



wwPDB X-ray Structure Validation Summary Report ⓘ

Sep 10, 2026 – 10:34 am BST

PDB ID : 2WSF / pdb_00002wsf
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 : 4-5-2 with Phenix2.0
Mogul : 1.8.4, CSD as541be (2020)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.015 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.50

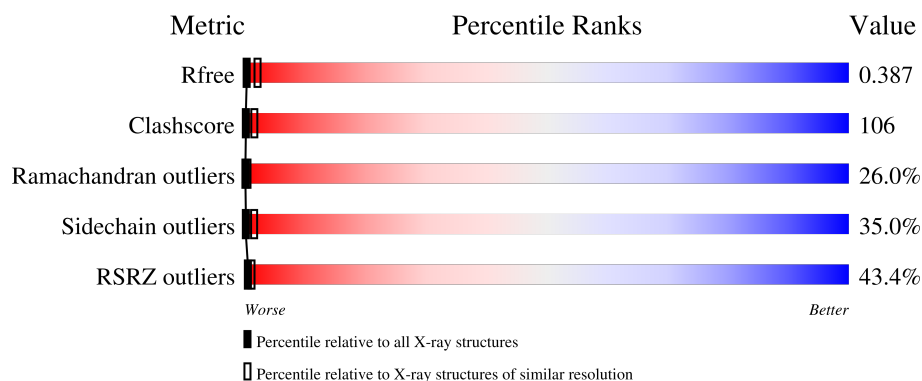
1 Overall quality at a glance

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}	180053	1083 (3.52-3.44)
Clashscore	190562	1139 (3.52-3.44)
Ramachandran outliers	187476	1111 (3.52-3.44)
Sidechain outliers	187428	1112 (3.52-3.44)
RSRZ outliers	180081	1082 (3.52-3.44)

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	26% 26% 27% 12% . 32%
2	2	269	19% 9% 24% 22% 12% 35%
3	3	276	36% 15% 19% 14% 7% 45%
4	4	251	20% 6% 20% 23% 17% 34%
5	A	758	47% 9% 44% 34% 9% .

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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	-	-	-
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	FRU	X	2	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	206	X	-	-	-
20	CLA	1	207	X	-	-	-
20	CLA	1	211	X	-	-	-
20	CLA	1	213	X	-	-	-
20	CLA	1	215	X	-	-	-
20	CLA	2	303	X	-	X	-
20	CLA	2	307	X	-	X	-
20	CLA	2	312	X	-	-	-
20	CLA	2	316	X	-	-	-
20	CLA	3	310	X	-	-	-
20	CLA	3	311	X	-	-	-
20	CLA	3	314	X	-	-	-
20	CLA	4	301	X	-	X	-
20	CLA	4	303	X	-	-	-
20	CLA	4	304	X	-	X	-
20	CLA	4	306	X	-	-	-
20	CLA	4	310	-	-	X	-
20	CLA	A	801	X	-	-	-
20	CLA	A	804	X	-	X	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
20	CLA	A	806	X	-	-	-
20	CLA	A	807	-	-	X	-
20	CLA	A	808	X	-	-	-
20	CLA	A	809	-	-	X	-
20	CLA	A	811	X	-	-	-
20	CLA	A	818	X	-	X	-
20	CLA	A	819	X	-	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	830	X	-	X	-
20	CLA	A	831	X	-	X	-
20	CLA	A	835	X	-	-	-
20	CLA	A	838	X	-	X	-
20	CLA	A	839	X	-	X	-
20	CLA	A	840	X	-	-	-
20	CLA	A	849	X	-	-	-
20	CLA	A	850	X	-	X	-
20	CLA	A	851	X	-	X	-
20	CLA	B	803	X	-	X	-
20	CLA	B	806	X	-	X	-
20	CLA	B	808	X	-	X	-
20	CLA	B	809	X	-	X	-
20	CLA	B	810	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	820	X	-	-	-
20	CLA	B	823	X	-	-	-
20	CLA	B	824	X	-	X	-
20	CLA	B	825	-	-	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	832	X	-	X	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
20	CLA	B	834	-	-	X	-
20	CLA	B	835	-	-	X	-
20	CLA	B	837	X	-	-	-
20	CLA	B	838	X	-	X	-
20	CLA	B	839	-	-	X	-
20	CLA	B	840	X	-	-	-
20	CLA	B	841	X	-	-	-
20	CLA	B	850	X	-	-	-
20	CLA	F	201	-	-	X	-
20	CLA	F	207	X	-	-	-
20	CLA	H	101	X	-	-	-
20	CLA	H	102	X	-	-	-
20	CLA	H	108	X	-	X	-
20	CLA	H	109	X	-	-	-
20	CLA	I	102	X	-	-	-
20	CLA	J	103	X	-	-	-
20	CLA	K	102	-	-	X	-
20	CLA	K	104	X	-	-	-
20	CLA	L	201	X	-	X	-
20	CLA	L	202	X	-	-	-
20	CLA	L	203	X	-	X	-
20	CLA	L	204	X	-	-	-
20	CLA	L	207	-	-	X	-
20	CLA	L	208	X	-	-	-
20	CLA	R	107	X	-	-	-
20	CLA	R	108	X	-	-	-
21	LMU	2	313	-	-	X	-
21	LMU	A	853	-	-	X	-
21	LMU	G	101	-	-	X	-
21	LMU	K	107	-	-	X	-
22	BCR	A	843	-	-	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	-
22	BCR	F	204	-	-	X	-
22	BCR	I	103	-	-	X	-
22	BCR	J	102	-	-	X	-
22	BCR	L	209	-	-	X	-
23	PQN	A	842	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
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			

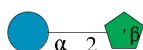
- Molecule 17 is a protein called PHOTOSYSTEM I-N SUBUNIT.

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.



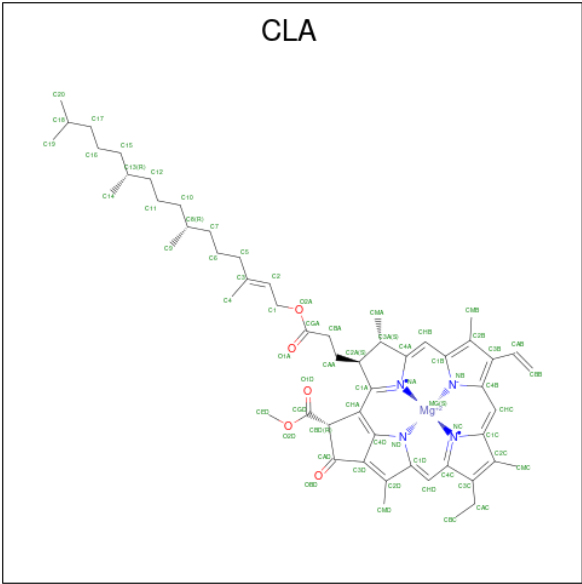
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace
19	M	2	Total	C	O	0	0	0
			23	12	11			
19	O	2	Total	C	O	0	0	0
			22	12	10			
19	P	2	Total	C	O	0	0	0
			23	12	11			

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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 (CCD ID: CLA) (formula: C₅₅H₇₂MgN₄O₅).



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

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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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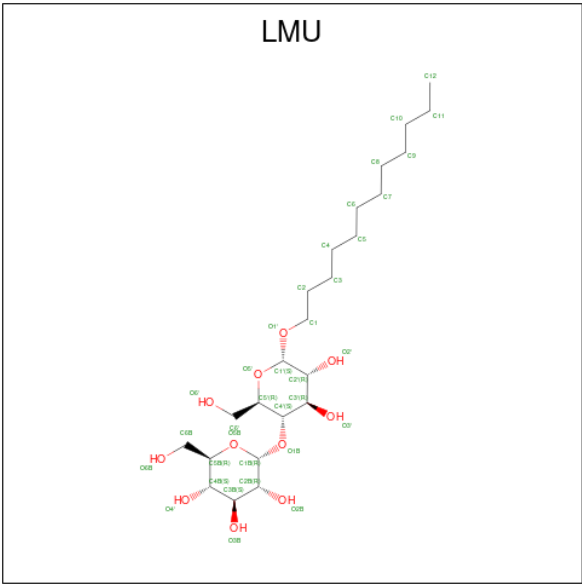
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
20	F	1	Total	C	Mg	N	O	0	0
			50	40	1	4	5		
20	F	1	Total	C	Mg	N	O	0	0
			36	30	1	4	1		
20	F	1	Total	C	Mg	N	O	0	0
			41	33	1	4	3		
20	F	1	Total	C	Mg	N	O	0	0
			53	43	1	4	5		
20	G	1	Total	C	Mg	N	O	0	0
			51	41	1	4	5		
20	H	1	Total	C	Mg	N	O	0	0
			55	45	1	4	5		
20	H	1	Total	C	Mg	N	O	0	0
			55	45	1	4	5		
20	H	1	Total	C	Mg	N	O	0	0
			58	48	1	4	5		
20	H	1	Total	C	Mg	N	O	0	0
			55	45	1	4	5		
20	H	1	Total	C	Mg	N	O	0	0
			50	40	1	4	5		
20	I	1	Total	C	Mg	N	O	0	0
			60	50	1	4	5		
20	J	1	Total	C	Mg	N	O	0	0
			48	38	1	4	5		
20	J	1	Total	C	Mg	N	O	0	0
			61	51	1	4	5		
20	K	1	Total	C	Mg	N	O	0	0
			46	36	1	4	5		
20	K	1	Total	C	Mg	N	O	0	0
			50	40	1	4	5		
20	K	1	Total	C	Mg	N	O	0	0
			50	40	1	4	5		
20	K	1	Total	C	Mg	N	O	0	0
			56	46	1	4	5		
20	L	1	Total	C	Mg	N	O	0	0
			60	50	1	4	5		
20	L	1	Total	C	Mg	N	O	0	0
			55	45	1	4	5		
20	L	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
20	L	1	Total	C	Mg	N	O	0	0
			55	45	1	4	5		

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

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



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

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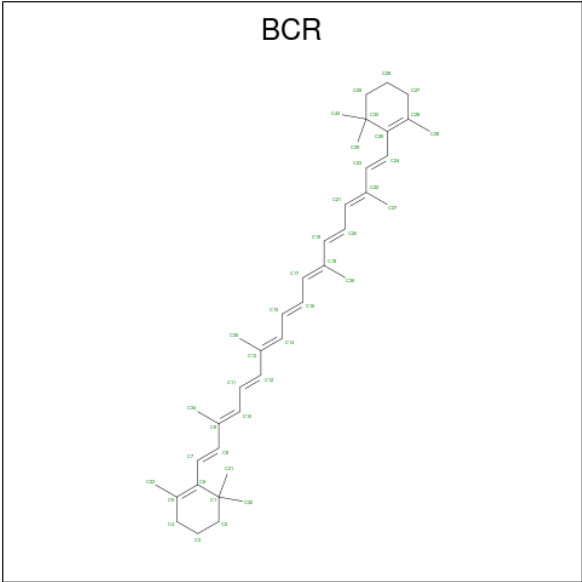
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
21	2	1	Total	C	O	0	0
			35	24	11		
21	3	1	Total	C	O	0	0
			35	24	11		
21	3	1	Total	C	O	0	0
			35	24	11		
21	4	1	Total	C	O	0	0
			35	24	11		
21	4	1	Total	C	O	0	0
			34	23	11		
21	4	1	Total	C	O	0	0
			35	24	11		
21	4	1	Total	C	O	0	0
			35	24	11		
21	A	1	Total	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 (CCD ID: BCR) (formula: $C_{40}H_{56}$).



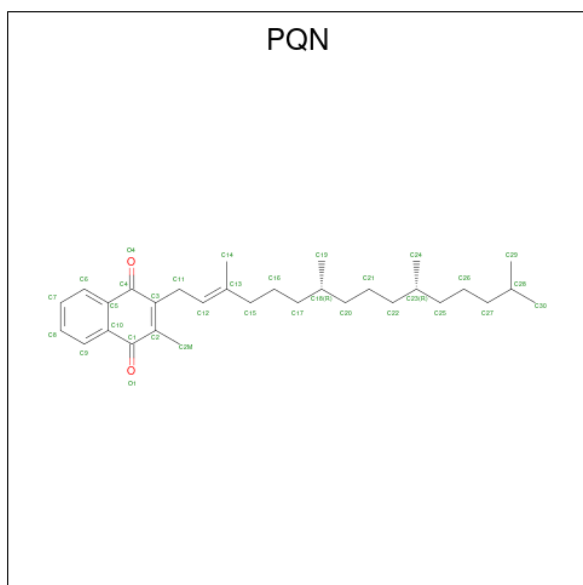
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
22	2	1	Total C 40 40	0	0
22	A	1	Total C 40 40	0	0
22	A	1	Total C 40 40	0	0
22	A	1	Total C 40 40	0	0
22	B	1	Total C 40 40	0	0
22	B	1	Total C 40 40	0	0
22	B	1	Total C 40 40	0	0
22	B	1	Total C 40 40	0	0
22	B	1	Total C 40 40	0	0
22	F	1	Total C 40 40	0	0
22	F	1	Total 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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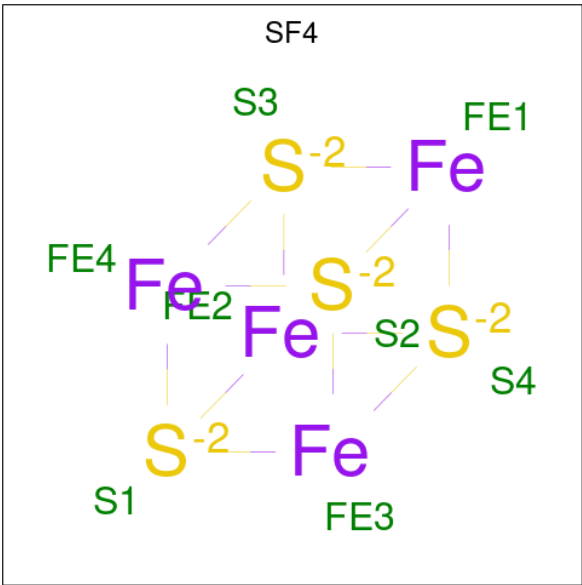
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
22	J	1	Total C 40 40	0	0
22	L	1	Total C 40 40	0	0

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



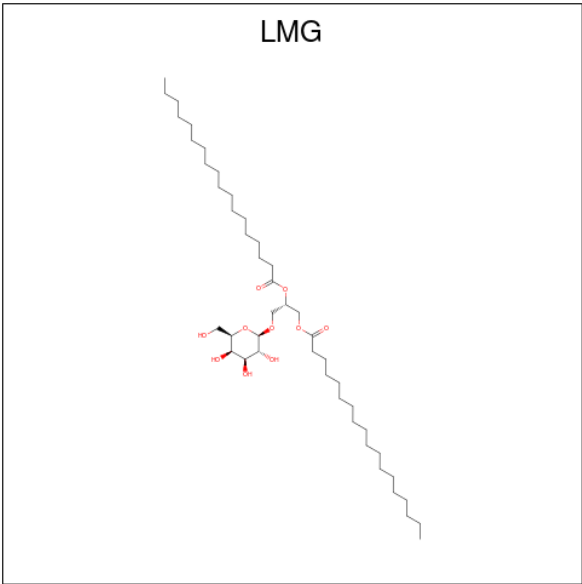
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
23	A	1	Total C O 33 31 2	0	0
23	B	1	Total C O 33 31 2	0	0

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



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

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

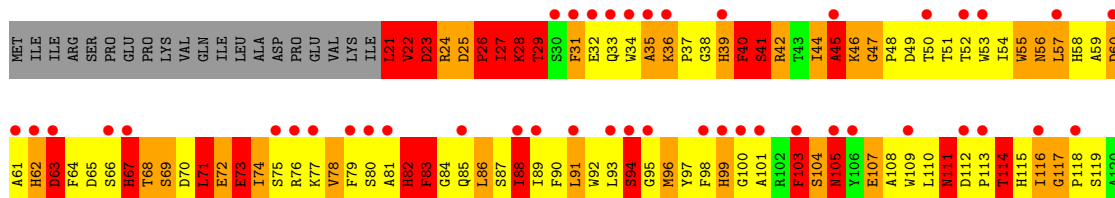
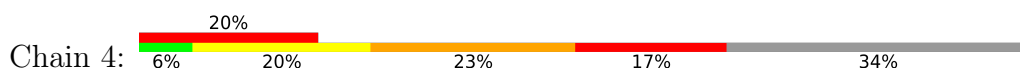


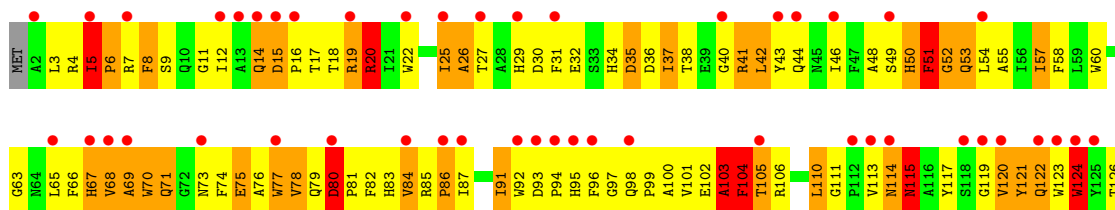
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
25	B	1	Total	C	O	0	0
			49	39	10		

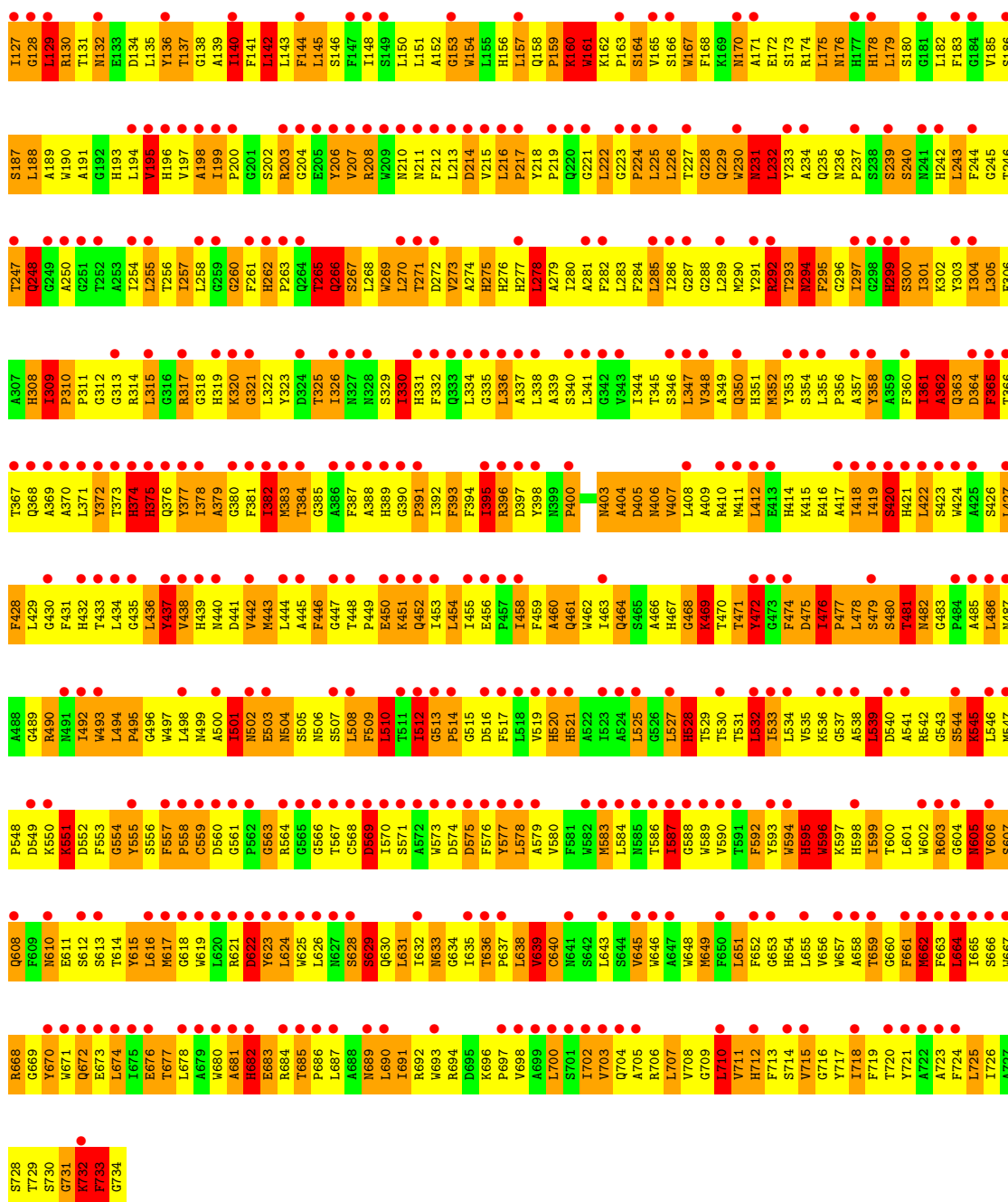
- Molecule 26 is UNKNOWN LIGAND (CCD ID: UNL) (formula:).

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

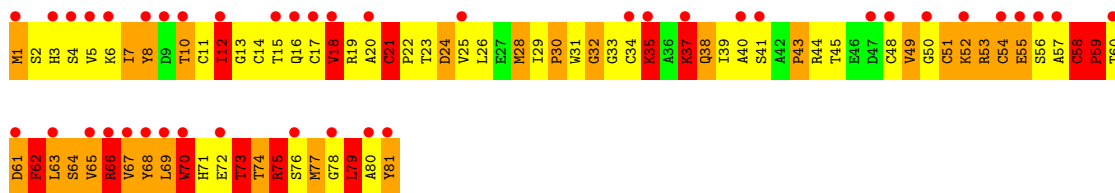
Chain 3: 36% 15% 19% 14% 7% 45%



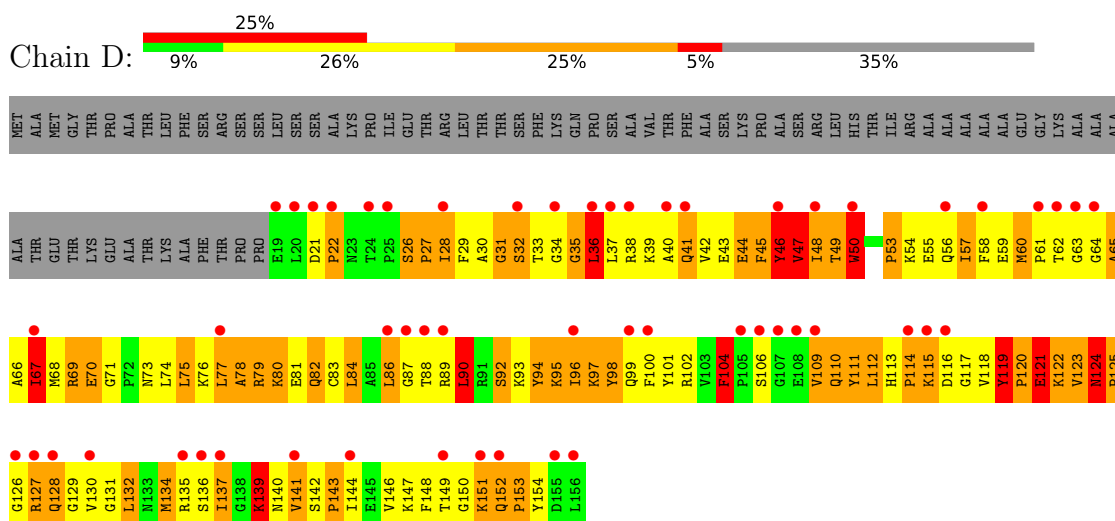




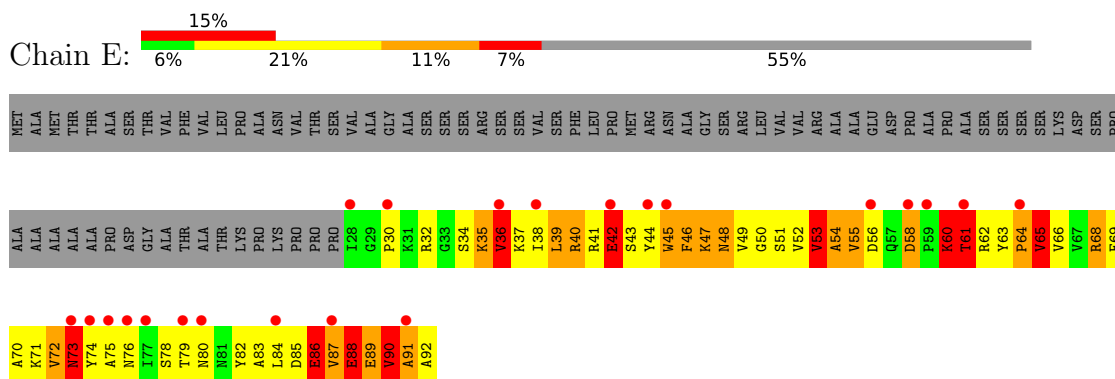
● Molecule 7: PHOTOSYSTEM I IRON-SULFUR CENTER



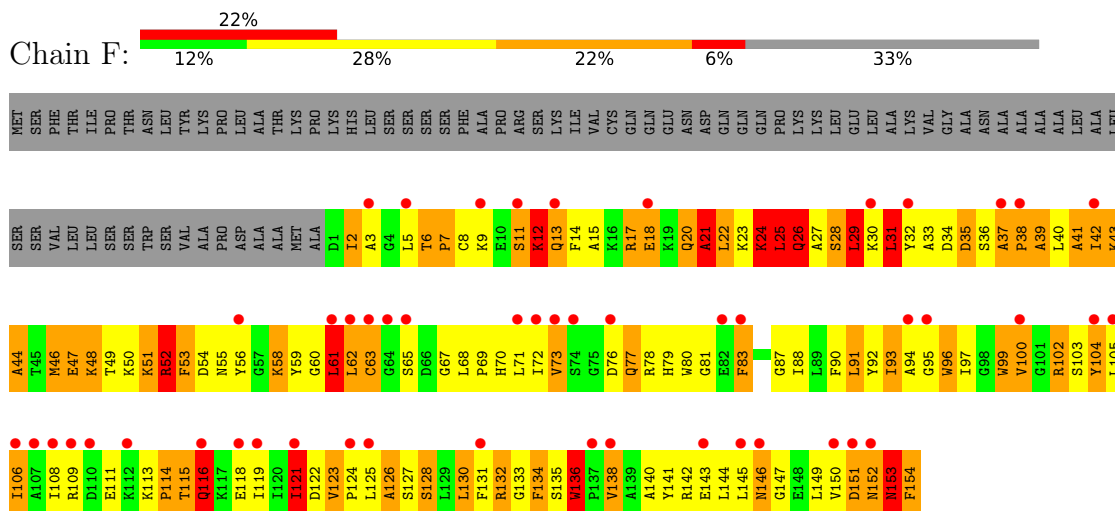
● Molecule 8: PHOTOSYSTEM I REACTION CENTER SUBUNIT II, CHLOROPLASTIC



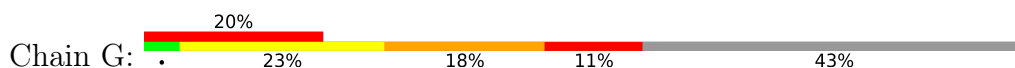
- Molecule 9: PHOTOSYSTEM I REACTION CENTER SUBUNIT IV A, CHLOROPLASTIC

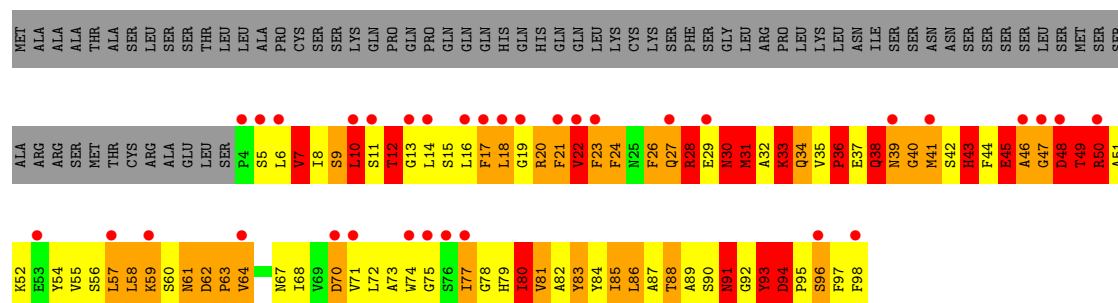


- Molecule 10: PHOTOSYSTEM I REACTION CENTER SUBUNIT III, CHLOROPLASTIC

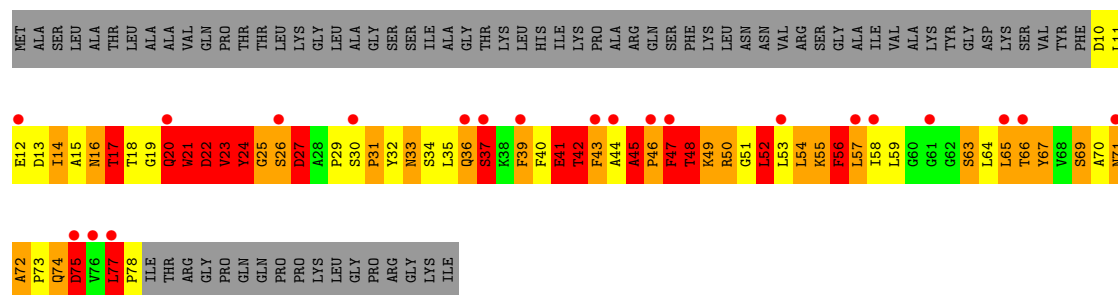
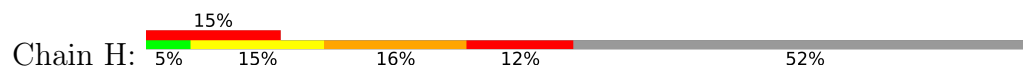


- Molecule 11: PHOTOSYSTEM I REACTION CENTER SUBUNIT V, CHLOROPLASTIC

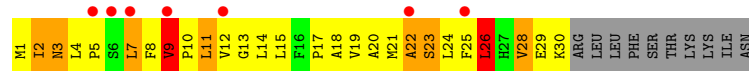




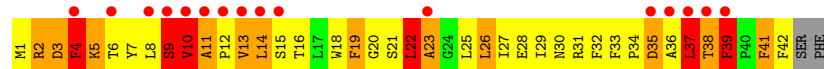
• Molecule 12: PHOTOSYSTEM I REACTION CENTER SUBUNIT VI, CHLOROPLASTIC



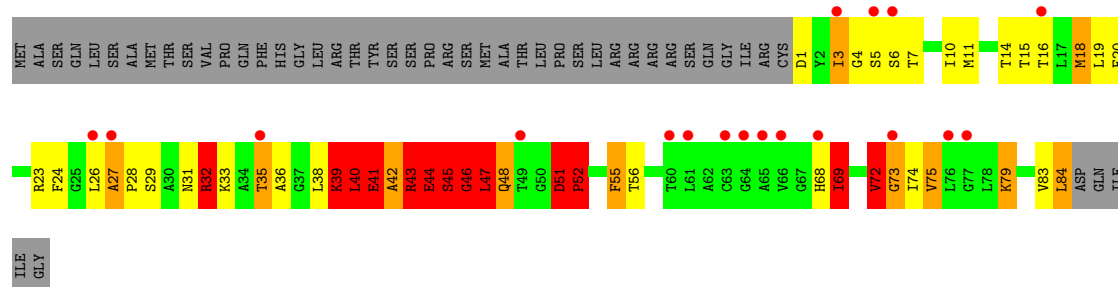
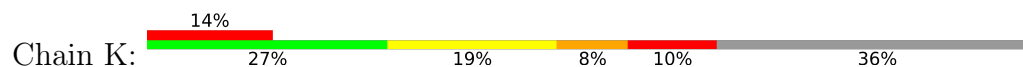
• Molecule 13: PHOTOSYSTEM I REACTION CENTER SUBUNIT VIII



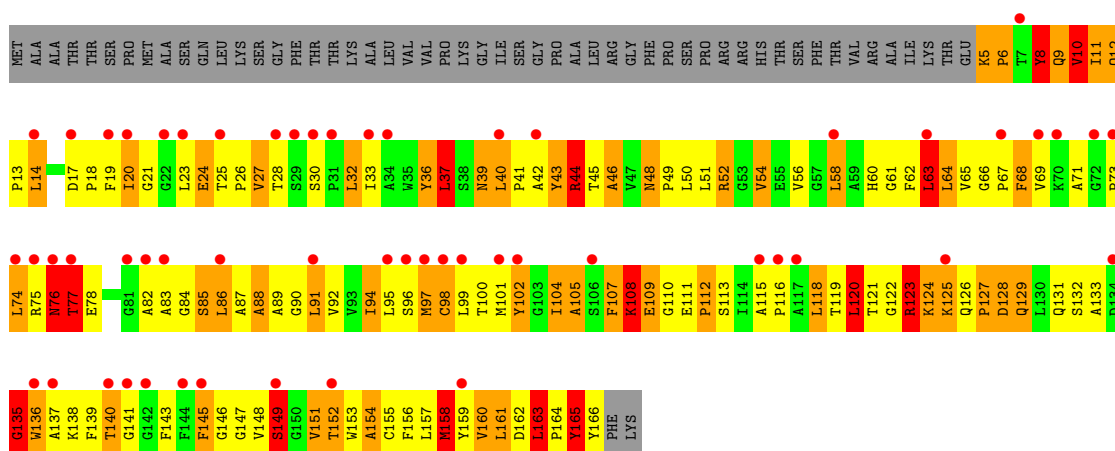
• Molecule 14: PHOTOSYSTEM I REACTION CENTER SUBUNIT IX



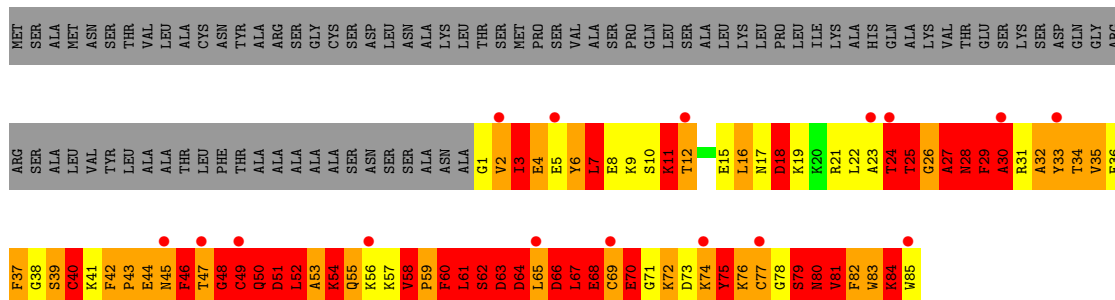
• Molecule 15: PHOTOSYSTEM I REACTION CENTER SUBUNIT PSAK, CHLOROPLASTIC



Chain L:



Chain N: 9% 12% 16% 19% 50%



Chain R: 30% 43% 26%



Chain M:



Chain O: 100%



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

Chain P:  100%

GLC1
FRU2

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

Chain Q:  100%

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:  50% 50%

GLC1
FRU2

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

Chain X:  50% 50%



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

Chain Y:  100%



- 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 50.00 – 3.48	Depositor EDS
% Data completeness (in resolution range)	96.4 (50.00-3.48) 96.6 (50.00-3.48)	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 (1.95%)	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)	0.10 , 14.2	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 ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: PQN, LMG, CLA, GLC, LMU, BCR, SF4, UNL, 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	0.67	0/1303	1.07	7/1774 (0.4%)
2	2	0.85	0/1420	1.50	23/1943 (1.2%)
3	3	0.66	0/1221	1.38	13/1642 (0.8%)
4	4	1.05	5/1359 (0.4%)	1.59	32/1851 (1.7%)
5	A	0.79	4/5938 (0.1%)	1.27	59/8104 (0.7%)
6	B	0.76	1/6058 (0.0%)	1.18	44/8278 (0.5%)
7	C	0.96	0/632	1.50	9/856 (1.1%)
8	D	0.96	0/1122	1.33	17/1514 (1.1%)
9	E	0.95	0/530	1.25	3/718 (0.4%)
10	F	0.82	0/1250	1.27	9/1687 (0.5%)
11	G	1.13	7/760 (0.9%)	1.83	19/1031 (1.8%)
12	H	0.90	0/543	1.48	11/741 (1.5%)
13	I	0.84	0/235	1.11	1/320 (0.3%)
14	J	0.81	0/349	1.40	7/475 (1.5%)
15	K	0.86	1/599 (0.2%)	1.25	6/810 (0.7%)
16	L	0.84	0/1251	1.25	12/1709 (0.7%)
17	N	1.17	5/699 (0.7%)	1.61	18/936 (1.9%)
All	All	0.84	23/25269 (0.1%)	1.32	290/34389 (0.8%)

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

The worst 5 of 23 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	4	39	TRP	CA-C	-7.67	1.42	1.52
5	A	22	VAL	CA-CB	-7.58	1.44	1.54
17	N	51	ASP	N-CA	7.28	1.55	1.46
17	N	40	CYS	C-O	7.01	1.32	1.24
17	N	52	LEU	N-CA	-6.99	1.41	1.46

The worst 5 of 290 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	G	46	ALA	N-CA-C	-25.52	83.47	111.28
3	3	180	LYS	CA-C-N	-16.91	95.85	123.91
3	3	180	LYS	C-N-CA	-16.91	95.85	123.91
11	G	51	ALA	N-CA-C	13.21	128.32	110.35
11	G	45	GLU	N-CA-C	13.08	125.07	111.07

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
2	2	42	ARG	Peptide

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Mol	Chain	Res	Type	Group
2	2	73	ILE	Peptide

5.2 Too-close contacts [i](#)

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	143	3
2	2	1374	0	1331	304	2
3	3	1186	0	1147	303	16
4	4	1319	0	1282	628	5
5	A	5745	0	5597	1401	0
6	B	5848	0	5655	1231	15
7	C	619	0	608	206	0
8	D	1095	0	1112	193	0
9	E	520	0	528	129	0
10	F	1221	0	1249	214	0
11	G	740	0	708	199	1
12	H	529	0	514	108	0
13	I	229	0	252	56	0
14	J	338	0	340	64	0
15	K	593	0	619	111	0
16	L	1215	0	1222	317	5
17	N	685	0	668	330	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	2	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	28
19	Z	23	0	21	14	0
19	a	23	0	21	1	0
20	1	617	0	388	89	1

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
20	2	650	0	465	142	0
20	3	620	0	362	70	0
20	4	694	0	443	168	0
20	A	2346	0	2062	697	0
20	B	2226	0	2061	666	0
20	F	180	0	123	47	0
20	G	51	0	40	4	0
20	H	273	0	235	58	0
20	I	60	0	58	11	0
20	J	109	0	95	26	0
20	K	202	0	158	51	1
20	L	332	0	297	94	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	28
21	H	140	0	184	42	0
21	K	105	0	138	40	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	117	0
22	F	80	0	108	61	0
22	G	40	0	54	4	0
22	I	79	0	105	44	0
22	J	40	0	54	34	0
22	L	40	0	54	36	0
23	A	33	0	46	7	0
23	B	33	0	46	27	0
24	A	8	0	0	18	0
24	C	16	0	0	5	0
25	B	49	0	71	16	0
26	H	23	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	36033	0	34504	7467	56

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 106.

The worst 5 of 7467 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
3:3:132:TRP:CH2	3:3:155:GLU:CD	1.76	1.58

The worst 5 of 56 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 ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	1	161/241 (67%)	84 (52%)	39 (24%)	38 (24%)	0 0
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	6

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	2	140/216 (65%)	83 (59%)	57 (41%)	0	0
3	3	112/215 (52%)	73 (65%)	39 (35%)	0	2
4	4	138/201 (69%)	79 (57%)	59 (43%)	0	0
5	A	592/618 (96%)	387 (65%)	205 (35%)	0	2
6	B	598/600 (100%)	392 (66%)	206 (34%)	0	2
7	C	70/70 (100%)	41 (59%)	29 (41%)	0	0
8	D	118/173 (68%)	77 (65%)	41 (35%)	0	2
9	E	56/114 (49%)	39 (70%)	17 (30%)	0	2
10	F	127/190 (67%)	83 (65%)	44 (35%)	0	2
11	G	79/144 (55%)	50 (63%)	29 (37%)	0	1
12	H	57/115 (50%)	28 (49%)	29 (51%)	0	0
13	I	26/36 (72%)	21 (81%)	5 (19%)	1	8
14	J	36/39 (92%)	23 (64%)	13 (36%)	0	1
15	K	61/102 (60%)	43 (70%)	18 (30%)	0	2
16	L	125/169 (74%)	87 (70%)	38 (30%)	0	2
17	N	74/139 (53%)	43 (58%)	31 (42%)	0	0
All	All	2536/3331 (76%)	1649 (65%)	887 (35%)	0	1

5 of 887 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
6	B	294	ASN
17	N	84	LYS
6	B	670	TYR
17	N	61	LEU
14	J	41	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 112 such sidechains are listed below:

Mol	Chain	Res	Type
6	B	177	HIS
17	N	45	ASN
6	B	504	ASN
16	L	129	GLN
10	F	152	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

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	0.54	0	15,15,17	2.23	2 (13%)
19	FRU	M	2	19	11,12,12	0.71	0	10,18,18	0.74	0
19	GLC	O	1	19	10,10,12	0.91	0	14,14,17	2.46	4 (28%)
19	FRU	O	2	19	11,12,12	0.62	0	10,18,18	1.15	1 (10%)
19	GLC	P	1	19	11,11,12	0.52	0	15,15,17	1.77	4 (26%)
19	FRU	P	2	19	11,12,12	0.70	0	10,18,18	1.23	2 (20%)
19	GLC	Q	1	19	11,11,12	0.60	0	15,15,17	2.44	5 (33%)
19	FRU	Q	2	19	11,12,12	0.78	0	10,18,18	1.18	1 (10%)
19	GLC	S	1	19	11,11,12	0.63	0	15,15,17	1.10	1 (6%)
19	FRU	S	2	19	11,12,12	0.79	0	10,18,18	1.56	2 (20%)
19	GLC	T	1	19	11,11,12	0.51	0	15,15,17	0.79	1 (6%)
19	FRU	T	2	19	11,12,12	0.64	0	10,18,18	1.26	1 (10%)
19	GLC	U	1	19	11,11,12	0.64	0	15,15,17	2.64	4 (26%)
19	FRU	U	2	19	11,12,12	0.65	0	10,18,18	1.39	3 (30%)
19	GLC	V	1	19	11,11,12	0.57	0	15,15,17	1.97	4 (26%)
19	FRU	V	2	19	11,12,12	0.76	0	10,18,18	1.22	1 (10%)
19	GLC	W	1	19	11,11,12	0.59	0	15,15,17	1.01	2 (13%)
19	FRU	W	2	19	11,12,12	0.55	0	10,18,18	1.18	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
19	GLC	X	1	19	10,10,12	0.91	0	14,14,17	2.11	5 (35%)
19	FRU	X	2	19	11,12,12	0.57	0	10,18,18	0.64	0
19	GLC	Y	1	21,19	11,11,12	1.69	3 (27%)	15,15,17	2.66	6 (40%)
19	FRU	Y	2	21,19	11,12,12	1.41	1 (9%)	10,18,18	1.43	2 (20%)
19	GLC	Z	1	19	11,11,12	0.43	0	15,15,17	1.12	2 (13%)
19	FRU	Z	2	19	11,12,12	0.68	0	10,18,18	1.12	0
19	GLC	a	1	19	11,11,12	0.78	0	15,15,17	1.58	2 (13%)
19	FRU	a	2	19	11,12,12	0.42	0	10,18,18	1.12	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	3/5/24/24	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	0/5/24/24	0/1/1/1
19	GLC	T	1	19	-	2/2/19/22	0/1/1/1
19	FRU	T	2	19	1/1/4/4	2/5/24/24	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	21,19	-	0/2/19/22	0/1/1/1
19	FRU	Y	2	21,19	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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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
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	4.27	1.48	1.40
19	Y	1	GLC	C1-C2	3.36	1.59	1.52
19	Y	1	GLC	C2-C3	2.99	1.56	1.52
19	Y	1	GLC	O2-C2	2.25	1.48	1.43

The worst 5 of 55 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	M	1	GLC	C1-O5-C5	7.84	122.82	112.19
19	U	1	GLC	C1-O5-C5	7.72	122.65	112.19
19	O	1	GLC	C1-C2-C3	7.09	118.38	109.67
19	Y	1	GLC	C6-C5-C4	5.98	127.01	113.00
19	V	1	GLC	C1-O5-C5	4.74	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 43 torsion outliers are listed below:

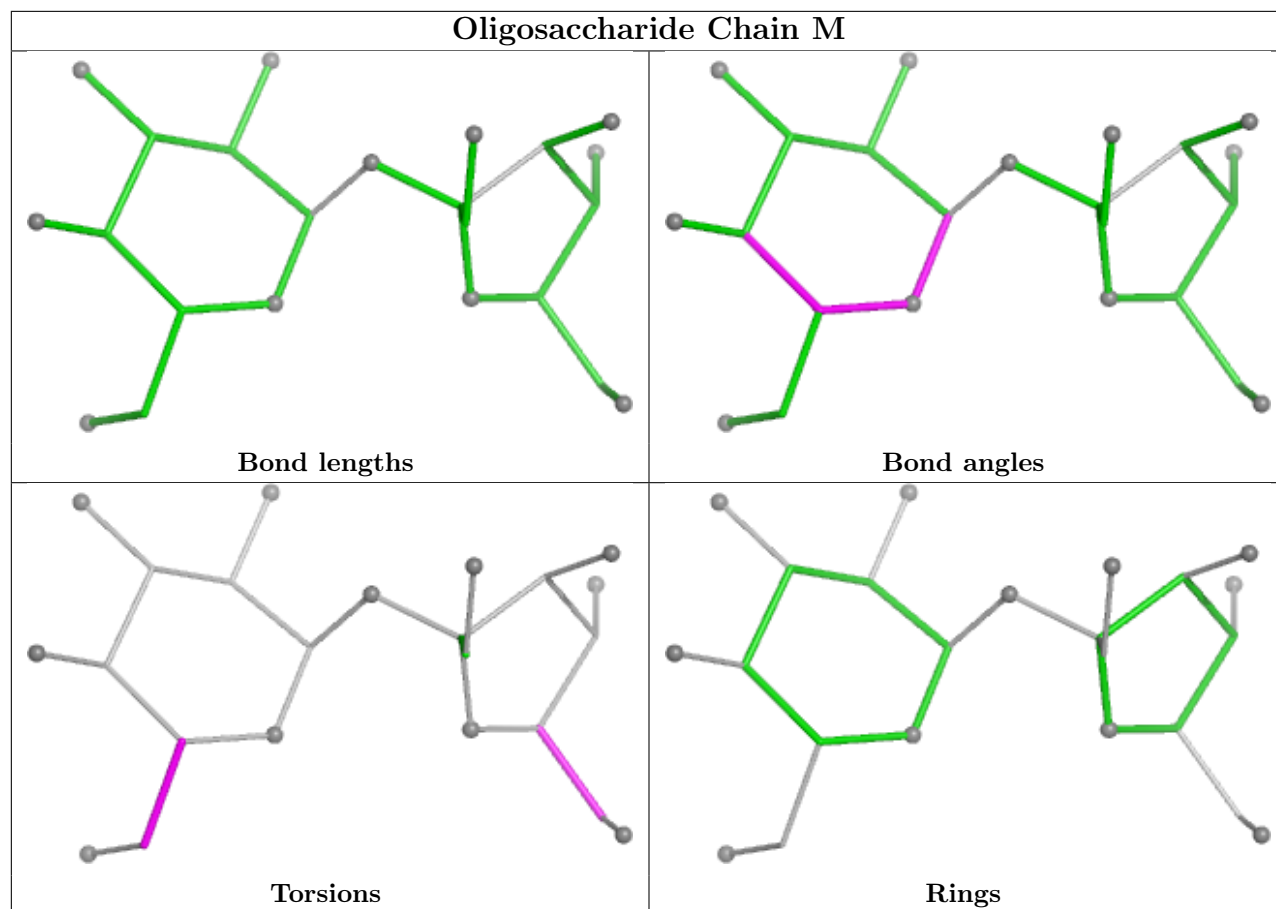
Mol	Chain	Res	Type	Atoms
19	P	2	FRU	C4-C5-C6-O6
19	P	2	FRU	O5-C5-C6-O6
19	Q	2	FRU	O1-C1-C2-C3
19	Q	2	FRU	O1-C1-C2-O2
19	V	2	FRU	O1-C1-C2-C3

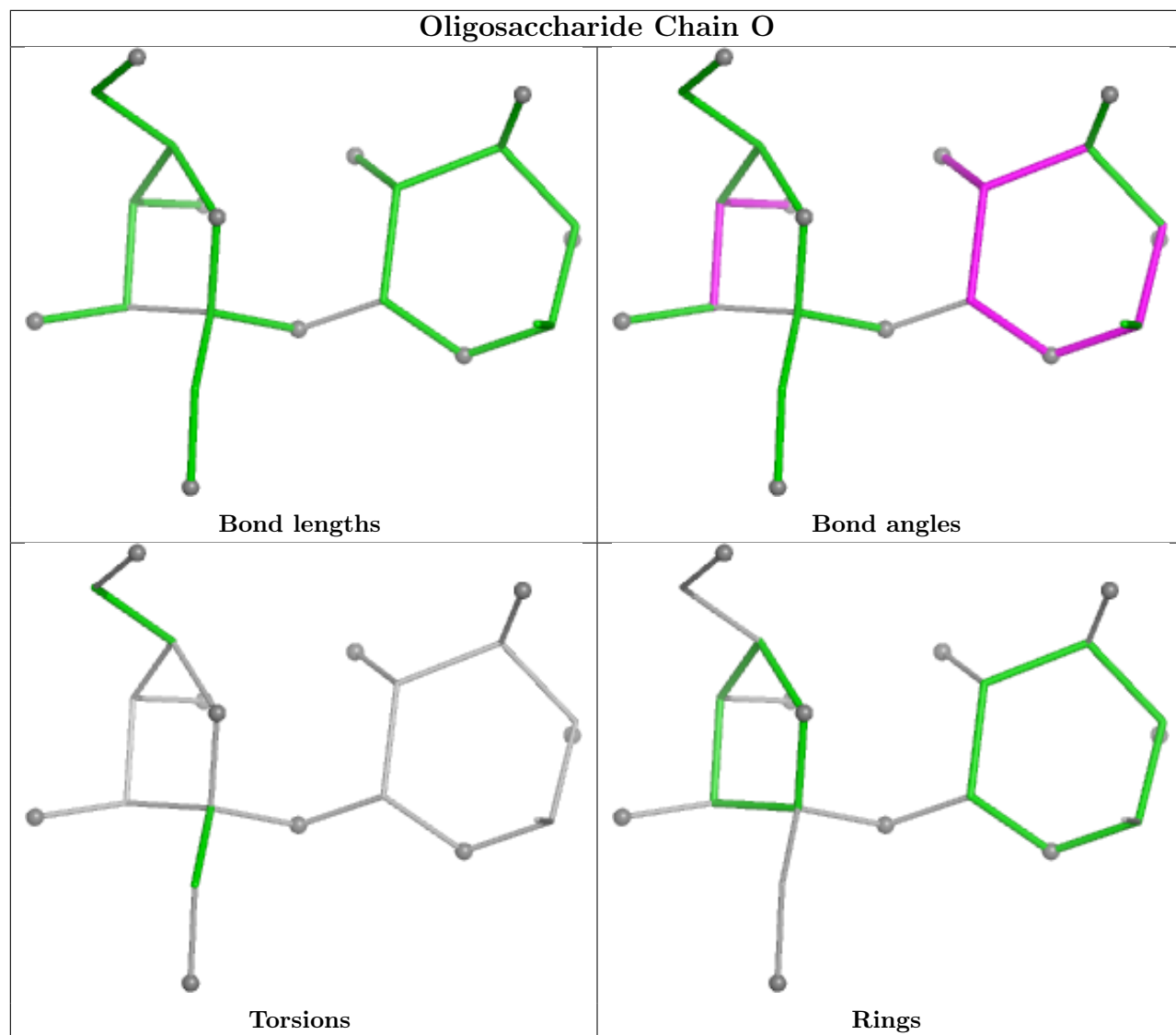
There are no ring outliers.

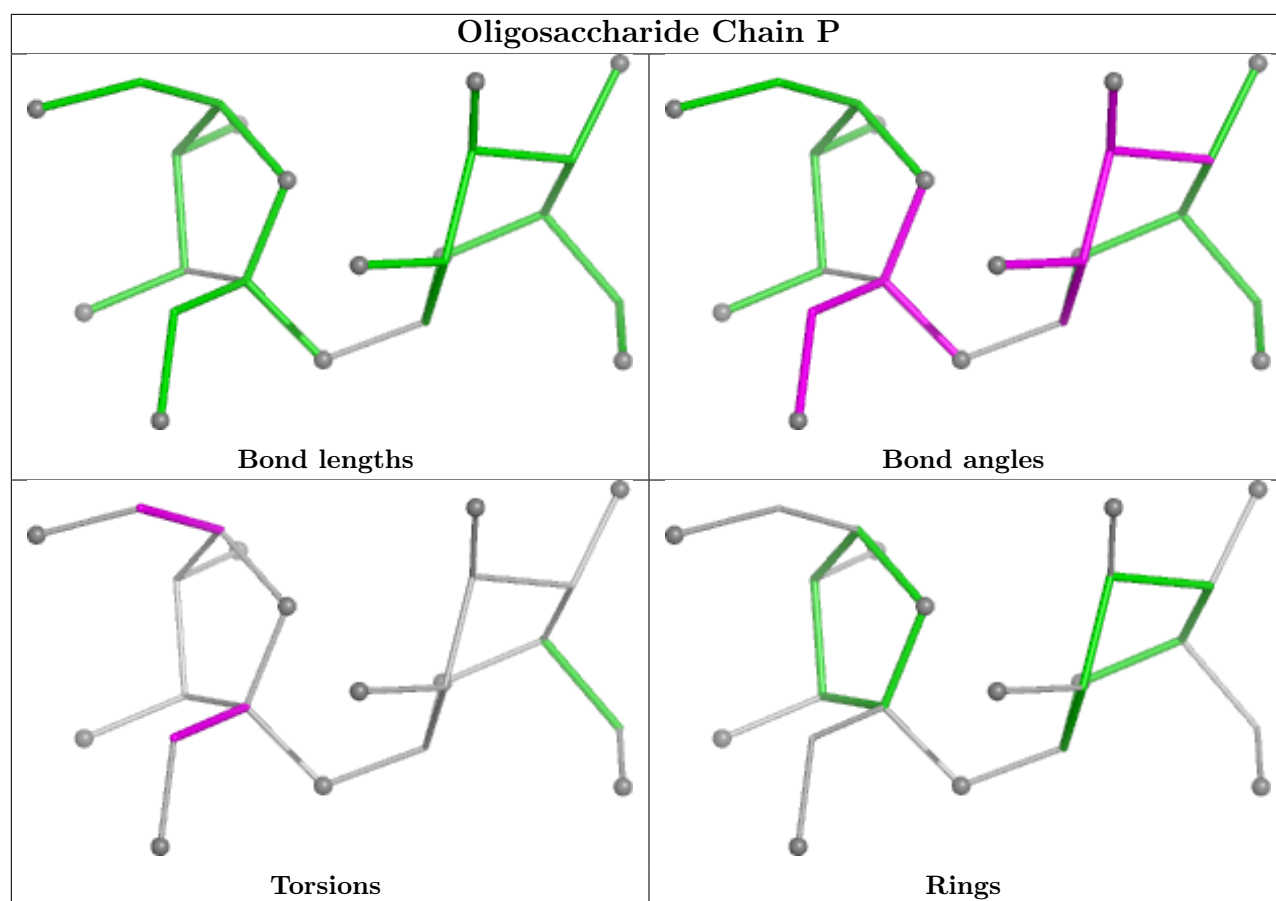
23 monomers are involved in 84 short contacts:

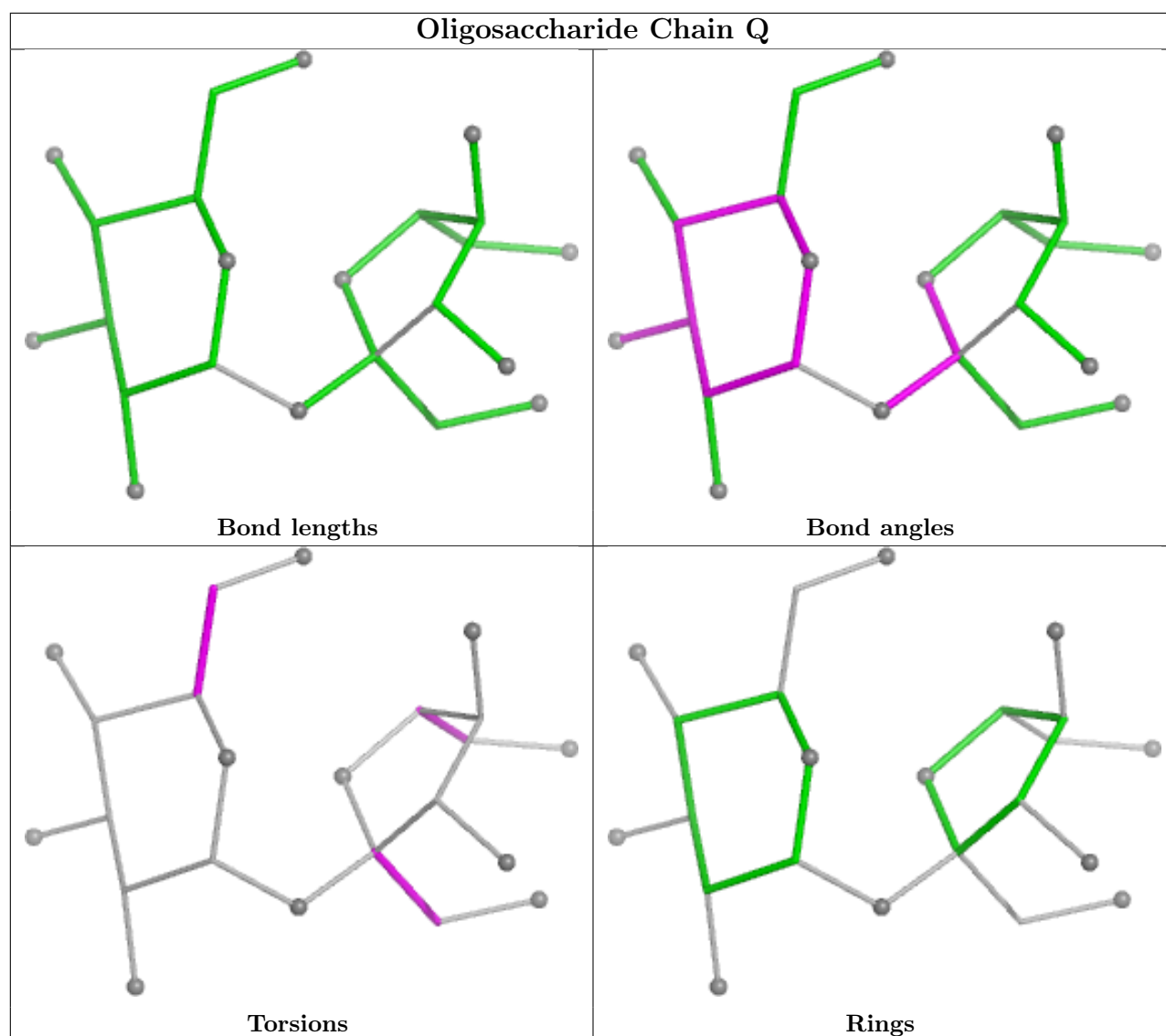
Mol	Chain	Res	Type	Clashes	Symm-Clashes
19	T	2	FRU	2	0
19	W	2	FRU	3	0
19	a	2	FRU	1	0
19	U	2	FRU	1	0
19	T	1	GLC	2	0
19	W	1	GLC	3	0
19	Y	2	FRU	1	16
19	Z	1	GLC	1	0
19	U	1	GLC	1	0
19	V	1	GLC	3	0
19	Y	1	GLC	0	12
19	P	1	GLC	8	0
19	X	2	FRU	3	0
19	Q	2	FRU	6	0
19	S	2	FRU	1	0
19	Z	2	FRU	13	0
19	V	2	FRU	4	0
19	X	1	GLC	3	0
19	O	2	FRU	3	0
19	O	1	GLC	10	0
19	Q	1	GLC	3	0
19	a	1	GLC	1	0
19	P	2	FRU	9	0

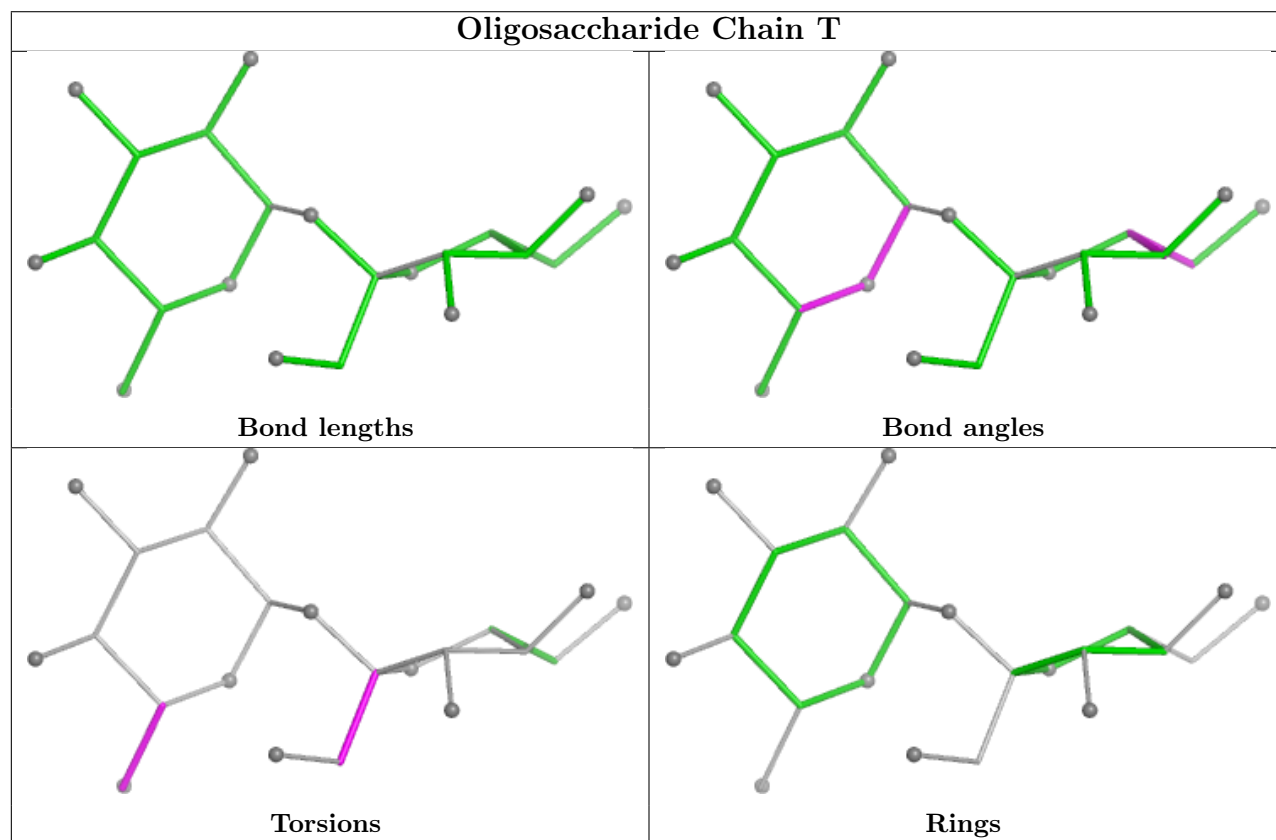
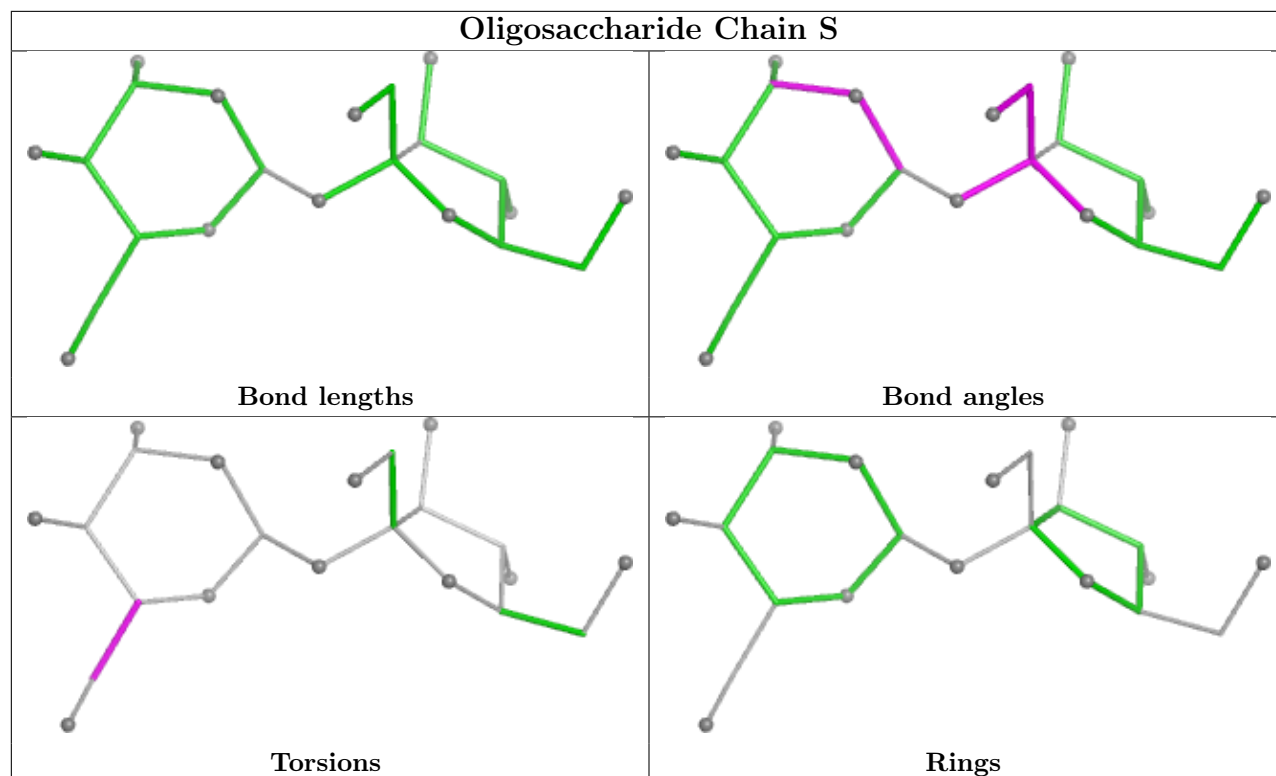
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

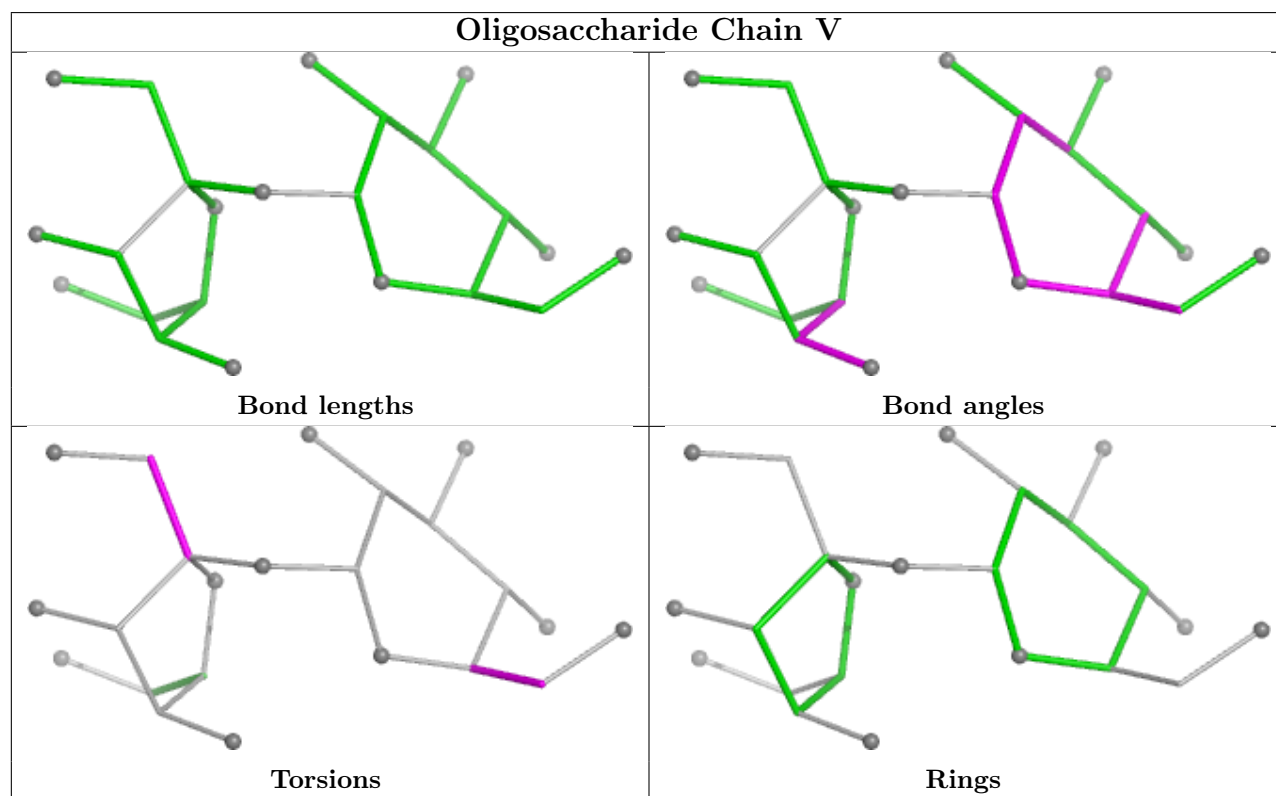
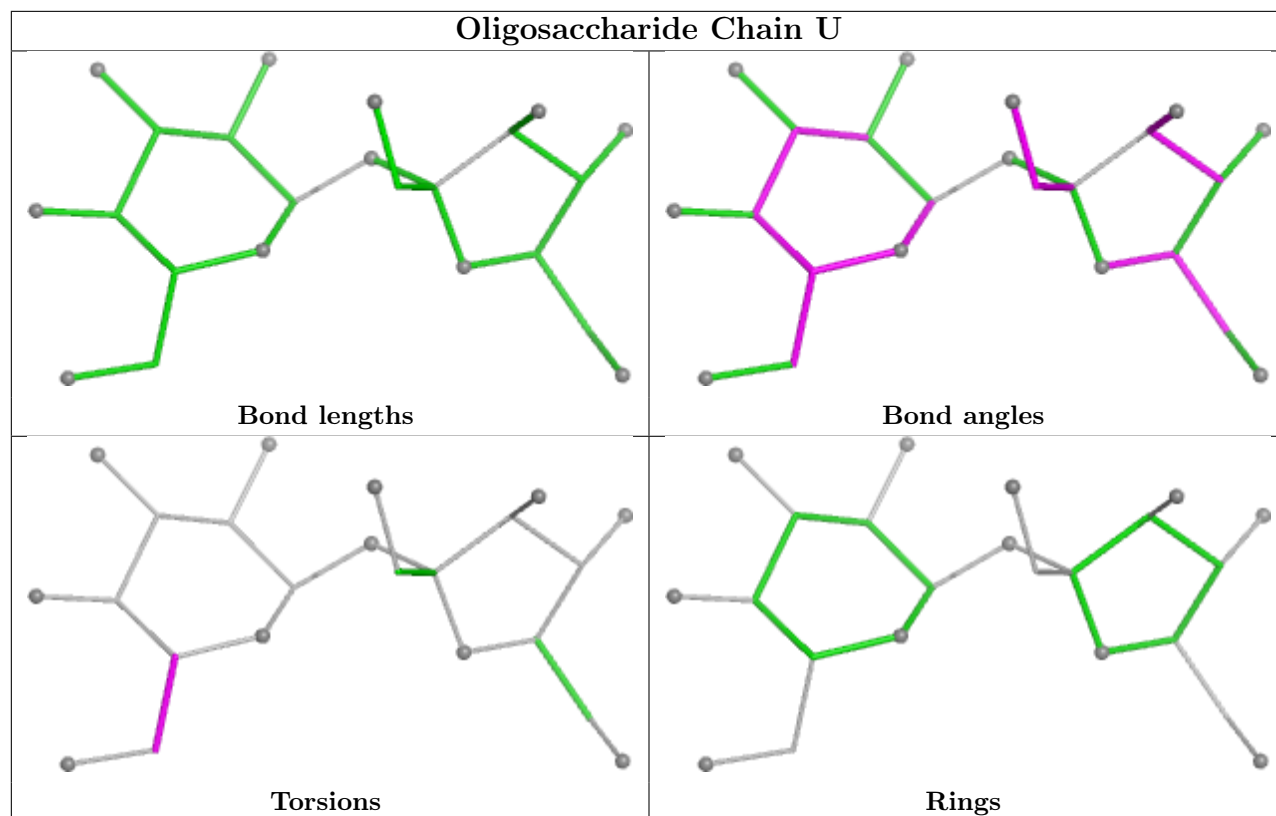


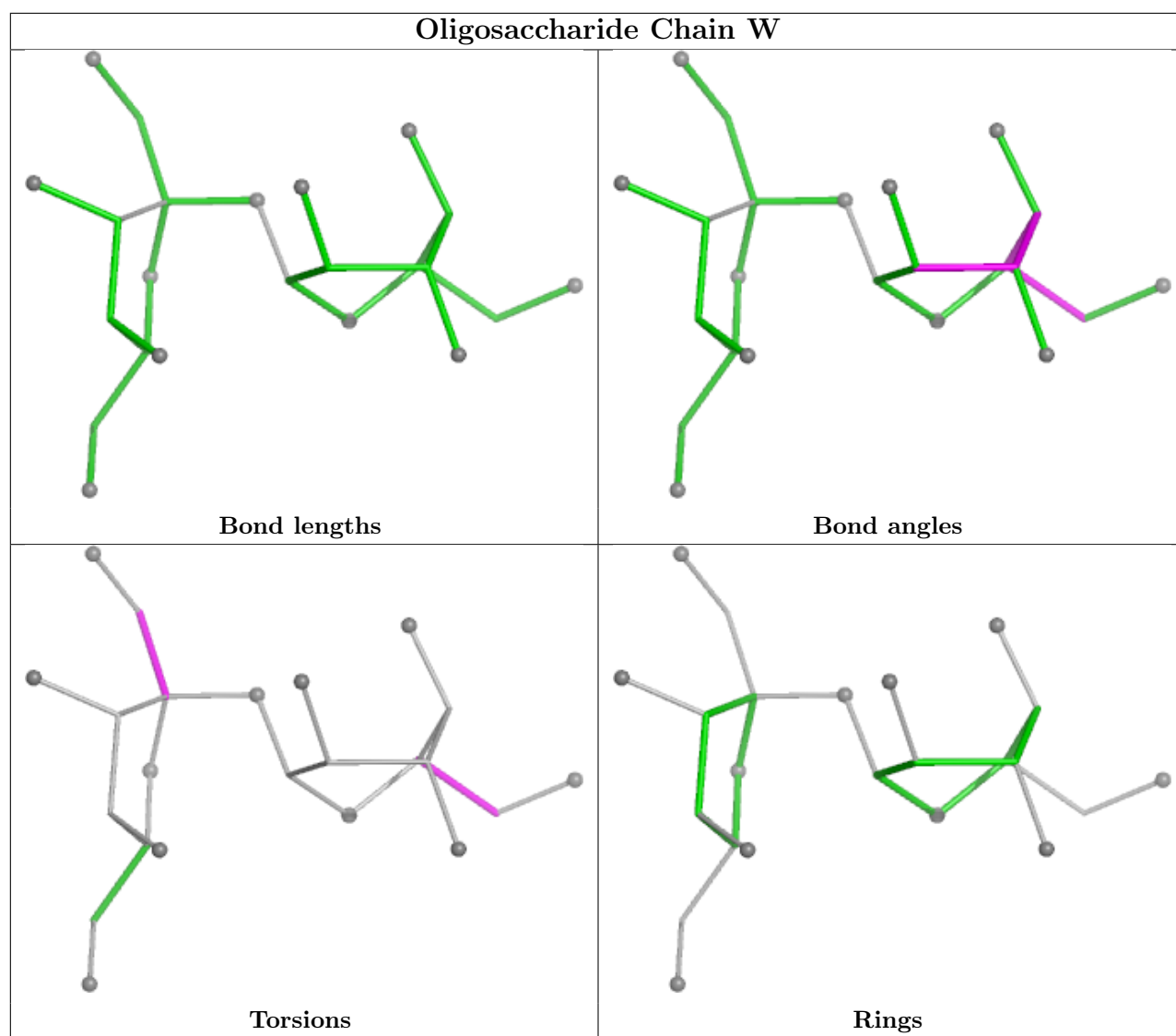


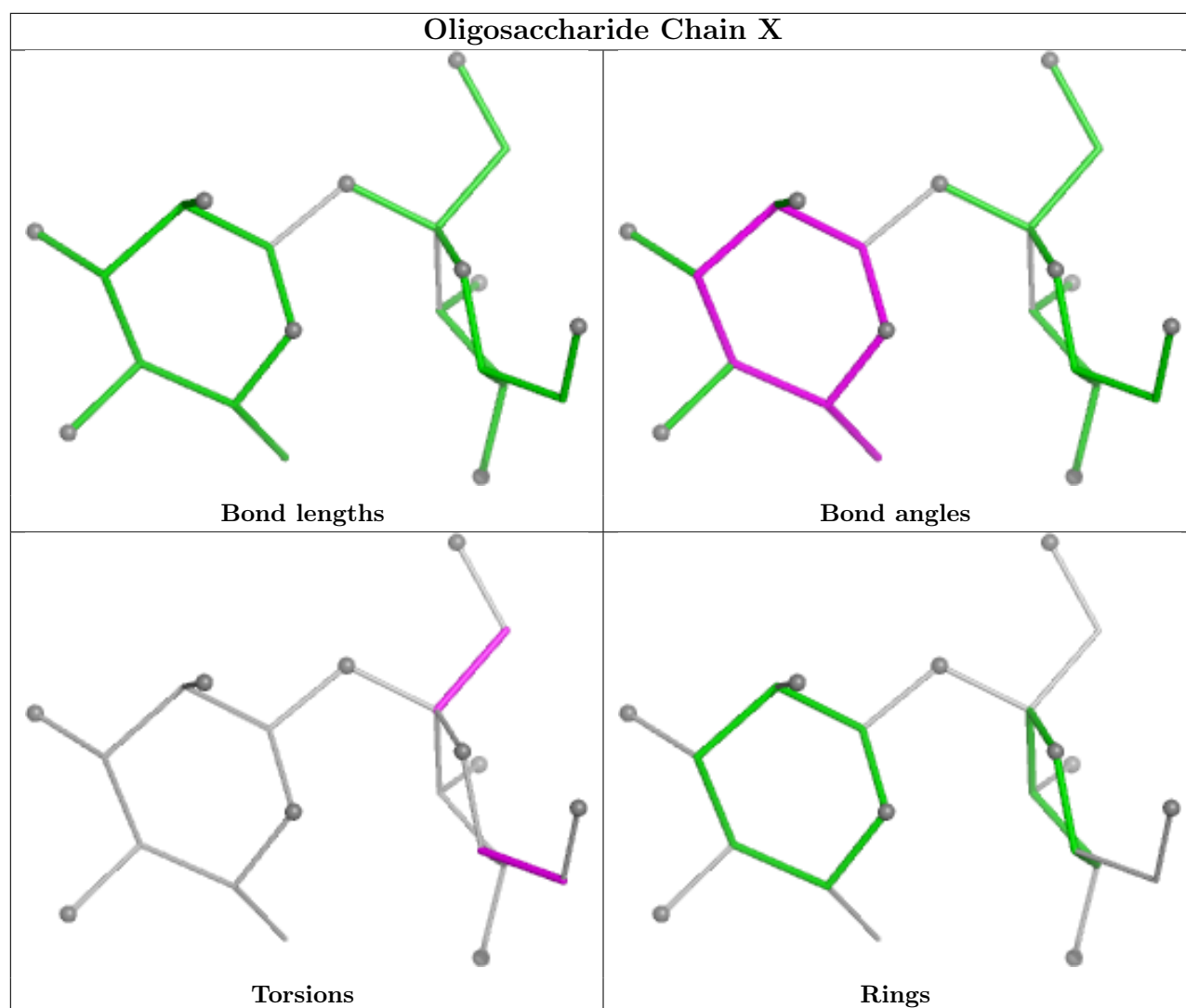


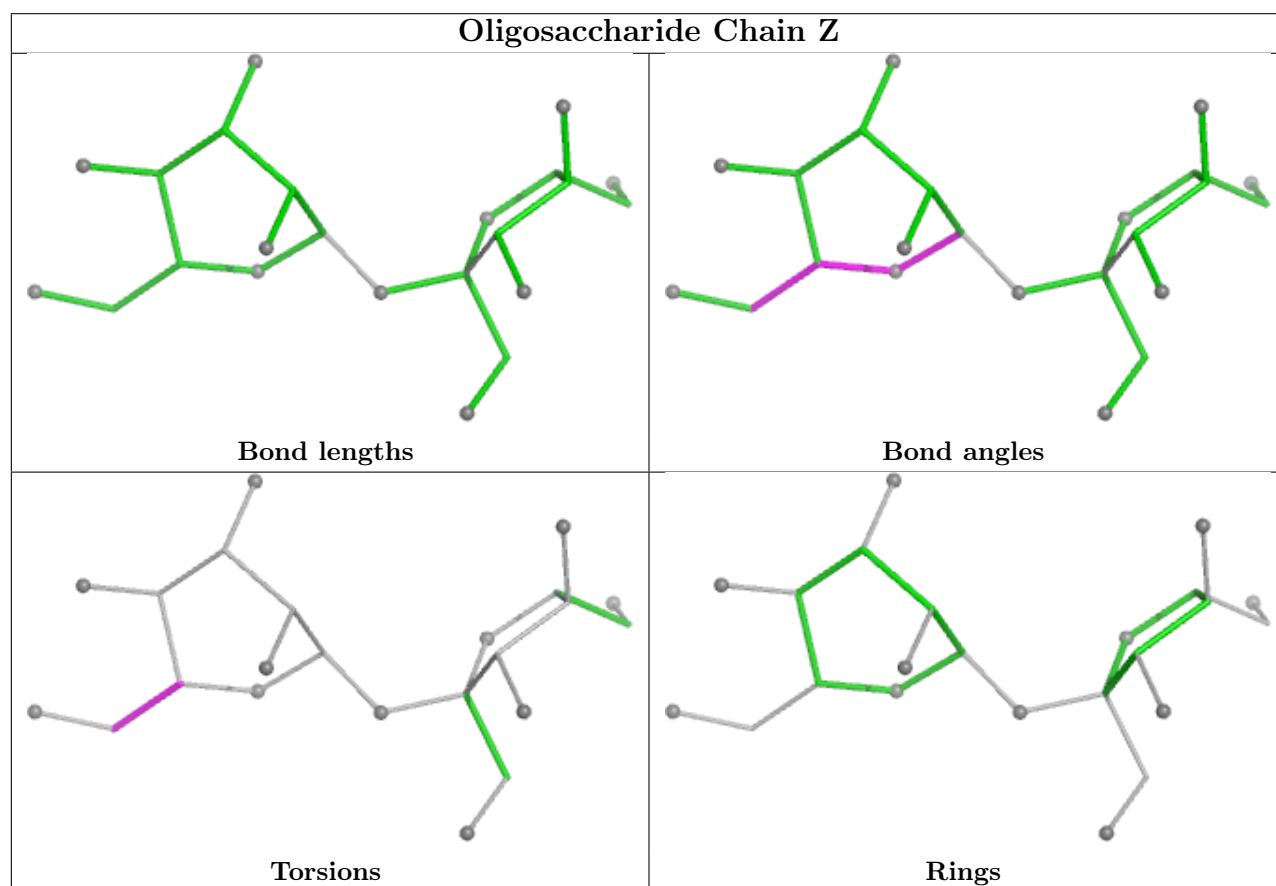
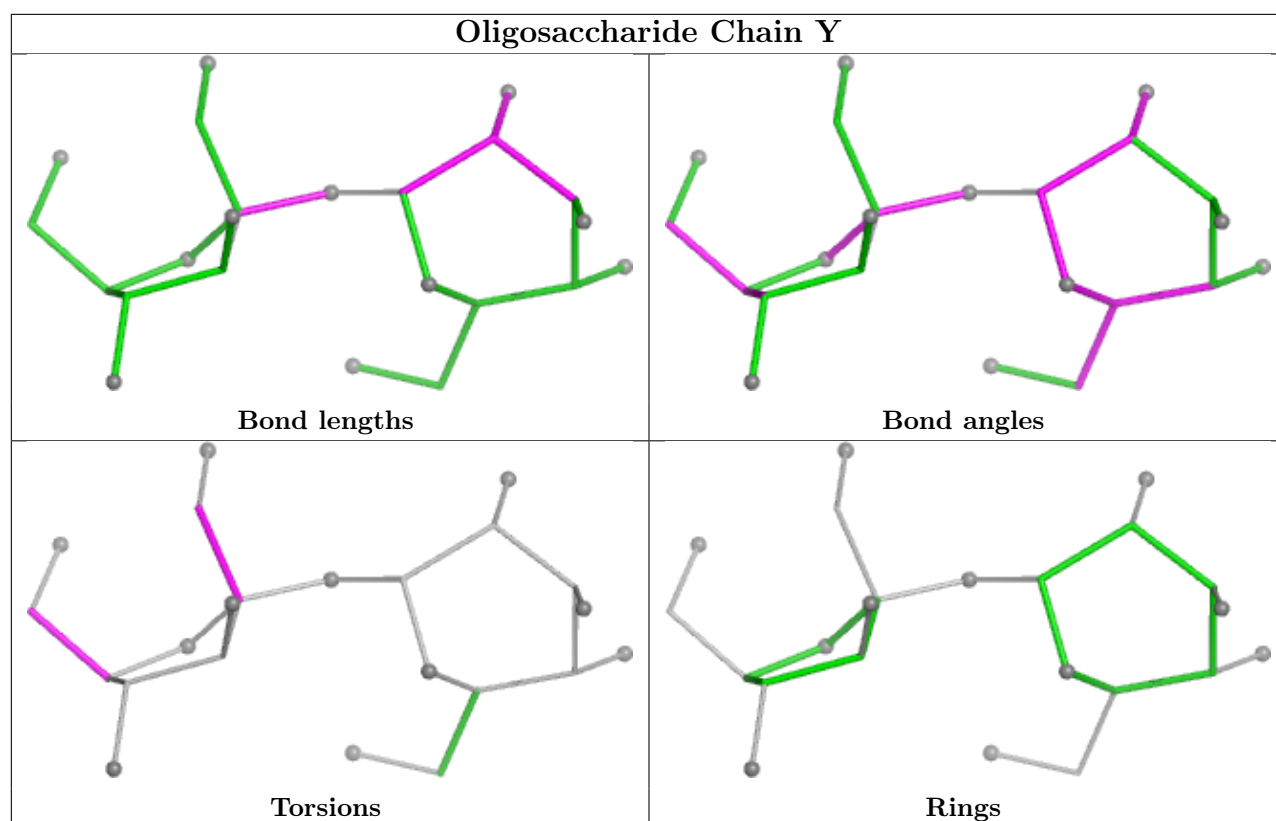


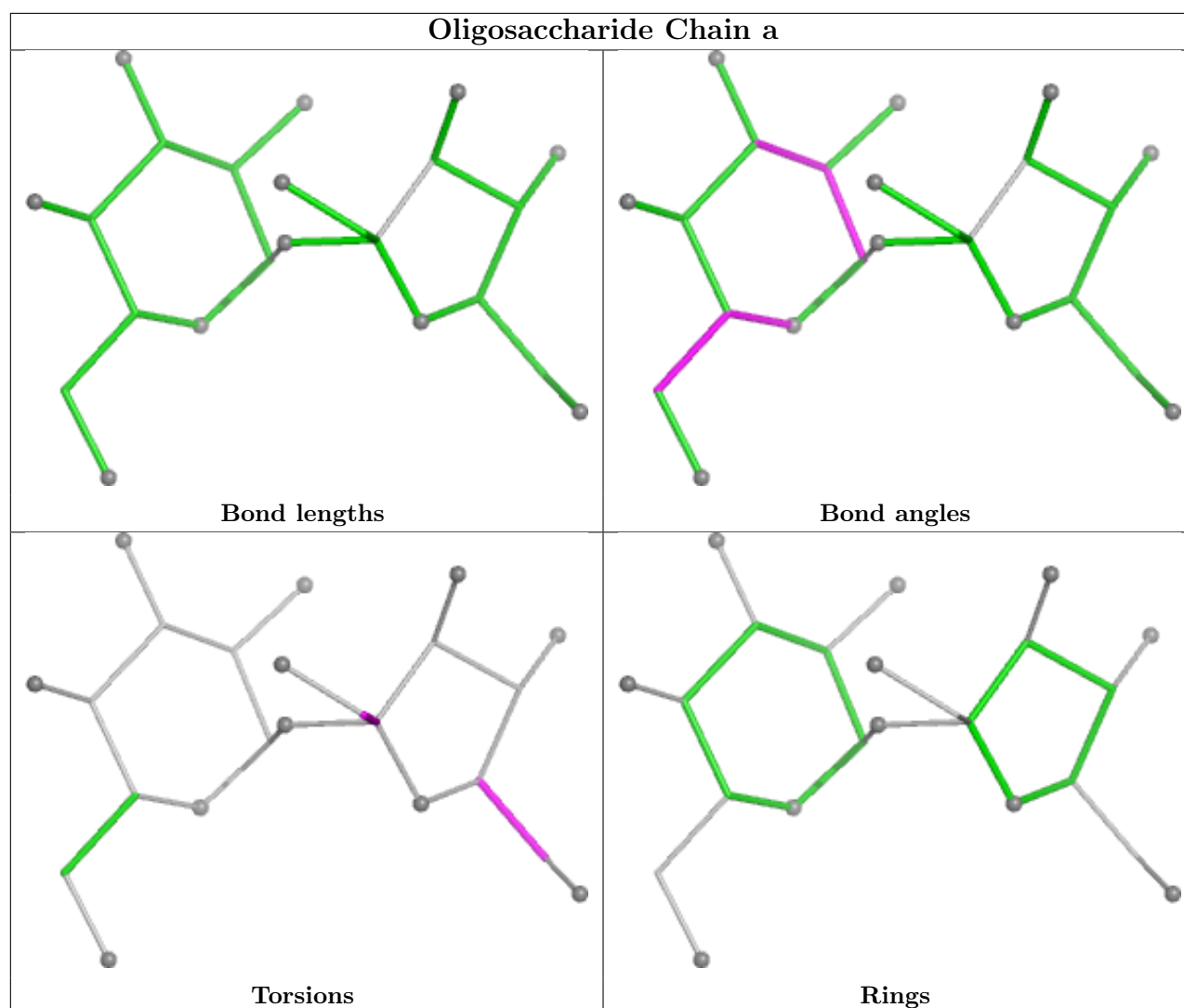












5.6 Ligand geometry [i](#)

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	A	822	5	54,58,73	2.45	16 (29%)	65,95,113	2.86	24 (36%)
20	CLA	A	851	-	69,73,73	2.23	15 (21%)	83,113,113	2.77	29 (34%)
20	CLA	A	808	5	64,68,73	2.29	17 (26%)	77,107,113	2.82	29 (37%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
21	LMU	D	201	-	36,36,36	0.47	0	47,47,47	1.44	6 (12%)
21	LMU	4	321	-	36,36,36	0.46	0	47,47,47	1.46	7 (14%)
21	LMU	L	210	-	36,36,36	0.71	1 (2%)	47,47,47	1.29	4 (8%)
21	LMU	R	106	-	36,36,36	0.52	0	47,47,47	1.23	4 (8%)
20	CLA	3	301	-	39,44,73	2.76	13 (33%)	52,78,113	3.38	22 (42%)
21	LMU	R	101	-	36,36,36	0.86	2 (5%)	47,47,47	2.08	11 (23%)
21	LMU	B	849	-	26,26,36	0.77	1 (3%)	37,37,47	1.28	6 (16%)
20	CLA	K	103	-	54,58,73	2.58	19 (35%)	65,95,113	3.04	26 (40%)
20	CLA	1	214	-	26,32,73	2.36	8 (30%)	34,54,113	3.17	21 (61%)
20	CLA	A	821	5	46,50,73	2.52	12 (26%)	55,85,113	3.34	22 (40%)
20	CLA	B	831	6	54,58,73	2.51	16 (29%)	65,95,113	2.83	26 (40%)
20	CLA	1	206	-	65,69,73	2.21	15 (23%)	78,108,113	2.71	30 (38%)
20	CLA	B	802	-	58,62,73	2.32	15 (25%)	69,99,113	2.99	27 (39%)
20	CLA	J	101	-	52,56,73	2.48	16 (30%)	62,92,113	2.96	22 (35%)
20	CLA	B	818	-	57,61,73	2.39	14 (24%)	68,98,113	2.74	22 (32%)
20	CLA	L	204	-	59,63,73	2.35	14 (23%)	71,101,113	2.77	29 (40%)
20	CLA	B	842	-	39,44,73	2.82	13 (33%)	52,78,113	3.33	26 (50%)
20	CLA	3	307	-	46,50,73	2.69	15 (32%)	55,85,113	3.39	27 (49%)
20	CLA	2	314	-	54,58,73	2.52	19 (35%)	65,95,113	3.34	24 (36%)
20	CLA	4	308	-	26,32,73	2.38	10 (38%)	34,54,113	3.06	21 (61%)
20	CLA	A	817	-	56,60,73	2.41	16 (28%)	67,97,113	2.97	25 (37%)
20	CLA	4	301	-	59,63,73	2.36	16 (27%)	71,101,113	2.86	25 (35%)
20	CLA	B	806	-	69,73,73	2.16	16 (23%)	83,113,113	2.70	27 (32%)
20	CLA	K	104	-	60,64,73	2.40	19 (31%)	72,102,113	3.01	27 (37%)
20	CLA	B	810	-	64,68,73	2.29	16 (25%)	77,107,113	2.83	27 (35%)
21	LMU	2	313	-	36,36,36	0.52	0	47,47,47	1.60	6 (12%)
21	LMU	4	319	-	35,35,36	0.80	2 (5%)	46,46,47	1.81	11 (23%)
20	CLA	A	801	-	50,54,73	2.68	15 (30%)	63,90,113	3.62	31 (49%)
24	SF4	C	103	7	0,12,12	-	-	-	-	-
20	CLA	3	312	-	26,32,73	2.39	9 (34%)	34,54,113	3.00	21 (61%)
21	LMU	A	847	-	36,36,36	0.68	1 (2%)	47,47,47	1.42	7 (14%)
20	CLA	2	304	-	26,32,73	2.35	11 (42%)	34,54,113	3.05	21 (61%)
21	LMU	B	805	-	36,36,36	0.67	1 (2%)	47,47,47	1.66	12 (25%)
20	CLA	L	202	-	59,63,73	2.36	16 (27%)	71,101,113	2.85	26 (36%)
20	CLA	A	841	-	26,32,73	2.41	9 (34%)	34,54,113	3.11	23 (67%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
20	CLA	B	809	-	69,73,73	2.18	15 (21%)	83,113,113	2.95	30 (36%)
20	CLA	A	816	-	58,62,73	2.44	21 (36%)	69,99,113	2.96	26 (37%)
21	LMU	H	104	-	36,36,36	0.60	0	47,47,47	1.63	7 (14%)
20	CLA	B	832	6	63,67,73	2.32	16 (25%)	75,105,113	2.92	26 (34%)
21	LMU	4	320	-	36,36,36	0.77	1 (2%)	47,47,47	1.28	7 (14%)
21	LMU	R	103	-	36,36,36	0.70	1 (2%)	47,47,47	1.46	6 (12%)
20	CLA	B	836	-	55,59,73	2.48	21 (38%)	66,96,113	3.16	24 (36%)
20	CLA	4	314	4	26,32,73	2.36	8 (30%)	34,54,113	2.94	20 (58%)
20	CLA	B	825	-	58,62,73	2.39	18 (31%)	69,99,113	2.85	26 (37%)
22	BCR	B	845	-	41,41,41	1.76	3 (7%)	56,56,56	4.78	19 (33%)
21	LMU	A	852	-	36,36,36	0.55	1 (2%)	47,47,47	0.85	1 (2%)
21	LMU	K	105	-	36,36,36	0.68	1 (2%)	47,47,47	1.54	8 (17%)
21	LMU	E	101	-	36,36,36	0.61	0	47,47,47	1.88	13 (27%)
20	CLA	B	835	20	49,53,73	2.60	16 (32%)	59,89,113	2.92	19 (32%)
20	CLA	H	109	-	59,63,73	2.34	14 (23%)	71,101,113	2.73	25 (35%)
20	CLA	A	807	5	50,54,73	2.51	16 (32%)	60,90,113	2.96	25 (41%)
21	LMU	2	321	-	36,36,36	0.82	1 (2%)	47,47,47	1.18	4 (8%)
21	LMU	K	106	-	36,36,36	0.37	0	47,47,47	1.06	4 (8%)
21	LMU	R	104	-	36,36,36	0.57	0	47,47,47	1.29	5 (10%)
20	CLA	B	814	-	69,73,73	2.17	15 (21%)	83,113,113	2.52	27 (32%)
20	CLA	B	807	6	49,53,73	2.61	16 (32%)	59,89,113	3.14	22 (37%)
20	CLA	A	805	5	58,62,73	2.29	13 (22%)	69,99,113	2.90	25 (36%)
20	CLA	4	304	-	59,63,73	2.32	14 (23%)	71,101,113	2.87	25 (35%)
21	LMU	3	318	-	36,36,36	0.49	0	47,47,47	0.72	1 (2%)
20	CLA	A	830	5	69,73,73	2.17	15 (21%)	83,113,113	2.61	21 (25%)
21	LMU	H	103	-	36,36,36	0.86	1 (2%)	47,47,47	2.09	12 (25%)
21	LMU	G	102	-	36,36,36	0.61	0	47,47,47	1.59	8 (17%)
21	LMU	R	109	-	36,36,36	0.49	0	47,47,47	0.82	1 (2%)
20	CLA	L	208	-	54,58,73	2.48	18 (33%)	65,95,113	3.13	24 (36%)
22	BCR	B	801	-	41,41,41	2.52	6 (14%)	56,56,56	6.08	21 (37%)
22	BCR	B	847	-	41,41,41	1.95	3 (7%)	56,56,56	5.45	17 (30%)
21	LMU	C	101	-	36,36,36	0.70	1 (2%)	47,47,47	1.26	4 (8%)
20	CLA	A	836	-	51,55,73	2.51	14 (27%)	61,91,113	2.85	22 (36%)
21	LMU	F	202	-	35,35,36	0.57	0	46,46,47	1.36	5 (10%)
20	CLA	4	311	-	26,32,73	2.33	11 (42%)	34,54,113	3.13	21 (61%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
20	CLA	A	828	5	69,73,73	2.14	14 (20%)	83,113,113	2.57	28 (33%)
20	CLA	3	305	-	26,32,73	2.30	8 (30%)	34,54,113	2.98	19 (55%)
20	CLA	A	835	5	69,73,73	2.22	17 (24%)	83,113,113	2.79	31 (37%)
20	CLA	1	215	-	55,59,73	2.50	23 (41%)	66,96,113	3.10	26 (39%)
20	CLA	2	316	-	69,73,73	2.33	23 (33%)	83,113,113	2.80	26 (31%)
20	CLA	A	806	-	60,64,73	2.29	14 (23%)	72,102,113	2.95	27 (37%)
20	CLA	K	101	-	50,54,73	2.58	18 (36%)	60,90,113	3.02	23 (38%)
20	CLA	B	824	-	69,73,73	2.43	23 (33%)	83,113,113	2.73	26 (31%)
20	CLA	3	317	-	39,44,73	2.79	13 (33%)	52,78,113	3.30	25 (48%)
20	CLA	A	814	5	26,32,73	2.38	10 (38%)	34,54,113	3.14	19 (55%)
20	CLA	H	102	-	59,63,73	2.31	13 (22%)	71,101,113	2.90	26 (36%)
20	CLA	B	833	6	54,58,73	2.45	17 (31%)	65,95,113	3.06	25 (38%)
20	CLA	1	204	-	50,54,73	2.73	21 (42%)	60,90,113	3.45	28 (46%)
21	LMU	A	846	-	36,36,36	0.70	0	47,47,47	1.27	7 (14%)
22	BCR	I	101	-	39,40,41	1.67	3 (7%)	52,53,56	4.25	19 (36%)
20	CLA	G	105	-	55,59,73	2.49	19 (34%)	66,96,113	3.00	24 (36%)
20	CLA	3	304	-	26,32,73	2.34	10 (38%)	34,54,113	3.22	21 (61%)
21	LMU	1	216	-	36,36,36	0.45	0	47,47,47	1.38	6 (12%)
20	CLA	H	101	-	59,63,73	2.39	15 (25%)	71,101,113	2.92	27 (38%)
20	CLA	4	318	-	51,55,73	2.54	19 (37%)	61,91,113	3.23	29 (47%)
20	CLA	B	829	-	69,73,73	2.11	15 (21%)	83,113,113	2.75	28 (33%)
20	CLA	A	834	-	50,54,73	2.53	15 (30%)	60,90,113	3.03	25 (41%)
22	BCR	B	844	-	41,41,41	1.86	3 (7%)	56,56,56	5.19	24 (42%)
20	CLA	4	305	-	54,58,73	2.53	19 (35%)	65,95,113	2.97	27 (41%)
20	CLA	4	312	-	26,32,73	2.44	8 (30%)	34,54,113	3.12	21 (61%)
20	CLA	3	314	-	69,73,73	2.30	24 (34%)	83,113,113	2.90	28 (33%)
20	CLA	B	823	6	59,63,73	2.38	17 (28%)	71,101,113	2.74	27 (38%)
20	CLA	H	110	16	54,58,73	2.45	13 (24%)	65,95,113	2.87	26 (40%)
20	CLA	A	824	-	63,67,73	2.25	16 (25%)	75,105,113	2.77	28 (37%)
20	CLA	A	826	-	69,73,73	2.15	17 (24%)	83,113,113	2.69	27 (32%)
22	BCR	G	104	-	41,41,41	1.87	3 (7%)	56,56,56	5.73	17 (30%)
20	CLA	2	303	-	62,66,73	2.42	21 (33%)	74,104,113	3.13	29 (39%)
20	CLA	3	311	-	69,73,73	2.18	16 (23%)	83,113,113	2.70	24 (28%)
20	CLA	K	102	-	54,58,73	2.46	16 (29%)	65,95,113	2.99	24 (36%)
20	CLA	B	811	6	26,32,73	2.40	11 (42%)	34,54,113	2.87	20 (58%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
25	LMG	B	848	-	49,49,55	0.99	2 (4%)	57,57,63	1.08	3 (5%)
20	CLA	I	102	-	64,68,73	2.24	14 (21%)	77,107,113	2.70	23 (29%)
20	CLA	2	312	-	65,69,73	2.29	20 (30%)	78,108,113	2.95	32 (41%)
20	CLA	B	821	-	54,58,73	2.40	14 (25%)	65,95,113	2.99	26 (40%)
22	BCR	F	203	-	41,41,41	2.01	3 (7%)	56,56,56	5.47	19 (33%)
20	CLA	A	804	20	59,63,73	2.37	15 (25%)	71,101,113	2.96	27 (38%)
20	CLA	1	211	-	55,59,73	2.57	22 (40%)	66,96,113	3.42	29 (43%)
20	CLA	B	819	6	45,49,73	2.93	23 (51%)	54,84,113	3.52	25 (46%)
21	LMU	H	105	-	36,36,36	0.72	1 (2%)	47,47,47	1.66	9 (19%)
20	CLA	B	834	20	49,53,73	2.61	15 (30%)	59,89,113	3.00	20 (33%)
20	CLA	B	822	-	50,54,73	2.48	15 (30%)	60,90,113	3.14	20 (33%)
20	CLA	2	306	-	26,32,73	2.26	9 (34%)	34,54,113	3.03	21 (61%)
24	SF4	A	856	6,5	0,12,12	-	-	-	-	-
20	CLA	B	850	6	69,73,73	2.14	16 (23%)	83,113,113	2.76	32 (38%)
20	CLA	R	107	-	61,65,73	2.31	13 (21%)	73,103,113	2.85	28 (38%)
20	CLA	R	108	-	69,73,73	2.17	13 (18%)	83,113,113	2.62	28 (33%)
21	LMU	R	102	-	36,36,36	0.57	0	47,47,47	1.51	9 (19%)
24	SF4	C	102	7	0,12,12	-	-	-	-	-
20	CLA	B	841	-	69,73,73	2.09	16 (23%)	83,113,113	2.68	25 (30%)
20	CLA	1	209	-	26,32,73	2.40	8 (30%)	34,54,113	3.07	23 (67%)
21	LMU	R	105	-	36,36,36	0.75	1 (2%)	47,47,47	1.39	8 (17%)
20	CLA	F	201	6,10	54,58,73	2.53	23 (42%)	65,95,113	3.18	26 (40%)
20	CLA	F	205	-	39,44,73	2.75	15 (38%)	52,78,113	3.20	25 (48%)
20	CLA	3	310	-	69,73,73	2.26	21 (30%)	83,113,113	2.81	32 (38%)
20	CLA	L	201	5	64,68,73	2.28	15 (23%)	77,107,113	2.65	25 (32%)
20	CLA	4	309	-	26,32,73	2.37	8 (30%)	34,54,113	3.10	19 (55%)
20	CLA	3	316	-	26,32,73	2.39	11 (42%)	34,54,113	3.14	20 (58%)
20	CLA	4	315	-	50,54,73	2.52	18 (36%)	60,90,113	3.01	23 (38%)
20	CLA	A	818	-	64,68,73	2.41	22 (34%)	77,107,113	2.96	32 (41%)
22	BCR	A	845	-	41,41,41	2.01	4 (9%)	56,56,56	5.71	26 (46%)
23	PQN	A	842	-	34,34,34	1.69	2 (5%)	42,45,45	1.21	5 (11%)
20	CLA	F	206	20	45,49,73	2.68	16 (35%)	54,84,113	3.16	23 (42%)
20	CLA	B	827	6	69,73,73	2.15	16 (23%)	83,113,113	2.57	25 (30%)
20	CLA	A	837	-	55,59,73	2.42	16 (29%)	66,96,113	3.15	25 (37%)
21	LMU	L	206	-	36,36,36	0.51	0	47,47,47	1.00	3 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
20	CLA	L	203	-	69,73,73	2.09	13 (18%)	83,113,113	2.71	29 (34%)
20	CLA	A	819	-	62,66,73	2.31	17 (27%)	74,104,113	2.80	25 (33%)
20	CLA	2	310	2	54,58,73	2.61	18 (33%)	65,95,113	3.06	26 (40%)
20	CLA	3	313	-	54,58,73	2.46	13 (24%)	65,95,113	2.80	25 (38%)
20	CLA	A	850	-	69,73,73	2.19	16 (23%)	83,113,113	2.69	26 (31%)
21	LMU	4	316	-	36,36,36	0.72	1 (2%)	47,47,47	1.08	3 (6%)
20	CLA	1	212	-	26,32,73	2.36	8 (30%)	34,54,113	3.02	21 (61%)
22	BCR	A	844	-	41,41,41	2.02	3 (7%)	56,56,56	5.57	21 (37%)
20	CLA	B	840	-	69,73,73	2.15	15 (21%)	83,113,113	2.63	27 (32%)
20	CLA	F	207	20	57,61,73	2.69	25 (43%)	68,98,113	3.05	30 (44%)
20	CLA	A	838	5	69,73,73	2.17	16 (23%)	83,113,113	2.67	31 (37%)
20	CLA	A	823	-	62,66,73	2.23	14 (22%)	74,104,113	2.68	25 (33%)
20	CLA	A	815	5	54,58,73	2.48	13 (24%)	65,95,113	2.91	28 (43%)
20	CLA	L	207	16	51,55,73	2.50	13 (25%)	61,91,113	3.19	26 (42%)
21	LMU	B	804	-	36,36,36	0.70	0	47,47,47	1.75	12 (25%)
21	LMU	2	320	-	36,36,36	0.46	0	47,47,47	1.27	3 (6%)
20	CLA	B	826	-	62,66,73	2.29	16 (25%)	74,104,113	2.73	24 (32%)
20	CLA	A	827	5	59,63,73	2.31	16 (27%)	71,101,113	2.85	27 (38%)
20	CLA	3	303	-	39,44,73	2.84	11 (28%)	52,78,113	3.20	23 (44%)
20	CLA	3	308	-	26,32,73	2.33	8 (30%)	34,54,113	3.15	20 (58%)
21	LMU	1	217	-	36,36,36	0.57	0	47,47,47	0.98	1 (2%)
20	CLA	A	810	-	49,53,73	2.62	14 (28%)	59,89,113	3.21	26 (44%)
21	LMU	2	318	-	36,36,36	0.56	0	47,47,47	0.68	0
21	LMU	G	101	19	36,36,36	1.11	4 (11%)	47,47,47	2.03	11 (23%)
22	BCR	A	843	-	41,41,41	1.95	3 (7%)	56,56,56	5.48	21 (37%)
20	CLA	2	305	2	54,58,73	2.43	13 (24%)	65,95,113	2.77	25 (38%)
20	CLA	1	202	1	45,49,73	2.66	14 (31%)	54,84,113	3.09	21 (38%)
20	CLA	3	315	-	26,32,73	2.43	10 (38%)	34,54,113	3.20	23 (67%)
20	CLA	4	317	-	56,60,73	2.44	16 (28%)	67,97,113	3.20	30 (44%)
20	CLA	J	103	-	65,69,73	2.27	20 (30%)	78,108,113	2.62	24 (30%)
20	CLA	4	310	-	54,58,73	2.50	19 (35%)	65,95,113	3.10	25 (38%)
21	LMU	3	319	-	36,36,36	0.44	0	47,47,47	1.12	4 (8%)
22	BCR	J	102	-	41,41,41	1.92	3 (7%)	56,56,56	5.54	18 (32%)
20	CLA	2	311	-	54,58,73	2.46	15 (27%)	65,95,113	3.00	30 (46%)
20	CLA	B	838	6	69,73,73	2.10	14 (20%)	83,113,113	2.60	26 (31%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
20	CLA	A	849	-	69,73,73	2.11	17 (24%)	83,113,113	2.78	27 (32%)
20	CLA	A	812	5	58,62,73	2.32	16 (27%)	69,99,113	2.70	21 (30%)
20	CLA	2	308	-	26,32,73	2.37	12 (46%)	34,54,113	3.24	21 (61%)
20	CLA	A	832	5	54,58,73	2.44	15 (27%)	65,95,113	2.89	25 (38%)
20	CLA	A	840	-	59,63,73	2.29	14 (23%)	71,101,113	2.93	24 (33%)
23	PQN	B	843	-	34,34,34	1.66	2 (5%)	42,45,45	1.35	6 (14%)
20	CLA	4	303	-	69,73,73	2.28	22 (31%)	83,113,113	2.99	32 (38%)
20	CLA	2	301	-	26,32,73	2.33	8 (30%)	34,54,113	3.07	23 (67%)
22	BCR	L	209	-	41,41,41	2.00	4 (9%)	56,56,56	5.64	17 (30%)
21	LMU	2	319	-	36,36,36	0.82	1 (2%)	47,47,47	1.56	11 (23%)
21	LMU	A	855	-	36,36,36	0.66	1 (2%)	47,47,47	1.38	7 (14%)
20	CLA	2	309	-	26,32,73	2.34	10 (38%)	34,54,113	3.07	21 (61%)
20	CLA	2	315	-	26,32,73	2.36	10 (38%)	34,54,113	3.03	19 (55%)
20	CLA	A	825	5	69,73,73	2.15	16 (23%)	83,113,113	2.45	22 (26%)
20	CLA	4	306	4	56,60,73	2.66	21 (37%)	67,97,113	3.25	35 (52%)
20	CLA	B	813	6	59,63,73	2.28	15 (25%)	71,101,113	2.80	24 (33%)
20	CLA	3	302	6	26,32,73	2.37	8 (30%)	34,54,113	2.99	19 (55%)
20	CLA	B	828	-	69,73,73	2.23	15 (21%)	83,113,113	2.74	27 (32%)
20	CLA	1	201	1	50,54,73	2.53	19 (38%)	60,90,113	3.54	31 (51%)
20	CLA	1	205	-	39,44,73	2.89	13 (33%)	52,78,113	3.14	22 (42%)
20	CLA	A	839	20	63,67,73	2.47	21 (33%)	75,105,113	3.02	31 (41%)
20	CLA	4	302	-	39,44,73	2.98	16 (41%)	52,78,113	3.37	24 (46%)
21	LMU	K	107	-	36,36,36	0.52	0	47,47,47	1.31	6 (12%)
21	LMU	H	106	-	36,36,36	0.60	1 (2%)	47,47,47	1.58	11 (23%)
20	CLA	A	829	5	54,58,73	2.46	13 (24%)	65,95,113	2.95	25 (38%)
20	CLA	2	302	-	55,59,73	2.62	21 (38%)	66,96,113	3.11	26 (39%)
20	CLA	B	803	-	69,73,73	2.18	15 (21%)	83,113,113	2.69	27 (32%)
20	CLA	1	203	-	51,55,73	2.61	18 (35%)	61,91,113	3.42	30 (49%)
20	CLA	B	812	6	58,62,73	2.71	24 (41%)	73,100,113	3.20	28 (38%)
21	LMU	L	205	-	36,36,36	0.65	0	47,47,47	1.92	13 (27%)
20	CLA	1	210	1	39,44,73	2.78	12 (30%)	52,78,113	3.22	22 (42%)
20	CLA	2	307	-	69,73,73	2.17	17 (24%)	83,113,113	2.76	30 (36%)
20	CLA	A	820	-	55,59,73	2.44	14 (25%)	66,96,113	2.96	22 (33%)
20	CLA	B	808	-	65,69,73	2.25	20 (30%)	78,108,113	2.75	29 (37%)
22	BCR	B	846	-	41,41,41	1.98	4 (9%)	56,56,56	5.56	21 (37%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
20	CLA	4	313	-	39,44,73	2.75	14 (35%)	52,78,113	3.41	25 (48%)
20	CLA	A	813	5	54,58,73	2.39	15 (27%)	65,95,113	2.93	27 (41%)
21	LMU	1	218	-	36,36,36	0.70	0	47,47,47	1.65	8 (17%)
22	BCR	I	103	-	41,41,41	2.13	5 (12%)	56,56,56	6.16	28 (50%)
20	CLA	1	207	-	55,59,73	2.48	17 (30%)	66,96,113	3.36	26 (39%)
20	CLA	3	306	-	26,32,73	2.33	10 (38%)	34,54,113	3.06	20 (58%)
20	CLA	B	816	6	64,68,73	2.20	12 (18%)	77,107,113	2.61	26 (33%)
21	LMU	A	854	-	36,36,36	0.51	0	47,47,47	1.28	7 (14%)
20	CLA	3	309	-	26,32,73	2.33	9 (34%)	34,54,113	3.19	21 (61%)
20	CLA	A	833	20,5	49,53,73	2.61	15 (30%)	59,89,113	3.21	27 (45%)
22	BCR	F	204	-	41,41,41	2.16	5 (12%)	56,56,56	5.75	24 (42%)
20	CLA	A	811	20,5	69,73,73	2.16	13 (18%)	83,113,113	2.82	29 (34%)
20	CLA	B	815	-	64,68,73	2.24	13 (20%)	77,107,113	2.66	25 (32%)
20	CLA	A	831	5	69,73,73	2.33	25 (36%)	83,113,113	3.17	31 (37%)
20	CLA	B	820	-	65,69,73	2.15	15 (23%)	78,108,113	2.77	25 (32%)
20	CLA	B	839	-	51,55,73	2.73	23 (45%)	61,91,113	3.55	27 (44%)
21	LMU	G	103	-	36,36,36	0.50	0	47,47,47	0.93	1 (2%)
20	CLA	B	837	6	64,68,73	2.20	14 (21%)	77,107,113	2.75	22 (28%)
20	CLA	A	809	5	56,60,73	2.37	14 (25%)	67,97,113	2.93	32 (47%)
20	CLA	A	802	-	26,32,73	2.41	8 (30%)	34,54,113	3.13	22 (64%)
20	CLA	1	208	-	26,32,73	2.31	8 (30%)	34,54,113	2.94	21 (61%)
20	CLA	B	830	6	69,73,73	2.16	16 (23%)	83,113,113	2.77	28 (33%)
20	CLA	H	108	-	62,66,73	2.52	22 (35%)	74,104,113	3.06	31 (41%)
20	CLA	4	307	-	26,32,73	2.38	9 (34%)	34,54,113	3.03	21 (61%)
20	CLA	A	803	-	50,54,73	2.64	21 (42%)	60,90,113	3.36	24 (40%)
21	LMU	A	848	-	36,36,36	0.49	0	47,47,47	0.86	3 (6%)
21	LMU	A	853	-	36,36,36	0.50	0	47,47,47	1.42	6 (12%)
20	CLA	B	817	-	50,54,73	2.45	13 (26%)	60,90,113	2.97	27 (45%)
22	BCR	2	317	-	41,41,41	1.96	3 (7%)	56,56,56	5.70	19 (33%)
20	CLA	1	213	-	55,59,73	2.73	26 (47%)	66,96,113	3.22	29 (43%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
20	CLA	A	822	5	-	6/21/97/115	-
20	CLA	A	851	-	1/1/15/20	25/39/115/115	-
20	CLA	A	808	5	1/1/14/20	16/33/109/115	-
21	LMU	D	201	-	-	9/21/61/61	0/2/2/2
21	LMU	4	321	-	-	15/21/61/61	0/2/2/2
21	LMU	L	210	-	-	16/21/61/61	0/2/2/2
21	LMU	R	106	-	-	12/21/61/61	0/2/2/2
21	LMU	R	101	-	-	13/21/61/61	0/2/2/2
21	LMU	B	849	-	-	5/11/51/61	0/2/2/2
20	CLA	K	103	-	-	12/21/97/115	-
20	CLA	A	821	5	-	3/12/88/115	-
20	CLA	B	831	6	-	11/21/97/115	-
20	CLA	1	206	-	1/1/14/20	21/35/111/115	-
20	CLA	B	802	-	-	11/26/102/115	-
20	CLA	J	101	-	-	10/19/95/115	-
20	CLA	B	818	-	-	9/25/101/115	-
20	CLA	L	204	-	1/1/13/20	8/27/103/115	-
20	CLA	3	307	-	-	9/12/88/115	-
20	CLA	2	314	-	-	9/21/97/115	-
20	CLA	B	806	-	1/1/15/20	21/39/115/115	-
20	CLA	A	817	-	-	15/24/100/115	-
20	CLA	4	301	-	1/1/13/20	14/27/103/115	-
20	CLA	K	104	-	1/1/13/20	11/29/105/115	-
21	LMU	2	313	-	-	16/21/61/61	0/2/2/2
20	CLA	B	810	-	1/1/14/20	11/33/109/115	-
21	LMU	4	319	-	-	13/20/60/61	0/2/2/2
20	CLA	A	801	-	2/2/11/20	11/16/92/115	-
24	SF4	C	103	7	-	-	0/6/5/5
21	LMU	A	847	-	-	13/21/61/61	0/2/2/2
21	LMU	B	805	-	-	13/21/61/61	0/2/2/2
20	CLA	L	202	-	1/1/13/20	14/27/103/115	-
20	CLA	B	809	-	1/1/15/20	18/39/115/115	-
20	CLA	A	816	-	-	11/26/102/115	-
21	LMU	H	104	-	-	12/21/61/61	0/2/2/2
20	CLA	B	832	6	1/1/13/20	17/32/108/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
21	LMU	4	320	-	-	16/21/61/61	0/2/2/2
21	LMU	R	103	-	-	11/21/61/61	0/2/2/2
20	CLA	B	836	-	-	11/23/99/115	-
20	CLA	B	825	-	-	10/26/102/115	-
22	BCR	B	845	-	-	9/29/63/63	0/2/2/2
21	LMU	A	852	-	-	20/21/61/61	0/2/2/2
21	LMU	K	105	-	-	12/21/61/61	0/2/2/2
21	LMU	E	101	-	-	14/21/61/61	0/2/2/2
20	CLA	B	835	20	-	8/15/91/115	-
20	CLA	H	109	-	1/1/13/20	9/27/103/115	-
20	CLA	A	807	5	-	9/17/93/115	-
21	LMU	2	321	-	-	8/21/61/61	0/2/2/2
21	LMU	K	106	-	-	13/21/61/61	0/2/2/2
21	LMU	R	104	-	-	14/21/61/61	0/2/2/2
20	CLA	B	814	-	1/1/15/20	23/39/115/115	-
20	CLA	B	807	6	-	6/15/91/115	-
20	CLA	A	805	5	-	14/26/102/115	-
20	CLA	4	304	-	1/1/13/20	13/27/103/115	-
21	LMU	3	318	-	-	12/21/61/61	0/2/2/2
20	CLA	A	830	5	1/1/15/20	20/39/115/115	-
21	LMU	H	103	-	-	14/21/61/61	0/2/2/2
21	LMU	G	102	-	-	14/21/61/61	0/2/2/2
21	LMU	R	109	-	-	14/21/61/61	0/2/2/2
20	CLA	L	208	-	1/1/12/20	11/21/97/115	-
22	BCR	B	801	-	-	13/29/63/63	0/2/2/2
22	BCR	B	847	-	-	12/29/63/63	0/2/2/2
21	LMU	C	101	-	-	14/21/61/61	0/2/2/2
20	CLA	A	836	-	-	8/18/94/115	-
21	LMU	F	202	-	-	13/20/60/61	0/2/2/2
20	CLA	A	828	5	1/1/15/20	21/39/115/115	-
20	CLA	A	835	5	1/1/15/20	16/39/115/115	-
20	CLA	1	215	-	1/1/12/20	9/23/99/115	-
20	CLA	2	316	-	1/1/15/20	16/39/115/115	-
20	CLA	A	806	-	1/1/13/20	7/29/105/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
20	CLA	K	101	-	-	7/17/93/115	-
20	CLA	B	824	-	1/1/15/20	21/39/115/115	-
20	CLA	H	102	-	1/1/13/20	15/27/103/115	-
20	CLA	B	833	6	-	8/21/97/115	-
20	CLA	1	204	-	-	11/17/93/115	-
21	LMU	A	846	-	-	17/21/61/61	0/2/2/2
22	BCR	I	101	-	-	10/29/60/63	0/2/2/2
20	CLA	G	105	-	-	11/23/99/115	-
21	LMU	1	216	-	-	11/21/61/61	0/2/2/2
20	CLA	H	101	-	2/2/13/20	11/27/103/115	-
20	CLA	4	318	-	-	13/18/94/115	-
20	CLA	B	829	-	1/1/15/20	20/39/115/115	-
20	CLA	A	834	-	-	9/17/93/115	-
22	BCR	B	844	-	-	7/29/63/63	0/2/2/2
20	CLA	4	305	-	-	11/21/97/115	-
20	CLA	3	314	-	1/1/15/20	18/39/115/115	-
20	CLA	B	823	6	1/1/13/20	11/27/103/115	-
20	CLA	H	110	16	-	9/21/97/115	-
20	CLA	A	824	-	1/1/13/20	15/32/108/115	-
20	CLA	A	826	-	1/1/15/20	15/39/115/115	-
22	BCR	G	104	-	-	14/29/63/63	0/2/2/2
20	CLA	2	303	-	1/1/13/20	16/31/107/115	-
20	CLA	3	311	-	1/1/15/20	22/39/115/115	-
20	CLA	K	102	-	-	5/21/97/115	-
25	LMG	B	848	-	-	27/44/64/70	0/1/1/1
20	CLA	I	102	-	1/1/14/20	14/33/109/115	-
20	CLA	2	312	-	1/1/14/20	23/35/111/115	-
20	CLA	B	821	-	-	7/21/97/115	-
22	BCR	F	203	-	-	13/29/63/63	0/2/2/2
20	CLA	A	804	20	1/1/13/20	12/27/103/115	-
20	CLA	1	211	-	1/1/12/20	9/23/99/115	-
20	CLA	B	819	6	-	2/10/86/115	-
21	LMU	H	105	-	-	17/21/61/61	0/2/2/2
20	CLA	B	834	20	-	11/15/91/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
20	CLA	B	822	-	-	13/17/93/115	-
24	SF4	A	856	6,5	-	-	0/6/5/5
20	CLA	B	850	6	1/1/15/20	23/39/115/115	-
20	CLA	R	107	-	1/1/13/20	15/30/106/115	-
20	CLA	R	108	-	1/1/15/20	21/39/115/115	-
21	LMU	R	102	-	-	11/21/61/61	0/2/2/2
24	SF4	C	102	7	-	-	0/6/5/5
20	CLA	B	841	-	1/1/15/20	19/39/115/115	-
21	LMU	R	105	-	-	14/21/61/61	0/2/2/2
20	CLA	F	201	6,10	-	11/21/97/115	-
20	CLA	3	310	-	1/1/15/20	18/39/115/115	-
20	CLA	L	201	5	1/1/14/20	14/33/109/115	-
20	CLA	4	315	-	-	10/17/93/115	-
23	PQN	A	842	-	1/1/8/9	11/23/43/43	0/2/2/2
20	CLA	A	818	-	1/1/14/20	15/33/109/115	-
22	BCR	A	845	-	-	10/29/63/63	0/2/2/2
20	CLA	F	206	20	-	5/10/86/115	-
20	CLA	B	827	6	1/1/15/20	22/39/115/115	-
20	CLA	A	837	-	-	15/23/99/115	-
21	LMU	L	206	-	-	14/21/61/61	0/2/2/2
20	CLA	L	203	-	1/1/15/20	17/39/115/115	-
20	CLA	A	819	-	1/1/13/20	11/31/107/115	-
20	CLA	2	310	2	-	6/21/97/115	-
20	CLA	A	850	-	1/1/15/20	18/39/115/115	-
20	CLA	3	313	-	-	10/21/97/115	-
21	LMU	4	316	-	-	13/21/61/61	0/2/2/2
22	BCR	A	844	-	-	14/29/63/63	0/2/2/2
20	CLA	B	840	-	1/1/15/20	18/39/115/115	-
20	CLA	F	207	20	3/3/12/20	12/25/101/115	-
20	CLA	A	838	5	1/1/15/20	19/39/115/115	-
20	CLA	A	823	-	1/1/13/20	13/31/107/115	-
20	CLA	A	815	5	-	11/21/97/115	-
20	CLA	L	207	16	-	11/18/94/115	-
21	LMU	B	804	-	-	16/21/61/61	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
21	LMU	2	320	-	-	18/21/61/61	0/2/2/2
20	CLA	B	826	-	1/1/13/20	19/31/107/115	-
20	CLA	A	827	5	1/1/13/20	10/27/103/115	-
21	LMU	1	217	-	-	9/21/61/61	0/2/2/2
21	LMU	2	318	-	-	13/21/61/61	0/2/2/2
20	CLA	A	810	-	-	5/15/91/115	-
21	LMU	G	101	19	-	13/21/61/61	0/2/2/2
22	BCR	A	843	-	-	14/29/63/63	0/2/2/2
22	BCR	J	102	-	-	11/29/63/63	0/2/2/2
20	CLA	2	305	2	-	7/21/97/115	-
20	CLA	1	202	1	-	5/10/86/115	-
20	CLA	J	103	-	1/1/14/20	21/35/111/115	-
20	CLA	4	317	-	-	12/24/100/115	-
21	LMU	3	319	-	-	11/21/61/61	0/2/2/2
20	CLA	4	310	-	-	11/21/97/115	-
20	CLA	B	838	6	1/1/15/20	13/39/115/115	-
20	CLA	2	311	-	-	12/21/97/115	-
20	CLA	A	849	-	1/1/15/20	26/39/115/115	-
20	CLA	A	840	-	1/1/13/20	8/27/103/115	-
20	CLA	A	812	5	-	14/26/102/115	-
20	CLA	A	832	5	-	12/21/97/115	-
23	PQN	B	843	-	1/1/8/9	10/23/43/43	0/2/2/2
20	CLA	4	303	-	2/2/15/20	23/39/115/115	-
22	BCR	L	209	-	-	10/29/63/63	0/2/2/2
21	LMU	2	319	-	-	11/21/61/61	0/2/2/2
21	LMU	A	855	-	-	13/21/61/61	0/2/2/2
20	CLA	A	825	5	1/1/15/20	25/39/115/115	-
20	CLA	4	306	4	1/1/12/20	8/24/100/115	-
20	CLA	B	813	6	1/1/13/20	13/27/103/115	-
20	CLA	B	828	-	1/1/15/20	17/39/115/115	-
20	CLA	1	201	1	-	12/17/93/115	-
20	CLA	A	839	20	1/1/13/20	15/31/107/115	-
21	LMU	K	107	-	-	17/21/61/61	0/2/2/2
21	LMU	H	106	-	-	9/21/61/61	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
20	CLA	A	829	5	-	6/21/97/115	-
20	CLA	2	302	-	-	13/23/99/115	-
20	CLA	B	803	-	1/1/15/20	20/39/115/115	-
20	CLA	1	203	-	-	10/18/94/115	-
20	CLA	B	812	6	1/1/13/20	8/25/101/115	-
21	LMU	L	205	-	-	13/21/61/61	0/2/2/2
20	CLA	2	307	-	1/1/15/20	22/39/115/115	-
20	CLA	B	808	-	1/1/14/20	20/35/111/115	-
20	CLA	A	820	-	-	9/23/99/115	-
22	BCR	B	846	-	-	14/29/63/63	0/2/2/2
20	CLA	A	813	5	-	10/21/97/115	-
21	LMU	1	218	-	-	13/21/61/61	0/2/2/2
22	BCR	I	103	-	-	15/29/63/63	0/2/2/2
20	CLA	1	207	-	1/1/12/20	10/23/99/115	-
20	CLA	B	816	6	1/1/14/20	16/33/109/115	-
21	LMU	A	854	-	-	16/21/61/61	0/2/2/2
20	CLA	A	833	20,5	-	7/15/91/115	-
22	BCR	F	204	-	-	9/29/63/63	0/2/2/2
20	CLA	A	811	20,5	1/1/15/20	25/39/115/115	-
20	CLA	B	815	-	1/1/14/20	19/33/109/115	-
20	CLA	A	831	5	1/1/15/20	20/39/115/115	-
20	CLA	B	820	-	1/1/14/20	15/35/111/115	-
20	CLA	B	839	-	-	11/18/94/115	-
21	LMU	G	103	-	-	14/21/61/61	0/2/2/2
20	CLA	B	837	6	1/1/14/20	15/33/109/115	-
20	CLA	A	809	5	-	11/24/100/115	-
20	CLA	H	108	-	1/1/13/20	20/31/107/115	-
20	CLA	B	830	6	1/1/15/20	27/39/115/115	-
21	LMU	A	848	-	-	12/21/61/61	0/2/2/2
20	CLA	A	803	-	-	5/17/93/115	-
21	LMU	A	853	-	-	11/21/61/61	0/2/2/2
20	CLA	B	817	-	-	13/17/93/115	-
22	BCR	2	317	-	-	15/29/63/63	0/2/2/2
20	CLA	1	213	-	2/2/12/20	11/23/99/115	-

The worst 5 of 2740 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	B	801	BCR	C21-C22	-9.91	1.22	1.35
22	B	801	BCR	C20-C21	-9.21	1.14	1.43
22	F	204	BCR	C21-C22	-8.47	1.24	1.35
22	A	843	BCR	C20-C21	-8.38	1.17	1.43
22	A	844	BCR	C20-C21	-8.34	1.17	1.43

The worst 5 of 5036 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	G	104	BCR	C20-C21-C22	36.27	179.07	127.31
22	L	209	BCR	C20-C21-C22	35.78	178.38	127.31
22	A	845	BCR	C20-C21-C22	35.54	178.03	127.31
22	J	102	BCR	C20-C21-C22	35.47	177.93	127.31
22	B	846	BCR	C20-C21-C22	35.39	177.82	127.31

5 of 85 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
20	1	206	CLA	C8
20	1	207	CLA	C2A
20	1	211	CLA	CBD
20	1	213	CLA	C2A
20	1	213	CLA	C3A

5 of 2678 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.

222 monomers are involved in 2653 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
20	A	822	CLA	19	0
20	A	851	CLA	26	0
20	A	808	CLA	19	0
21	D	201	LMU	3	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
21	4	321	LMU	13	0
21	L	210	LMU	1	0
21	R	106	LMU	9	0
21	R	101	LMU	3	0
21	B	849	LMU	1	0
20	K	103	CLA	8	0
20	A	821	CLA	8	0
20	B	831	CLA	8	0
20	1	206	CLA	10	0
20	B	802	CLA	16	0
20	J	101	CLA	12	0
20	B	818	CLA	15	0
20	L	204	CLA	14	0
20	B	842	CLA	2	0
20	3	307	CLA	14	0
20	2	314	CLA	17	0
20	A	817	CLA	6	0
20	4	301	CLA	36	0
20	B	806	CLA	24	0
20	K	104	CLA	17	0
20	B	810	CLA	18	0
21	2	313	LMU	29	0
21	4	319	LMU	8	3
20	A	801	CLA	9	0
24	C	103	SF4	1	0
21	A	847	LMU	4	0
20	2	304	CLA	2	0
21	B	805	LMU	3	0
20	L	202	CLA	10	0
20	A	841	CLA	1	0
20	B	809	CLA	21	0
20	A	816	CLA	20	0
21	H	104	LMU	9	0
20	B	832	CLA	22	0
21	4	320	LMU	2	0
21	R	103	LMU	9	0
20	B	836	CLA	9	0
20	4	314	CLA	10	0
20	B	825	CLA	24	0
22	B	845	BCR	16	0
21	A	852	LMU	4	0
21	K	105	LMU	12	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
21	E	101	LMU	11	0
20	B	835	CLA	34	0
20	H	109	CLA	13	0
20	A	807	CLA	33	0
21	K	106	LMU	8	0
21	R	104	LMU	5	0
20	B	814	CLA	28	0
20	B	807	CLA	8	0
20	A	805	CLA	13	0
20	4	304	CLA	21	0
21	3	318	LMU	2	0
20	A	830	CLA	30	0
21	H	103	LMU	6	0
21	G	102	LMU	7	0
21	R	109	LMU	9	3
20	L	208	CLA	8	0
22	B	801	BCR	24	0
22	B	847	BCR	34	0
20	A	836	CLA	4	0
21	F	202	LMU	8	0
20	4	311	CLA	3	0
20	A	828	CLA	14	0
20	3	305	CLA	3	0
20	A	835	CLA	15	0
20	1	215	CLA	1	0
20	2	316	CLA	11	0
20	A	806	CLA	12	0
20	K	101	CLA	15	1
20	B	824	CLA	32	0
20	A	814	CLA	14	0
20	H	102	CLA	2	0
20	B	833	CLA	15	0
20	1	204	CLA	14	0
21	A	846	LMU	5	0
22	I	101	BCR	7	0
20	G	105	CLA	4	0
20	3	304	CLA	2	0
21	1	216	LMU	3	0
20	H	101	CLA	14	0
20	4	318	CLA	13	0
20	B	829	CLA	26	0
20	A	834	CLA	7	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
22	B	844	BCR	7	0
20	4	305	CLA	5	0
20	4	312	CLA	4	0
20	3	314	CLA	11	0
20	B	823	CLA	15	0
20	H	110	CLA	3	0
20	A	824	CLA	46	0
20	A	826	CLA	47	0
22	G	104	BCR	4	0
20	2	303	CLA	23	0
20	3	311	CLA	10	0
20	K	102	CLA	25	0
20	B	811	CLA	4	0
25	B	848	LMG	16	0
20	I	102	CLA	11	0
20	2	312	CLA	19	0
20	B	821	CLA	8	0
22	F	203	BCR	27	0
20	A	804	CLA	36	0
20	1	211	CLA	7	0
20	B	819	CLA	9	0
21	H	105	LMU	18	0
20	B	834	CLA	23	0
20	B	822	CLA	15	0
24	A	856	SF4	18	0
20	B	850	CLA	18	0
20	R	107	CLA	10	0
20	R	108	CLA	4	0
21	R	102	LMU	8	0
24	C	102	SF4	4	0
20	B	841	CLA	17	0
20	1	209	CLA	1	0
20	F	201	CLA	30	0
20	F	205	CLA	1	0
20	3	310	CLA	16	0
20	L	201	CLA	21	0
20	4	315	CLA	5	0
20	A	818	CLA	44	0
22	A	845	BCR	48	0
23	A	842	PQN	7	0
20	F	206	CLA	6	0
20	B	827	CLA	33	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
20	A	837	CLA	16	0
20	L	203	CLA	27	0
20	A	819	CLA	34	0
20	2	310	CLA	20	0
20	3	313	CLA	1	0
20	A	850	CLA	28	0
21	4	316	LMU	1	0
20	1	212	CLA	2	0
22	A	844	BCR	23	0
20	B	840	CLA	13	0
20	F	207	CLA	12	0
20	A	838	CLA	31	0
20	A	823	CLA	11	0
20	A	815	CLA	3	0
20	L	207	CLA	24	0
21	B	804	LMU	7	0
21	2	320	LMU	5	0
20	B	826	CLA	40	0
20	A	827	CLA	20	0
20	3	303	CLA	3	0
20	3	308	CLA	2	0
21	1	217	LMU	20	0
20	A	810	CLA	5	0
21	2	318	LMU	6	0
21	G	101	LMU	4	28
22	A	843	BCR	32	0
20	2	305	CLA	15	0
20	4	317	CLA	3	0
20	J	103	CLA	14	0
20	4	310	CLA	26	0
21	3	319	LMU	14	0
22	J	102	BCR	34	0
20	2	311	CLA	5	0
20	B	838	CLA	42	0
20	A	849	CLA	17	0
20	A	812	CLA	2	0
20	2	308	CLA	1	0
20	A	832	CLA	20	0
20	A	840	CLA	8	0
23	B	843	PQN	27	0
20	4	303	CLA	19	0
22	L	209	BCR	36	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
21	2	319	LMU	5	0
20	A	825	CLA	51	0
20	4	306	CLA	17	0
20	B	813	CLA	7	0
20	B	828	CLA	15	0
20	1	201	CLA	12	0
20	1	205	CLA	7	0
20	A	839	CLA	28	0
20	4	302	CLA	3	0
21	K	107	LMU	21	0
21	H	106	LMU	9	0
20	A	829	CLA	5	0
20	2	302	CLA	13	0
20	B	803	CLA	41	0
20	1	203	CLA	8	0
20	B	812	CLA	7	0
21	L	205	LMU	1	0
20	1	210	CLA	8	0
20	2	307	CLA	21	0
20	A	820	CLA	6	0
20	B	808	CLA	31	0
22	B	846	BCR	36	0
20	4	313	CLA	4	0
20	A	813	CLA	16	0
21	1	218	LMU	9	0
22	I	103	BCR	38	0
20	1	207	CLA	5	1
20	3	306	CLA	7	0
20	B	816	CLA	7	0
21	A	854	LMU	16	0
20	3	309	CLA	1	0
20	A	833	CLA	13	0
22	F	204	BCR	34	0
20	A	811	CLA	19	0
20	B	815	CLA	17	0
20	A	831	CLA	36	0
20	B	820	CLA	18	0
20	B	839	CLA	49	0
21	G	103	LMU	16	0
20	B	837	CLA	10	0
20	A	809	CLA	30	0
20	1	208	CLA	4	0

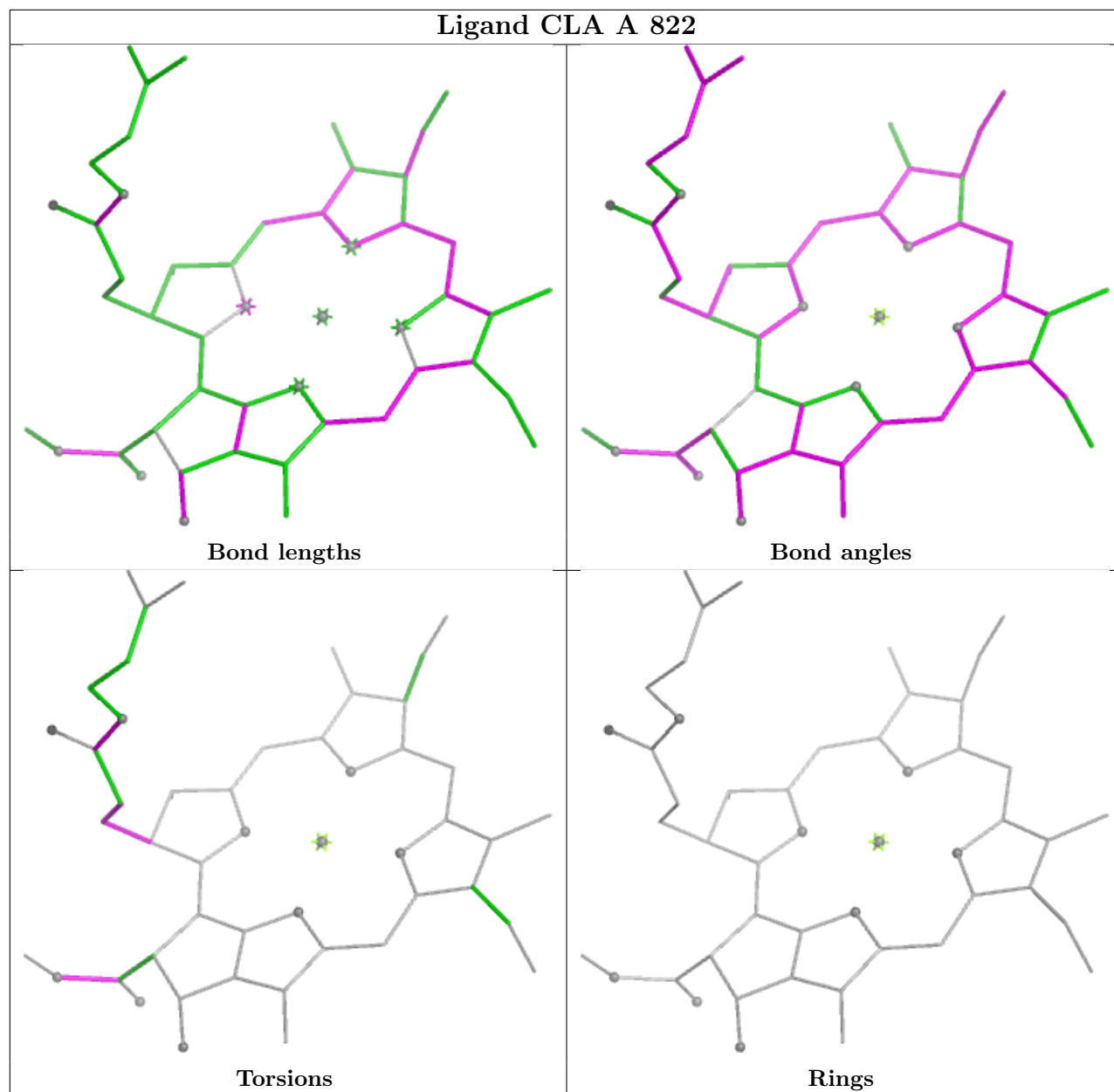
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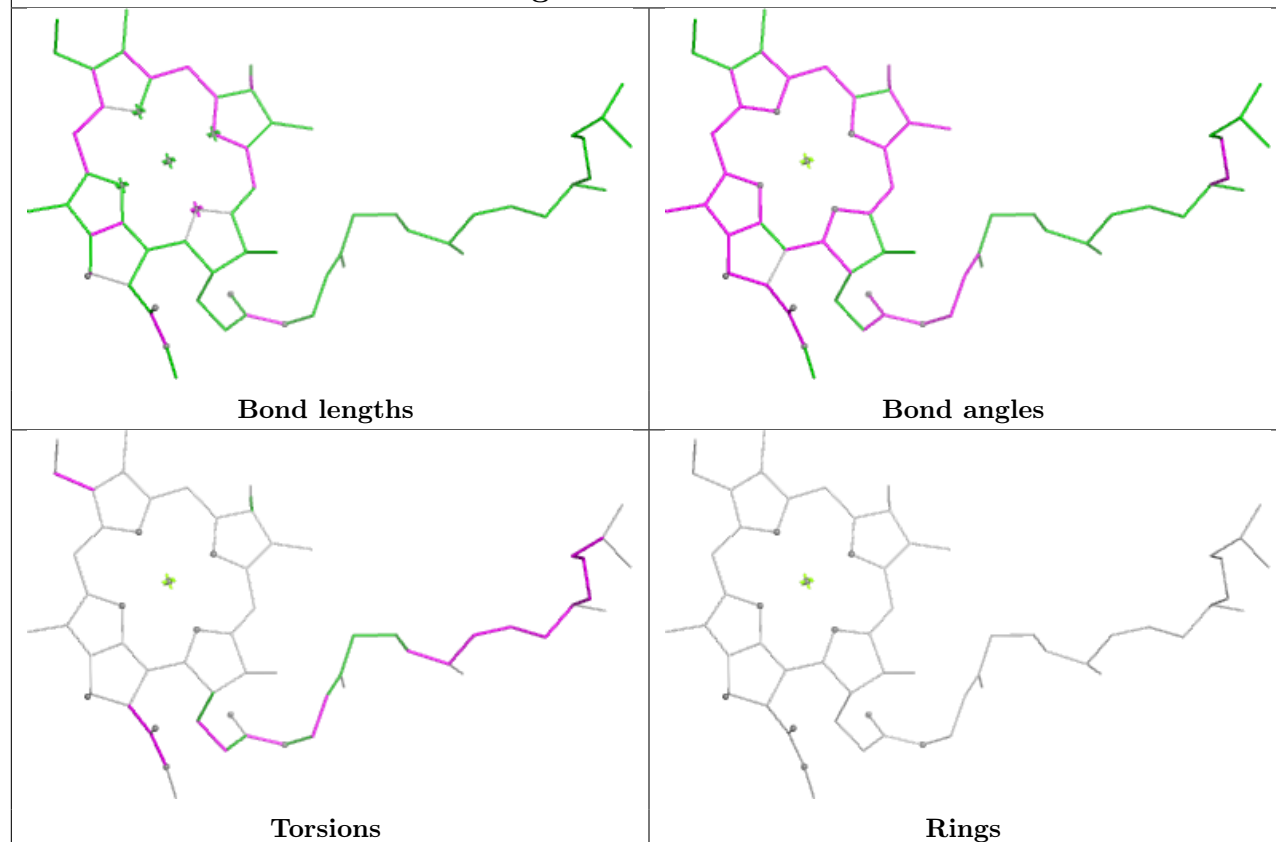
Mol	Chain	Res	Type	Clashes	Symm-Clashes
20	B	830	CLA	25	0
20	H	108	CLA	26	0
20	A	803	CLA	19	0
21	A	848	LMU	4	0
21	A	853	LMU	21	0
20	B	817	CLA	19	0
22	2	317	BCR	9	0
20	1	213	CLA	18	0

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.

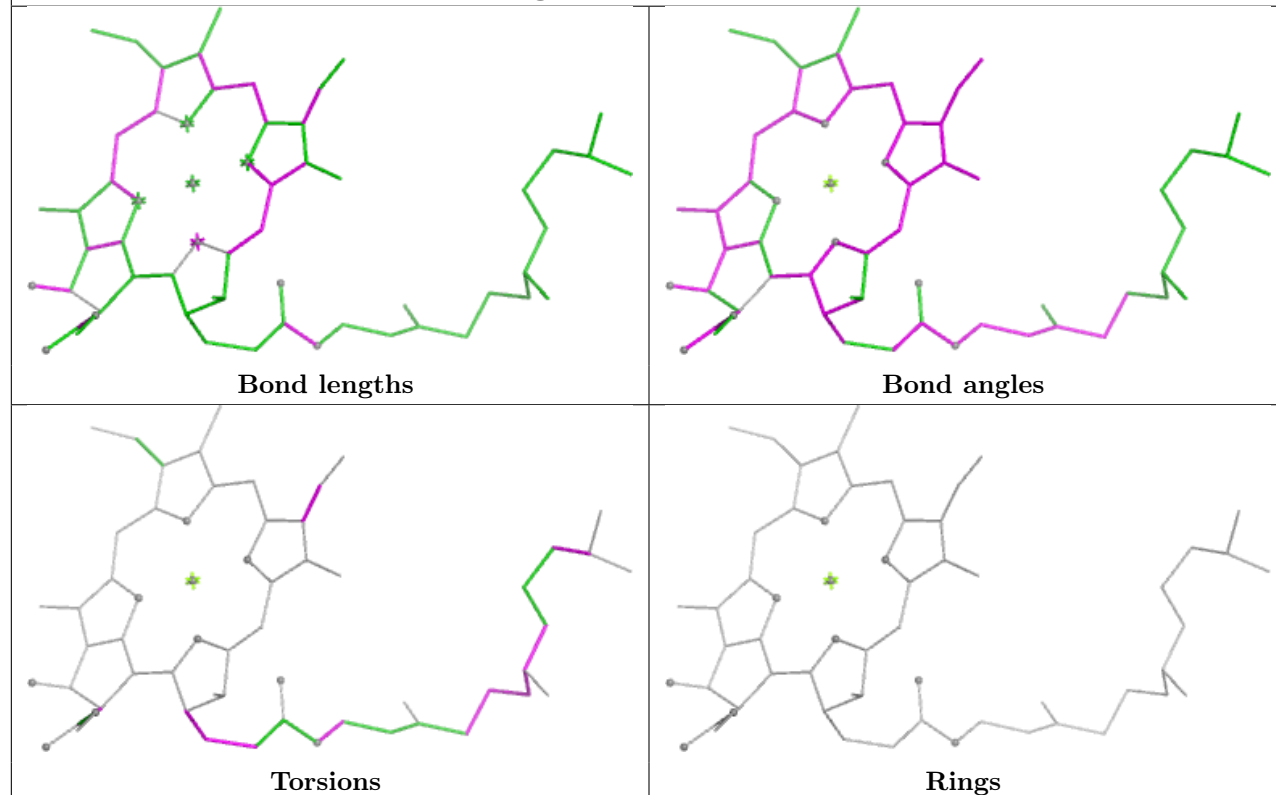
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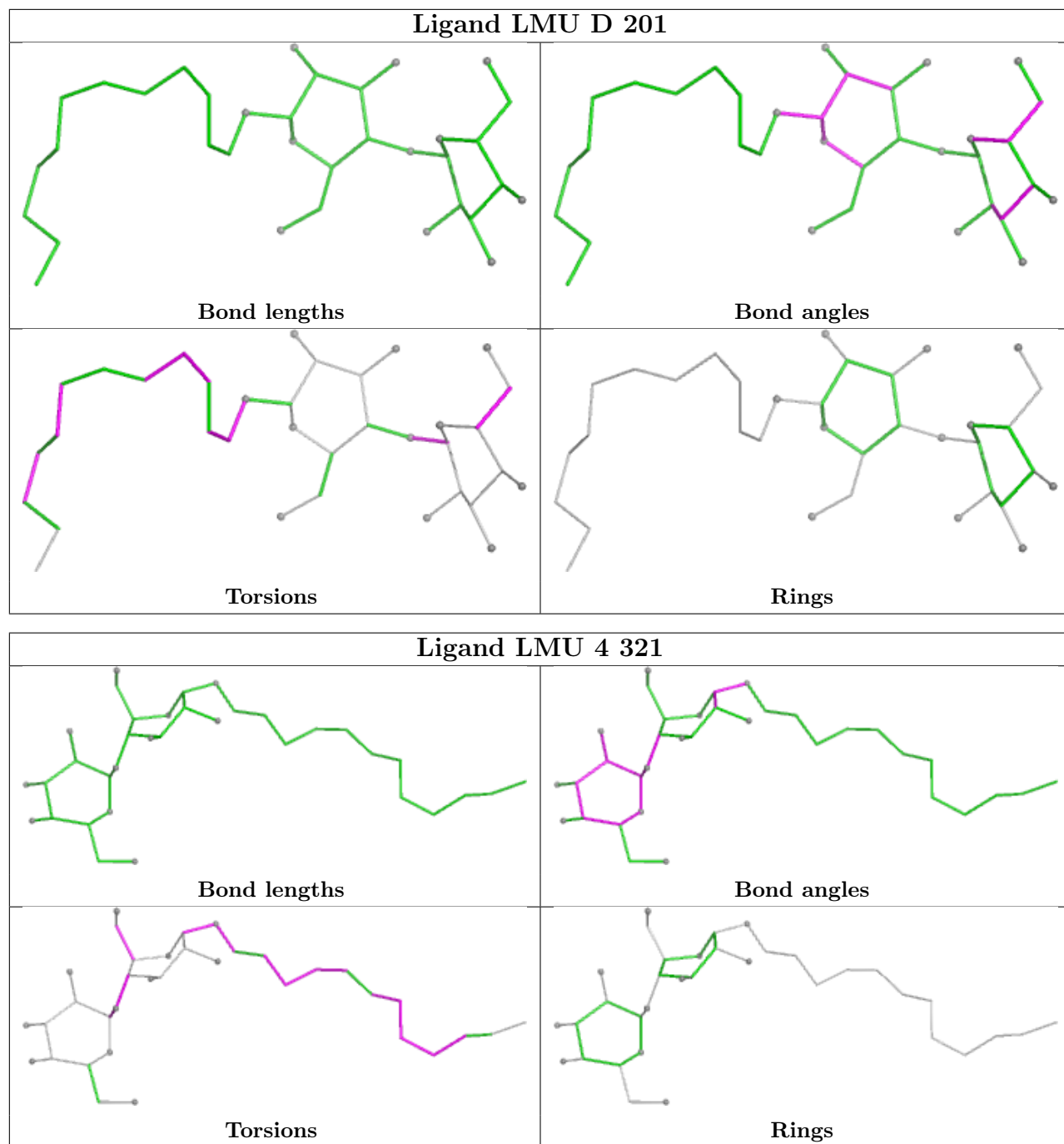


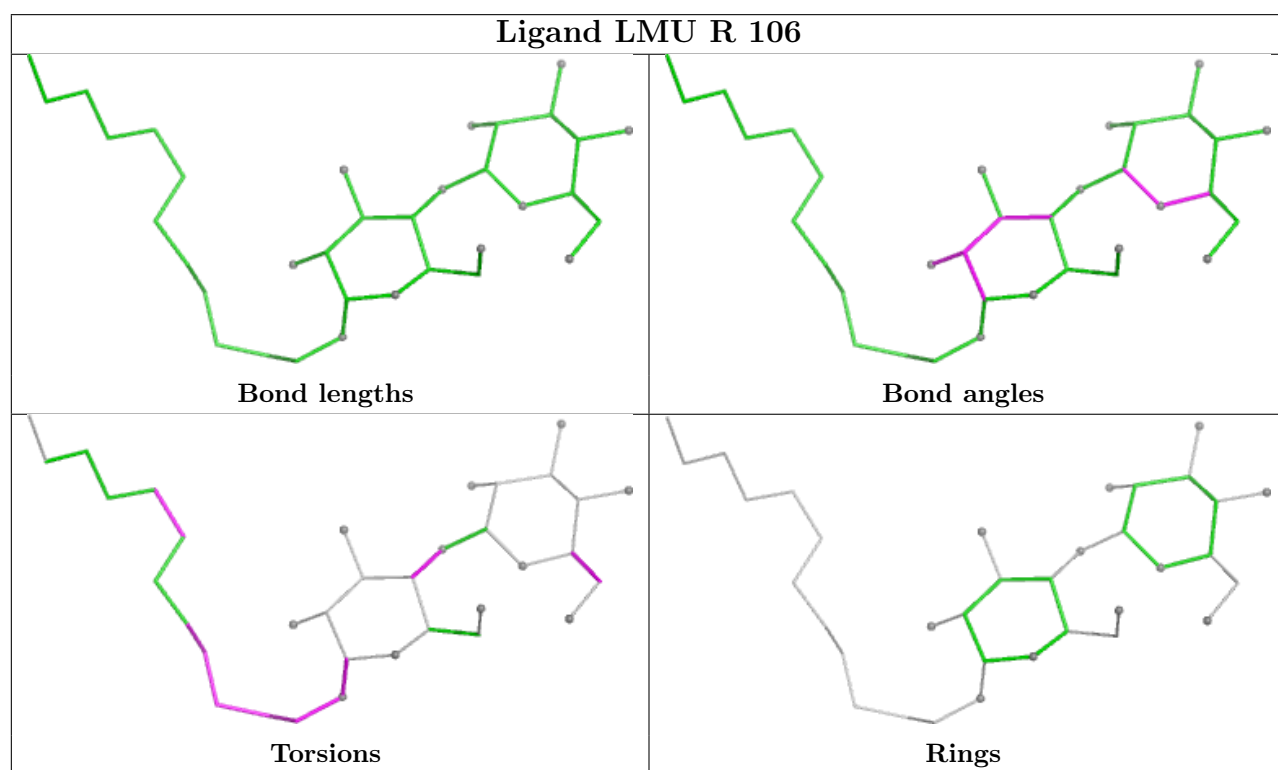
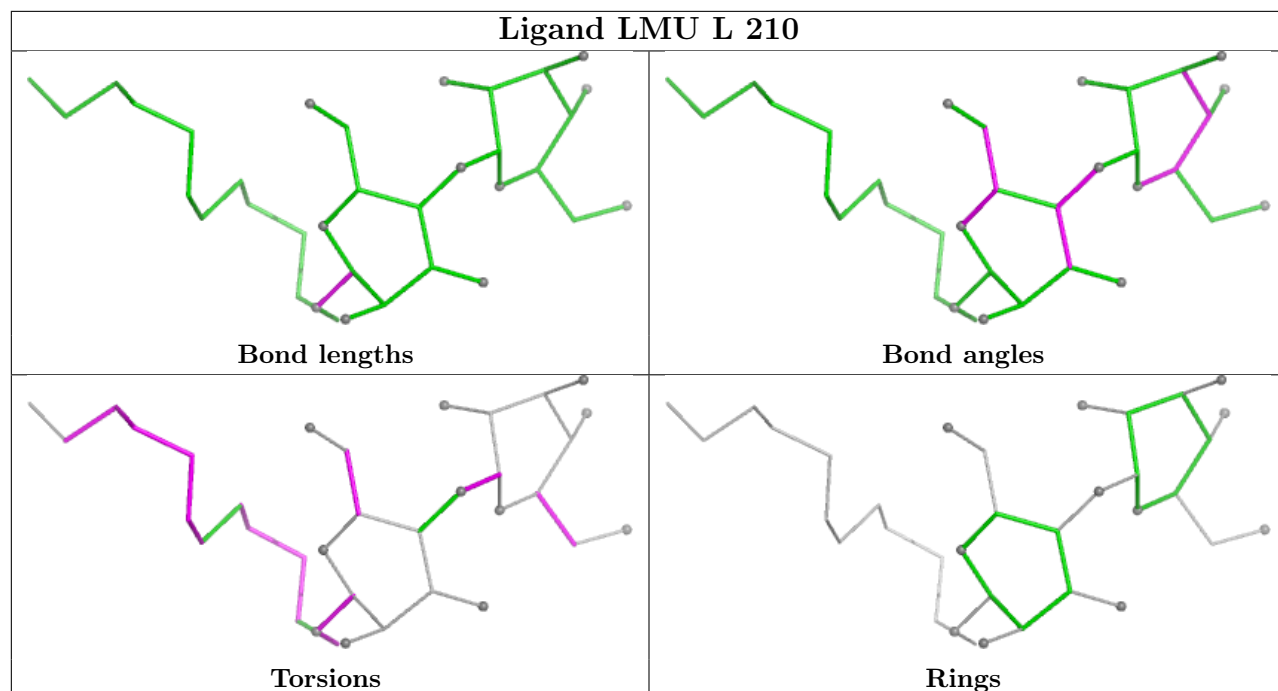
Ligand CLA A 851



