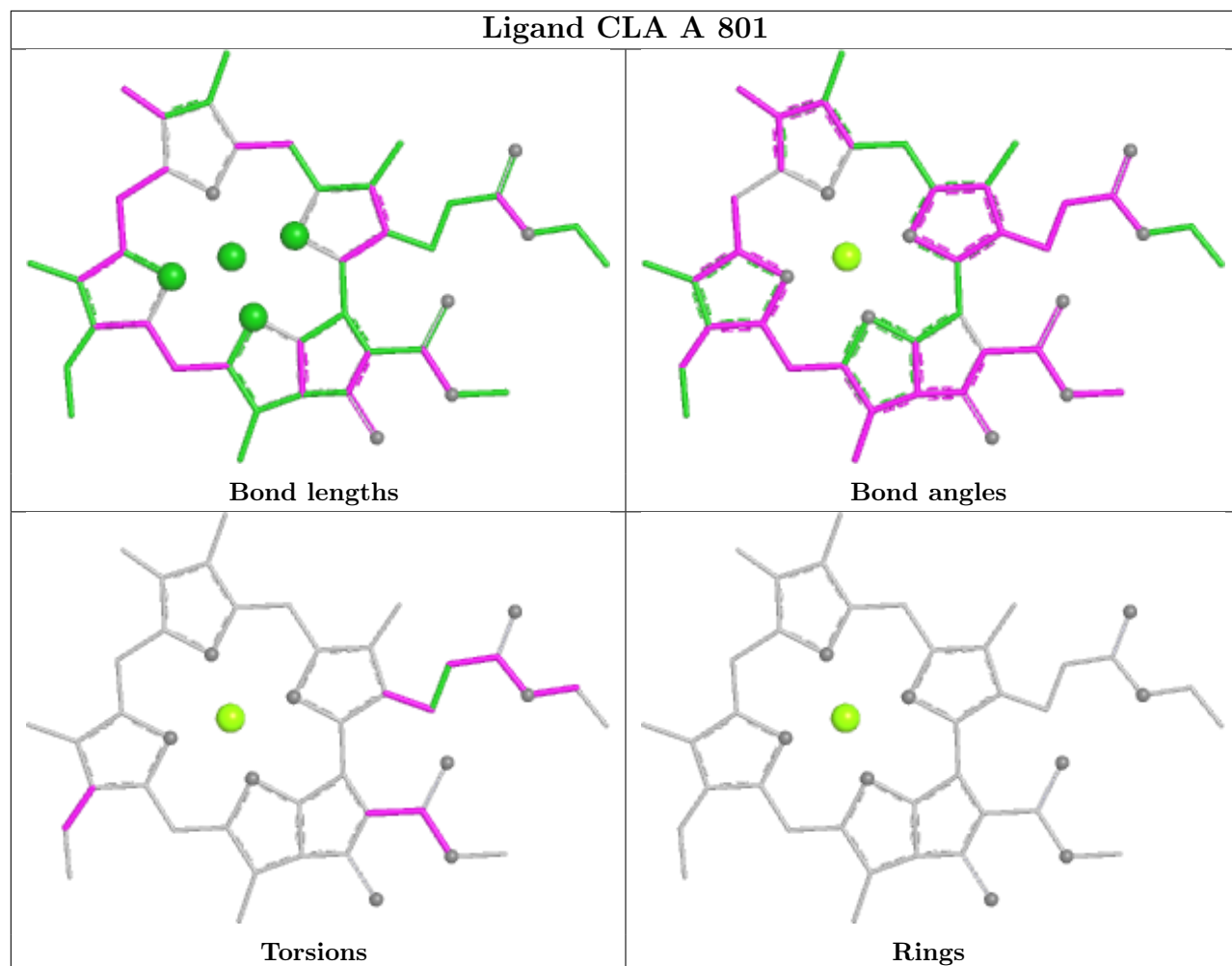


Torsions

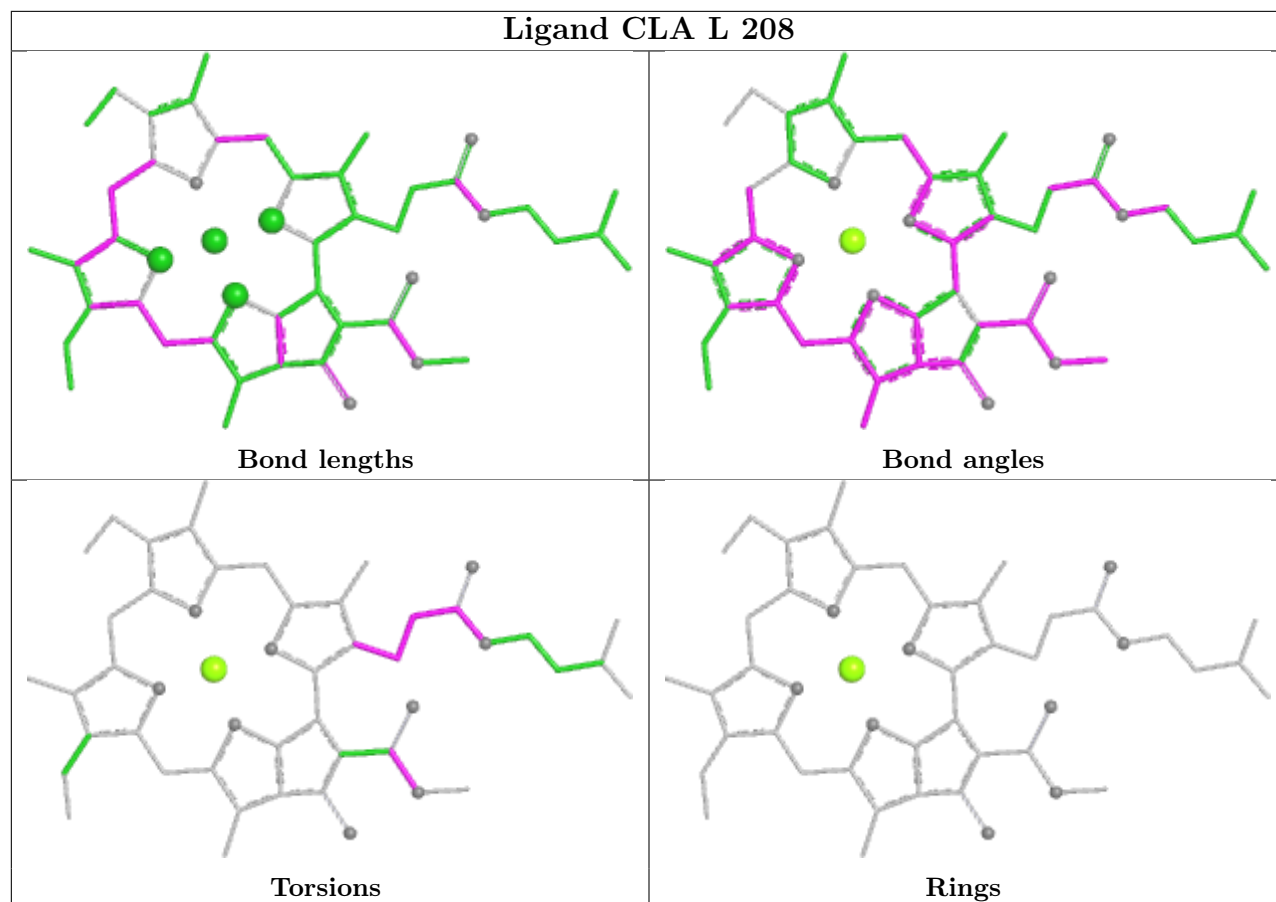


Rings

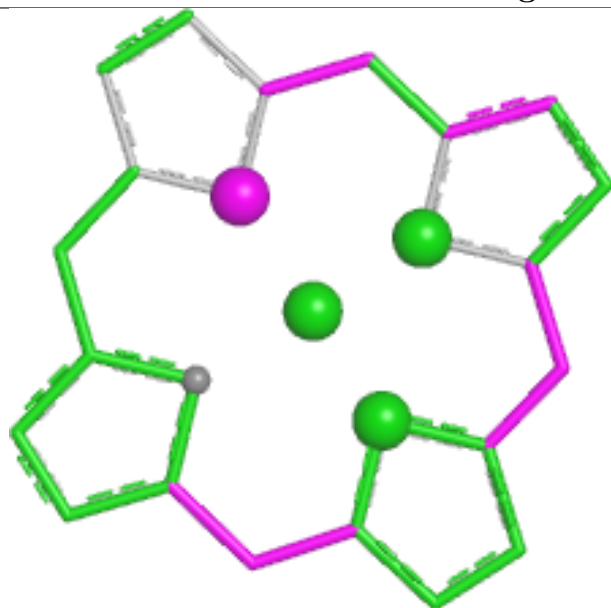
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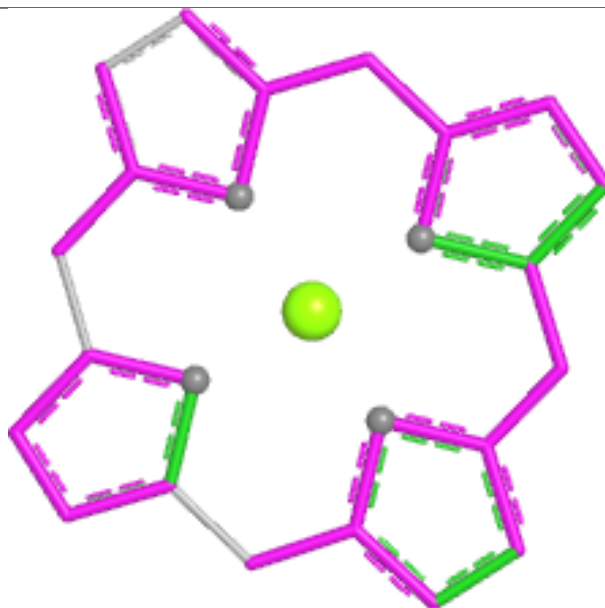
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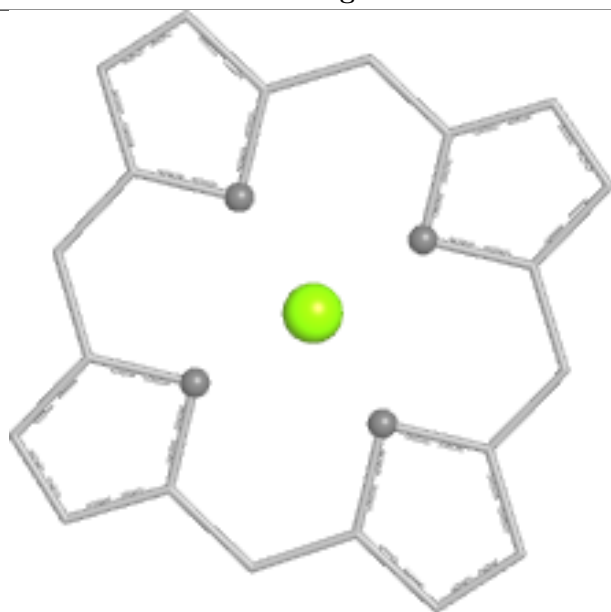
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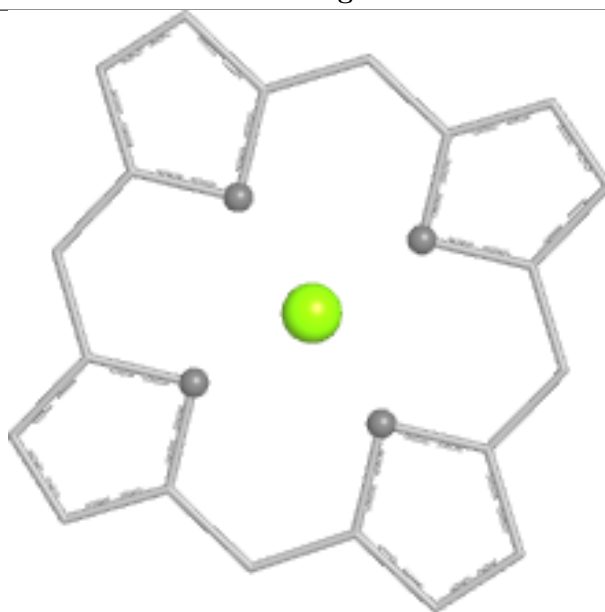
Bond lengths



Bond angles

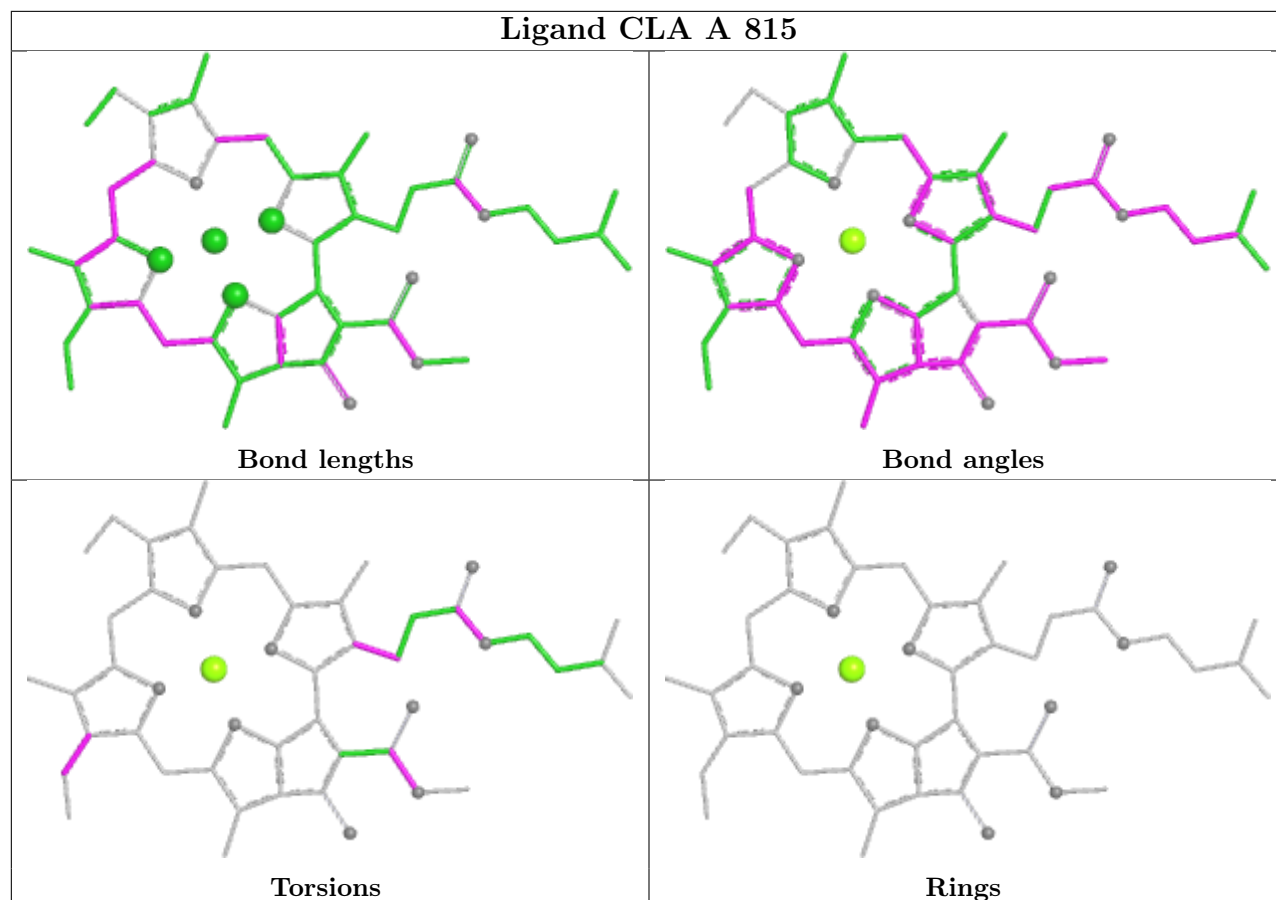


Torsions

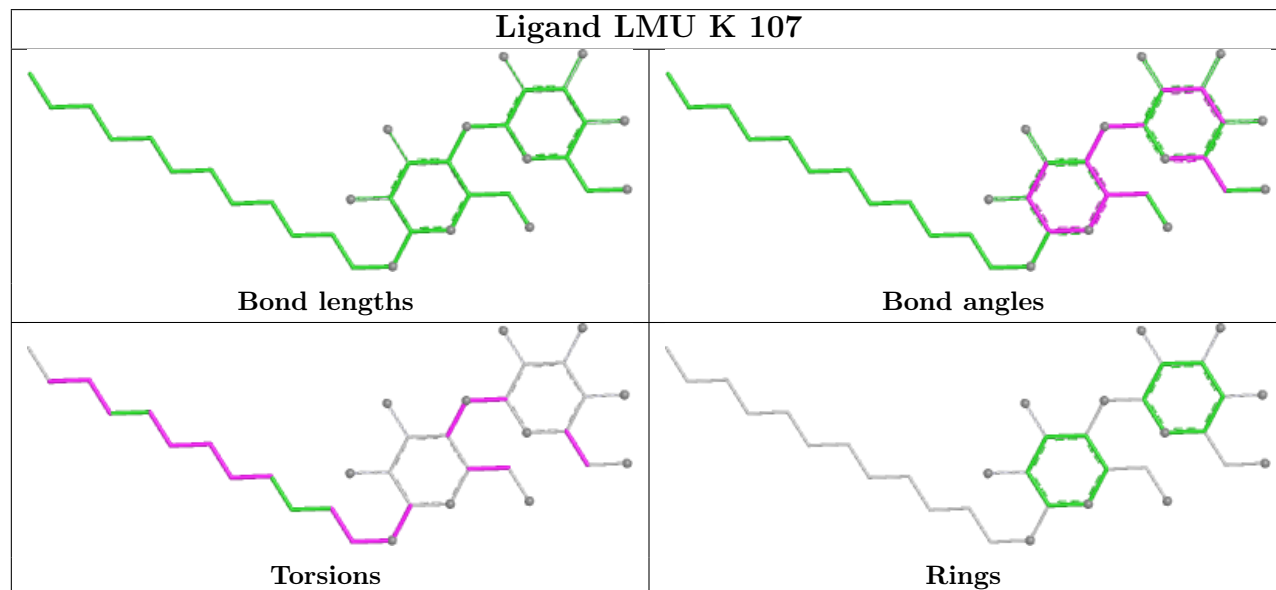


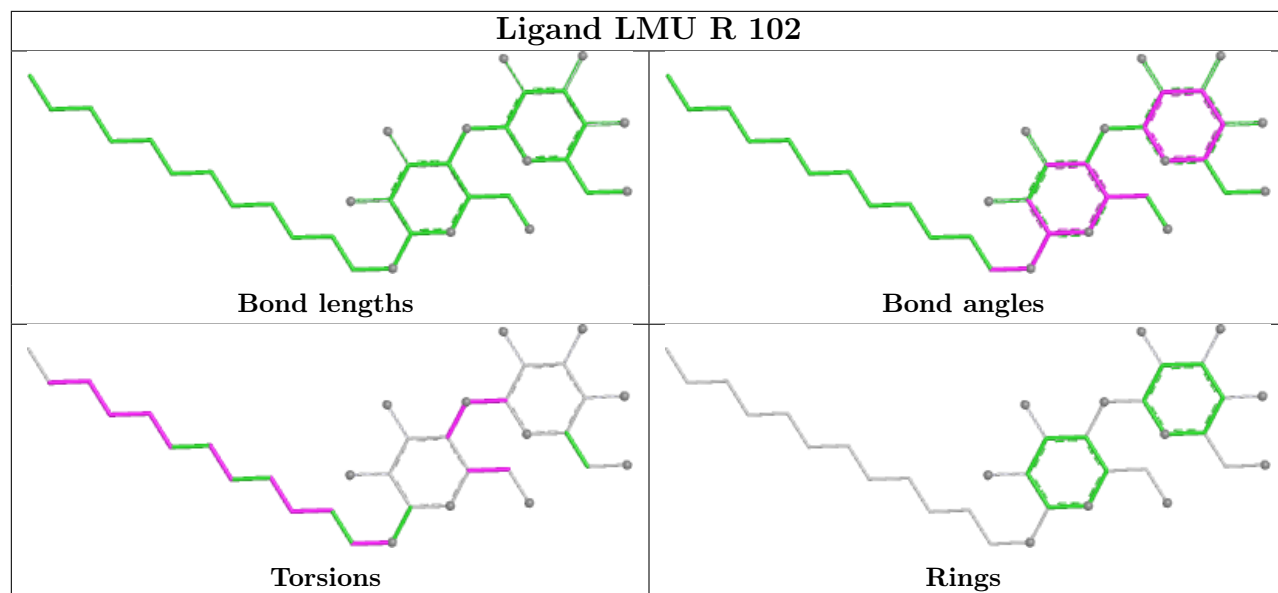
Rings

Ligand CLA A 815

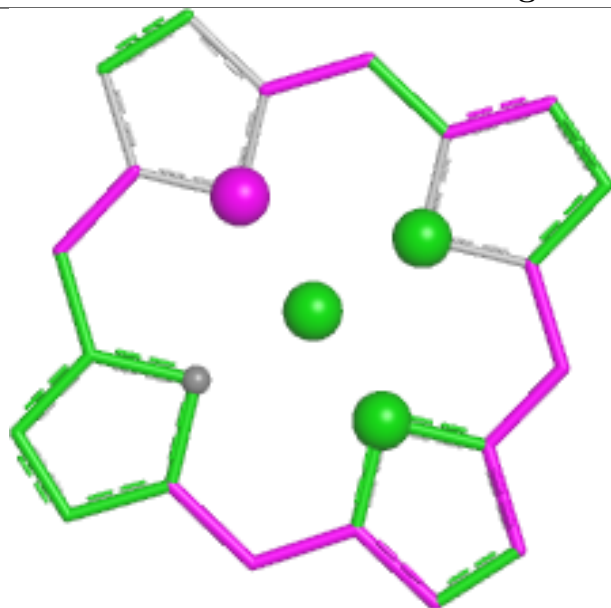


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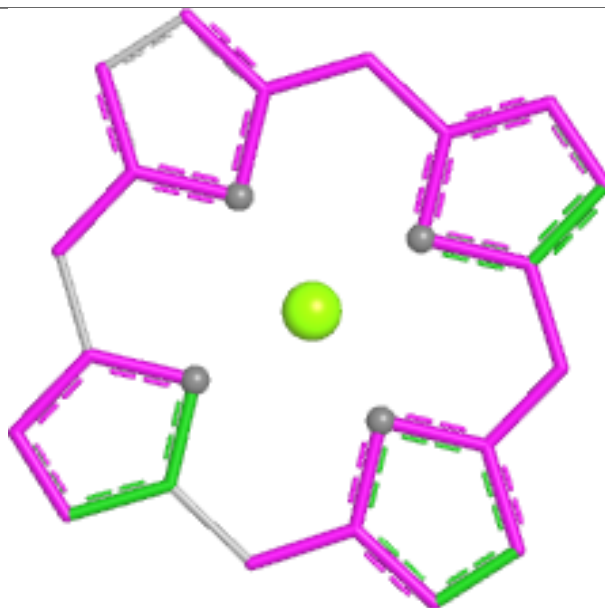




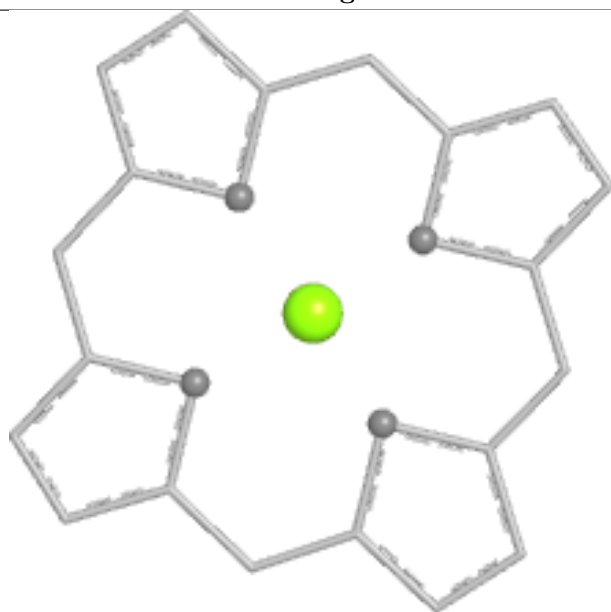
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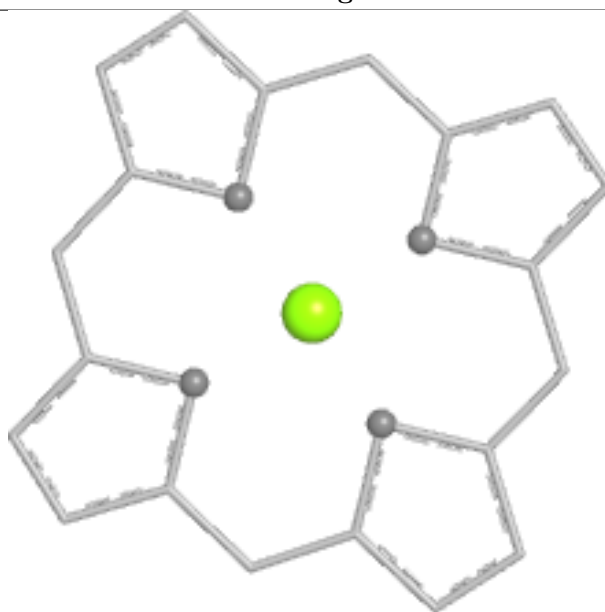
Bond lengths



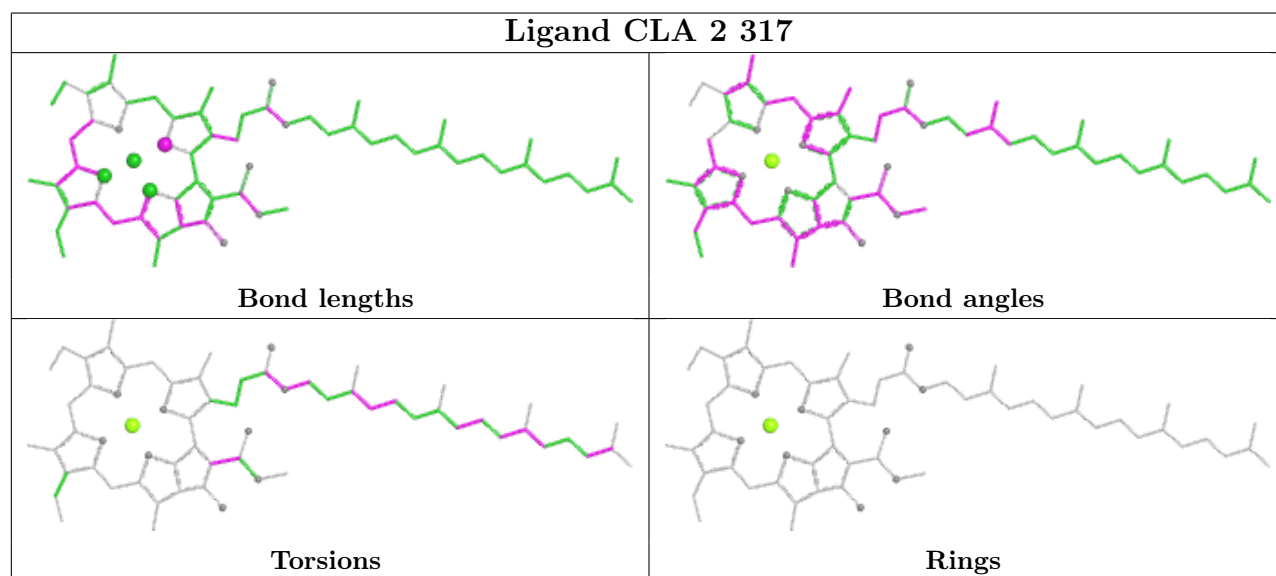
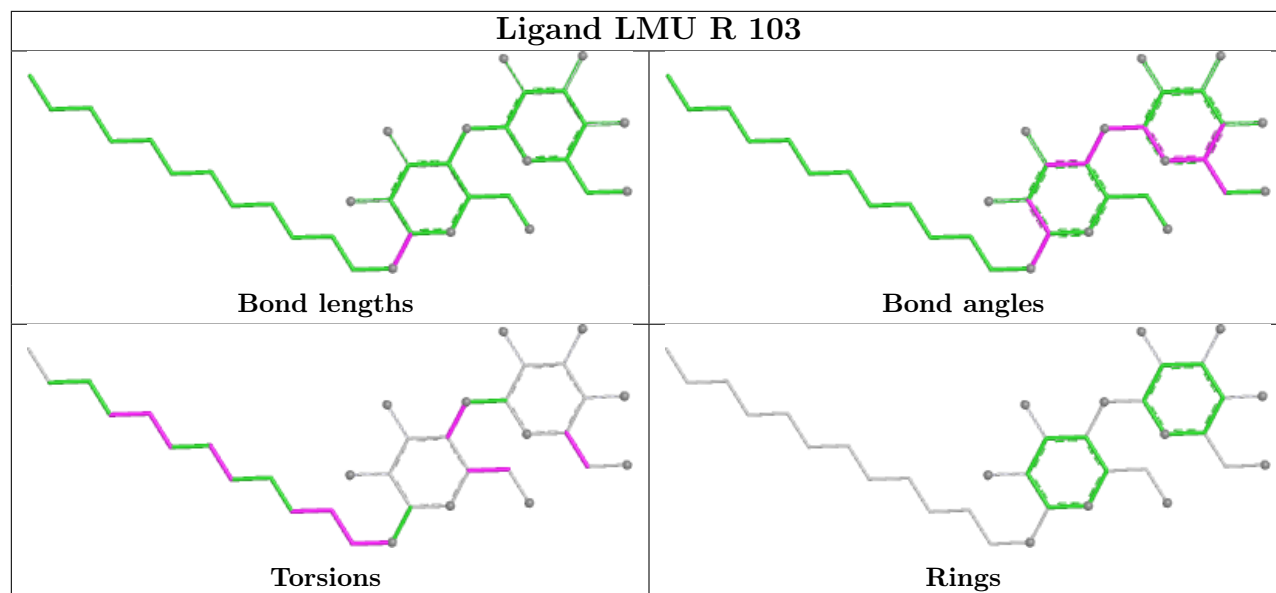
Bond angles



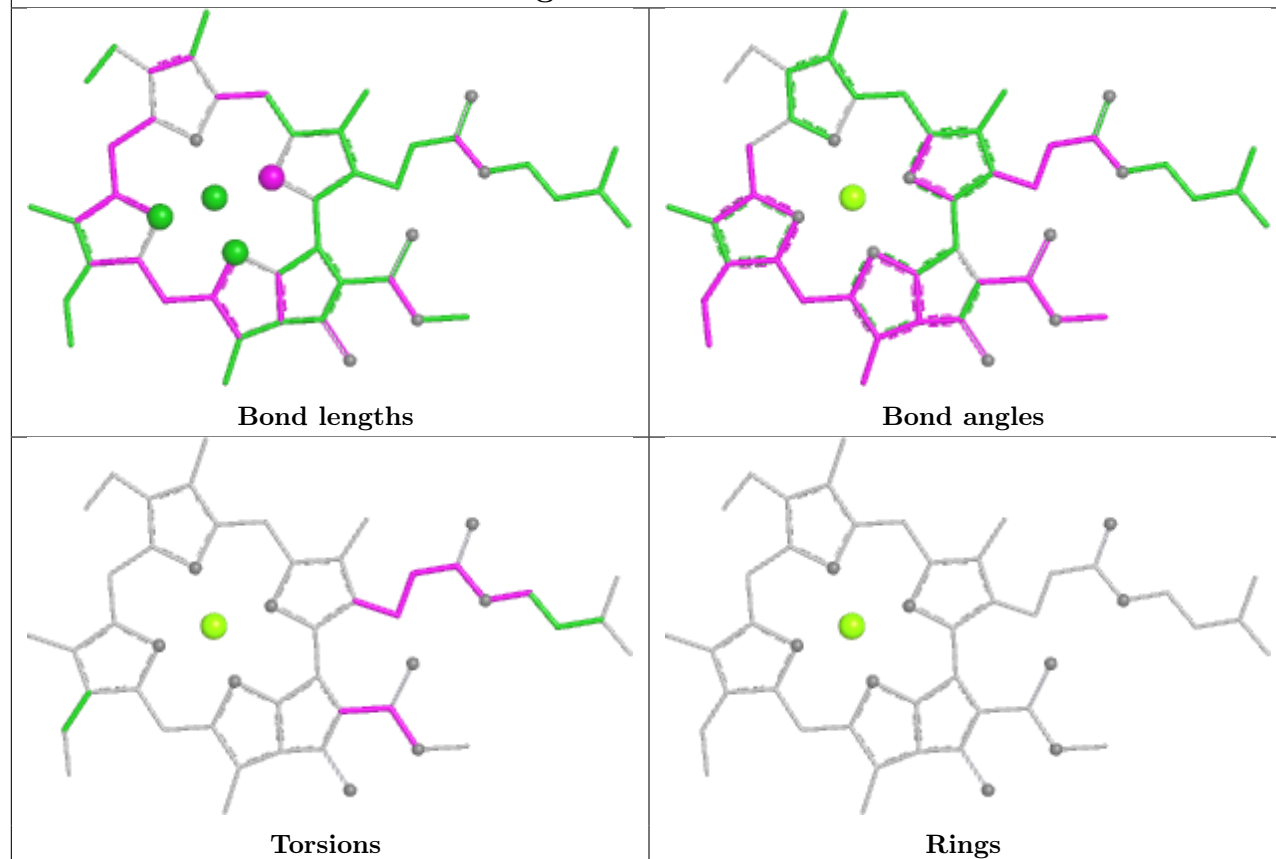
Torsions



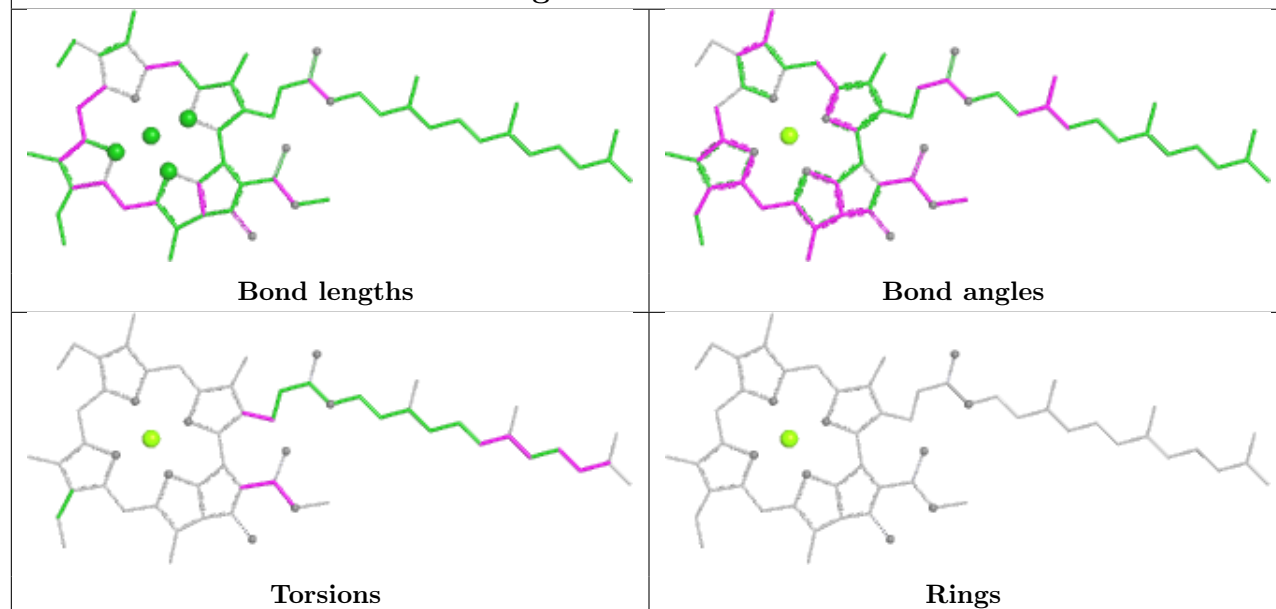
Rings

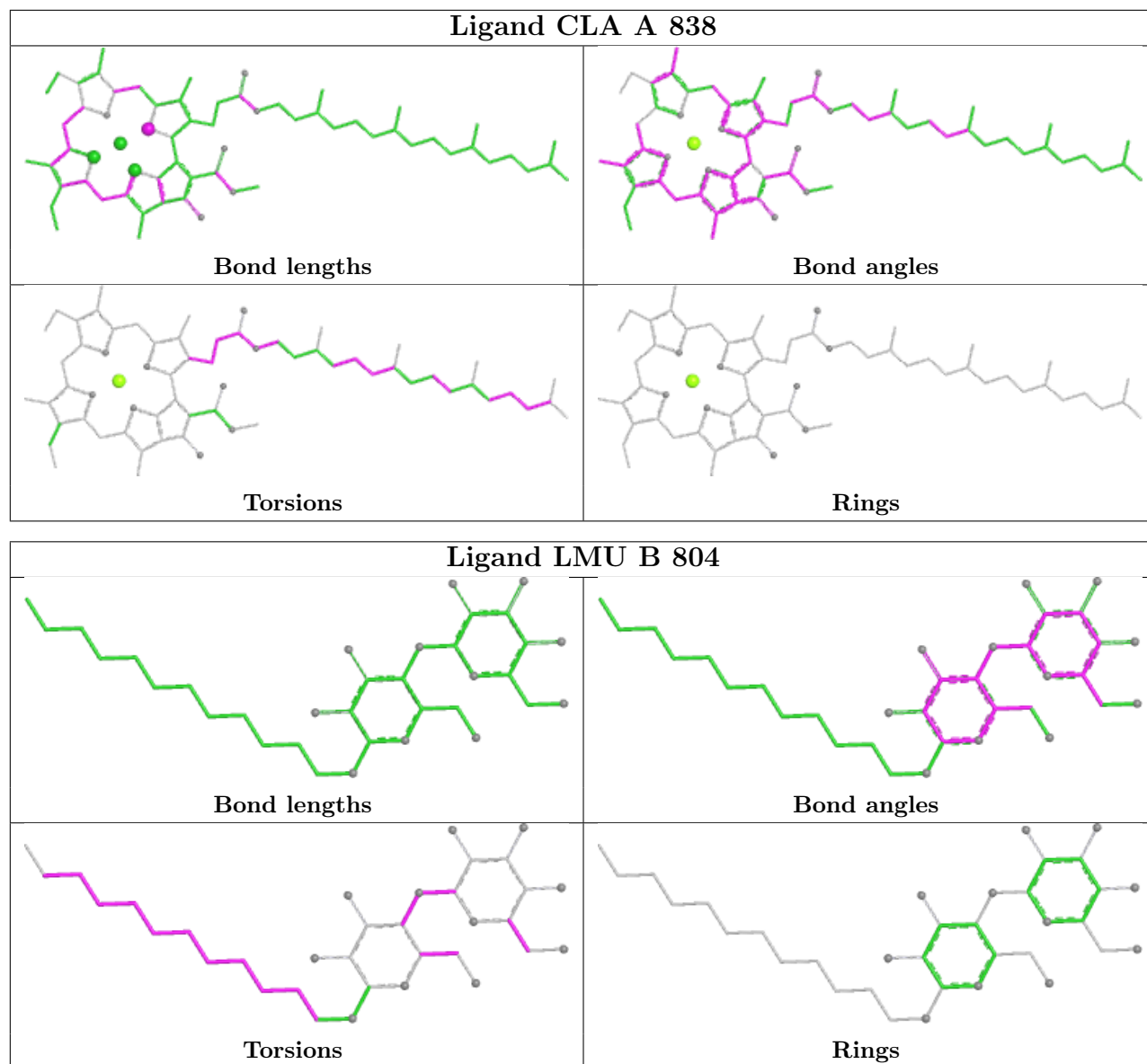


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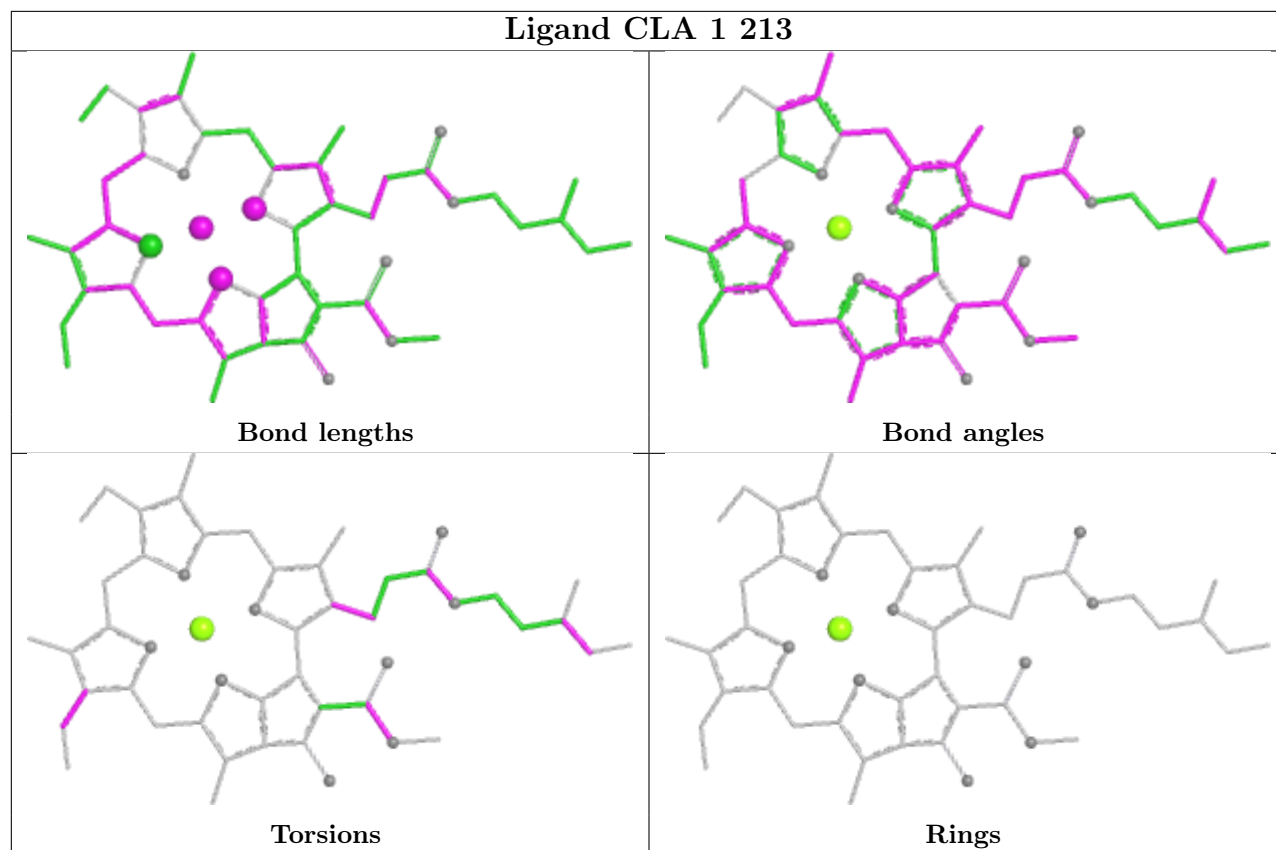


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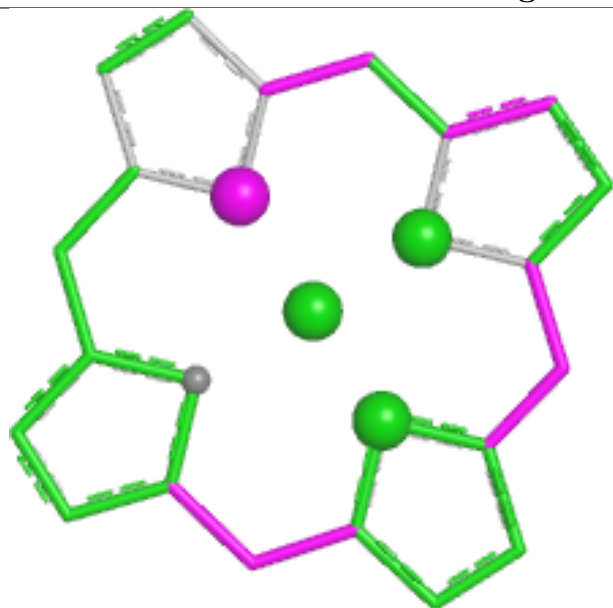




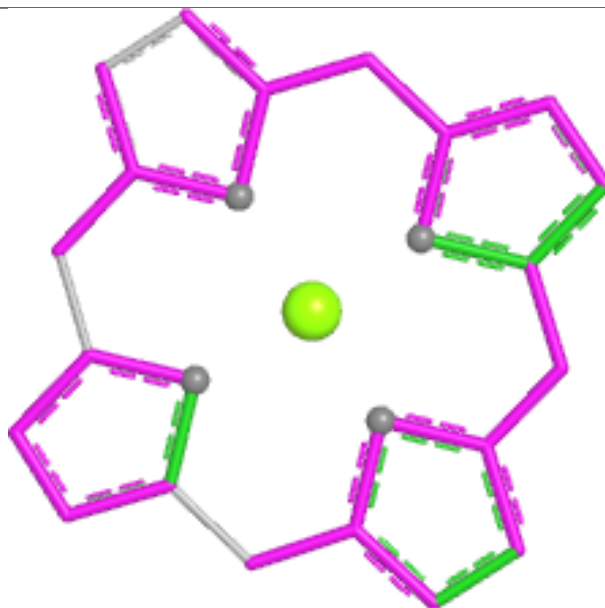
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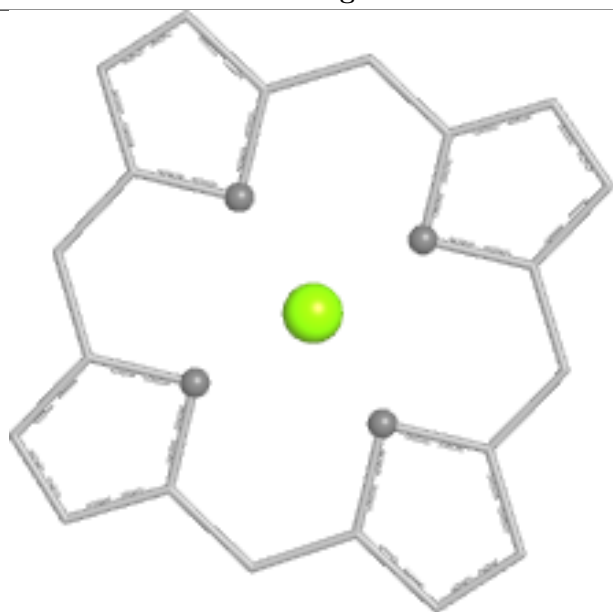
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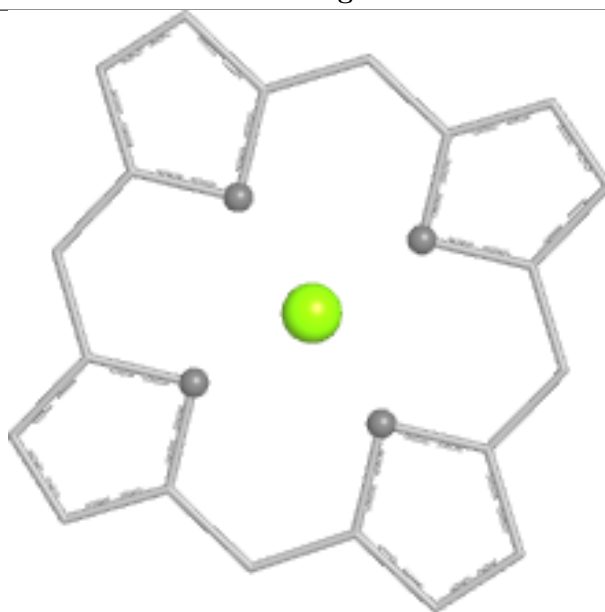
Bond lengths



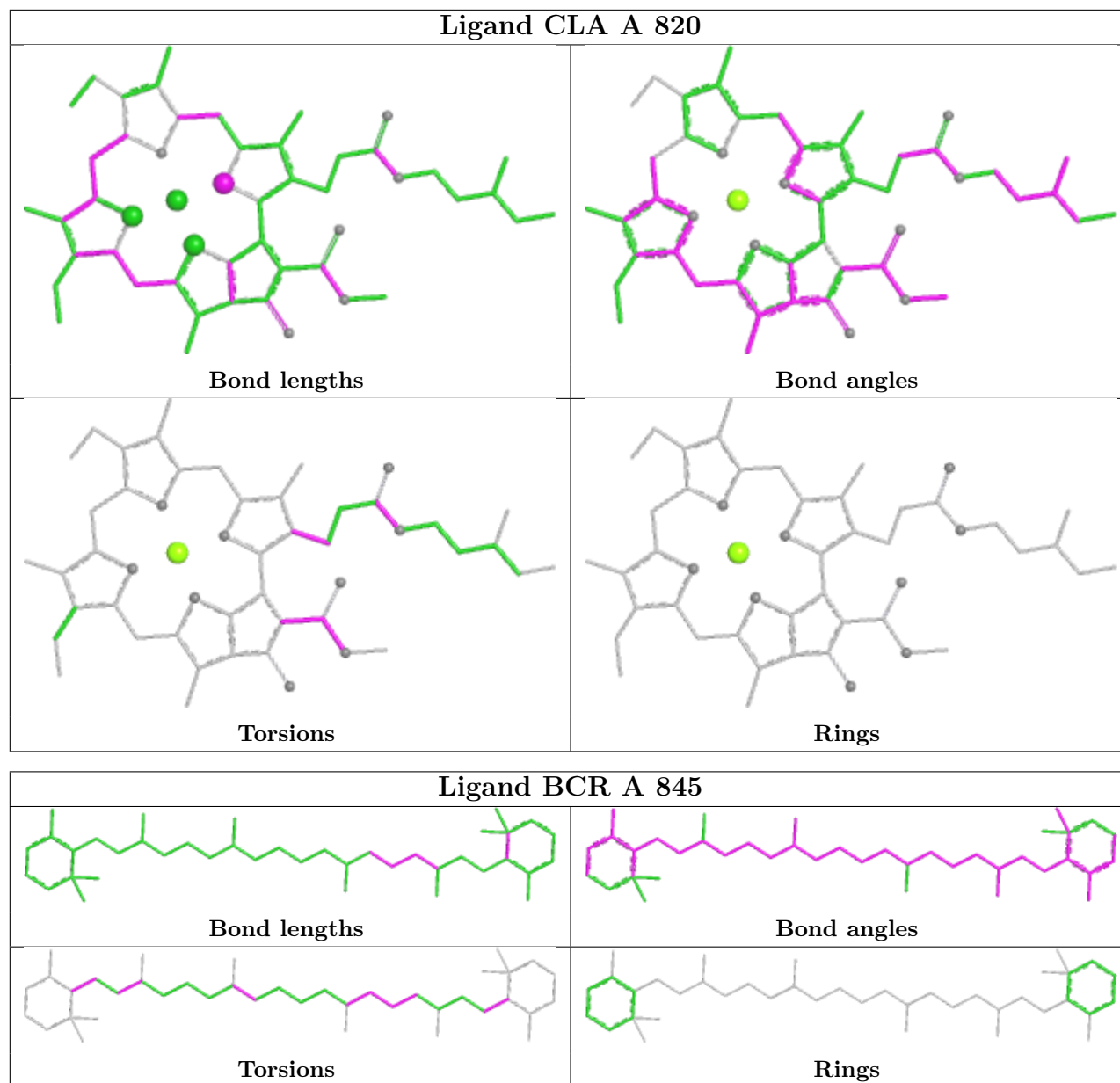
Bond angles

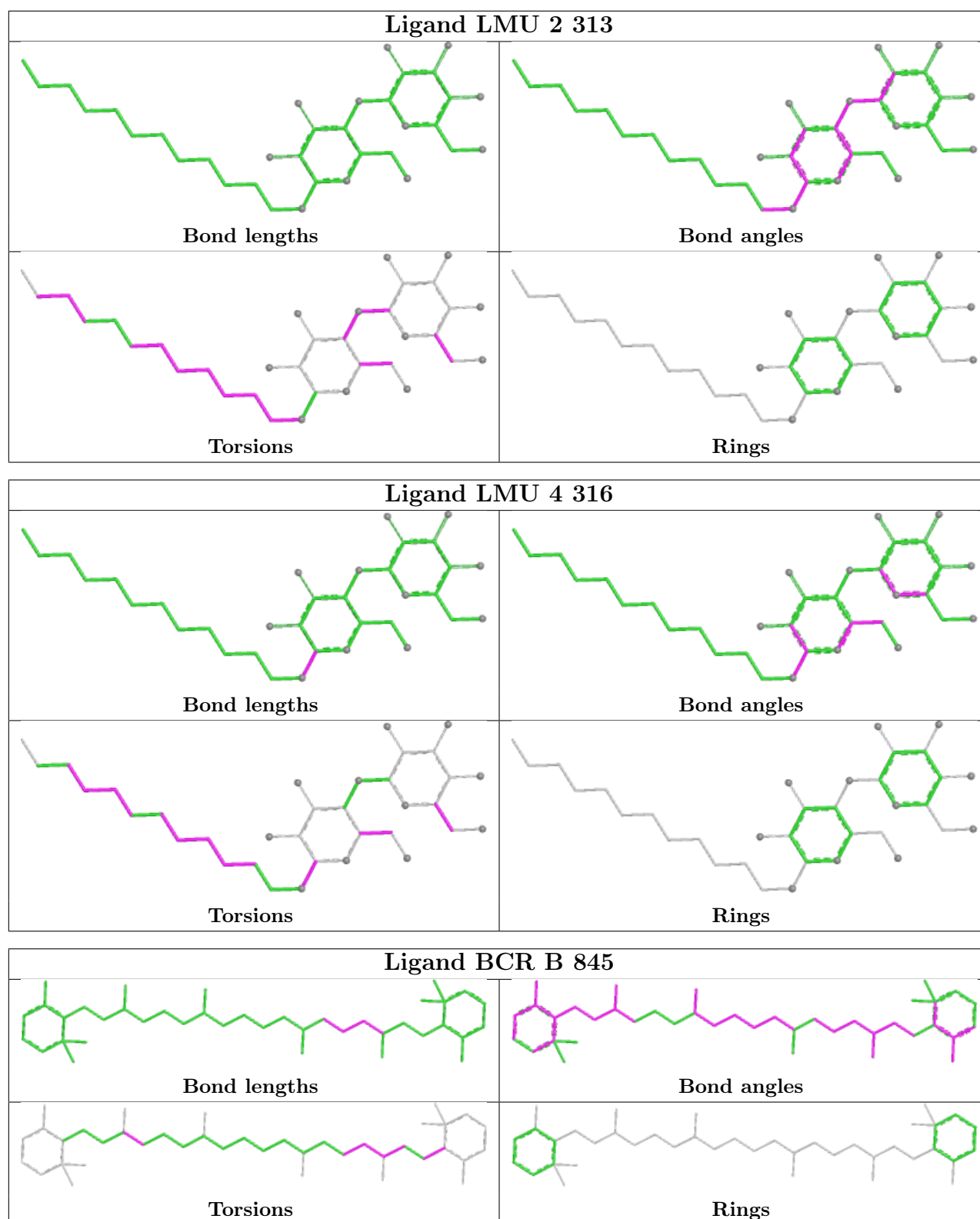


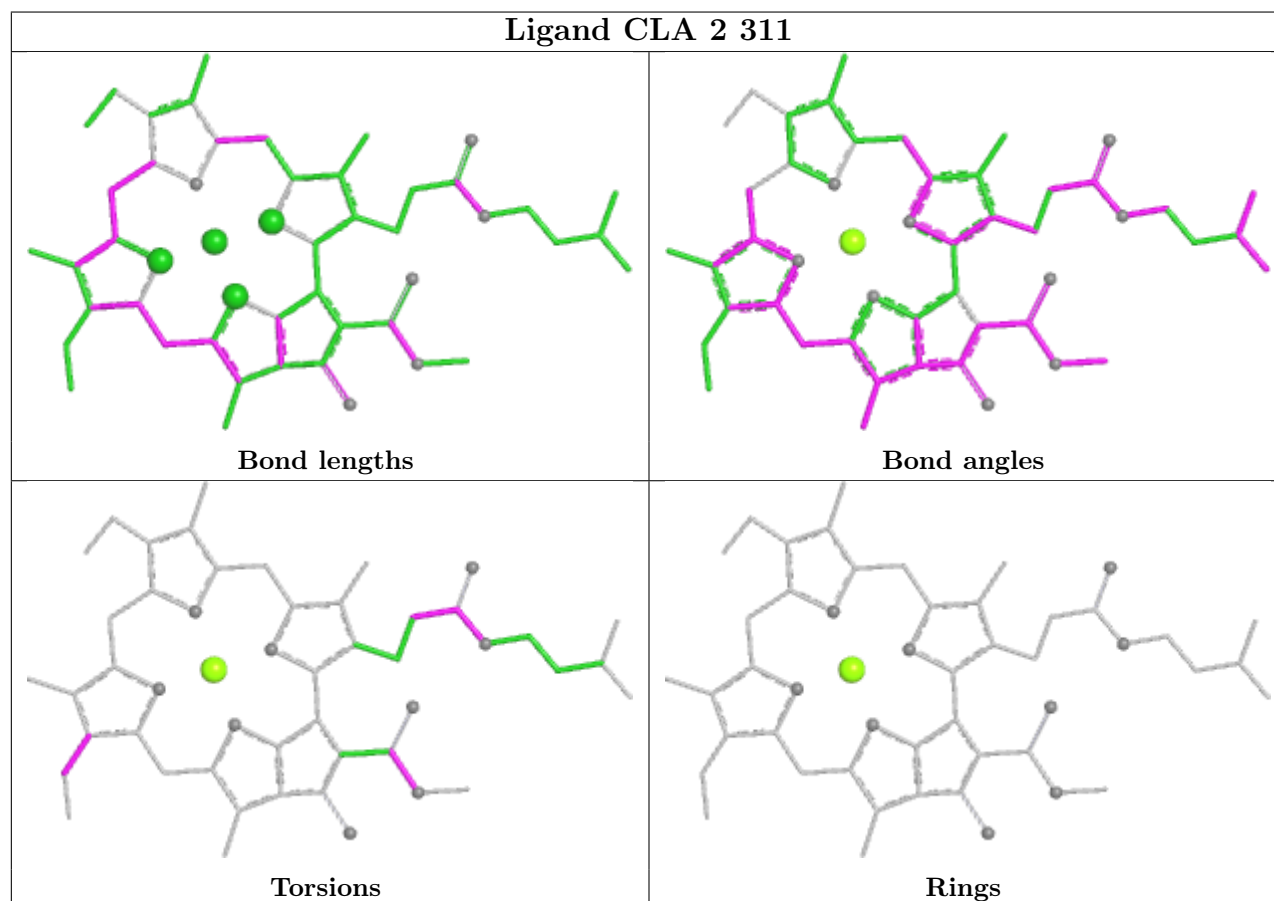
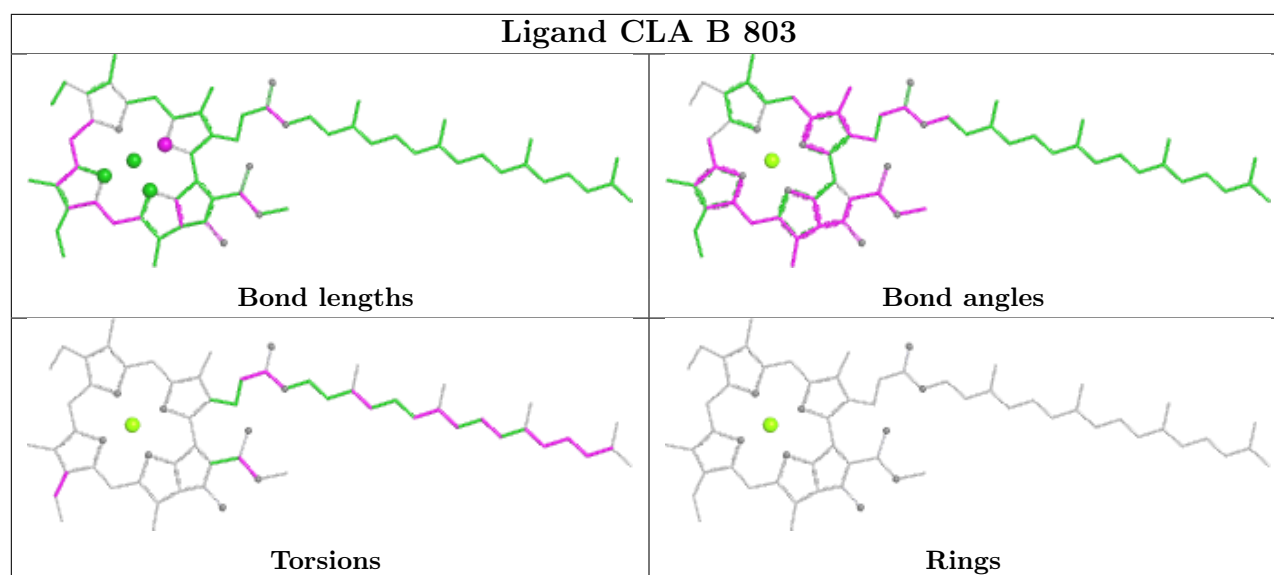
Torsions

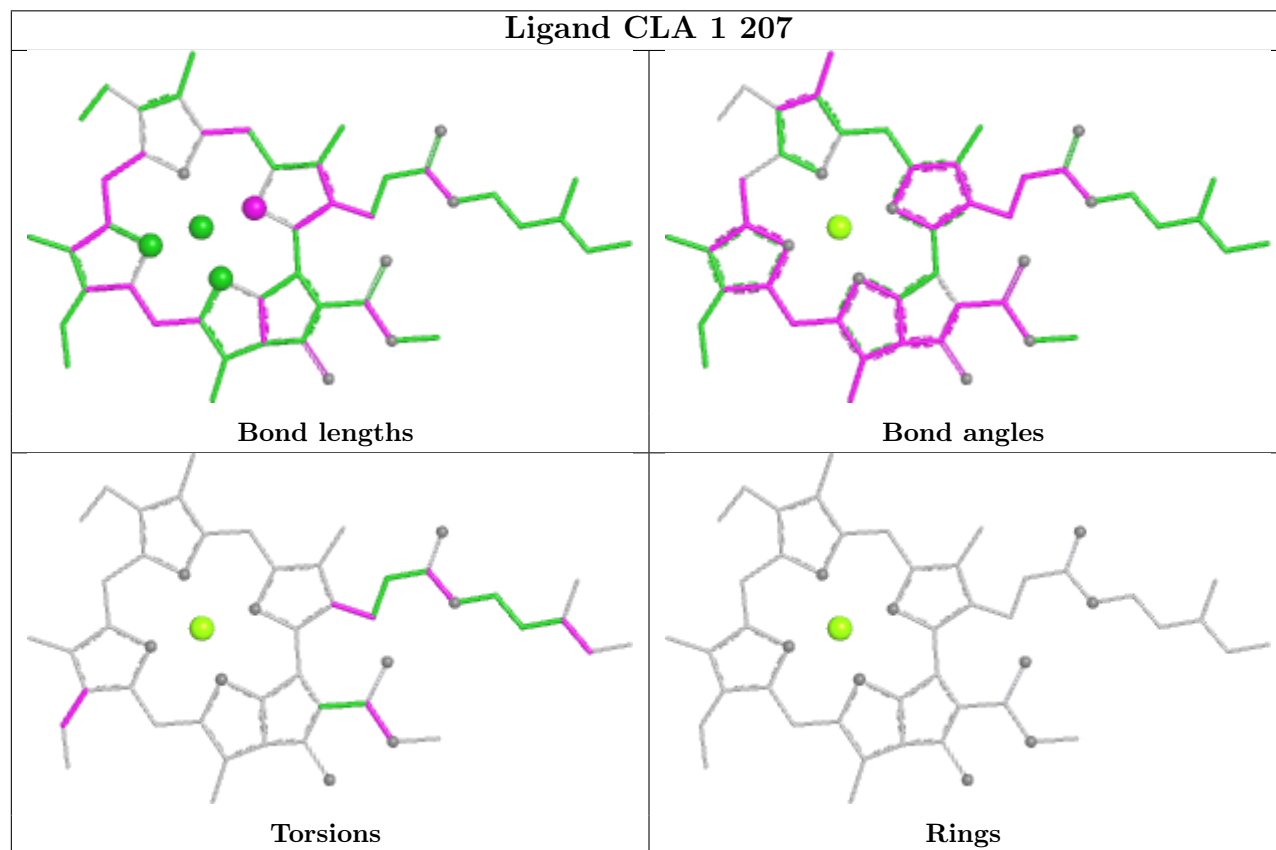
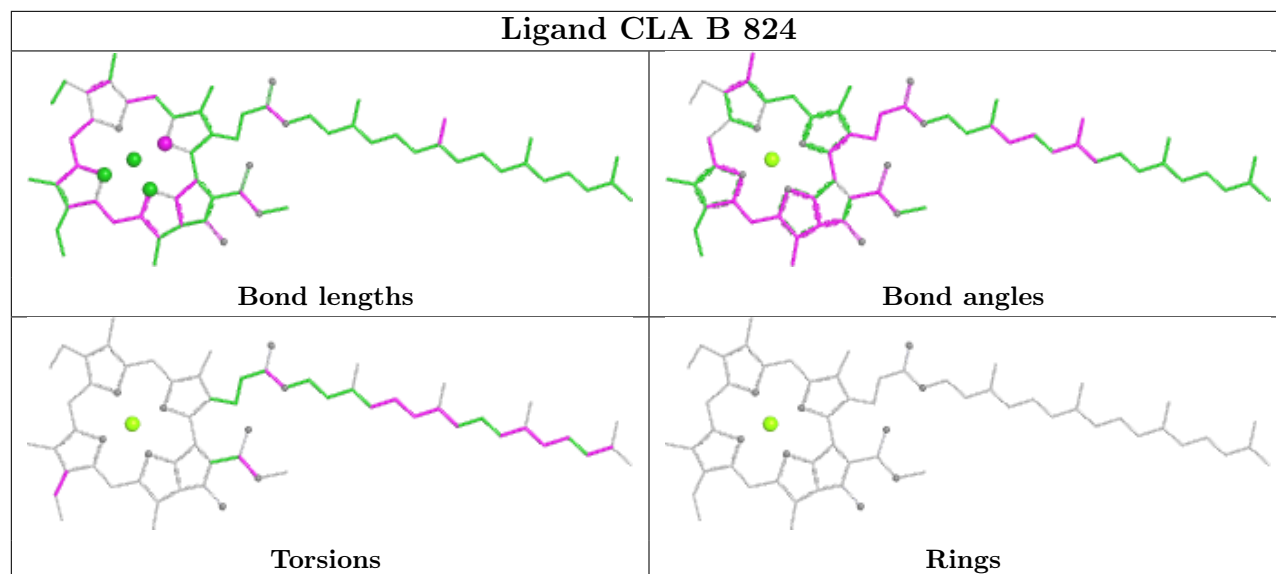


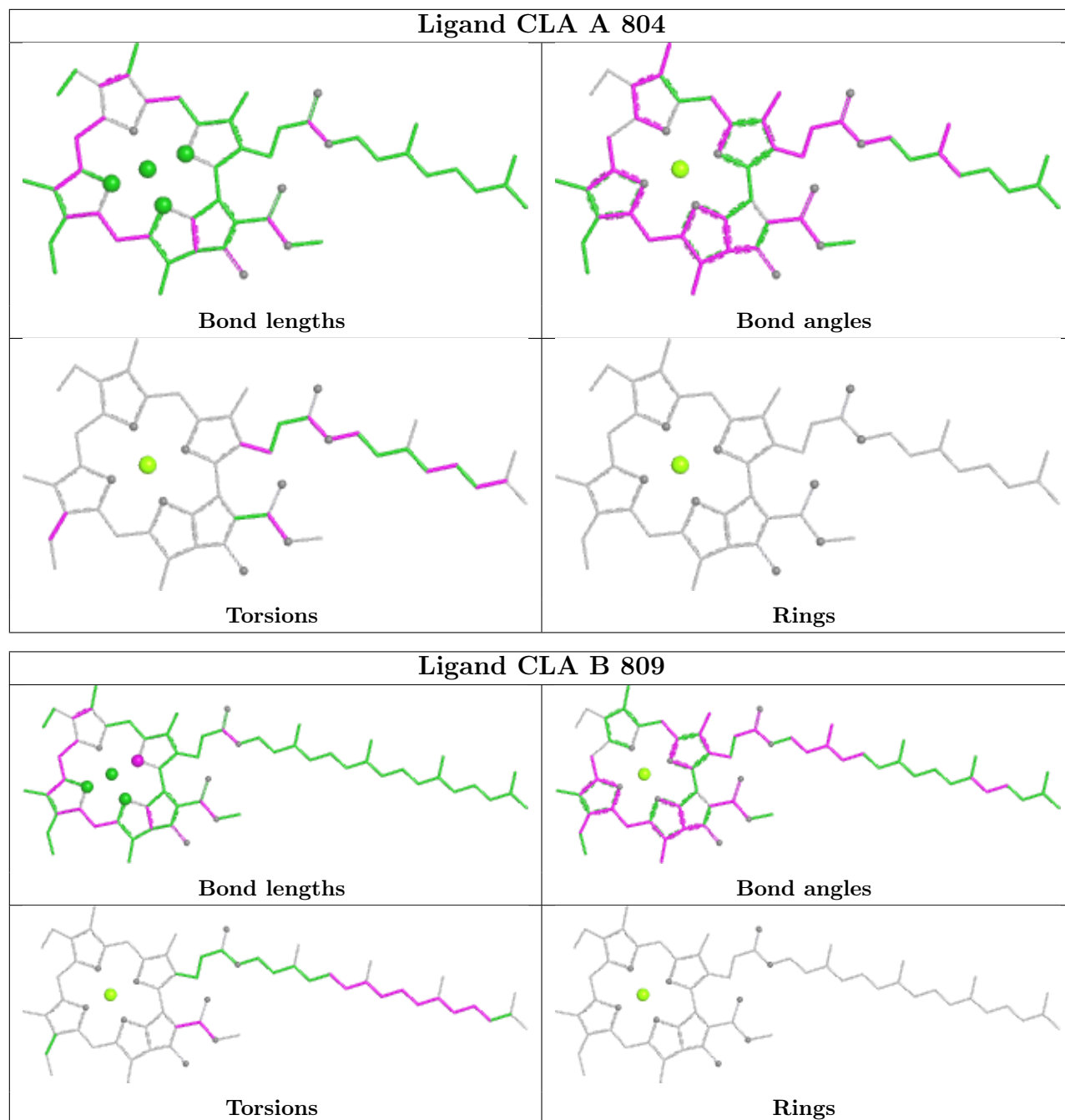
Rings



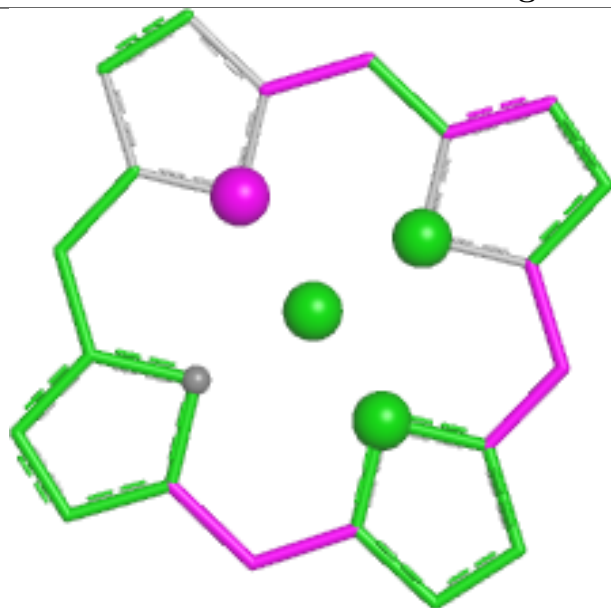




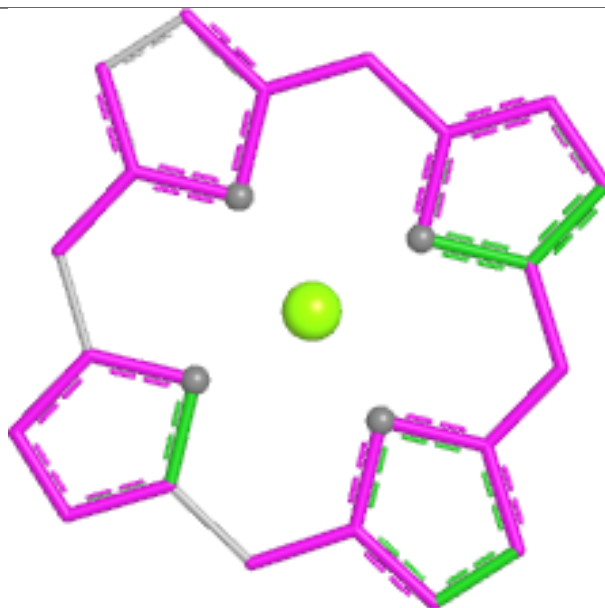




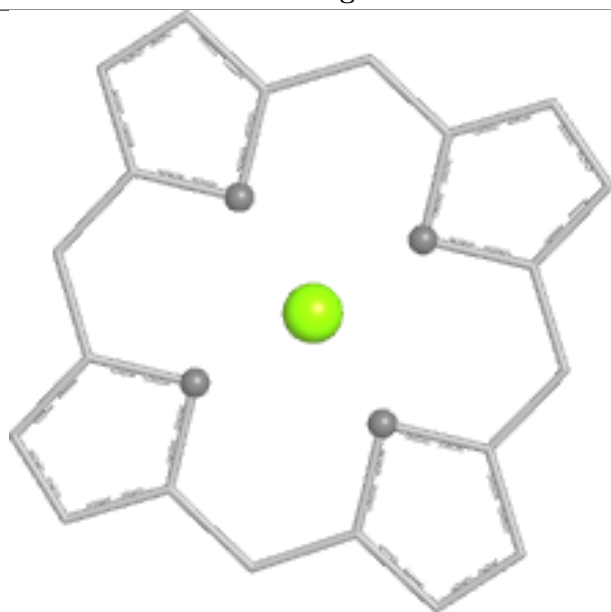
Ligand CLA 1 208



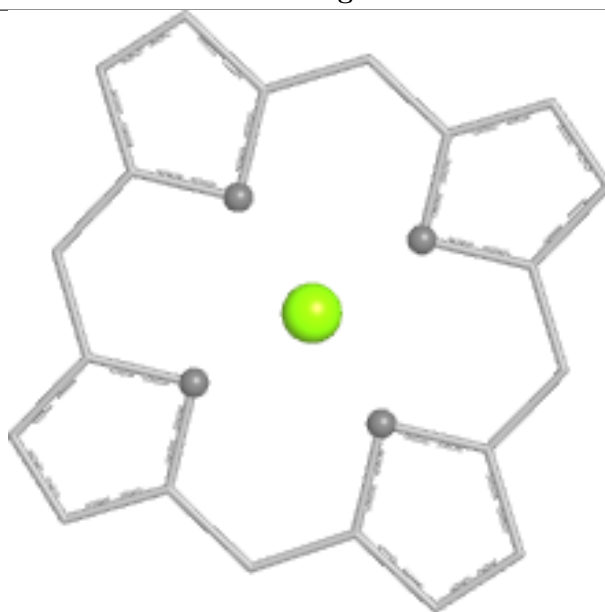
Bond lengths



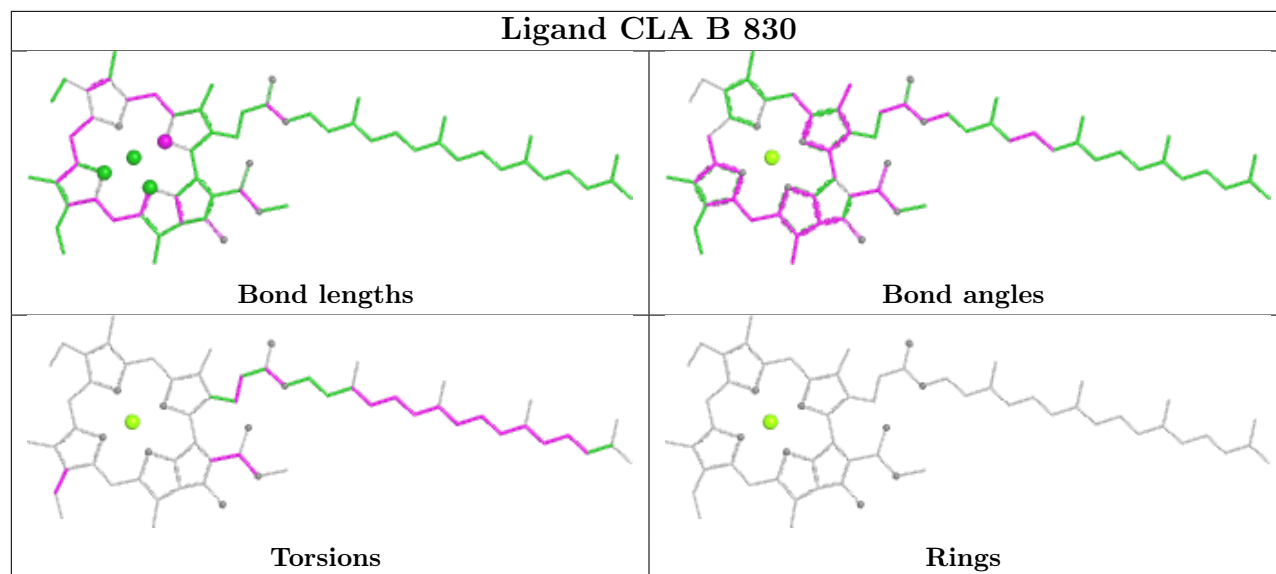
Bond angles



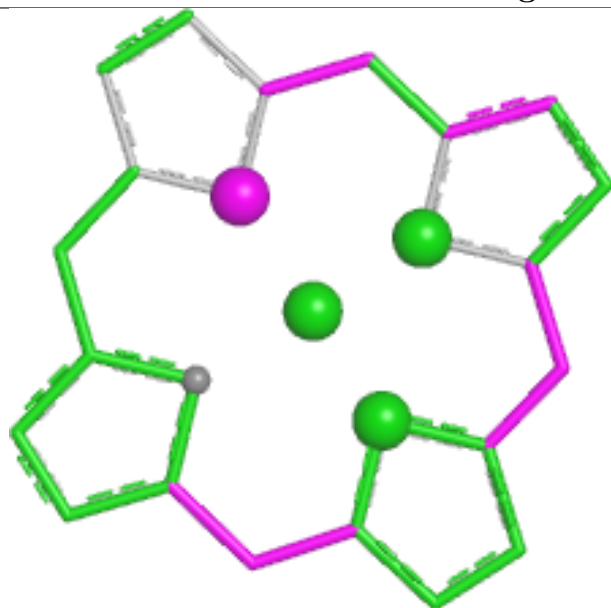
Torsions



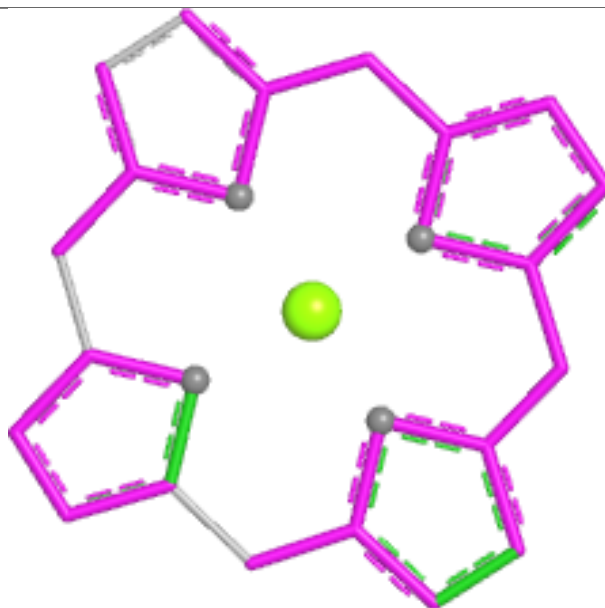
Rings



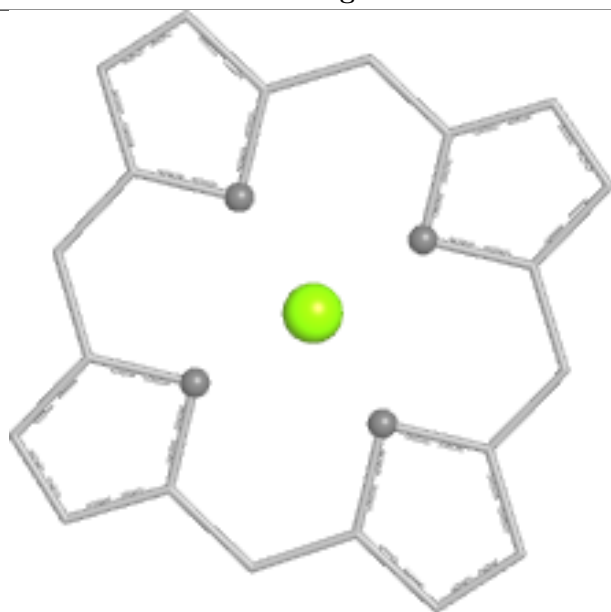
Ligand CLA 4 312



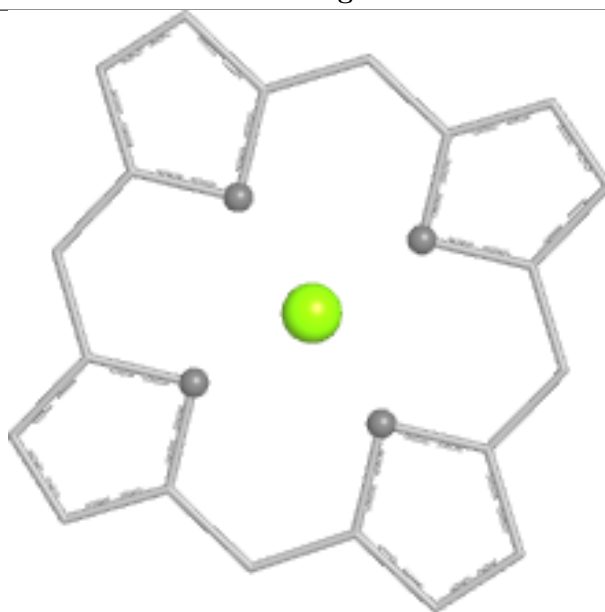
Bond lengths



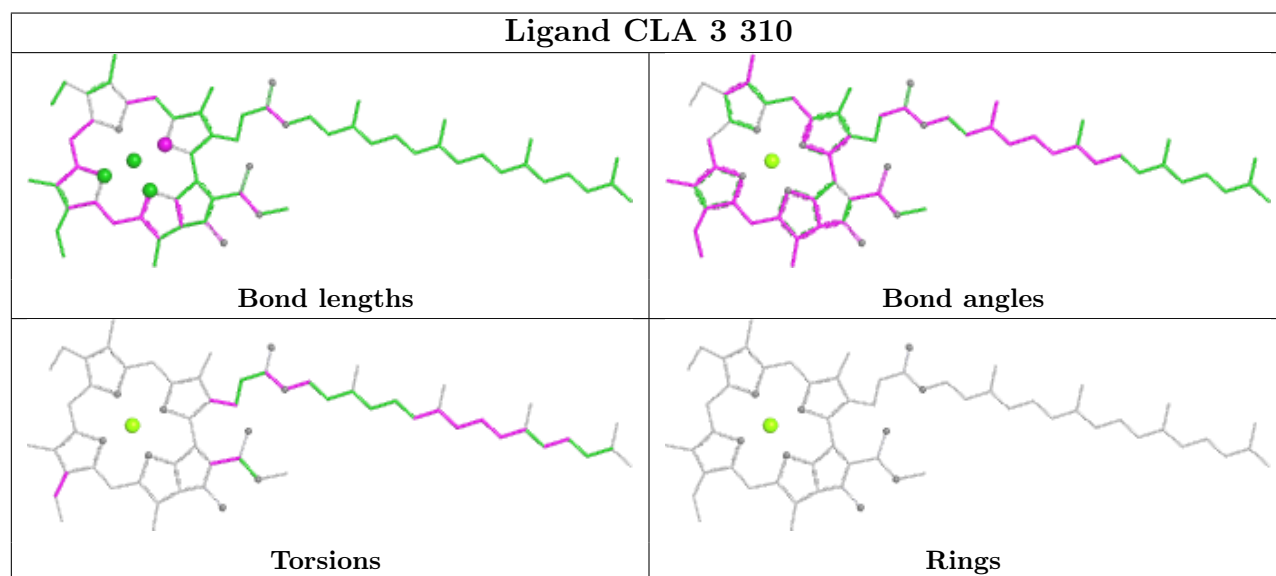
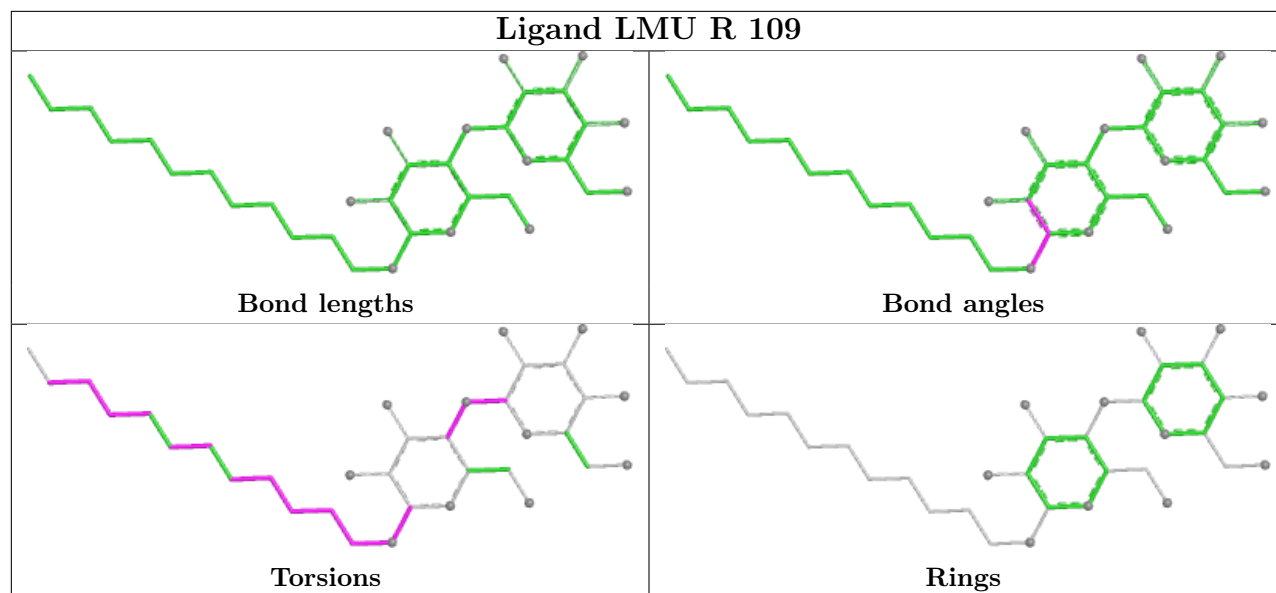
Bond angles



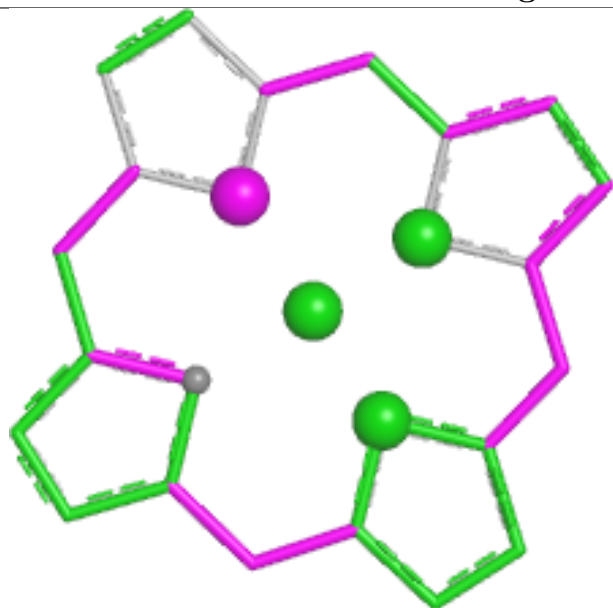
Torsions



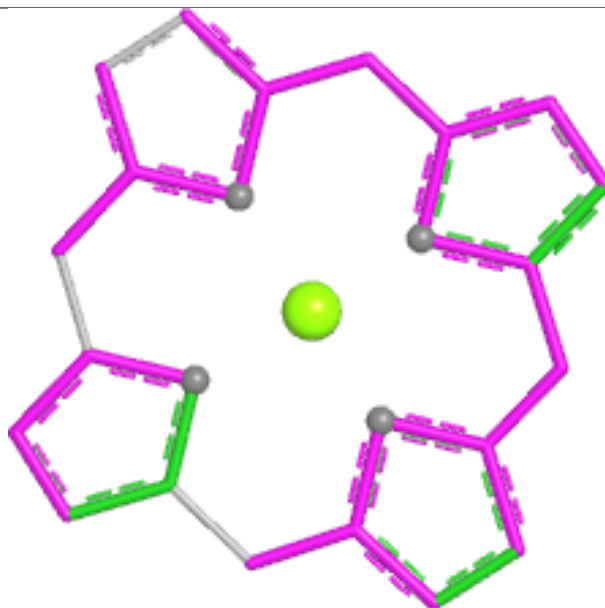
Rings



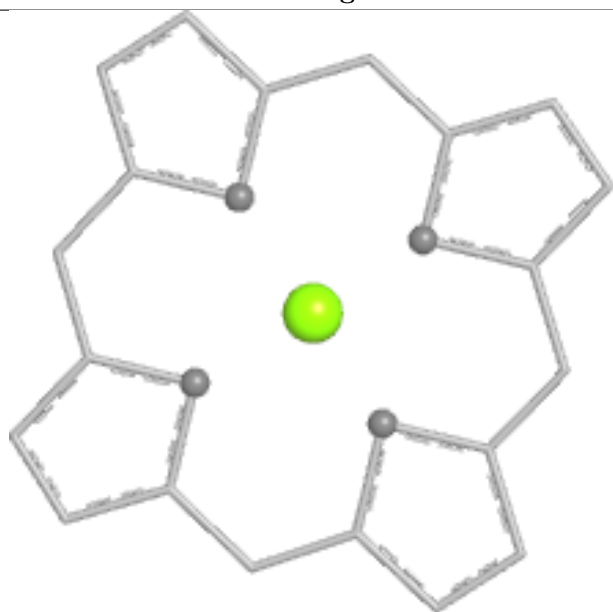
Ligand CLA 2 309



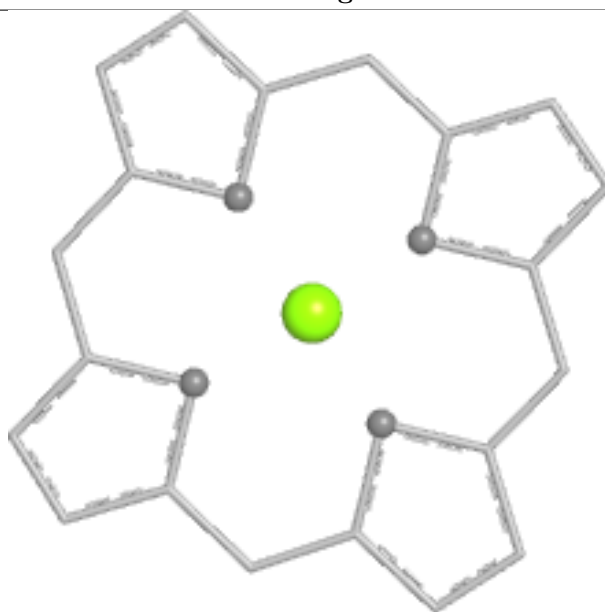
Bond lengths



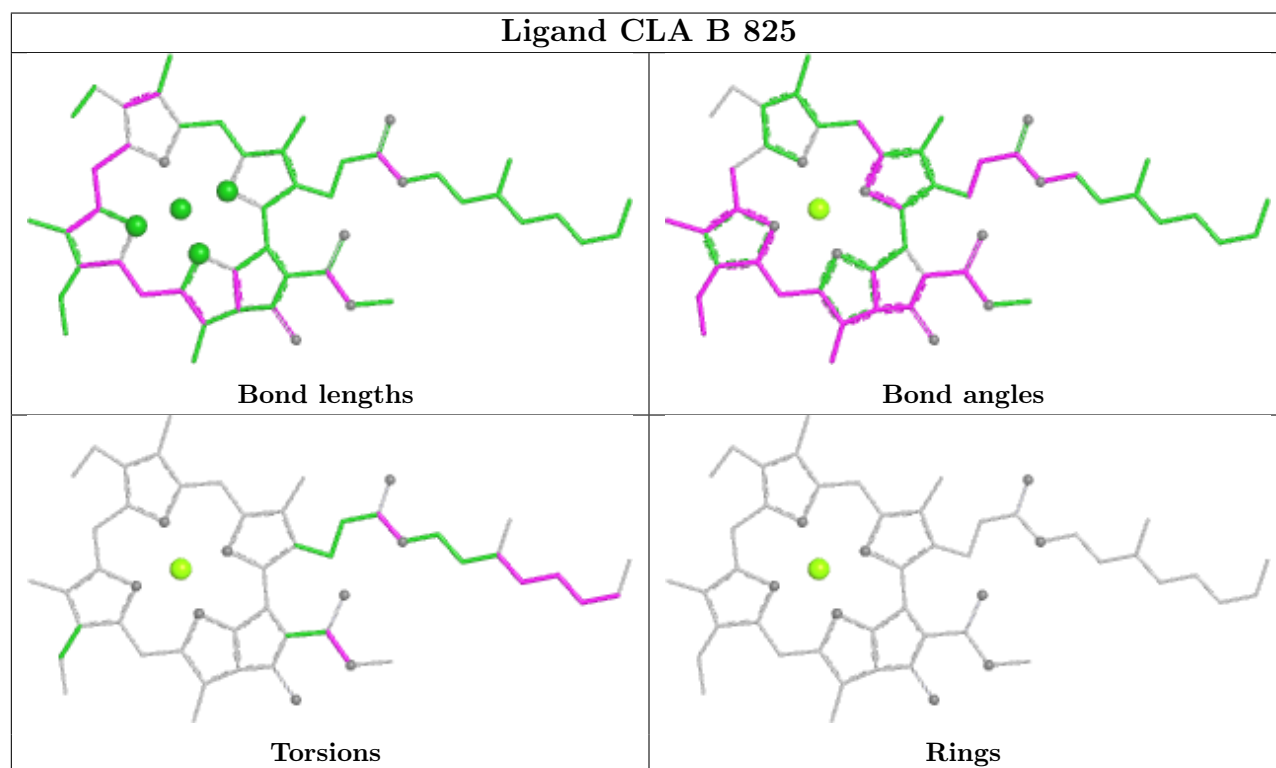
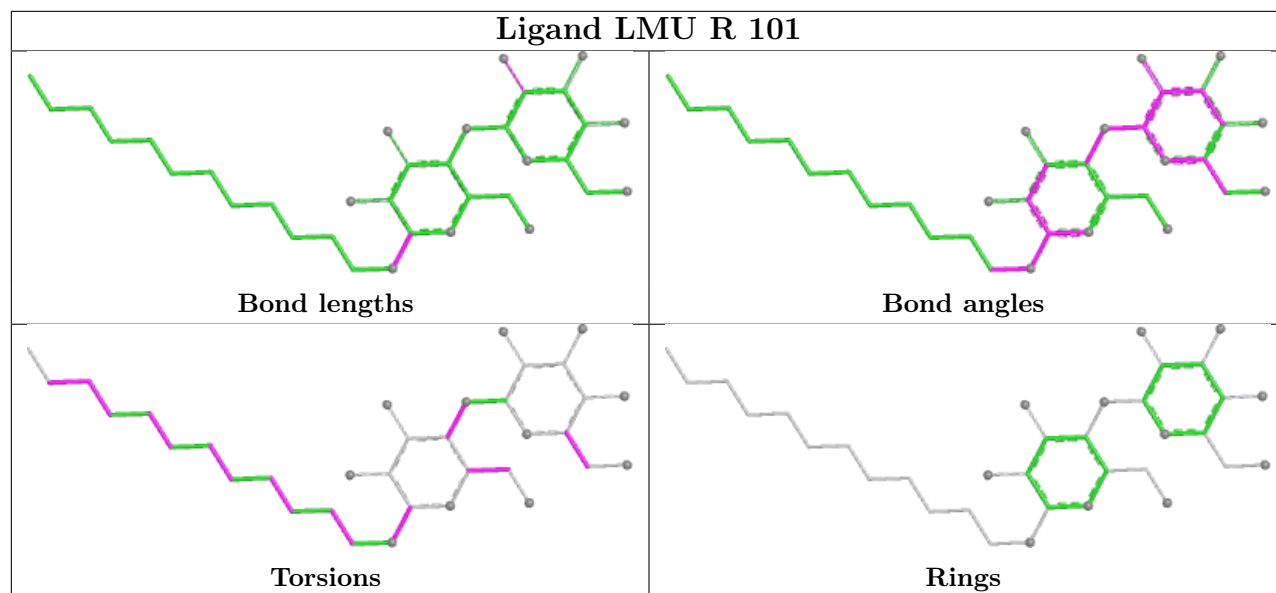
Bond angles



