



wwPDB X-ray Structure Validation Summary Report ⓘ

Sep 10, 2026 – 08:53 am BST

PDB ID : 2WSE / pdb_00002wse
Title : Improved Model of Plant Photosystem I
Authors : Amunts, A.; Toporik, H.; Borovikov, A.; Nelson, N.
Deposited on : 2009-09-05
Resolution : 3.49 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

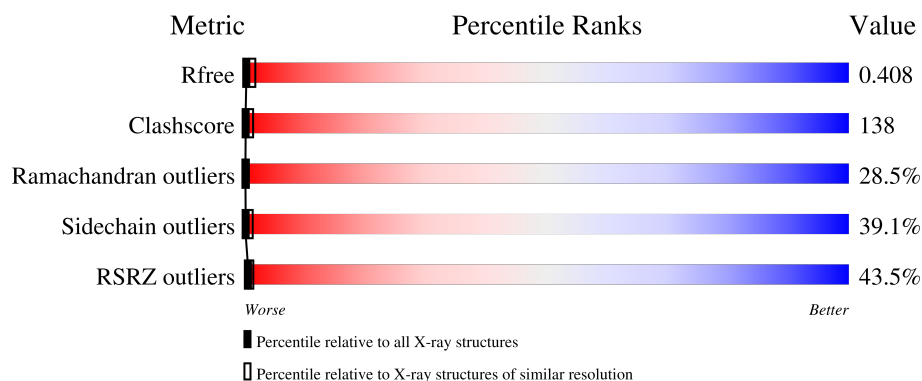
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.49 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	1085 (3.54-3.46)
Clashscore	190562	1140 (3.54-3.46)
Ramachandran outliers	187476	1113 (3.54-3.46)
Sidechain outliers	187428	1114 (3.54-3.46)
RSRZ outliers	180081	1084 (3.54-3.46)

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	37% 27% 24% 12% 5% 32%
2	2	269	20% 6% 19% 24% 16% 35%
3	3	276	37% 16% 16% 18% 7% 42%
4	4	251	20% 5% 14% 26% 21% 34%
5	A	758	49% 5% 43% 36% 12% .

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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	 100%

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
19	FRU	M	2	X	-	-	-
19	GLC	O	1	-	-	X	-
19	FRU	O	2	X	-	X	-
19	GLC	P	1	-	-	X	-
19	FRU	P	2	X	-	X	-
19	FRU	Q	2	X	-	X	-
19	FRU	S	2	X	-	X	-
19	GLC	T	1	-	-	X	-
19	FRU	T	2	X	-	X	-
19	GLC	U	1	-	-	X	-
19	FRU	U	2	X	-	X	-
19	FRU	V	2	X	-	-	-
19	FRU	W	2	X	-	-	-
19	GLC	X	1	-	-	X	-
19	FRU	X	2	X	-	X	-
19	GLC	Y	1	-	-	X	-
19	FRU	Y	2	X	-	X	-
19	GLC	Z	1	-	-	X	-
19	FRU	Z	2	X	-	X	-
19	FRU	a	2	X	-	-	-
20	CLA	1	202	X	-	X	-
20	CLA	1	206	X	-	-	-
20	CLA	1	207	X	-	-	-
20	CLA	1	210	X	-	-	-
20	CLA	1	215	X	-	X	-
20	CLA	2	303	X	-	-	-
20	CLA	2	307	X	-	-	-
20	CLA	2	308	X	-	-	-
20	CLA	2	315	X	-	-	-
20	CLA	2	320	X	-	X	-
20	CLA	3	302	-	-	X	-
20	CLA	3	311	X	-	-	-
20	CLA	3	313	X	-	X	-
20	CLA	3	317	X	-	-	-
20	CLA	4	302	X	-	X	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
20	CLA	4	304	X	-	X	-
20	CLA	4	305	X	-	-	-
20	CLA	4	307	X	-	-	-
20	CLA	4	311	X	-	-	-
20	CLA	A	801	X	-	-	-
20	CLA	A	804	X	-	X	-
20	CLA	A	805	X	-	X	-
20	CLA	A	806	X	-	-	-
20	CLA	A	807	-	-	X	-
20	CLA	A	808	X	-	X	-
20	CLA	A	809	-	-	X	-
20	CLA	A	811	X	-	X	-
20	CLA	A	814	-	-	X	-
20	CLA	A	815	-	-	X	-
20	CLA	A	816	-	-	X	-
20	CLA	A	818	X	-	X	-
20	CLA	A	819	X	-	X	-
20	CLA	A	822	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	-	X	-
20	CLA	A	828	X	-	-	-
20	CLA	A	830	X	-	X	-
20	CLA	A	831	X	-	-	-
20	CLA	A	835	X	-	-	-
20	CLA	A	838	X	-	X	-
20	CLA	A	839	X	-	X	-
20	CLA	A	841	X	-	X	-
20	CLA	A	850	X	-	-	-
20	CLA	A	851	X	-	X	-
20	CLA	A	852	X	-	X	-
20	CLA	B	803	X	-	X	-
20	CLA	B	805	X	-	-	-
20	CLA	B	806	X	-	-	-
20	CLA	B	807	X	-	X	-
20	CLA	B	808	X	-	-	-
20	CLA	B	809	X	-	-	-
20	CLA	B	810	X	-	-	-
20	CLA	B	811	X	-	X	-
20	CLA	B	812	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
20	CLA	B	813	X	-	-	-
20	CLA	B	815	X	-	-	-
20	CLA	B	816	X	-	-	-
20	CLA	B	817	X	-	-	-
20	CLA	B	820	X	-	-	-
20	CLA	B	821	-	-	X	-
20	CLA	B	822	-	-	X	-
20	CLA	B	823	X	-	X	-
20	CLA	B	824	X	-	X	-
20	CLA	B	825	X	-	X	-
20	CLA	B	826	X	-	X	-
20	CLA	B	827	X	-	X	-
20	CLA	B	830	X	-	X	-
20	CLA	B	833	-	-	X	-
20	CLA	B	835	X	-	-	-
20	CLA	B	836	X	-	X	-
20	CLA	B	837	-	-	X	-
20	CLA	B	838	X	-	X	-
20	CLA	B	839	X	-	X	-
20	CLA	B	849	X	-	X	-
20	CLA	B	850	X	-	X	-
20	CLA	B	851	X	-	X	-
20	CLA	F	206	X	-	-	-
20	CLA	H	101	X	-	X	-
20	CLA	H	102	X	-	-	-
20	CLA	H	103	X	-	-	-
20	CLA	H	109	X	-	-	-
20	CLA	I	102	X	-	-	-
20	CLA	J	101	-	-	X	-
20	CLA	J	103	X	-	X	-
20	CLA	K	103	X	-	-	-
20	CLA	K	107	-	-	X	-
20	CLA	L	201	X	-	X	-
20	CLA	L	202	X	-	X	-
20	CLA	L	203	X	-	-	-
20	CLA	L	206	-	-	X	-
20	CLA	L	207	X	-	-	-
20	CLA	R	107	X	-	-	-
20	CLA	R	108	X	-	-	-
21	LMU	A	854	-	-	X	-
21	LMU	A	855	-	-	X	-
21	LMU	B	847	-	-	X	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
21	LMU	E	101	-	-	X	-
21	LMU	H	106	-	-	X	-
21	LMU	H	108	-	-	X	-
21	LMU	K	105	-	-	X	-
21	LMU	K	106	-	-	X	-
21	LMU	N	101	-	-	X	-
21	LMU	R	101	X	-	-	-
21	LMU	R	102	-	-	X	-
21	LMU	R	103	-	-	X	-
21	LMU	R	109	-	-	X	-
22	BCR	3	314	-	-	X	-
22	BCR	A	843	-	-	X	-
22	BCR	A	844	-	-	X	-
22	BCR	A	845	-	-	X	-
22	BCR	A	846	-	-	X	-
22	BCR	A	847	-	-	X	-
22	BCR	B	845	-	-	X	-
22	BCR	B	846	-	-	X	-
22	BCR	F	202	-	-	X	-
22	BCR	F	203	-	-	X	-
22	BCR	I	103	-	-	X	-
22	BCR	J	102	-	-	X	-
22	BCR	L	208	-	-	X	-
23	PQN	A	842	X	-	-	-
23	PQN	B	841	X	-	X	-
24	SF4	A	857	-	-	X	-
24	SF4	C	102	-	-	X	-
24	SF4	C	103	-	-	X	-
25	LMG	B	848	-	-	X	-

2 Entry composition

There are 26 unique types of molecules in this entry. The entry contains 36461 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	164	Total	C	N	O	S	0	0	0
			1255	817	206	228	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
			1380	902	229	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	160	Total	C	N	O	S	0	0	0
			1233	811	200	217	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
			1322	864	219	236	3			

There is a discrepancy between the modelled and reference sequences:

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

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

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

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

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

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

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

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

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

There are 8 discrepancies between the modelled and reference sequences:

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

There is a discrepancy between the modelled and reference sequences:

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

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

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

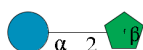
- Molecule 17 is a protein called PHOTOSYSTEM I-N SUBUNIT.

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

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

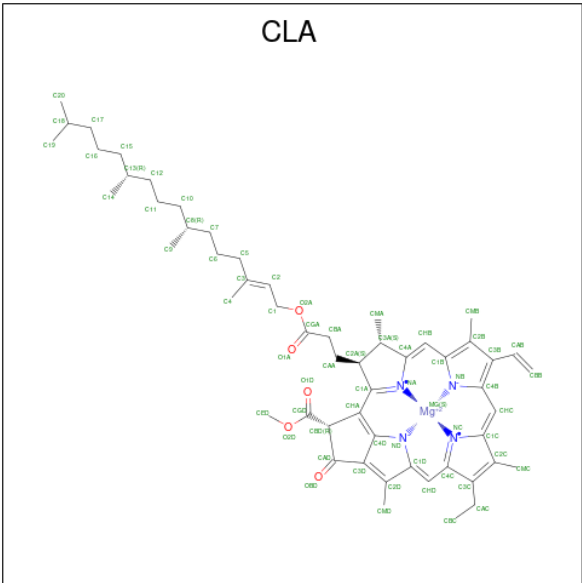
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
18	R	53	Total	C	N	O	0	0	0
			265	159	53	53			

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



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

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



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
20	1	1	Total	C	Mg	N	O	0	0
			46	36	1	4	5		
20	1	1	Total	C	Mg	N	O	0	0
			57	47	1	4	5		
20	1	1	Total	C	Mg	N	O	0	0
			47	37	1	4	5		
20	1	1	Total	C	Mg	N	O	0	0
			46	36	1	4	5		
20	1	1	Total	C	Mg	N		0	0
			25	20	1	4			
20	1	1	Total	C	Mg	N	O	0	0
			61	51	1	4	5		
20	1	1	Total	C	Mg	N	O	0	0
			51	41	1	4	5		
20	1	1	Total	C	Mg	N		0	0
			25	20	1	4			
20	1	1	Total	C	Mg	N	O	0	0
			36	30	1	4	1		
20	1	1	Total	C	Mg	N	O	0	0
			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		0	0
			25	20	1	4			
20	1	1	Total	C	Mg	N	O	0	0
			61	51	1	4	5		
20	1	1	Total	C	Mg	N		0	0
			25	20	1	4			
20	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
			65	55	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	C	Mg	N	O	0	0
			65	55	1	4	5		
20	2	1	Total	C	Mg	N		0	0
			25	20	1	4			
20	2	1	Total	C	Mg	N		0	0
			25	20	1	4			
20	2	1	Total	C	Mg	N	O	0	0
			50	40	1	4	5		
20	2	1	Total	C	Mg	N	O	0	0
			50	40	1	4	5		
20	2	1	Total	C	Mg	N		0	0
			25	20	1	4			
20	2	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
20	2	1	Total	C	Mg	N	O	0	0
			61	51	1	4	5		
20	3	1	Total	C	Mg	N	O	0	0
			36	30	1	4	1		
20	3	1	Total	C	Mg	N	O	0	0
			50	40	1	4	5		
20	3	1	Total	C	Mg	N		0	0
			25	20	1	4			
20	3	1	Total	C	Mg	N	O	0	0
			36	30	1	4	1		
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		0	0
			25	20	1	4			
20	3	1	Total	C	Mg	N	O	0	0
			42	34	1	4	3		
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
			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	O	0	0
			65	55	1	4	5		

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

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
20	4	1	Total	C	Mg	N	O	0	0
			47	37	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		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
			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
			55	45	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
			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
			54	44	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
			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
			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
			51	41	1	4	5		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
20	A	1	Total	C	Mg	N	O	0	0
			42	34	1	4	3		
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
			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
			55	45	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
			49	39	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
			47	37	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
			65	55	1	4	5		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
20	A	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
20	A	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
20	A	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
20	B	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
20	B	1	Total 45	C 35	Mg 1	N 4	O 5	0	0
20	B	1	Total 60	C 50	Mg 1	N 4	O 5	0	0
20	B	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
20	B	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
20	B	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
20	B	1	Total 54	C 44	Mg 1	N 4	O 5	0	0
20	B	1	Total 55	C 45	Mg 1	N 4	O 5	0	0
20	B	1	Total 58	C 48	Mg 1	N 4	O 5	0	0
20	B	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
20	B	1	Total 60	C 50	Mg 1	N 4	O 5	0	0
20	B	1	Total 46	C 36	Mg 1	N 4	O 5	0	0
20	B	1	Total 59	C 49	Mg 1	N 4	O 5	0	0
20	B	1	Total 60	C 50	Mg 1	N 4	O 5	0	0
20	B	1	Total 61	C 51	Mg 1	N 4	O 5	0	0
20	B	1	Total 50	C 40	Mg 1	N 4	O 5	0	0
20	B	1	Total 46	C 36	Mg 1	N 4	O 5	0	0
20	B	1	Total 55	C 45	Mg 1	N 4	O 5	0	0

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

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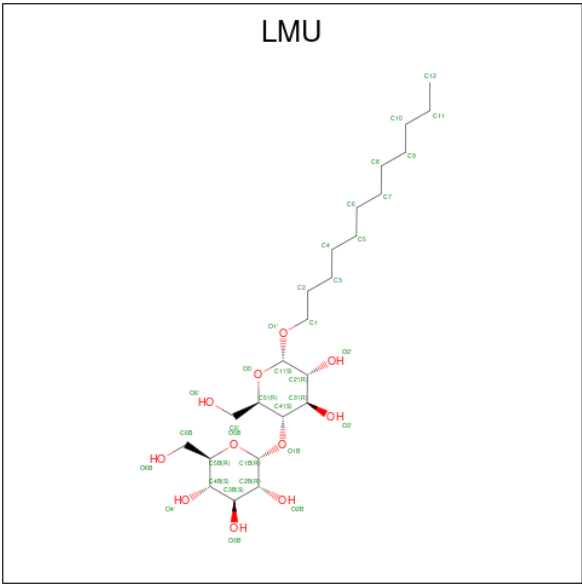
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
20	B	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
20	B	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
20	F	1	Total 36	C 30	Mg 1	N 4	O 1	0	0
20	F	1	Total 41	C 33	Mg 1	N 4	O 3	0	0
20	F	1	Total 53	C 43	Mg 1	N 4	O 5	0	0
20	G	1	Total 51	C 41	Mg 1	N 4	O 5	0	0
20	H	1	Total 55	C 45	Mg 1	N 4	O 5	0	0
20	H	1	Total 55	C 45	Mg 1	N 4	O 5	0	0
20	H	1	Total 55	C 45	Mg 1	N 4	O 5	0	0
20	H	1	Total 60	C 50	Mg 1	N 4	O 5	0	0
20	H	1	Total 50	C 40	Mg 1	N 4	O 5	0	0
20	I	1	Total 60	C 50	Mg 1	N 4	O 5	0	0
20	J	1	Total 48	C 38	Mg 1	N 4	O 5	0	0
20	J	1	Total 61	C 51	Mg 1	N 4	O 5	0	0
20	K	1	Total 45	C 35	Mg 1	N 4	O 5	0	0
20	K	1	Total 50	C 40	Mg 1	N 4	O 5	0	0
20	K	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
20	K	1	Total 50	C 40	Mg 1	N 4	O 5	0	0
20	L	1	Total 55	C 45	Mg 1	N 4	O 5	0	0
20	L	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
20	L	1	Total 55	C 45	Mg 1	N 4	O 5	0	0

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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
			58	48	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	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		

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

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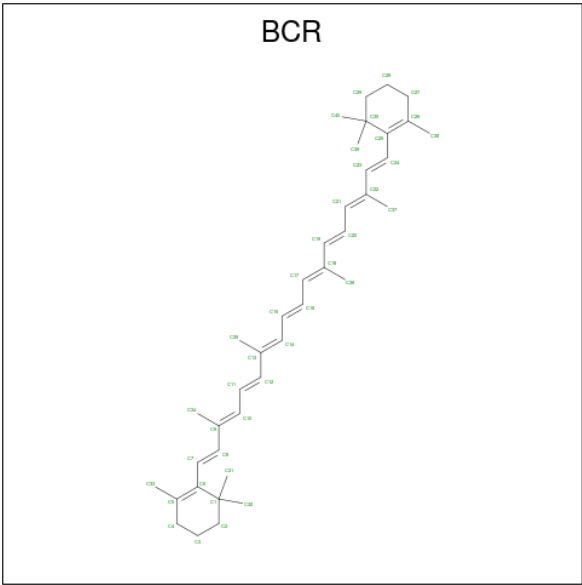
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
21	E	1	Total	C	O	0	0
			35	24	11		
21	F	1	Total	C	O	0	0
			34	23	11		
21	G	1	Total	C	O	0	0
			35	24	11		
21	H	1	Total	C	O	0	0
			35	24	11		
21	H	1	Total	C	O	0	0
			35	24	11		
21	H	1	Total	C	O	0	0
			35	24	11		
21	H	1	Total	C	O	0	0
			35	24	11		
21	K	1	Total	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	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	N	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		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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: C₄₀H₅₆).



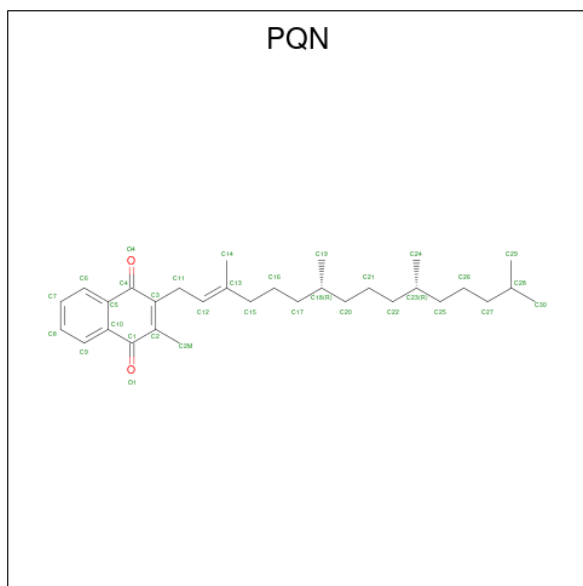
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
22	3	1	Total	C	0	0
			40	40		
22	A	1	Total	C	0	0
			40	40		
22	A	1	Total	C	0	0
			40	40		
22	A	1	Total	C	0	0
			40	40		
22	A	1	Total	C	0	0
			40	40		
22	A	1	Total	C	0	0
			40	40		
22	B	1	Total	C	0	0
			40	40		
22	B	1	Total	C	0	0
			40	40		
22	B	1	Total	C	0	0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

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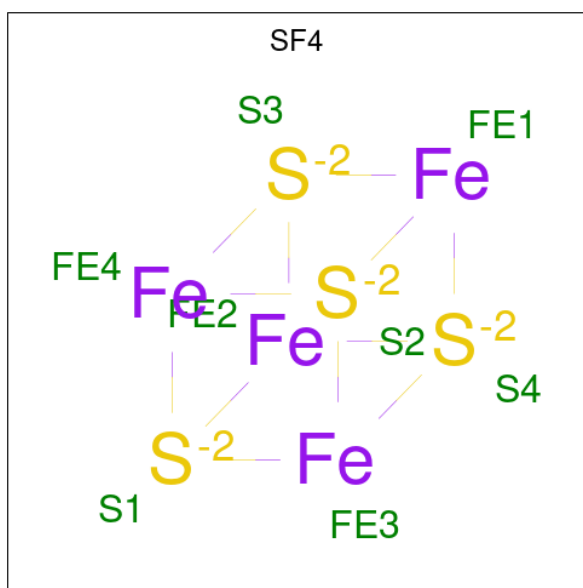
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
22	B	1	Total C 40 40	0	0
22	B	1	Total C 40 40	0	0
22	B	1	Total C 40 40	0	0
22	F	1	Total C 40 40	0	0
22	F	1	Total C 40 40	0	0
22	I	1	Total C 40 40	0	0
22	I	1	Total C 40 40	0	0
22	J	1	Total C 40 40	0	0
22	L	1	Total C 40 40	0	0

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



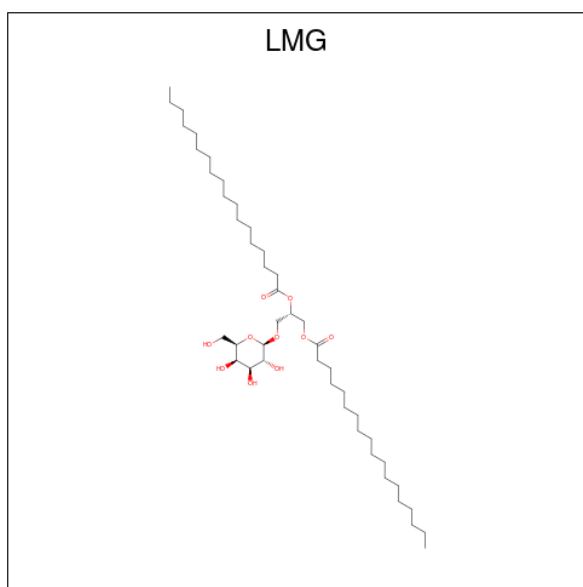
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
23	A	1	Total C O 33 31 2	0	0
23	B	1	Total C O 33 31 2	0	0

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



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

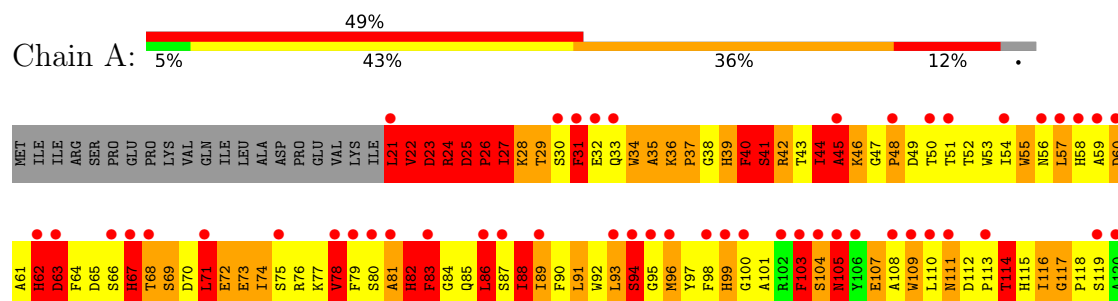
- Molecule 25 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (CCD ID: LMG) (formula: $\text{C}_{45}\text{H}_{86}\text{O}_{10}$).

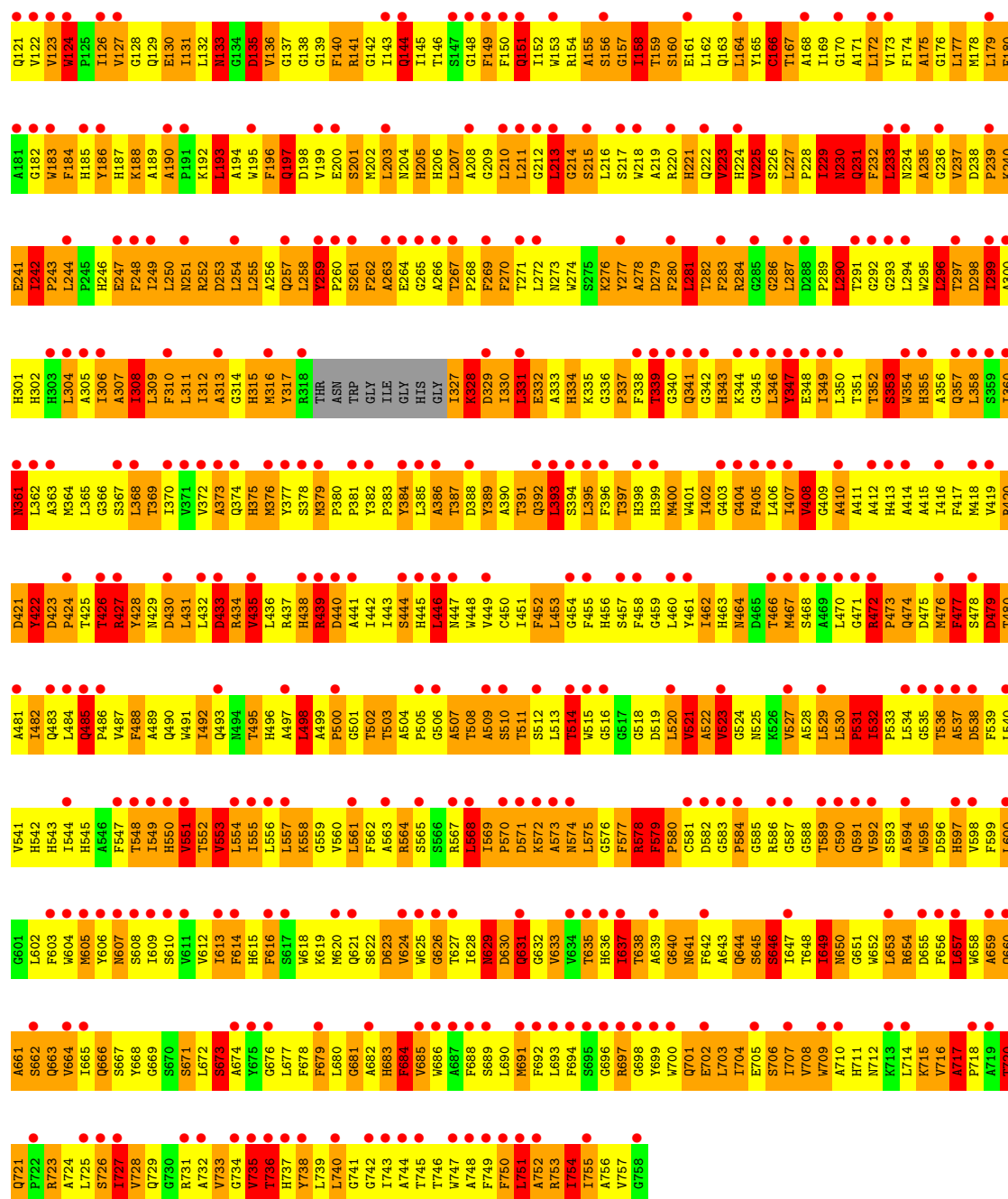


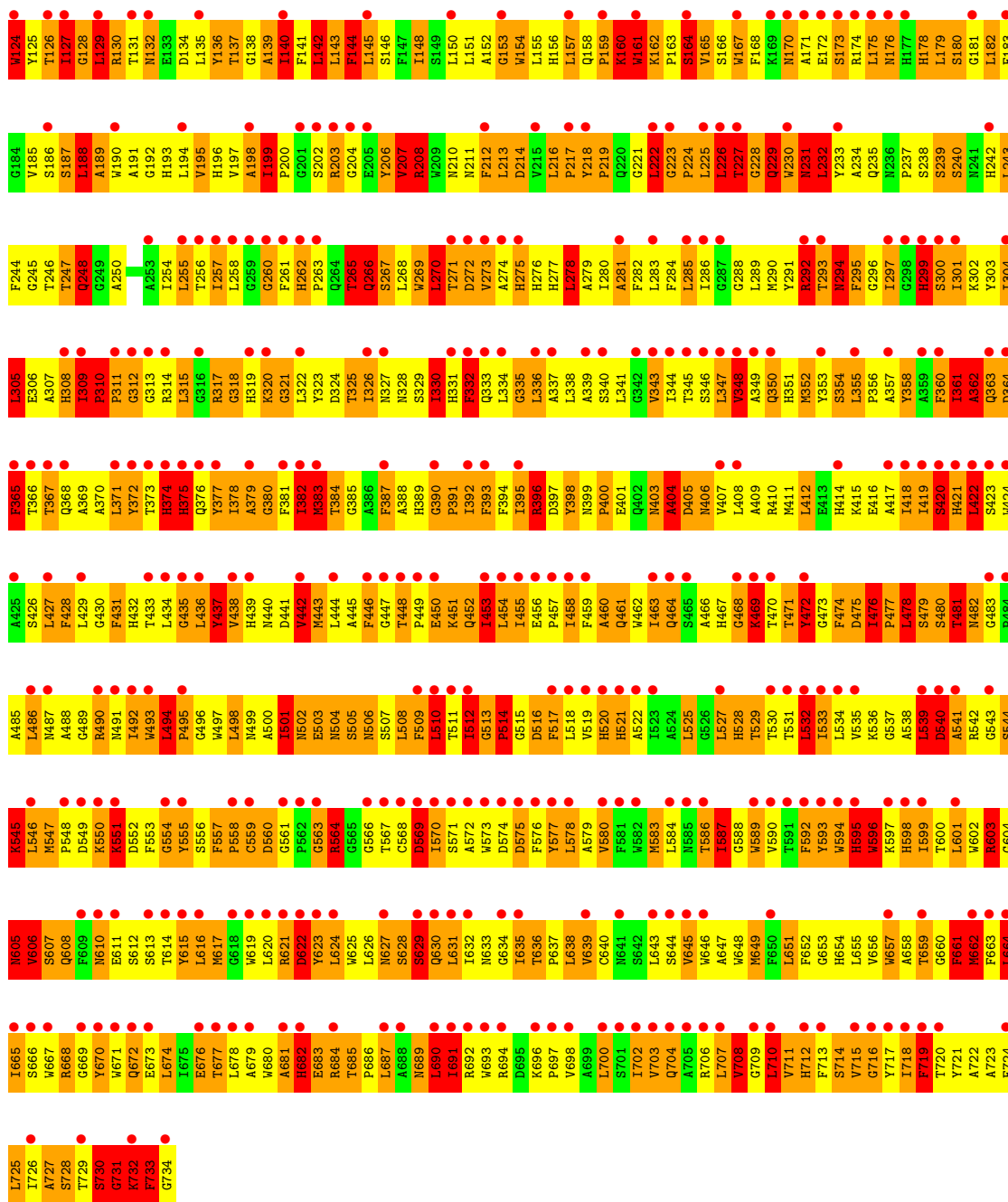
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
25	B	1	Total	C	O	0	0
			49	39	10		

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

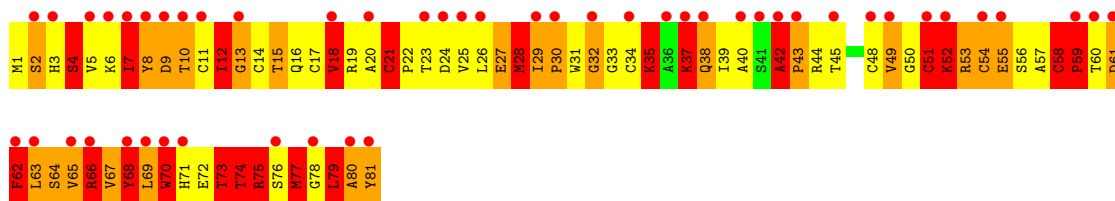
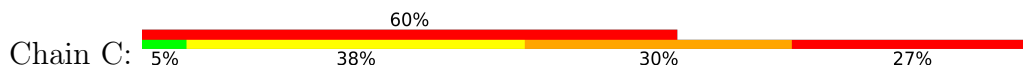
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
26	H	1	Total	C	O	0	0
			23	12	11		



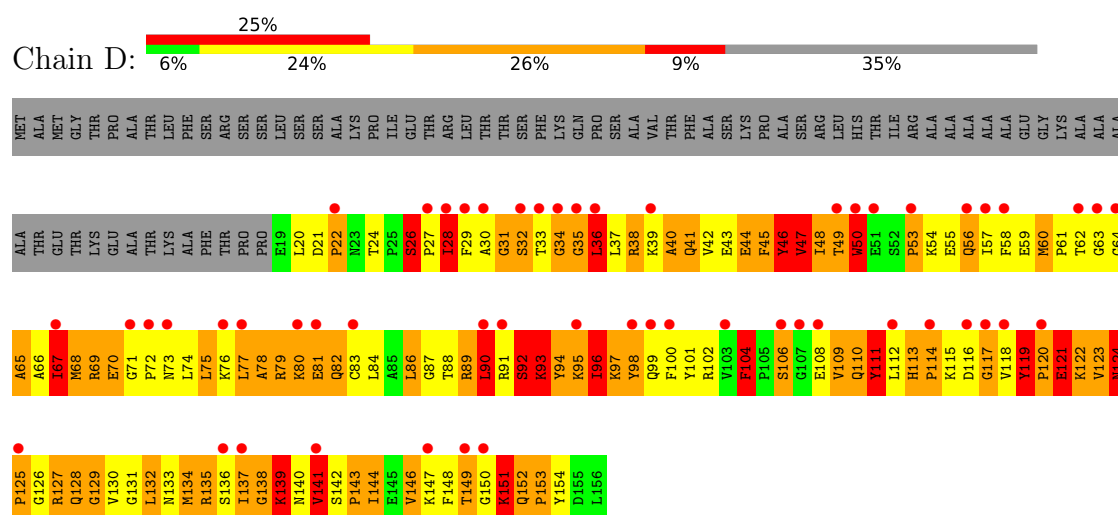




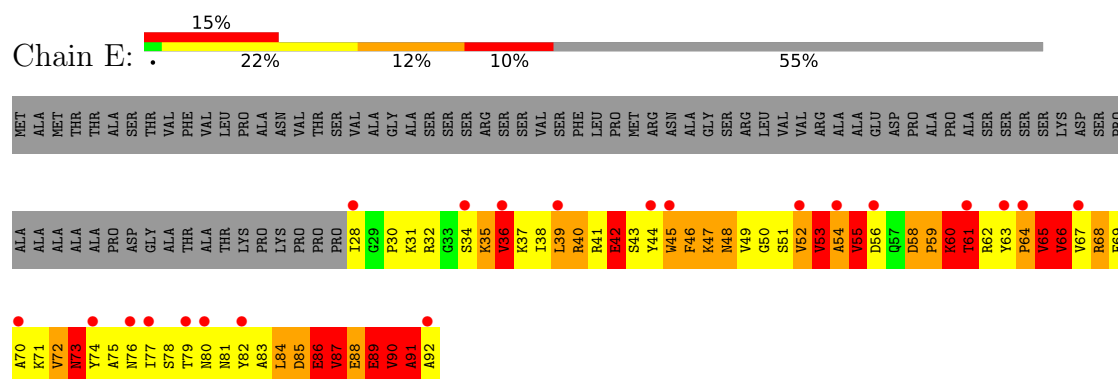
- Molecule 7: PHOTOSYSTEM I IRON-SULFUR CENTER



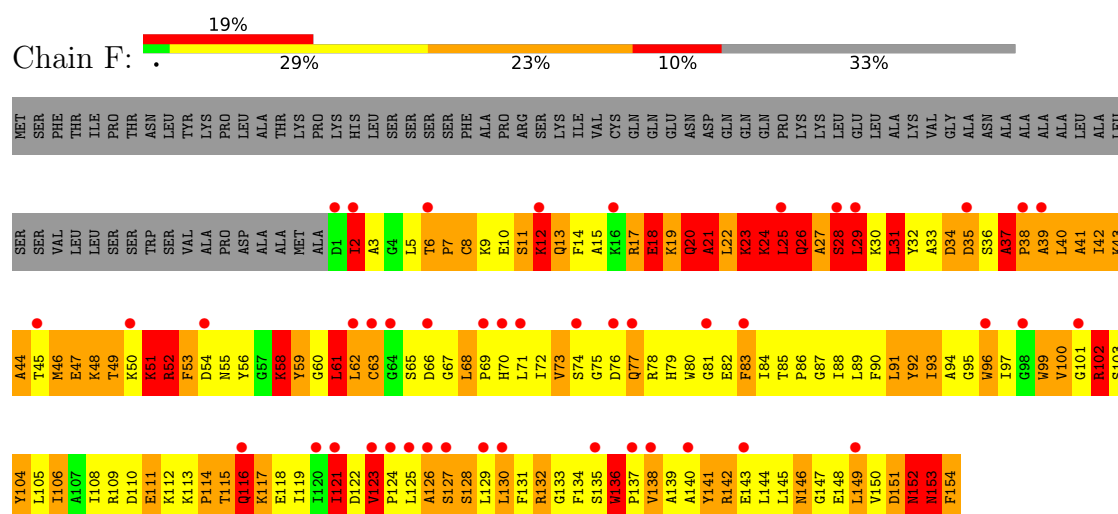
- Molecule 8: PHOTOSYSTEM I REACTION CENTER SUBUNIT II, CHLOROPLASTIC



- 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 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:  100%

GLC1
FRU2

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

Chain T:  100%

GLC1
FRU2

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

Chain U:  100%

GLC1
FRU2

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

Chain V:  100%

GLC1
FRU2

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

Chain W:  100%

GLC1
FRU2

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

Chain X:  100%

GLC1
FRU2

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

Chain Y:  100%GLC1
FRU2

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

Chain Z:  100%GLC1
FRU2

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

Chain a:  100%GLC1
FRU2

4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	120.66Å 189.09Å 129.39Å 90.00° 91.24° 90.00°	Depositor
Resolution (Å)	30.00 – 3.49 30.00 – 3.49	Depositor EDS
% Data completeness (in resolution range)	91.2 (30.00-3.49) 90.6 (30.00-3.49)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.56 (at 3.48Å)	Xtriage
Refinement program	REFMAC 5.5.0072	Depositor
R, R_{free}	0.369 , 0.375 0.387 , 0.408	Depositor DCC
R_{free} test set	1334 reflections (1.91%)	wwPDB-VP
Wilson B-factor (Å ²)	90.9	Xtriage
Anisotropy	0.544	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.20 , 98.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	0.034 for h,-k,-l	Xtriage
F_o, F_c correlation	0.72	EDS
Total number of atoms	36461	wwPDB-VP
Average B, all atoms (Å ²)	23.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.09% 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: BCR, LMU, GLC, SF4, LMG, UNL, PQN, FRU, CLA

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	0.73	0/1294	1.35	12/1762 (0.7%)
2	2	1.31	7/1426 (0.5%)	1.74	40/1950 (2.1%)
3	3	0.78	3/1270 (0.2%)	1.34	18/1714 (1.1%)
4	4	1.61	15/1362 (1.1%)	1.87	46/1855 (2.5%)
5	A	1.14	9/5938 (0.2%)	1.45	85/8104 (1.0%)
6	B	1.14	16/6058 (0.3%)	1.37	70/8278 (0.8%)
7	C	1.65	7/632 (1.1%)	1.82	23/856 (2.7%)
8	D	1.29	3/1122 (0.3%)	1.43	19/1514 (1.3%)
9	E	1.43	5/530 (0.9%)	1.51	7/718 (1.0%)
10	F	1.38	10/1250 (0.8%)	1.52	25/1687 (1.5%)
11	G	1.34	5/760 (0.7%)	1.87	28/1031 (2.7%)
12	H	1.32	2/543 (0.4%)	1.62	11/741 (1.5%)
13	I	1.19	0/235	1.32	2/320 (0.6%)
14	J	1.11	0/349	1.58	7/475 (1.5%)
15	K	0.86	0/599	1.86	31/810 (3.8%)
16	L	1.29	4/1238 (0.3%)	1.50	21/1691 (1.2%)
17	N	1.51	3/699 (0.4%)	1.65	15/936 (1.6%)
All	All	1.21	89/25305 (0.4%)	1.52	460/34442 (1.3%)

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	6
2	2	3	22
3	3	0	19
4	4	0	22
5	A	0	30
6	B	0	20

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Mol	Chain	#Chirality outliers	#Planarity outliers
7	C	0	3
8	D	0	6
9	E	0	6
10	F	0	12
11	G	1	16
12	H	0	9
15	K	0	3
16	L	0	5
17	N	0	21
18	R	0	17
All	All	4	217

The worst 5 of 89 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	4	39	TRP	CA-C	-10.24	1.39	1.52
3	3	92	TRP	CB-CG	9.80	1.80	1.50
4	4	93	ILE	CA-C	9.77	1.65	1.52
7	C	73	THR	CA-C	-8.68	1.41	1.52
4	4	93	ILE	C-O	8.54	1.34	1.24

The worst 5 of 460 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1	57	ILE	N-CA-C	24.21	135.32	110.62
11	G	44	PHE	N-CA-C	-15.90	94.78	113.38
5	A	152	ILE	N-CA-C	-13.07	98.24	110.53
11	G	21	PHE	N-CA-C	12.78	124.90	110.97
5	A	532	ILE	CA-C-N	12.68	133.49	119.92

All (4) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	2	67	PHE	CA
2	2	101	PHE	CA
2	2	174	VAL	CA
11	G	21	PHE	CA

5 of 217 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	1	184	PRO	Peptide

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Mol	Chain	Res	Type	Group
1	1	56	GLY	Peptide
1	1	57	ILE	Peptide
1	1	60	PRO	Peptide
1	1	63	LEU	Peptide

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	1	1255	0	1222	210	0
2	2	1380	0	1341	496	0
3	3	1233	0	1199	294	12
4	4	1322	0	1287	760	8
5	A	5745	0	5595	1697	0
6	B	5848	0	5653	1518	13
7	C	619	0	608	238	0
8	D	1095	0	1112	227	0
9	E	520	0	528	156	0
10	F	1221	0	1246	328	1
11	G	740	0	709	306	11
12	H	529	0	514	127	0
13	I	229	0	252	66	0
14	J	338	0	340	79	0
15	K	593	0	618	127	0
16	L	1203	0	1213	380	8
17	N	685	0	670	456	11
18	R	265	0	65	65	0
19	M	23	0	21	0	0
19	O	22	0	18	10	0
19	P	23	0	21	16	0
19	Q	23	0	21	14	0
19	S	23	0	21	6	0
19	T	23	0	21	6	0
19	U	23	0	21	21	0
19	V	23	0	21	2	0
19	W	23	0	18	5	0
19	X	23	0	21	12	0
19	Y	23	0	20	19	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
19	Z	23	0	21	13	0
19	a	23	0	21	4	0
20	1	606	0	376	169	1
20	2	672	0	513	137	0
20	3	659	0	382	131	0
20	4	710	0	463	178	0
20	A	2449	0	2260	957	1
20	B	2360	0	2255	804	0
20	F	130	0	86	30	0
20	G	51	0	40	19	0
20	H	275	0	239	80	0
20	I	60	0	58	10	0
20	J	109	0	95	54	0
20	K	210	0	177	41	1
20	L	272	0	239	100	0
20	R	115	0	106	22	0
21	1	175	0	230	45	0
21	2	175	0	230	25	3
21	3	70	0	92	12	0
21	4	174	0	224	23	4
21	A	210	0	276	85	0
21	B	105	0	138	45	15
21	C	35	0	46	0	0
21	D	35	0	40	12	0
21	E	35	0	41	30	0
21	F	34	0	41	19	0
21	G	35	0	46	19	0
21	H	175	0	230	108	0
21	K	140	0	183	95	0
21	L	105	0	138	10	0
21	N	35	0	45	35	0
21	R	245	0	321	84	4
22	3	40	0	54	19	13
22	A	200	0	269	213	0
22	B	240	0	321	144	0
22	F	80	0	108	73	0
22	I	80	0	108	64	0
22	J	40	0	52	42	0
22	L	40	0	54	51	0
23	A	33	0	46	9	0
23	B	33	0	46	31	0
24	A	8	0	0	19	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
24	C	16	0	0	8	0
25	B	49	0	71	29	0
26	H	23	0	0	2	0
All	All	36461	0	35177	9873	53

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 138.

The worst 5 of 9873 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)
2:2:43:TRP:CZ3	2:2:125:PHE:CG	1.81	1.63
4:4:69:ILE:CD1	4:4:175:LYS:HG2	1.30	1.61
2:2:43:TRP:CH2	2:2:125:PHE:CE1	1.88	1.61
4:4:69:ILE:HD11	4:4:175:LYS:CG	1.24	1.61
2:2:43:TRP:CH2	2:2:125:PHE:CZ	1.85	1.60

The worst 5 of 53 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)
22:3:314:BCR:C28	21:B:847:LMU:C5[2_556]	0.48	1.72
22:3:314:BCR:C40	21:B:847:LMU:C8[2_556]	0.57	1.63
4:4:130:GLU:O	16:L:159:TYR:OH[1_655]	0.69	1.51
3:3:181:LEU:CG	6:B:490:ARG:NH2[1_556]	0.72	1.48
11:G:31:MET:CE	17:N:85:TRP:NE1[2_546]	0.72	1.48

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	160/241 (66%)	83 (52%)	47 (29%)	30 (19%)	0	1
2	2	174/269 (65%)	62 (36%)	48 (28%)	64 (37%)	0	0
3	3	154/276 (56%)	77 (50%)	42 (27%)	35 (23%)	0	1
4	4	164/251 (65%)	56 (34%)	47 (29%)	61 (37%)	0	0
5	A	726/758 (96%)	333 (46%)	198 (27%)	195 (27%)	0	0
6	B	731/734 (100%)	362 (50%)	186 (25%)	183 (25%)	0	0
7	C	79/81 (98%)	23 (29%)	29 (37%)	27 (34%)	0	0
8	D	136/212 (64%)	49 (36%)	41 (30%)	46 (34%)	0	0
9	E	63/143 (44%)	28 (44%)	15 (24%)	20 (32%)	0	0
10	F	152/231 (66%)	69 (45%)	41 (27%)	42 (28%)	0	0
11	G	93/167 (56%)	37 (40%)	25 (27%)	31 (33%)	0	0
12	H	67/144 (46%)	28 (42%)	15 (22%)	24 (36%)	0	0
13	I	28/40 (70%)	10 (36%)	11 (39%)	7 (25%)	0	0
14	J	40/44 (91%)	19 (48%)	11 (28%)	10 (25%)	0	0
15	K	82/131 (63%)	54 (66%)	12 (15%)	16 (20%)	0	1
16	L	159/216 (74%)	65 (41%)	46 (29%)	48 (30%)	0	0
17	N	83/170 (49%)	22 (26%)	19 (23%)	42 (51%)	0	0
All	All	3091/4108 (75%)	1377 (44%)	833 (27%)	881 (28%)	0	0

5 of 881 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	1	25	ASP
1	1	30	GLY
1	1	35	ASN
1	1	90	PRO
1	1	130	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	1	126/190 (66%)	96 (76%)	30 (24%)	1	4
2	2	141/216 (65%)	77 (55%)	64 (45%)	0	0
3	3	118/215 (55%)	75 (64%)	43 (36%)	0	1
4	4	139/201 (69%)	68 (49%)	71 (51%)	0	0
5	A	592/618 (96%)	375 (63%)	217 (37%)	0	1
6	B	598/600 (100%)	362 (60%)	236 (40%)	0	1
7	C	70/70 (100%)	40 (57%)	30 (43%)	0	0
8	D	118/173 (68%)	78 (66%)	40 (34%)	0	2
9	E	56/114 (49%)	36 (64%)	20 (36%)	0	1
10	F	127/190 (67%)	77 (61%)	50 (39%)	0	1
11	G	79/144 (55%)	46 (58%)	33 (42%)	0	0
12	H	57/115 (50%)	28 (49%)	29 (51%)	0	0
13	I	26/36 (72%)	18 (69%)	8 (31%)	0	2
14	J	36/39 (92%)	23 (64%)	13 (36%)	0	1
15	K	61/102 (60%)	35 (57%)	26 (43%)	0	0
16	L	124/169 (73%)	81 (65%)	43 (35%)	0	2
17	N	74/139 (53%)	32 (43%)	42 (57%)	0	0
All	All	2542/3331 (76%)	1547 (61%)	995 (39%)	0	1

5 of 995 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
6	B	142	LEU
15	K	10	ILE
6	B	481	THR
14	J	14	LEU
16	L	151	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 113 such sidechains are listed below:

Mol	Chain	Res	Type
6	B	266	GLN
16	L	129	GLN
6	B	595	HIS
16	L	60	HIS
11	G	39	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	0.86	0	15,15,17	2.46	4 (26%)
19	FRU	M	2	19	11,12,12	1.15	2 (18%)	10,18,18	0.97	0
19	GLC	O	1	19	10,10,12	1.48	3 (30%)	14,14,17	3.32	9 (64%)
19	FRU	O	2	19	11,12,12	1.11	1 (9%)	10,18,18	2.31	3 (30%)
19	GLC	P	1	19	11,11,12	1.51	2 (18%)	15,15,17	2.88	10 (66%)
19	FRU	P	2	19	11,12,12	1.38	2 (18%)	10,18,18	2.17	2 (20%)
19	GLC	Q	1	19	11,11,12	1.02	0	15,15,17	3.55	8 (53%)
19	FRU	Q	2	19	11,12,12	1.29	1 (9%)	10,18,18	1.71	2 (20%)
19	GLC	S	1	19	11,11,12	1.19	1 (9%)	15,15,17	1.61	3 (20%)
19	FRU	S	2	19	11,12,12	2.16	4 (36%)	10,18,18	2.83	4 (40%)
19	GLC	T	1	19	11,11,12	1.36	2 (18%)	15,15,17	1.81	3 (20%)
19	FRU	T	2	19	11,12,12	1.74	2 (18%)	10,18,18	2.33	4 (40%)
19	GLC	U	1	19	11,11,12	1.37	1 (9%)	15,15,17	1.56	3 (20%)
19	FRU	U	2	19	11,12,12	1.25	1 (9%)	10,18,18	1.61	2 (20%)
19	GLC	V	1	19	11,11,12	1.15	1 (9%)	15,15,17	3.47	6 (40%)
19	FRU	V	2	19	11,12,12	1.16	0	10,18,18	2.27	4 (40%)
19	GLC	W	1	19	11,11,12	1.16	1 (9%)	15,15,17	1.60	3 (20%)
19	FRU	W	2	19	11,12,12	1.23	1 (9%)	10,18,18	2.21	3 (30%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
19	GLC	X	1	19	11,11,12	1.29	1 (9%)	15,15,17	2.17	4 (26%)
19	FRU	X	2	19	11,12,12	1.17	1 (9%)	10,18,18	1.83	4 (40%)
19	GLC	Y	1	19	11,11,12	1.95	3 (27%)	15,15,17	4.48	8 (53%)
19	FRU	Y	2	21,19	11,12,12	1.17	2 (18%)	10,18,18	2.41	3 (30%)
19	GLC	Z	1	19	11,11,12	1.08	0	15,15,17	2.04	5 (33%)
19	FRU	Z	2	19	11,12,12	0.70	0	10,18,18	1.67	4 (40%)
19	GLC	a	1	19	11,11,12	1.73	2 (18%)	15,15,17	2.10	5 (33%)
19	FRU	a	2	19	11,12,12	1.06	0	10,18,18	2.02	5 (50%)

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	2/5/24/24	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	-	1/2/19/22	0/1/1/1
19	FRU	P	2	19	1/1/4/4	2/5/24/24	0/1/1/1
19	GLC	Q	1	19	-	1/2/19/22	0/1/1/1
19	FRU	Q	2	19	1/1/4/4	4/5/24/24	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	3/5/24/24	0/1/1/1
19	GLC	T	1	19	-	2/2/19/22	0/1/1/1
19	FRU	T	2	19	1/1/4/4	3/5/24/24	0/1/1/1
19	GLC	U	1	19	-	2/2/19/22	0/1/1/1
19	FRU	U	2	19	1/1/4/4	5/5/24/24	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	1/5/24/24	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	2/5/24/24	0/1/1/1
19	GLC	X	1	19	-	2/2/19/22	0/1/1/1
19	FRU	X	2	19	1/1/4/4	3/5/24/24	0/1/1/1
19	GLC	Y	1	19	-	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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
19	GLC	Z	1	19	-	2/2/19/22	0/1/1/1
19	FRU	Z	2	19	1/1/4/4	1/5/24/24	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	3/5/24/24	0/1/1/1

The worst 5 of 34 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	Y	1	GLC	O5-C1	-4.80	1.36	1.43
19	S	2	FRU	O5-C2	-3.61	1.37	1.43
19	U	2	FRU	O5-C2	-3.34	1.38	1.43
19	Q	2	FRU	O5-C2	-3.19	1.38	1.43
19	T	2	FRU	O5-C2	-3.14	1.38	1.43

The worst 5 of 111 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	Y	1	GLC	C1-O5-C5	-11.22	97.00	112.19
19	M	1	GLC	C1-O5-C5	7.92	122.92	112.19
19	O	1	GLC	C1-C2-C3	7.69	119.11	109.67
19	V	1	GLC	C1-O5-C5	7.47	122.31	112.19
19	Y	1	GLC	O5-C1-C2	-7.39	99.37	110.77

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 50 torsion outliers are listed below:

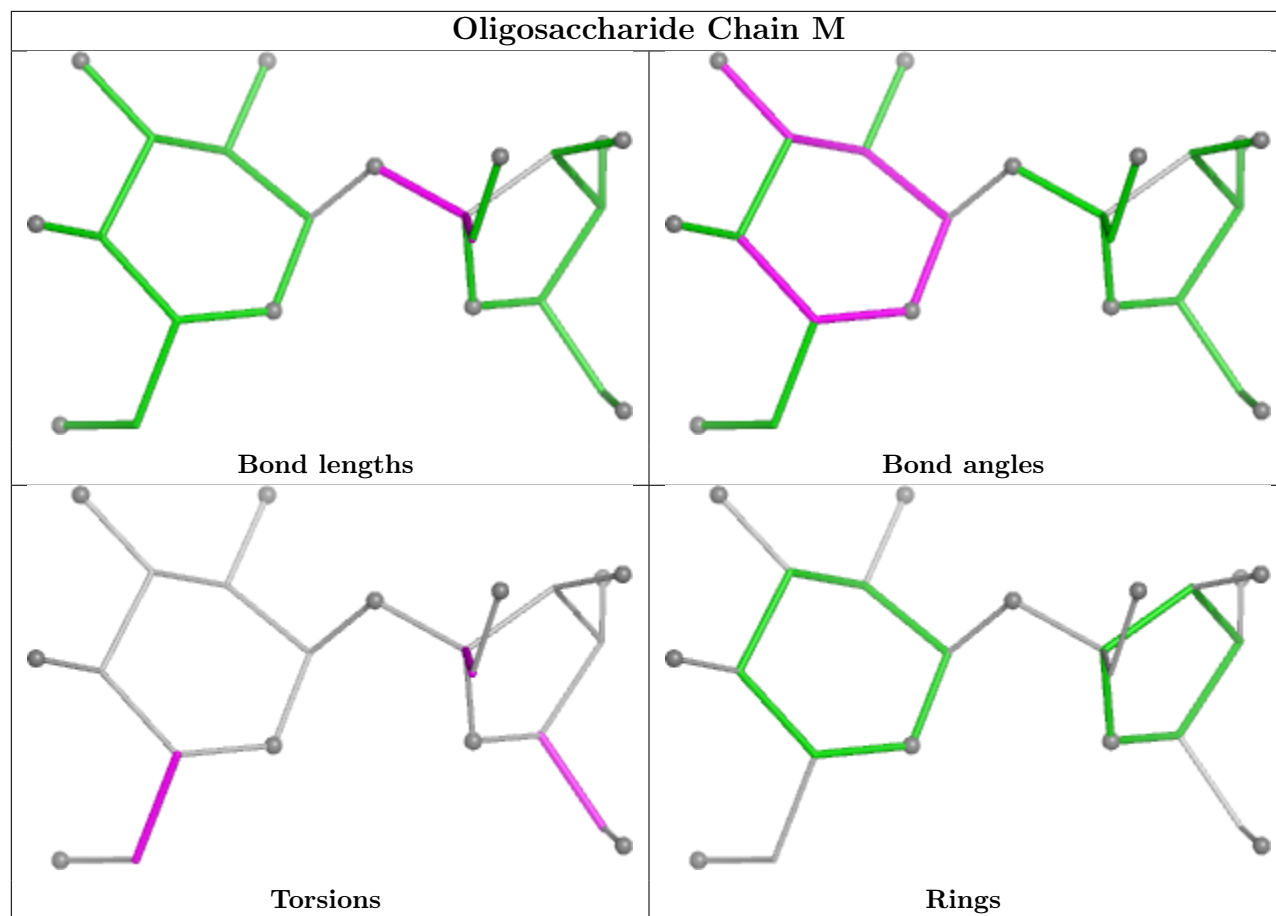
Mol	Chain	Res	Type	Atoms
19	Q	2	FRU	O1-C1-C2-C3
19	Q	2	FRU	O1-C1-C2-O2
19	U	2	FRU	O1-C1-C2-C3
19	U	2	FRU	O1-C1-C2-O2
19	U	2	FRU	C4-C5-C6-O6

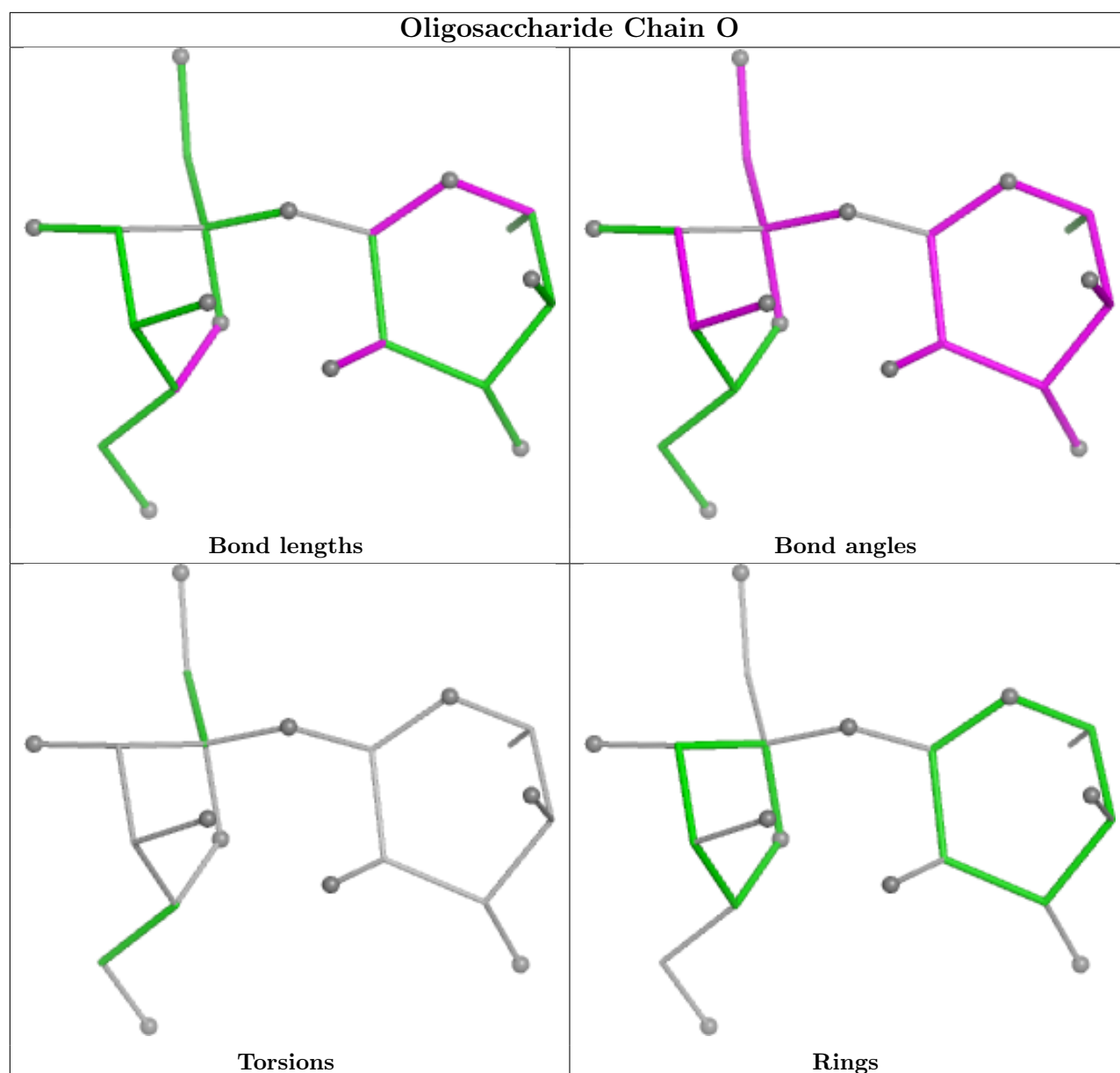
There are no ring outliers.

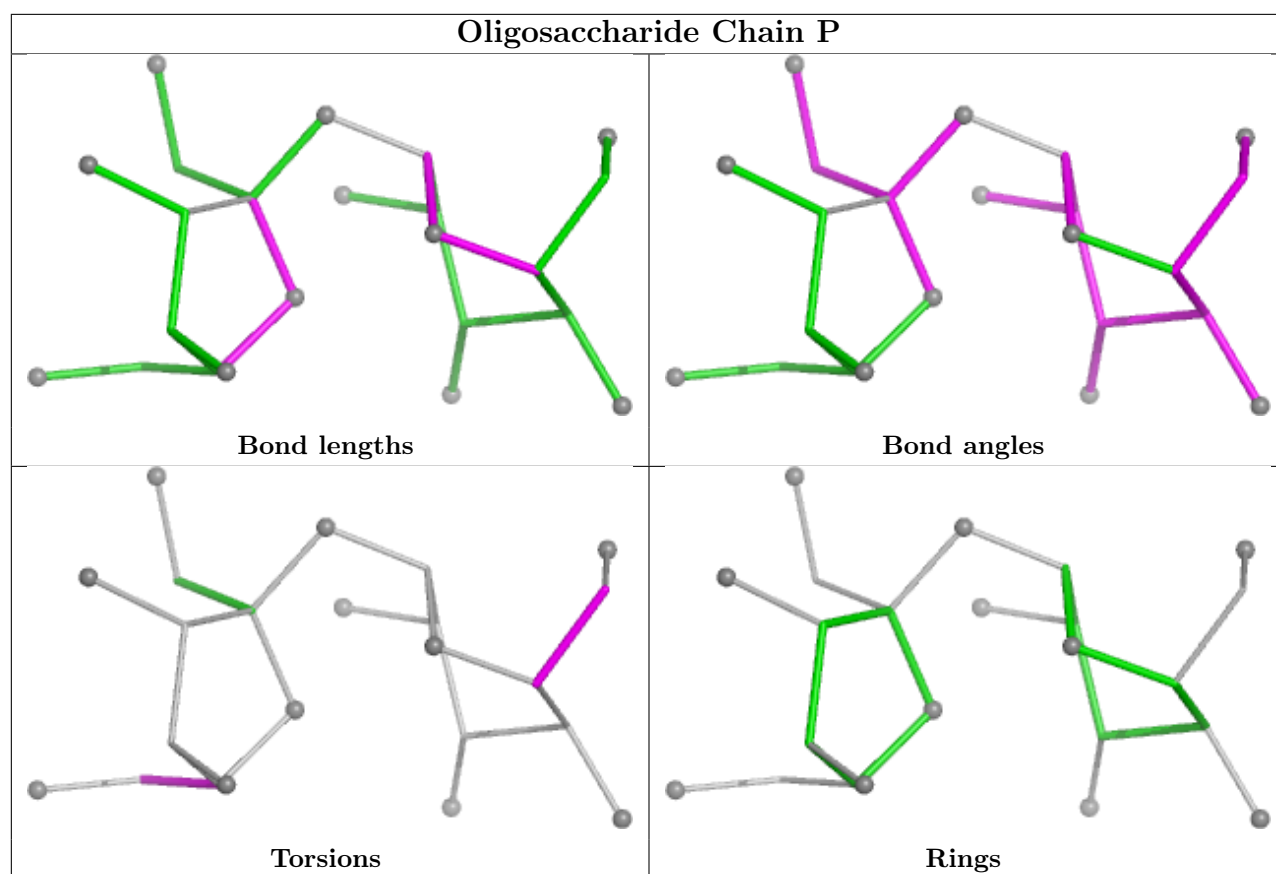
24 monomers are involved in 128 short contacts:

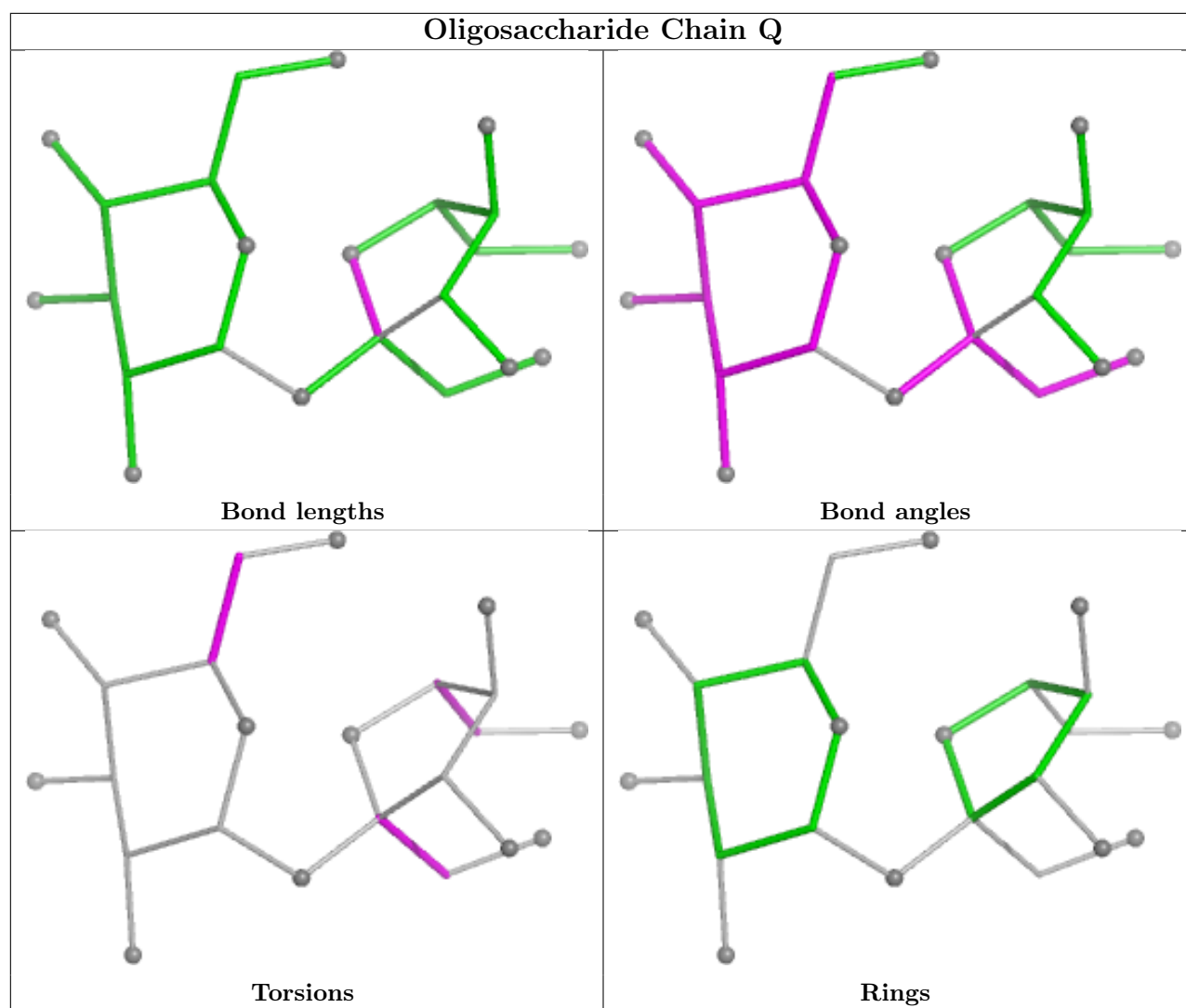
Mol	Chain	Res	Type	Clashes	Symm-Clashes
19	Z	2	FRU	9	0
19	Z	1	GLC	13	0
19	Q	2	FRU	14	0
19	Y	2	FRU	17	0
19	W	2	FRU	3	0
19	U	1	GLC	11	0
19	P	2	FRU	15	0
19	P	1	GLC	10	0
19	Q	1	GLC	5	0
19	U	2	FRU	20	0
19	Y	1	GLC	7	0
19	V	2	FRU	2	0
19	W	1	GLC	2	0
19	X	2	FRU	9	0
19	X	1	GLC	11	0
19	a	2	FRU	4	0
19	S	2	FRU	6	0
19	O	2	FRU	6	0
19	S	1	GLC	5	0
19	T	2	FRU	6	0
19	V	1	GLC	1	0
19	a	1	GLC	3	0
19	O	1	GLC	10	0
19	T	1	GLC	6	0

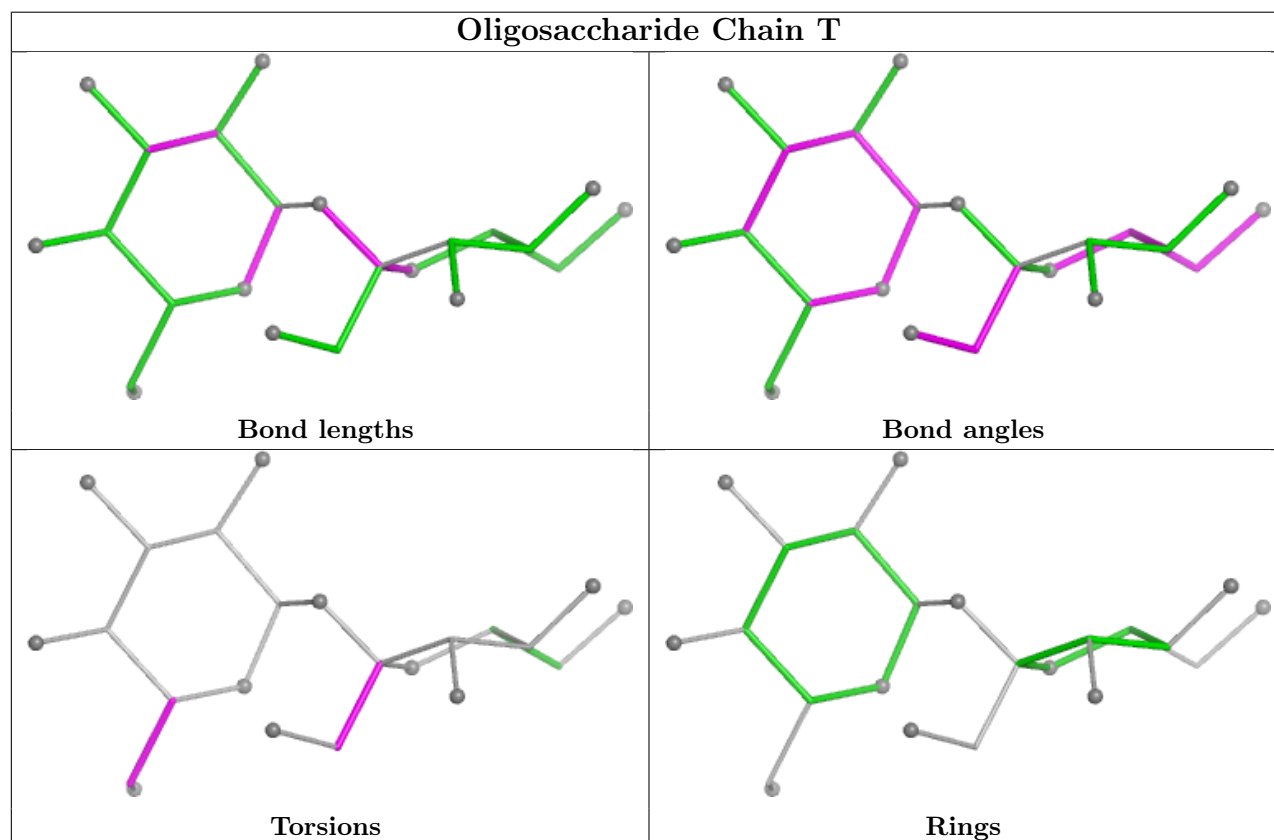
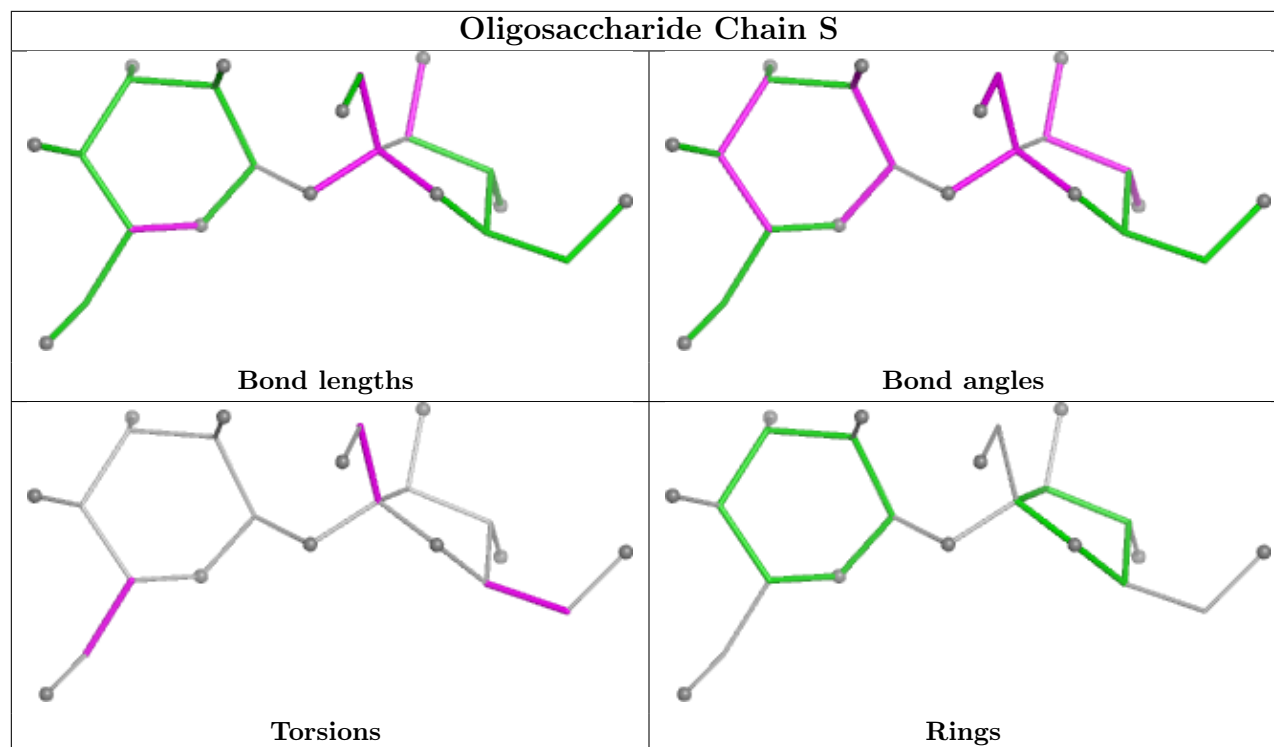
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

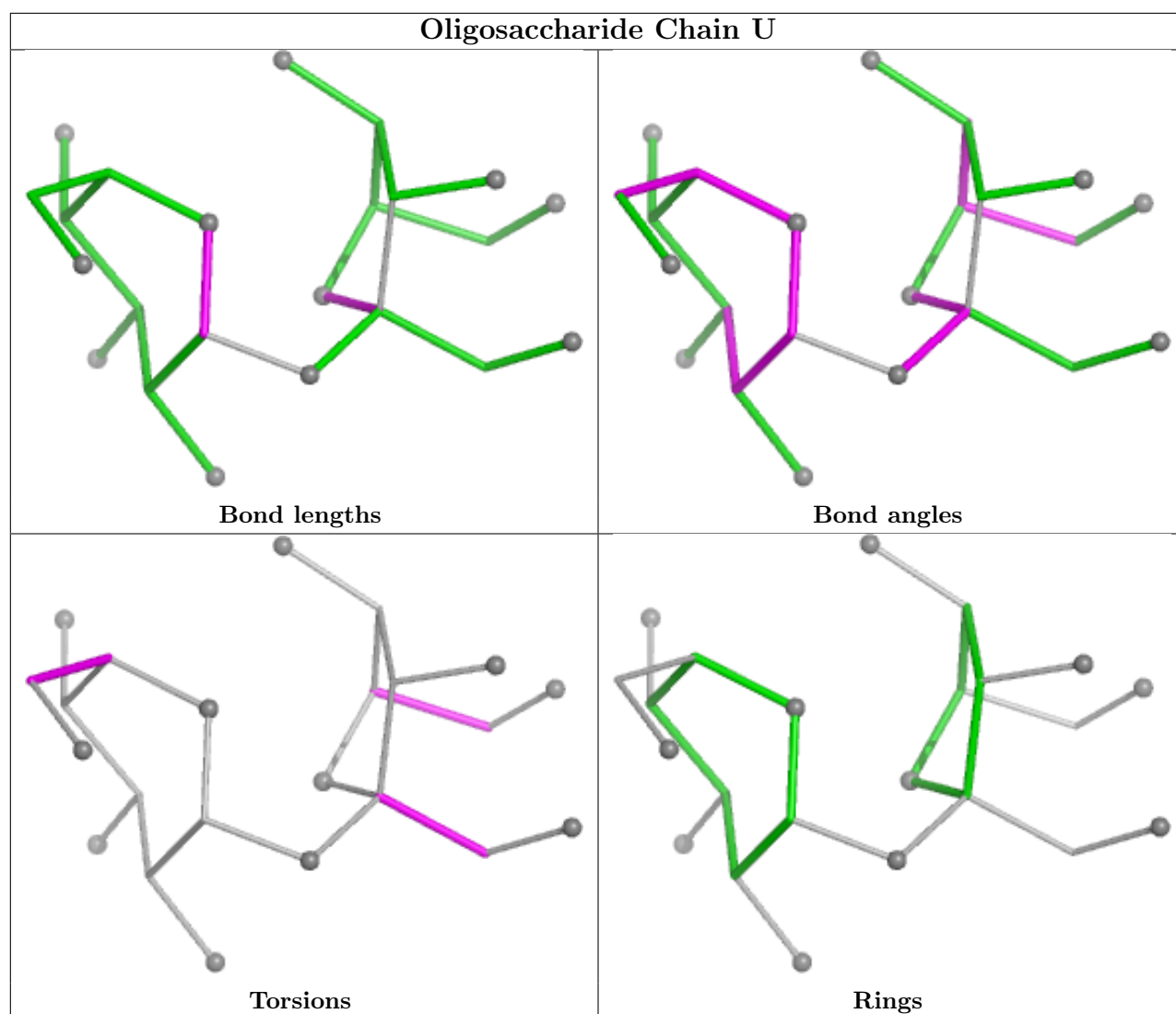


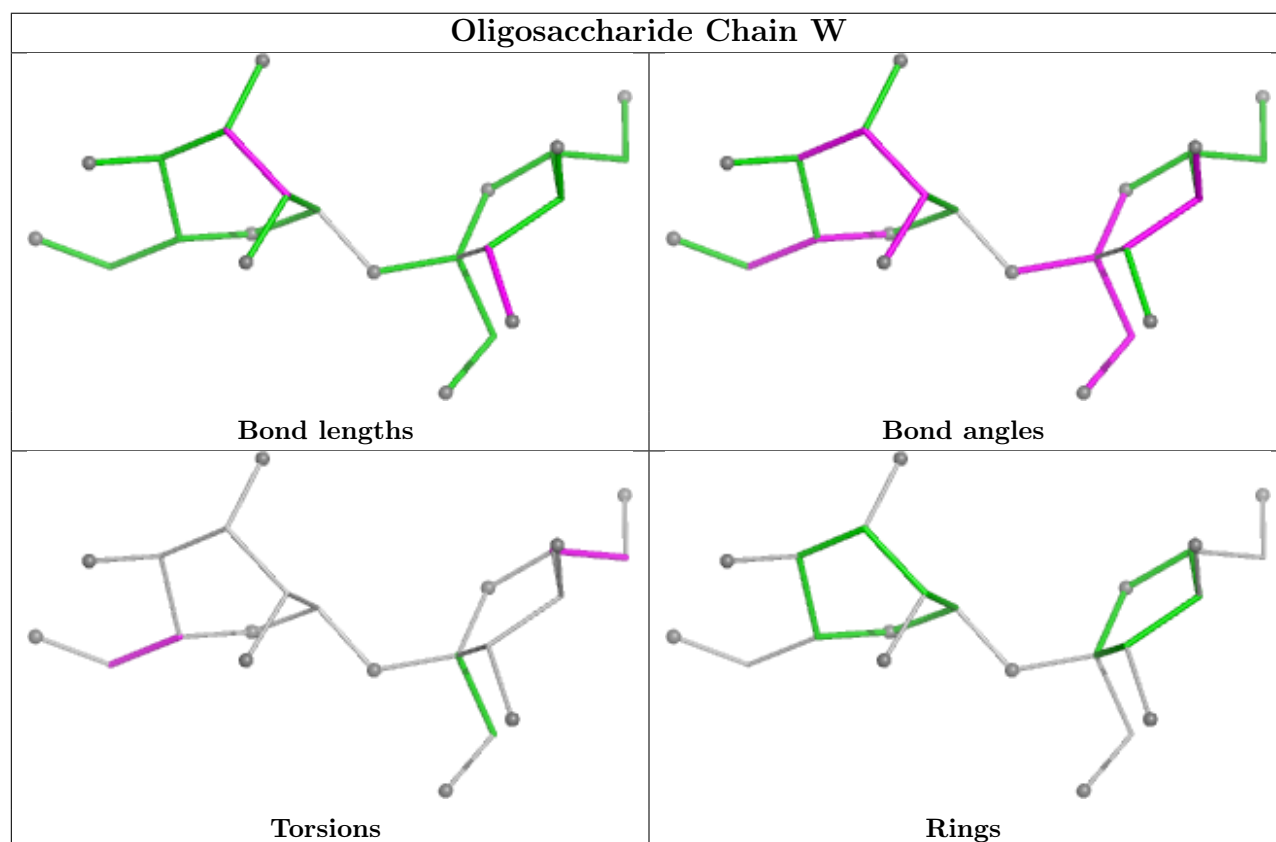
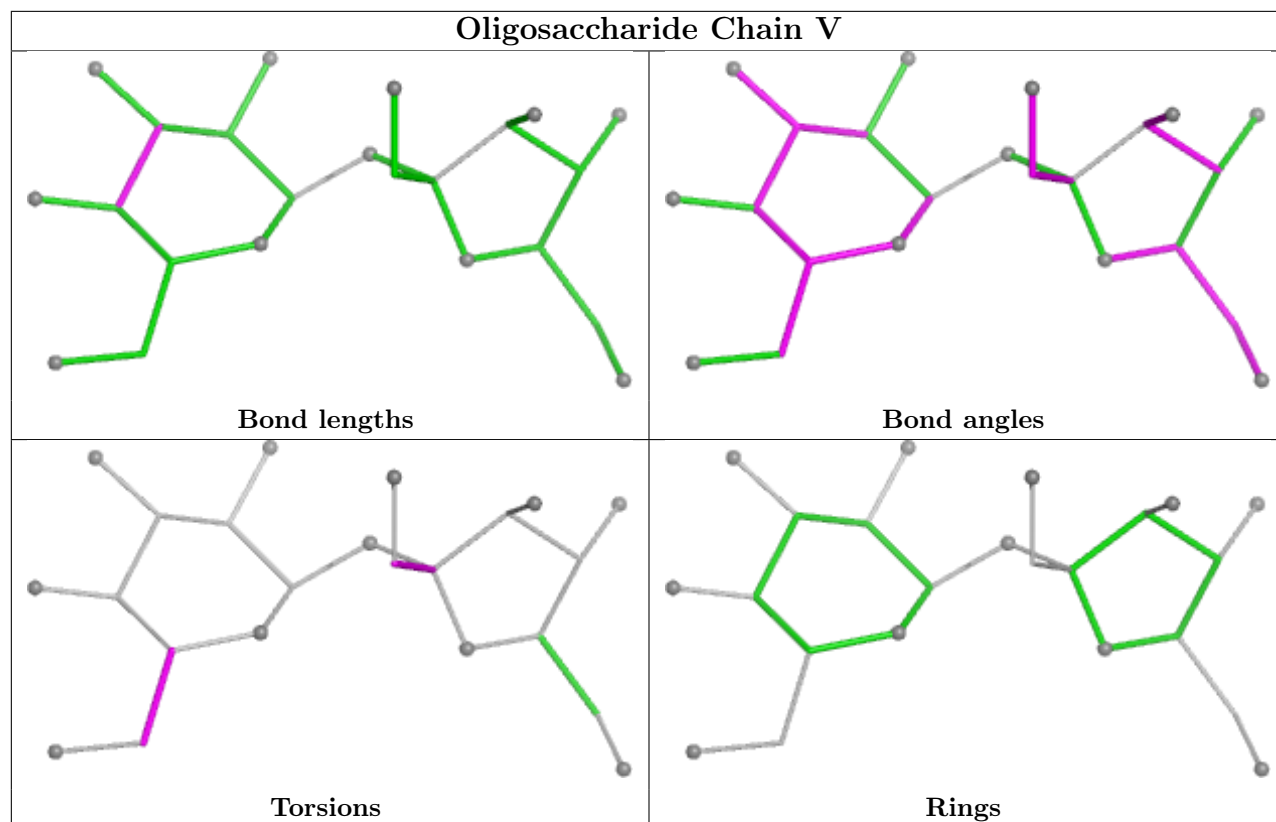