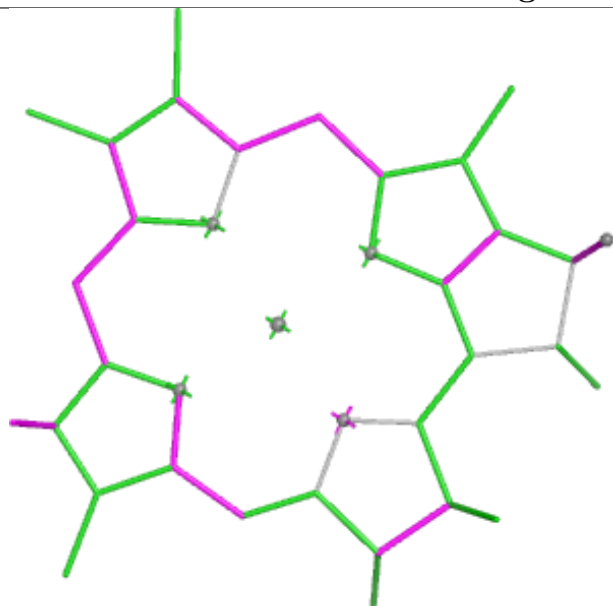
Ligand CLA A 808



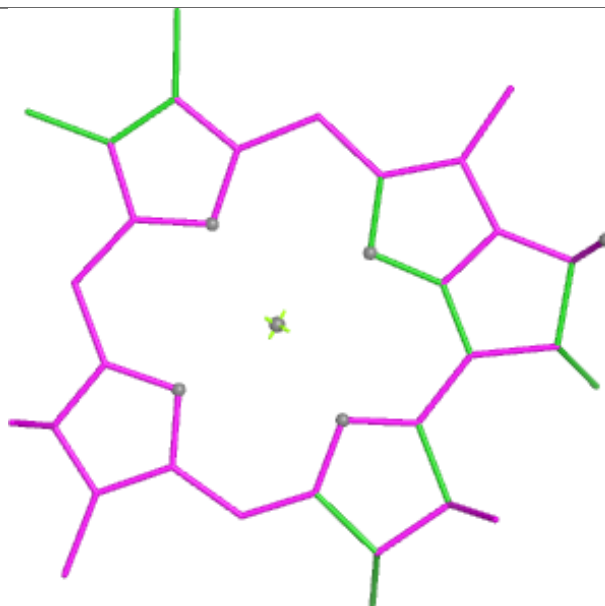




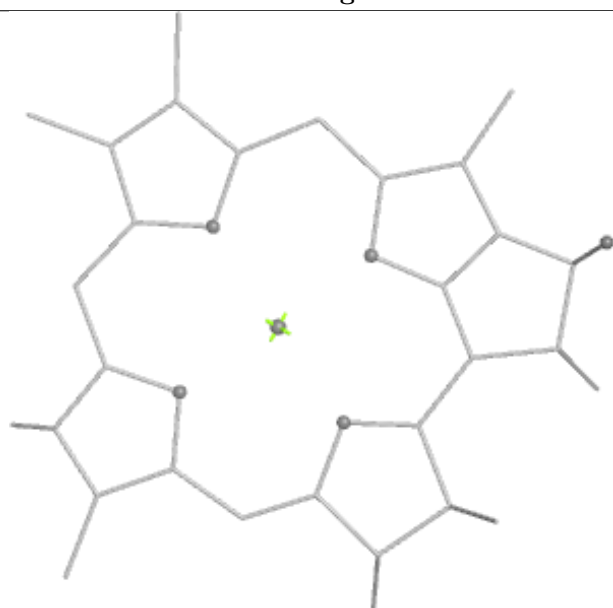
Ligand CLA 3 301



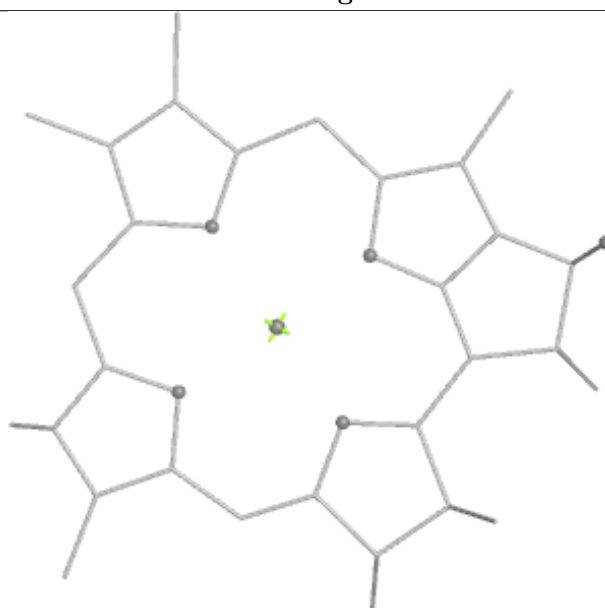
Bond lengths



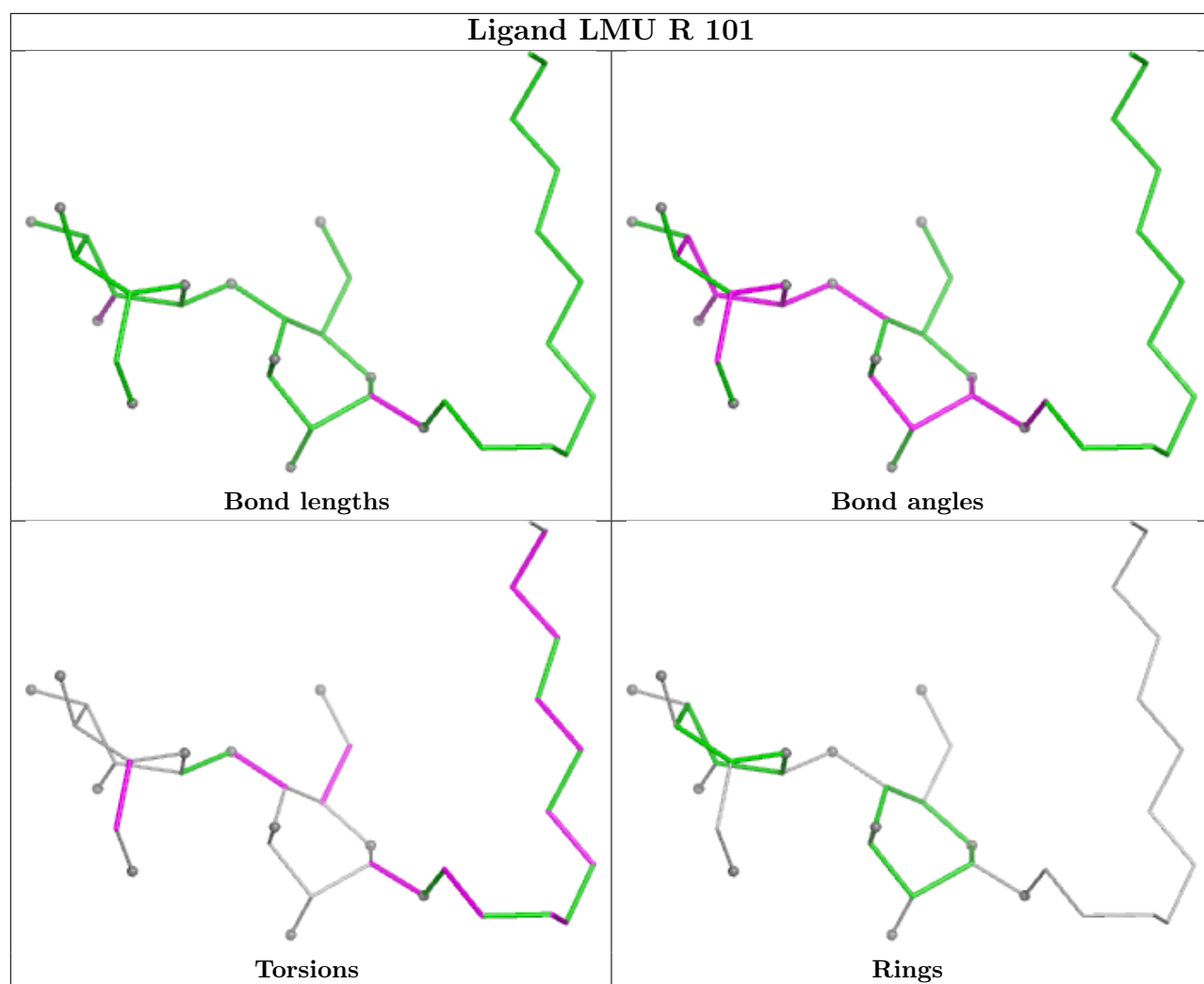
Bond angles

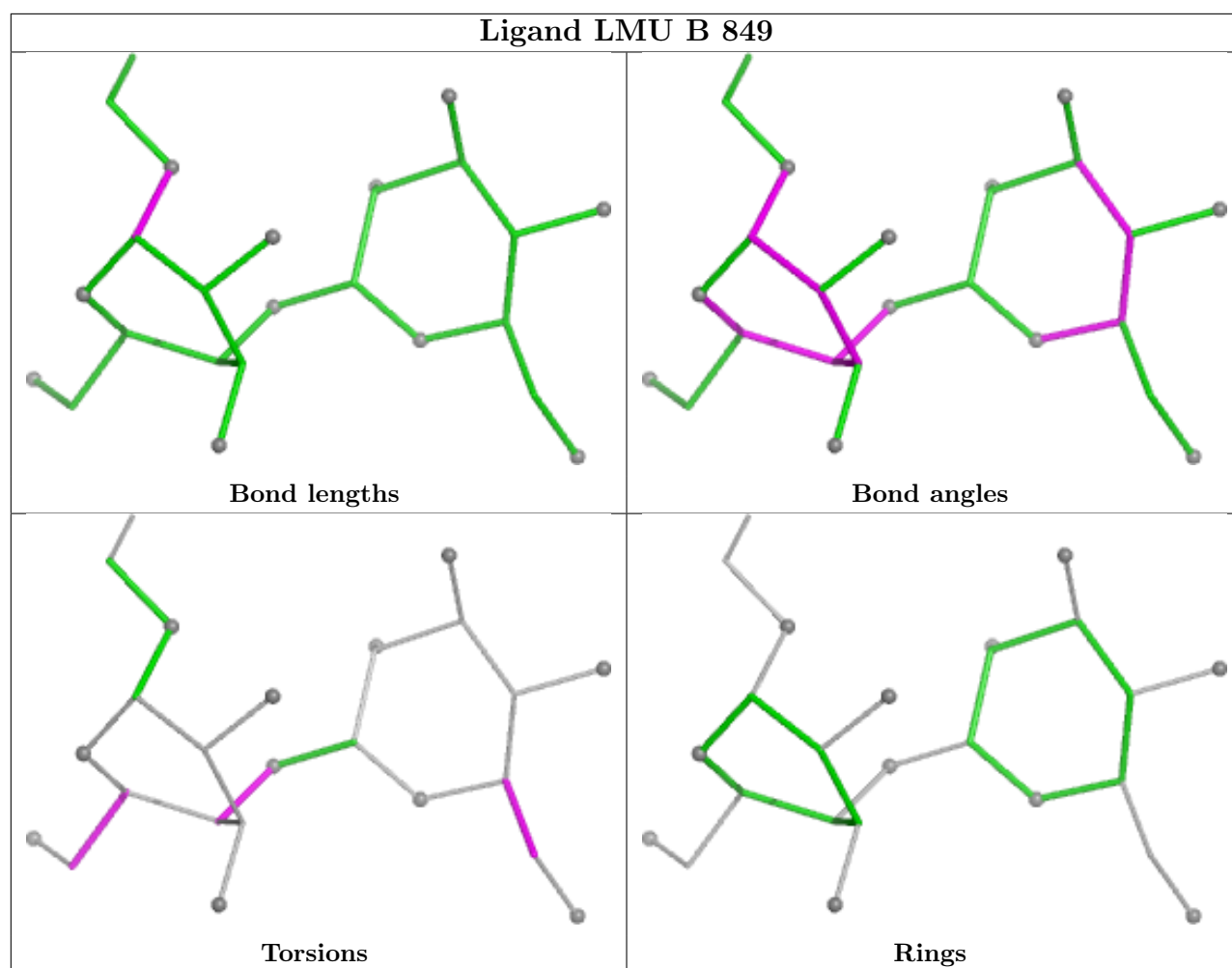


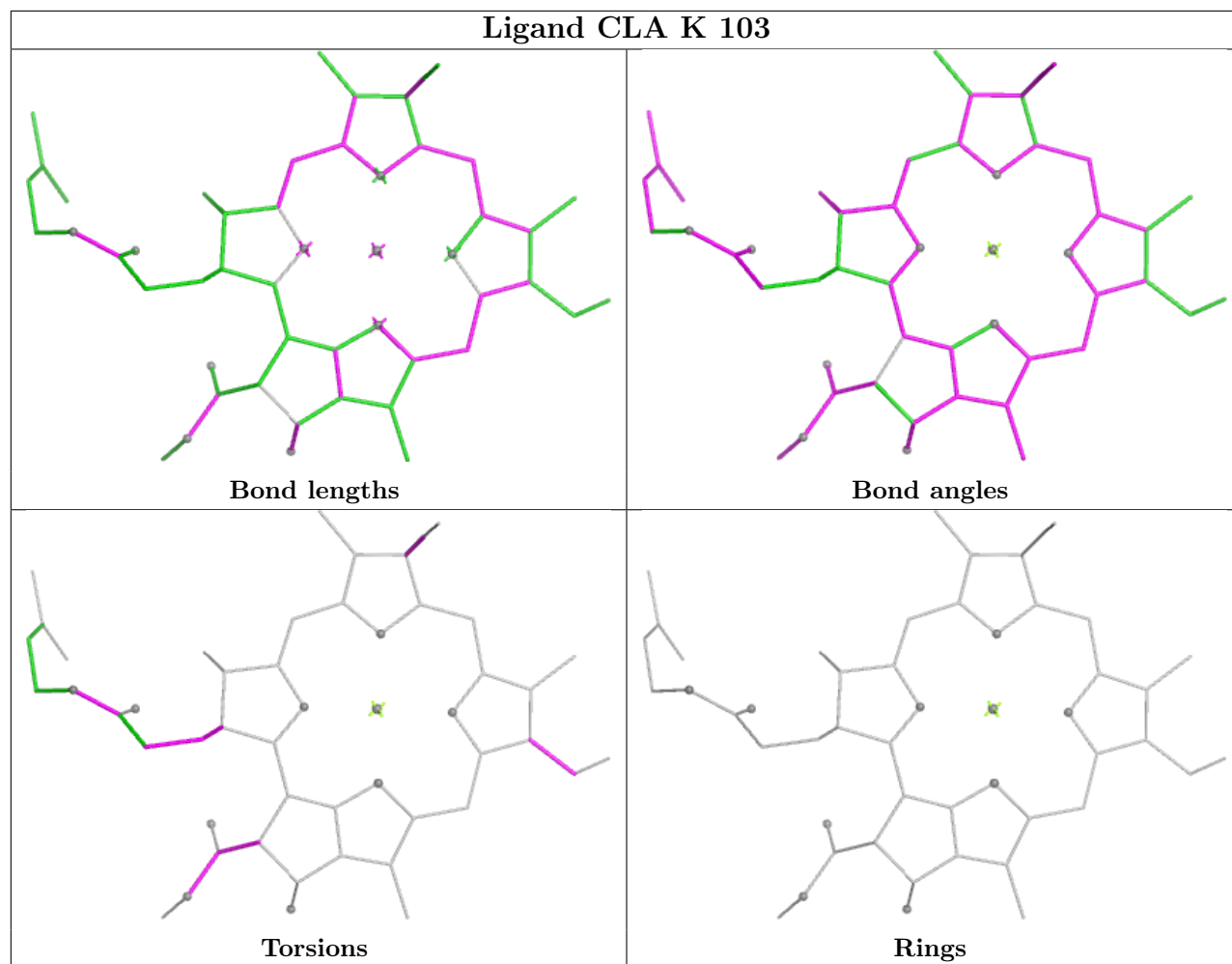
Torsions



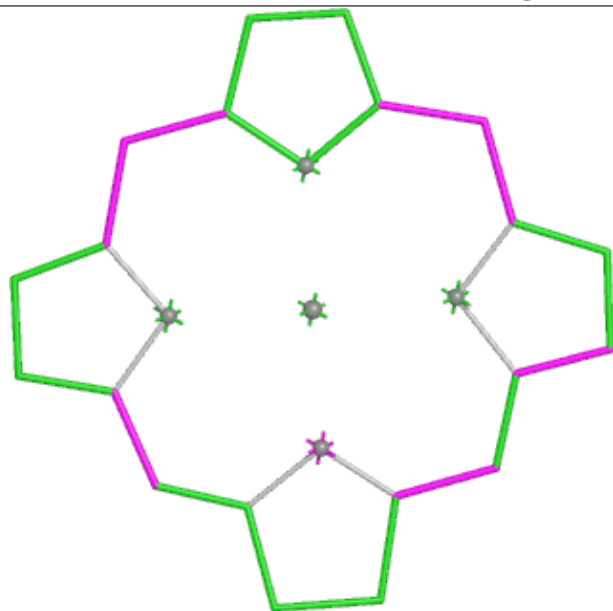
Rings



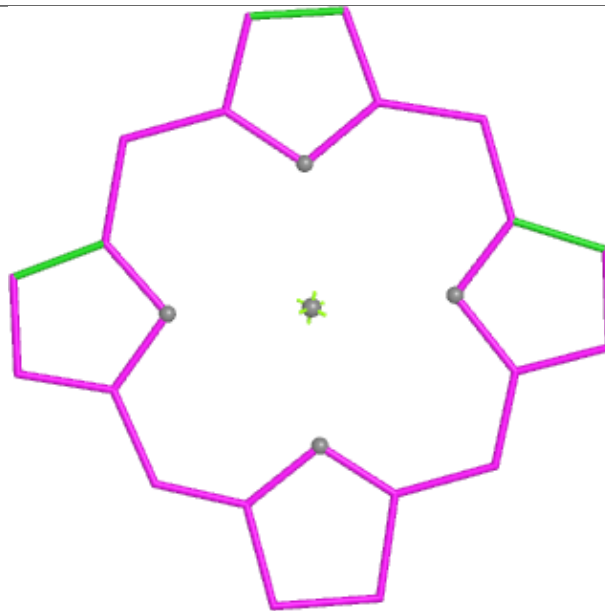




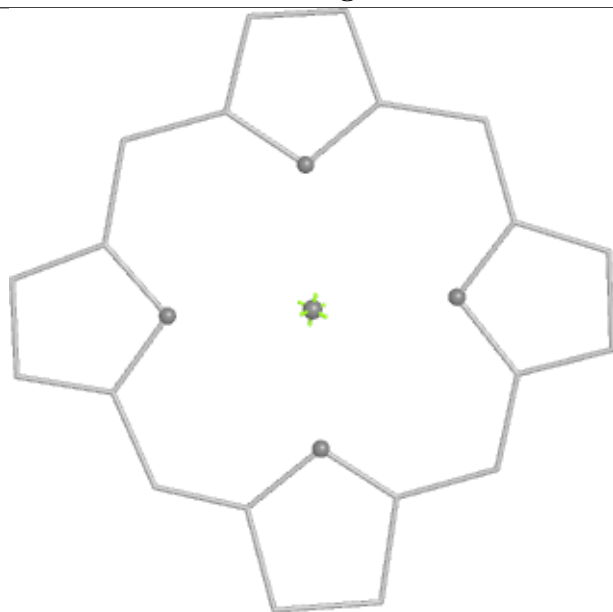
Ligand CLA 1 214



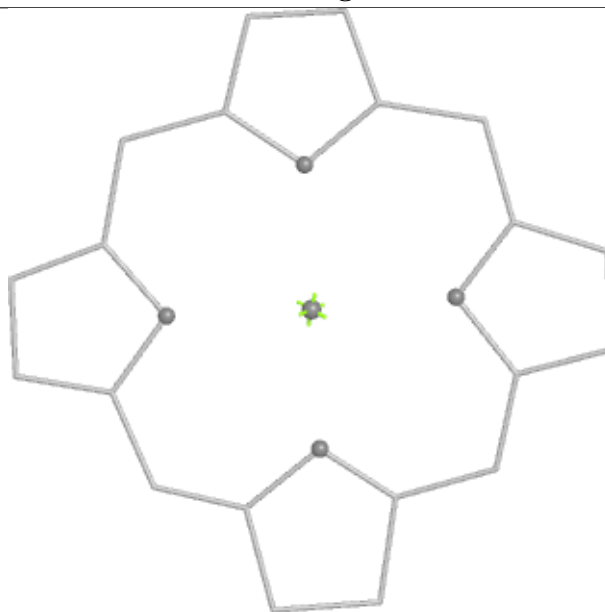
Bond lengths



Bond angles

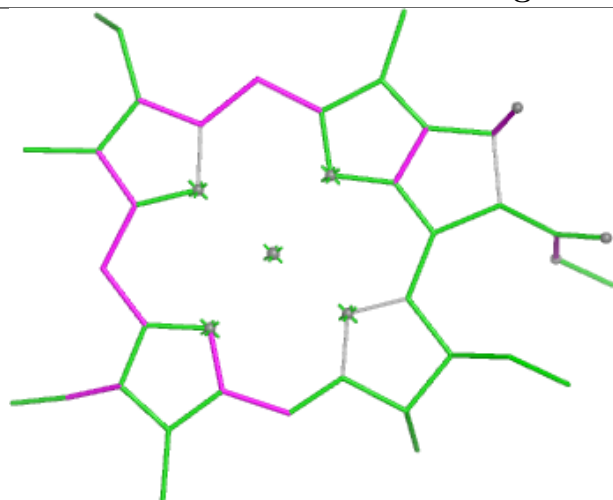


Torsions

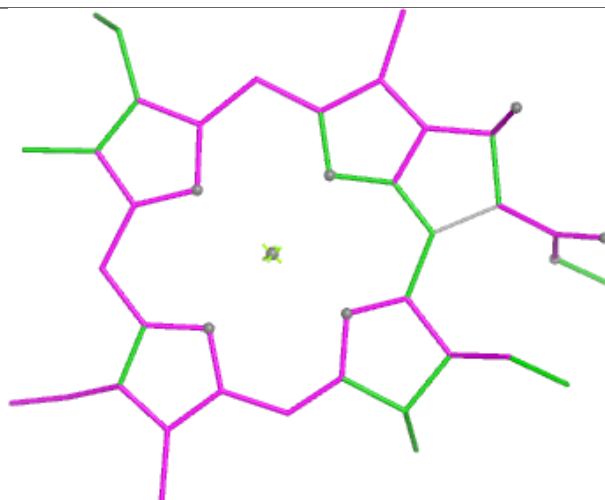


Rings

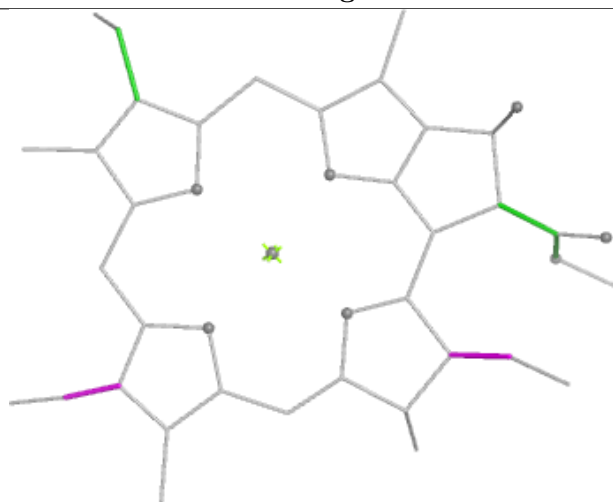
Ligand CLA A 821



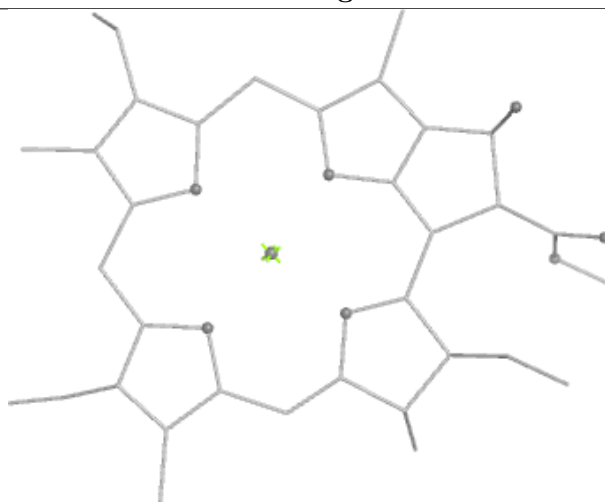
Bond lengths



Bond angles

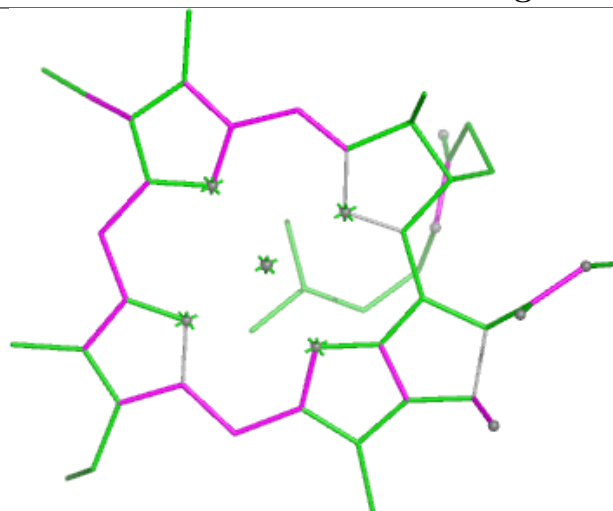


Torsions

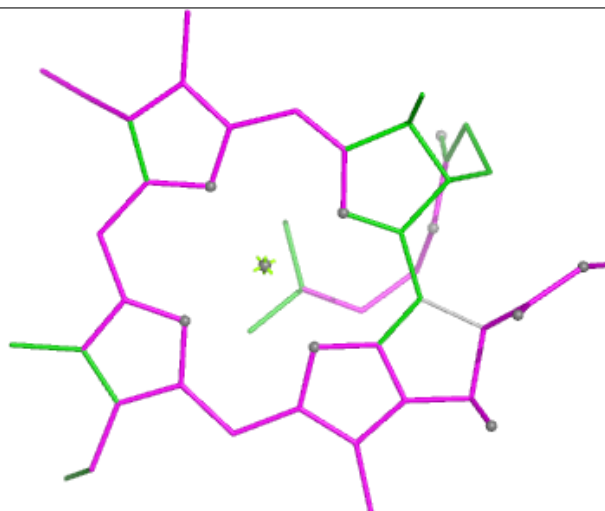


Rings

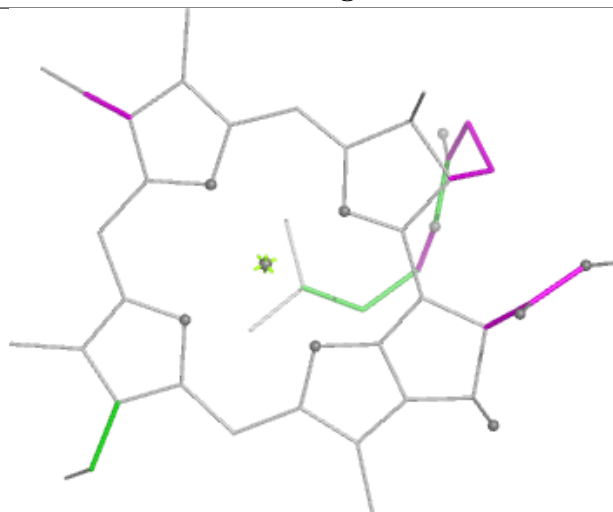
Ligand CLA B 831



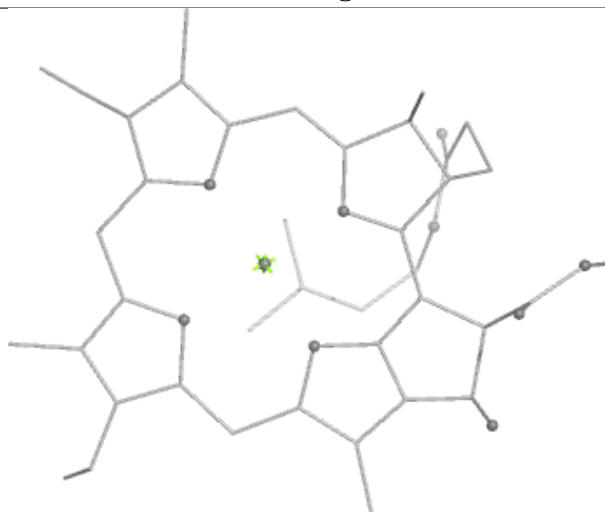
Bond lengths



Bond angles

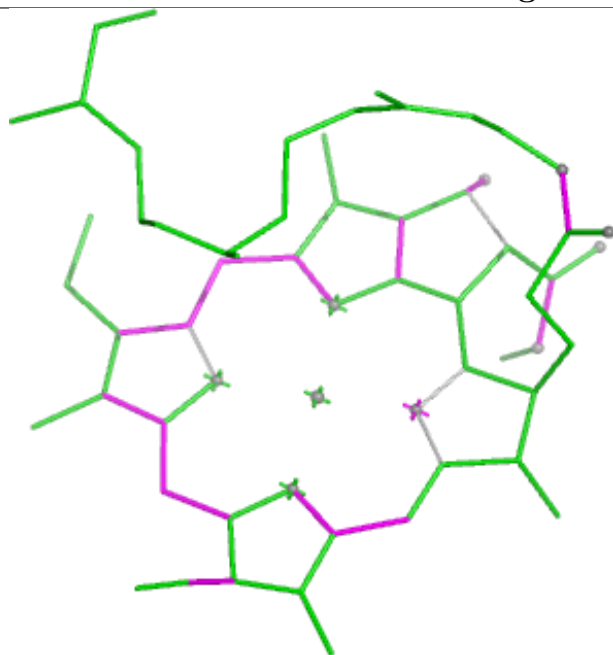


Torsions

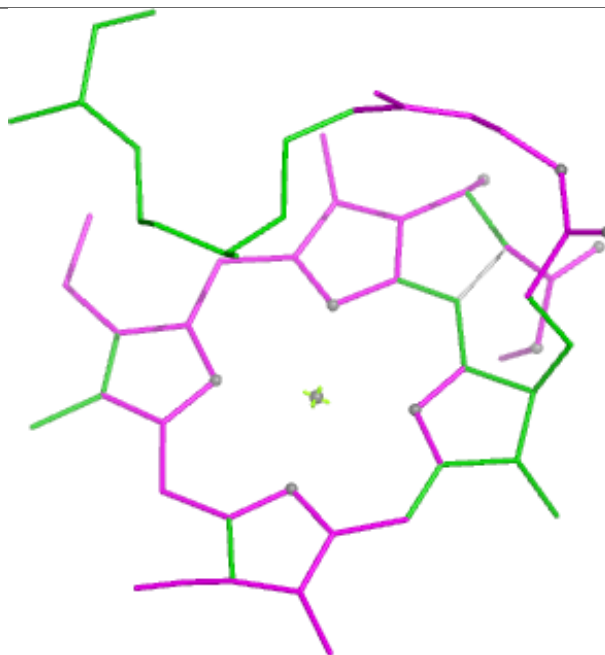


Rings

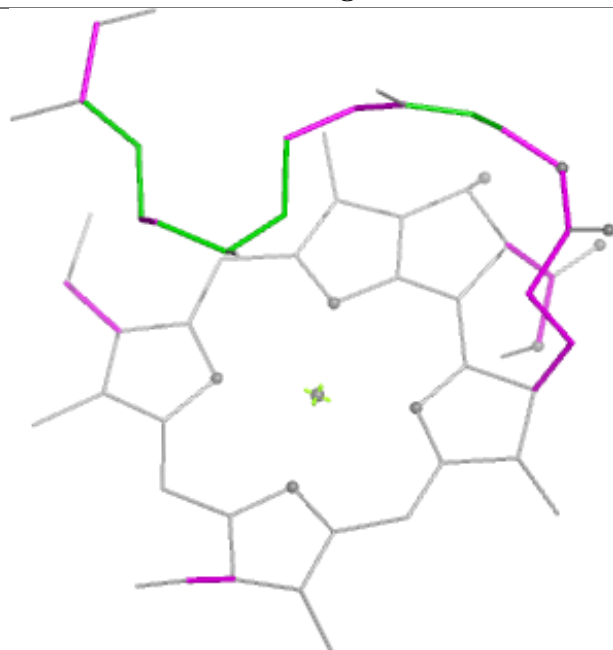
Ligand CLA 1 206



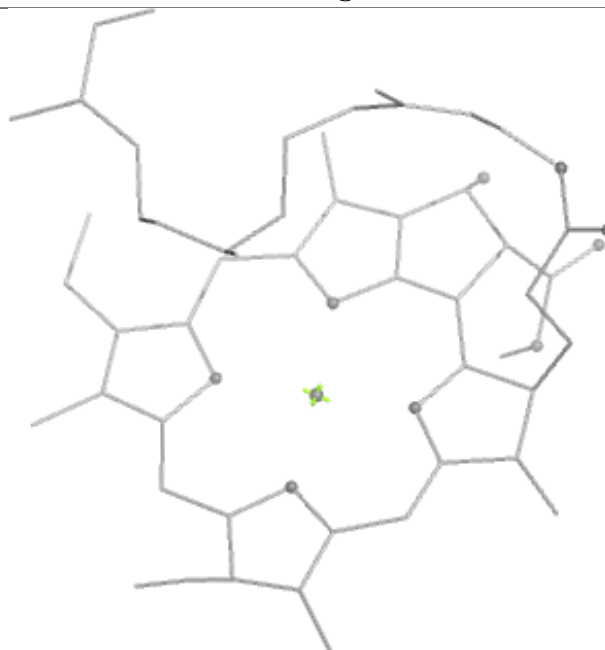
Bond lengths



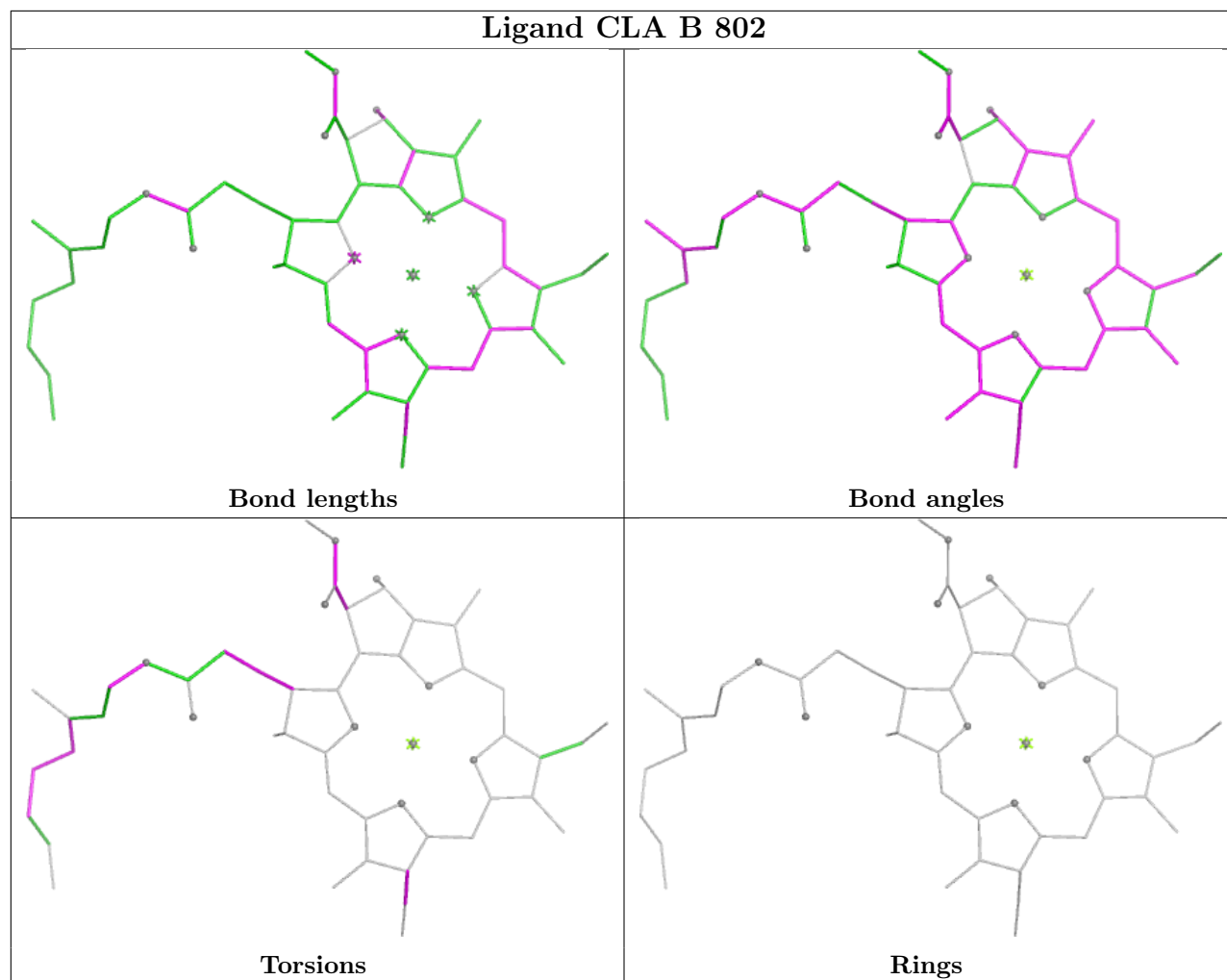
Bond angles



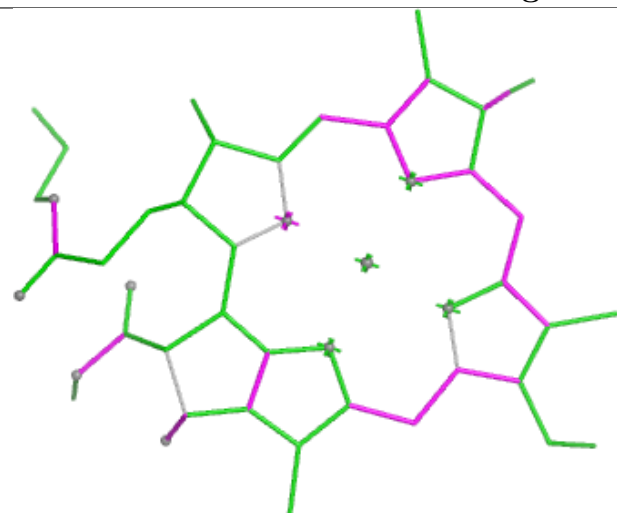
Torsions



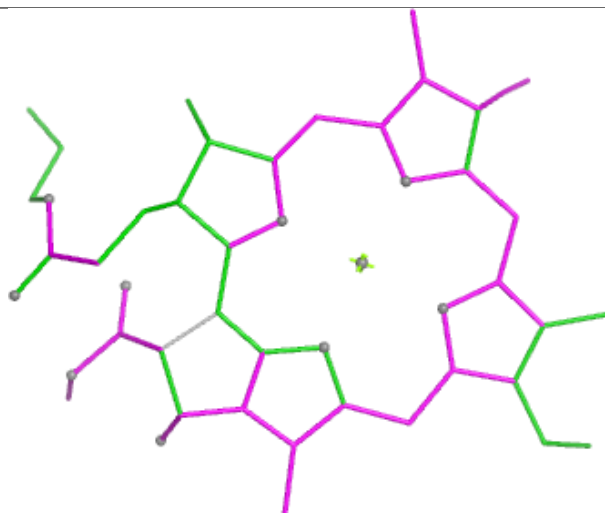
Rings



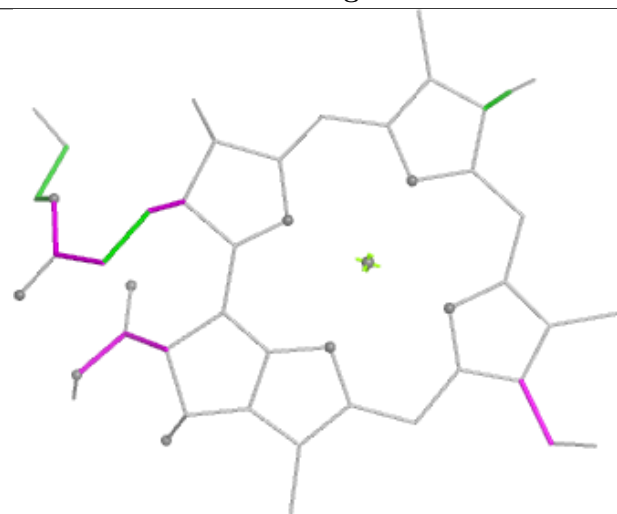
Ligand CLA J 101



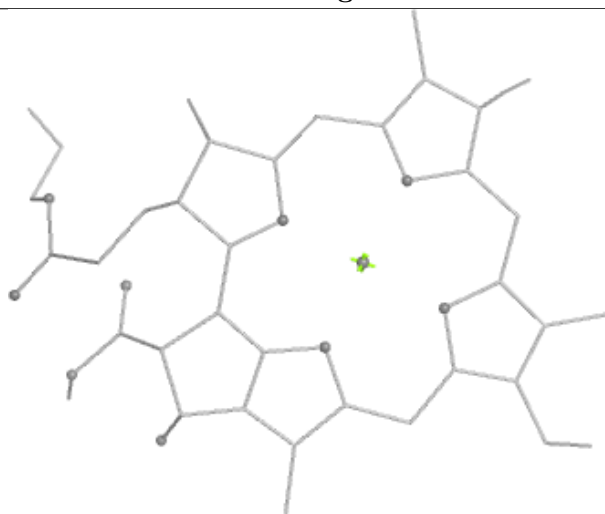
Bond lengths



Bond angles

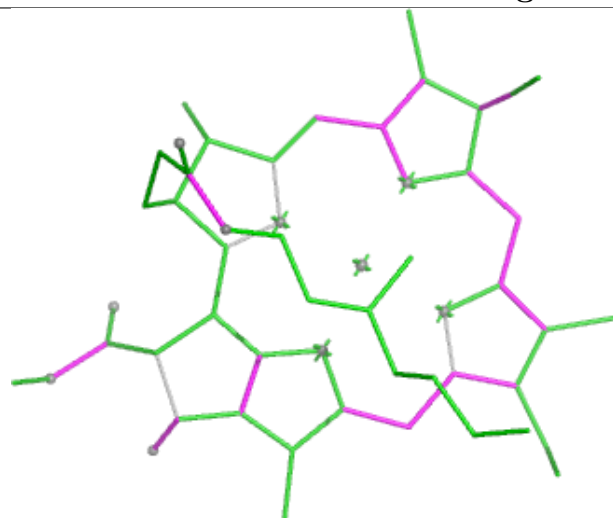


Torsions

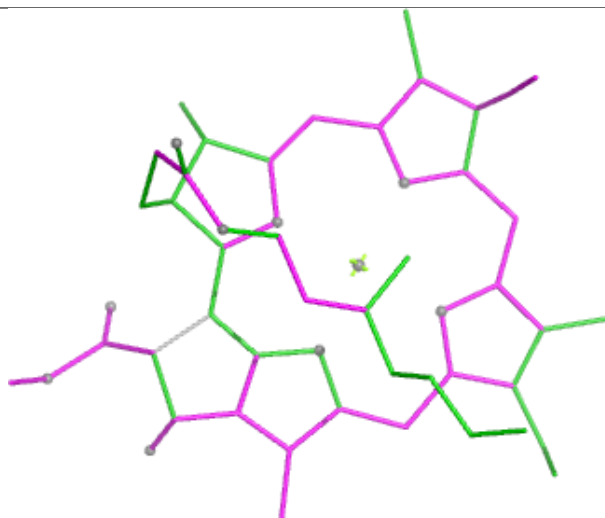


Rings

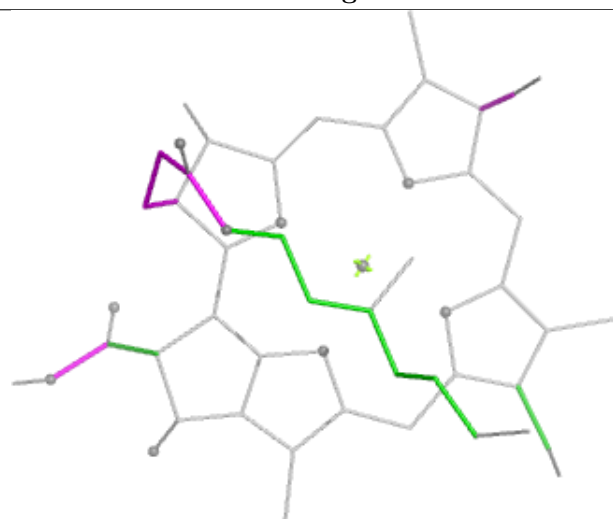
Ligand CLA B 818



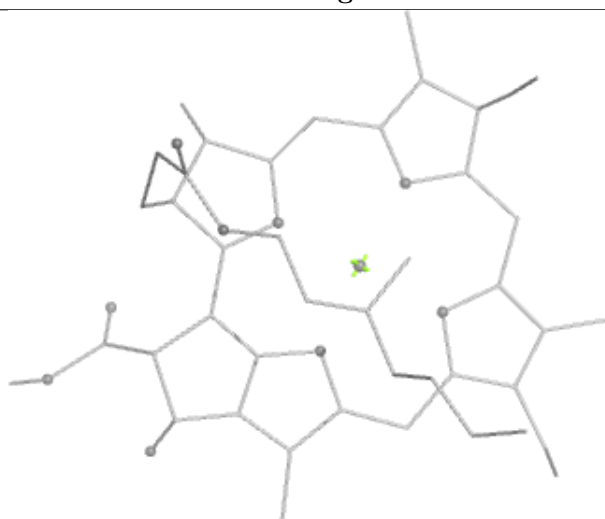
Bond lengths



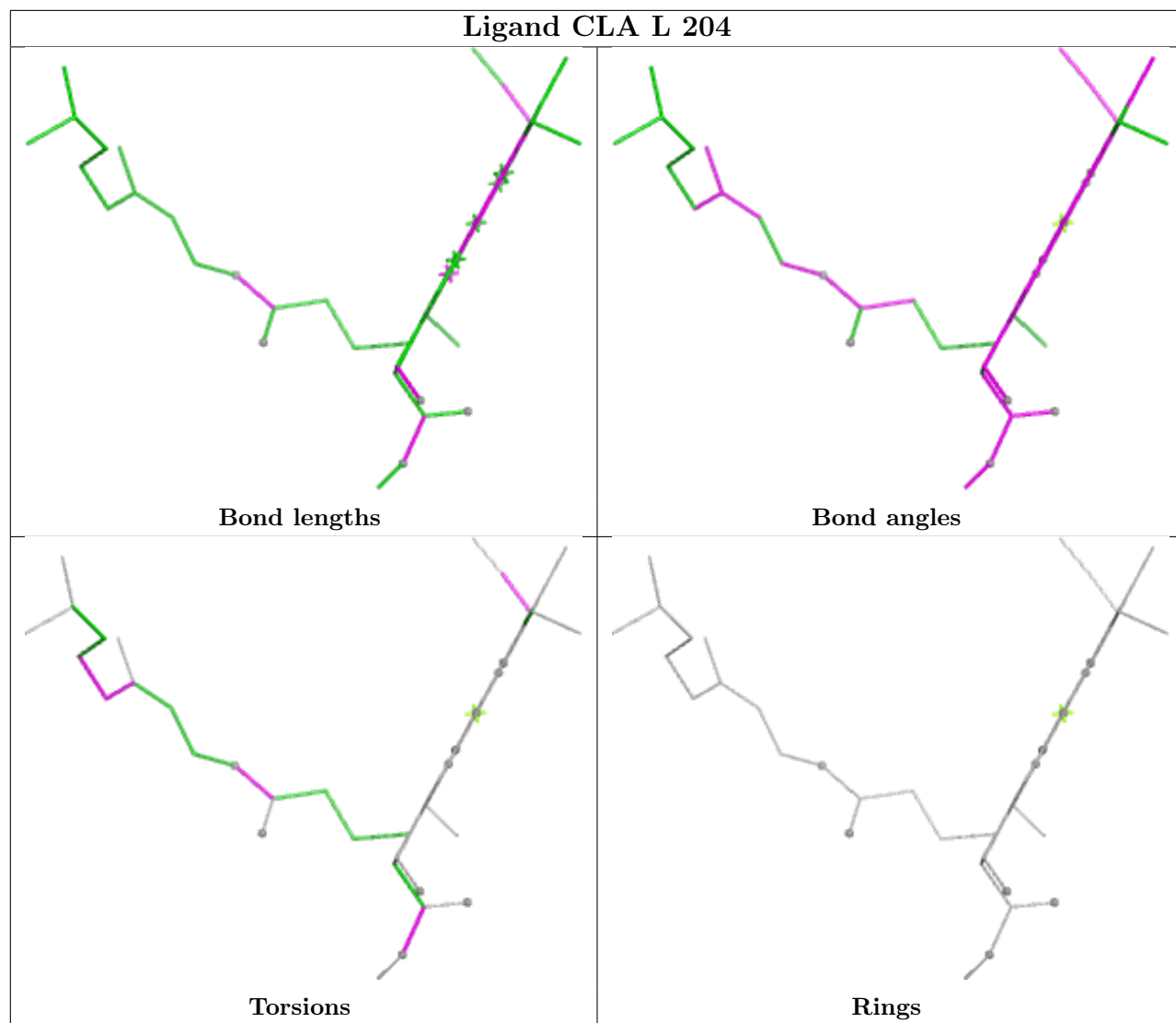
Bond angles



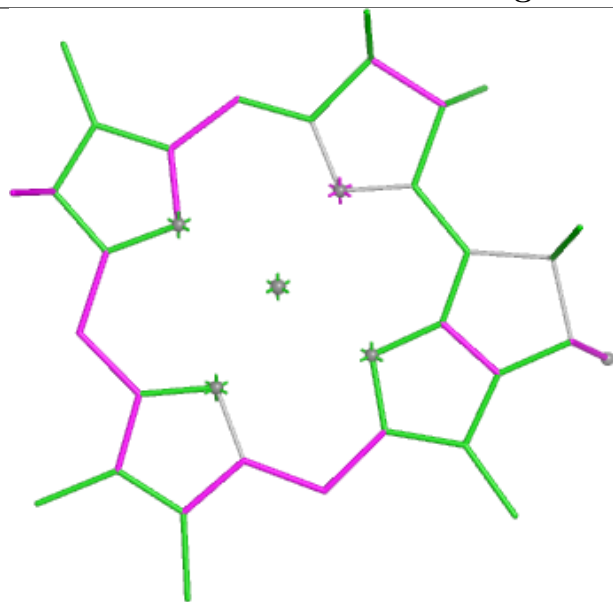
Torsions



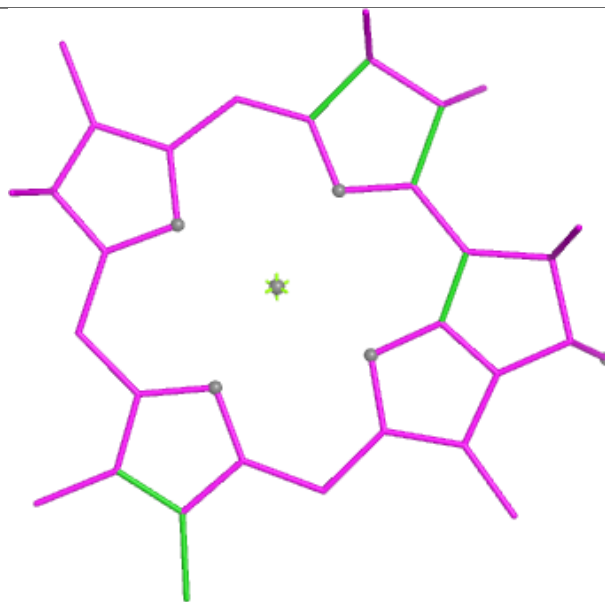
Rings



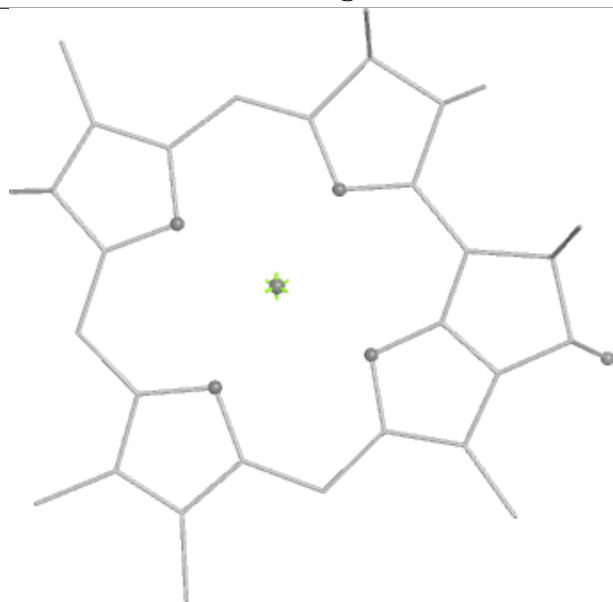
Ligand CLA B 842



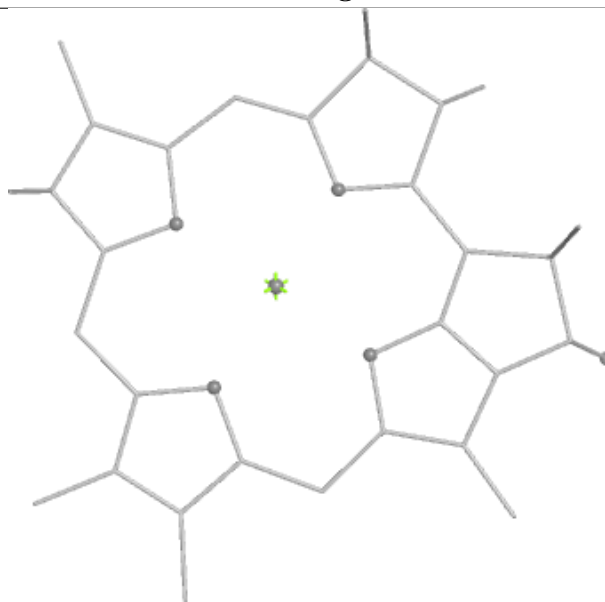
Bond lengths



Bond angles

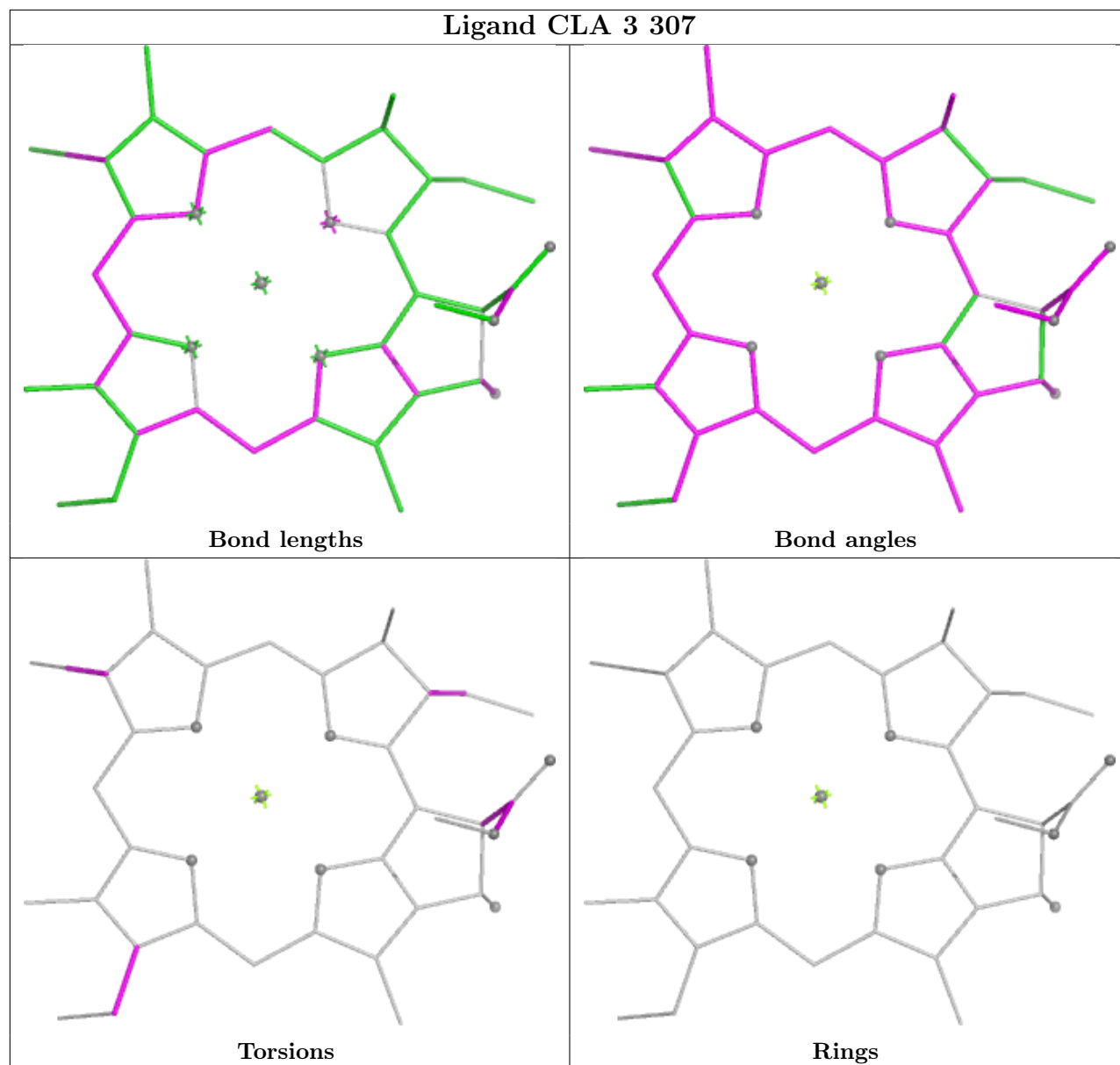


Torsions

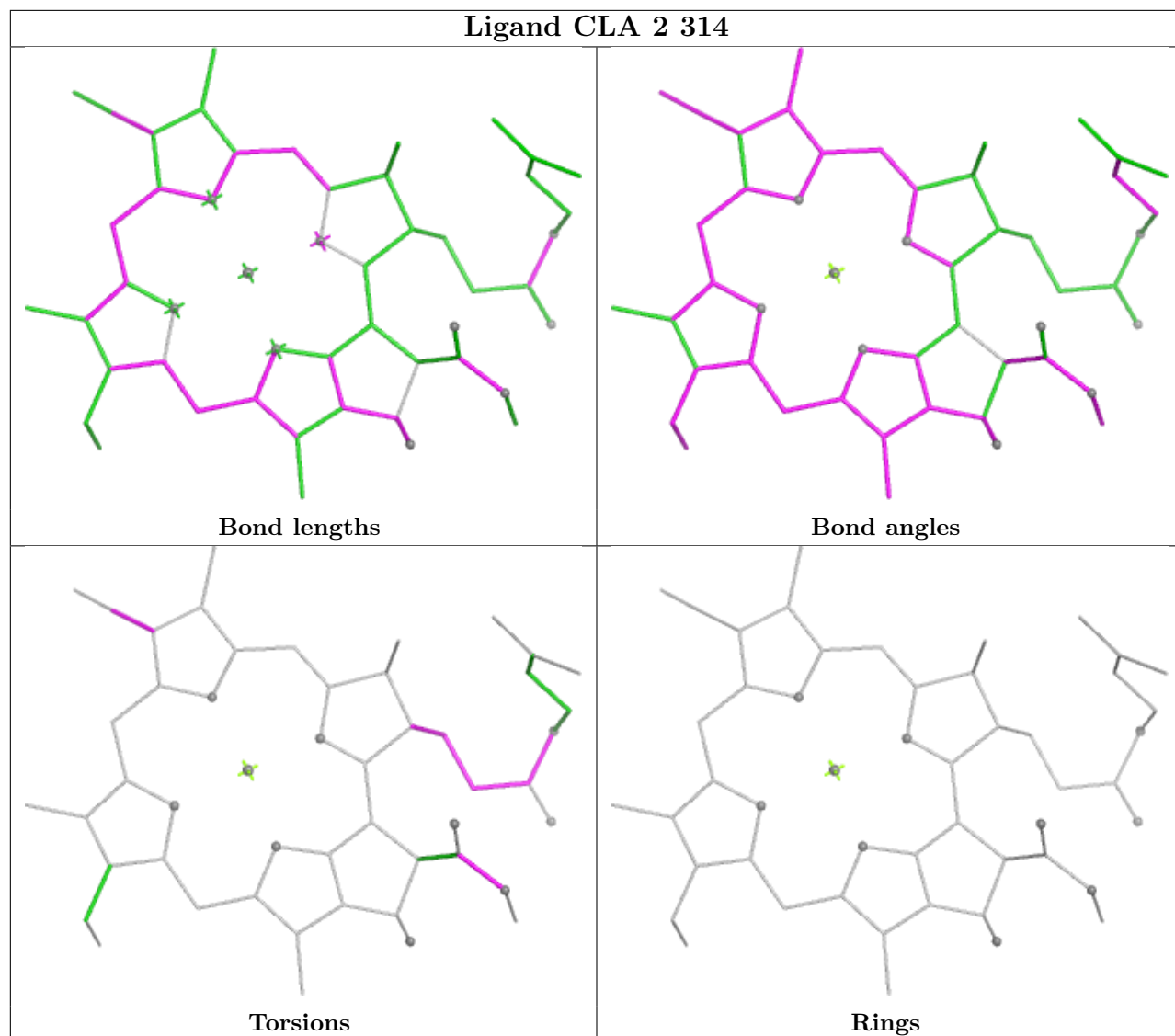


Rings

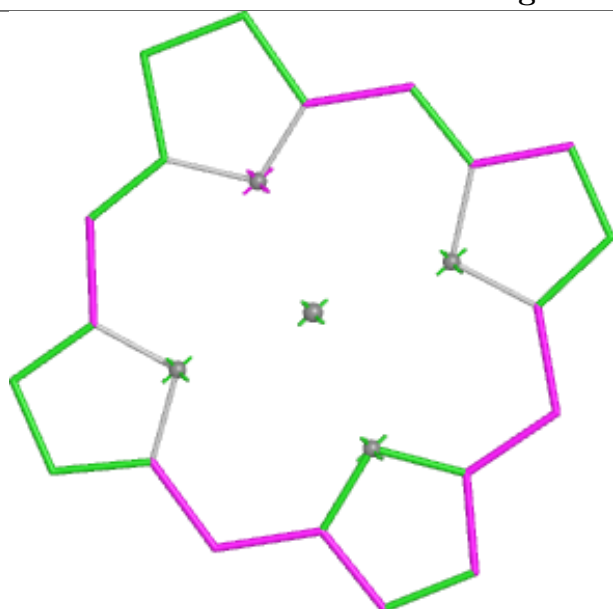
Ligand CLA 3 307



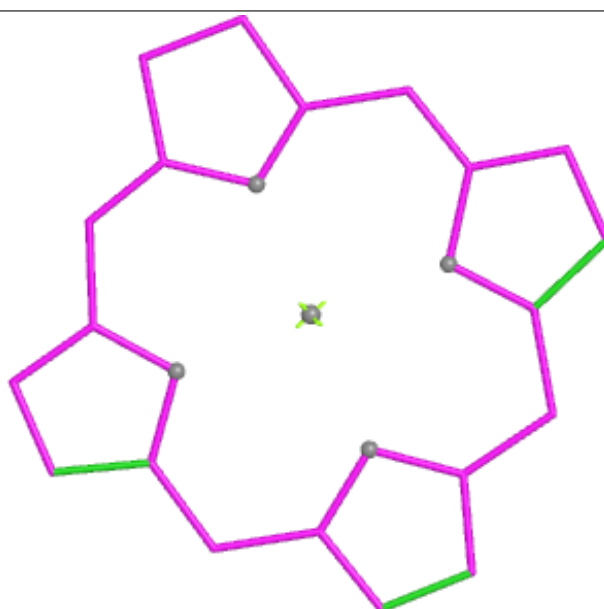
Ligand CLA 2 314



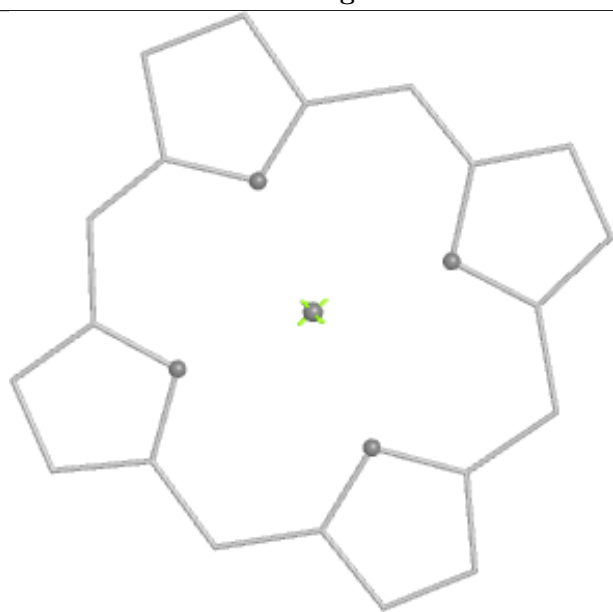
Ligand CLA 4 308



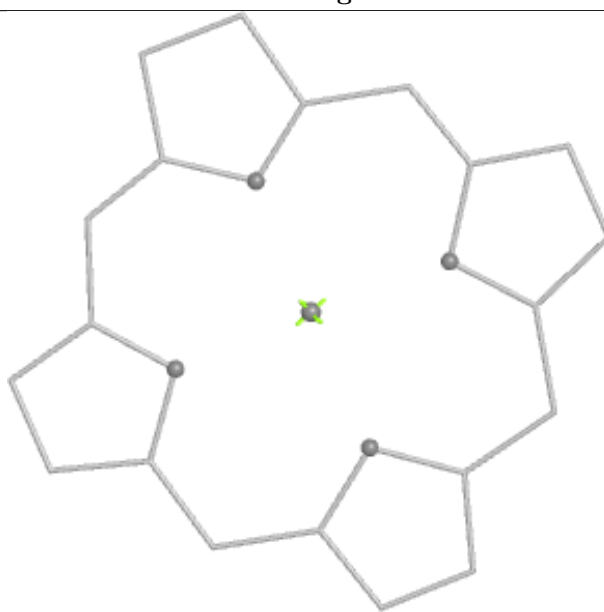
Bond lengths



Bond angles

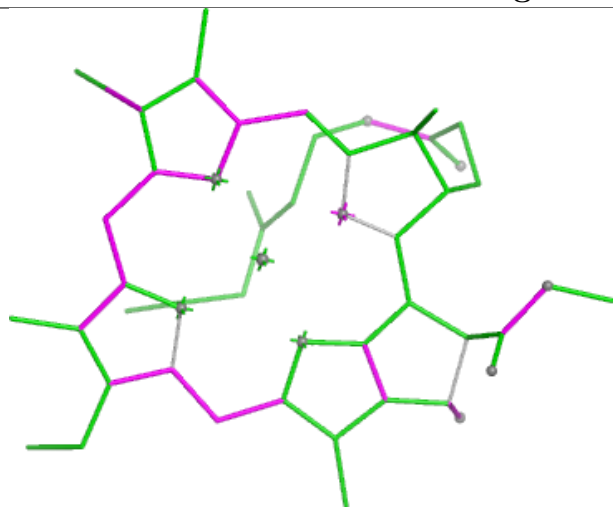


Torsions

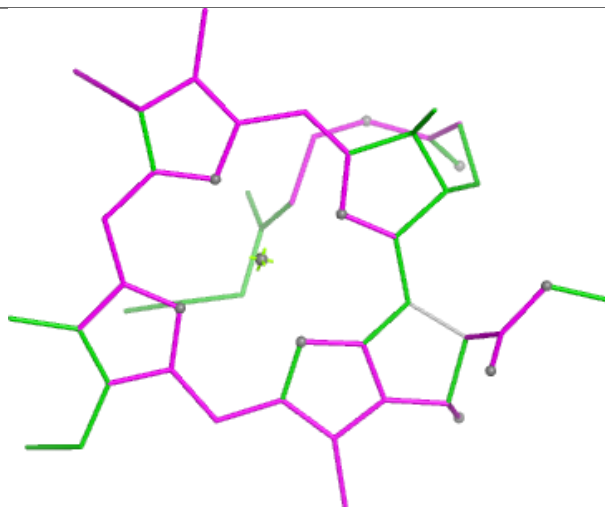


Rings

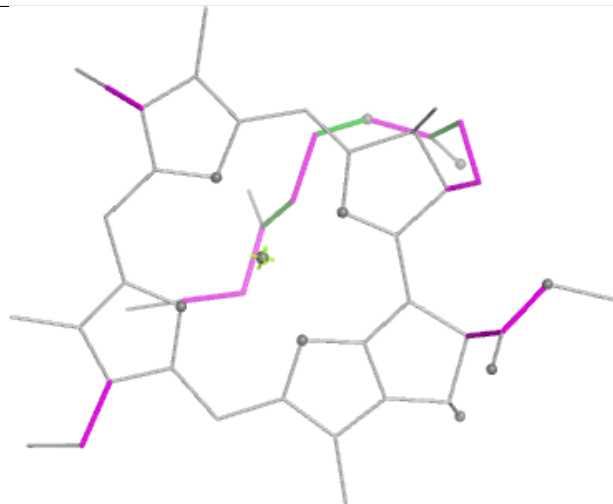
Ligand CLA A 817



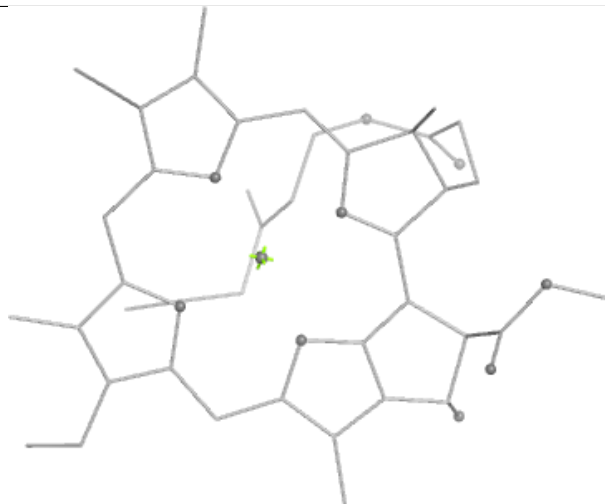
Bond lengths



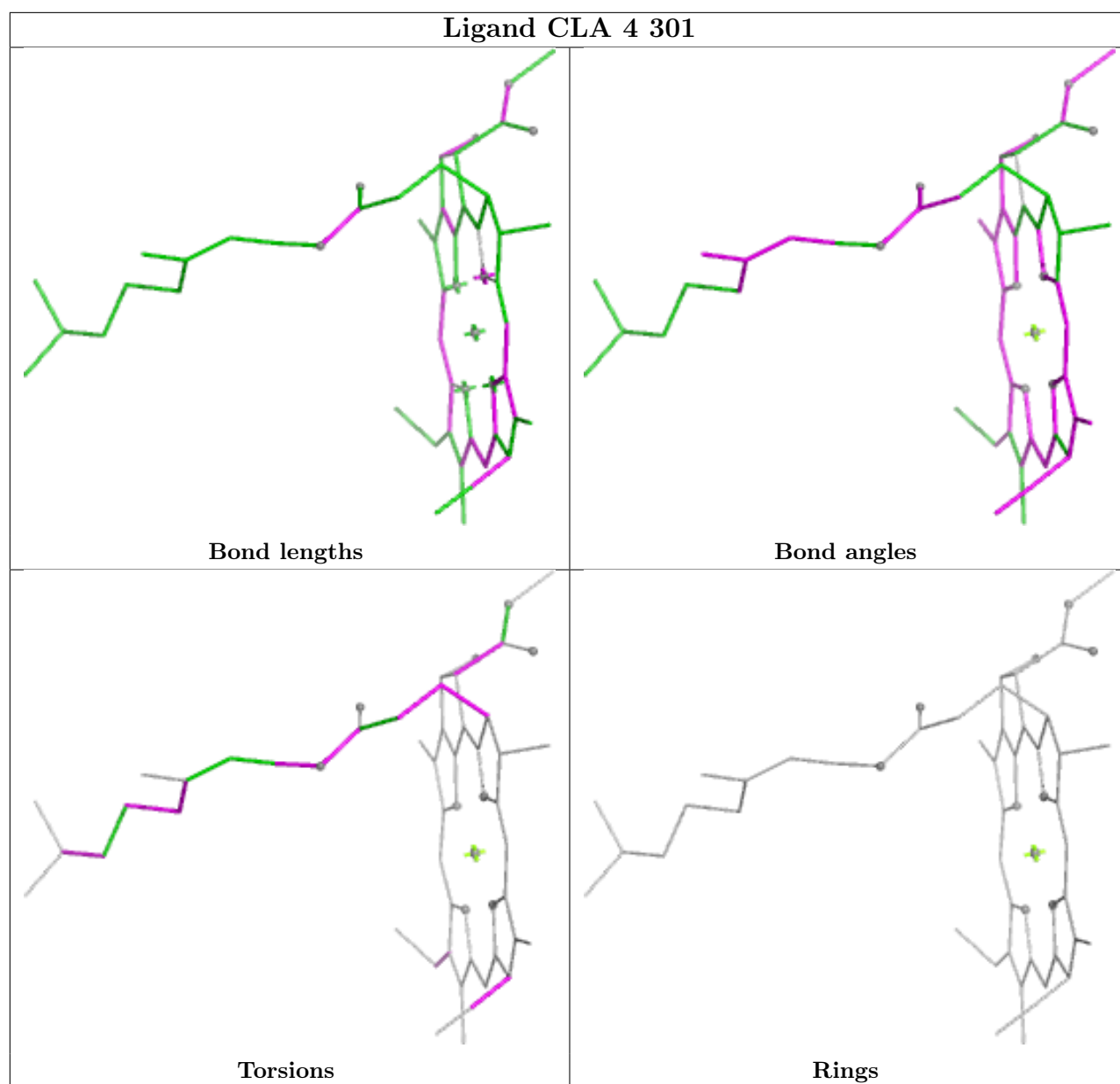
Bond angles

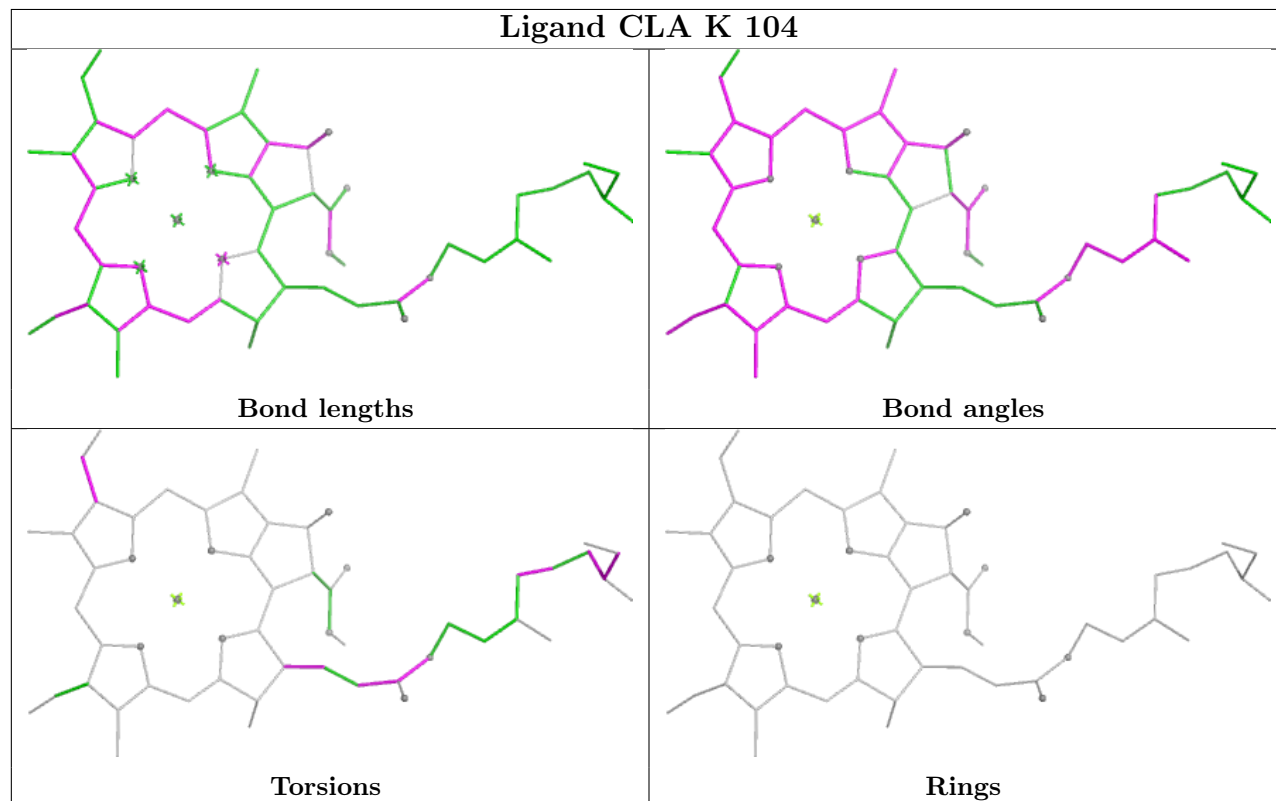
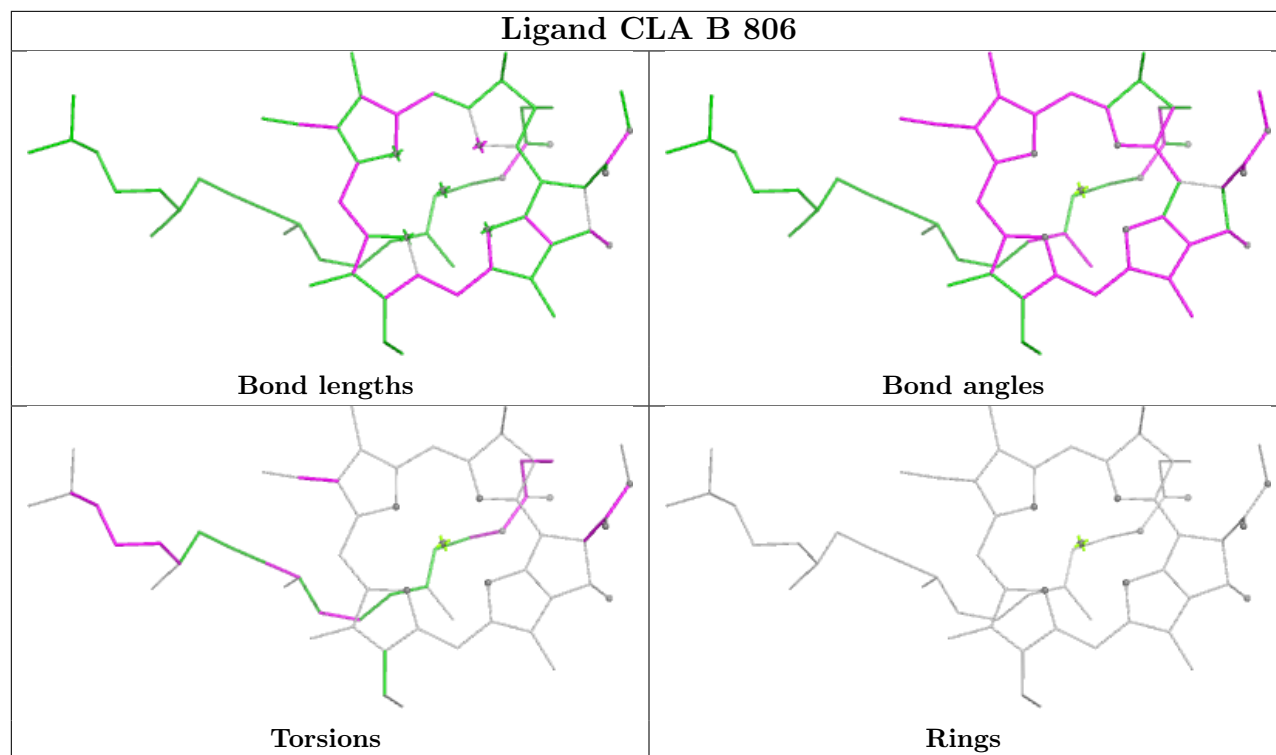


Torsions

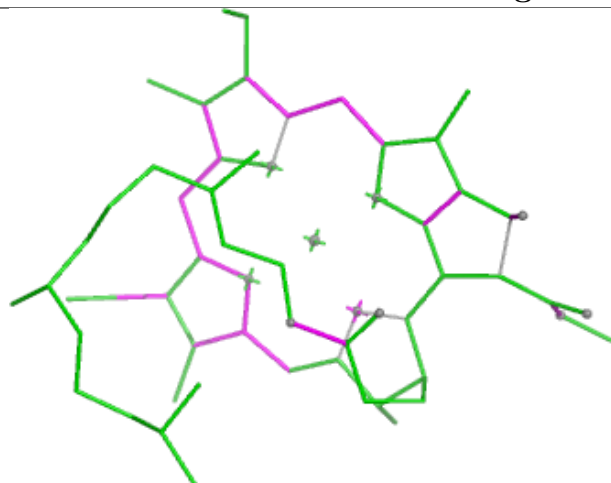


Rings

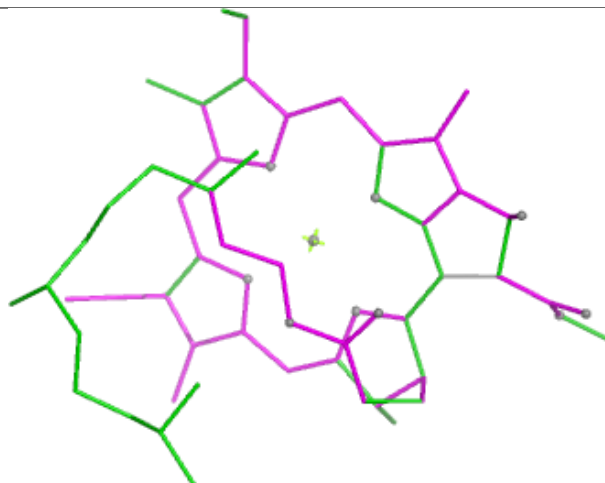




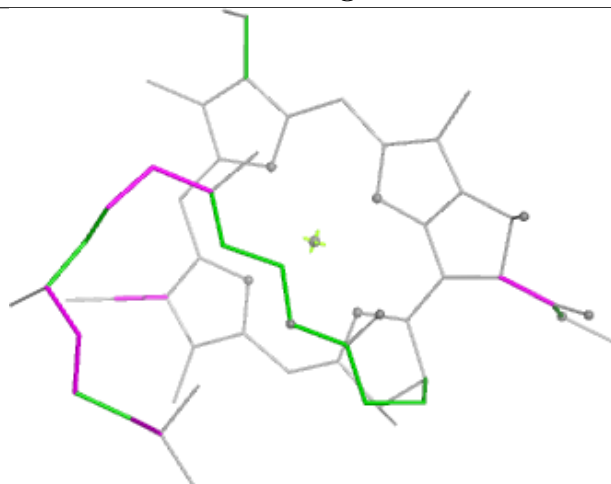
Ligand CLA B 810



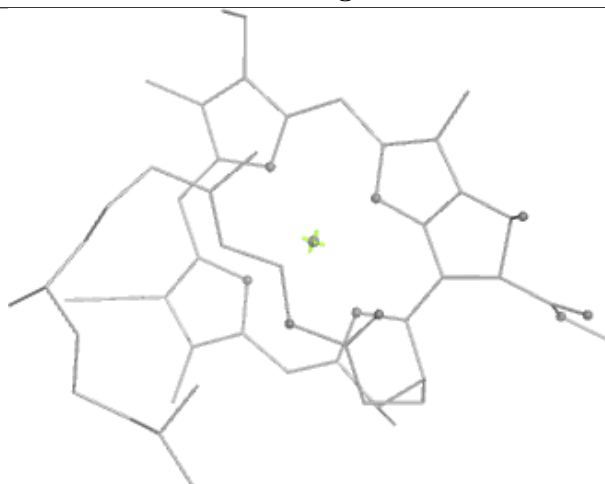
Bond lengths



Bond angles

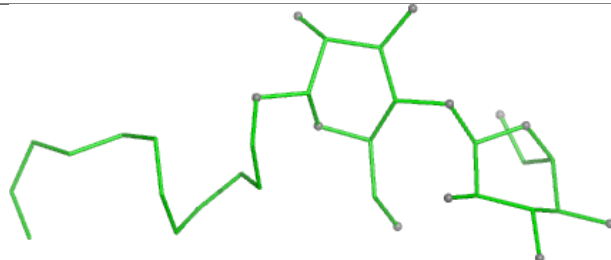


Torsions

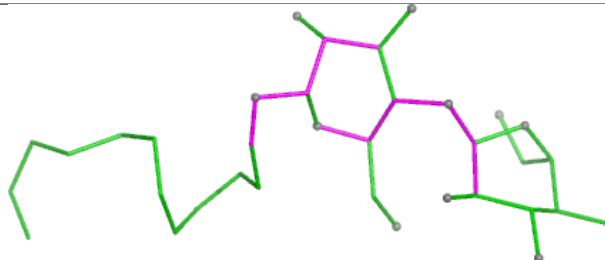


Rings

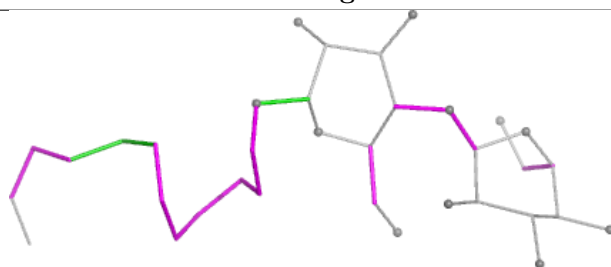
Ligand LMU 2 313



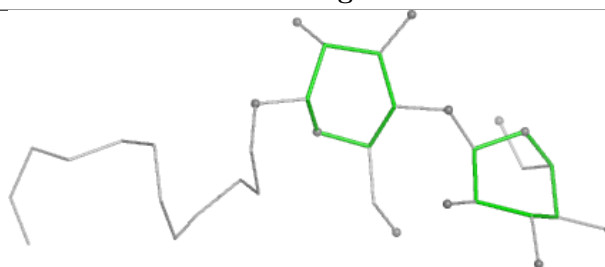
Bond lengths



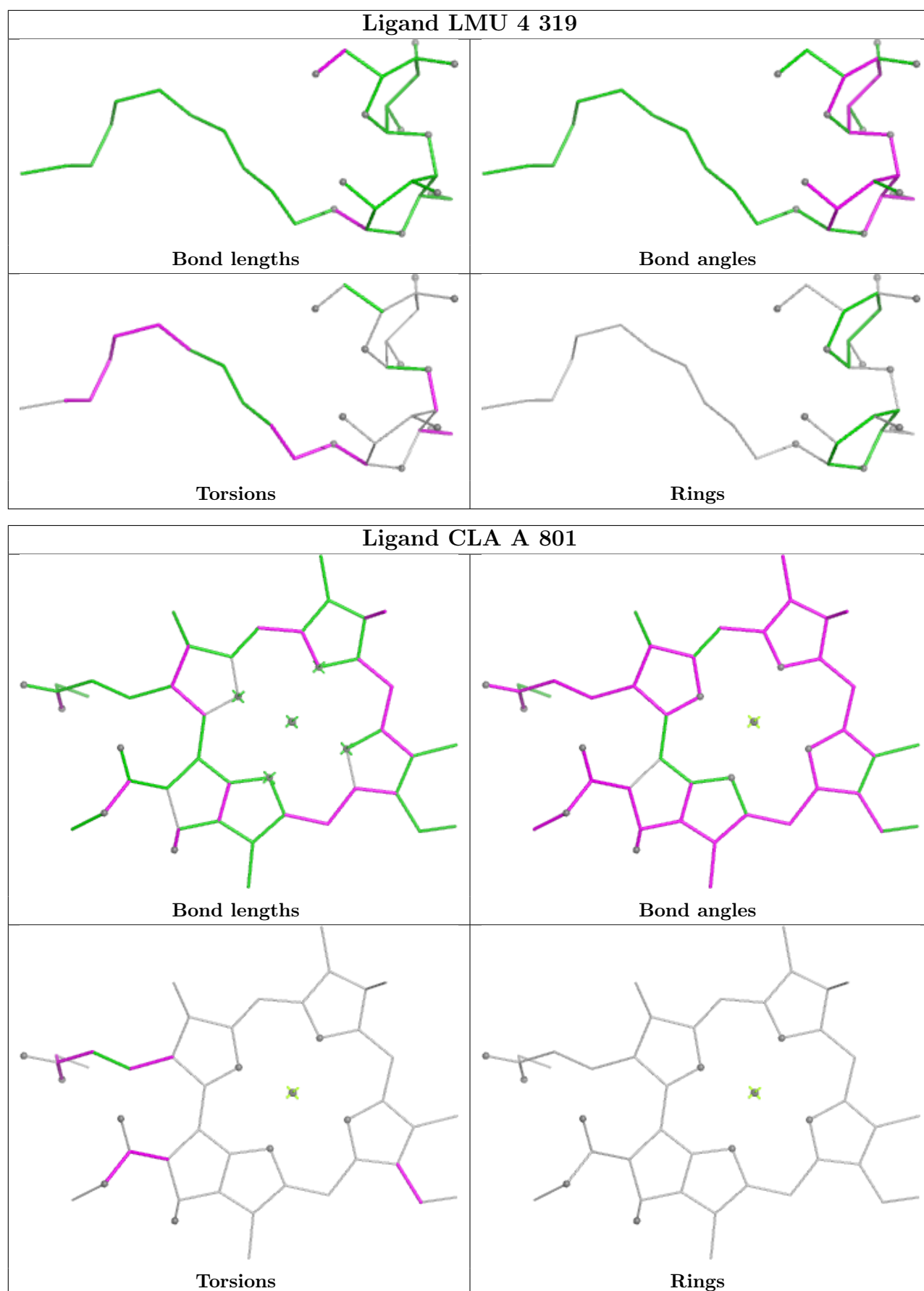
Bond angles



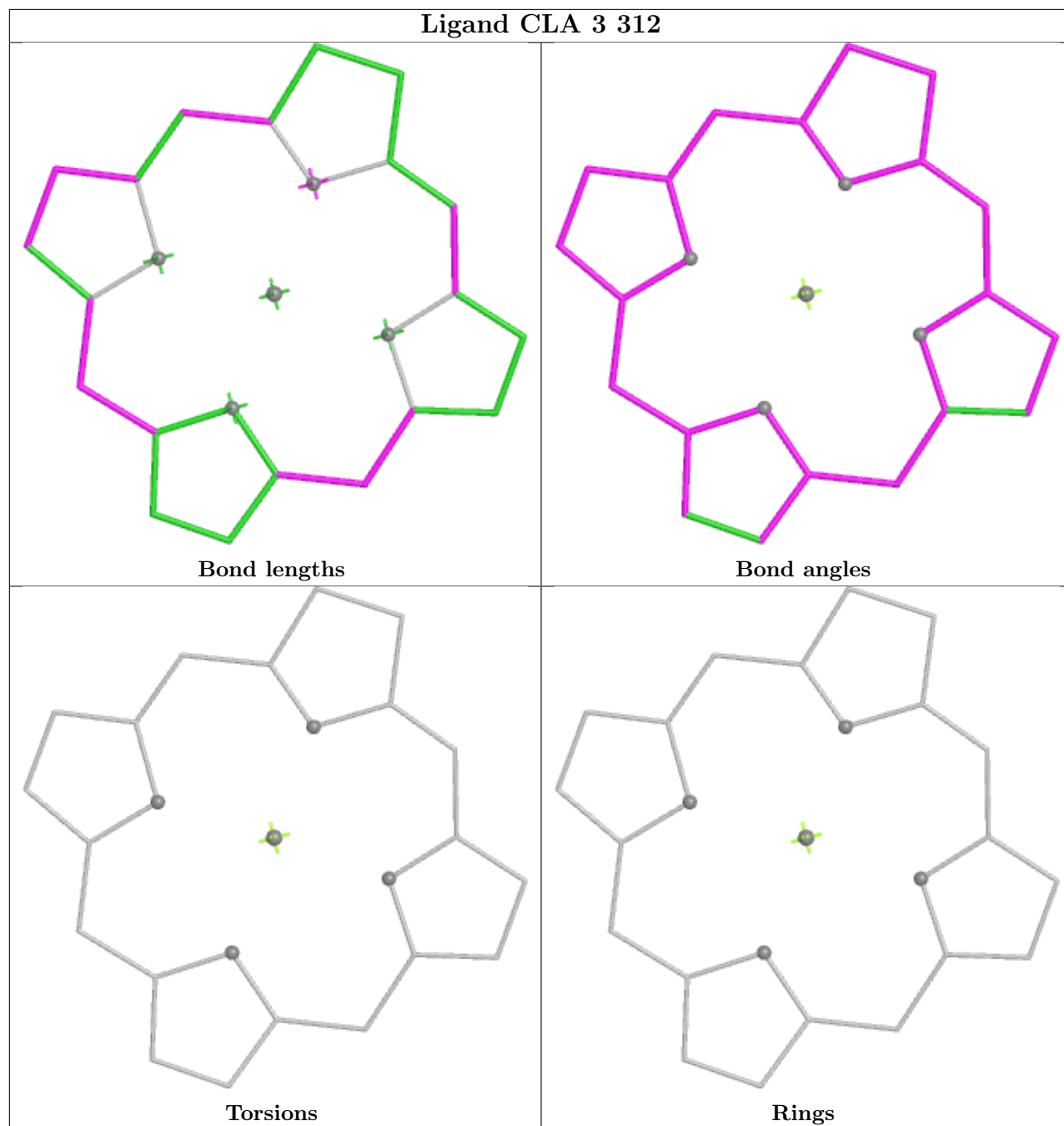
Torsions

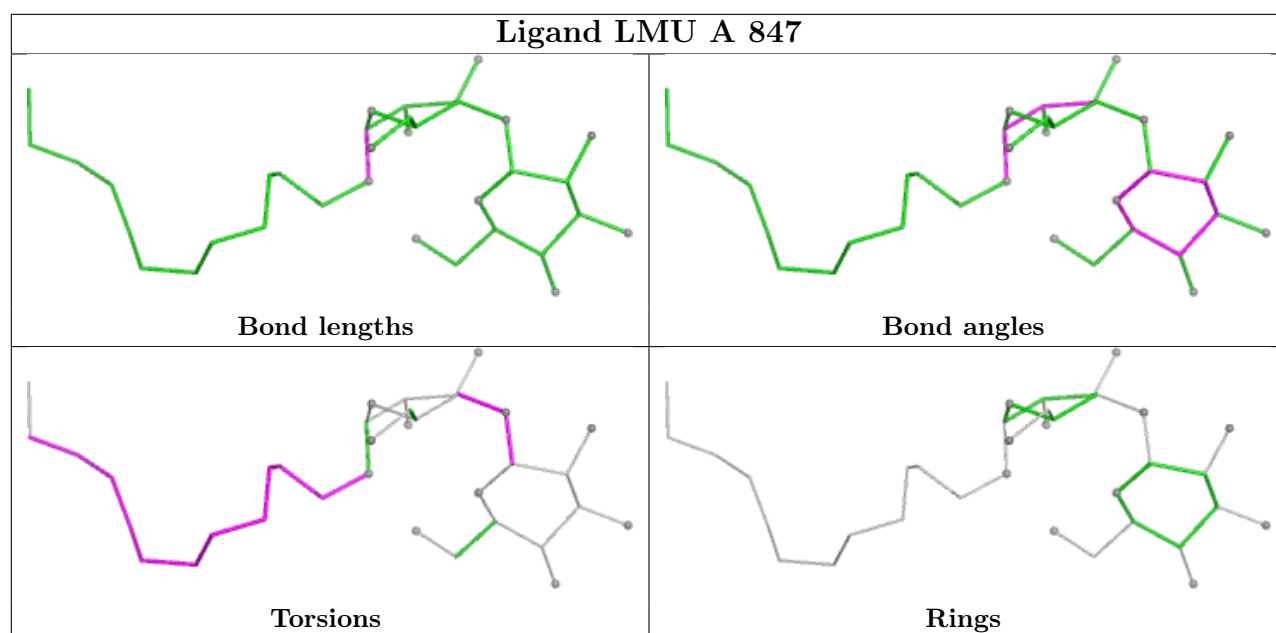


Rings

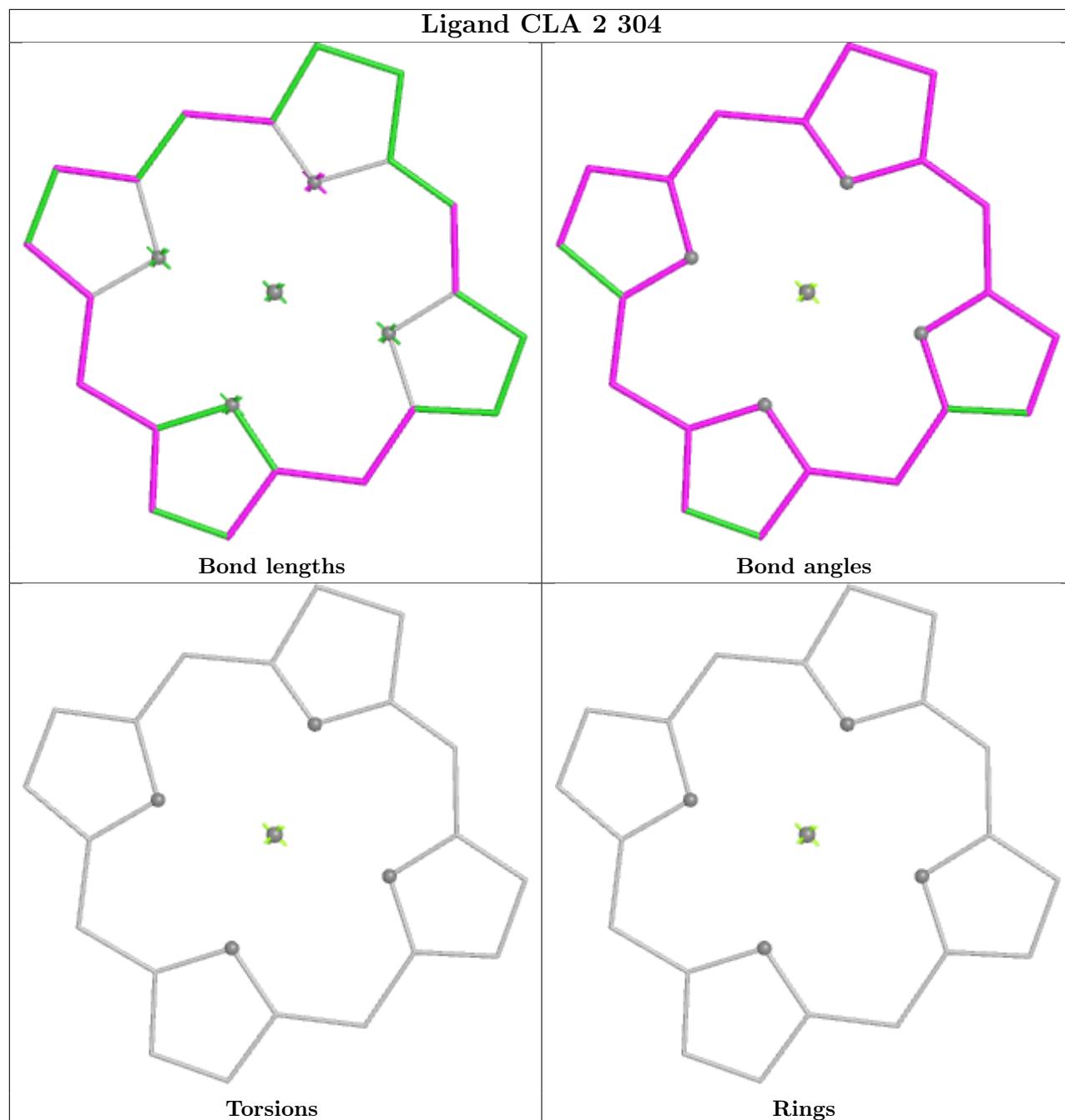


Ligand CLA 3 312

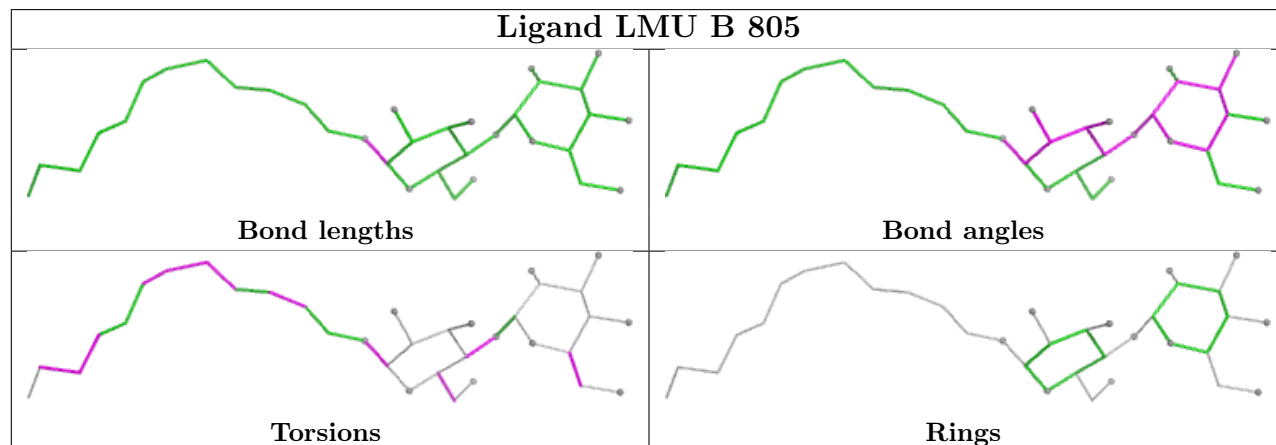




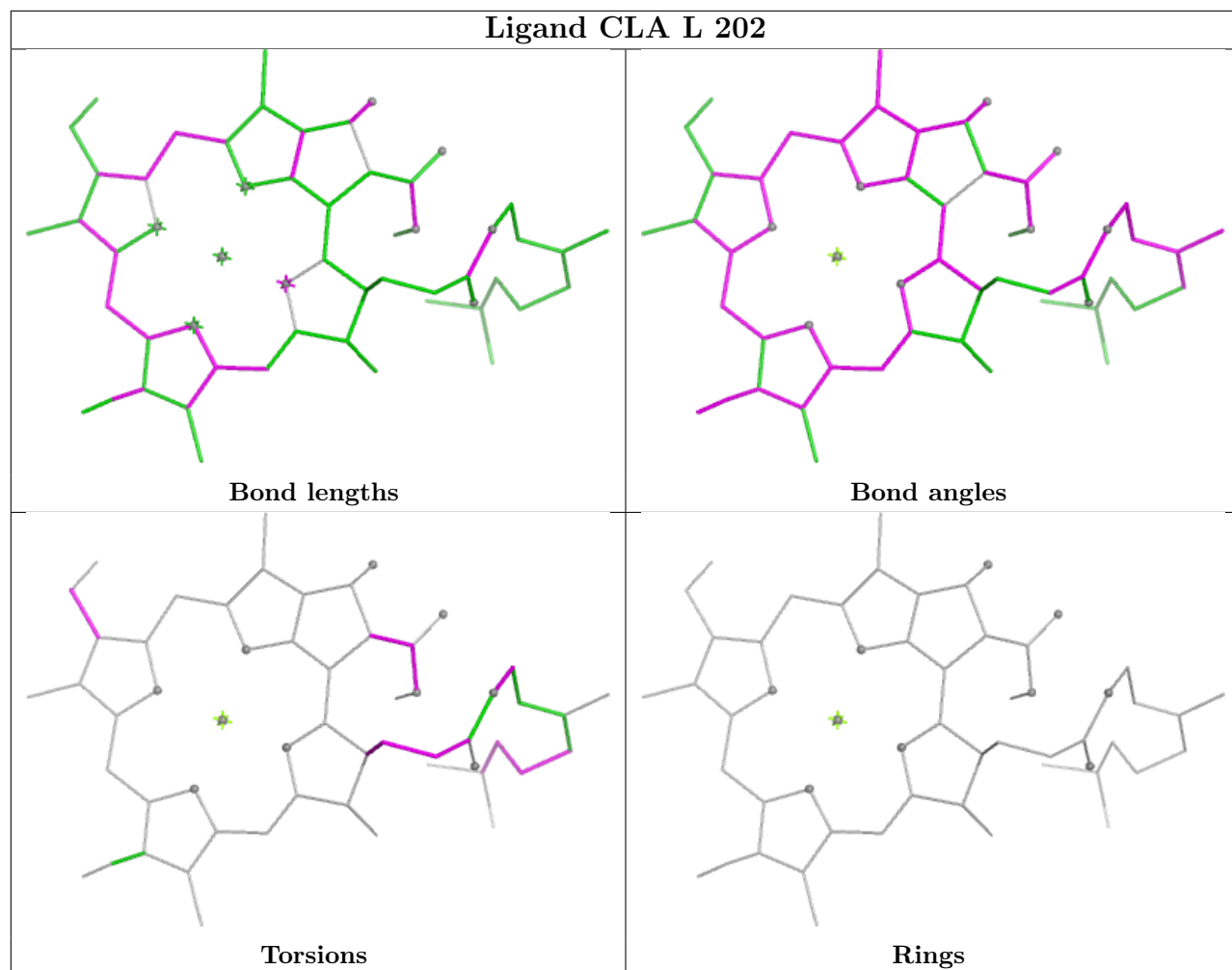
Ligand CLA 2 304



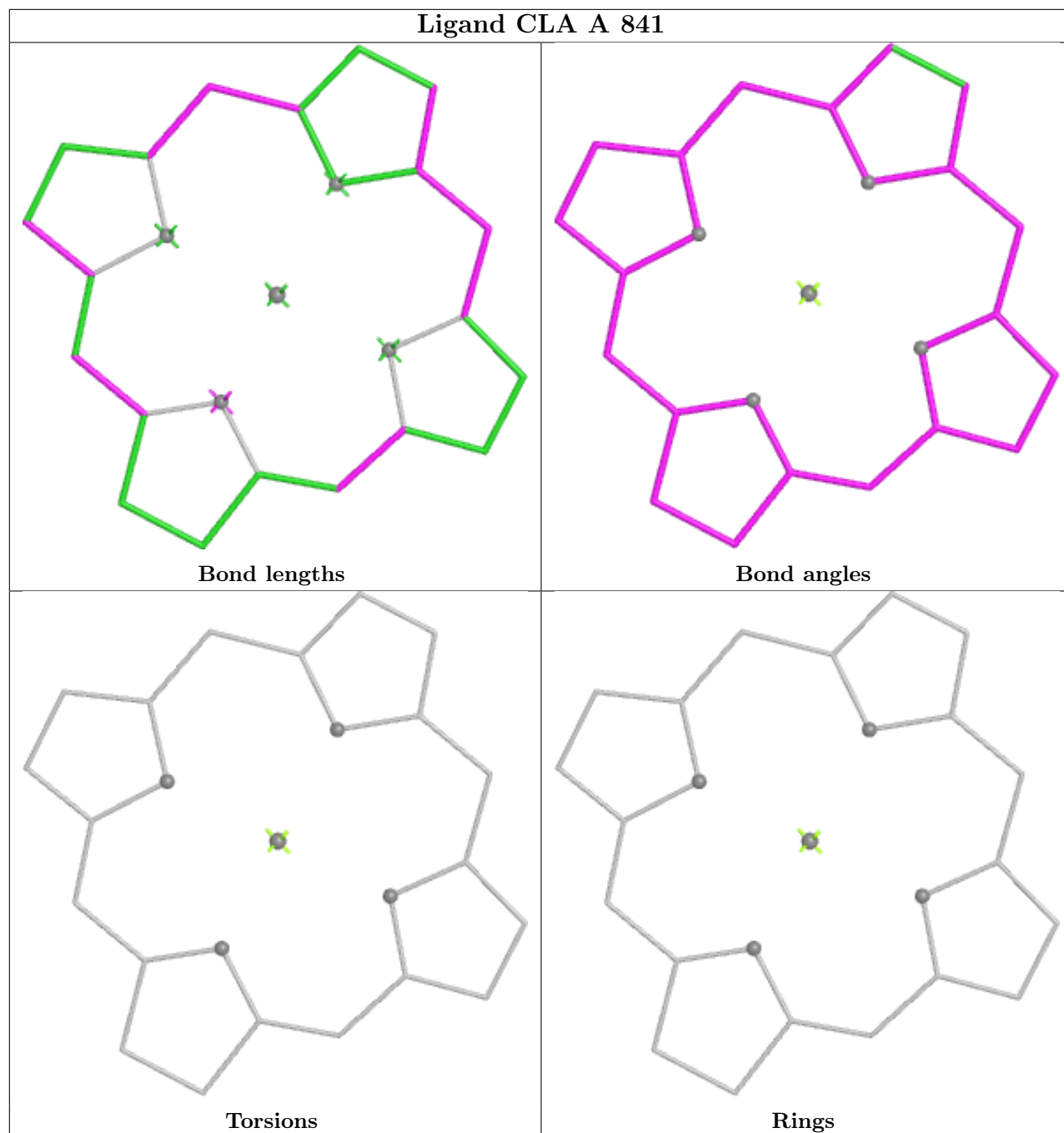
Ligand LMU B 805



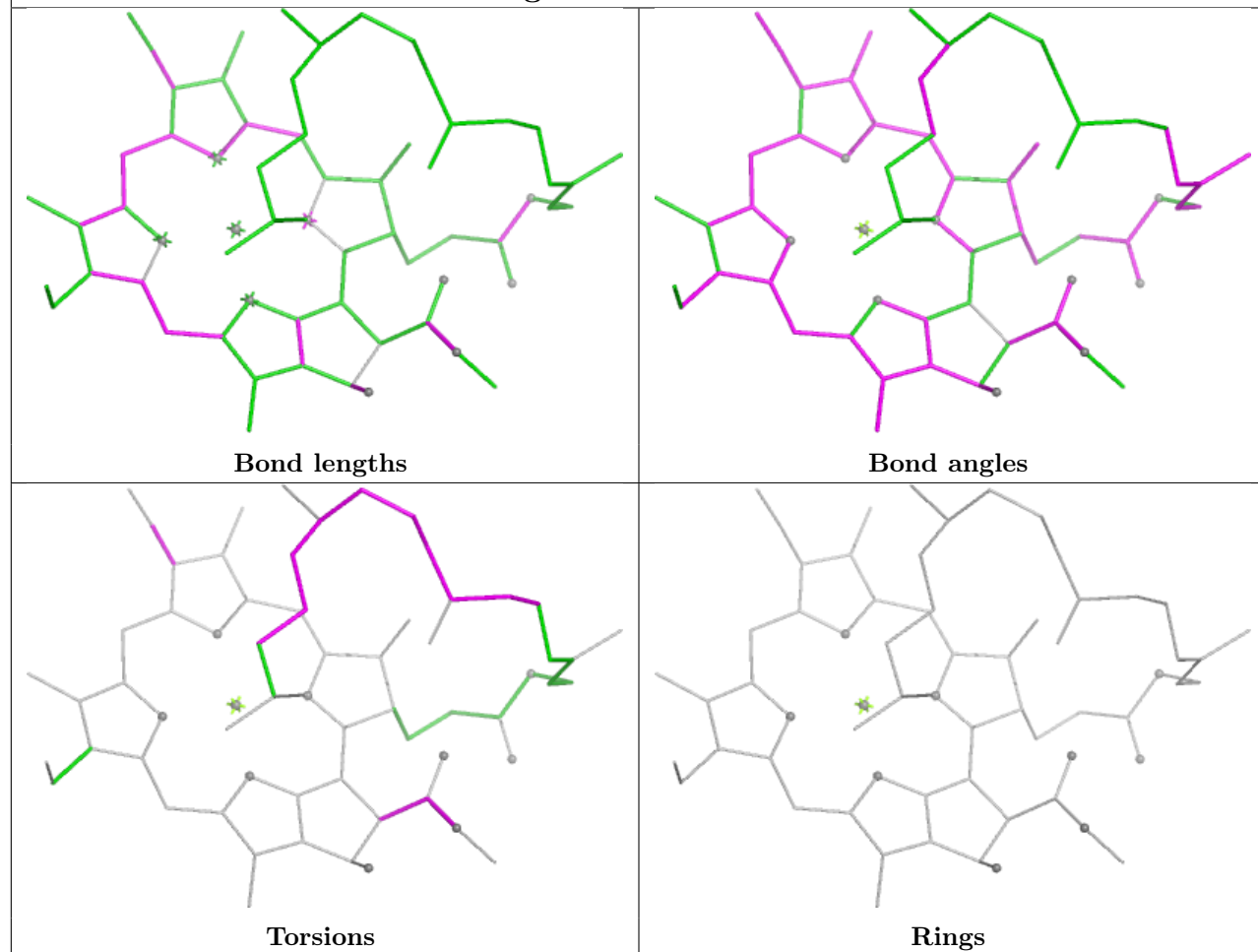
Ligand CLA L 202



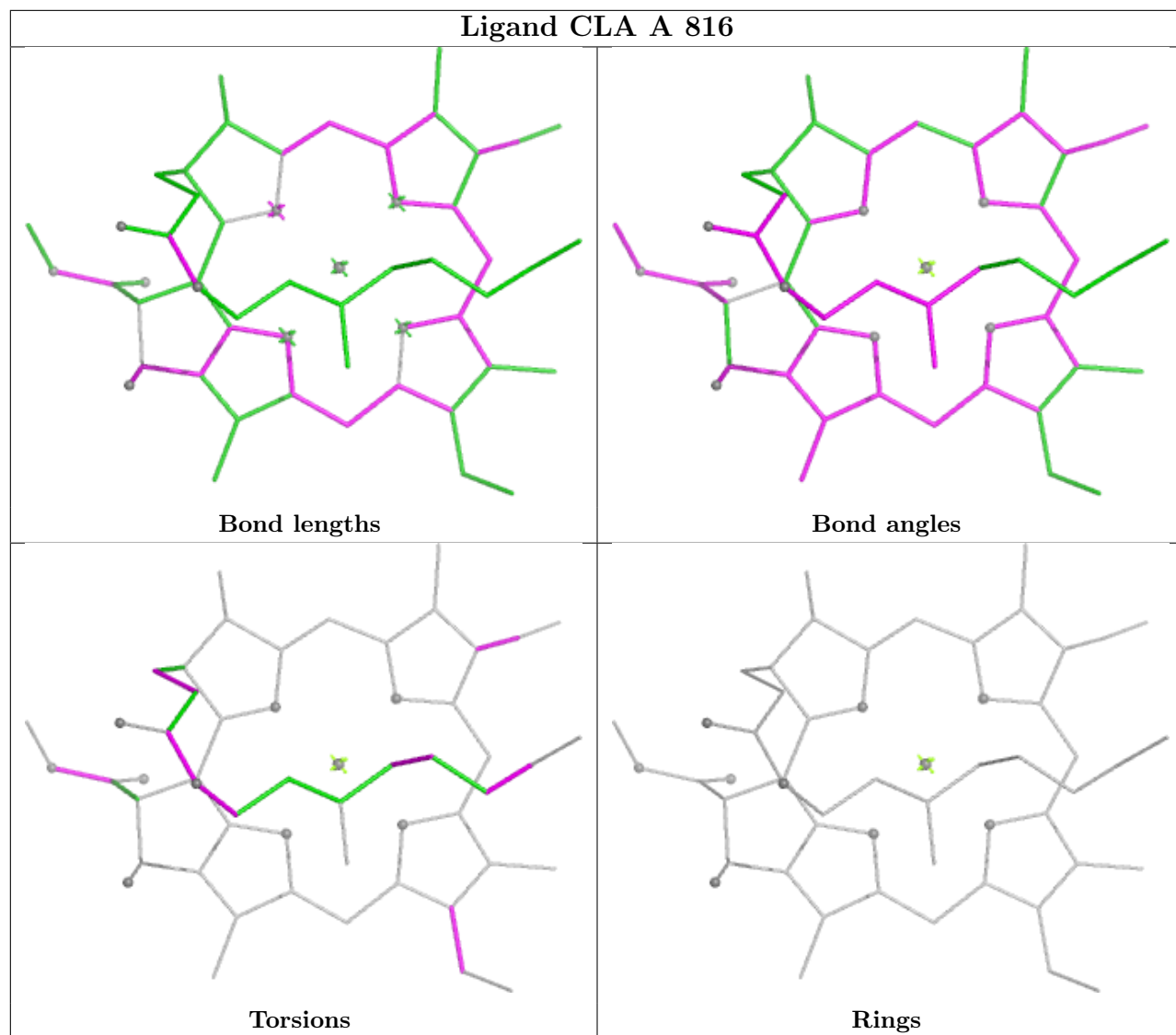
Ligand CLA A 841



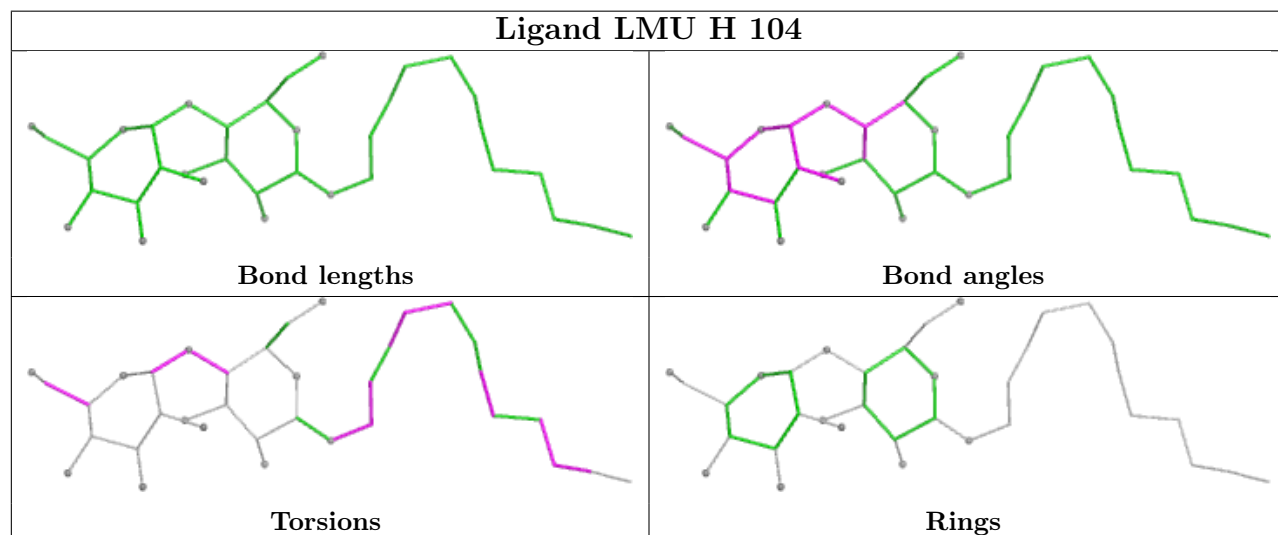
Ligand CLA B 809

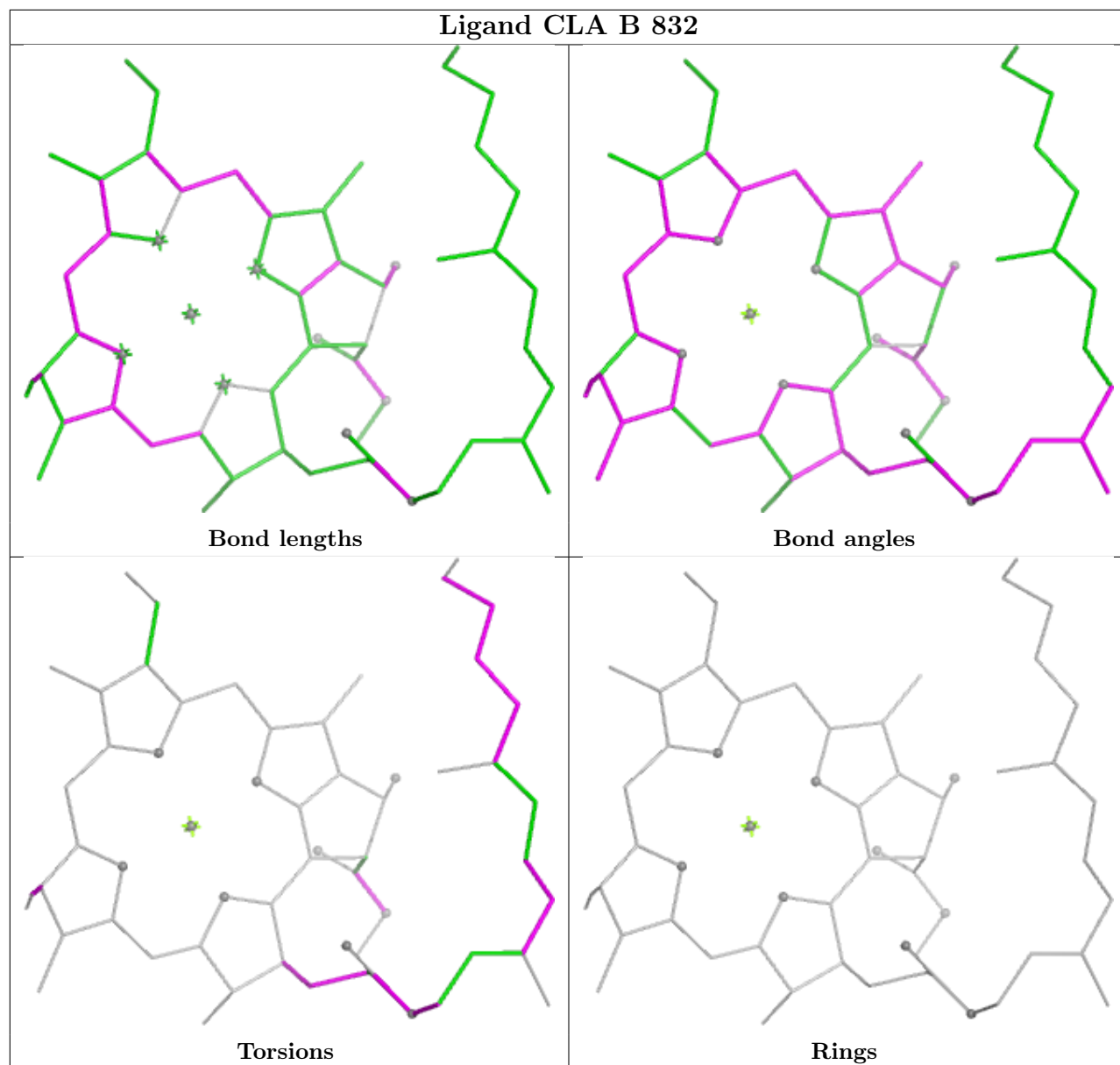


Ligand CLA A 816

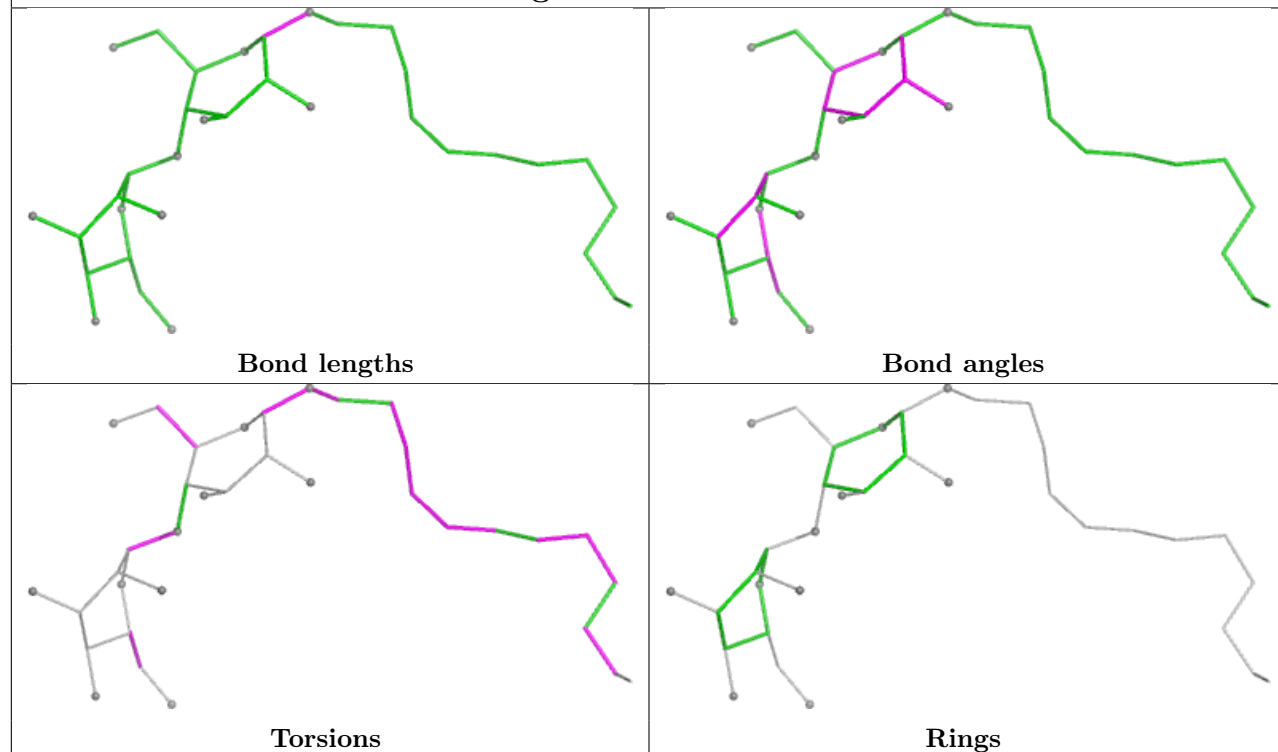


Ligand LMU H 104

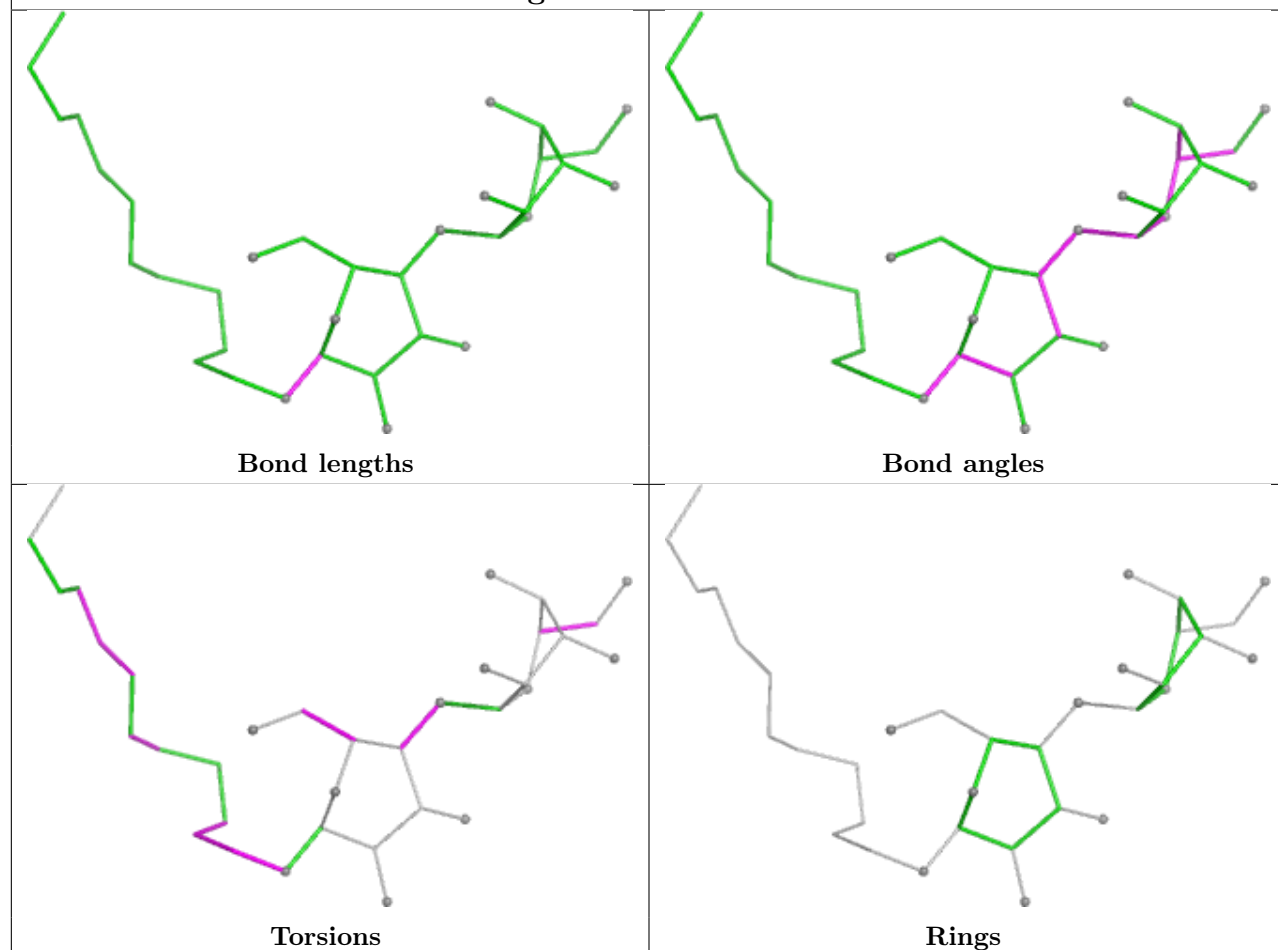




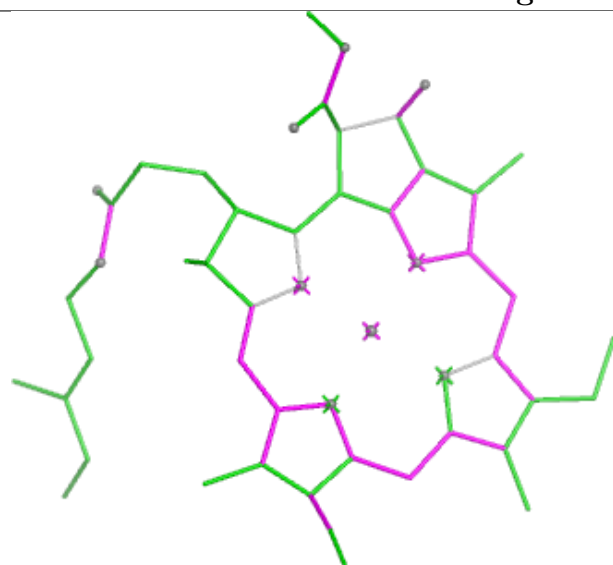
Ligand LMU 4 320



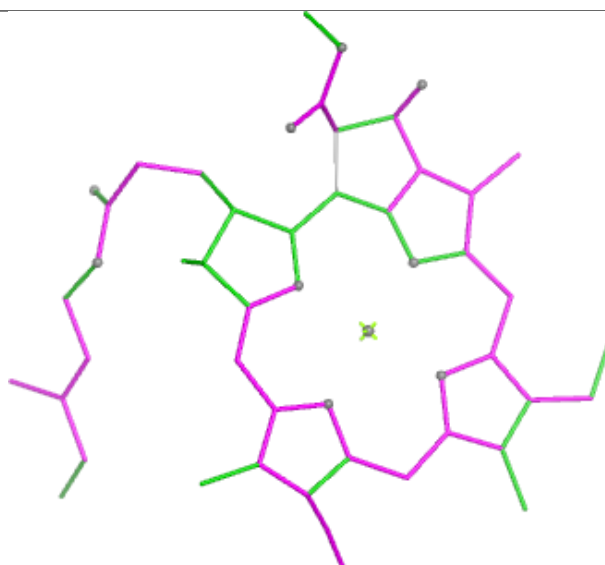
Ligand LMU R 103



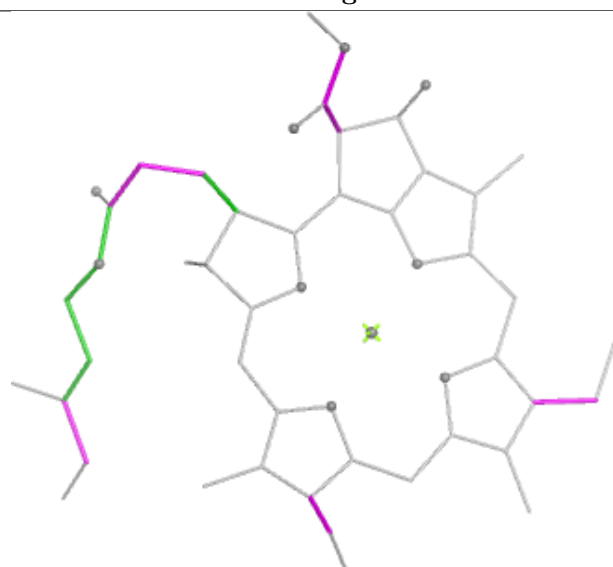
Ligand CLA B 836



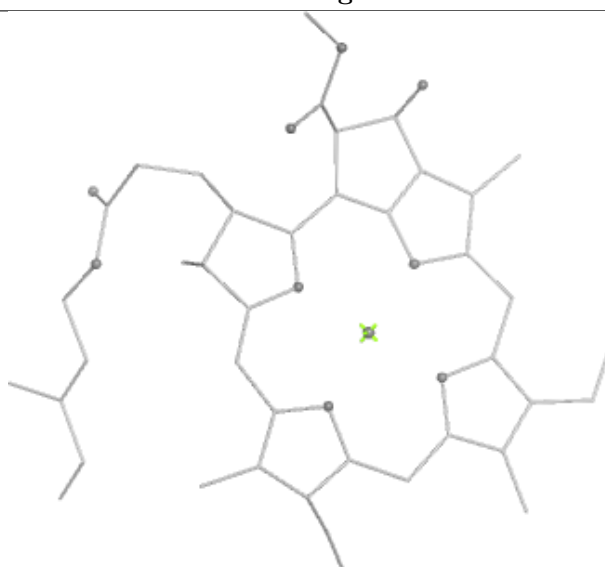
Bond lengths



Bond angles

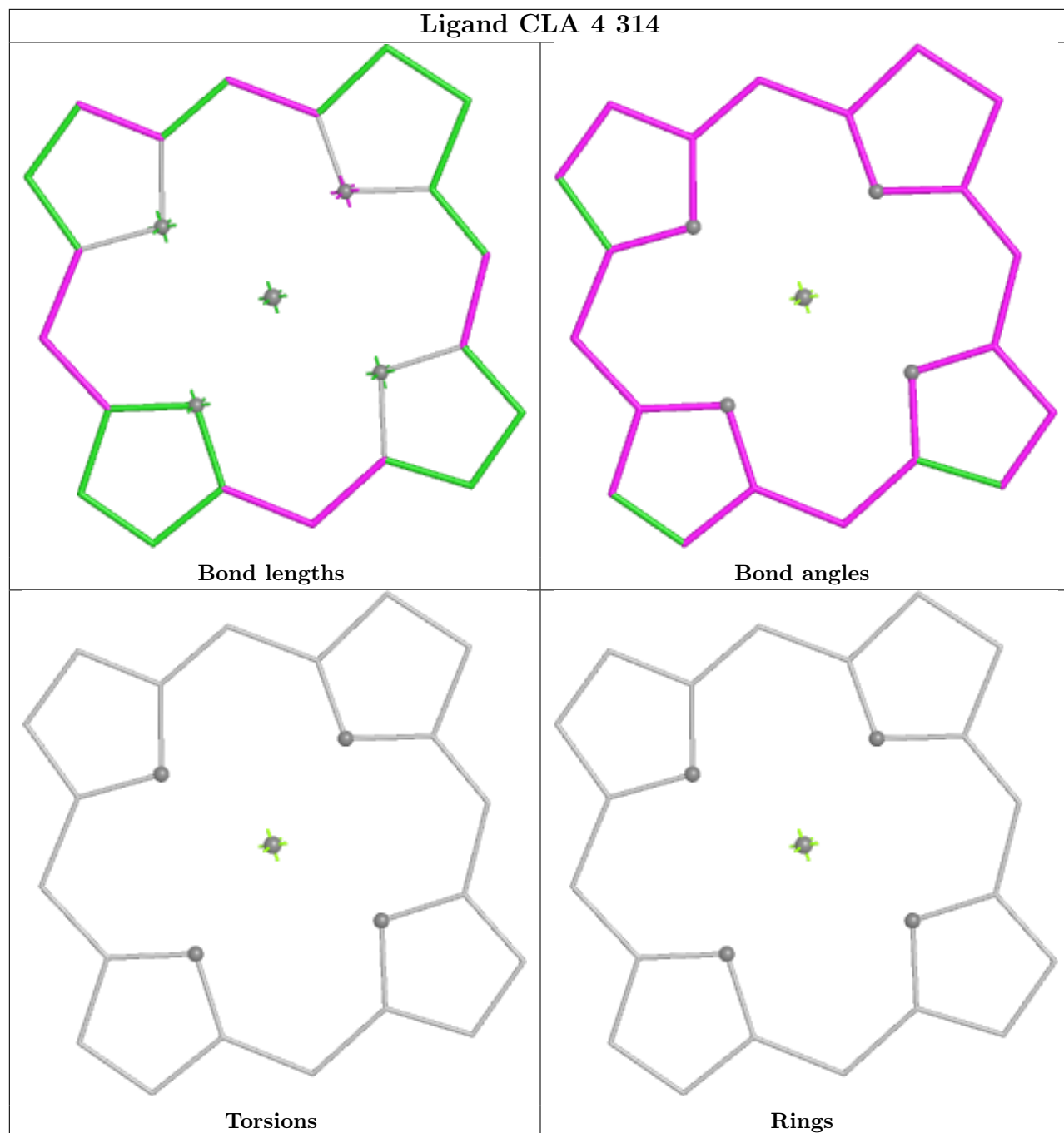


Torsions

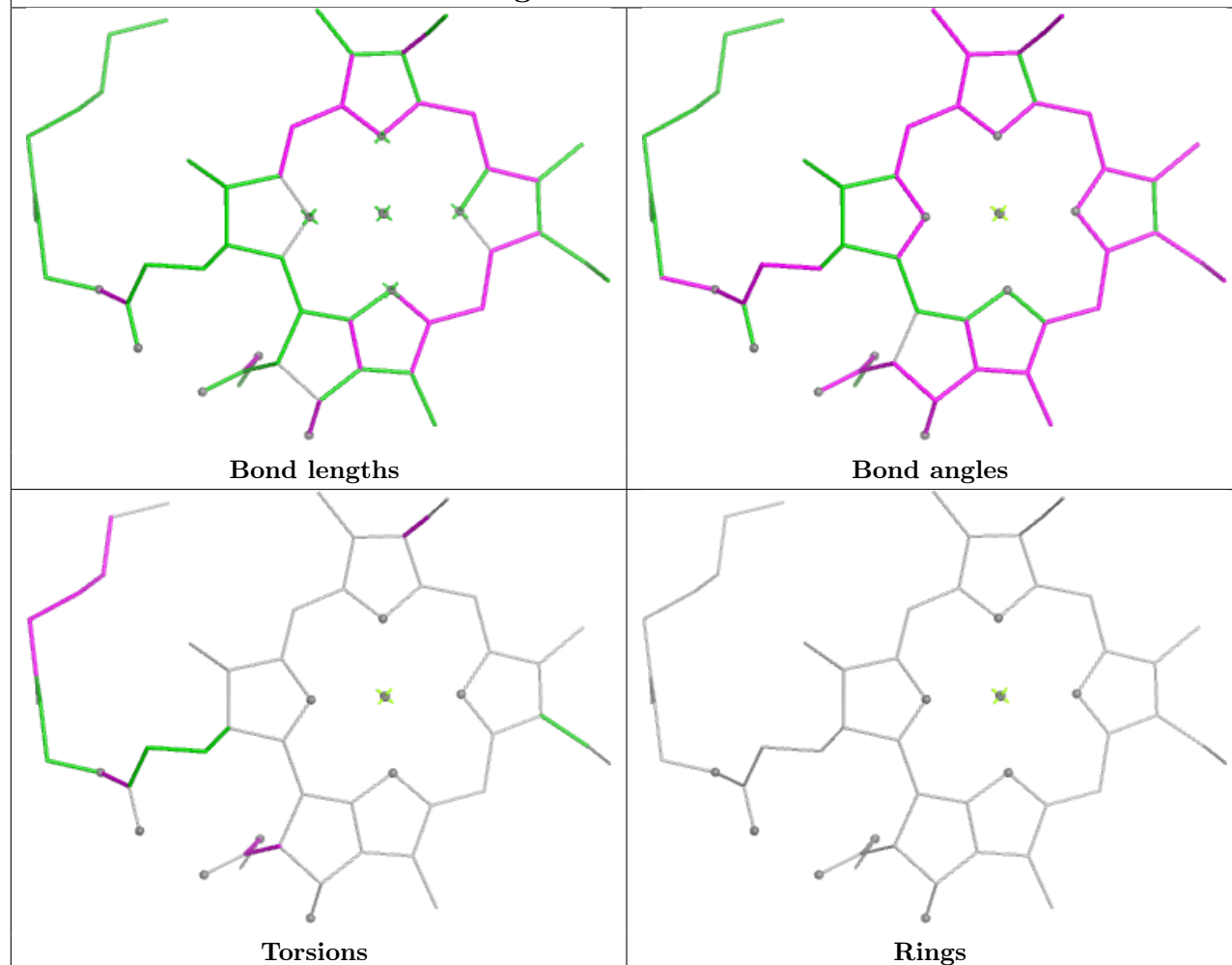


Rings

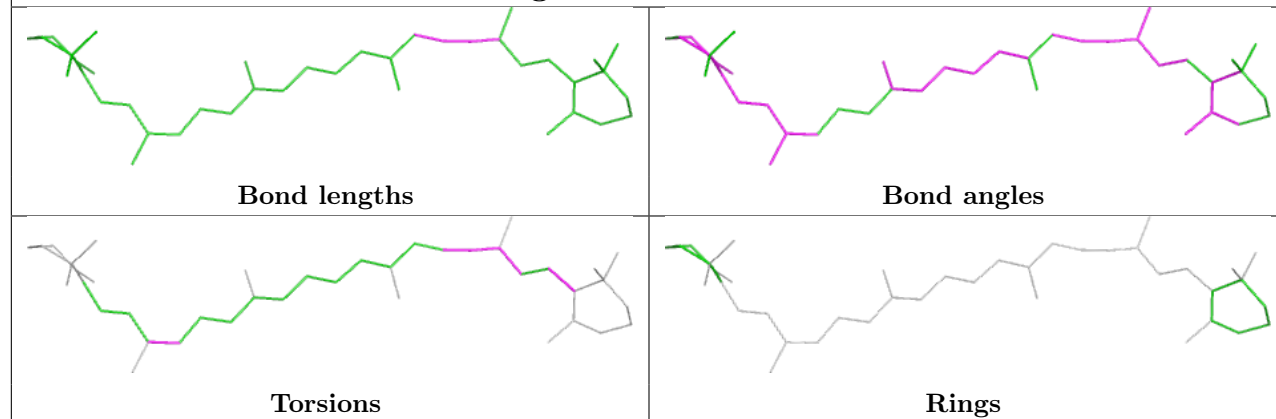
Ligand CLA 4 314

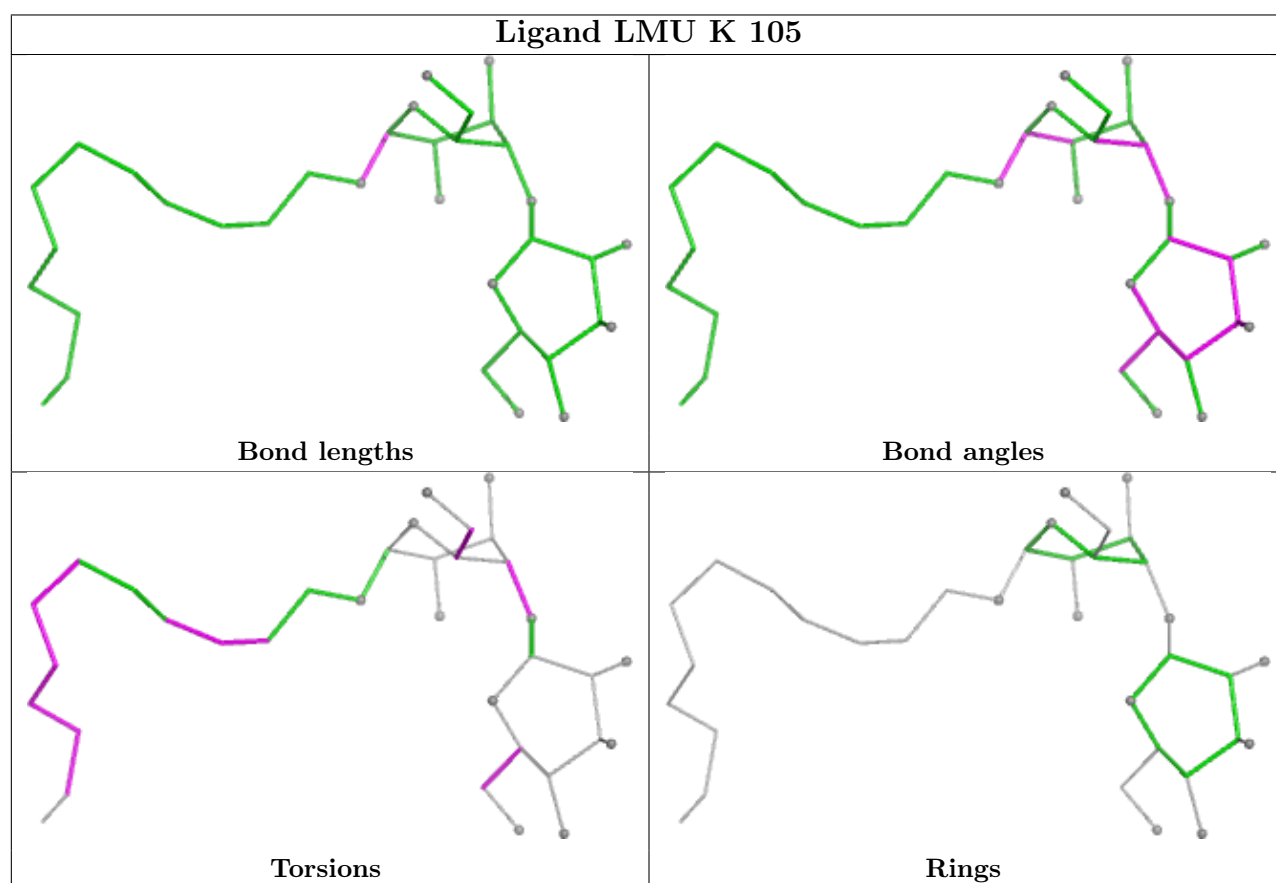
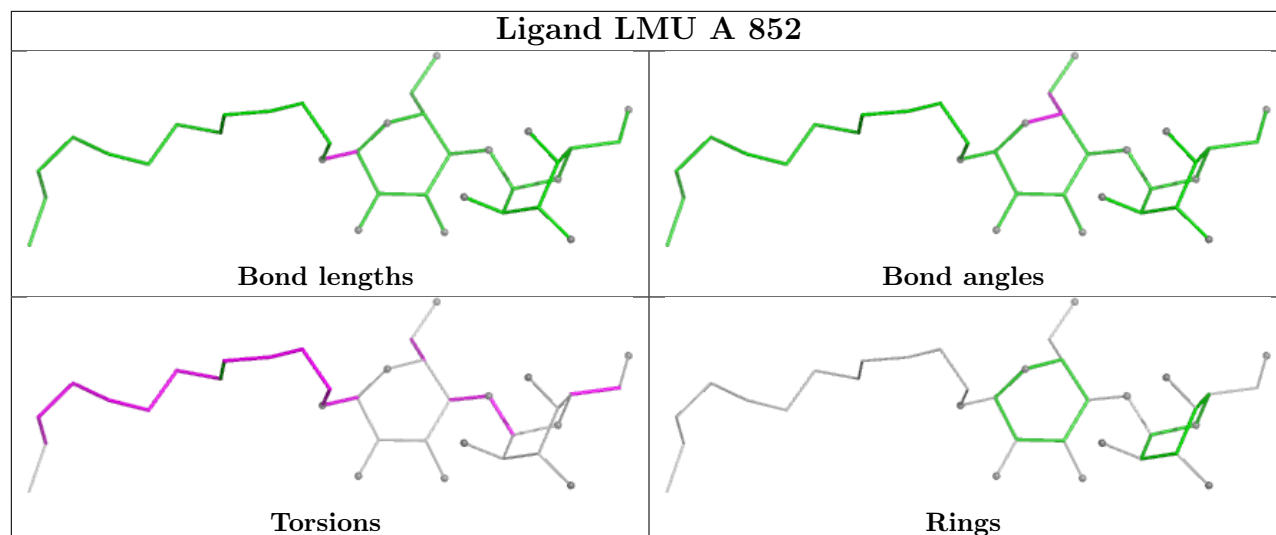


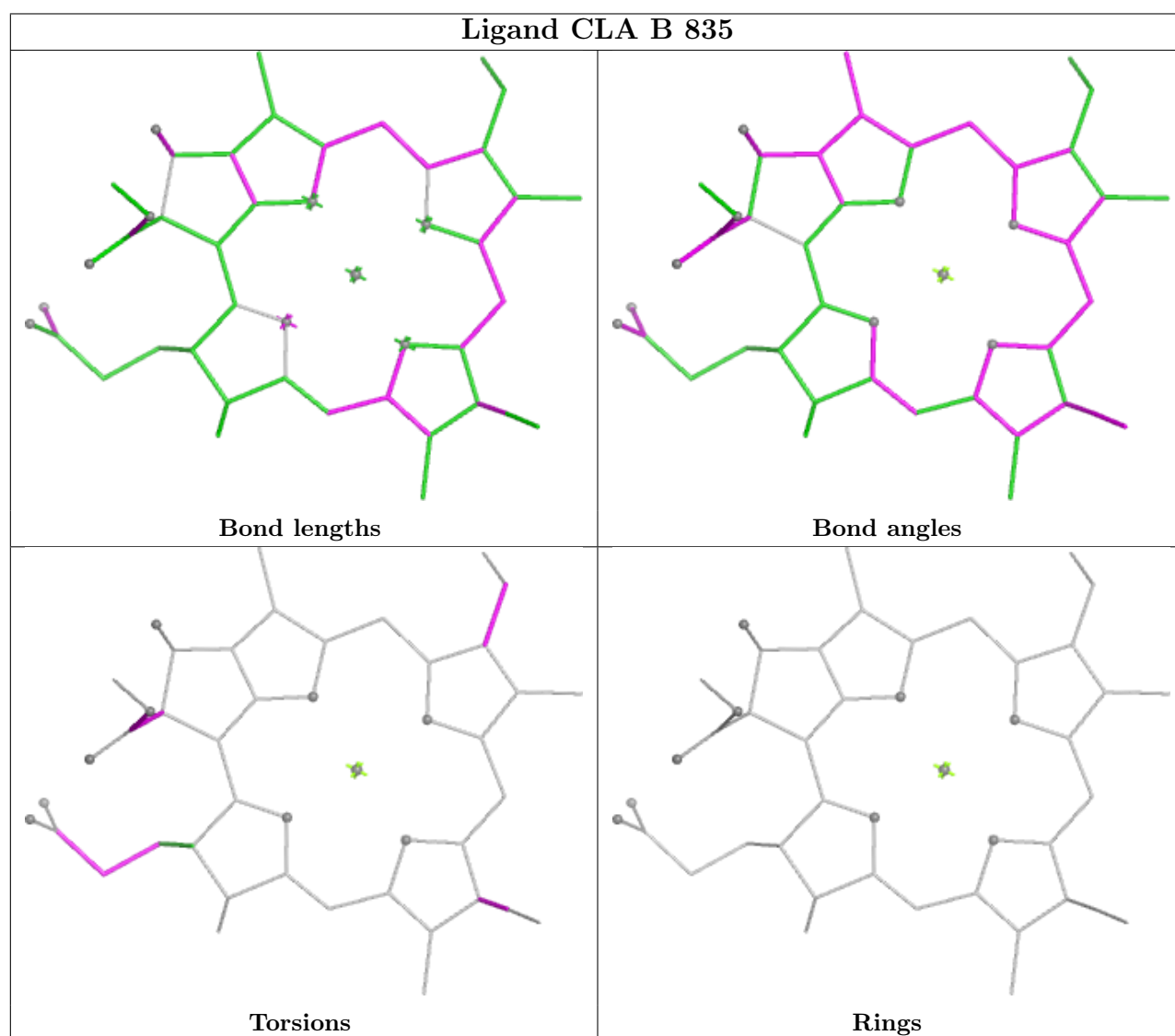
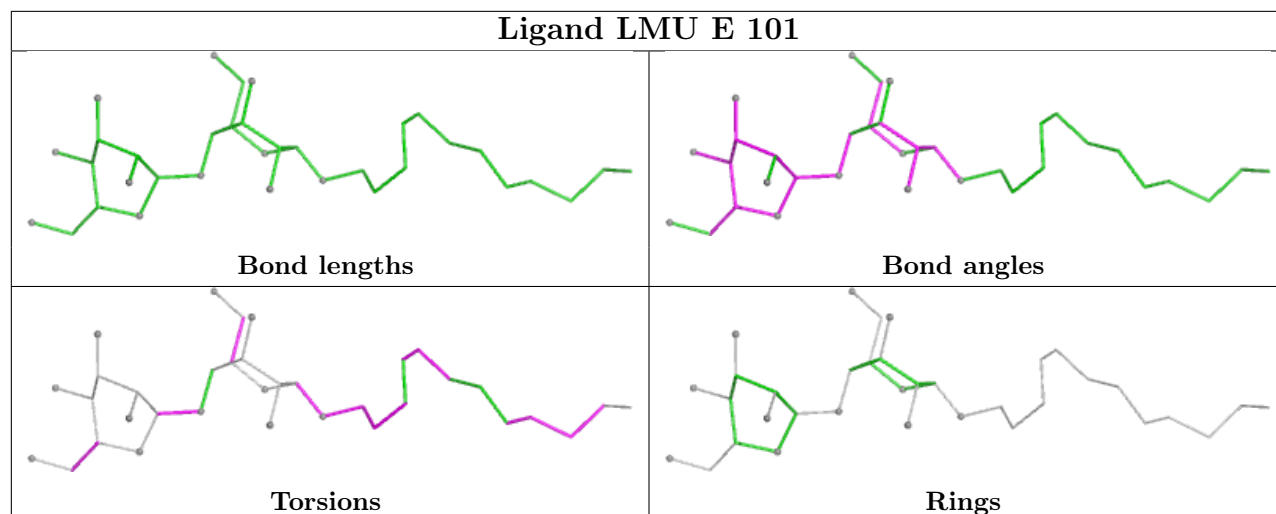
Ligand CLA B 825

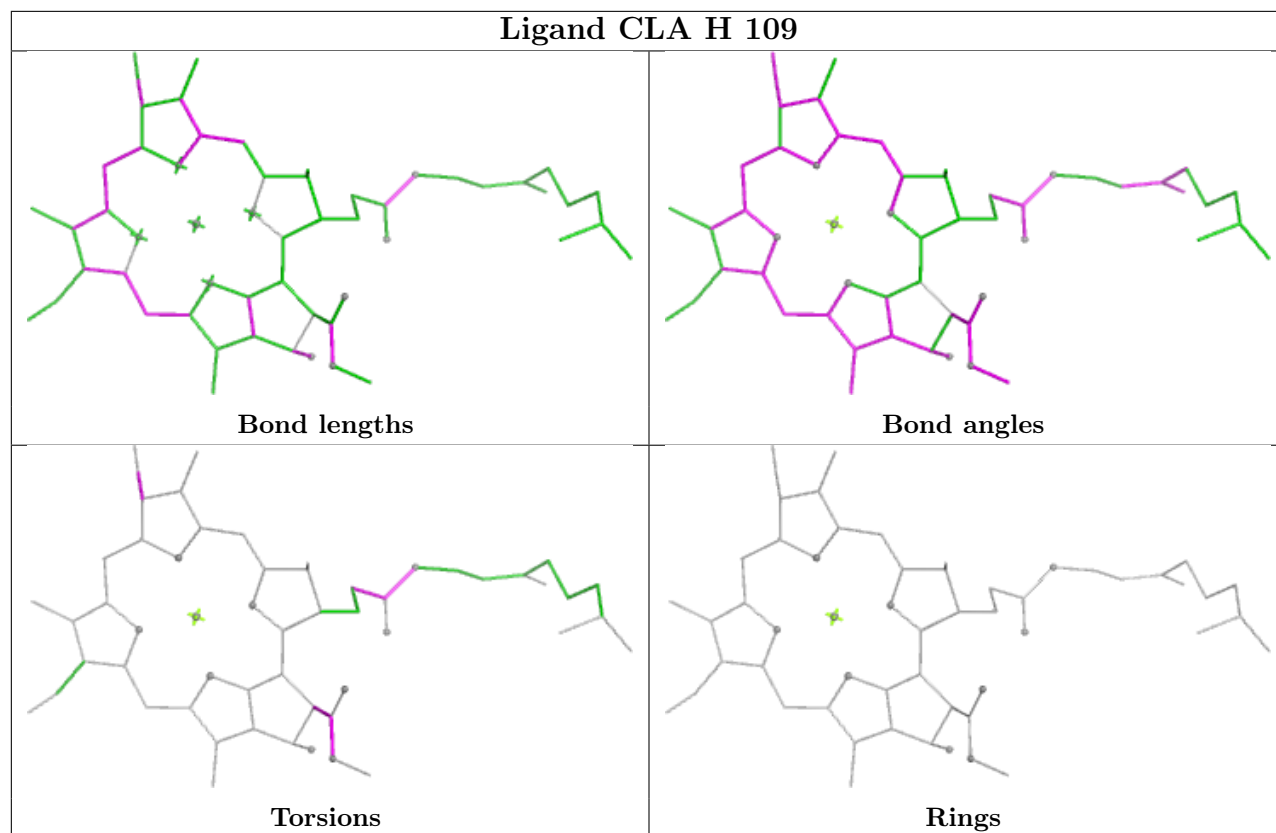


Ligand BCR B 845

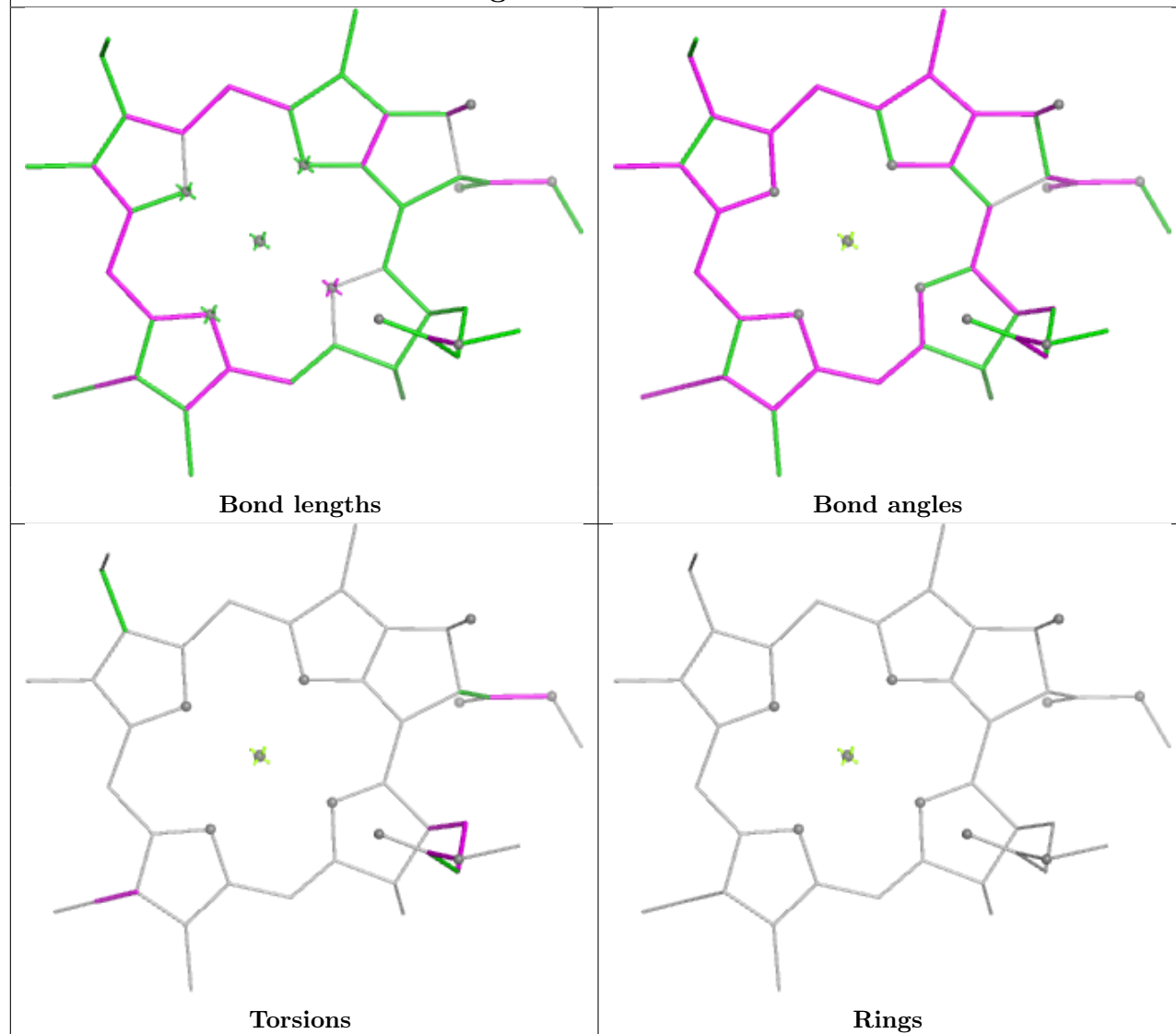




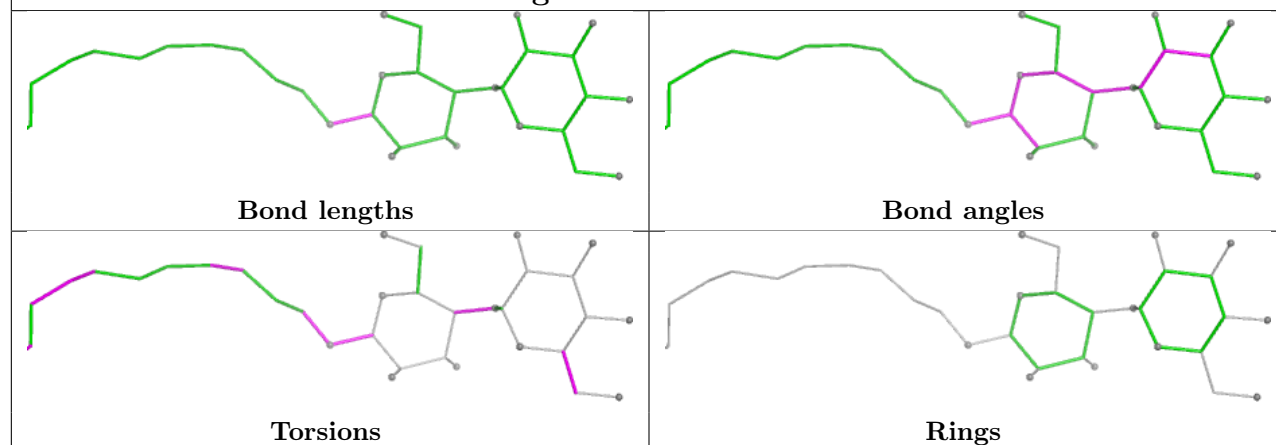


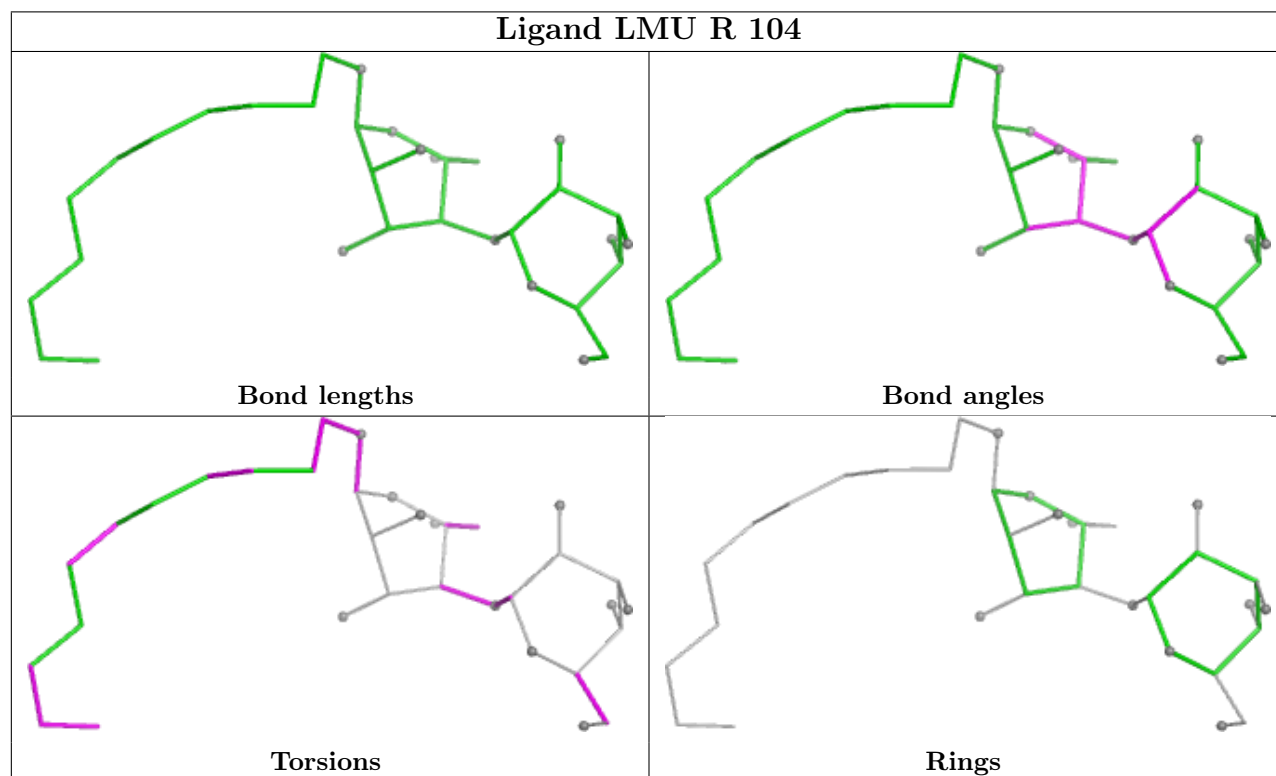
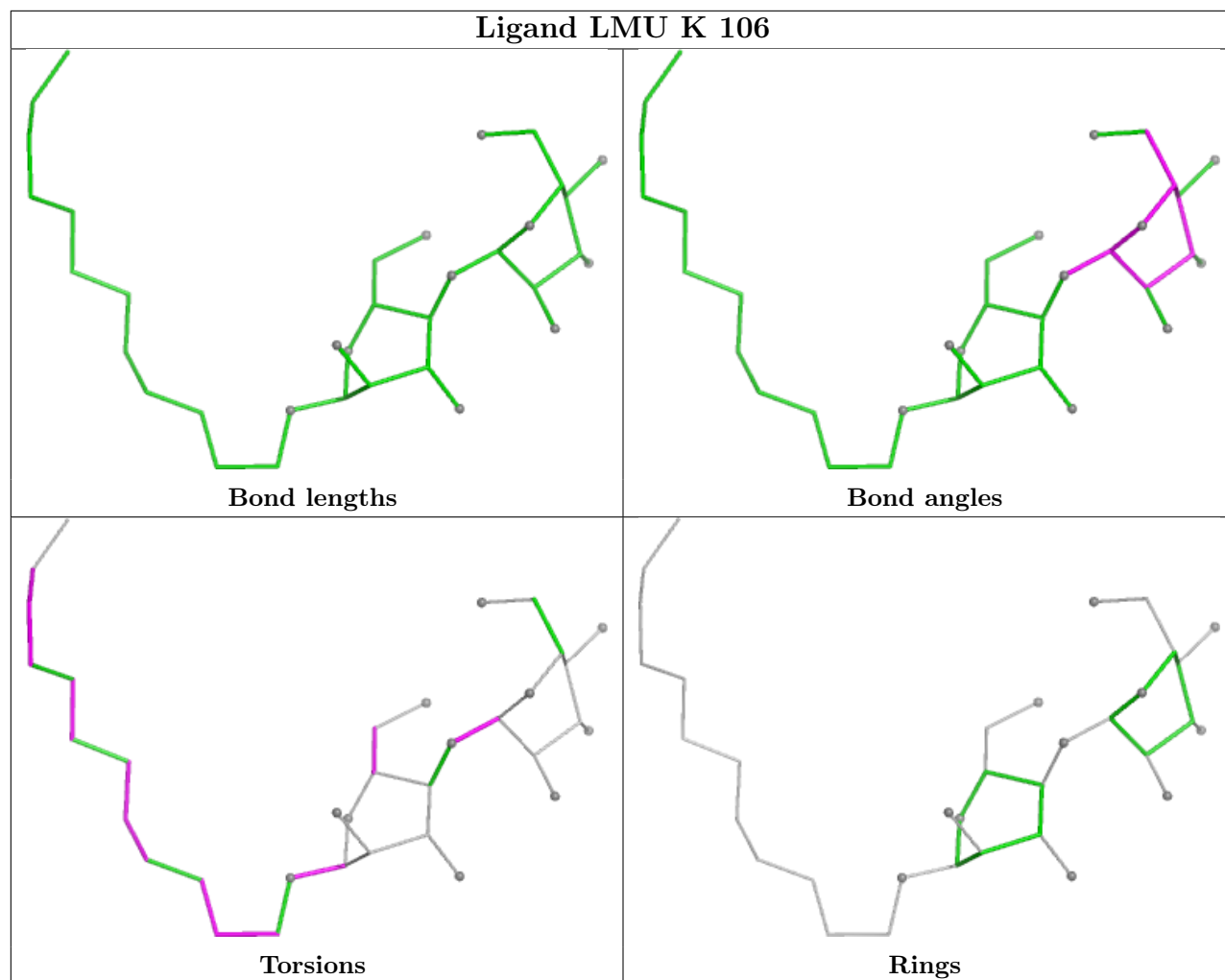


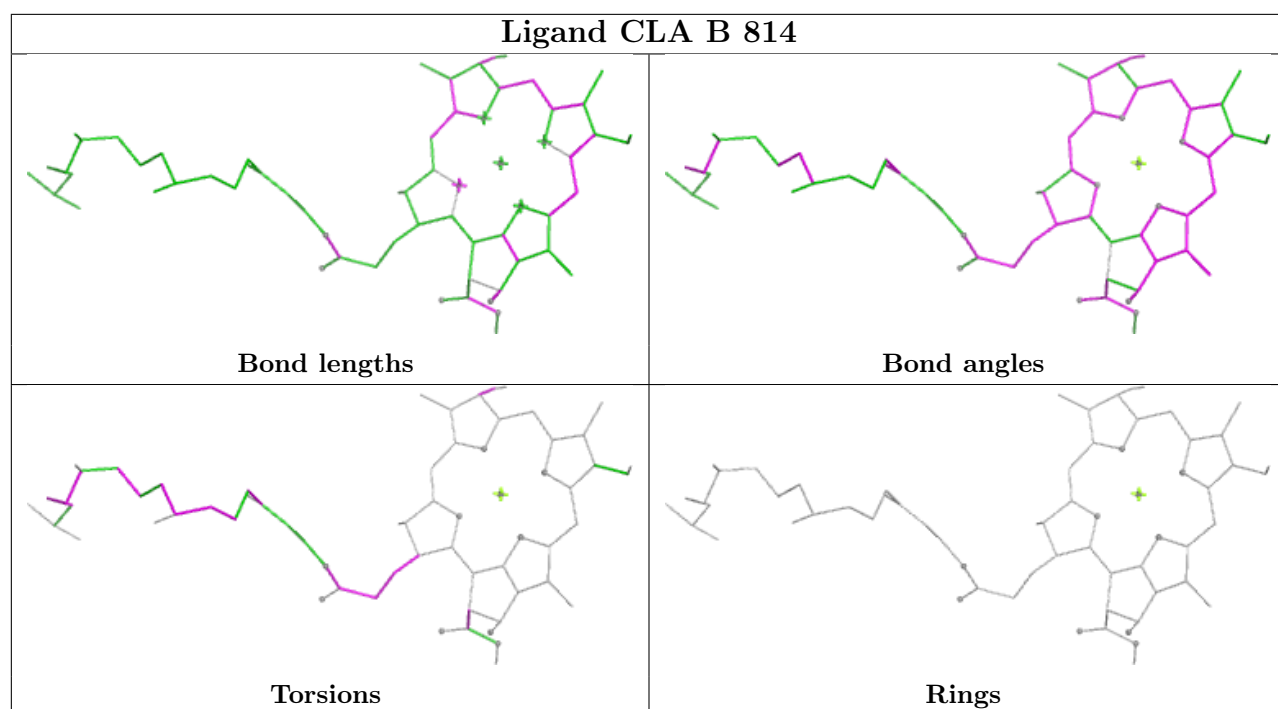
Ligand CLA A 807



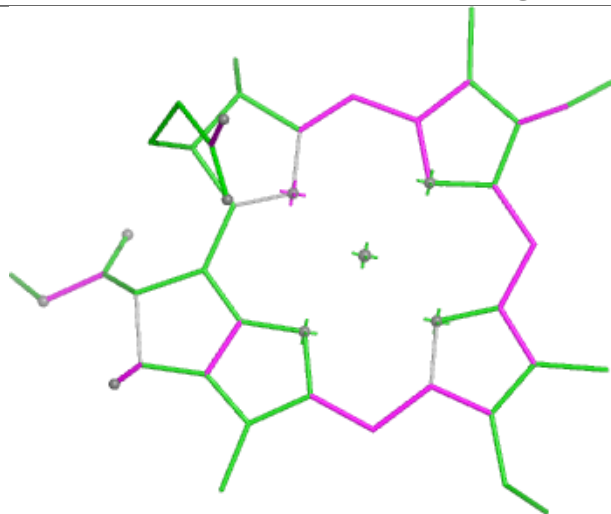
Ligand LMU 2 321



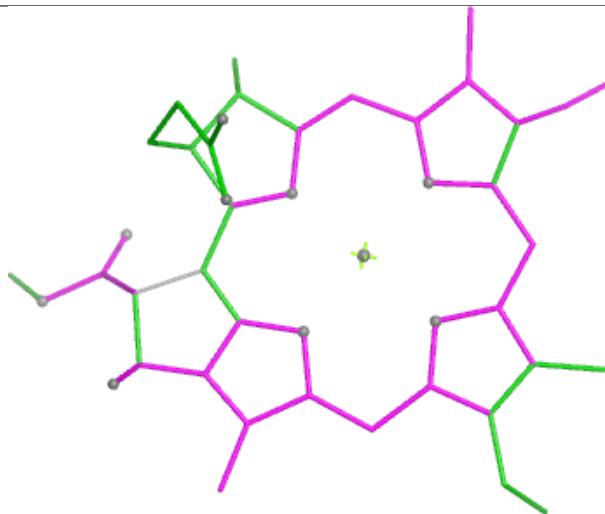




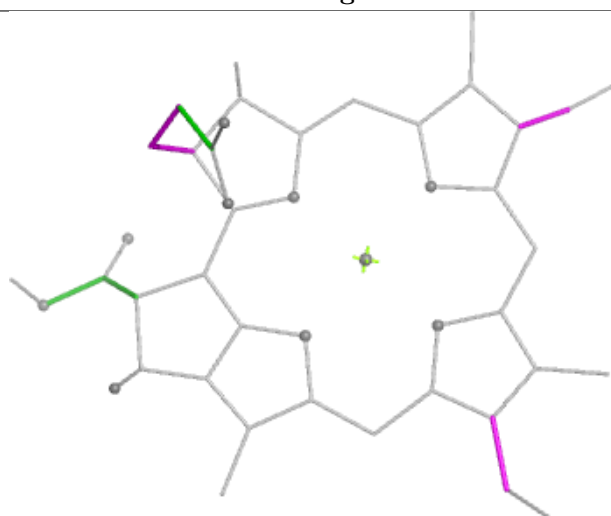
Ligand CLA B 807



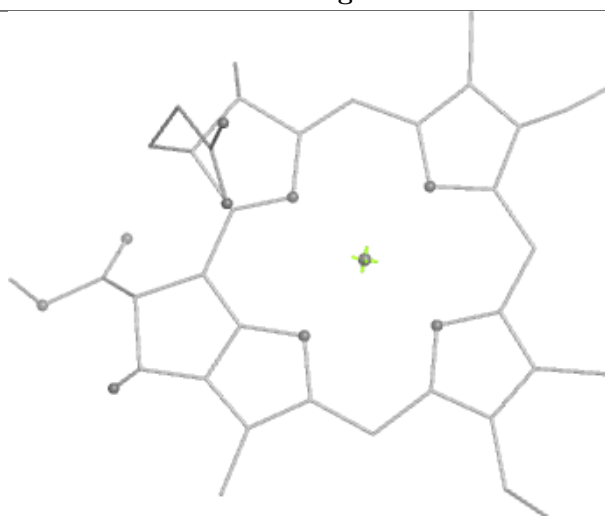
Bond lengths



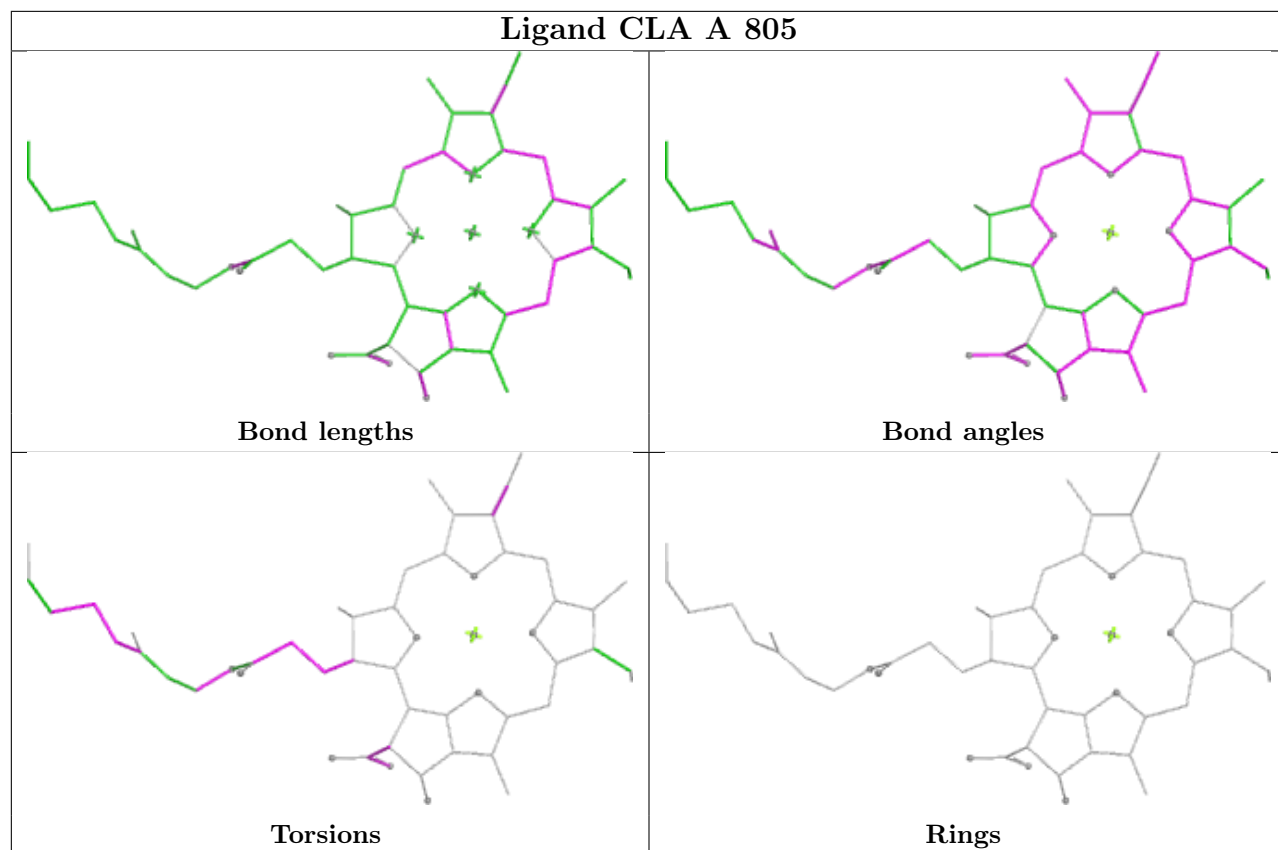
Bond angles



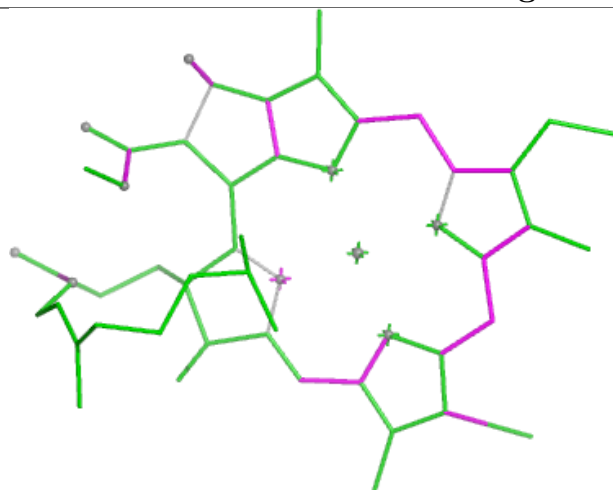
Torsions



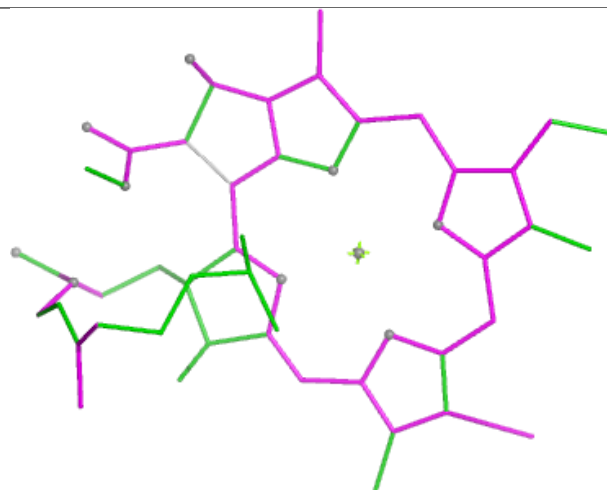
Rings



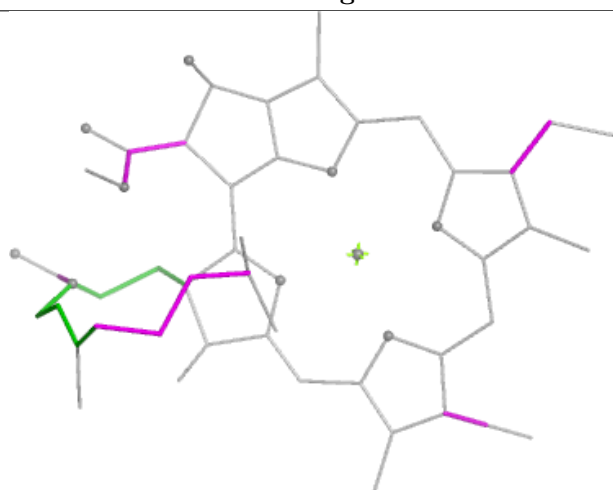
Ligand CLA 4 304



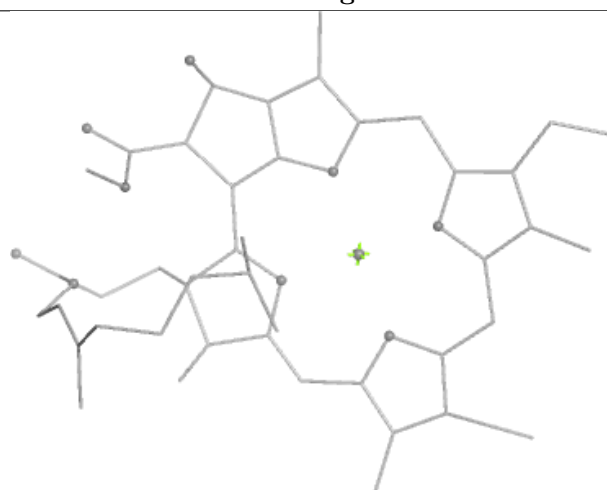
Bond lengths



Bond angles

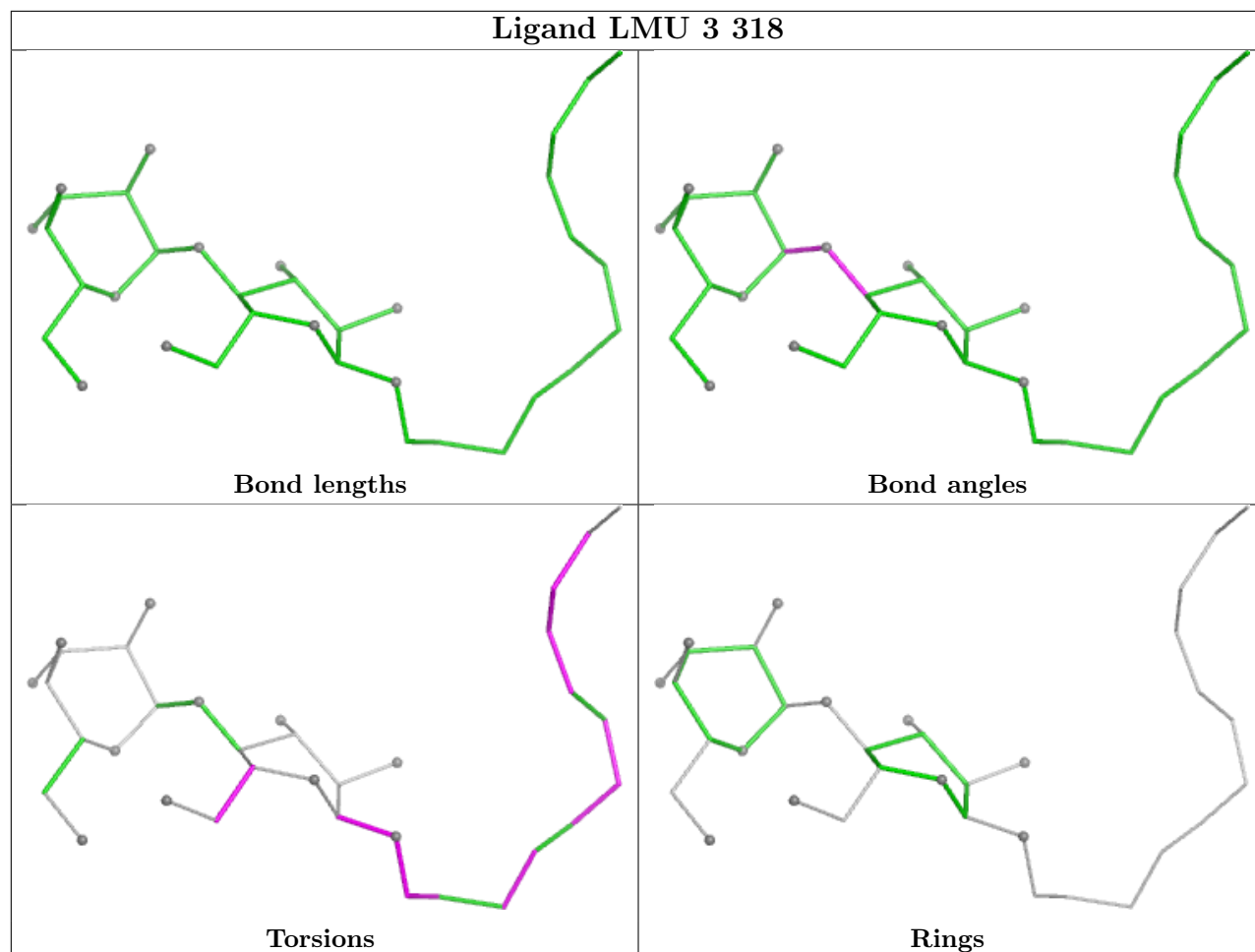


Torsions

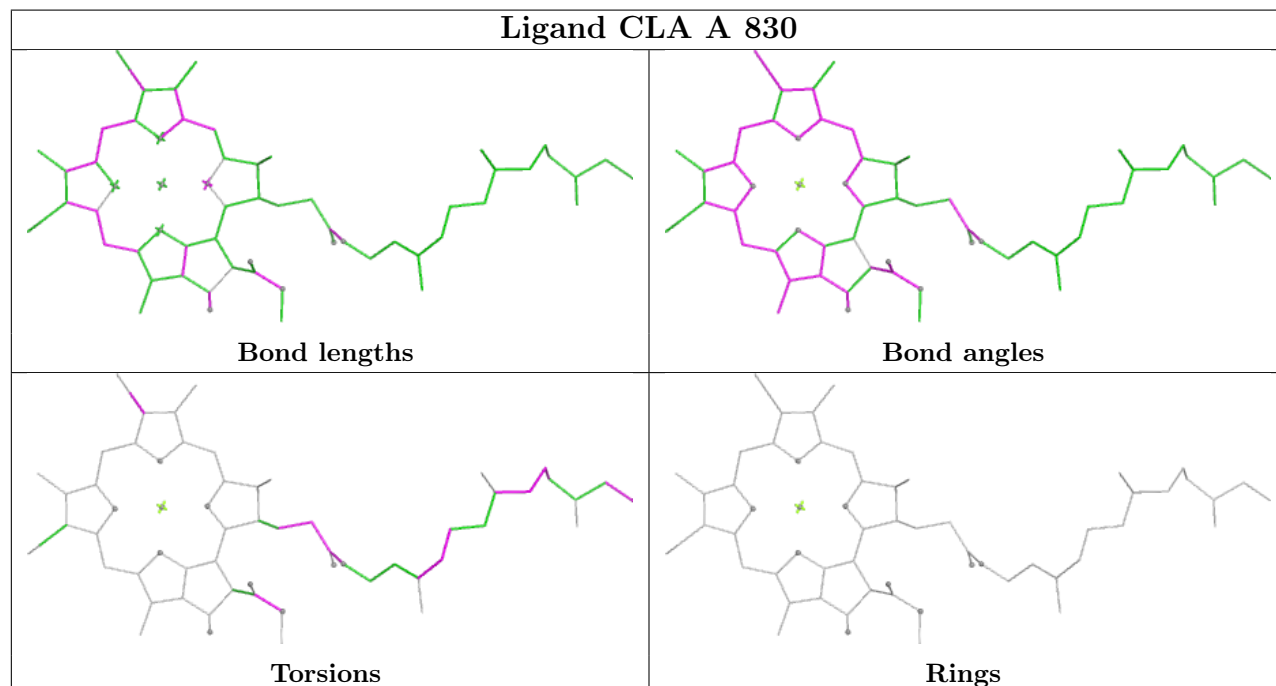


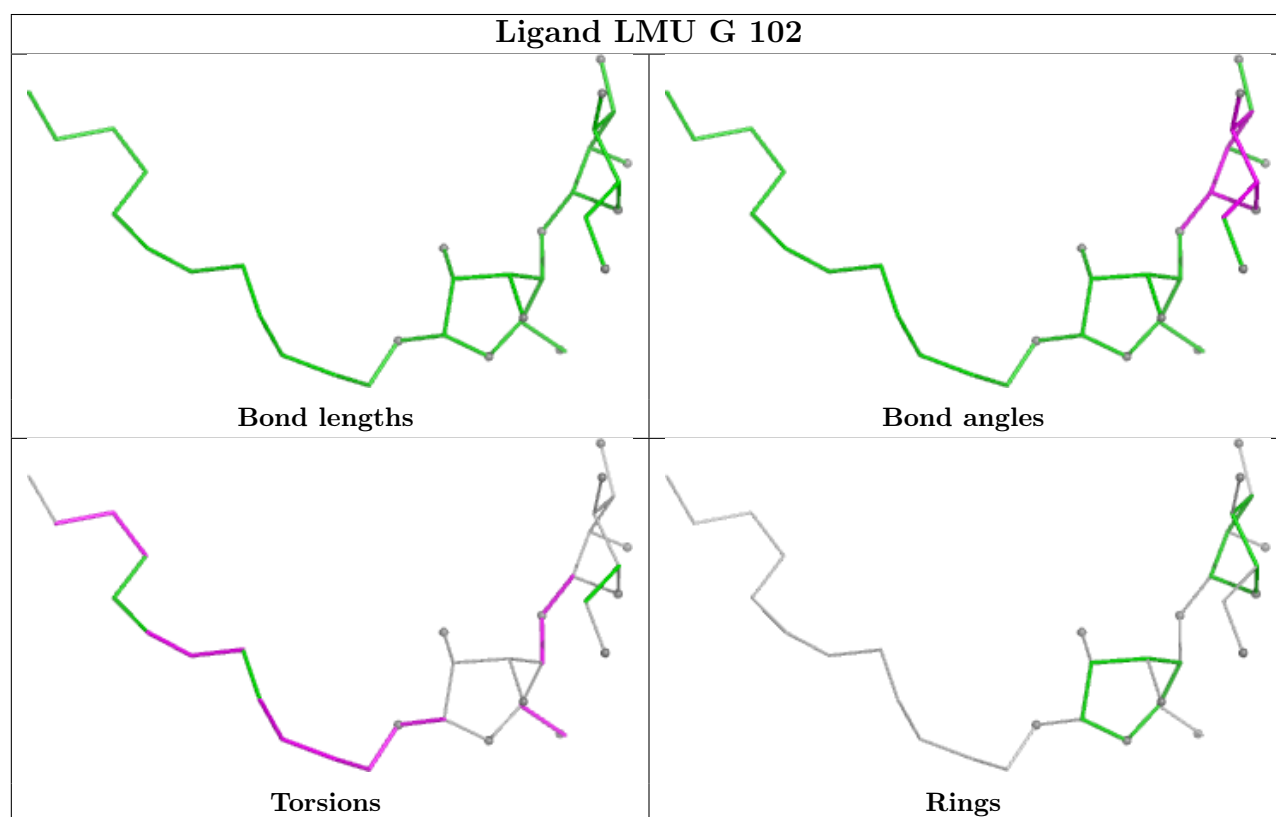
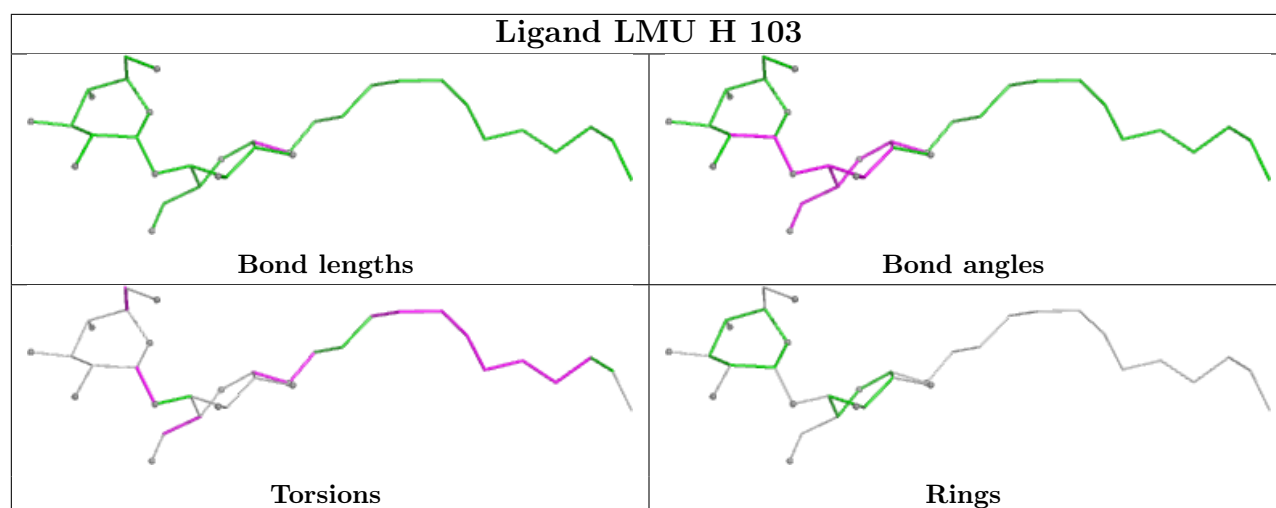
Rings

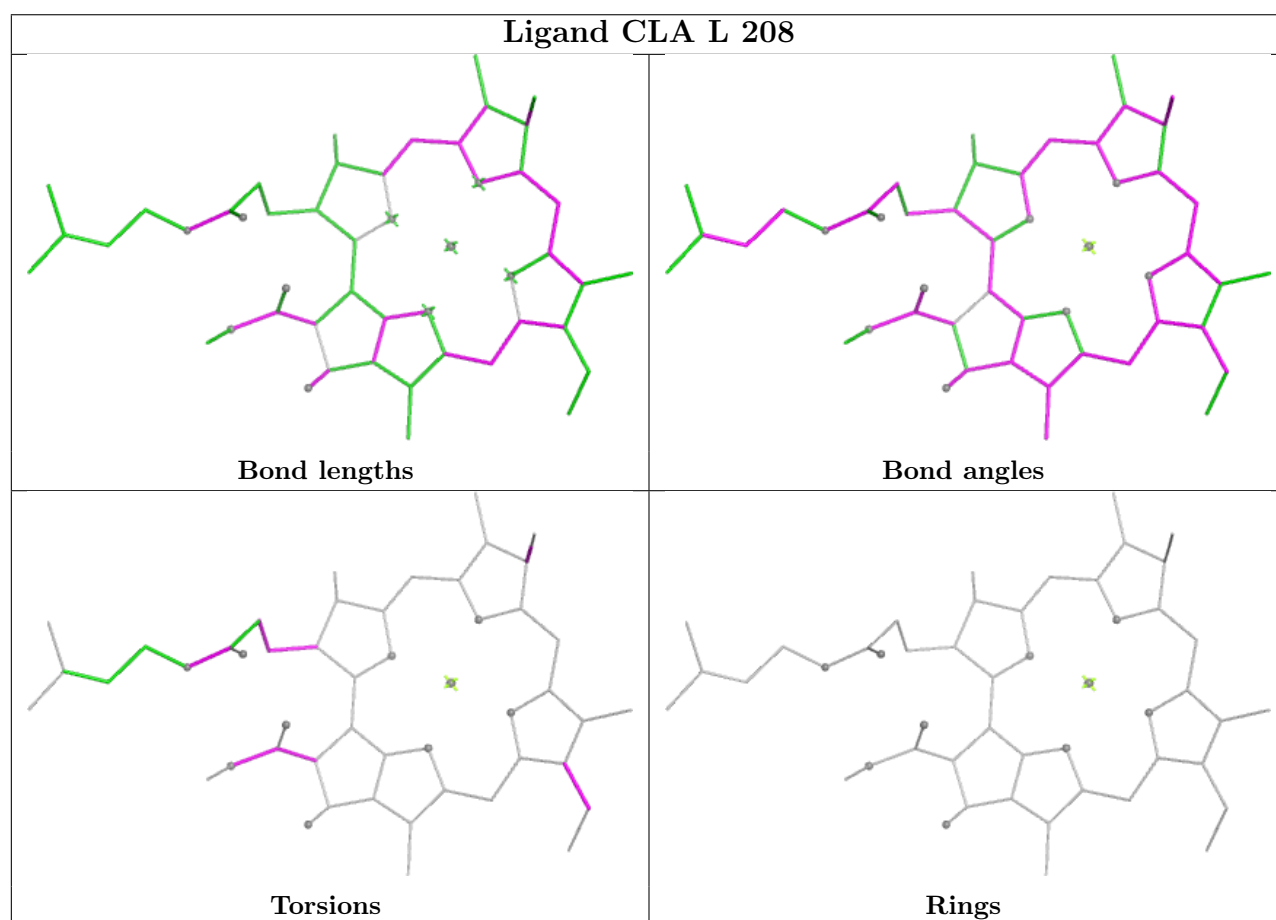
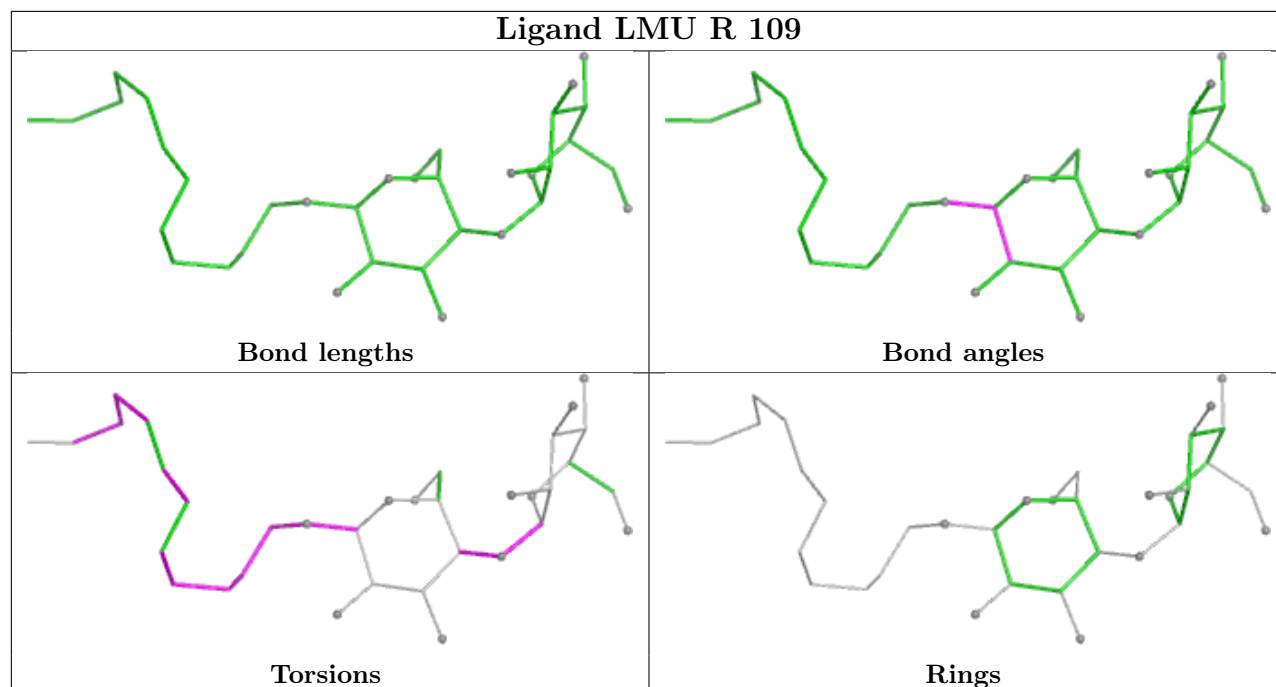
Ligand LMU 3 318