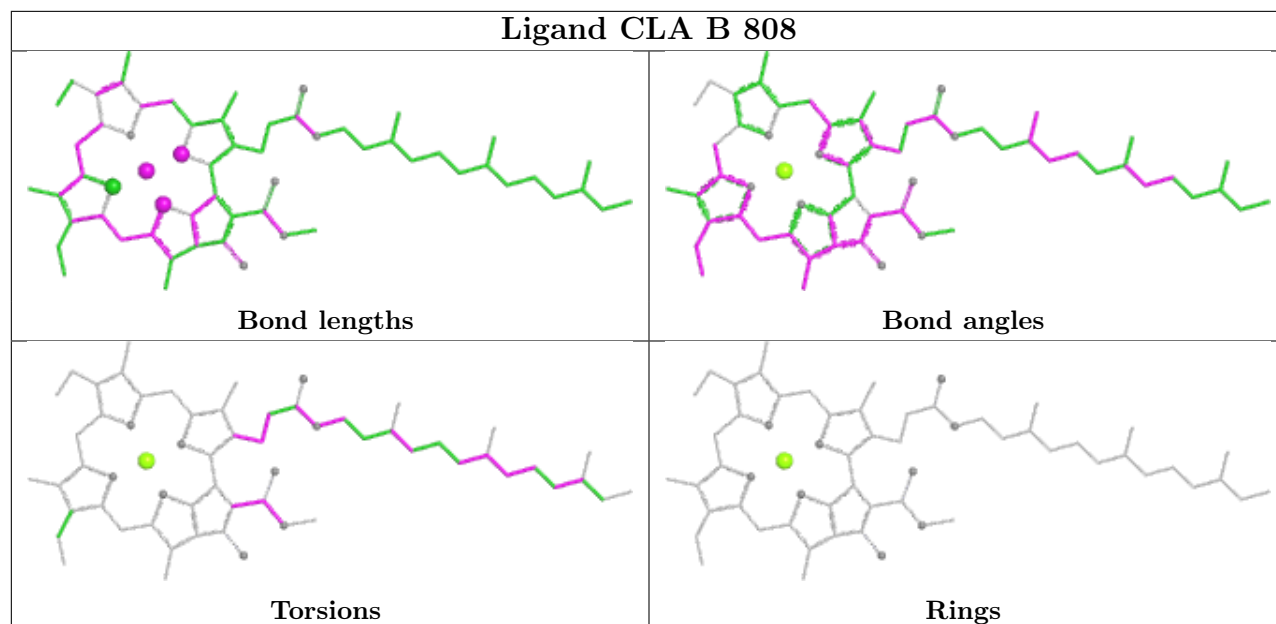
Torsions



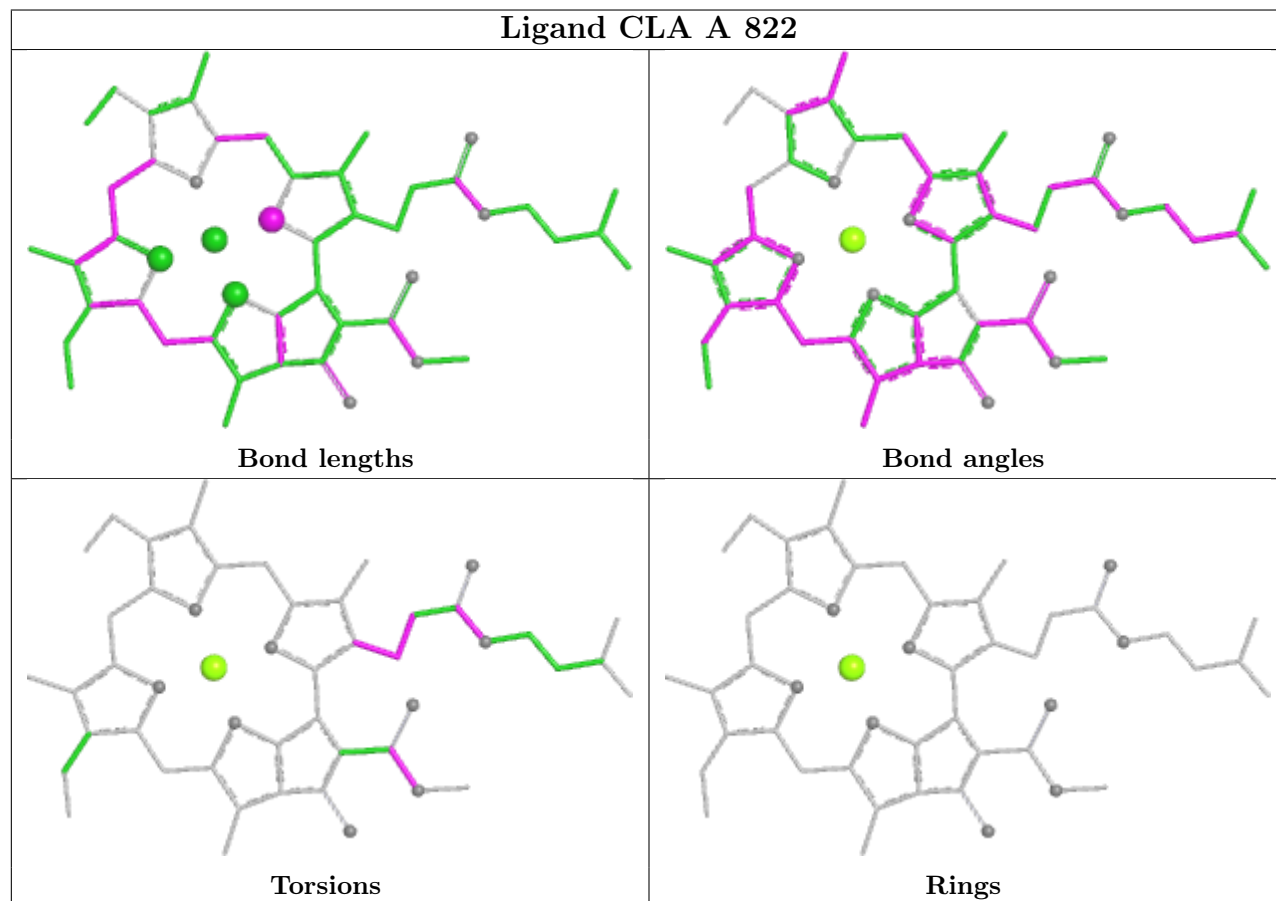
Rings

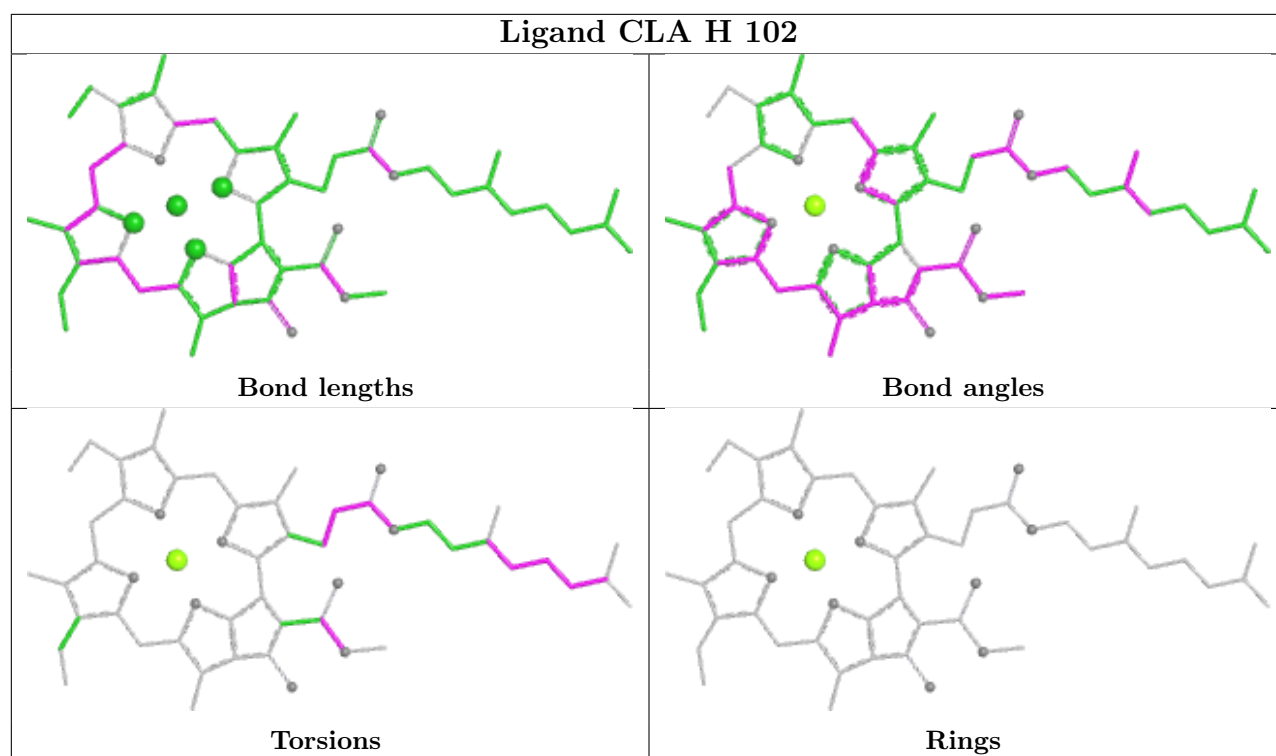


Ligand CLA B 808

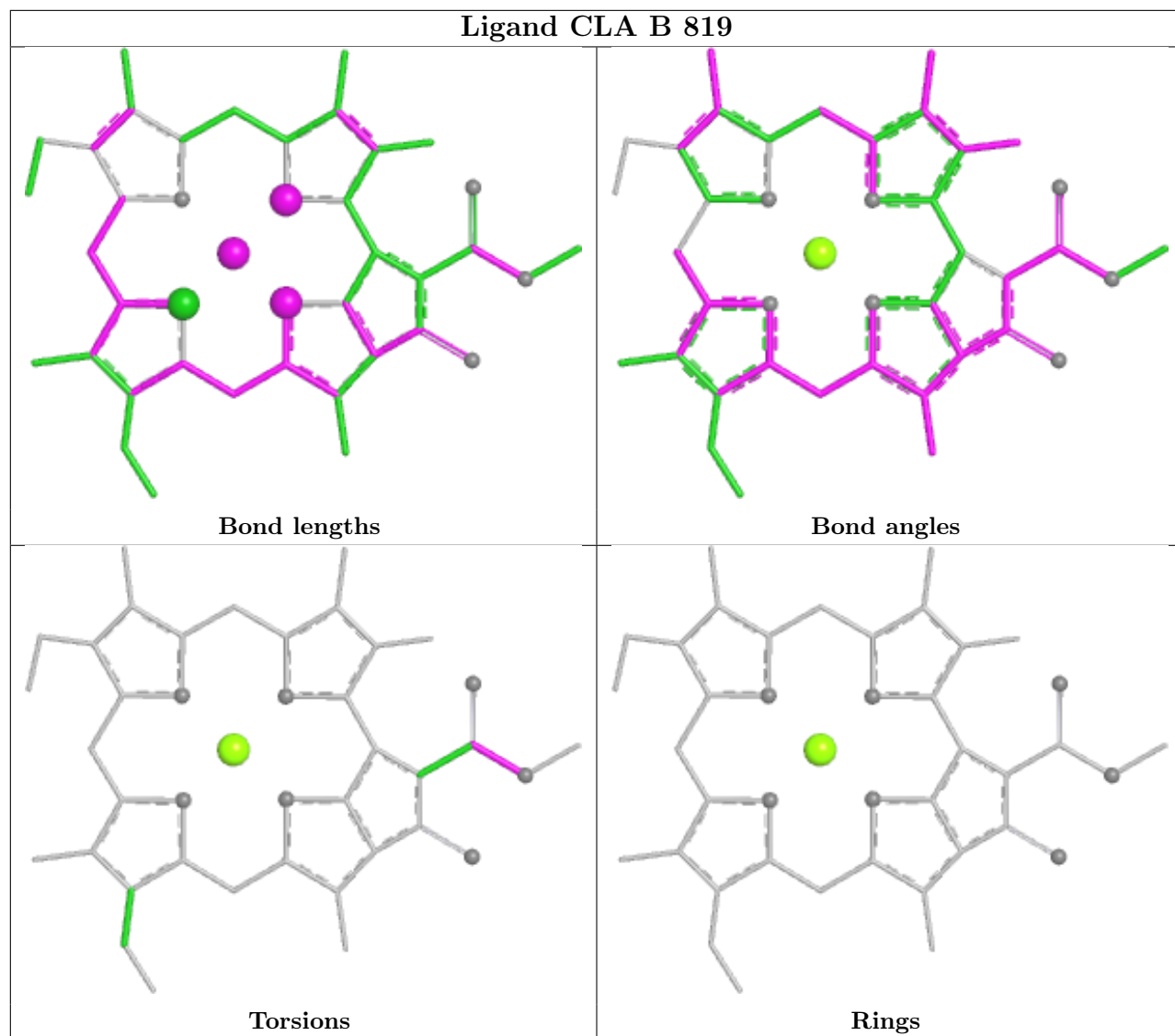


Ligand CLA A 822

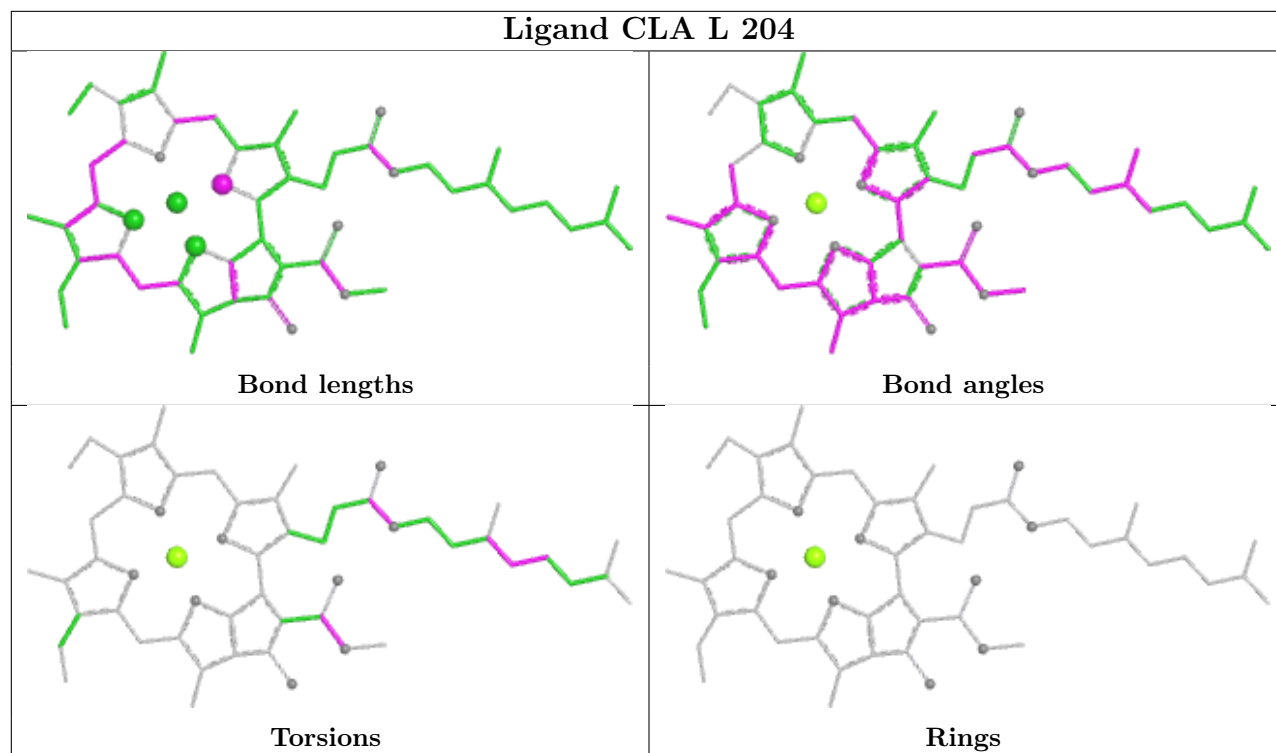




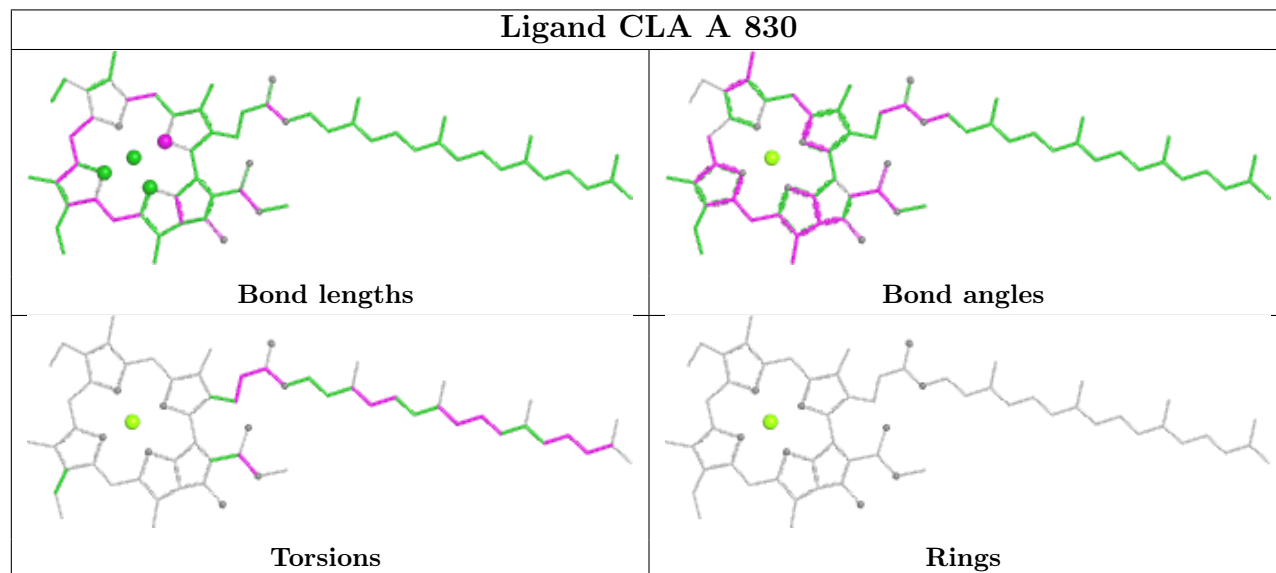
Ligand CLA B 819



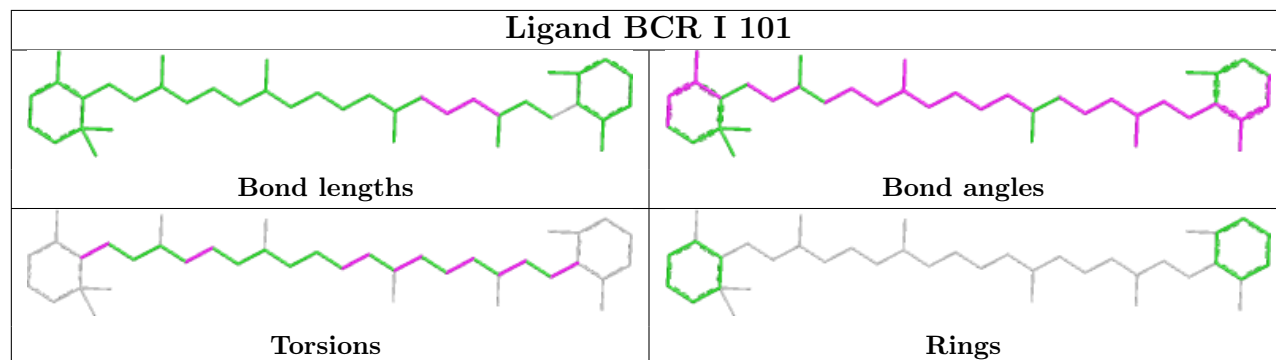
Ligand CLA L 204



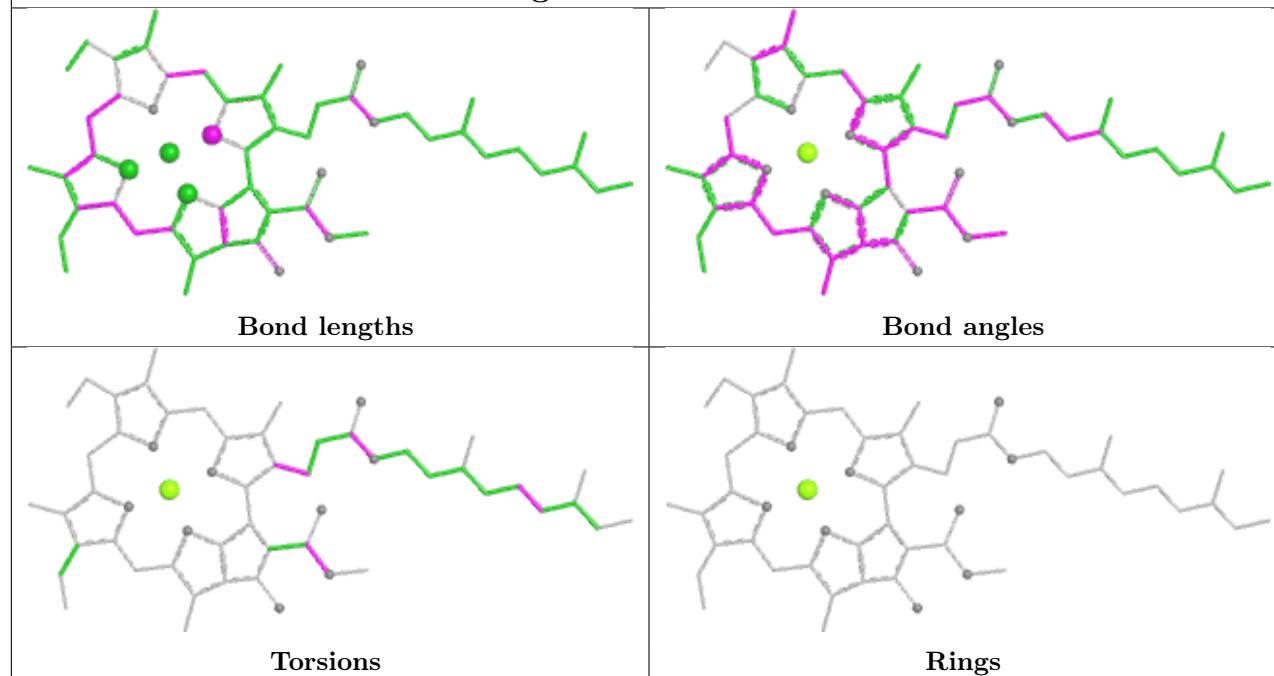
Ligand CLA A 830



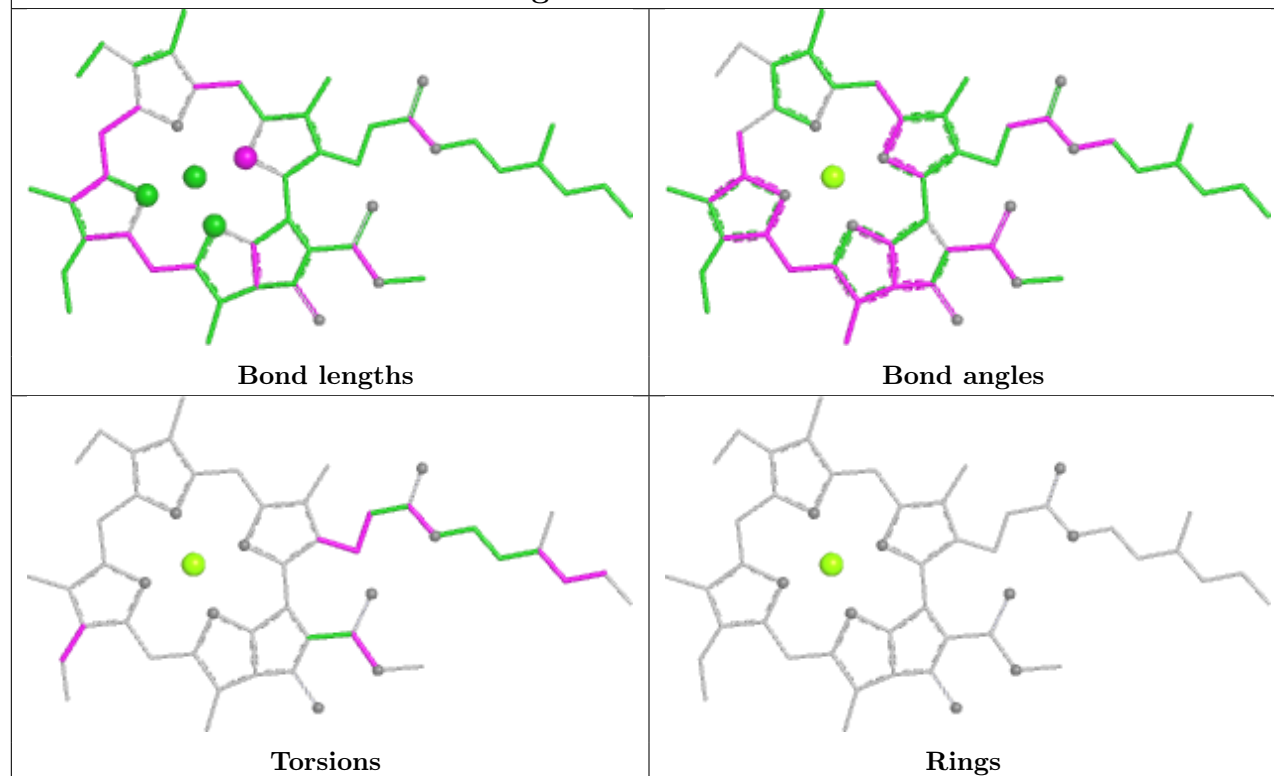
Ligand BCR I 101



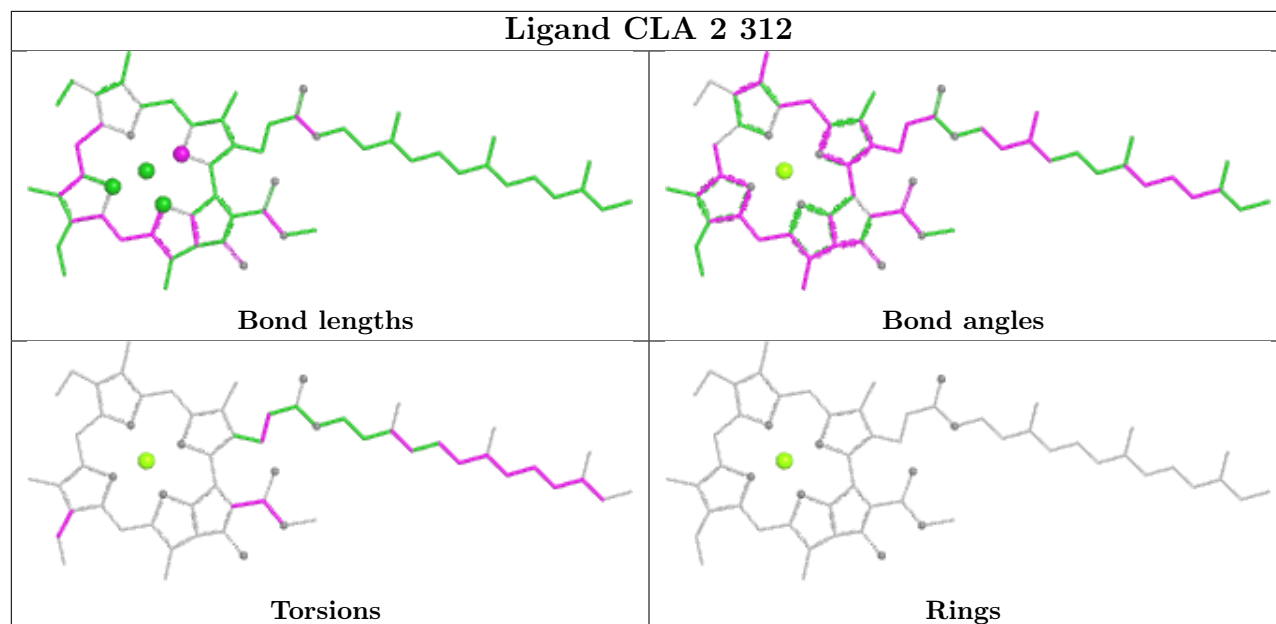
Ligand CLA A 806



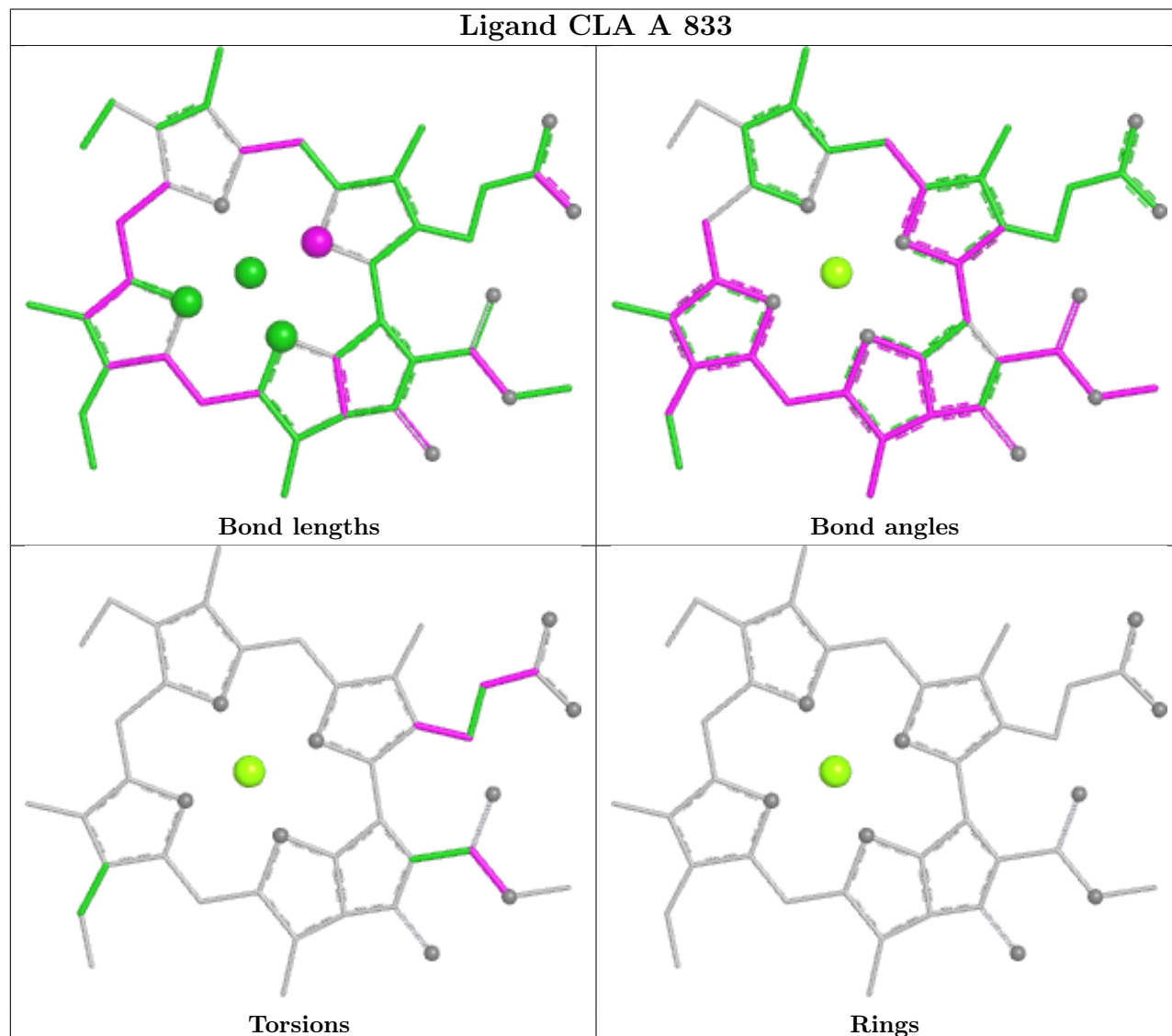
Ligand CLA A 817



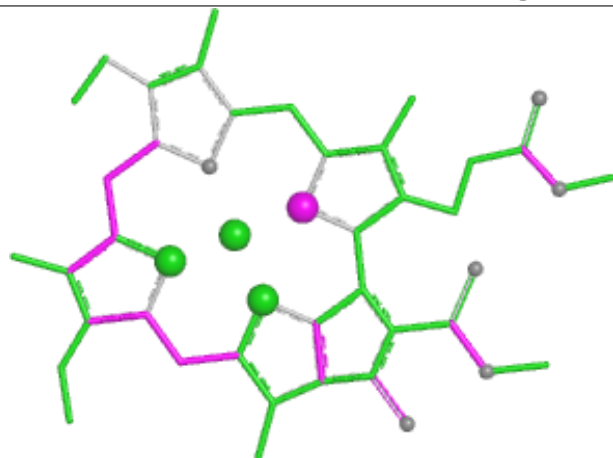
Ligand CLA 2 312



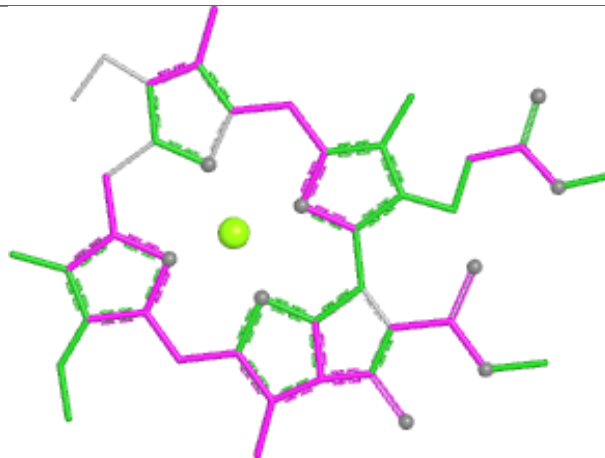
Ligand CLA A 833



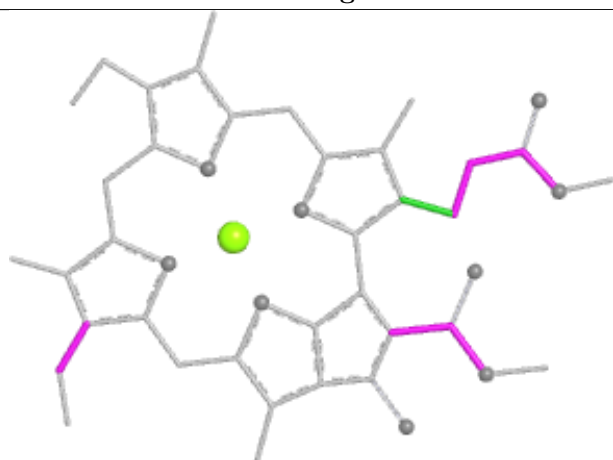
Ligand CLA B 822



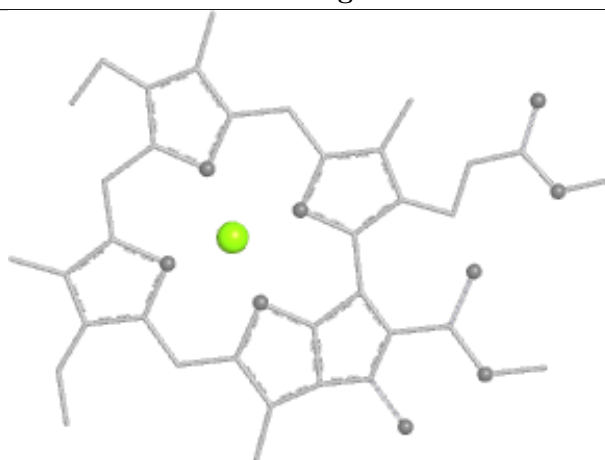
Bond lengths



Bond angles

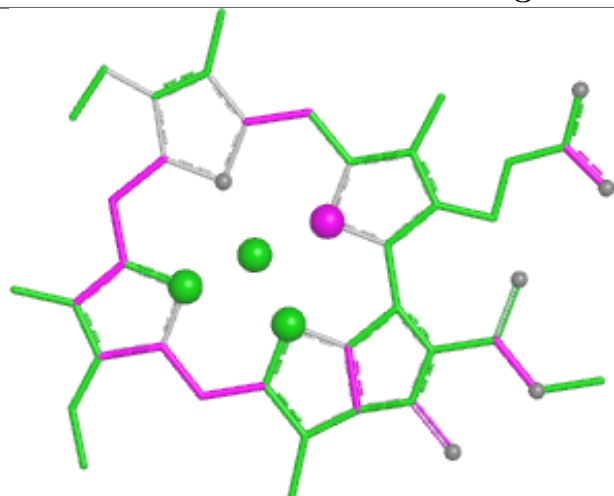


Torsions

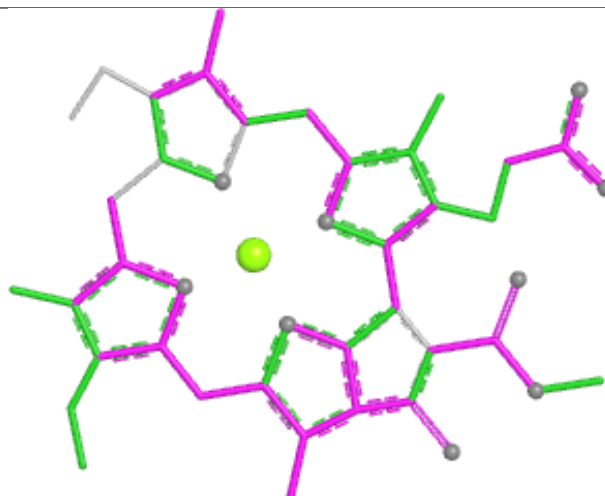


Rings

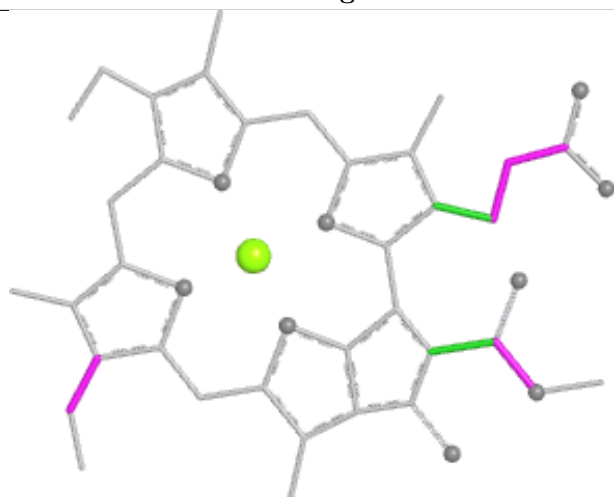
Ligand CLA B 835



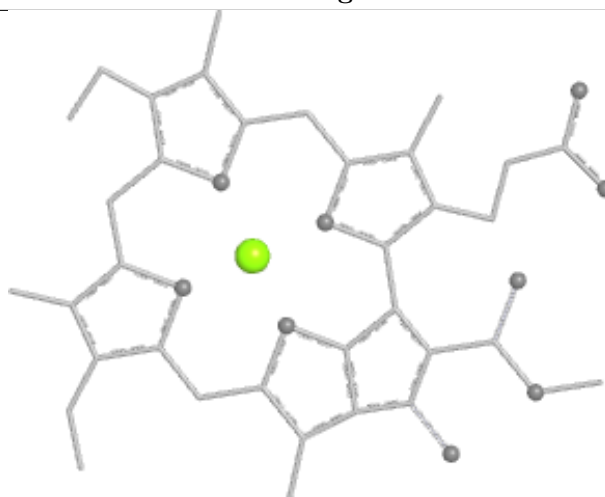
Bond lengths



Bond angles

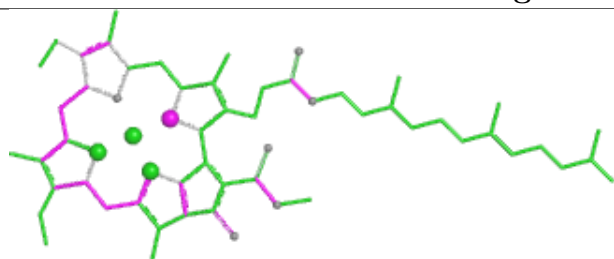


Torsions

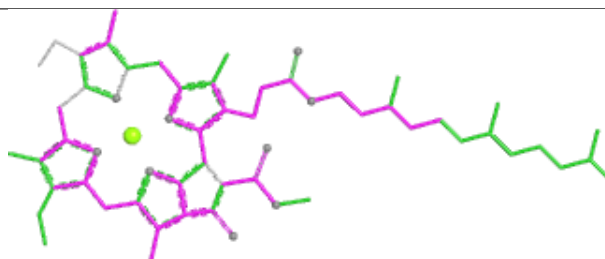


Rings

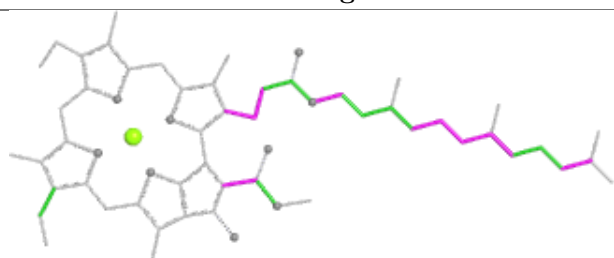
Ligand CLA A 808



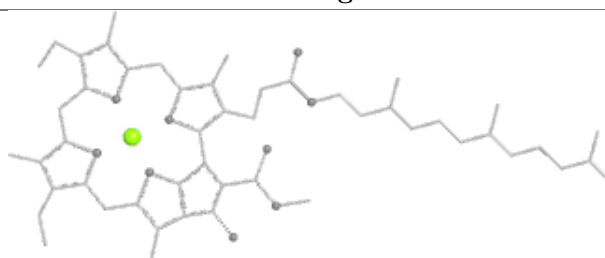
Bond lengths



Bond angles

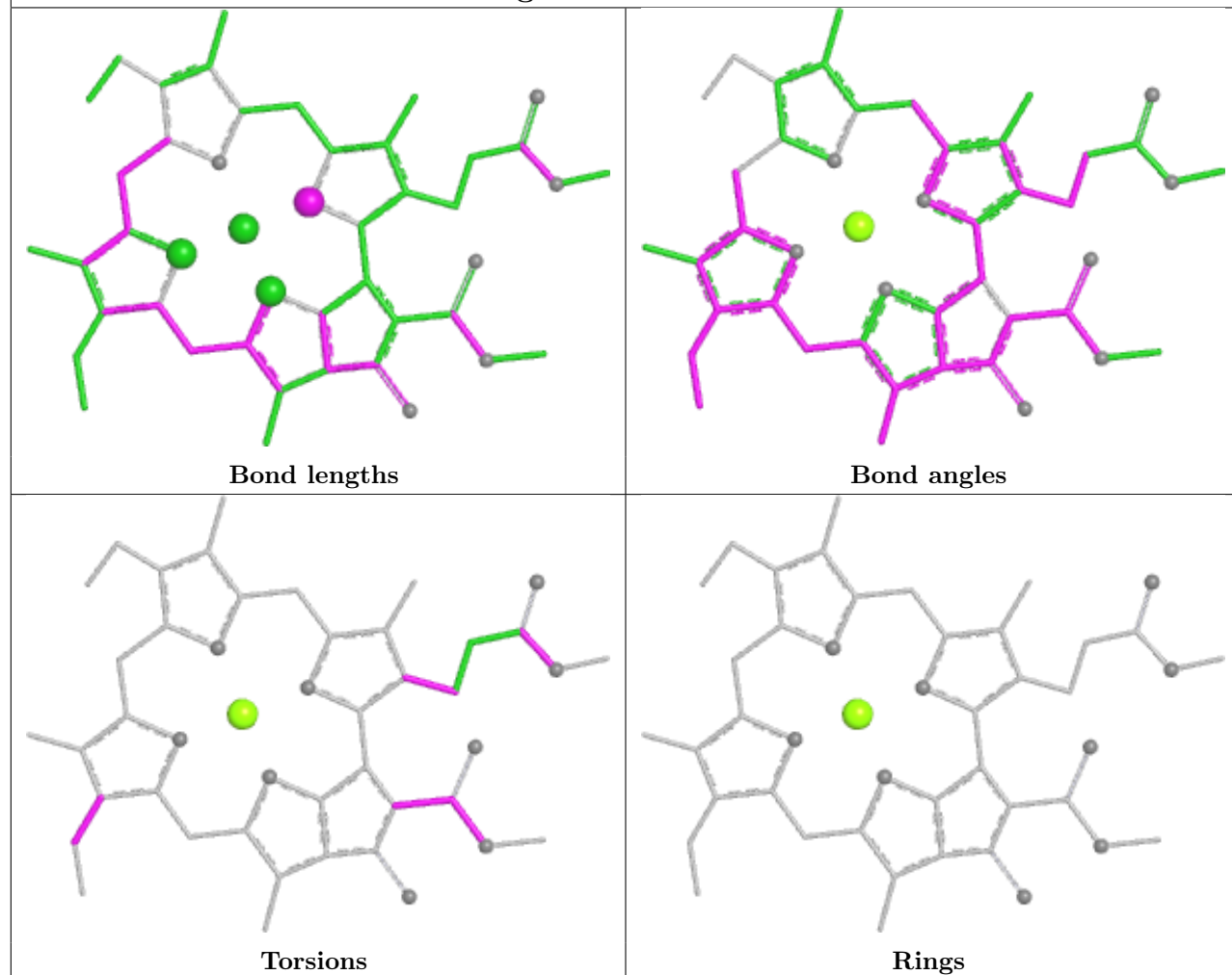


Torsions

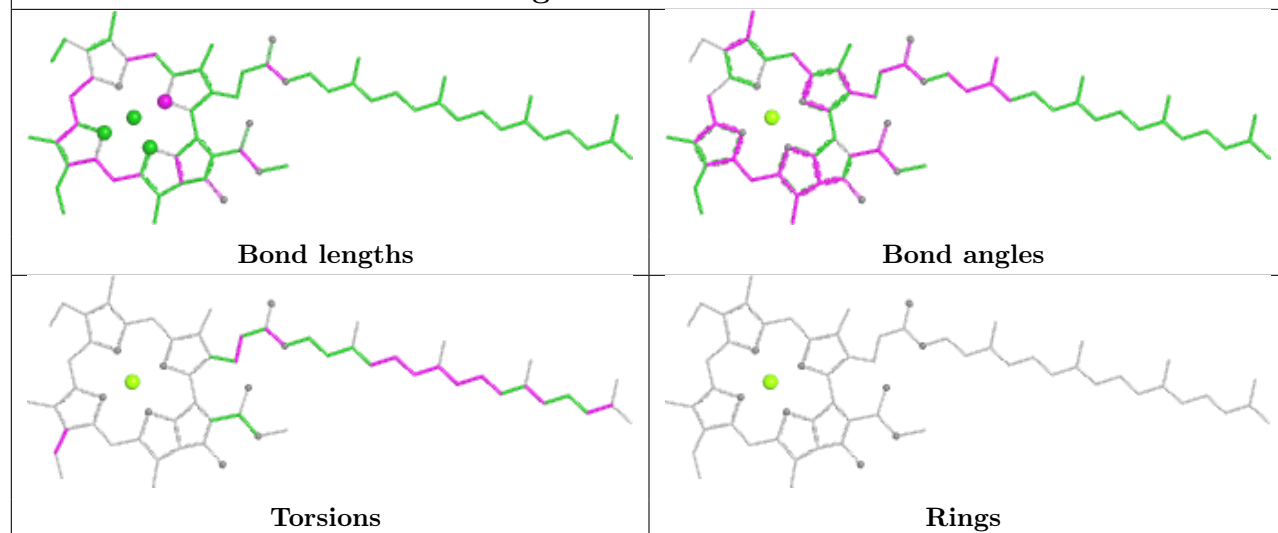


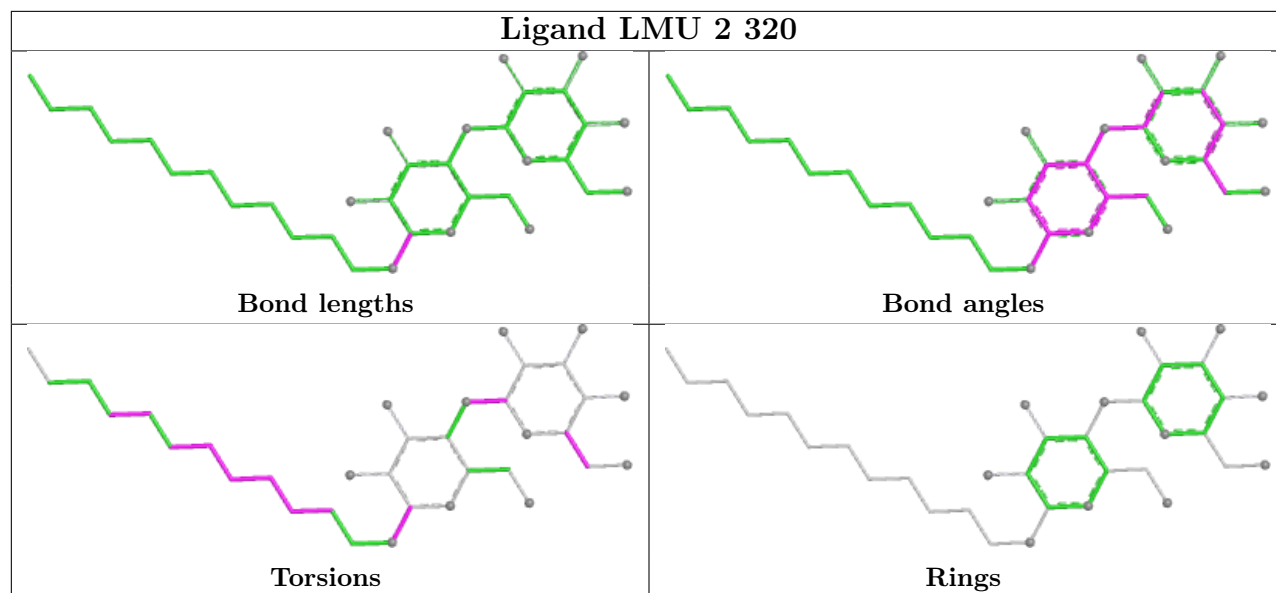
Rings

Ligand CLA 1 201

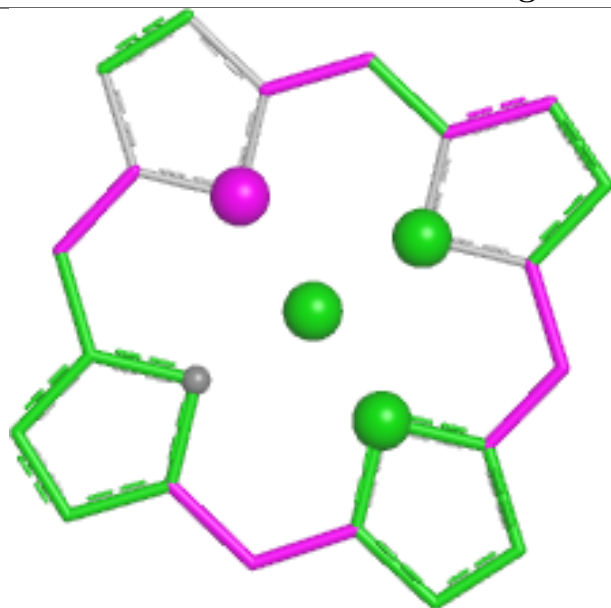


Ligand CLA B 840

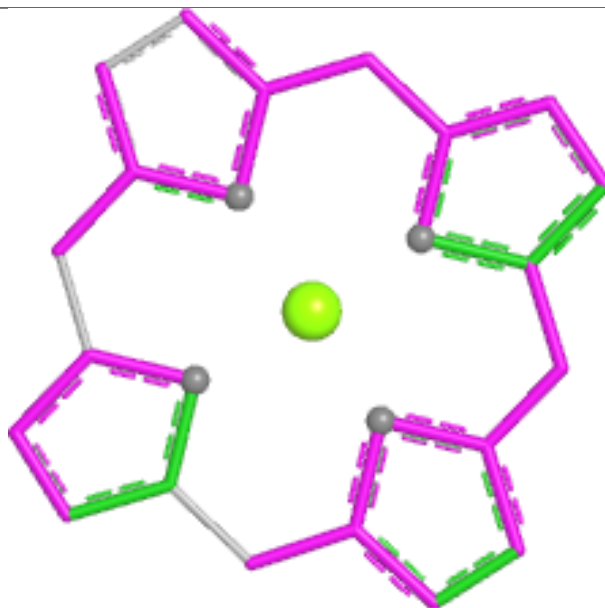




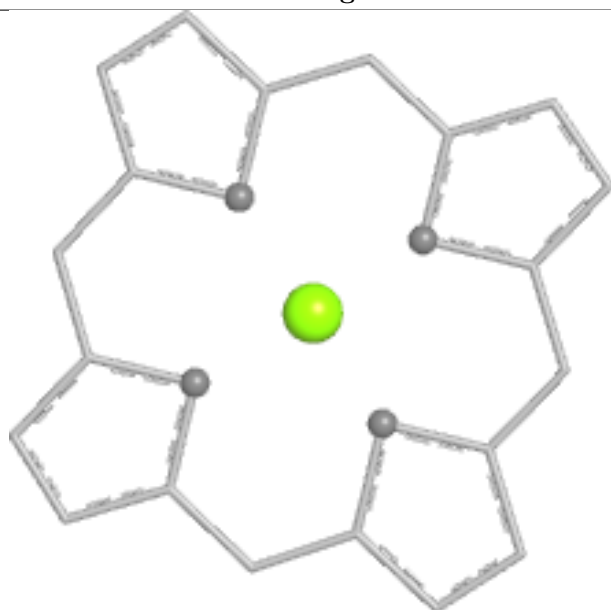
Ligand CLA 2 306



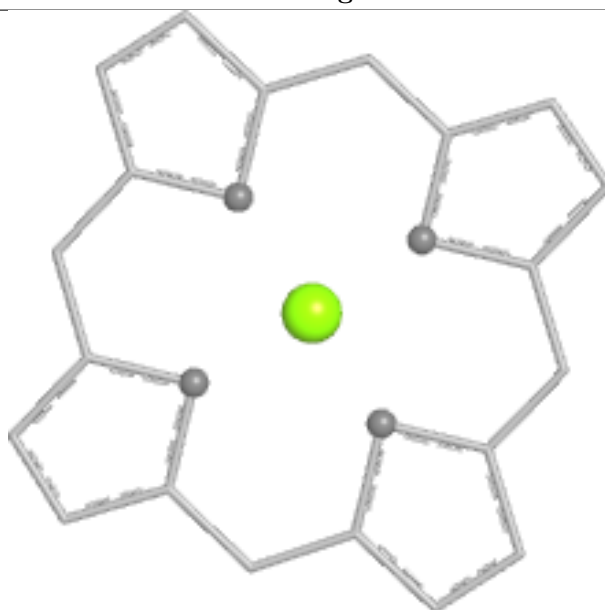
Bond lengths



Bond angles

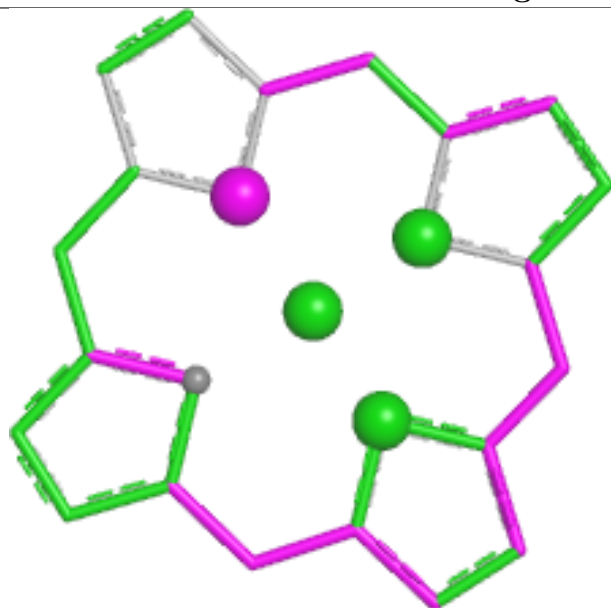


Torsions

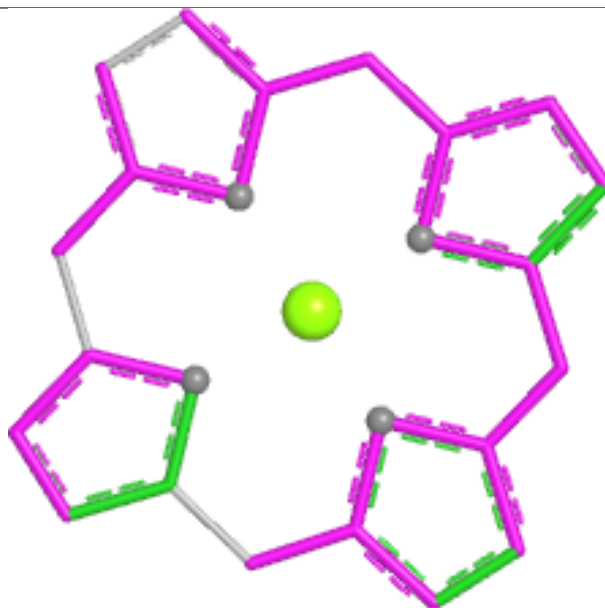


Rings

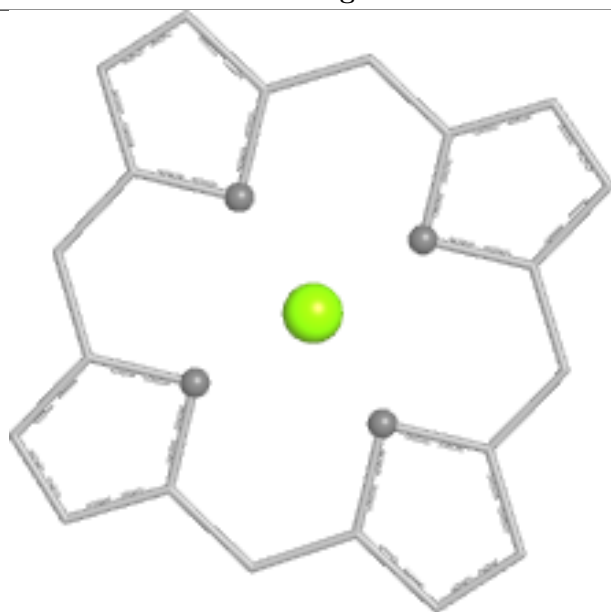
Ligand CLA A 814



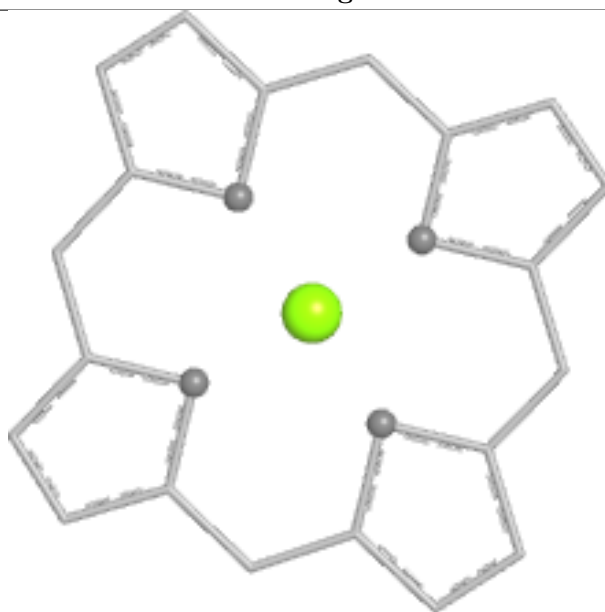
Bond lengths



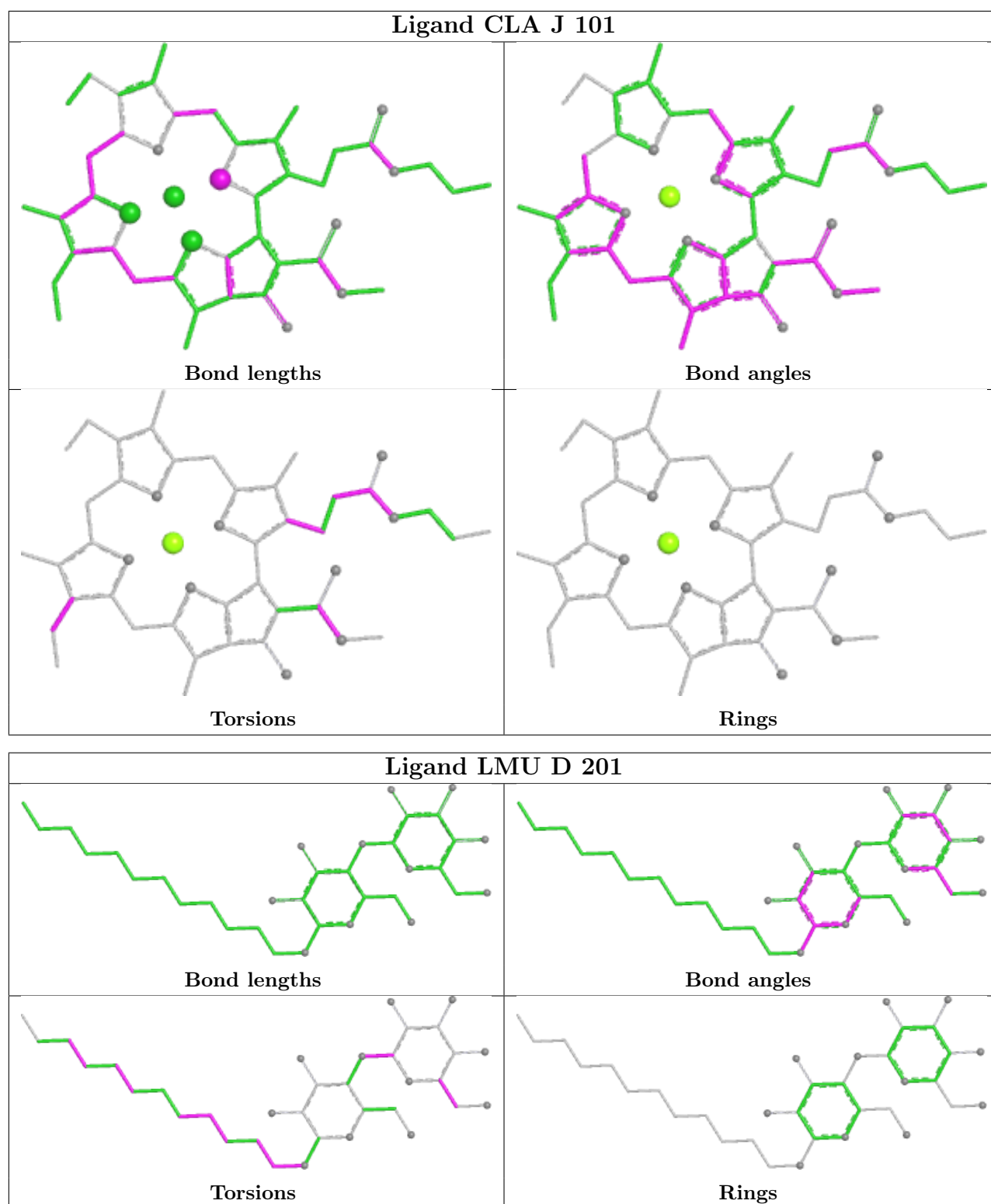
Bond angles



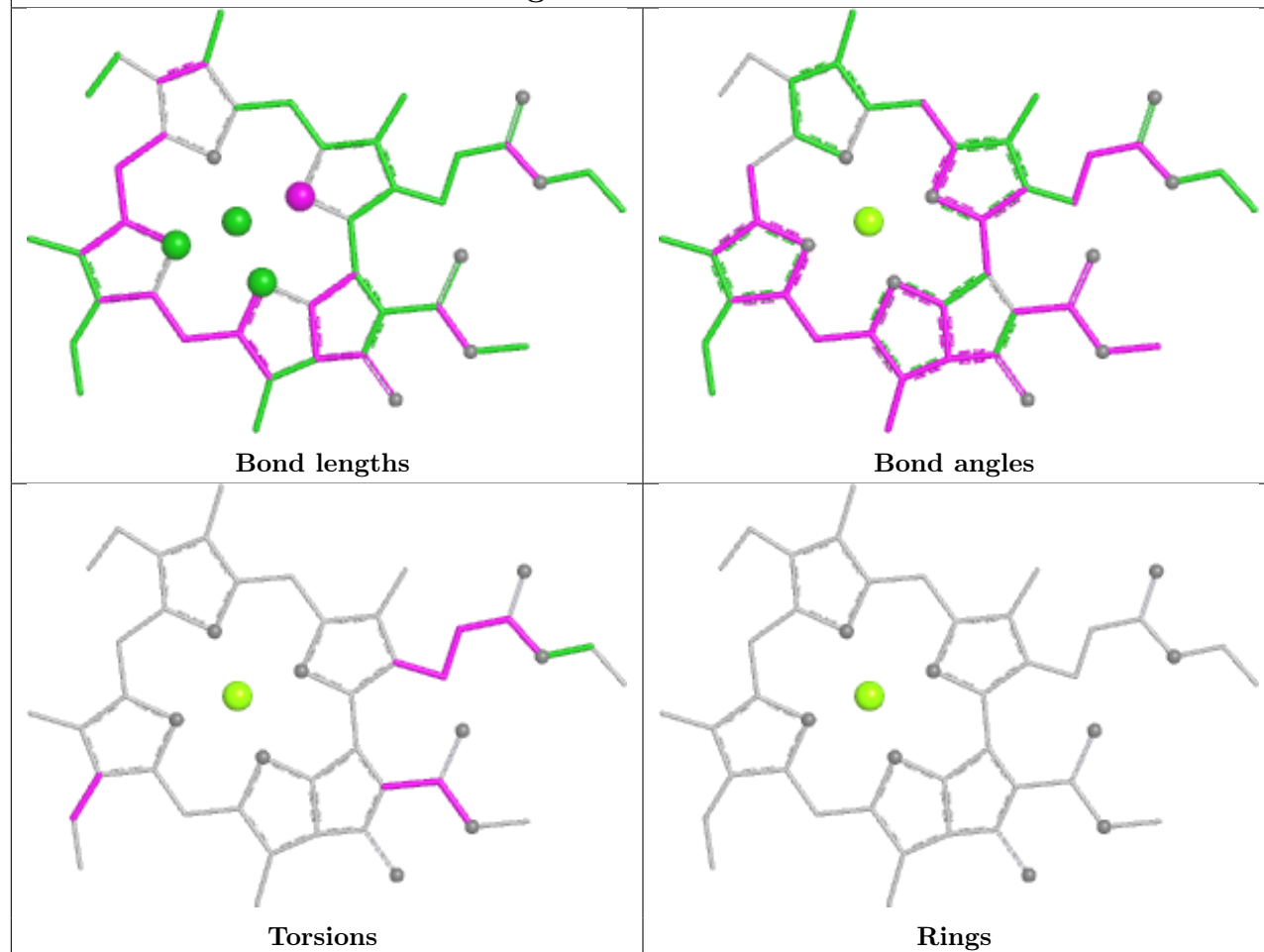
Torsions



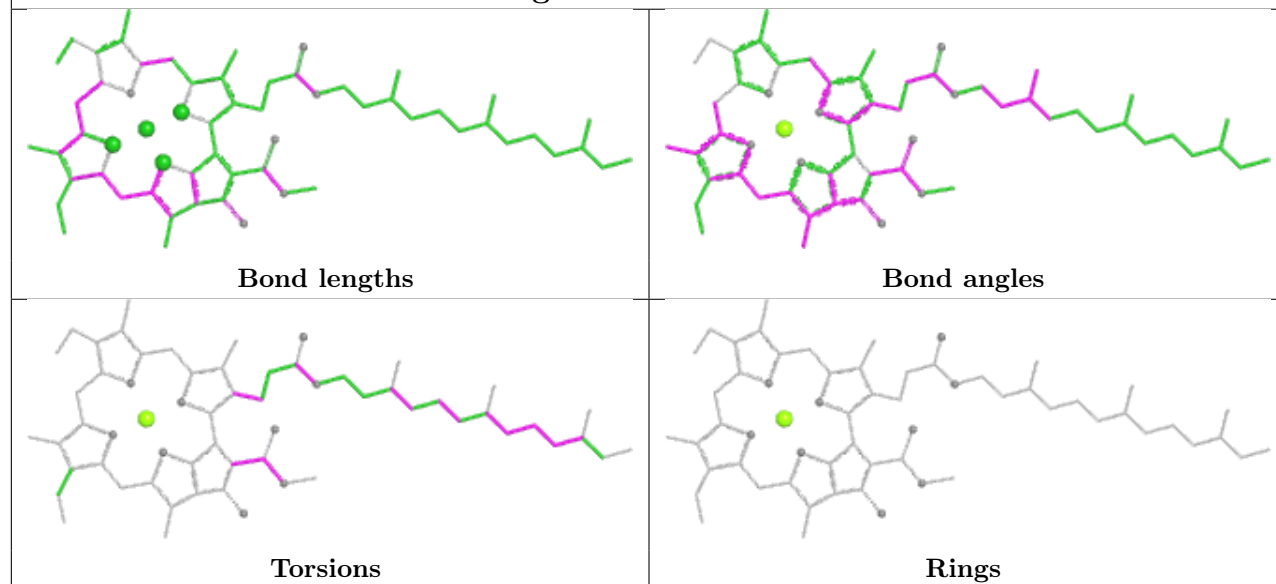
Rings

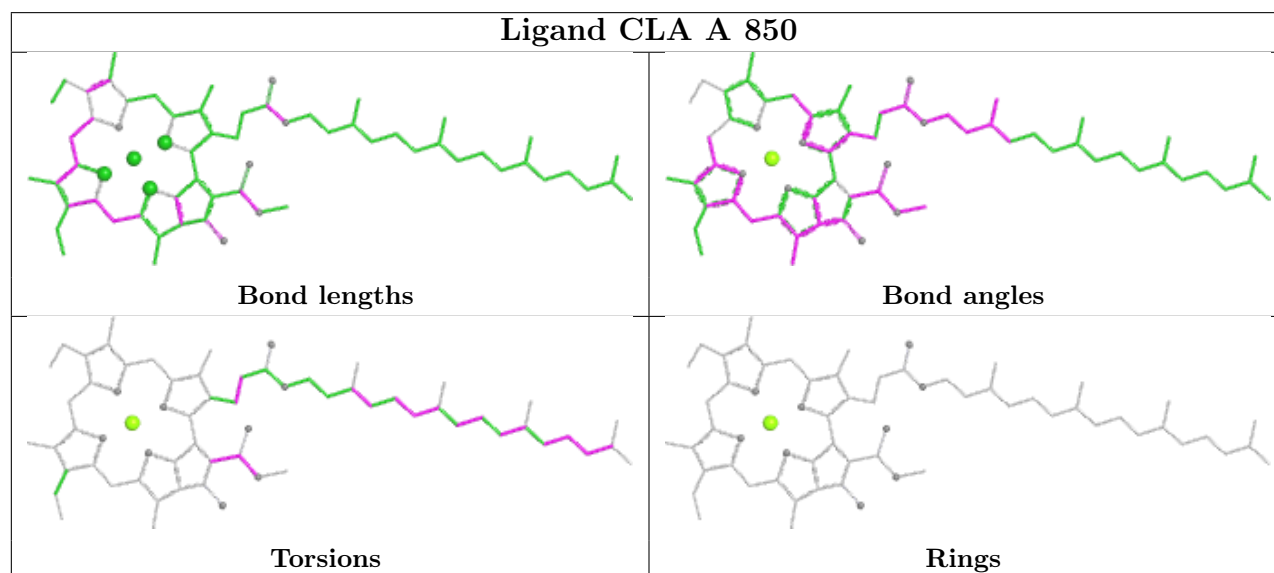
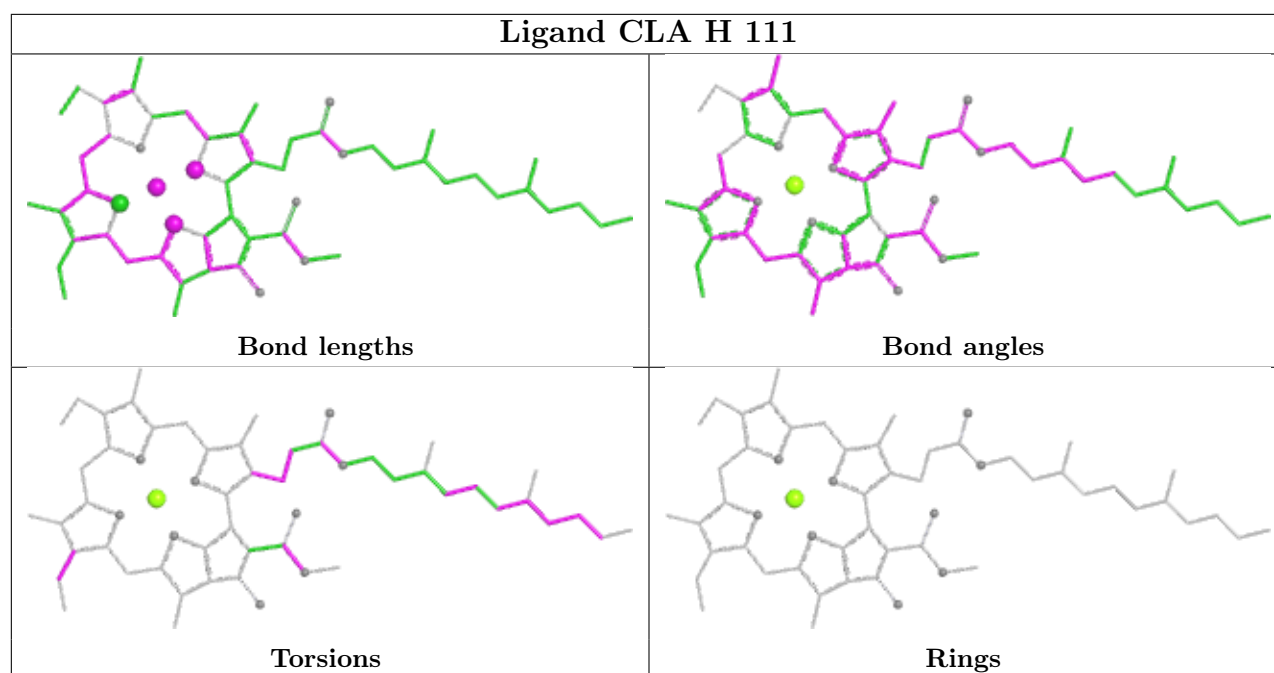


Ligand CLA B 839

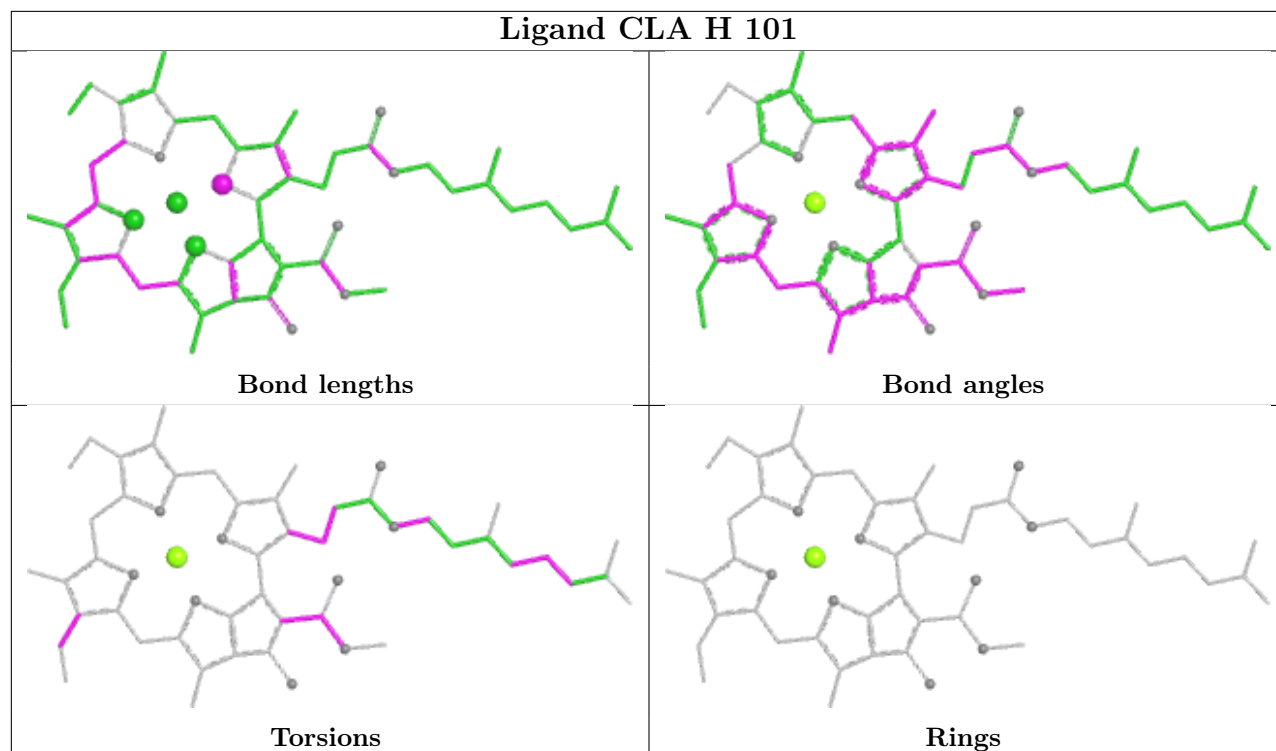


Ligand CLA B 820

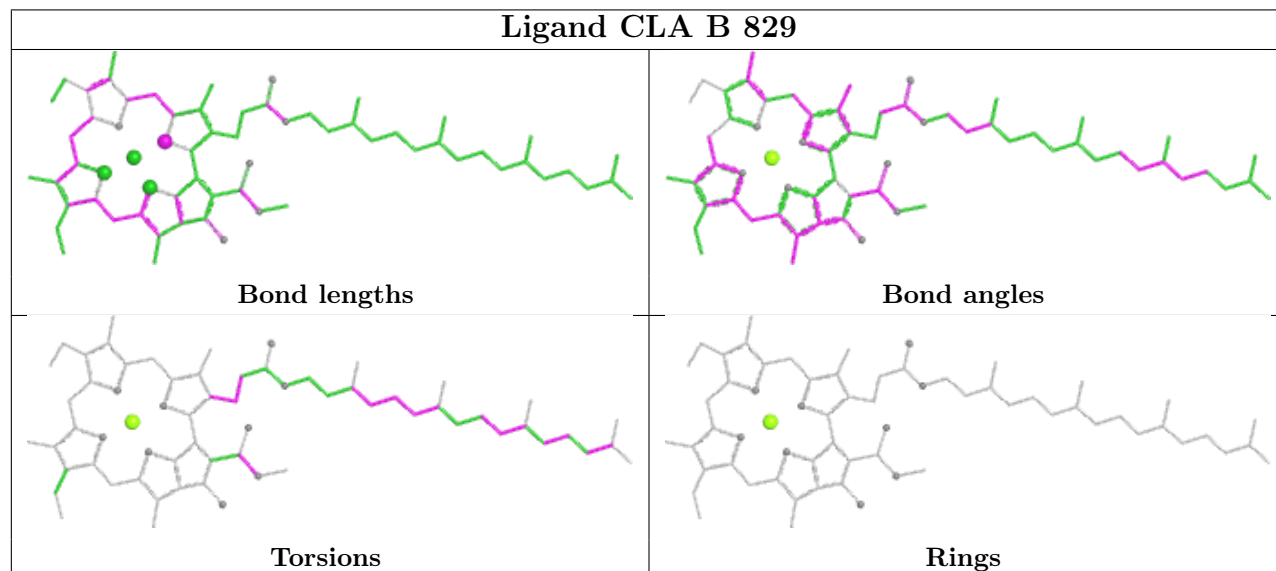


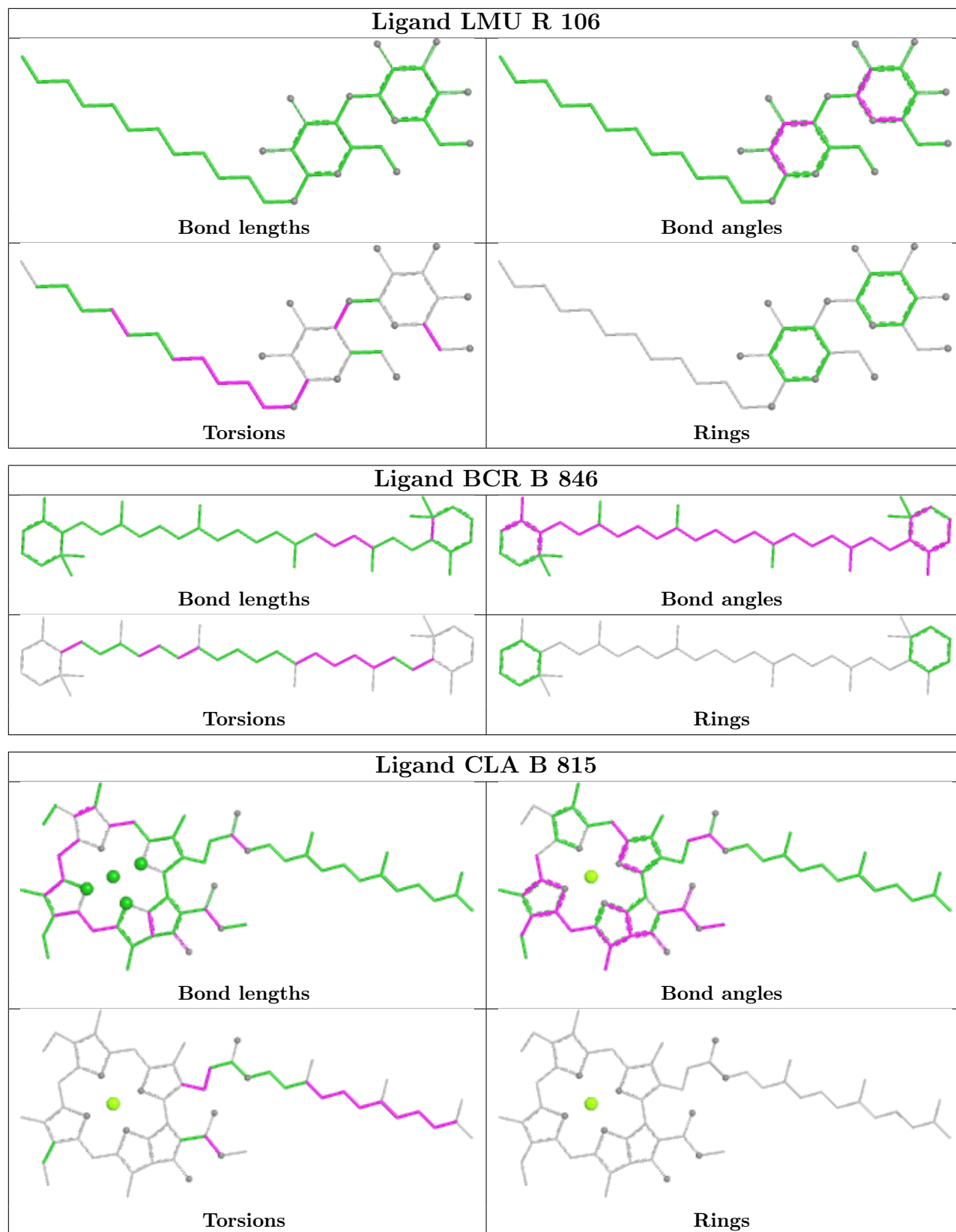


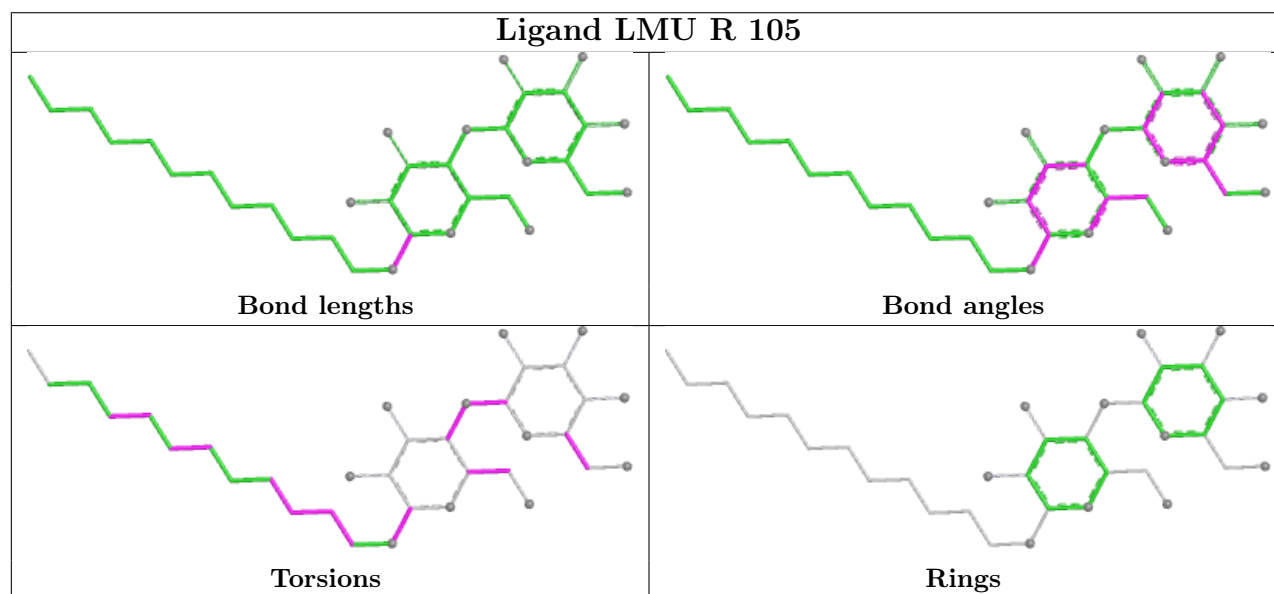
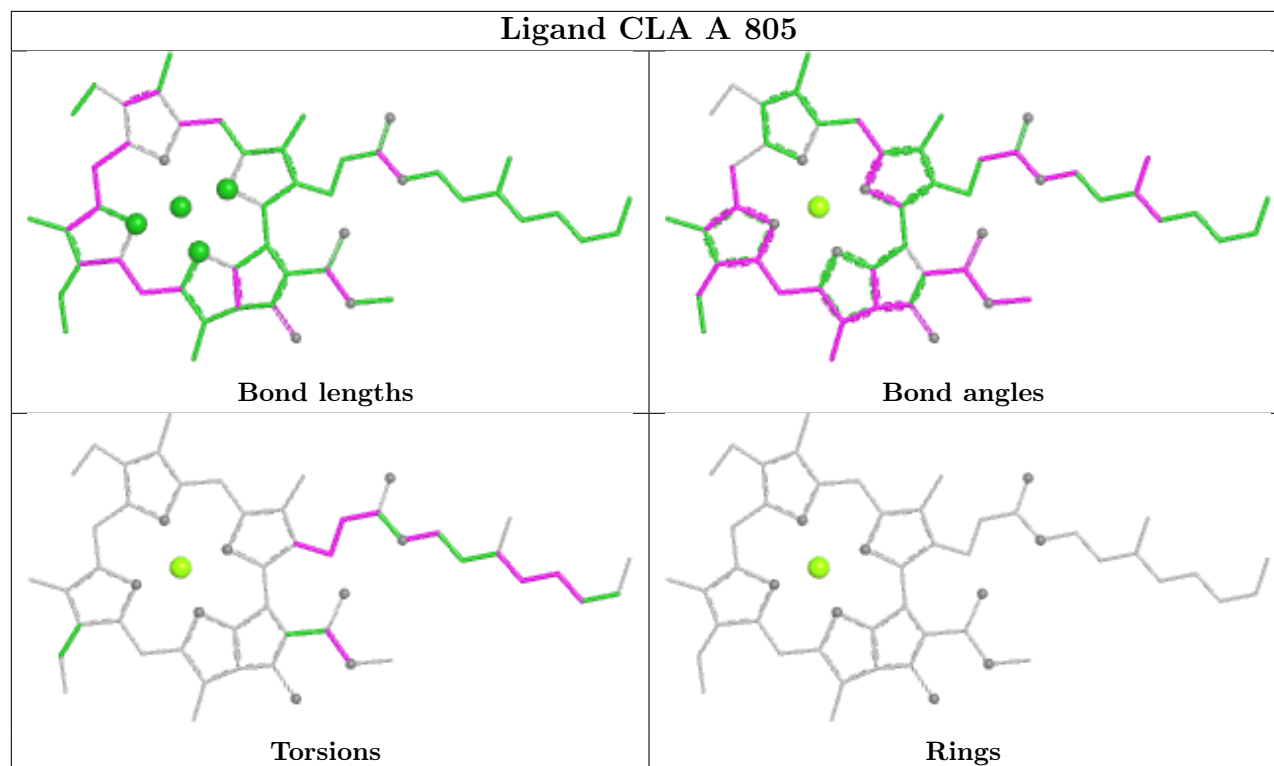
Ligand CLA H 101



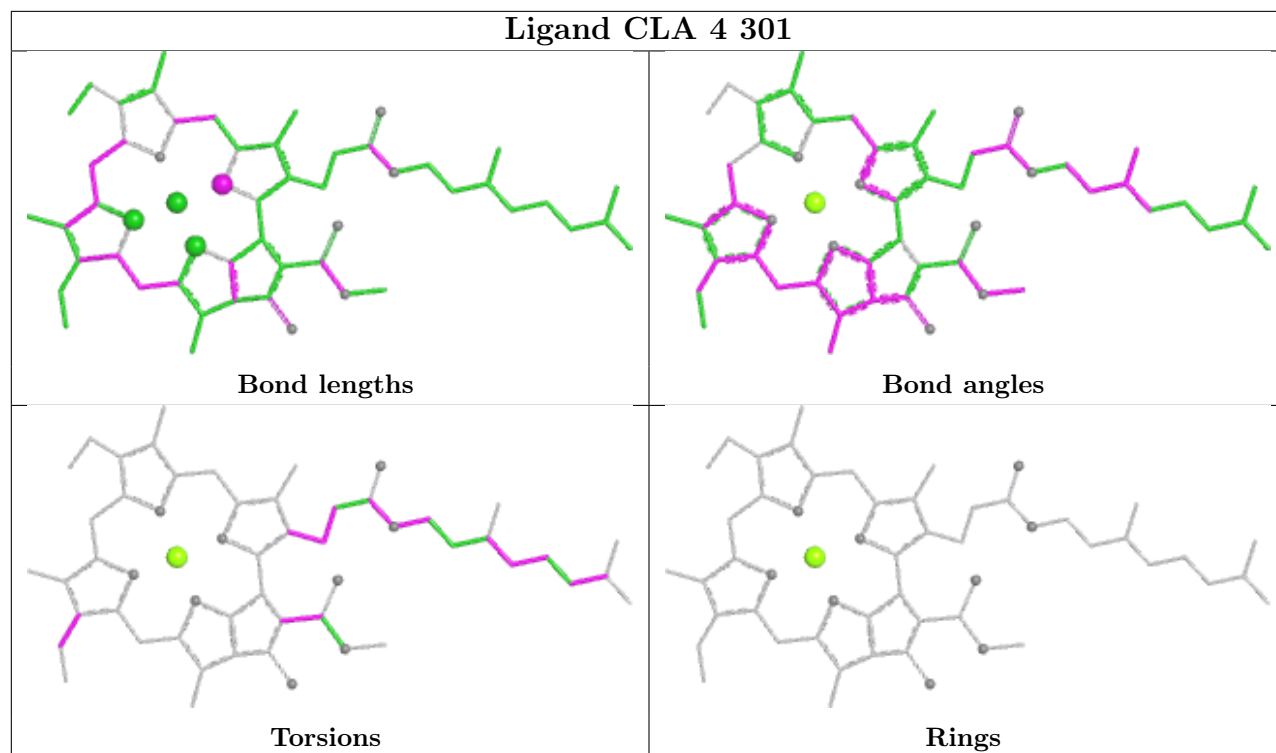
Ligand CLA B 829



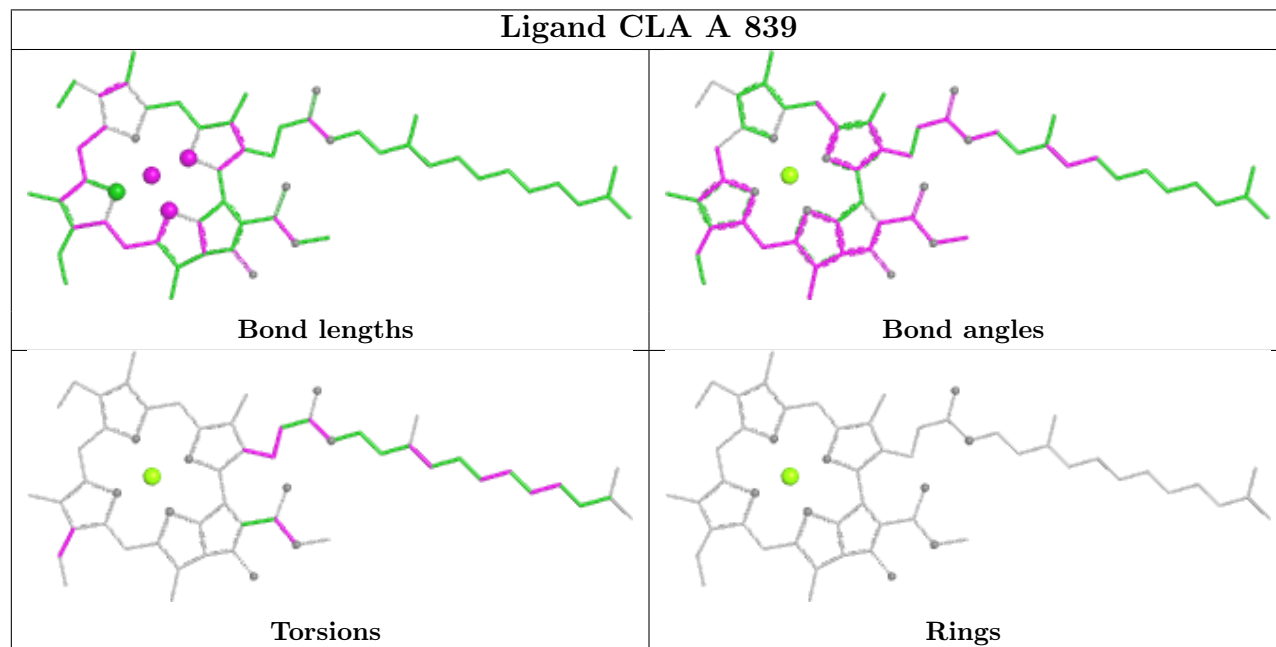




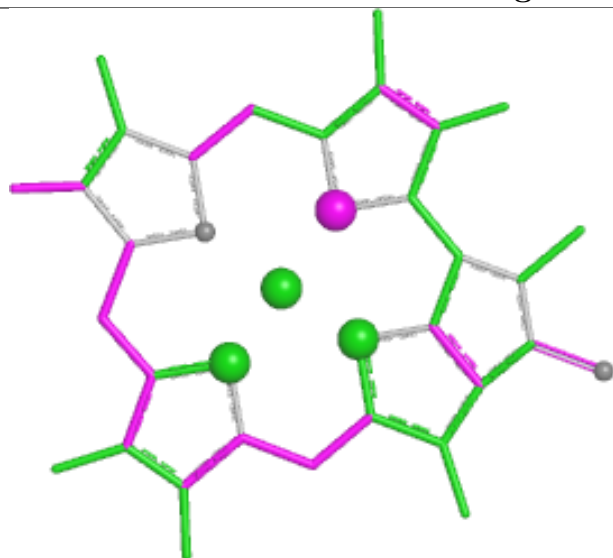
Ligand CLA 4 301



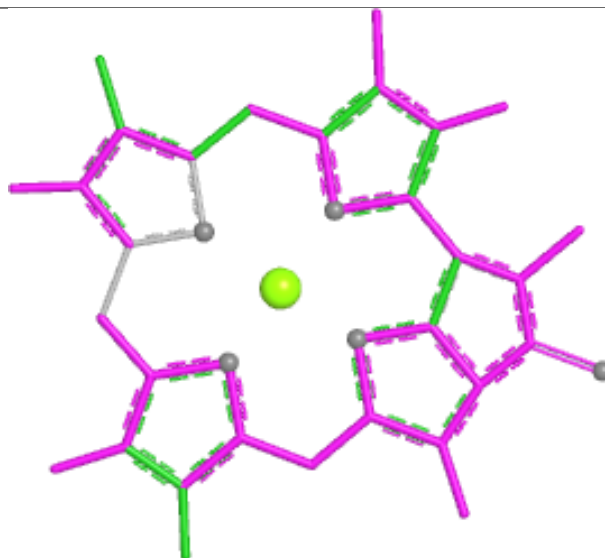
Ligand CLA A 839



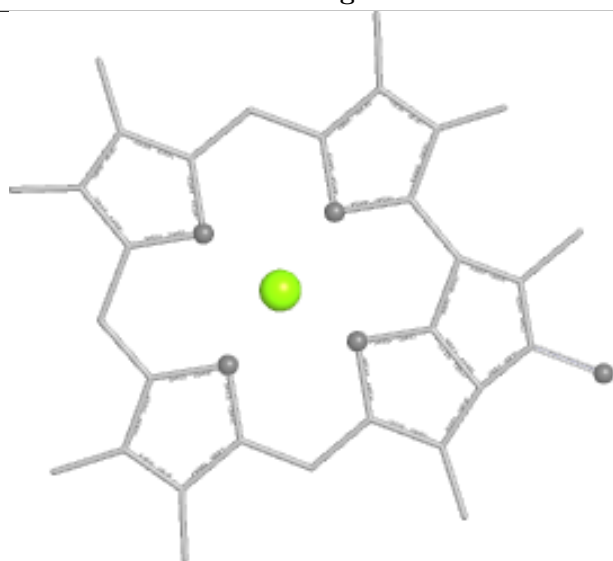
Ligand CLA B 842



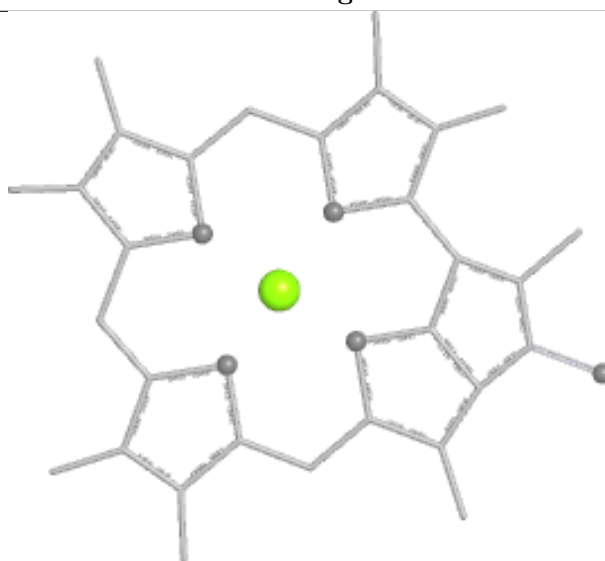
Bond lengths



Bond angles

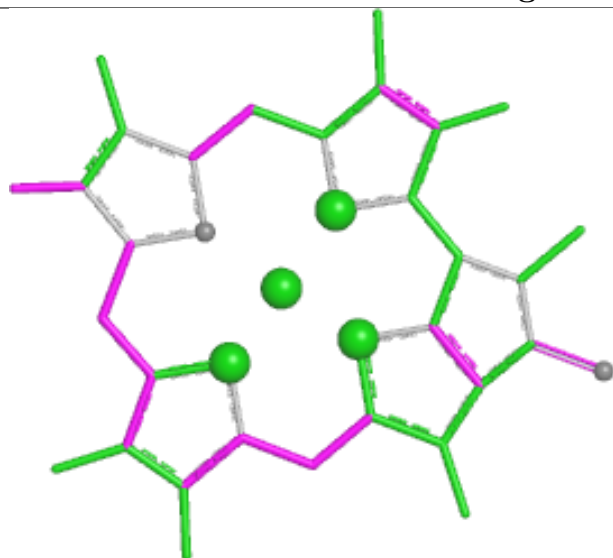


Torsions

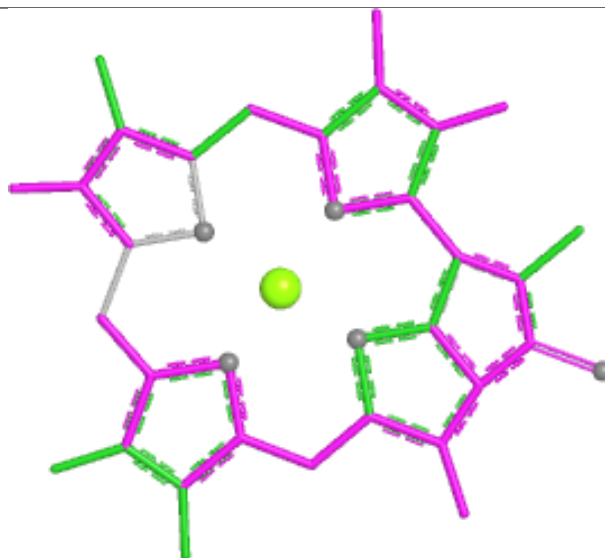


Rings

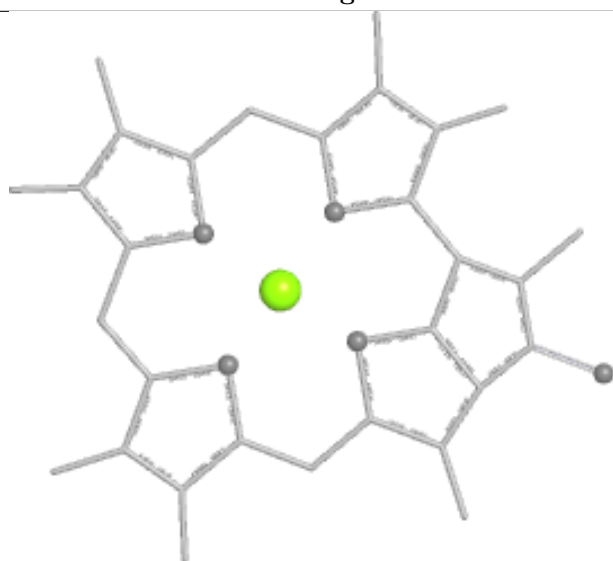
Ligand CLA 1 205



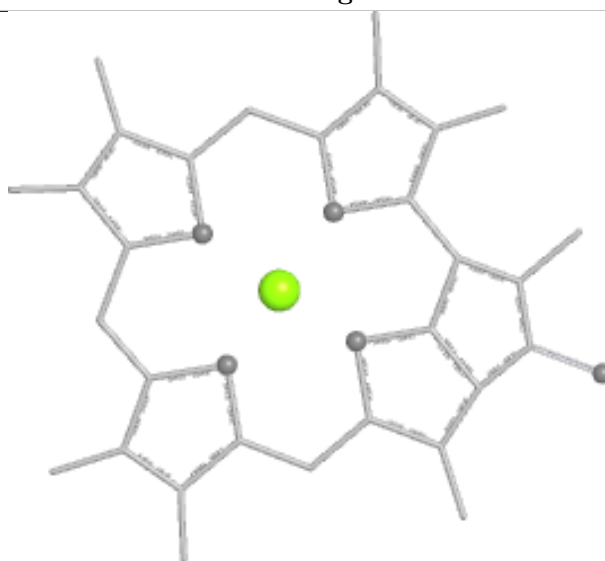
Bond lengths



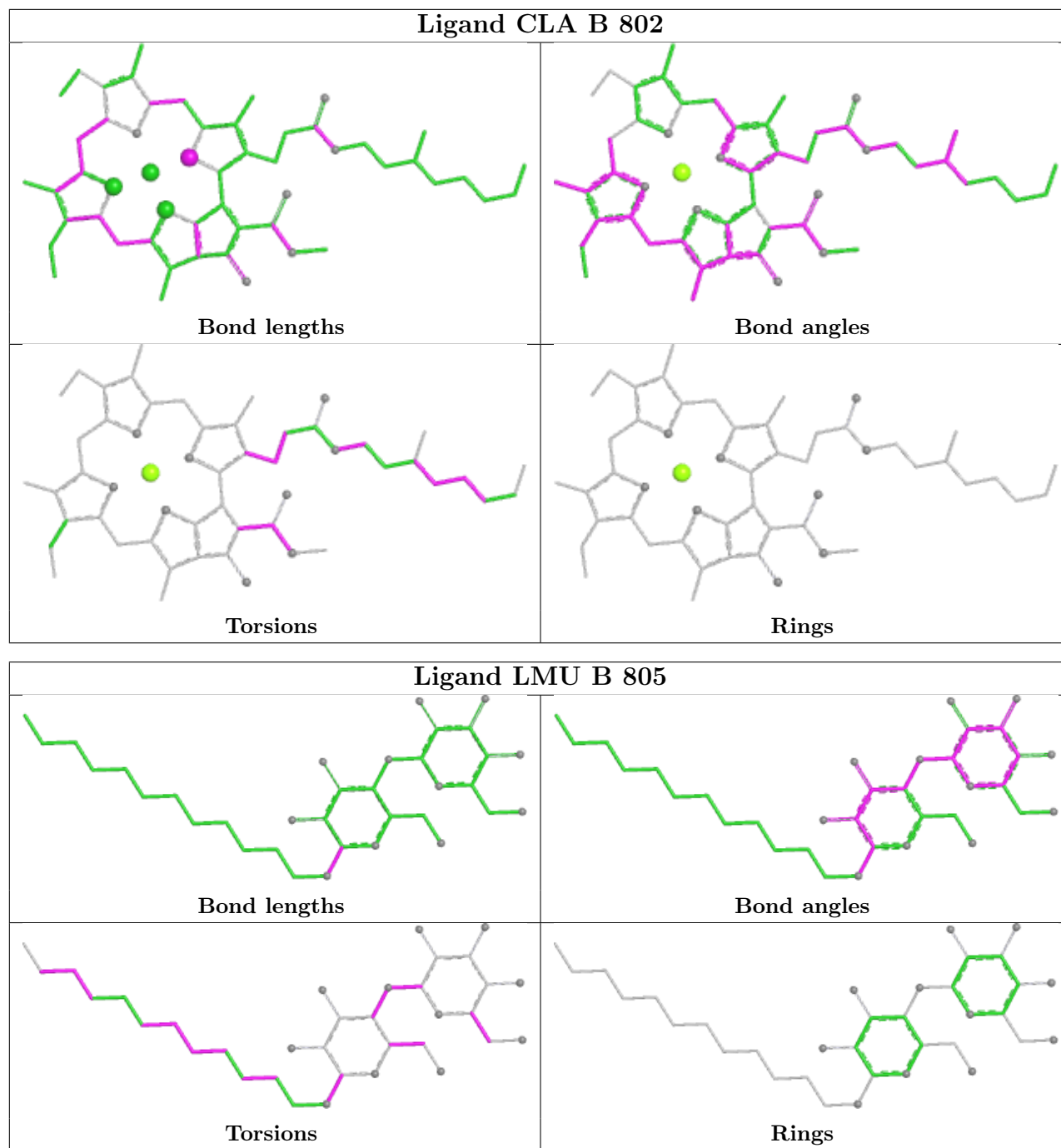
Bond angles



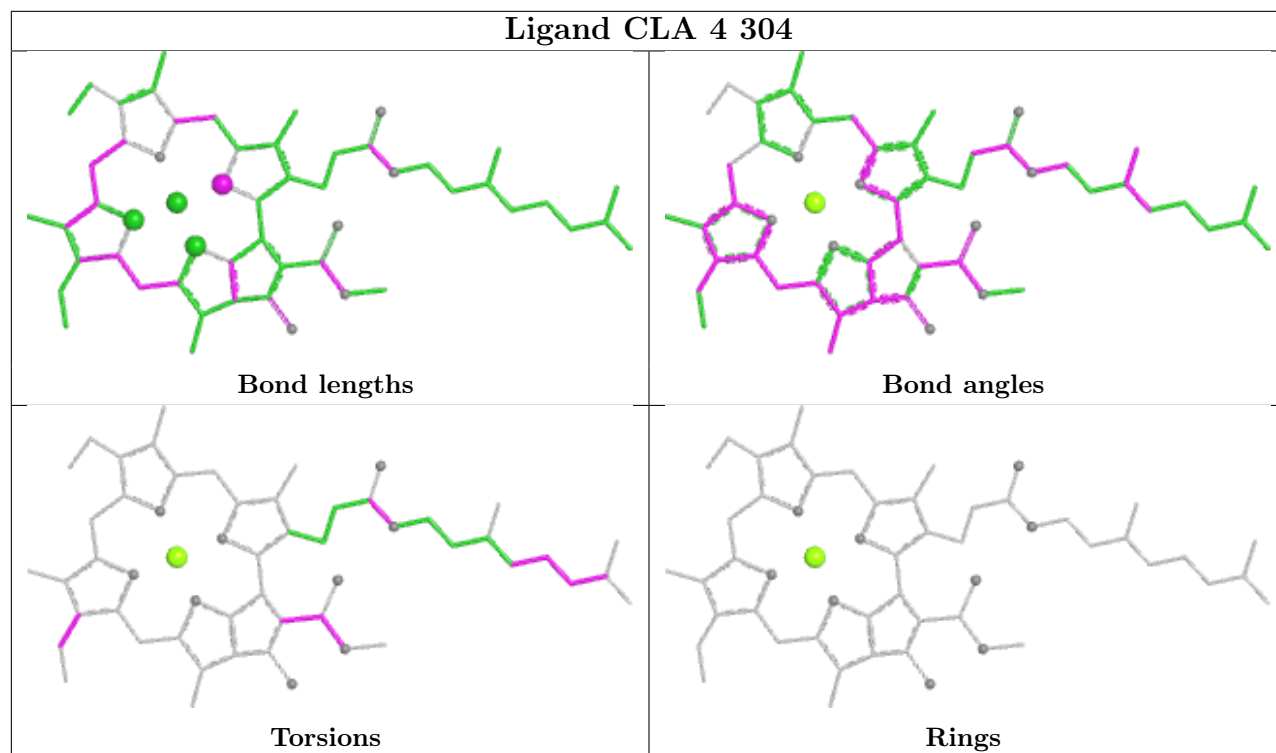
Torsions



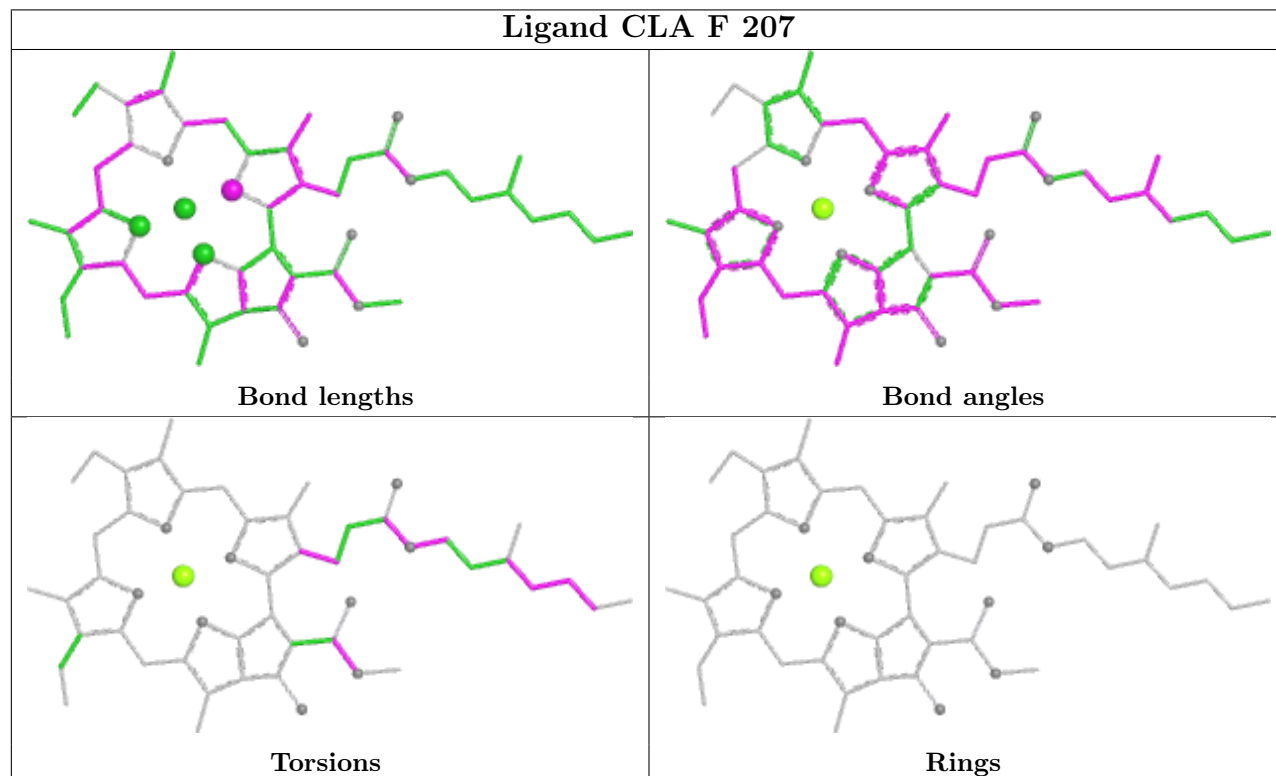
Rings

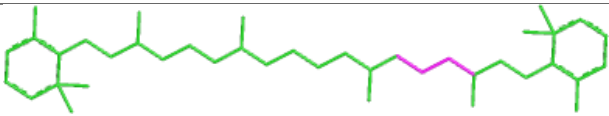
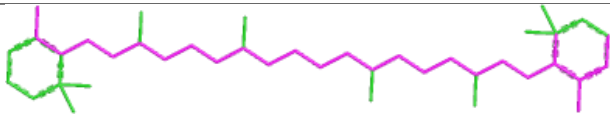
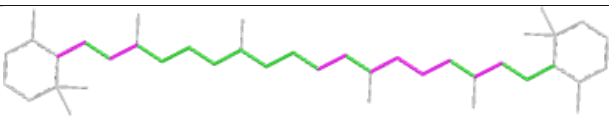
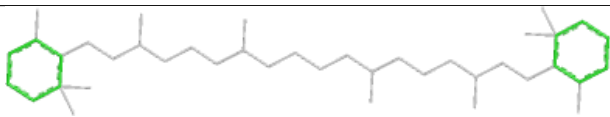


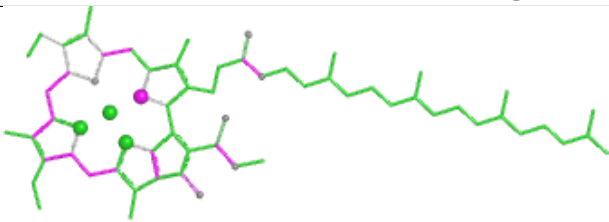
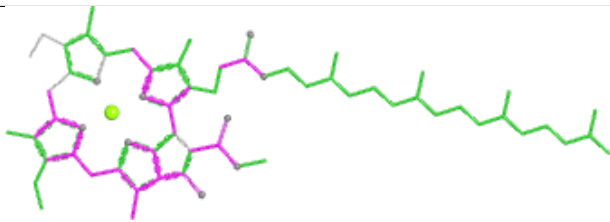
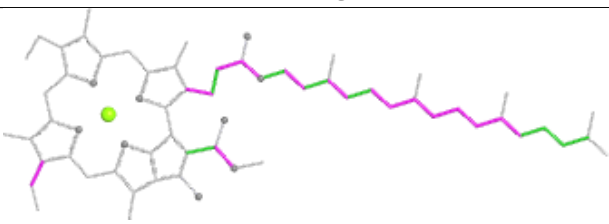
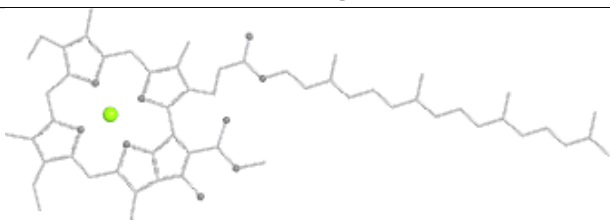
Ligand CLA 4 304

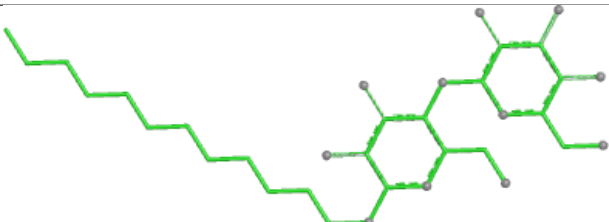
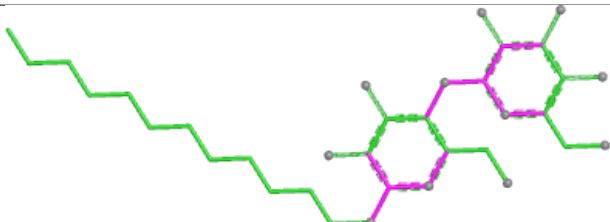
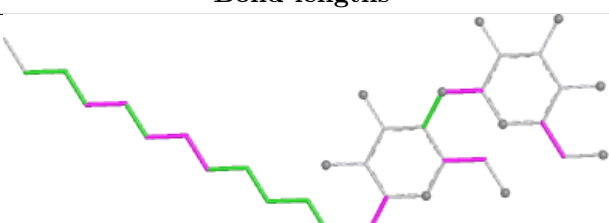
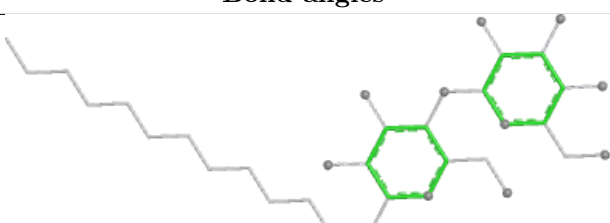


Ligand CLA F 207

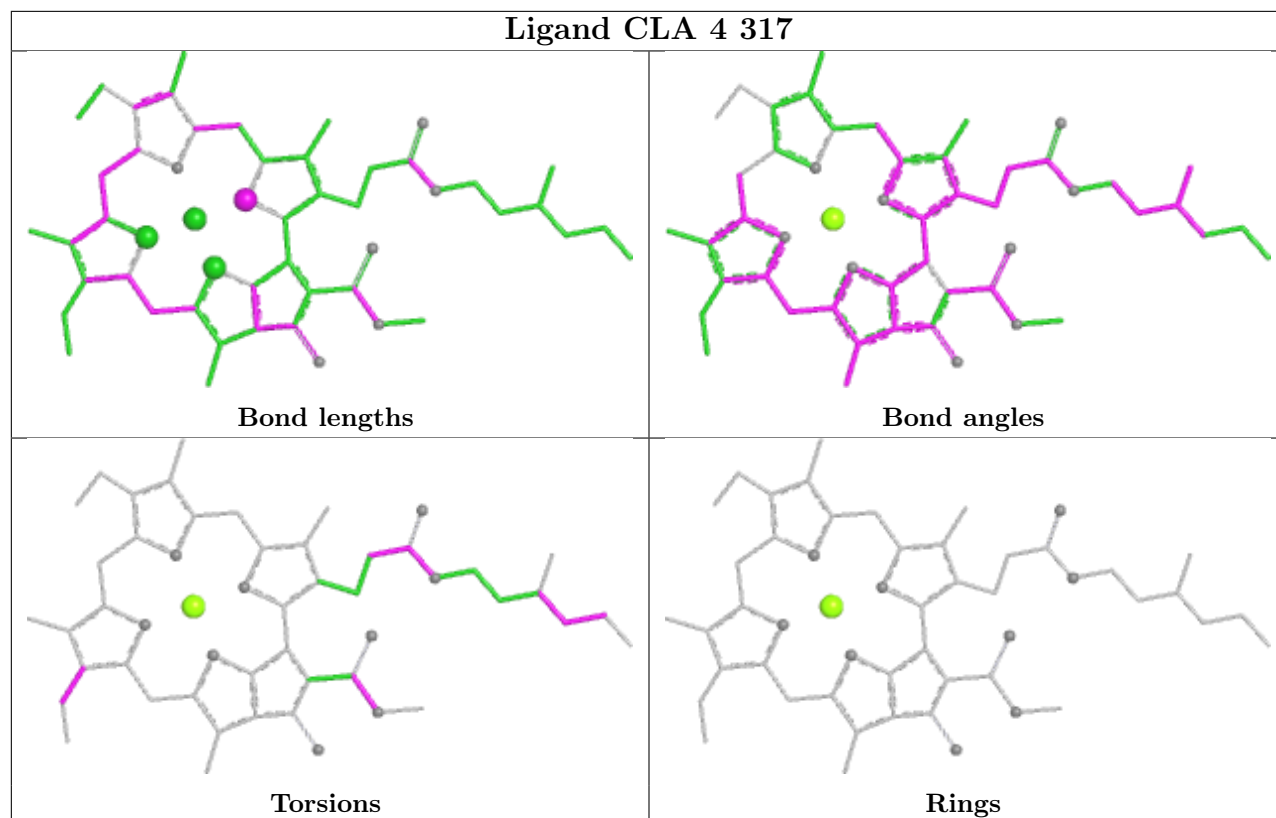


Ligand BCR J 102	
	
Bond lengths	Bond angles
	
Torsions	Rings

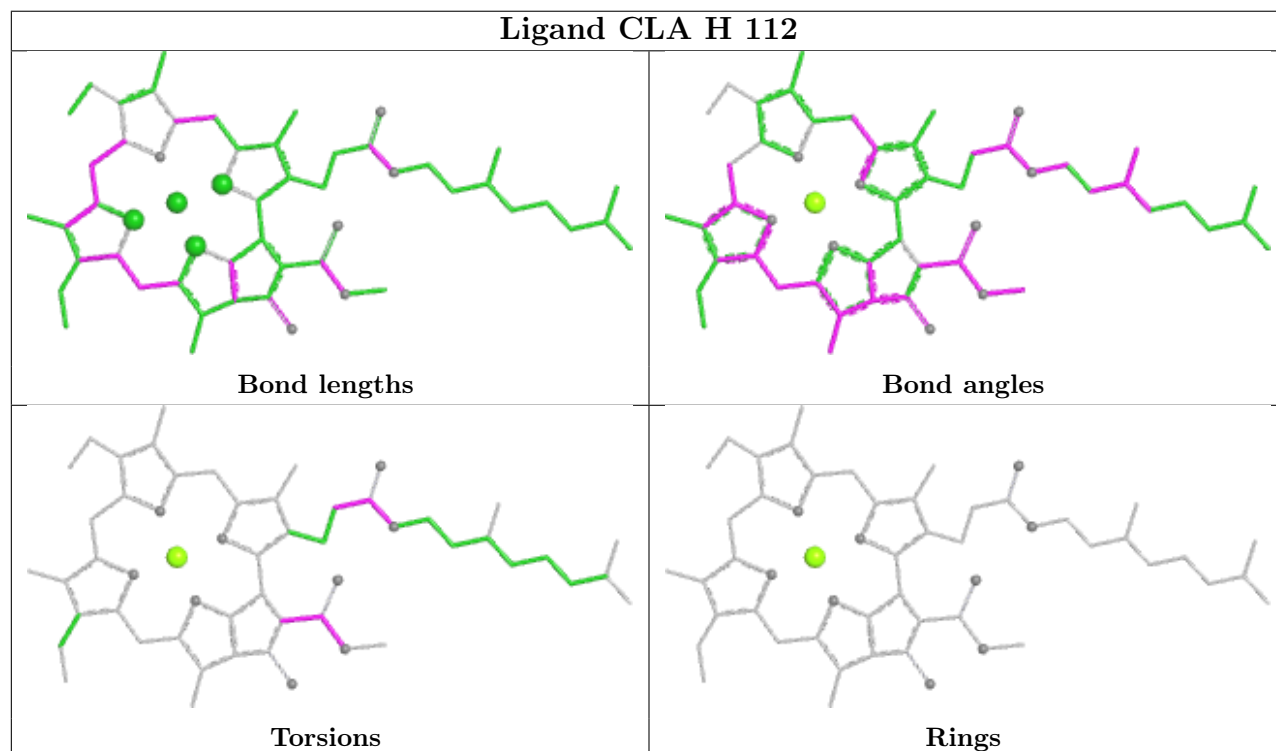
Ligand CLA A 825	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand LMU 1 216	
	
Bond lengths	Bond angles
	
Torsions	Rings

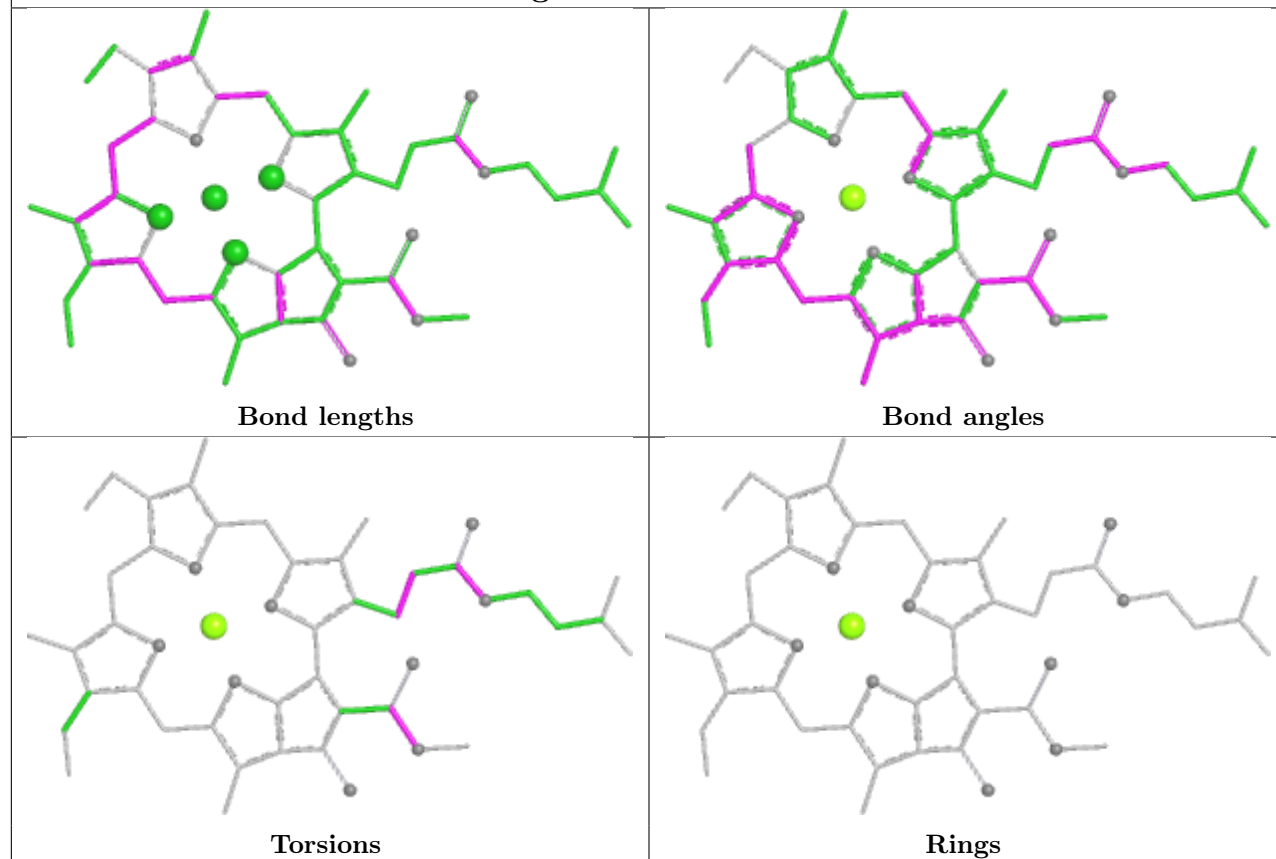
Ligand CLA 4 317



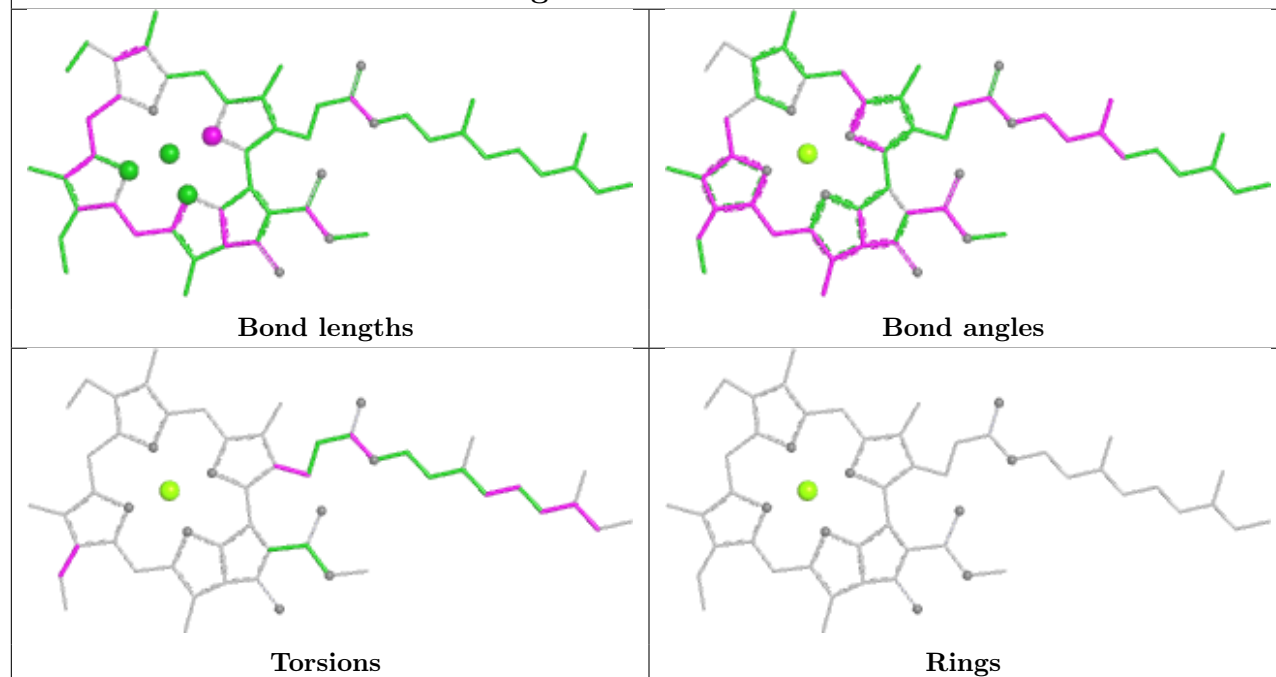
Ligand CLA H 112



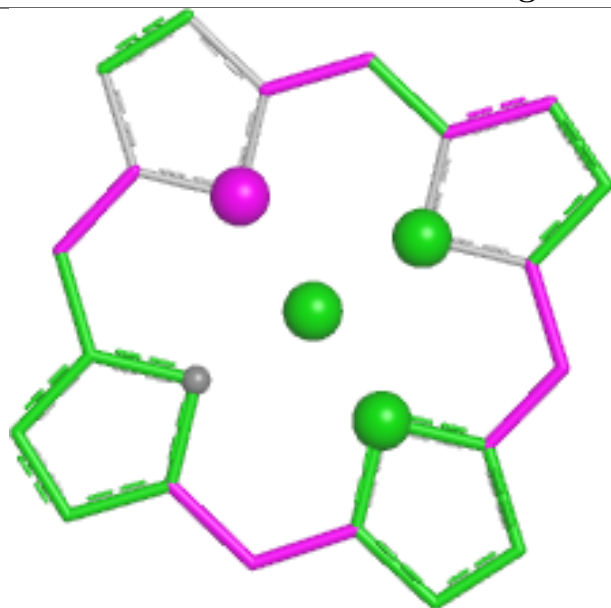
Ligand CLA A 829



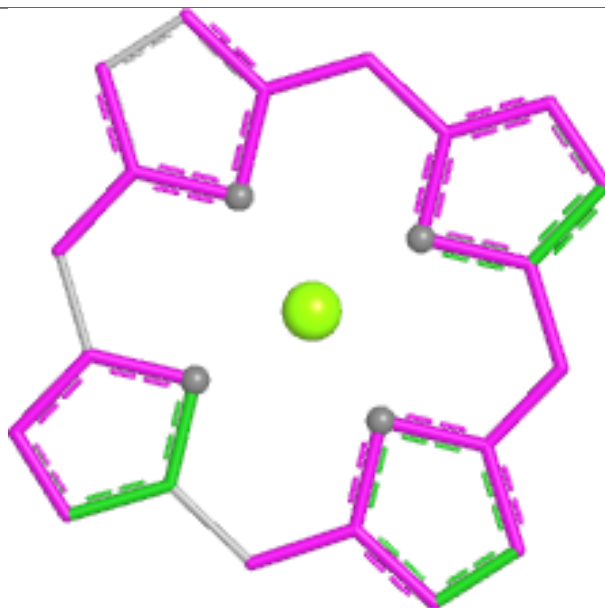
Ligand CLA K 104



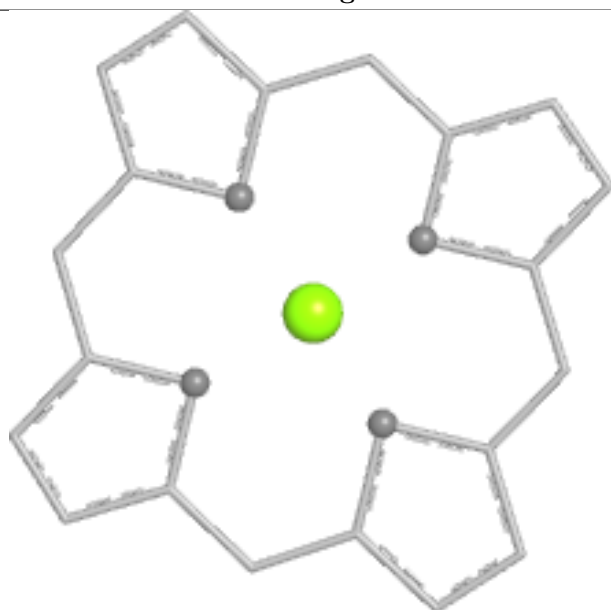
Ligand CLA 1 214



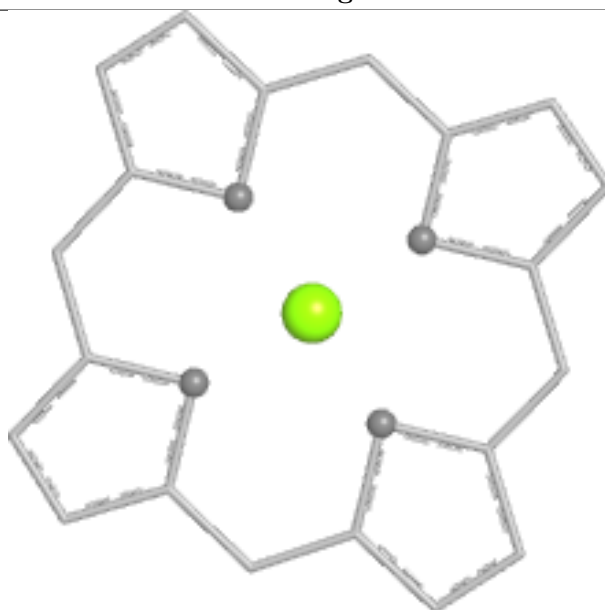
Bond lengths



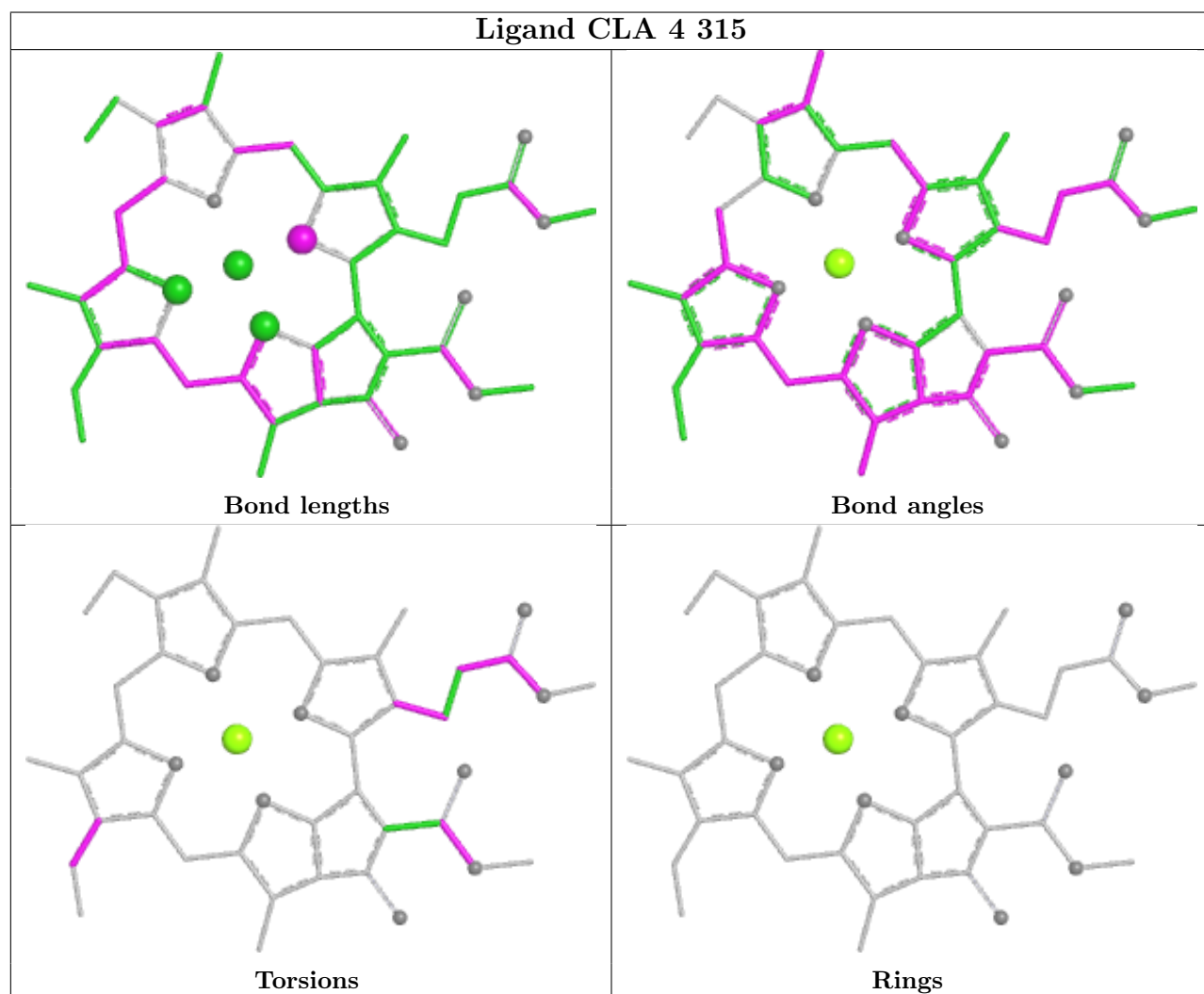
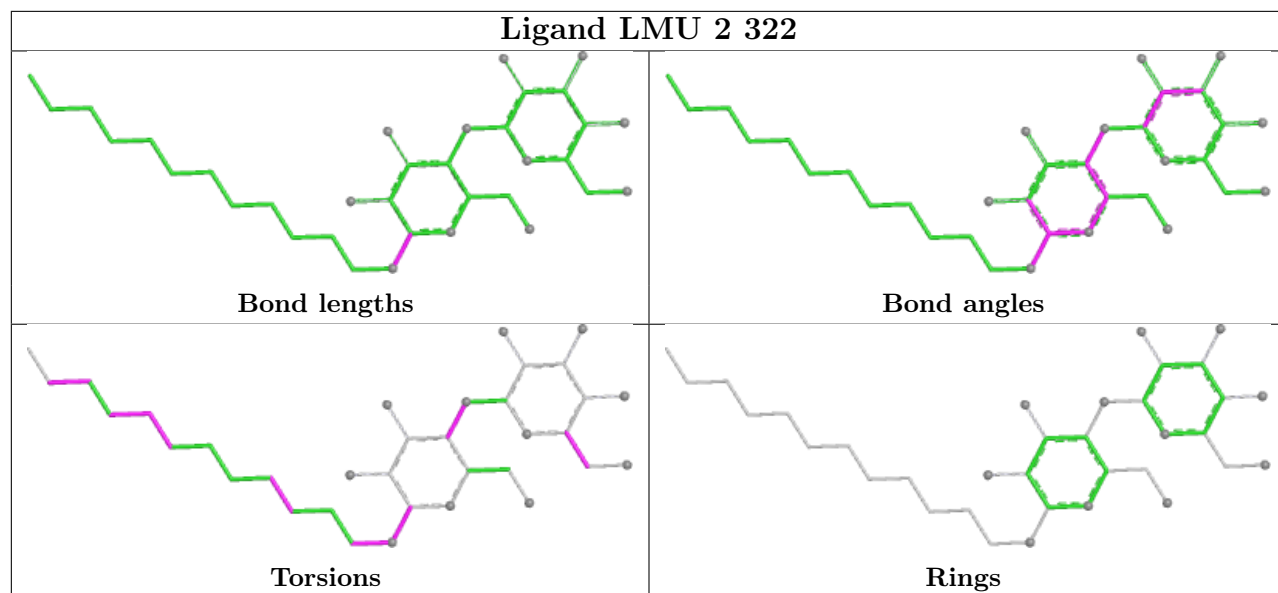
Bond angles



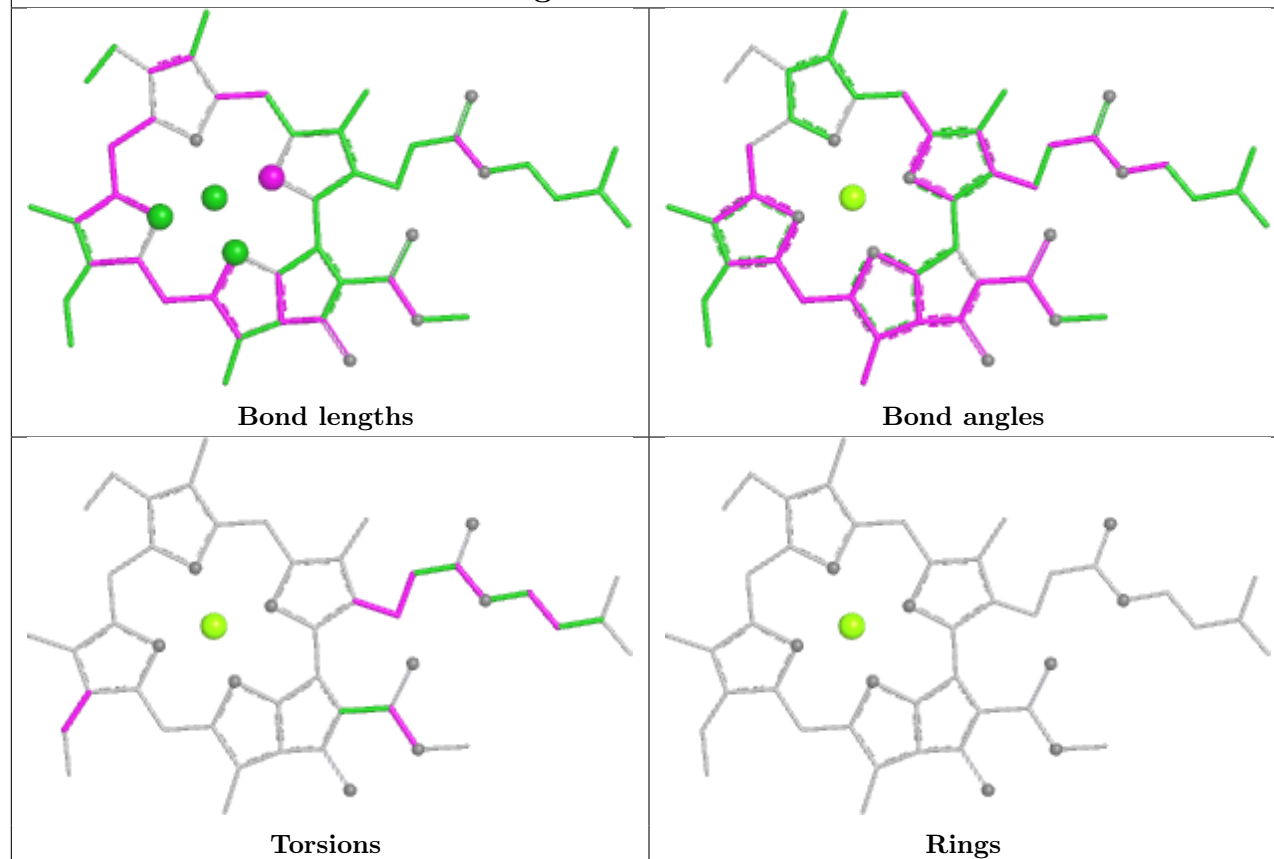
Torsions



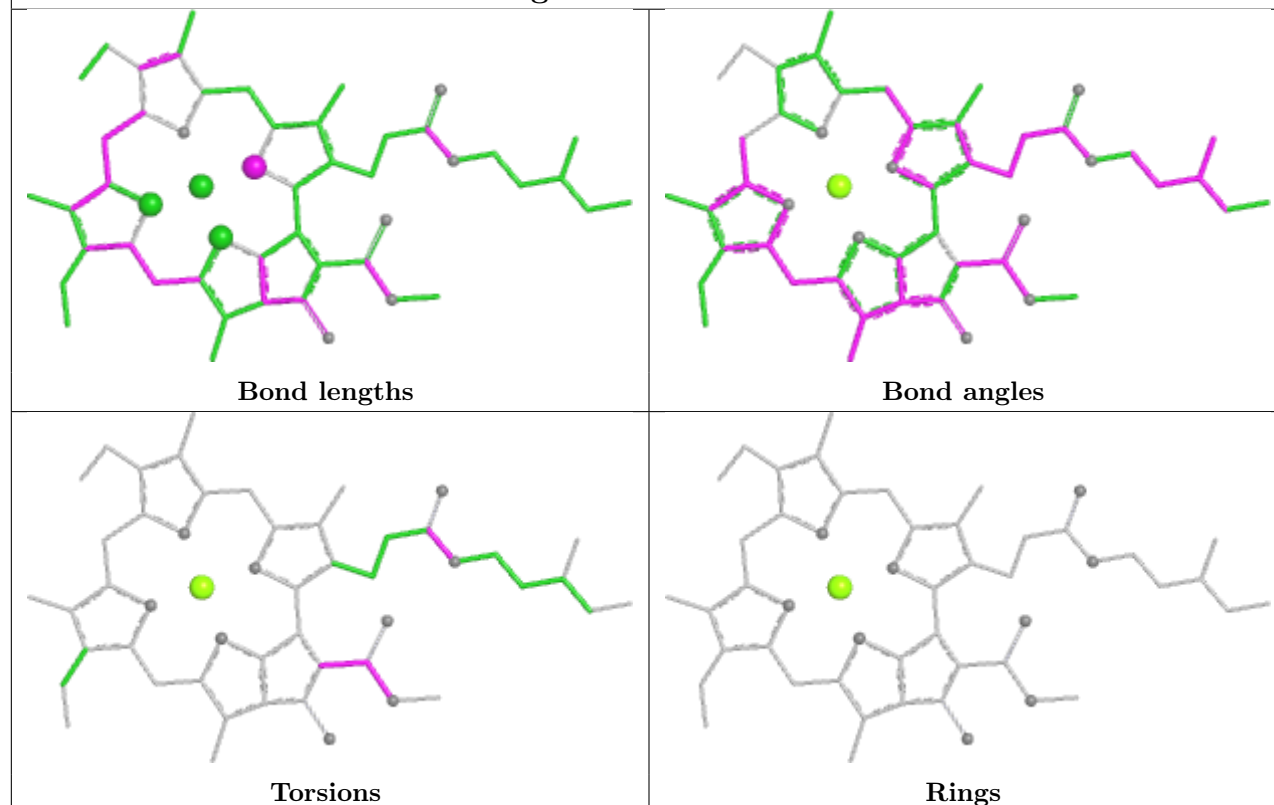
Rings

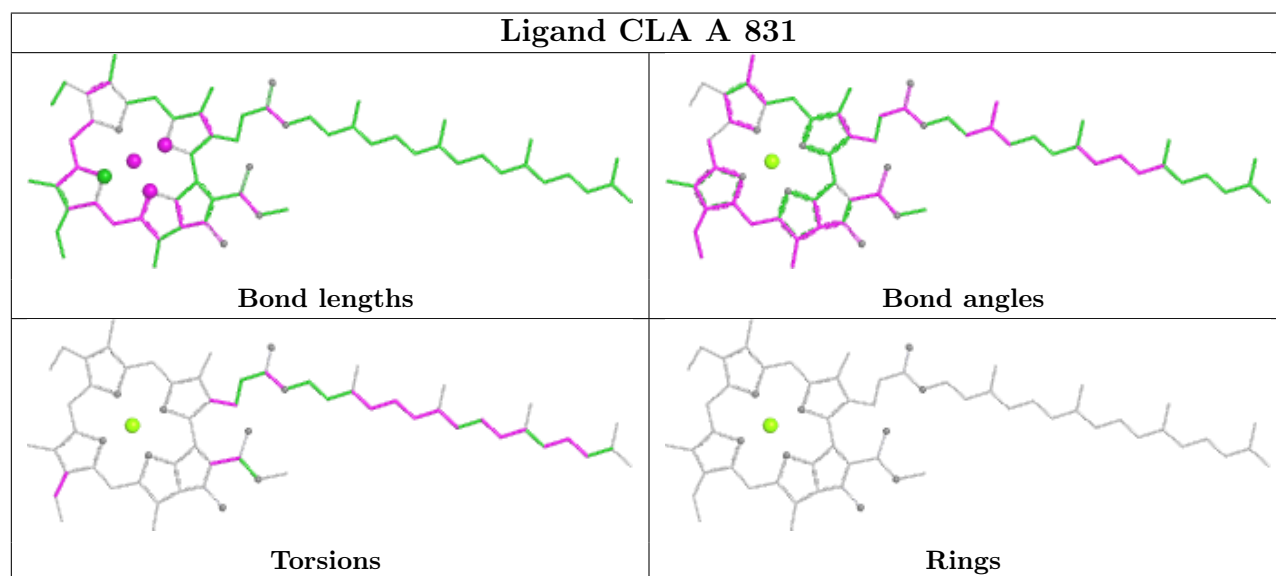
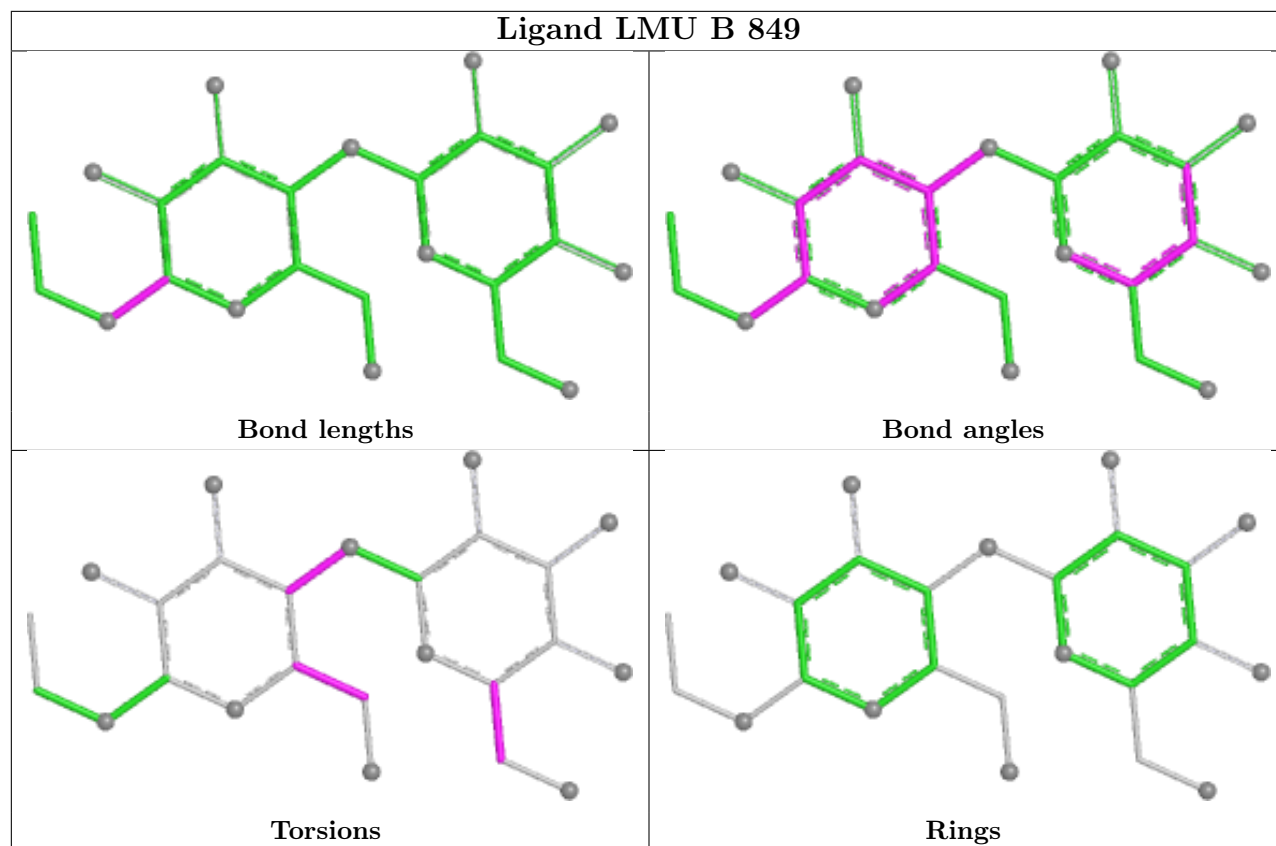


Ligand CLA F 201

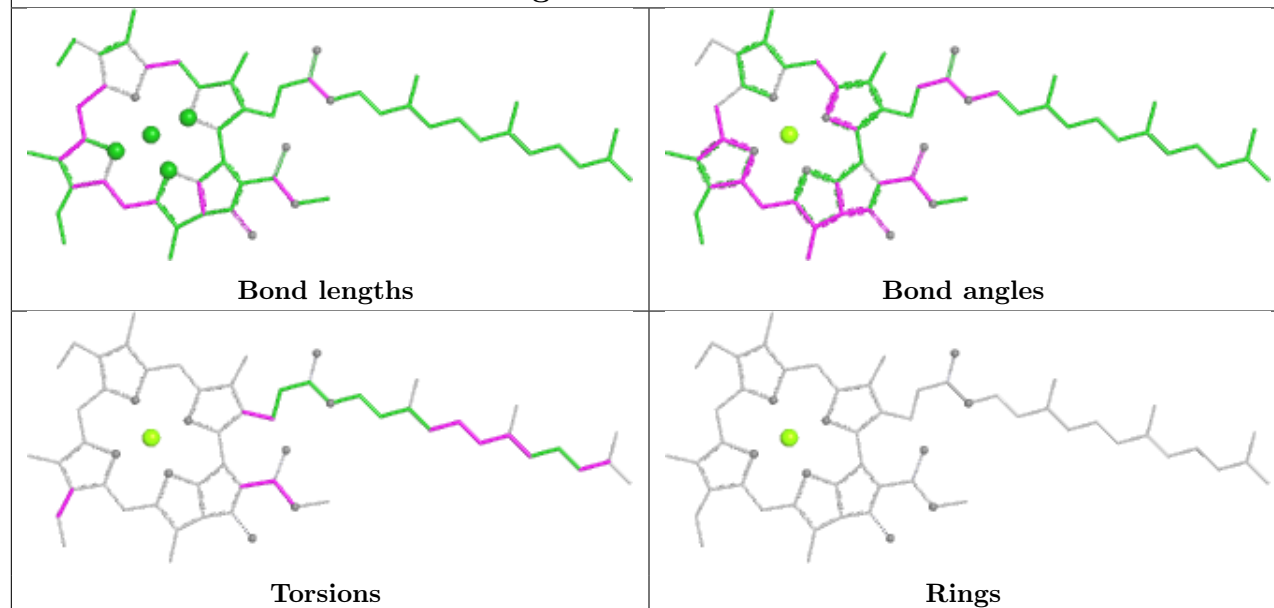


Ligand CLA G 105

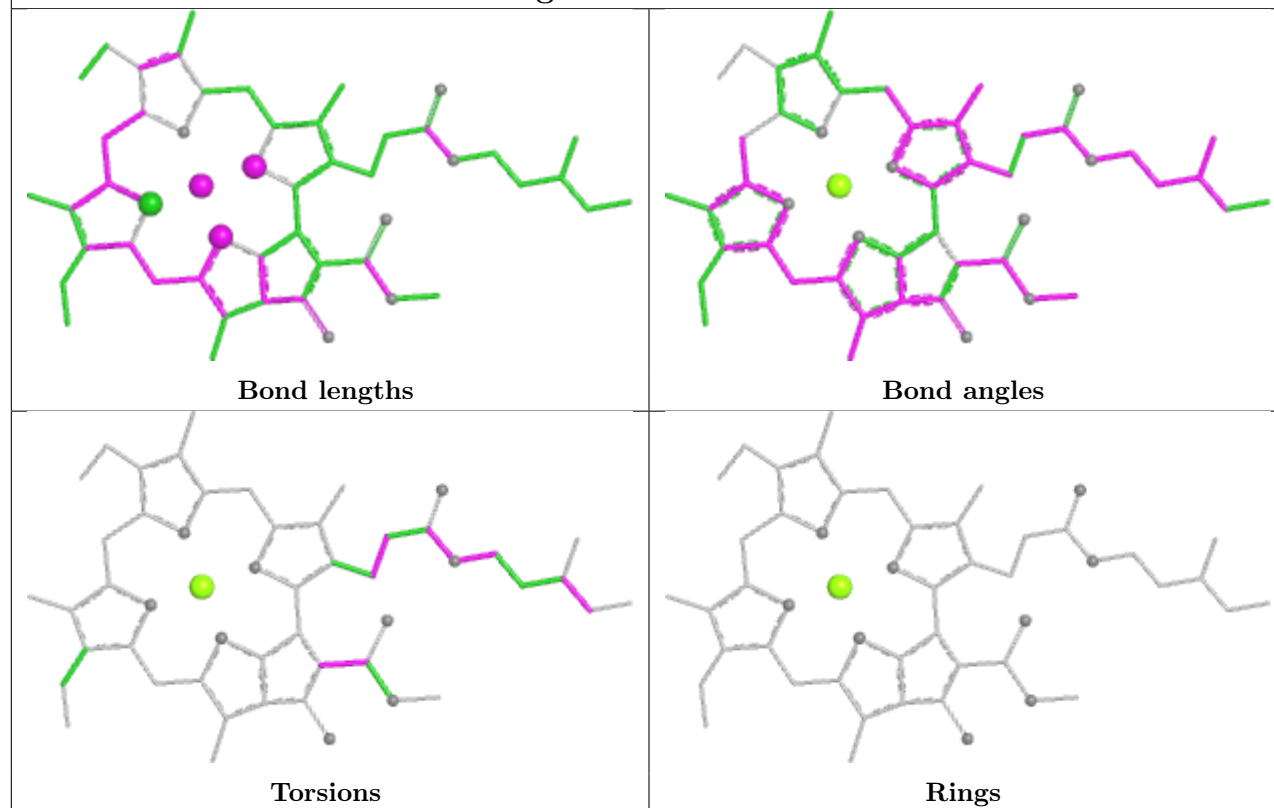




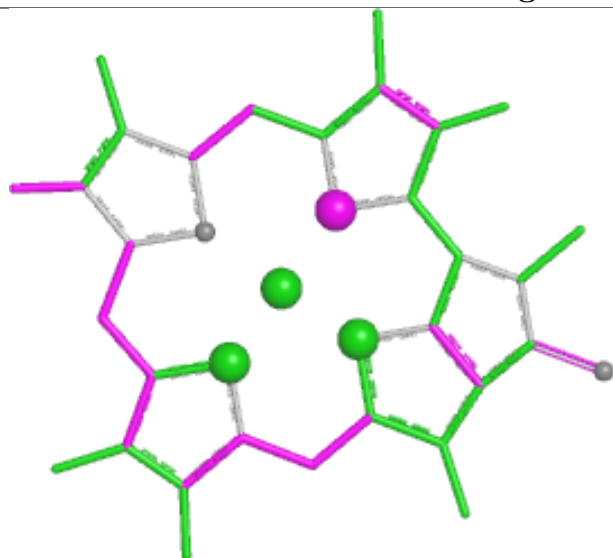
Ligand CLA B 837



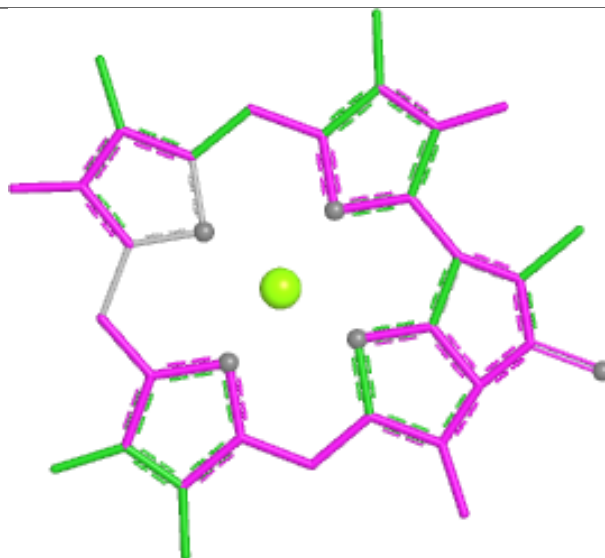
Ligand CLA 1 215



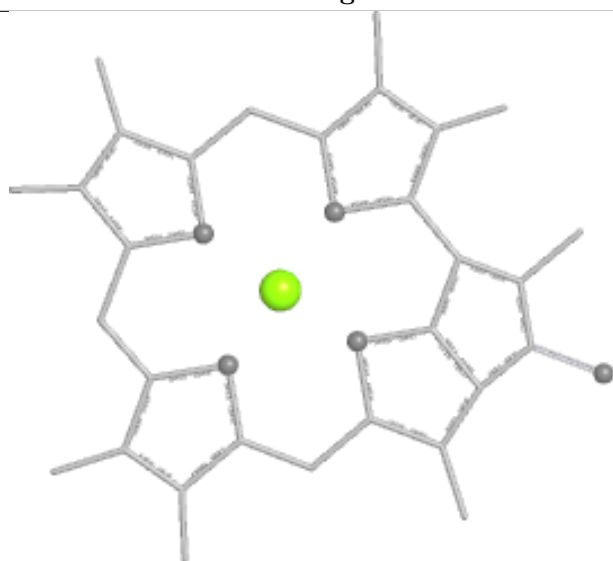
Ligand CLA 3 301



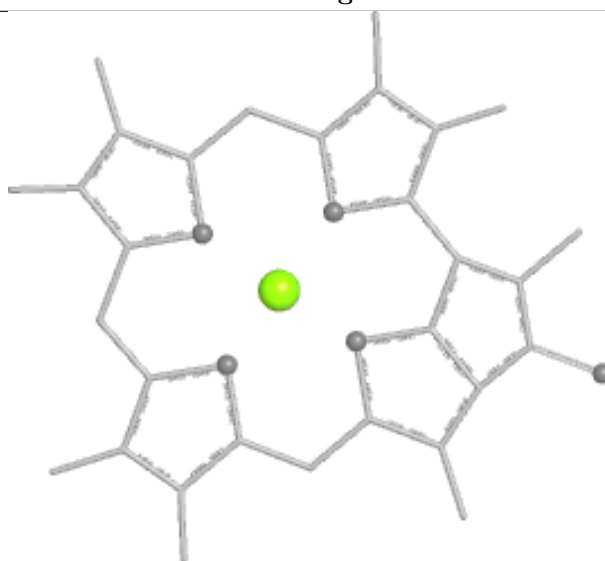
Bond lengths



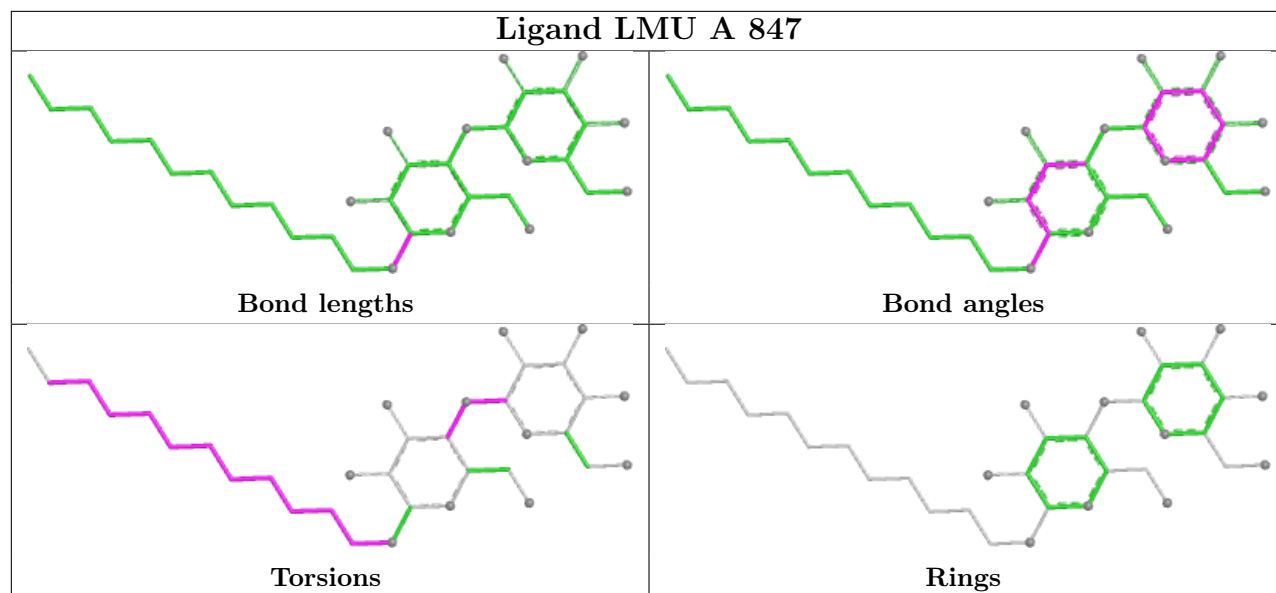
Bond angles



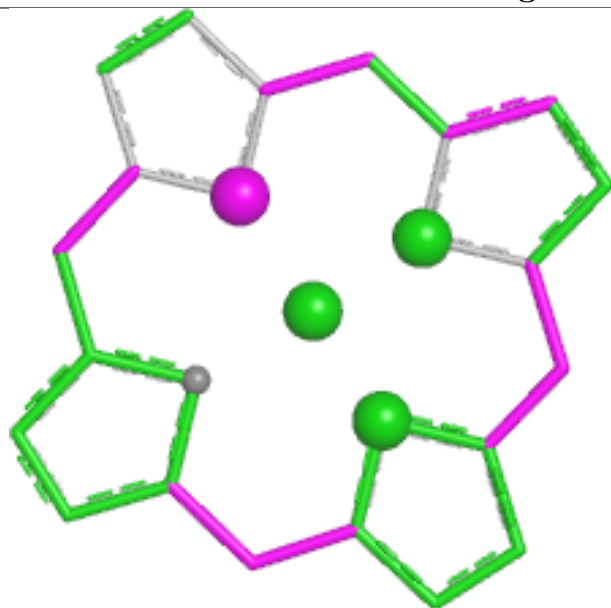
Torsions



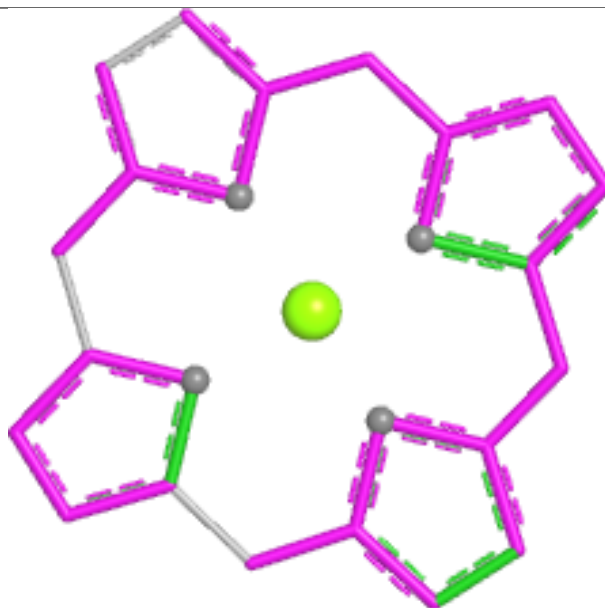
Rings



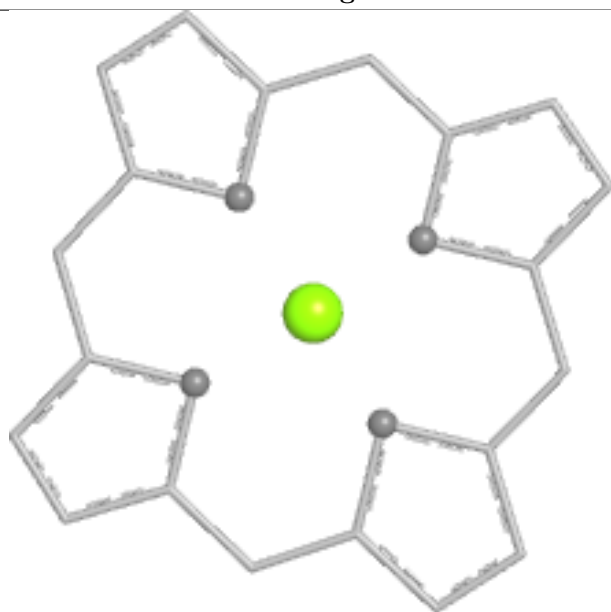
Ligand CLA 2 301



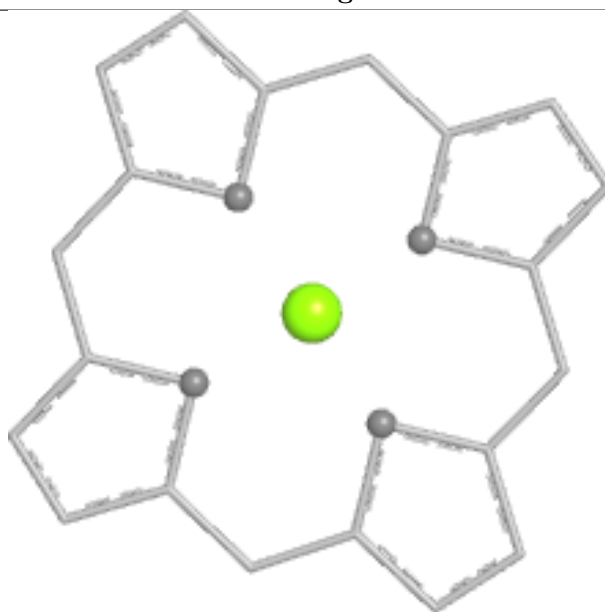
Bond lengths



Bond angles

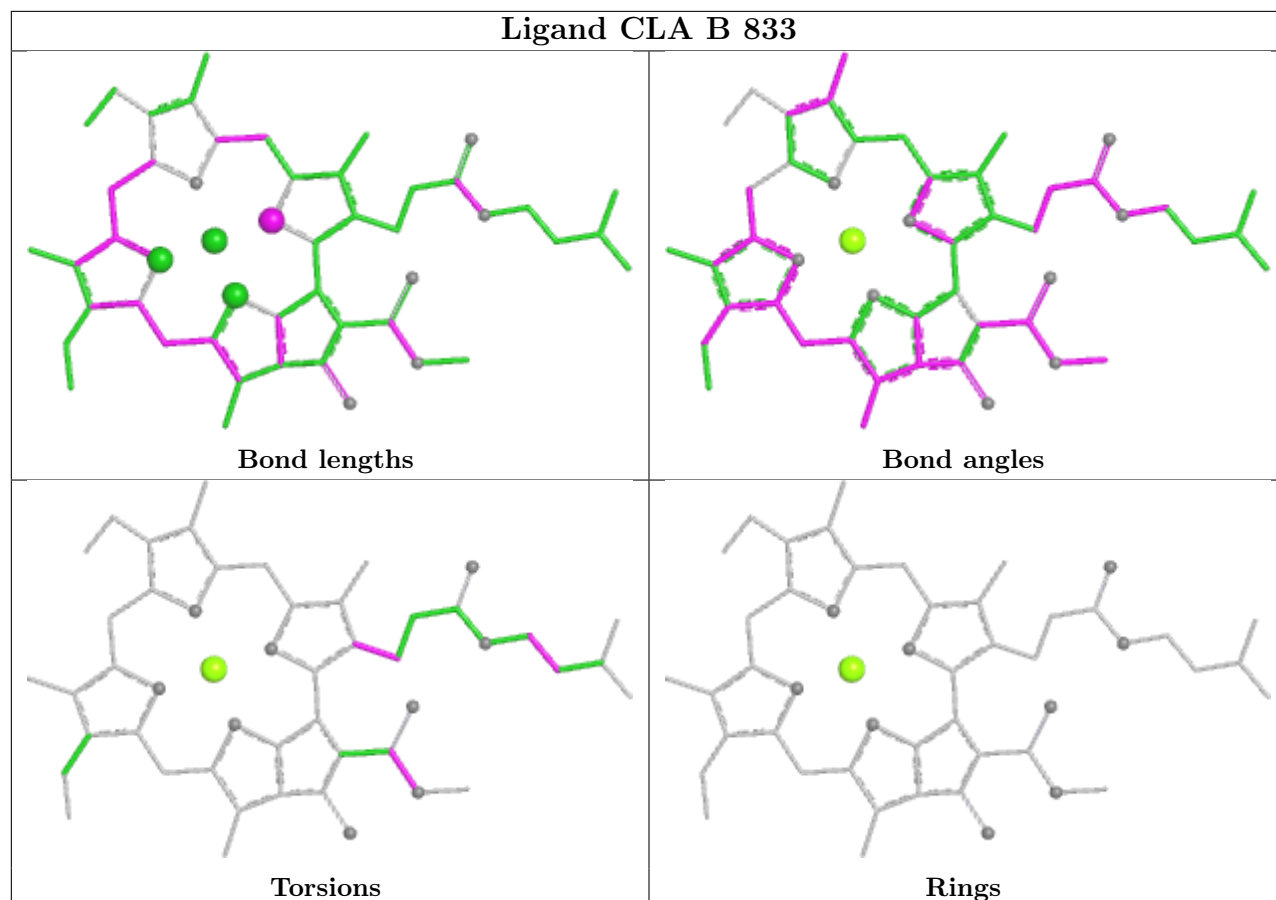


Torsions

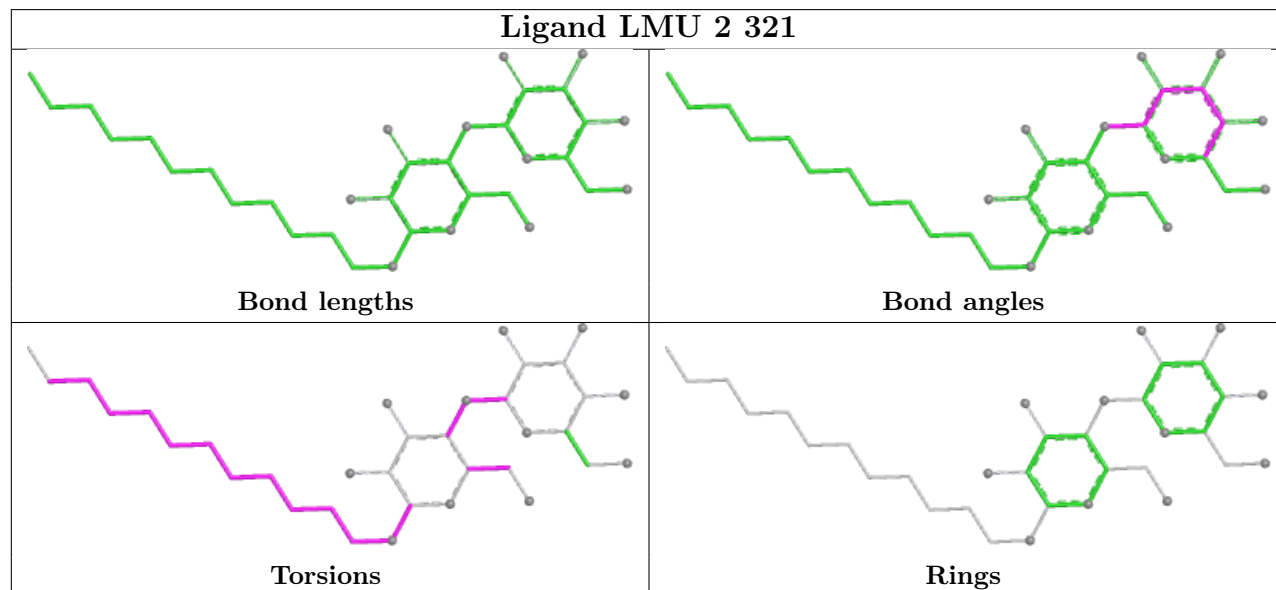


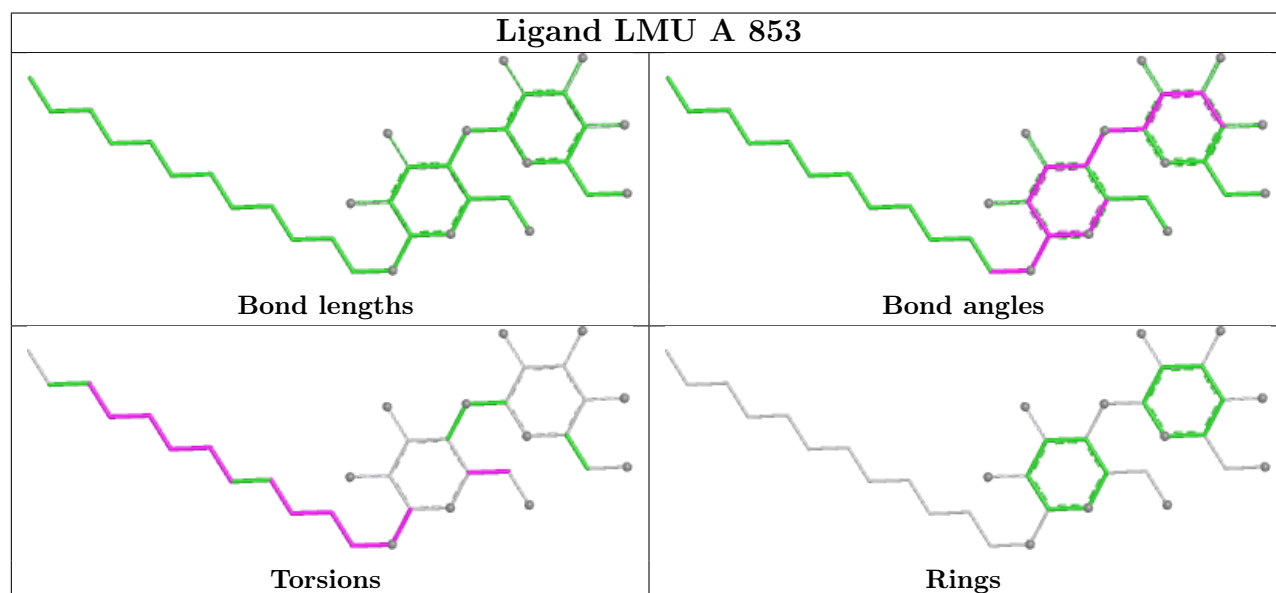
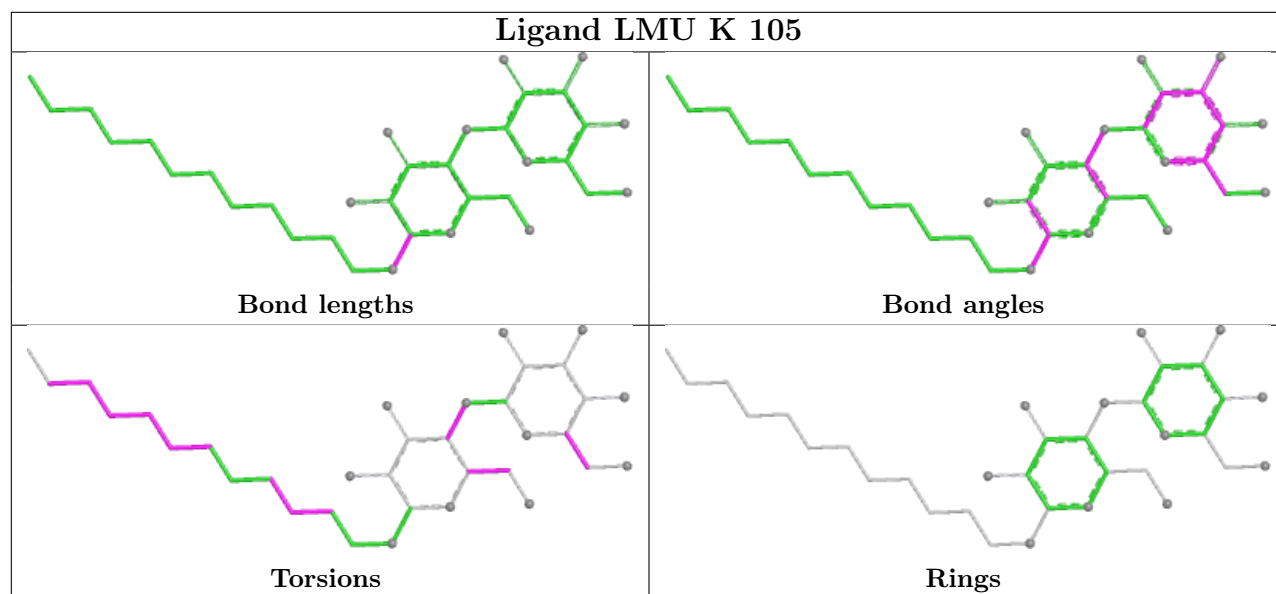
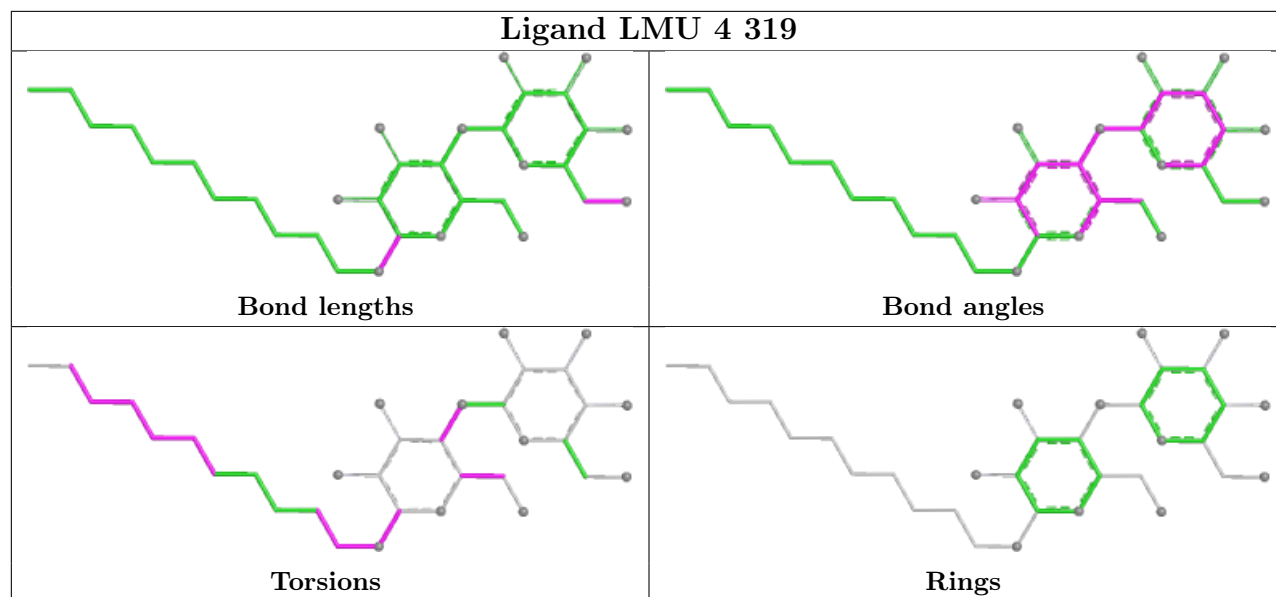
Rings

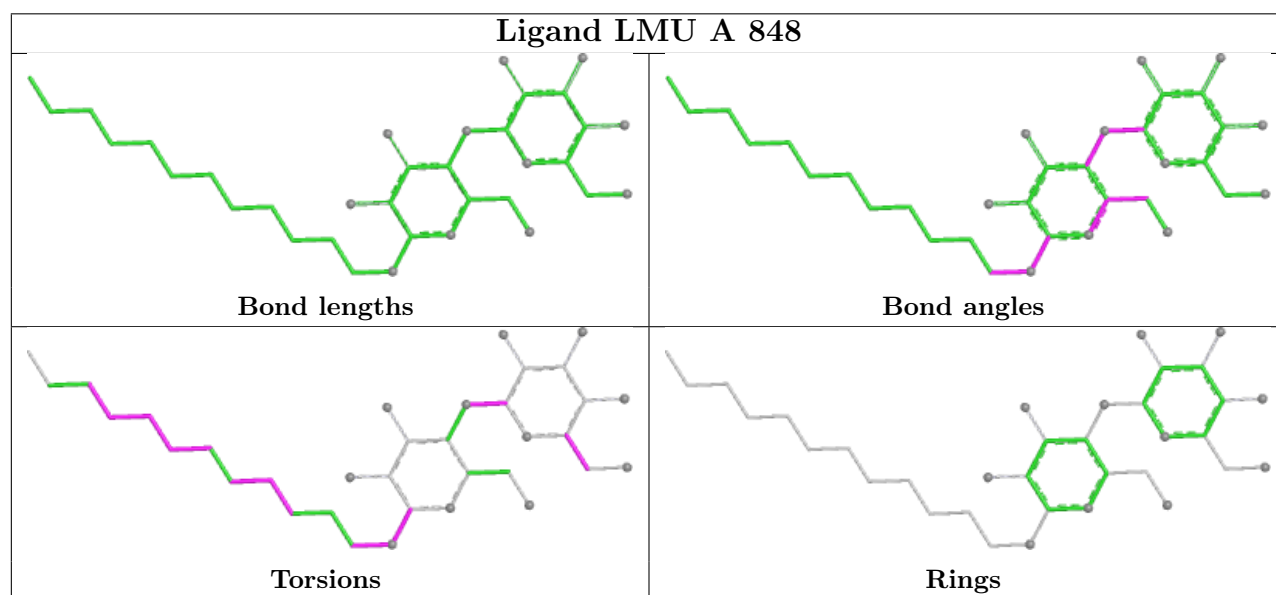
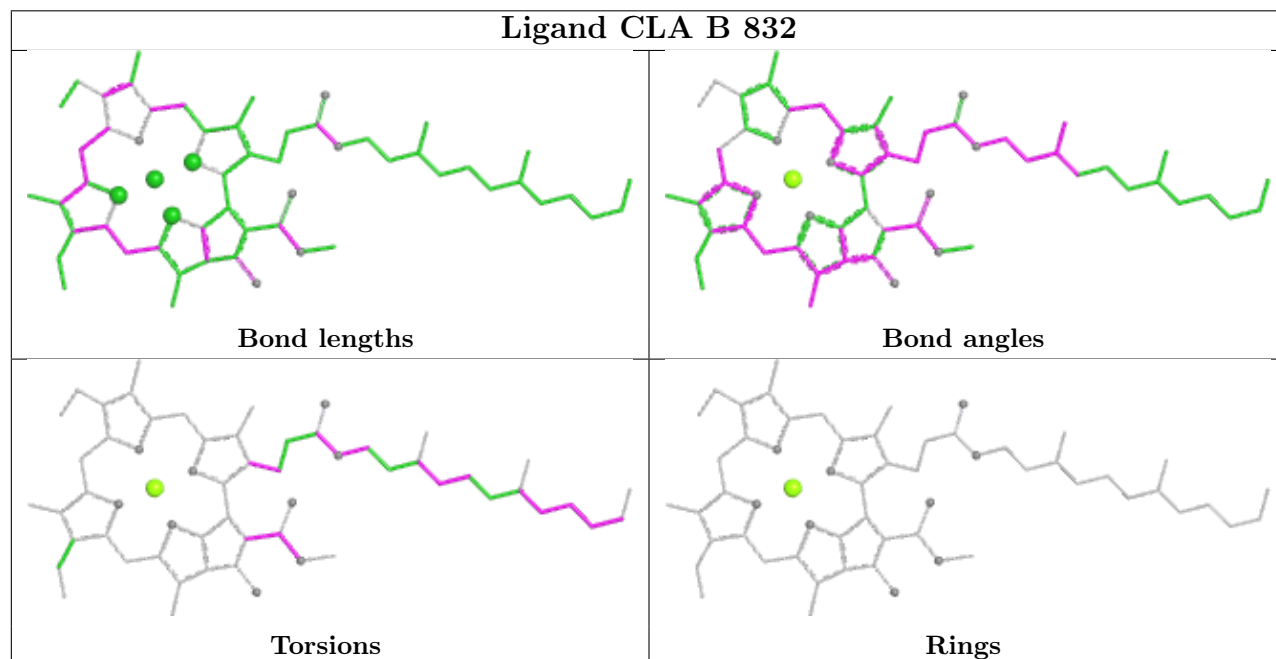
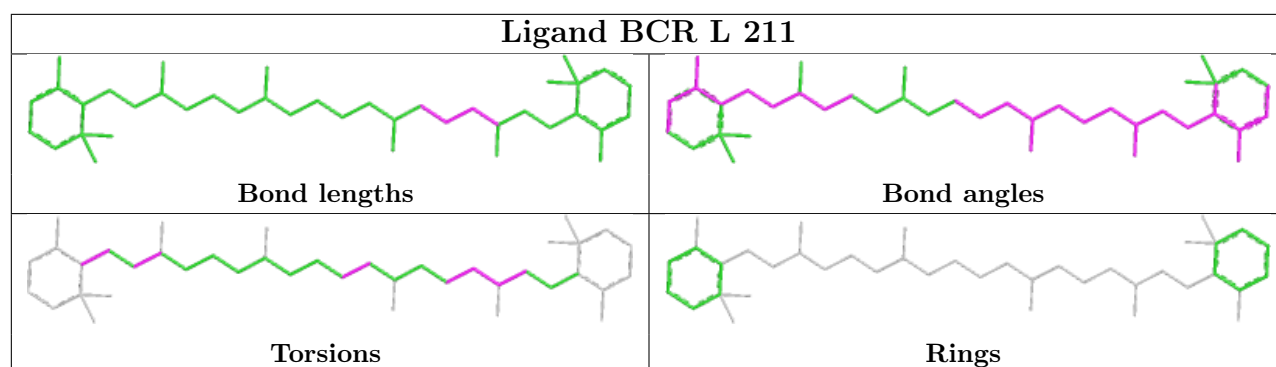
Ligand CLA B 833



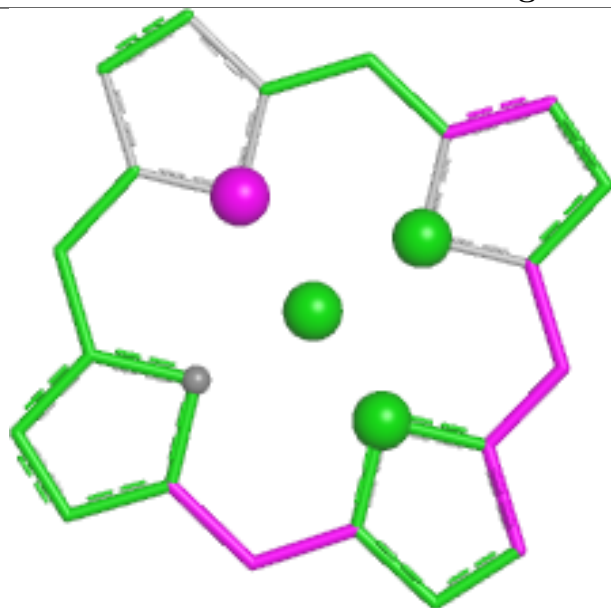
Ligand LMU 2 321



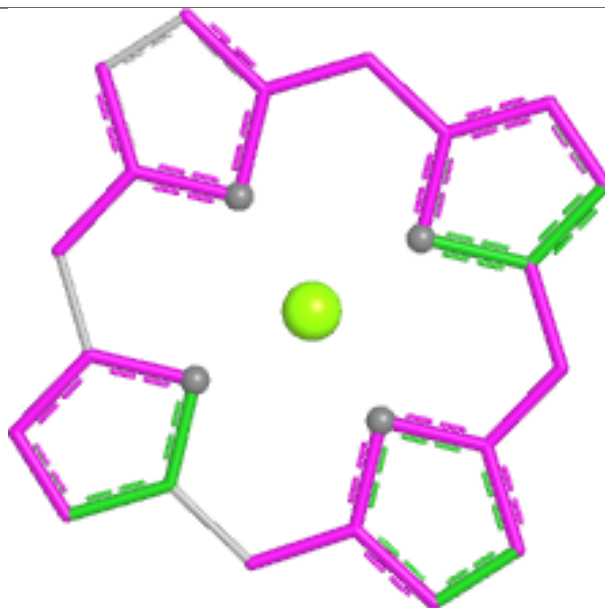




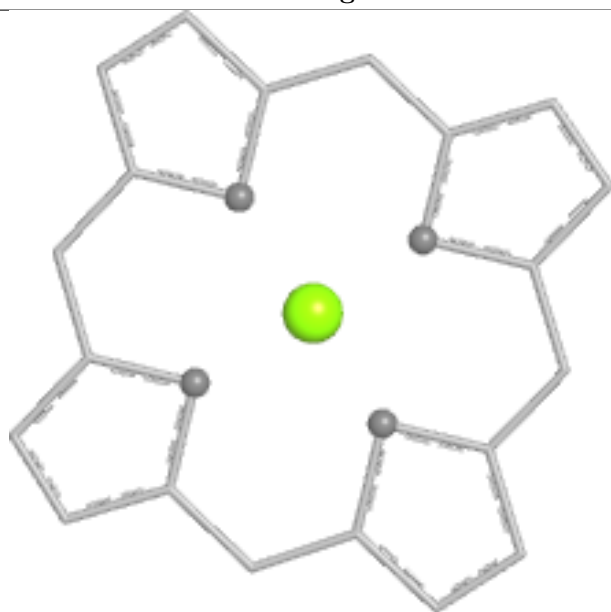
Ligand CLA 3 317



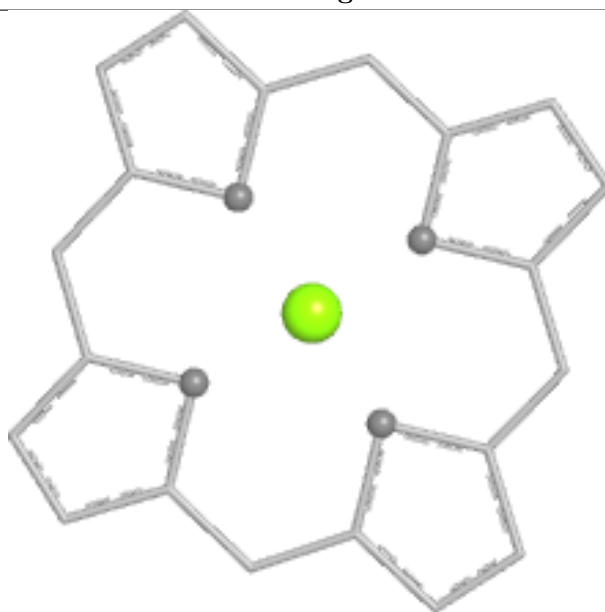
Bond lengths



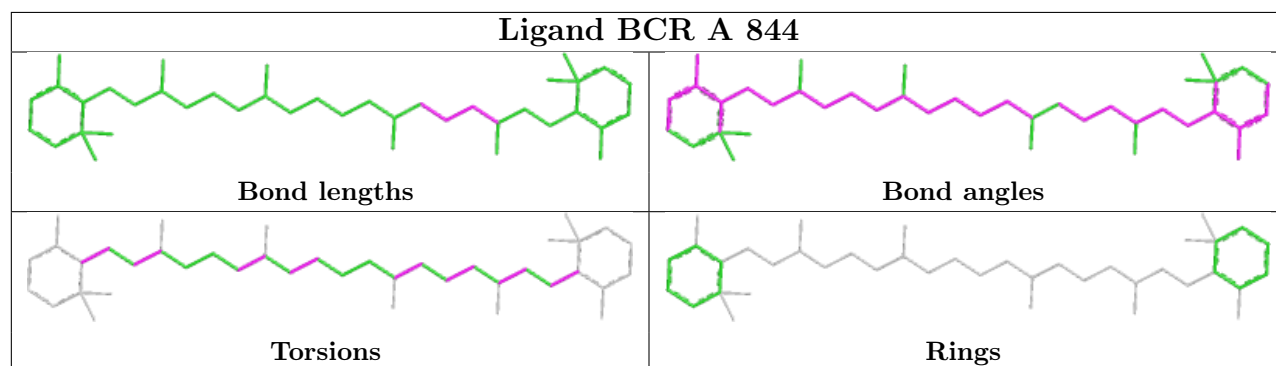
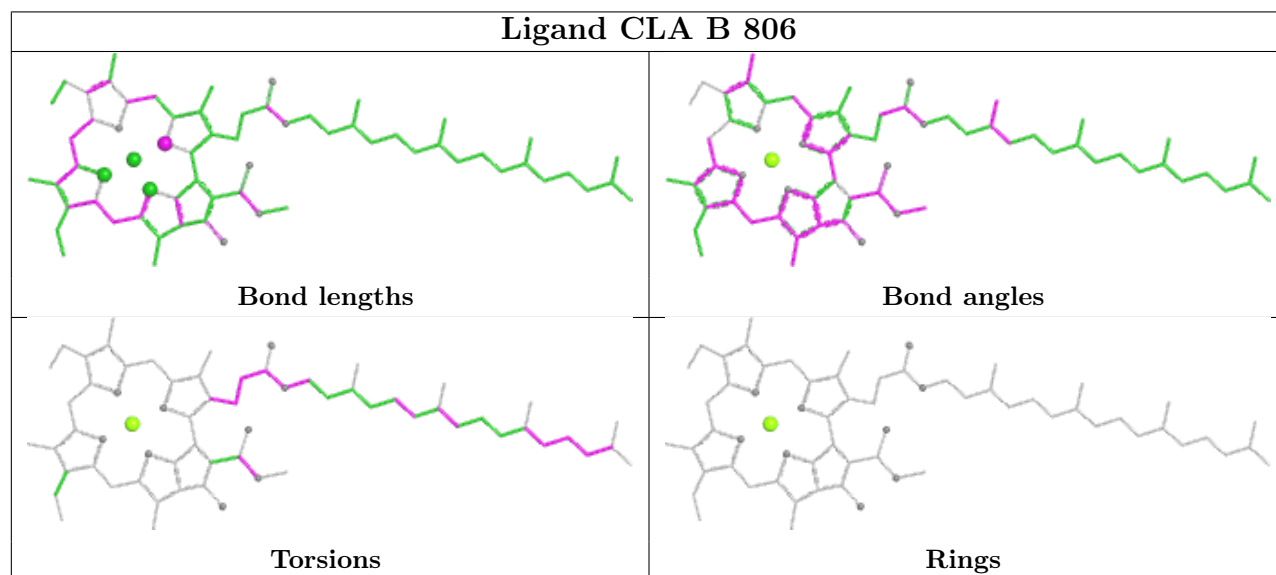
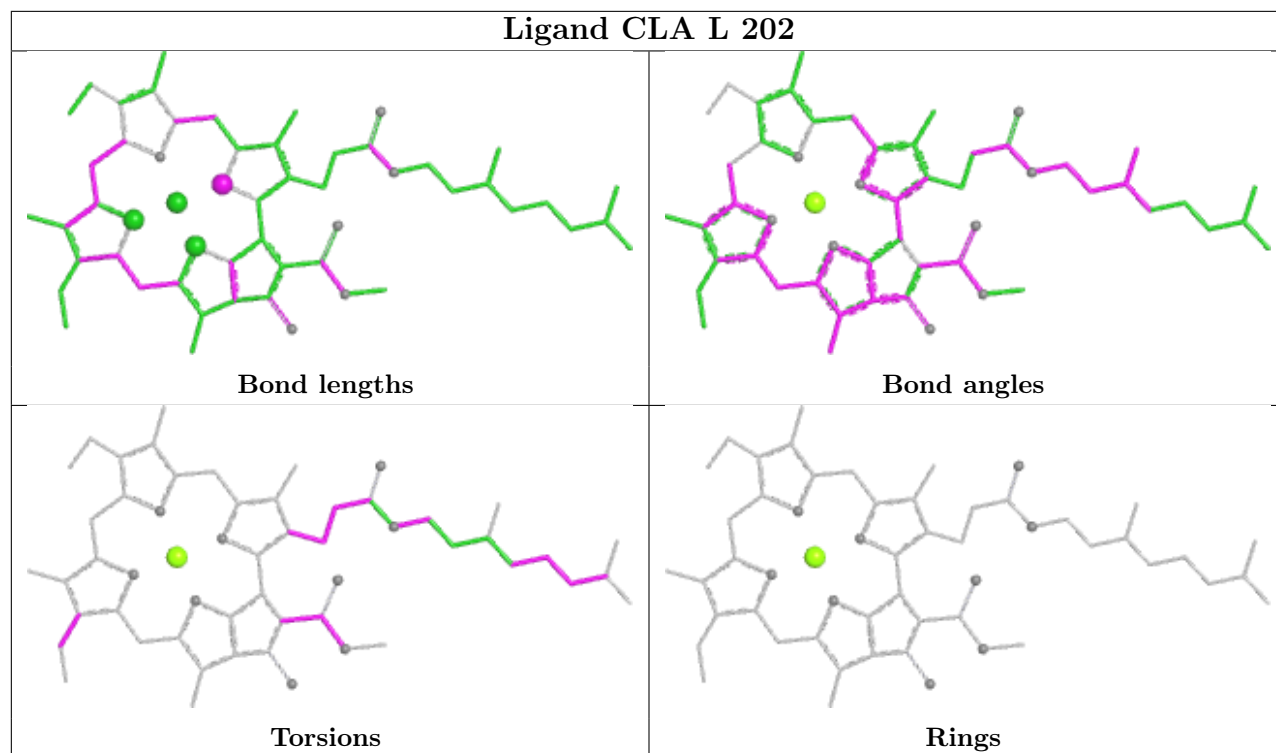
Bond angles