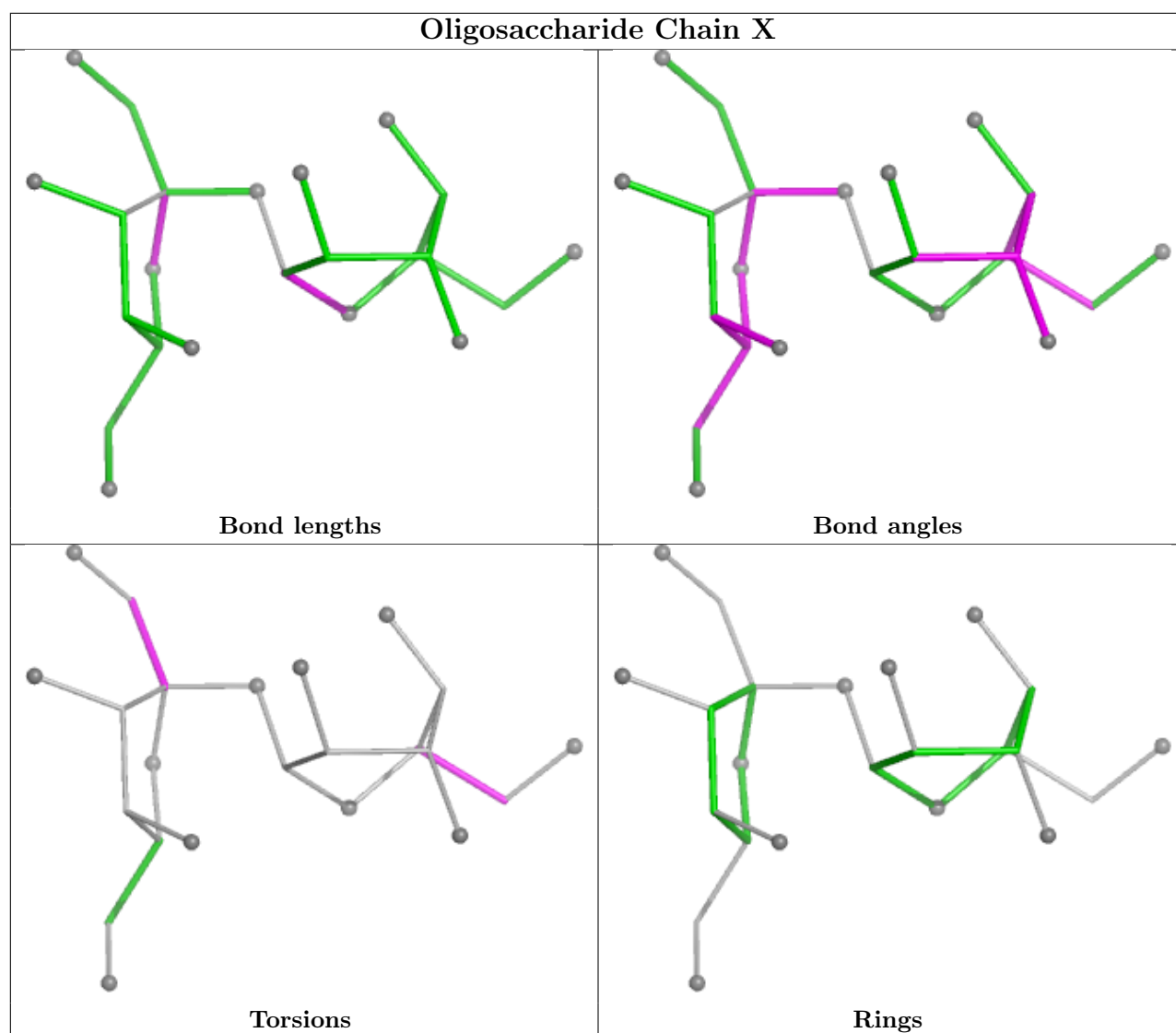


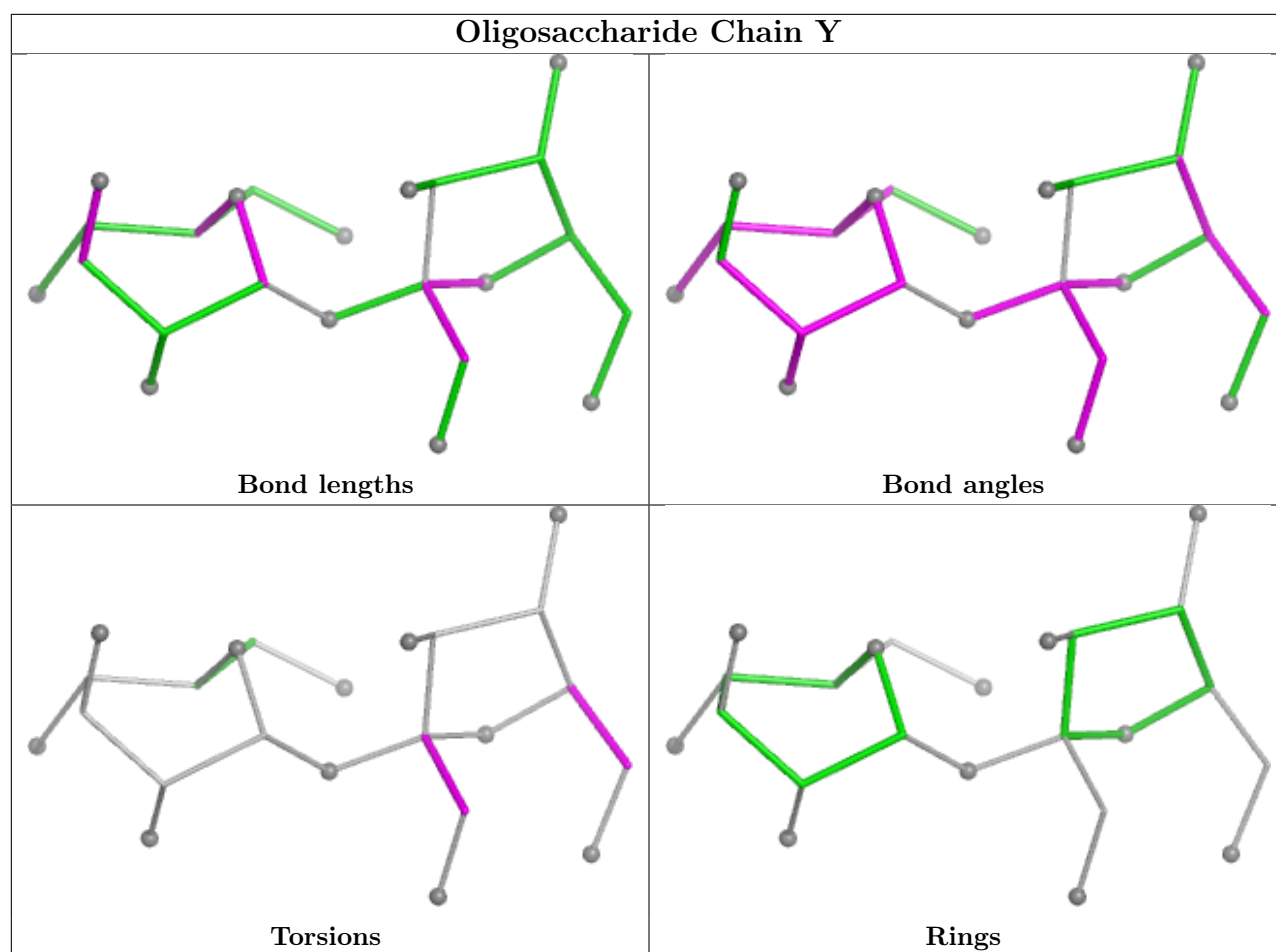


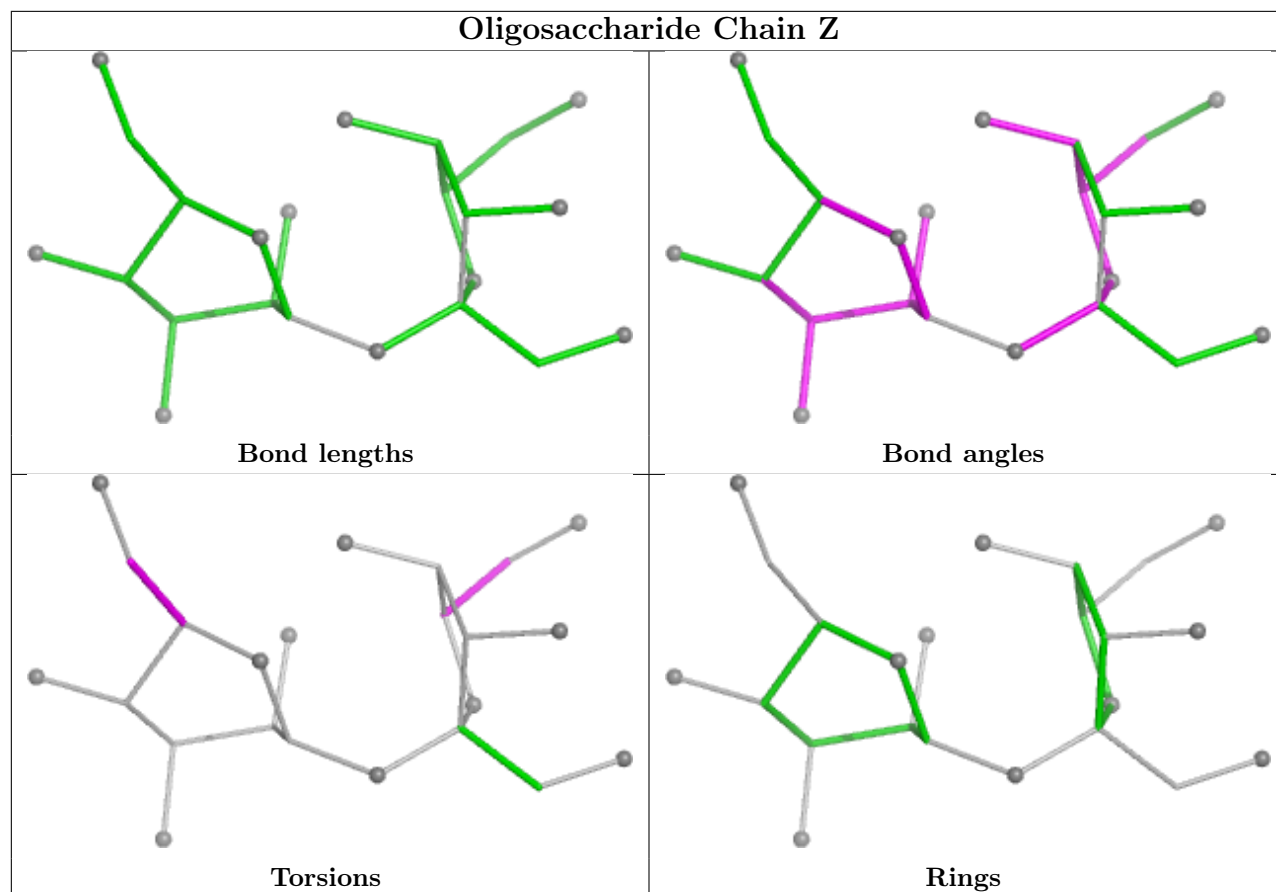


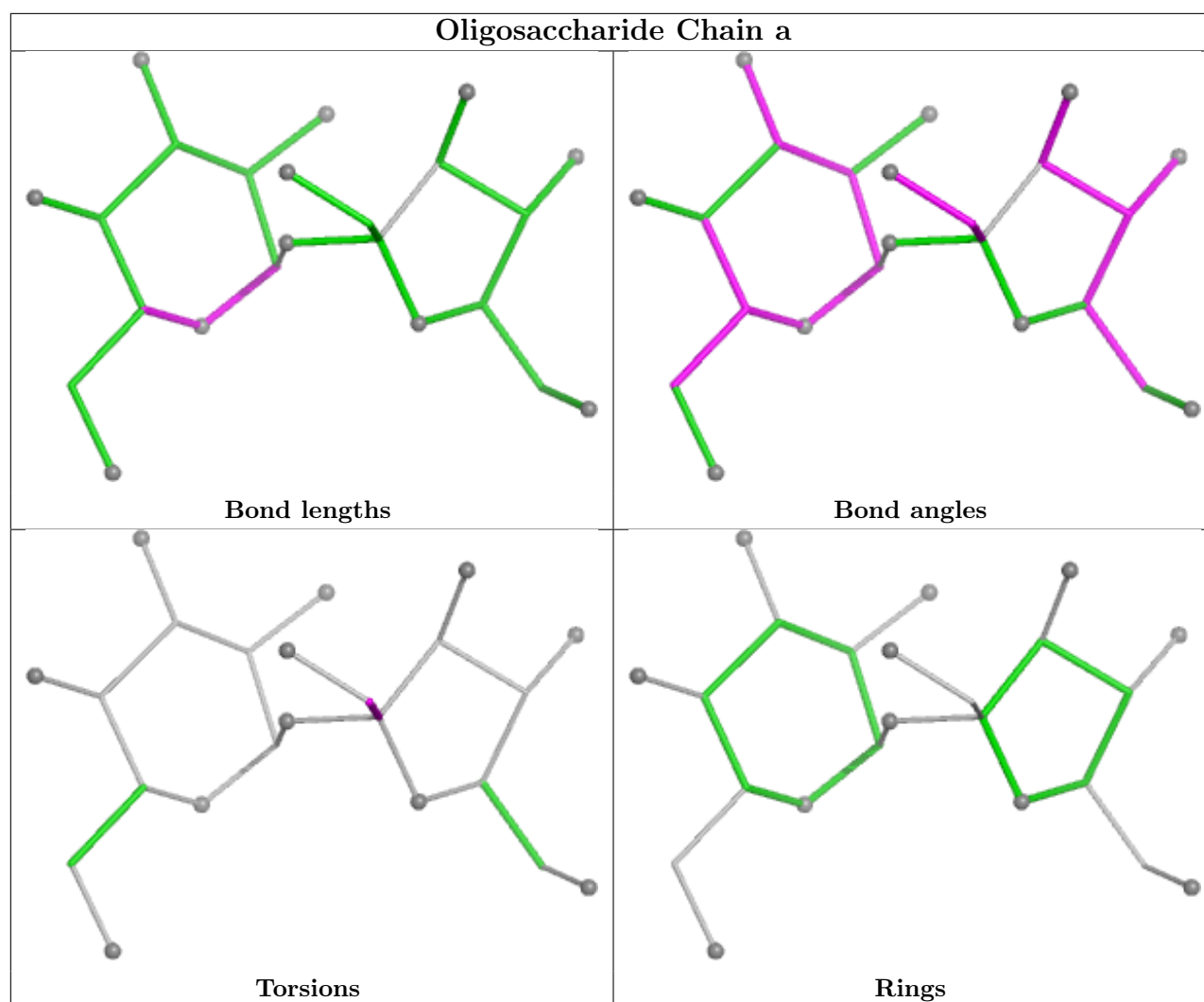












5.6 Ligand geometry [i](#)

Of 249 ligands modelled in this entry, 1 is unknown - leaving 248 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	4	319	21	51,55,73	2.52	16 (31%)	61,91,113	3.00	21 (34%)
20	CLA	R	107	-	61,65,73	2.34	13 (21%)	73,103,113	2.92	28 (38%)
21	LMU	4	322	20	36,36,36	0.75	1 (2%)	47,47,47	1.26	4 (8%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
20	CLA	L	206	22,16	51,55,73	2.43	13 (25%)	61,91,113	3.36	28 (45%)
20	CLA	4	304	-	69,73,73	2.60	30 (43%)	83,113,113	3.57	38 (45%)
20	CLA	A	836	-	51,55,73	2.48	15 (29%)	61,91,113	2.81	23 (37%)
21	LMU	4	301	-	36,36,36	0.41	0	47,47,47	0.72	1 (2%)
20	CLA	3	318	-	26,32,73	2.78	13 (50%)	34,54,113	3.53	22 (64%)
21	LMU	L	209	-	36,36,36	0.87	1 (2%)	47,47,47	1.50	9 (19%)
20	CLA	B	807	-	69,73,73	2.25	17 (24%)	83,113,113	2.85	29 (34%)
20	CLA	B	816	6	64,68,73	2.18	13 (20%)	77,107,113	2.76	29 (37%)
21	LMU	A	853	-	36,36,36	0.40	0	47,47,47	0.72	1 (2%)
25	LMG	B	848	-	49,49,55	0.96	2 (4%)	57,57,63	1.02	3 (5%)
20	CLA	3	307	-	26,32,73	2.34	10 (38%)	34,54,113	3.15	23 (67%)
20	CLA	3	316	-	54,58,73	2.55	13 (24%)	65,95,113	2.68	25 (38%)
20	CLA	2	312	-	54,58,73	2.56	13 (24%)	65,95,113	3.05	27 (41%)
20	CLA	B	813	6	64,68,73	2.25	14 (21%)	77,107,113	2.67	26 (33%)
20	CLA	1	208	-	26,32,73	2.63	12 (46%)	34,54,113	3.37	22 (64%)
20	CLA	B	817	-	65,69,73	2.18	16 (24%)	78,108,113	2.88	30 (38%)
20	CLA	H	103	-	59,63,73	2.35	14 (23%)	71,101,113	3.06	28 (39%)
20	CLA	3	310	-	26,32,73	2.45	11 (42%)	34,54,113	3.41	21 (61%)
22	BCR	I	101	-	41,41,41	2.84	17 (41%)	56,56,56	5.37	31 (55%)
20	CLA	2	315	-	69,73,73	2.21	15 (21%)	83,113,113	2.73	25 (30%)
20	CLA	A	811	20,5	69,73,73	2.18	12 (17%)	83,113,113	3.07	30 (36%)
20	CLA	B	806	-	69,73,73	2.20	16 (23%)	83,113,113	3.09	34 (40%)
21	LMU	3	321	-	36,36,36	0.71	0	47,47,47	1.91	11 (23%)
21	LMU	F	201	-	35,35,36	1.30	4 (11%)	46,46,47	2.37	15 (32%)
20	CLA	A	814	5	49,53,73	2.64	15 (30%)	59,89,113	3.05	24 (40%)
20	CLA	1	210	-	55,59,73	2.95	26 (47%)	66,96,113	4.11	31 (46%)
22	BCR	B	842	-	41,41,41	1.97	4 (9%)	56,56,56	5.89	20 (35%)
20	CLA	B	811	-	62,66,73	2.68	24 (38%)	74,104,113	3.38	33 (44%)
21	LMU	R	101	-	36,36,36	1.04	2 (5%)	47,47,47	2.44	13 (27%)
20	CLA	3	302	-	54,58,73	3.17	24 (44%)	65,95,113	3.14	27 (41%)
20	CLA	A	851	-	69,73,73	2.21	18 (26%)	83,113,113	2.72	27 (32%)
20	CLA	1	202	20,1	61,65,73	2.79	28 (45%)	73,103,113	3.45	34 (46%)
20	CLA	3	309	-	26,32,73	2.33	9 (34%)	34,54,113	3.01	22 (64%)
20	CLA	A	806	-	59,63,73	2.36	15 (25%)	71,101,113	3.04	26 (36%)
20	CLA	A	823	-	69,73,73	2.09	15 (21%)	83,113,113	2.61	26 (31%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
20	CLA	4	310	-	26,32,73	2.46	15 (57%)	34,54,113	3.27	20 (58%)
20	CLA	I	102	-	64,68,73	2.27	15 (23%)	77,107,113	2.87	24 (31%)
21	LMU	G	101	-	36,36,36	1.02	2 (5%)	47,47,47	2.58	13 (27%)
20	CLA	B	815	-	63,67,73	2.28	16 (25%)	75,105,113	2.41	21 (28%)
21	LMU	1	218	-	36,36,36	0.44	0	47,47,47	1.61	9 (19%)
20	CLA	3	315	-	26,32,73	2.52	9 (34%)	34,54,113	3.07	21 (61%)
20	CLA	H	101	-	59,63,73	2.73	25 (42%)	71,101,113	3.37	34 (47%)
20	CLA	B	835	6	64,68,73	2.18	12 (18%)	77,107,113	2.98	22 (28%)
20	CLA	B	828	6	54,58,73	2.69	16 (29%)	65,95,113	2.75	29 (44%)
21	LMU	H	107	-	36,36,36	0.77	0	47,47,47	2.24	14 (29%)
21	LMU	H	108	-	36,36,36	1.03	3 (8%)	47,47,47	2.76	19 (40%)
20	CLA	2	308	-	69,73,73	2.17	12 (17%)	83,113,113	2.78	28 (33%)
20	CLA	1	204	-	50,54,73	2.64	18 (36%)	60,90,113	2.87	24 (40%)
22	BCR	B	843	-	41,41,41	2.11	5 (12%)	56,56,56	5.92	21 (37%)
22	BCR	A	845	-	41,41,41	2.00	5 (12%)	56,56,56	5.92	23 (41%)
20	CLA	2	303	-	69,73,73	2.22	16 (23%)	83,113,113	2.78	32 (38%)
20	CLA	3	319	-	26,32,73	2.49	8 (30%)	34,54,113	3.41	18 (52%)
21	LMU	2	317	-	36,36,36	1.06	1 (2%)	47,47,47	1.93	15 (31%)
20	CLA	1	201	1	50,54,73	2.94	28 (56%)	60,90,113	4.17	38 (63%)
20	CLA	2	301	-	26,32,73	2.57	14 (53%)	34,54,113	3.40	20 (58%)
20	CLA	2	314	-	26,32,73	2.42	10 (38%)	34,54,113	2.93	20 (58%)
20	CLA	A	816	-	58,62,73	2.77	24 (41%)	69,99,113	3.03	25 (36%)
21	LMU	2	318	-	36,36,36	1.01	1 (2%)	47,47,47	1.28	6 (12%)
20	CLA	B	839	-	69,73,73	2.11	16 (23%)	83,113,113	2.87	28 (33%)
21	LMU	4	317	-	36,36,36	0.75	1 (2%)	47,47,47	1.15	3 (6%)
21	LMU	B	847	22	36,36,36	1.00	1 (2%)	47,47,47	2.37	16 (34%)
21	LMU	D	201	21	36,36,36	0.40	0	47,47,47	0.69	1 (2%)
20	CLA	A	835	5	69,73,73	2.25	16 (23%)	83,113,113	2.94	31 (37%)
20	CLA	B	833	20	49,53,73	2.64	15 (30%)	59,89,113	3.17	23 (38%)
21	LMU	1	219	-	36,36,36	1.02	2 (5%)	47,47,47	2.24	13 (27%)
20	CLA	A	840	-	54,58,73	2.51	16 (29%)	65,95,113	2.95	25 (38%)
21	LMU	H	104	19	36,36,36	1.13	4 (11%)	47,47,47	3.11	22 (46%)
22	BCR	B	846	-	41,41,41	2.10	4 (9%)	56,56,56	5.93	21 (37%)
20	CLA	B	803	-	69,73,73	2.19	18 (26%)	83,113,113	2.69	32 (38%)
20	CLA	K	101	-	49,53,73	2.62	18 (36%)	59,89,113	3.15	23 (38%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
20	CLA	A	852	-	69,73,73	2.34	16 (23%)	83,113,113	2.94	28 (33%)
22	BCR	B	844	-	41,41,41	1.91	4 (9%)	56,56,56	5.05	24 (42%)
22	BCR	J	102	-	41,41,41	1.93	4 (9%)	56,56,56	5.92	19 (33%)
20	CLA	4	315	4	26,32,73	2.34	8 (30%)	34,54,113	2.91	19 (55%)
20	CLA	B	849	6	69,73,73	2.19	16 (23%)	83,113,113	2.82	33 (39%)
21	LMU	K	104	-	36,36,36	0.67	1 (2%)	47,47,47	1.90	13 (27%)
20	CLA	2	307	2	69,73,73	2.54	27 (39%)	83,113,113	3.00	32 (38%)
20	CLA	4	318	-	56,60,73	2.88	21 (37%)	67,97,113	3.65	29 (43%)
21	LMU	R	104	-	36,36,36	0.77	1 (2%)	47,47,47	2.17	18 (38%)
20	CLA	2	310	-	26,32,73	2.33	9 (34%)	34,54,113	3.04	22 (64%)
22	BCR	L	208	-	41,41,41	2.56	11 (26%)	56,56,56	5.71	20 (35%)
20	CLA	3	311	3	69,73,73	2.60	26 (37%)	83,113,113	3.22	30 (36%)
20	CLA	K	107	21	54,58,73	2.51	16 (29%)	65,95,113	2.95	25 (38%)
20	CLA	1	206	20	65,69,73	2.25	16 (24%)	78,108,113	2.62	27 (34%)
20	CLA	A	839	-	69,73,73	2.57	22 (31%)	83,113,113	3.51	34 (40%)
20	CLA	J	103	-	65,69,73	2.27	17 (26%)	78,108,113	2.81	26 (33%)
21	LMU	L	204	-	36,36,36	0.69	2 (5%)	47,47,47	2.38	14 (29%)
20	CLA	4	308	-	39,44,73	2.93	16 (41%)	52,78,113	3.29	22 (42%)
20	CLA	B	827	6	69,73,73	2.23	19 (27%)	83,113,113	2.97	26 (31%)
20	CLA	B	840	-	39,44,73	2.82	13 (33%)	52,78,113	3.40	28 (53%)
20	CLA	L	203	-	59,63,73	2.39	12 (20%)	71,101,113	2.74	28 (39%)
20	CLA	4	314	-	39,44,73	2.70	12 (30%)	52,78,113	3.48	26 (50%)
20	CLA	A	825	20,5	69,73,73	2.21	16 (23%)	83,113,113	2.69	25 (30%)
24	SF4	A	857	6,5	0,12,12	-	-	-	-	-
20	CLA	H	111	16	54,58,73	2.46	15 (27%)	65,95,113	2.96	25 (38%)
20	CLA	2	302	-	55,59,73	2.48	16 (29%)	66,96,113	2.96	23 (34%)
20	CLA	4	305	-	59,63,73	2.28	14 (23%)	71,101,113	2.97	28 (39%)
20	CLA	2	309	-	26,32,73	2.38	8 (30%)	34,54,113	3.11	21 (61%)
21	LMU	R	109	21	36,36,36	0.37	0	47,47,47	0.70	1 (2%)
20	CLA	B	838	-	69,73,73	2.18	14 (20%)	83,113,113	2.91	32 (38%)
20	CLA	A	807	5	50,54,73	3.08	26 (52%)	60,90,113	3.42	31 (51%)
20	CLA	B	814	-	50,54,73	2.50	12 (24%)	60,90,113	2.98	23 (38%)
20	CLA	A	801	-	50,54,73	2.74	16 (32%)	63,90,113	3.86	35 (55%)
20	CLA	B	804	6	49,53,73	2.63	18 (36%)	59,89,113	3.19	23 (38%)
20	CLA	B	822	-	58,62,73	2.42	19 (32%)	69,99,113	2.85	31 (44%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
21	LMU	L	205	-	36,36,36	0.80	2 (5%)	47,47,47	1.89	16 (34%)
21	LMU	2	319	-	36,36,36	1.04	1 (2%)	47,47,47	1.37	3 (6%)
20	CLA	B	831	6	54,58,73	2.60	19 (35%)	65,95,113	3.16	27 (41%)
20	CLA	1	214	-	26,32,73	2.30	9 (34%)	34,54,113	2.99	22 (64%)
20	CLA	A	832	20,5	54,58,73	2.44	15 (27%)	65,95,113	2.94	25 (38%)
20	CLA	L	201	-	59,63,73	3.01	25 (42%)	71,101,113	3.56	32 (45%)
21	LMU	E	101	21	36,36,36	0.93	2 (5%)	47,47,47	3.05	25 (53%)
20	CLA	B	836	6	69,73,73	2.12	15 (21%)	83,113,113	2.73	24 (28%)
20	CLA	1	212	-	26,32,73	2.50	10 (38%)	34,54,113	3.44	21 (61%)
20	CLA	3	304	-	39,44,73	2.74	11 (28%)	52,78,113	3.02	20 (38%)
20	CLA	4	306	-	54,58,73	2.94	23 (42%)	65,95,113	3.24	23 (35%)
22	BCR	3	314	21	41,41,41	2.06	5 (12%)	56,56,56	5.89	21 (37%)
20	CLA	L	202	5	69,73,73	2.22	16 (23%)	83,113,113	2.62	26 (31%)
23	PQN	A	842	-	34,34,34	1.73	3 (8%)	42,45,45	1.52	7 (16%)
20	CLA	B	825	-	69,73,73	2.34	16 (23%)	83,113,113	2.91	29 (34%)
20	CLA	L	207	-	54,58,73	2.61	19 (35%)	65,95,113	3.23	25 (38%)
20	CLA	3	301	-	39,44,73	2.67	10 (25%)	52,78,113	3.42	26 (50%)
20	CLA	A	818	-	69,73,73	2.17	16 (23%)	83,113,113	2.69	32 (38%)
20	CLA	B	830	6	69,73,73	2.26	19 (27%)	83,113,113	2.95	28 (33%)
20	CLA	B	851	-	69,73,73	2.24	16 (23%)	83,113,113	2.68	29 (34%)
20	CLA	F	206	20	57,61,73	2.77	24 (42%)	68,98,113	2.83	26 (38%)
21	LMU	2	313	-	36,36,36	0.82	1 (2%)	47,47,47	0.91	2 (4%)
20	CLA	4	316	-	50,54,73	2.83	24 (48%)	60,90,113	3.23	25 (41%)
22	BCR	A	843	5	41,41,41	1.93	4 (9%)	56,56,56	5.89	19 (33%)
20	CLA	2	320	-	65,69,73	2.49	25 (38%)	78,108,113	3.04	33 (42%)
20	CLA	A	809	5	56,60,73	2.38	15 (26%)	67,97,113	3.17	31 (46%)
22	BCR	A	847	-	41,41,41	2.06	5 (12%)	56,56,56	5.93	22 (39%)
21	LMU	K	105	-	36,36,36	0.53	0	47,47,47	2.04	15 (31%)
24	SF4	C	102	7	0,12,12	-	-	-	-	-
20	CLA	A	826	-	69,73,73	2.15	16 (23%)	83,113,113	2.73	30 (36%)
21	LMU	B	801	-	36,36,36	0.67	0	47,47,47	2.44	16 (34%)
21	LMU	1	213	-	36,36,36	0.81	0	47,47,47	2.10	16 (34%)
20	CLA	1	216	-	26,32,73	2.35	14 (53%)	34,54,113	3.00	23 (67%)
20	CLA	1	211	-	26,32,73	2.44	8 (30%)	34,54,113	3.11	21 (61%)
20	CLA	B	812	6	69,73,73	2.20	14 (20%)	83,113,113	2.55	28 (33%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
20	CLA	1	215	-	65,69,73	2.48	23 (35%)	78,108,113	3.44	35 (44%)
20	CLA	G	102	-	55,59,73	2.70	24 (43%)	66,96,113	3.40	29 (43%)
20	CLA	B	805	-	64,68,73	2.25	14 (21%)	77,107,113	3.22	32 (41%)
21	LMU	A	854	-	36,36,36	0.69	1 (2%)	47,47,47	1.89	11 (23%)
21	LMU	N	101	-	36,36,36	0.55	1 (2%)	47,47,47	2.05	13 (27%)
21	LMU	R	103	-	36,36,36	0.78	0	47,47,47	2.05	14 (29%)
20	CLA	3	306	-	26,32,73	2.35	10 (38%)	34,54,113	3.17	22 (64%)
22	BCR	I	103	-	41,41,41	2.82	11 (26%)	56,56,56	6.56	29 (51%)
20	CLA	4	302	4	59,63,73	2.41	17 (28%)	71,101,113	2.94	26 (36%)
20	CLA	A	819	-	69,73,73	2.17	15 (21%)	83,113,113	2.63	23 (27%)
20	CLA	B	829	6	54,58,73	2.31	14 (25%)	65,95,113	3.02	28 (43%)
20	CLA	A	828	5	69,73,73	2.16	16 (23%)	83,113,113	2.64	30 (36%)
20	CLA	B	808	6	69,73,73	2.18	19 (27%)	83,113,113	2.73	25 (30%)
20	CLA	B	809	6	58,62,73	2.63	15 (25%)	73,100,113	2.82	30 (41%)
20	CLA	A	831	-	59,63,73	2.42	15 (25%)	71,101,113	3.21	30 (42%)
22	BCR	B	852	20	41,41,41	3.47	21 (51%)	56,56,56	6.45	26 (46%)
22	BCR	A	844	-	41,41,41	2.03	4 (9%)	56,56,56	5.93	20 (35%)
20	CLA	4	311	-	59,63,73	2.40	13 (22%)	71,101,113	2.86	28 (39%)
20	CLA	B	824	6	69,73,73	2.23	18 (26%)	83,113,113	2.64	23 (27%)
20	CLA	B	819	-	50,54,73	2.46	14 (28%)	60,90,113	3.20	20 (33%)
20	CLA	A	802	-	26,32,73	2.53	12 (46%)	34,54,113	3.63	20 (58%)
21	LMU	A	856	-	36,36,36	0.78	1 (2%)	47,47,47	1.59	8 (17%)
20	CLA	F	205	20	45,49,73	2.70	15 (33%)	54,84,113	3.17	25 (46%)
21	LMU	B	802	-	36,36,36	1.02	4 (11%)	47,47,47	2.47	13 (27%)
20	CLA	F	204	-	39,44,73	2.76	12 (30%)	52,78,113	3.31	27 (51%)
20	CLA	A	841	-	69,73,73	2.10	15 (21%)	83,113,113	2.84	28 (33%)
20	CLA	B	850	-	69,73,73	2.11	15 (21%)	83,113,113	2.89	31 (37%)
20	CLA	A	813	5	58,62,73	2.26	16 (27%)	69,99,113	2.86	26 (37%)
20	CLA	H	102	-	59,63,73	2.40	17 (28%)	71,101,113	2.87	26 (36%)
20	CLA	A	850	-	69,73,73	2.23	17 (24%)	83,113,113	2.87	27 (32%)
20	CLA	A	817	-	56,60,73	2.47	15 (26%)	67,97,113	3.05	27 (40%)
20	CLA	A	820	-	55,59,73	2.50	17 (30%)	66,96,113	2.97	23 (34%)
21	LMU	2	316	-	36,36,36	0.39	0	47,47,47	0.71	1 (2%)
20	CLA	K	102	-	54,58,73	2.99	27 (50%)	65,95,113	3.31	28 (43%)
20	CLA	A	821	5	46,50,73	2.58	14 (30%)	55,85,113	3.32	23 (41%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
21	LMU	1	220	-	36,36,36	0.59	1 (2%)	47,47,47	1.36	7 (14%)
20	CLA	3	303	6	26,32,73	2.59	12 (46%)	34,54,113	3.22	20 (58%)
22	BCR	F	202	-	41,41,41	1.99	4 (9%)	56,56,56	5.89	20 (35%)
21	LMU	C	101	-	36,36,36	0.85	1 (2%)	47,47,47	1.37	7 (14%)
20	CLA	4	307	4	56,60,73	3.24	30 (53%)	67,97,113	3.80	40 (59%)
20	CLA	B	820	6	59,63,73	2.46	16 (27%)	71,101,113	2.83	24 (33%)
20	CLA	4	313	-	26,32,73	2.54	8 (30%)	34,54,113	3.19	22 (64%)
20	CLA	K	103	-	69,73,73	2.20	12 (17%)	83,113,113	2.56	26 (31%)
23	PQN	B	841	-	34,34,34	1.67	2 (5%)	42,45,45	1.60	6 (14%)
21	LMU	R	105	-	36,36,36	0.86	1 (2%)	47,47,47	1.64	11 (23%)
20	CLA	B	821	-	69,73,73	3.10	31 (44%)	83,113,113	3.02	30 (36%)
21	LMU	K	106	-	36,36,36	0.46	0	47,47,47	2.20	17 (36%)
21	LMU	3	320	-	36,36,36	0.40	0	47,47,47	0.71	1 (2%)
20	CLA	A	810	-	49,53,73	2.67	17 (34%)	59,89,113	3.23	25 (42%)
20	CLA	B	834	-	55,59,73	2.51	13 (23%)	66,96,113	3.02	26 (39%)
20	CLA	4	303	-	39,44,73	3.05	16 (41%)	52,78,113	3.56	23 (44%)
20	CLA	H	109	-	64,68,73	2.36	14 (21%)	77,107,113	2.98	28 (36%)
20	CLA	3	308	-	46,50,73	2.52	12 (26%)	55,85,113	3.23	28 (50%)
20	CLA	A	838	5	69,73,73	2.26	17 (24%)	83,113,113	2.82	32 (38%)
20	CLA	A	827	5	59,63,73	2.32	16 (27%)	71,101,113	2.83	27 (38%)
20	CLA	1	205	-	26,32,73	2.48	12 (46%)	34,54,113	3.66	21 (61%)
20	CLA	B	832	20	49,53,73	2.76	17 (34%)	59,89,113	3.11	23 (38%)
21	LMU	R	106	-	36,36,36	0.88	1 (2%)	47,47,47	1.57	10 (21%)
20	CLA	2	305	-	54,58,73	2.44	15 (27%)	65,95,113	2.79	26 (40%)
20	CLA	3	317	-	69,73,73	2.15	16 (23%)	83,113,113	2.56	24 (28%)
21	LMU	A	848	-	36,36,36	0.87	0	47,47,47	1.41	6 (12%)
22	BCR	B	845	-	41,41,41	2.16	5 (12%)	56,56,56	5.93	23 (41%)
20	CLA	3	313	-	69,73,73	2.65	27 (39%)	83,113,113	3.20	32 (38%)
20	CLA	B	818	-	54,58,73	2.41	15 (27%)	65,95,113	2.95	24 (36%)
20	CLA	J	101	-	52,56,73	2.54	18 (34%)	62,92,113	3.07	24 (38%)
20	CLA	2	311	2	54,58,73	2.44	13 (24%)	65,95,113	3.01	26 (40%)
20	CLA	A	803	-	54,58,73	2.42	15 (27%)	65,95,113	3.30	29 (44%)
20	CLA	4	312	-	26,32,73	2.35	10 (38%)	34,54,113	3.23	21 (61%)
21	LMU	A	855	-	36,36,36	0.78	1 (2%)	47,47,47	1.95	17 (36%)
21	LMU	1	217	-	36,36,36	0.38	0	47,47,47	0.70	1 (2%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
21	LMU	R	102	-	36,36,36	0.43	0	47,47,47	1.74	12 (25%)
20	CLA	A	830	5	69,73,73	2.29	18 (26%)	83,113,113	2.71	25 (30%)
20	CLA	2	306	-	26,32,73	2.45	12 (46%)	34,54,113	3.33	21 (61%)
20	CLA	B	810	6	59,63,73	2.28	14 (23%)	71,101,113	2.77	27 (38%)
20	CLA	A	805	5	69,73,73	2.11	13 (18%)	83,113,113	2.78	29 (34%)
21	LMU	K	108	20	36,36,36	0.79	1 (2%)	47,47,47	2.27	12 (25%)
24	SF4	C	103	7	0,12,12	-	-	-	-	-
20	CLA	A	833	5	49,53,73	2.55	16 (32%)	59,89,113	3.52	27 (45%)
20	CLA	A	808	5	69,73,73	2.24	17 (24%)	83,113,113	3.03	32 (38%)
20	CLA	2	304	-	26,32,73	2.57	15 (57%)	34,54,113	3.34	23 (67%)
20	CLA	1	203	-	51,55,73	2.55	12 (23%)	61,91,113	3.26	27 (44%)
20	CLA	A	815	5	54,58,73	3.16	27 (50%)	65,95,113	3.69	36 (55%)
20	CLA	A	837	-	51,55,73	2.61	17 (33%)	61,91,113	3.31	27 (44%)
20	CLA	3	305	-	26,32,73	2.50	12 (46%)	34,54,113	3.44	19 (55%)
20	CLA	4	309	-	26,32,73	2.74	14 (53%)	34,54,113	3.58	21 (61%)
20	CLA	A	804	20	59,63,73	2.41	16 (27%)	71,101,113	2.91	27 (38%)
20	CLA	A	812	5	58,62,73	2.36	13 (22%)	69,99,113	2.64	23 (33%)
21	LMU	H	106	-	36,36,36	1.05	4 (11%)	47,47,47	2.75	19 (40%)
20	CLA	A	834	-	53,57,73	2.53	15 (28%)	62,93,113	2.97	24 (38%)
20	CLA	B	837	-	51,55,73	2.45	14 (27%)	61,91,113	3.00	25 (40%)
21	LMU	A	849	-	36,36,36	0.86	1 (2%)	47,47,47	1.67	10 (21%)
20	CLA	A	829	5	54,58,73	2.47	12 (22%)	65,95,113	3.06	29 (44%)
22	BCR	A	846	-	41,41,41	2.08	4 (9%)	56,56,56	5.92	22 (39%)
21	LMU	4	320	21	35,35,36	0.30	0	46,46,47	0.72	1 (2%)
20	CLA	1	209	1	39,44,73	2.83	12 (30%)	52,78,113	3.07	22 (42%)
22	BCR	F	203	-	41,41,41	3.03	14 (34%)	56,56,56	6.09	31 (55%)
21	LMU	H	105	-	36,36,36	0.98	1 (2%)	47,47,47	2.33	16 (34%)
20	CLA	R	108	-	62,66,73	2.67	25 (40%)	74,104,113	3.14	31 (41%)
20	CLA	3	312	-	26,32,73	2.79	14 (53%)	34,54,113	3.85	26 (76%)
20	CLA	1	207	-	55,59,73	2.50	16 (29%)	66,96,113	3.42	30 (45%)
20	CLA	B	823	-	62,66,73	2.32	16 (25%)	74,104,113	2.87	25 (33%)
21	LMU	4	321	-	36,36,36	0.95	1 (2%)	47,47,47	1.40	8 (17%)
20	CLA	A	824	-	69,73,73	2.19	16 (23%)	83,113,113	2.67	26 (31%)
20	CLA	B	826	-	69,73,73	2.18	15 (21%)	83,113,113	2.83	31 (37%)
20	CLA	A	822	-	59,63,73	2.38	16 (27%)	71,101,113	2.90	24 (33%)

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	4	319	21	-	10/18/94/115	-
20	CLA	R	107	-	1/1/13/20	15/30/106/115	-
21	LMU	4	322	20	-	14/21/61/61	0/2/2/2
20	CLA	L	206	22,16	-	10/18/94/115	-
20	CLA	4	304	-	2/2/15/20	20/39/115/115	-
20	CLA	A	836	-	-	8/18/94/115	-
21	LMU	4	301	-	-	13/21/61/61	0/2/2/2
21	LMU	L	209	-	-	14/21/61/61	0/2/2/2
20	CLA	B	807	-	1/1/15/20	11/39/115/115	-
20	CLA	B	816	6	1/1/14/20	15/33/109/115	-
21	LMU	A	853	-	-	19/21/61/61	0/2/2/2
25	LMG	B	848	-	-	23/44/64/70	0/1/1/1
20	CLA	3	316	-	-	10/21/97/115	-
20	CLA	B	813	6	1/1/14/20	16/33/109/115	-
20	CLA	2	312	-	-	12/21/97/115	-
20	CLA	B	817	-	1/1/14/20	17/35/111/115	-
20	CLA	H	103	-	1/1/13/20	15/27/103/115	-
22	BCR	I	101	-	-	7/29/63/63	0/2/2/2
20	CLA	2	315	-	1/1/15/20	18/39/115/115	-
20	CLA	A	811	20,5	1/1/15/20	25/39/115/115	-
20	CLA	B	806	-	1/1/15/20	19/39/115/115	-
21	LMU	3	321	-	-	15/21/61/61	0/2/2/2
21	LMU	F	201	-	-	14/20/60/61	0/2/2/2
20	CLA	A	814	5	-	11/15/91/115	-
20	CLA	1	210	-	1/1/12/20	10/23/99/115	-
22	BCR	B	842	-	-	13/29/63/63	0/2/2/2
20	CLA	B	811	-	1/1/13/20	18/31/107/115	-
21	LMU	R	101	-	1/1/10/10	11/21/61/61	0/2/2/2
20	CLA	3	302	-	-	4/21/97/115	-
20	CLA	A	851	-	1/1/15/20	19/39/115/115	-
20	CLA	1	202	20,1	1/1/13/20	17/30/106/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
20	CLA	A	806	-	1/1/13/20	8/27/103/115	-
20	CLA	A	823	-	1/1/15/20	21/39/115/115	-
20	CLA	I	102	-	1/1/14/20	14/33/109/115	-
21	LMU	G	101	-	-	15/21/61/61	0/2/2/2
20	CLA	B	815	-	1/1/13/20	12/32/108/115	-
21	LMU	1	218	-	-	10/21/61/61	0/2/2/2
20	CLA	H	101	-	1/1/13/20	17/27/103/115	-
20	CLA	B	835	6	1/1/14/20	16/33/109/115	-
20	CLA	B	828	6	-	11/21/97/115	-
21	LMU	H	107	-	-	12/21/61/61	0/2/2/2
21	LMU	H	108	-	-	14/21/61/61	0/2/2/2
20	CLA	2	308	-	1/1/15/20	15/39/115/115	-
20	CLA	1	204	-	-	8/17/93/115	-
22	BCR	B	843	-	-	7/29/63/63	0/2/2/2
22	BCR	A	845	-	-	14/29/63/63	0/2/2/2
20	CLA	2	303	-	1/1/15/20	18/39/115/115	-
21	LMU	2	317	-	-	13/21/61/61	0/2/2/2
21	LMU	2	318	-	-	13/21/61/61	0/2/2/2
20	CLA	1	201	1	-	12/17/93/115	-
21	LMU	D	201	21	-	14/21/61/61	0/2/2/2
20	CLA	A	816	-	-	13/26/102/115	-
21	LMU	B	847	22	-	10/21/61/61	0/2/2/2
20	CLA	B	839	-	1/1/15/20	18/39/115/115	-
21	LMU	4	317	-	-	13/21/61/61	0/2/2/2
20	CLA	A	835	5	1/1/15/20	18/39/115/115	-
20	CLA	B	833	20	-	8/15/91/115	-
21	LMU	1	219	-	-	13/21/61/61	0/2/2/2
20	CLA	A	840	-	-	12/21/97/115	-
21	LMU	H	104	19	-	14/21/61/61	0/2/2/2
22	BCR	B	846	-	-	12/29/63/63	0/2/2/2
20	CLA	B	803	-	1/1/15/20	21/39/115/115	-
20	CLA	K	101	-	-	5/15/91/115	-
20	CLA	A	852	-	1/1/15/20	24/39/115/115	-
22	BCR	B	844	-	-	11/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	BCR	J	102	-	-	12/29/63/63	0/2/2/2
20	CLA	B	849	6	1/1/15/20	21/39/115/115	-
21	LMU	K	104	-	-	12/21/61/61	0/2/2/2
20	CLA	2	307	2	1/1/15/20	21/39/115/115	-
20	CLA	4	318	-	-	13/24/100/115	-
21	LMU	R	104	-	-	17/21/61/61	0/2/2/2
22	BCR	L	208	-	-	10/29/63/63	0/2/2/2
20	CLA	3	311	3	1/1/15/20	23/39/115/115	-
20	CLA	K	107	21	-	6/21/97/115	-
20	CLA	1	206	20	1/1/14/20	21/35/111/115	-
20	CLA	A	839	-	1/1/15/20	23/39/115/115	-
20	CLA	J	103	-	1/1/14/20	25/35/111/115	-
21	LMU	L	204	-	-	14/21/61/61	0/2/2/2
20	CLA	B	827	6	1/1/15/20	27/39/115/115	-
20	CLA	L	203	-	1/1/13/20	8/27/103/115	-
20	CLA	A	825	20,5	1/1/15/20	23/39/115/115	-
24	SF4	A	857	6,5	-	-	0/6/5/5
20	CLA	H	111	16	-	10/21/97/115	-
20	CLA	2	302	-	-	12/23/99/115	-
20	CLA	4	305	-	1/1/13/20	13/27/103/115	-
21	LMU	R	109	21	-	16/21/61/61	0/2/2/2
20	CLA	B	838	-	1/1/15/20	20/39/115/115	-
20	CLA	A	807	5	-	7/17/93/115	-
20	CLA	B	814	-	-	9/17/93/115	-
20	CLA	A	801	-	2/2/11/20	12/16/92/115	-
20	CLA	B	804	6	-	7/15/91/115	-
20	CLA	B	822	-	-	9/26/102/115	-
21	LMU	L	205	-	-	14/21/61/61	0/2/2/2
21	LMU	2	319	-	-	8/21/61/61	0/2/2/2
20	CLA	B	831	6	-	6/21/97/115	-
20	CLA	A	832	20,5	-	13/21/97/115	-
20	CLA	L	201	-	2/2/13/20	14/27/103/115	-
21	LMU	E	101	21	-	14/21/61/61	0/2/2/2
20	CLA	B	836	6	1/1/15/20	17/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
20	CLA	4	306	-	-	10/21/97/115	-
22	BCR	3	314	21	-	13/29/63/63	0/2/2/2
20	CLA	L	202	5	1/1/15/20	16/39/115/115	-
23	PQN	A	842	-	1/1/8/9	11/23/43/43	0/2/2/2
20	CLA	B	825	-	1/1/15/20	17/39/115/115	-
20	CLA	L	207	-	1/1/12/20	11/21/97/115	-
20	CLA	A	818	-	1/1/15/20	18/39/115/115	-
20	CLA	B	830	6	1/1/15/20	22/39/115/115	-
20	CLA	B	851	-	1/1/15/20	19/39/115/115	-
20	CLA	F	206	20	3/3/12/20	10/25/101/115	-
21	LMU	2	313	-	-	16/21/61/61	0/2/2/2
20	CLA	4	316	-	-	11/17/93/115	-
22	BCR	A	843	5	-	11/29/63/63	0/2/2/2
20	CLA	2	320	-	1/1/14/20	22/35/111/115	-
20	CLA	A	809	5	-	11/24/100/115	-
22	BCR	A	847	-	-	10/29/63/63	0/2/2/2
21	LMU	K	105	-	-	18/21/61/61	0/2/2/2
24	SF4	C	102	7	-	-	0/6/5/5
20	CLA	A	826	-	1/1/15/20	17/39/115/115	-
21	LMU	B	801	-	-	16/21/61/61	0/2/2/2
21	LMU	1	213	-	-	13/21/61/61	0/2/2/2
20	CLA	B	812	6	1/1/15/20	26/39/115/115	-
20	CLA	1	215	-	1/1/14/20	22/35/111/115	-
20	CLA	G	102	-	-	10/23/99/115	-
20	CLA	B	805	-	1/1/14/20	21/33/109/115	-
21	LMU	A	854	-	-	11/21/61/61	0/2/2/2
21	LMU	N	101	-	-	15/21/61/61	0/2/2/2
21	LMU	R	103	-	-	13/21/61/61	0/2/2/2
22	BCR	I	103	-	-	13/29/63/63	0/2/2/2
20	CLA	4	302	4	1/1/13/20	15/27/103/115	-
20	CLA	A	819	-	1/1/15/20	16/39/115/115	-
20	CLA	B	829	6	-	13/21/97/115	-
20	CLA	A	828	5	1/1/15/20	18/39/115/115	-
20	CLA	B	808	6	1/1/15/20	20/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
20	CLA	B	809	6	1/1/13/20	11/25/101/115	-
20	CLA	A	831	-	1/1/13/20	15/27/103/115	-
22	BCR	B	852	20	-	12/29/63/63	0/2/2/2
22	BCR	A	844	-	-	12/29/63/63	0/2/2/2
20	CLA	4	311	-	1/1/13/20	14/27/103/115	-
20	CLA	B	824	6	1/1/15/20	22/39/115/115	-
20	CLA	B	819	-	-	14/17/93/115	-
21	LMU	A	856	-	-	14/21/61/61	0/2/2/2
20	CLA	F	205	20	-	6/10/86/115	-
21	LMU	B	802	-	-	11/21/61/61	0/2/2/2
20	CLA	H	102	-	1/1/13/20	10/27/103/115	-
20	CLA	A	841	-	1/1/15/20	17/39/115/115	-
20	CLA	B	850	-	1/1/15/20	15/39/115/115	-
20	CLA	A	813	5	-	12/26/102/115	-
20	CLA	A	850	-	1/1/15/20	25/39/115/115	-
20	CLA	A	817	-	-	15/24/100/115	-
20	CLA	A	820	-	-	9/23/99/115	-
21	LMU	2	316	-	-	14/21/61/61	0/2/2/2
20	CLA	K	102	-	-	10/21/97/115	-
20	CLA	A	821	5	-	3/12/88/115	-
21	LMU	1	220	-	-	13/21/61/61	0/2/2/2
22	BCR	F	202	-	-	12/29/63/63	0/2/2/2
21	LMU	C	101	-	-	14/21/61/61	0/2/2/2
20	CLA	4	307	4	1/1/12/20	8/24/100/115	-
20	CLA	B	820	6	1/1/13/20	10/27/103/115	-
20	CLA	K	103	-	1/1/15/20	21/39/115/115	-
23	PQN	B	841	-	1/1/8/9	10/23/43/43	0/2/2/2
21	LMU	R	105	-	-	15/21/61/61	0/2/2/2
20	CLA	B	821	-	-	21/39/115/115	-
21	LMU	K	106	-	-	15/21/61/61	0/2/2/2
21	LMU	3	320	-	-	11/21/61/61	0/2/2/2
20	CLA	A	810	-	-	5/15/91/115	-
20	CLA	B	834	-	-	9/23/99/115	-
20	CLA	H	109	-	1/1/14/20	15/33/109/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
20	CLA	3	308	-	-	6/12/88/115	-
20	CLA	A	838	5	1/1/15/20	20/39/115/115	-
20	CLA	A	827	5	1/1/13/20	11/27/103/115	-
20	CLA	B	832	20	-	13/15/91/115	-
21	LMU	R	106	-	-	13/21/61/61	0/2/2/2
20	CLA	2	305	-	-	9/21/97/115	-
20	CLA	3	317	-	1/1/15/20	20/39/115/115	-
21	LMU	A	848	-	-	16/21/61/61	0/2/2/2
22	BCR	B	845	-	-	14/29/63/63	0/2/2/2
20	CLA	3	313	-	1/1/15/20	19/39/115/115	-
20	CLA	B	818	-	-	7/21/97/115	-
20	CLA	J	101	-	-	11/19/95/115	-
20	CLA	2	311	2	-	7/21/97/115	-
20	CLA	A	803	-	-	5/21/97/115	-
21	LMU	A	855	-	-	14/21/61/61	0/2/2/2
21	LMU	1	217	-	-	14/21/61/61	0/2/2/2
21	LMU	R	102	-	-	11/21/61/61	0/2/2/2
20	CLA	A	830	5	1/1/15/20	22/39/115/115	-
20	CLA	B	810	6	1/1/13/20	12/27/103/115	-
20	CLA	A	805	5	1/1/15/20	24/39/115/115	-
21	LMU	K	108	20	-	12/21/61/61	0/2/2/2
24	SF4	C	103	7	-	-	0/6/5/5
20	CLA	A	833	5	-	7/15/91/115	-
20	CLA	A	808	5	1/1/15/20	21/39/115/115	-
20	CLA	1	203	-	-	9/18/94/115	-
20	CLA	A	815	5	-	9/21/97/115	-
20	CLA	A	837	-	-	12/18/94/115	-
20	CLA	A	804	20	1/1/13/20	13/27/103/115	-
20	CLA	A	812	5	-	14/26/102/115	-
21	LMU	H	106	-	-	13/21/61/61	0/2/2/2
20	CLA	A	834	-	-	11/20/96/115	-
20	CLA	B	837	-	-	7/18/94/115	-
21	LMU	A	849	-	-	13/21/61/61	0/2/2/2
20	CLA	A	829	5	-	4/21/97/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	BCR	A	846	-	-	17/29/63/63	0/2/2/2
21	LMU	4	320	21	-	15/20/60/61	0/2/2/2
22	BCR	F	203	-	-	12/29/63/63	0/2/2/2
21	LMU	H	105	-	-	17/21/61/61	0/2/2/2
20	CLA	R	108	-	1/1/13/20	18/31/107/115	-
20	CLA	1	207	-	1/1/12/20	10/23/99/115	-
20	CLA	B	823	-	1/1/13/20	17/31/107/115	-
21	LMU	4	321	-	-	15/21/61/61	0/2/2/2
20	CLA	A	824	-	1/1/15/20	18/39/115/115	-
20	CLA	B	826	-	1/1/15/20	17/39/115/115	-
20	CLA	A	822	-	1/1/13/20	10/27/103/115	-

The worst 5 of 2975 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	B	852	BCR	C21-C22	-11.54	1.20	1.35
22	I	101	BCR	C21-C22	-10.73	1.21	1.35
22	F	203	BCR	C21-C22	-10.22	1.22	1.35
22	B	852	BCR	C20-C21	-10.12	1.12	1.43
22	I	103	BCR	C21-C22	-9.51	1.23	1.35

The worst 5 of 5552 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	A	846	BCR	C20-C21-C22	36.89	179.96	127.31
22	J	102	BCR	C20-C21-C22	36.89	179.96	127.31
22	B	846	BCR	C20-C21-C22	36.87	179.93	127.31
22	A	845	BCR	C20-C21-C22	36.86	179.91	127.31
22	A	844	BCR	C20-C21-C22	36.84	179.89	127.31

5 of 91 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
20	1	202	CLA	C8
20	1	206	CLA	C8
20	1	207	CLA	C2A
20	1	210	CLA	CBD
20	1	215	CLA	C8

5 of 2900 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	C4B-C3B-CAB-CBB
20	1	201	CLA	CHA-CBD-CGD-O1D

There are no ring outliers.

228 monomers are involved in 3635 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
20	4	319	CLA	11	0
20	R	107	CLA	10	0
21	4	322	LMU	2	0
20	L	206	CLA	21	0
20	4	304	CLA	22	0
20	A	836	CLA	16	0
21	4	301	LMU	7	0
21	L	209	LMU	3	0
20	B	807	CLA	23	0
20	B	816	CLA	16	0
21	A	853	LMU	9	0
25	B	848	LMG	29	0
20	3	307	CLA	16	0
20	3	316	CLA	2	0
20	2	312	CLA	11	0
20	B	813	CLA	13	0
20	B	817	CLA	17	0
20	H	103	CLA	3	0
20	3	310	CLA	7	0
22	I	101	BCR	19	0
20	2	315	CLA	6	0
20	A	811	CLA	22	0
20	B	806	CLA	17	0
21	3	321	LMU	8	0
21	F	201	LMU	19	0
20	A	814	CLA	34	0
20	1	210	CLA	8	0
22	B	842	BCR	9	0
20	B	811	CLA	29	0
21	R	101	LMU	6	0
20	3	302	CLA	26	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
20	A	851	CLA	35	0
20	1	202	CLA	39	0
20	3	309	CLA	5	0
20	A	806	CLA	17	0
20	A	823	CLA	17	0
20	4	310	CLA	3	0
20	I	102	CLA	10	0
21	G	101	LMU	19	0
20	B	815	CLA	20	0
21	1	218	LMU	8	0
20	H	101	CLA	36	0
20	B	835	CLA	12	0
20	B	828	CLA	13	0
21	H	107	LMU	11	0
21	H	108	LMU	37	0
20	2	308	CLA	8	0
20	1	204	CLA	7	0
22	B	843	BCR	18	0
22	A	845	BCR	45	0
20	2	303	CLA	12	0
21	2	317	LMU	6	0
20	1	201	CLA	14	0
20	A	816	CLA	35	0
21	2	318	LMU	4	0
20	B	839	CLA	25	0
21	4	317	LMU	4	0
21	B	847	LMU	28	15
21	D	201	LMU	12	0
20	A	835	CLA	17	0
20	B	833	CLA	22	0
21	1	219	LMU	20	0
20	A	840	CLA	9	0
21	H	104	LMU	20	0
22	B	846	BCR	53	0
20	B	803	CLA	28	0
20	K	101	CLA	19	1
20	A	852	CLA	27	0
22	B	844	BCR	18	0
22	J	102	BCR	42	0
20	4	315	CLA	3	0
20	B	849	CLA	21	0
21	K	104	LMU	8	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
20	2	307	CLA	18	0
20	4	318	CLA	19	0
21	R	104	LMU	10	0
22	L	208	BCR	51	0
20	3	311	CLA	20	0
20	K	107	CLA	24	0
20	1	206	CLA	15	0
20	A	839	CLA	43	0
20	J	103	CLA	27	0
21	L	204	LMU	3	0
20	4	308	CLA	2	0
20	B	827	CLA	30	0
20	B	840	CLA	2	0
20	L	203	CLA	19	0
20	4	314	CLA	8	0
20	A	825	CLA	76	0
24	A	857	SF4	19	0
20	H	111	CLA	9	0
20	2	302	CLA	15	0
20	4	305	CLA	20	0
20	2	309	CLA	1	0
21	R	109	LMU	20	4
20	B	838	CLA	25	0
20	A	807	CLA	31	0
20	B	814	CLA	20	0
20	A	801	CLA	8	0
20	B	804	CLA	7	0
20	B	822	CLA	25	0
21	L	205	LMU	4	0
21	2	319	LMU	0	2
20	B	831	CLA	18	0
20	A	832	CLA	16	0
20	L	201	CLA	35	0
21	E	101	LMU	30	0
20	B	836	CLA	43	0
20	3	304	CLA	14	0
20	4	306	CLA	10	0
22	3	314	BCR	19	13
20	L	202	CLA	23	0
23	A	842	PQN	9	0
20	B	825	CLA	24	0
20	L	207	CLA	12	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
20	A	818	CLA	28	0
20	B	830	CLA	27	0
20	B	851	CLA	48	0
20	F	206	CLA	15	0
21	2	313	LMU	3	1
20	4	316	CLA	6	0
22	A	843	BCR	46	0
20	2	320	CLA	34	0
20	A	809	CLA	26	0
22	A	847	BCR	63	0
21	K	105	LMU	35	0
24	C	102	SF4	4	0
20	A	826	CLA	60	0
21	B	801	LMU	13	0
21	1	213	LMU	8	0
20	1	211	CLA	6	0
20	B	812	CLA	20	0
20	1	215	CLA	54	0
20	G	102	CLA	19	0
20	B	805	CLA	17	0
21	A	854	LMU	42	0
21	N	101	LMU	35	0
21	R	103	LMU	25	0
20	3	306	CLA	3	0
22	I	103	BCR	46	0
20	4	302	CLA	28	0
20	A	819	CLA	45	0
20	B	829	CLA	13	0
20	A	828	CLA	14	0
20	B	808	CLA	19	0
20	B	809	CLA	5	0
20	A	831	CLA	15	0
22	B	852	BCR	13	0
22	A	844	BCR	24	0
20	4	311	CLA	17	0
20	B	824	CLA	50	0
20	B	819	CLA	17	0
20	F	205	CLA	13	0
21	B	802	LMU	4	0
20	F	204	CLA	2	0
20	A	841	CLA	29	0
20	B	850	CLA	40	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
20	A	813	CLA	19	0
20	H	102	CLA	15	0
20	A	850	CLA	18	0
20	A	817	CLA	10	0
20	A	820	CLA	15	0
21	2	316	LMU	12	0
20	K	102	CLA	10	0
20	A	821	CLA	10	0
22	F	202	BCR	31	0
20	4	307	CLA	17	0
20	B	820	CLA	14	0
20	4	313	CLA	5	0
20	K	103	CLA	3	0
23	B	841	PQN	31	0
20	B	821	CLA	41	0
21	K	106	LMU	47	0
21	3	320	LMU	4	0
20	A	810	CLA	5	0
20	B	834	CLA	4	0
20	4	303	CLA	3	0
20	H	109	CLA	17	0
20	3	308	CLA	2	0
20	A	838	CLA	39	0
20	A	827	CLA	22	0
20	B	832	CLA	20	0
21	R	106	LMU	2	0
20	2	305	CLA	12	0
20	3	317	CLA	18	0
21	A	848	LMU	3	0
22	B	845	BCR	33	0
20	3	313	CLA	27	0
20	B	818	CLA	8	0
20	J	101	CLA	27	0
20	2	311	CLA	18	0
20	A	803	CLA	13	0
20	4	312	CLA	4	0
21	A	855	LMU	27	0
21	1	217	LMU	9	0
21	R	102	LMU	21	0
20	A	830	CLA	38	0
20	B	810	CLA	19	0
20	A	805	CLA	25	0

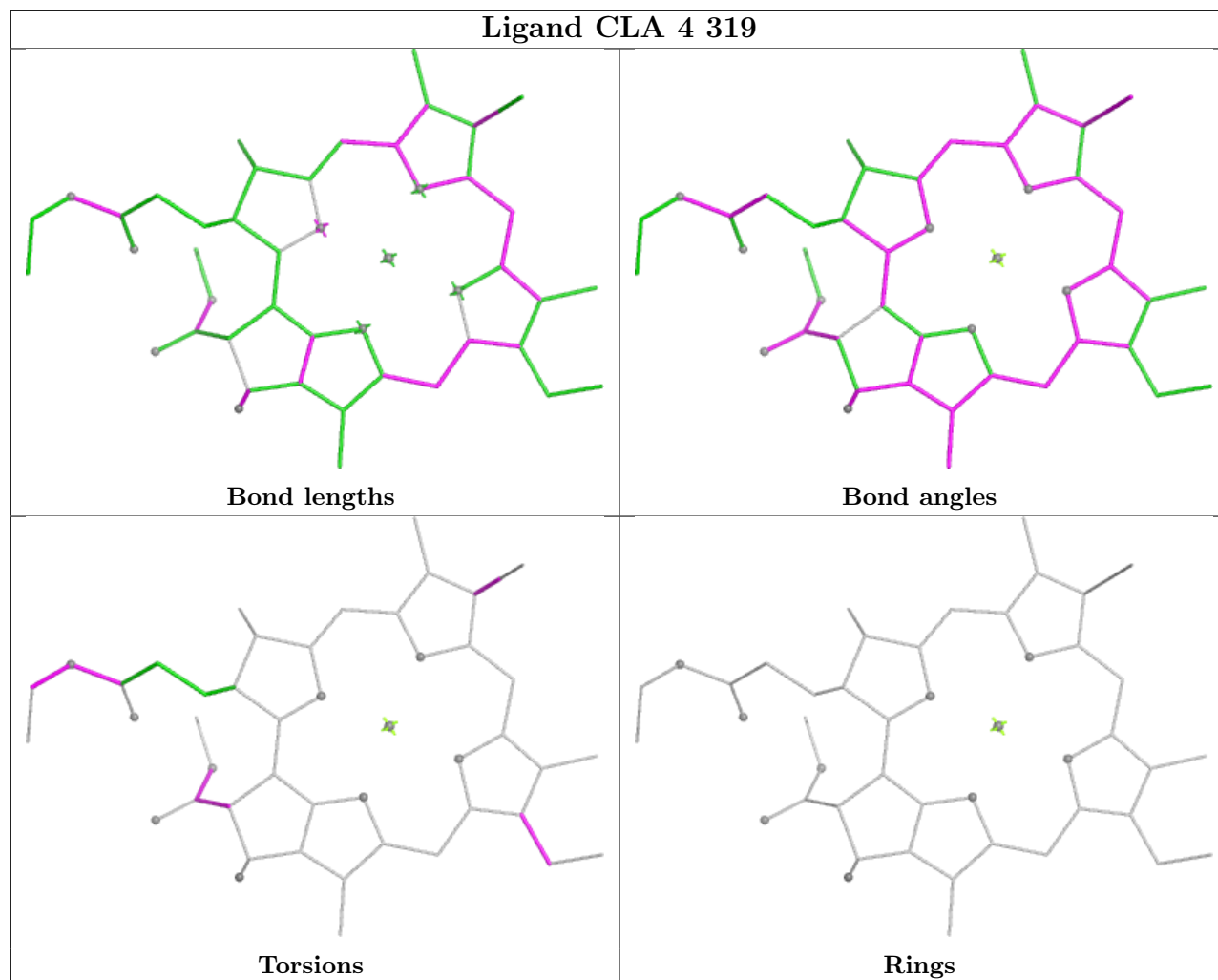
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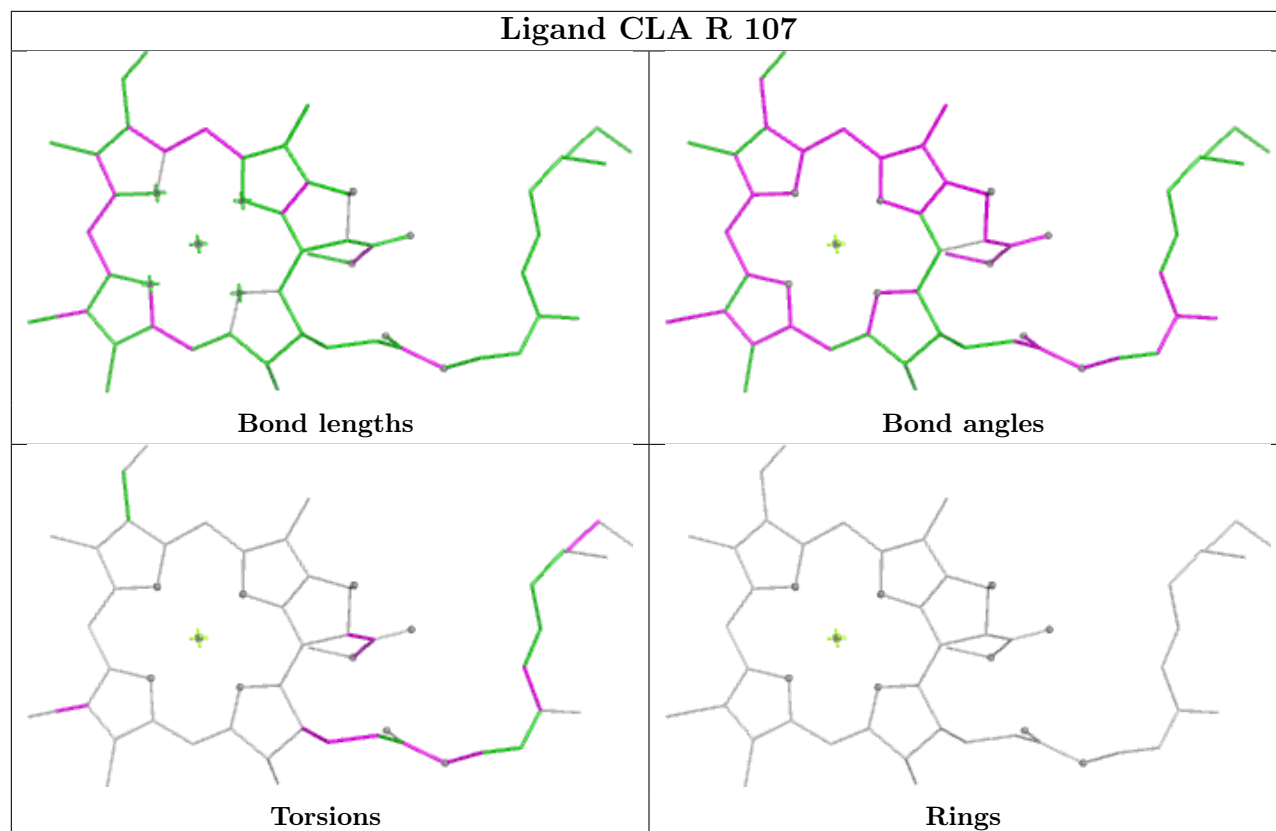
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21	K	108	LMU	6	0
24	C	103	SF4	4	0
20	A	833	CLA	18	1
20	A	808	CLA	26	0
20	2	304	CLA	5	0
20	1	203	CLA	13	0
20	A	815	CLA	45	0
20	A	837	CLA	17	0
20	3	305	CLA	1	0
20	4	309	CLA	1	0
20	A	804	CLA	28	0
20	A	812	CLA	2	0
21	H	106	LMU	29	0
20	A	834	CLA	12	0
20	B	837	CLA	26	0
21	A	849	LMU	4	0
20	A	829	CLA	6	0
22	A	846	BCR	35	0
21	4	320	LMU	8	4
20	1	209	CLA	11	0
22	F	203	BCR	42	0
21	H	105	LMU	12	0
20	R	108	CLA	12	0
20	1	207	CLA	6	1
20	B	823	CLA	64	0
21	4	321	LMU	2	0
20	A	824	CLA	84	0
20	B	826	CLA	33	0
20	A	822	CLA	34	0

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

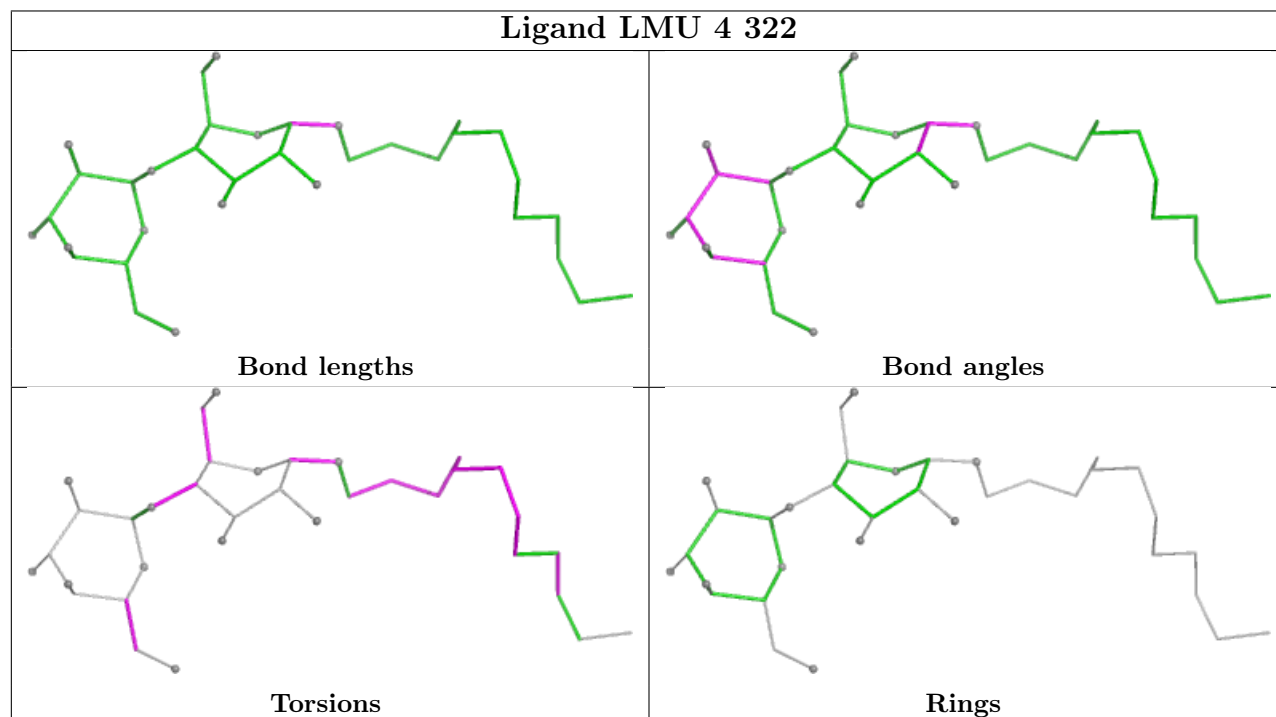
Ligand CLA 4 319



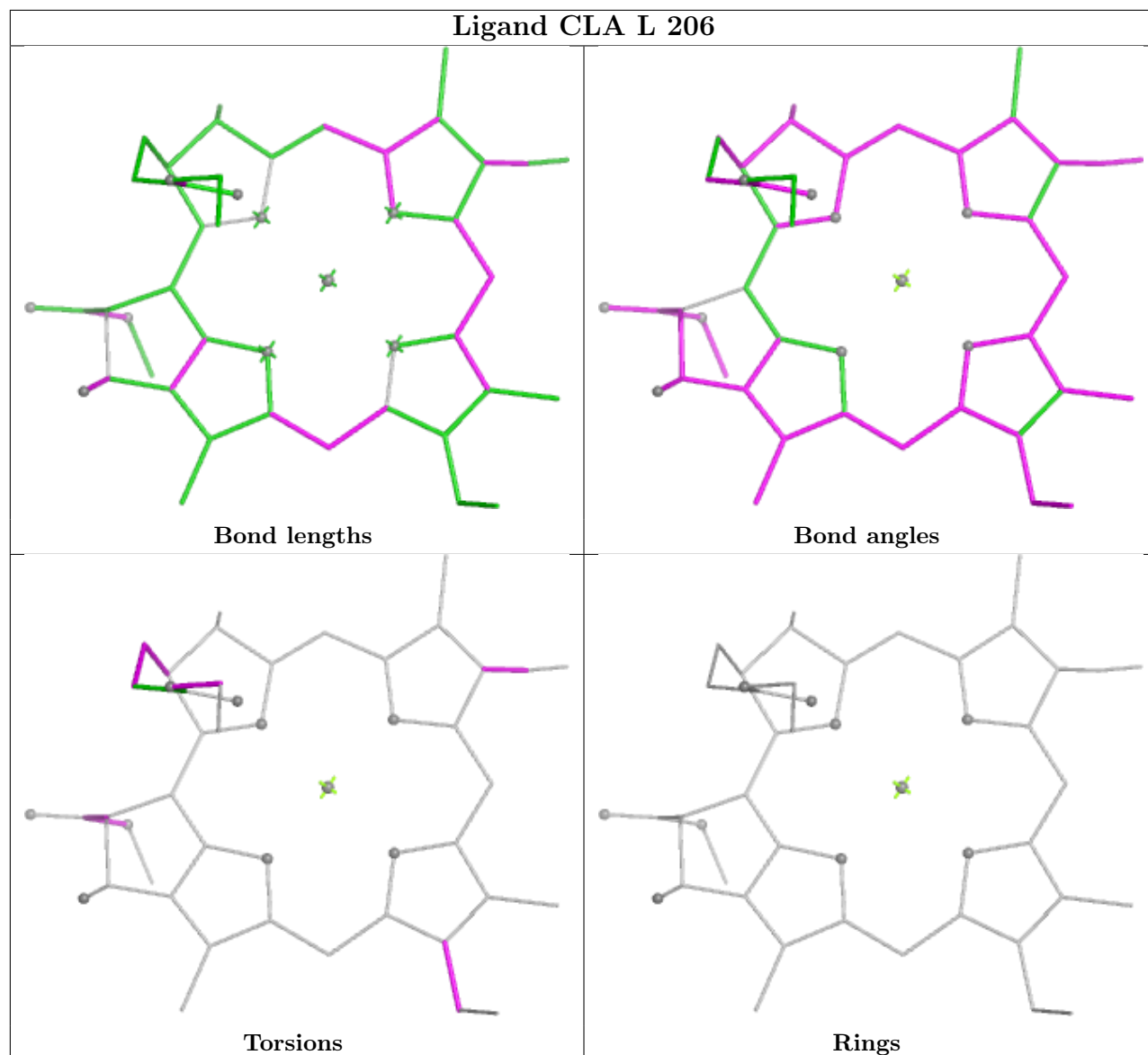
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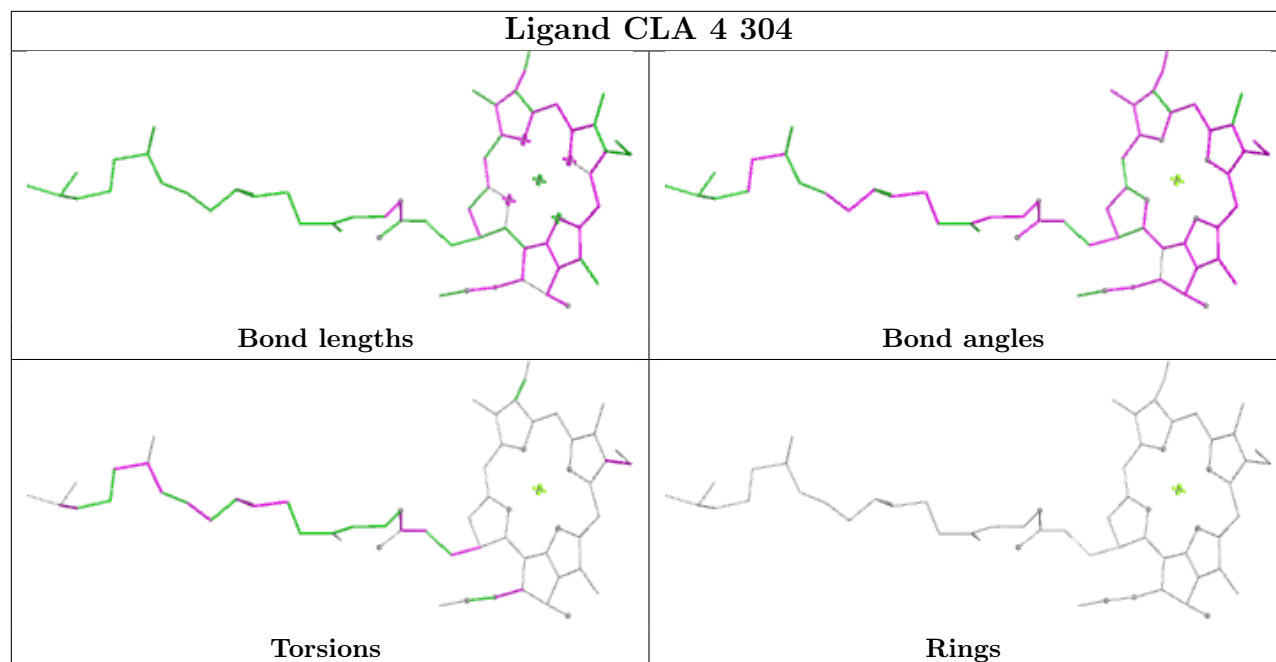
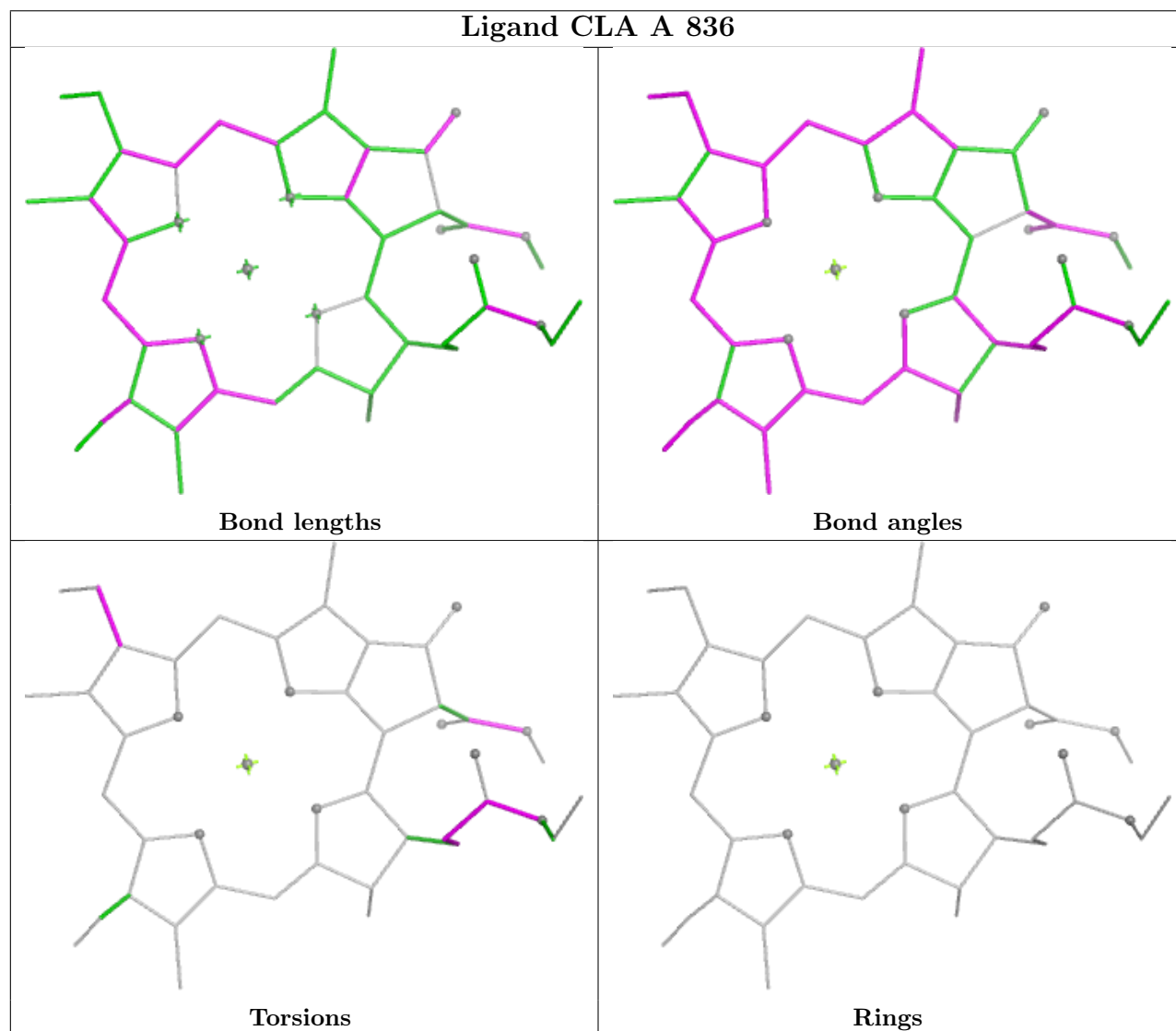


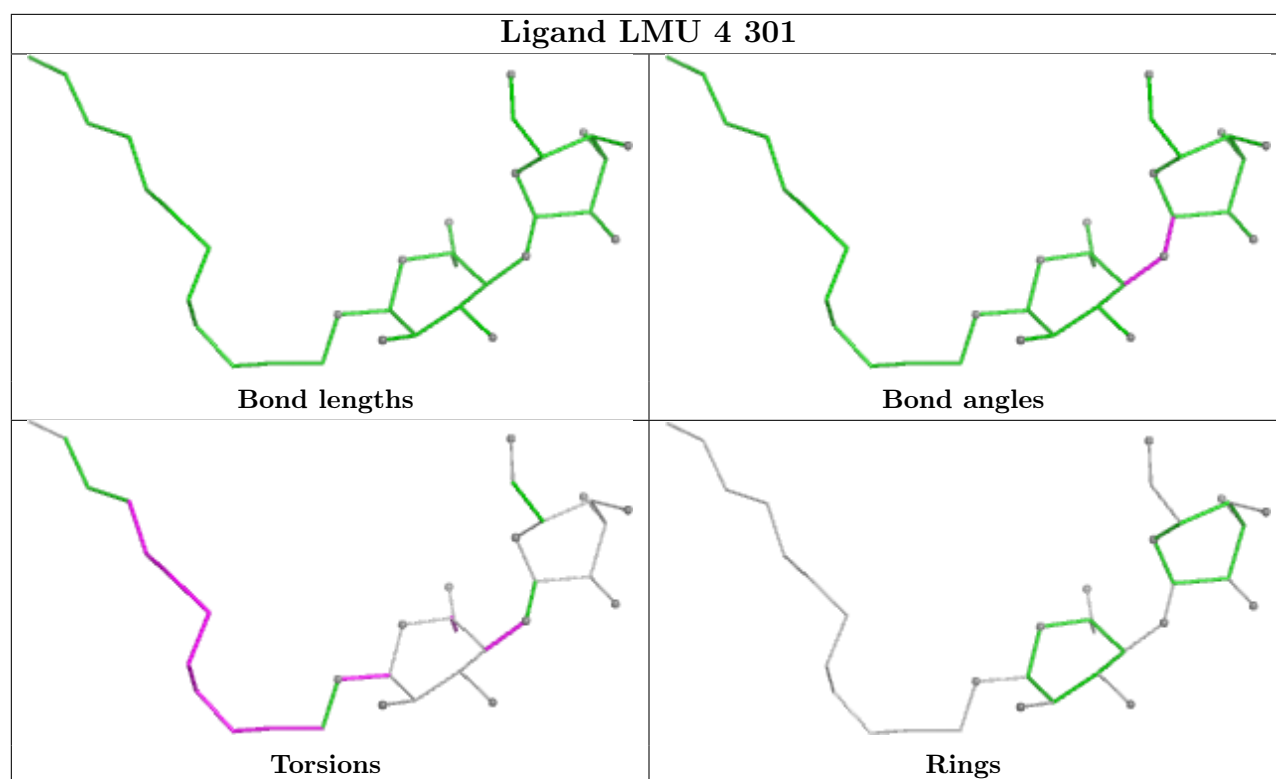
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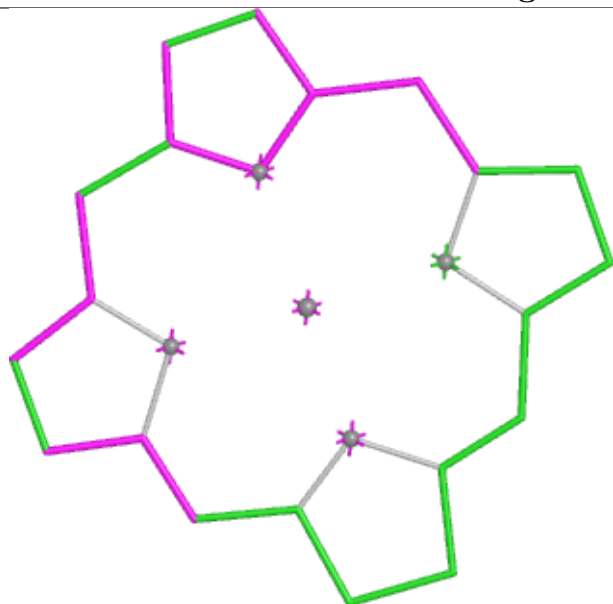
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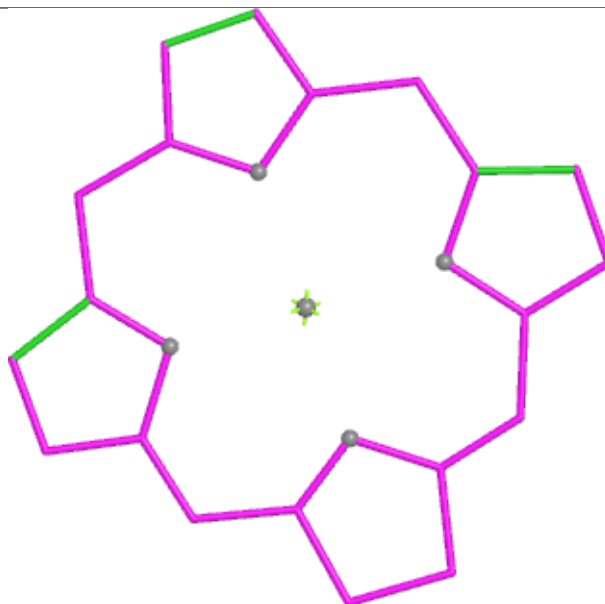
Ligand CLA 4 304**Ligand CLA A 836**



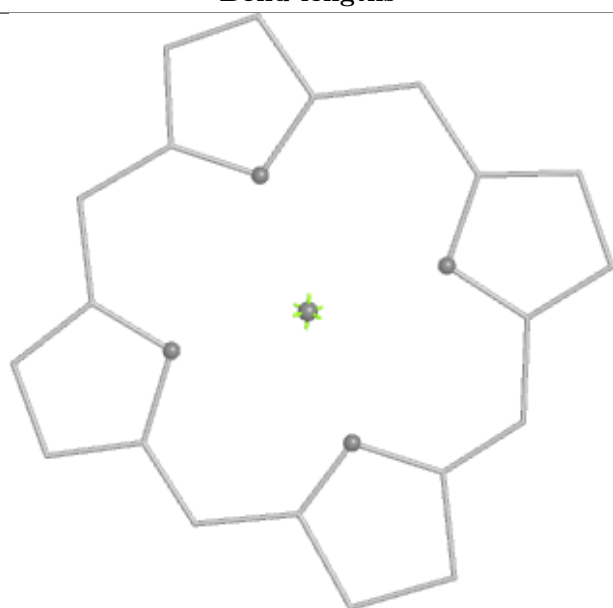
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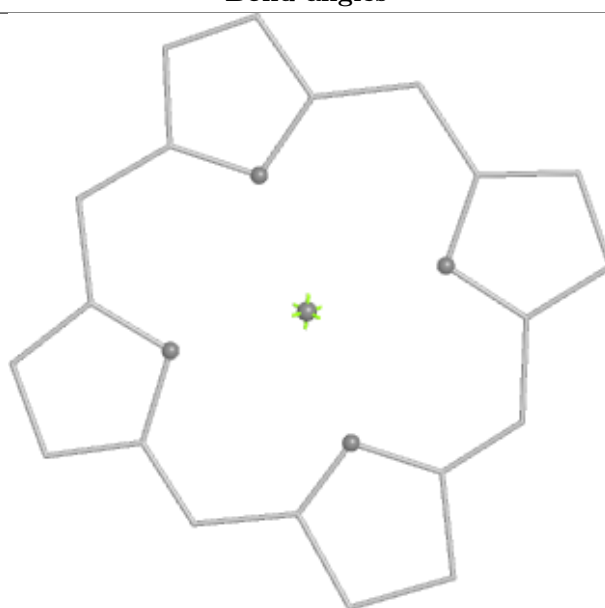
Bond lengths



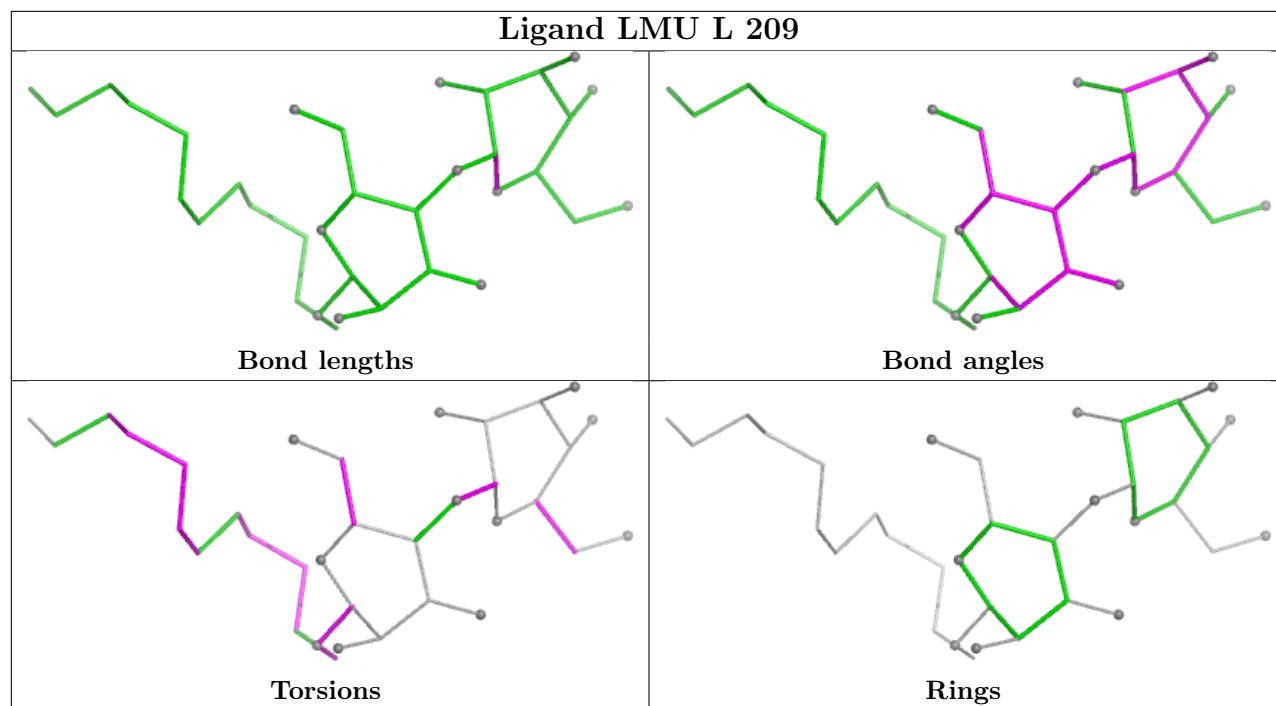
Bond angles



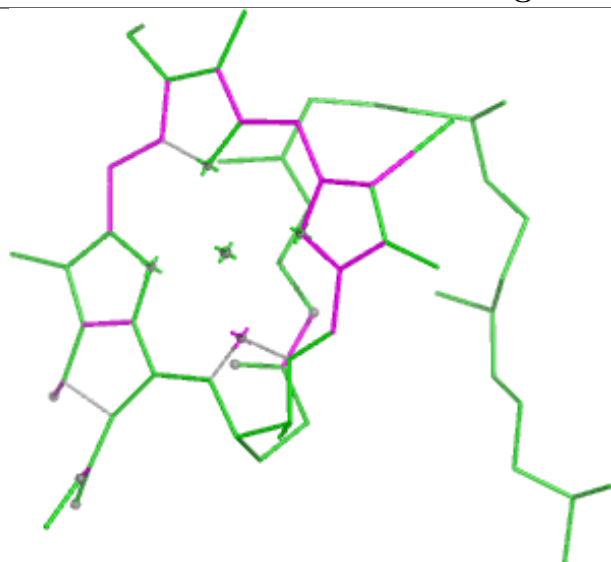
Torsions



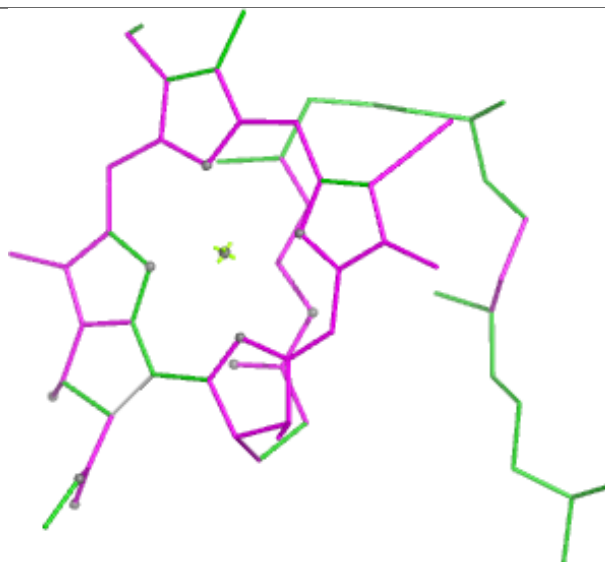
Rings



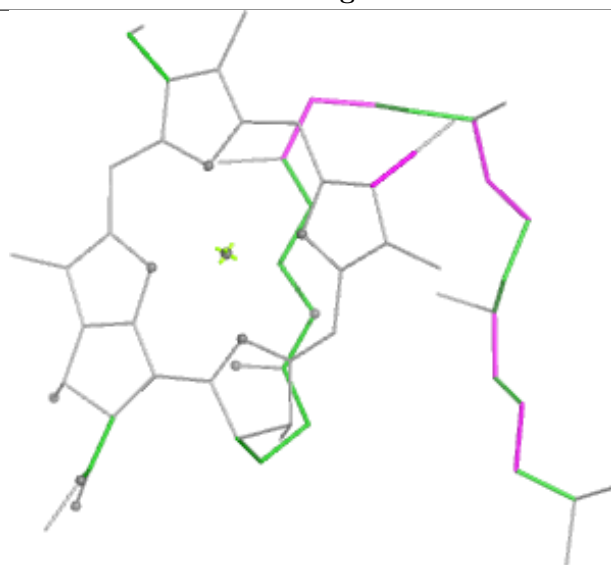
Ligand CLA B 807



Bond lengths



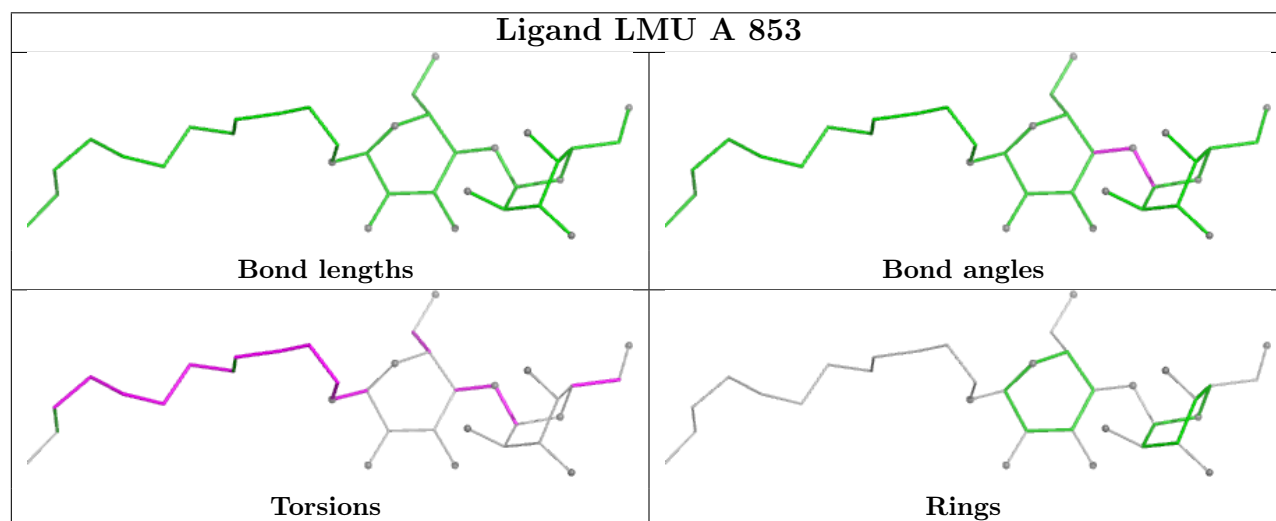
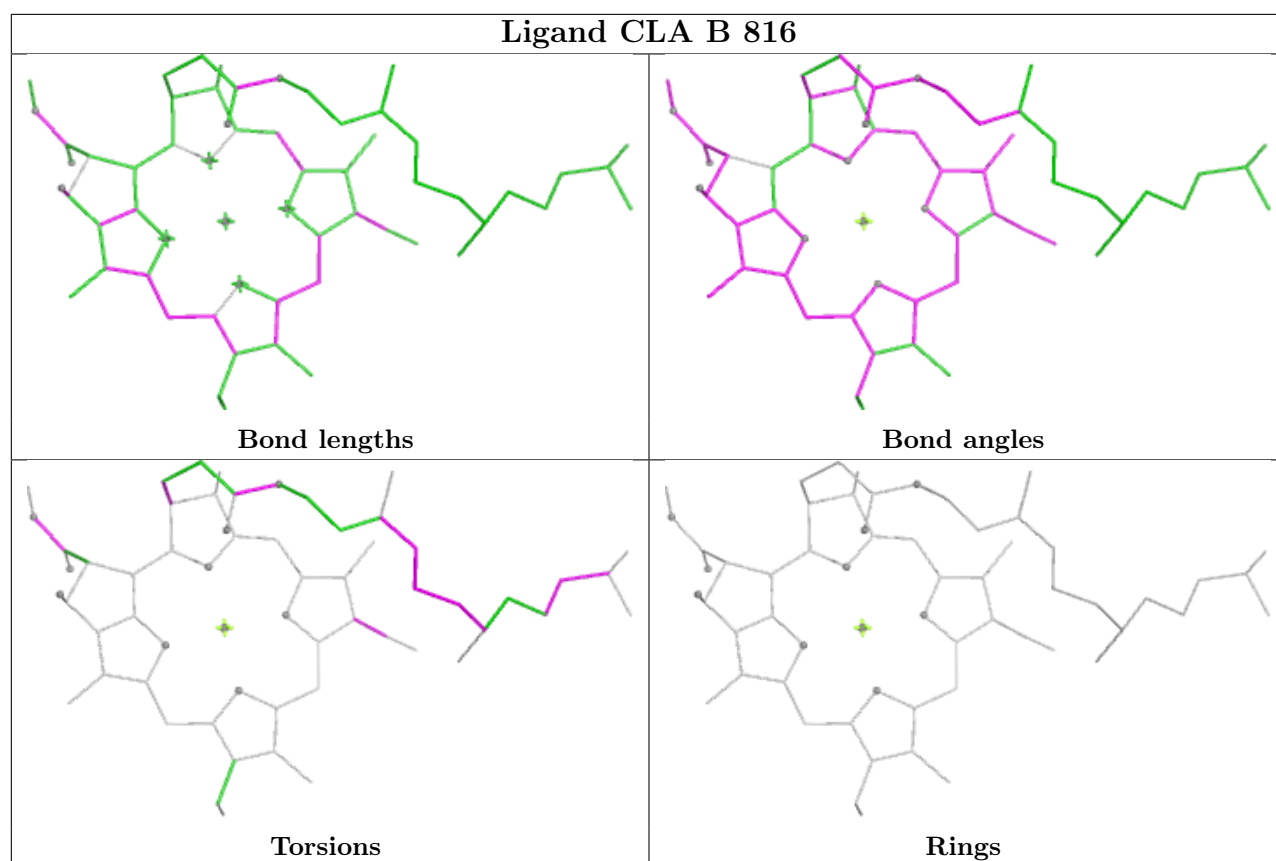
Bond angles