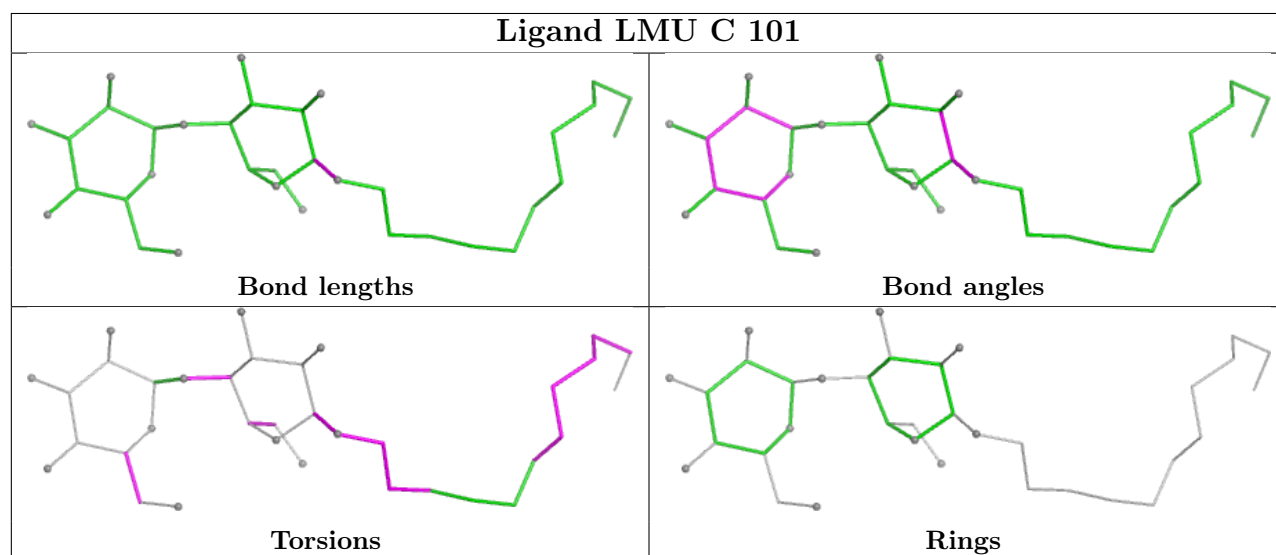
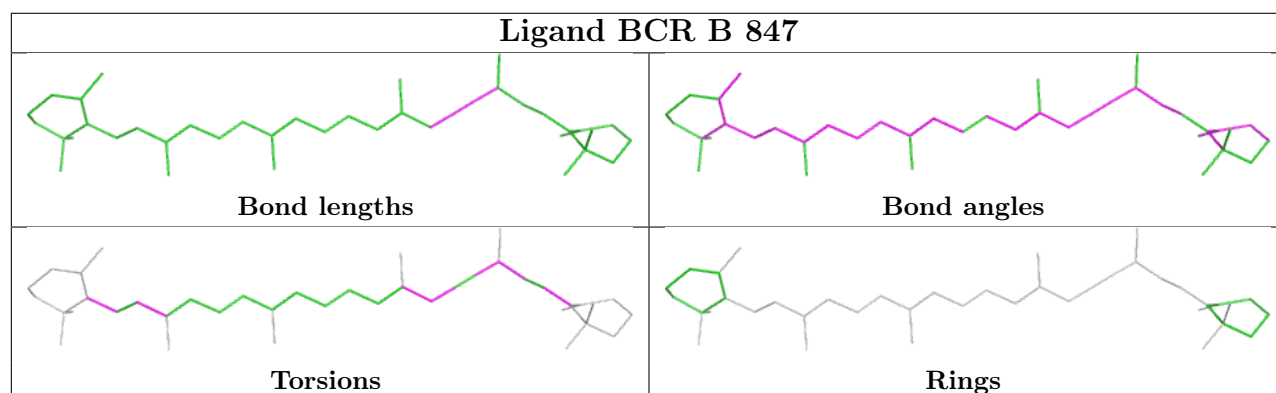
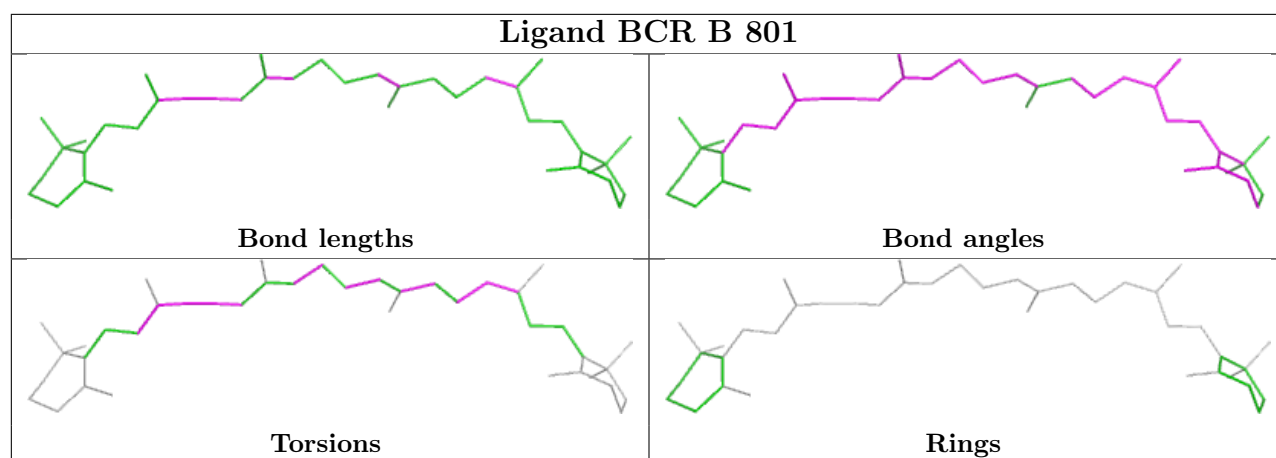


Ligand CLA A 830

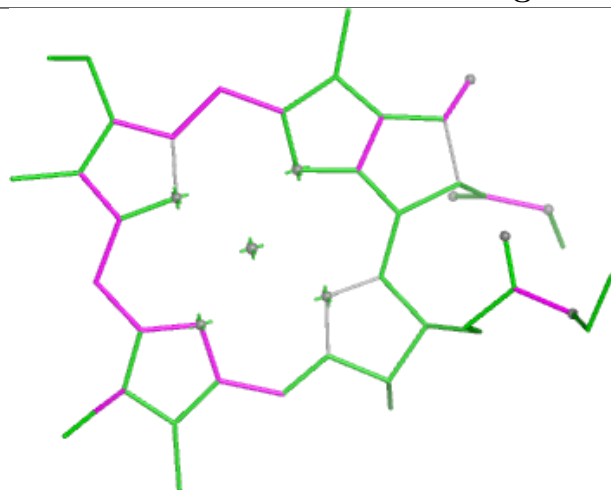




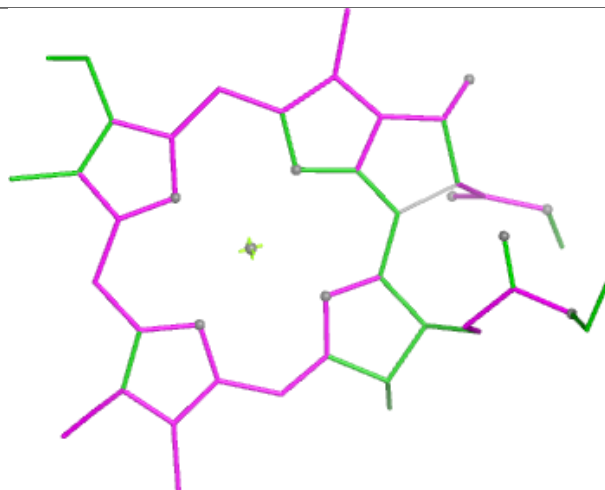




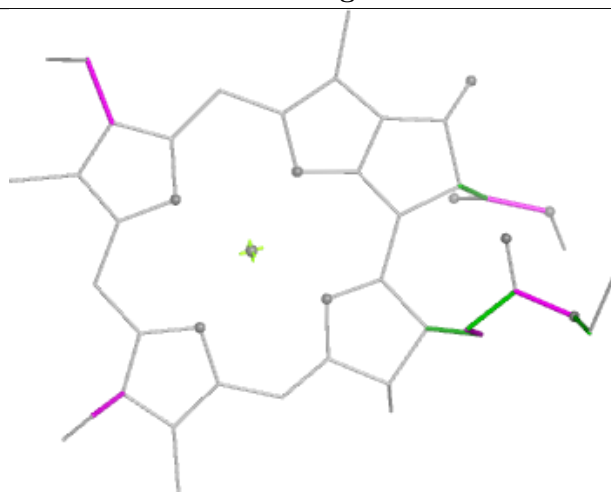
Ligand CLA A 836



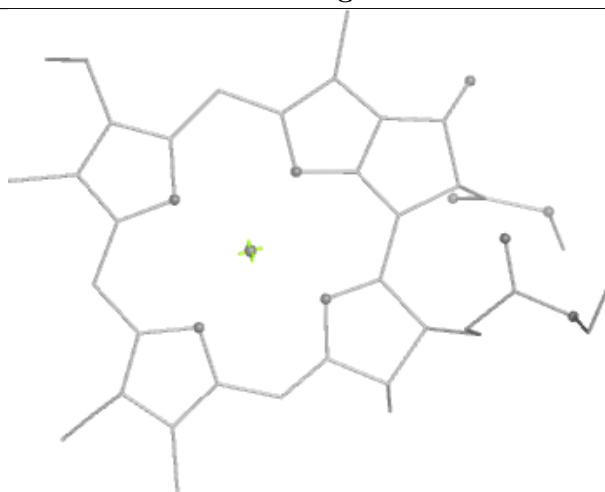
Bond lengths



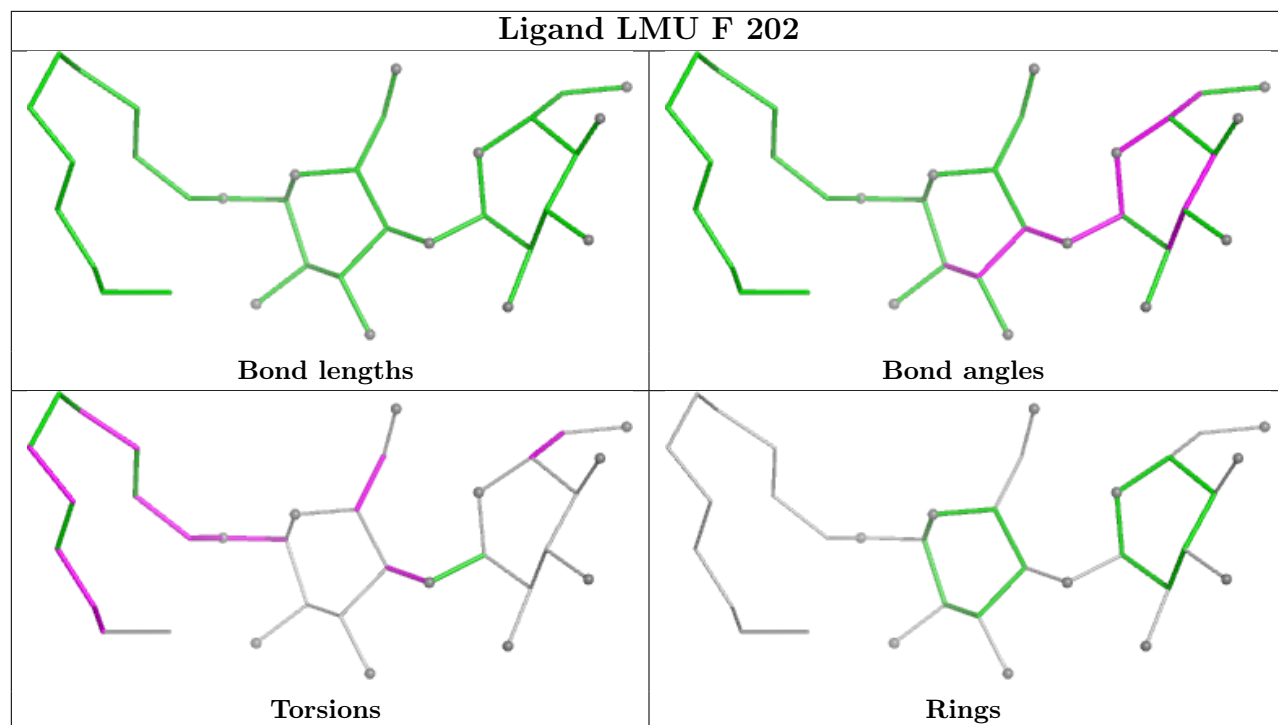
Bond angles



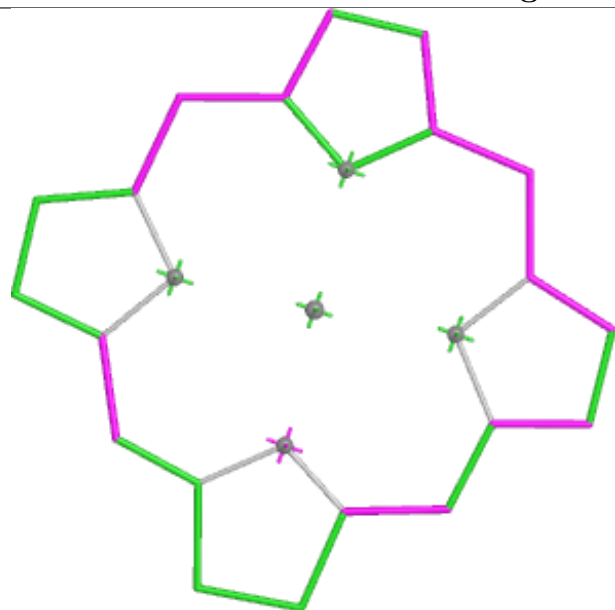
Torsions



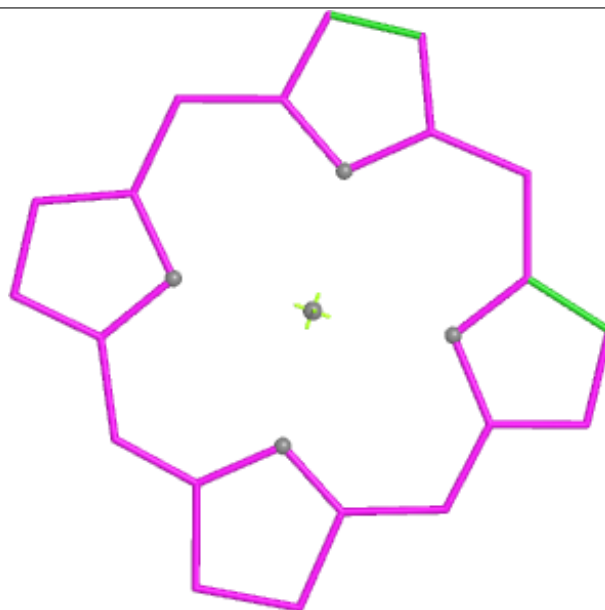
Rings



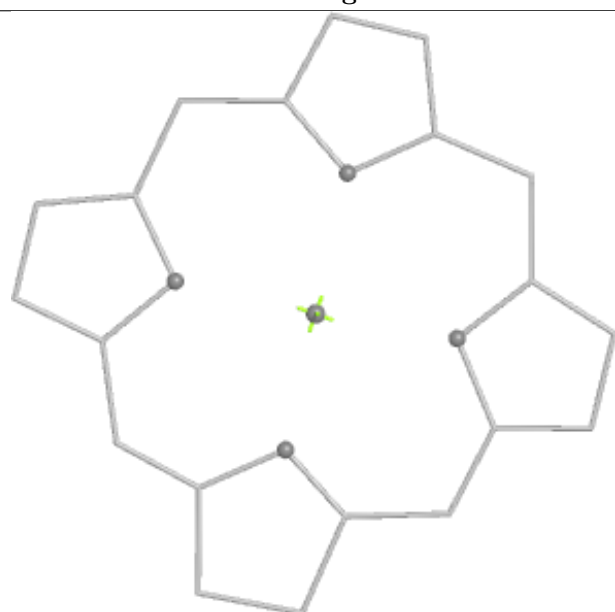
Ligand CLA 4 311



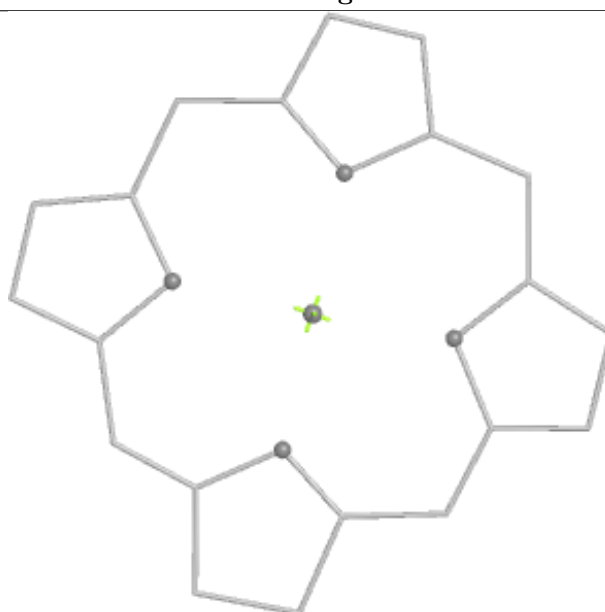
Bond lengths



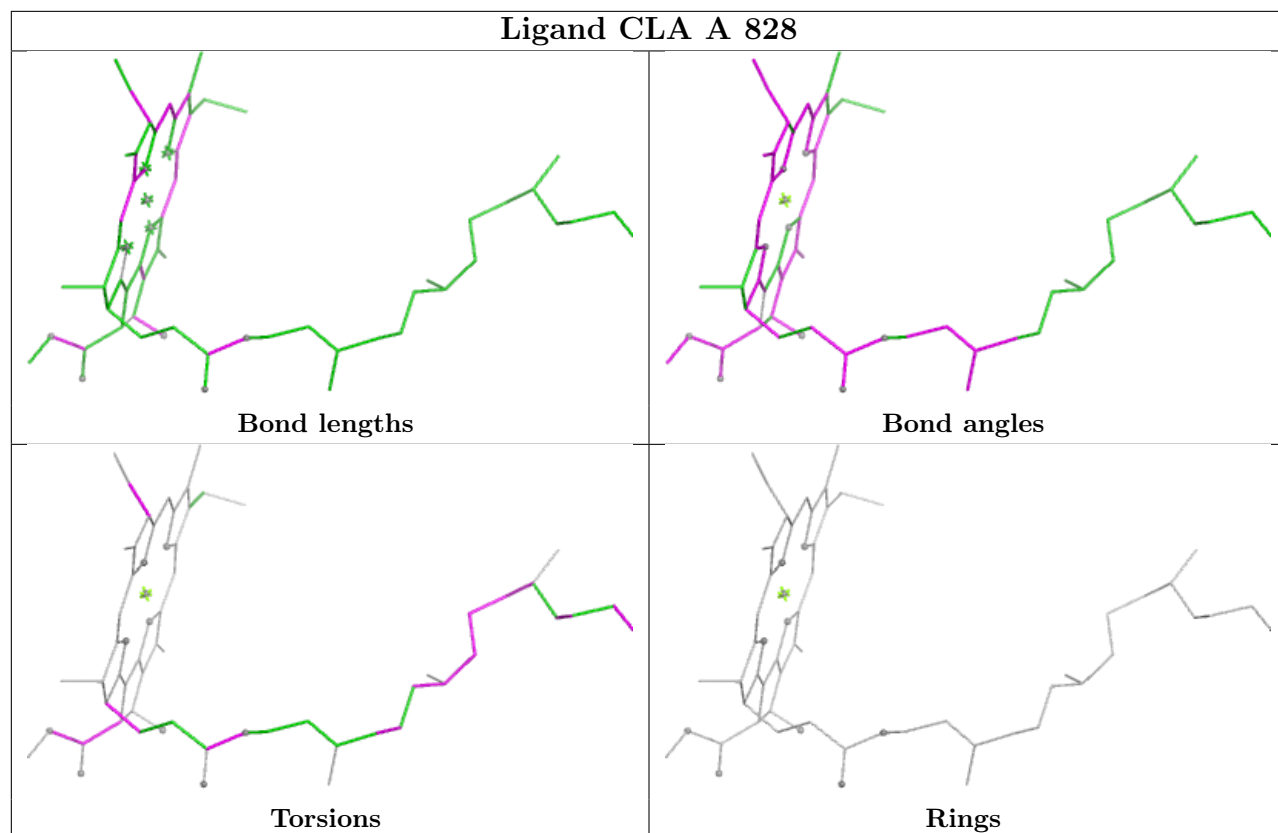
Bond angles



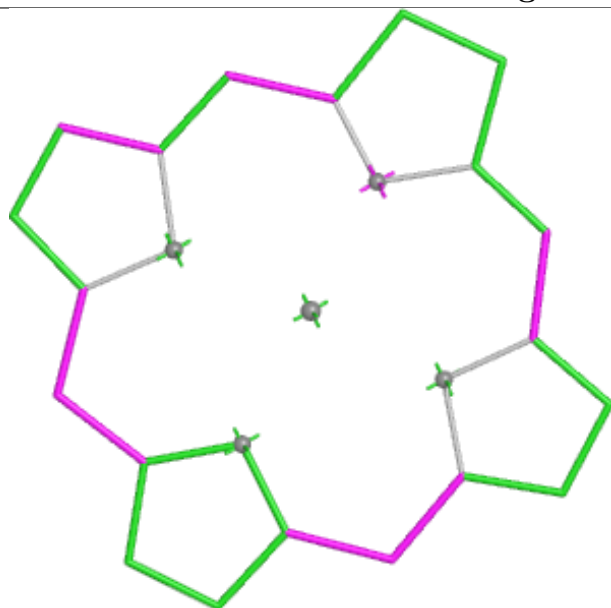
Torsions



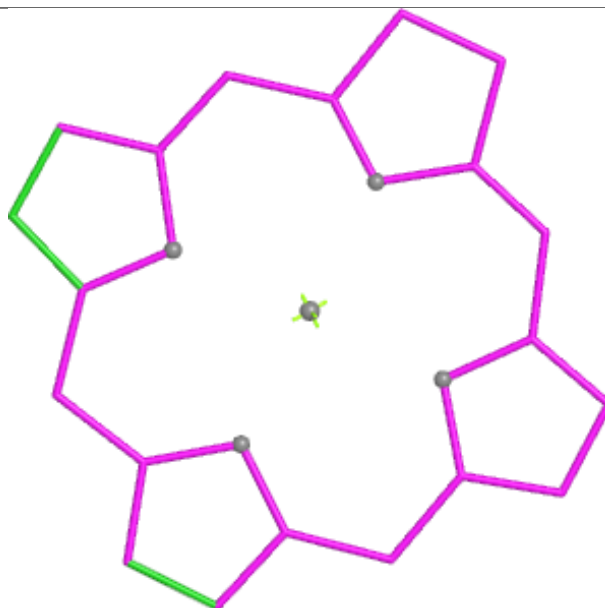
Rings



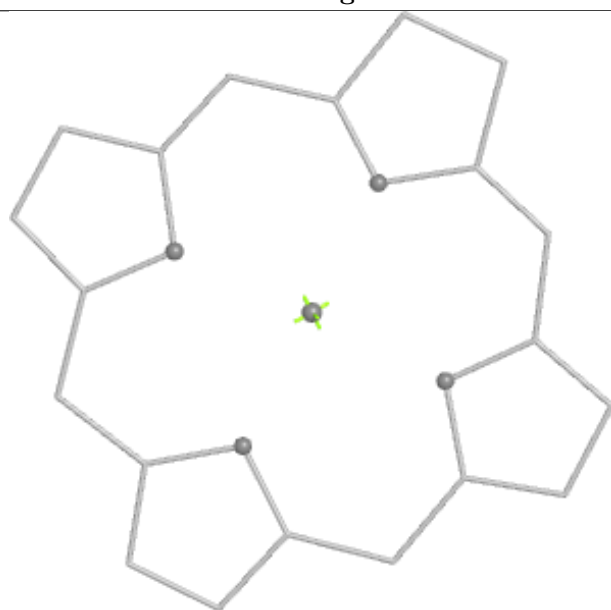
Ligand CLA 3 305



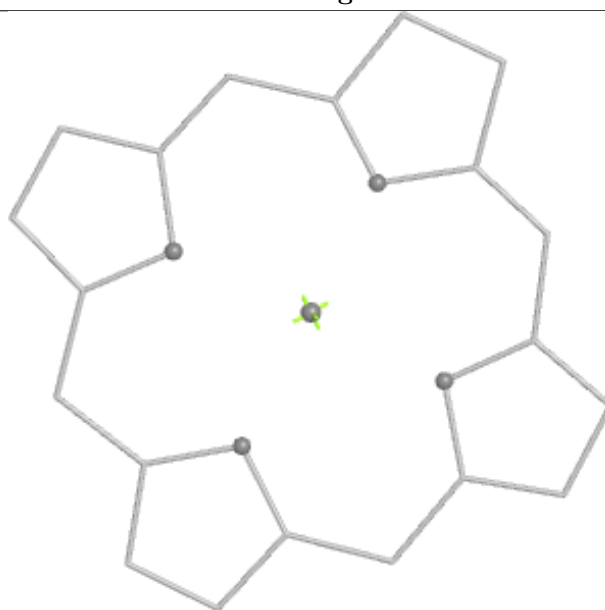
Bond lengths



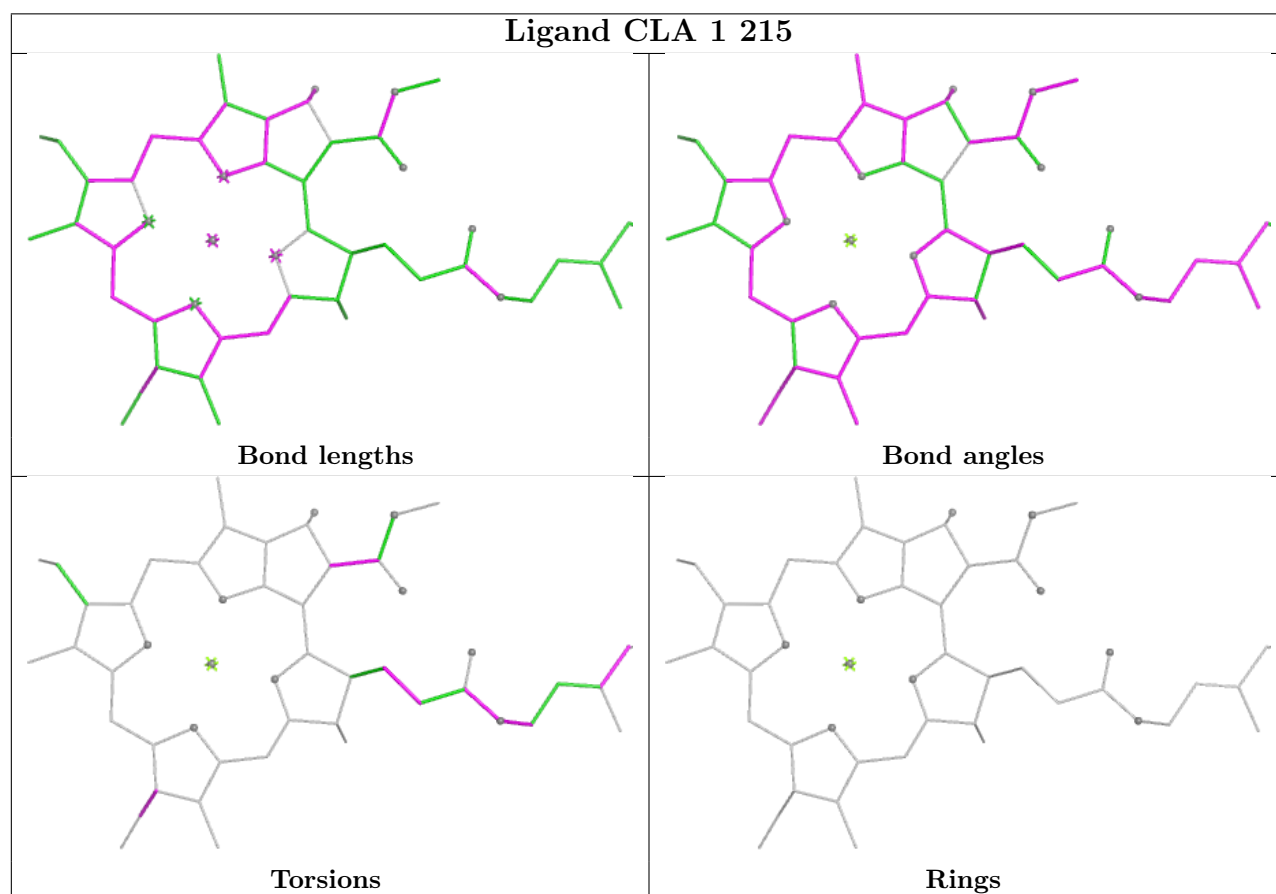
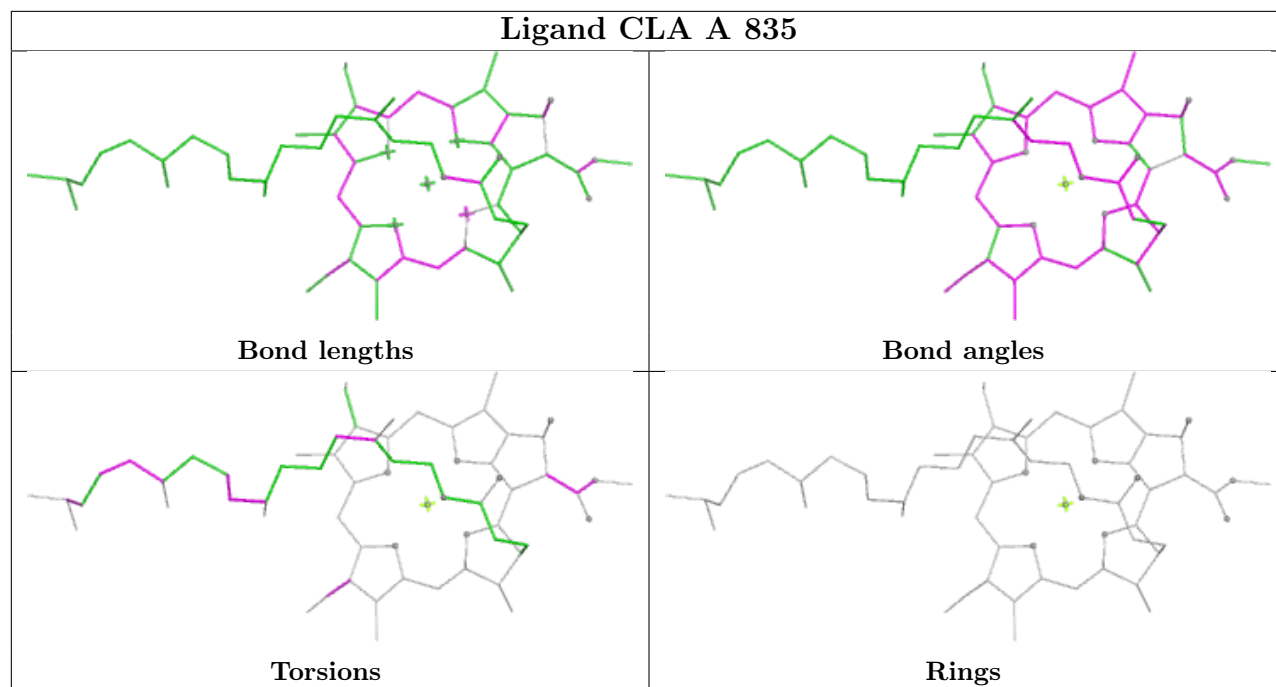
Bond angles



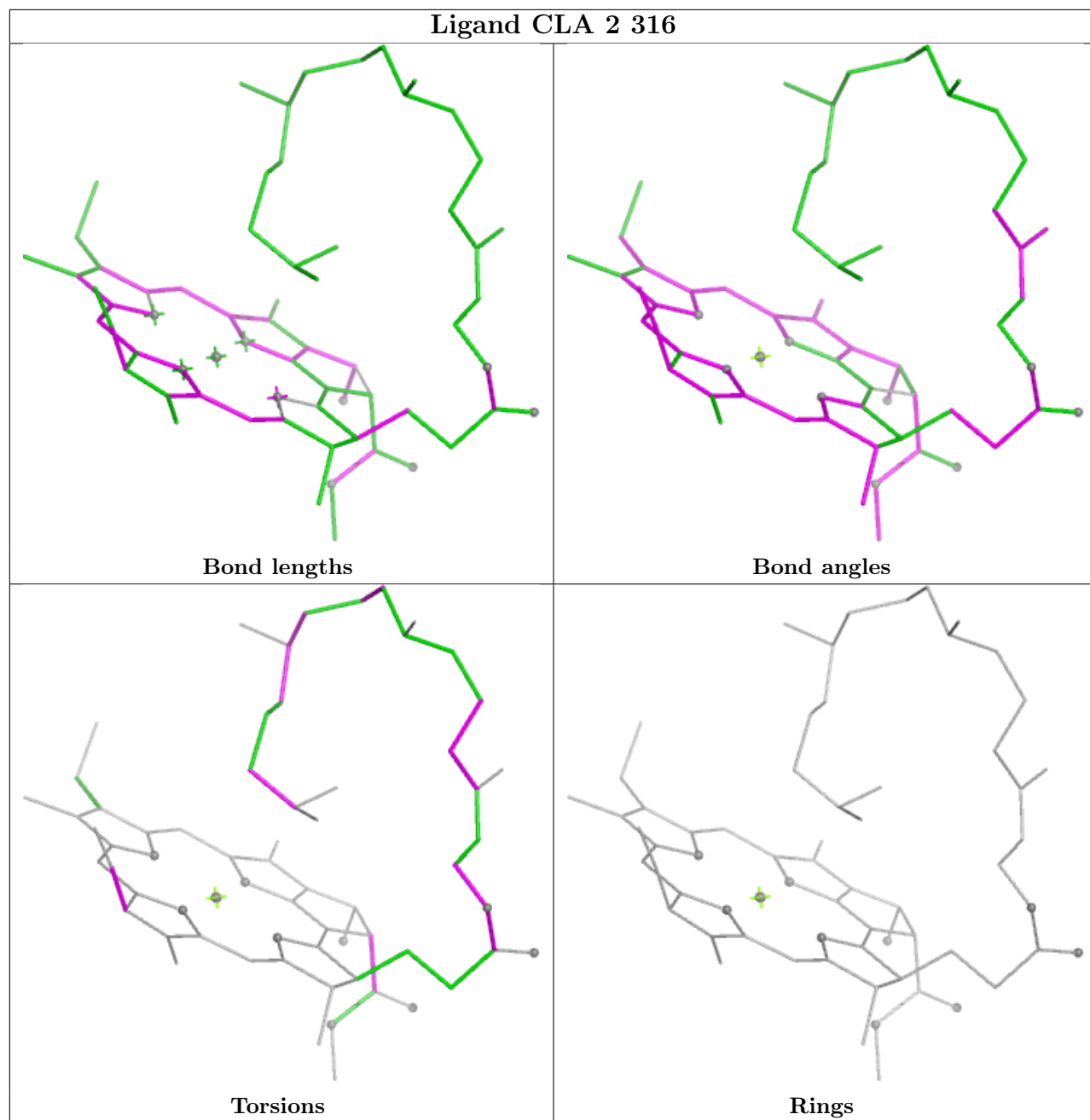
Torsions



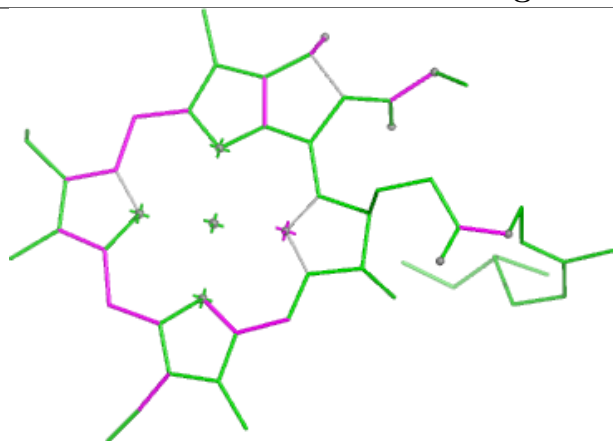
Rings



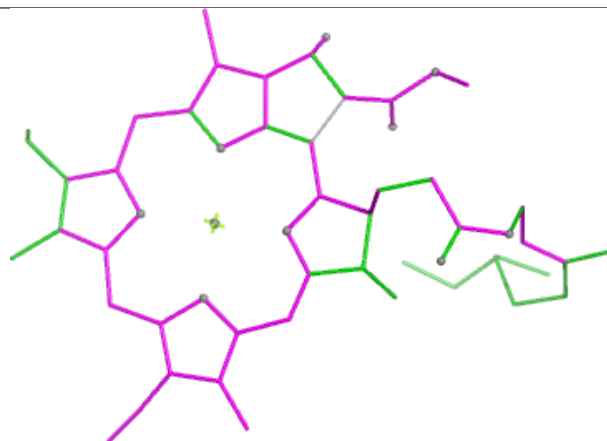
Ligand CLA 2 316



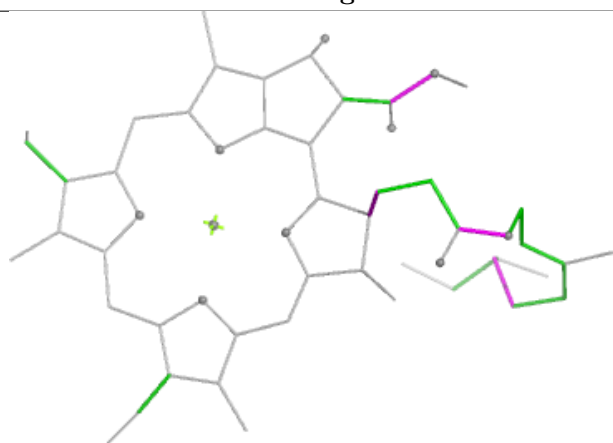
Ligand CLA A 806



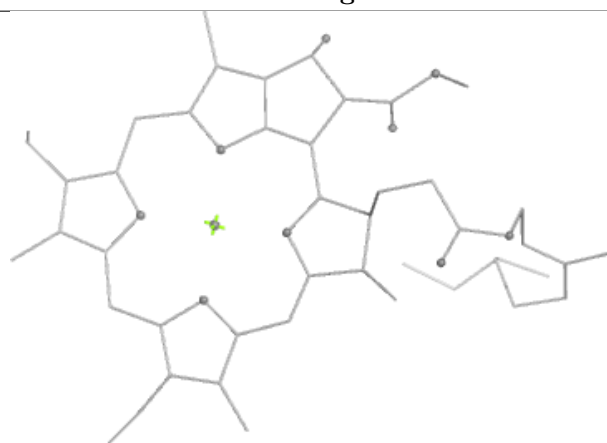
Bond lengths



Bond angles

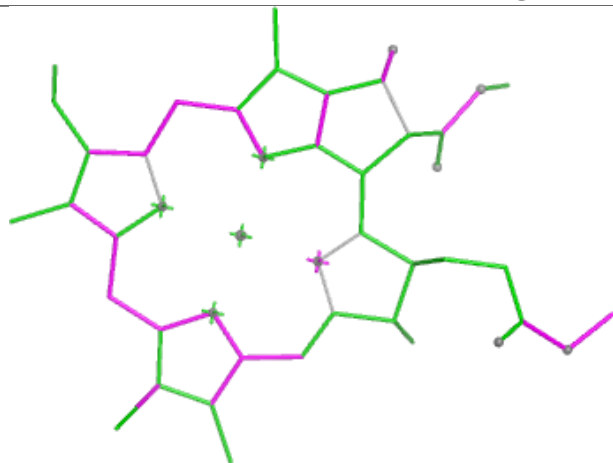


Torsions

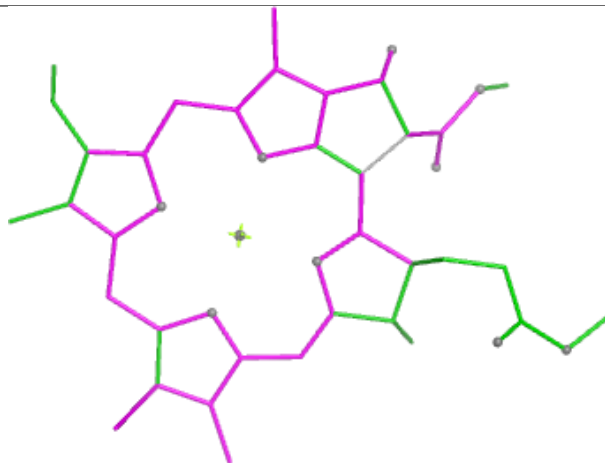


Rings

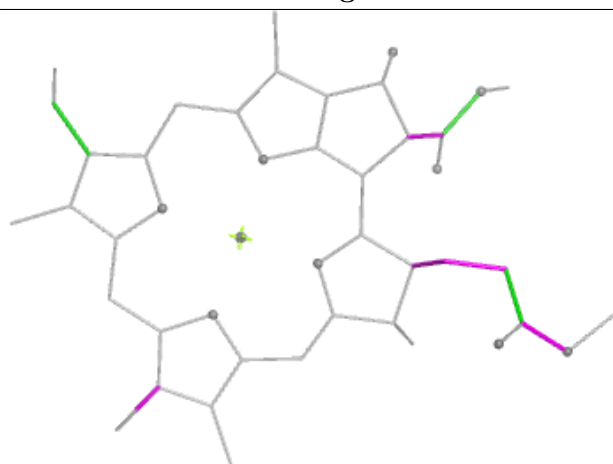
Ligand CLA K 101



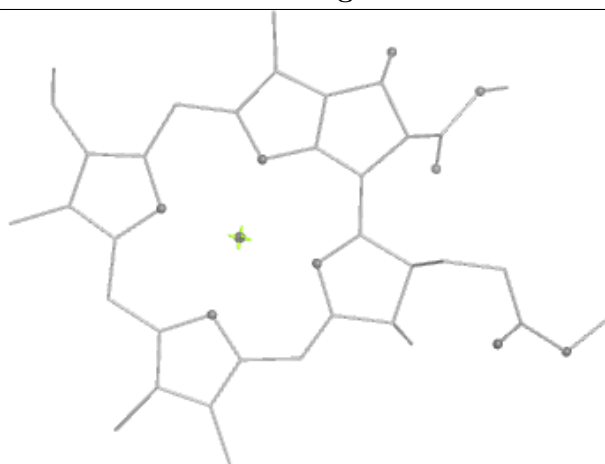
Bond lengths



Bond angles

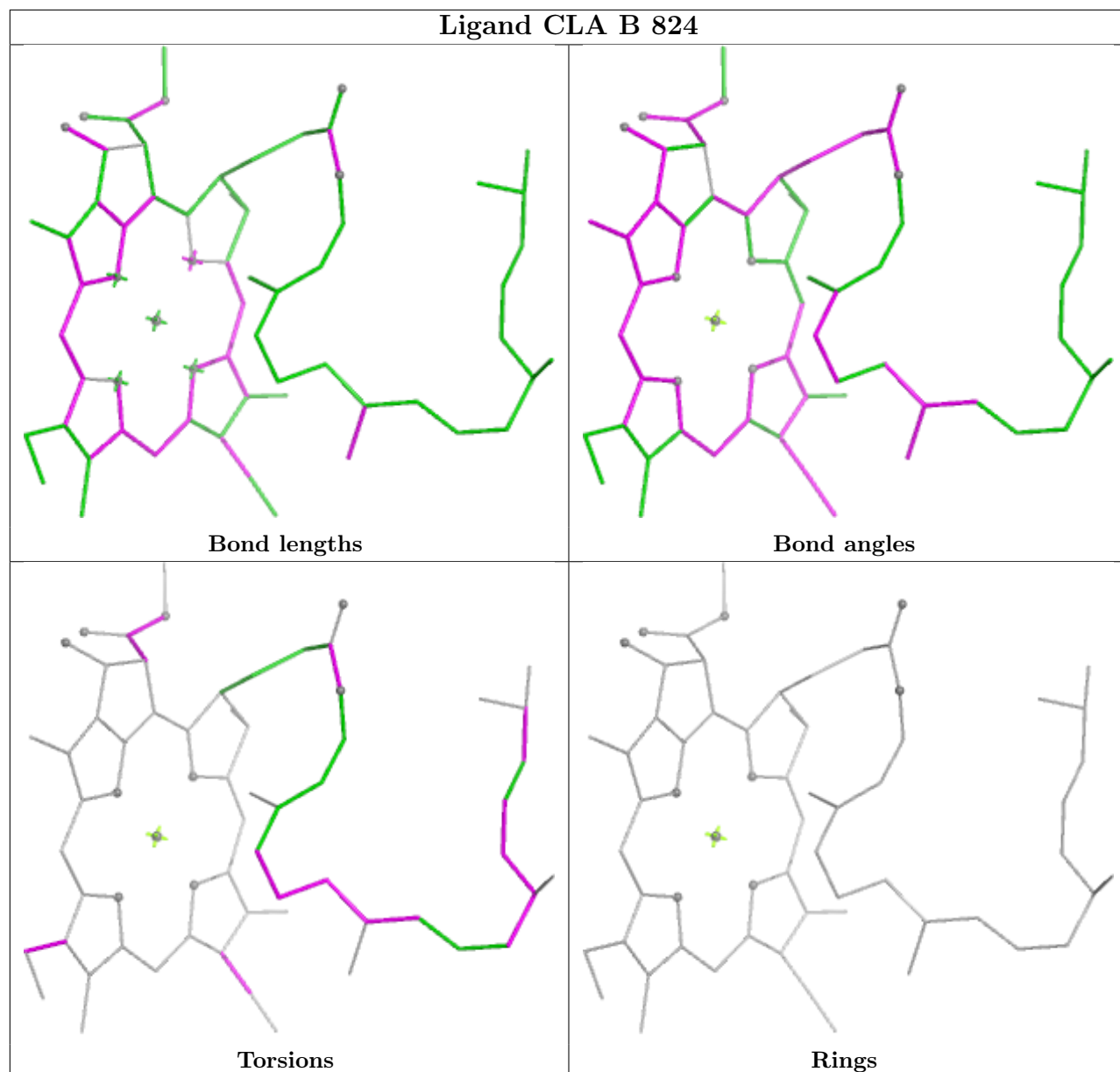


Torsions

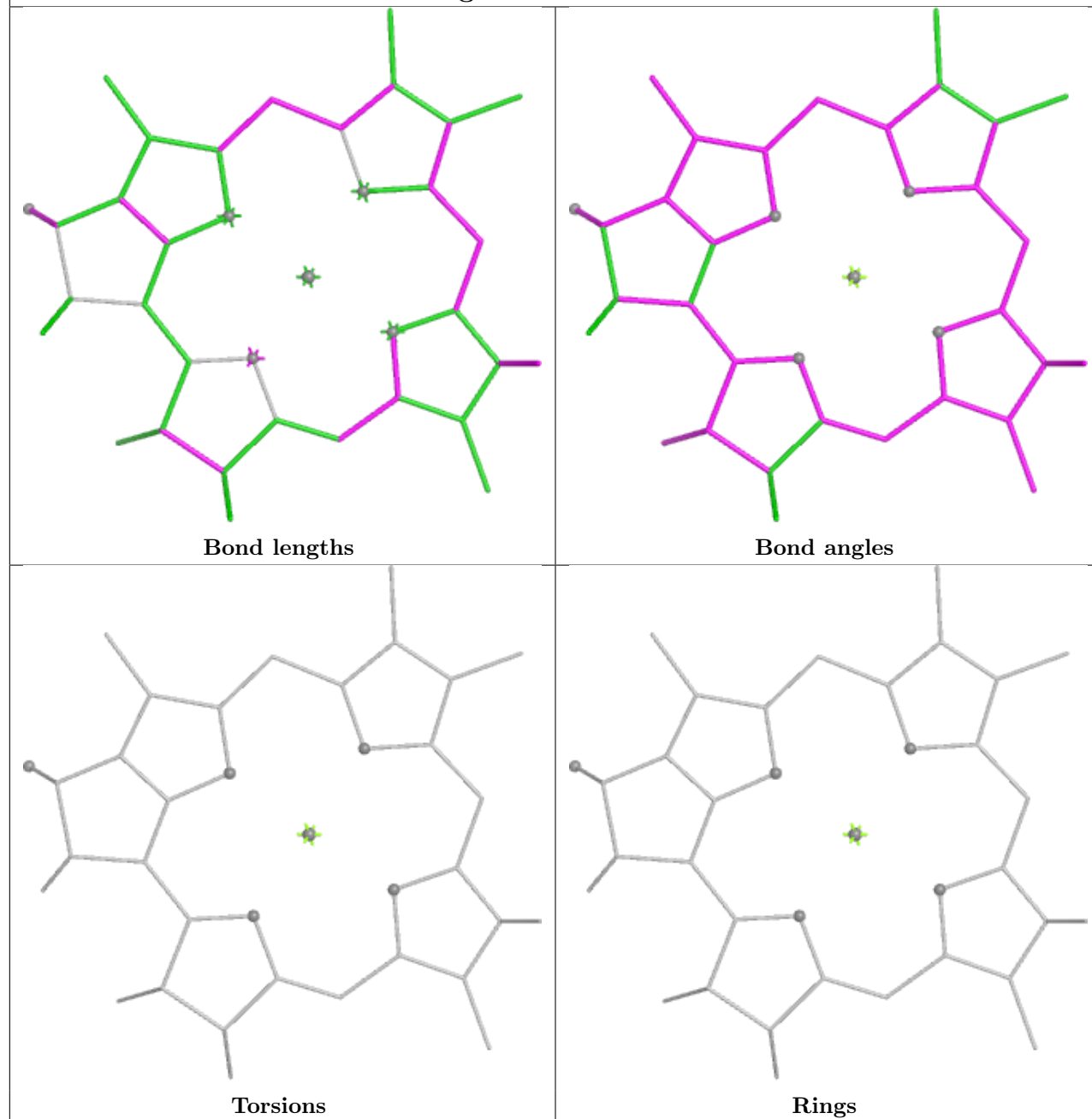


Rings

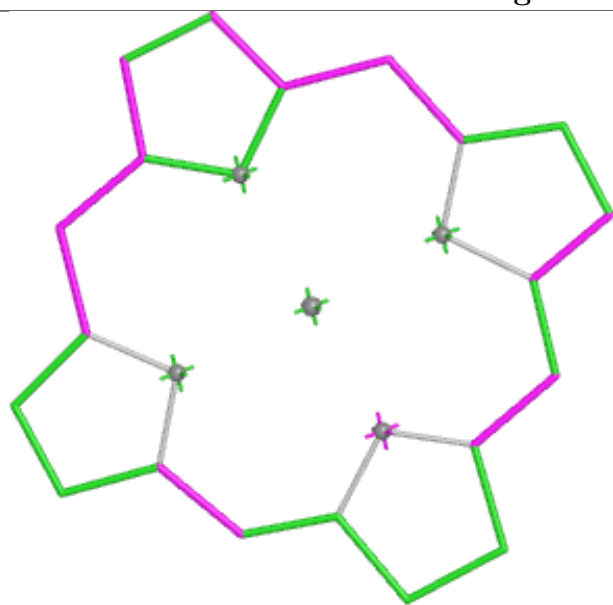
Ligand CLA B 824



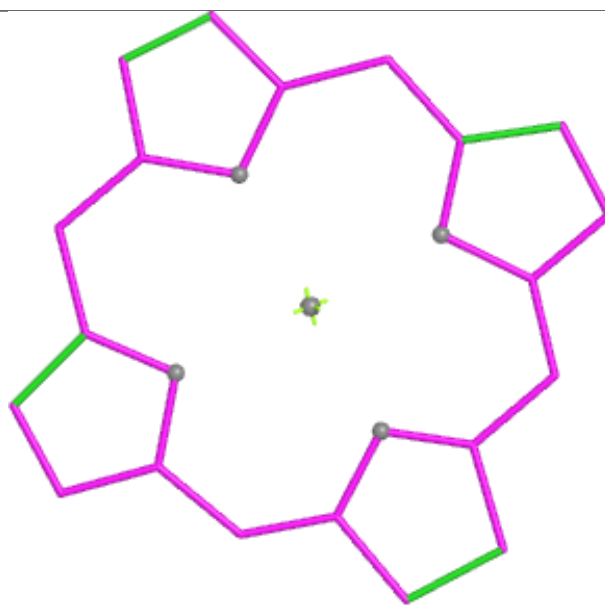
Ligand CLA 3 317



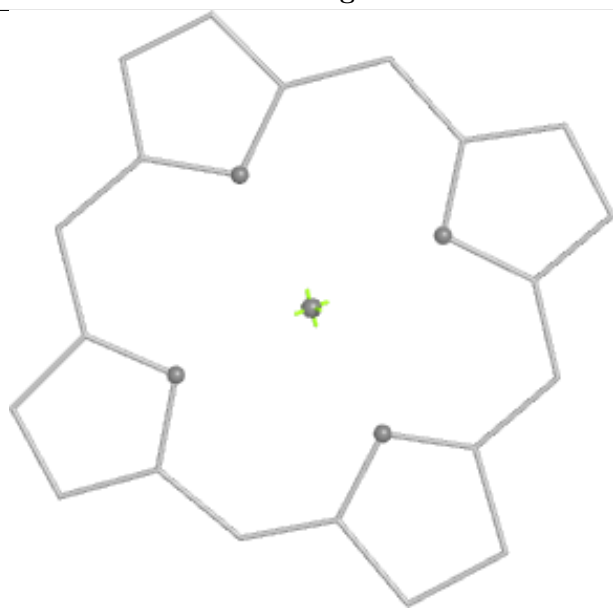
Ligand CLA A 814



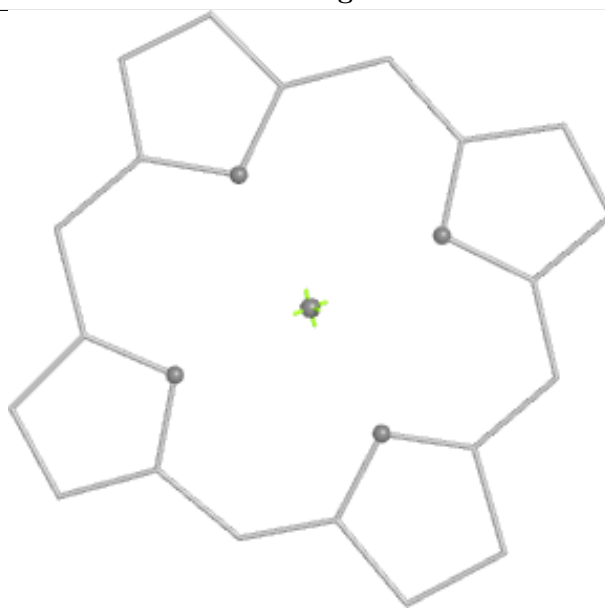
Bond lengths



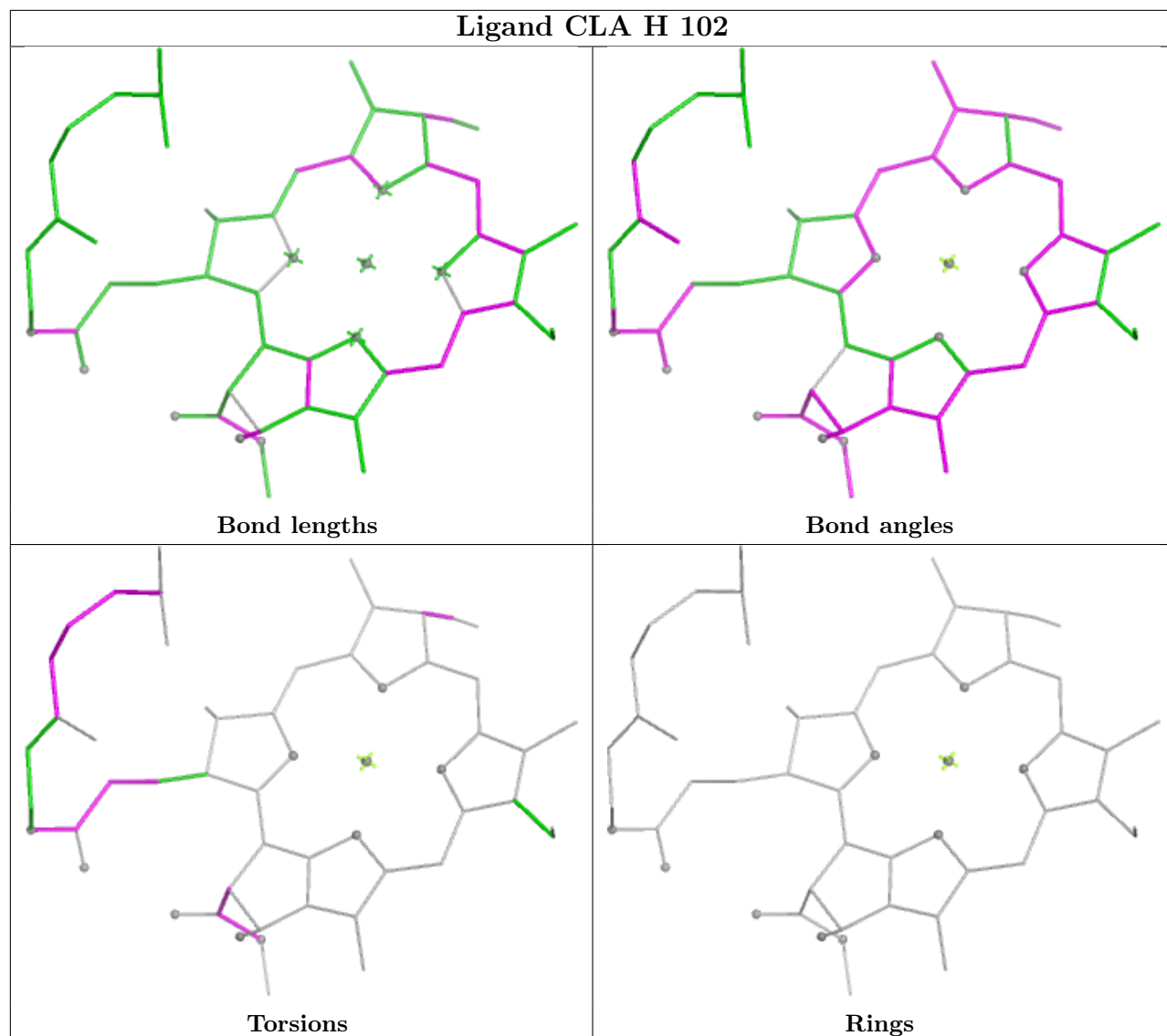
Bond angles



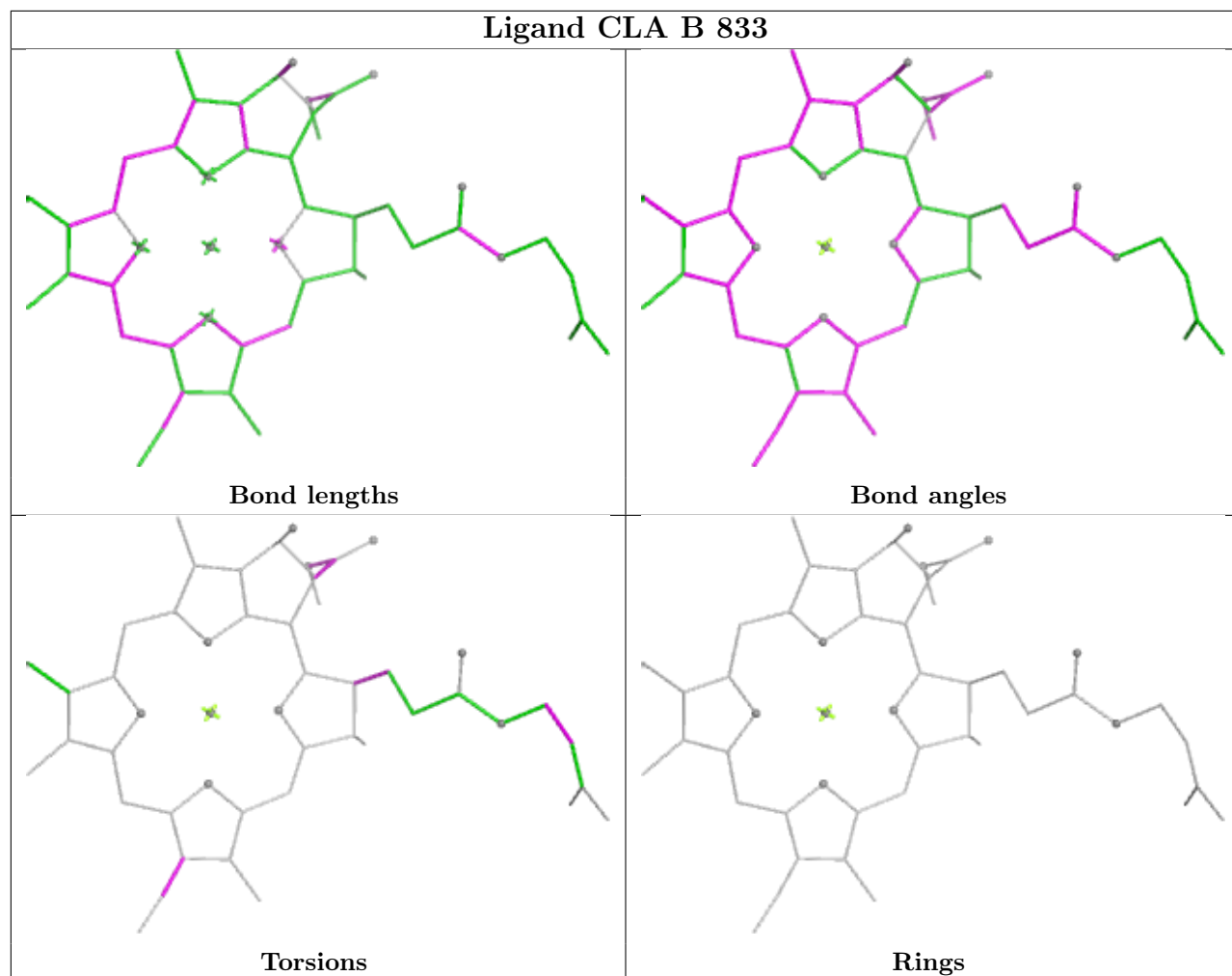
Torsions



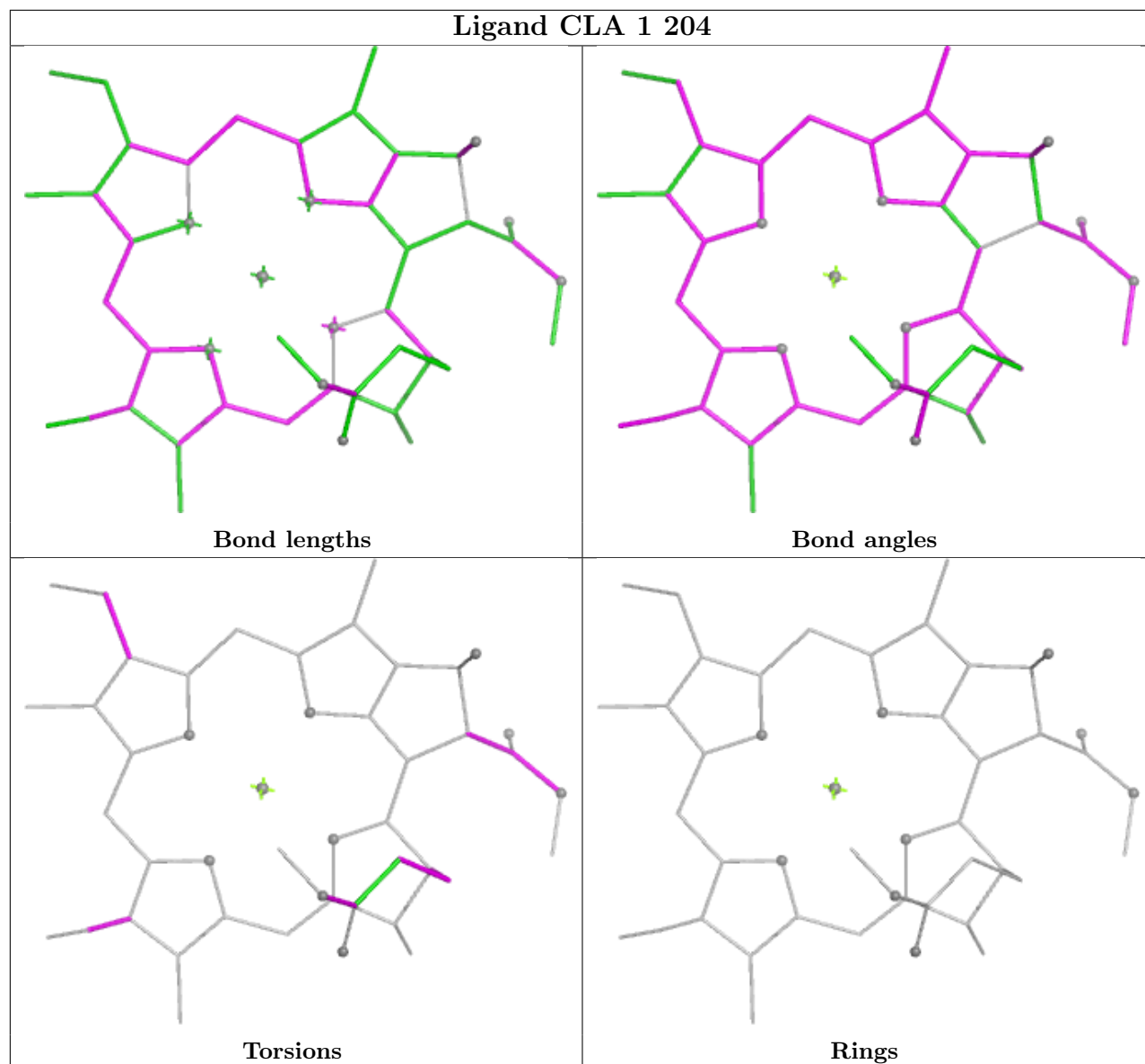
Rings



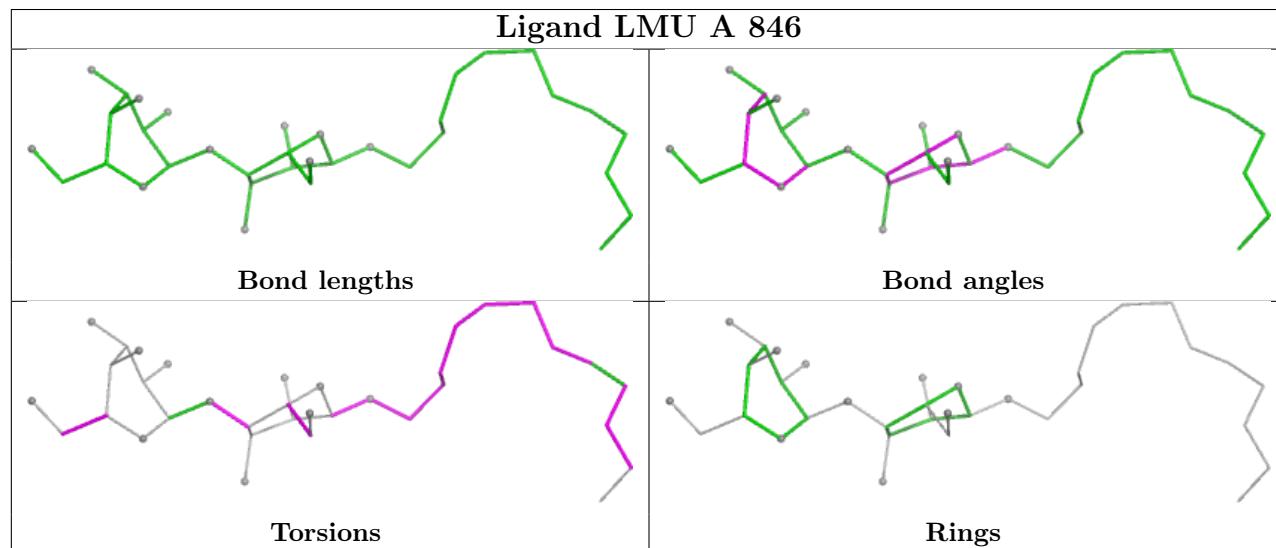
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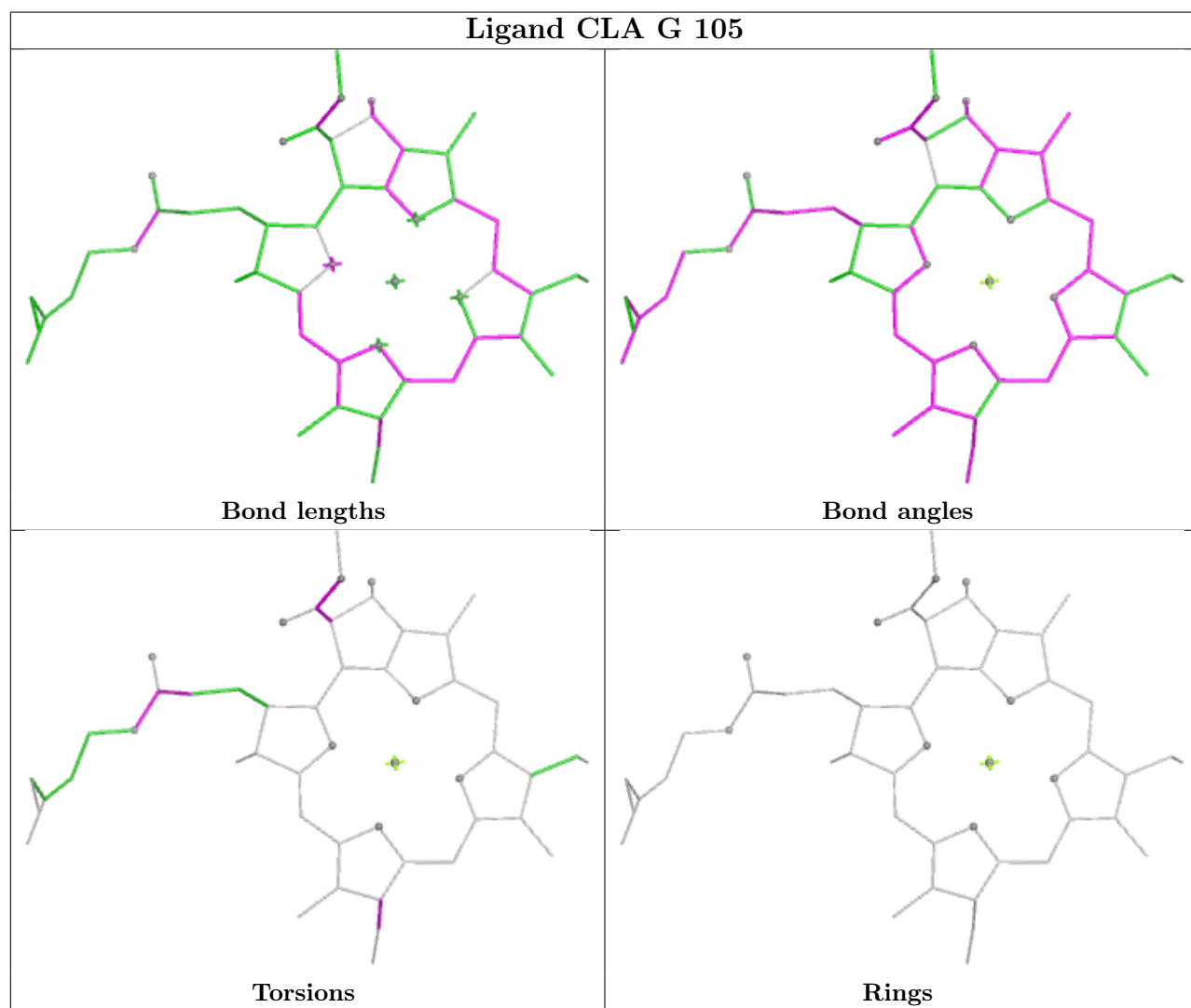
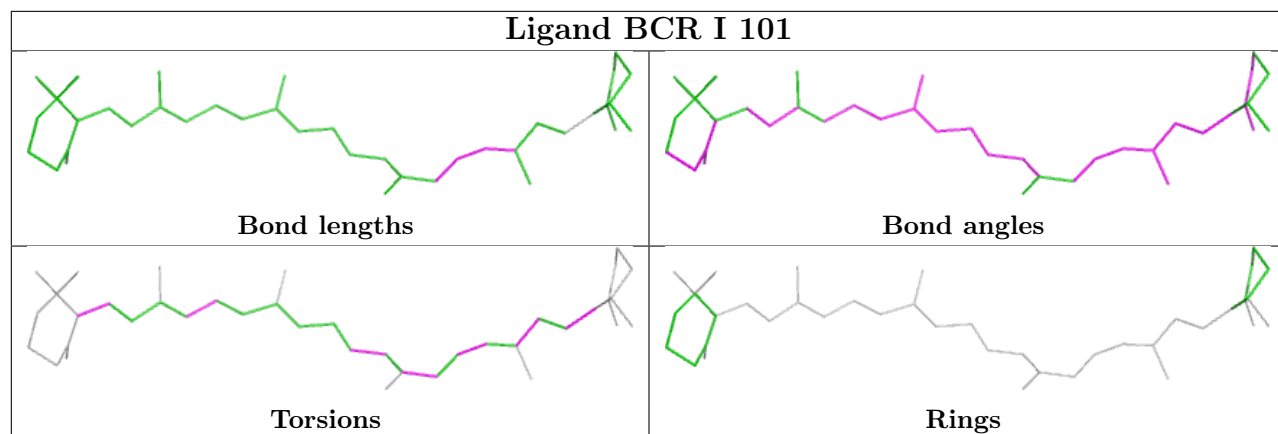


Ligand CLA 1 204

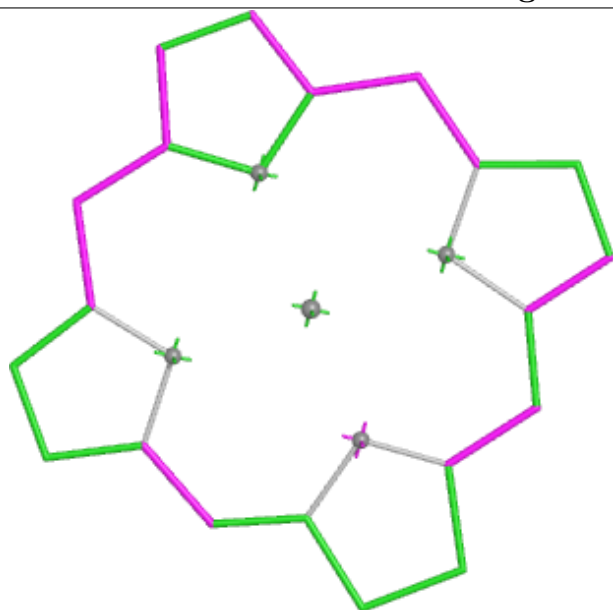


Ligand LMU A 846

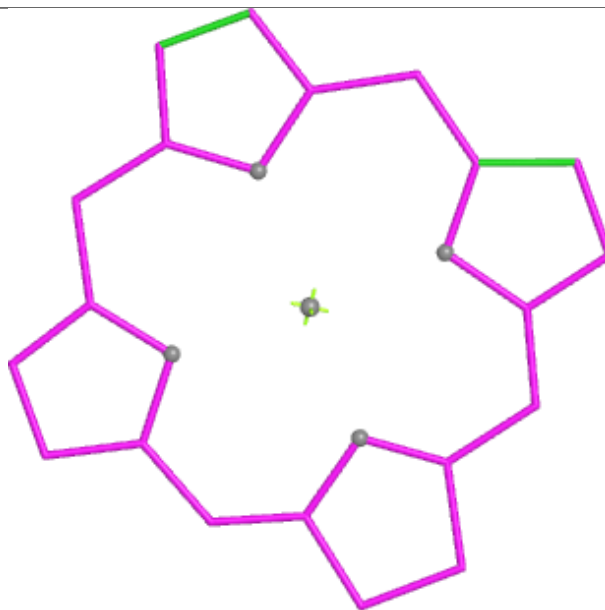




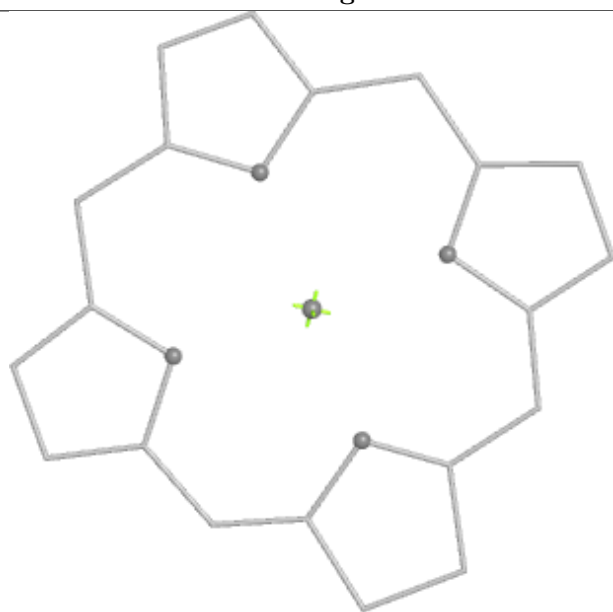
Ligand CLA 3 304



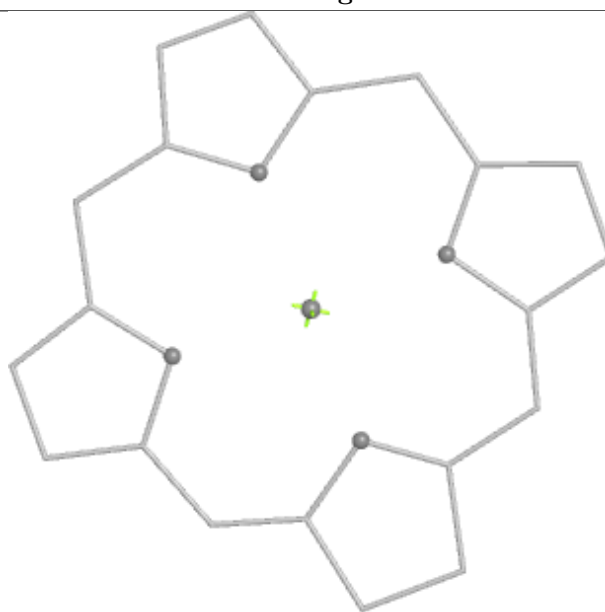
Bond lengths



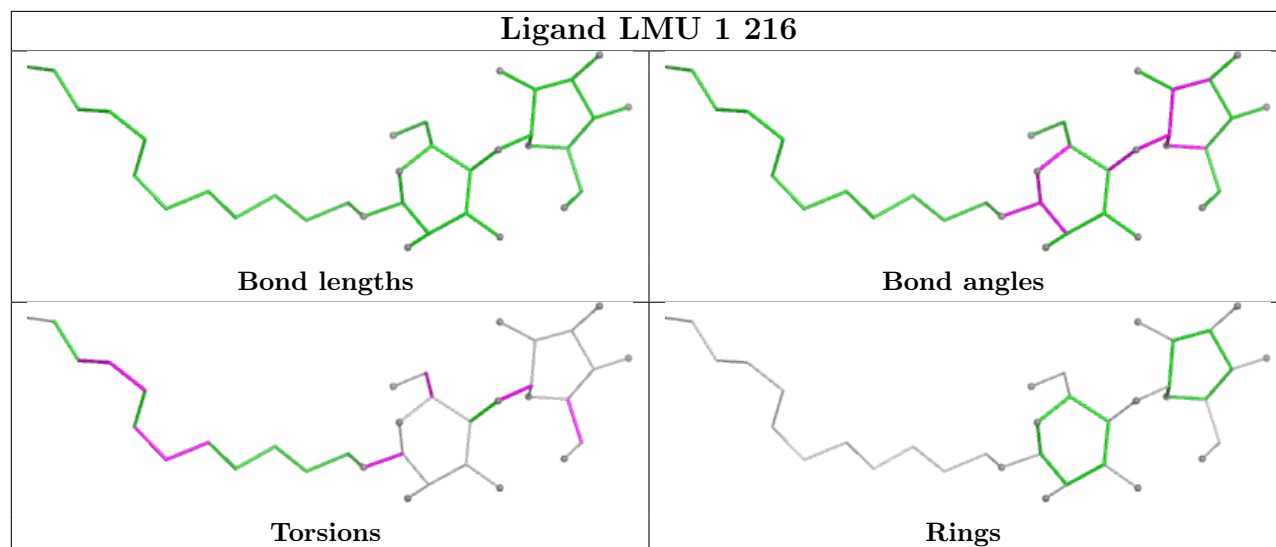
Bond angles



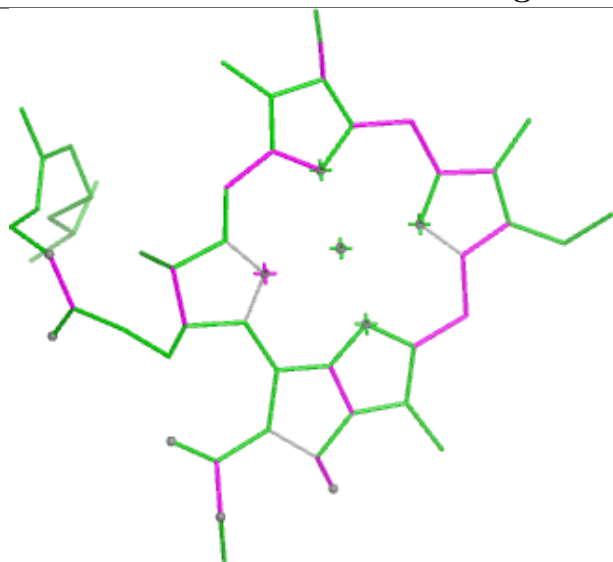
Torsions



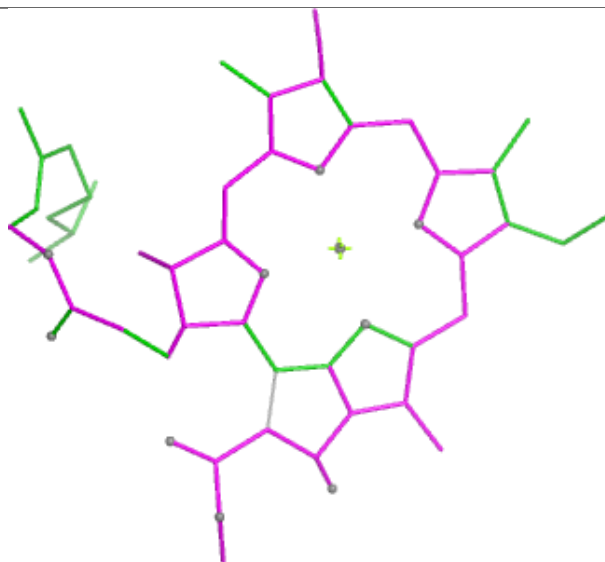
Rings



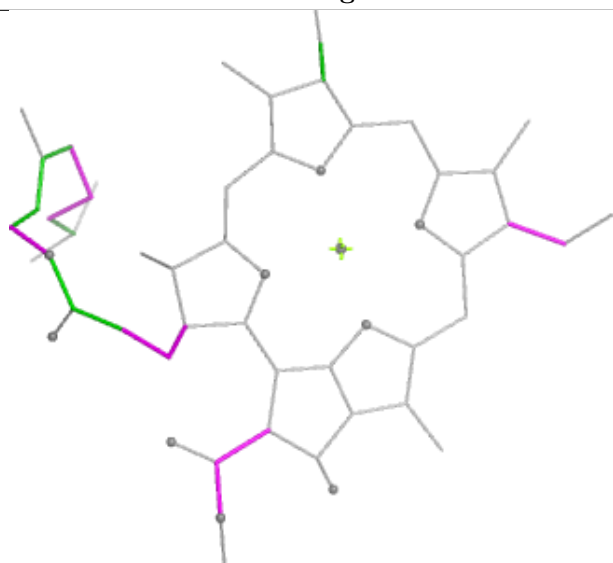
Ligand CLA H 101



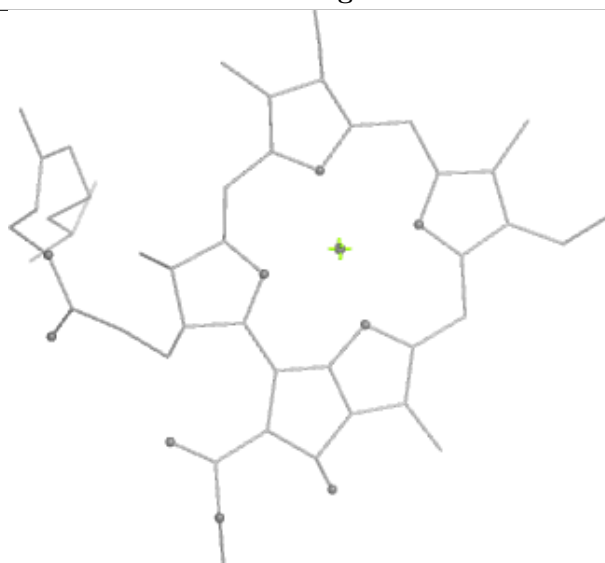
Bond lengths



Bond angles

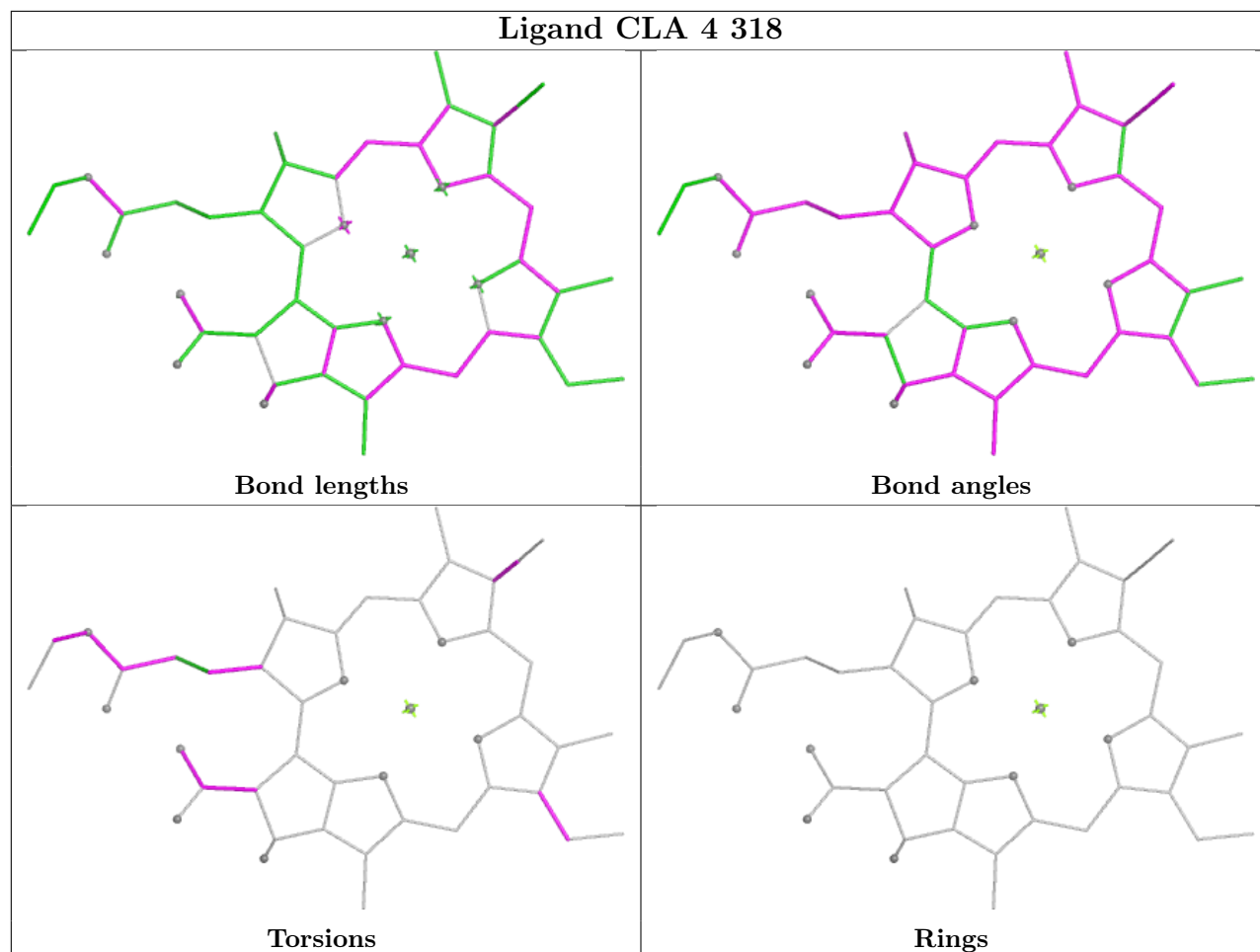


Torsions

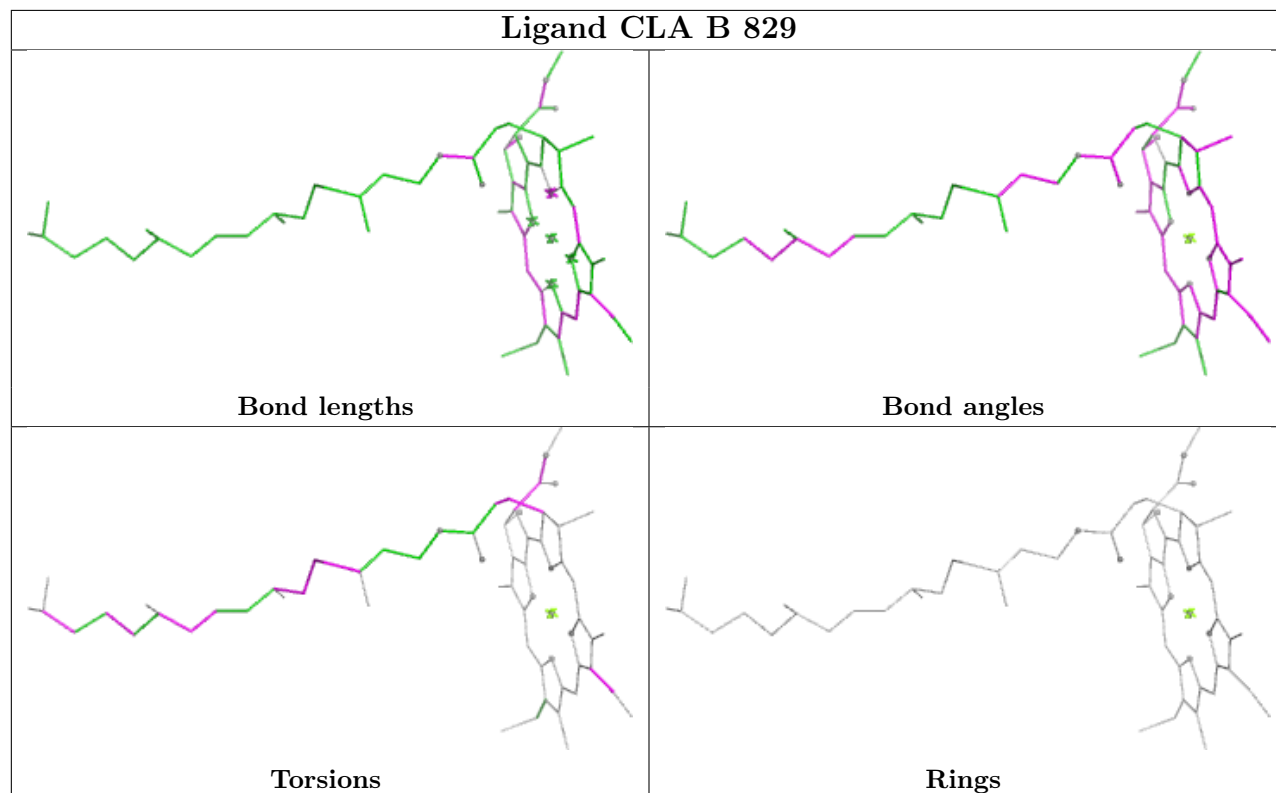


Rings

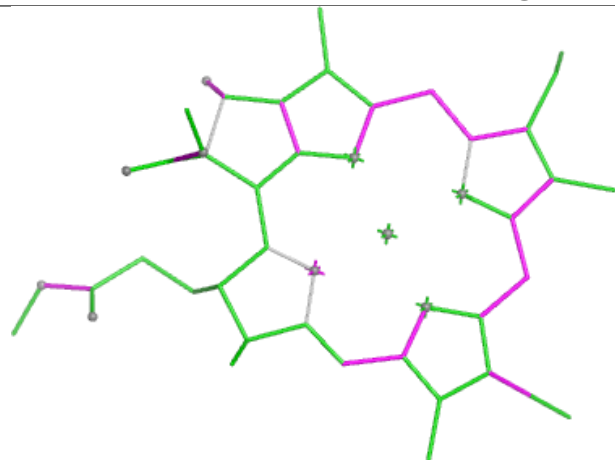
Ligand CLA 4 318



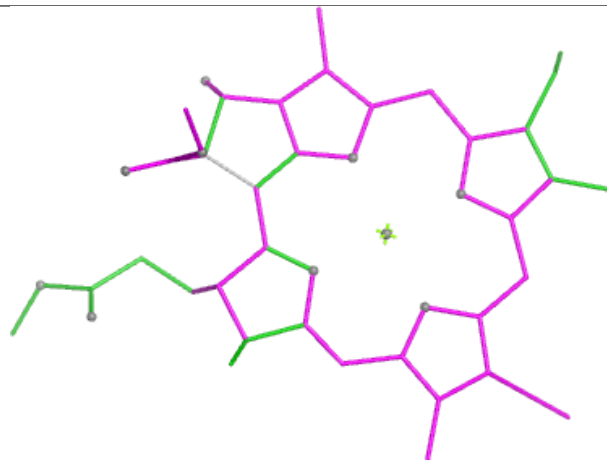
Ligand CLA B 829



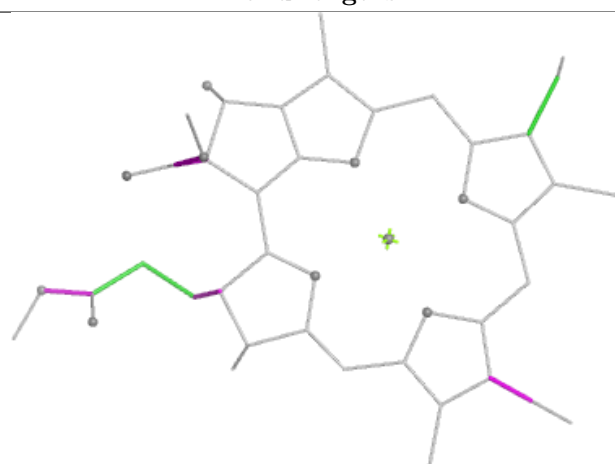
Ligand CLA A 834



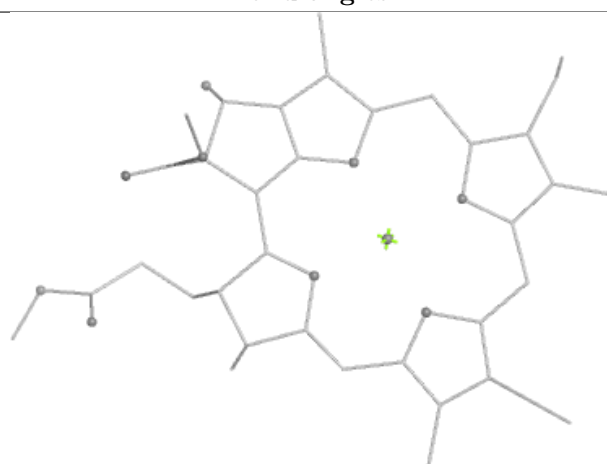
Bond lengths



Bond angles

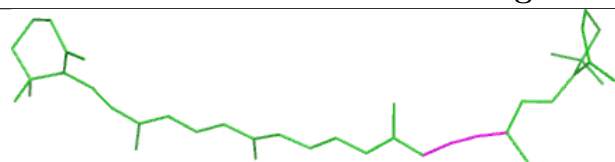


Torsions

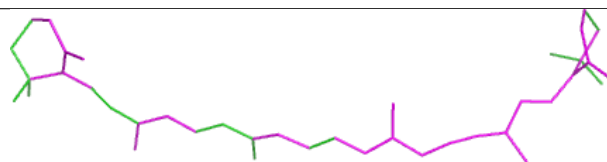


Rings

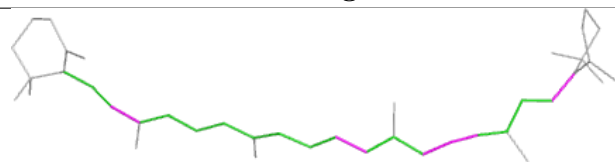
Ligand BCR B 844



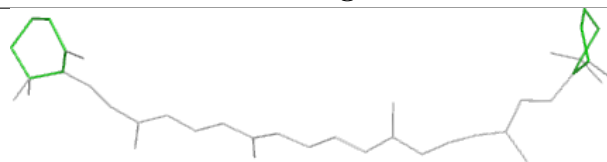
Bond lengths



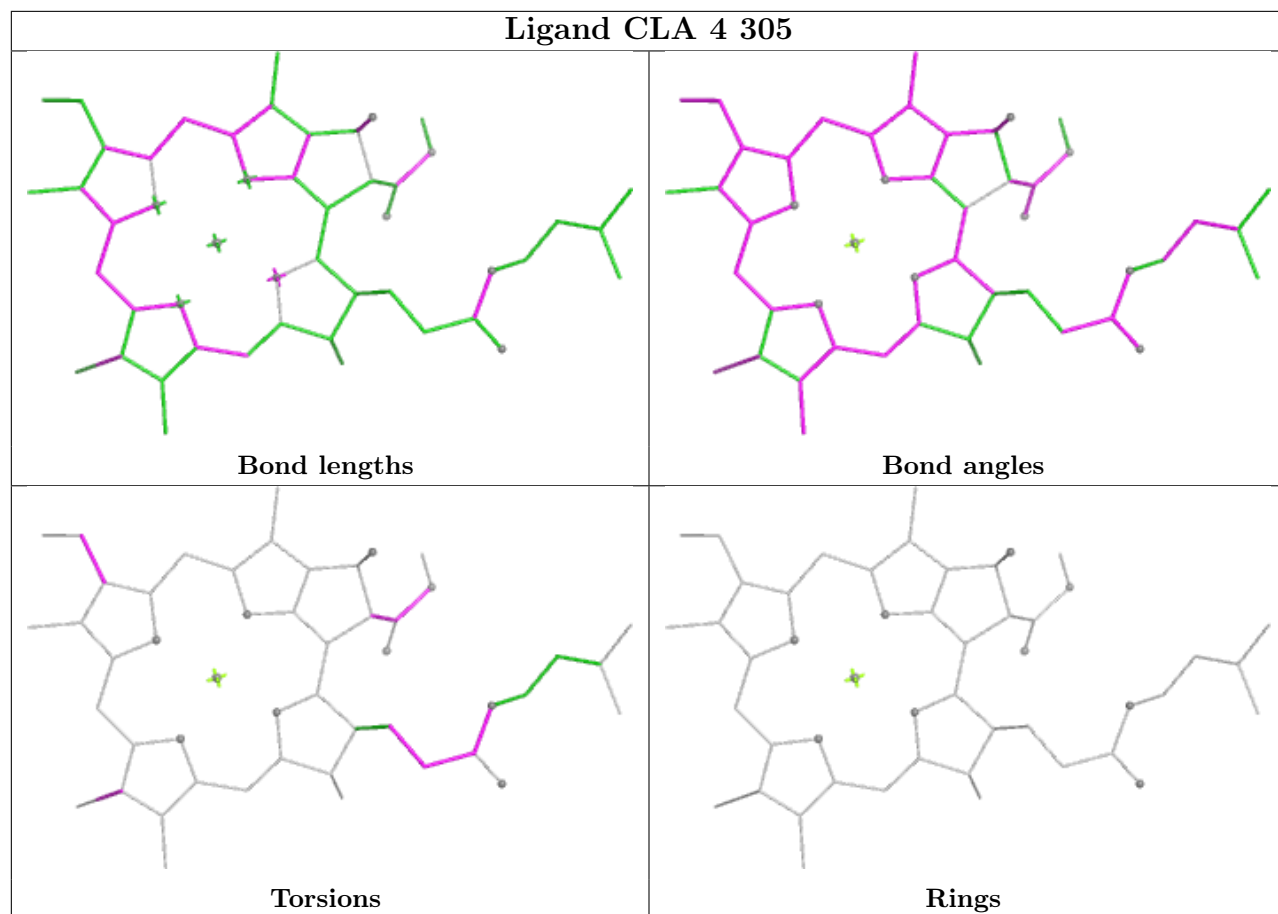
Bond angles



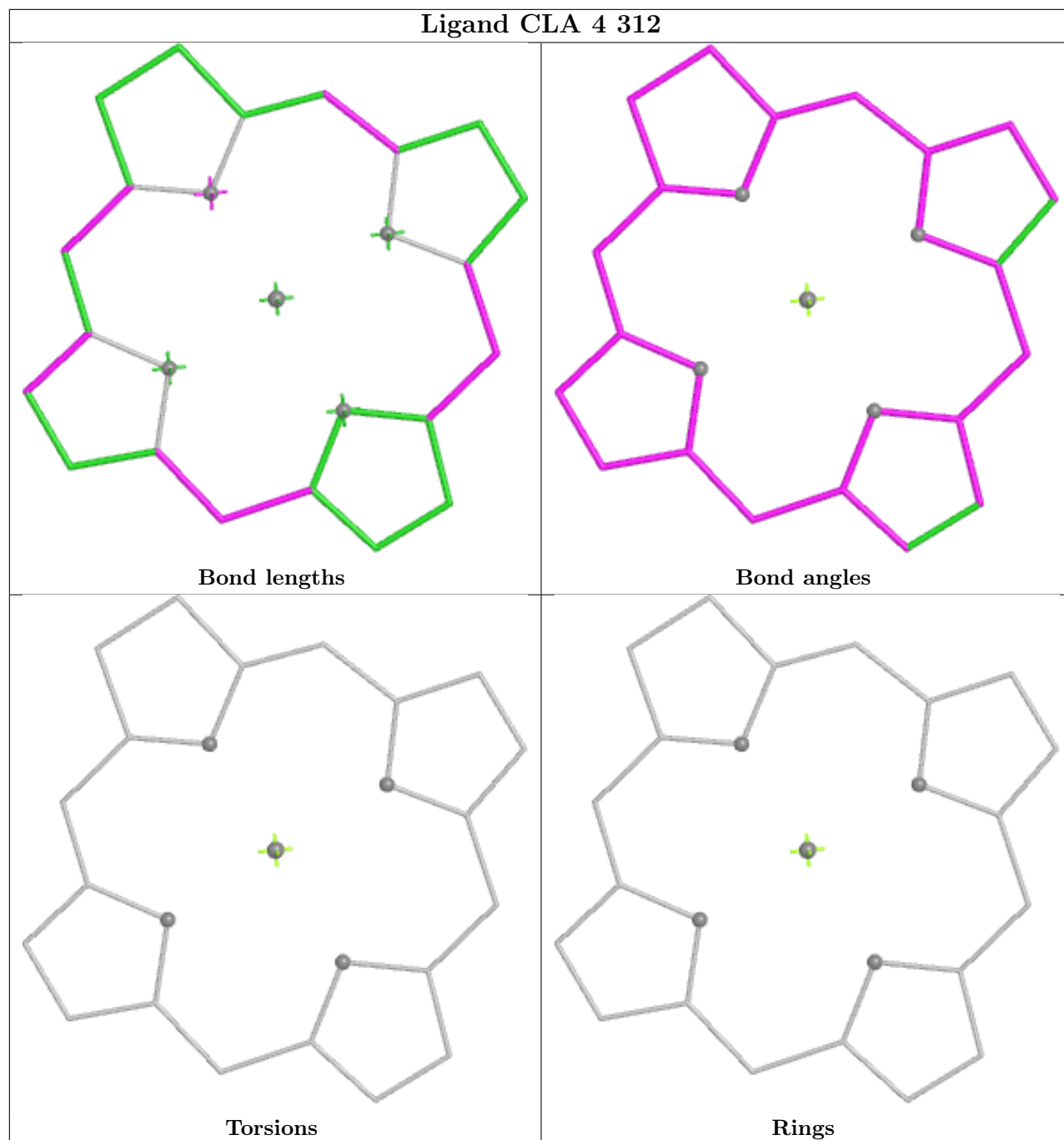
Torsions

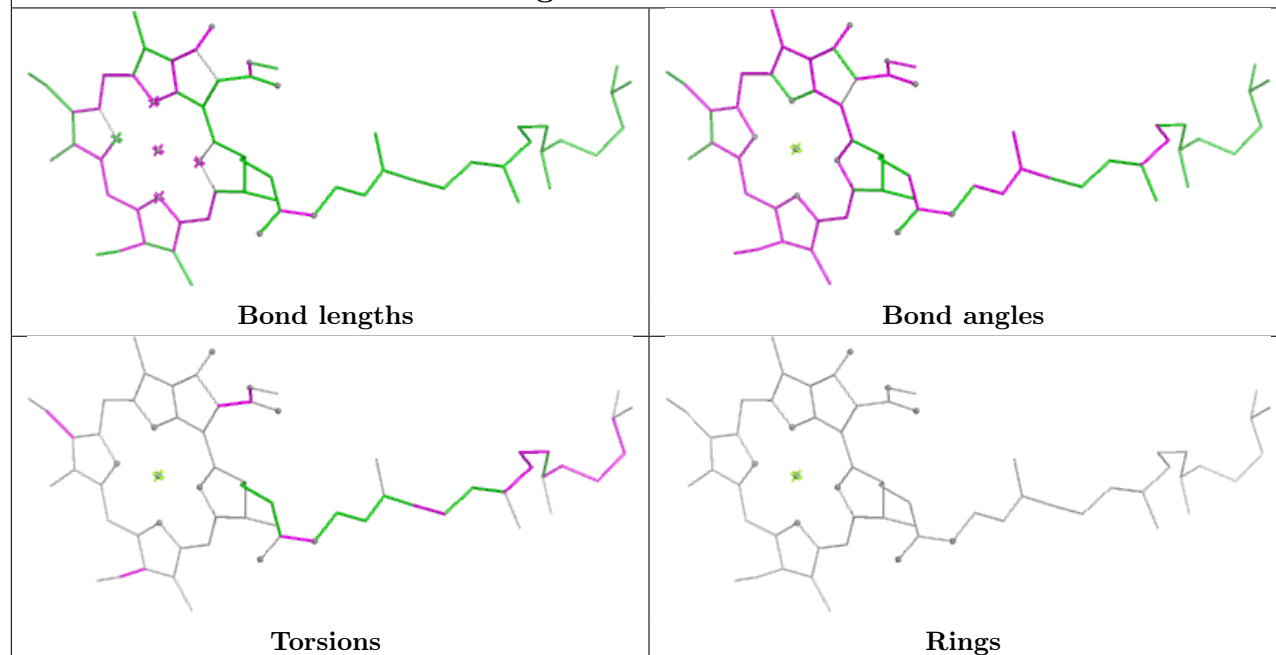
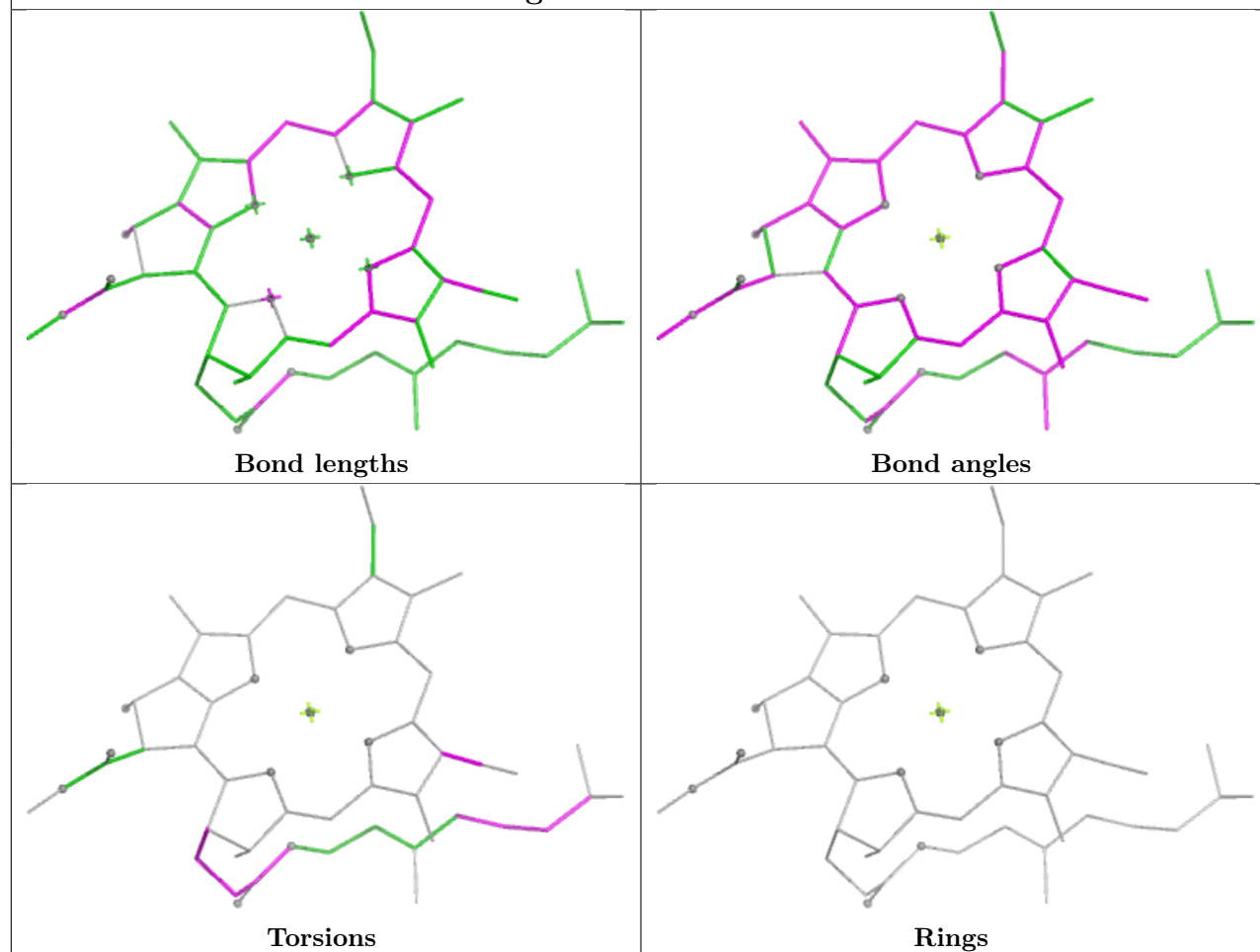


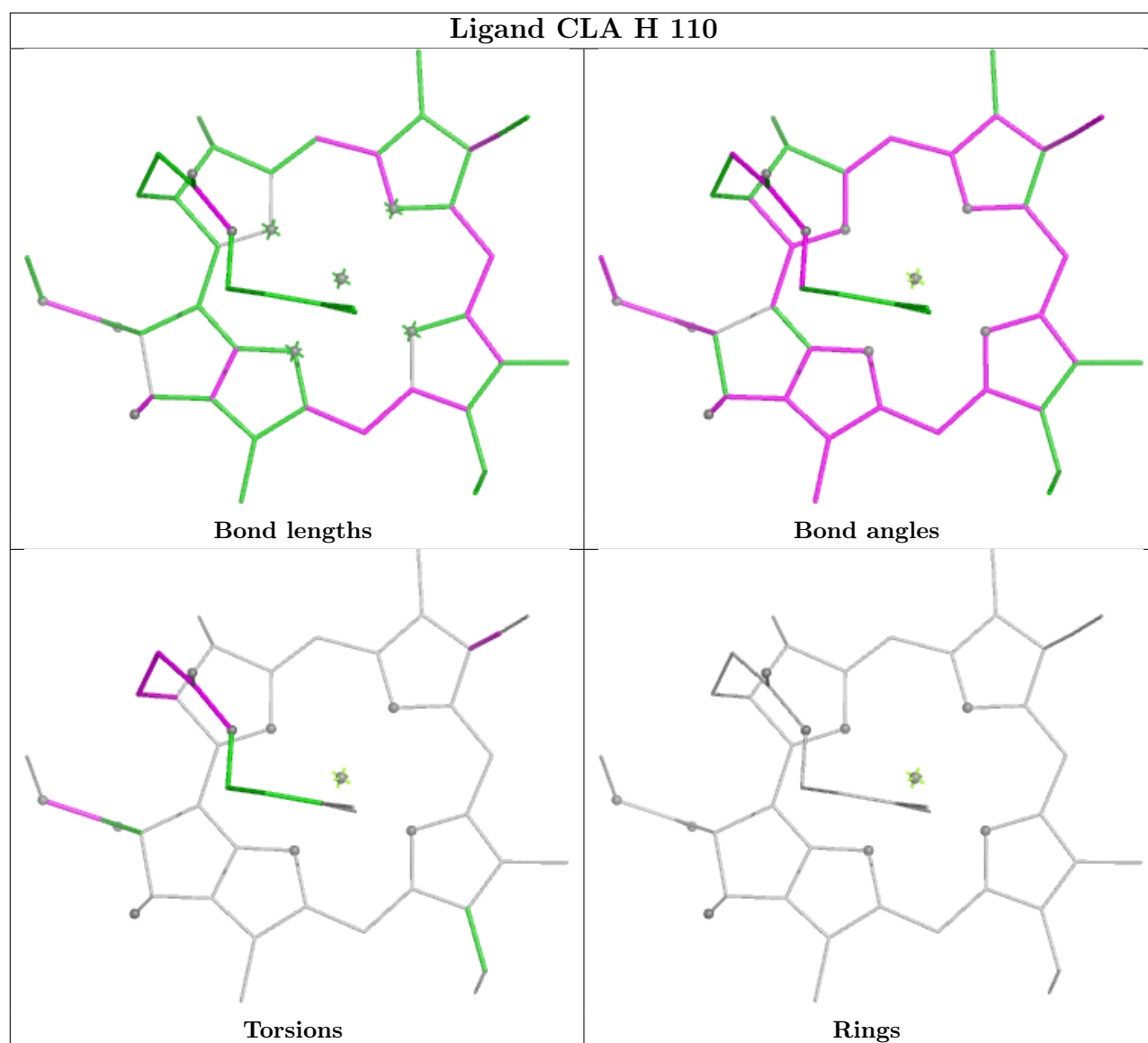
Rings

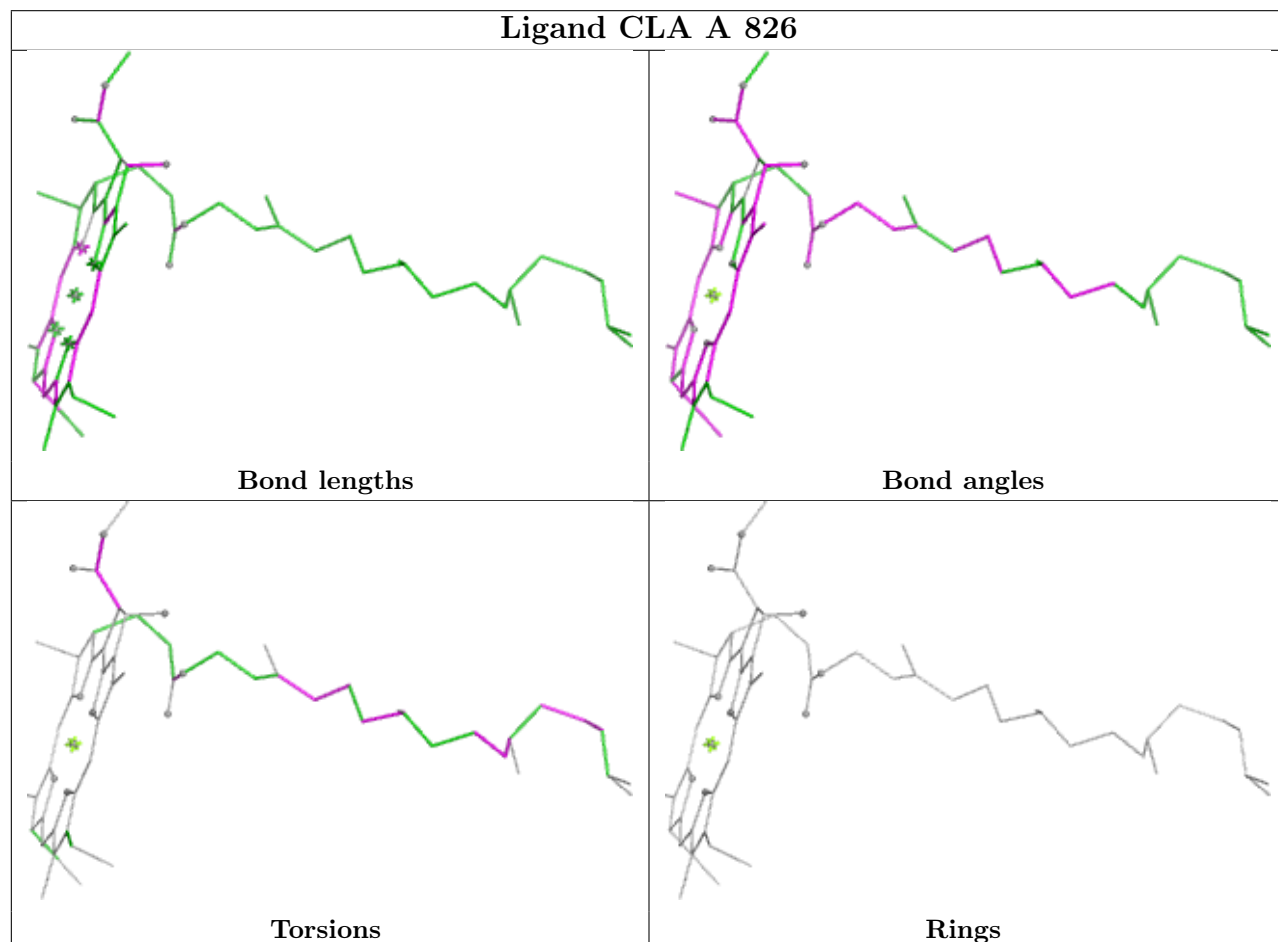
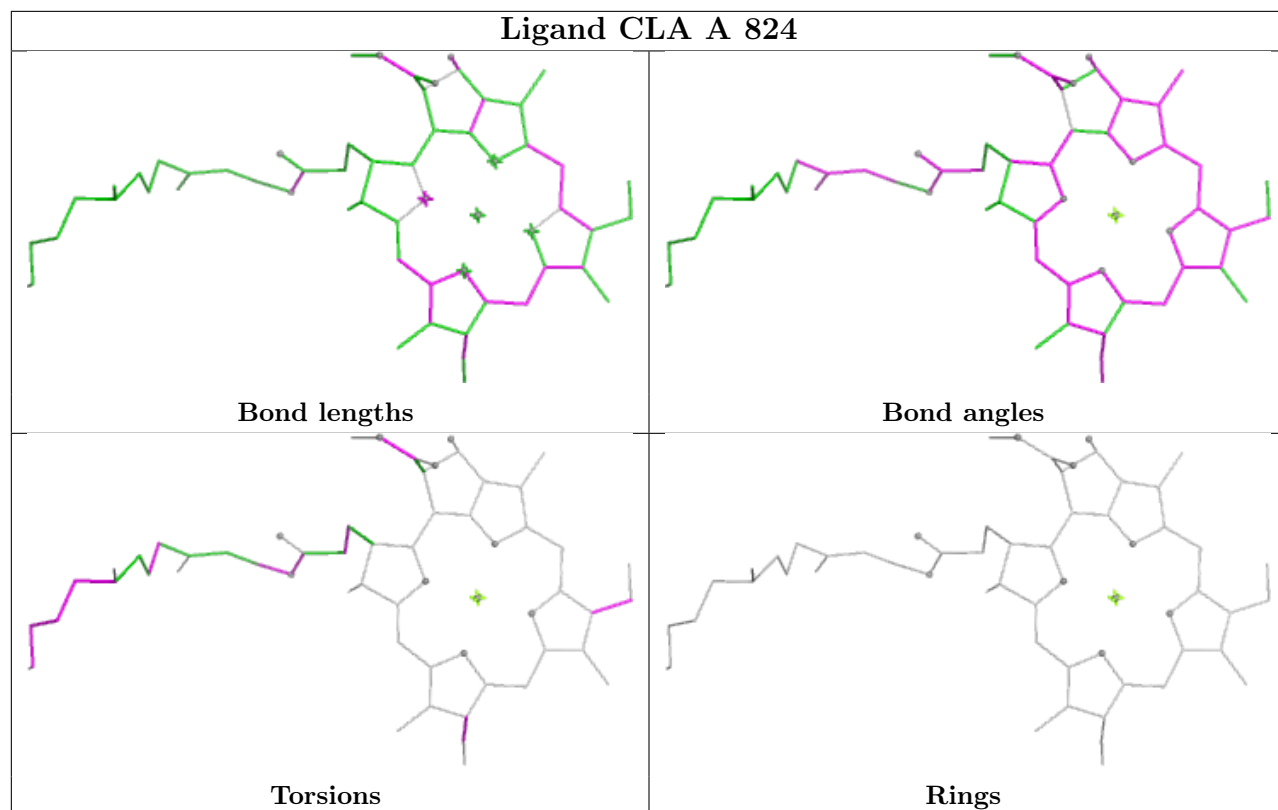


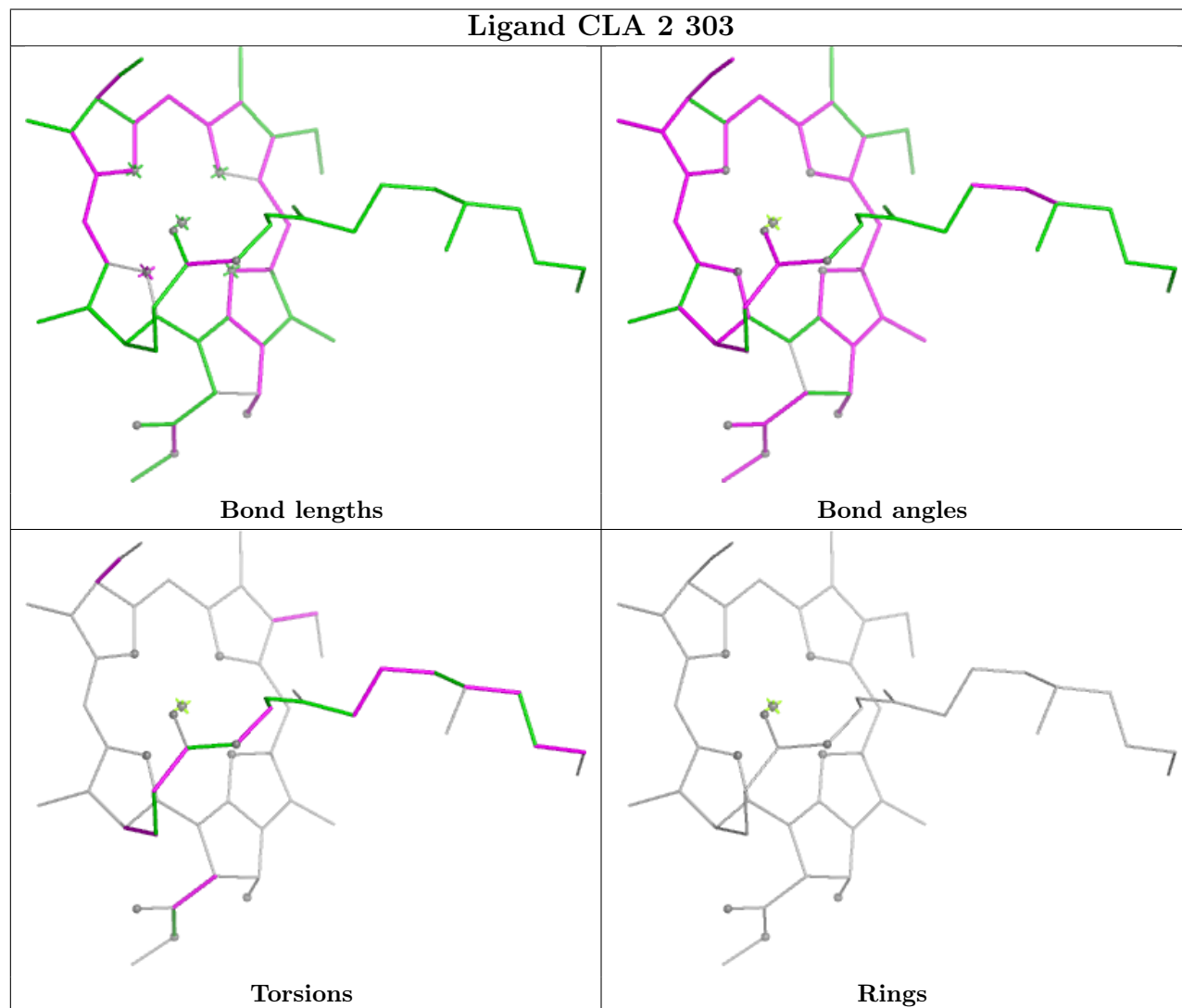
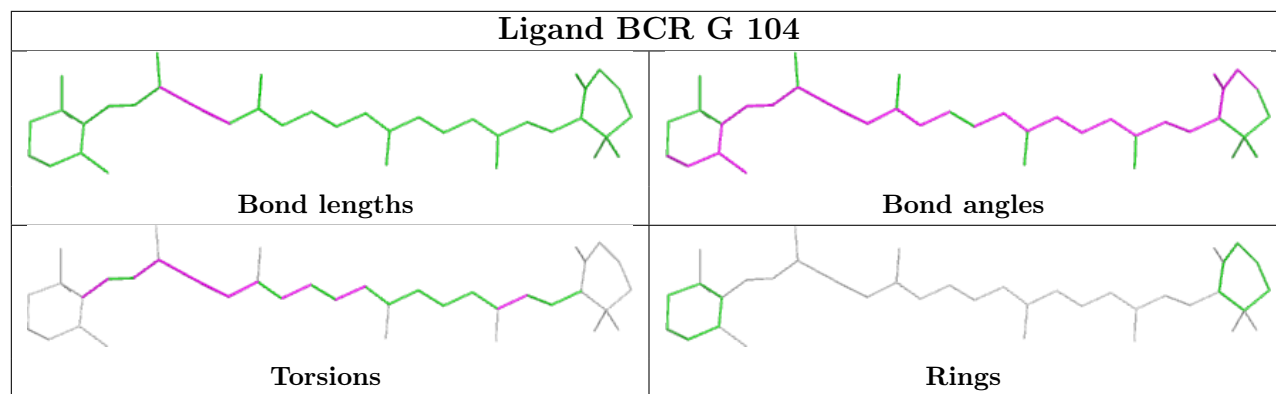
Ligand CLA 4 312



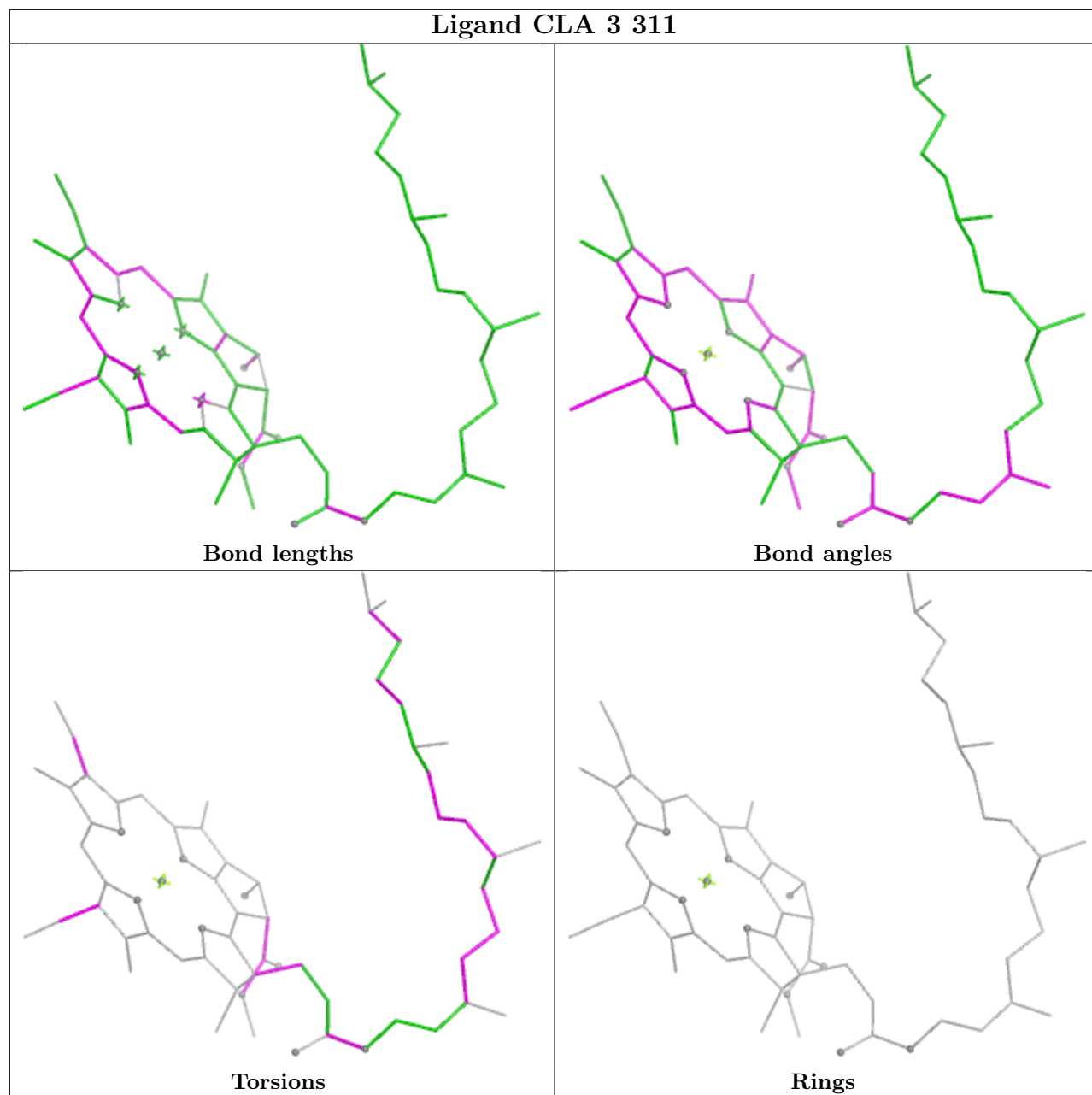
Ligand CLA 3 314**Ligand CLA B 823**

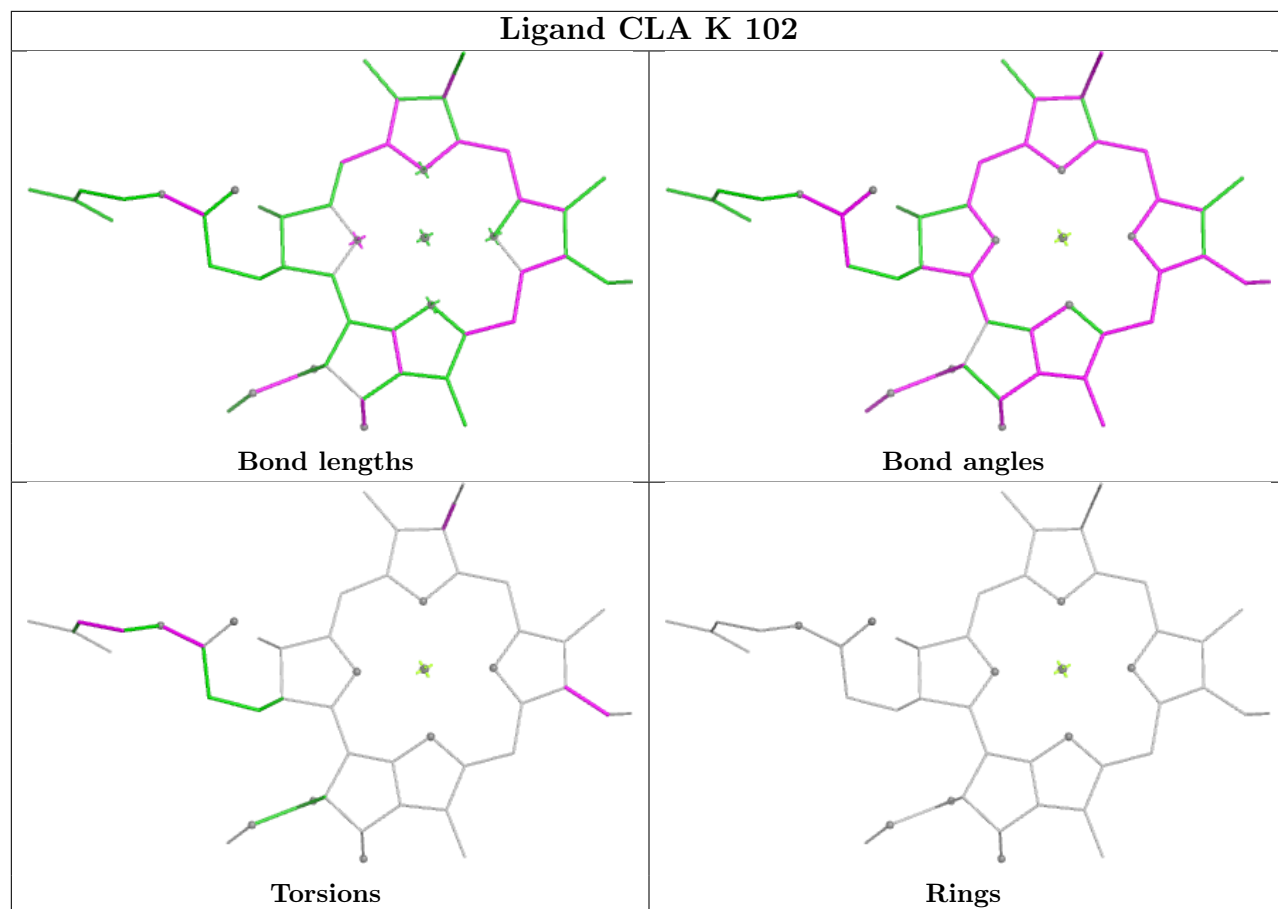




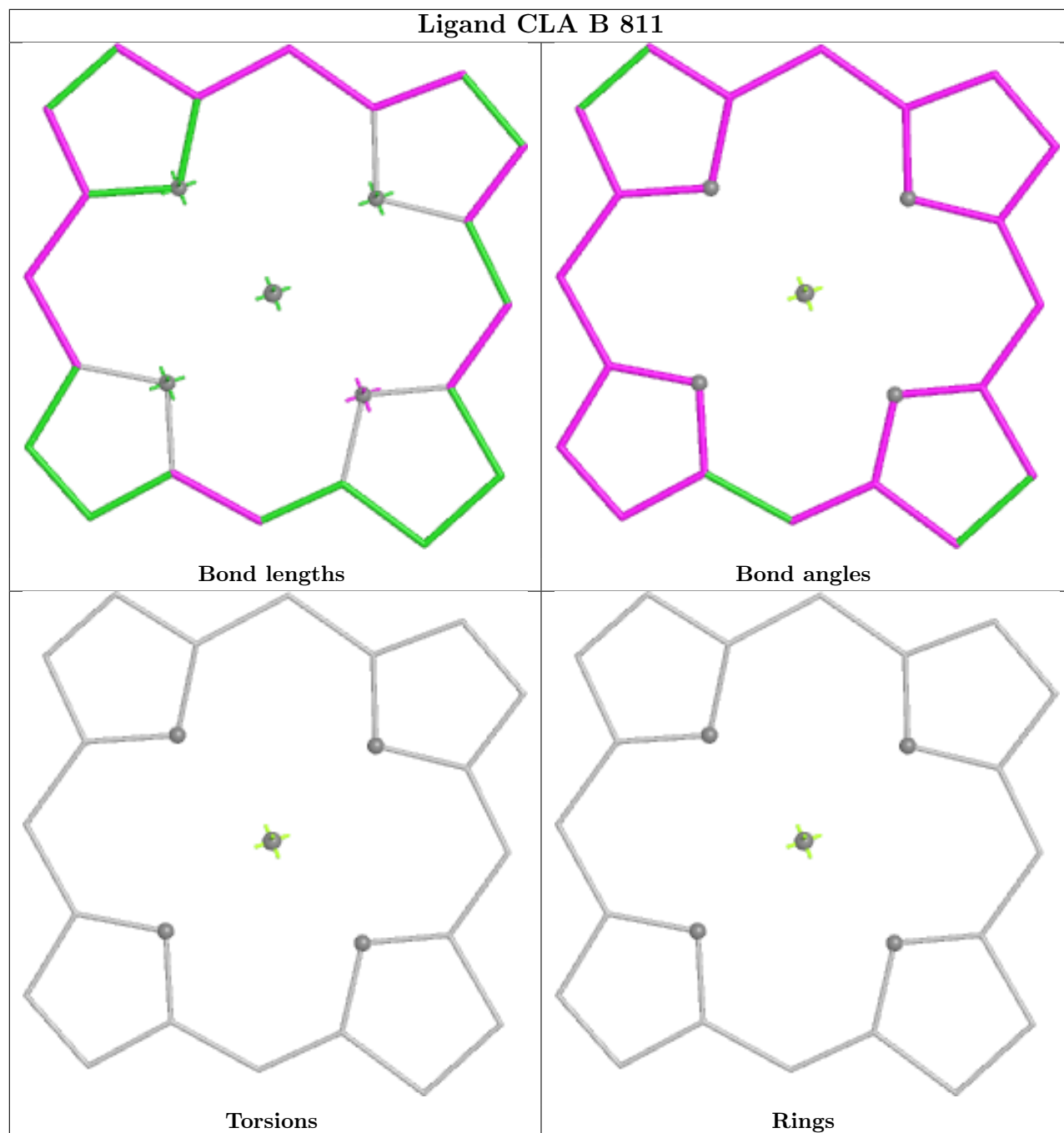


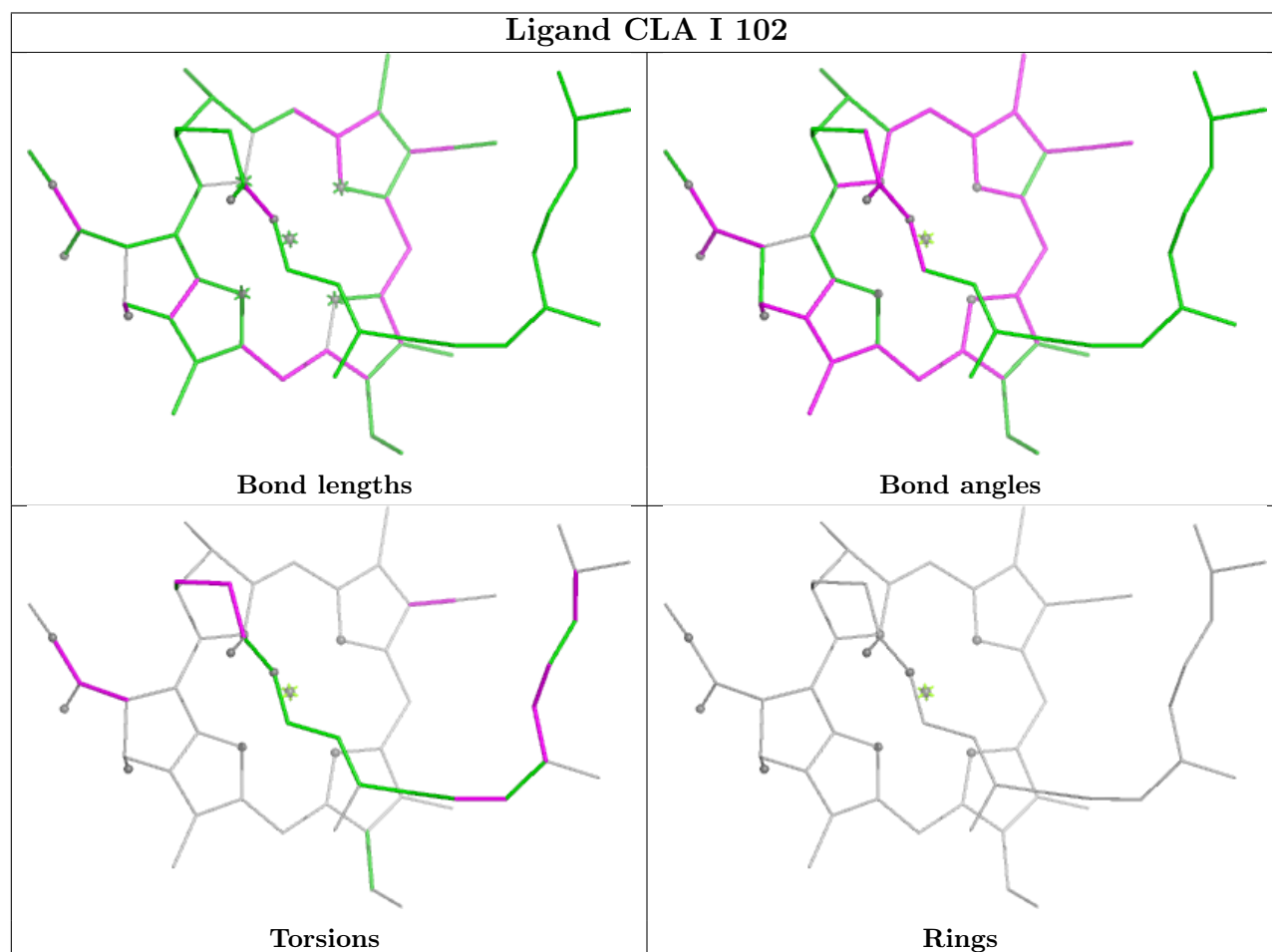
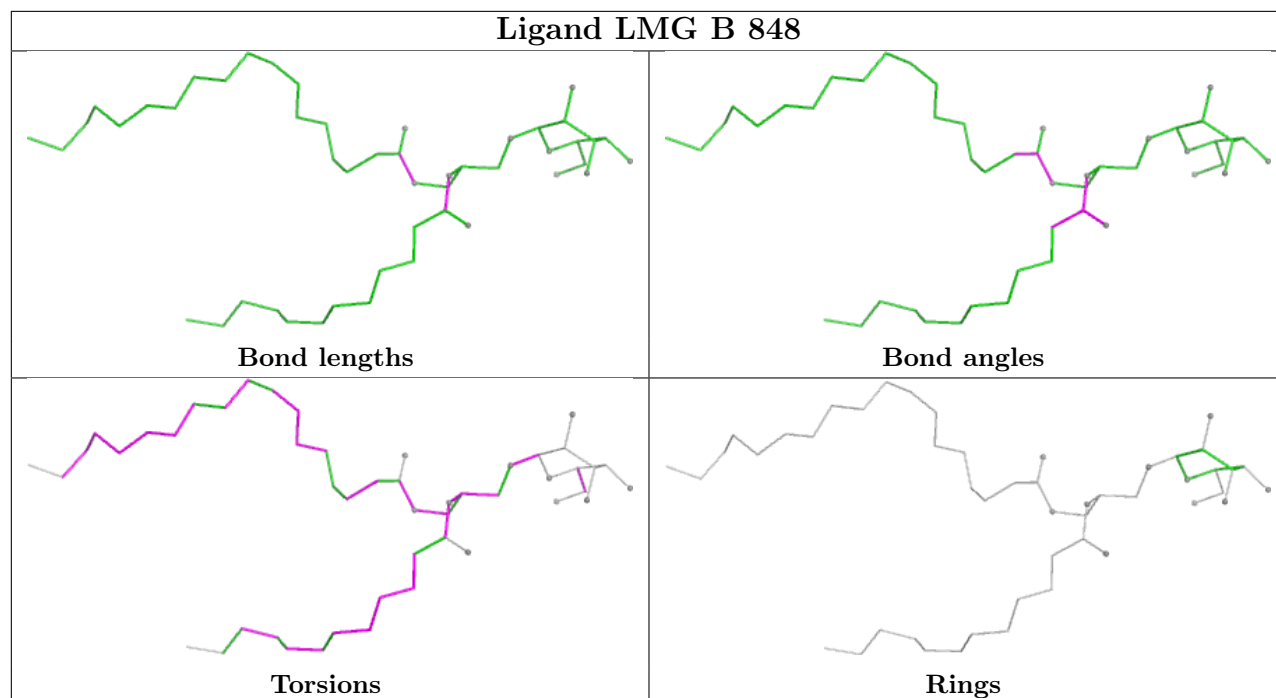
Ligand CLA 3 311