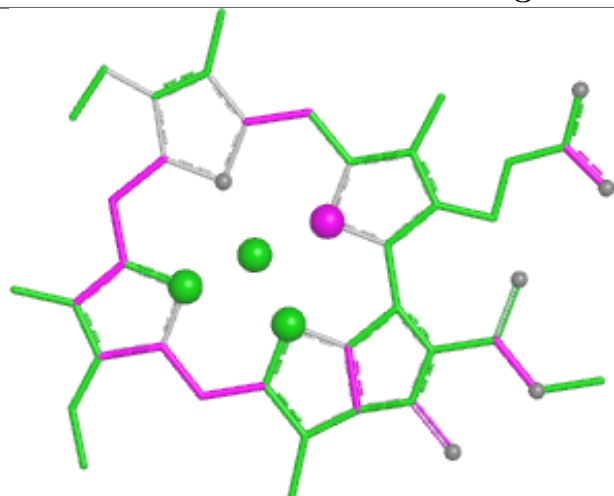
Torsions



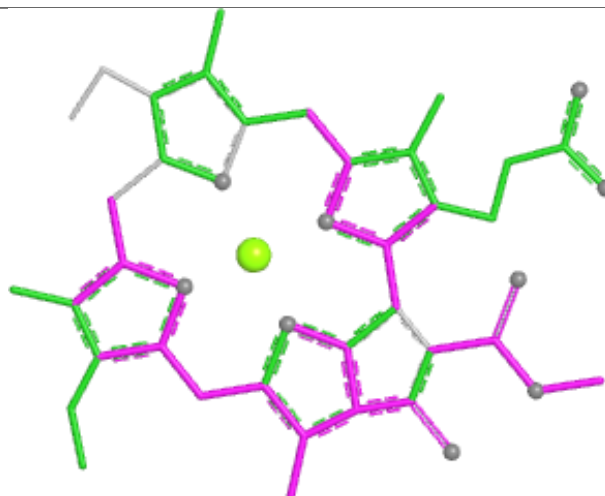
Rings



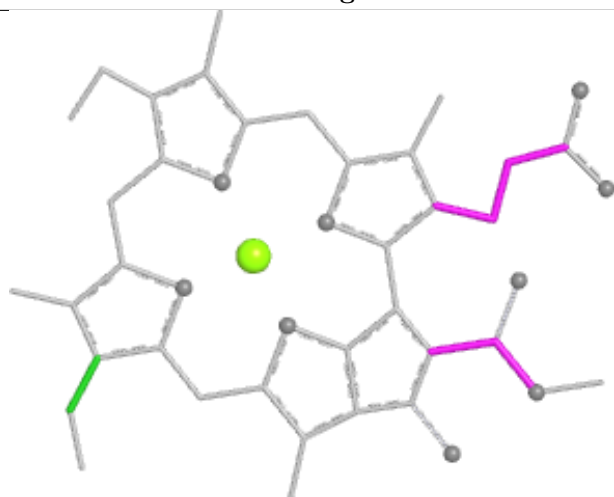
Ligand CLA B 834



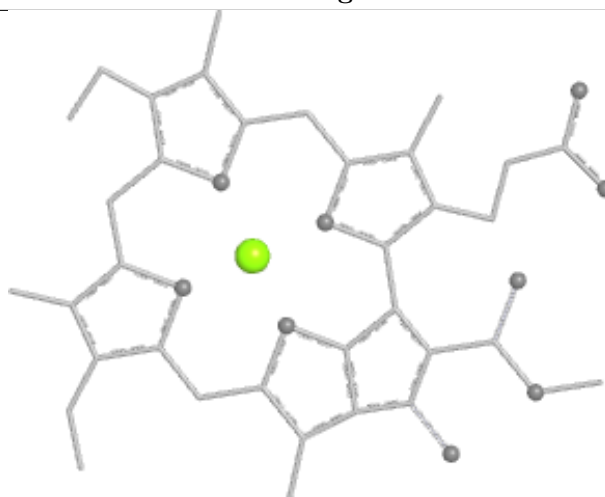
Bond lengths



Bond angles

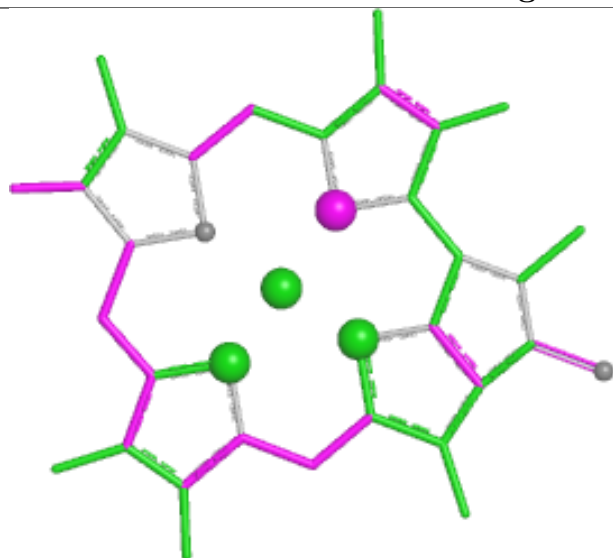


Torsions

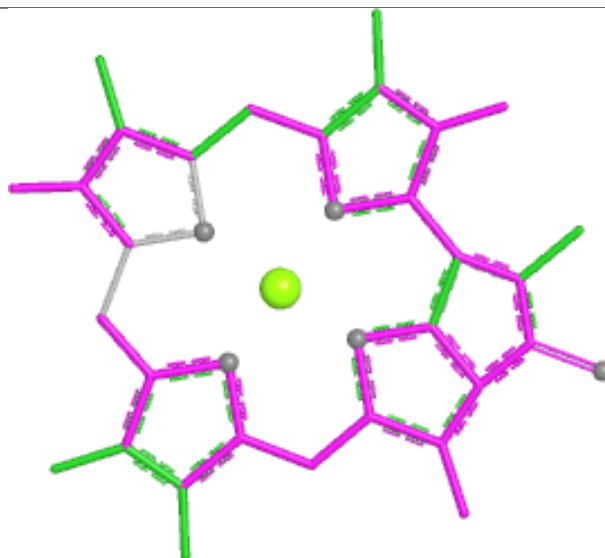


Rings

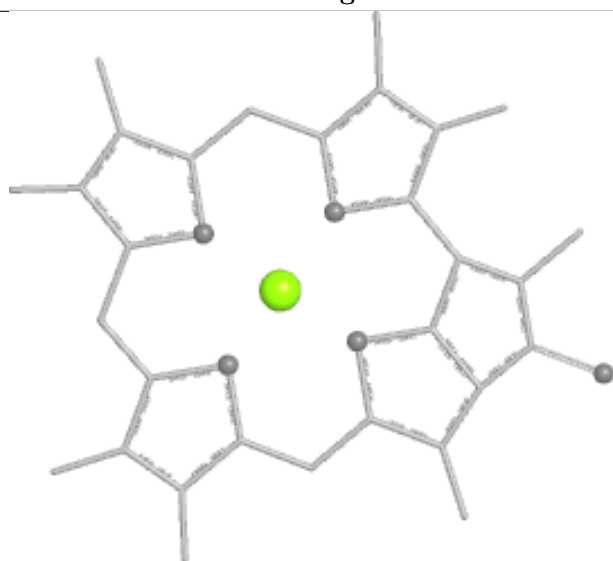
Ligand CLA 3 318



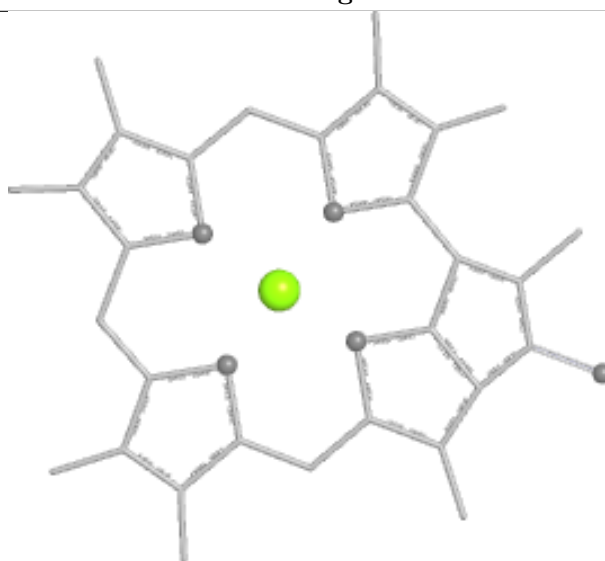
Bond lengths



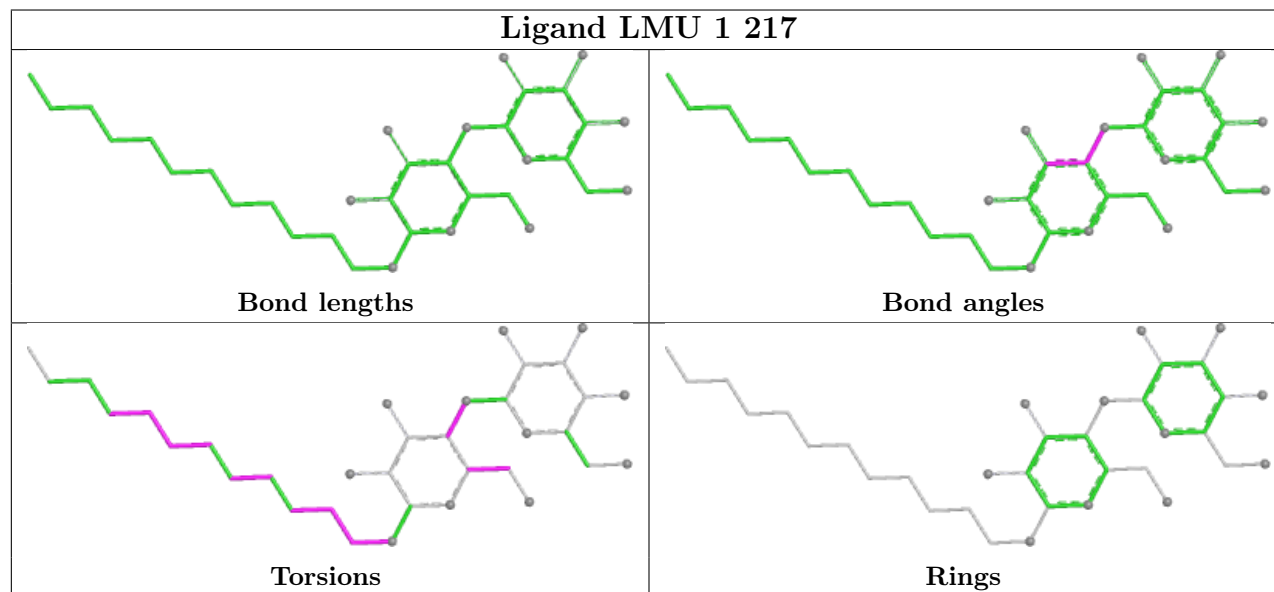
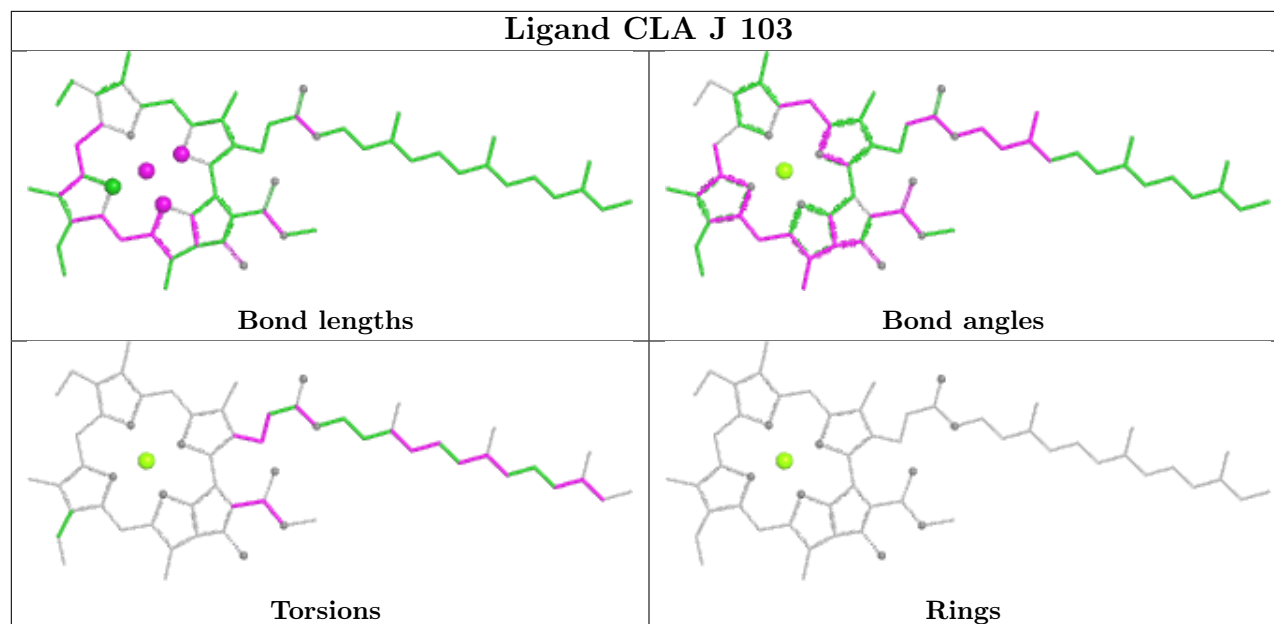
Bond angles



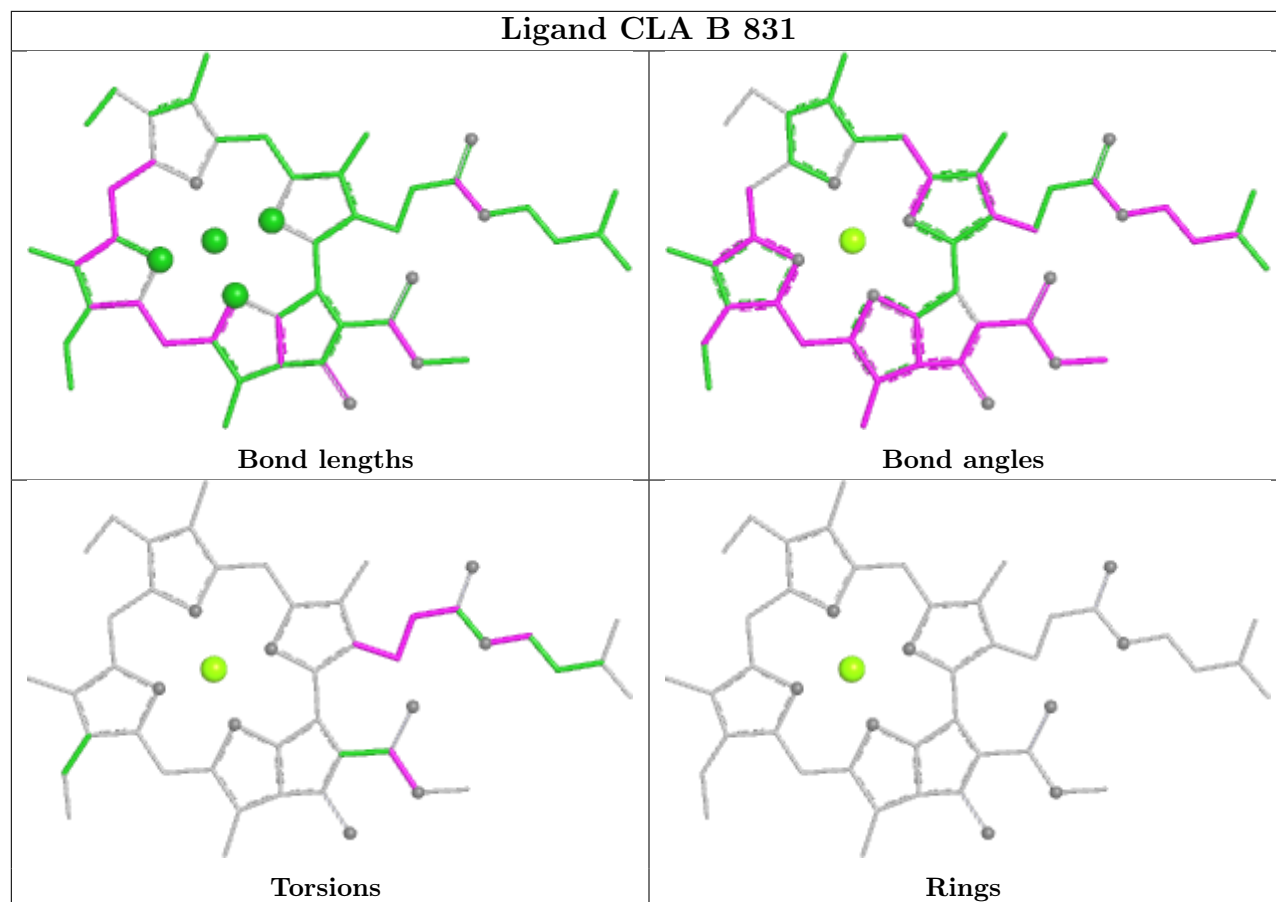
Torsions



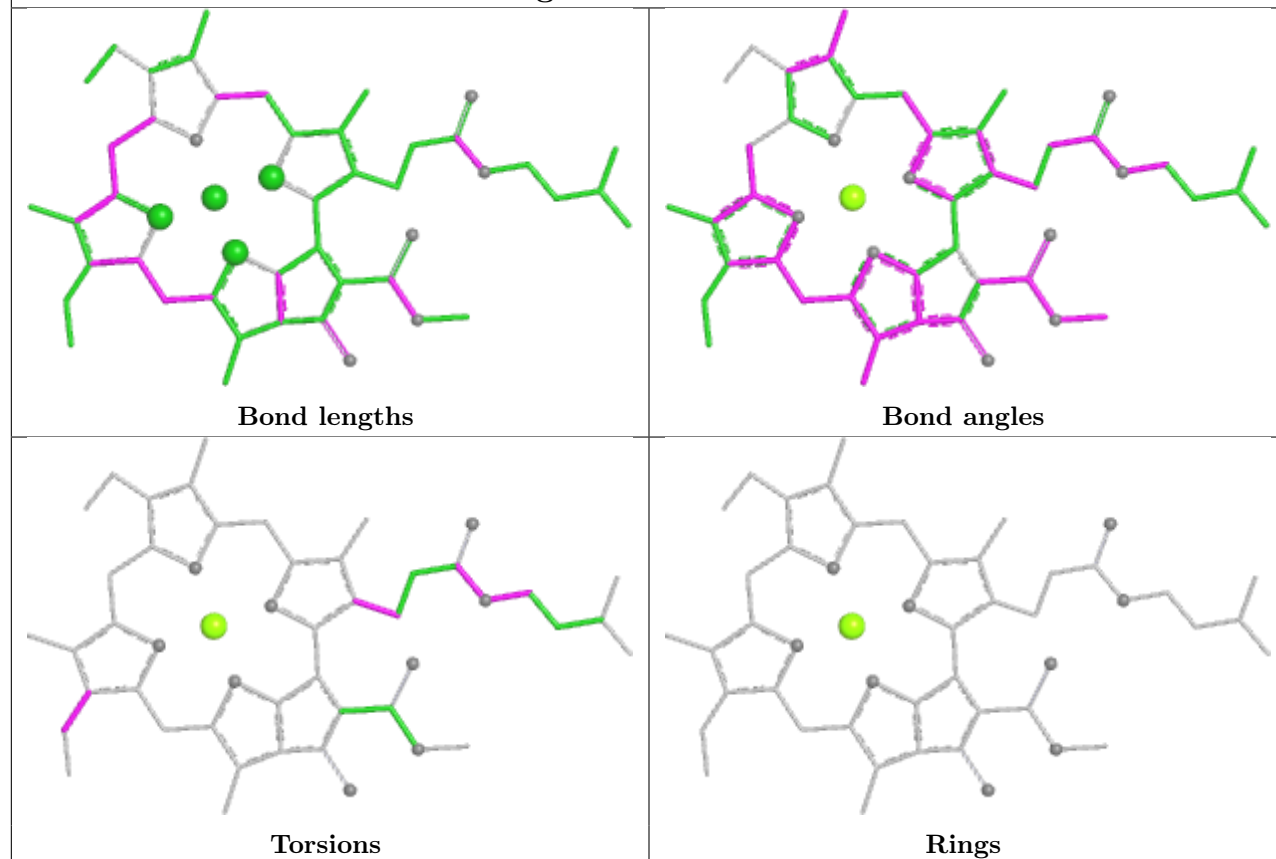
Rings



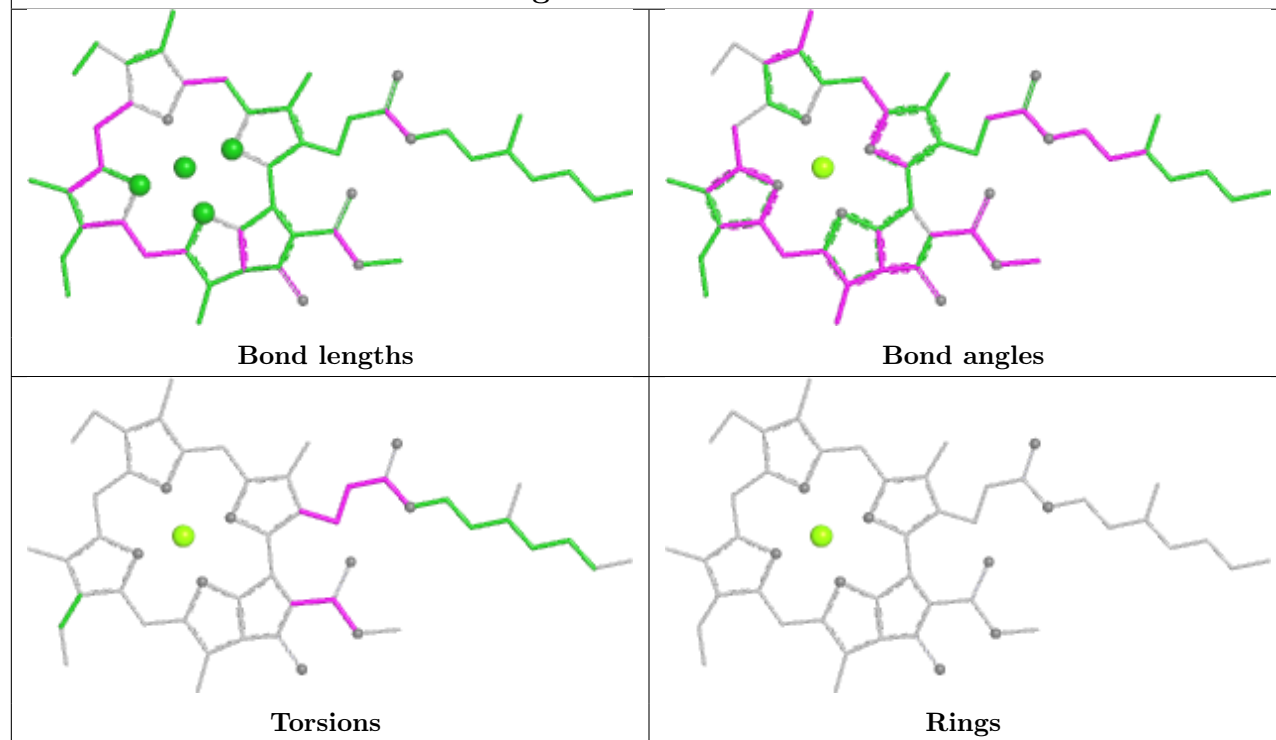
Ligand CLA B 831



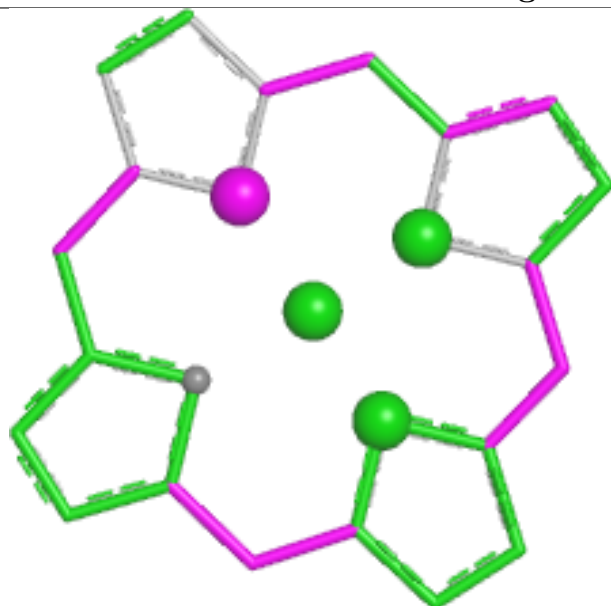
Ligand CLA 2 305



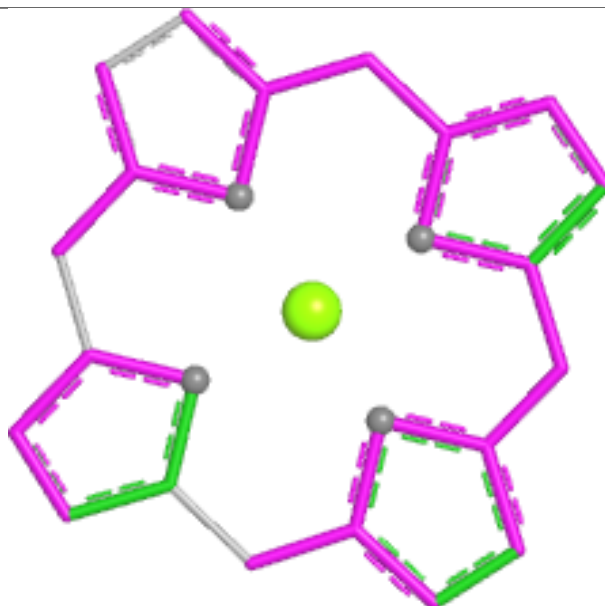
Ligand CLA B 818



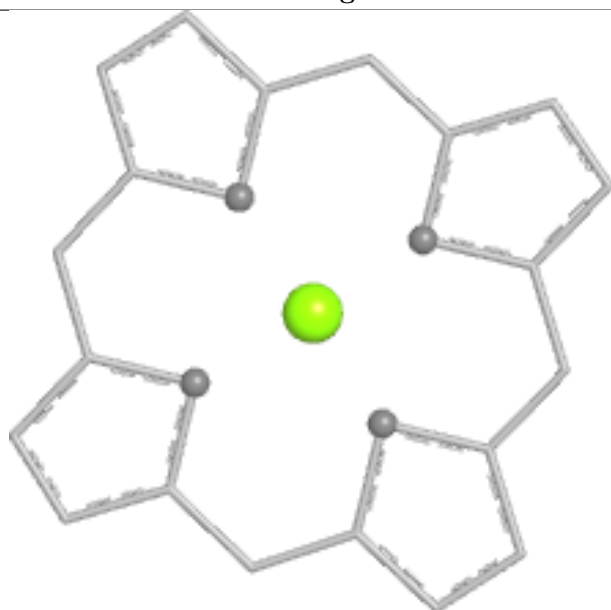
Ligand CLA 1 212



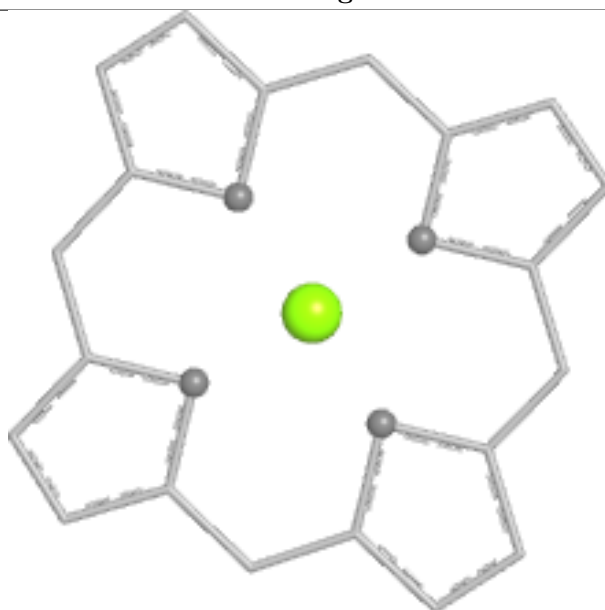
Bond lengths



Bond angles

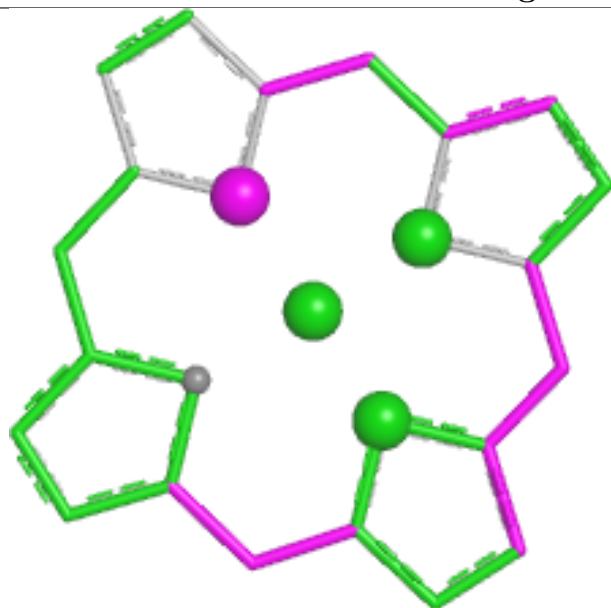


Torsions

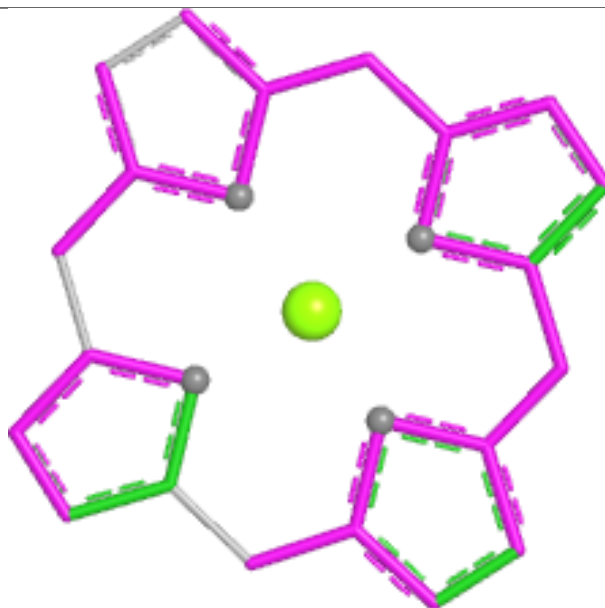


Rings

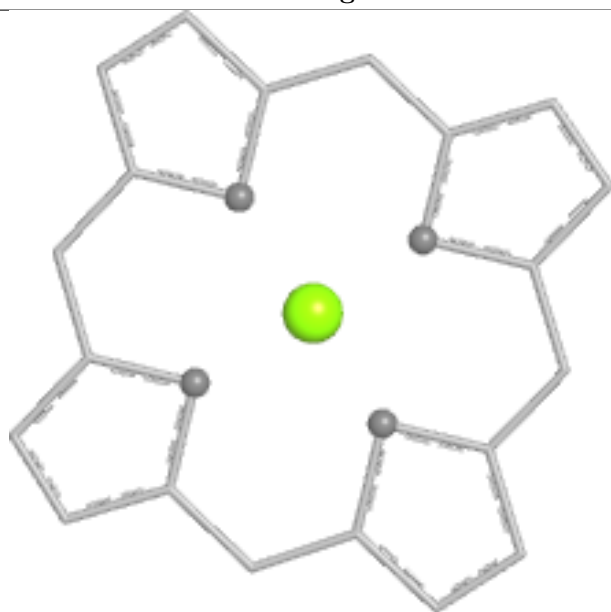
Ligand CLA 4 311



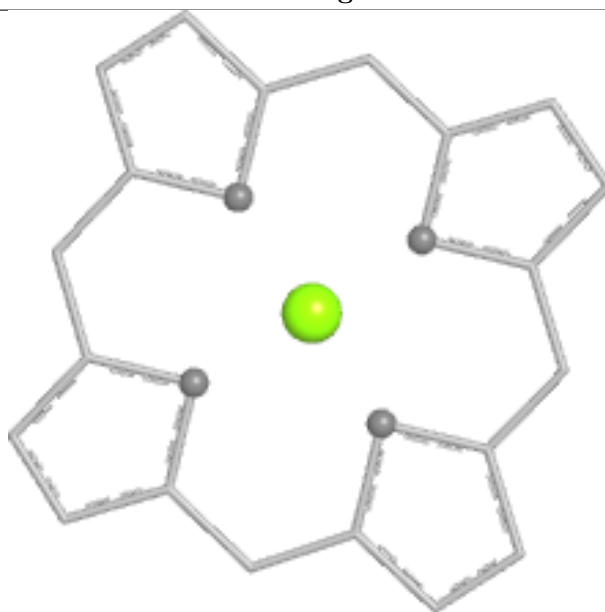
Bond lengths



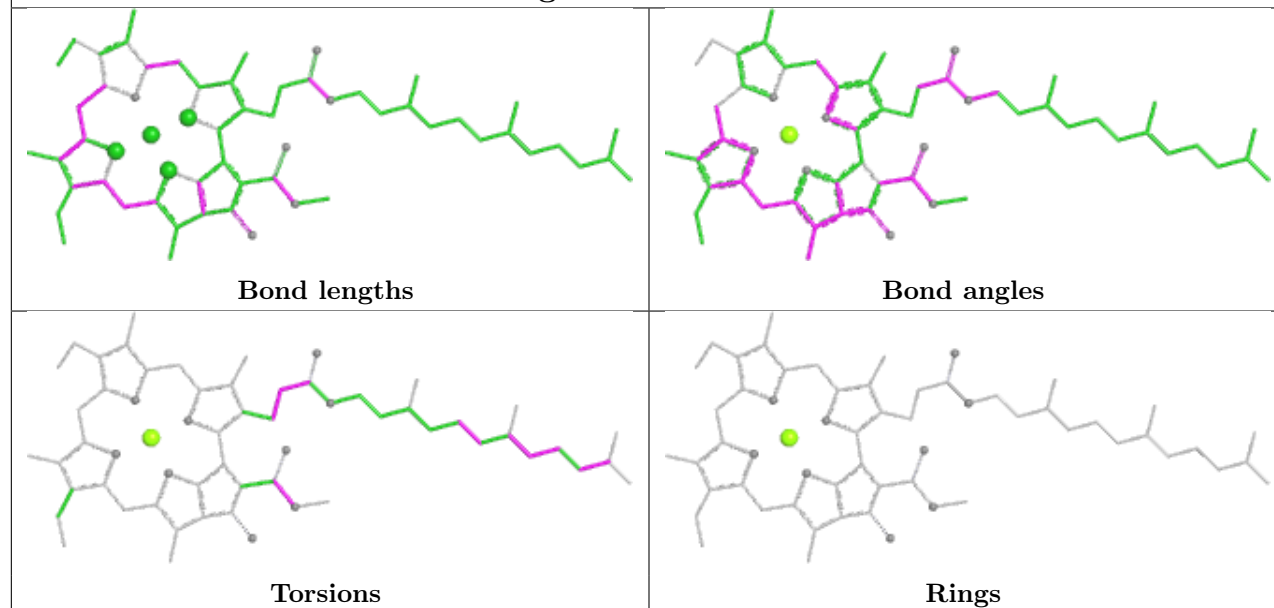
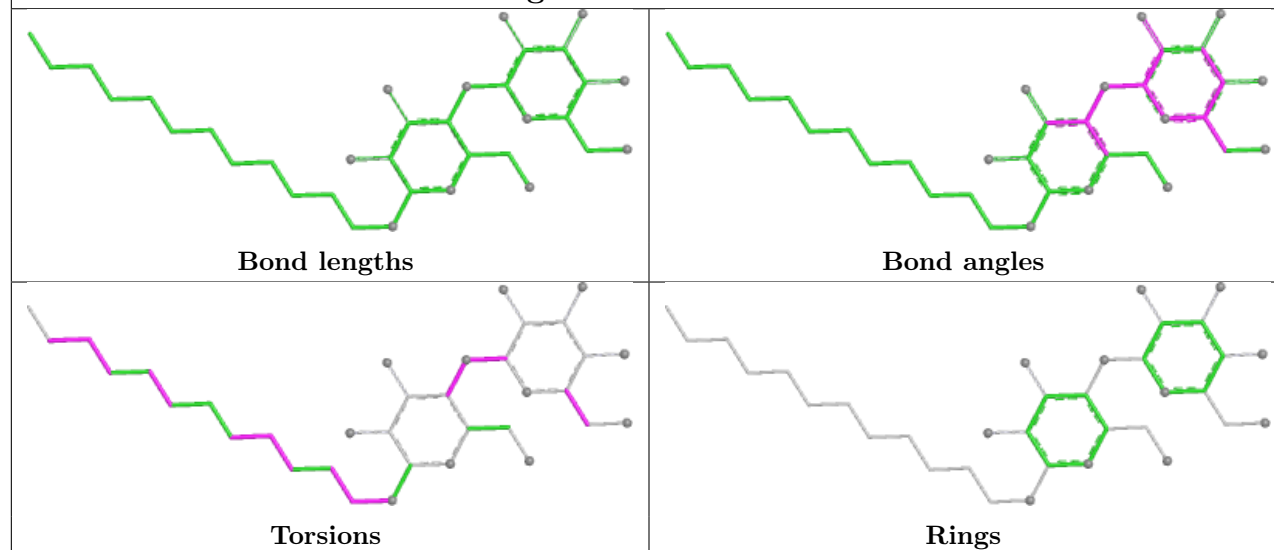
Bond angles

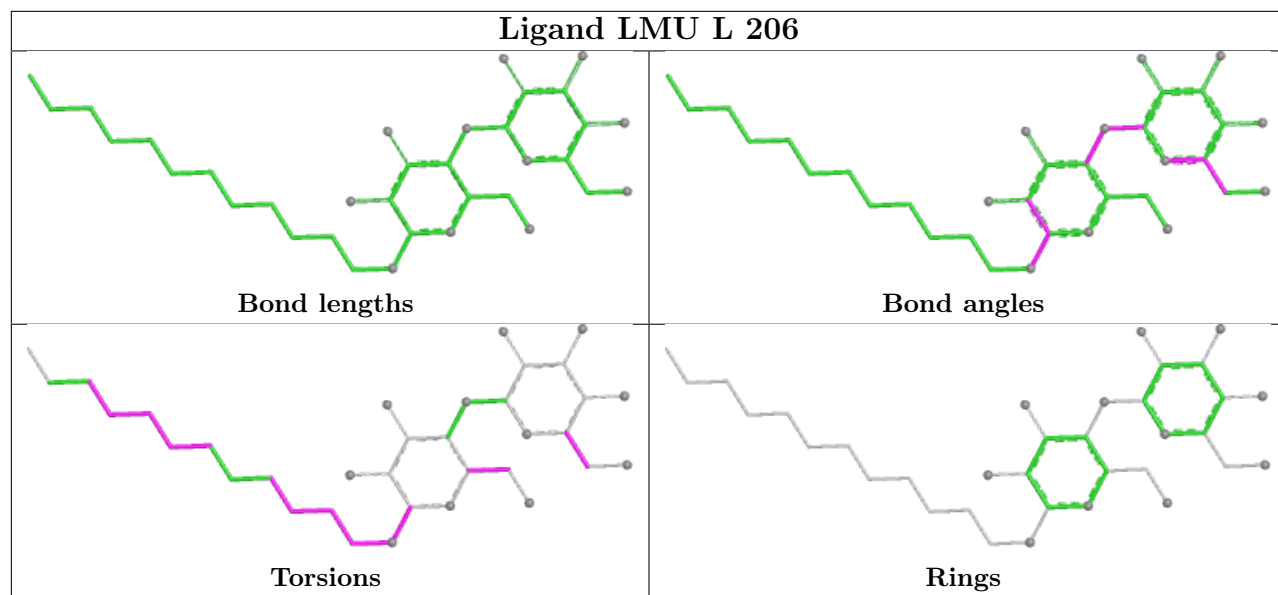


Torsions

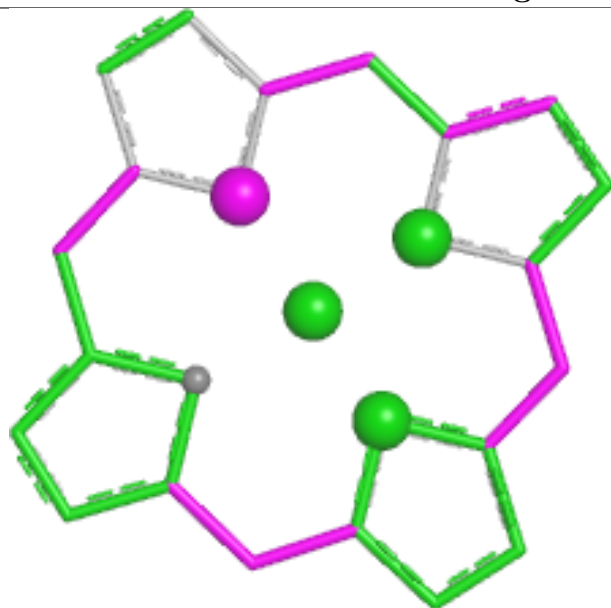


Rings

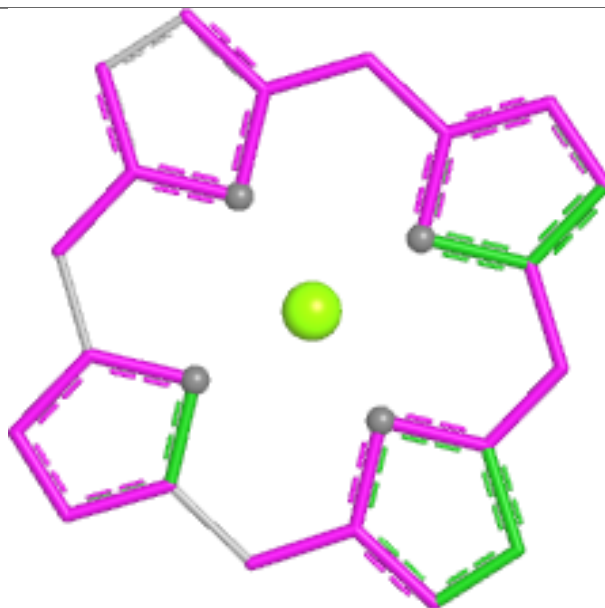
Ligand CLA I 102**Ligand LMU H 104**



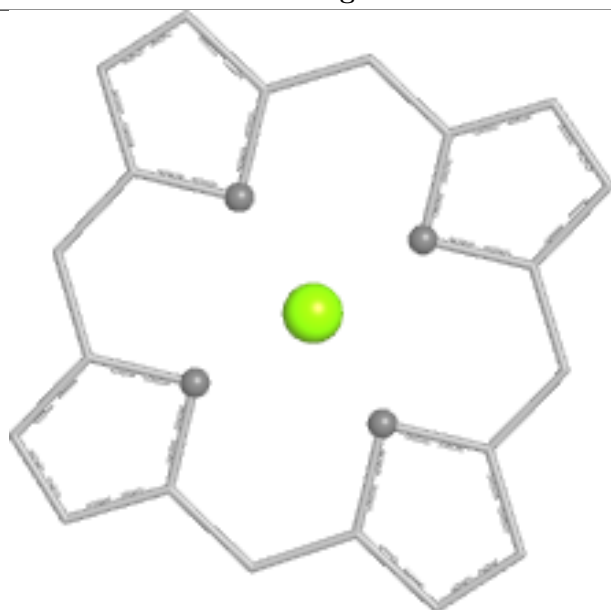
Ligand CLA A 841



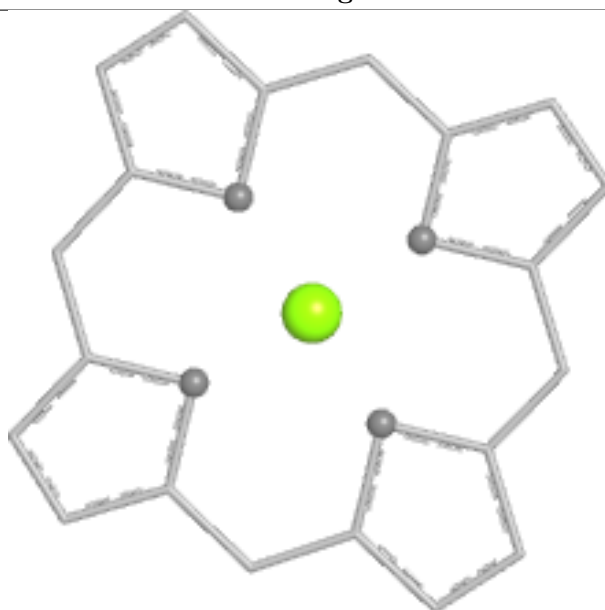
Bond lengths



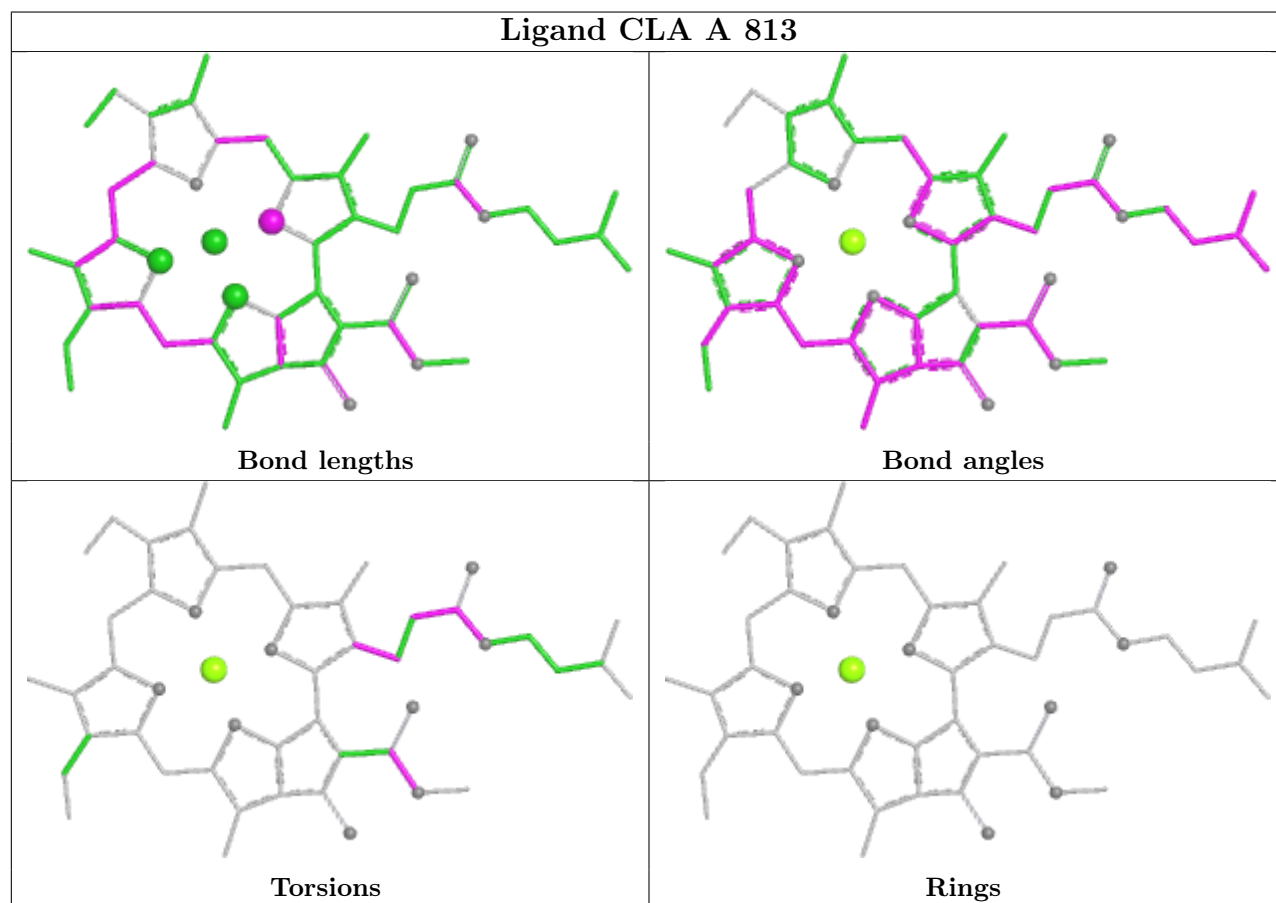
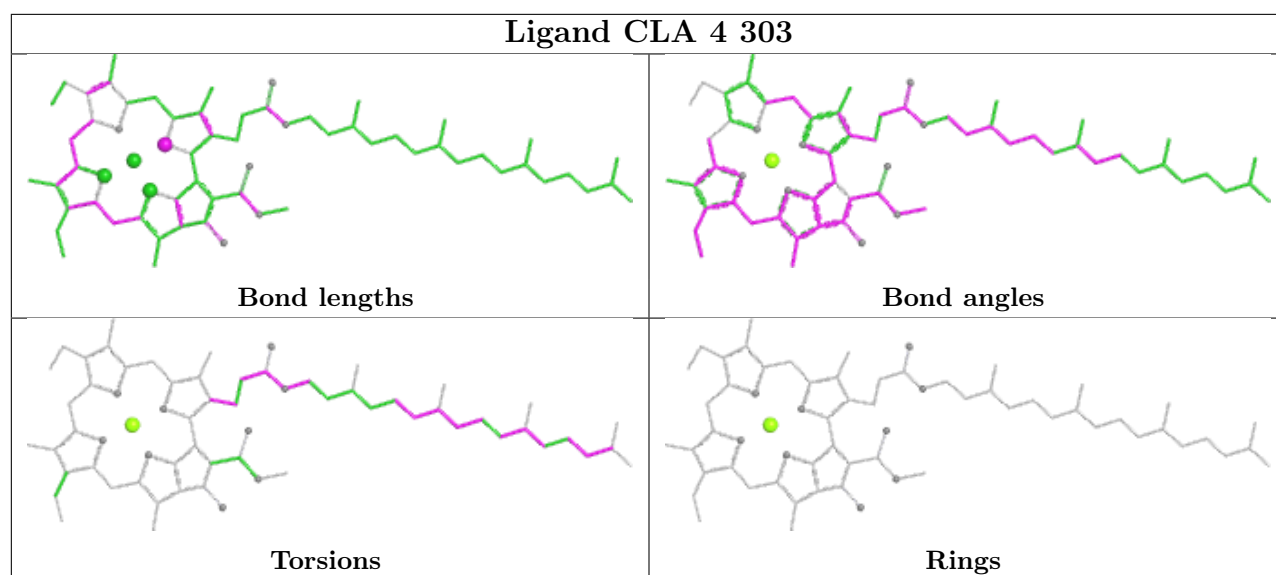
Bond angles

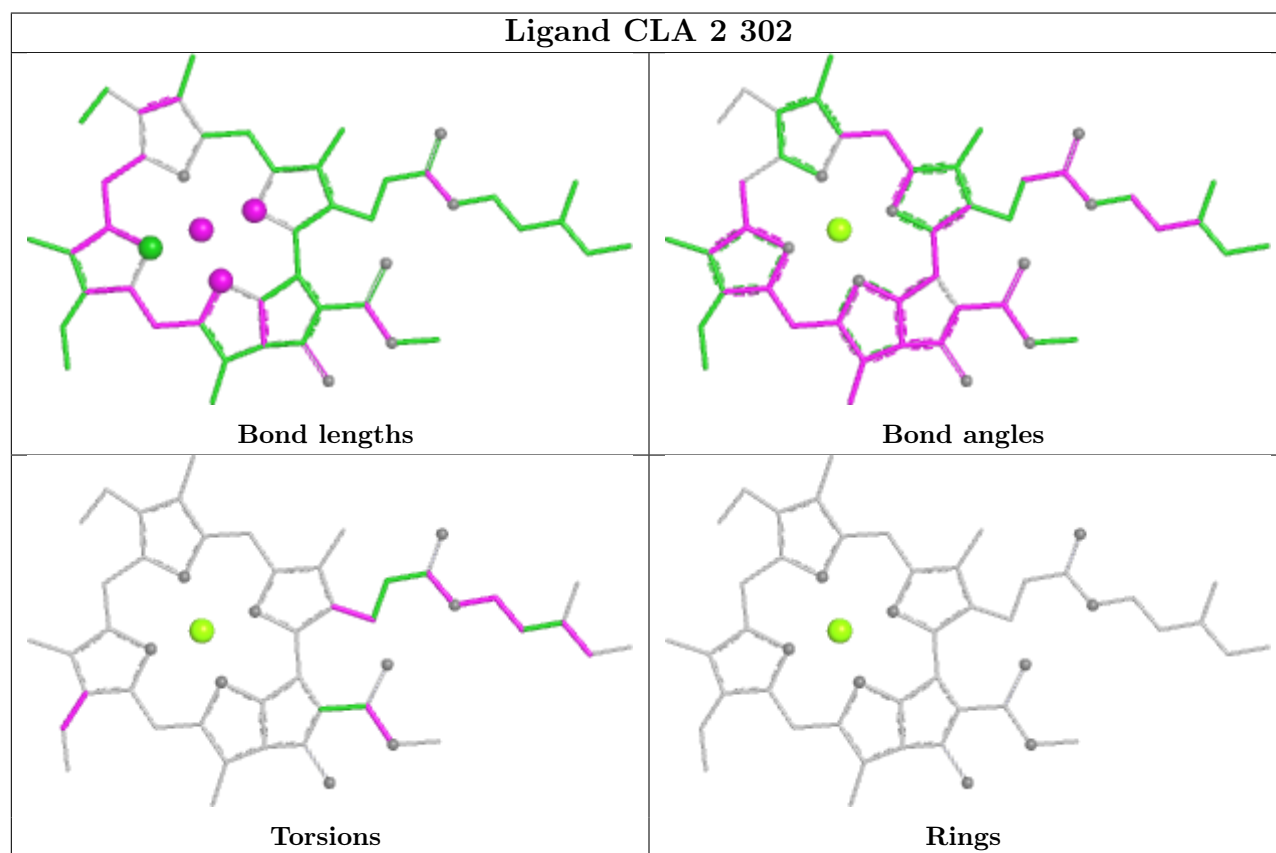
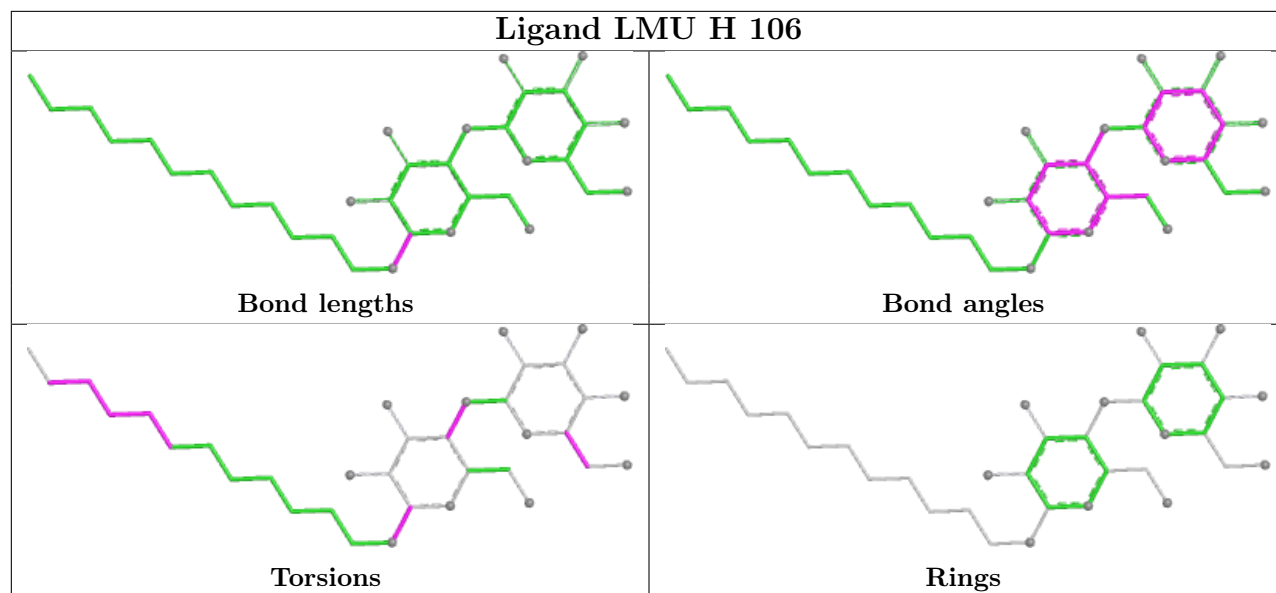


Torsions

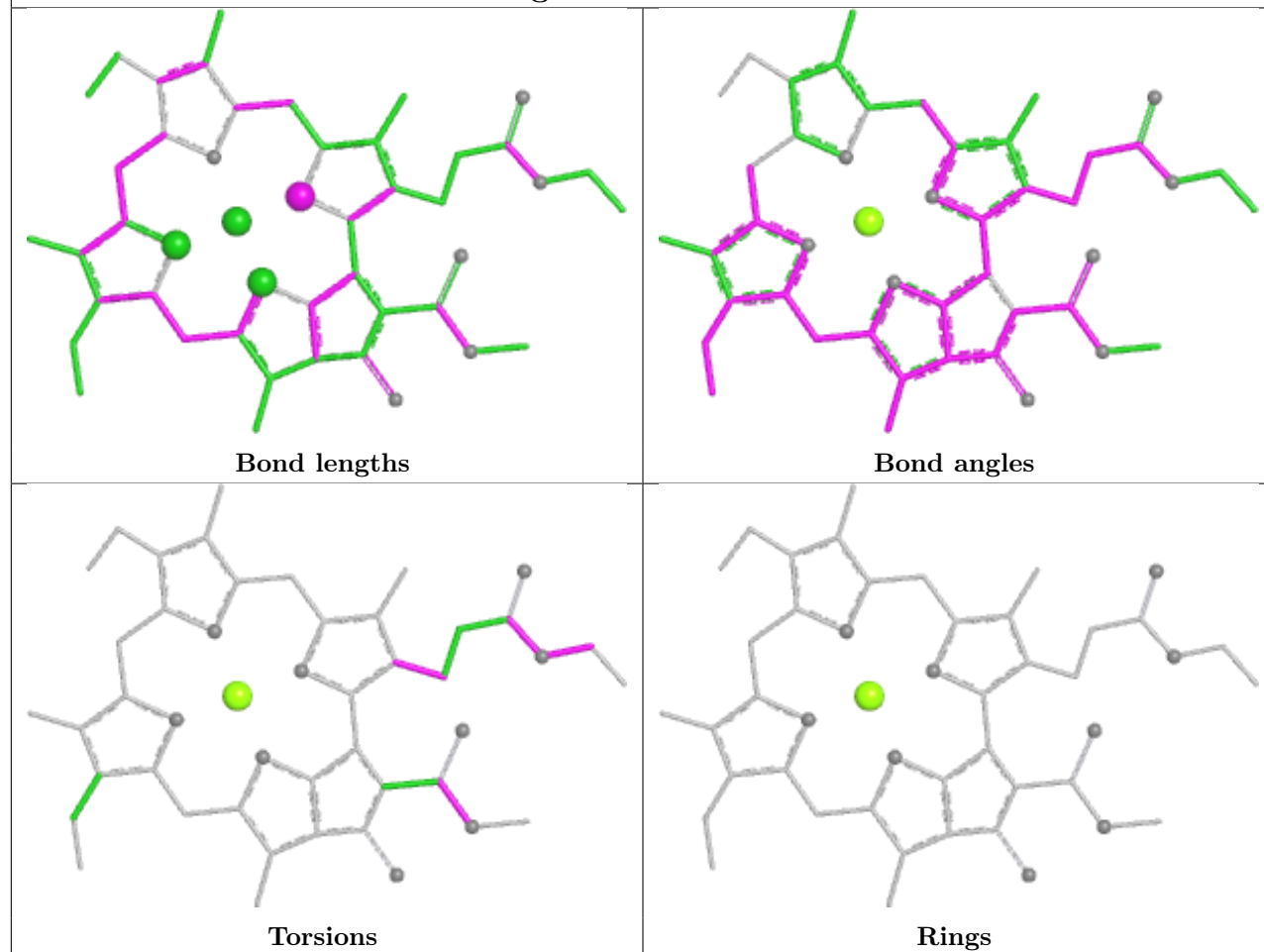


Rings

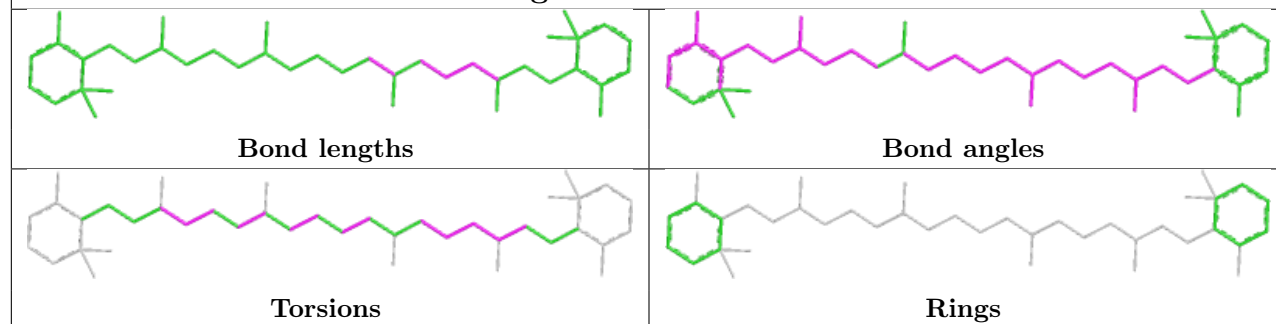




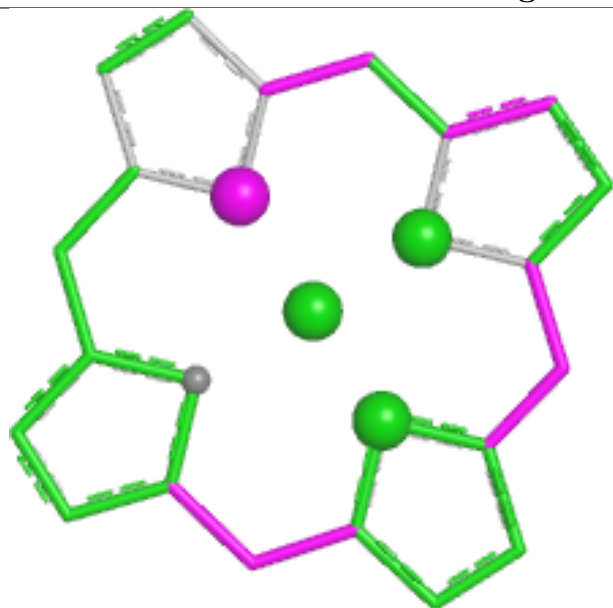
Ligand CLA 1 203



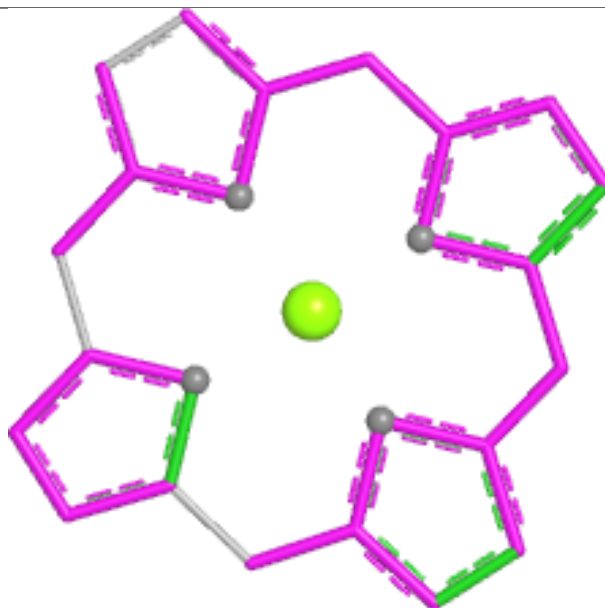
Ligand BCR B 801



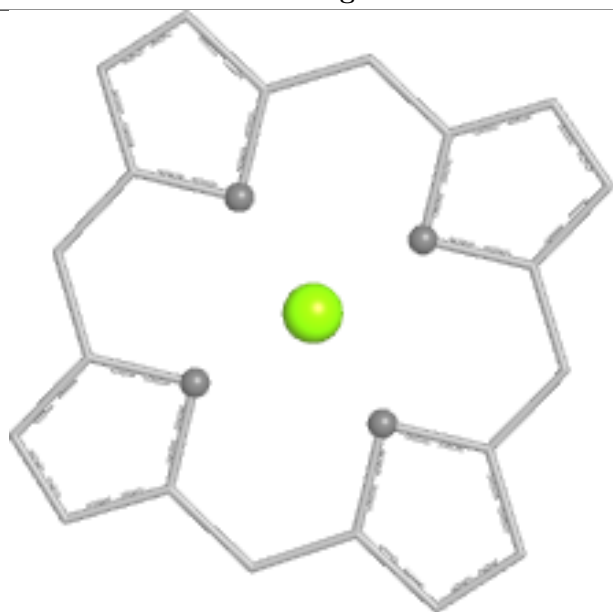
Ligand CLA 4 314



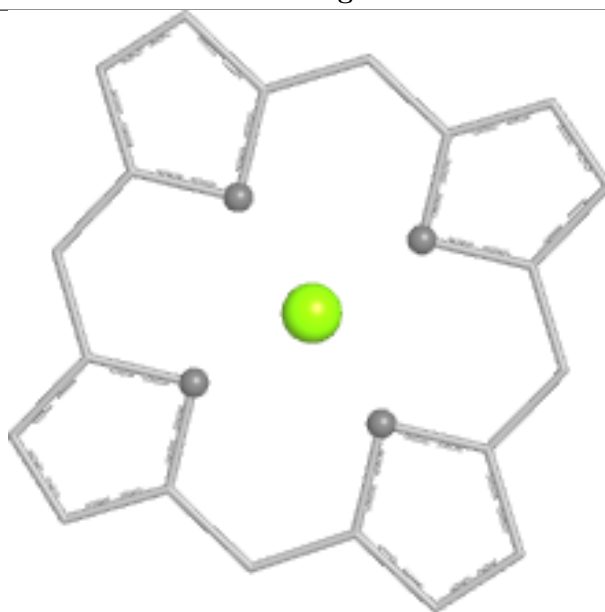
Bond lengths



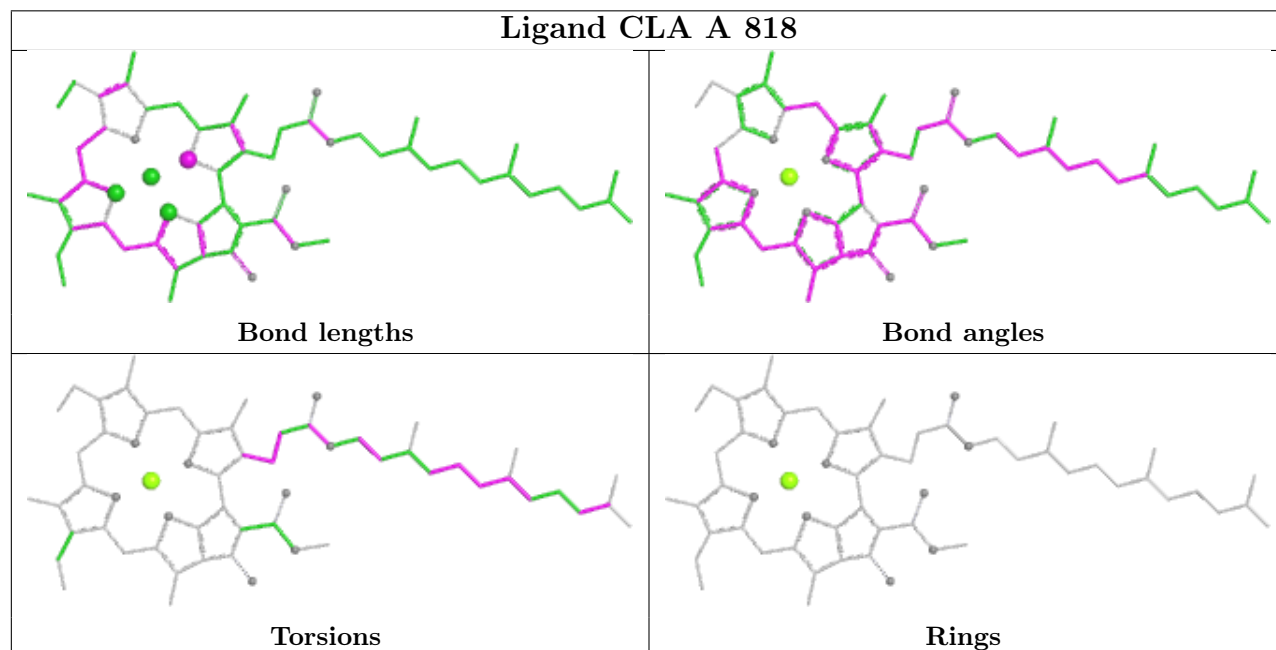
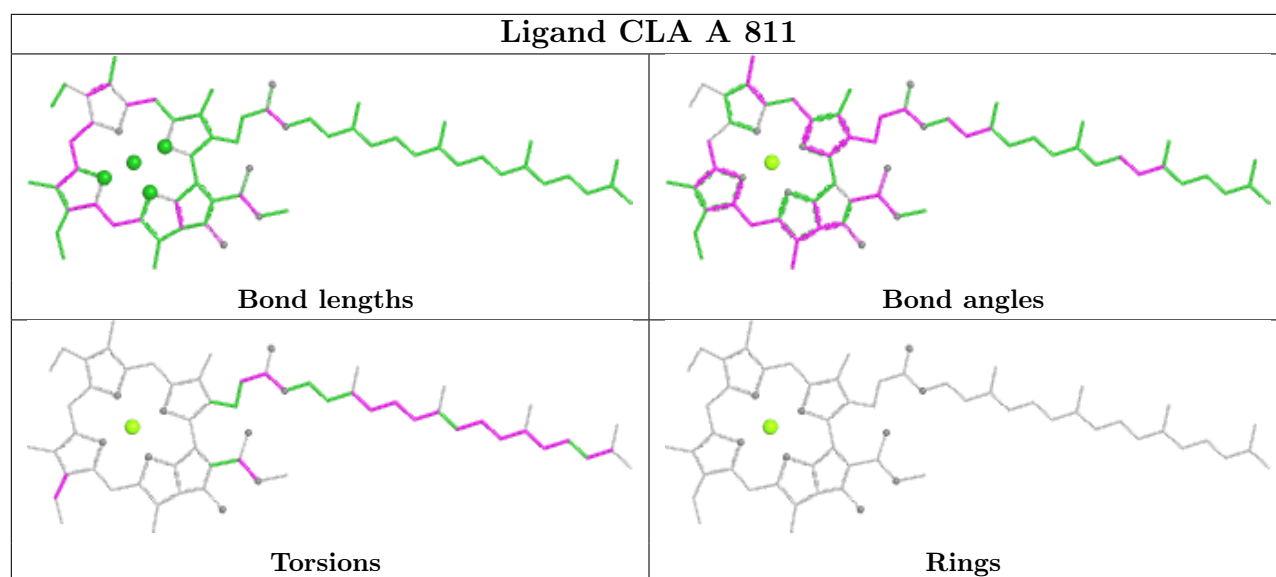
Bond angles

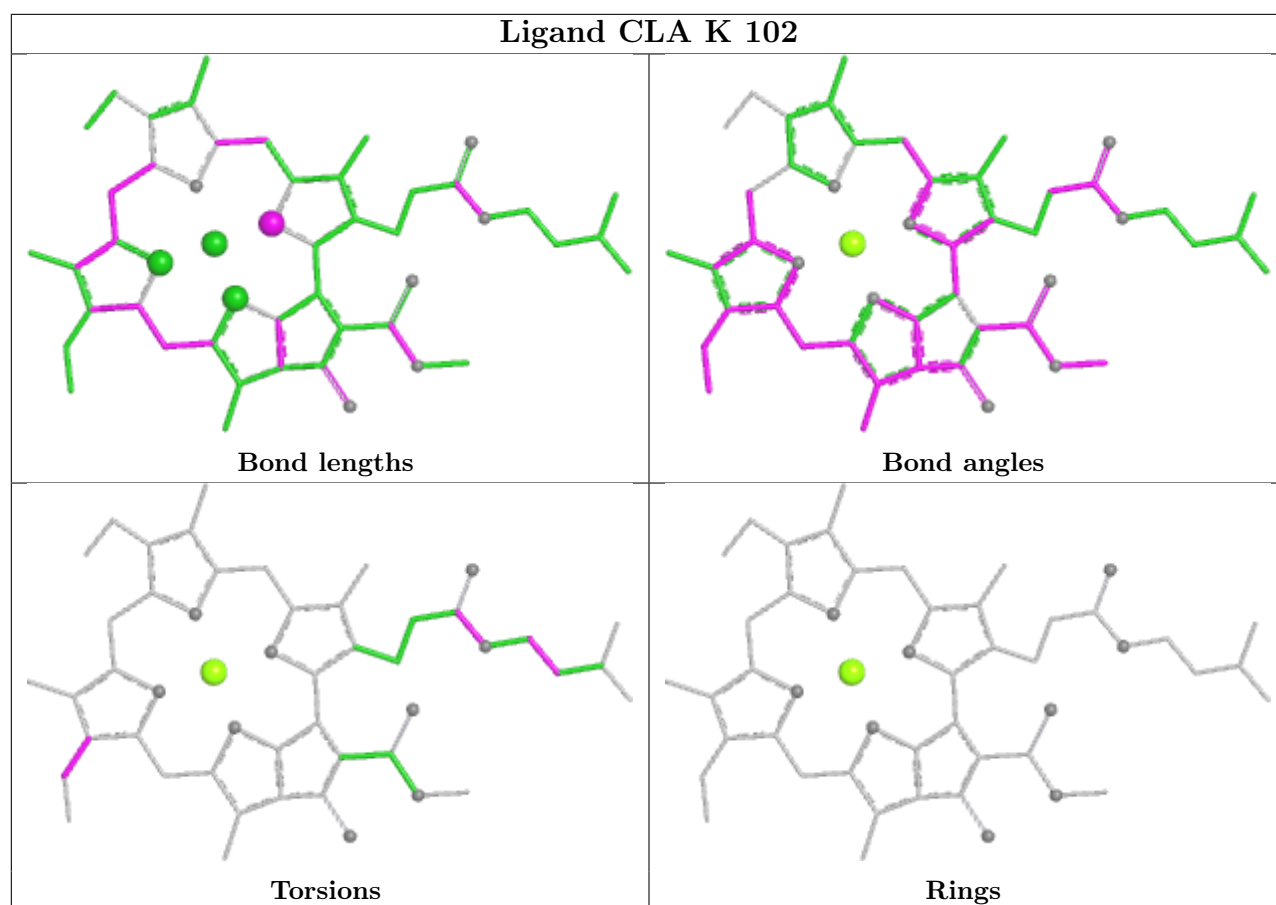


Torsions

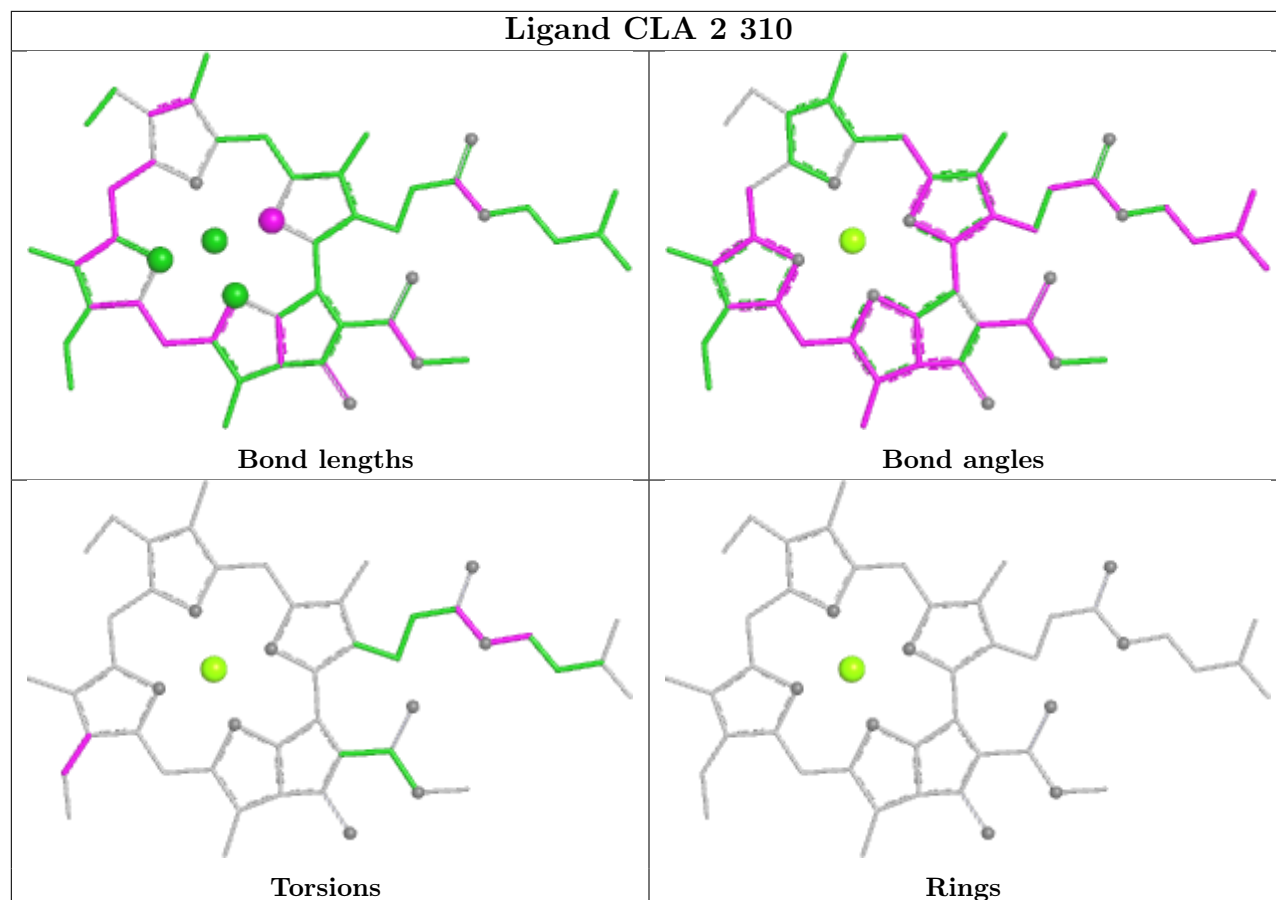


Rings

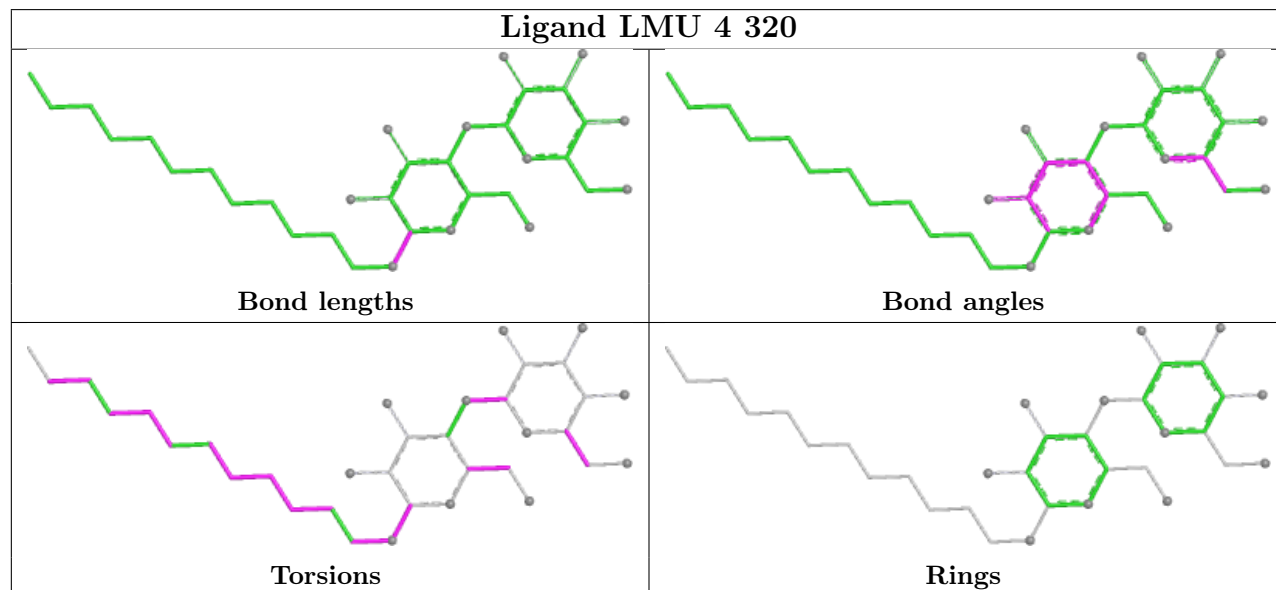


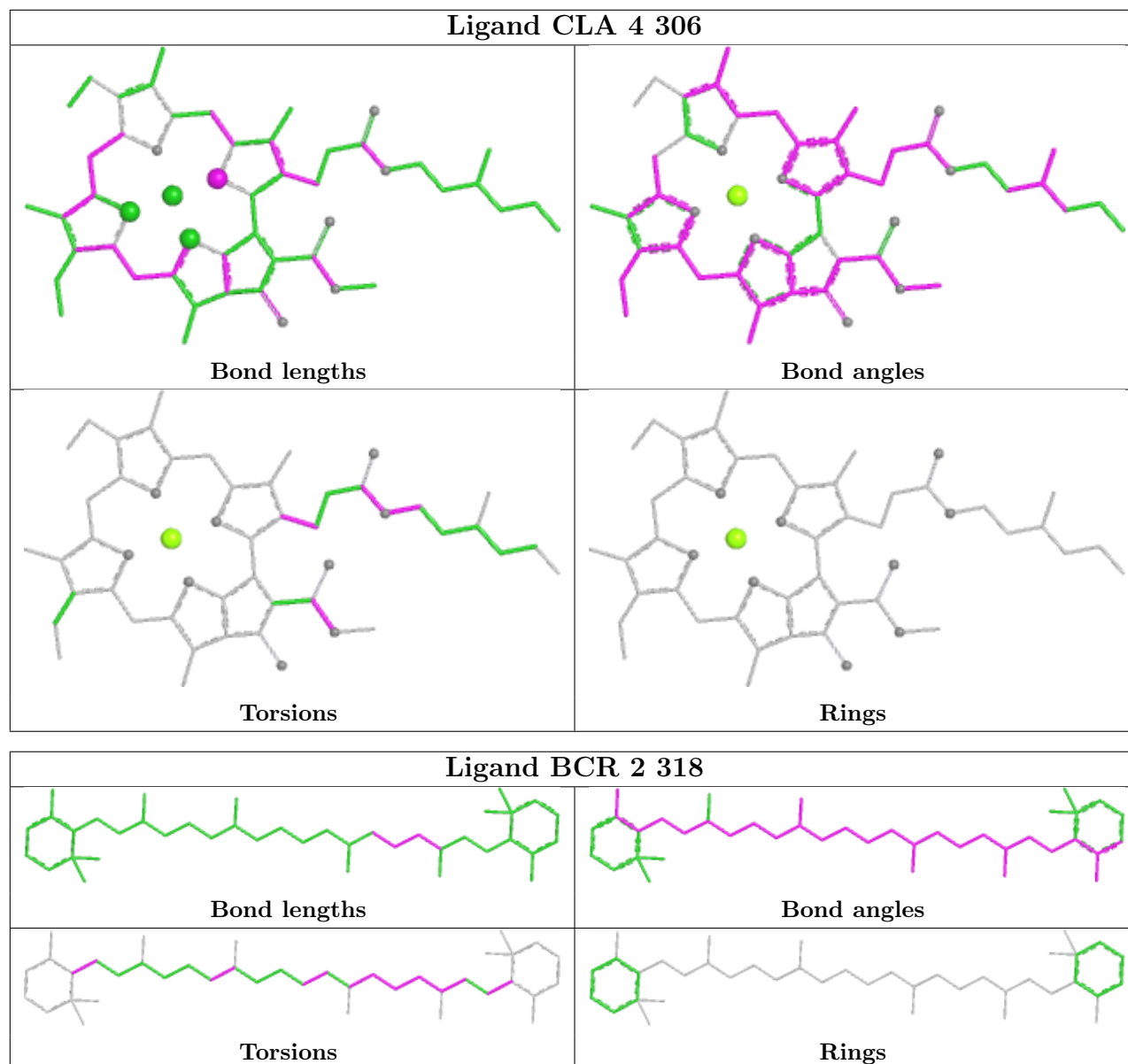


Ligand CLA 2 310

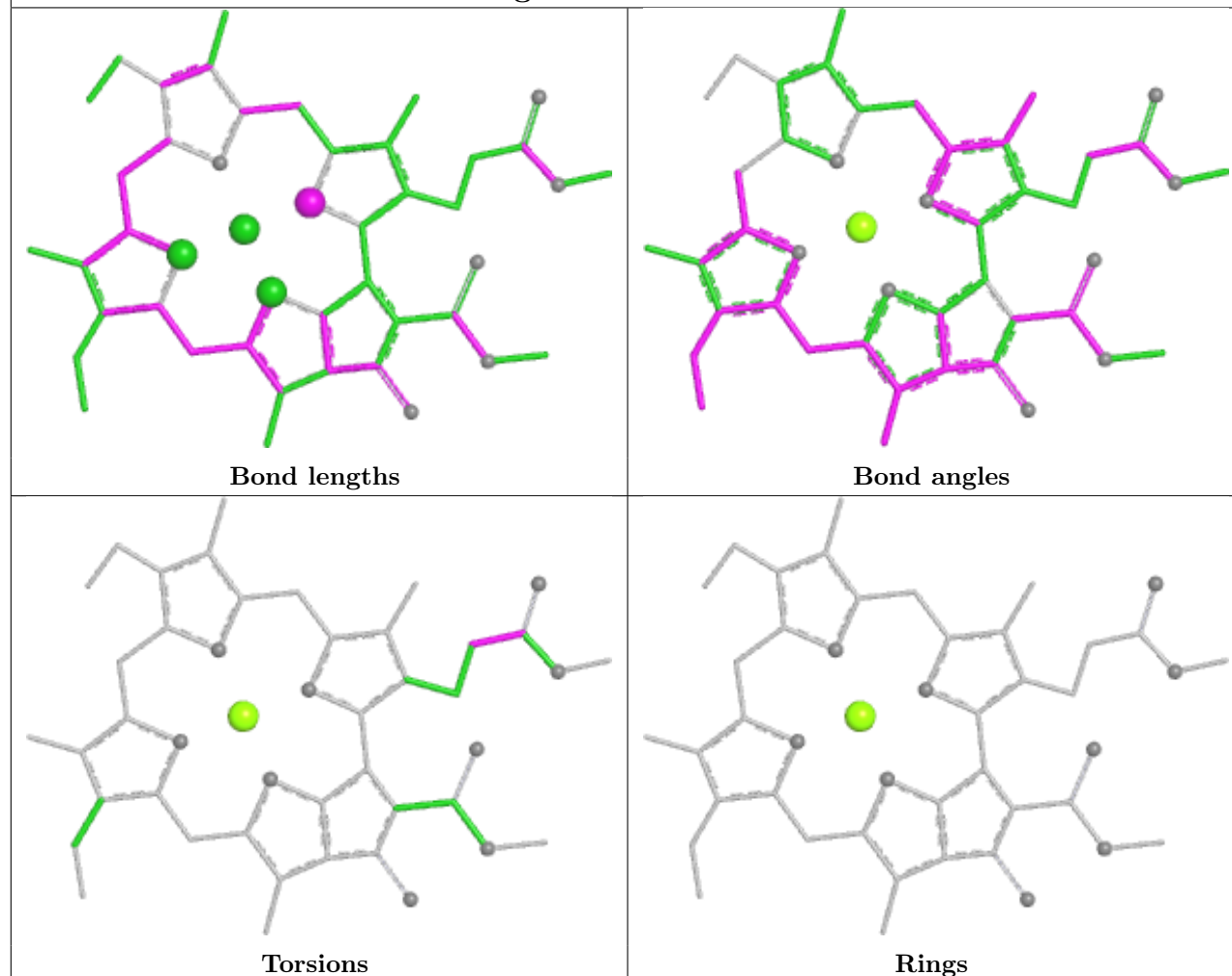


Ligand LMU 4 320

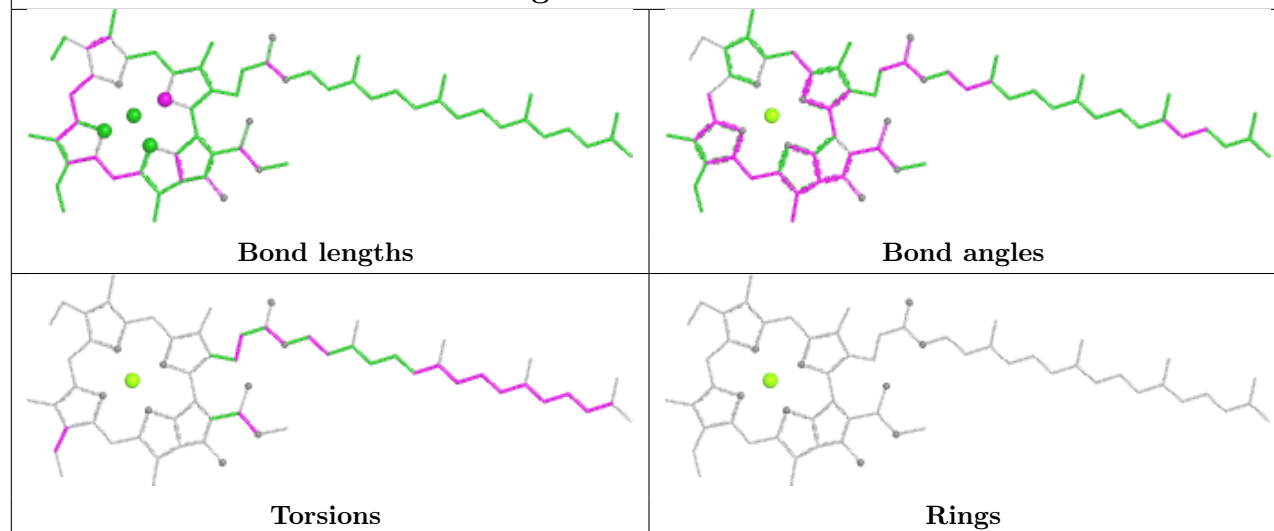




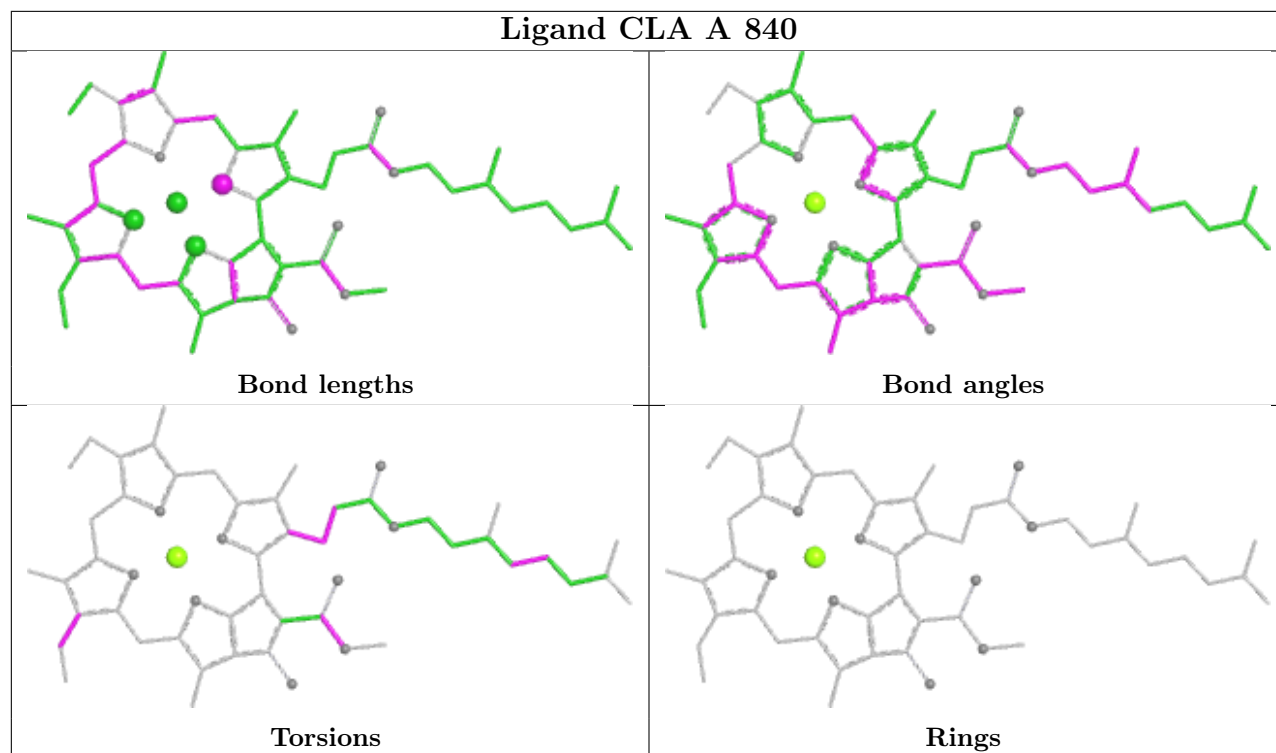
Ligand CLA A 803



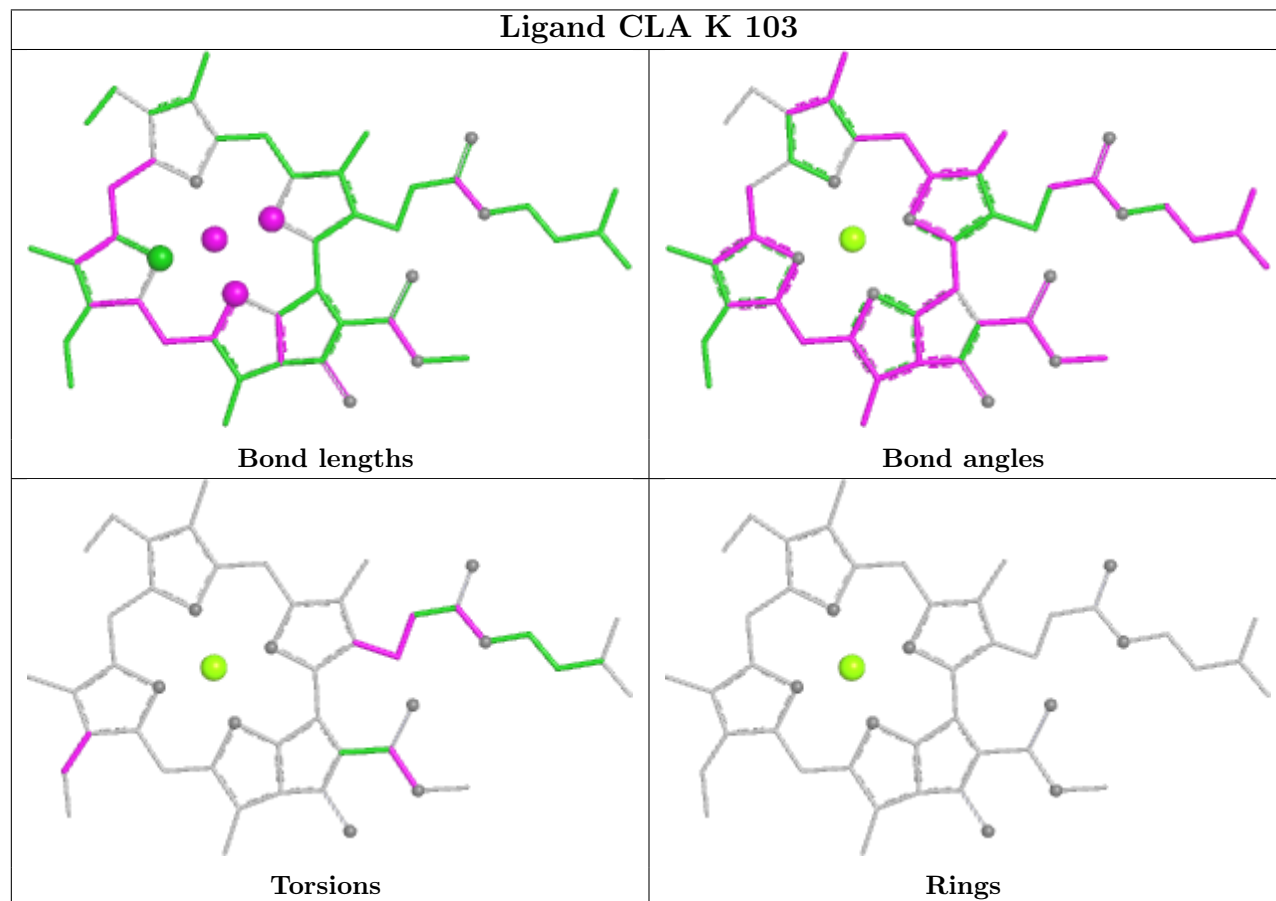
Ligand CLA A 851



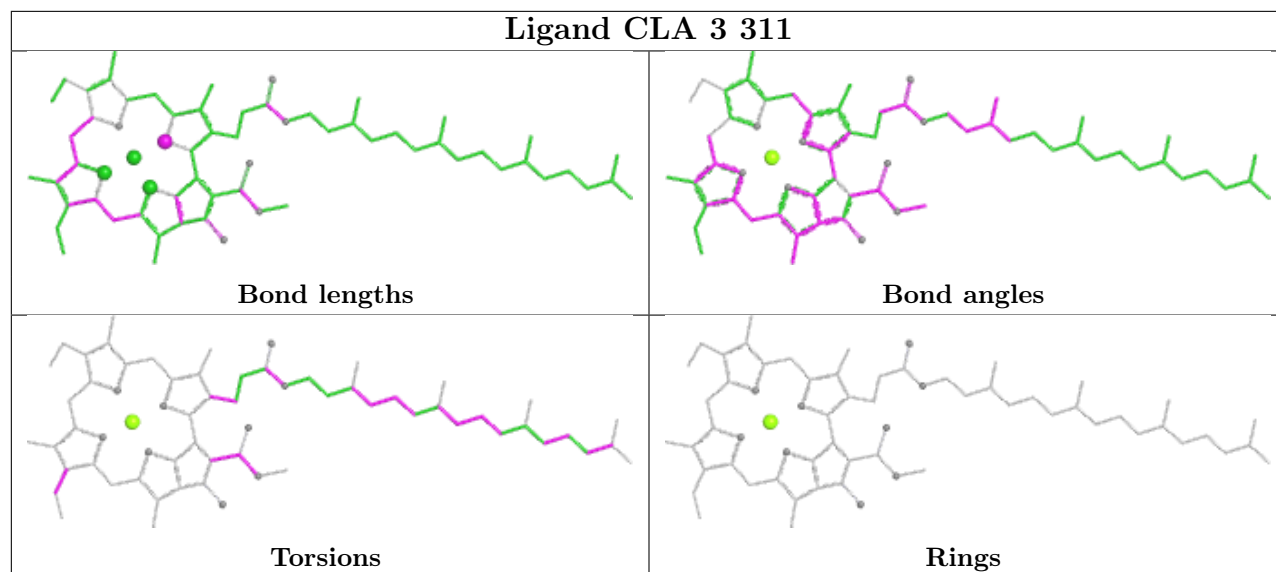
Ligand CLA A 840



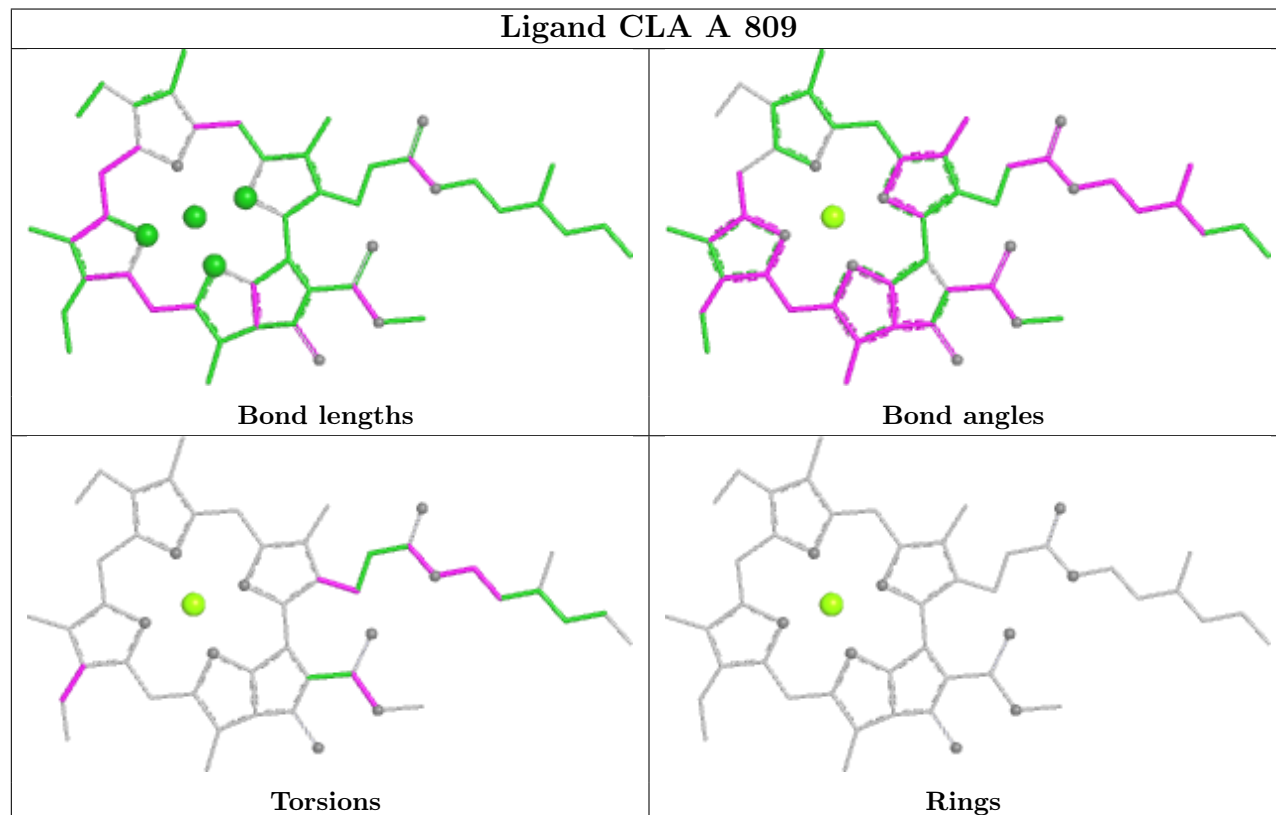
Ligand CLA K 103



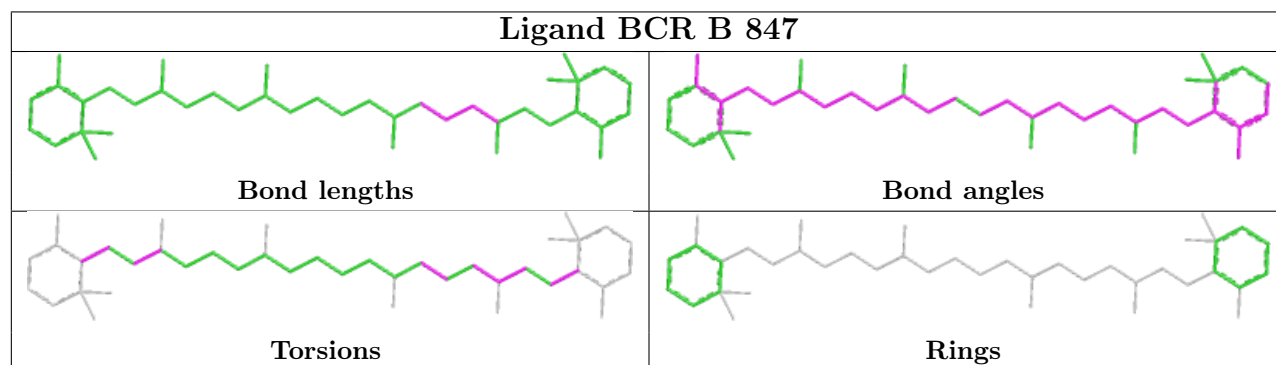
Ligand CLA 3 311

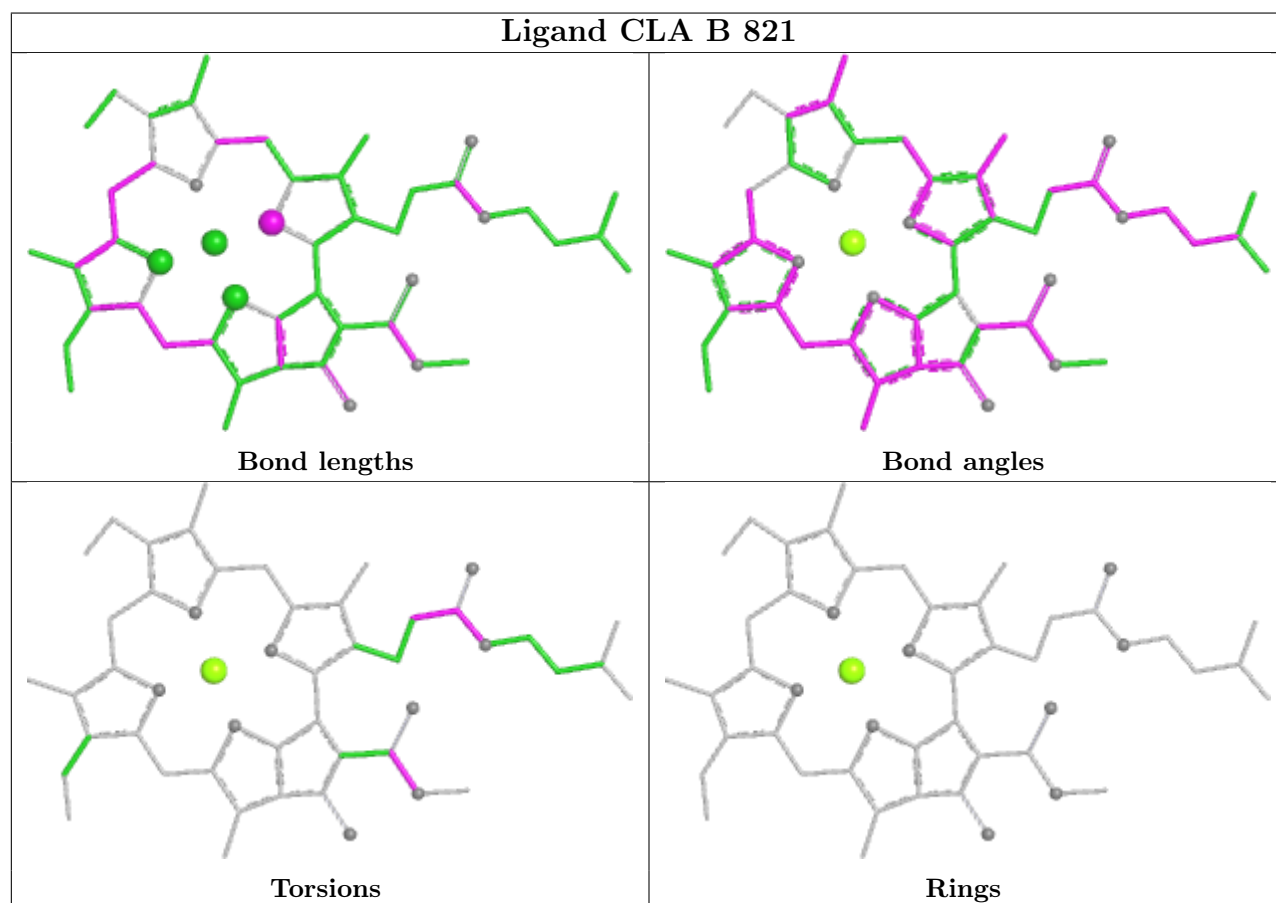
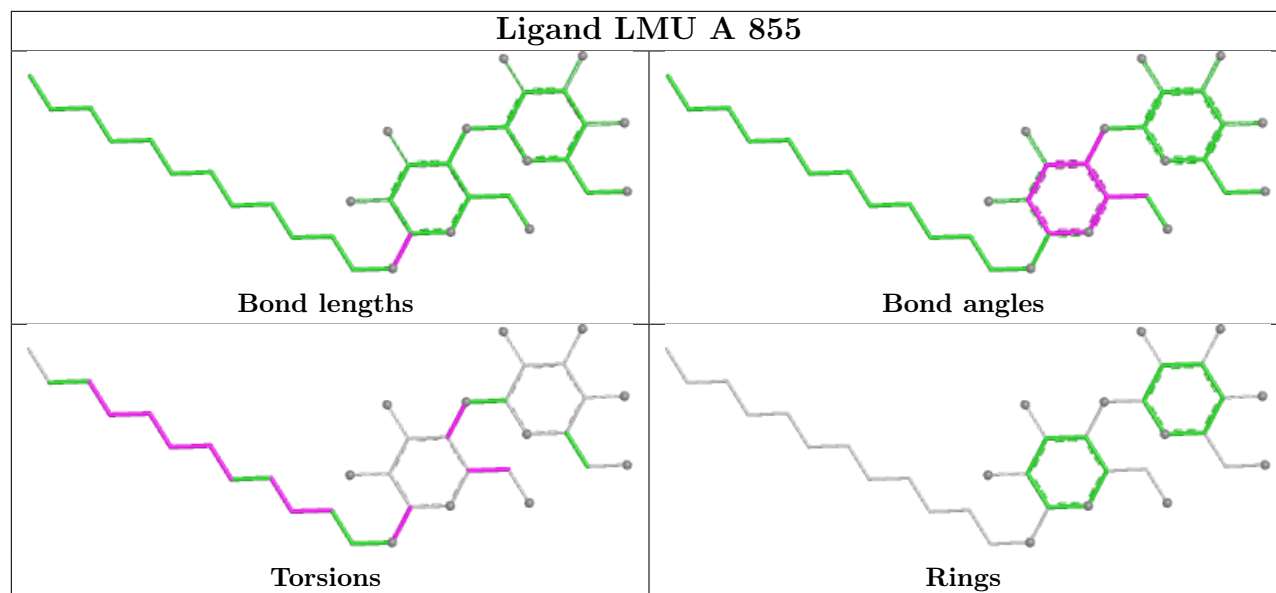


Ligand CLA A 809

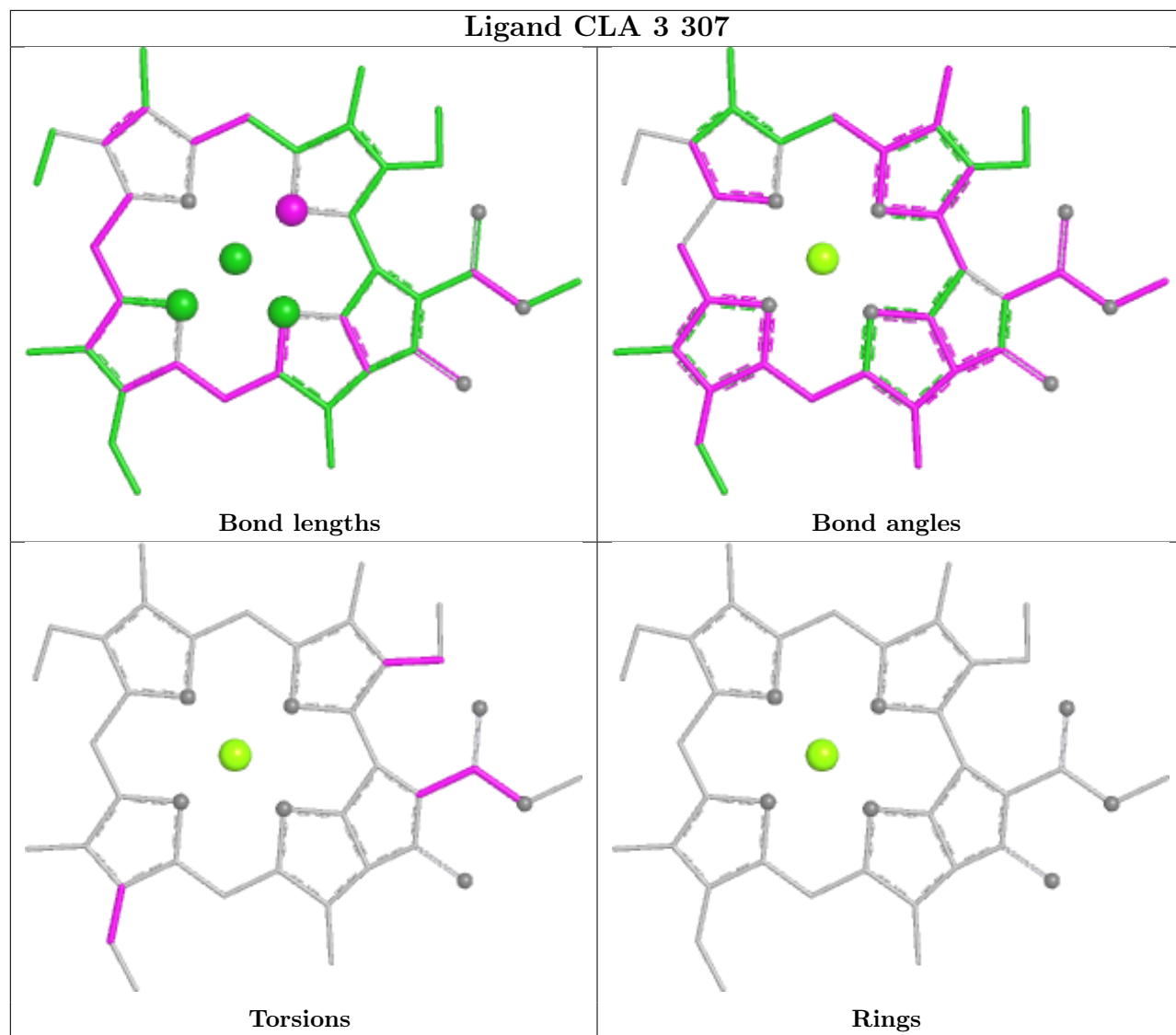


Ligand BCR B 847

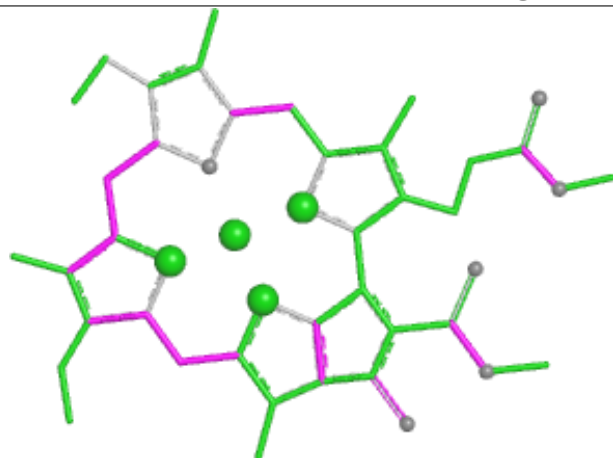




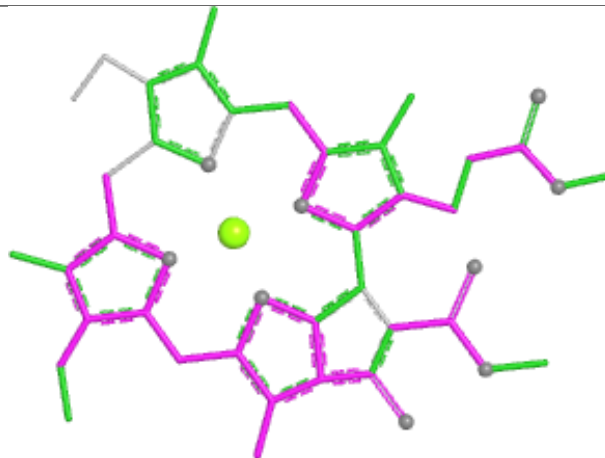
Ligand CLA 3 307



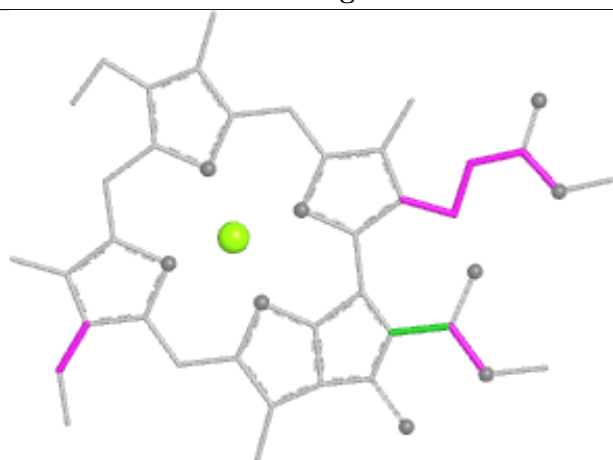
Ligand CLA B 817



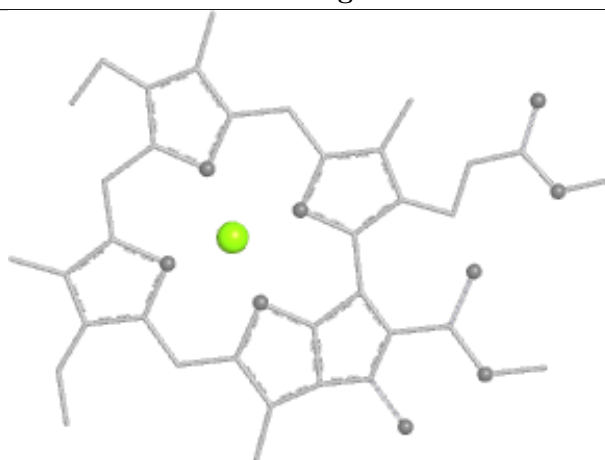
Bond lengths



Bond angles

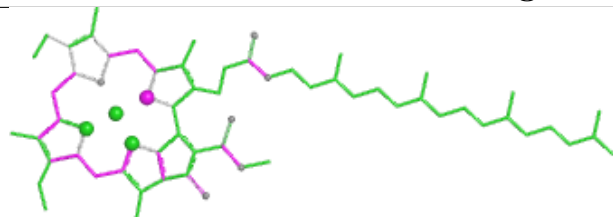


Torsions

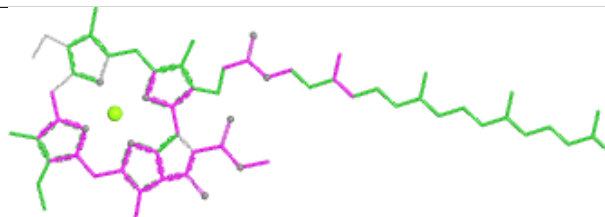


Rings

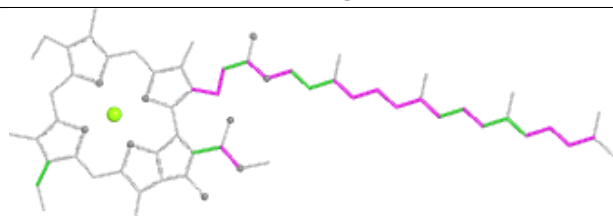
Ligand CLA 2 307



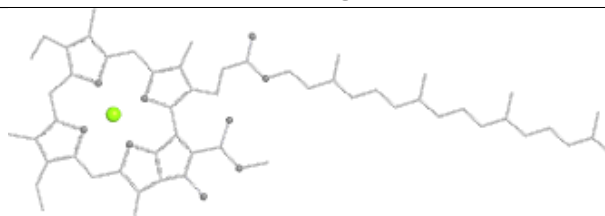
Bond lengths



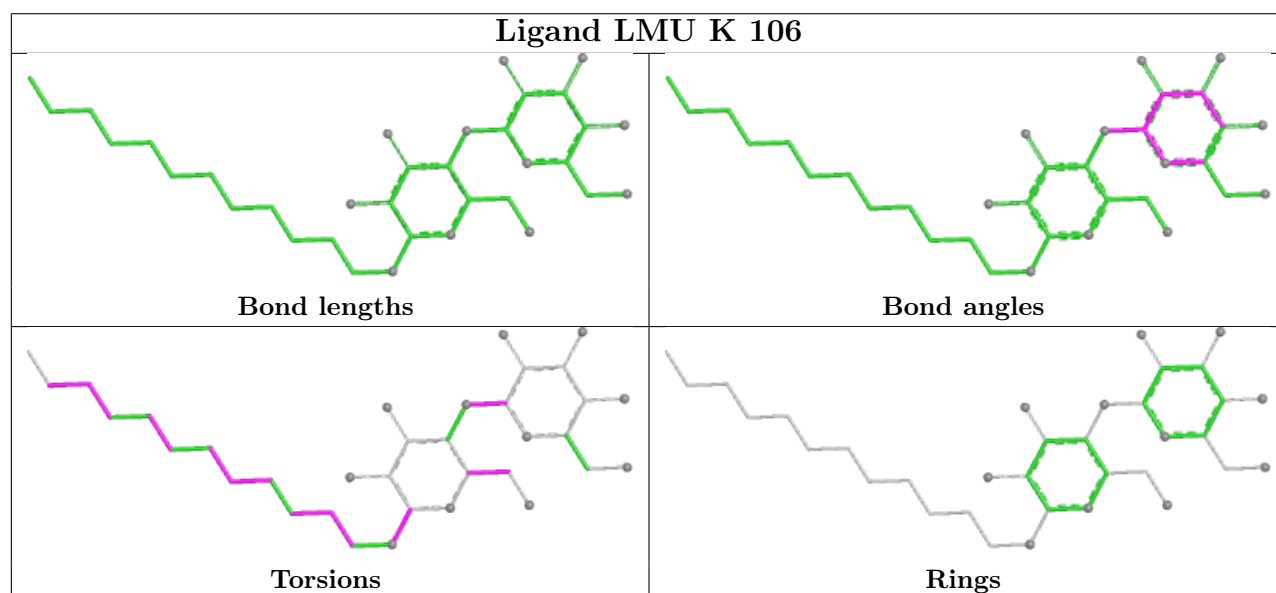
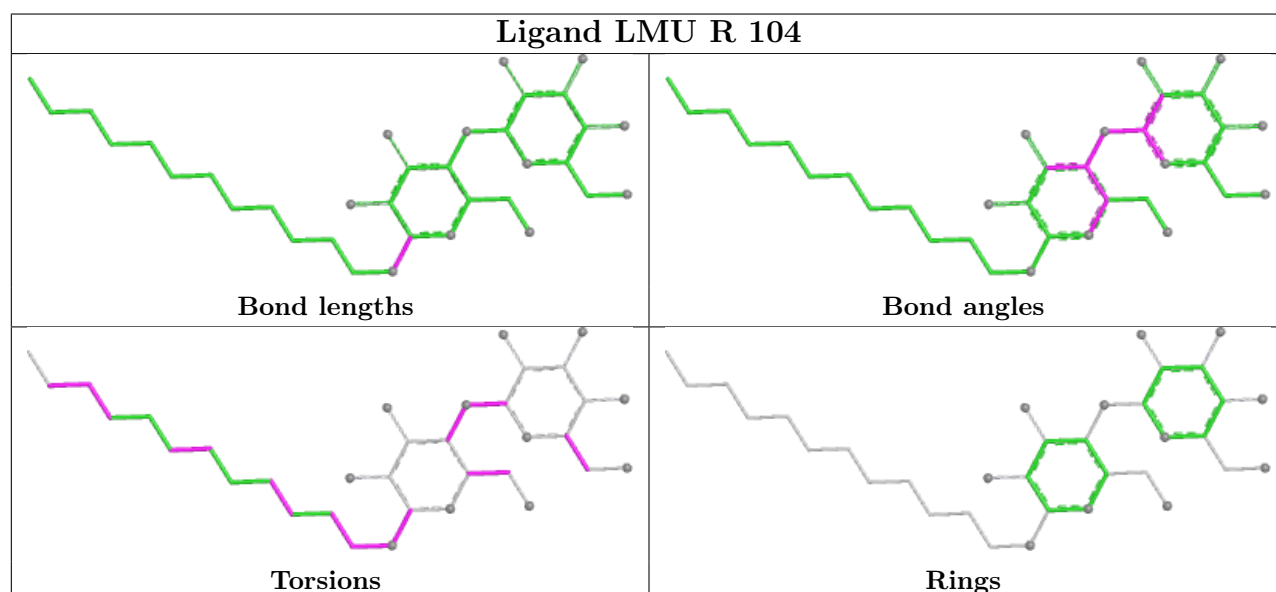
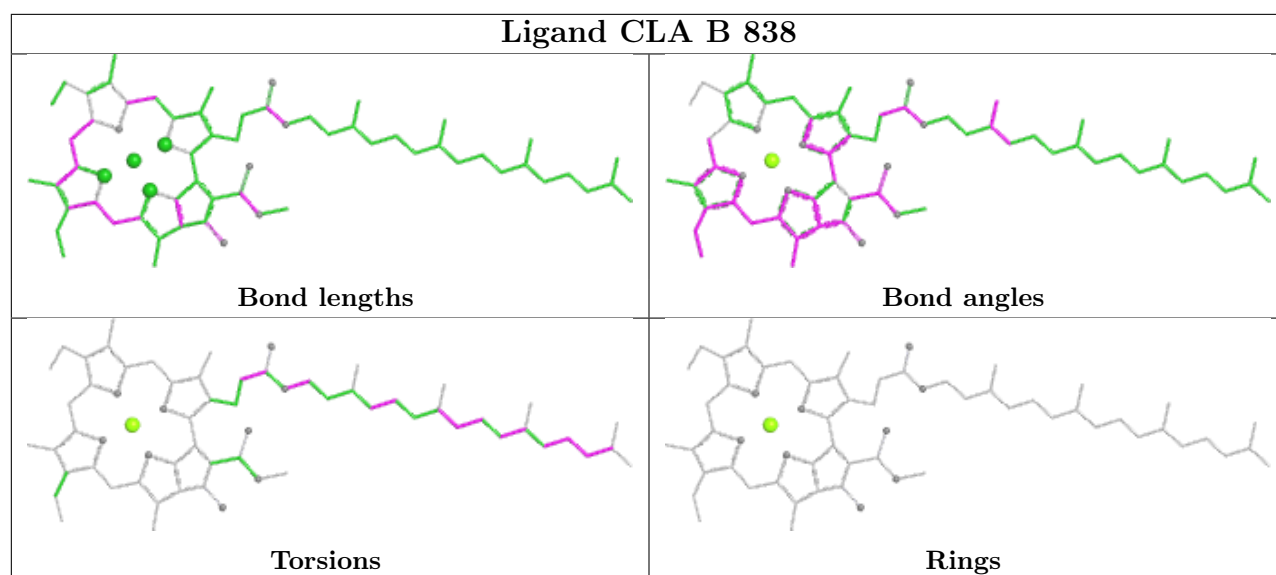
Bond angles

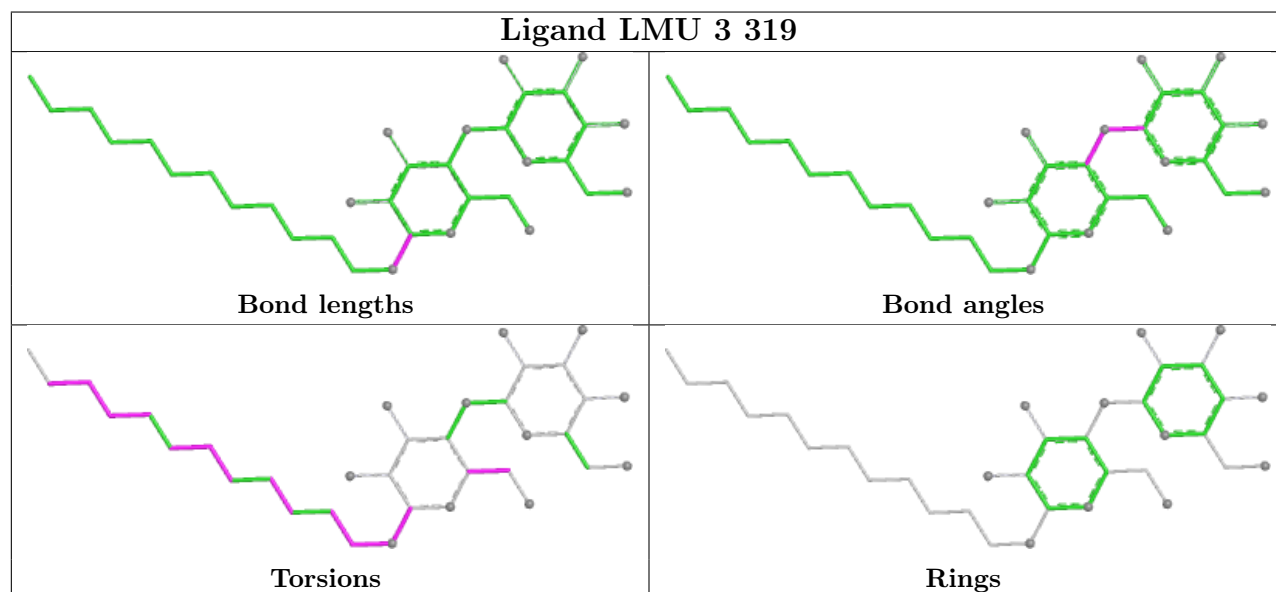
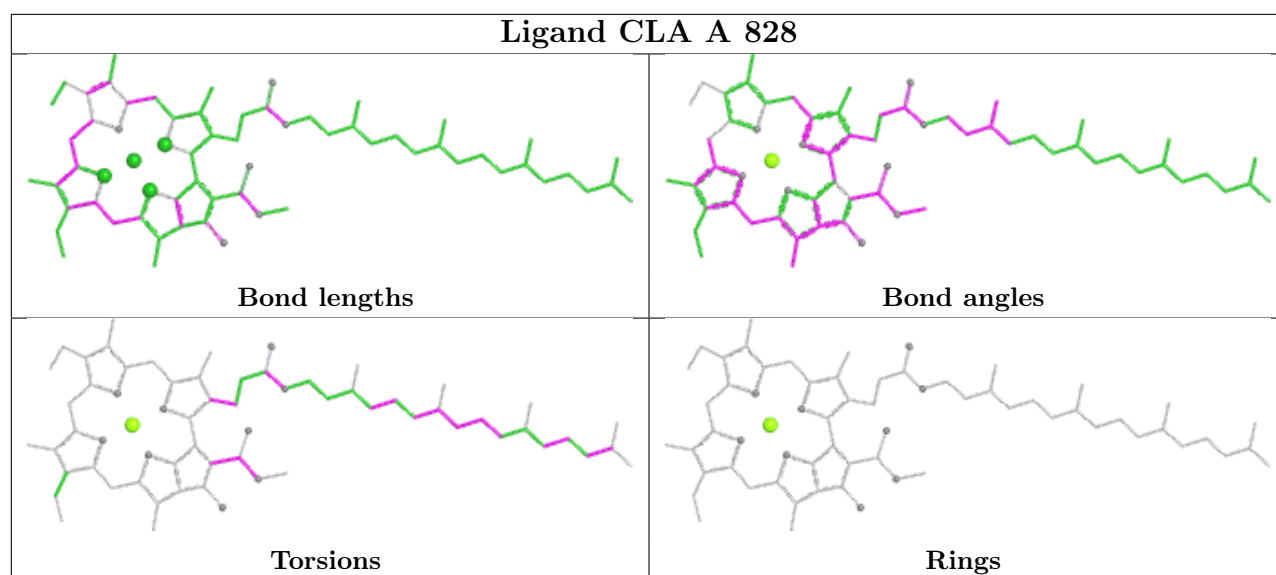


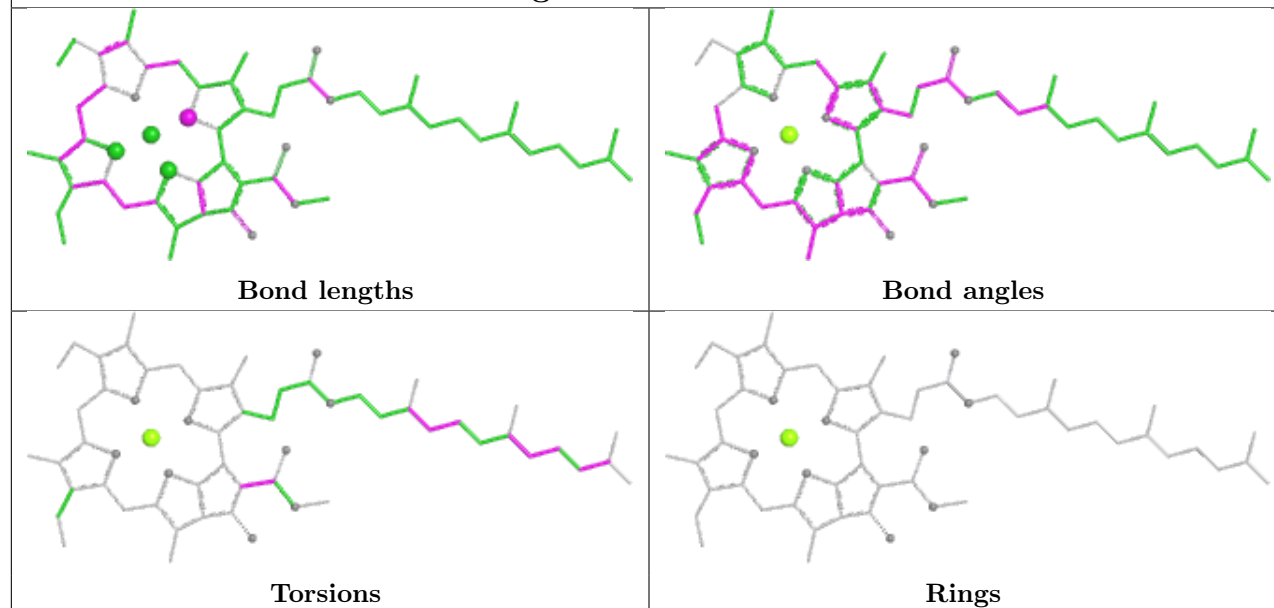
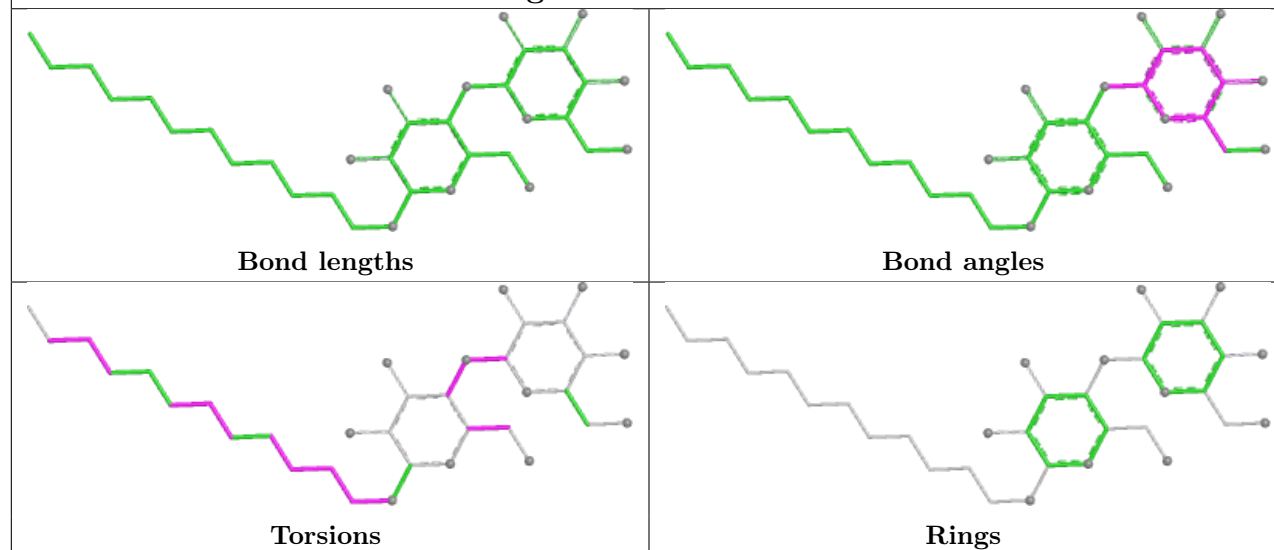
Torsions