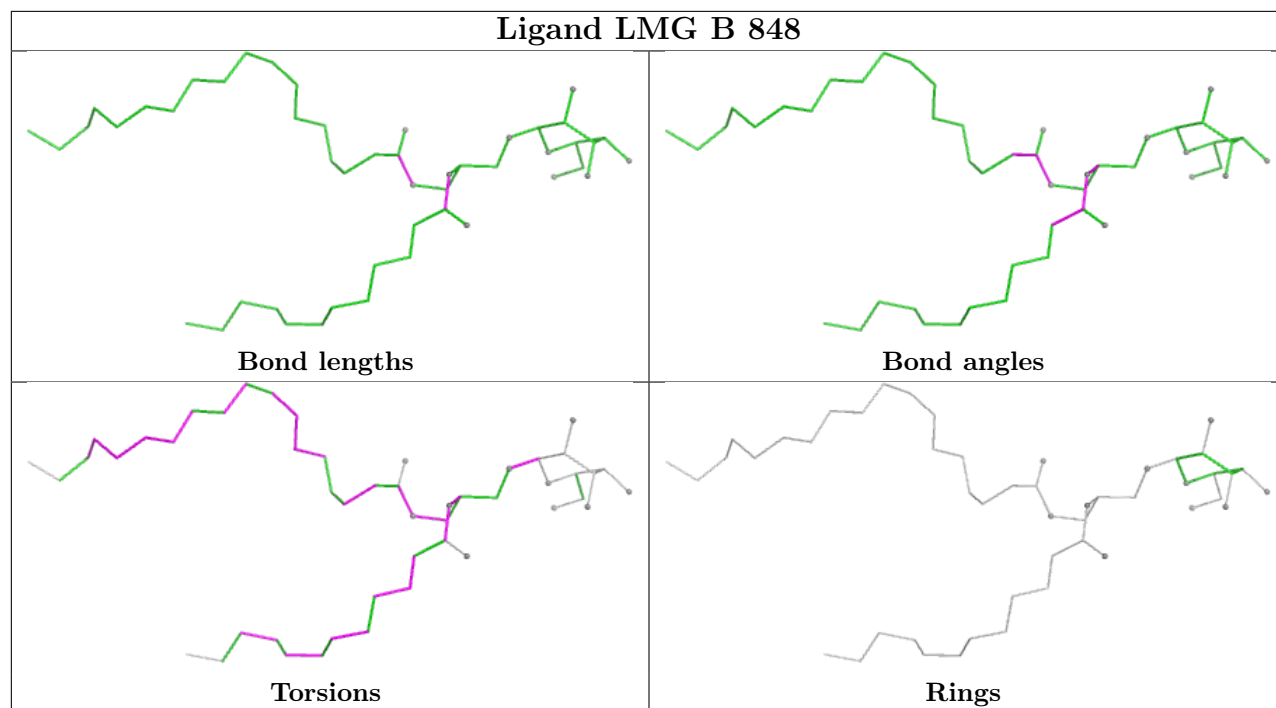


Torsions

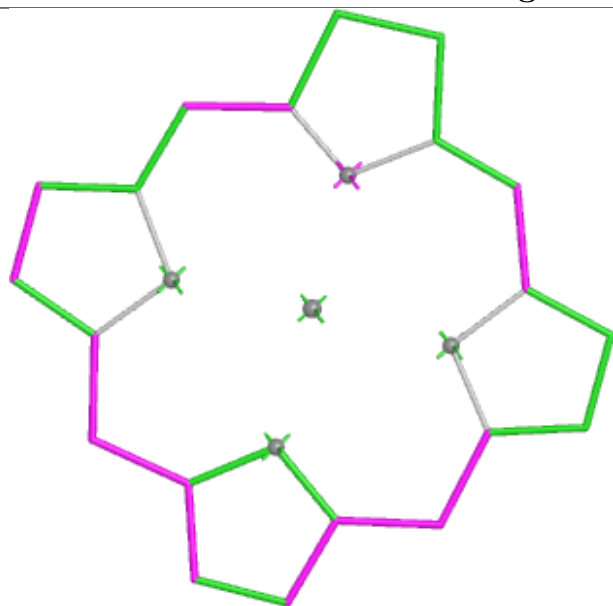


Rings

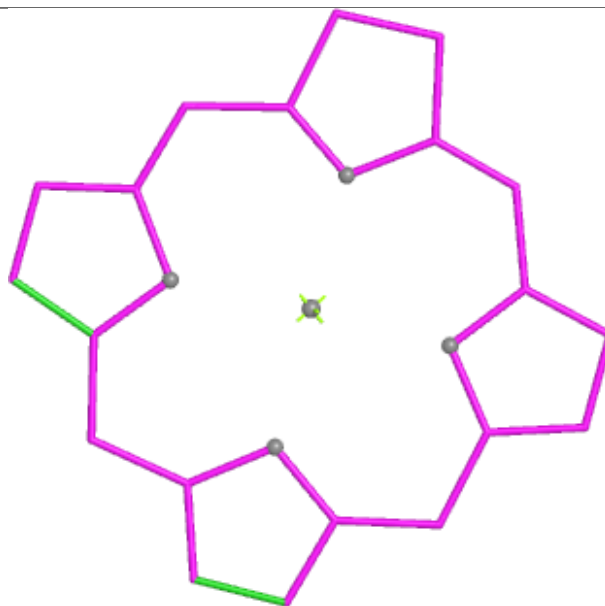




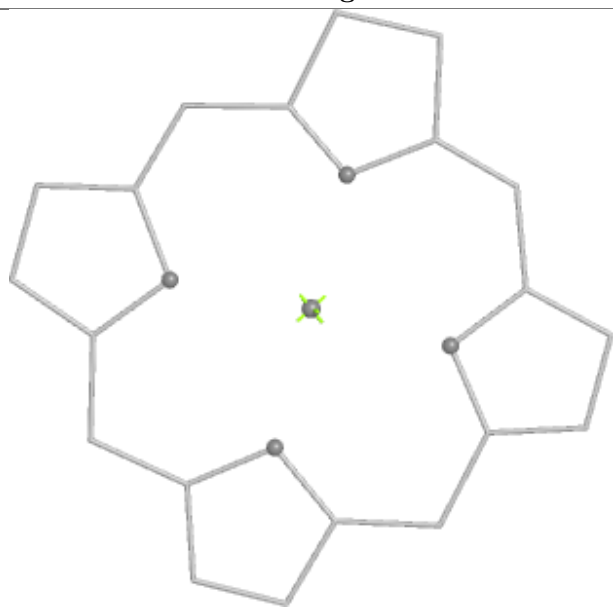
Ligand CLA 3 307



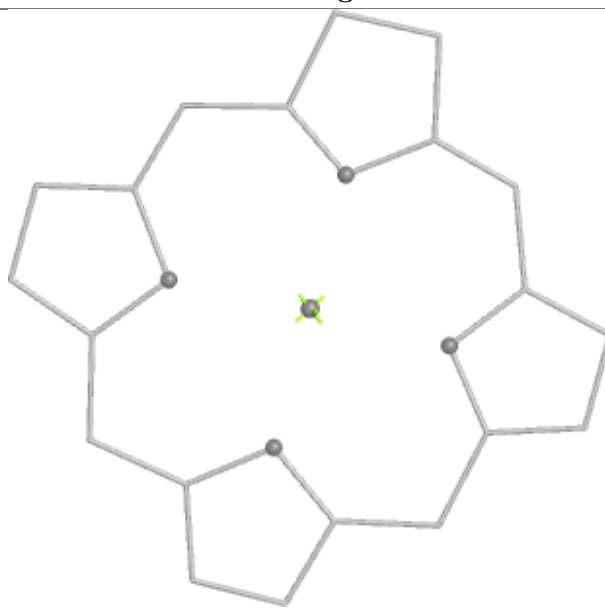
Bond lengths



Bond angles

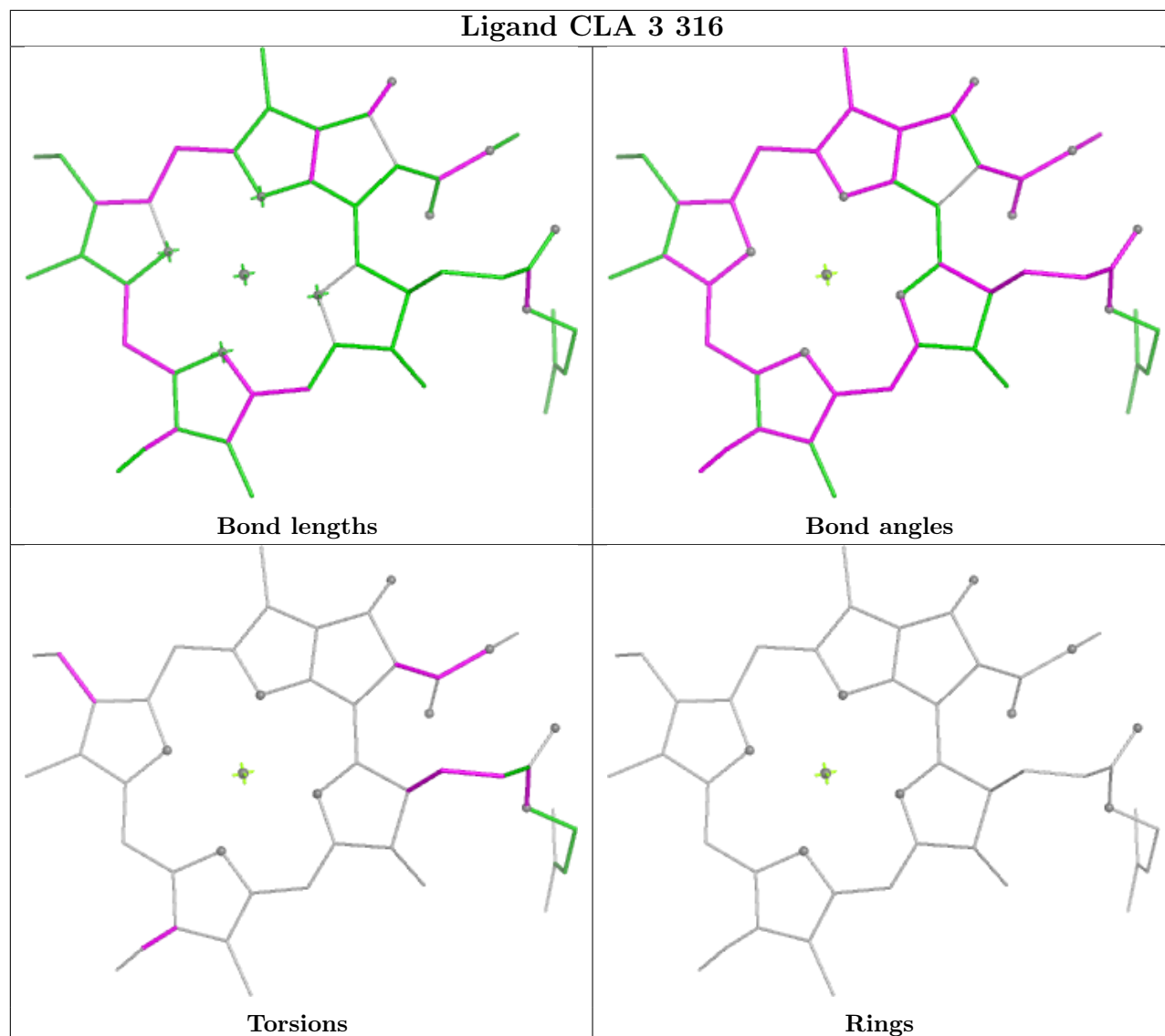


Torsions

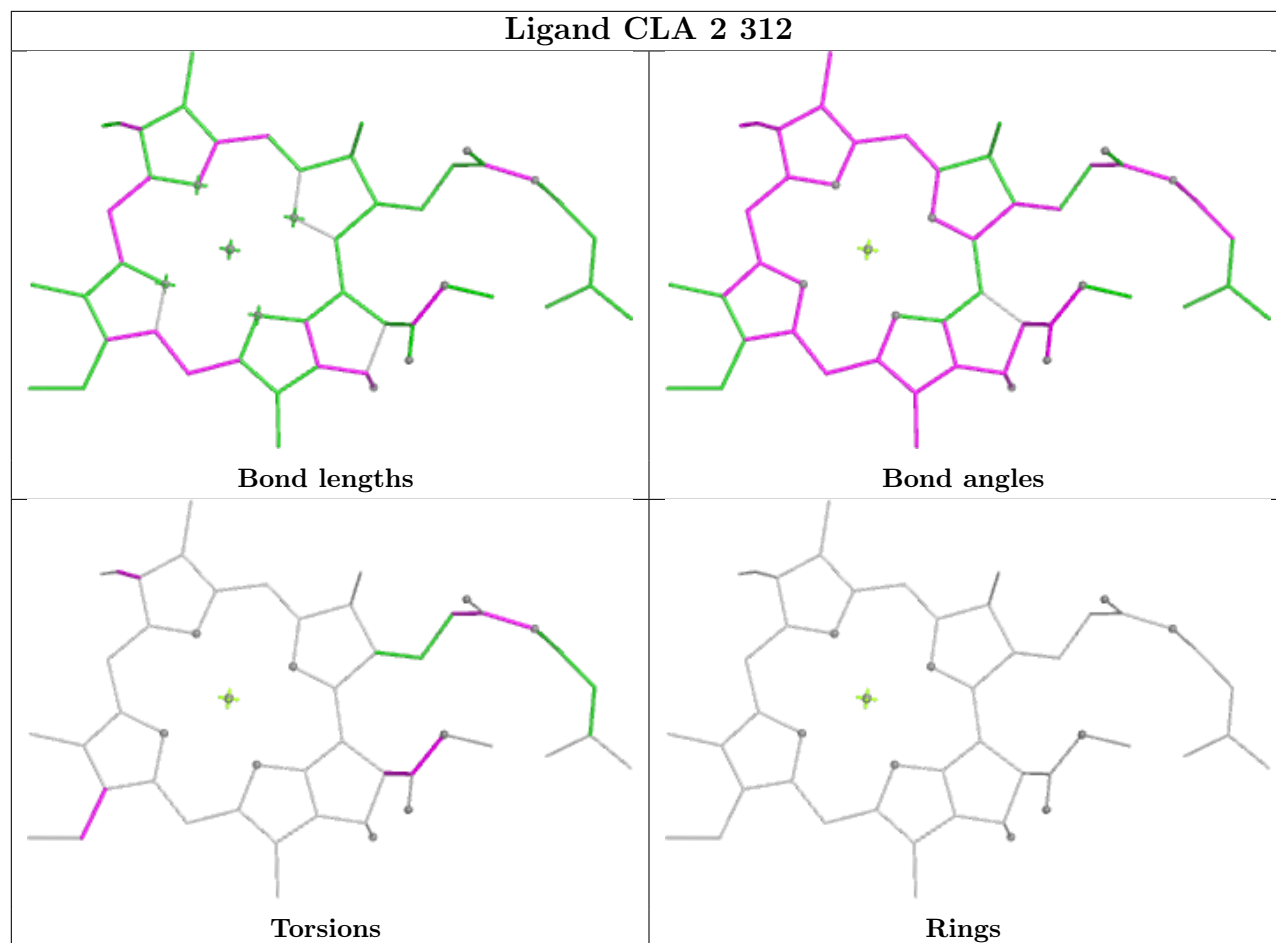


Rings

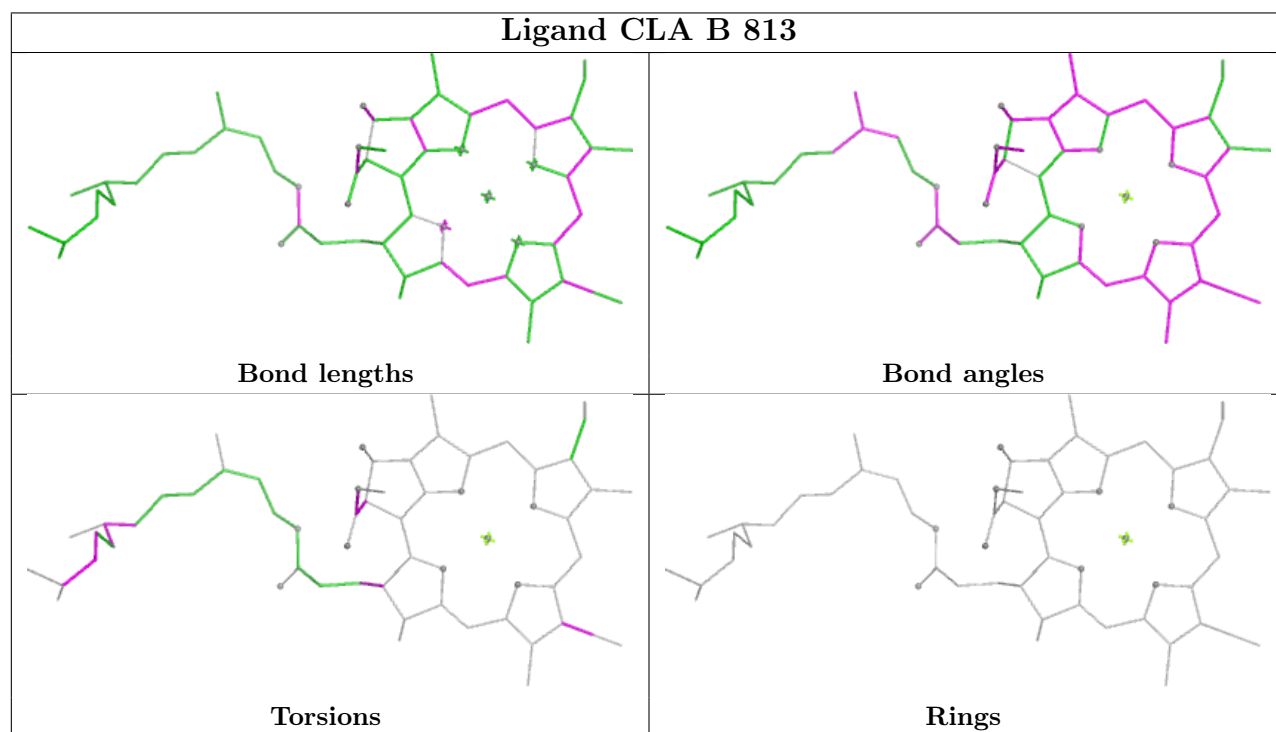
Ligand CLA 3 316



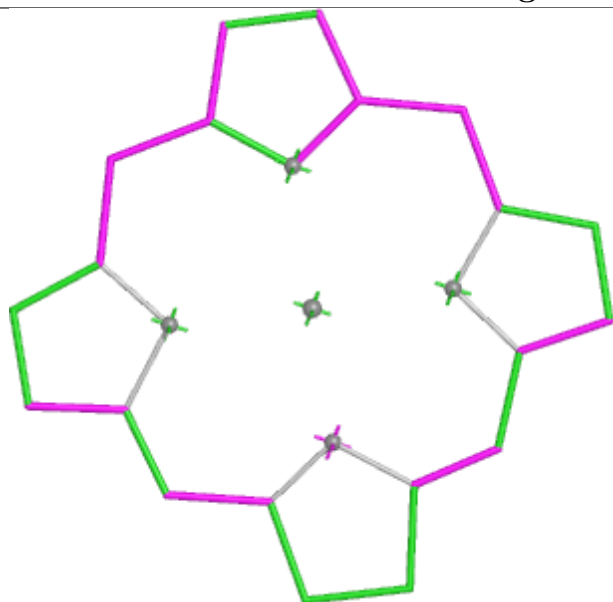
Ligand CLA 2 312



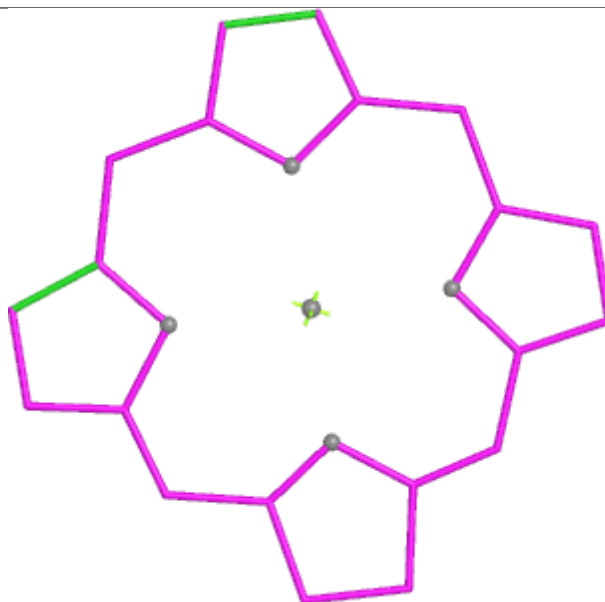
Ligand CLA B 813



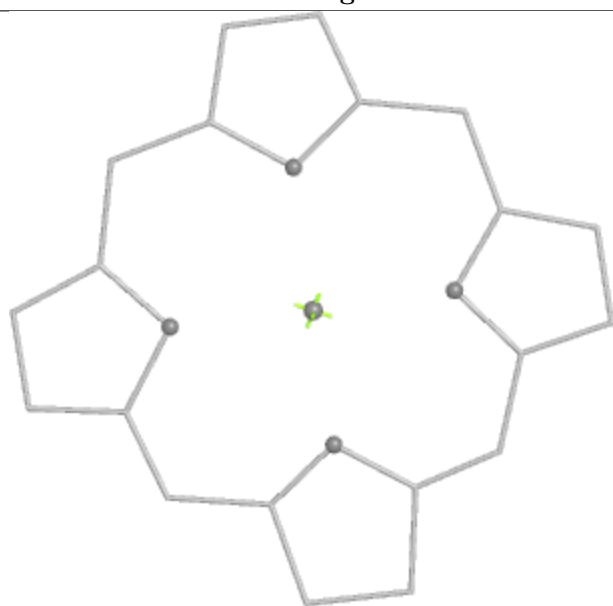
Ligand CLA 1 208



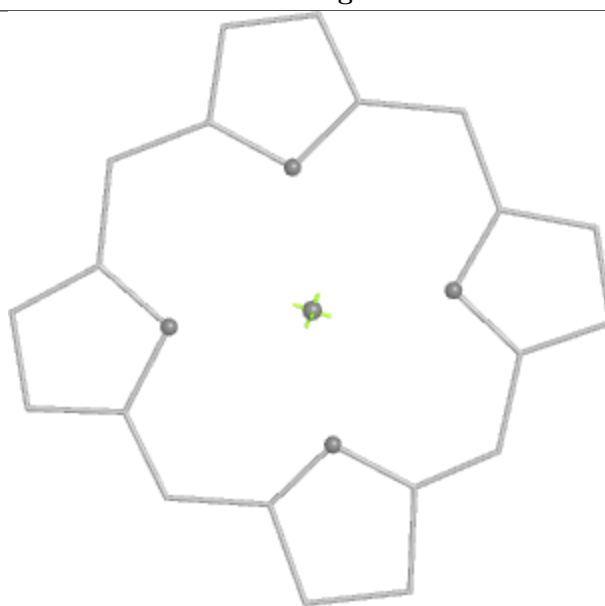
Bond lengths



Bond angles

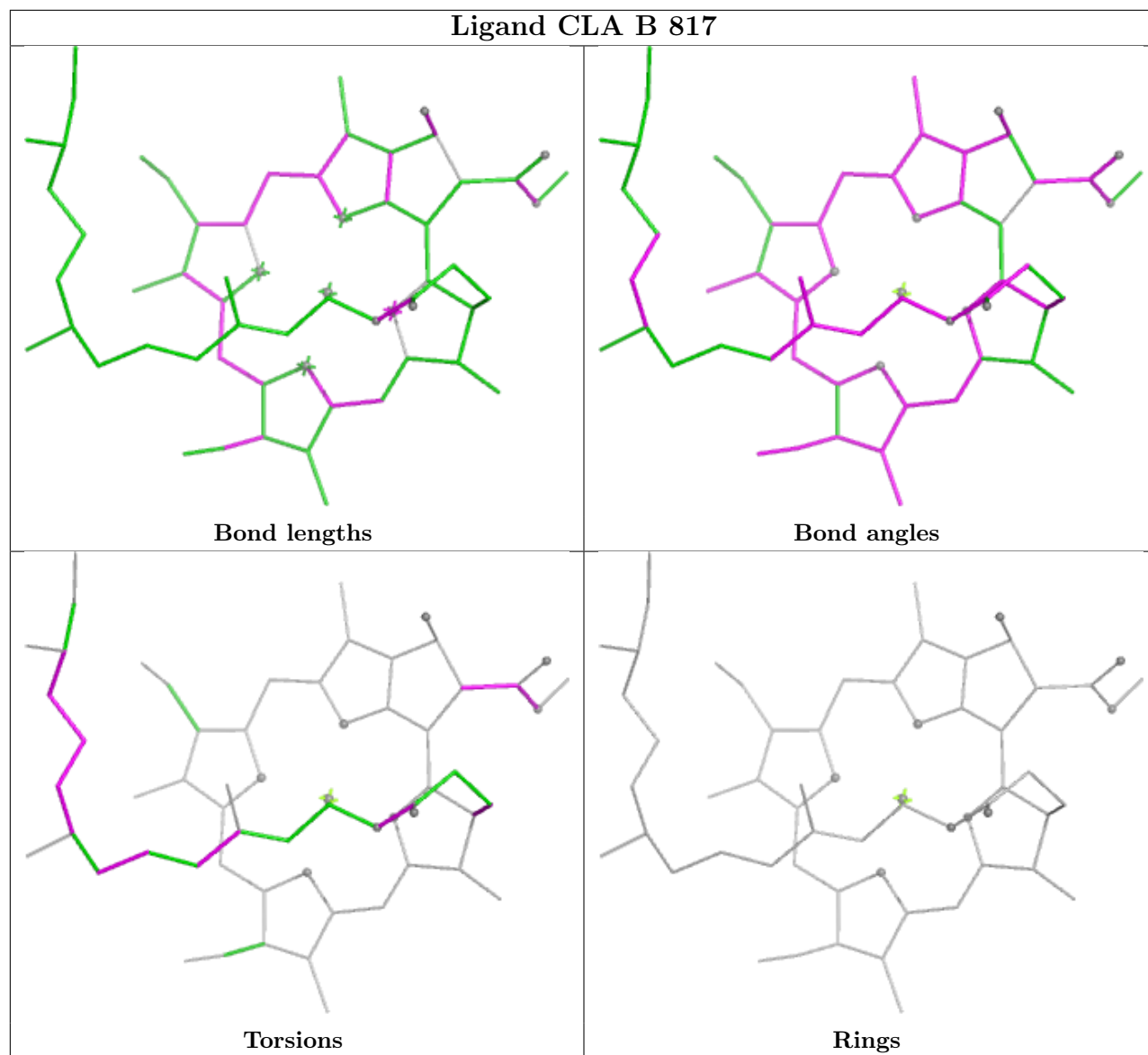


Torsions

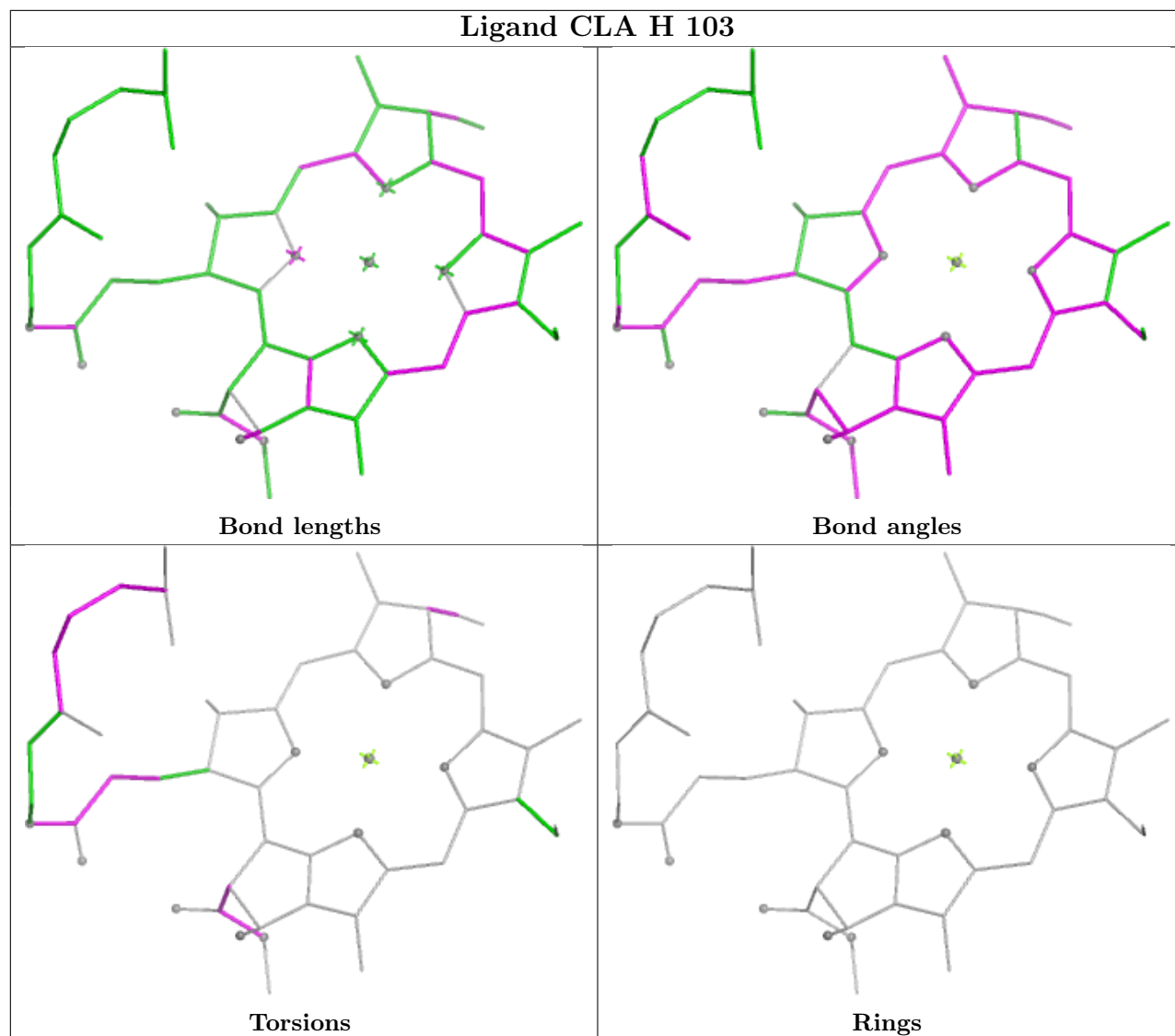


Rings

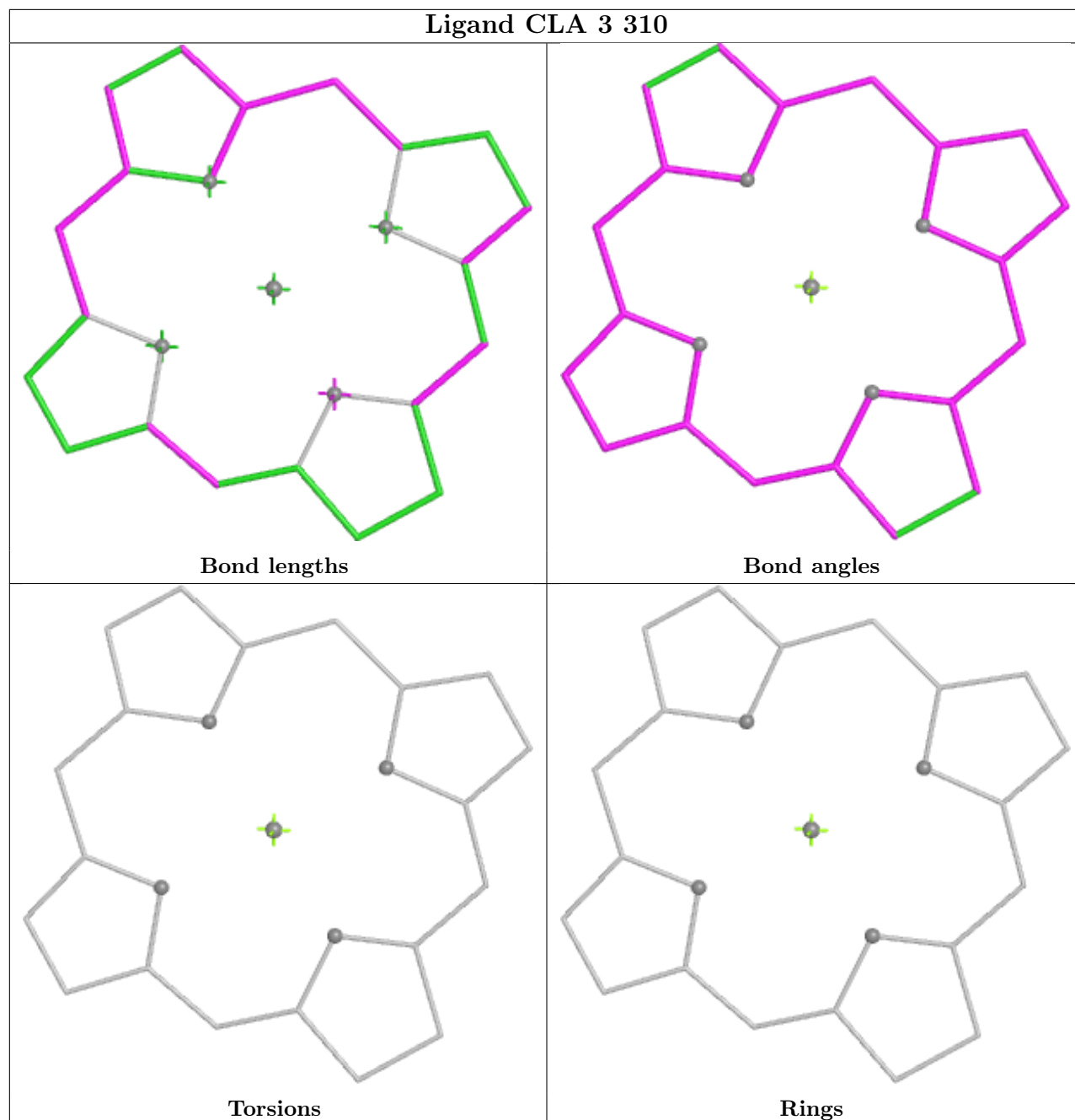
Ligand CLA B 817



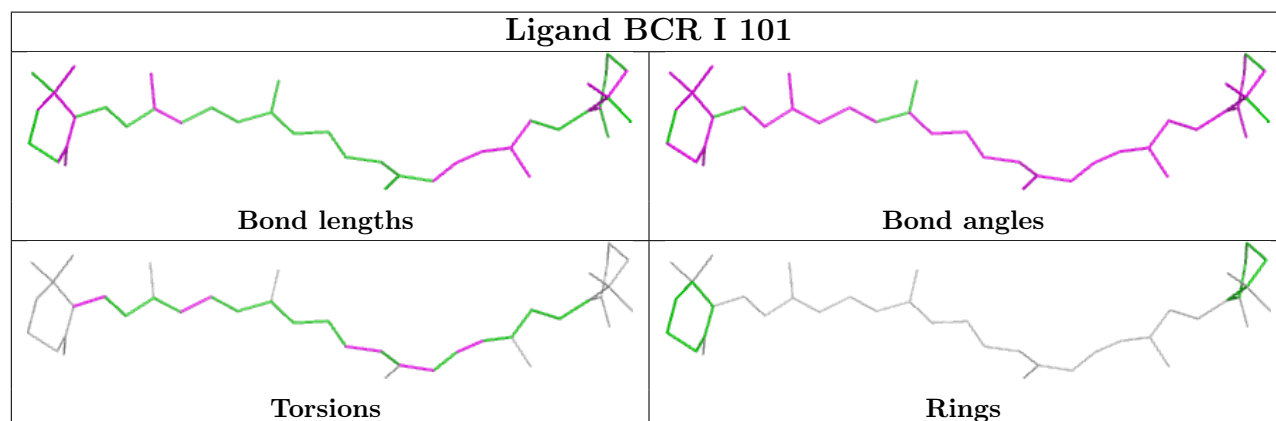
Ligand CLA H 103



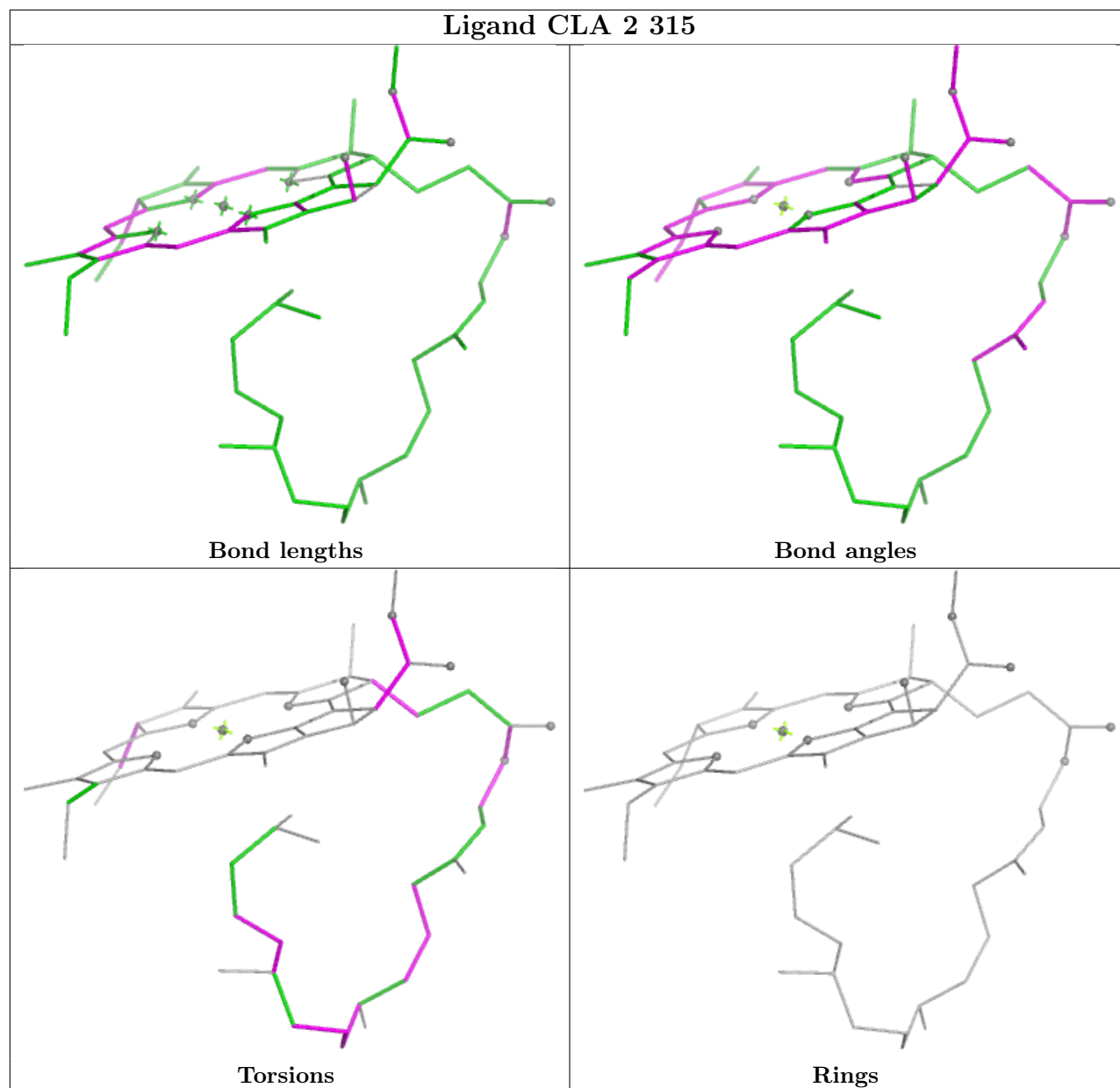
Ligand CLA 3 310

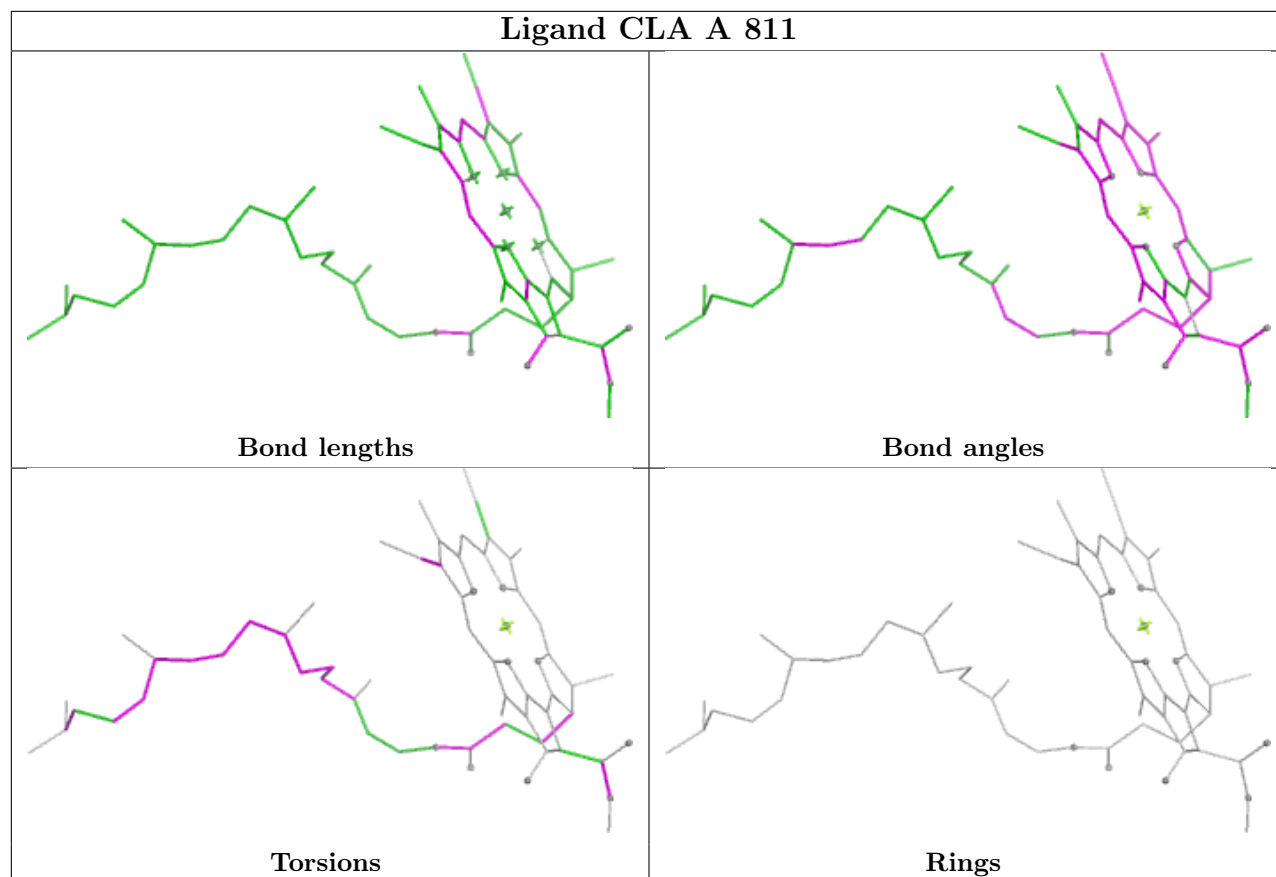


Ligand BCR I 101

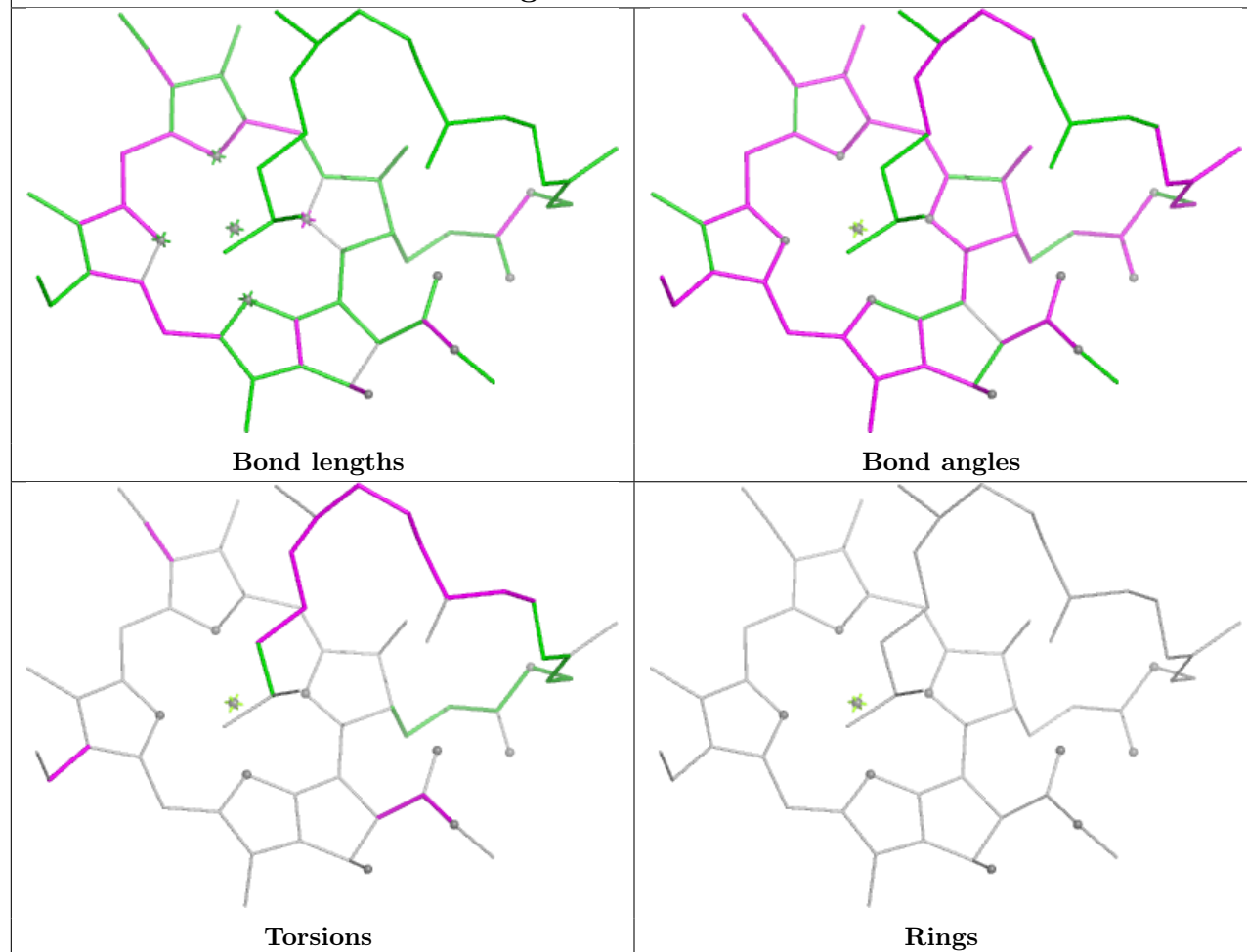


Ligand CLA 2 315

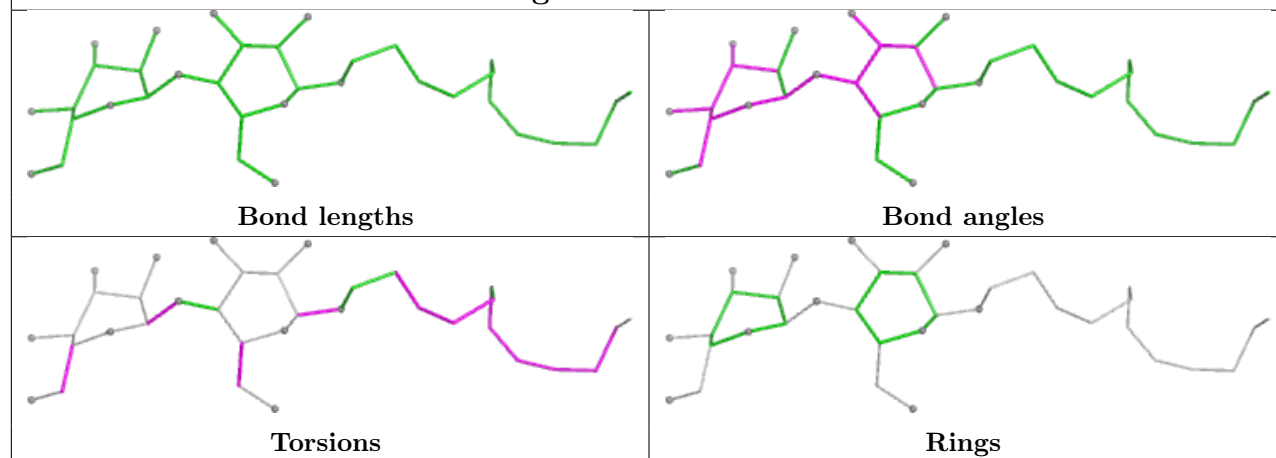


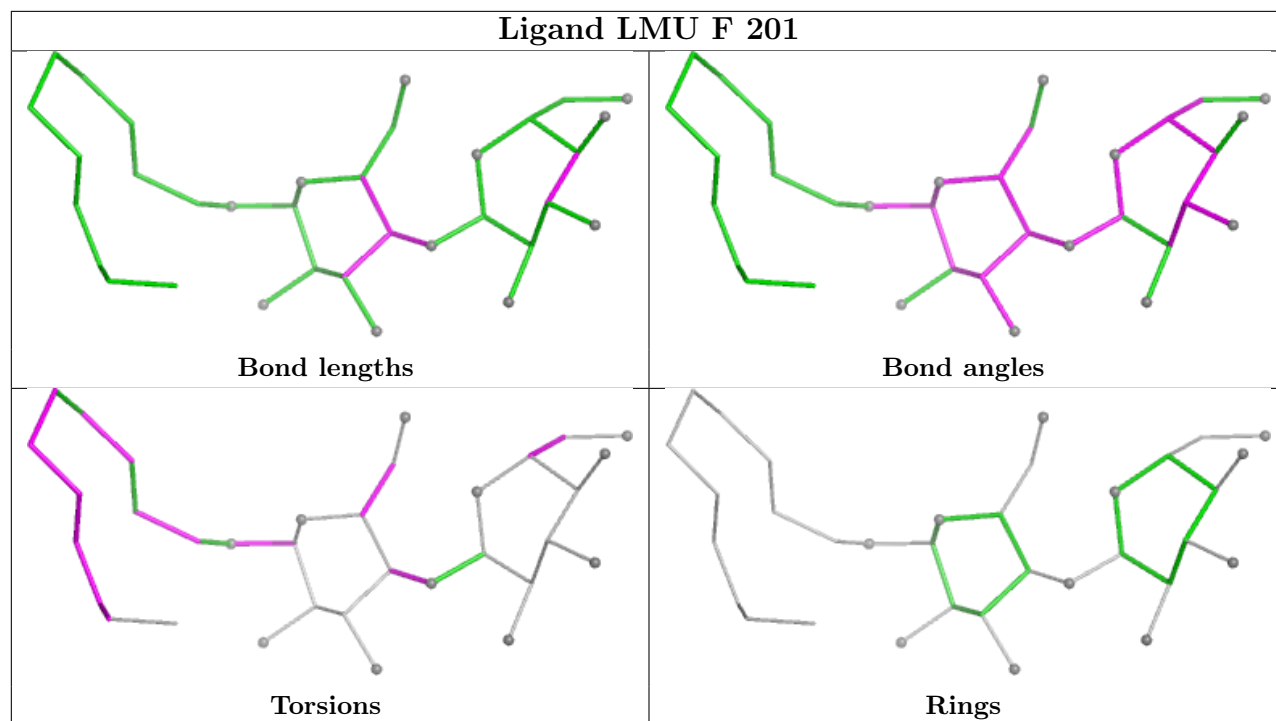


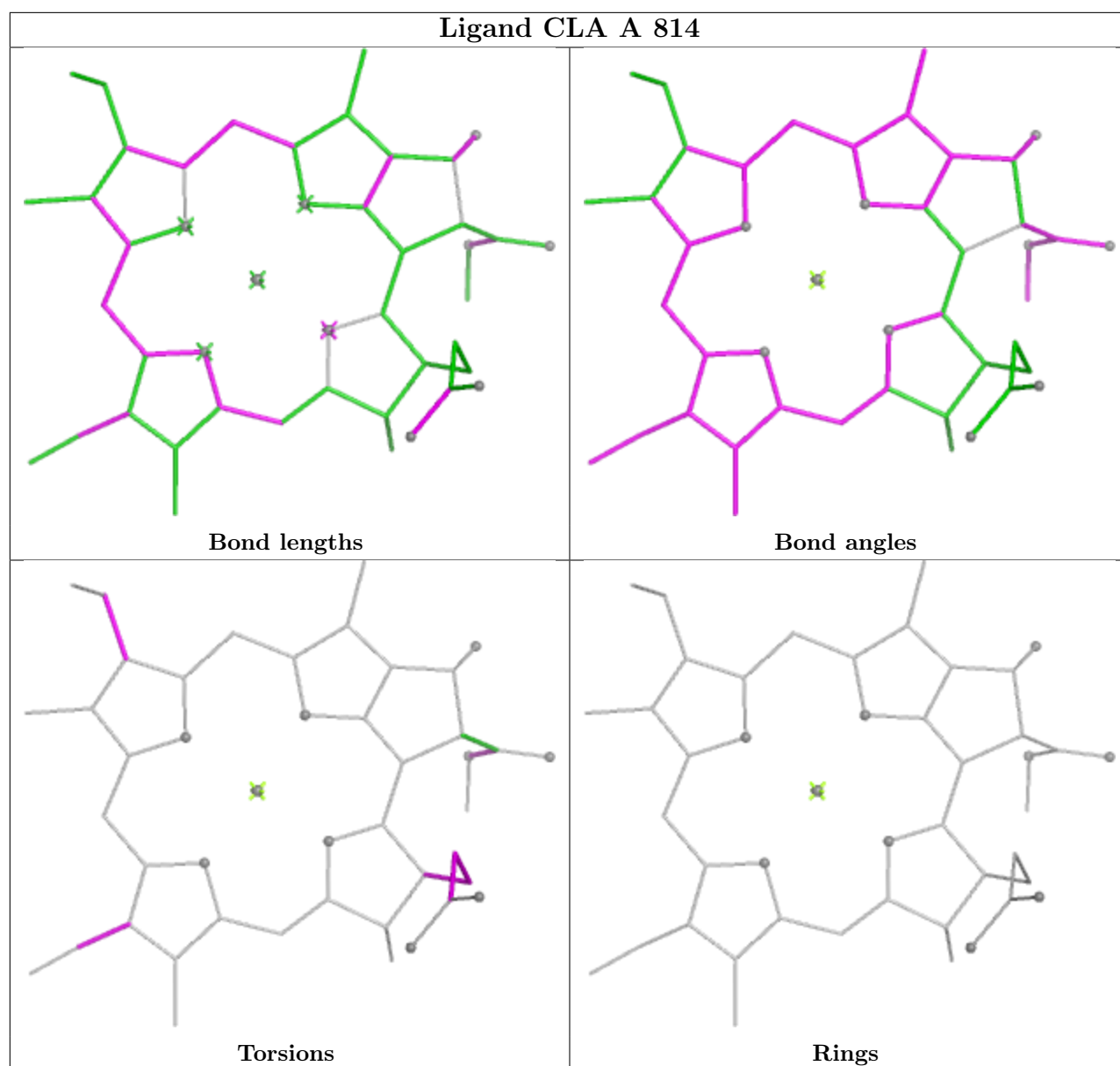
Ligand CLA B 806



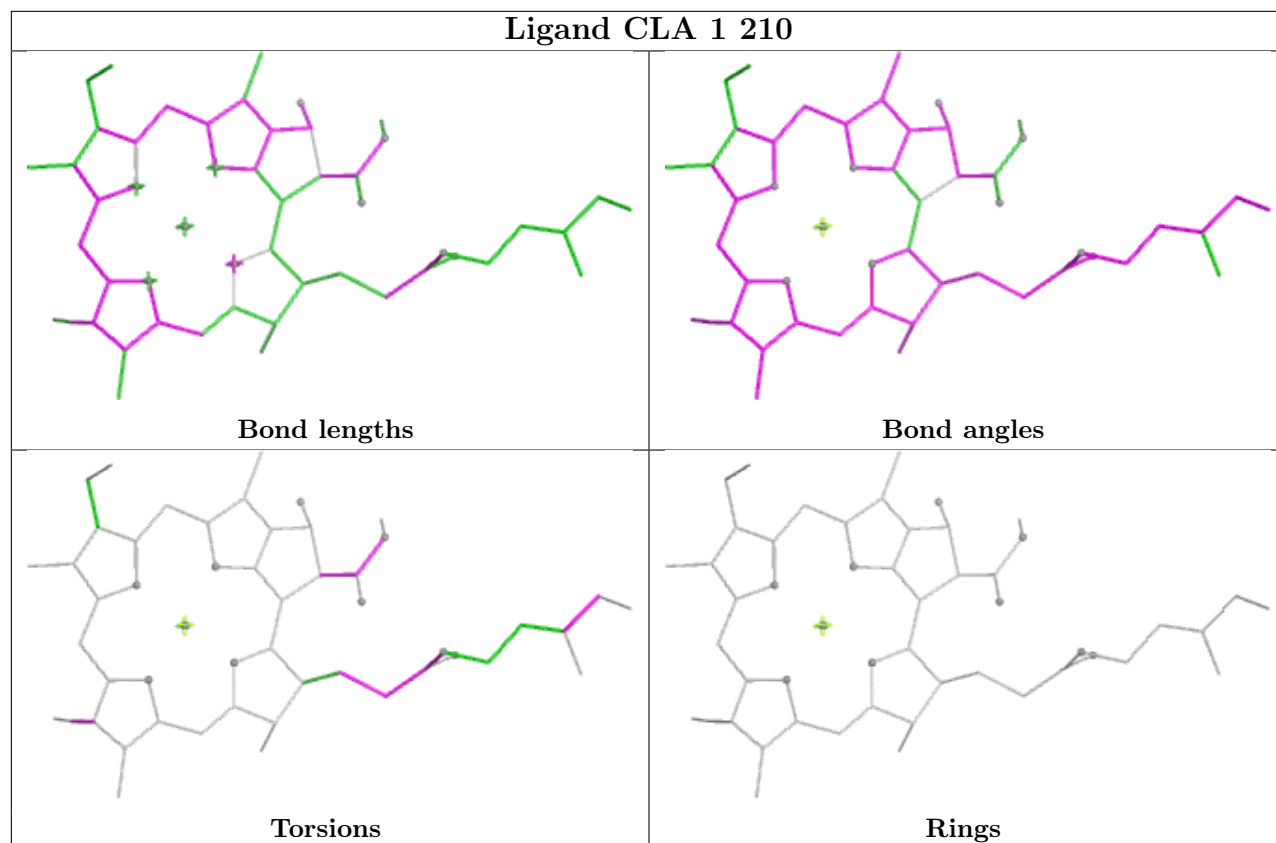
Ligand LMU 3 321



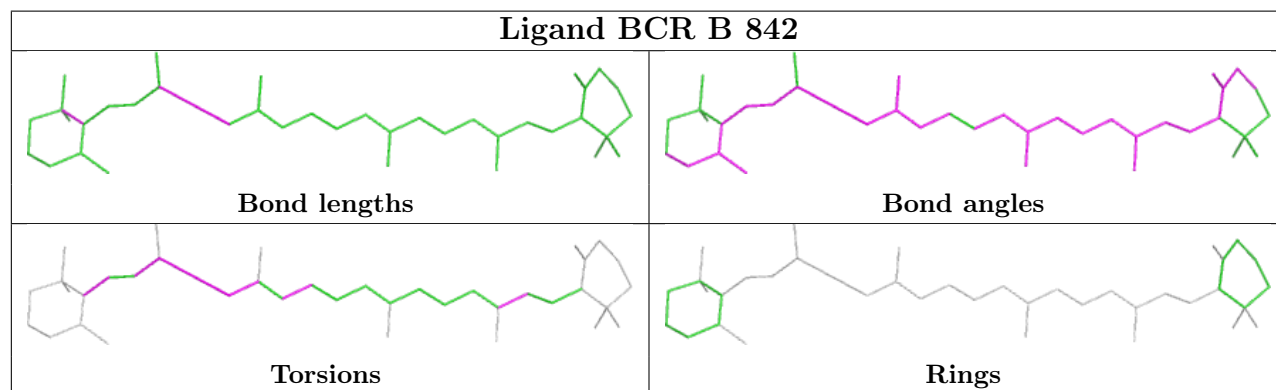


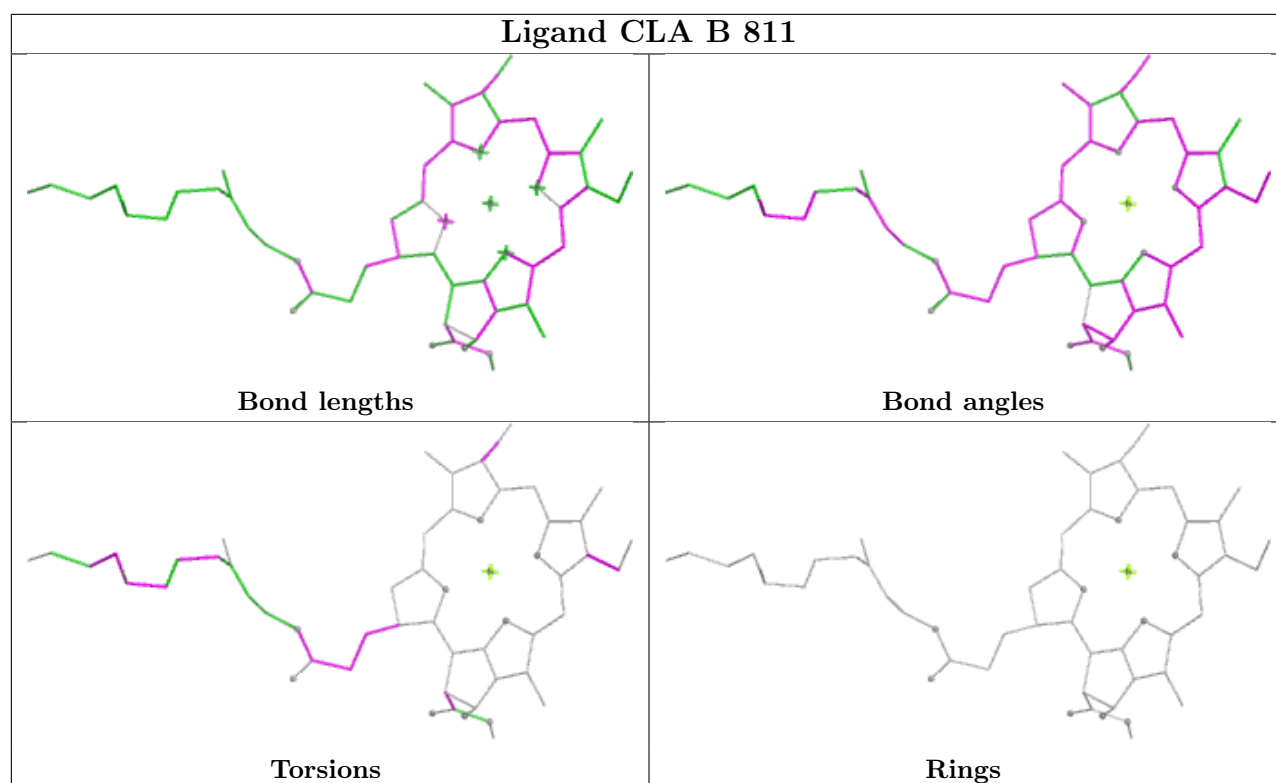


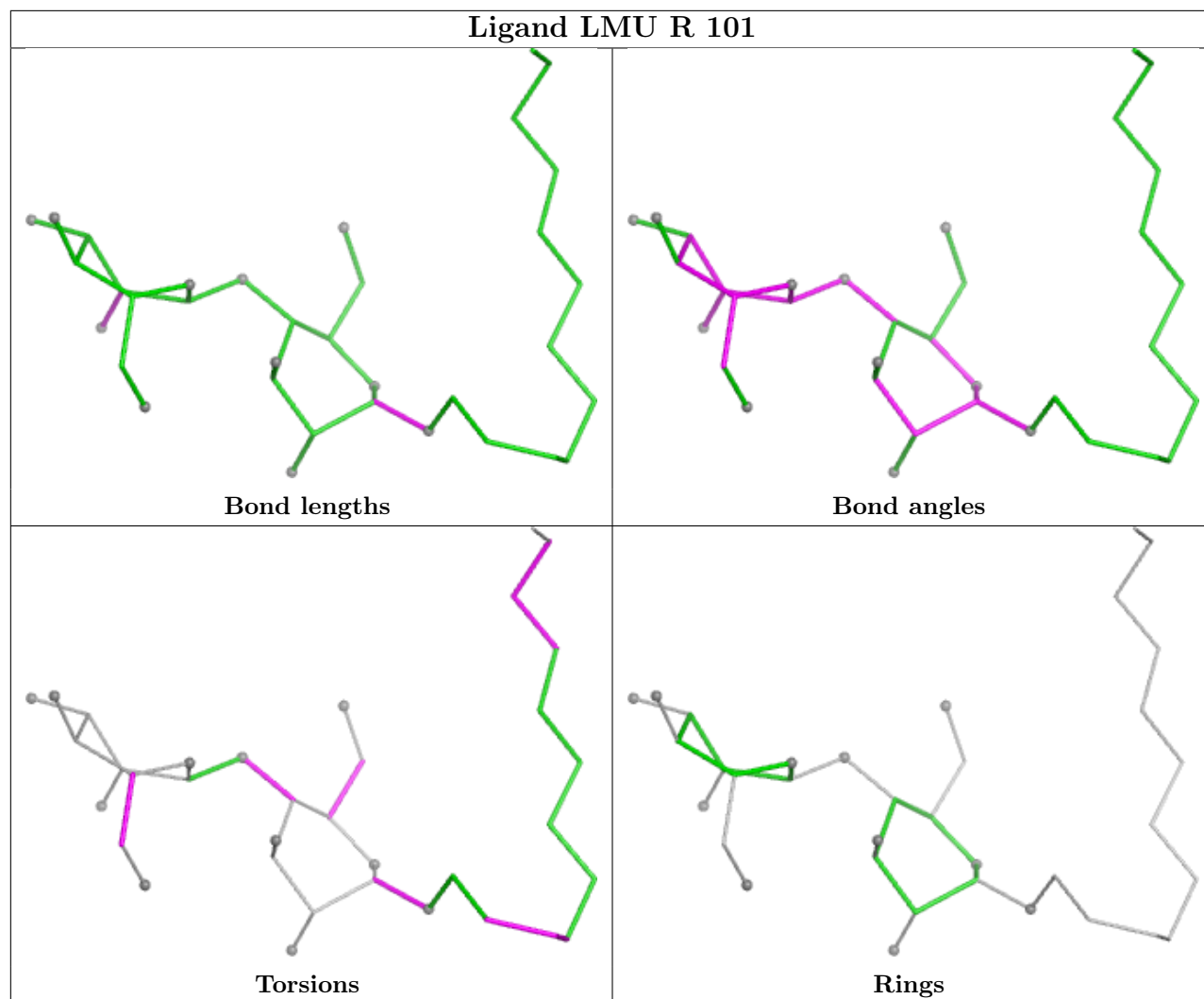
Ligand CLA 1 210

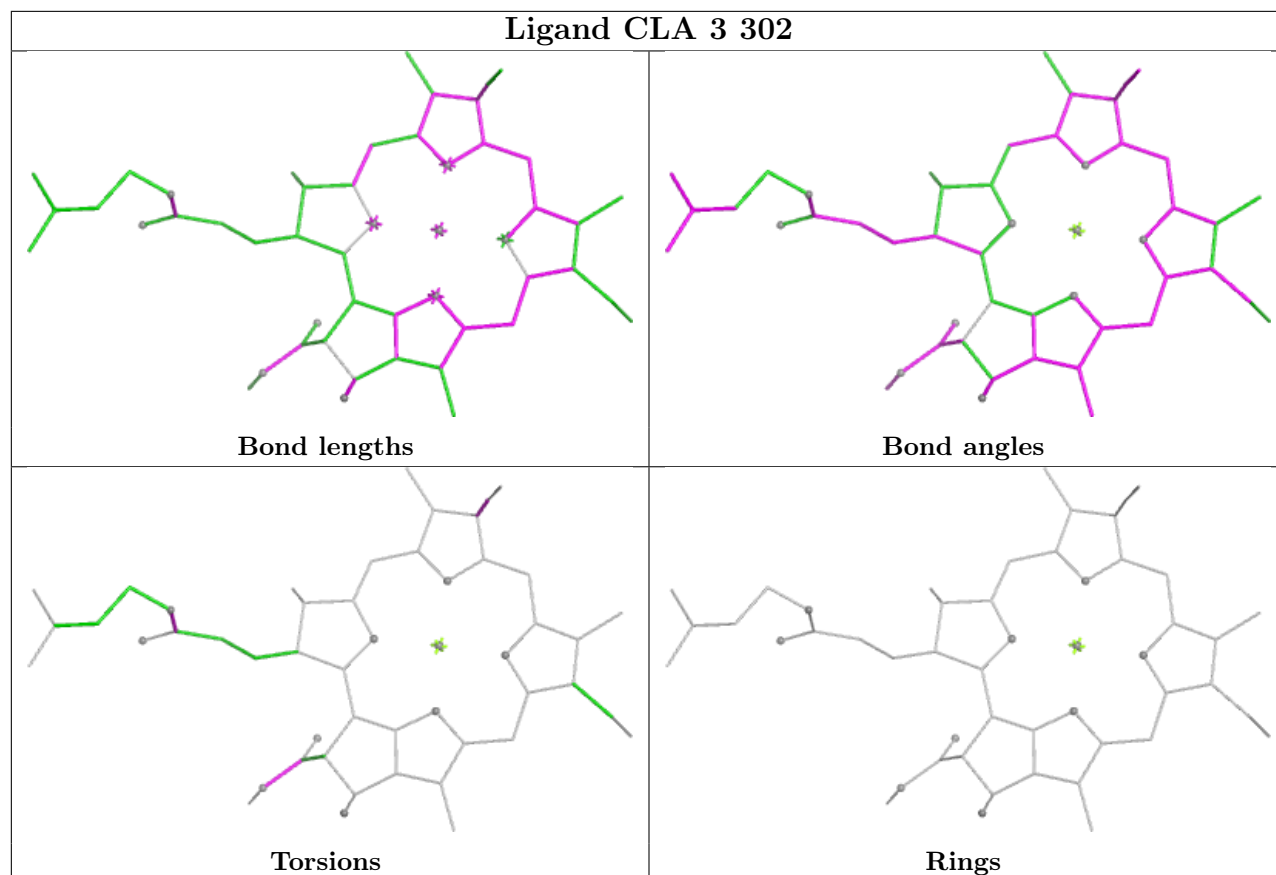
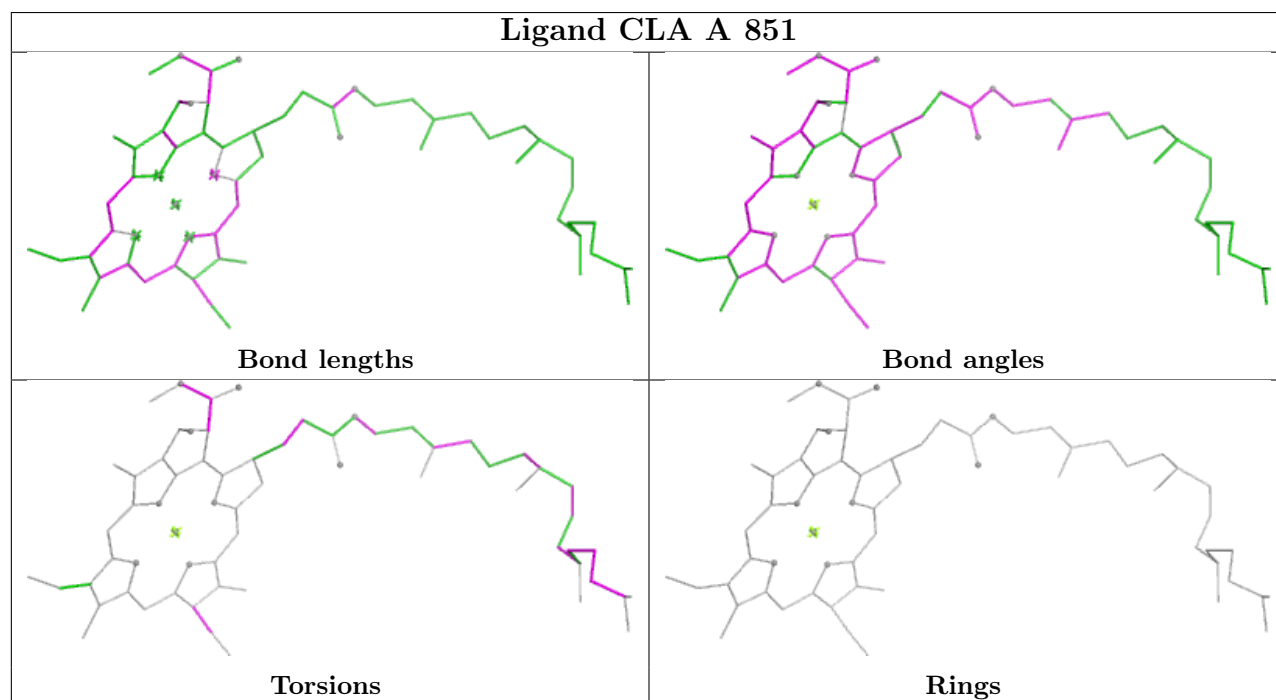


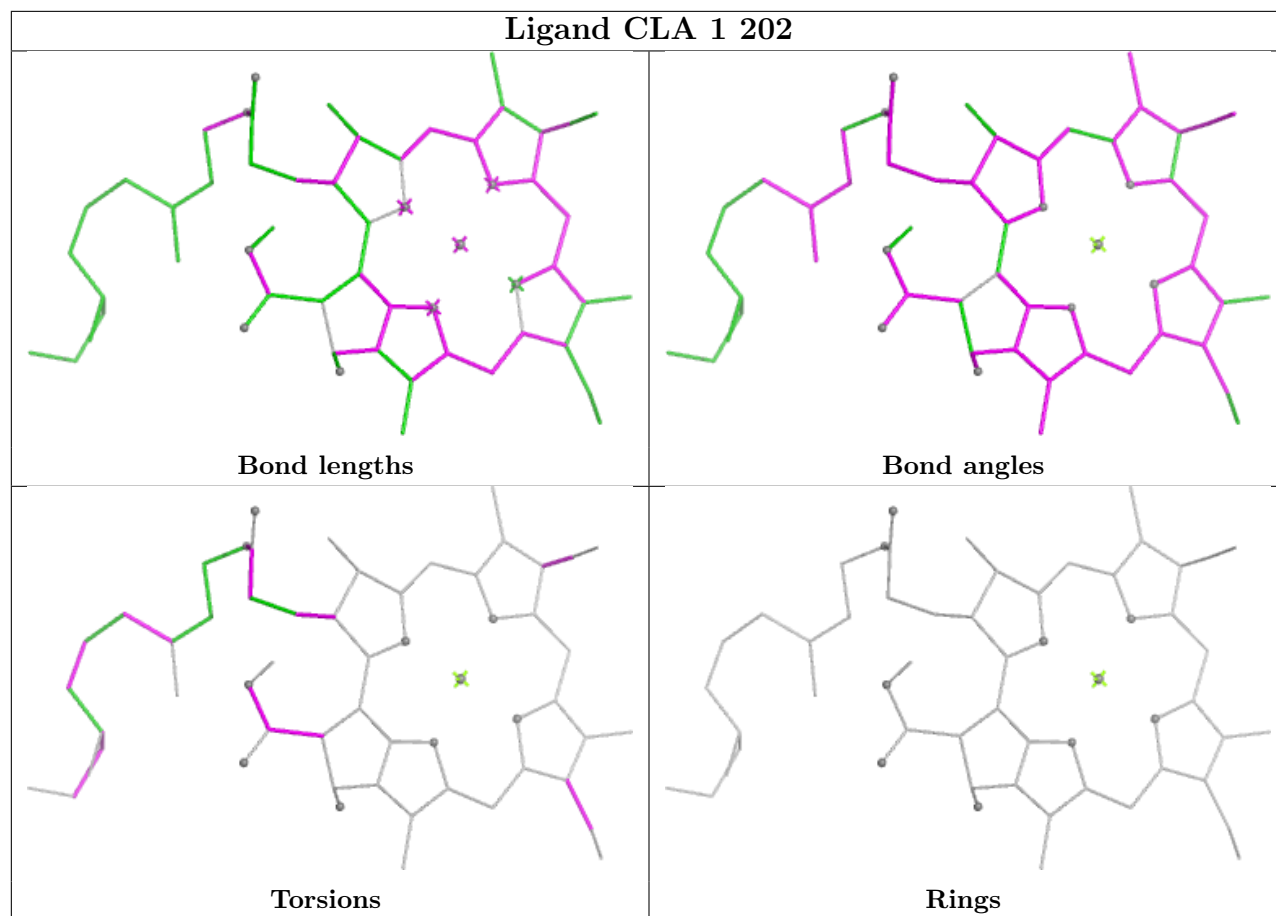
Ligand BCR B 842



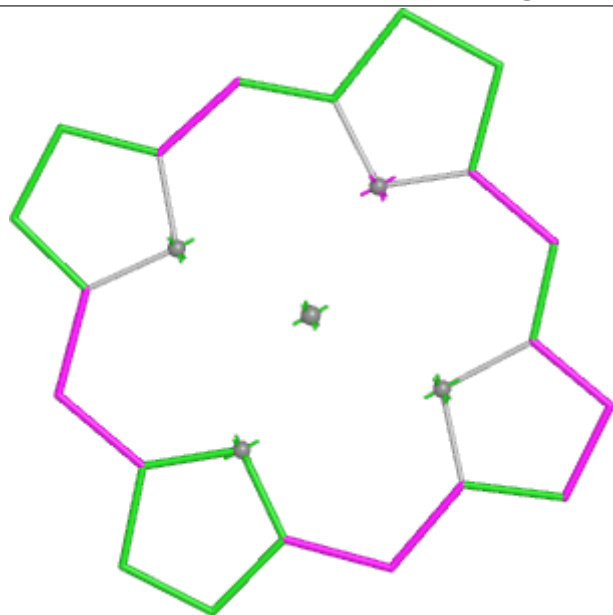




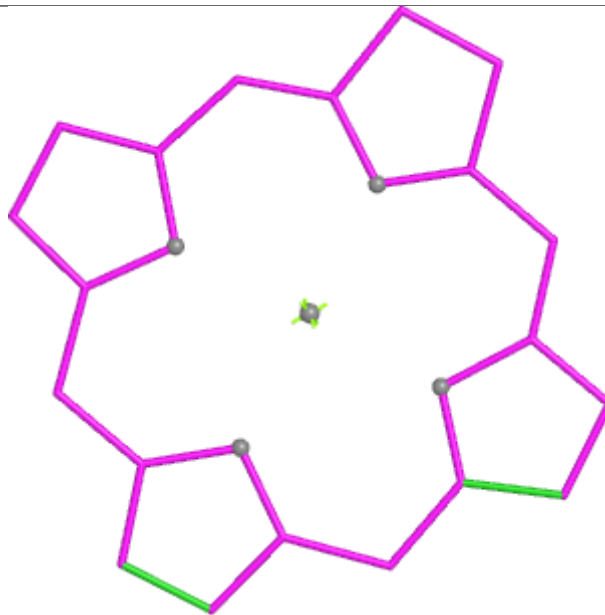
Ligand CLA 3 302**Ligand CLA A 851**



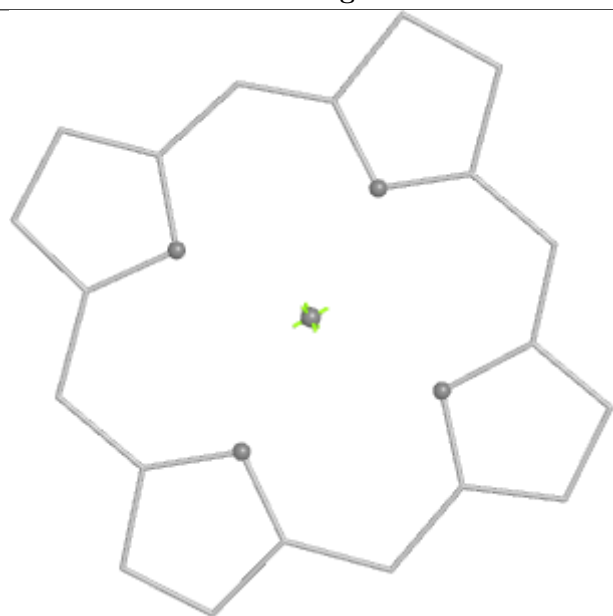
Ligand CLA 3 309



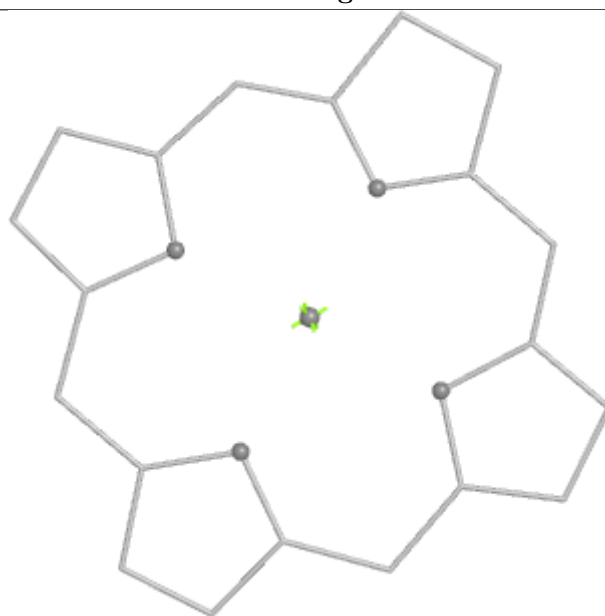
Bond lengths



Bond angles

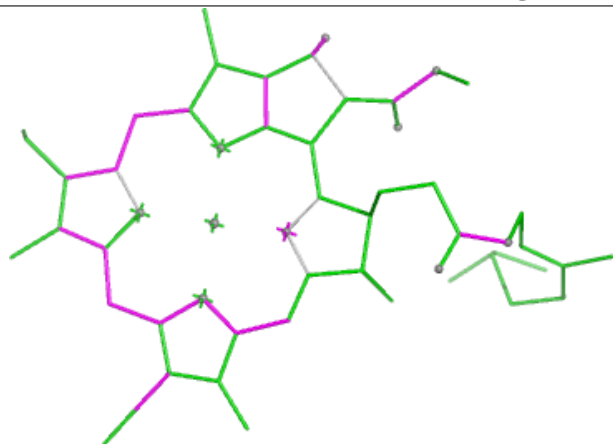


Torsions

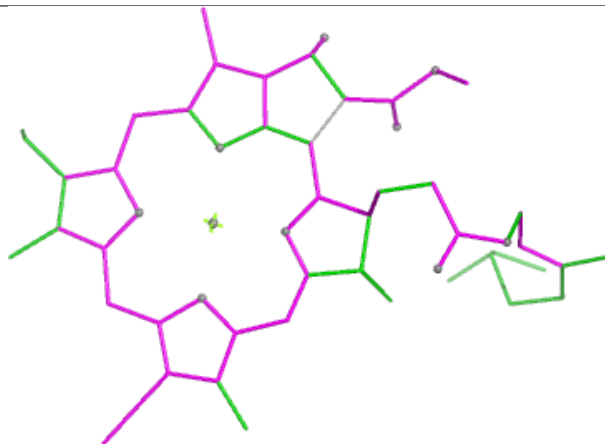


Rings

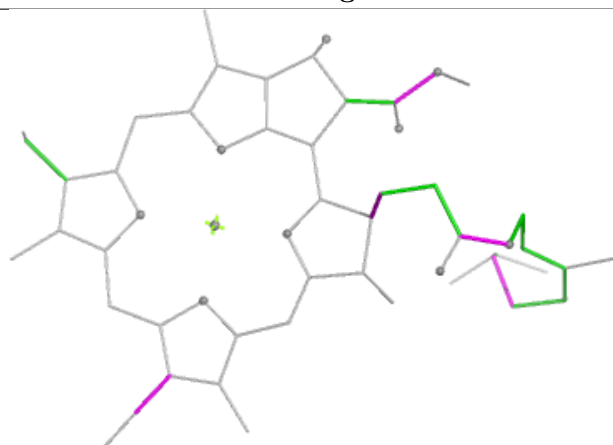
Ligand CLA A 806



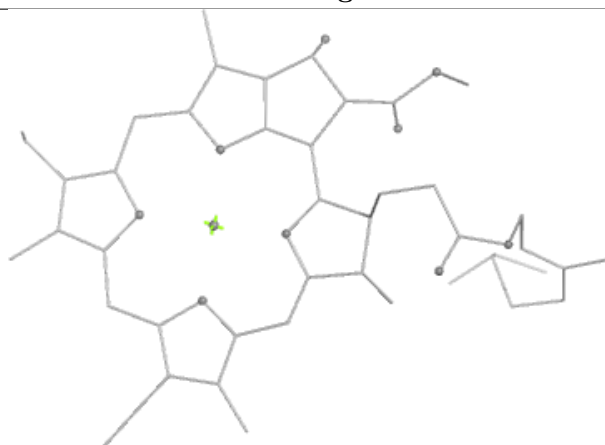
Bond lengths



Bond angles

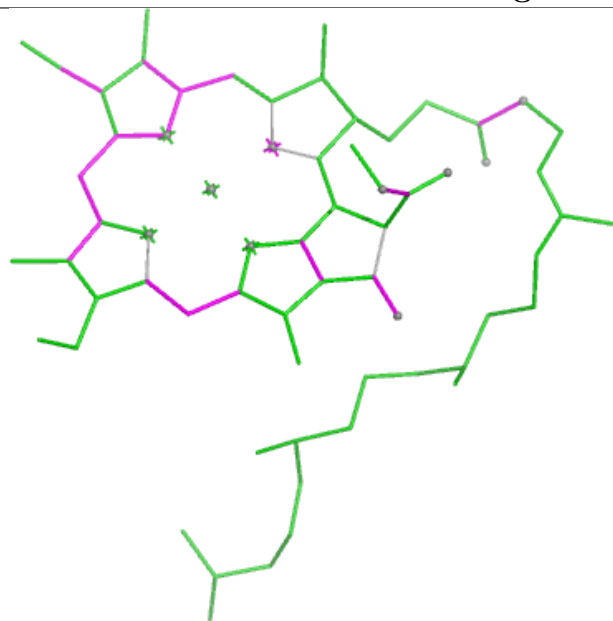


Torsions

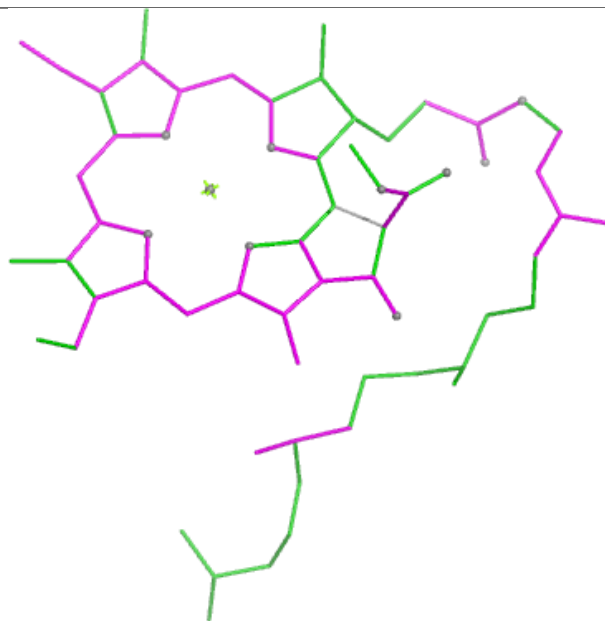


Rings

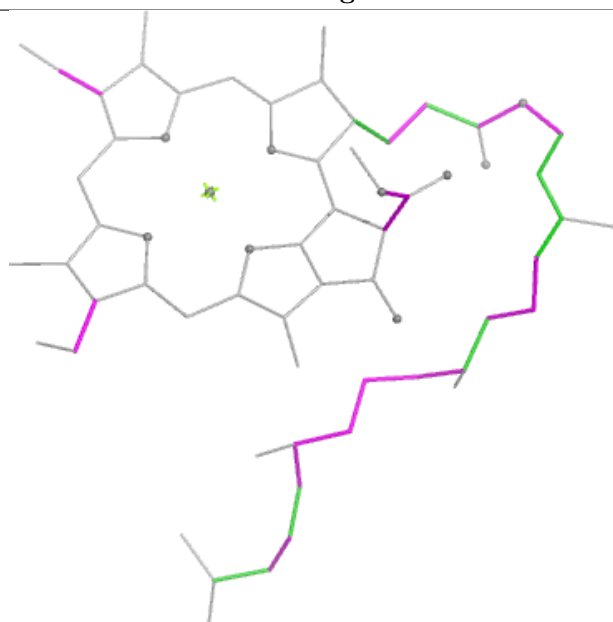
Ligand CLA A 823



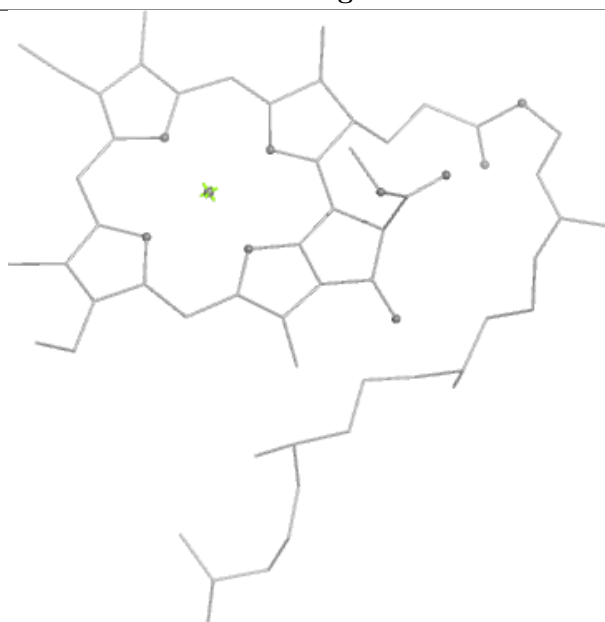
Bond lengths



Bond angles

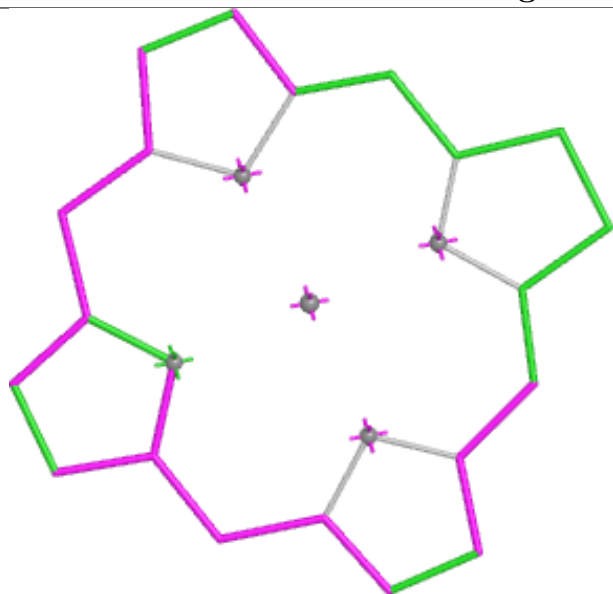


Torsions

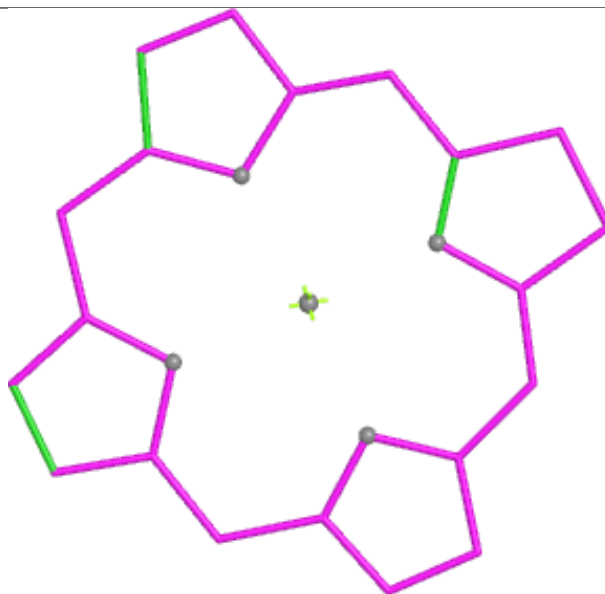


Rings

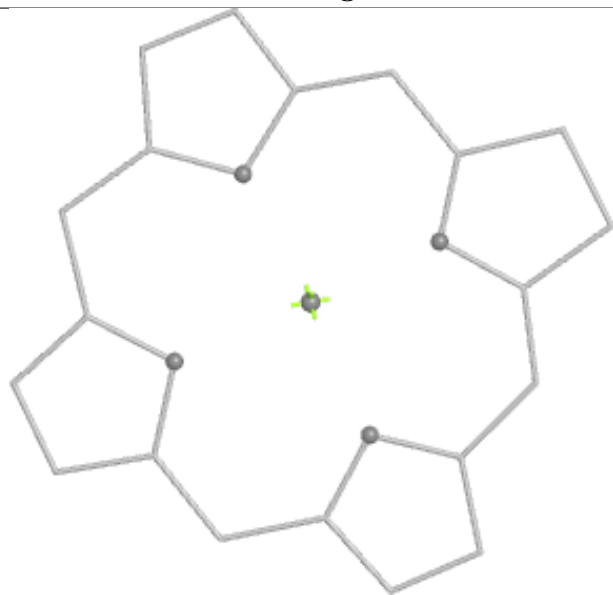
Ligand CLA 4 310



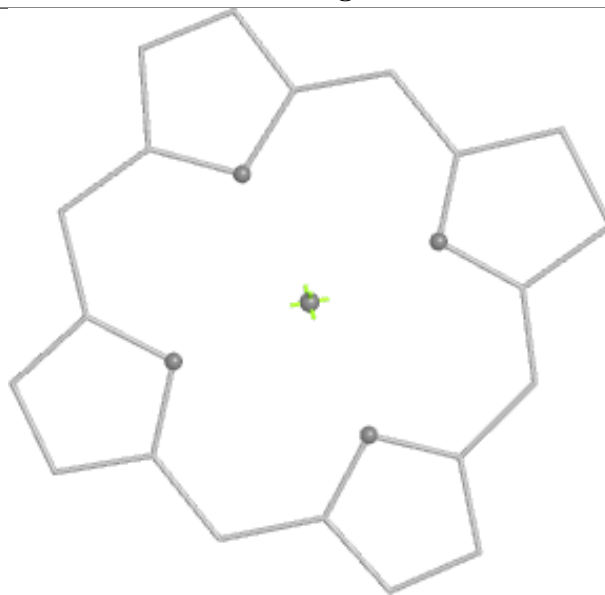
Bond lengths



Bond angles

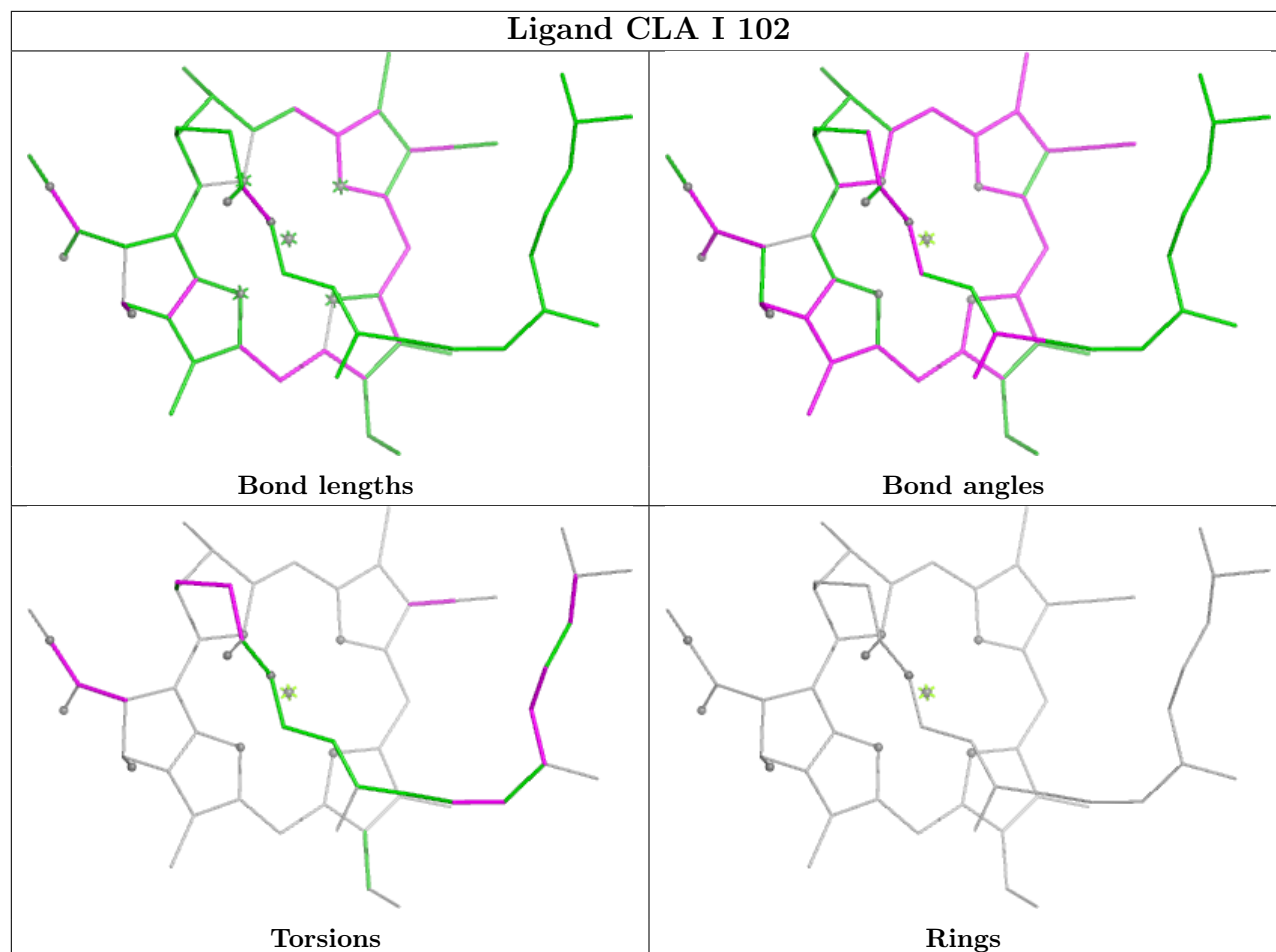


Torsions

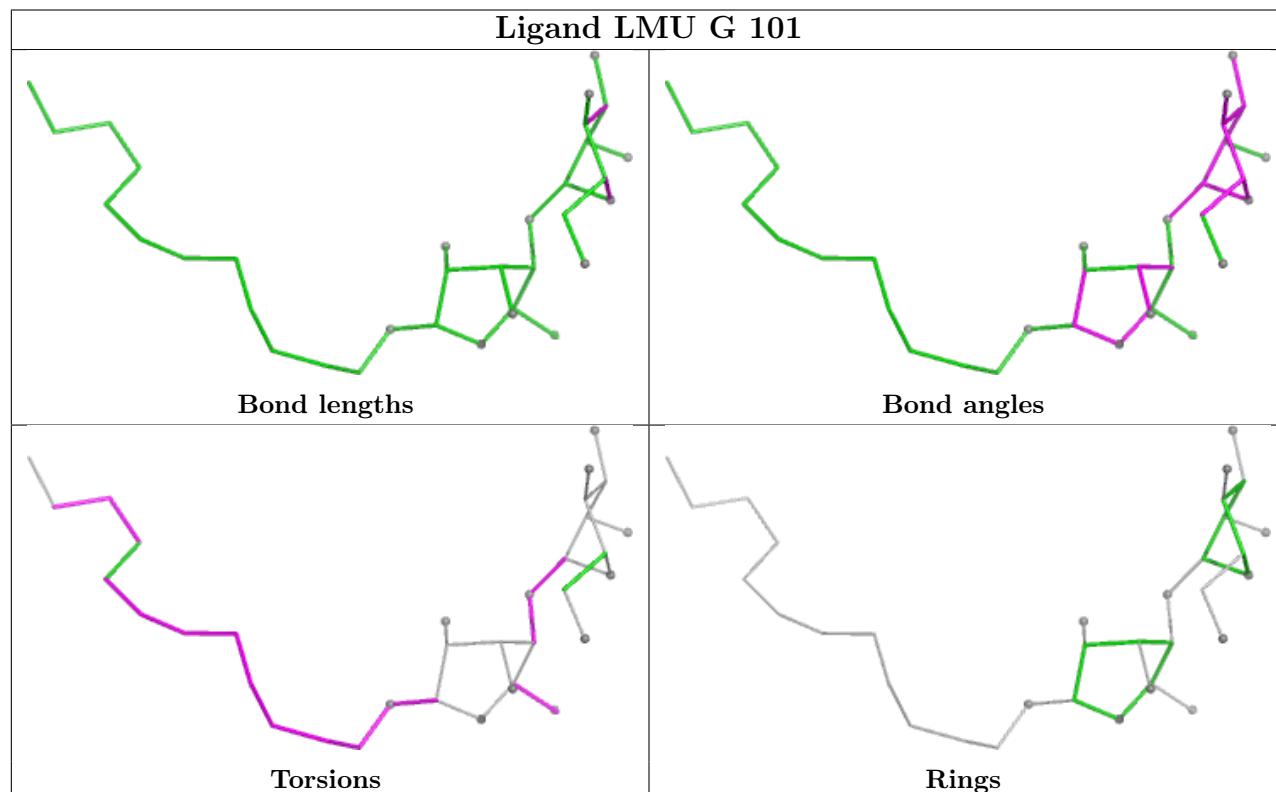


Rings

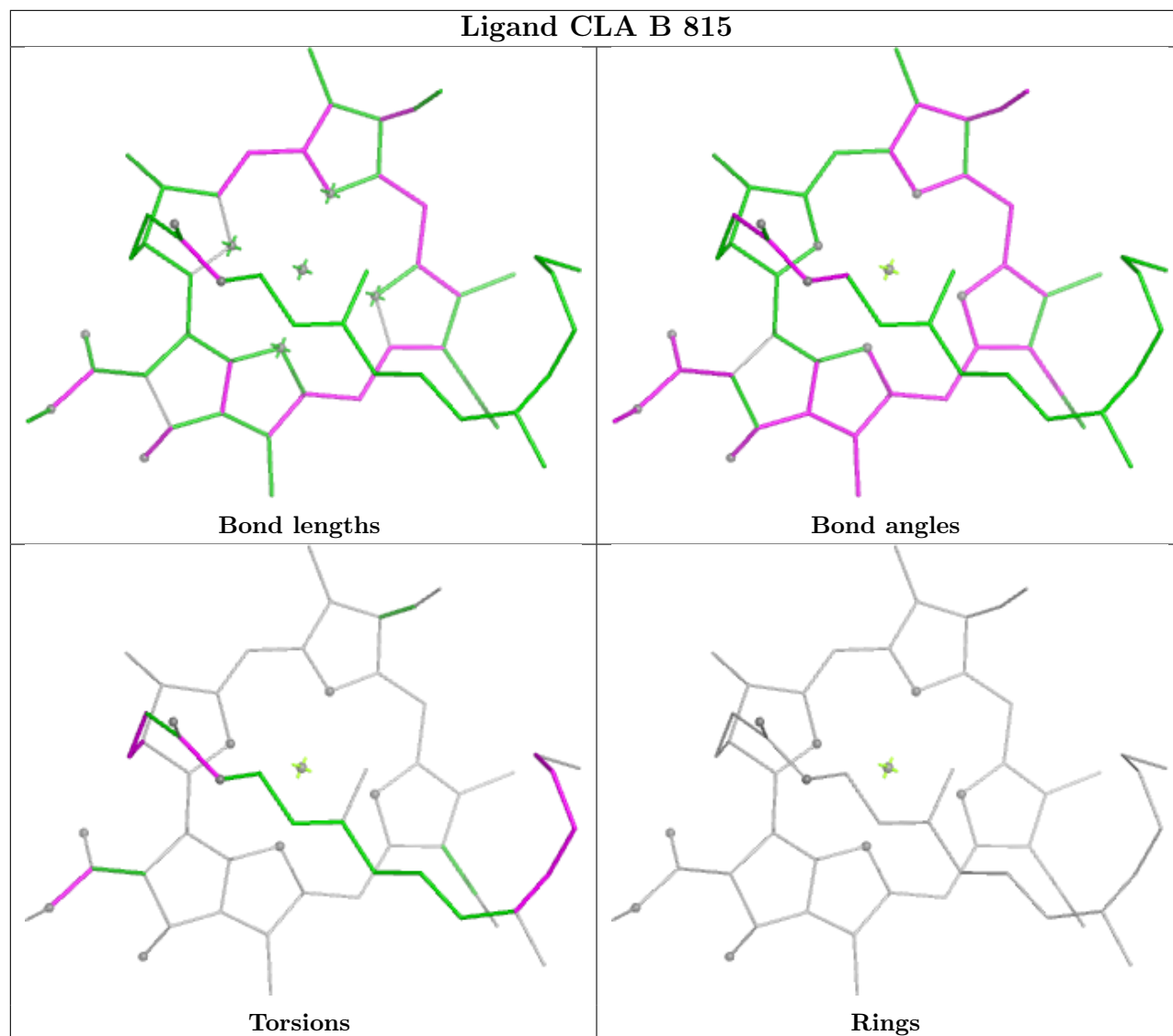
Ligand CLA I 102

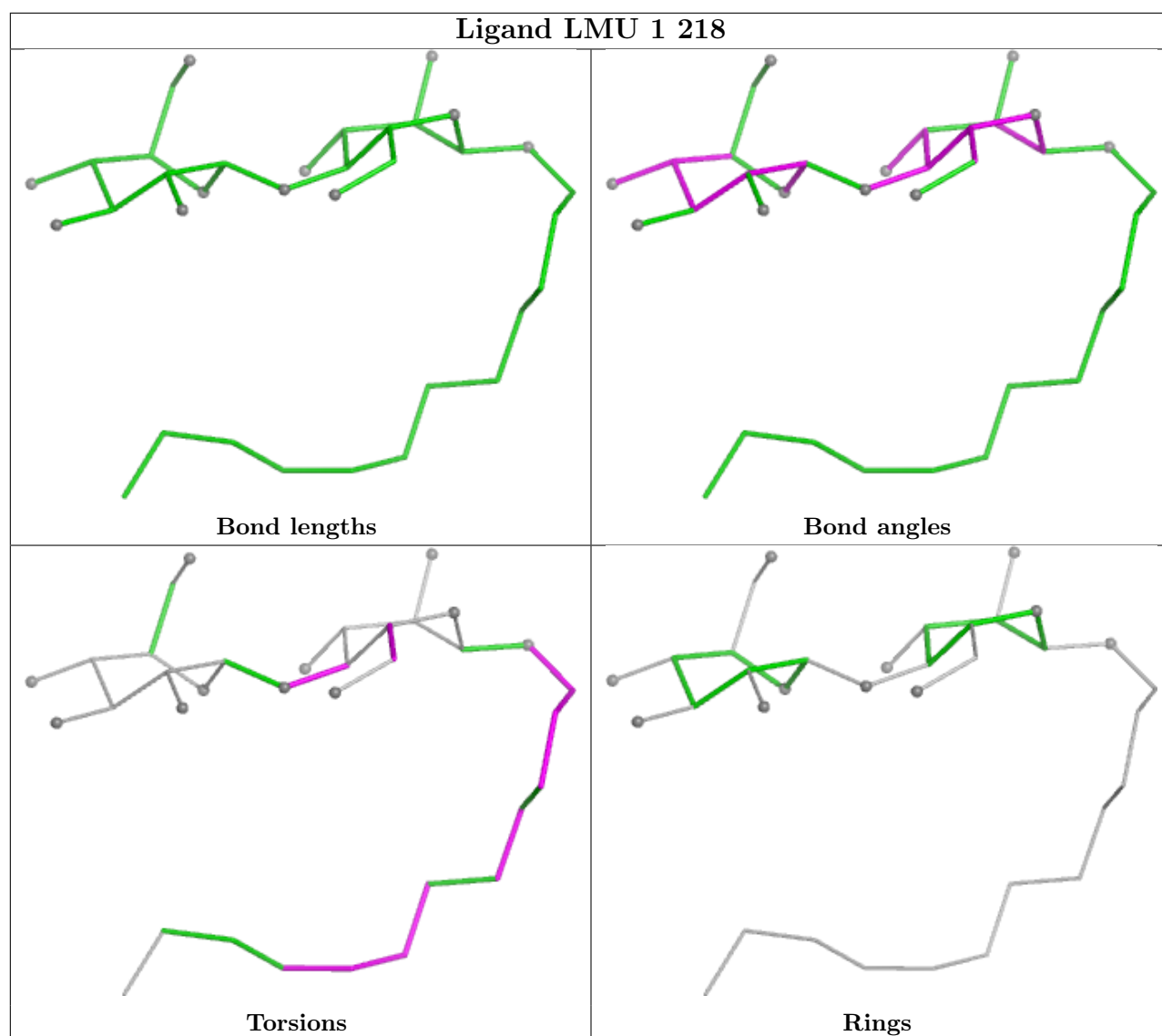


Ligand LMU G 101

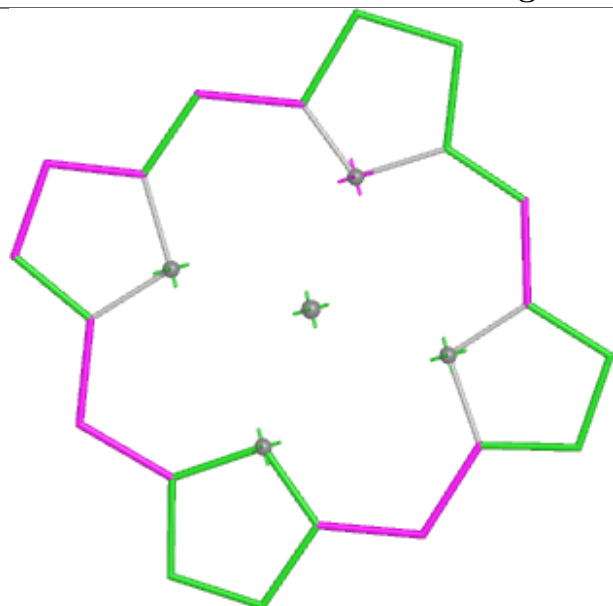


Ligand CLA B 815

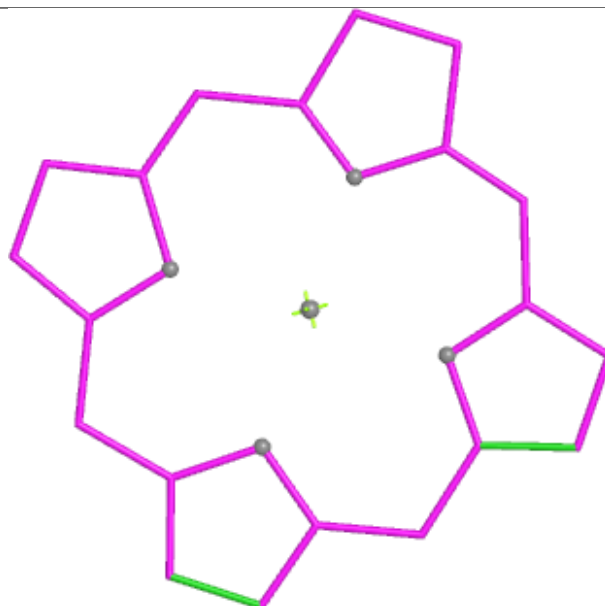




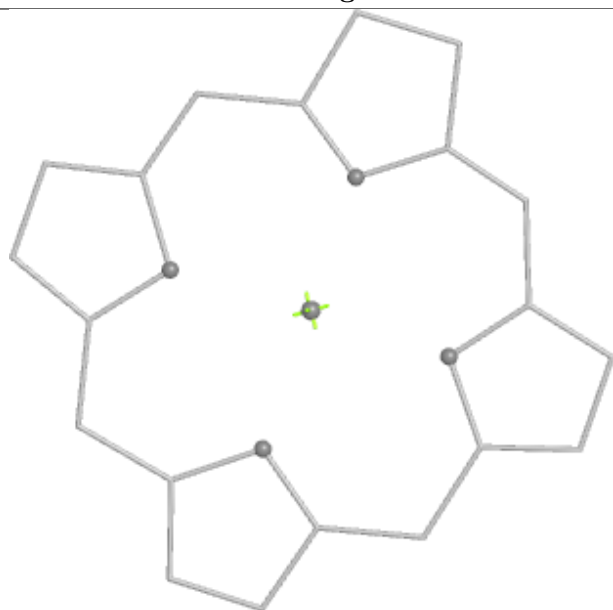
Ligand CLA 3 315



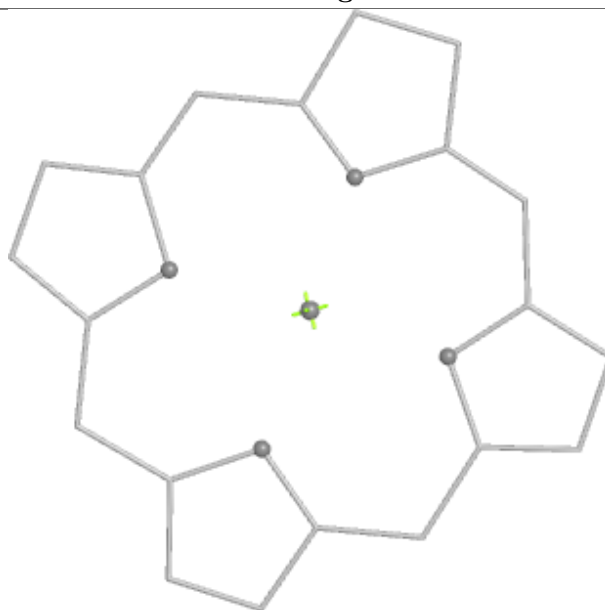
Bond lengths



Bond angles

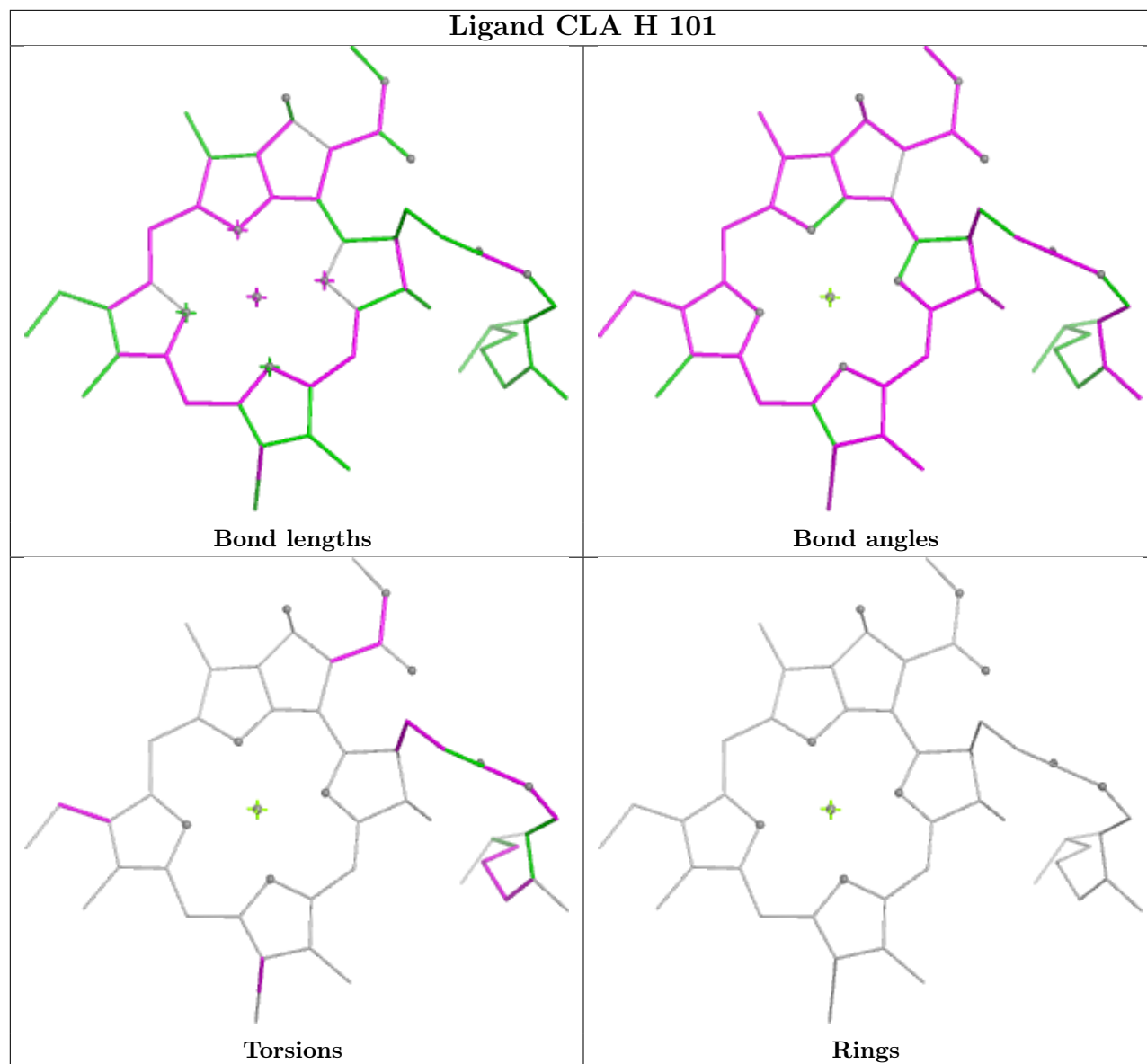


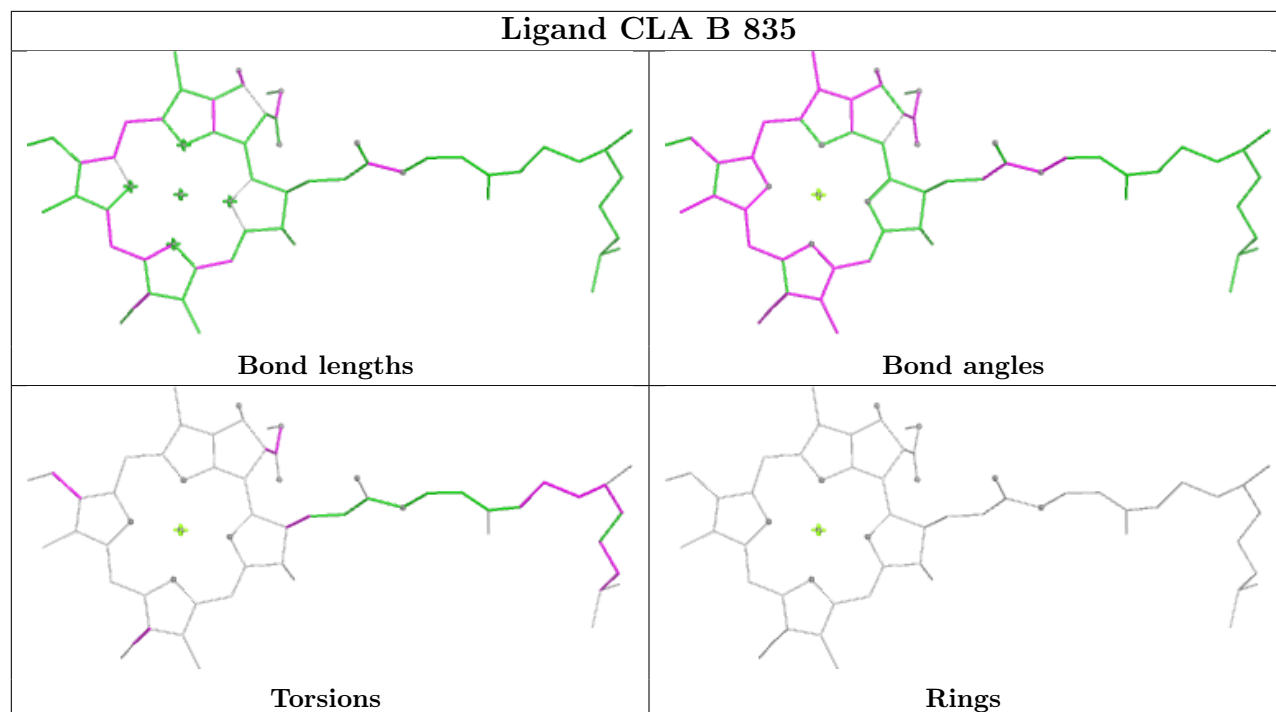
Torsions



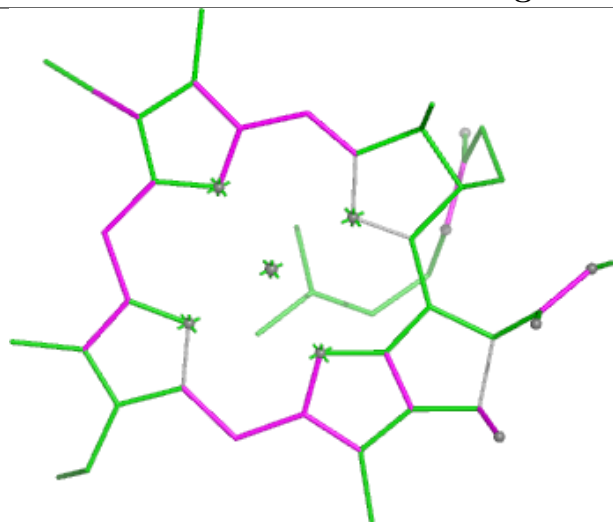
Rings

Ligand CLA H 101

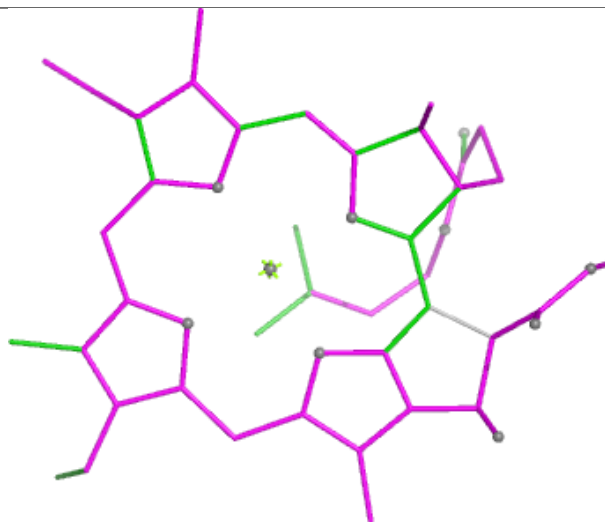




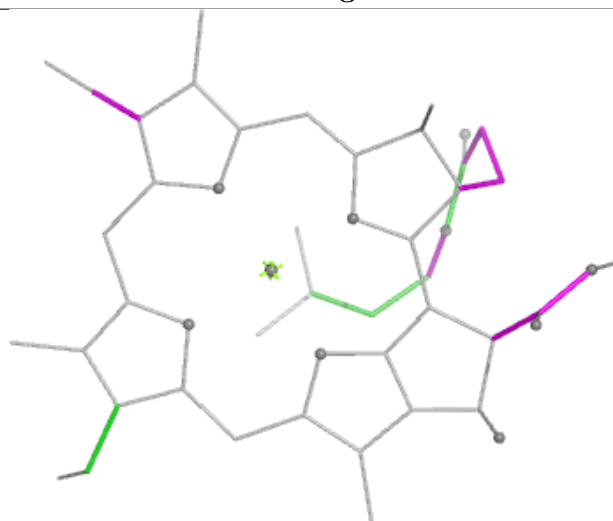
Ligand CLA B 828



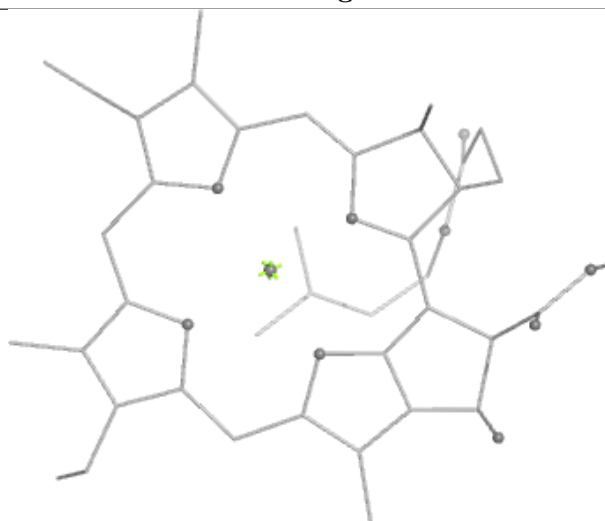
Bond lengths



Bond angles

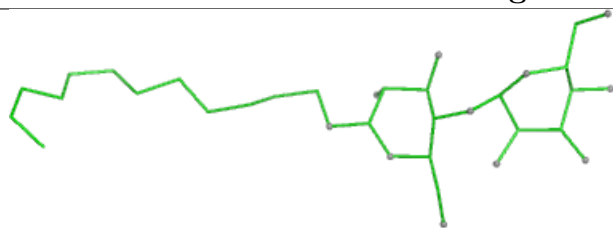


Torsions

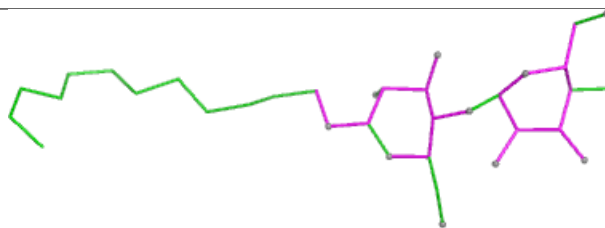


Rings

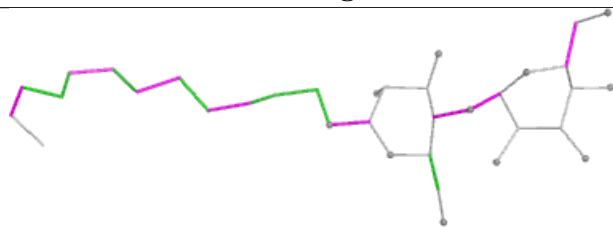
Ligand LMU H 107



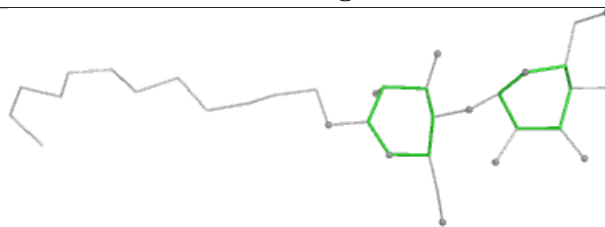
Bond lengths



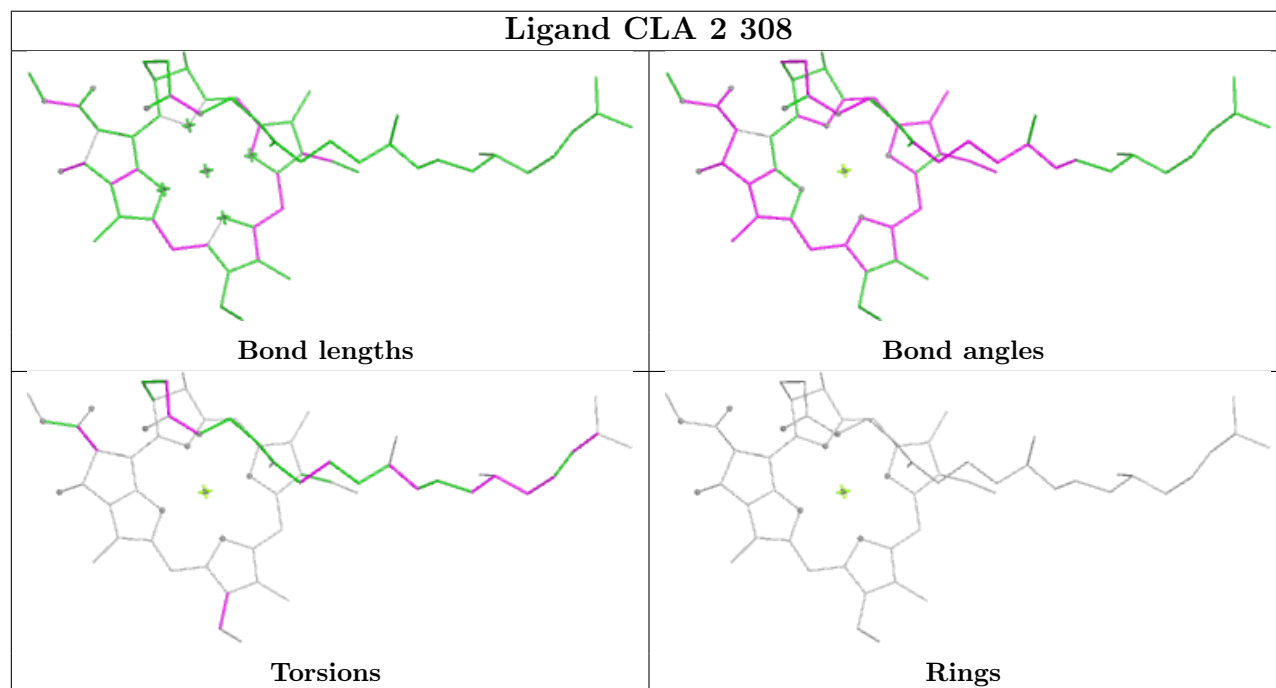
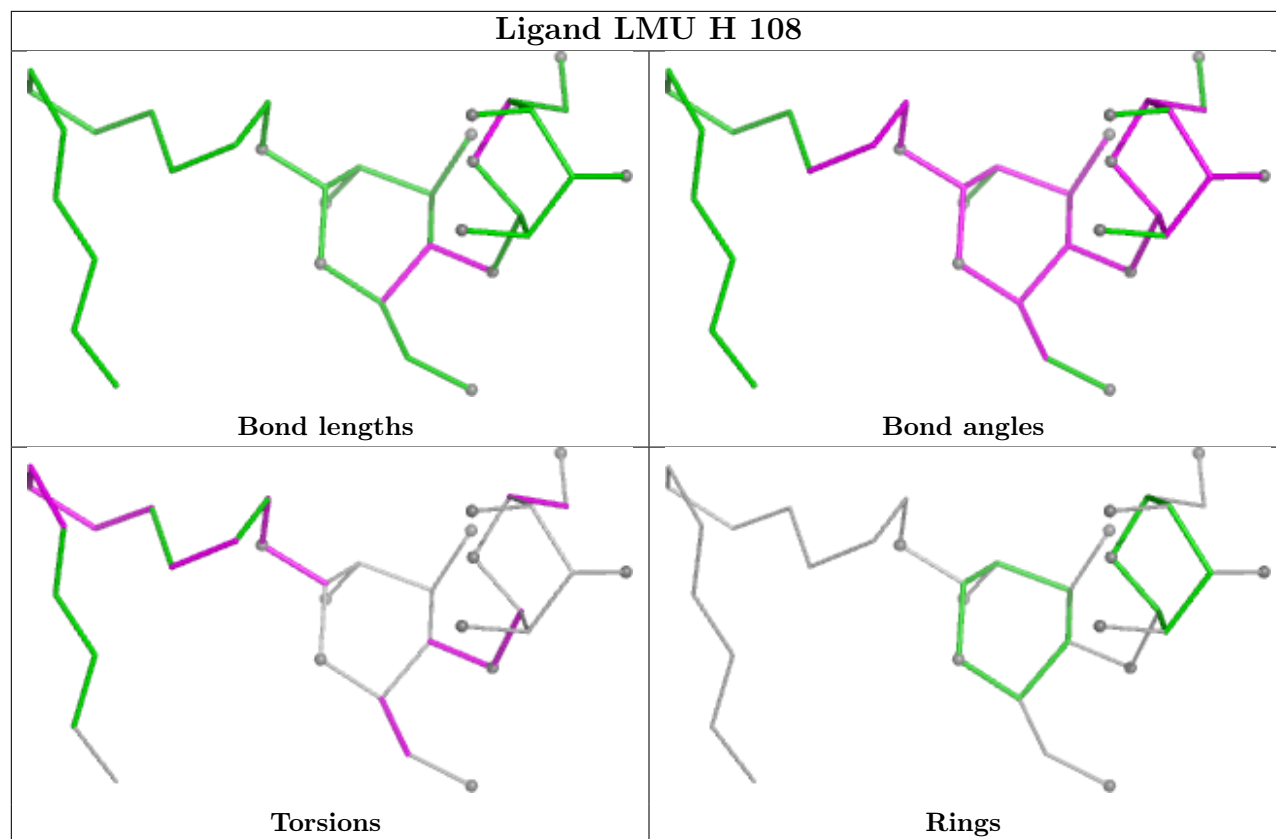
Bond angles