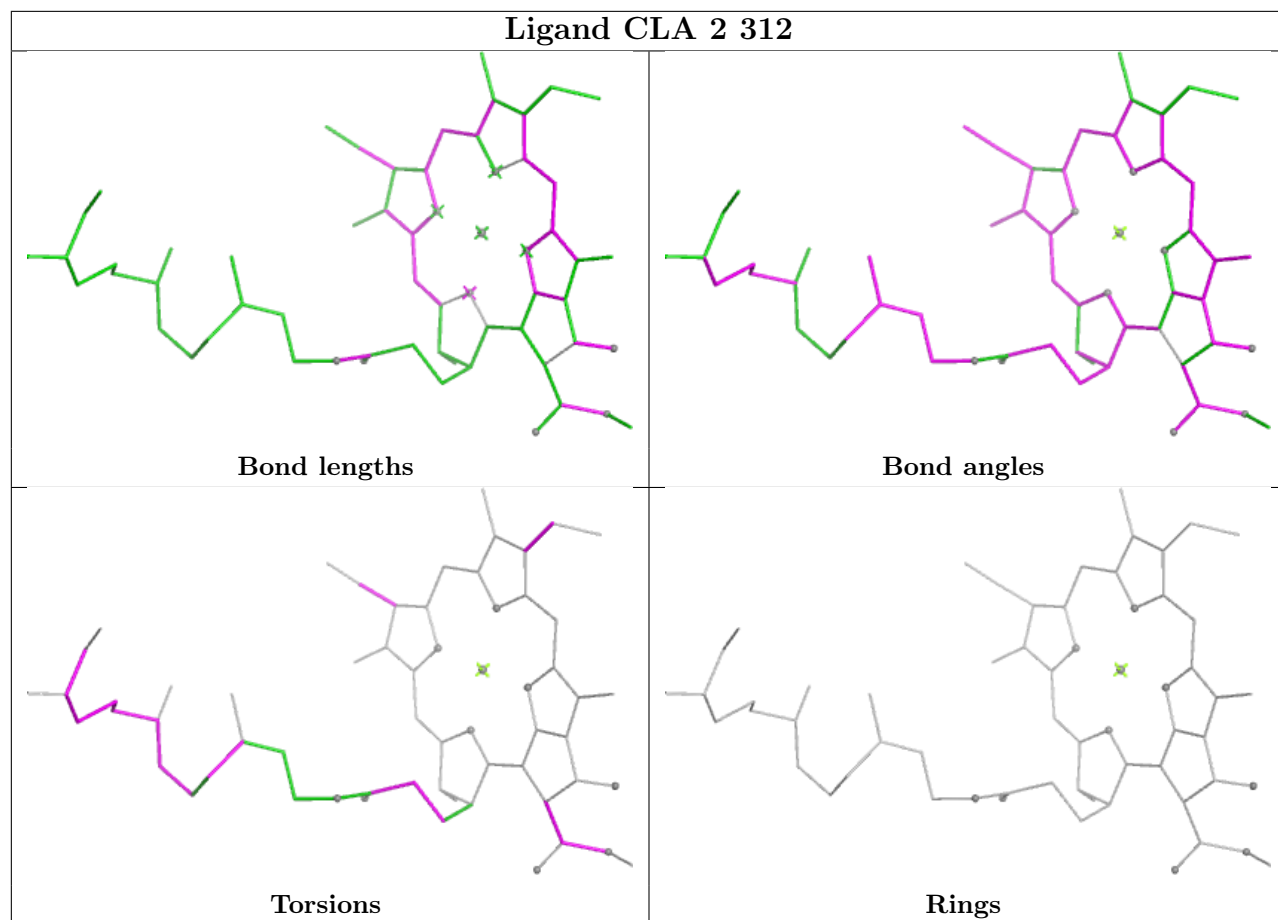




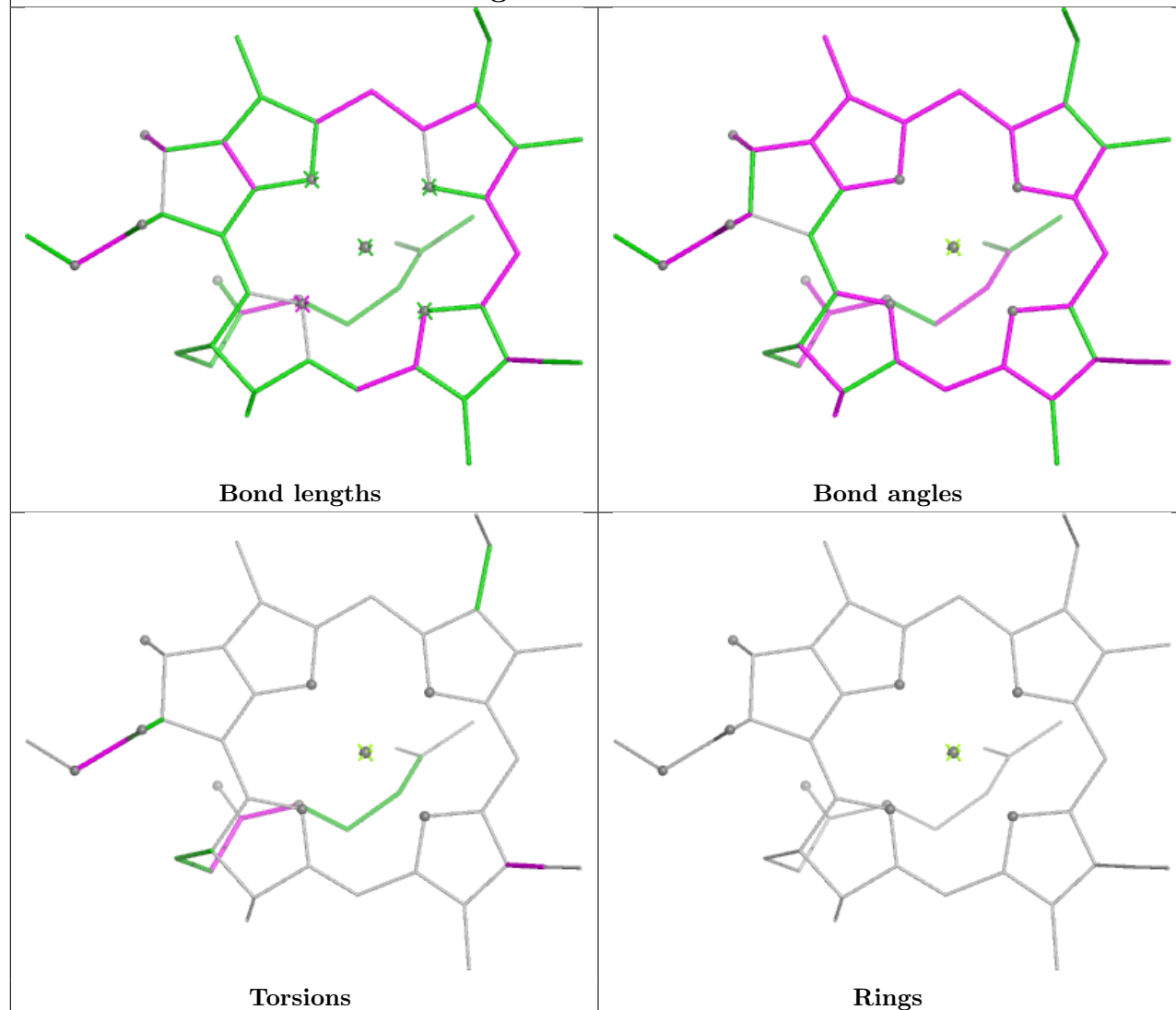
Ligand CLA B 811



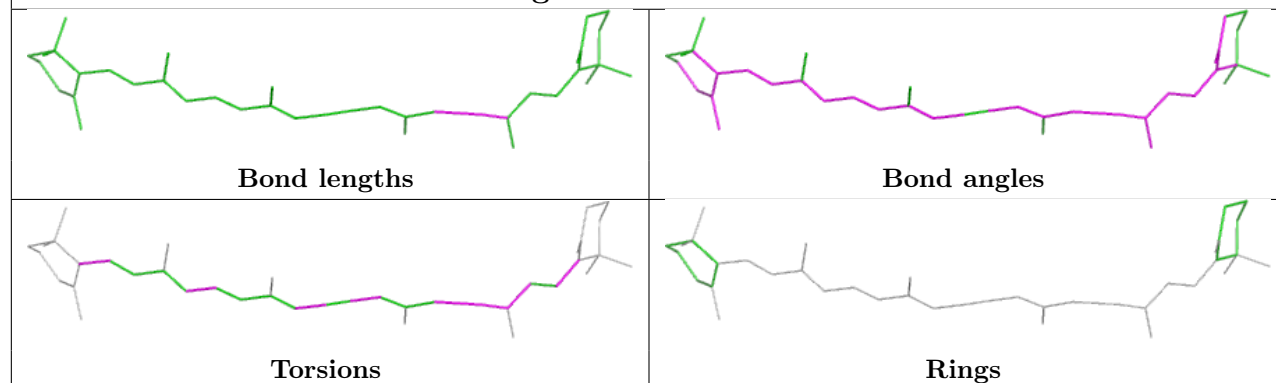


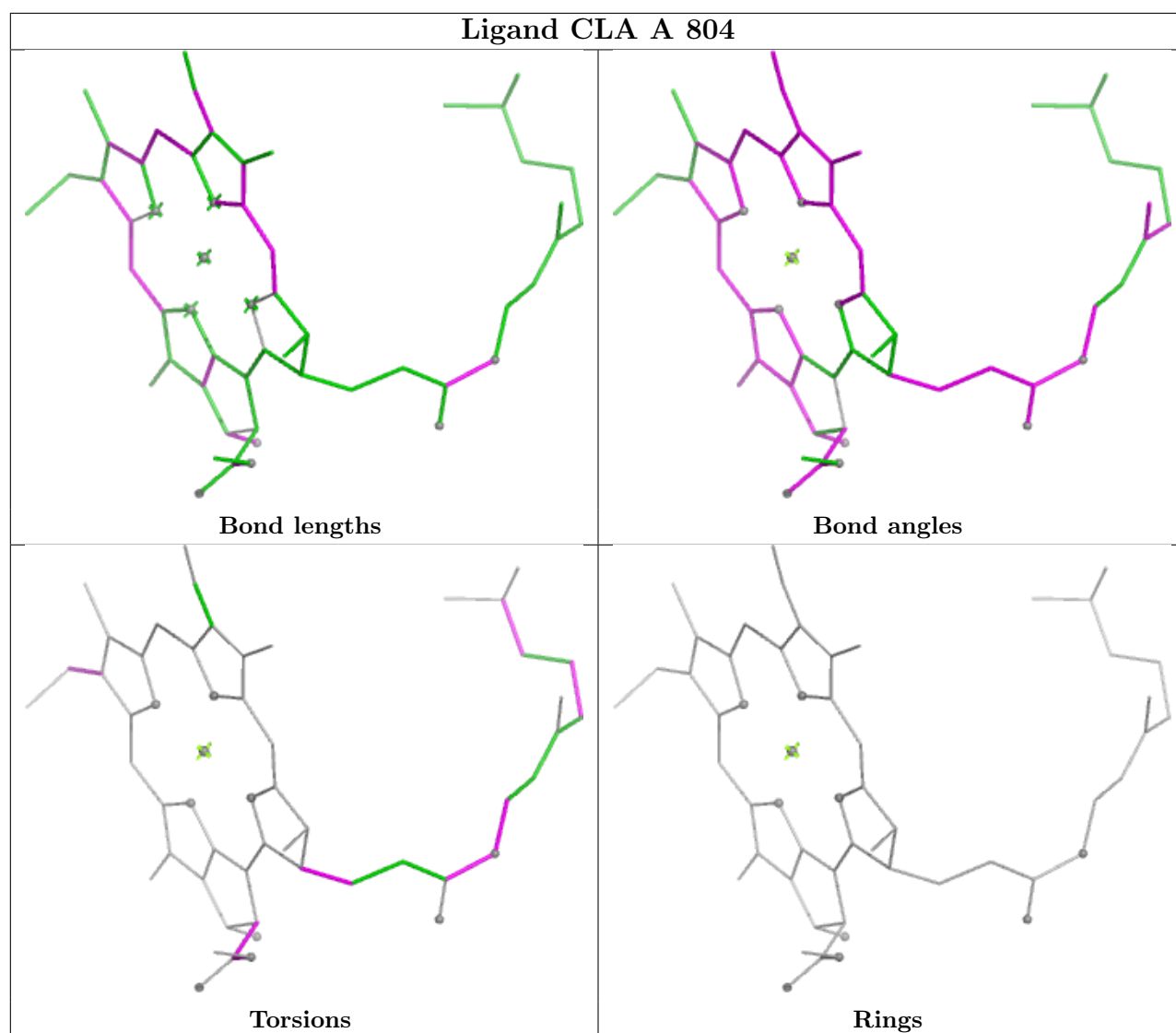


Ligand CLA B 821

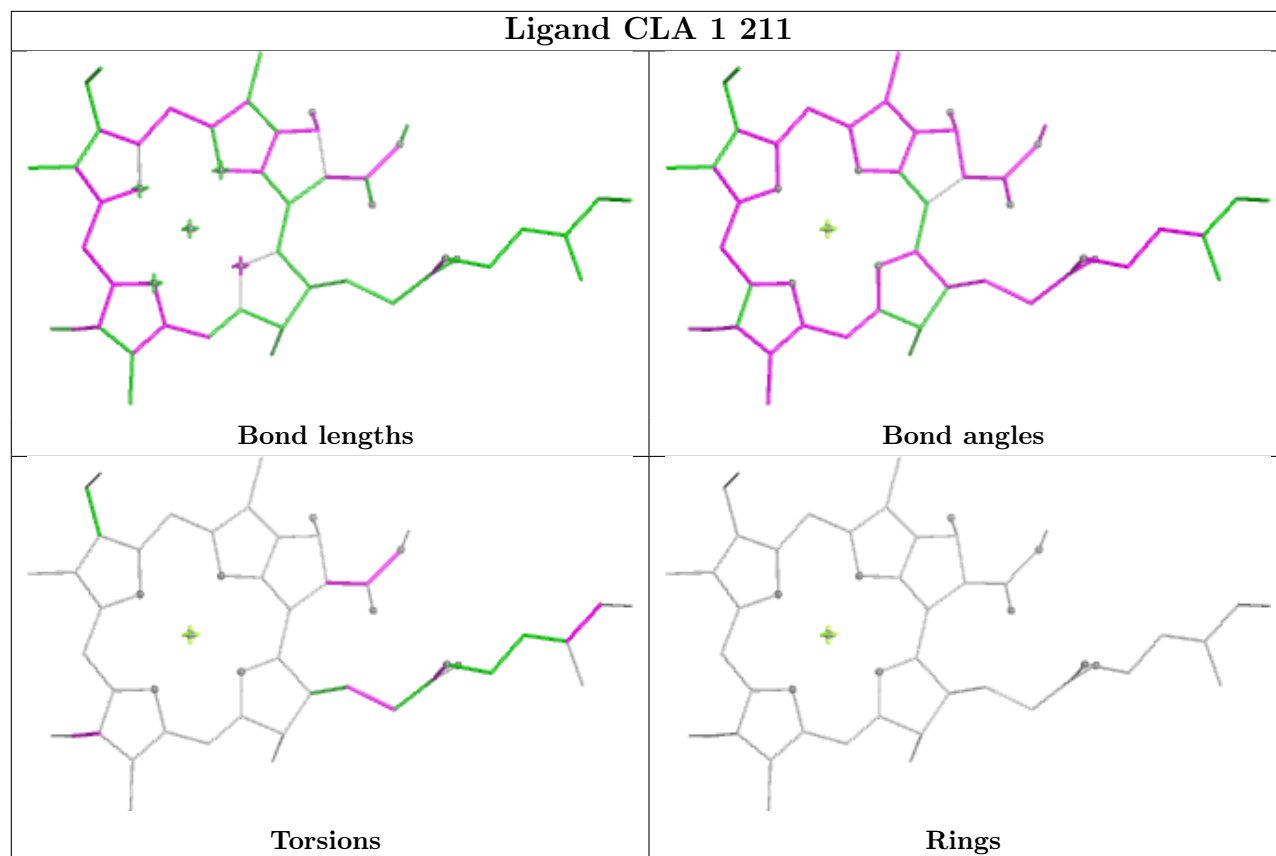


Ligand BCR F 203

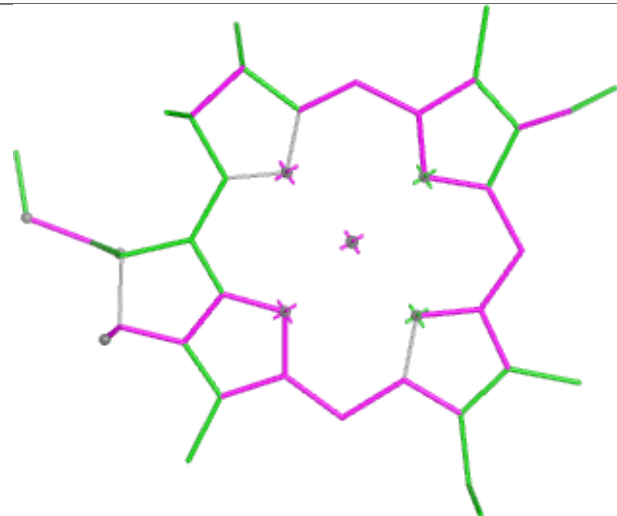




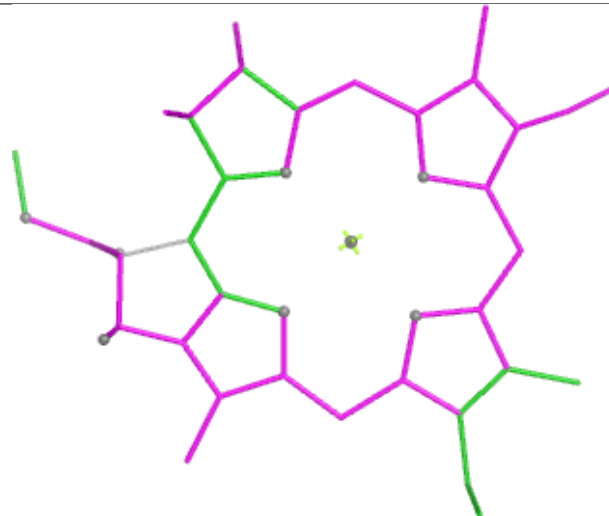
Ligand CLA 1 211



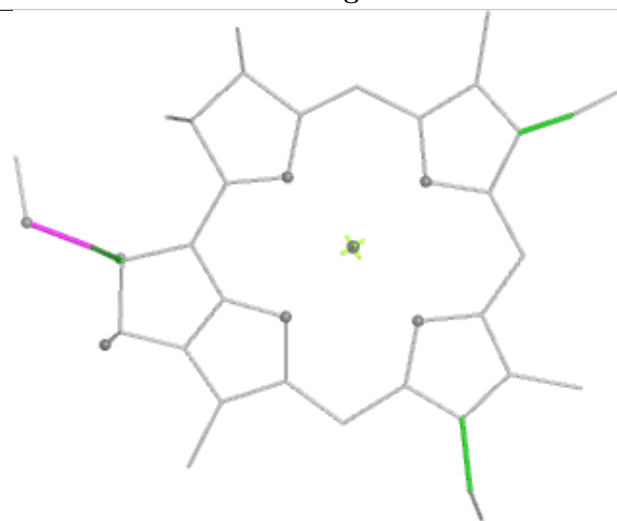
Ligand CLA B 819



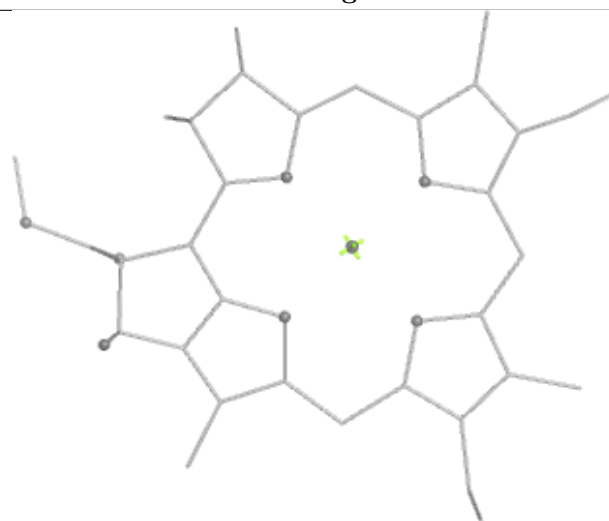
Bond lengths



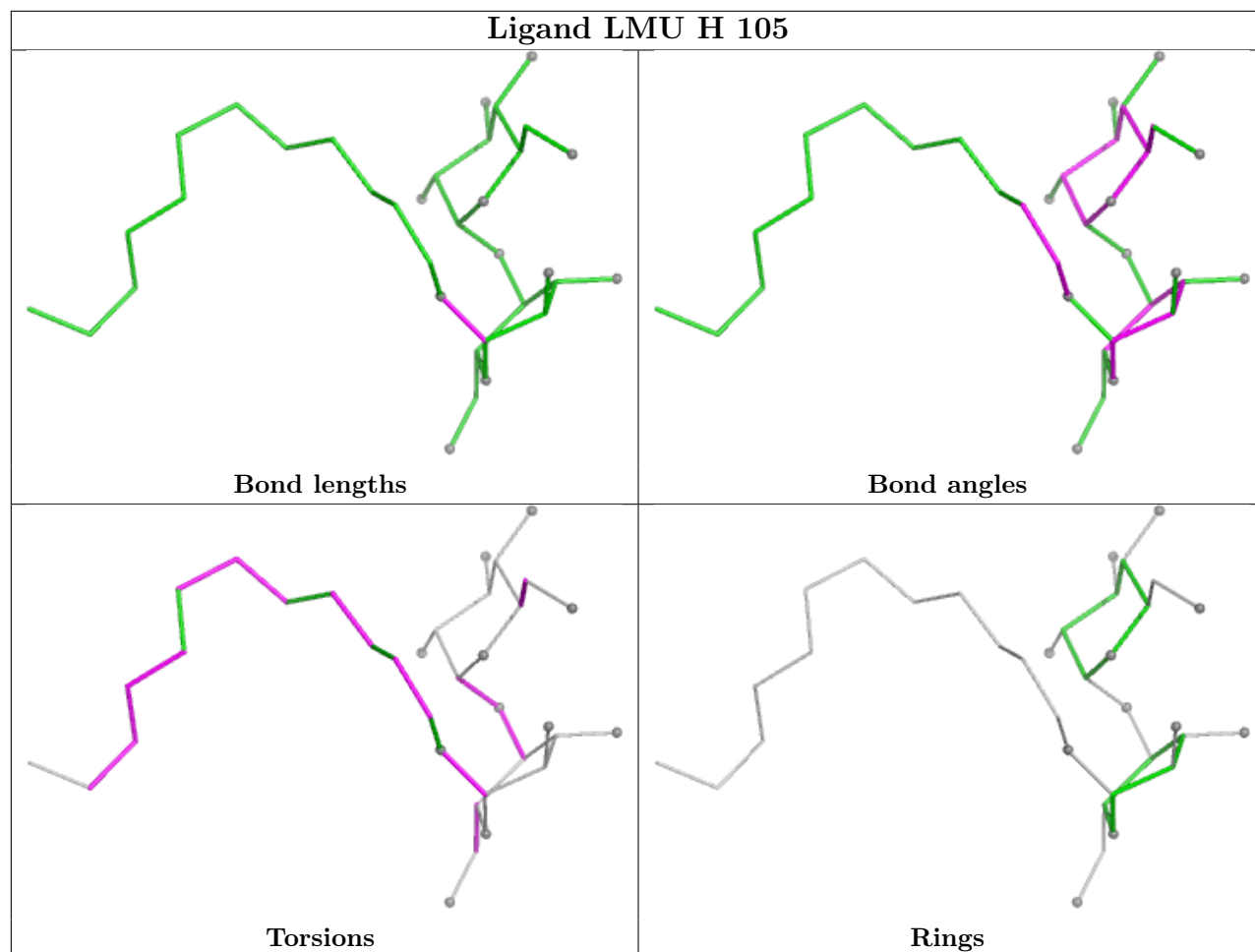
Bond angles



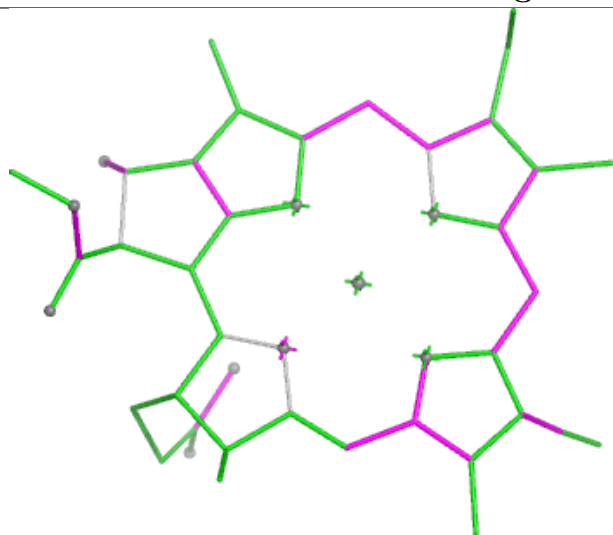
Torsions



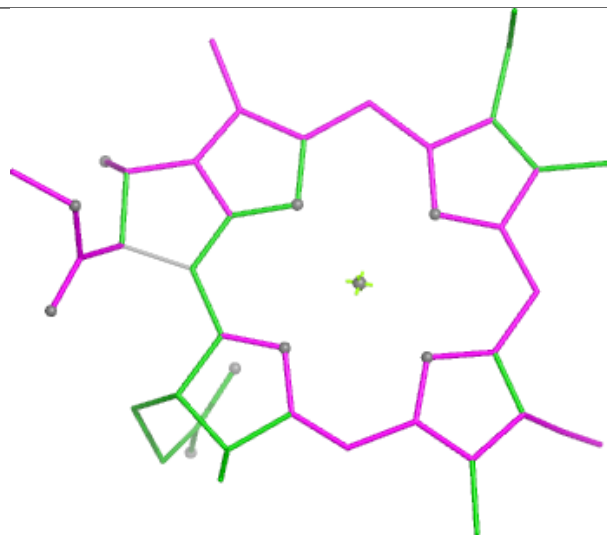
Rings



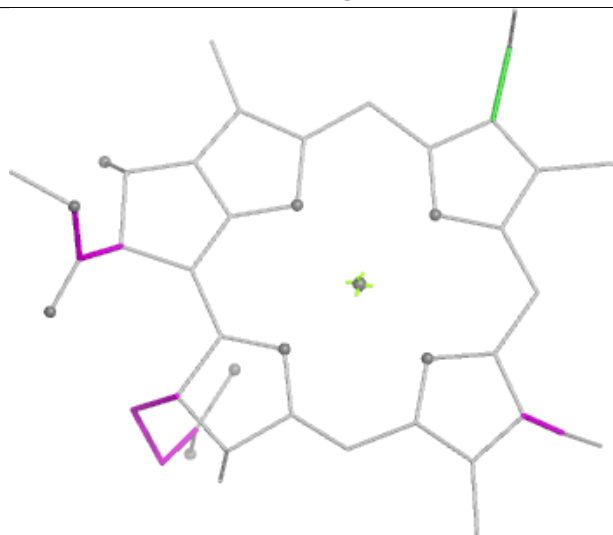
Ligand CLA B 834



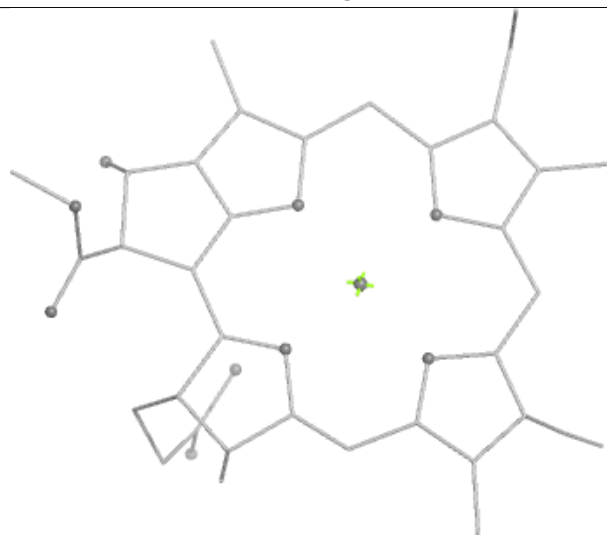
Bond lengths



Bond angles

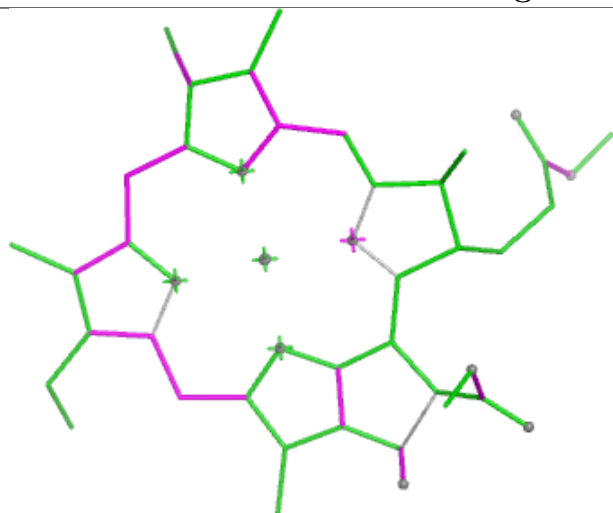


Torsions

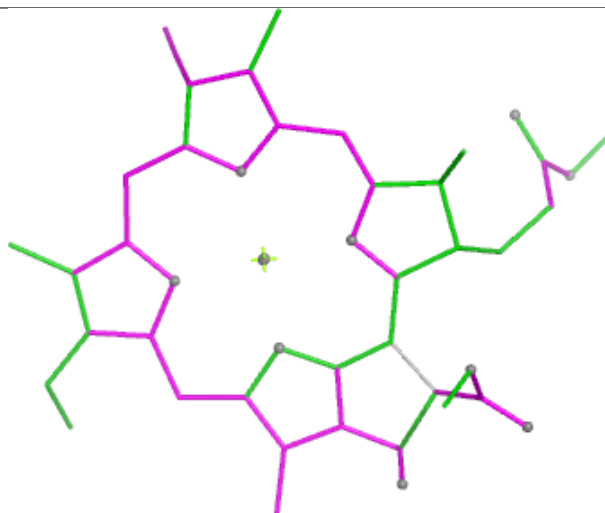


Rings

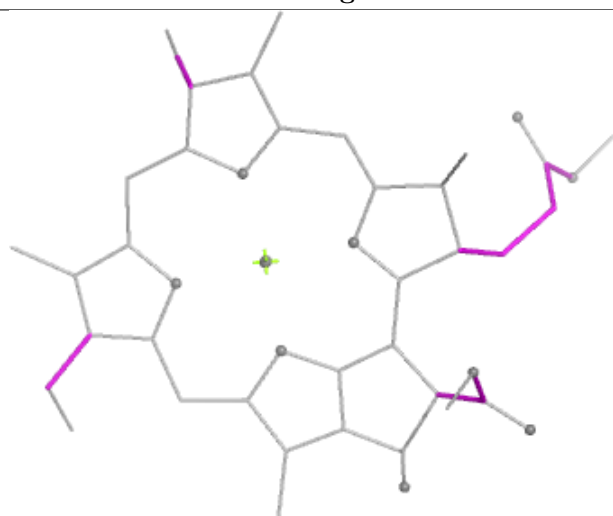
Ligand CLA B 822



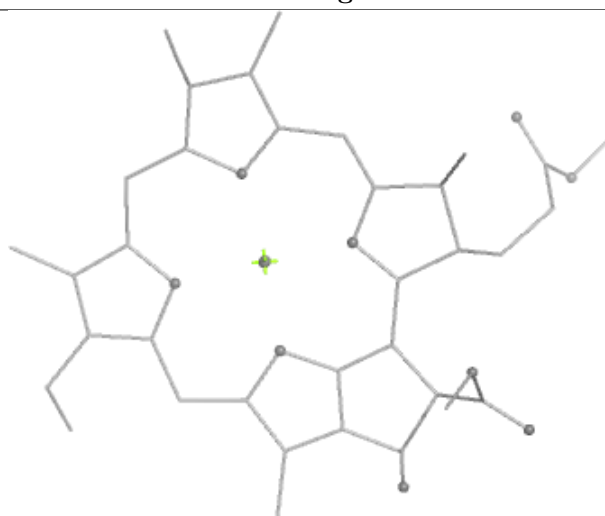
Bond lengths



Bond angles

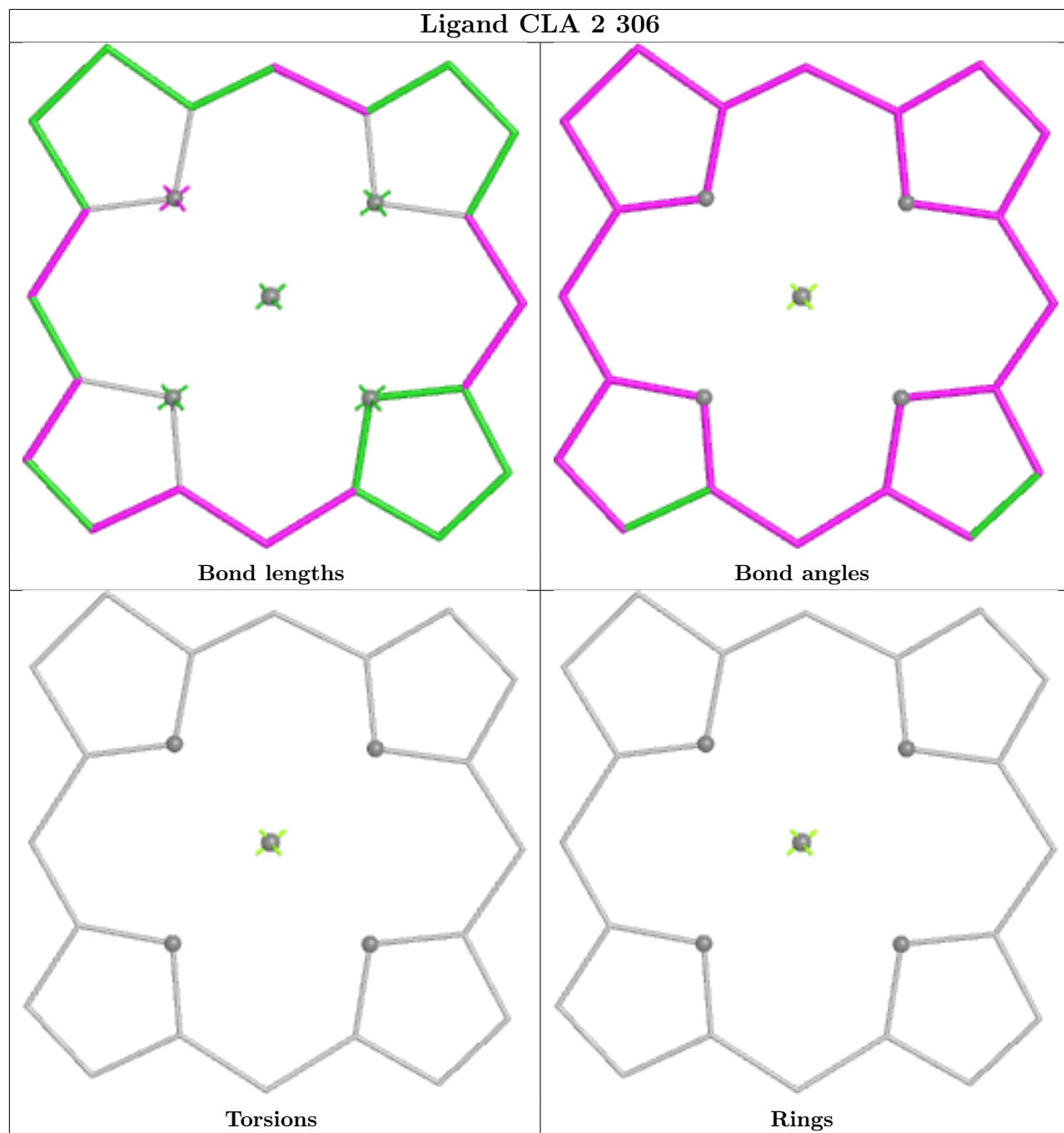


Torsions

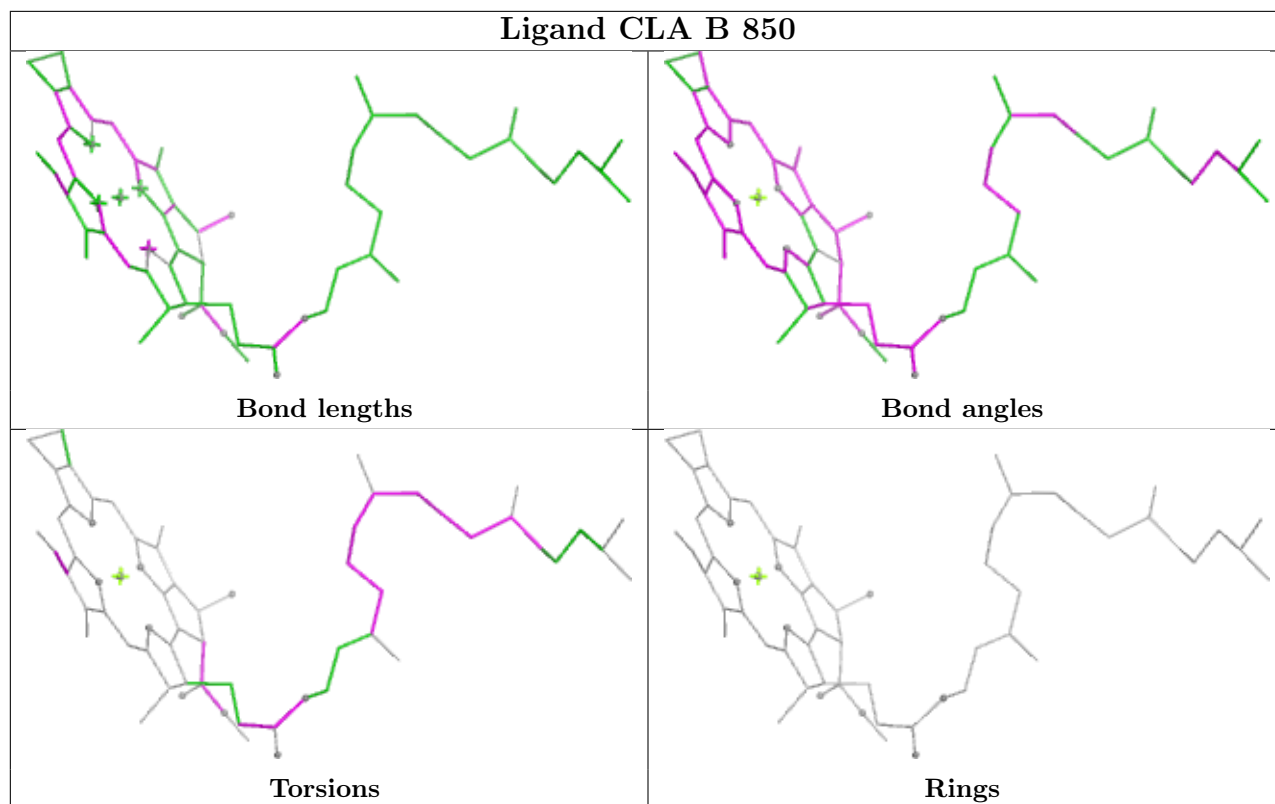


Rings

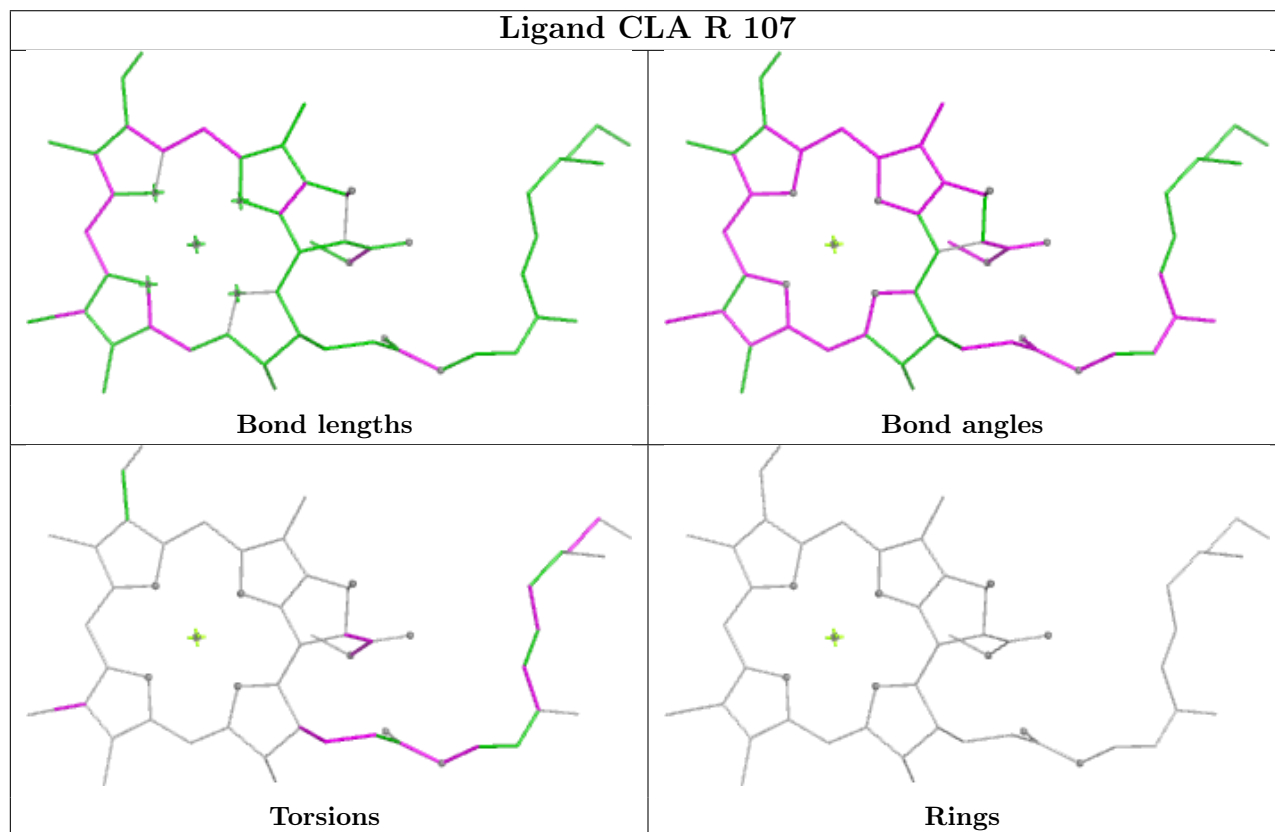
Ligand CLA 2 306



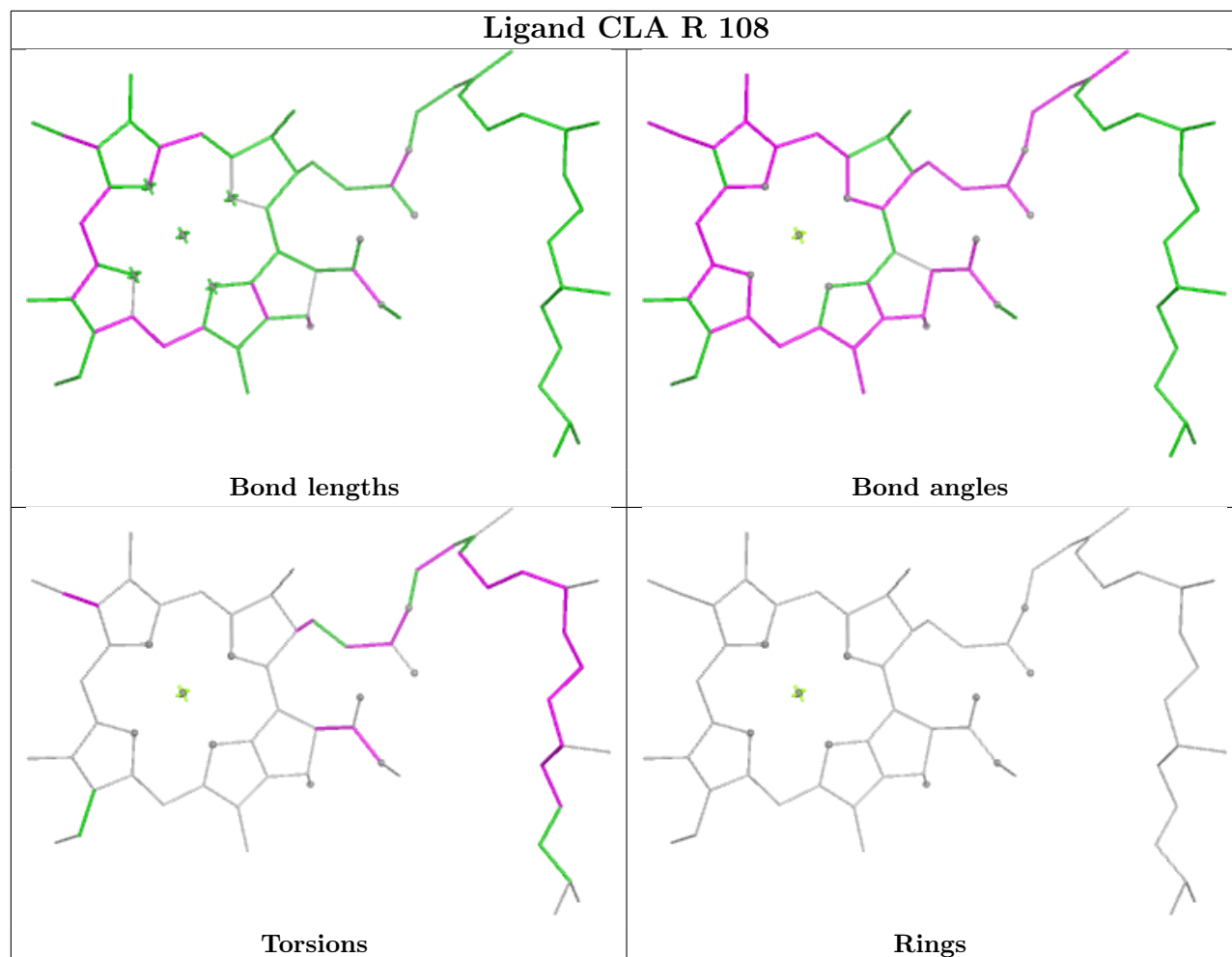
Ligand CLA B 850



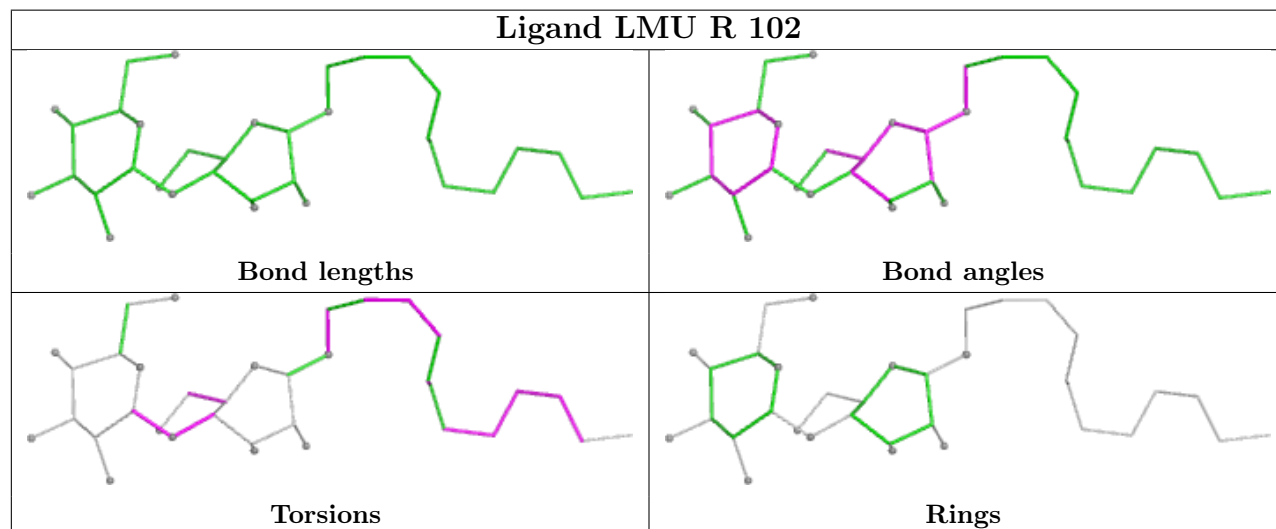
Ligand CLA R 107

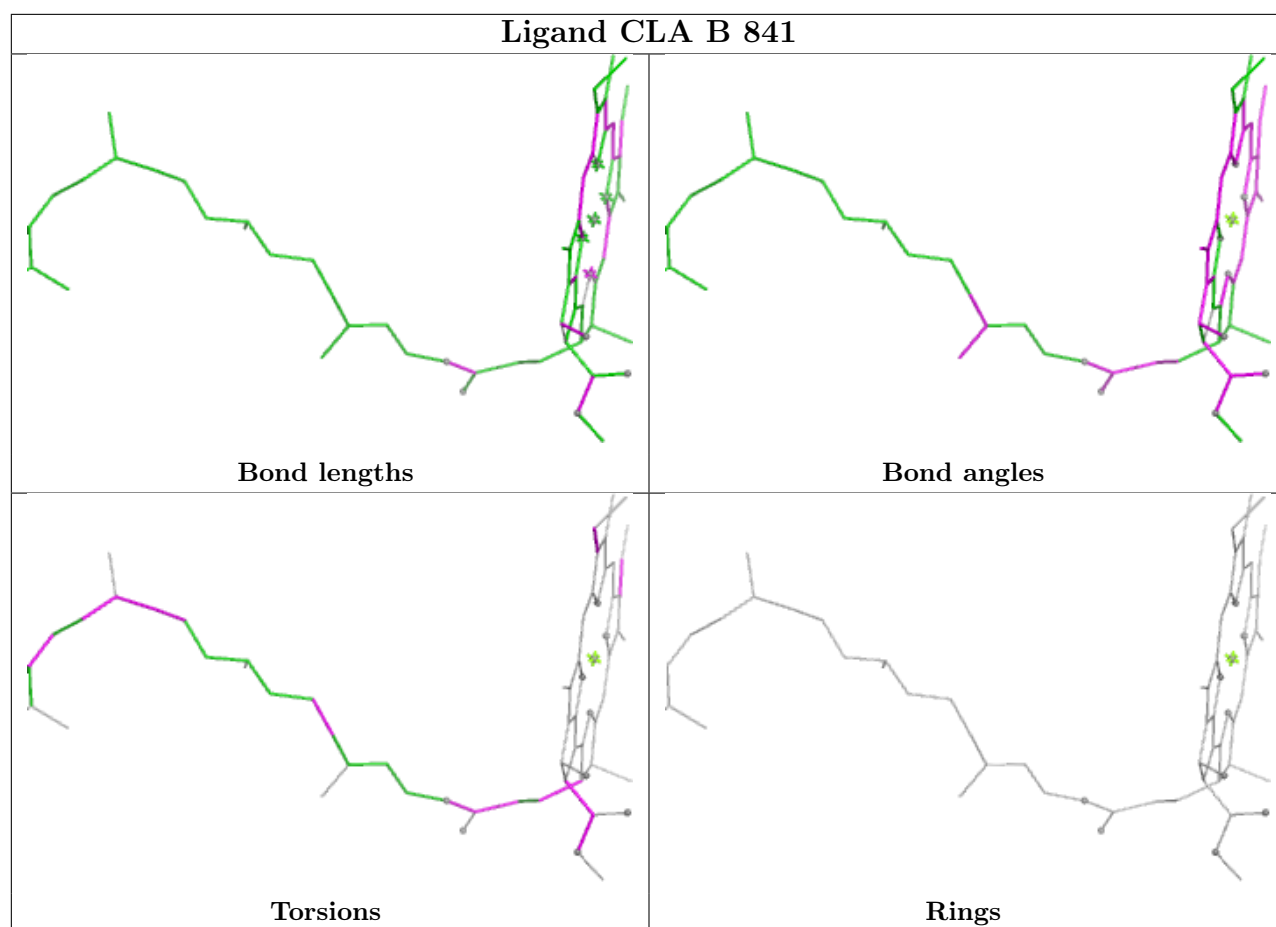


Ligand CLA R 108

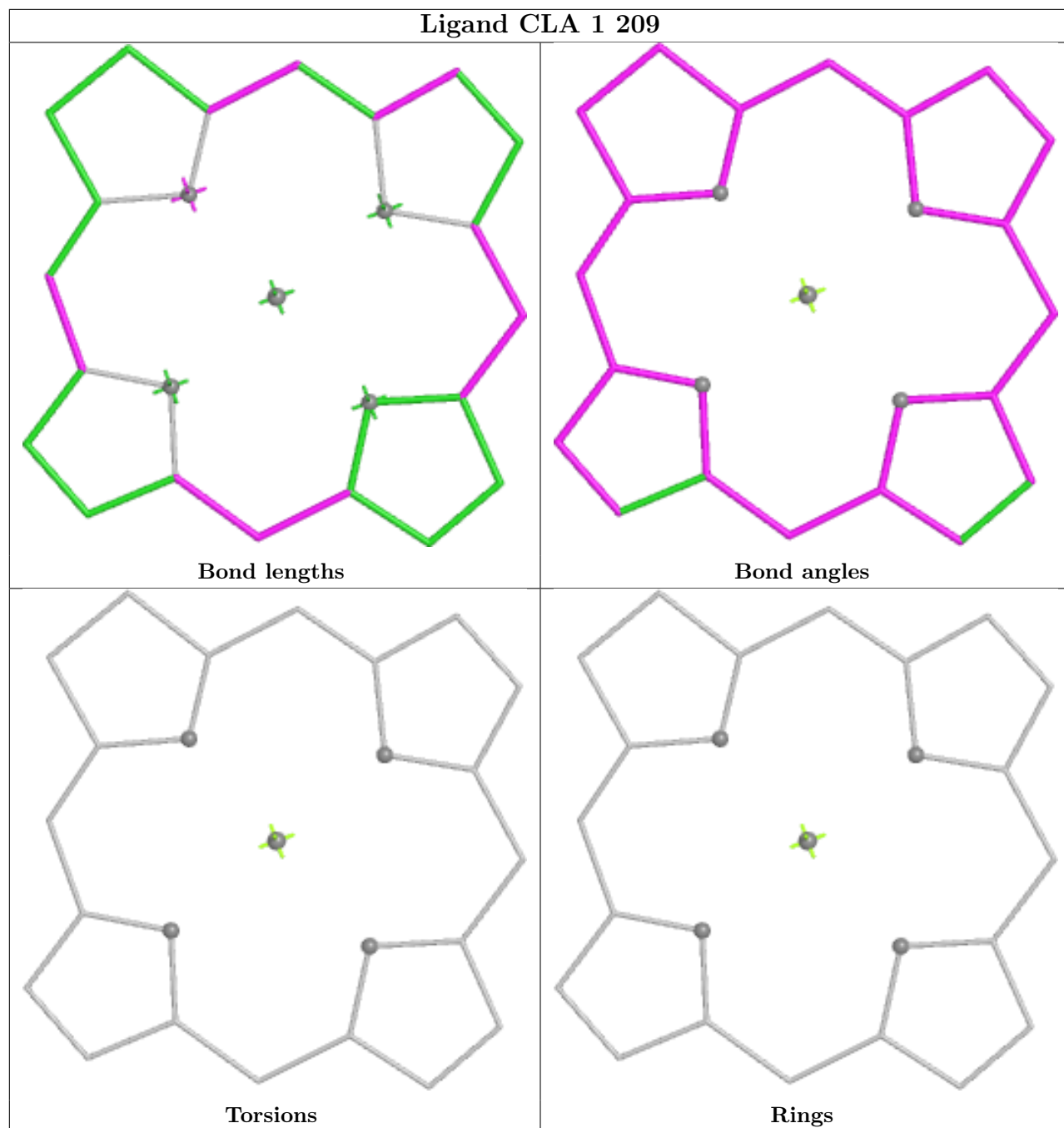


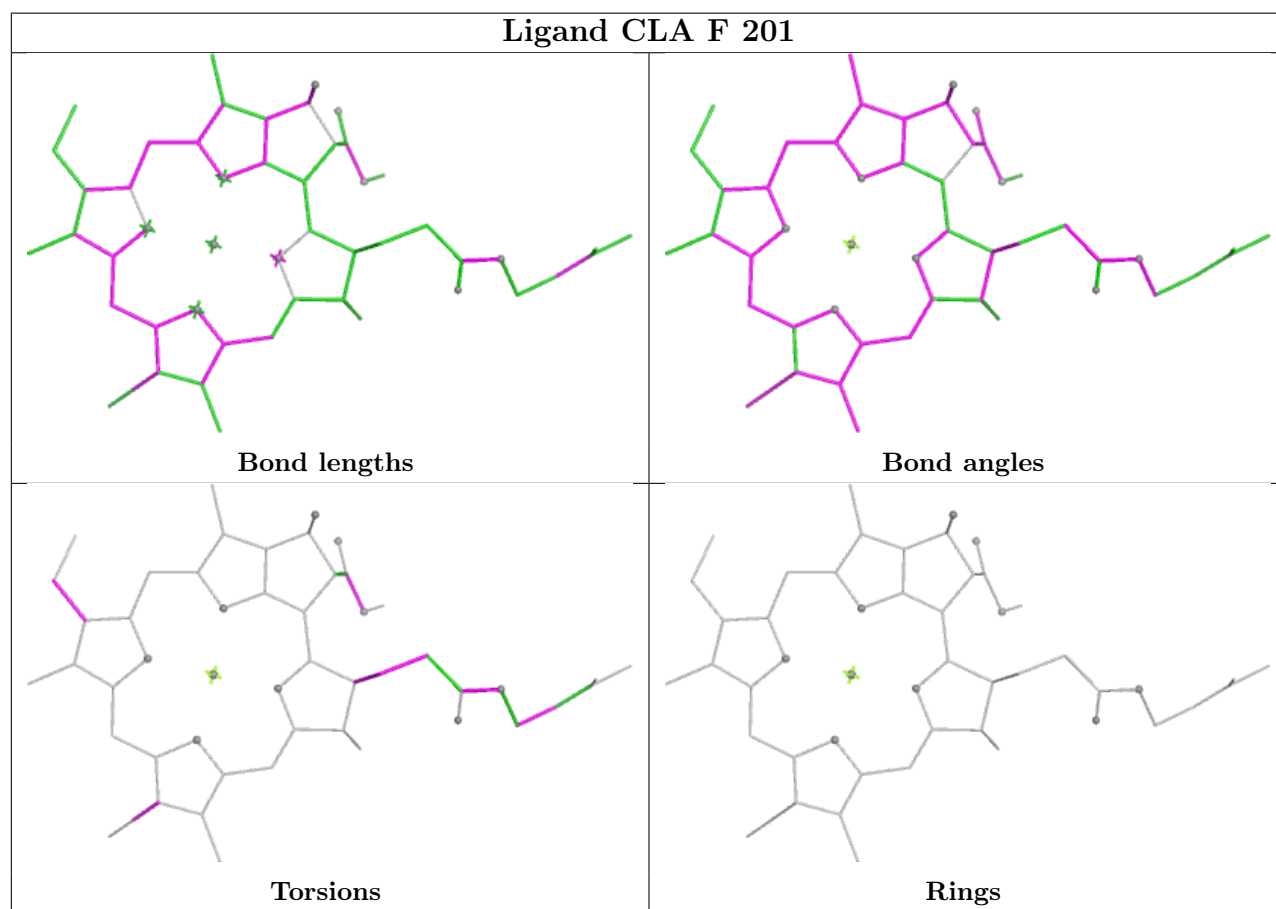
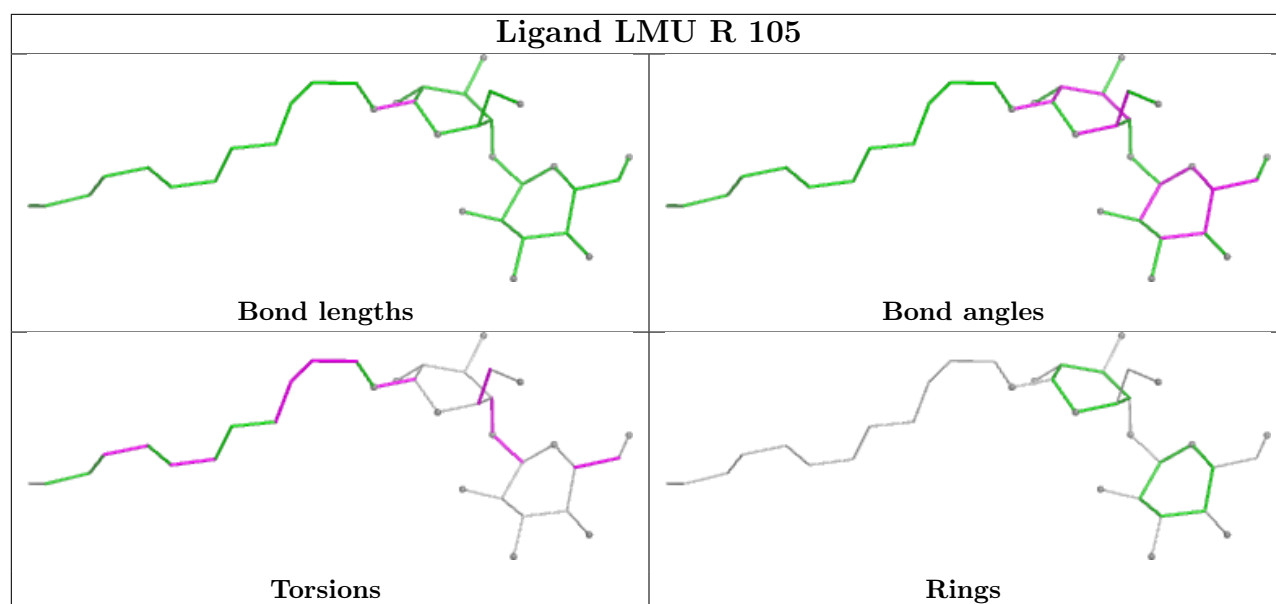
Ligand LMU R 102



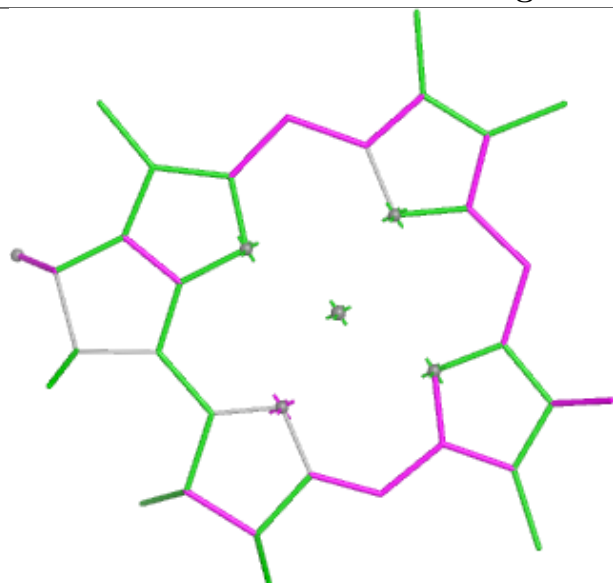


Ligand CLA 1 209

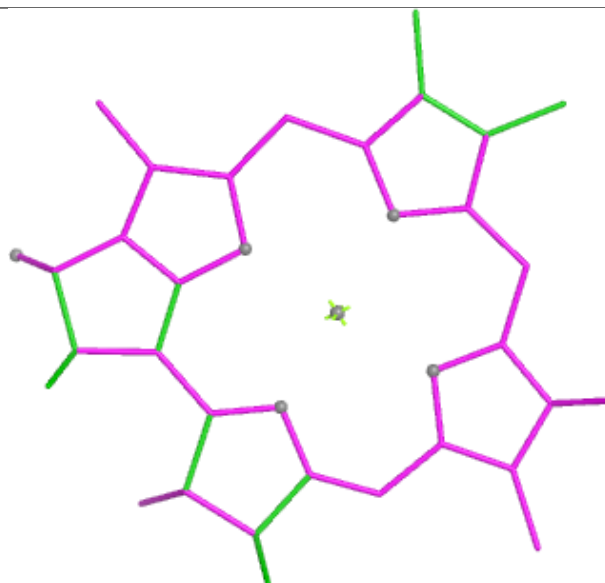




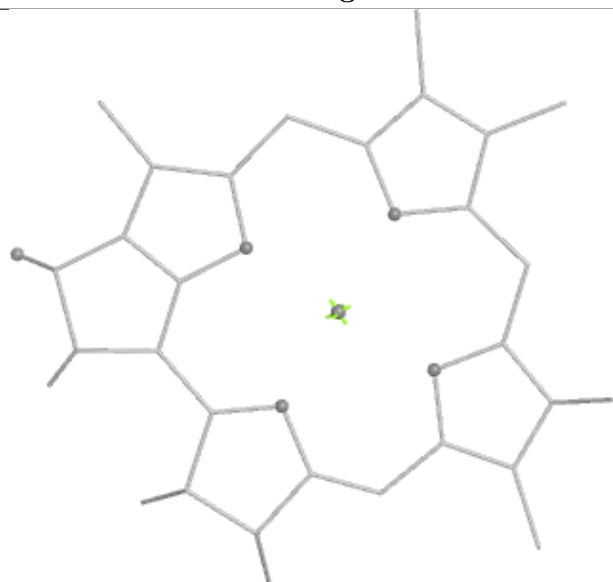
Ligand CLA F 205



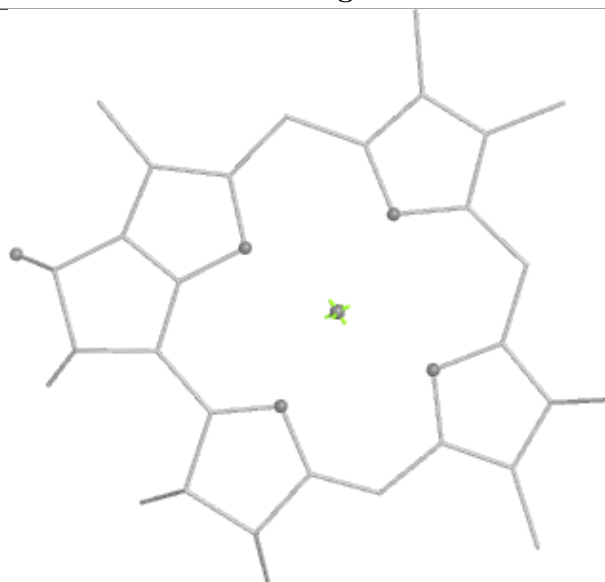
Bond lengths



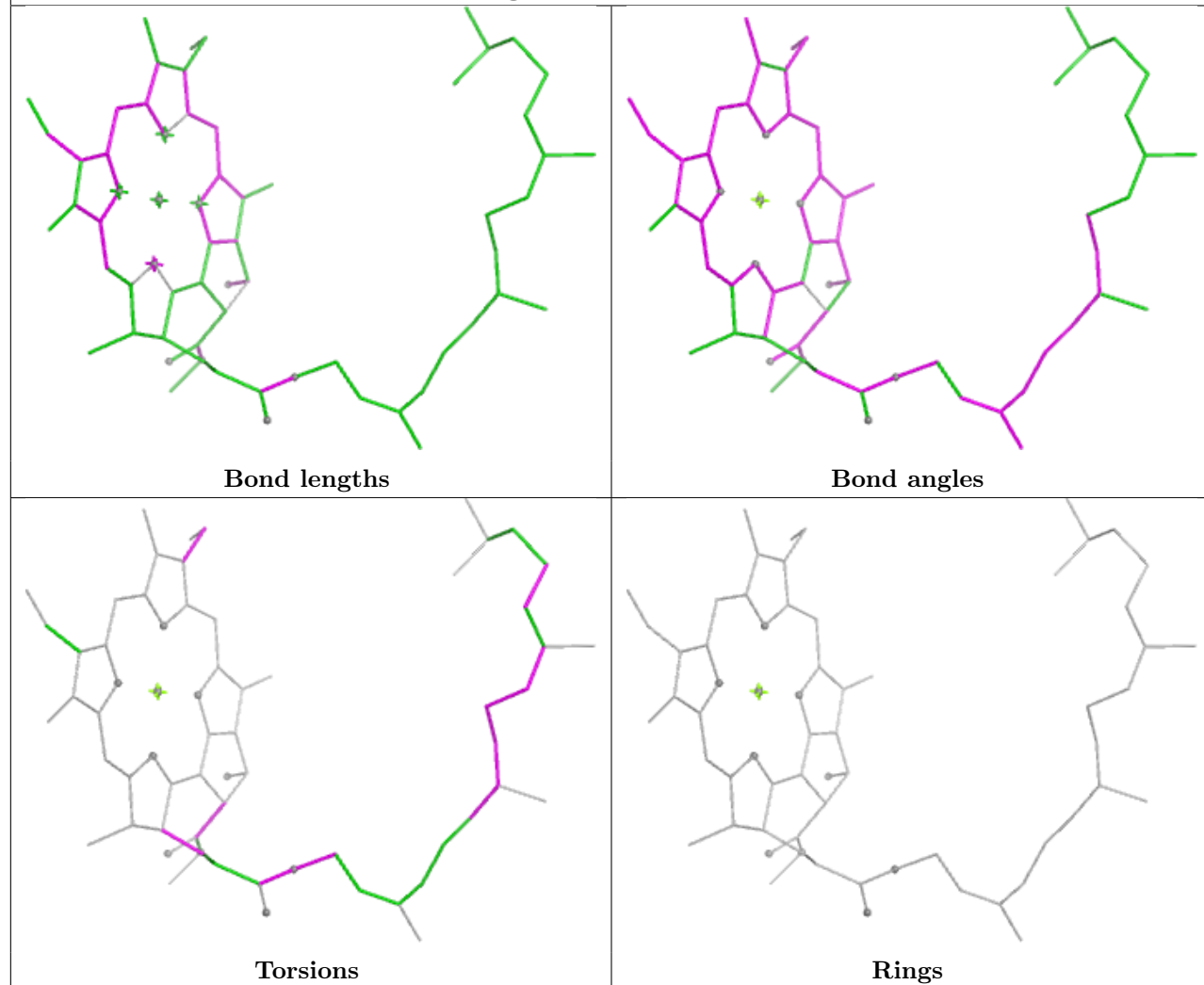
Bond angles

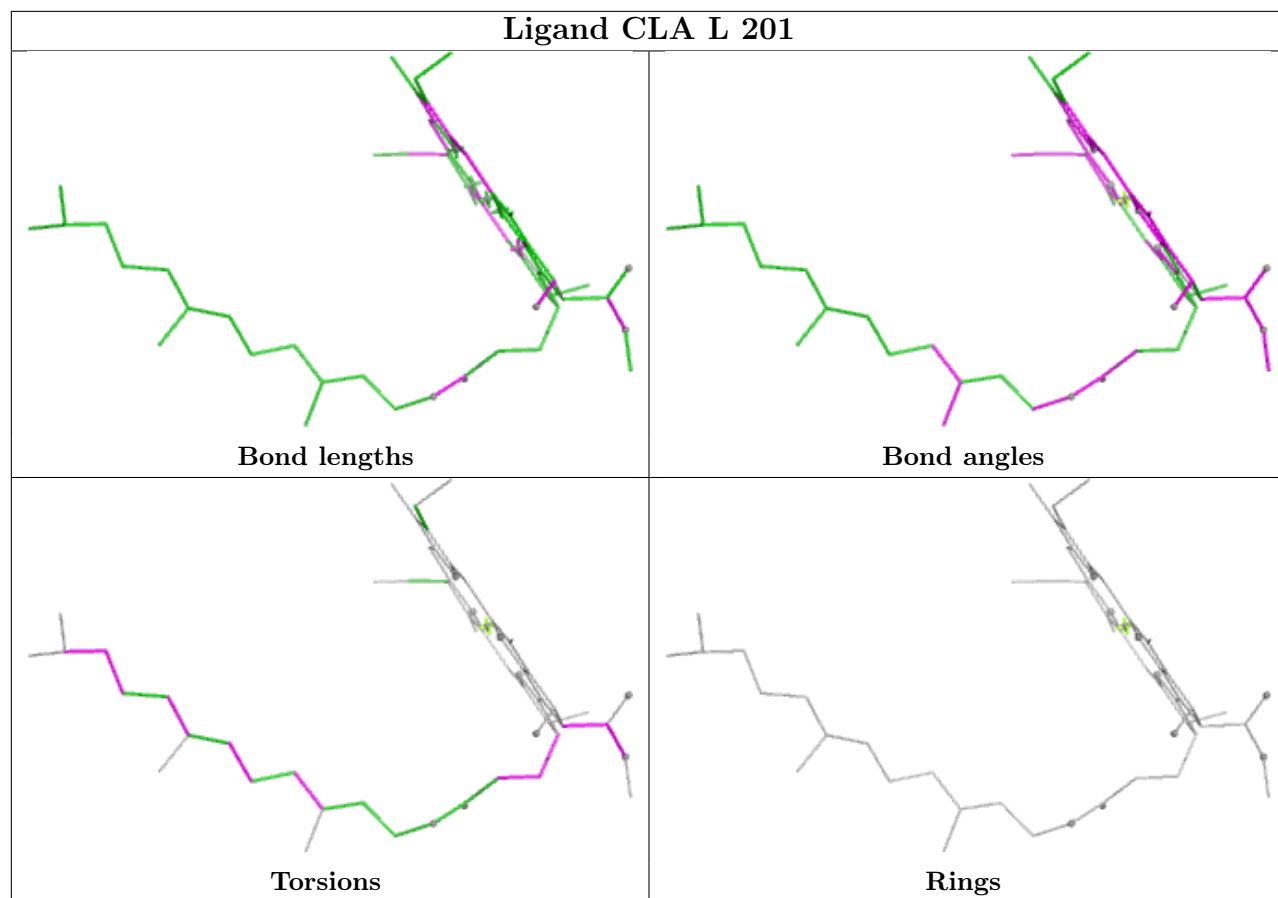


Torsions

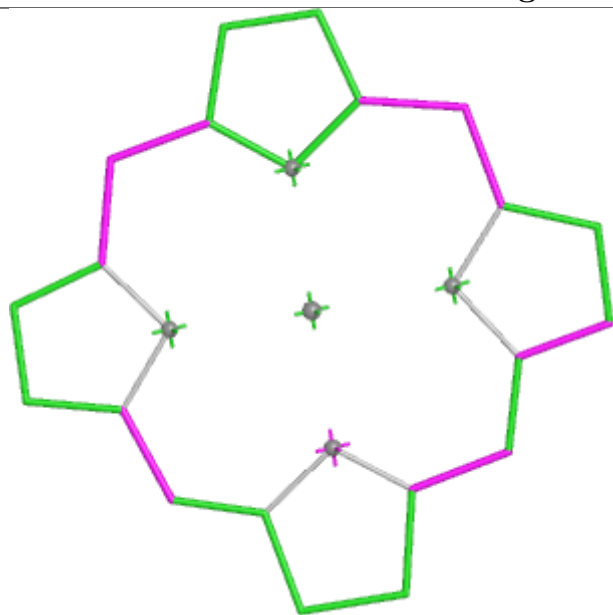


Rings

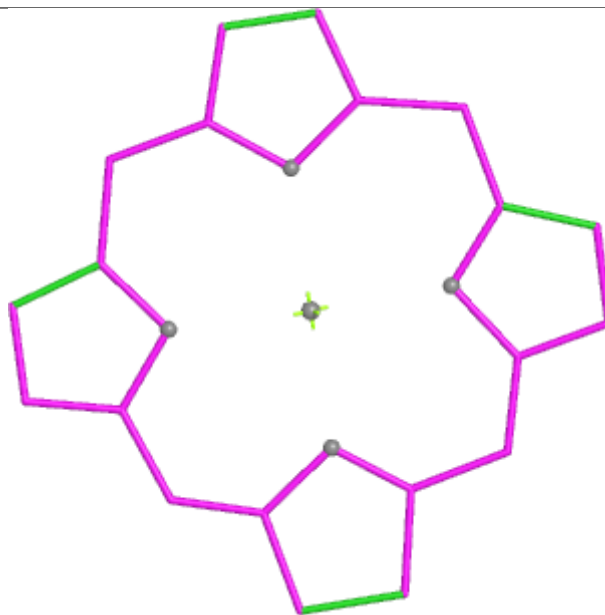
Ligand CLA 3 310



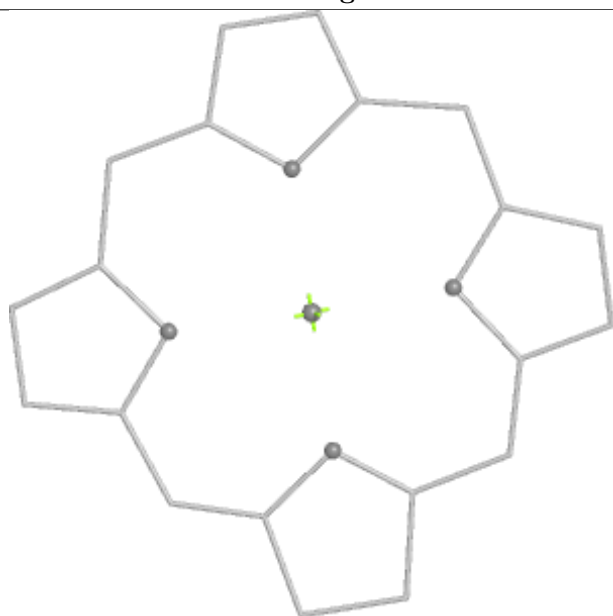
Ligand CLA 4 309



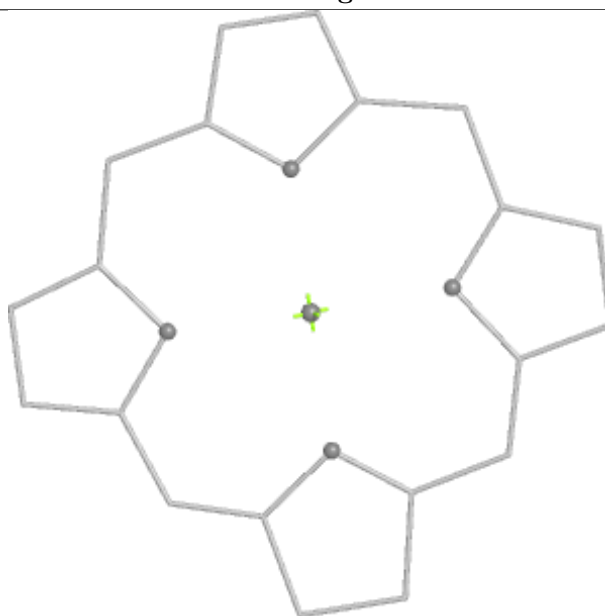
Bond lengths



Bond angles

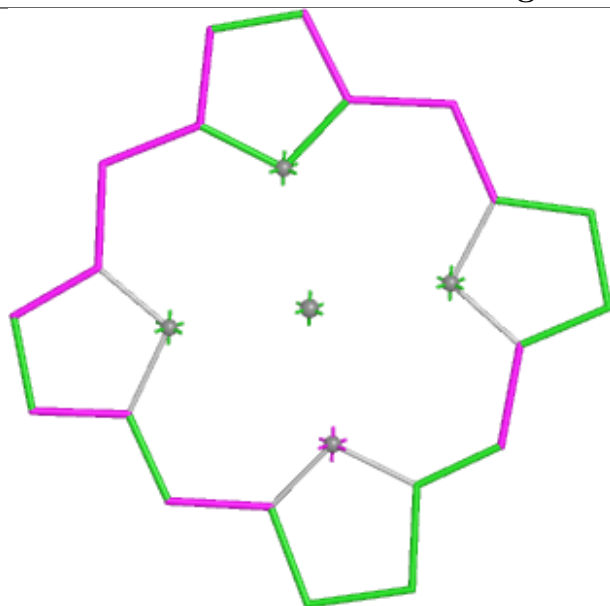


Torsions

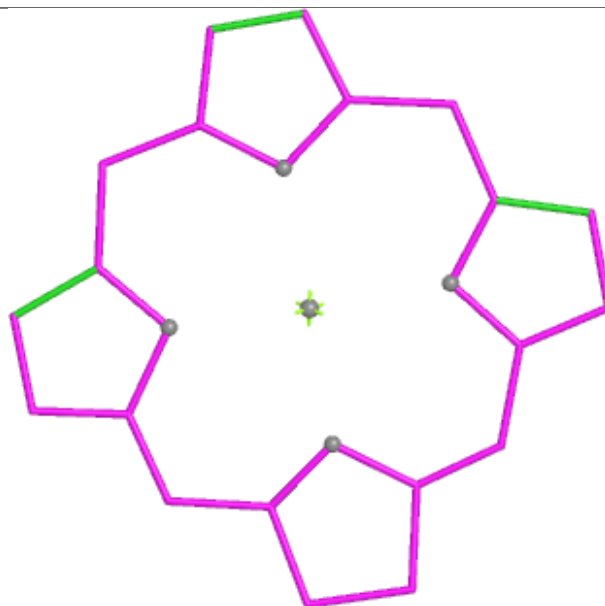


Rings

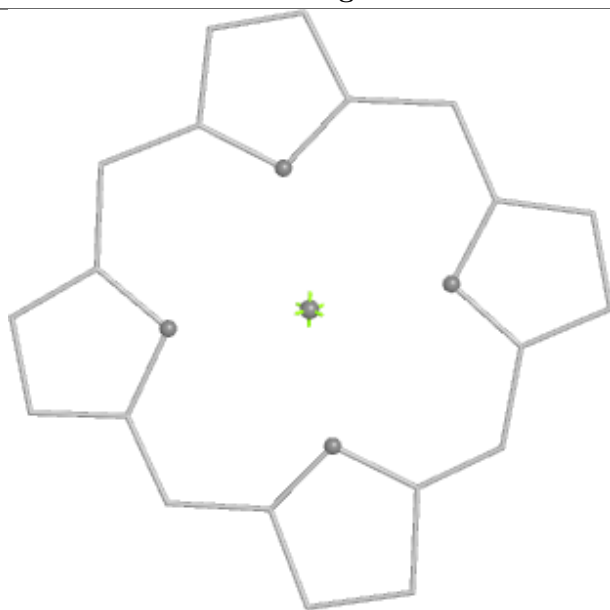
Ligand CLA 3 316



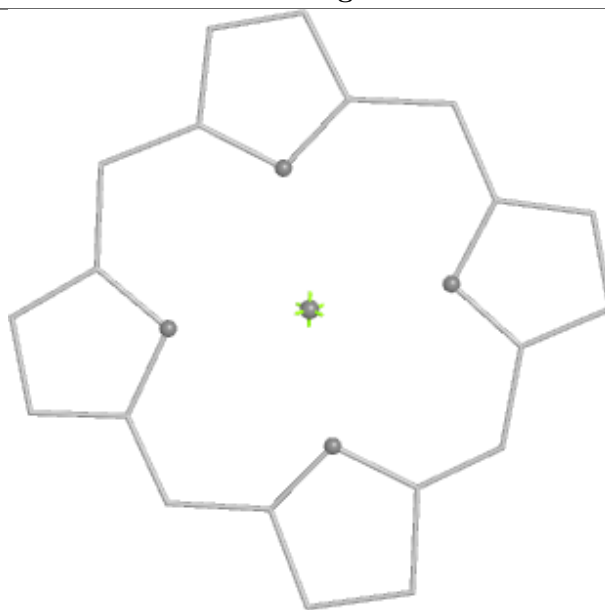
Bond lengths



Bond angles

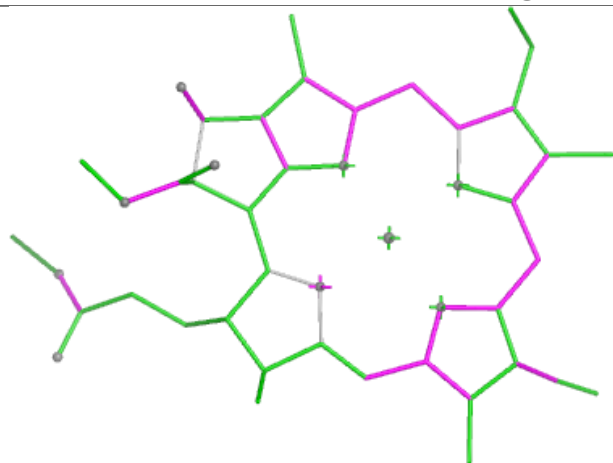


Torsions

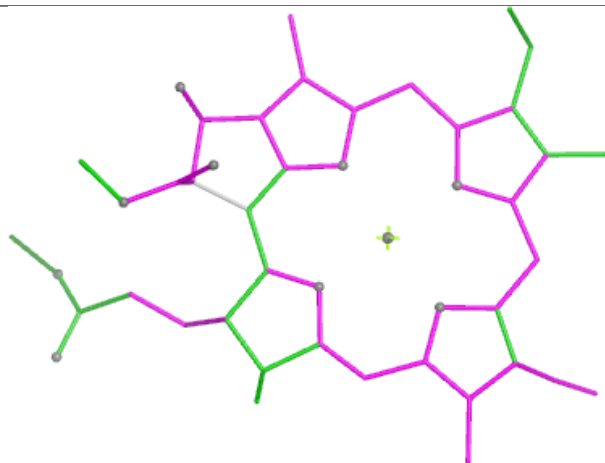


Rings

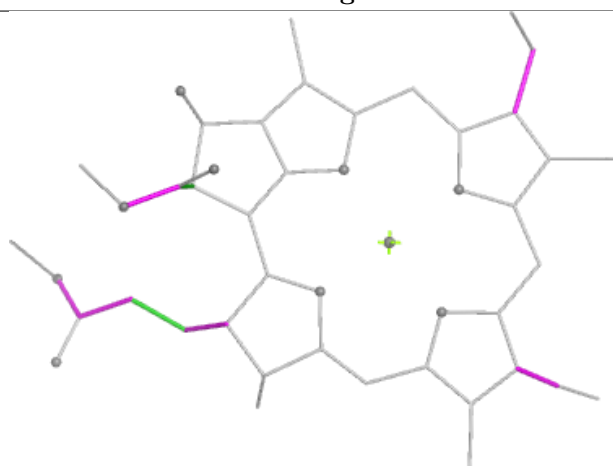
Ligand CLA 4 315



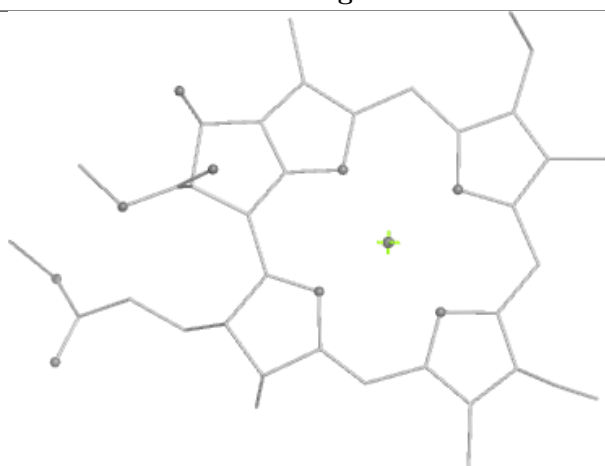
Bond lengths



Bond angles

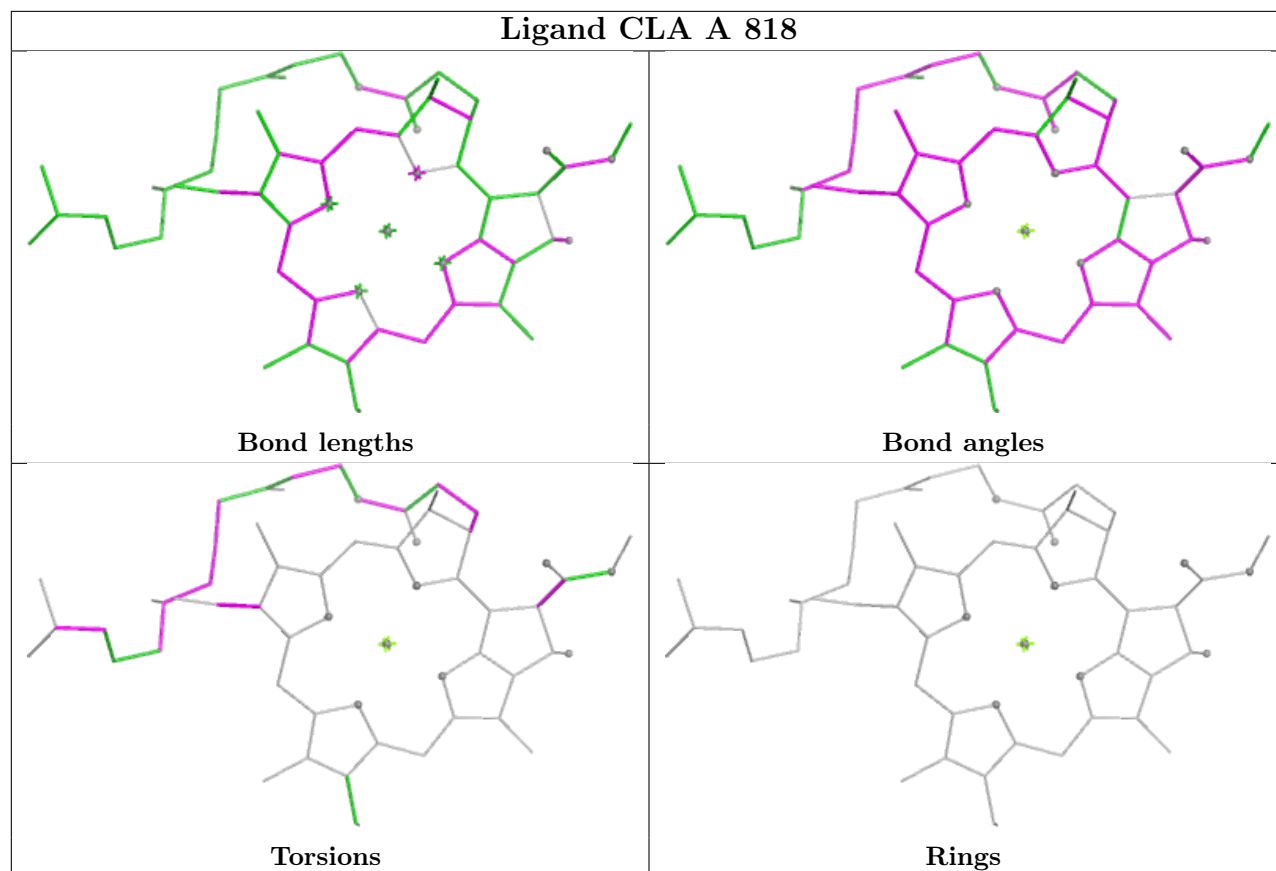


Torsions

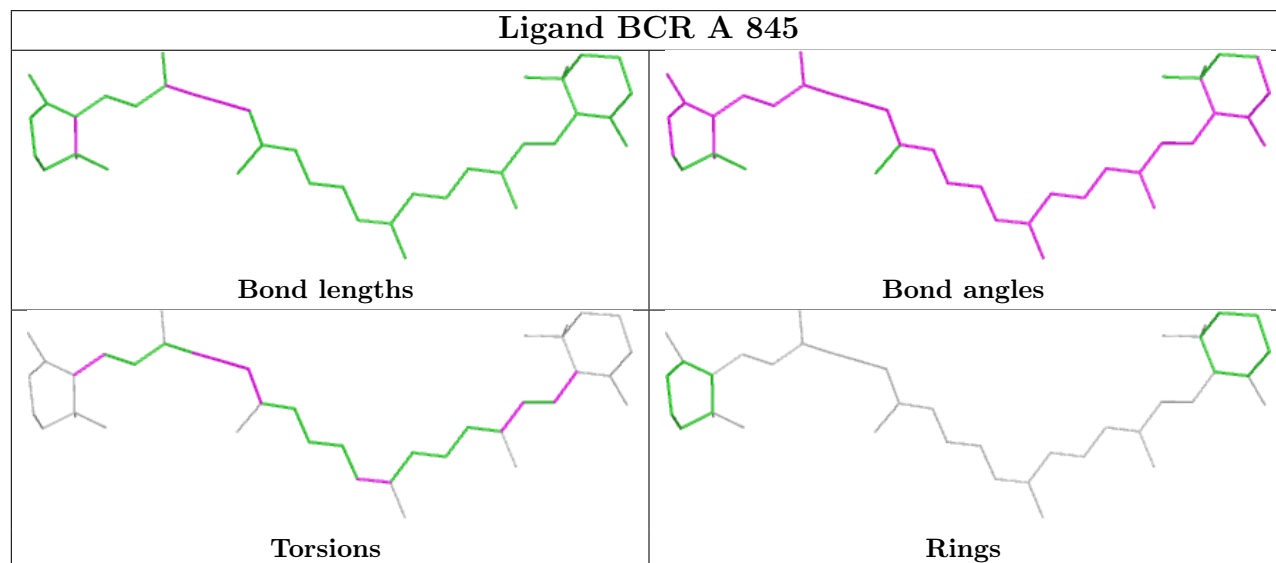


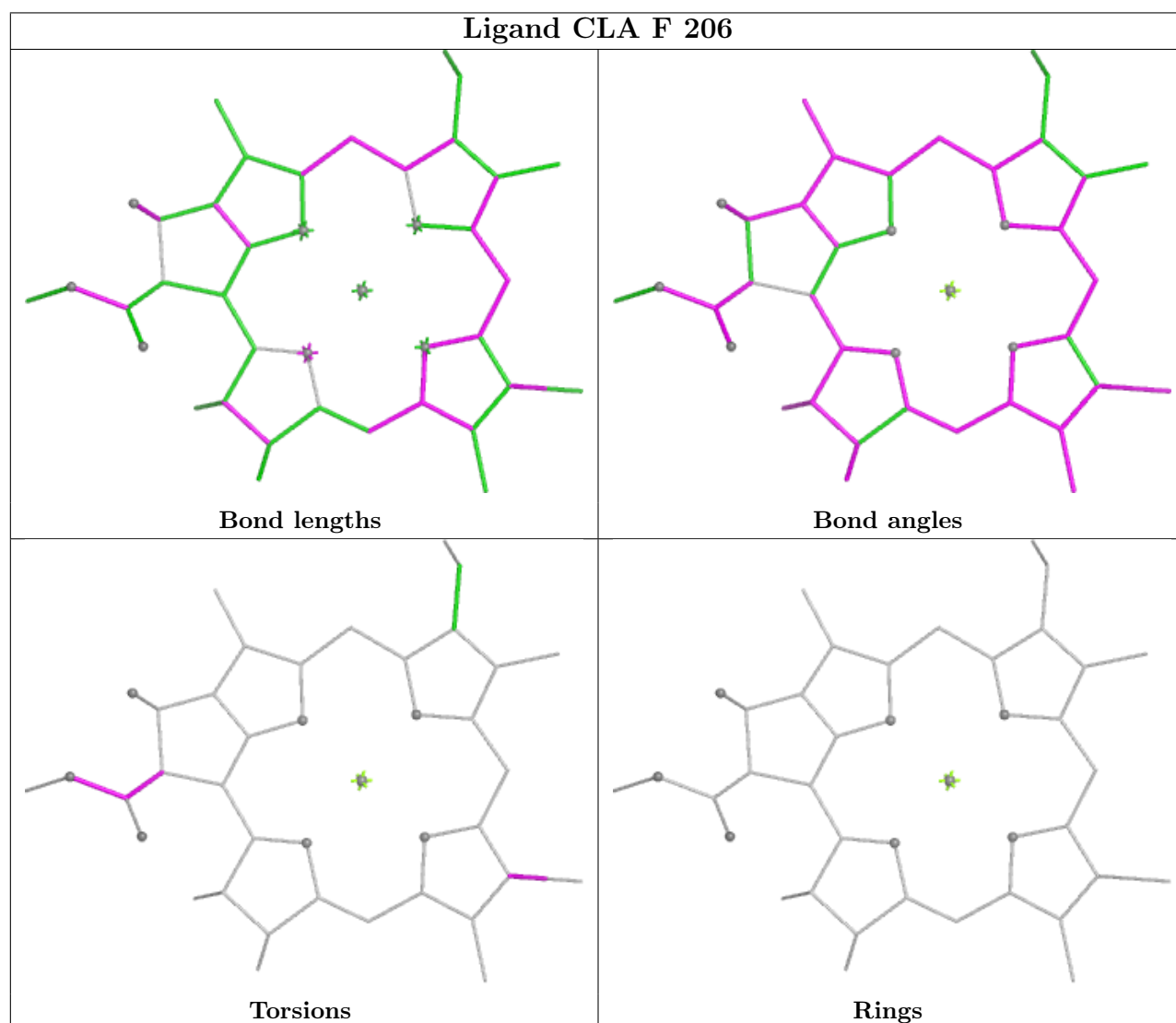
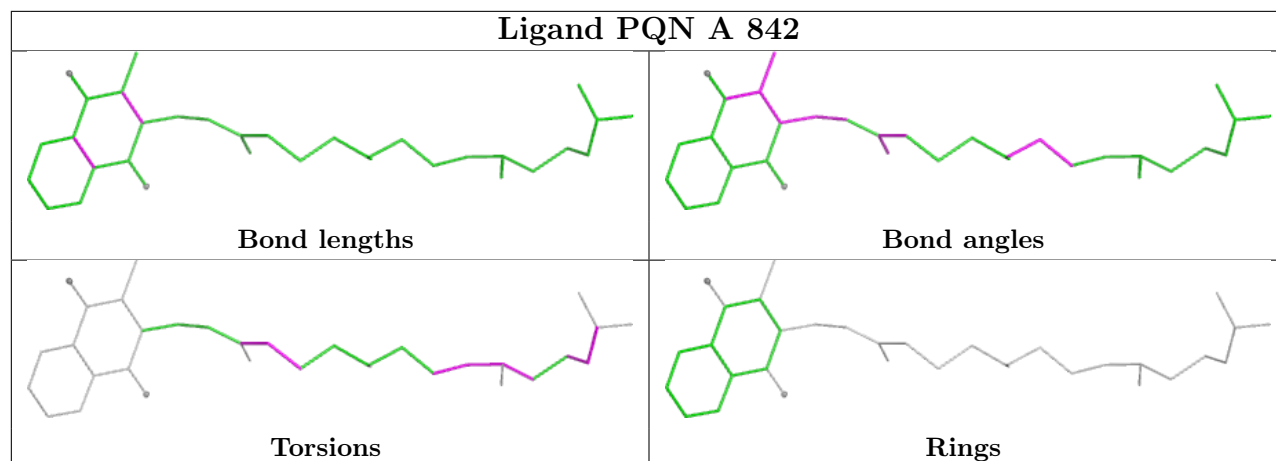
Rings

Ligand CLA A 818

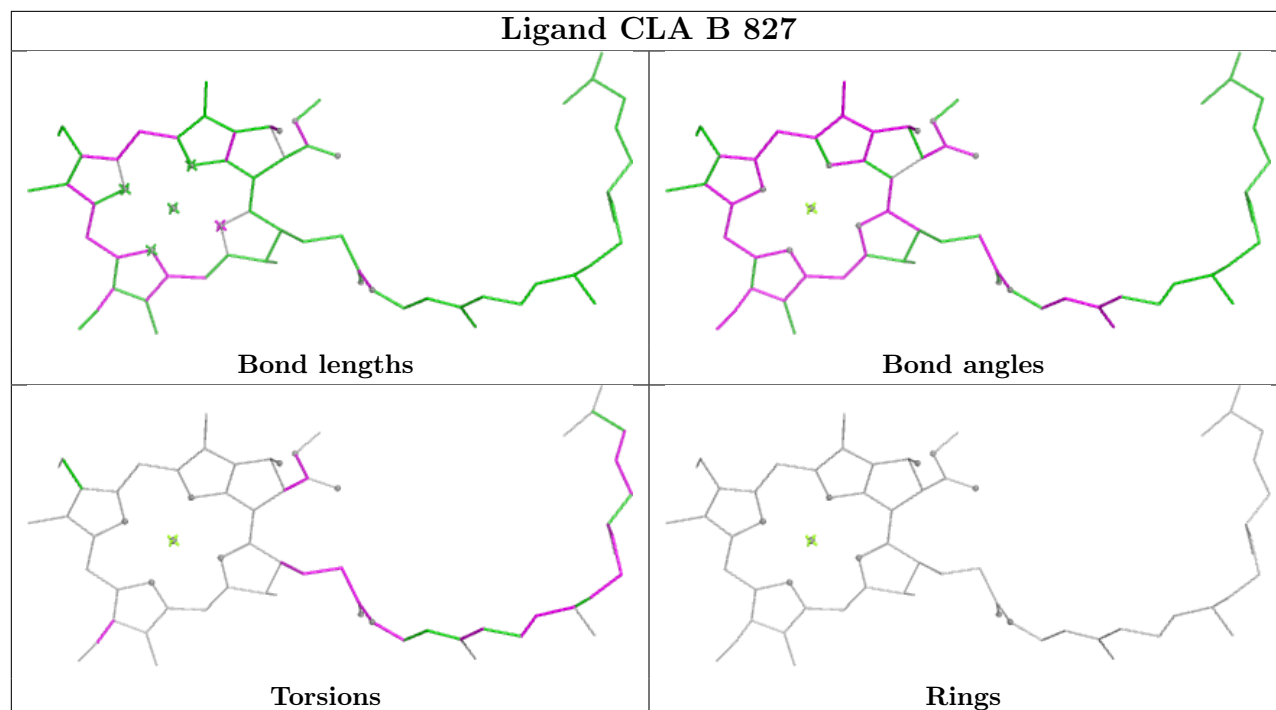


Ligand BCR A 845

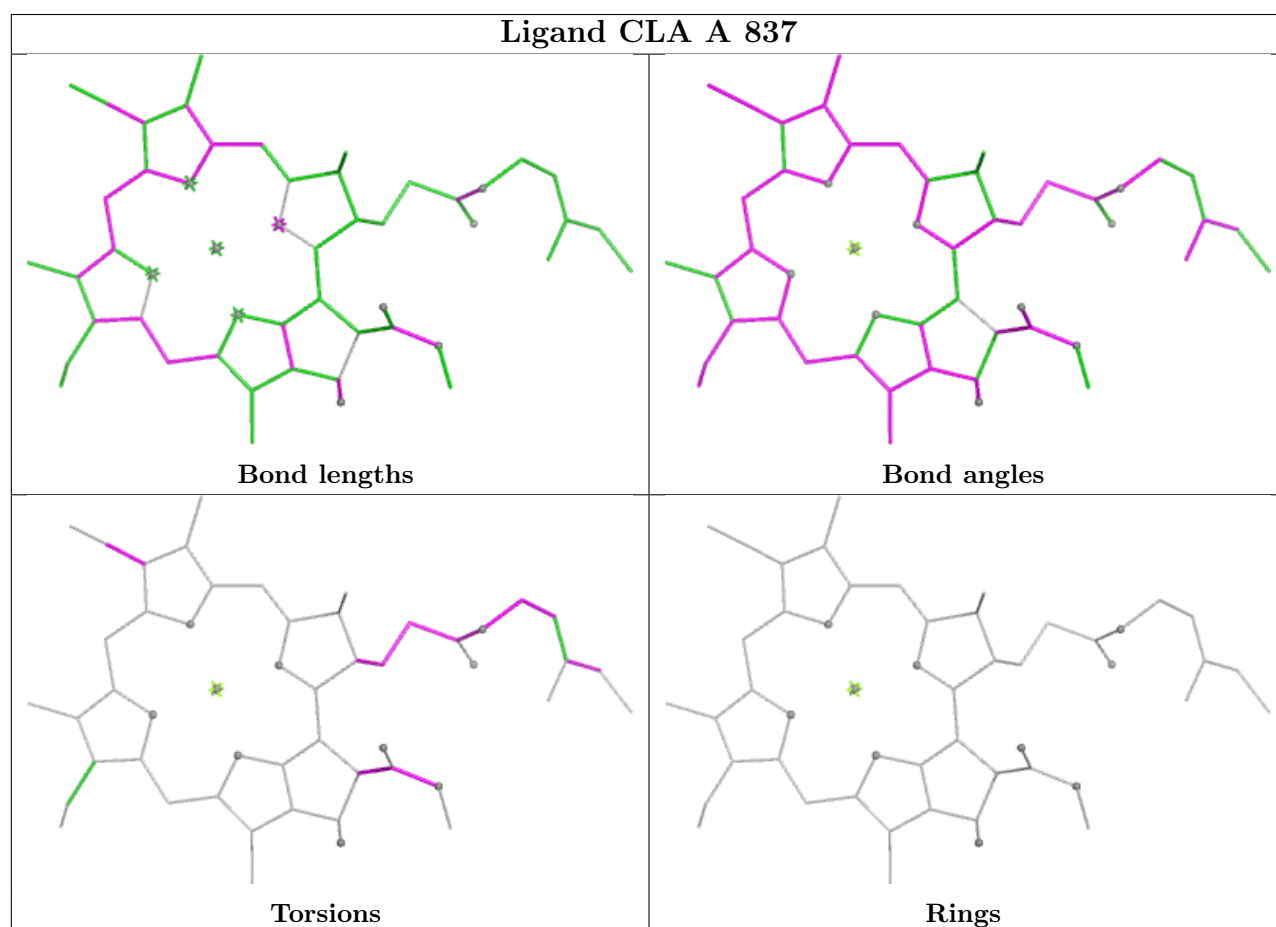


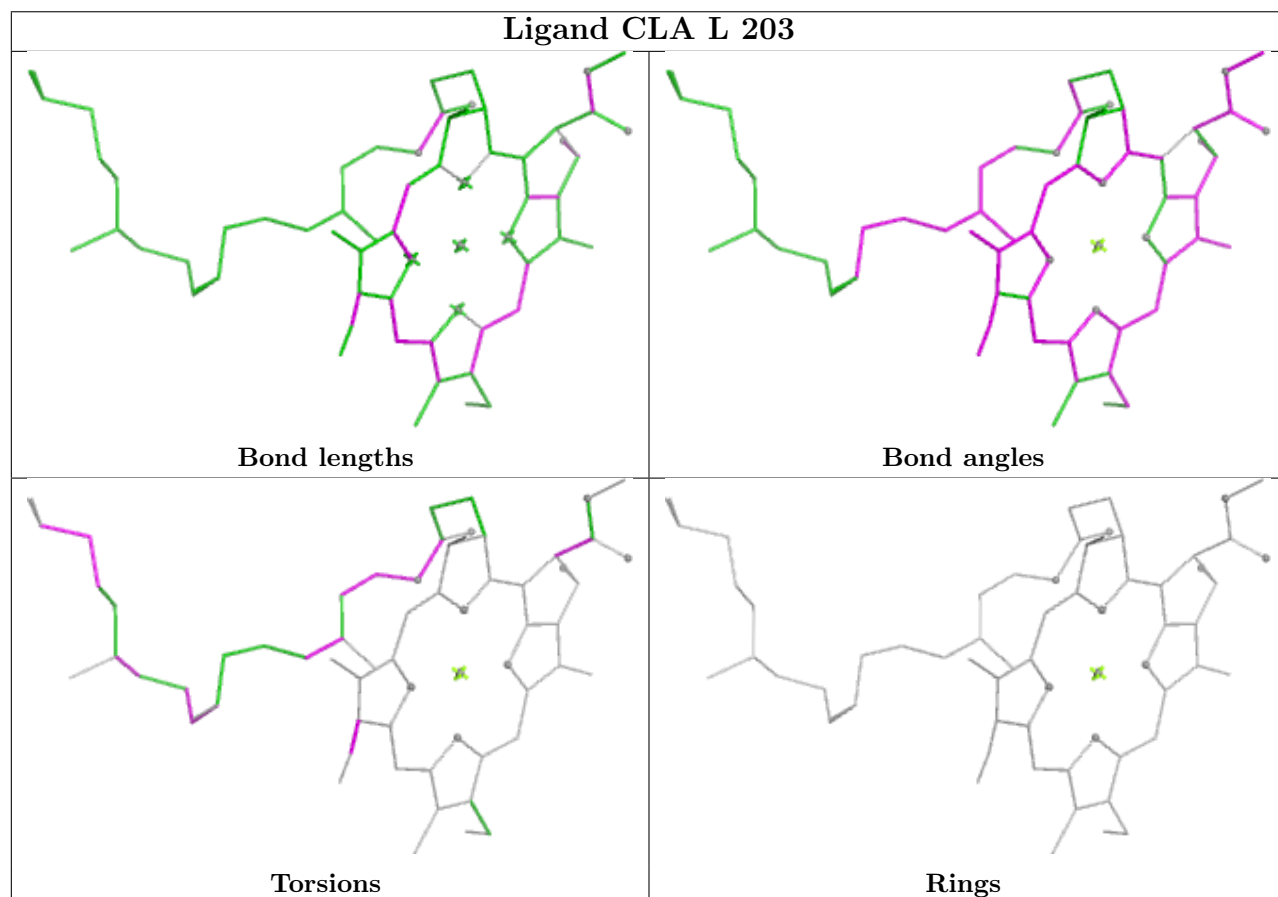
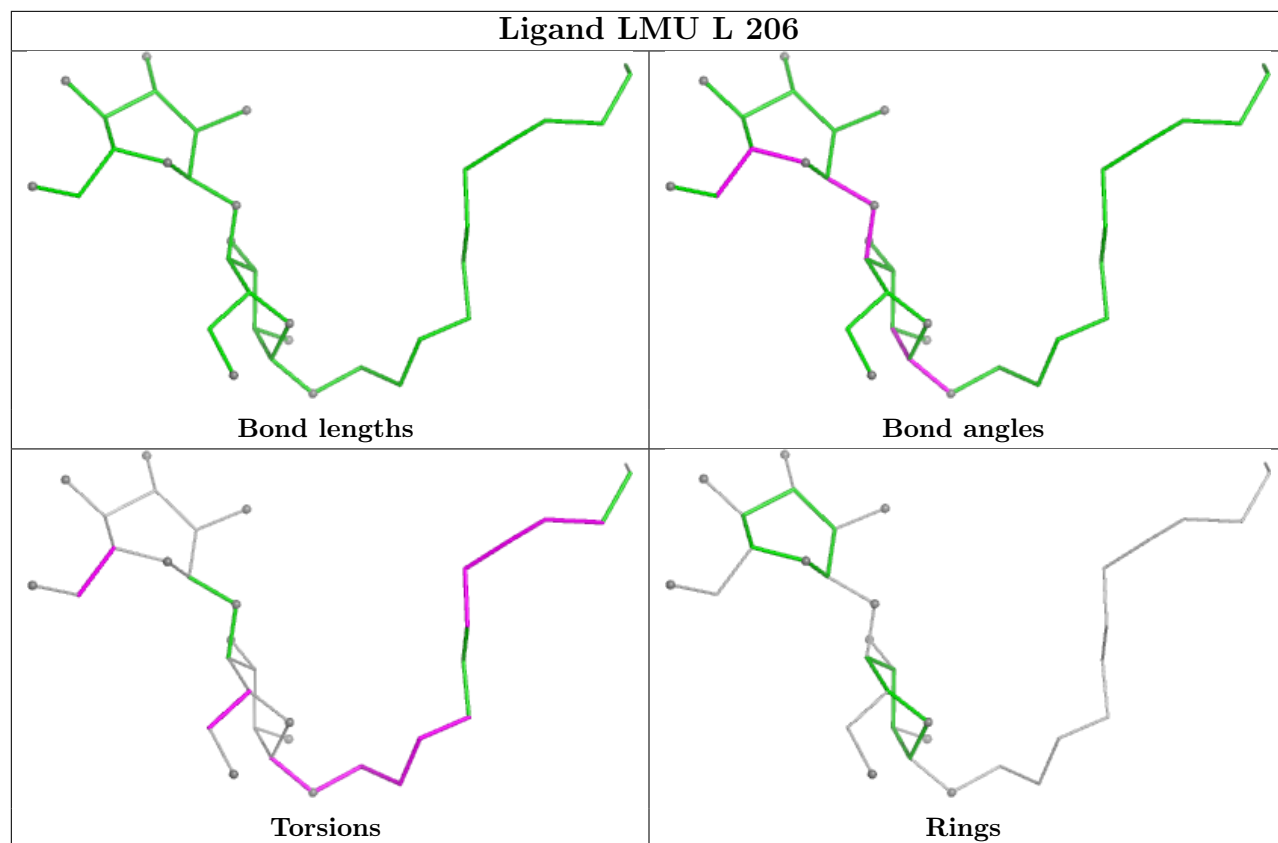


Ligand CLA B 827

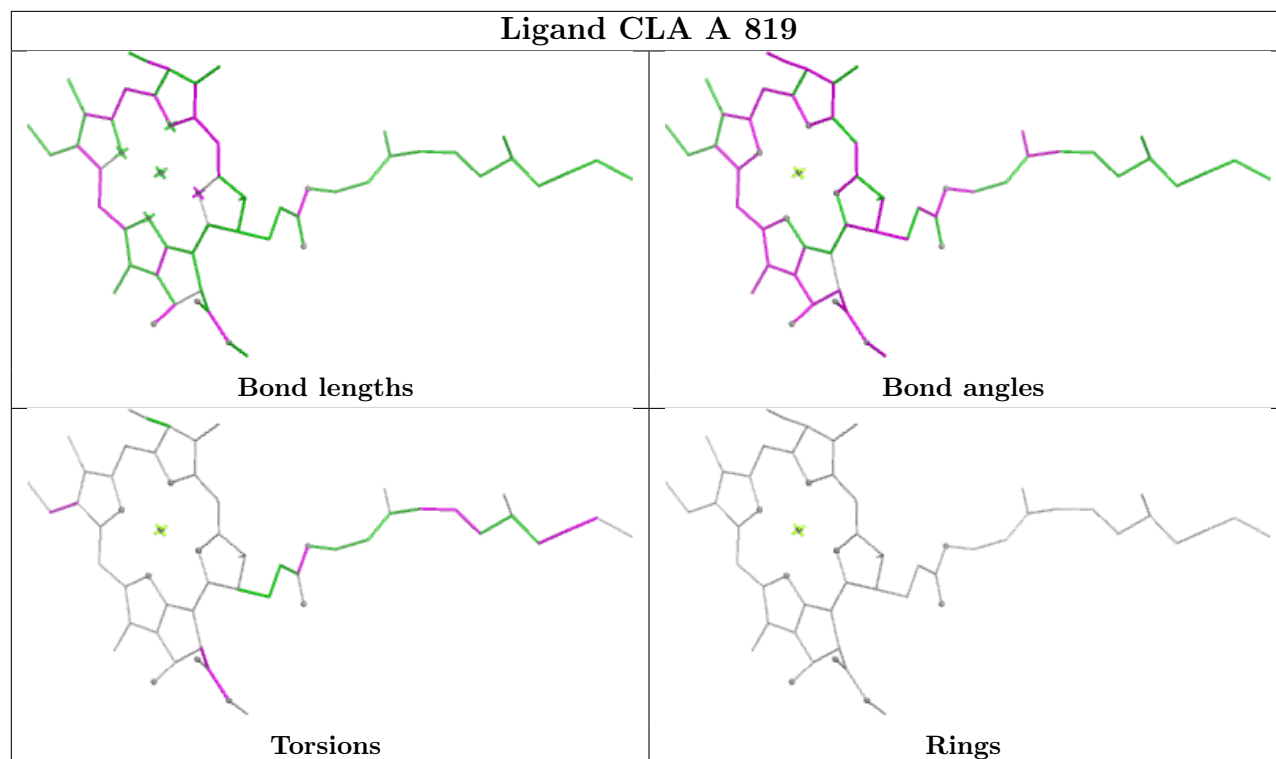


Ligand CLA A 837

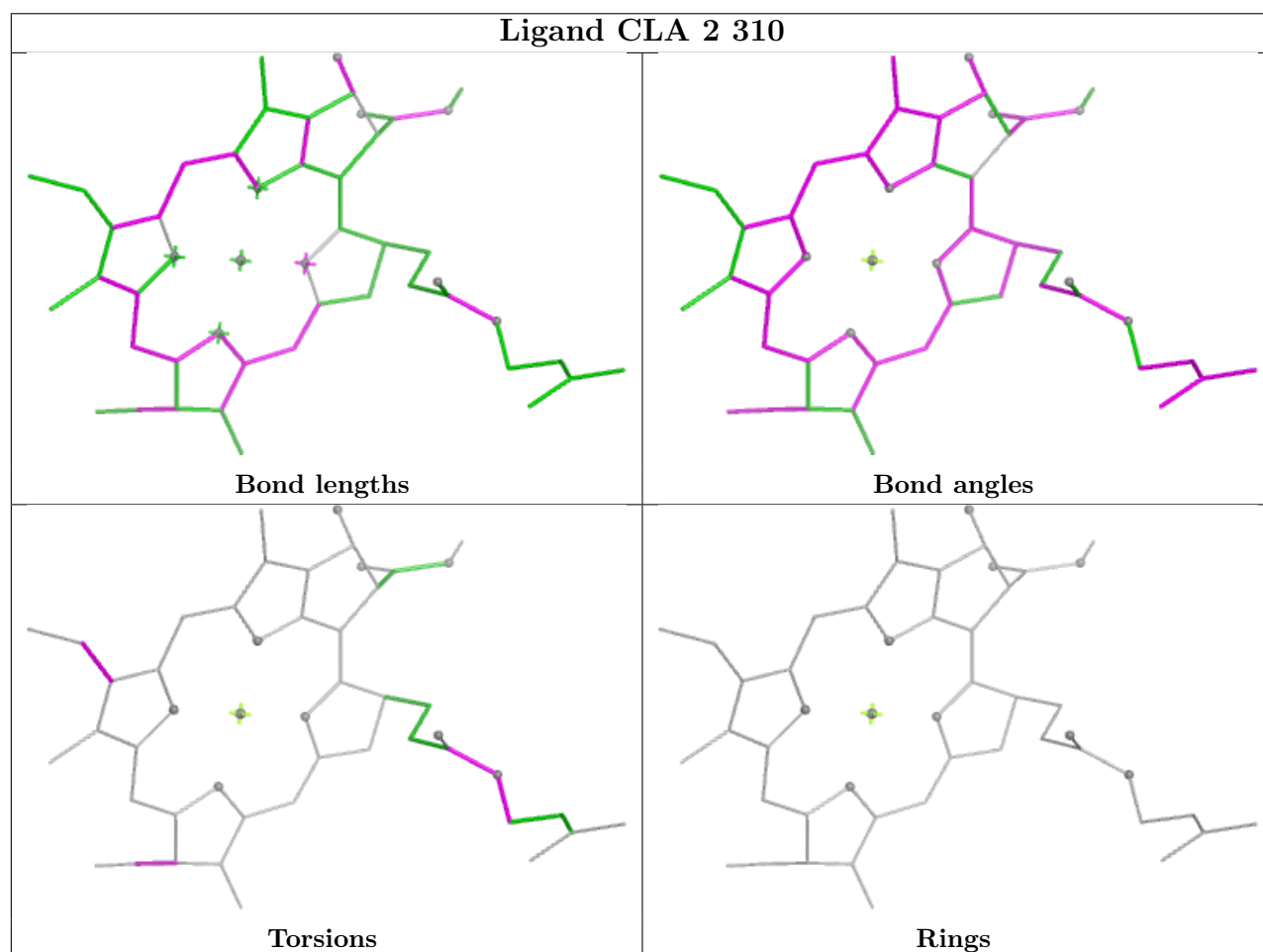




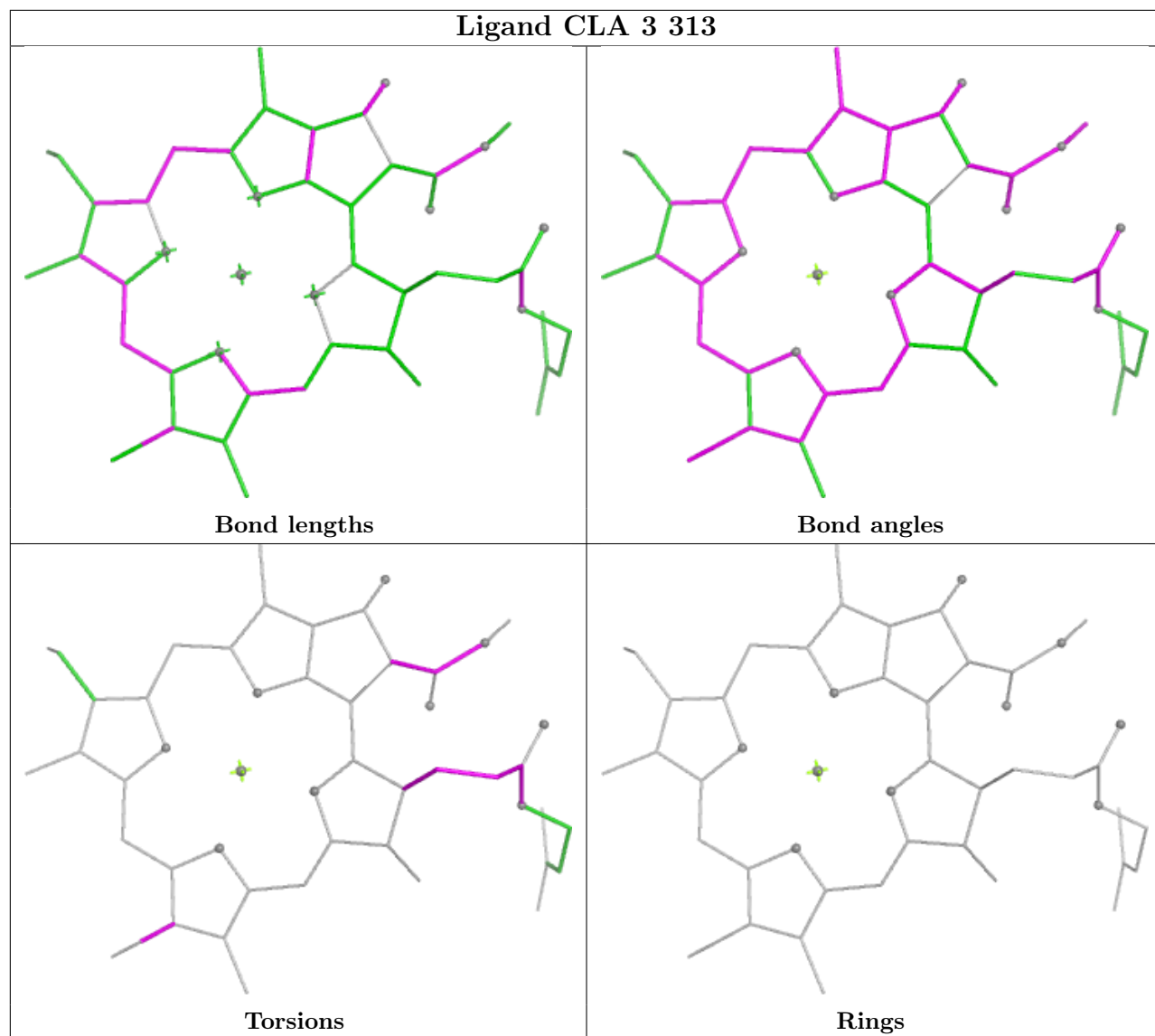
Ligand CLA A 819

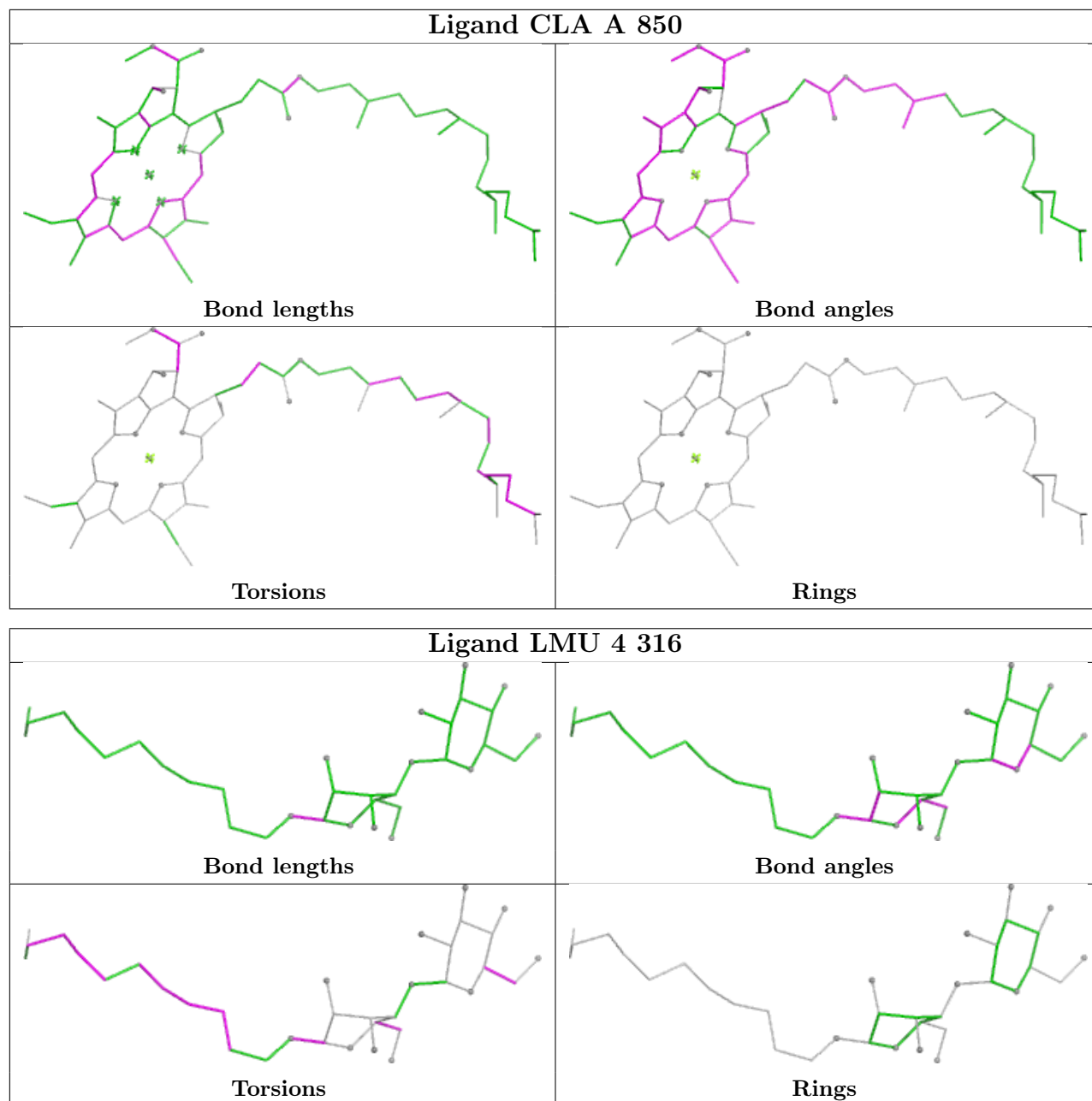


Ligand CLA 2 310

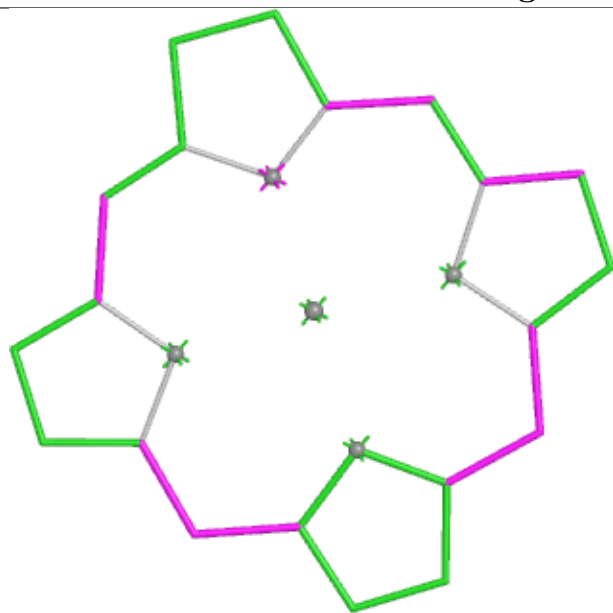


Ligand CLA 3 313

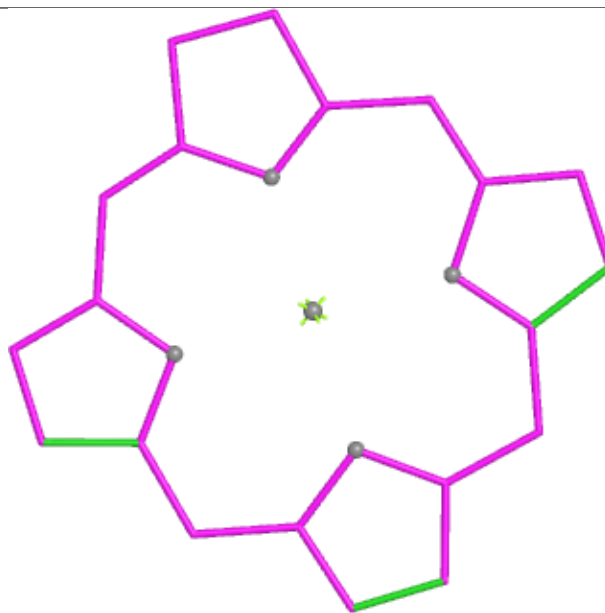




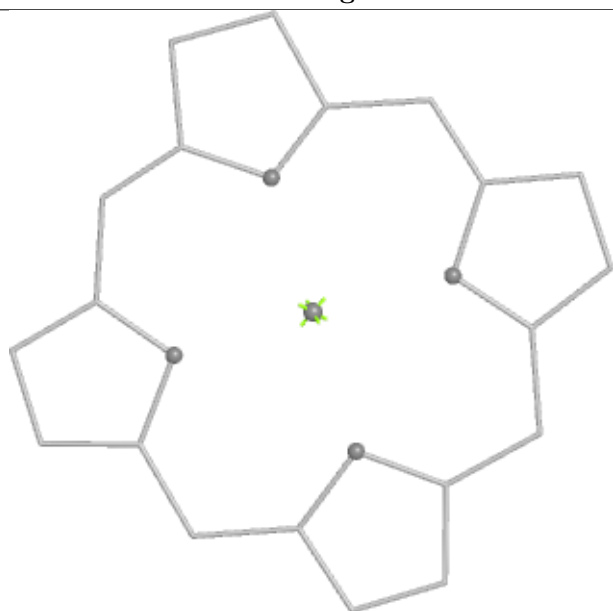
Ligand CLA 1 212



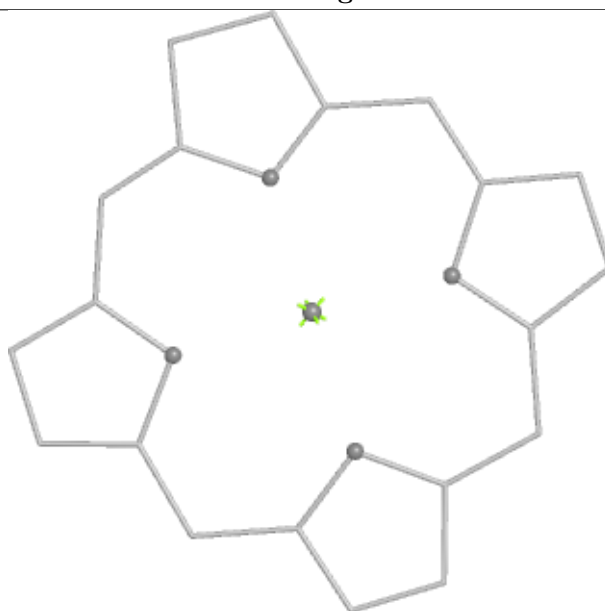
Bond lengths



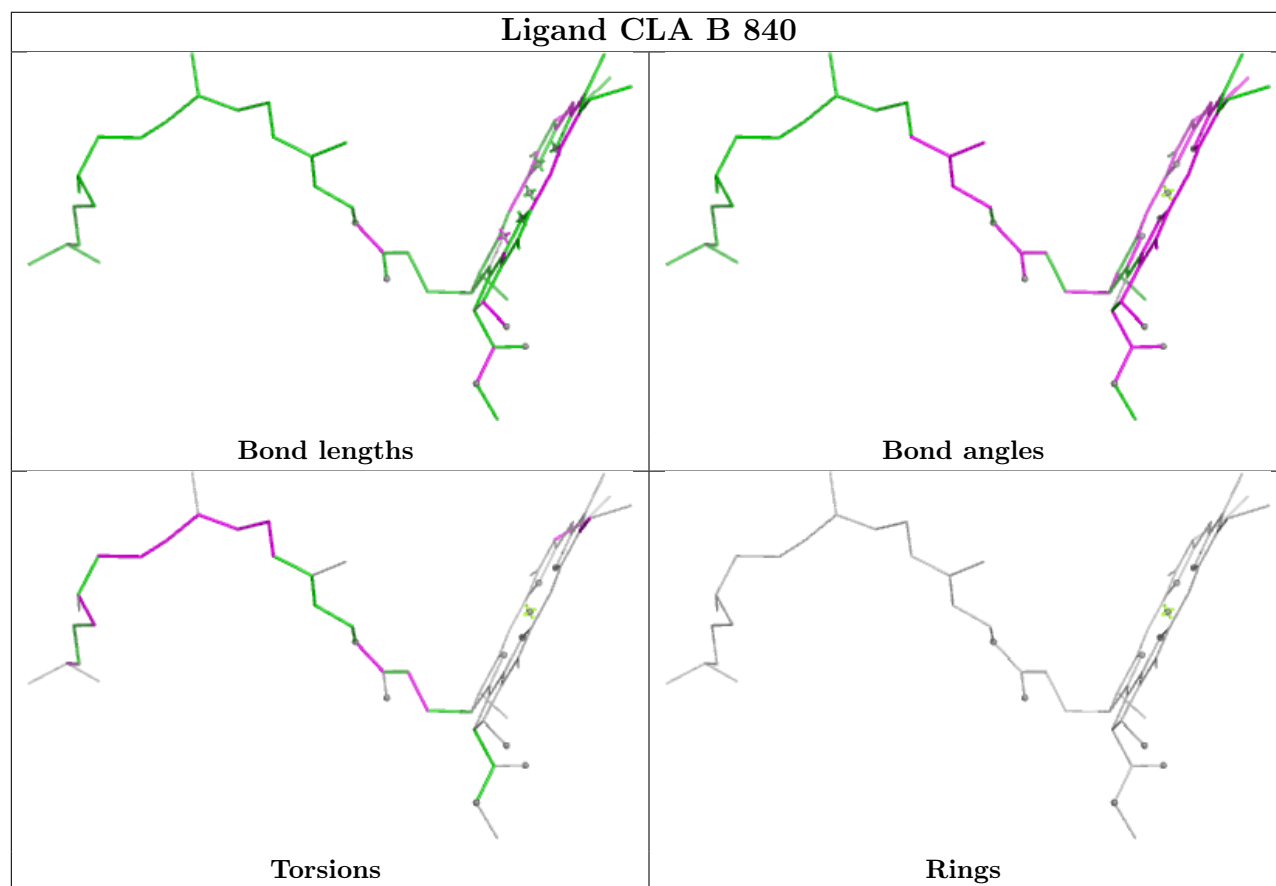
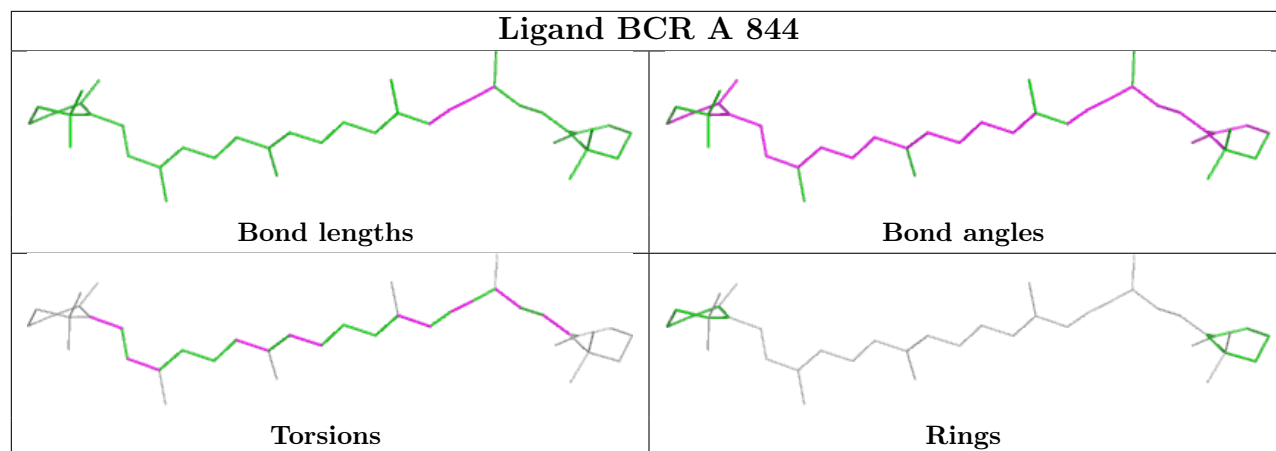
Bond angles



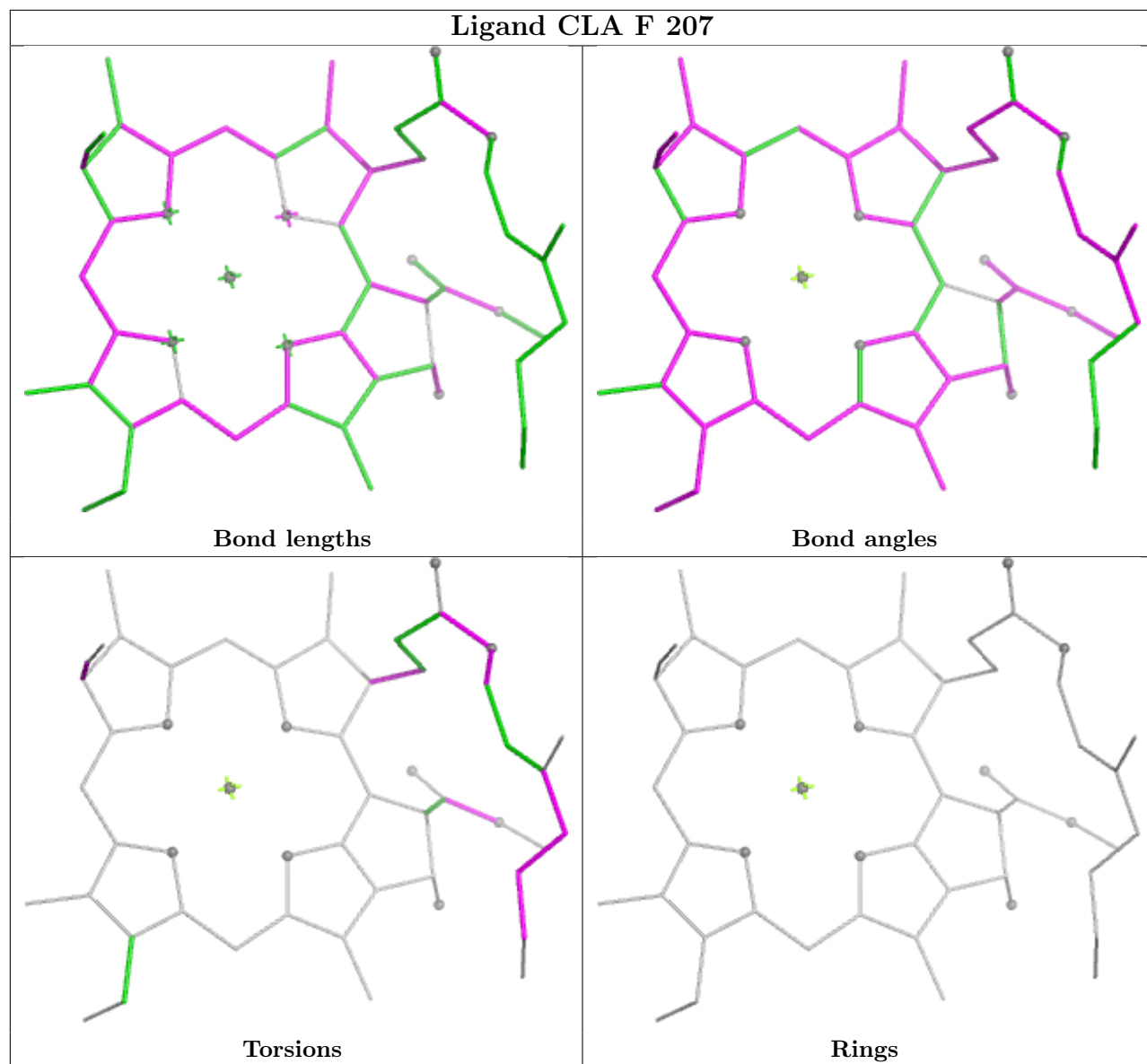
Torsions



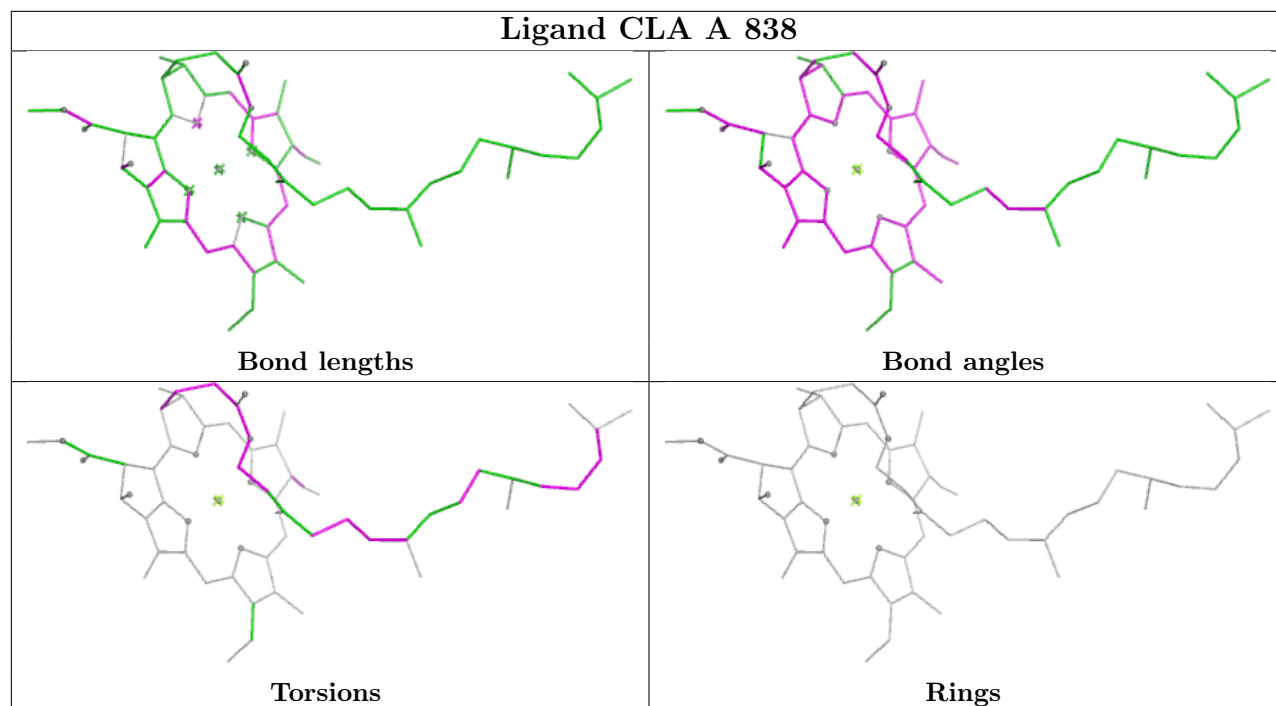
Rings



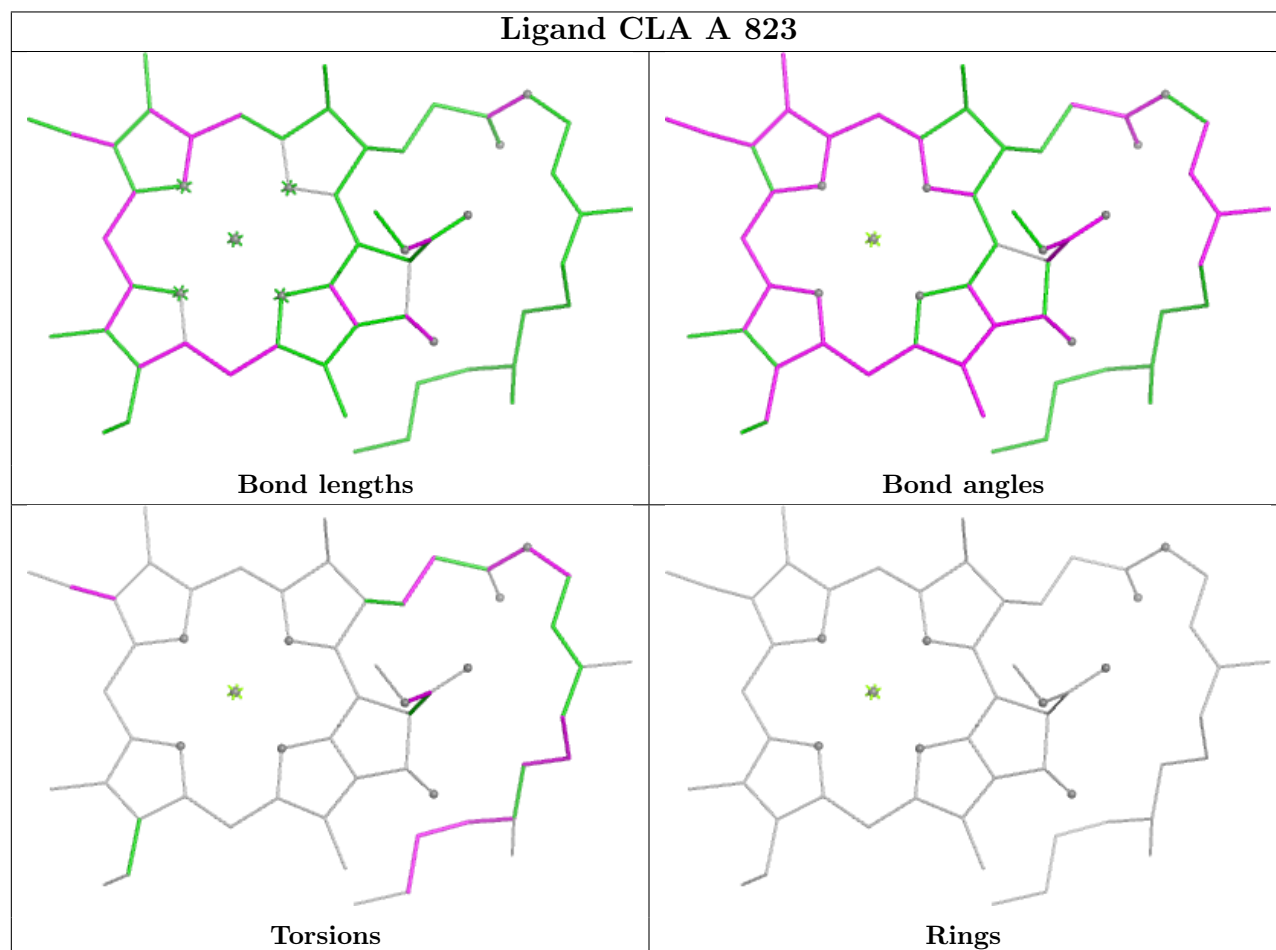
Ligand CLA F 207

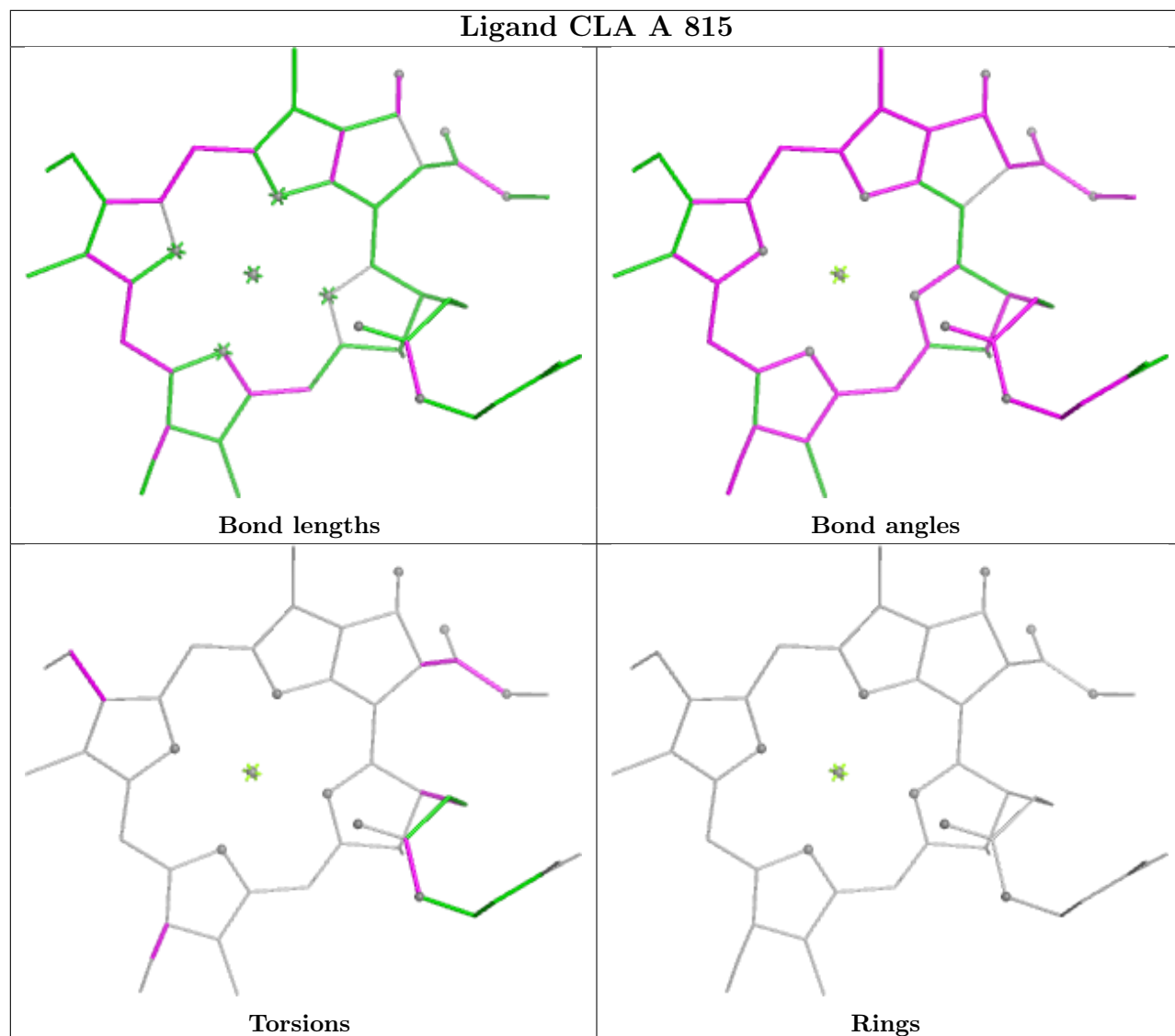


Ligand CLA A 838

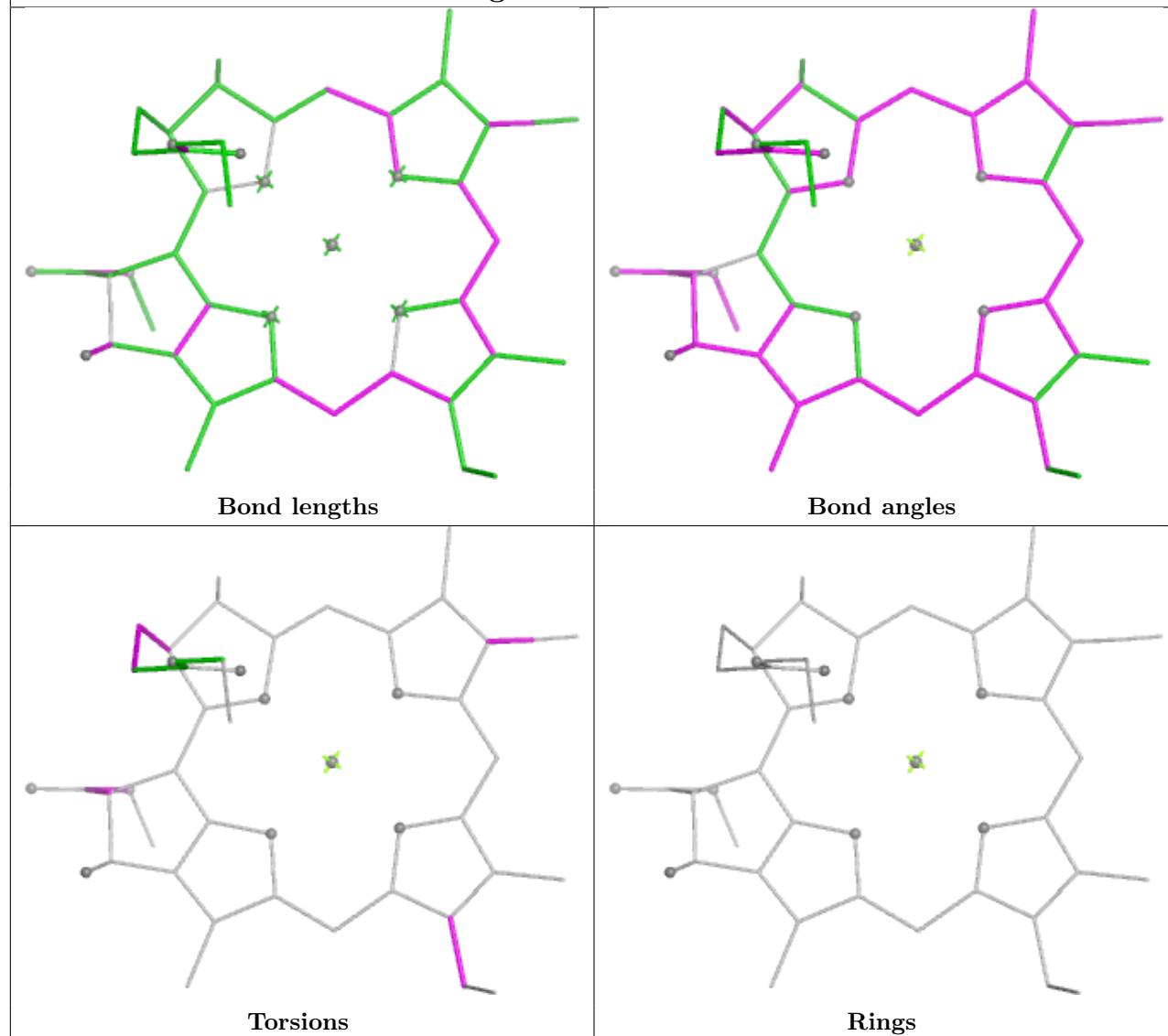


Ligand CLA A 823

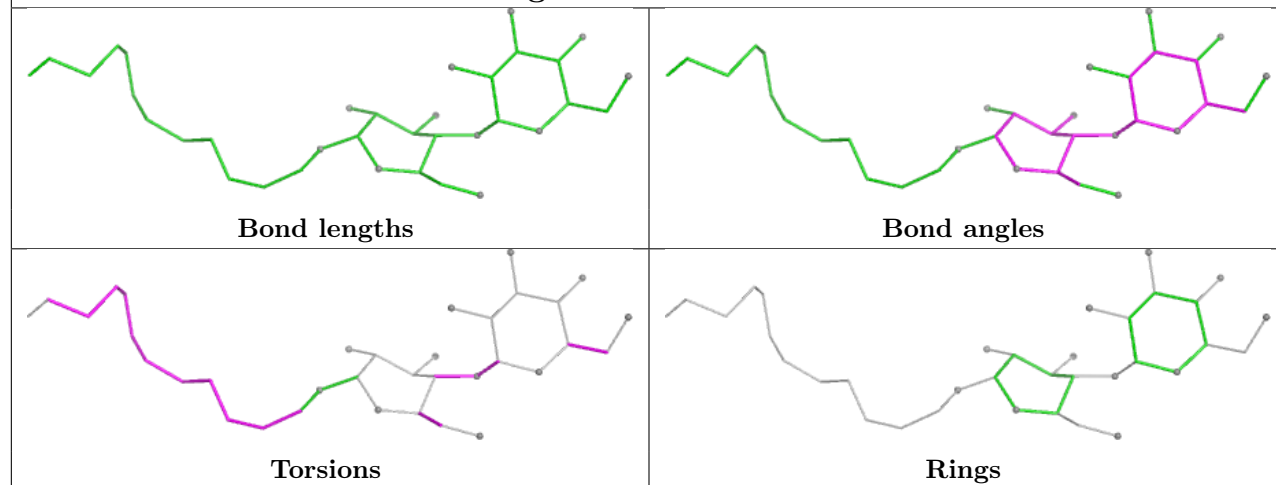


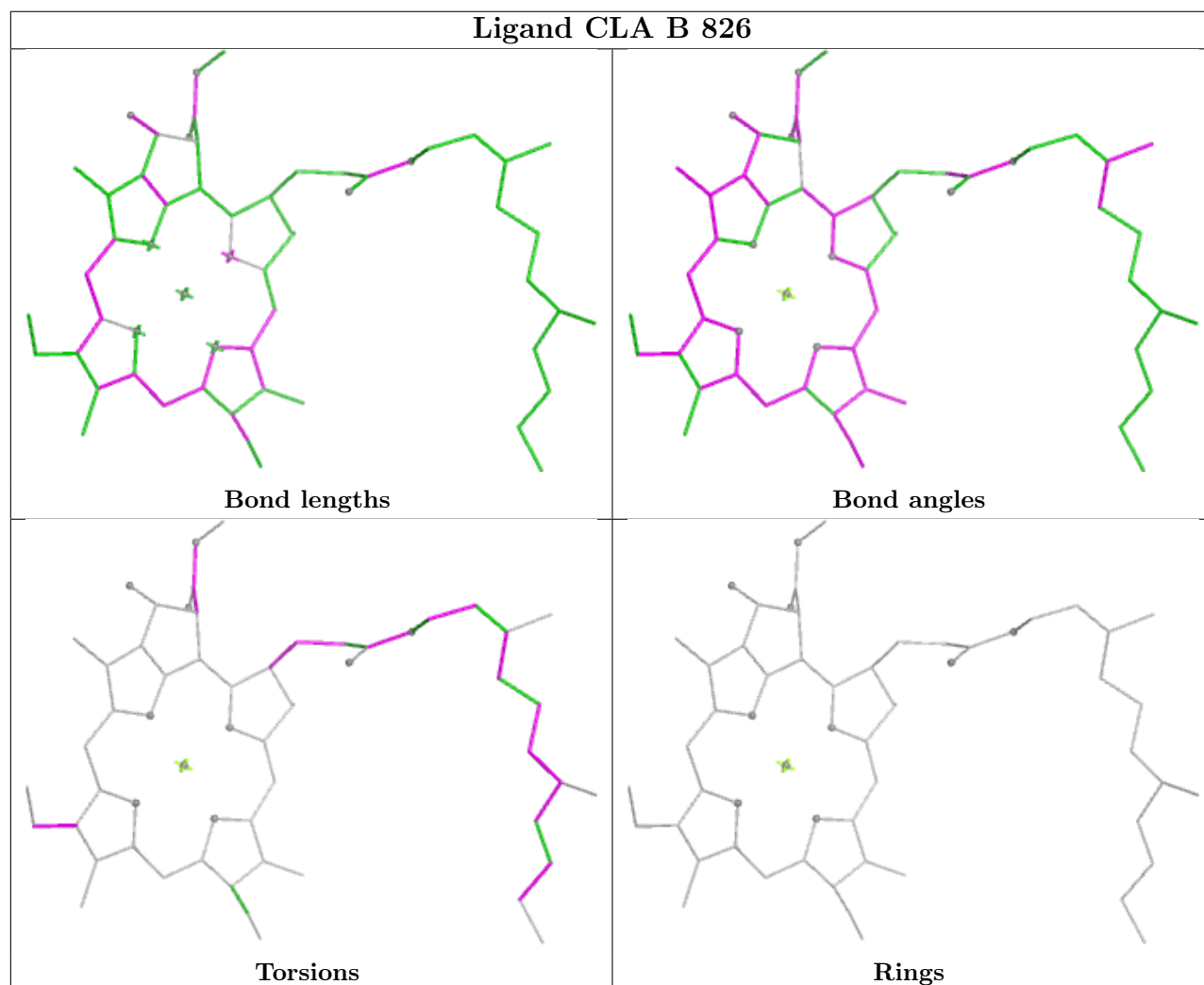
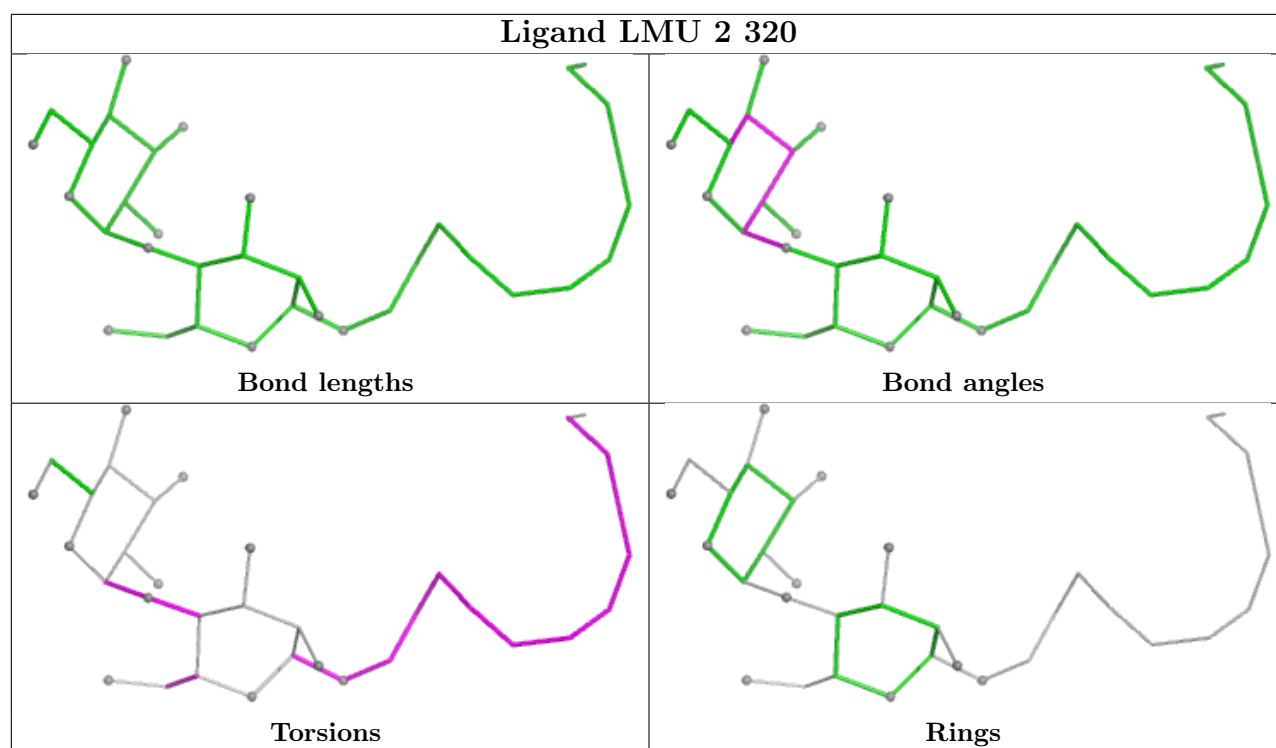


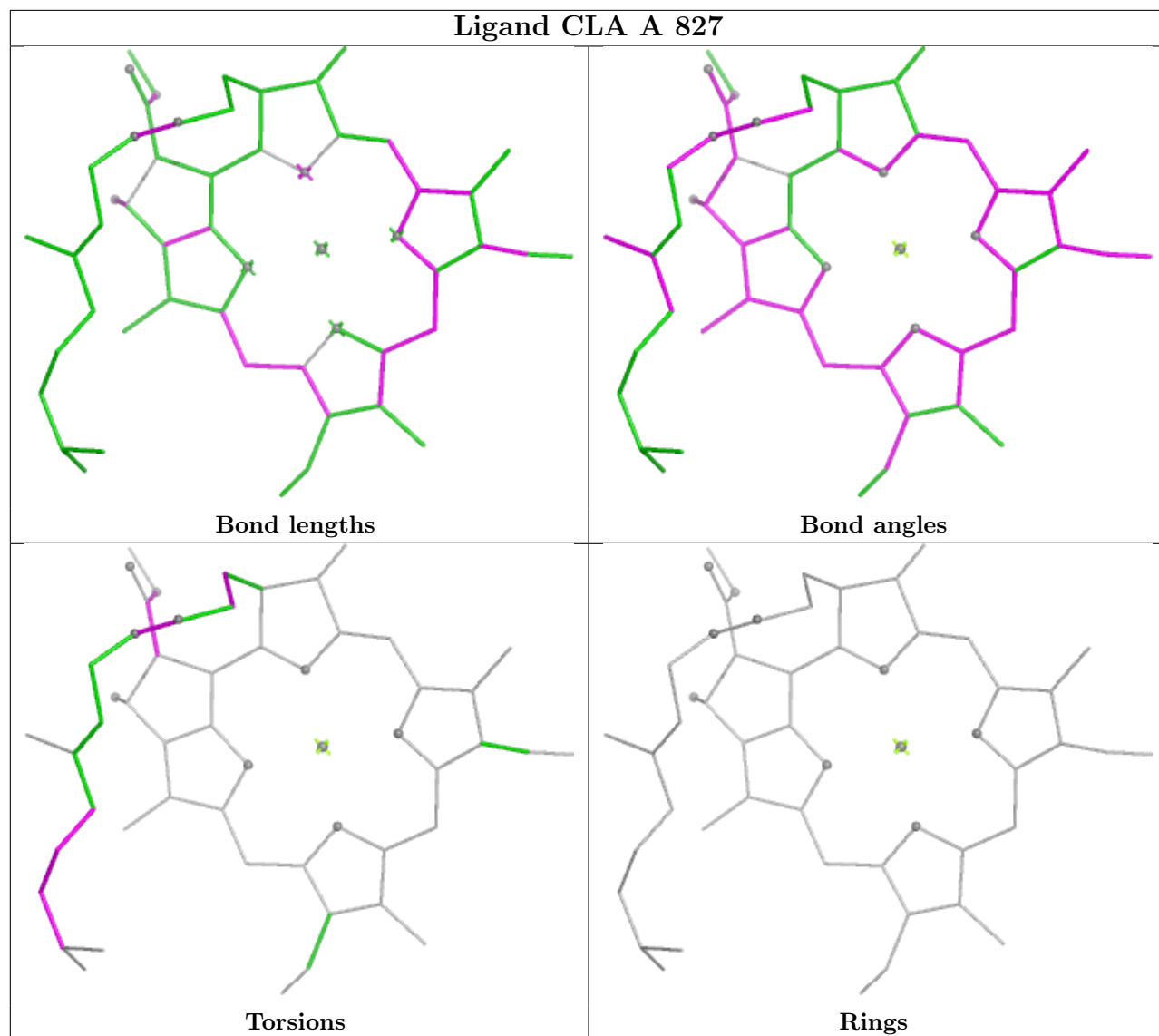
Ligand CLA L 207



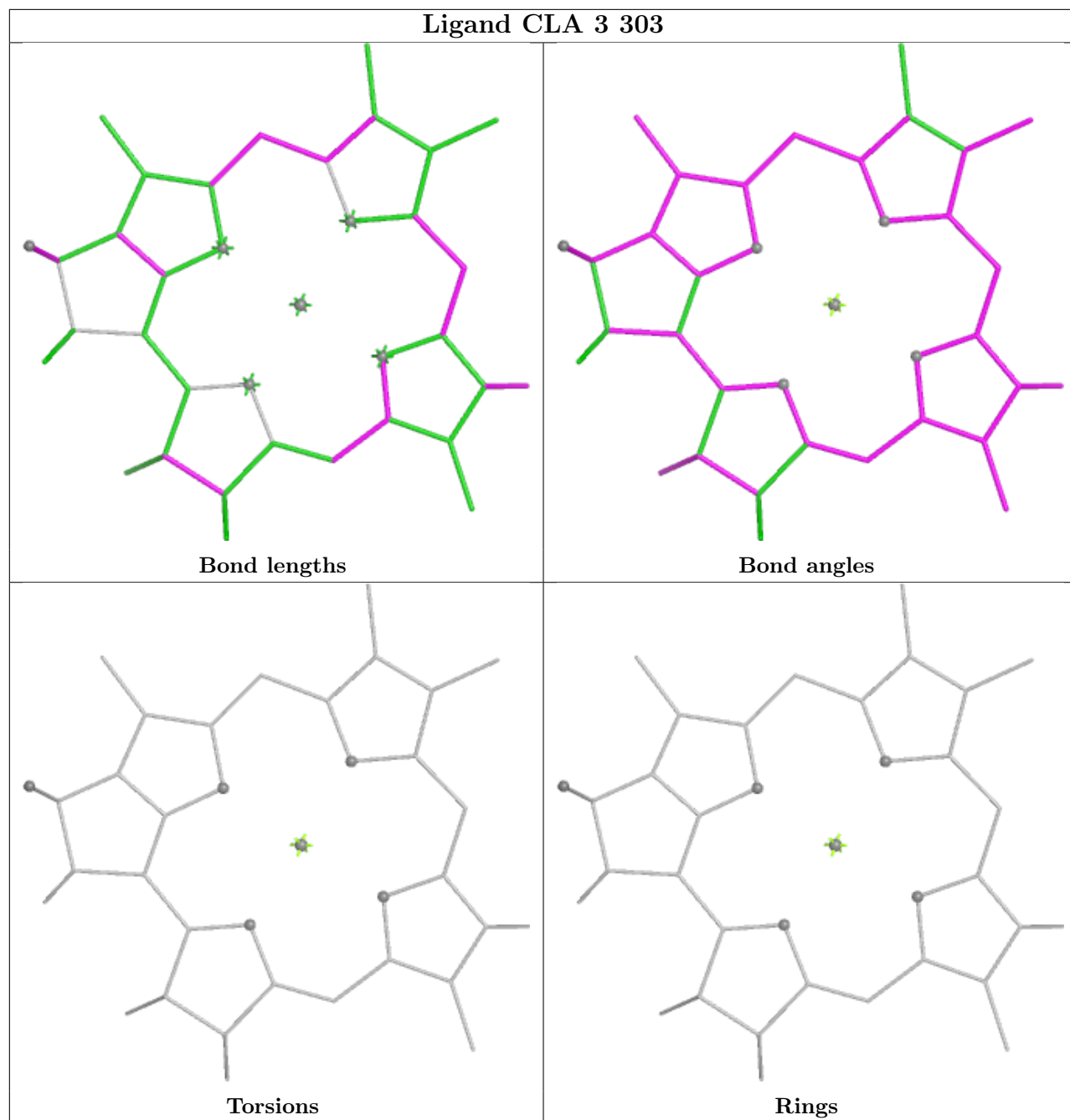
Ligand LMU B 804



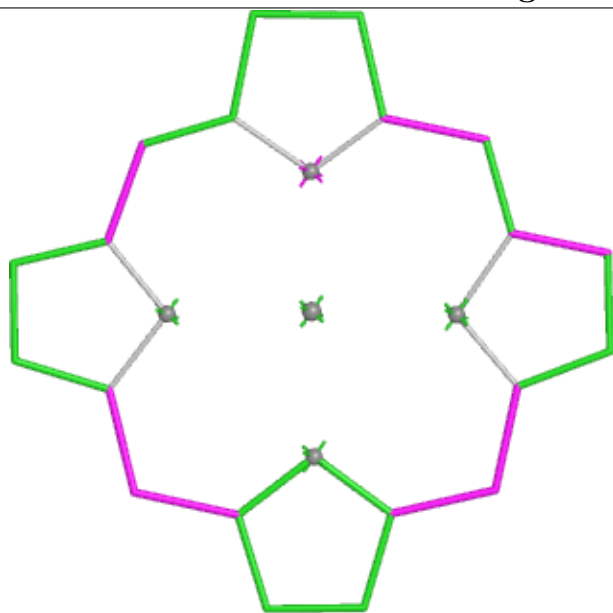




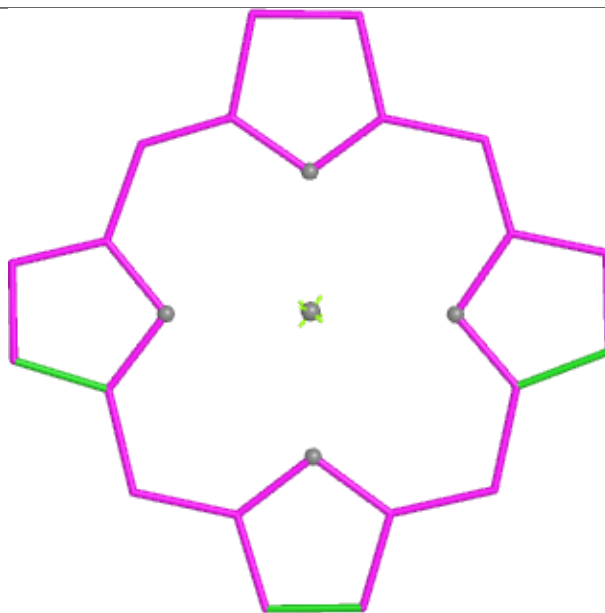
Ligand CLA 3 303



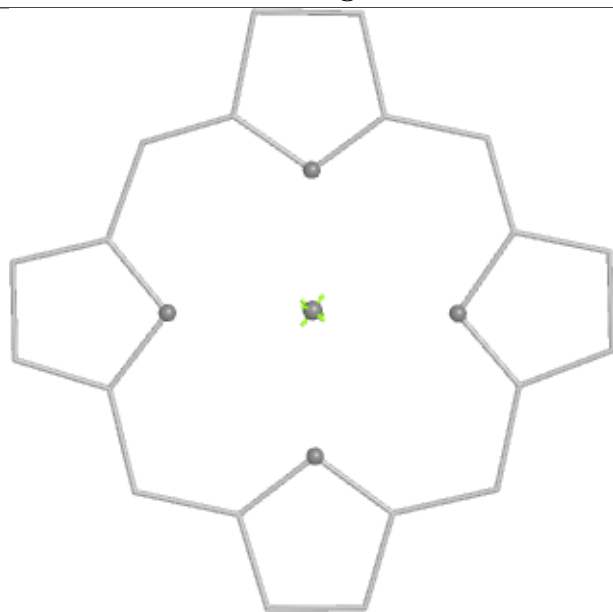
Ligand CLA 3 308



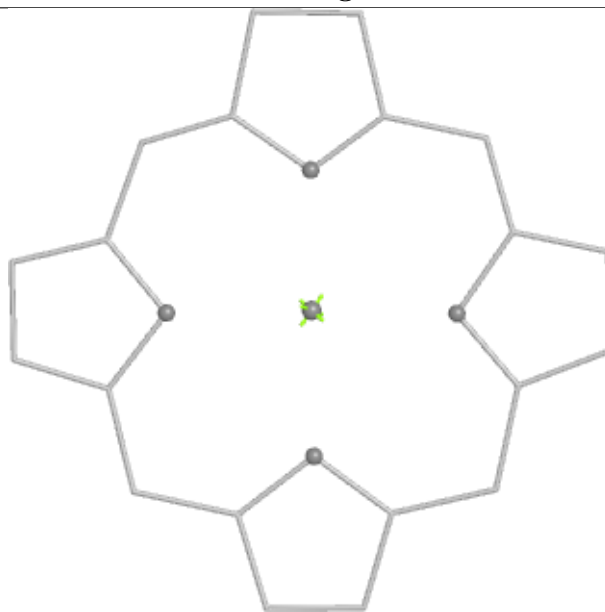
Bond lengths



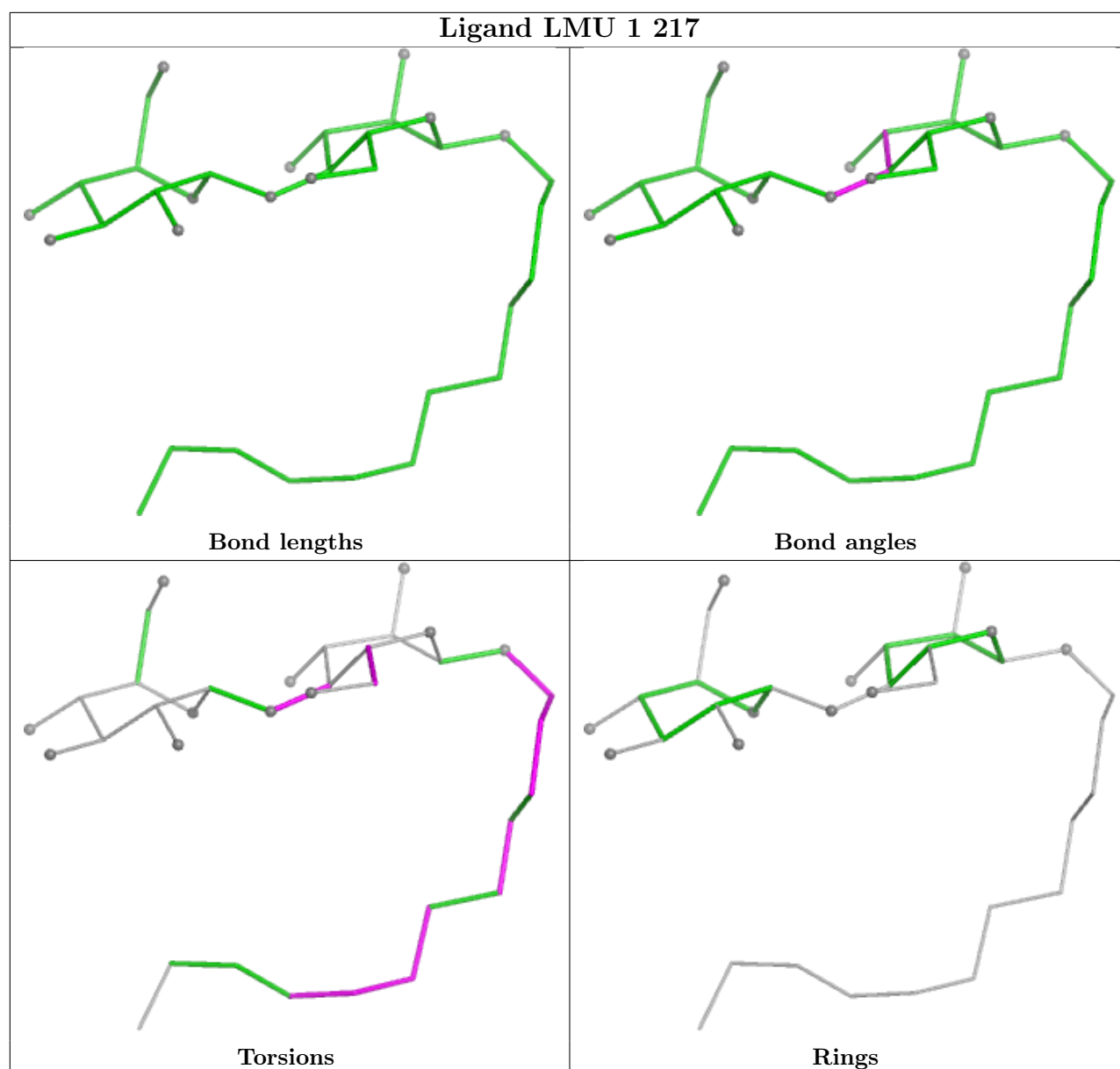
Bond angles



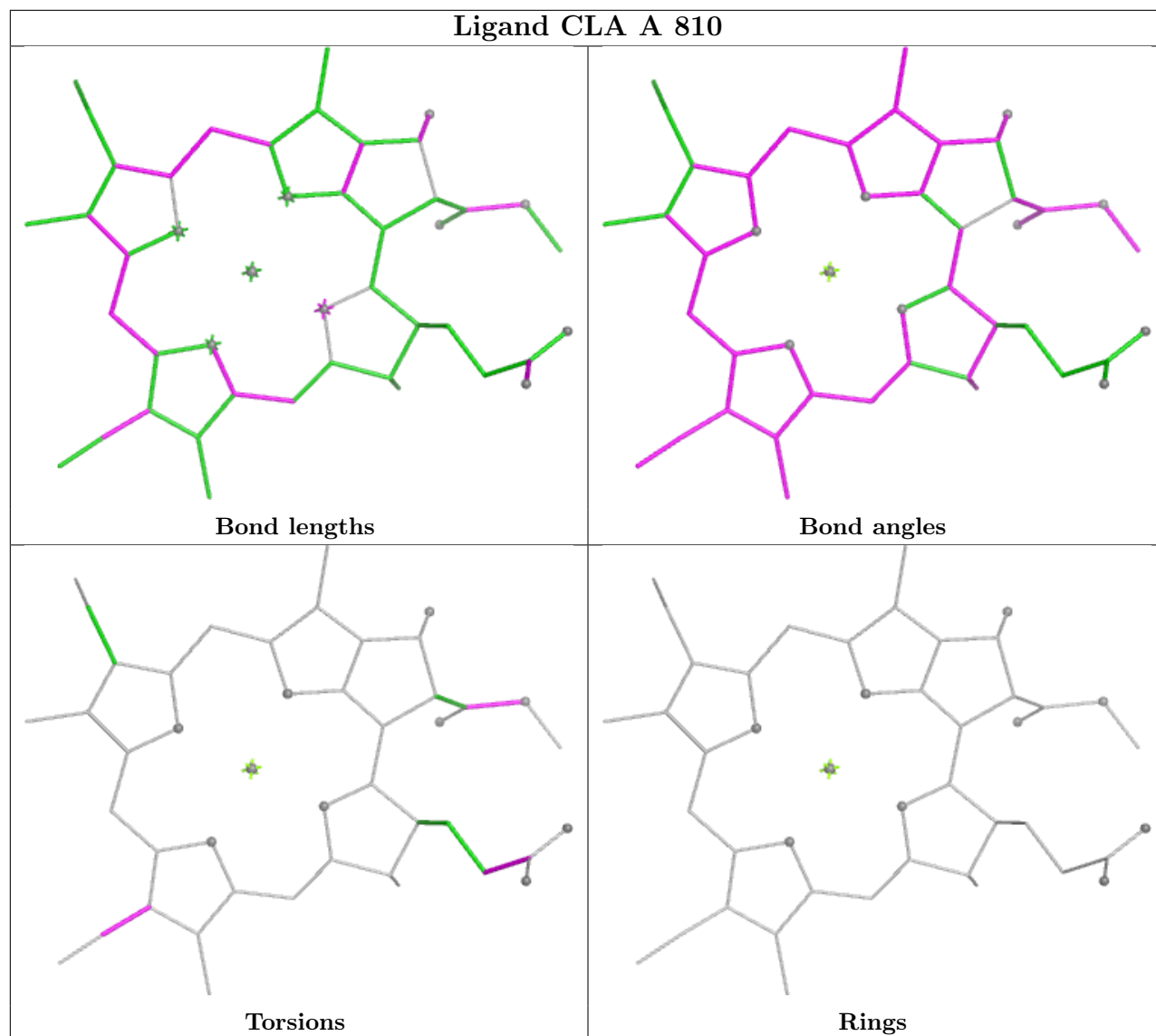
Torsions

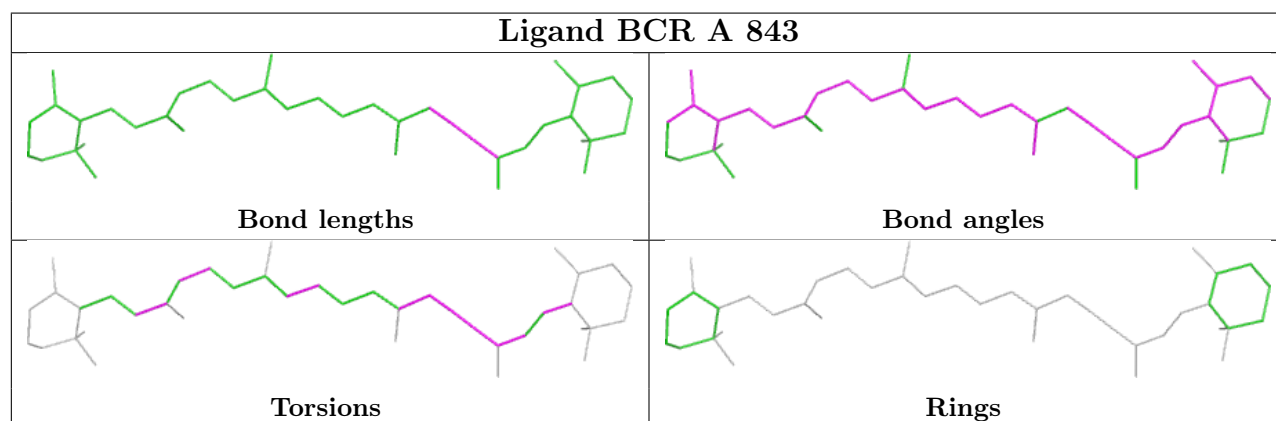
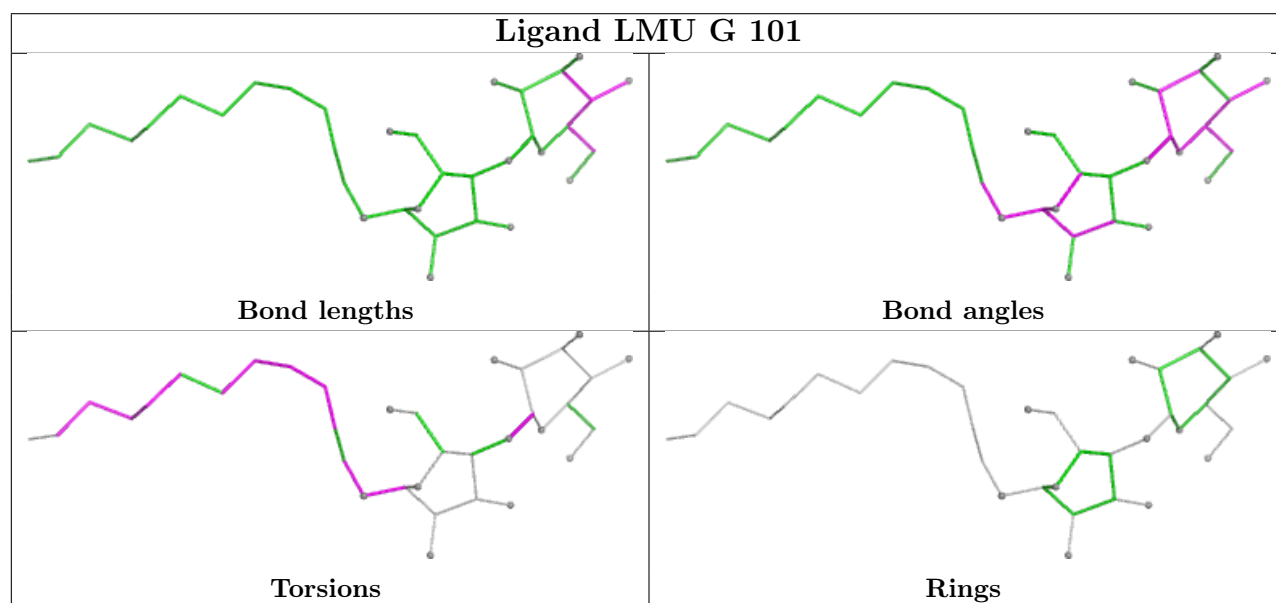
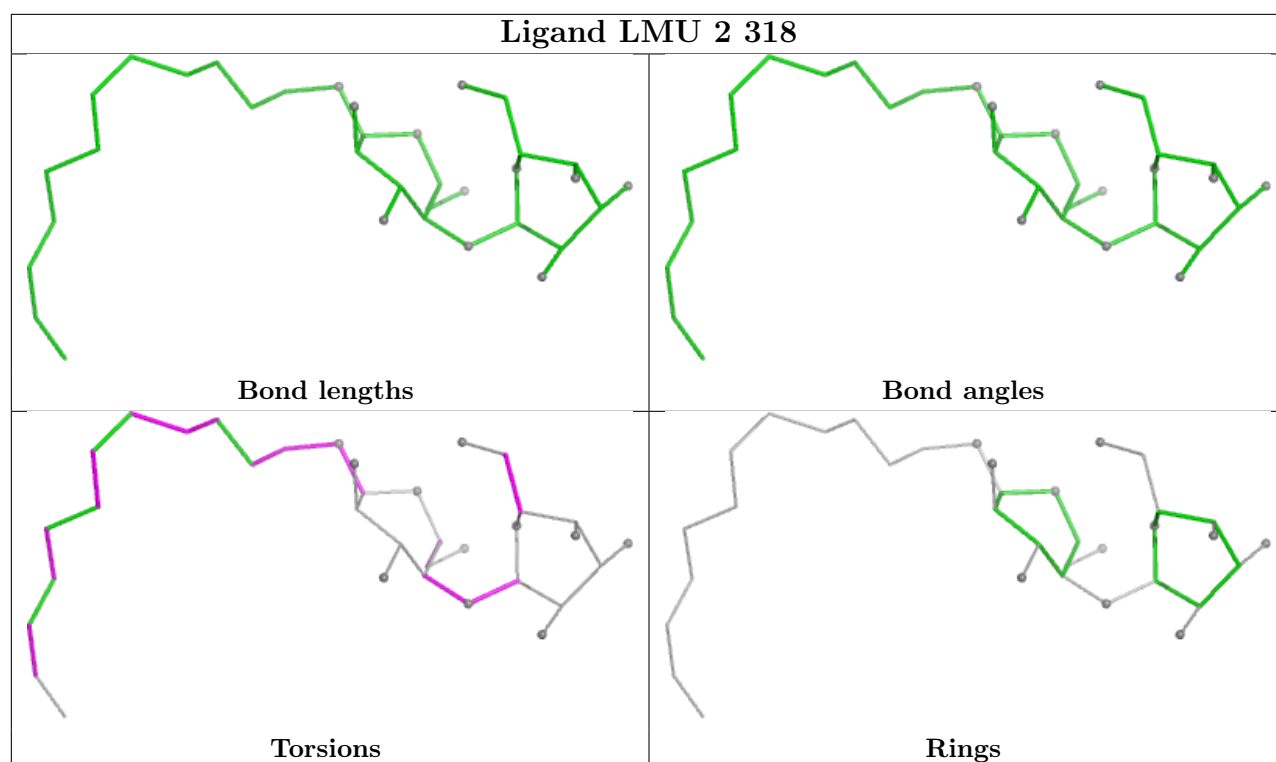


Rings

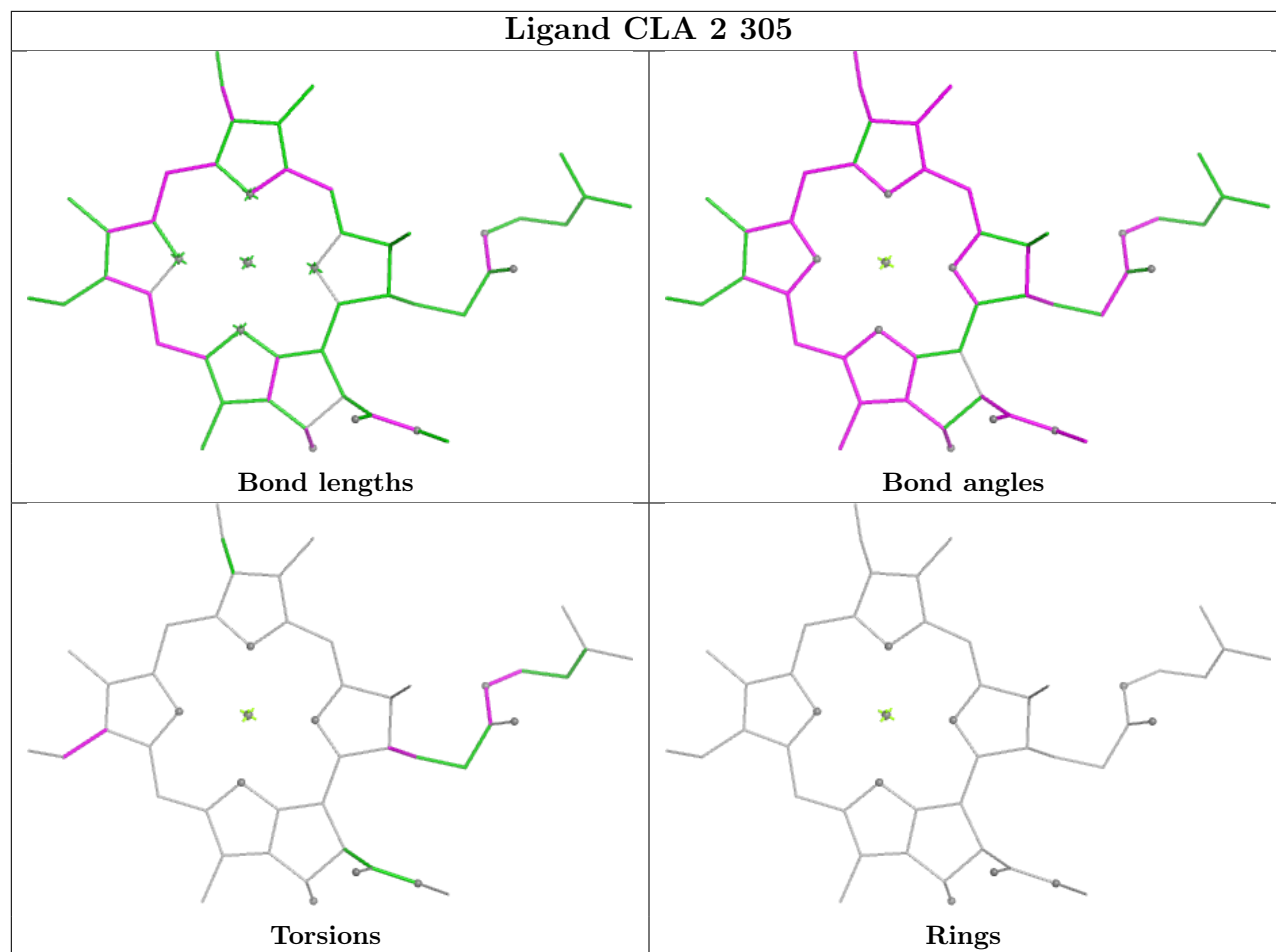


Ligand CLA A 810

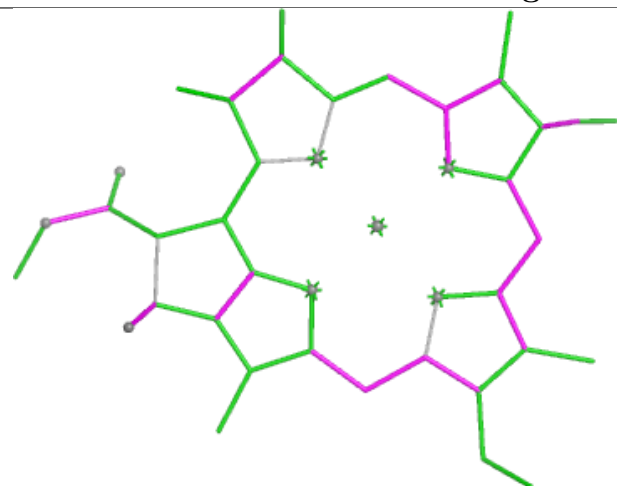




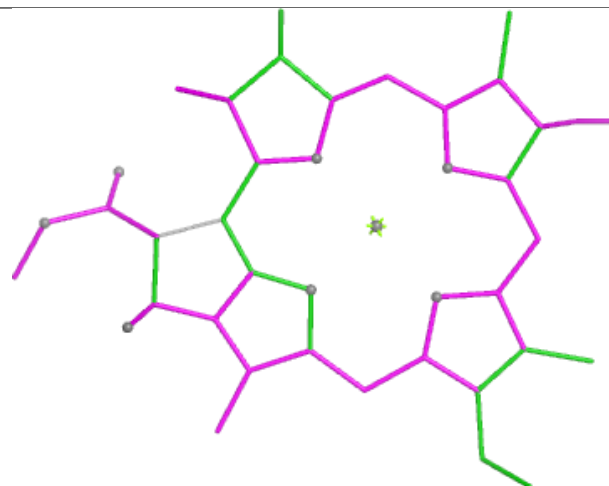
Ligand CLA 2 305



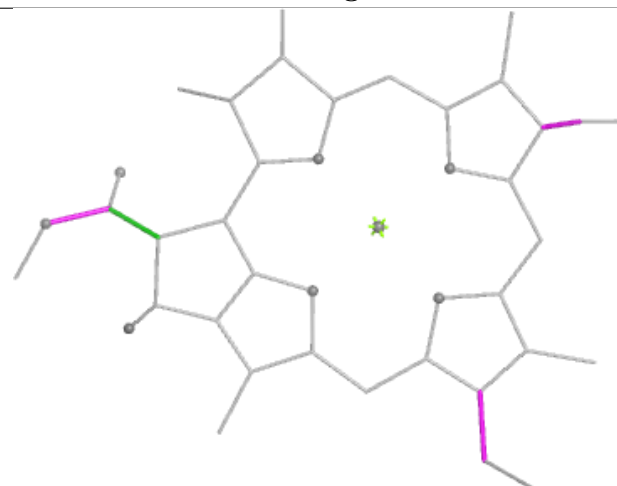
Ligand CLA 1 202



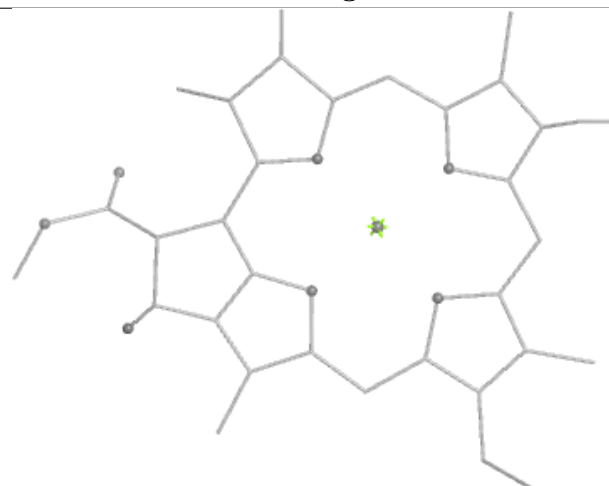
Bond lengths



Bond angles

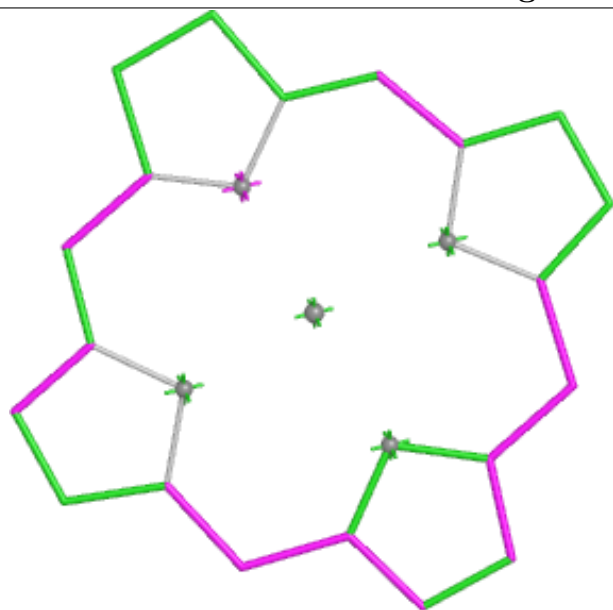


Torsions

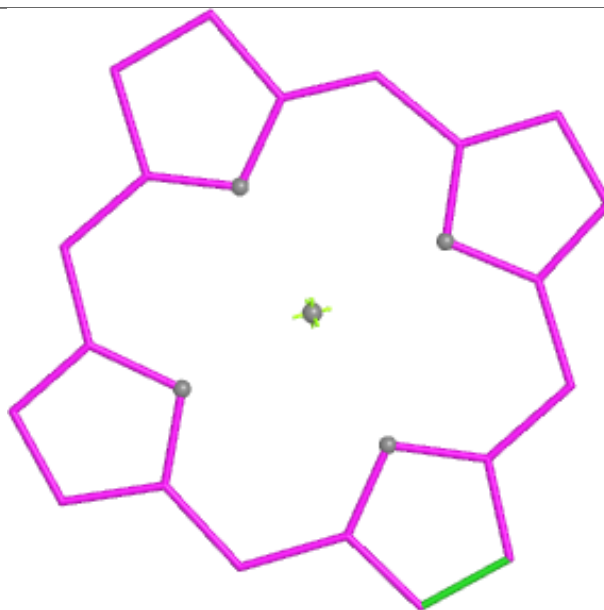


Rings

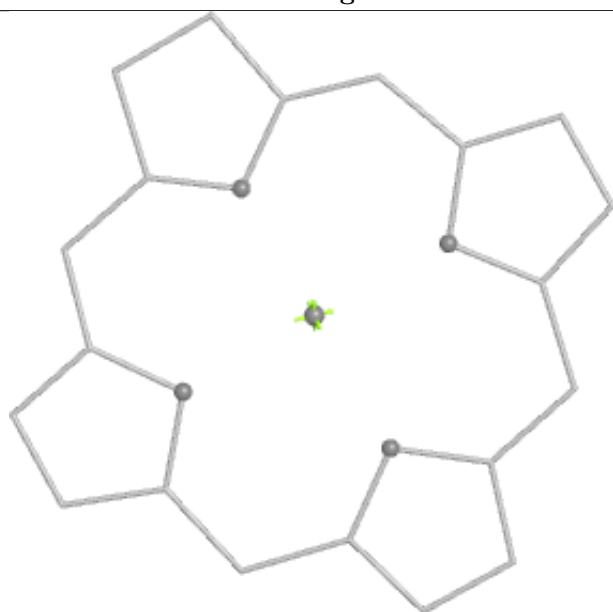
Ligand CLA 3 315



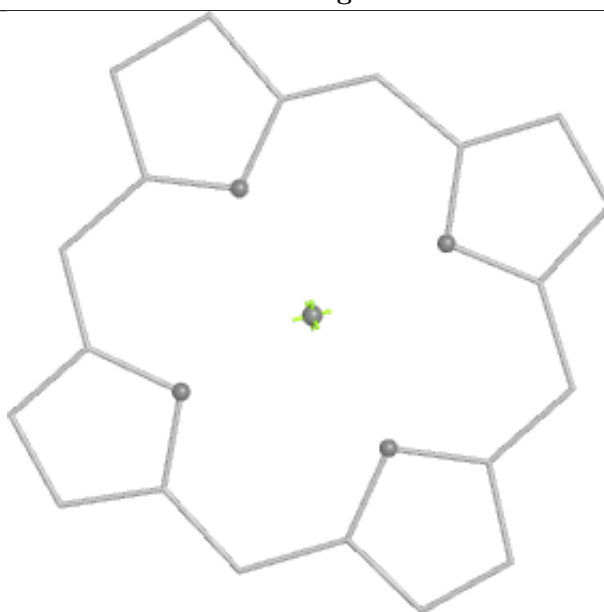
Bond lengths



Bond angles

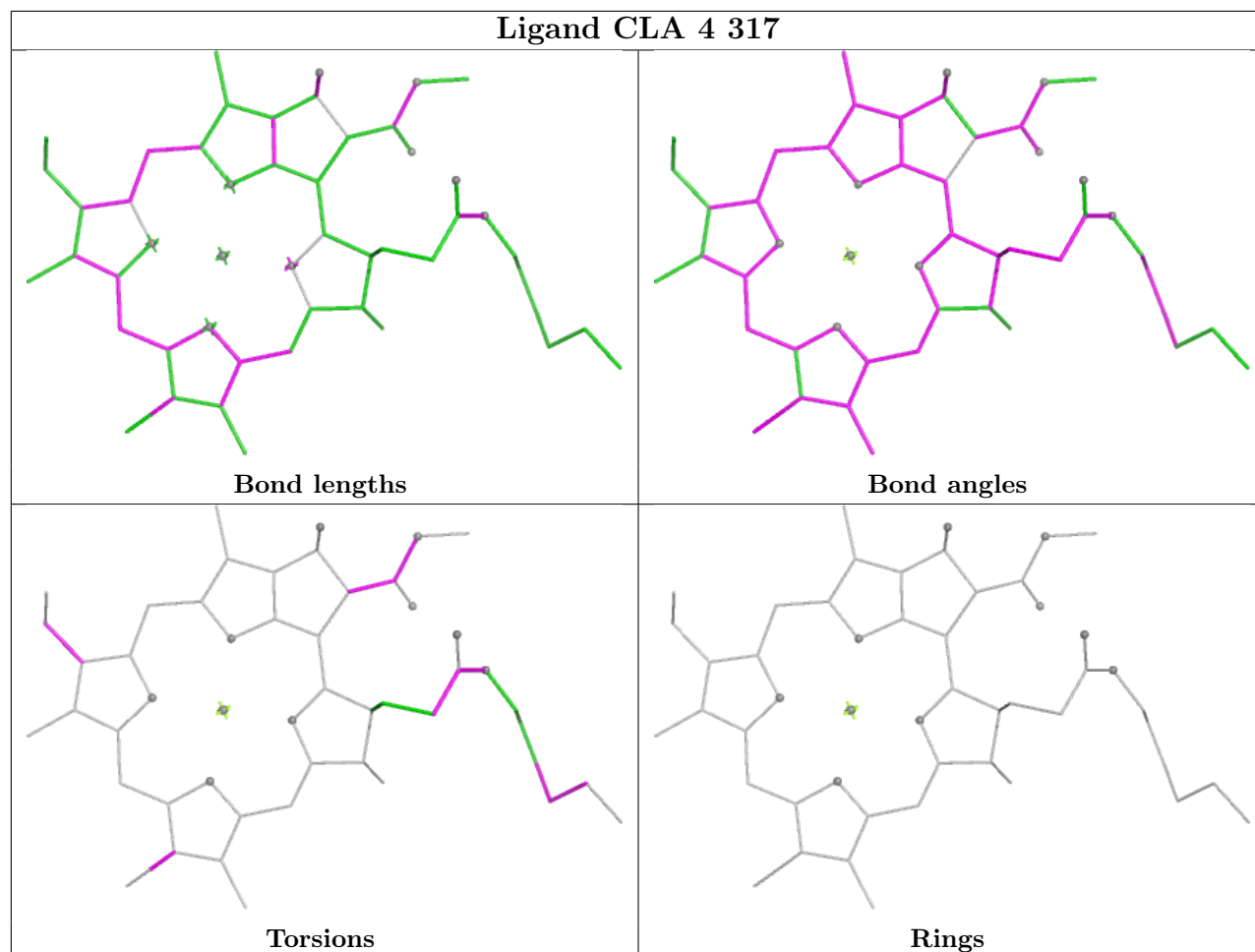


Torsions

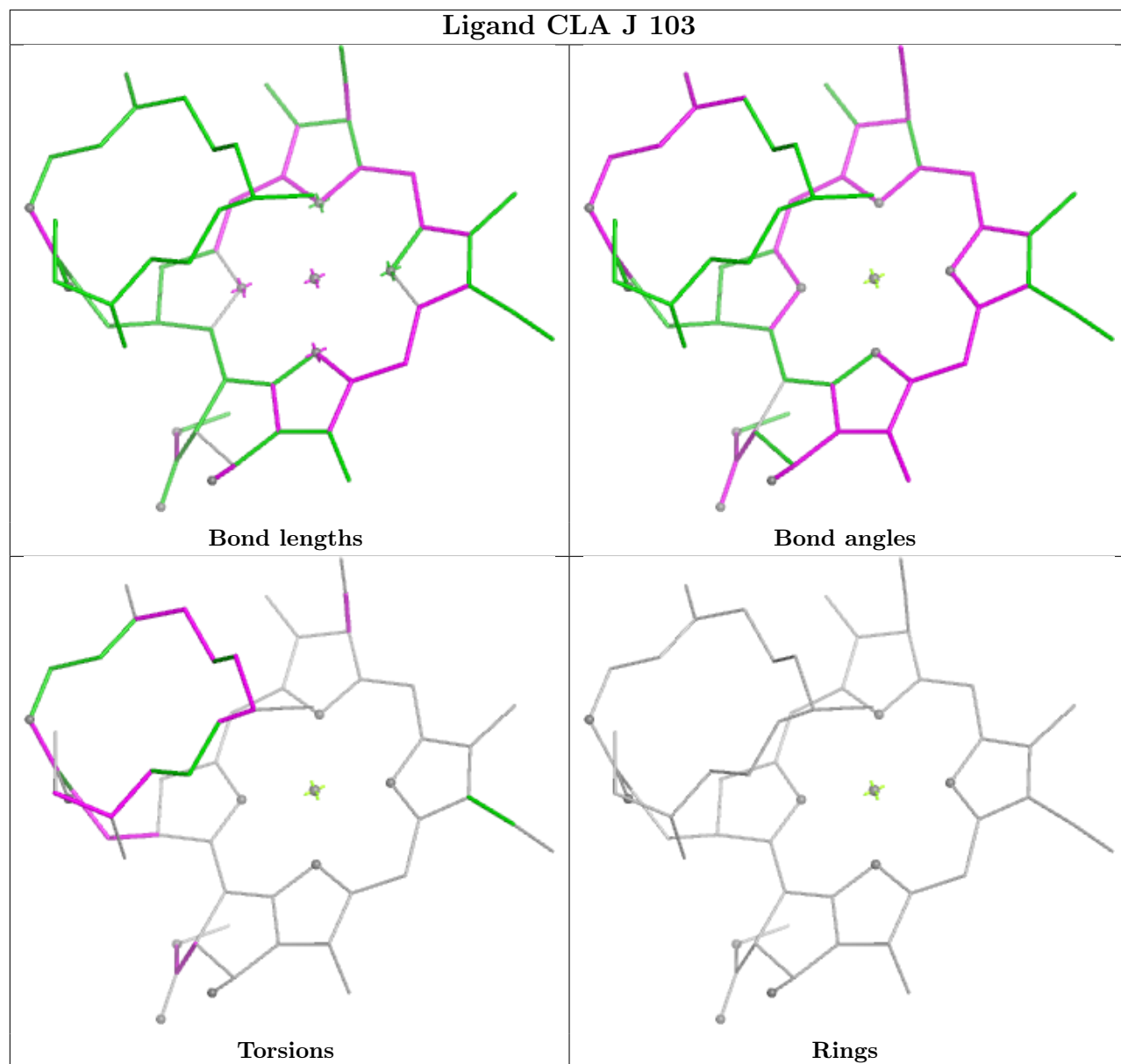


Rings

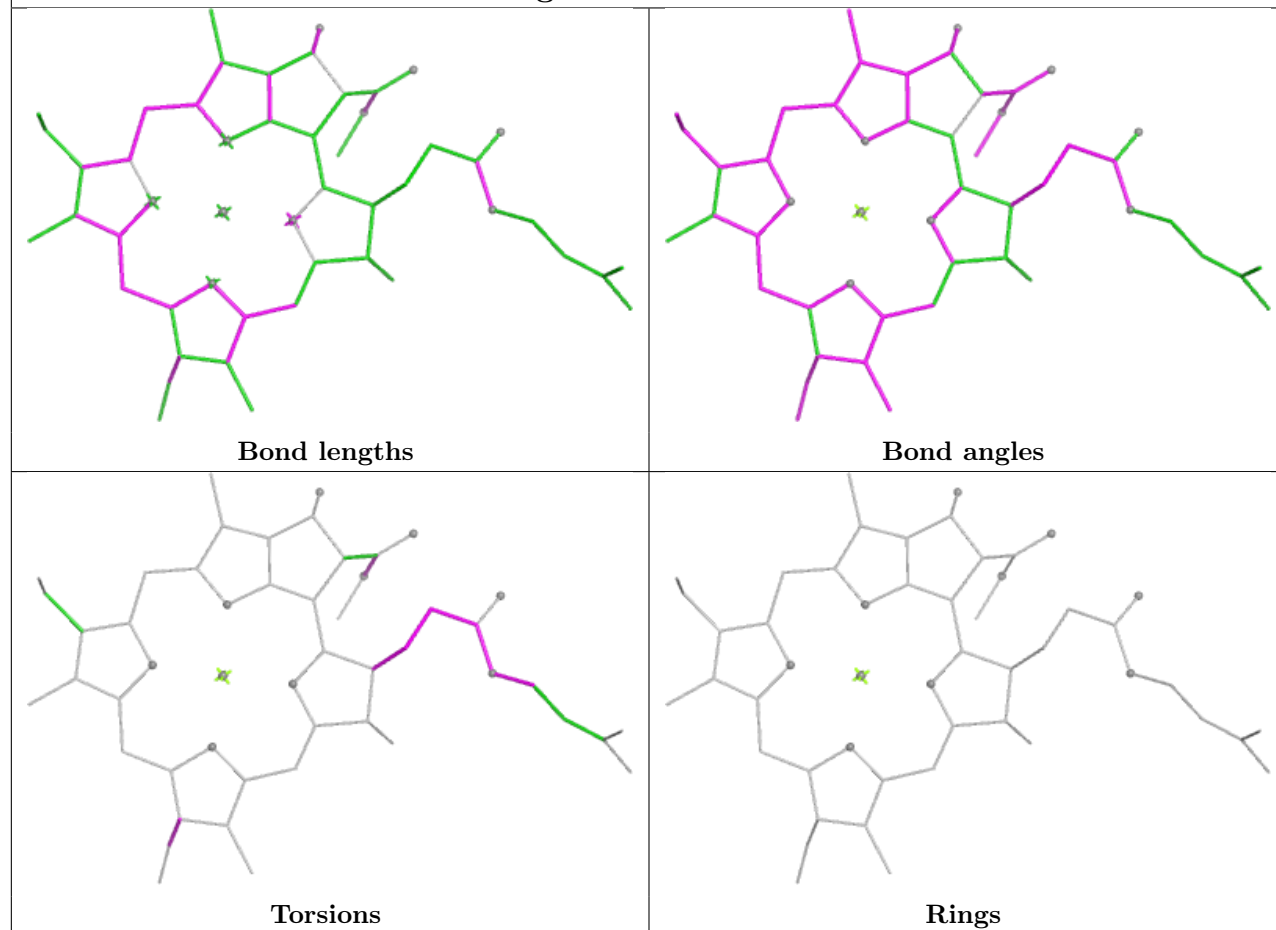
Ligand CLA 4 317



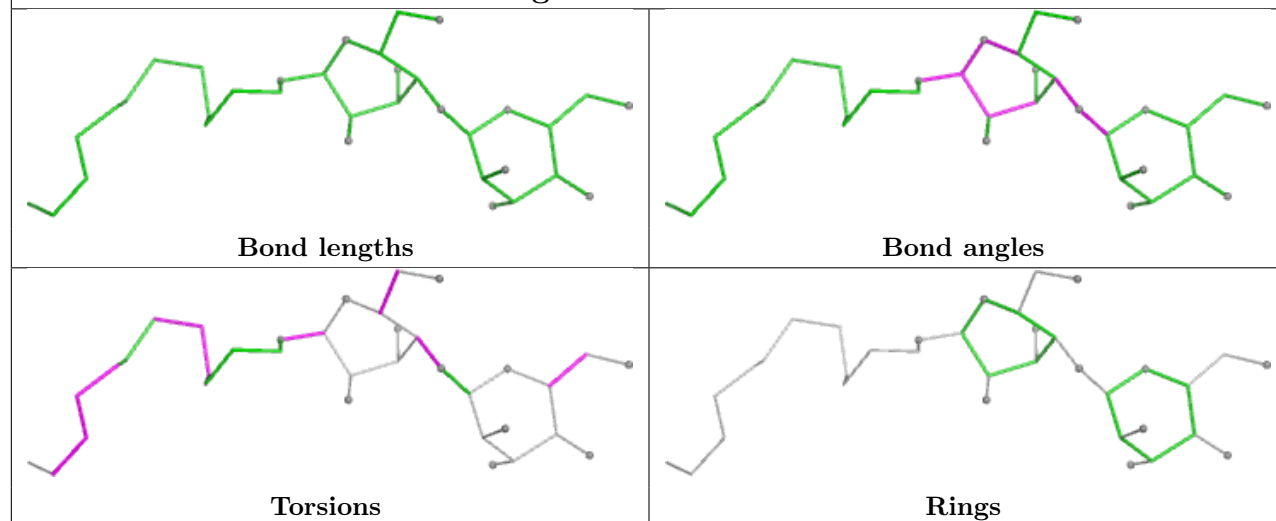
Ligand CLA J 103

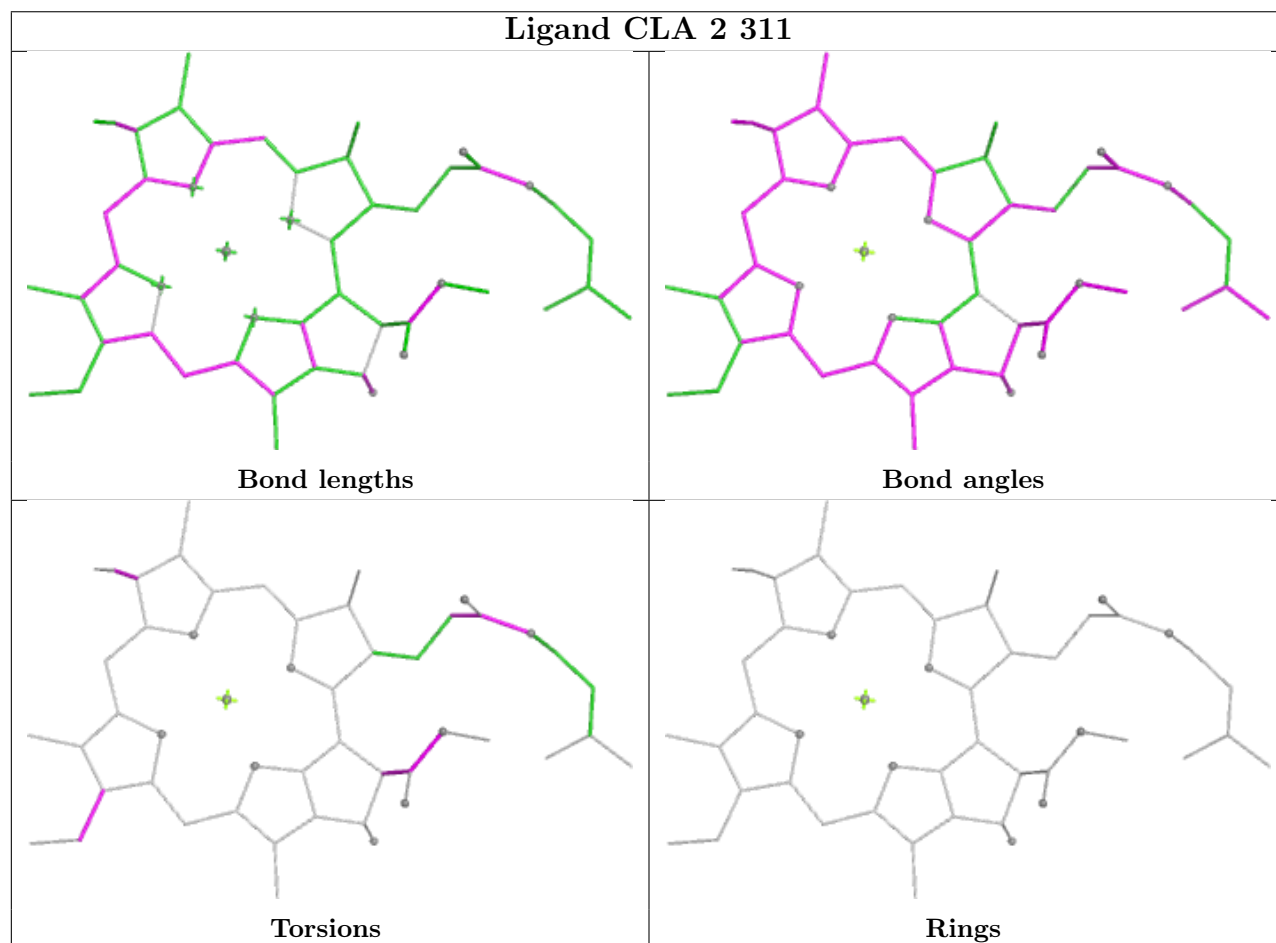
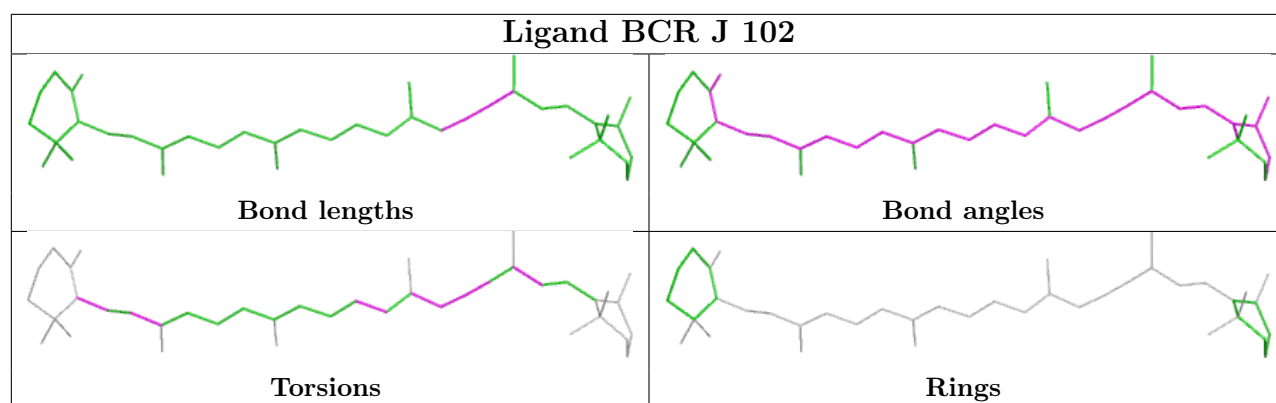