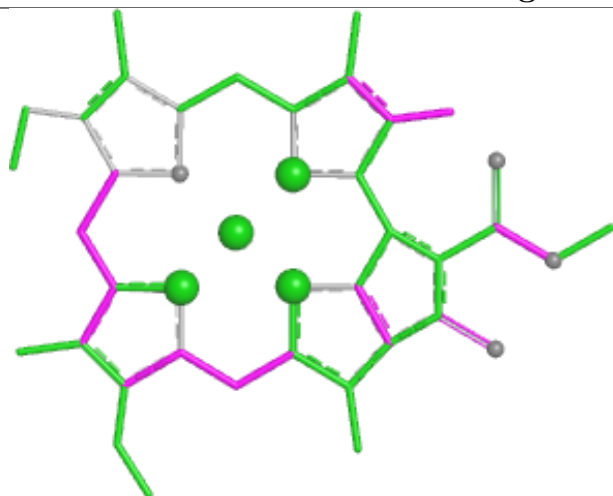
Rings



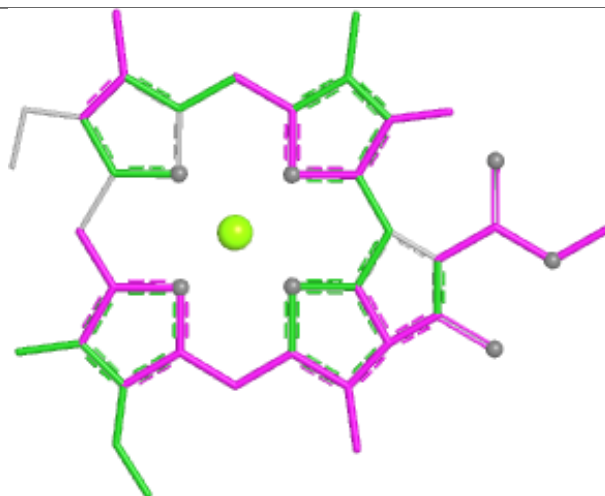


Ligand CLA B 810**Ligand LMU G 102**

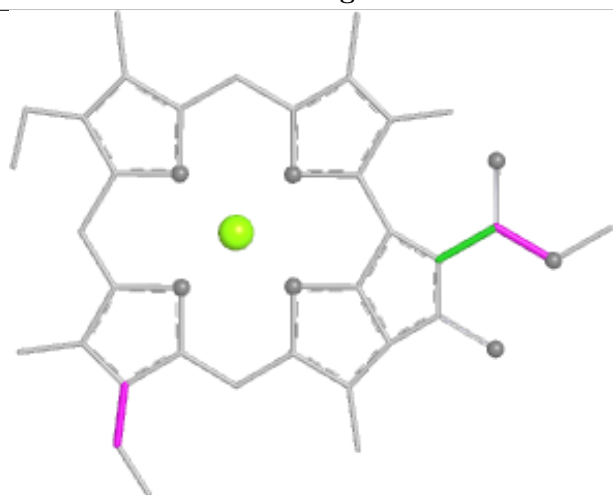
Ligand CLA 1 202



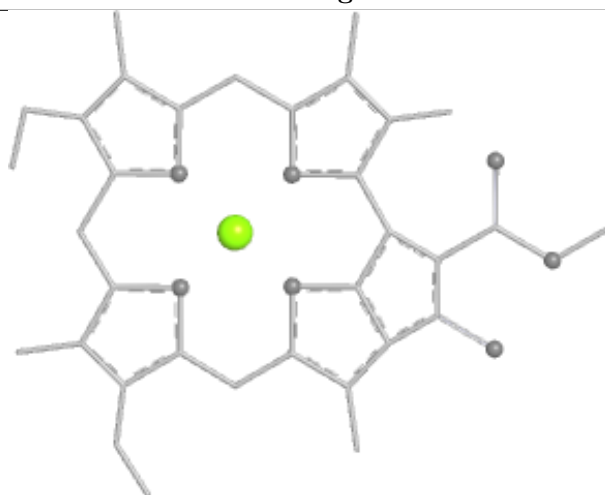
Bond lengths



Bond angles

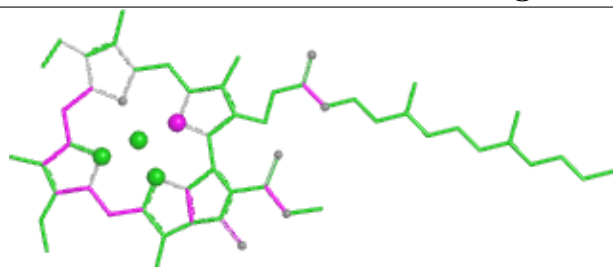


Torsions

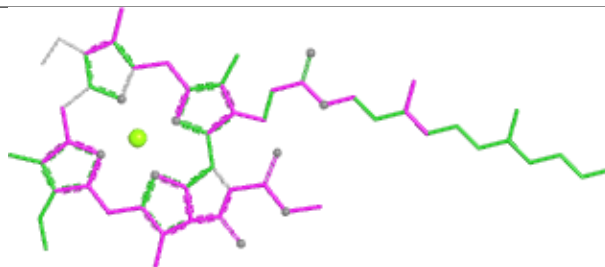


Rings

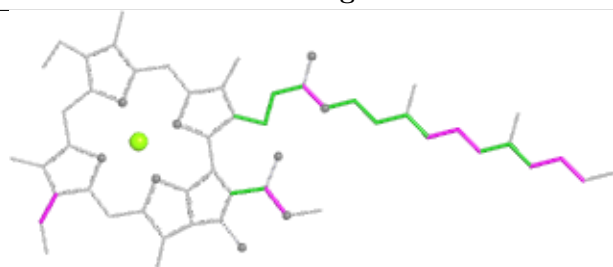
Ligand CLA A 819



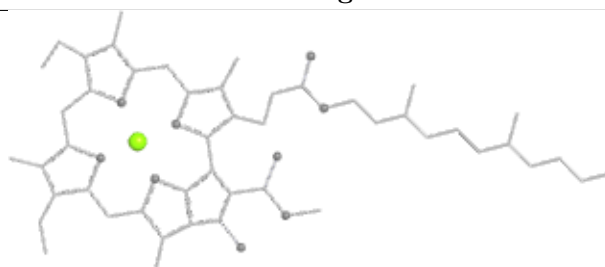
Bond lengths



Bond angles

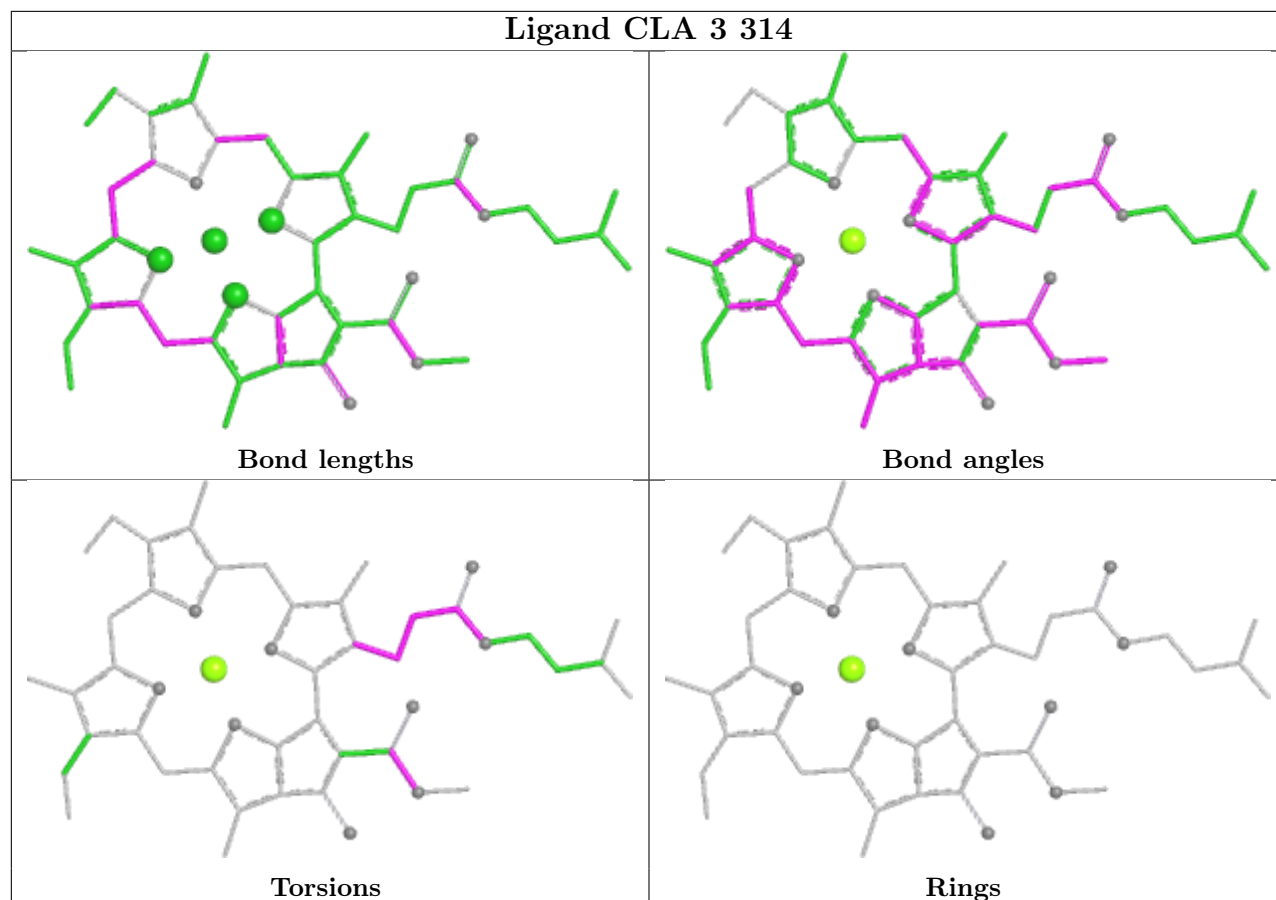


Torsions

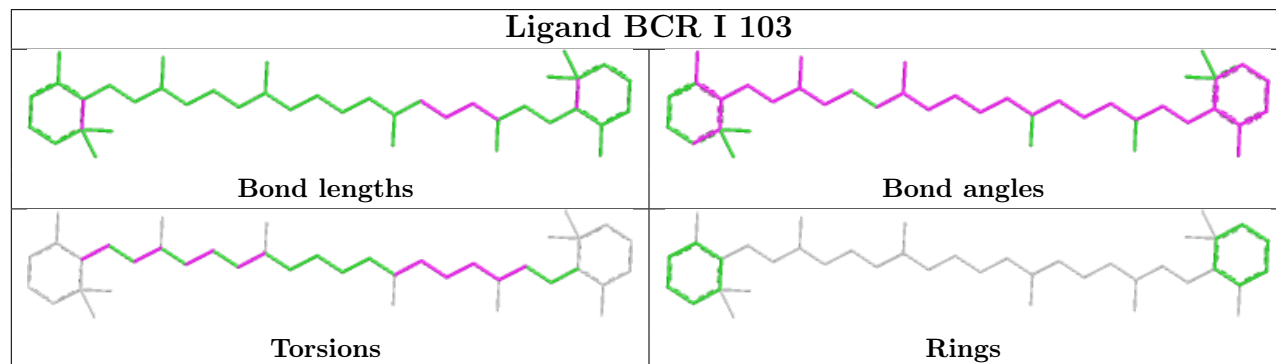


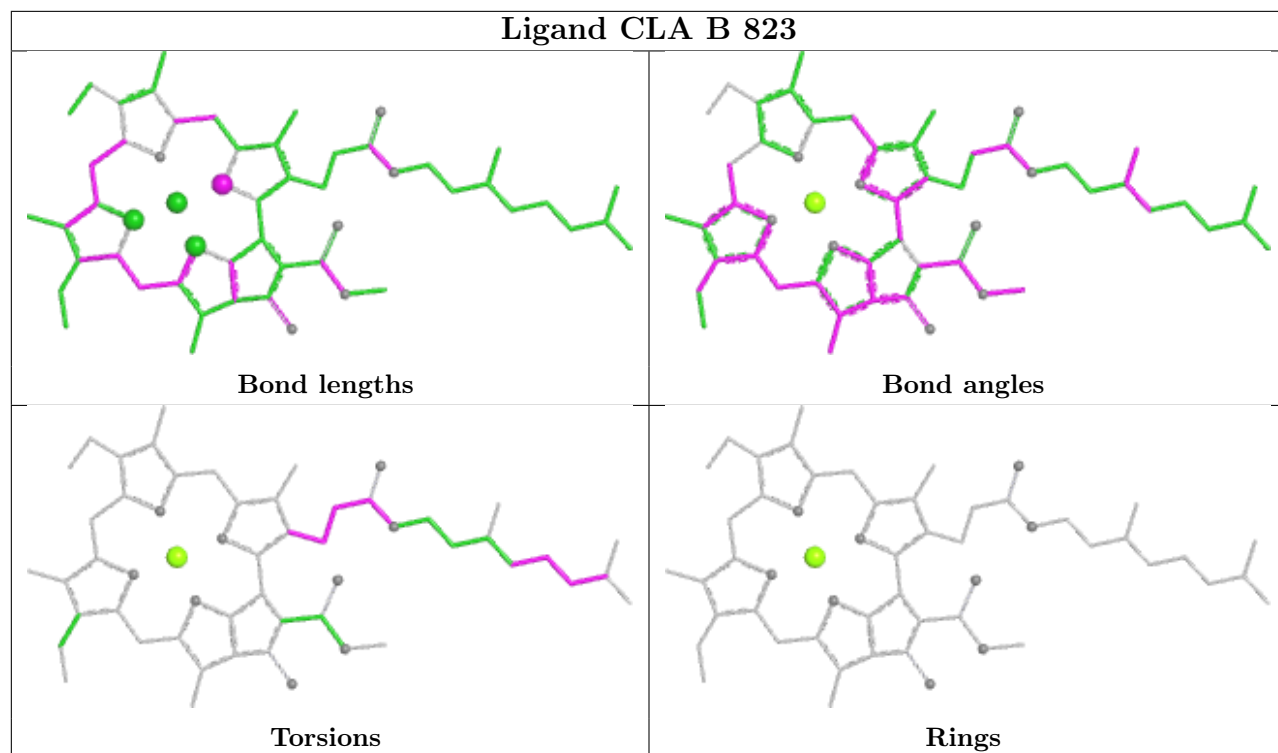
Rings

Ligand CLA 3 314

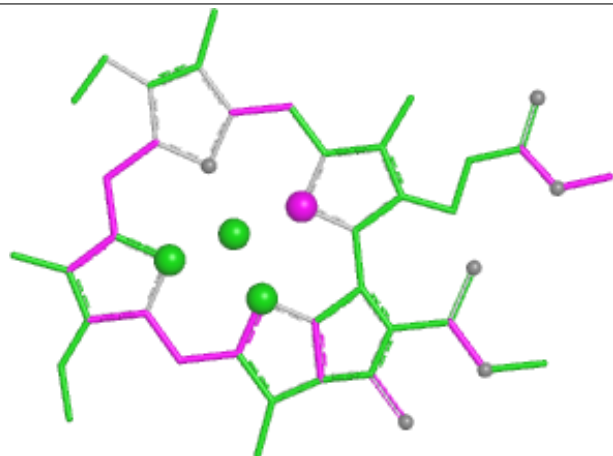


Ligand BCR I 103

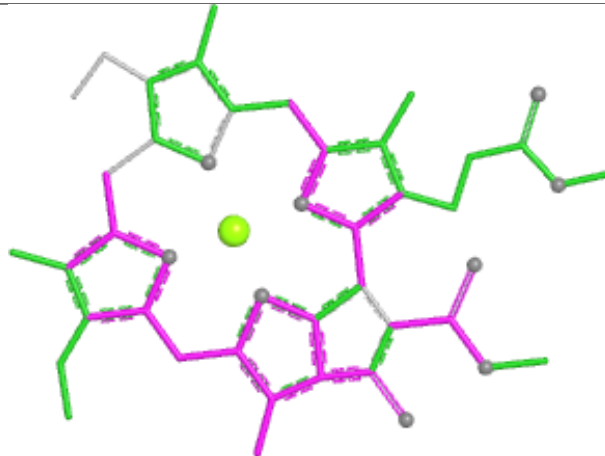




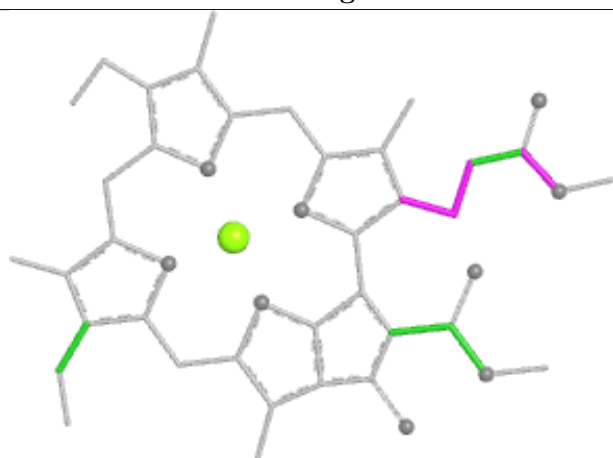
Ligand CLA K 101



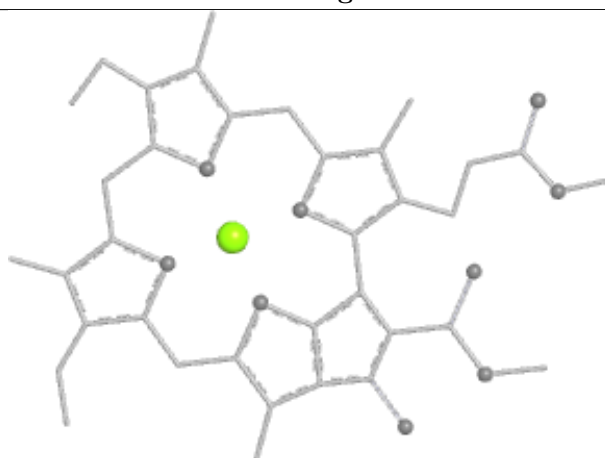
Bond lengths



Bond angles

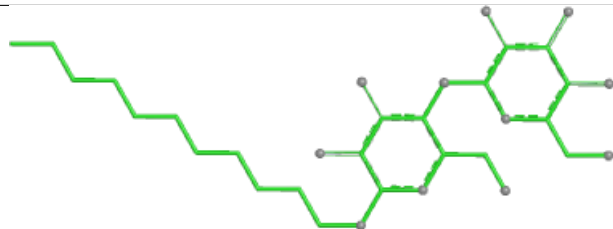


Torsions

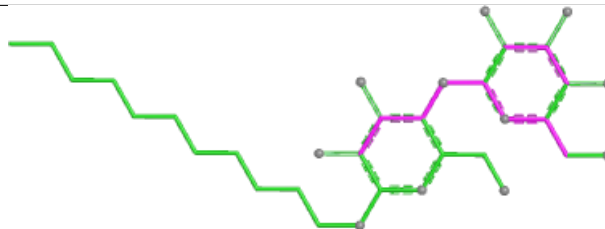


Rings

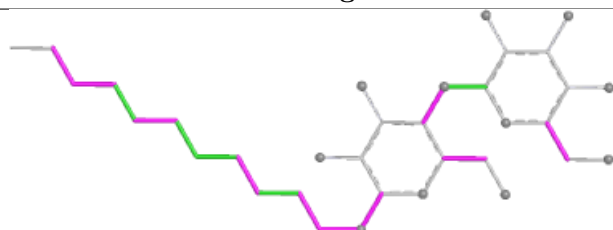
Ligand LMU F 202



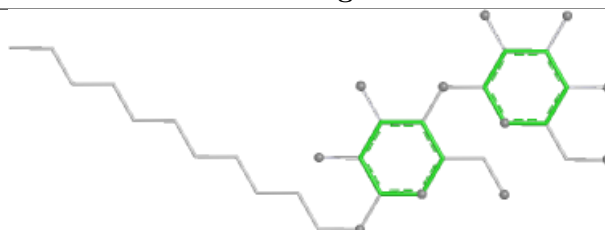
Bond lengths



Bond angles

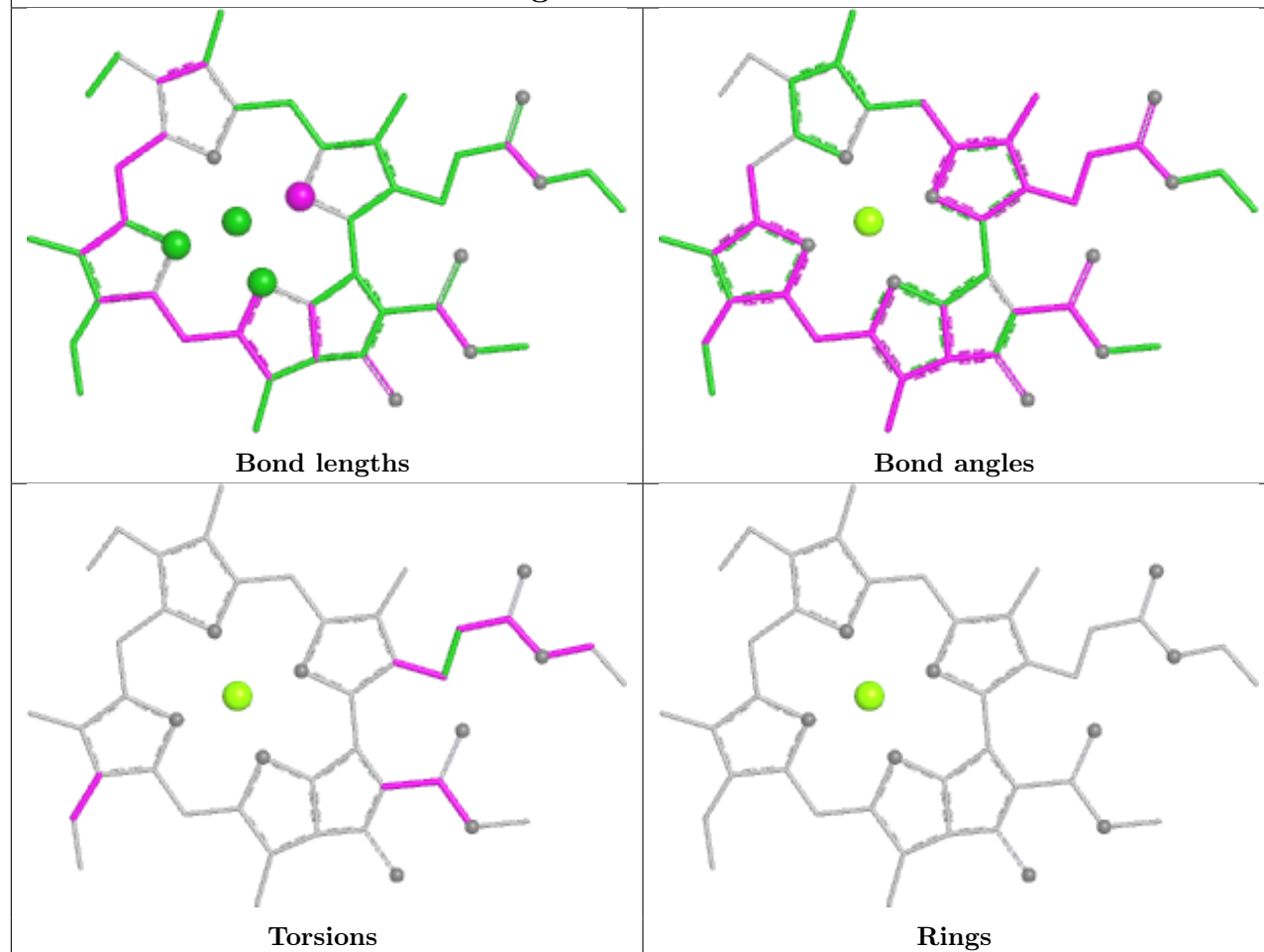


Torsions

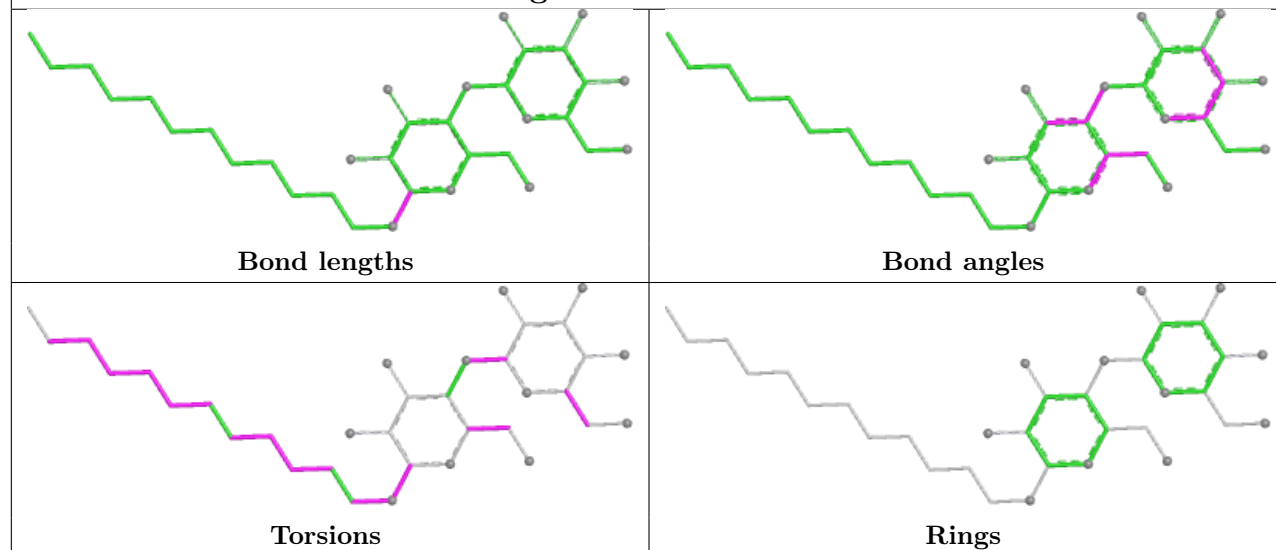


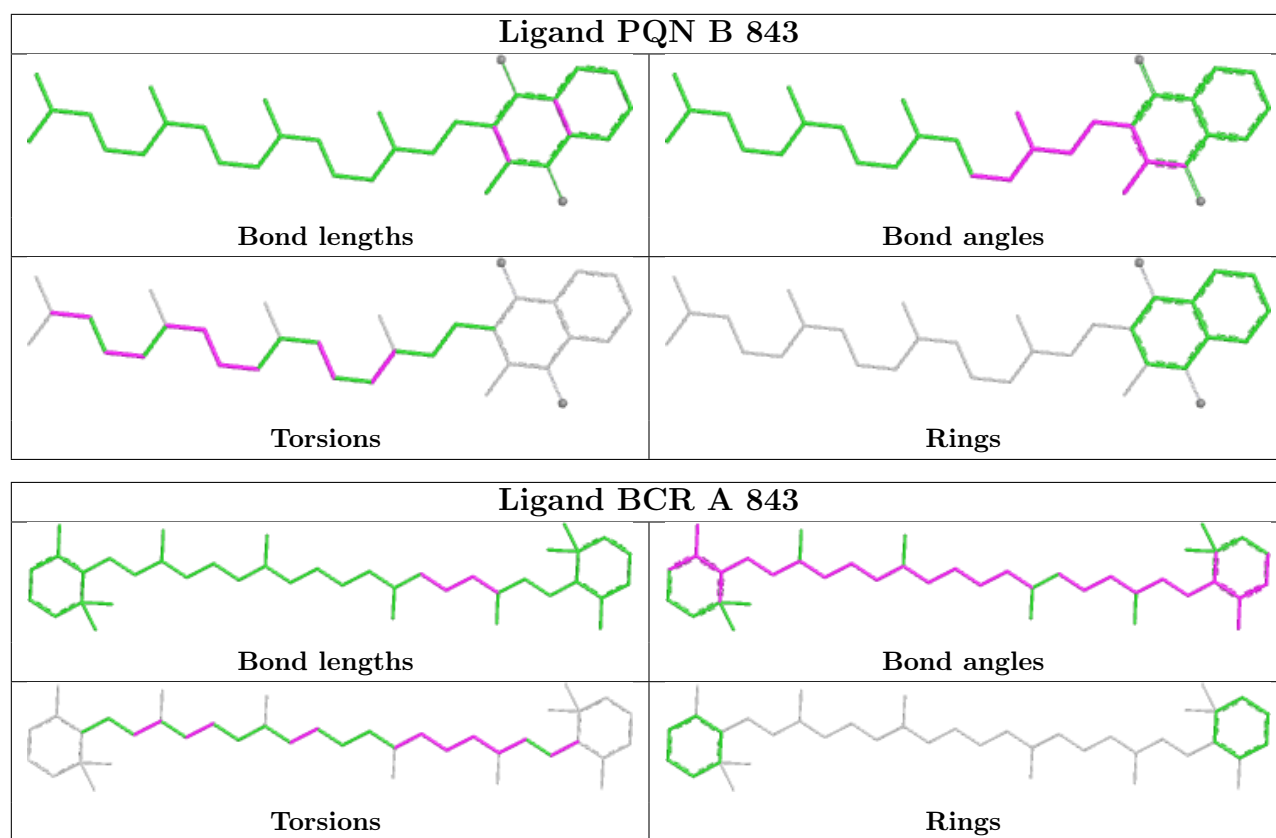
Rings

Ligand CLA 4 318

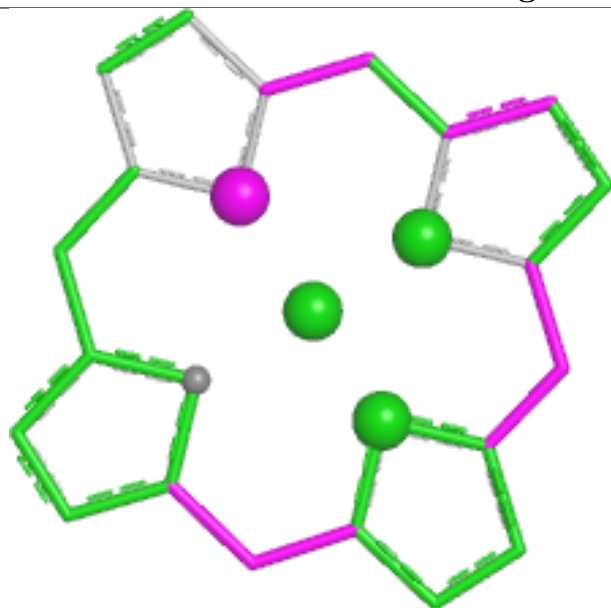


Ligand LMU L 212

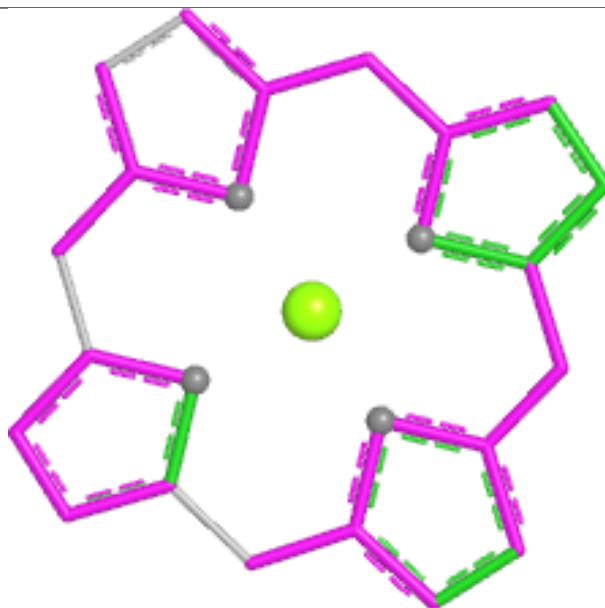




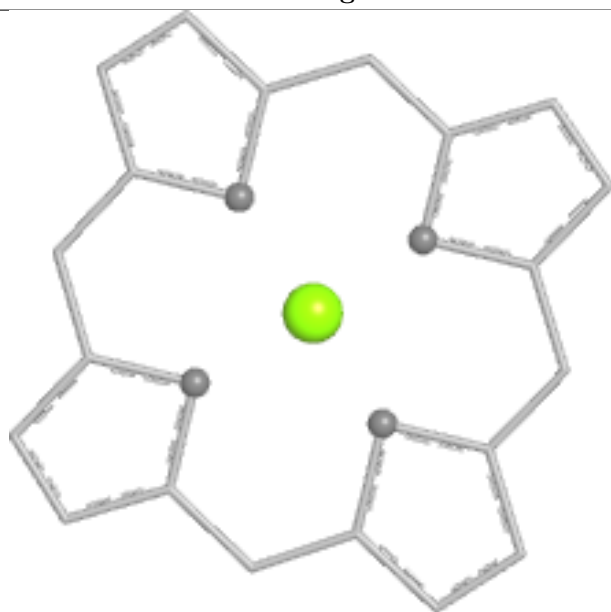
Ligand CLA 3 305



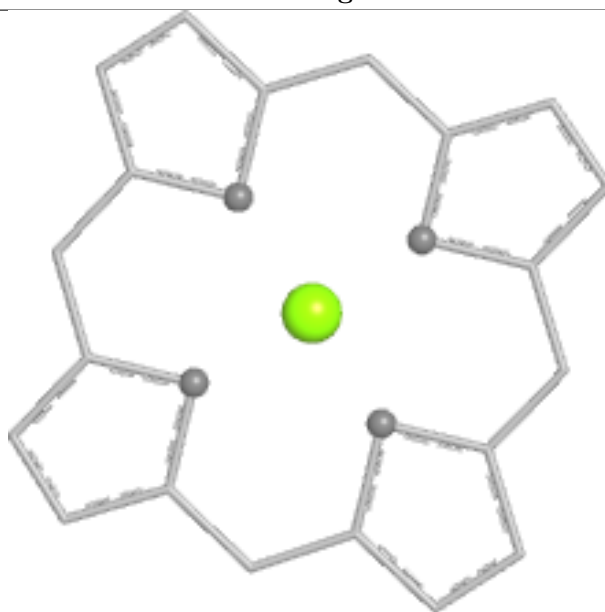
Bond lengths



Bond angles

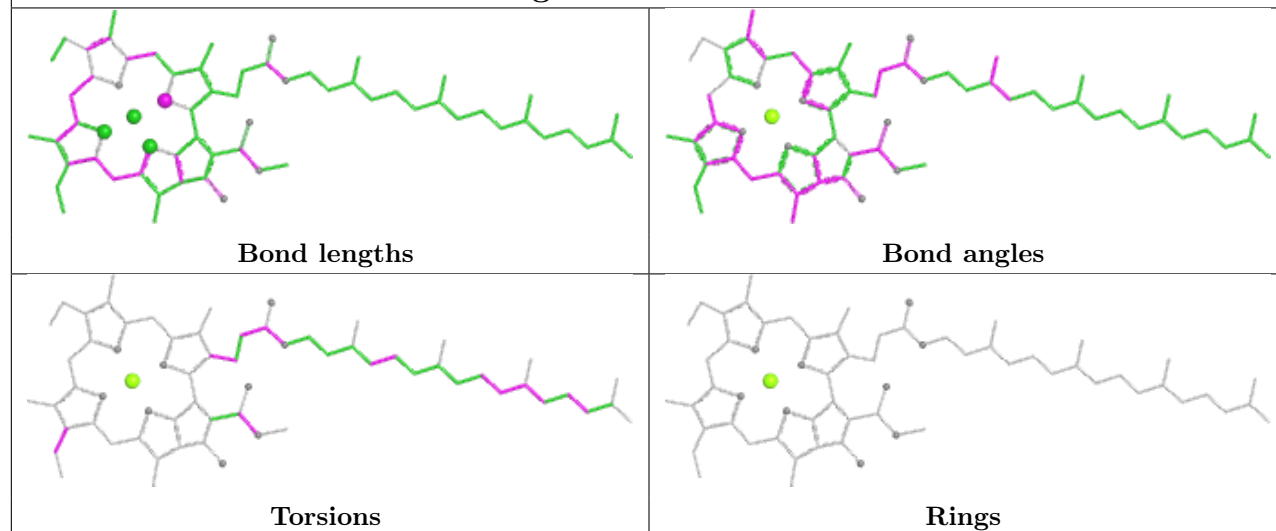


Torsions

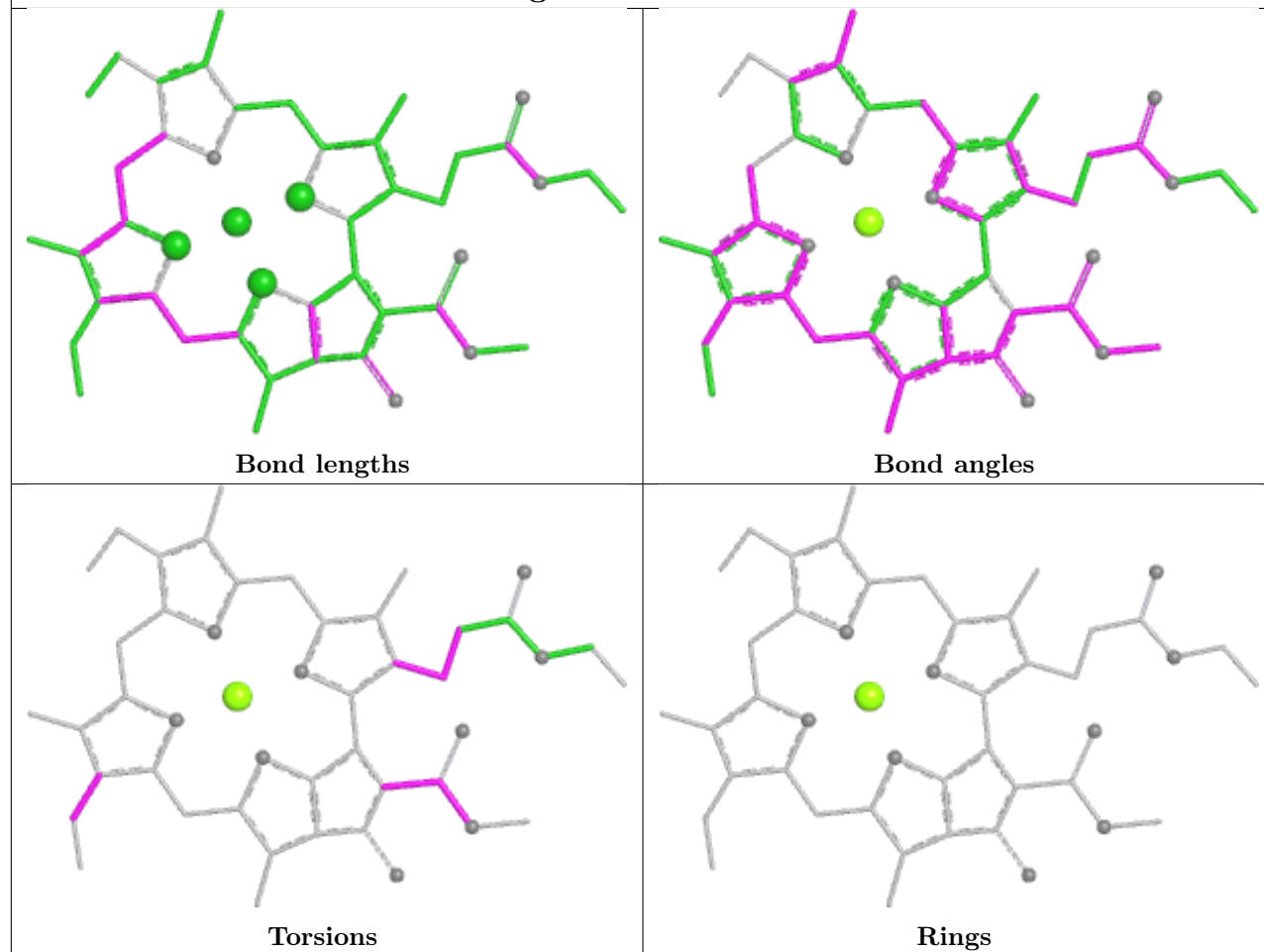


Rings

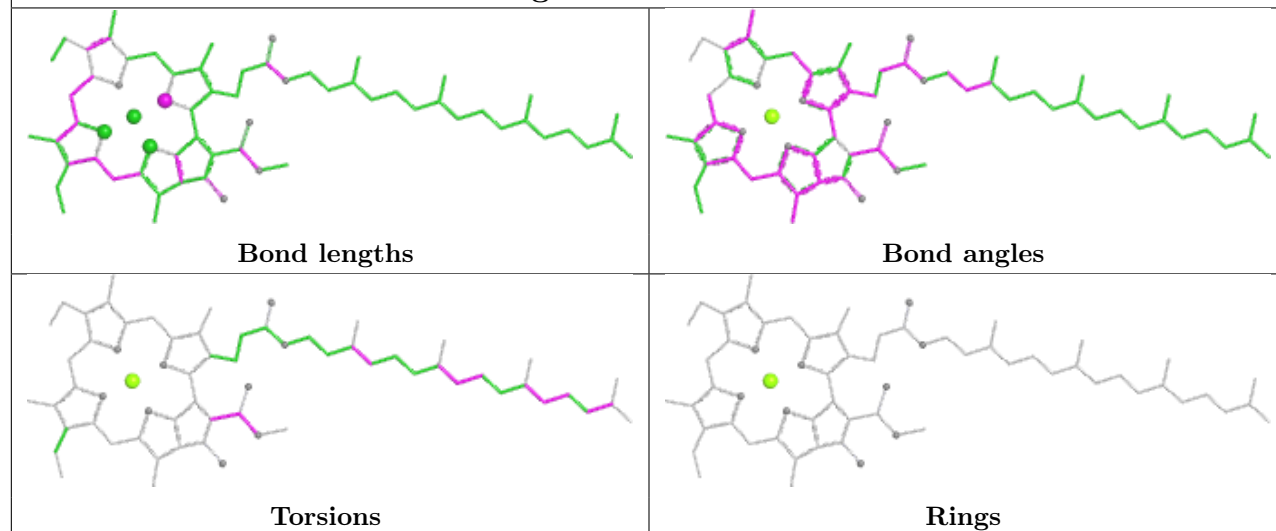
Ligand CLA B 841



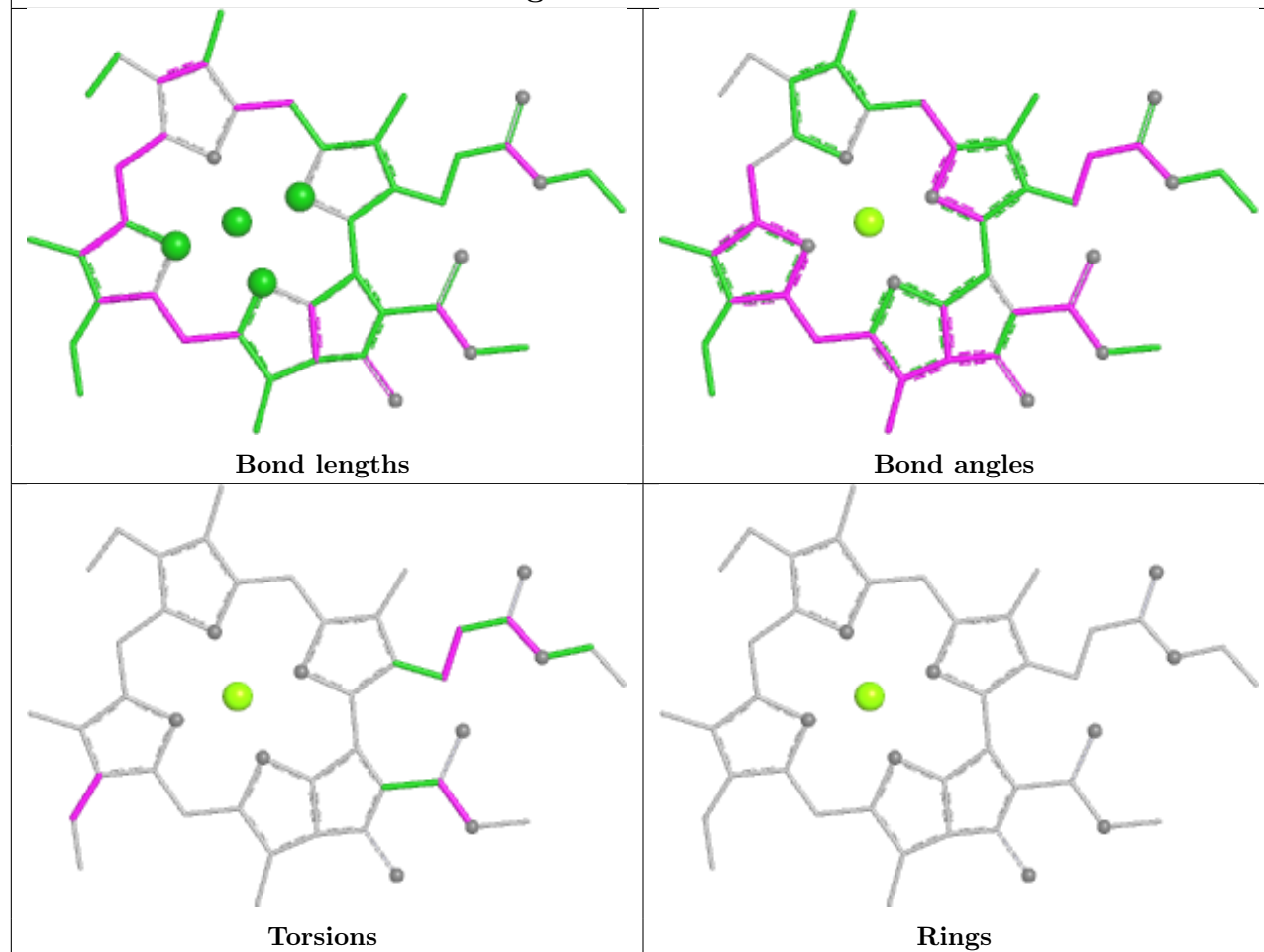
Ligand CLA L 209



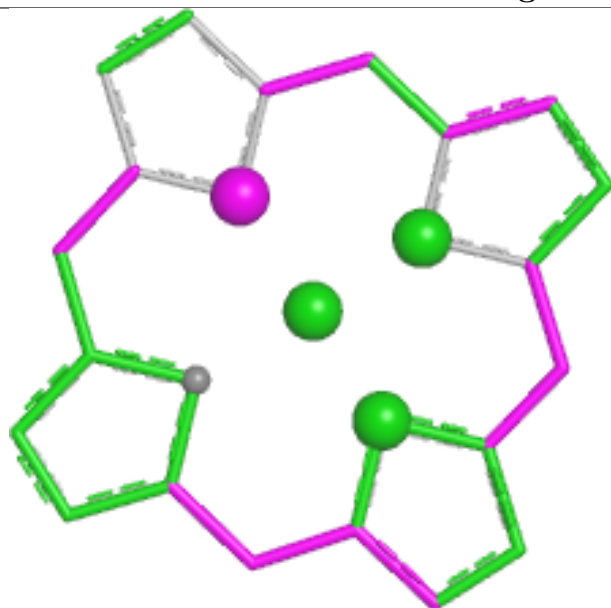
Ligand CLA A 835



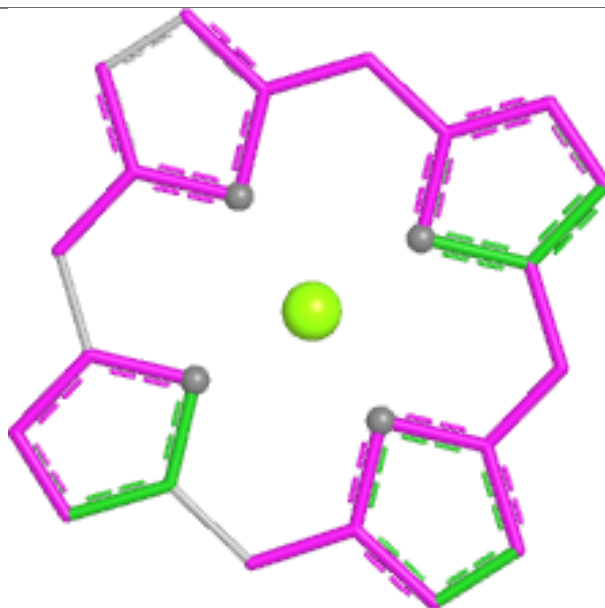
Ligand CLA A 836



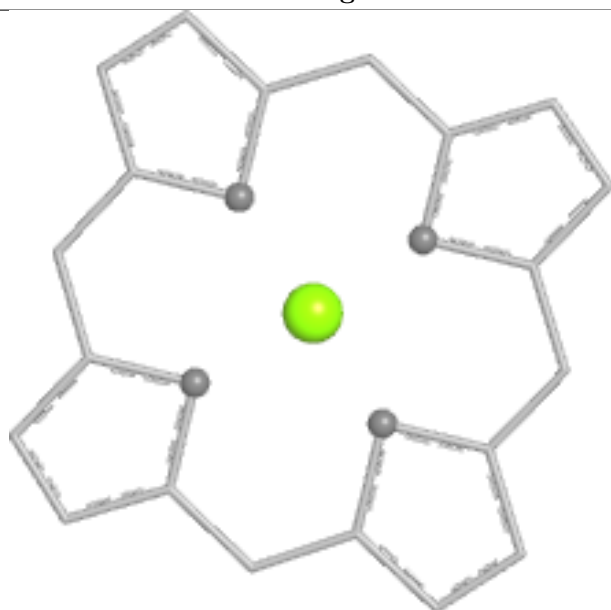
Ligand CLA 3 304



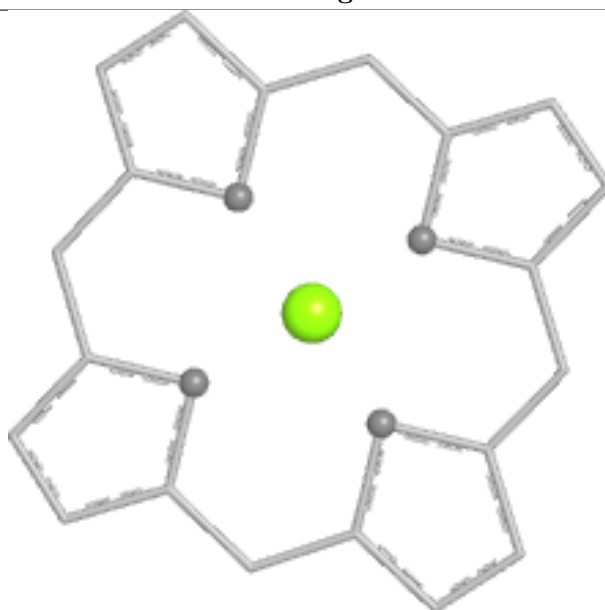
Bond lengths



Bond angles

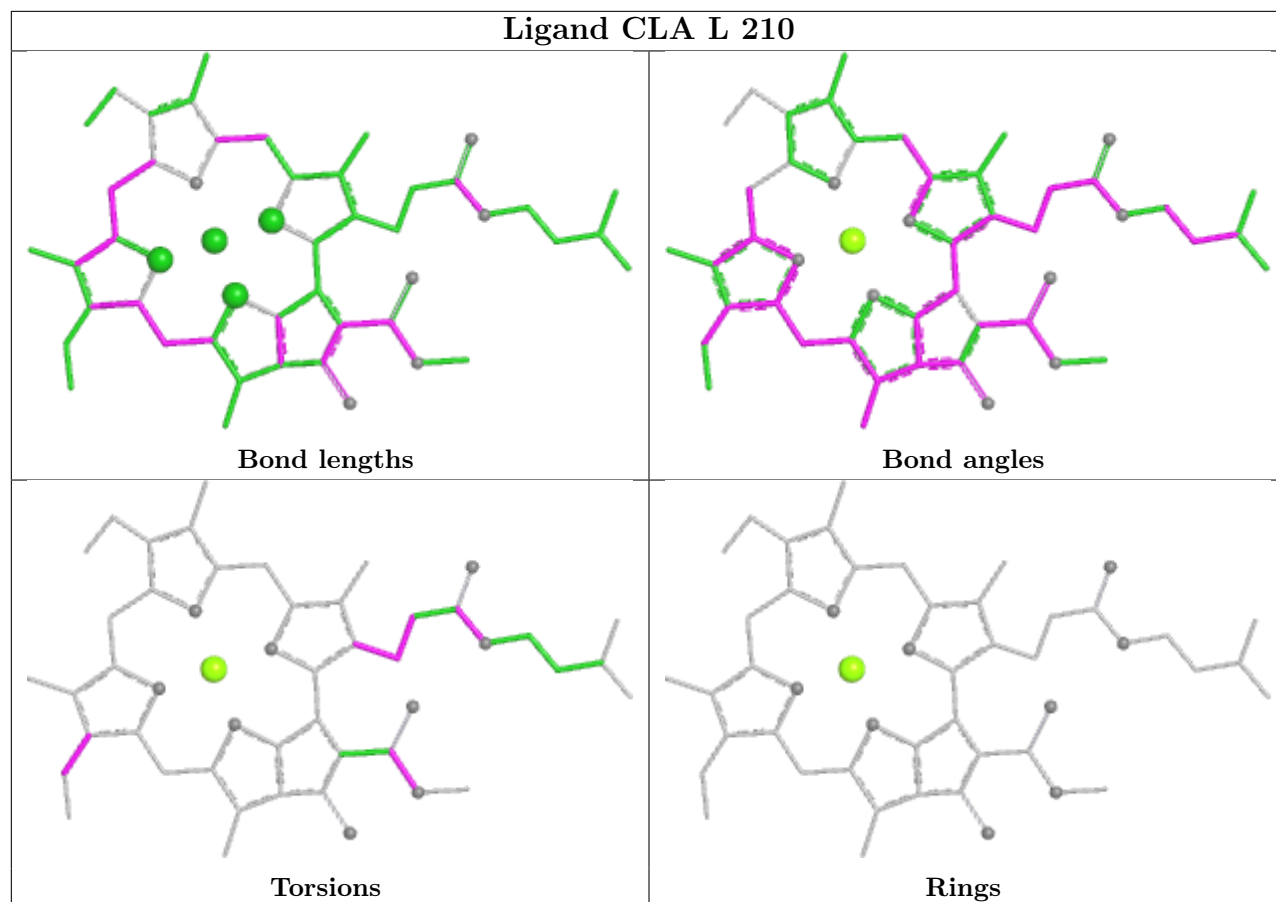


Torsions

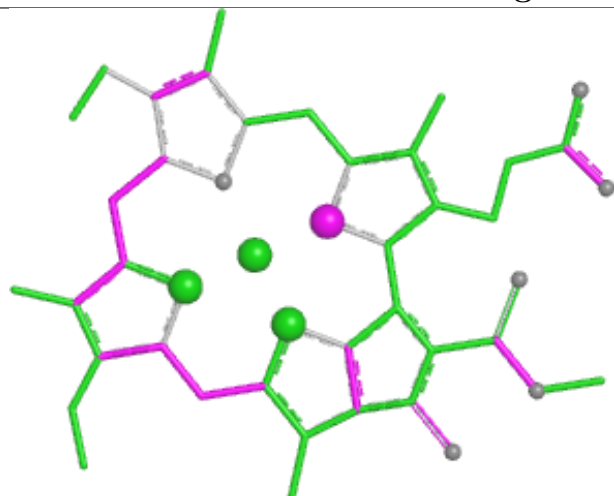


Rings

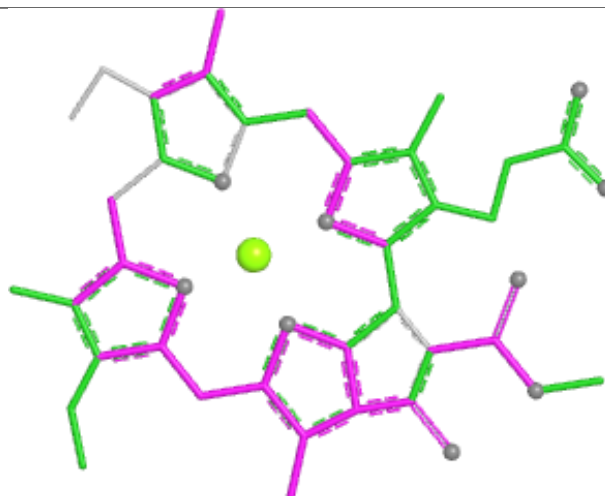
Ligand CLA L 210



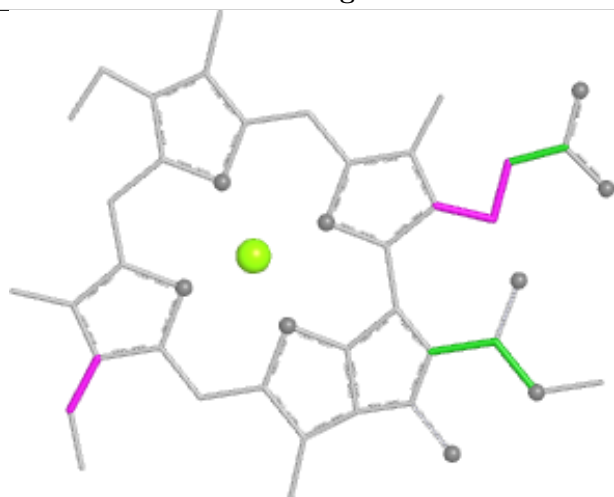
Ligand CLA B 807



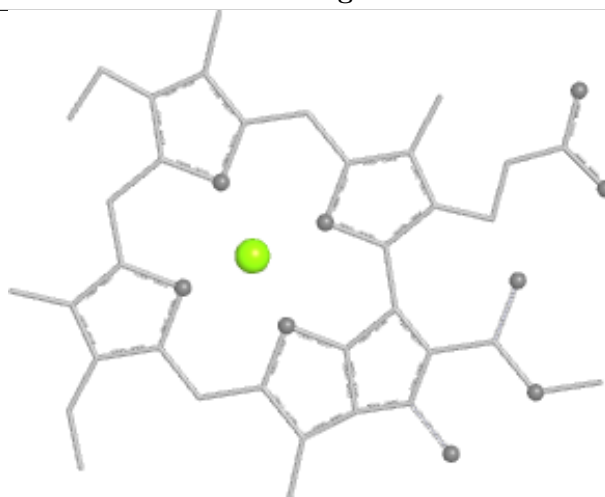
Bond lengths



Bond angles

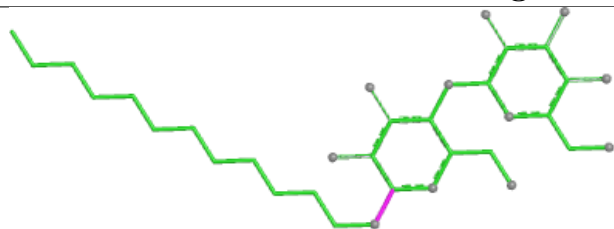


Torsions

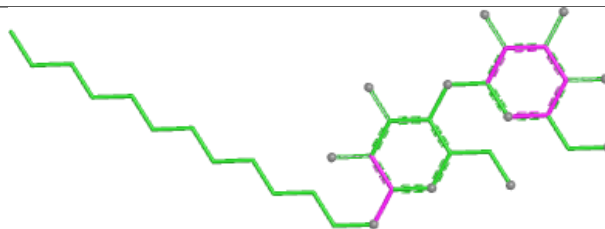


Rings

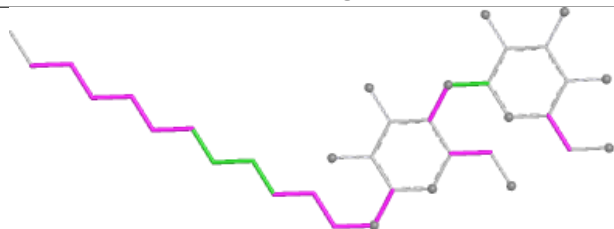
Ligand LMU C 101



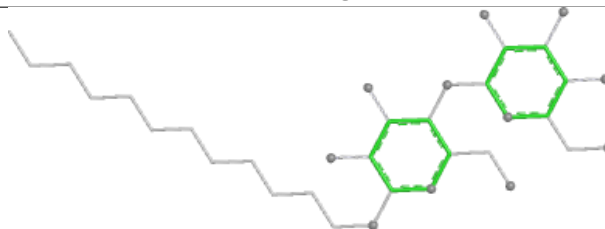
Bond lengths



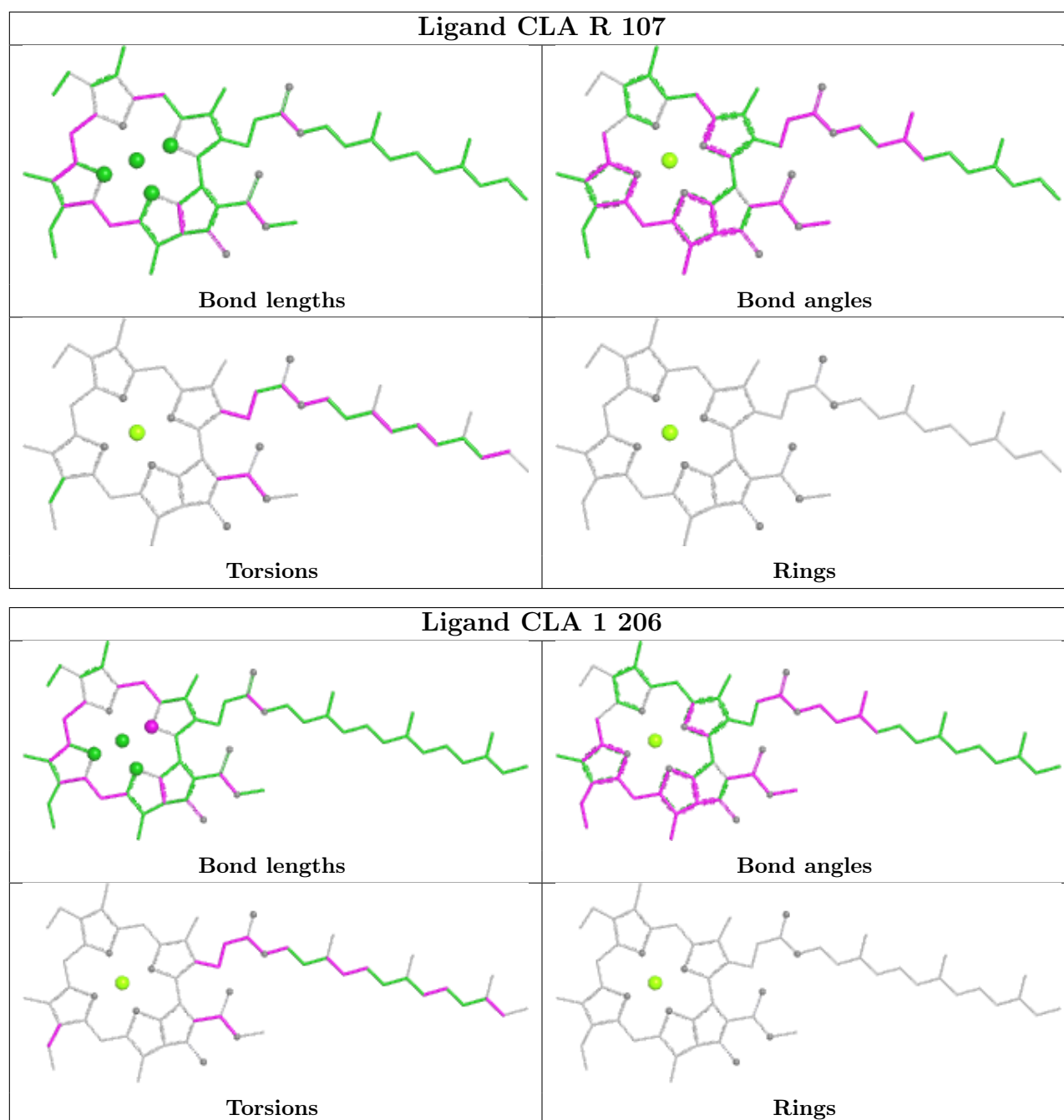
Bond angles

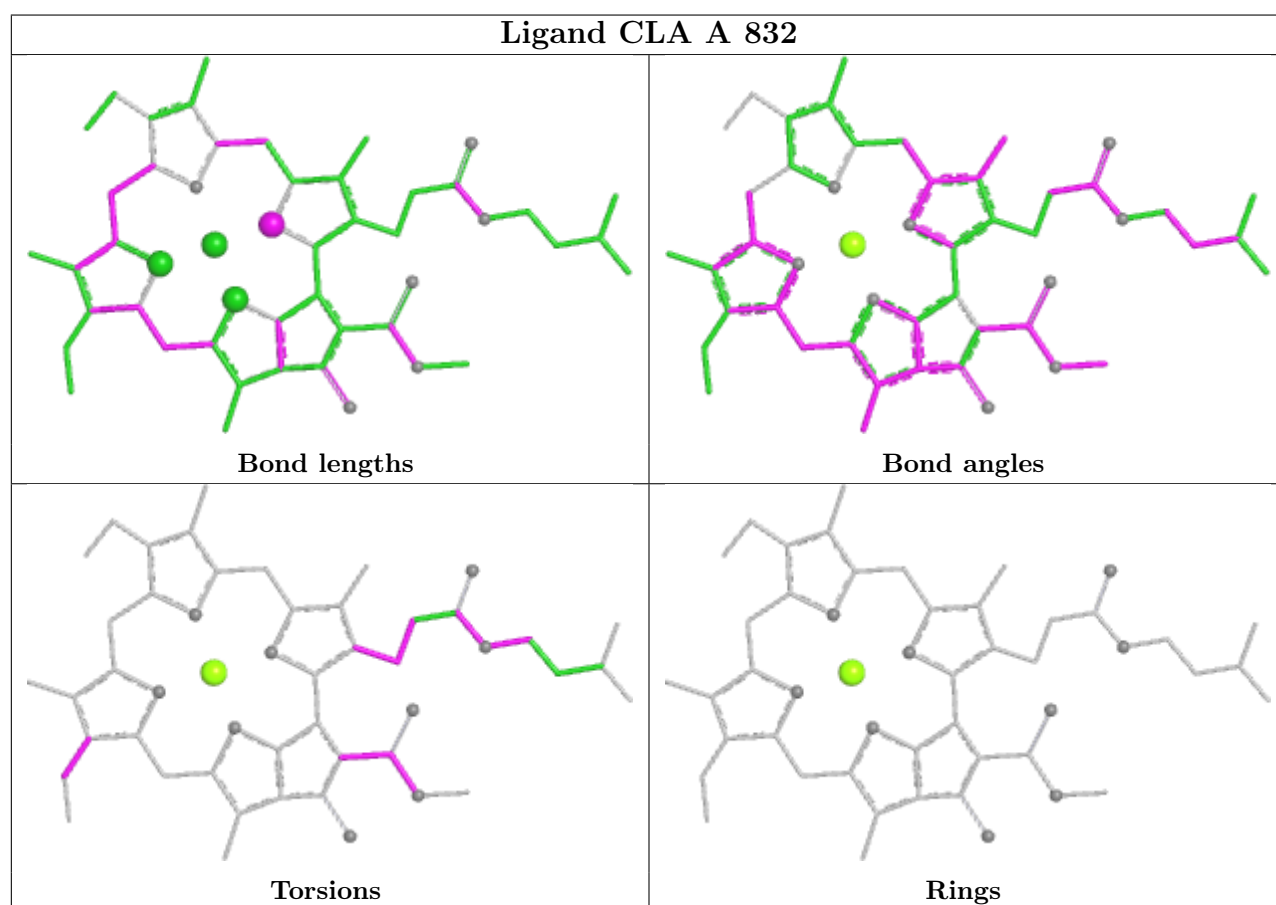
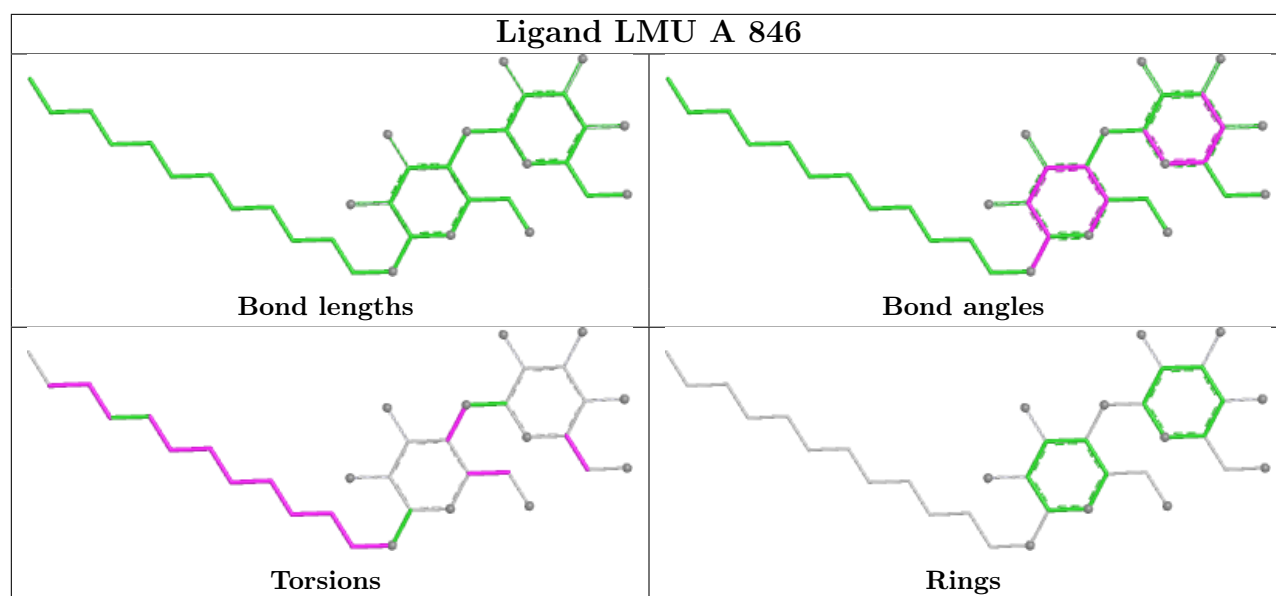


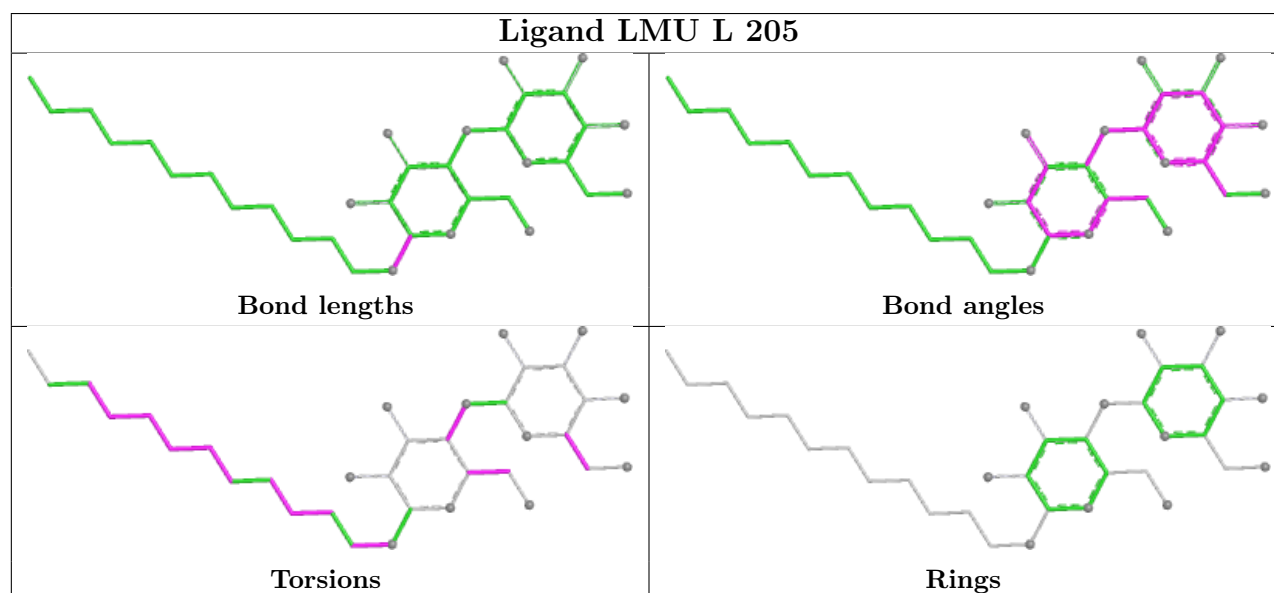
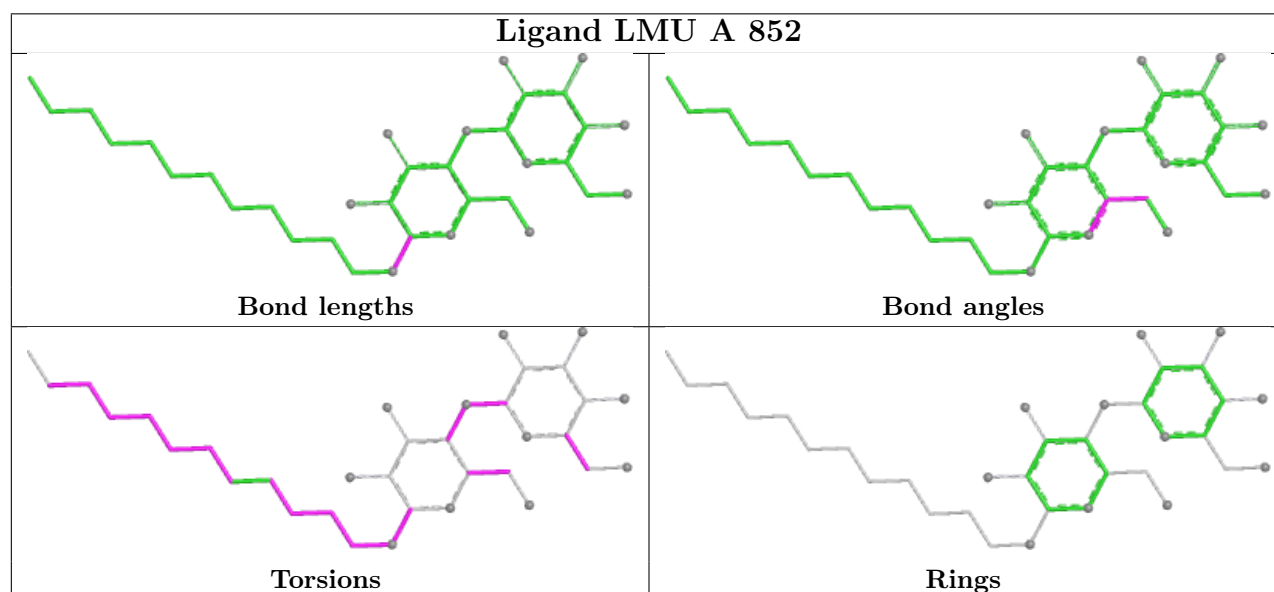
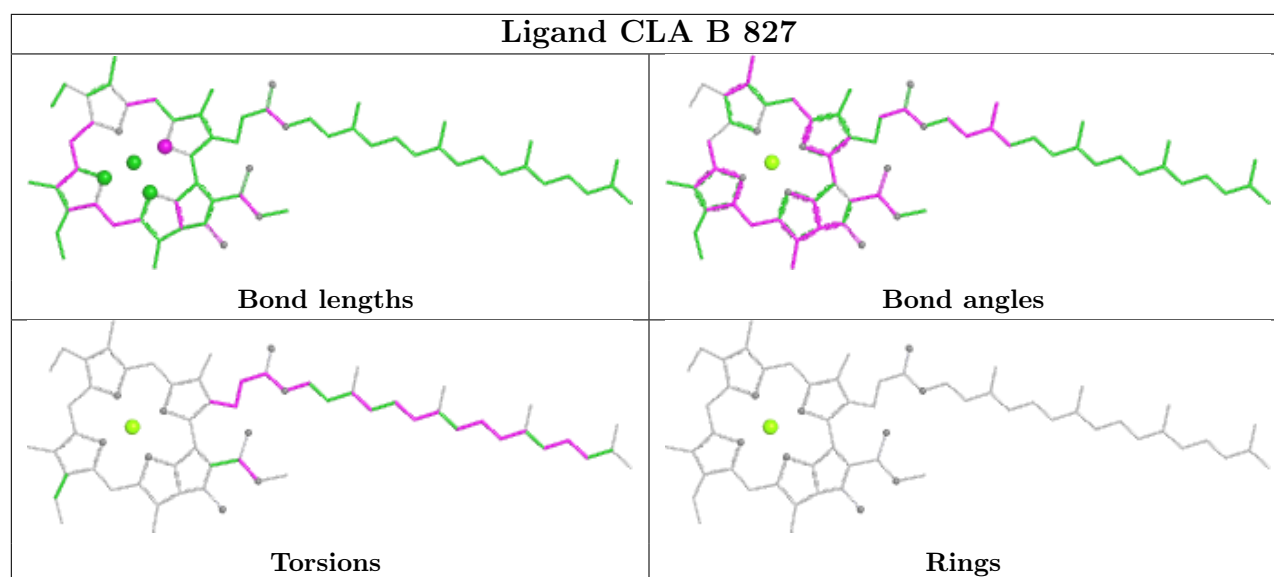
Torsions

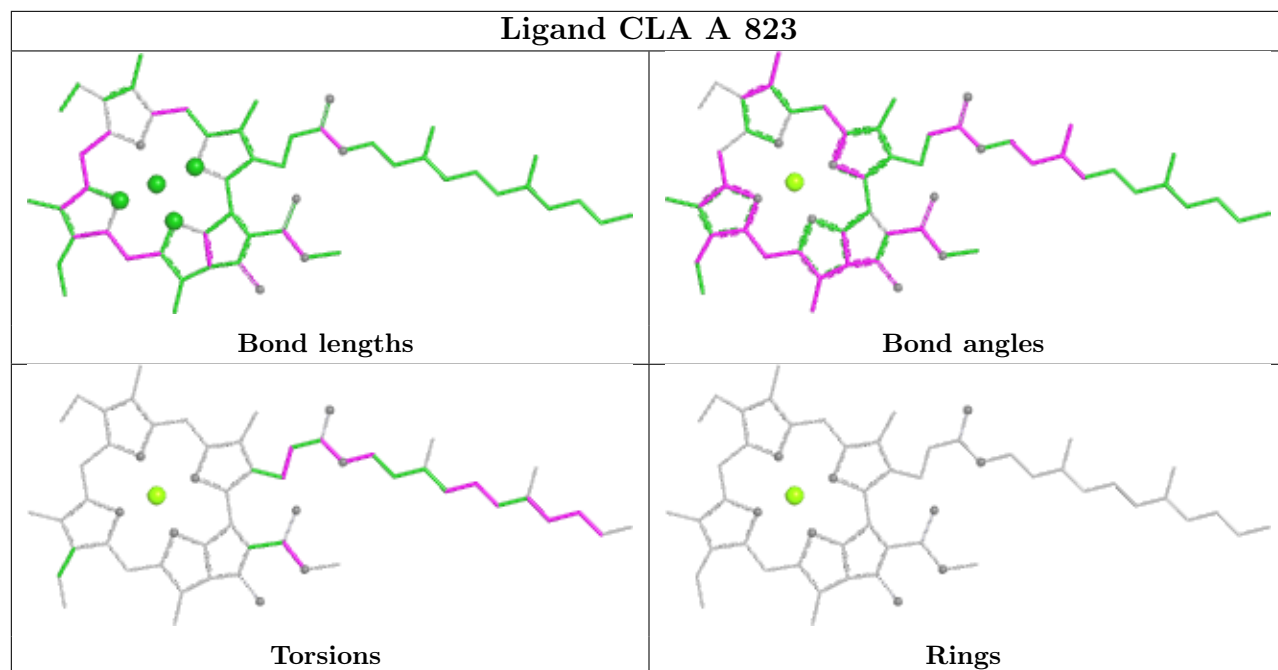


Rings

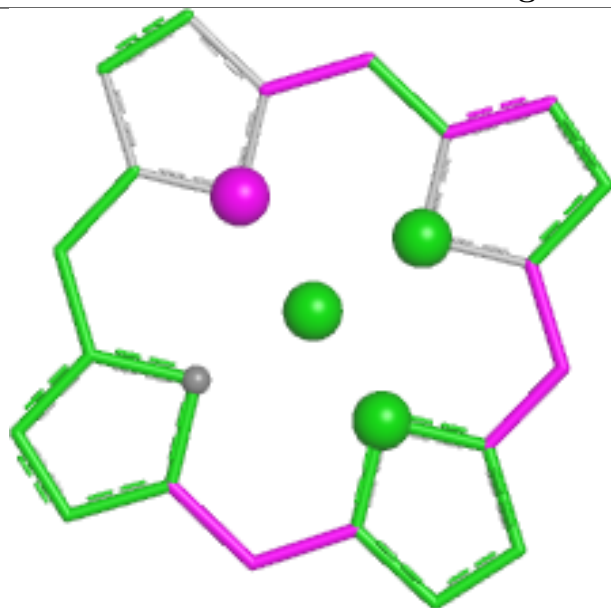




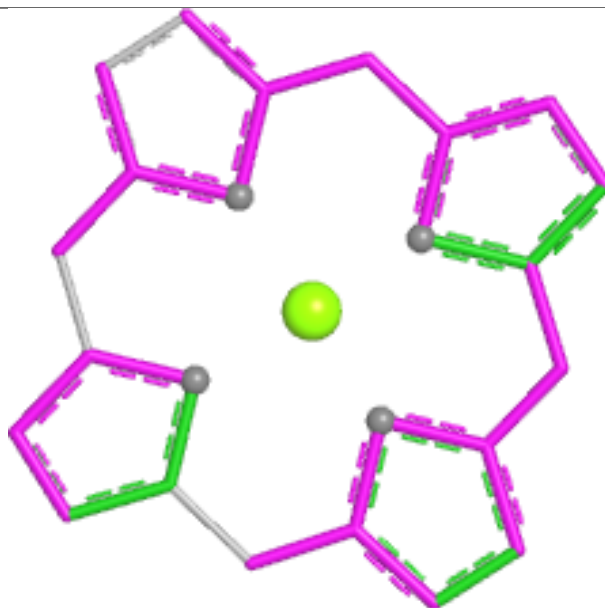




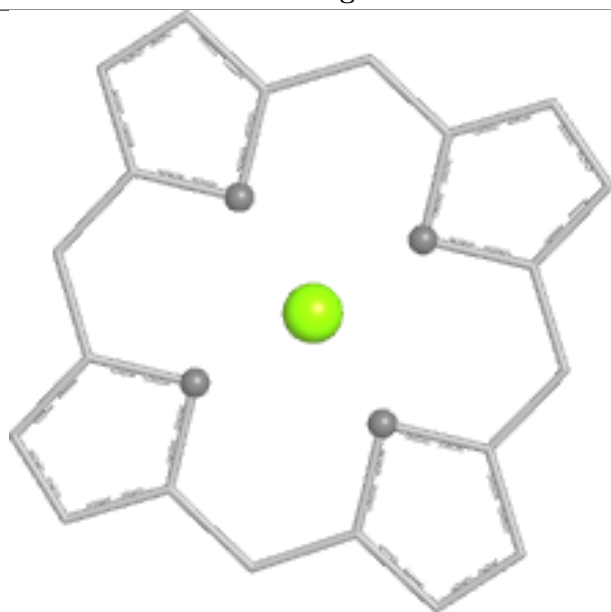
Ligand CLA 3 302



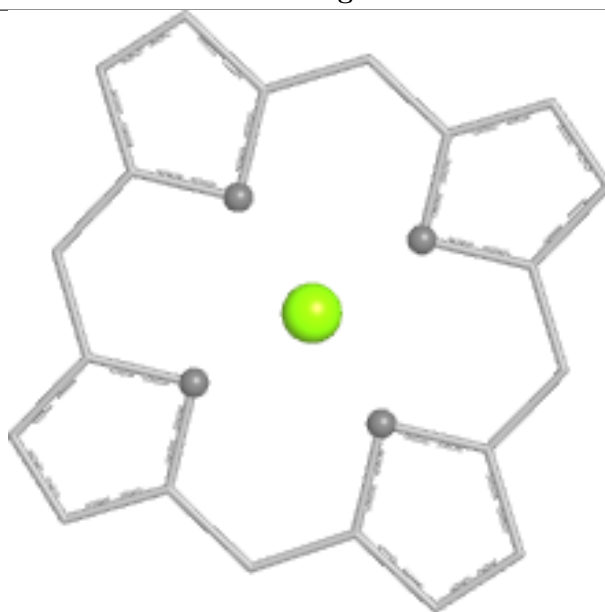
Bond lengths



Bond angles

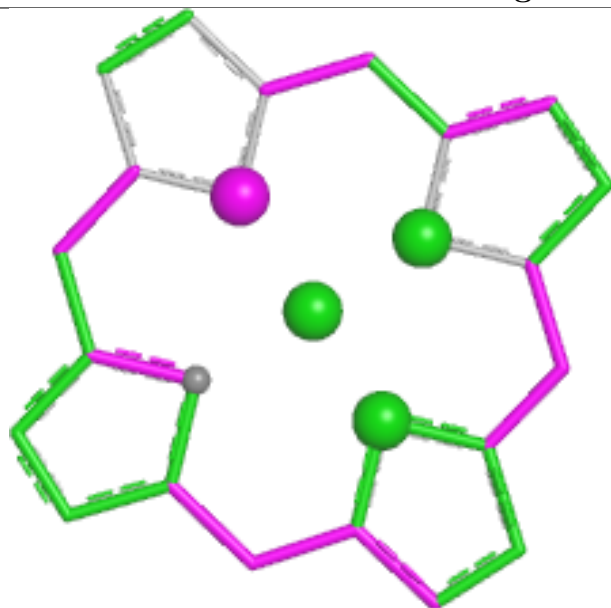


Torsions

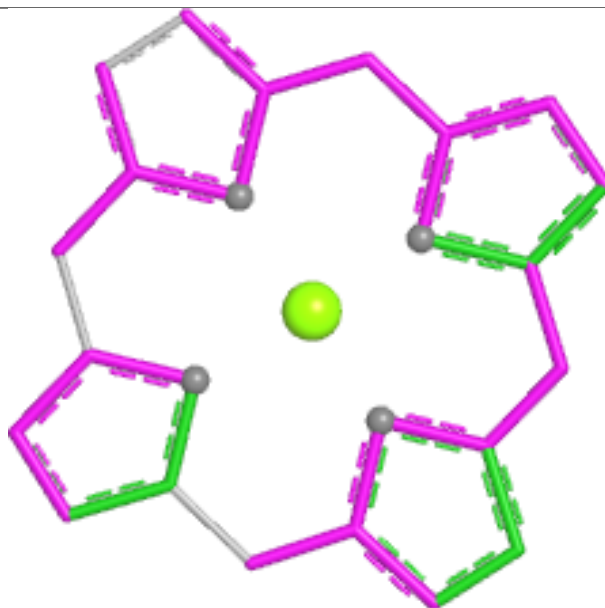


Rings

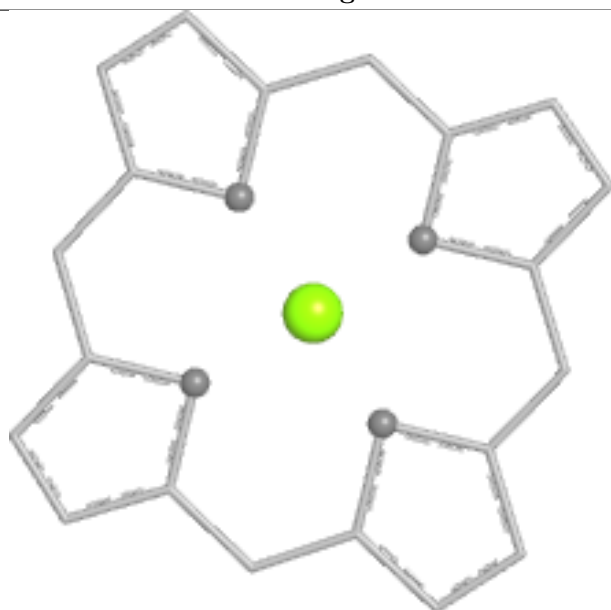
Ligand CLA B 811



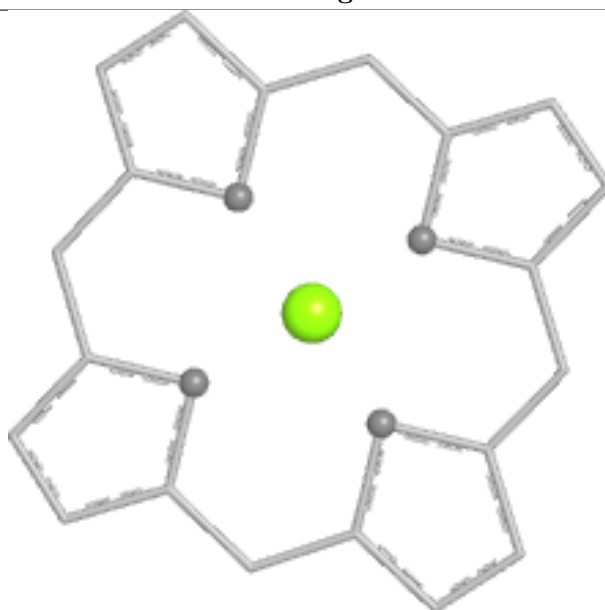
Bond lengths



Bond angles

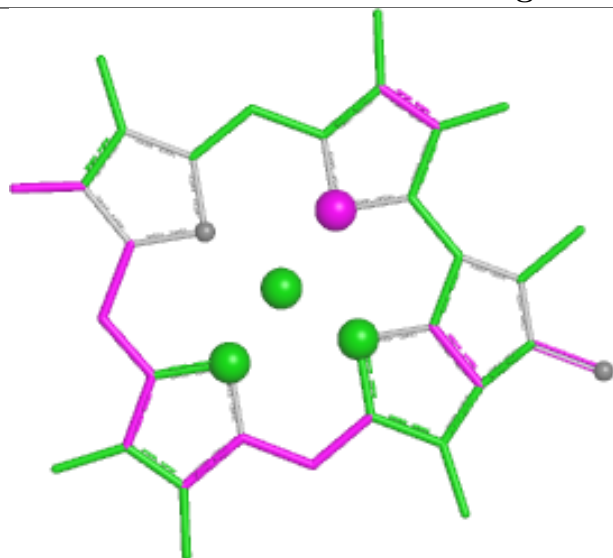


Torsions

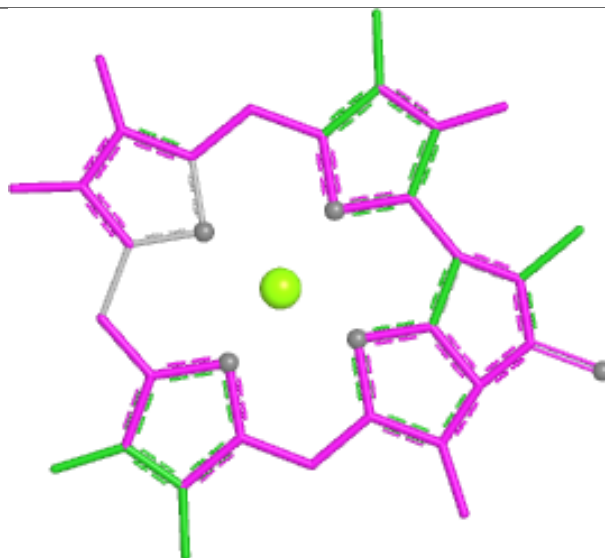


Rings

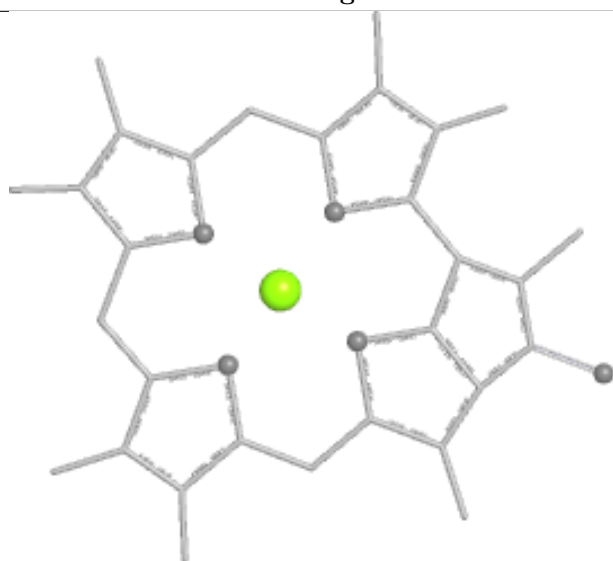
Ligand CLA F 205



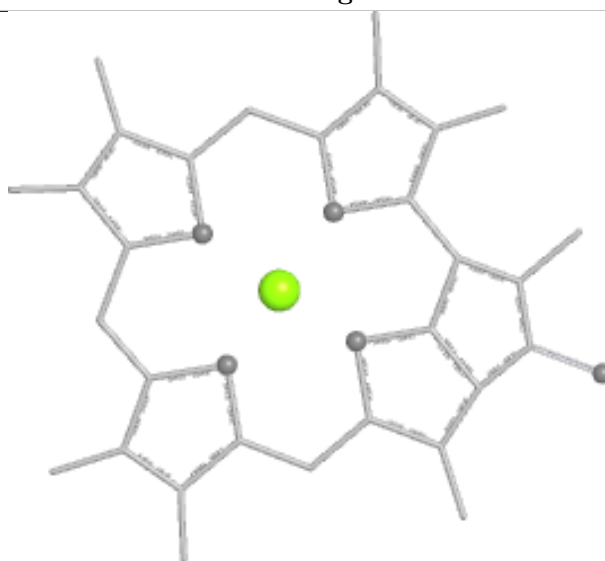
Bond lengths



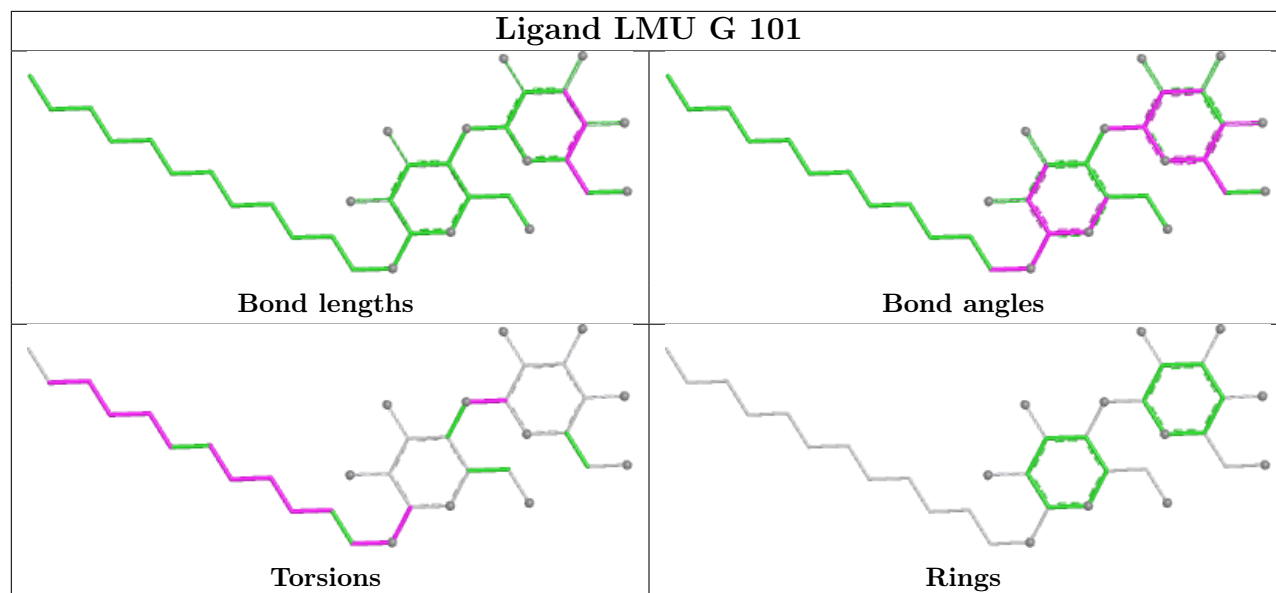
Bond angles



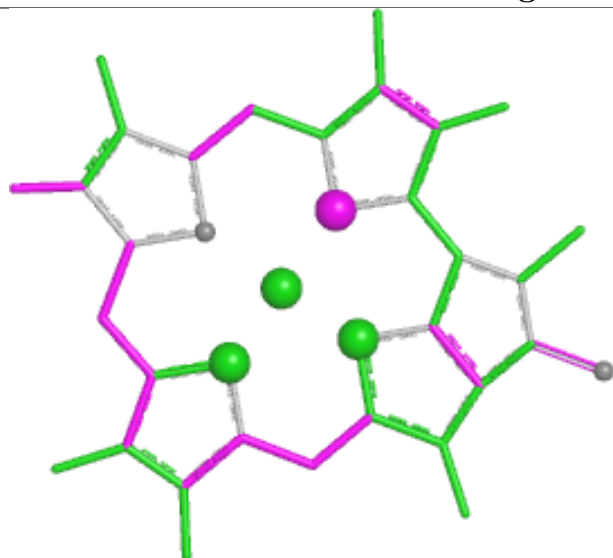
Torsions



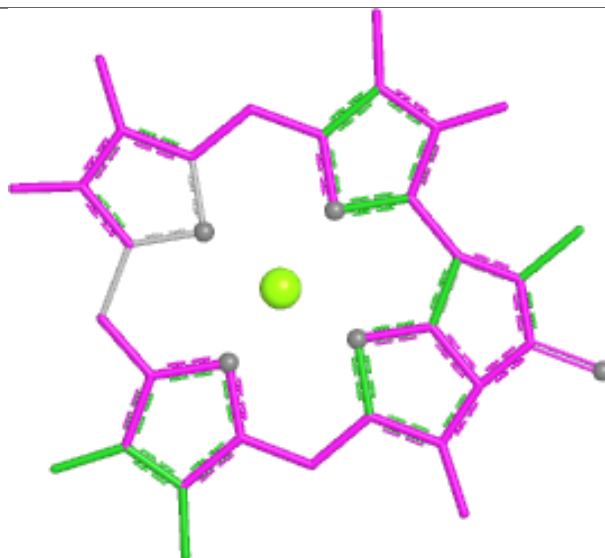
Rings



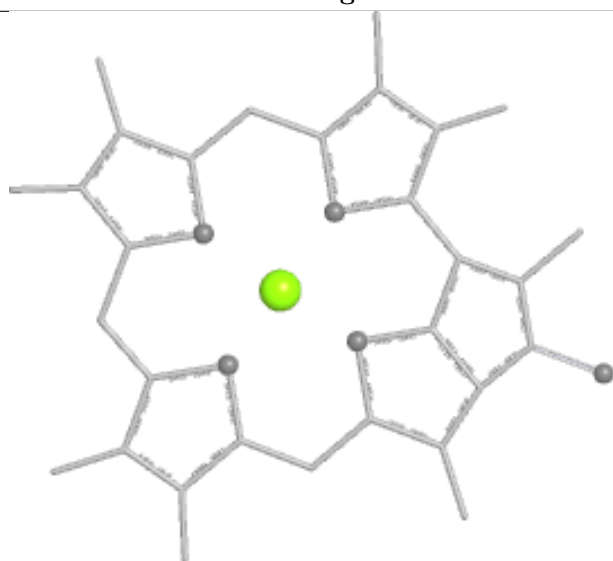
Ligand CLA 4 302



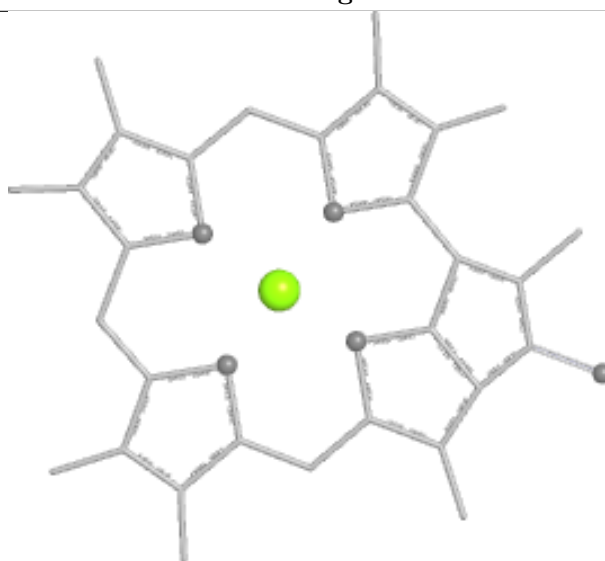
Bond lengths



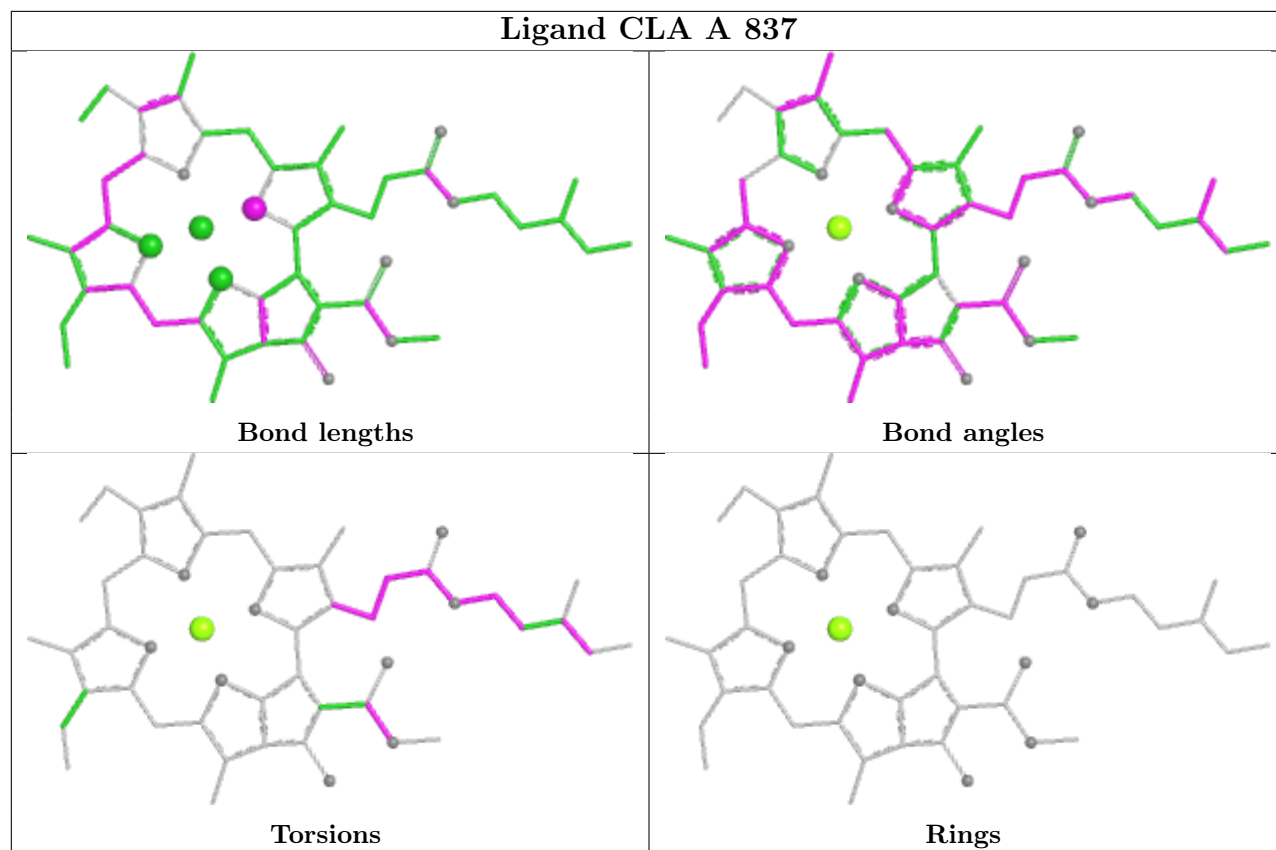
Bond angles



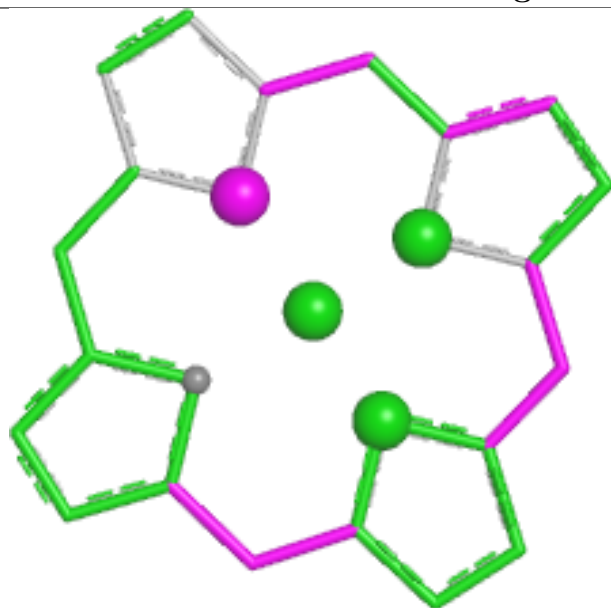
Torsions



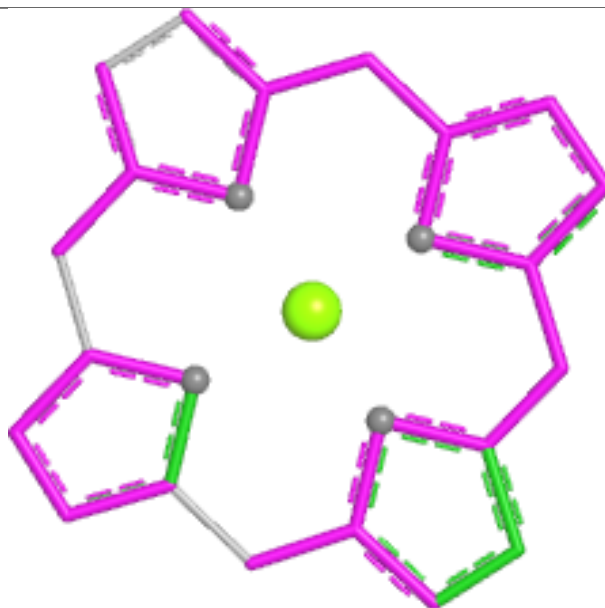
Rings



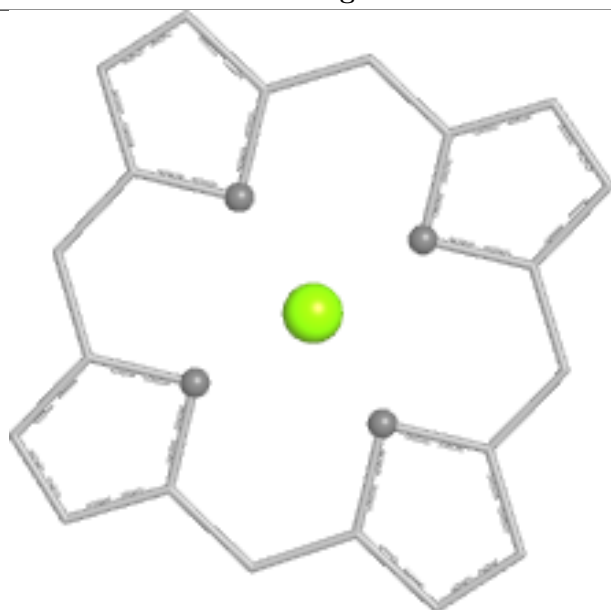
Ligand CLA A 802



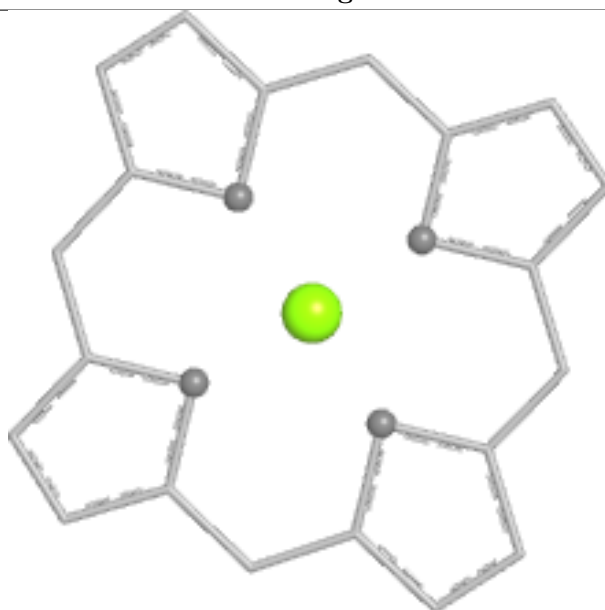
Bond lengths



Bond angles

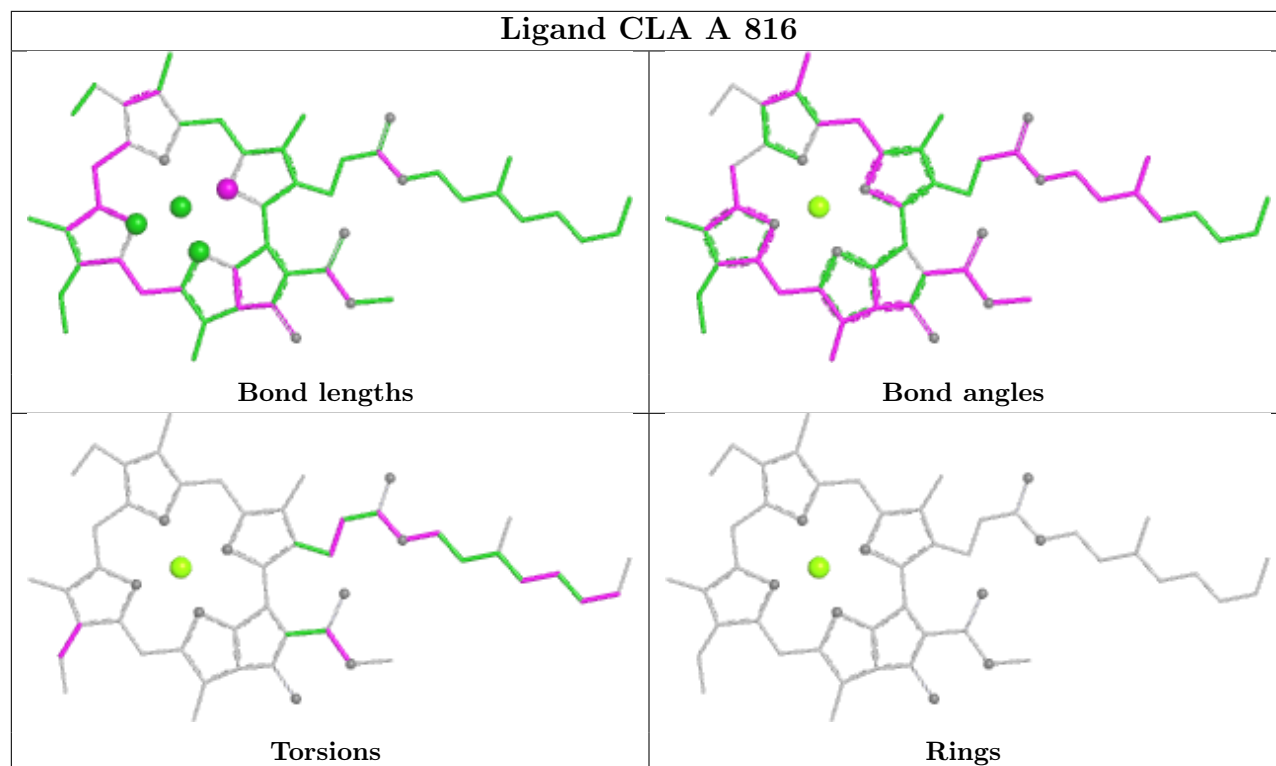


Torsions

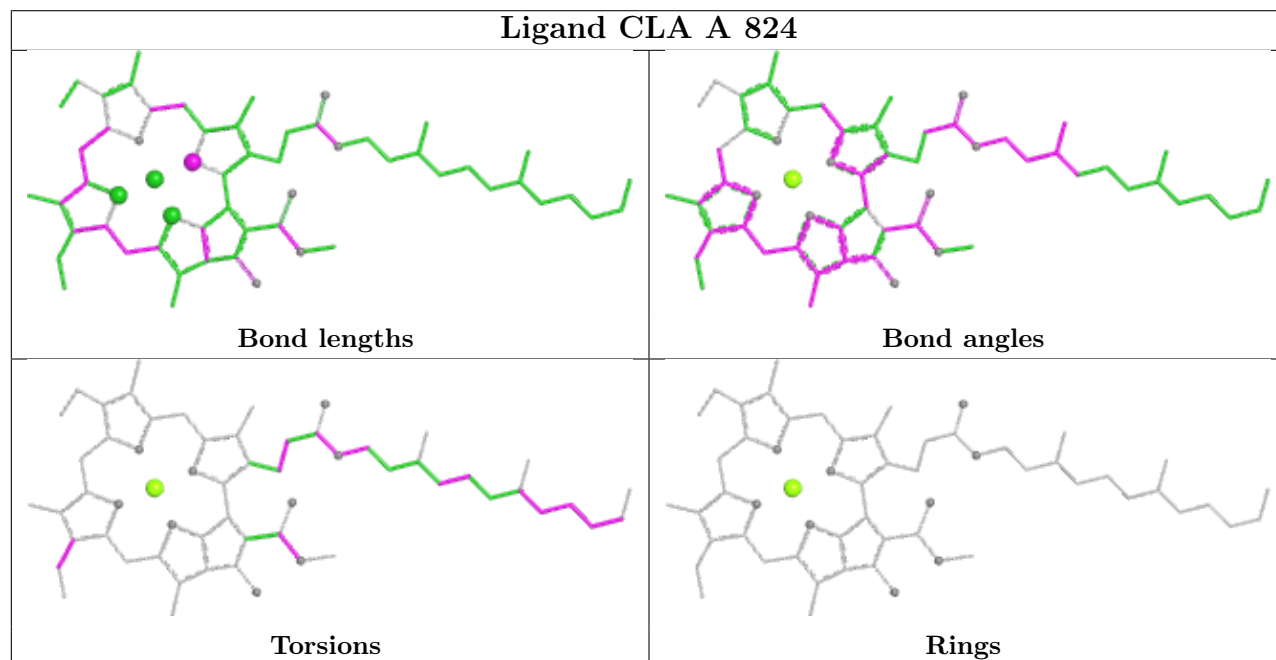


Rings

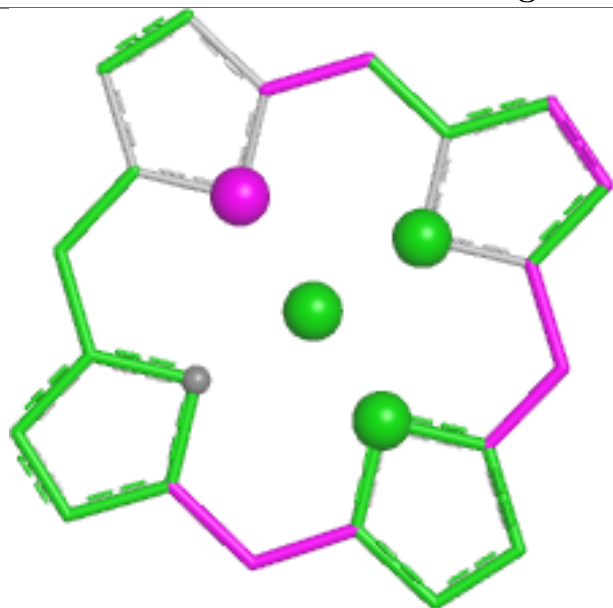
Ligand CLA A 816



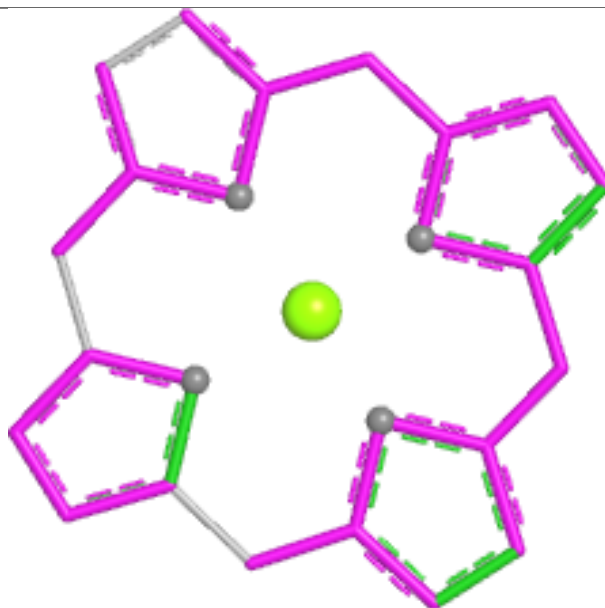
Ligand CLA A 824



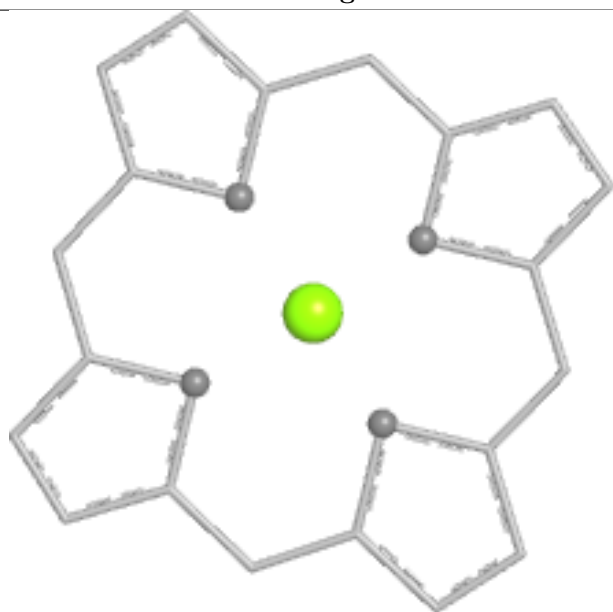
Ligand CLA 3 306



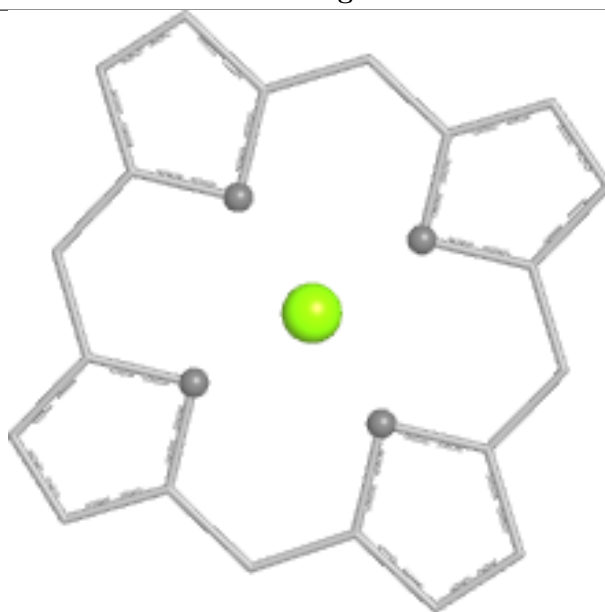
Bond lengths



Bond angles

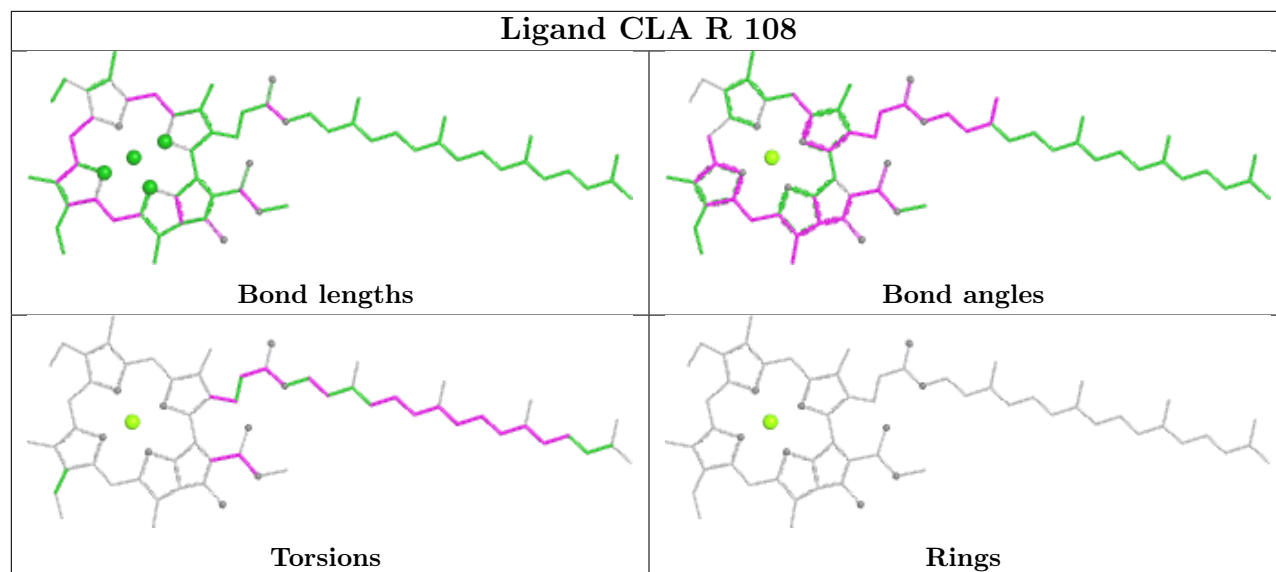


Torsions

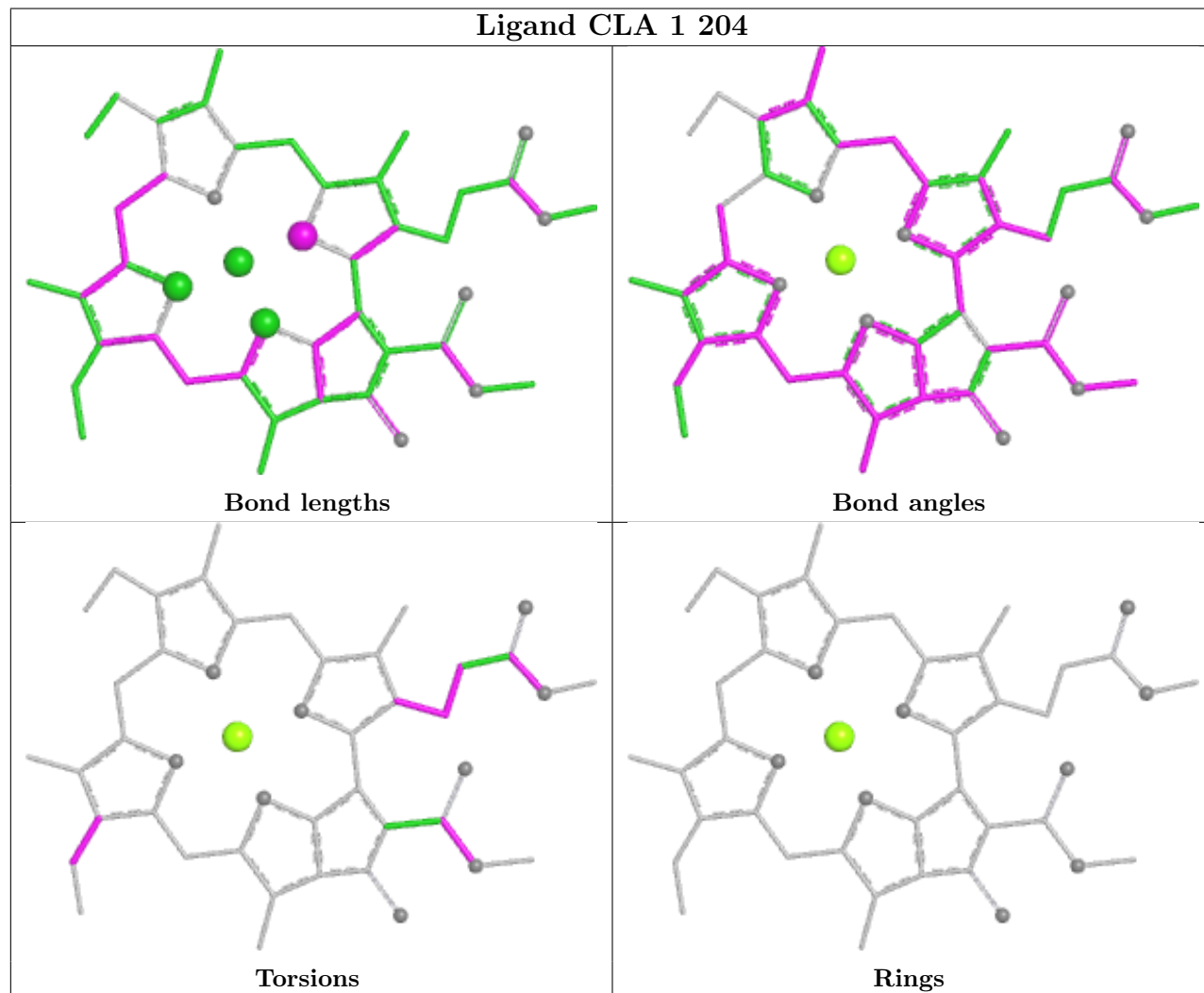


Rings

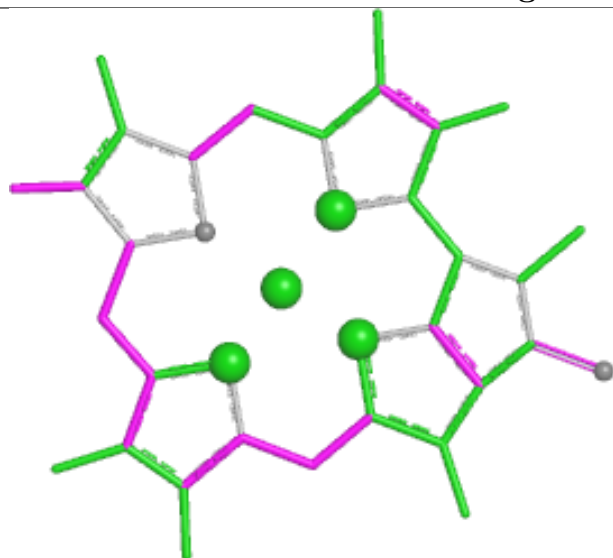
Ligand CLA R 108



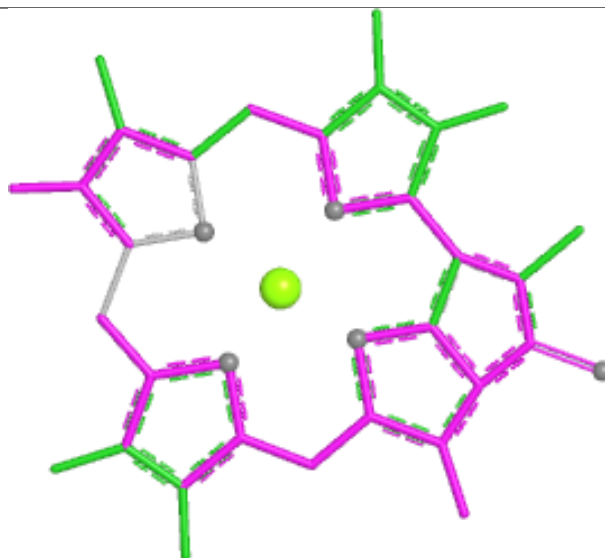
Ligand CLA 1 204



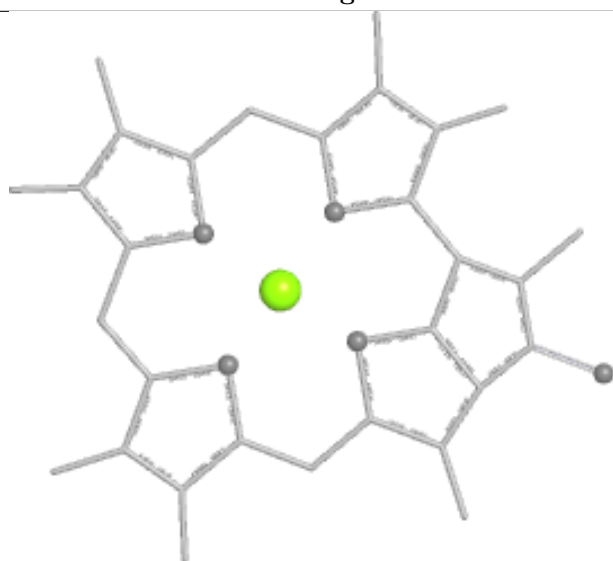
Ligand CLA 1 210



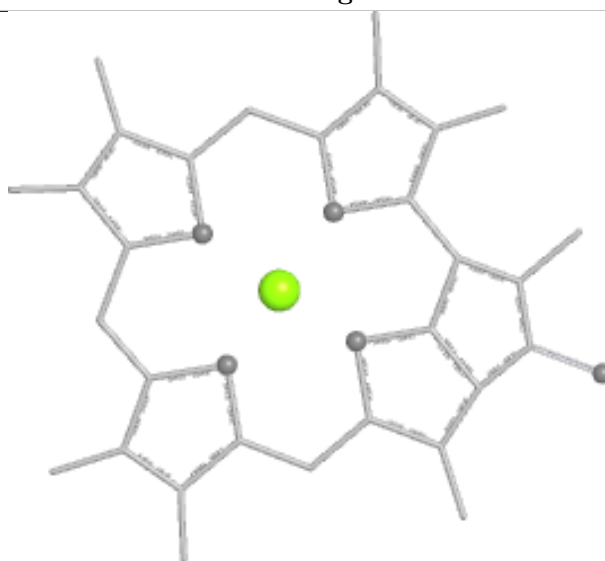
Bond lengths



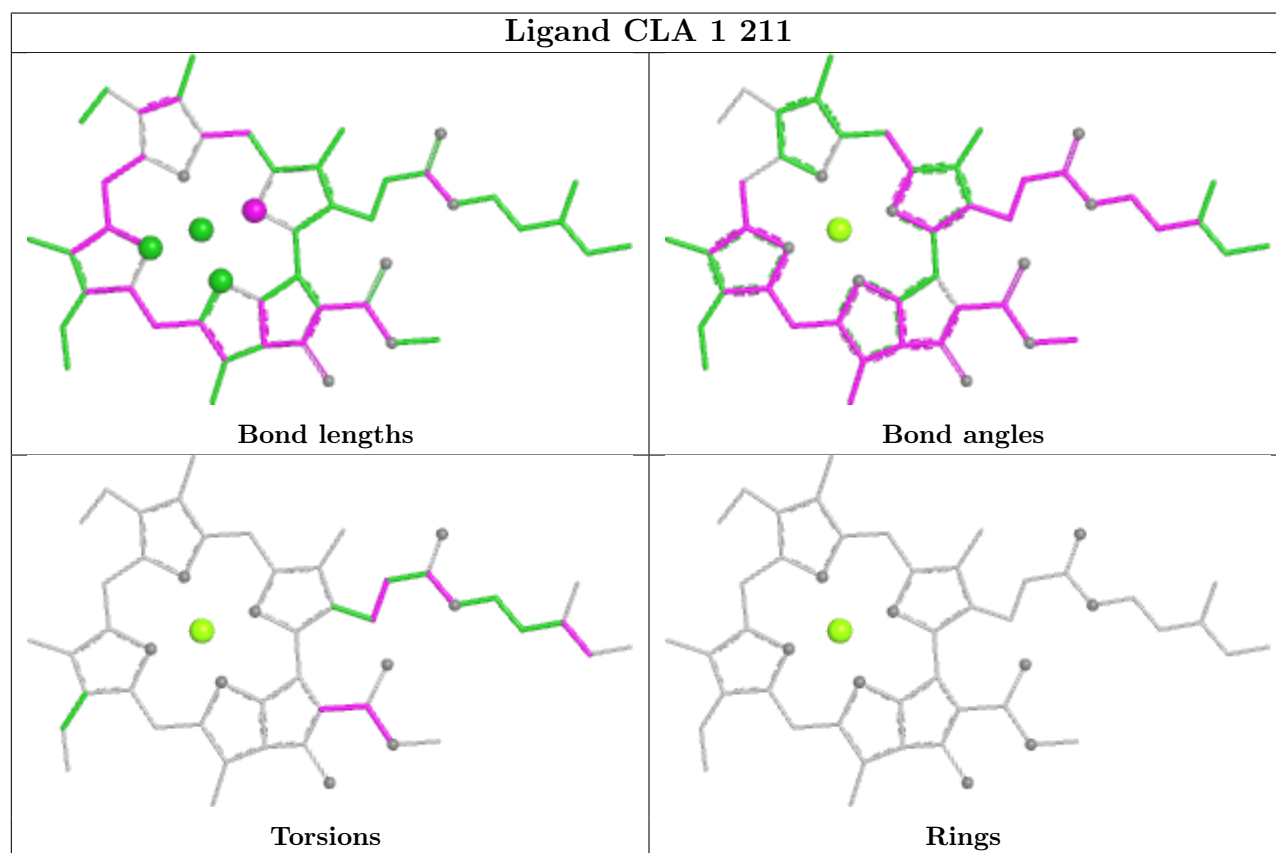
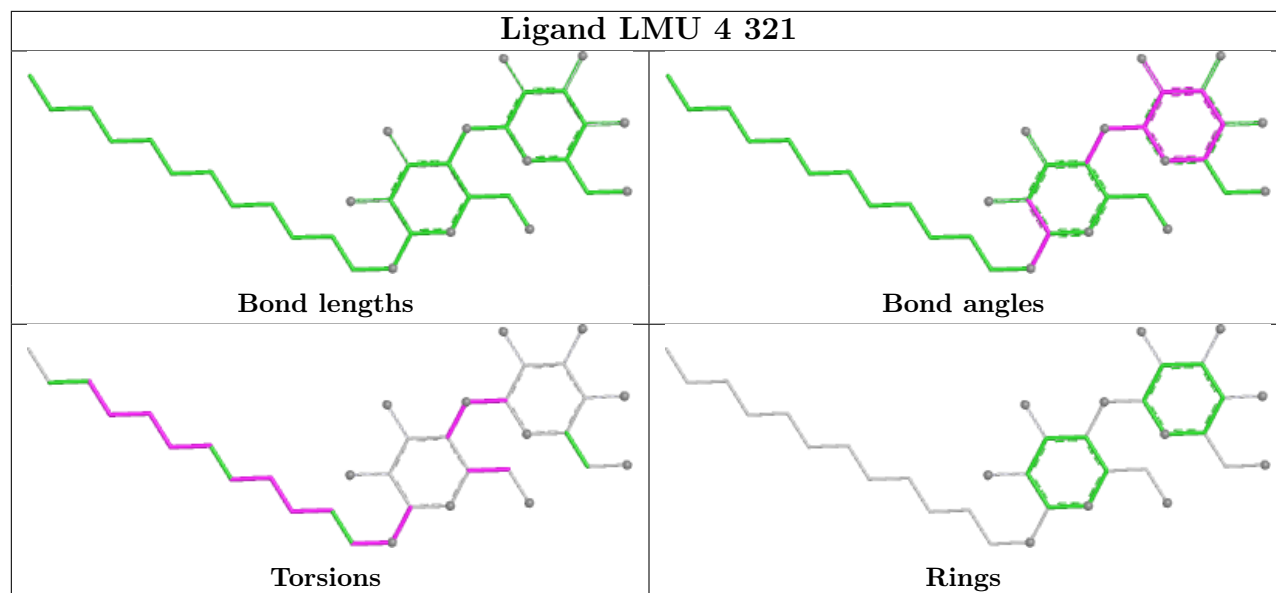
Bond angles