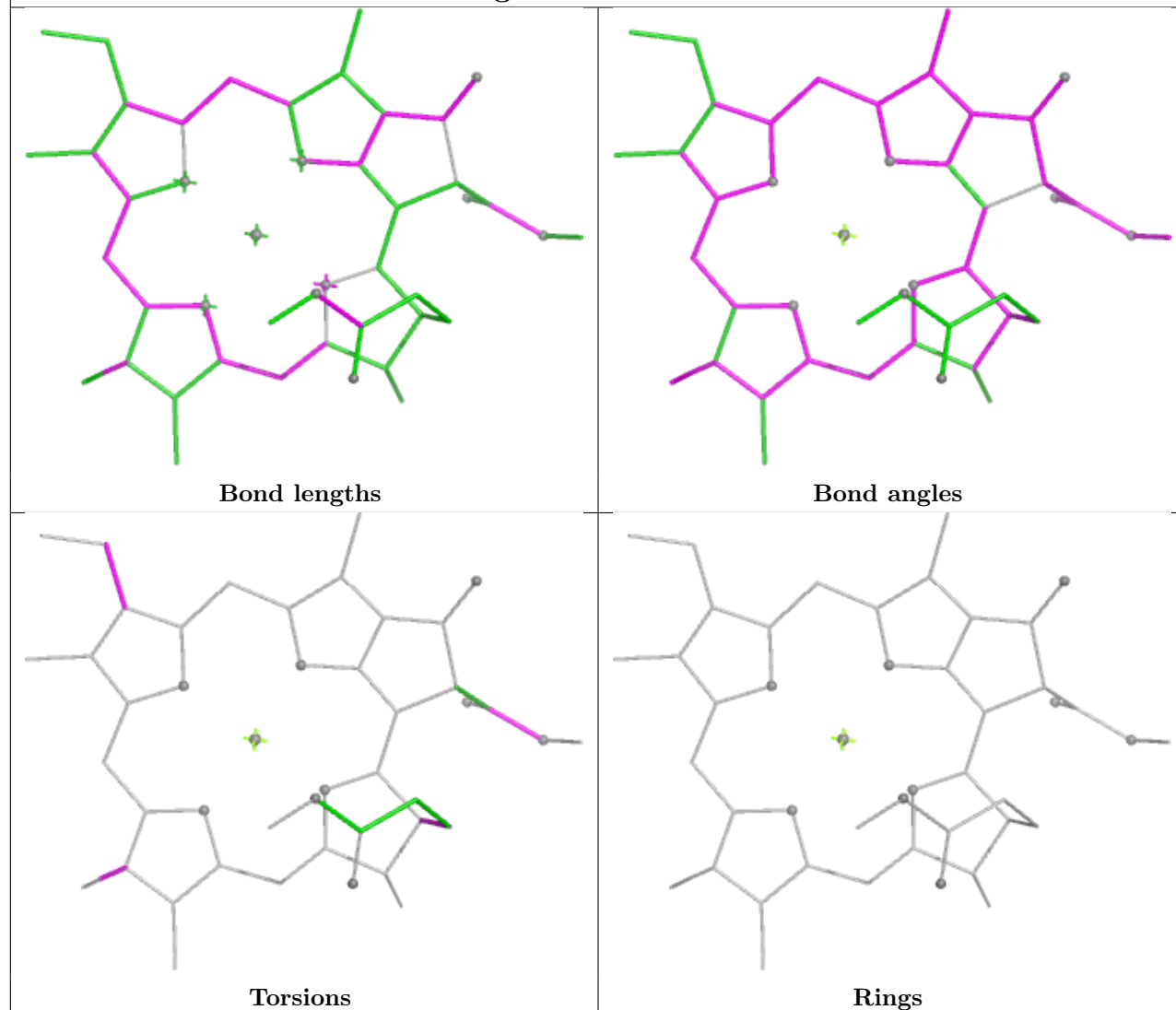
Torsions



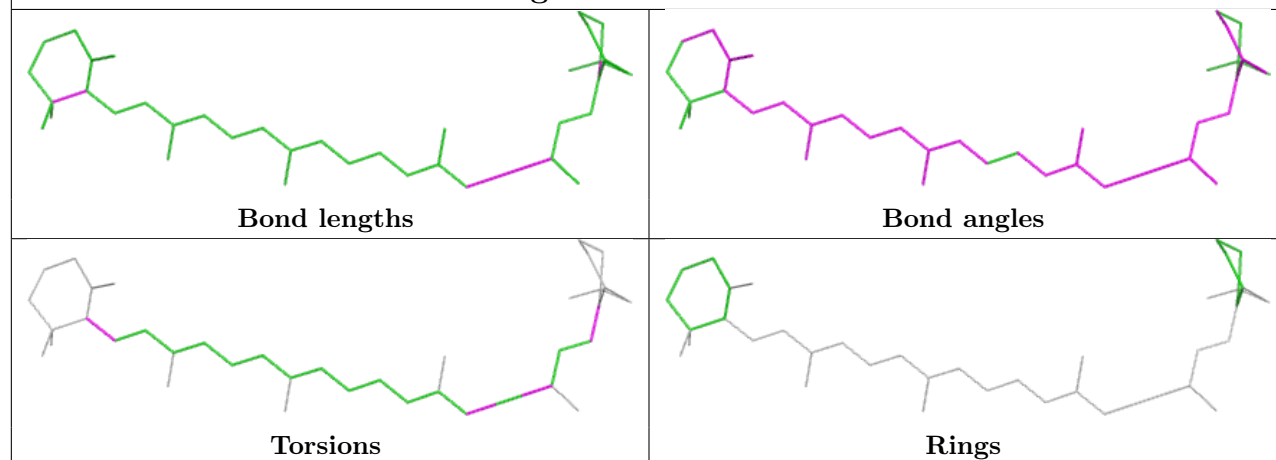
Rings

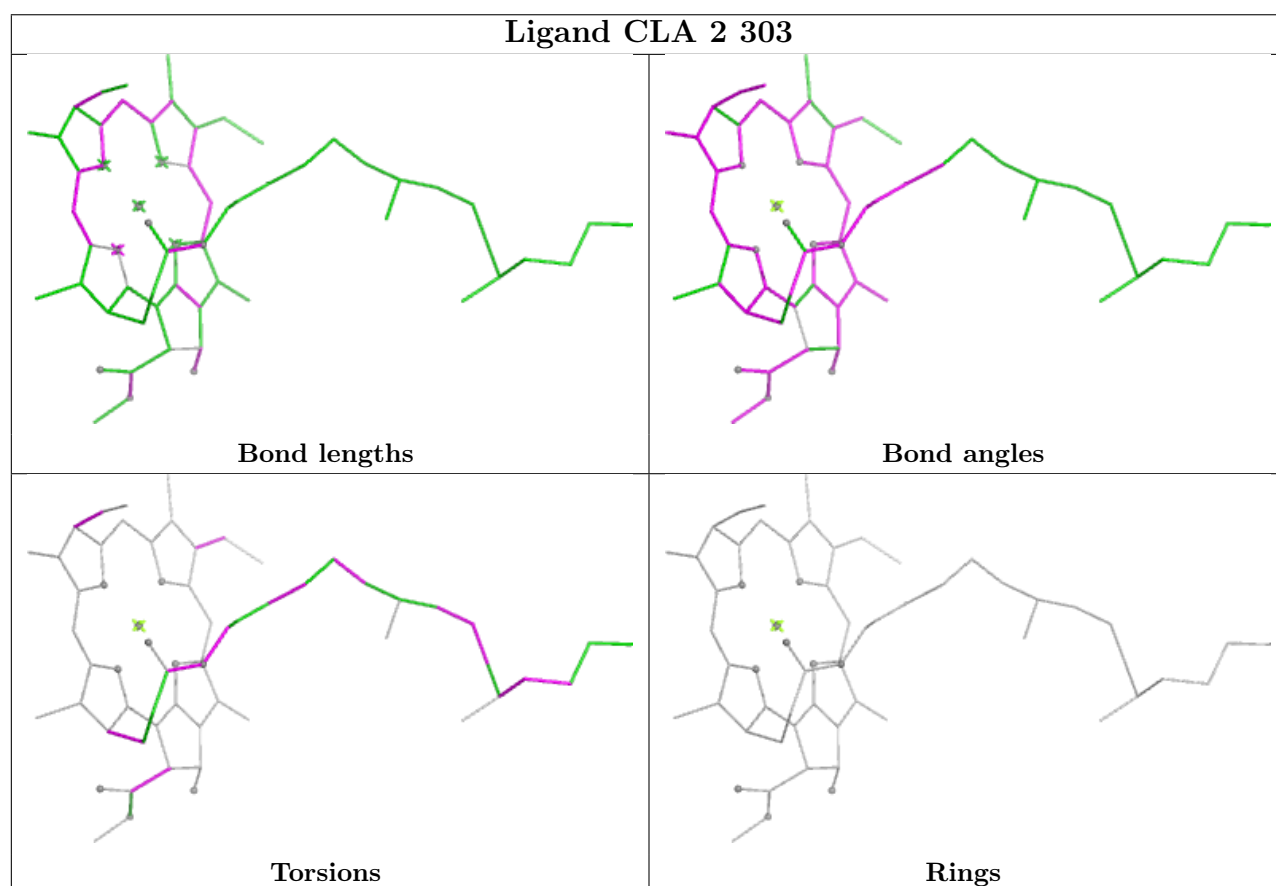
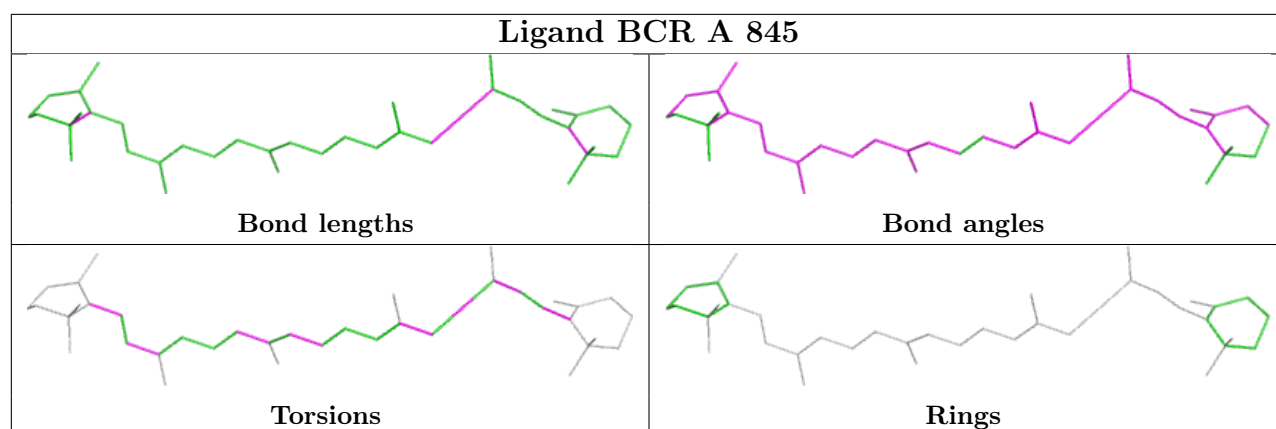


Ligand CLA 1 204

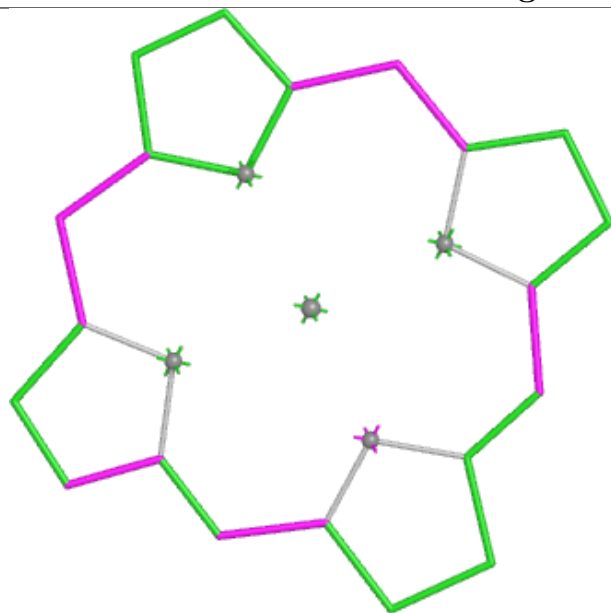


Ligand BCR B 843

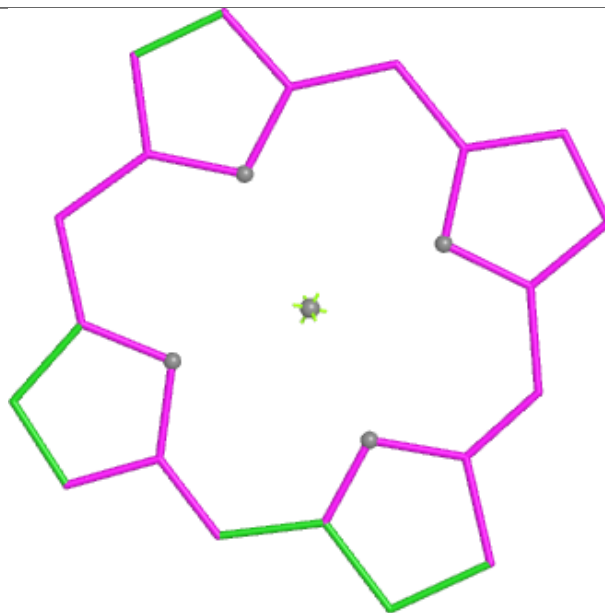




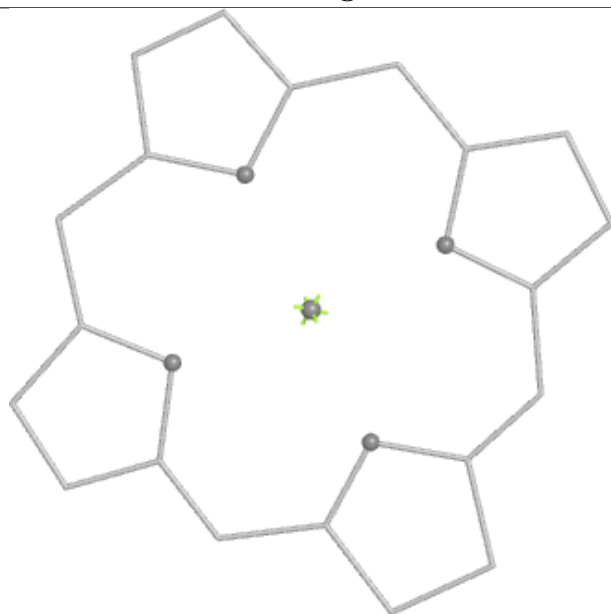
Ligand CLA 3 319



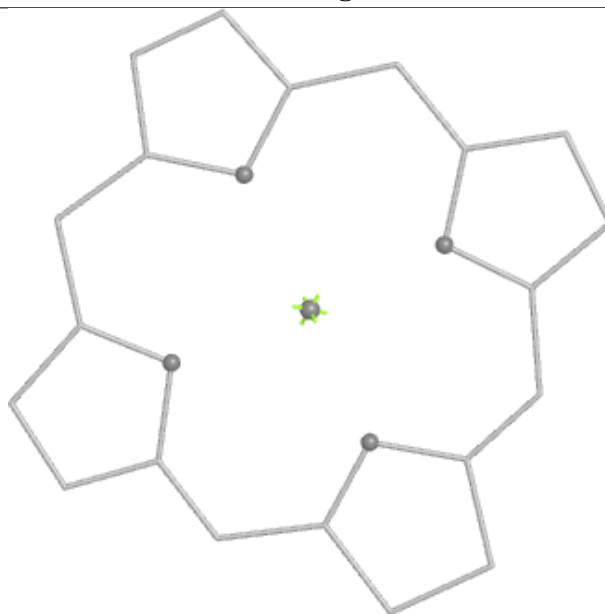
Bond lengths



Bond angles

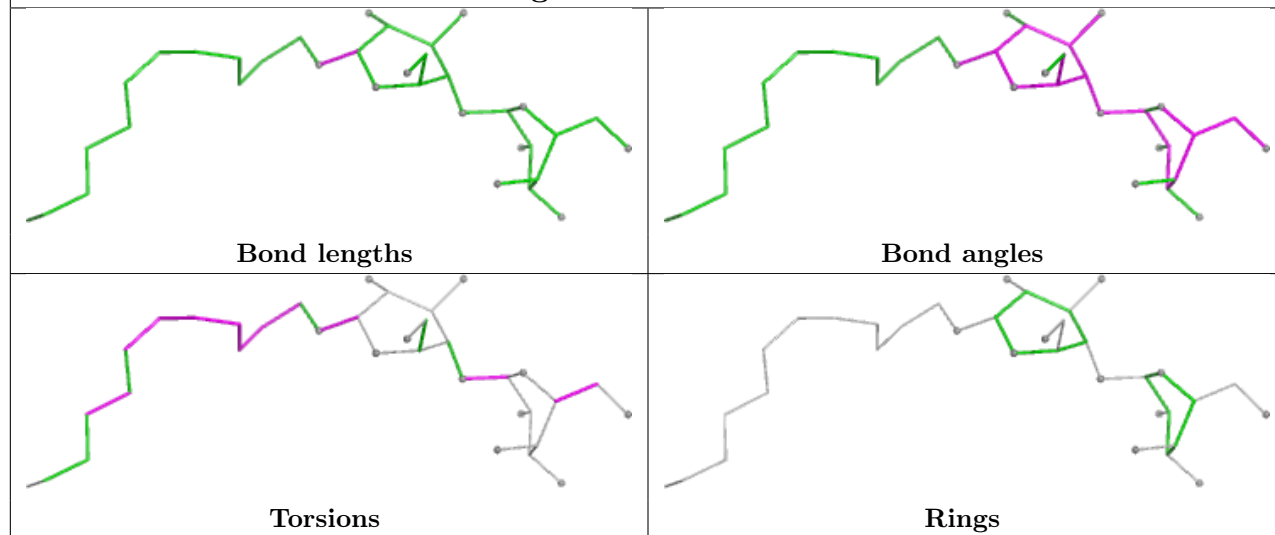


Torsions

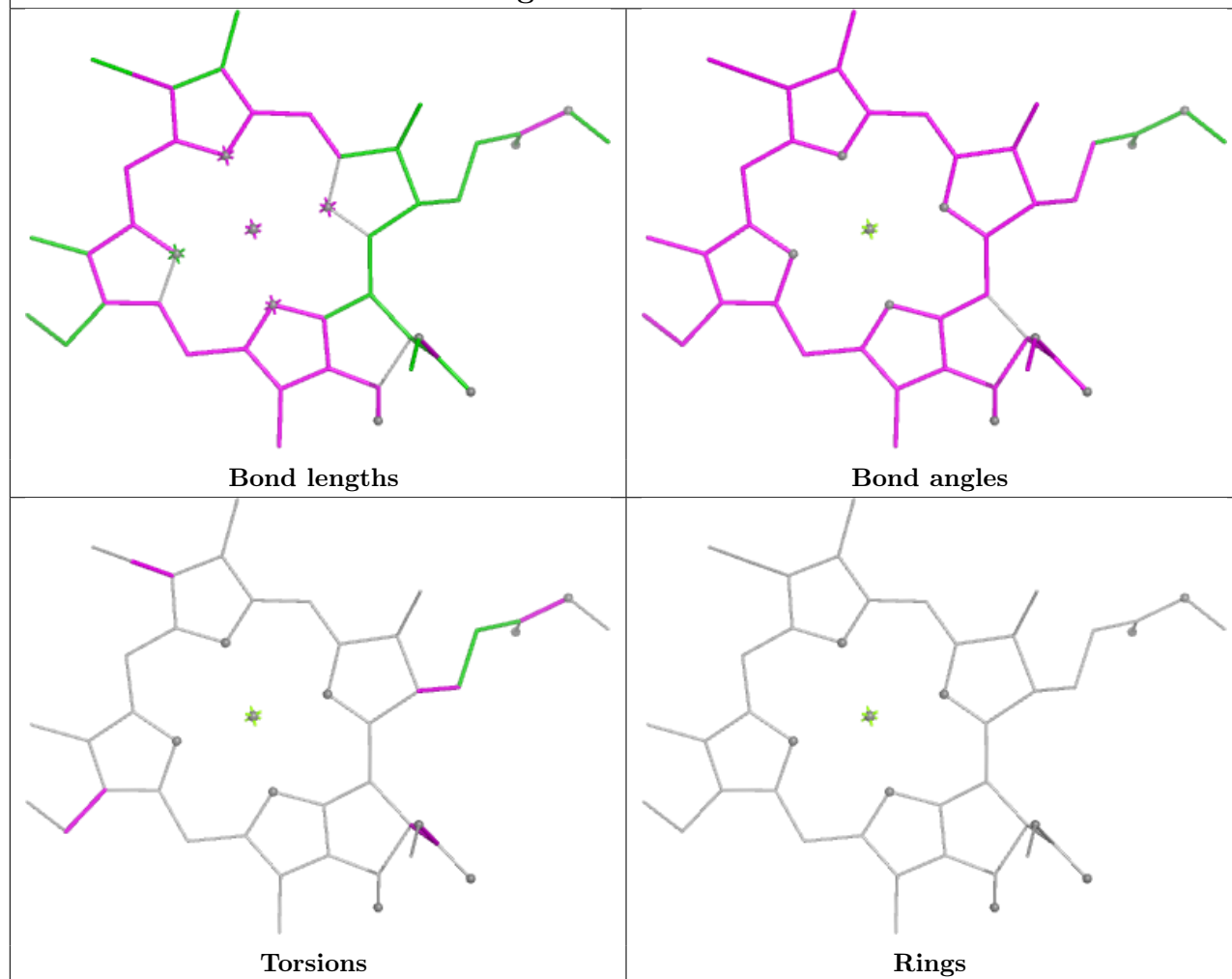


Rings

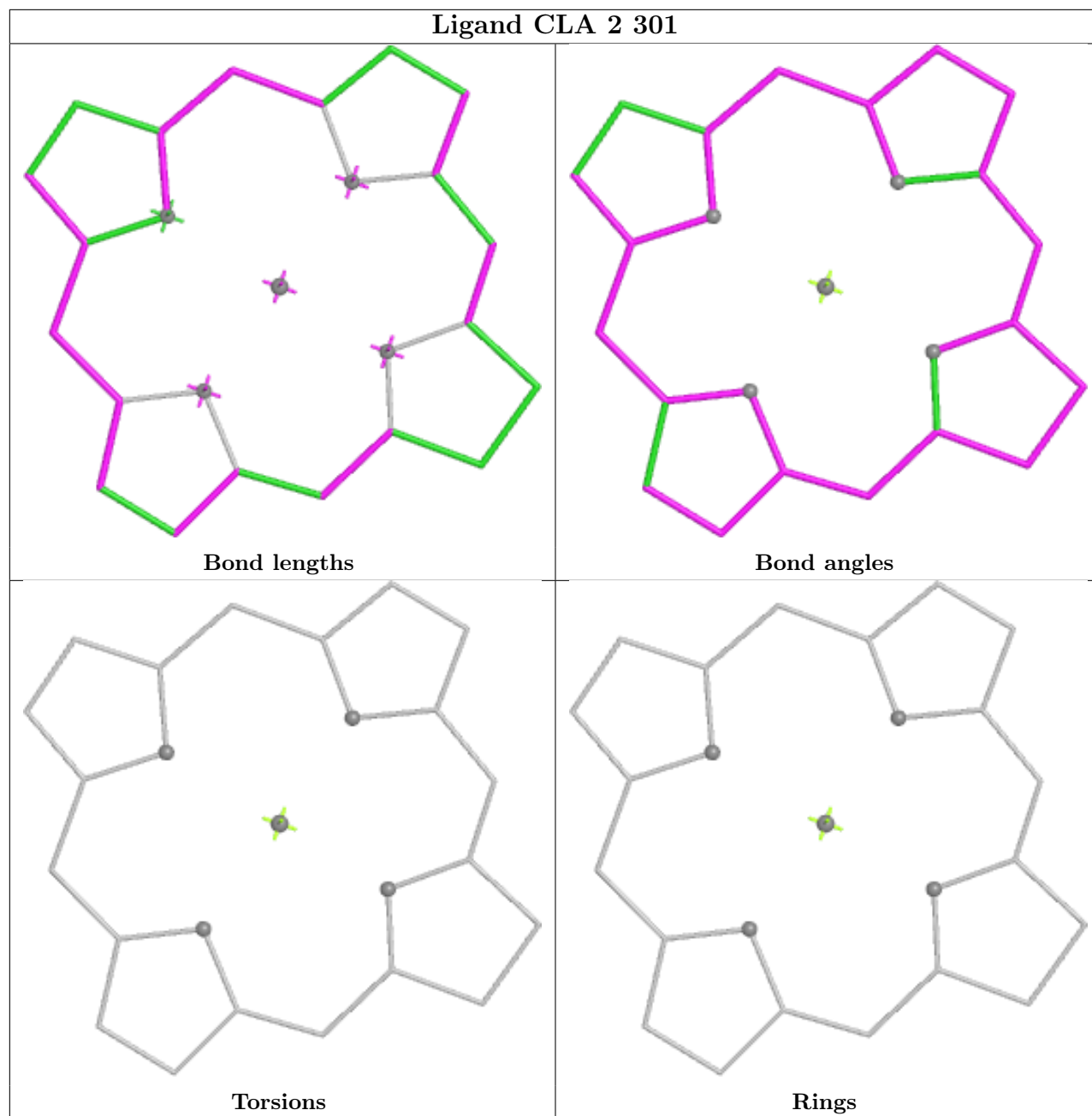
Ligand LMU 2 317



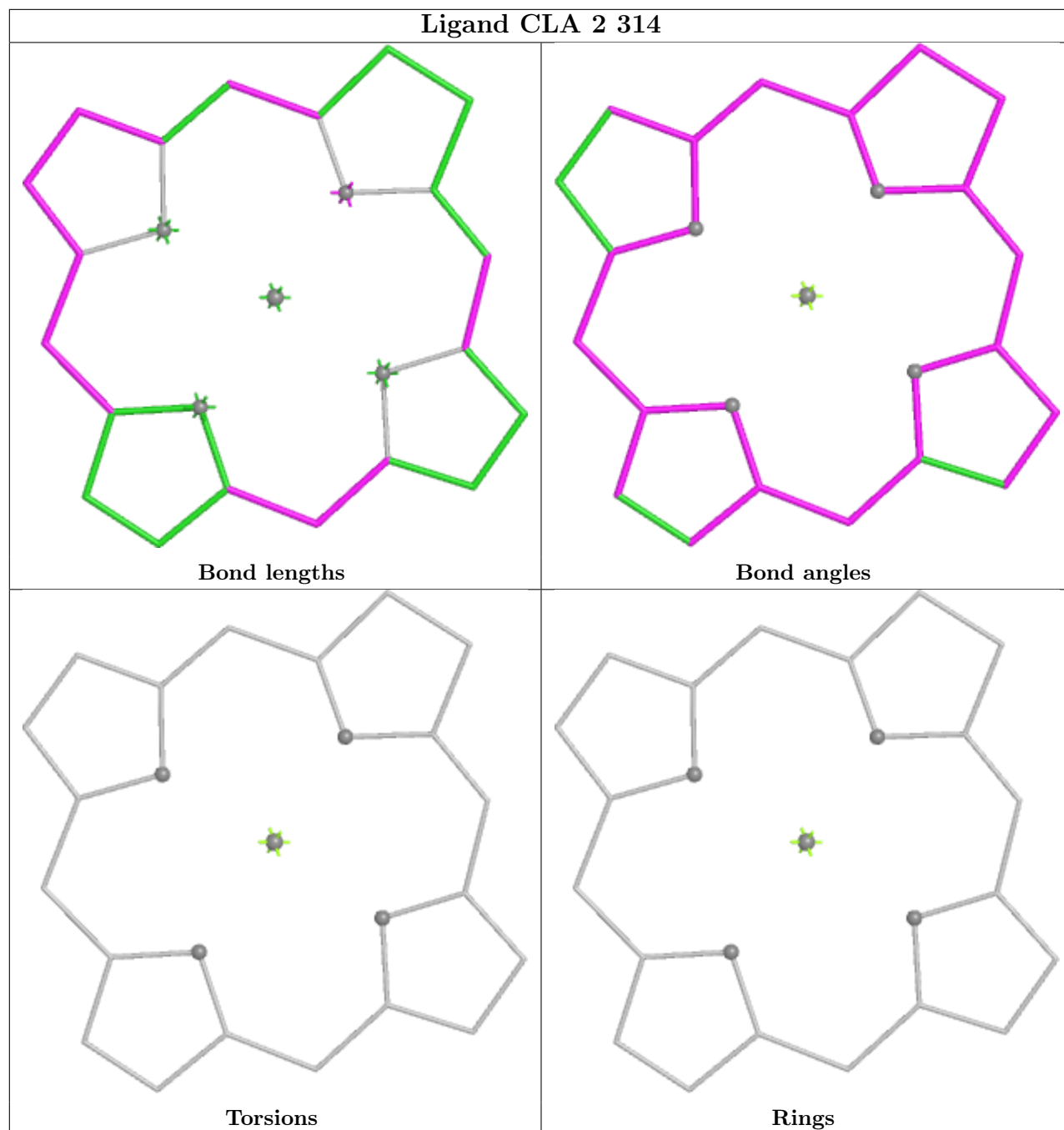
Ligand CLA 1 201



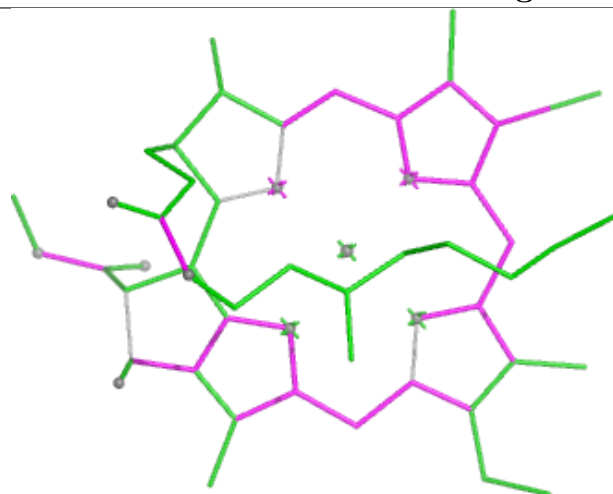
Ligand CLA 2 301



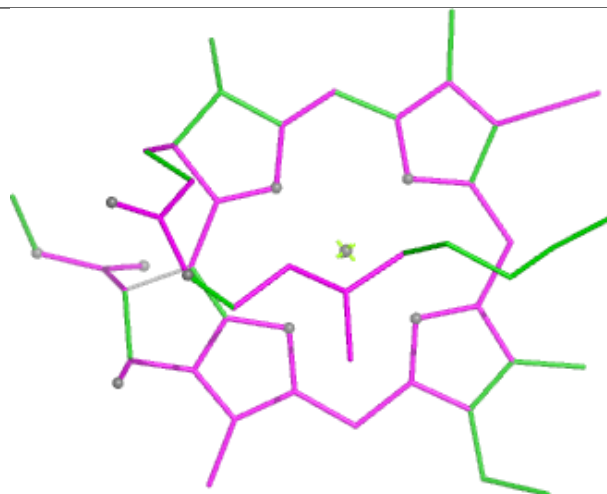
Ligand CLA 2 314



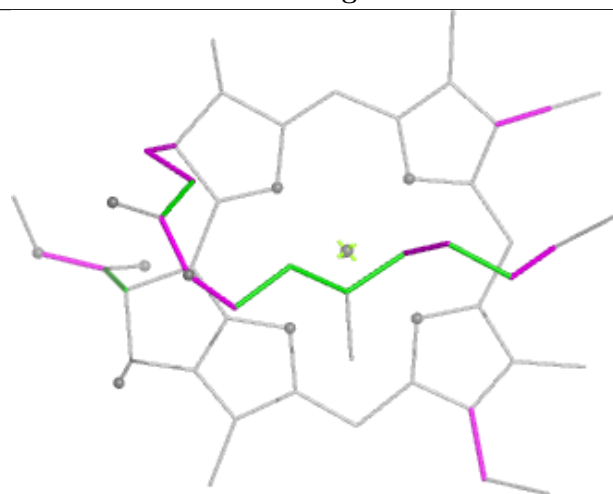
Ligand CLA A 816



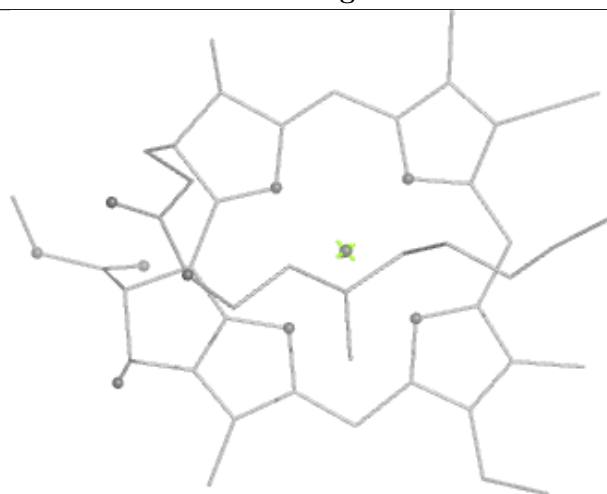
Bond lengths



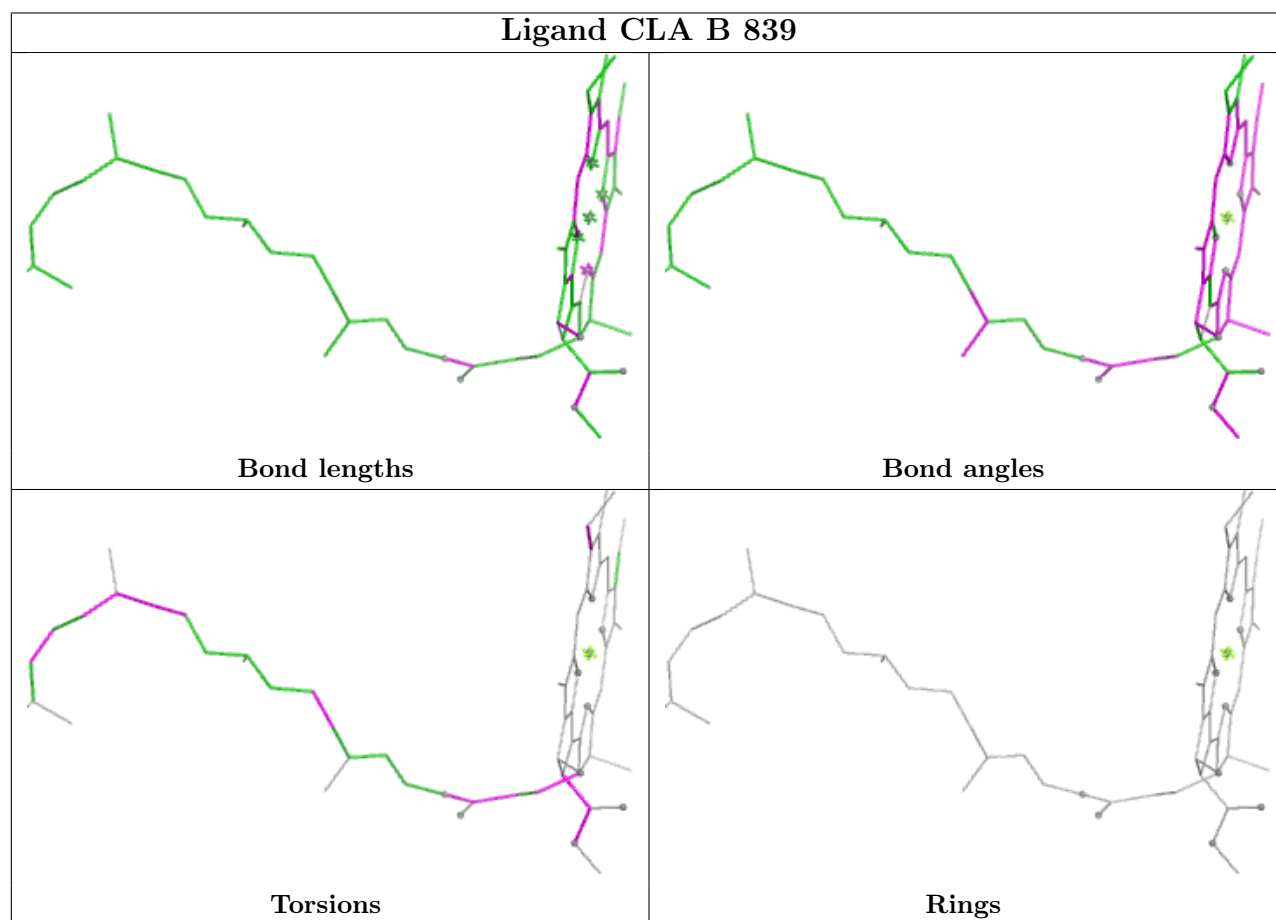
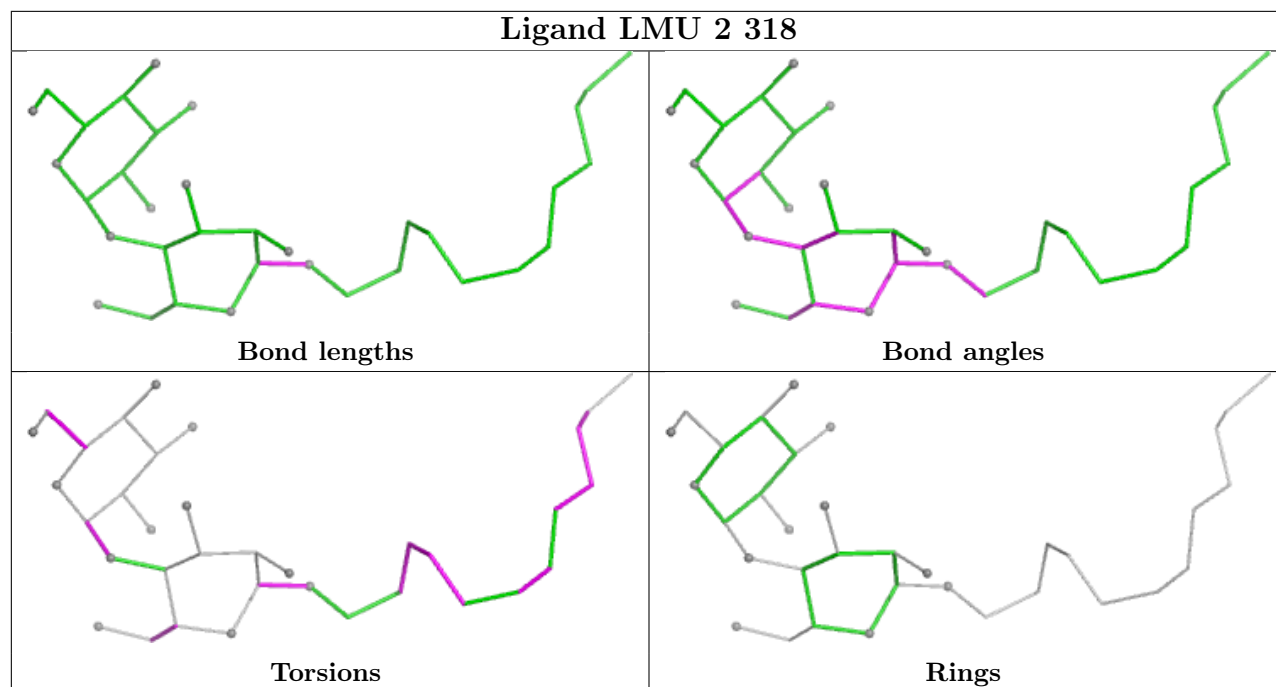
Bond angles

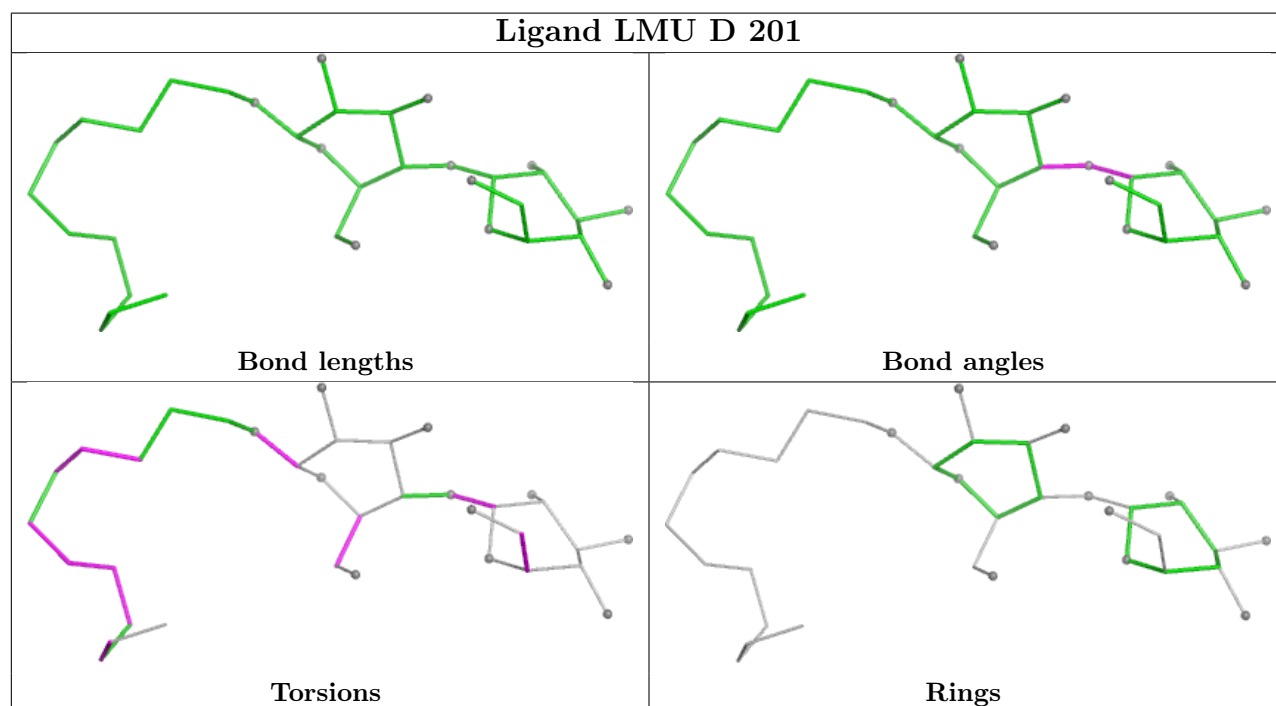
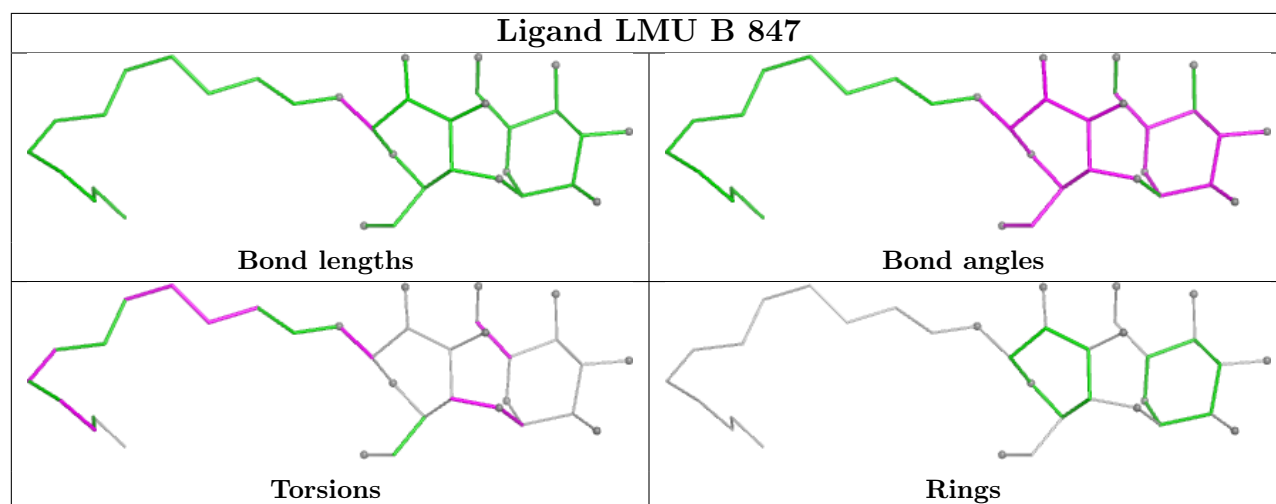
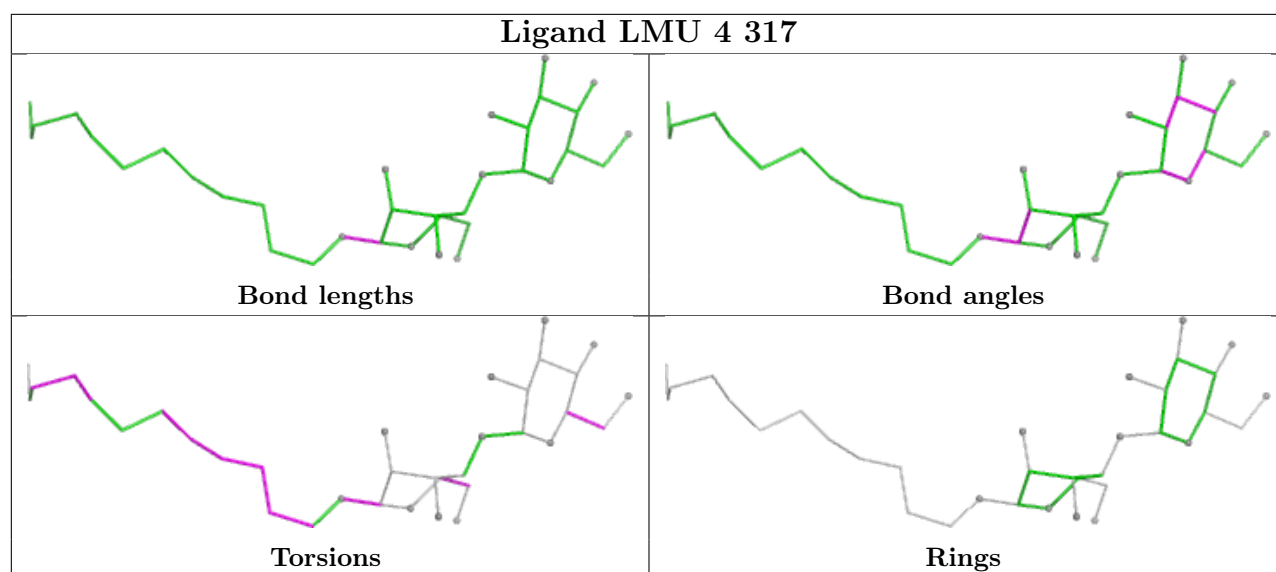


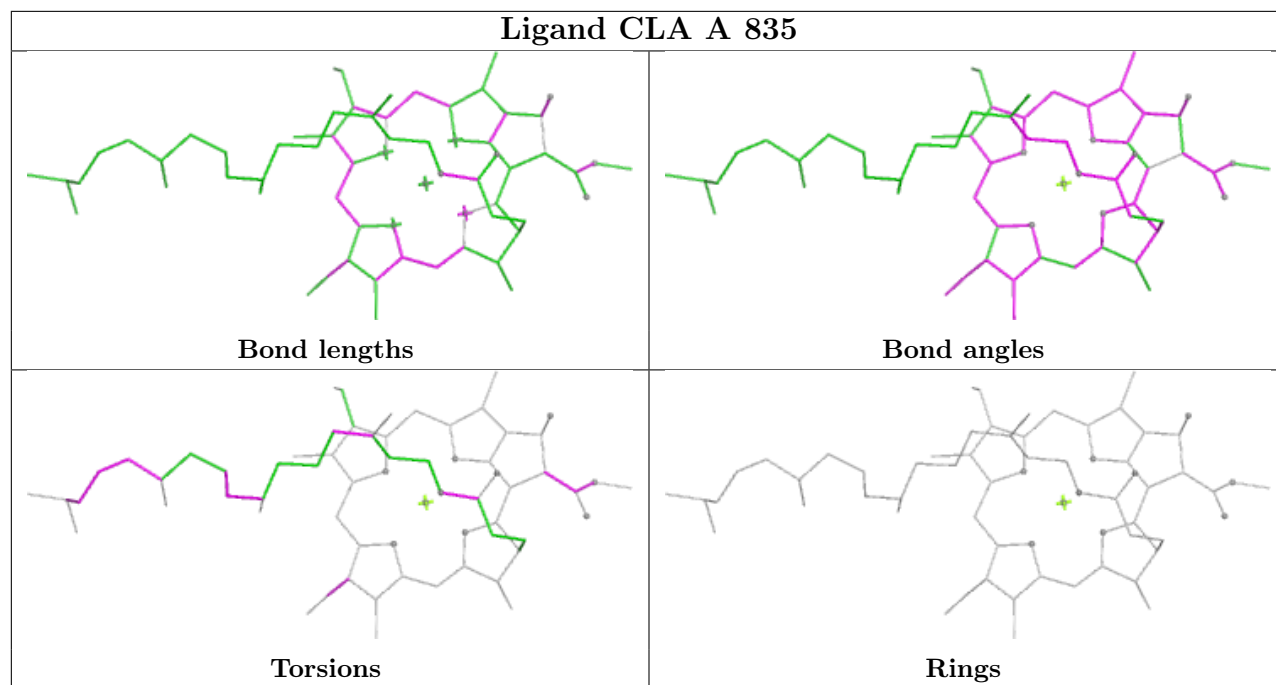
Torsions



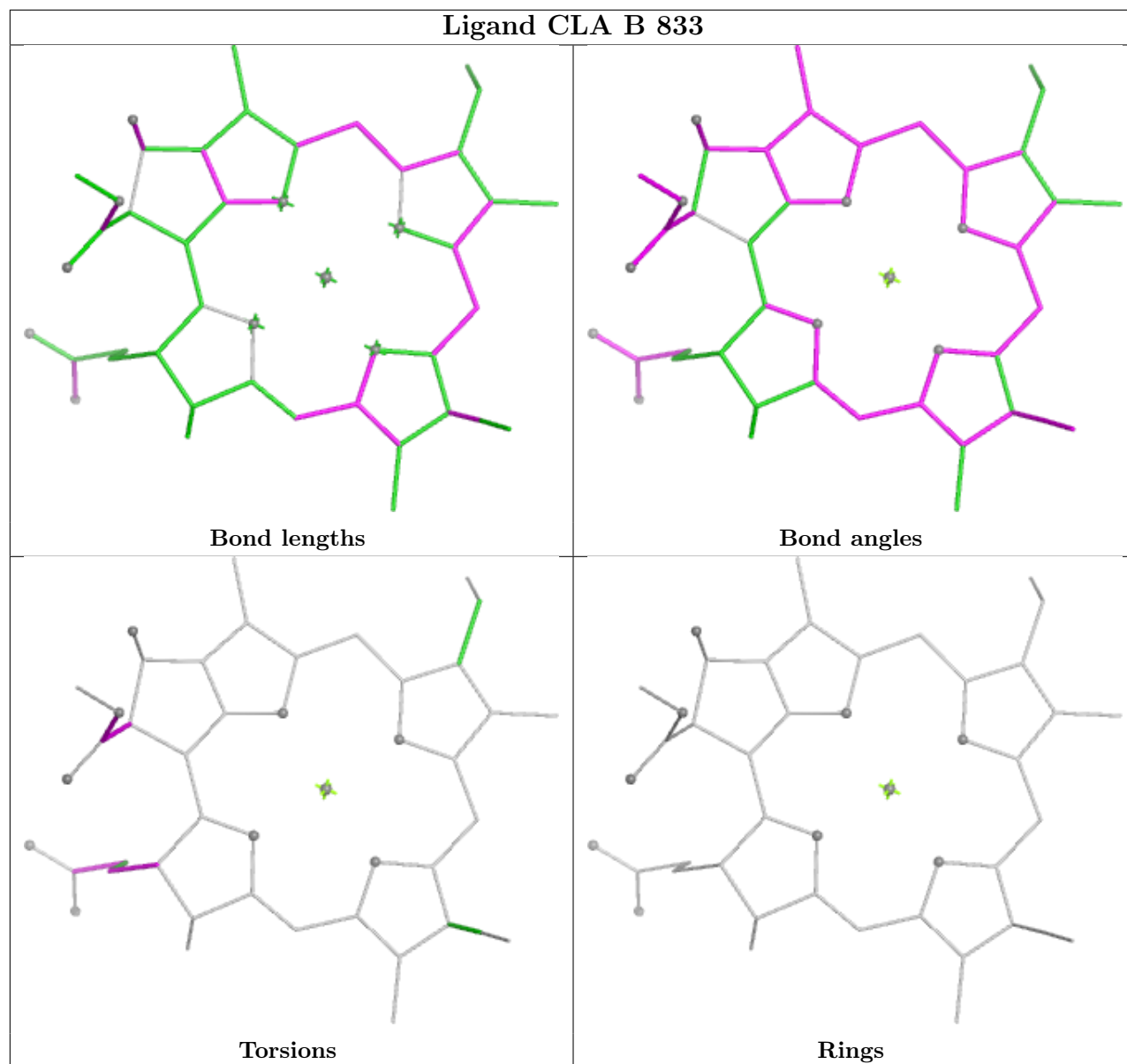
Rings



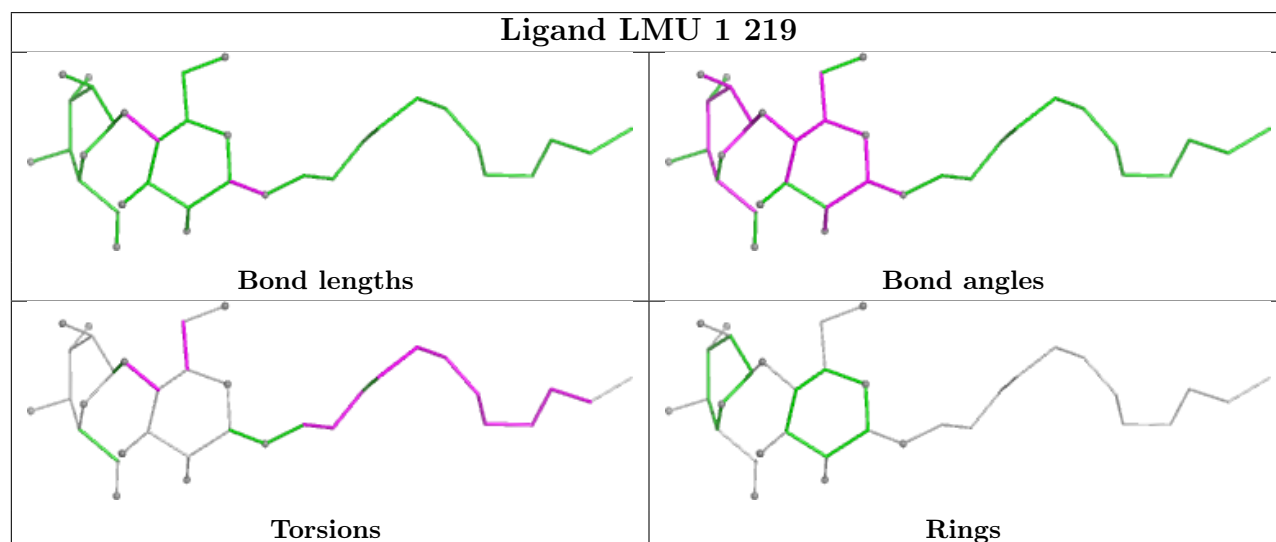




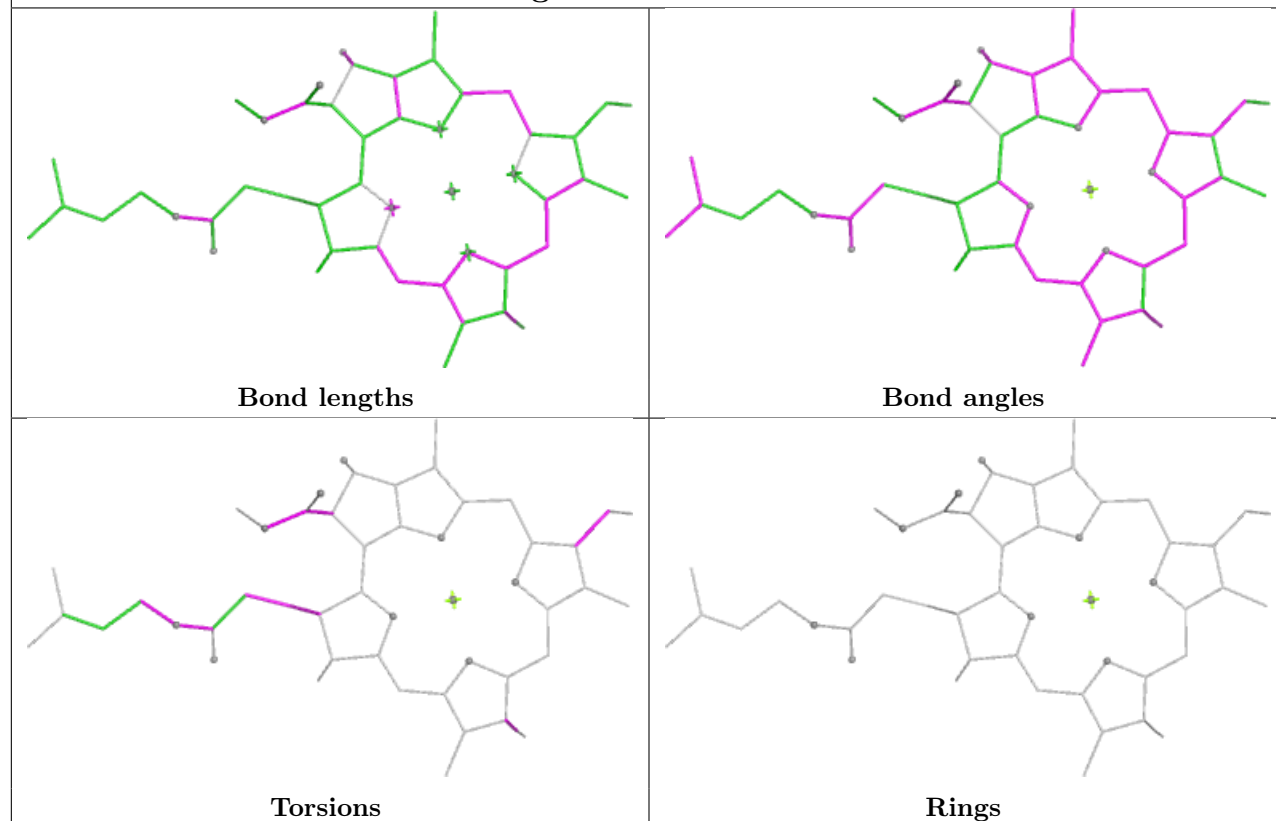
Ligand CLA B 833



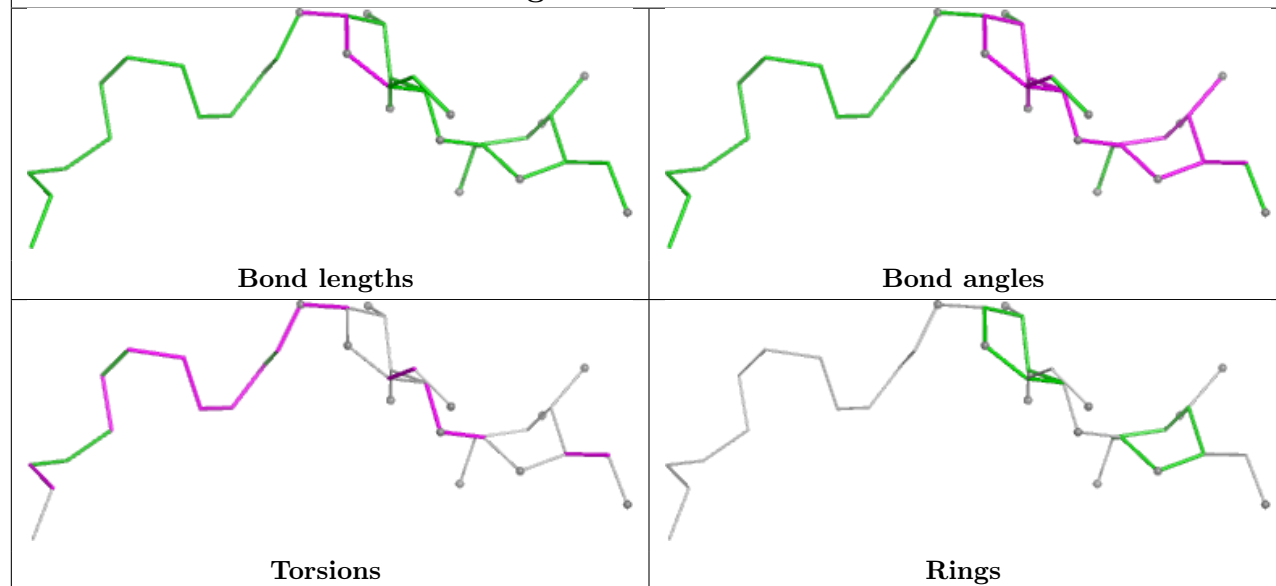
Ligand LMU 1 219

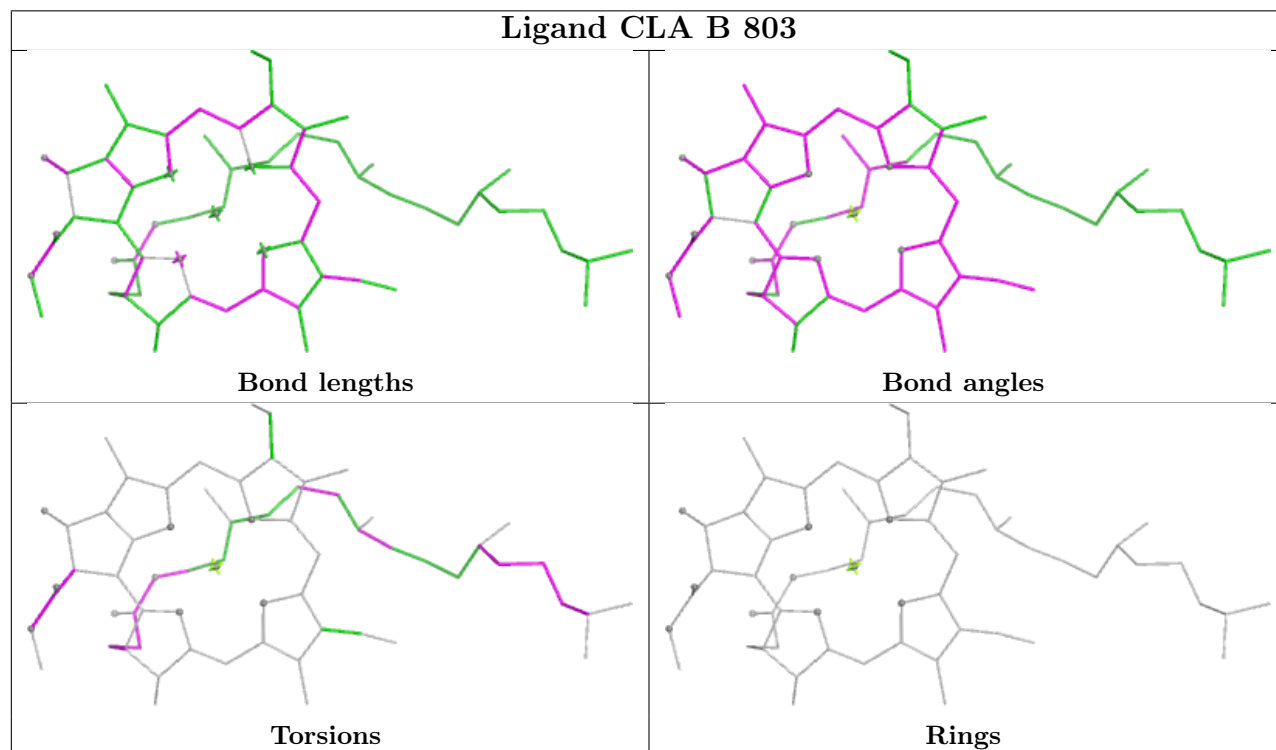
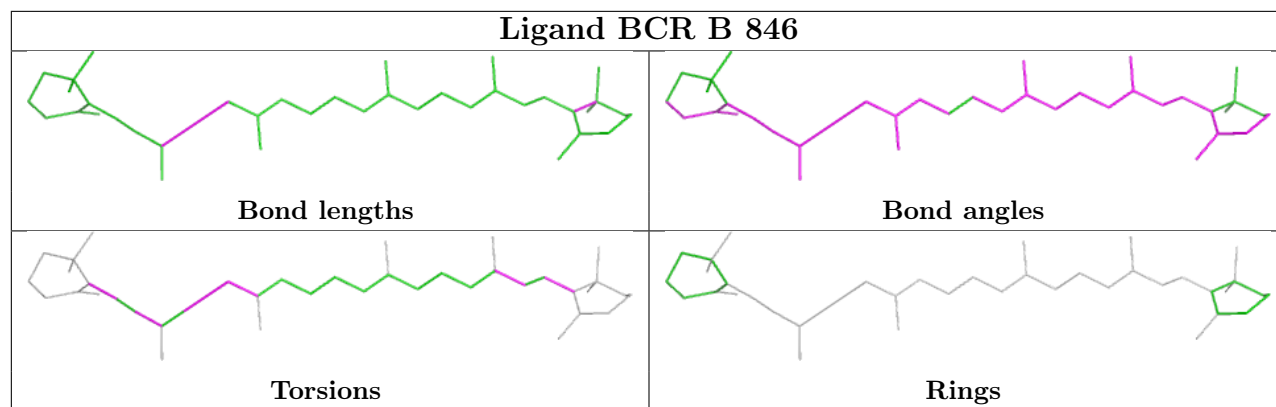


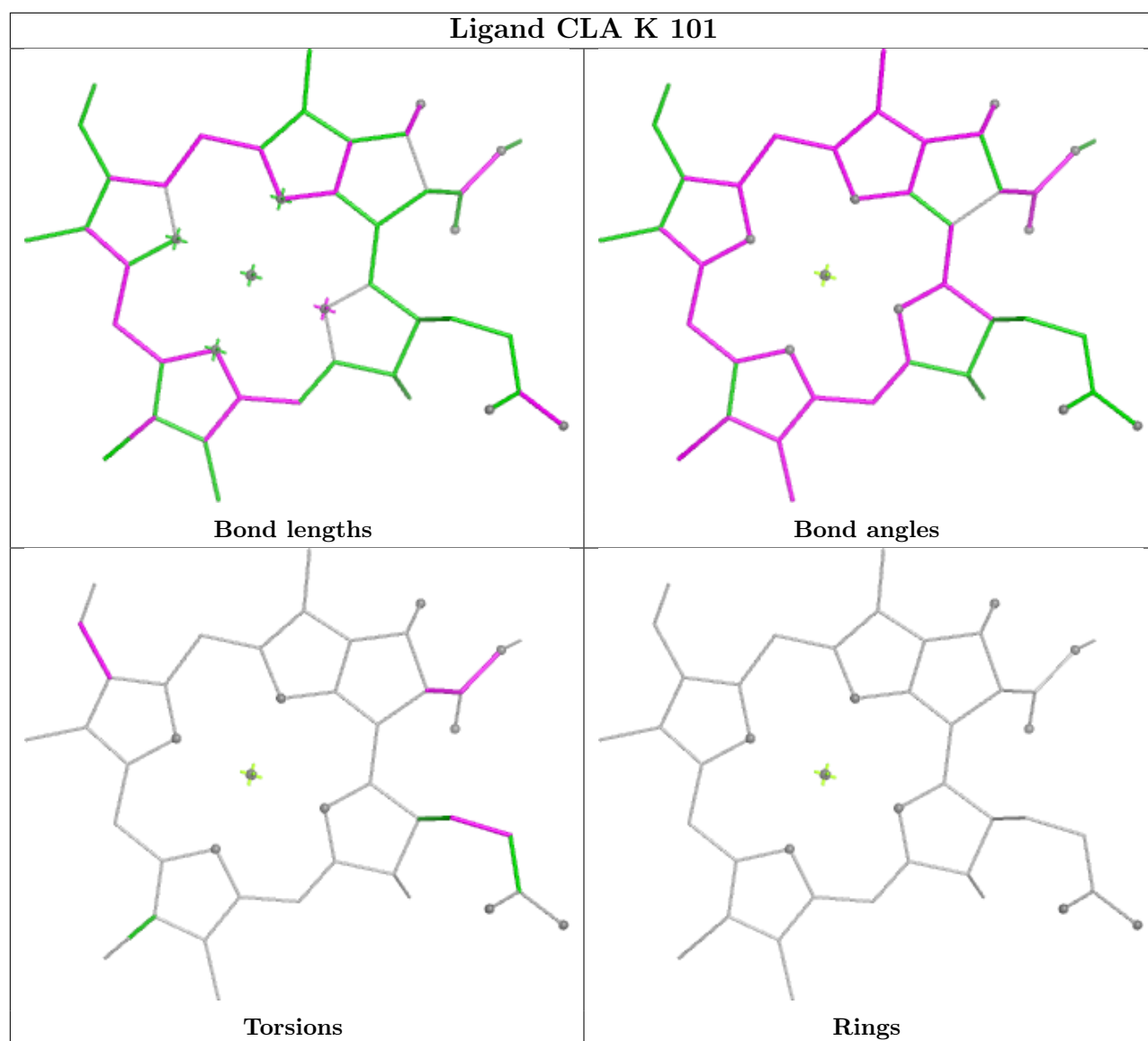
Ligand CLA A 840

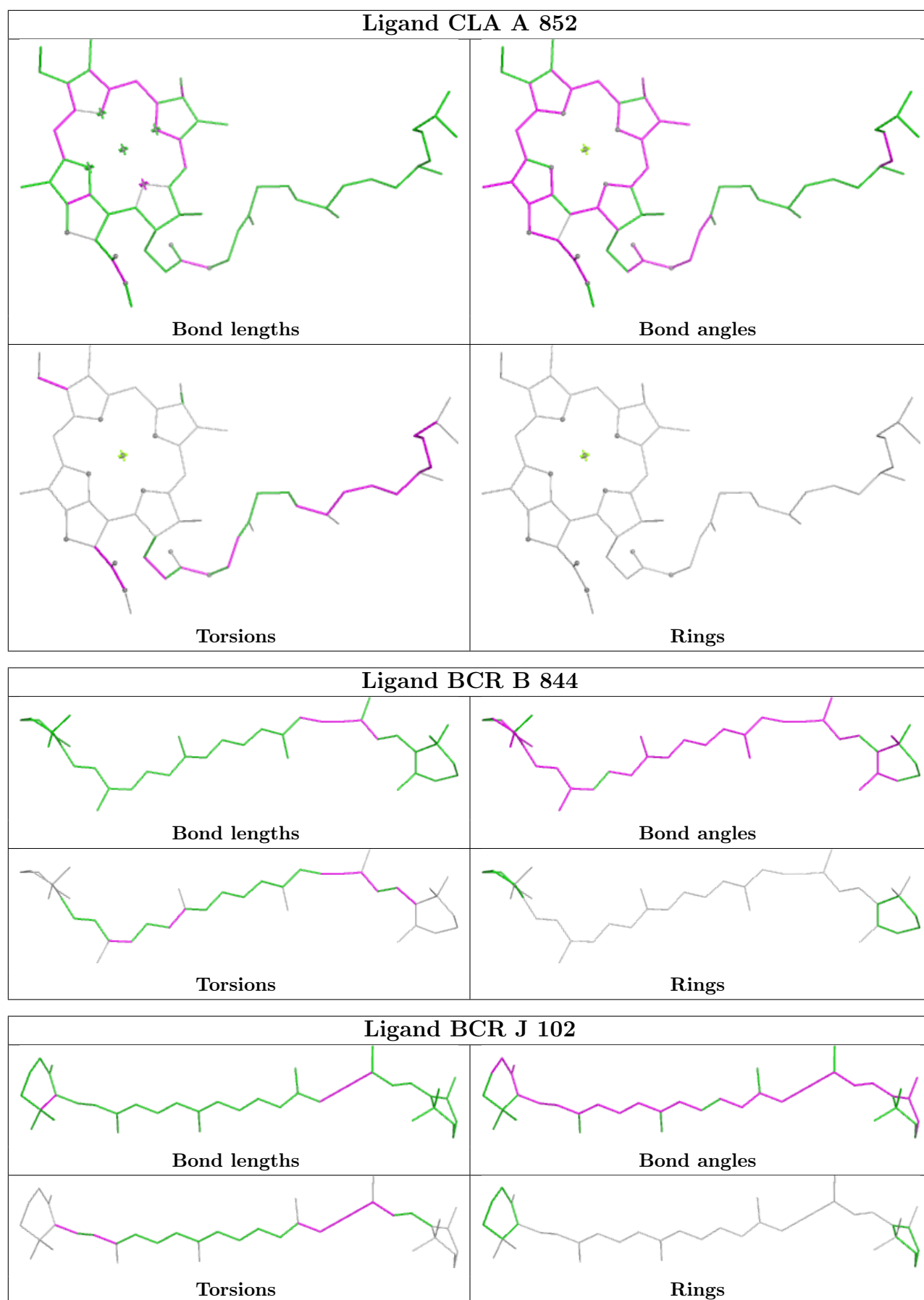


Ligand LMU H 104

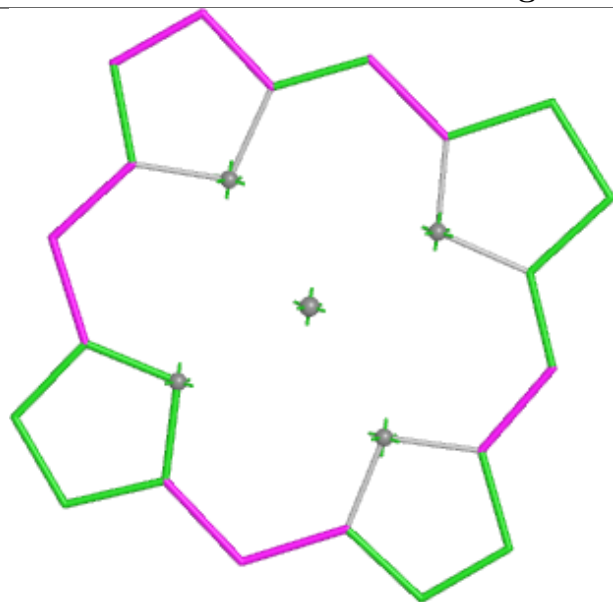




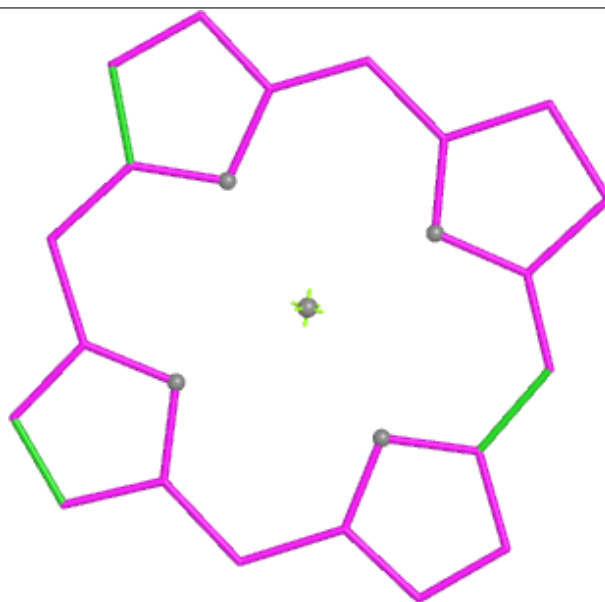




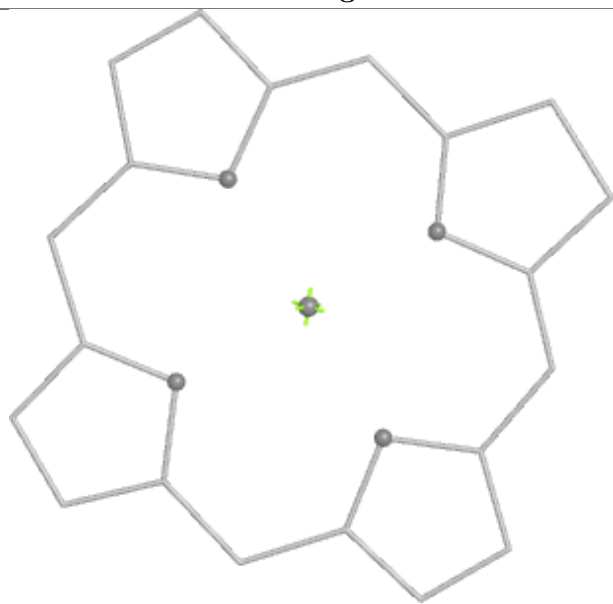
Ligand CLA 4 315



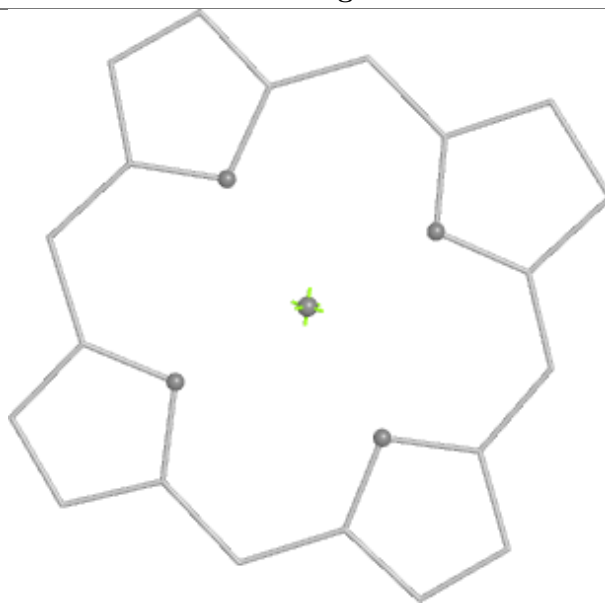
Bond lengths



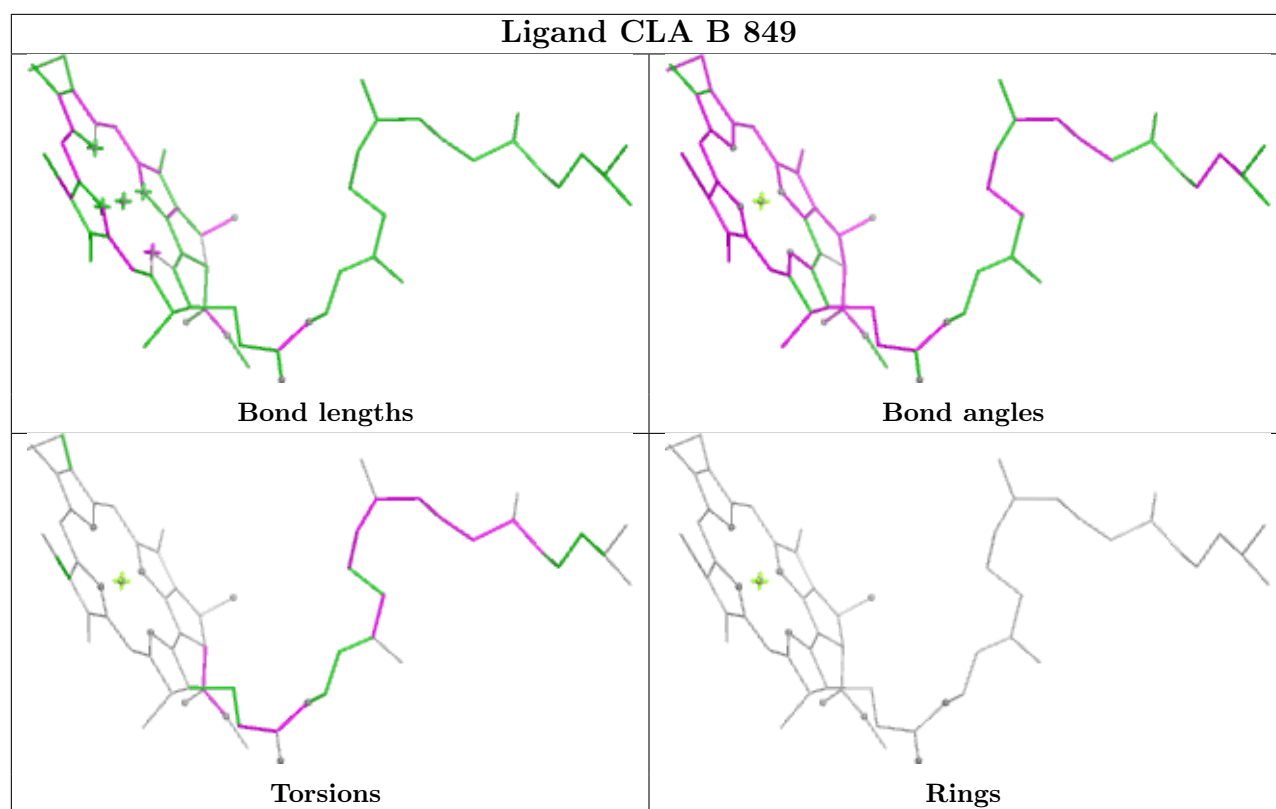
Bond angles

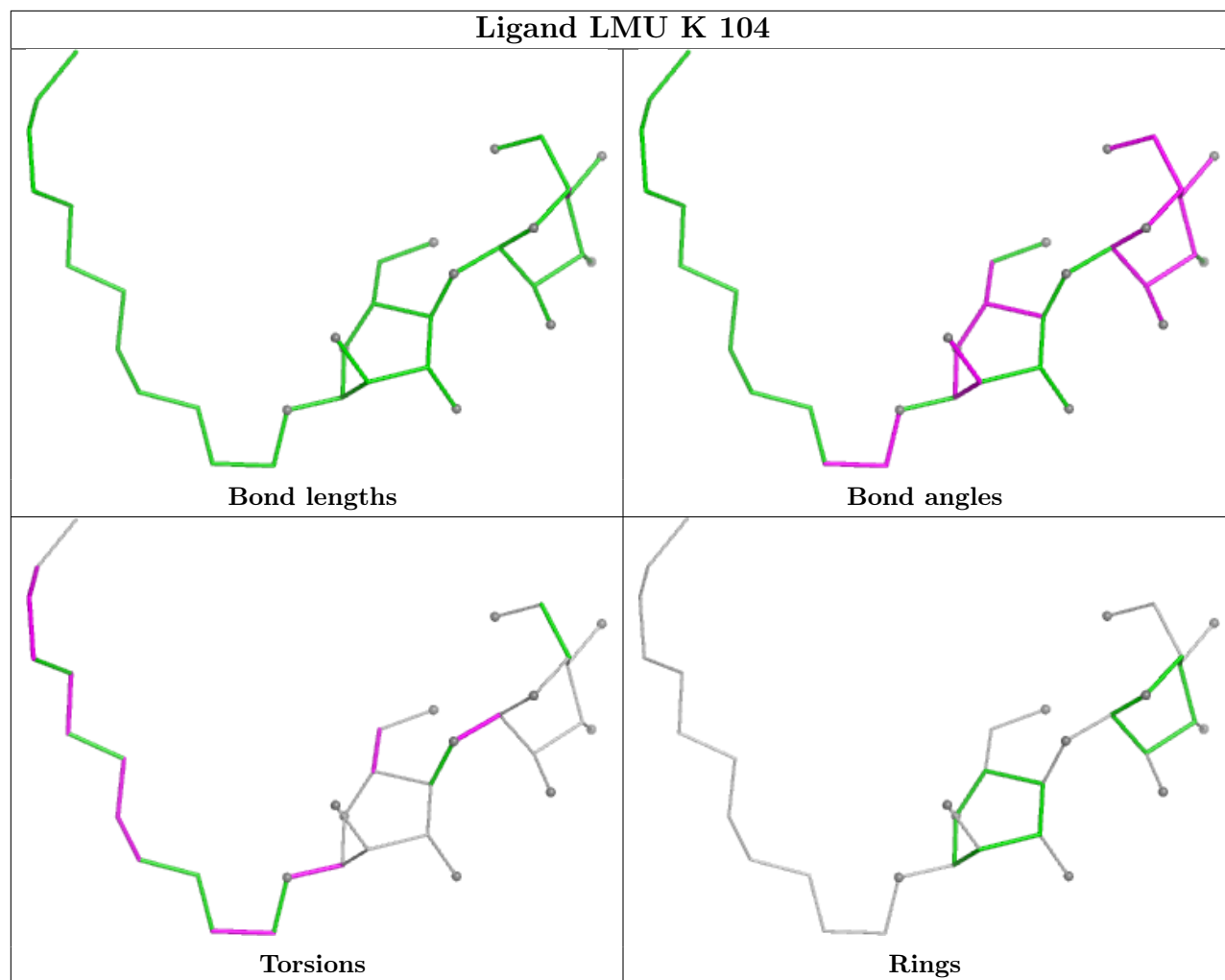


Torsions

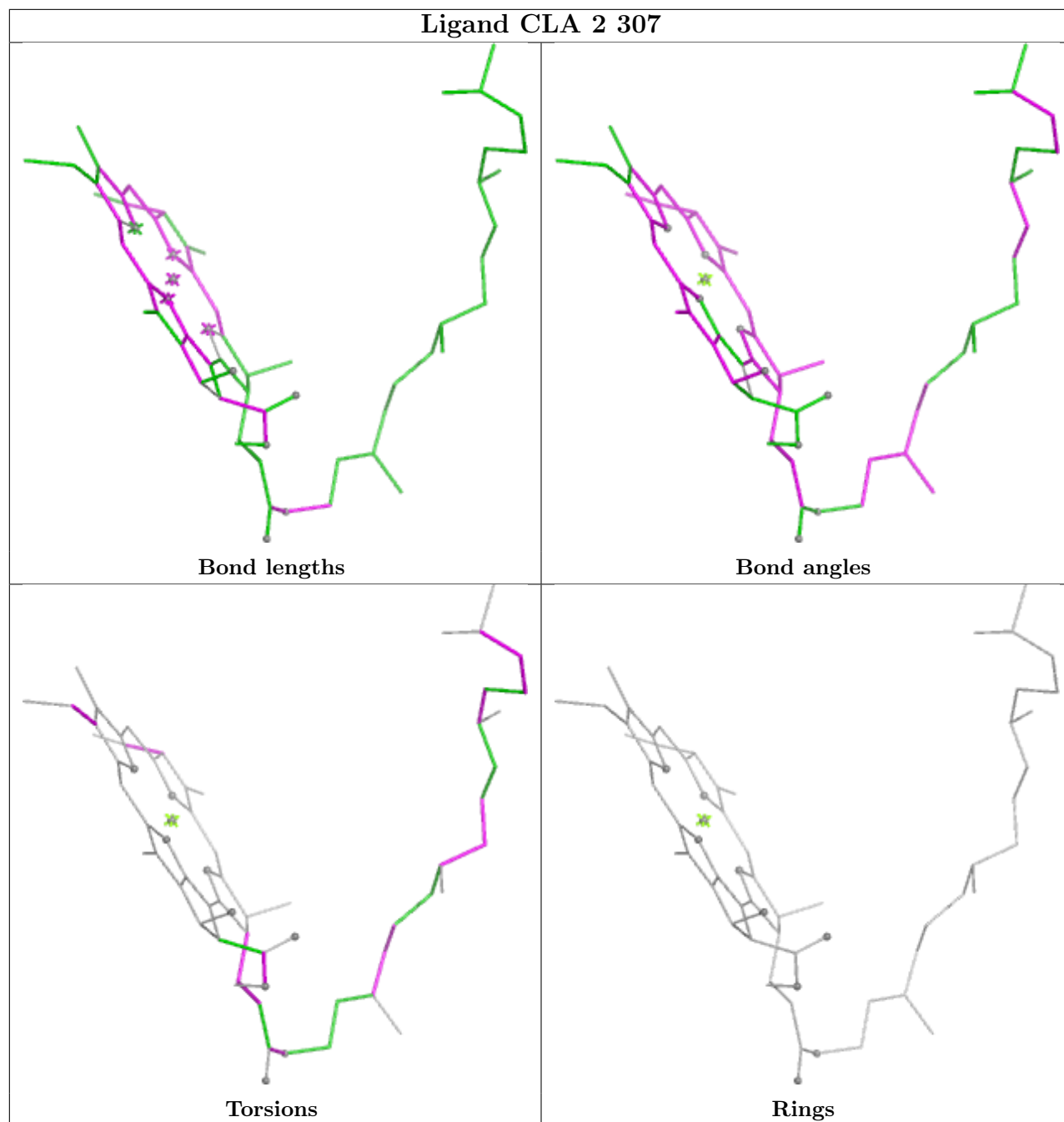


Rings

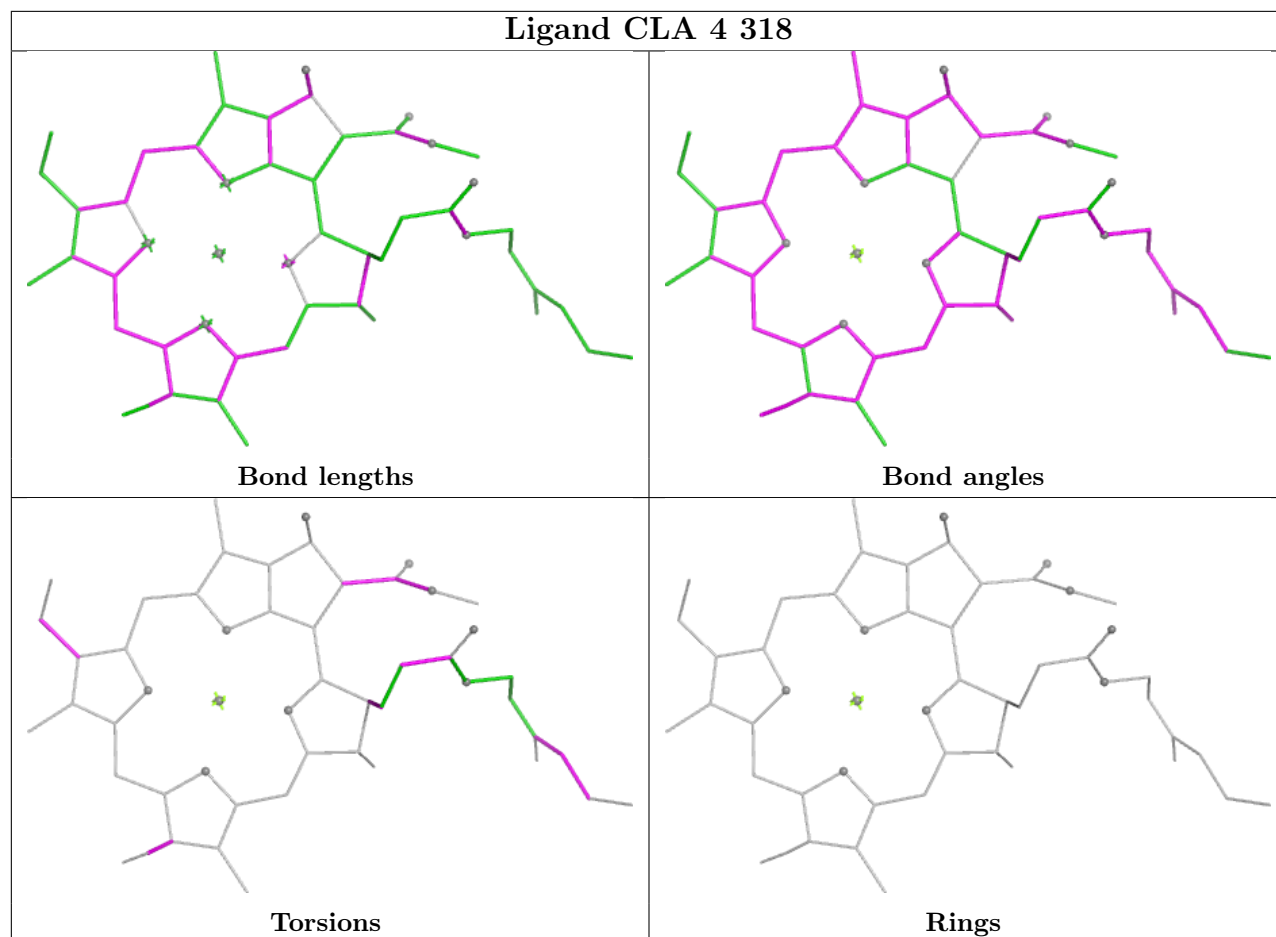




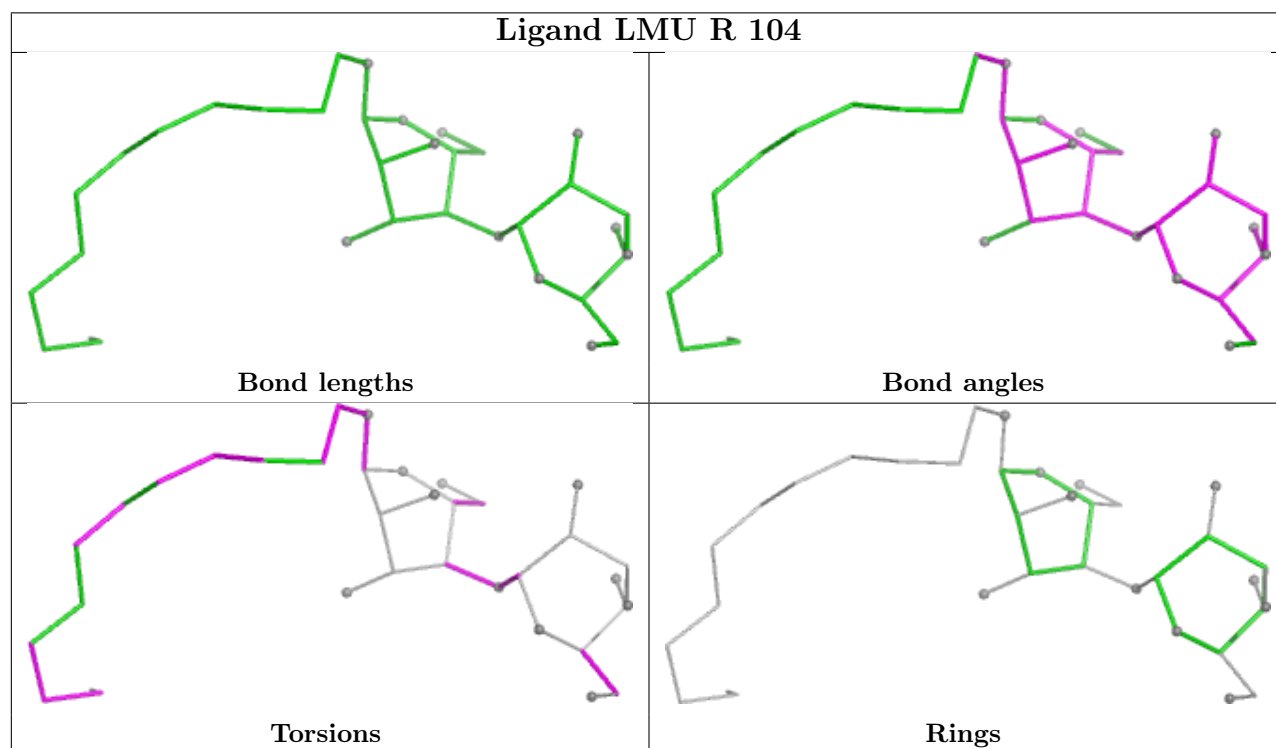
Ligand CLA 2 307



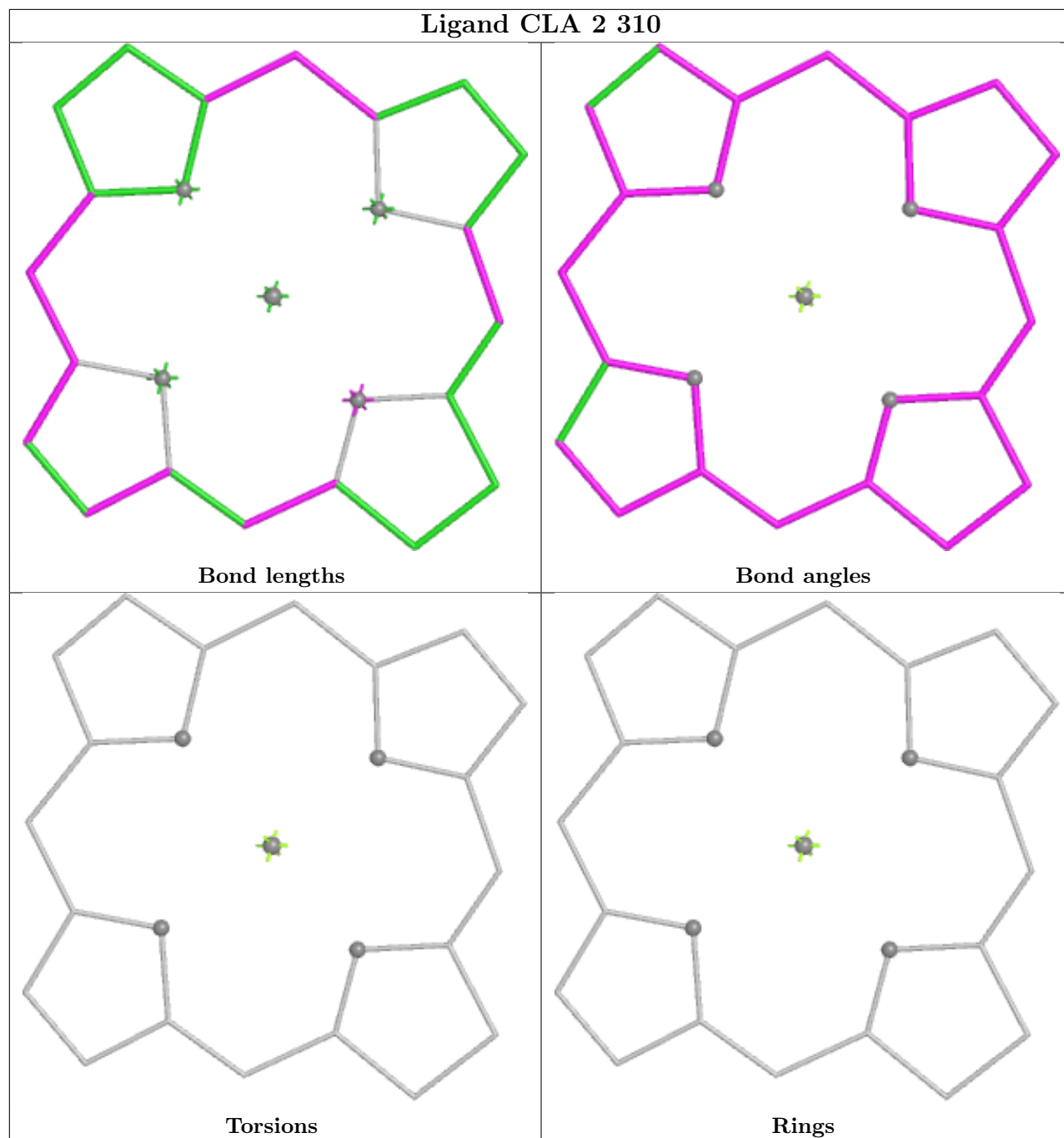
Ligand CLA 4 318



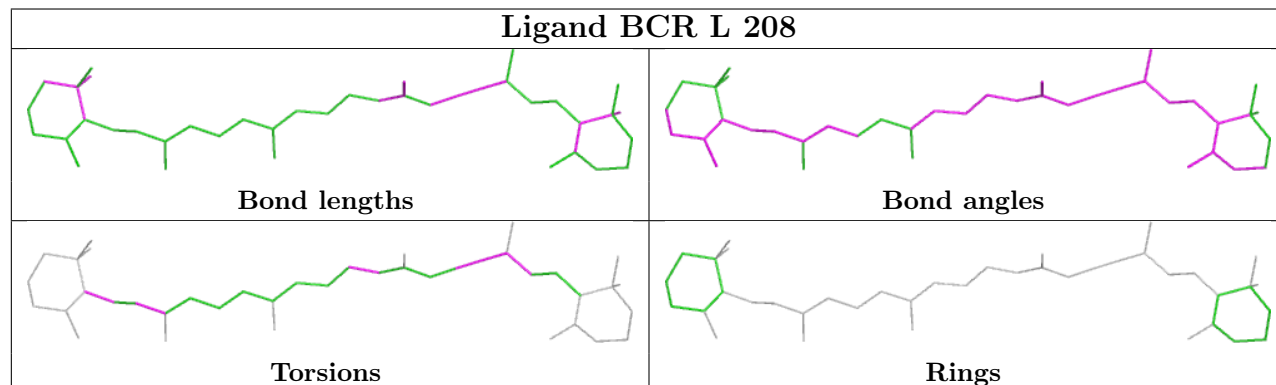
Ligand LMU R 104

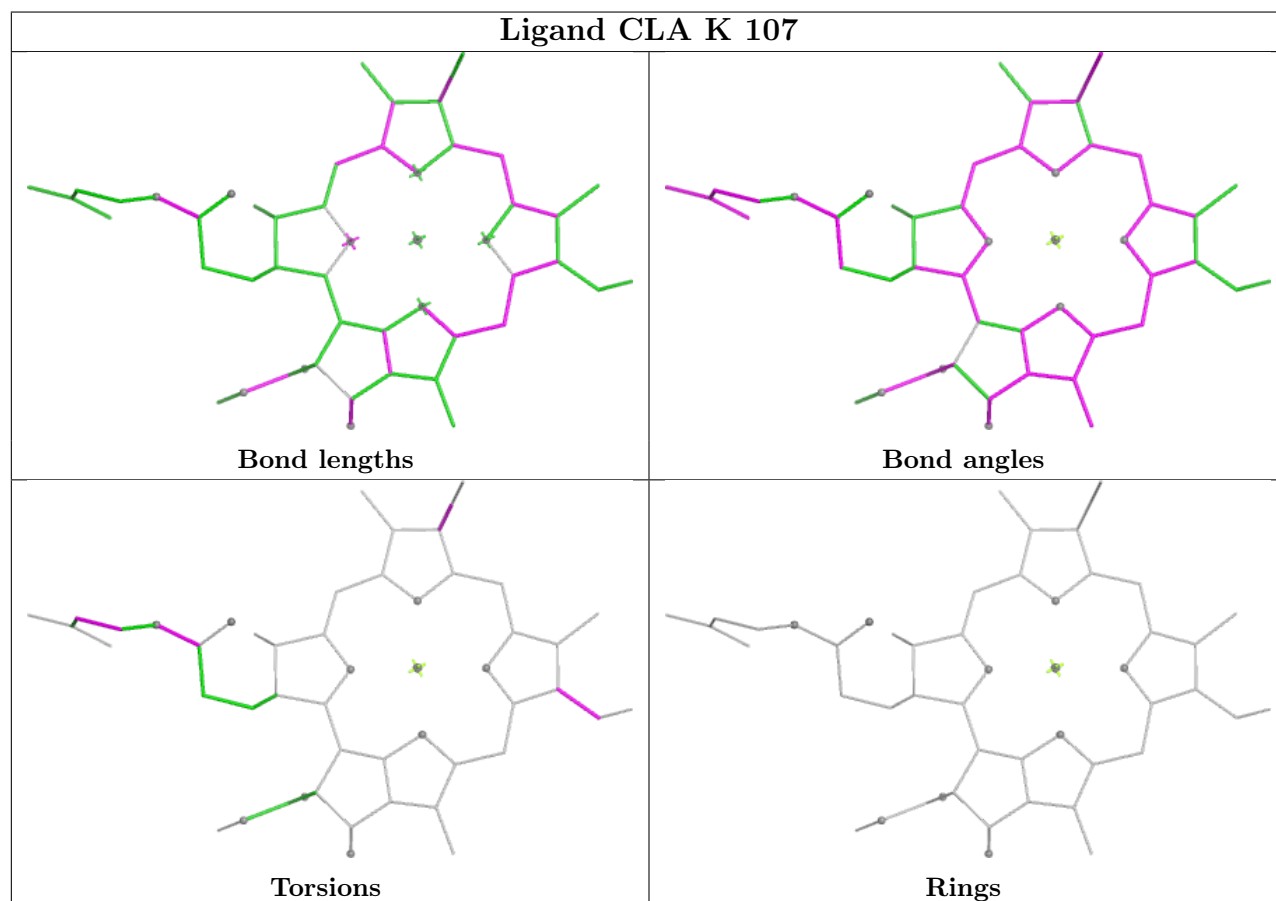
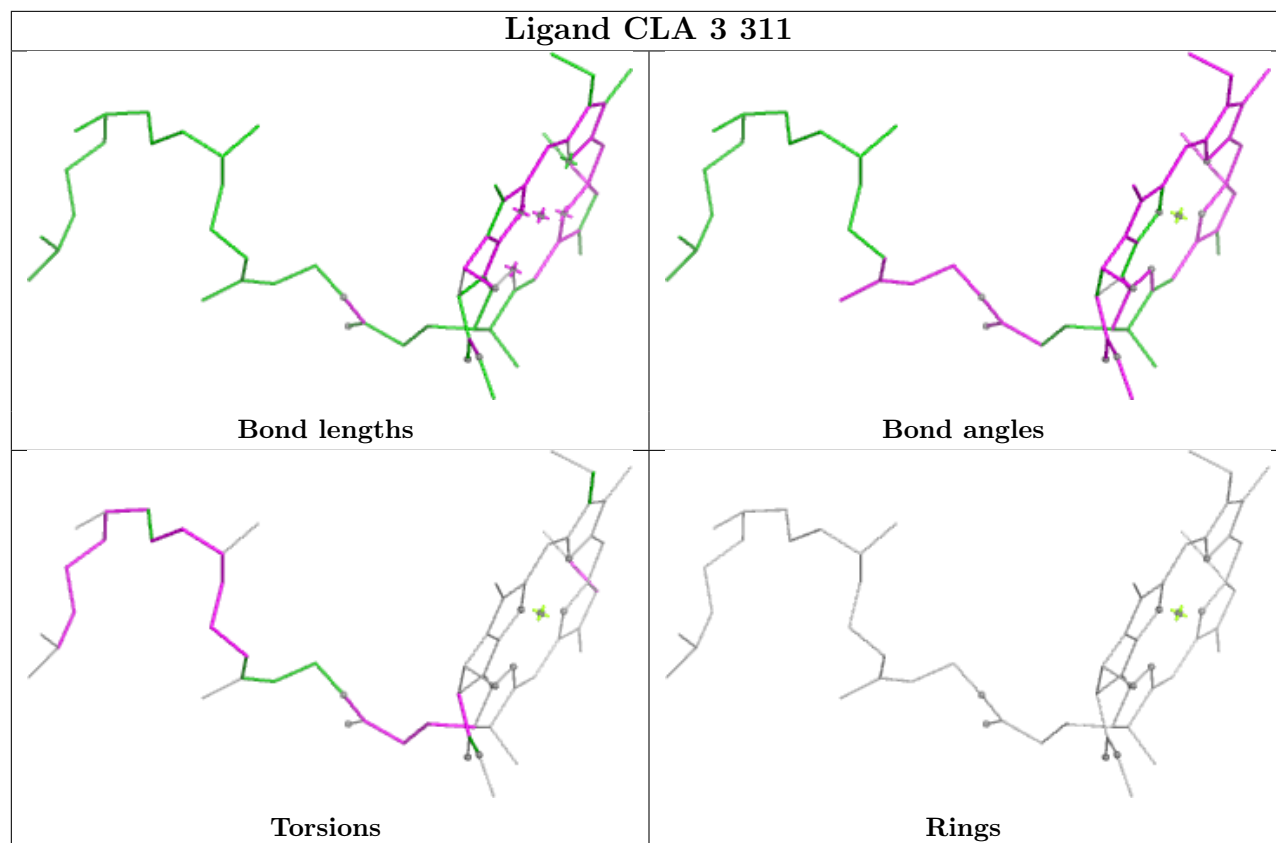