Ligand CLA 4 310

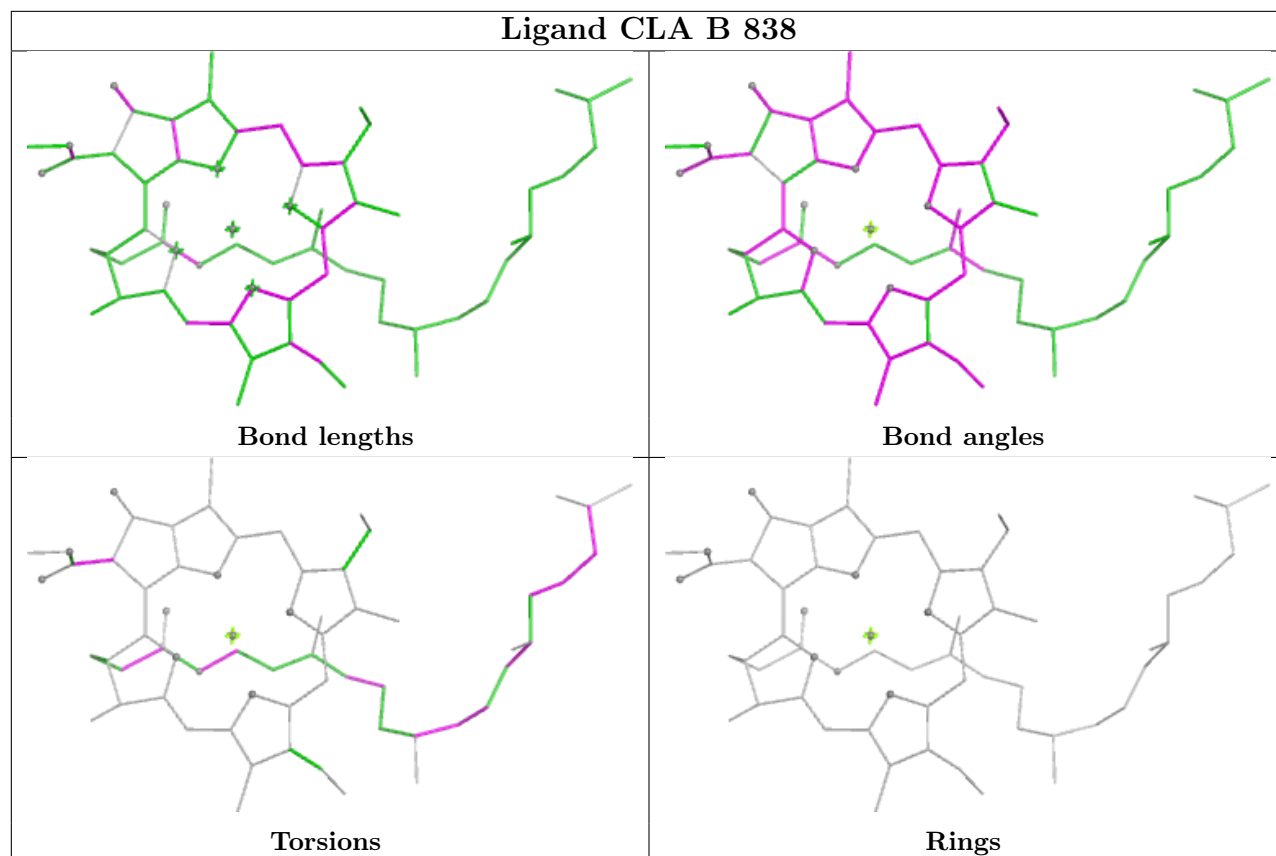


Ligand LMU 3 319

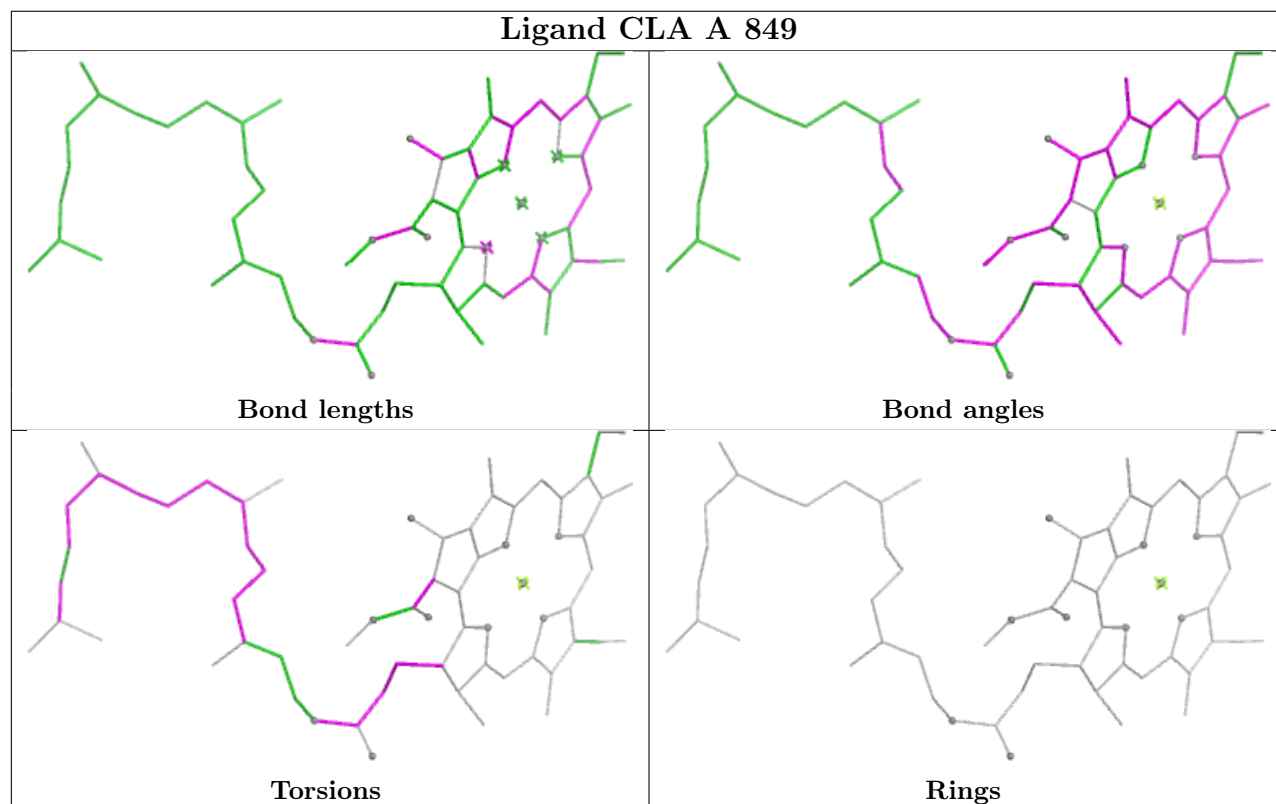




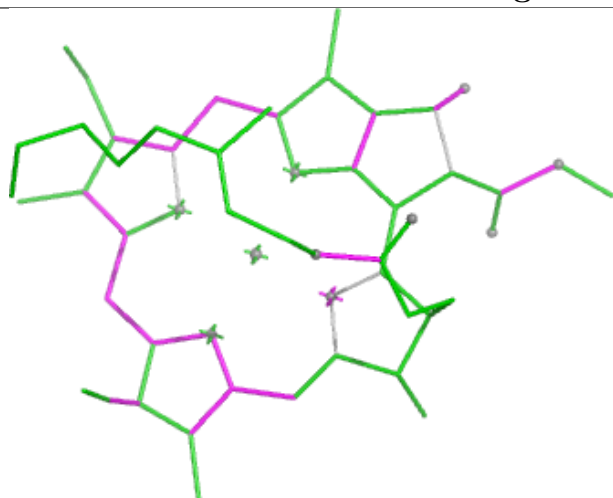
Ligand CLA B 838



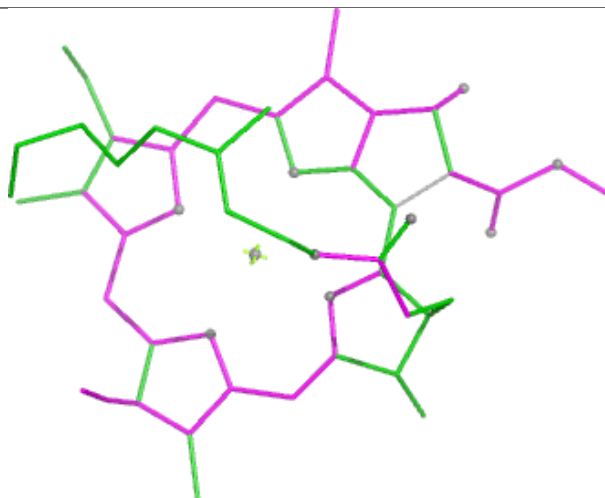
Ligand CLA A 849



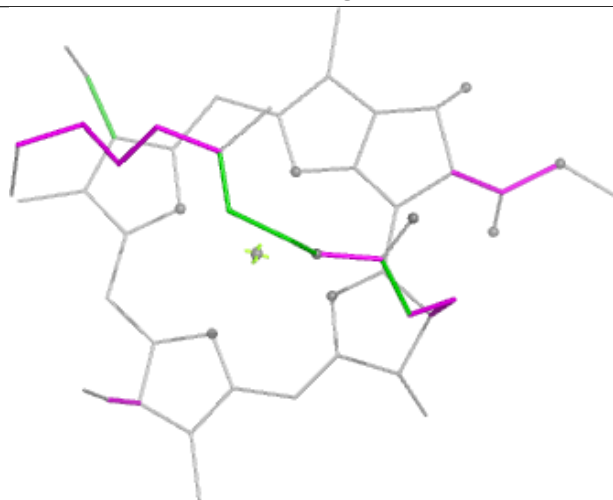
Ligand CLA A 812



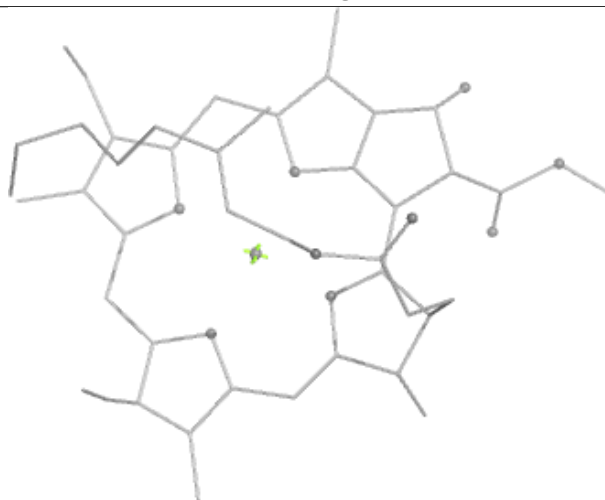
Bond lengths



Bond angles

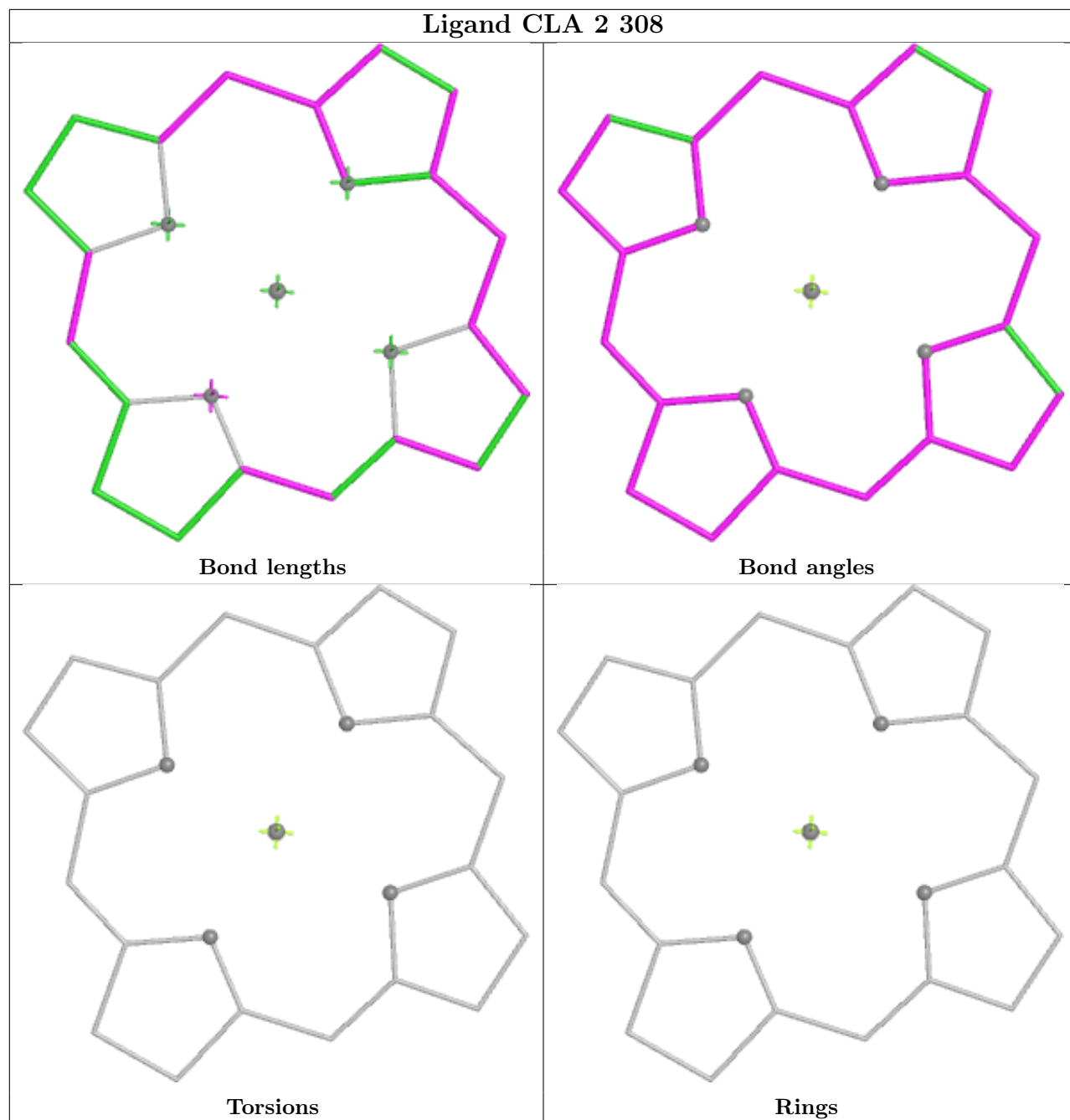


Torsions

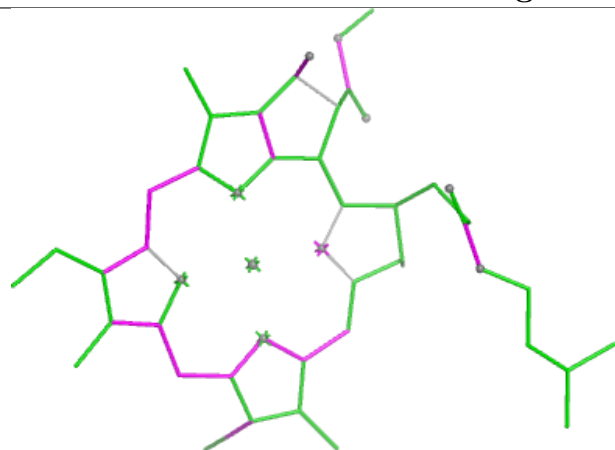


Rings

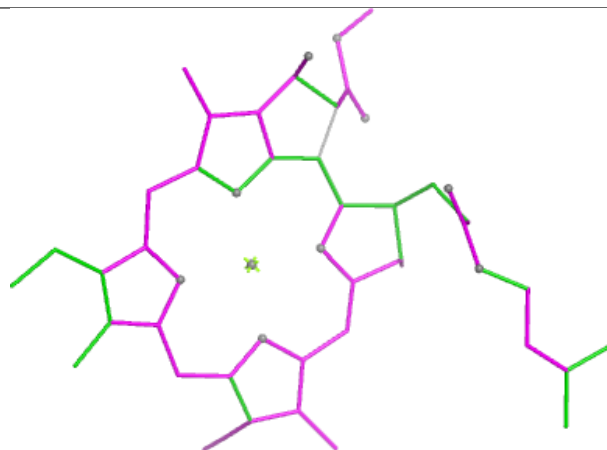
Ligand CLA 2 308



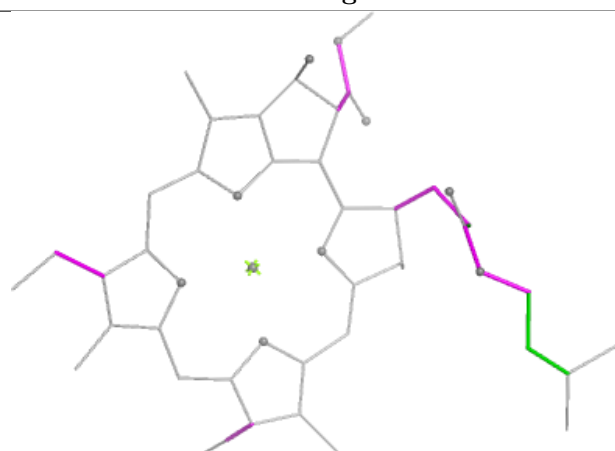
Ligand CLA A 832



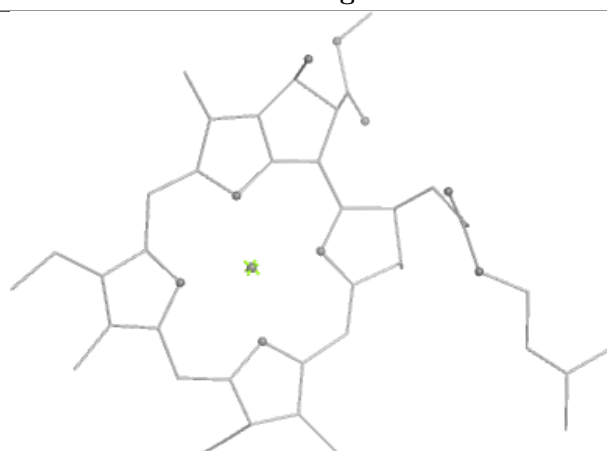
Bond lengths



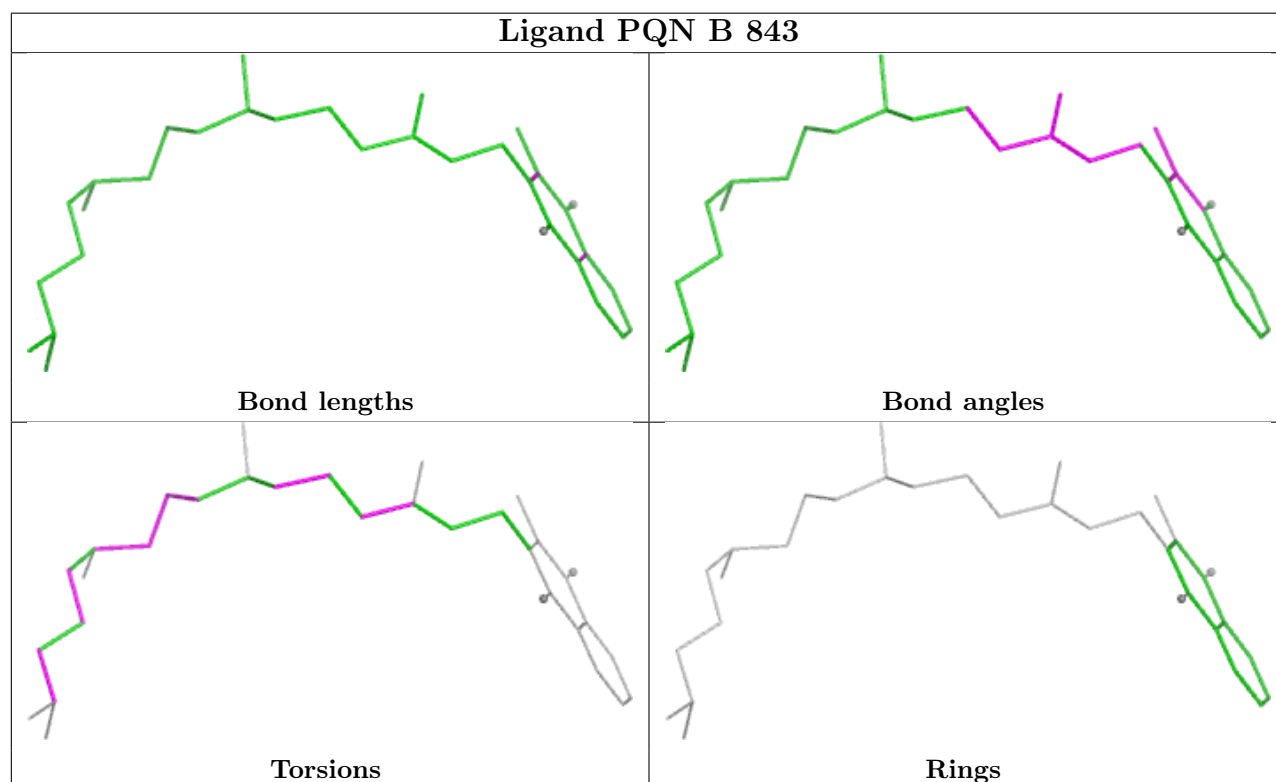
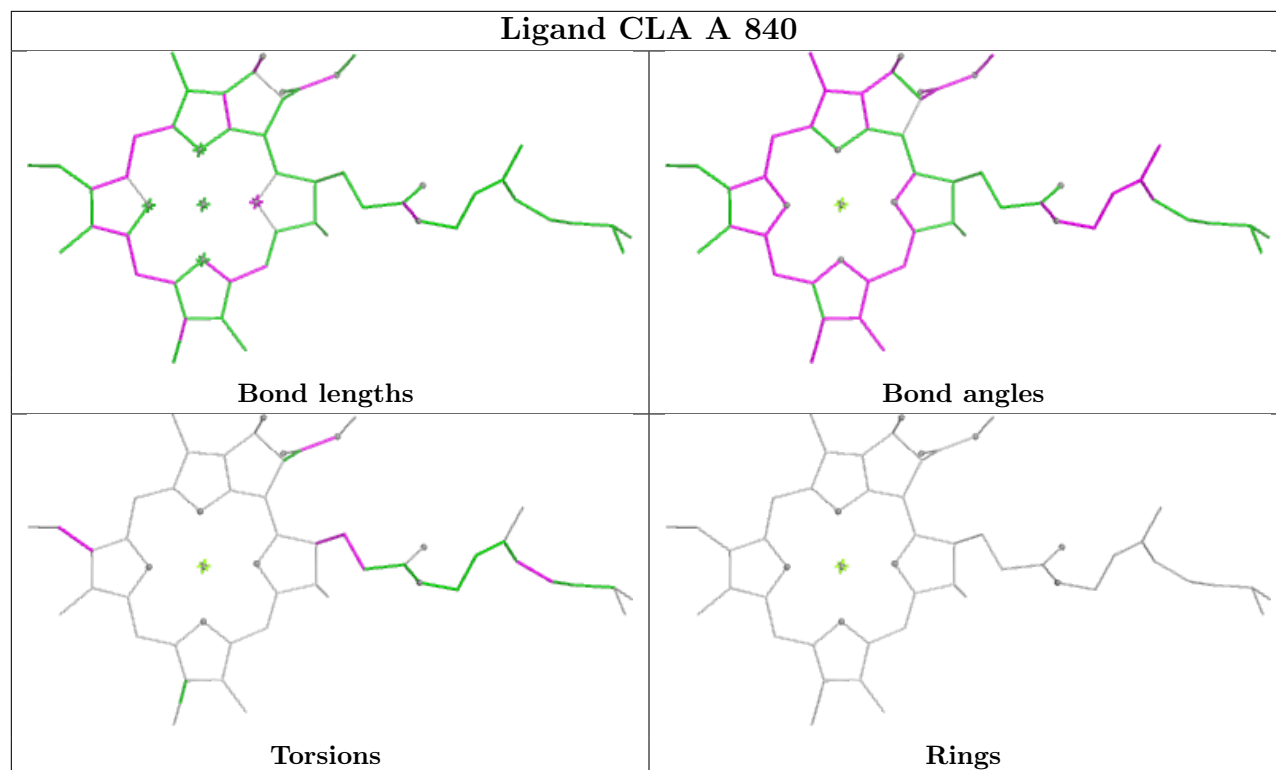
Bond angles

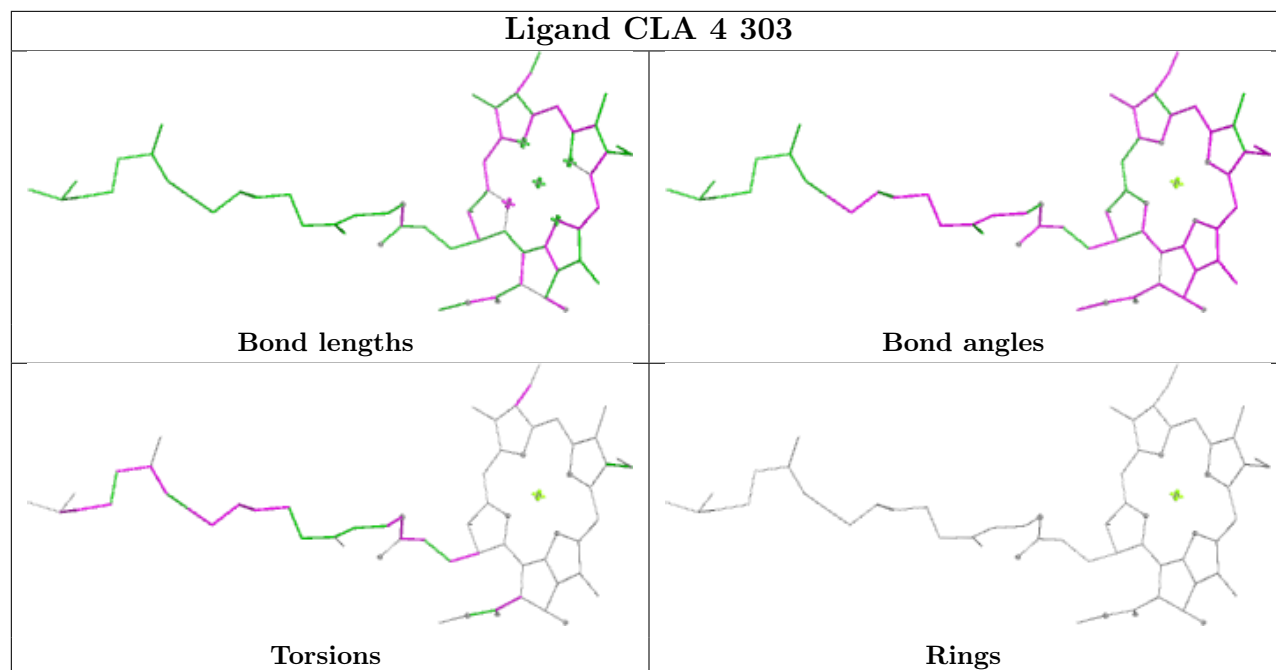


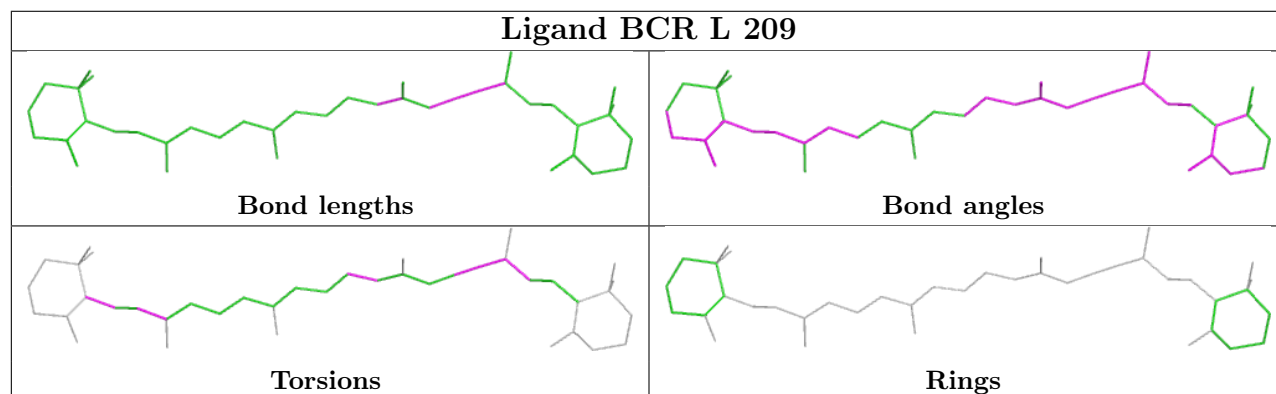
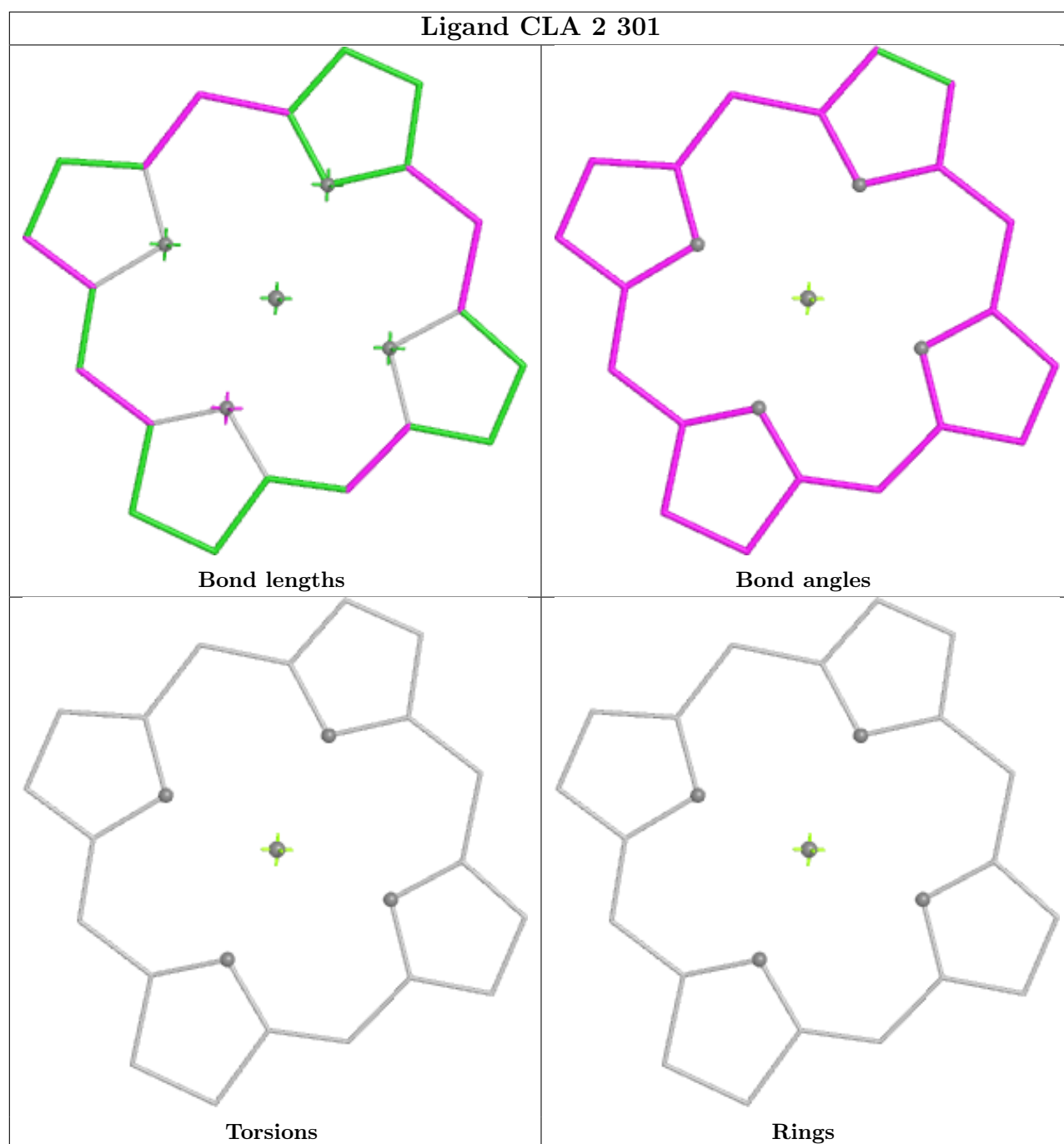
Torsions

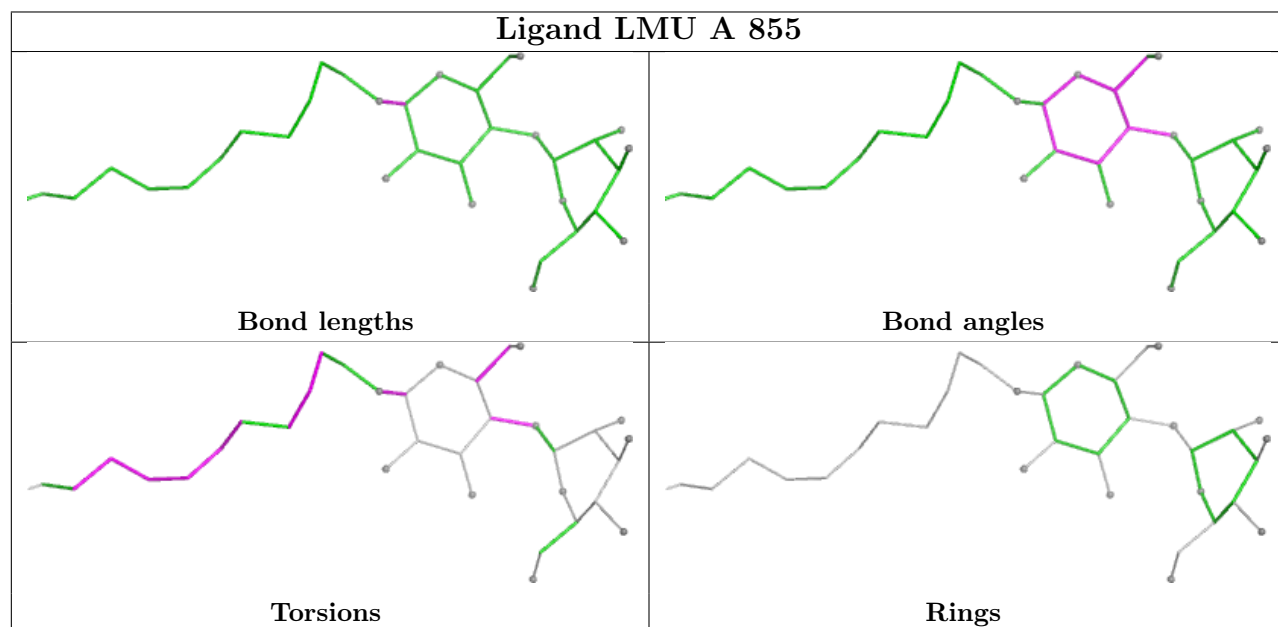
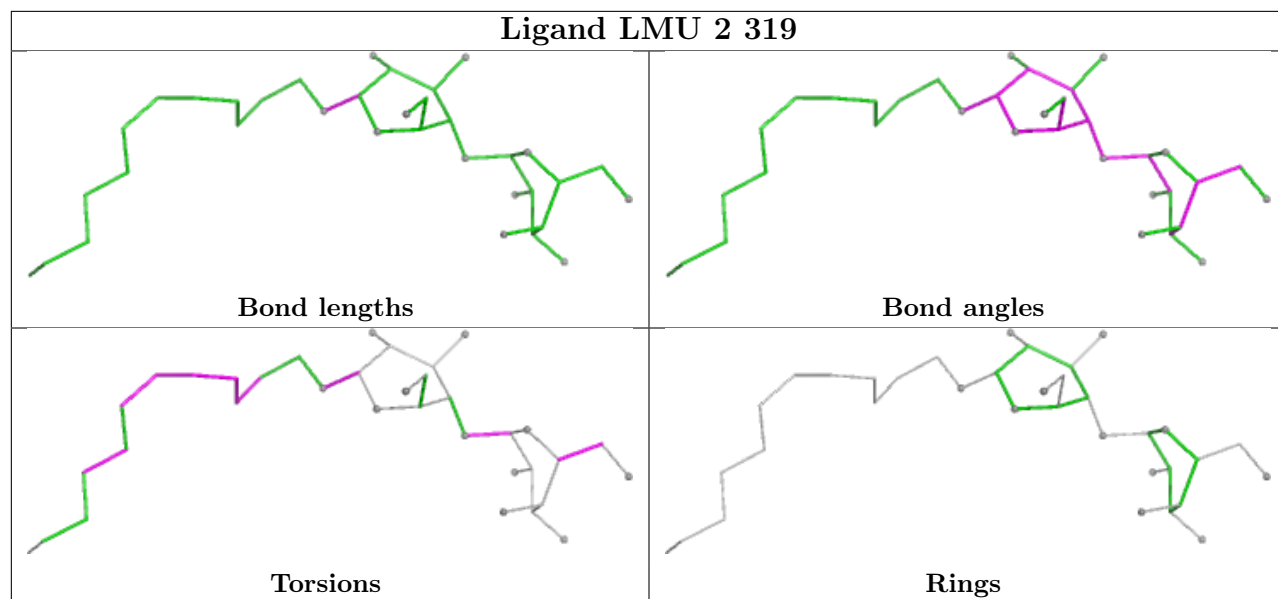


Rings

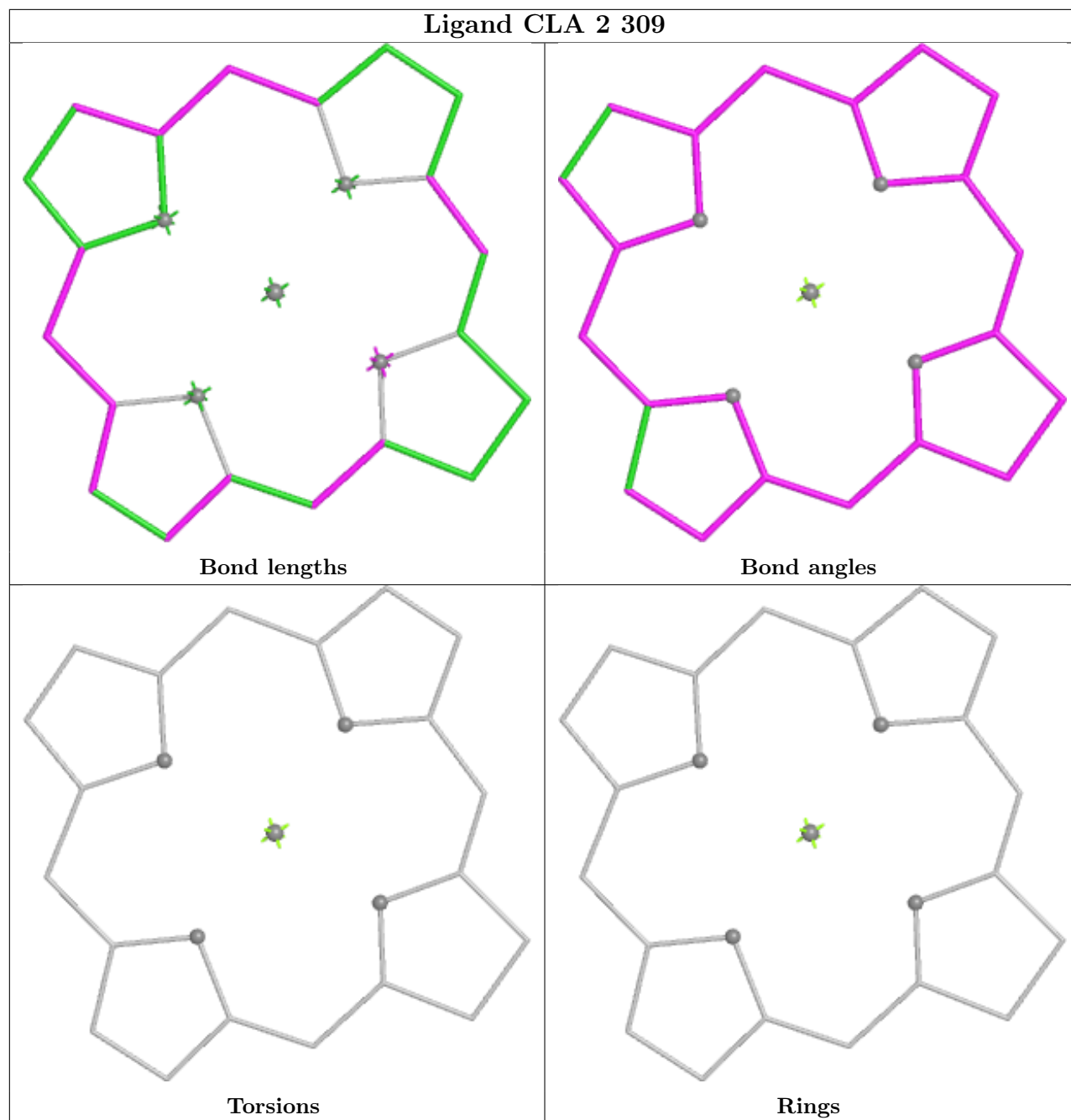




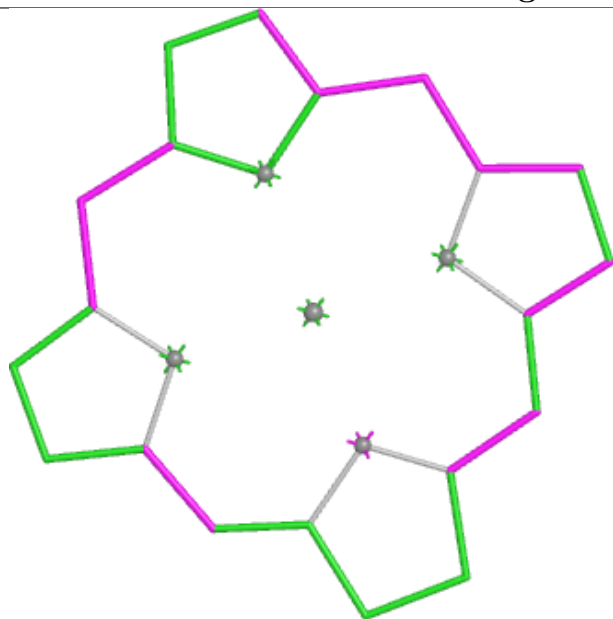




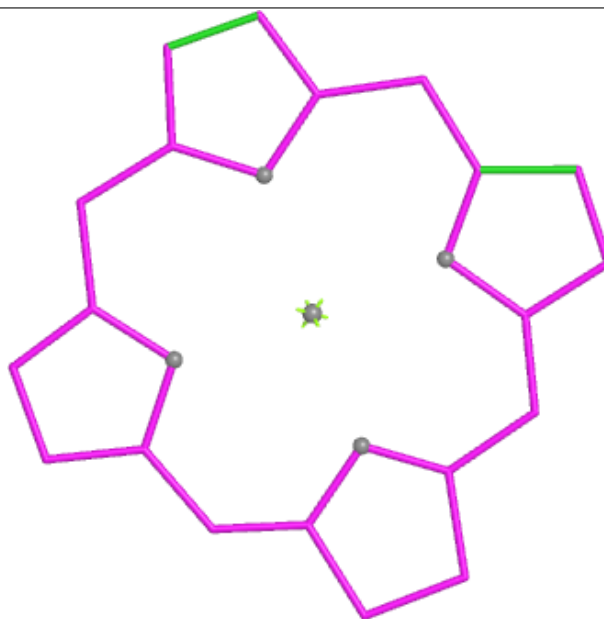
Ligand CLA 2 309



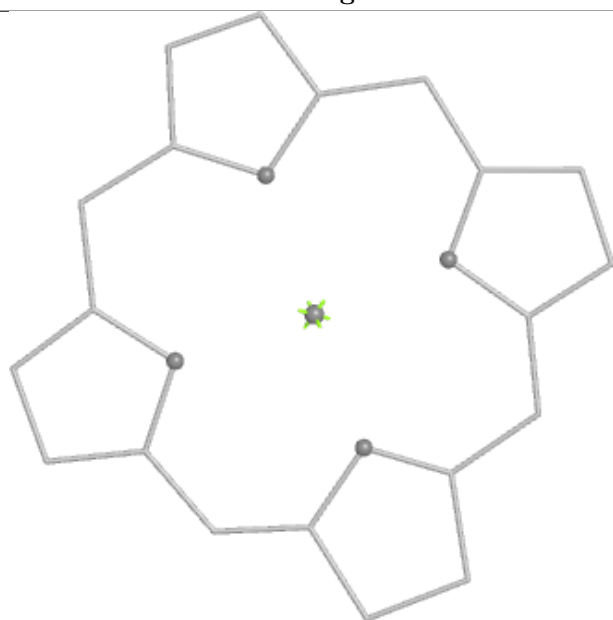
Ligand CLA 2 315



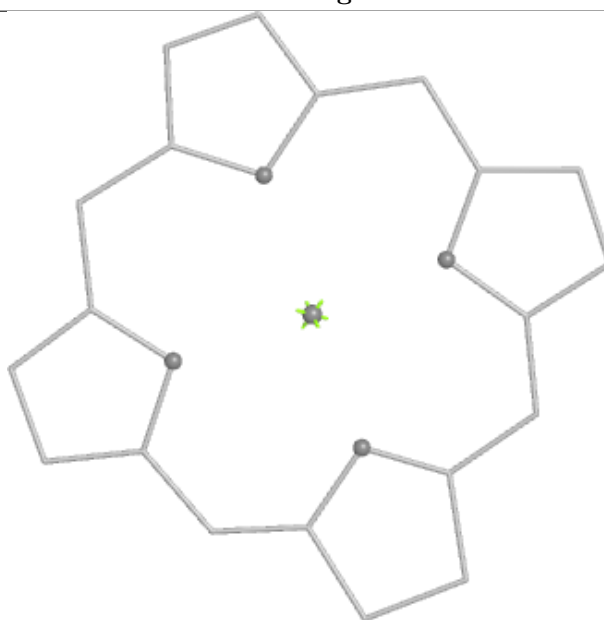
Bond lengths



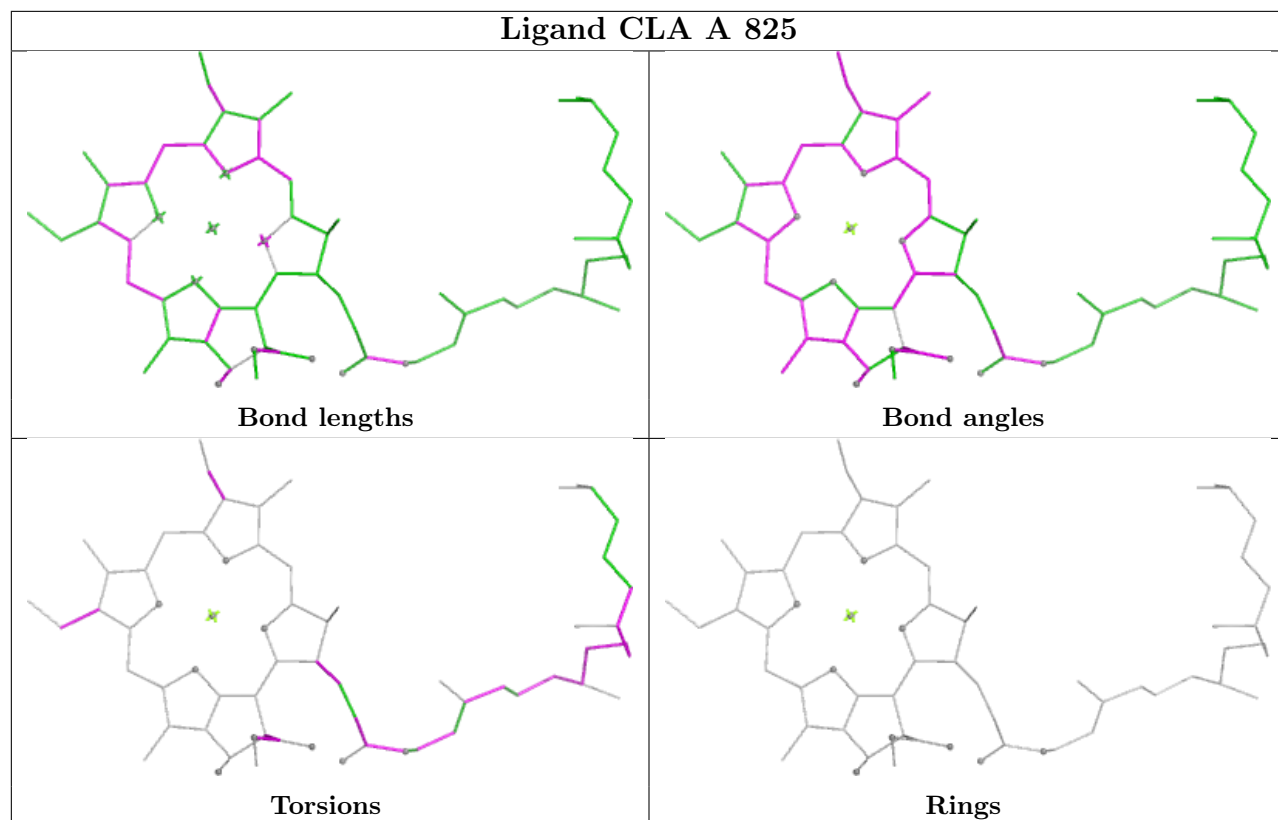
Bond angles



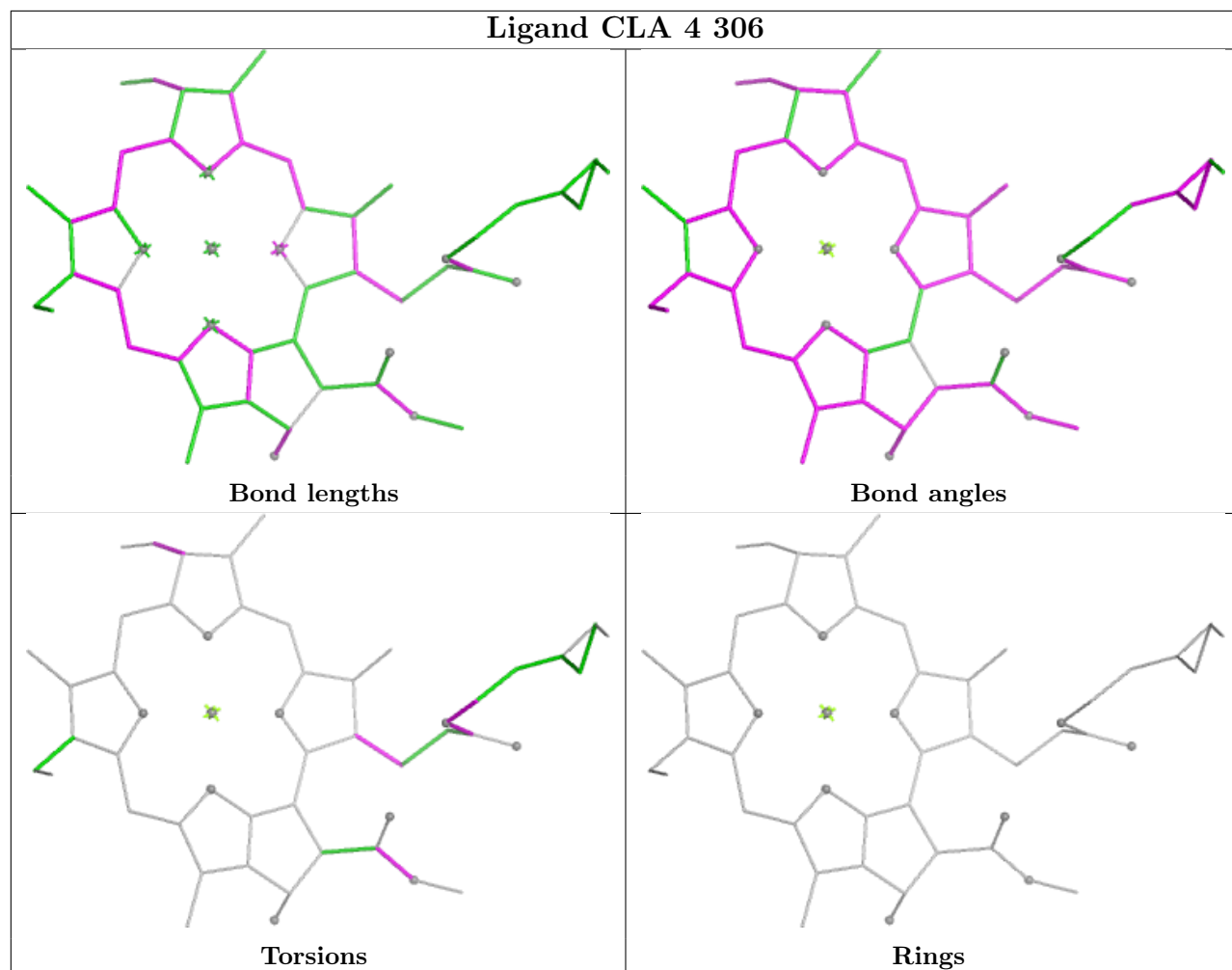
Torsions



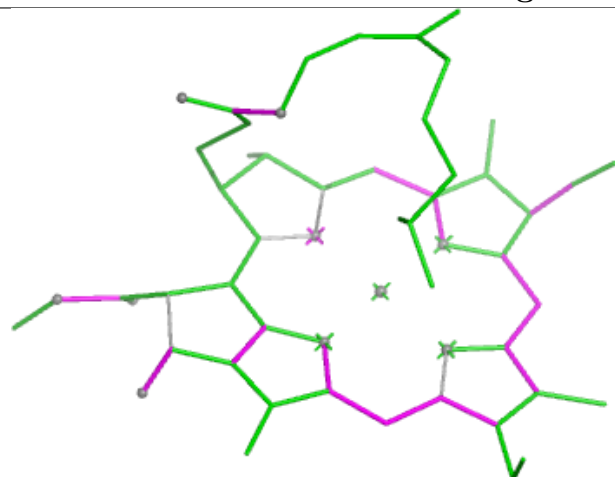
Rings



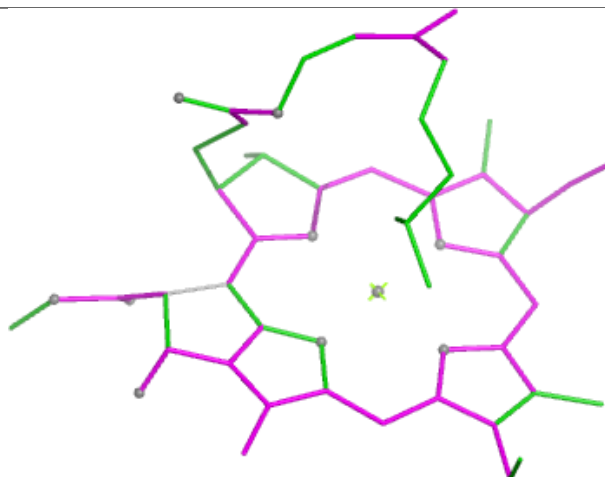
Ligand CLA 4 306



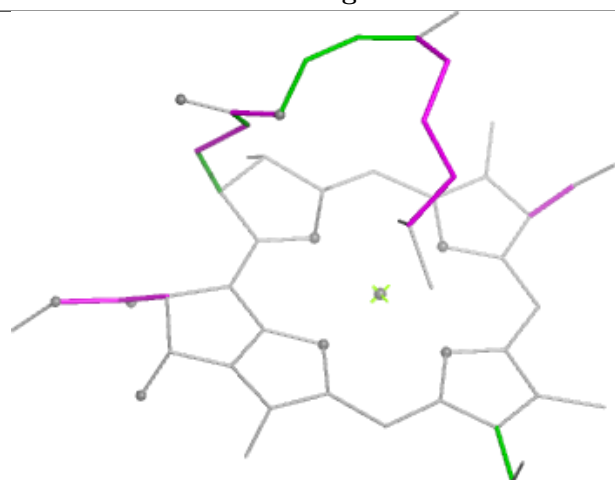
Ligand CLA B 813



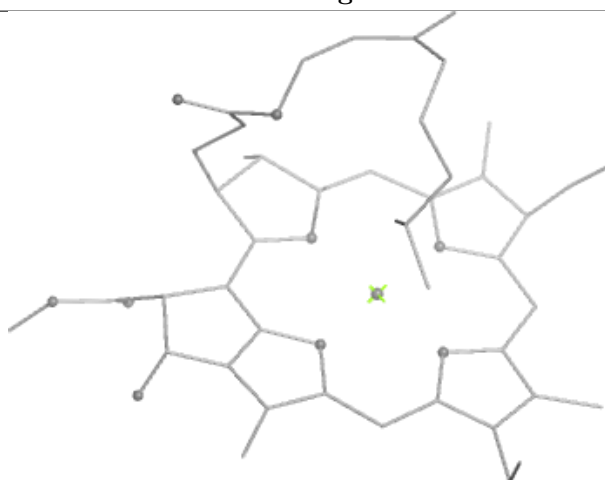
Bond lengths



Bond angles

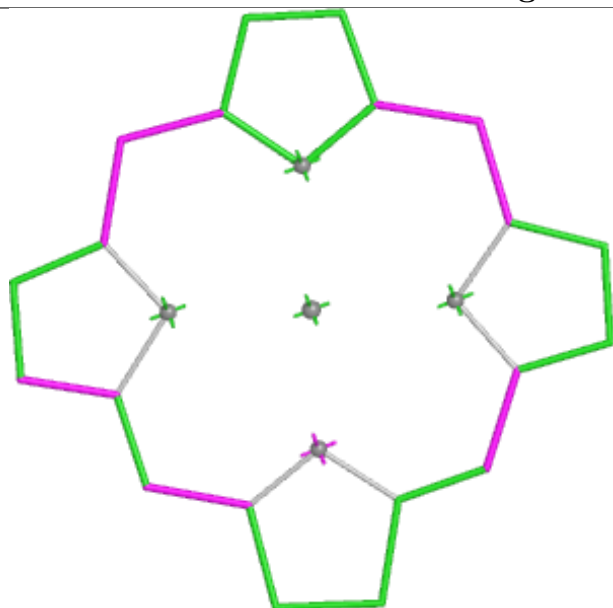


Torsions

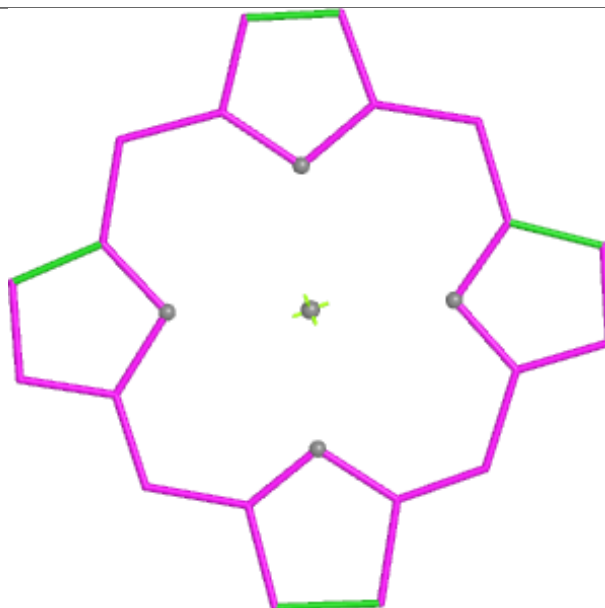


Rings

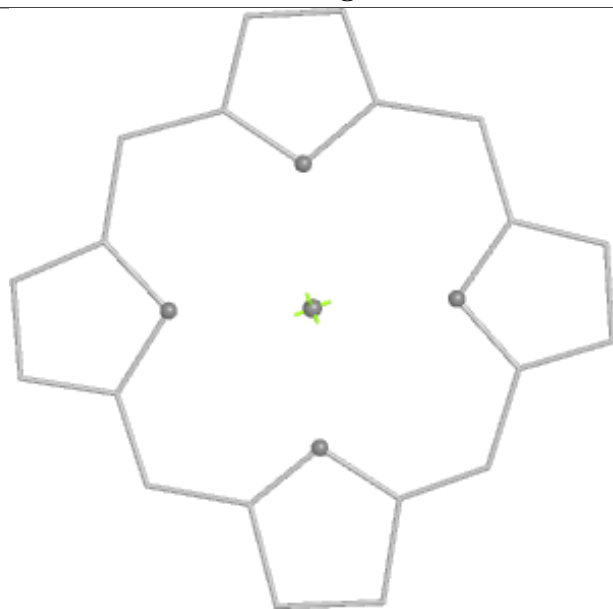
Ligand CLA 3 302



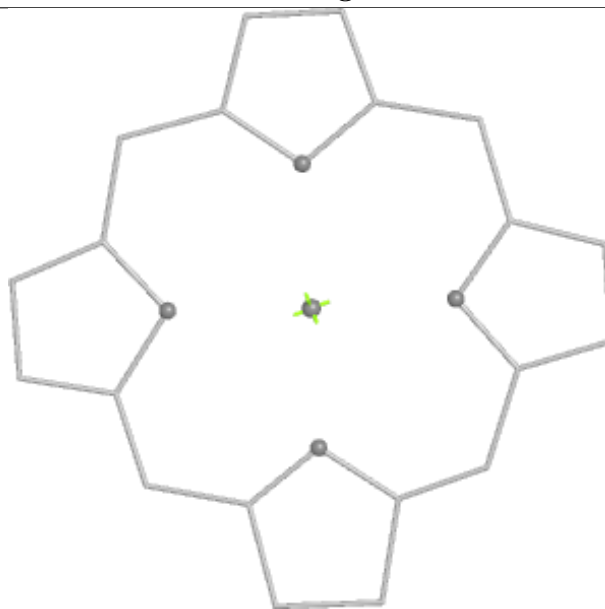
Bond lengths



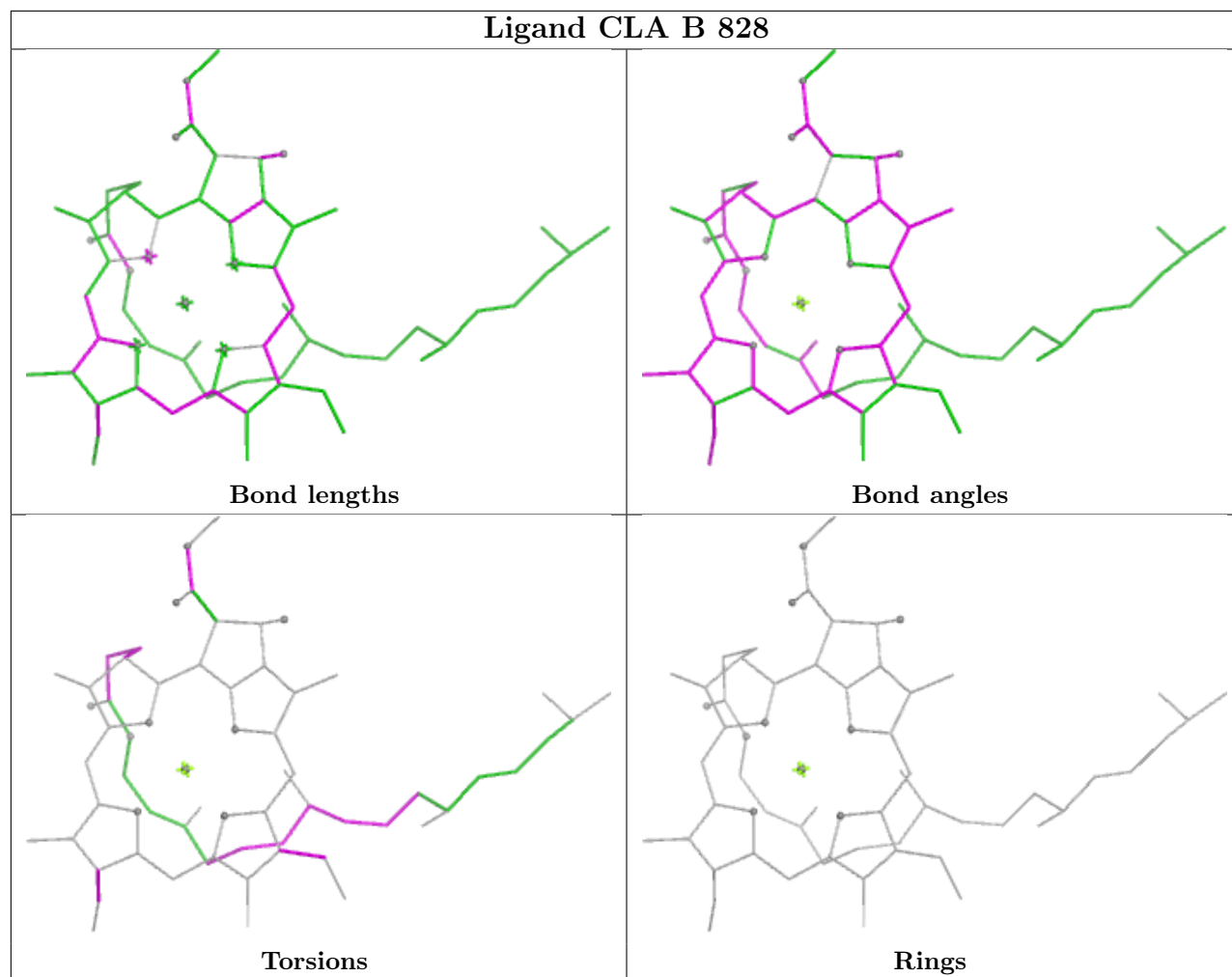
Bond angles



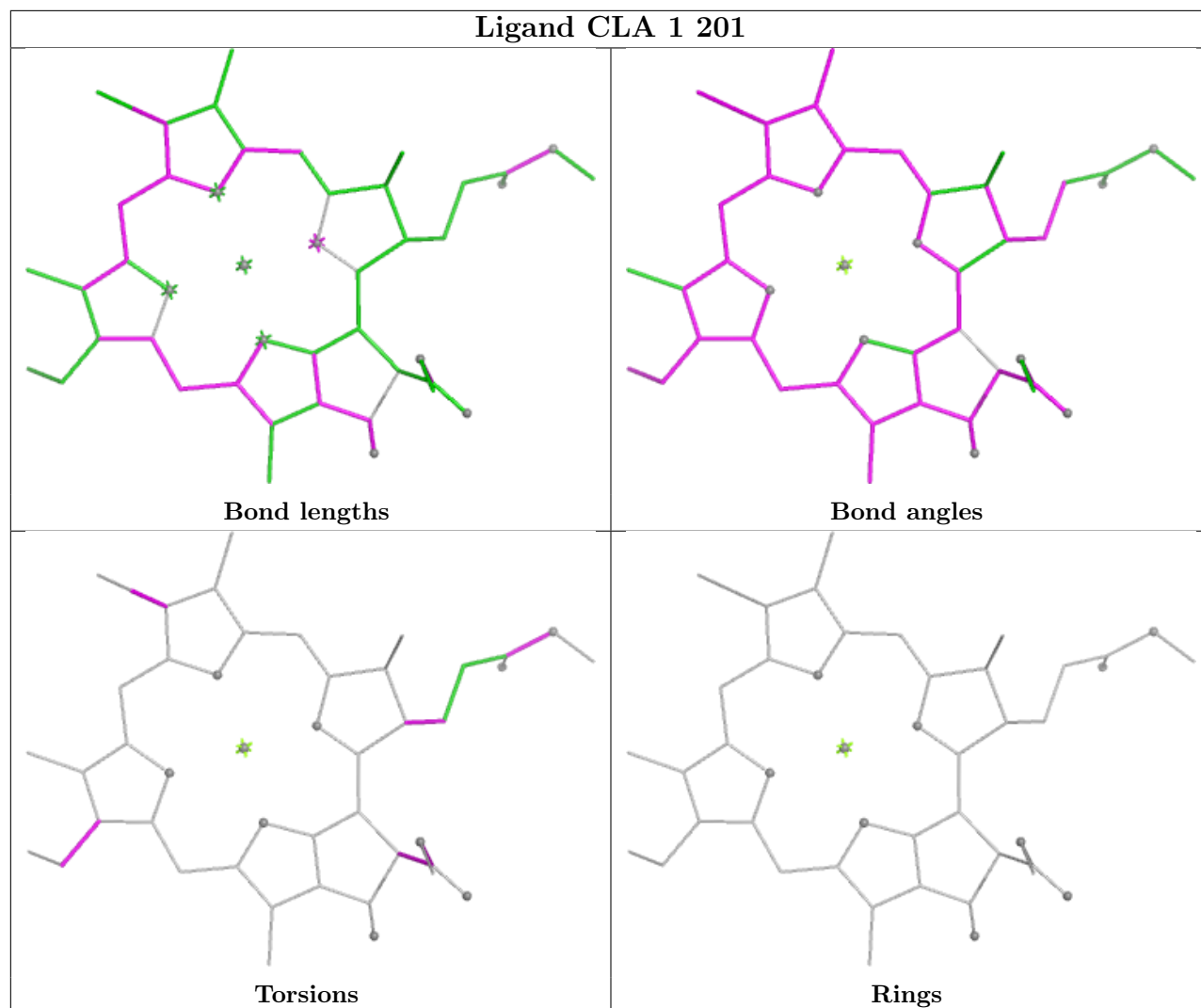
Torsions



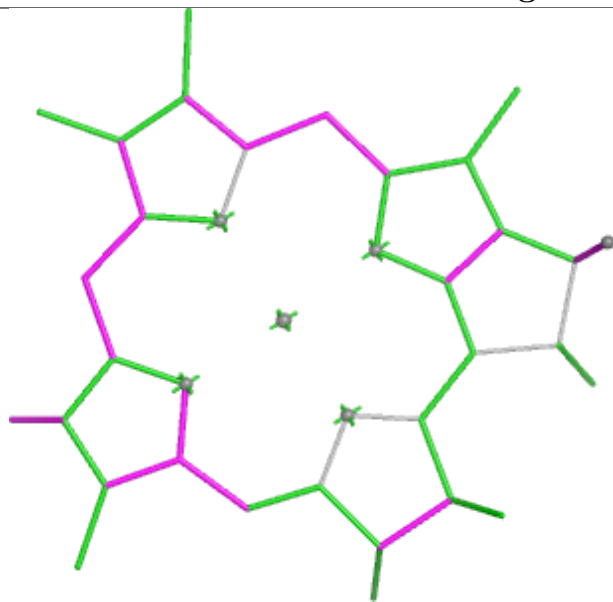
Rings



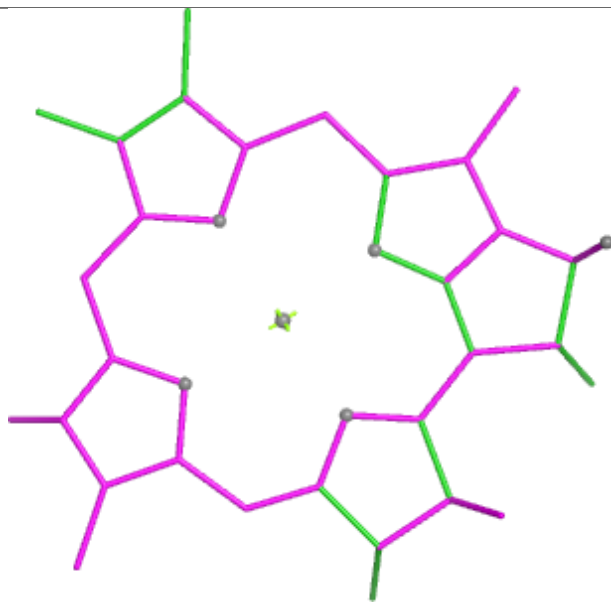
Ligand CLA 1 201



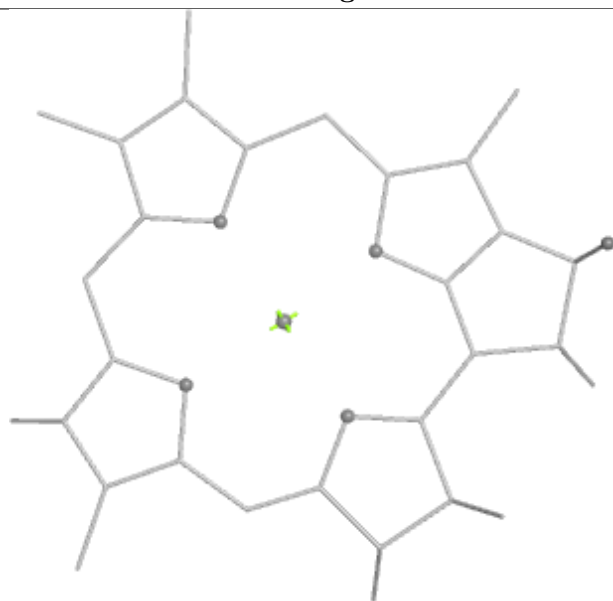
Ligand CLA 1 205



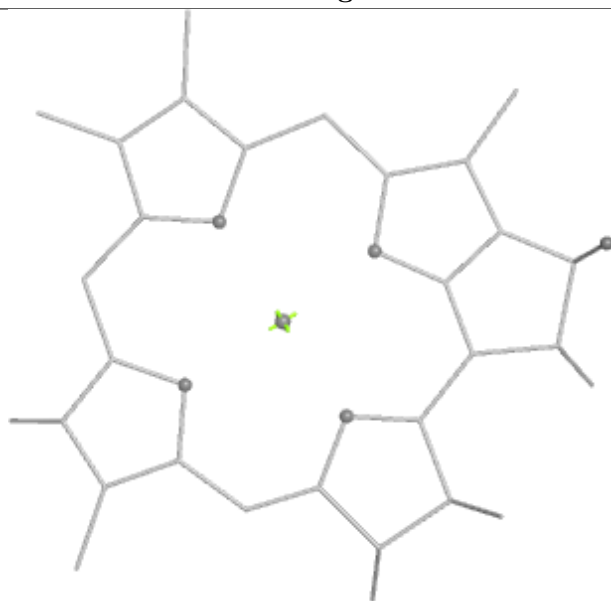
Bond lengths



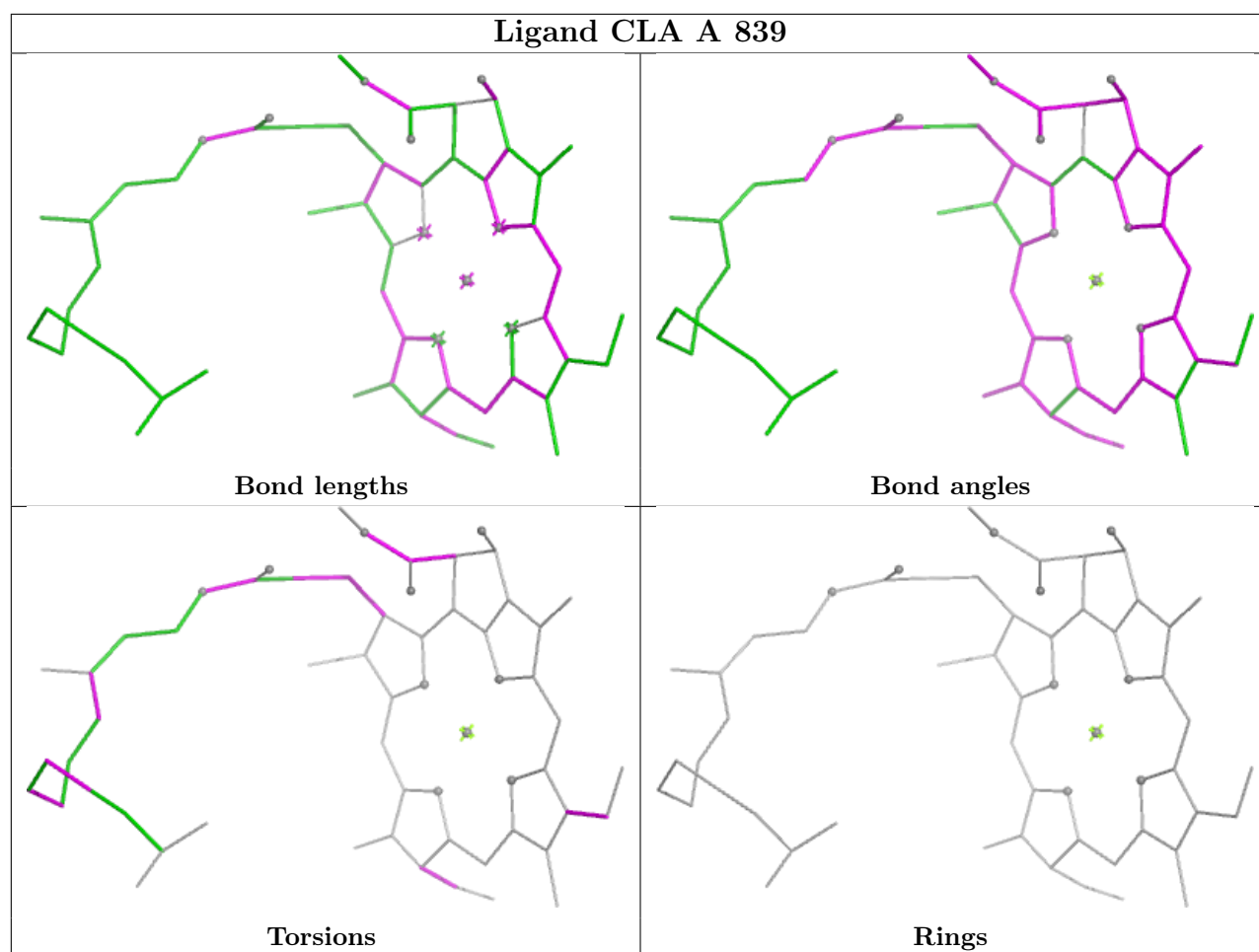
Bond angles



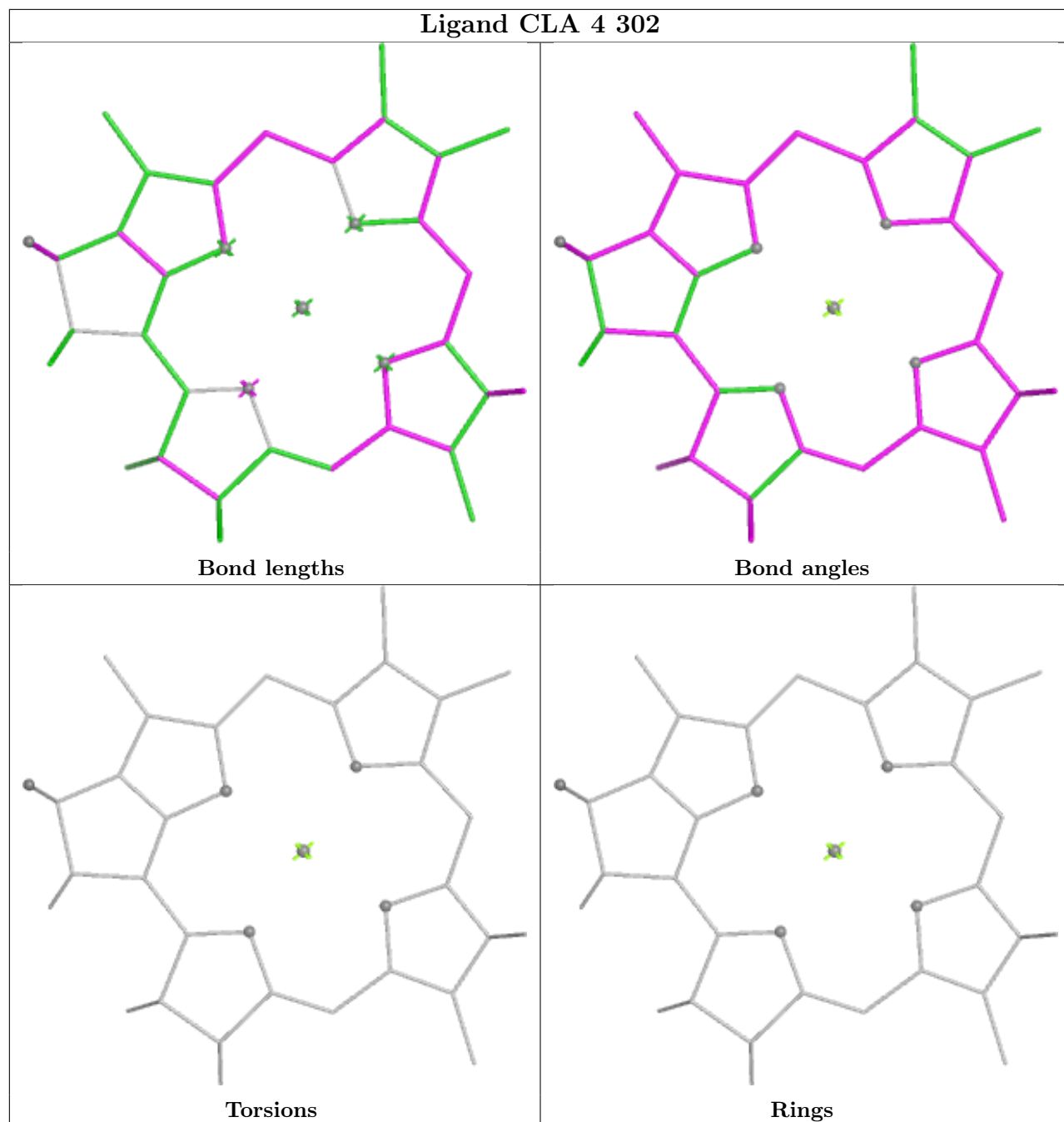
Torsions

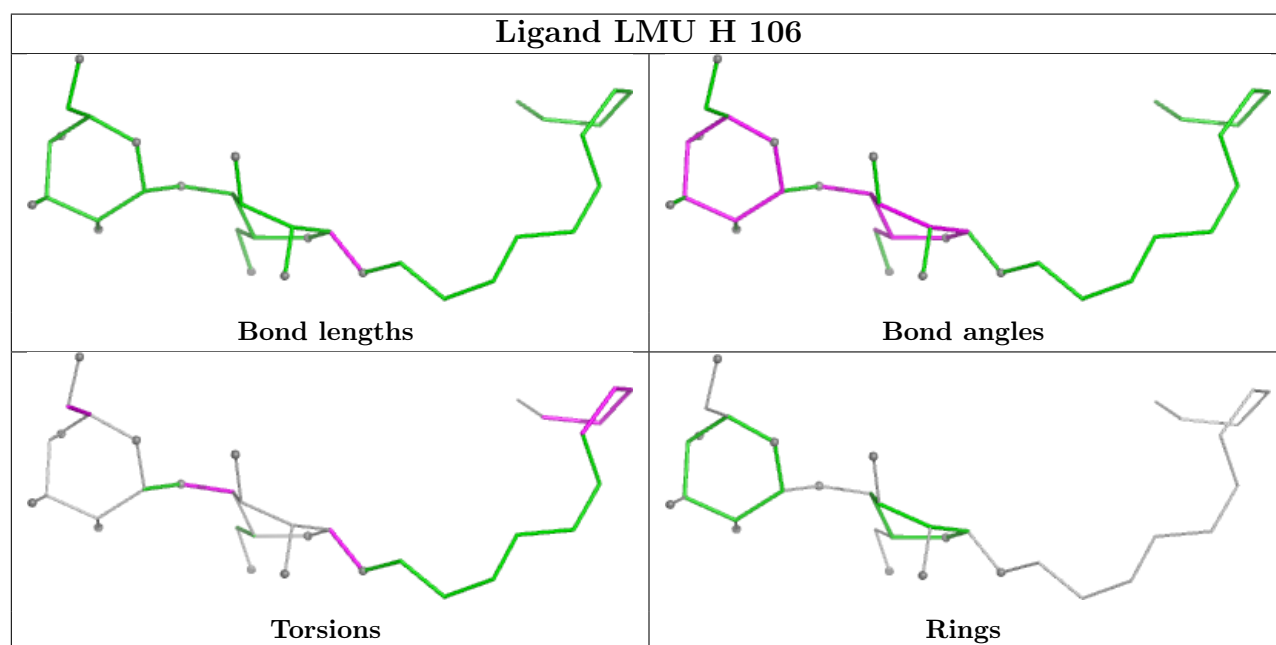
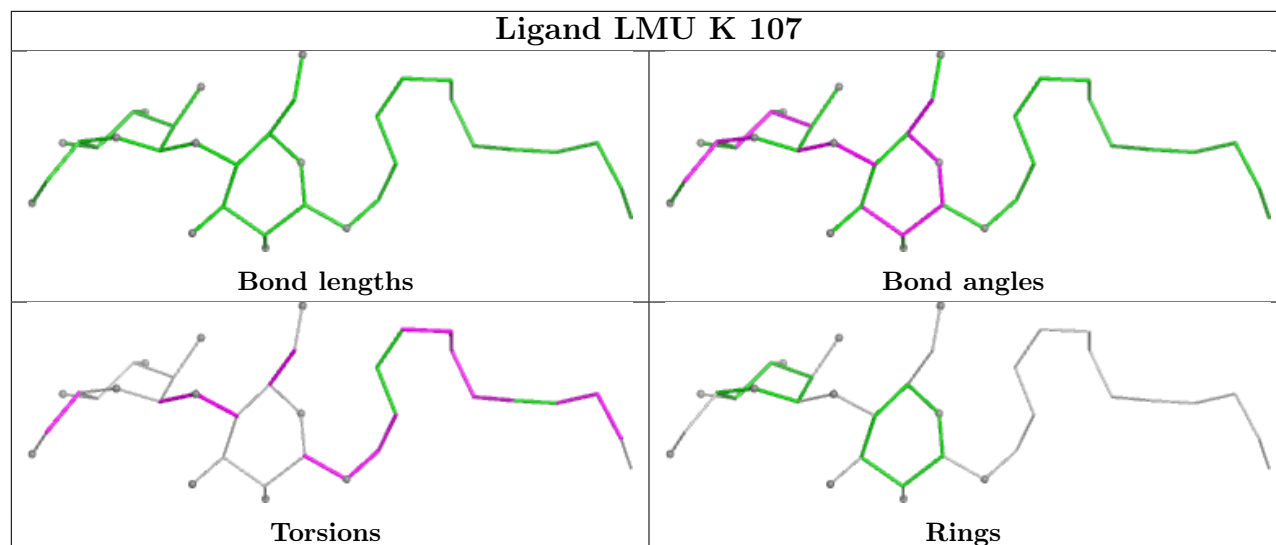


Rings

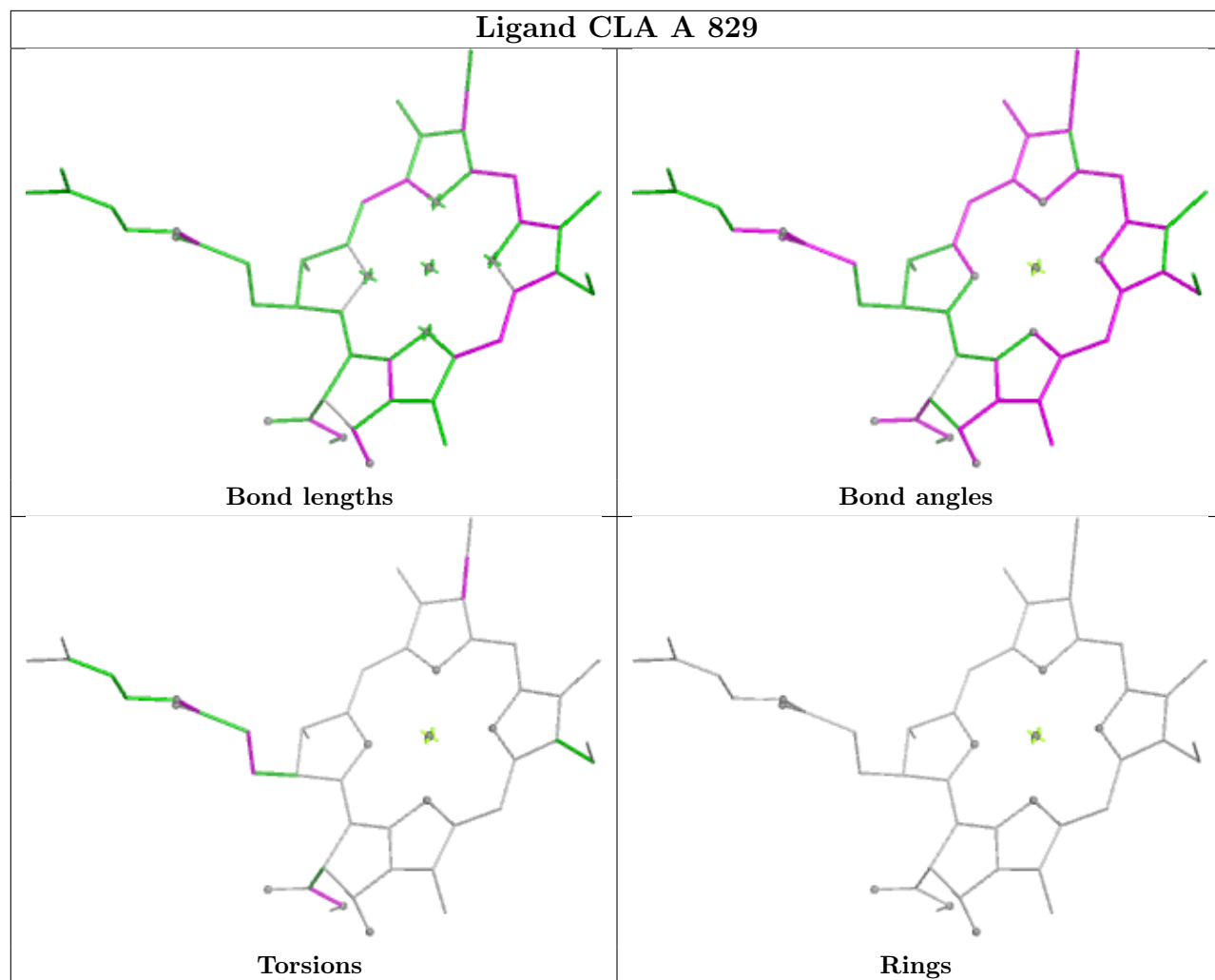


Ligand CLA 4 302

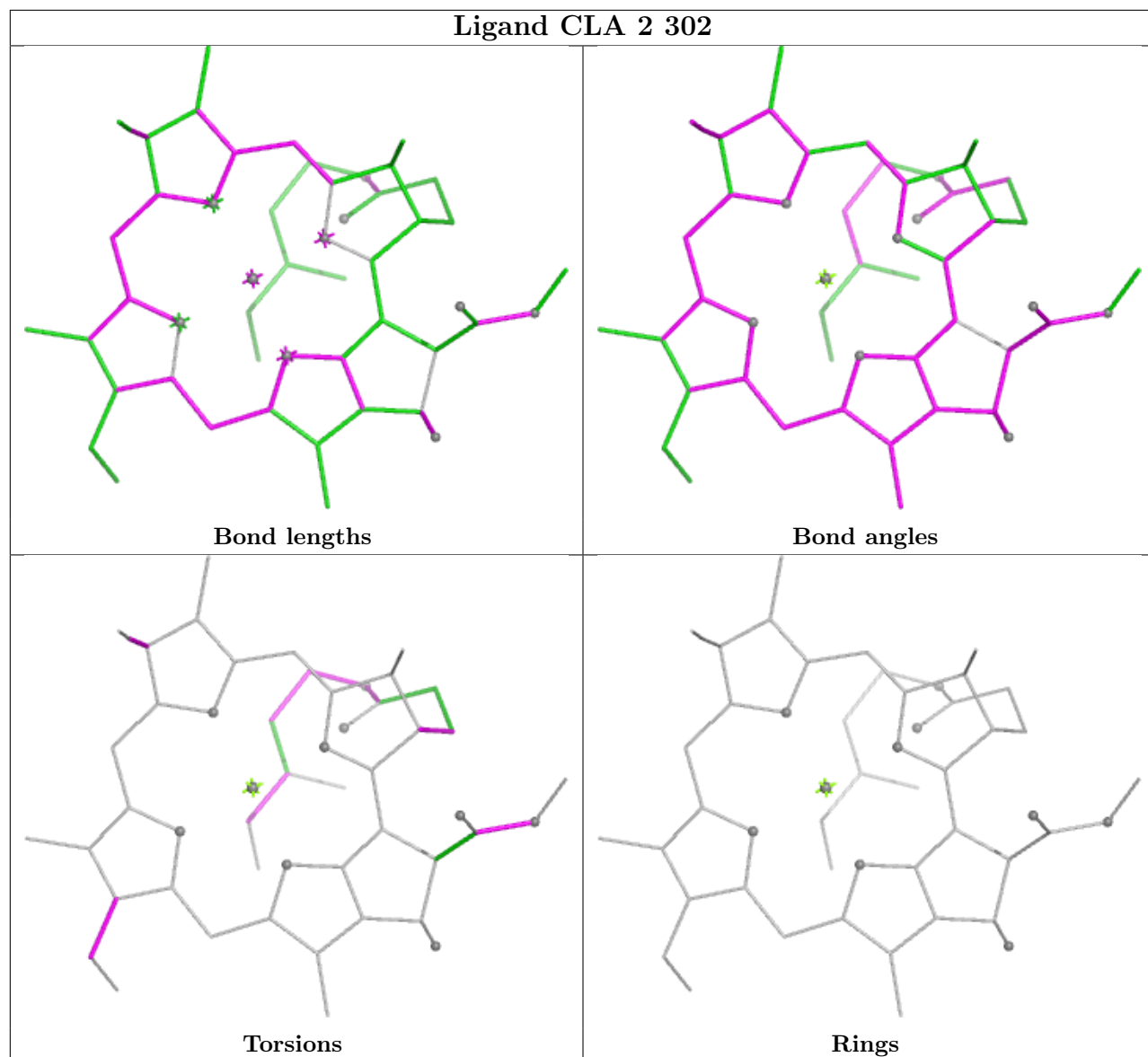


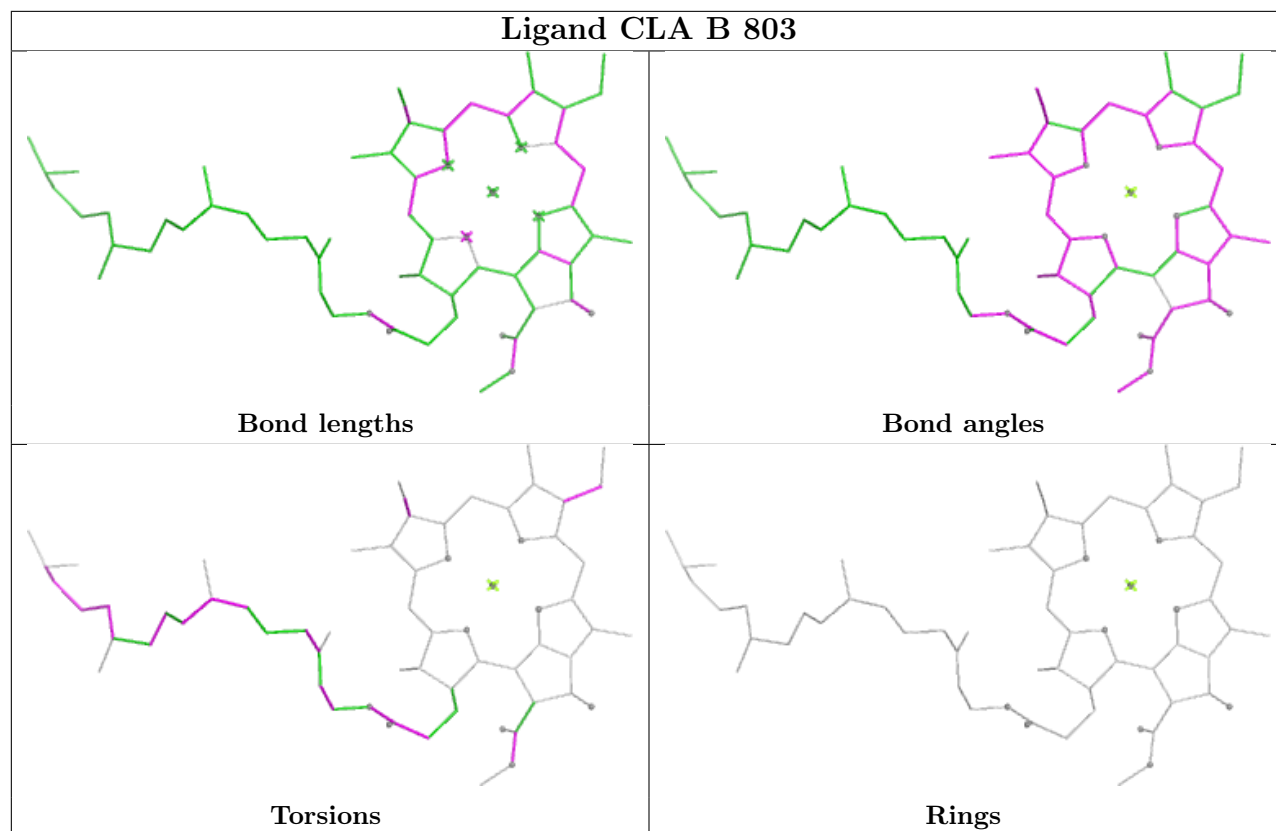


Ligand CLA A 829

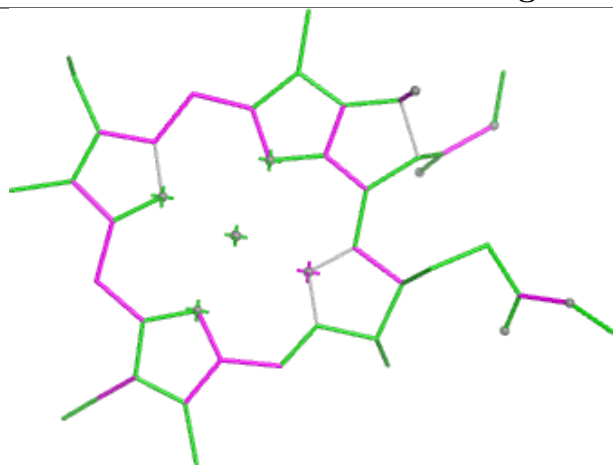


Ligand CLA 2 302

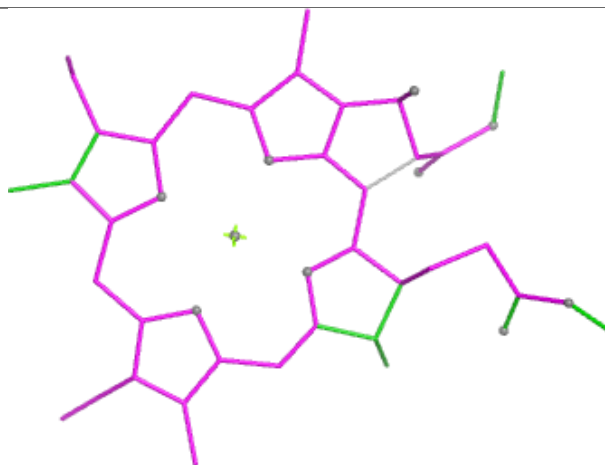




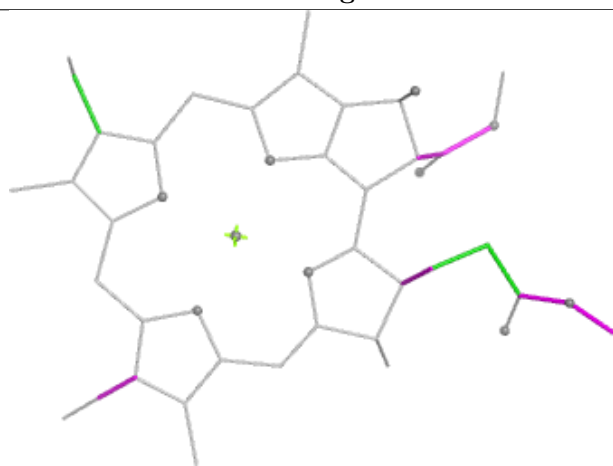
Ligand CLA 1 203



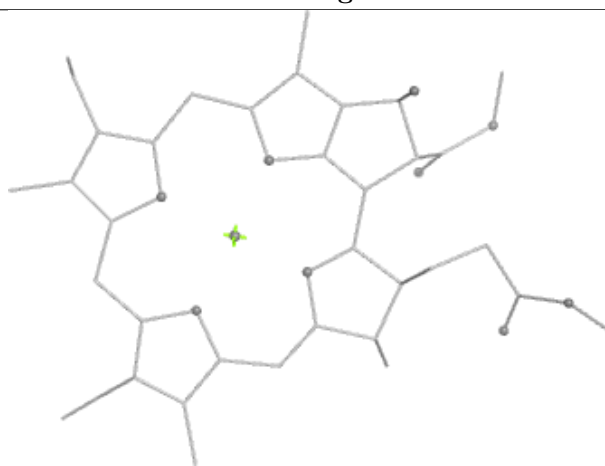
Bond lengths



Bond angles

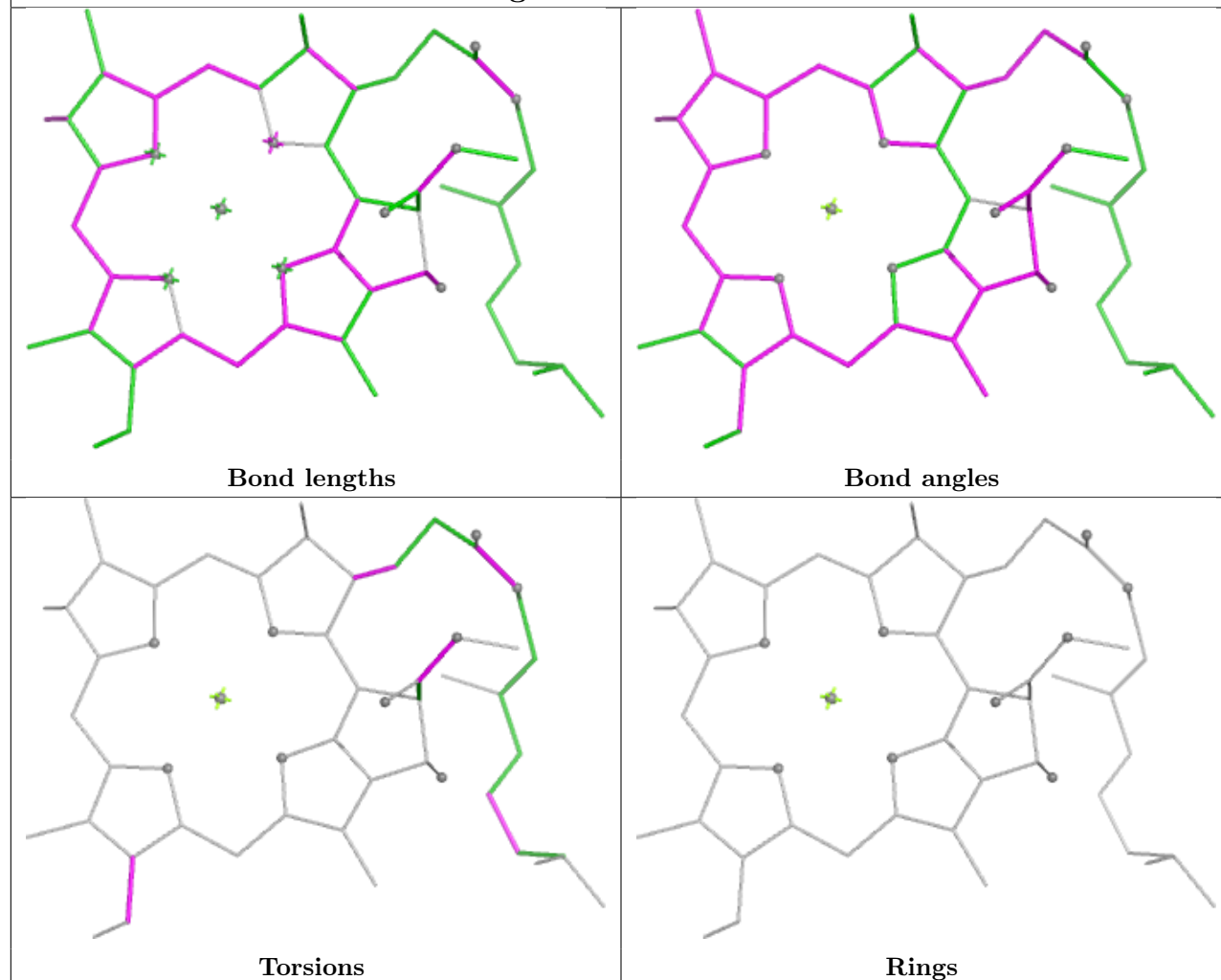


Torsions

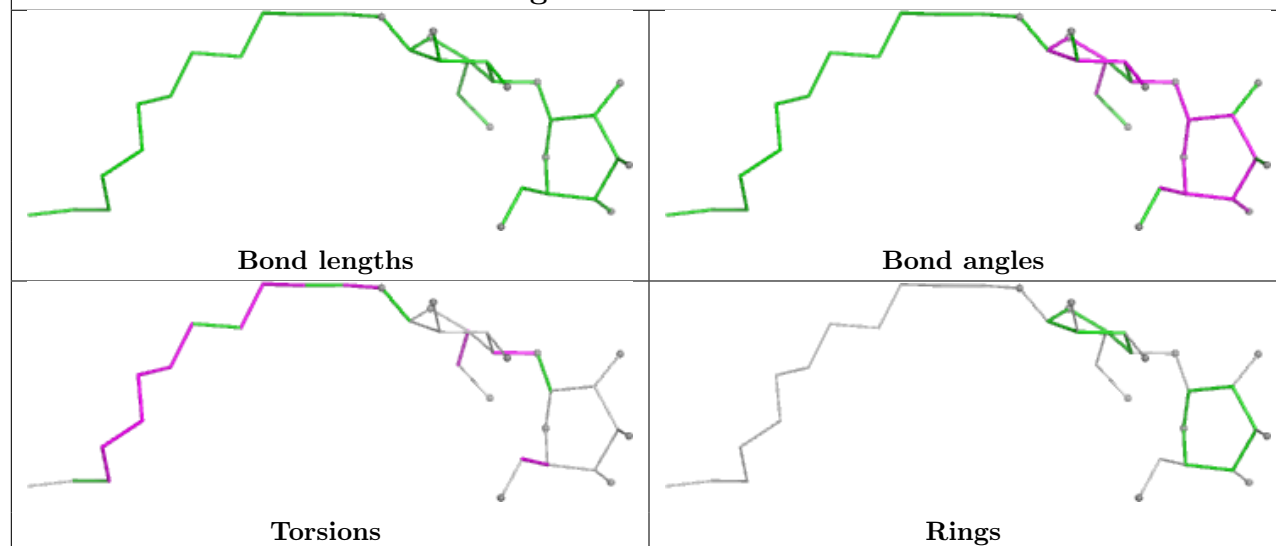


Rings

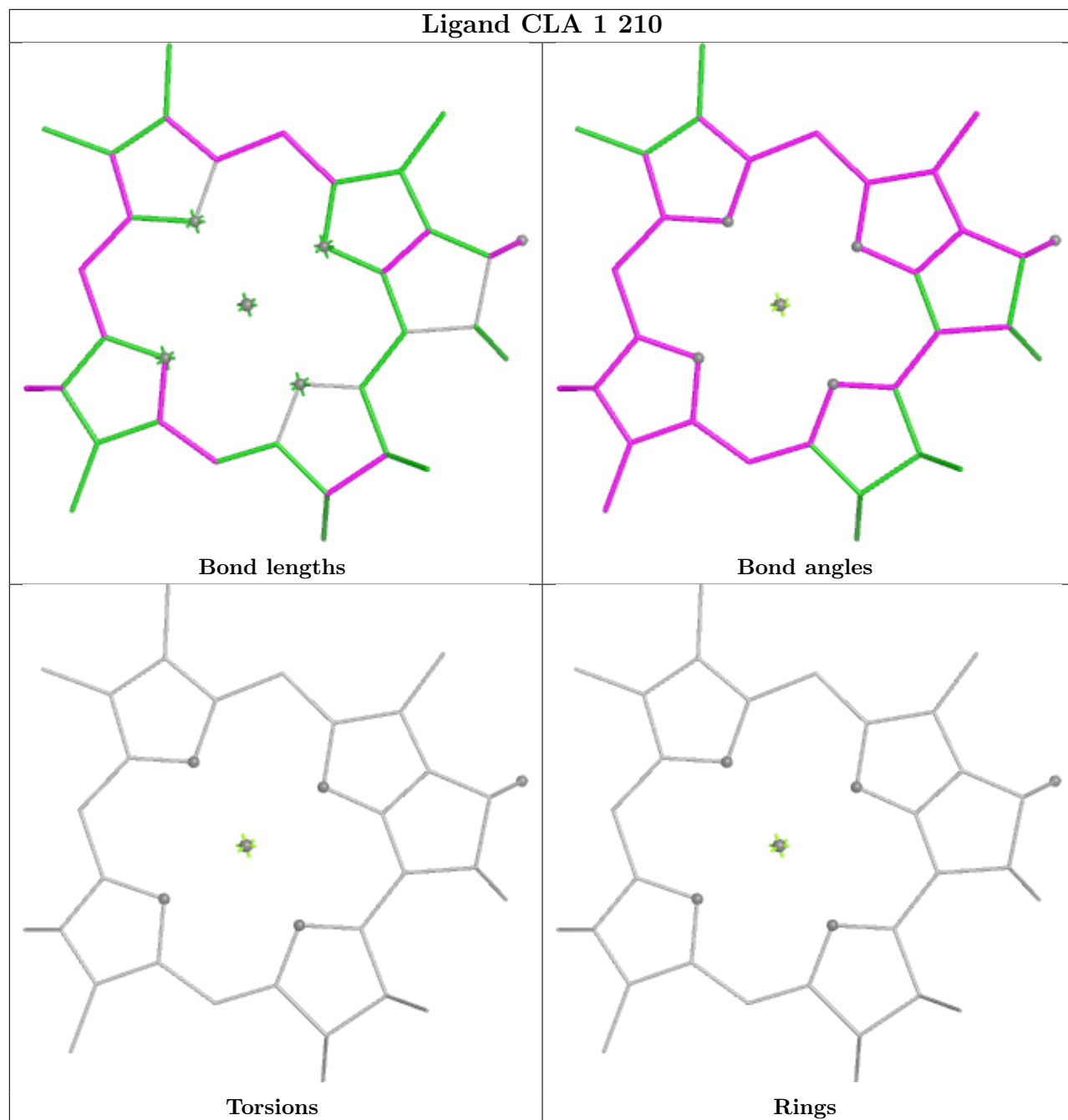
Ligand CLA B 812

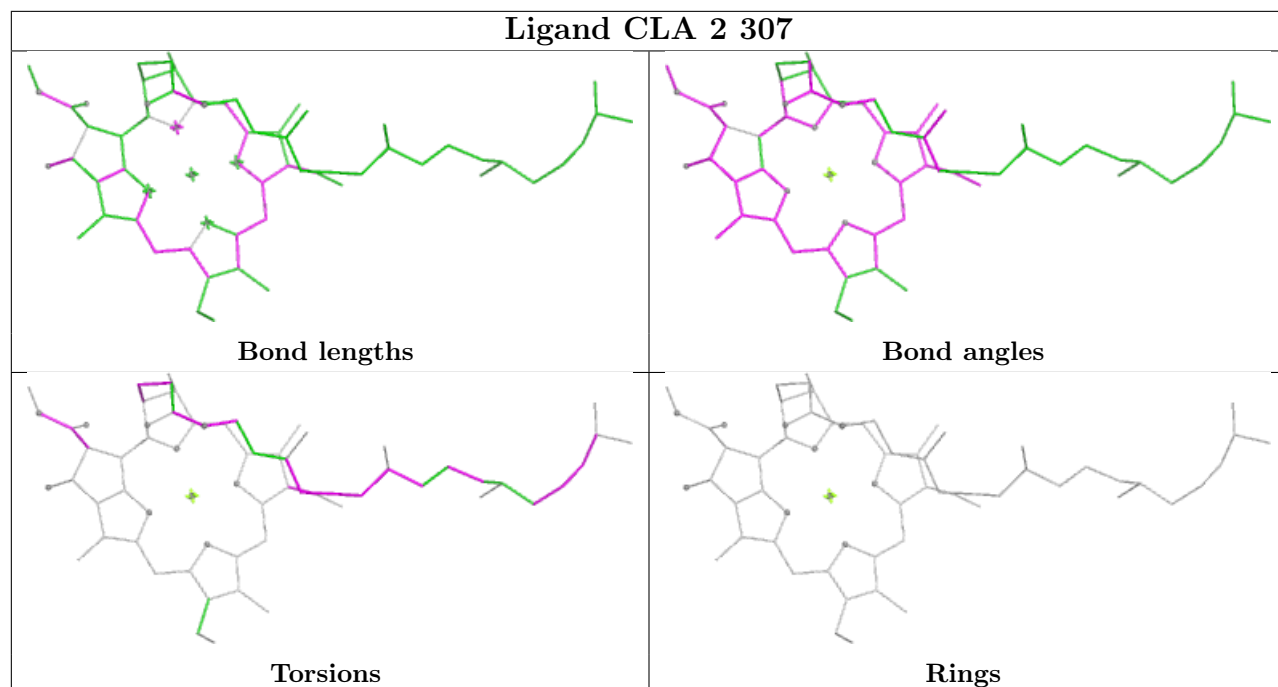


Ligand LMU L 205

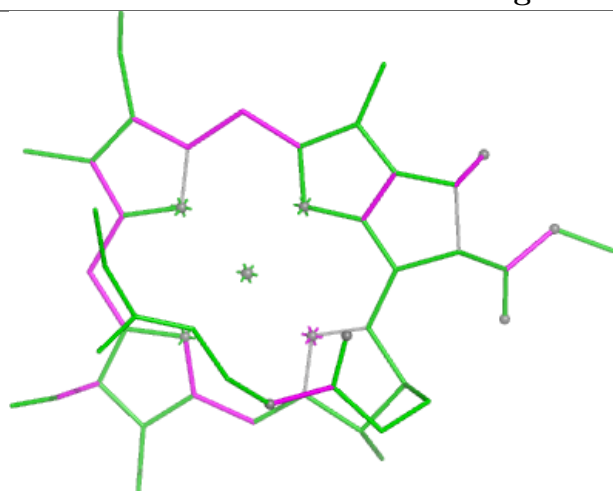


Ligand CLA 1 210

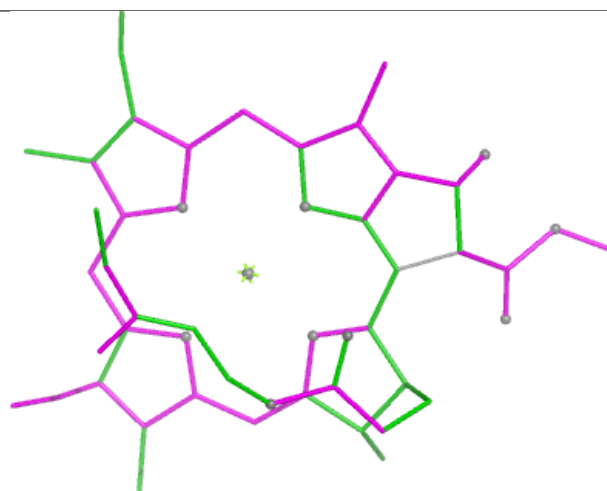




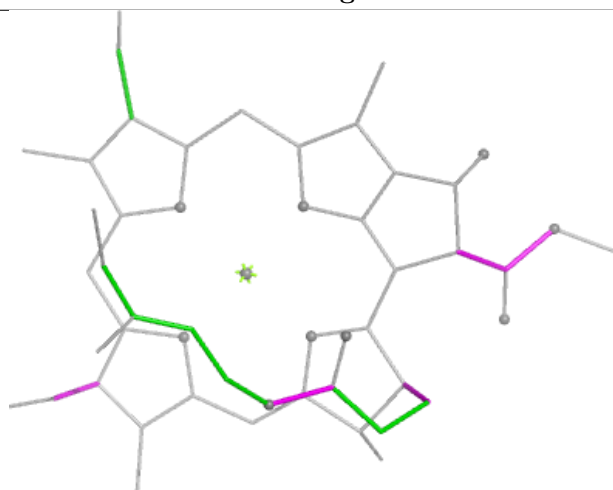
Ligand CLA A 820



Bond lengths



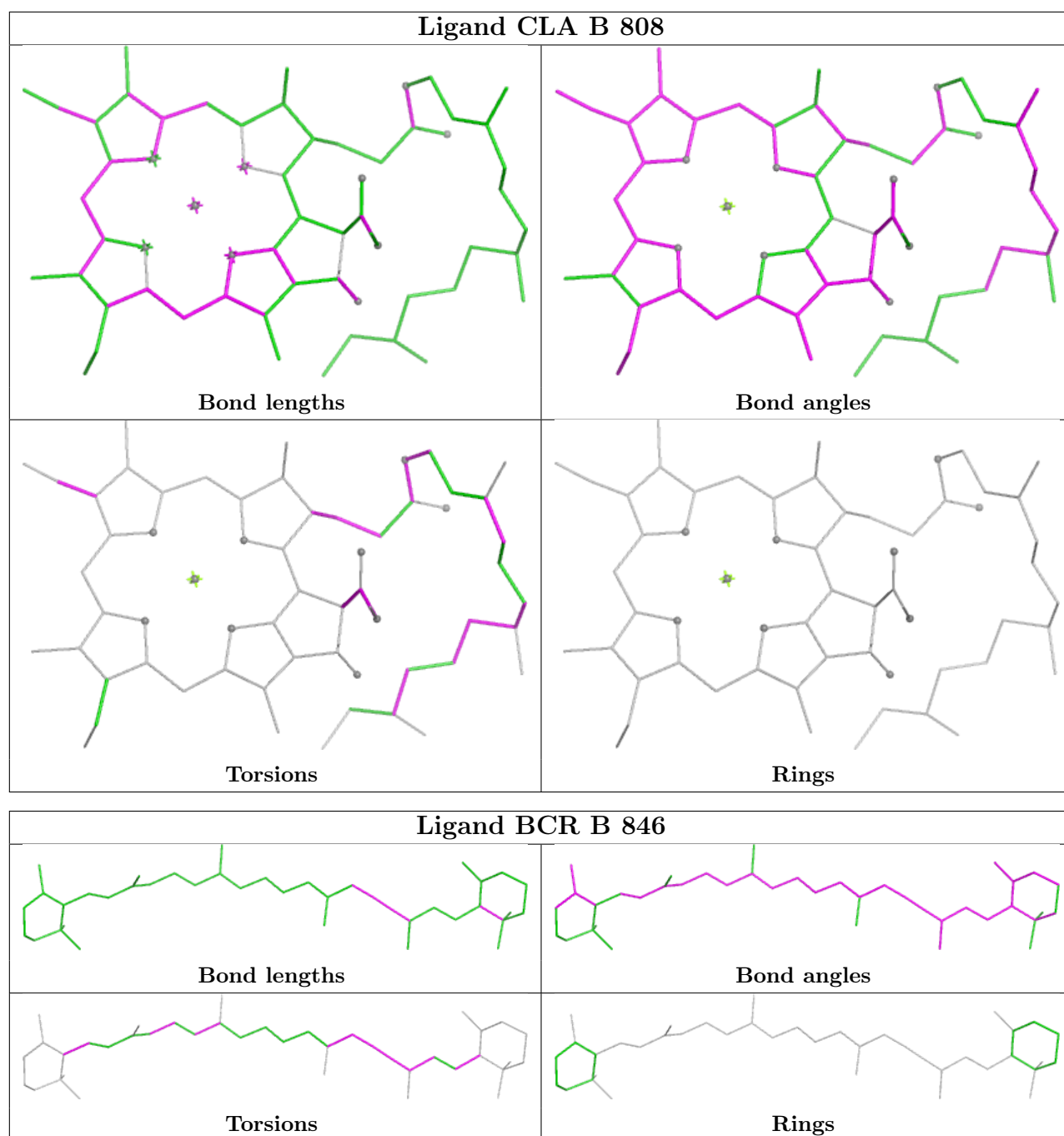
Bond angles



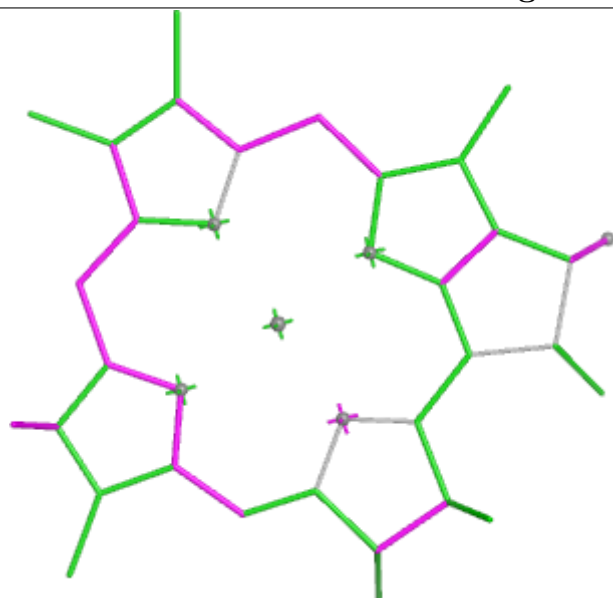
Torsions



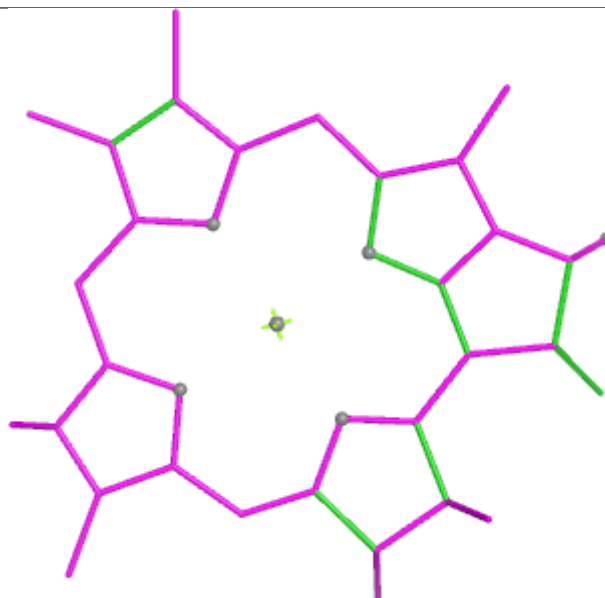
Rings



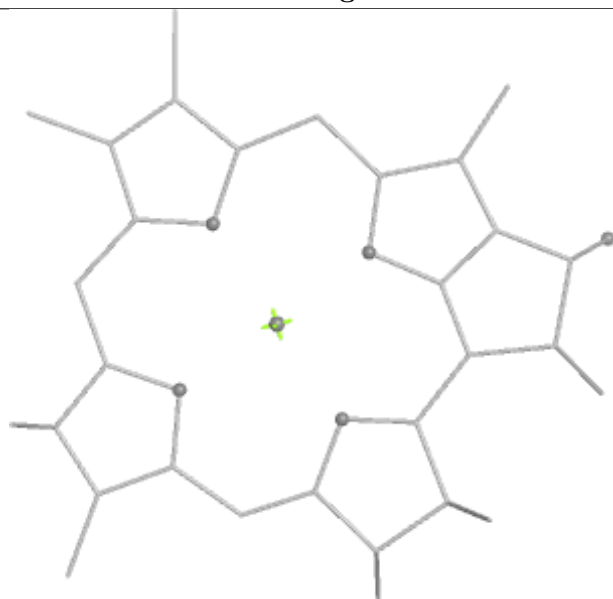
Ligand CLA 4 313



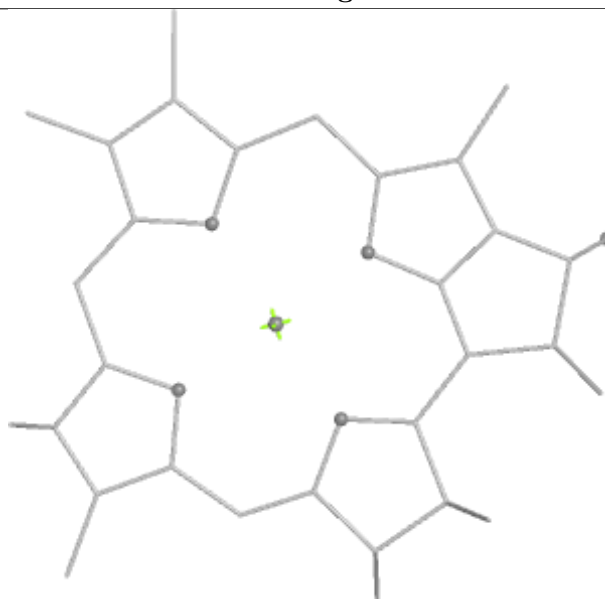
Bond lengths



Bond angles

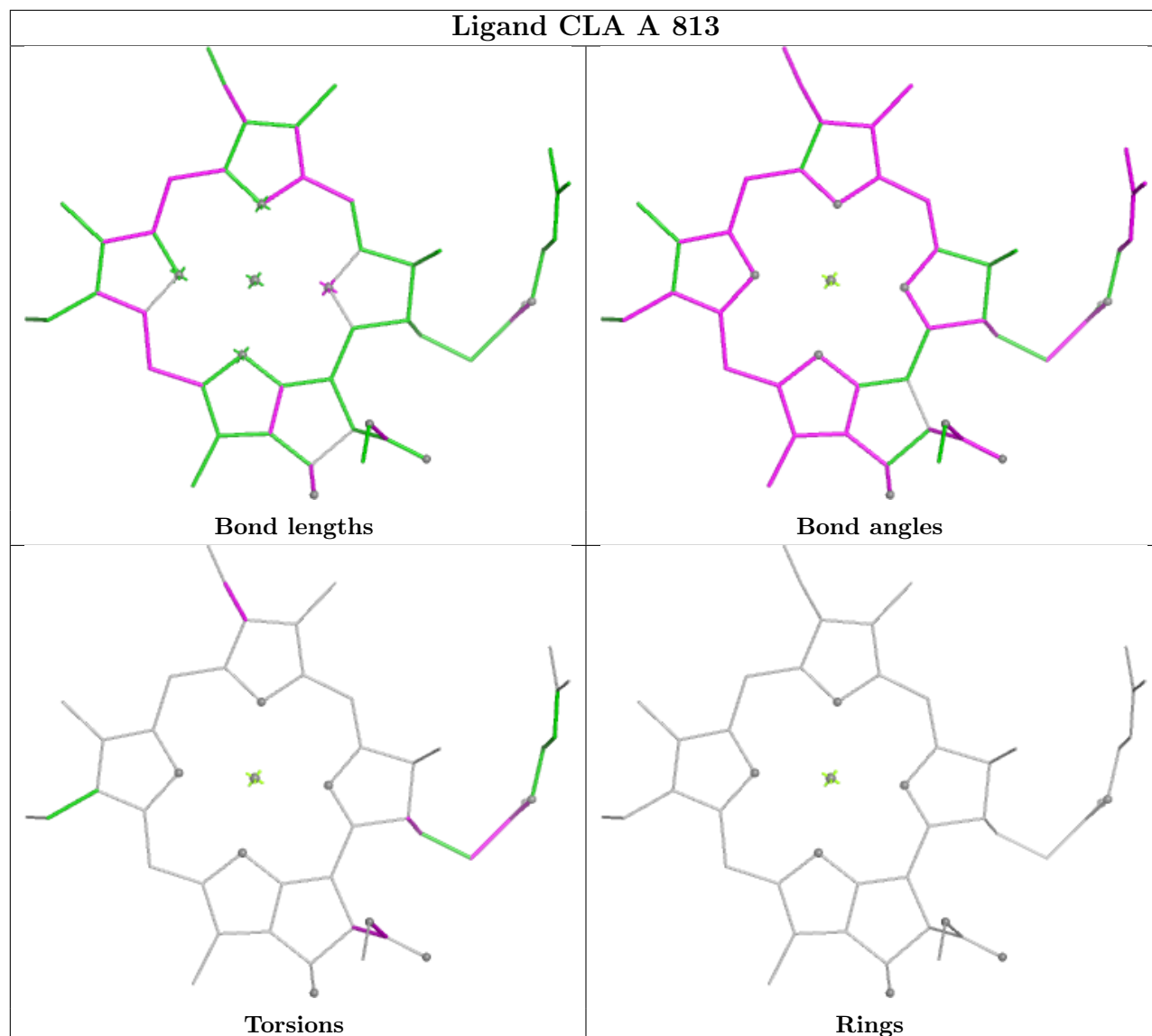


Torsions

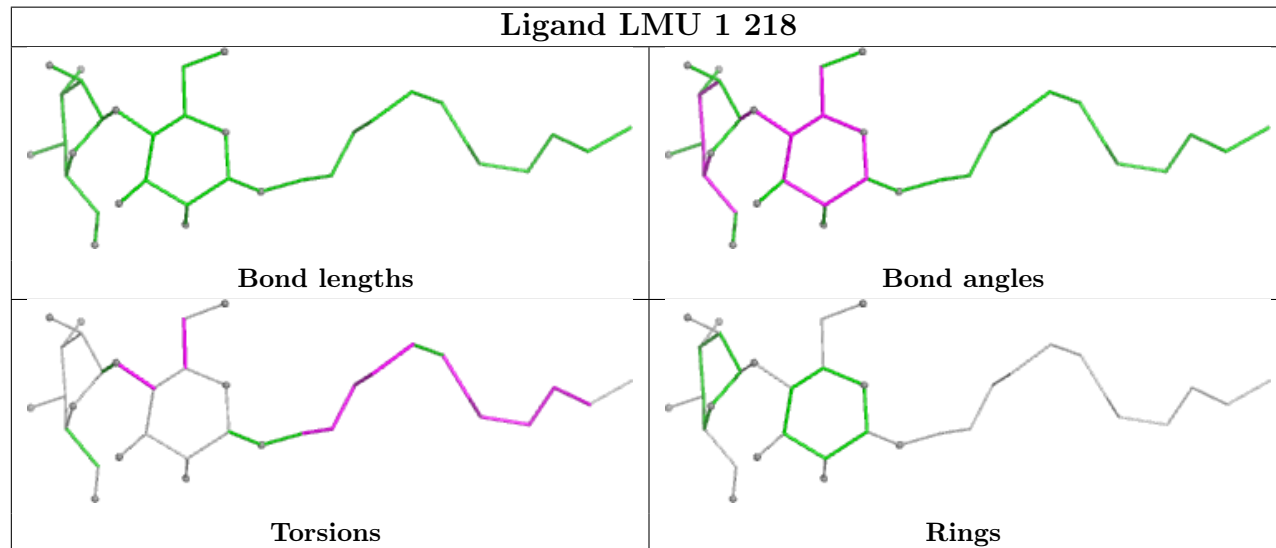


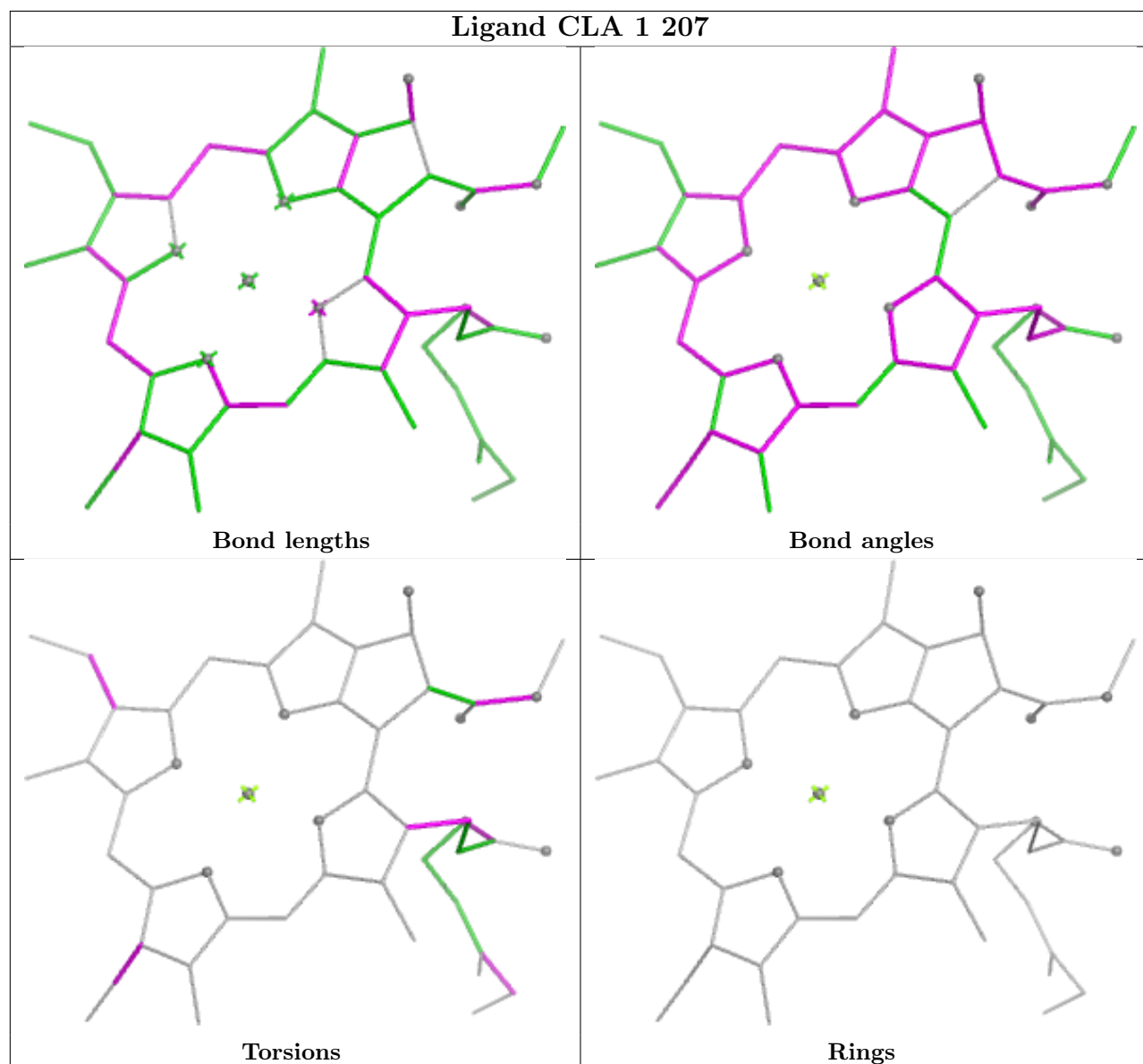
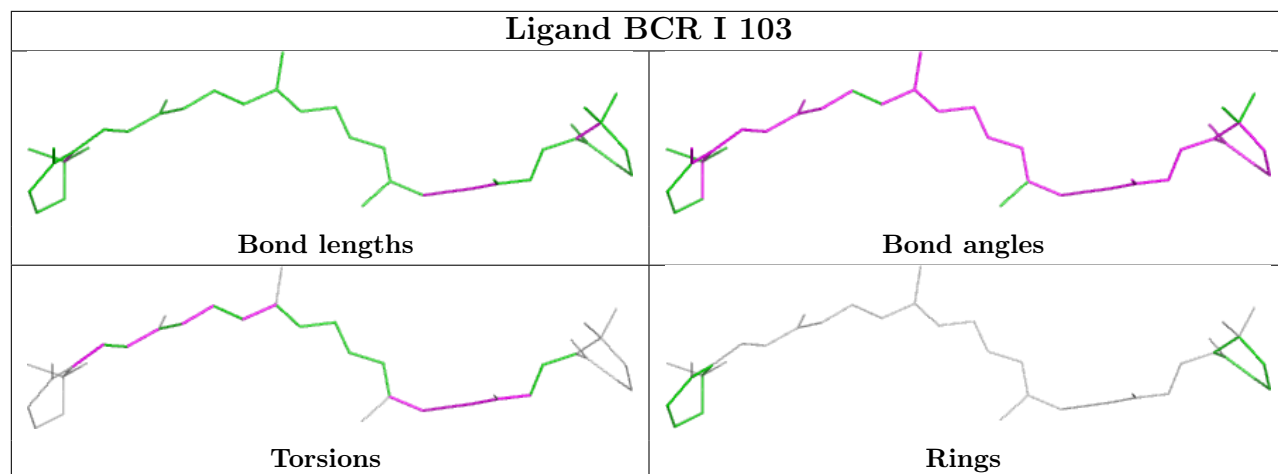
Rings

Ligand CLA A 813

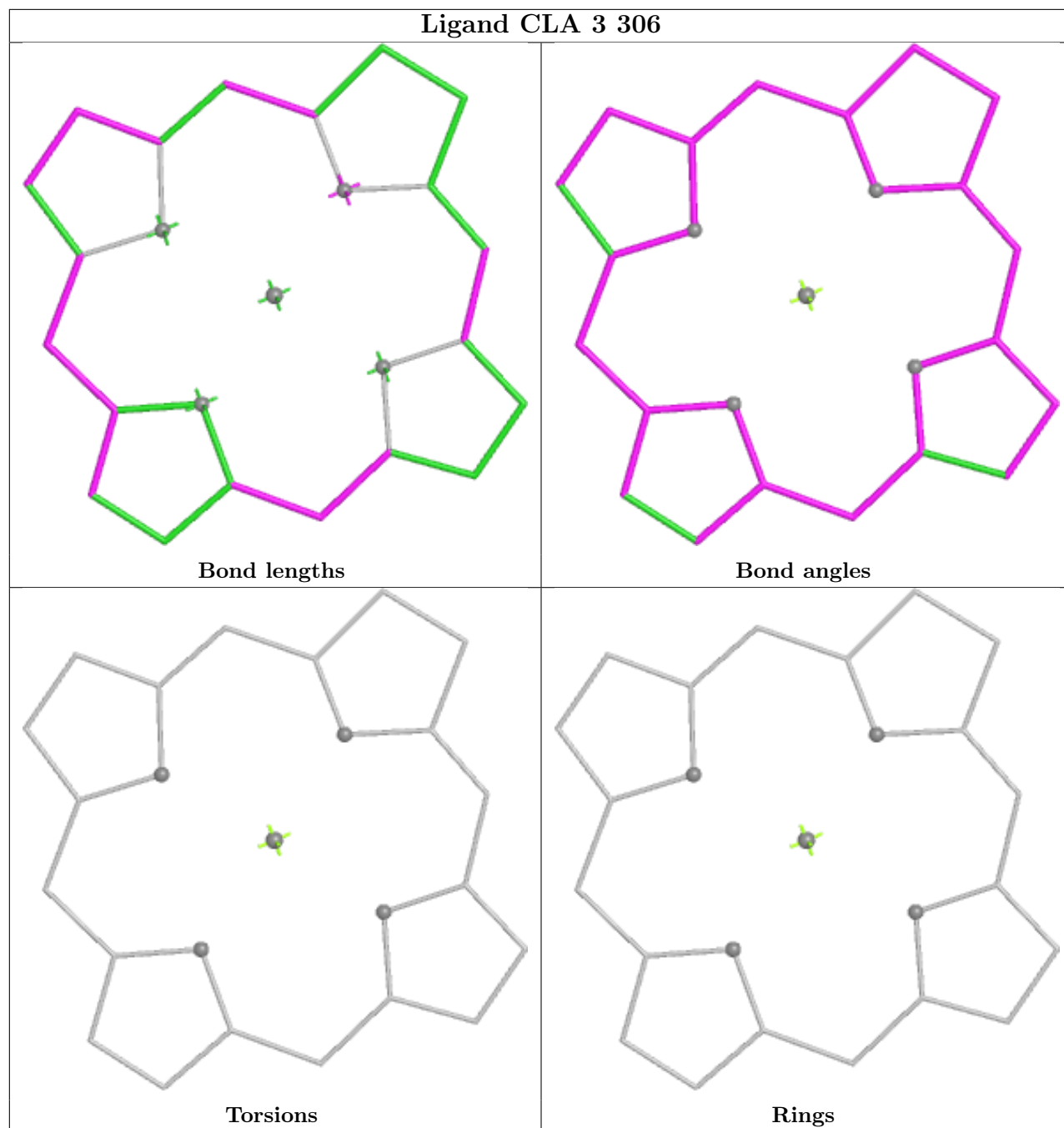


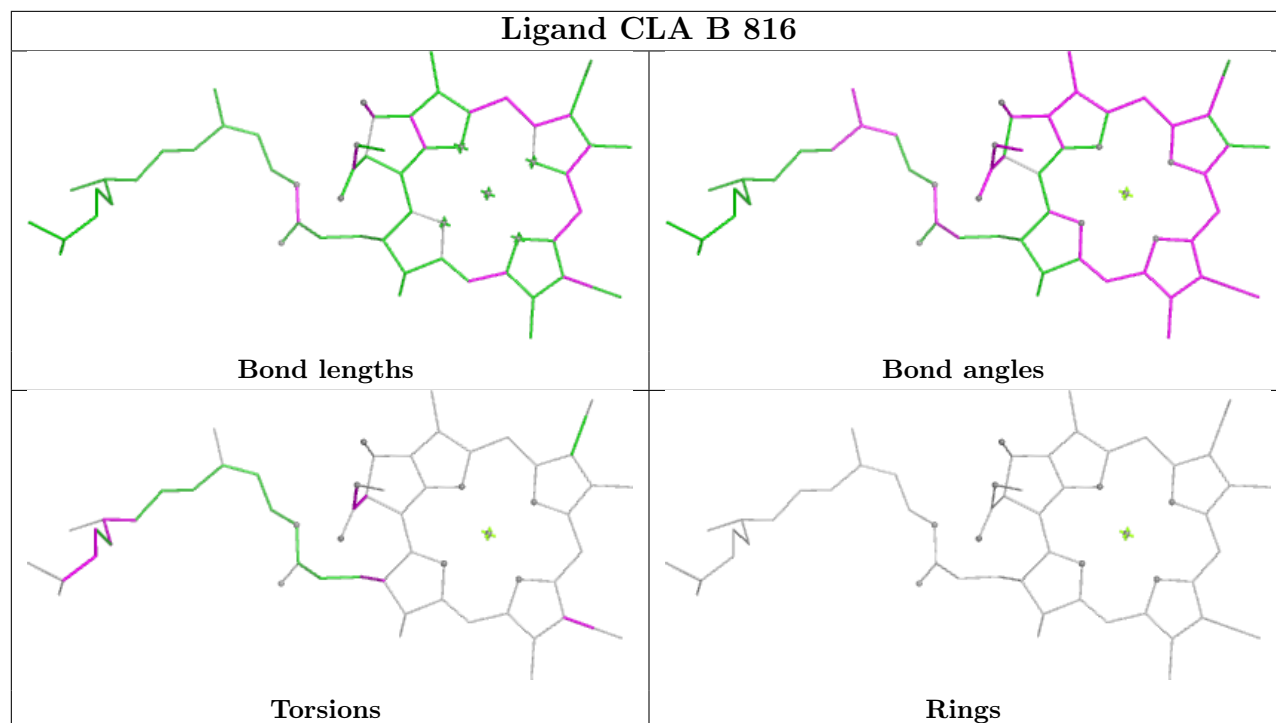
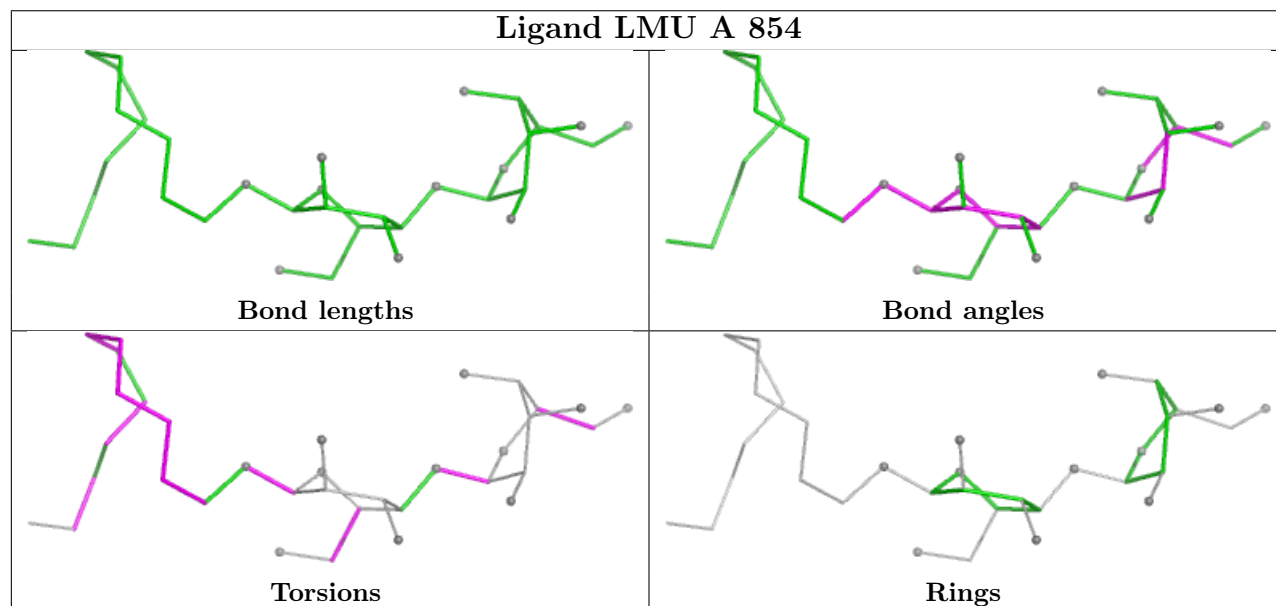
Ligand LMU 1 218



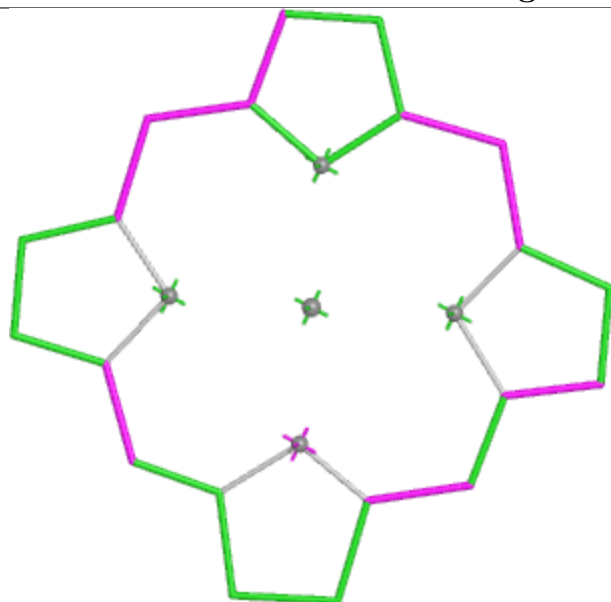


Ligand CLA 3 306

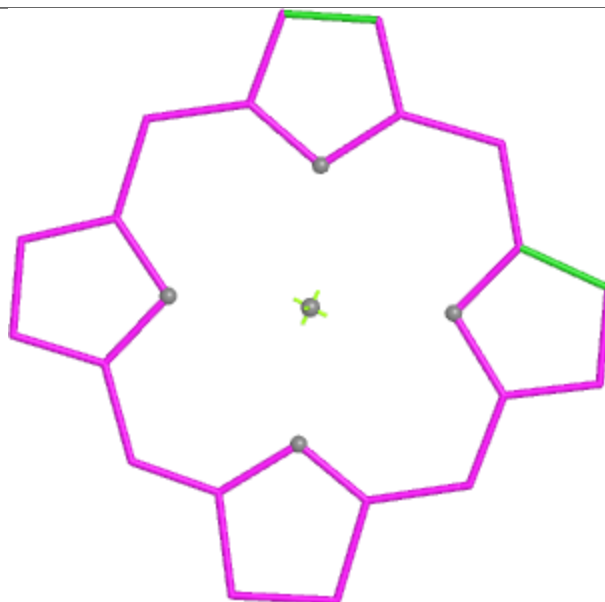


Ligand CLA B 816**Ligand LMU A 854**

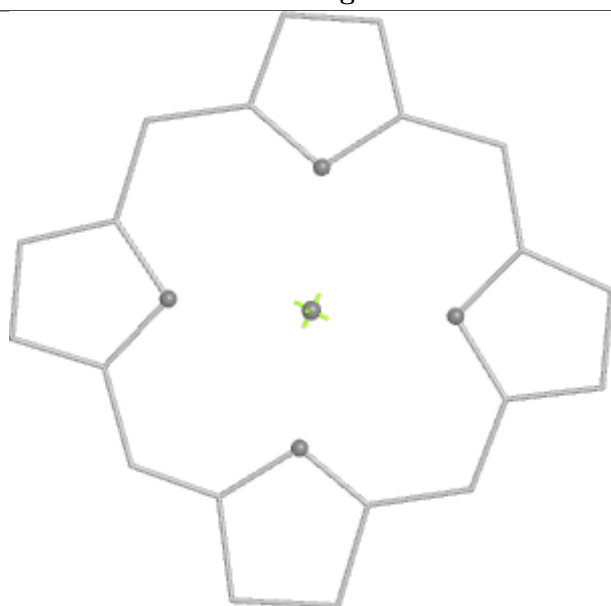
Ligand CLA 3 309



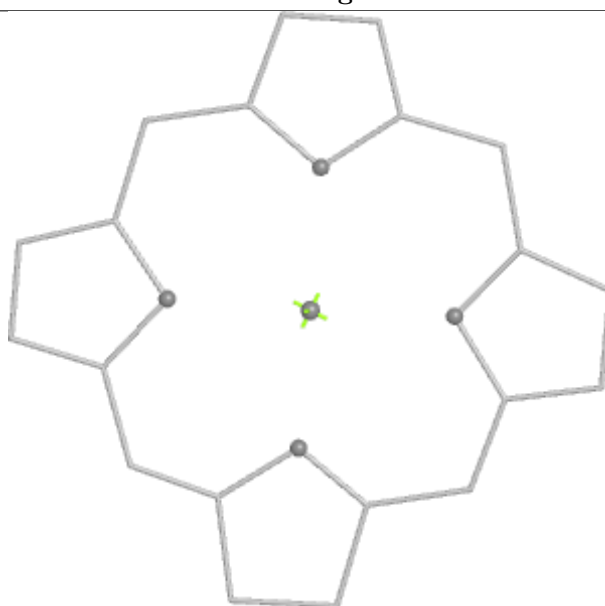
Bond lengths



Bond angles

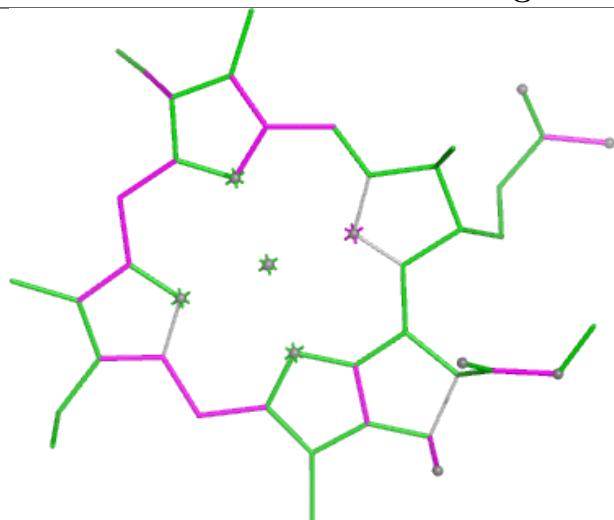


Torsions

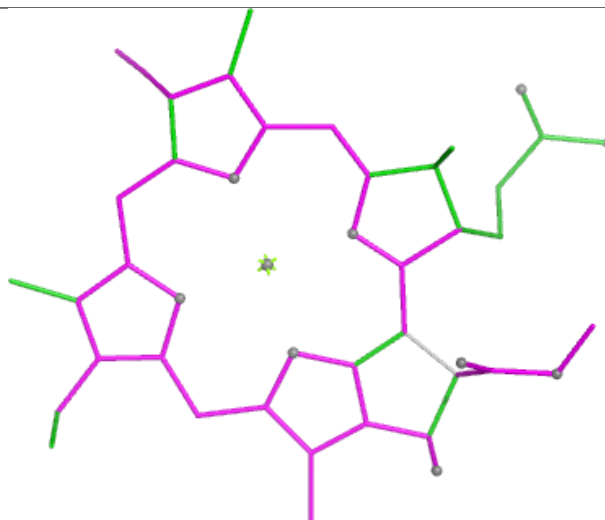


Rings

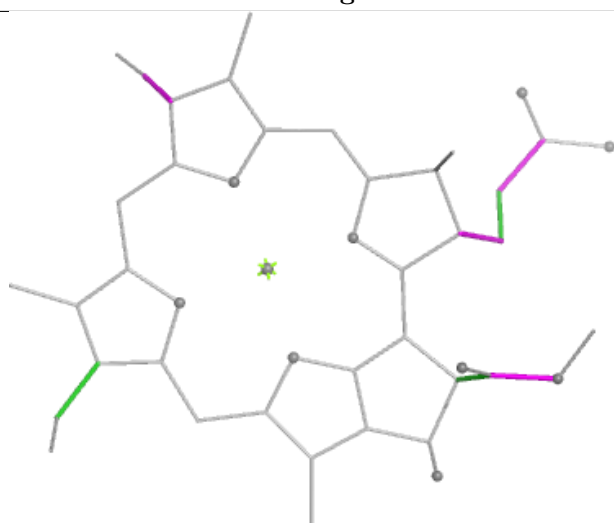
Ligand CLA A 833



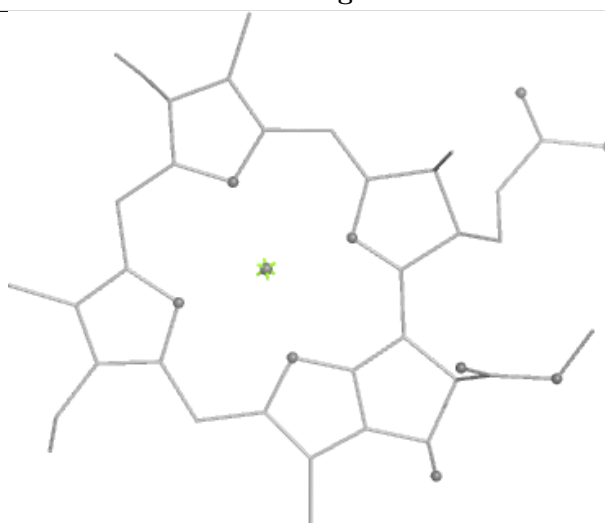
Bond lengths



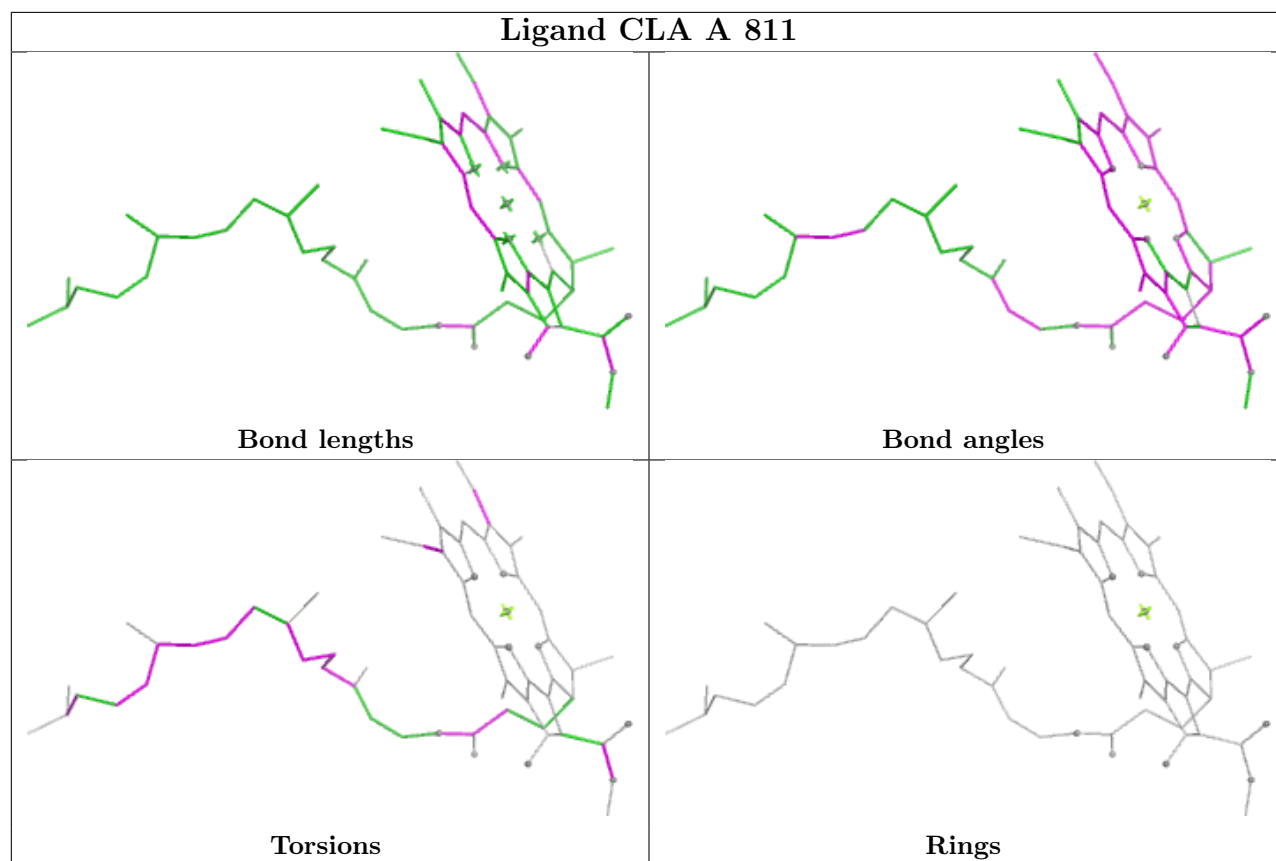
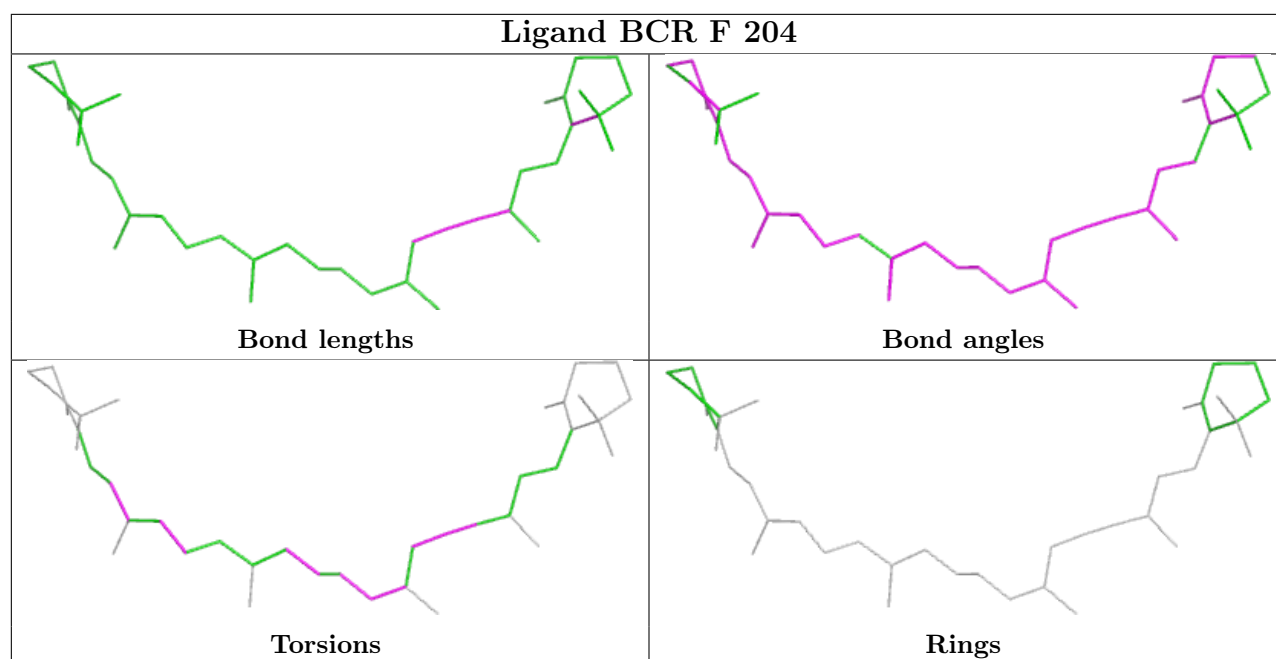
Bond angles



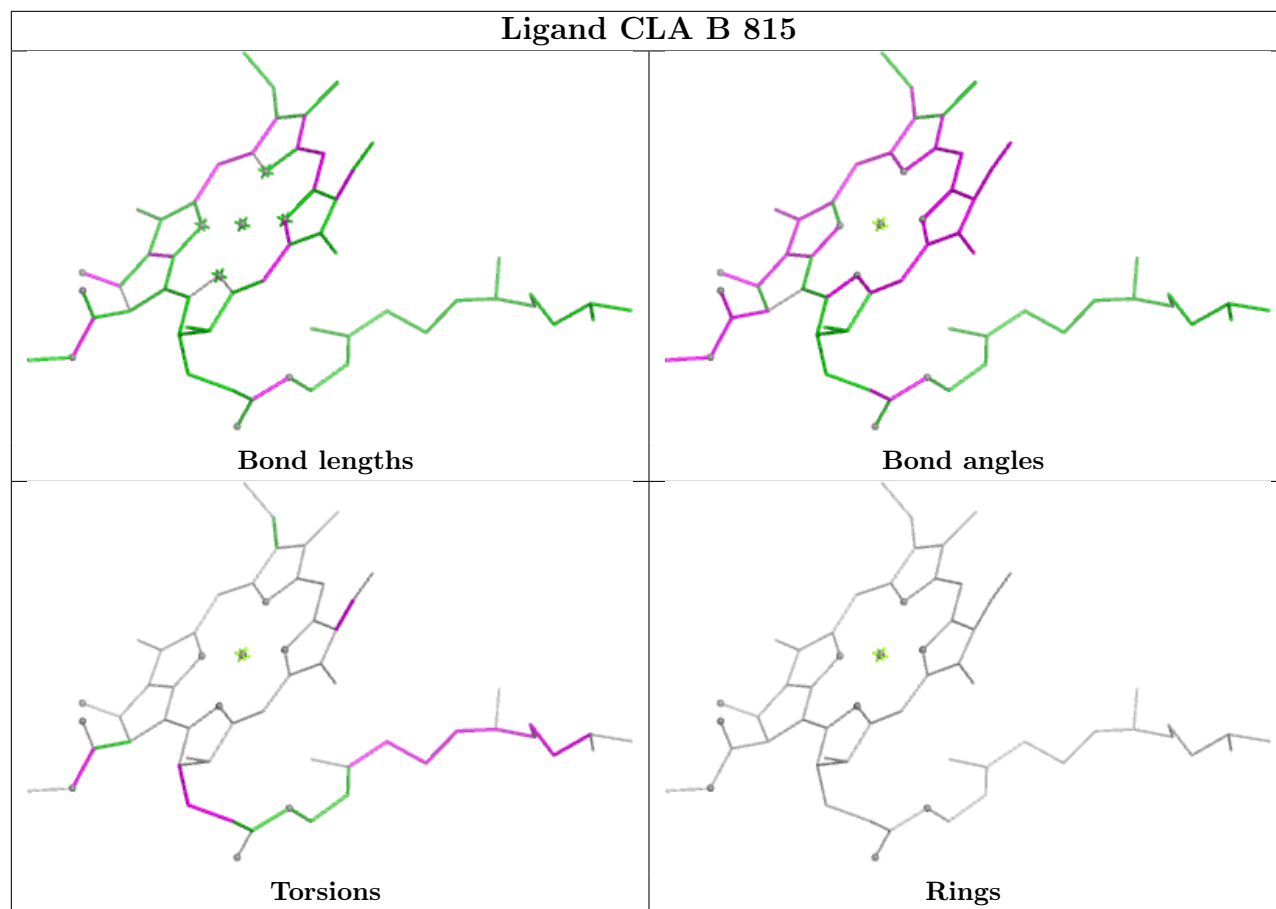
Torsions



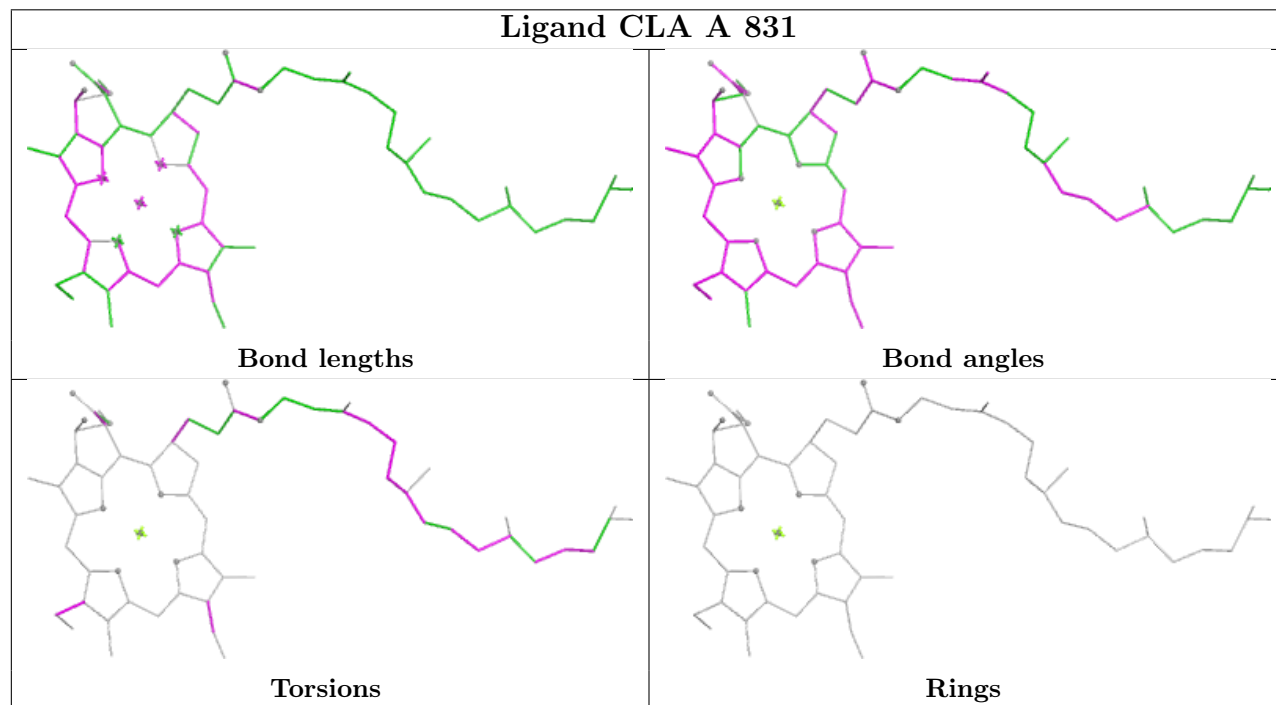
Rings



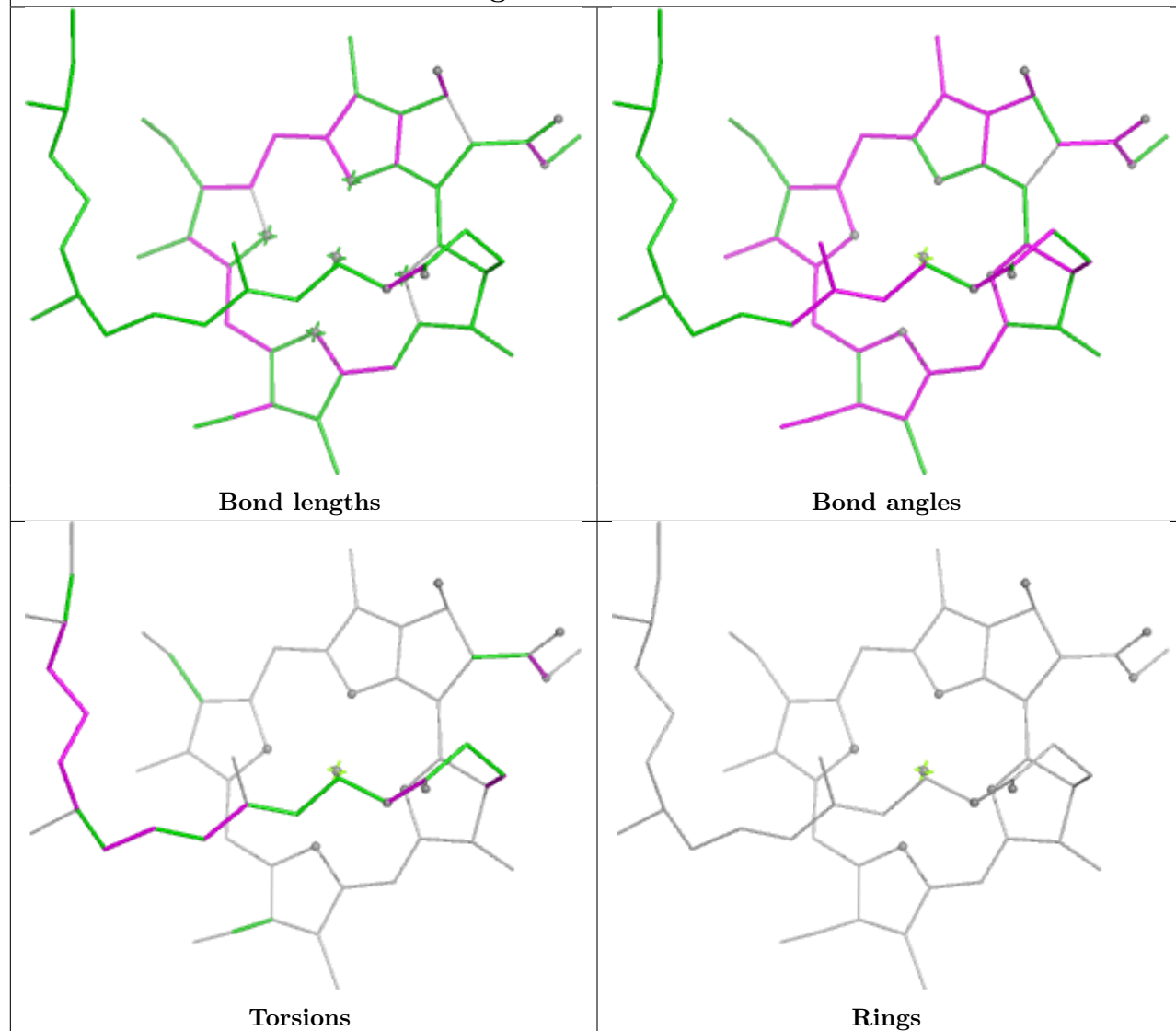
Ligand CLA B 815

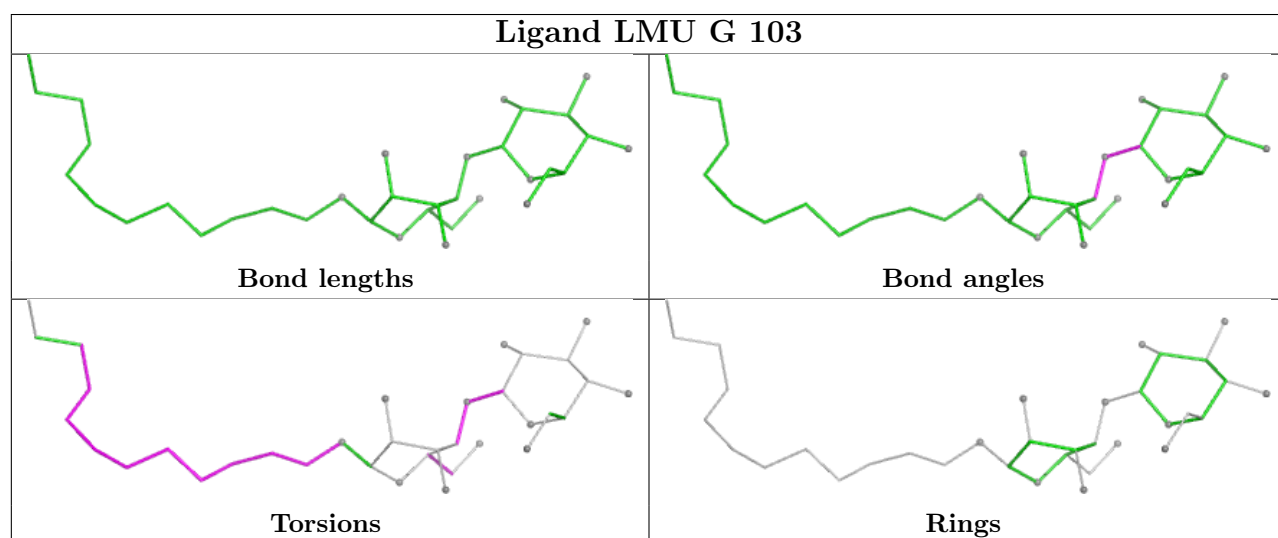
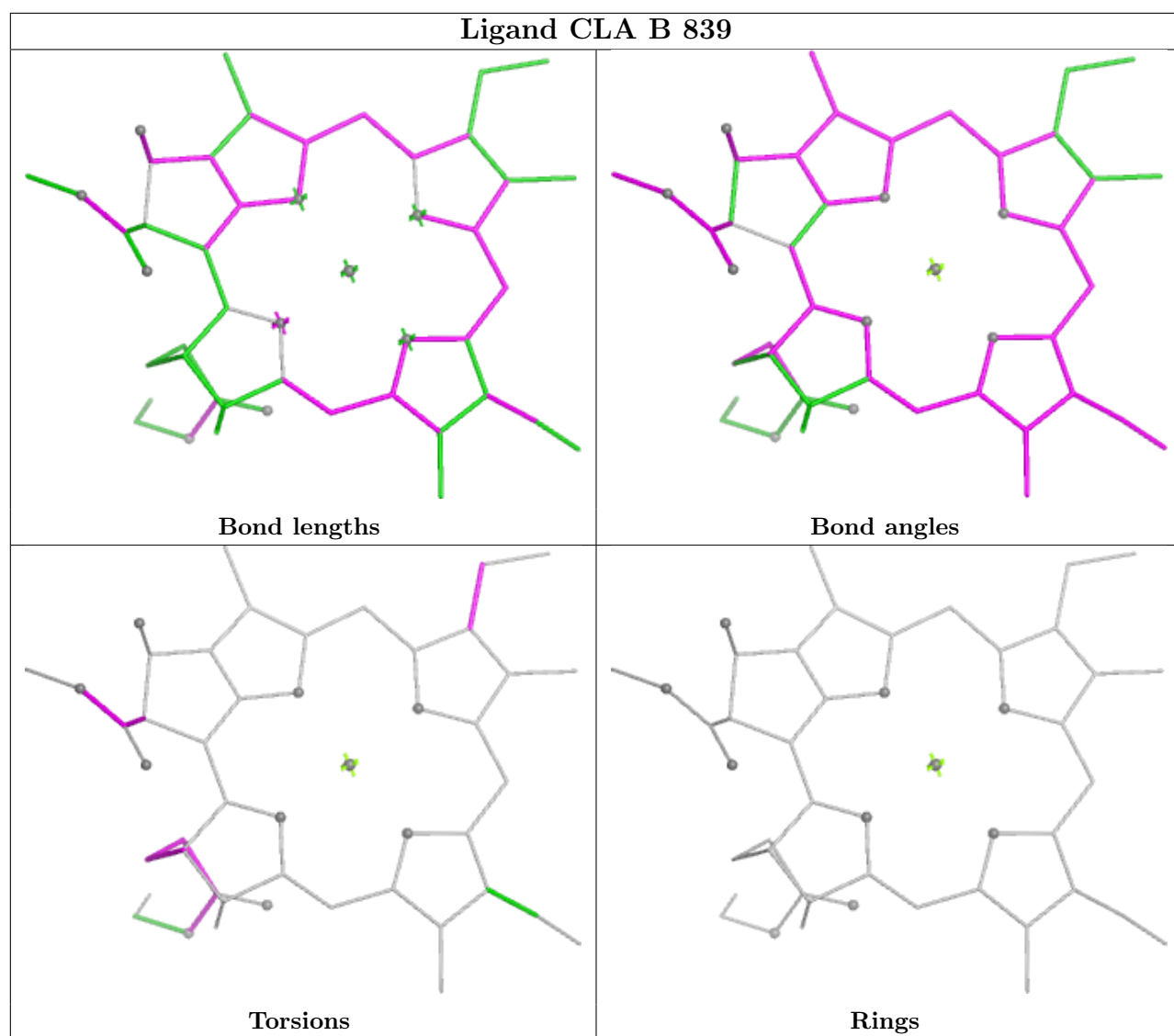