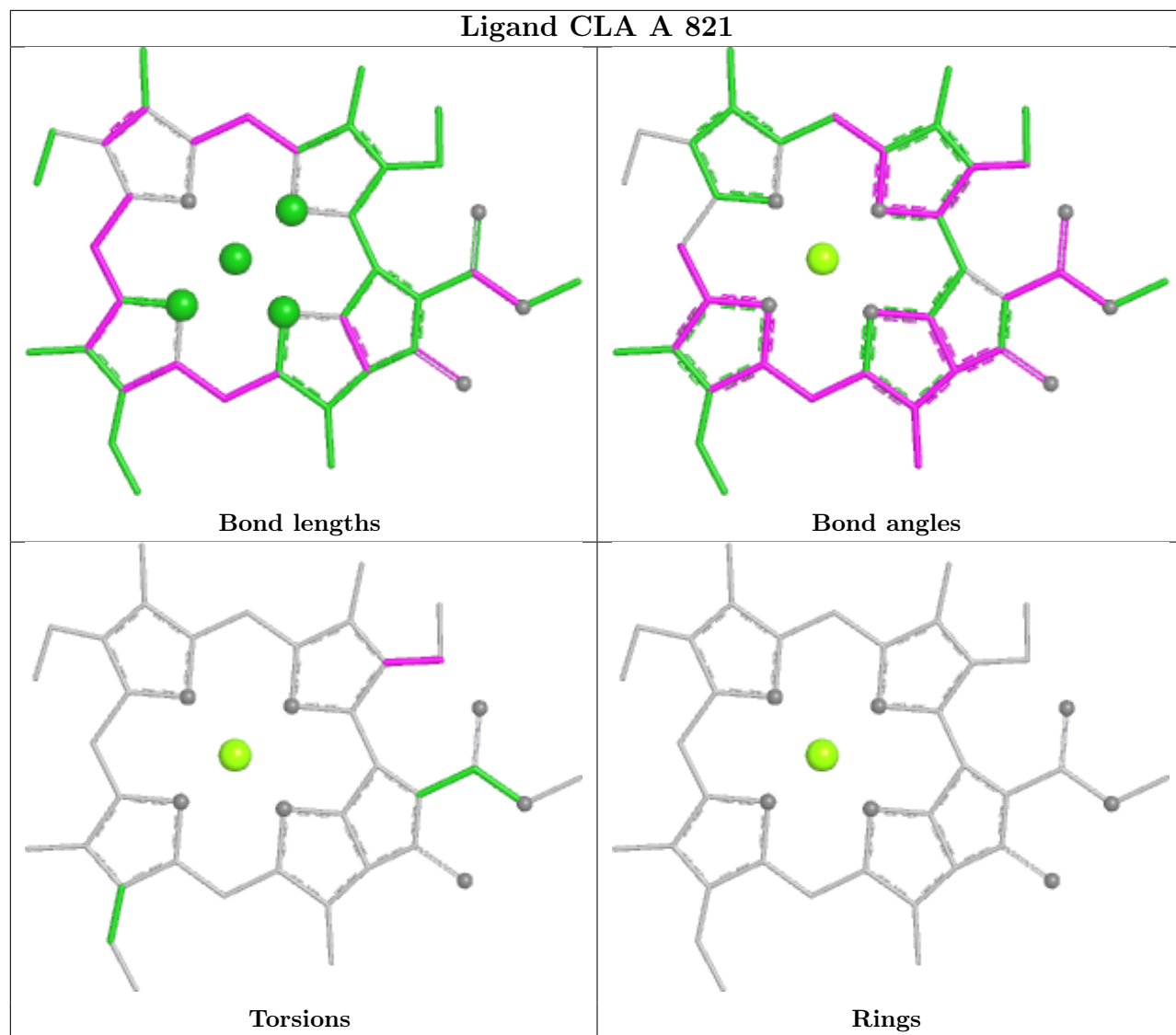
Torsions



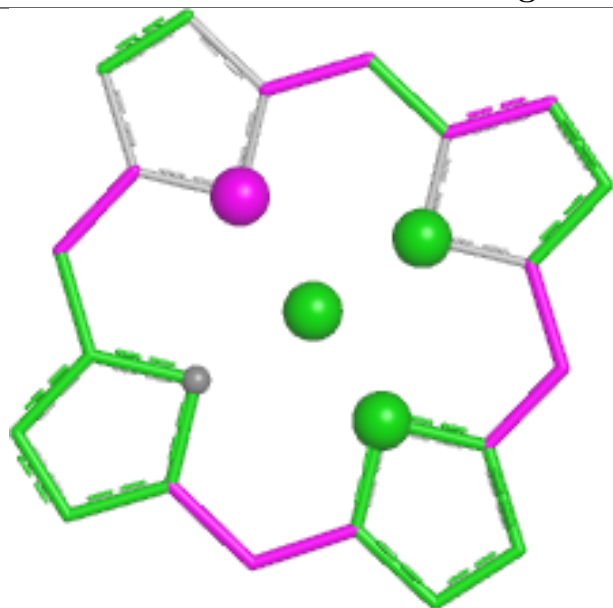
Rings



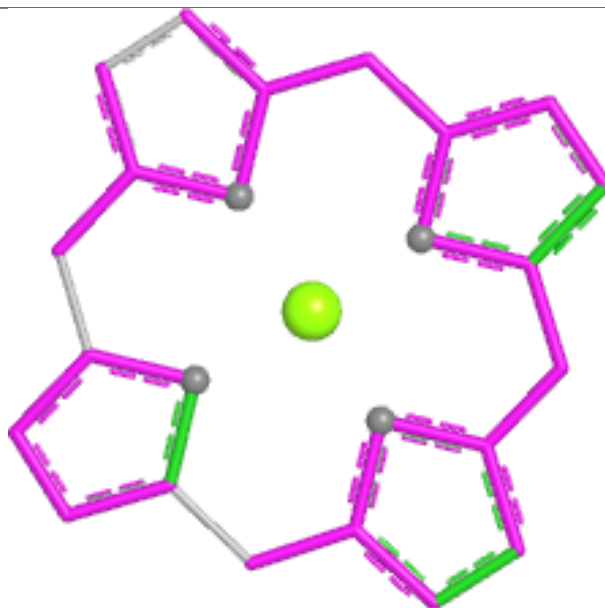
Ligand CLA A 821



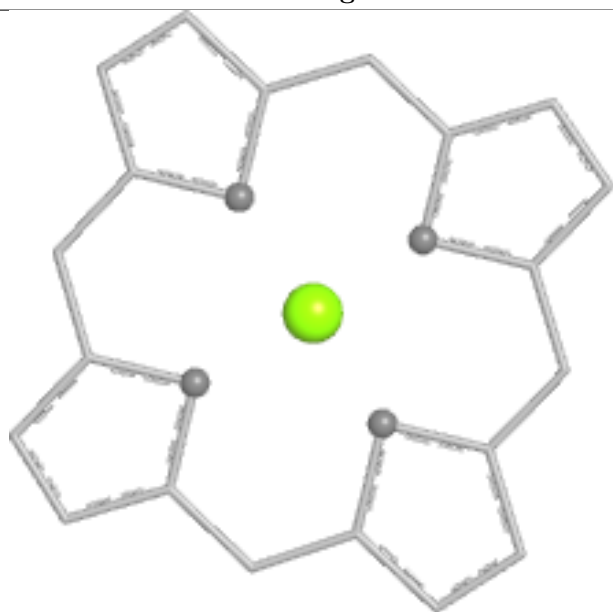
Ligand CLA 1 209



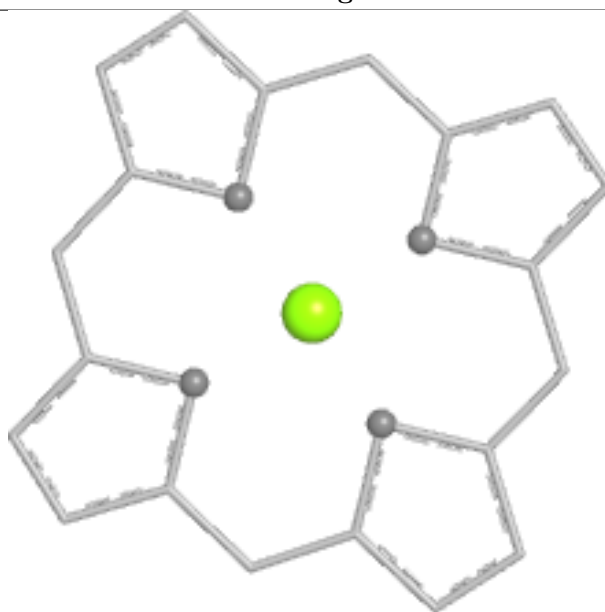
Bond lengths



Bond angles

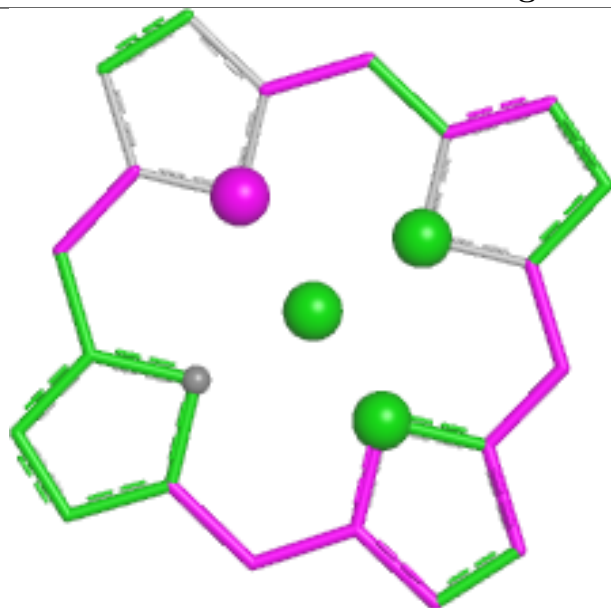


Torsions

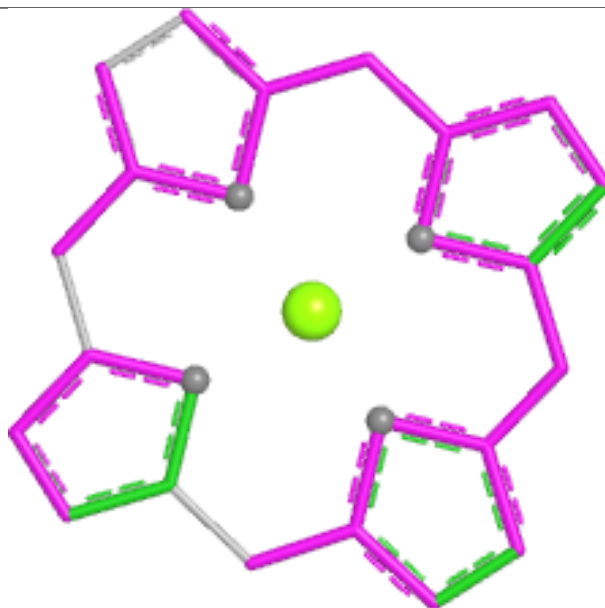


Rings

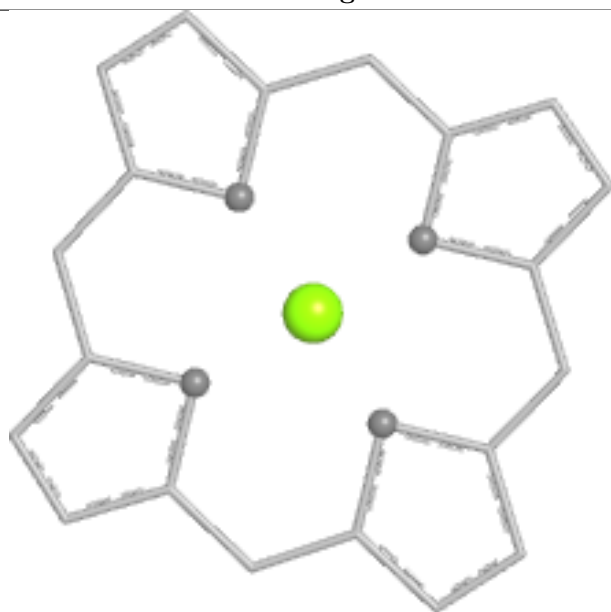
Ligand CLA 2 308



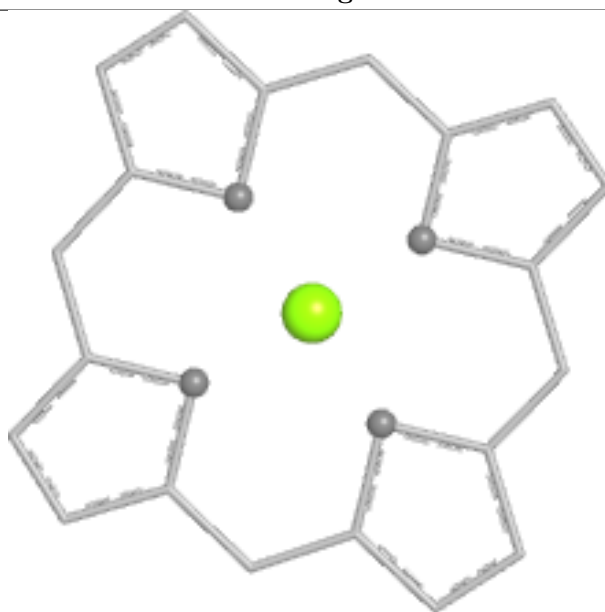
Bond lengths



Bond angles

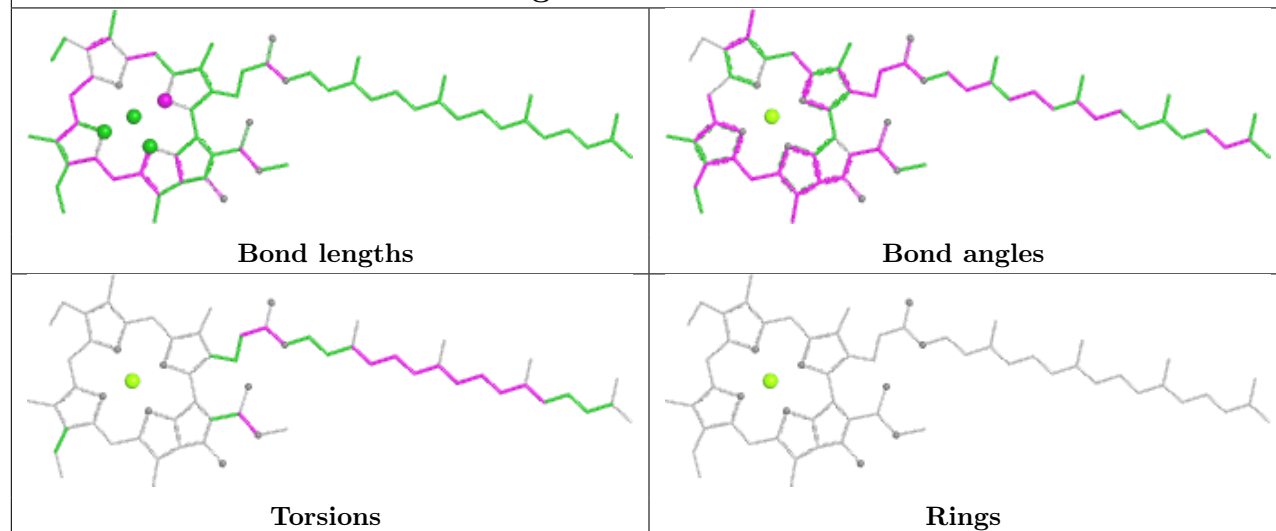


Torsions

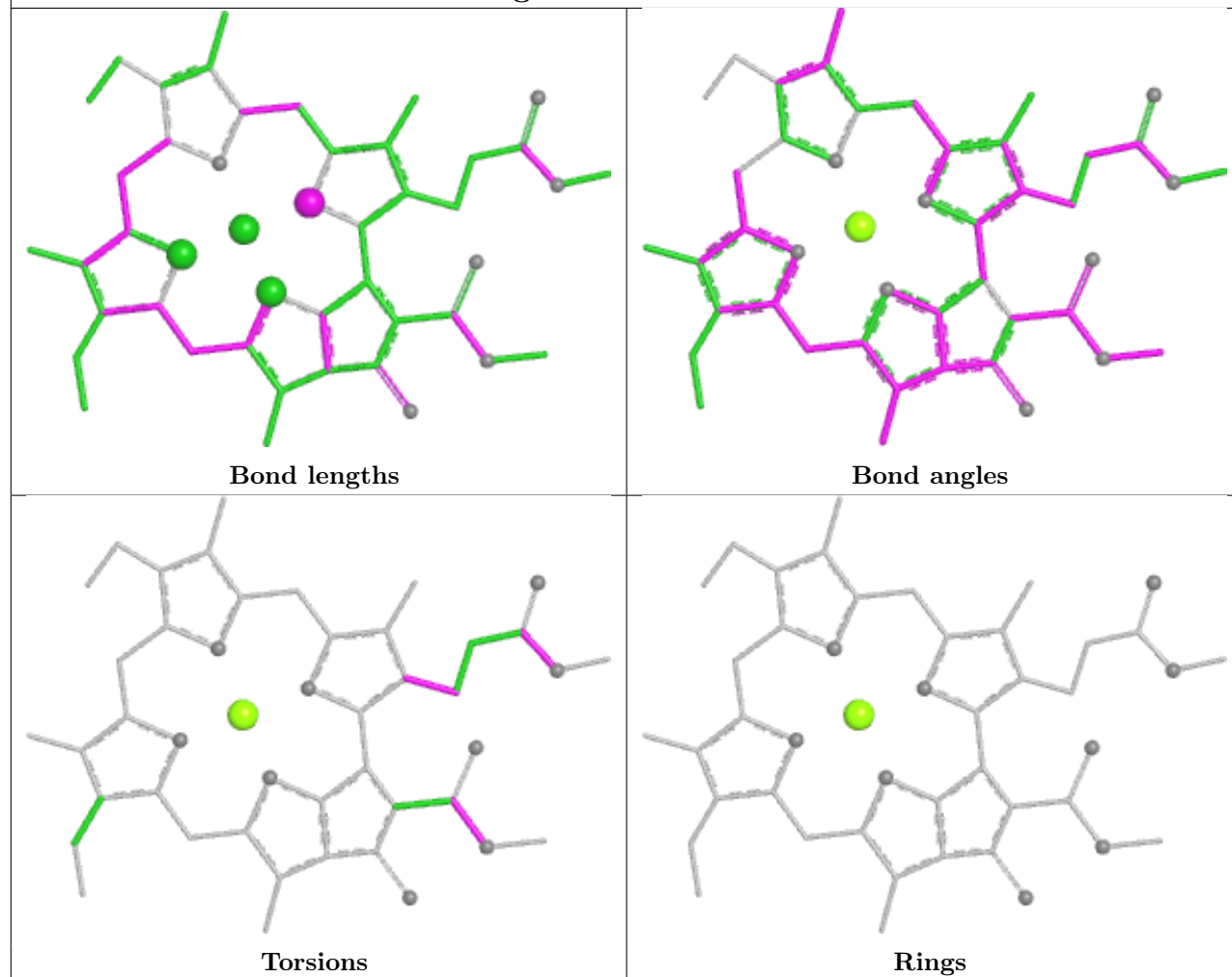


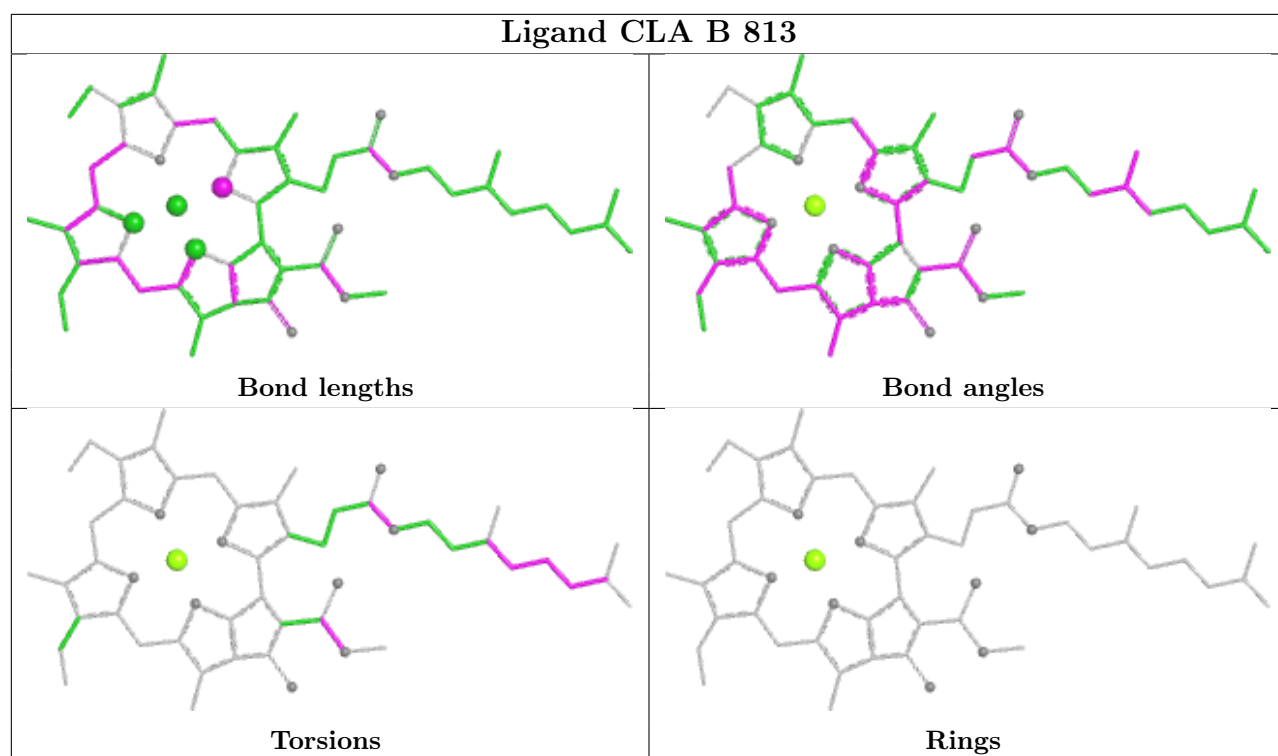
Rings

Ligand CLA B 850

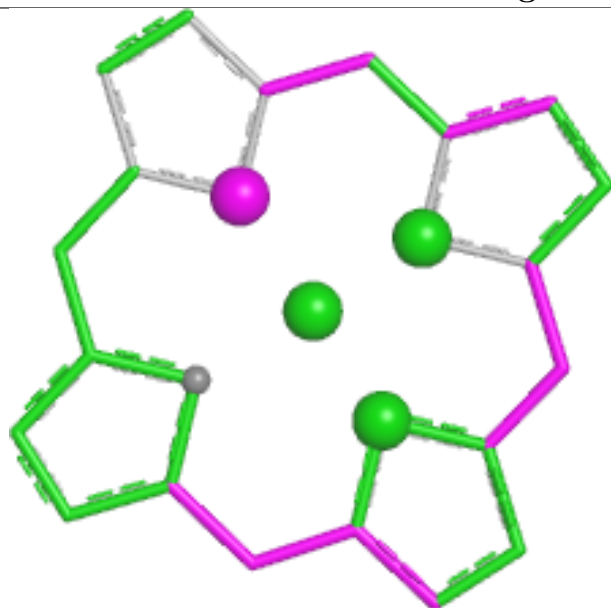


Ligand CLA A 834

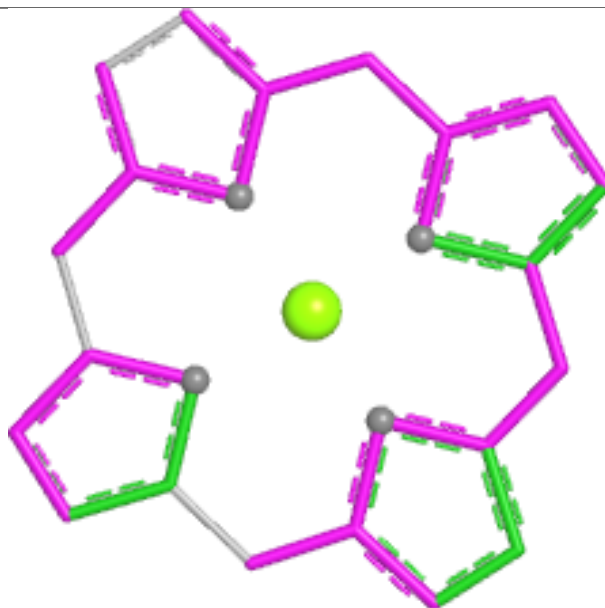




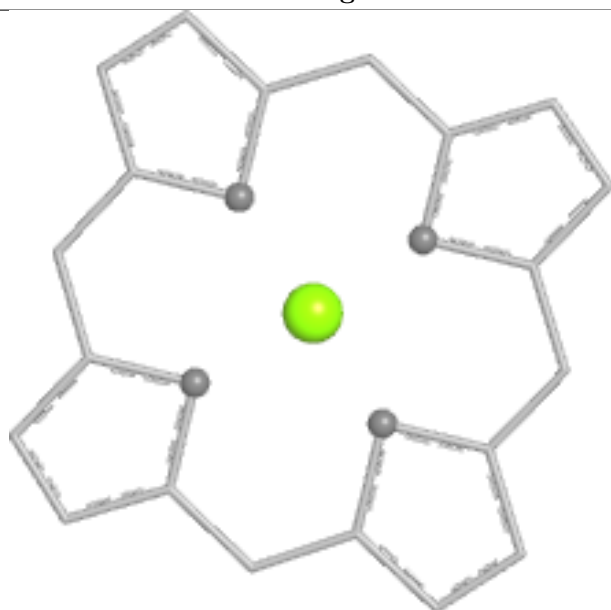
Ligand CLA 4 307



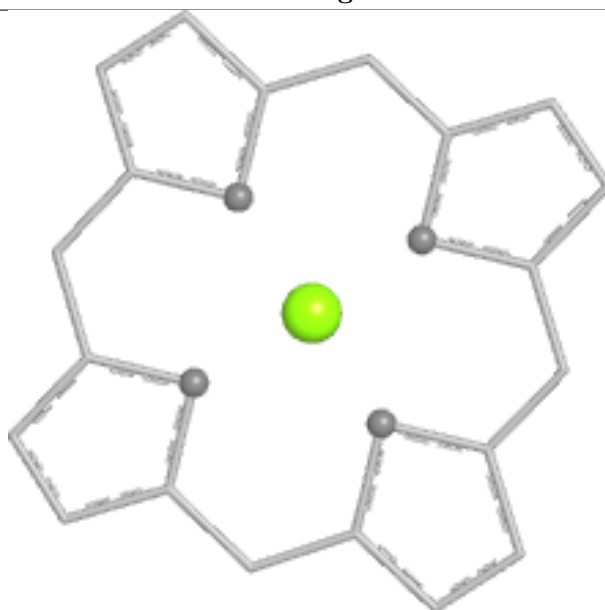
Bond lengths



Bond angles

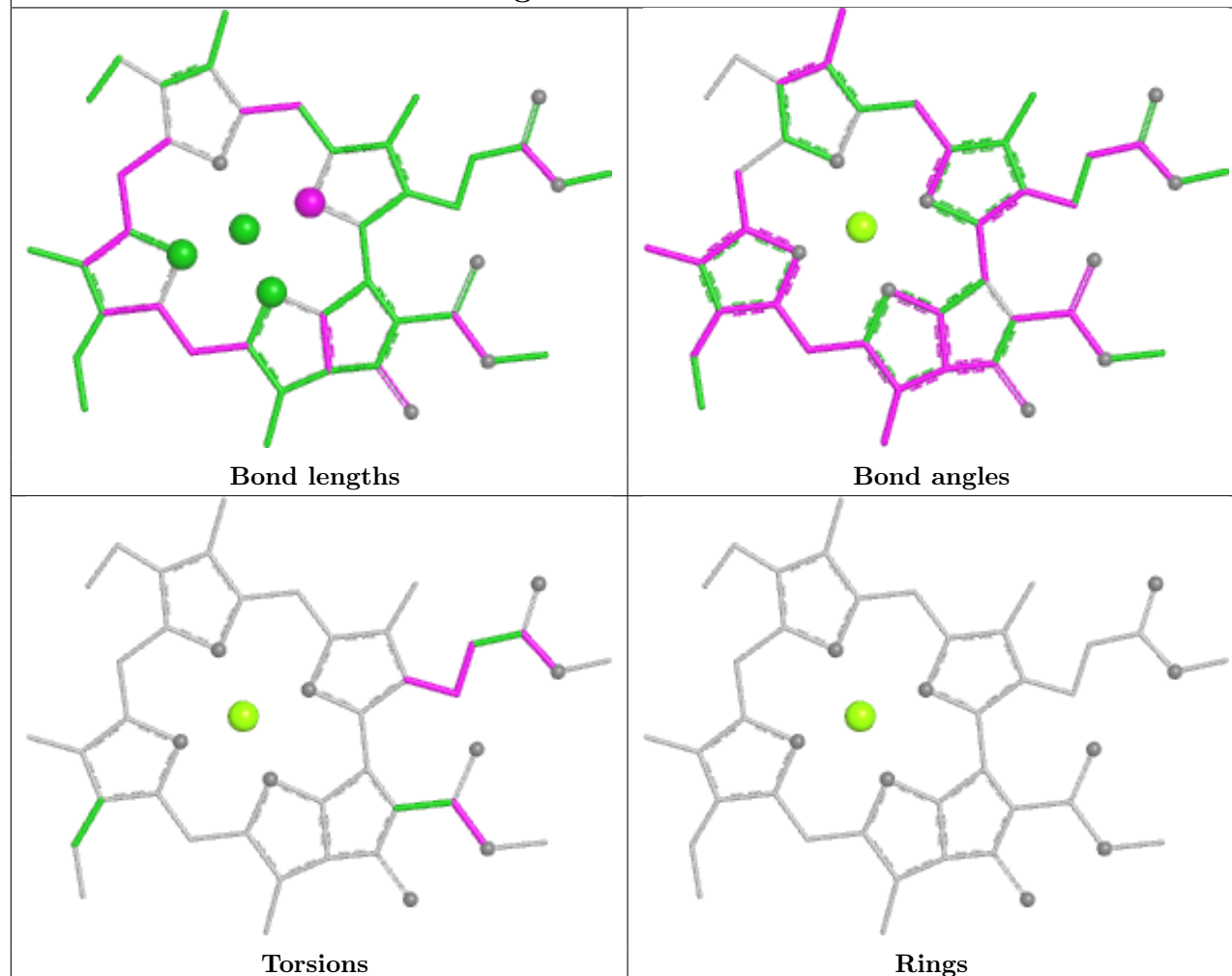


Torsions

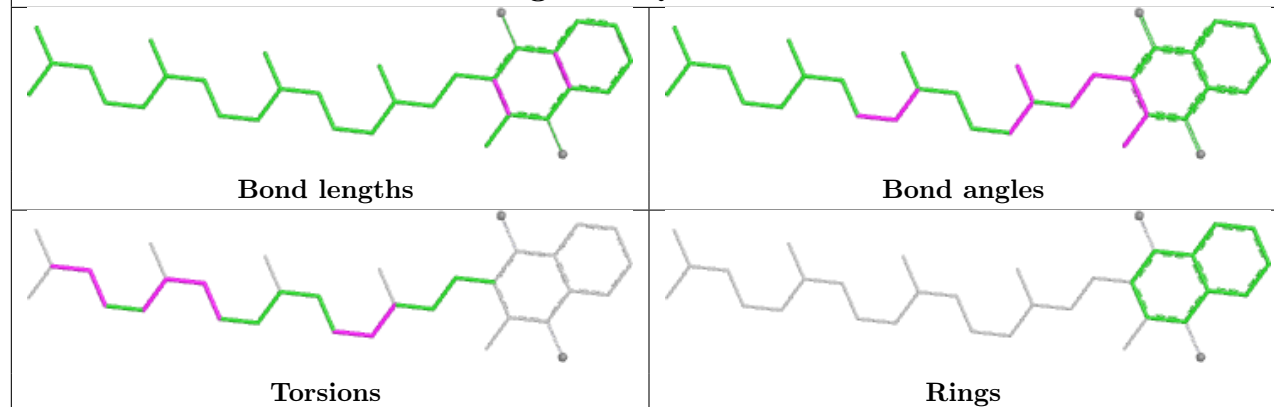


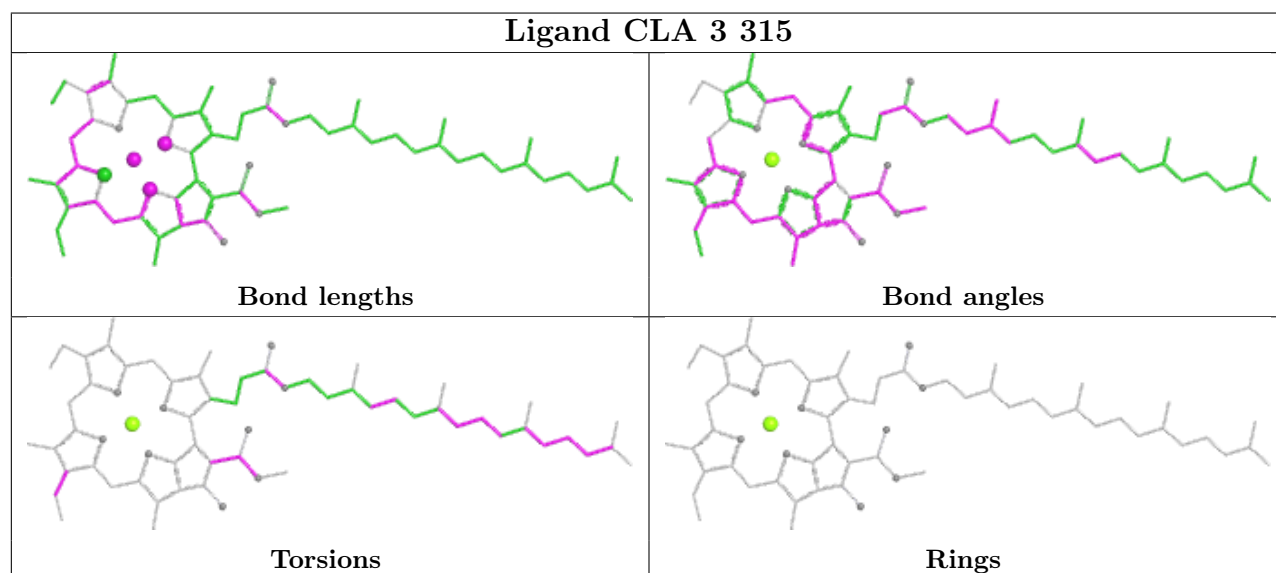
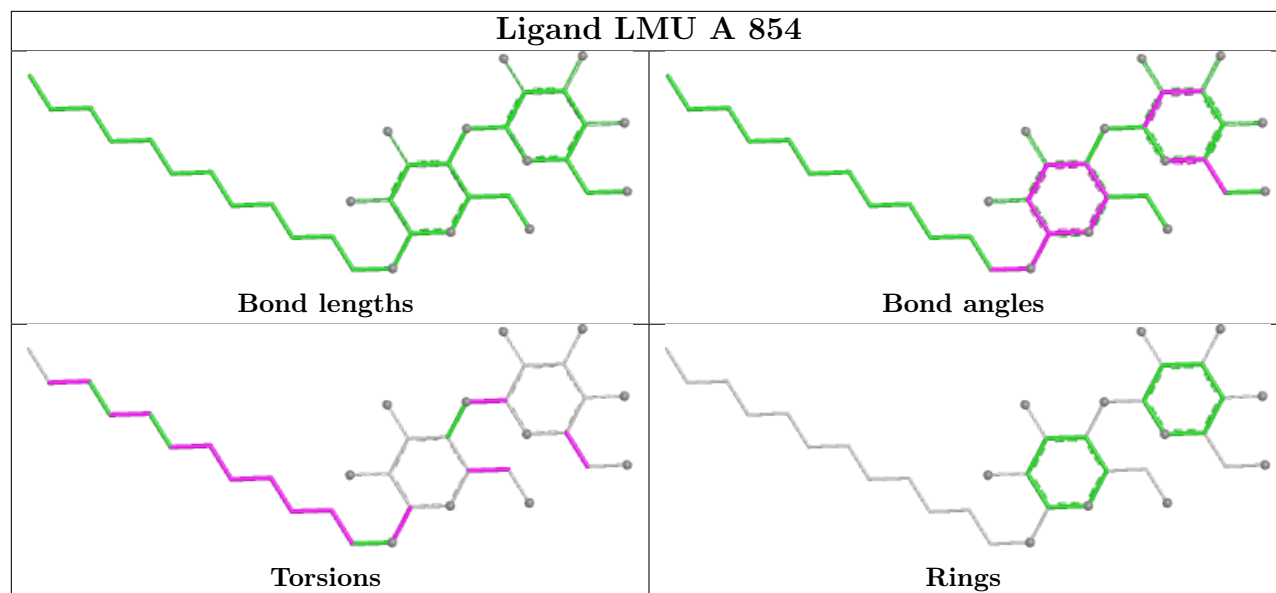
Rings

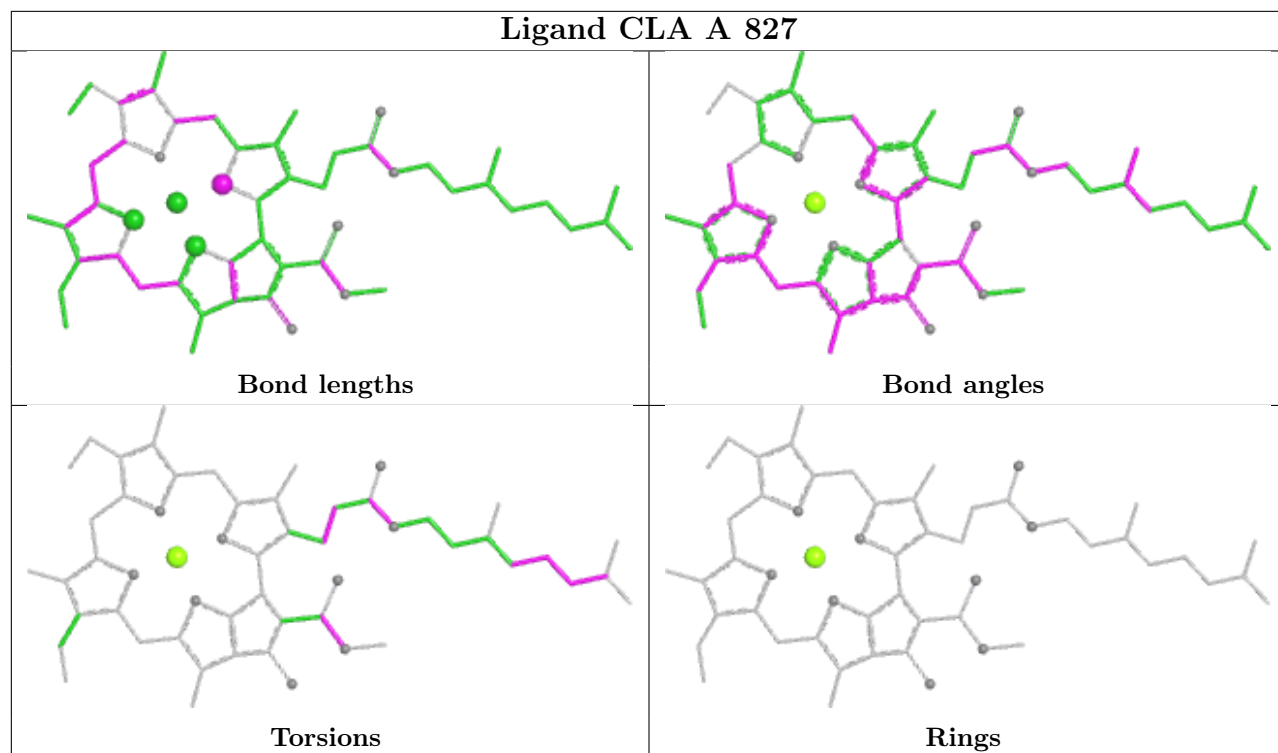
Ligand CLA A 807



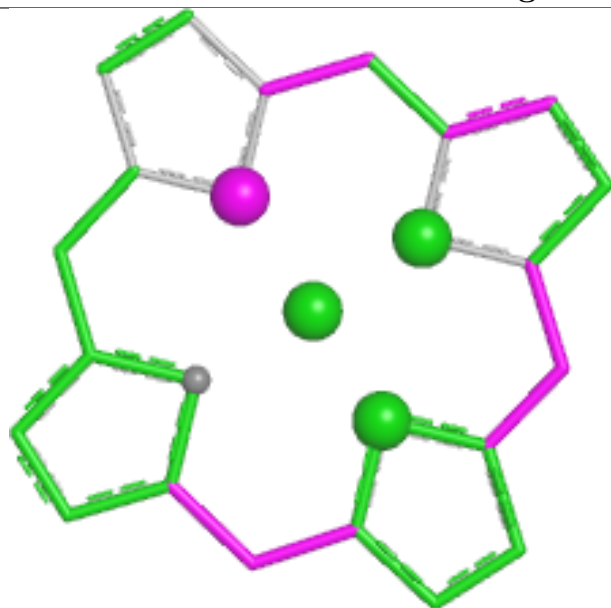
Ligand PQN A 842



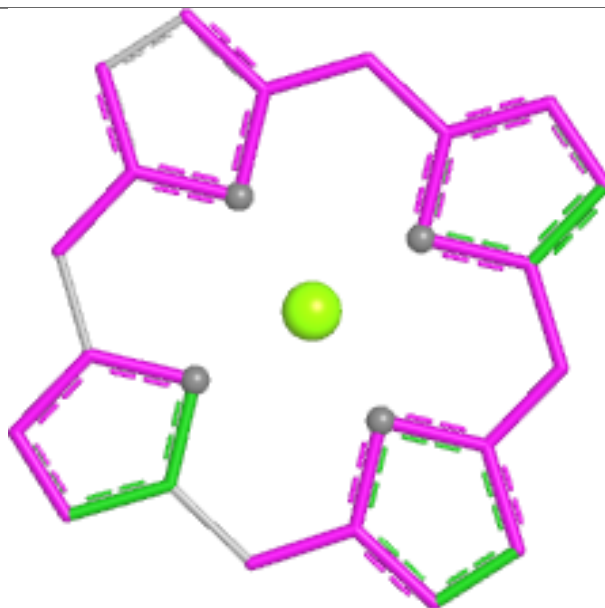




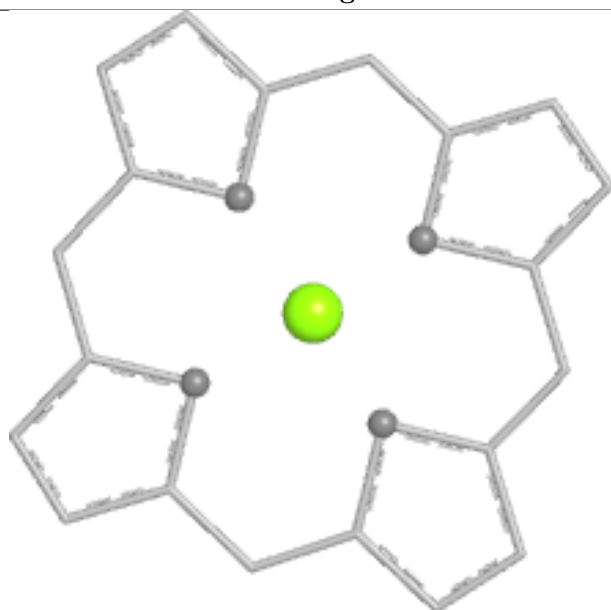
Ligand CLA 4 309



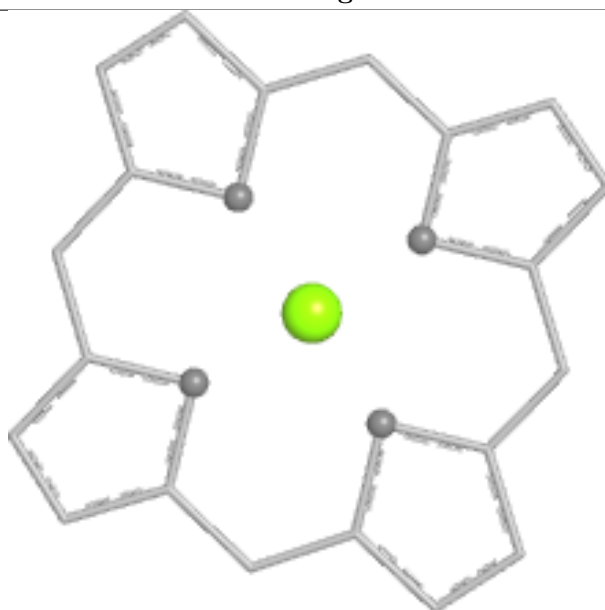
Bond lengths



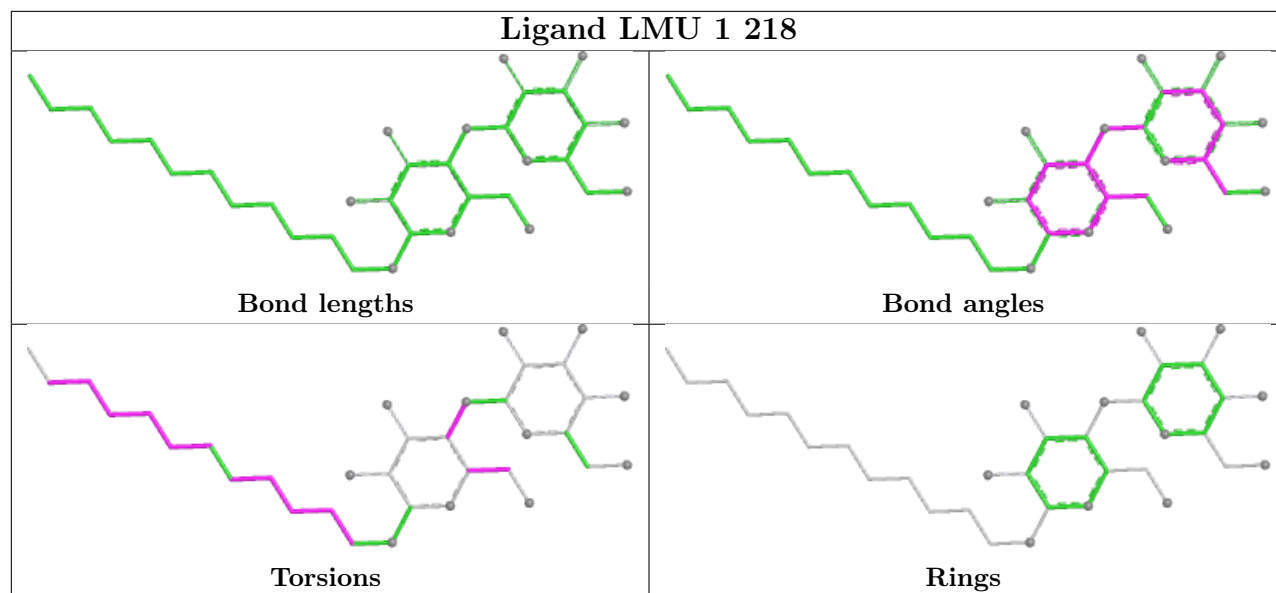
Bond angles



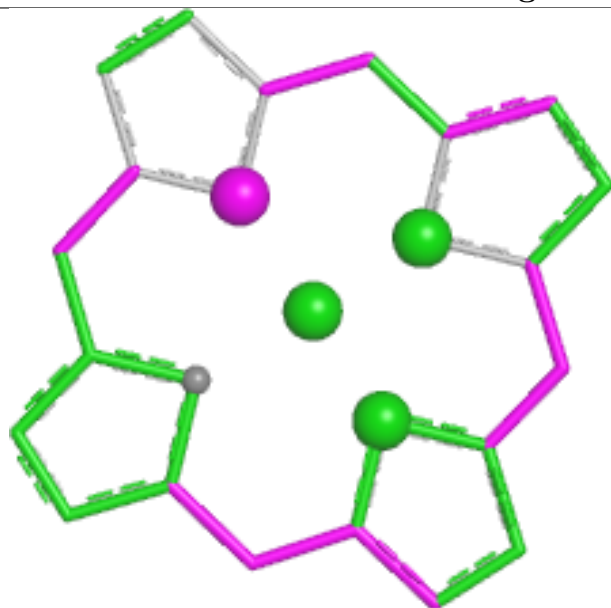
Torsions



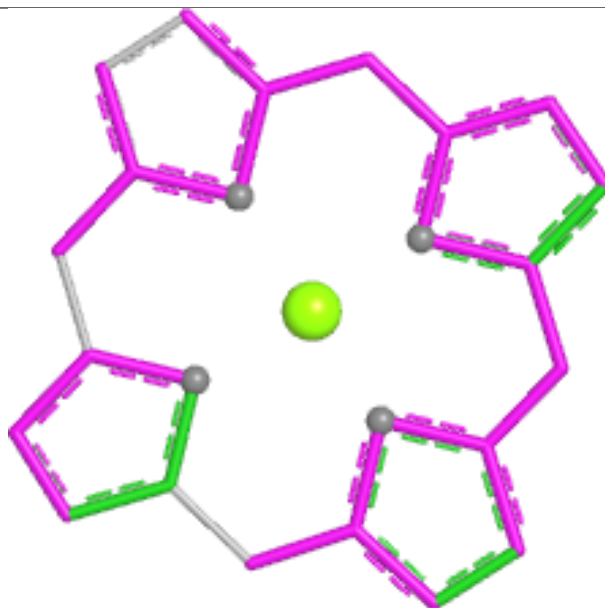
Rings



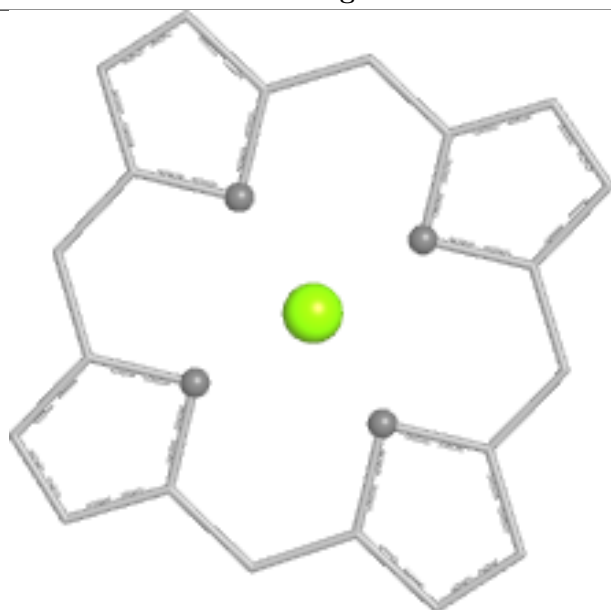
Ligand CLA 3 309



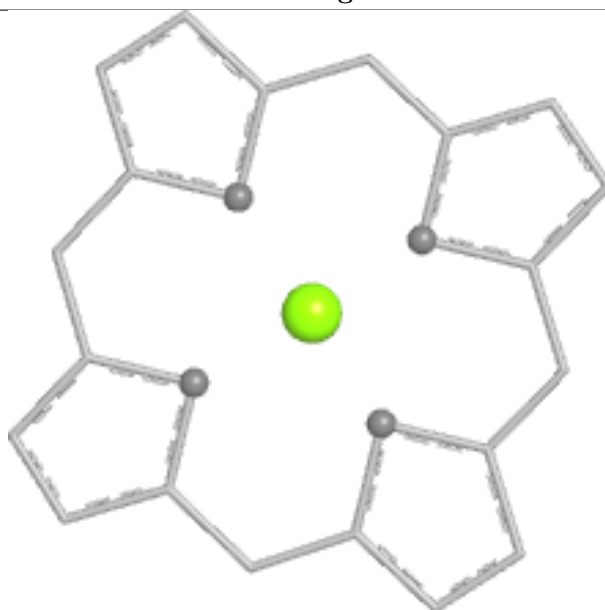
Bond lengths



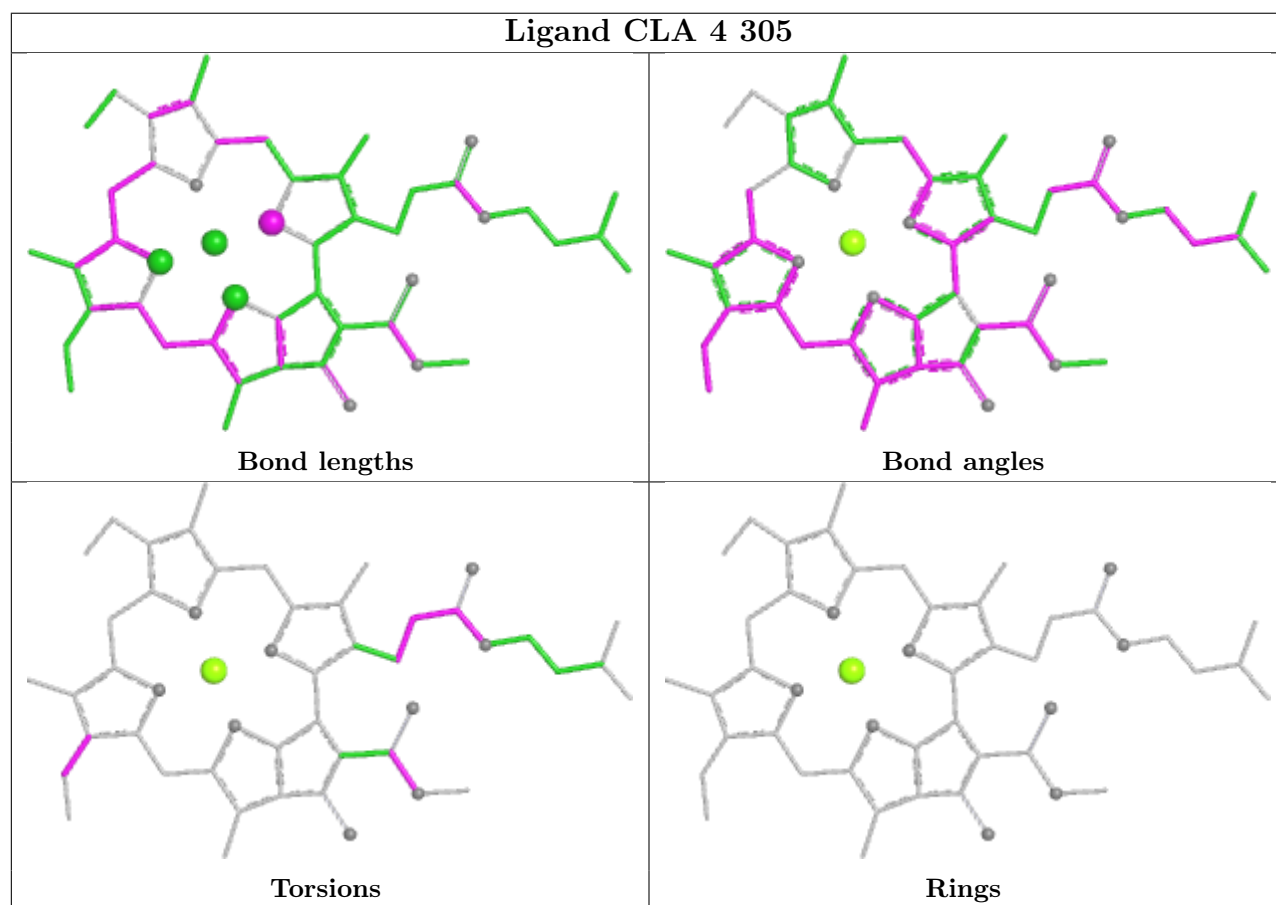
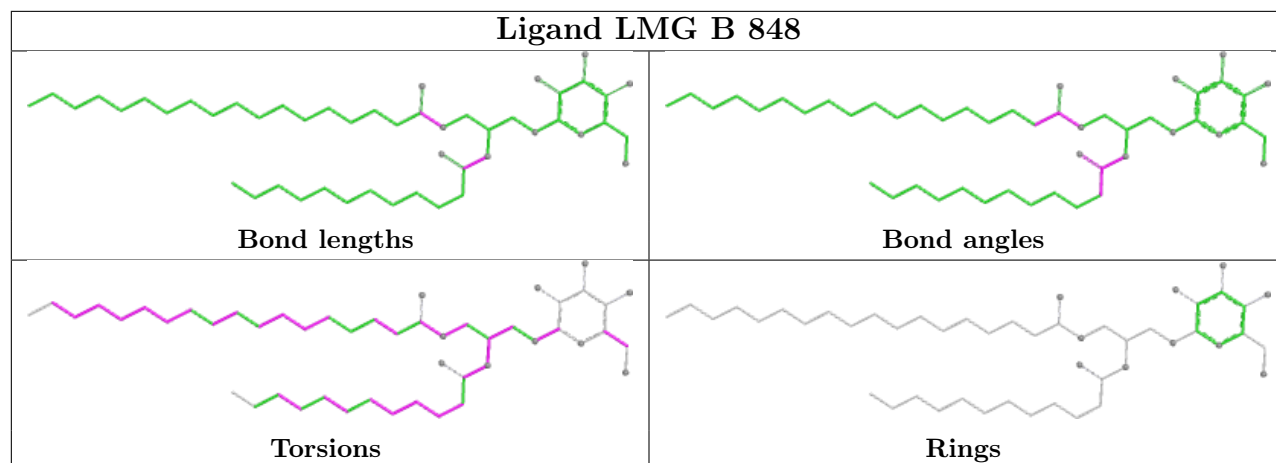
Bond angles



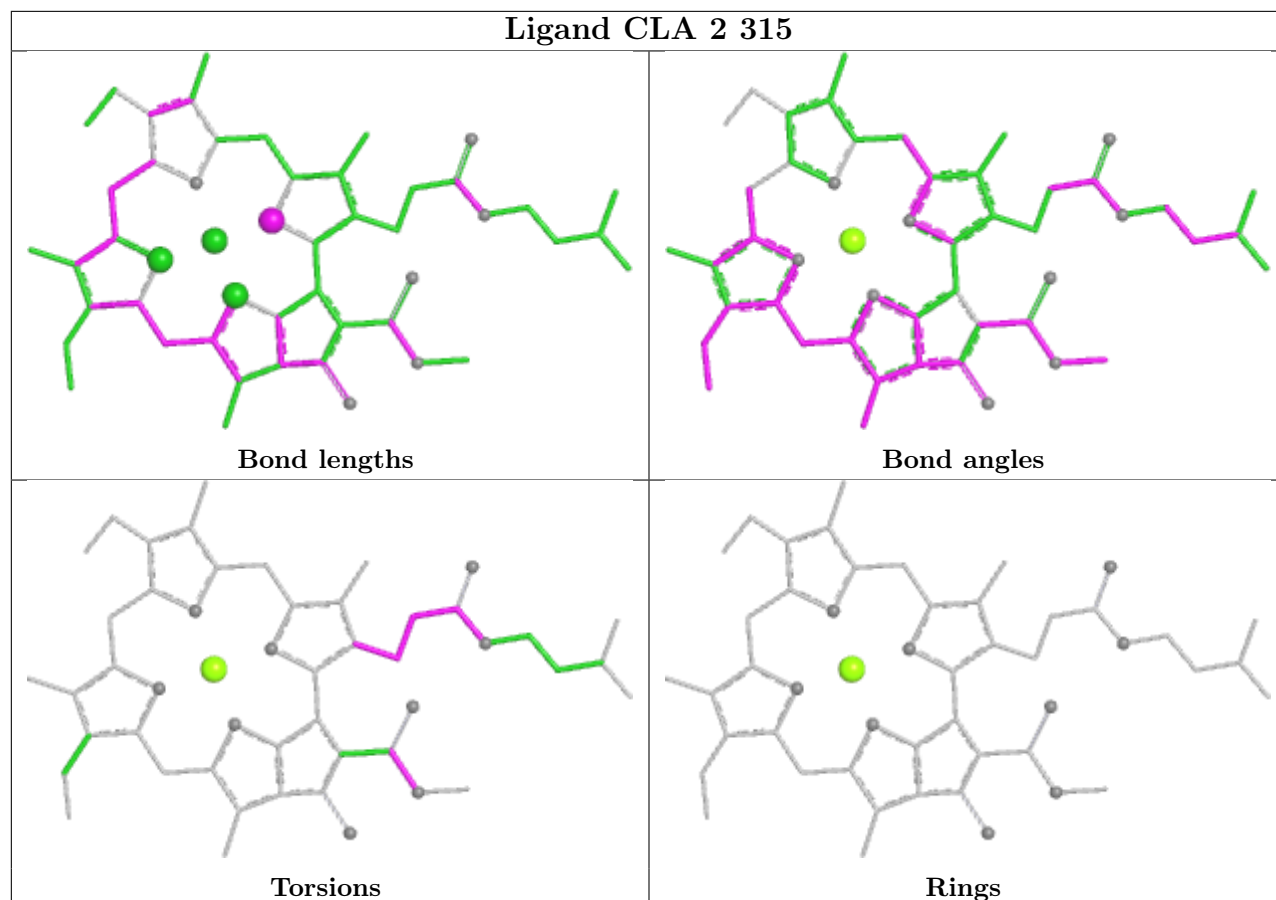
Torsions



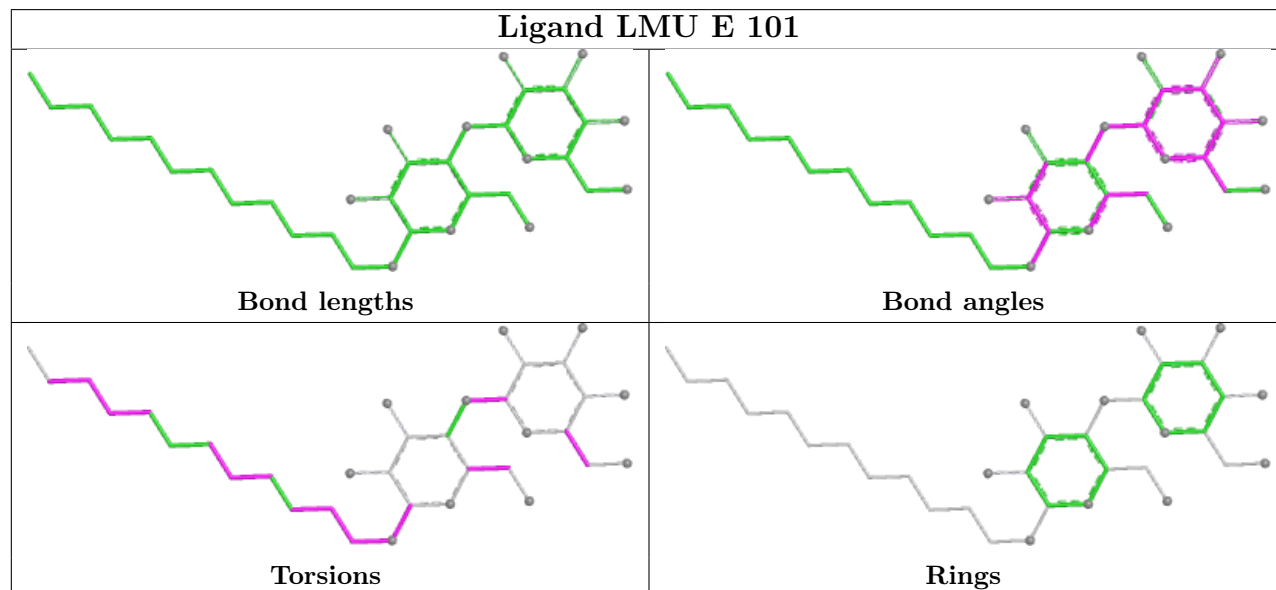
Rings

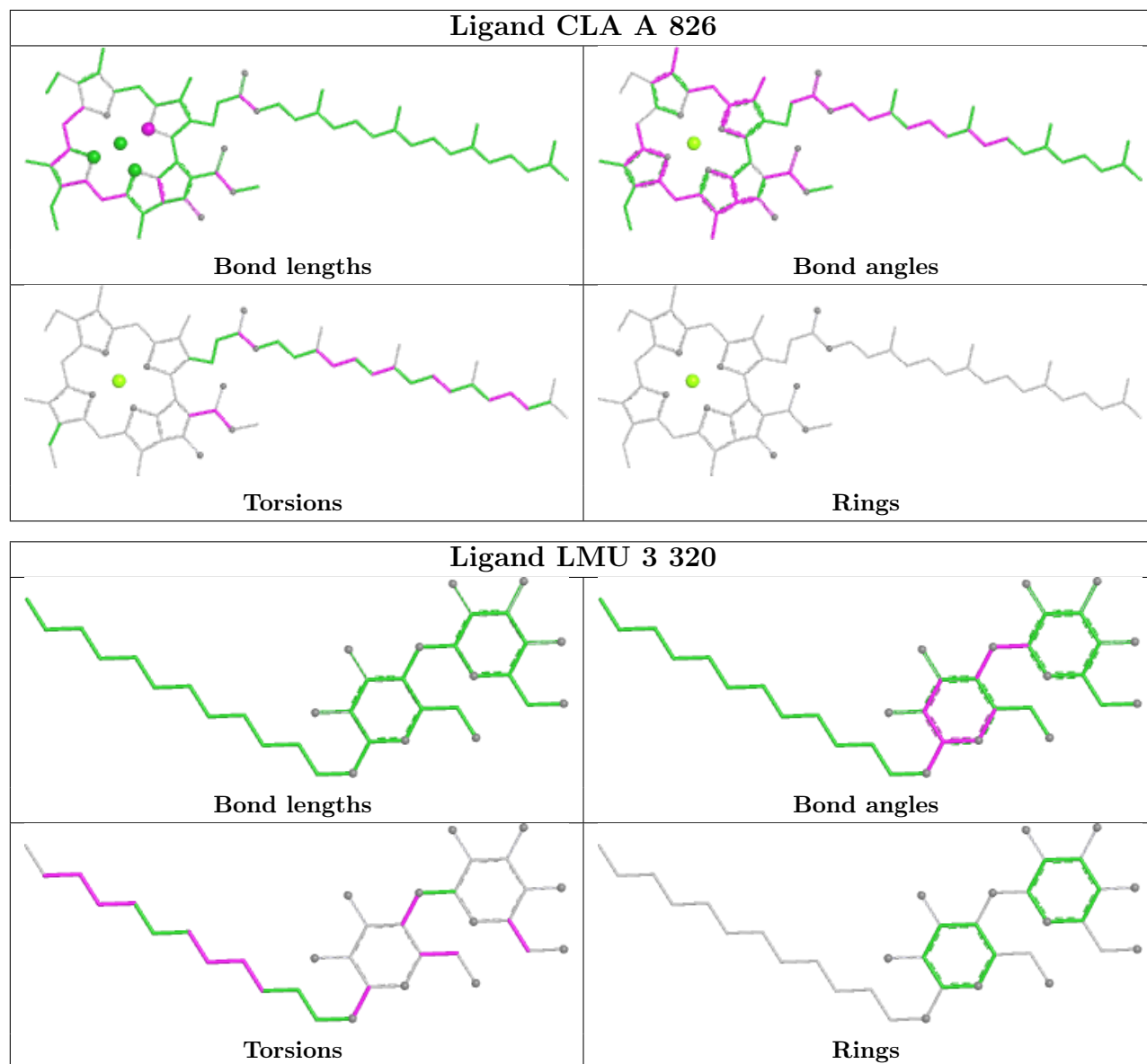


Ligand CLA 2 315

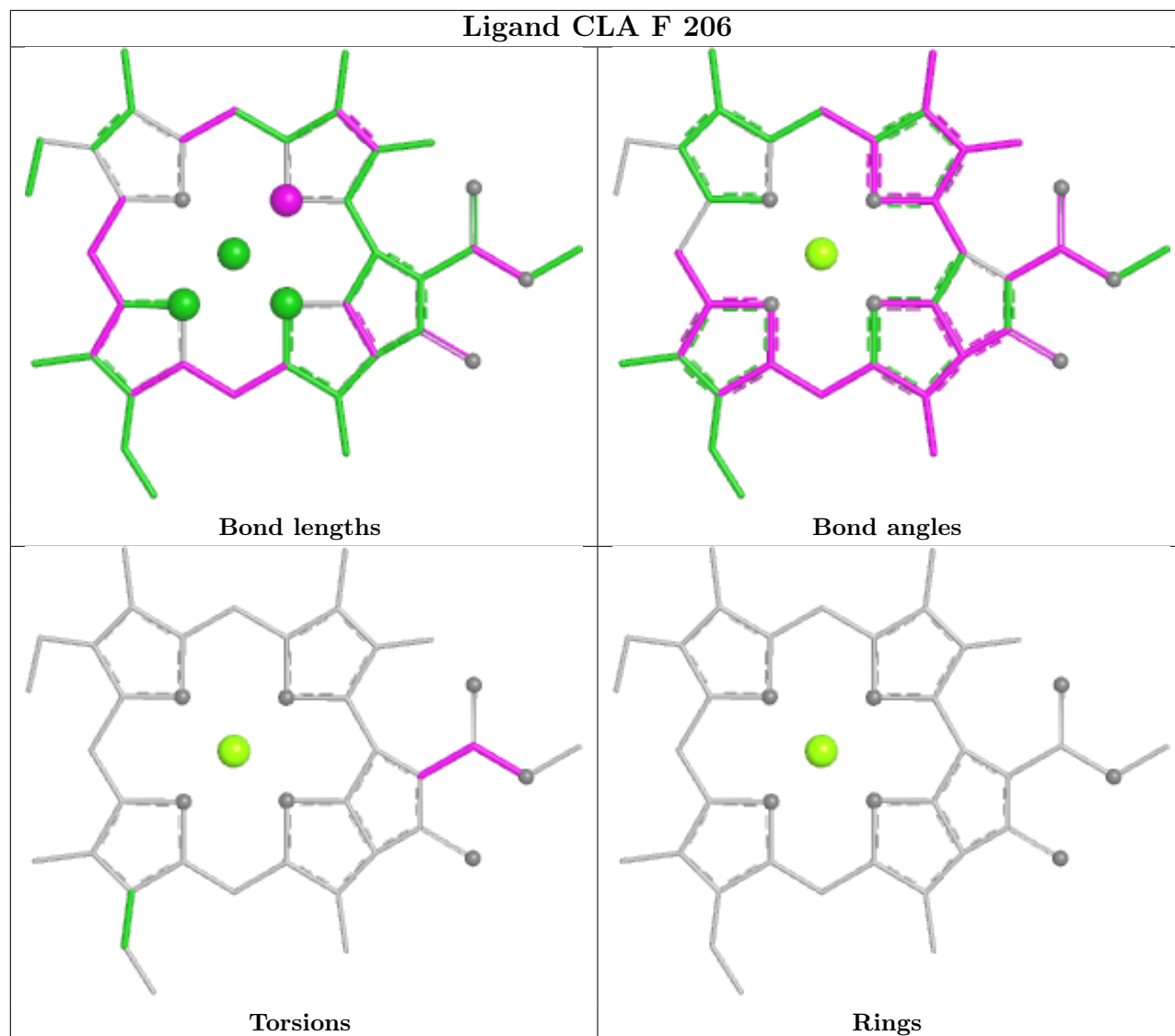


Ligand LMU E 101

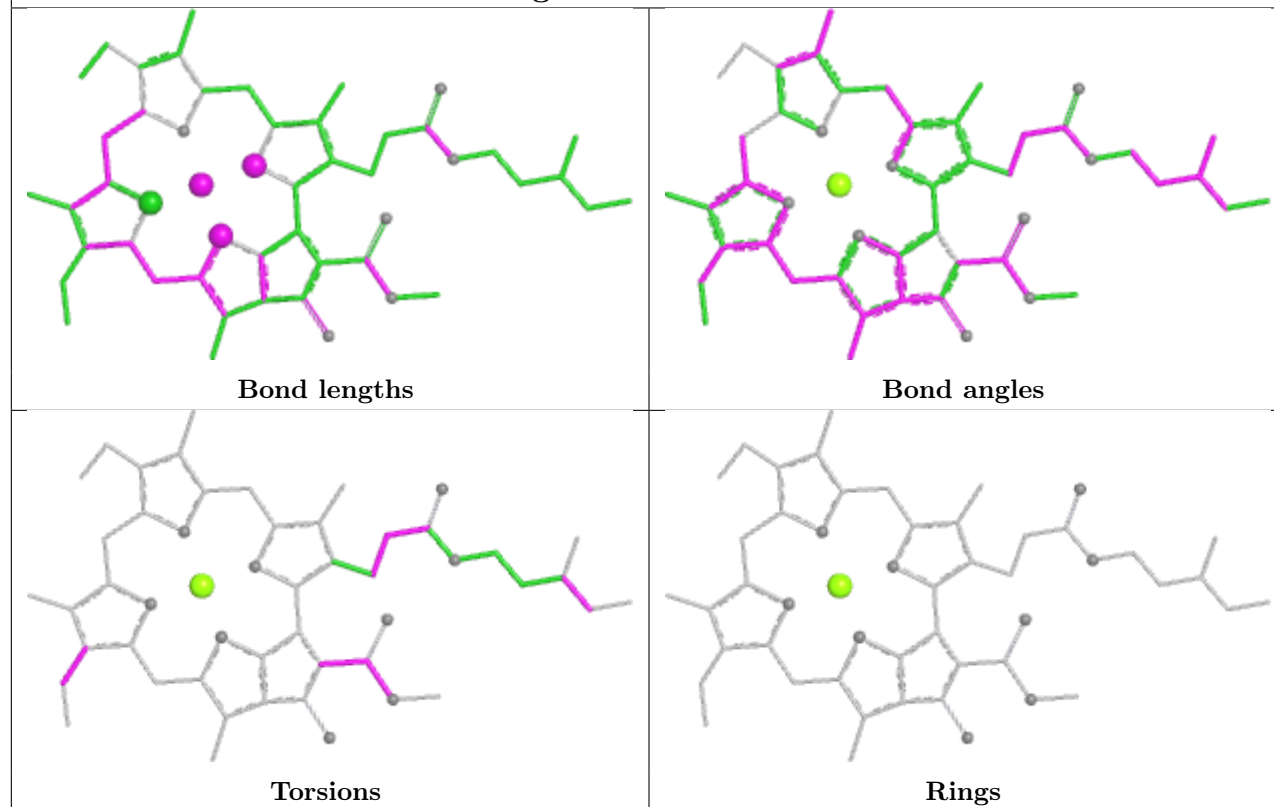




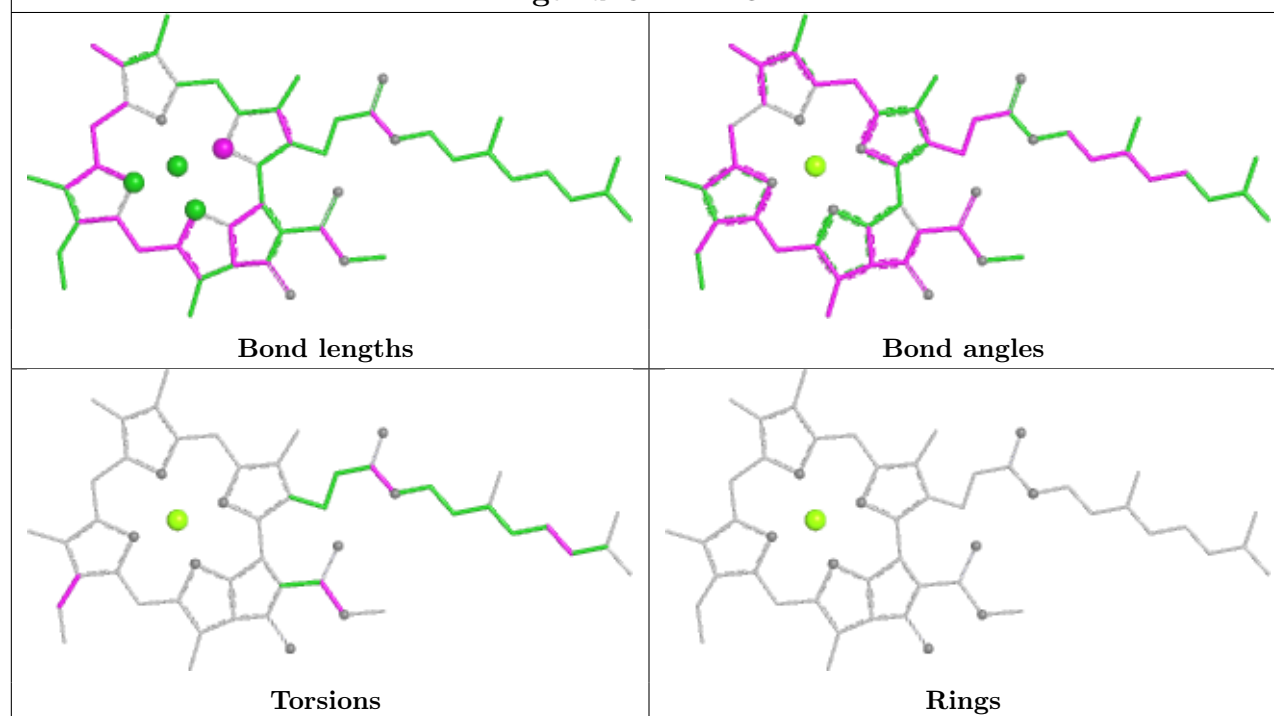
Ligand CLA F 206

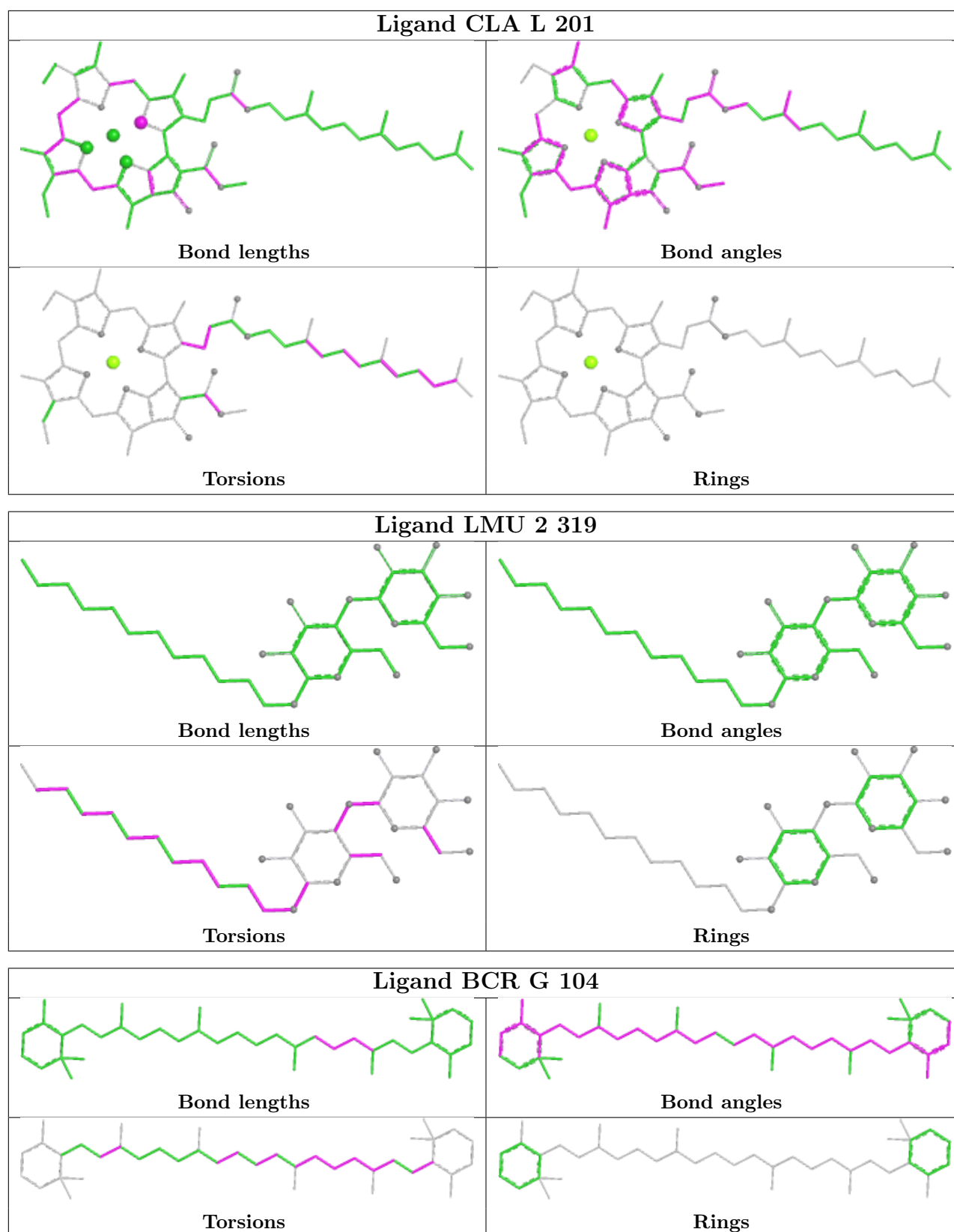


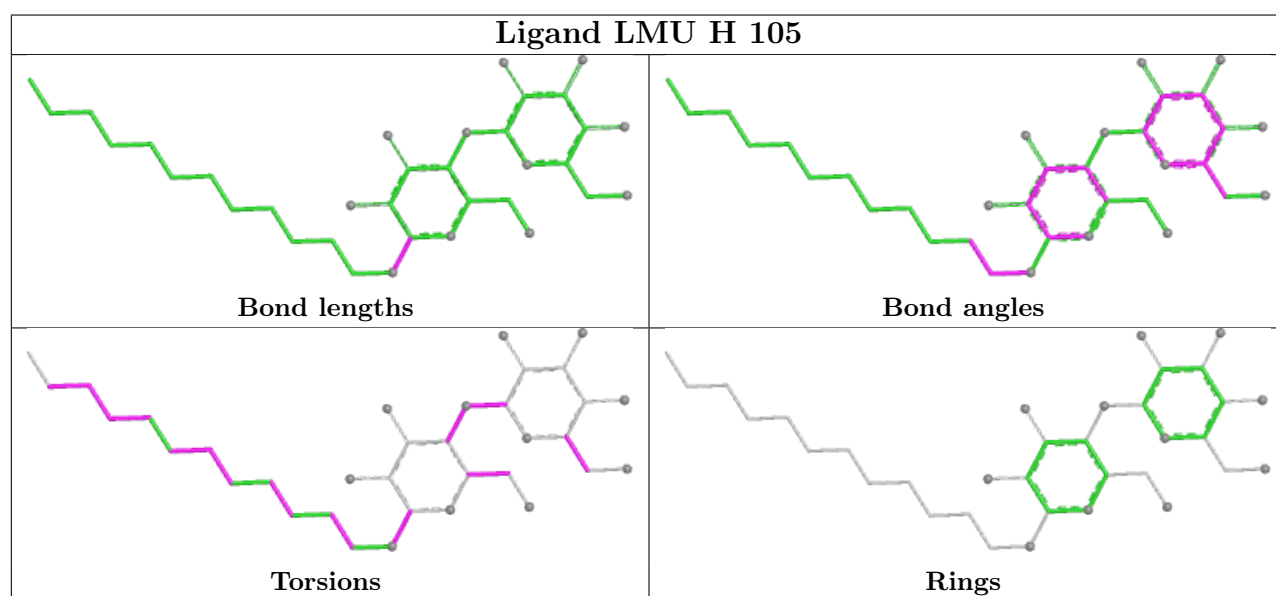
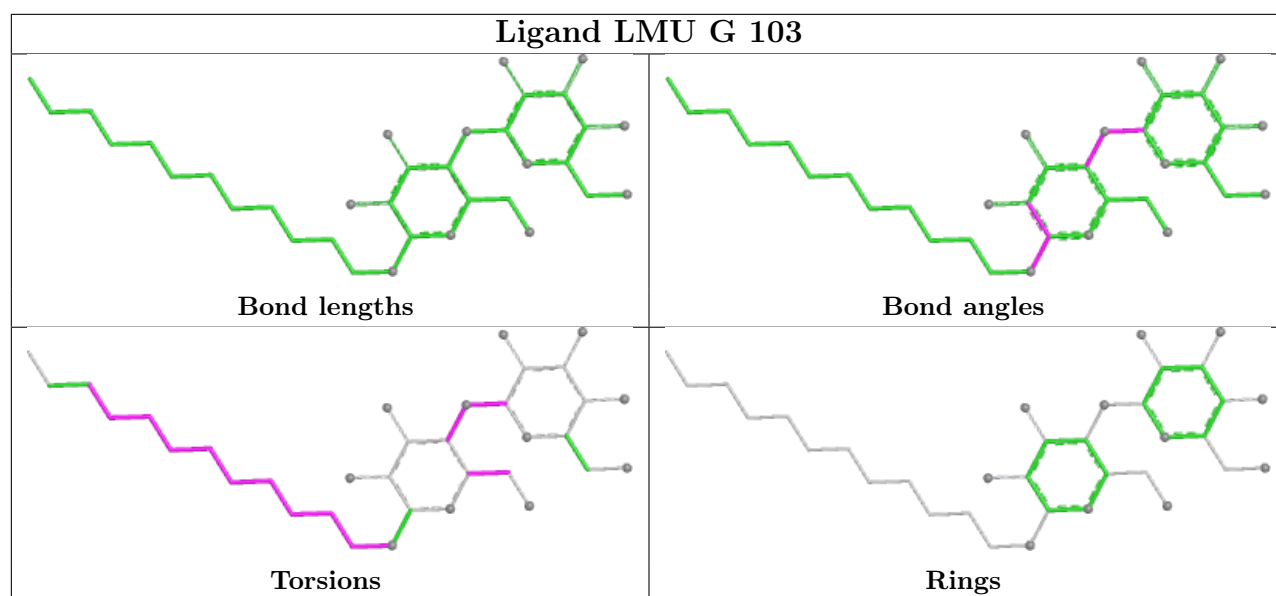
Ligand CLA B 836



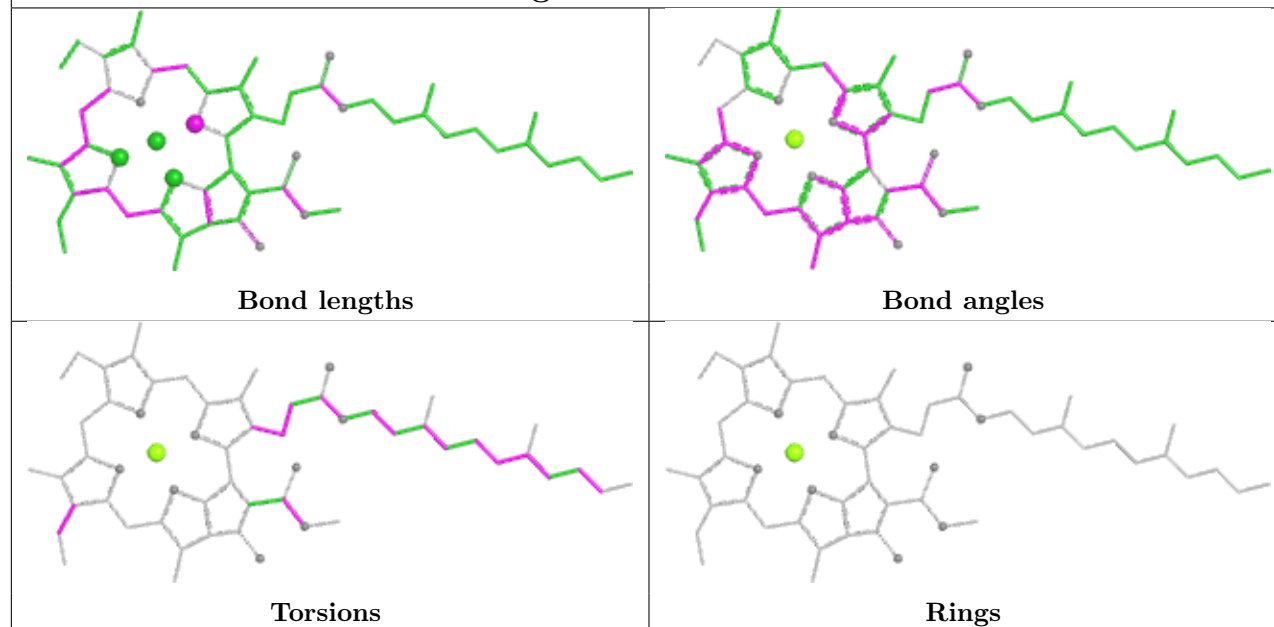
Ligand CLA B 812



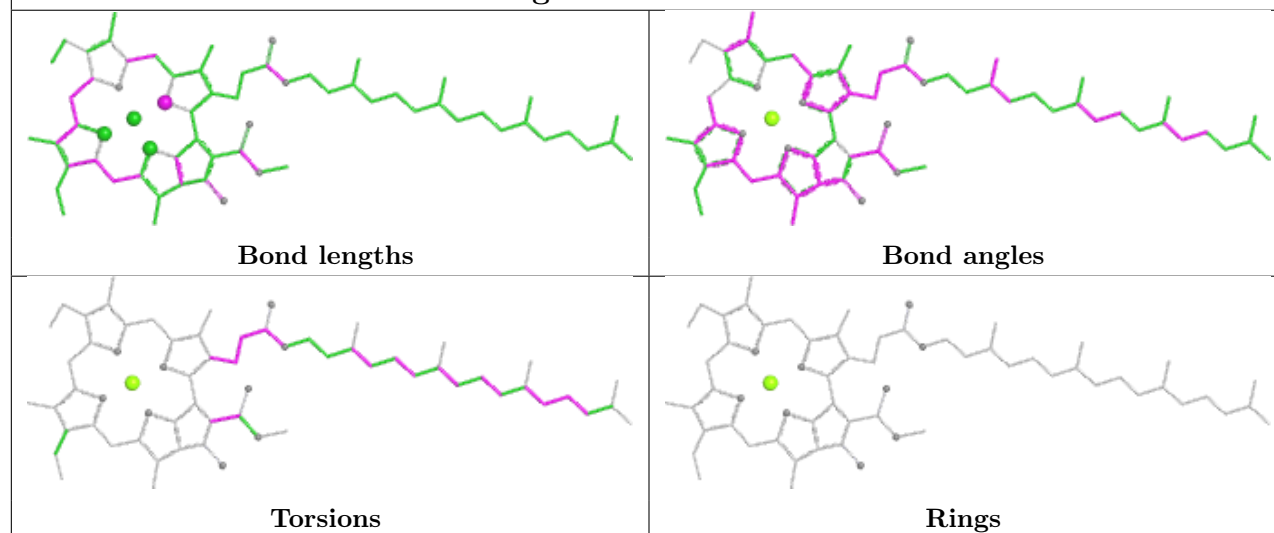




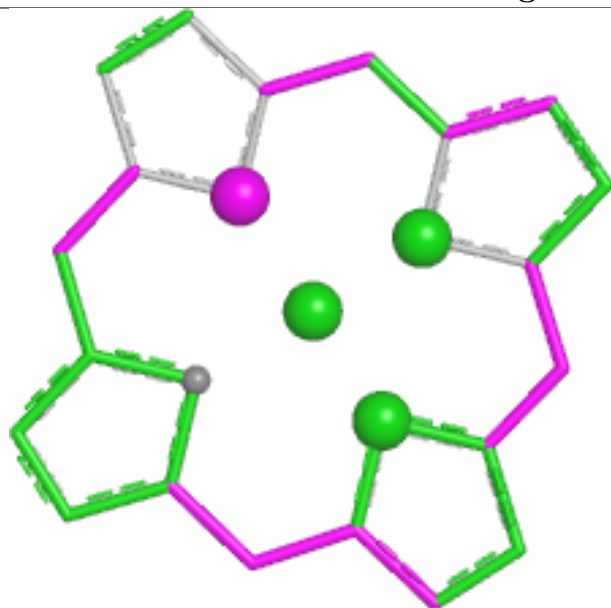
Ligand CLA B 826



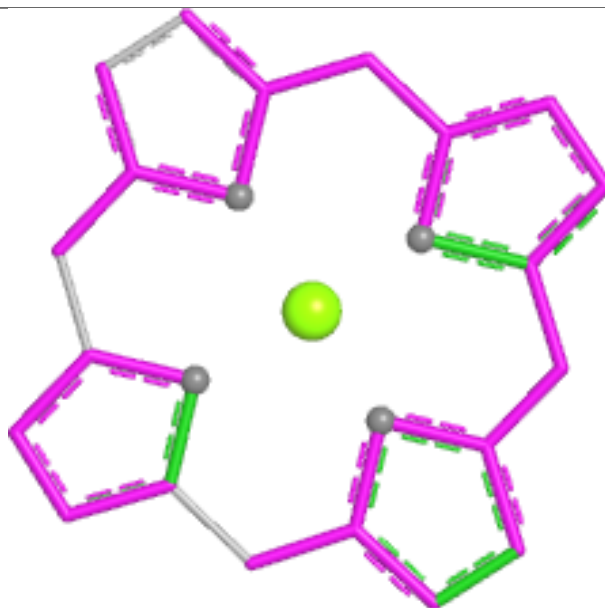
Ligand CLA B 814



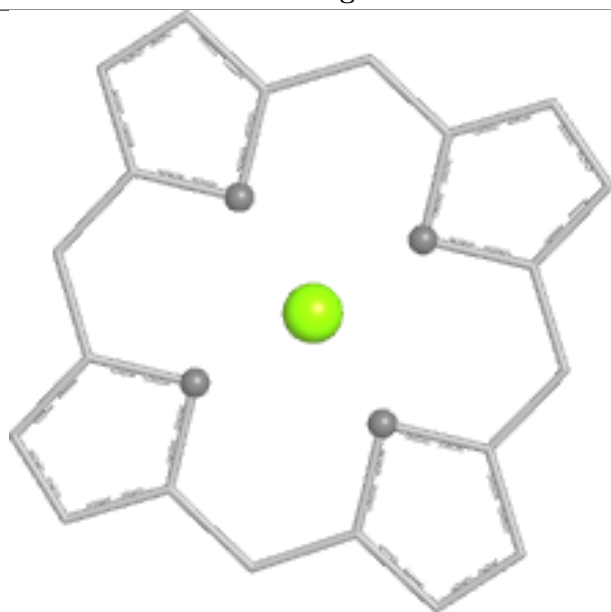
Ligand CLA 3 316



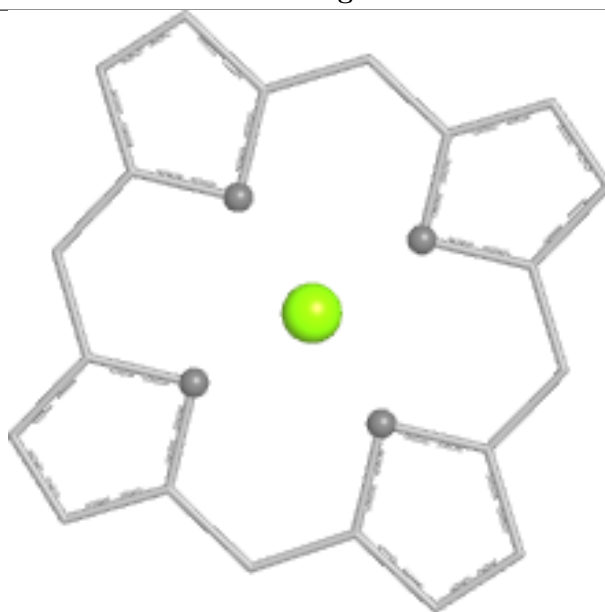
Bond lengths



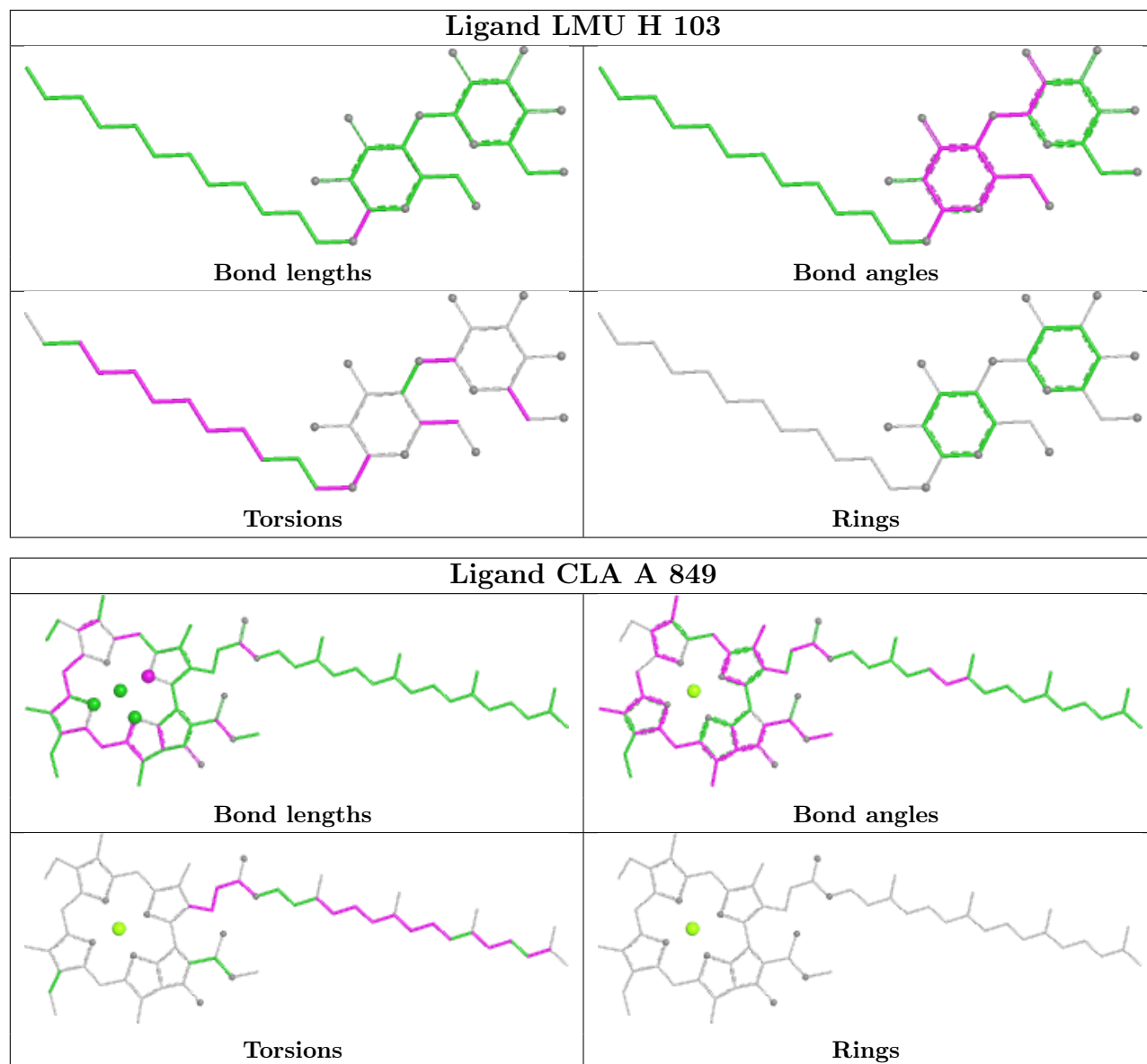
Bond angles



Torsions



Rings



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	1	165/241 (68%)	1.34	39 (23%) 0 0	21, 24, 25, 25	0
2	2	176/269 (65%)	0.89	34 (19%) 1 1	21, 23, 24, 25	0
3	3	153/276 (55%)	1.12	30 (19%) 1 1	49, 78, 110, 112	0
4	4	166/251 (66%)	0.57	15 (9%) 9 11	21, 23, 24, 25	0
5	A	730/758 (96%)	0.62	56 (7%) 13 15	20, 22, 23, 25	0
6	B	733/734 (99%)	0.67	53 (7%) 15 17	20, 22, 24, 25	0
7	C	81/81 (100%)	0.83	11 (13%) 3 4	21, 22, 23, 23	0
8	D	138/212 (65%)	0.90	25 (18%) 1 2	21, 23, 24, 25	0
9	E	65/143 (45%)	0.71	10 (15%) 2 3	21, 22, 24, 24	0
10	F	154/231 (66%)	0.60	12 (7%) 13 15	21, 22, 23, 24	0
11	G	95/167 (56%)	0.95	12 (12%) 3 5	21, 23, 24, 25	0
12	H	69/144 (47%)	0.83	10 (14%) 2 3	21, 23, 24, 25	0
13	I	30/40 (75%)	0.32	1 (3%) 46 43	21, 22, 23, 23	0
14	J	42/44 (95%)	0.51	3 (7%) 16 17	21, 23, 23, 24	0
15	K	84/131 (64%)	1.48	19 (22%) 0 0	21, 24, 24, 26	0
16	L	162/216 (75%)	0.60	18 (11%) 5 7	20, 23, 24, 25	0
17	N	85/170 (50%)	0.60	7 (8%) 11 13	22, 23, 24, 25	0
18	R	0/53	-	-	-	-
All	All	3128/4161 (75%)	0.76	355 (11%) 5 6	20, 23, 25, 112	0

The worst 5 of 355 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
15	K	16	THR	10.2
3	3	40	SER	8.6
1	1	92	GLY	7.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	1	87	ASN	7.4
15	K	64	GLY	7.0

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

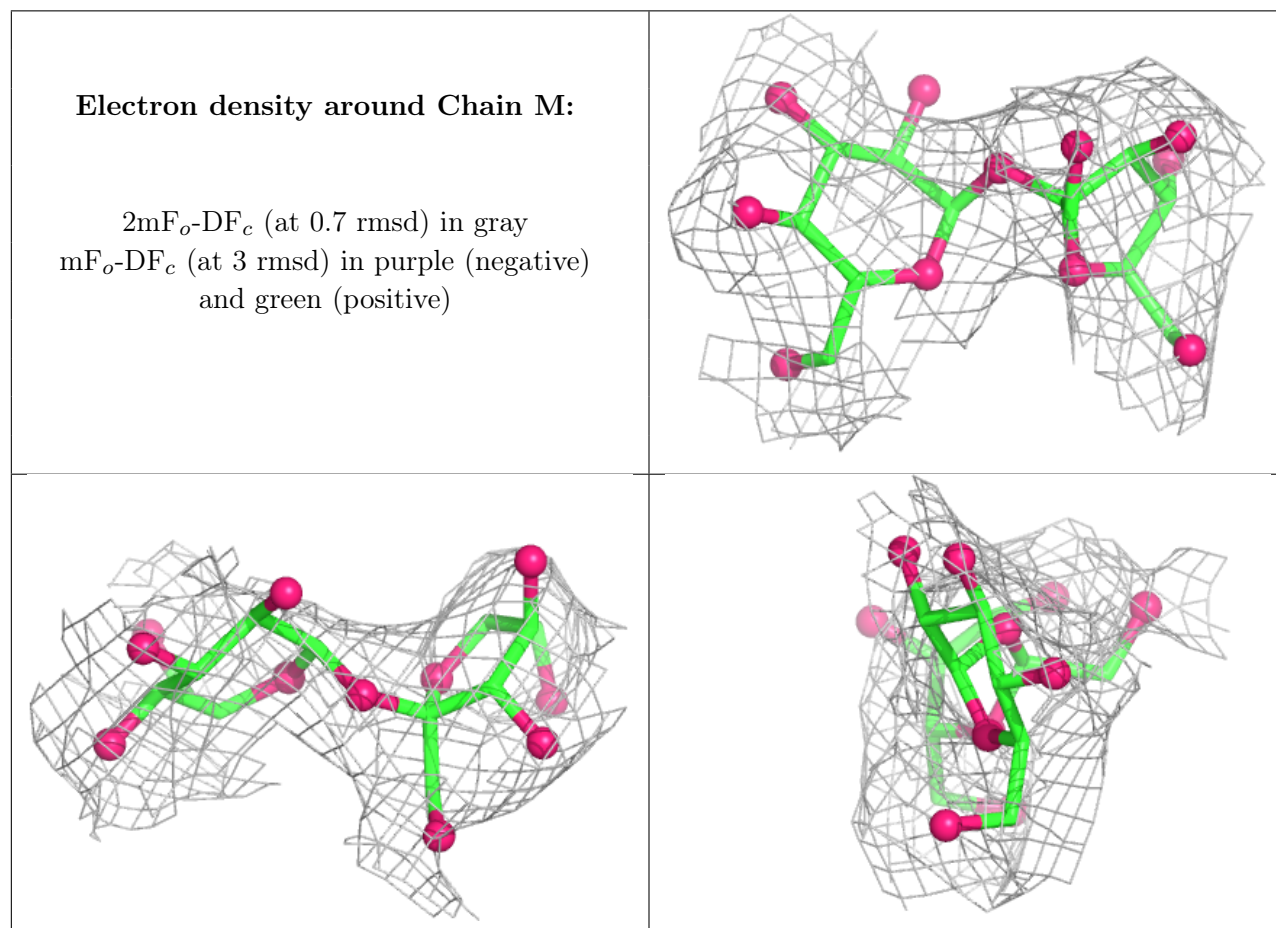
There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates [i](#)

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.

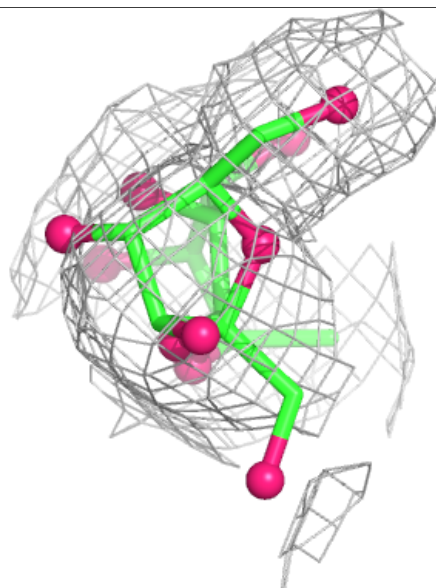
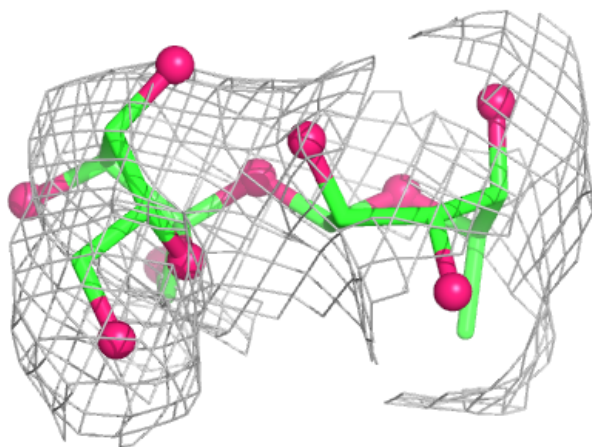
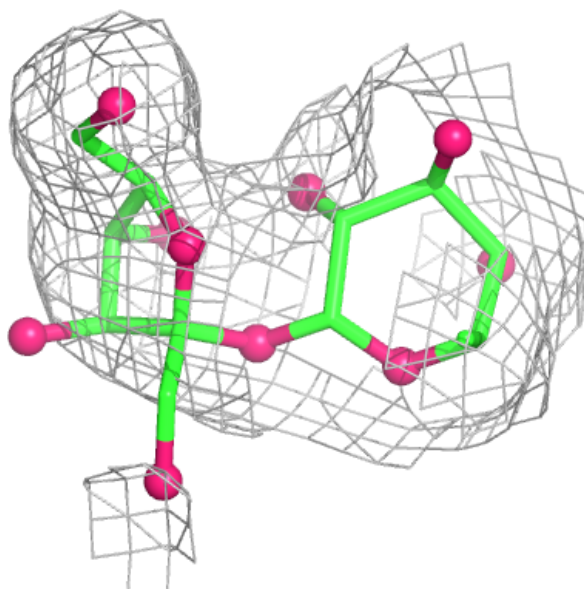
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
19	GLC	X	1	10/12	0.65	0.43	6,52,60,60	0
19	GLC	M	1	11/12	0.66	0.33	2,44,60,60	0
19	FRU	X	2	12/12	0.67	0.49	11,32,60,60	0
19	FRU	U	2	12/12	0.68	0.29	2,34,60,60	0
19	GLC	W	1	11/12	0.69	0.35	9,40,60,60	0
19	FRU	W	2	12/12	0.69	0.33	17,37,60,60	0
19	GLC	S	1	11/12	0.71	0.39	2,19,60,60	0
19	GLC	U	1	11/12	0.74	0.31	2,60,60,60	0
19	GLC	Z	1	11/12	0.74	0.28	4,31,60,60	0
19	GLC	V	1	11/12	0.76	0.22	2,57,60,60	0
19	FRU	O	2	12/12	0.76	0.43	2,28,60,60	0
19	FRU	Z	2	12/12	0.76	0.25	3,43,60,60	0
19	GLC	a	1	11/12	0.76	0.21	2,23,50,54	0
19	FRU	S	2	12/12	0.79	0.21	2,32,60,60	0
19	GLC	T	1	11/12	0.79	0.22	13,47,60,60	0
19	FRU	a	2	12/12	0.80	0.21	6,32,60,60	0
19	GLC	Y	1	11/12	0.81	0.28	2,34,60,60	0
19	FRU	Q	2	12/12	0.82	0.32	2,28,60,60	0
19	GLC	Q	1	11/12	0.83	0.23	2,27,60,60	0
19	FRU	Y	2	12/12	0.83	0.28	2,30,60,60	0
19	FRU	V	2	12/12	0.83	0.25	2,33,60,60	0
19	FRU	M	2	12/12	0.84	0.39	9,35,60,60	0
19	GLC	P	1	11/12	0.85	0.24	2,13,57,60	0
19	FRU	T	2	12/12	0.85	0.24	6,39,60,60	0
19	FRU	P	2	12/12	0.85	0.20	2,36,60,60	0
19	GLC	O	1	10/12	0.85	0.16	4,38,60,60	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.



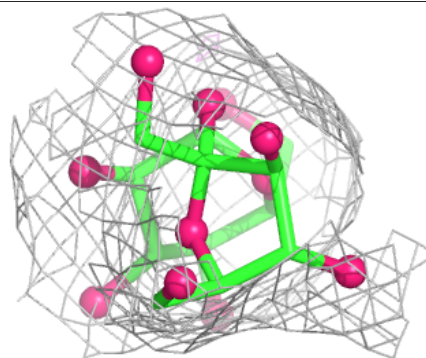
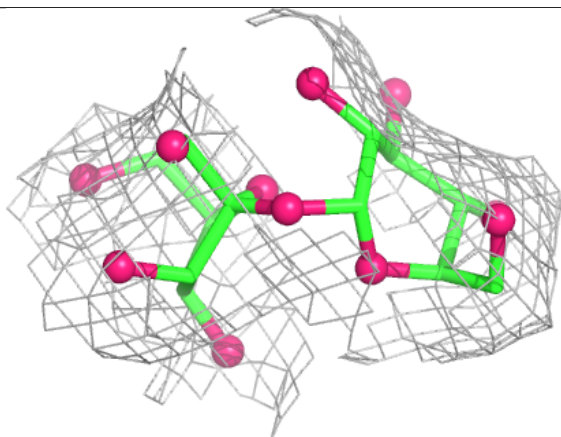
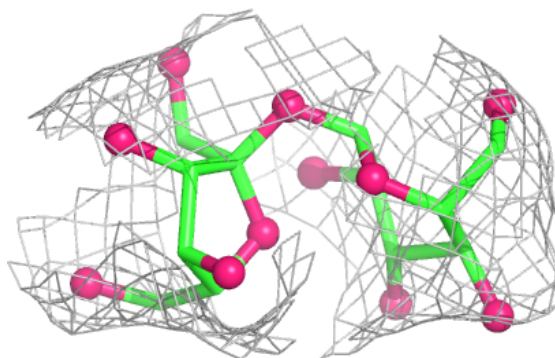
Electron density around Chain O:

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



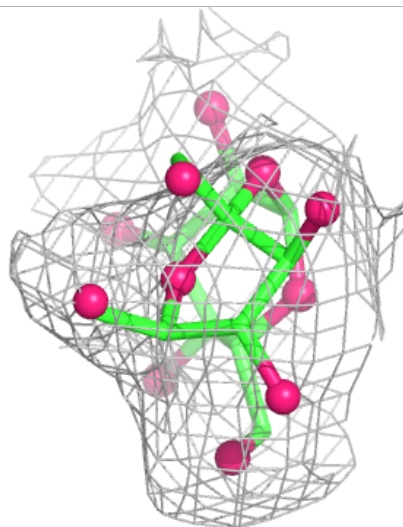
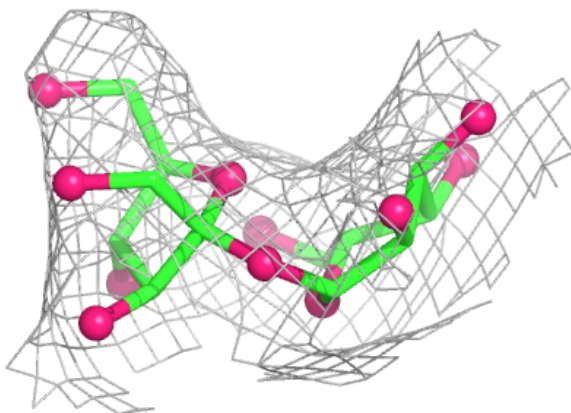
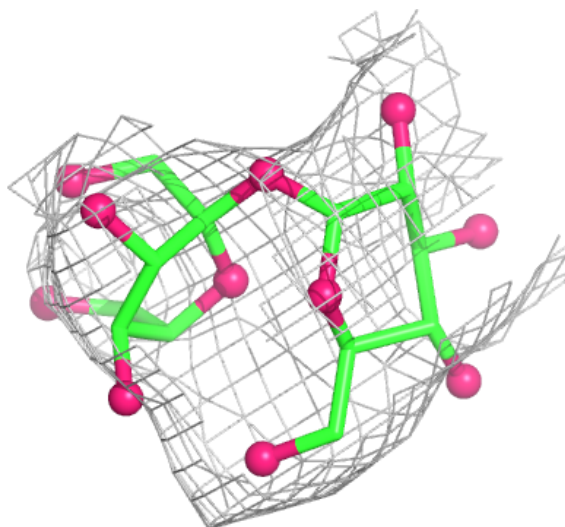
Electron density around Chain P:

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



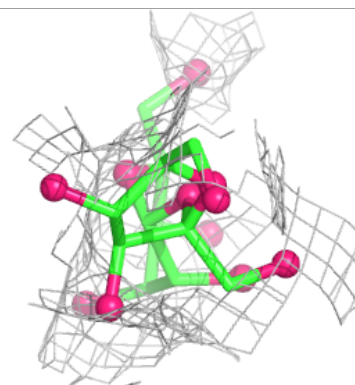
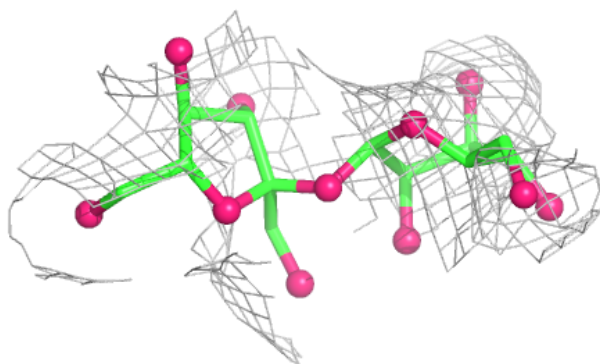
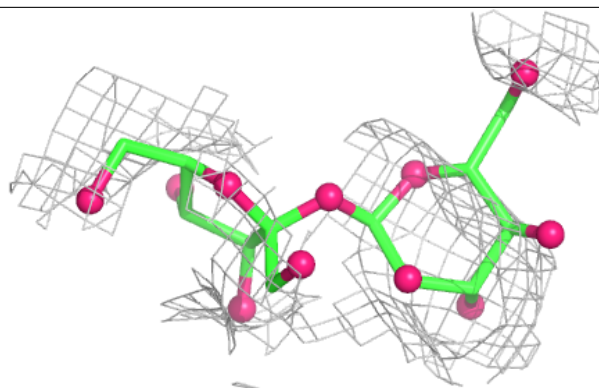
Electron density around Chain Q:

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

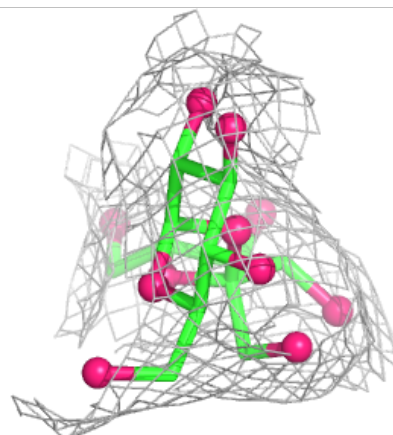
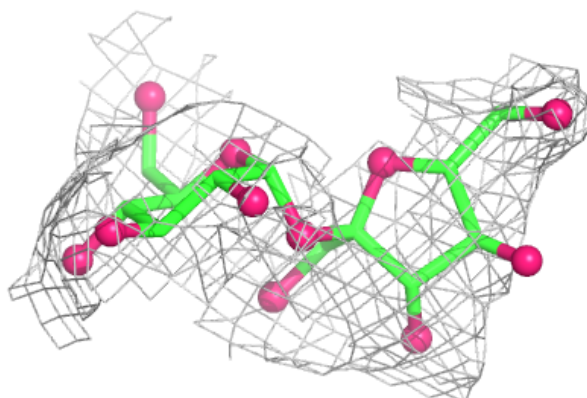
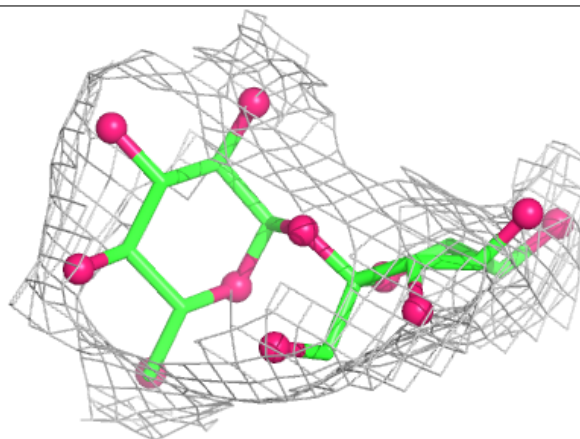


Electron density around Chain S:

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

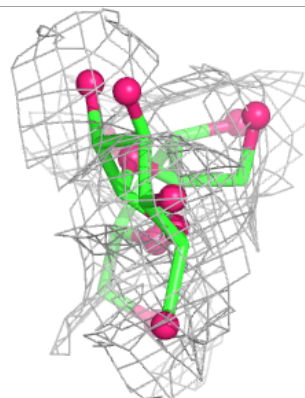
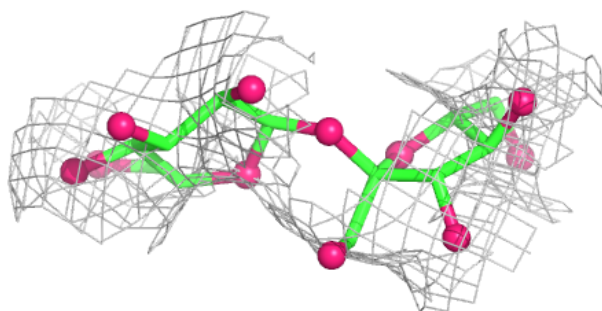
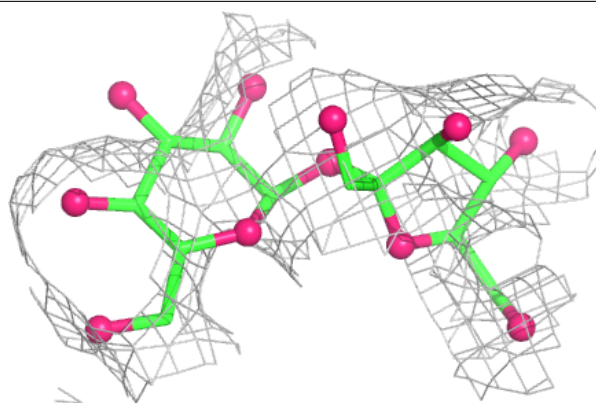
**Electron density around Chain T:**

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

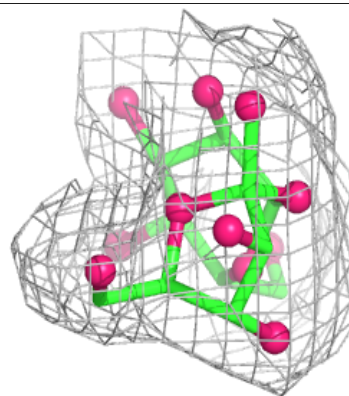
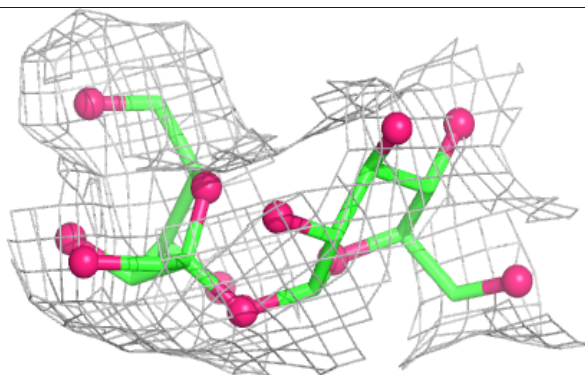
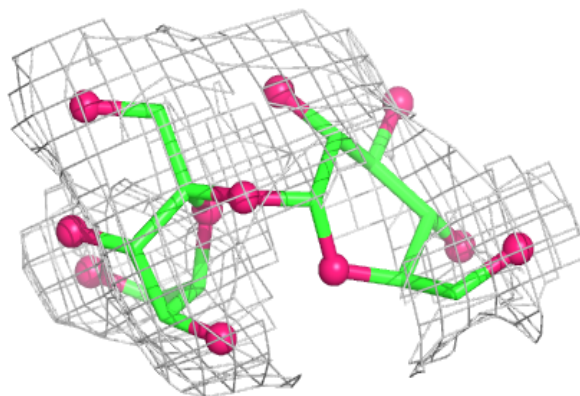


Electron density around Chain U:

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

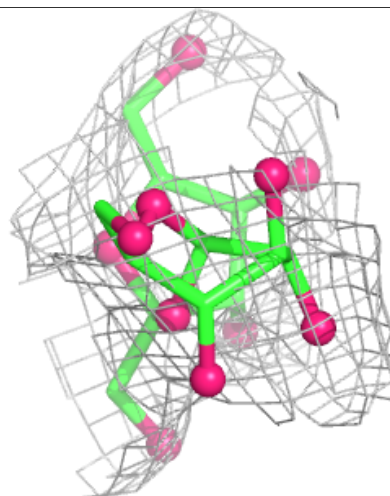
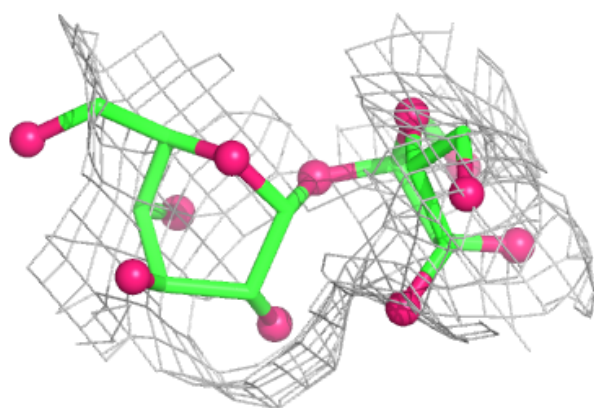
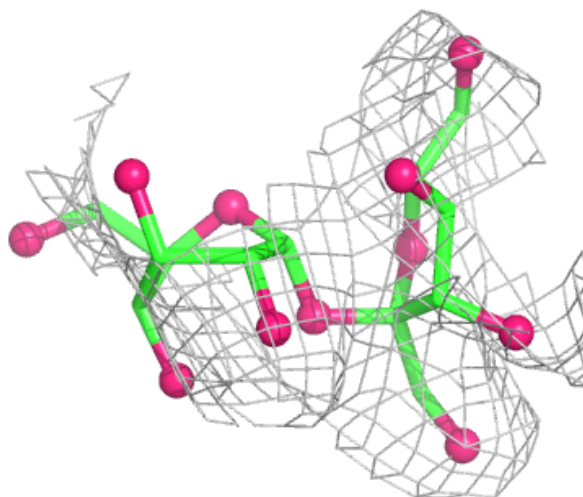
**Electron density around Chain V:**

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



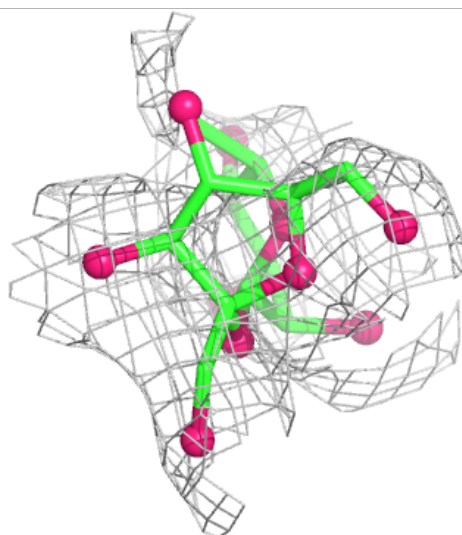
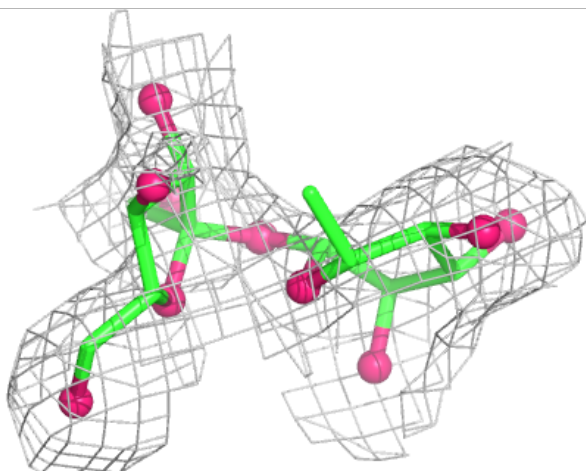
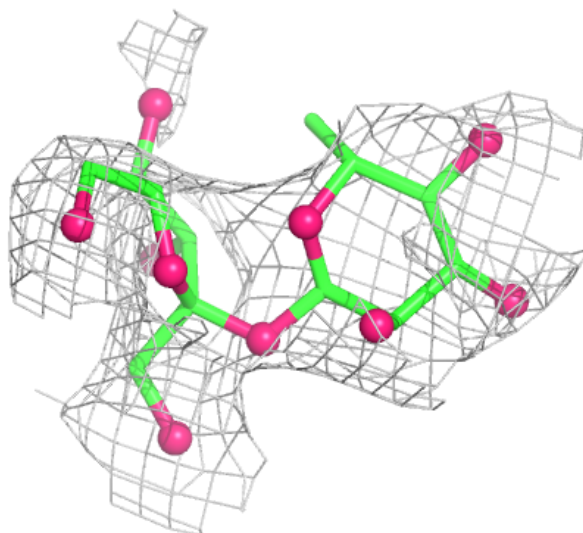
Electron density around Chain W:

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



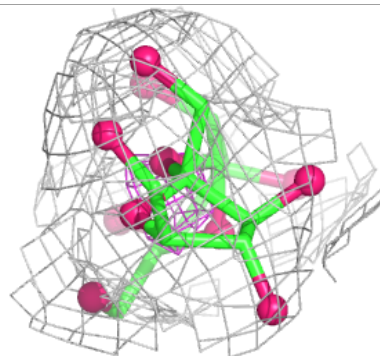
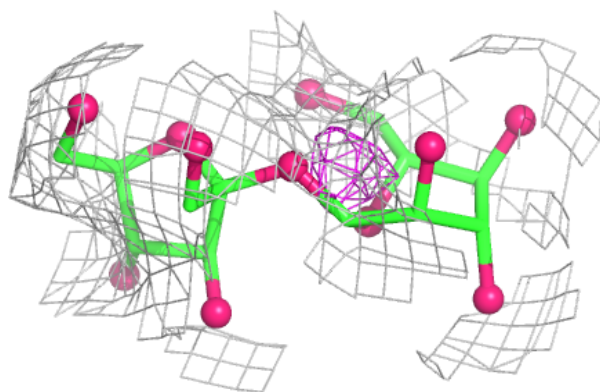
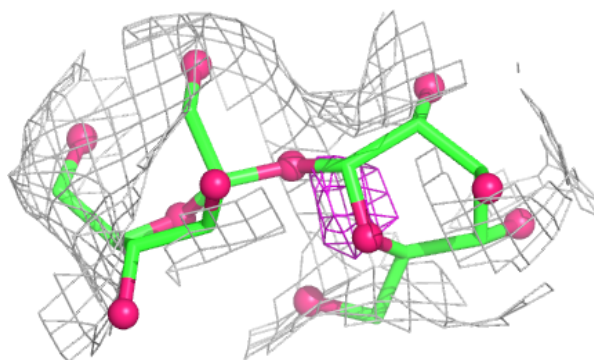
Electron density around Chain X:

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

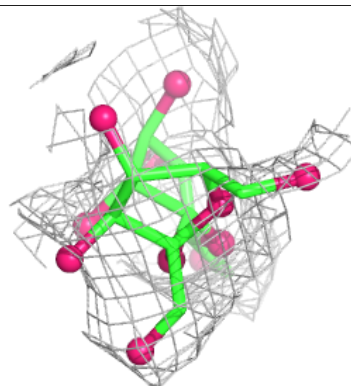
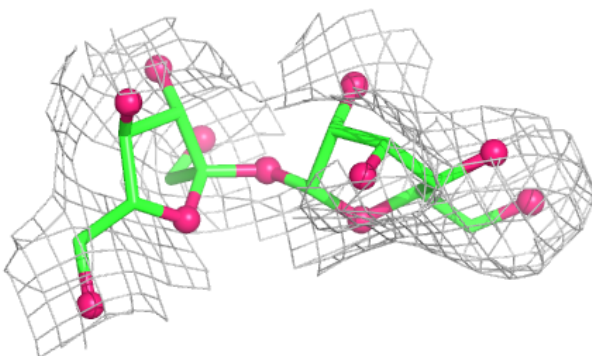


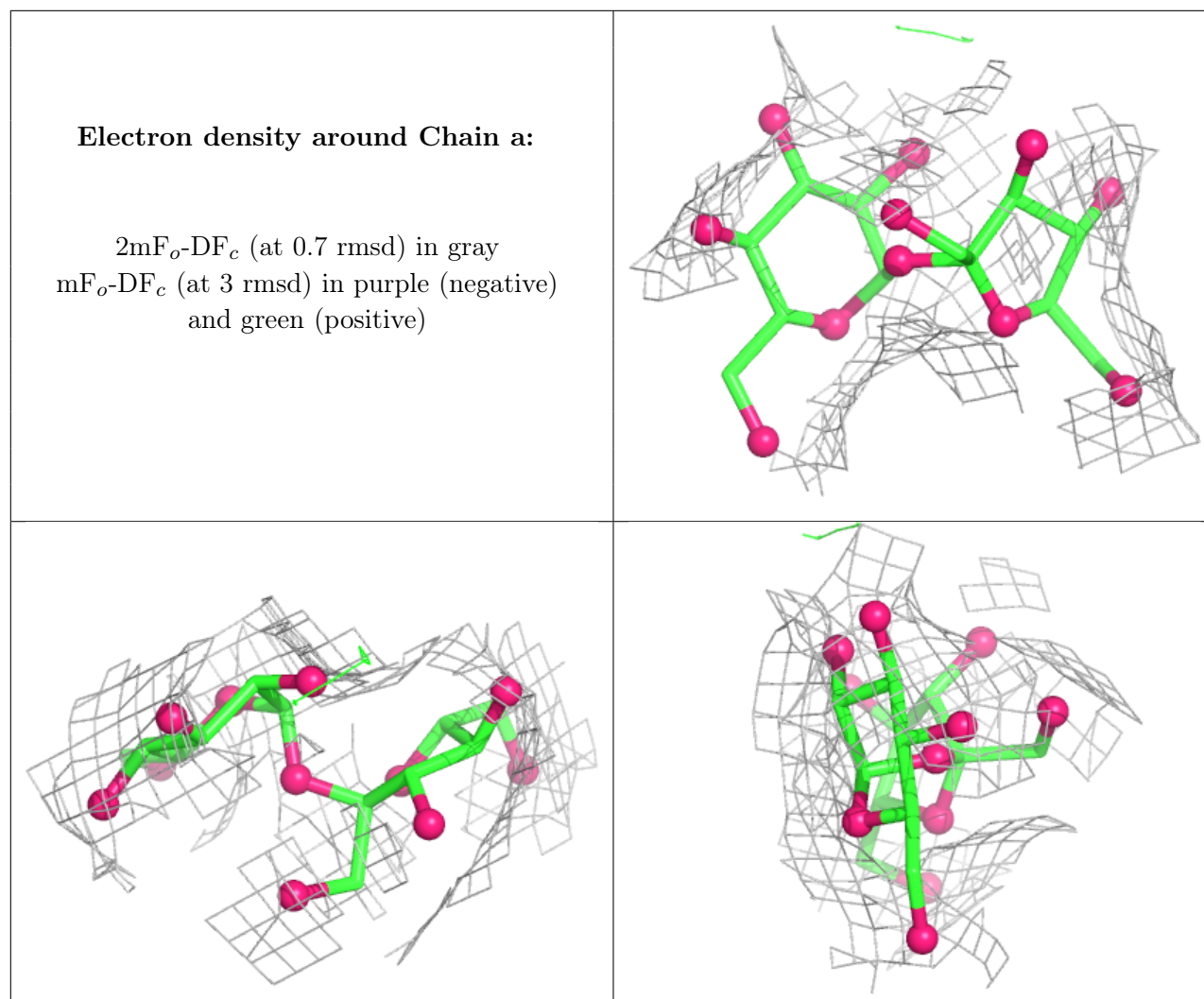
Electron density around Chain Y:

$2mF_o-DF_c$ (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)





6.4 Ligands ⓘ

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
21	LMU	A	852	35/35	0.54	0.49	2,39,60,60	0
20	CLA	H	102	55/65	0.56	0.39	2,49,60,60	0
21	LMU	A	853	35/35	0.57	0.37	2,45,60,60	0
21	LMU	4	320	35/35	0.58	0.27	2,43,60,60	0
21	LMU	B	804	35/35	0.58	0.32	2,34,60,60	0
21	LMU	G	103	35/35	0.58	0.30	2,51,60,60	0
20	CLA	1	211	51/65	0.59	0.52	2,42,60,60	0
21	LMU	2	321	35/35	0.60	0.39	2,40,60,60	0
22	BCR	2	318	40/40	0.60	0.40	2,32,60,60	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
20	CLA	4	317	52/65	0.61	0.42	2,34,60,60	0
20	CLA	3	314	50/65	0.62	0.41	2,56,60,60	0
21	LMU	L	205	35/35	0.62	0.22	2,31,60,60	0
20	CLA	B	835	45/65	0.62	0.36	12,37,60,60	0
20	CLA	1	215	51/65	0.63	0.40	2,51,60,60	0
21	LMU	H	103	35/35	0.63	0.33	2,15,60,60	0
21	LMU	2	322	35/35	0.63	0.33	2,40,60,60	0
20	CLA	A	802	25/65	0.63	0.53	2,42,60,60	0
22	BCR	A	843	40/40	0.63	0.45	2,45,60,60	0
20	CLA	L	204	55/65	0.64	0.45	2,44,60,60	0
20	CLA	B	817	46/65	0.64	0.43	2,28,60,60	0
20	CLA	3	305	25/65	0.64	0.34	17,42,60,60	0
20	CLA	4	303	65/65	0.64	0.36	2,32,60,60	0
20	CLA	K	103	50/65	0.65	0.32	2,60,60,60	0
21	LMU	A	848	35/35	0.65	0.29	2,45,60,60	0
20	CLA	3	311	65/65	0.66	0.41	2,46,60,60	0
20	CLA	3	318	36/65	0.66	0.40	2,51,60,60	0
20	CLA	H	112	55/65	0.67	0.34	2,33,60,60	0
20	CLA	B	836	51/65	0.67	0.37	2,45,60,60	0
20	CLA	A	840	55/65	0.67	0.36	2,44,60,60	0
21	LMU	H	106	35/35	0.68	0.29	2,41,60,60	0
20	CLA	F	206	41/65	0.68	0.33	2,41,60,60	0
21	LMU	R	104	35/35	0.68	0.23	2,36,60,60	0
20	CLA	H	101	55/65	0.68	0.47	2,47,60,60	0
20	CLA	4	308	25/65	0.68	0.30	2,29,60,60	0
22	BCR	I	103	40/40	0.68	0.40	2,38,60,60	0
20	CLA	4	304	55/65	0.69	0.36	4,39,60,60	0
20	CLA	4	307	25/65	0.69	0.35	2,39,60,60	0
21	LMU	A	846	35/35	0.69	0.25	2,26,60,60	0
21	LMU	K	106	35/35	0.69	0.24	2,38,60,60	0
20	CLA	1	201	46/65	0.69	0.25	2,56,60,60	0
21	LMU	1	217	35/35	0.69	0.23	2,44,60,60	0
21	LMU	2	313	35/35	0.69	0.27	2,21,60,60	0
20	CLA	3	309	25/65	0.69	0.27	2,47,60,60	0
22	BCR	G	104	40/40	0.69	0.48	2,33,60,60	0
21	LMU	E	101	35/35	0.69	0.28	2,30,60,60	0
21	LMU	B	805	35/35	0.70	0.29	2,37,60,60	0
20	CLA	G	105	51/65	0.70	0.42	2,44,60,60	0
21	LMU	R	105	35/35	0.70	0.27	2,35,60,60	0
20	CLA	3	310	65/65	0.70	0.33	2,26,60,60	0
20	CLA	3	302	25/65	0.70	0.41	15,54,60,60	0
21	LMU	A	854	35/35	0.70	0.27	2,32,60,60	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
20	CLA	3	303	36/65	0.70	0.26	2,53,60,60	0
21	LMU	R	103	35/35	0.71	0.38	2,35,60,60	0
20	CLA	3	313	25/65	0.71	0.43	2,30,60,60	0
20	CLA	R	108	65/65	0.71	0.34	2,35,60,60	0
20	CLA	2	312	61/65	0.71	0.25	2,34,60,60	0
20	CLA	K	101	46/65	0.71	0.25	2,51,60,60	0
21	LMU	K	107	35/35	0.71	0.26	2,38,60,60	0
20	CLA	A	841	25/65	0.71	0.30	2,43,60,60	0
20	CLA	L	202	55/65	0.72	0.44	2,46,60,60	0
21	LMU	R	106	35/35	0.72	0.23	2,27,60,60	0
20	CLA	B	816	60/65	0.72	0.34	2,40,60,60	0
21	LMU	R	101	35/35	0.72	0.32	2,45,60,60	0
22	BCR	B	845	40/40	0.72	0.38	2,21,60,60	0
21	LMU	3	319	35/35	0.72	0.31	2,44,60,60	0
20	CLA	R	107	57/65	0.72	0.30	2,38,60,60	0
22	BCR	L	211	40/40	0.72	0.47	2,18,60,60	0
21	LMU	G	102	35/35	0.73	0.26	2,33,60,60	0
20	CLA	A	833	45/65	0.73	0.27	2,37,60,60	0
20	CLA	2	301	25/65	0.73	0.47	2,48,60,60	0
20	CLA	2	304	25/65	0.73	0.45	2,27,60,60	0
20	CLA	1	207	51/65	0.73	0.31	2,36,60,60	0
22	BCR	A	844	40/40	0.73	0.39	2,34,60,60	0
20	CLA	1	208	25/65	0.73	0.27	2,31,60,60	0
20	CLA	1	205	36/65	0.73	0.29	2,52,60,60	0
20	CLA	A	801	46/65	0.73	0.35	2,43,60,60	0
20	CLA	1	206	61/65	0.73	0.29	2,35,60,60	0
20	CLA	2	305	50/65	0.74	0.30	2,48,60,60	0
20	CLA	A	820	51/65	0.74	0.30	2,44,60,60	0
20	CLA	4	301	55/65	0.74	0.35	2,33,60,60	0
21	LMU	C	101	35/35	0.74	0.38	2,35,60,60	0
20	CLA	1	203	47/65	0.75	0.27	2,17,60,60	0
20	CLA	K	102	50/65	0.75	0.32	2,28,60,60	0
21	LMU	2	320	35/35	0.75	0.25	2,29,60,60	0
20	CLA	2	311	50/65	0.75	0.31	2,25,60,60	0
21	LMU	K	105	35/35	0.75	0.26	2,37,60,60	0
20	CLA	3	317	25/65	0.75	0.27	2,42,60,60	0
20	CLA	4	305	50/65	0.75	0.41	2,21,60,60	0
20	CLA	A	811	65/65	0.75	0.40	2,15,60,60	0
21	LMU	L	206	35/35	0.75	0.24	2,23,60,60	0
21	LMU	L	212	35/35	0.75	0.30	2,22,60,60	0
20	CLA	3	307	42/65	0.75	0.26	2,53,60,60	0
20	CLA	4	318	47/65	0.76	0.28	2,37,60,60	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
20	CLA	3	316	25/65	0.76	0.48	2,47,60,60	0
20	CLA	2	302	51/65	0.76	0.23	2,33,60,60	0
20	CLA	3	306	25/65	0.76	0.28	2,56,60,60	0
20	CLA	2	307	65/65	0.76	0.25	2,24,60,60	0
20	CLA	4	314	25/65	0.76	0.30	2,35,60,60	0
21	LMU	4	316	35/35	0.76	0.38	2,37,60,60	0
20	CLA	4	315	46/65	0.76	0.31	2,45,60,60	0
20	CLA	1	213	51/65	0.76	0.40	2,39,60,60	0
21	LMU	A	847	35/35	0.76	0.26	2,27,60,60	0
20	CLA	J	101	48/65	0.77	0.28	2,34,60,60	0
20	CLA	3	301	36/65	0.77	0.28	2,34,60,60	0
20	CLA	1	210	36/65	0.77	0.31	2,35,60,60	0
20	CLA	2	310	50/65	0.77	0.32	2,18,60,60	0
20	CLA	K	104	56/65	0.77	0.31	2,36,60,60	0
21	LMU	H	104	35/35	0.77	0.23	2,16,60,60	0
21	LMU	R	102	35/35	0.77	0.22	2,38,60,60	0
21	LMU	4	321	35/35	0.77	0.27	2,21,55,60	0
20	CLA	2	315	50/65	0.77	0.40	2,33,60,60	0
25	LMG	B	848	49/55	0.77	0.35	2,20,60,60	0
20	CLA	J	103	61/65	0.78	0.24	2,19,60,60	0
20	CLA	4	302	36/65	0.78	0.35	2,26,60,60	0
20	CLA	2	306	25/65	0.78	0.22	2,57,60,60	0
20	CLA	B	815	60/65	0.78	0.35	2,19,60,60	0
20	CLA	A	821	42/65	0.78	0.29	2,46,60,60	0
20	CLA	A	823	58/65	0.78	0.36	2,18,60,60	0
20	CLA	B	822	46/65	0.78	0.34	2,34,60,60	0
22	BCR	J	102	40/40	0.78	0.35	2,31,60,60	0
20	CLA	L	208	50/65	0.78	0.31	2,27,60,60	0
20	CLA	4	309	25/65	0.78	0.39	2,40,60,60	0
21	LMU	F	202	34/35	0.79	0.22	2,23,60,60	0
20	CLA	A	817	52/65	0.79	0.36	2,33,60,60	0
20	CLA	B	813	55/65	0.79	0.29	2,28,60,60	0
21	LMU	3	320	35/35	0.79	0.20	2,28,59,60	0
20	CLA	3	308	25/65	0.79	0.26	2,37,60,60	0
20	CLA	2	316	25/65	0.79	0.28	2,36,60,60	0
20	CLA	A	810	45/65	0.79	0.33	2,38,60,60	0
20	CLA	3	315	65/65	0.79	0.29	2,33,60,60	0
20	CLA	A	814	25/65	0.79	0.29	2,31,60,60	0
21	LMU	4	319	34/35	0.80	0.24	2,22,60,60	0
21	LMU	2	319	35/35	0.80	0.20	2,25,60,60	0
20	CLA	A	805	54/65	0.80	0.29	2,10,60,60	0
20	CLA	A	834	46/65	0.80	0.39	2,20,60,60	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
20	CLA	A	839	59/65	0.80	0.29	2,30,60,60	0
20	CLA	1	212	25/65	0.80	0.26	2,42,60,60	0
20	CLA	1	204	46/65	0.80	0.28	2,35,60,60	0
20	CLA	4	310	50/65	0.80	0.24	2,20,60,60	0
26	UNL	H	109	23/-	0.80	0.22	2,31,60,60	0
21	LMU	D	201	35/35	0.81	0.22	2,12,50,57	0
20	CLA	1	214	25/65	0.81	0.29	5,42,60,60	0
20	CLA	A	819	58/65	0.81	0.35	2,20,60,60	0
20	CLA	A	825	65/65	0.81	0.32	2,16,60,60	0
21	LMU	1	218	35/35	0.81	0.20	2,46,60,60	0
20	CLA	L	201	60/65	0.81	0.29	2,18,60,60	0
20	CLA	B	842	36/65	0.81	0.30	2,52,60,60	0
20	CLA	2	309	25/65	0.81	0.42	2,34,60,60	0
21	LMU	B	849	25/35	0.81	0.21	2,36,60,60	0
20	CLA	B	820	61/65	0.81	0.30	2,16,60,60	0
20	CLA	A	812	54/65	0.82	0.25	2,28,60,60	0
21	LMU	R	109	35/35	0.82	0.24	2,21,60,60	0
20	CLA	A	807	46/65	0.82	0.29	2,20,60,60	0
20	CLA	A	815	50/65	0.82	0.27	2,21,60,60	0
20	CLA	A	824	59/65	0.82	0.29	2,25,60,60	0
22	BCR	A	845	40/40	0.82	0.34	2,5,44,60	0
20	CLA	H	111	58/65	0.82	0.32	2,15,60,60	0
22	BCR	B	846	40/40	0.82	0.33	2,11,60,60	0
22	BCR	B	847	40/40	0.82	0.33	2,10,60,60	0
20	CLA	B	827	65/65	0.82	0.32	2,15,60,60	0
20	CLA	B	812	54/65	0.82	0.25	2,17,60,60	0
20	CLA	L	210	50/65	0.82	0.26	2,18,60,60	0
20	CLA	3	304	25/65	0.82	0.19	2,28,60,60	0
21	LMU	A	855	35/35	0.82	0.22	2,29,60,60	0
20	CLA	2	303	58/65	0.82	0.23	2,22,60,60	0
20	CLA	B	806	65/65	0.83	0.28	2,11,60,60	0
21	LMU	G	101	35/35	0.83	0.25	2,34,60,60	0
20	CLA	A	816	54/65	0.83	0.28	2,31,60,60	0
20	CLA	4	306	52/65	0.83	0.25	2,26,60,60	0
21	LMU	1	216	35/35	0.83	0.25	2,11,50,60	0
20	CLA	B	834	45/65	0.83	0.28	2,16,60,60	0
22	BCR	I	101	39/40	0.83	0.31	2,8,60,60	0
20	CLA	A	804	55/65	0.83	0.32	2,11,60,60	0
20	CLA	2	317	65/65	0.83	0.26	2,15,60,60	0
20	CLA	L	203	65/65	0.83	0.31	2,22,60,60	0
20	CLA	B	837	60/65	0.83	0.32	2,2,60,60	0
20	CLA	A	829	50/65	0.83	0.30	2,32,60,60	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
20	CLA	L	209	47/65	0.84	0.26	2,13,45,60	0
20	CLA	I	102	60/65	0.84	0.29	2,18,60,60	0
20	CLA	A	813	50/65	0.84	0.27	2,29,60,60	0
22	BCR	B	844	40/40	0.84	0.30	2,5,60,60	0
20	CLA	A	835	65/65	0.84	0.29	2,6,60,60	0
20	CLA	A	818	60/65	0.84	0.33	2,11,52,60	0
20	CLA	4	311	25/65	0.84	0.26	2,15,60,60	0
20	CLA	A	806	56/65	0.84	0.30	2,2,54,60	0
20	CLA	F	207	53/65	0.84	0.28	2,22,60,60	0
20	CLA	B	821	50/65	0.84	0.30	2,37,60,60	0
20	CLA	A	832	50/65	0.84	0.26	2,18,56,60	0
20	CLA	B	823	55/65	0.84	0.28	2,30,60,60	0
23	PQN	A	842	33/33	0.84	0.32	2,4,59,60	0
20	CLA	B	807	45/65	0.84	0.27	2,14,56,60	0
20	CLA	1	209	25/65	0.84	0.31	11,37,60,60	0
20	CLA	B	803	65/65	0.85	0.31	2,14,56,60	0
20	CLA	A	838	65/65	0.85	0.31	2,8,60,60	0
21	LMU	H	105	35/35	0.85	0.20	2,31,60,60	0
20	CLA	B	818	53/65	0.85	0.28	2,14,60,60	0
20	CLA	B	824	65/65	0.85	0.26	2,17,60,60	0
20	CLA	B	840	65/65	0.85	0.30	2,11,60,60	0
20	CLA	B	825	54/65	0.85	0.31	2,15,60,60	0
20	CLA	B	826	58/65	0.85	0.31	2,13,60,60	0
20	CLA	A	828	65/65	0.85	0.29	2,12,60,60	0
20	CLA	B	832	59/65	0.85	0.28	2,6,60,60	0
20	CLA	B	833	50/65	0.85	0.29	2,11,53,60	0
20	CLA	B	841	65/65	0.86	0.32	2,2,55,60	0
20	CLA	4	313	36/65	0.86	0.24	2,21,60,60	0
20	CLA	F	201	50/65	0.86	0.23	2,7,51,60	0
20	CLA	A	803	46/65	0.86	0.30	2,14,49,60	0
20	CLA	A	851	65/65	0.86	0.28	2,2,60,60	0
20	CLA	A	837	51/65	0.86	0.28	2,12,60,60	0
20	CLA	1	202	41/65	0.86	0.22	2,41,60,60	0
23	PQN	B	843	33/33	0.86	0.28	2,2,46,51	0
20	CLA	A	827	55/65	0.86	0.30	2,12,60,60	0
20	CLA	B	811	25/65	0.86	0.28	2,2,60,60	0
20	CLA	2	308	25/65	0.87	0.19	2,12,60,60	0
20	CLA	B	829	65/65	0.87	0.26	2,11,46,60	0
20	CLA	F	205	36/65	0.88	0.24	2,17,60,60	0
20	CLA	4	312	25/65	0.88	0.19	2,2,26,32	0
20	CLA	B	838	65/65	0.88	0.24	2,7,60,60	0
20	CLA	A	830	65/65	0.88	0.25	2,9,59,60	0

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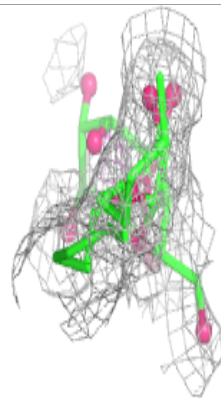
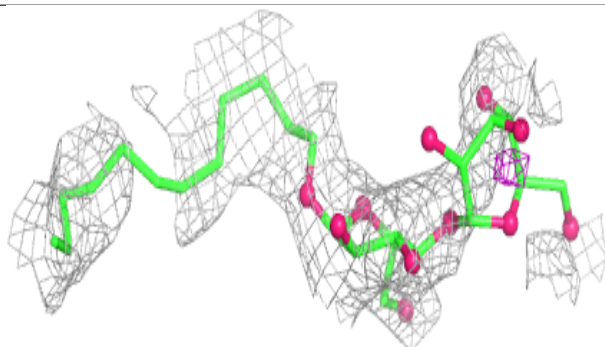
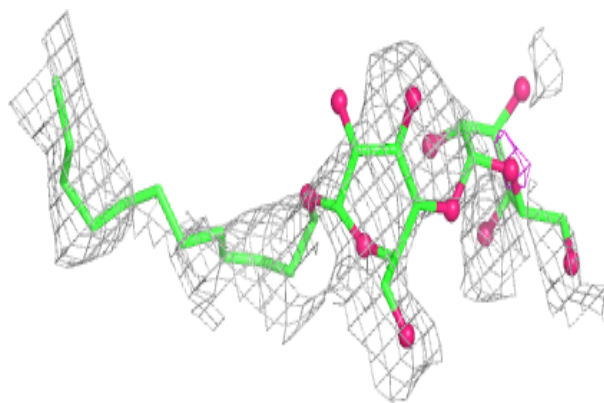
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
20	CLA	A	831	65/65	0.88	0.25	2,14,60,60	0
20	CLA	A	826	65/65	0.88	0.29	2,2,50,60	0
20	CLA	B	850	65/65	0.88	0.28	2,2,55,60	0
20	CLA	A	850	65/65	0.88	0.27	2,4,48,60	0
22	BCR	F	203	40/40	0.88	0.28	2,2,60,60	0
20	CLA	A	836	47/65	0.89	0.23	2,8,50,60	0
20	CLA	B	839	47/65	0.89	0.25	2,5,55,60	0
20	CLA	B	808	61/65	0.89	0.27	2,9,48,60	0
20	CLA	B	810	60/65	0.89	0.27	2,2,60,60	0
22	BCR	F	204	40/40	0.89	0.22	2,6,60,60	0
20	CLA	B	831	50/65	0.89	0.26	2,12,60,60	0
20	CLA	A	822	50/65	0.89	0.23	2,7,60,60	0
20	CLA	B	828	65/65	0.90	0.26	2,10,56,60	0
20	CLA	B	809	65/65	0.90	0.26	2,2,53,60	0
20	CLA	B	830	65/65	0.90	0.24	2,6,53,60	0
20	CLA	B	814	65/65	0.90	0.26	2,13,60,60	0
20	CLA	A	849	65/65	0.90	0.27	2,2,48,60	0
20	CLA	B	819	41/65	0.90	0.27	2,5,40,60	0
20	CLA	A	809	52/65	0.91	0.24	2,10,60,60	0
20	CLA	A	808	60/65	0.91	0.29	2,10,60,60	0
22	BCR	B	801	40/40	0.91	0.23	2,4,50,60	0
20	CLA	B	802	54/65	0.92	0.27	2,6,45,60	0
24	SF4	C	103	8/8	0.96	0.08	12,19,20,24	0
24	SF4	C	102	8/8	0.97	0.08	18,22,26,32	0
24	SF4	A	856	8/8	0.98	0.05	23,24,24,25	0

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

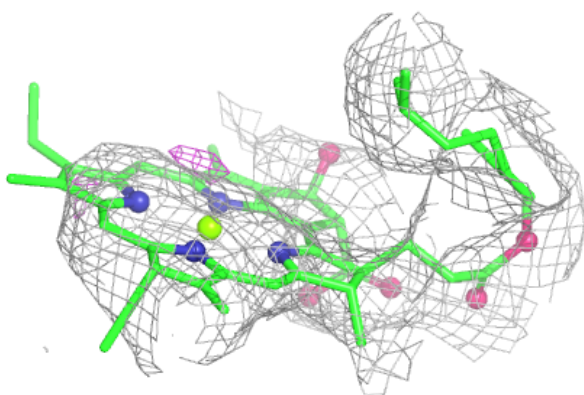
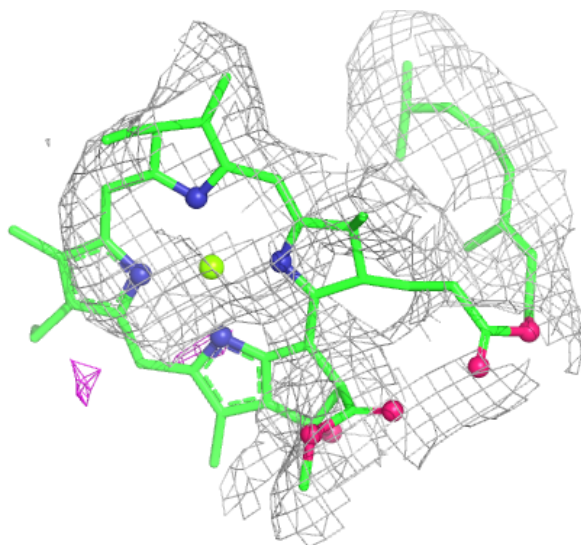
Electron density around LMU A 852:

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



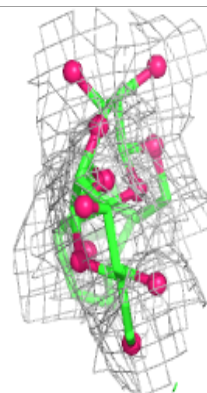
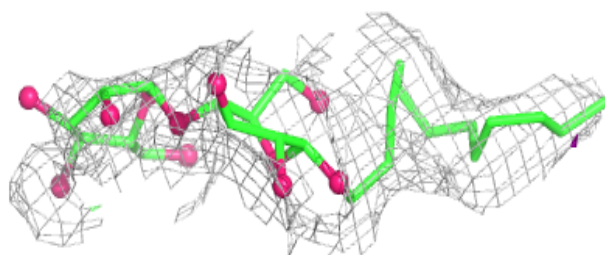
Electron density around CLA H 102:

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

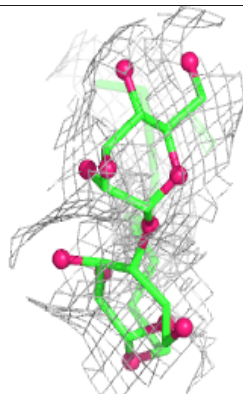
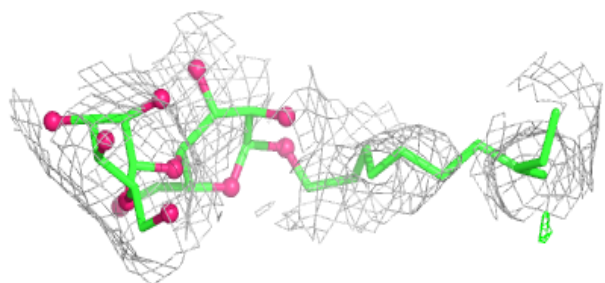
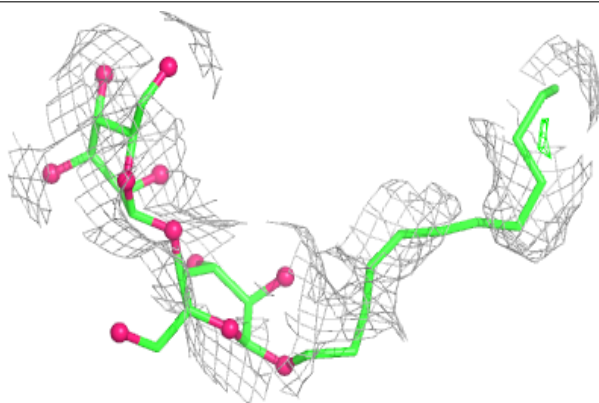


Electron density around LMU A 853:

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

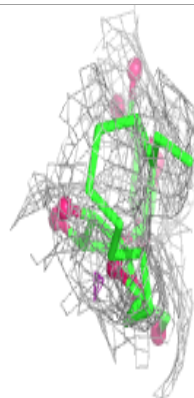
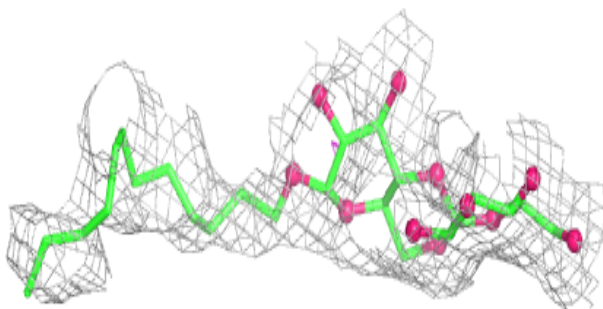
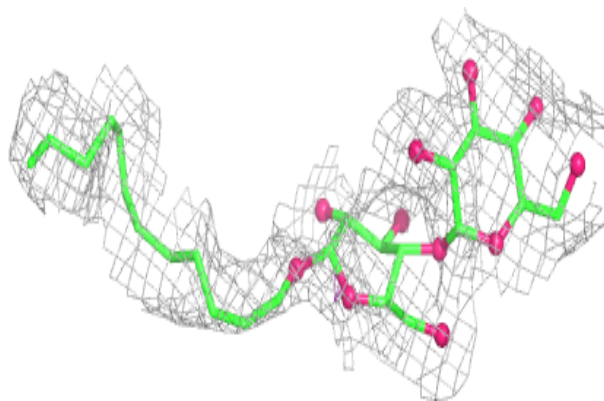
**Electron density around LMU 4 320:**

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

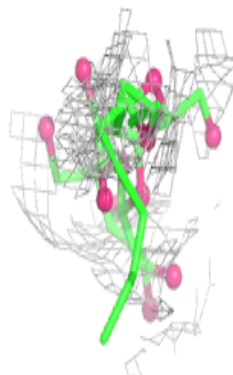
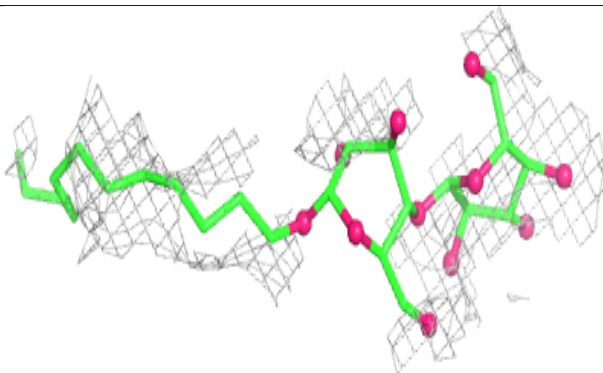
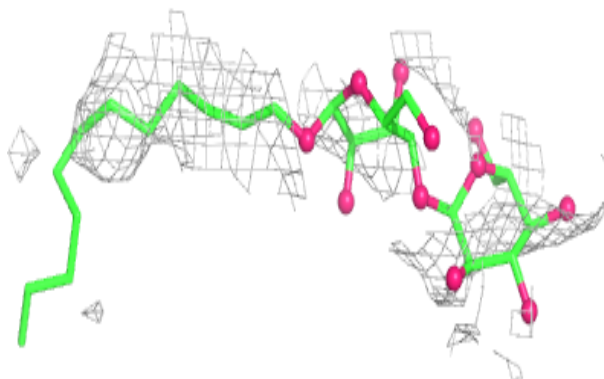


Electron density around LMU B 804:

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

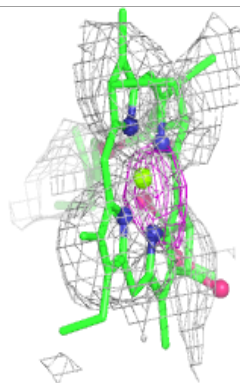
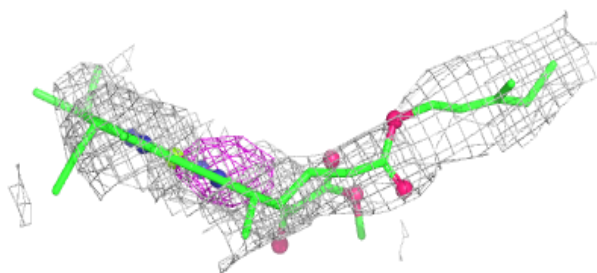
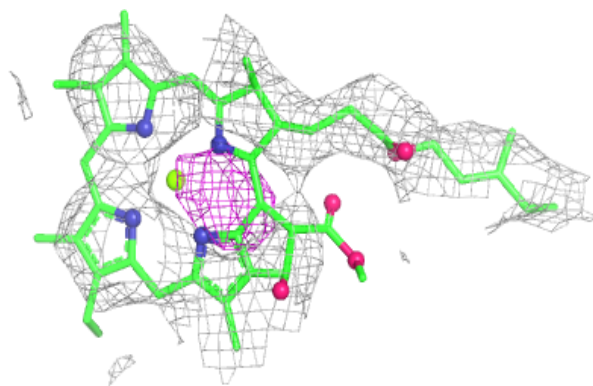
**Electron density around LMU G 103:**

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

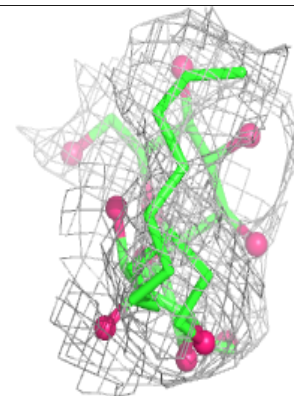
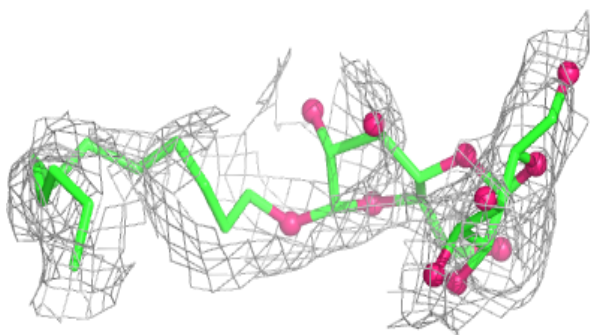
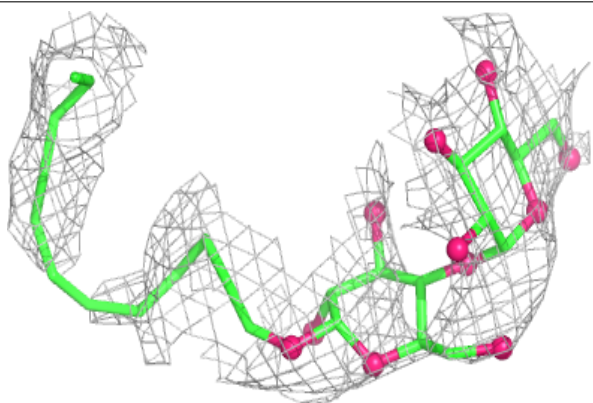