Ligand CLA 2 310

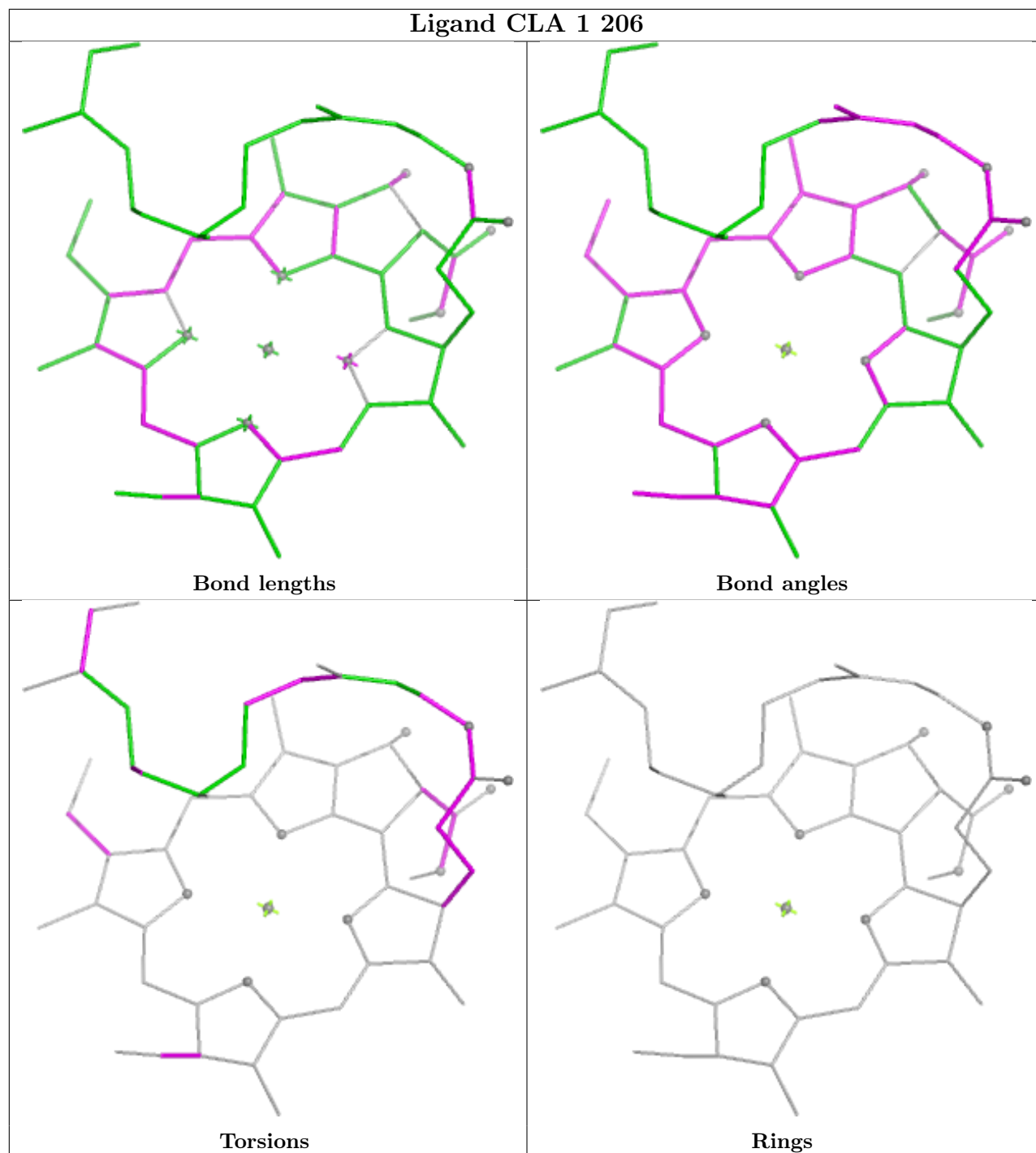


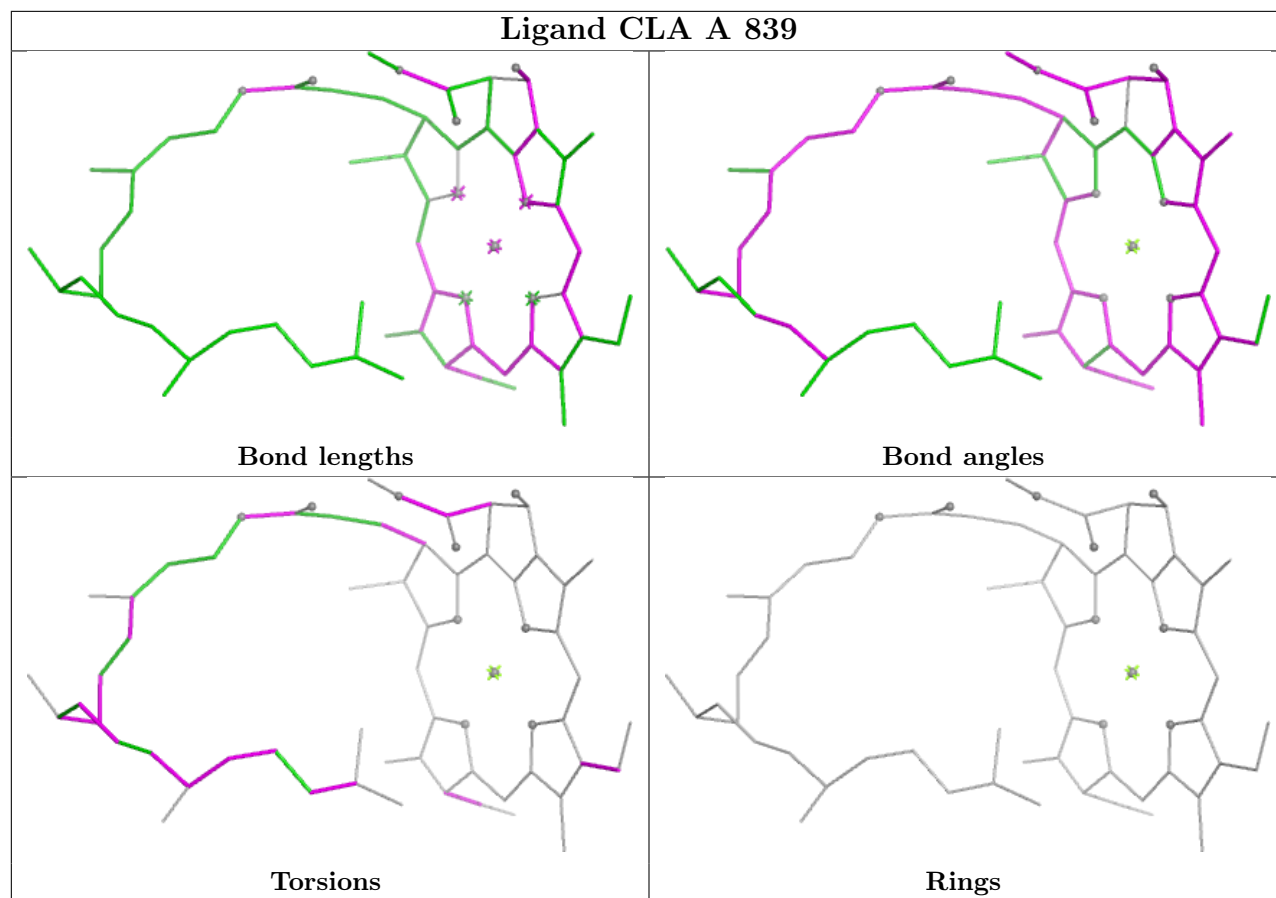
Ligand BCR L 208



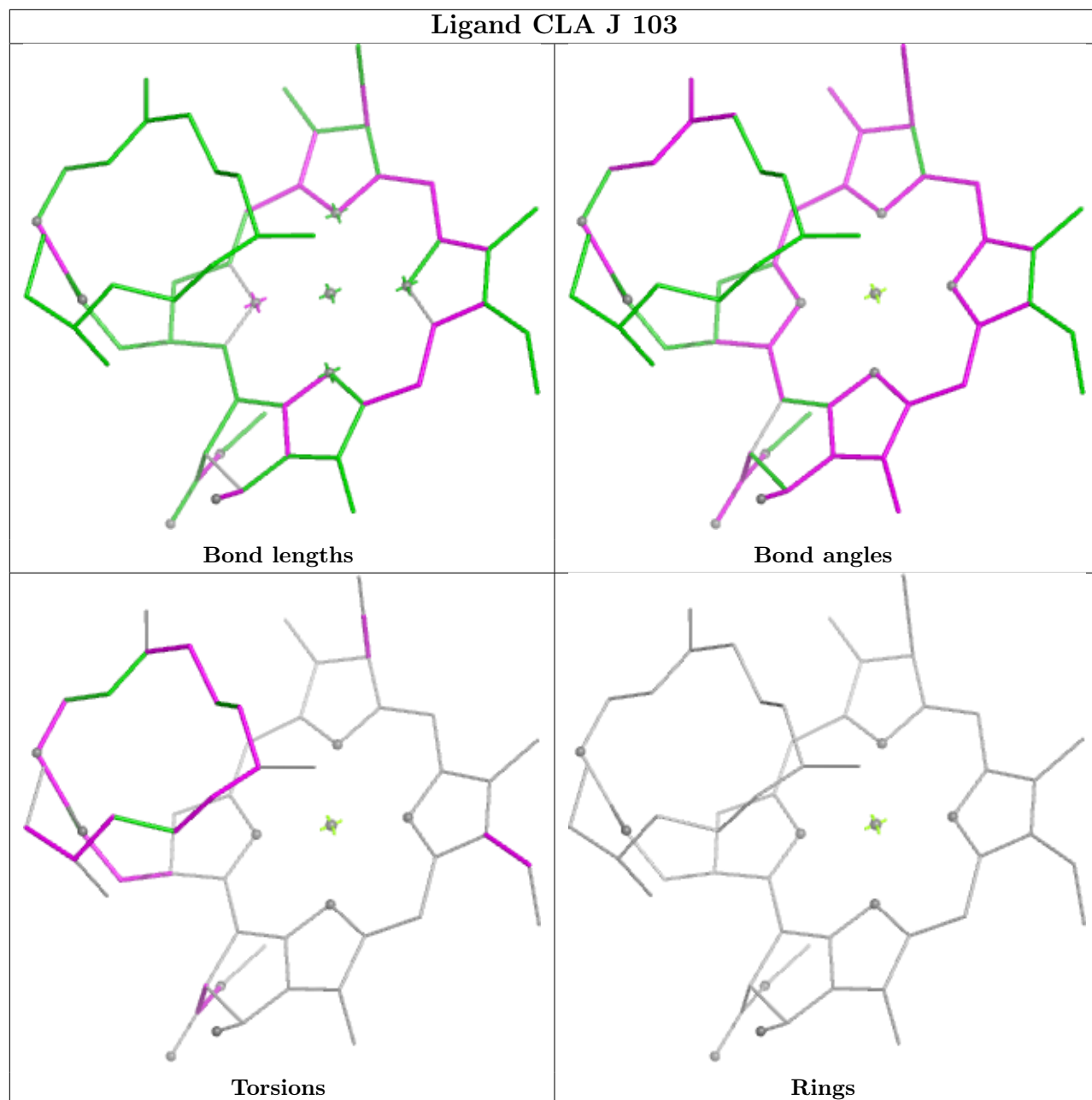


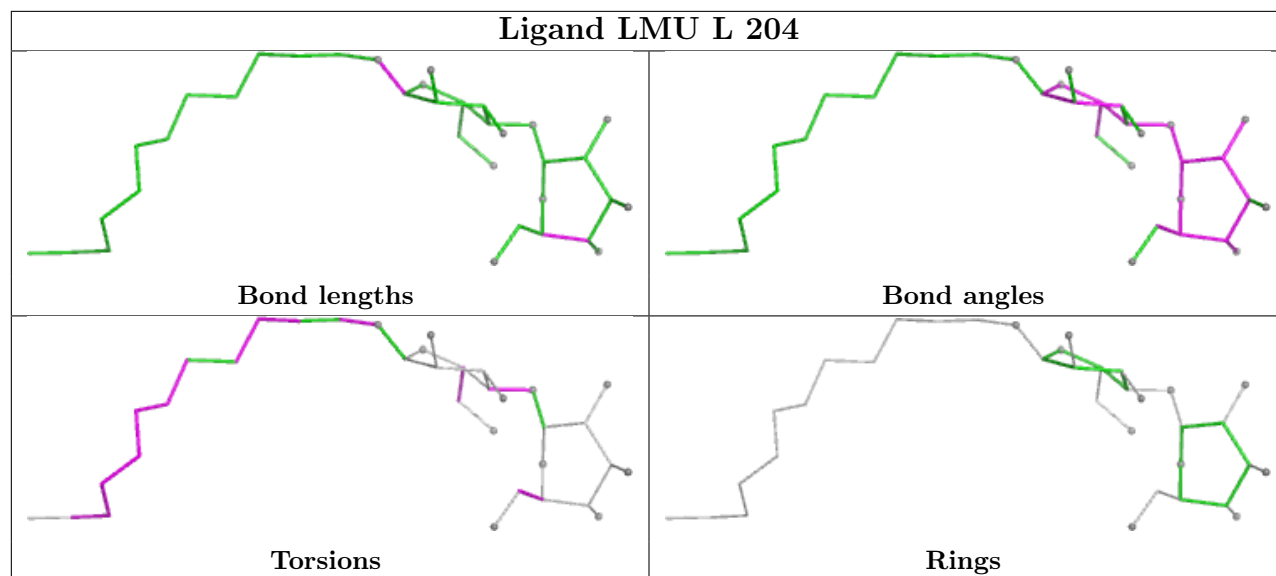
Ligand CLA 1 206



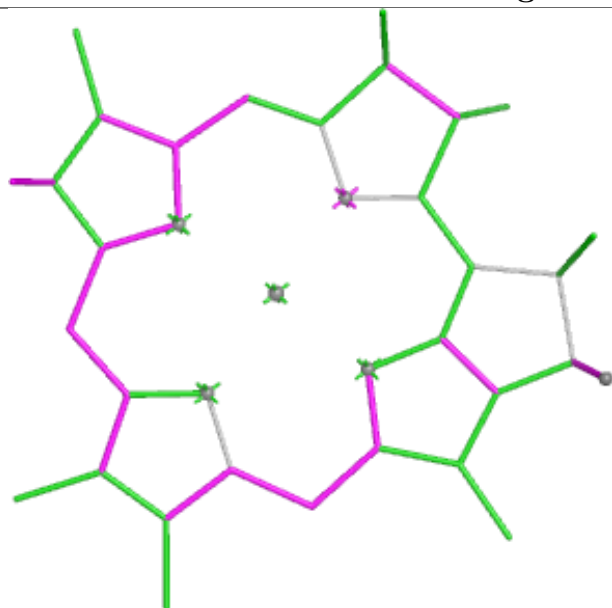


Ligand CLA J 103

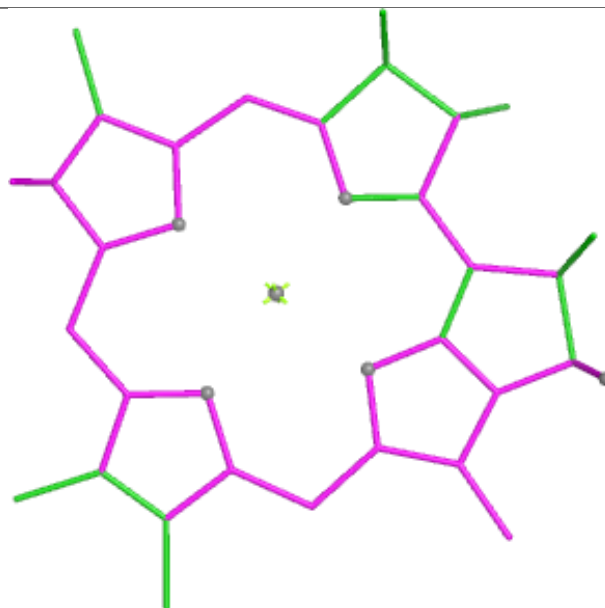




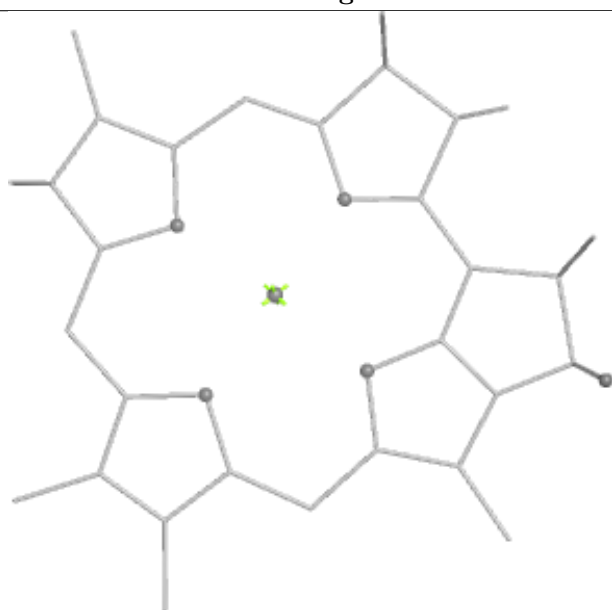
Ligand CLA 4 308



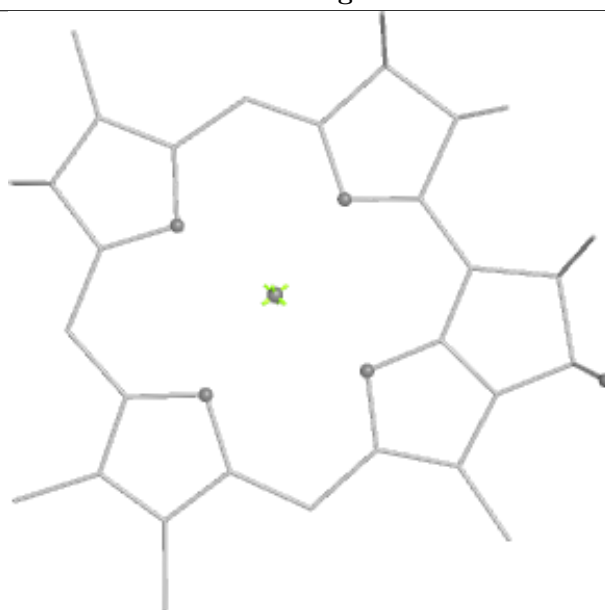
Bond lengths



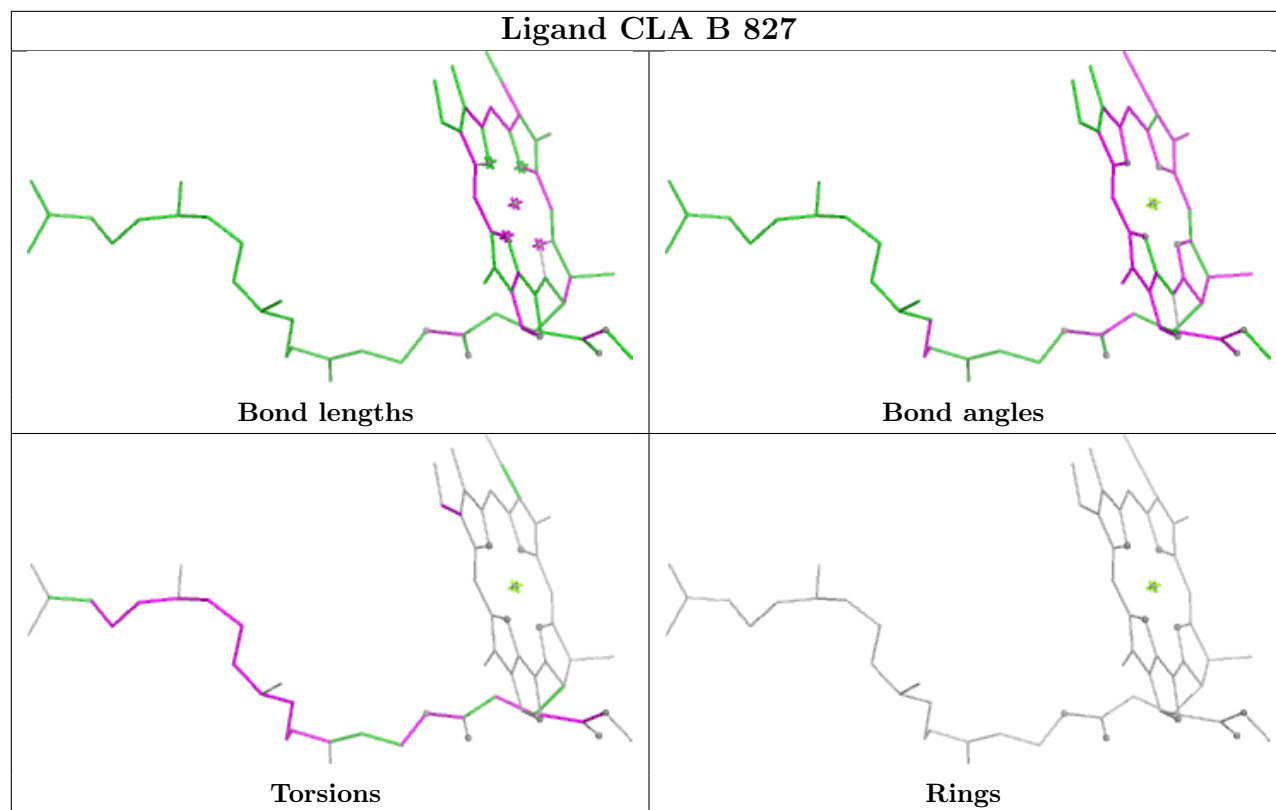
Bond angles



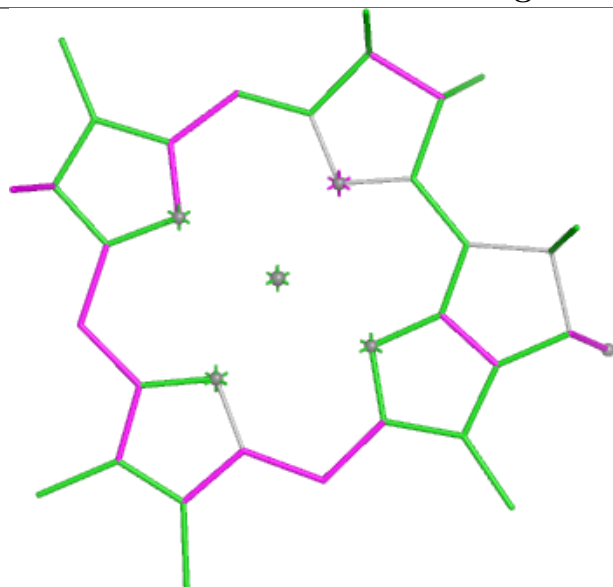
Torsions



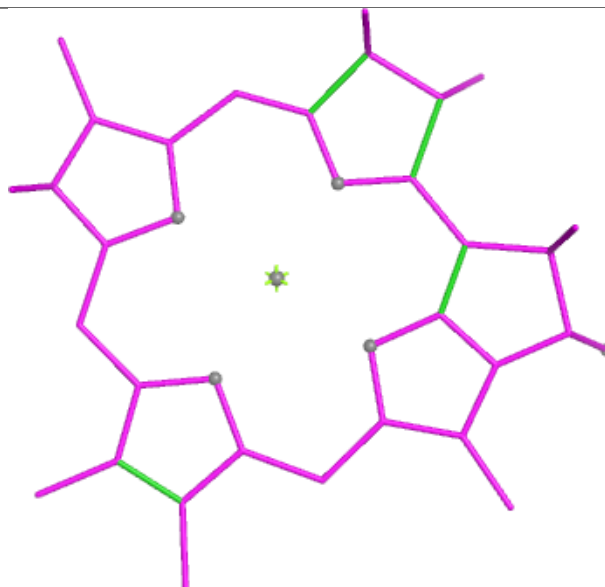
Rings



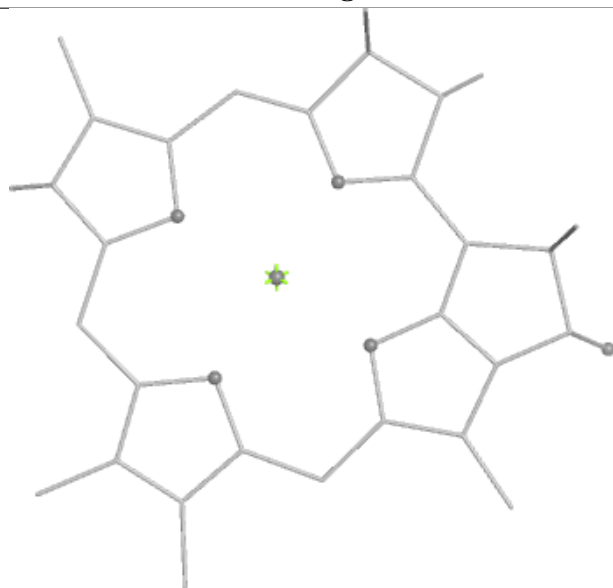
Ligand CLA B 840



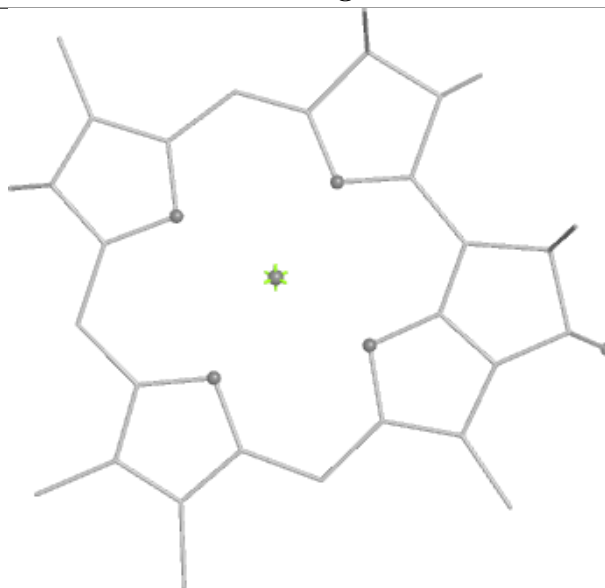
Bond lengths



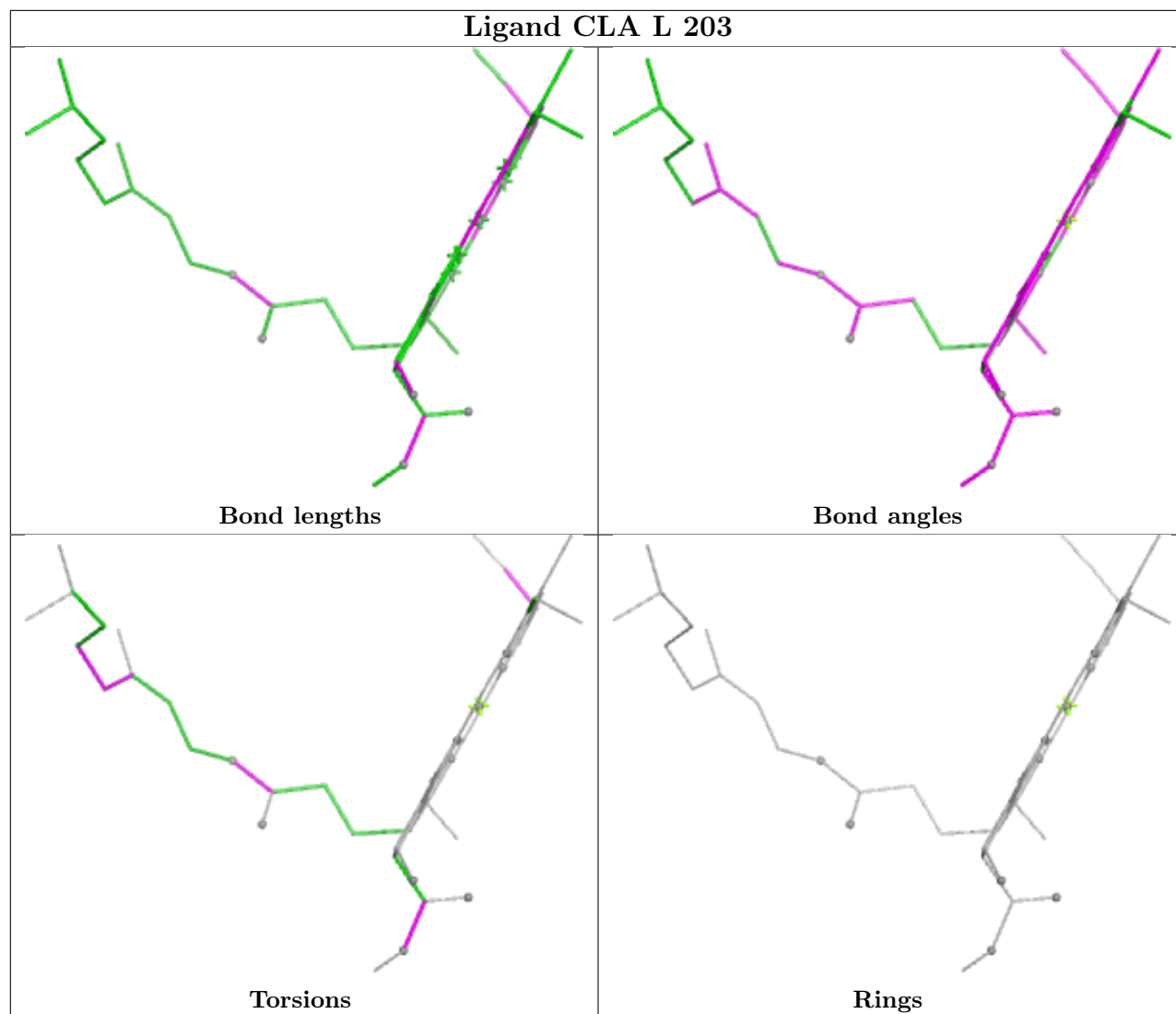
Bond angles



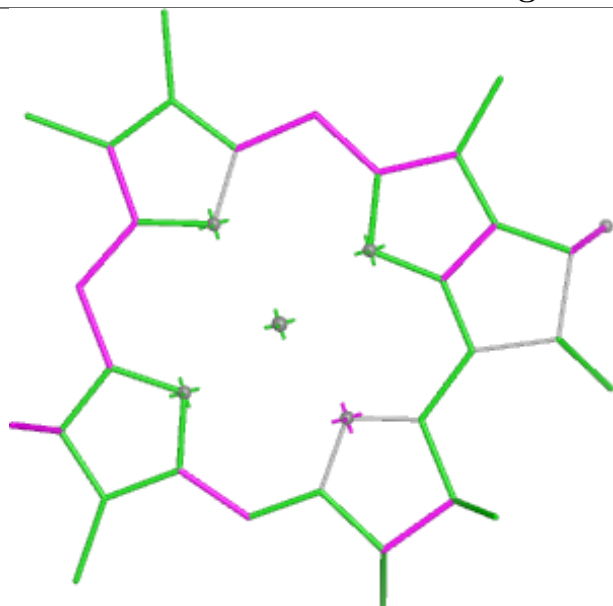
Torsions



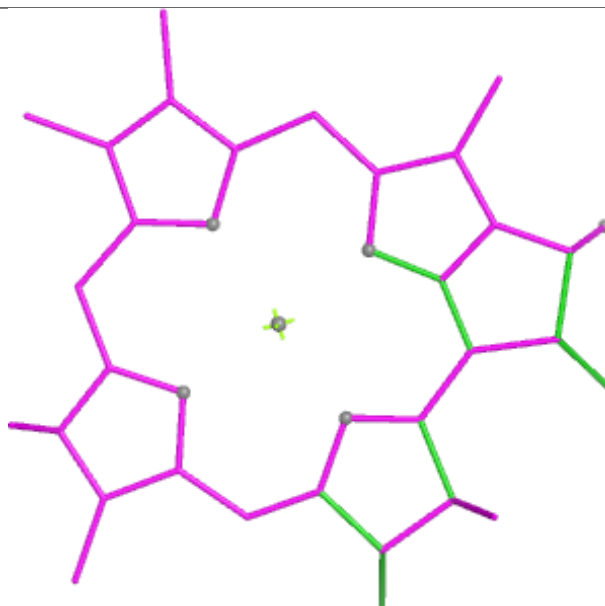
Rings



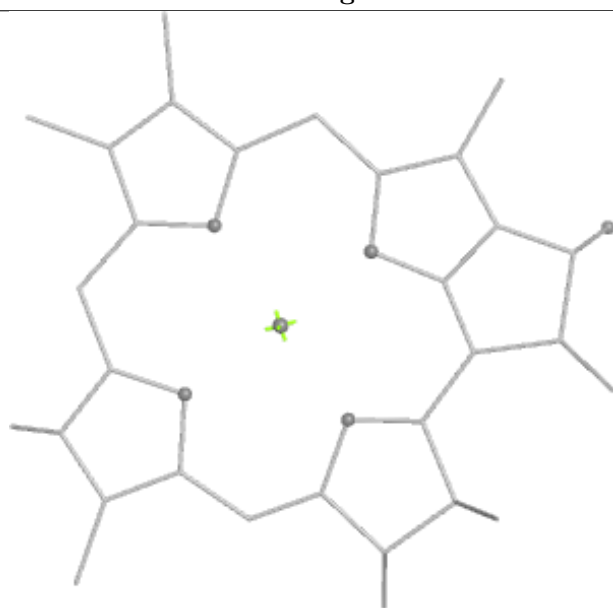
Ligand CLA 4 314



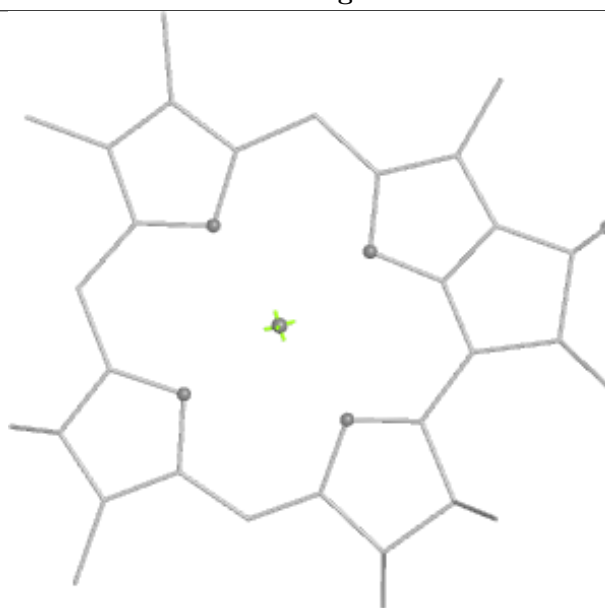
Bond lengths



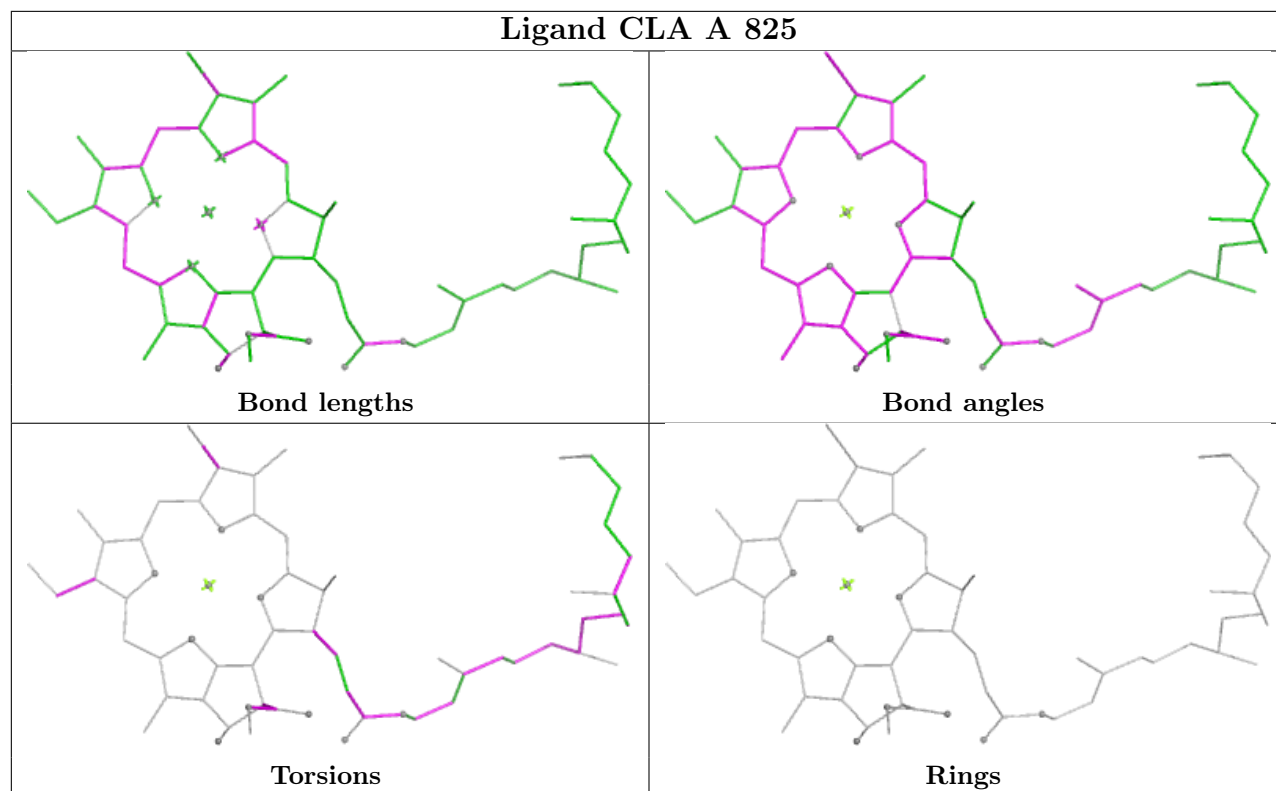
Bond angles

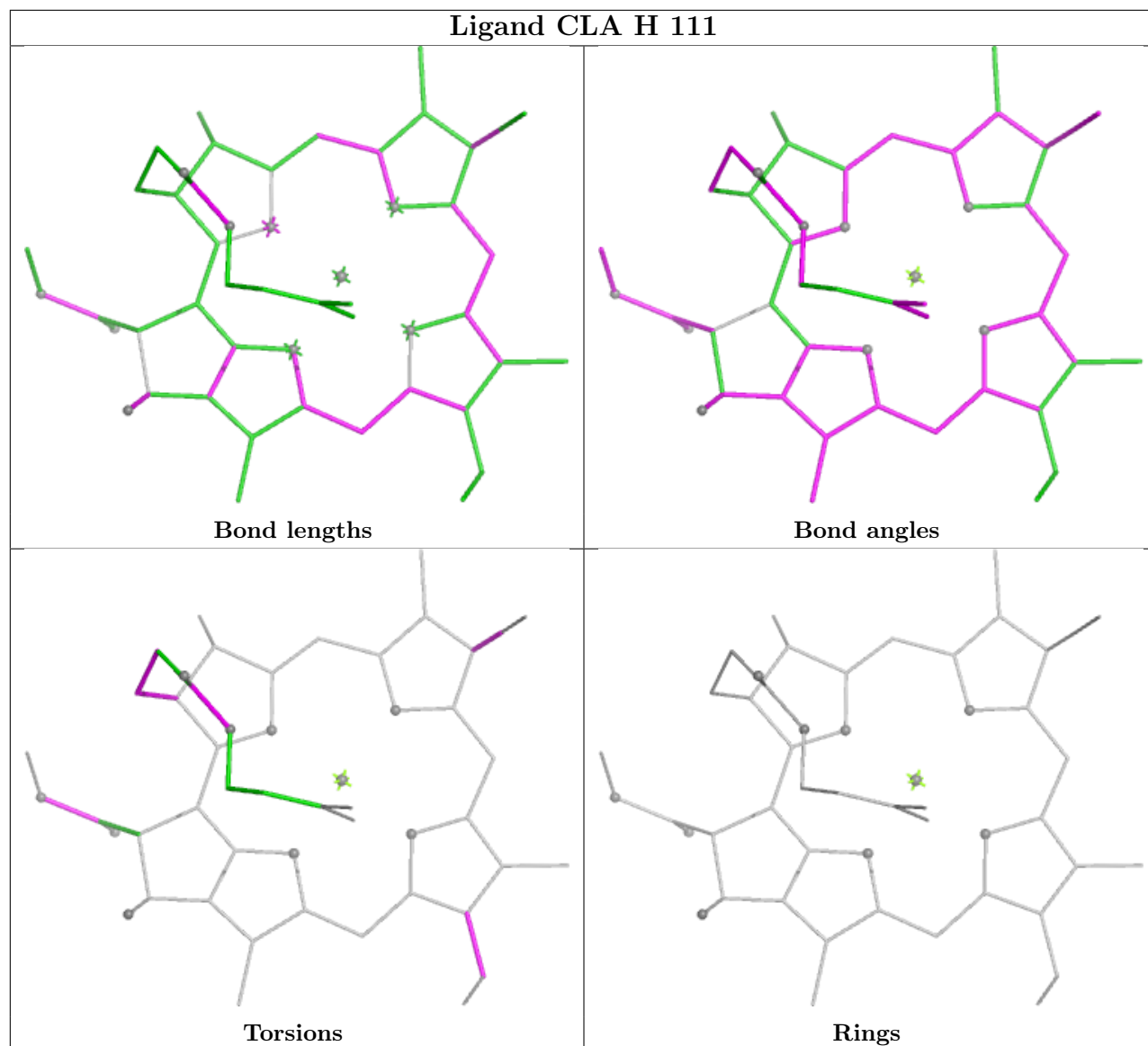


Torsions

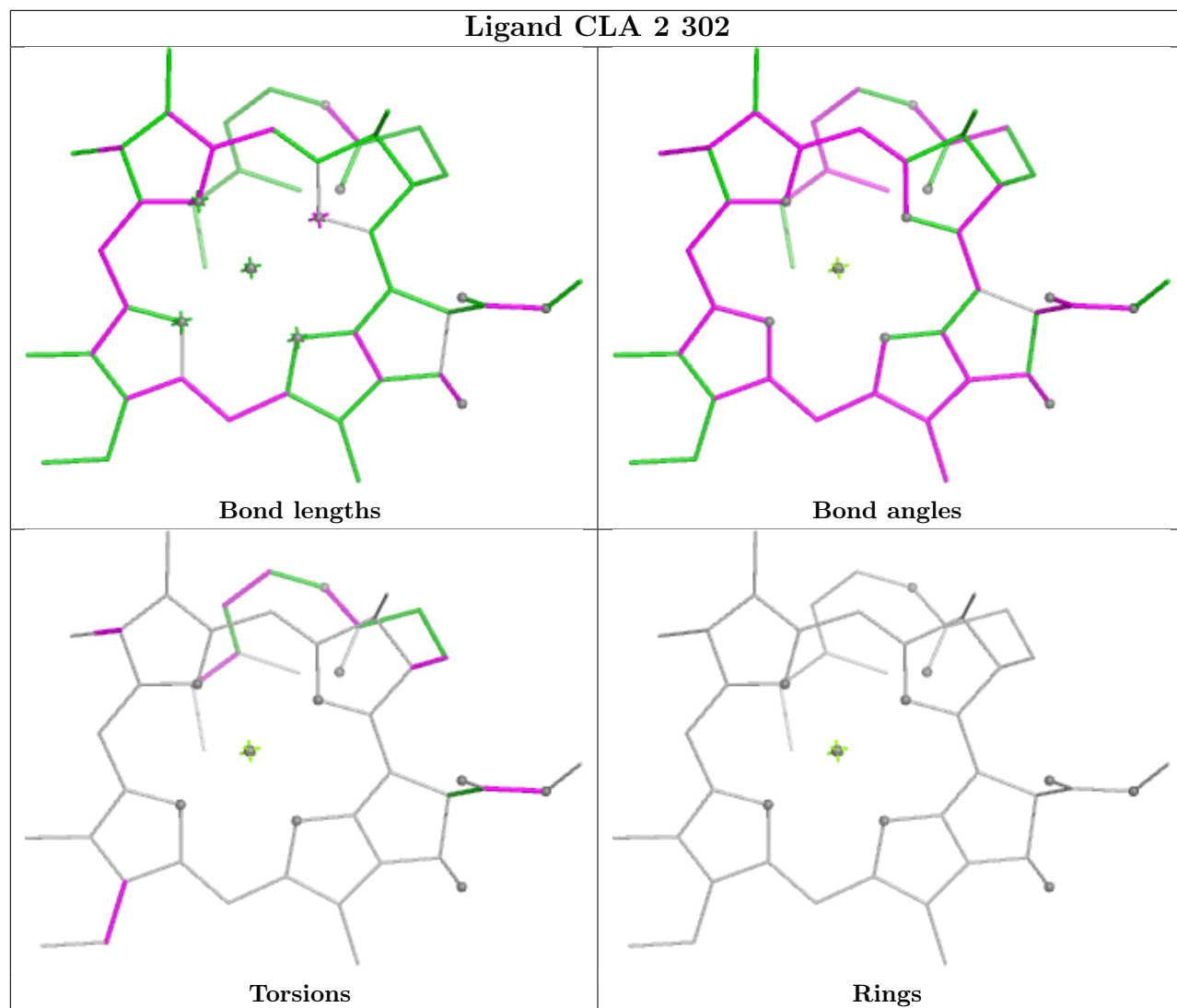


Rings

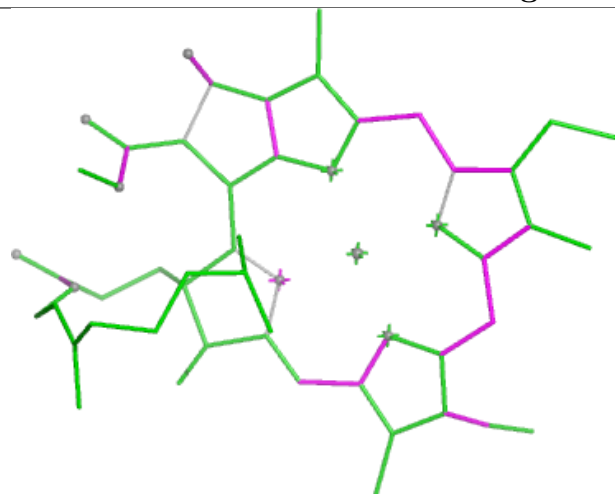




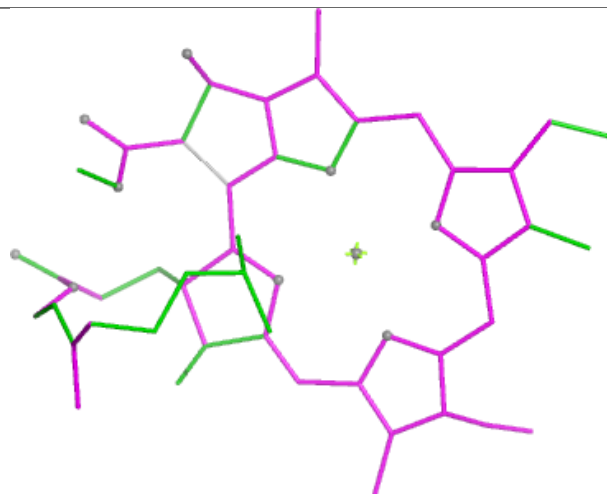
Ligand CLA 2 302



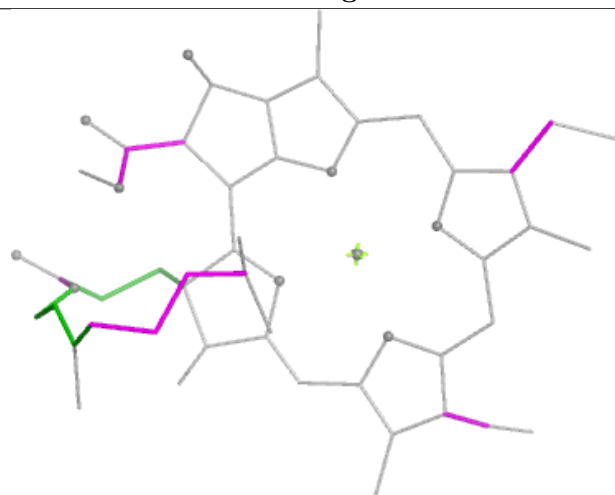
Ligand CLA 4 305



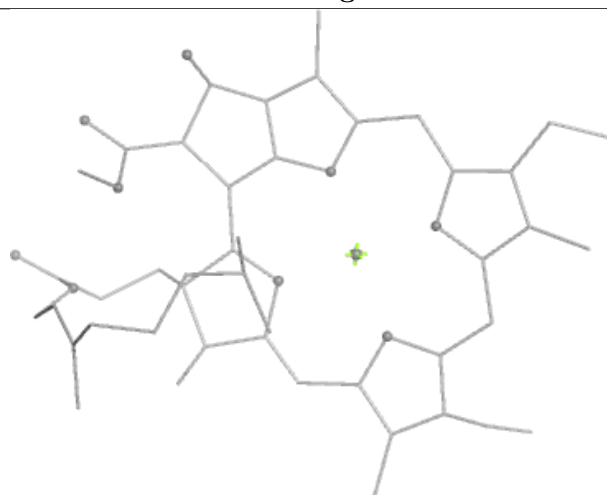
Bond lengths



Bond angles

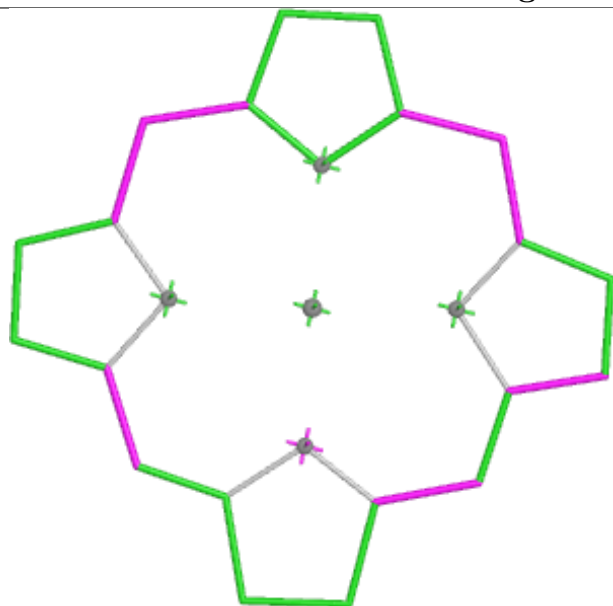


Torsions

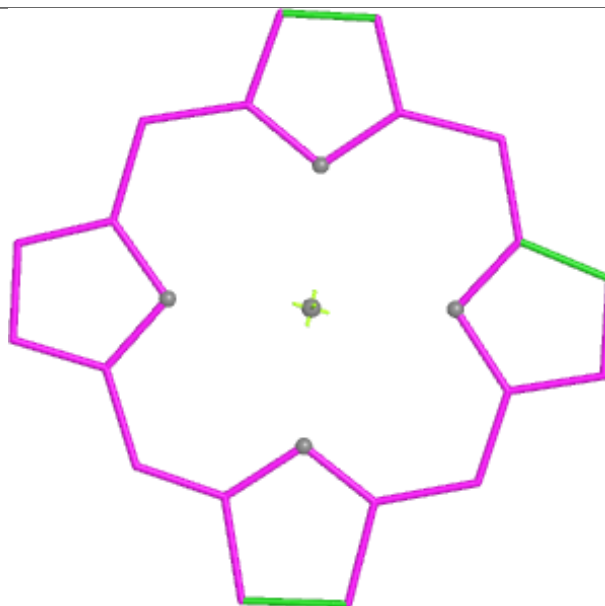


Rings

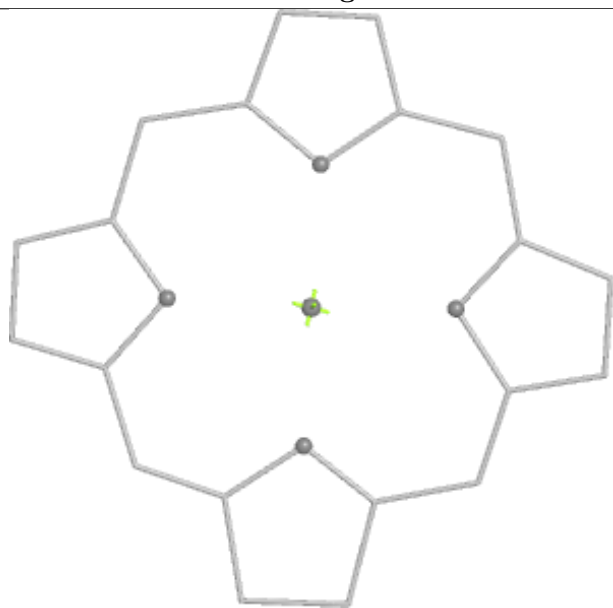
Ligand CLA 2 309



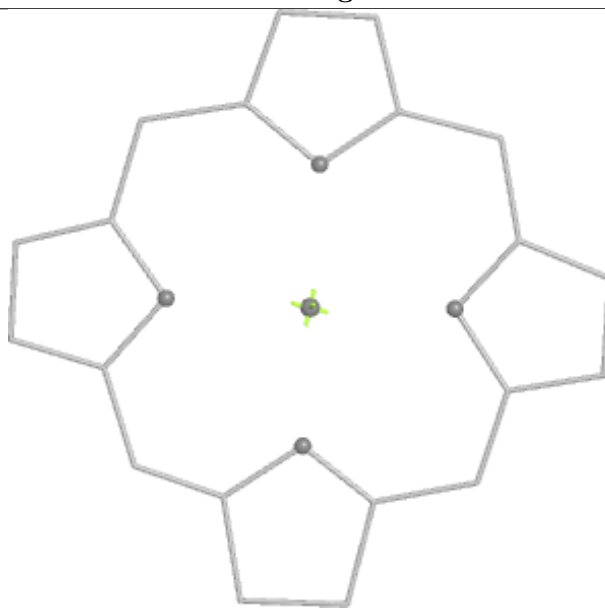
Bond lengths



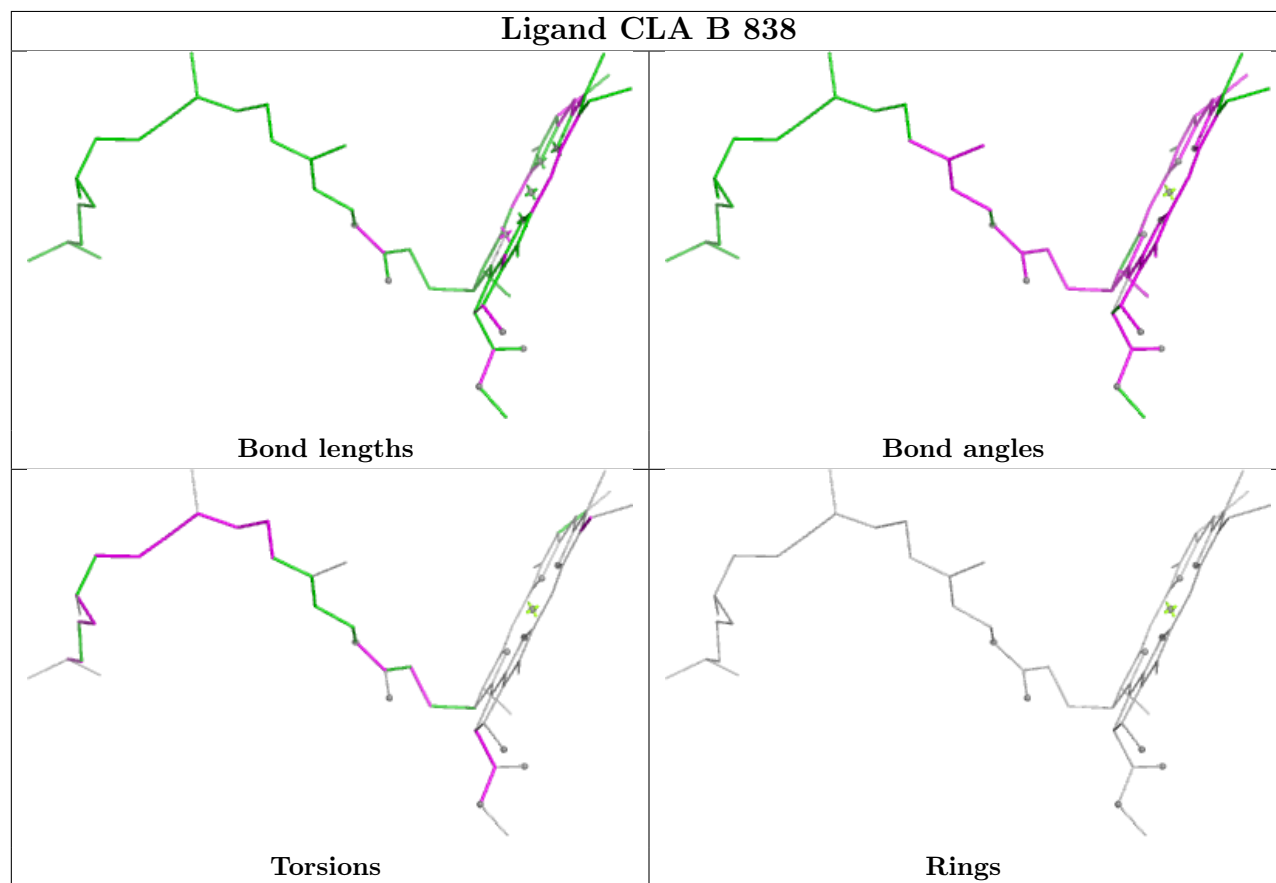
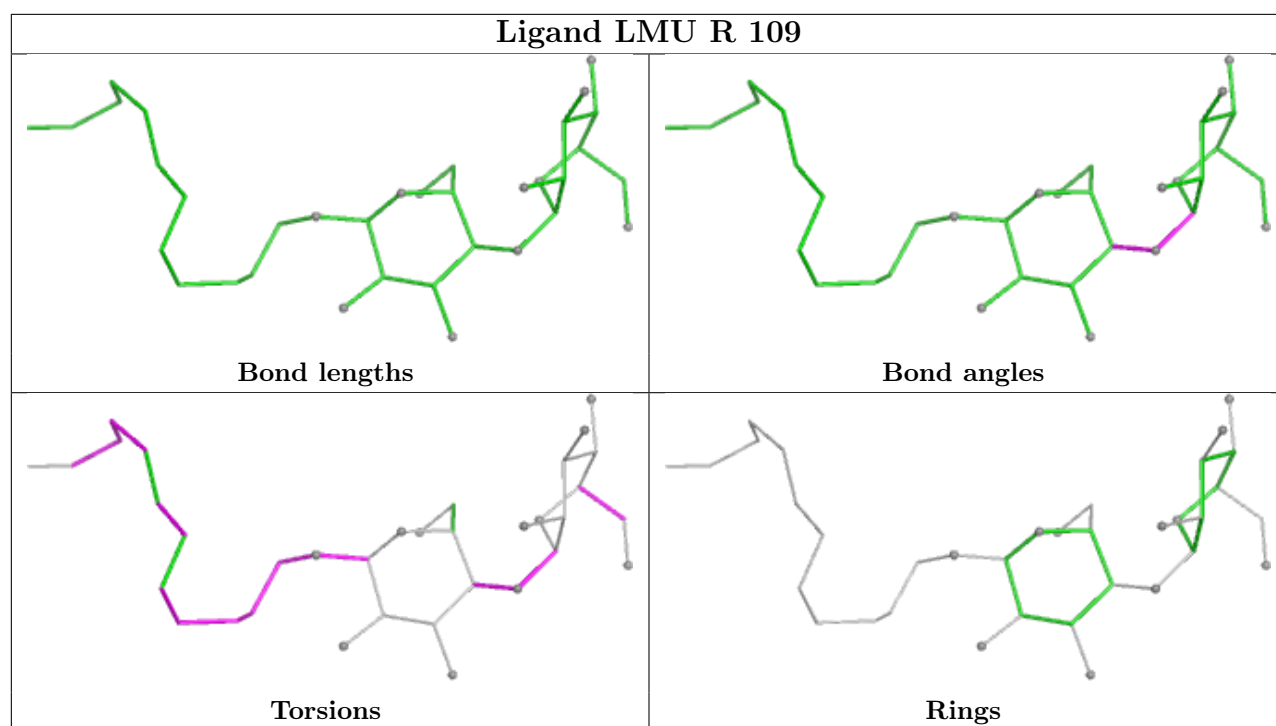
Bond angles



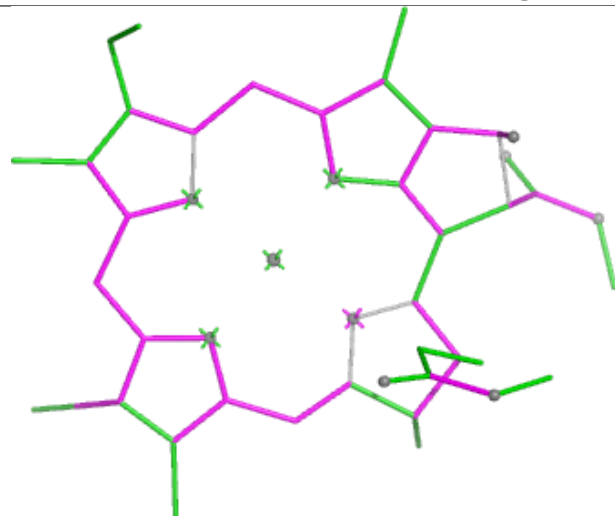
Torsions



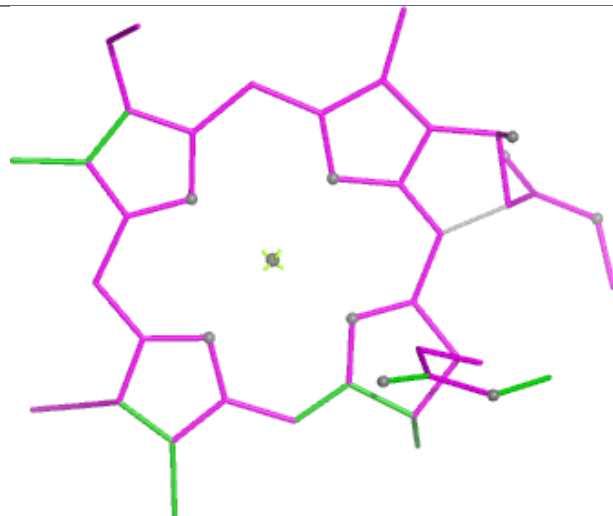
Rings



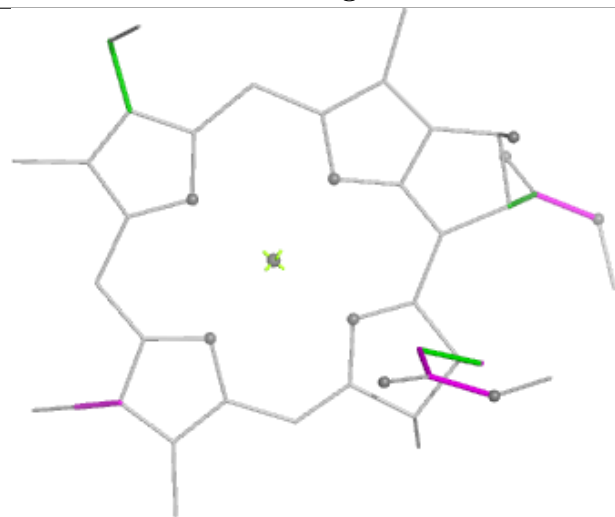
Ligand CLA A 807



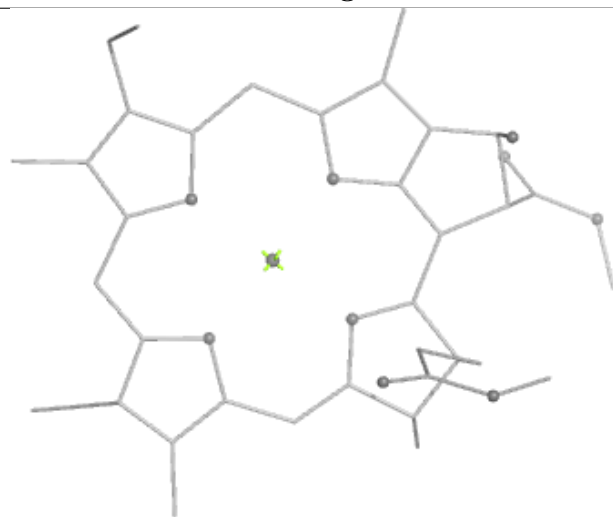
Bond lengths



Bond angles

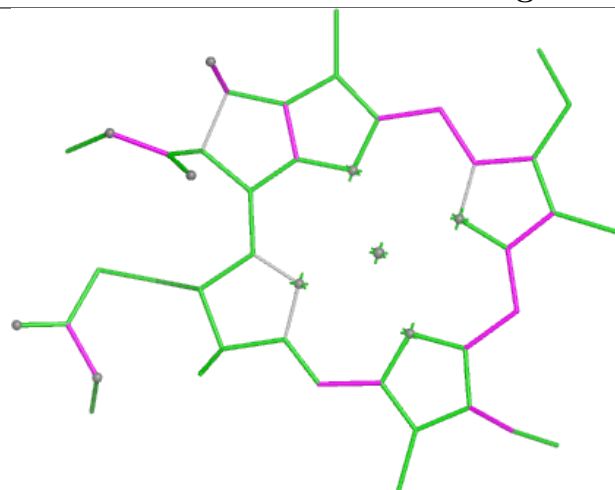


Torsions

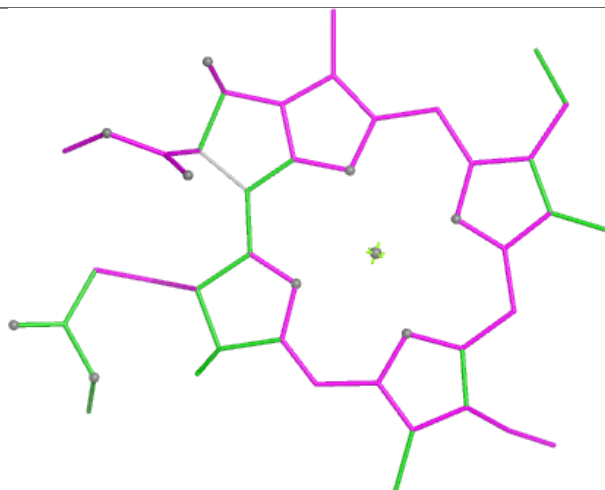


Rings

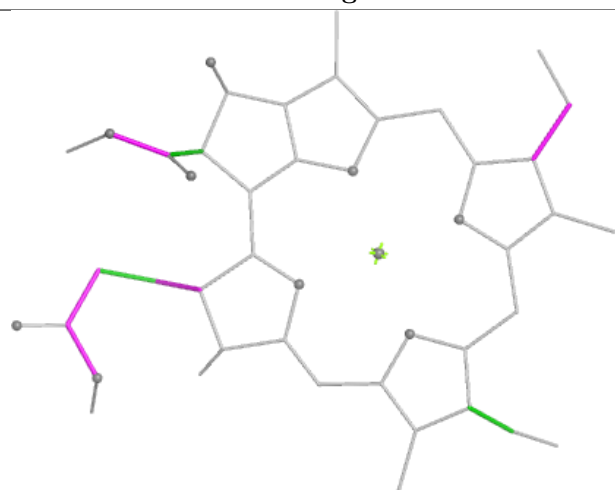
Ligand CLA B 814



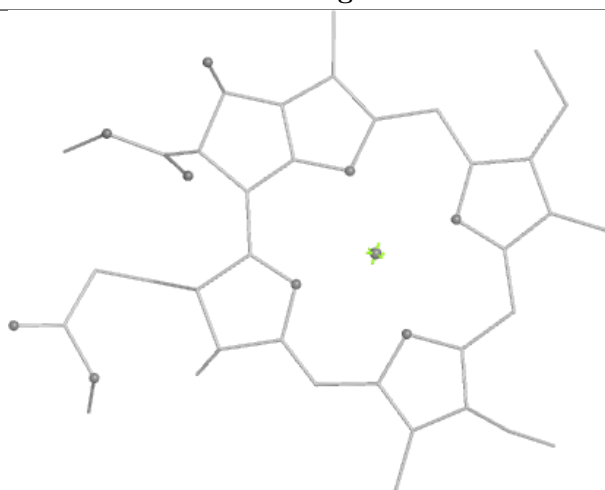
Bond lengths



Bond angles

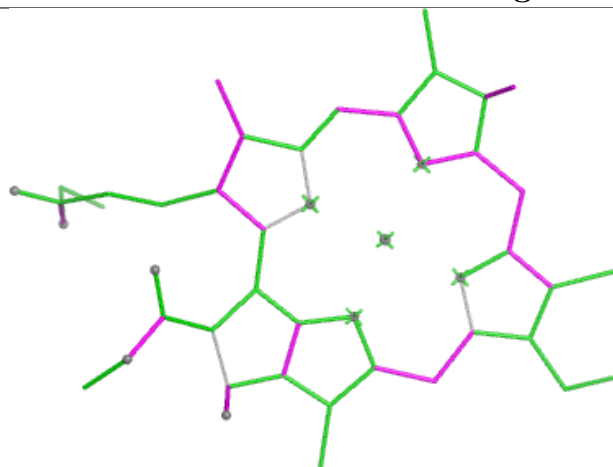


Torsions

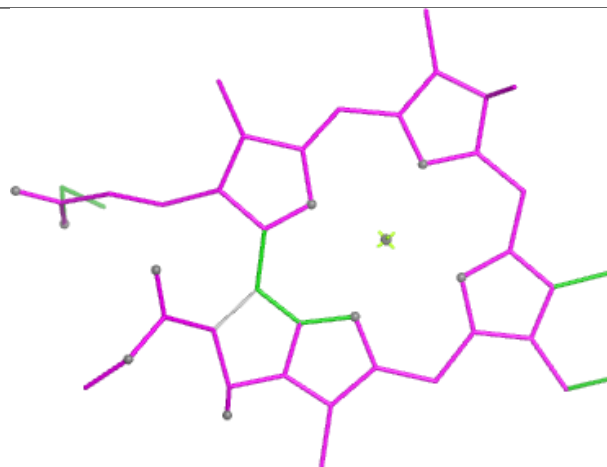


Rings

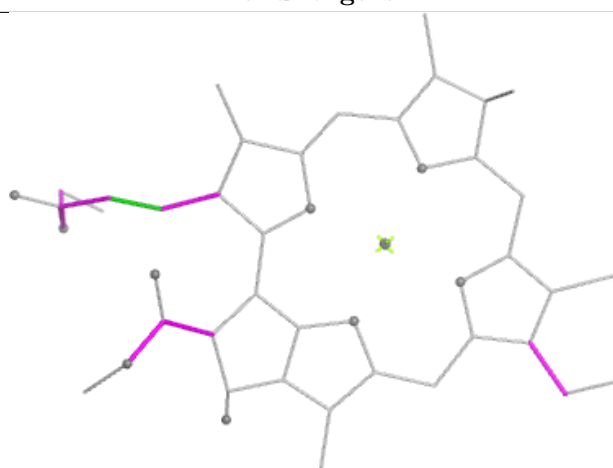
Ligand CLA A 801



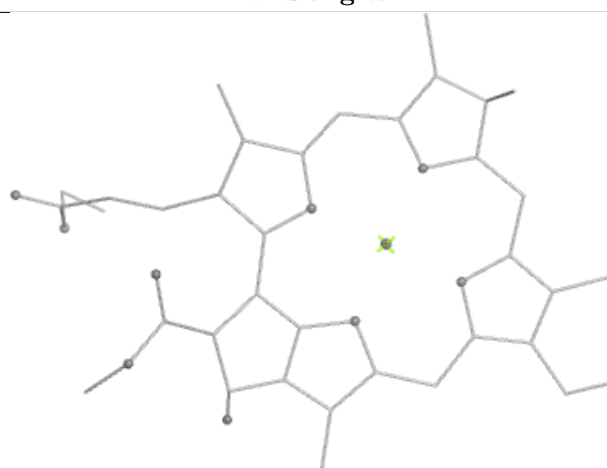
Bond lengths



Bond angles

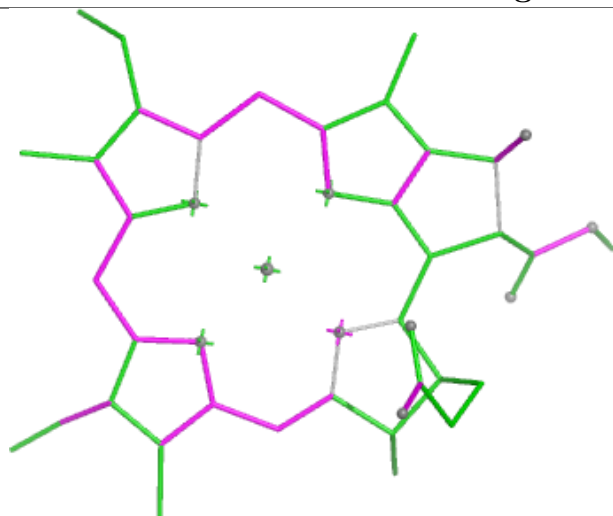


Torsions

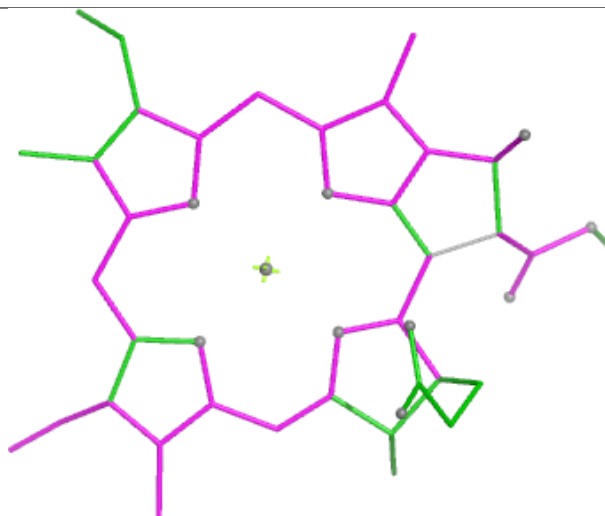


Rings

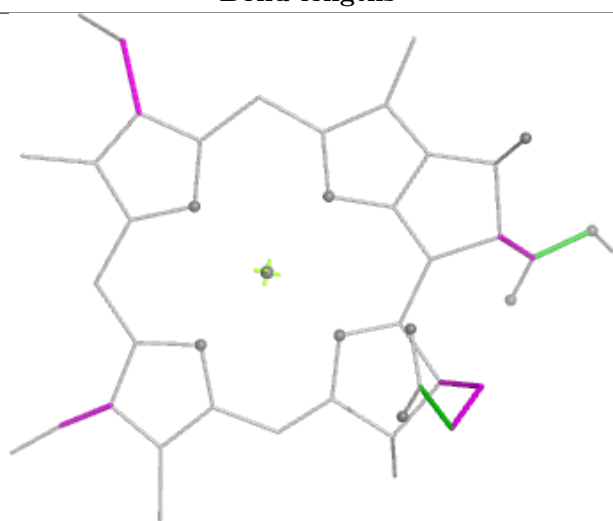
Ligand CLA B 804



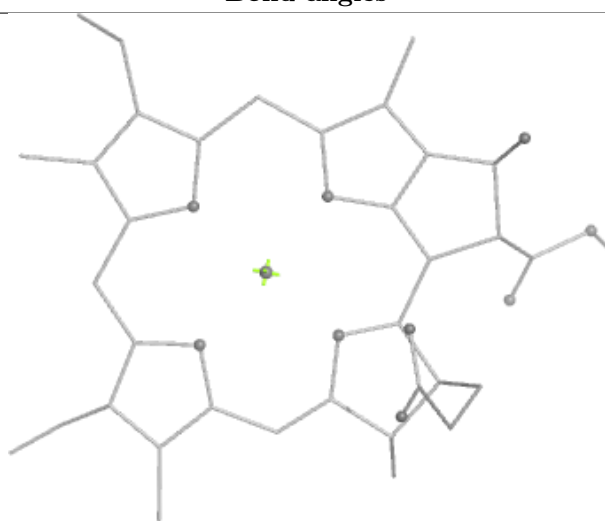
Bond lengths



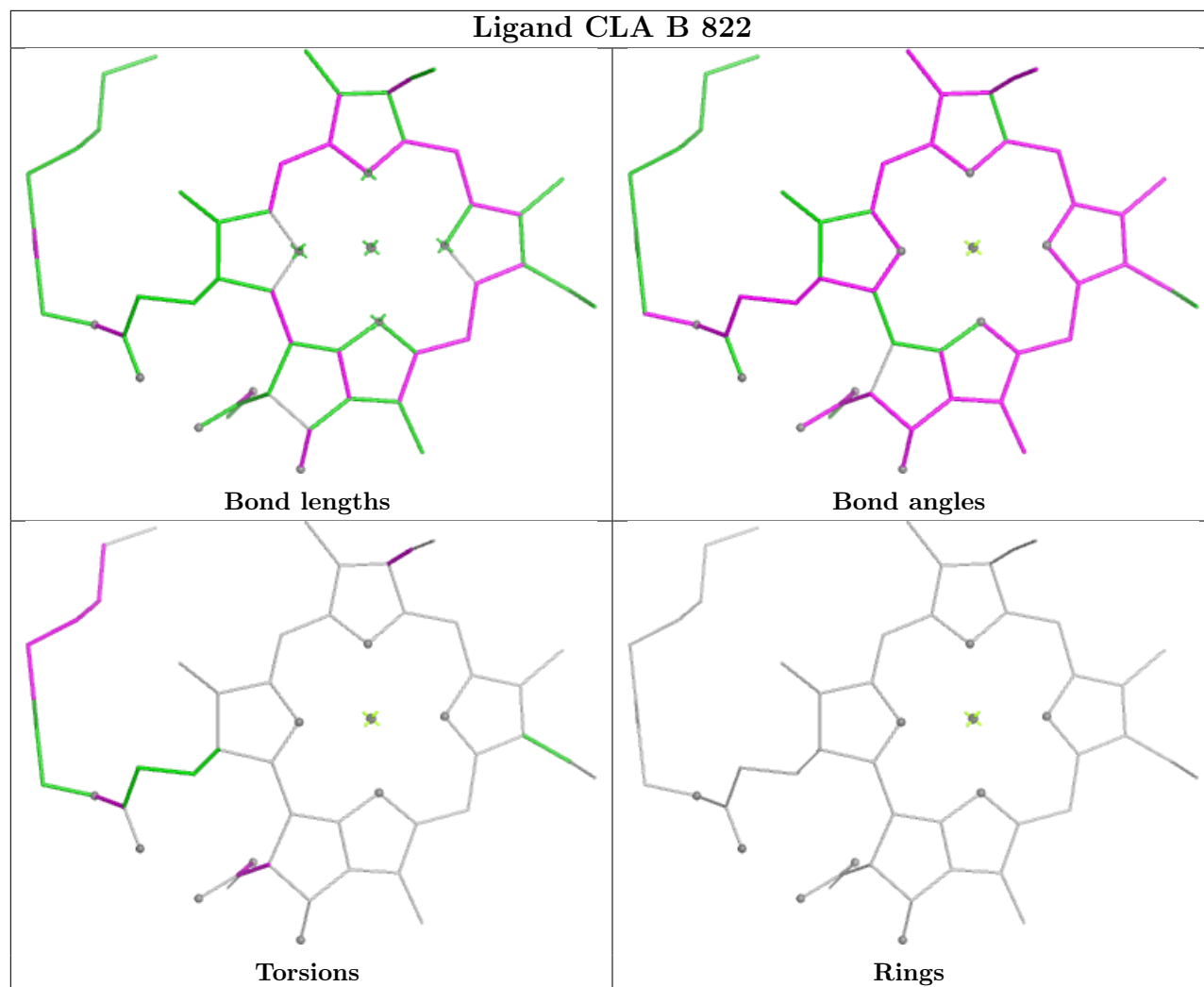
Bond angles

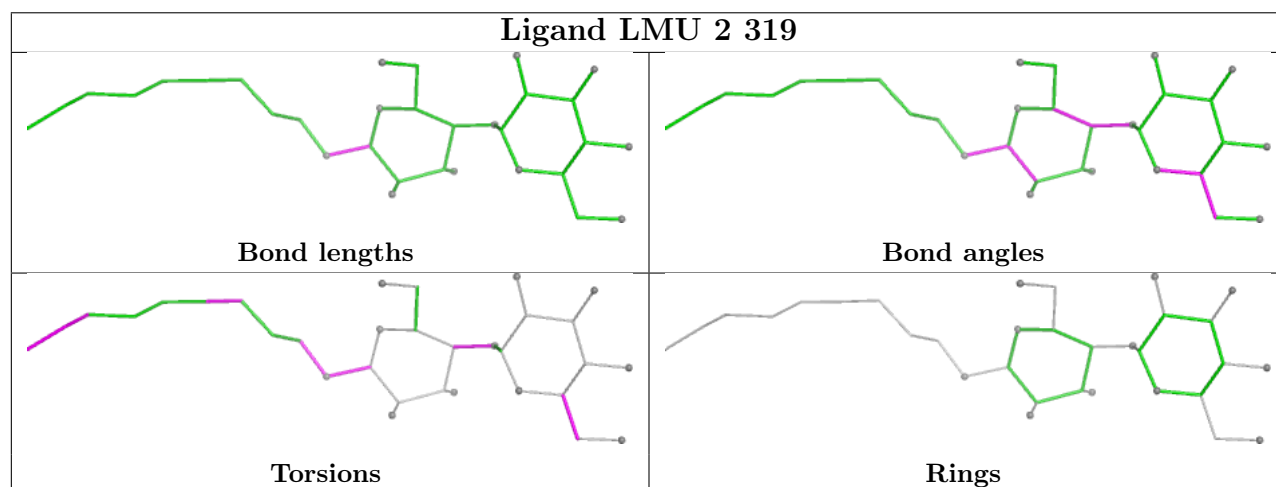
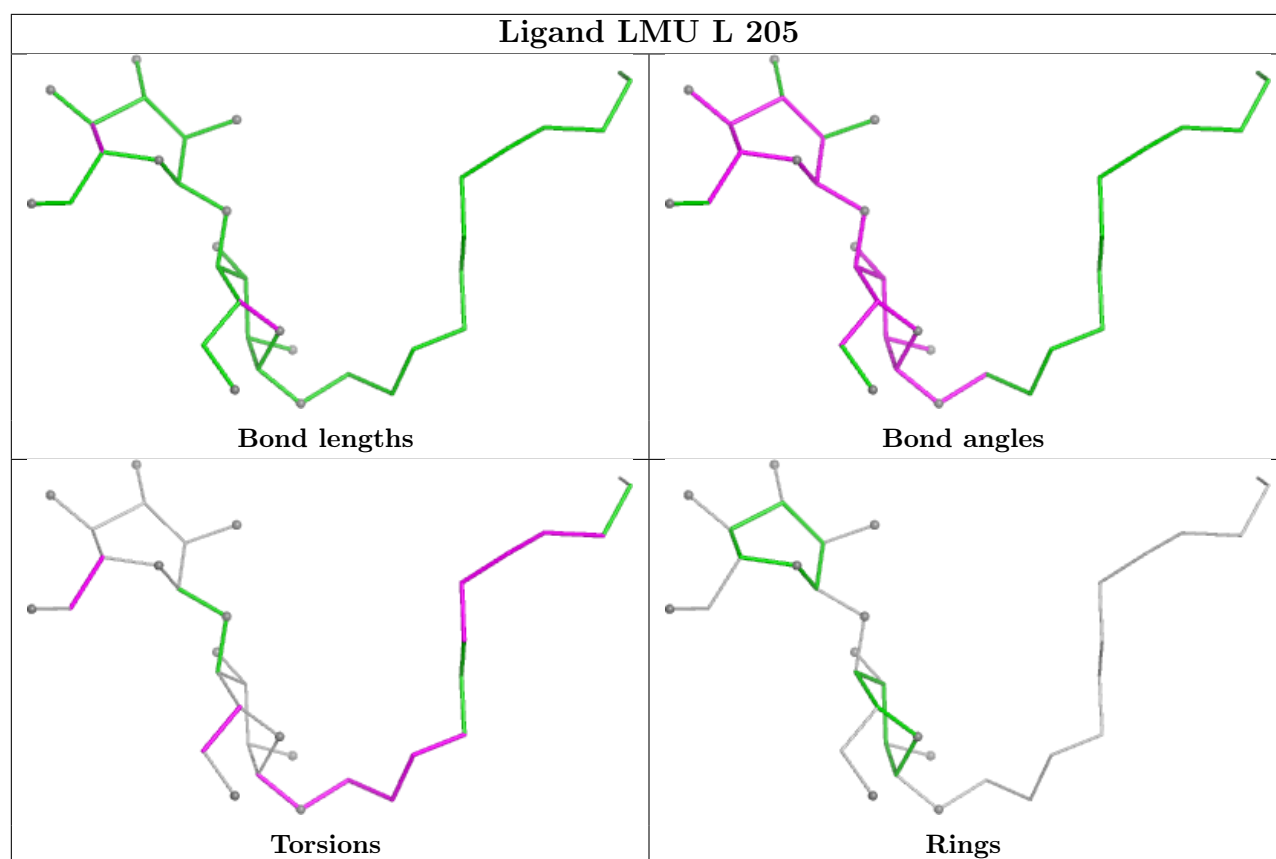