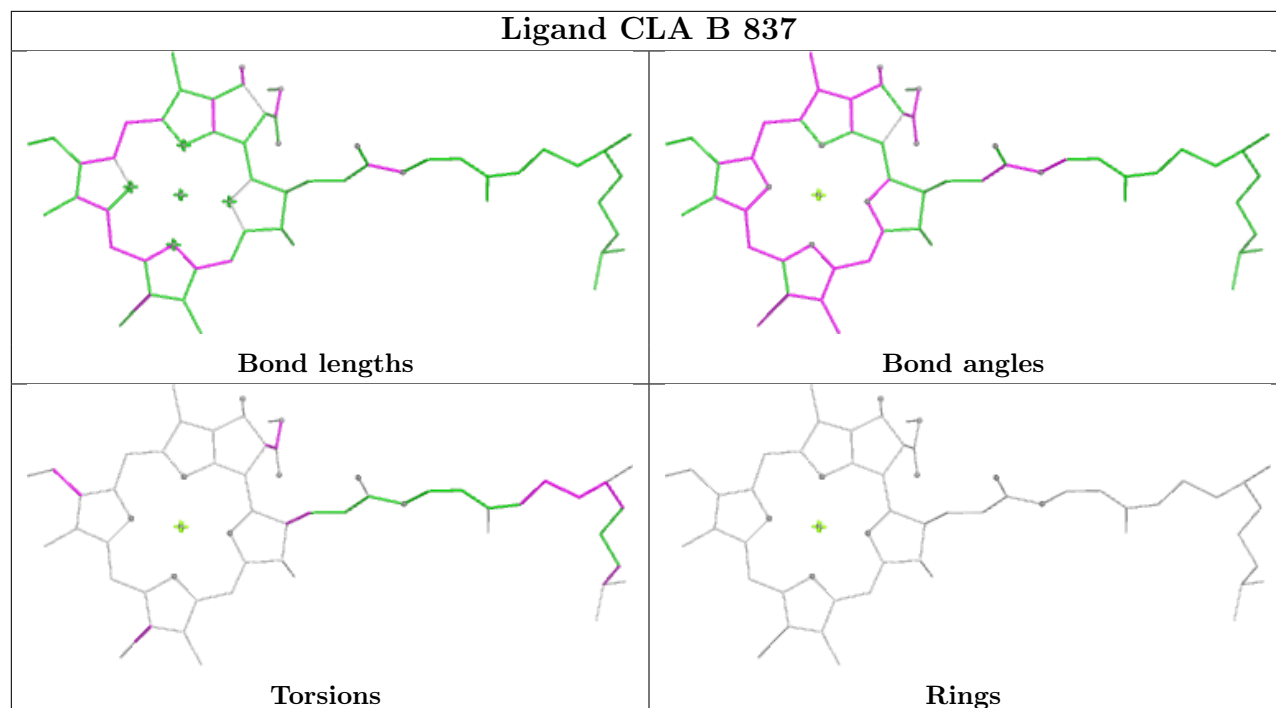
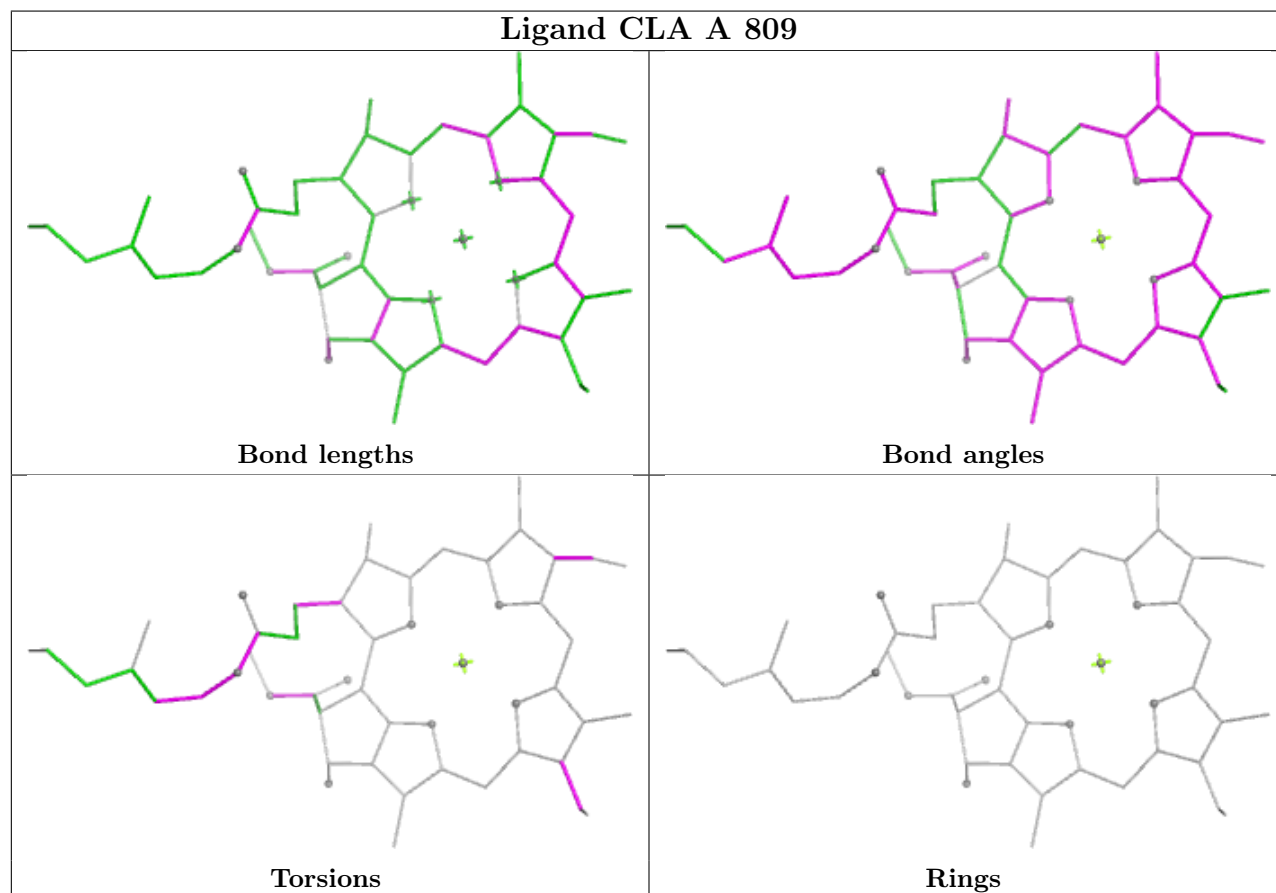
Ligand CLA A 831



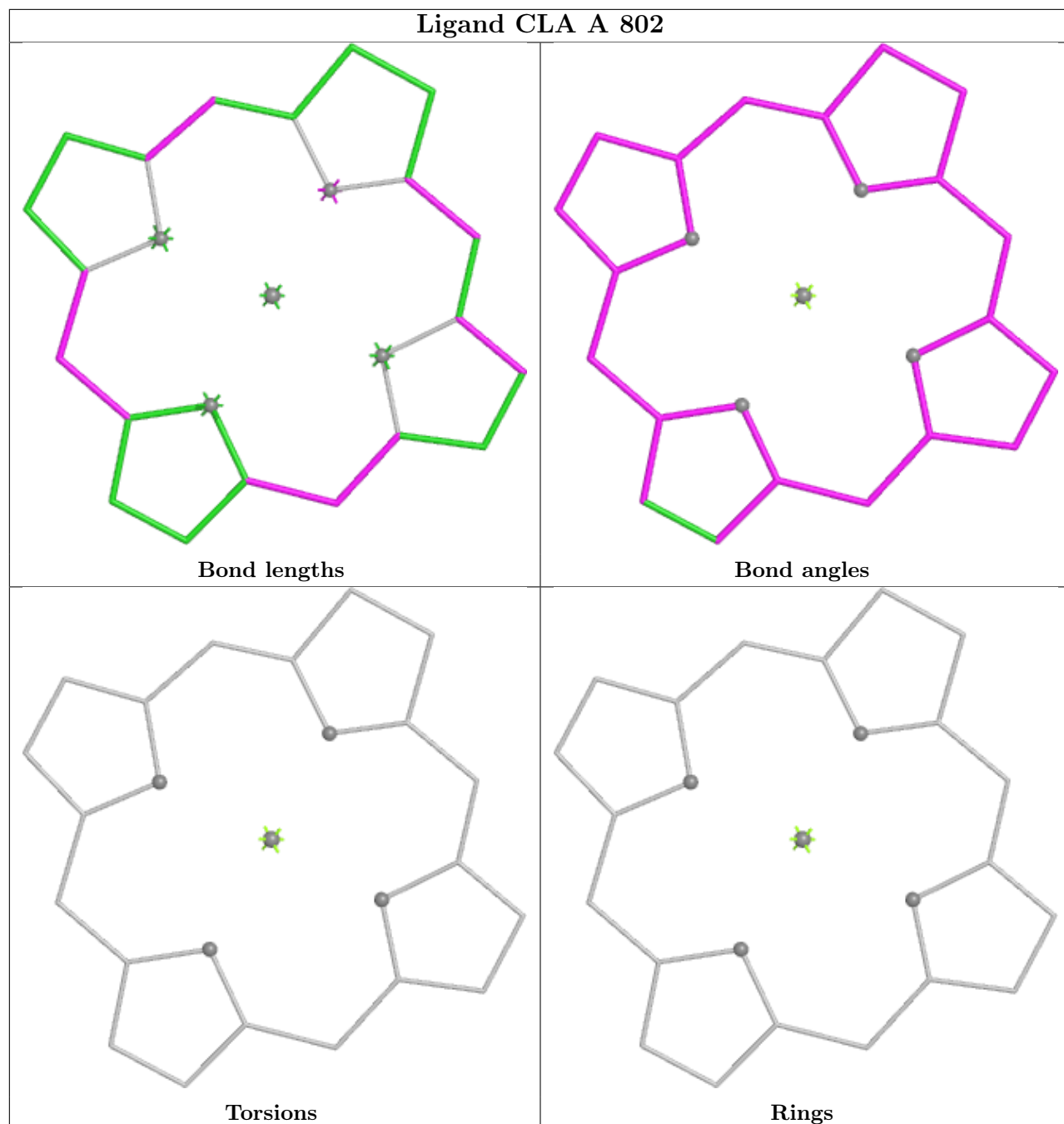
Ligand CLA B 820



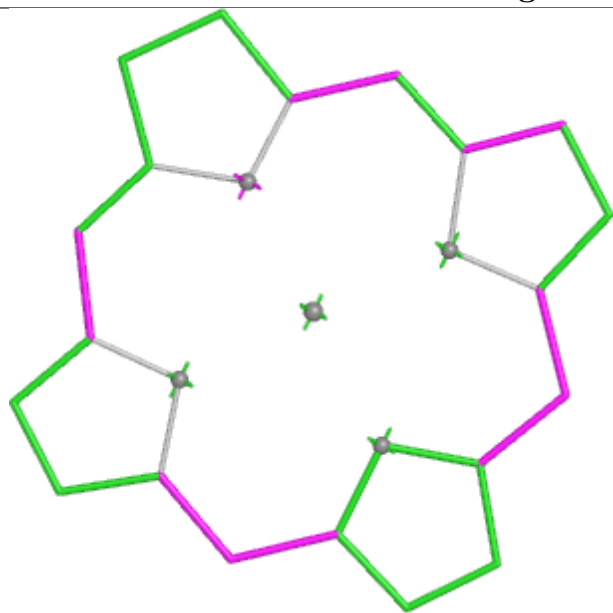


Ligand CLA B 837**Ligand CLA A 809**

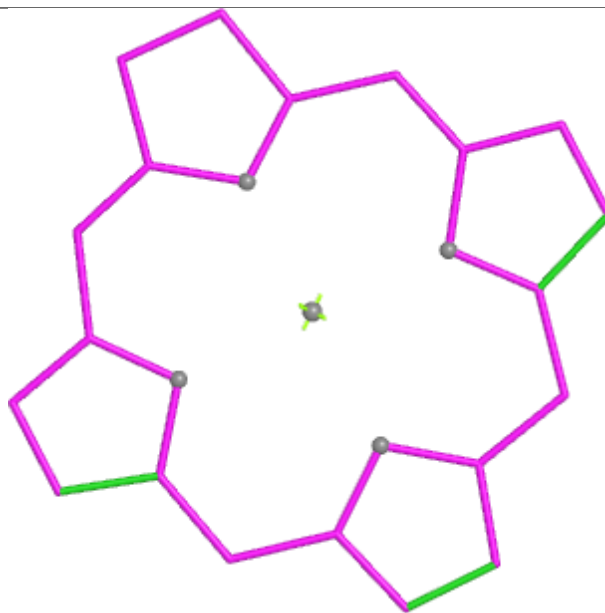
Ligand CLA A 802



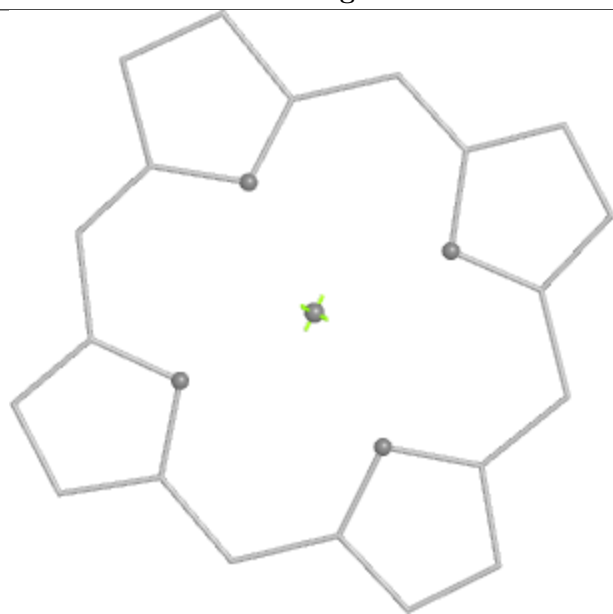
Ligand CLA 1 208



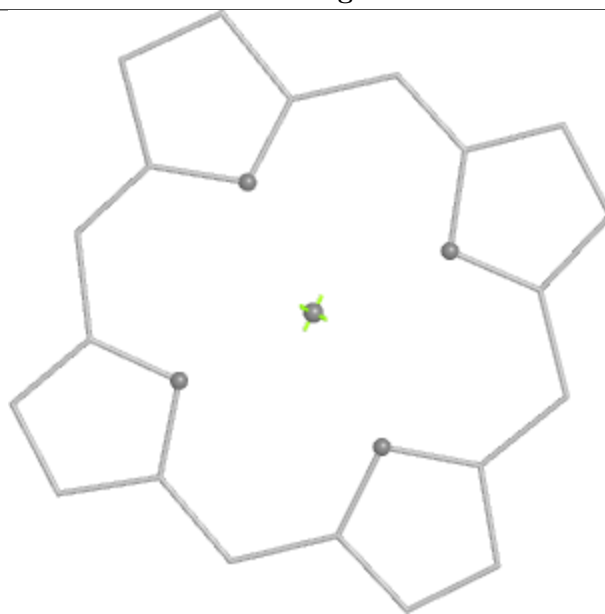
Bond lengths



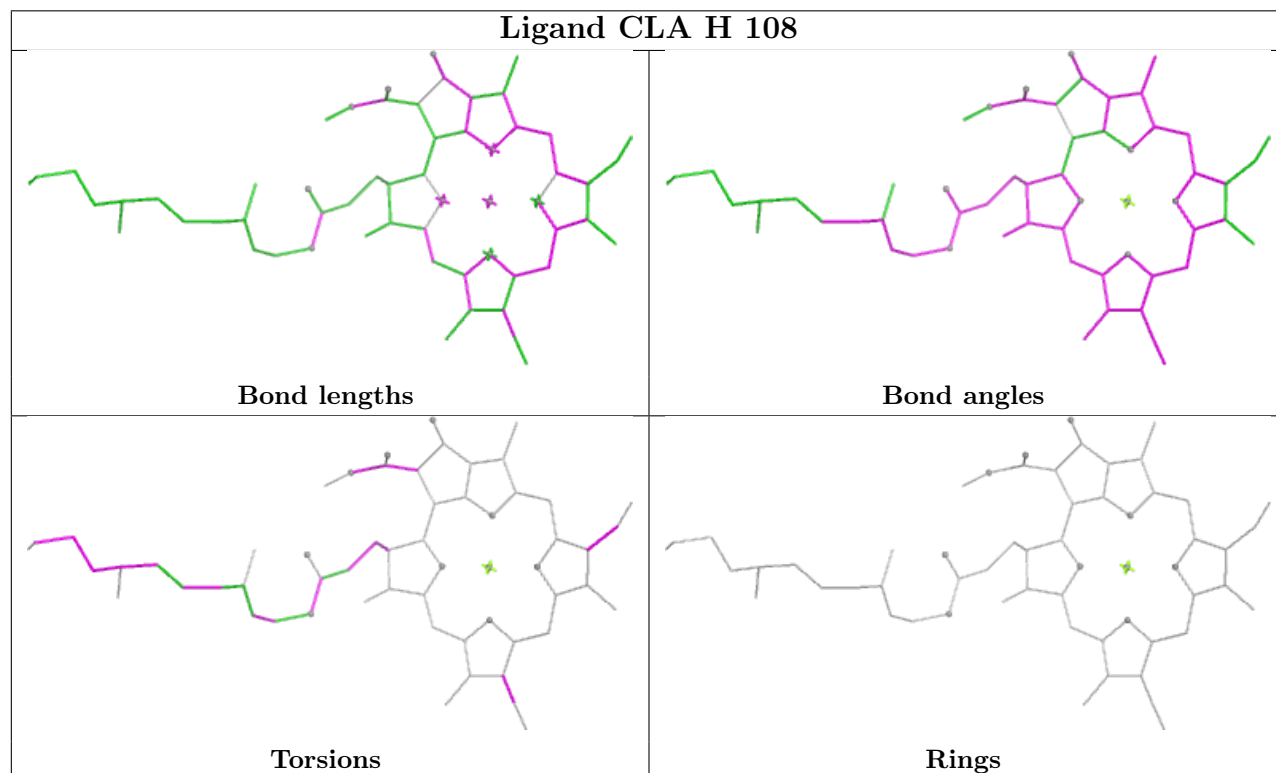
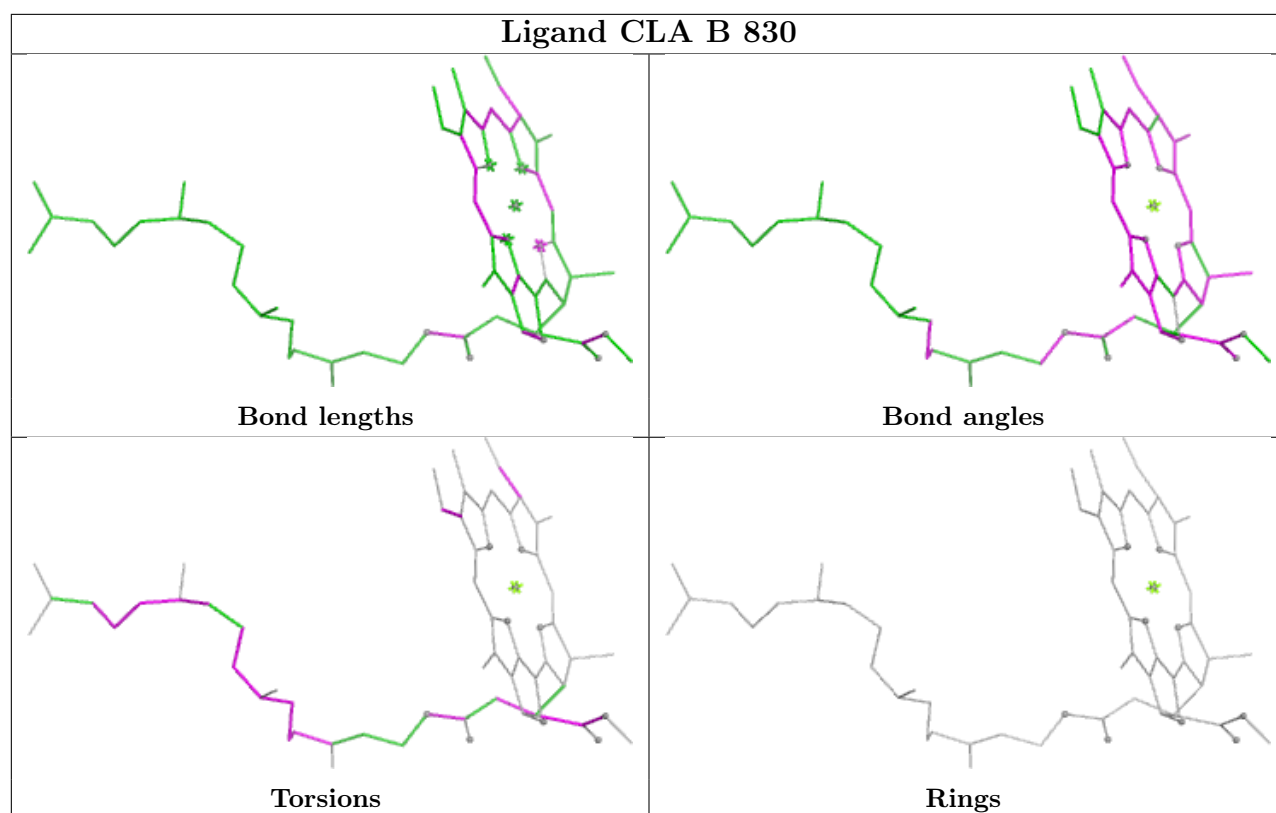
Bond angles



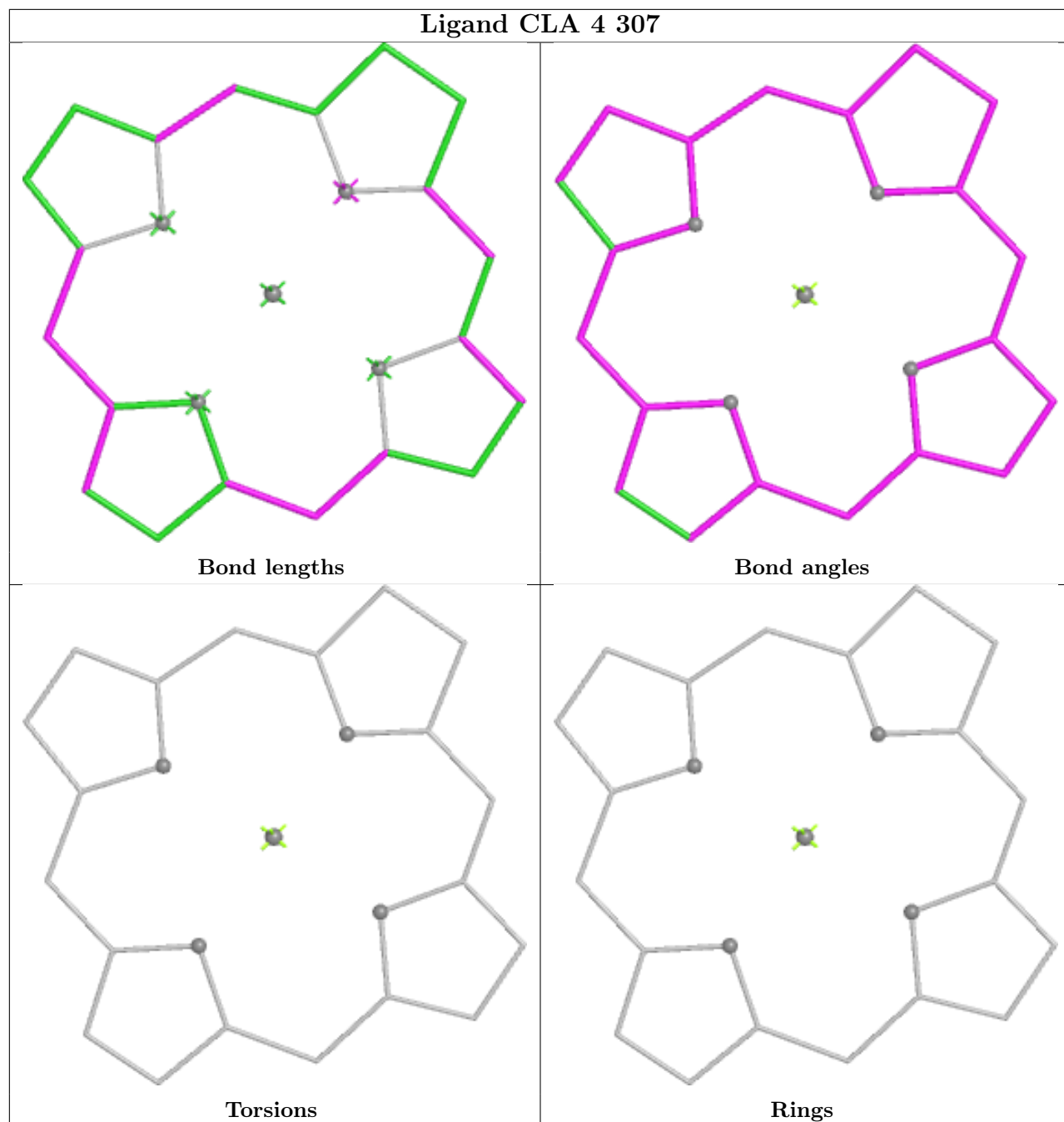
Torsions



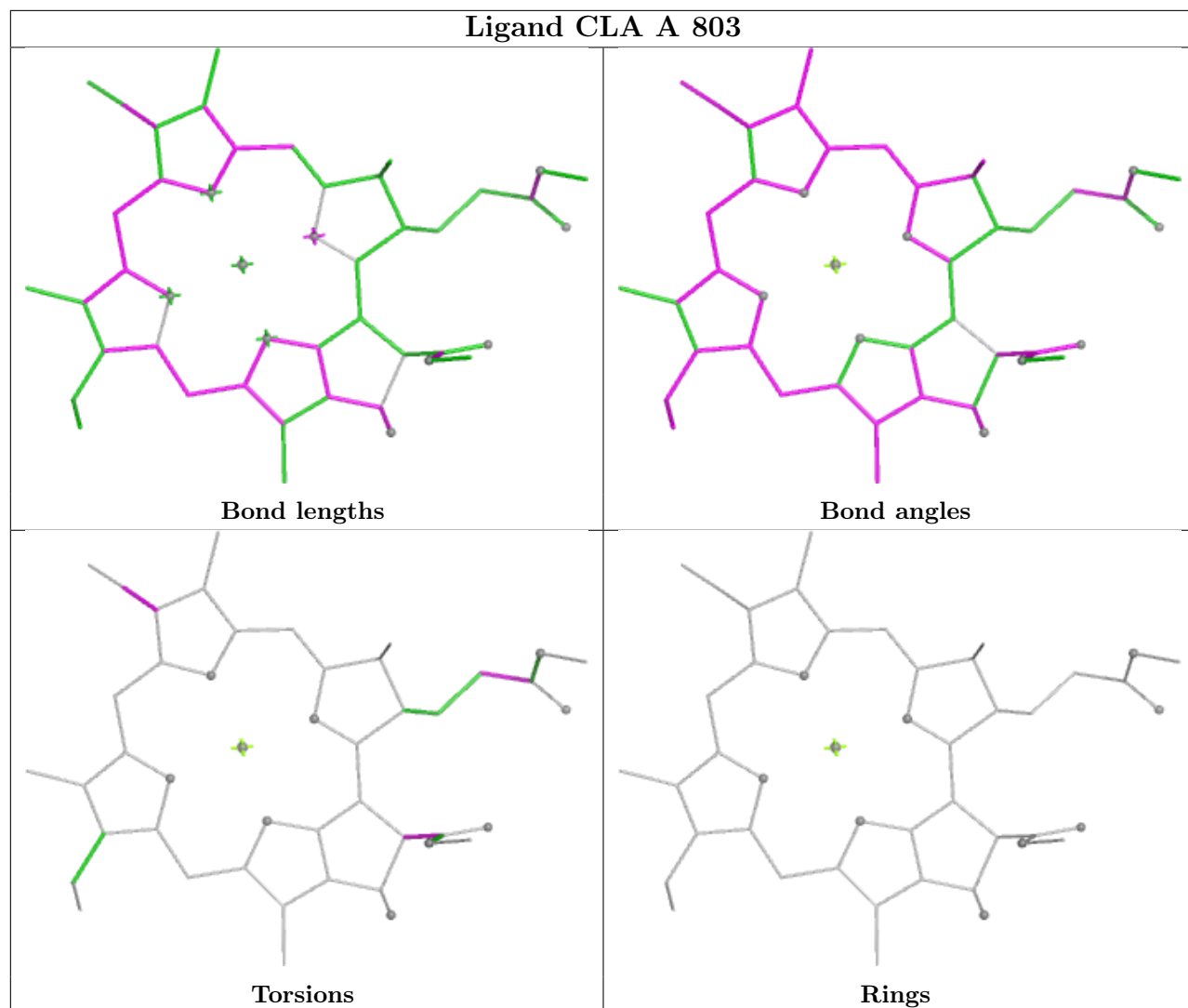
Rings

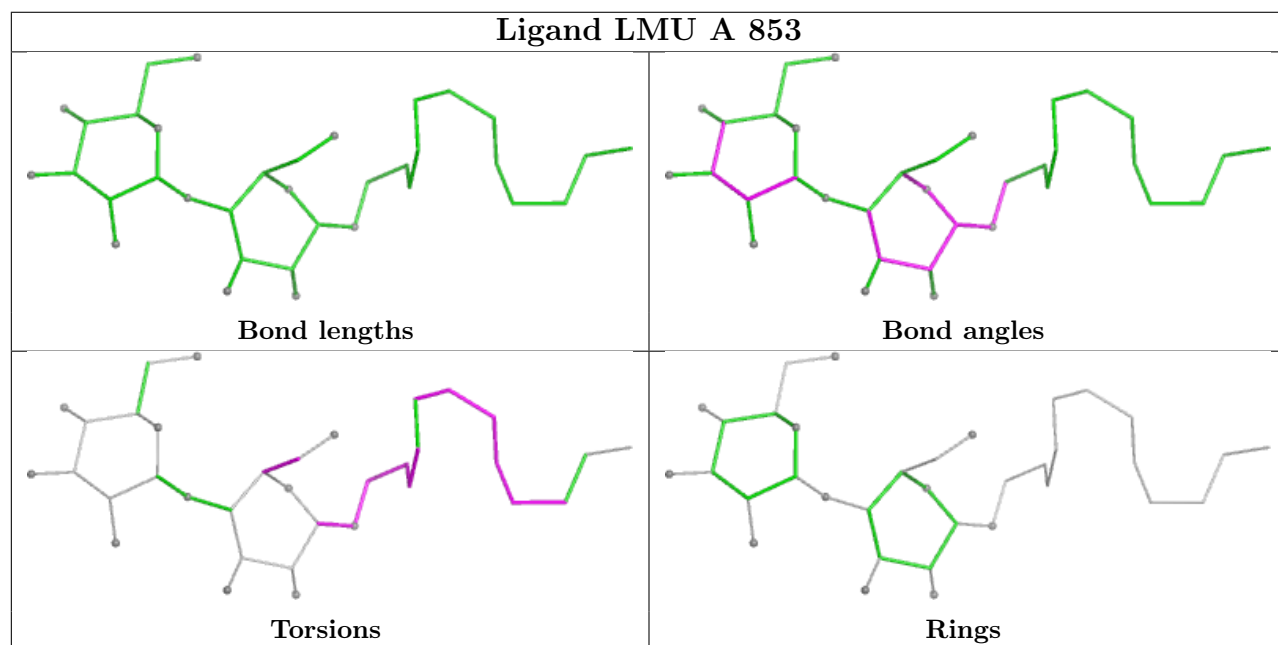
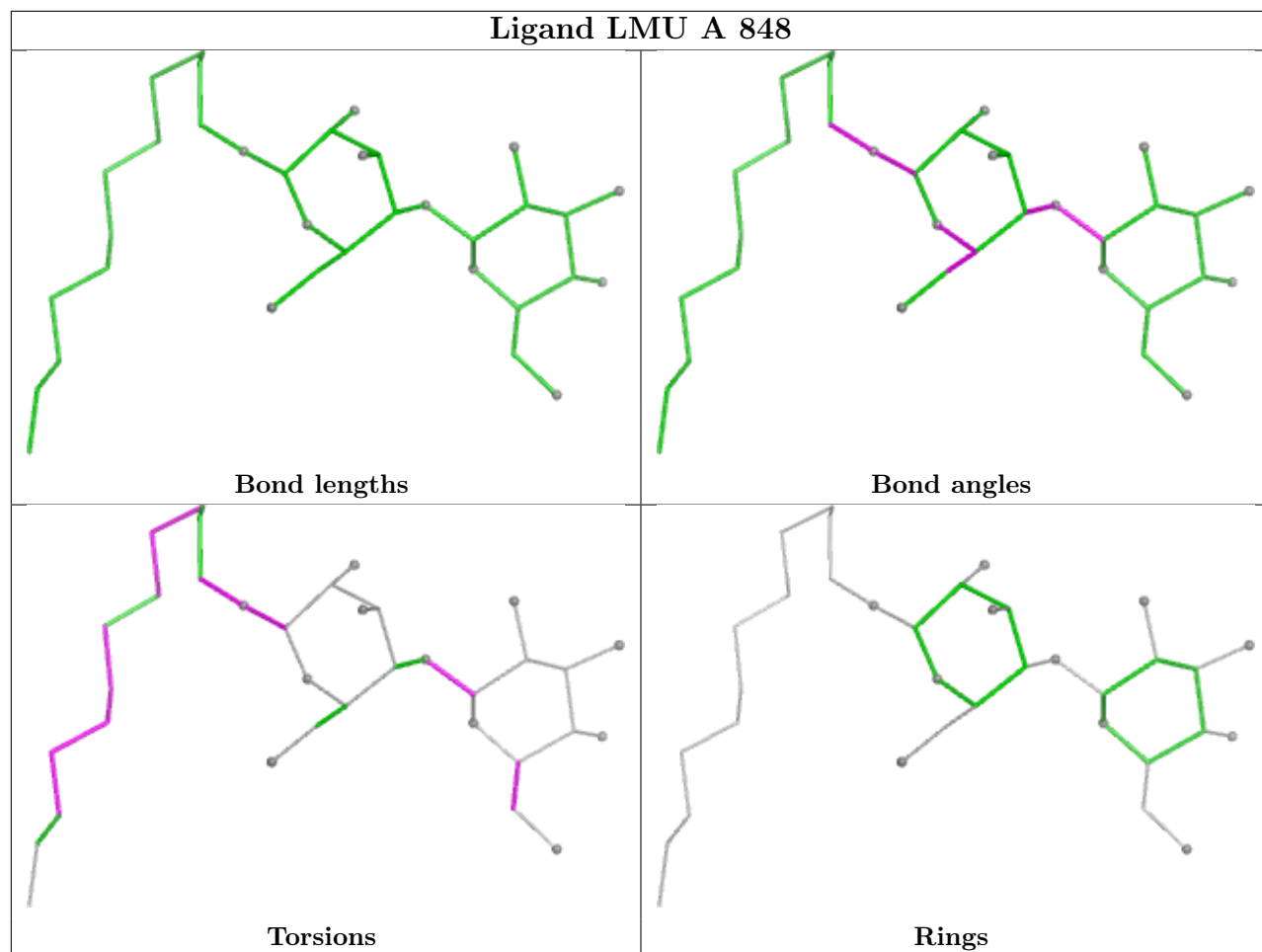


Ligand CLA 4 307

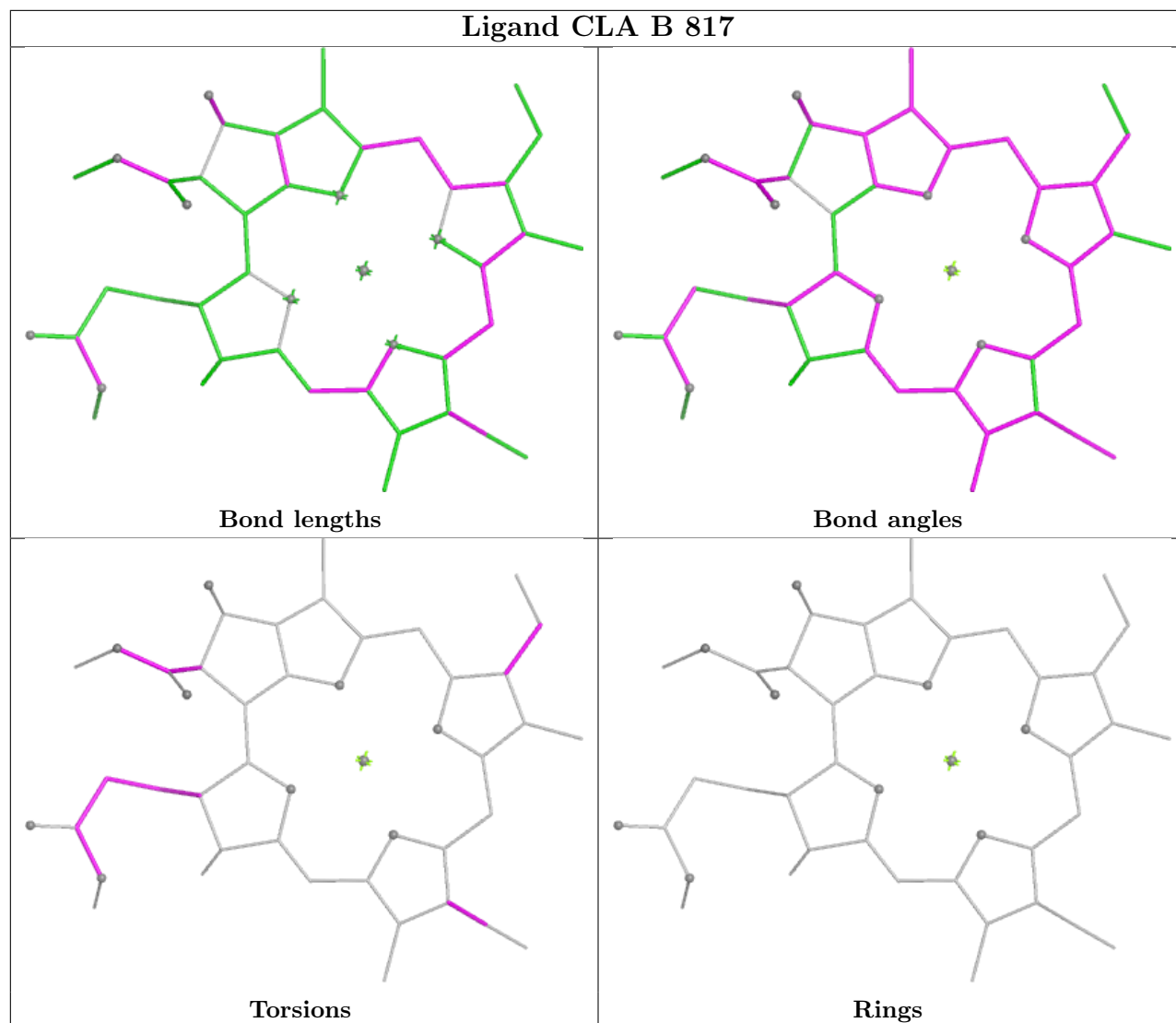


Ligand CLA A 803

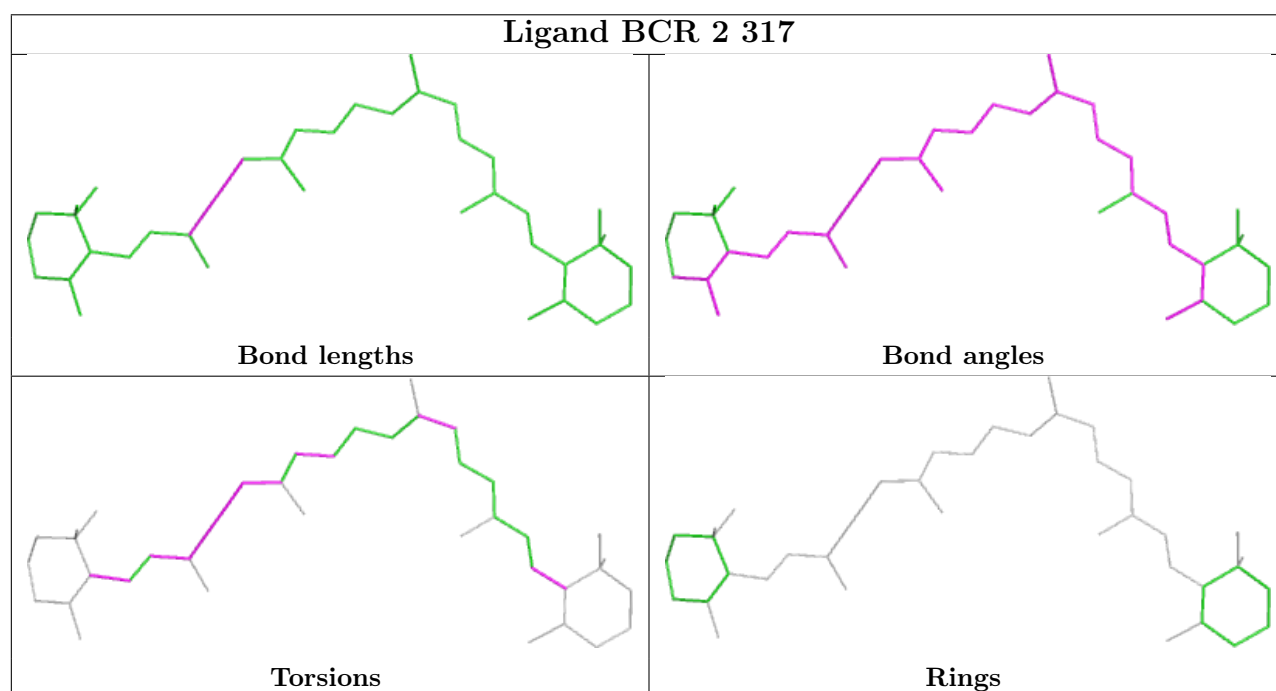


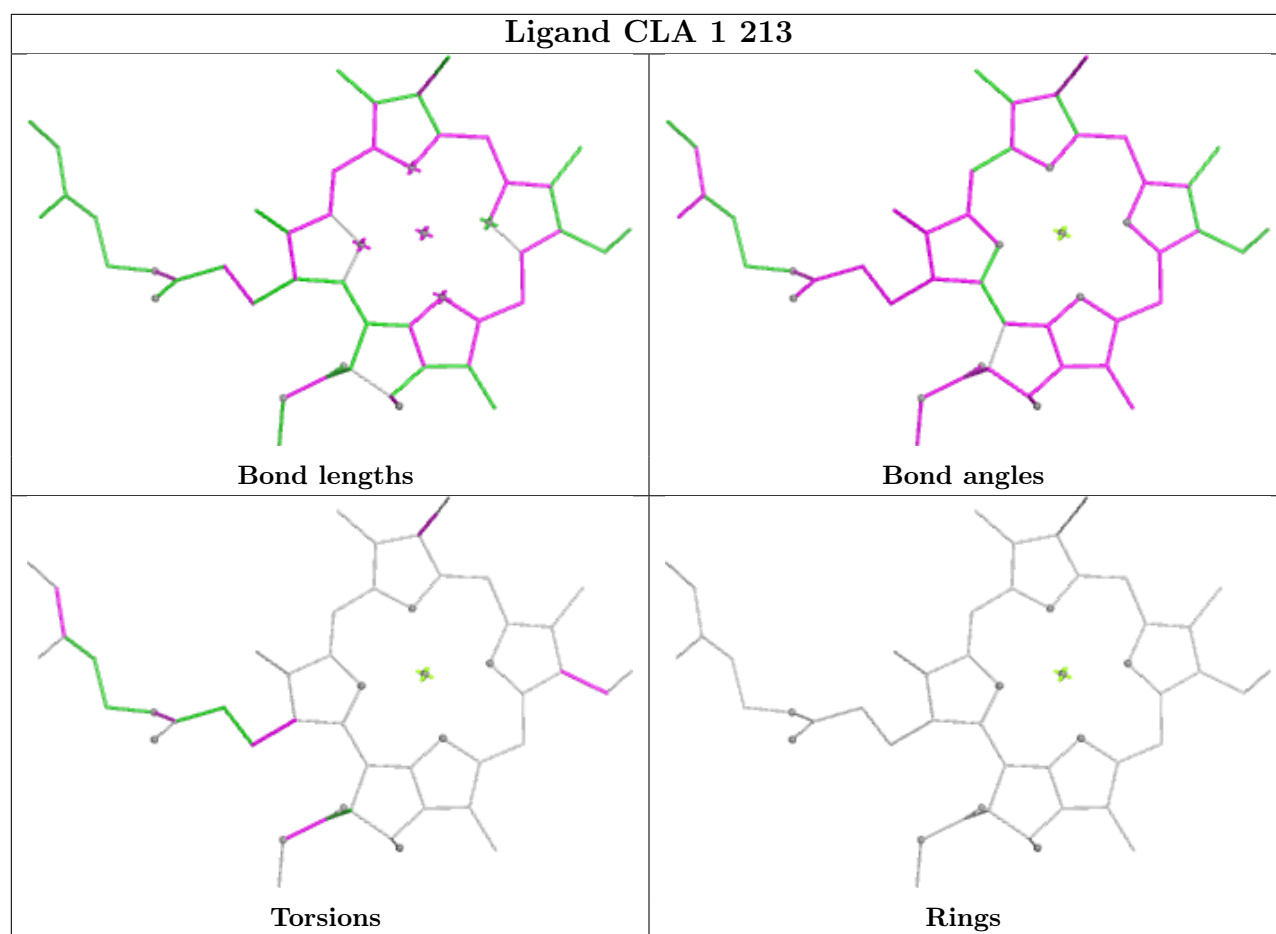


Ligand CLA B 817



Ligand BCR 2 317





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%)	2.01	62 (37%) 1 1	21, 24, 25, 25	0
2	2	176/269 (65%)	1.61	50 (28%) 1 2	21, 23, 24, 25	0
3	3	153/276 (55%)	2.87	99 (64%) 0 0	49, 78, 110, 112	0
4	4	166/251 (66%)	1.67	51 (30%) 1 2	21, 23, 24, 25	0
5	A	730/758 (96%)	2.29	356 (48%) 0 1	20, 22, 23, 25	0
6	B	733/734 (99%)	2.38	403 (54%) 0 0	20, 22, 24, 25	0
7	C	81/81 (100%)	2.19	42 (51%) 0 1	21, 22, 23, 23	0
8	D	138/212 (65%)	1.93	54 (39%) 1 1	21, 23, 24, 25	0
9	E	65/143 (45%)	1.78	22 (33%) 1 1	21, 22, 24, 24	0
10	F	154/231 (66%)	1.73	50 (32%) 1 1	21, 22, 23, 24	0
11	G	95/167 (56%)	1.87	34 (35%) 1 1	21, 23, 24, 25	0
12	H	69/144 (47%)	1.54	21 (30%) 1 2	21, 23, 24, 25	0
13	I	30/40 (75%)	1.40	7 (23%) 2 2	21, 22, 23, 23	0
14	J	42/44 (95%)	1.85	16 (38%) 1 1	21, 23, 23, 24	0
15	K	84/131 (64%)	1.47	18 (21%) 2 3	21, 24, 24, 26	0
16	L	162/216 (75%)	1.94	55 (33%) 1 1	20, 23, 24, 25	0
17	N	85/170 (50%)	1.24	16 (18%) 3 3	22, 23, 24, 25	0
18	R	0/53	-	-	-	-
All	All	3128/4161 (75%)	2.08	1356 (43%) 0 1	20, 23, 25, 112	0

The worst 5 of 1356 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
6	B	204	GLY	10.5
16	L	141	GLY	10.3
6	B	197	VAL	10.1

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Mol	Chain	Res	Type	RSRZ
5	A	130	GLU	10.0
6	B	566	GLY	9.4

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

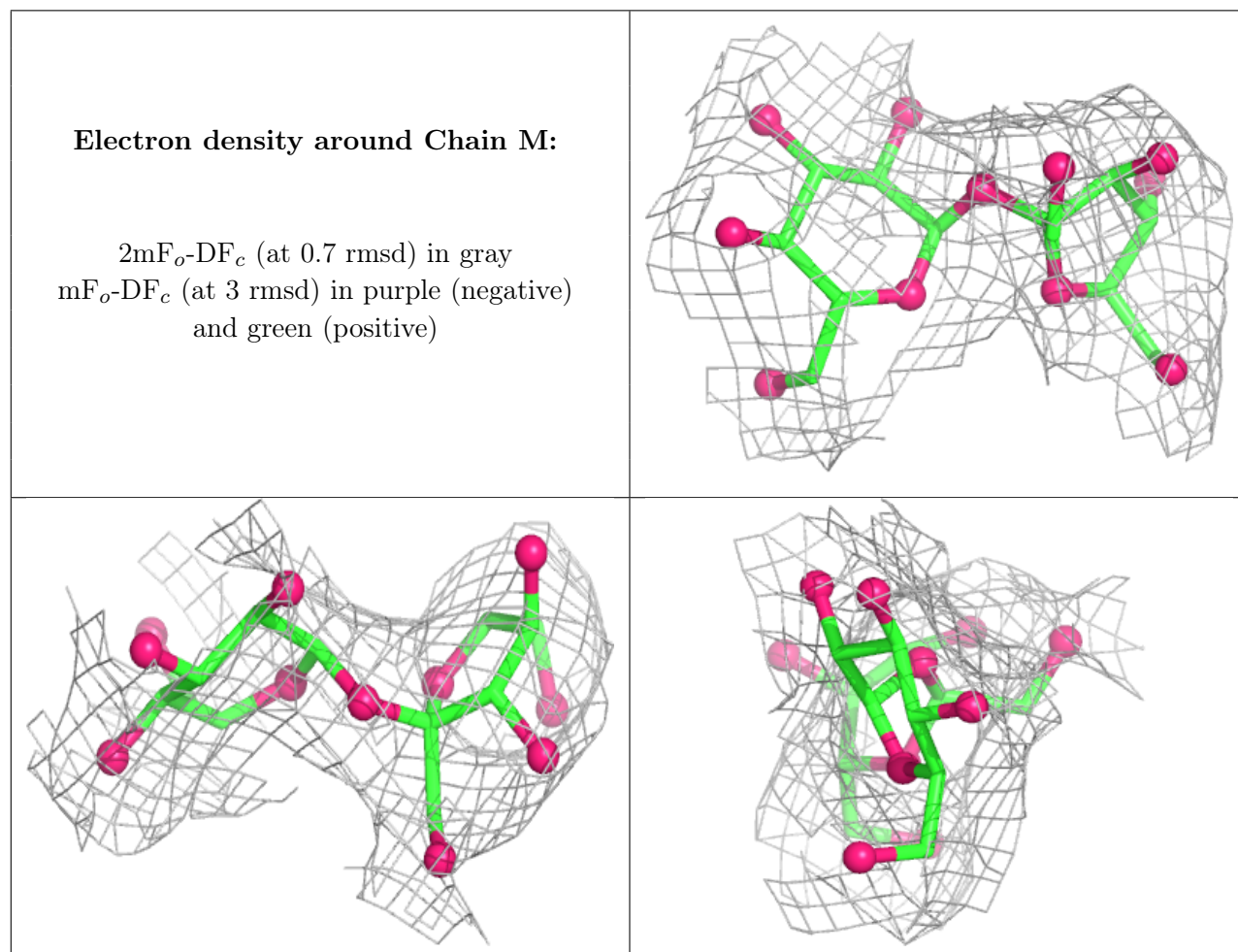
There are no non-standard protein/DNA/RNA residues in this entry.

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.

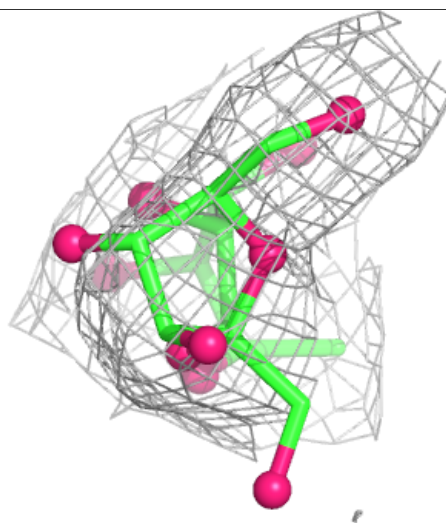
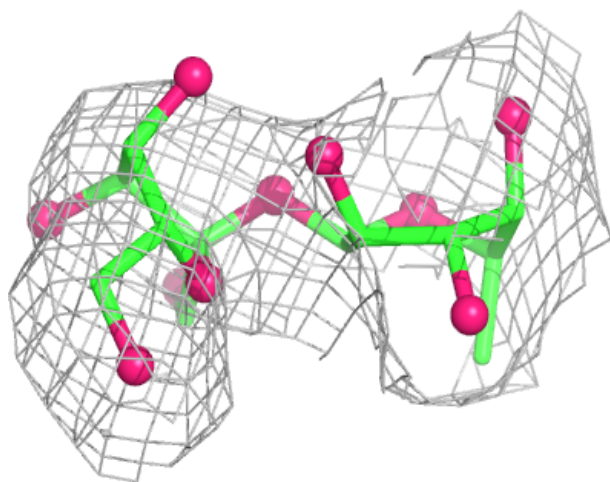
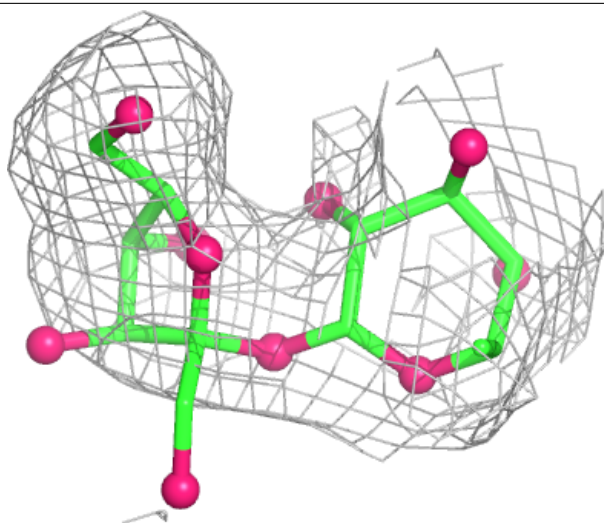
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
19	GLC	M	1	11/12	-	-	2,44,60,60	0
19	FRU	M	2	12/12	-	-	9,35,60,60	0
19	GLC	O	1	10/12	-	-	4,38,60,60	0
19	FRU	O	2	12/12	-	-	2,28,60,60	0
19	GLC	P	1	11/12	-	-	2,13,57,60	0
19	FRU	P	2	12/12	-	-	2,36,60,60	0
19	GLC	Q	1	11/12	-	-	2,27,60,60	0
19	FRU	Q	2	12/12	-	-	2,28,60,60	0
19	GLC	Y	1	11/12	0.64	0.15	2,34,60,60	0
19	GLC	S	1	11/12	0.67	0.15	2,19,60,60	0
19	FRU	S	2	12/12	0.73	0.12	2,32,60,60	0
19	FRU	T	2	12/12	0.74	0.18	6,39,60,60	0
19	GLC	W	1	11/12	0.76	0.19	9,40,60,60	0
19	GLC	T	1	11/12	0.78	0.14	13,47,60,60	0
19	FRU	Y	2	12/12	0.78	0.15	2,30,60,60	0
19	GLC	X	1	10/12	0.80	0.12	6,52,60,60	0
19	FRU	U	2	12/12	0.81	0.12	2,34,60,60	0
19	GLC	V	1	11/12	0.81	0.12	2,57,60,60	0
19	FRU	W	2	12/12	0.82	0.13	17,37,60,60	0
19	FRU	X	2	12/12	0.83	0.13	11,32,60,60	0
19	GLC	U	1	11/12	0.85	0.13	2,60,60,60	0
19	GLC	Z	1	11/12	0.85	0.10	4,31,60,60	0
19	FRU	V	2	12/12	0.87	0.10	2,33,60,60	0
19	FRU	Z	2	12/12	0.87	0.10	3,43,60,60	0
19	GLC	a	1	11/12	-	-	2,23,50,54	0
19	FRU	a	2	12/12	-	-	6,32,60,60	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.



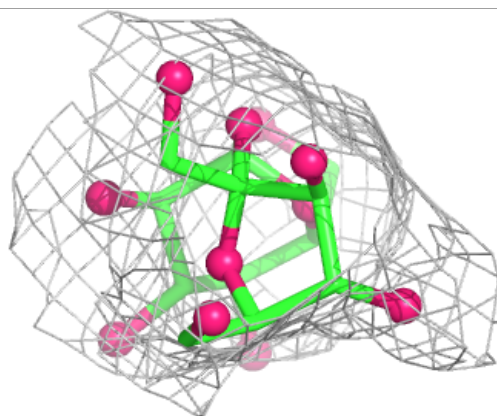
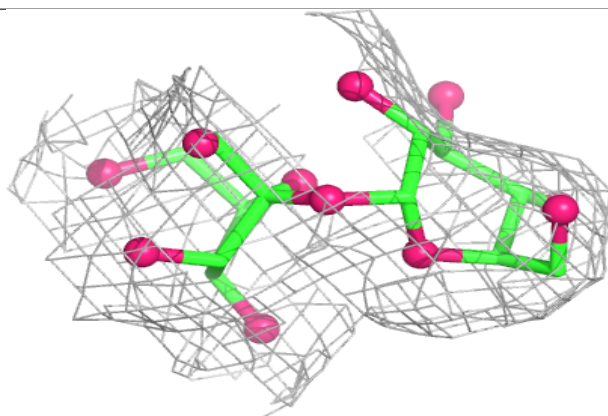
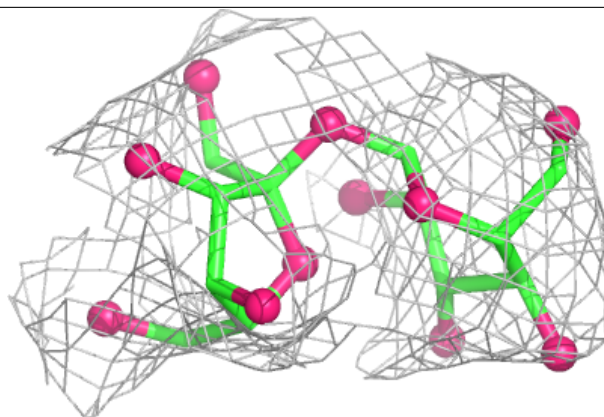
Electron density around Chain O:

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



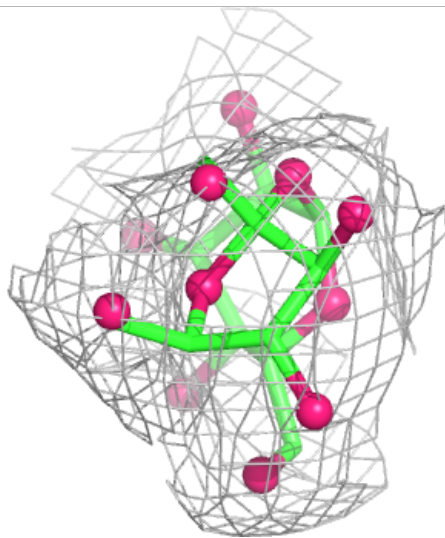
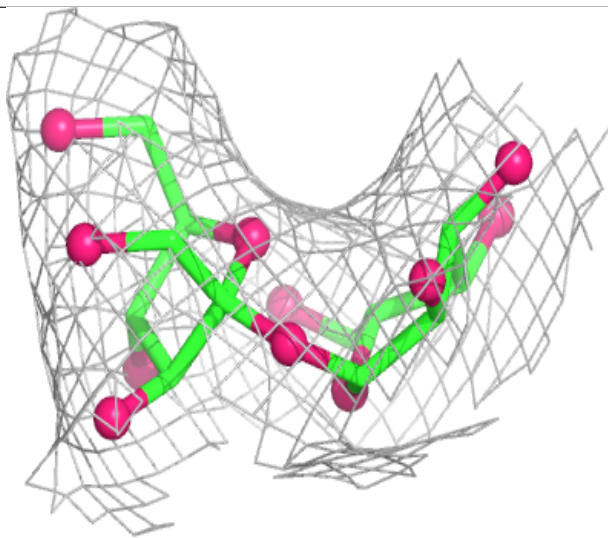
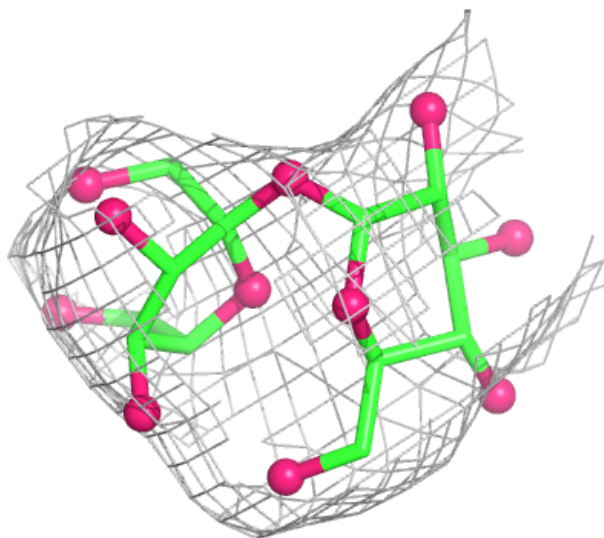
Electron density around Chain P:

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



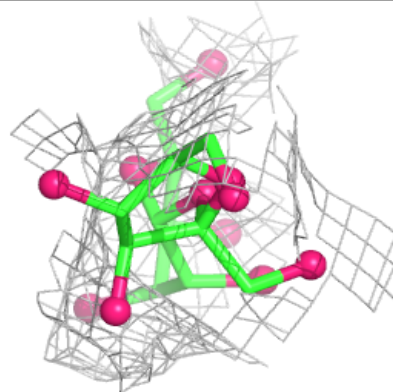
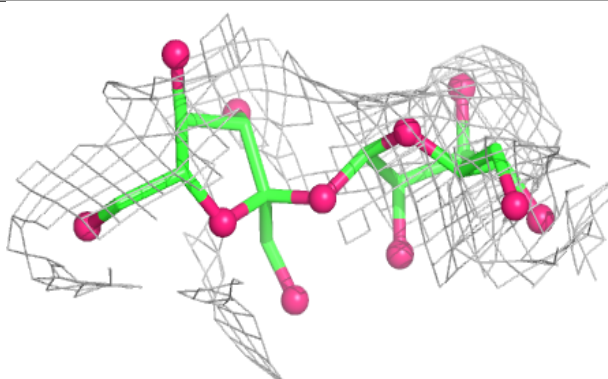
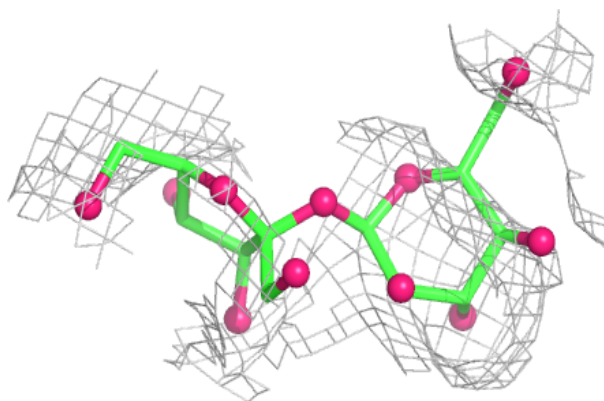
Electron density around Chain Q:

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

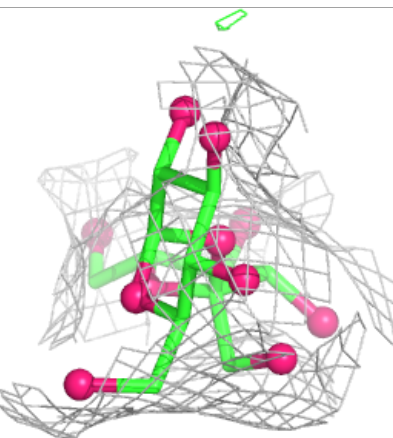
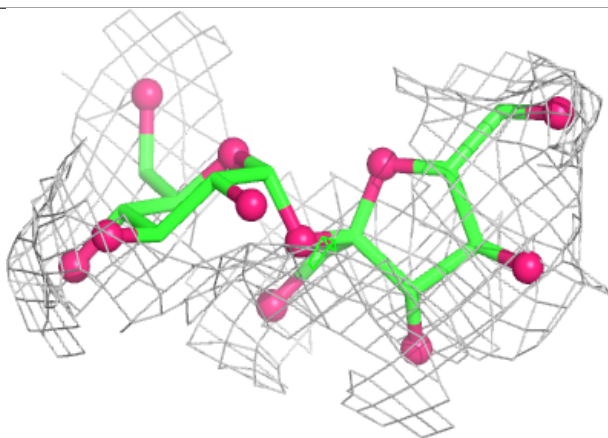
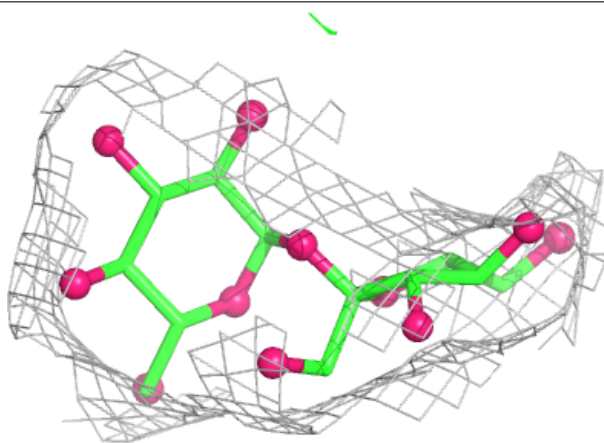


Electron density around Chain S:

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

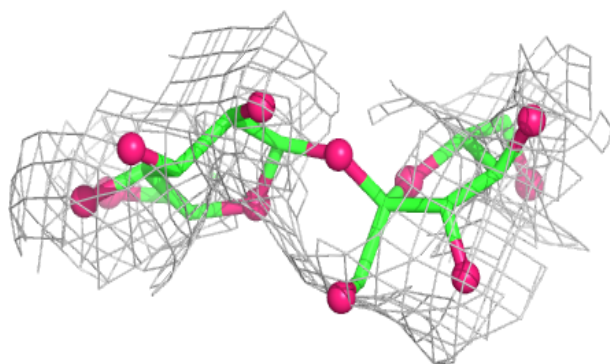
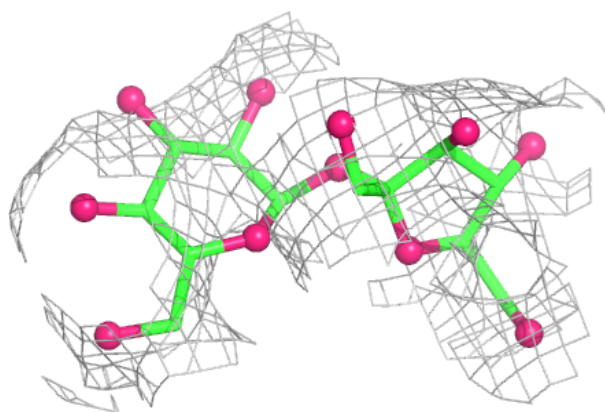
**Electron density around Chain T:**

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

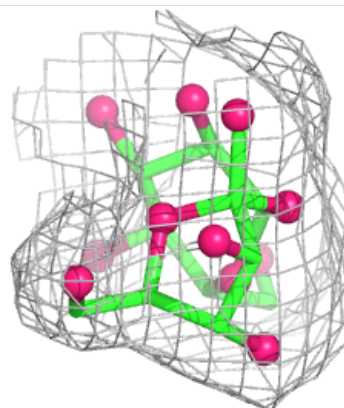
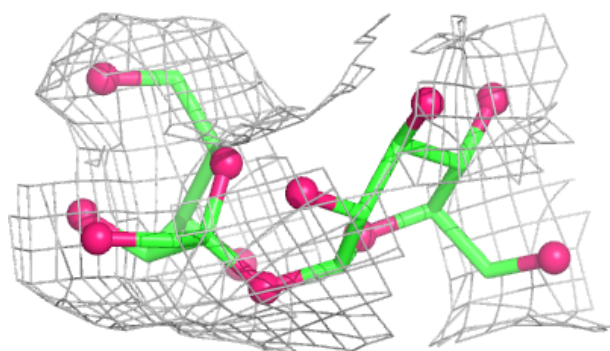
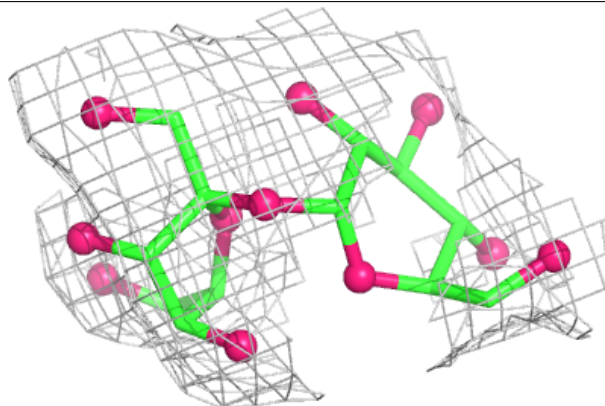


Electron density around Chain U:

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

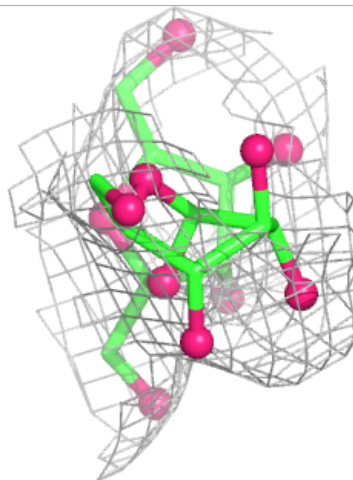
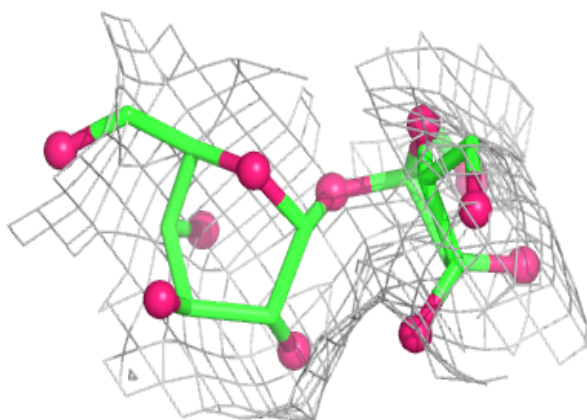
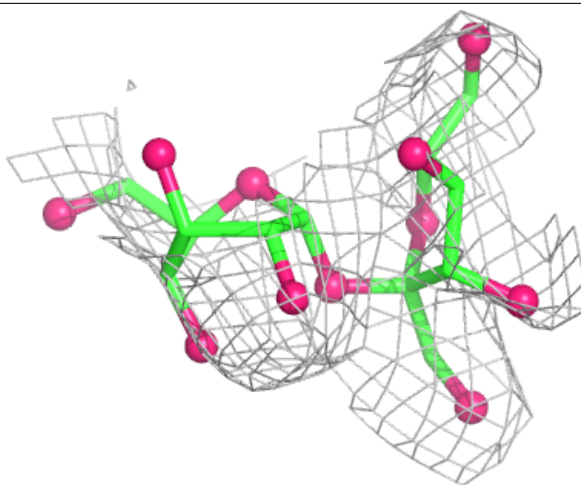
**Electron density around Chain V:**

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



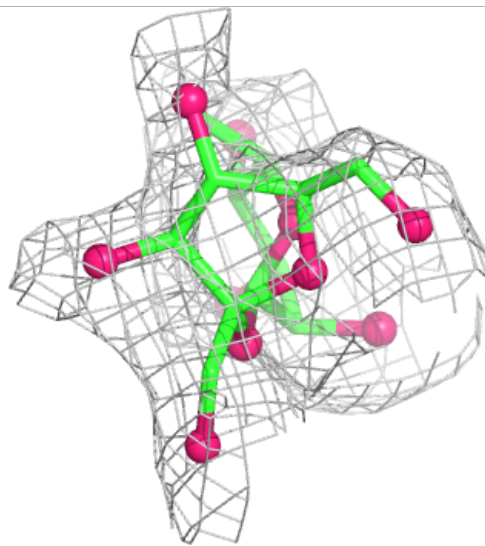
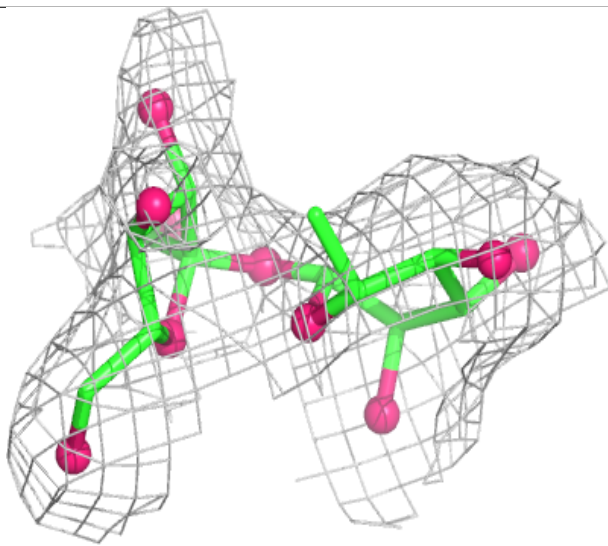
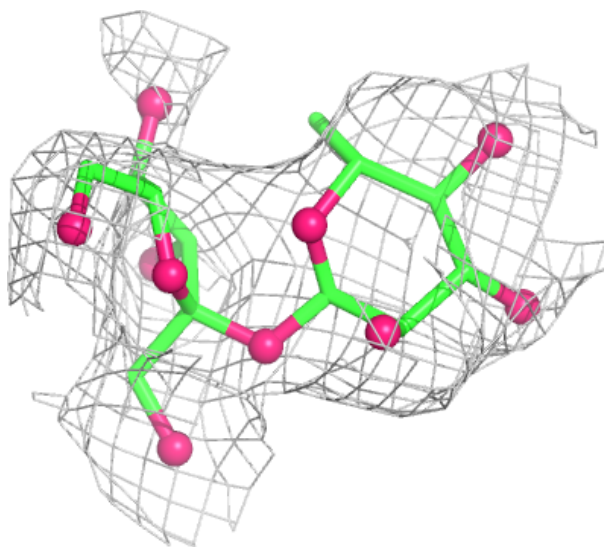
Electron density around Chain W:

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



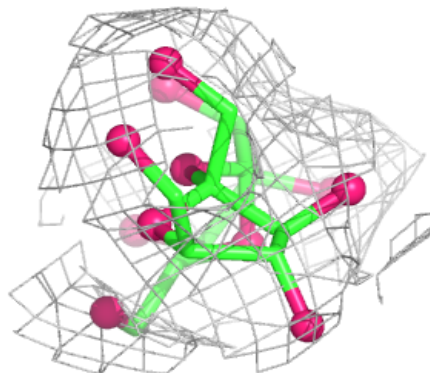
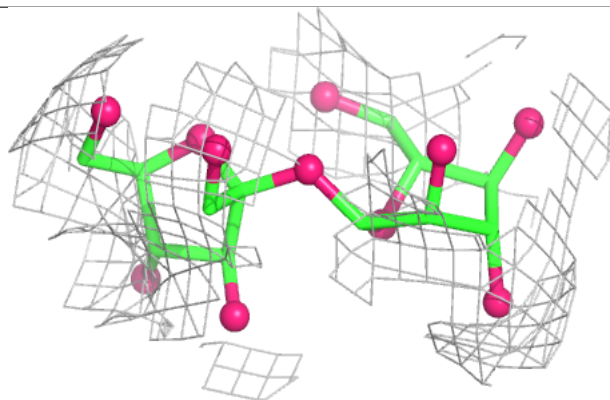
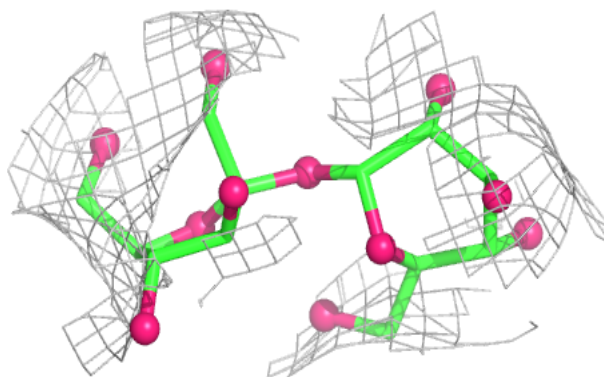
Electron density around Chain X:

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

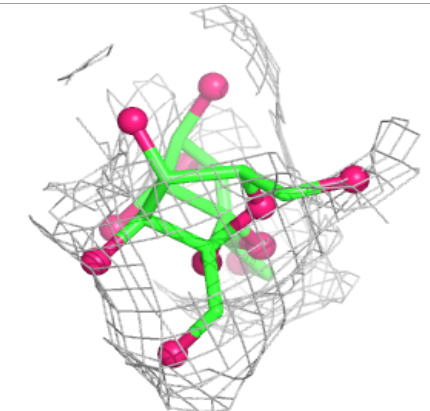
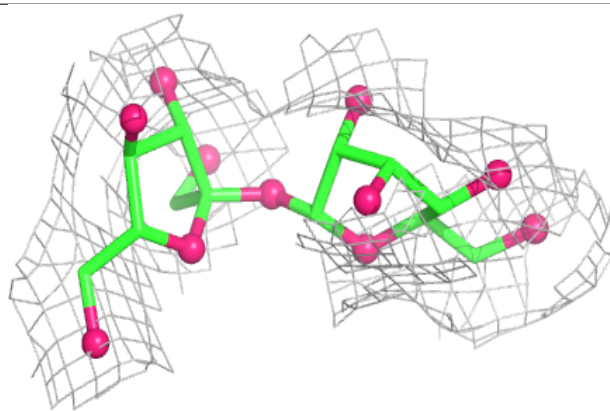
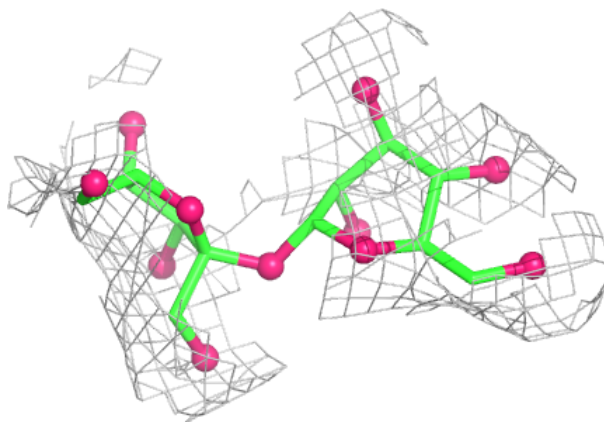


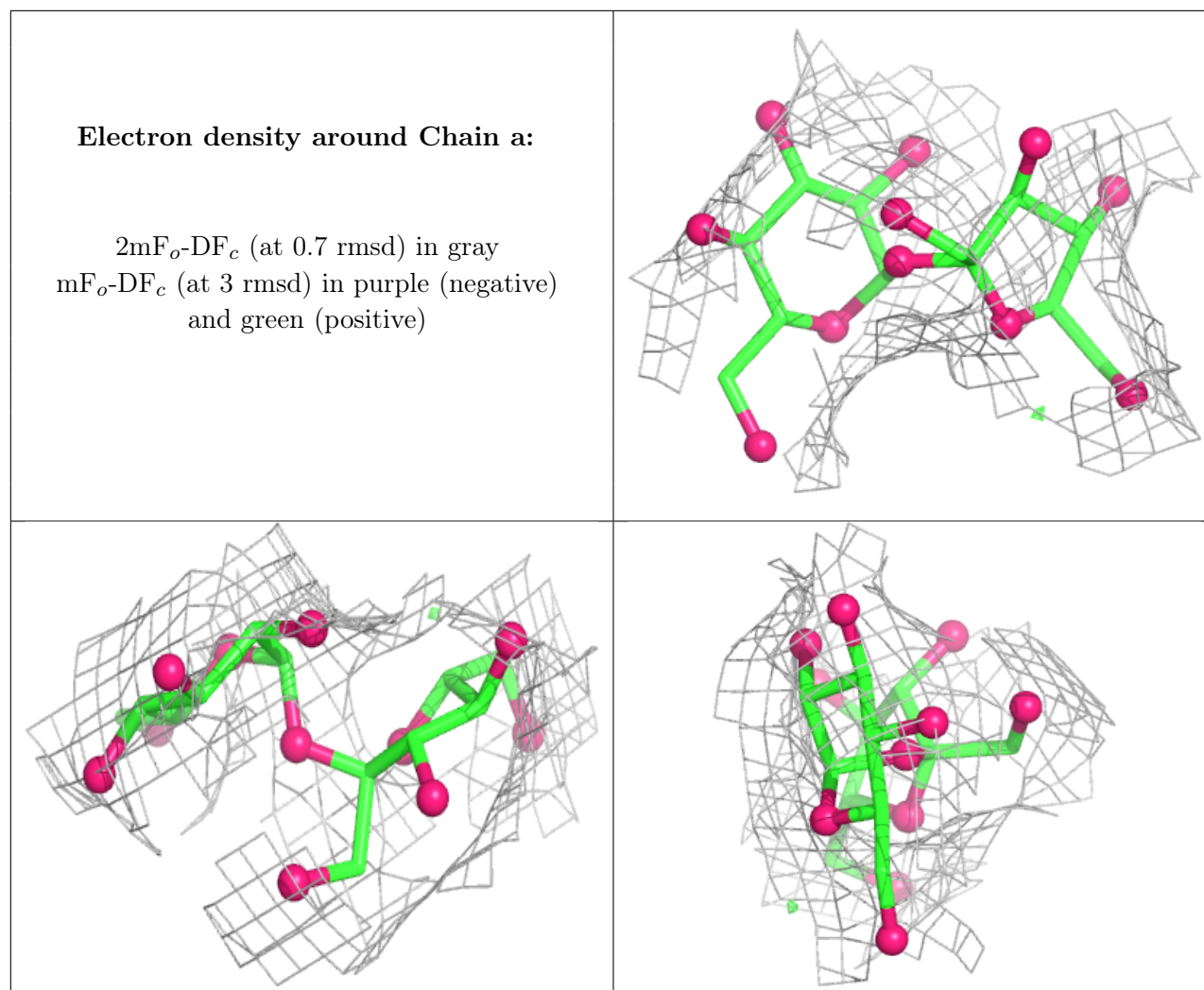
Electron density around Chain Y:

$2mF_o - DF_c$ (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 [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($\text{\AA}^2$)	Q<0.9
21	LMU	A	852	35/35	0.50	0.21	2,39,60,60	0
20	CLA	4	307	25/65	0.54	0.23	2,39,60,60	0
22	BCR	2	317	40/40	0.54	0.29	2,32,60,60	0
20	CLA	B	816	60/65	0.57	0.23	2,40,60,60	0
20	CLA	H	102	55/65	0.57	0.21	2,49,60,60	0
22	BCR	A	843	40/40	0.57	0.30	2,45,60,60	0
22	BCR	I	103	40/40	0.59	0.22	2,38,60,60	0
20	CLA	G	105	51/65	0.60	0.17	2,44,60,60	0
20	CLA	1	211	51/65	0.60	0.18	2,42,60,60	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
20	CLA	3	313	50/65	0.60	0.17	2,56,60,60	0
20	CLA	B	835	45/65	0.61	0.18	12,37,60,60	0
21	LMU	2	320	35/35	0.61	0.17	2,40,60,60	0
20	CLA	A	802	25/65	0.61	0.17	2,42,60,60	0
21	LMU	A	853	35/35	0.62	0.19	2,45,60,60	0
20	CLA	3	311	65/65	0.62	0.21	2,46,60,60	0
21	LMU	4	320	35/35	0.62	0.18	2,43,60,60	0
20	CLA	4	304	55/65	0.62	0.20	4,39,60,60	0
20	CLA	3	305	25/65	0.63	0.21	17,42,60,60	0
21	LMU	1	217	35/35	0.63	0.16	2,44,60,60	0
20	CLA	4	314	25/65	0.63	0.21	2,35,60,60	0
20	CLA	F	206	41/65	0.64	0.21	2,41,60,60	0
20	CLA	4	317	52/65	0.64	0.19	2,34,60,60	0
21	LMU	E	101	35/35	0.64	0.20	2,30,60,60	0
20	CLA	3	317	36/65	0.65	0.23	2,51,60,60	0
20	CLA	B	836	51/65	0.65	0.18	2,45,60,60	0
21	LMU	R	101	35/35	0.65	0.16	2,45,60,60	0
20	CLA	4	303	65/65	0.65	0.24	2,32,60,60	0
20	CLA	B	817	46/65	0.65	0.25	2,28,60,60	0
20	CLA	H	101	55/65	0.65	0.16	2,47,60,60	0
21	LMU	H	106	35/35	0.66	0.18	2,41,60,60	0
21	LMU	K	106	35/35	0.66	0.16	2,38,60,60	0
20	CLA	K	103	50/65	0.66	0.18	2,60,60,60	0
20	CLA	3	309	25/65	0.66	0.19	2,47,60,60	0
21	LMU	2	313	35/35	0.66	0.18	2,21,60,60	0
20	CLA	A	840	55/65	0.66	0.24	2,44,60,60	0
20	CLA	3	312	25/65	0.67	0.17	2,30,60,60	0
21	LMU	G	103	35/35	0.67	0.16	2,51,60,60	0
20	CLA	1	205	36/65	0.67	0.19	2,52,60,60	0
21	LMU	3	318	35/35	0.67	0.17	2,44,60,60	0
21	LMU	L	205	35/35	0.68	0.16	2,31,60,60	0
20	CLA	4	308	25/65	0.68	0.20	2,29,60,60	0
20	CLA	H	109	55/65	0.68	0.18	2,33,60,60	0
20	CLA	3	310	65/65	0.68	0.18	2,26,60,60	0
21	LMU	2	321	35/35	0.68	0.17	2,40,60,60	0
20	CLA	3	303	36/65	0.69	0.17	2,53,60,60	0
20	CLA	K	101	46/65	0.69	0.16	2,51,60,60	0
21	LMU	R	102	35/35	0.69	0.16	2,38,60,60	0
21	LMU	R	103	35/35	0.69	0.17	2,35,60,60	0
21	LMU	H	103	35/35	0.69	0.15	2,15,60,60	0
20	CLA	1	215	51/65	0.69	0.16	2,51,60,60	0
22	BCR	G	104	40/40	0.69	0.28	2,33,60,60	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
20	CLA	L	204	55/65	0.69	0.20	2,44,60,60	0
21	LMU	A	848	35/35	0.70	0.17	2,45,60,60	0
21	LMU	A	854	35/35	0.70	0.17	2,32,60,60	0
21	LMU	B	804	35/35	0.70	0.16	2,34,60,60	0
20	CLA	4	301	55/65	0.70	0.23	2,33,60,60	0
22	BCR	L	209	40/40	0.70	0.30	2,18,60,60	0
20	CLA	A	811	65/65	0.71	0.20	2,15,60,60	0
20	CLA	A	819	58/65	0.71	0.22	2,20,60,60	0
20	CLA	A	820	51/65	0.71	0.18	2,44,60,60	0
21	LMU	C	101	35/35	0.71	0.14	2,35,60,60	0
20	CLA	2	307	65/65	0.71	0.15	2,24,60,60	0
20	CLA	3	306	25/65	0.71	0.16	2,56,60,60	0
22	BCR	A	844	40/40	0.71	0.26	2,34,60,60	0
20	CLA	2	311	50/65	0.71	0.25	2,25,60,60	0
20	CLA	A	801	46/65	0.71	0.15	2,43,60,60	0
20	CLA	2	305	50/65	0.71	0.21	2,48,60,60	0
20	CLA	2	301	25/65	0.72	0.17	2,48,60,60	0
20	CLA	1	207	51/65	0.72	0.16	2,36,60,60	0
20	CLA	4	305	50/65	0.72	0.19	2,21,60,60	0
20	CLA	K	104	56/65	0.72	0.17	2,36,60,60	0
20	CLA	1	209	25/65	0.73	0.16	11,37,60,60	0
20	CLA	R	107	57/65	0.73	0.19	2,38,60,60	0
20	CLA	A	821	42/65	0.73	0.21	2,46,60,60	0
20	CLA	3	307	42/65	0.73	0.16	2,53,60,60	0
21	LMU	K	107	35/35	0.73	0.14	2,38,60,60	0
21	LMU	A	846	35/35	0.73	0.17	2,26,60,60	0
21	LMU	L	210	35/35	0.73	0.16	2,22,60,60	0
21	LMU	2	319	35/35	0.73	0.14	2,29,60,60	0
20	CLA	4	318	47/65	0.74	0.17	2,37,60,60	0
20	CLA	R	108	65/65	0.74	0.16	2,35,60,60	0
20	CLA	2	312	61/65	0.74	0.15	2,34,60,60	0
21	LMU	R	104	35/35	0.74	0.14	2,36,60,60	0
20	CLA	3	302	25/65	0.74	0.18	15,54,60,60	0
21	LMU	K	105	35/35	0.74	0.15	2,37,60,60	0
20	CLA	1	206	61/65	0.74	0.16	2,35,60,60	0
20	CLA	1	201	46/65	0.74	0.17	2,56,60,60	0
20	CLA	4	315	46/65	0.74	0.15	2,45,60,60	0
20	CLA	2	302	51/65	0.74	0.17	2,33,60,60	0
20	CLA	B	842	36/65	0.75	0.17	2,52,60,60	0
21	LMU	R	106	35/35	0.75	0.15	2,27,60,60	0
20	CLA	L	202	55/65	0.75	0.15	2,46,60,60	0
20	CLA	1	210	36/65	0.75	0.19	2,35,60,60	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
20	CLA	J	101	48/65	0.75	0.17	2,34,60,60	0
21	LMU	H	104	35/35	0.75	0.14	2,16,60,60	0
20	CLA	A	841	25/65	0.75	0.16	2,43,60,60	0
20	CLA	A	810	45/65	0.75	0.17	2,38,60,60	0
21	LMU	R	105	35/35	0.76	0.13	2,35,60,60	0
21	LMU	F	202	34/35	0.76	0.15	2,23,60,60	0
20	CLA	3	316	25/65	0.76	0.14	2,42,60,60	0
20	CLA	A	814	25/65	0.76	0.18	2,31,60,60	0
20	CLA	1	214	25/65	0.76	0.15	5,42,60,60	0
22	BCR	B	845	40/40	0.76	0.22	2,21,60,60	0
21	LMU	B	849	25/35	0.76	0.14	2,36,60,60	0
20	CLA	K	102	50/65	0.76	0.16	2,28,60,60	0
20	CLA	1	203	47/65	0.76	0.16	2,17,60,60	0
26	UNL	H	107	23/-	0.76	0.14	2,31,60,60	0
20	CLA	A	839	59/65	0.77	0.16	2,30,60,60	0
21	LMU	G	102	35/35	0.77	0.16	2,33,60,60	0
21	LMU	4	316	35/35	0.77	0.14	2,37,60,60	0
20	CLA	4	302	36/65	0.77	0.24	2,26,60,60	0
20	CLA	2	306	25/65	0.77	0.17	2,57,60,60	0
20	CLA	1	208	25/65	0.78	0.17	2,31,60,60	0
20	CLA	2	310	50/65	0.78	0.19	2,18,60,60	0
20	CLA	B	813	55/65	0.78	0.22	2,28,60,60	0
21	LMU	G	101	35/35	0.78	0.15	2,34,60,60	0
21	LMU	L	206	35/35	0.78	0.15	2,23,60,60	0
20	CLA	3	314	65/65	0.78	0.15	2,33,60,60	0
20	CLA	L	201	60/65	0.78	0.22	2,18,60,60	0
20	CLA	A	829	50/65	0.78	0.19	2,32,60,60	0
22	BCR	J	102	40/40	0.78	0.24	2,31,60,60	0
20	CLA	A	833	45/65	0.78	0.18	2,37,60,60	0
25	LMG	B	848	49/55	0.78	0.27	2,20,60,60	0
20	CLA	A	817	52/65	0.78	0.23	2,33,60,60	0
20	CLA	3	301	36/65	0.79	0.16	2,34,60,60	0
20	CLA	B	812	54/65	0.79	0.19	2,17,60,60	0
22	BCR	A	845	40/40	0.79	0.25	2,5,44,60	0
20	CLA	A	823	58/65	0.79	0.23	2,18,60,60	0
20	CLA	B	815	60/65	0.79	0.21	2,19,60,60	0
20	CLA	A	815	50/65	0.79	0.17	2,21,60,60	0
20	CLA	1	212	25/65	0.79	0.18	2,42,60,60	0
20	CLA	1	213	51/65	0.79	0.19	2,39,60,60	0
20	CLA	J	103	61/65	0.79	0.16	2,19,60,60	0
20	CLA	4	310	50/65	0.79	0.16	2,20,60,60	0
20	CLA	B	822	46/65	0.80	0.20	2,34,60,60	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
21	LMU	4	321	35/35	0.80	0.13	2,21,55,60	0
22	BCR	B	844	40/40	0.80	0.21	2,5,60,60	0
20	CLA	3	315	25/65	0.80	0.14	2,47,60,60	0
20	CLA	2	309	25/65	0.80	0.14	2,34,60,60	0
20	CLA	4	306	52/65	0.81	0.14	2,26,60,60	0
20	CLA	L	208	50/65	0.81	0.17	2,18,60,60	0
20	CLA	B	823	55/65	0.81	0.18	2,30,60,60	0
20	CLA	B	834	45/65	0.81	0.19	2,16,60,60	0
20	CLA	1	204	46/65	0.81	0.16	2,35,60,60	0
21	LMU	1	218	35/35	0.81	0.15	2,46,60,60	0
20	CLA	A	812	54/65	0.81	0.16	2,28,60,60	0
20	CLA	H	110	50/65	0.81	0.17	2,27,60,60	0
20	CLA	A	807	46/65	0.81	0.19	2,20,60,60	0
20	CLA	A	834	46/65	0.82	0.21	2,20,60,60	0
20	CLA	A	804	55/65	0.82	0.19	2,11,60,60	0
20	CLA	B	837	60/65	0.82	0.22	2,2,60,60	0
21	LMU	R	109	35/35	0.82	0.14	2,21,60,60	0
21	LMU	A	847	35/35	0.82	0.14	2,27,60,60	0
20	CLA	A	824	59/65	0.82	0.19	2,25,60,60	0
20	CLA	A	825	65/65	0.82	0.19	2,16,60,60	0
20	CLA	F	207	53/65	0.82	0.14	2,22,60,60	0
21	LMU	2	318	35/35	0.82	0.12	2,25,60,60	0
20	CLA	A	805	54/65	0.82	0.20	2,10,60,60	0
22	BCR	B	847	40/40	0.82	0.23	2,10,60,60	0
21	LMU	B	805	35/35	0.82	0.16	2,37,60,60	0
20	CLA	B	825	54/65	0.82	0.24	2,15,60,60	0
20	CLA	B	826	58/65	0.82	0.23	2,13,60,60	0
21	LMU	D	201	35/35	0.82	0.12	2,12,50,57	0
20	CLA	L	203	65/65	0.82	0.23	2,22,60,60	0
20	CLA	2	314	50/65	0.82	0.13	2,33,60,60	0
20	CLA	B	807	45/65	0.83	0.19	2,14,56,60	0
20	CLA	B	808	61/65	0.83	0.18	2,9,48,60	0
20	CLA	2	303	58/65	0.83	0.13	2,22,60,60	0
20	CLA	L	207	47/65	0.83	0.18	2,13,45,60	0
21	LMU	A	855	35/35	0.83	0.14	2,29,60,60	0
20	CLA	F	201	50/65	0.83	0.15	2,7,51,60	0
20	CLA	2	304	25/65	0.83	0.14	2,27,60,60	0
20	CLA	A	813	50/65	0.83	0.20	2,29,60,60	0
21	LMU	1	216	35/35	0.83	0.12	2,11,50,60	0
20	CLA	4	309	25/65	0.83	0.17	2,40,60,60	0
20	CLA	3	308	25/65	0.83	0.15	2,37,60,60	0
20	CLA	B	820	61/65	0.83	0.19	2,16,60,60	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
20	CLA	B	821	50/65	0.83	0.20	2,37,60,60	0
20	CLA	A	816	54/65	0.83	0.16	2,31,60,60	0
20	CLA	I	102	60/65	0.83	0.15	2,18,60,60	0
20	CLA	2	315	25/65	0.83	0.16	2,36,60,60	0
20	CLA	A	818	60/65	0.83	0.20	2,11,52,60	0
22	BCR	I	101	39/40	0.83	0.22	2,8,60,60	0
20	CLA	3	304	25/65	0.83	0.14	2,28,60,60	0
20	CLA	B	827	65/65	0.83	0.21	2,15,60,60	0
20	CLA	B	832	59/65	0.83	0.21	2,6,60,60	0
20	CLA	2	316	65/65	0.83	0.16	2,15,60,60	0
20	CLA	B	806	65/65	0.83	0.23	2,11,60,60	0
20	CLA	A	806	56/65	0.84	0.18	2,2,54,60	0
21	LMU	3	319	35/35	0.84	0.10	2,28,59,60	0
20	CLA	4	313	36/65	0.84	0.16	2,21,60,60	0
20	CLA	A	828	65/65	0.84	0.21	2,12,60,60	0
20	CLA	A	851	65/65	0.84	0.22	2,2,60,60	0
22	BCR	B	846	40/40	0.84	0.23	2,11,60,60	0
20	CLA	A	803	46/65	0.84	0.14	2,14,49,60	0
20	CLA	A	832	50/65	0.84	0.18	2,18,56,60	0
20	CLA	1	202	41/65	0.84	0.15	2,41,60,60	0
20	CLA	4	312	25/65	0.84	0.15	2,2,26,32	0
20	CLA	A	835	65/65	0.84	0.19	2,6,60,60	0
20	CLA	B	814	65/65	0.84	0.19	2,13,60,60	0
23	PQN	B	843	33/33	0.84	0.22	2,2,46,51	0
20	CLA	H	108	58/65	0.84	0.20	2,15,60,60	0
20	CLA	A	837	51/65	0.84	0.24	2,12,60,60	0
20	CLA	B	803	65/65	0.85	0.22	2,14,56,60	0
20	CLA	B	838	65/65	0.85	0.18	2,7,60,60	0
20	CLA	B	840	65/65	0.85	0.22	2,11,60,60	0
20	CLA	B	824	65/65	0.85	0.18	2,17,60,60	0
20	CLA	B	833	50/65	0.85	0.24	2,11,53,60	0
20	CLA	B	811	25/65	0.86	0.17	2,2,60,60	0
20	CLA	A	850	65/65	0.86	0.21	2,4,48,60	0
20	CLA	B	810	60/65	0.86	0.21	2,2,60,60	0
22	BCR	F	203	40/40	0.86	0.21	2,2,60,60	0
20	CLA	B	829	65/65	0.86	0.18	2,11,46,60	0
21	LMU	4	319	34/35	0.86	0.12	2,22,60,60	0
21	LMU	H	105	35/35	0.87	0.11	2,31,60,60	0
22	BCR	B	801	40/40	0.87	0.20	2,4,50,60	0
20	CLA	A	838	65/65	0.87	0.19	2,8,60,60	0
20	CLA	A	826	65/65	0.87	0.21	2,2,50,60	0
20	CLA	4	311	25/65	0.87	0.23	2,15,60,60	0

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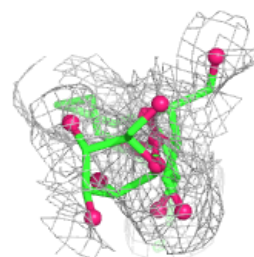
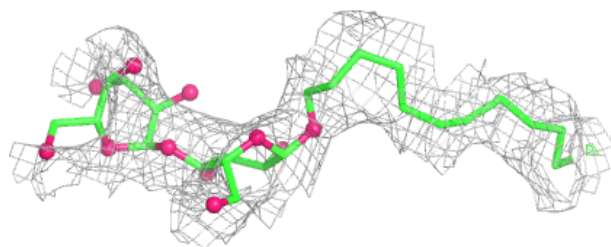
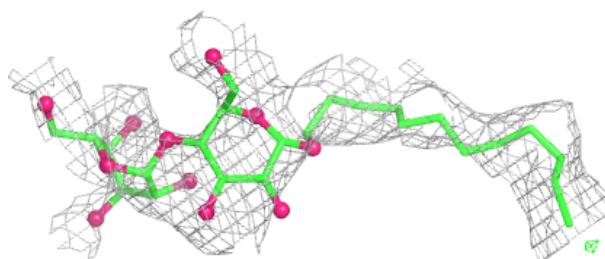
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
23	PQN	A	842	33/33	0.87	0.23	2,4,59,60	0
20	CLA	F	205	36/65	0.87	0.17	2,17,60,60	0
20	CLA	B	818	53/65	0.87	0.17	2,14,60,60	0
22	BCR	F	204	40/40	0.87	0.17	2,6,60,60	0
20	CLA	2	308	25/65	0.88	0.14	2,12,60,60	0
20	CLA	B	839	47/65	0.88	0.14	2,5,55,60	0
20	CLA	A	827	55/65	0.88	0.20	2,12,60,60	0
20	CLA	B	841	65/65	0.88	0.20	2,2,55,60	0
20	CLA	A	830	65/65	0.88	0.17	2,9,59,60	0
20	CLA	A	831	65/65	0.88	0.17	2,14,60,60	0
20	CLA	A	836	47/65	0.88	0.16	2,8,50,60	0
20	CLA	B	831	50/65	0.89	0.14	2,12,60,60	0
20	CLA	A	822	50/65	0.89	0.21	2,7,60,60	0
20	CLA	B	850	65/65	0.89	0.22	2,2,55,60	0
20	CLA	A	808	60/65	0.90	0.20	2,10,60,60	0
20	CLA	B	830	65/65	0.90	0.20	2,6,53,60	0
20	CLA	A	809	52/65	0.90	0.18	2,10,60,60	0
20	CLA	B	809	65/65	0.90	0.20	2,2,53,60	0
20	CLA	B	819	41/65	0.90	0.14	2,5,40,60	0
20	CLA	B	828	65/65	0.90	0.18	2,10,56,60	0
20	CLA	A	849	65/65	0.91	0.22	2,2,48,60	0
20	CLA	B	802	54/65	0.91	0.18	2,6,45,60	0
24	SF4	C	103	8/8	0.98	0.05	12,19,20,24	0
24	SF4	A	856	8/8	0.98	0.05	23,24,24,25	0
24	SF4	C	102	8/8	0.98	0.06	18,22,26,32	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.

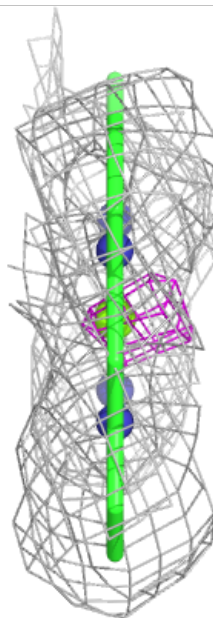
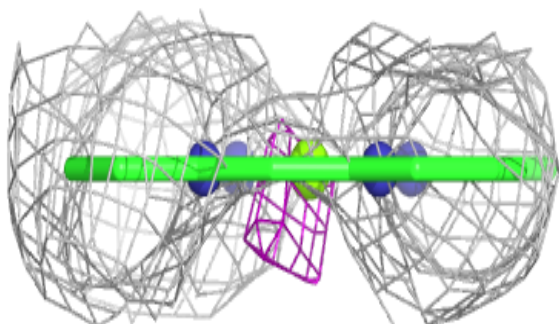
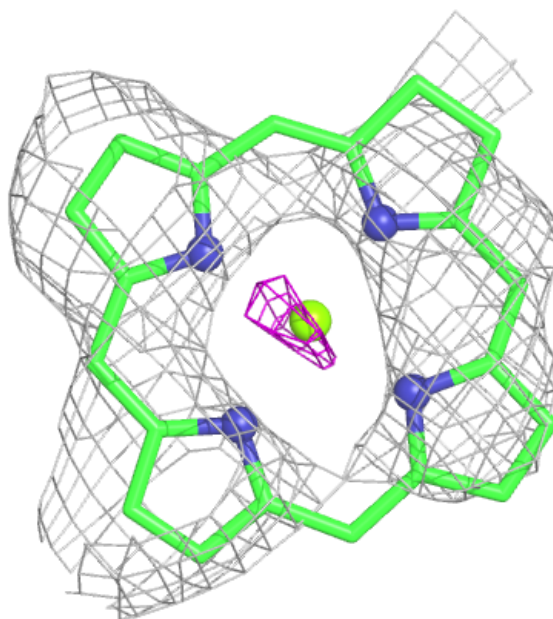
Electron density around LMU A 852:

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



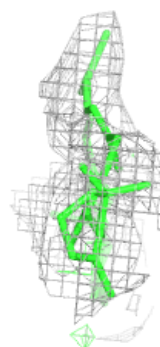
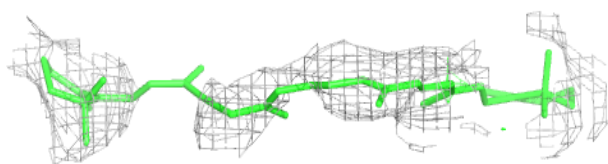
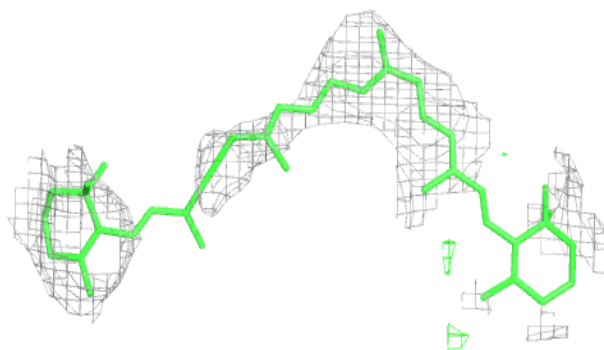
Electron density around CLA 4 307:

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

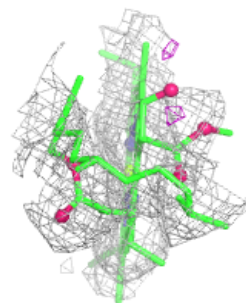
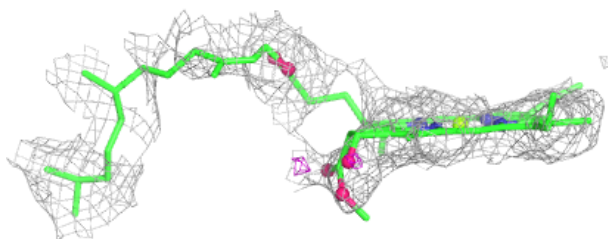
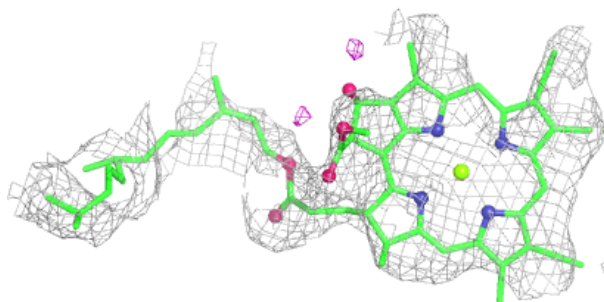


Electron density around BCR 2 317:

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

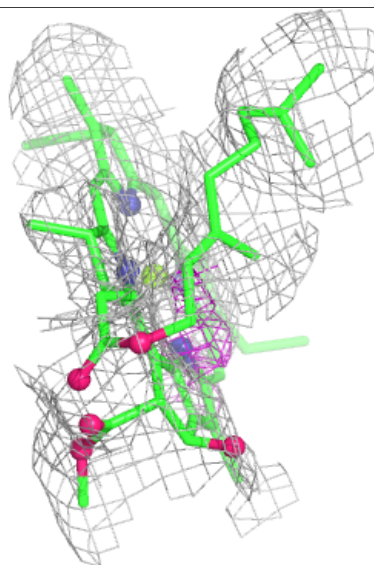
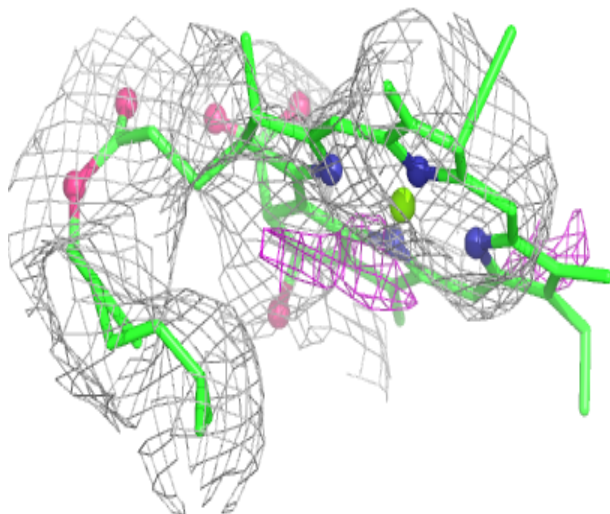
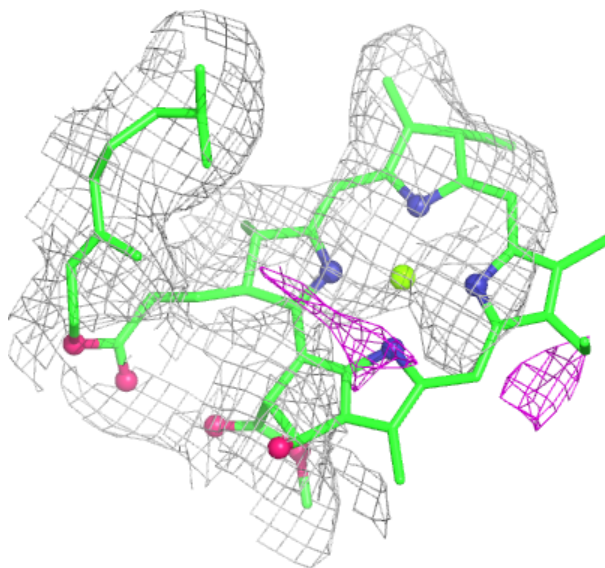
**Electron density around CLA B 816:**

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



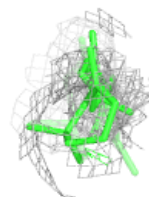
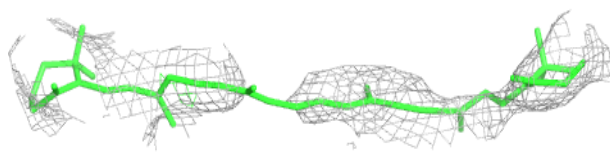
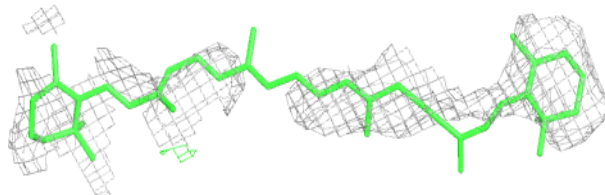
Electron density around CLA H 102:

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

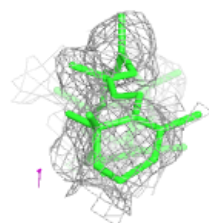
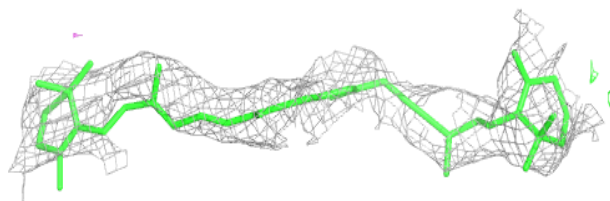
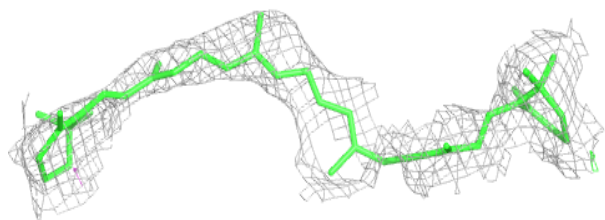


Electron density around BCR A 843:

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

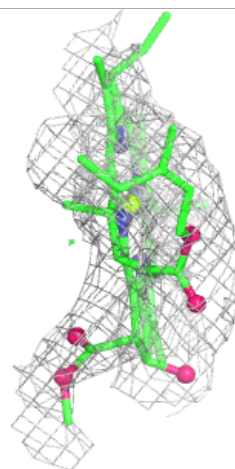
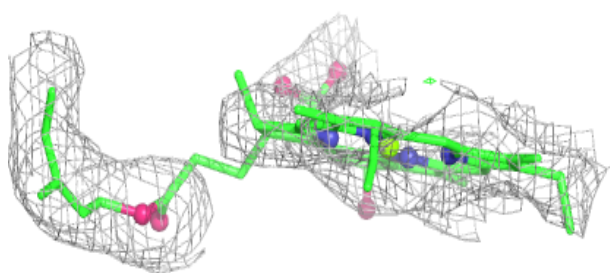
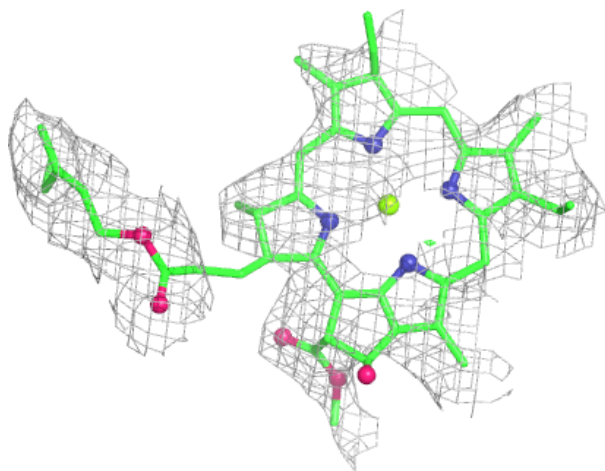
**Electron density around BCR I 103:**

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



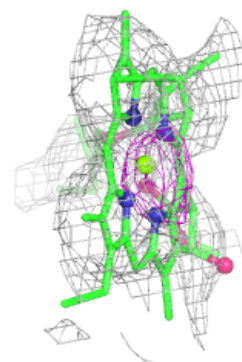
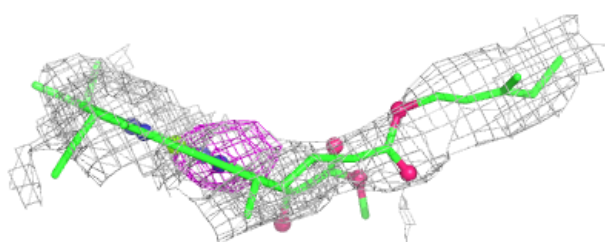
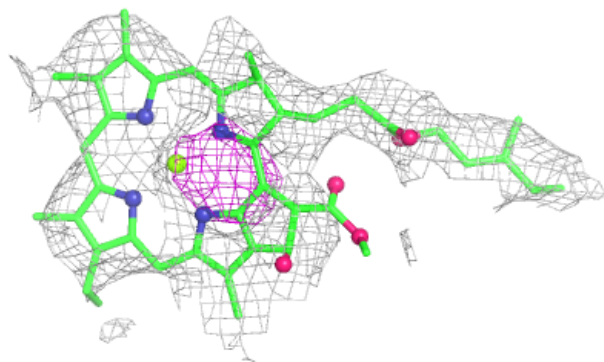
Electron density around CLA G 105:

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



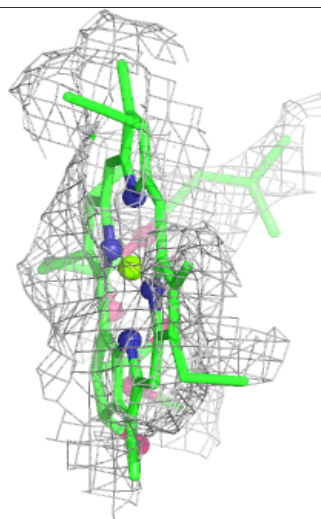
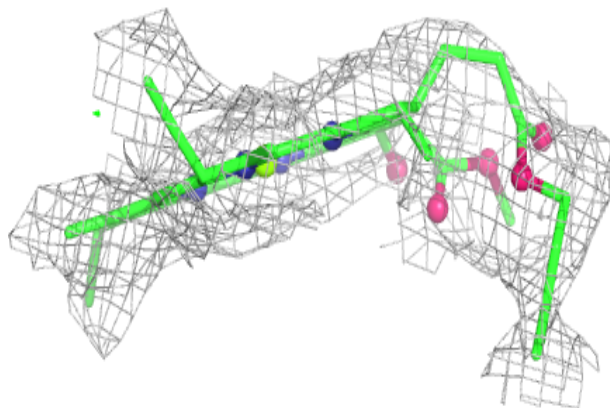
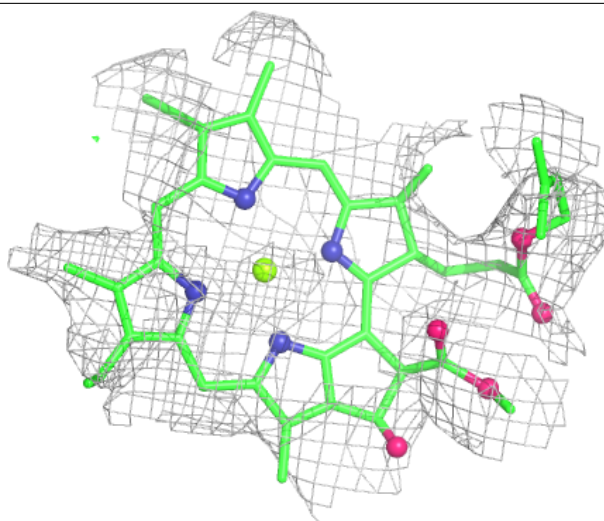
Electron density around CLA 1 211:

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



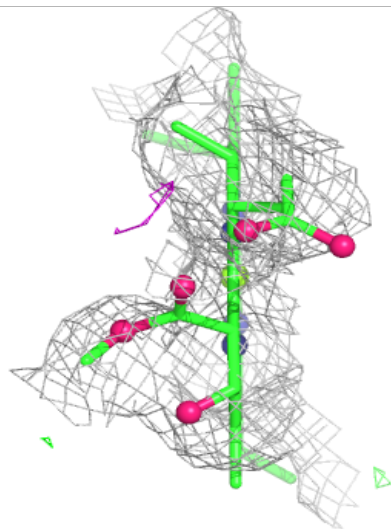
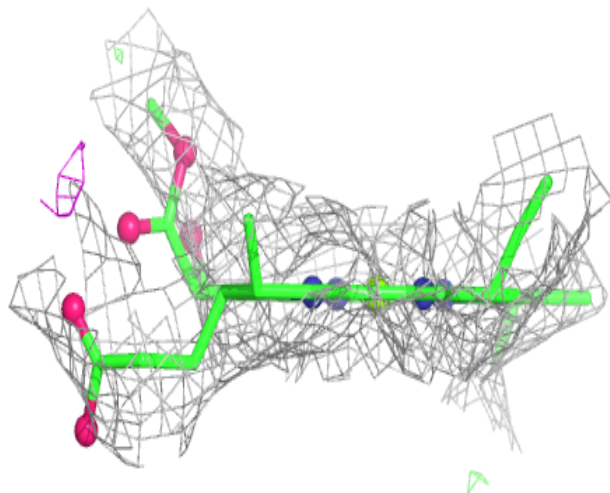
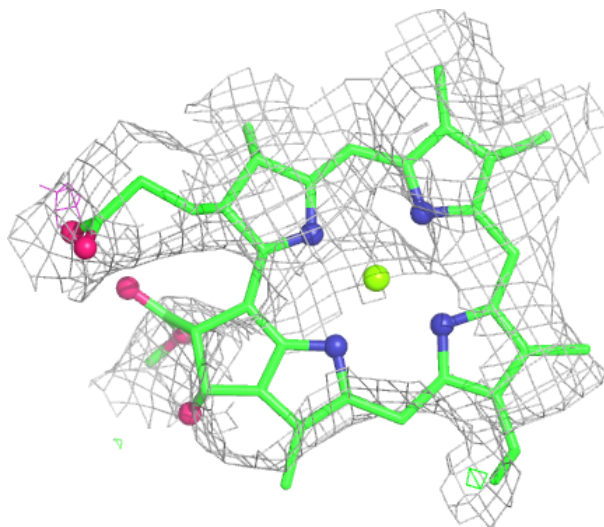
Electron density around CLA 3 313:

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



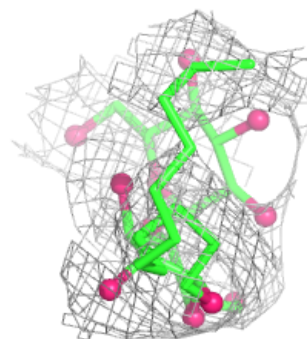
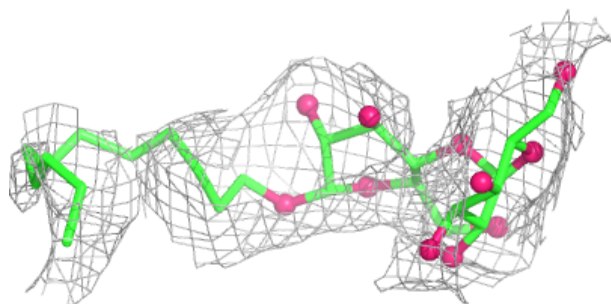
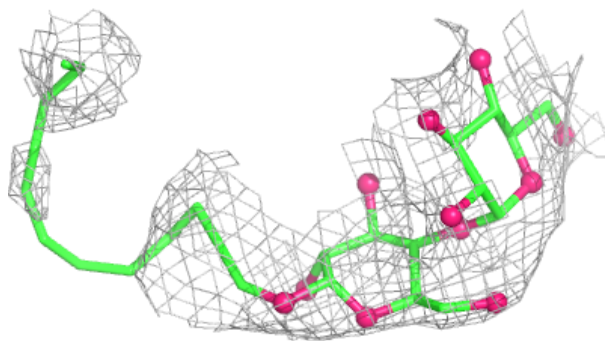
Electron density around CLA B 835:

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



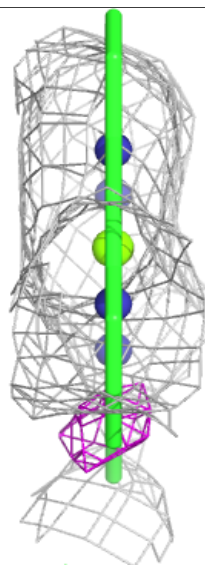
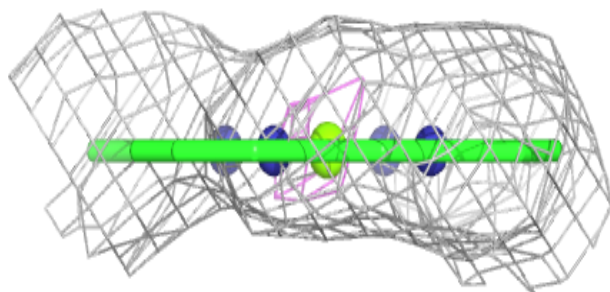
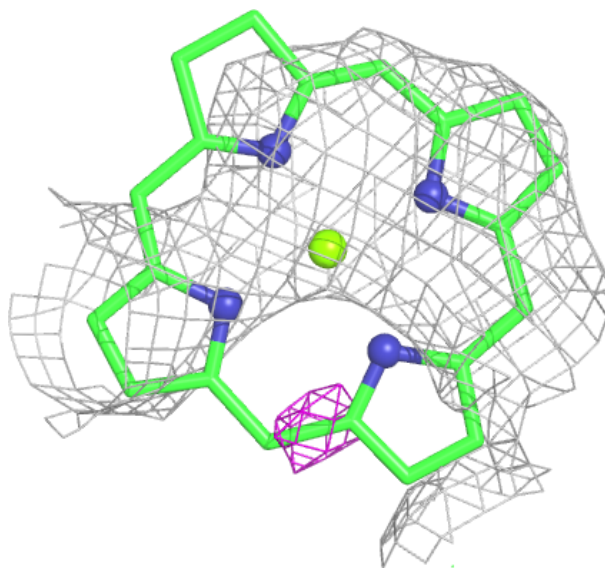
Electron density around LMU 2 320:

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



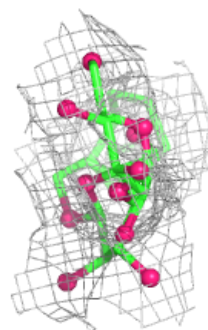
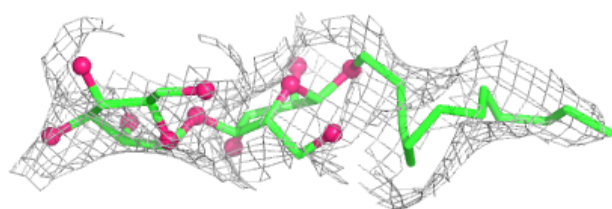
Electron density around CLA A 802:

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



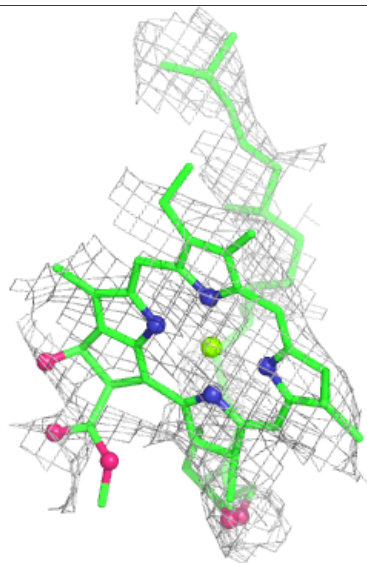
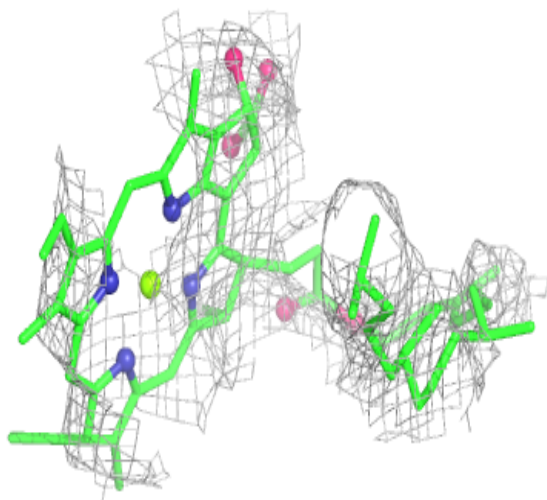
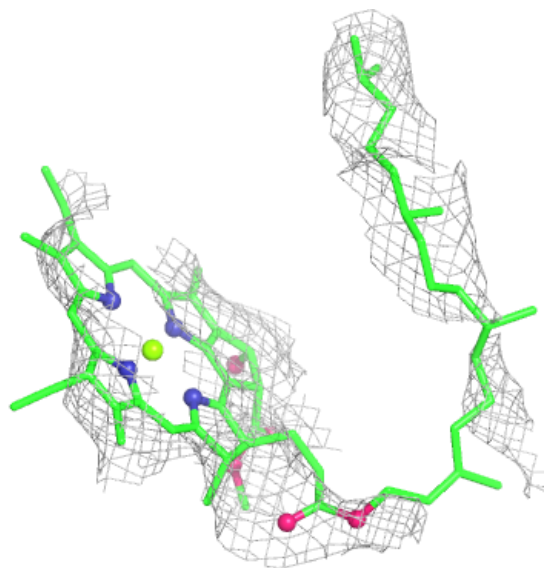
Electron density around LMU A 853:

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



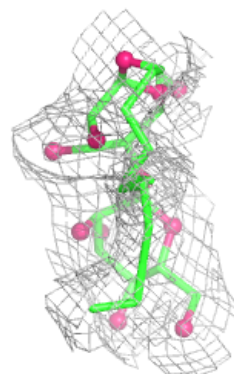
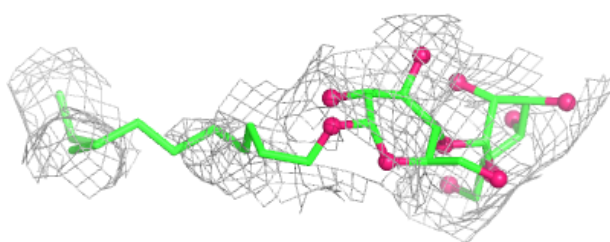
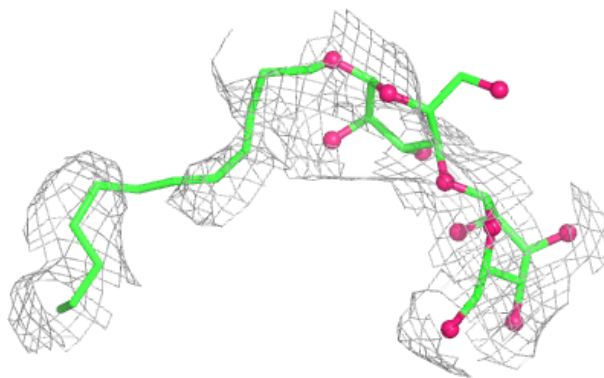
Electron density around CLA 3 311:

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



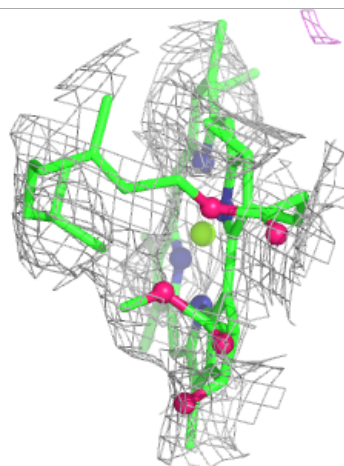
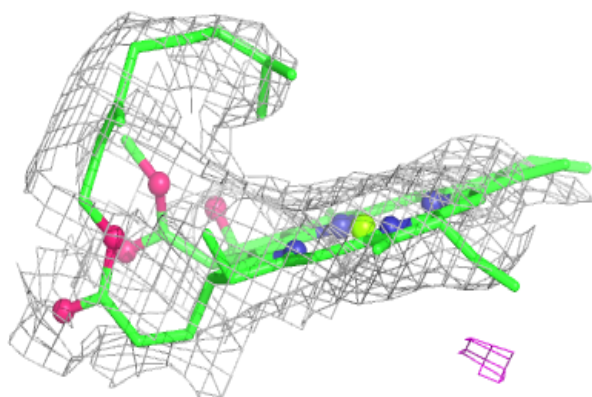
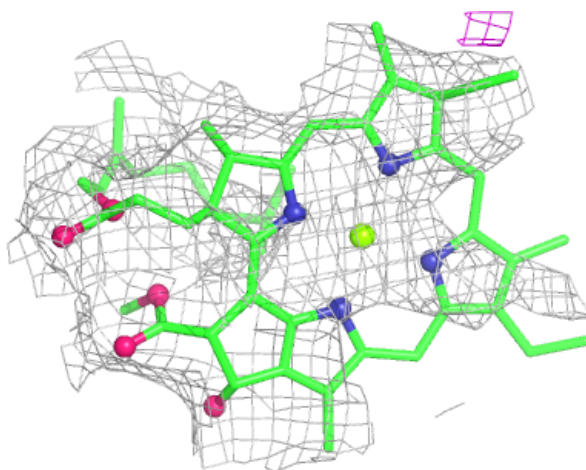
Electron density around LMU 4 320:

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



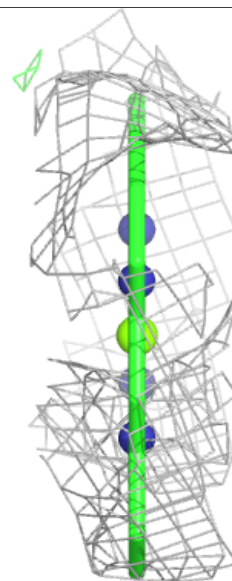
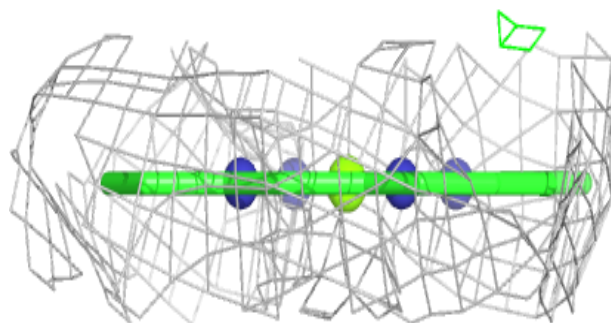
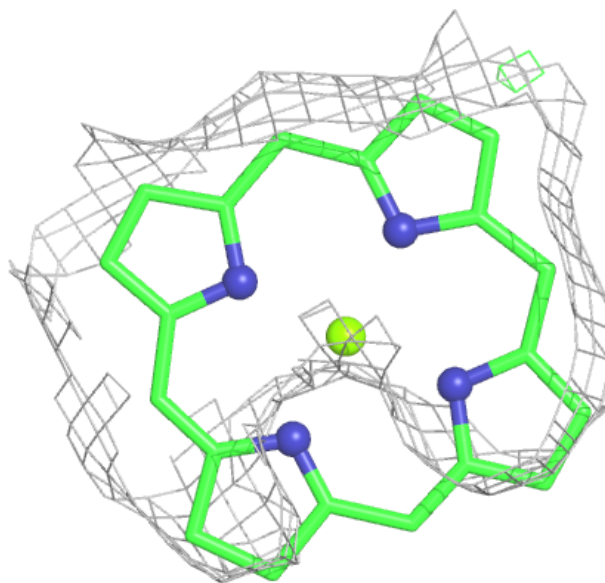
Electron density around CLA 4 304:

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



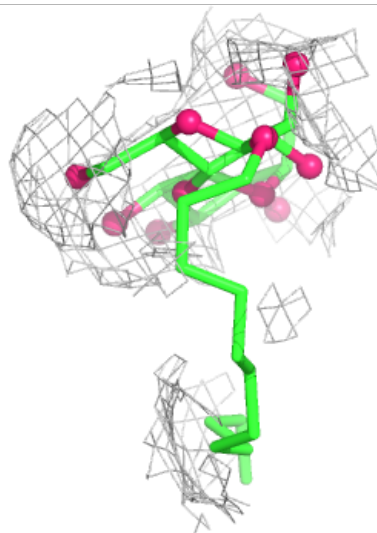
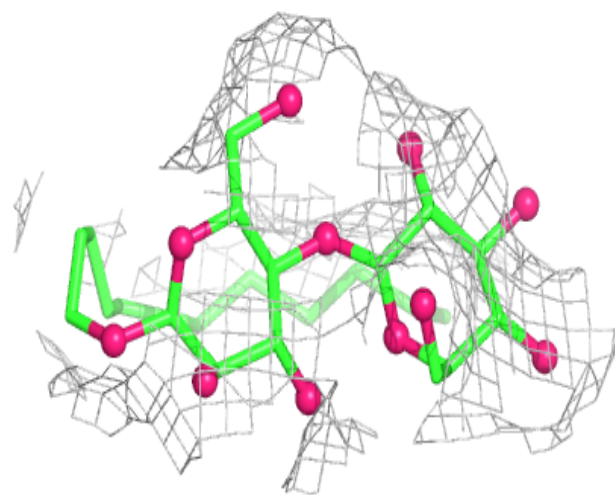
Electron density around CLA 3 305:

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



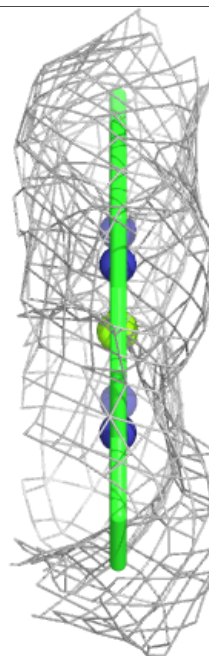
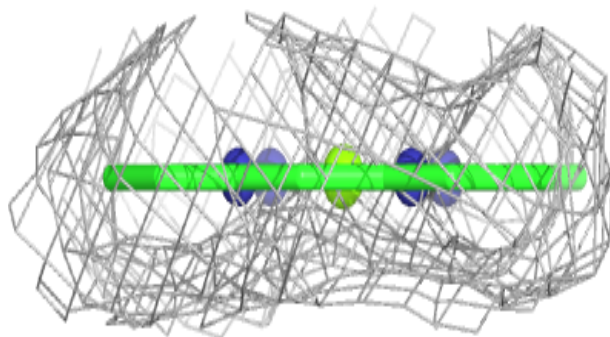
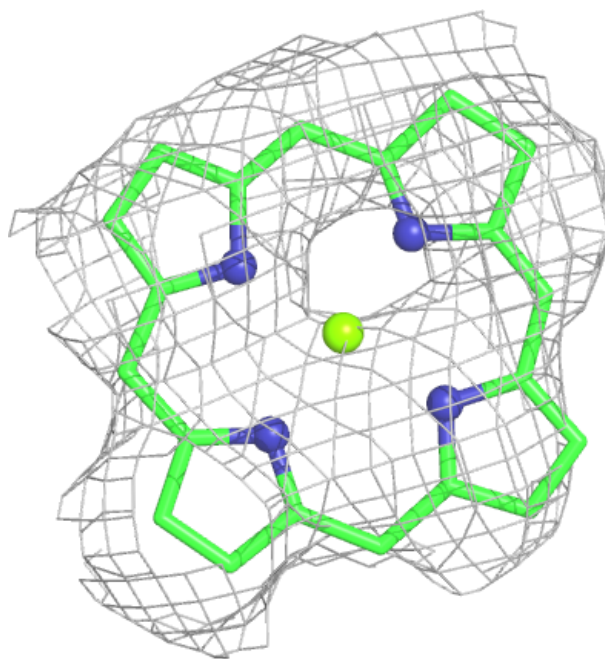
Electron density around LMU 1 217:

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



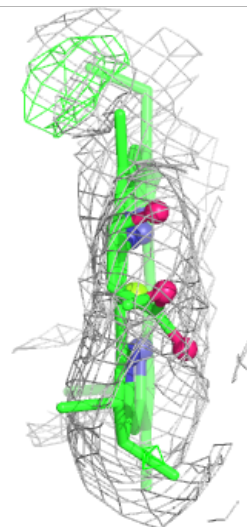
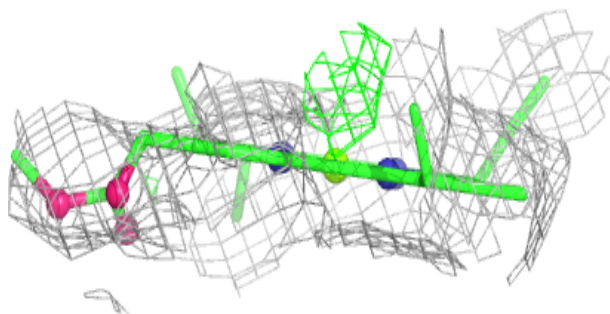
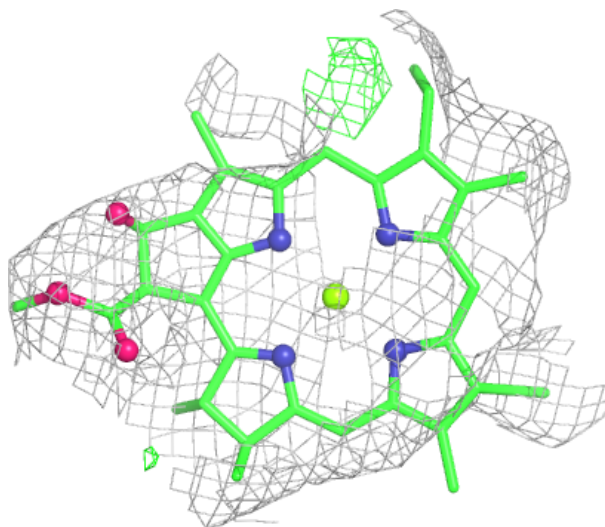
Electron density around CLA 4 314:

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



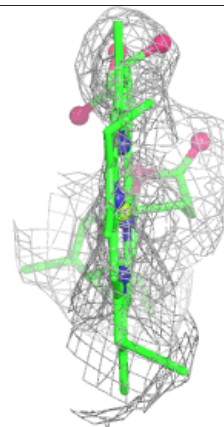
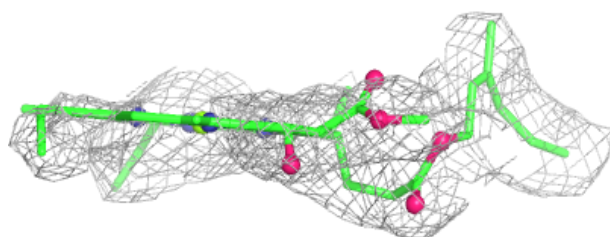
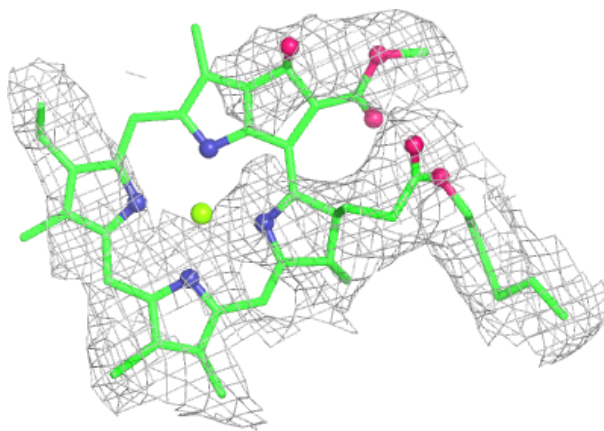
Electron density around CLA F 206:

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

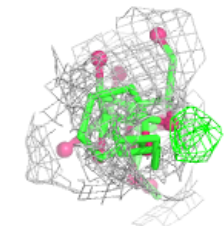
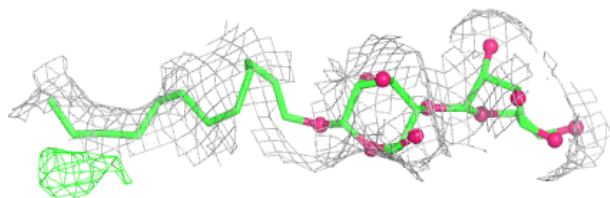
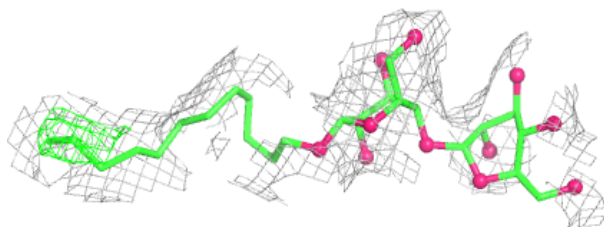


Electron density around CLA 4 317:

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

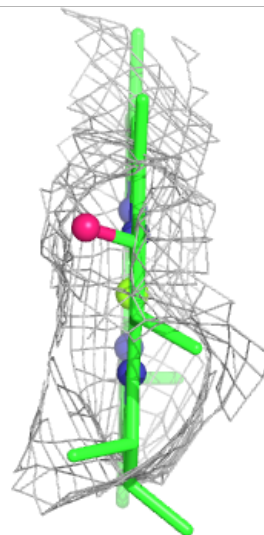
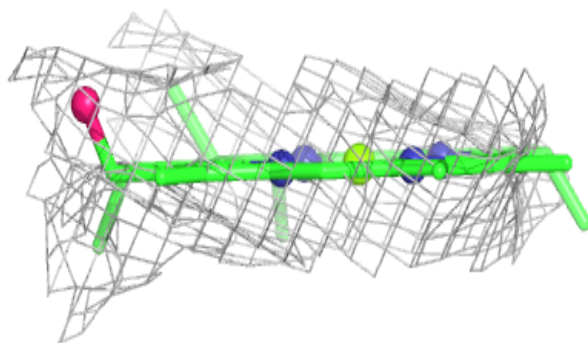
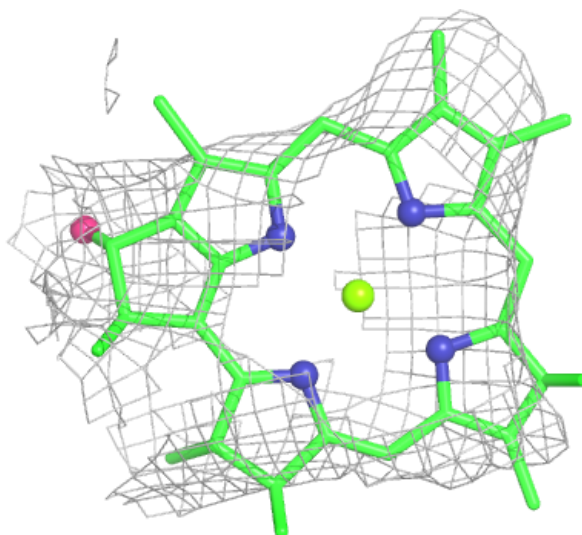
**Electron density around LMU E 101:**

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



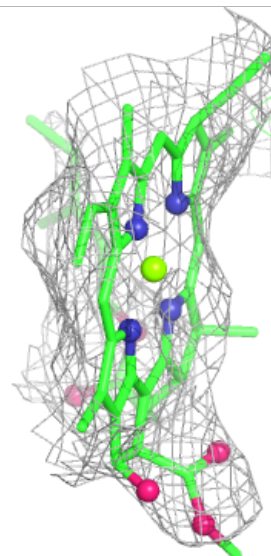
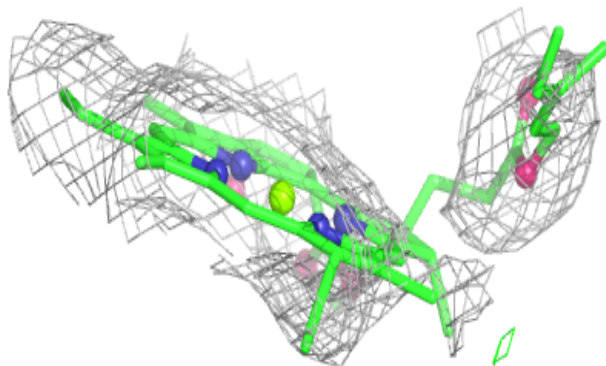
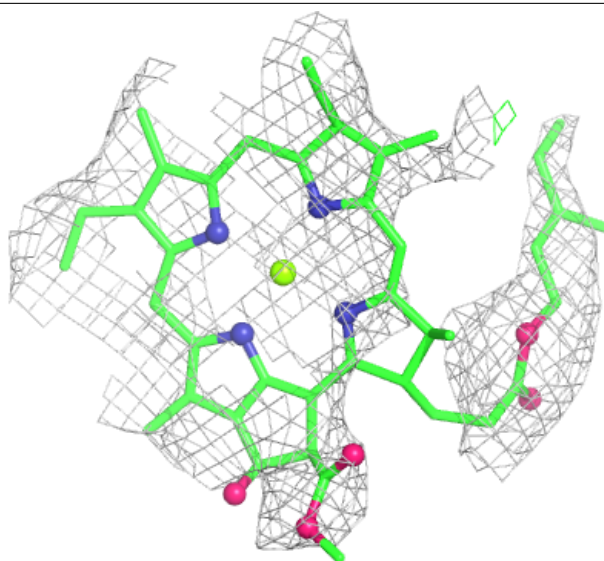
Electron density around CLA 3 317:

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



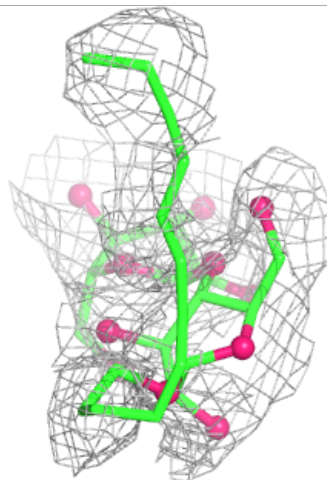
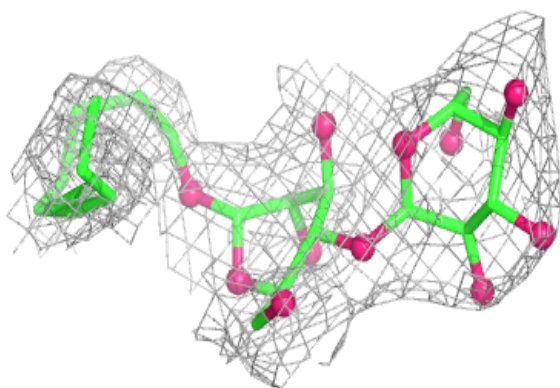
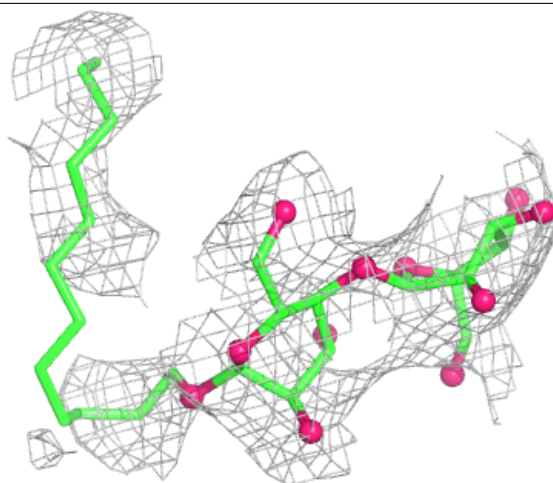
Electron density around CLA B 836:

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



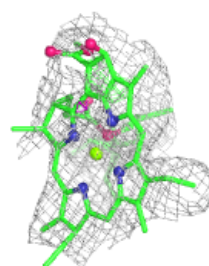
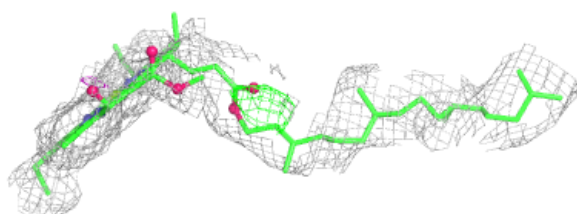
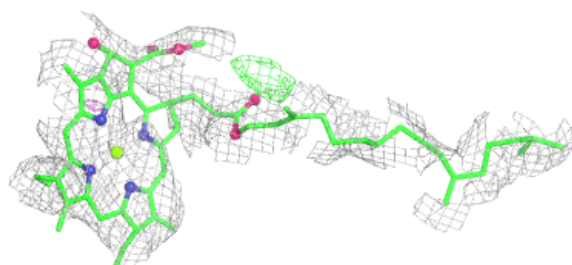
Electron density around LMU R 101:

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



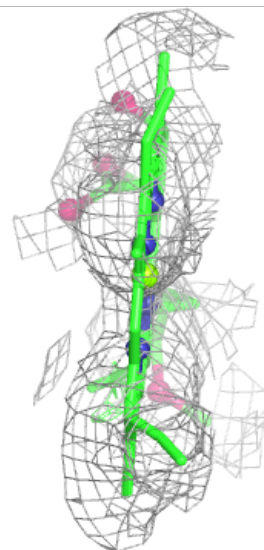
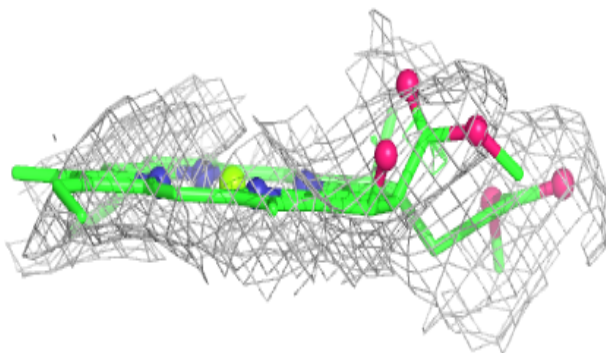
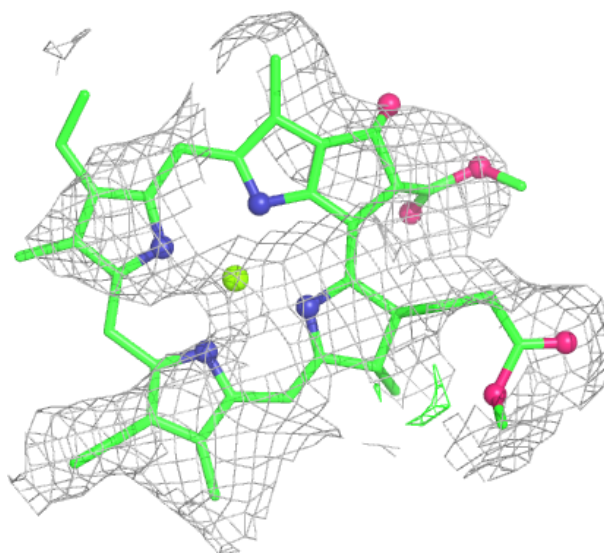
Electron density around CLA 4 303:

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



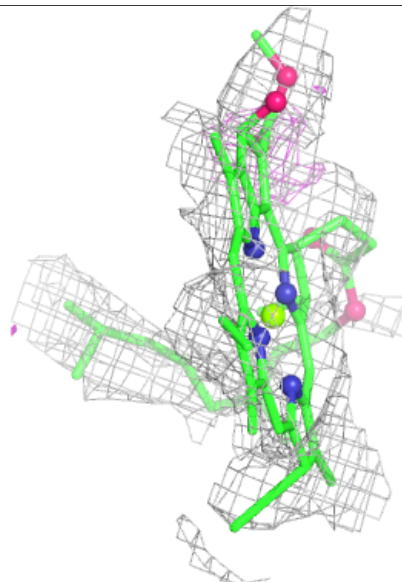
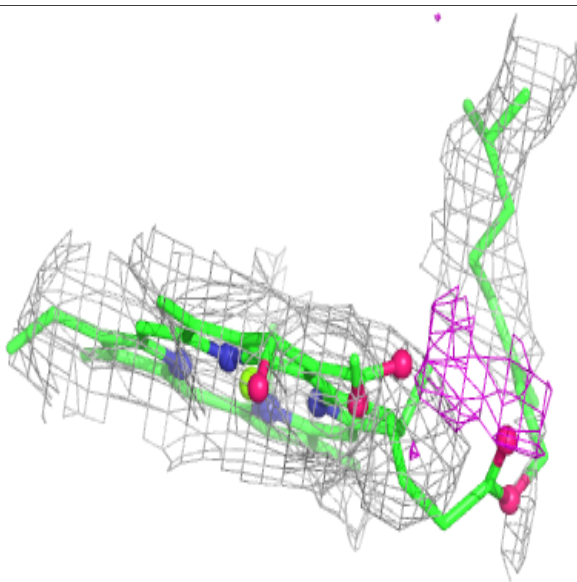
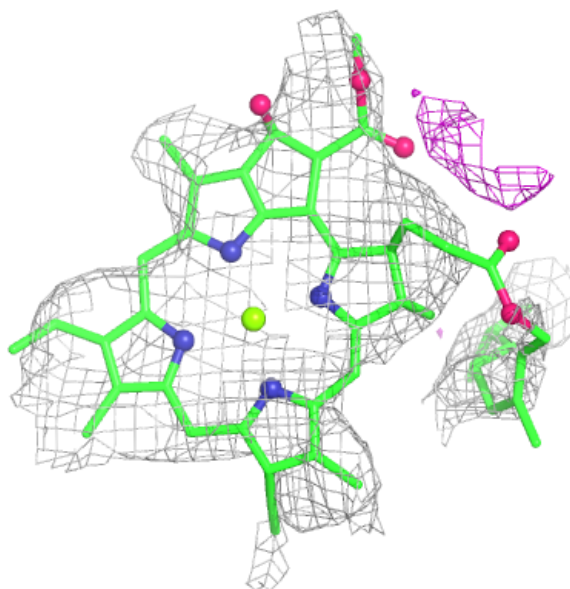
Electron density around CLA B 817:

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



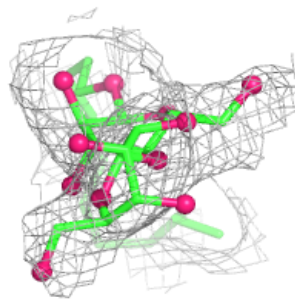
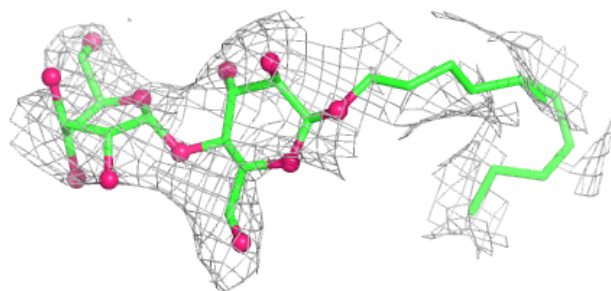
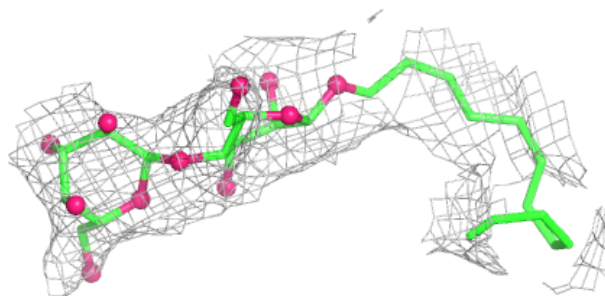
Electron density around CLA H 101:

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



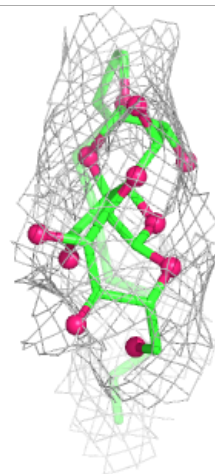
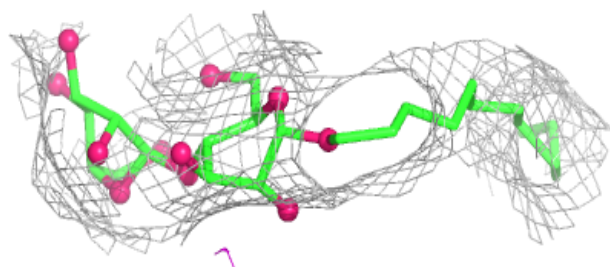
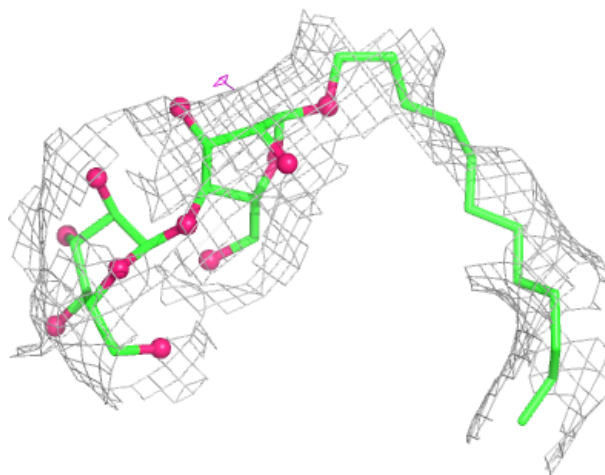
Electron density around LMU H 106:

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



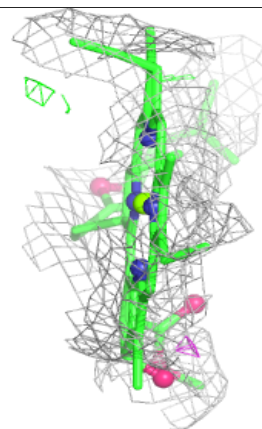
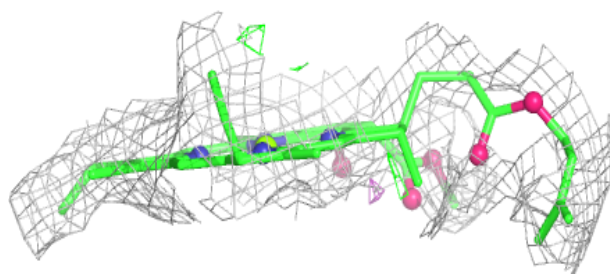
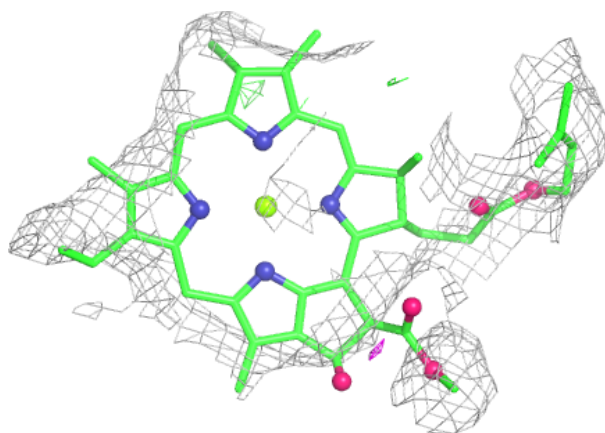
Electron density around LMU K 106:

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



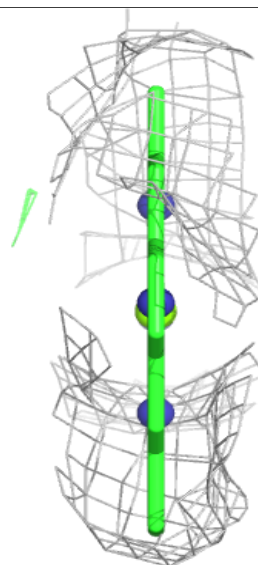
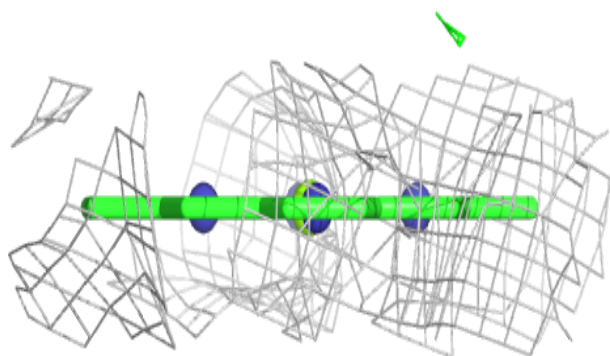
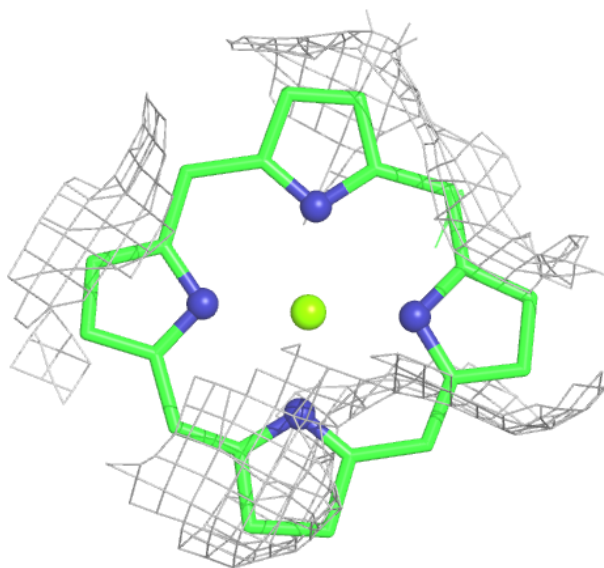
Electron density around CLA K 103:

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



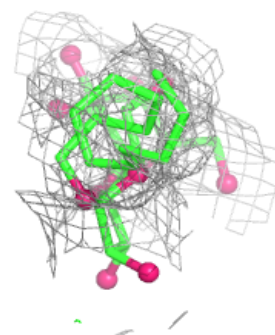
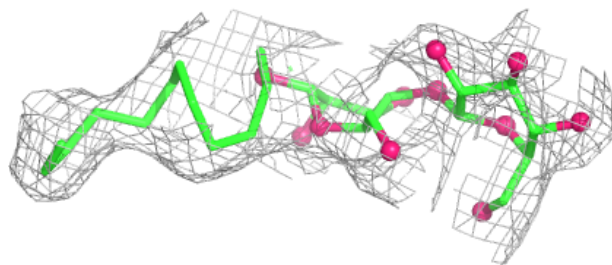
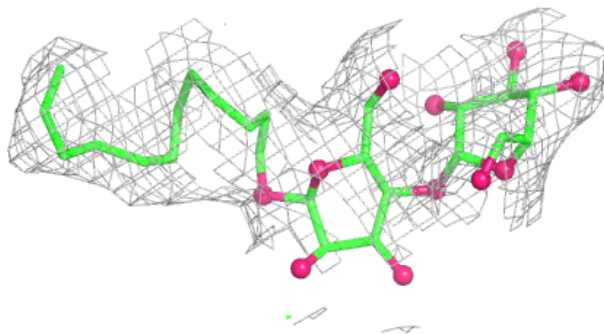
Electron density around CLA 3 309:

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

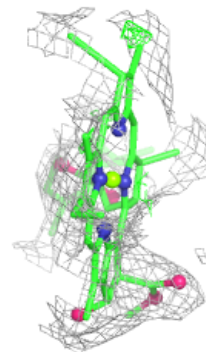
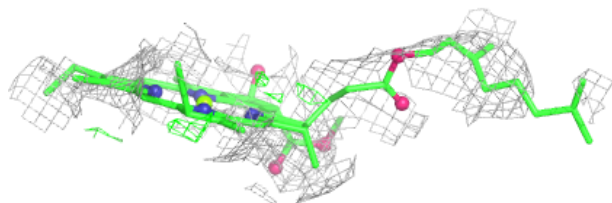
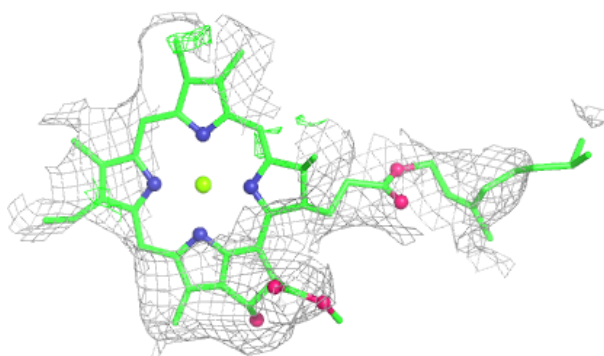


Electron density around LMU 2 313:

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

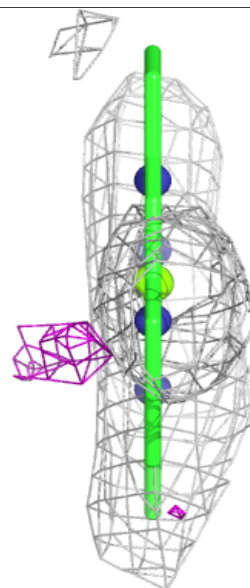
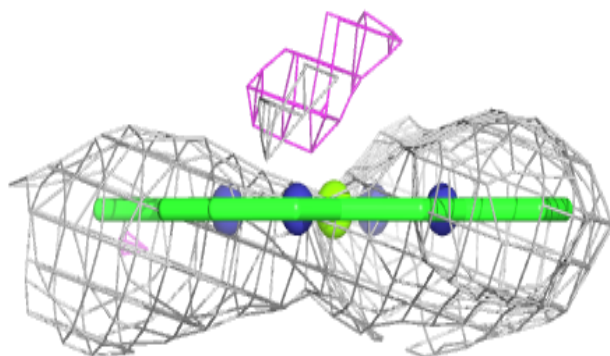
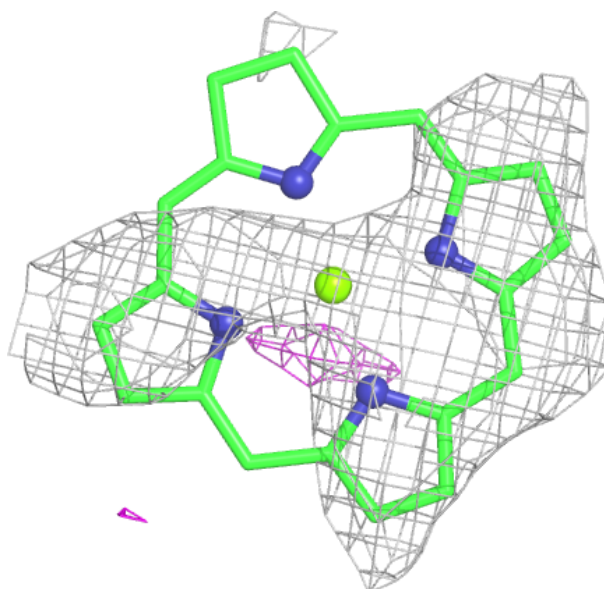
**Electron density around CLA A 840:**

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



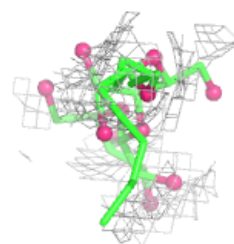
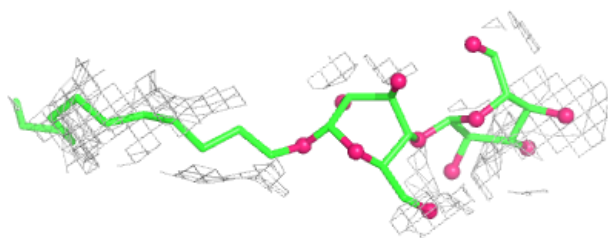
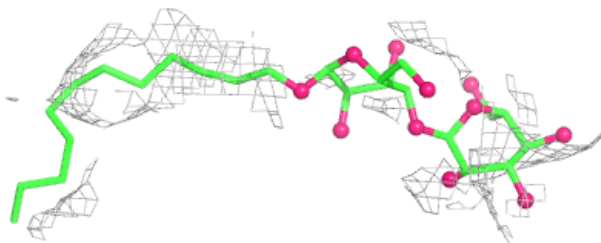
Electron density around CLA 3 312:

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



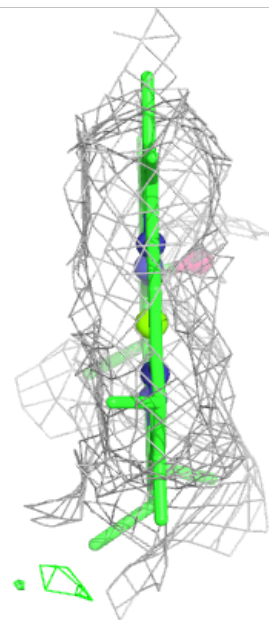
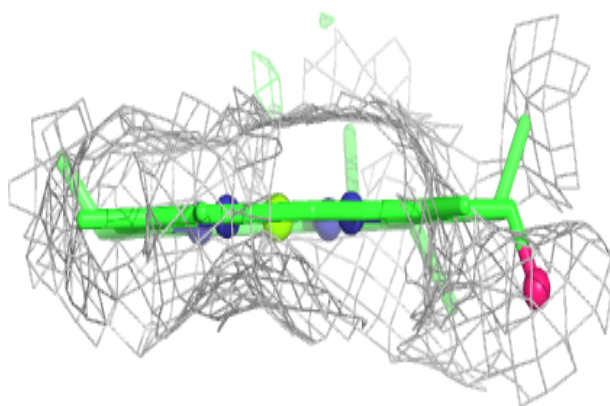
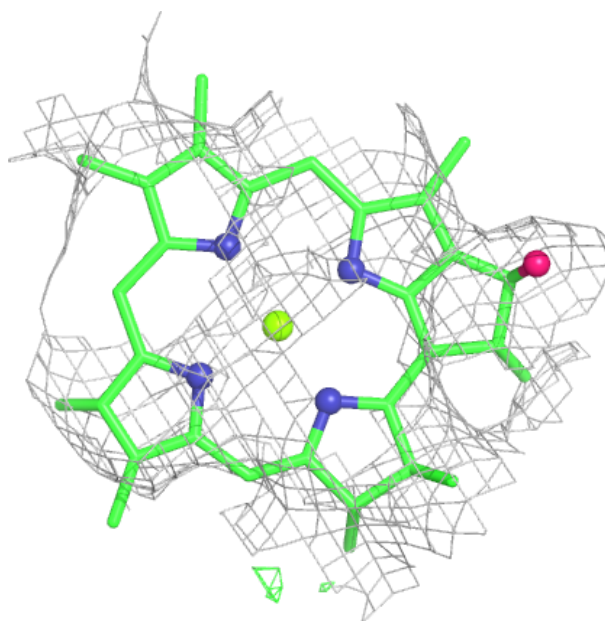
Electron density around LMU G 103:

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



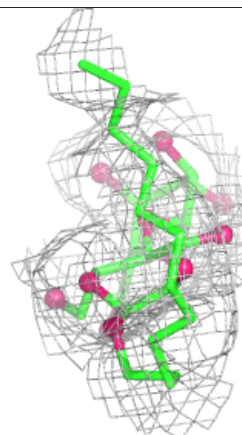
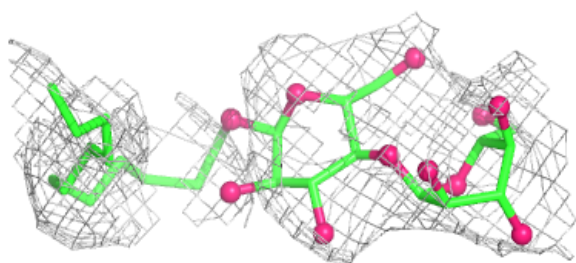
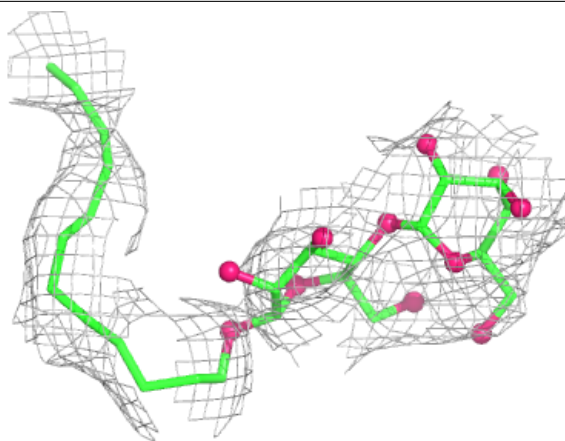
Electron density around CLA 1 205:

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



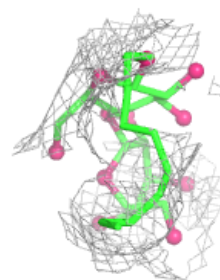
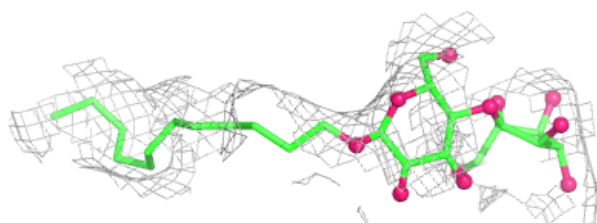
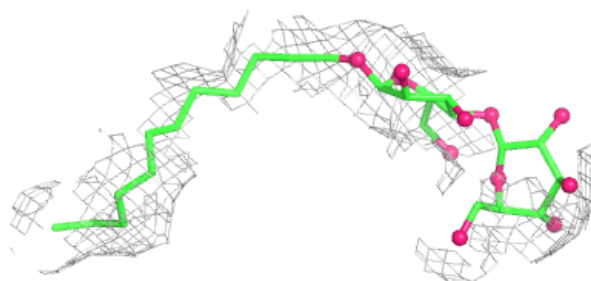
Electron density around LMU 3 318:

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



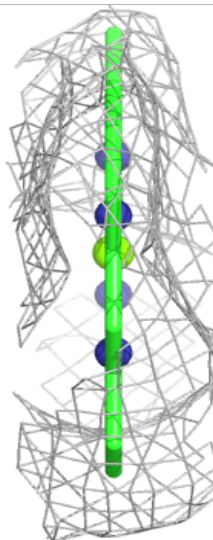
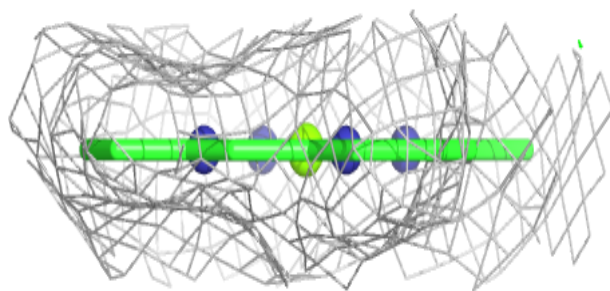
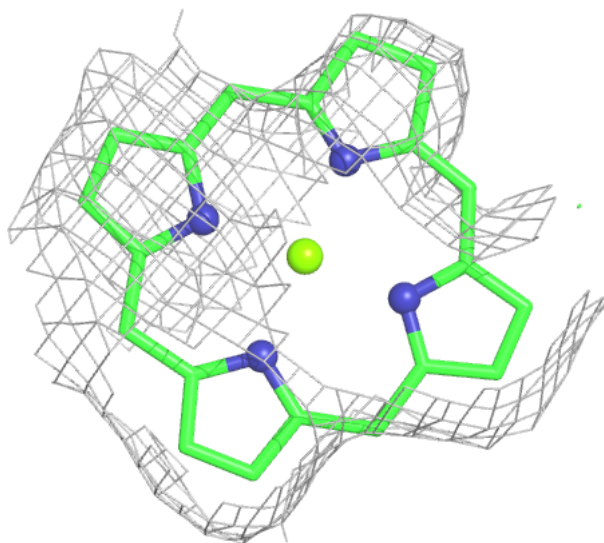
Electron density around LMU L 205:

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



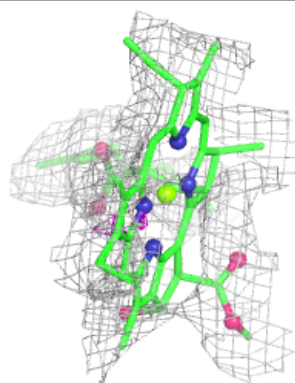
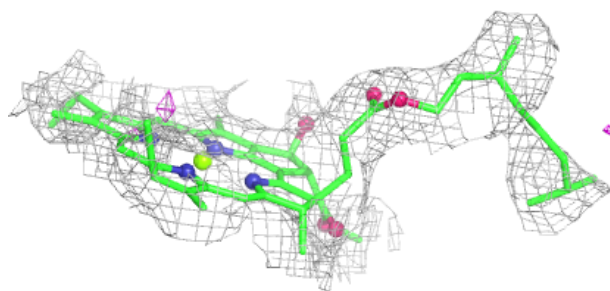
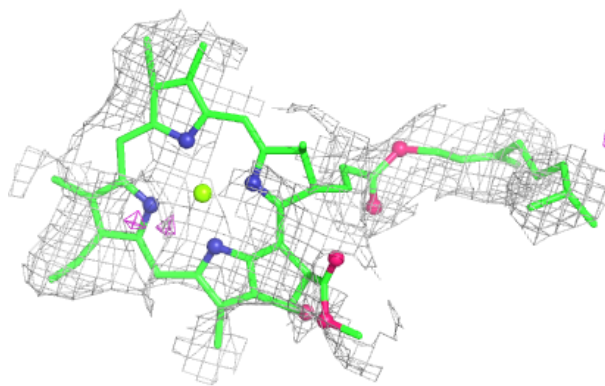
Electron density around CLA 4 308:

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



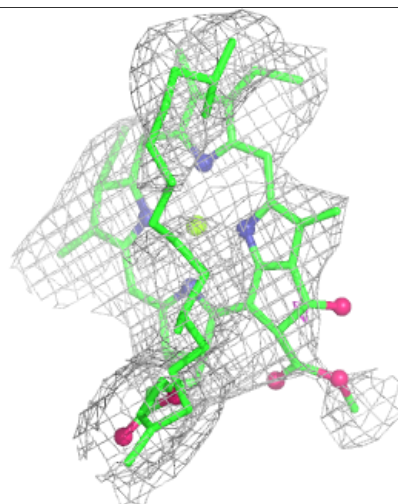
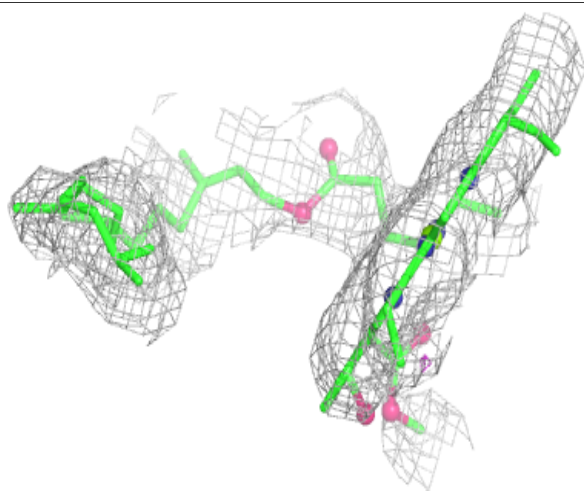
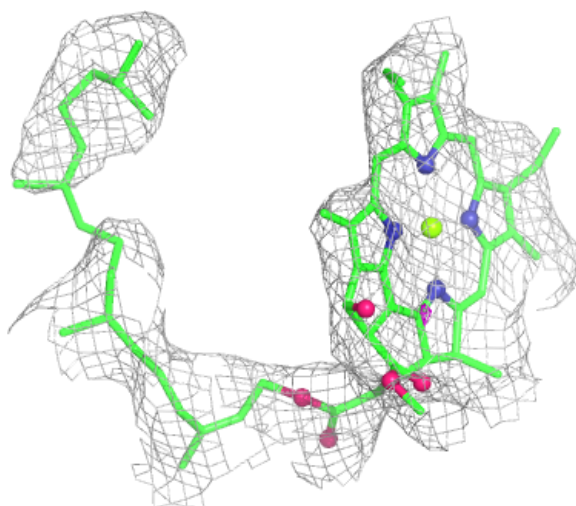
Electron density around CLA H 109:

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



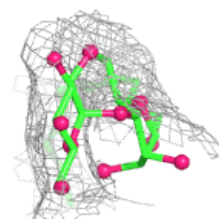
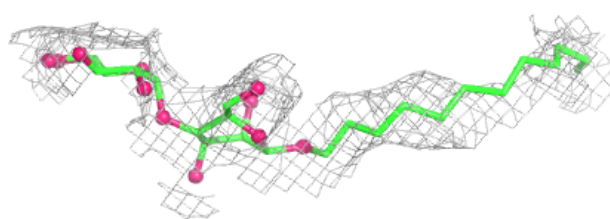
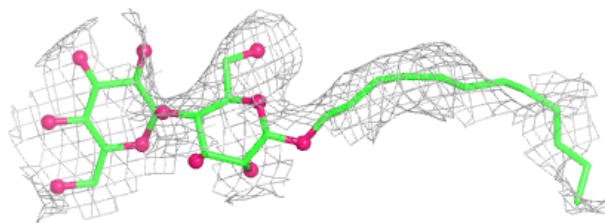
Electron density around CLA 3 310:

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



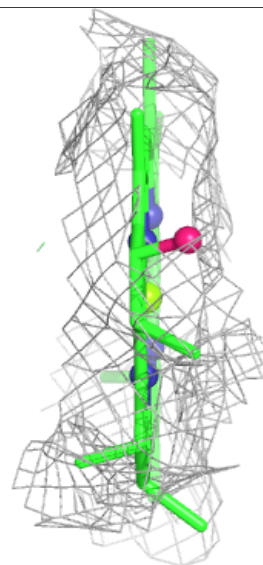
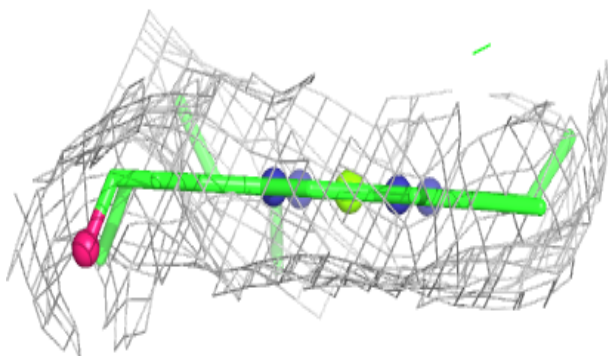
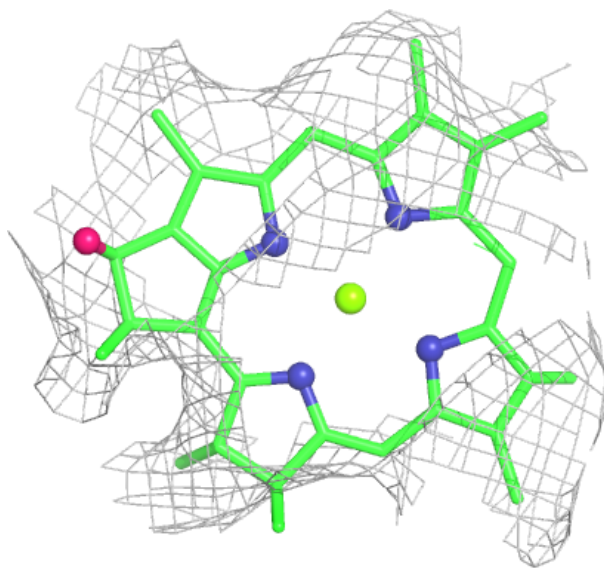
Electron density around LMU 2 321:

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



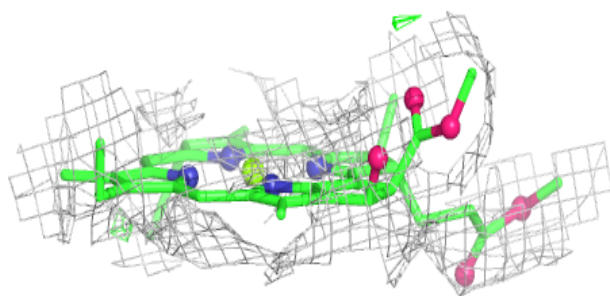
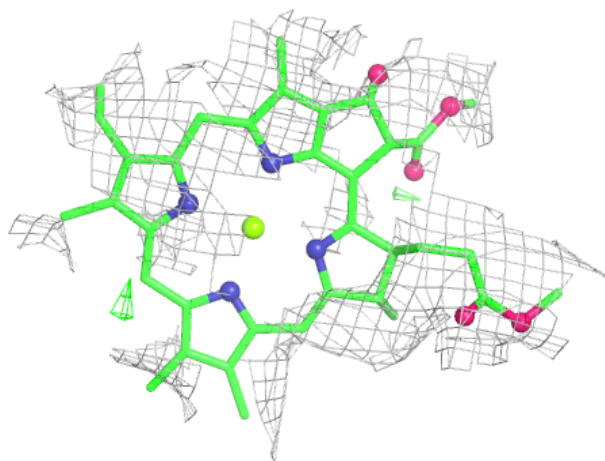
Electron density around CLA 3 303:

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



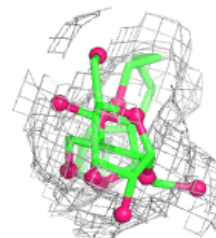
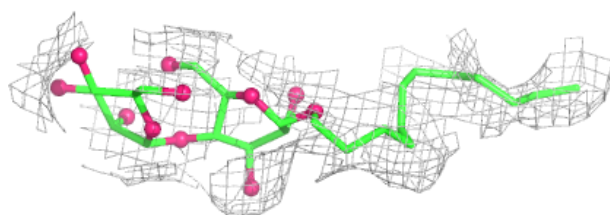
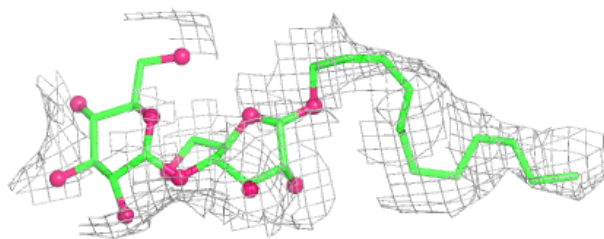
Electron density around CLA K 101:

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



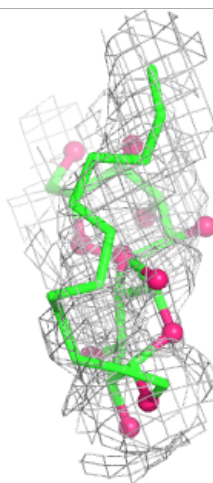
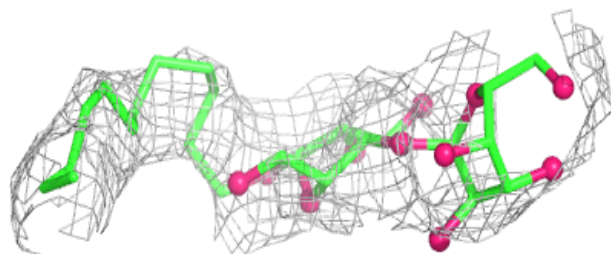
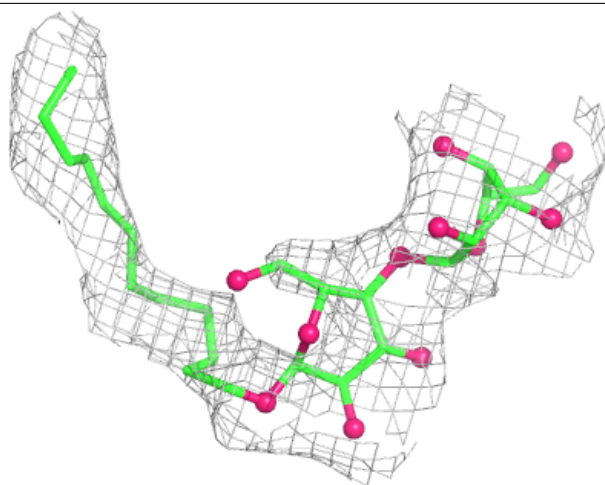
Electron density around LMU R 102:

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



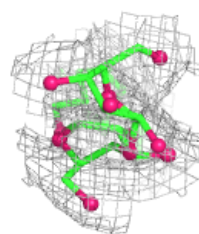
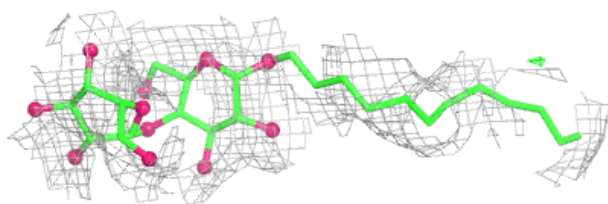
Electron density around LMU R 103:

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

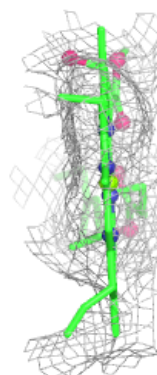
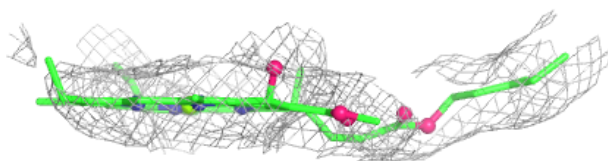
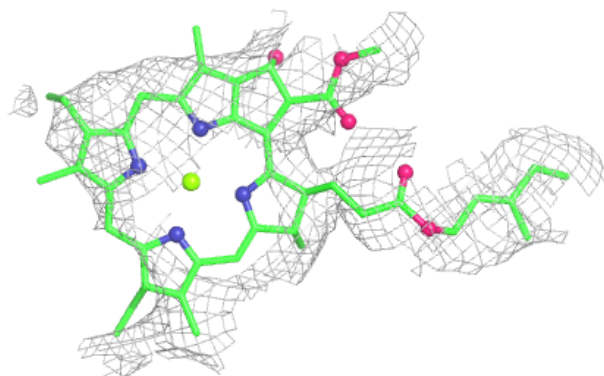


Electron density around LMU H 103:

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

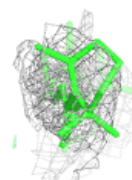
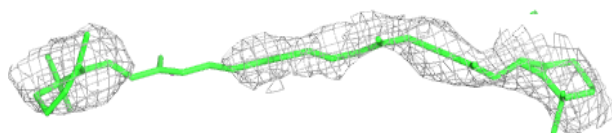
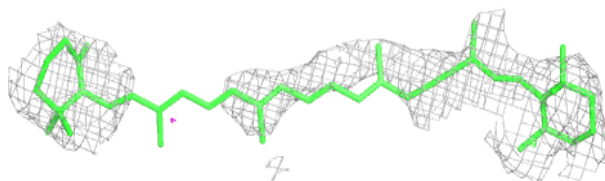
**Electron density around CLA 1 215:**

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

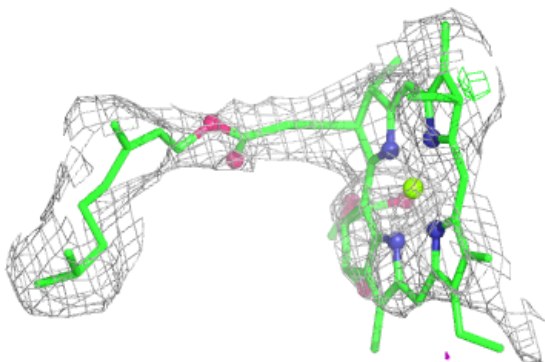
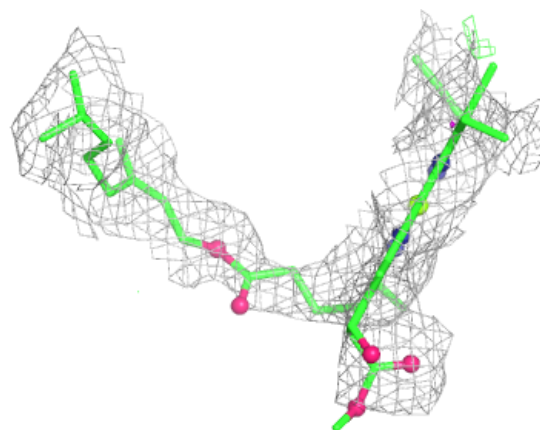


Electron density around BCR G 104:

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

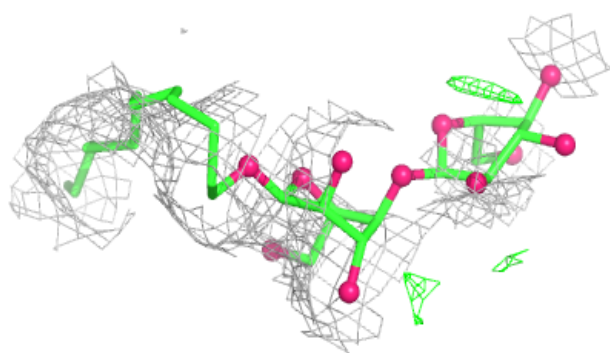
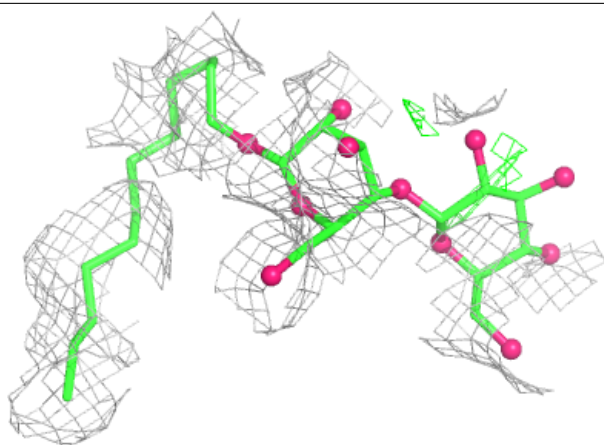
**Electron density around CLA L 204:**

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

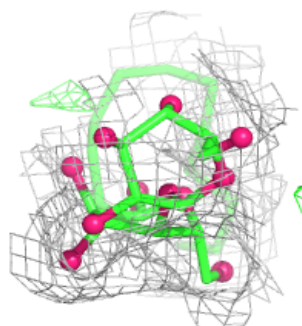
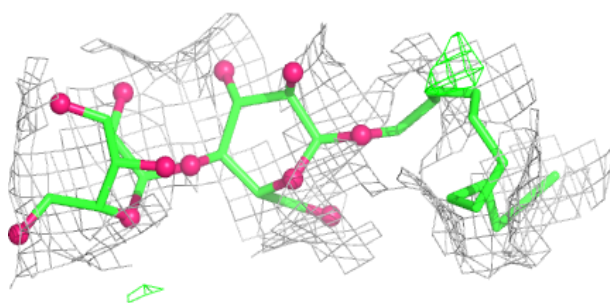
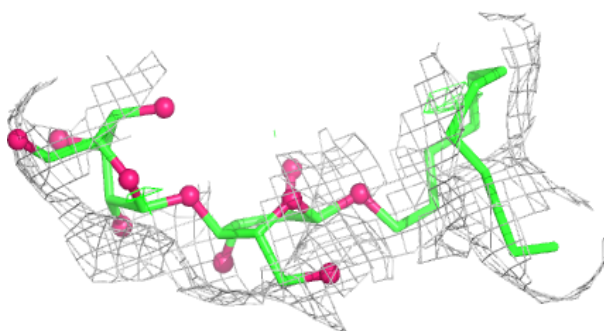


Electron density around LMU A 848:

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

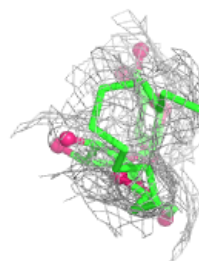
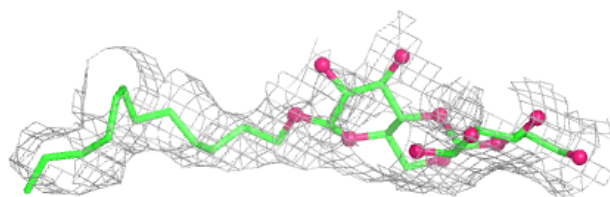
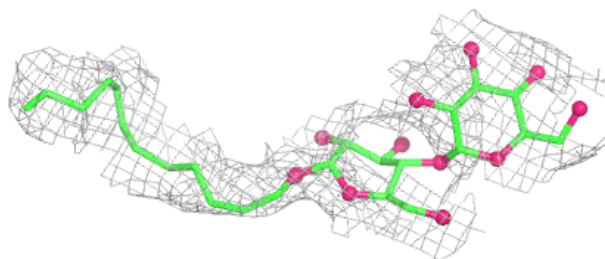
**Electron density around LMU A 854:**

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



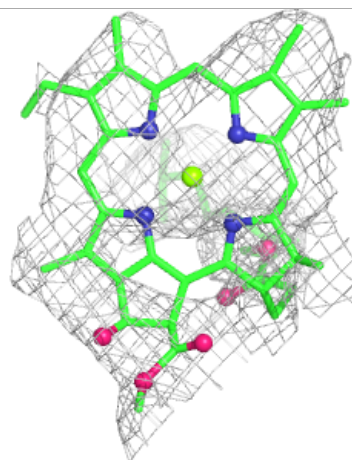
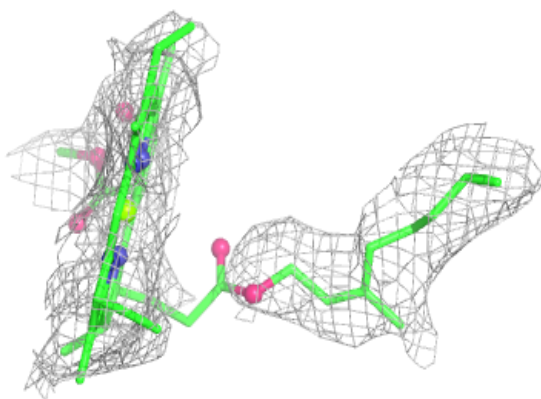
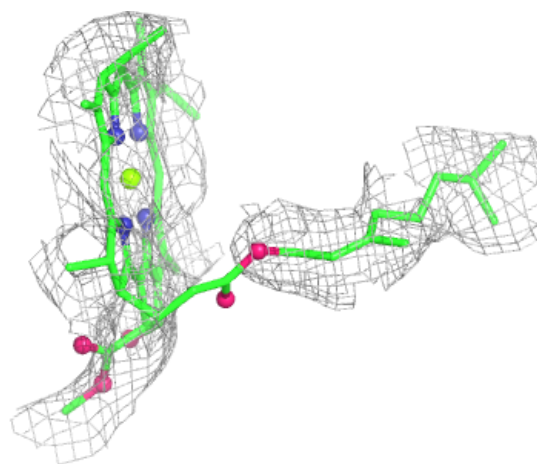
Electron density around LMU B 804:

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



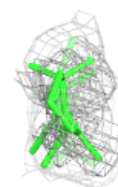
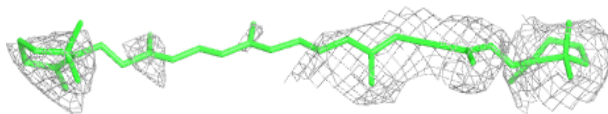
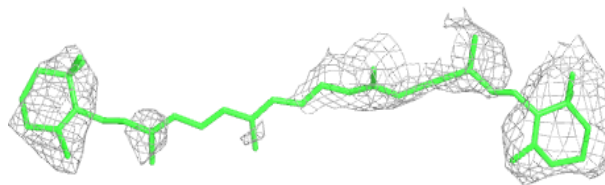
Electron density around CLA 4 301:

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

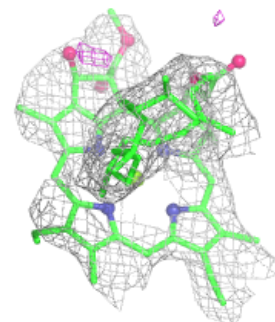
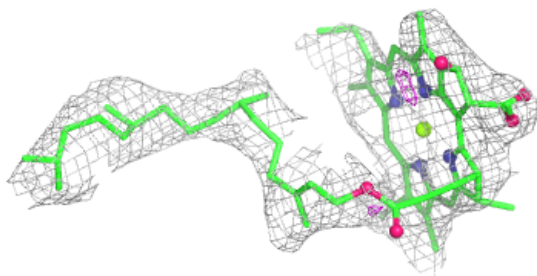
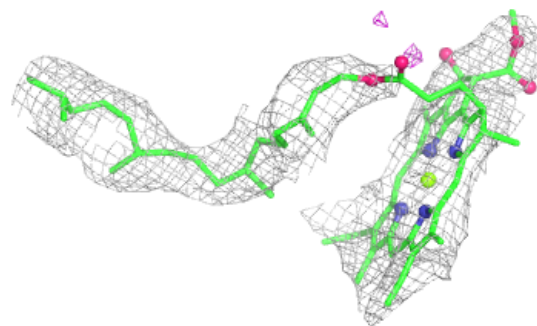


Electron density around BCR L 209:

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

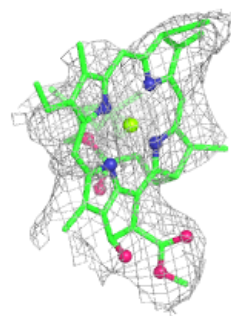
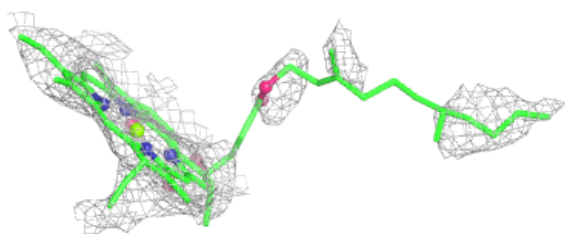
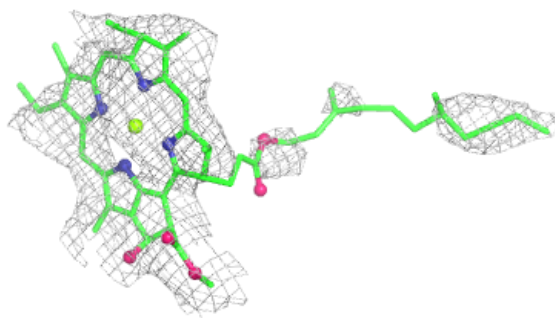
**Electron density around CLA A 811:**

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



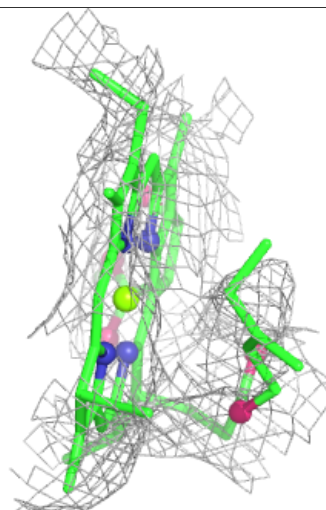
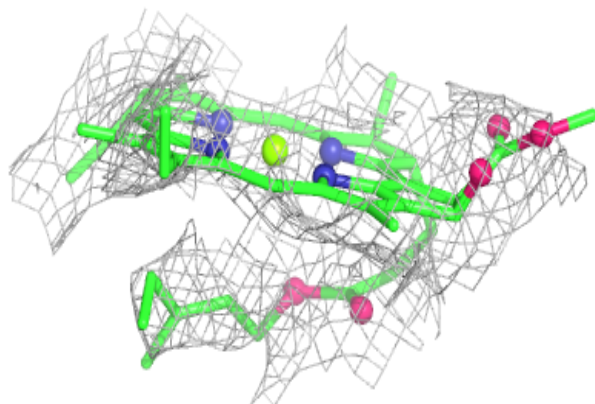
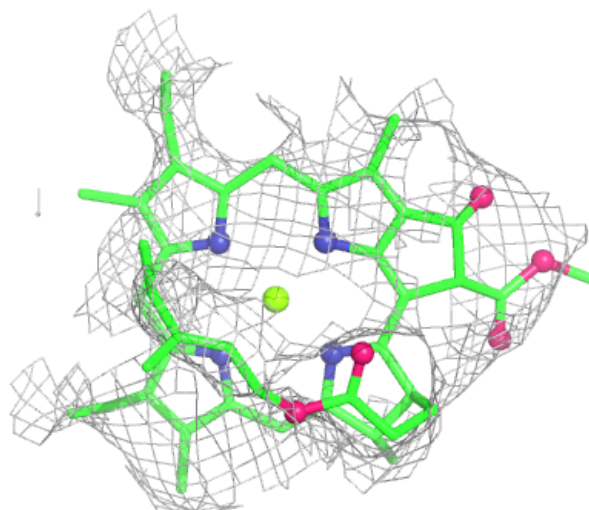
Electron density around CLA A 819:

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



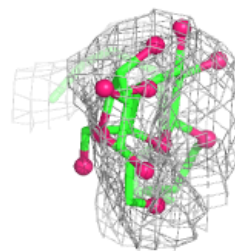
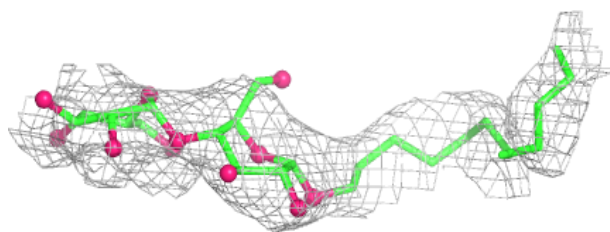
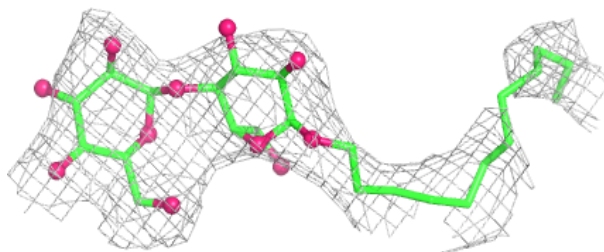
Electron density around CLA A 820:

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

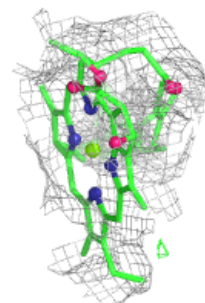
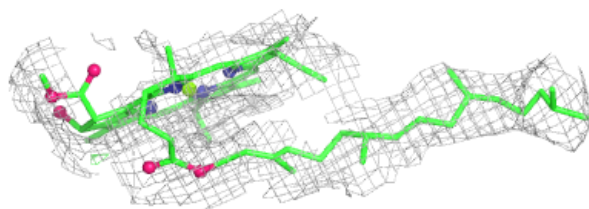
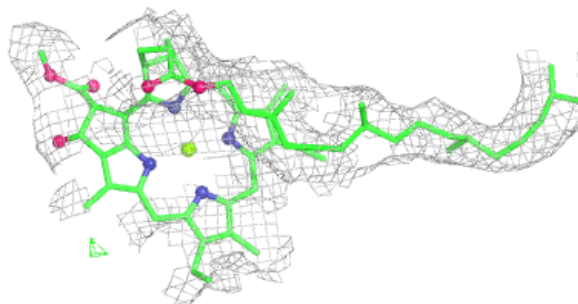


Electron density around LMU C 101:

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

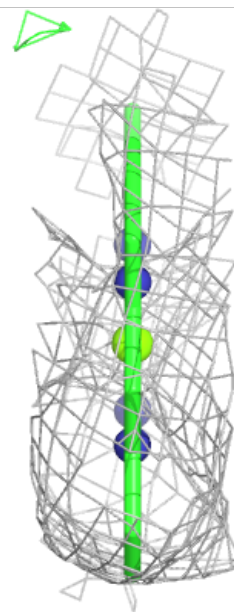
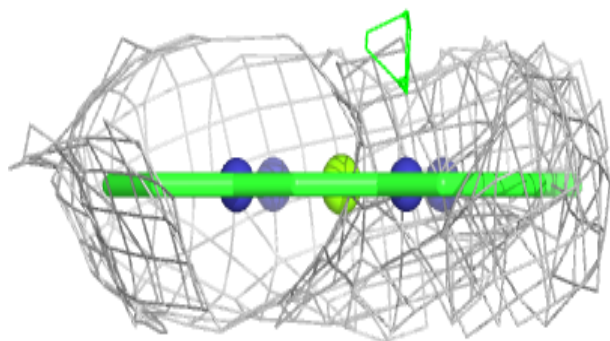
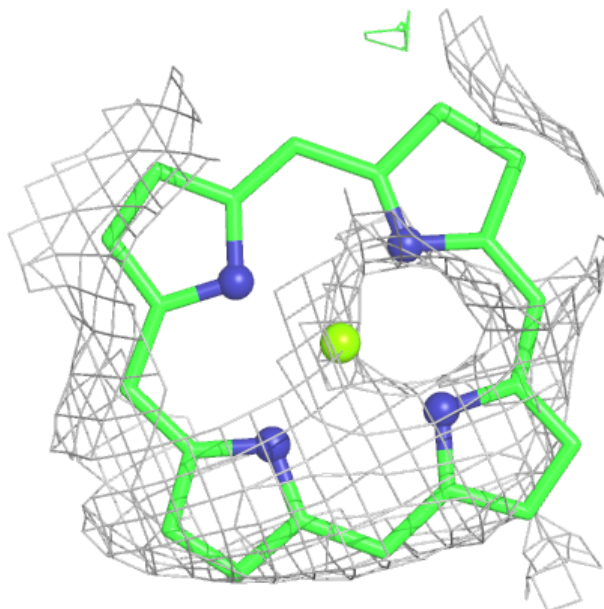
**Electron density around CLA 2 307:**

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



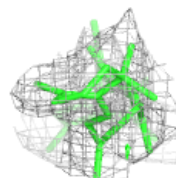
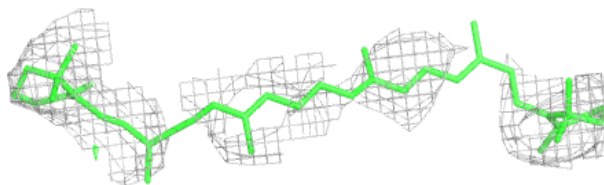
Electron density around CLA 3 306:

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

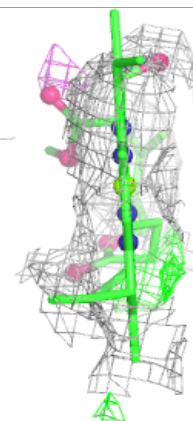
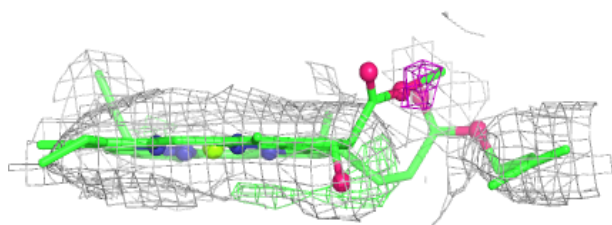
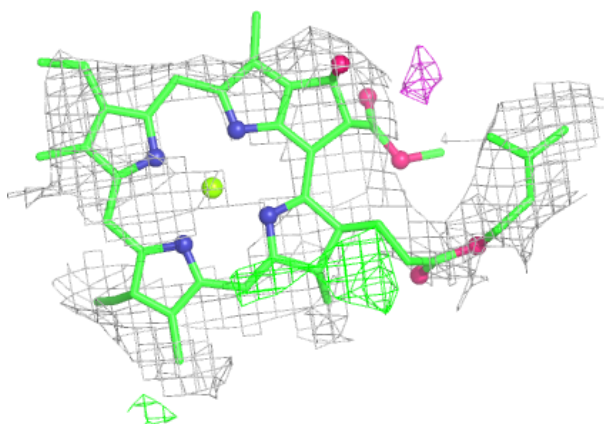


Electron density around BCR A 844:

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

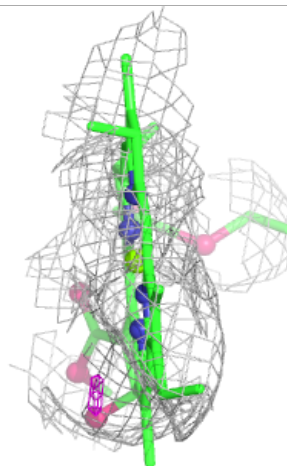
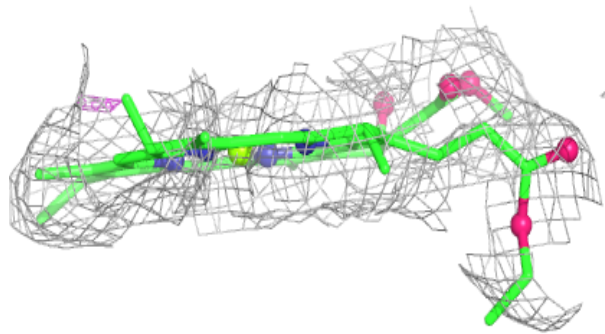
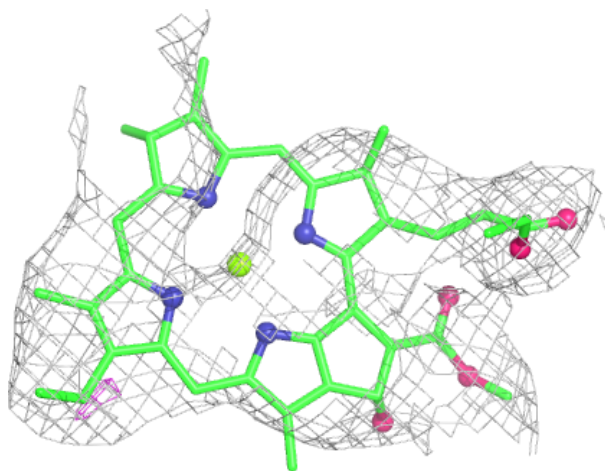
**Electron density around CLA 2 311:**

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



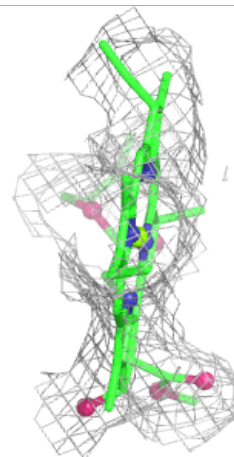
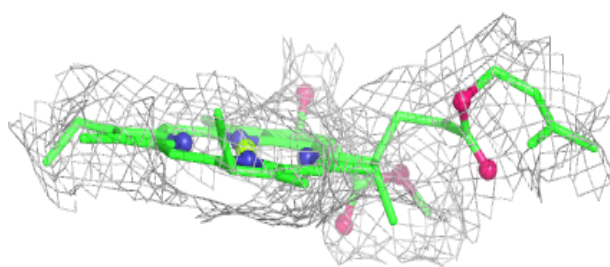
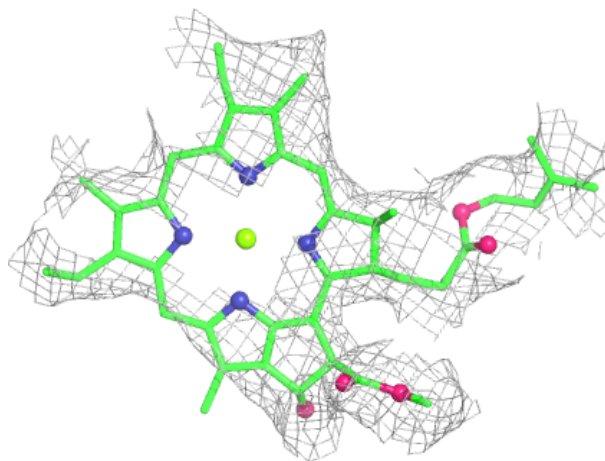
Electron density around CLA A 801:

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



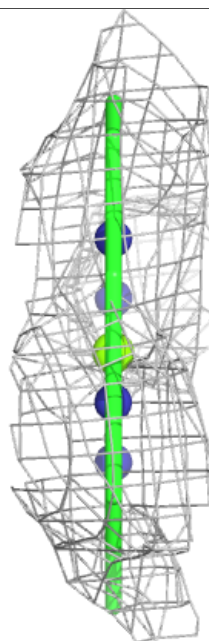
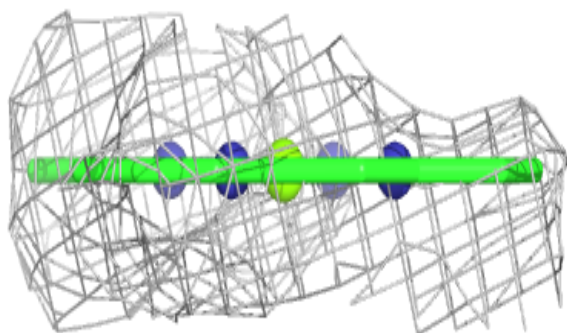
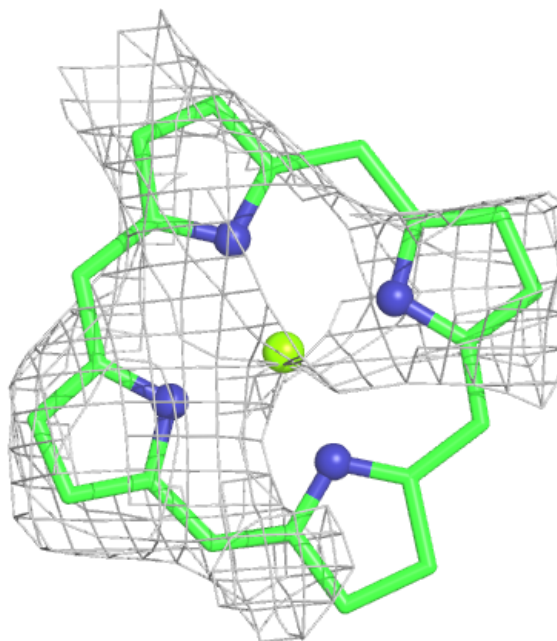
Electron density around CLA 2 305:

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



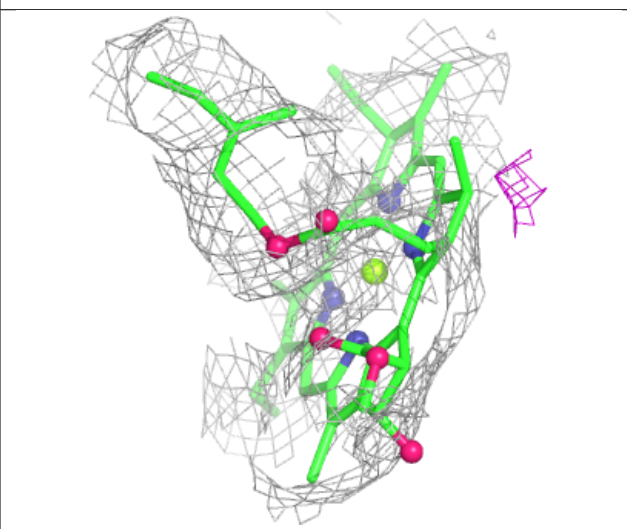
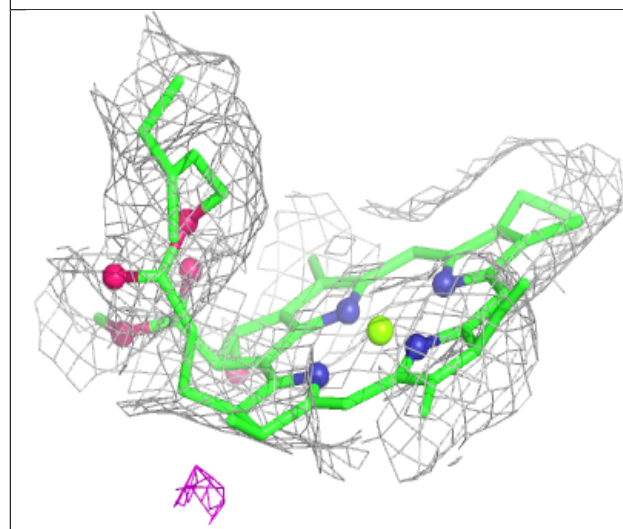
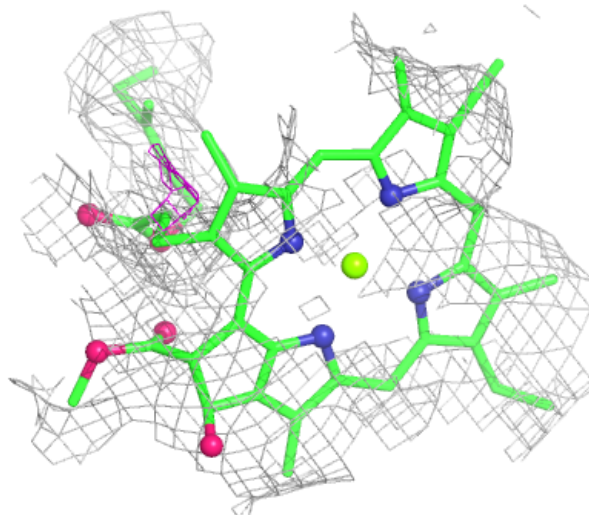
Electron density around CLA 2 301:

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



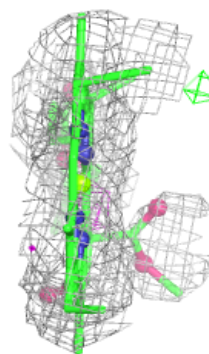
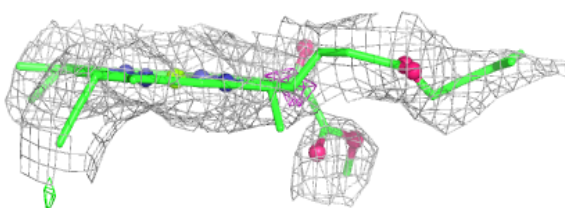
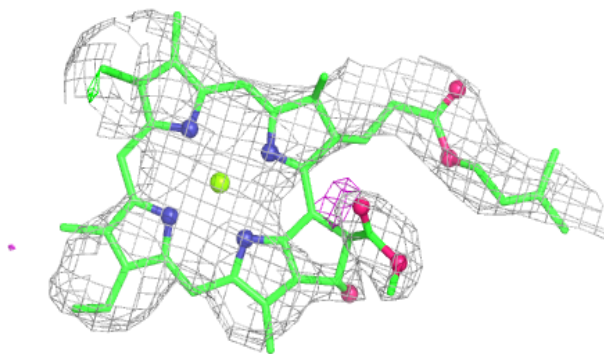
Electron density around CLA 1 207:

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

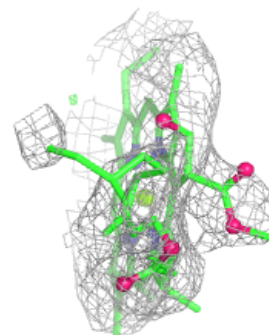
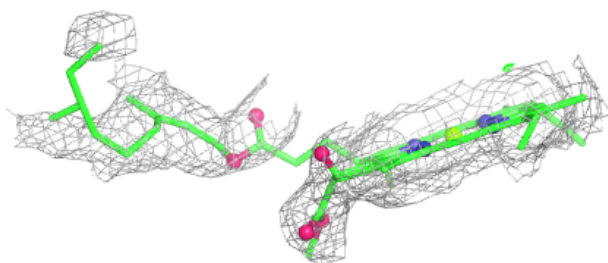
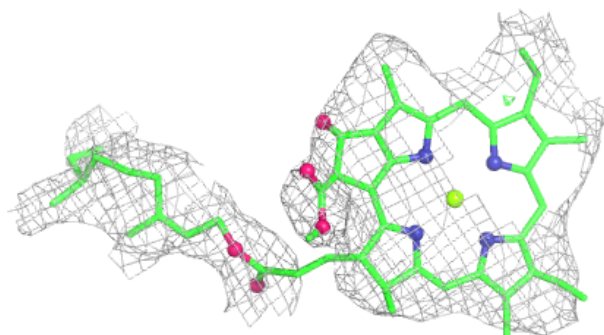


Electron density around CLA 4 305:

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

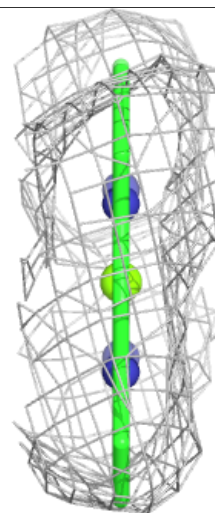
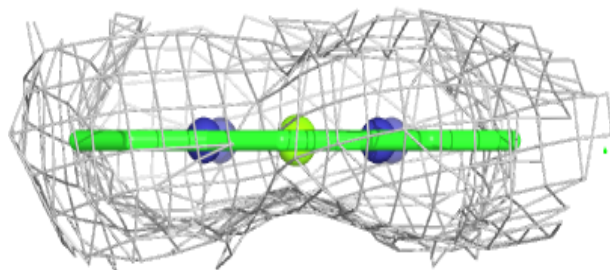
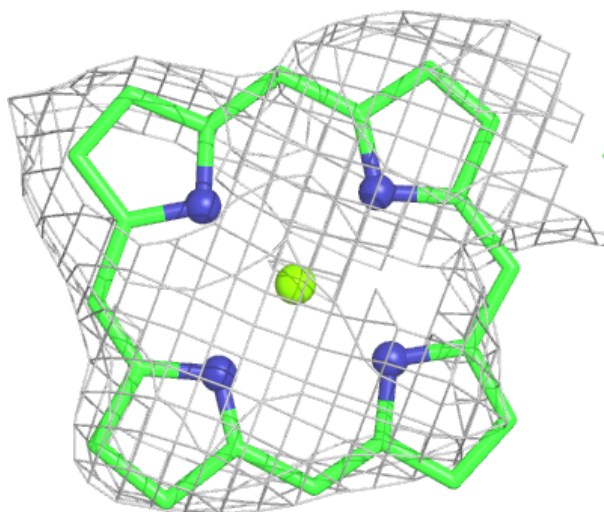
**Electron density around CLA K 104:**

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



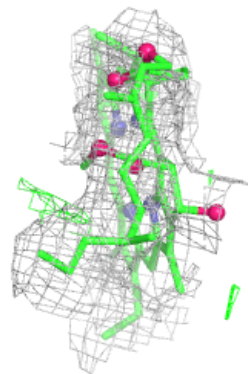
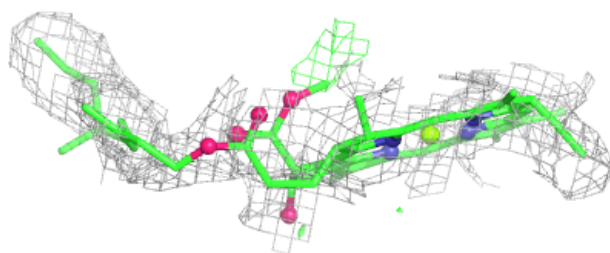
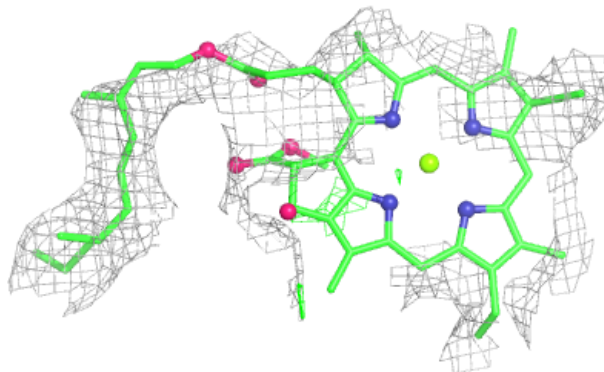
Electron density around CLA 1 209:

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



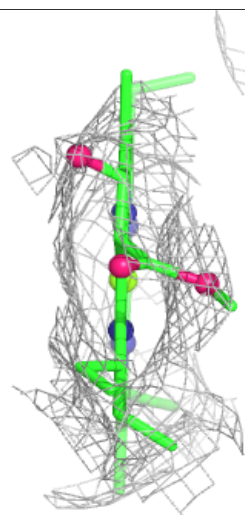
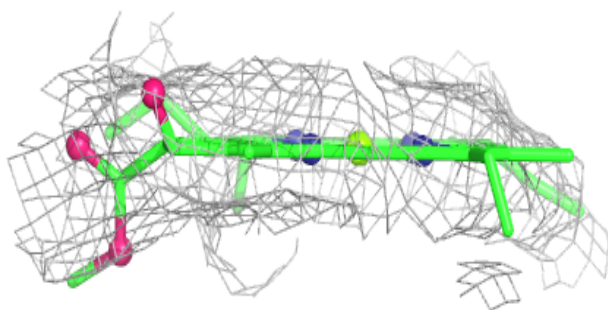
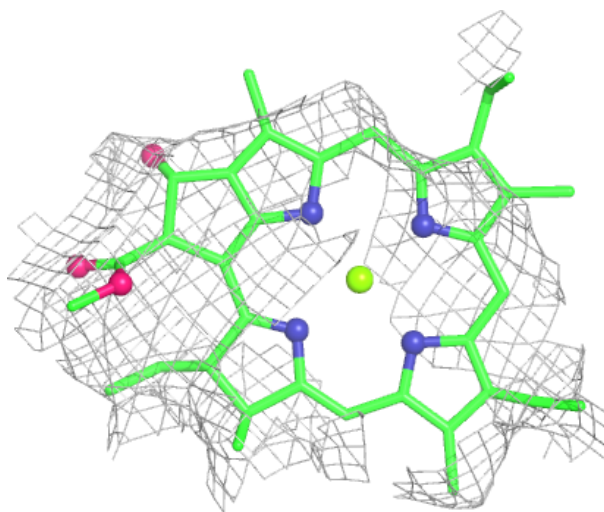
Electron density around CLA R 107:

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



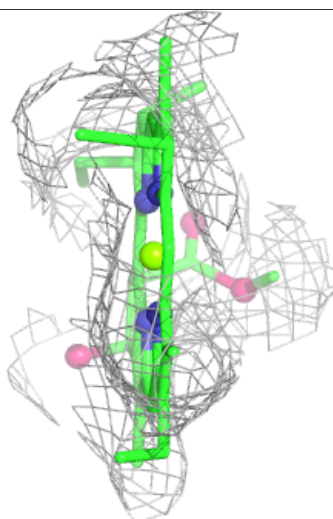
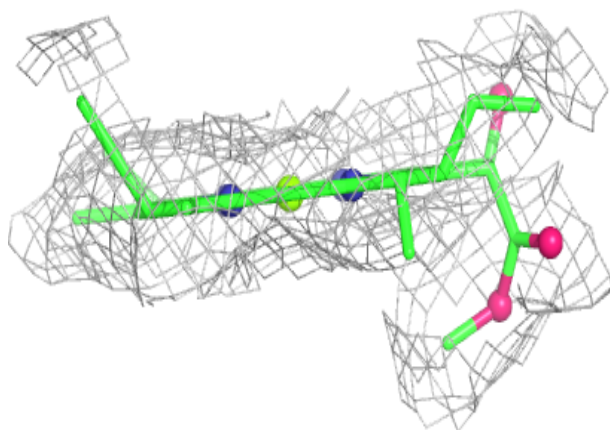
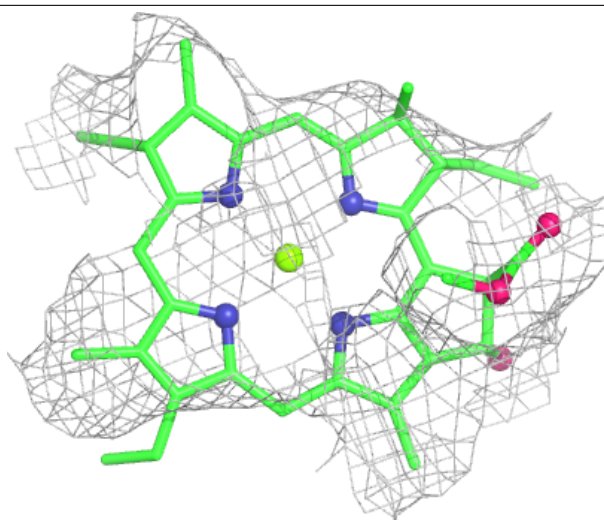
Electron density around CLA A 821:

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



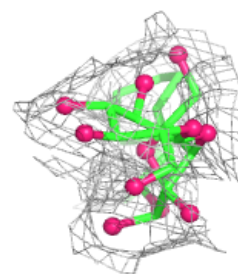
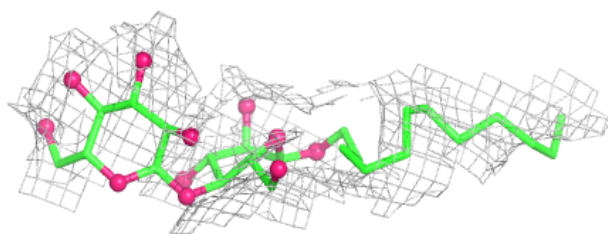
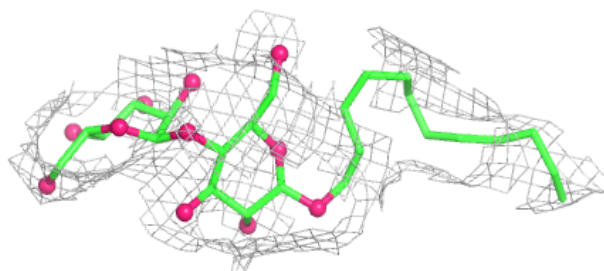
Electron density around CLA 3 307:

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

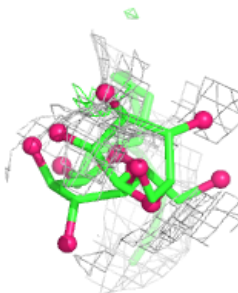
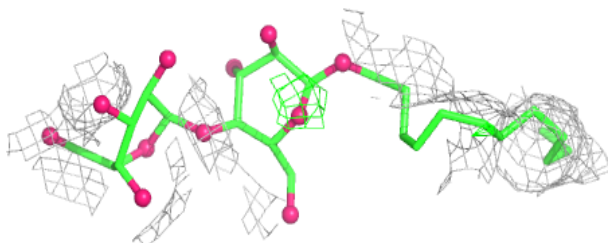
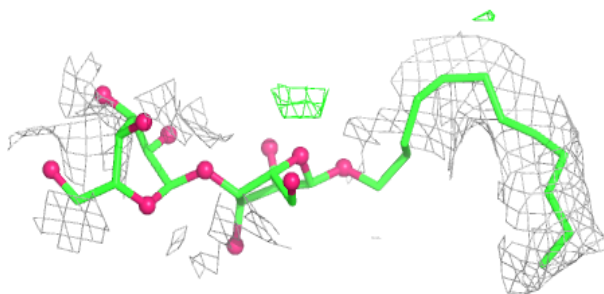


Electron density around LMU K 107:

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

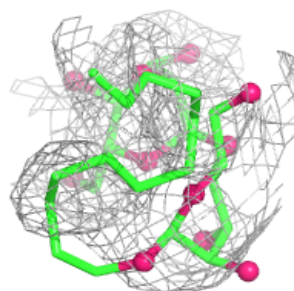
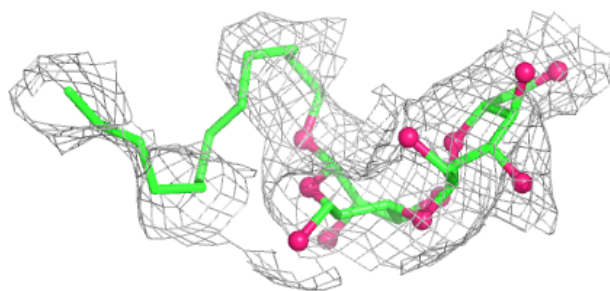
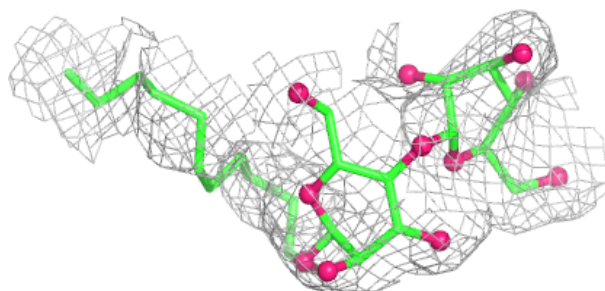
**Electron density around LMU A 846:**

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

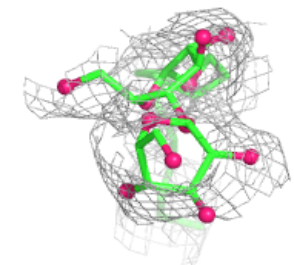
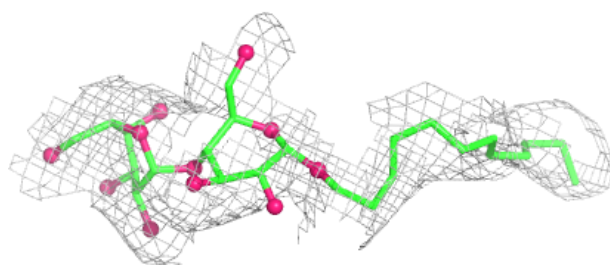
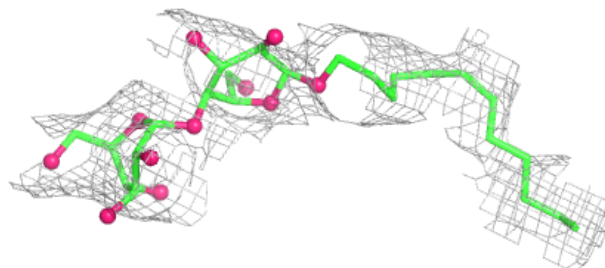


Electron density around LMU L 210:

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

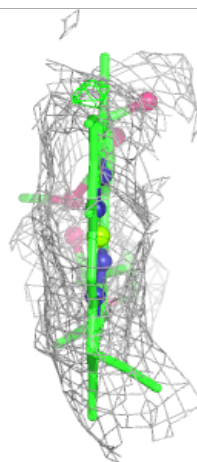
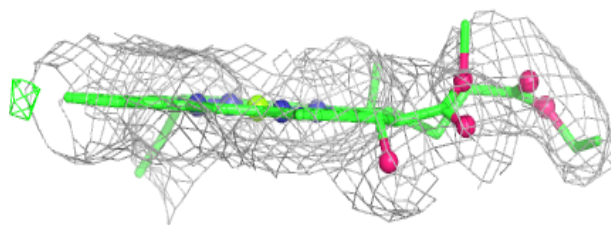
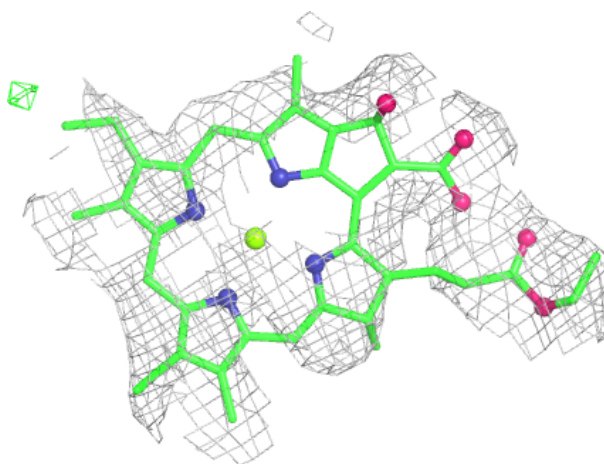
**Electron density around LMU 2 319:**

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



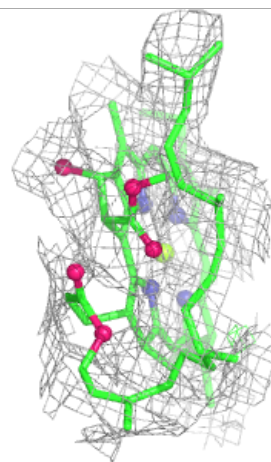
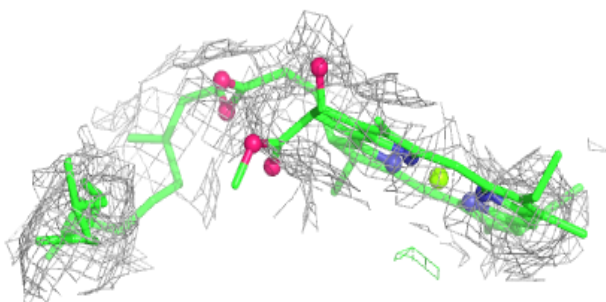
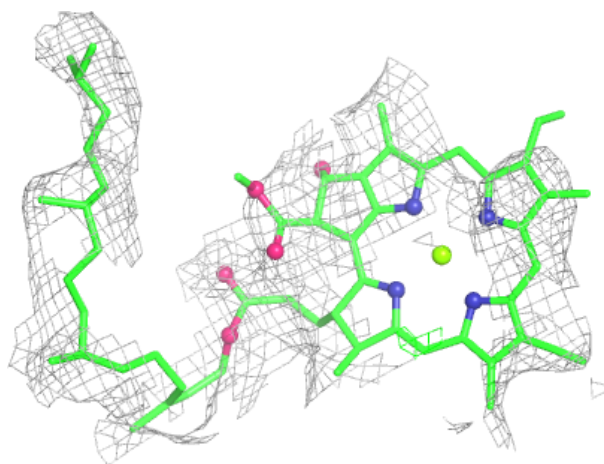
Electron density around CLA 4 318:

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



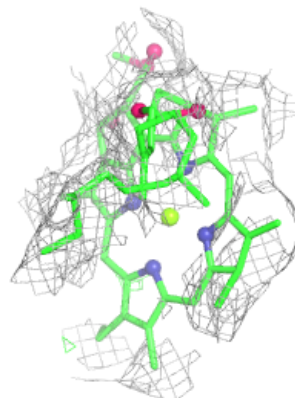
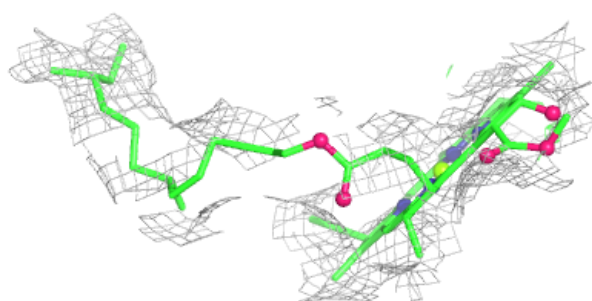
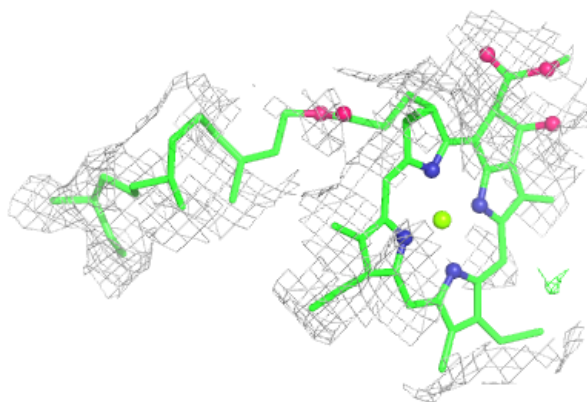
Electron density around CLA R 108:

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

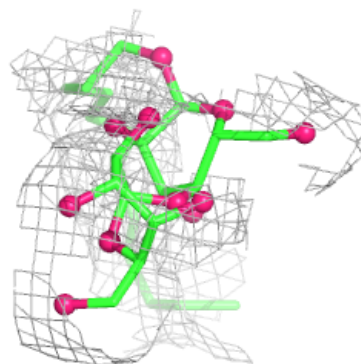
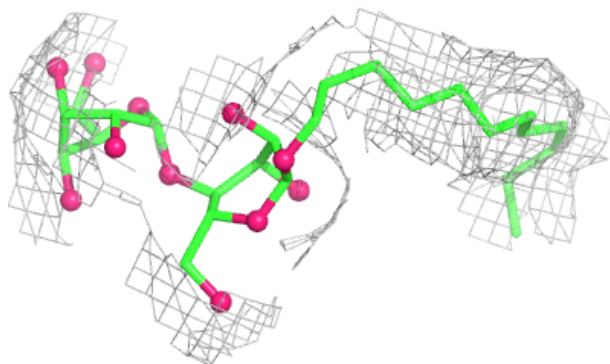


Electron density around CLA 2 312:

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

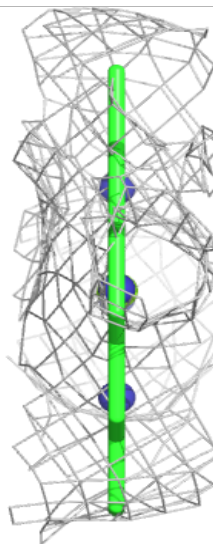
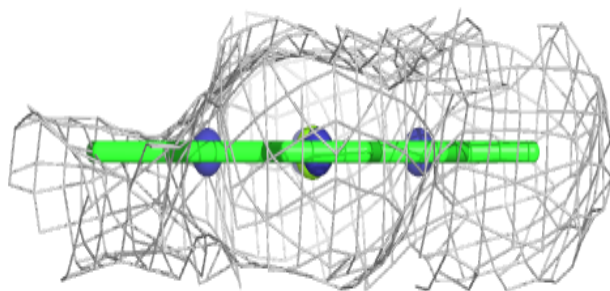
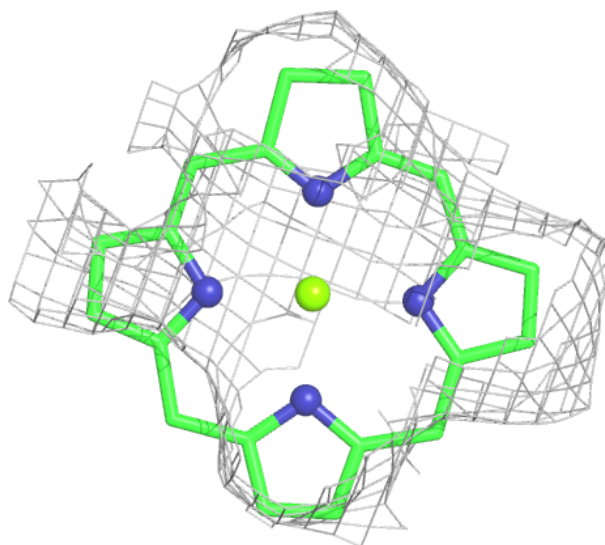
**Electron density around LMU R 104:**

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



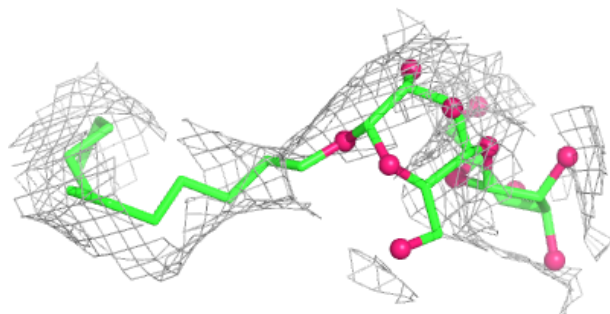
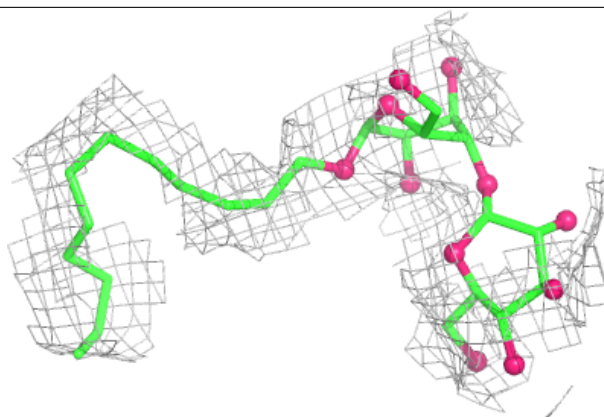
Electron density around CLA 3 302:

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



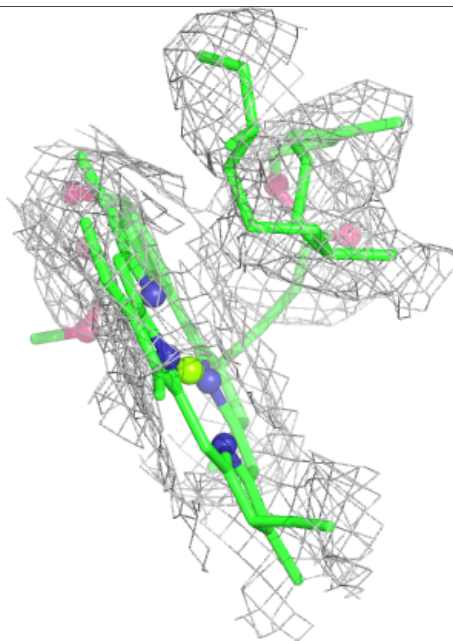
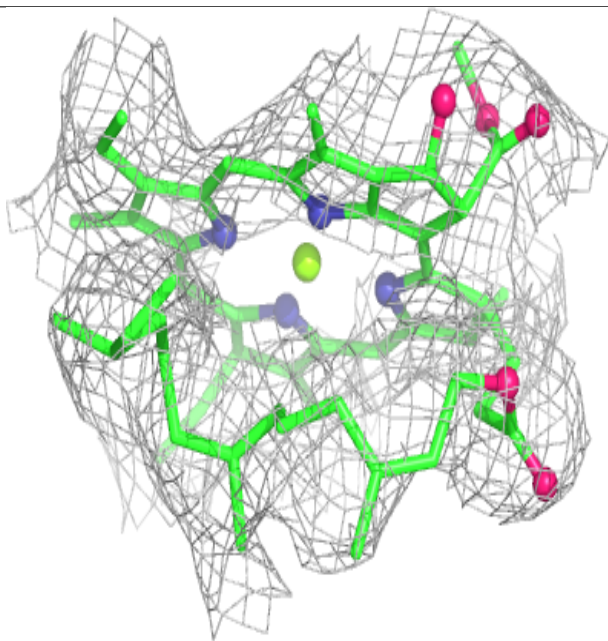
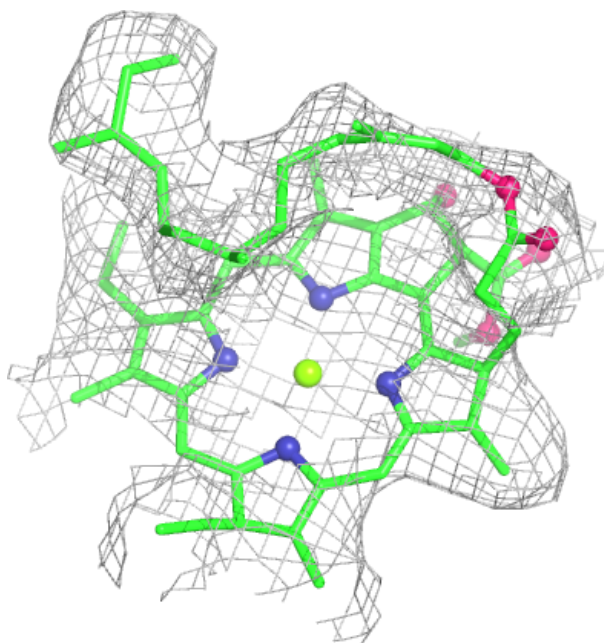
Electron density around LMU K 105:

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



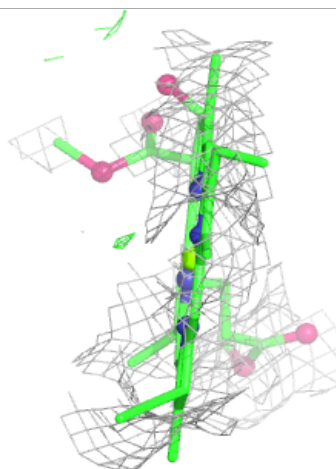
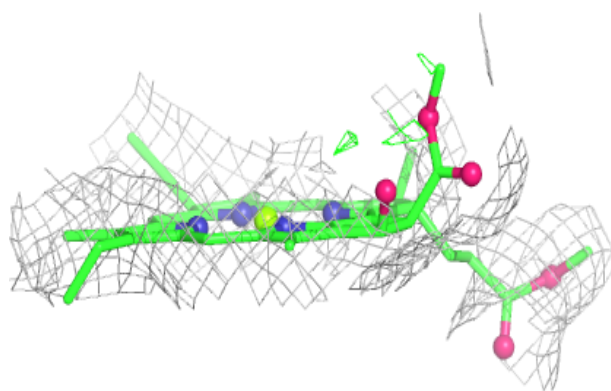
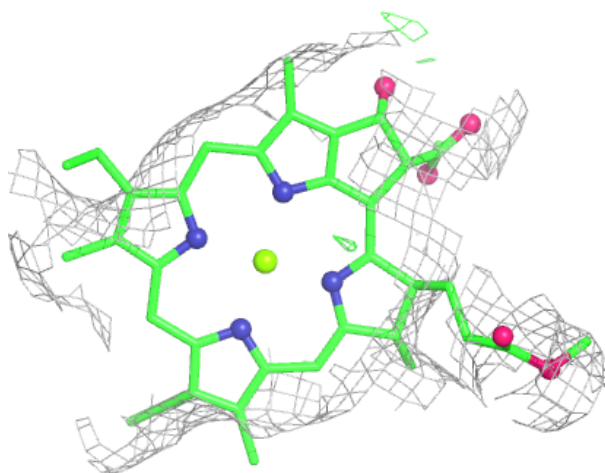
Electron density around CLA 1 206:

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



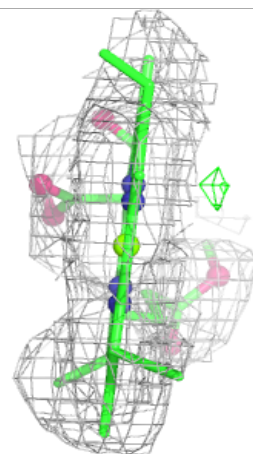
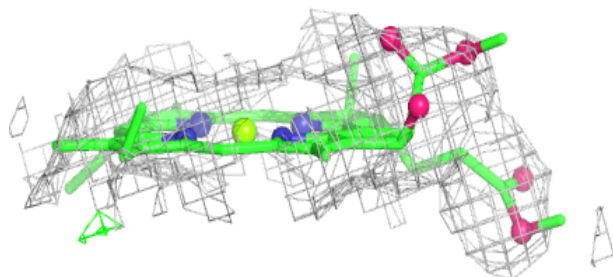
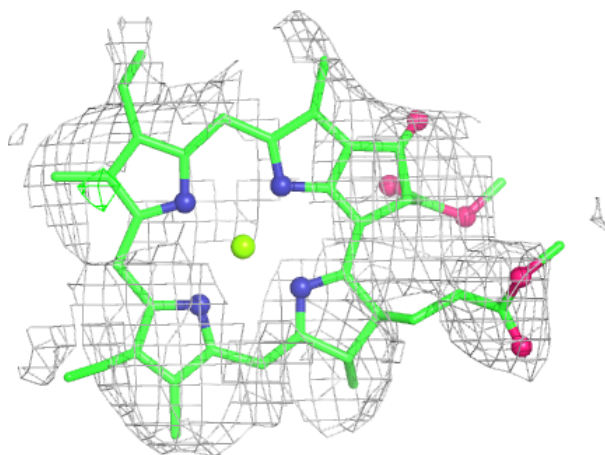
Electron density around CLA 1 201:

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



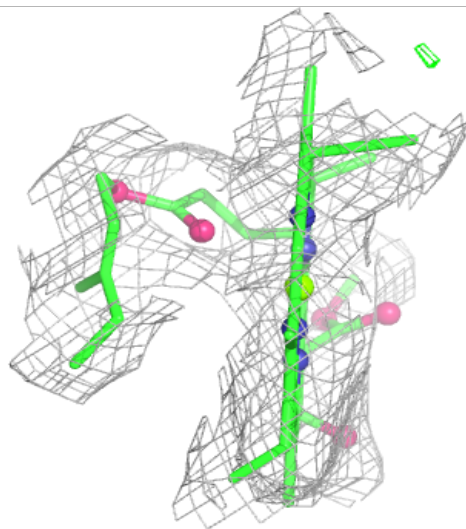
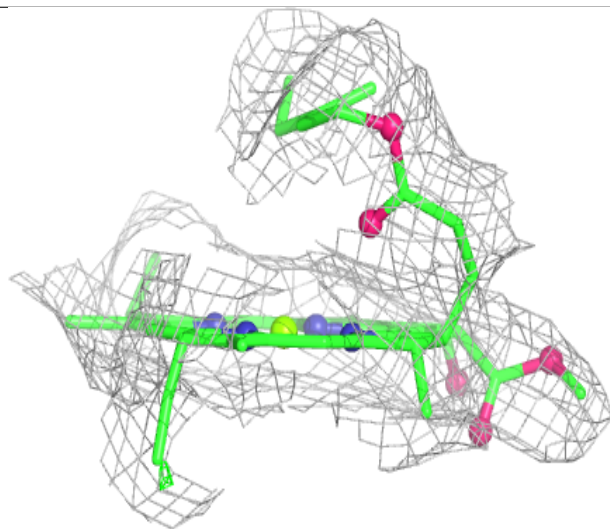
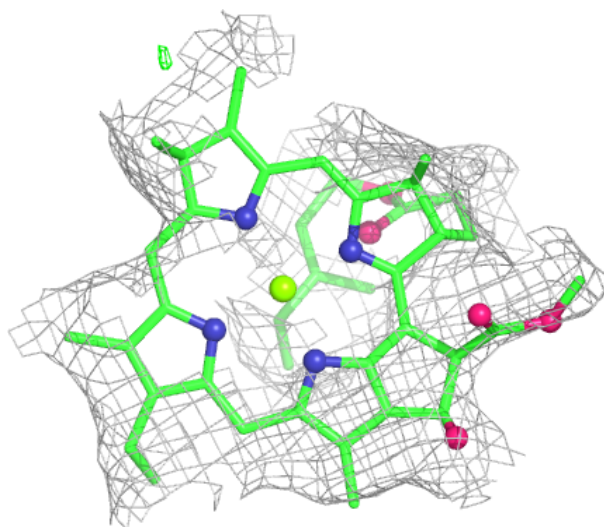
Electron density around CLA 4 315:

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



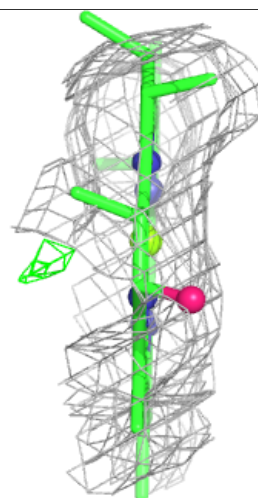
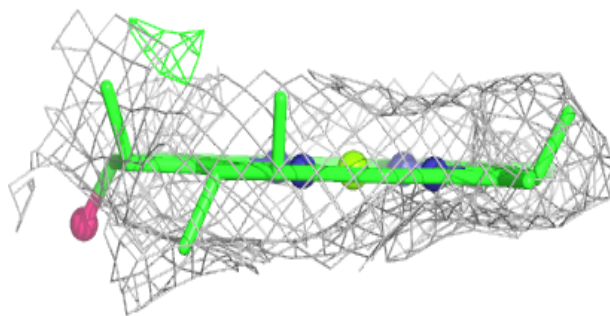
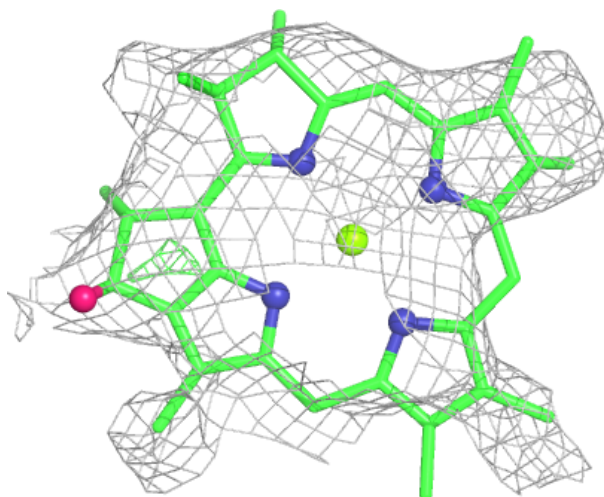
Electron density around CLA 2 302:

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



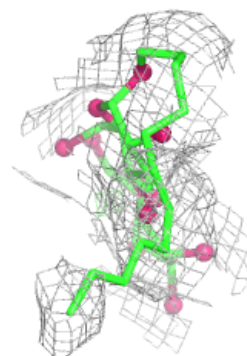
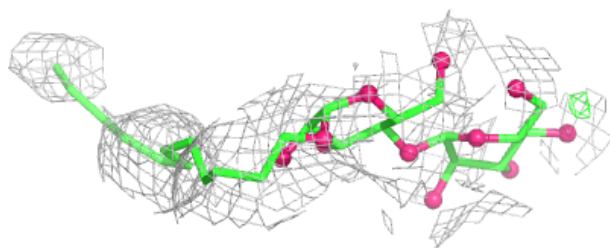
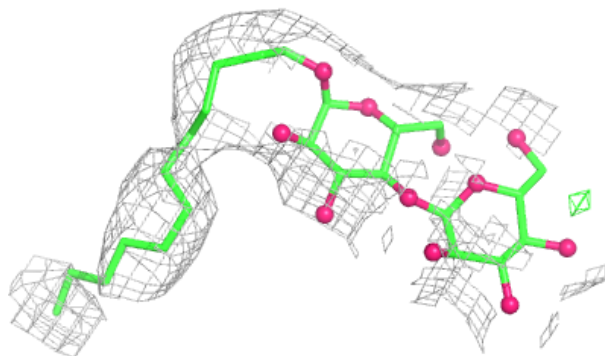
Electron density around CLA B 842:

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

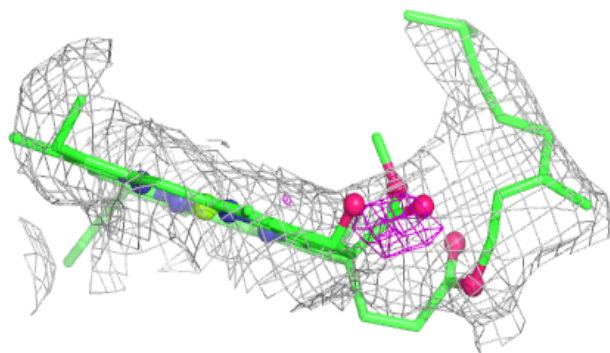
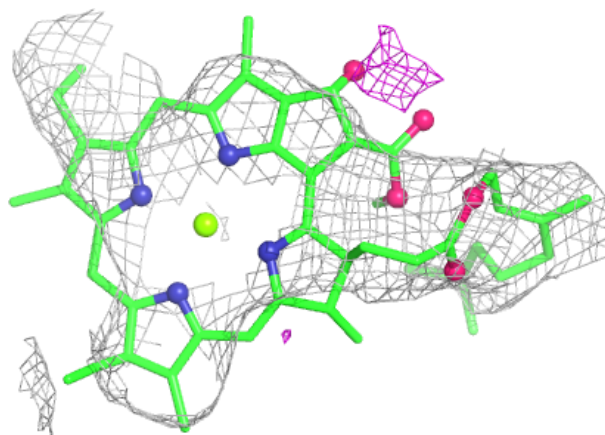


Electron density around LMU R 106:

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

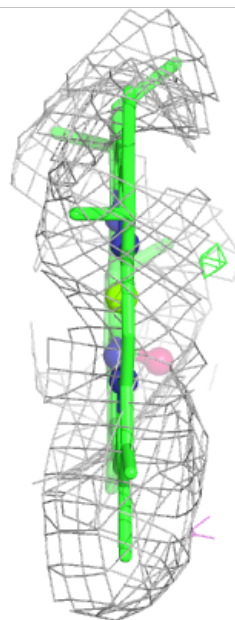
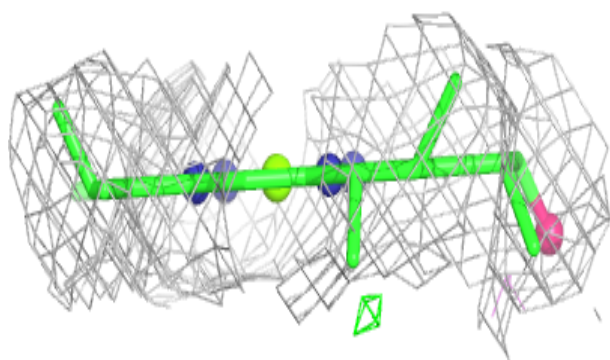
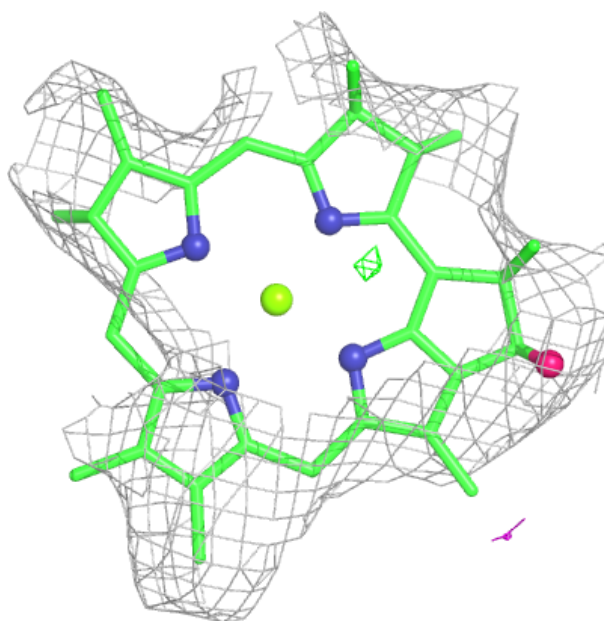
**Electron density around CLA L 202:**

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



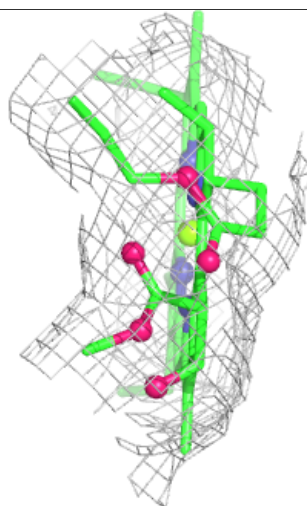
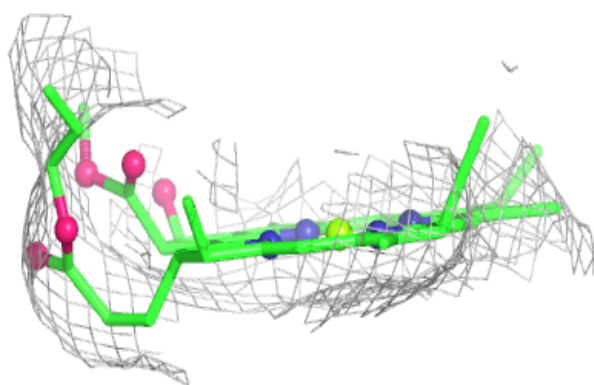
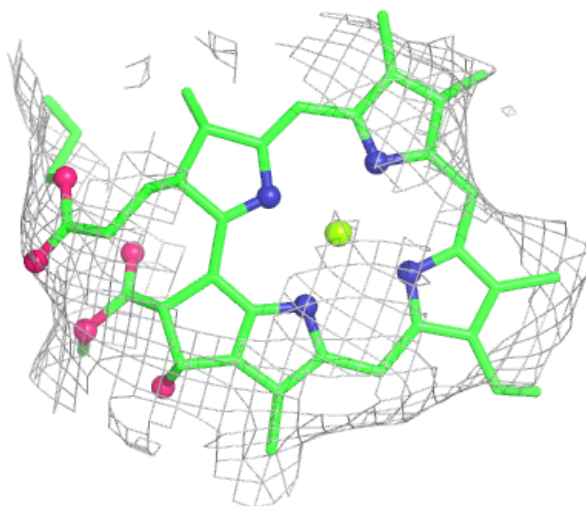
Electron density around CLA 1 210:

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



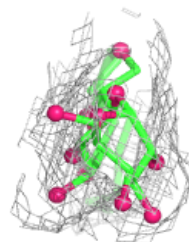
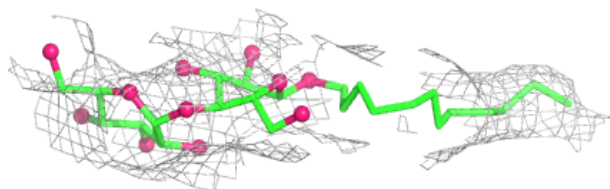
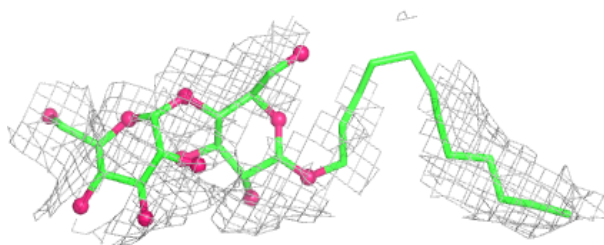
Electron density around CLA J 101:

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



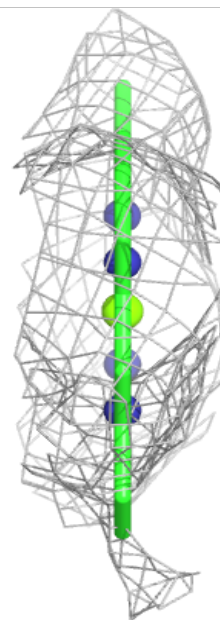
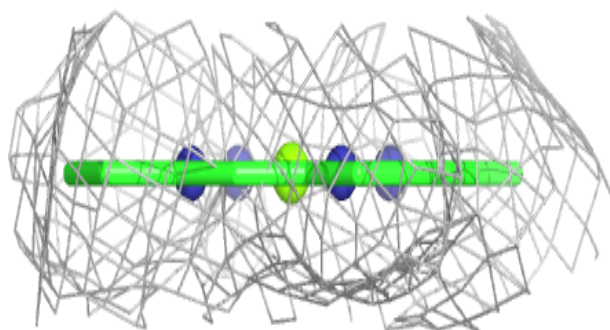
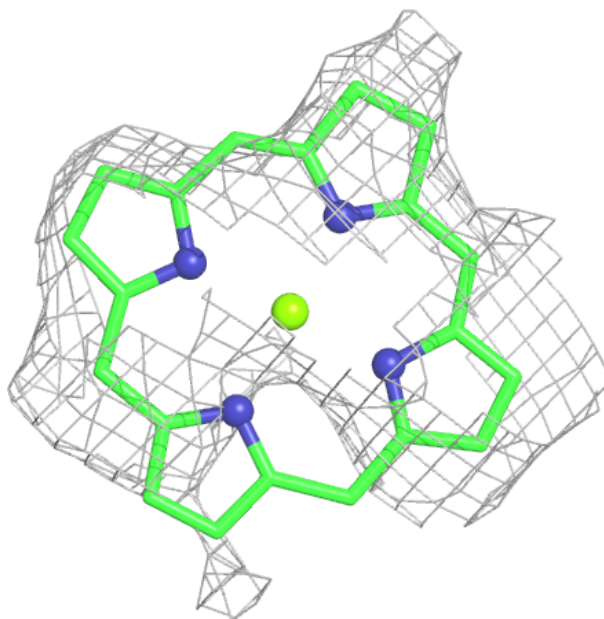
Electron density around LMU H 104:

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



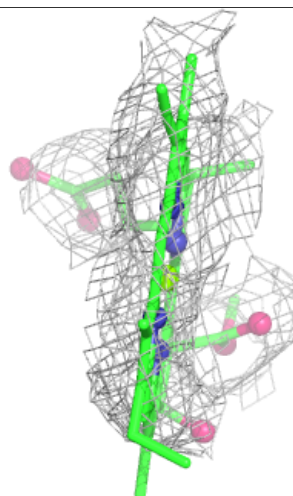
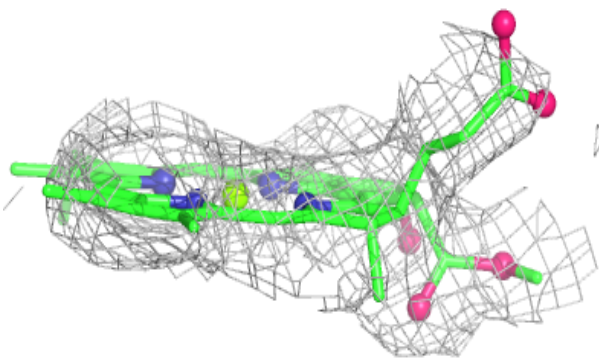
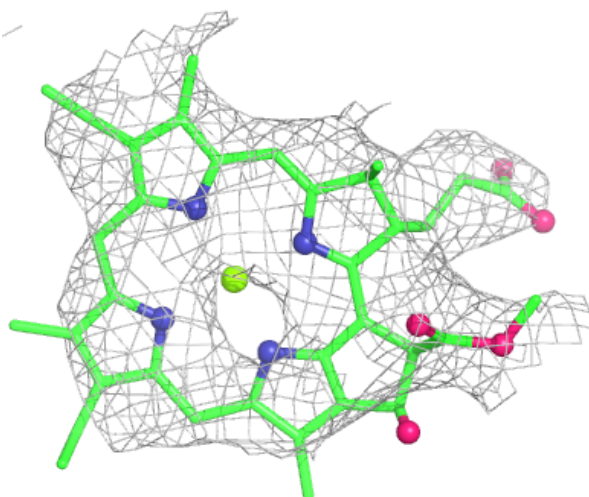
Electron density around CLA A 841:

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



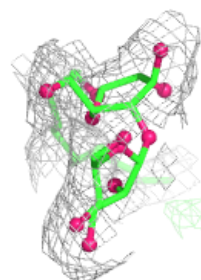
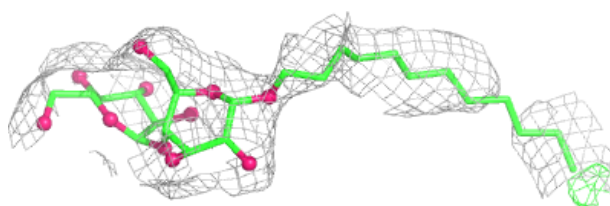
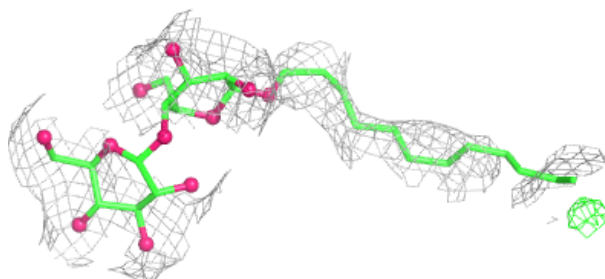
Electron density around CLA A 810:

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

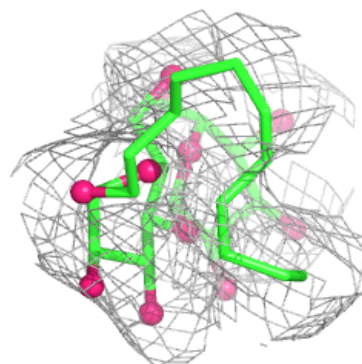
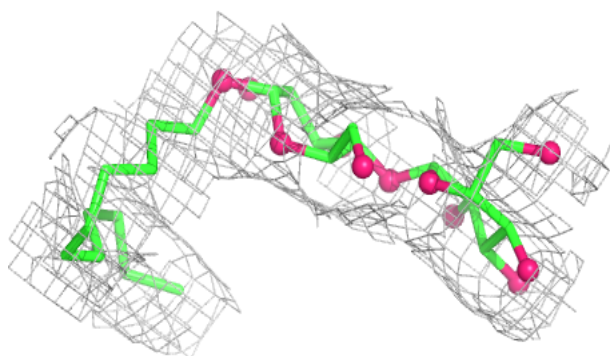
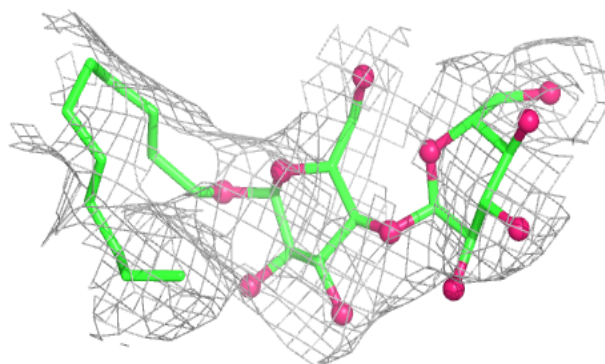


Electron density around LMU R 105:

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

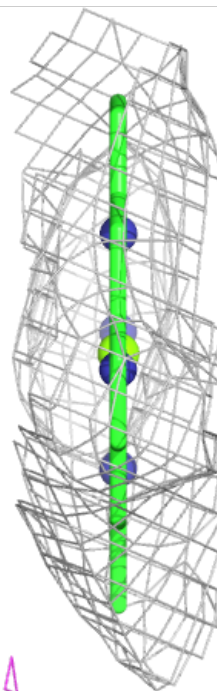
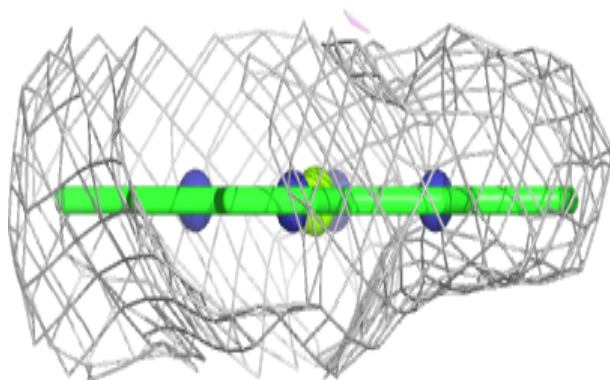
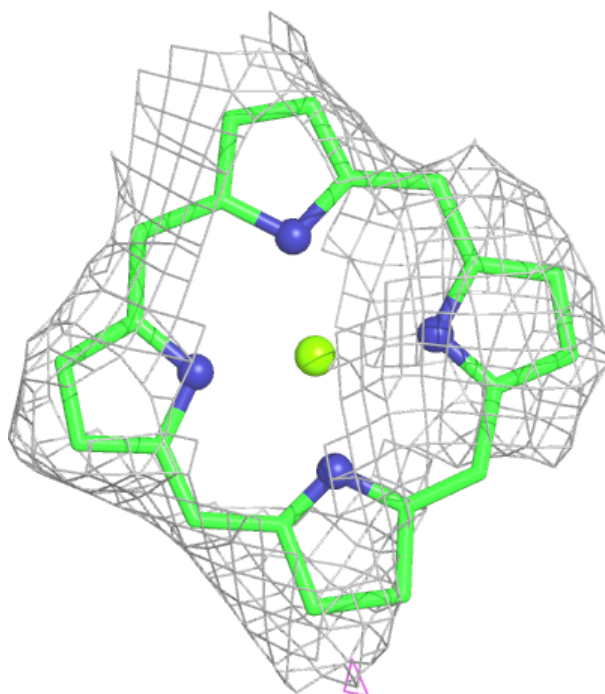
**Electron density around LMU F 202:**

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



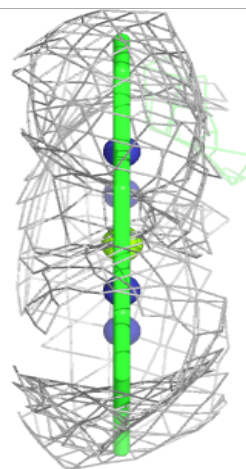
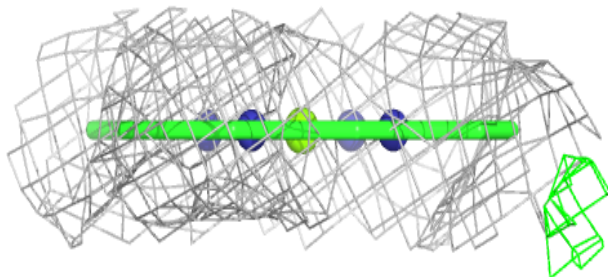
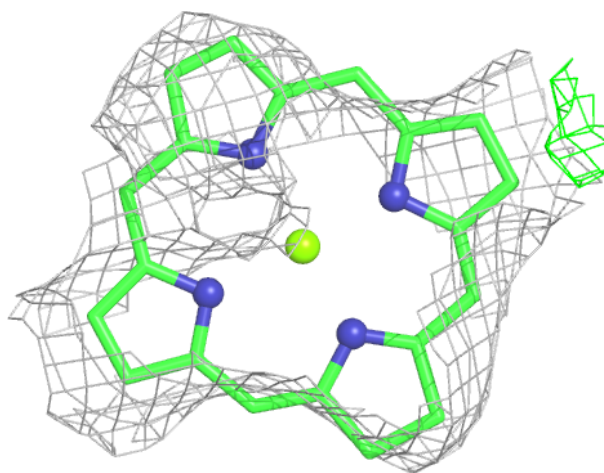
Electron density around CLA 3 316:

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



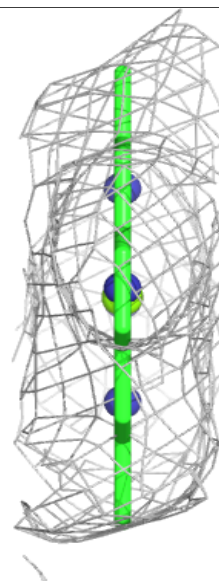
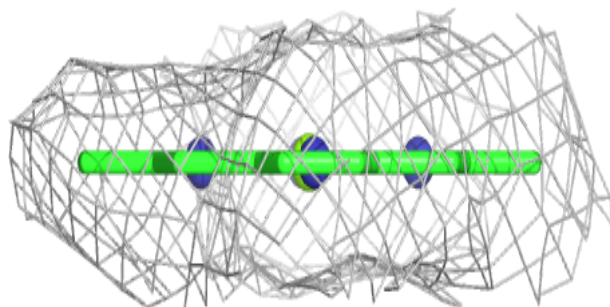
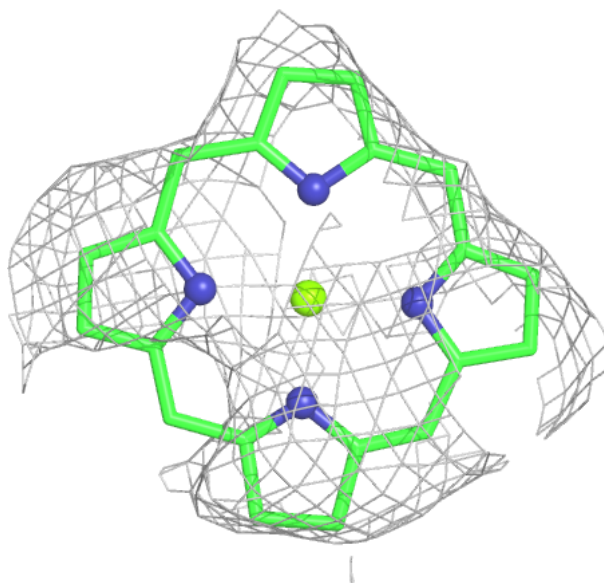
Electron density around CLA A 814:

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



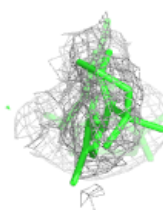
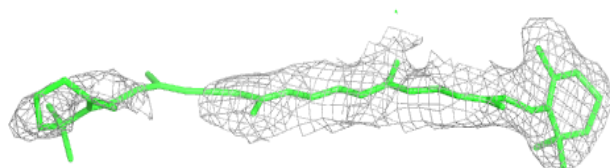
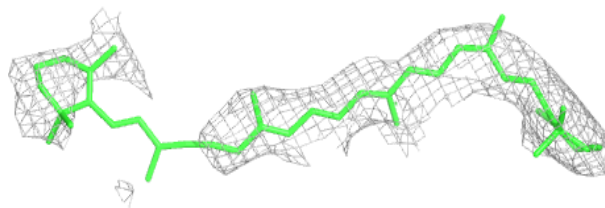
Electron density around CLA 1 214:

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

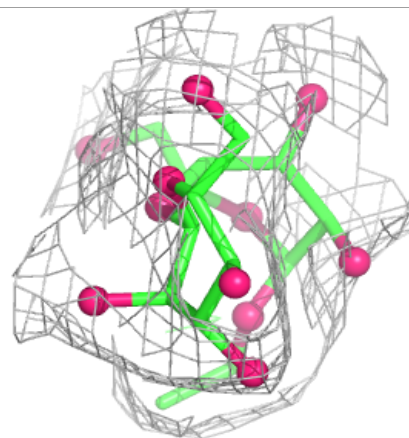
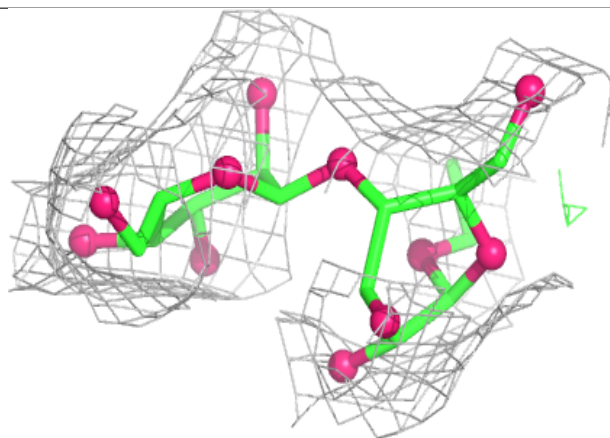
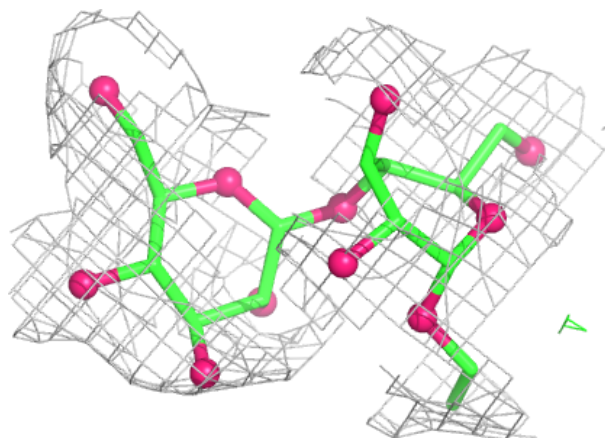


Electron density around BCR B 845:

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

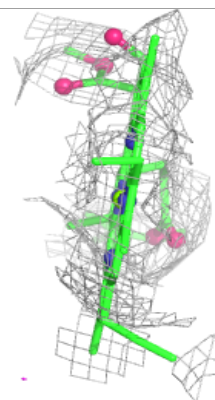
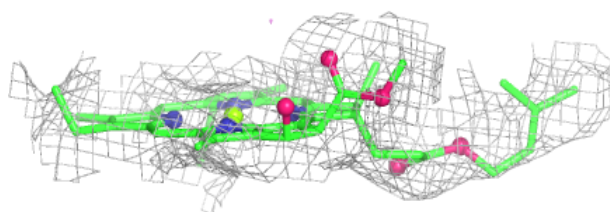
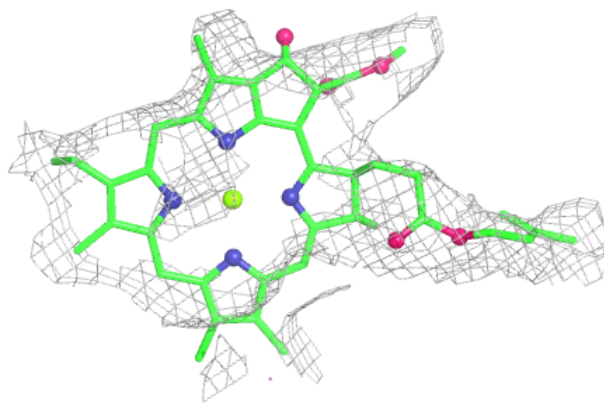
**Electron density around LMU B 849:**

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



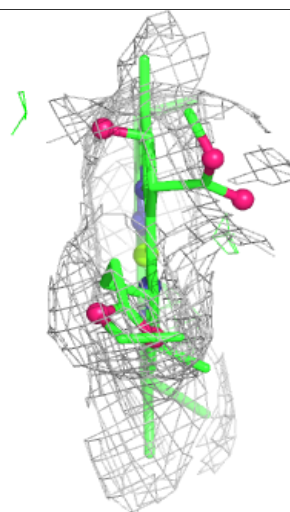
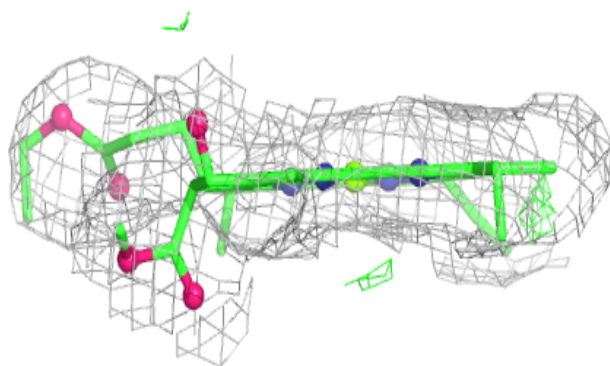
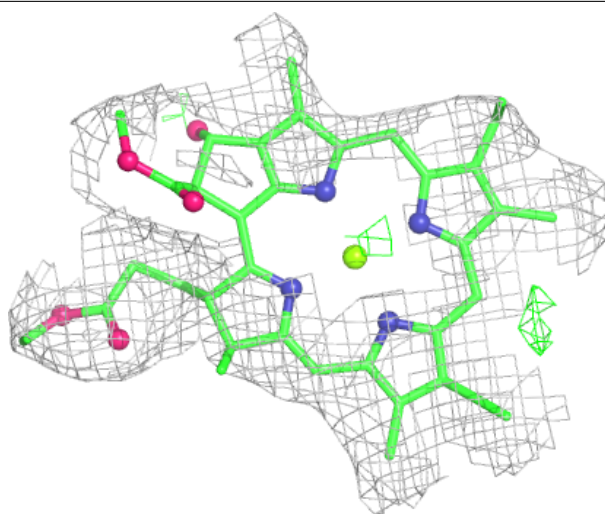
Electron density around CLA K 102:

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



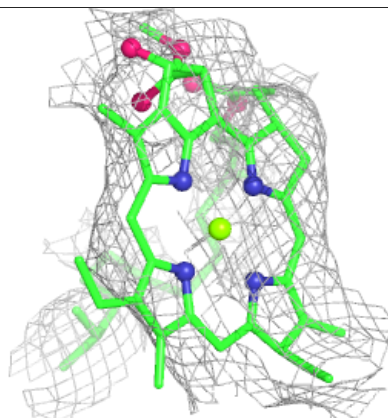
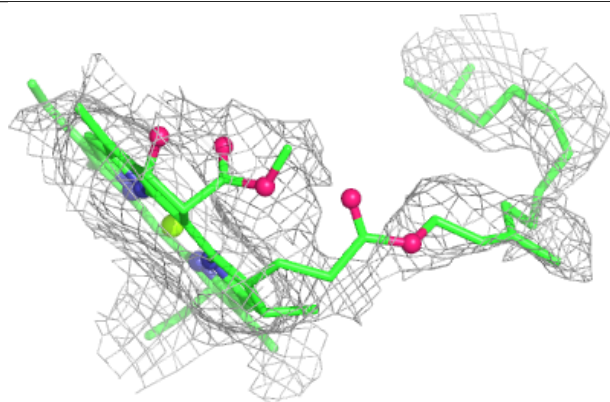
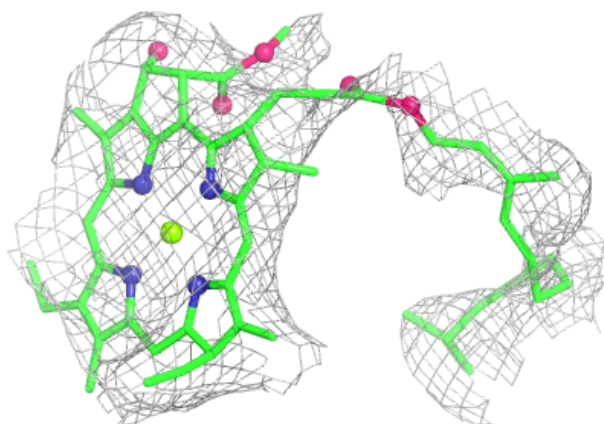
Electron density around CLA 1 203:

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

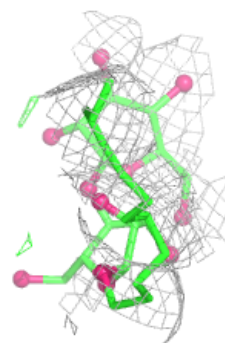
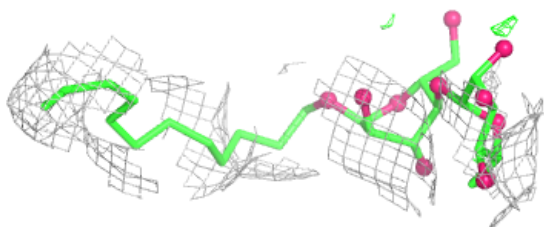
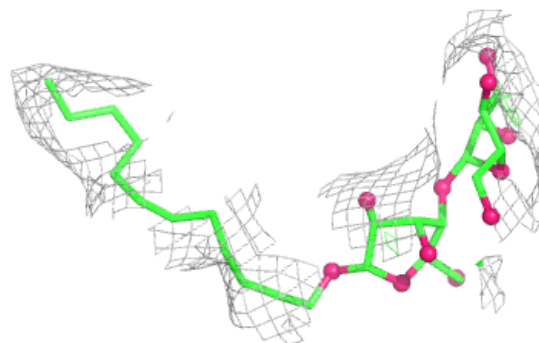


Electron density around CLA A 839:

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

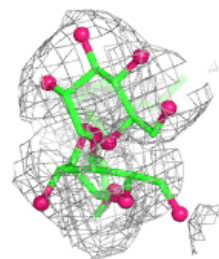
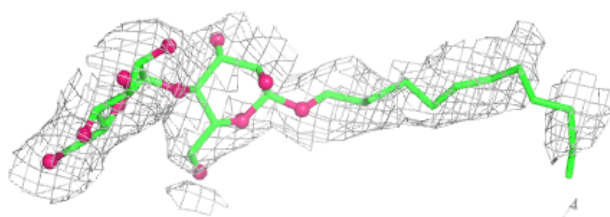
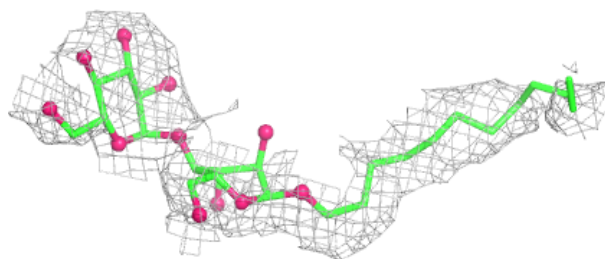
**Electron density around LMU G 102:**

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



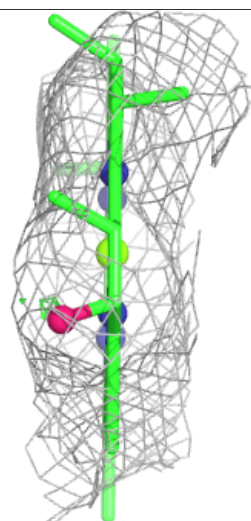
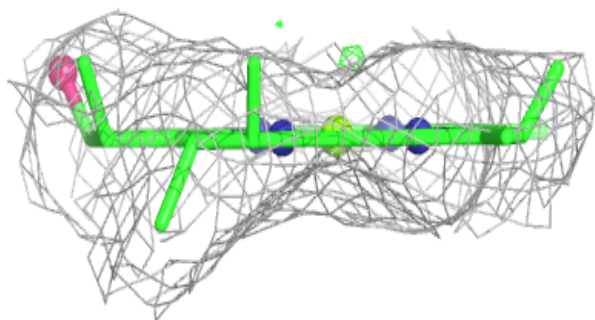
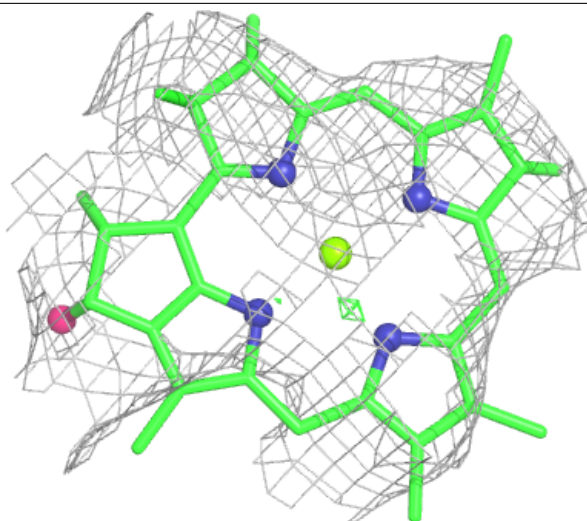
Electron density around LMU 4 316:

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



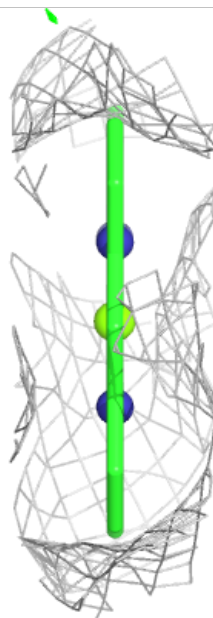
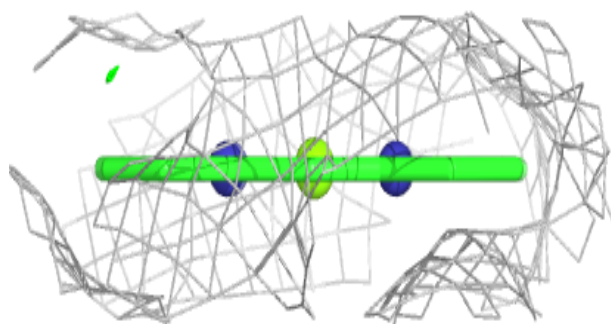
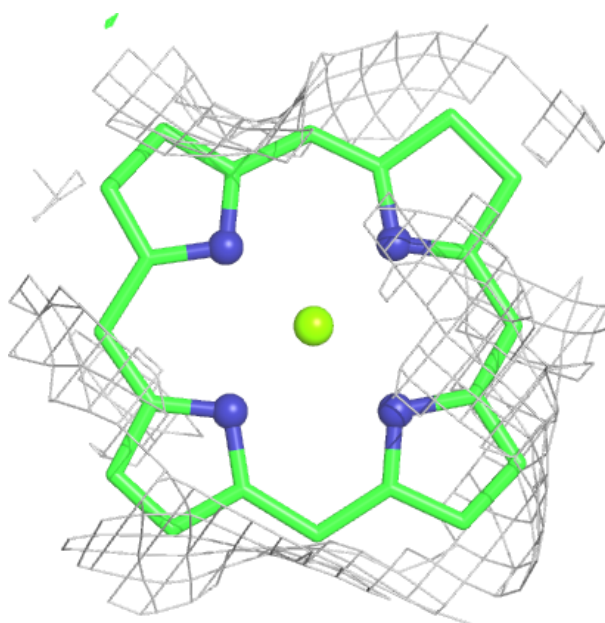
Electron density around CLA 4 302:

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



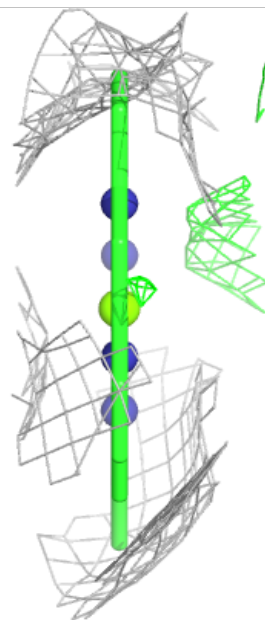
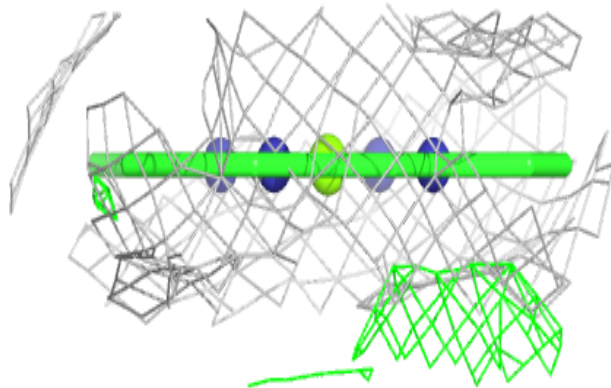
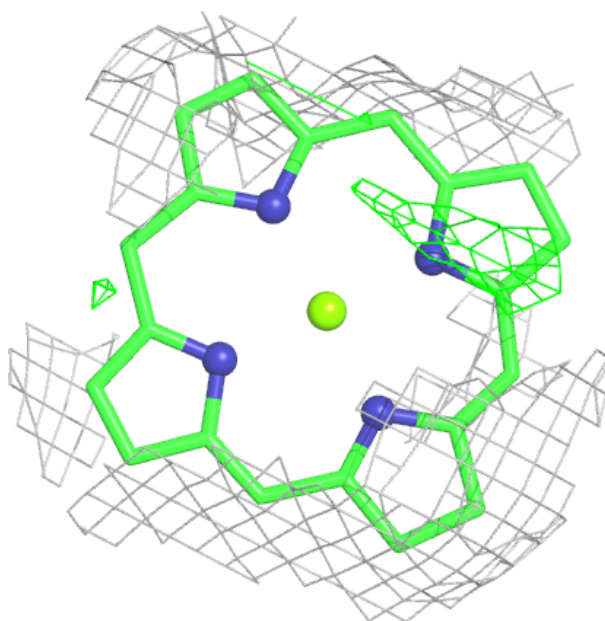
Electron density around CLA 2 306:

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



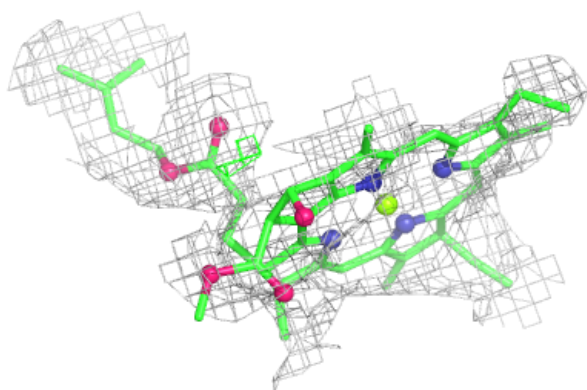
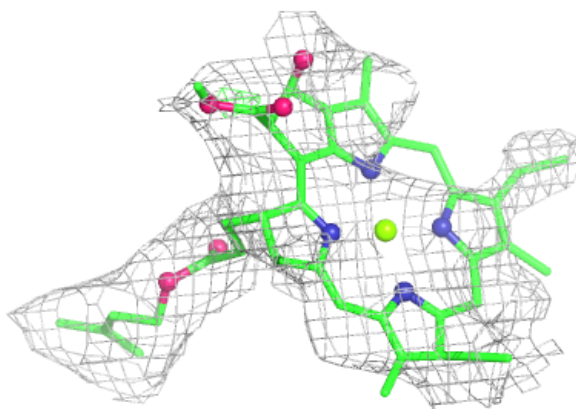
Electron density around CLA 1 208:

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



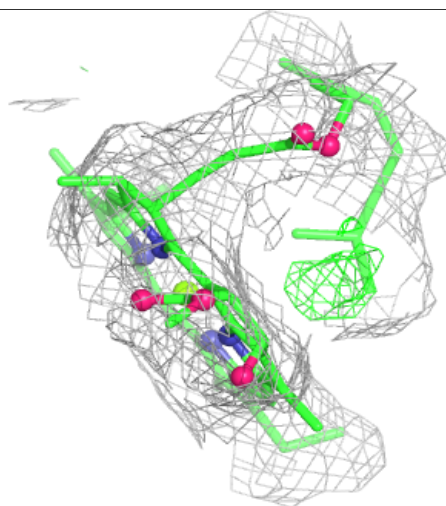
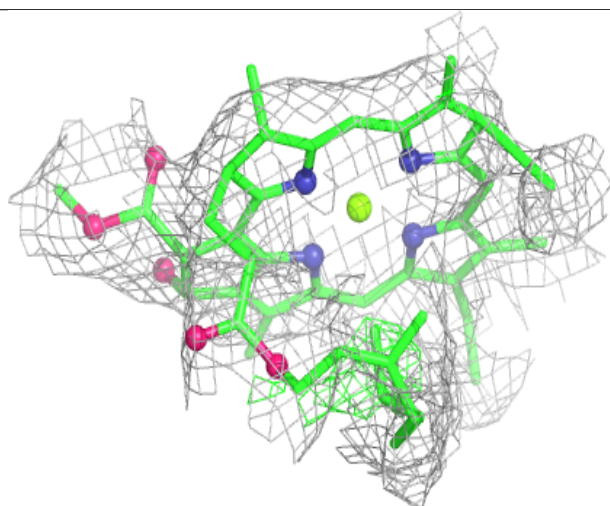
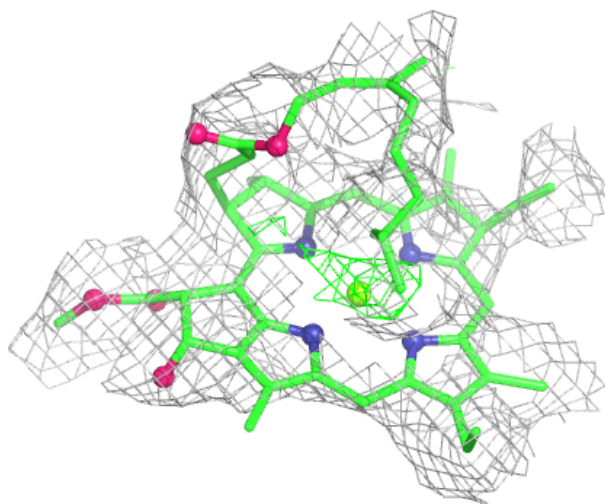
Electron density around CLA 2 310:

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



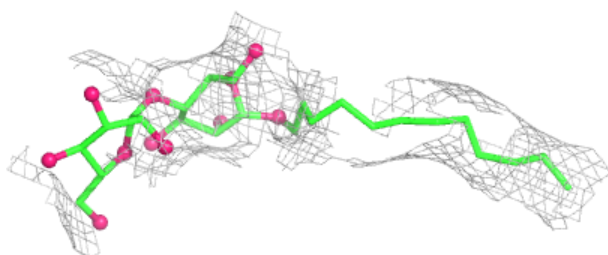
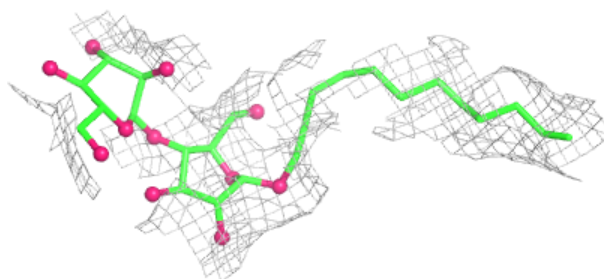
Electron density around CLA B 813:

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

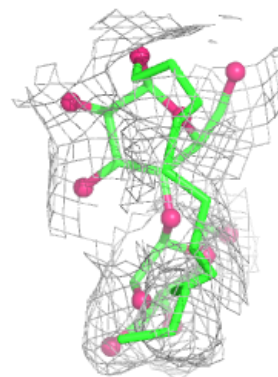
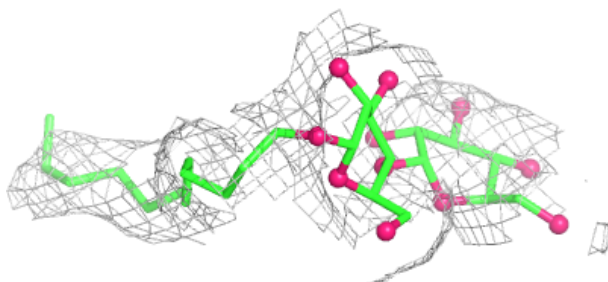
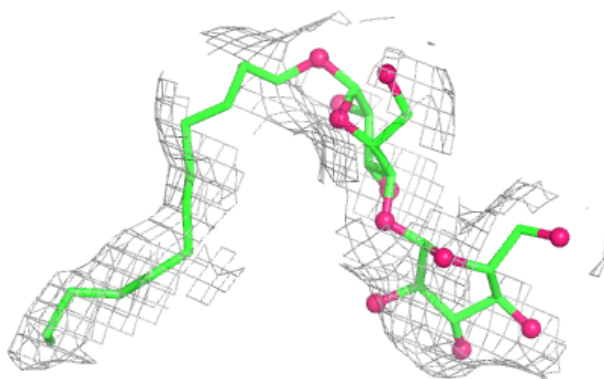


Electron density around LMU G 101:

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

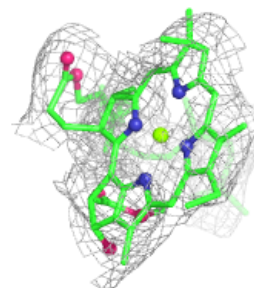
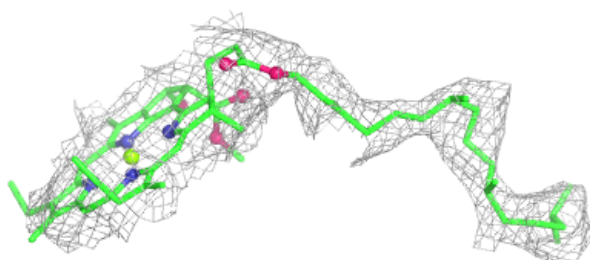
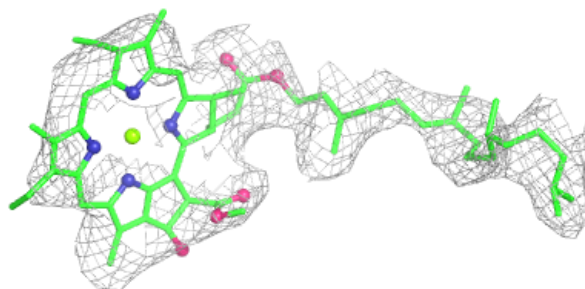
**Electron density around LMU L 206:**

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

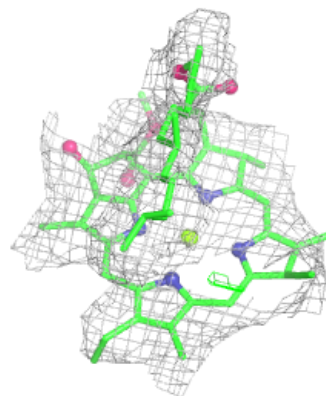
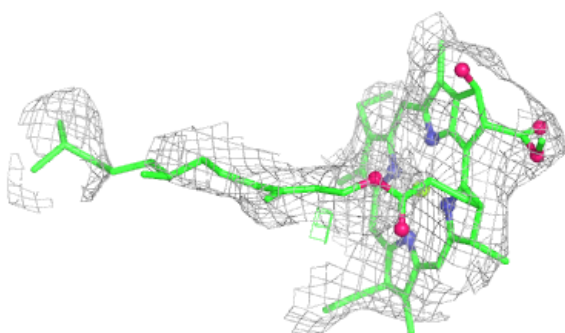
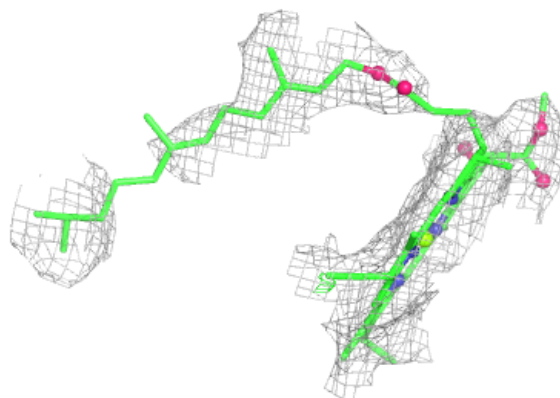


Electron density around CLA 3 314:

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

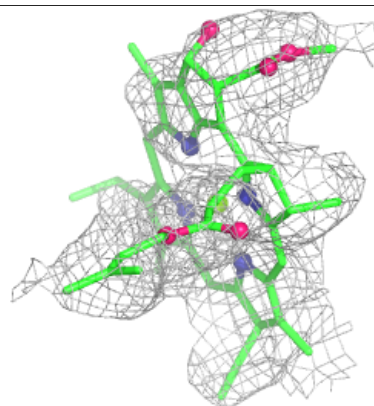
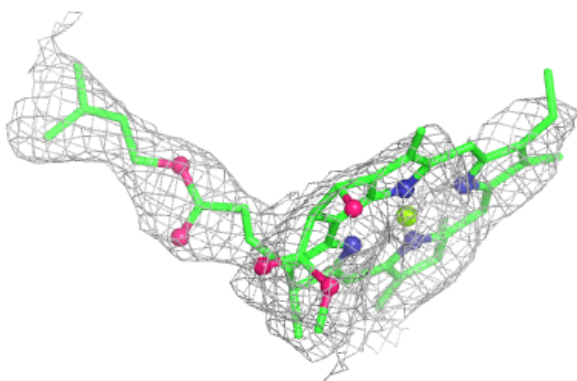
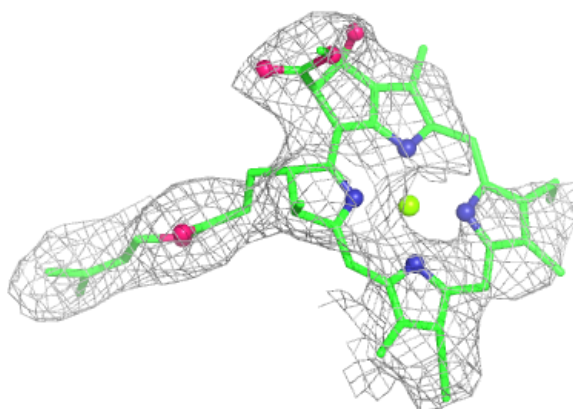
**Electron density around CLA L 201:**

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

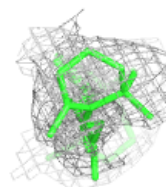
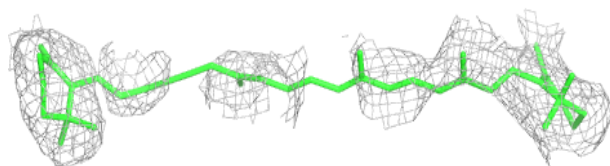
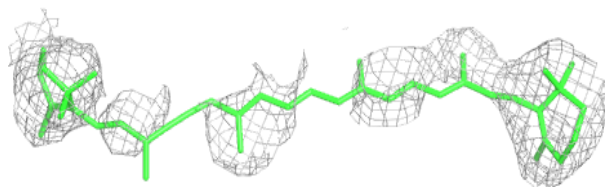


Electron density around CLA A 829:

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

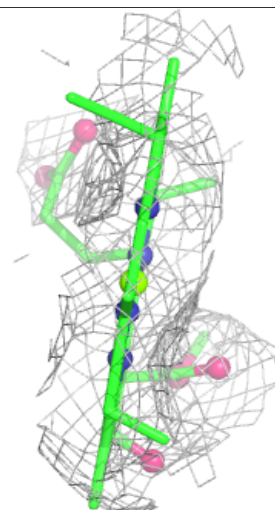
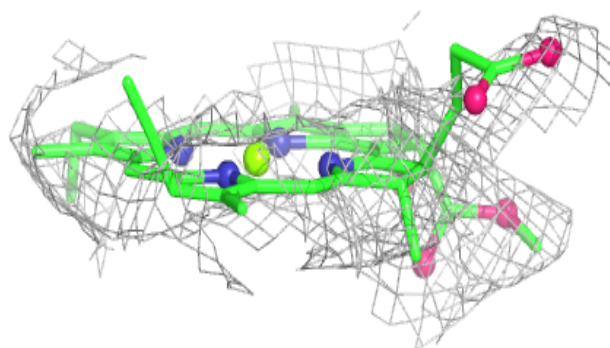
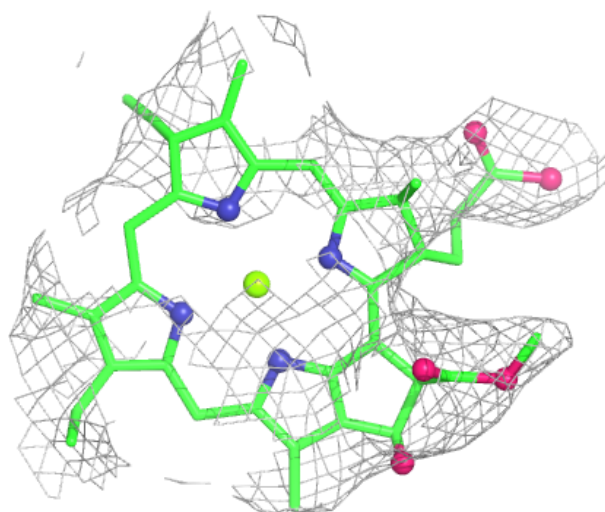
**Electron density around BCR J 102:**

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



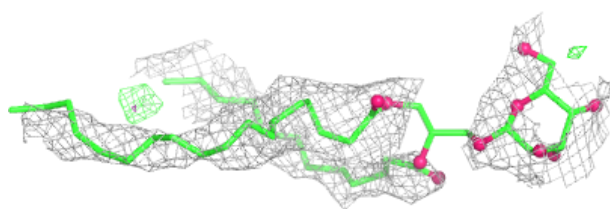
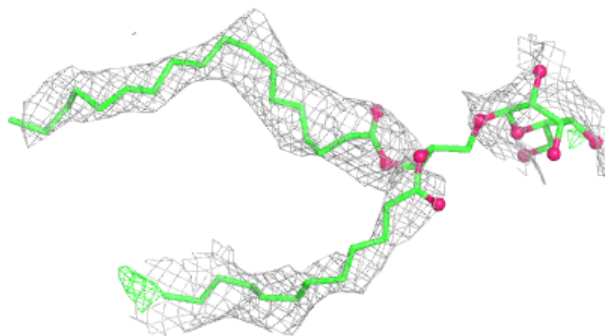
Electron density around CLA A 833:

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



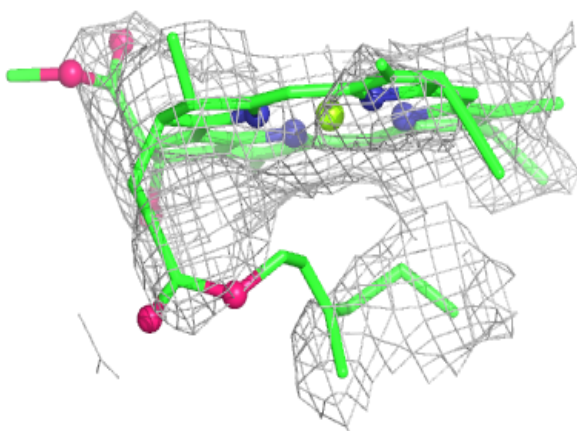
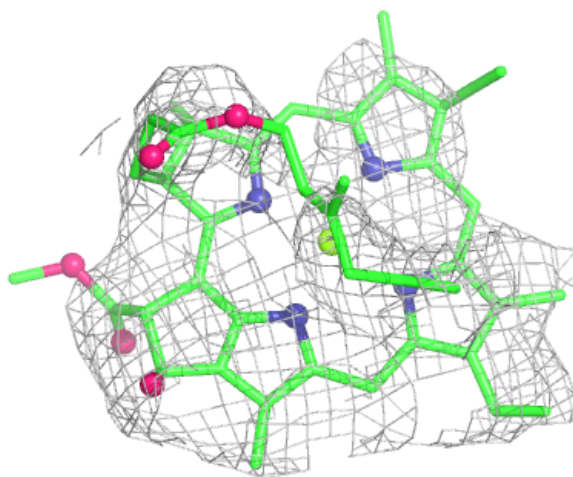
Electron density around LMG B 848:

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



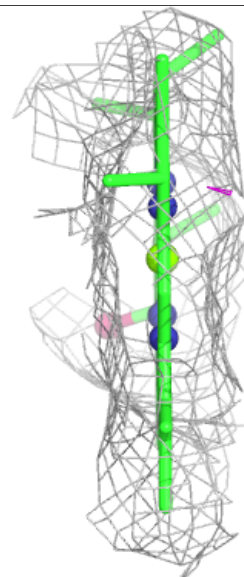
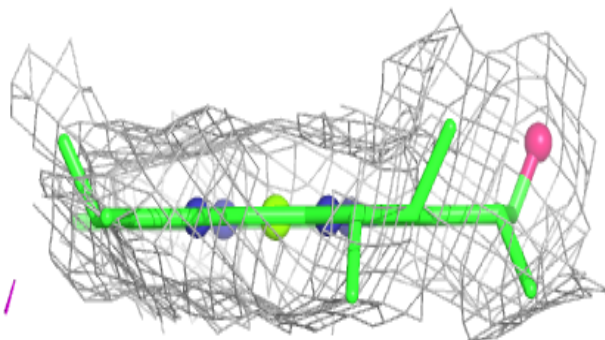
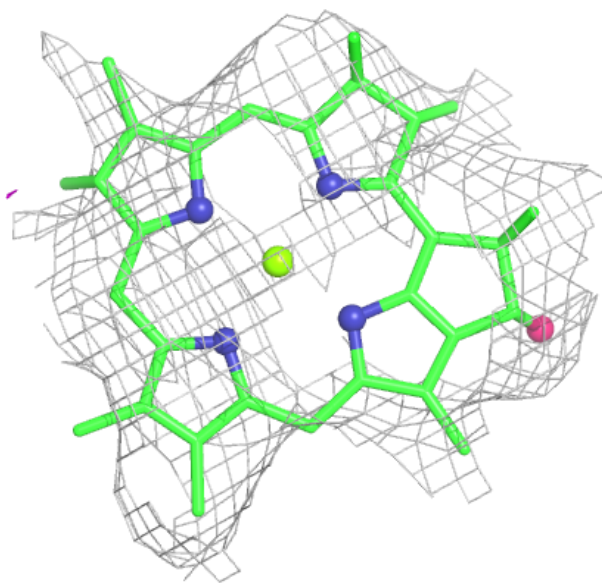
Electron density around CLA A 817:

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



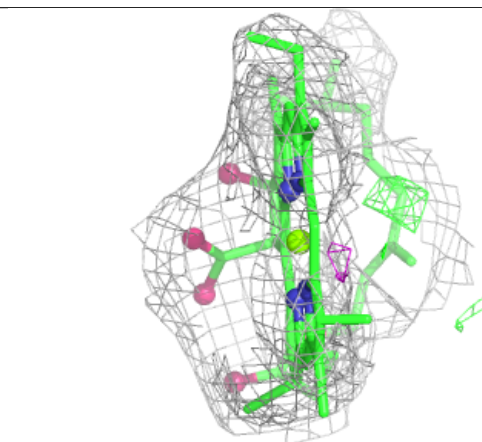
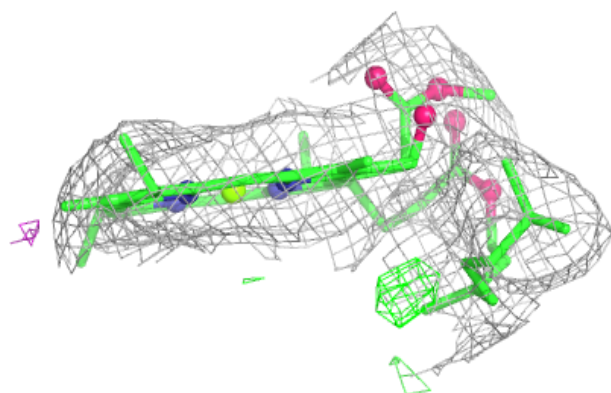
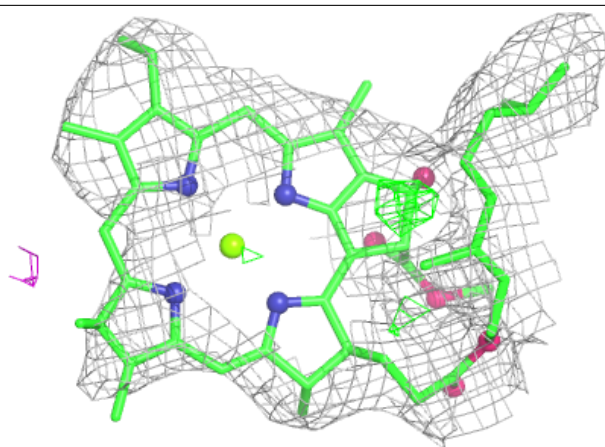
Electron density around CLA 3 301:

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

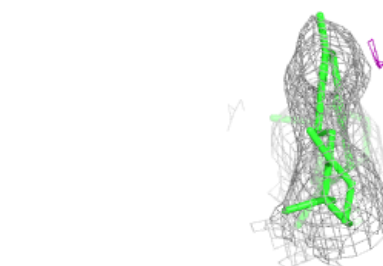
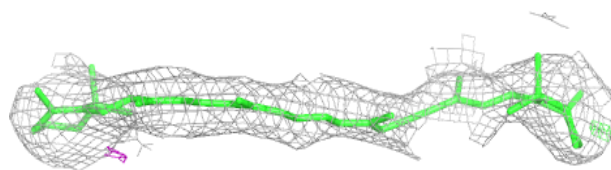
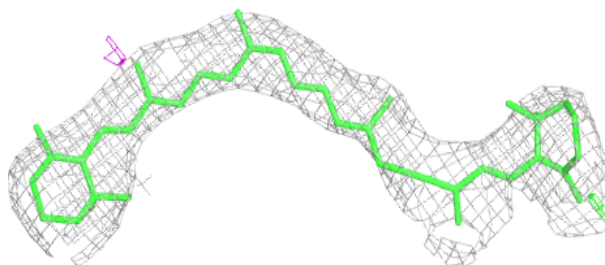


Electron density around CLA B 812:

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

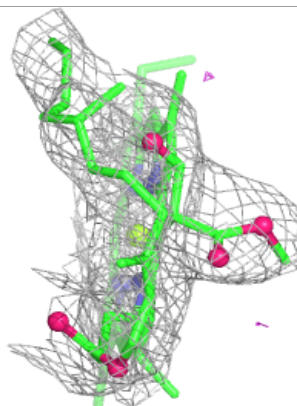
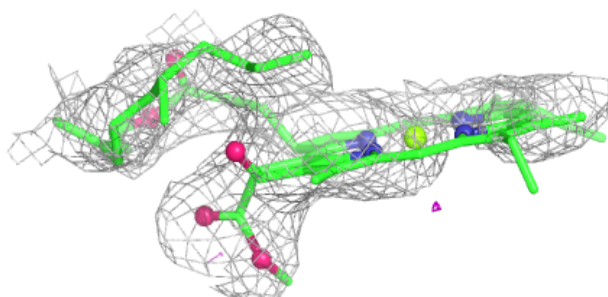
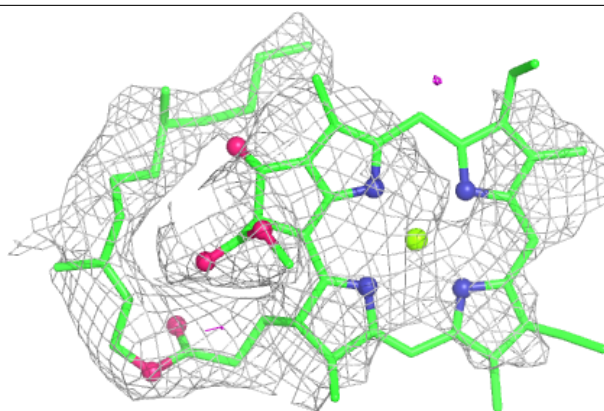
**Electron density around BCR A 845:**

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

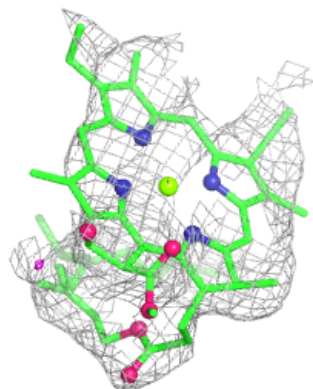
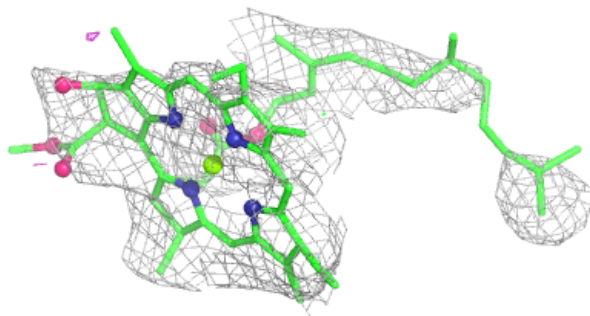
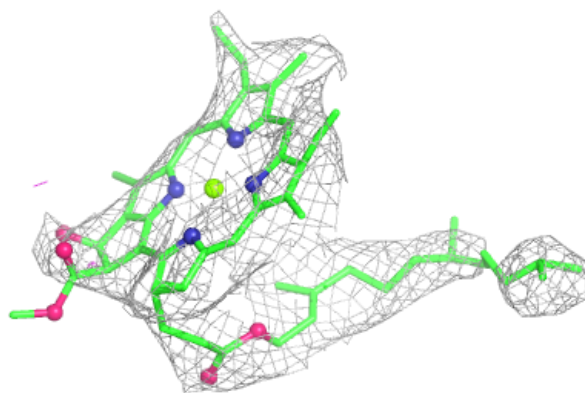


Electron density around CLA A 823:

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

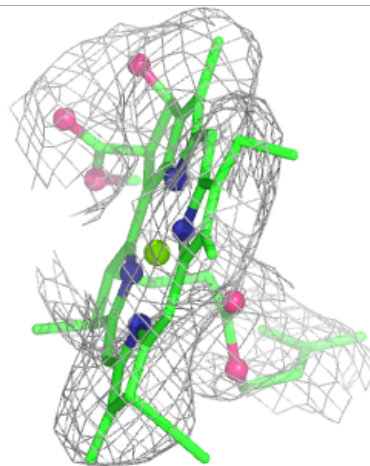
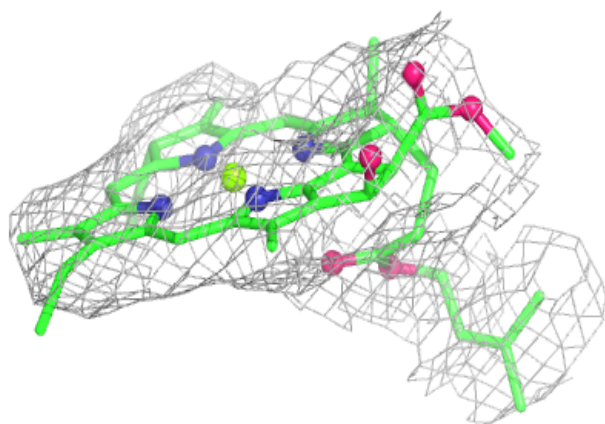
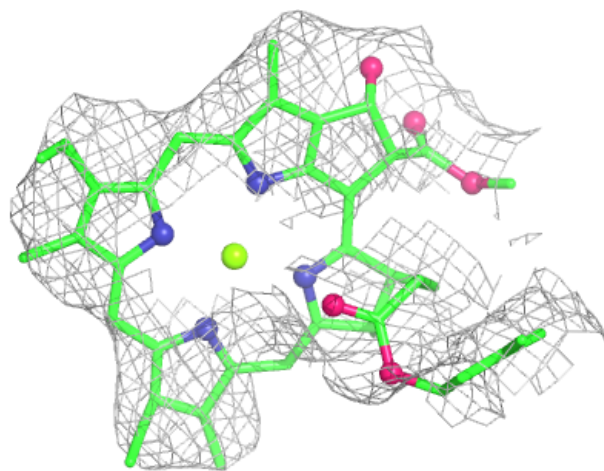
**Electron density around CLA B 815:**

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



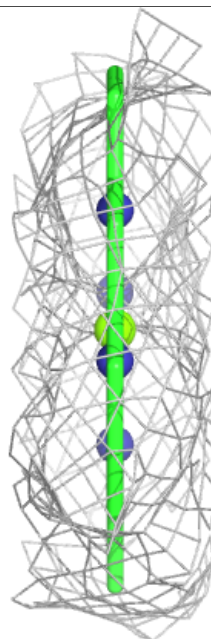
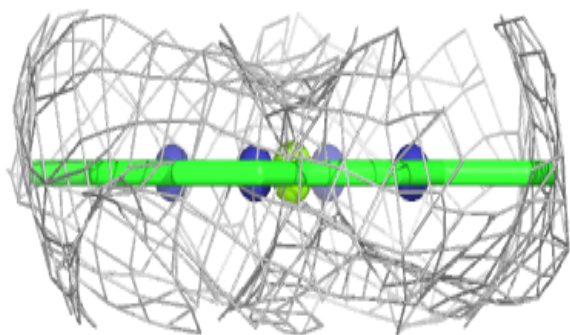
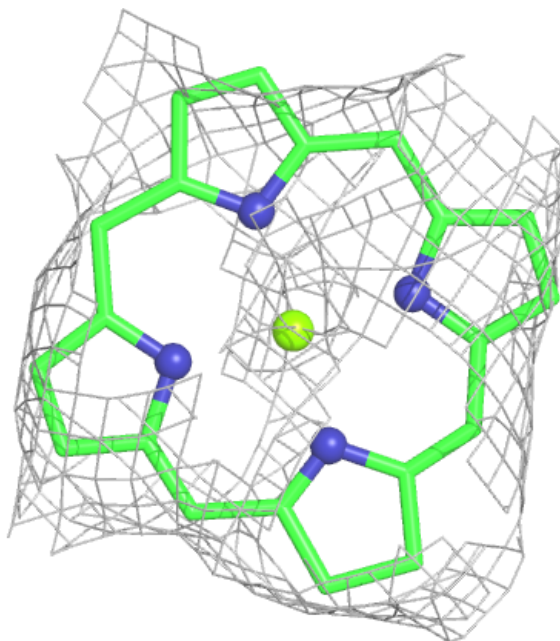
Electron density around CLA A 815:

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



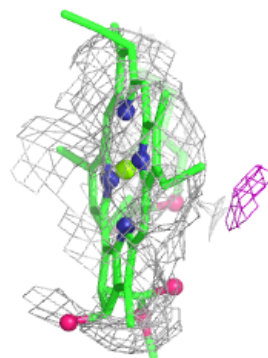
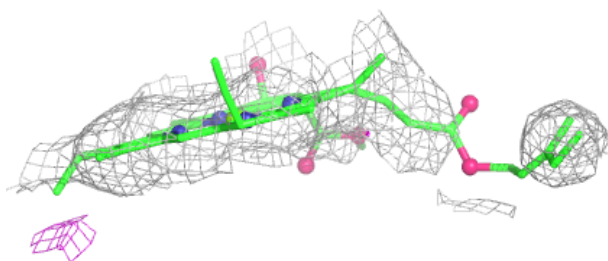
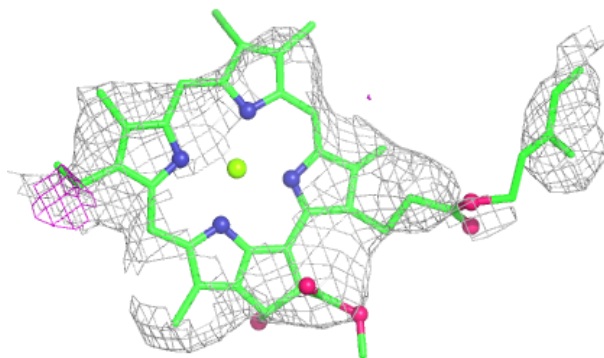
Electron density around CLA 1 212:

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



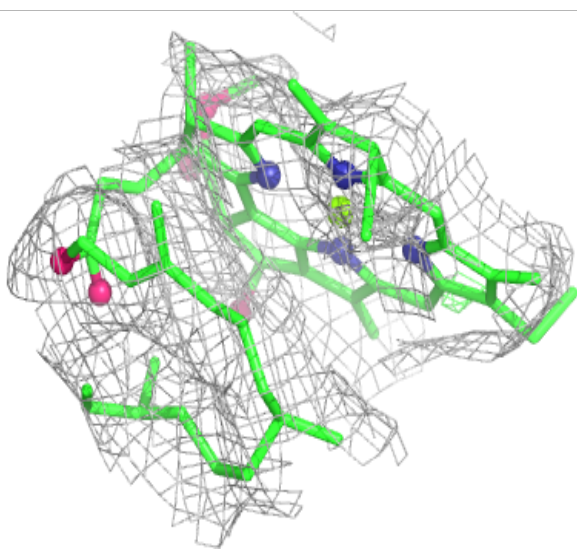
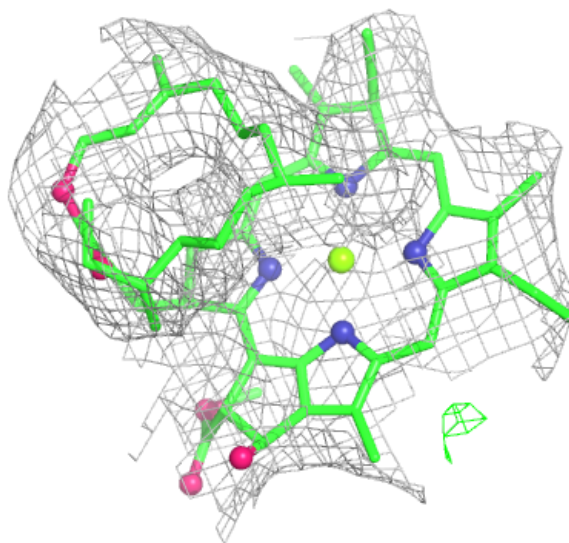
Electron density around CLA 1 213:

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



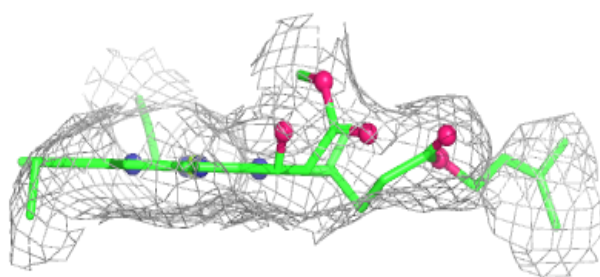
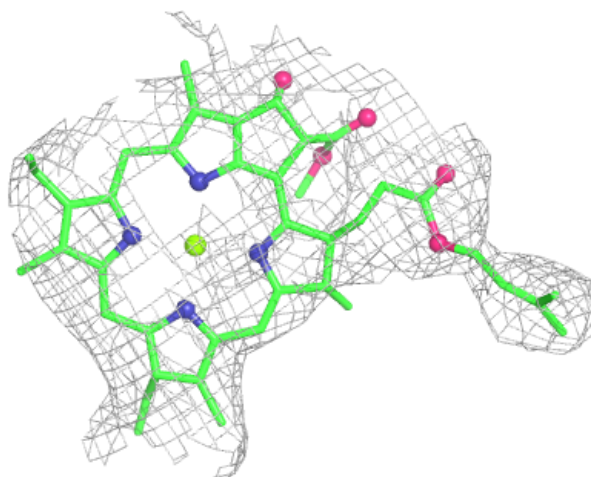
Electron density around CLA J 103:

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



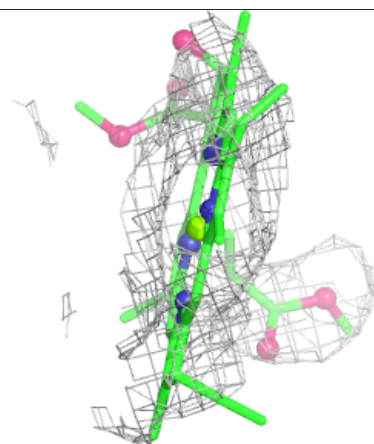
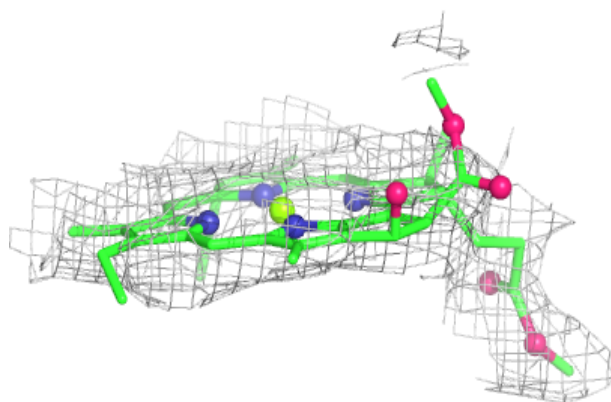
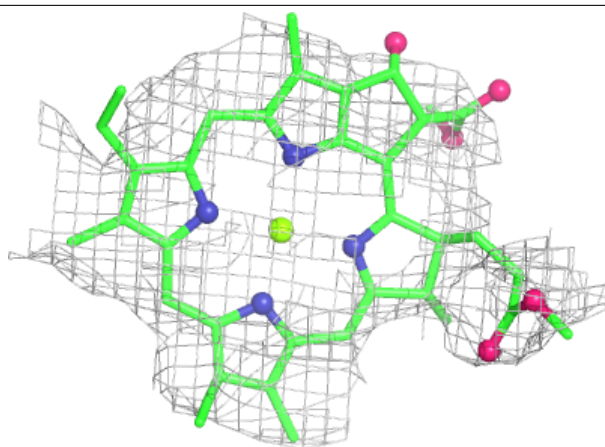
Electron density around CLA 4 310:

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

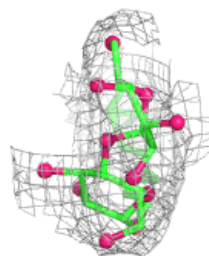
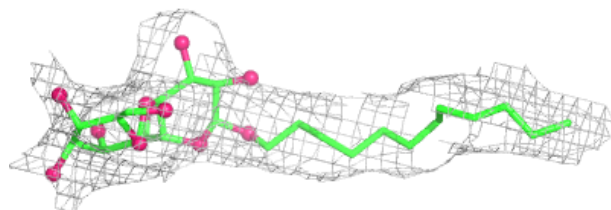
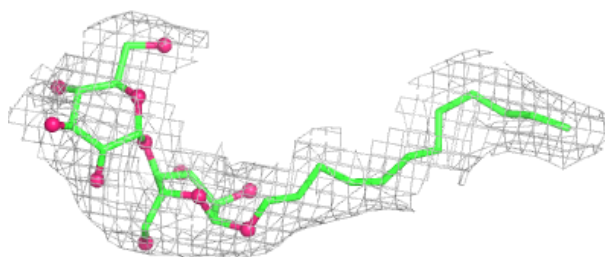


Electron density around CLA B 822:

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

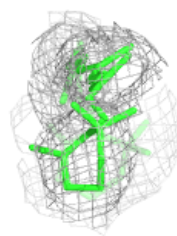
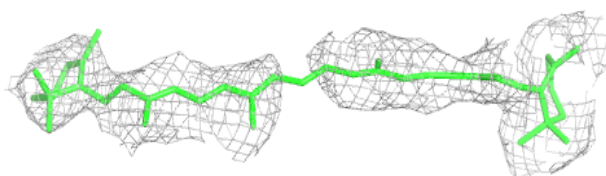
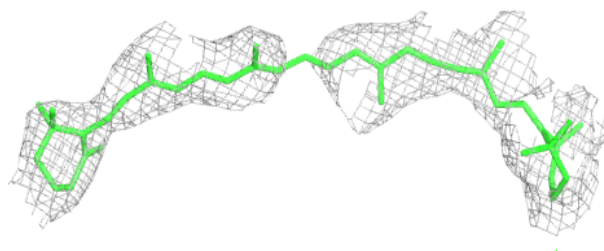
**Electron density around LMU 4 321:**

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



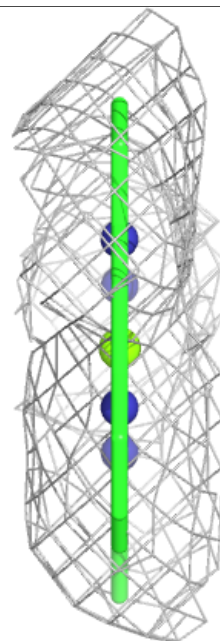
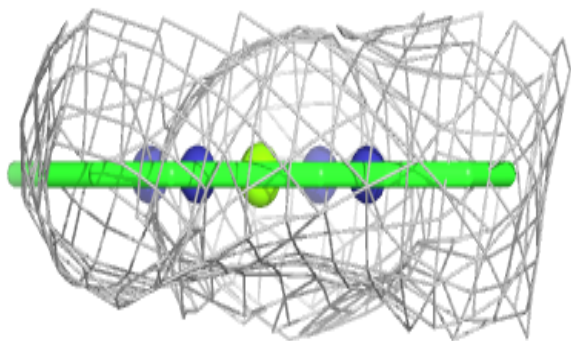
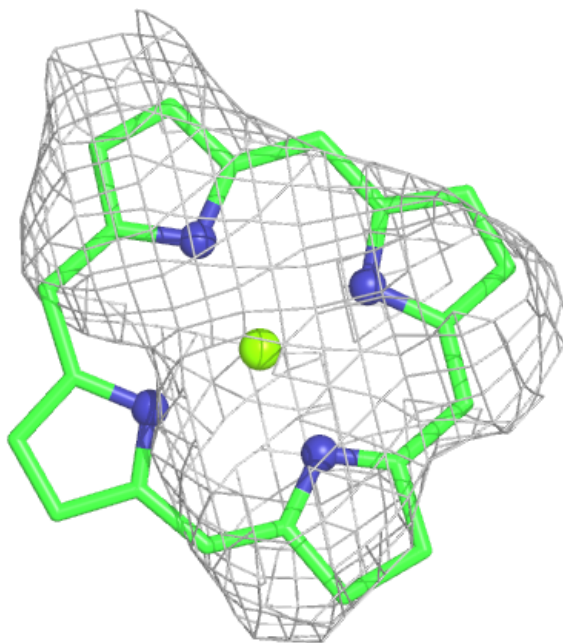
Electron density around BCR B 844:

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



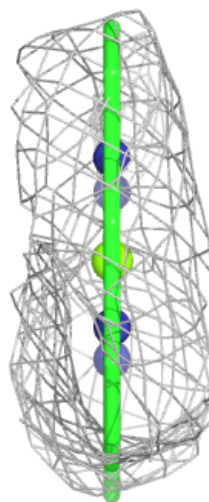
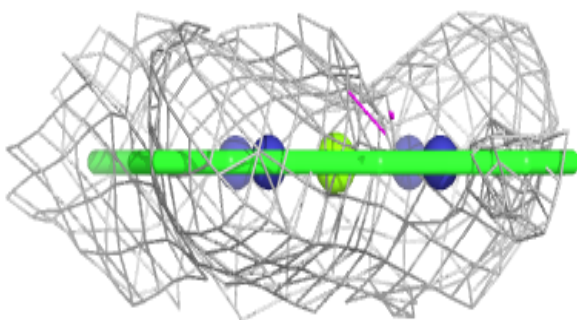
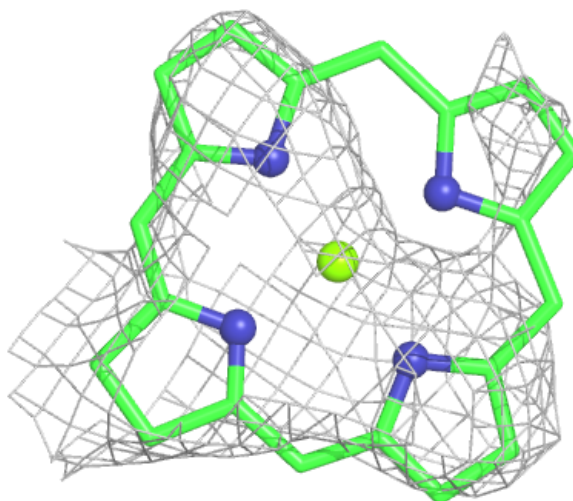
Electron density around CLA 3 315:

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



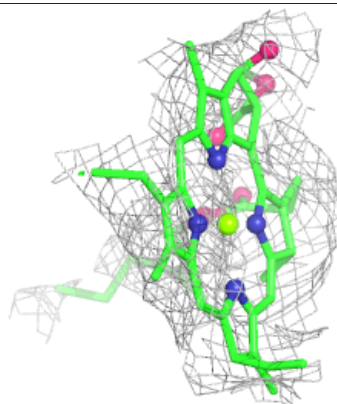
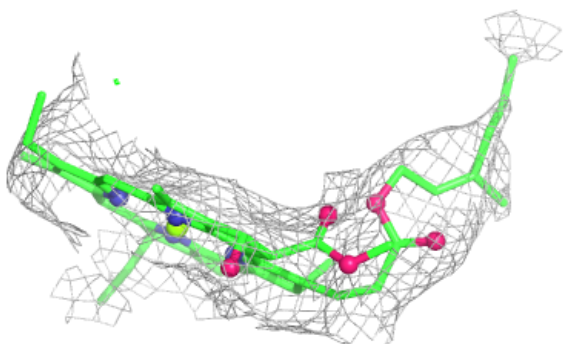
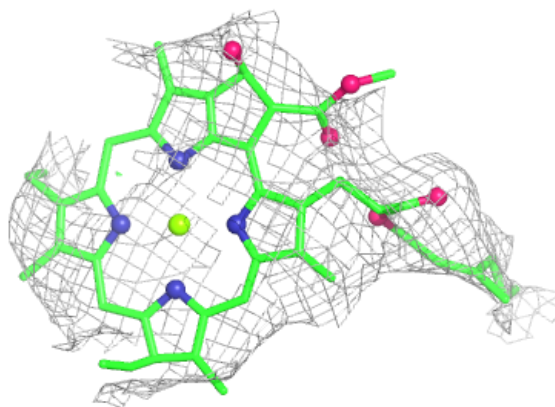
Electron density around CLA 2 309:

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

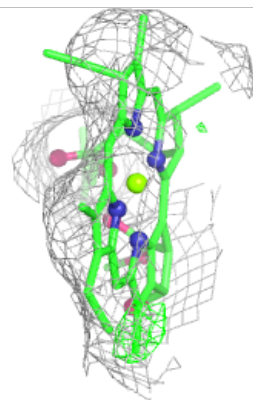
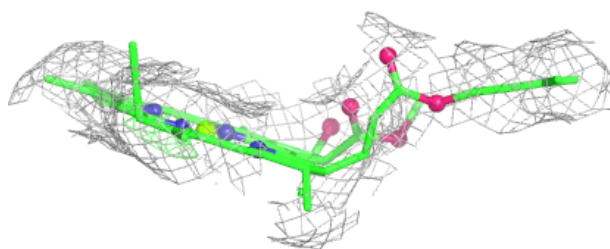
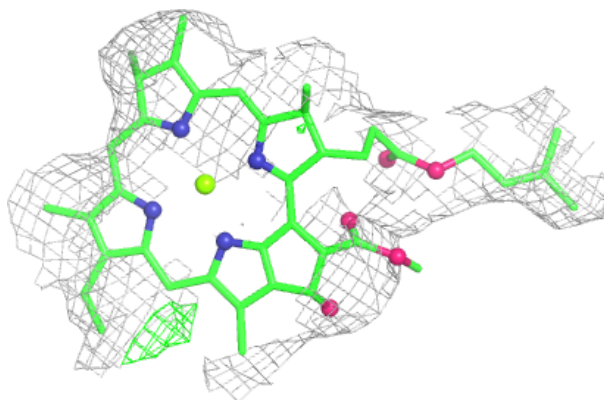


Electron density around CLA 4 306:

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

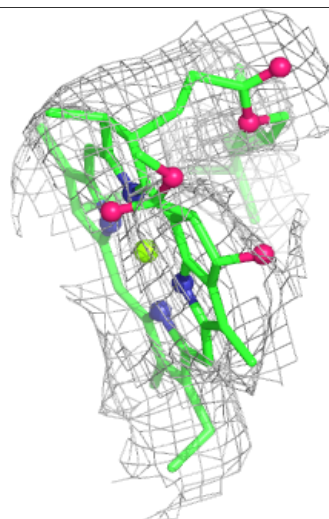
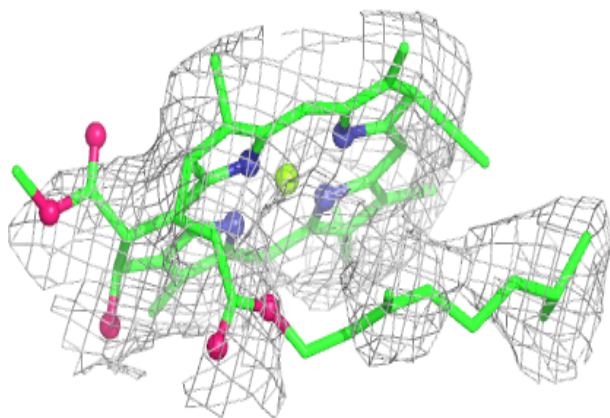
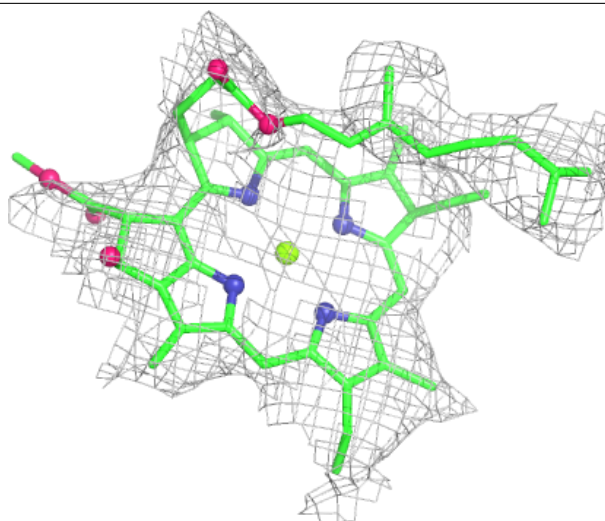
**Electron density around CLA L 208:**