Electron density around CLA 1 211:

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

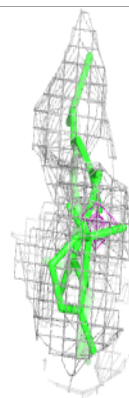
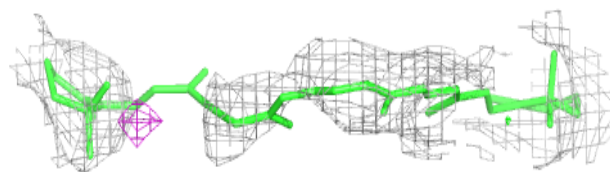
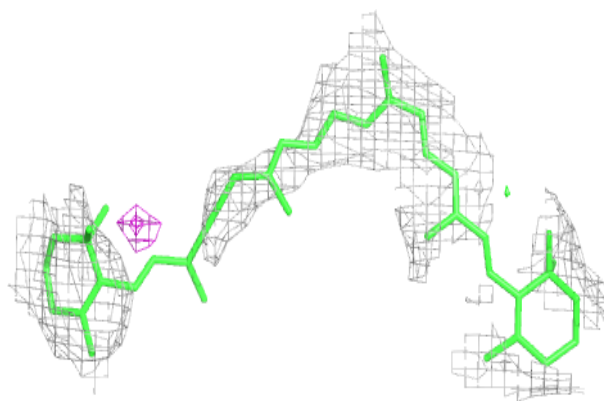
**Electron density around LMU 2 321:**

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



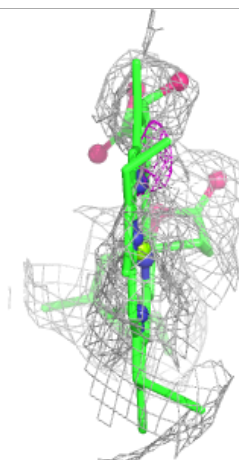
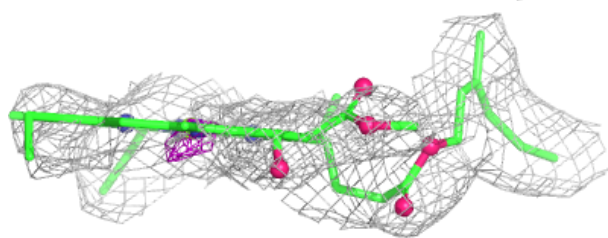
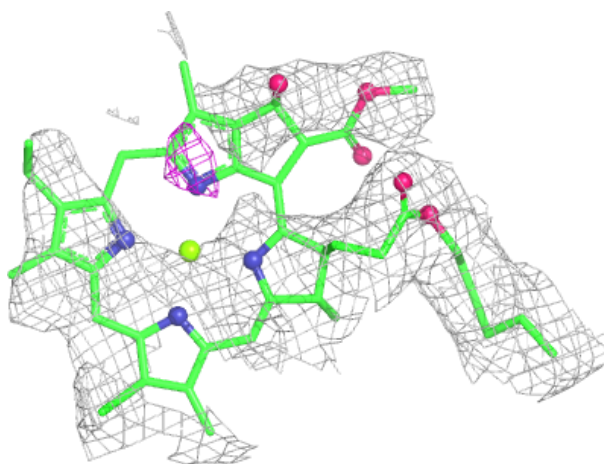
Electron density around BCR 2 318:

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



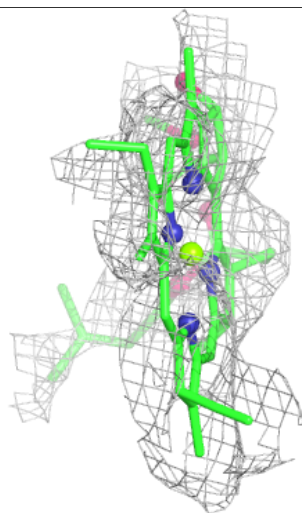
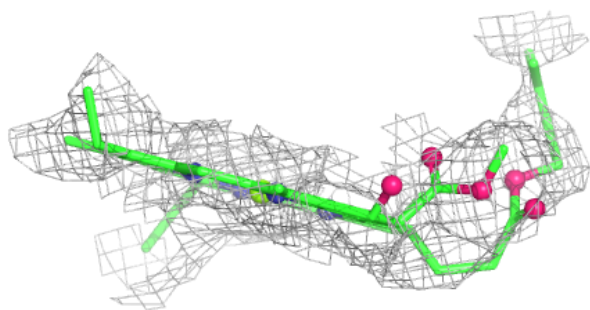
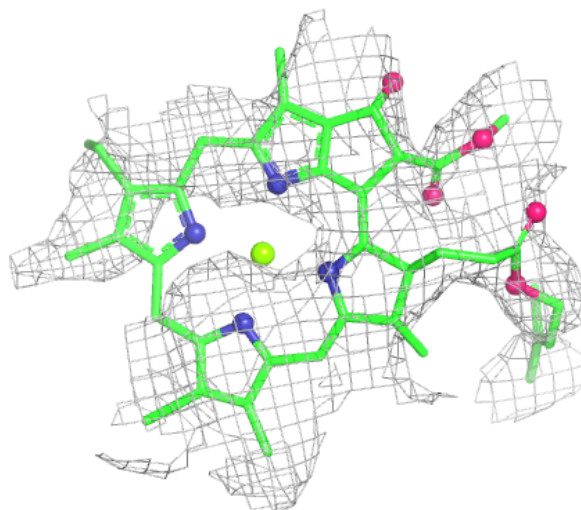
Electron density around CLA 4 317:

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



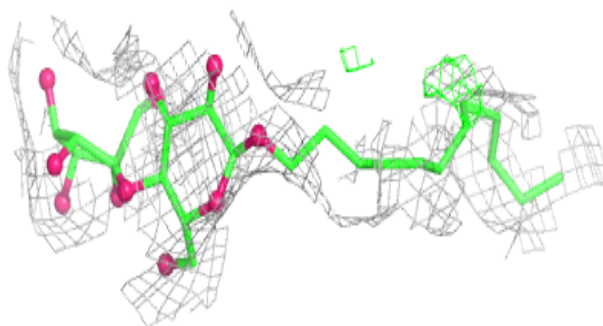
Electron density around CLA 3 314:

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



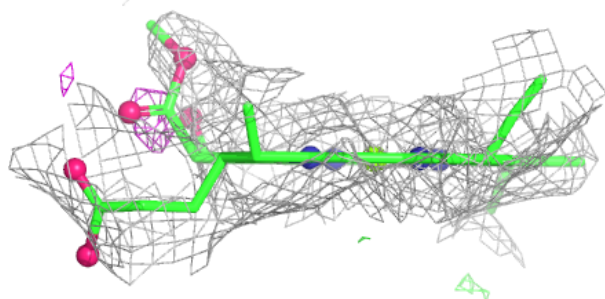
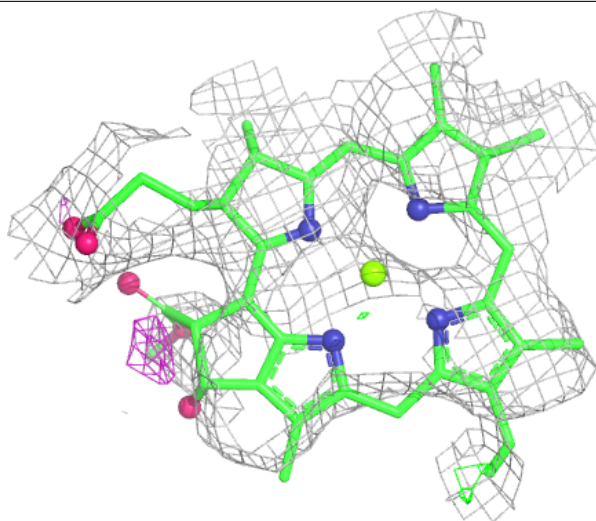
Electron density around LMU L 205:

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



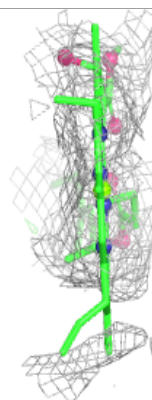
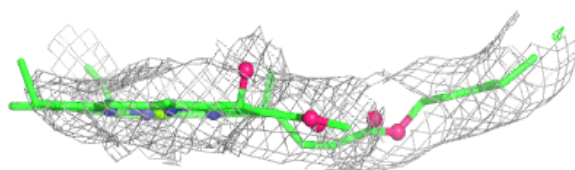
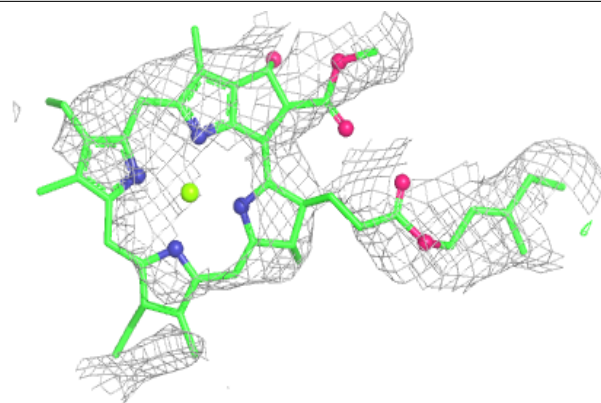
Electron density around CLA B 835:

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

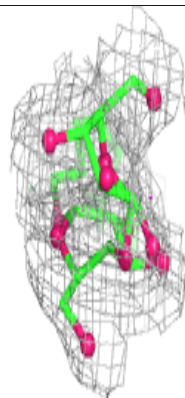
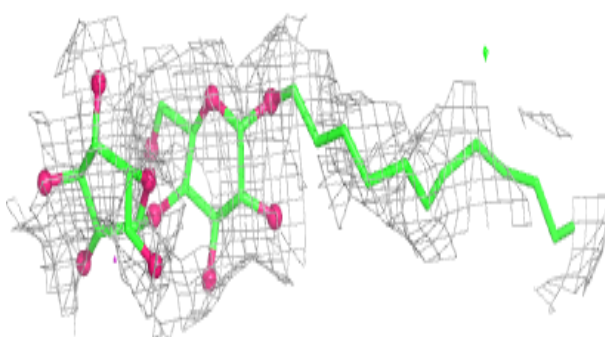
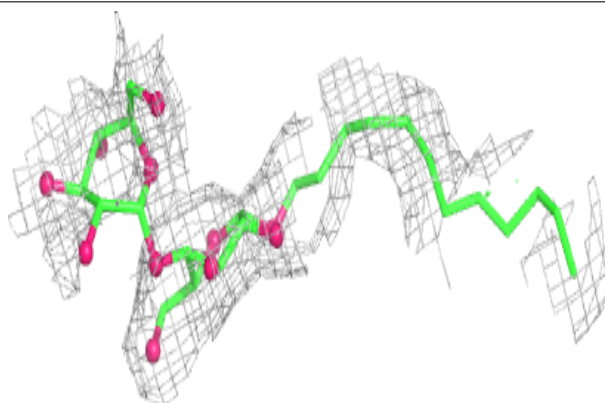


Electron density around CLA 1 215:

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

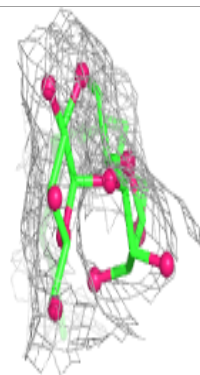
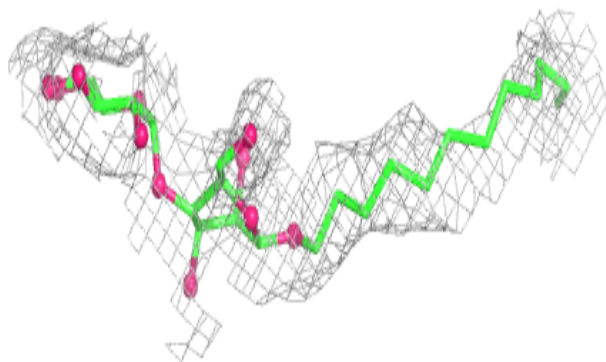
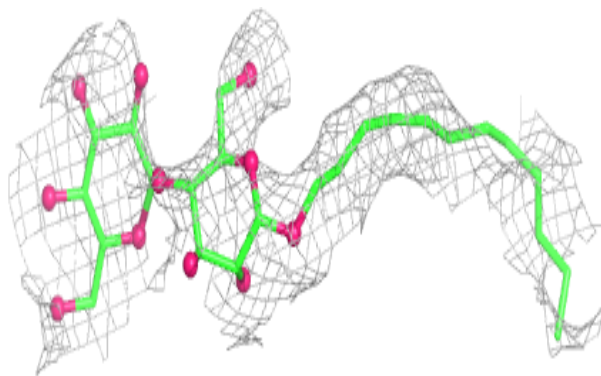
**Electron density around LMU H 103:**

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



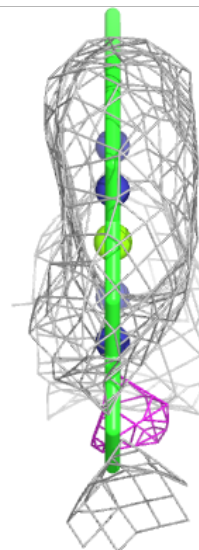
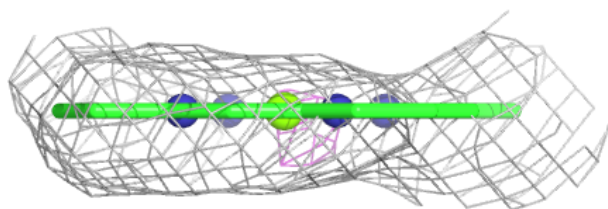
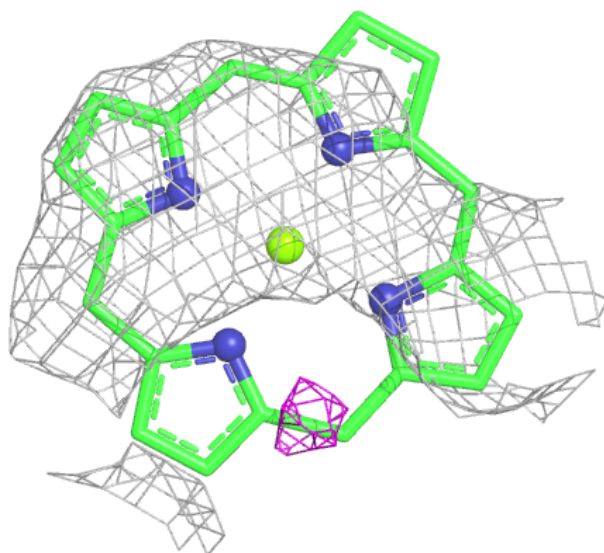
Electron density around LMU 2 322:

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



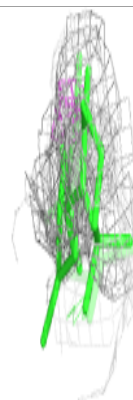
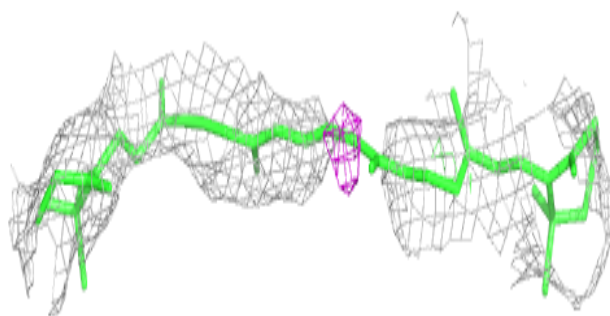
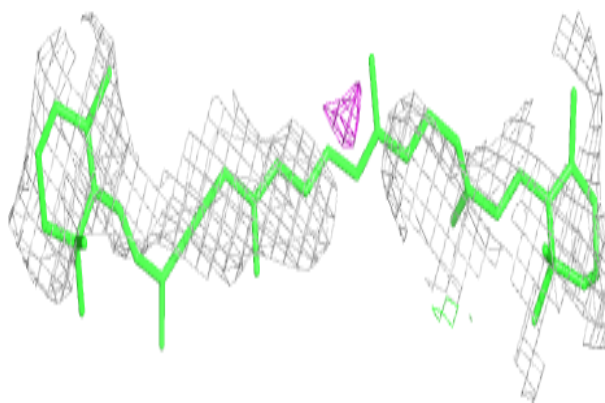
Electron density around CLA A 802:

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

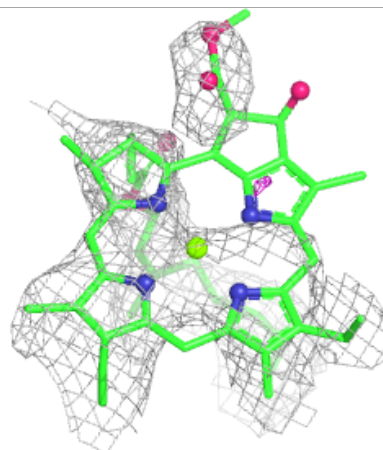
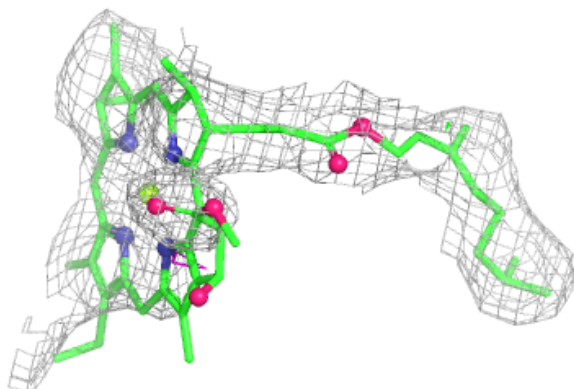
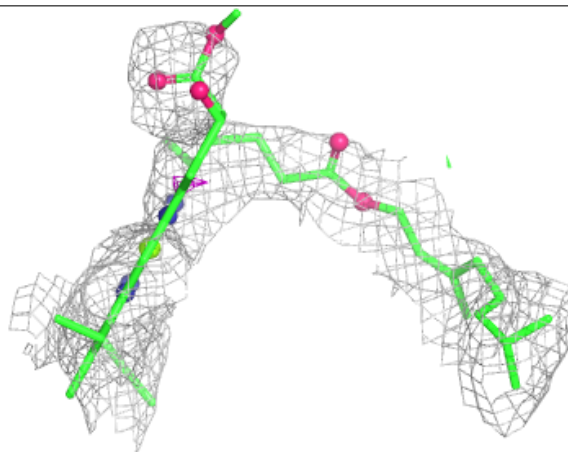


Electron density around BCR A 843:

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

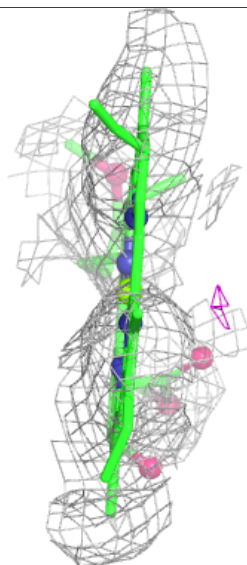
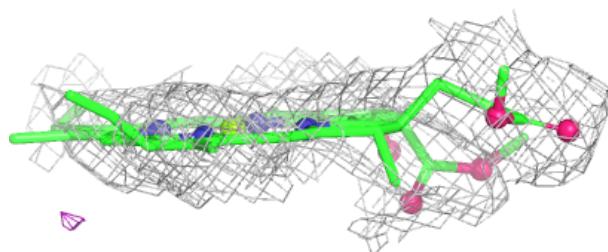
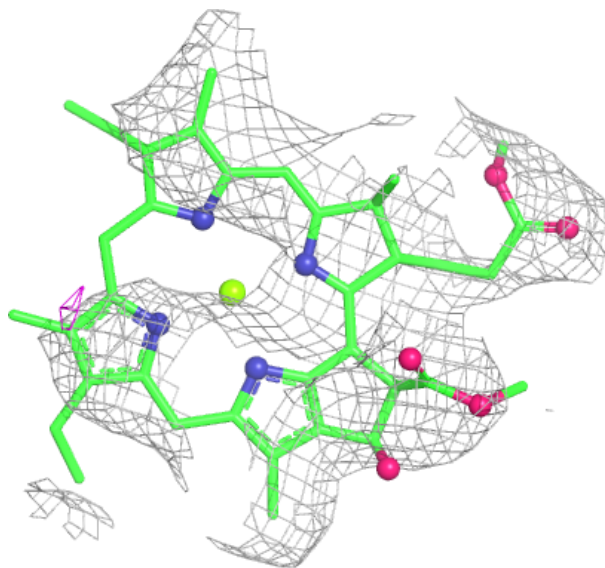
**Electron density around CLA L 204:**

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



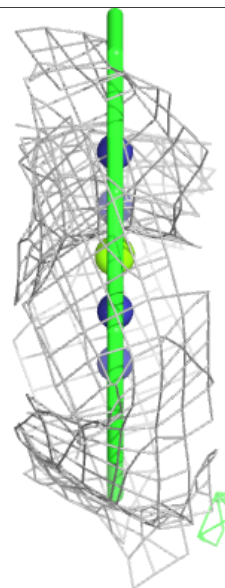
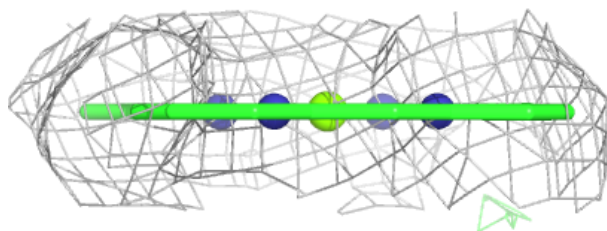
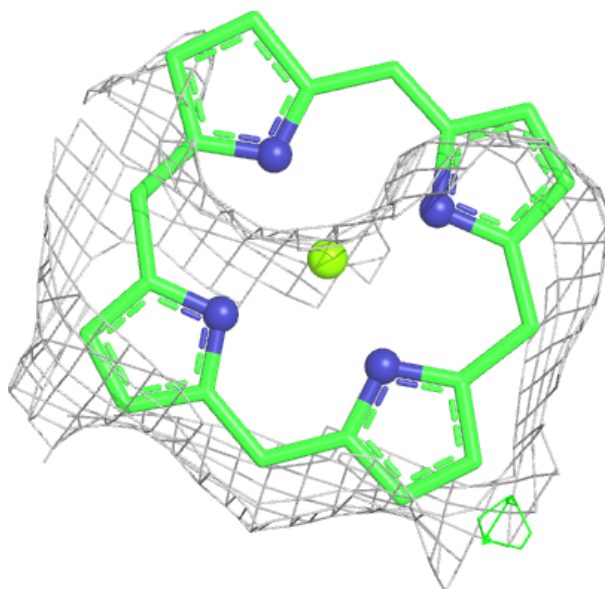
Electron density around CLA B 817:

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



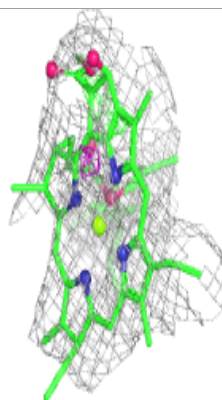
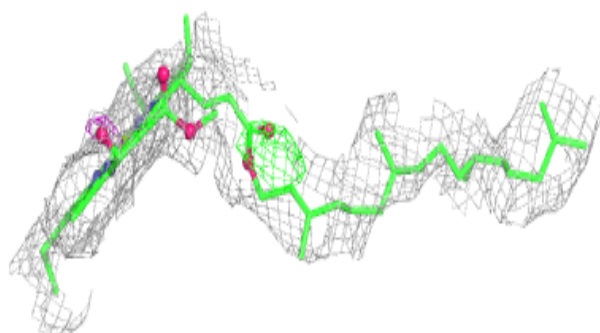
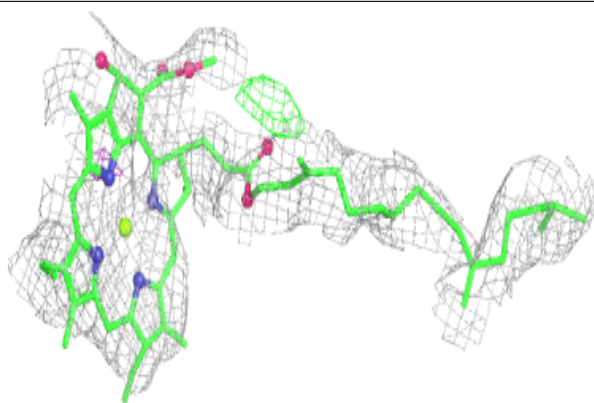
Electron density around CLA 3 305:

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

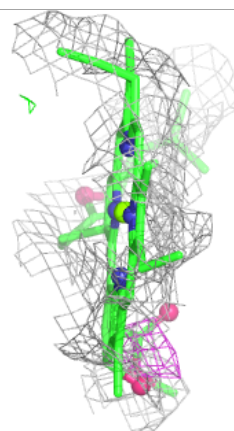
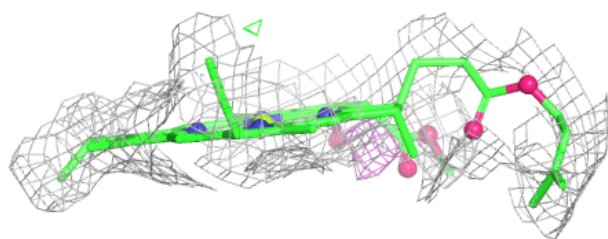
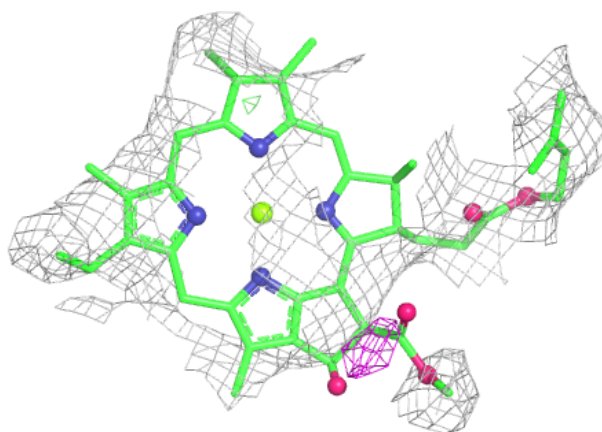


Electron density around CLA 4 303:

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

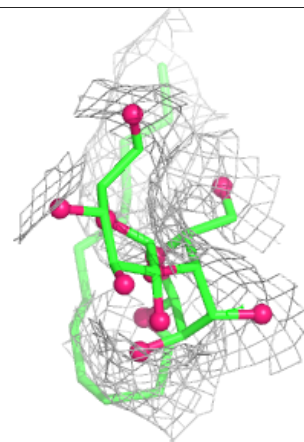
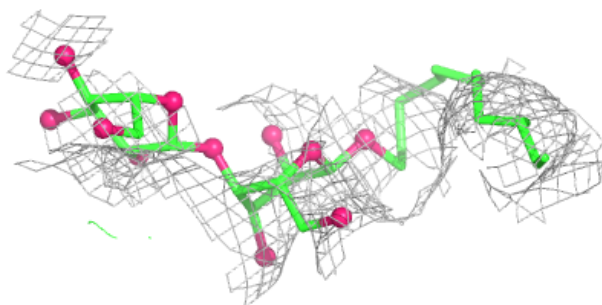
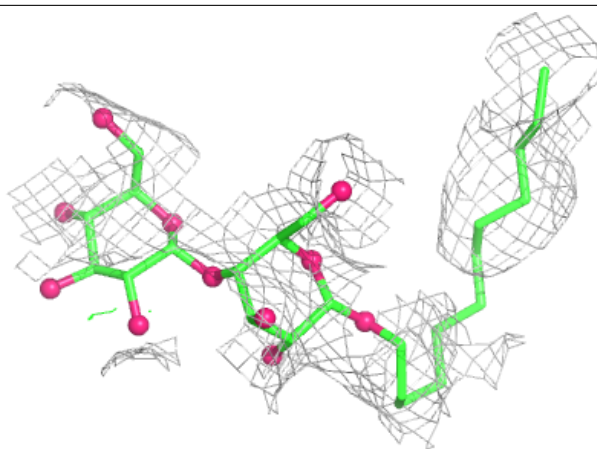
**Electron density around CLA K 103:**

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



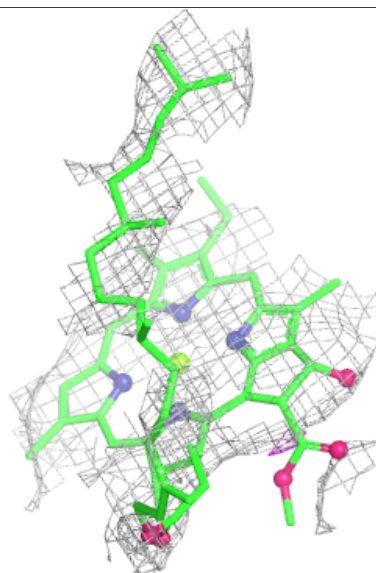
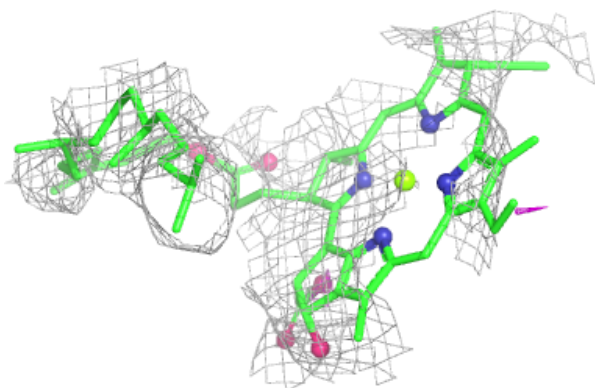
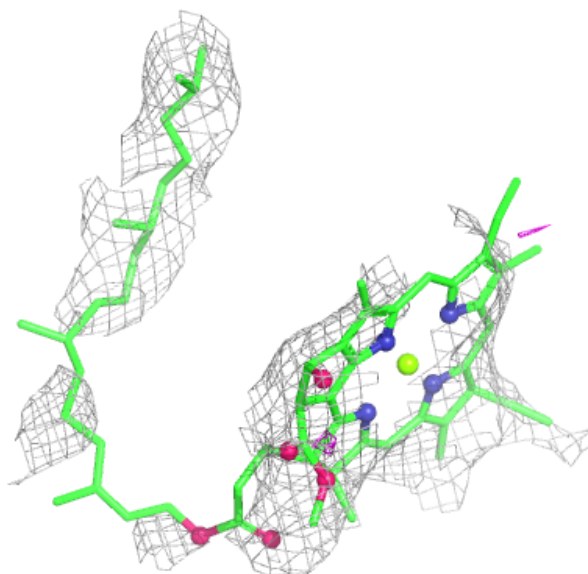
Electron density around LMU A 848:

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



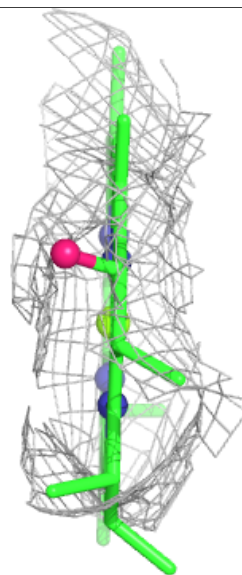
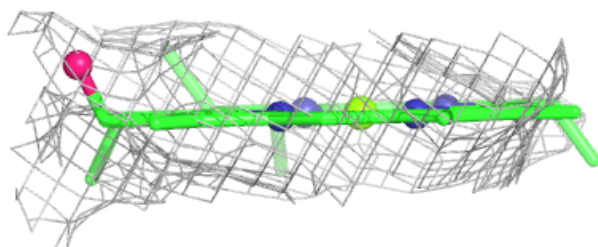
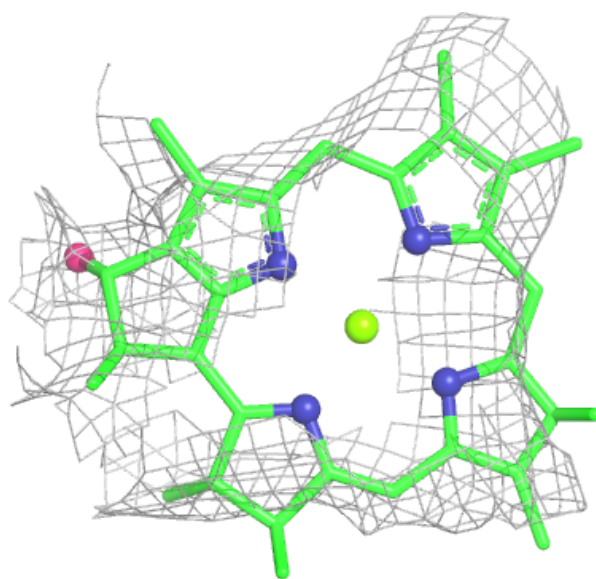
Electron density around CLA 3 311:

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



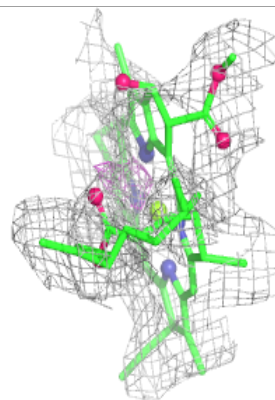
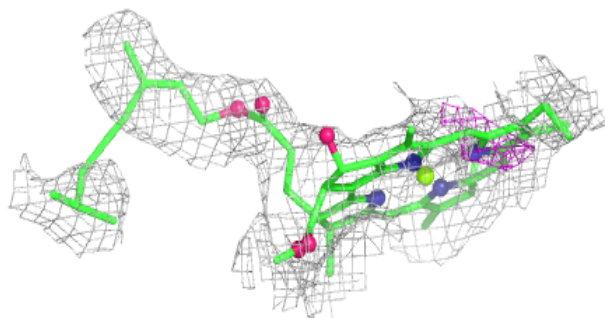
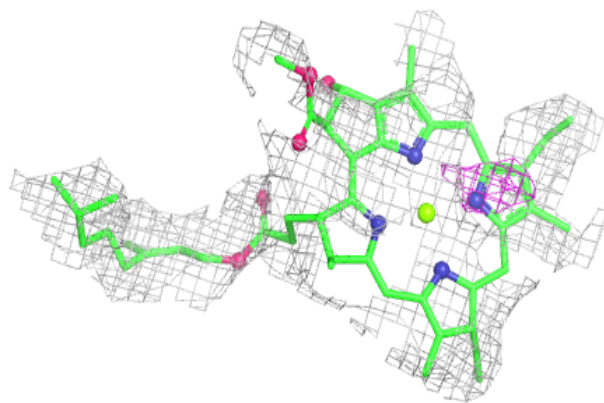
Electron density around CLA 3 318:

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



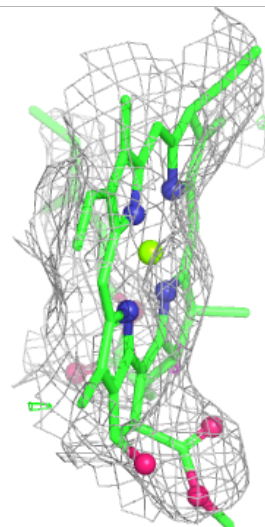
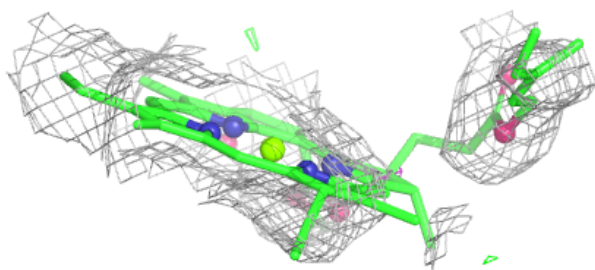
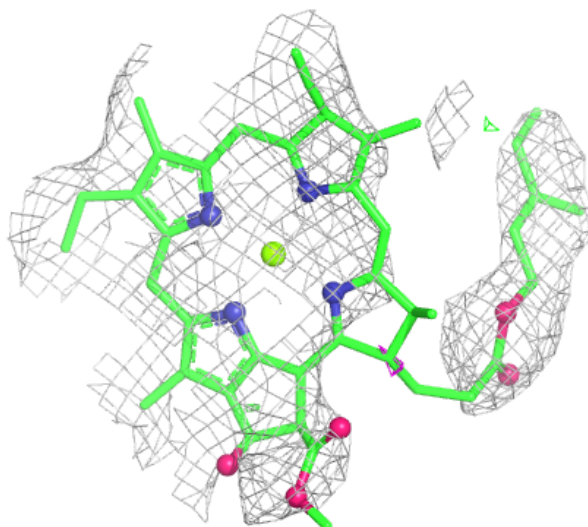
Electron density around CLA H 112:

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



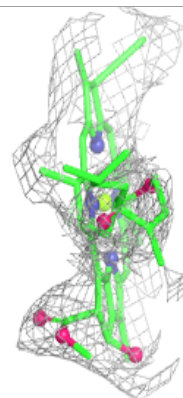
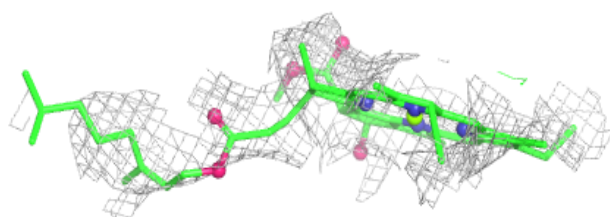
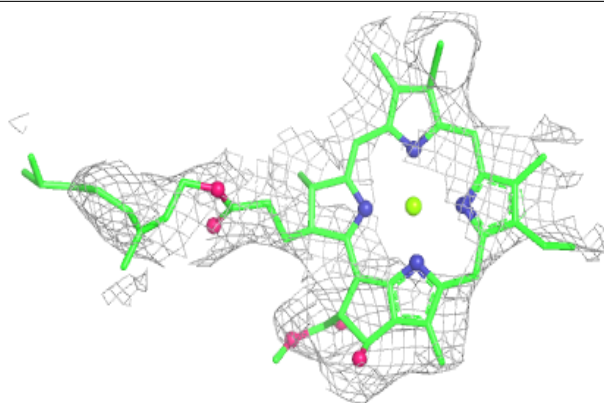
Electron density around CLA B 836:

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

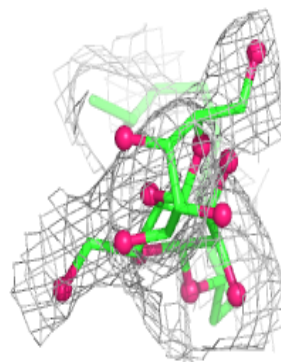
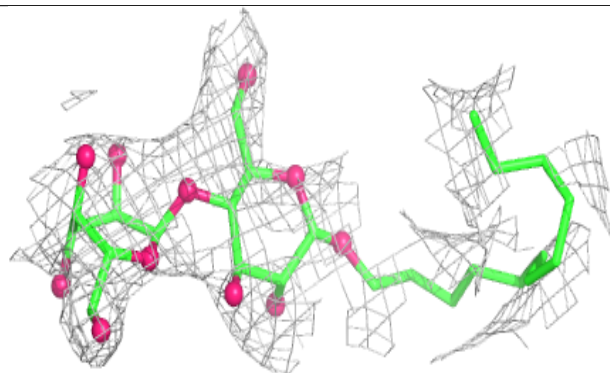
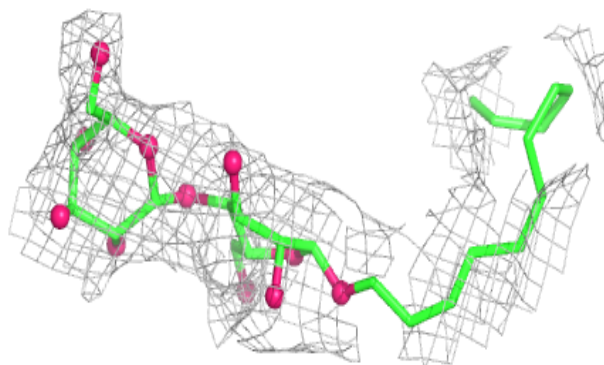


Electron density around CLA A 840:

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

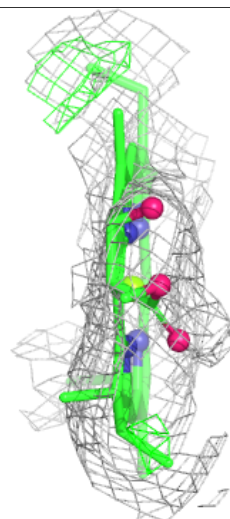
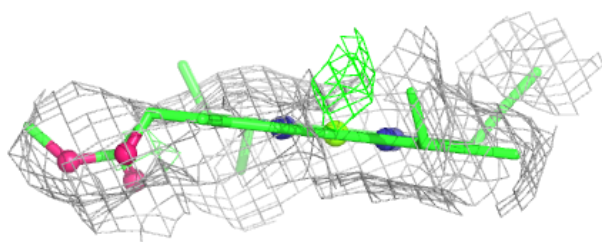
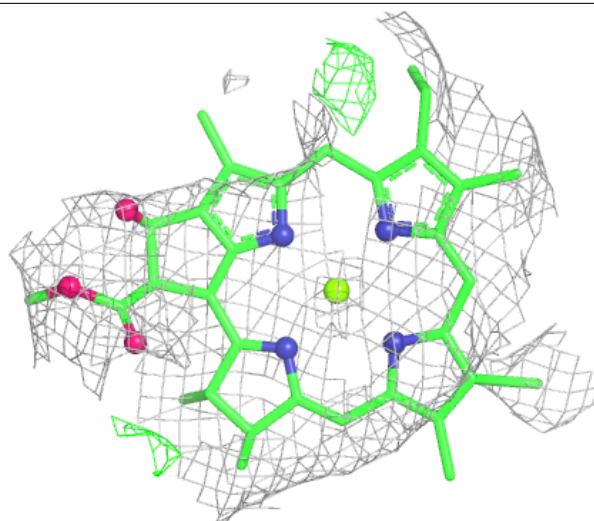
**Electron density around LMU H 106:**

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



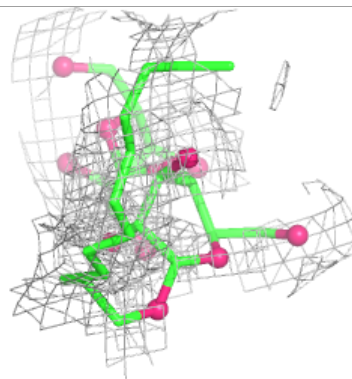
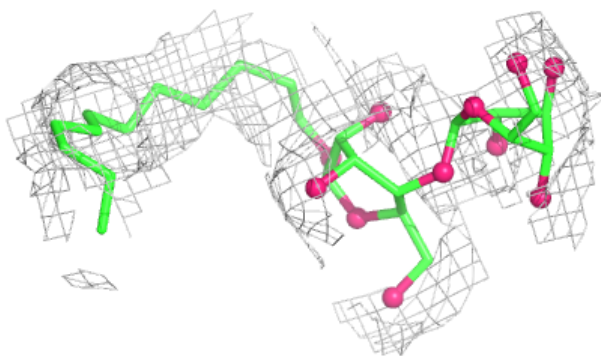
Electron density around CLA F 206:

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



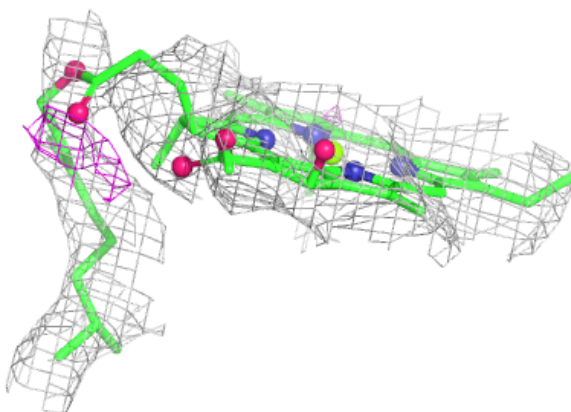
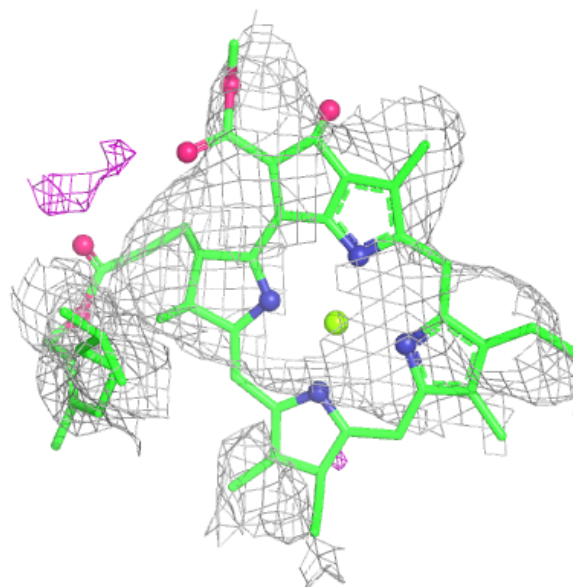
Electron density around LMU R 104:

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



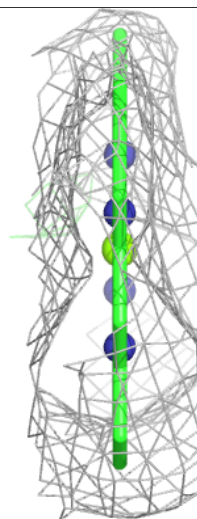
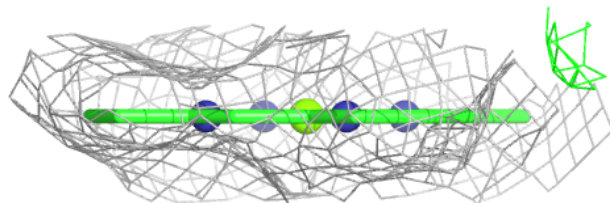
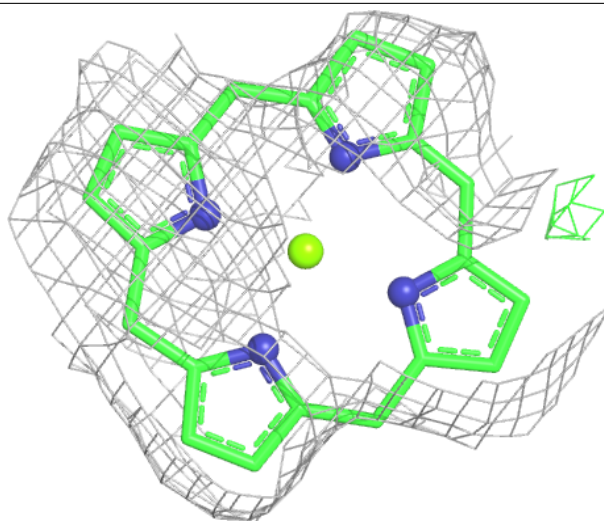
Electron density around CLA H 101:

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



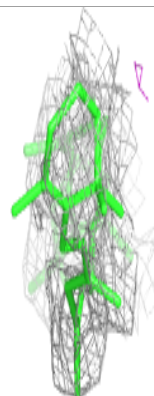
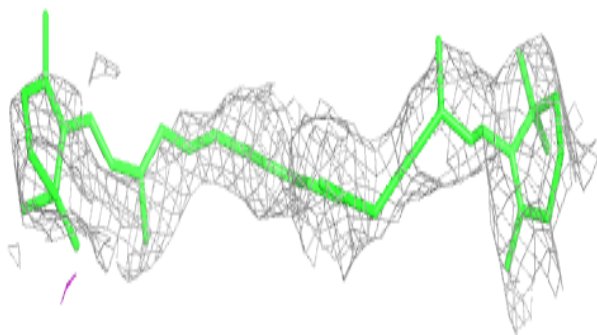
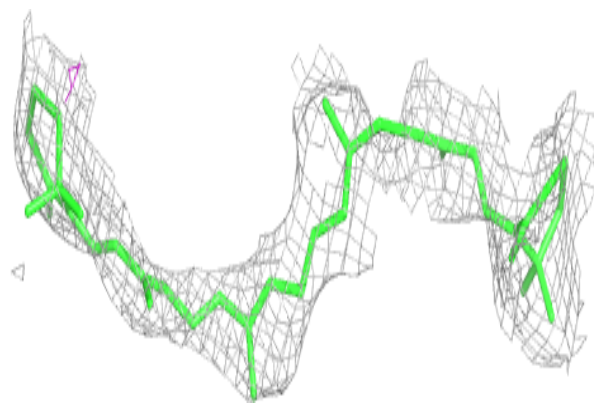
Electron density around CLA 4 308:

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

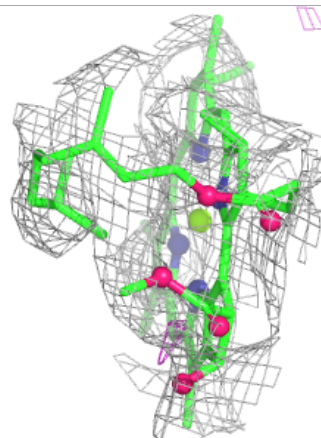
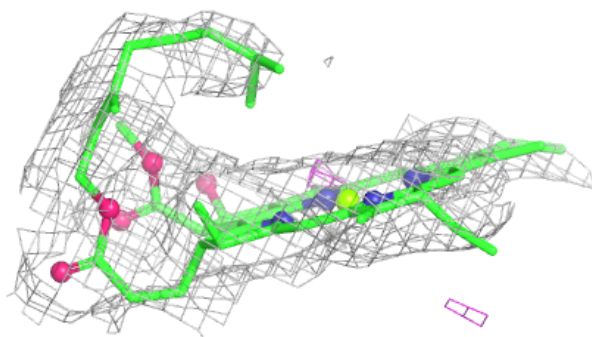
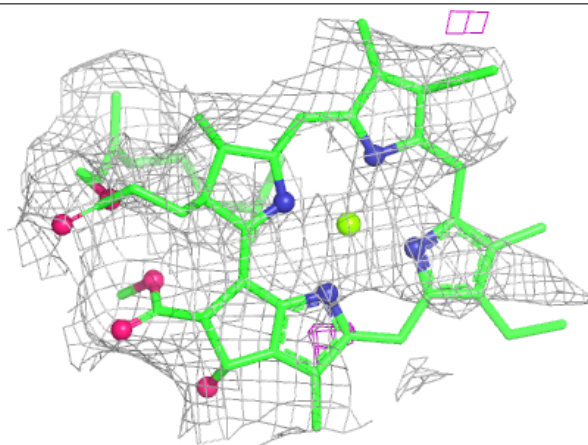


Electron density around BCR I 103:

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

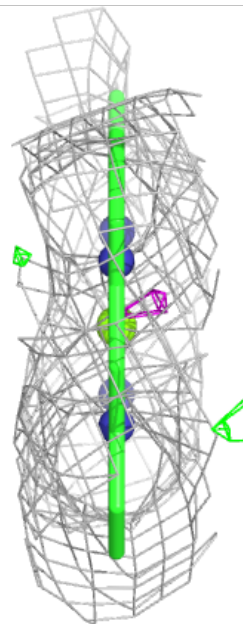
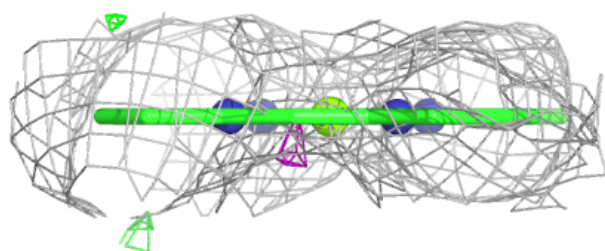
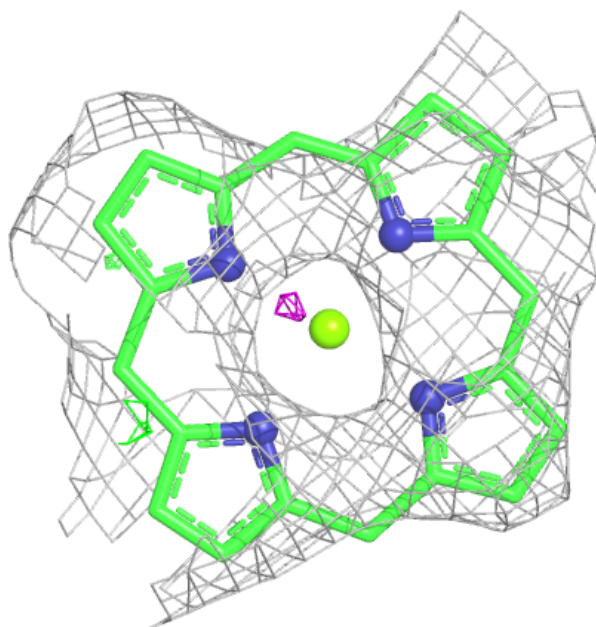
**Electron density around CLA 4 304:**

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



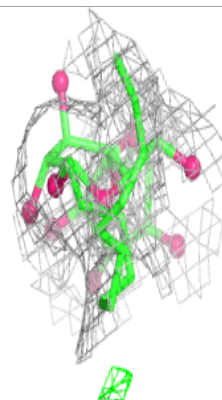
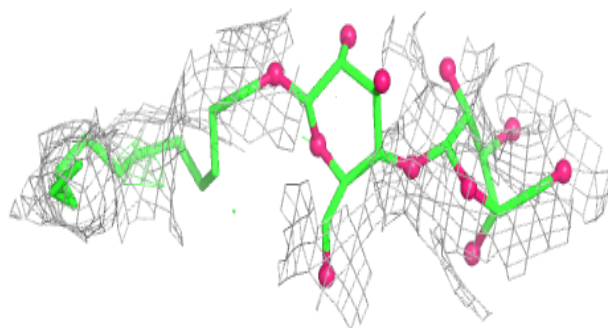
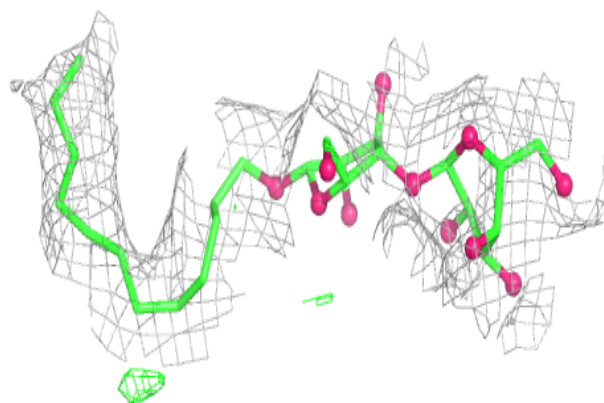
Electron density around CLA 4 307:

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

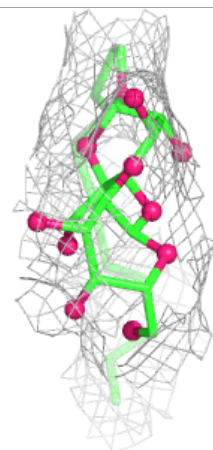
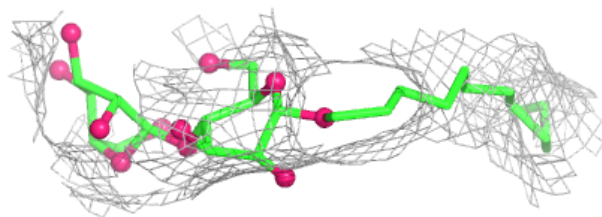
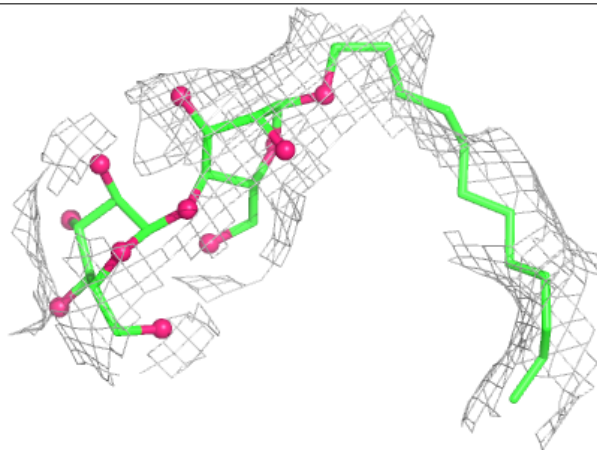


Electron density around LMU A 846:

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

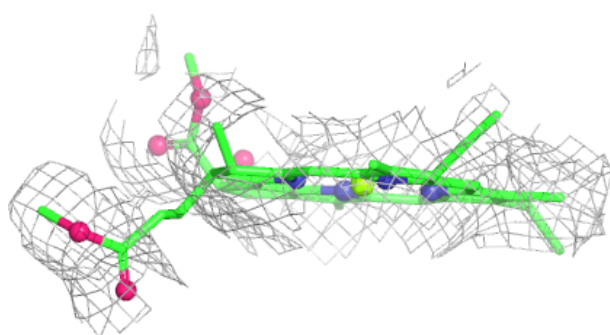
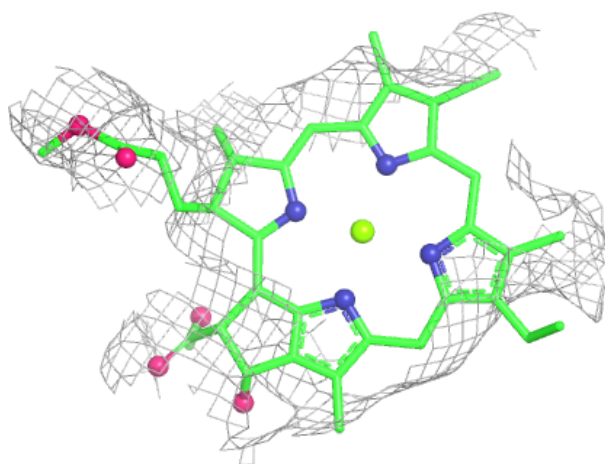
**Electron density around LMU K 106:**

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



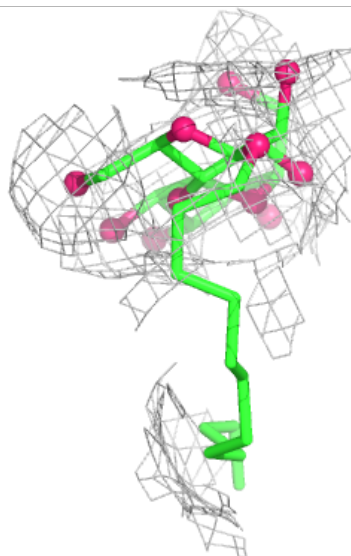
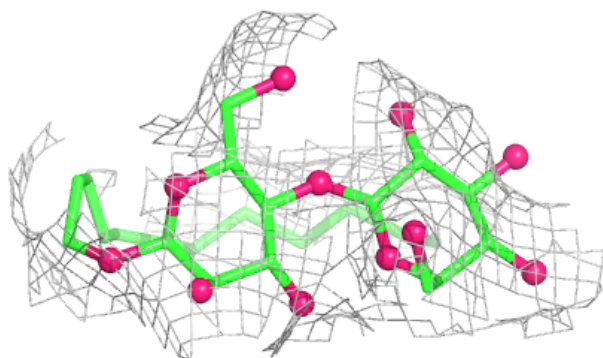
Electron density around CLA 1 201:

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



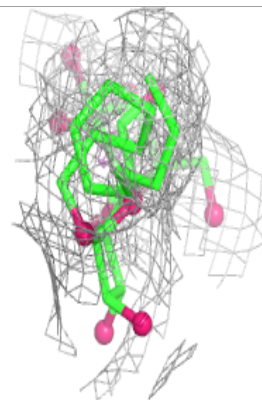
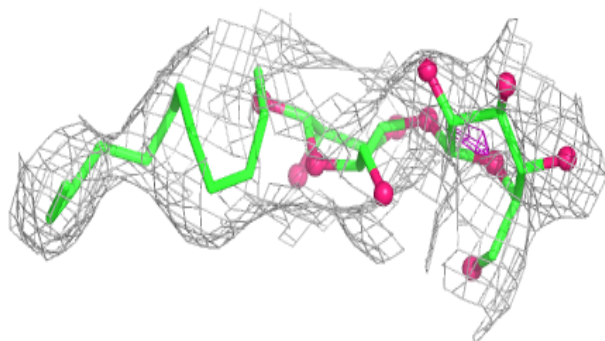
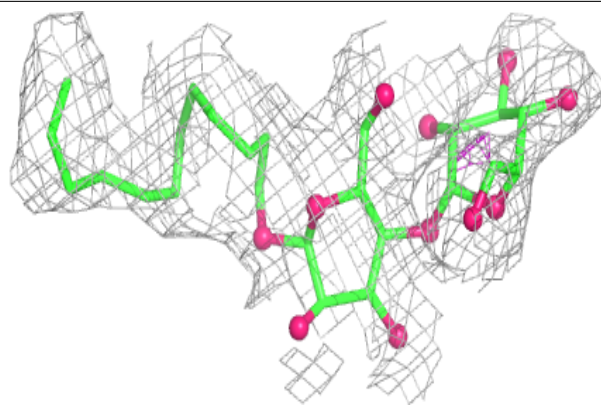
Electron density around LMU 1 217:

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



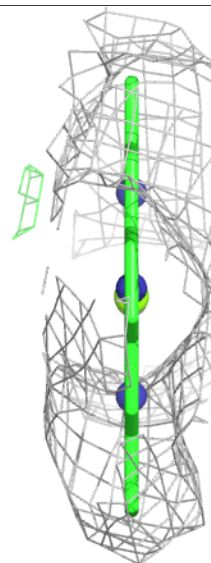
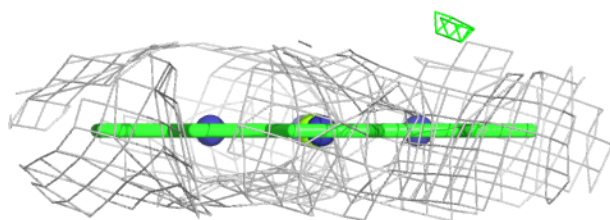
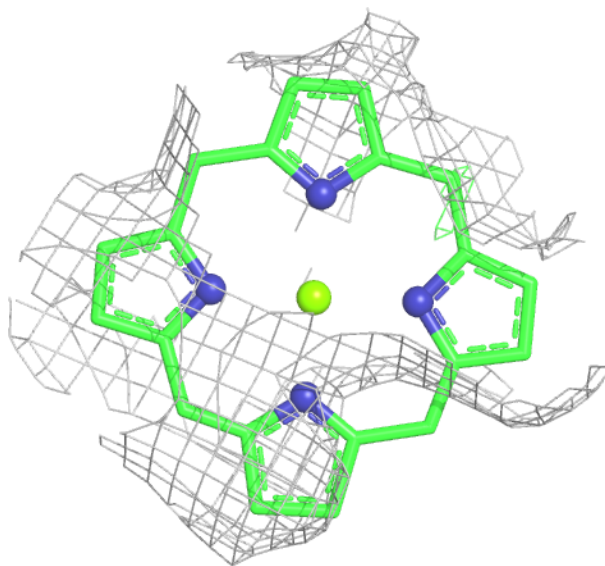
Electron density around LMU 2 313:

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



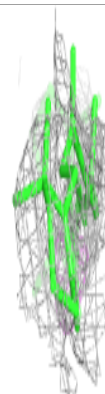
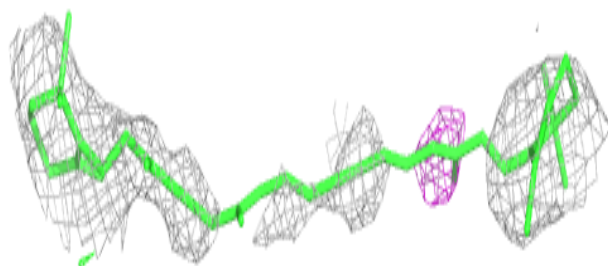
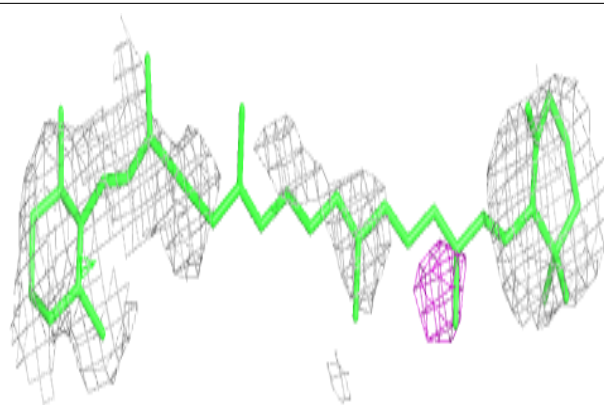
Electron density around CLA 3 309:

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

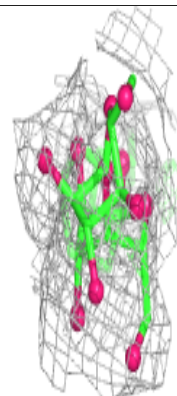
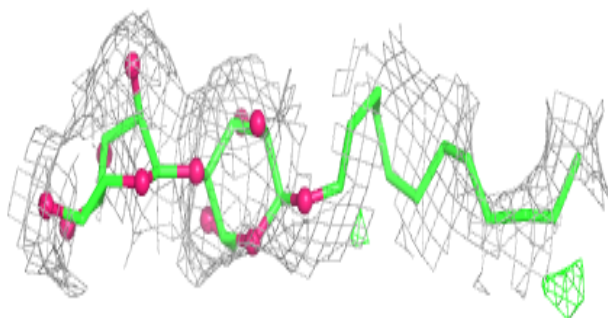
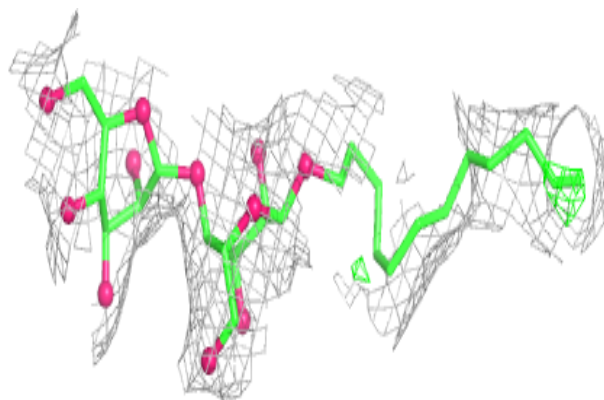


Electron density around BCR G 104:

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

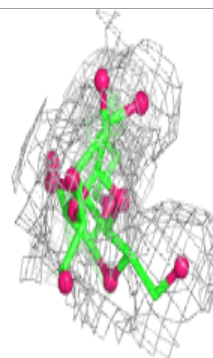
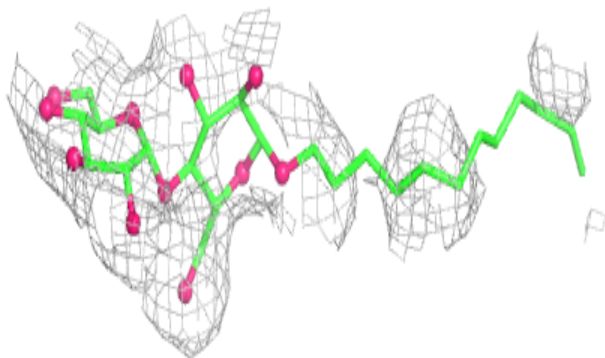
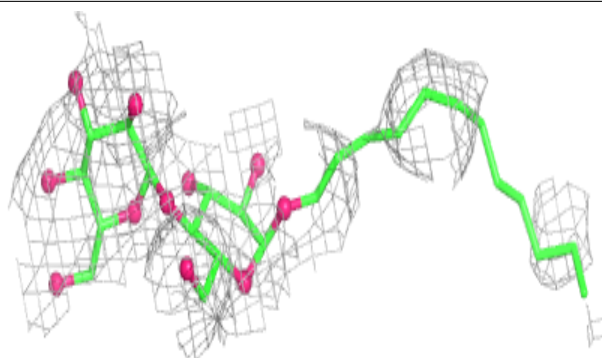
**Electron density around LMU E 101:**

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



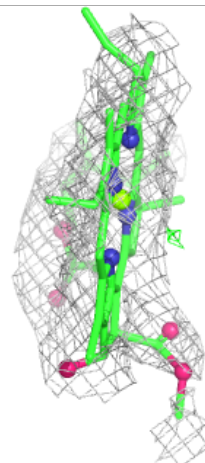
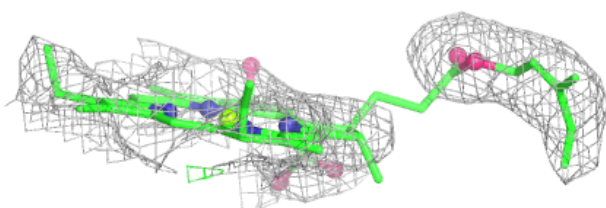
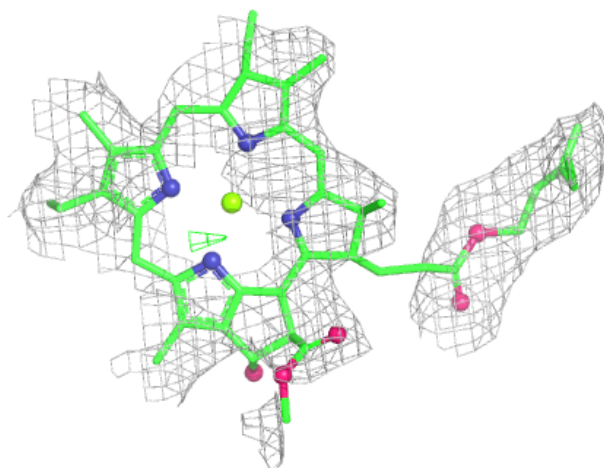
Electron density around LMU B 805:

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



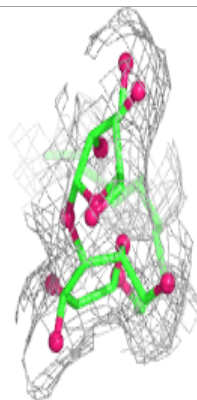
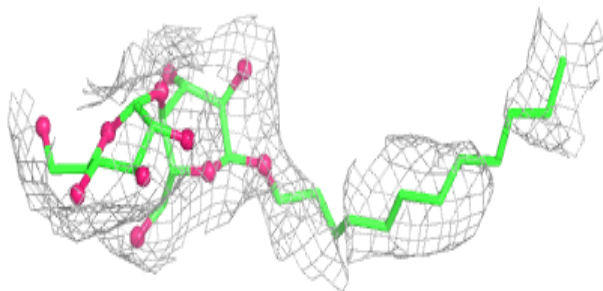
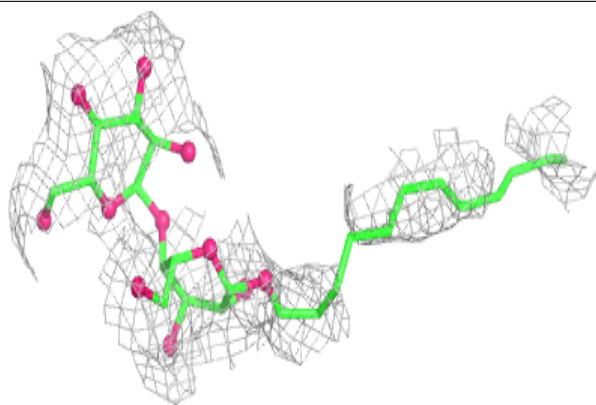
Electron density around CLA G 105:

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



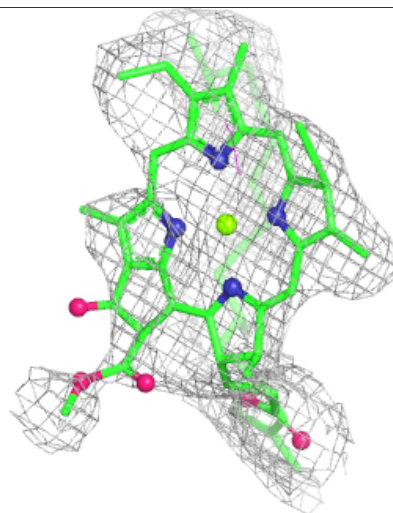
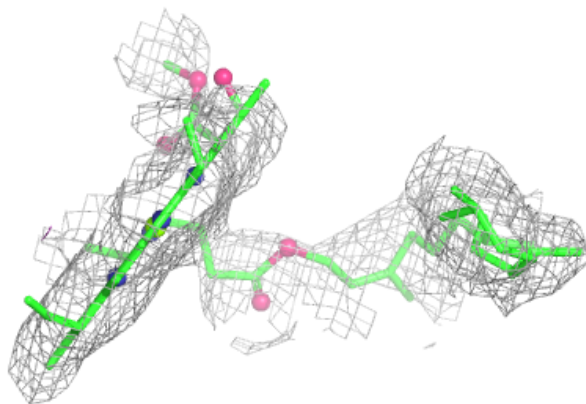
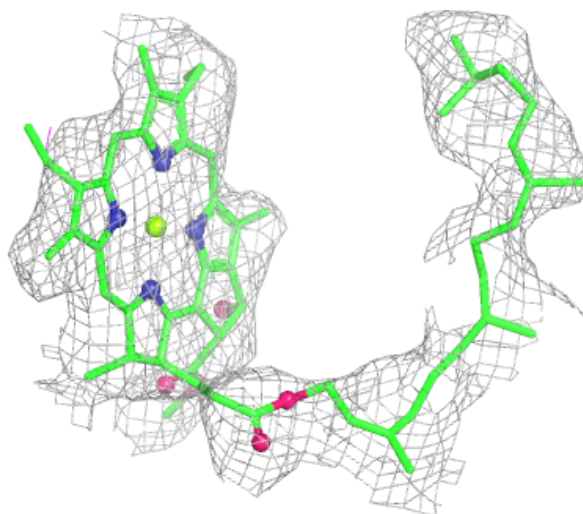
Electron density around LMU R 105:

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



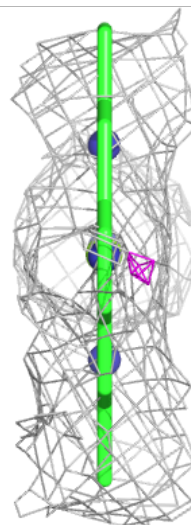
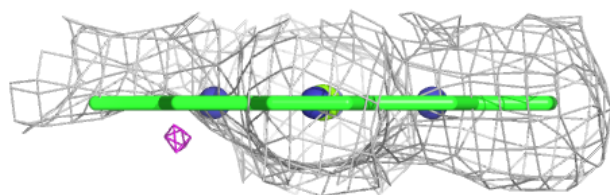
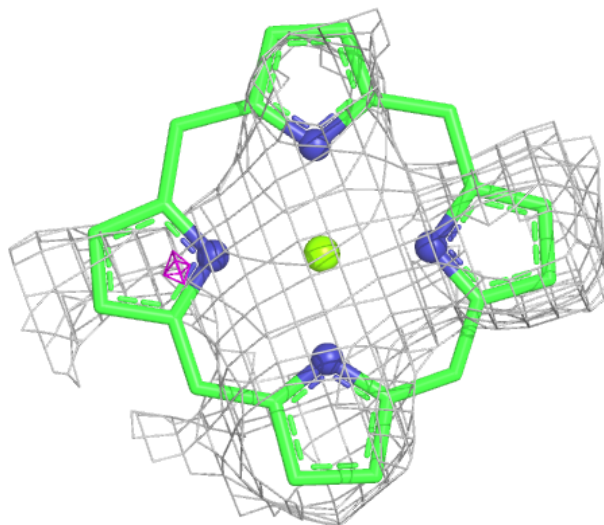
Electron density around CLA 3 310:

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



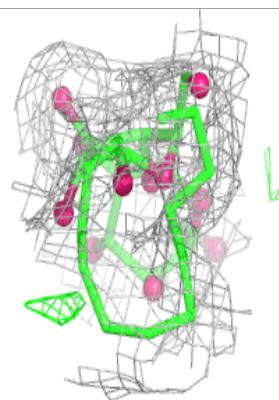
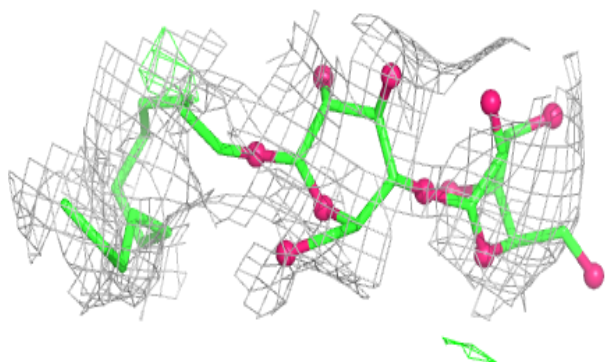
Electron density around CLA 3 302:

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



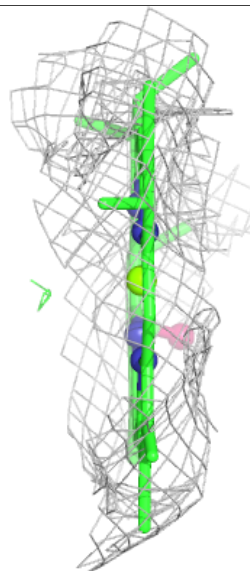
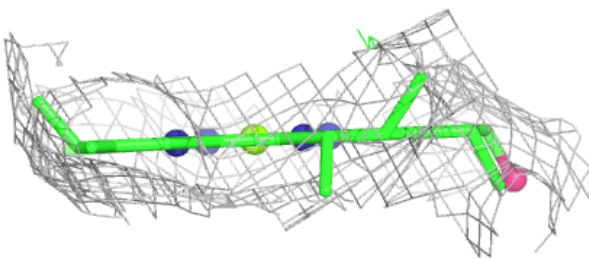
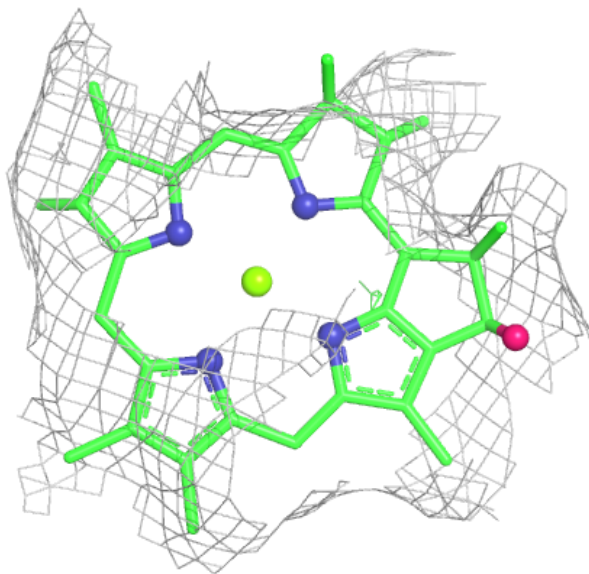
Electron density around LMU A 854:

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



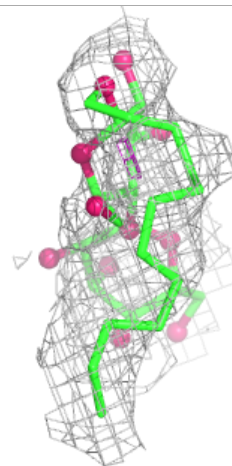
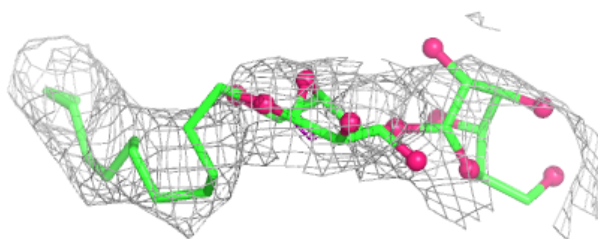
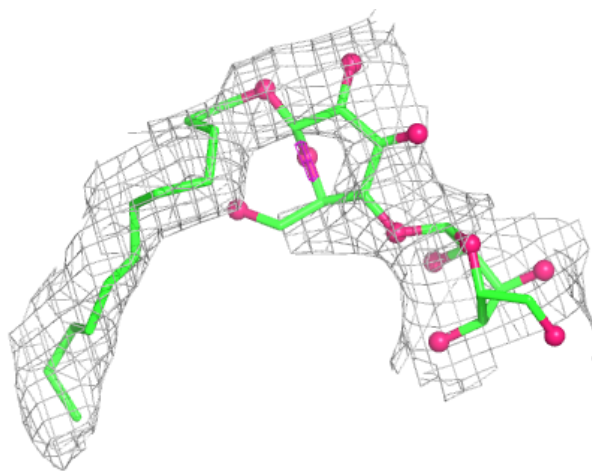
Electron density around CLA 3 303:

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



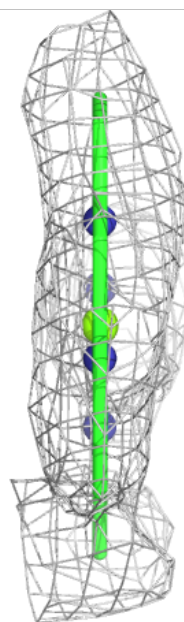
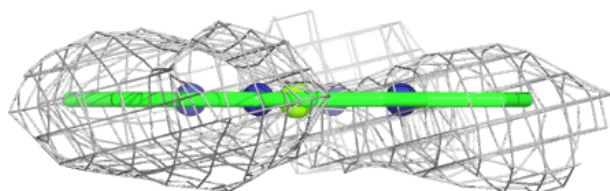
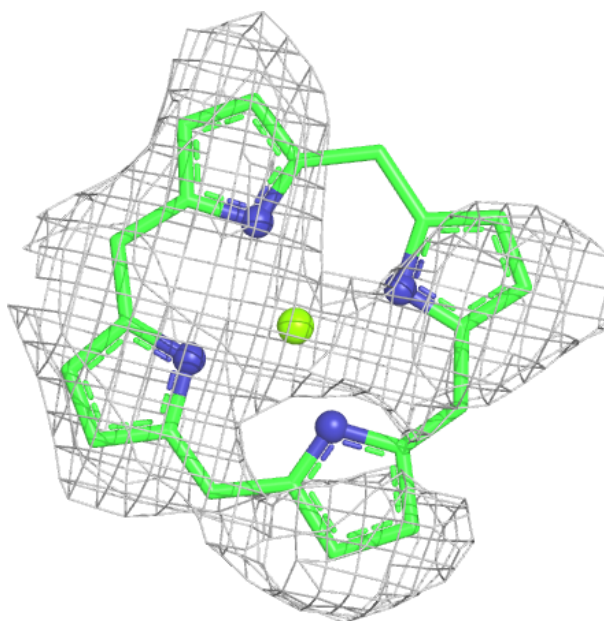
Electron density around LMU R 103:

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



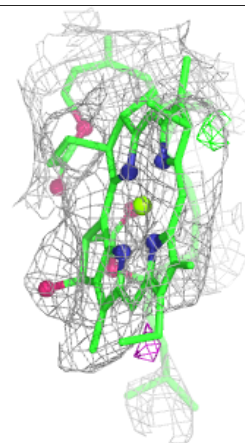
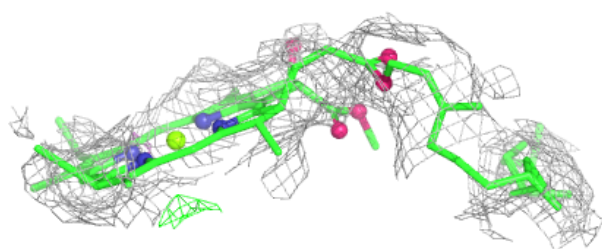
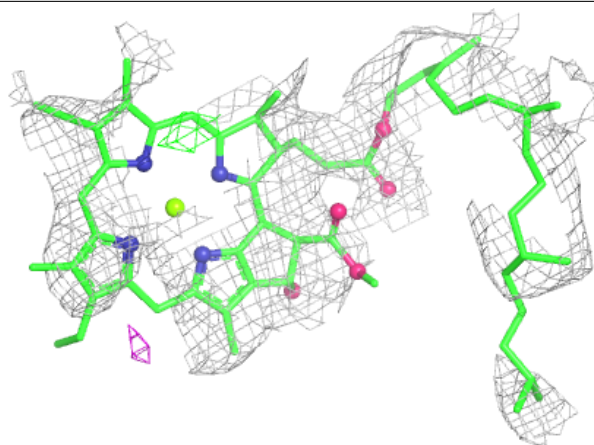
Electron density around CLA 3 313:

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

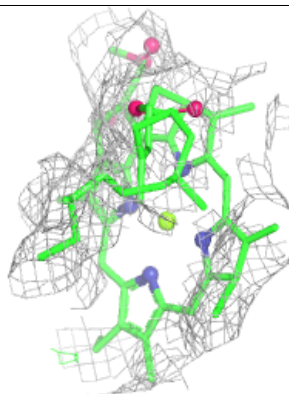
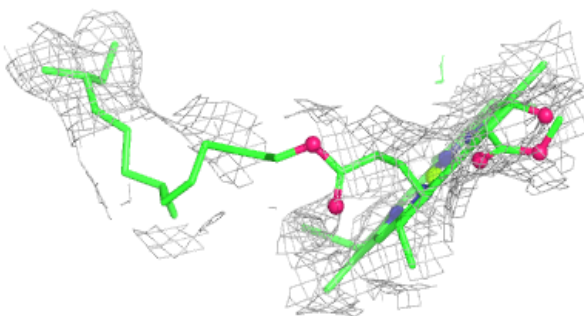
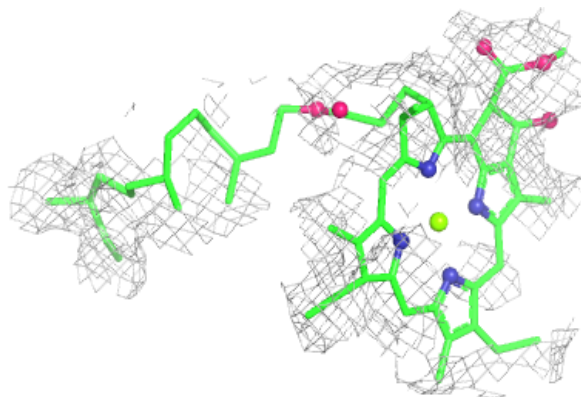


Electron density around CLA R 108:

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

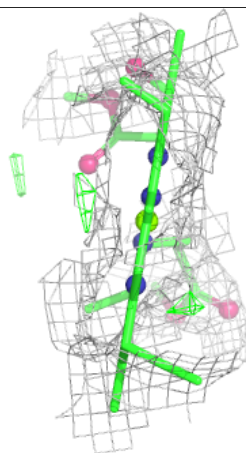
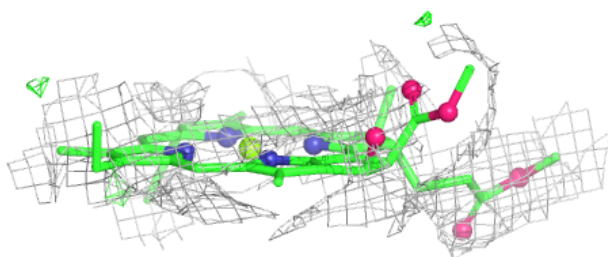
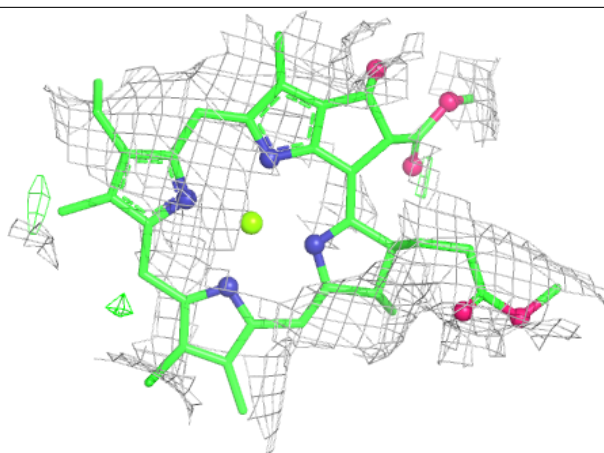
**Electron density around CLA 2 312:**

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

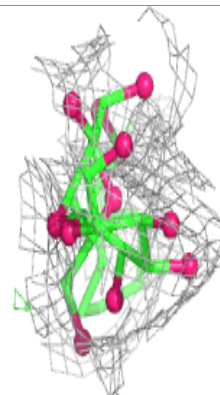
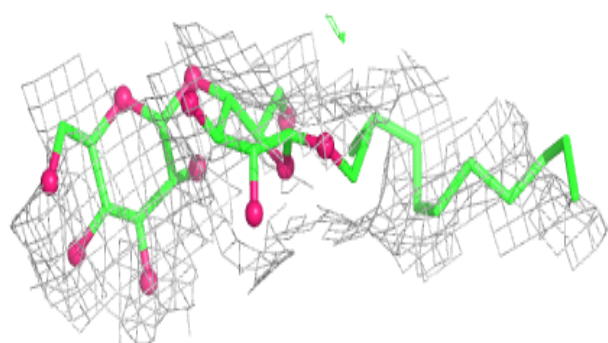
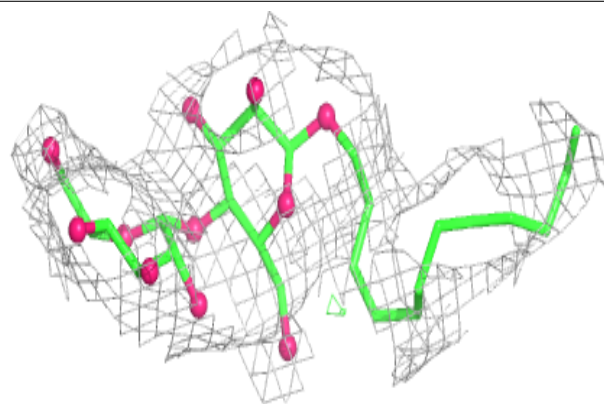


Electron density around CLA K 101:

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

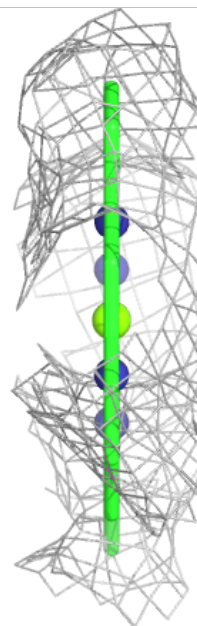
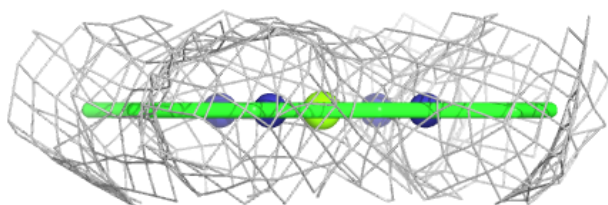
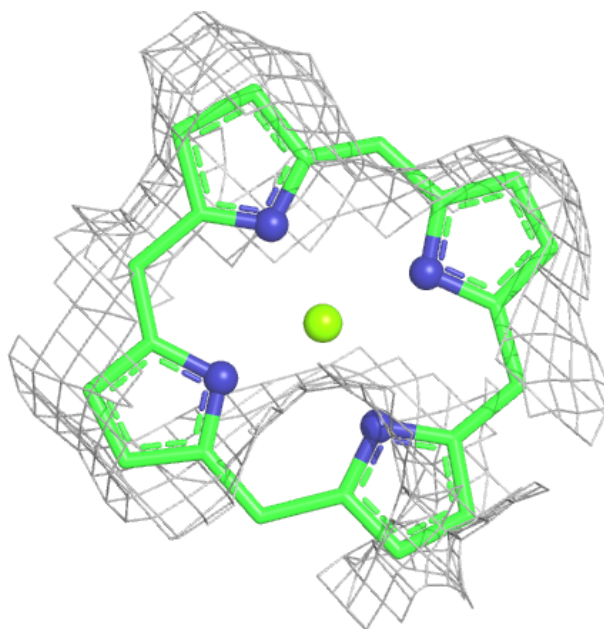
**Electron density around LMU K 107:**

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



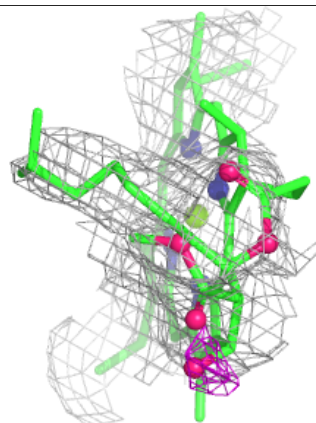
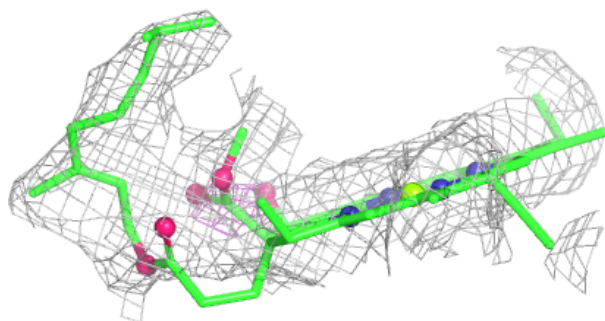
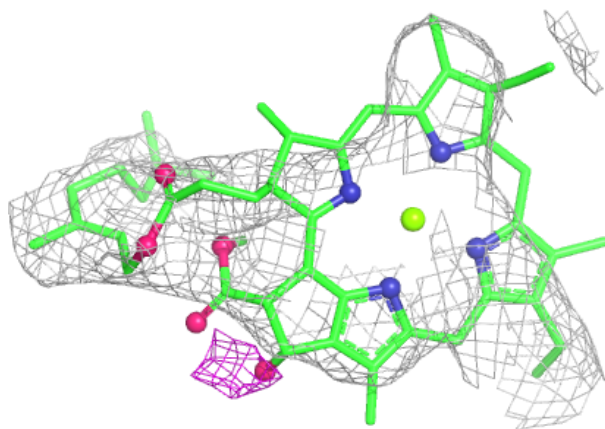
Electron density around CLA A 841:

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

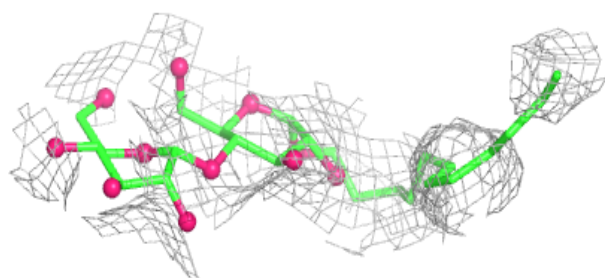
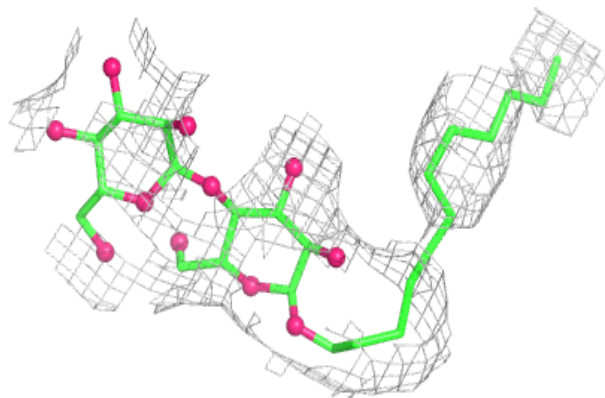


Electron density around CLA L 202:

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

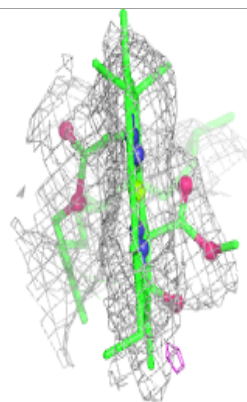
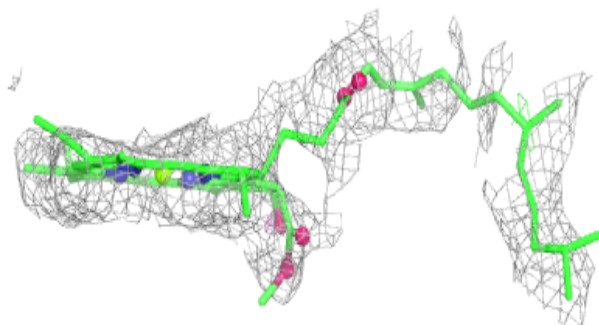
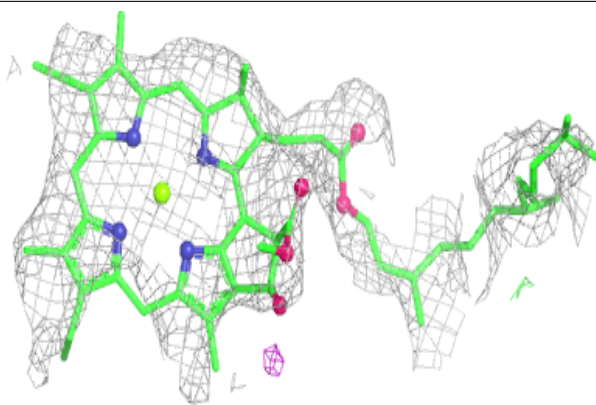
**Electron density around LMU R 106:**

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



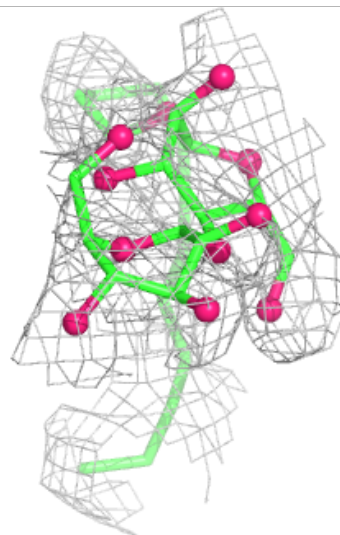
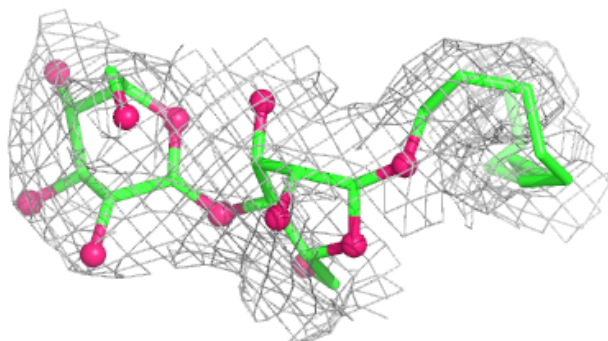
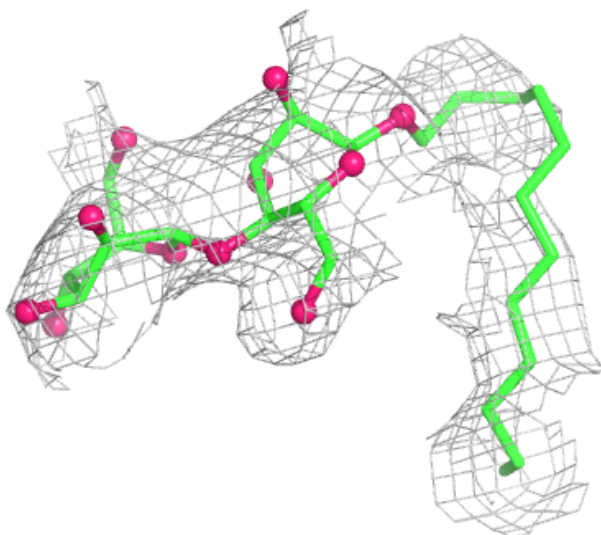
Electron density around CLA B 816:

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



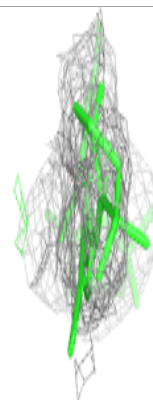
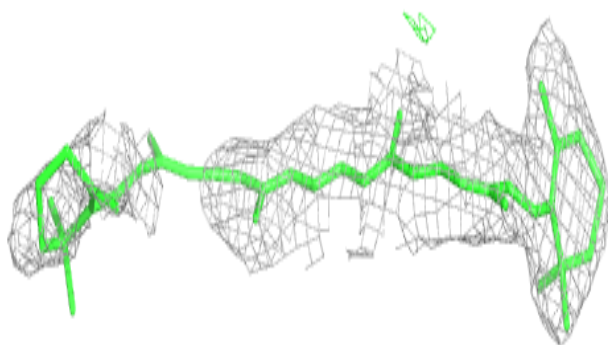
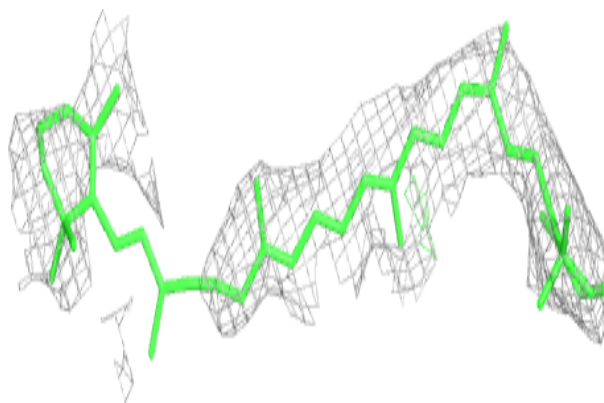
Electron density around LMU R 101:

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

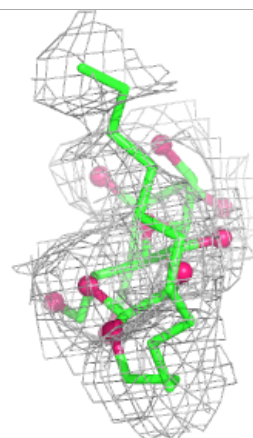
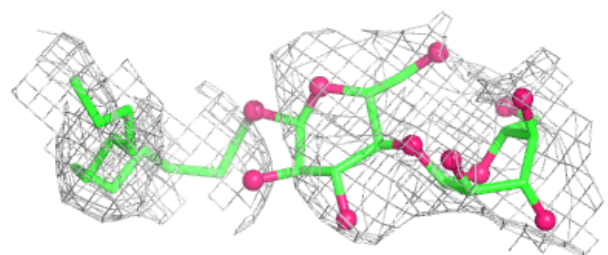
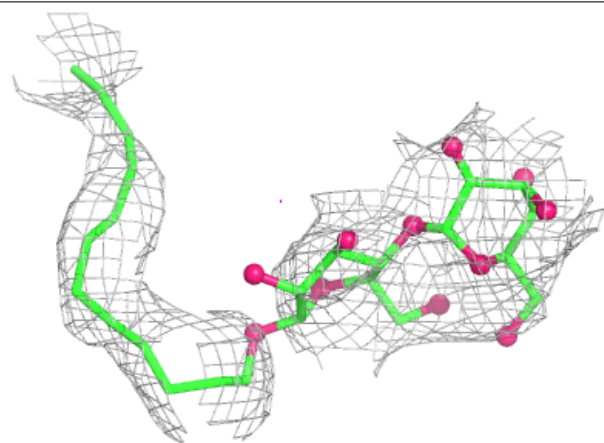


Electron density around BCR B 845:

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

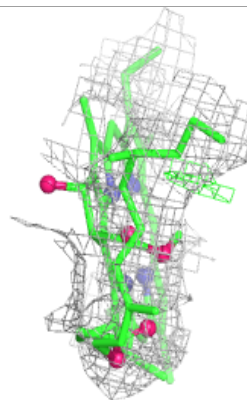
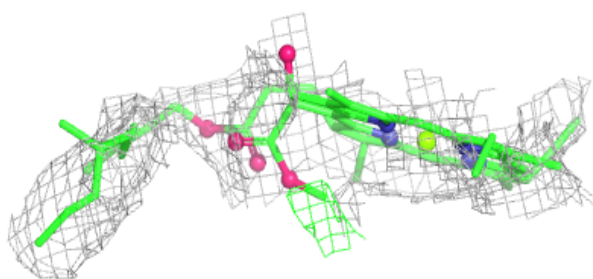
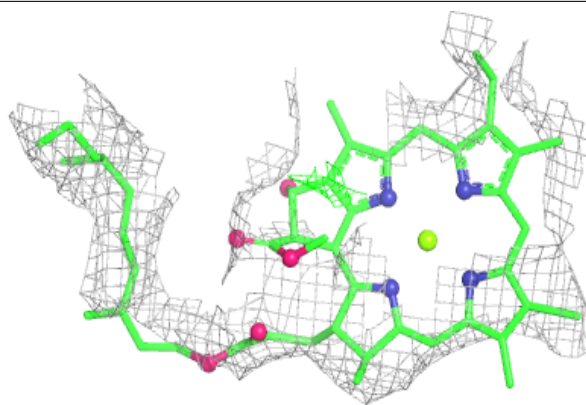
**Electron density around LMU 3 319:**

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

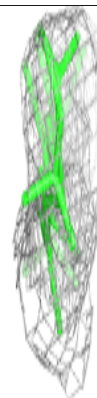
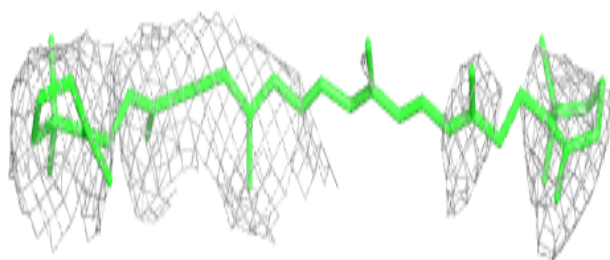
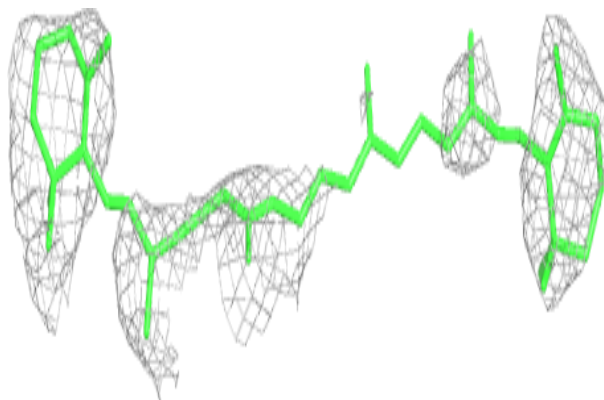


Electron density around CLA R 107:

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

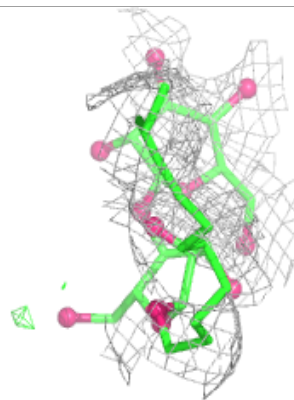
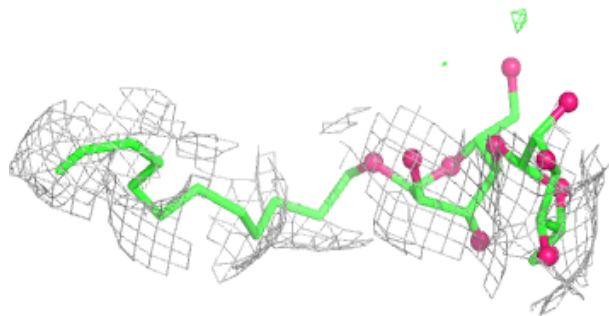
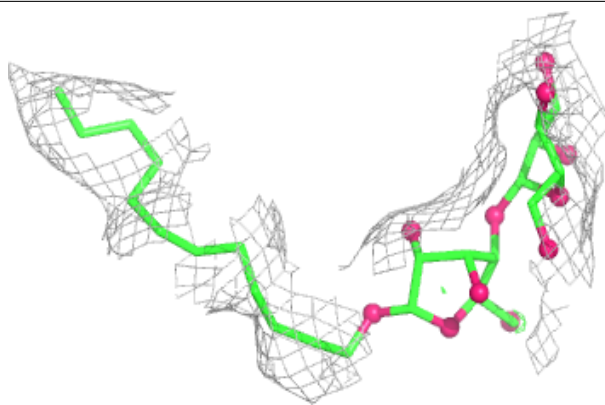
**Electron density around BCR L 211:**

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



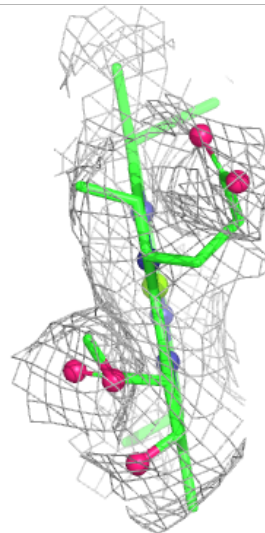
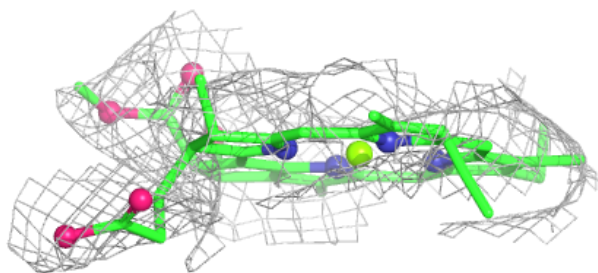
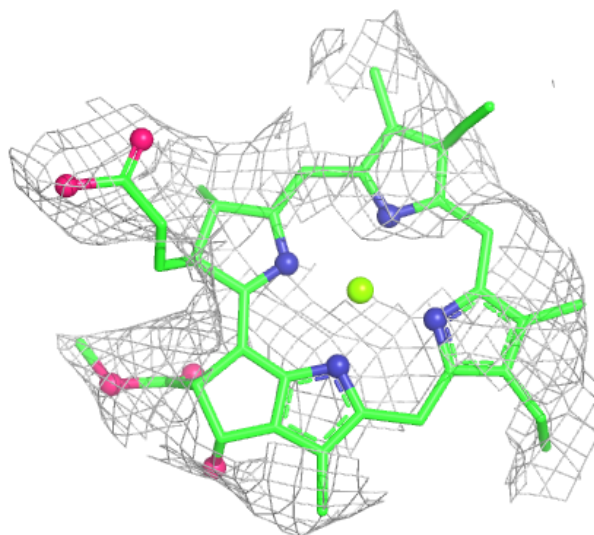
Electron density around LMU G 102:

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



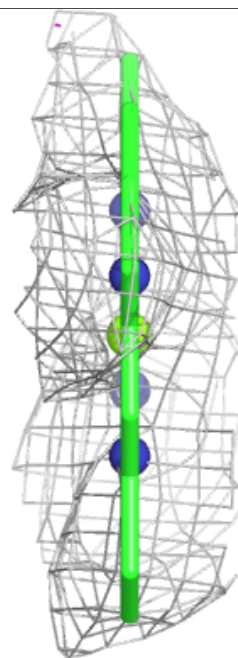
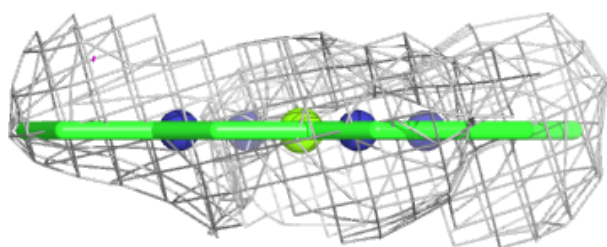
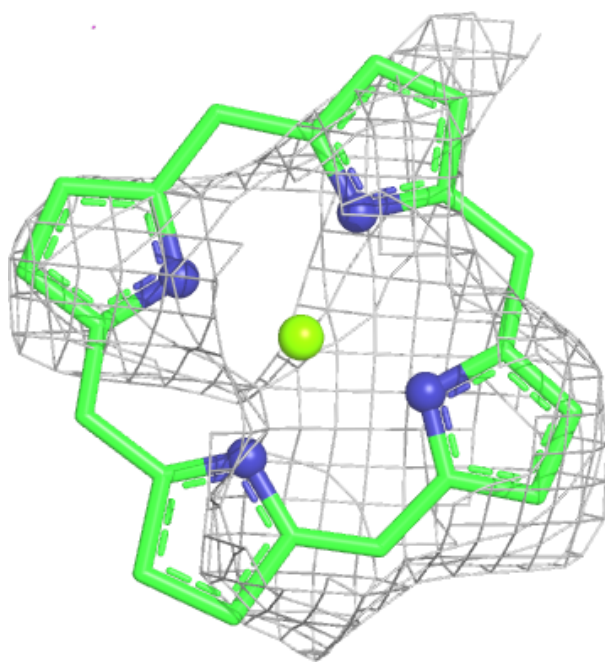
Electron density around CLA A 833:

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



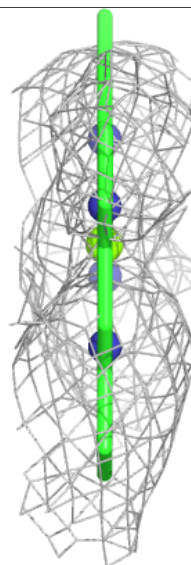
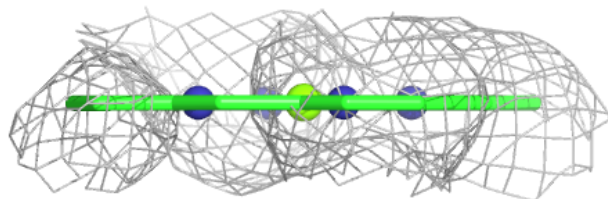
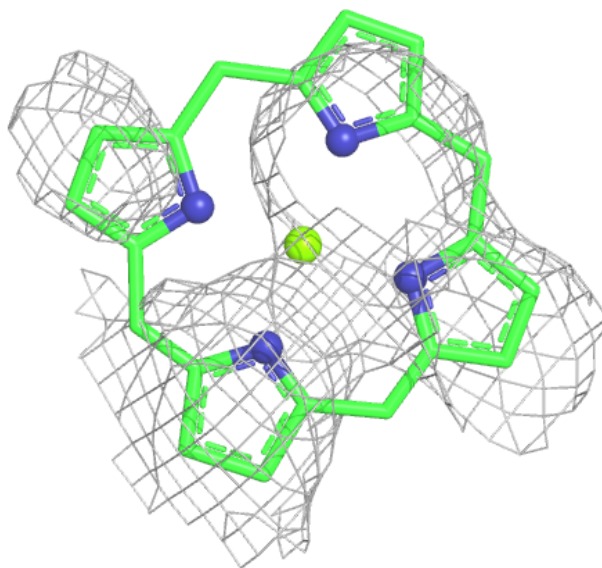
Electron density around CLA 2 301:

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



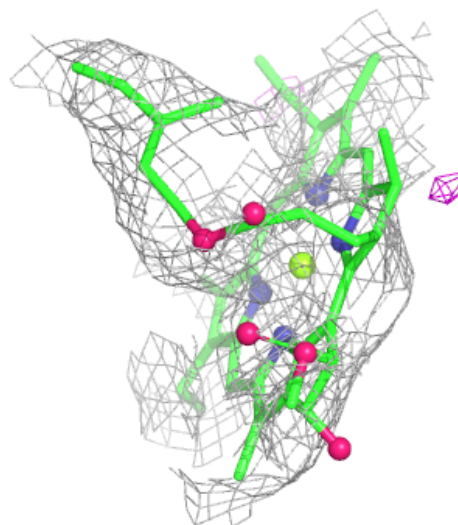
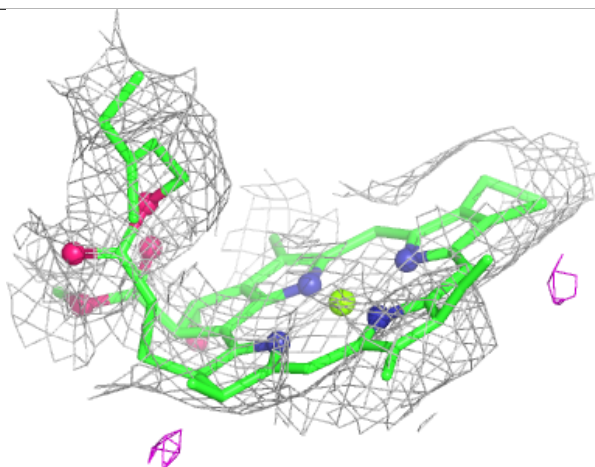
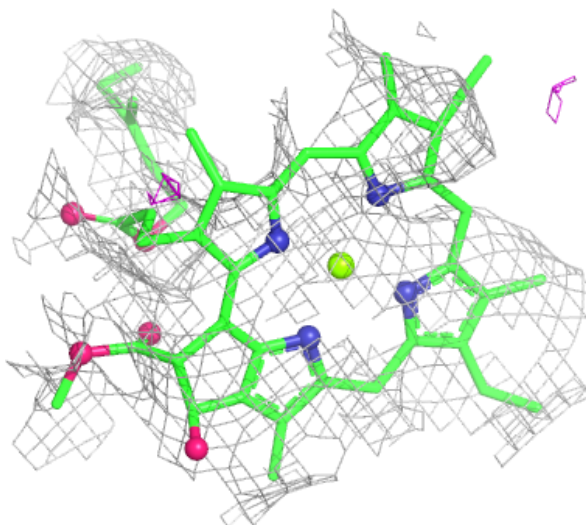
Electron density around CLA 2 304:

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



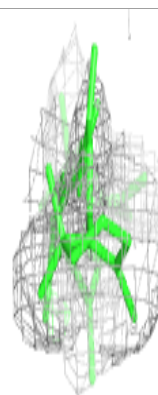
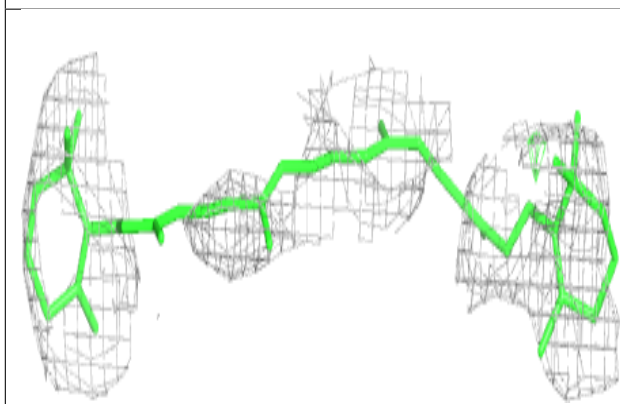
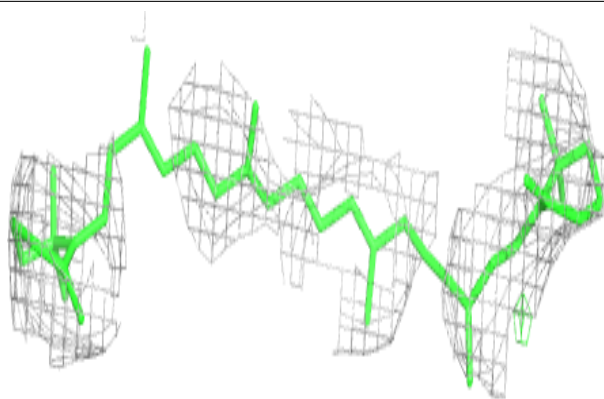
Electron density around CLA 1 207:

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



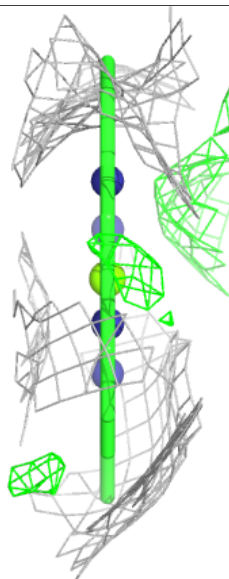
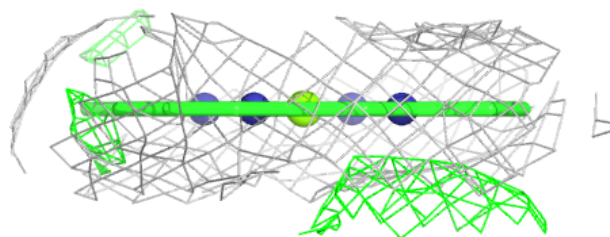
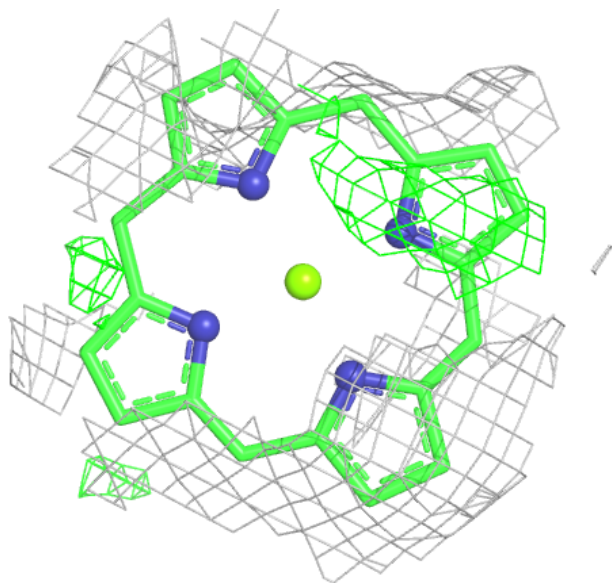
Electron density around BCR A 844:

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



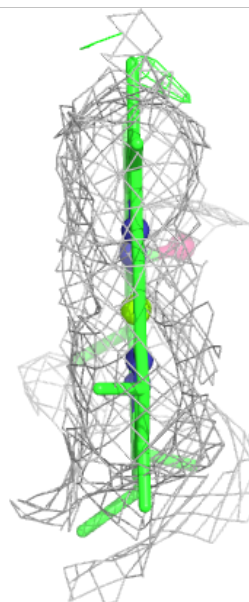
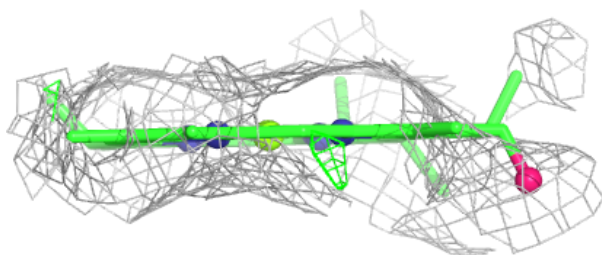
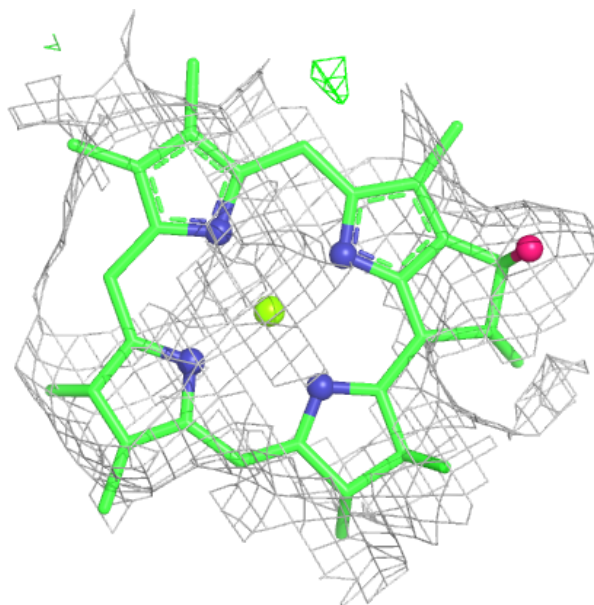
Electron density around CLA 1 208:

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



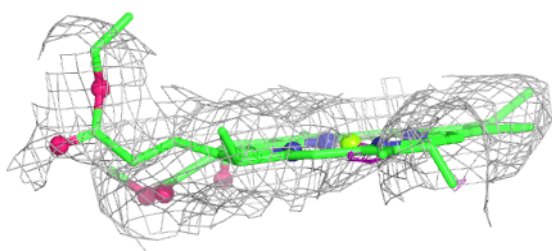
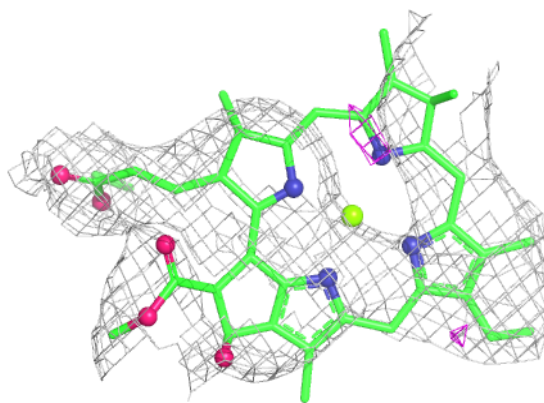
Electron density around CLA 1 205:

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



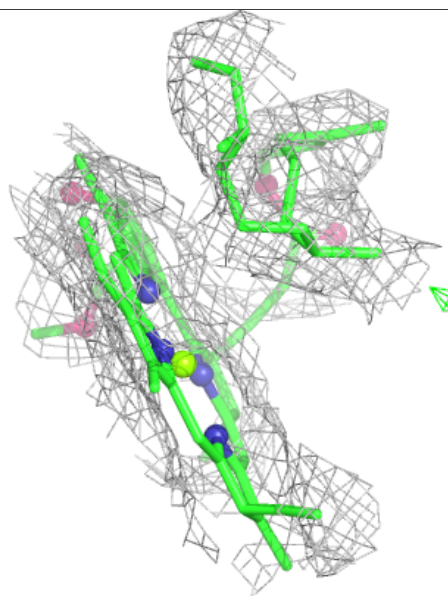
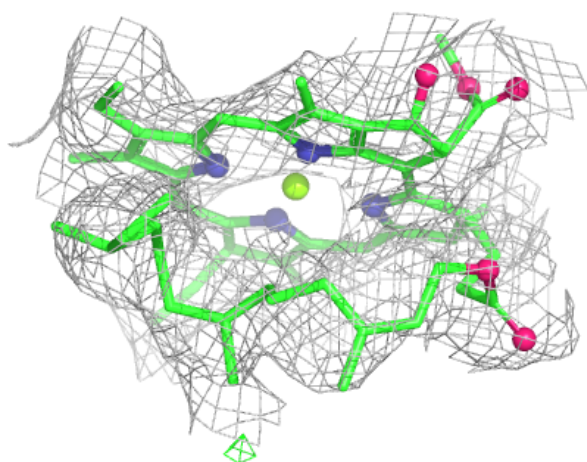
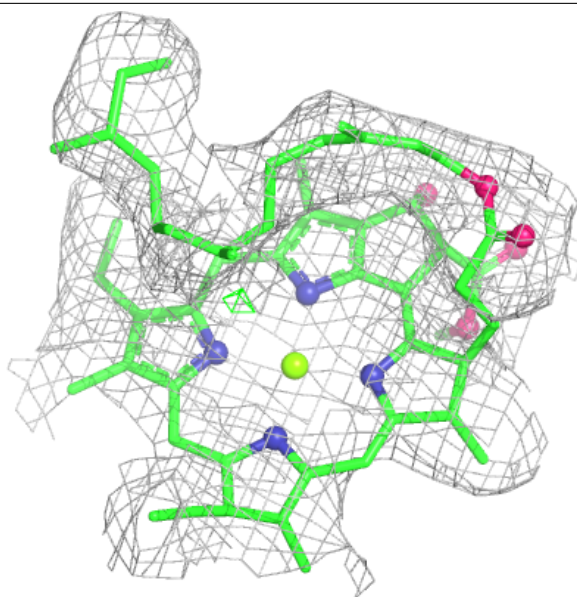
Electron density around CLA A 801:

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



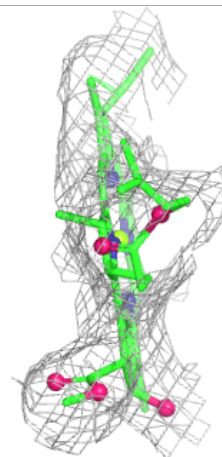
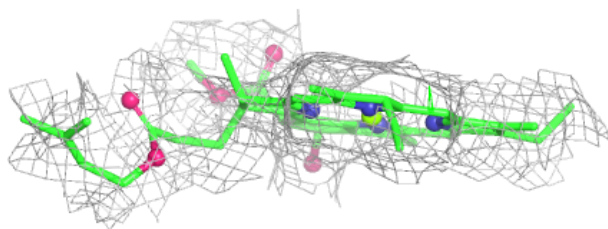
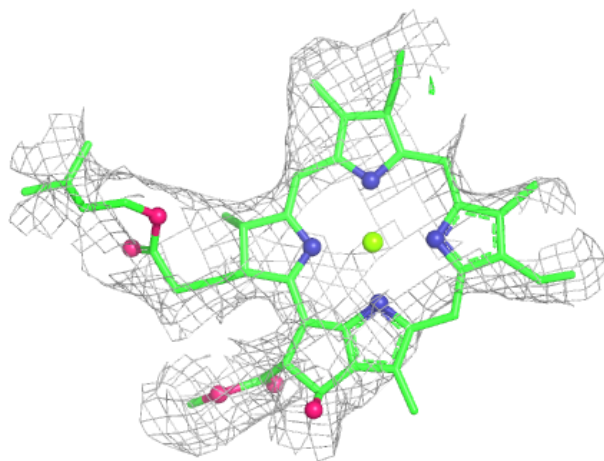
Electron density around CLA 1 206:

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



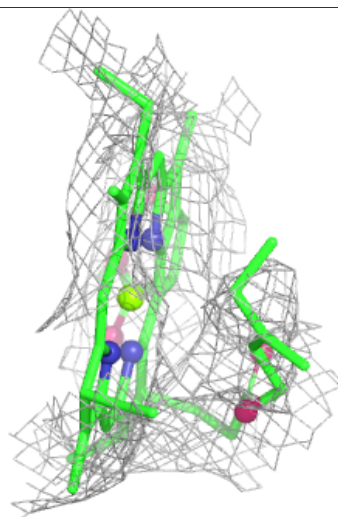
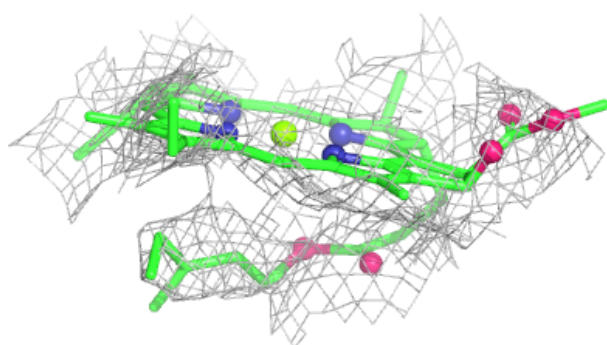
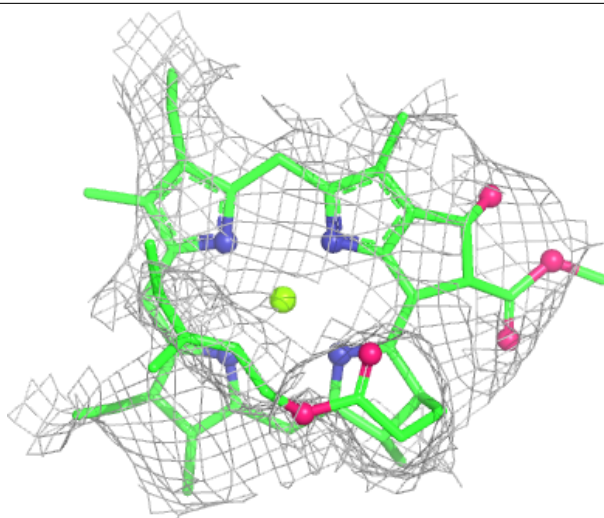
Electron density around CLA 2 305:

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



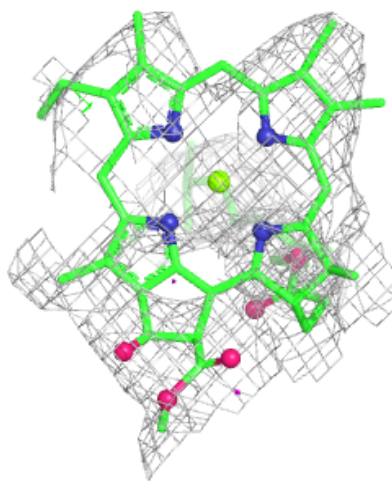
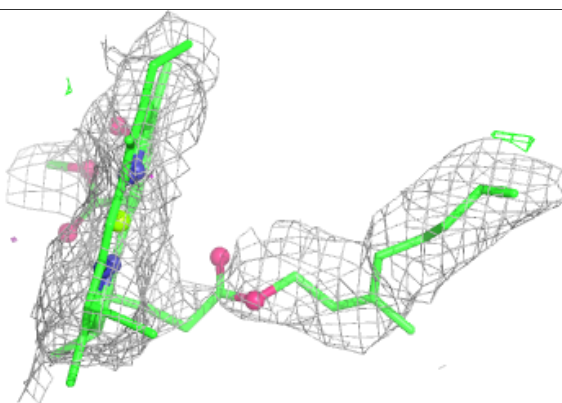
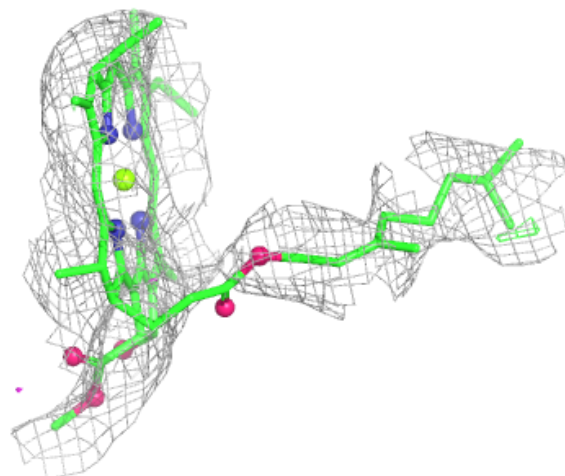
Electron density around CLA A 820:

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



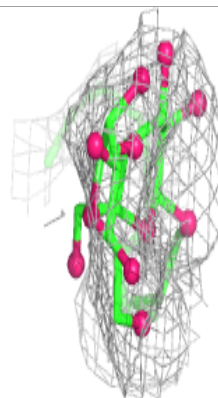
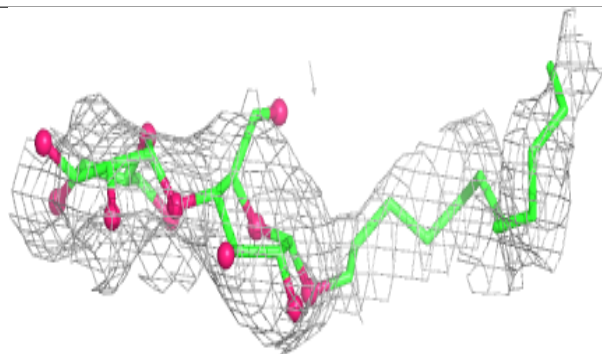
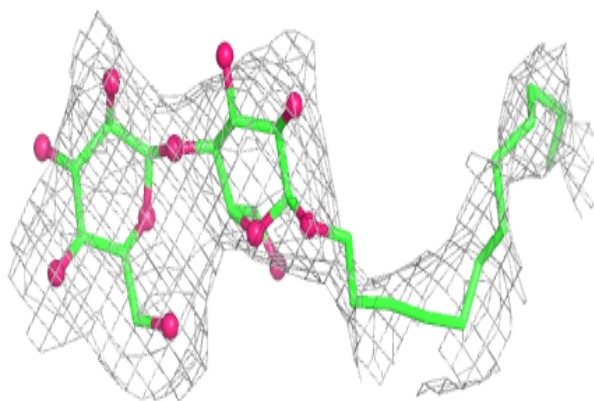
Electron density around CLA 4 301:

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



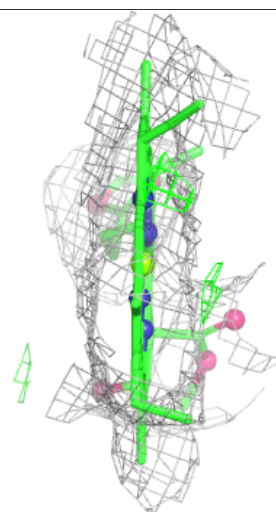
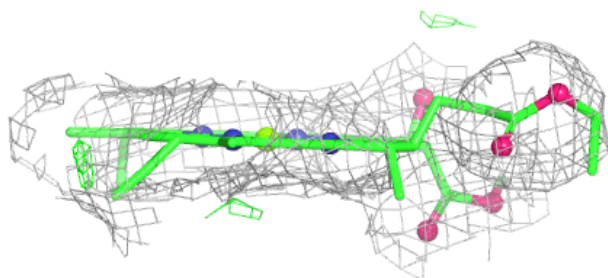
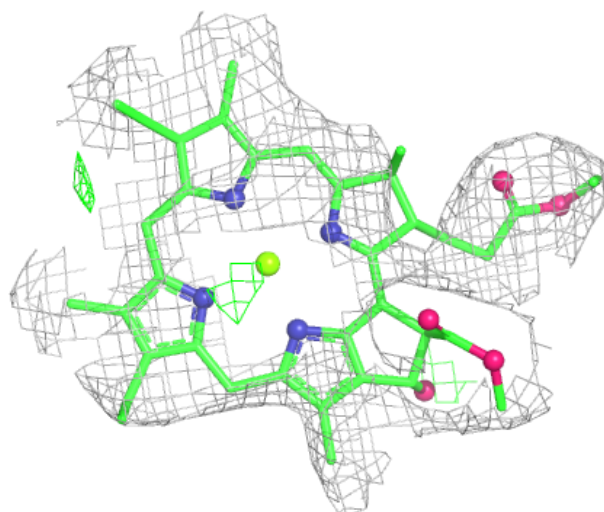
Electron density around LMU C 101:

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



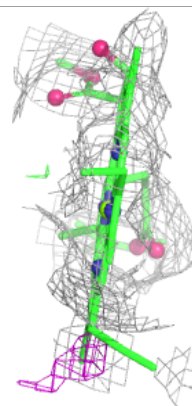
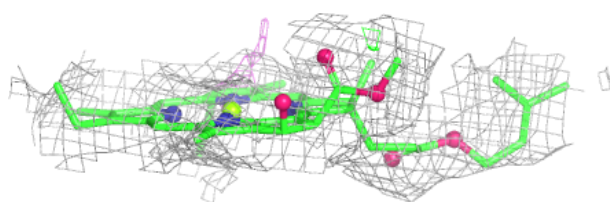
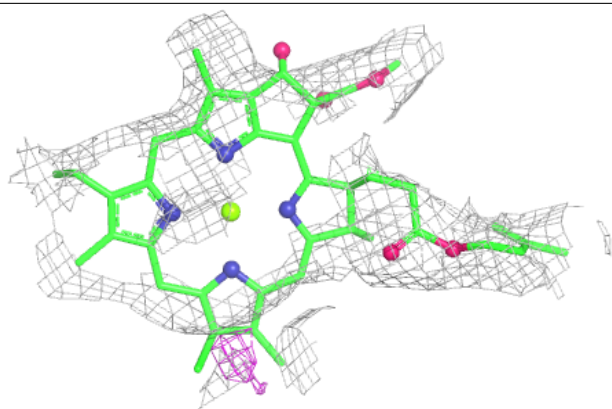
Electron density around CLA 1 203:

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

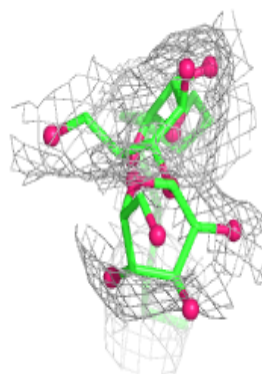
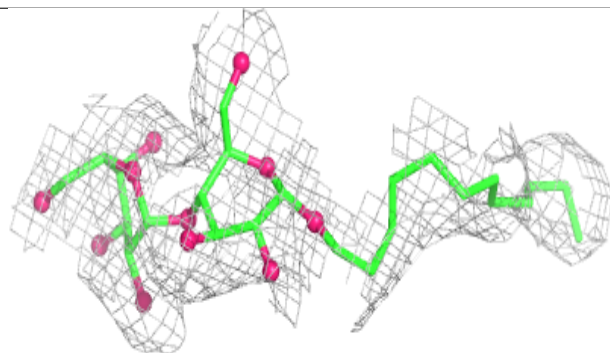
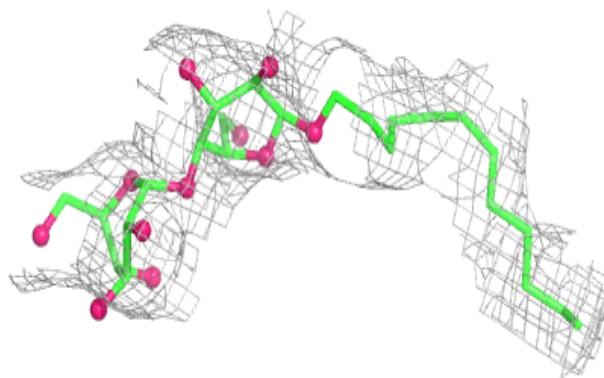


Electron density around CLA K 102:

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

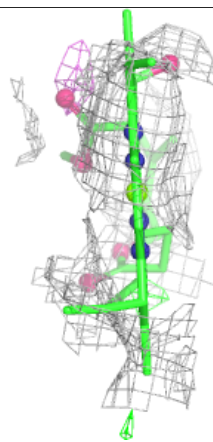
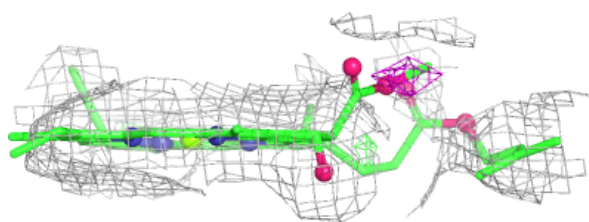
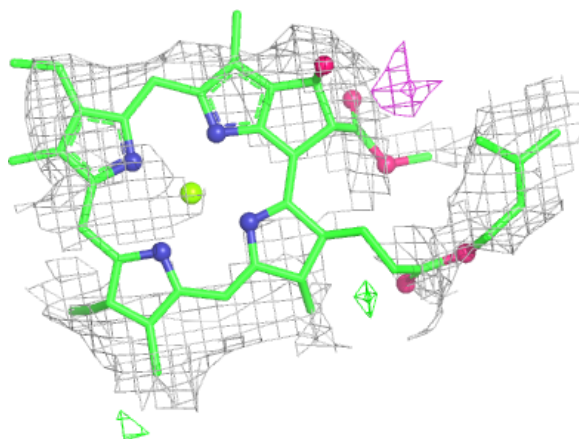
**Electron density around LMU 2 320:**

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



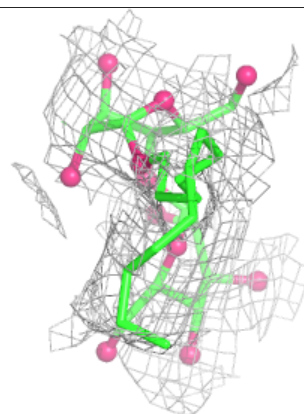
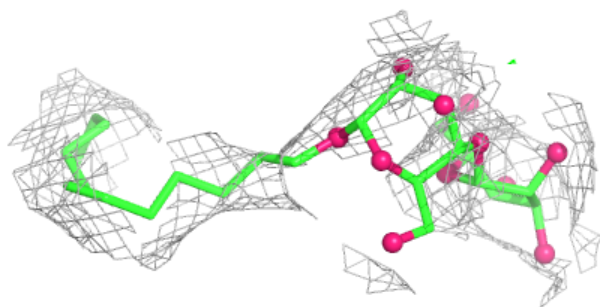
Electron density around CLA 2 311:

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



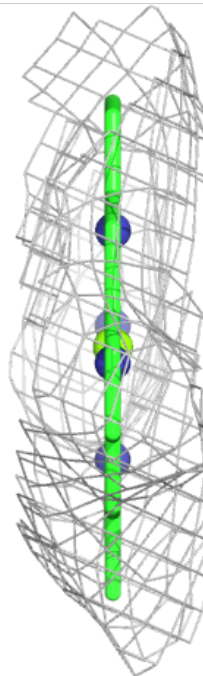
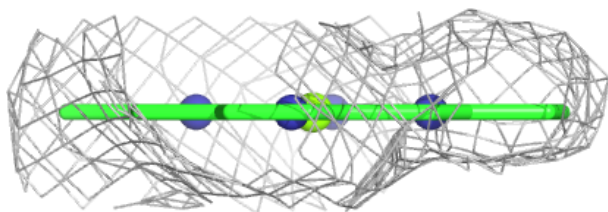
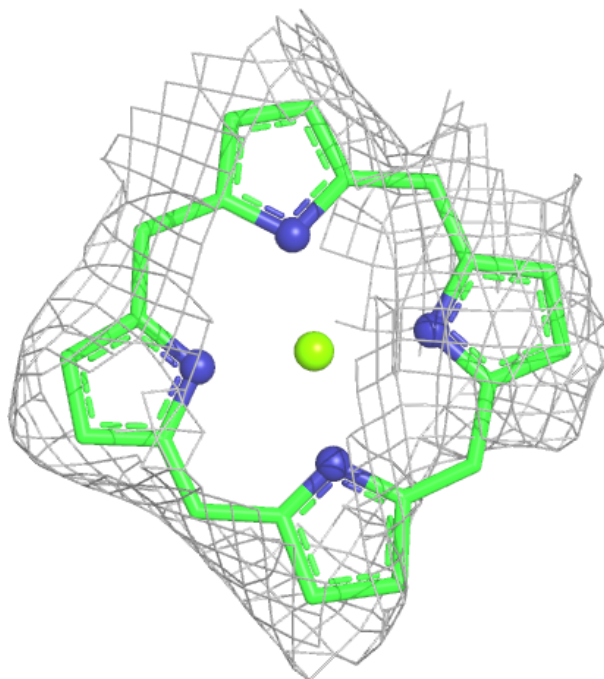
Electron density around LMU K 105:

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



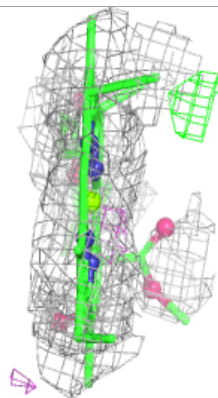
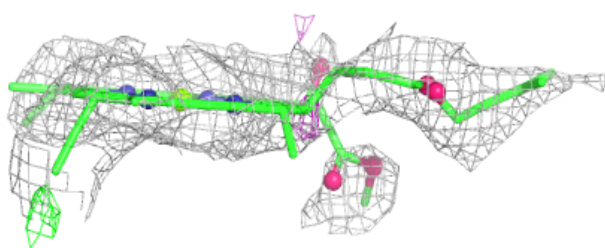
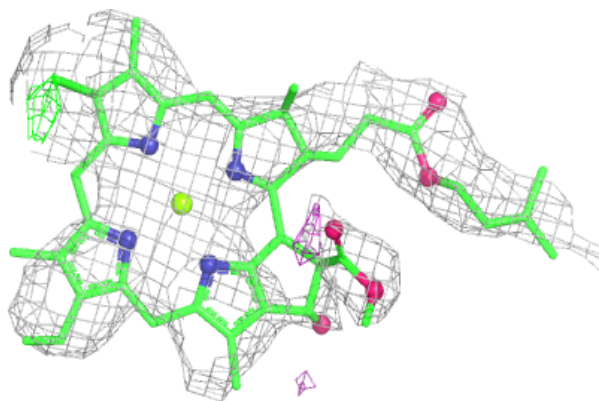
Electron density around CLA 3 317:

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

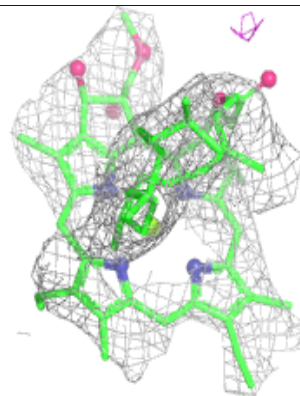
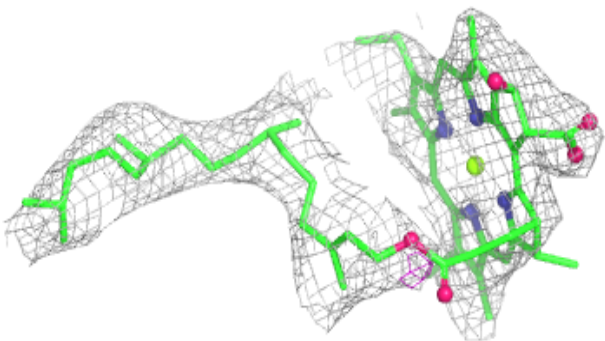
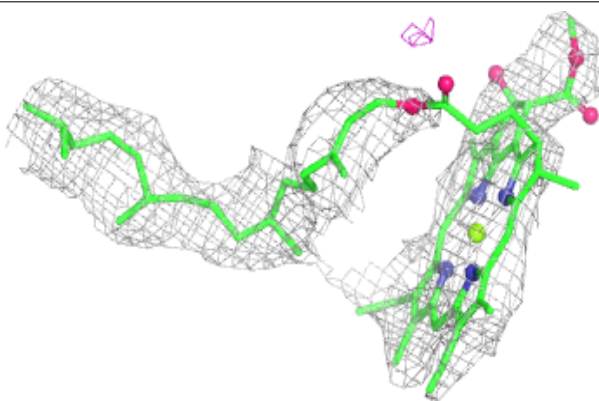


Electron density around CLA 4 305:

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

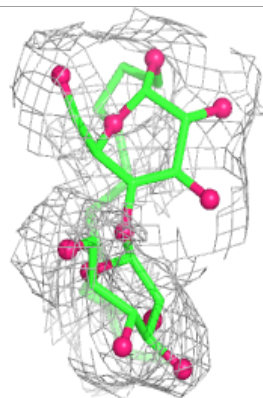
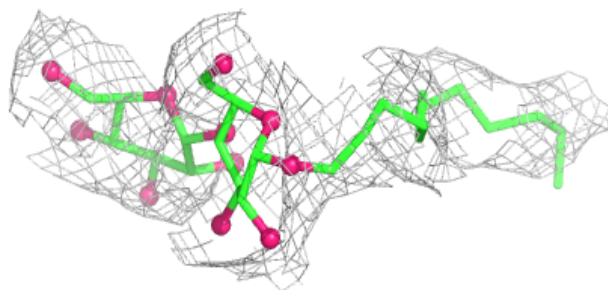
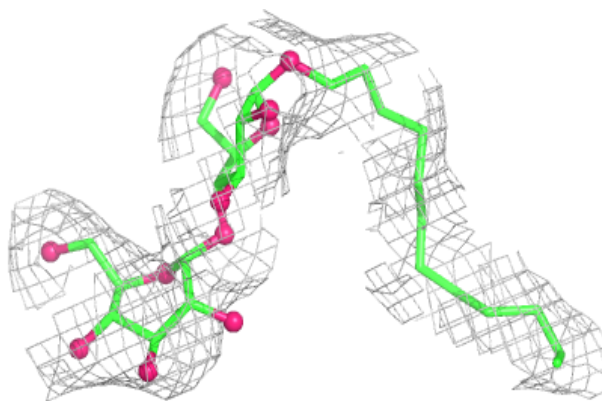
**Electron density around CLA A 811:**

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

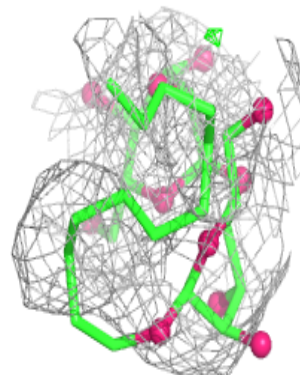
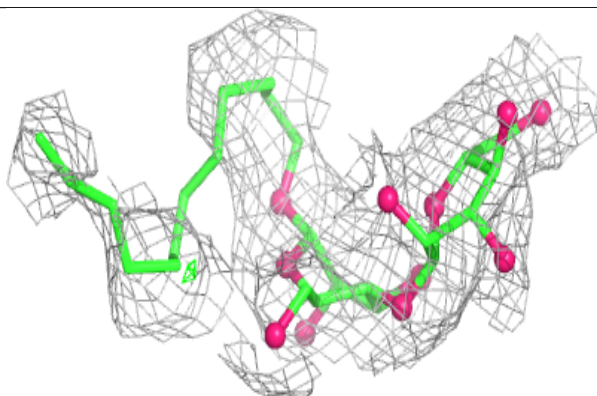
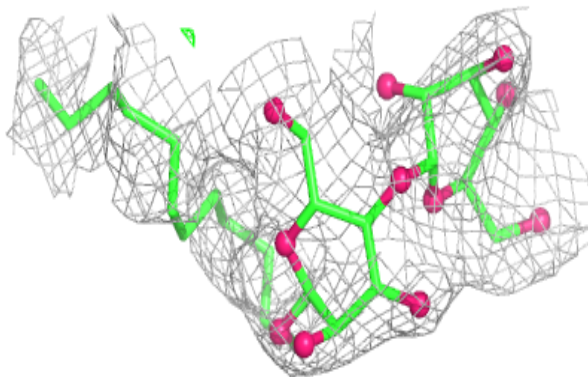


Electron density around LMU L 206:

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

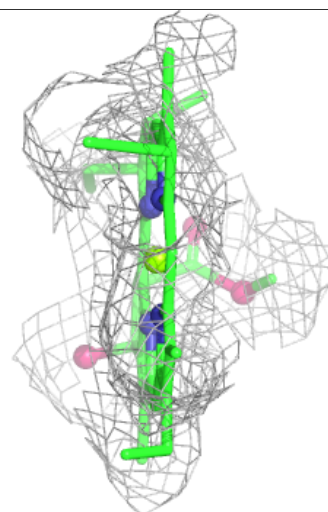
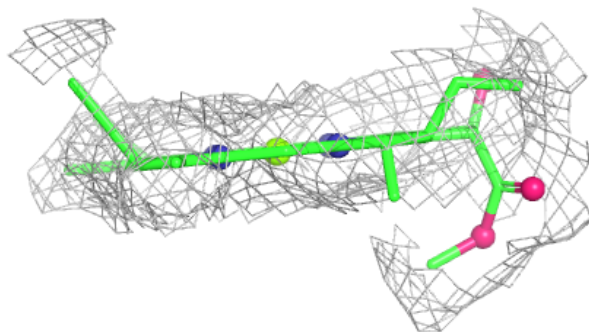
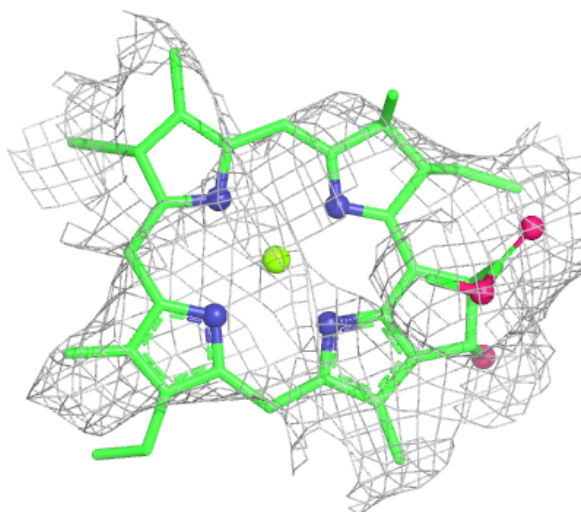
**Electron density around LMU L 212:**

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



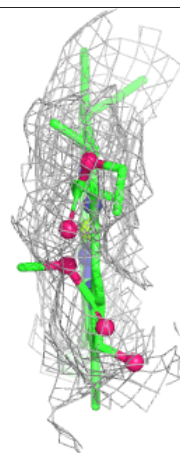
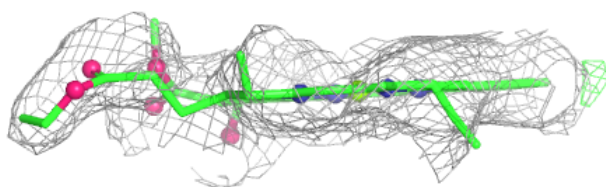
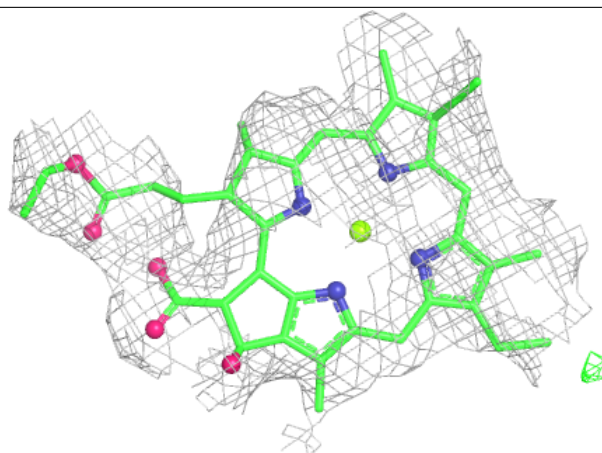
Electron density around CLA 3 307:

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



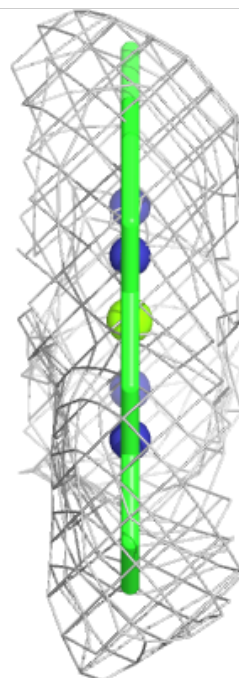
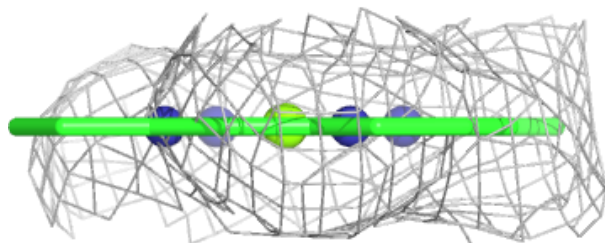
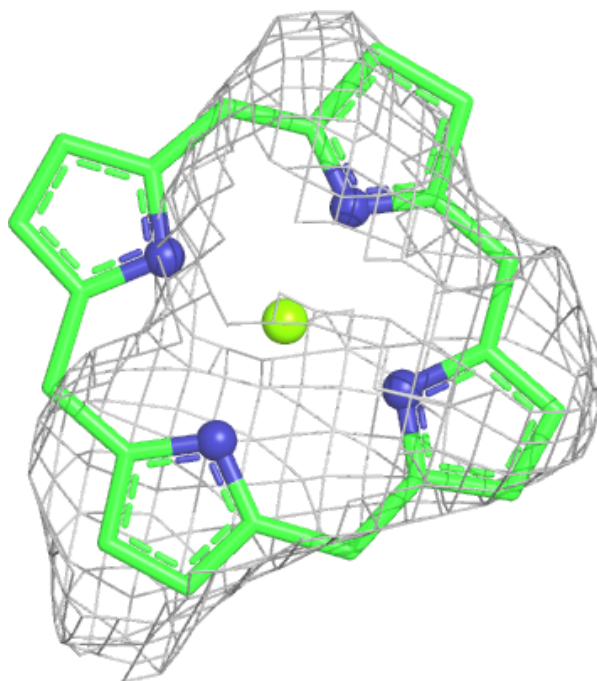
Electron density around CLA 4 318:

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



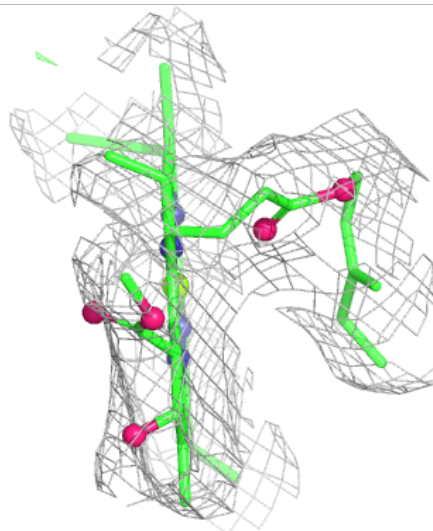
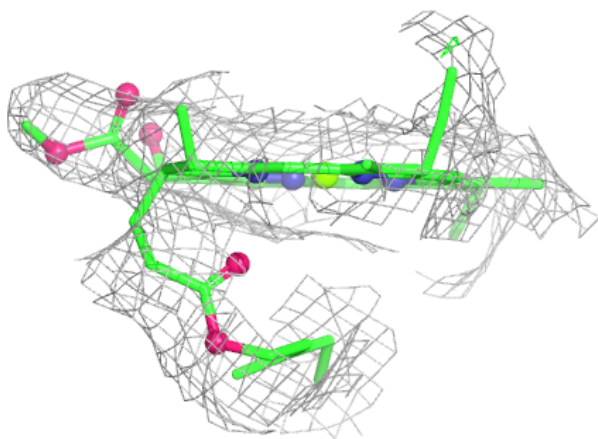
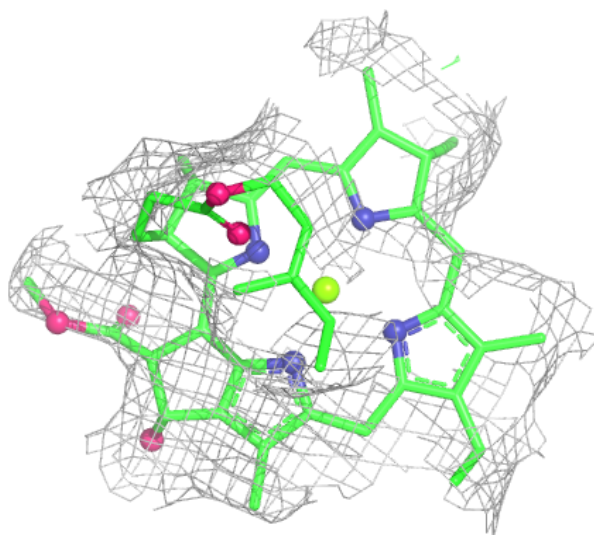
Electron density around CLA 3 316:

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



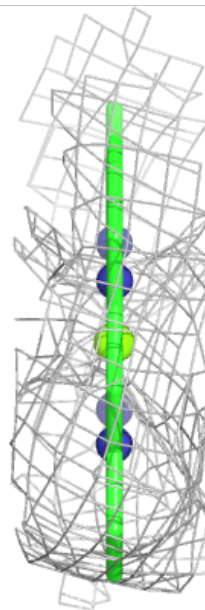
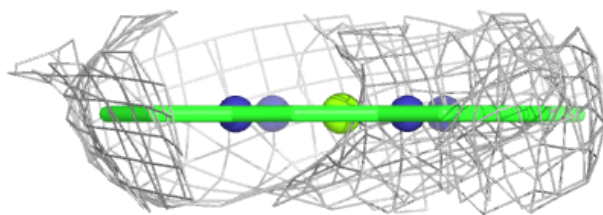
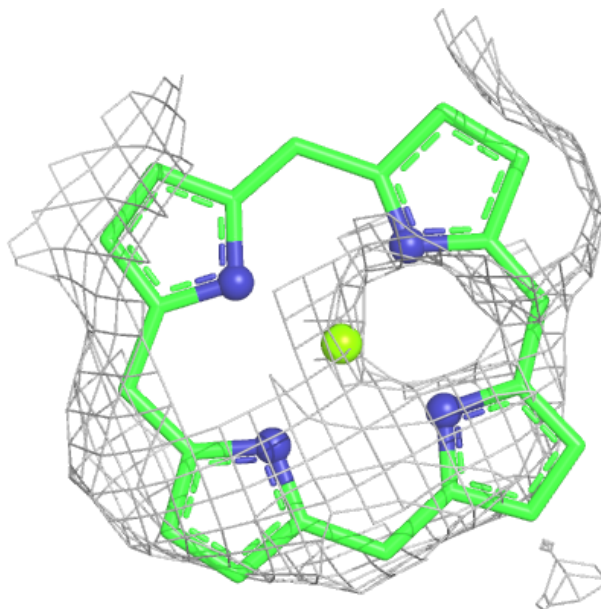
Electron density around CLA 2 302:

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



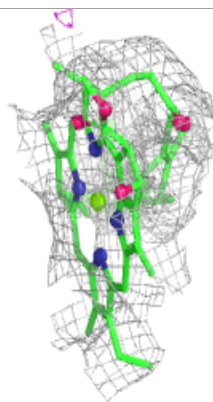
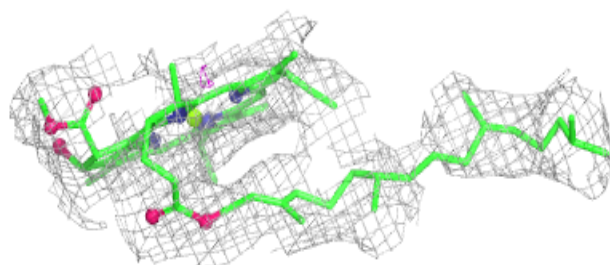
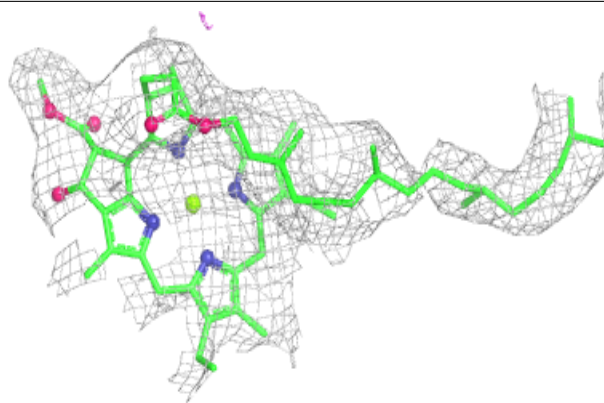
Electron density around CLA 3 306:

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



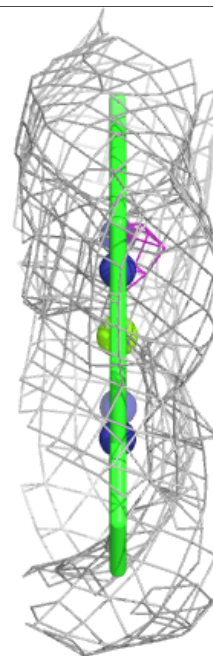
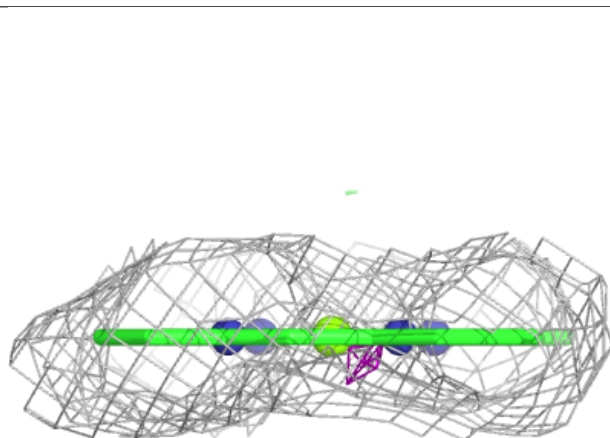
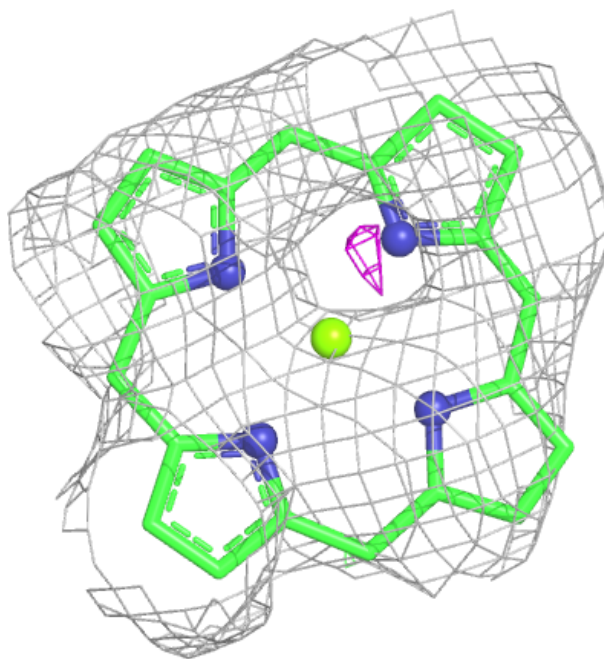
Electron density around CLA 2 307:

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



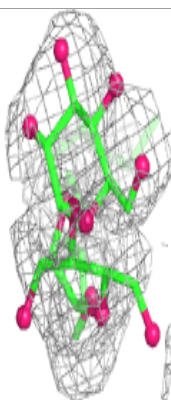
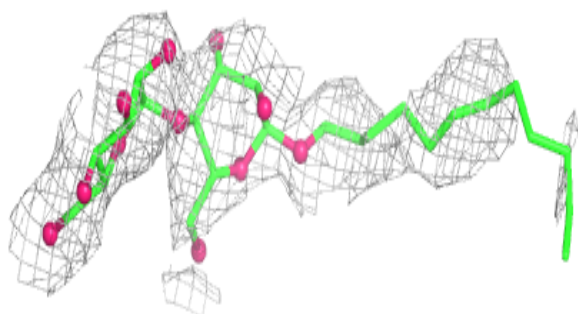
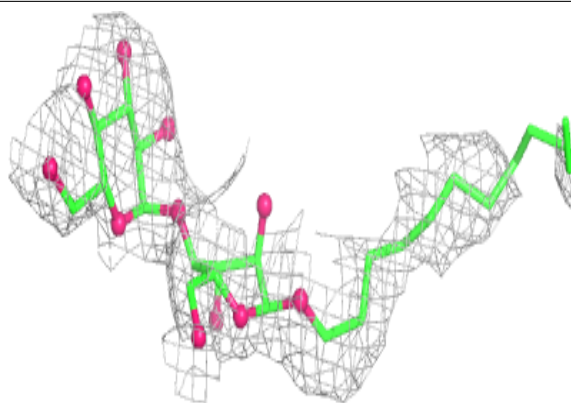
Electron density around CLA 4 314:

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

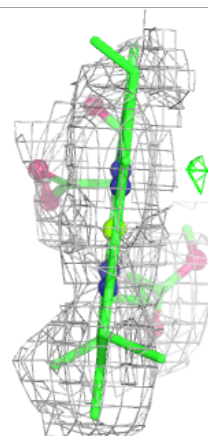
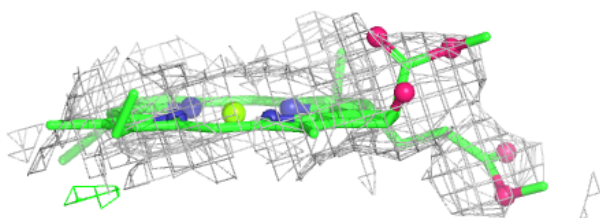
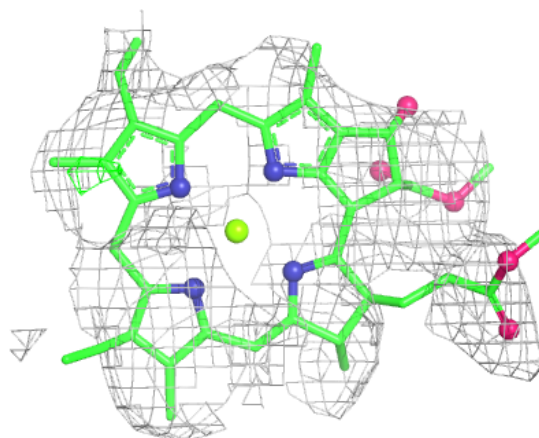


Electron density around LMU 4 316:

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

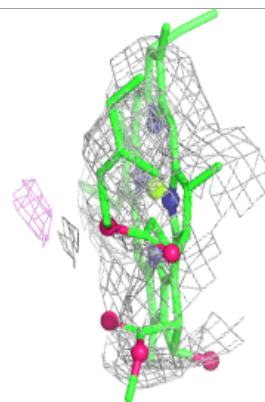
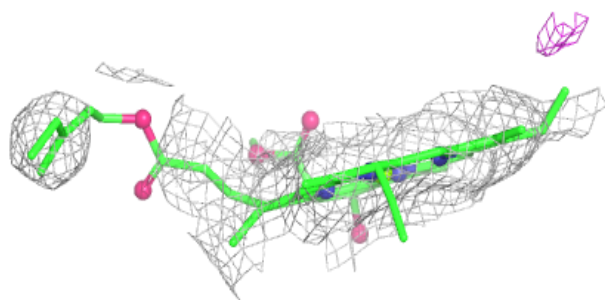
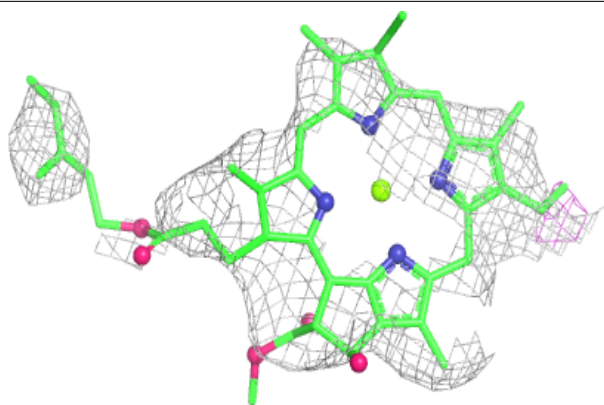
**Electron density around CLA 4 315:**

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

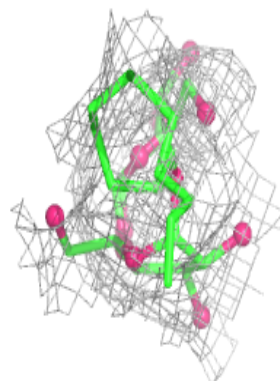
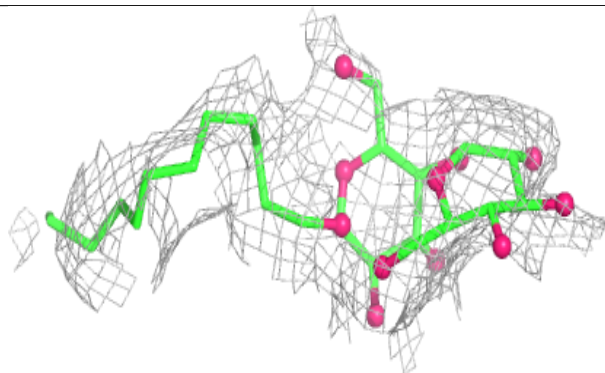
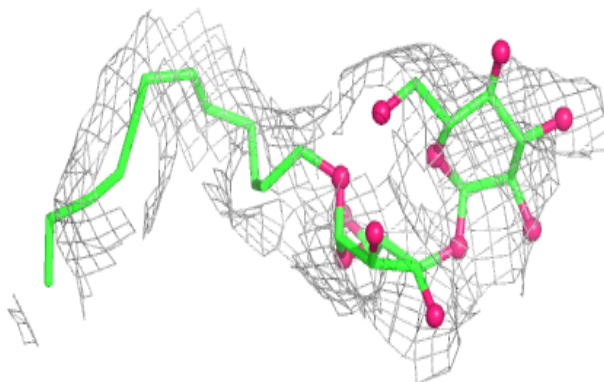


Electron density around CLA 1 213:

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

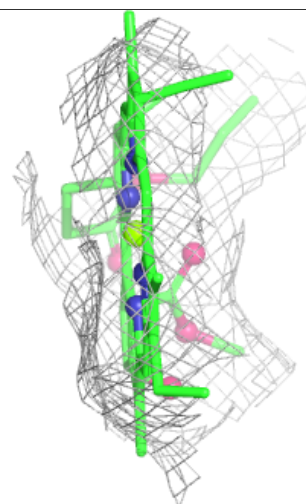
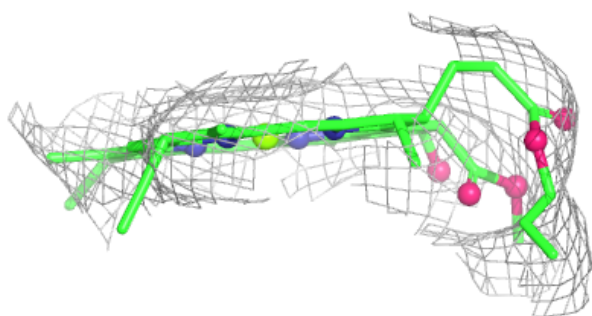
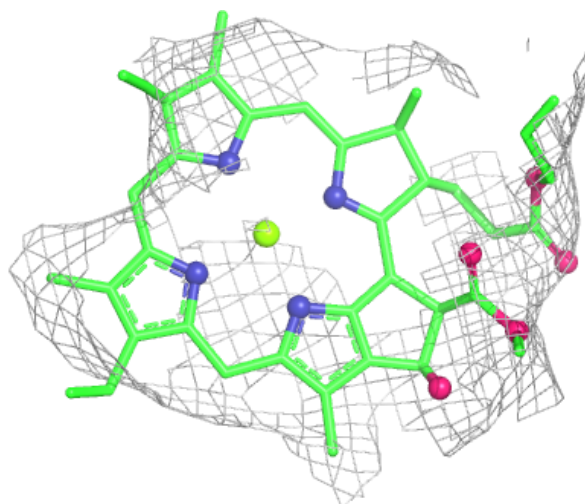
**Electron density around LMU A 847:**

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



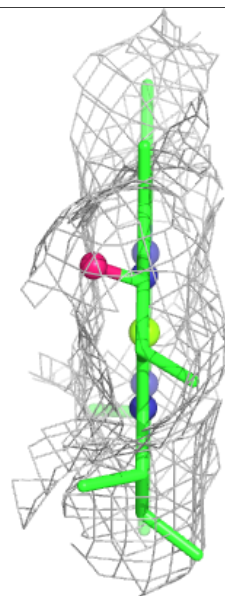
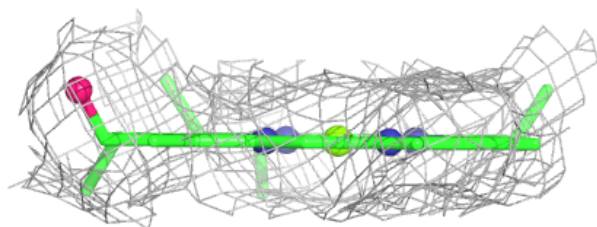
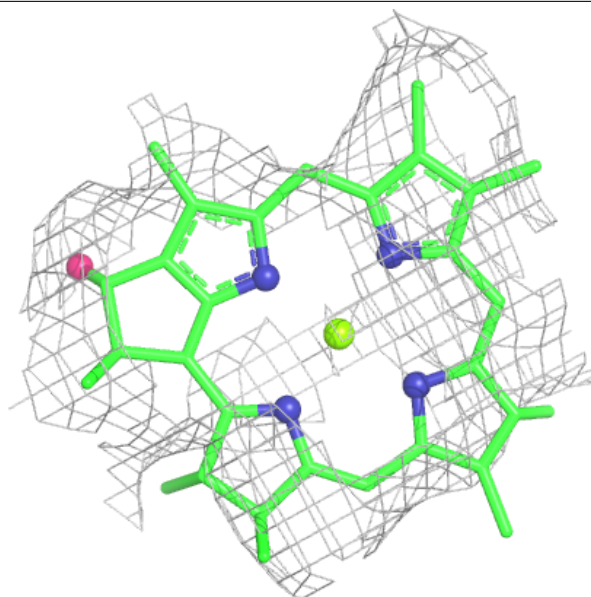
Electron density around CLA J 101:

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



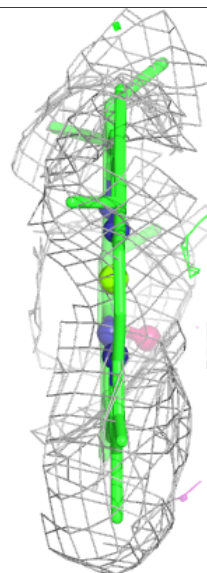
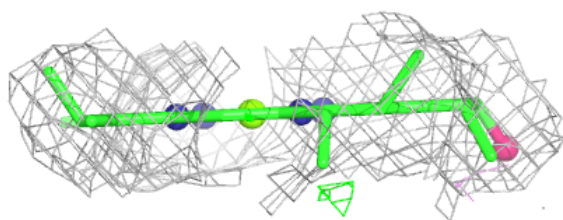
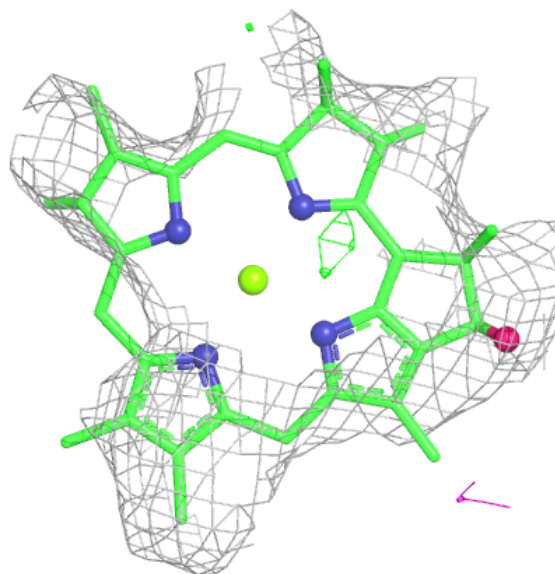
Electron density around CLA 3 301:

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



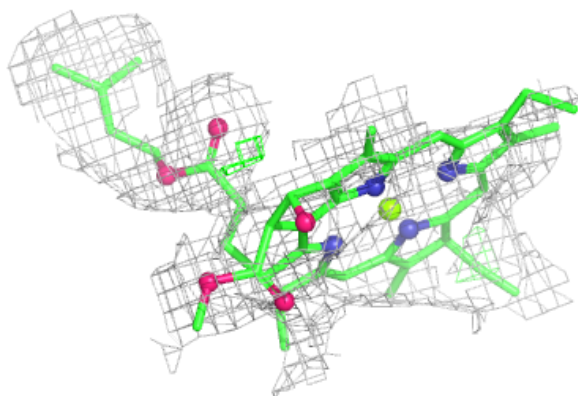
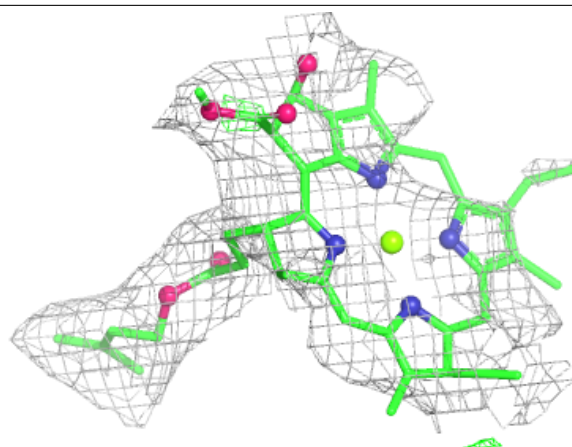
Electron density around CLA 1 210:

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

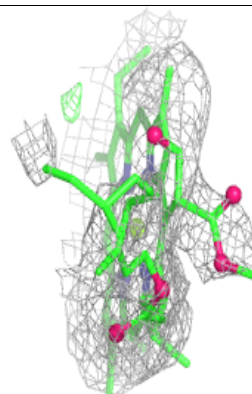
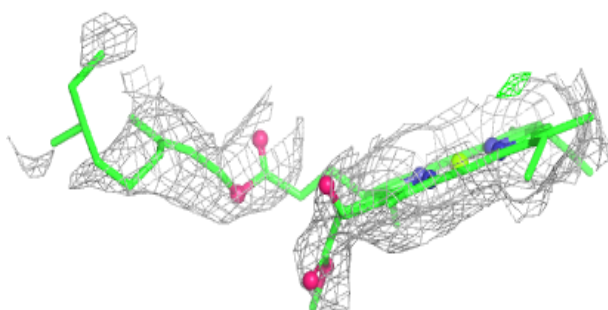
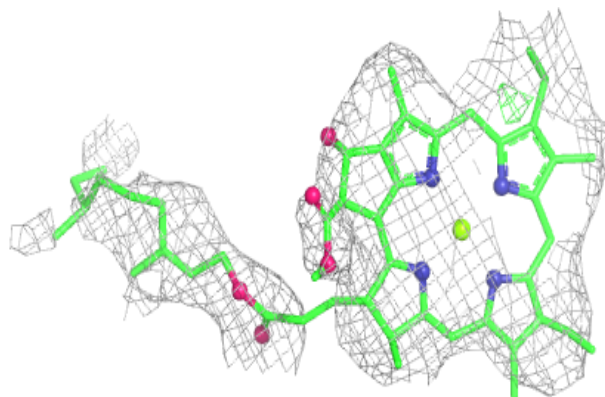


Electron density around CLA 2 310:

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

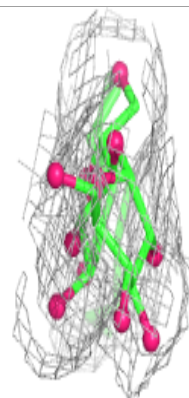
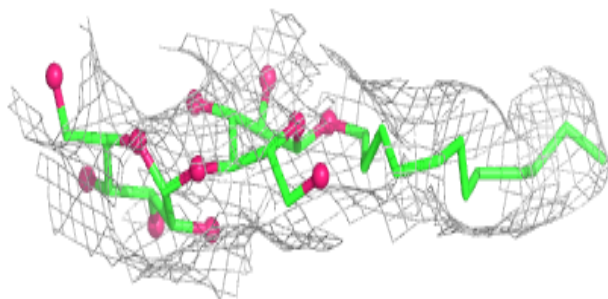
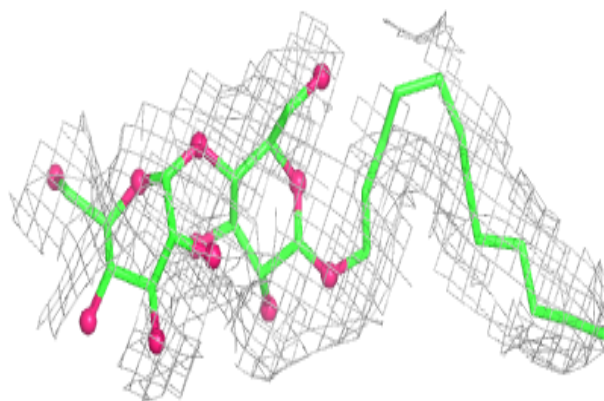
**Electron density around CLA K 104:**

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

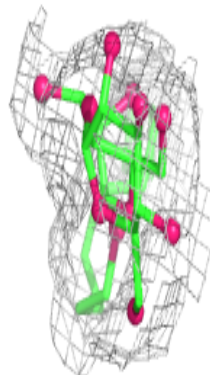
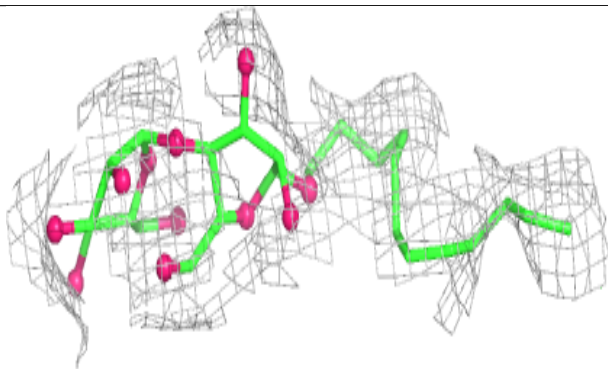
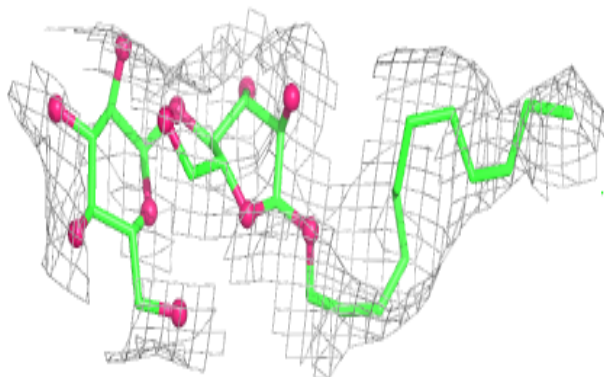


Electron density around LMU H 104:

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

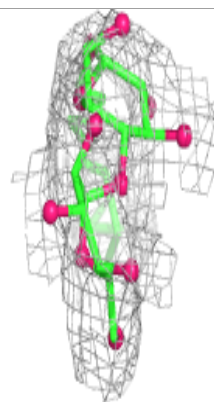
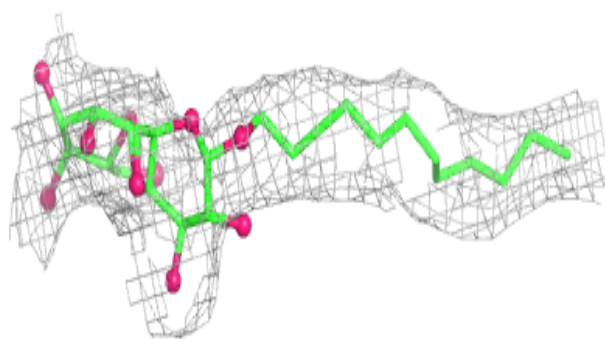
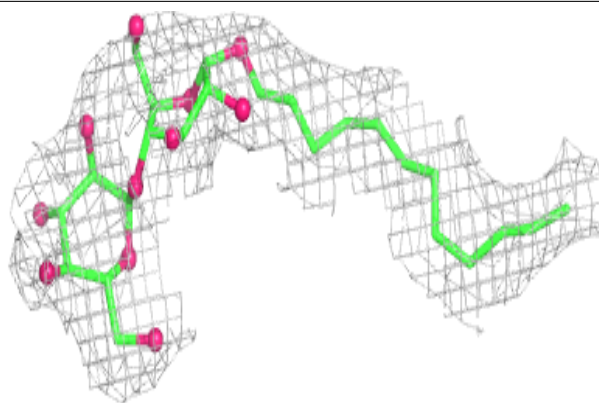
**Electron density around LMU R 102:**

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



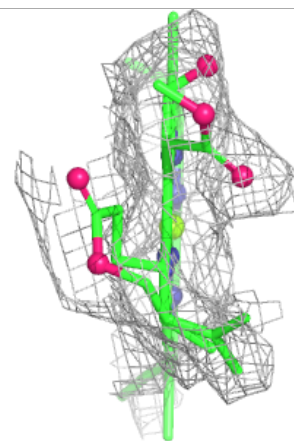
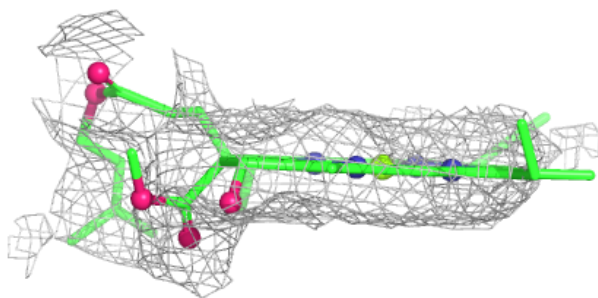
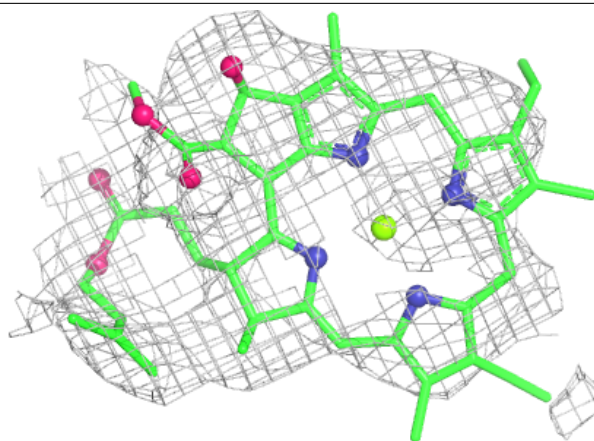
Electron density around LMU 4 321:

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



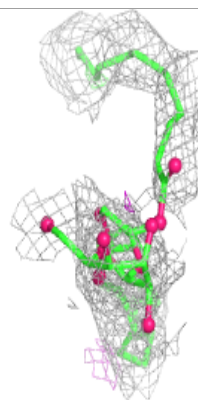
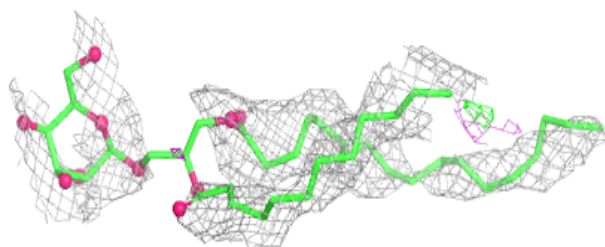
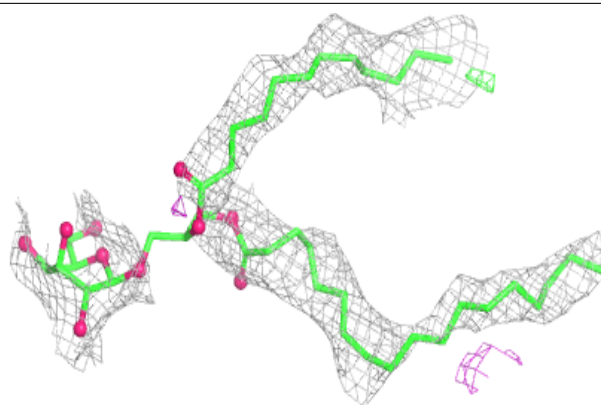
Electron density around CLA 2 315:

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



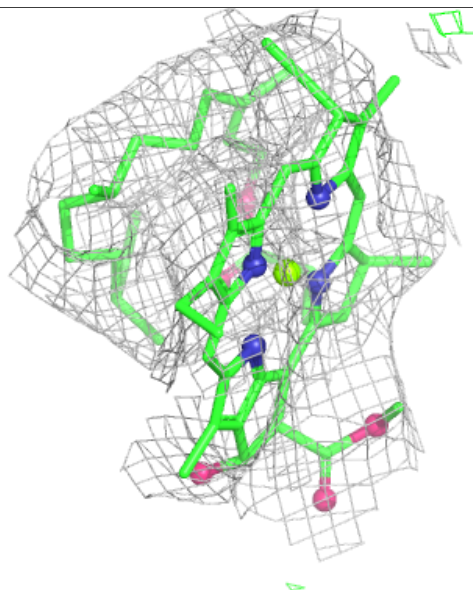
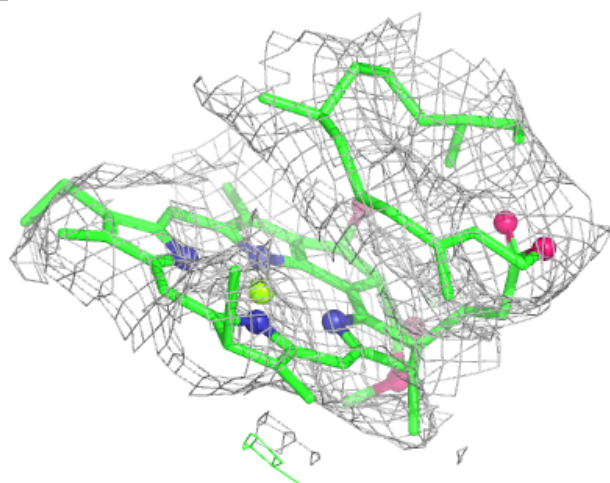
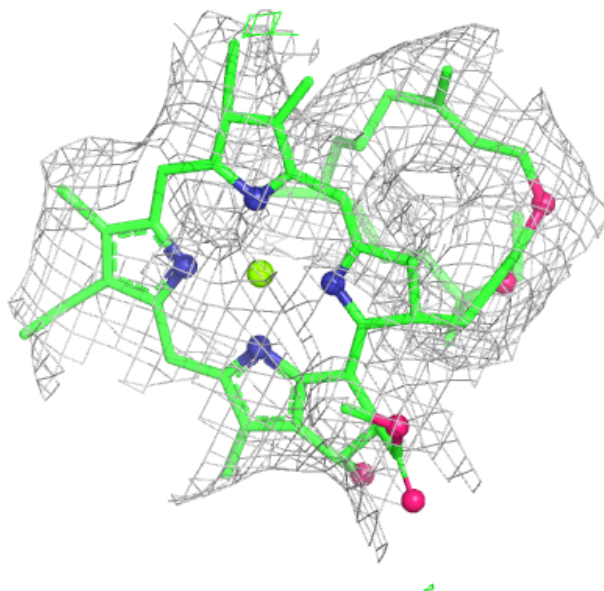
Electron density around LMG B 848:

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



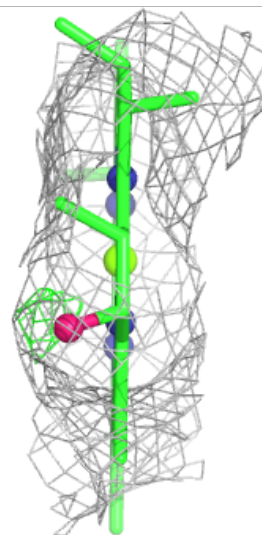
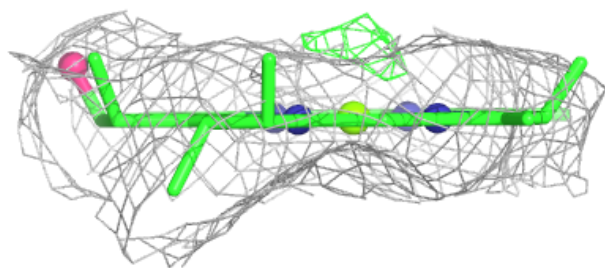
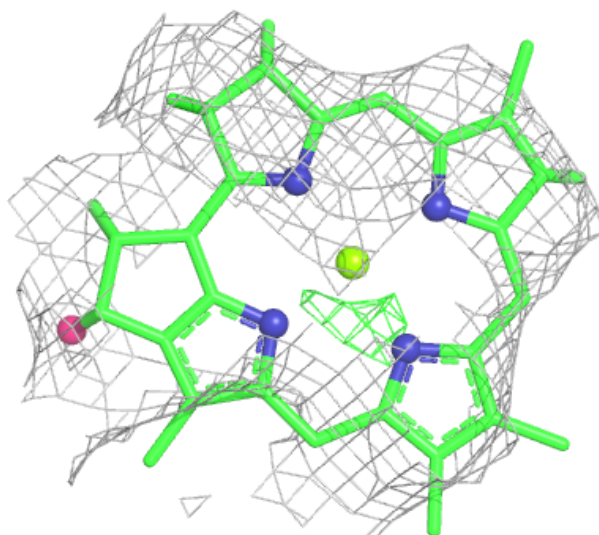
Electron density around CLA J 103:

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



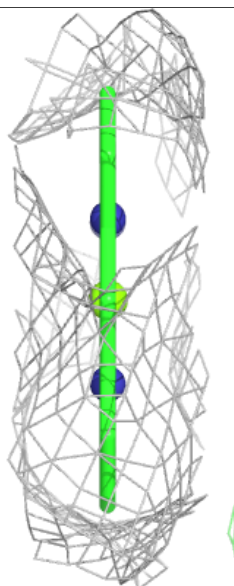
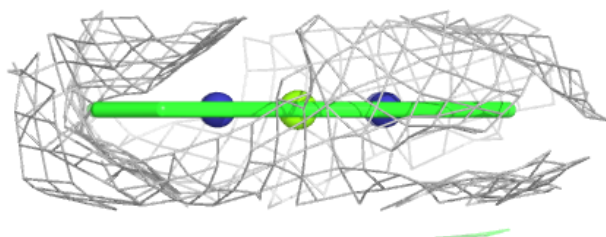
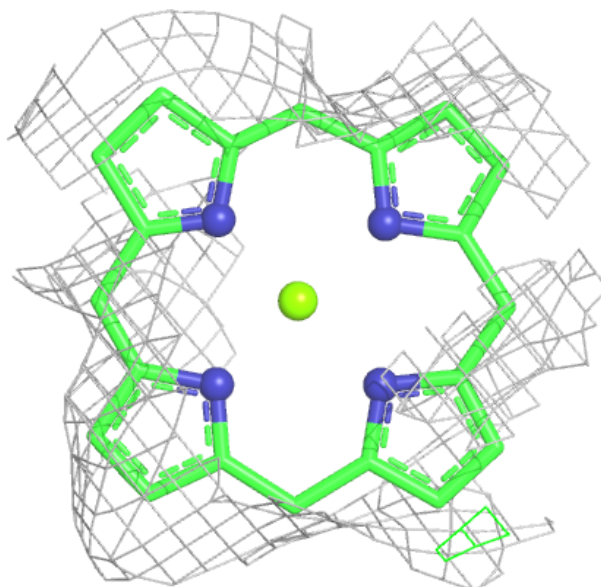
Electron density around CLA 4 302:

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



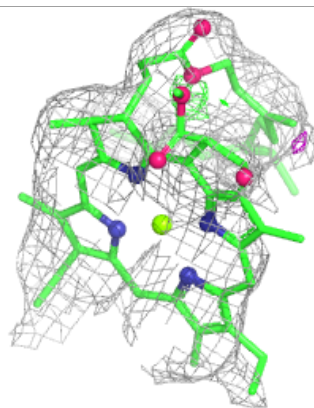
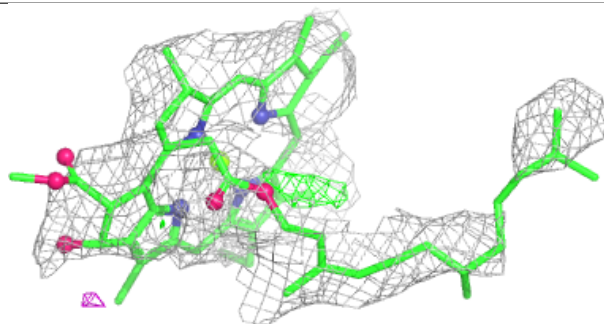
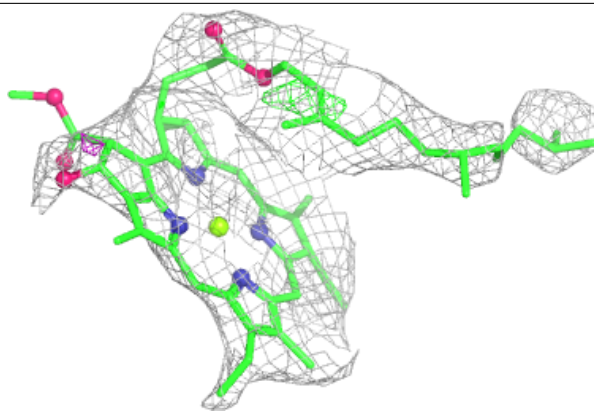
Electron density around CLA 2 306:

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



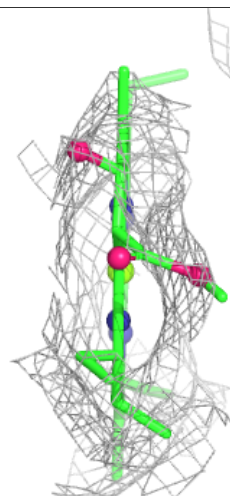
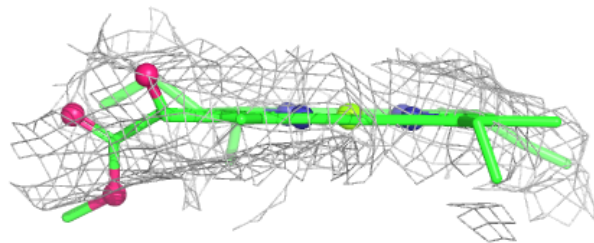
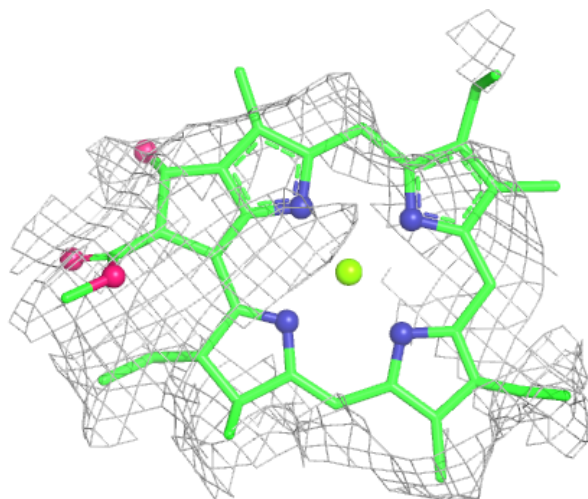
Electron density around CLA B 815:

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



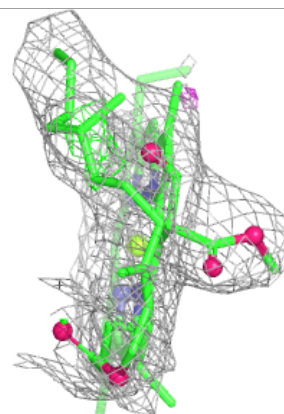
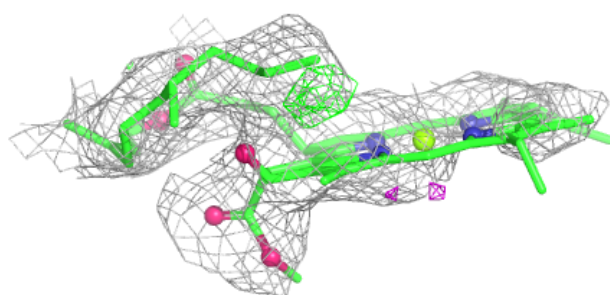
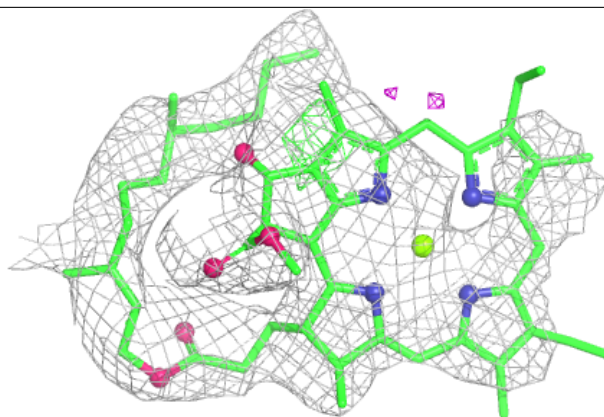
Electron density around CLA A 821:

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

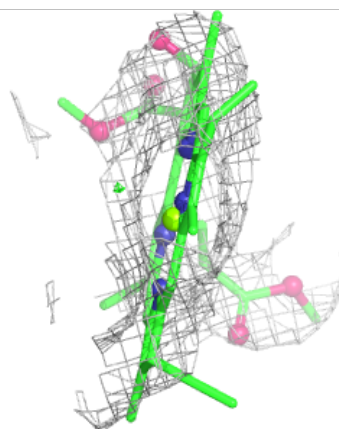
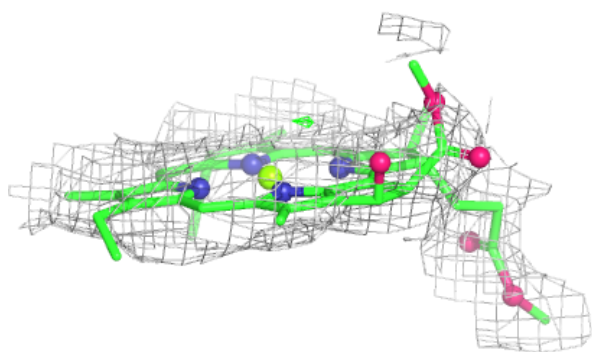
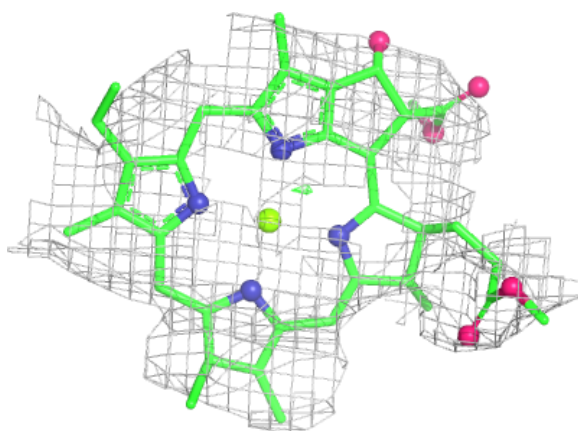


Electron density around CLA A 823:

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

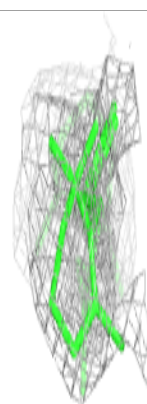
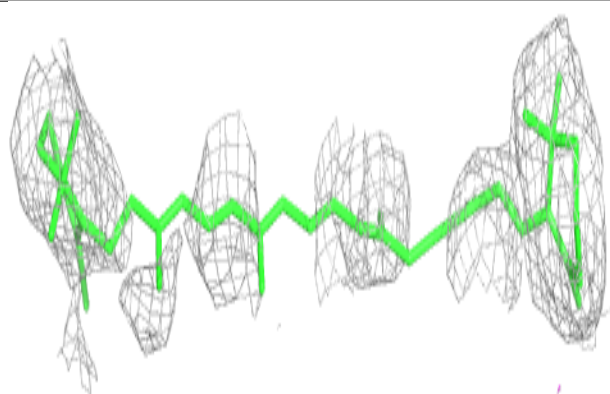
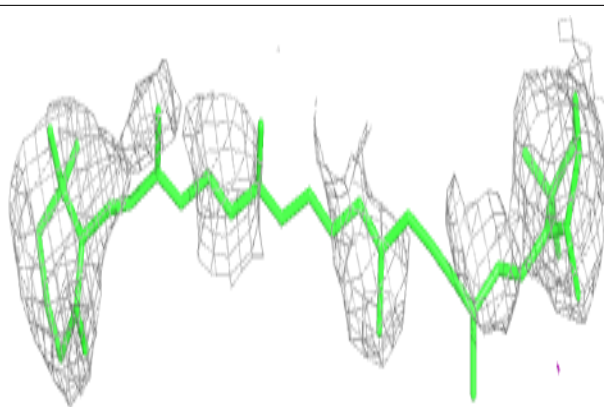
**Electron density around CLA B 822:**

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



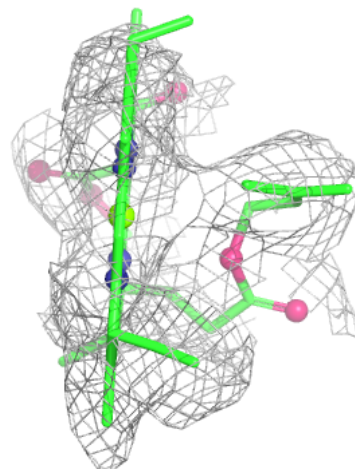
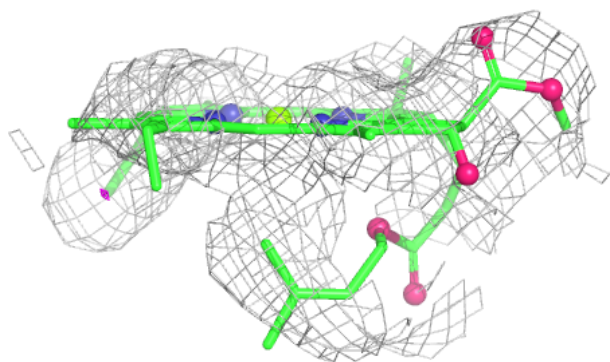
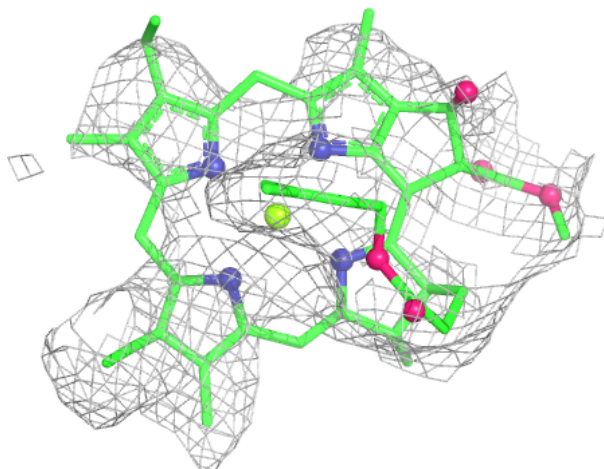
Electron density around BCR J 102:

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



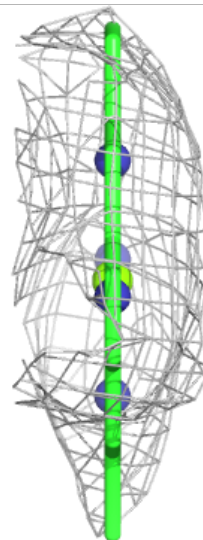
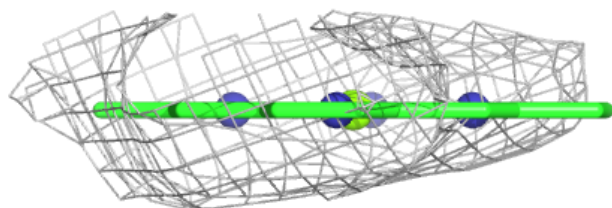
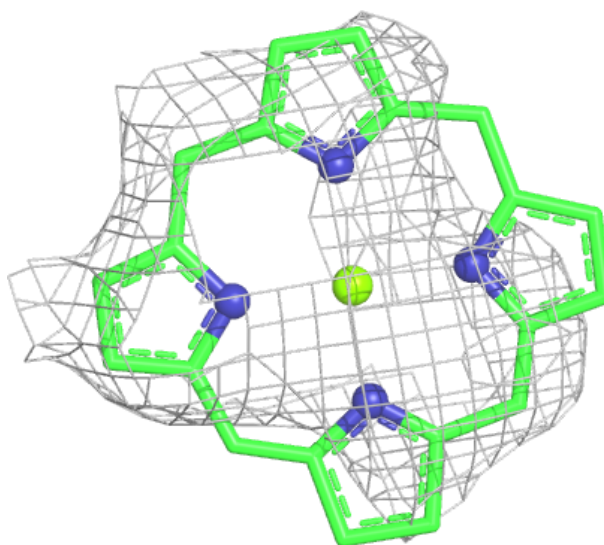
Electron density around CLA L 208:

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



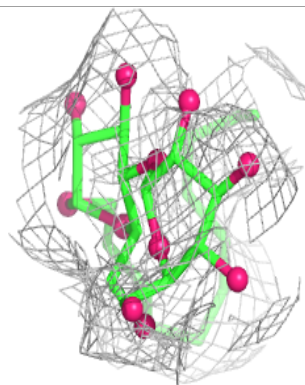
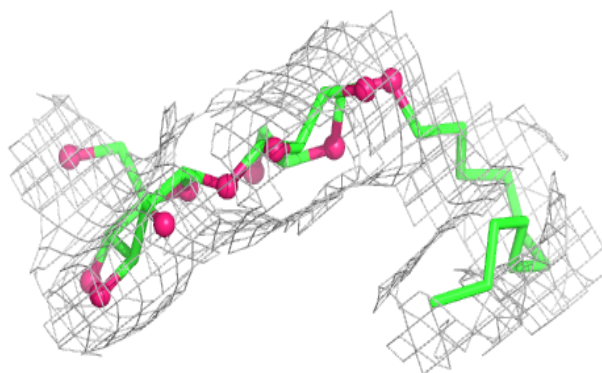
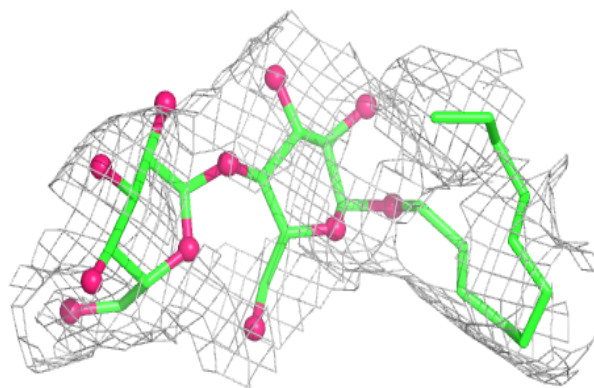
Electron density around CLA 4 309:

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



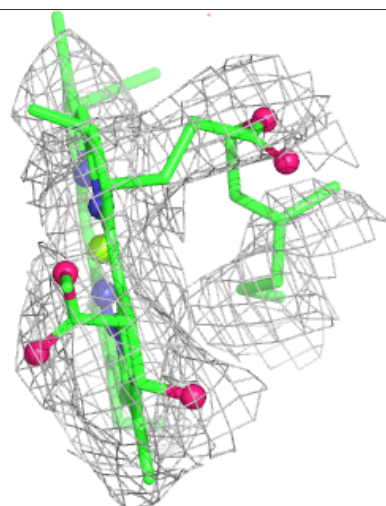
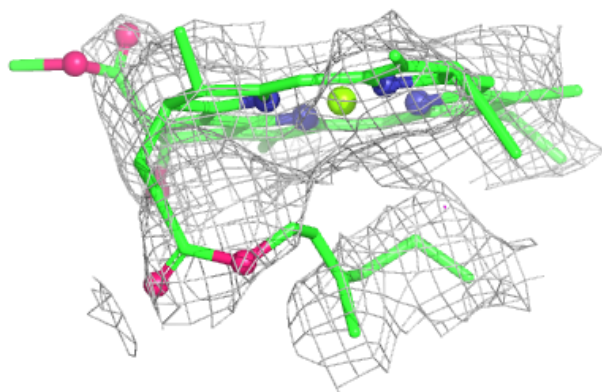
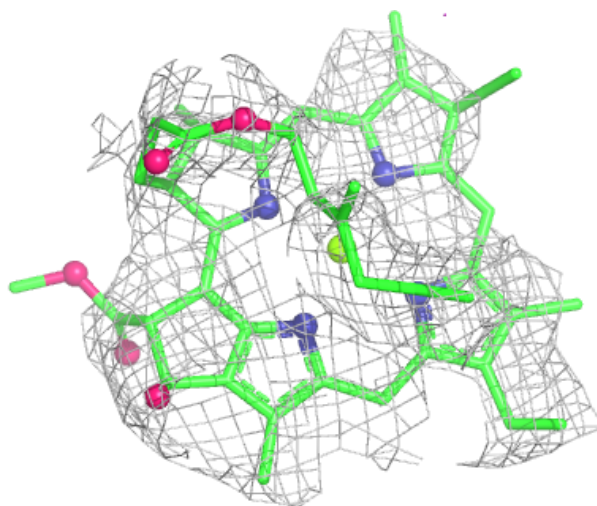
Electron density around LMU F 202:

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



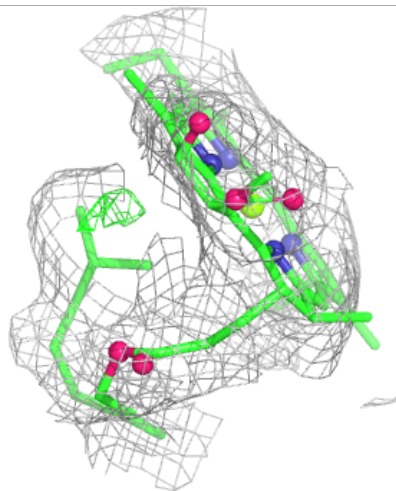
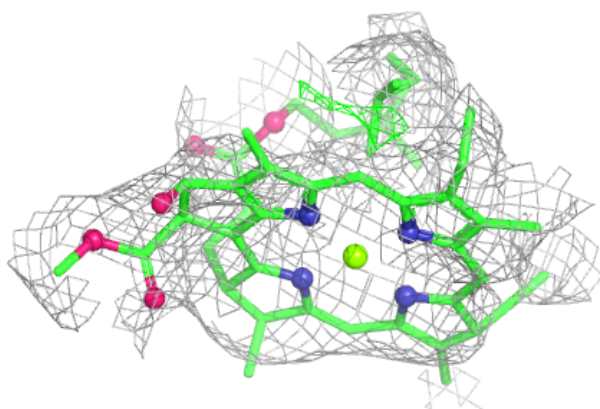
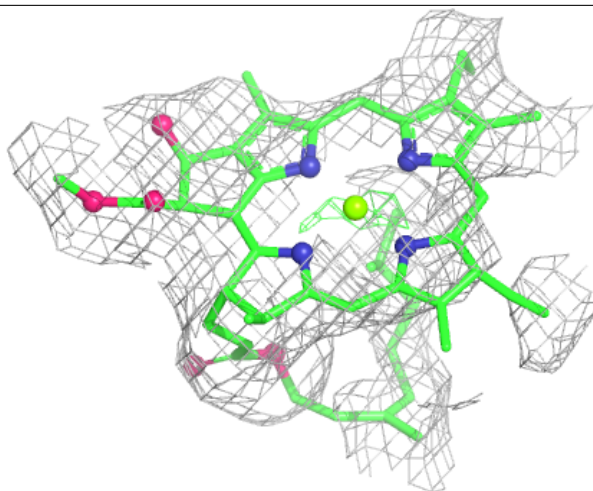
Electron density around CLA A 817:

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



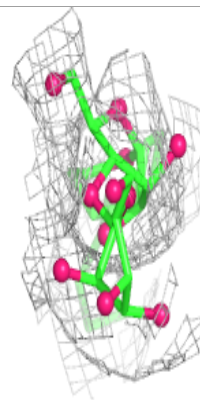
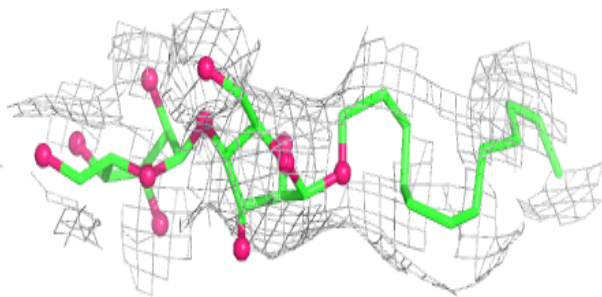
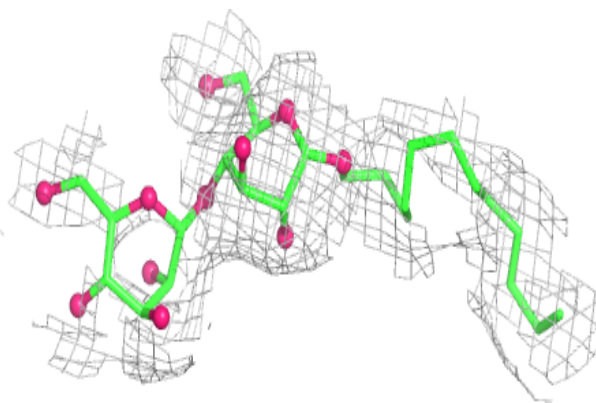
Electron density around CLA B 813:

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



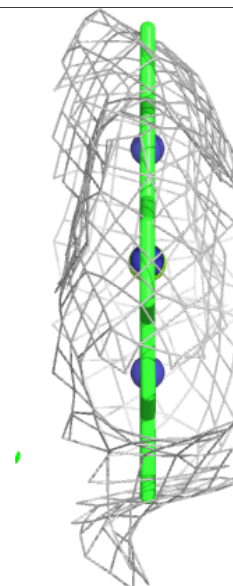
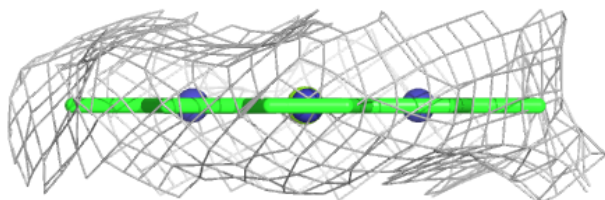
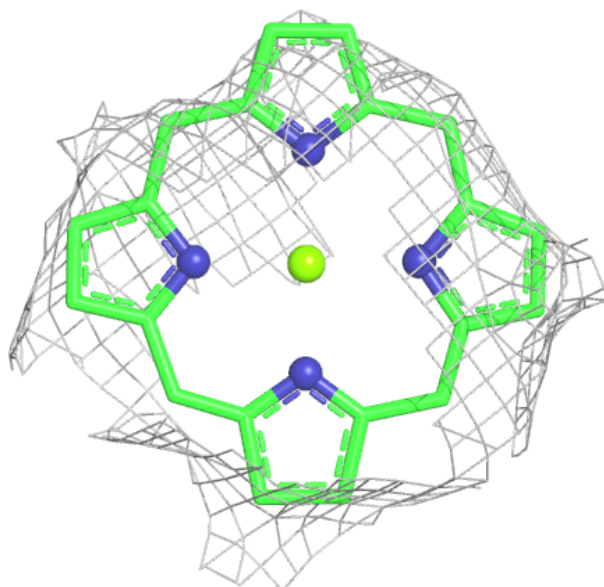
Electron density around LMU 3 320:

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



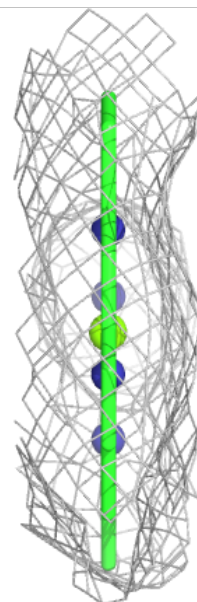
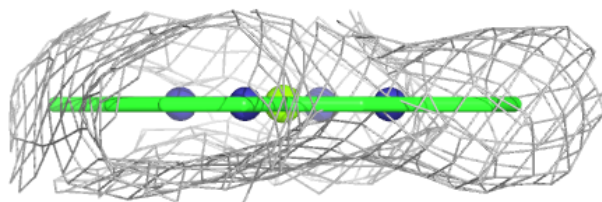
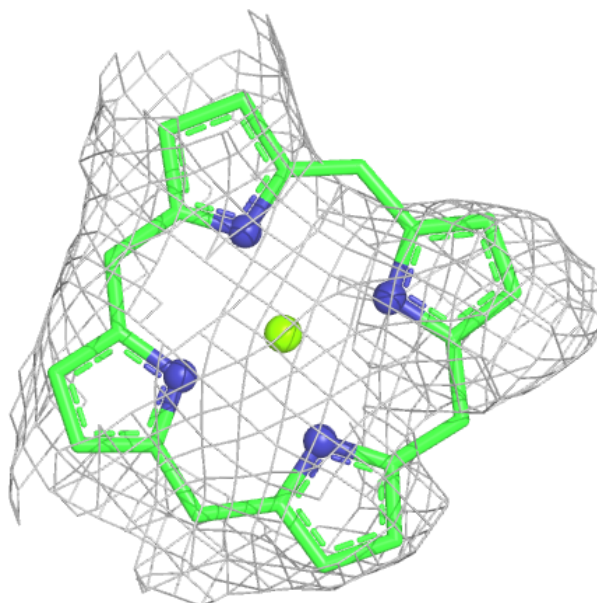
Electron density around CLA 3 308:

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



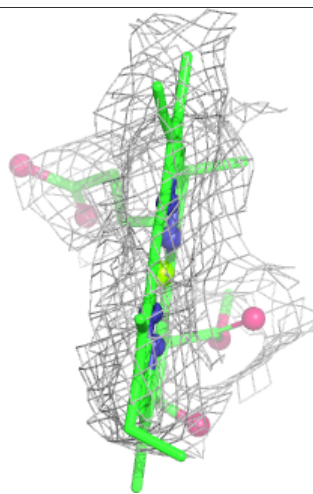
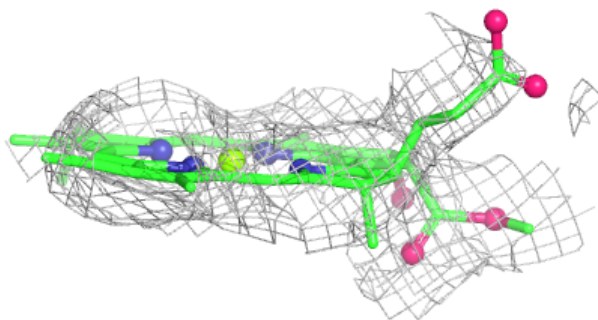
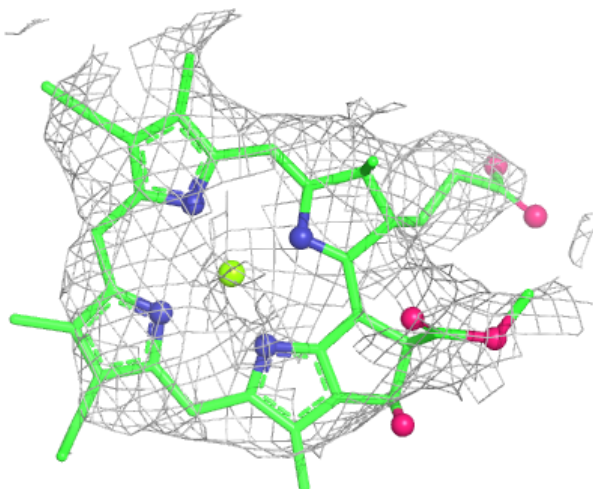
Electron density around CLA 2 316:

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



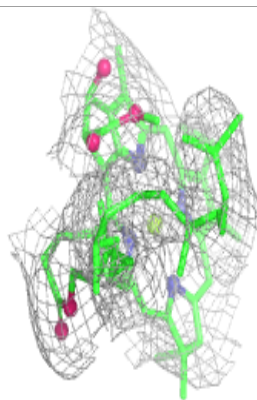
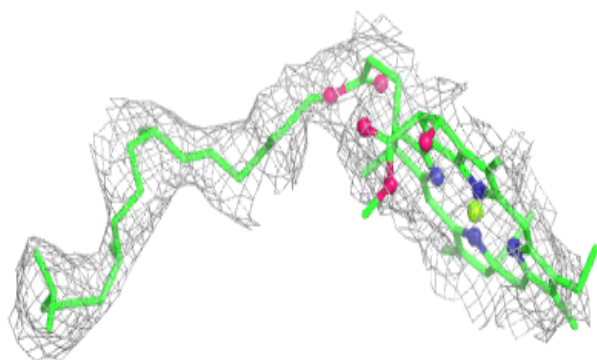
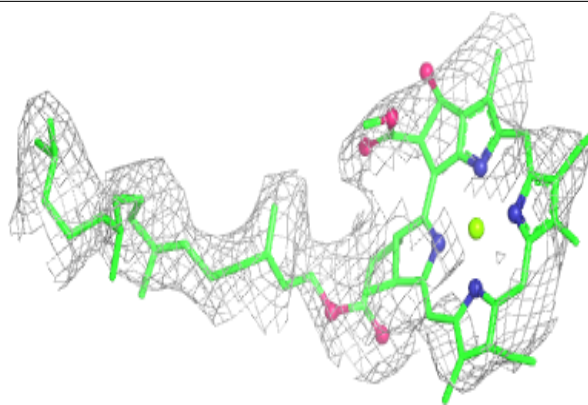
Electron density around CLA A 810:

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



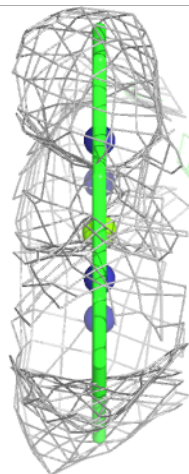
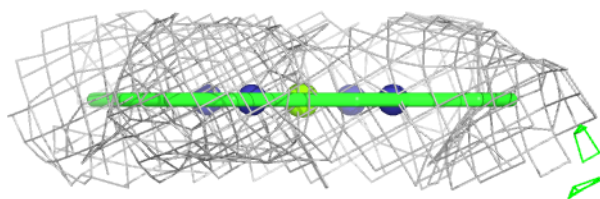
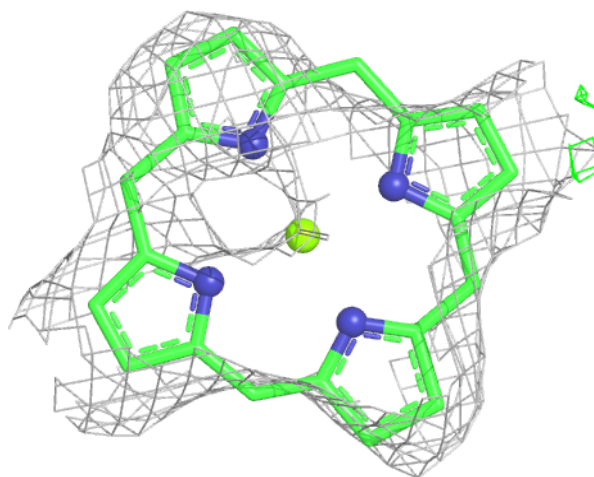
Electron density around CLA 3 315:

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



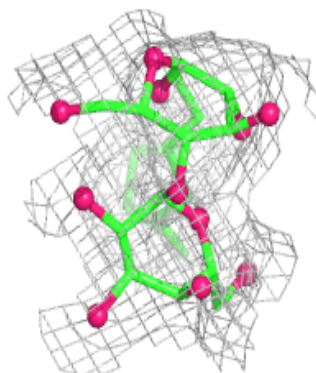
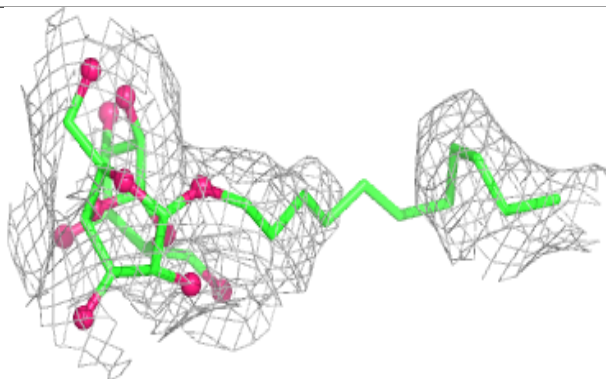
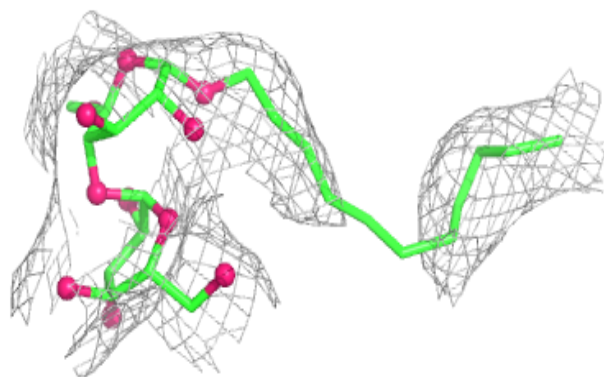
Electron density around CLA A 814:

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

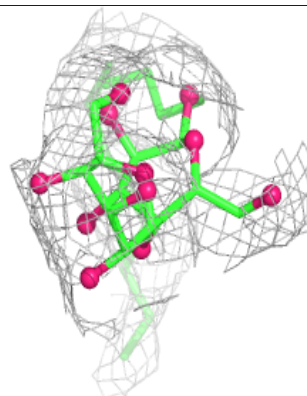
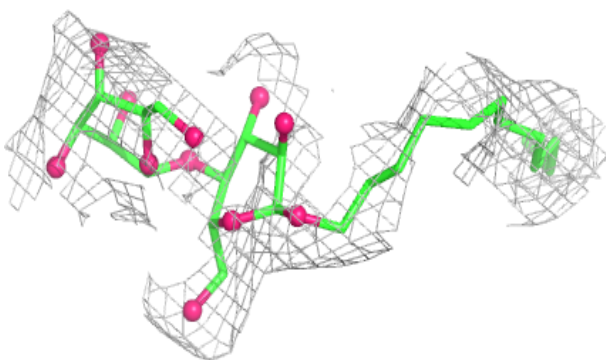
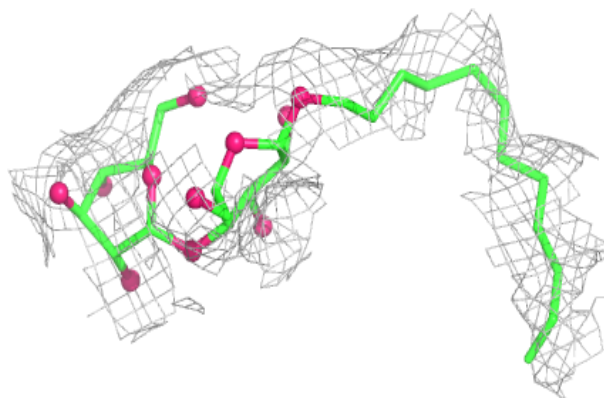


Electron density around LMU 4 319:

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

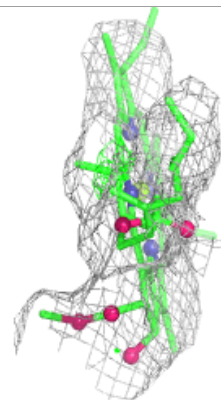
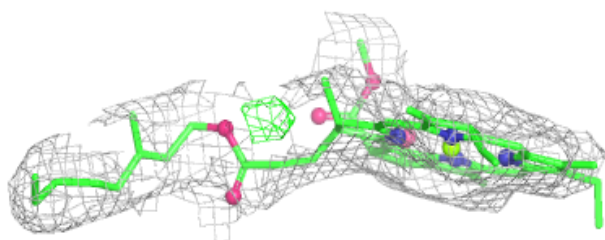
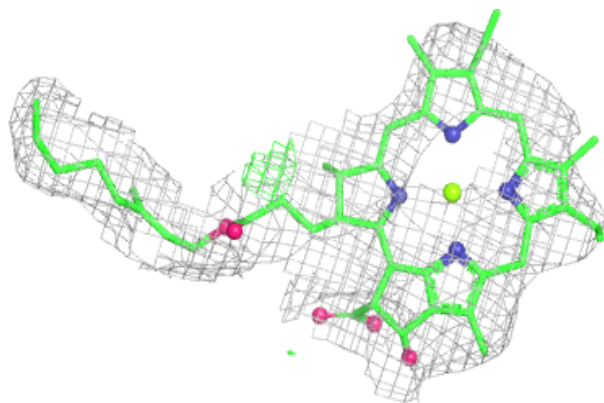
**Electron density around LMU 2 319:**

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

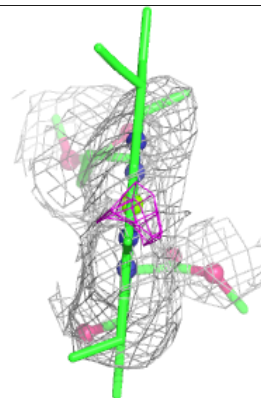
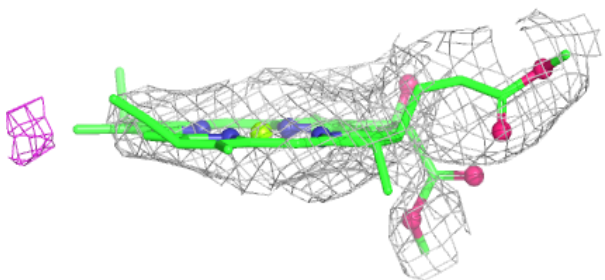
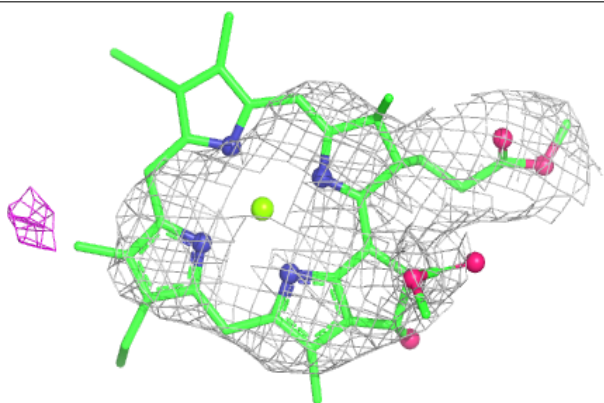


Electron density around CLA A 805:

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

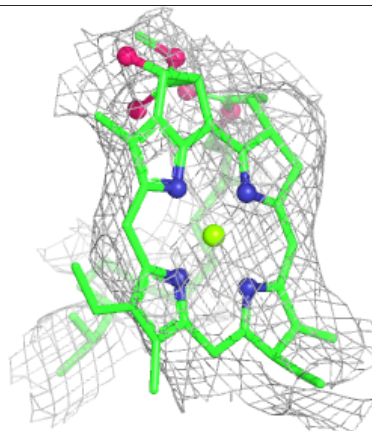
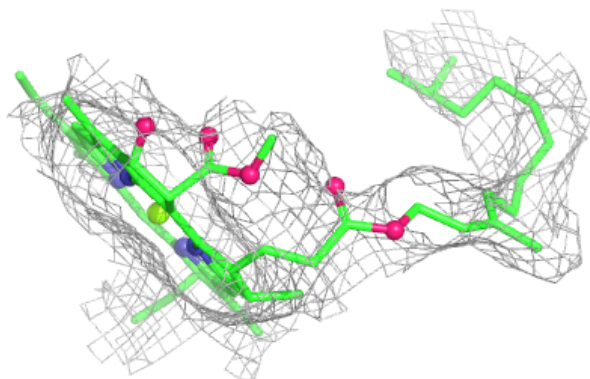
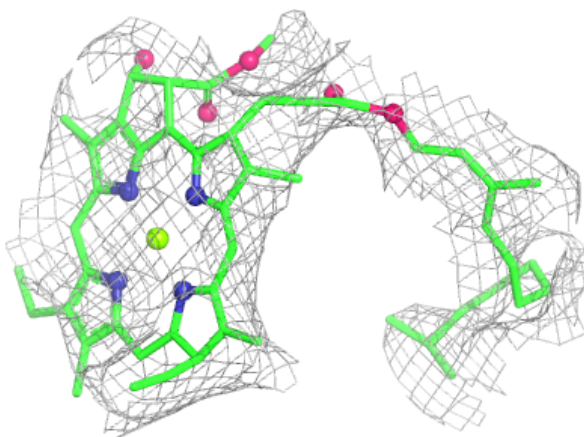
**Electron density around CLA A 834:**

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



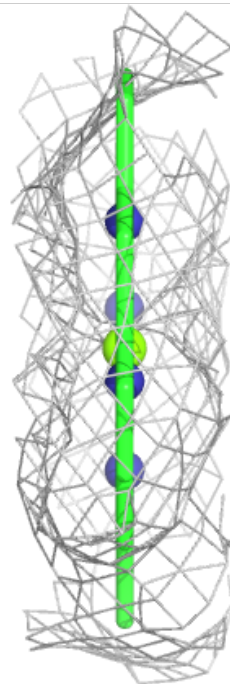
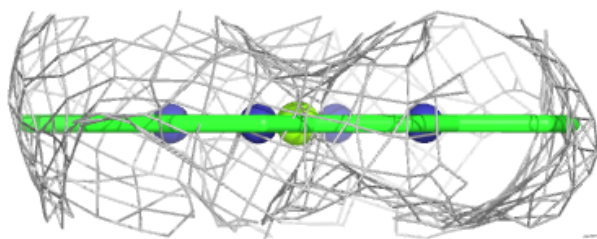
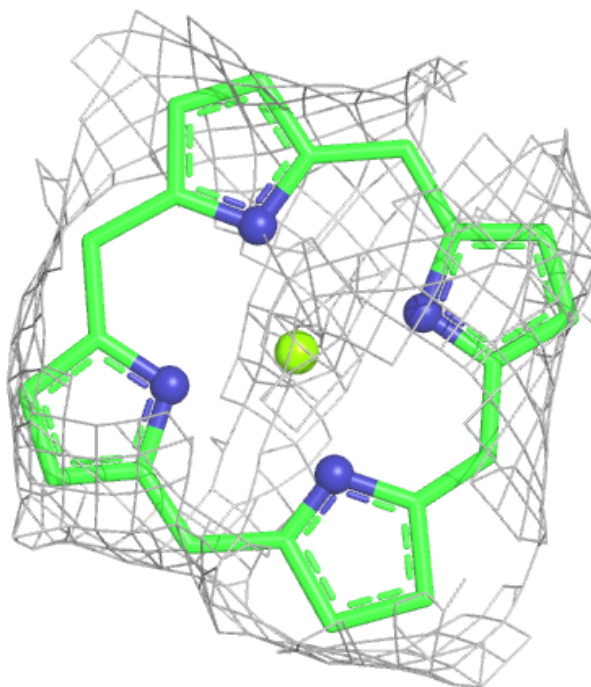
Electron density around CLA A 839:

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



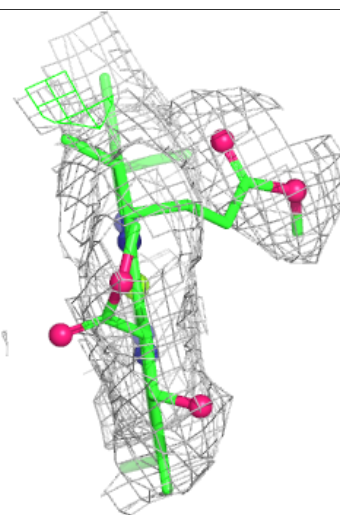
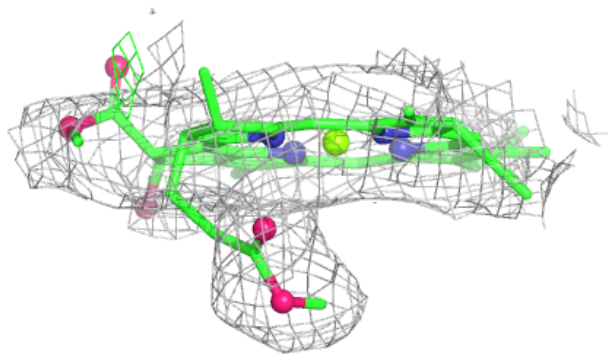
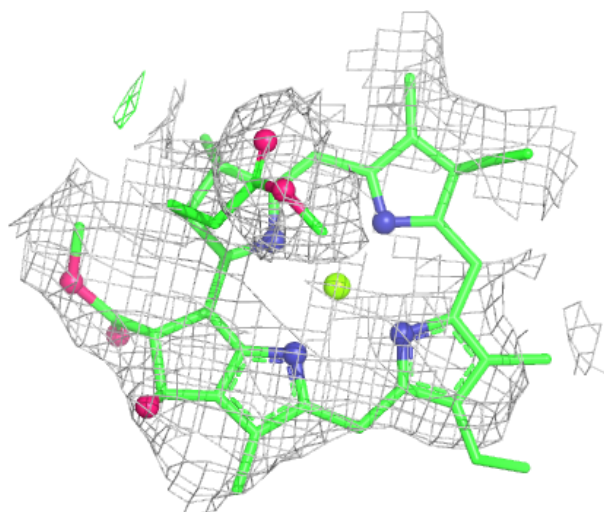
Electron density around CLA 1 212:

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



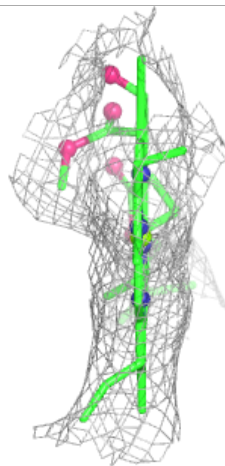
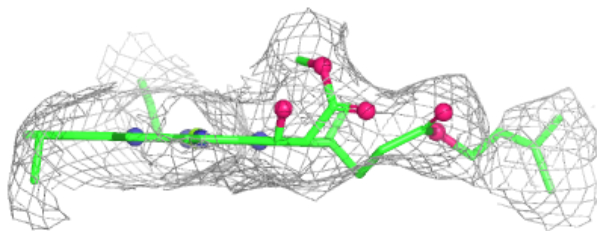
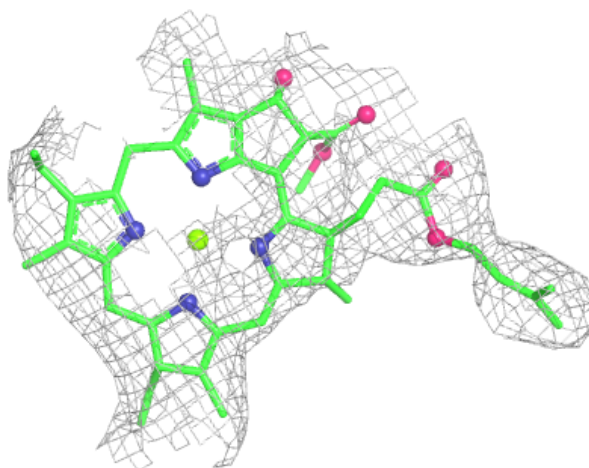
Electron density around CLA 1 204:

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



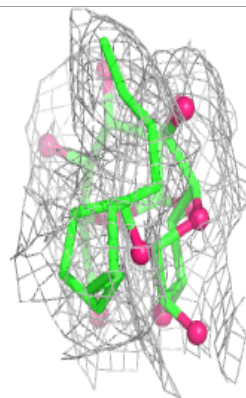
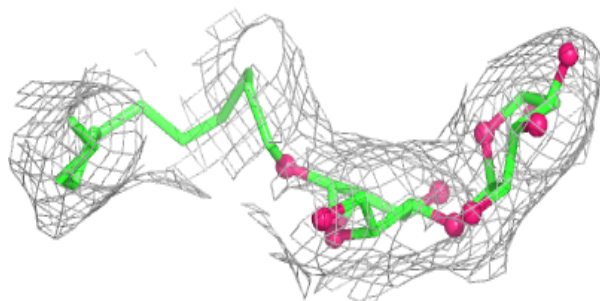
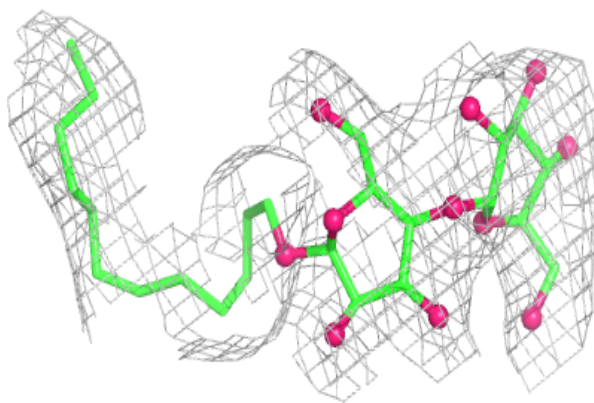
Electron density around CLA 4 310:

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



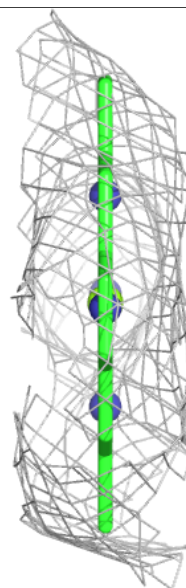
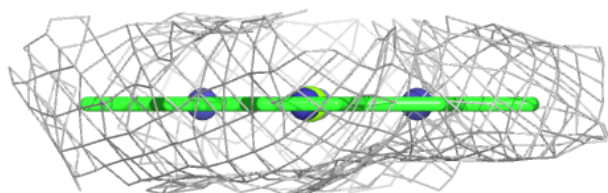
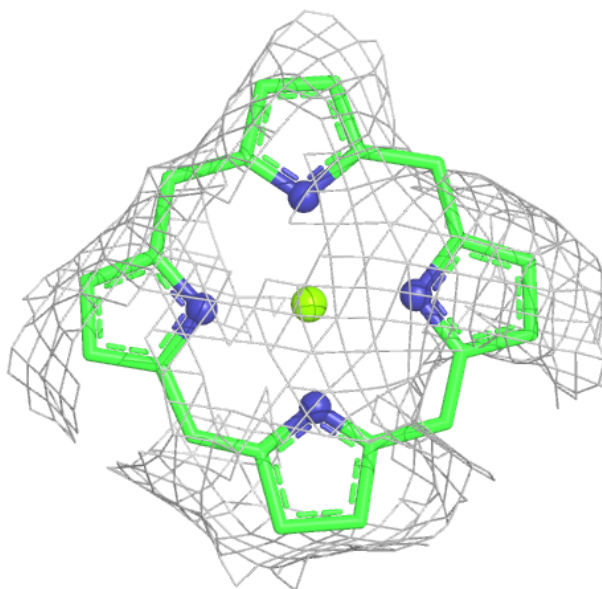
Electron density around LMU D 201:

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



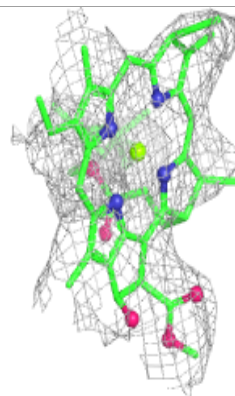
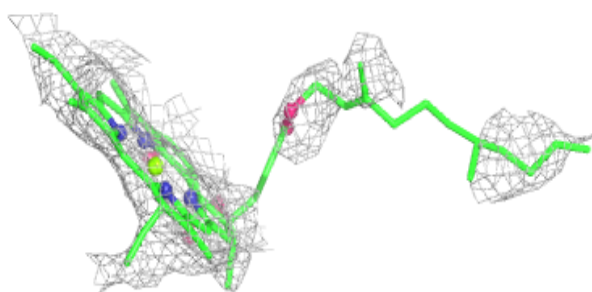
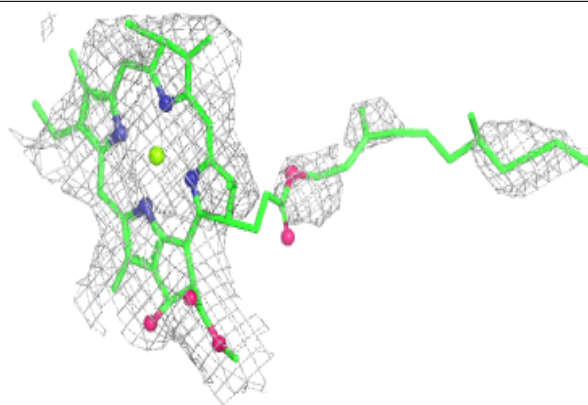
Electron density around CLA 1 214:

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

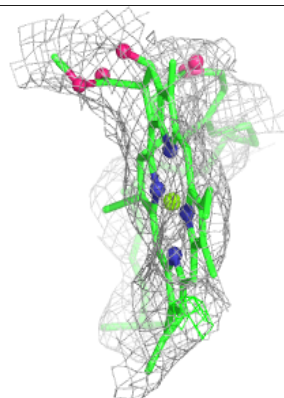
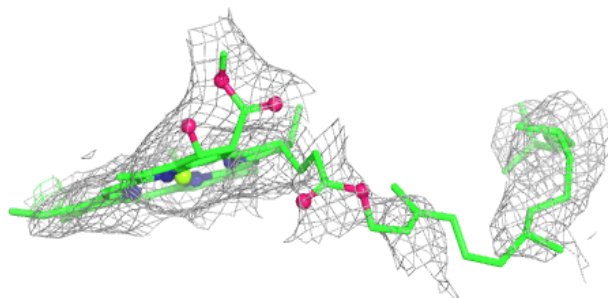
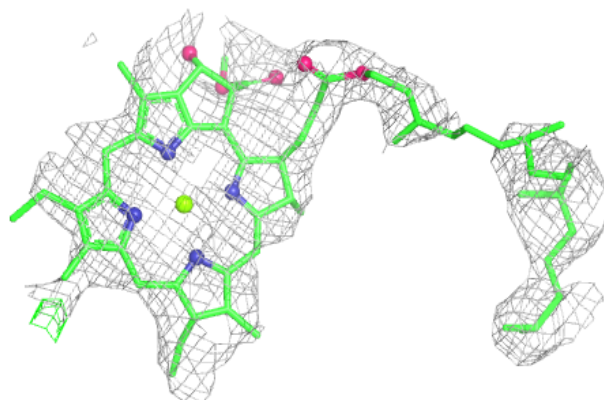


Electron density around CLA A 819:

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

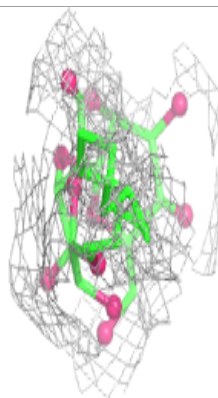
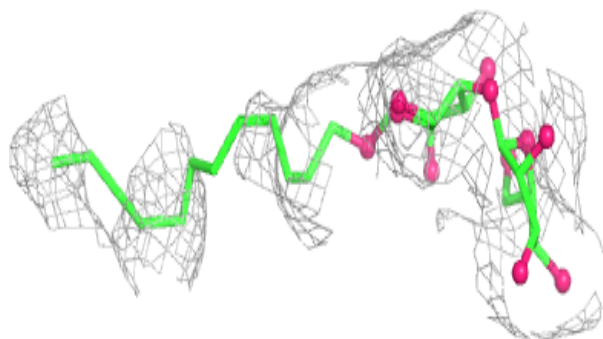
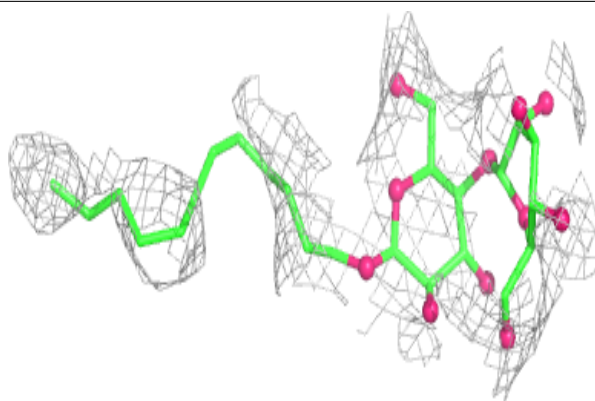
**Electron density around CLA A 825:**

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

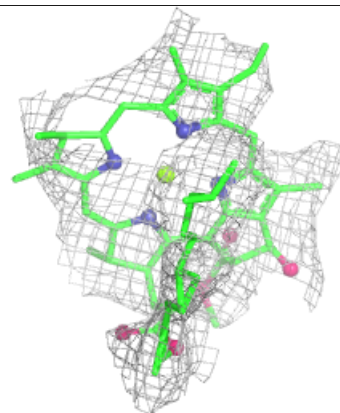
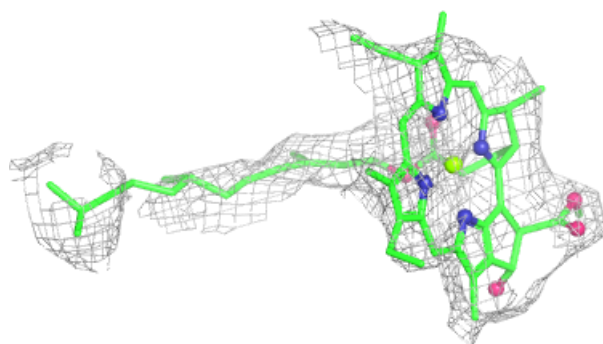
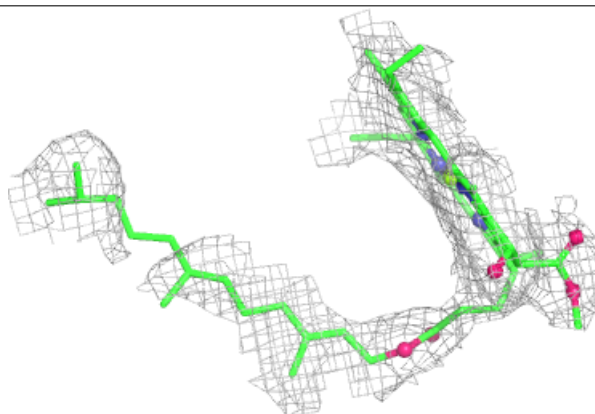


Electron density around LMU 1 218:

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

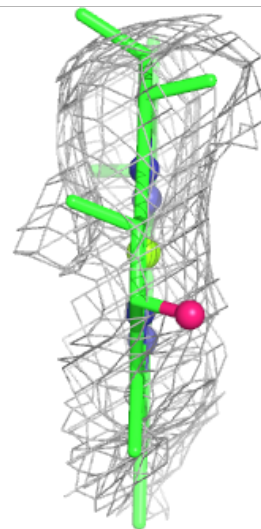
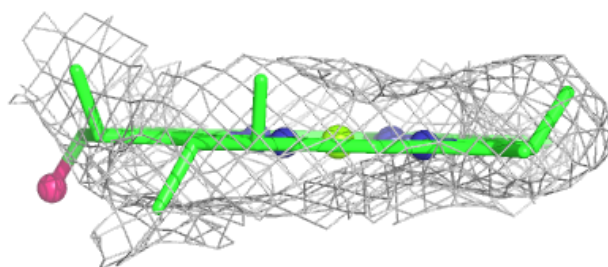
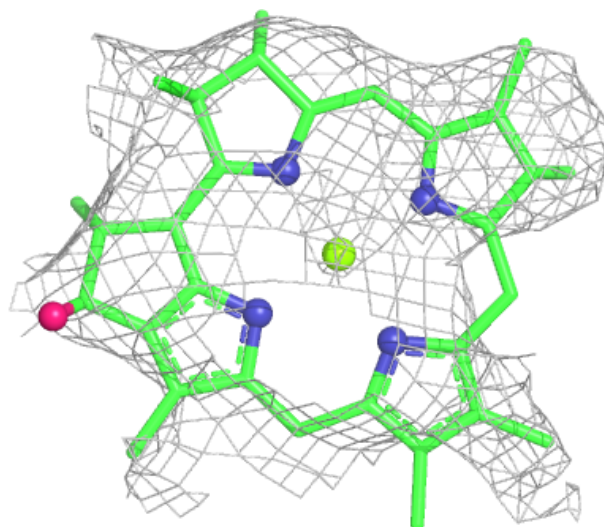
**Electron density around CLA L 201:**

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



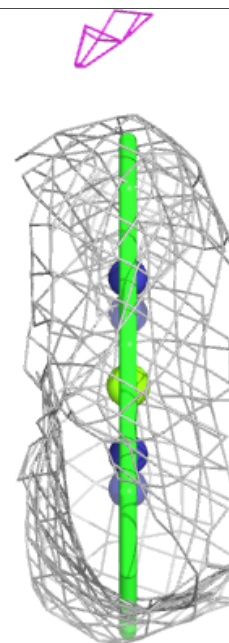
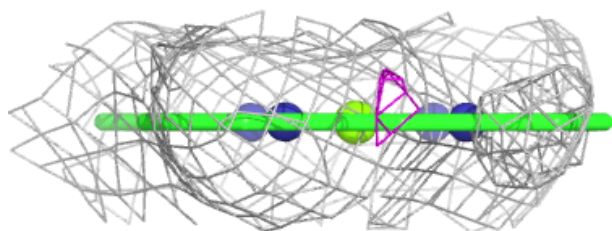
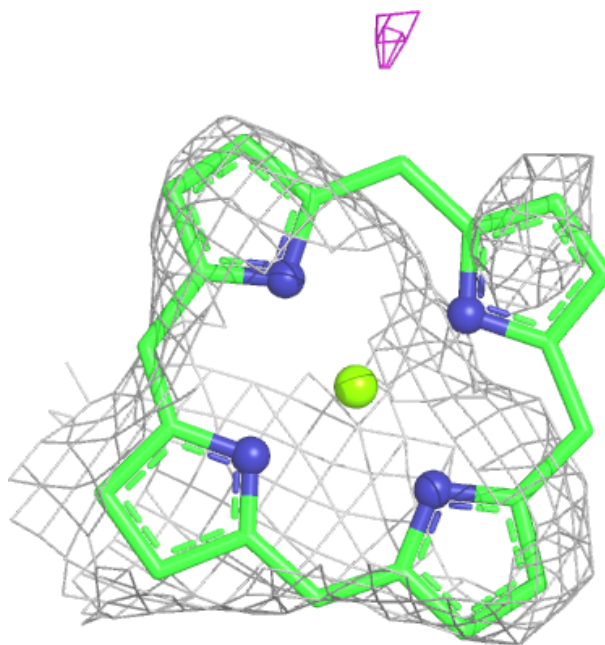
Electron density around CLA B 842:

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



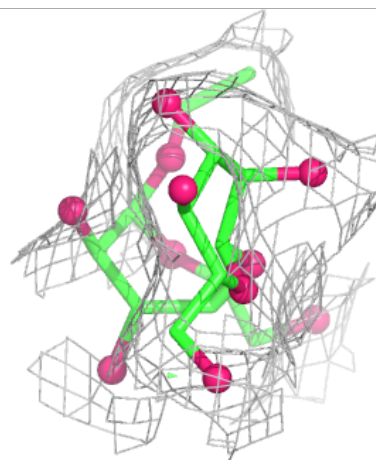
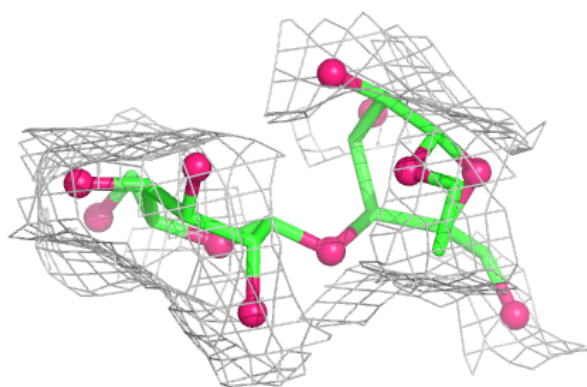
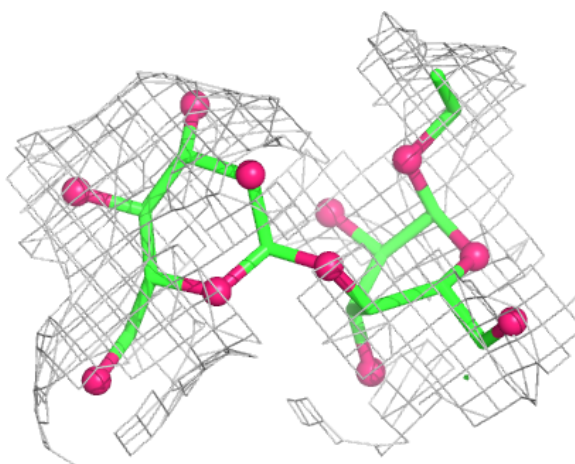
Electron density around CLA 2 309:

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



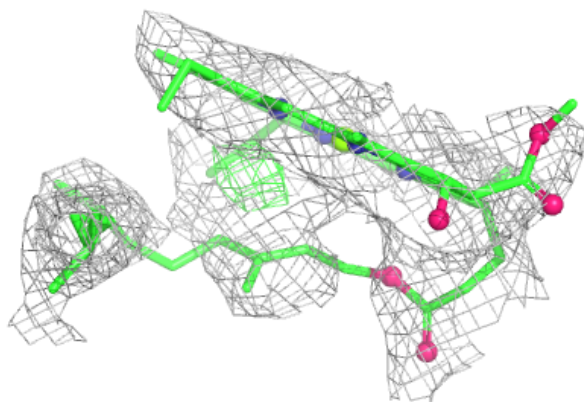
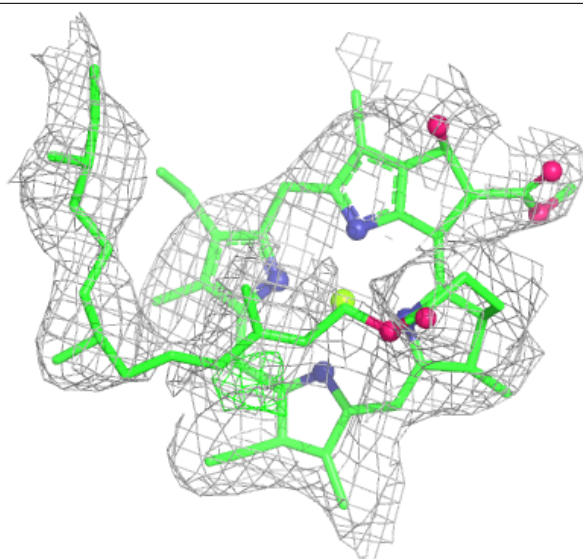
Electron density around LMU B 849:

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



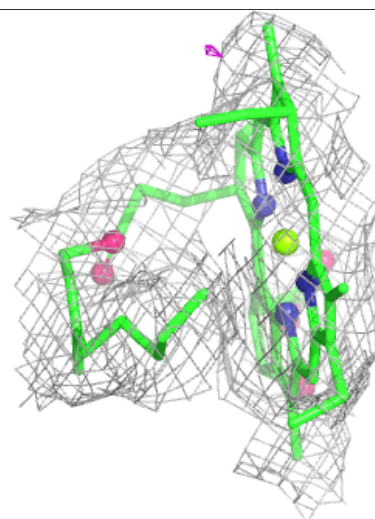
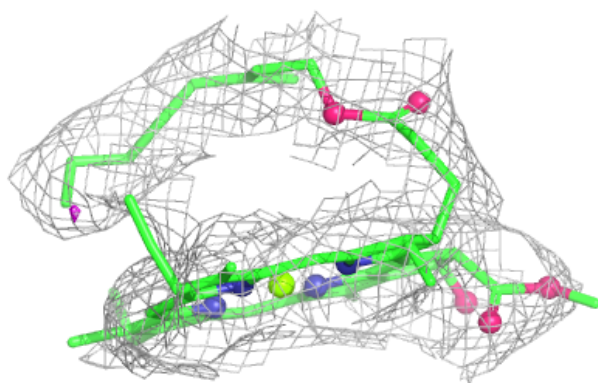
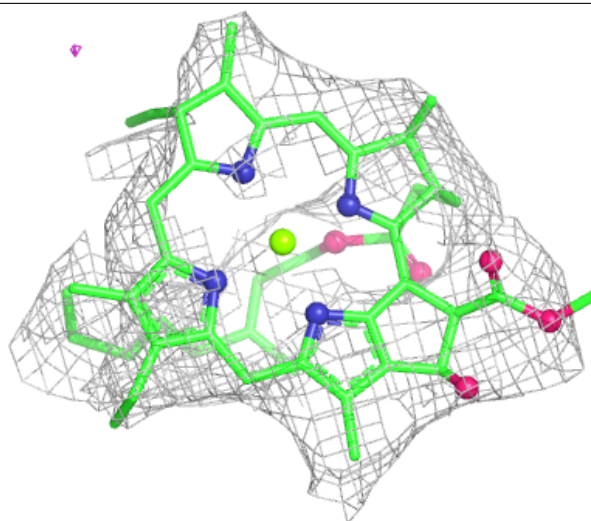
Electron density around CLA B 820:

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



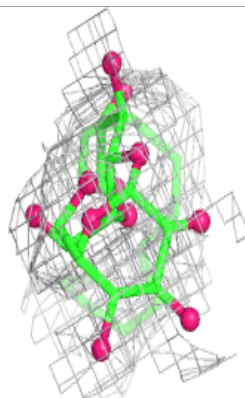
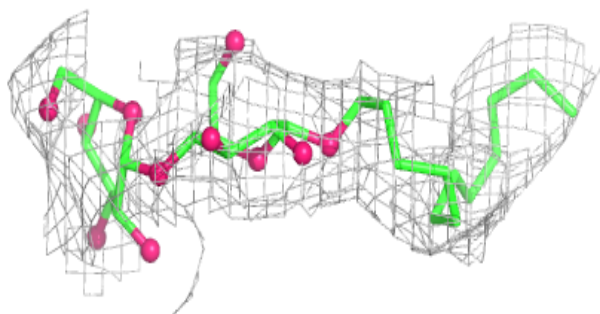
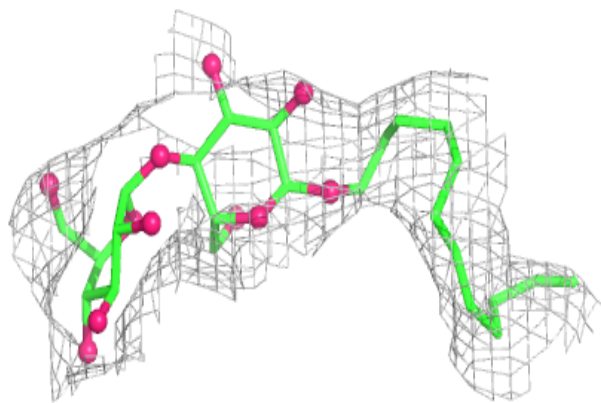
Electron density around CLA A 812:

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



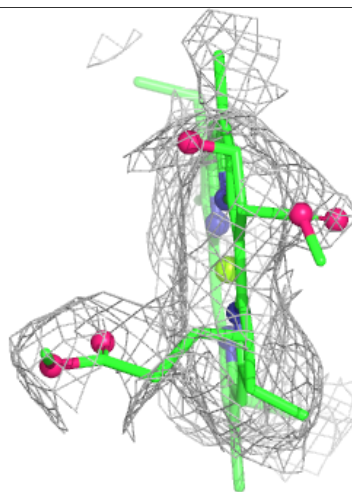
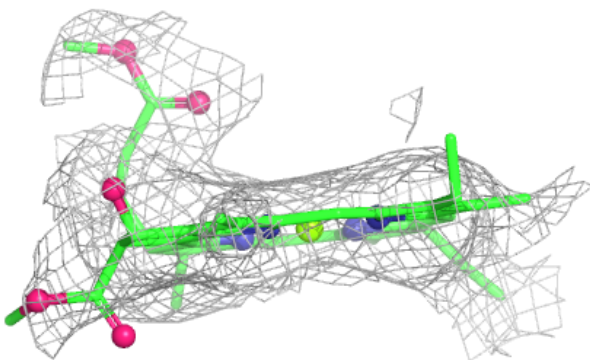
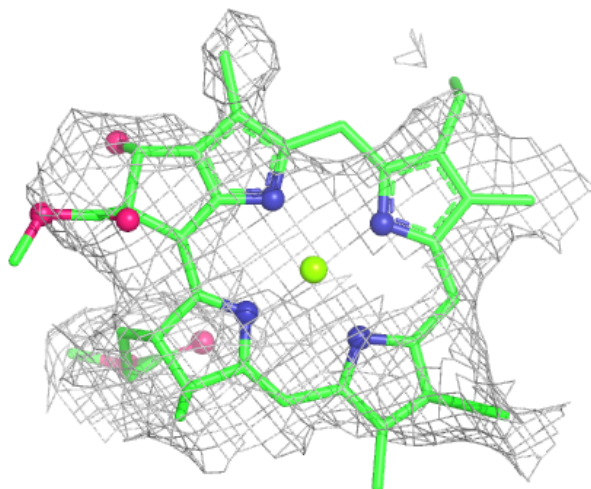
Electron density around LMU R 109:

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



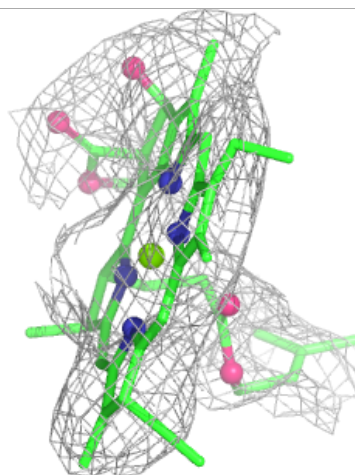
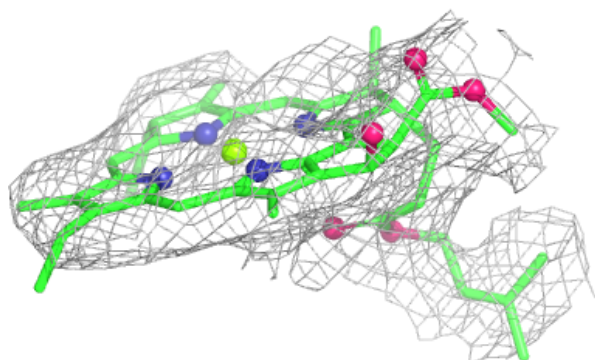
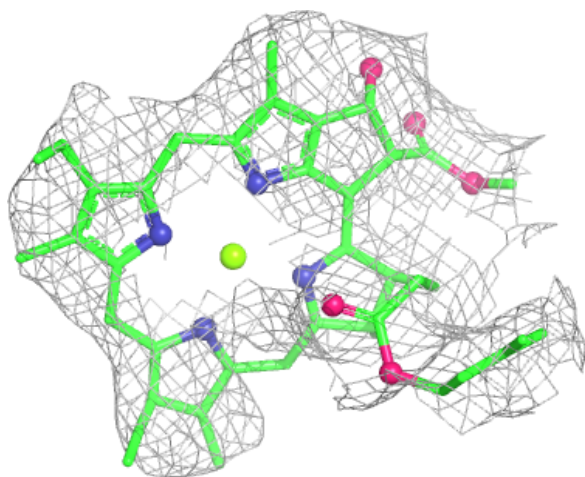
Electron density around CLA A 807:

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



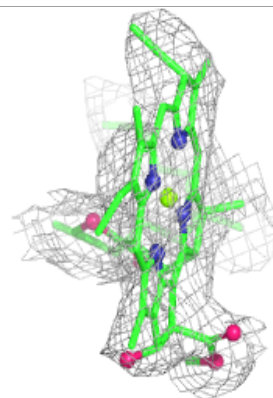
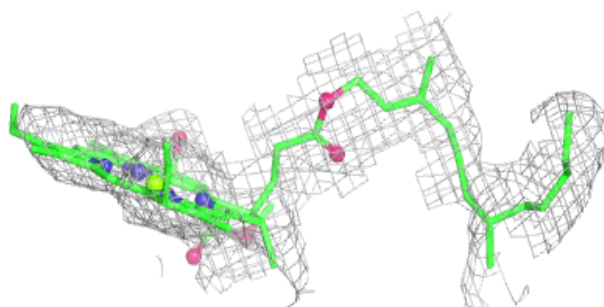
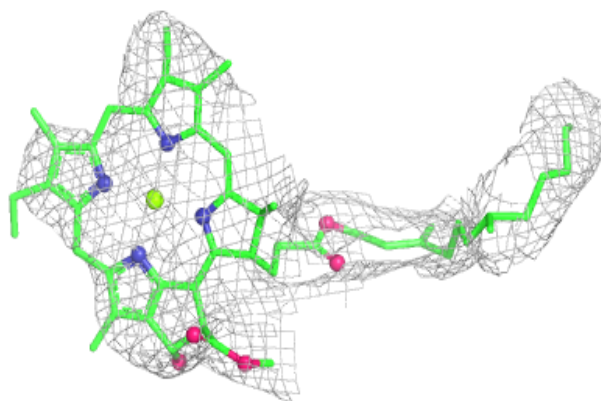
Electron density around CLA A 815:

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

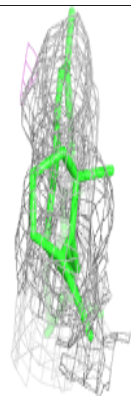
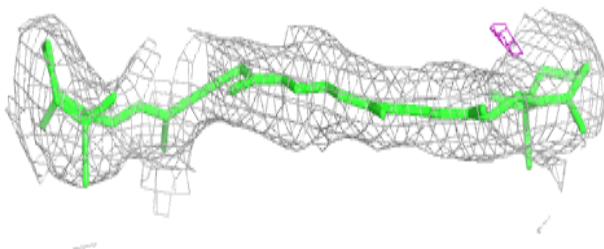
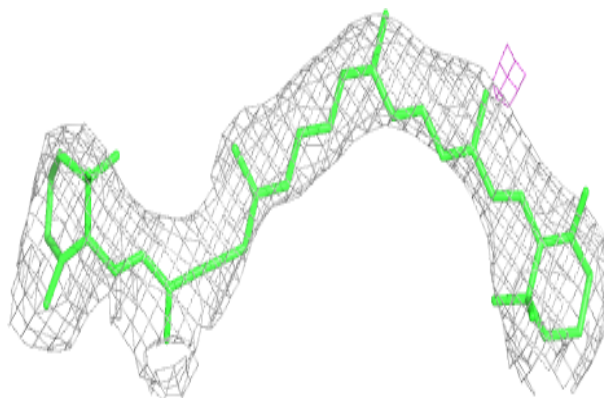


Electron density around CLA A 824:

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

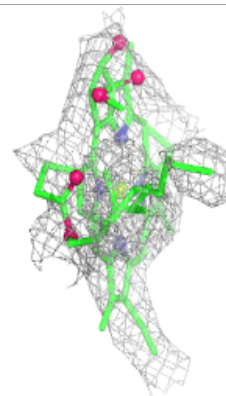
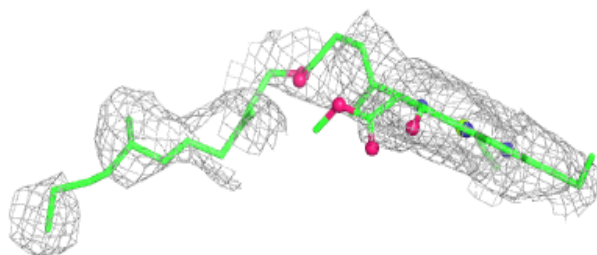
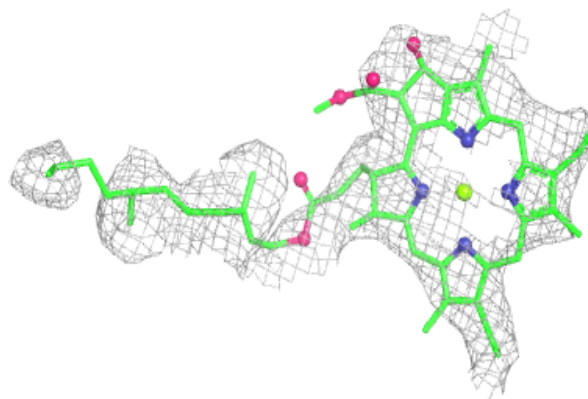
**Electron density around BCR A 845:**

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

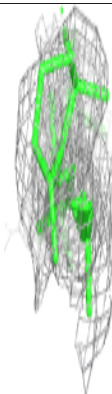
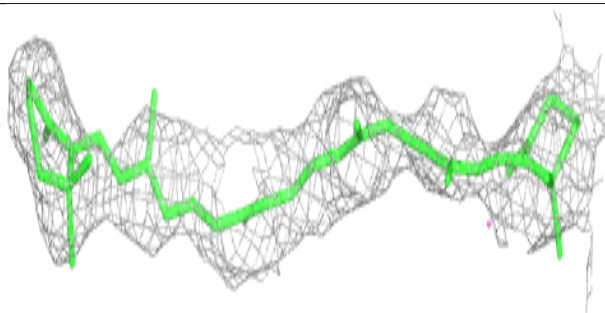
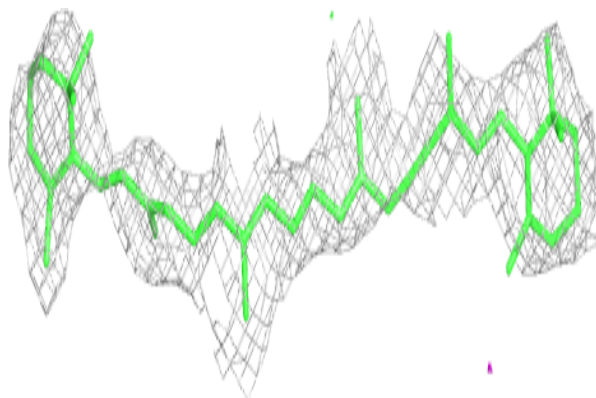


Electron density around CLA H 111:

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

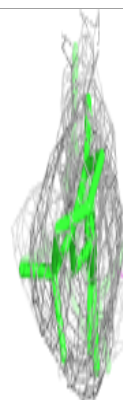
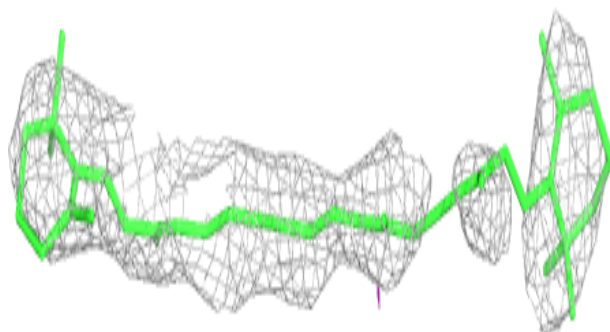
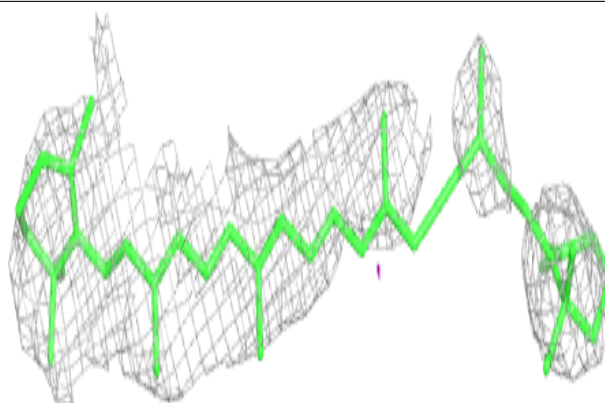
**Electron density around BCR B 846:**

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

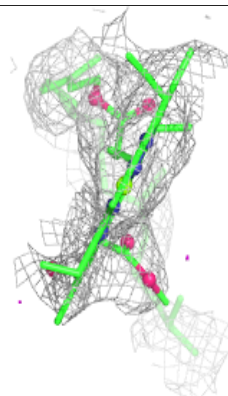
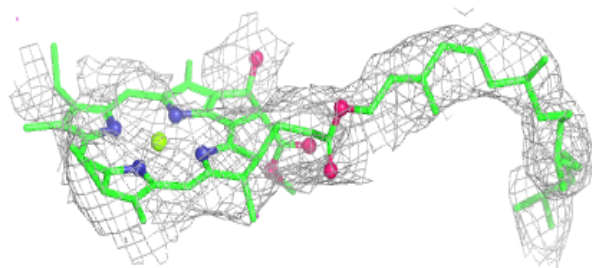
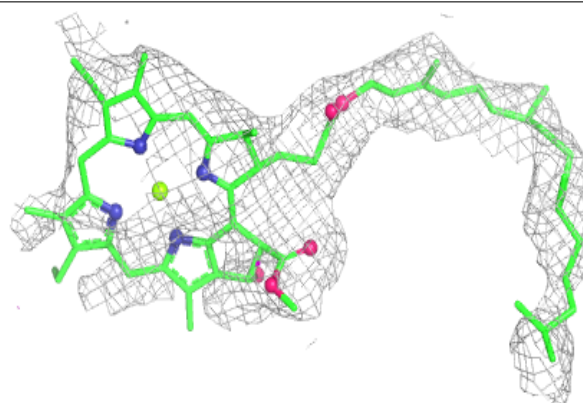


Electron density around BCR B 847:

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

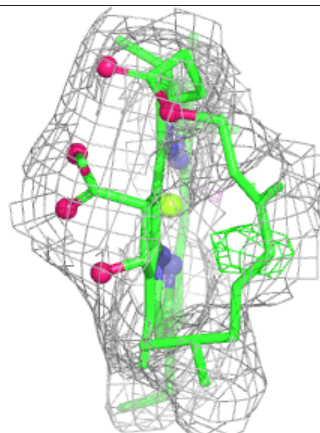
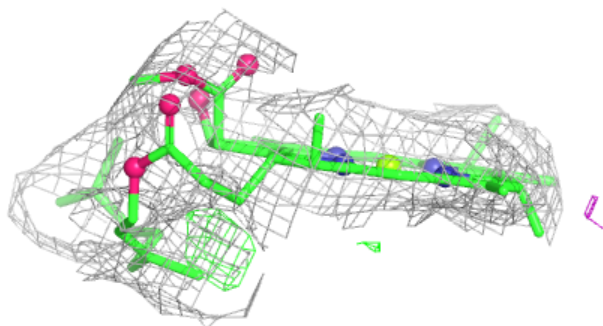
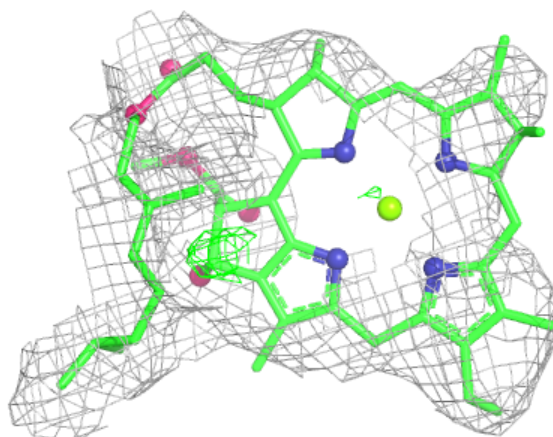
**Electron density around CLA B 827:**

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

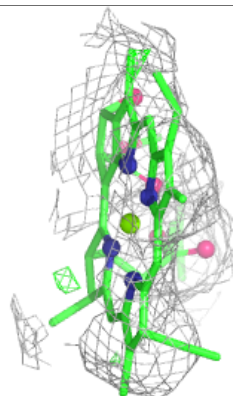
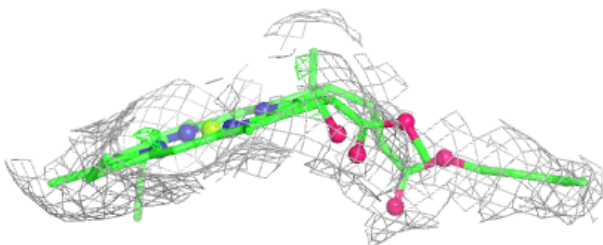
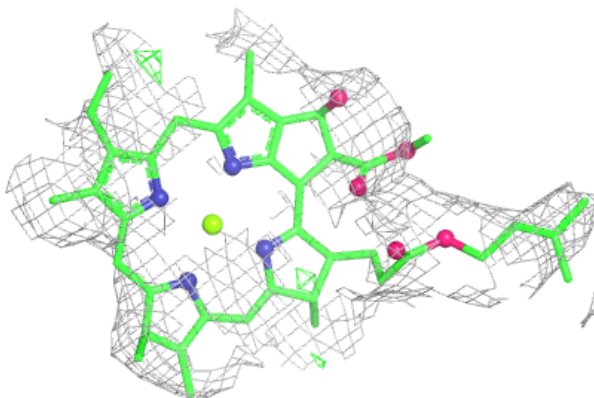


Electron density around CLA B 812:

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

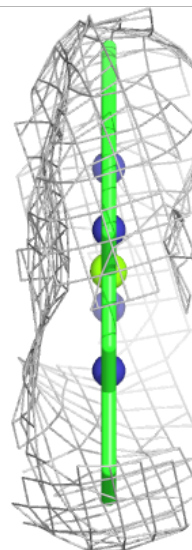
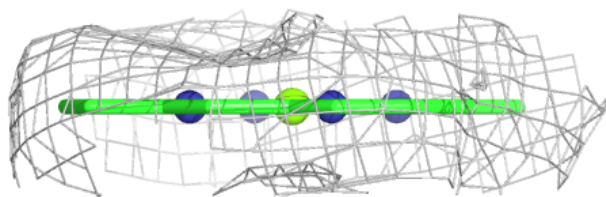
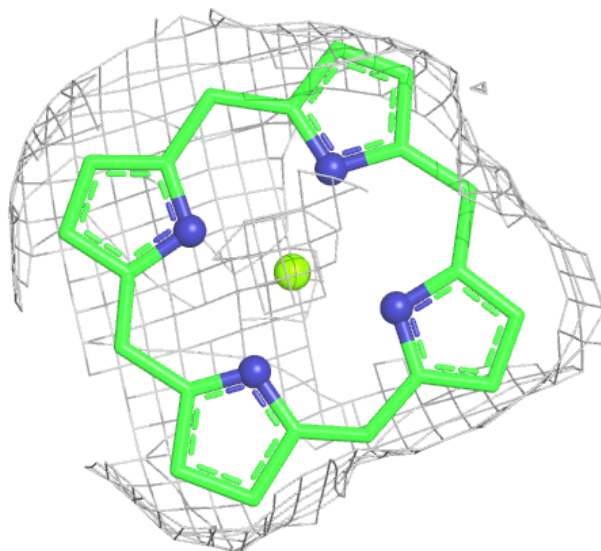
**Electron density around CLA L 210:**

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



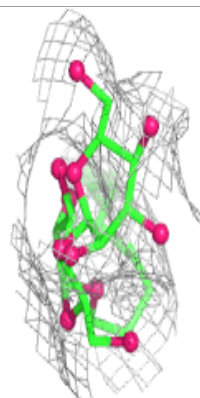
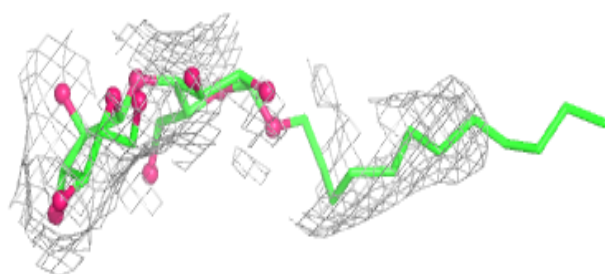
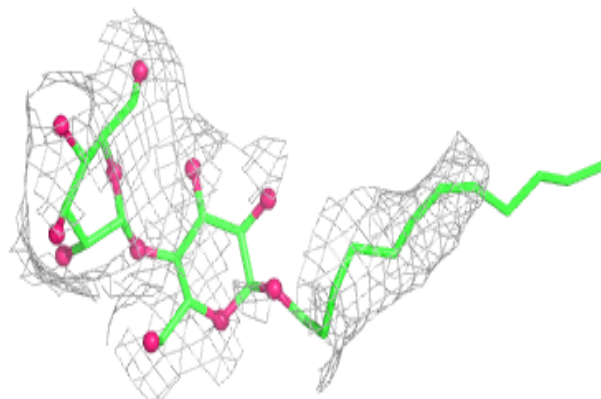
Electron density around CLA 3 304:

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



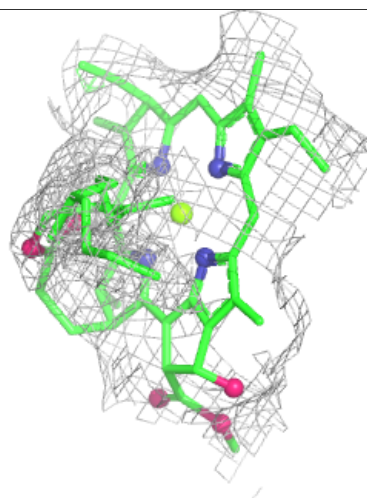
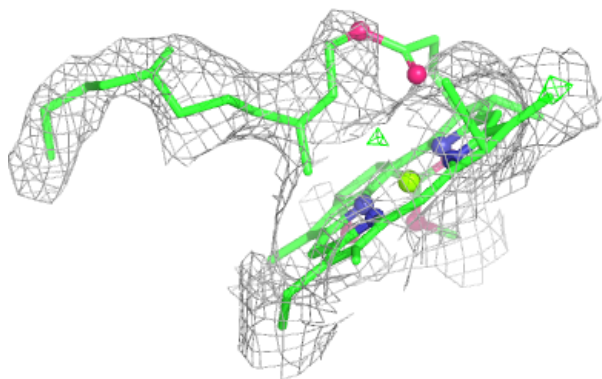
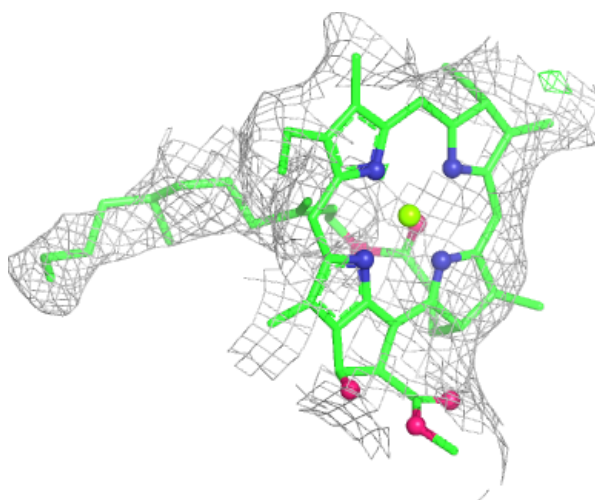
Electron density around LMU A 855:

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



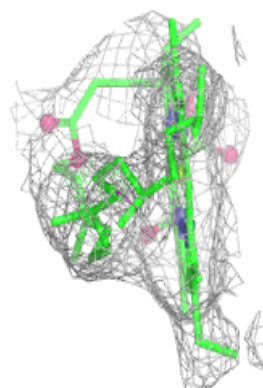
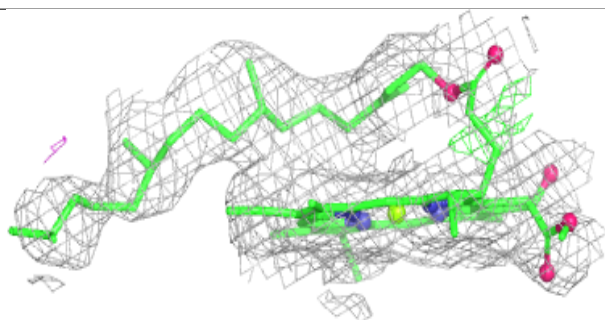
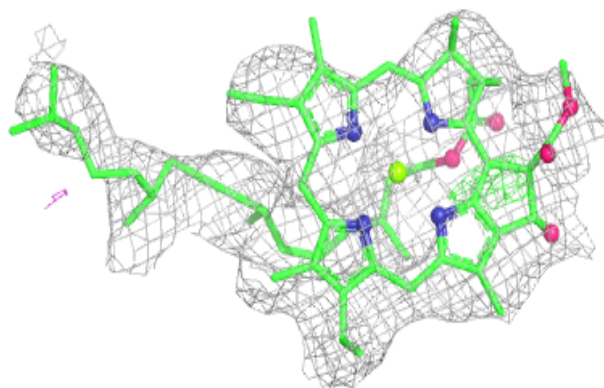
Electron density around CLA 2 303:

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

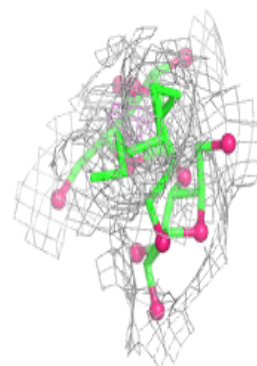
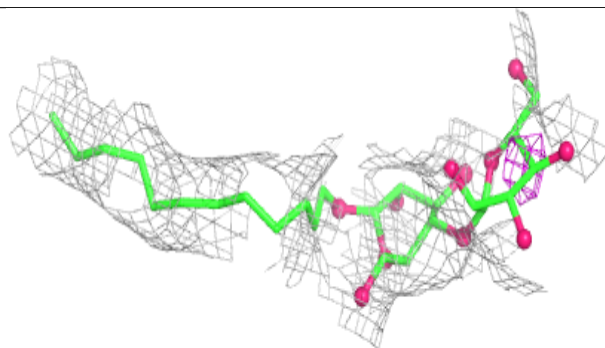
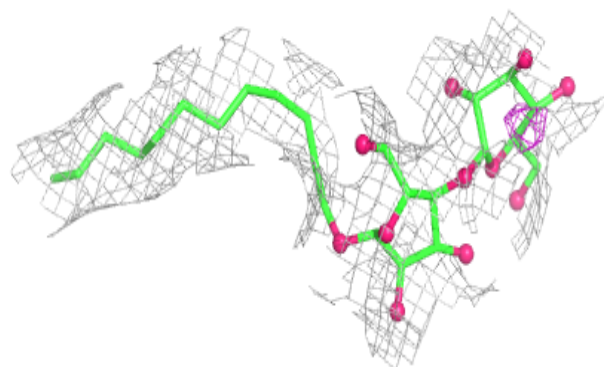


Electron density around CLA B 806:

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

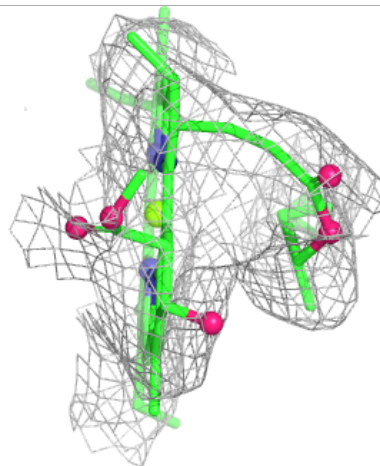
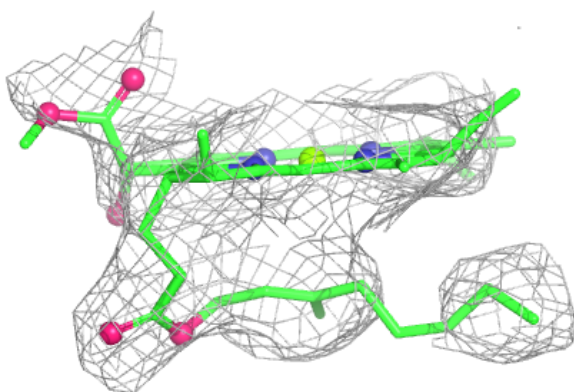
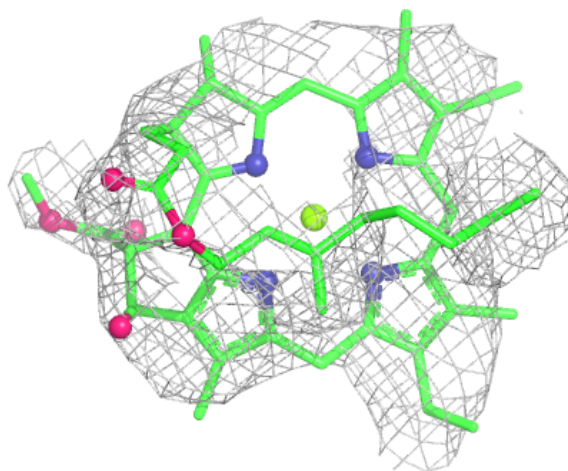
**Electron density around LMU G 101:**

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



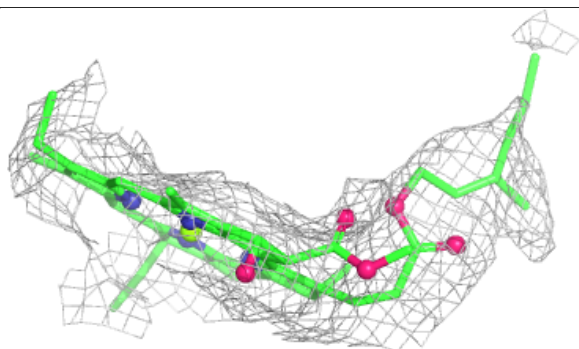
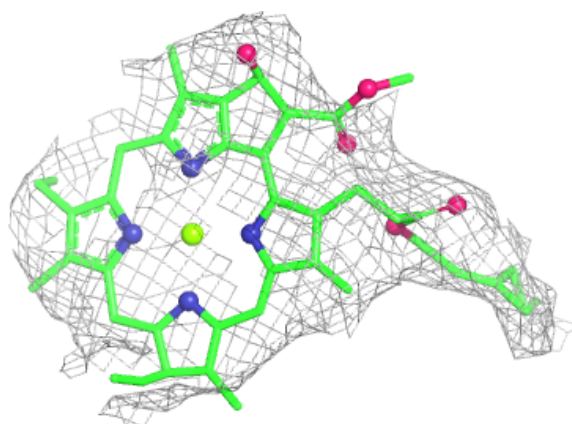
Electron density around CLA A 816:

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

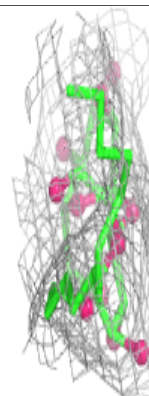
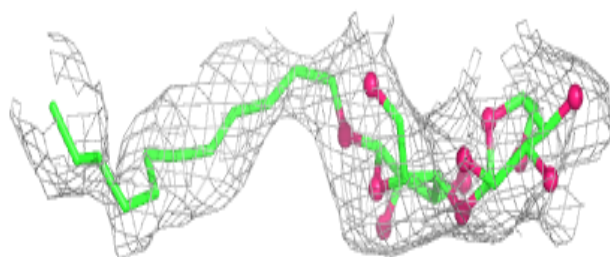
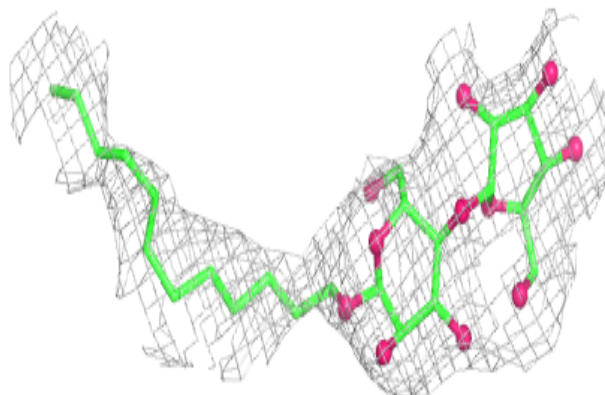


Electron density around CLA 4 306:

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

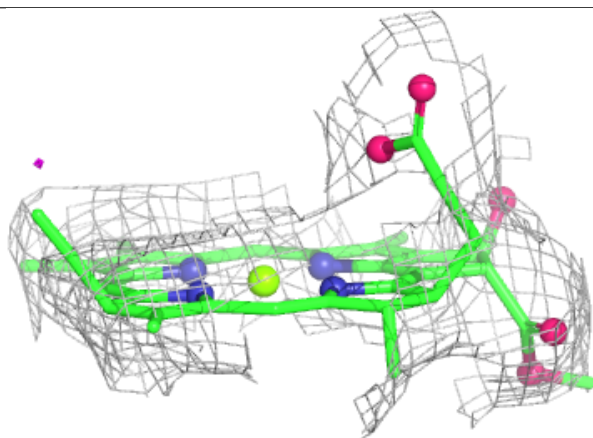
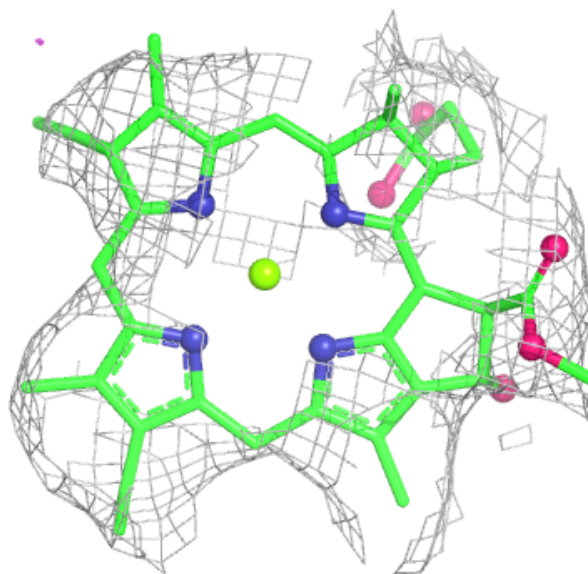
**Electron density around LMU 1 216:**

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



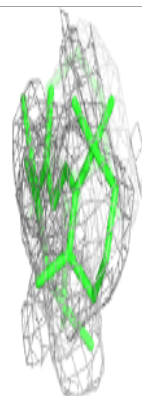
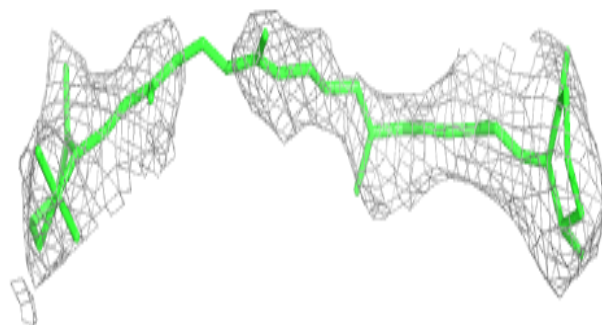
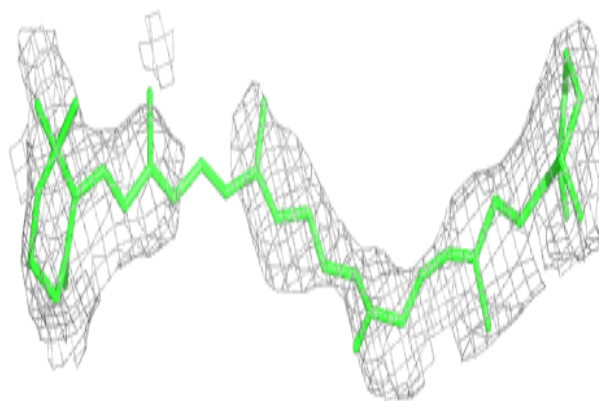
Electron density around CLA B 834:

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



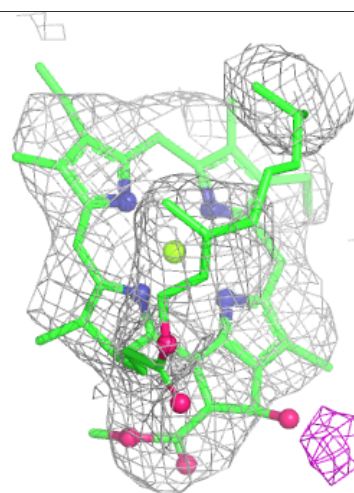
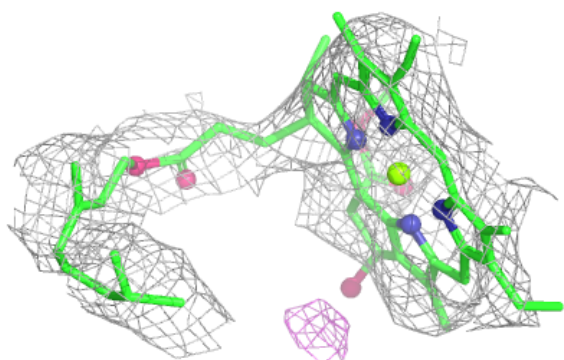
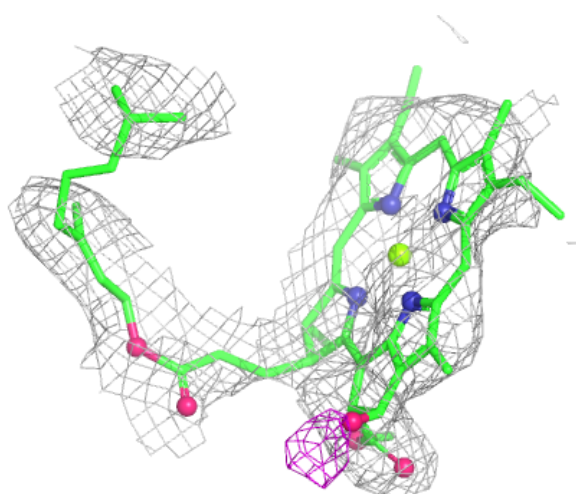
Electron density around BCR I 101:

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



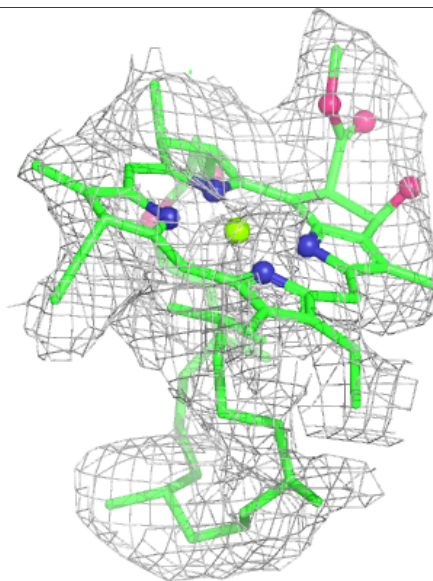
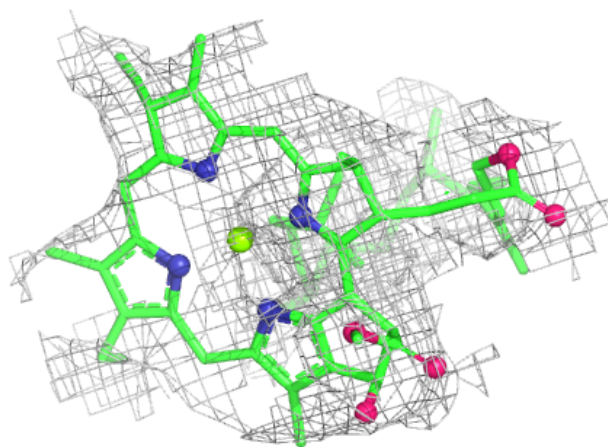
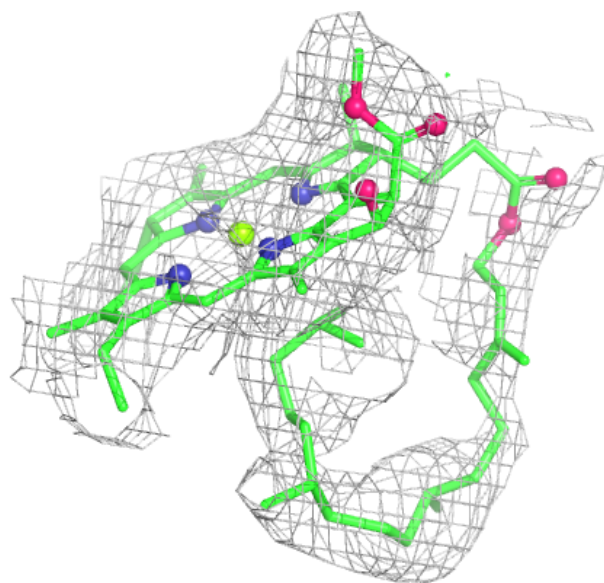
Electron density around CLA A 804:

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



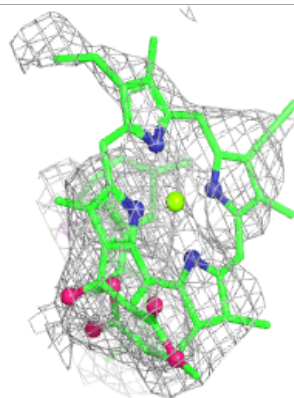
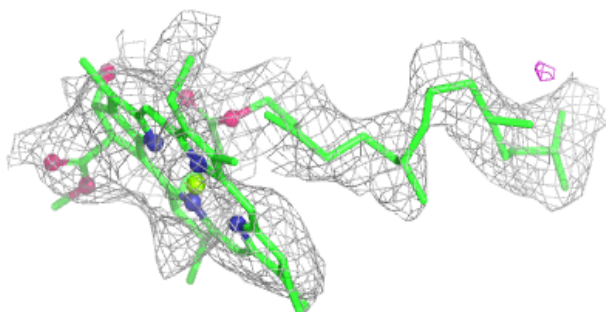
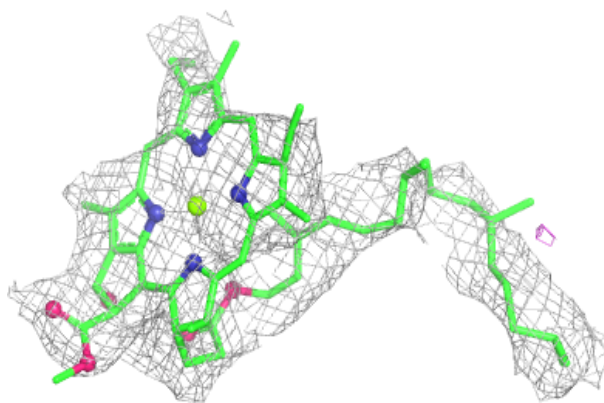
Electron density around CLA 2 317:

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

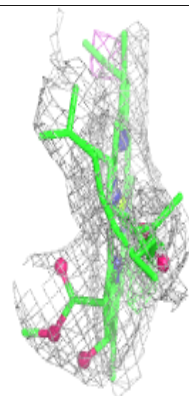
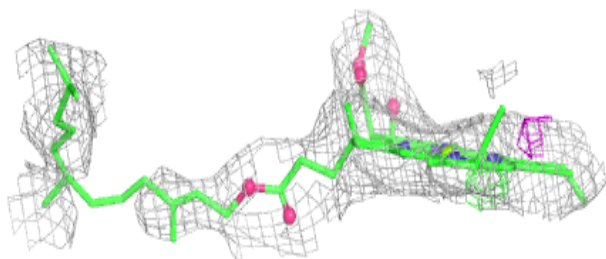
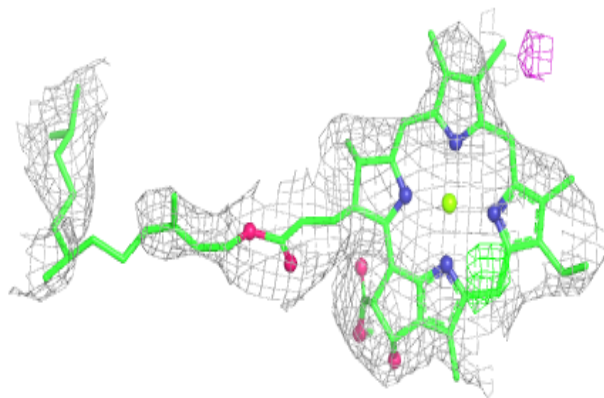


Electron density around CLA L 203:

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

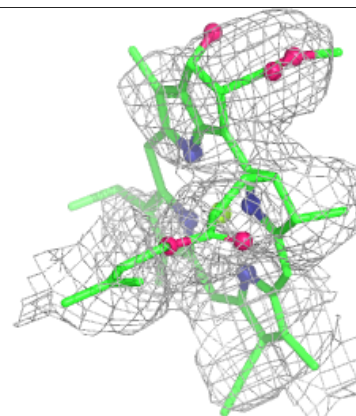
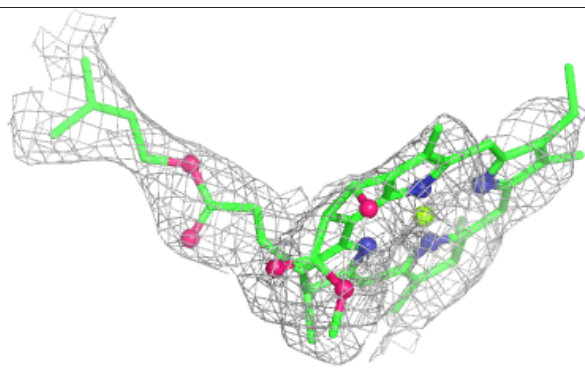
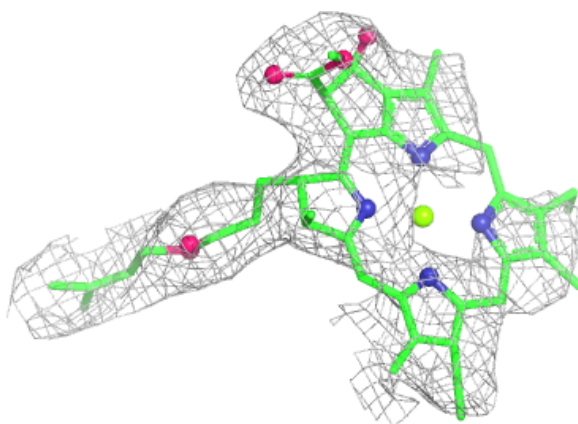
**Electron density around CLA B 837:**

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



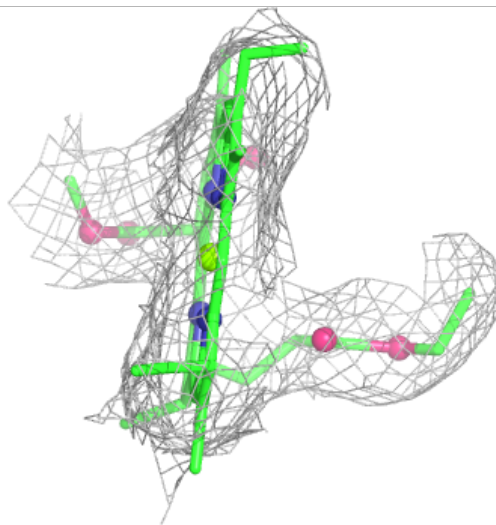
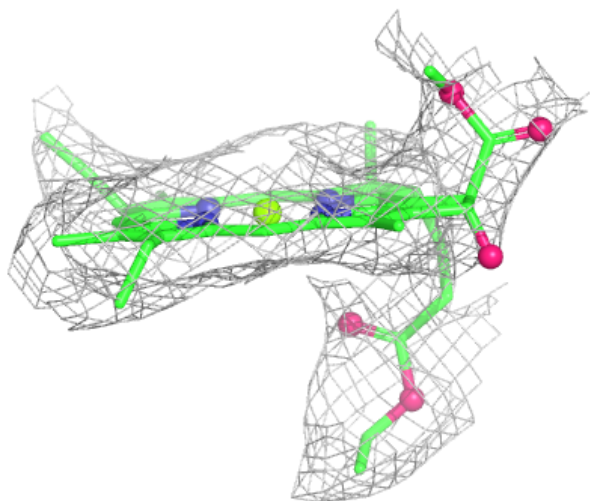
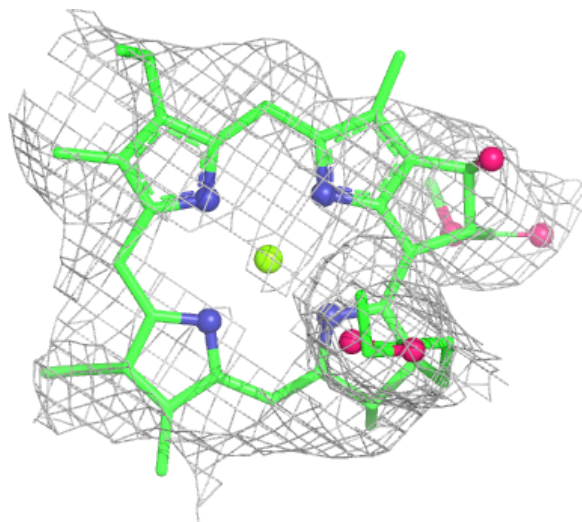
Electron density around CLA A 829:

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



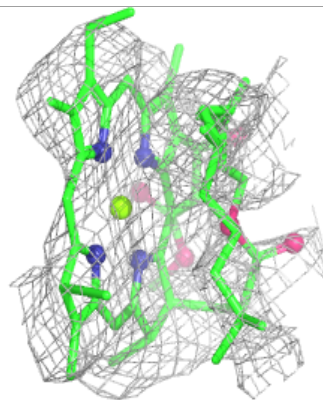
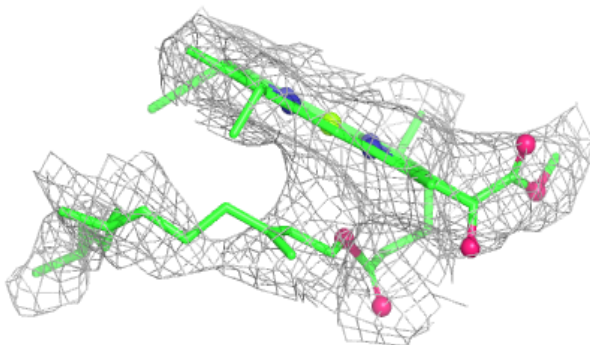
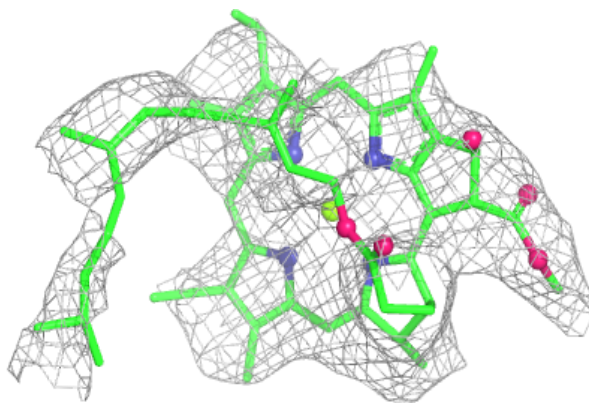
Electron density around CLA L 209:

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



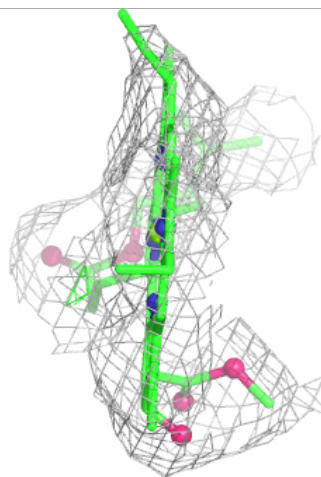
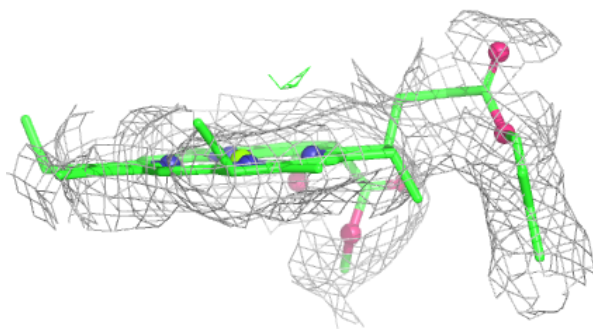
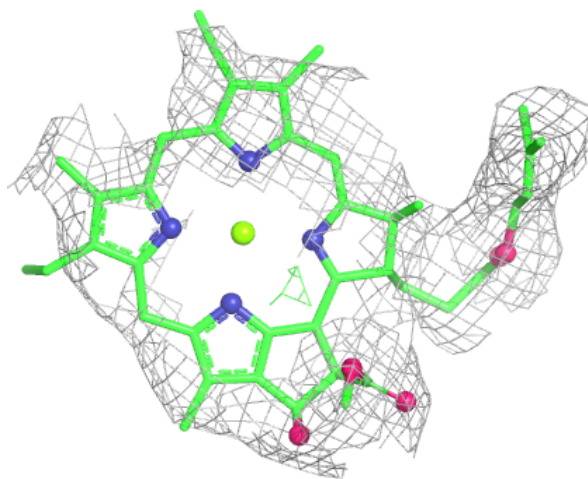
Electron density around CLA I 102:

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



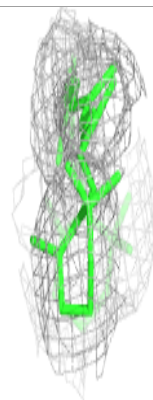
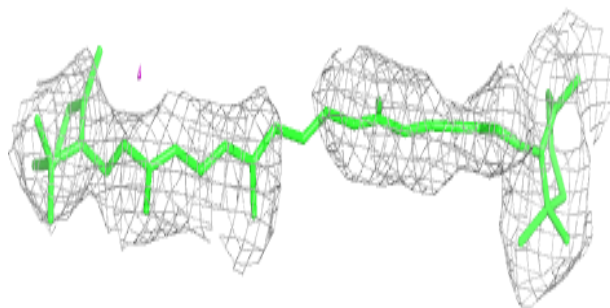
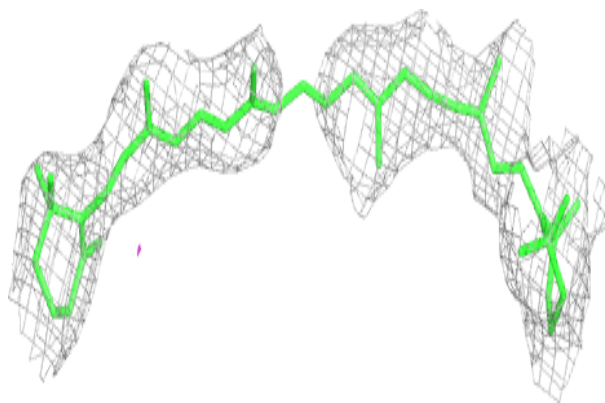
Electron density around CLA A 813:

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

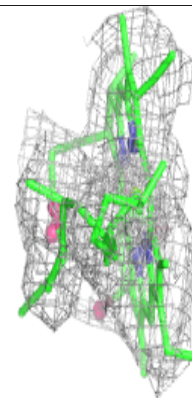
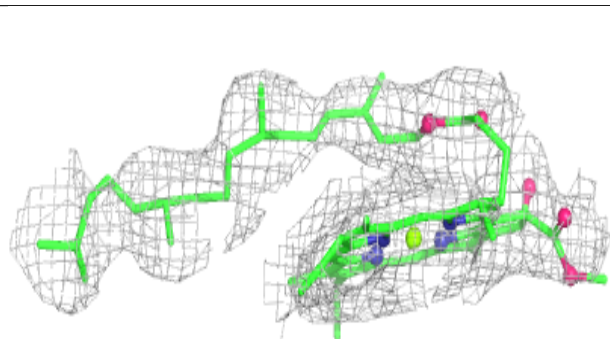
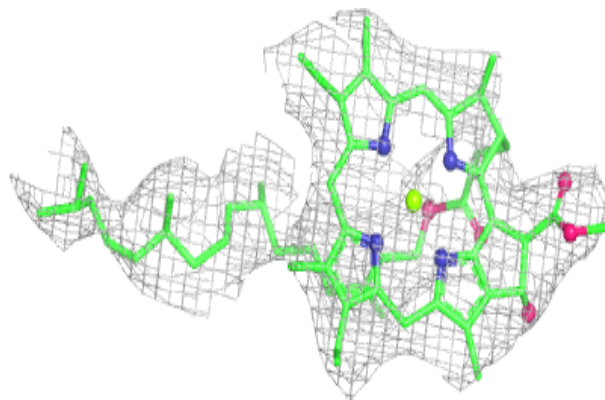


Electron density around BCR B 844:

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

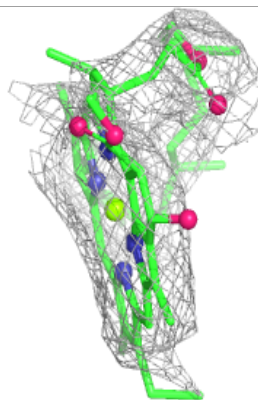
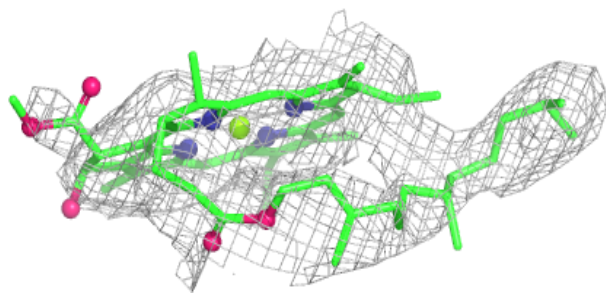
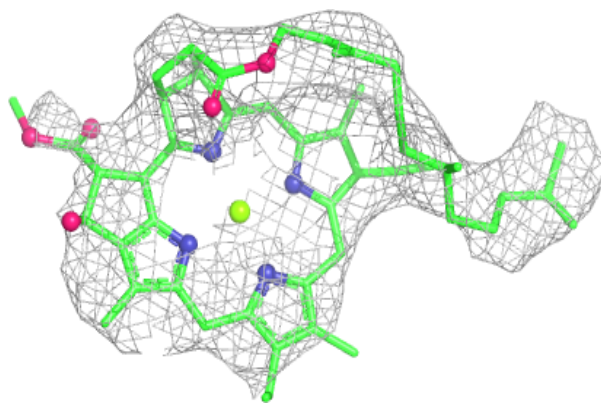
**Electron density around CLA A 835:**

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



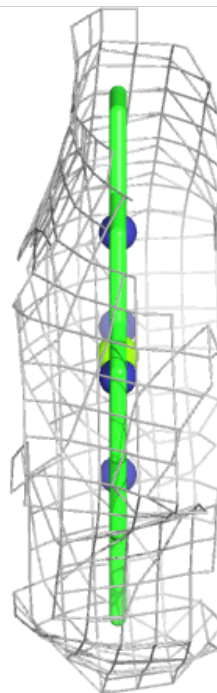
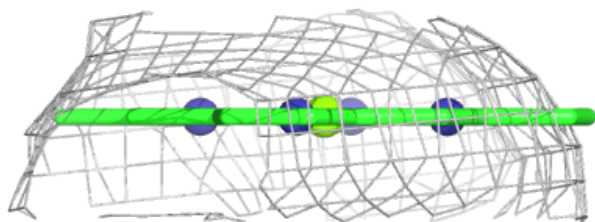
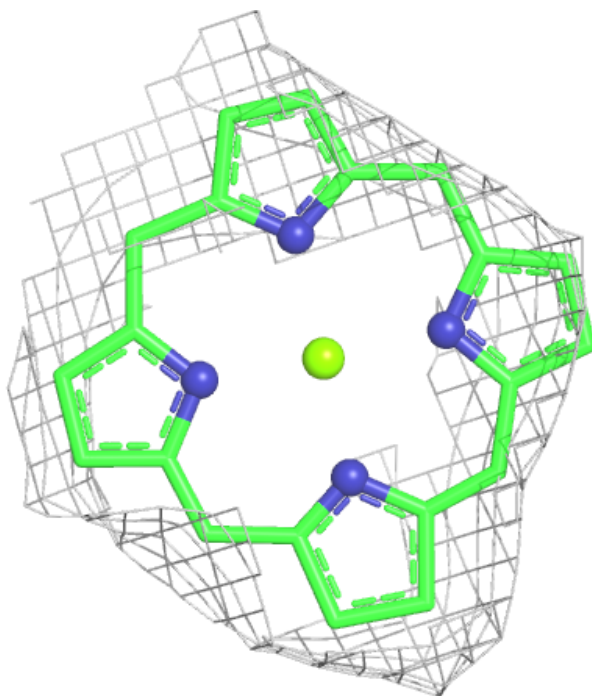
Electron density around CLA A 818:

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



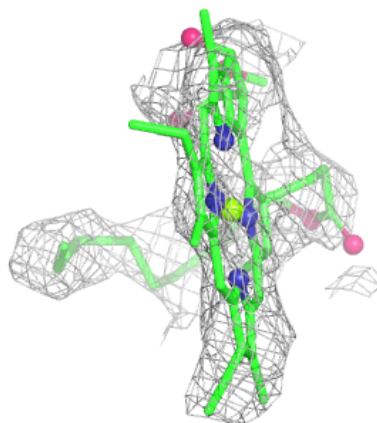
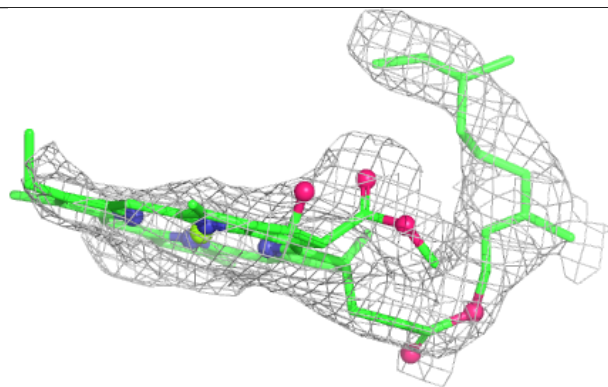
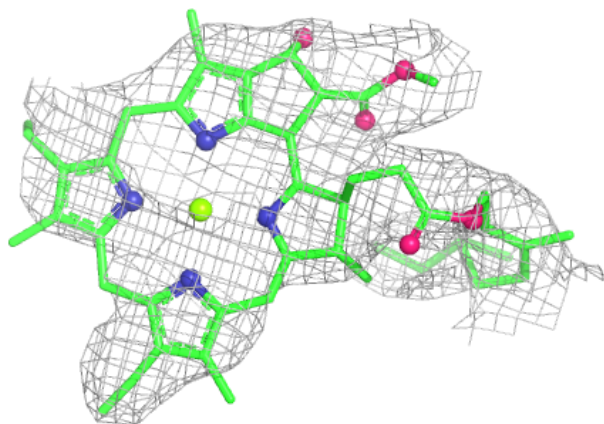
Electron density around CLA 4 311:

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



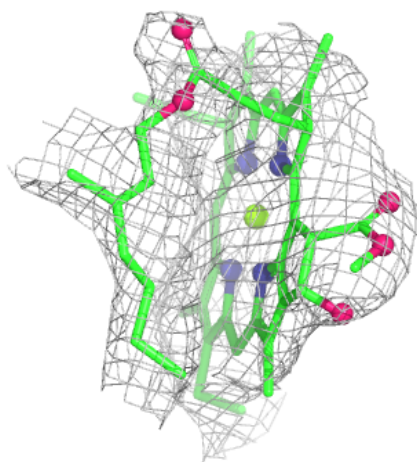
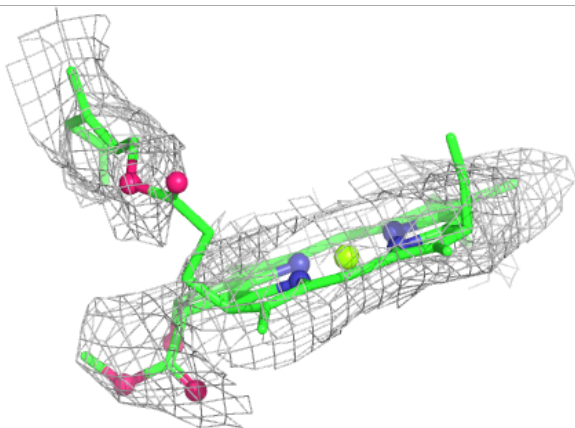
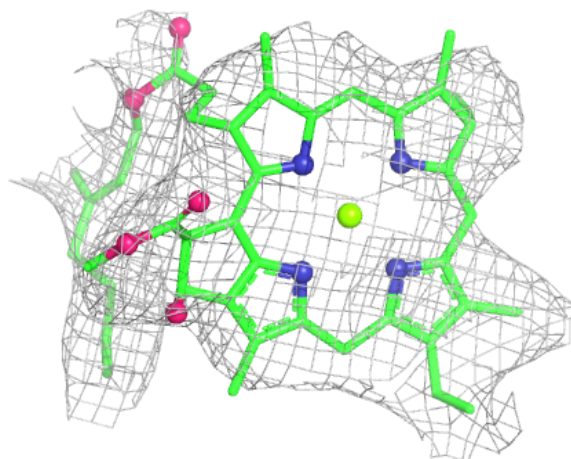
Electron density around CLA A 806:

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



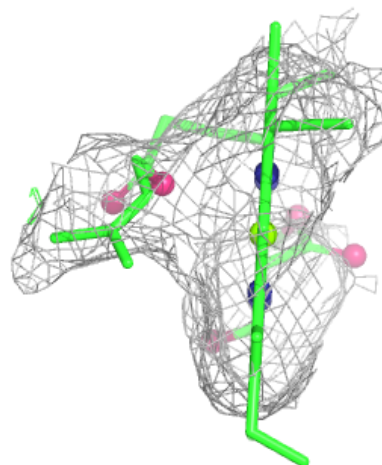
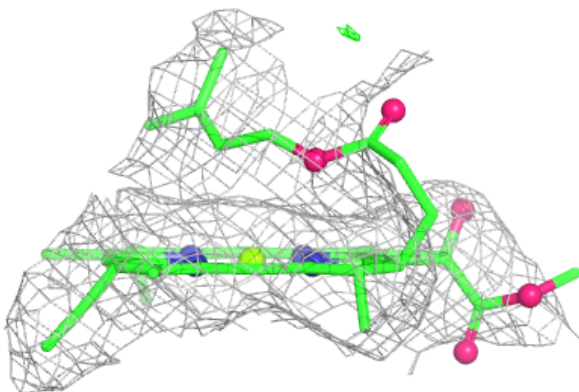
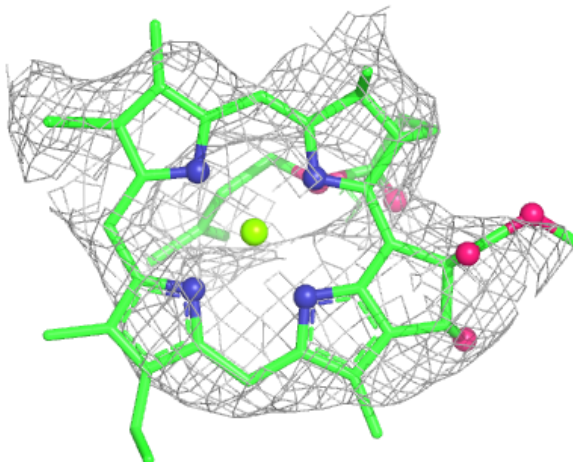
Electron density around CLA F 207:

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



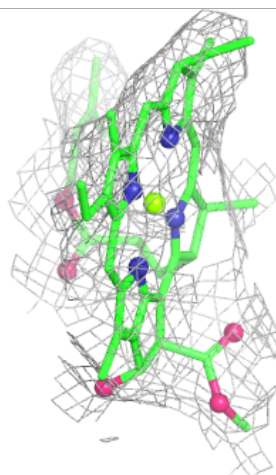
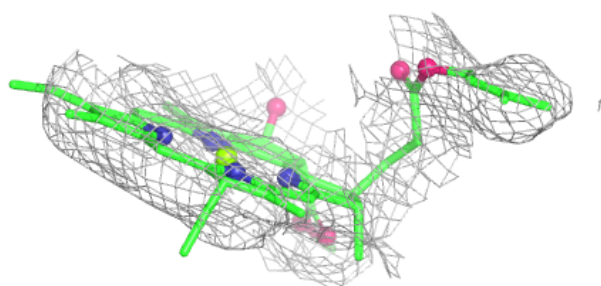
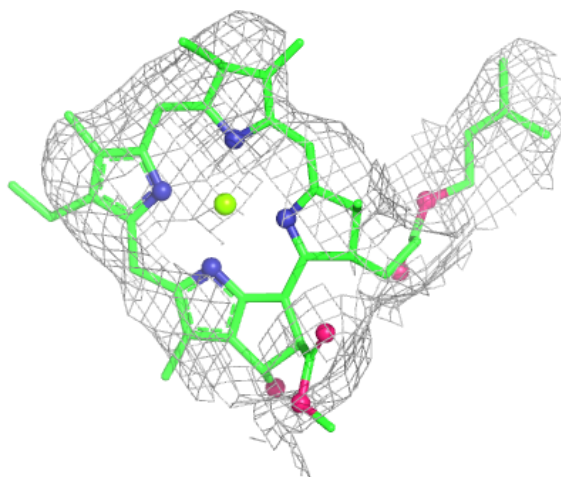
Electron density around CLA B 821:

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



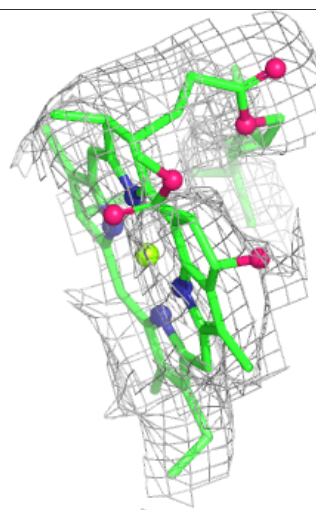
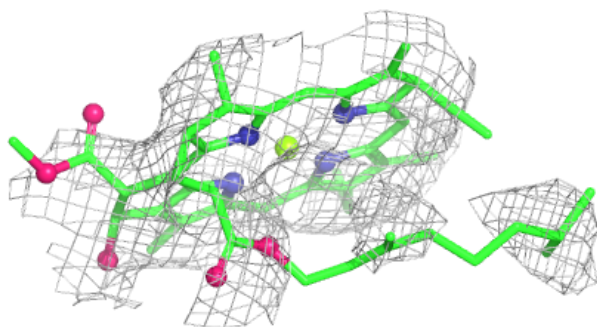
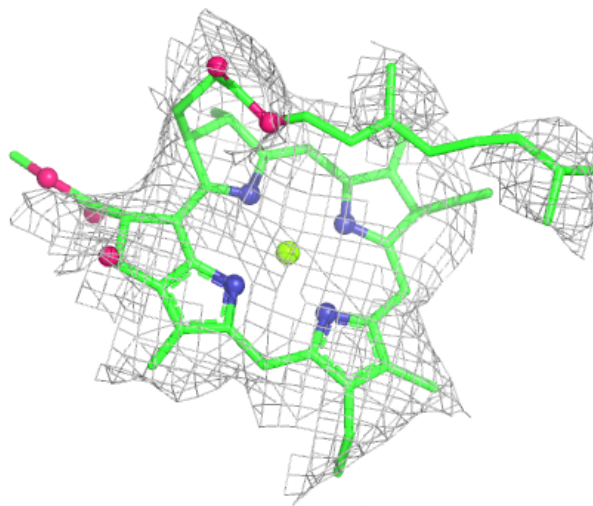
Electron density around CLA A 832:

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



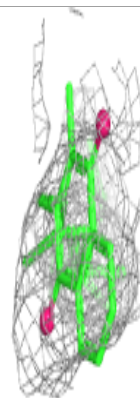
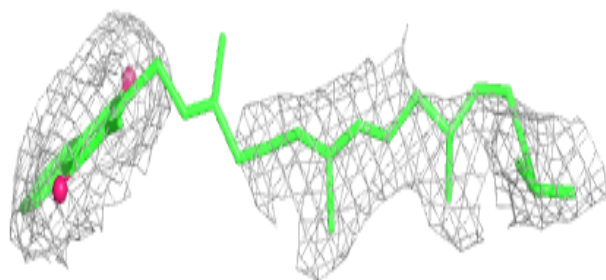
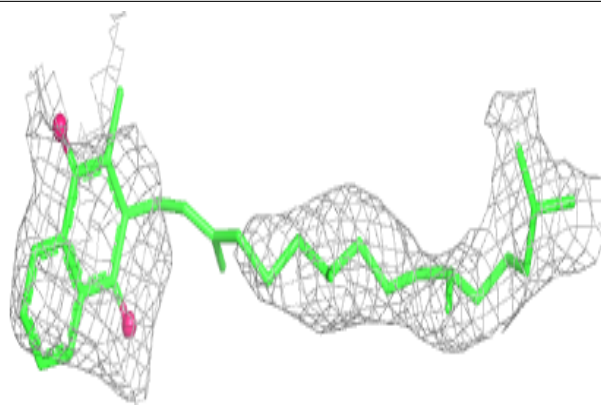
Electron density around CLA B 823:

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



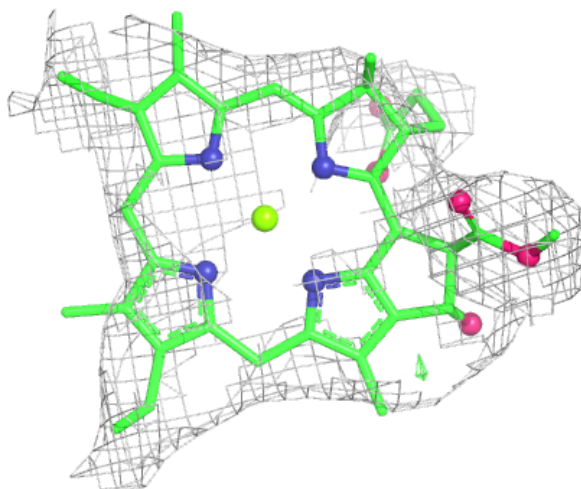
Electron density around PQN A 842:

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



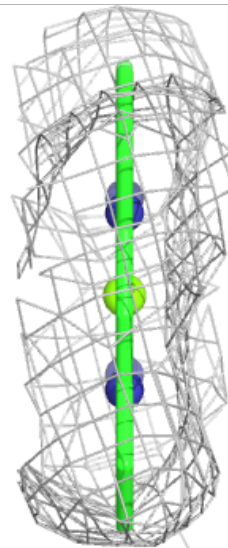
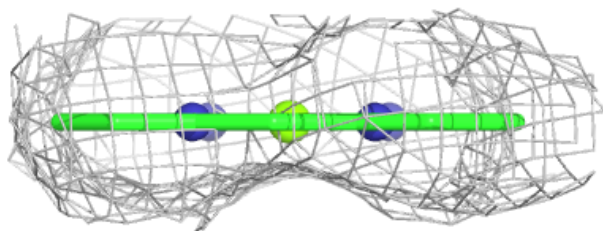
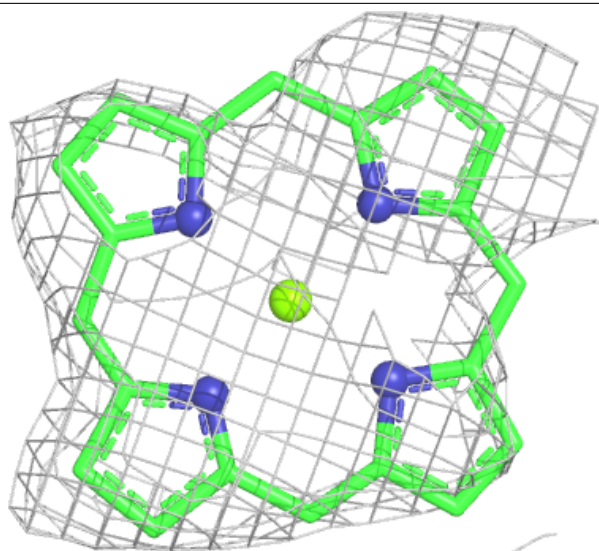
Electron density around CLA B 807:

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



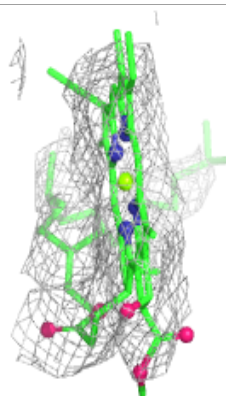
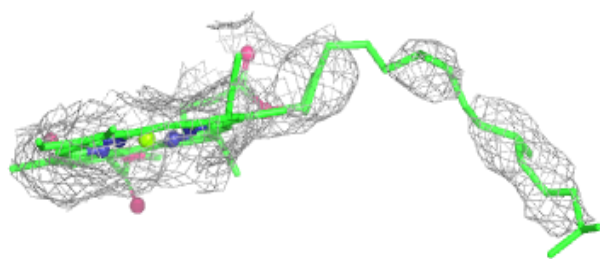
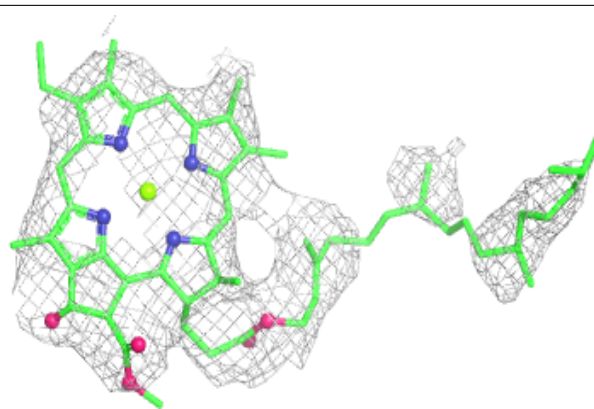
Electron density around CLA 1 209:

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

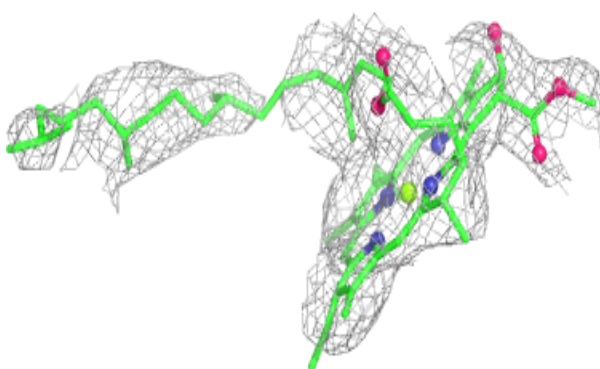
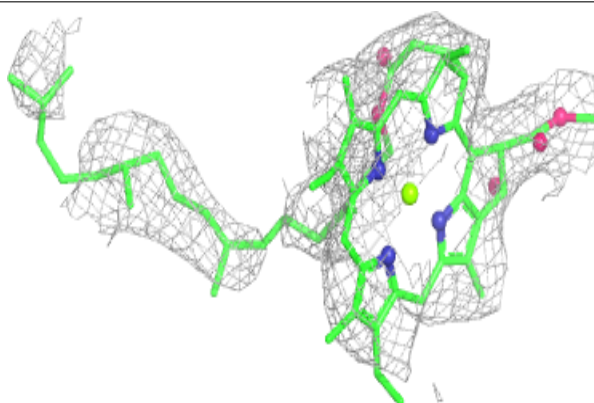


Electron density around CLA B 803:

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

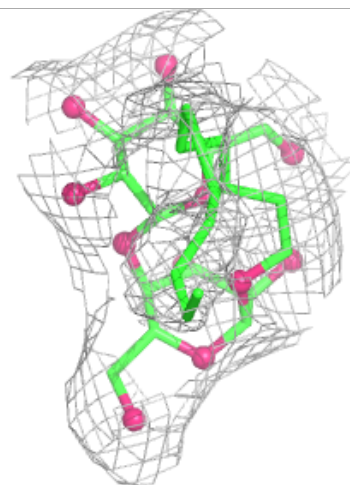
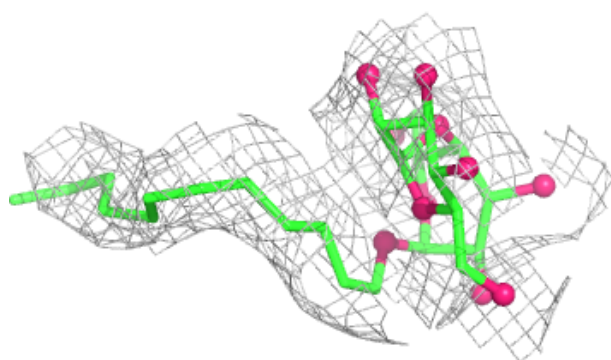
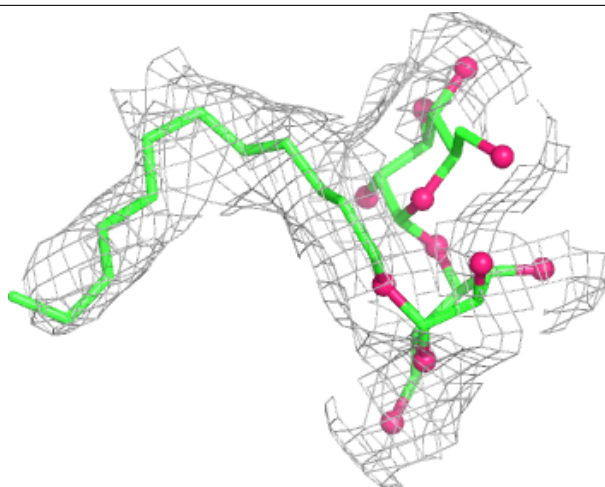
**Electron density around CLA A 838:**

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



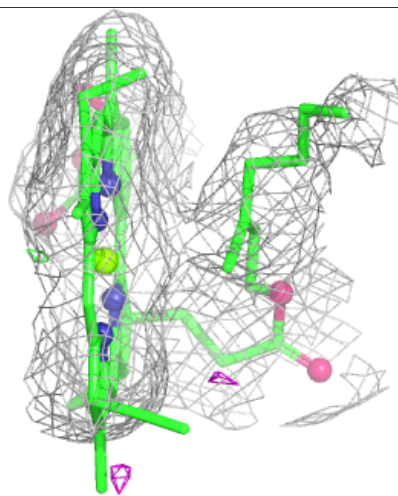
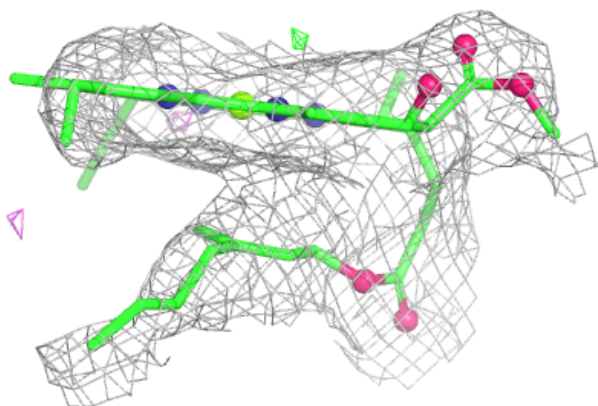
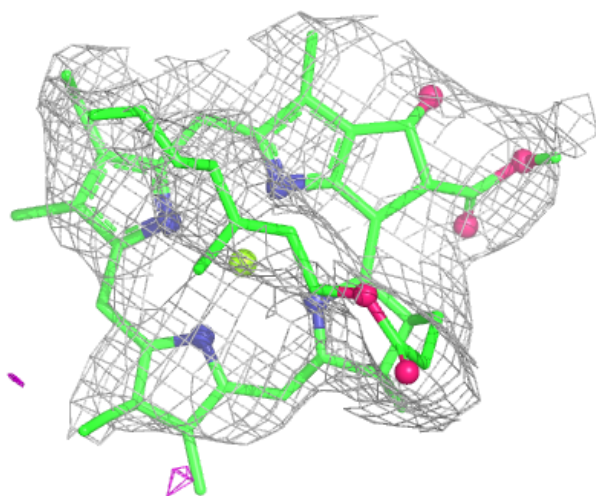
Electron density around LMU H 105:

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



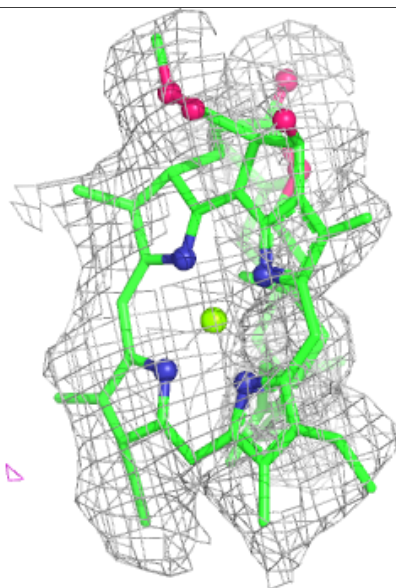
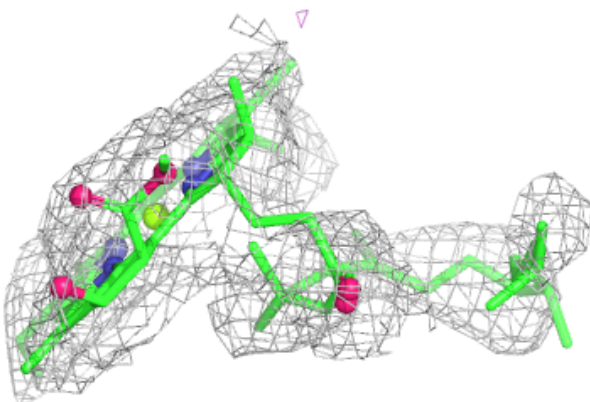
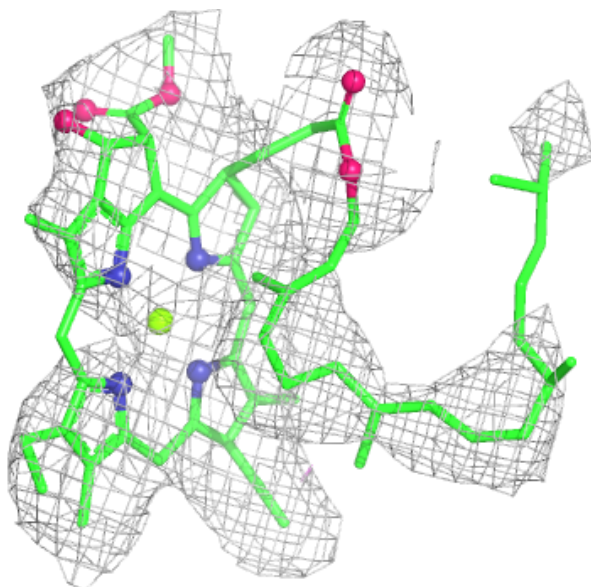
Electron density around CLA B 818:

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



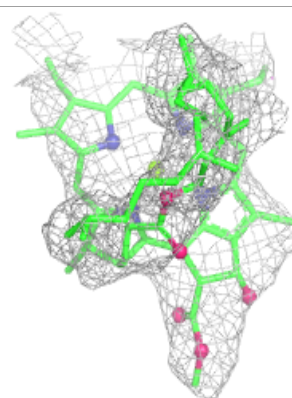
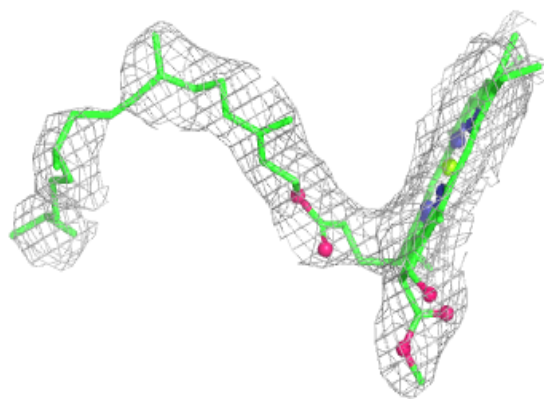
Electron density around CLA B 824:

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



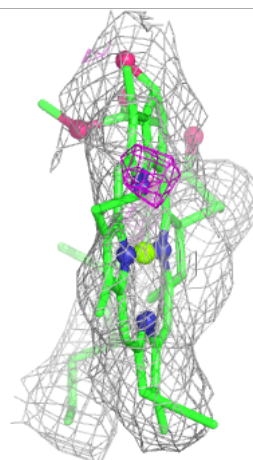
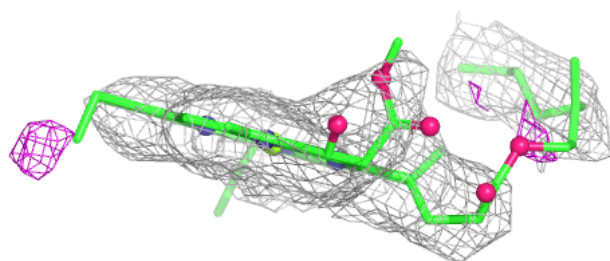
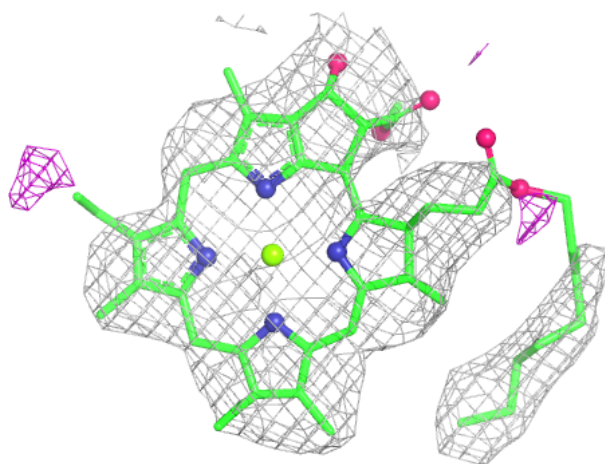
Electron density around CLA B 840:

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



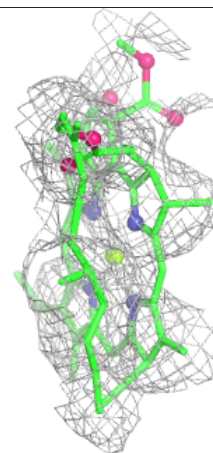
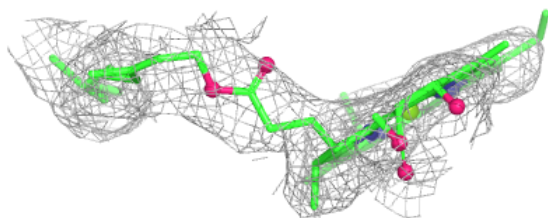
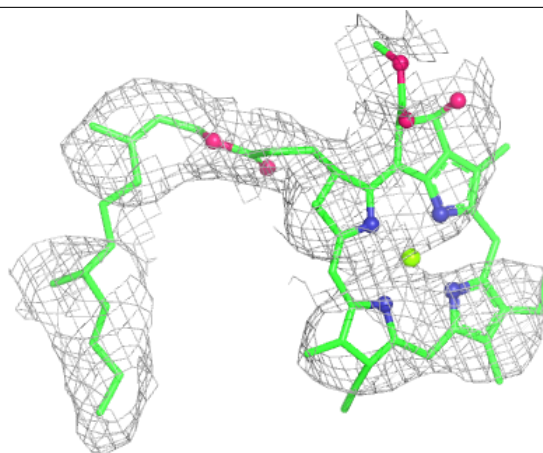
Electron density around CLA B 825:

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

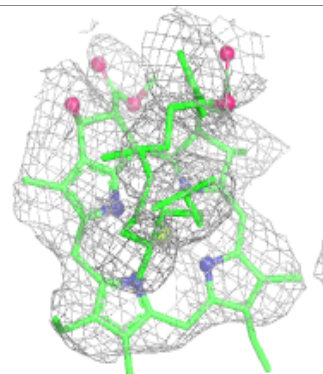
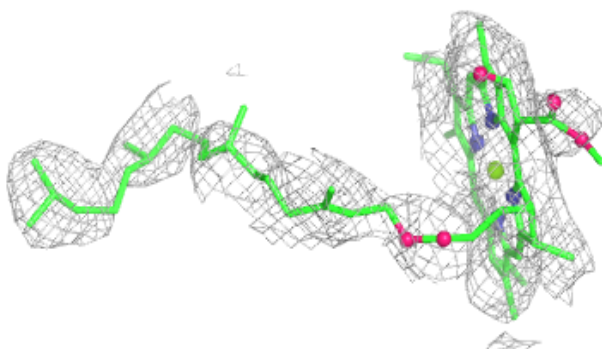
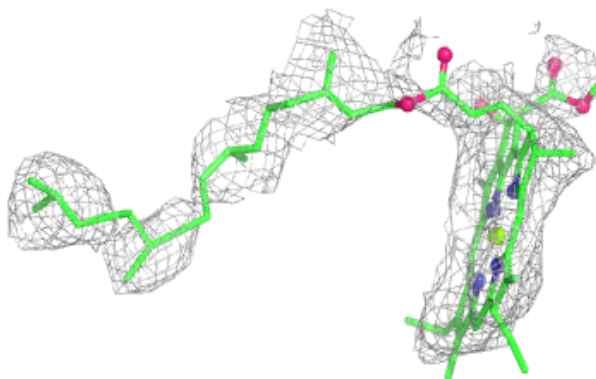


Electron density around CLA B 826:

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

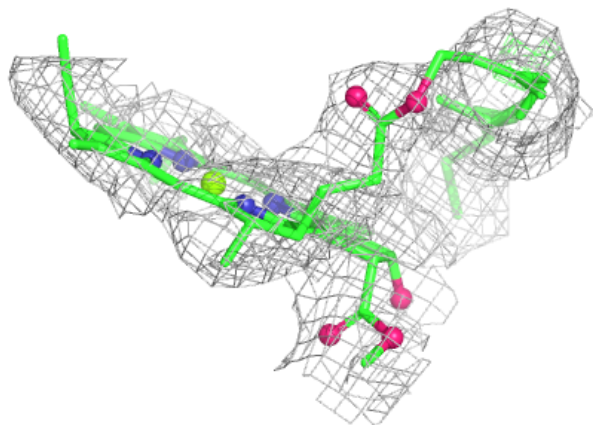
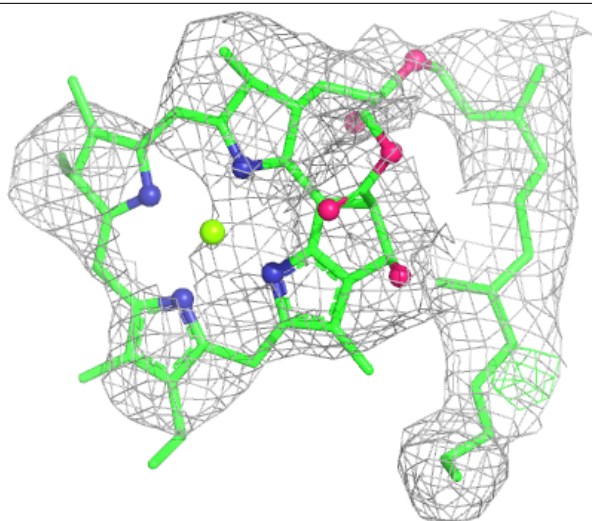
**Electron density around CLA A 828:**

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



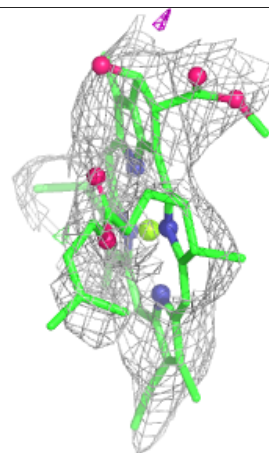
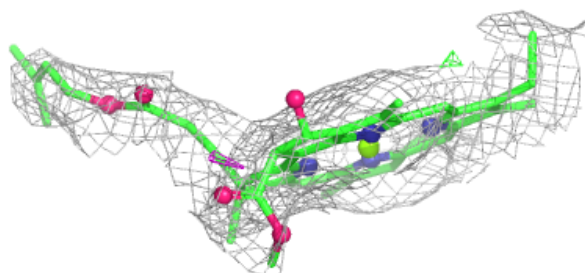
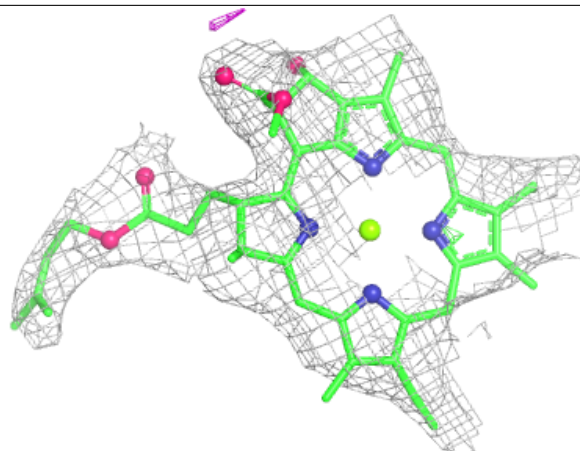
Electron density around CLA B 832:

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

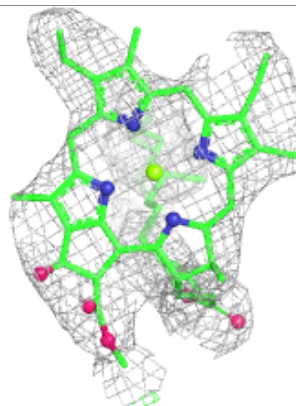
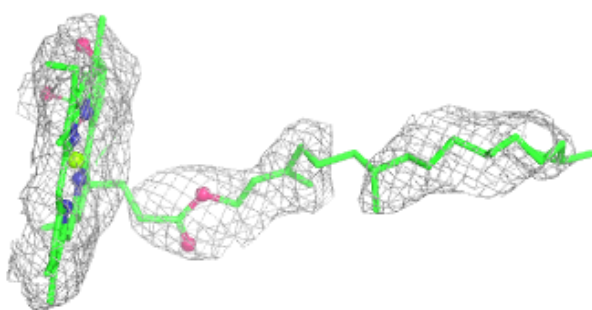


Electron density around CLA B 833:

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

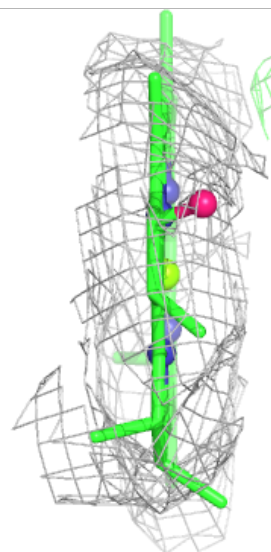
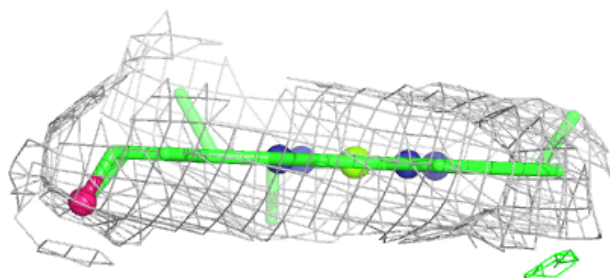
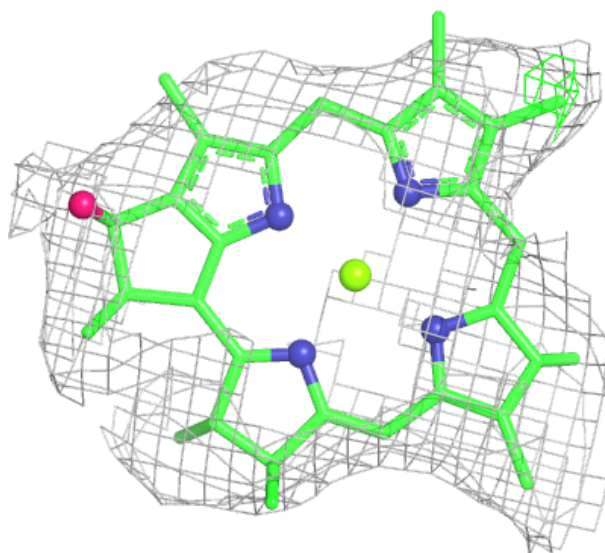
**Electron density around CLA B 841:**

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



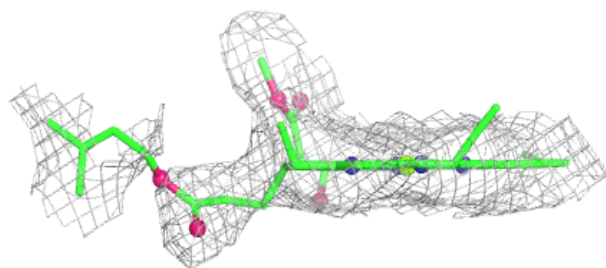
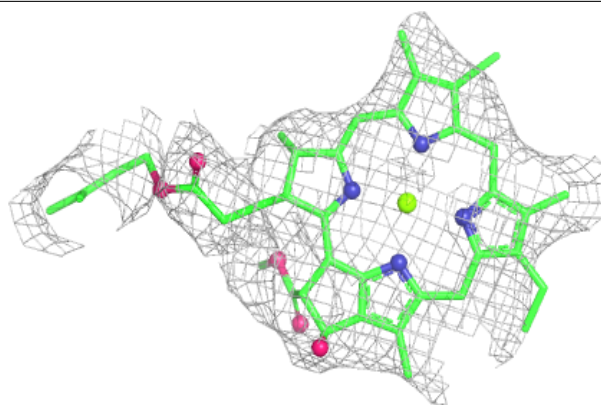
Electron density around CLA 4 313:

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



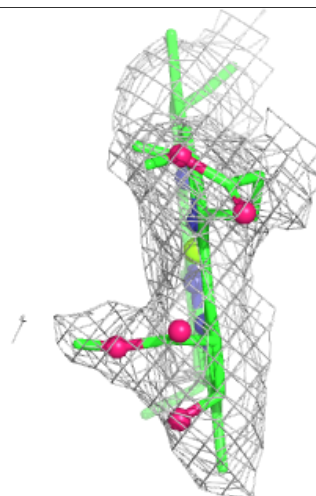
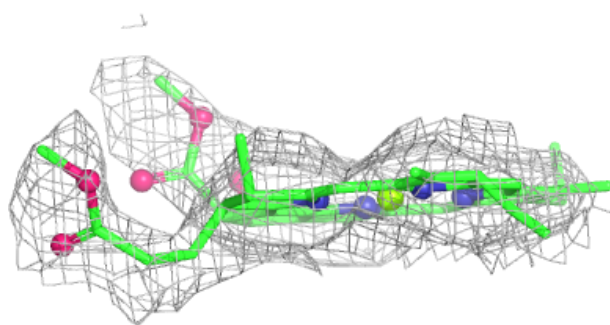
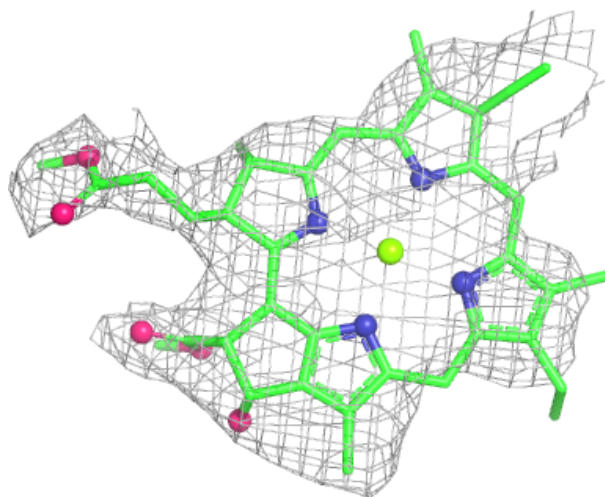
Electron density around CLA F 201:

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



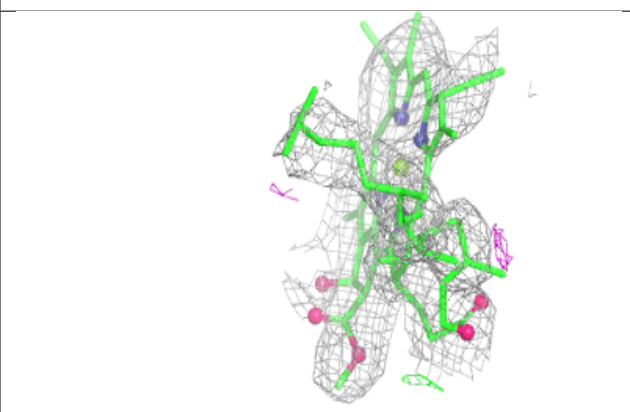
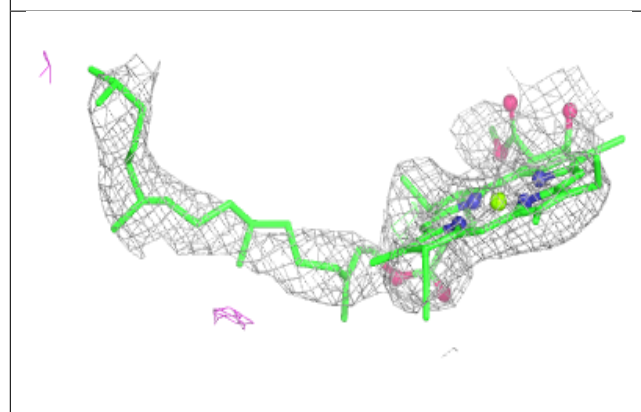
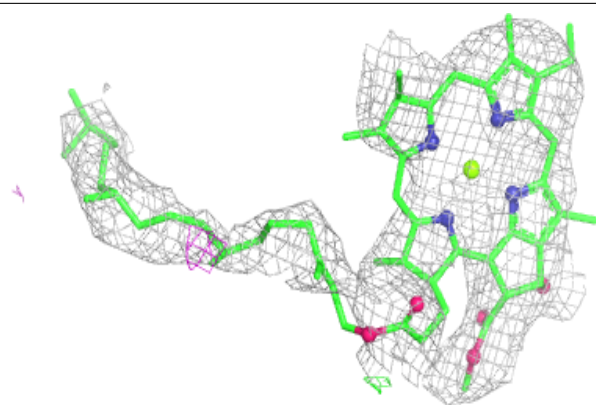
Electron density around CLA A 803:

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

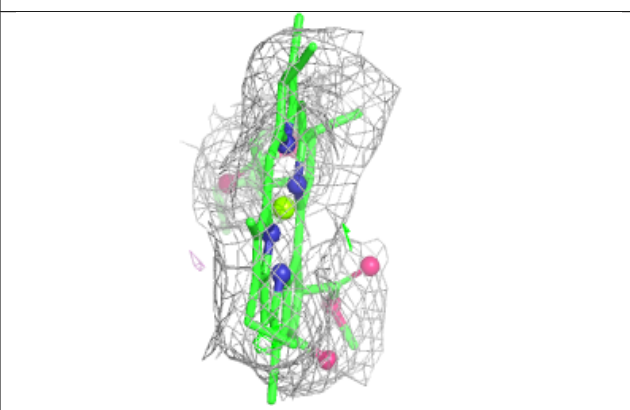
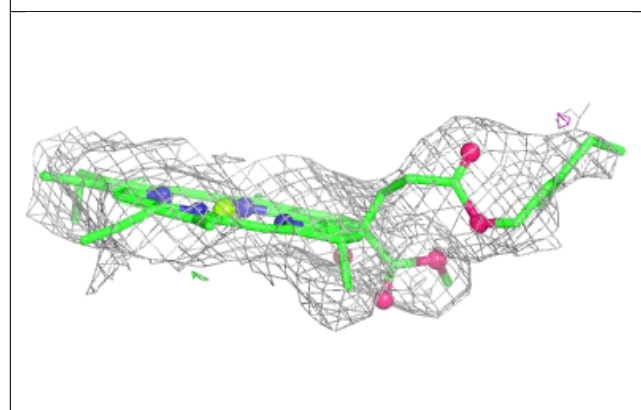
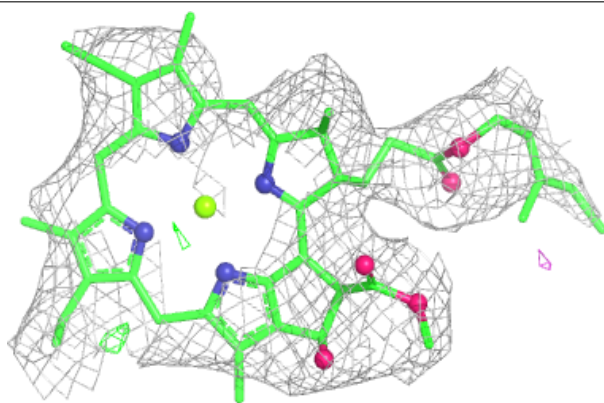


Electron density around CLA A 851:

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

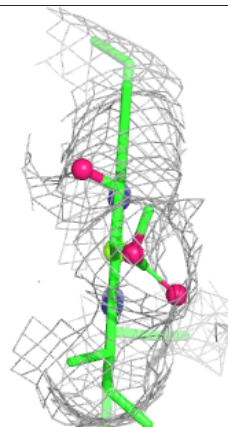
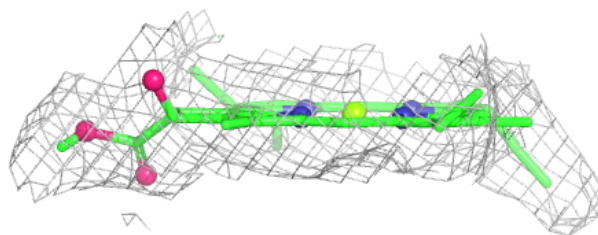
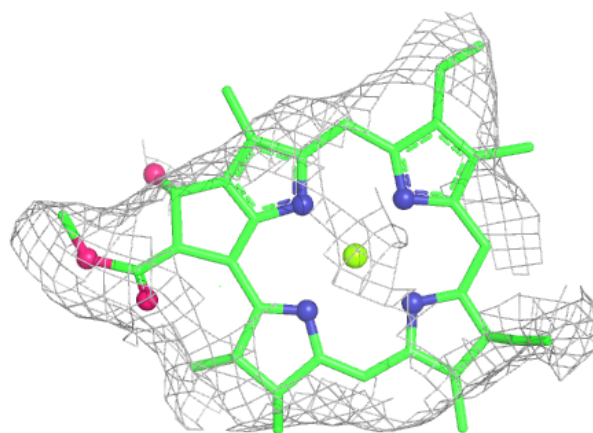
**Electron density around CLA A 837:**

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

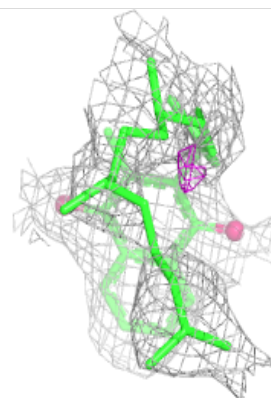
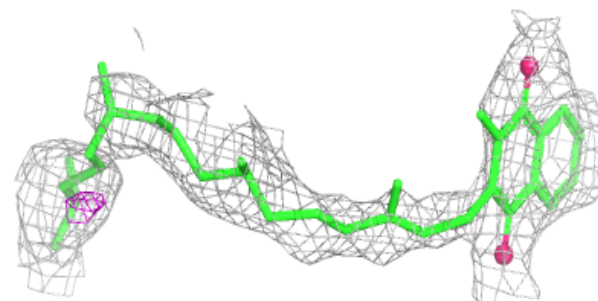
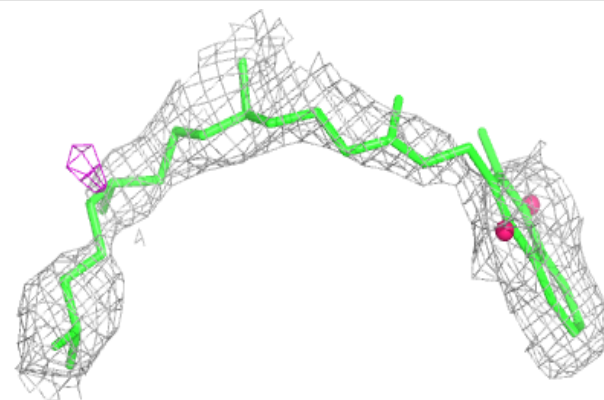


Electron density around CLA 1 202:

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

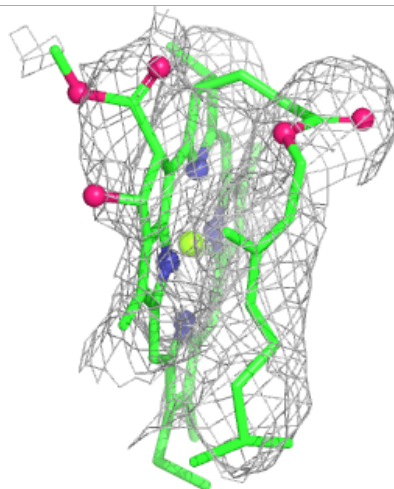
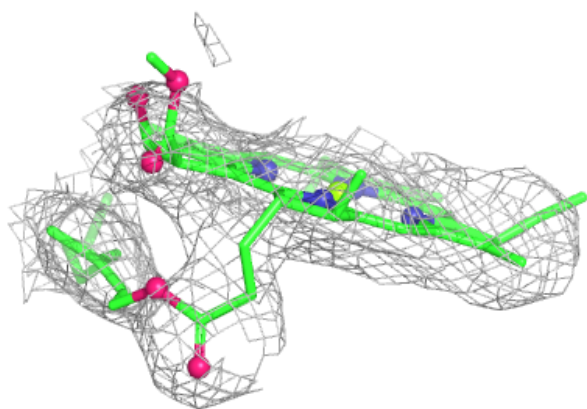
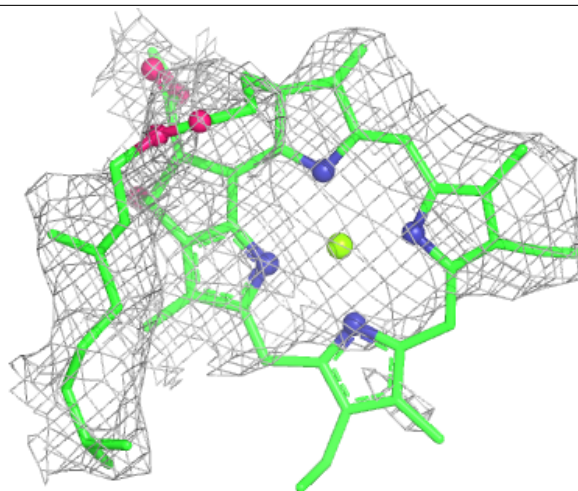
**Electron density around PQN B 843:**

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



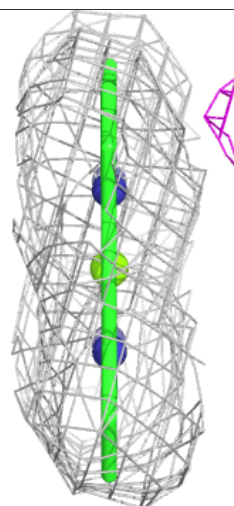
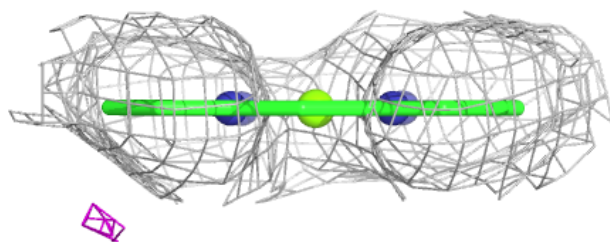
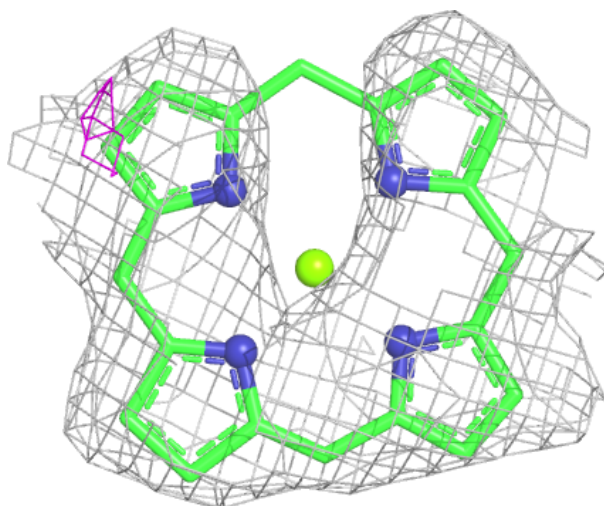
Electron density around CLA A 827:

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



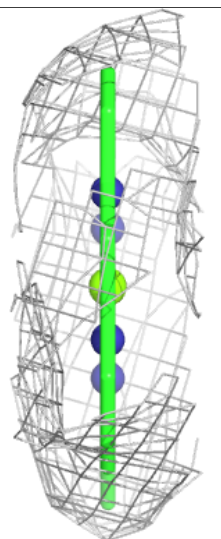
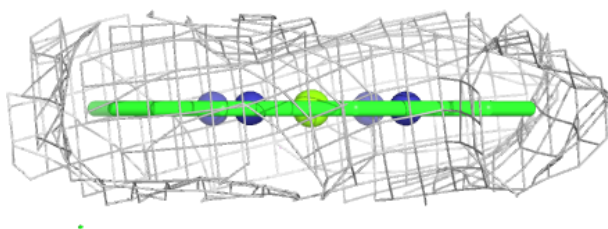
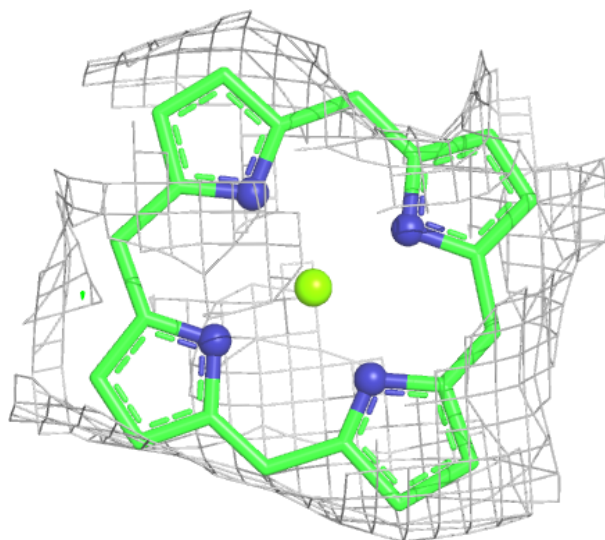
Electron density around CLA B 811:

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



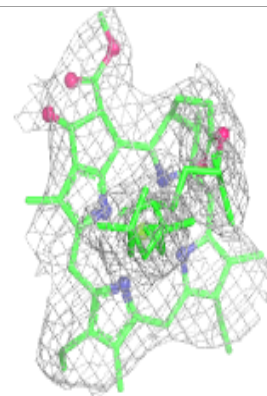
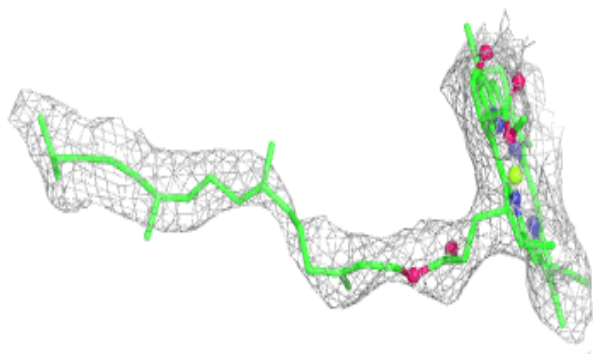
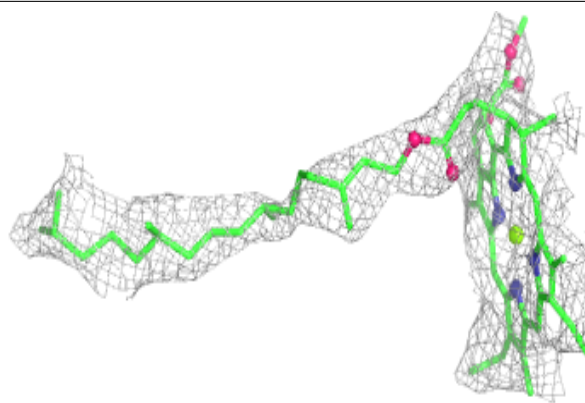
Electron density around CLA 2 308:

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



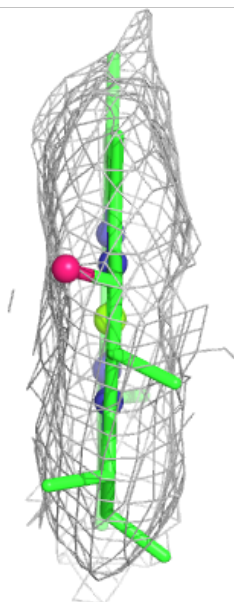
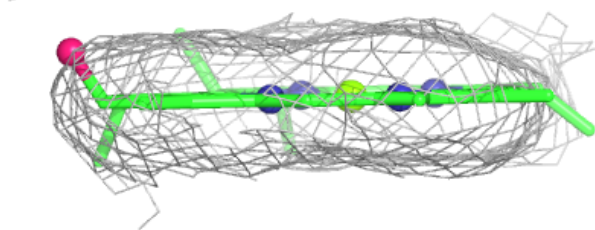
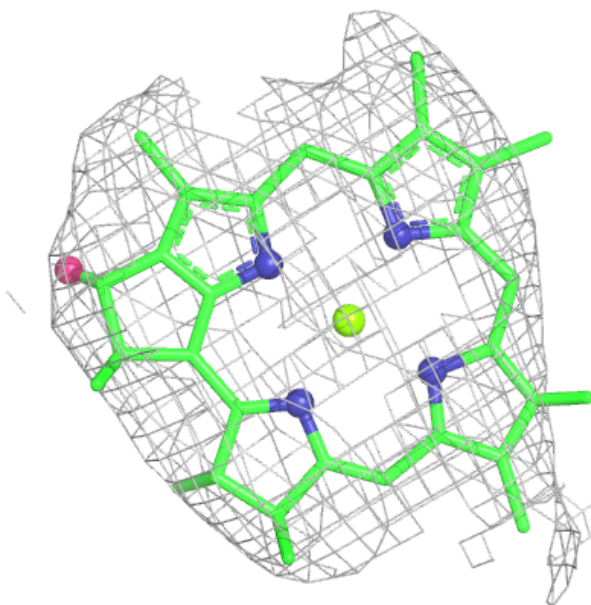
Electron density around CLA B 829:

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



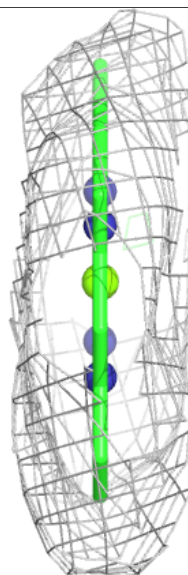
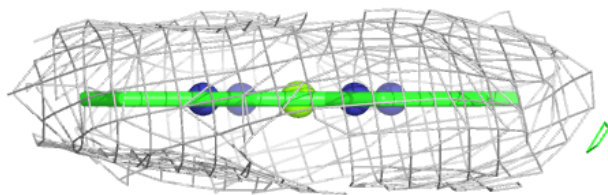
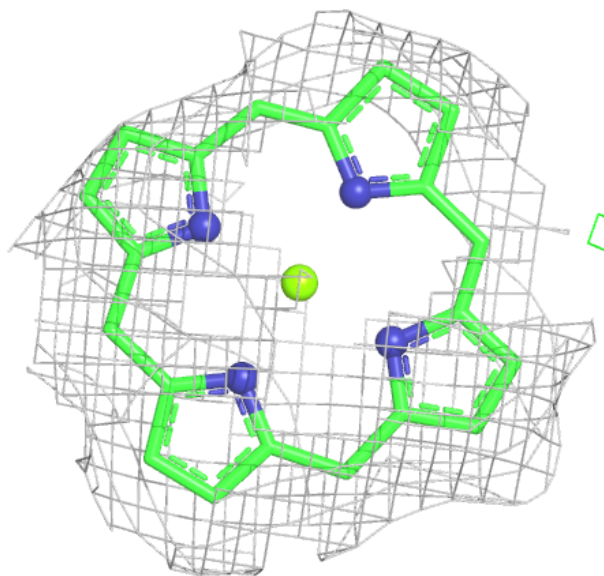
Electron density around CLA F 205:

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



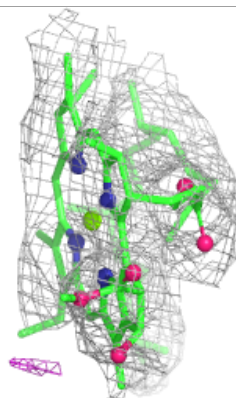
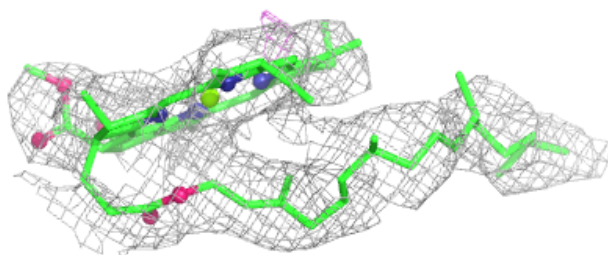
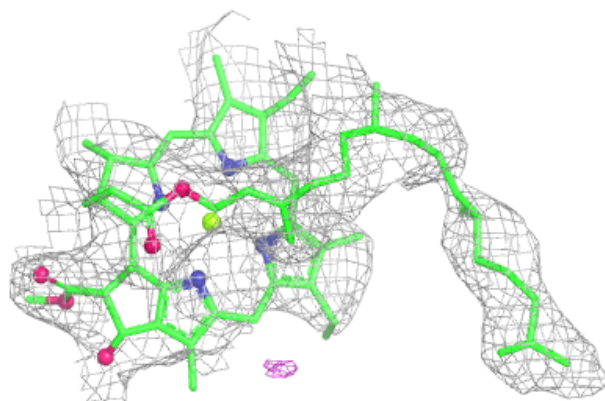
Electron density around CLA 4 312:

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

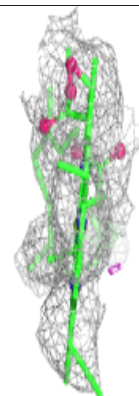
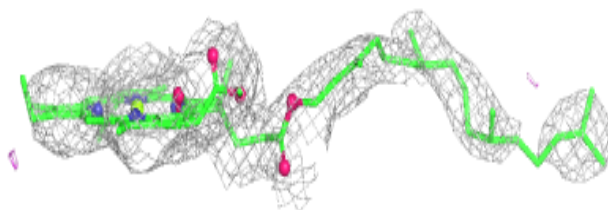
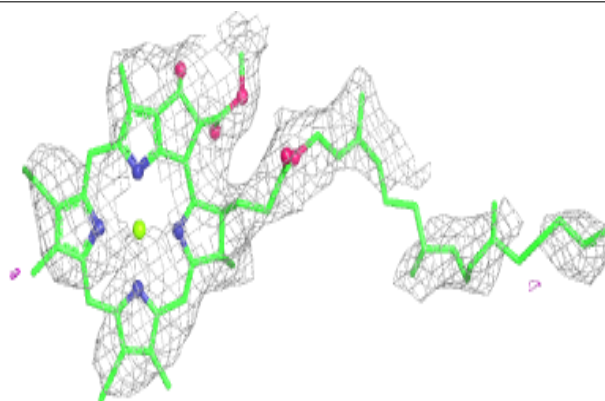


Electron density around CLA B 838:

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

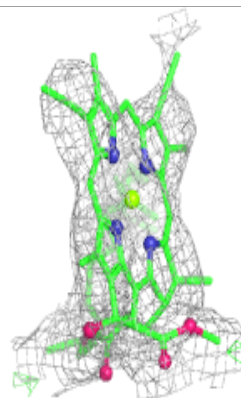
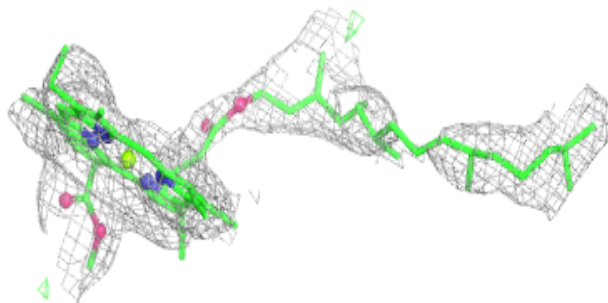
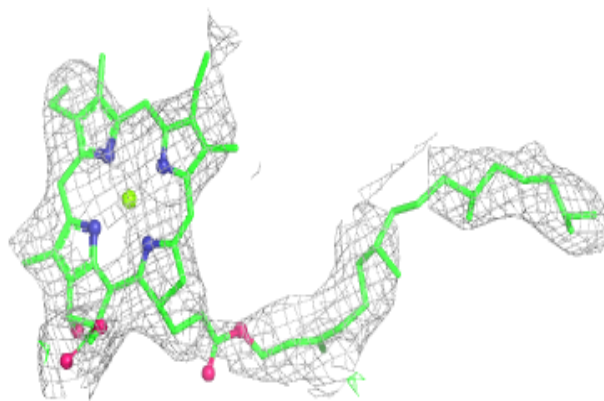
**Electron density around CLA A 830:**

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

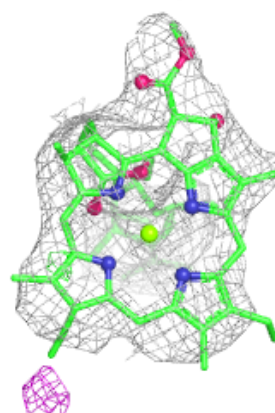
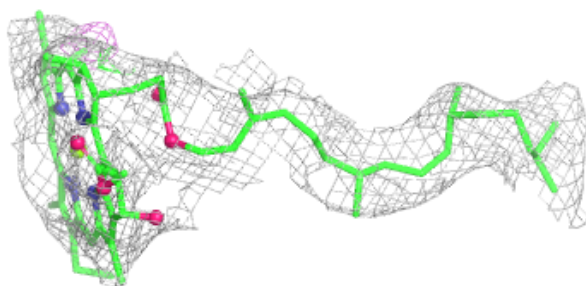
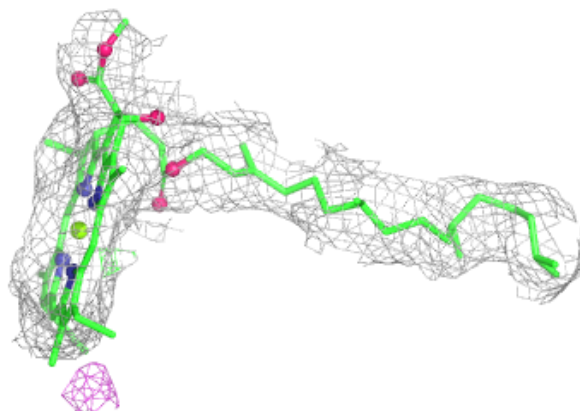


Electron density around CLA A 831:

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

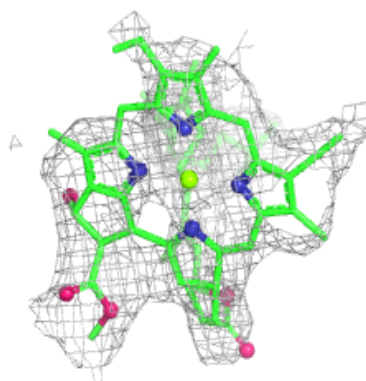
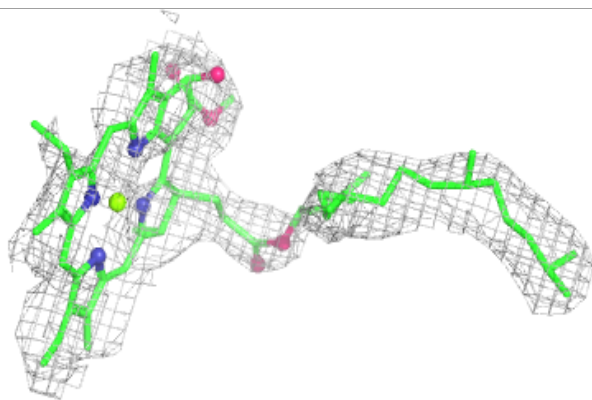
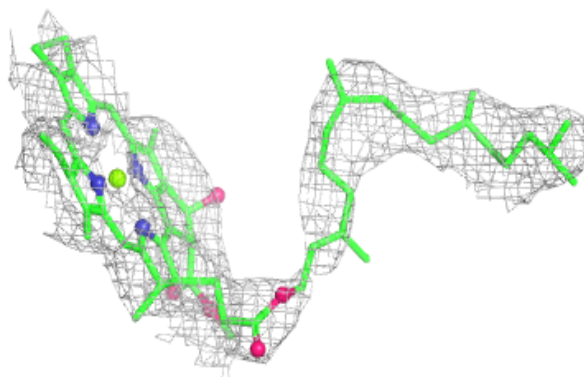
**Electron density around CLA A 826:**

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

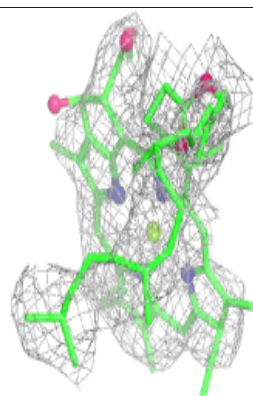
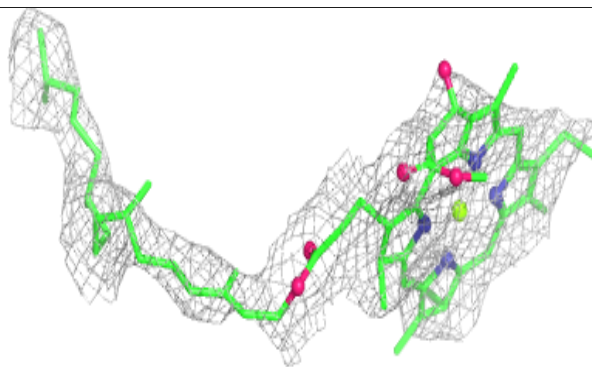
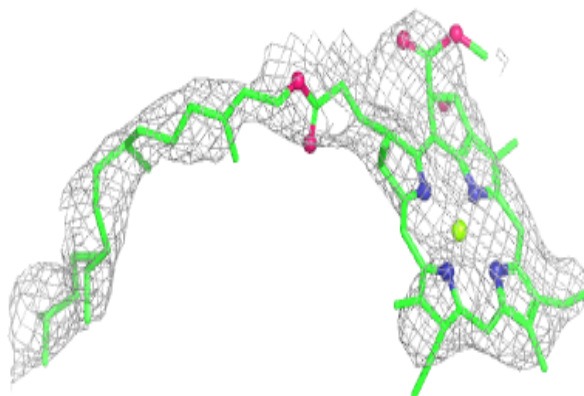


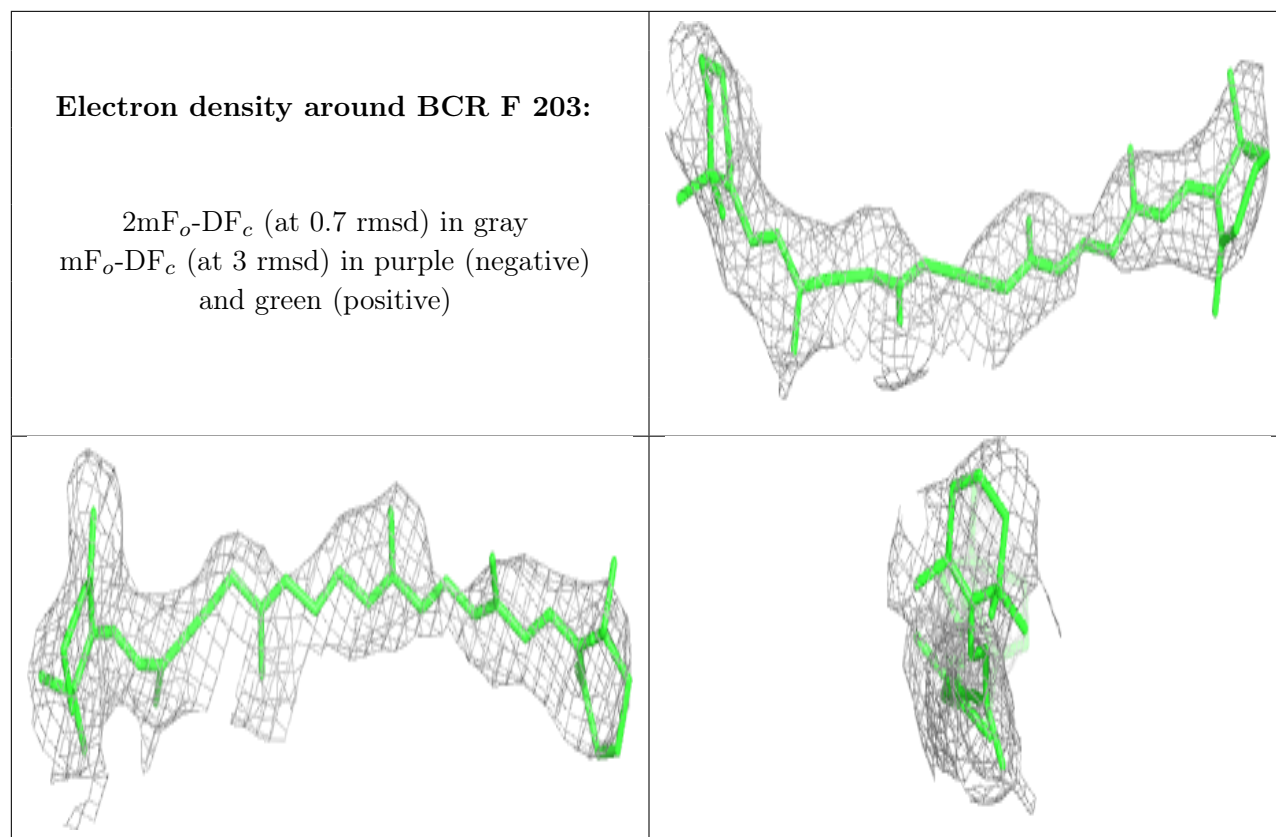
Electron density around CLA B 850:

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

**Electron density around CLA A 850:**

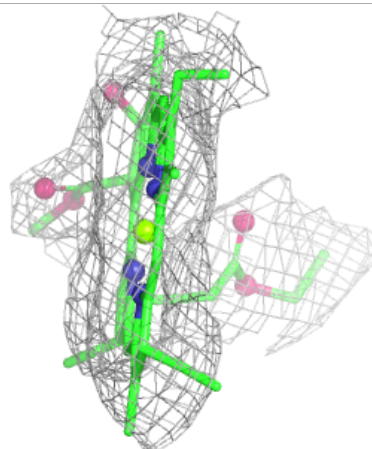
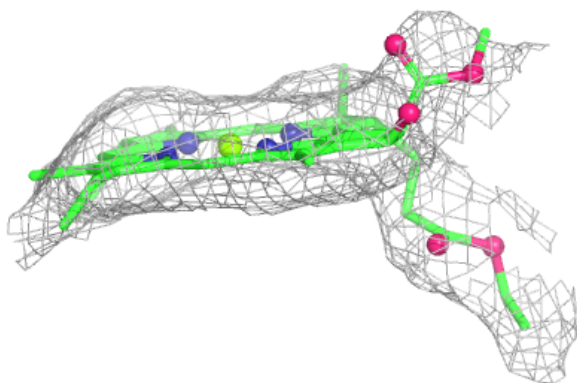
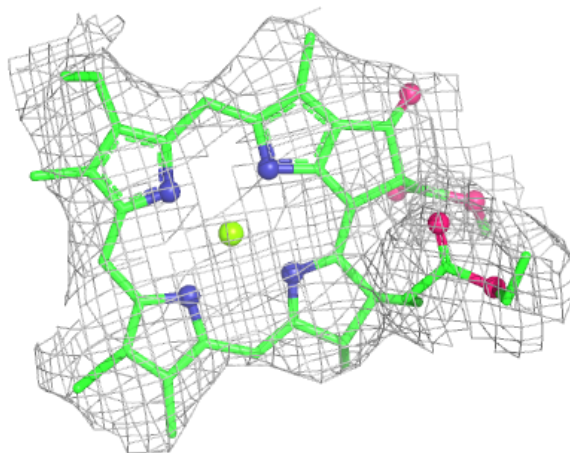
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





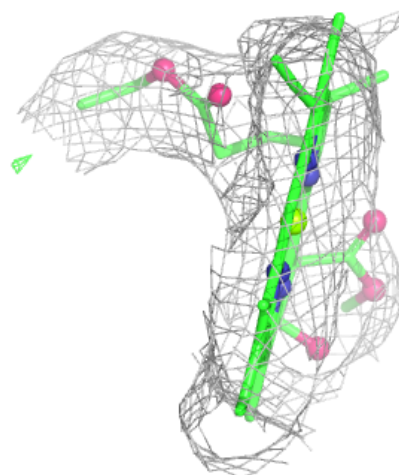
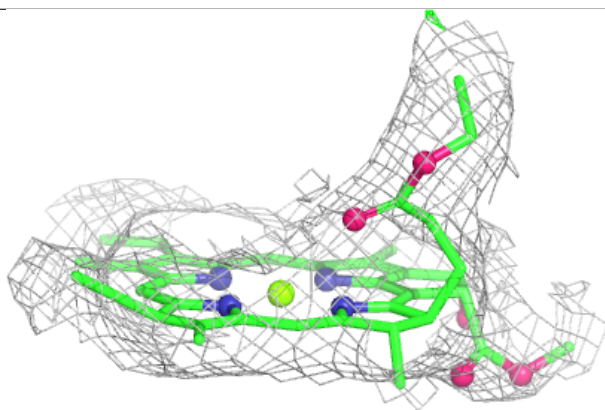
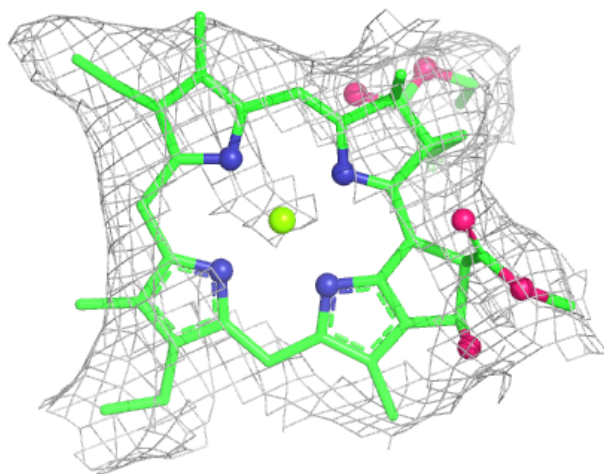
Electron density around CLA A 836:

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



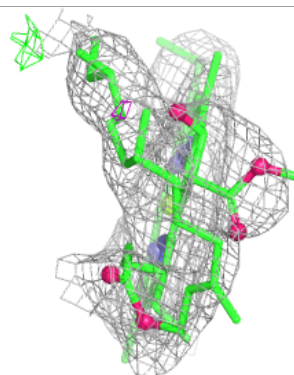
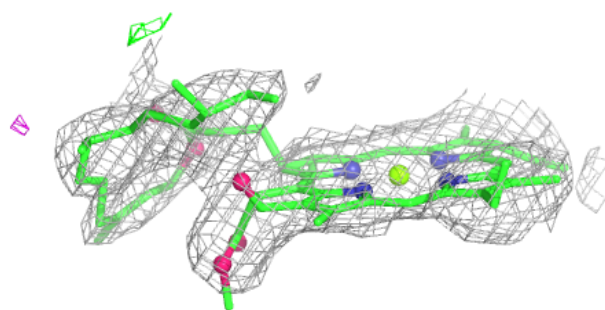
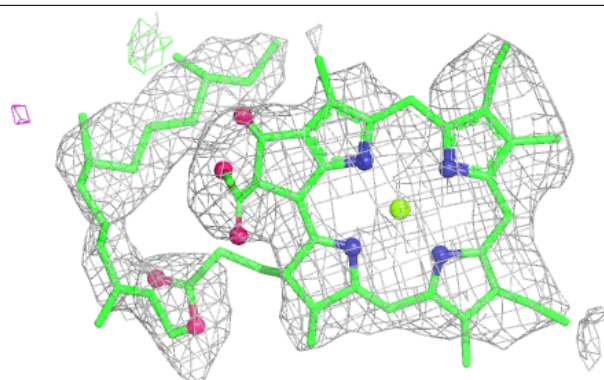
Electron density around CLA B 839:

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



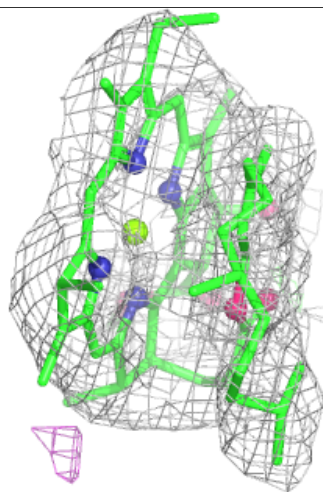
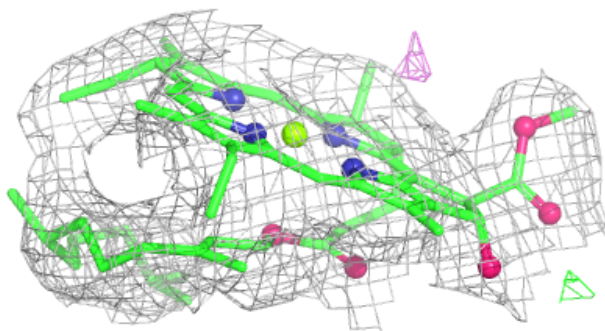
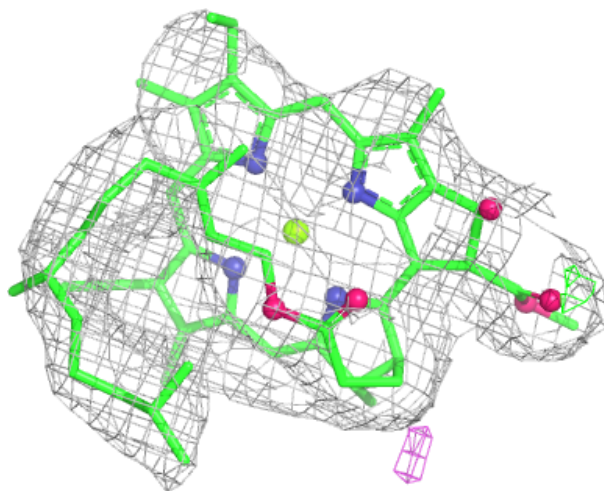
Electron density around CLA B 808:

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



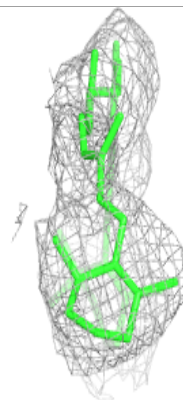
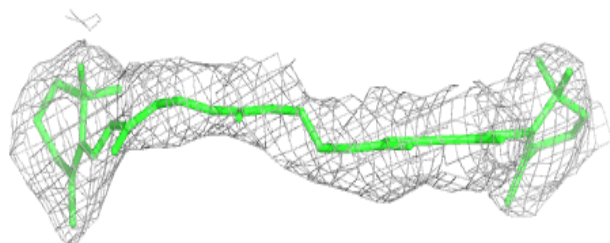
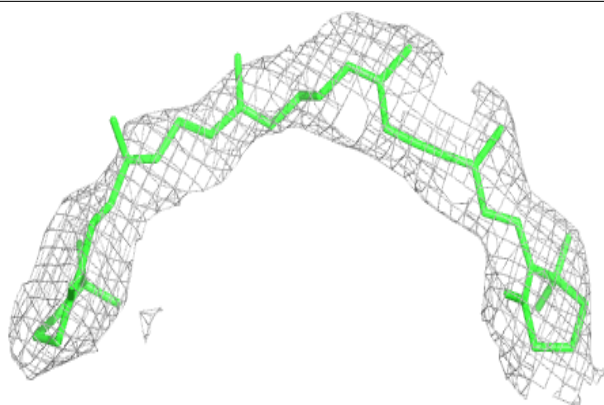
Electron density around CLA B 810:

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



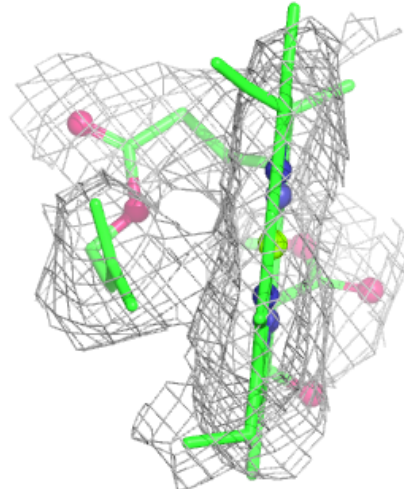
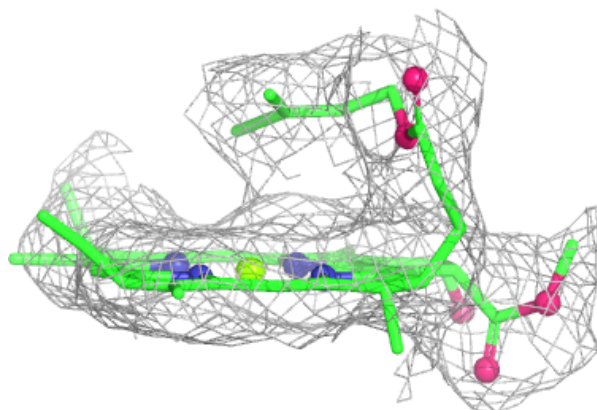
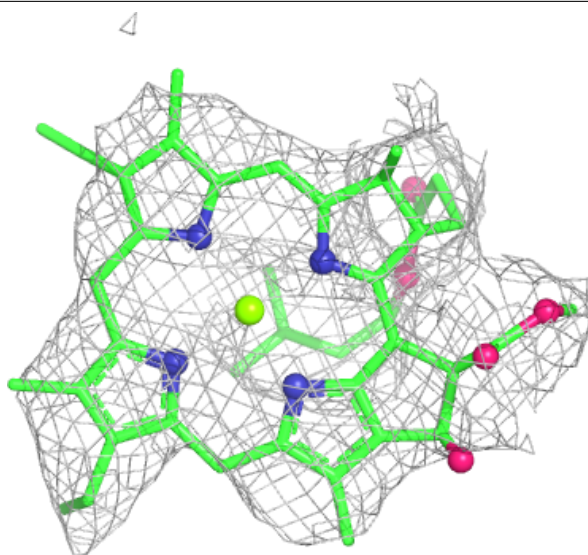
Electron density around BCR F 204:

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



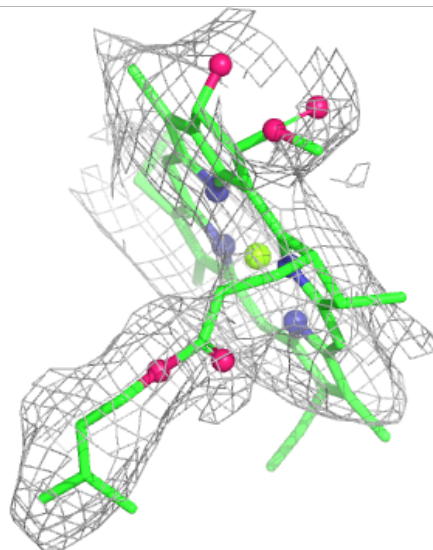
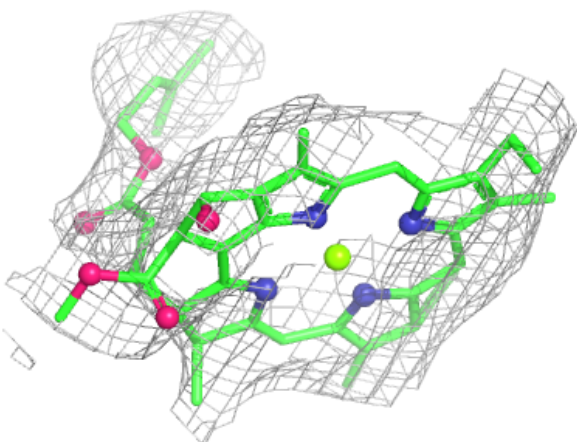
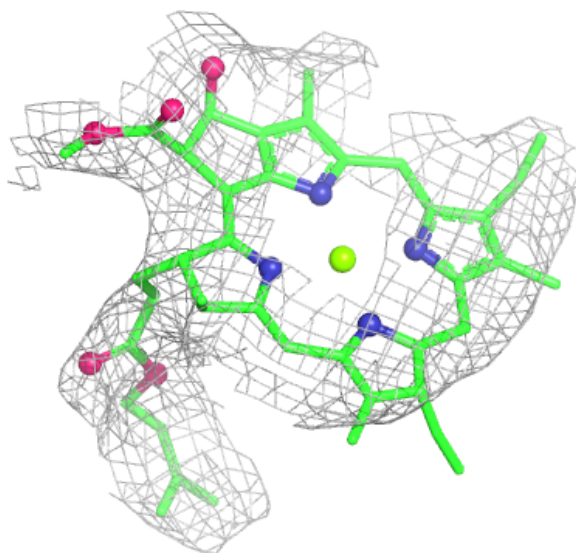
Electron density around CLA B 831:

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



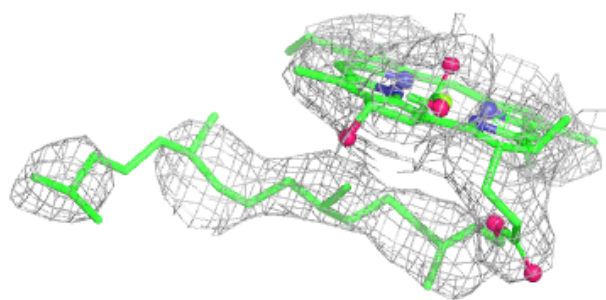
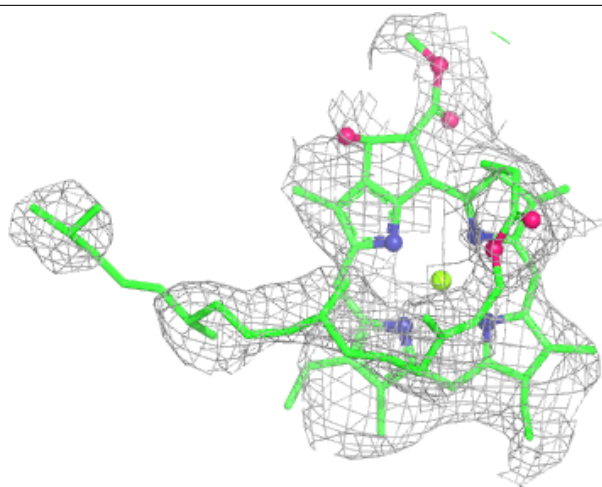
Electron density around CLA A 822:

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



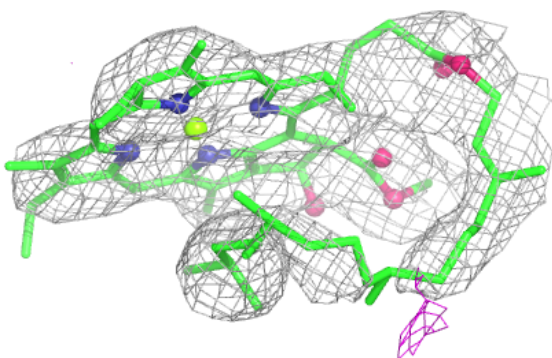
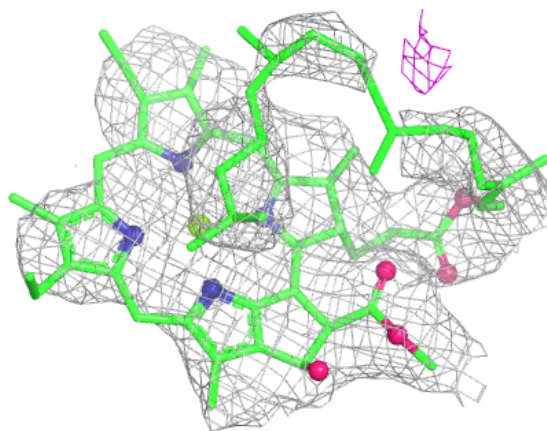
Electron density around CLA B 828:

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

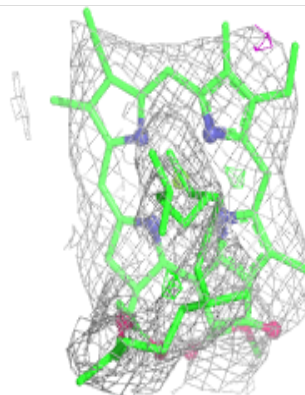
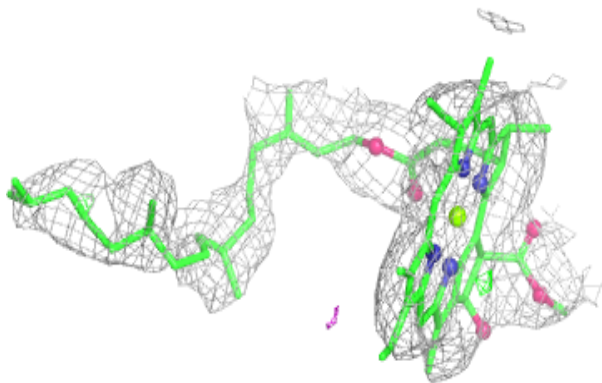
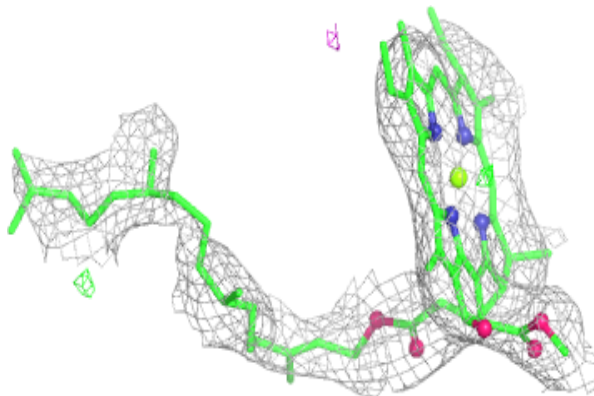


Electron density around CLA B 809:

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

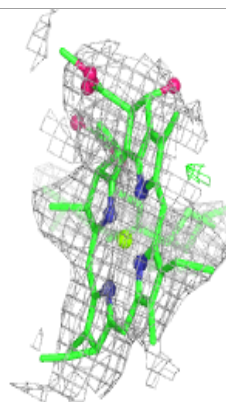
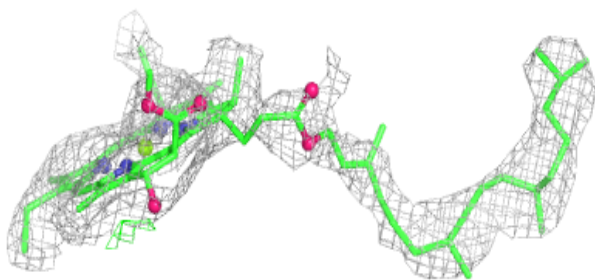
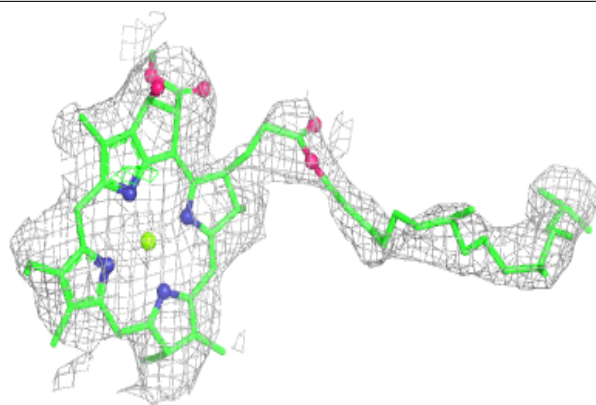
**Electron density around CLA B 830:**

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

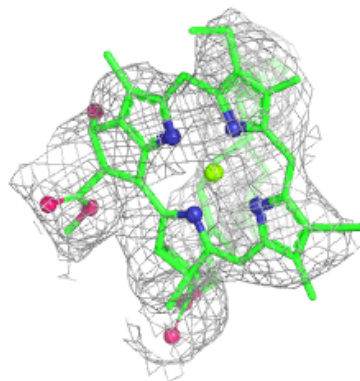
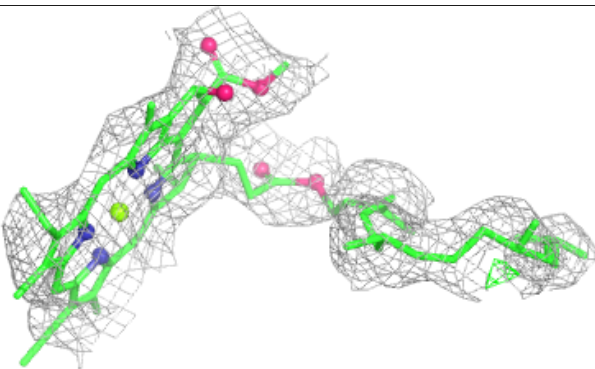
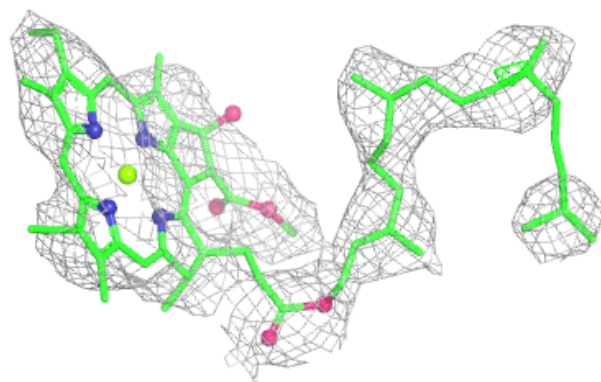


Electron density around CLA B 814:

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

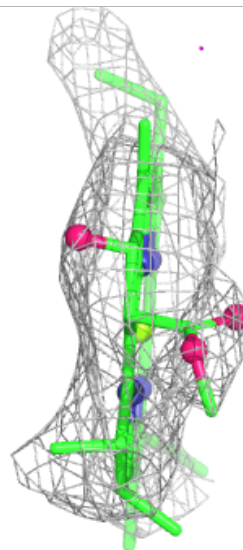
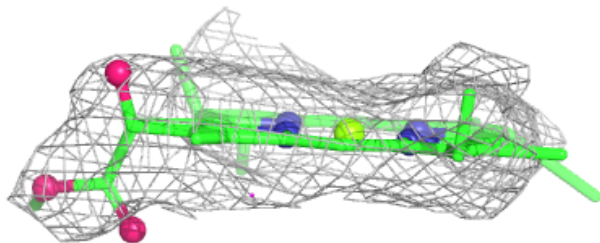
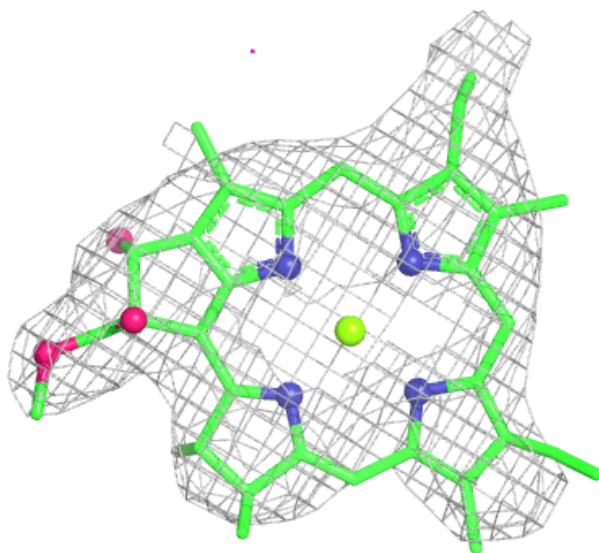
**Electron density around CLA A 849:**

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



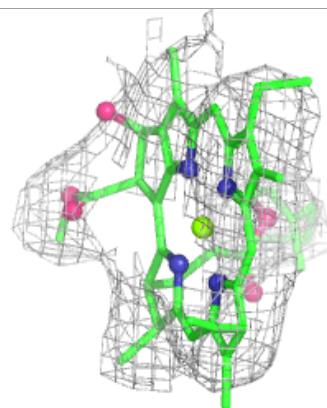
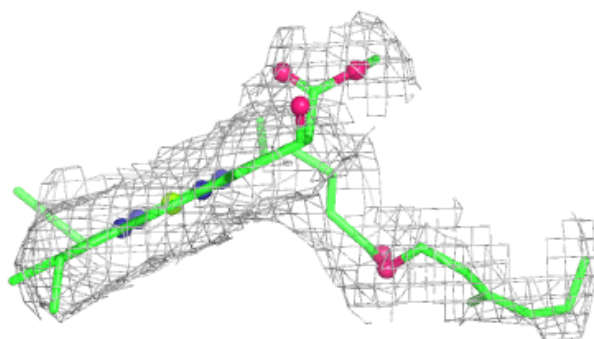
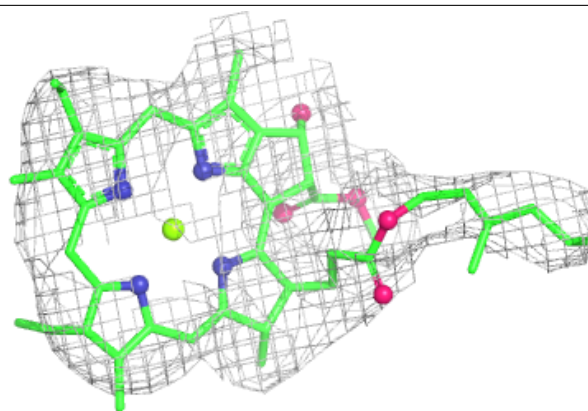
Electron density around CLA B 819:

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

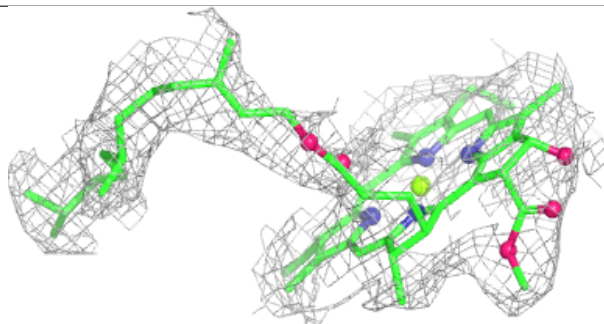
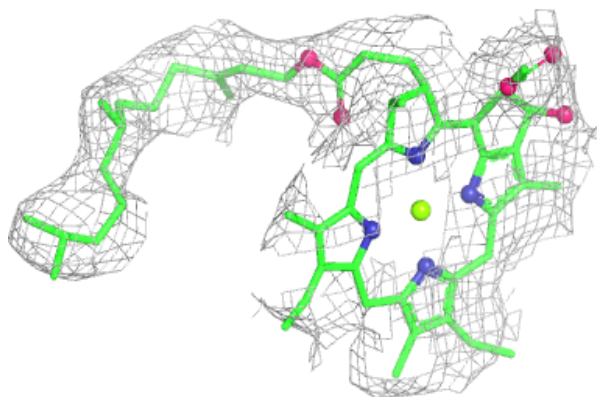


Electron density around CLA A 809:

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

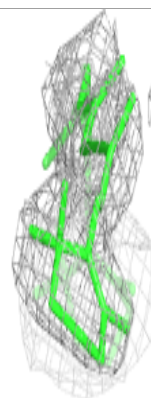
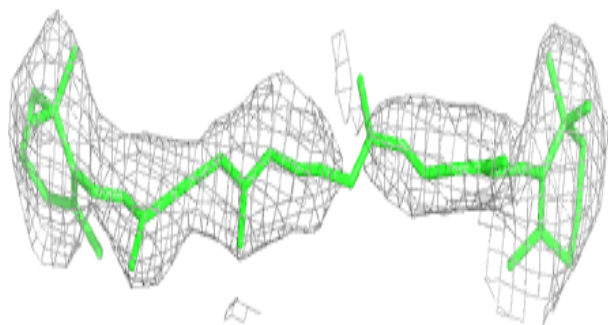
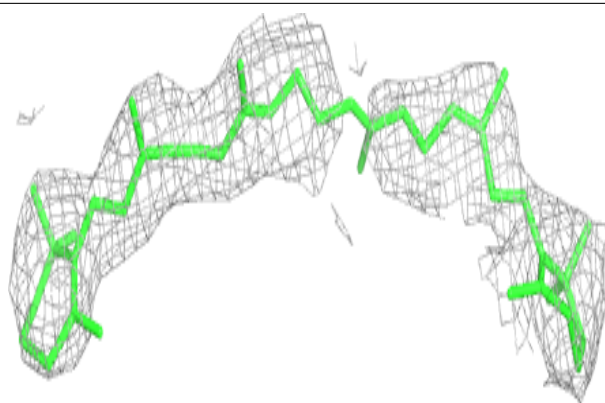
**Electron density around CLA A 808:**

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

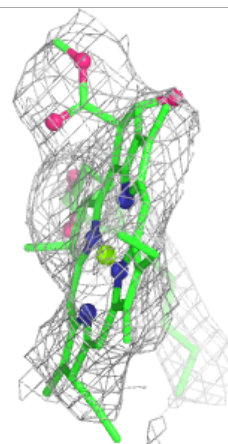
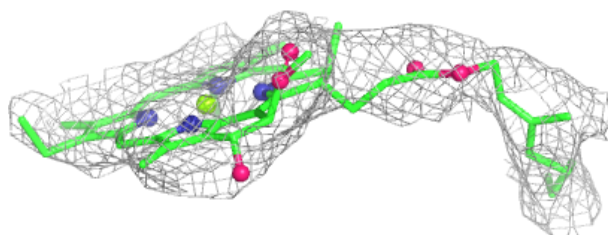
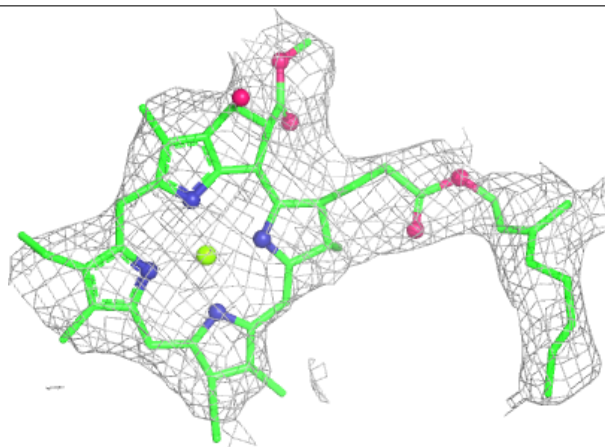


Electron density around BCR B 801:

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

**Electron density around CLA 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)



6.5 Other polymers [i](#)

There are no such residues in this entry.