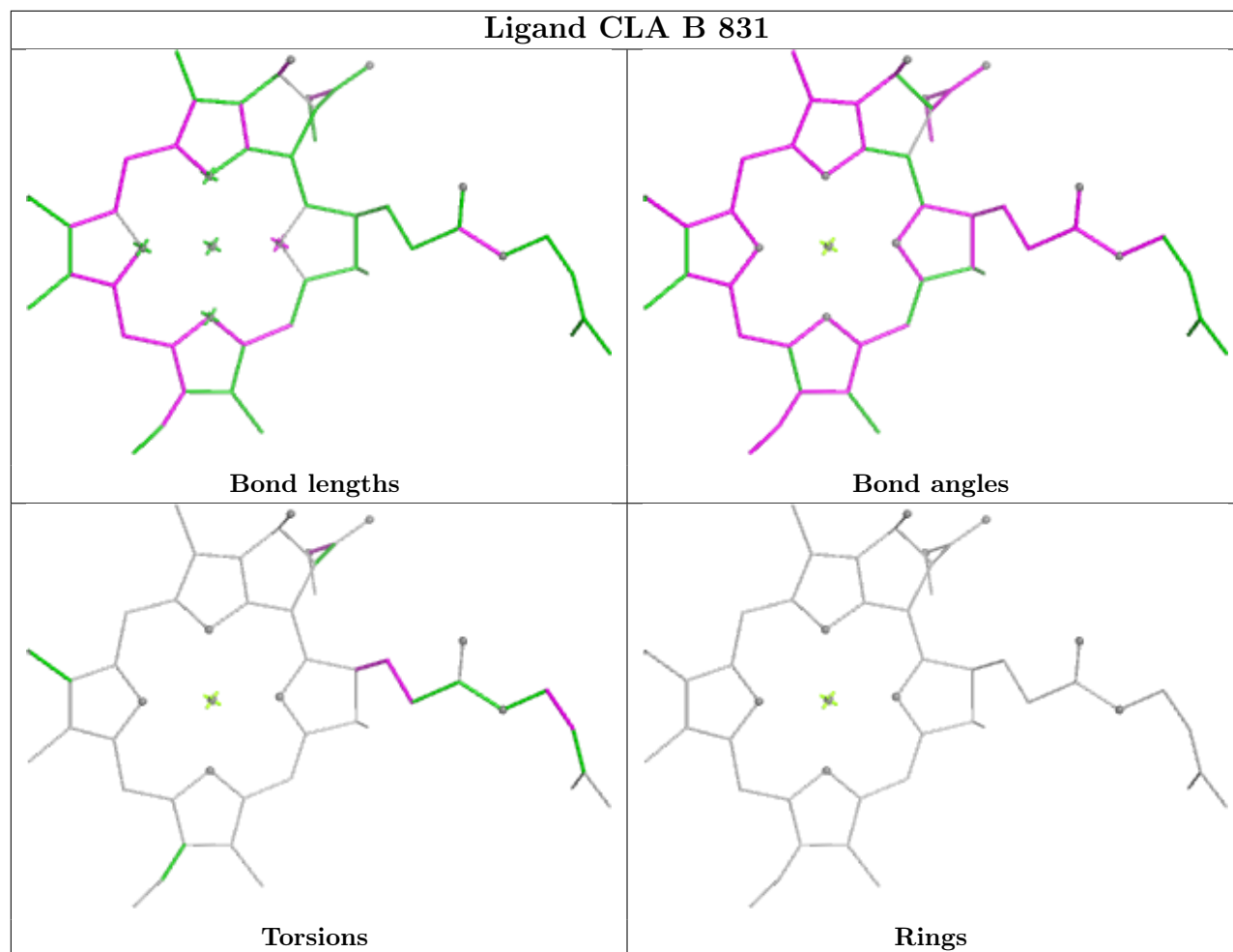
Torsions



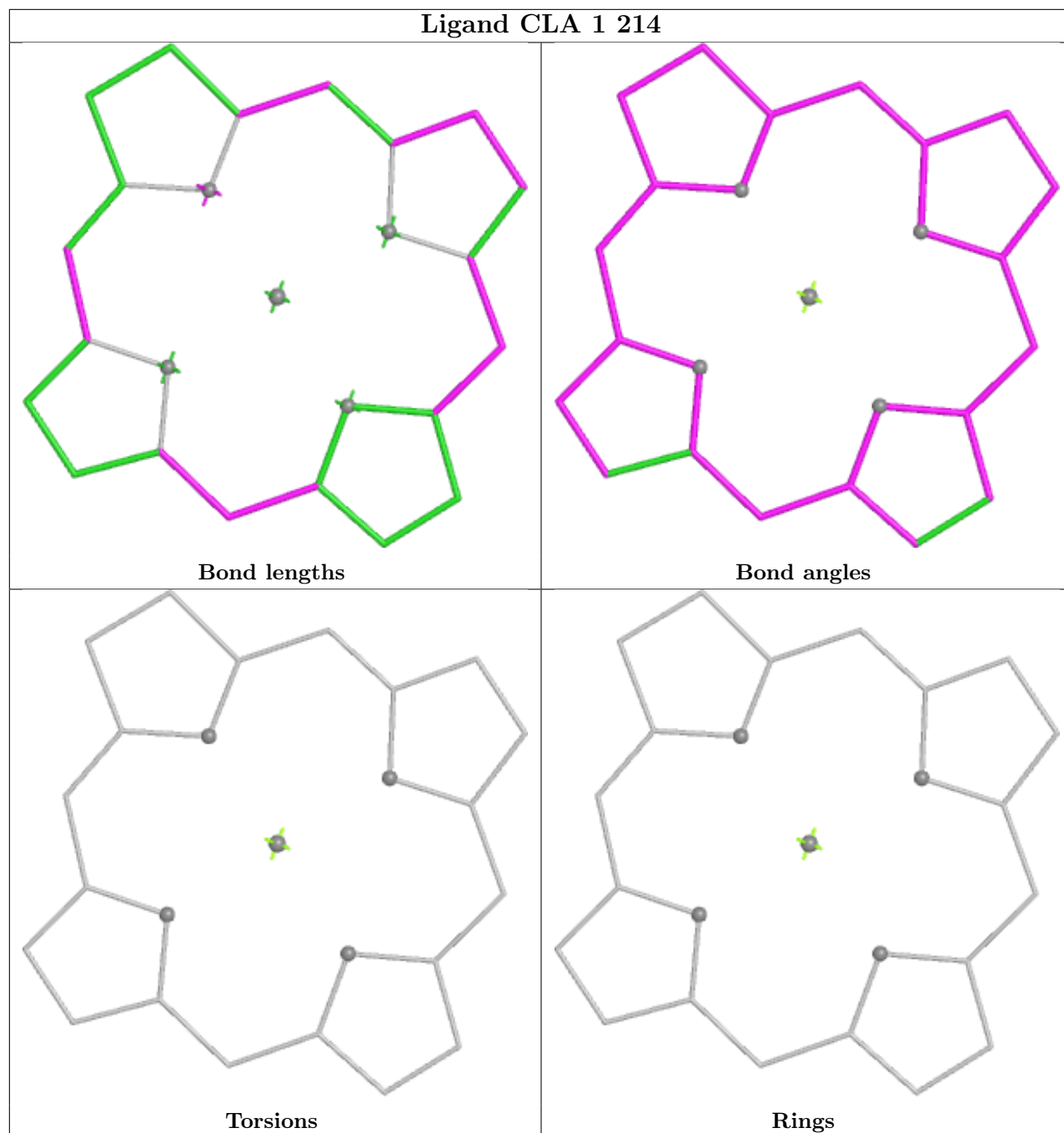
Rings



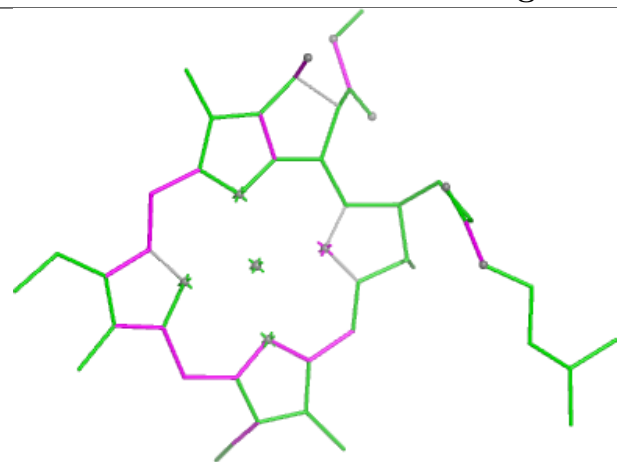




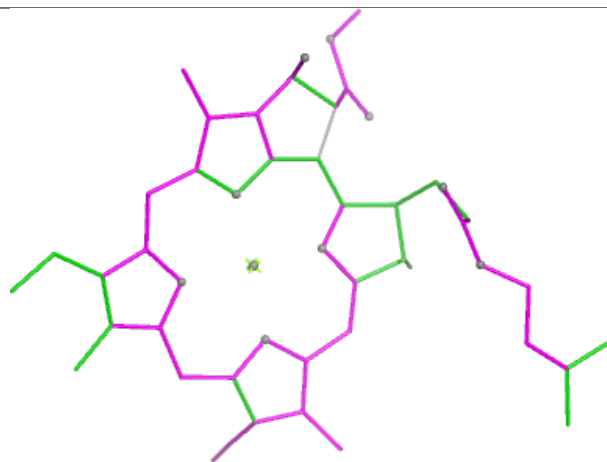
Ligand CLA 1 214



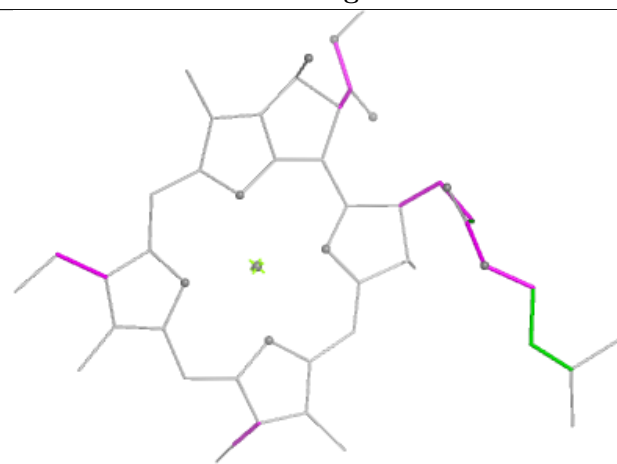
Ligand CLA A 832



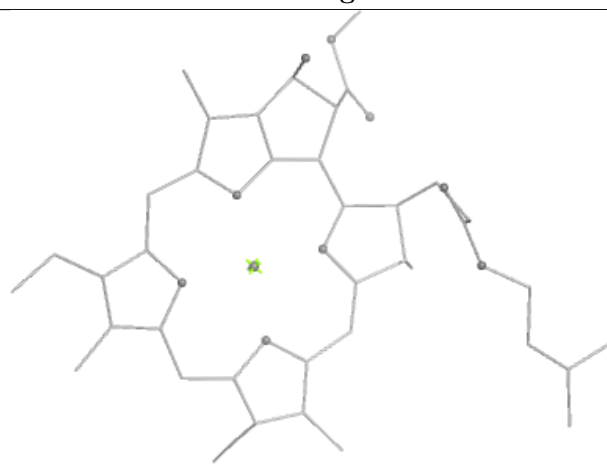
Bond lengths



Bond angles

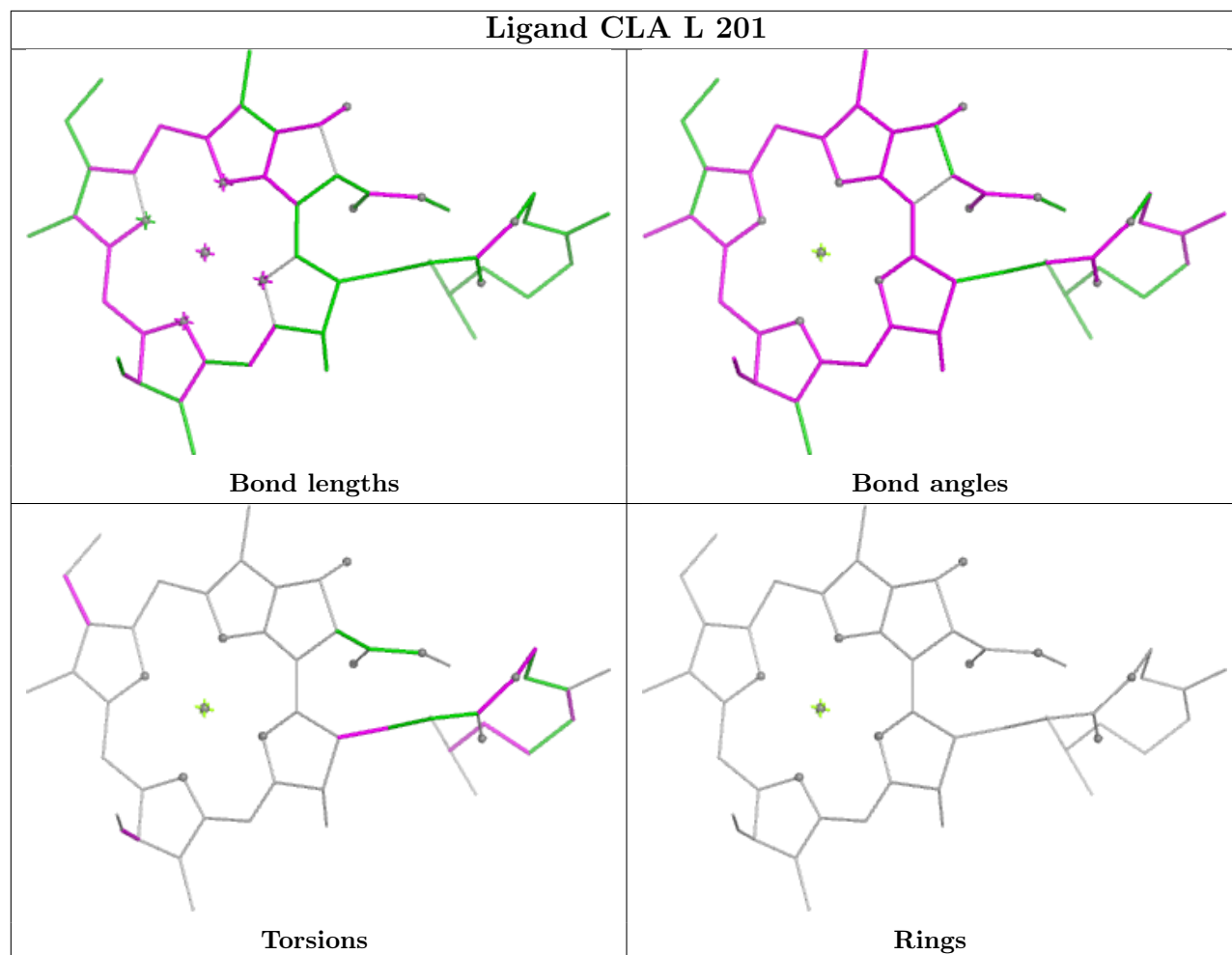


Torsions

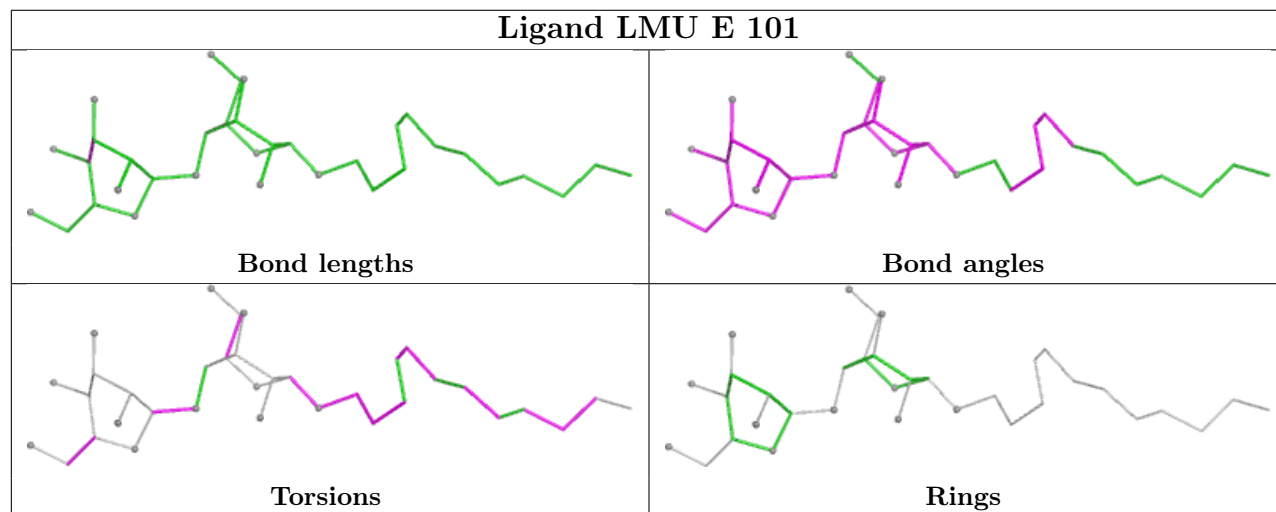


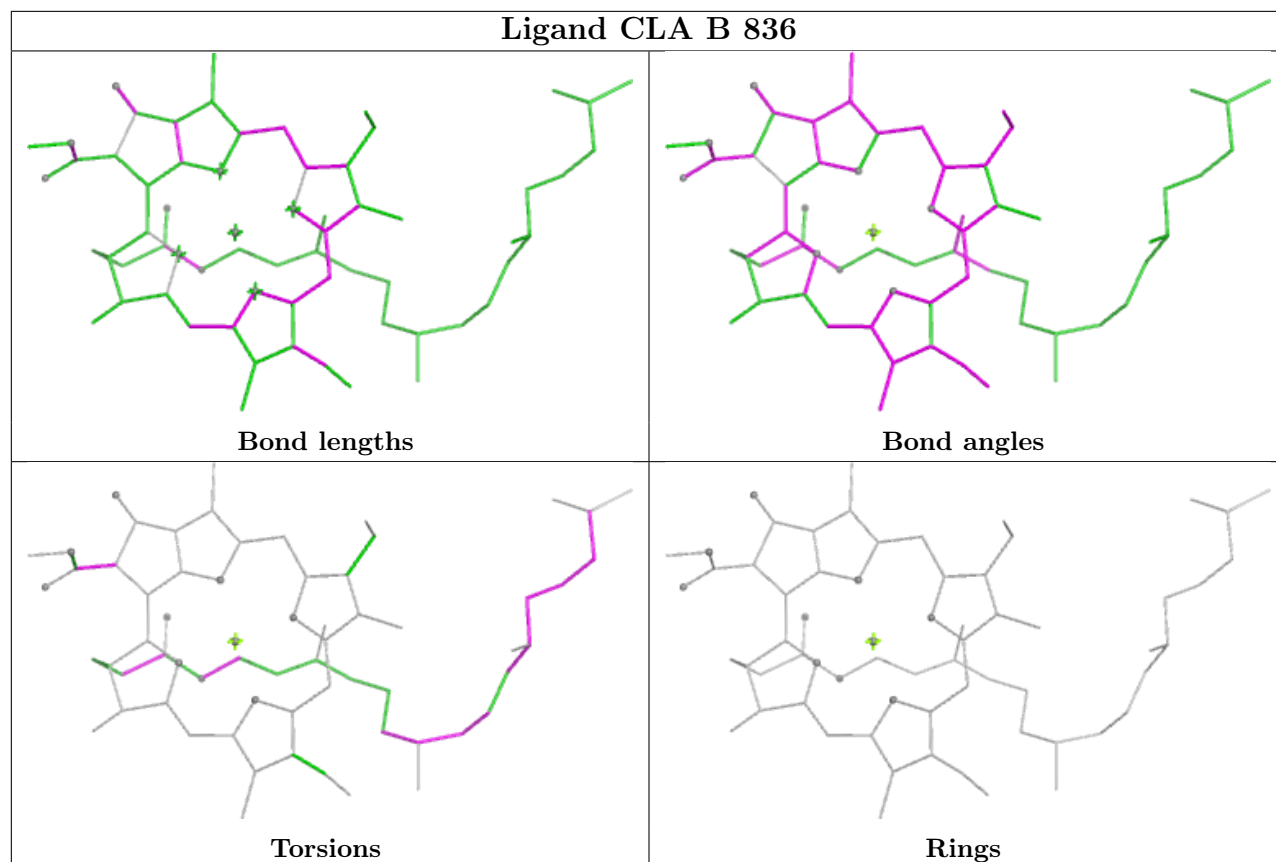
Rings

Ligand CLA L 201

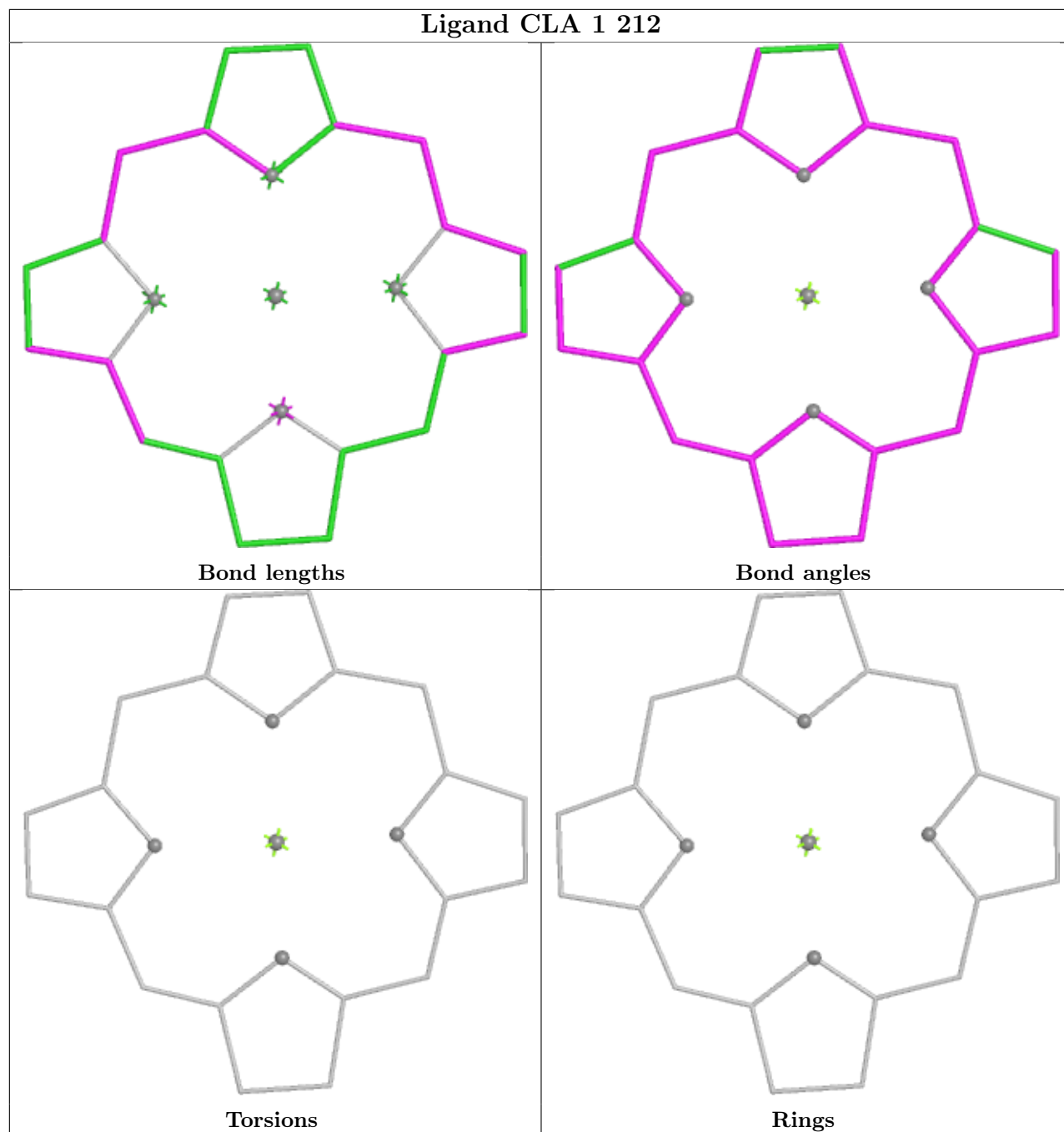


Ligand LMU E 101

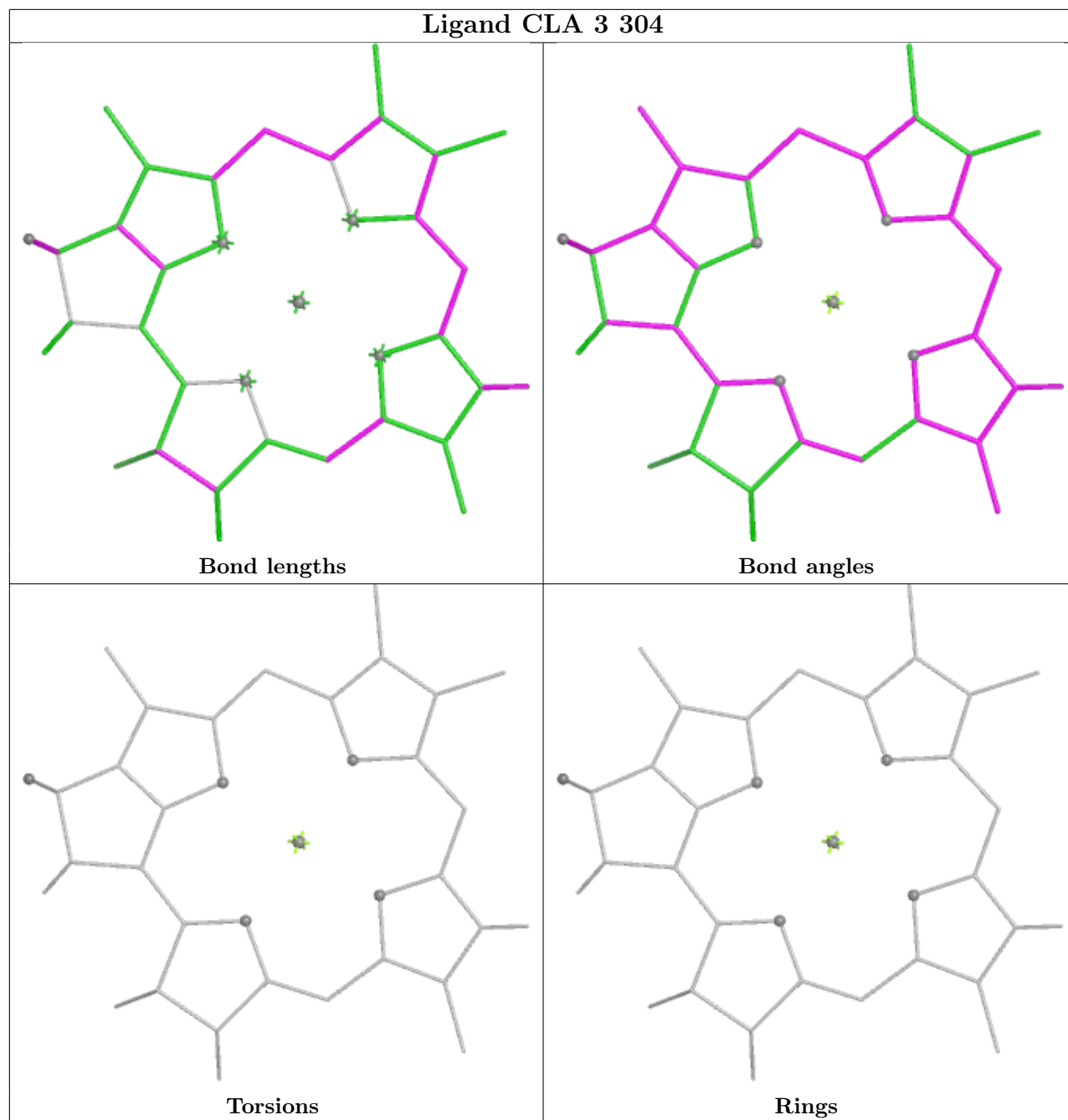




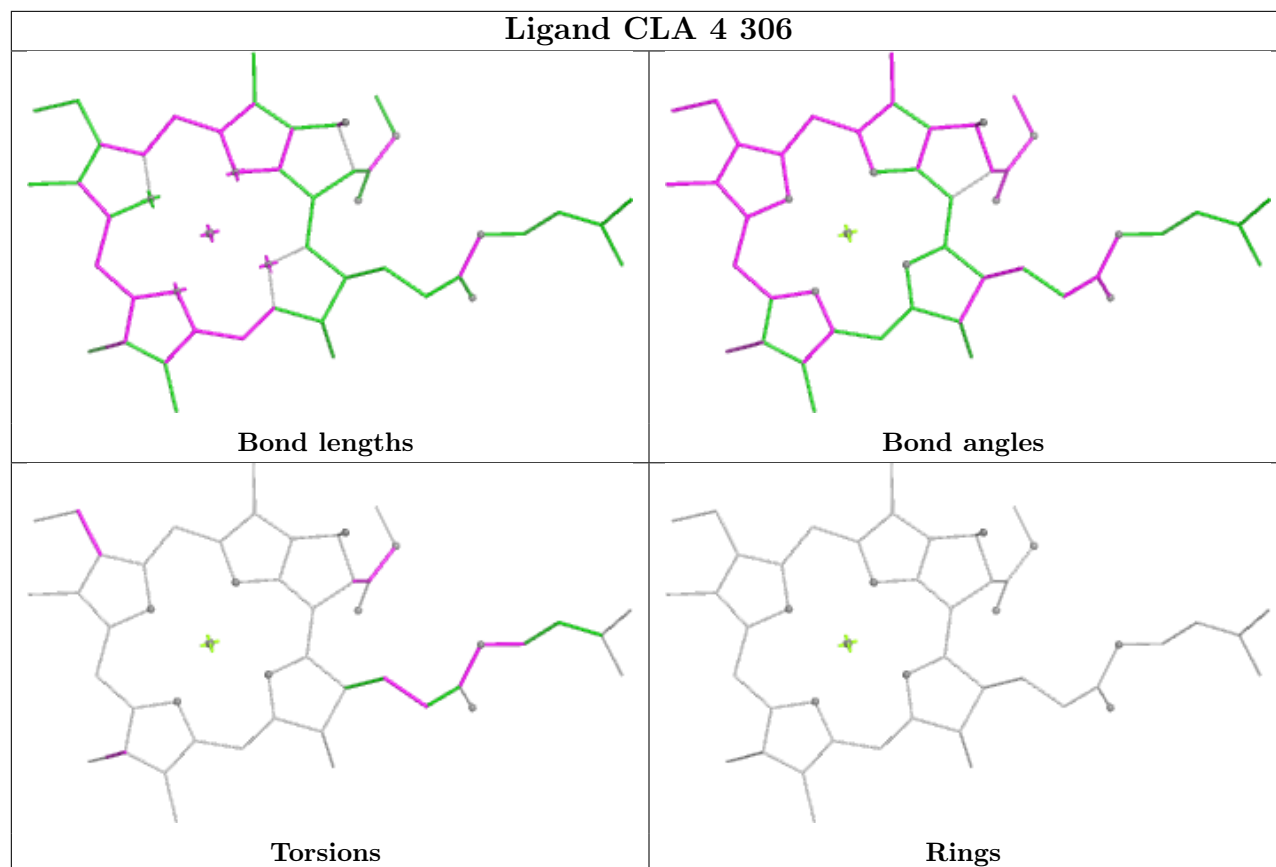
Ligand CLA 1 212



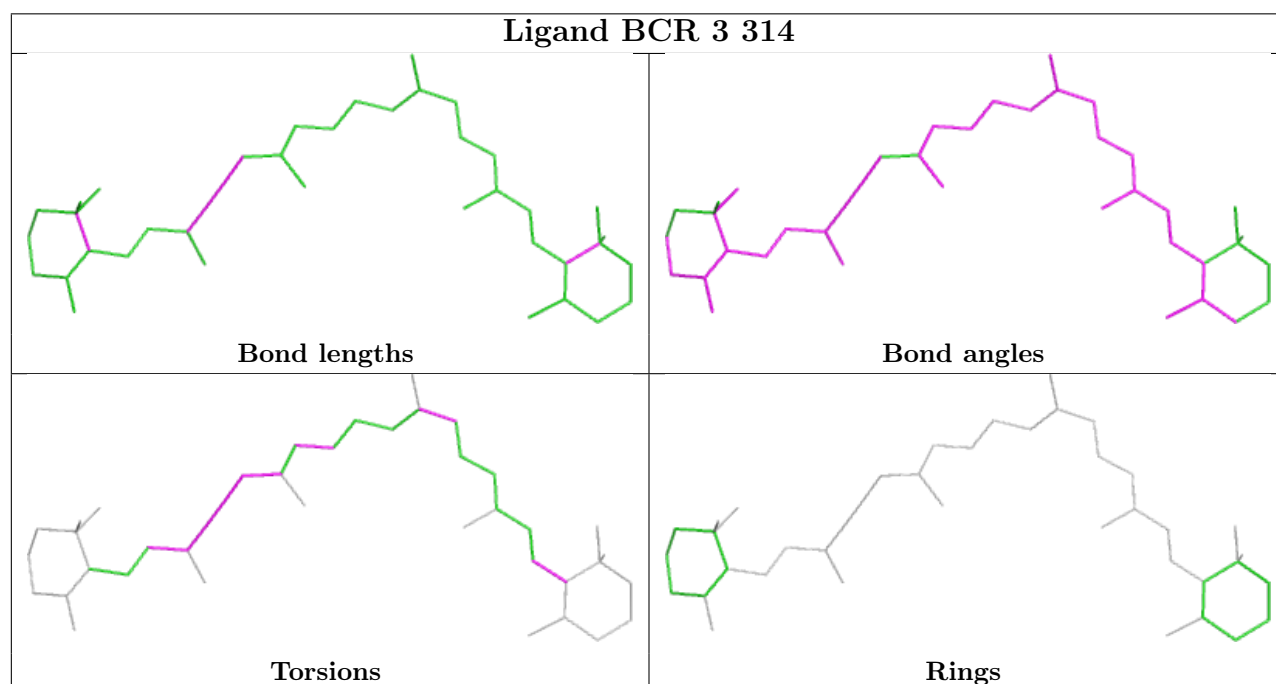
Ligand CLA 3 304



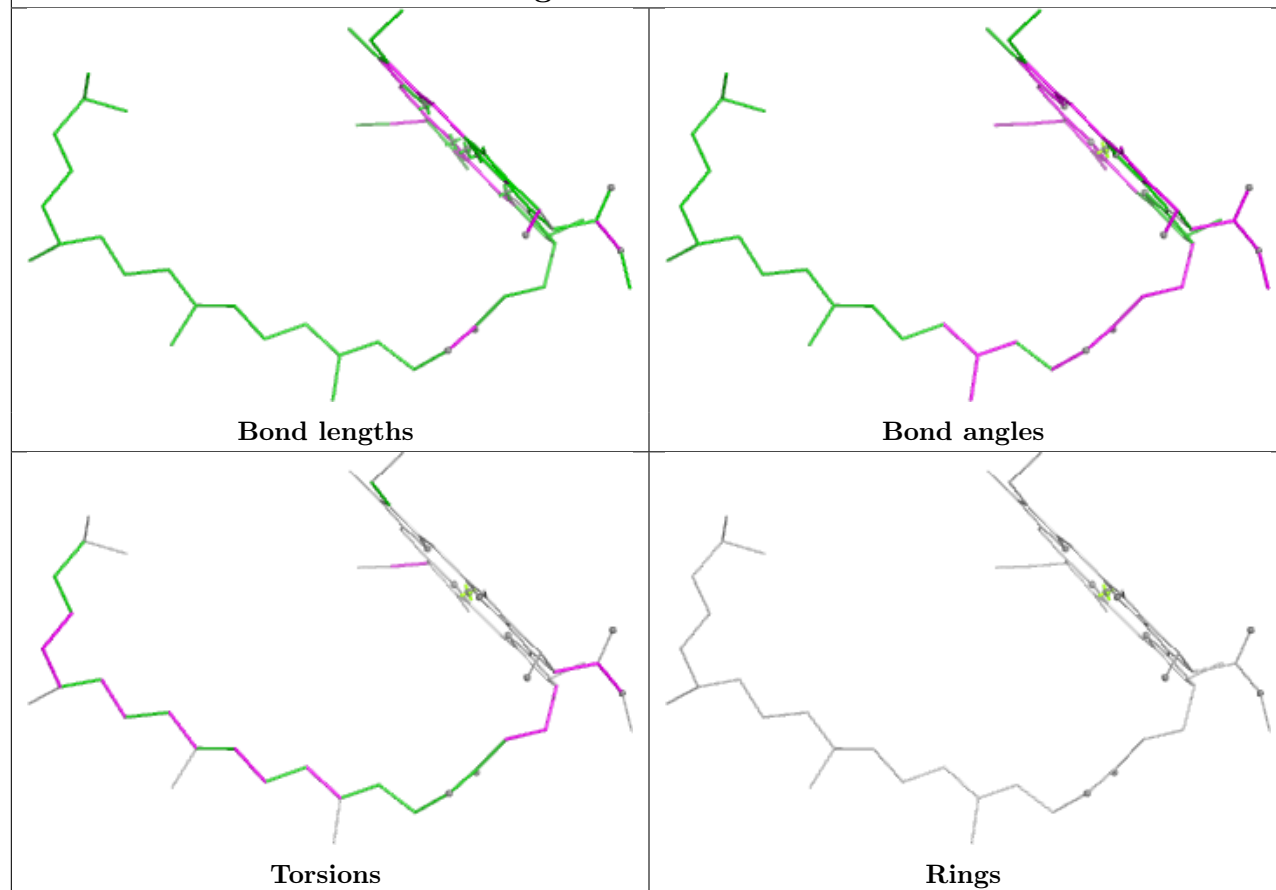
Ligand CLA 4 306



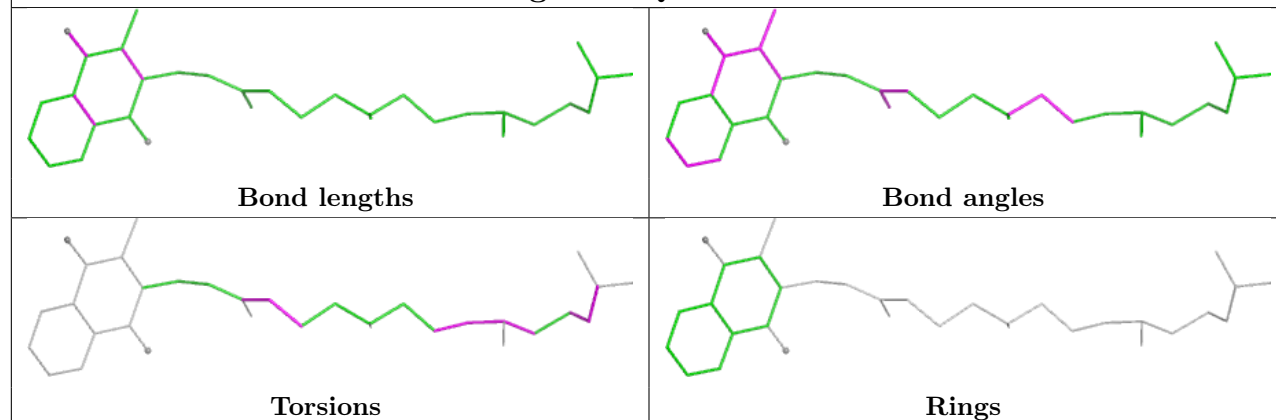
Ligand BCR 3 314

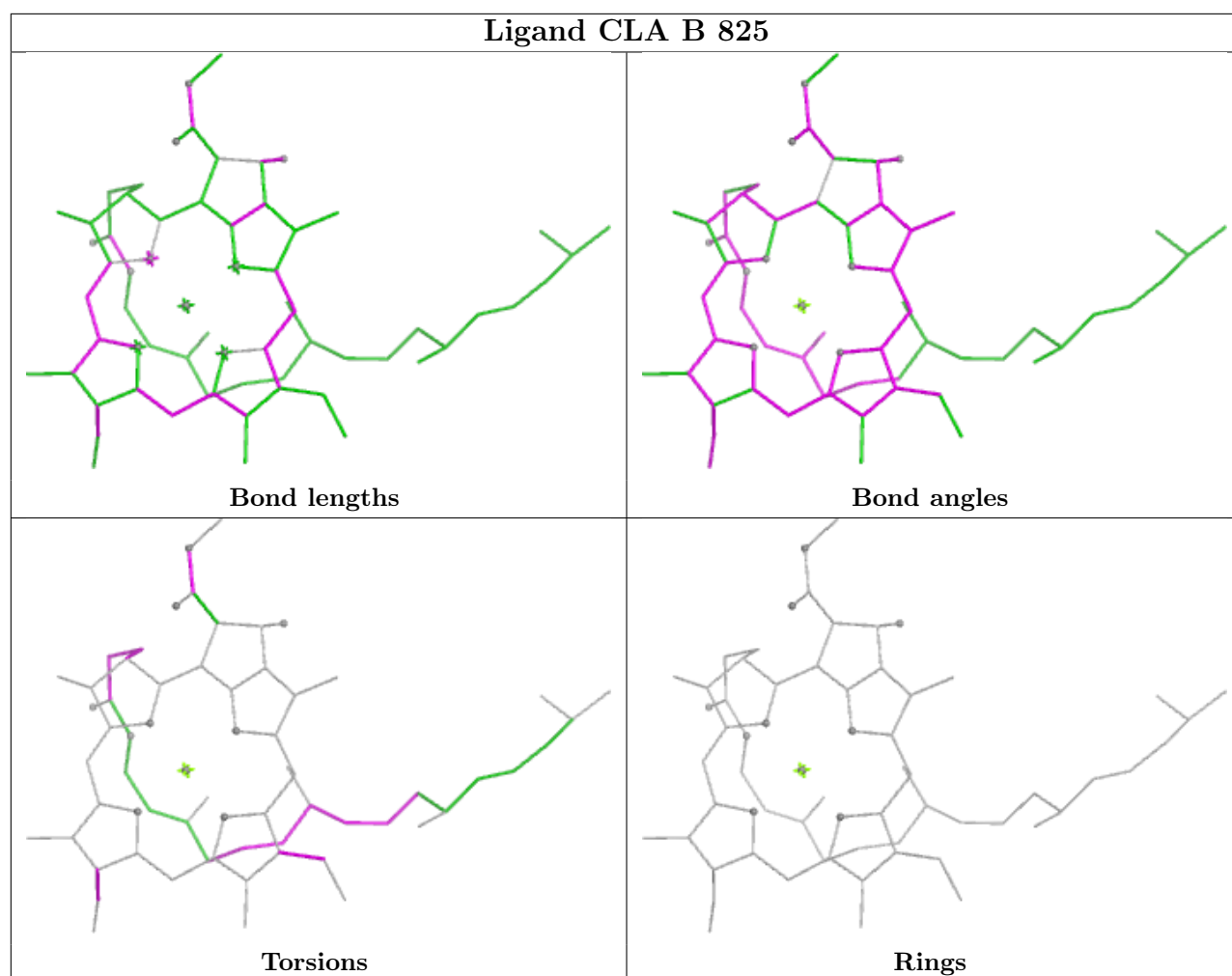


Ligand CLA L 202

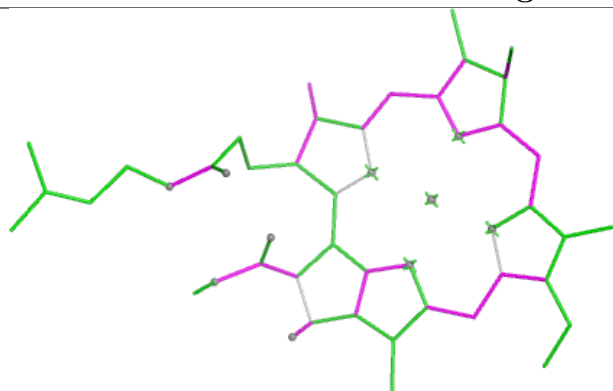


Ligand PQN A 842

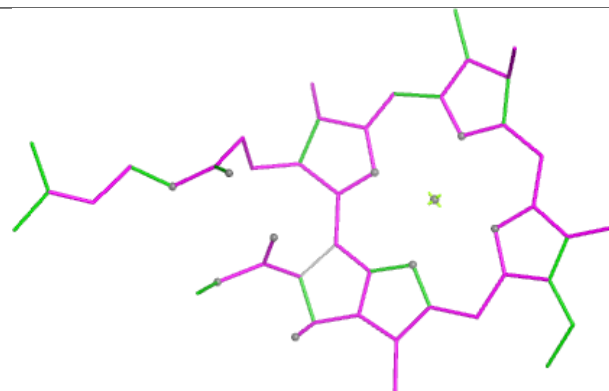




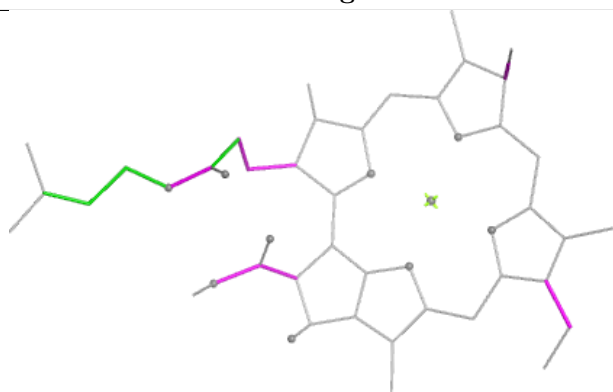
Ligand CLA L 207



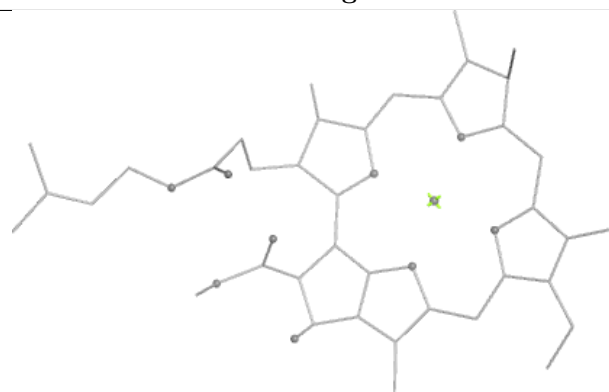
Bond lengths



Bond angles

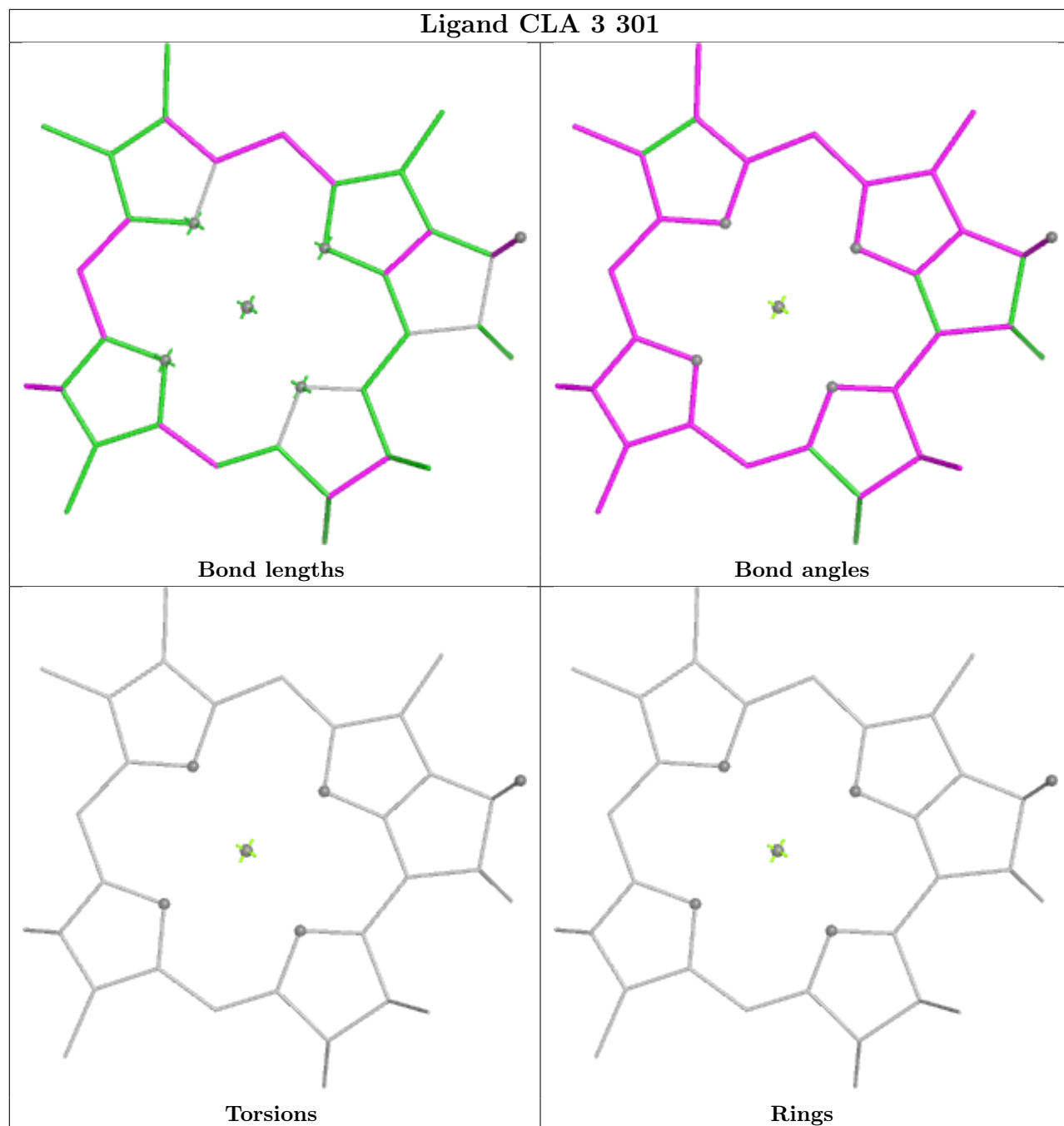


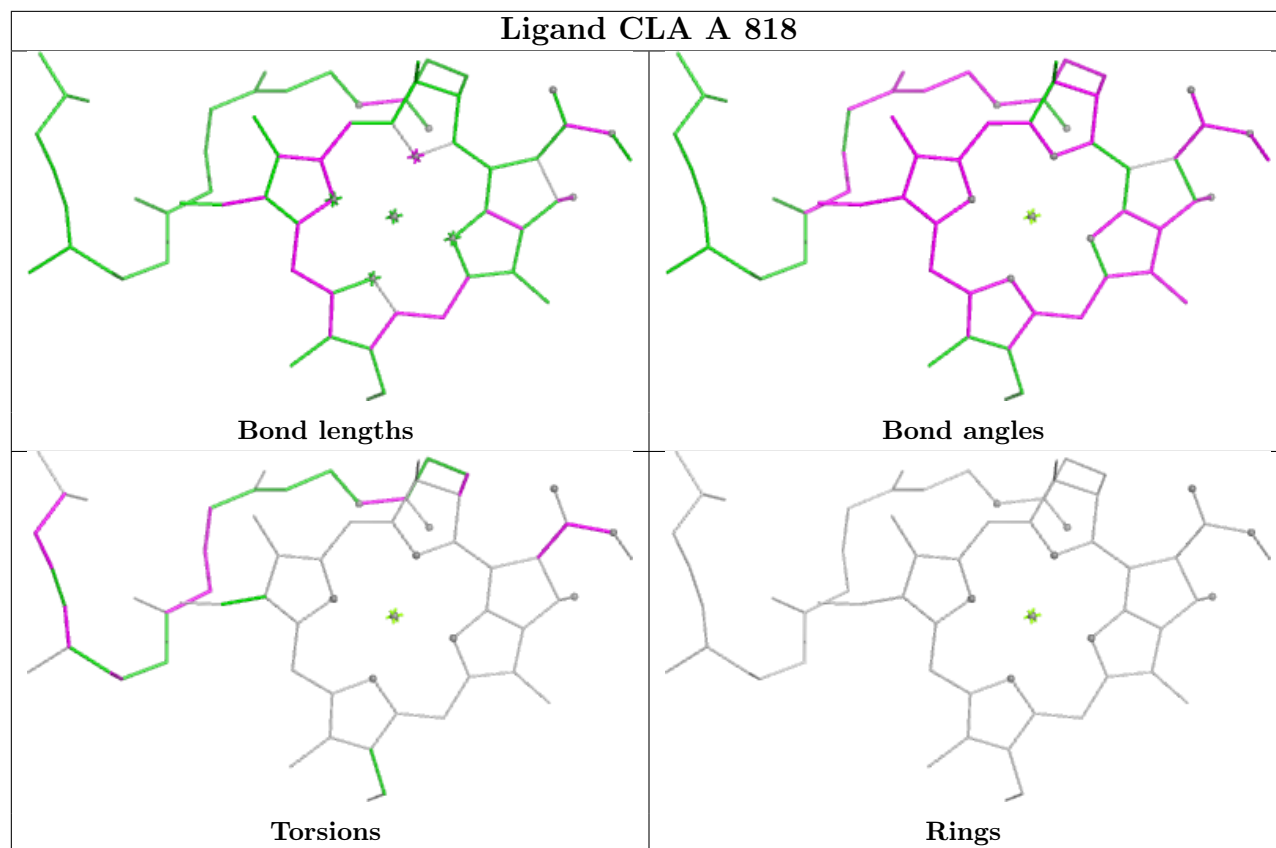
Torsions



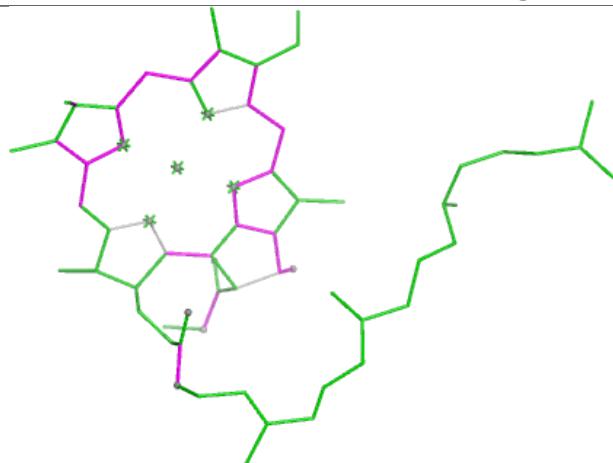
Rings

Ligand CLA 3 301

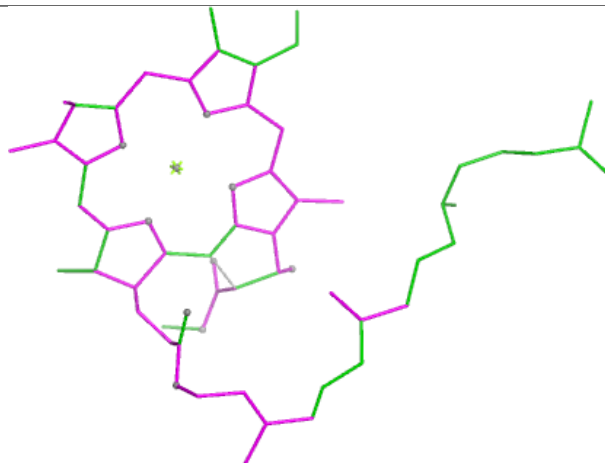




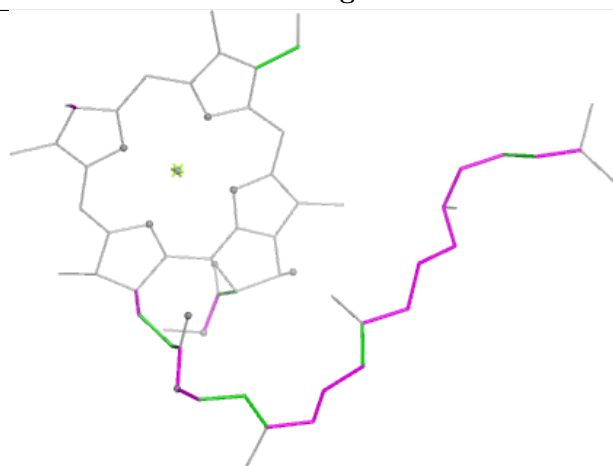
Ligand CLA B 830



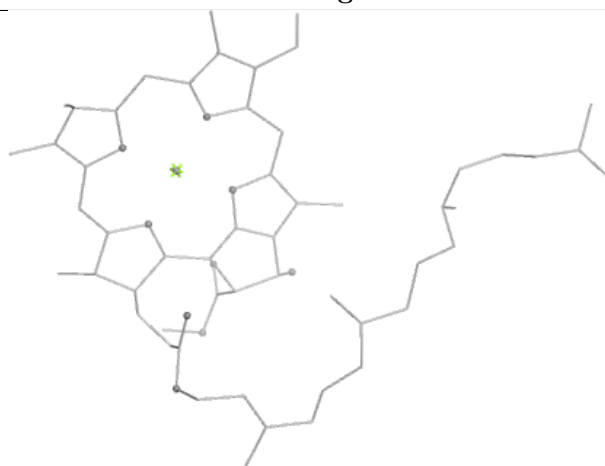
Bond lengths



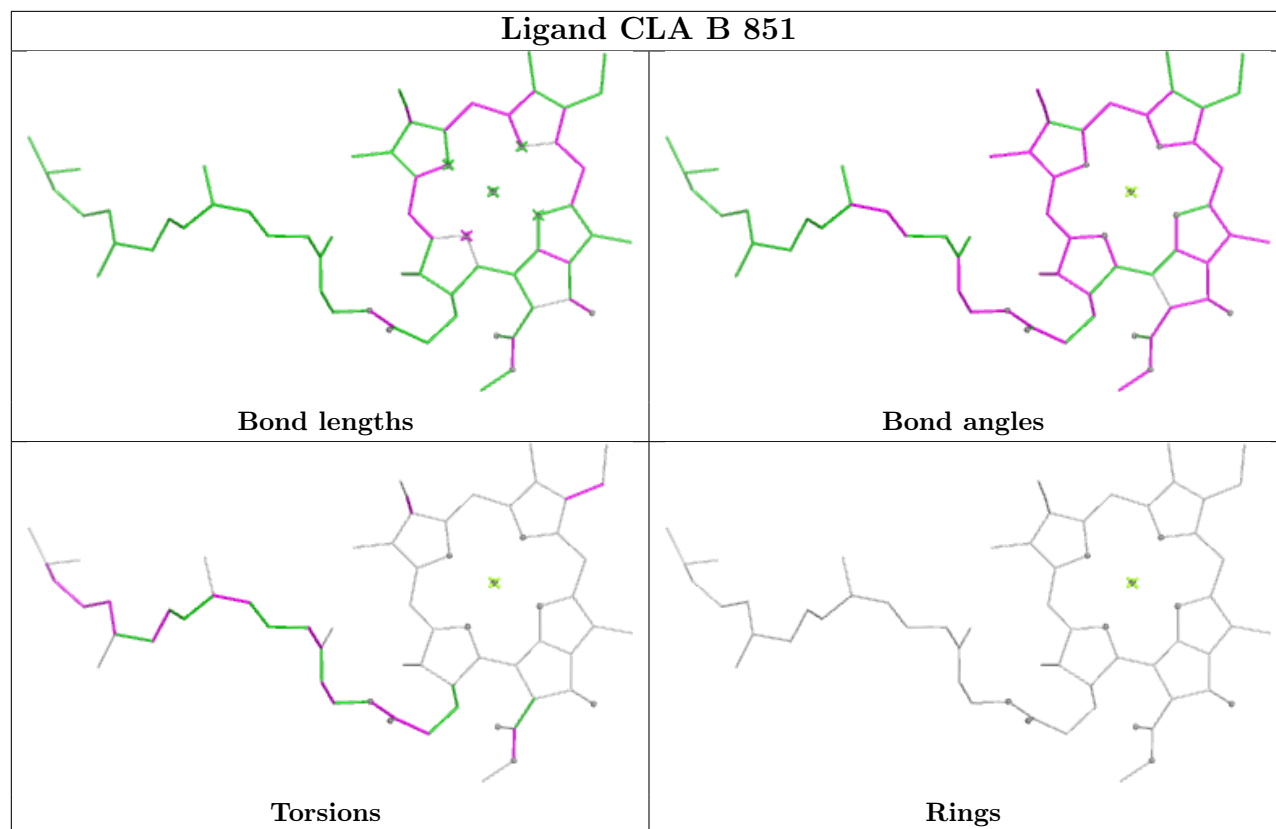
Bond angles

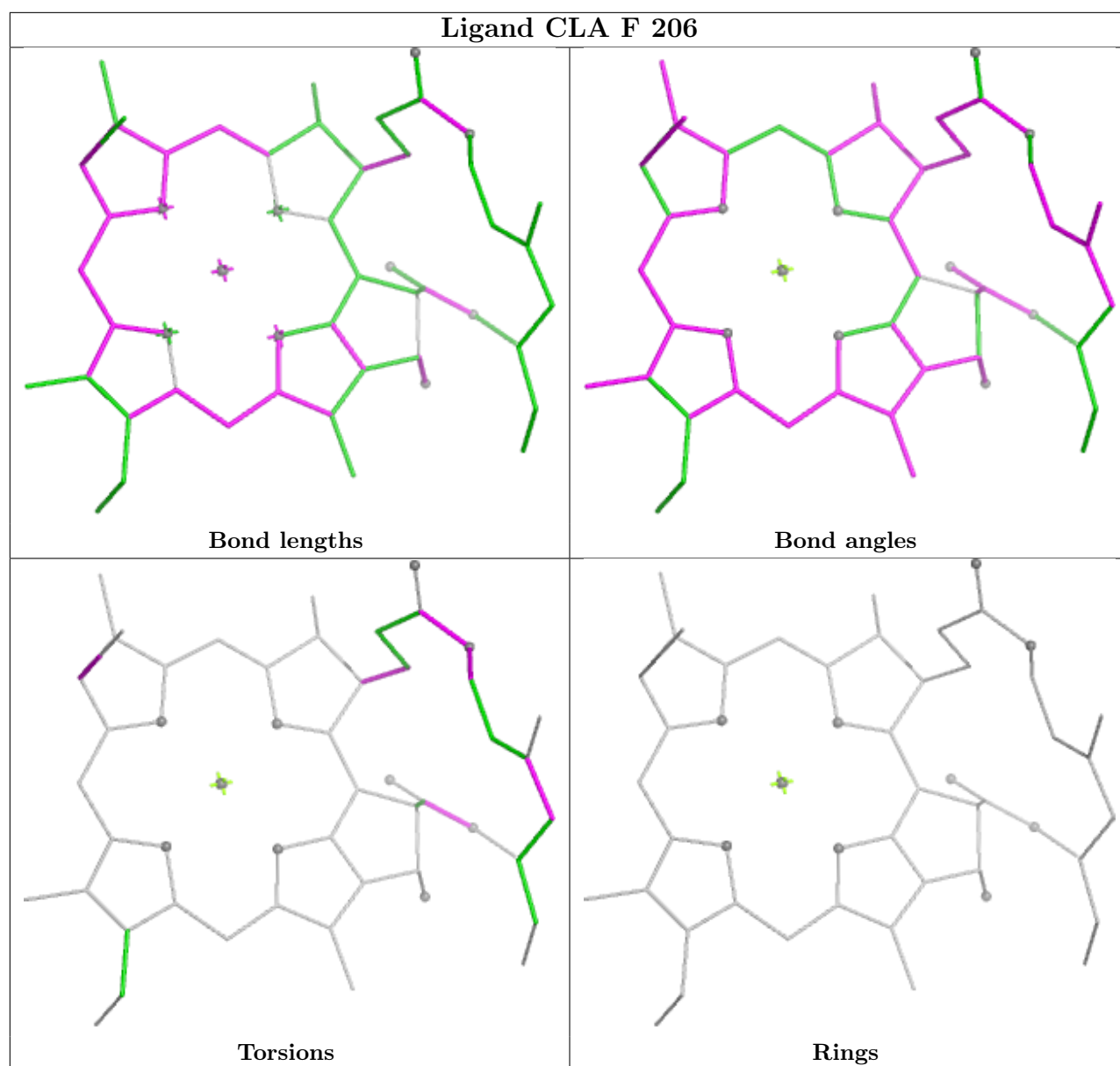


Torsions

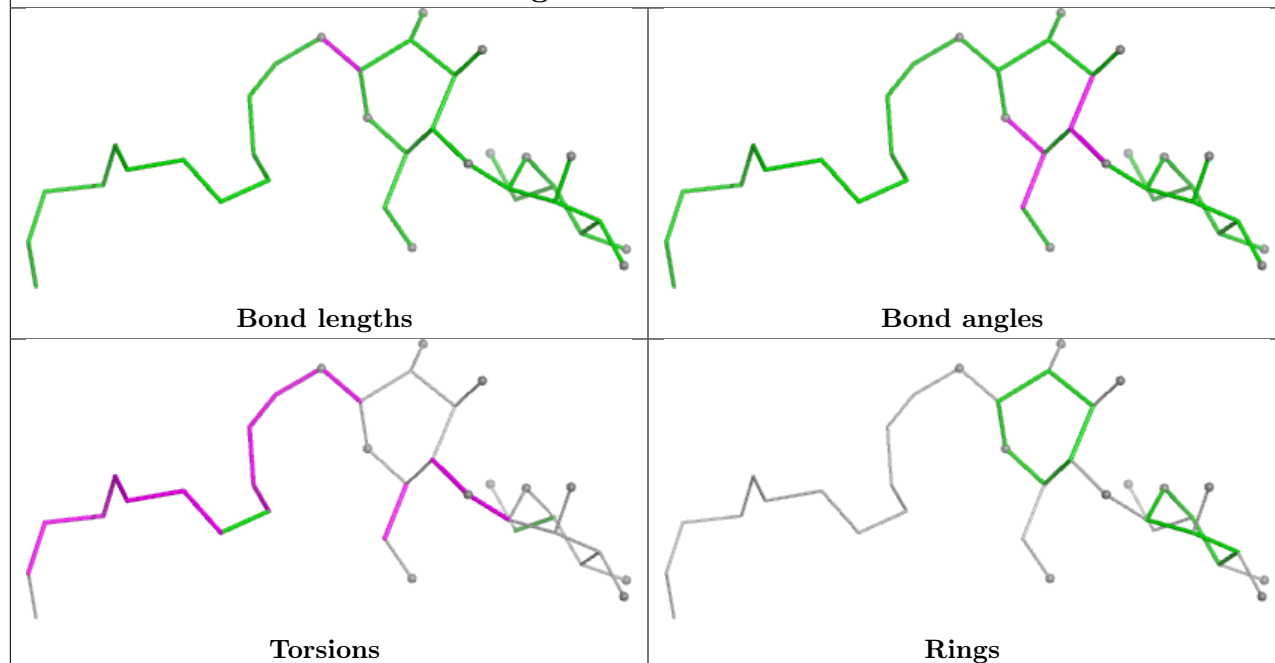


Rings

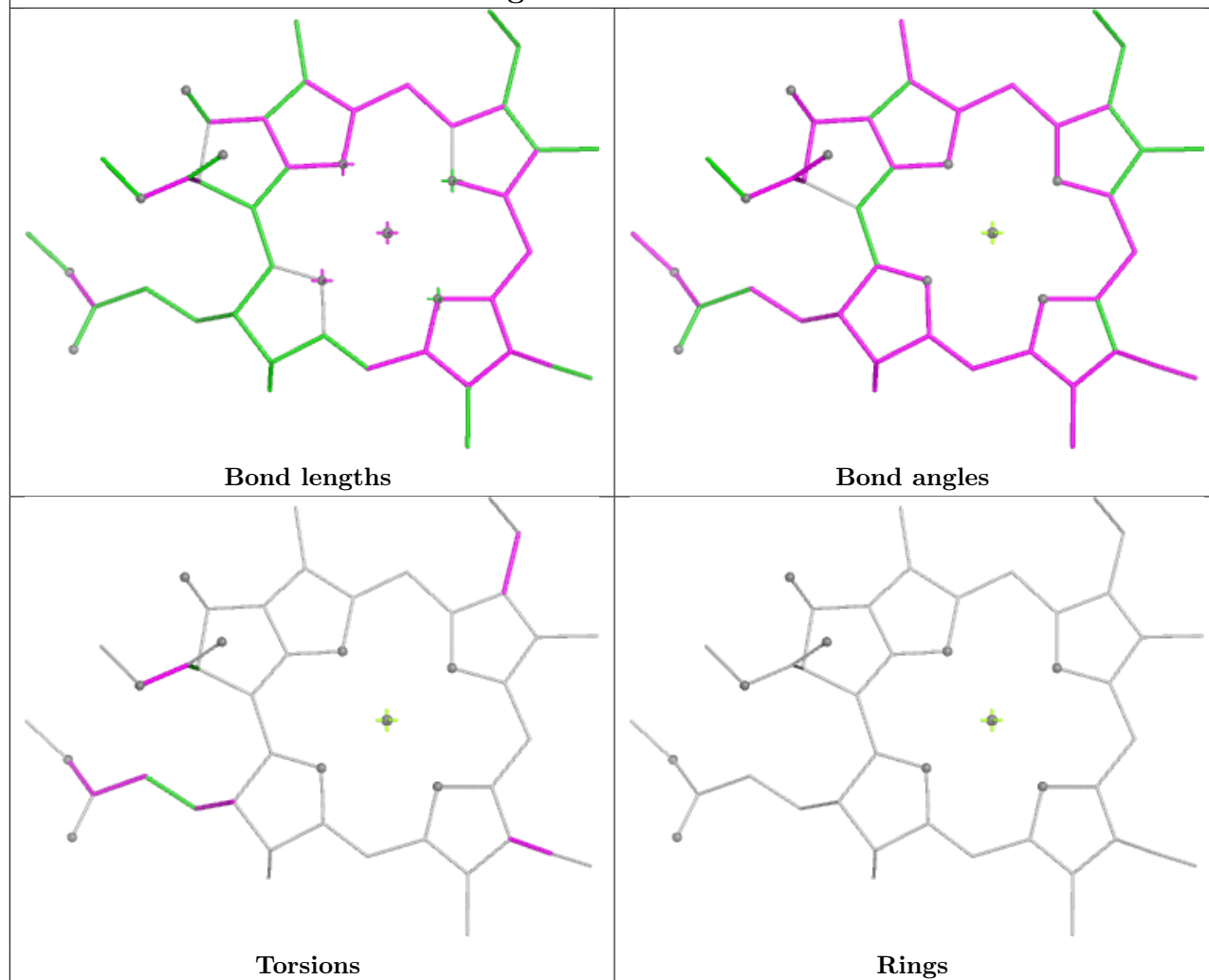


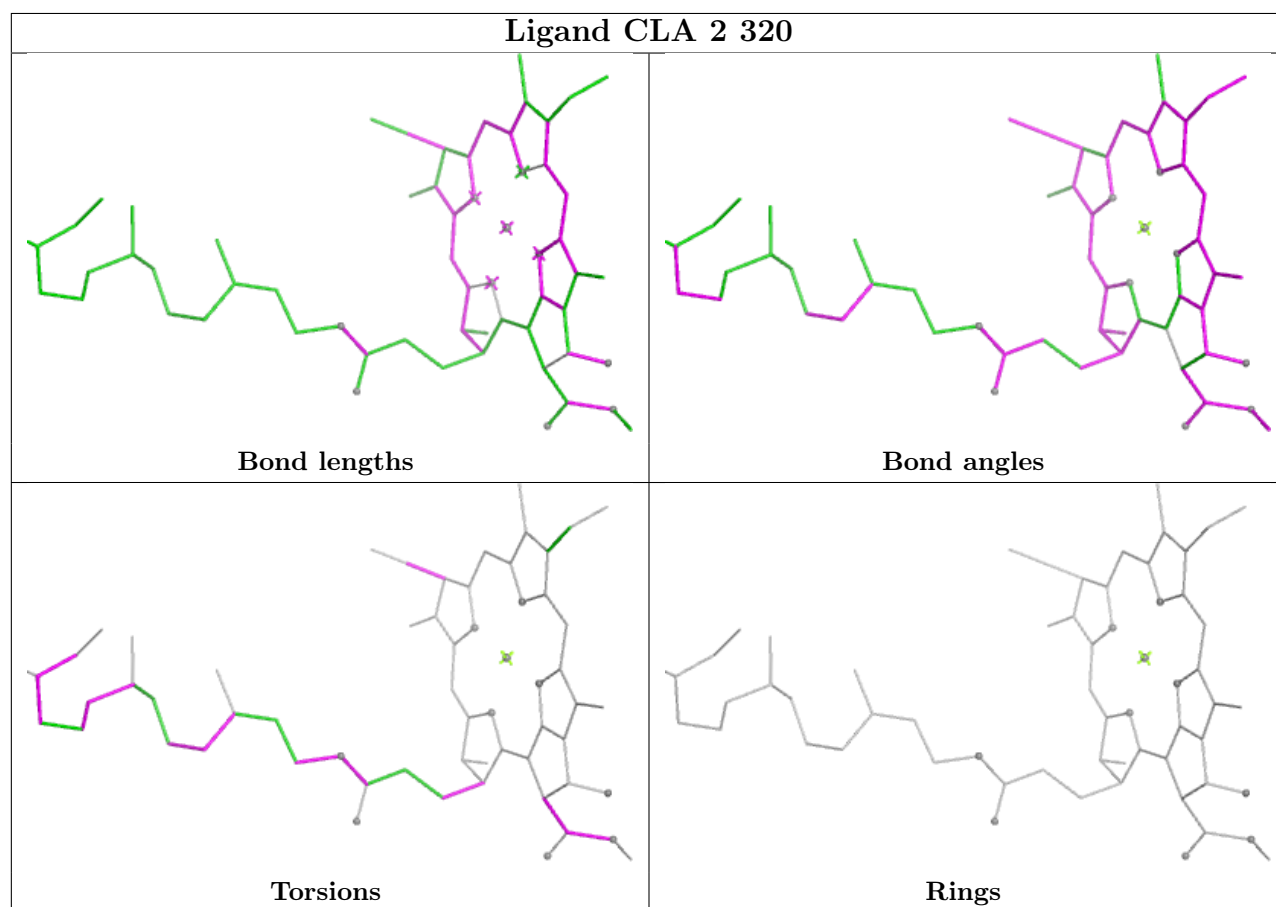
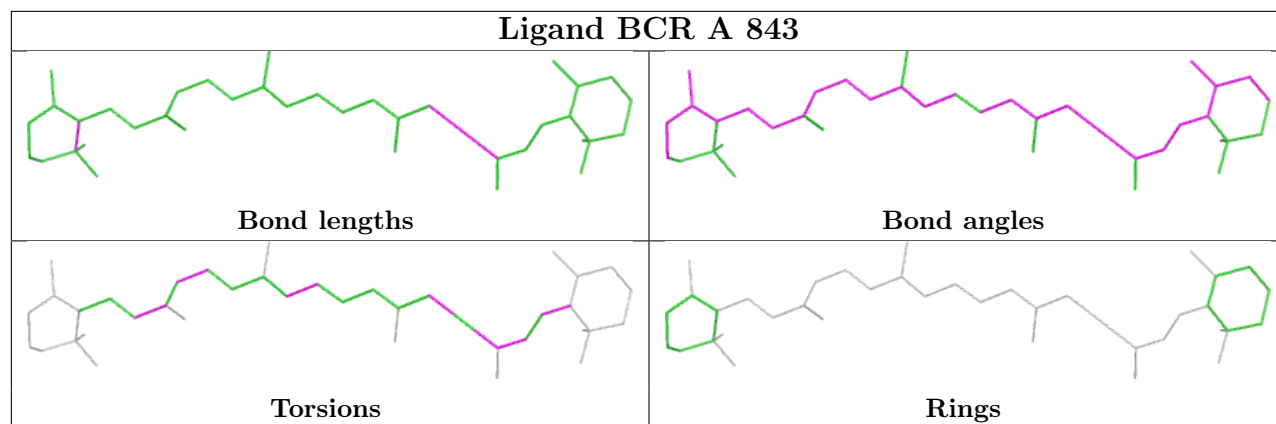


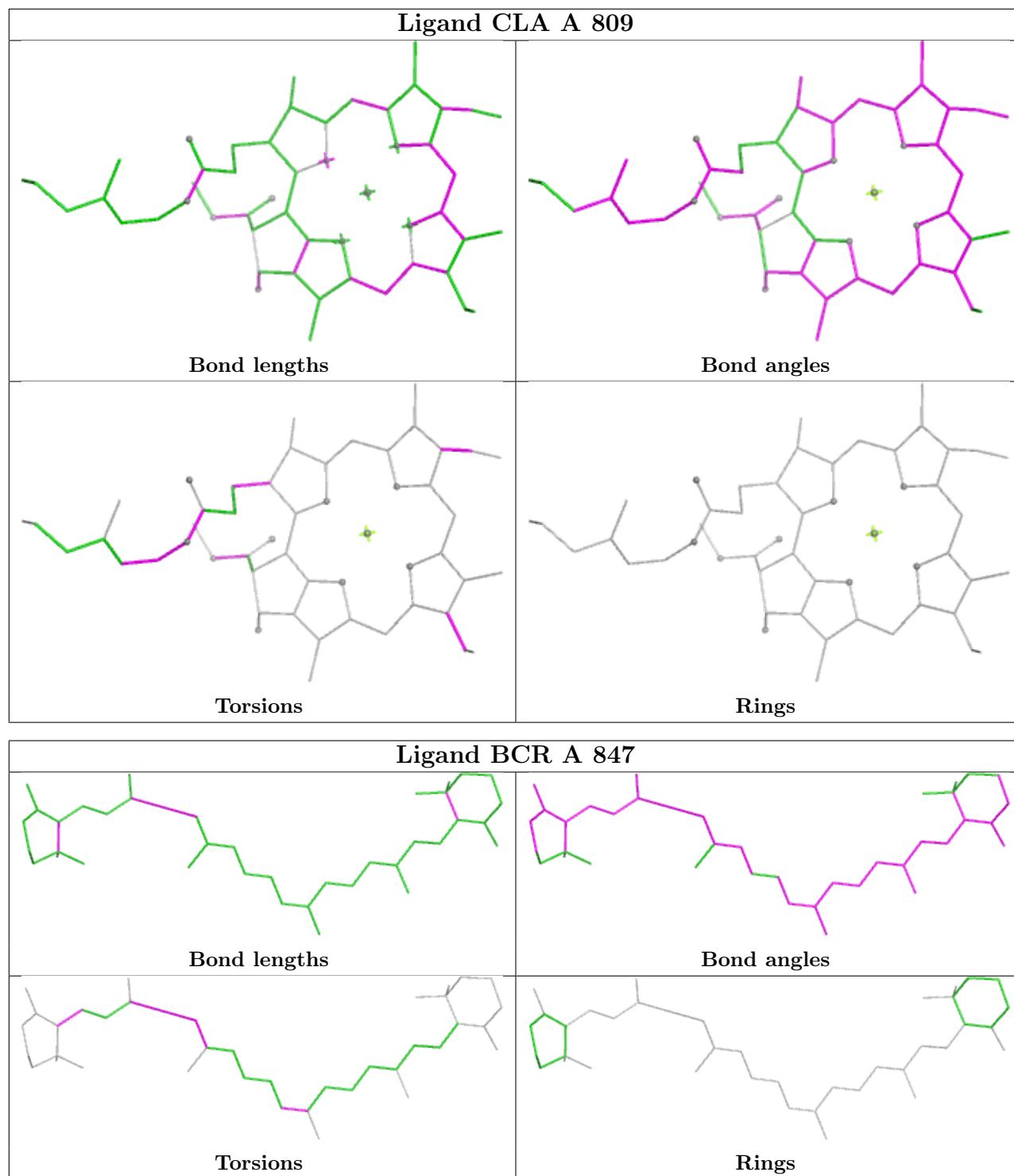
Ligand LMU 2 313

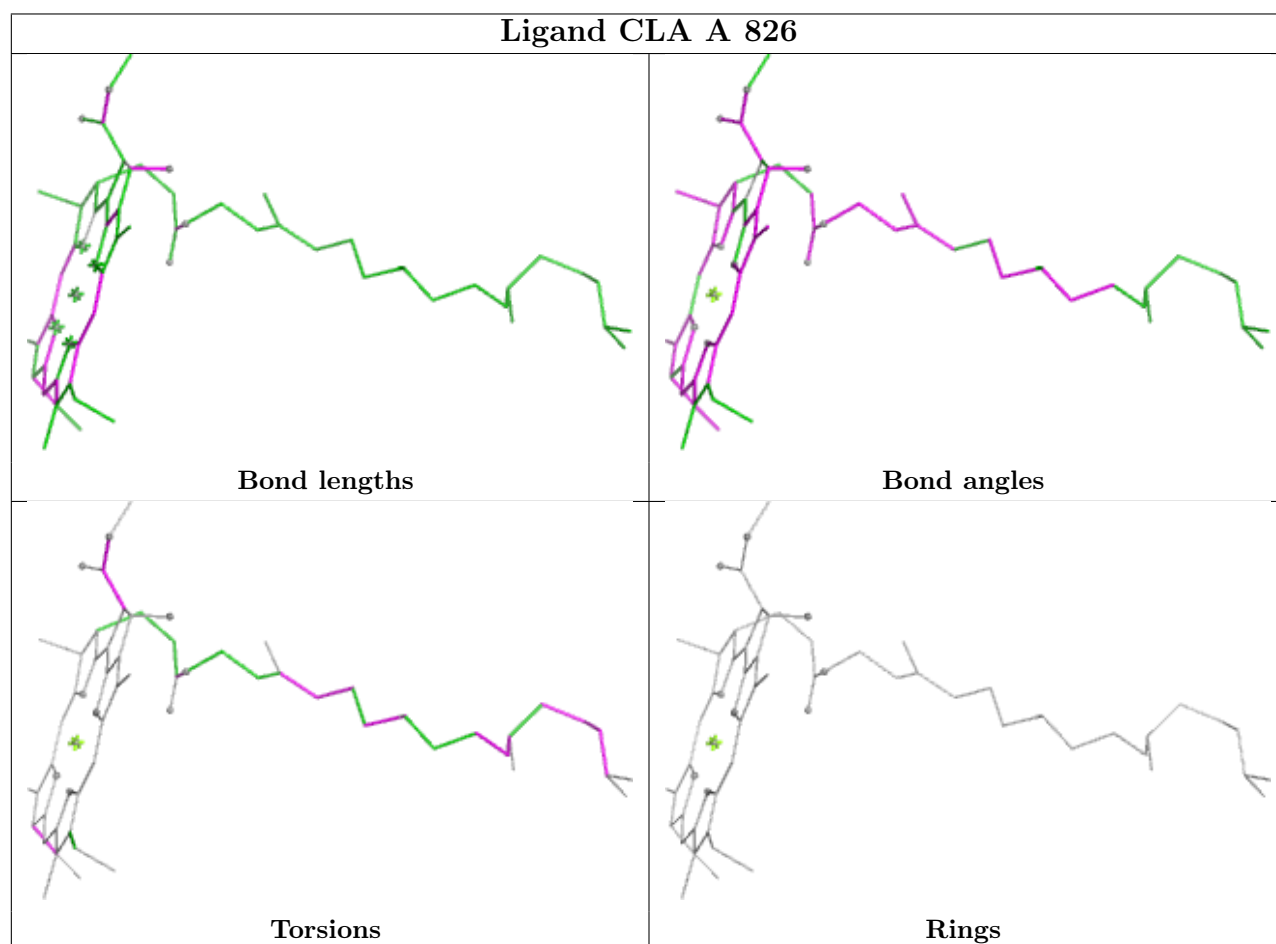
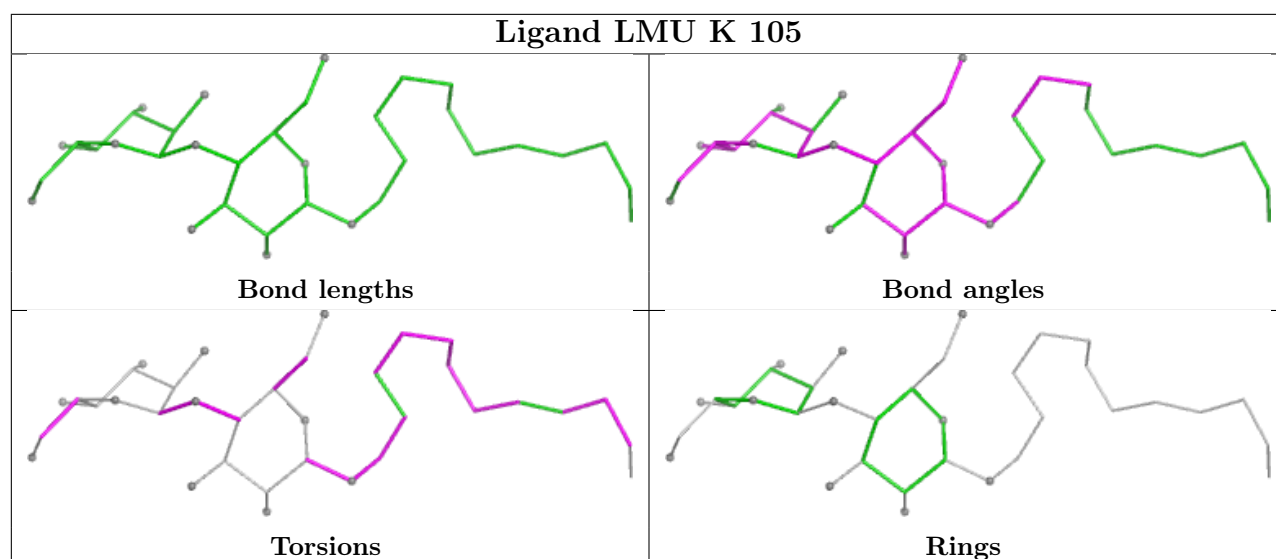


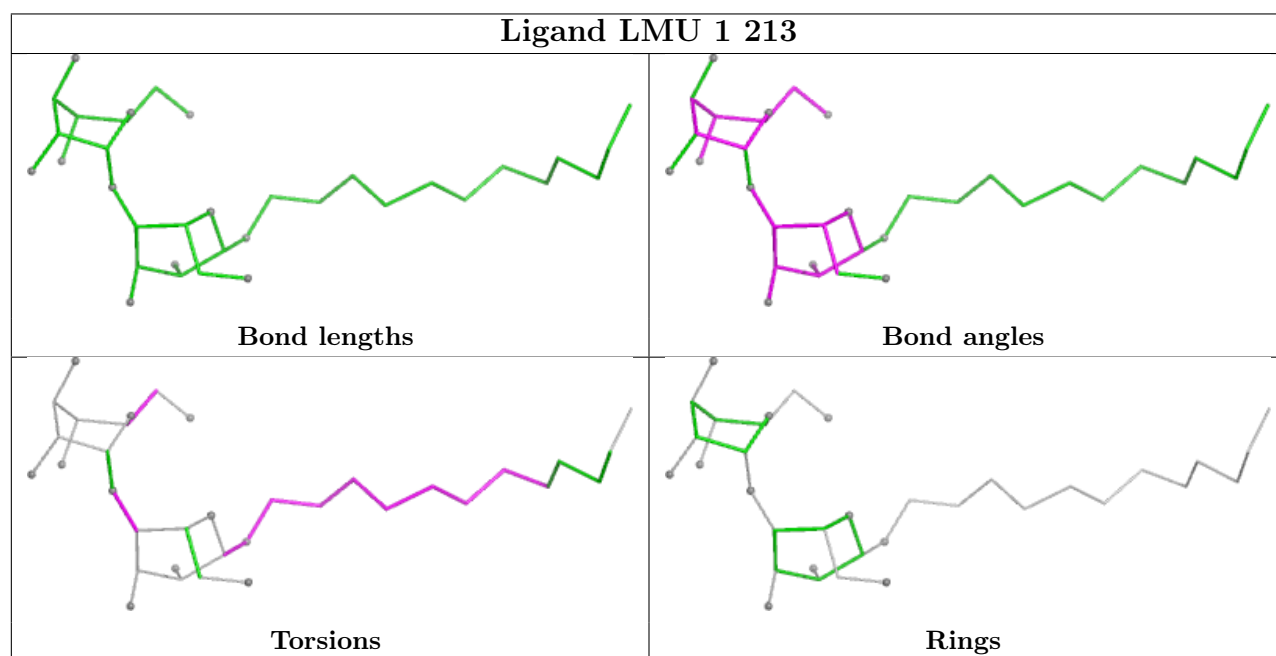
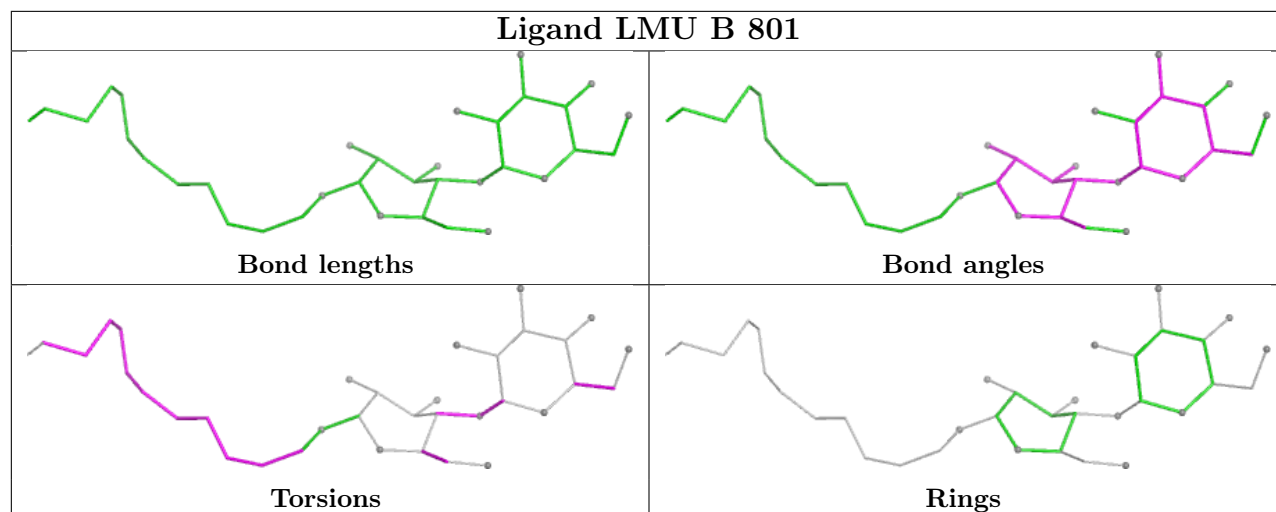
Ligand CLA 4 316



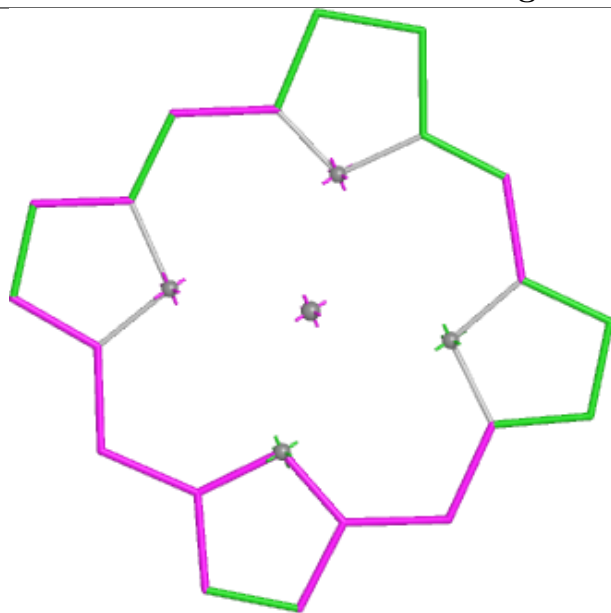




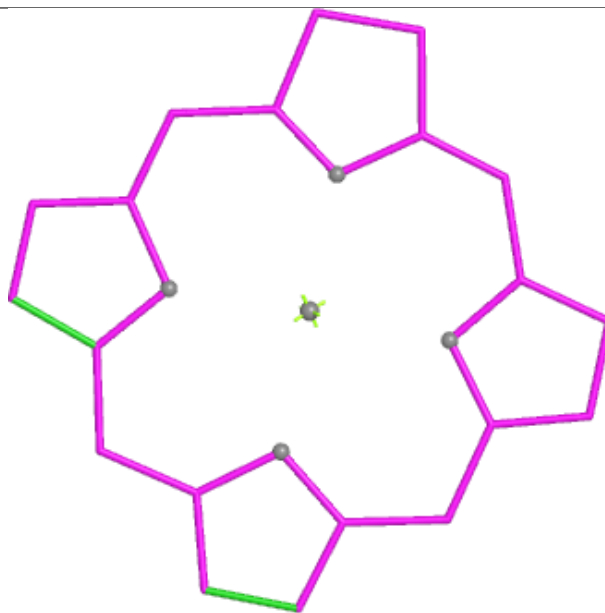




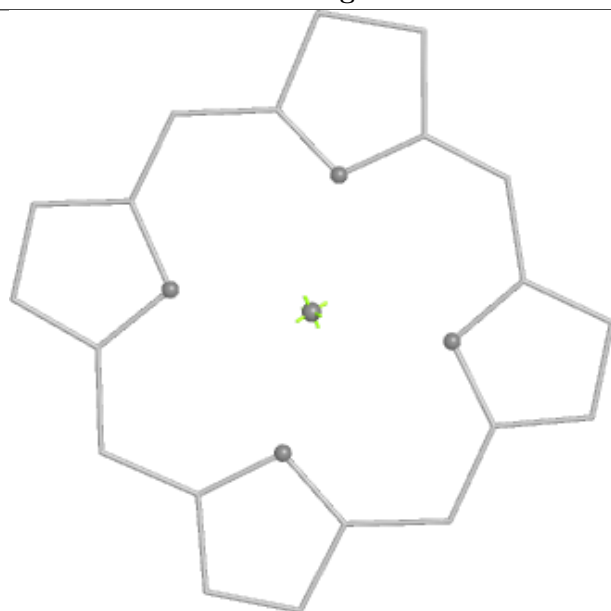
Ligand CLA 1 216



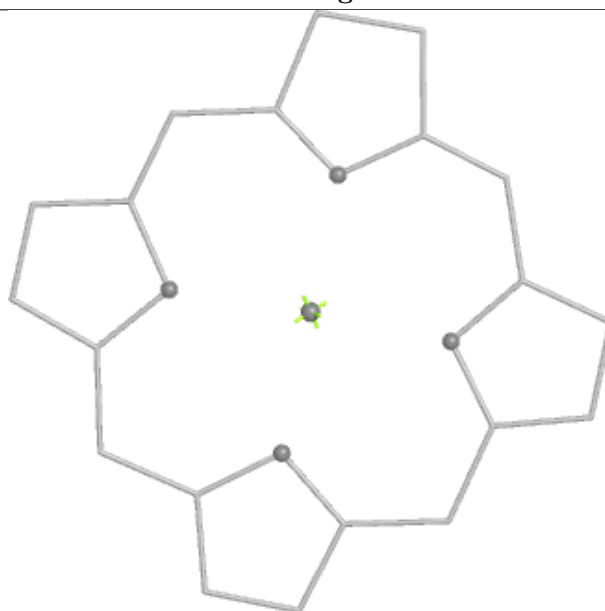
Bond lengths



Bond angles

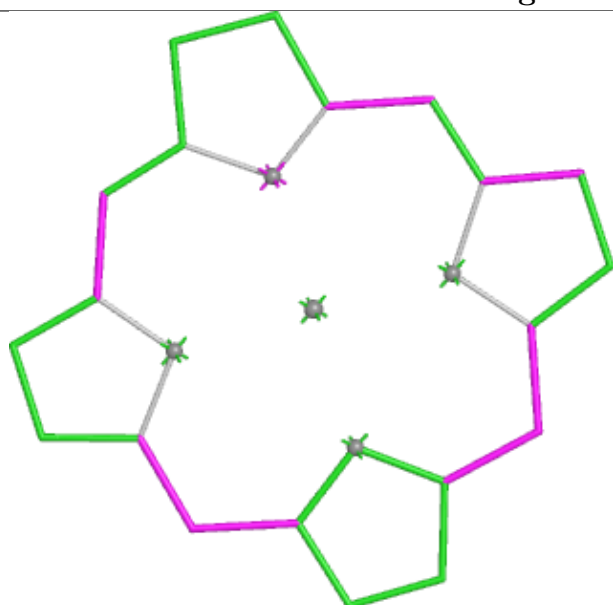


Torsions

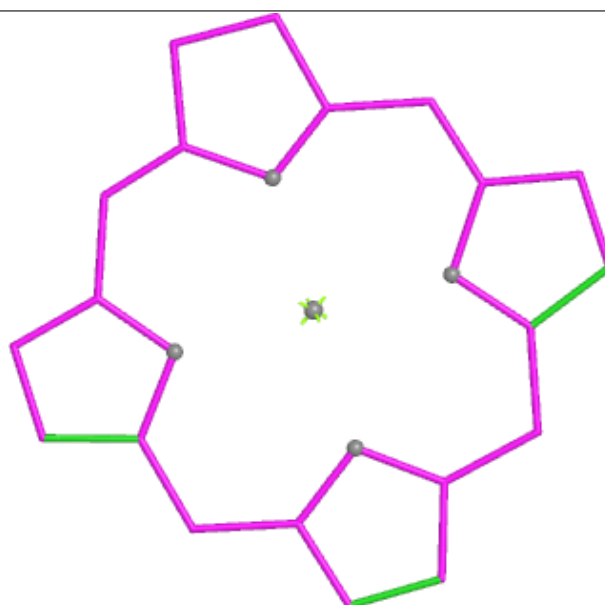


Rings

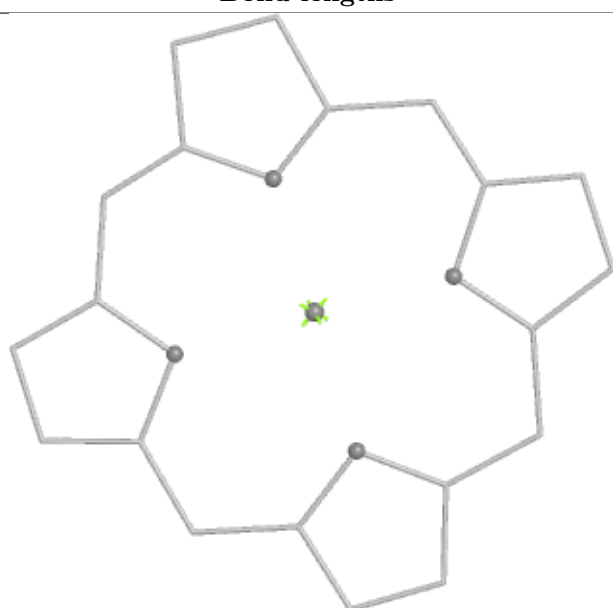
Ligand CLA 1 211



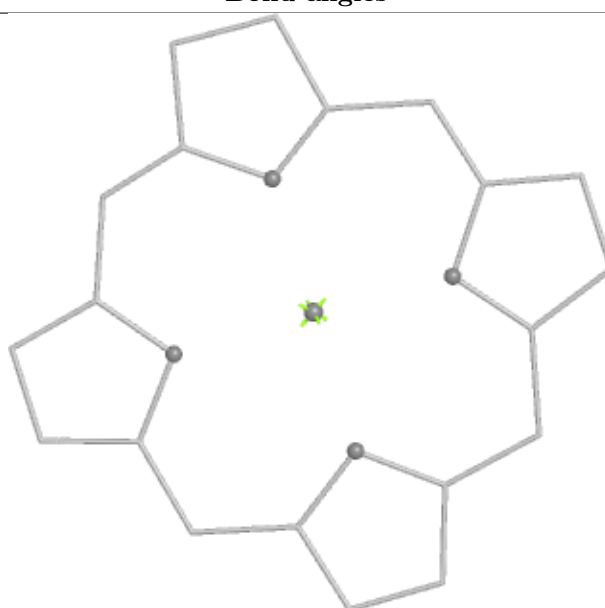
Bond lengths



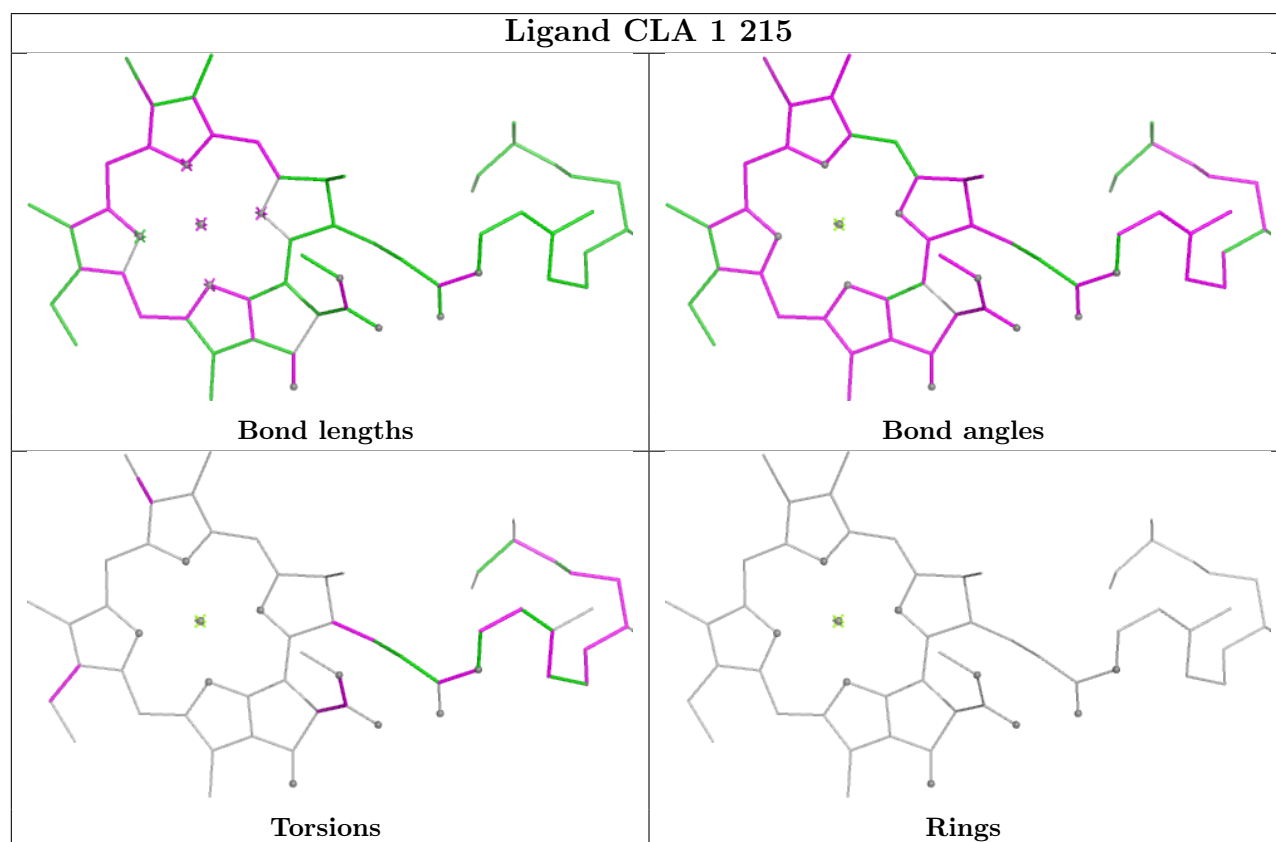
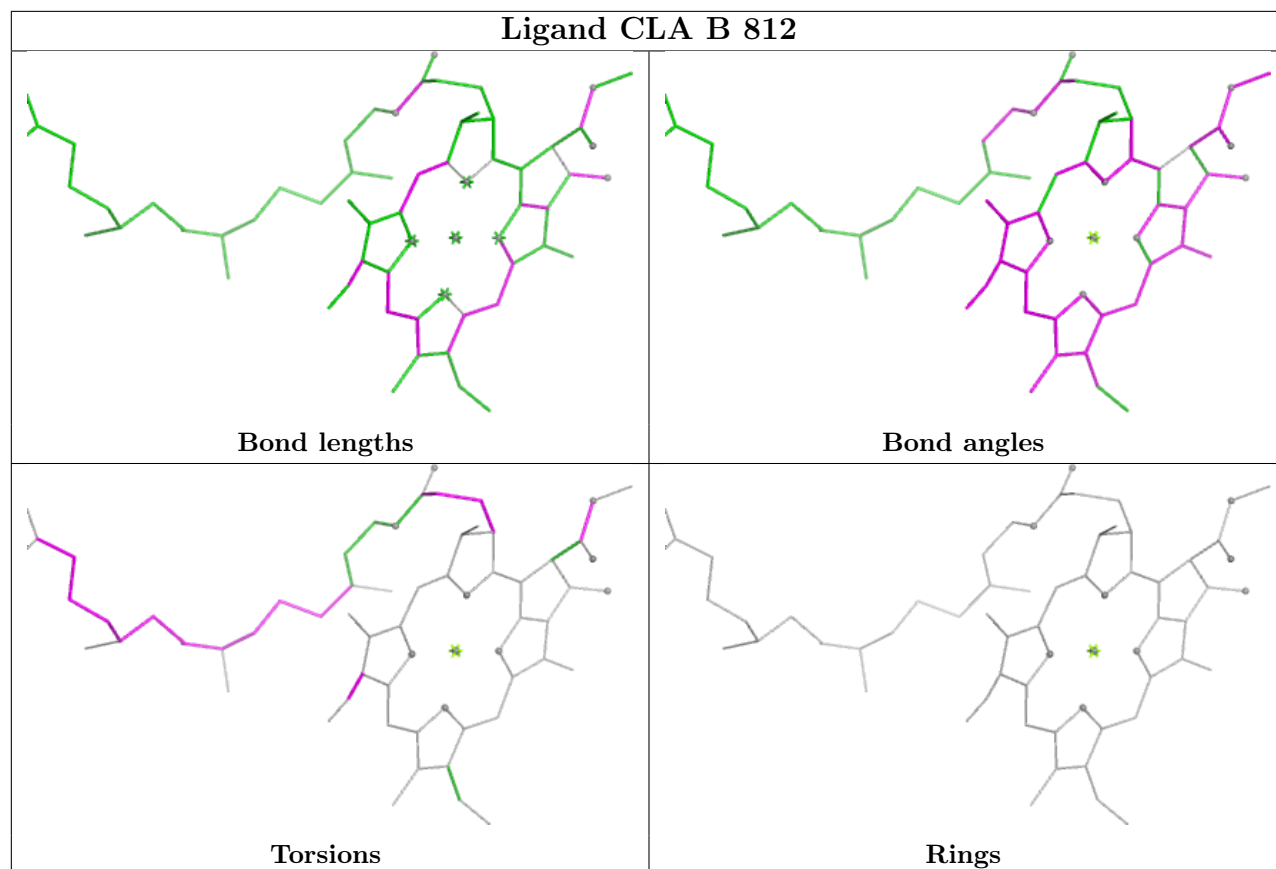
Bond angles