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



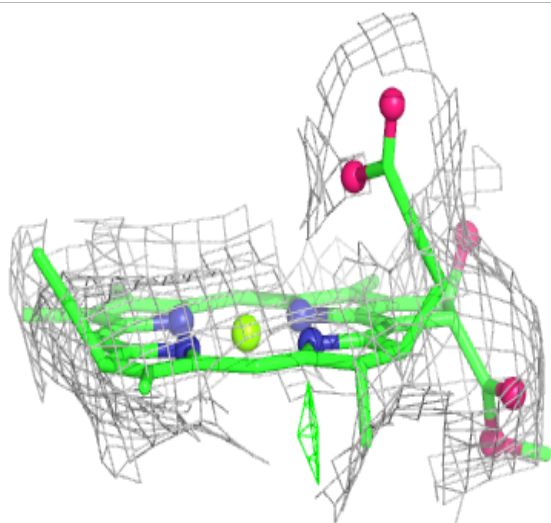
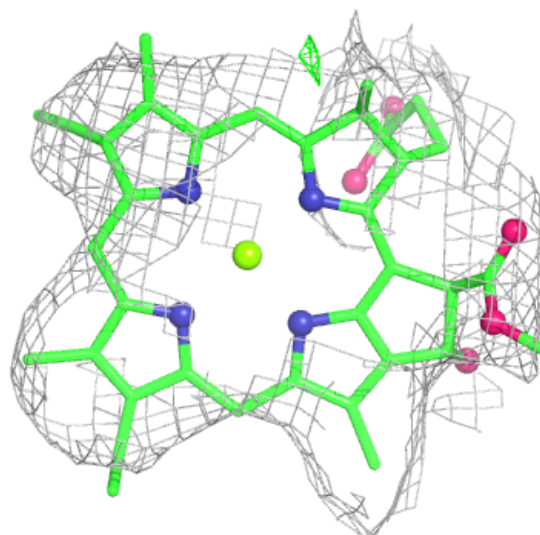
Electron density around CLA B 823:

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



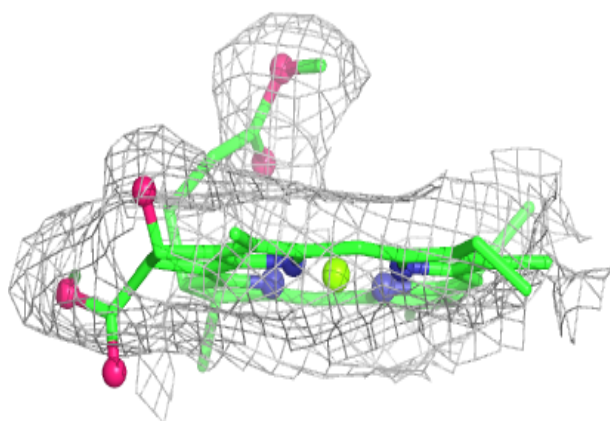
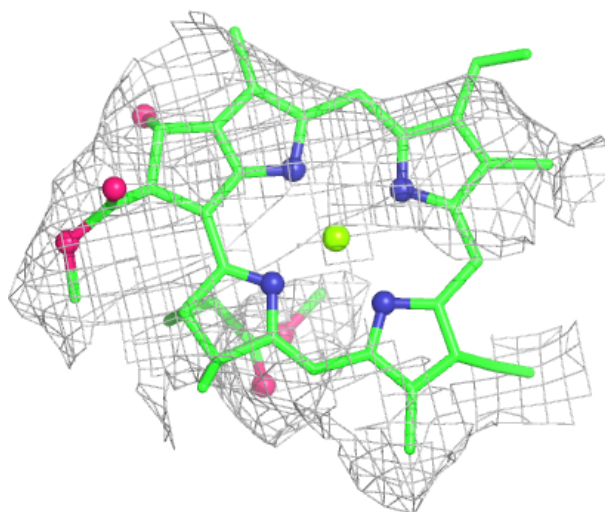
Electron density around CLA B 834:

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



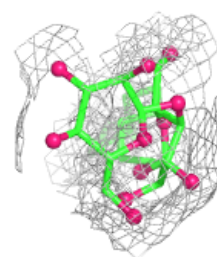
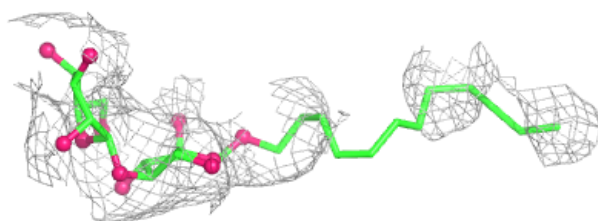
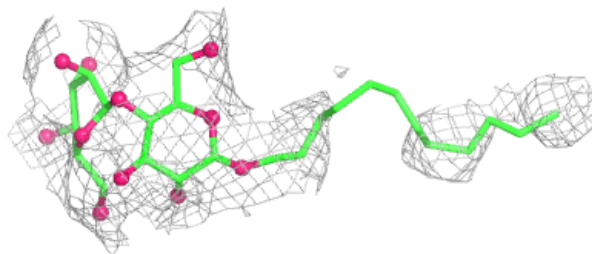
Electron density around CLA 1 204:

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



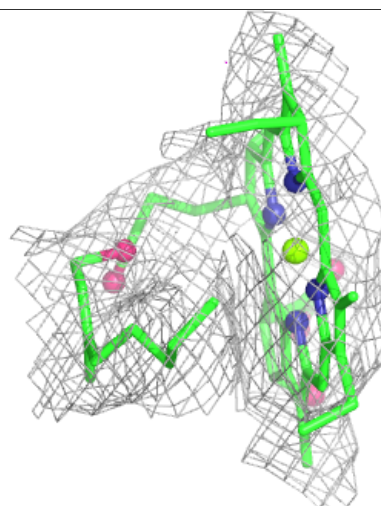
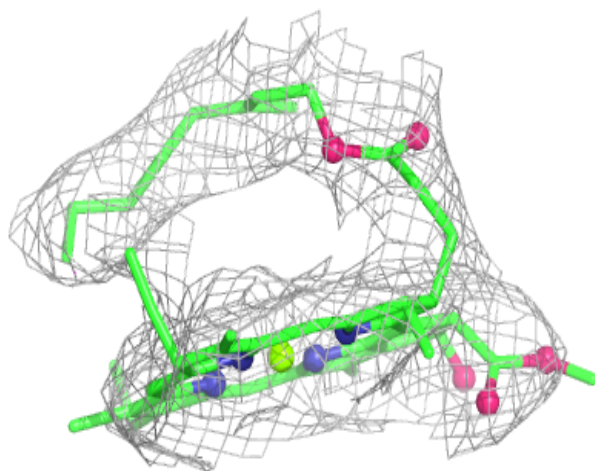
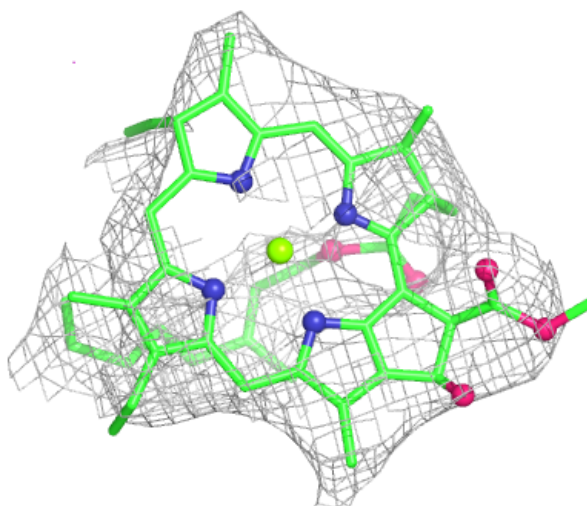
Electron density around LMU 1 218:

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



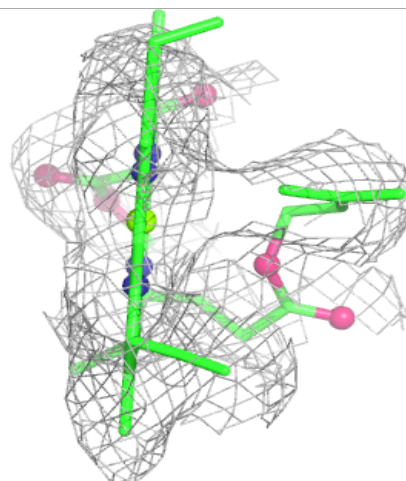
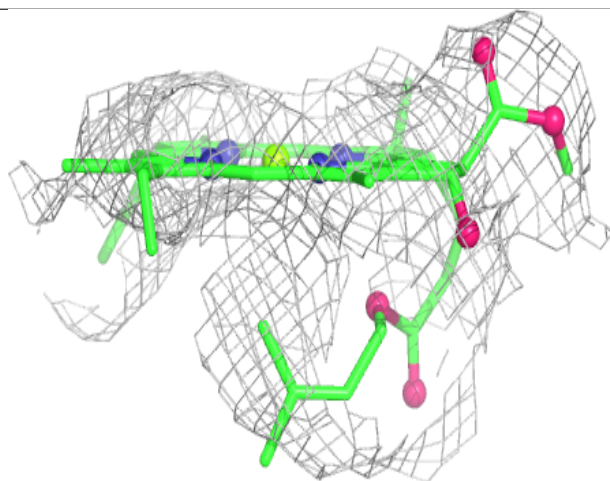
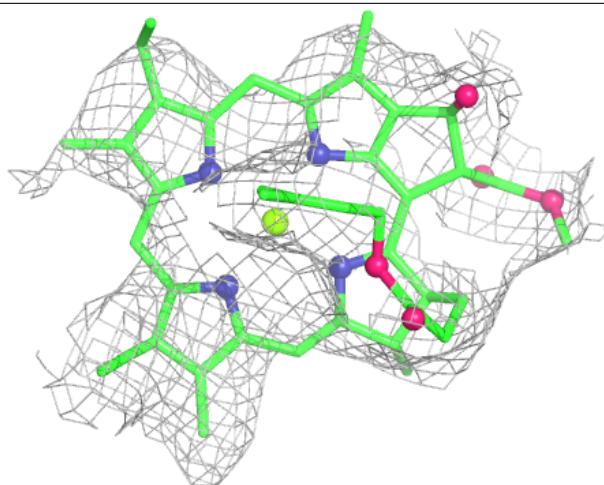
Electron density around CLA A 812:

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



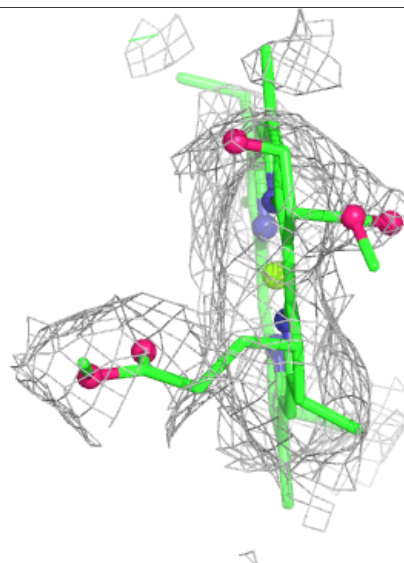
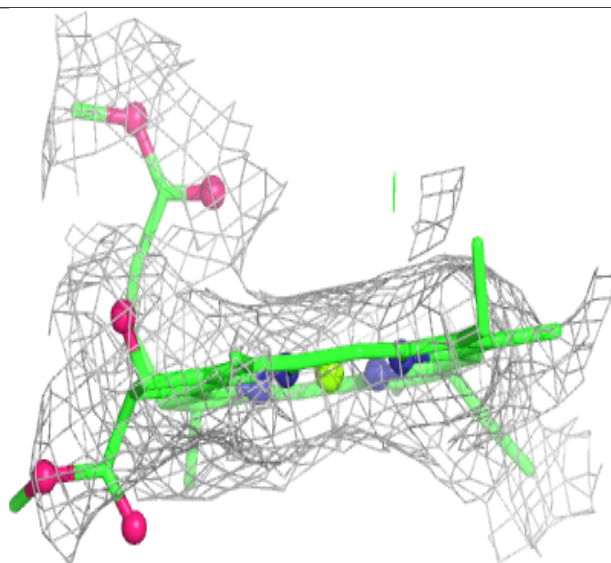
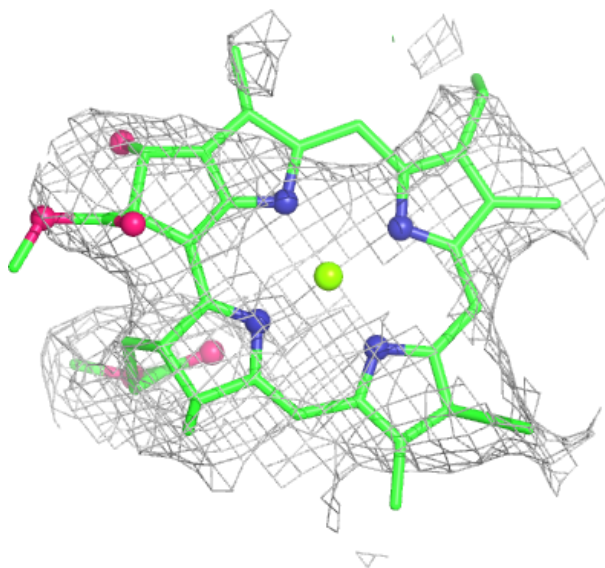
Electron density around CLA H 110:

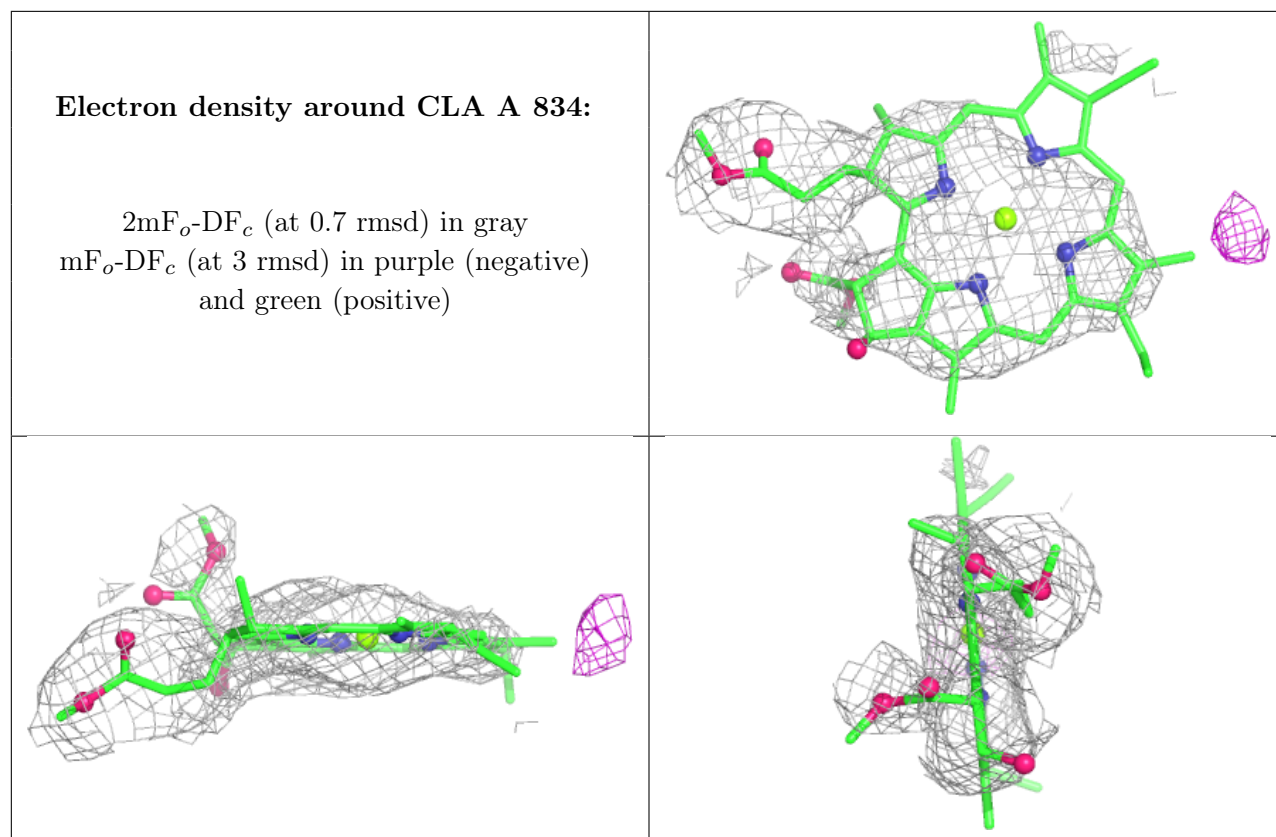
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around CLA A 807:

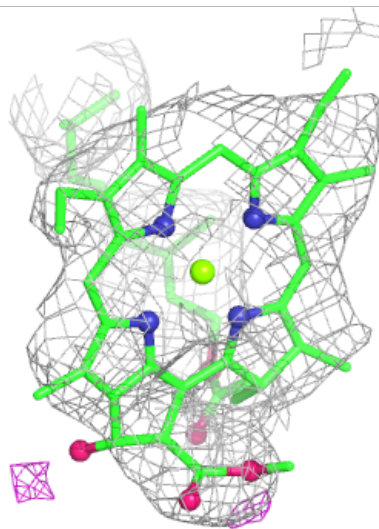
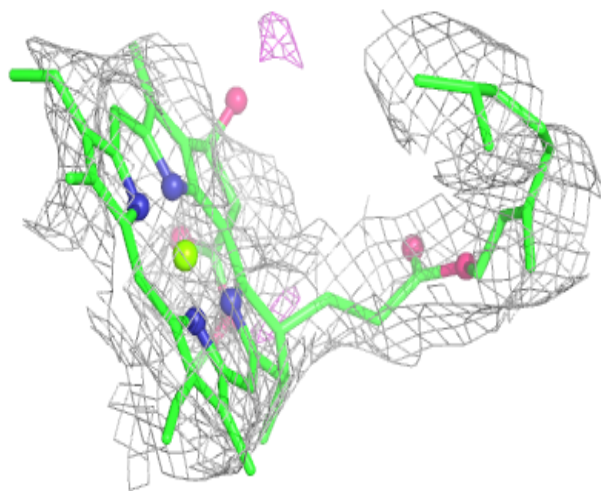
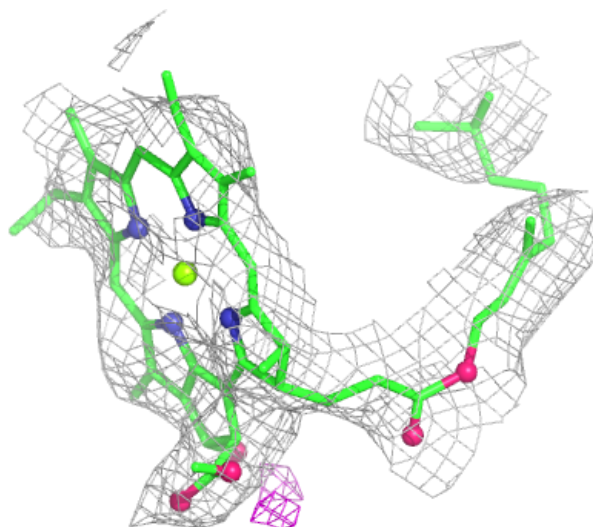
2mF_o-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





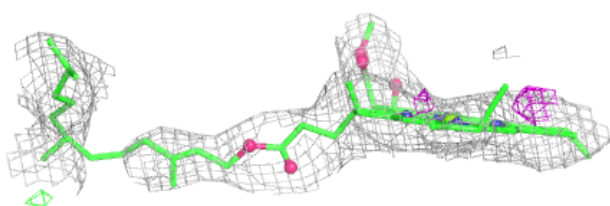
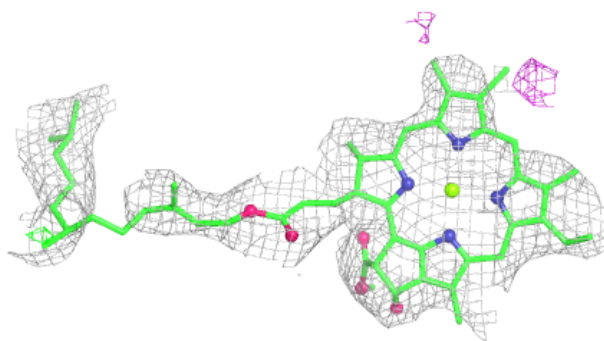
Electron density around CLA A 804:

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

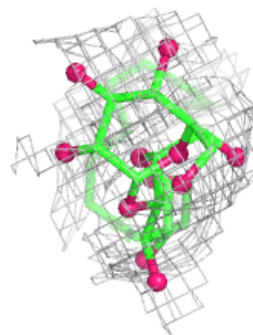
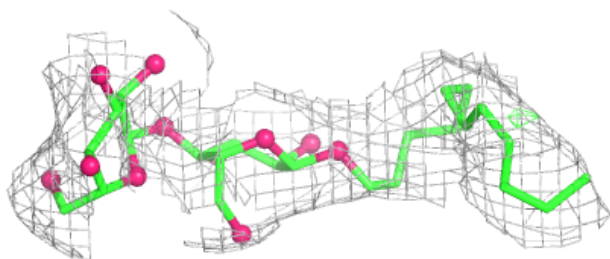
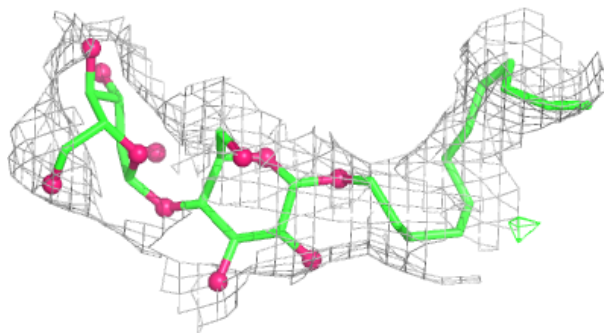


Electron density around CLA B 837:

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

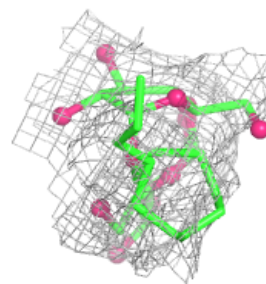
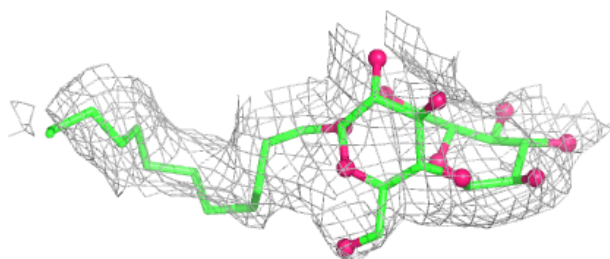
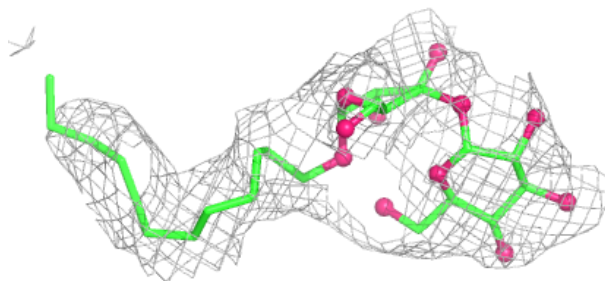
**Electron density around LMU R 109:**

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

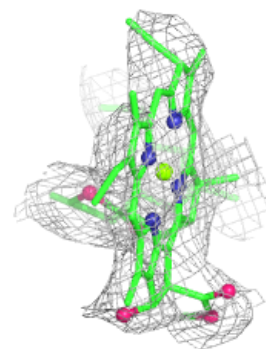
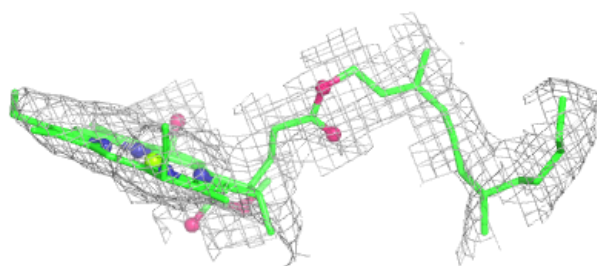
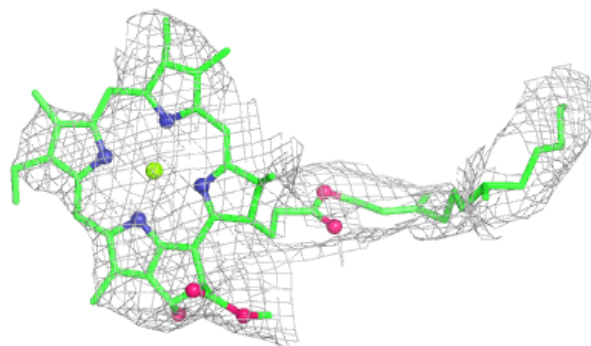


Electron density around LMU A 847:

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

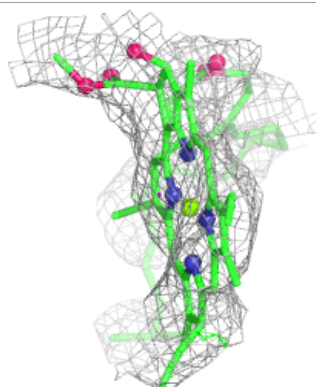
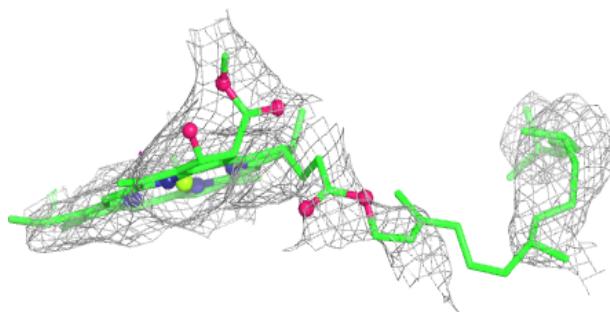
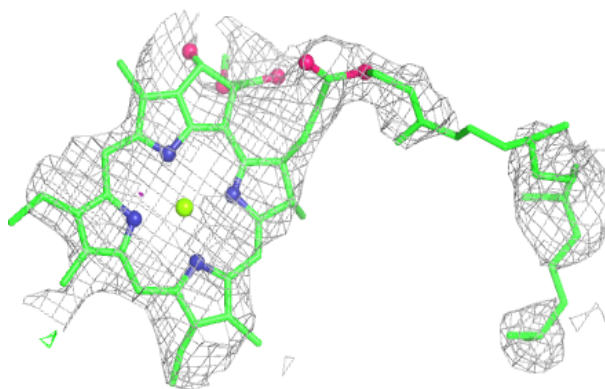
**Electron density around CLA A 824:**

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



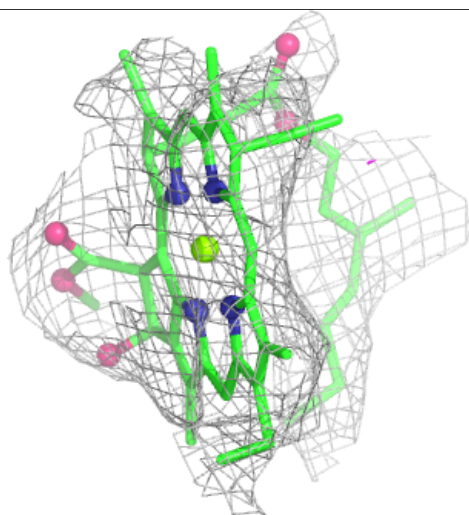
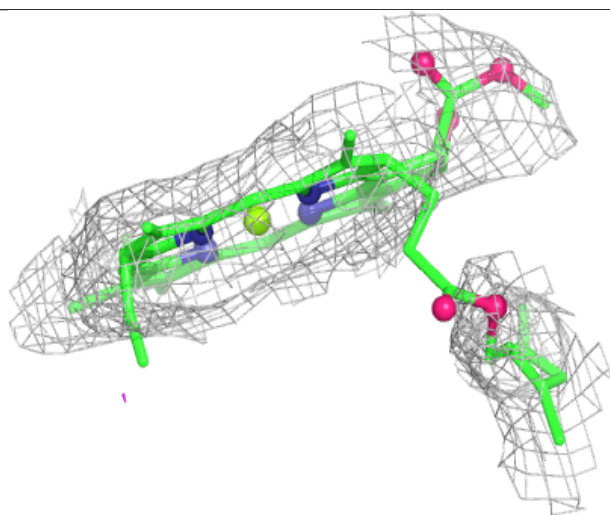
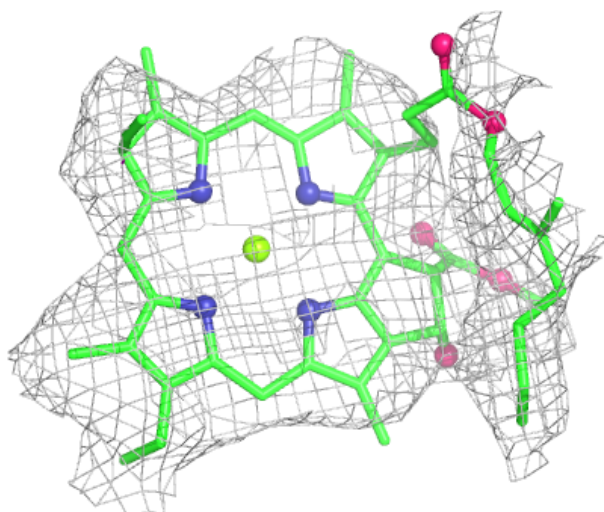
Electron density around CLA A 825:

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



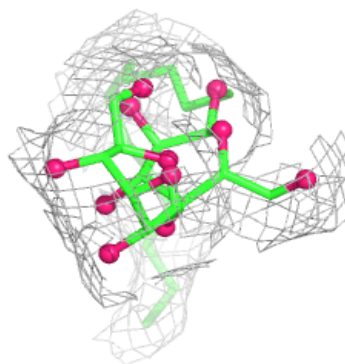
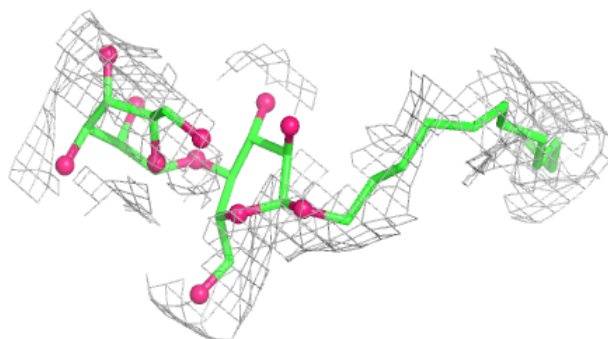
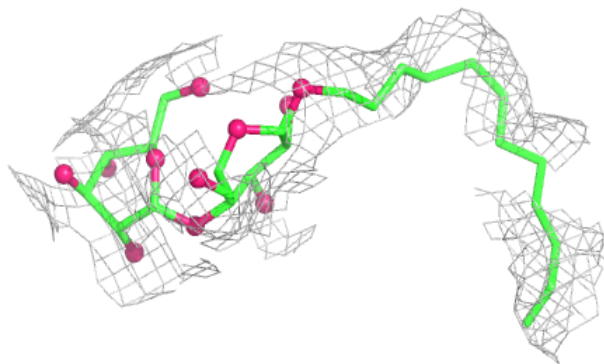
Electron density around CLA F 207:

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

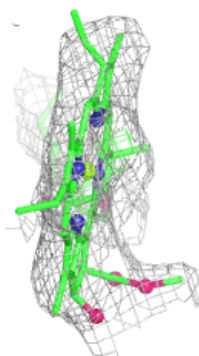
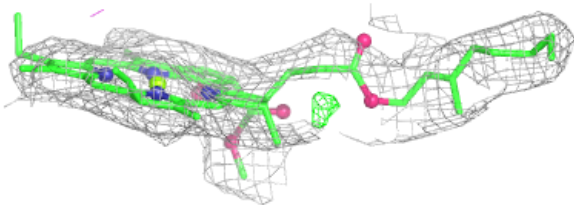
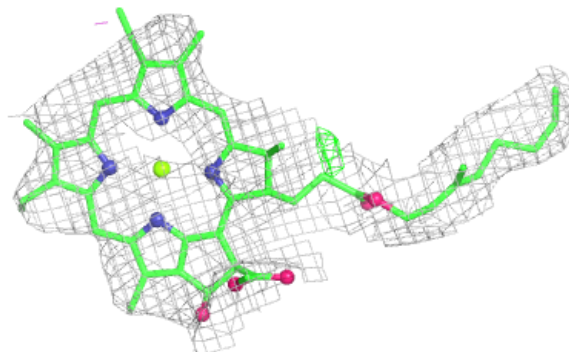


Electron density around LMU 2 318:

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

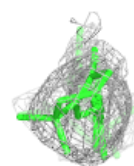
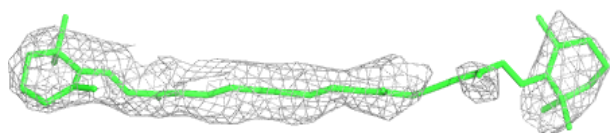
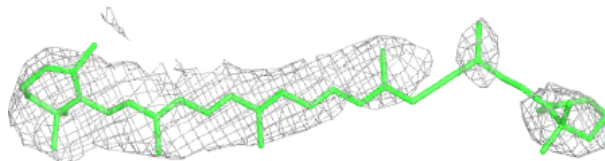
**Electron density around CLA A 805:**

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

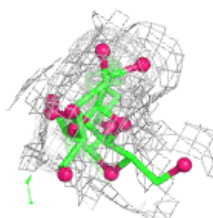
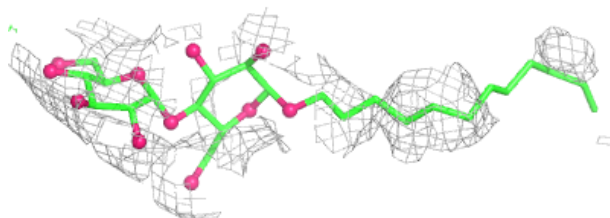
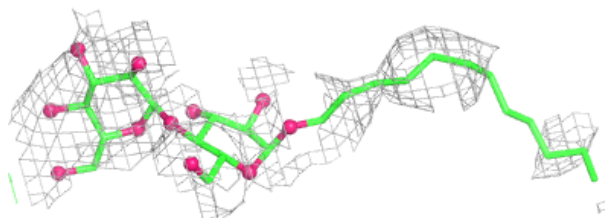


Electron density around BCR B 847:

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

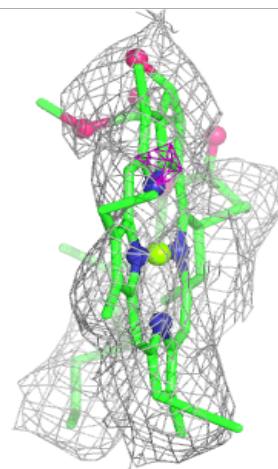
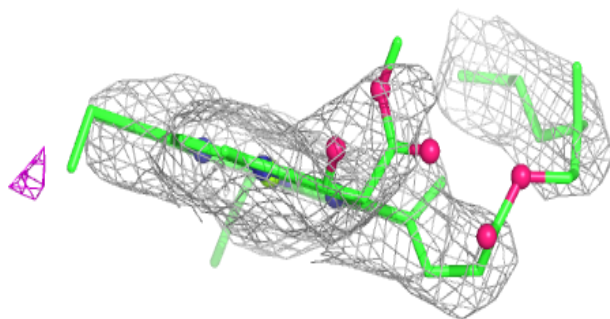
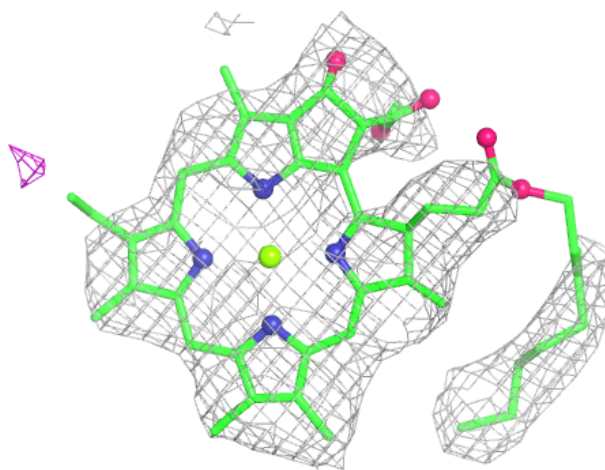
**Electron density around LMU B 805:**

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



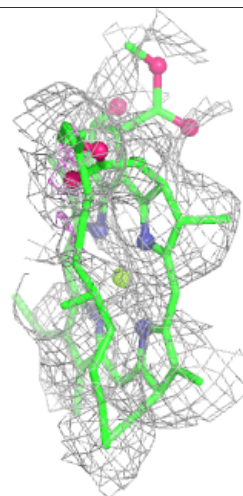
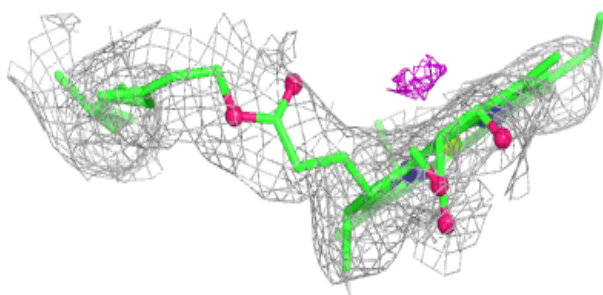
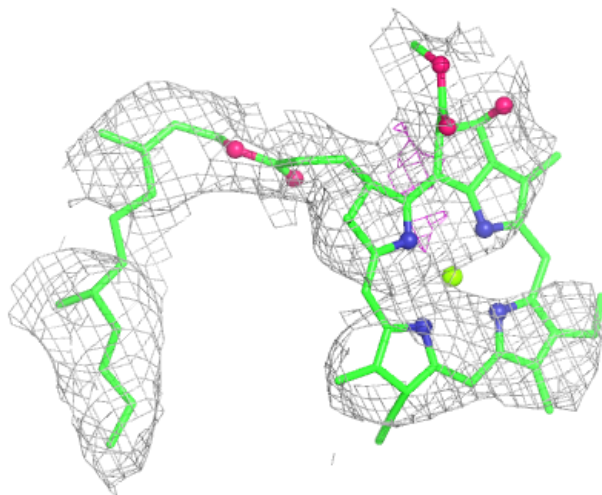
Electron density around CLA B 825:

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



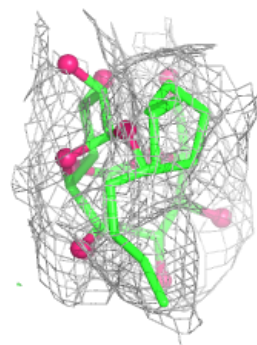
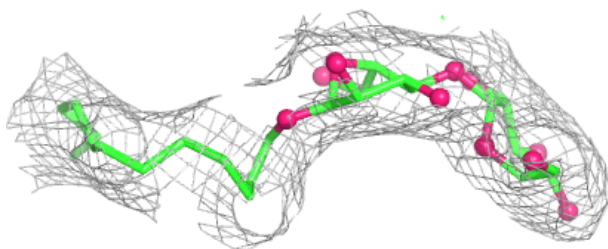
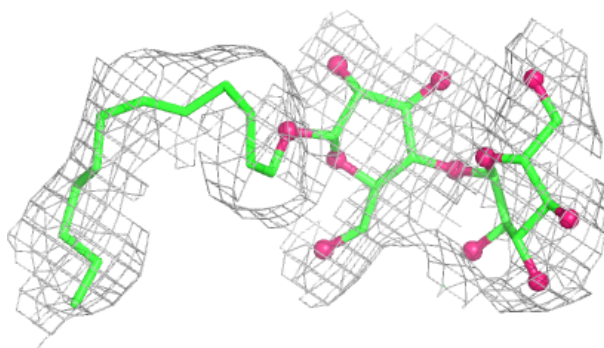
Electron density around CLA B 826:

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

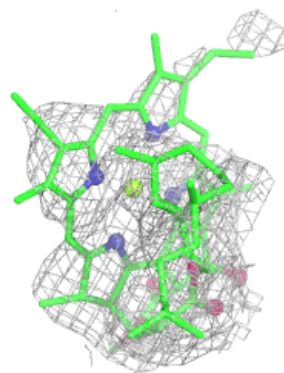
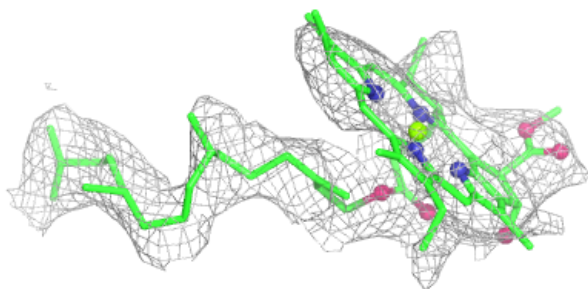
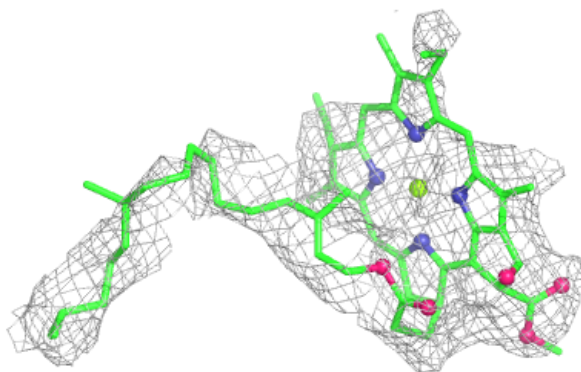


Electron density around LMU D 201:

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

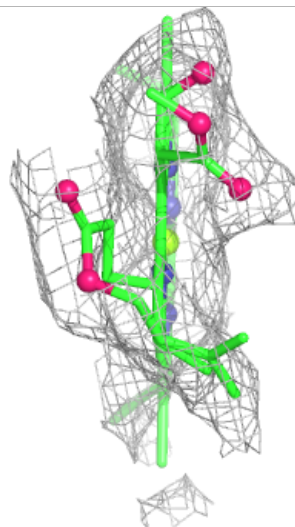
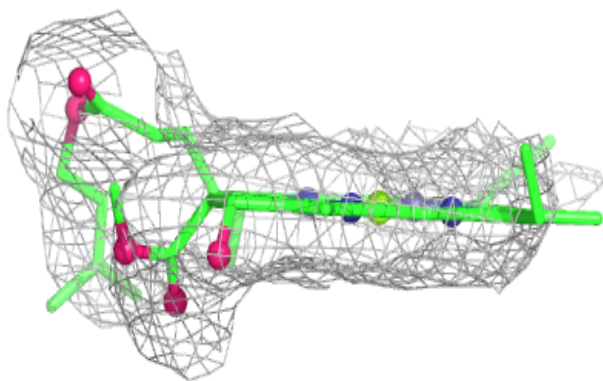
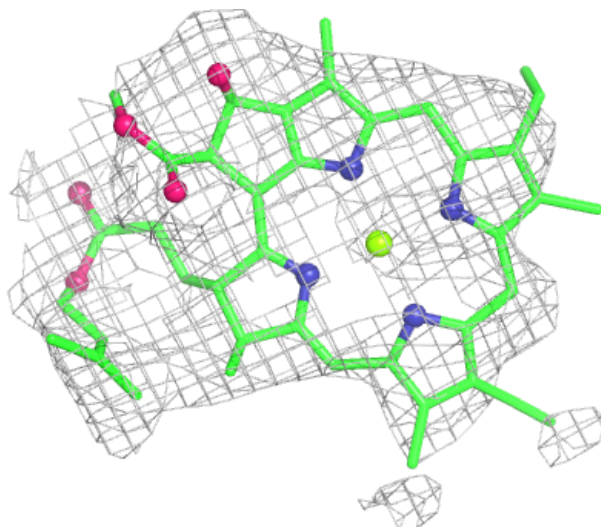
**Electron density around CLA L 203:**

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



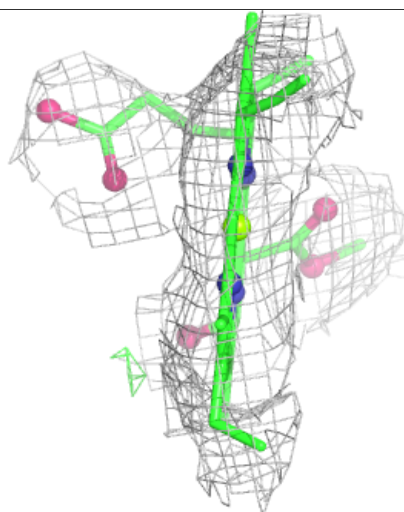
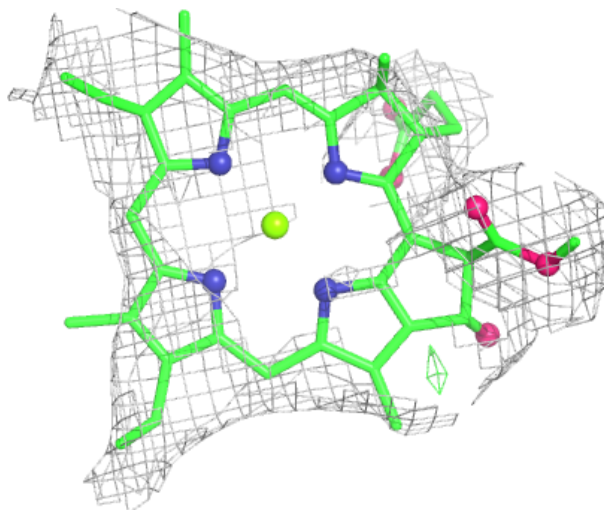
Electron density around CLA 2 314:

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



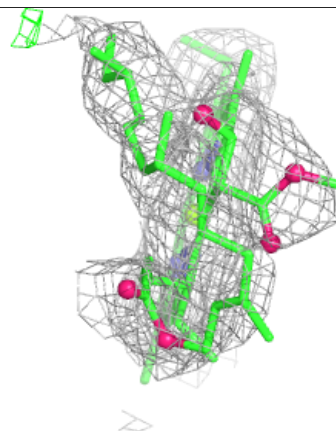
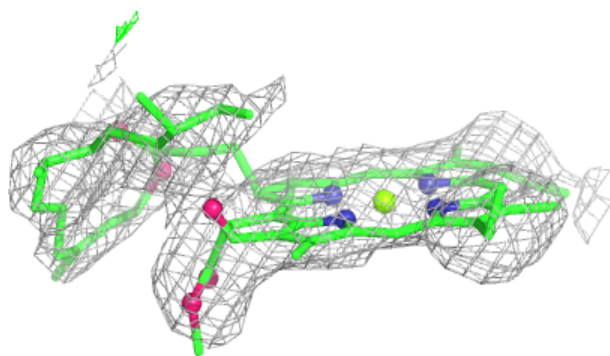
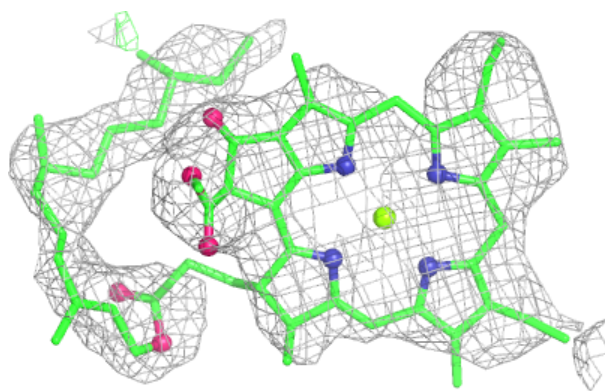
Electron density around CLA B 807:

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



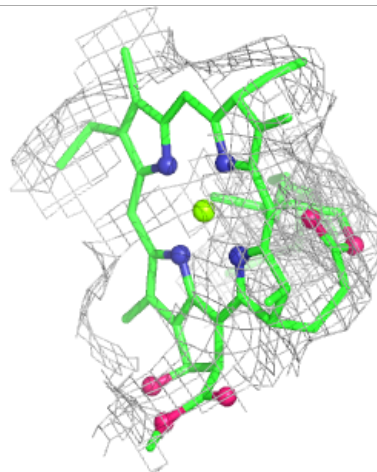
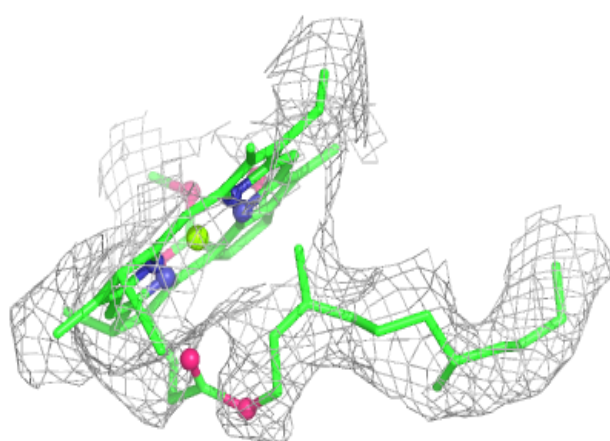
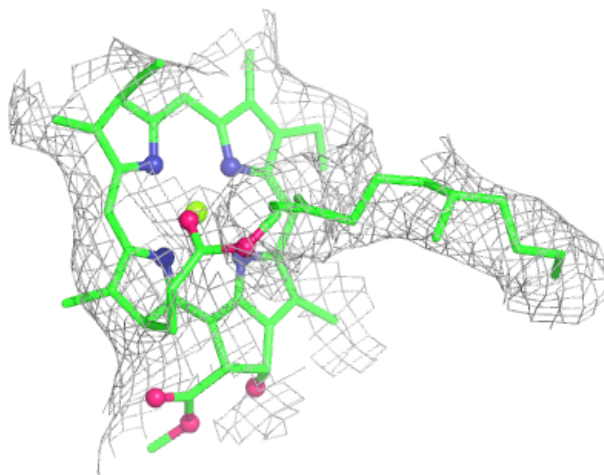
Electron density around CLA B 808:

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



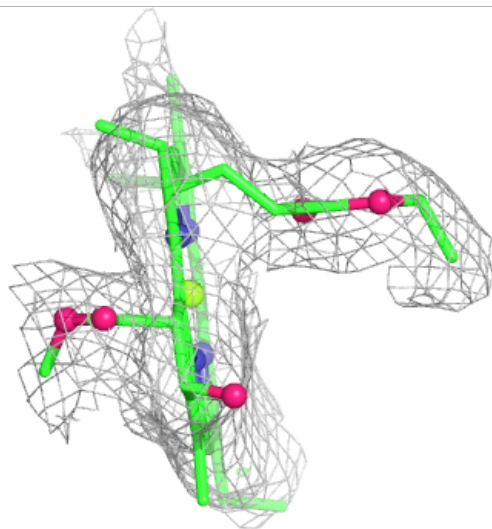
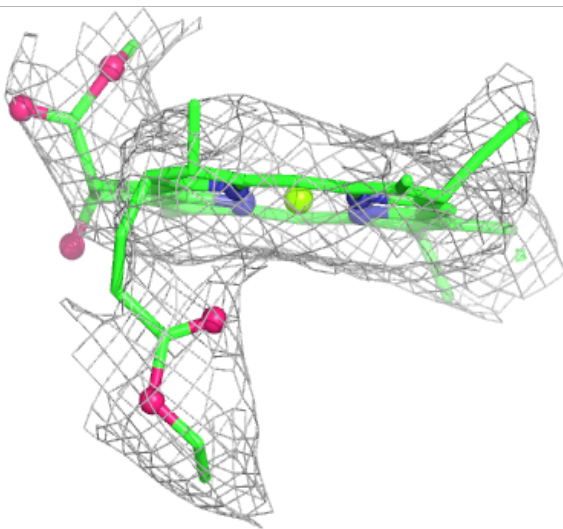
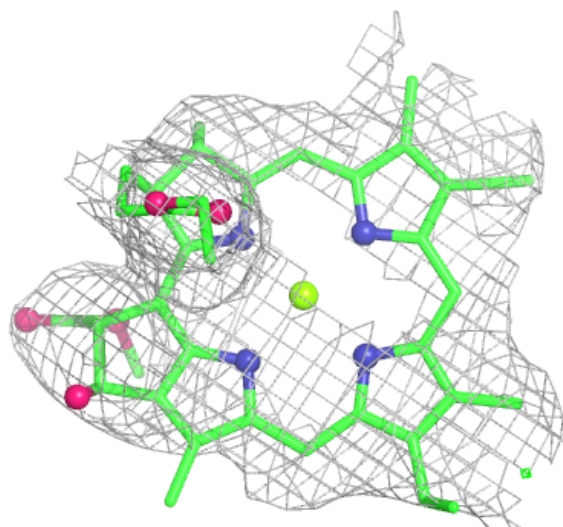
Electron density around CLA 2 303:

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



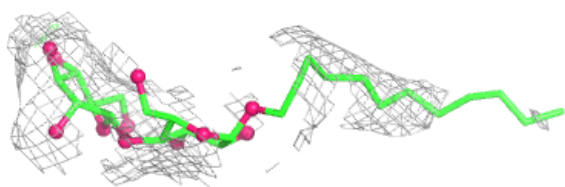
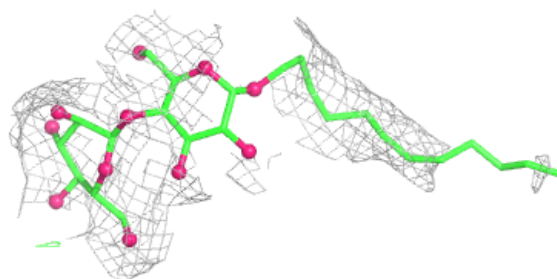
Electron density around CLA L 207:

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

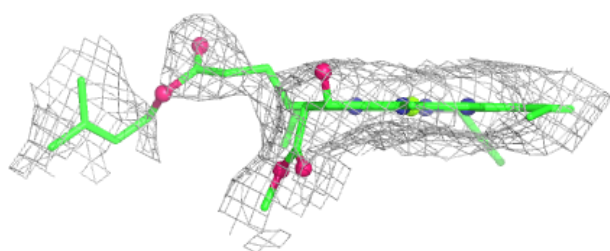
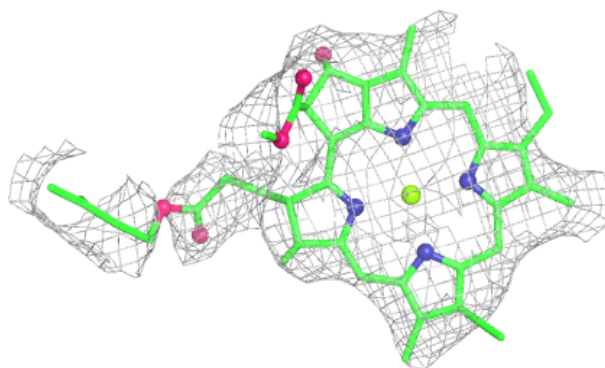


Electron density around LMU A 855:

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

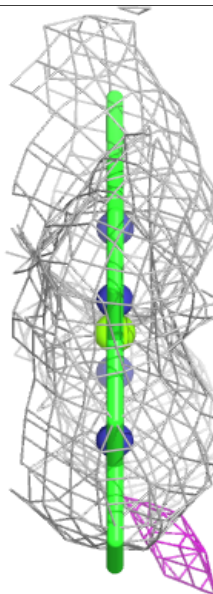
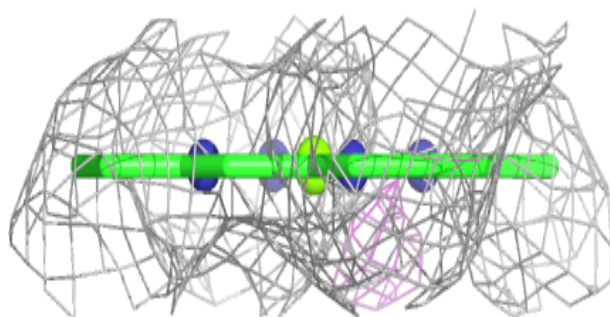
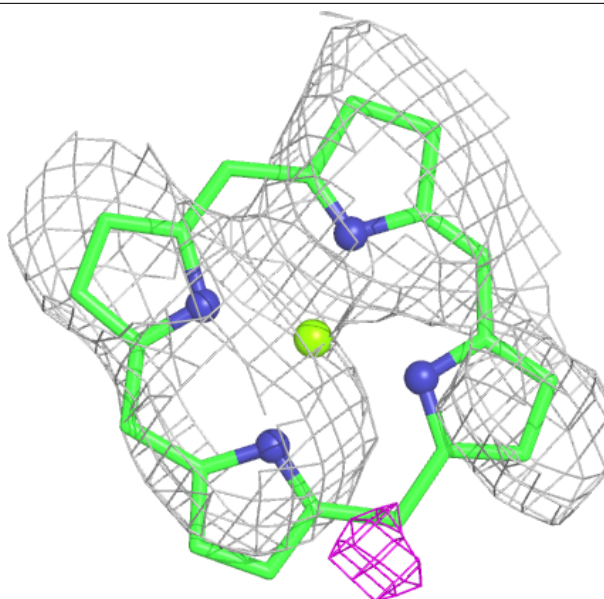
**Electron density around CLA F 201:**

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



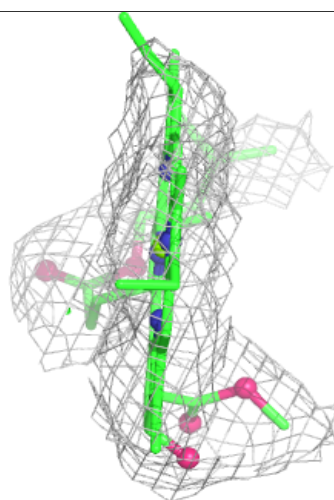
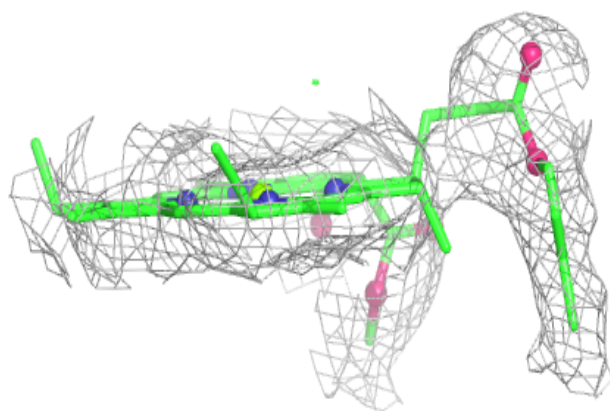
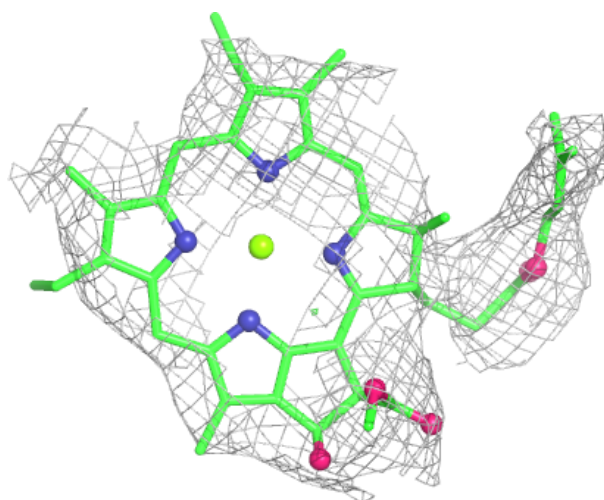
Electron density around CLA 2 304:

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



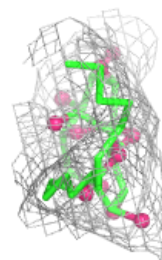
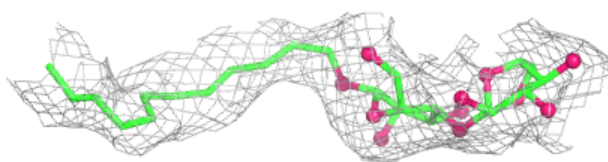
Electron density around CLA A 813:

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



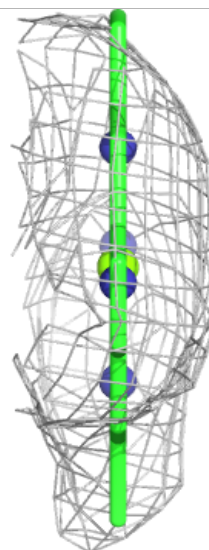
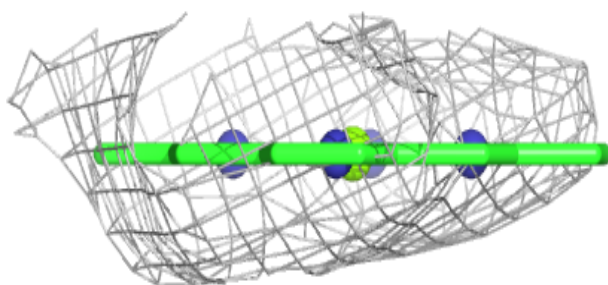
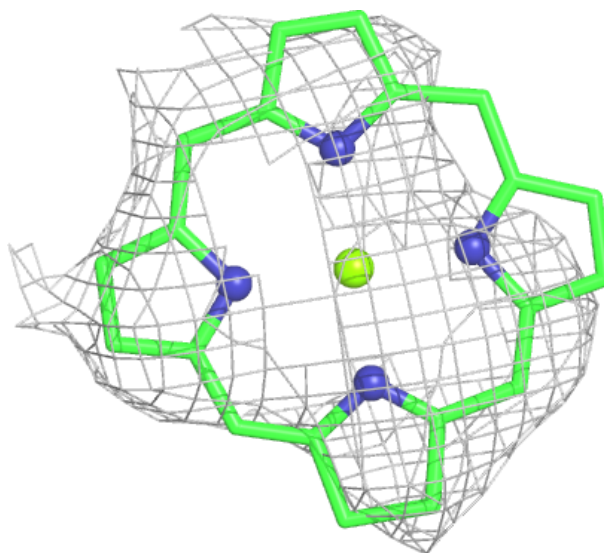
Electron density around LMU 1 216:

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



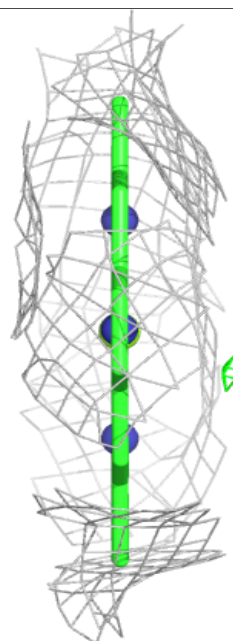
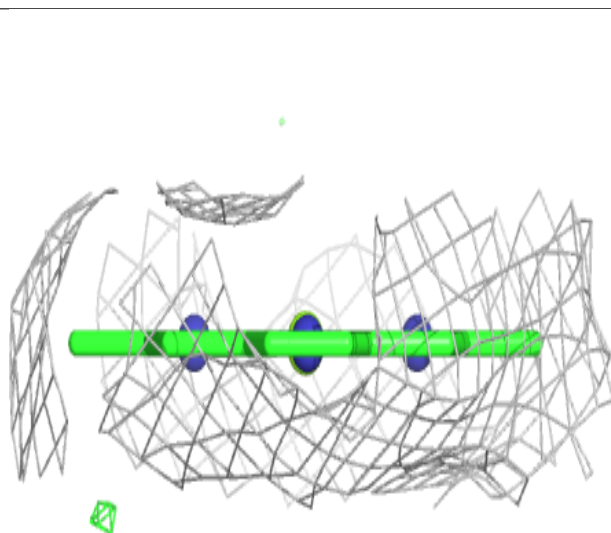
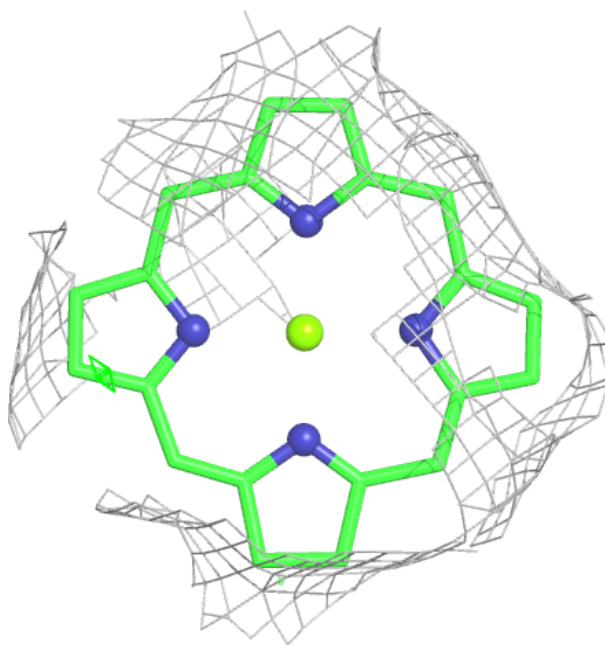
Electron density around CLA 4 309:

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



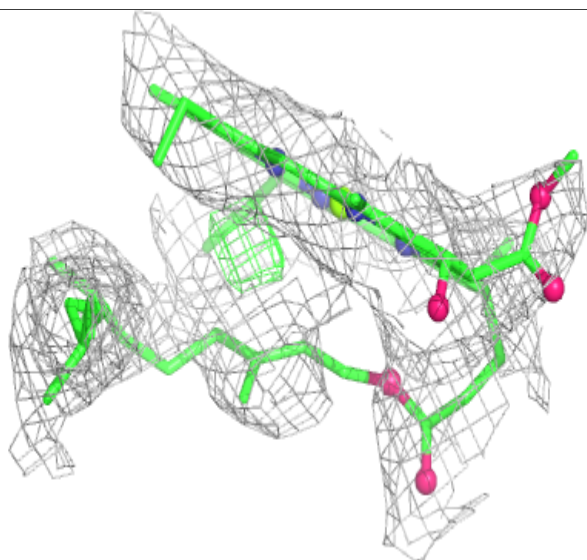
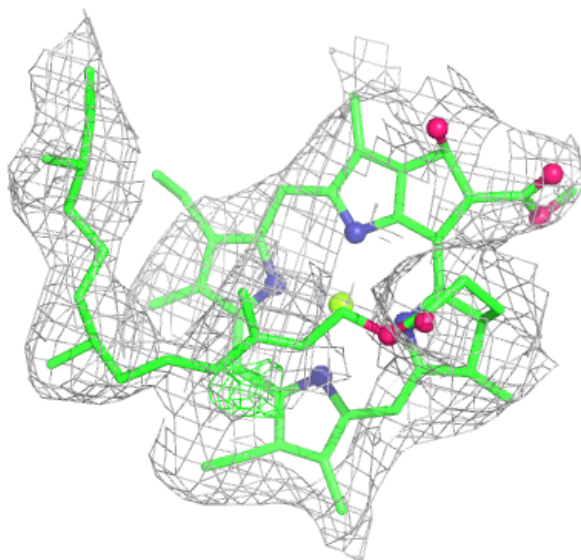
Electron density around CLA 3 308:

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



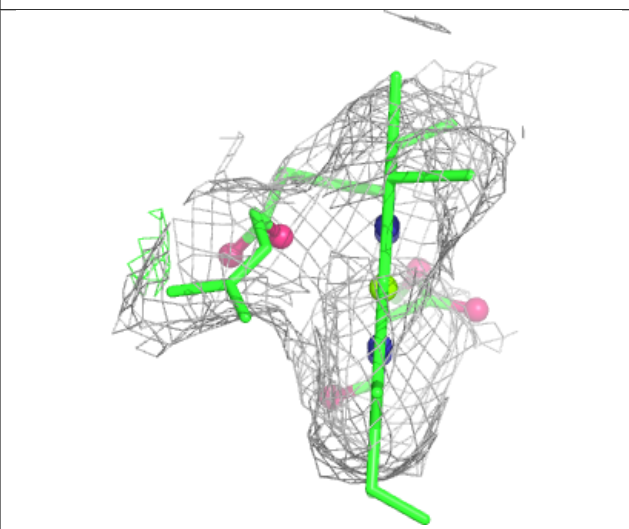
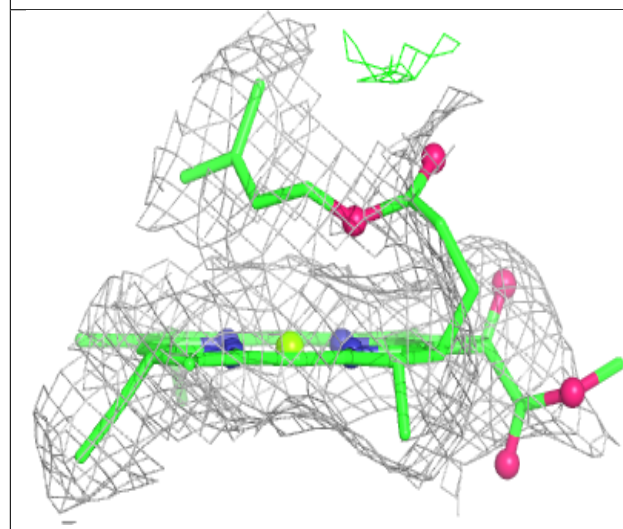
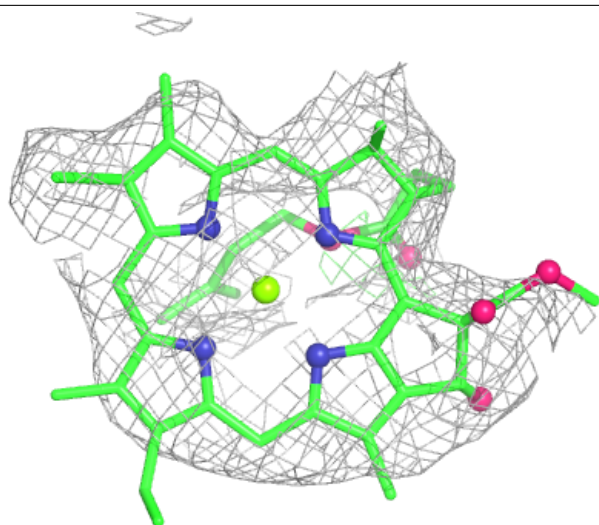
Electron density around CLA B 820:

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



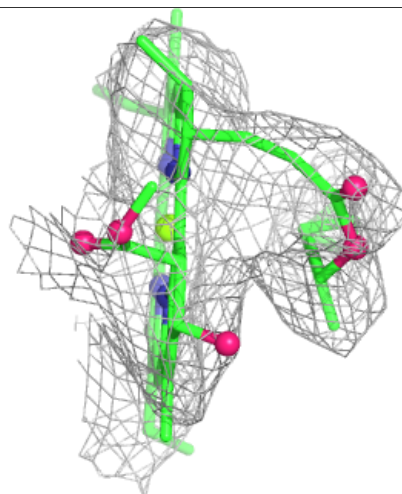
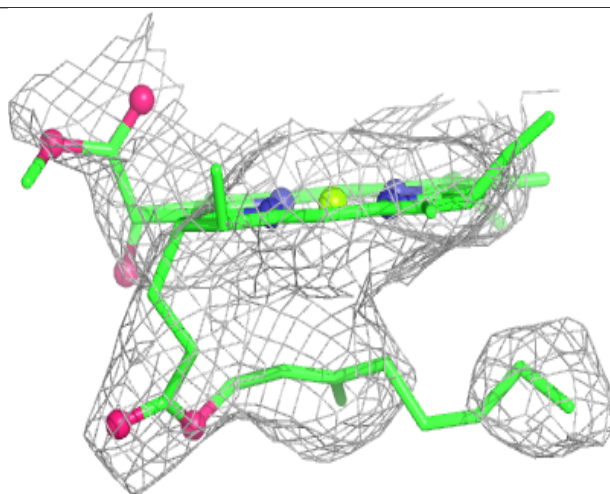
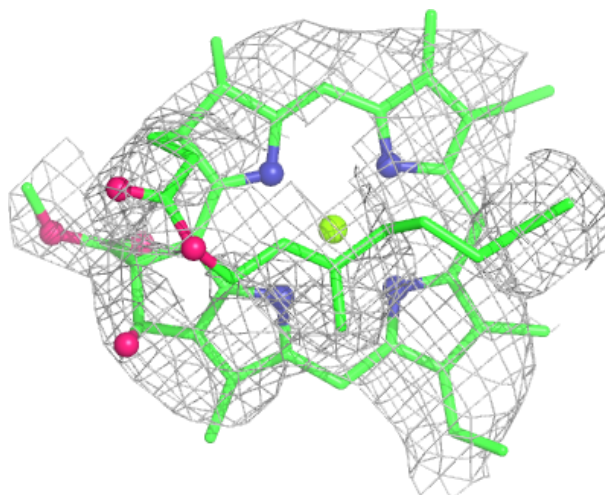
Electron density around CLA B 821:

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



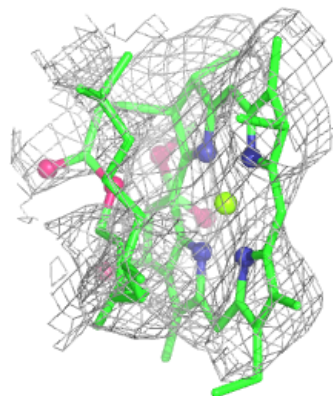
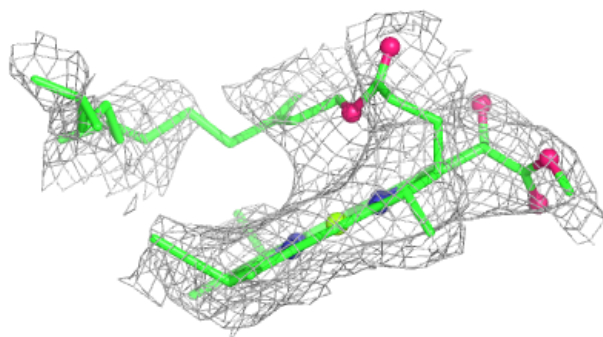
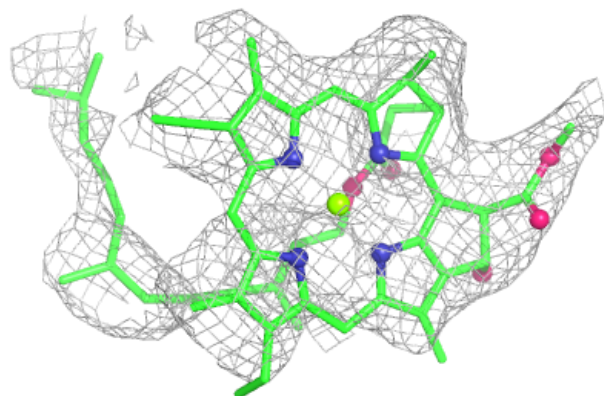
Electron density around CLA A 816:

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



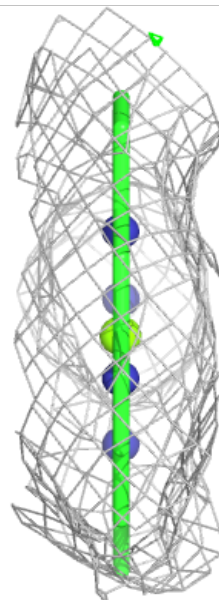
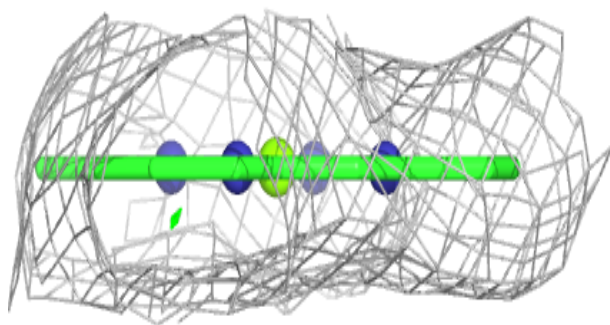
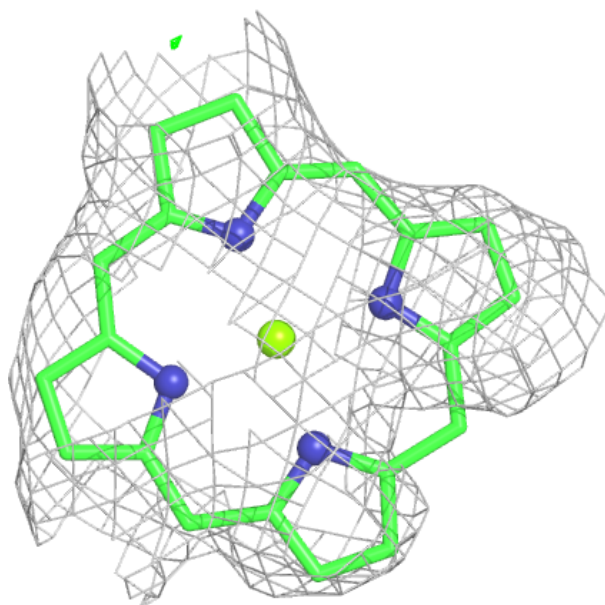
Electron density around CLA I 102:

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



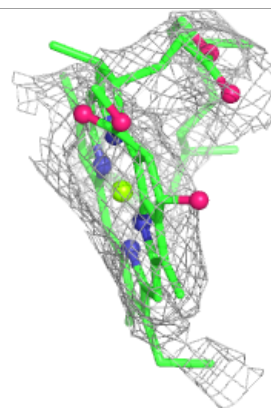
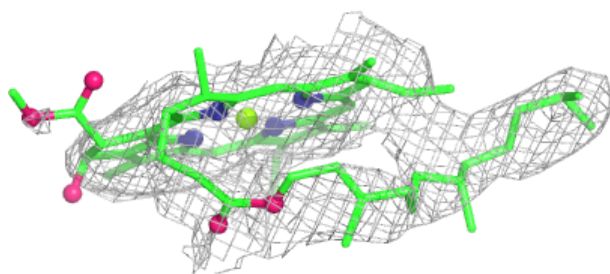
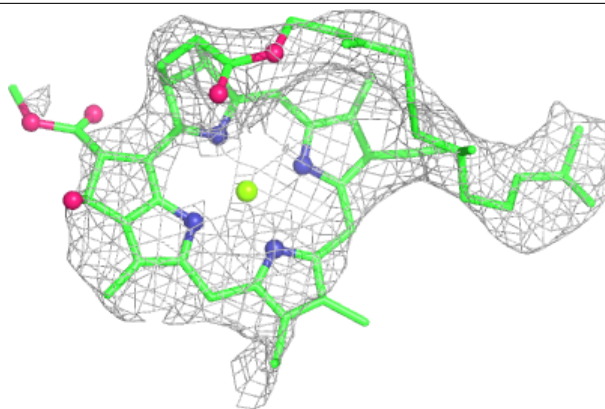
Electron density around CLA 2 315:

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

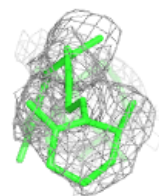
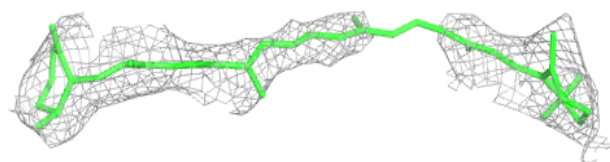
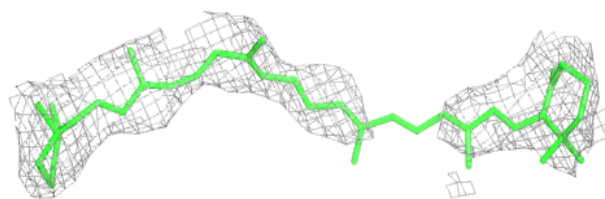


Electron density around CLA A 818:

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

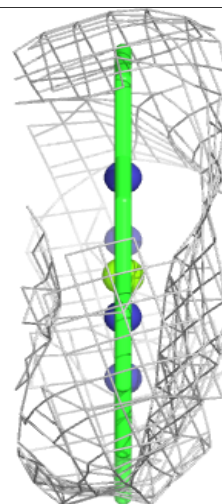
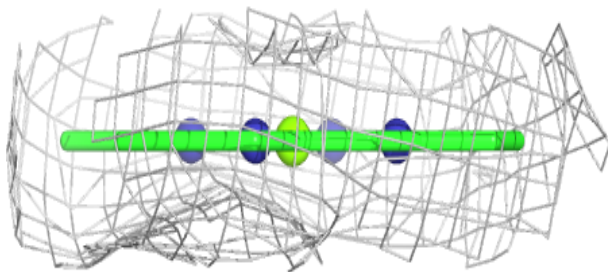
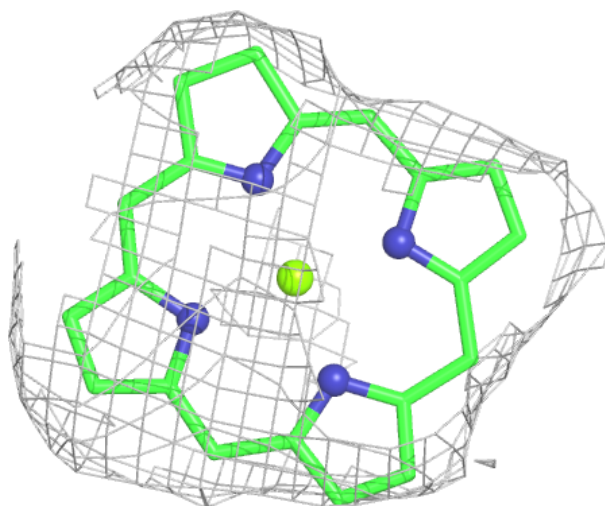
**Electron density around BCR I 101:**

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



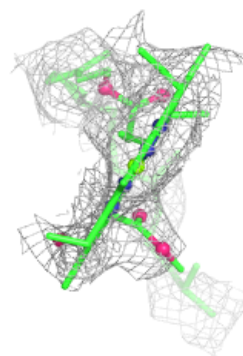
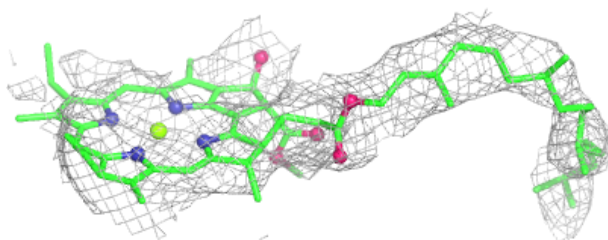
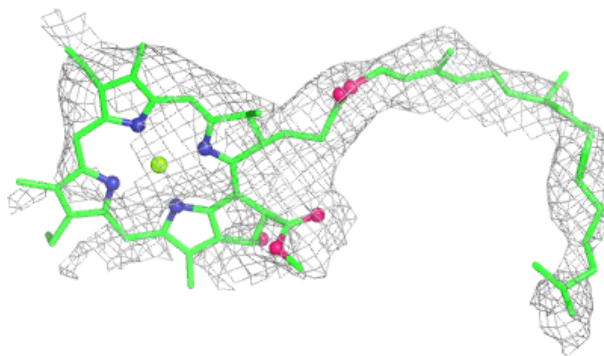
Electron density around CLA 3 304:

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



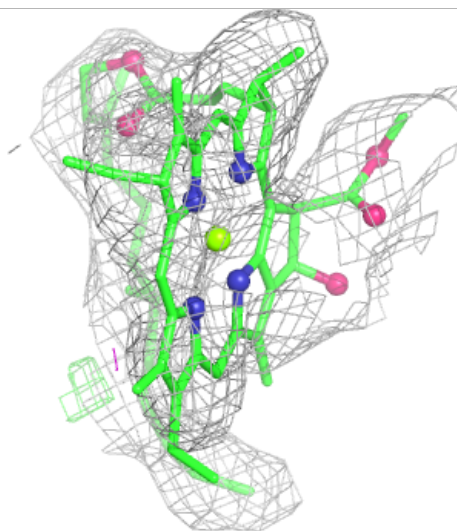
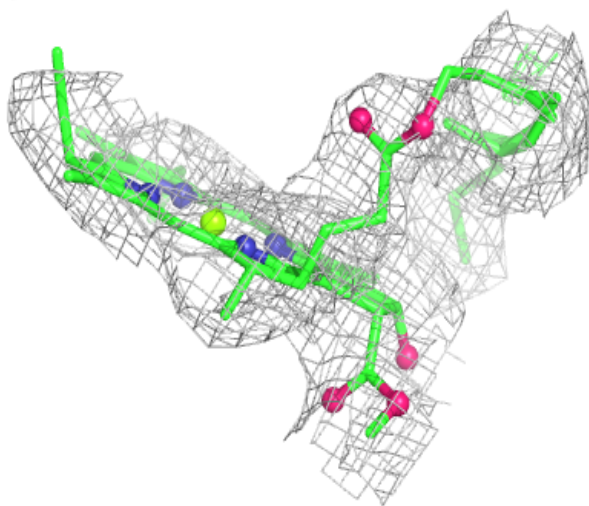
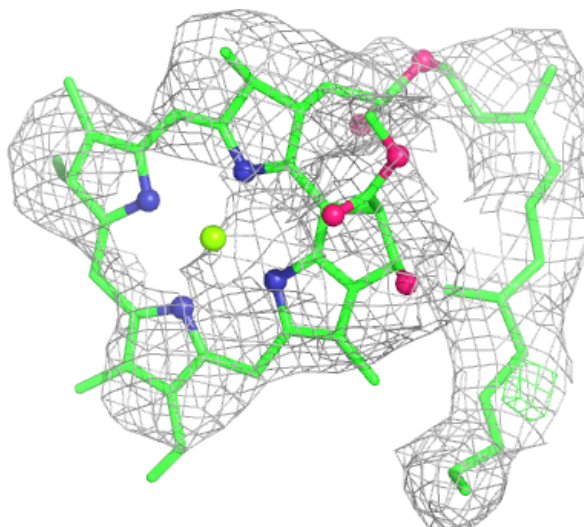
Electron density around CLA B 827:

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



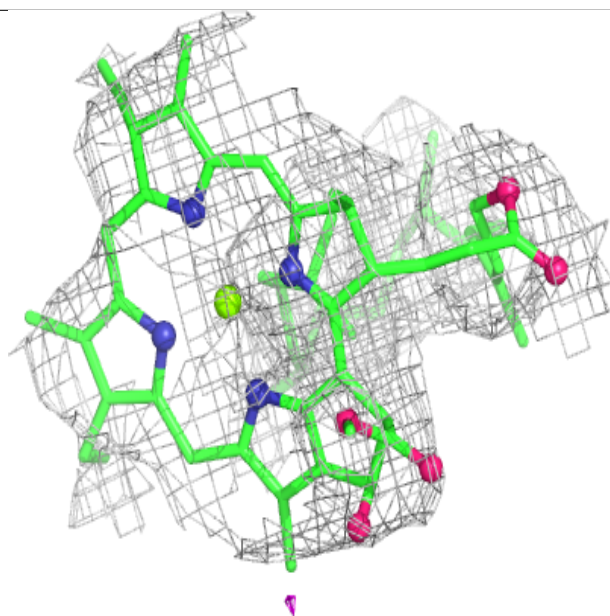
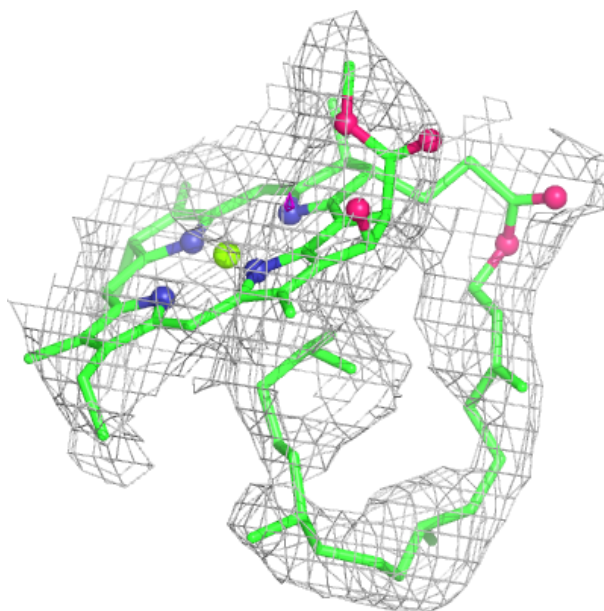
Electron density around CLA B 832:

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



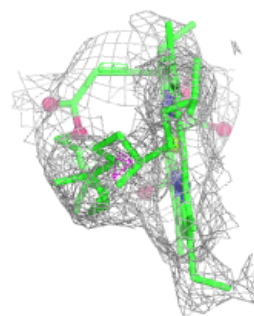
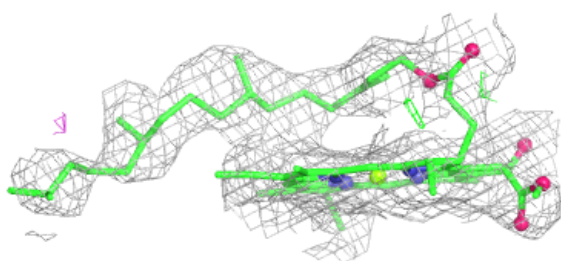
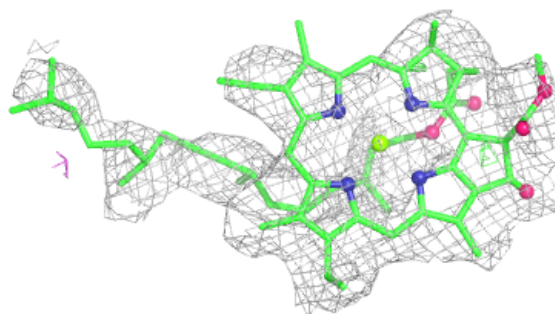
Electron density around CLA 2 316:

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



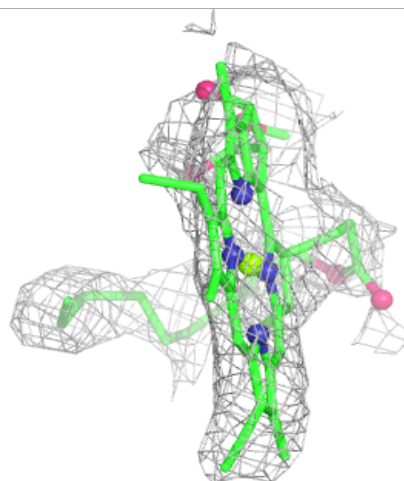
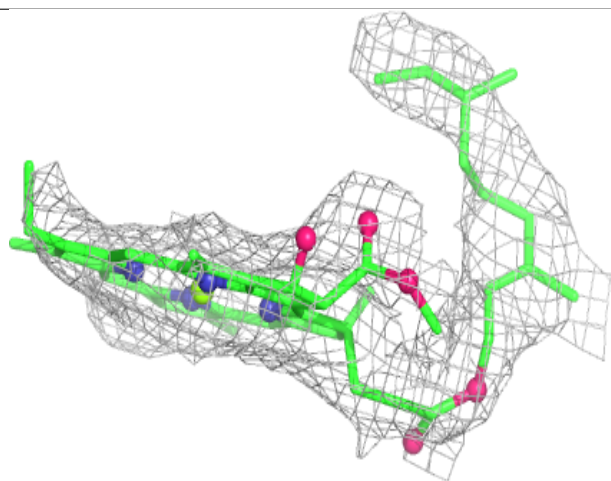
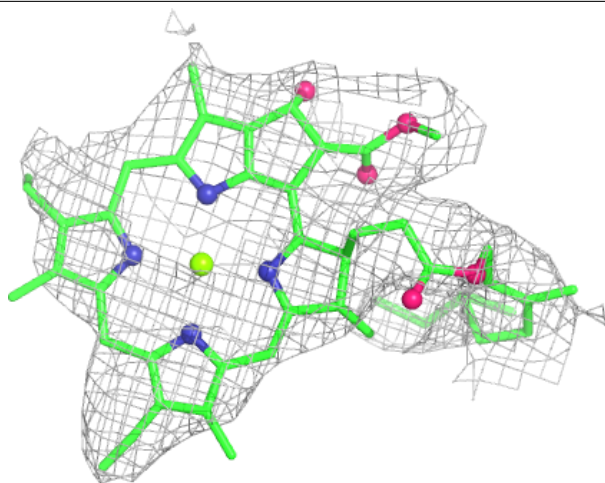
Electron density around CLA B 806:

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



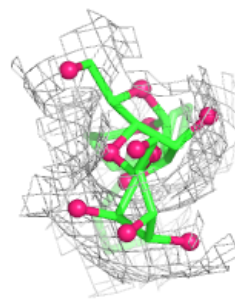
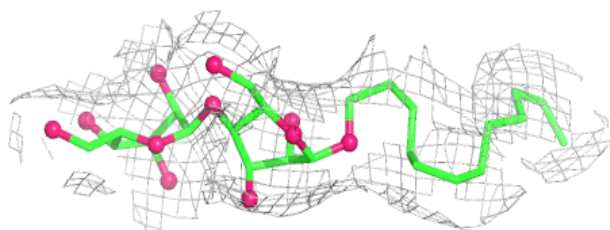
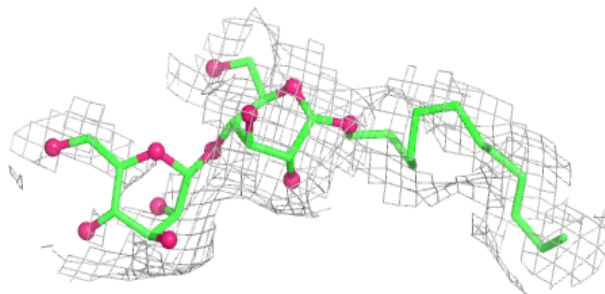
Electron density around CLA A 806:

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



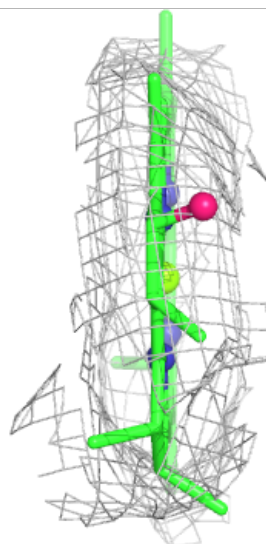
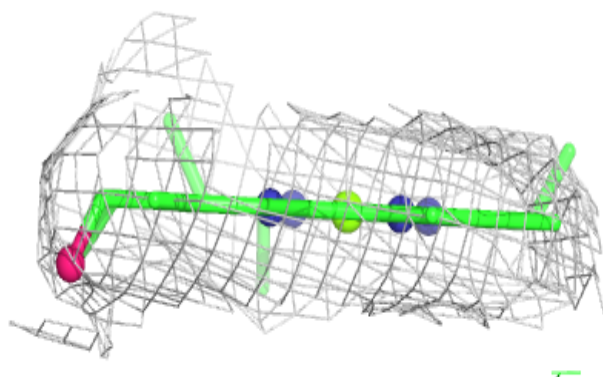
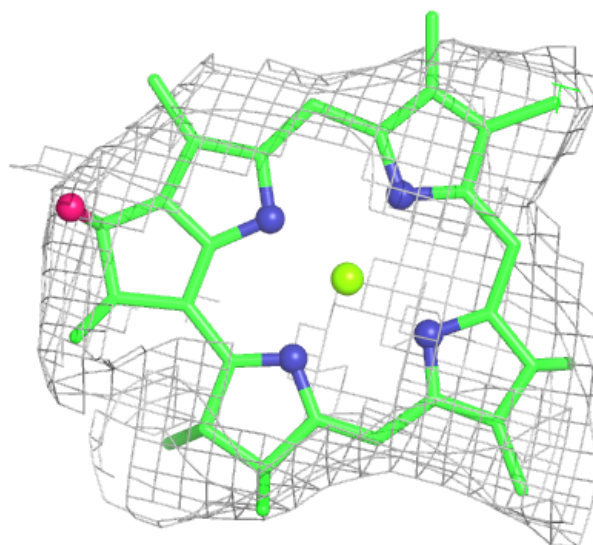
Electron density around LMU 3 319:

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



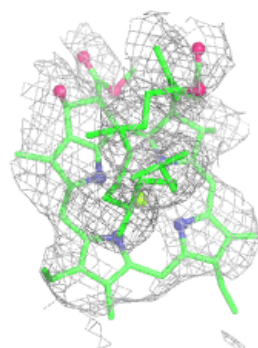
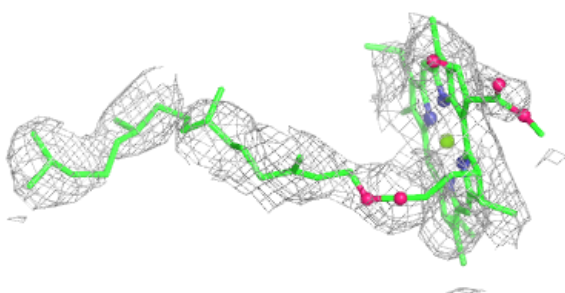
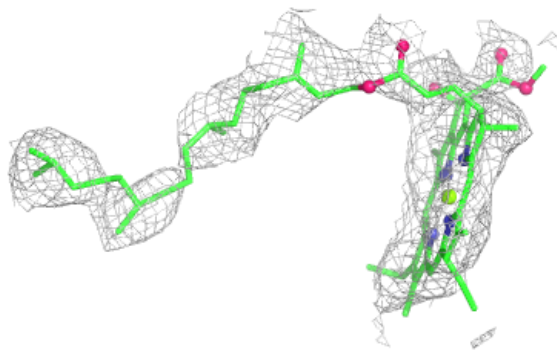
Electron density around CLA 4 313:

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

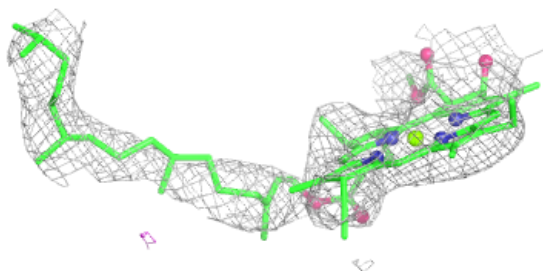
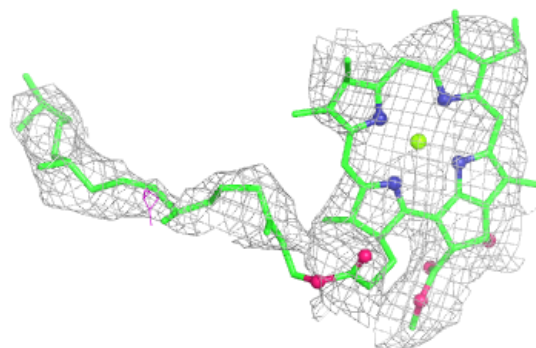


Electron density around CLA A 828:

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

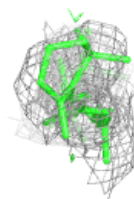
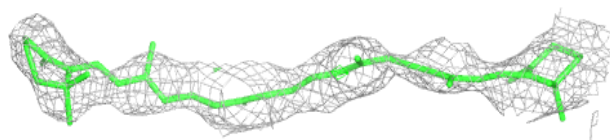
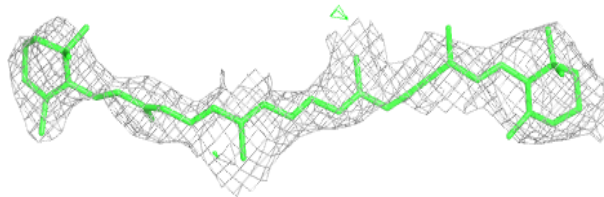
**Electron density around CLA A 851:**

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



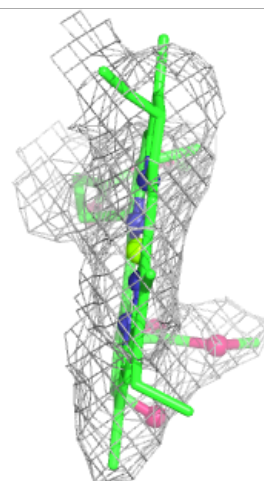
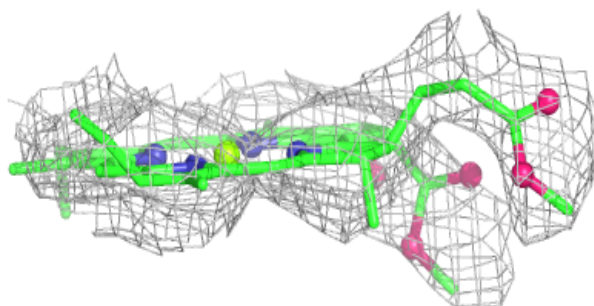
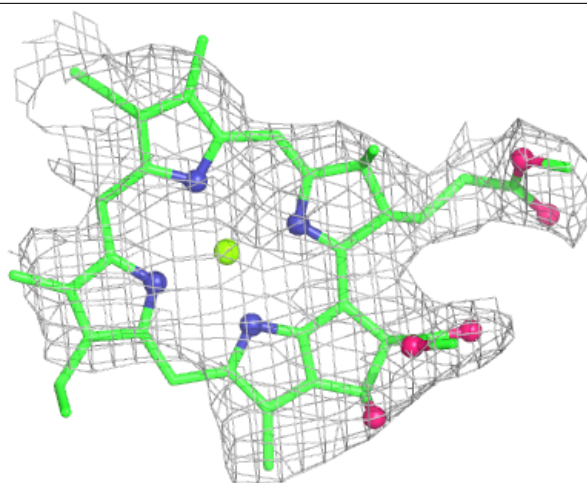
Electron density around BCR B 846:

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



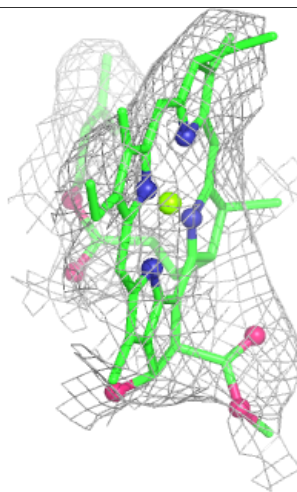
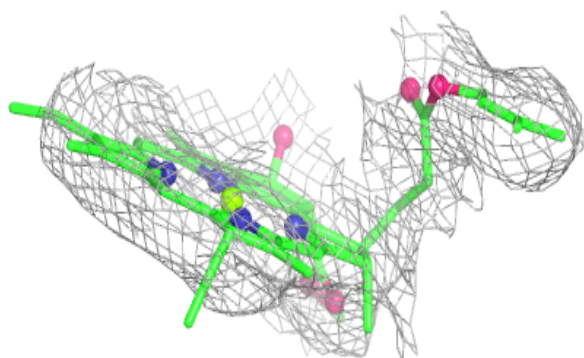
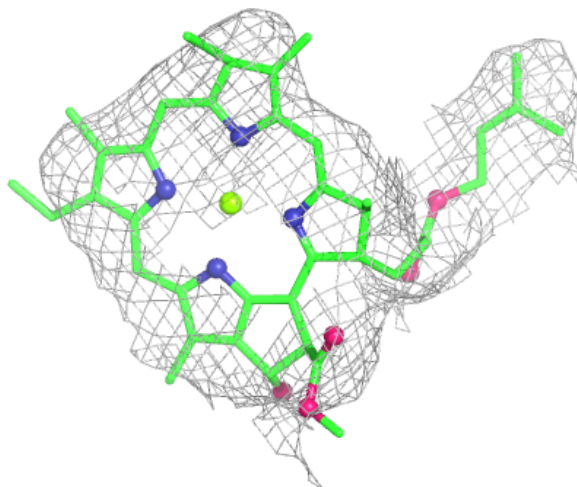
Electron density around CLA A 803:

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



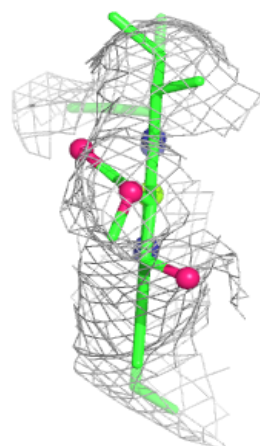
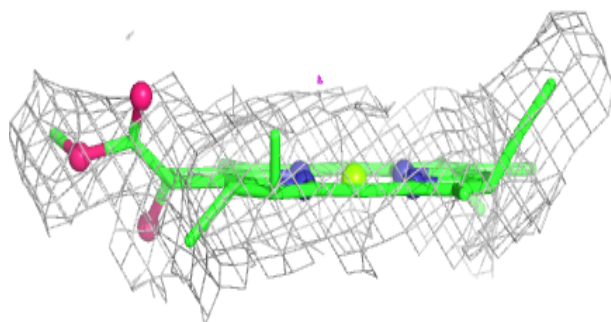
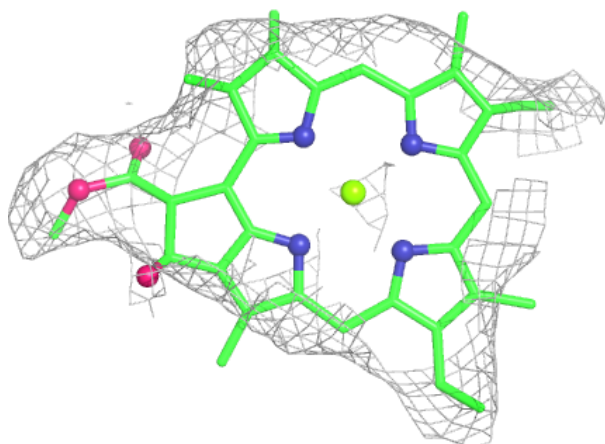
Electron density around CLA A 832:

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



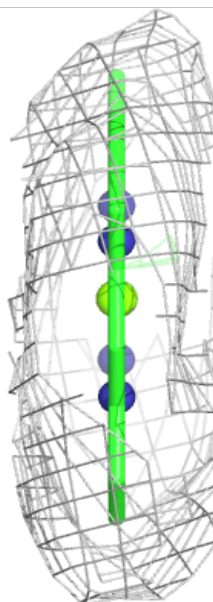
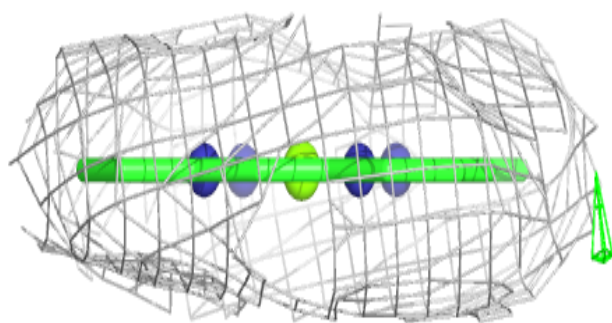
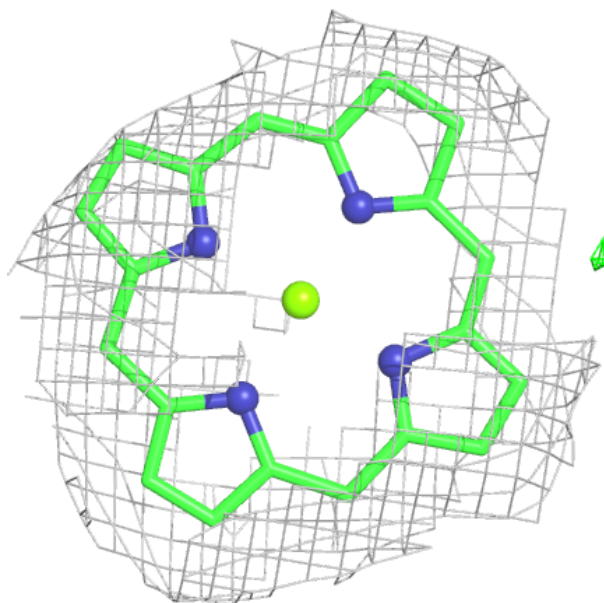
Electron density around CLA 1 202:

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



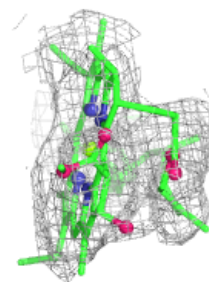
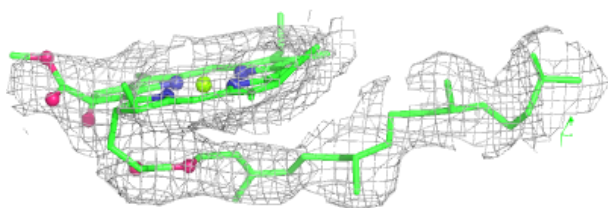
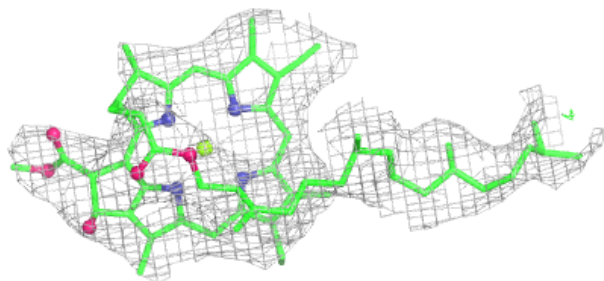
Electron density around CLA 4 312:

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

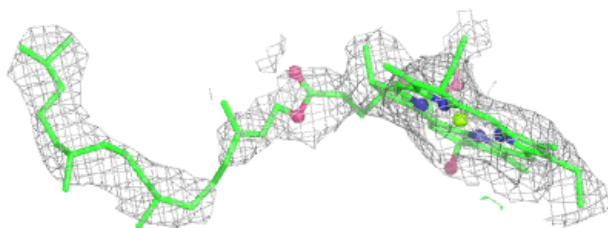
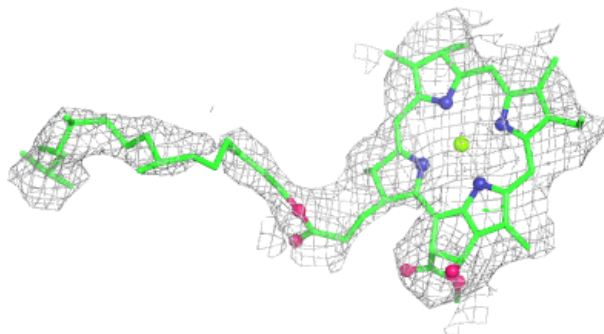


Electron density around CLA A 835:

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

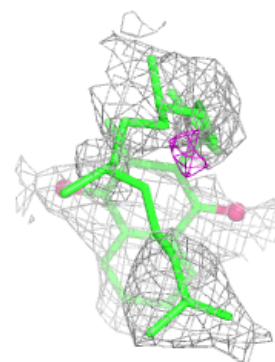
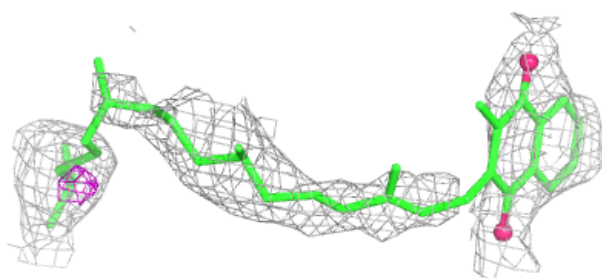
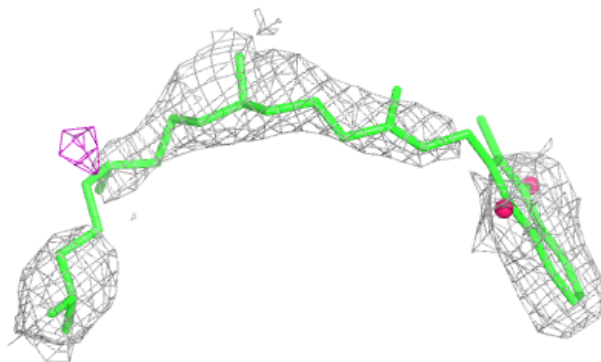
**Electron density around CLA B 814:**

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

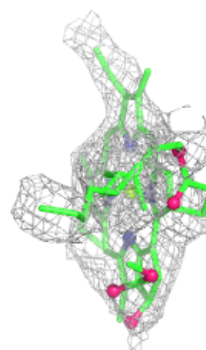
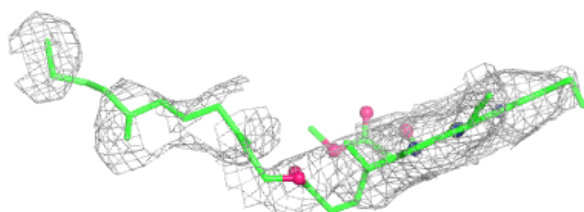
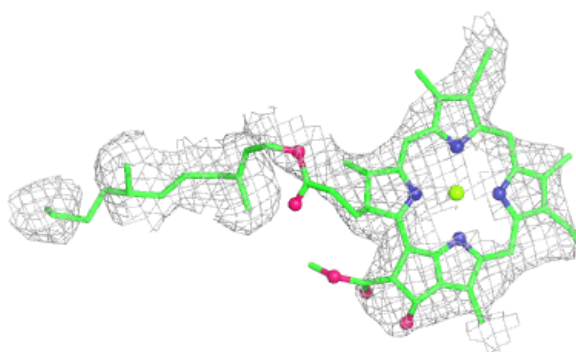


Electron density around PQN B 843:

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

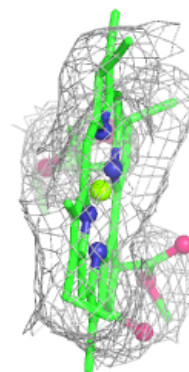
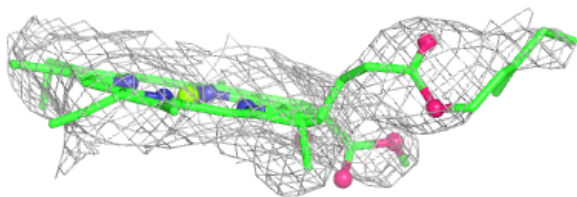
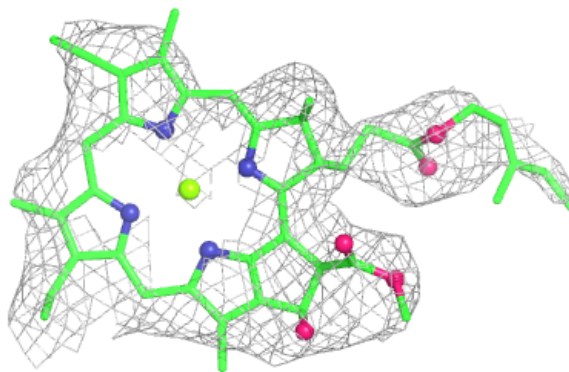
**Electron density around CLA H 108:**

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

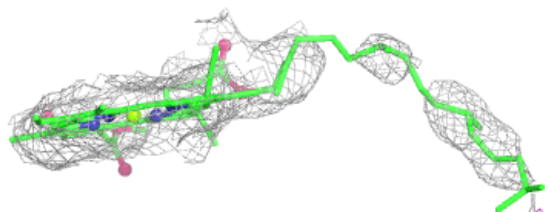
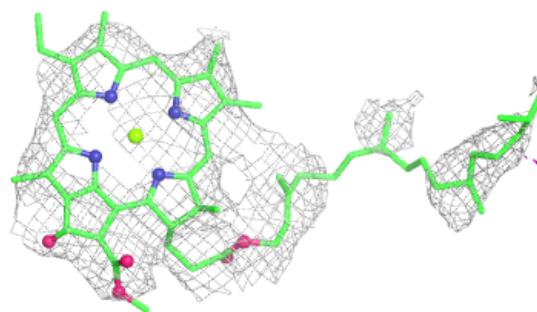


Electron density around CLA A 837:

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

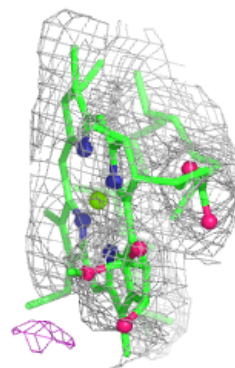
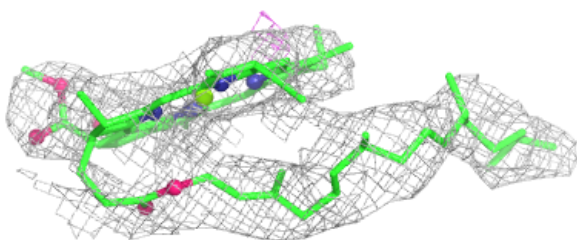
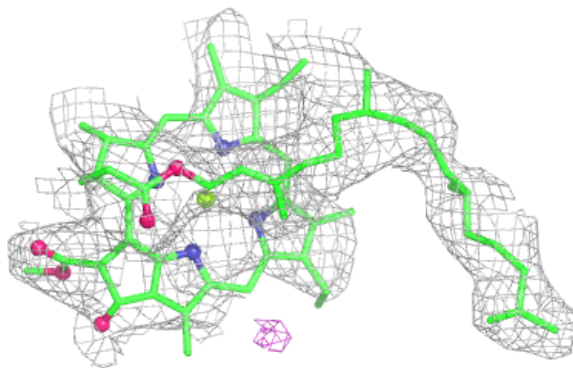
**Electron density around CLA B 803:**

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

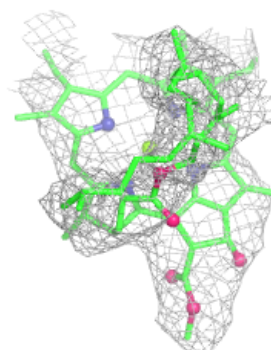
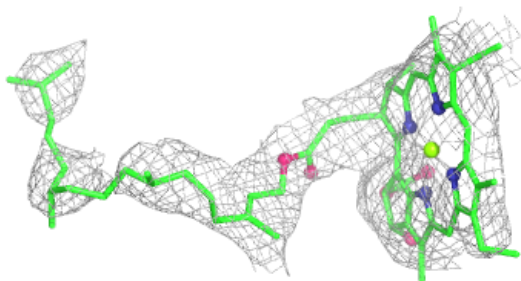
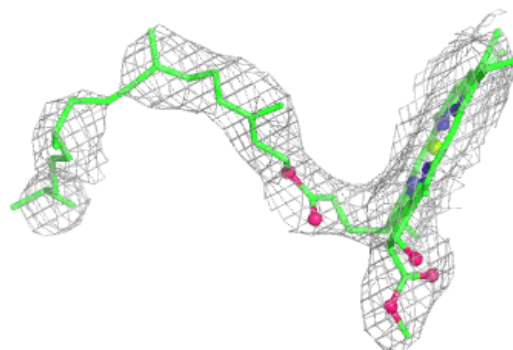


Electron density around CLA B 838:

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

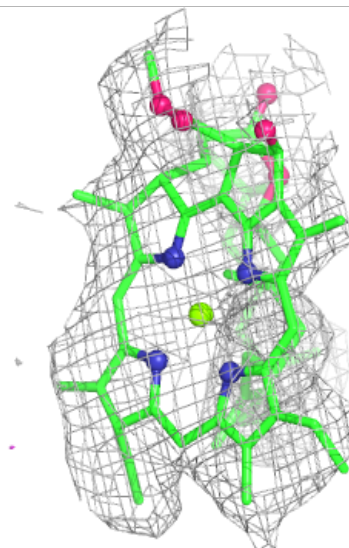
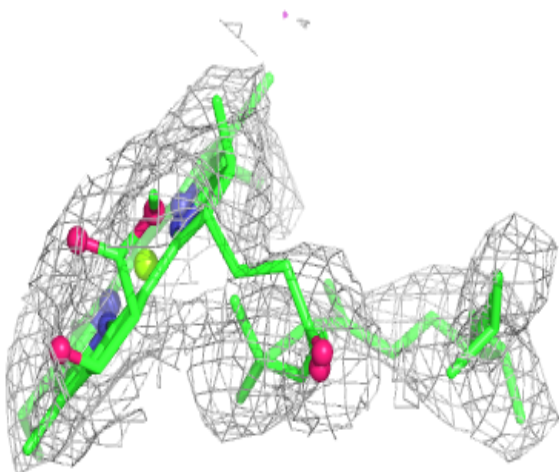
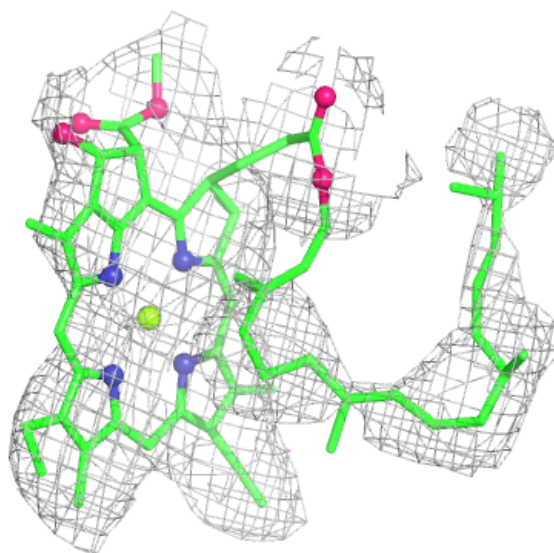
**Electron density around CLA B 840:**

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



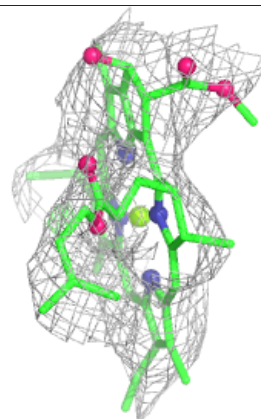
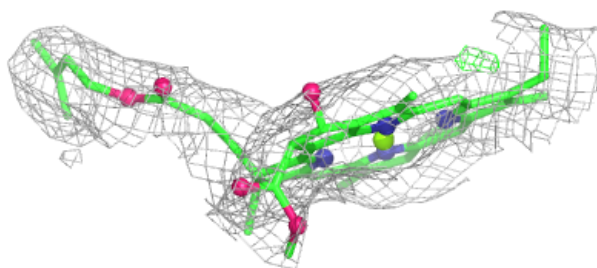
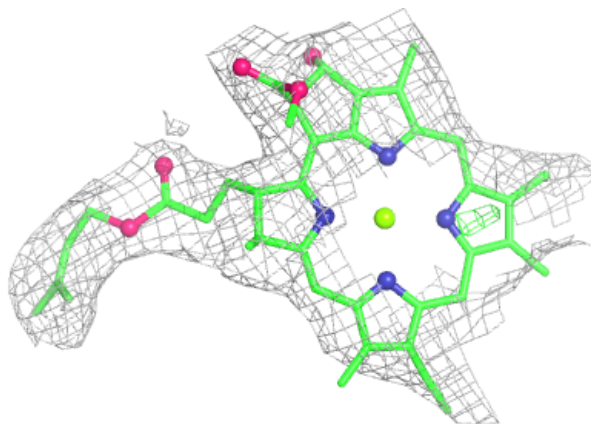
Electron density around CLA B 824:

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



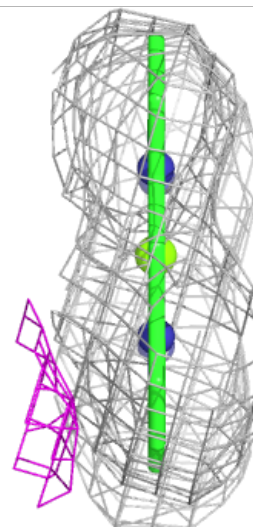
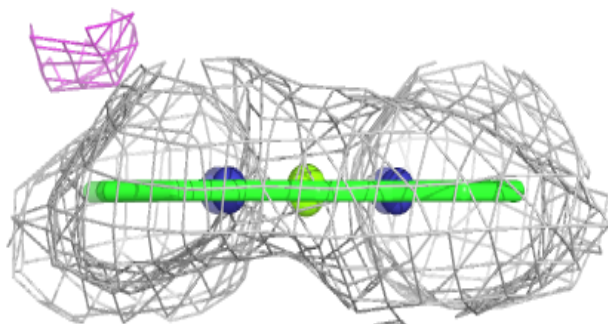
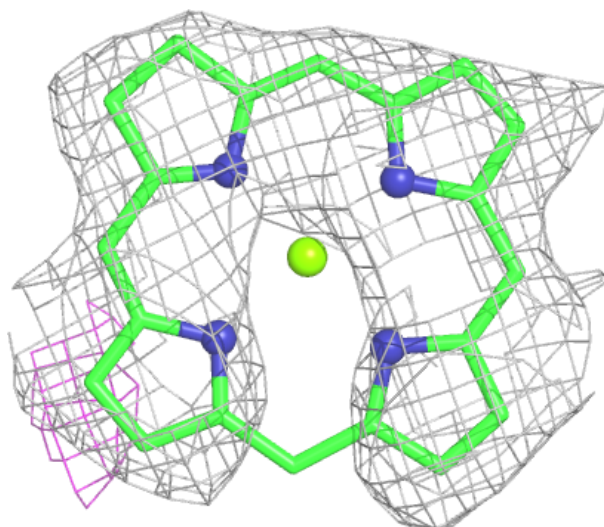
Electron density around CLA B 833:

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



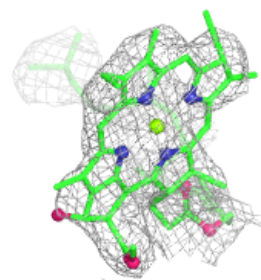
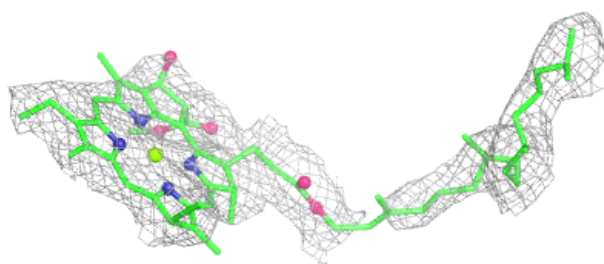
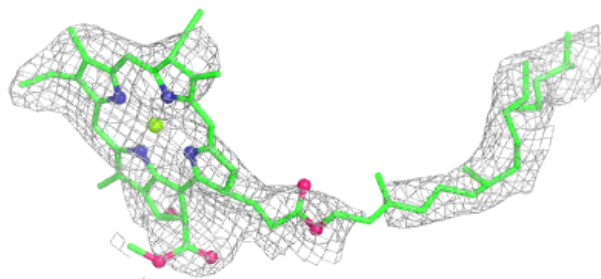
Electron density around CLA B 811:

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



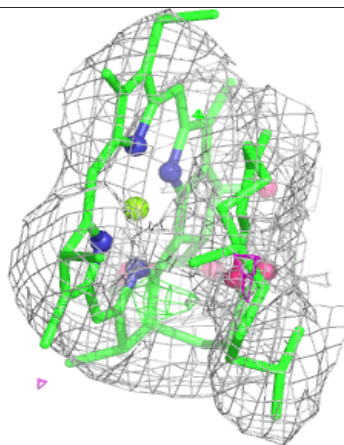
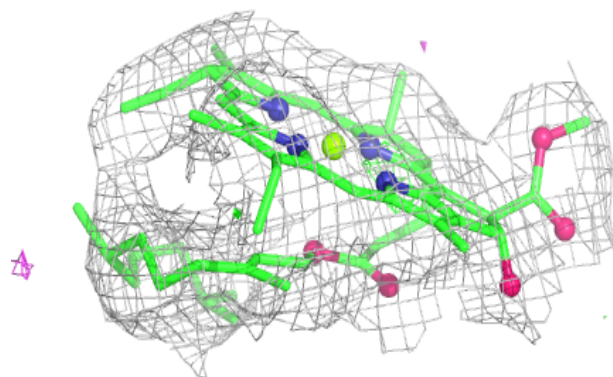
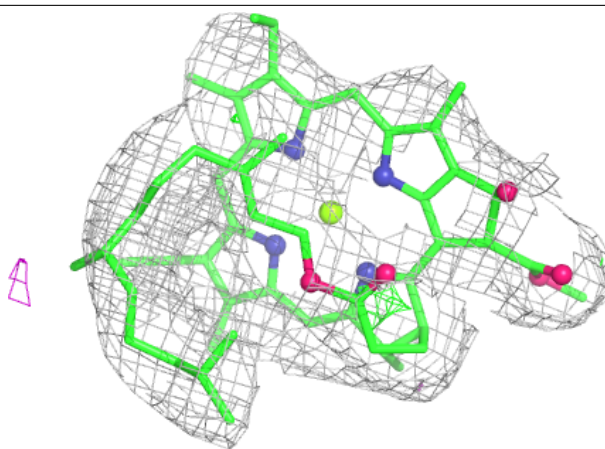
Electron density around CLA A 850:

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

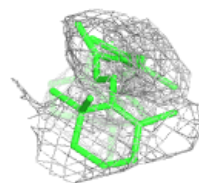
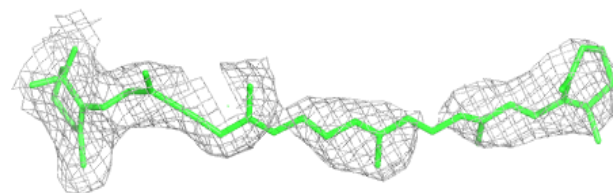
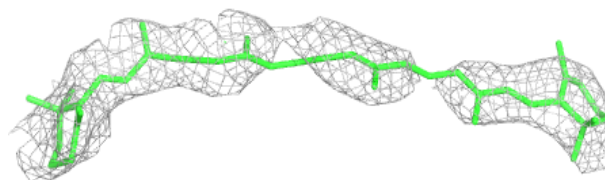


Electron density around CLA B 810:

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

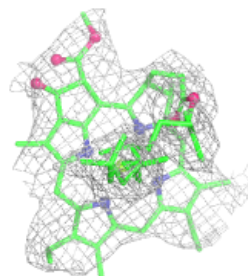
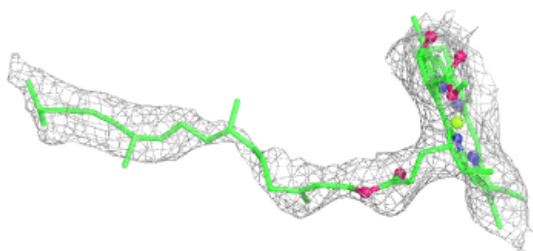
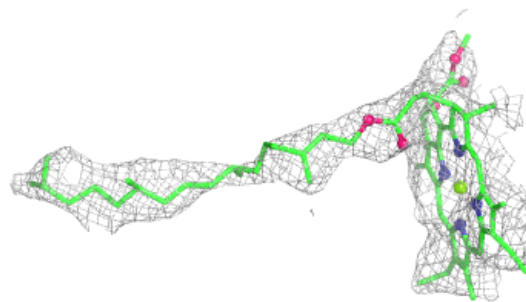
**Electron density around BCR F 203:**

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

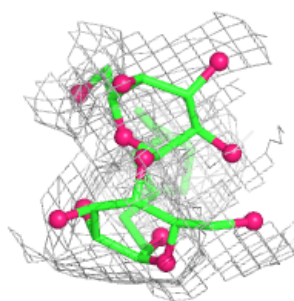
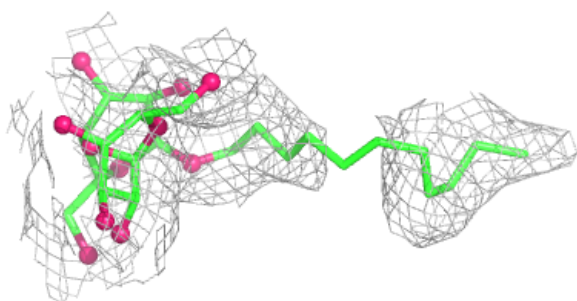
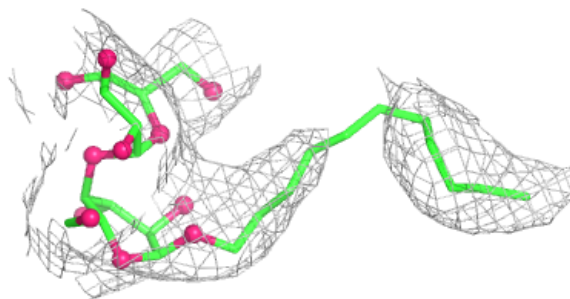


Electron density around CLA B 829:

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

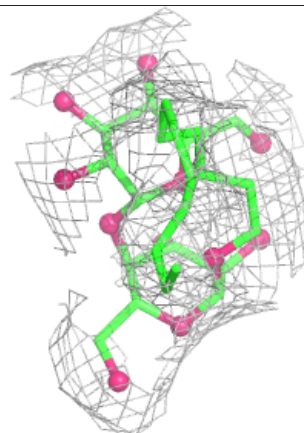
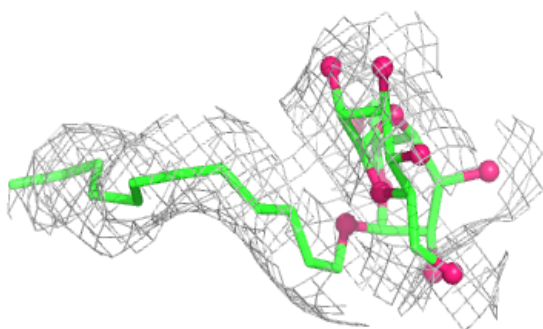
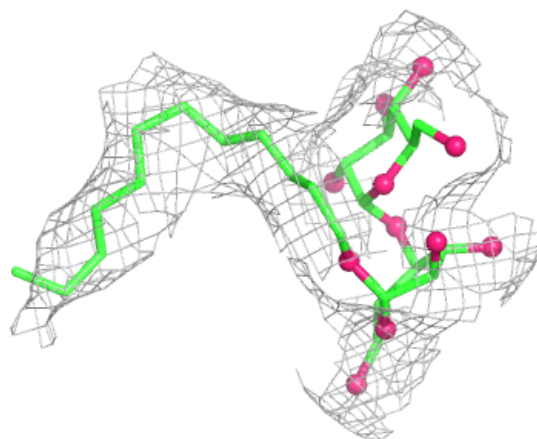
**Electron density around LMU 4 319:**

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

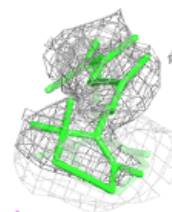
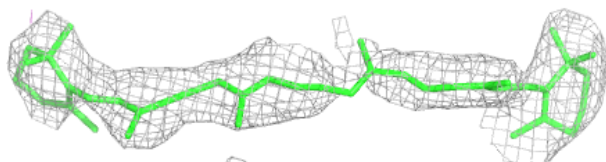
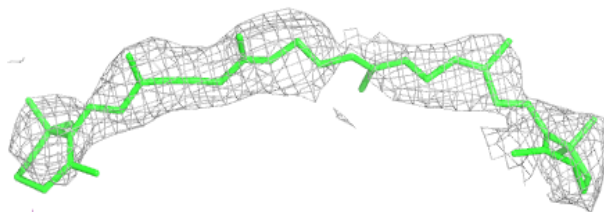


Electron density around LMU H 105:

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

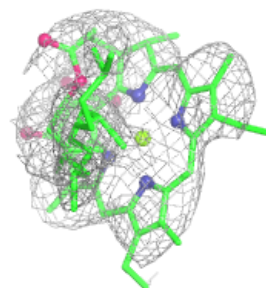
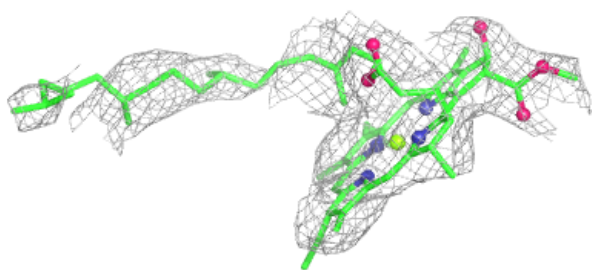
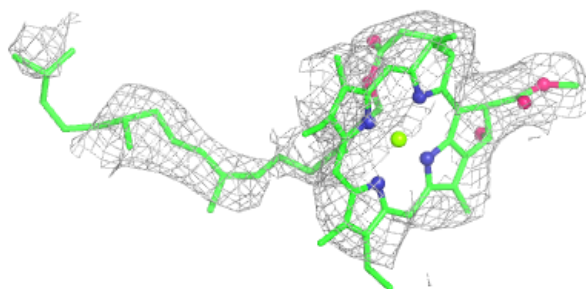
**Electron density around BCR B 801:**

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

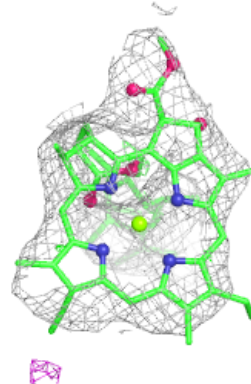
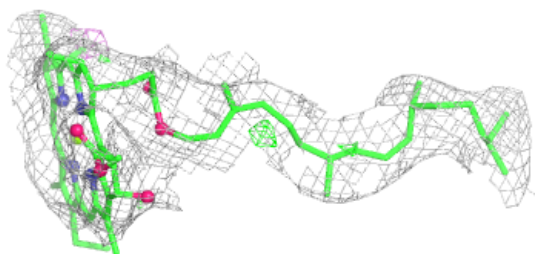
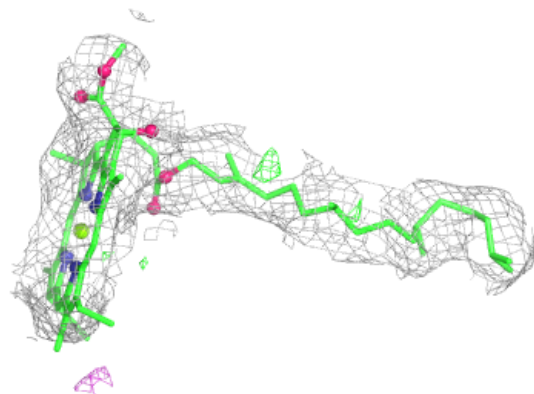


Electron density around CLA A 838:

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

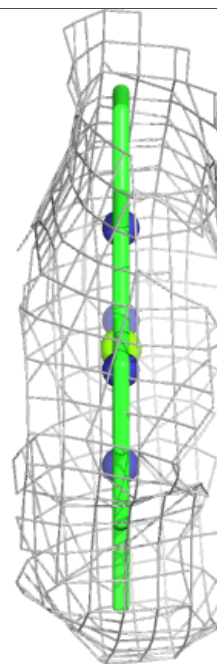
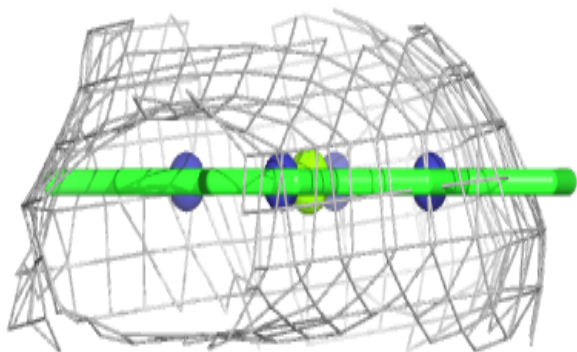
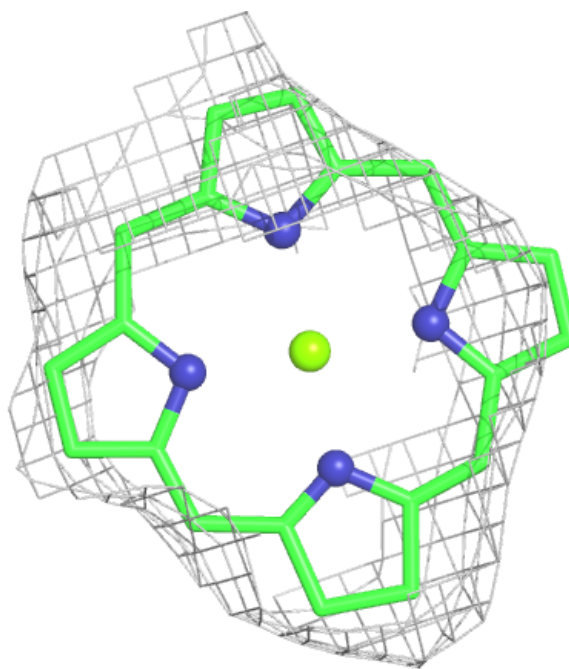
**Electron density around CLA A 826:**

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



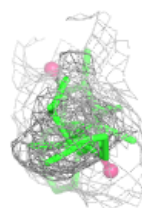
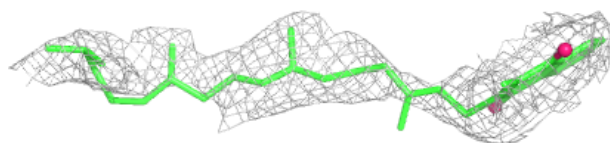
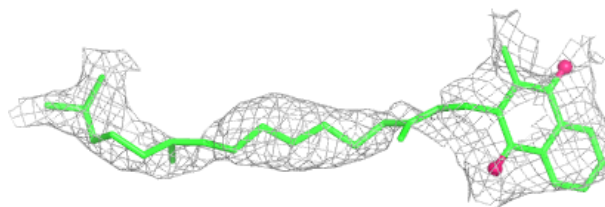
Electron density around CLA 4 311:

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



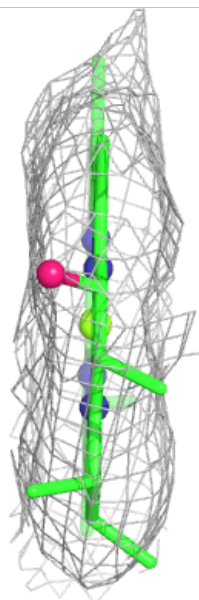
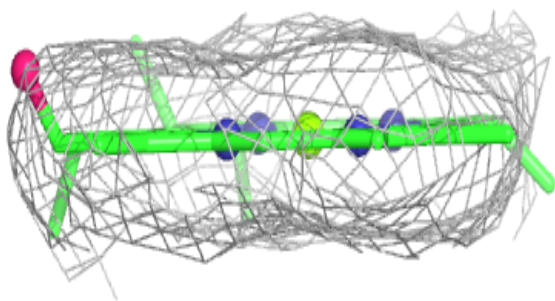
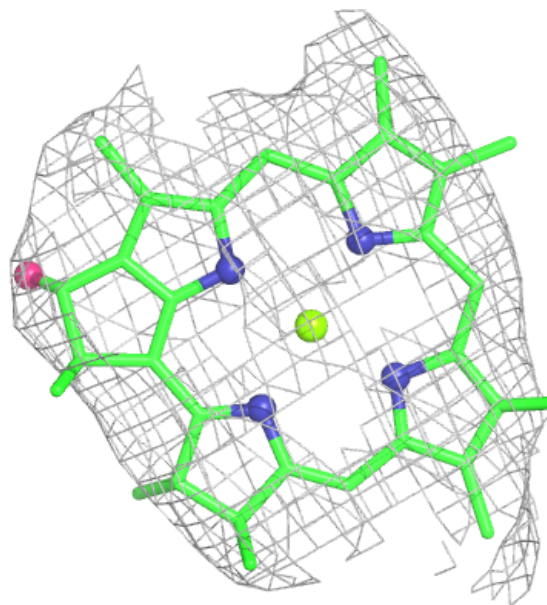
Electron density around PQN A 842:

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



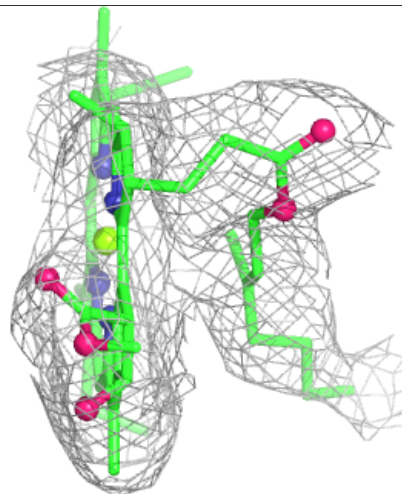
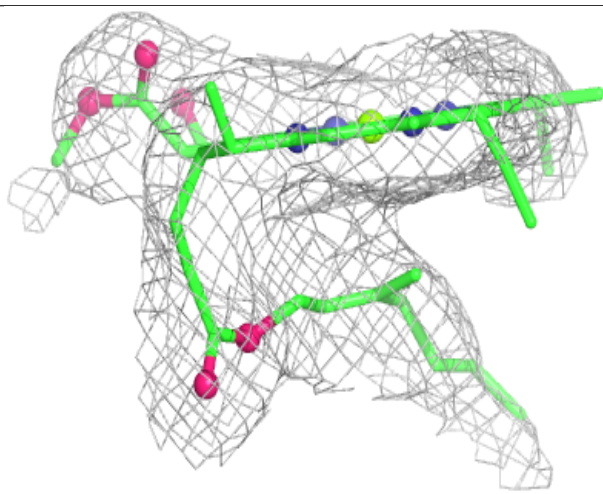
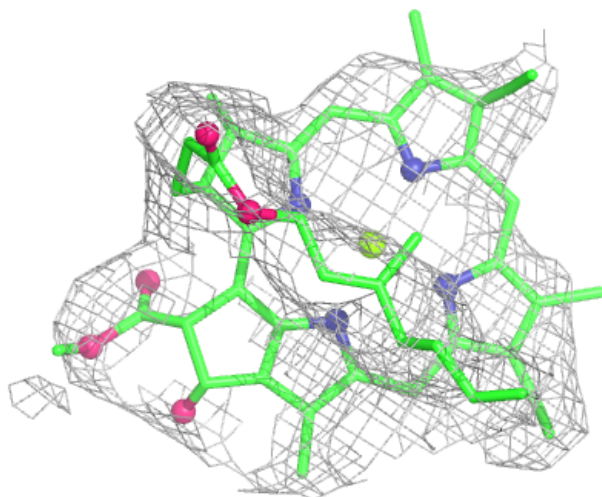
Electron density around CLA F 205:

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



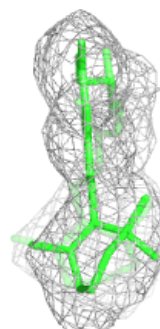
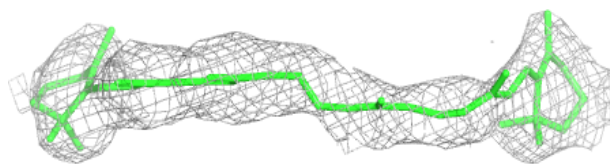
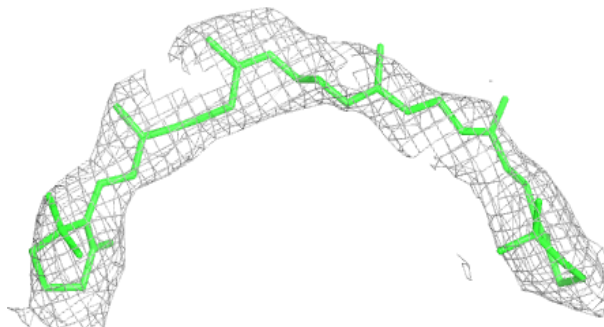
Electron density around CLA B 818:

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



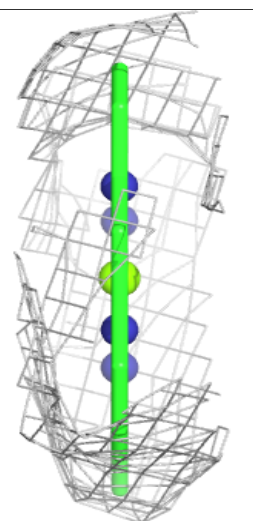
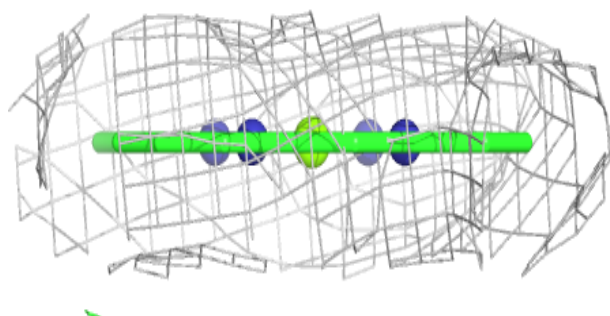
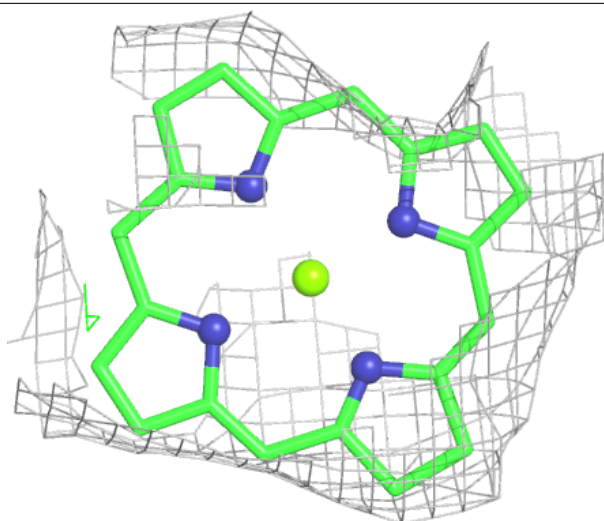
Electron density around BCR F 204:

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



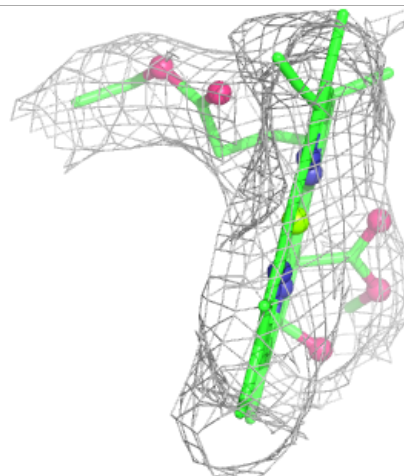
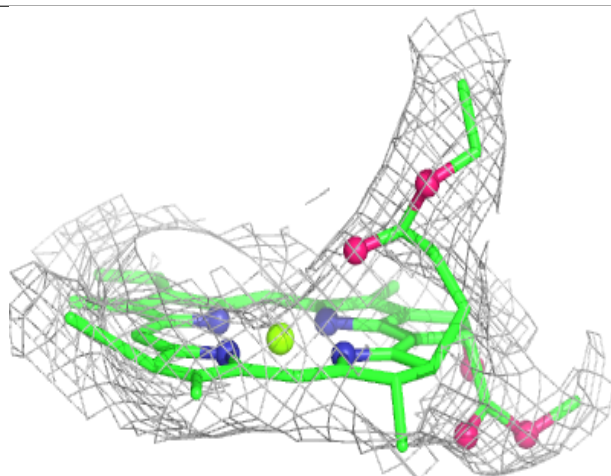
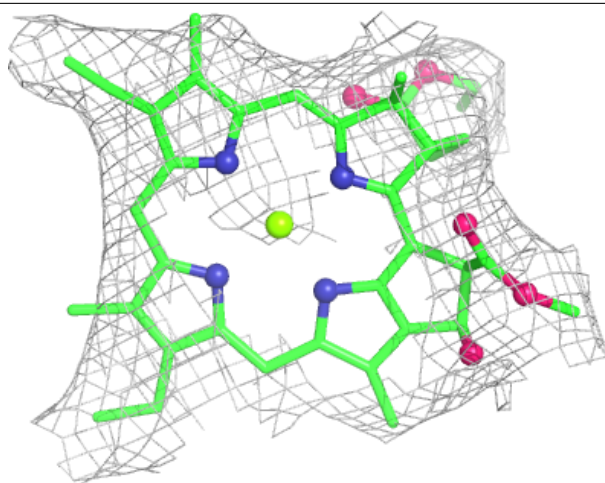
Electron density around CLA 2 308:

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



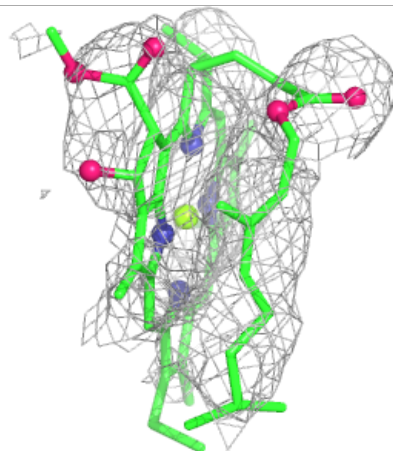
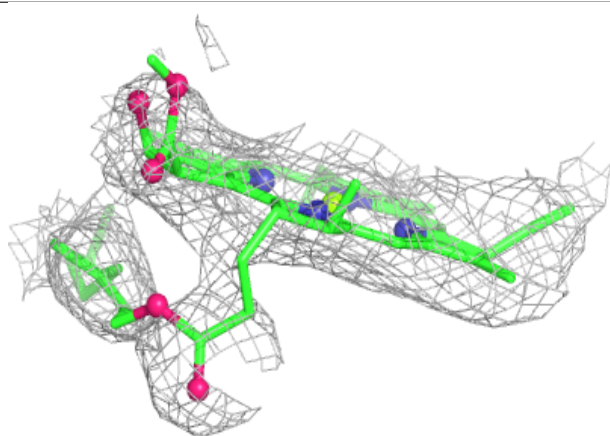
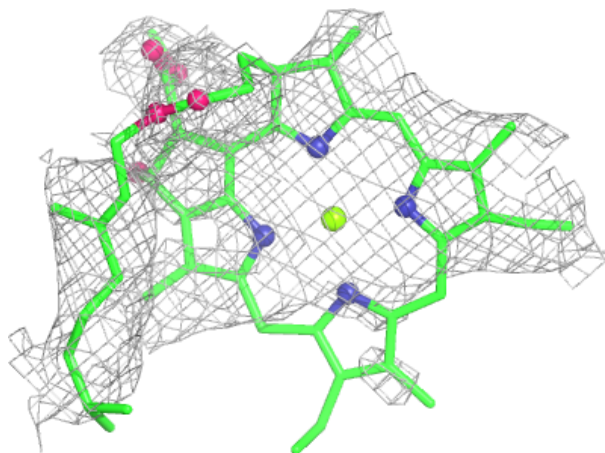
Electron density around CLA B 839:

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



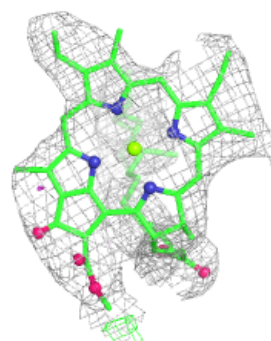
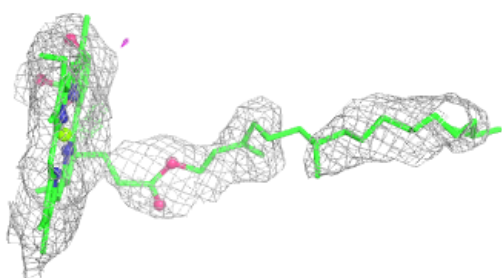
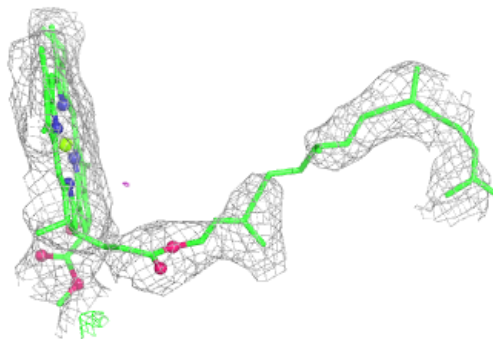
Electron density around CLA A 827:

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

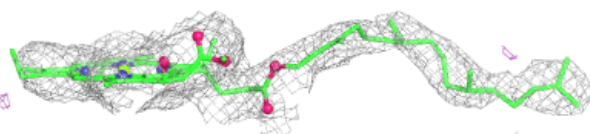
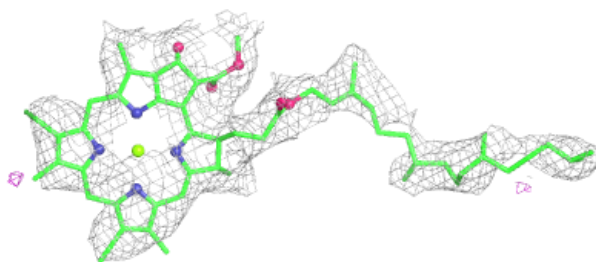


Electron density around CLA B 841:

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

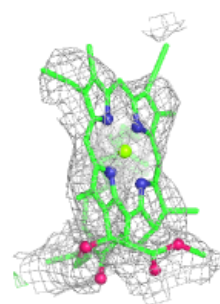
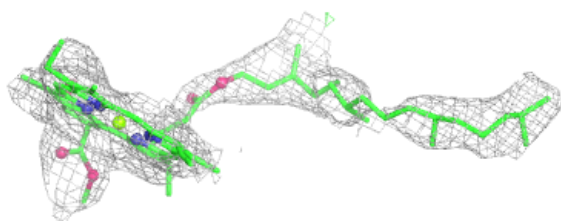
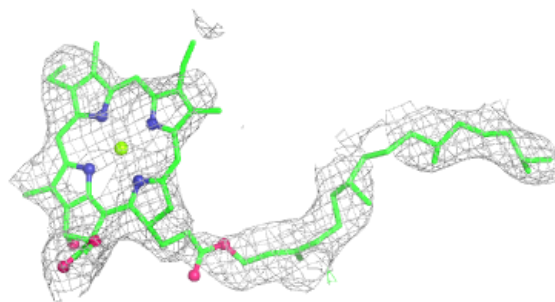
**Electron density around CLA A 830:**

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



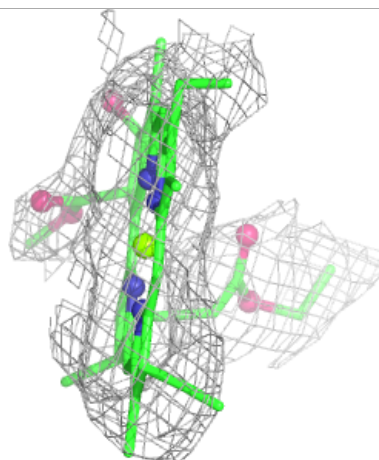
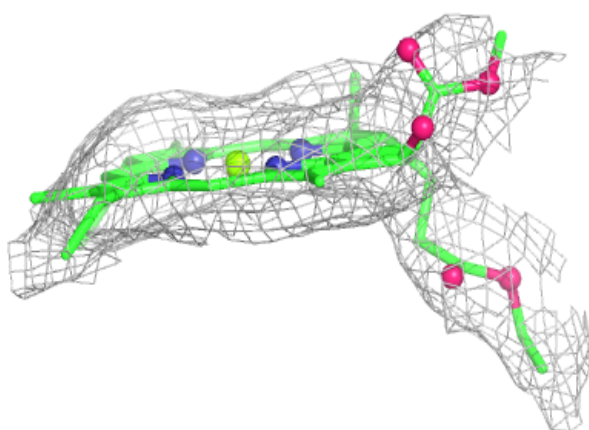
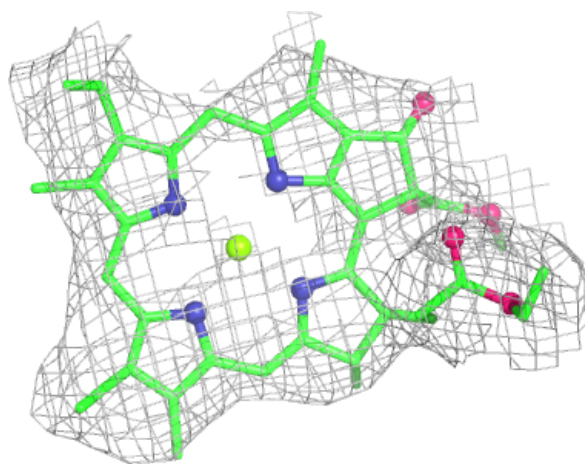
Electron density around CLA A 831:

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



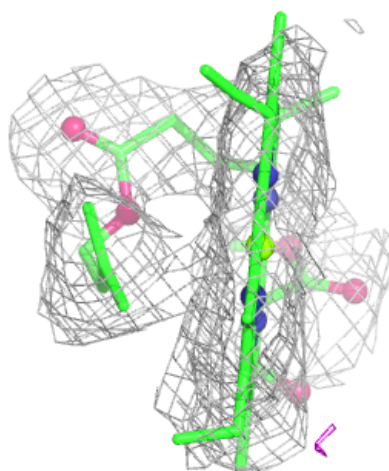
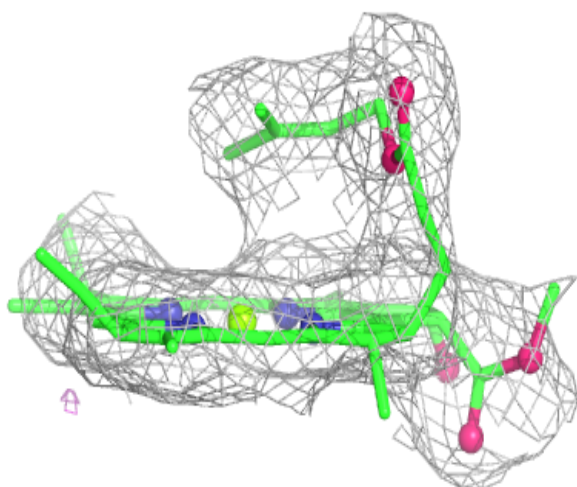
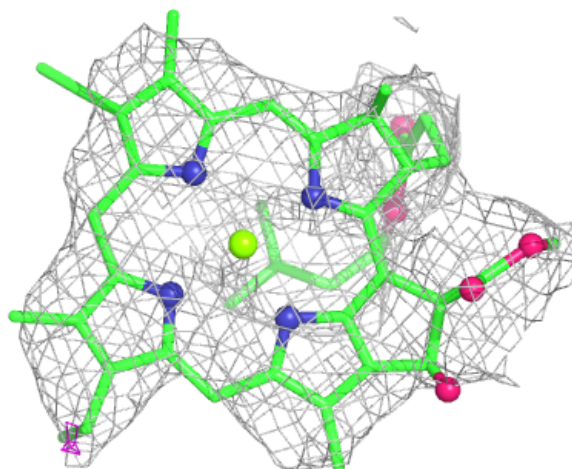
Electron density around CLA A 836:

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



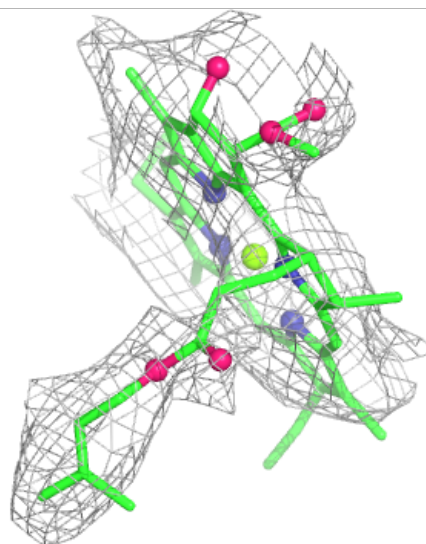
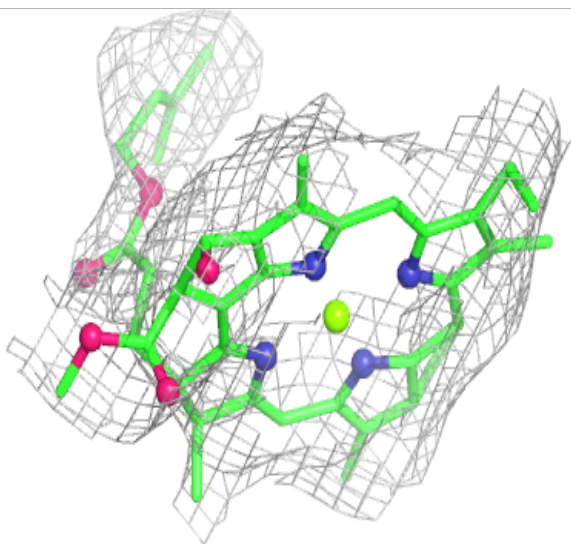
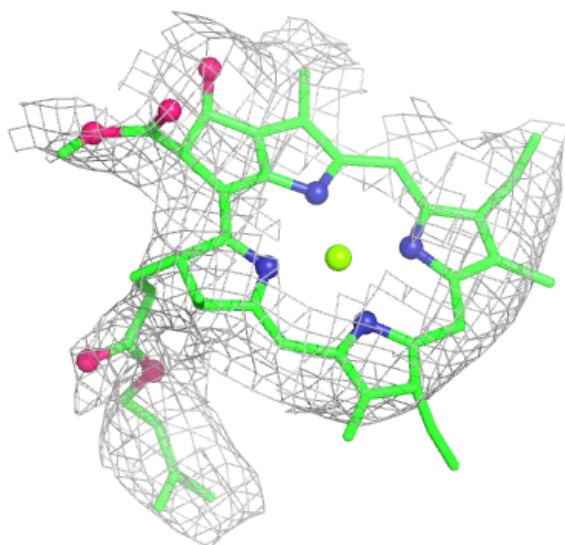
Electron density around CLA B 831:

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



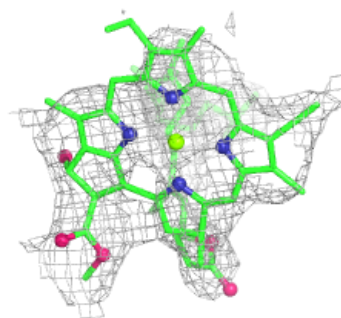
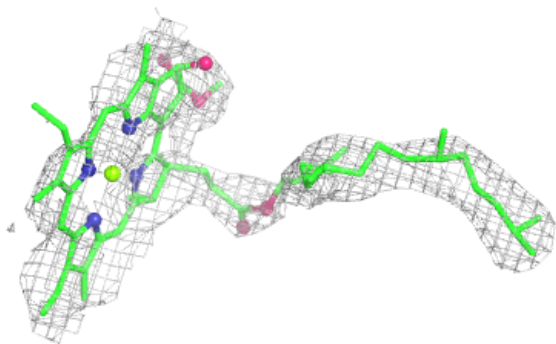
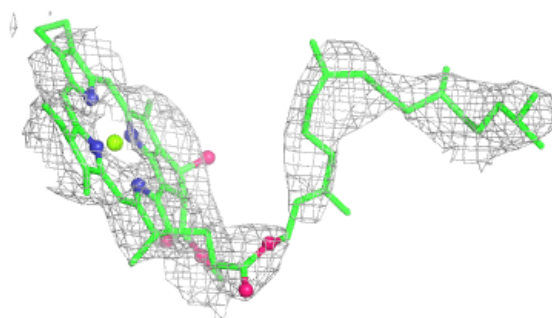
Electron density around CLA A 822:

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

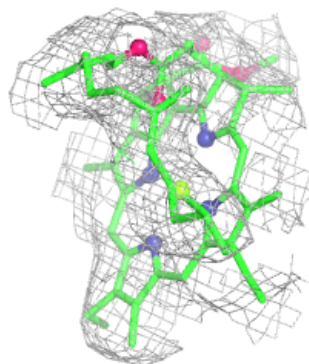
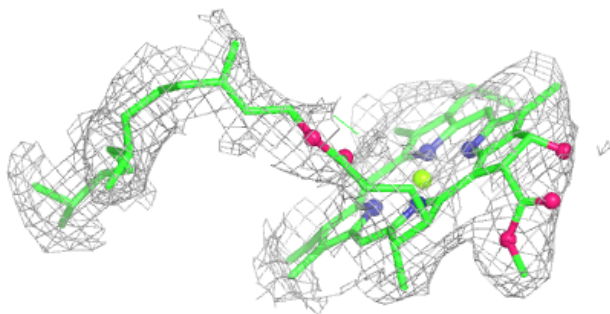
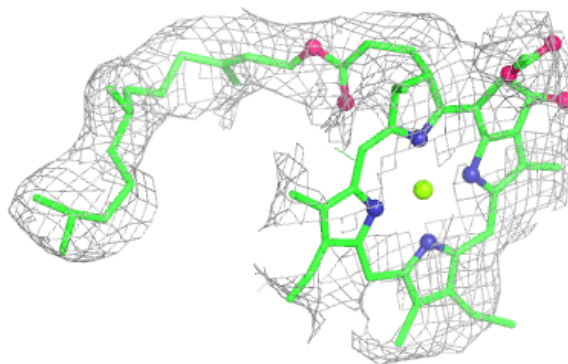


Electron density around CLA B 850:

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

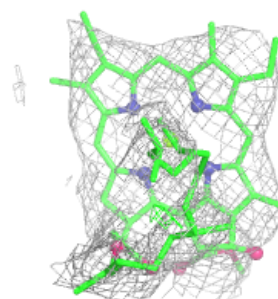
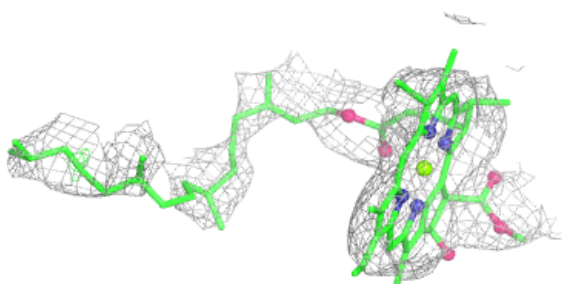
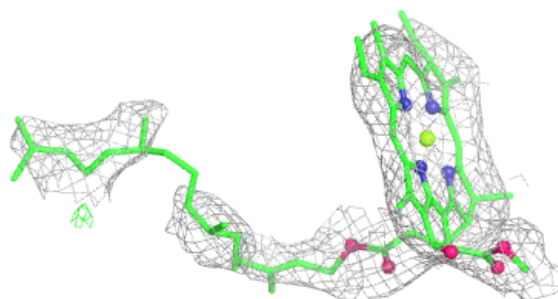
**Electron density around CLA A 808:**

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

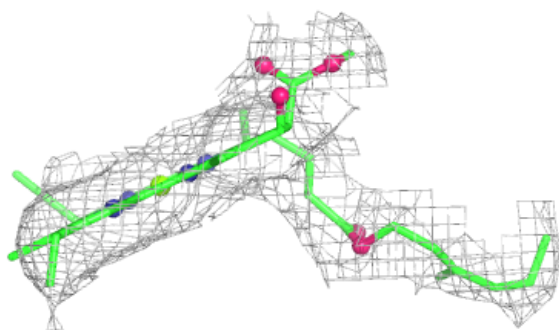
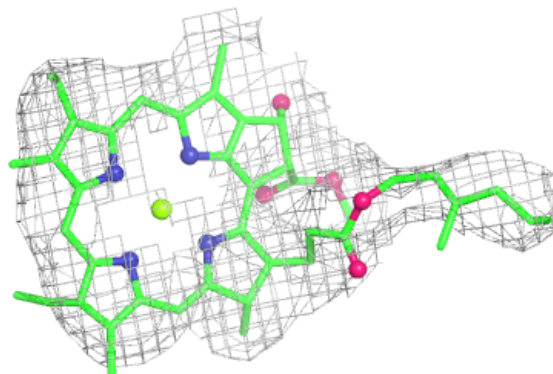


Electron density around CLA B 830:

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

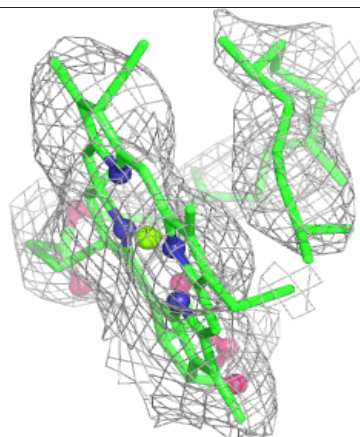
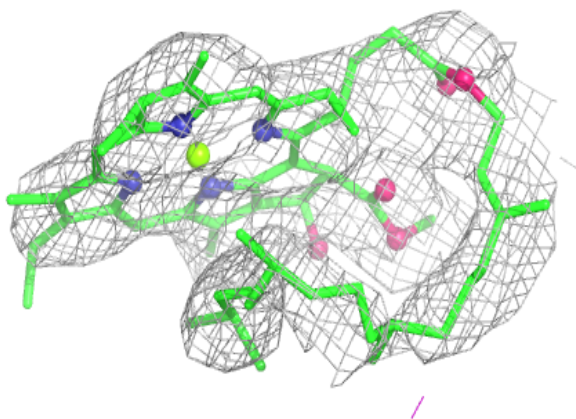
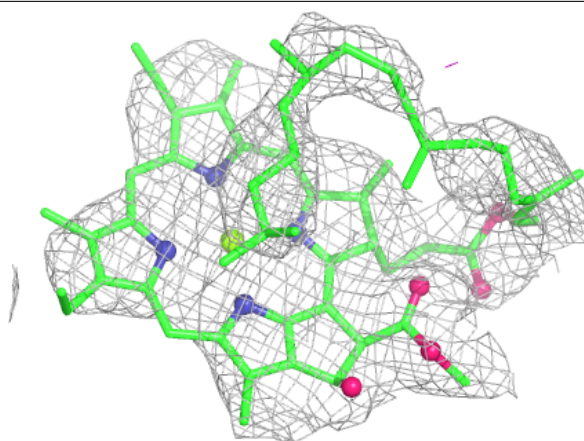
**Electron density around CLA A 809:**

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



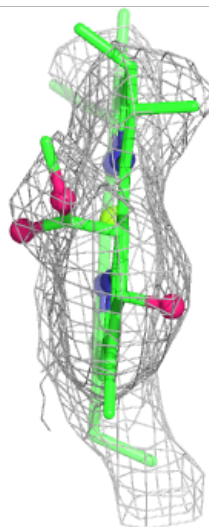
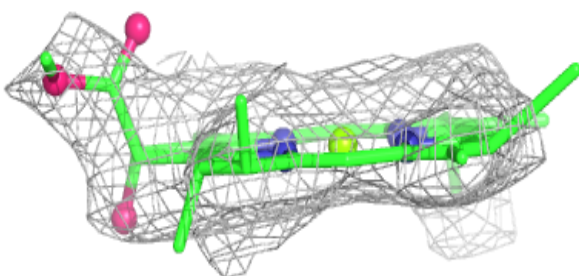
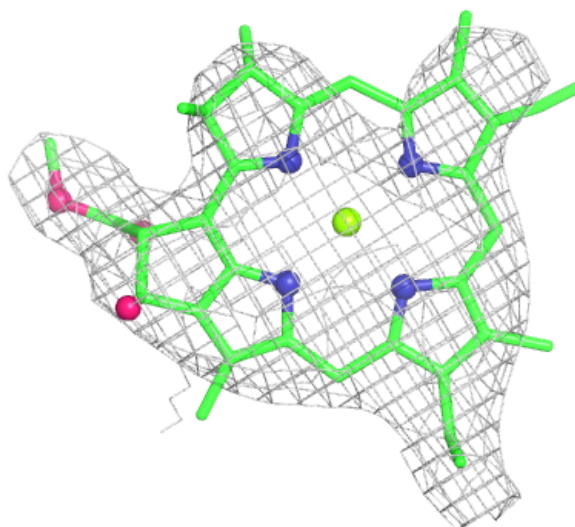
Electron density around CLA B 809:

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



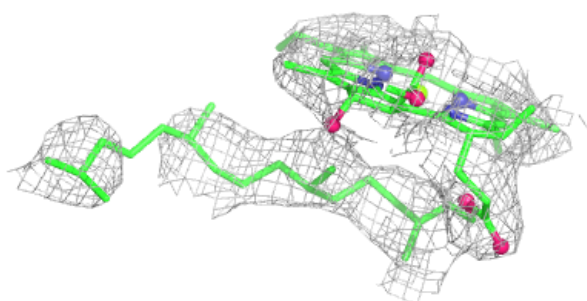
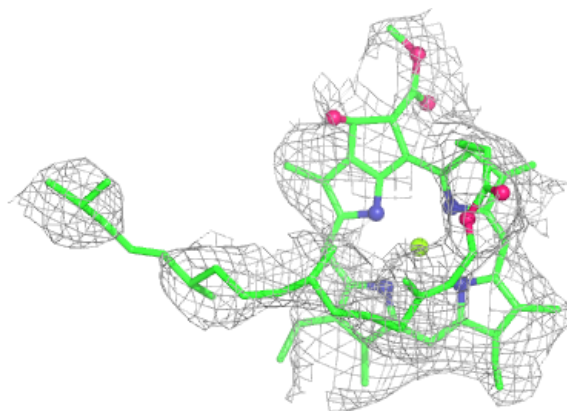
Electron density around CLA B 819:

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

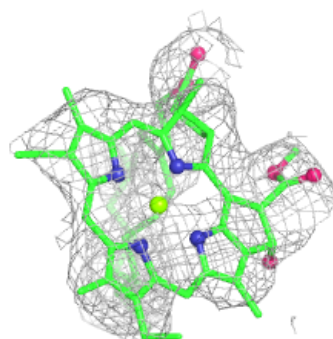
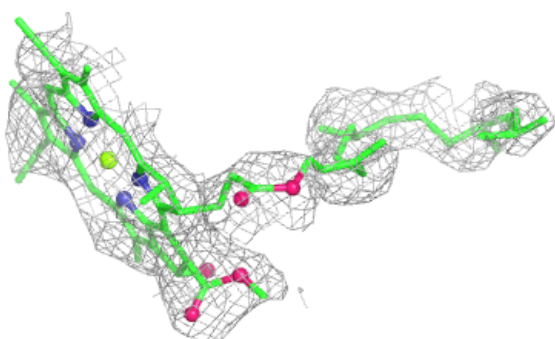
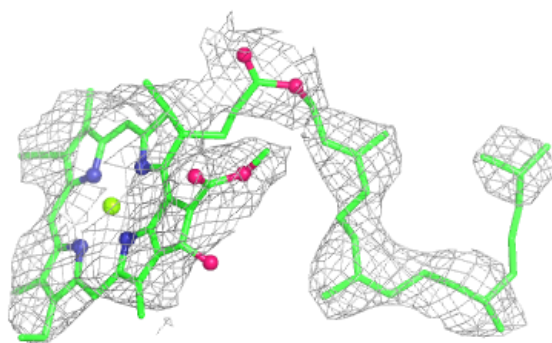


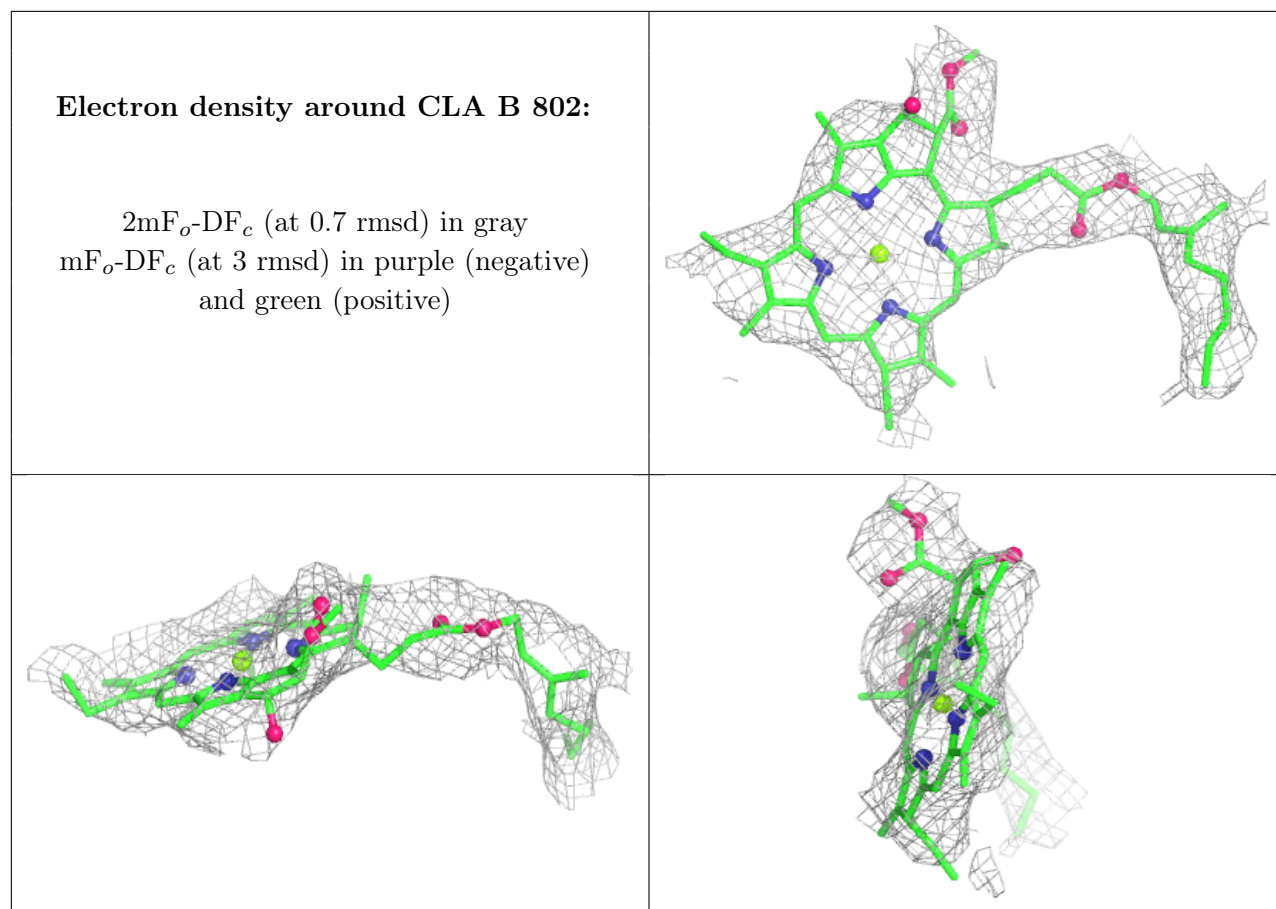
Electron density around CLA B 828:

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

**Electron density around CLA 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)





6.5 Other polymers ⓘ

There are no such residues in this entry.