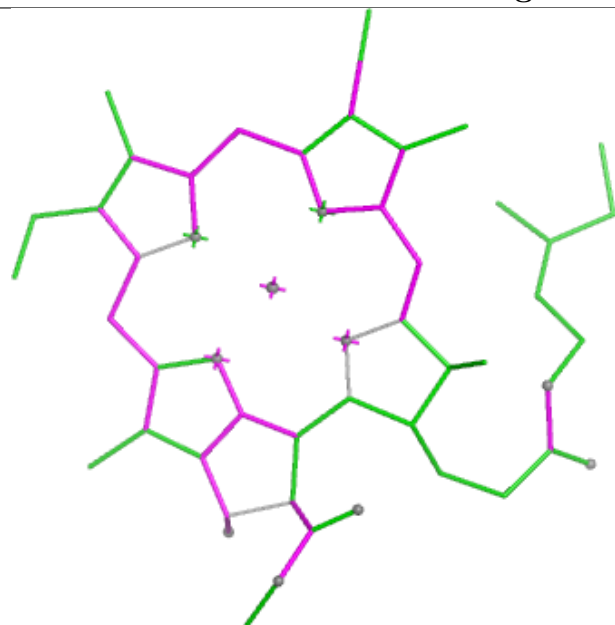
Torsions



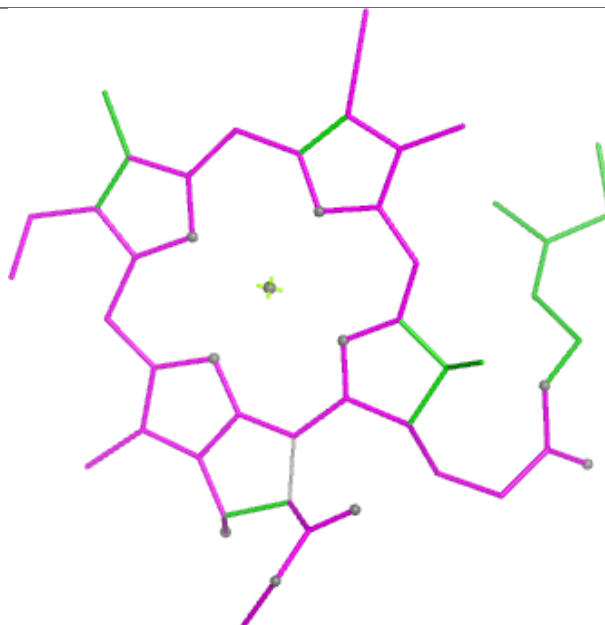
Rings



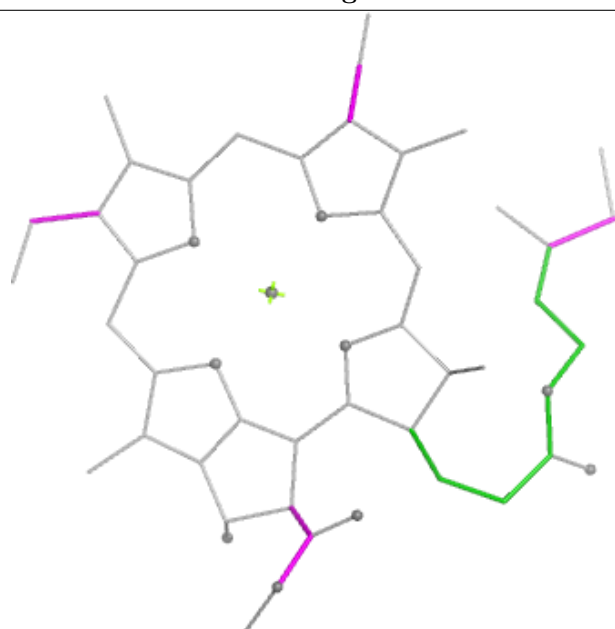
Ligand CLA G 102



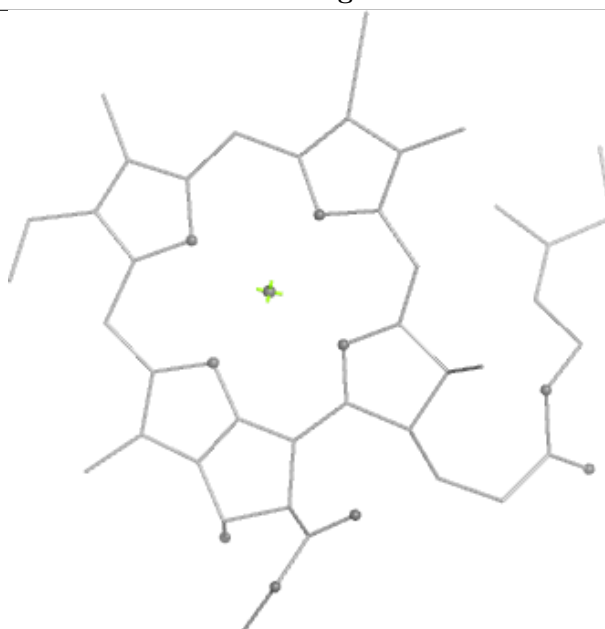
Bond lengths



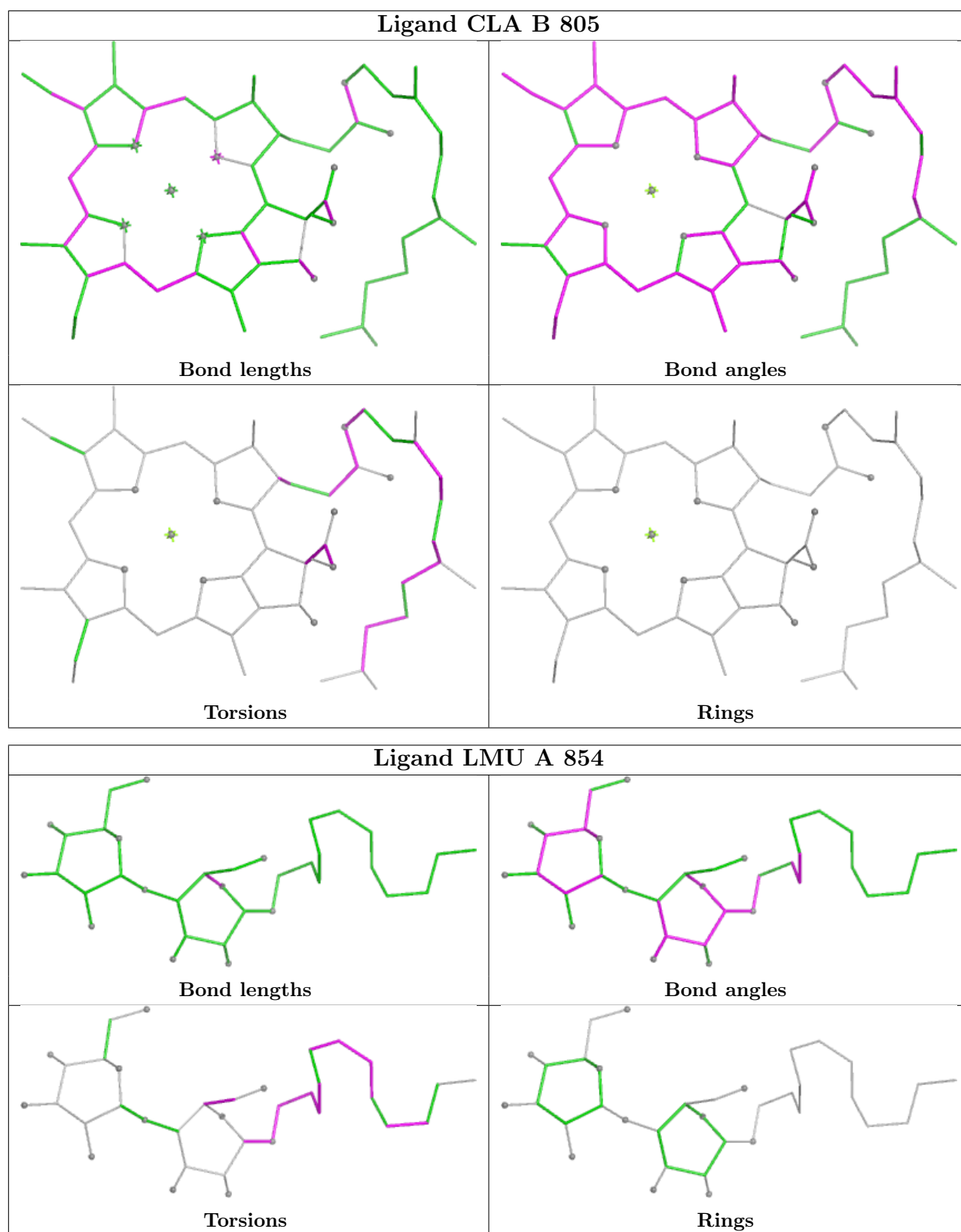
Bond angles

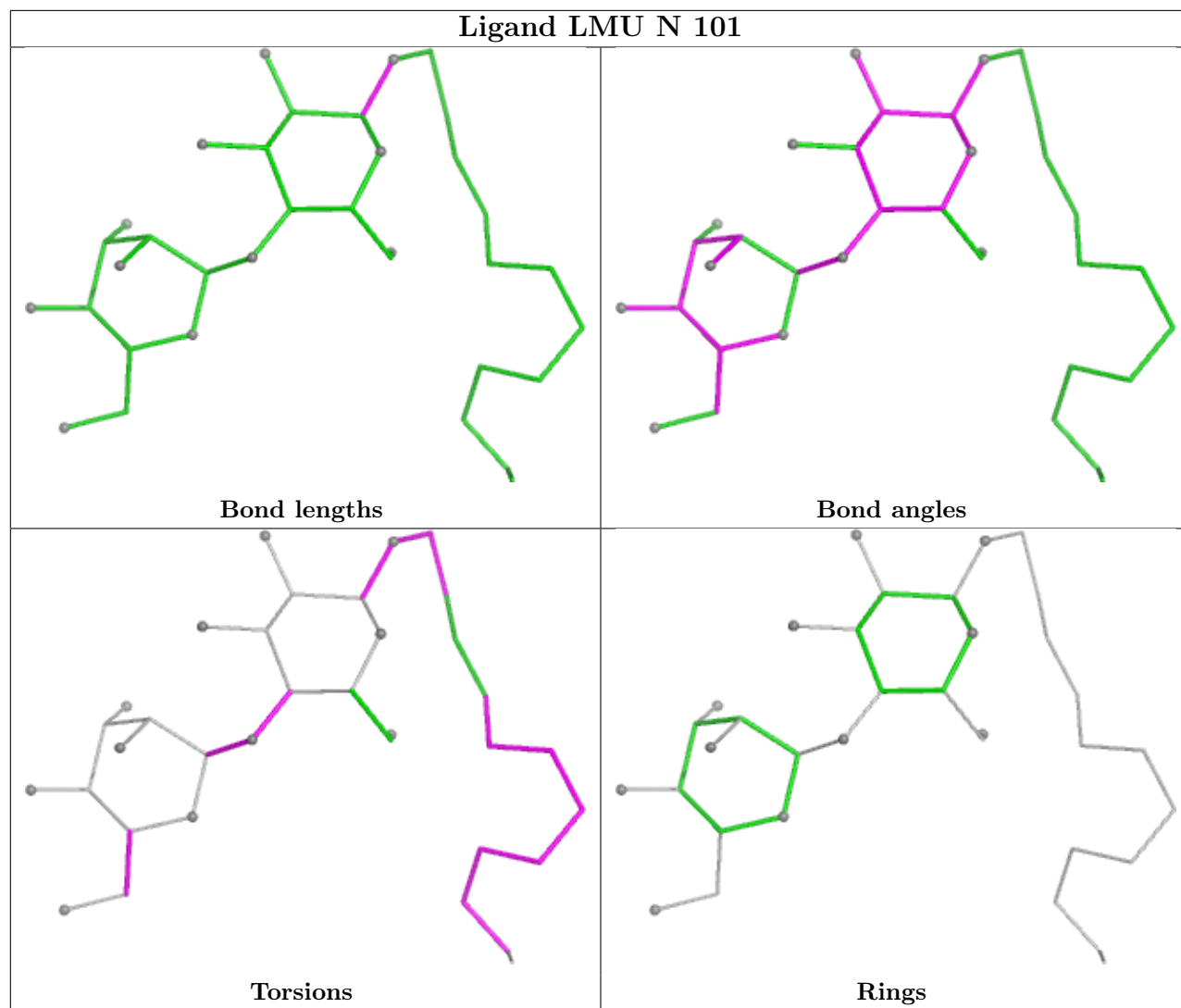


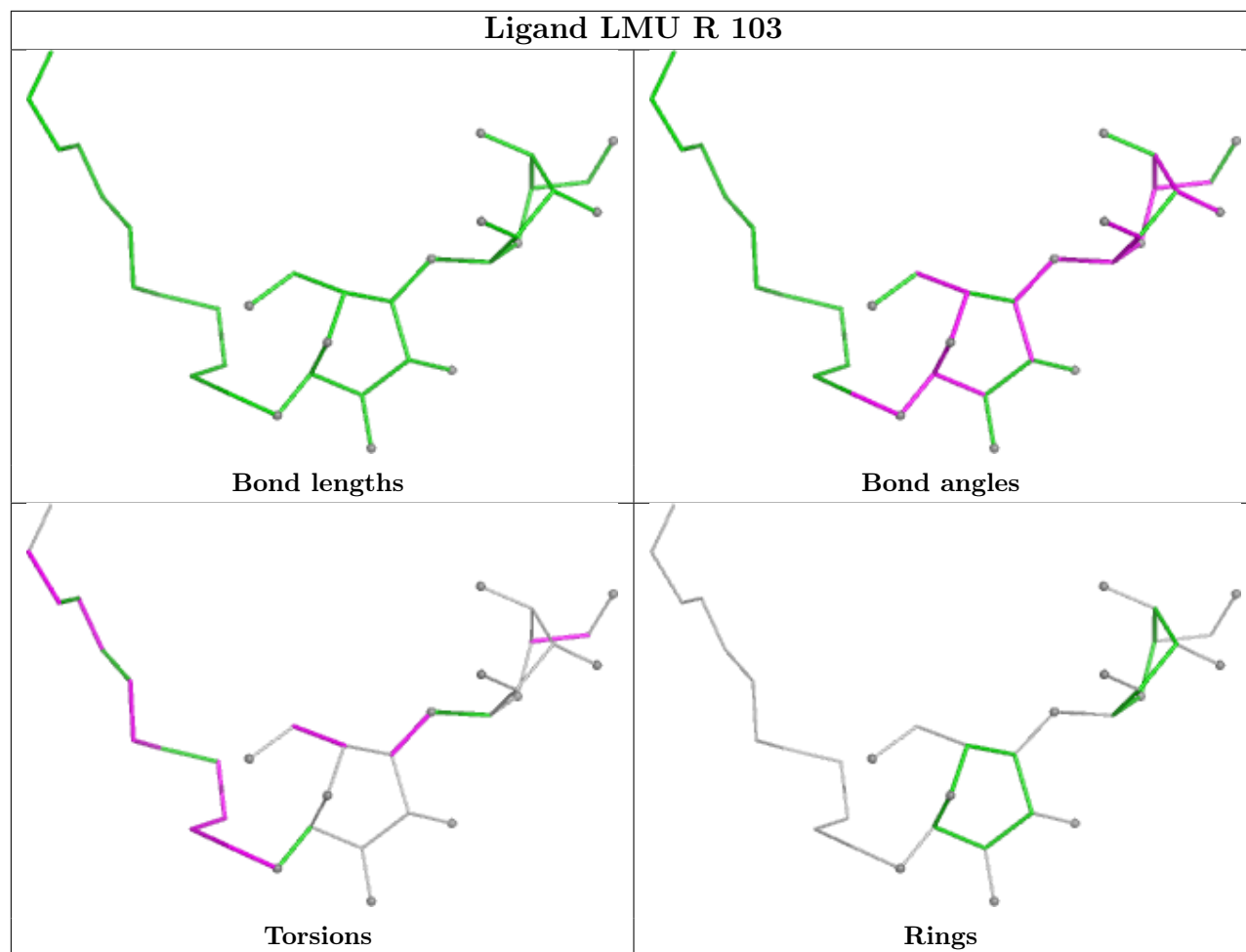
Torsions



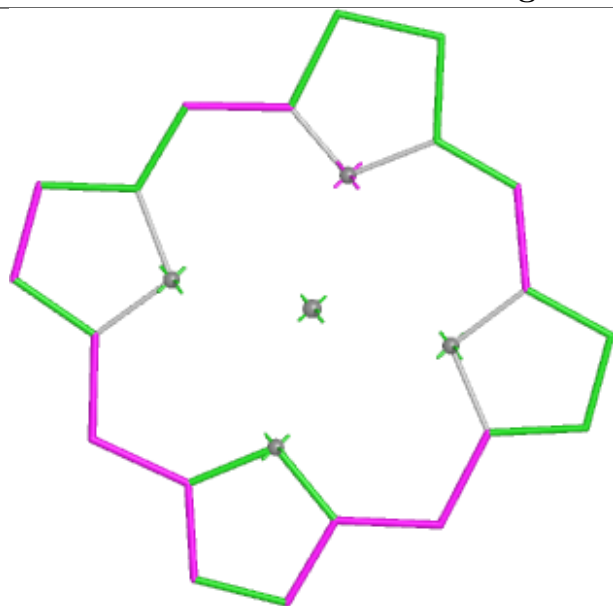
Rings



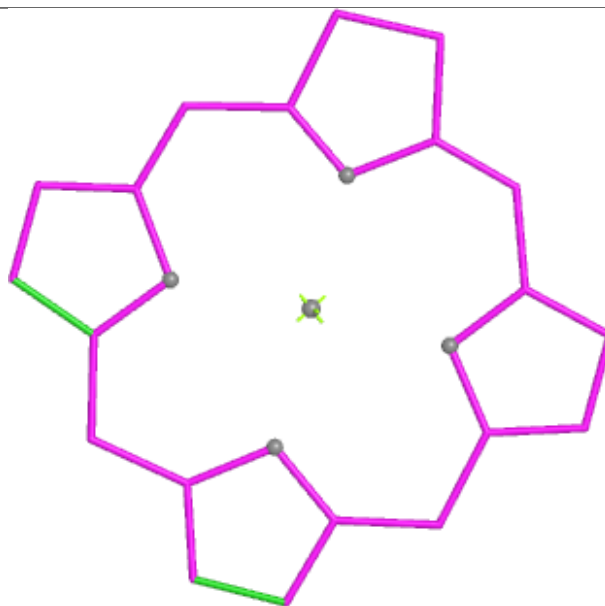




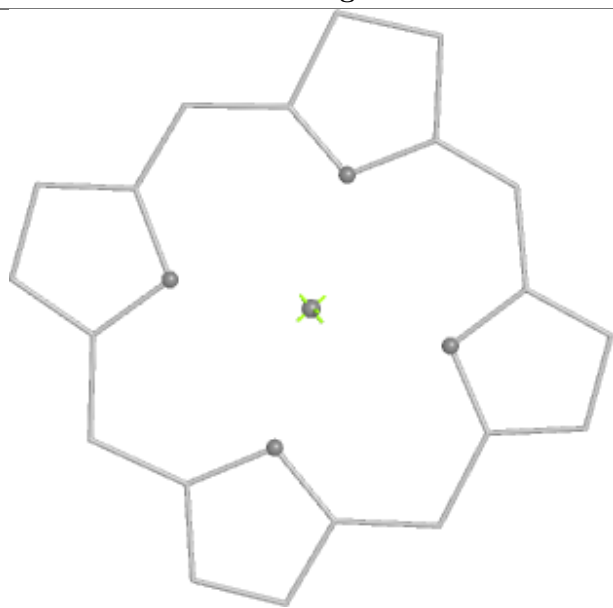
Ligand CLA 3 306



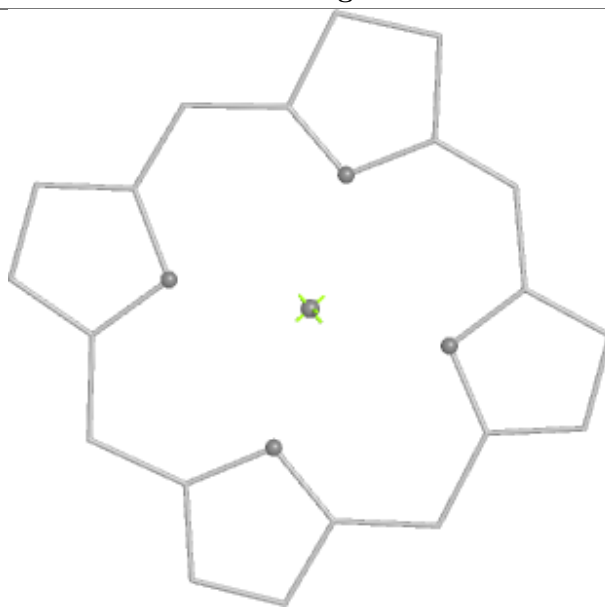
Bond lengths



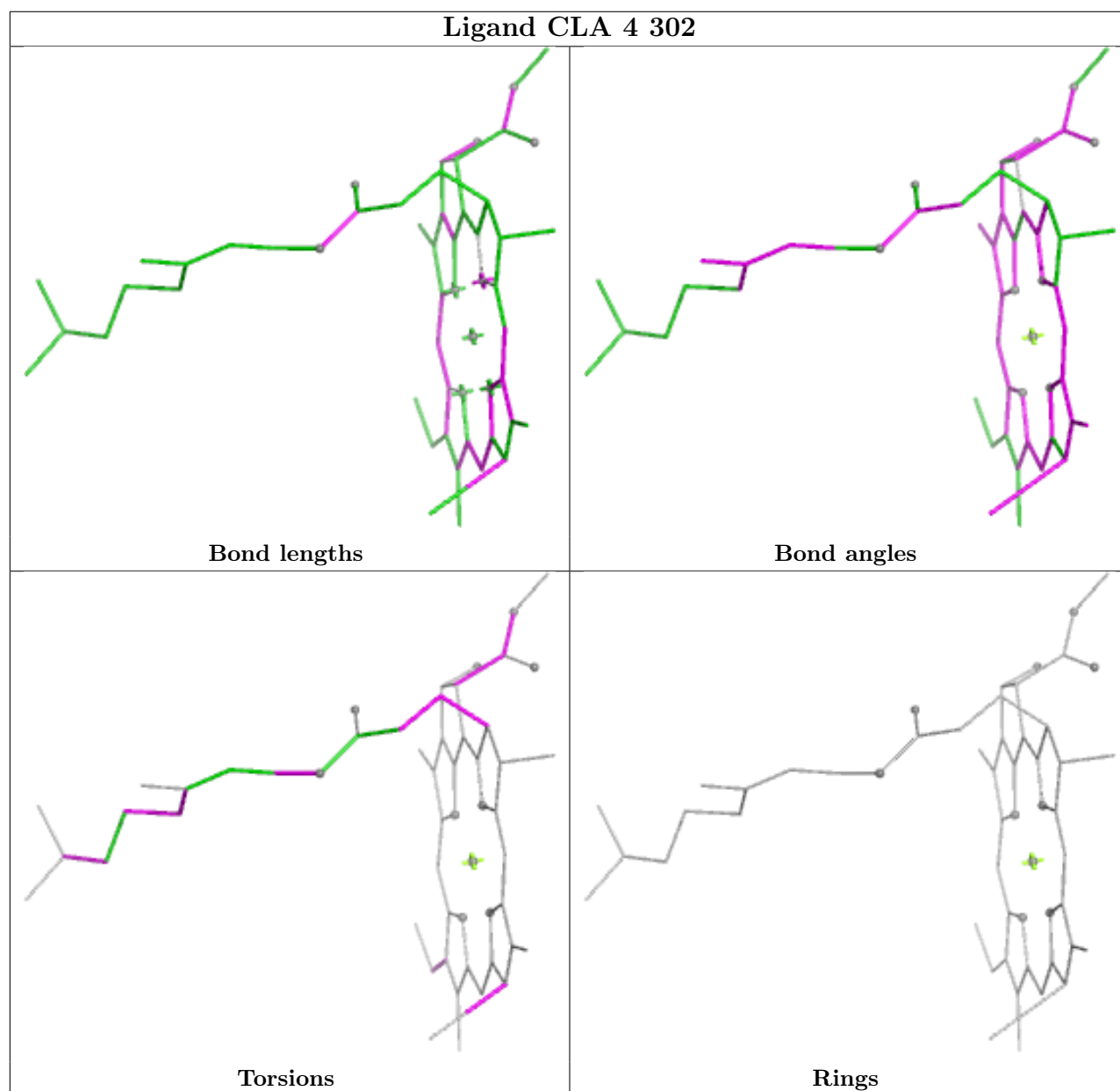
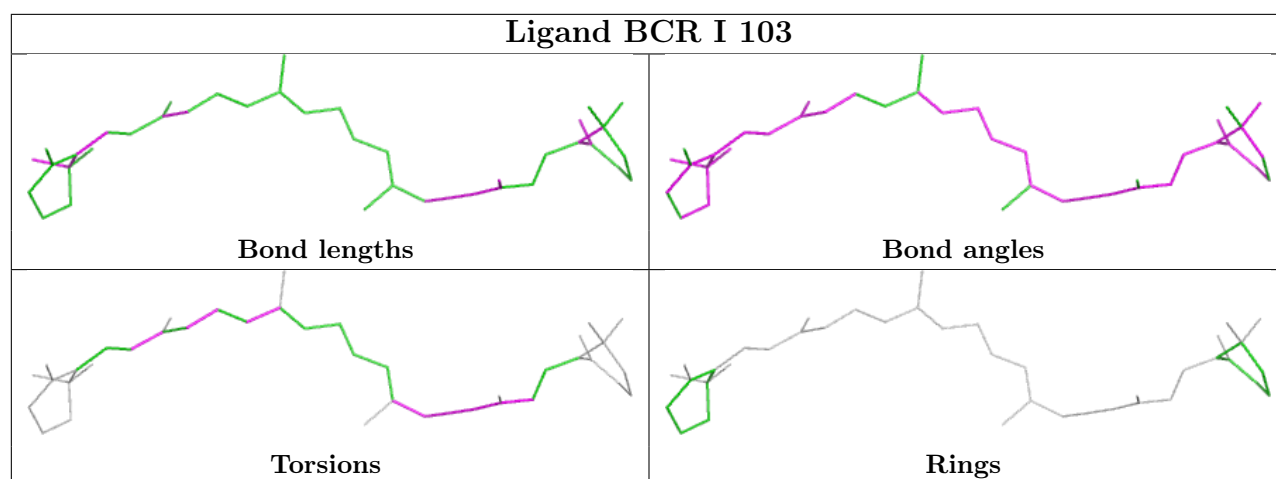
Bond angles



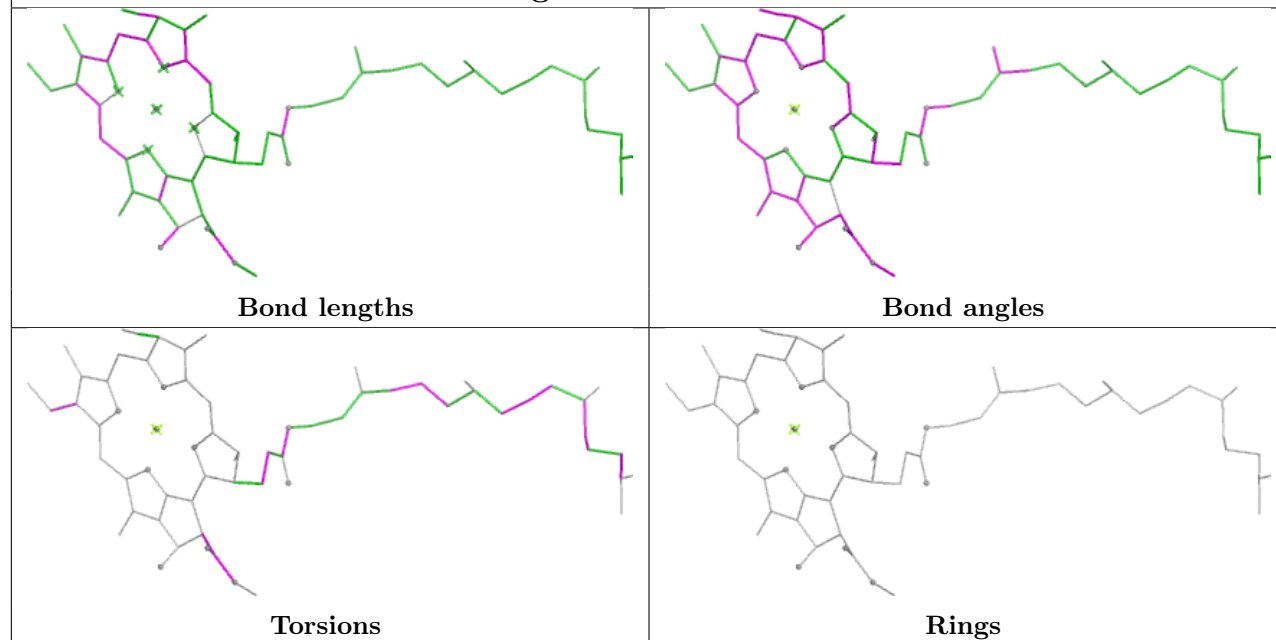
Torsions



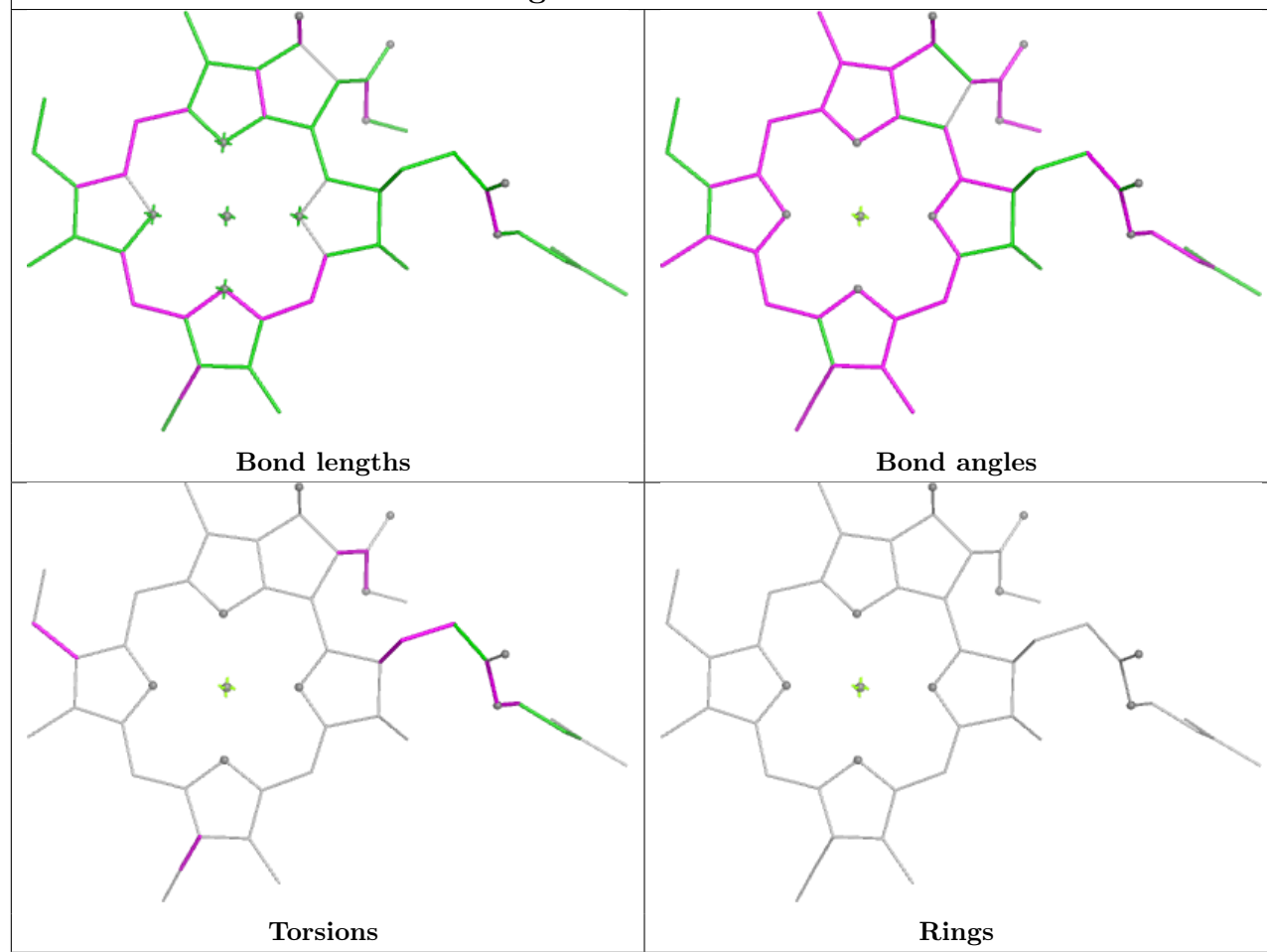
Rings



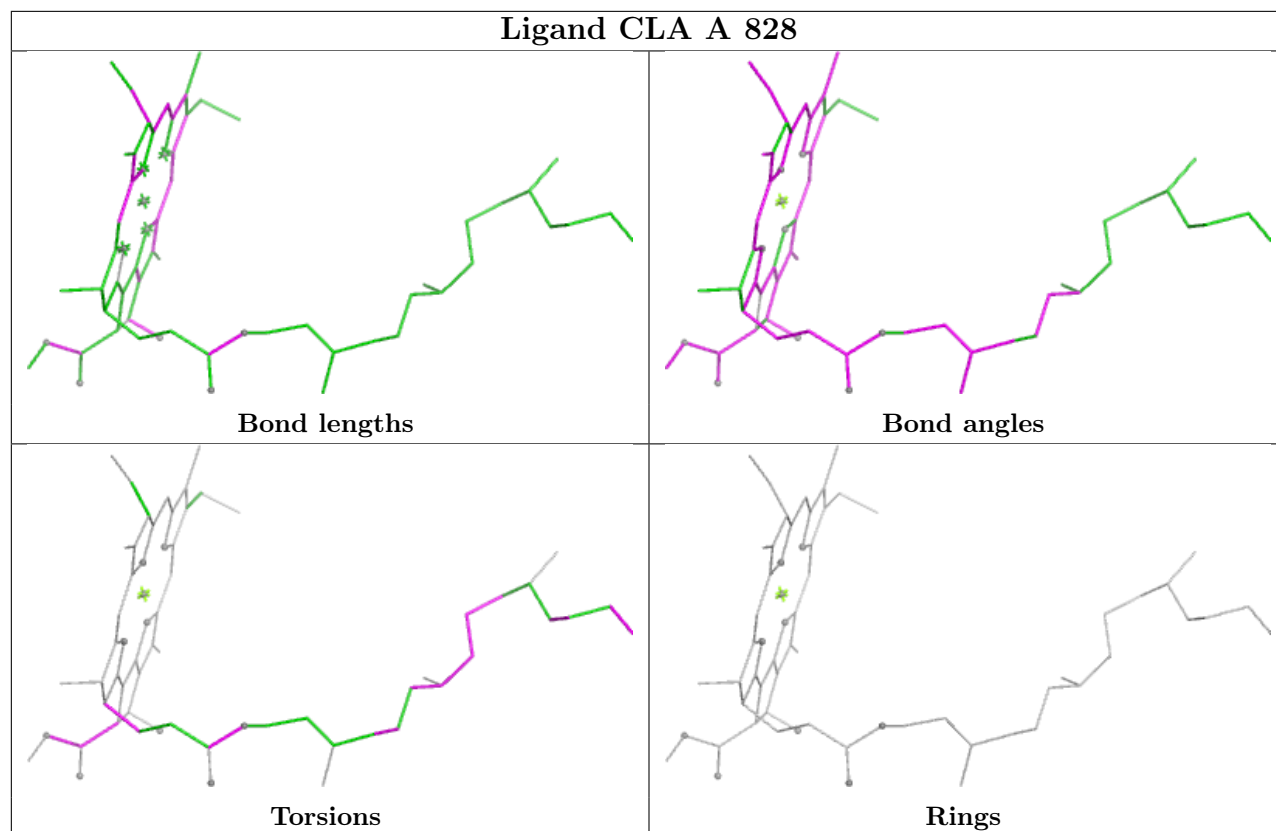
Ligand CLA A 819



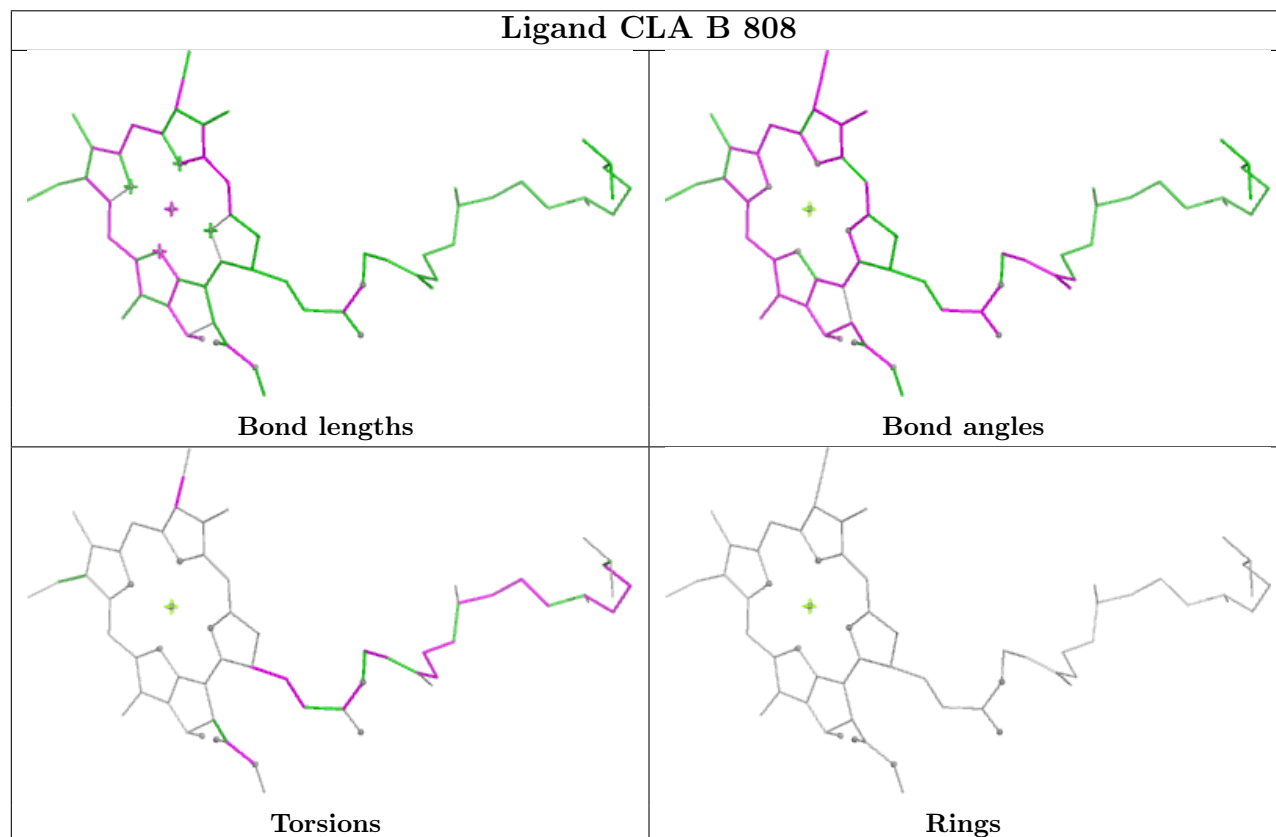
Ligand CLA B 829



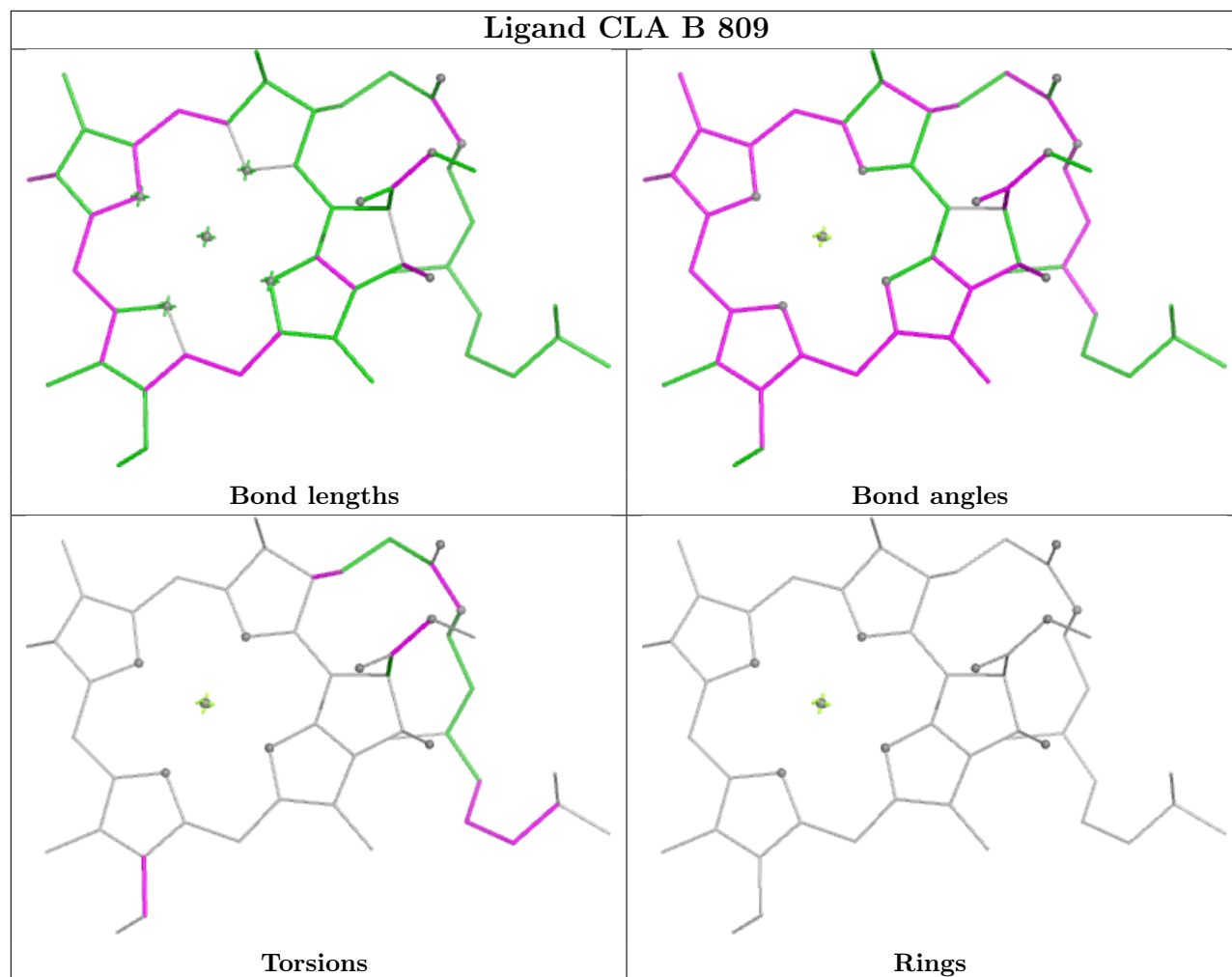
Ligand CLA A 828

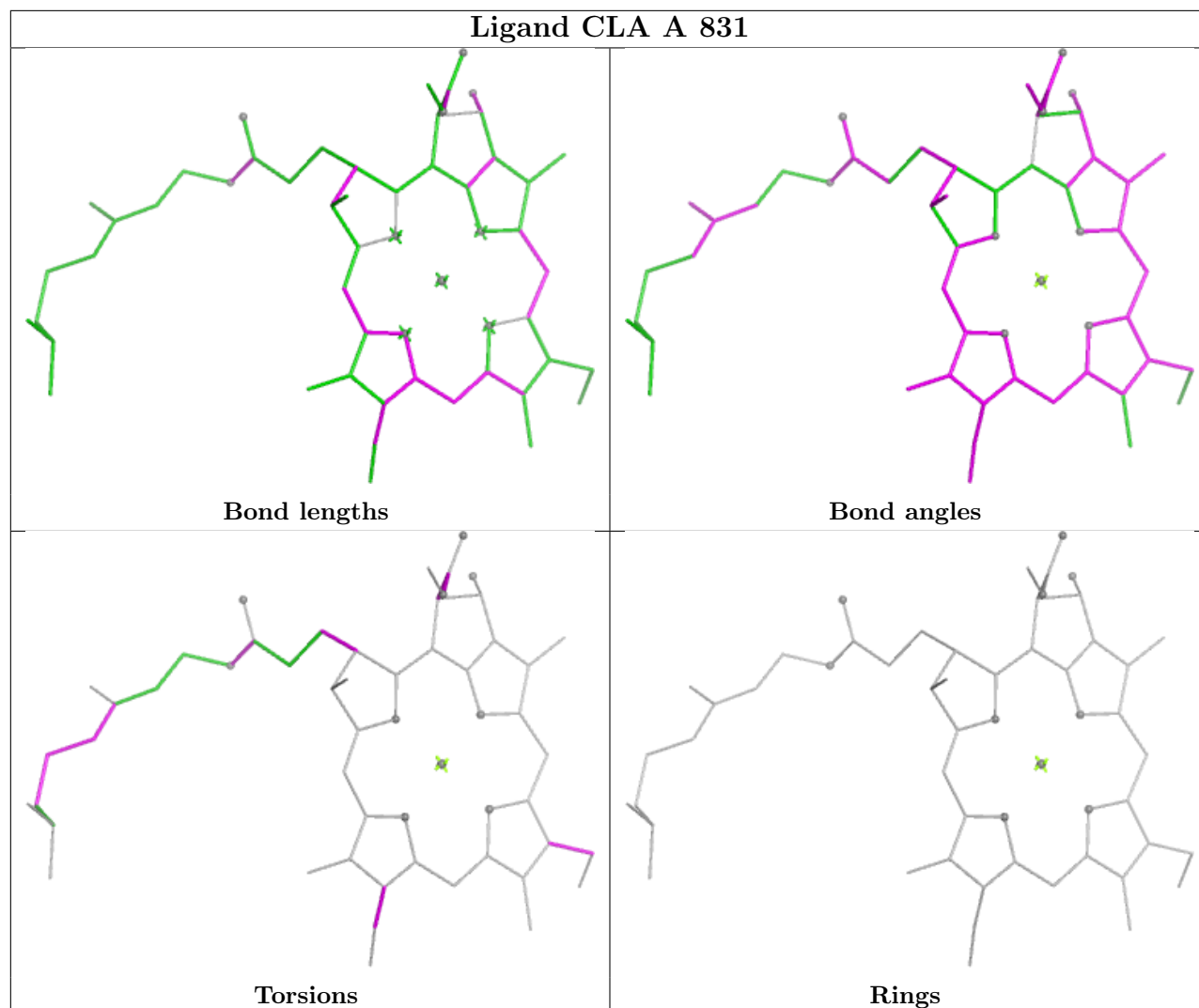
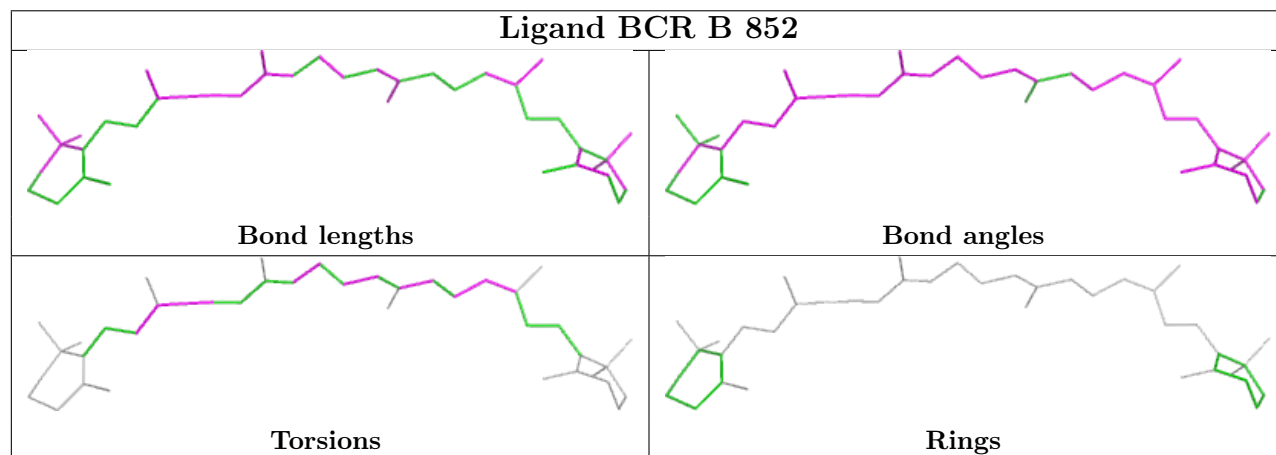


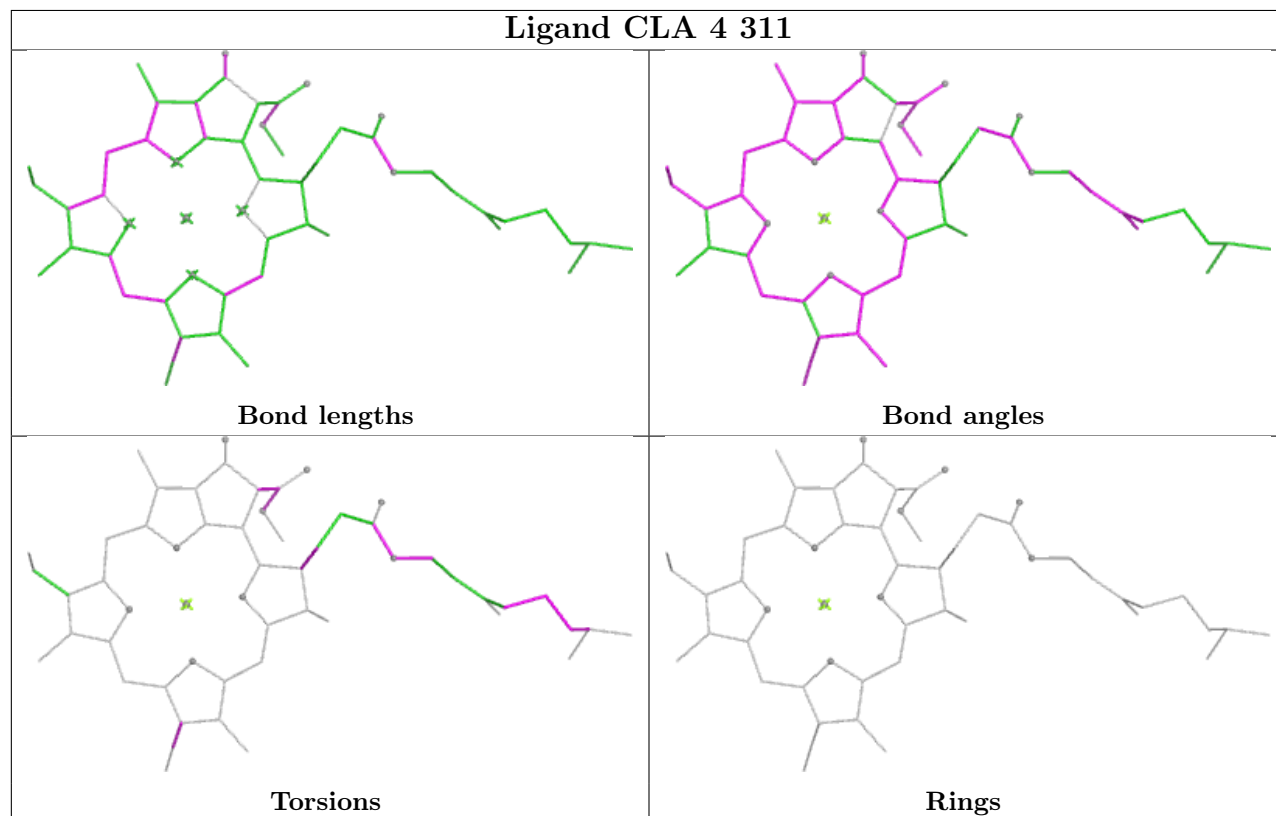
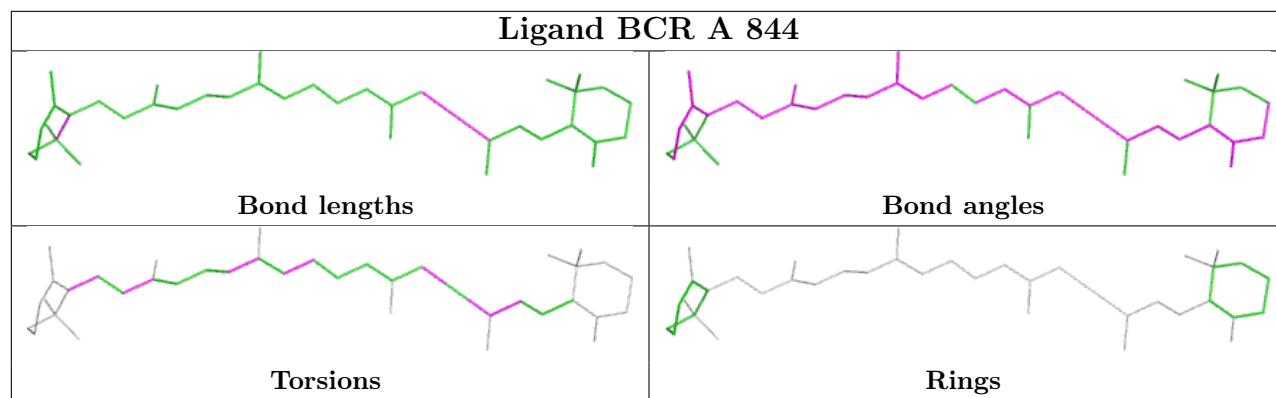
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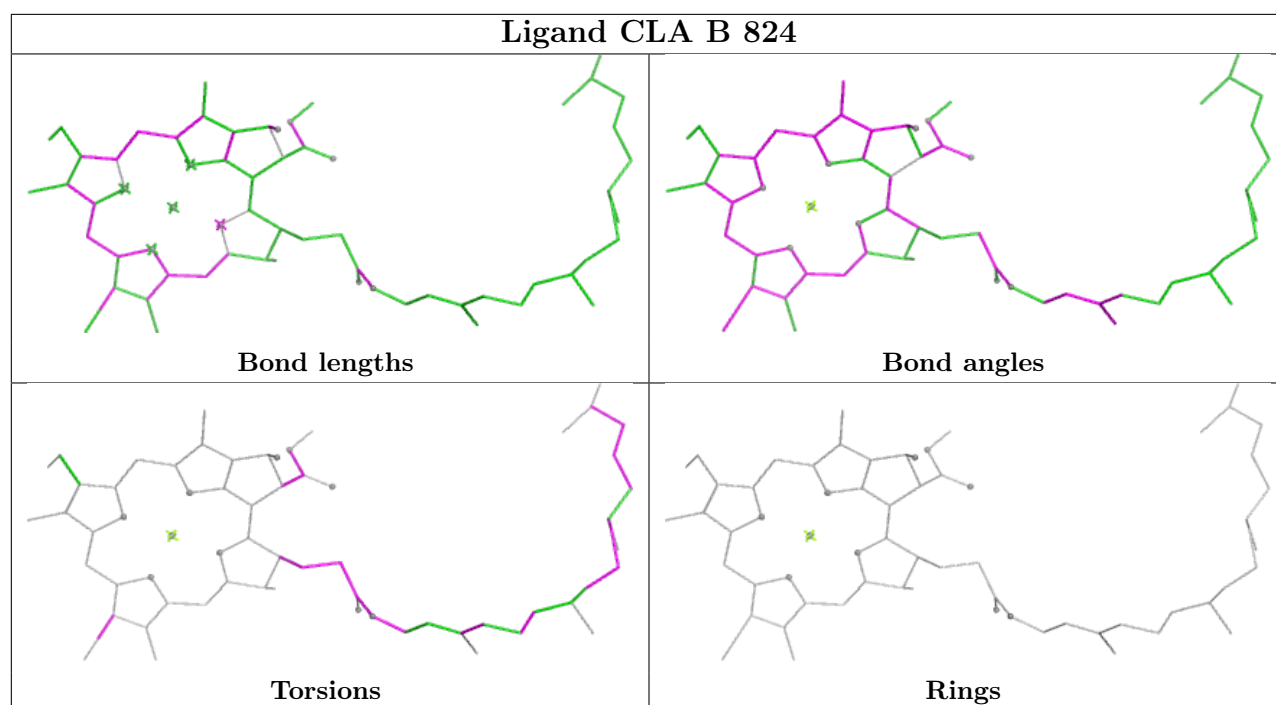


Ligand CLA B 809

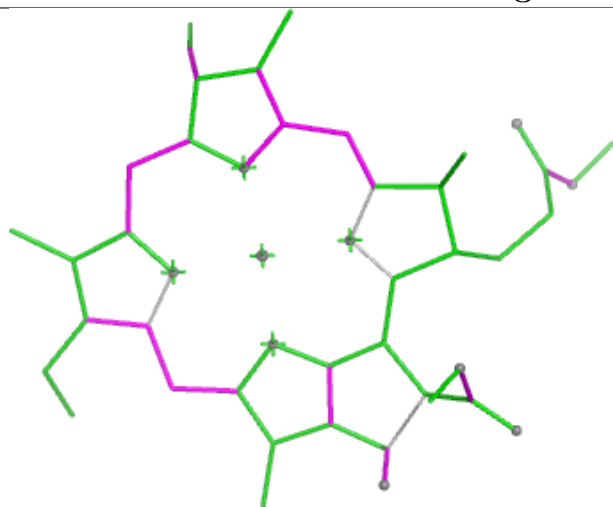


Ligand CLA A 831**Ligand BCR B 852**

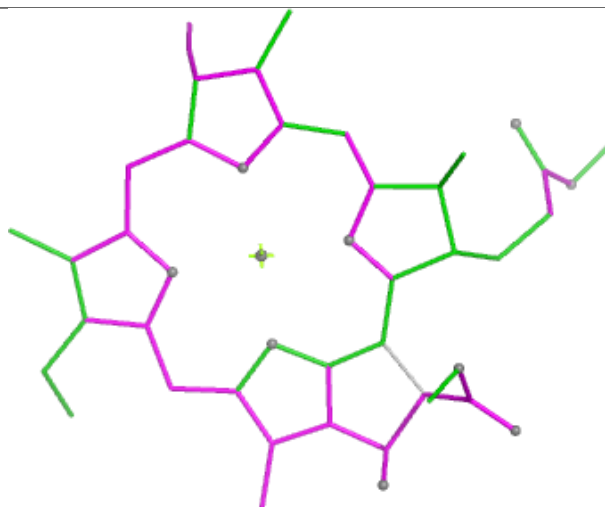




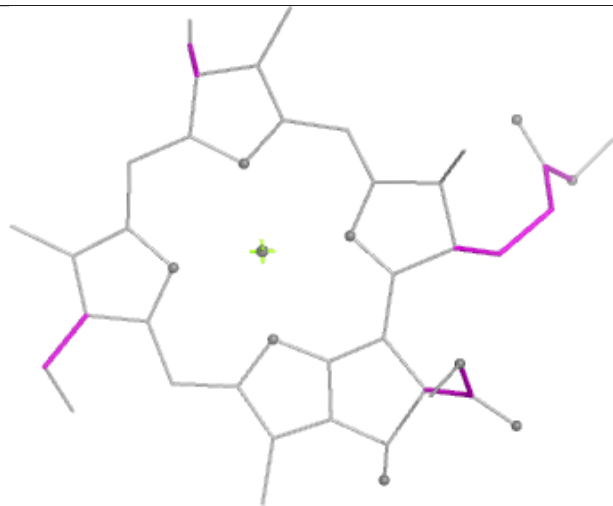
Ligand CLA B 819



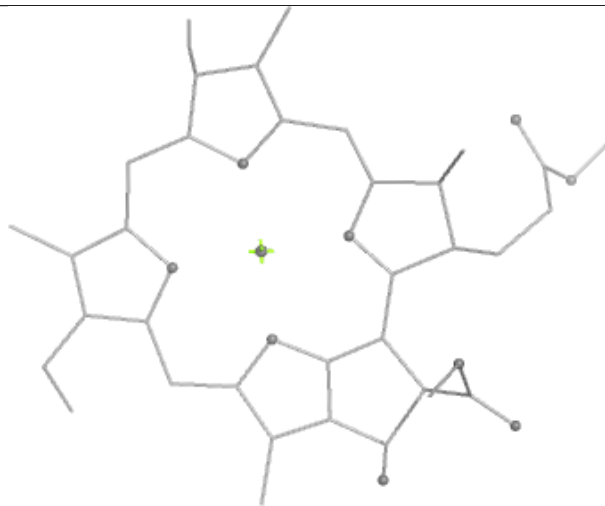
Bond lengths



Bond angles

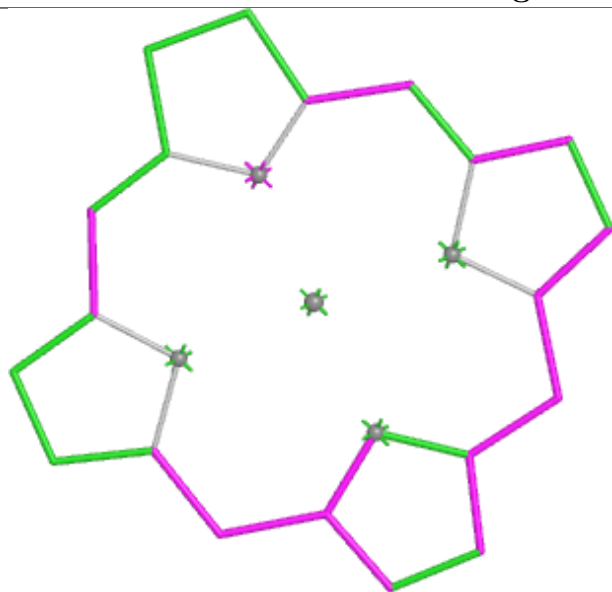


Torsions

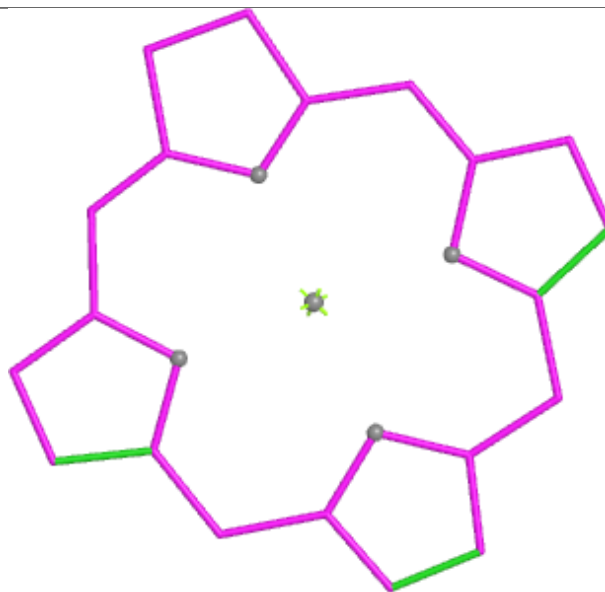


Rings

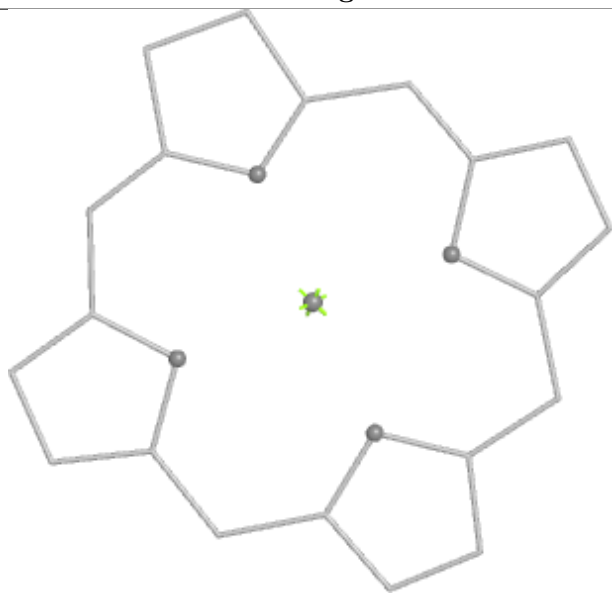
Ligand CLA A 802



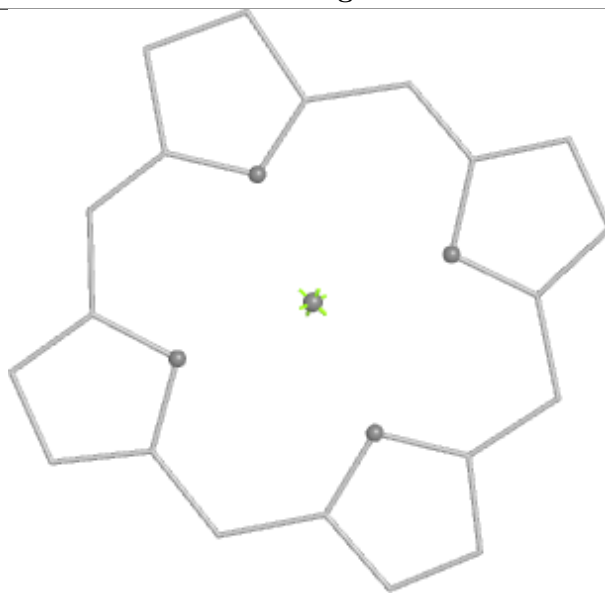
Bond lengths



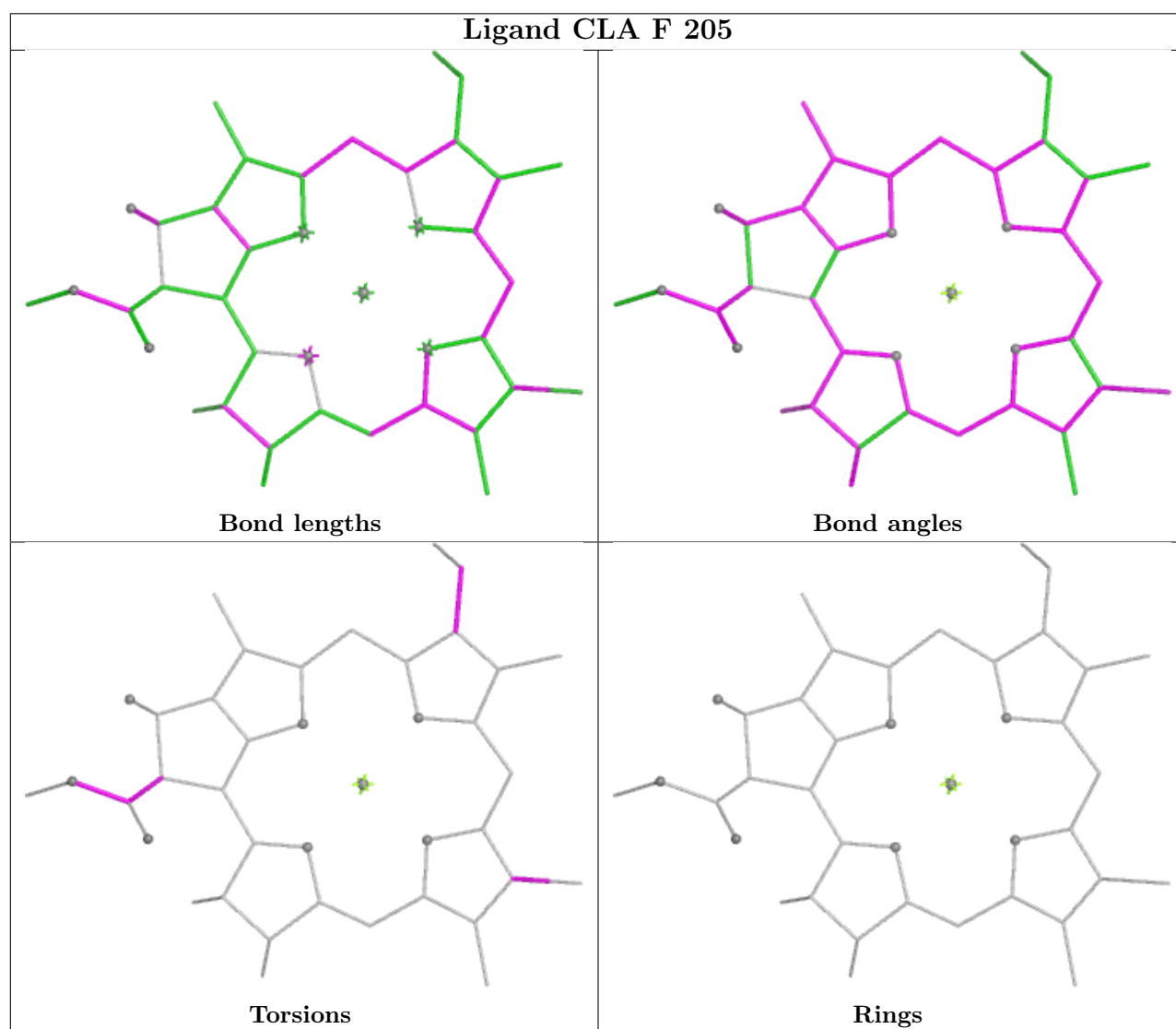
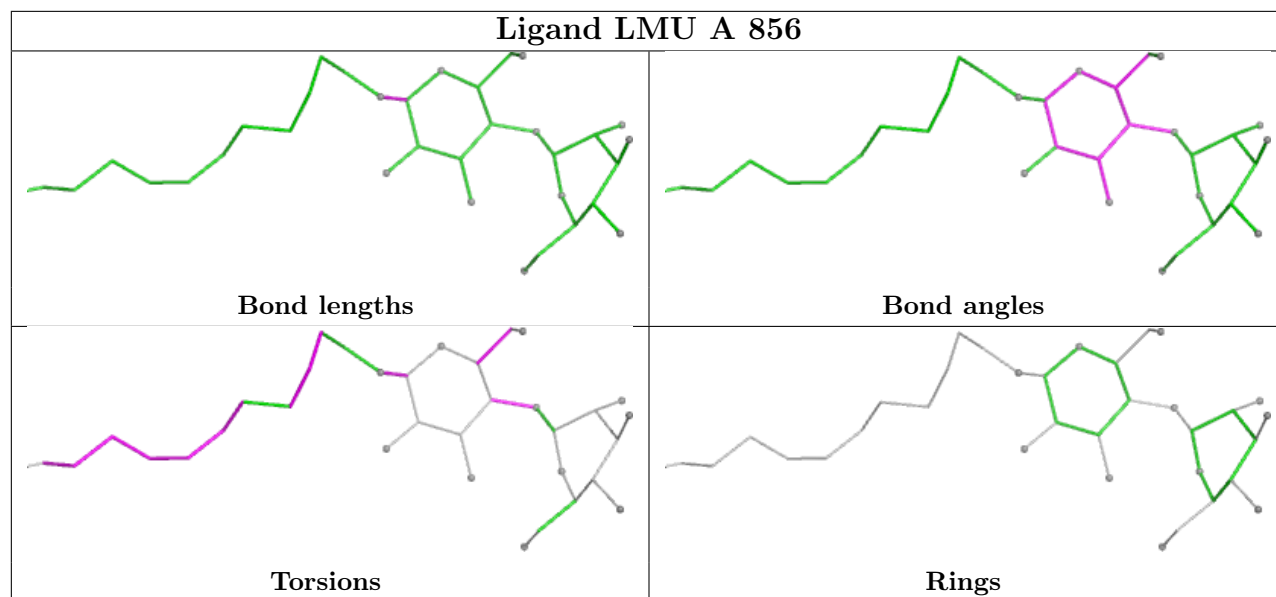
Bond angles

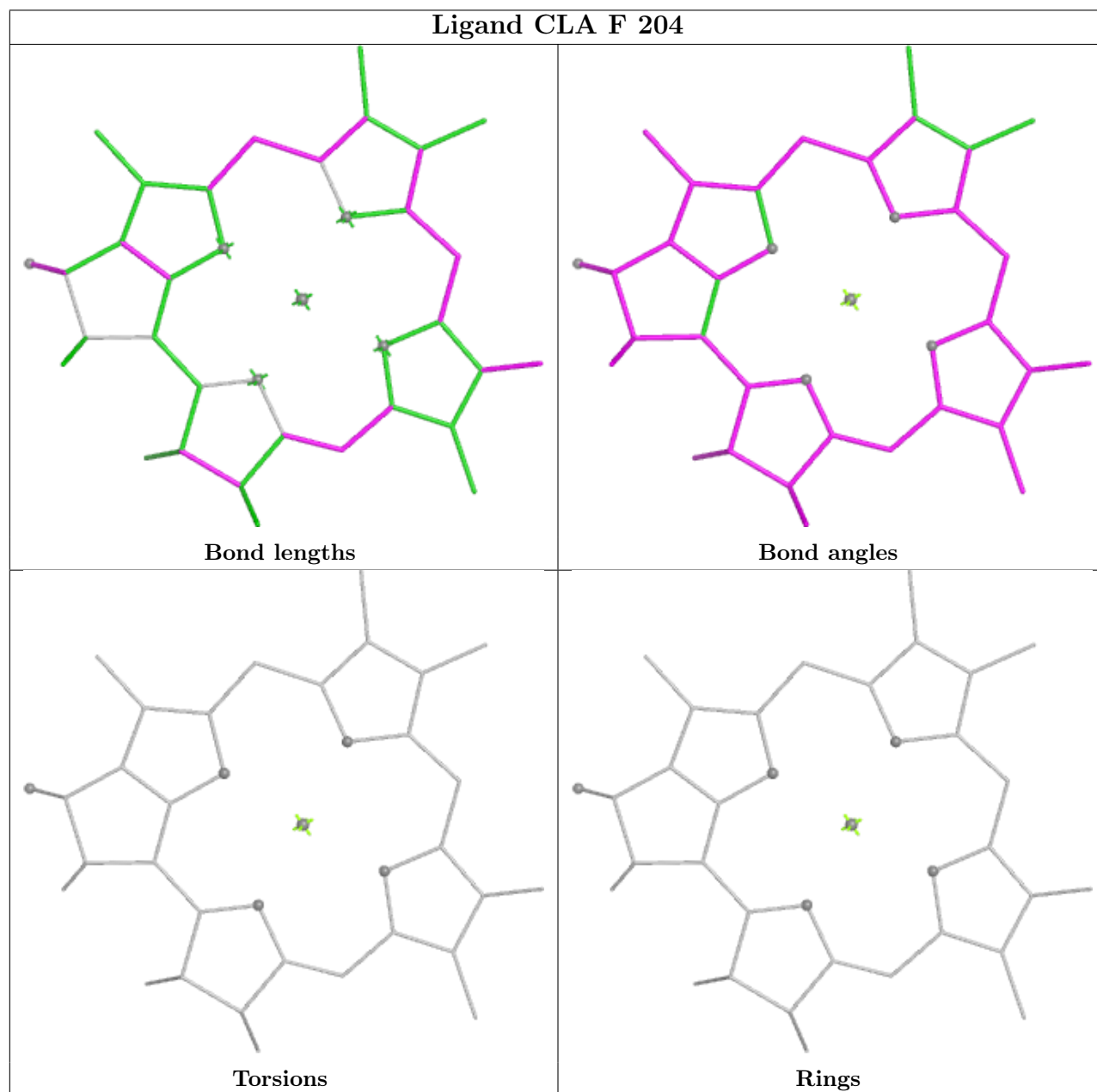
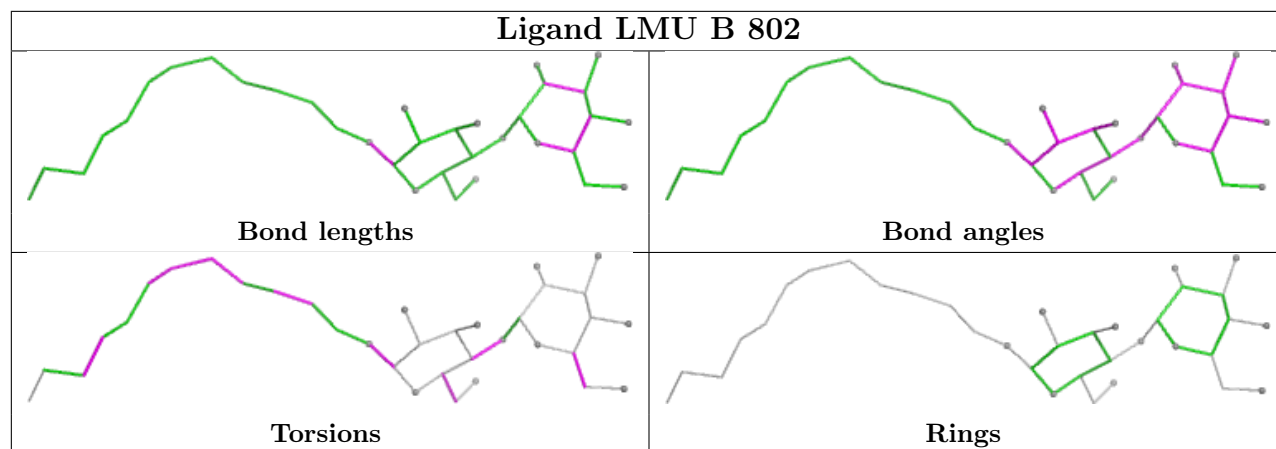


Torsions

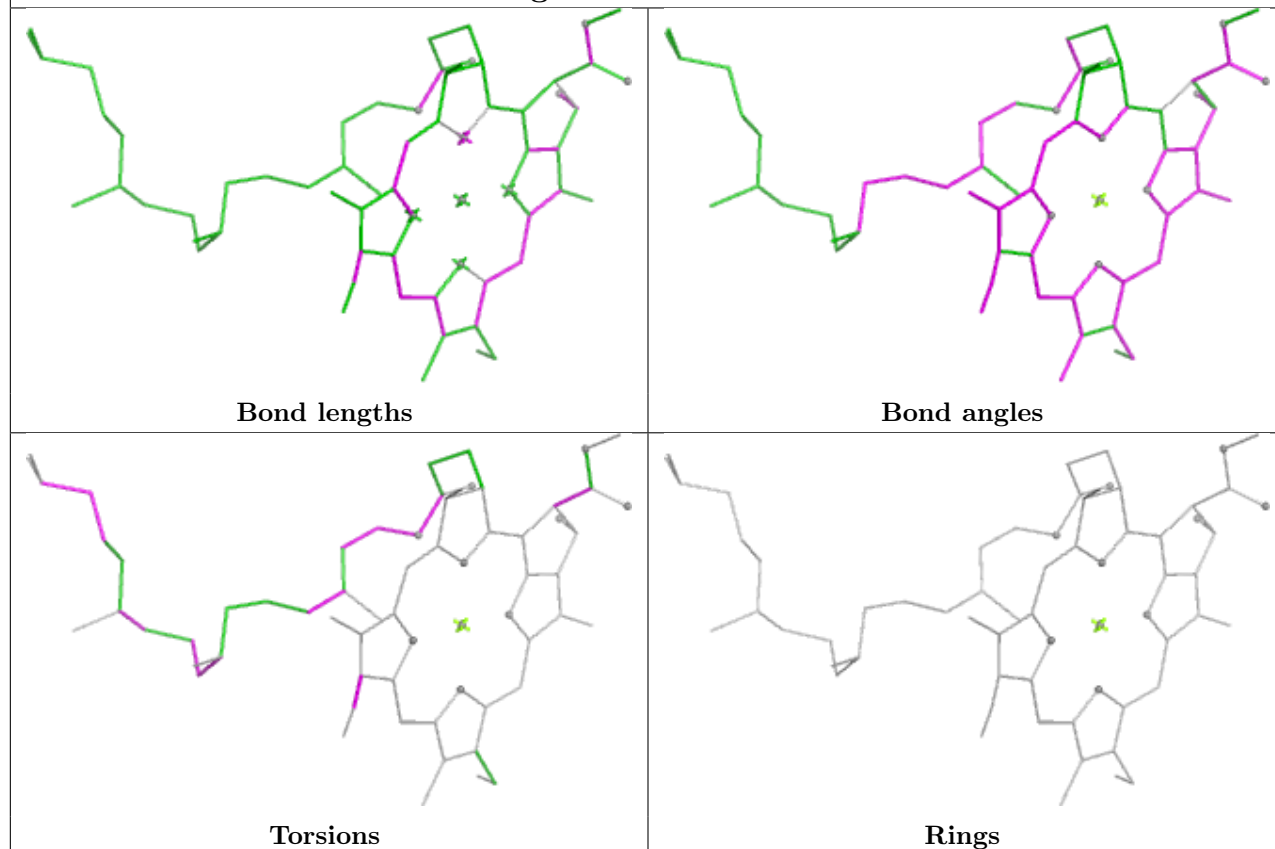


Rings

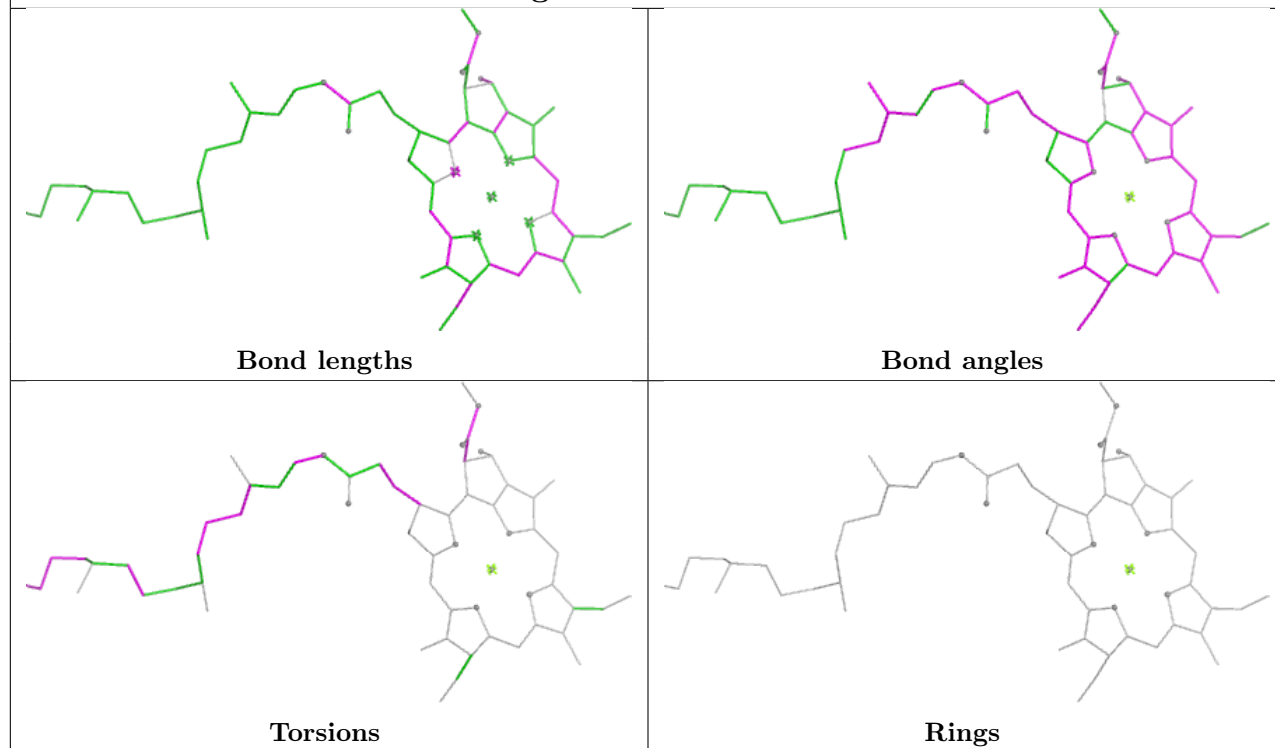




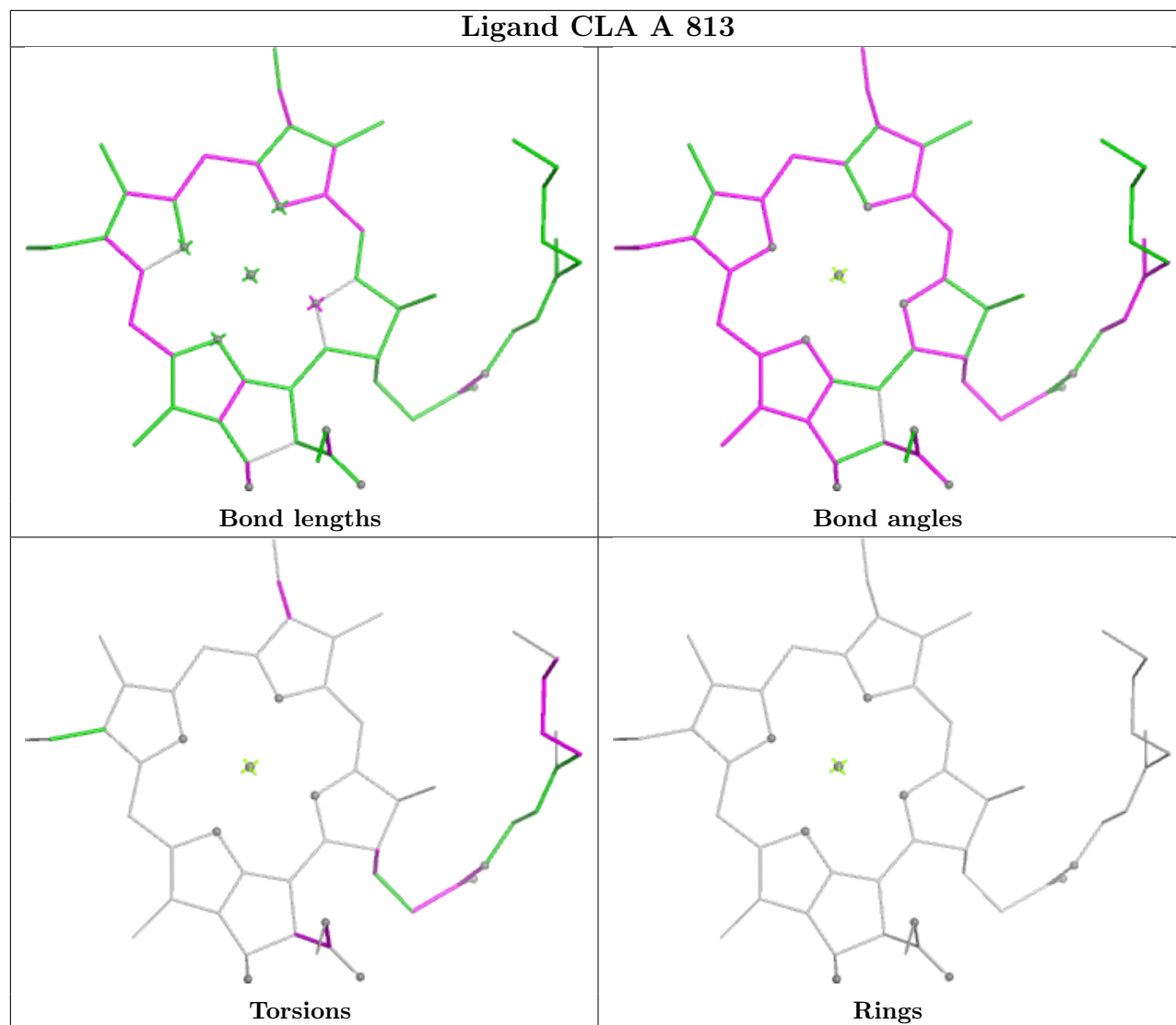
Ligand CLA A 841



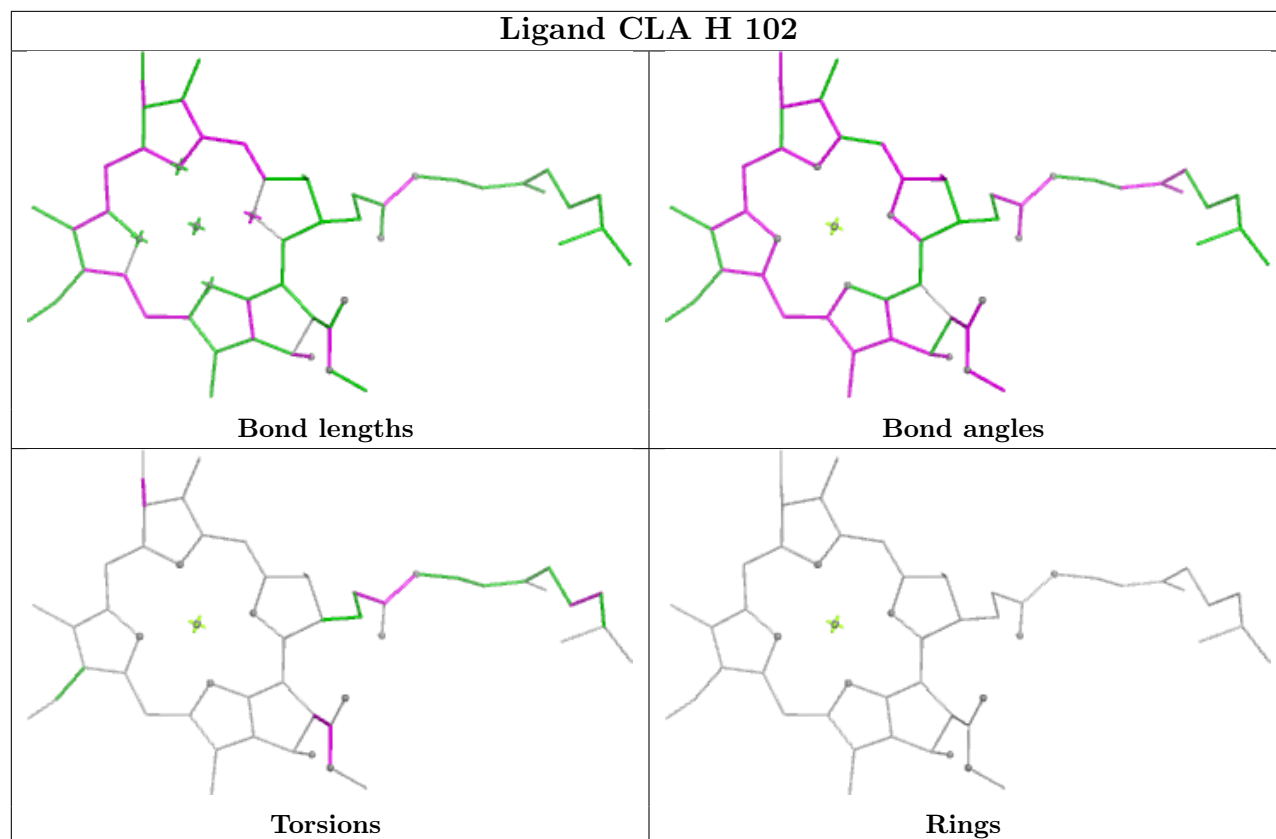
Ligand CLA B 850



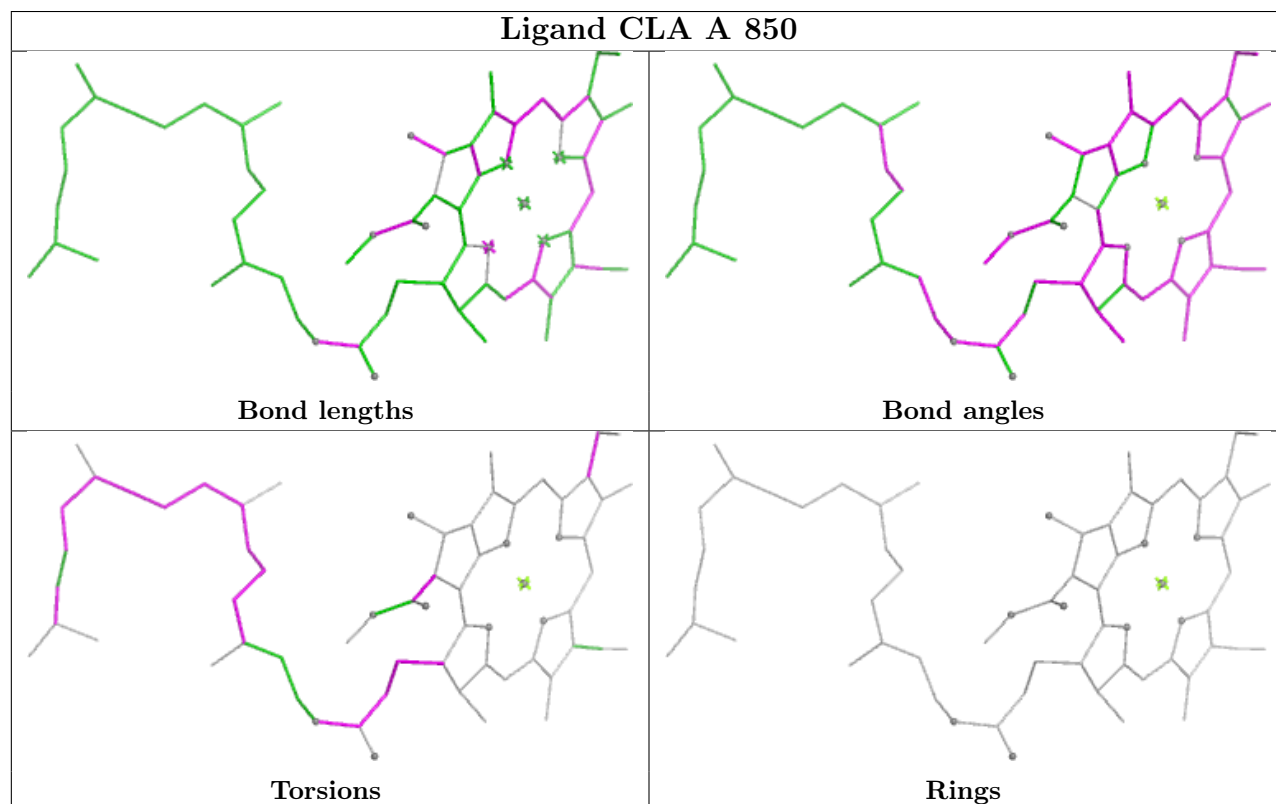
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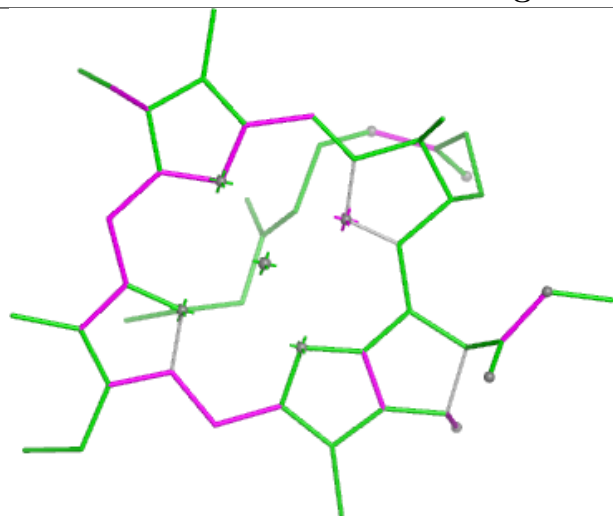
Ligand CLA H 102



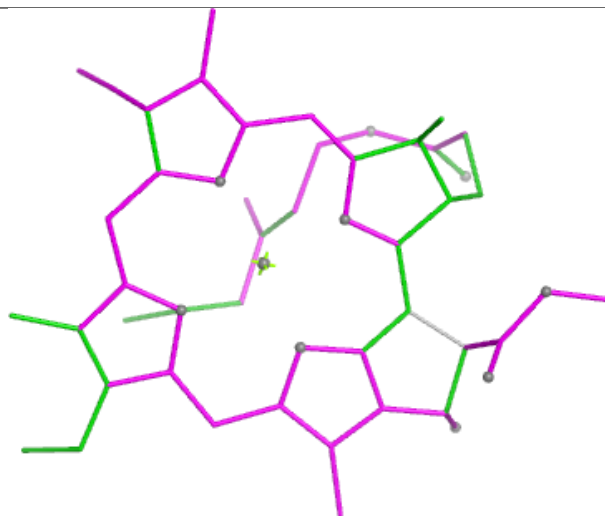
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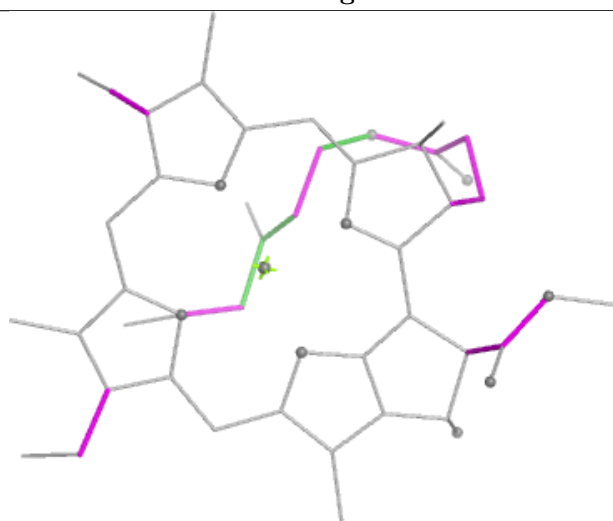
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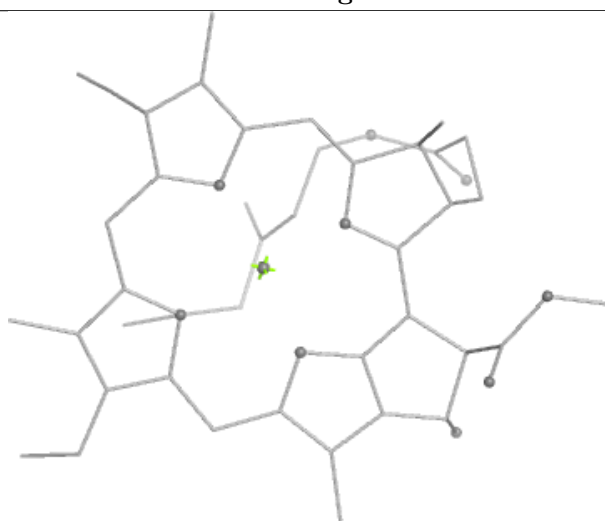
Bond lengths



Bond angles

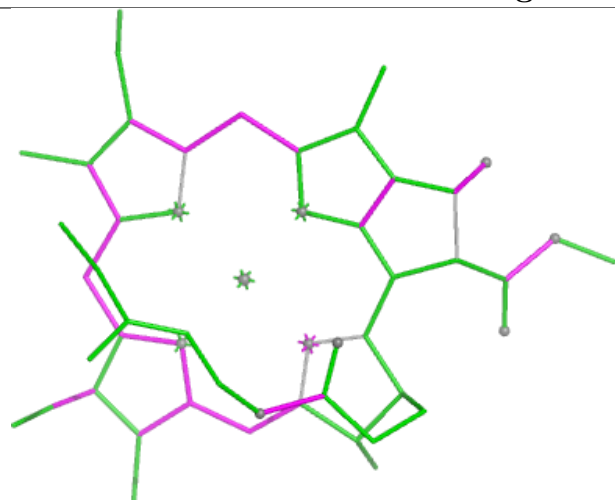


Torsions

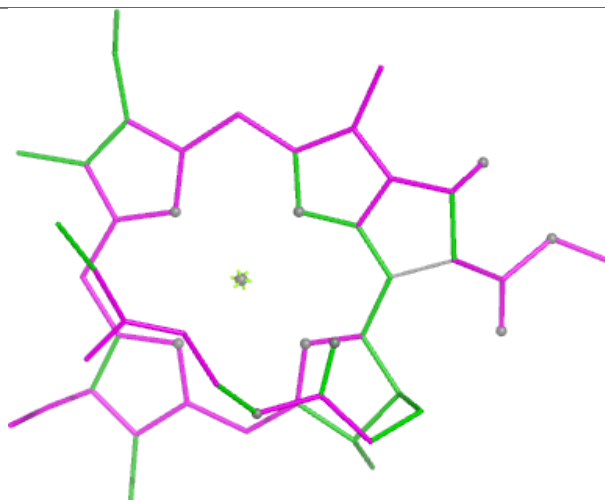


Rings

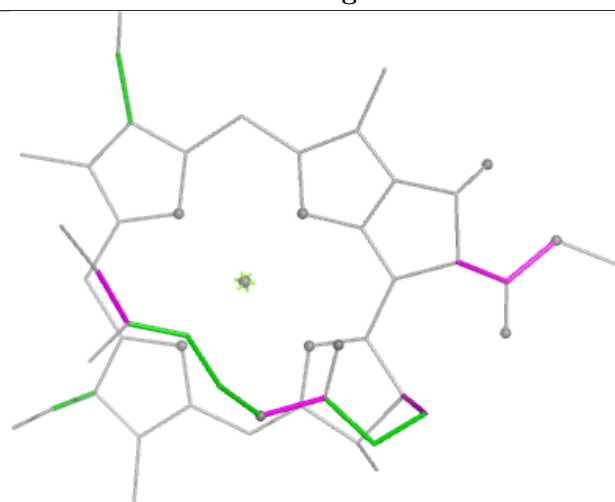
Ligand CLA A 820



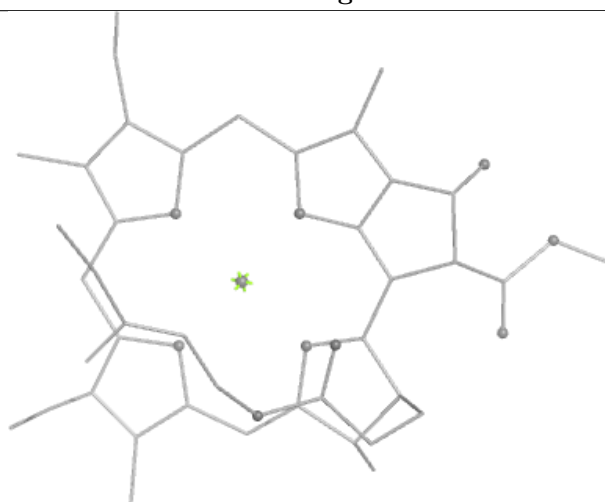
Bond lengths



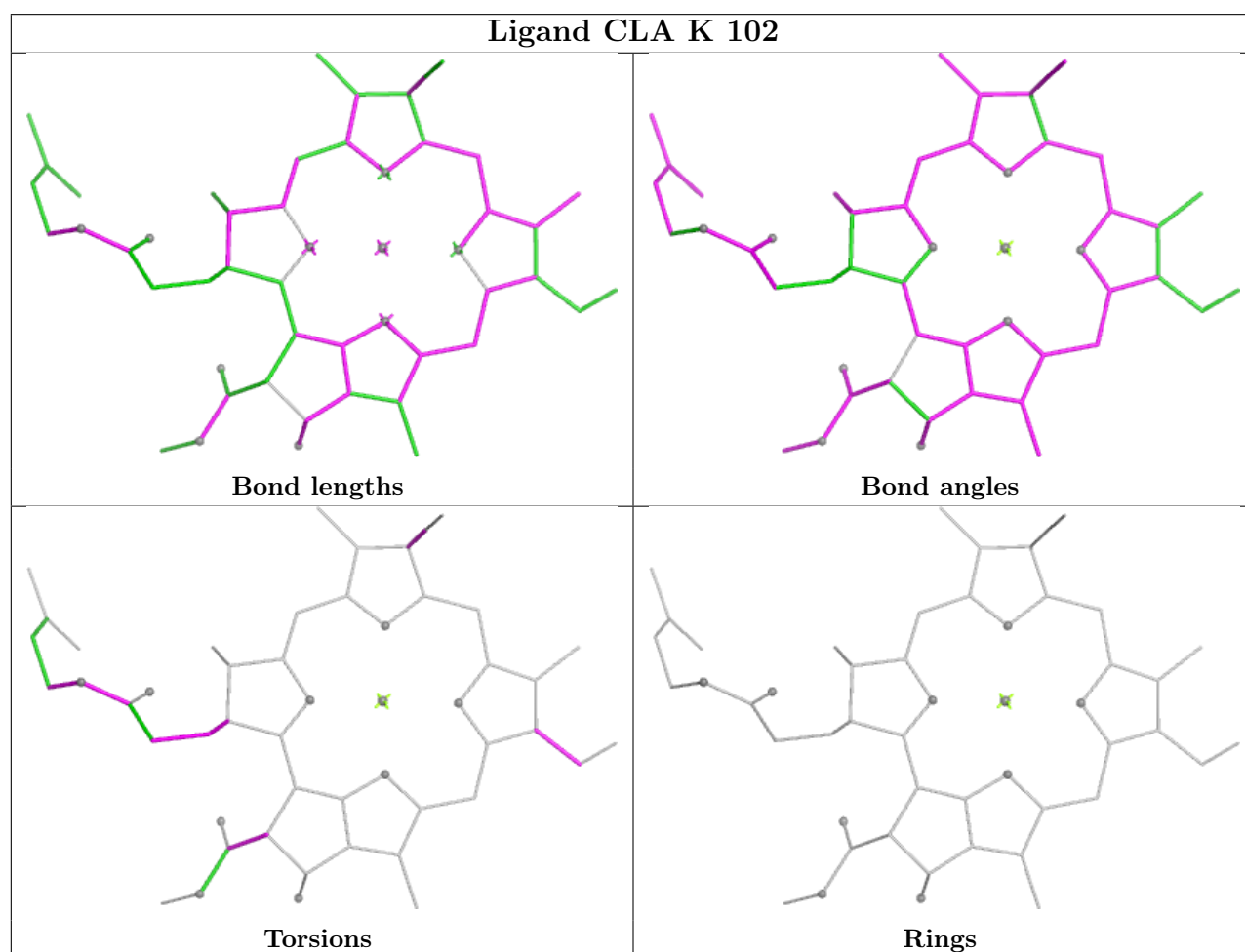
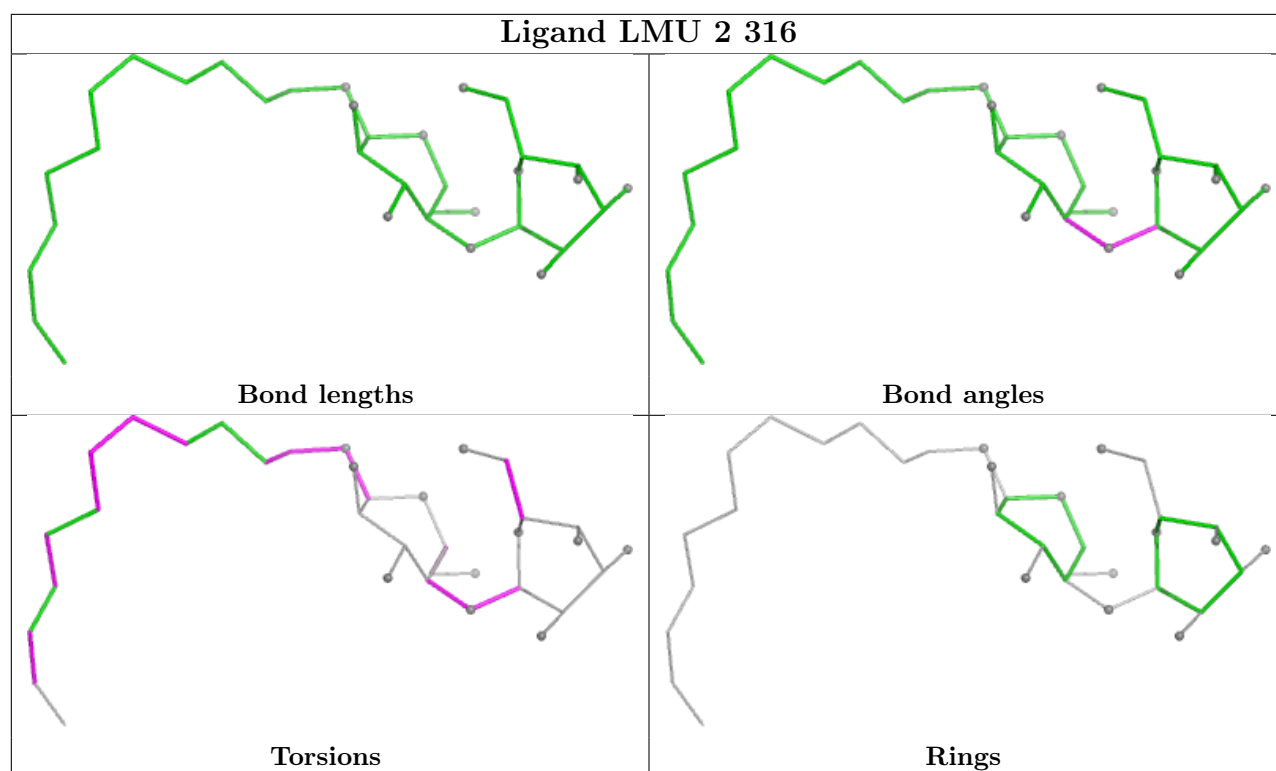
Bond angles



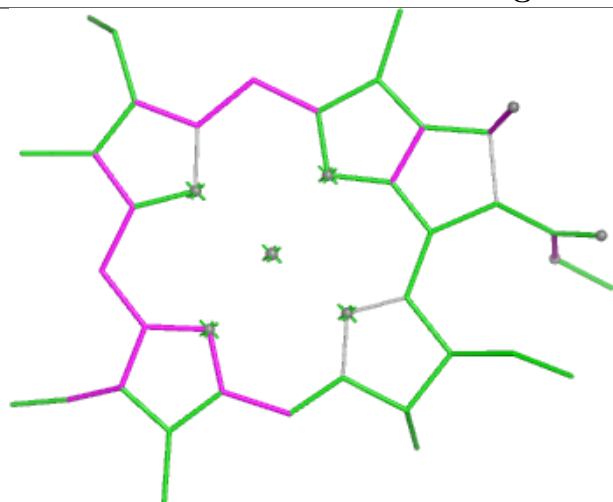
Torsions



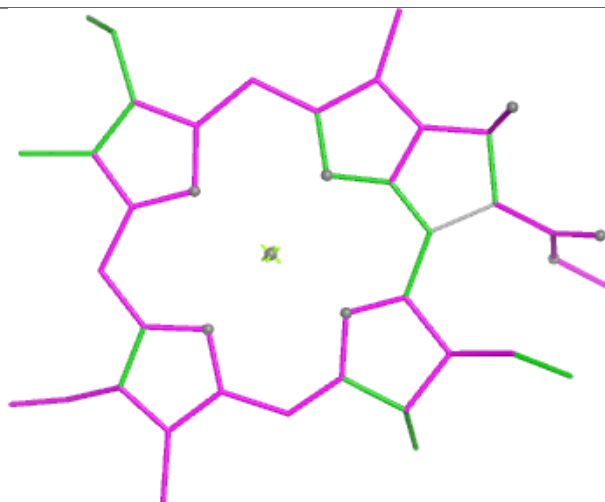
Rings



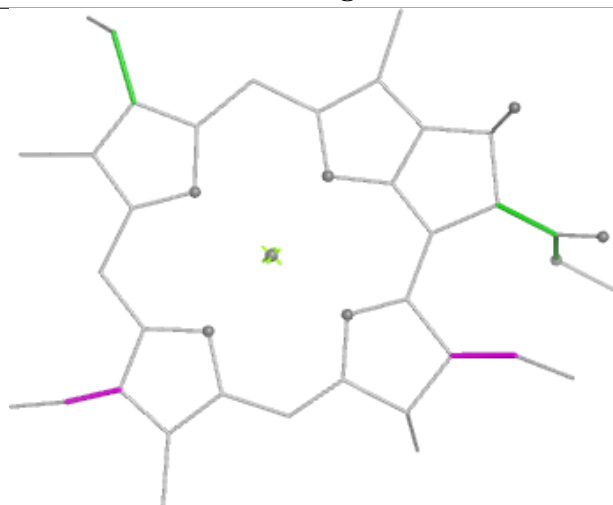
Ligand CLA A 821



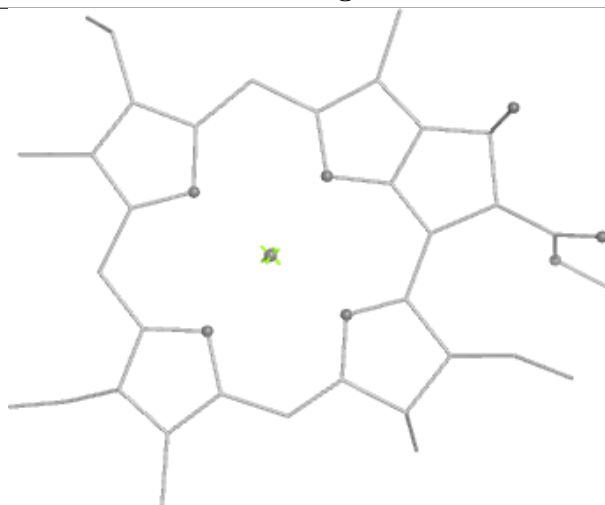
Bond lengths



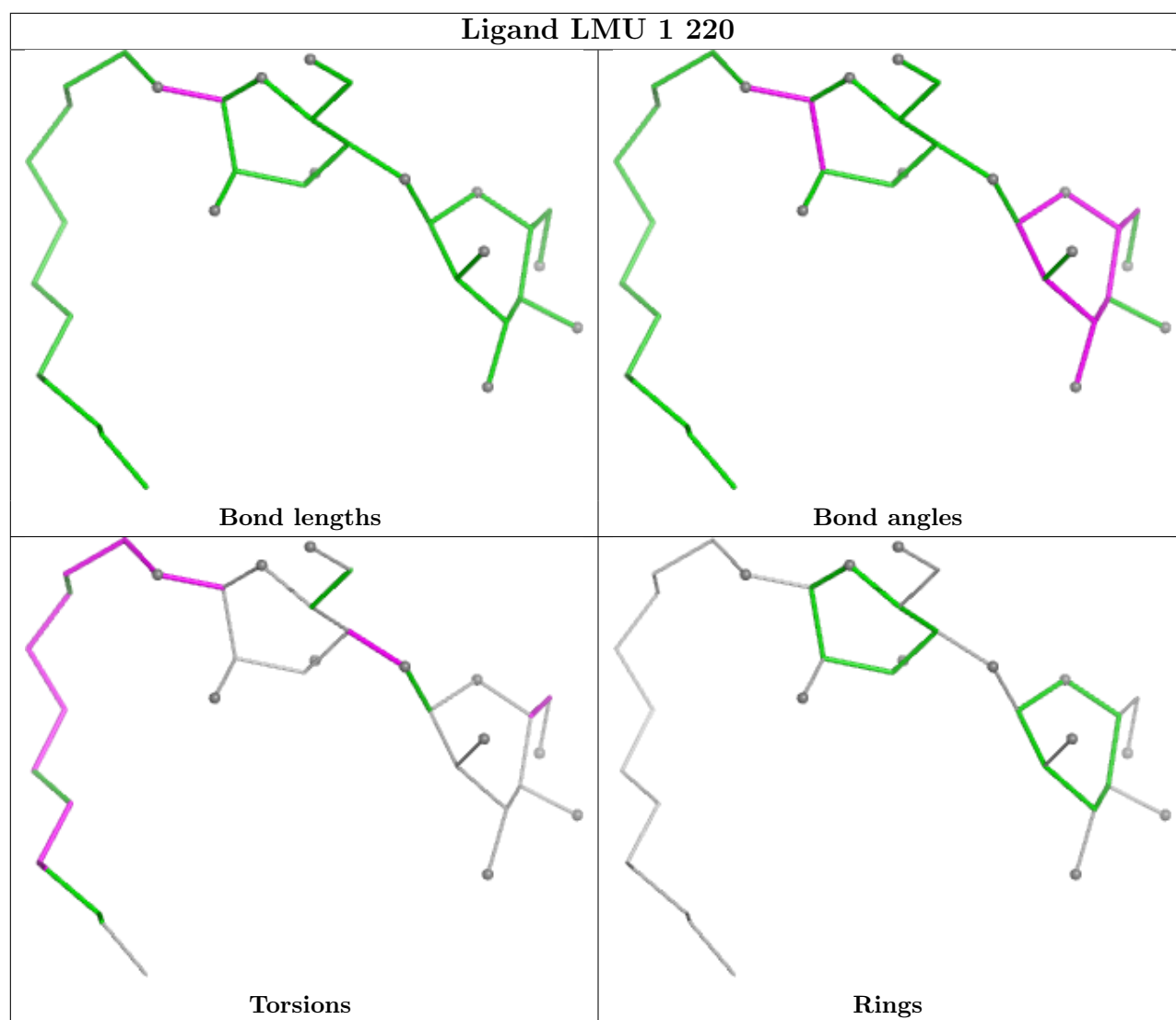
Bond angles



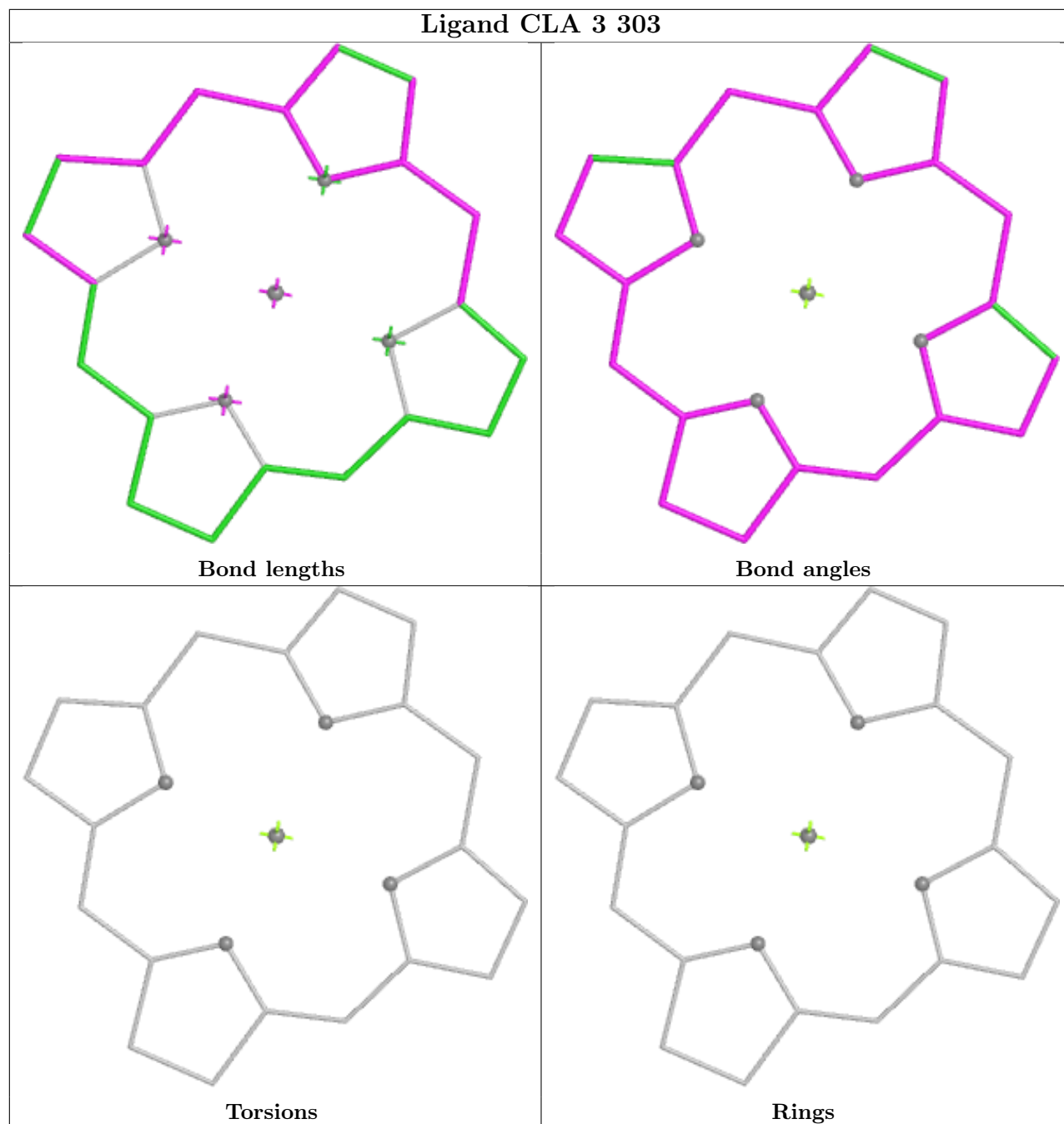
Torsions



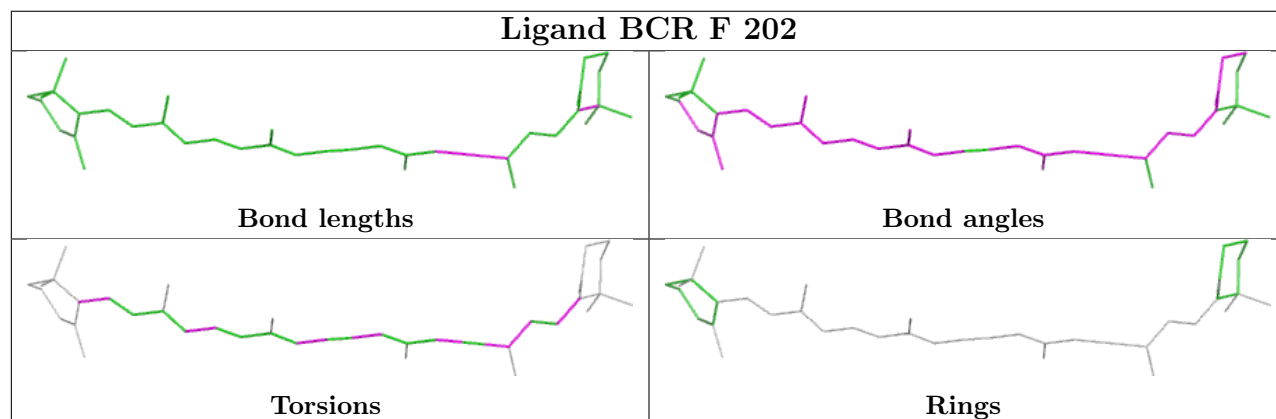
Rings

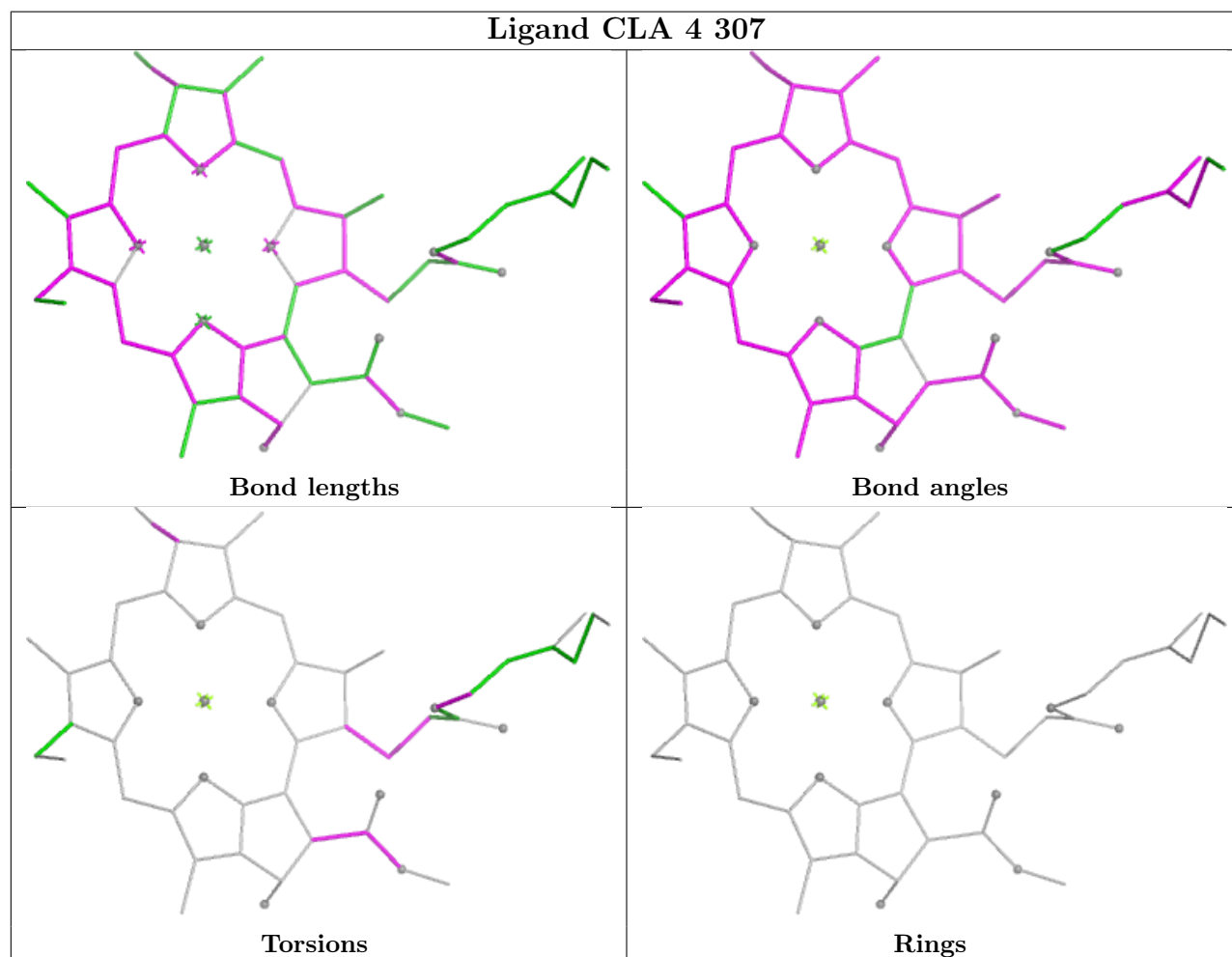
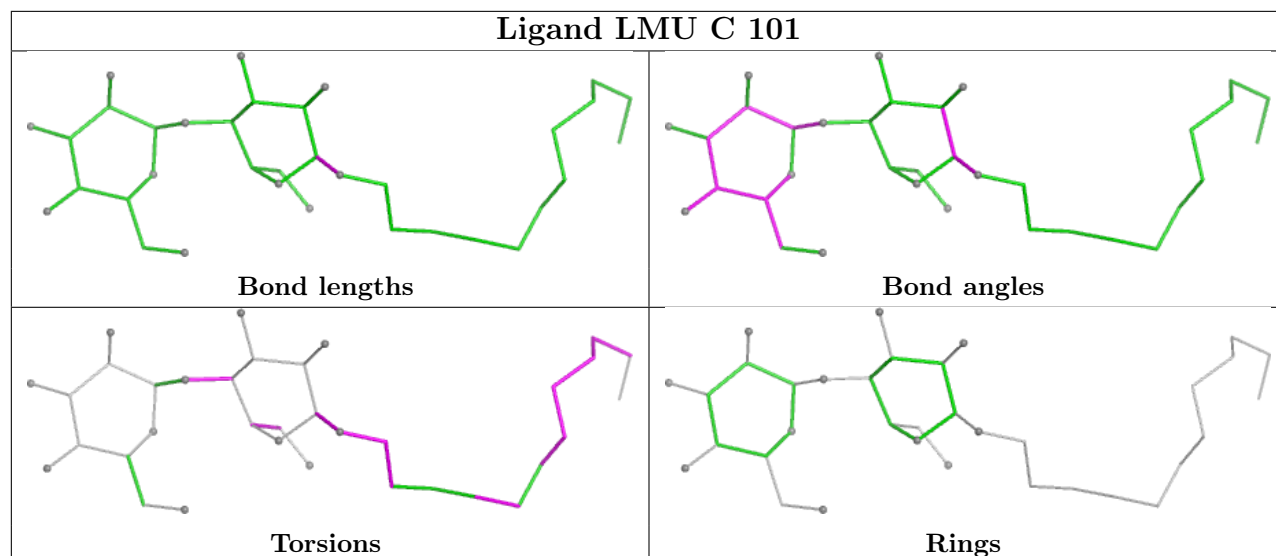


Ligand CLA 3 303

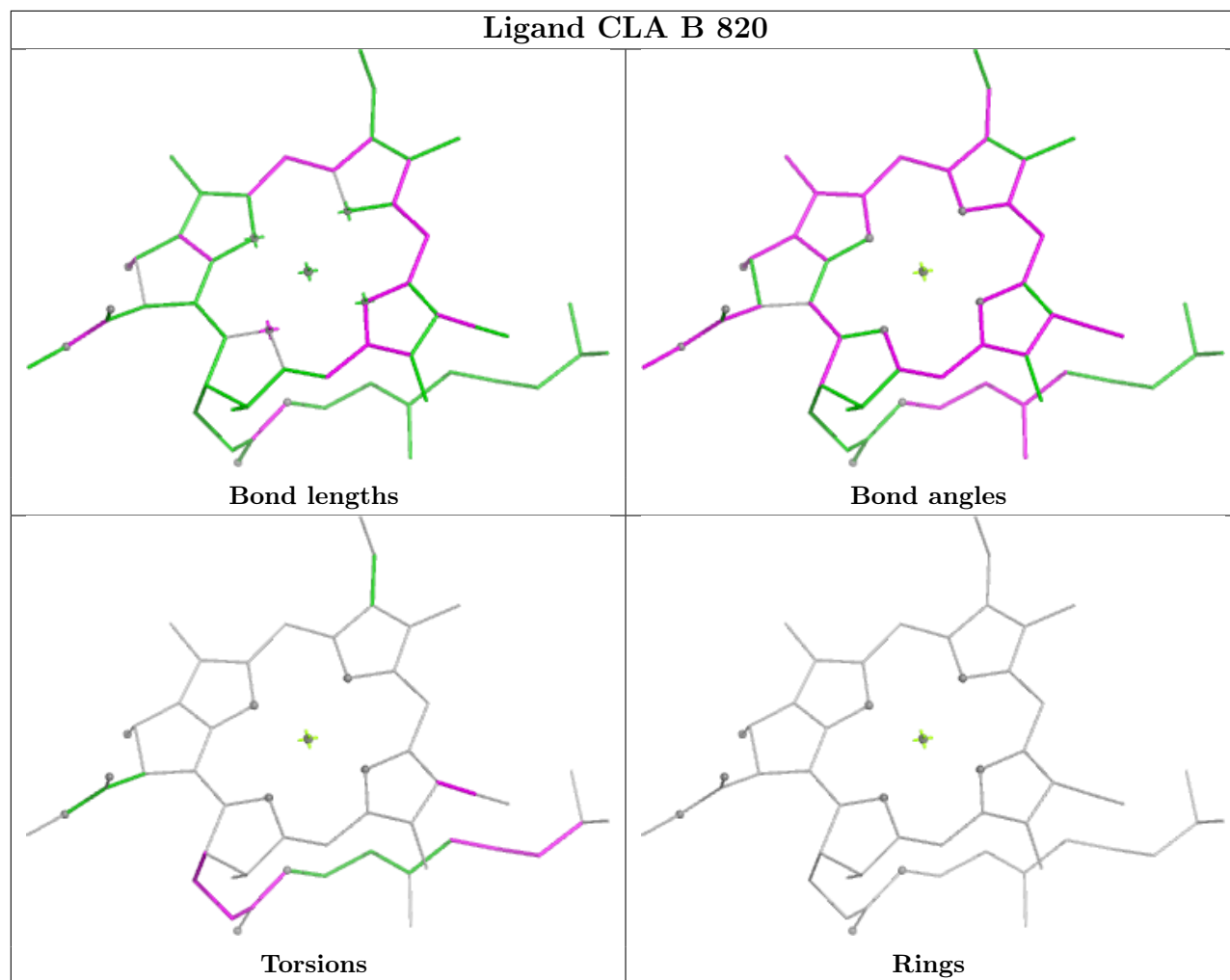


Ligand BCR F 202

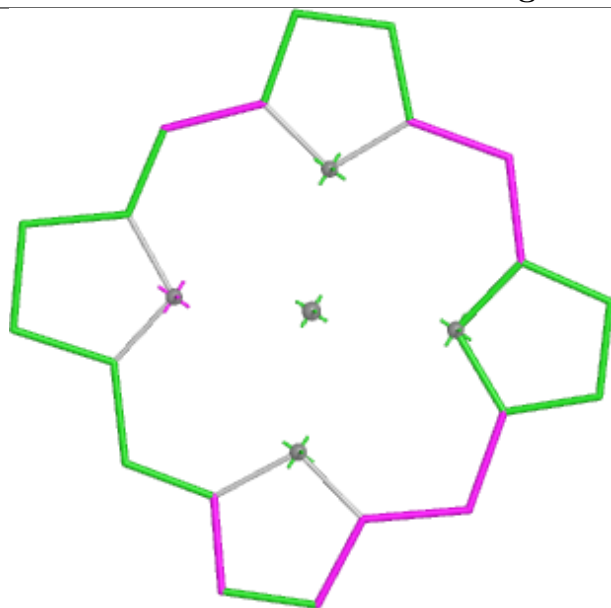




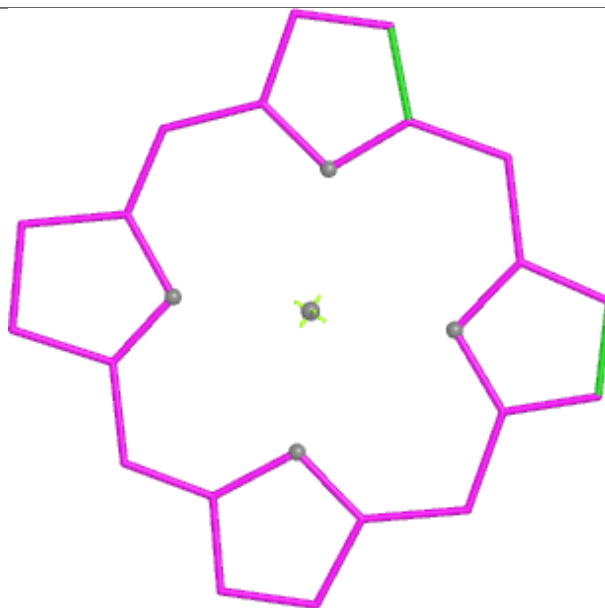
Ligand CLA B 820



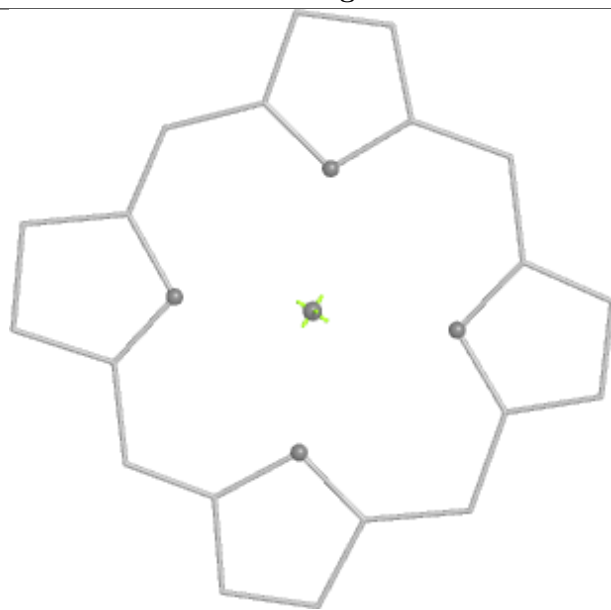
Ligand CLA 4 313



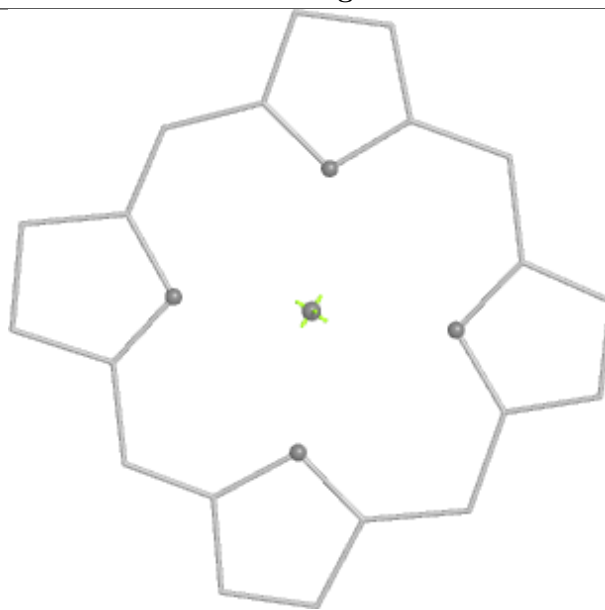
Bond lengths



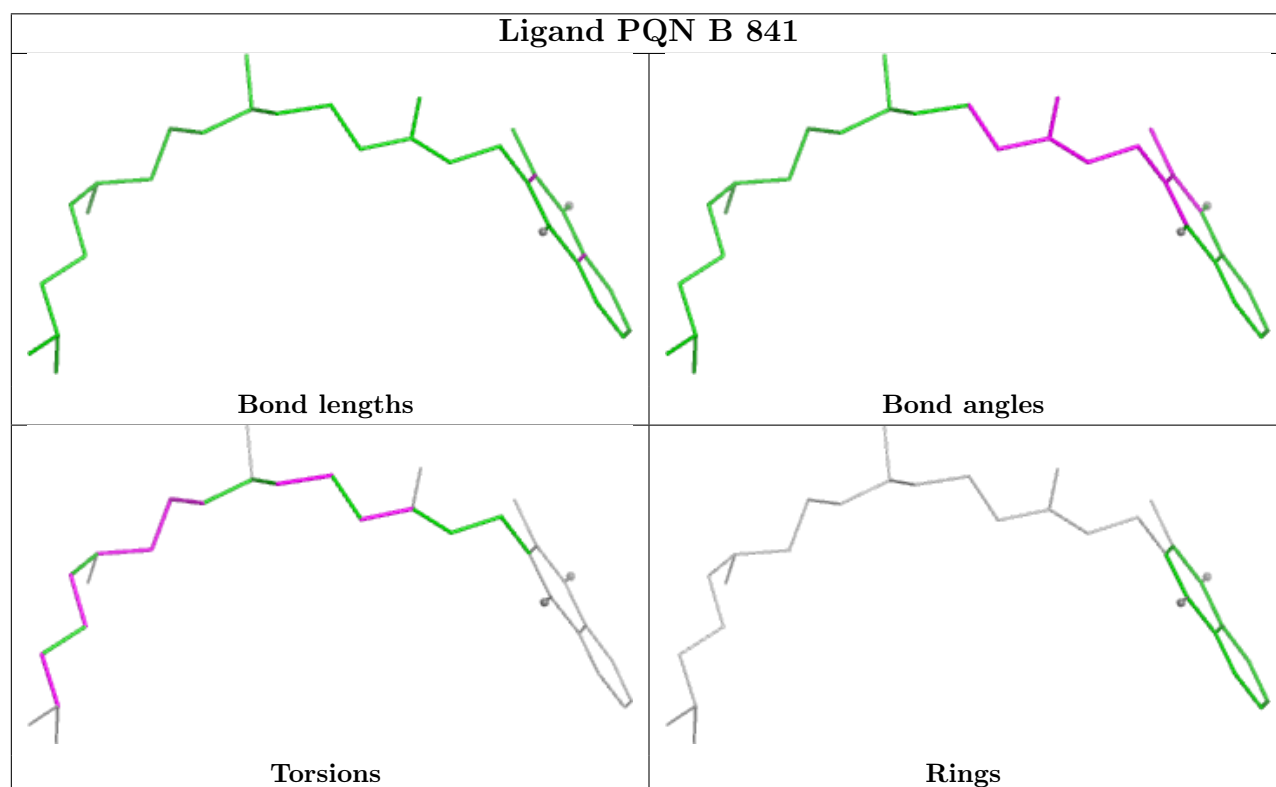
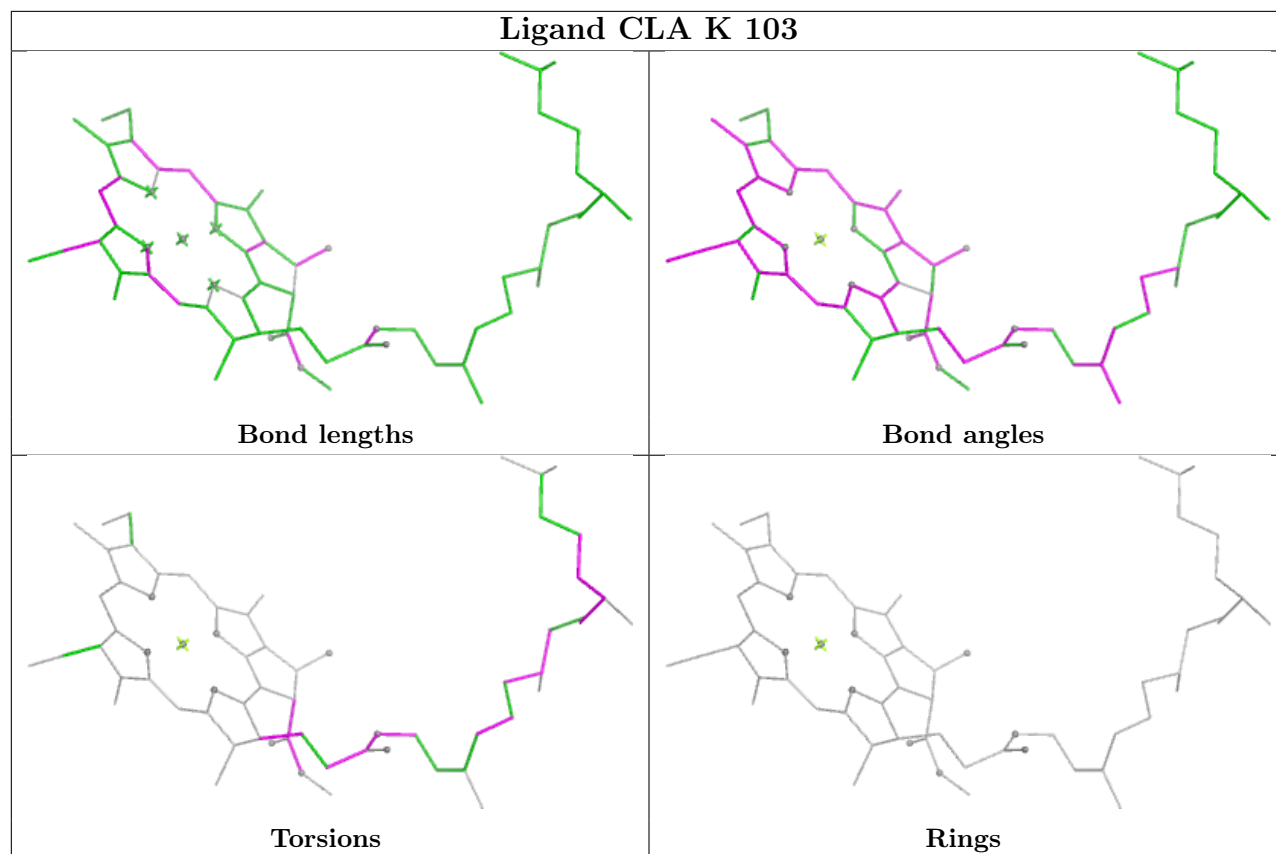
Bond angles

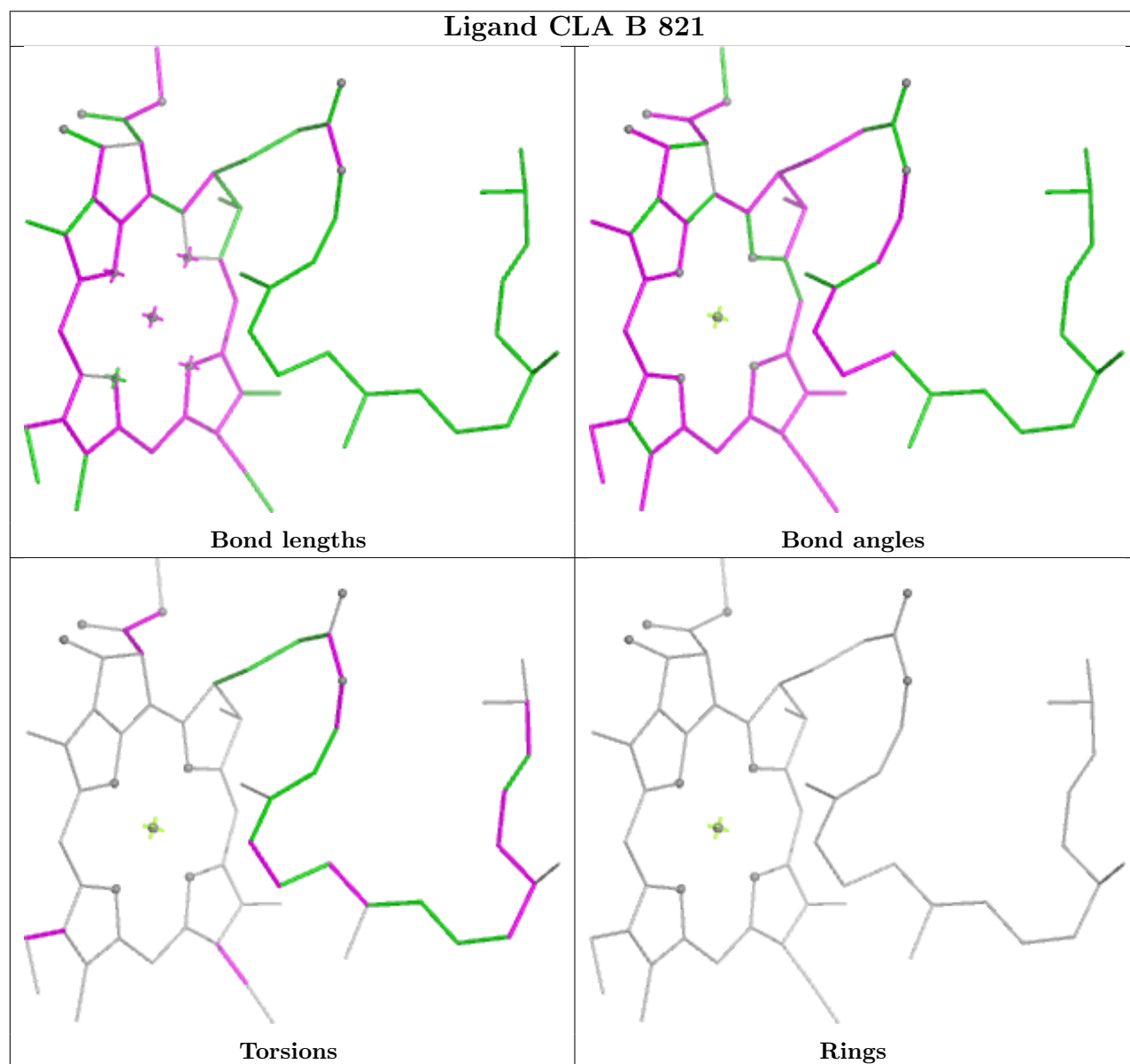
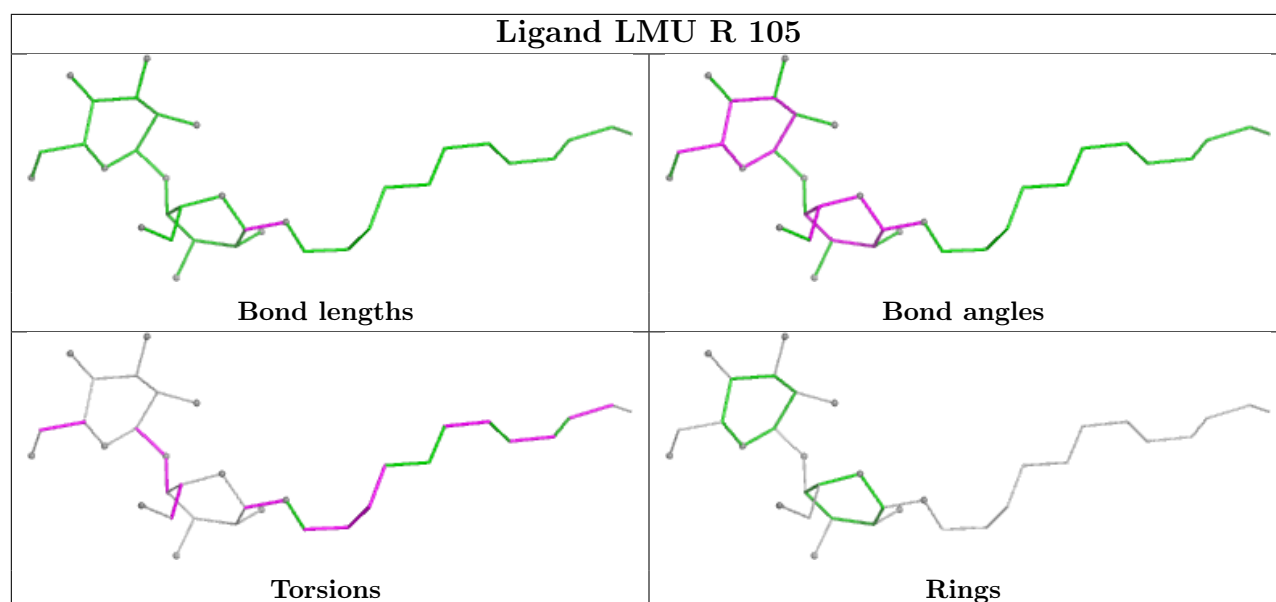


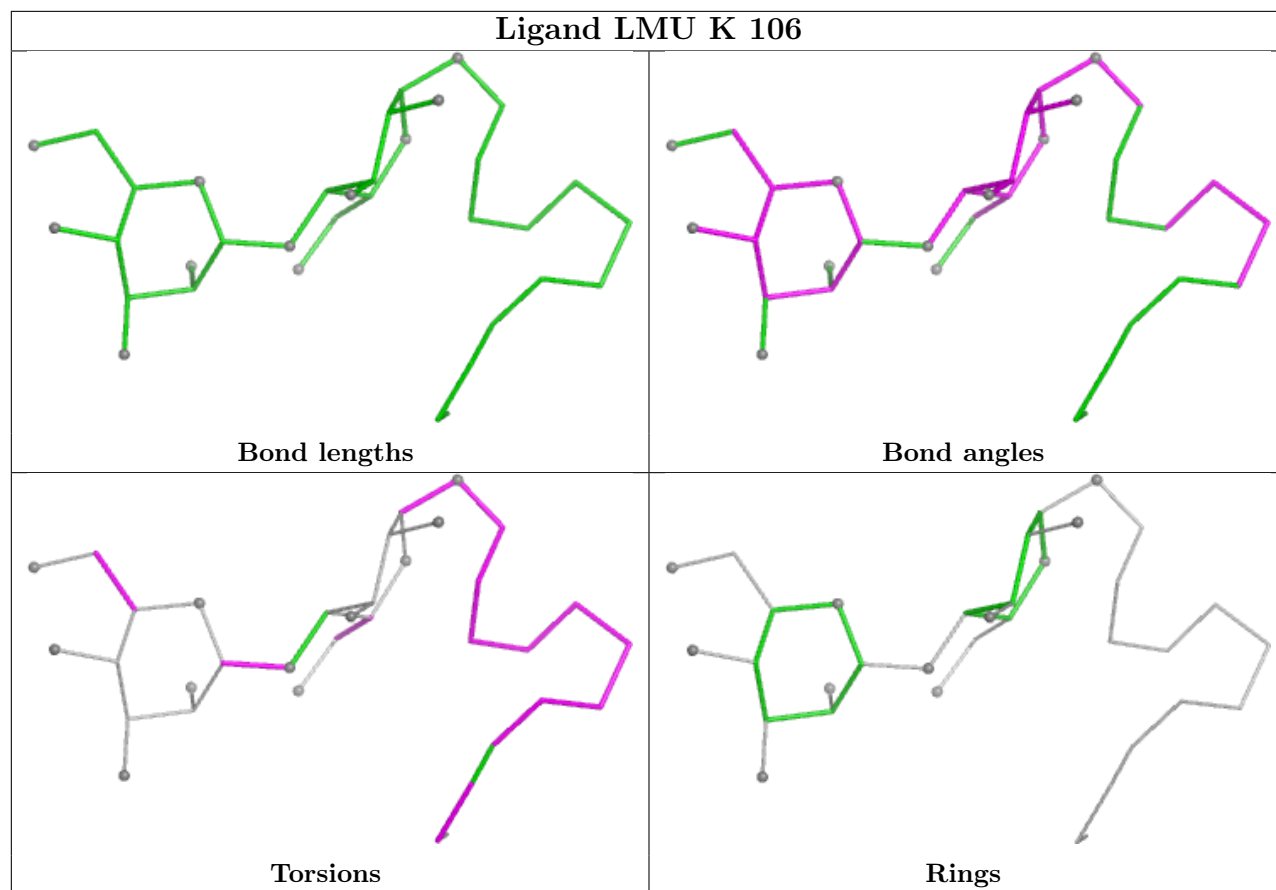
Torsions



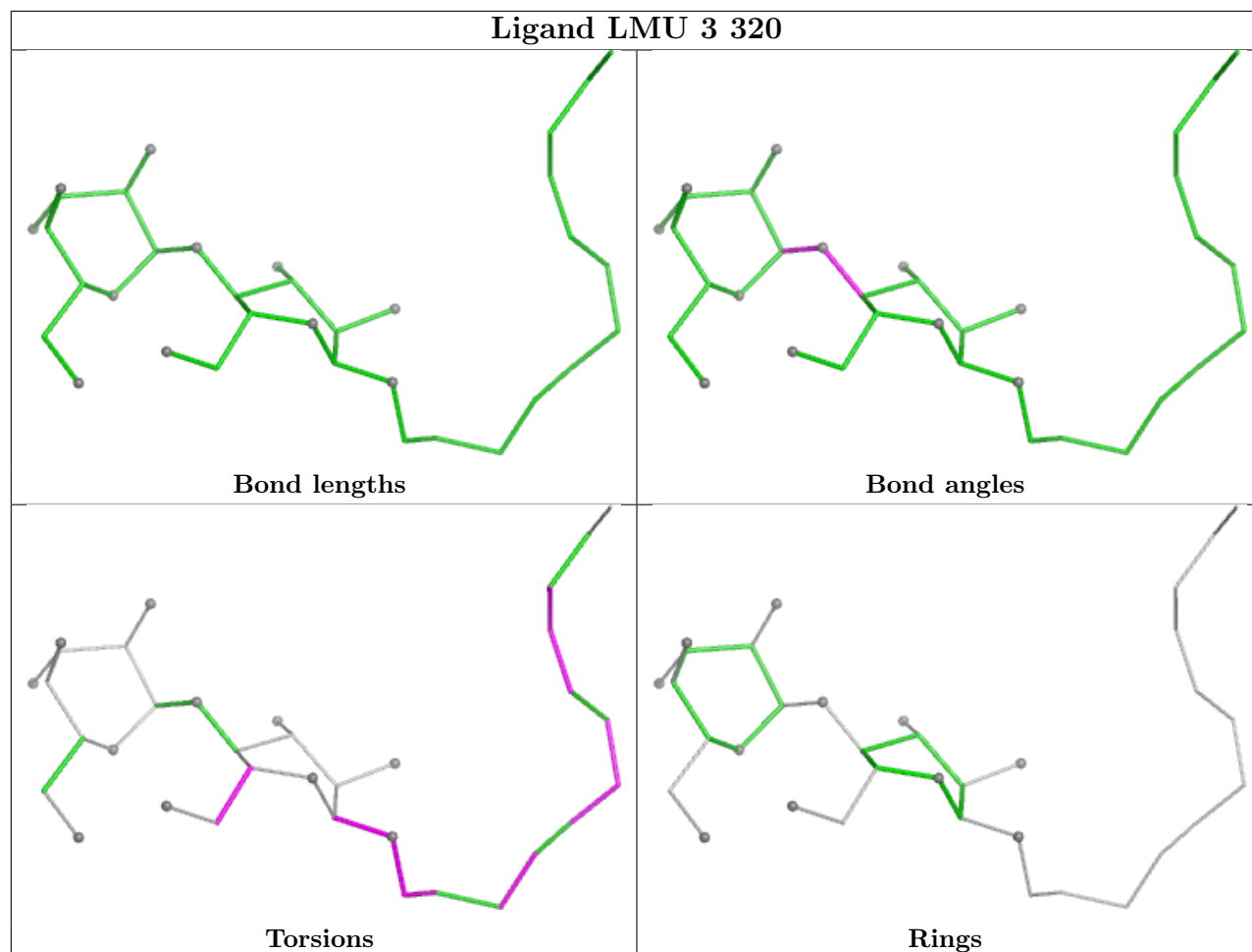
Rings



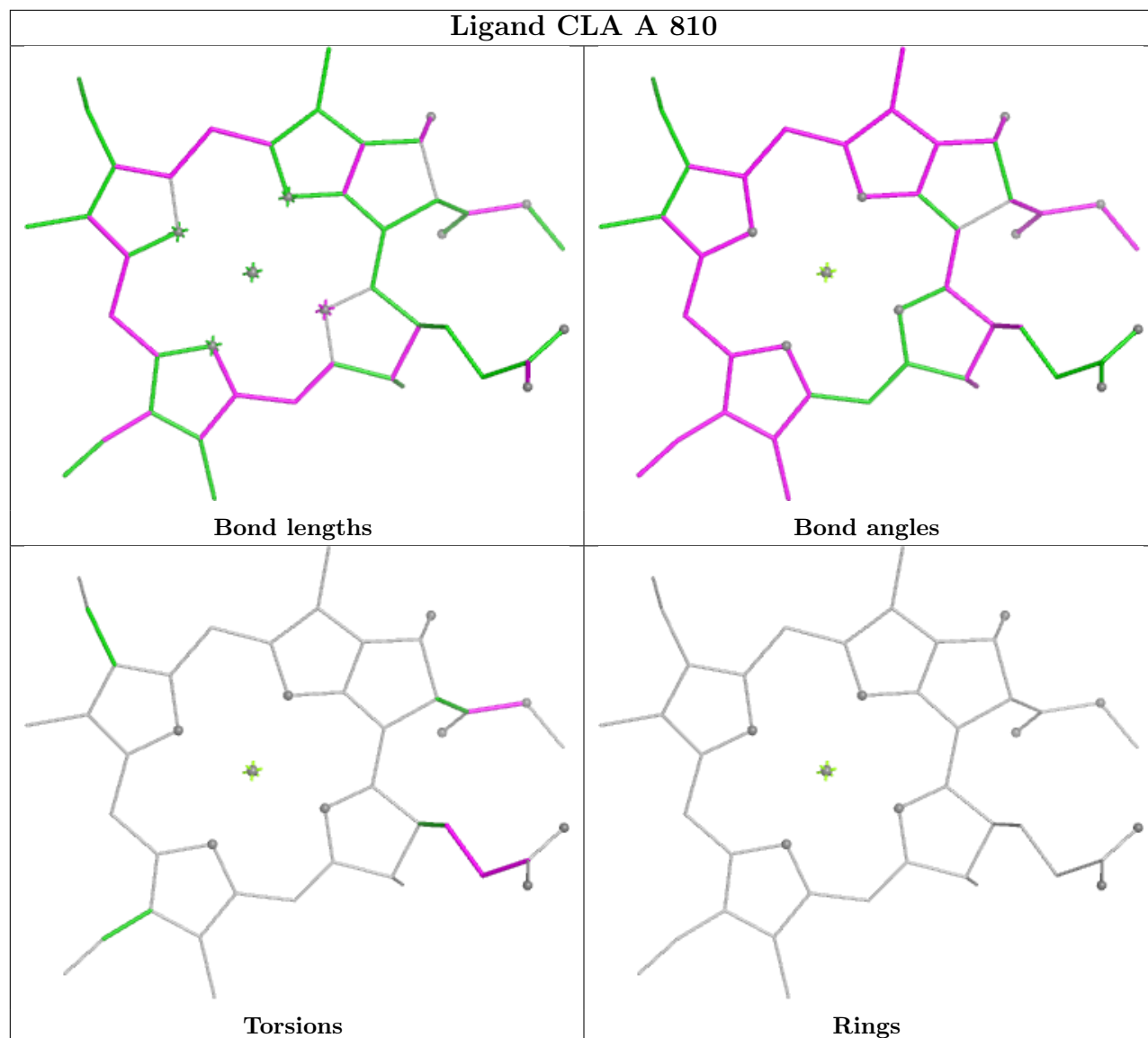


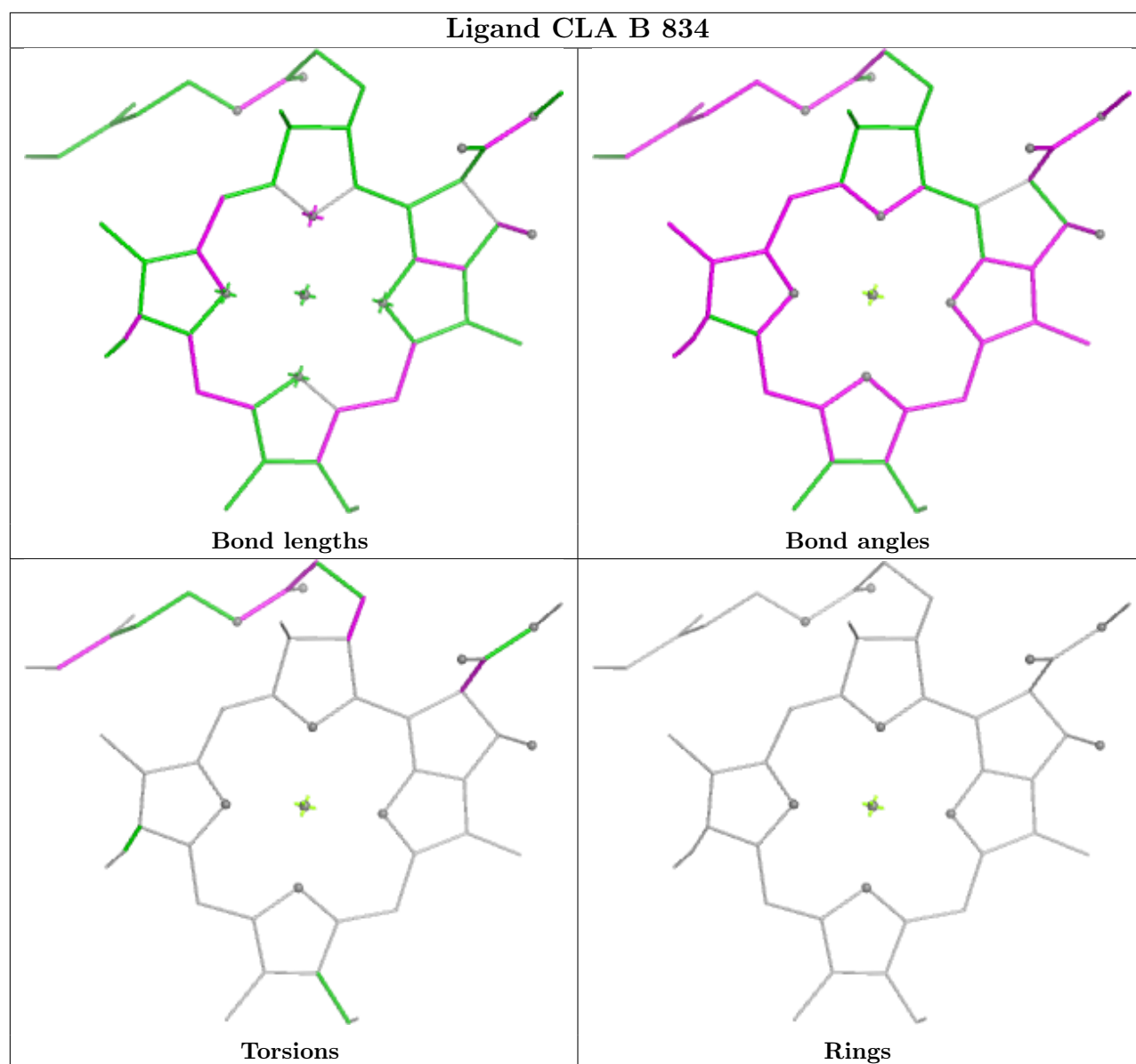


Ligand LMU 3 320

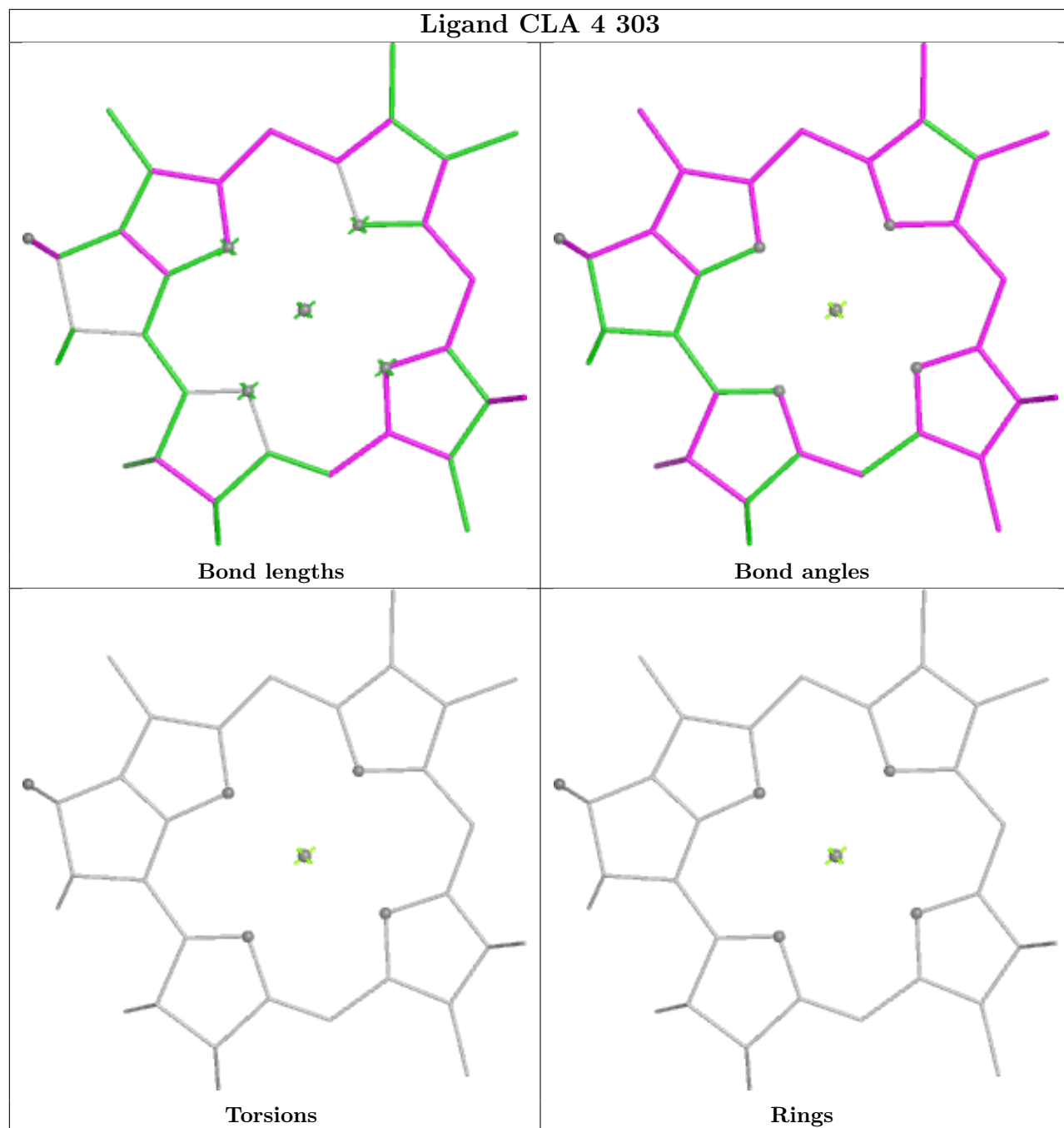


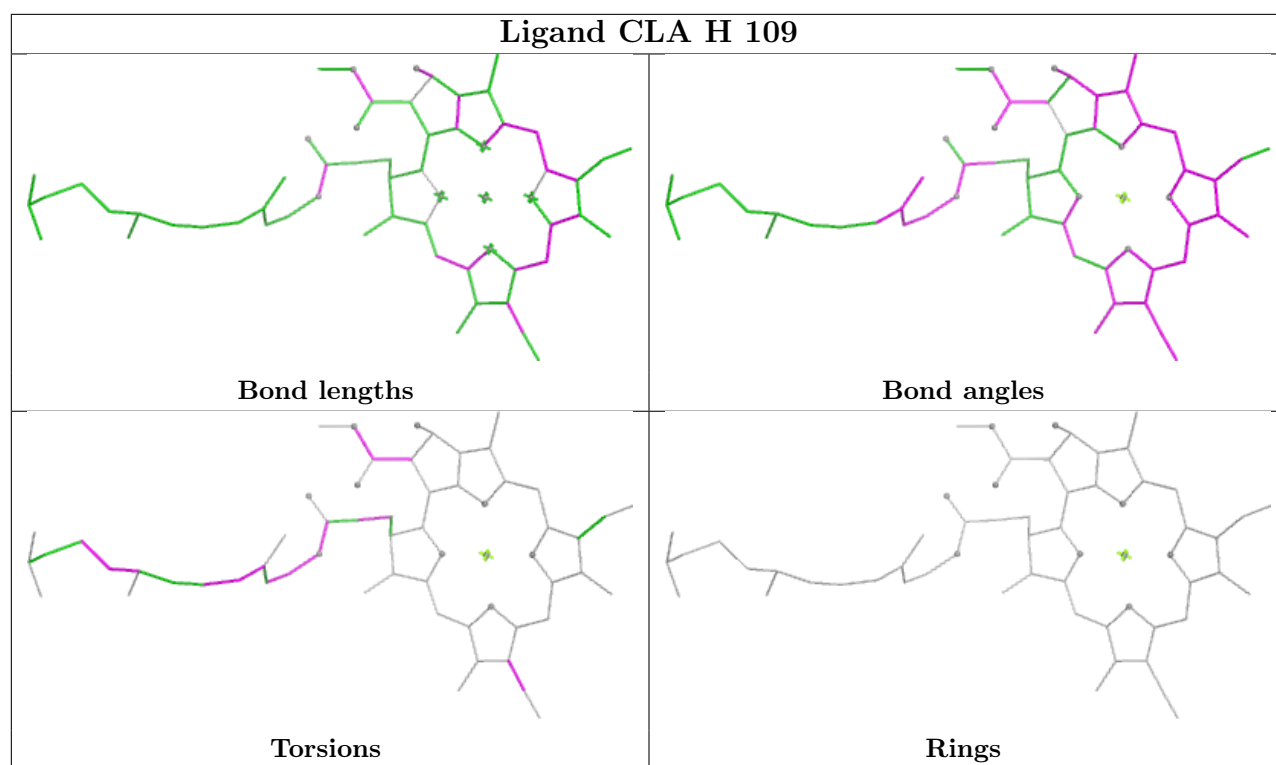
Ligand CLA A 810



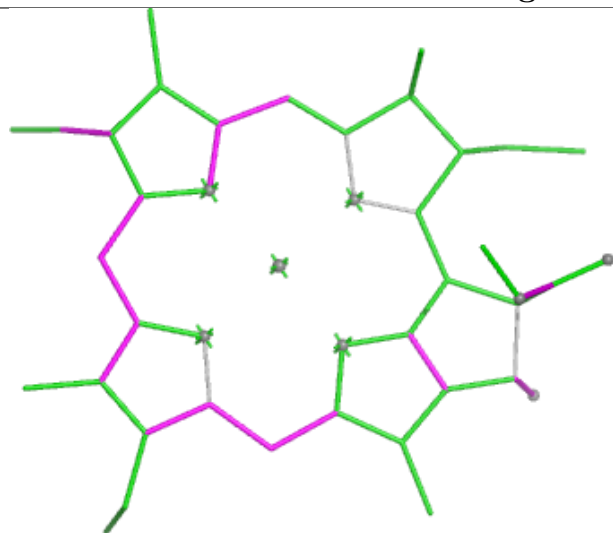


Ligand CLA 4 303

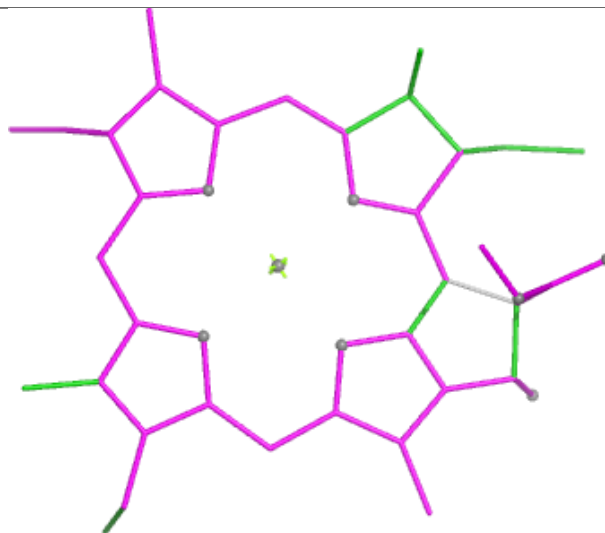




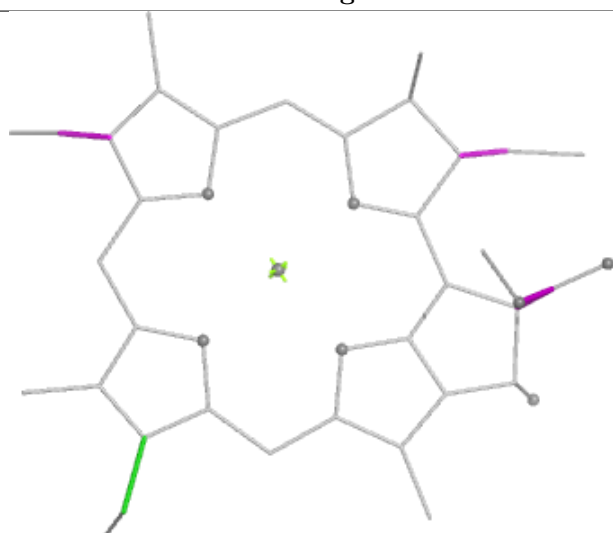
Ligand CLA 3 308



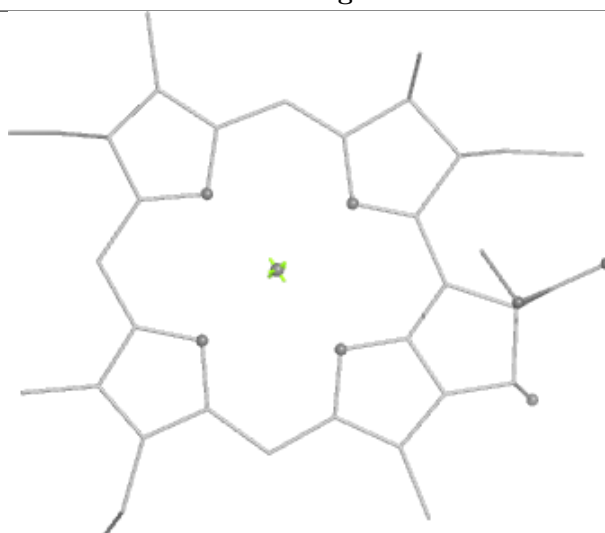
Bond lengths



Bond angles

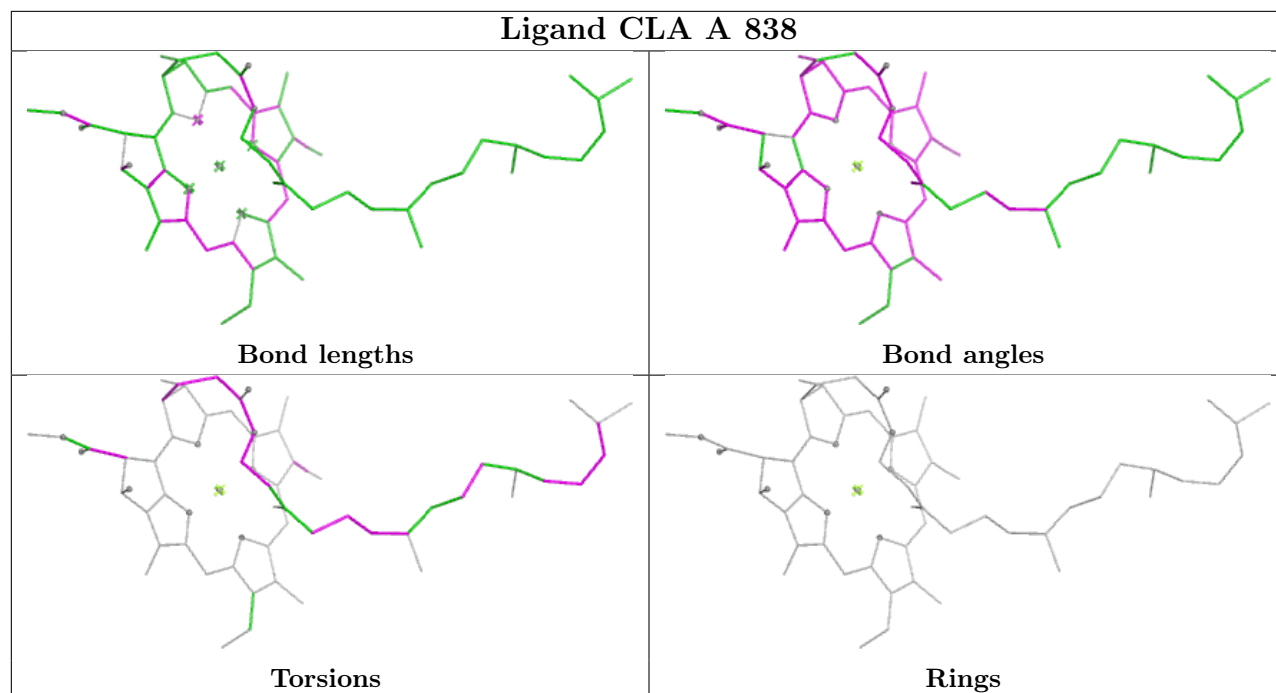


Torsions

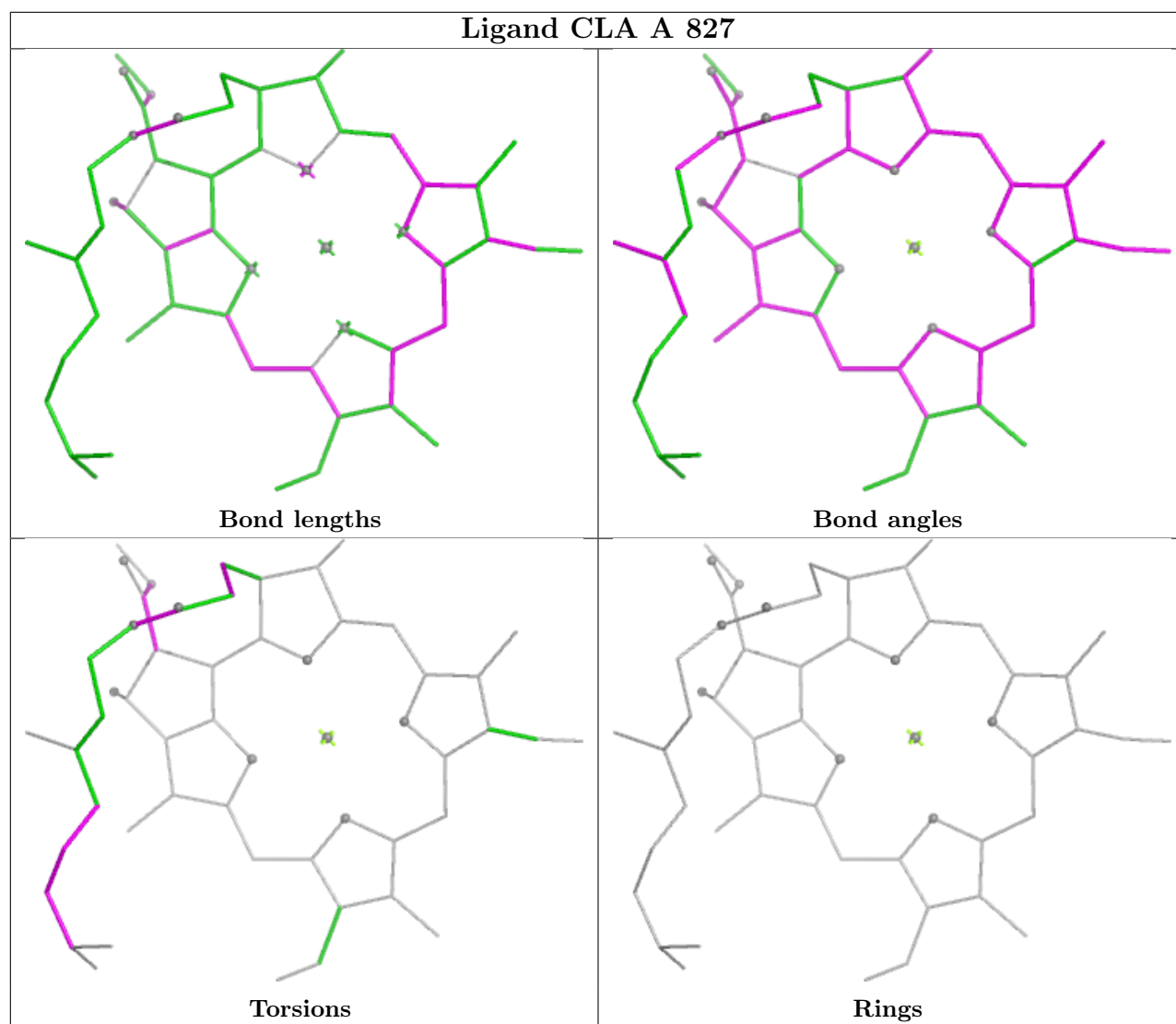


Rings

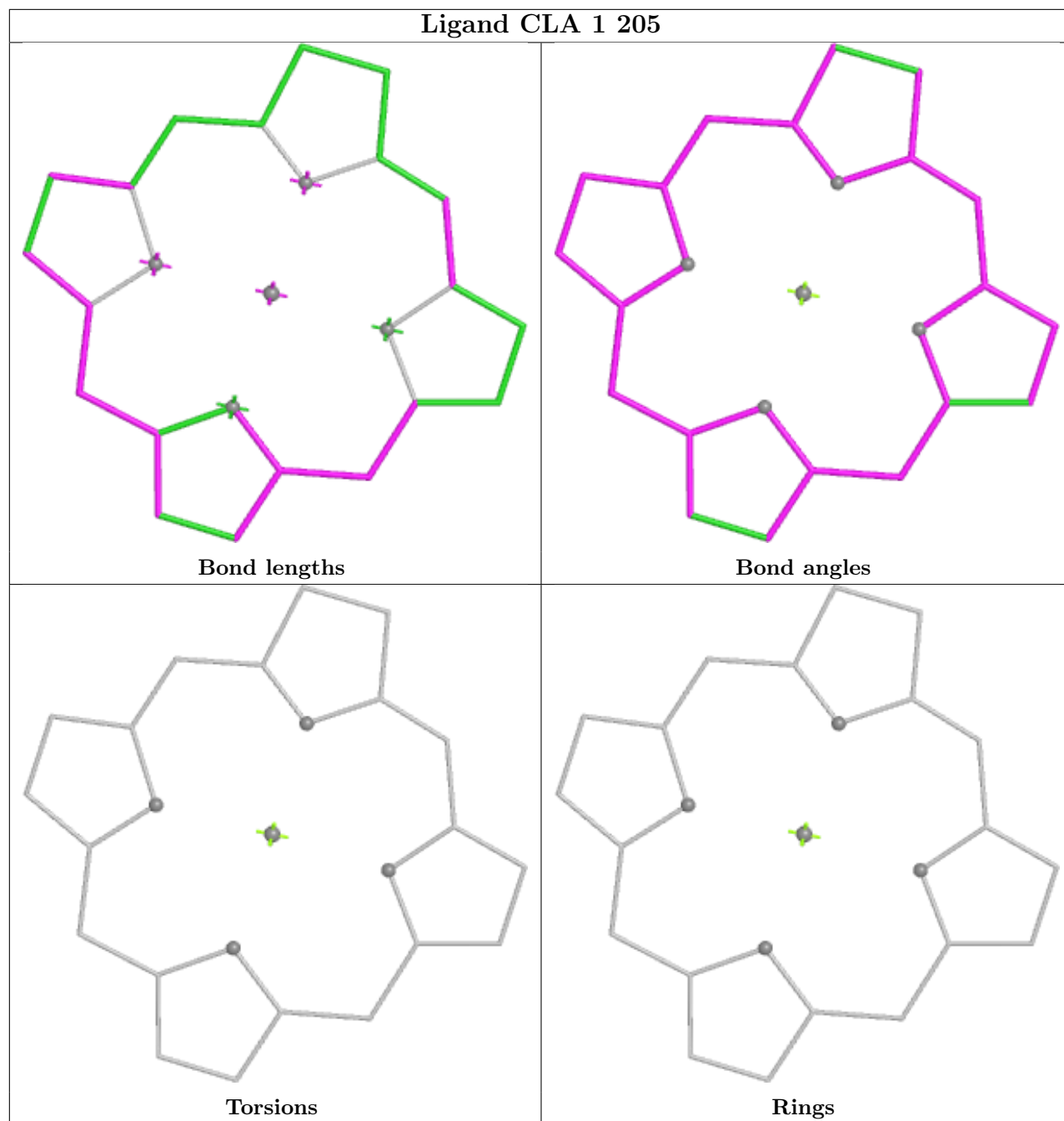
Ligand CLA A 838



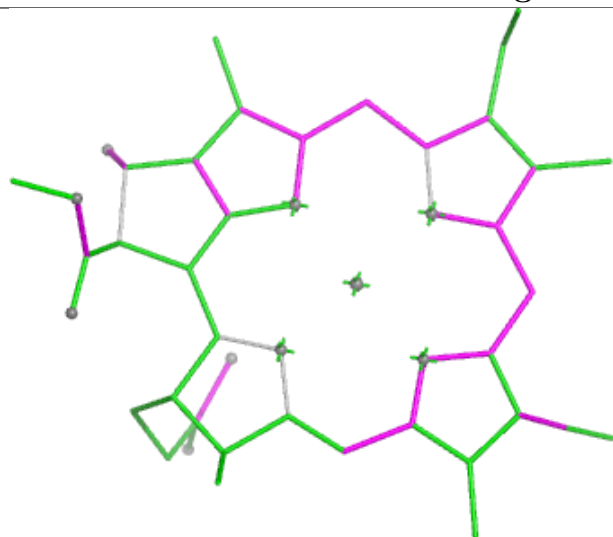
Ligand CLA A 827



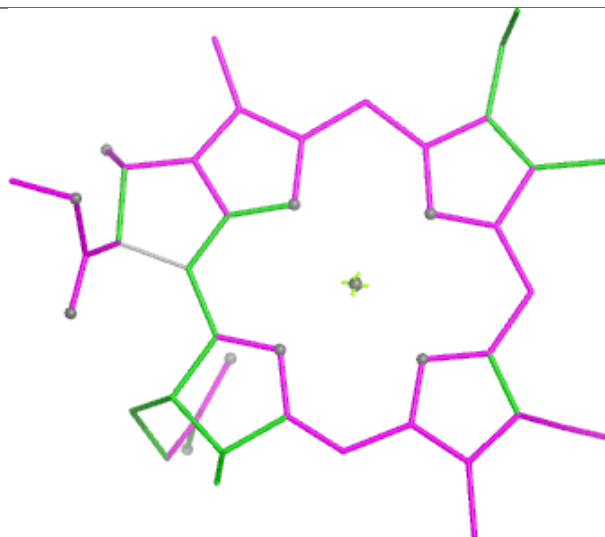
Ligand CLA 1 205



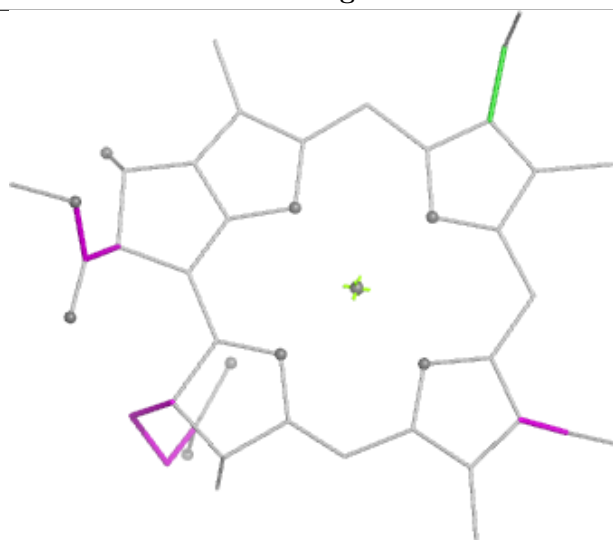
Ligand CLA B 832



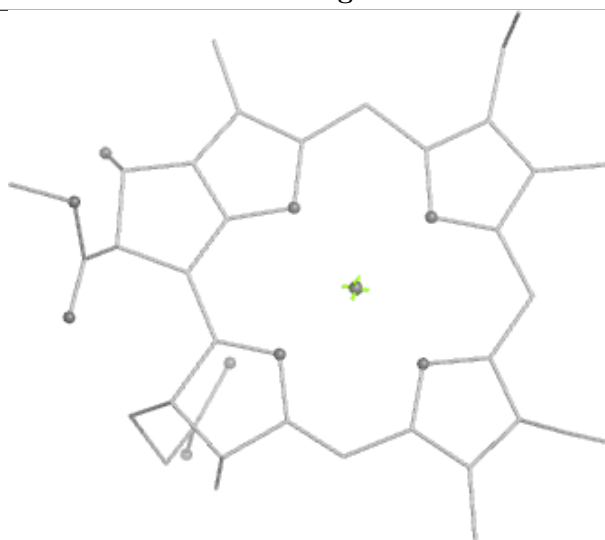
Bond lengths



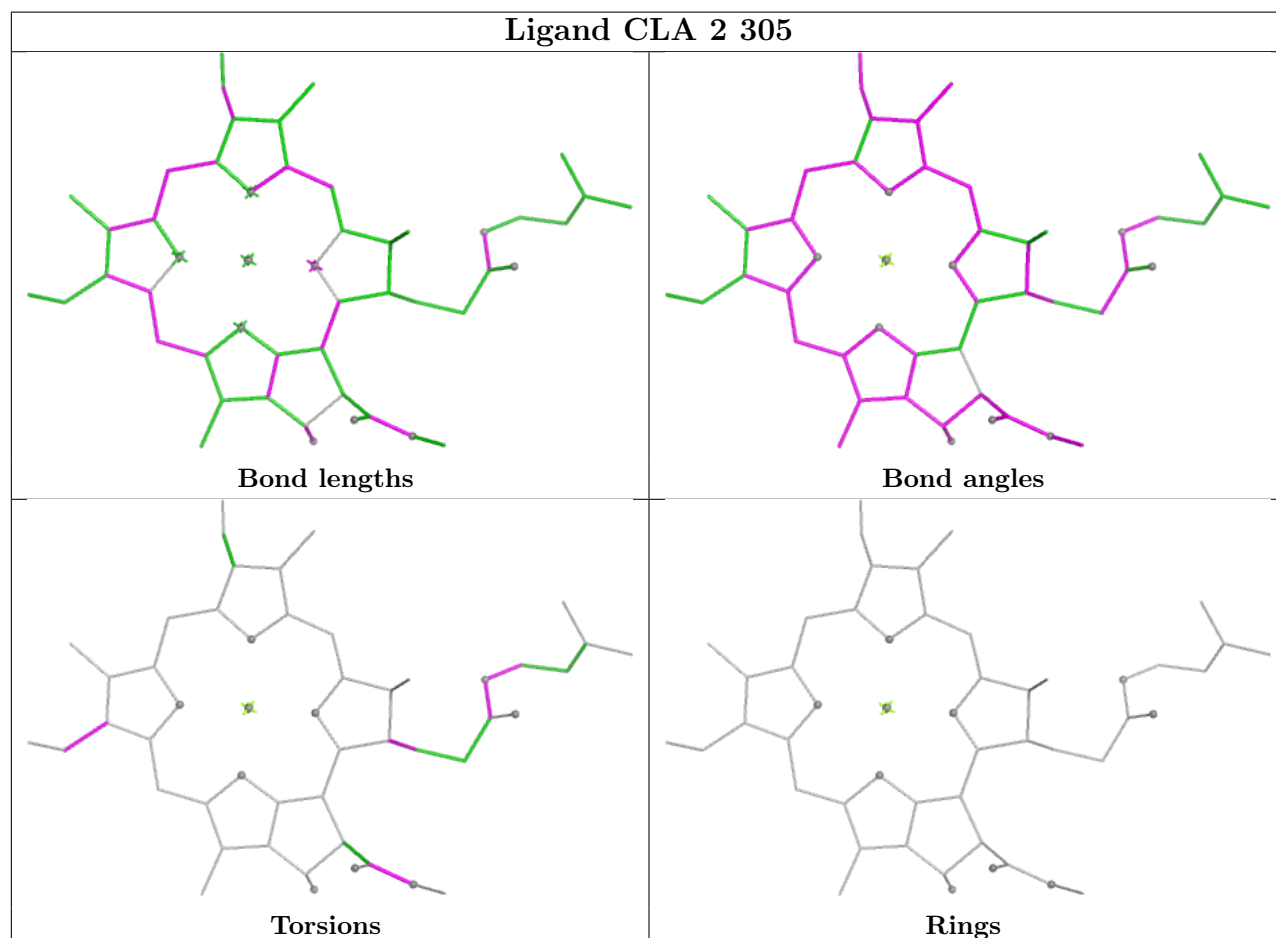
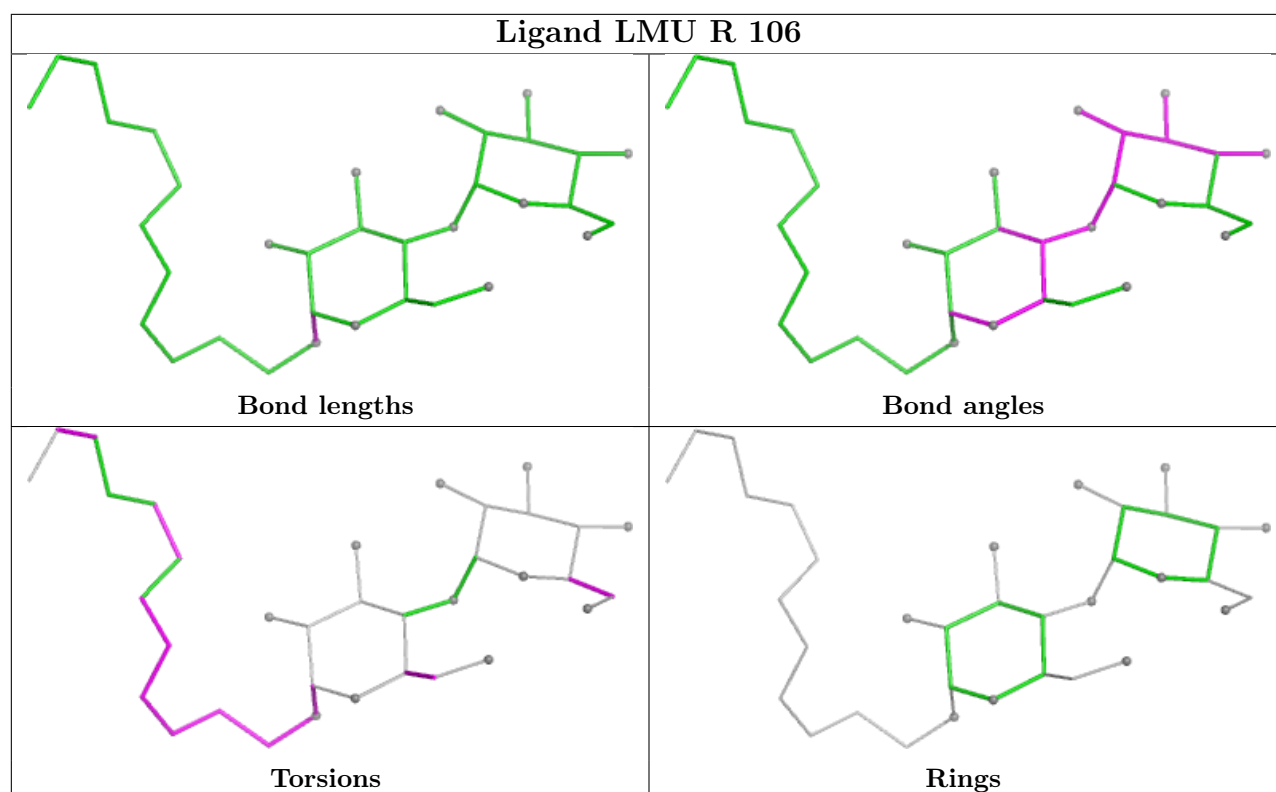
Bond angles

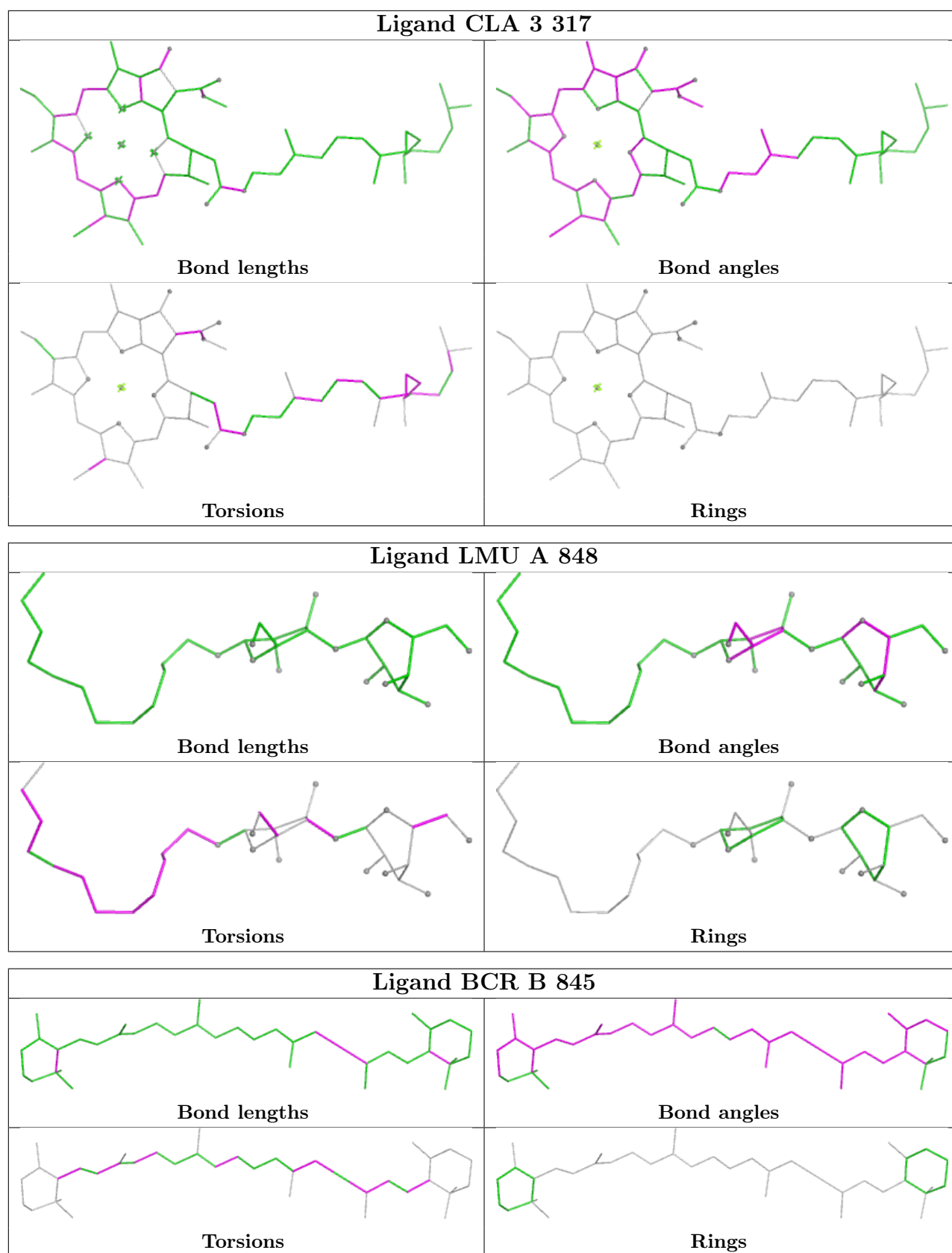


Torsions

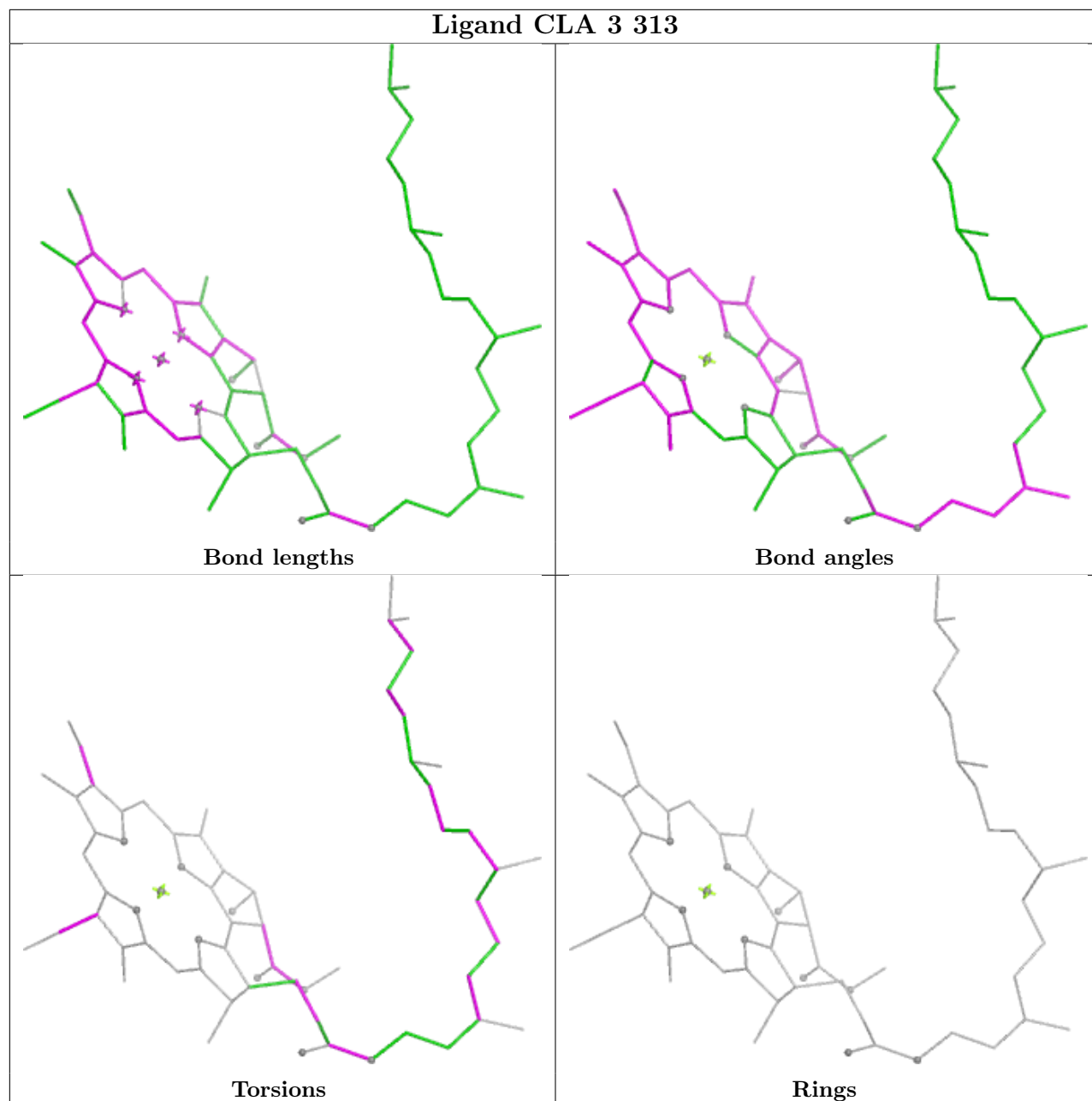


Rings

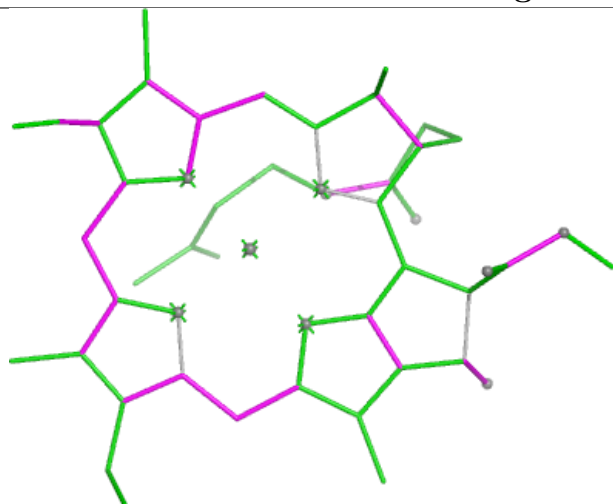




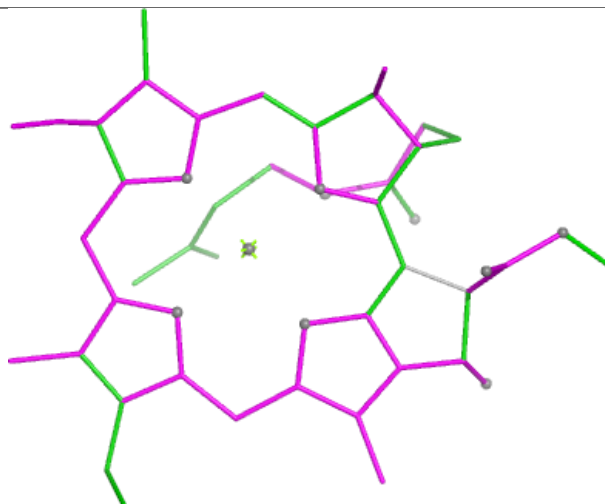
Ligand CLA 3 313



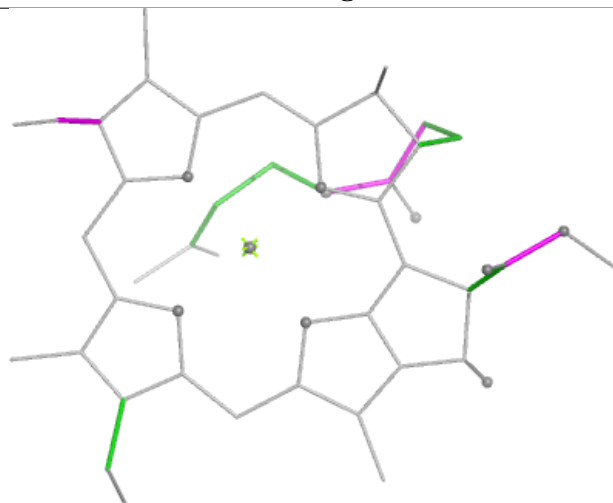
Ligand CLA B 818



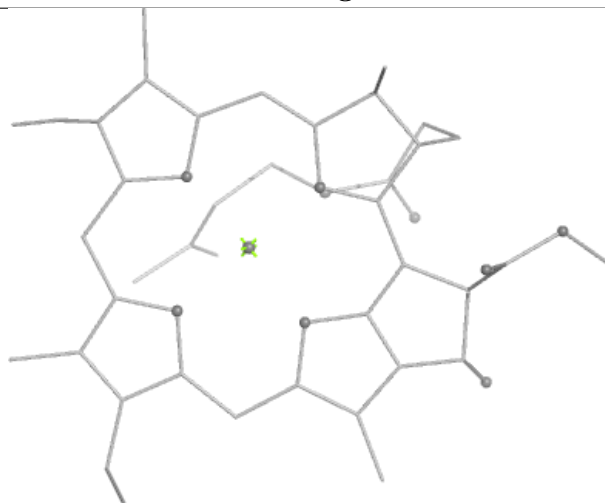
Bond lengths



Bond angles

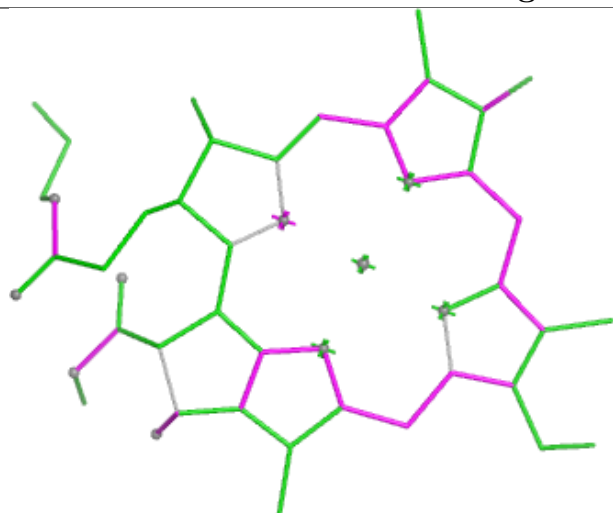


Torsions

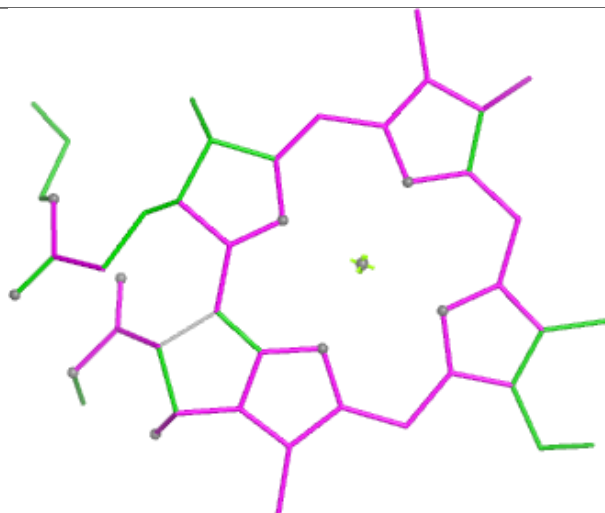


Rings

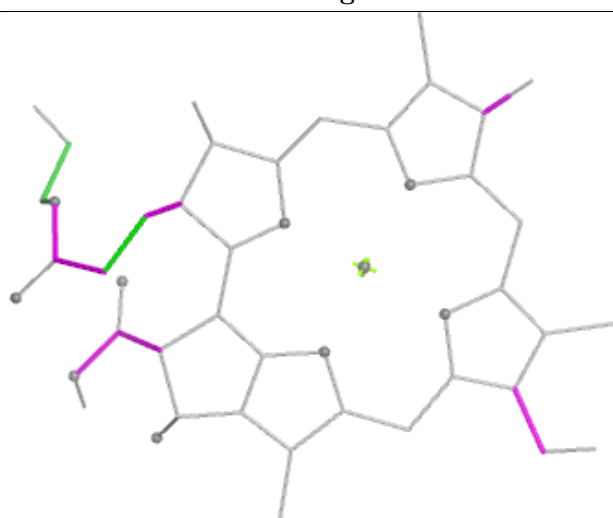
Ligand CLA J 101



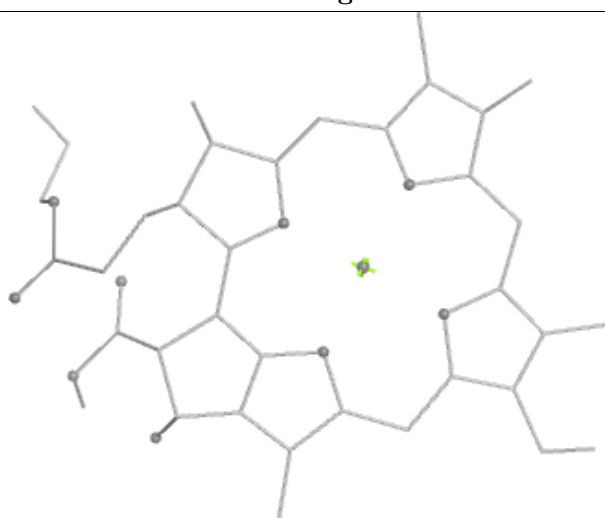
Bond lengths



Bond angles

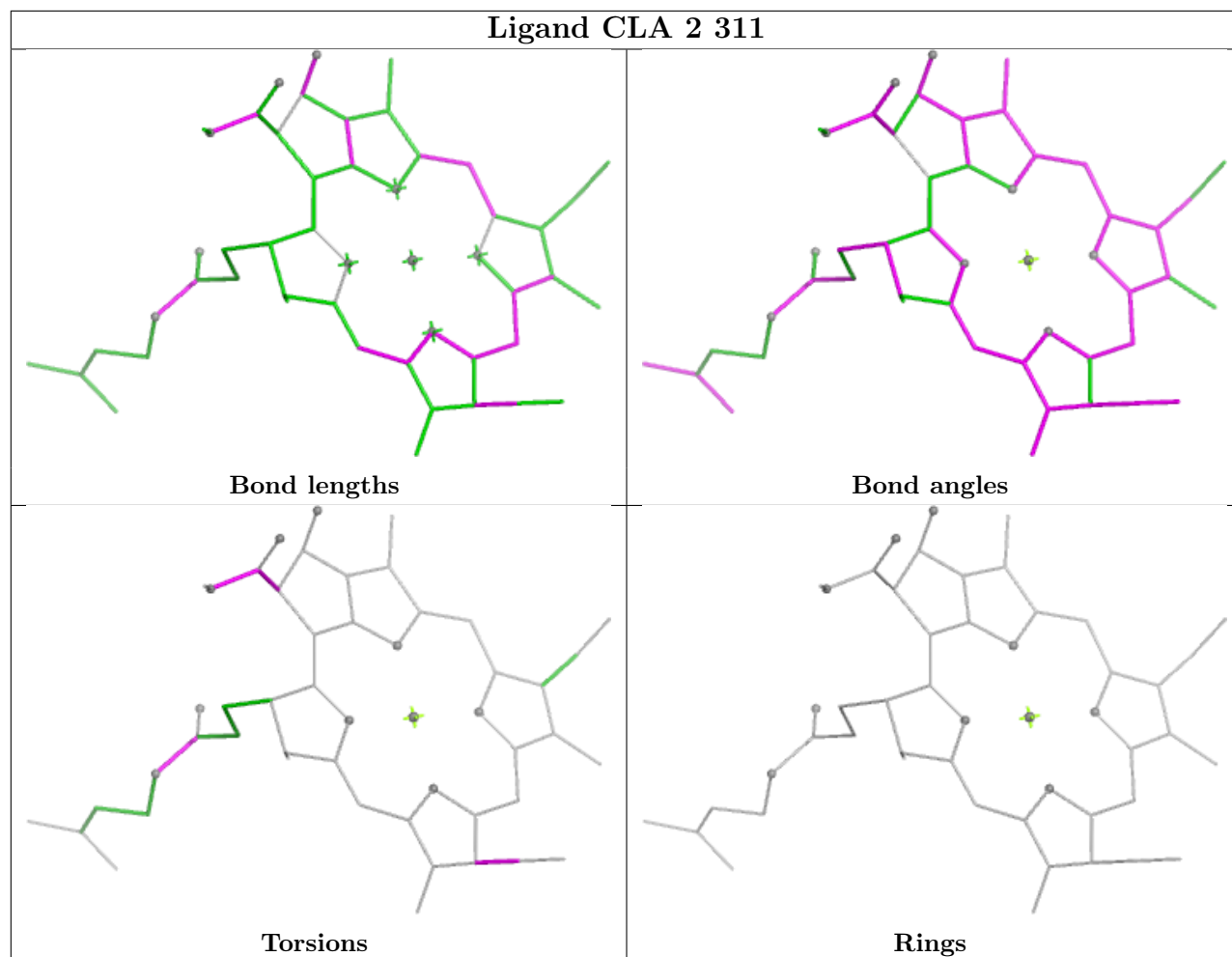


Torsions

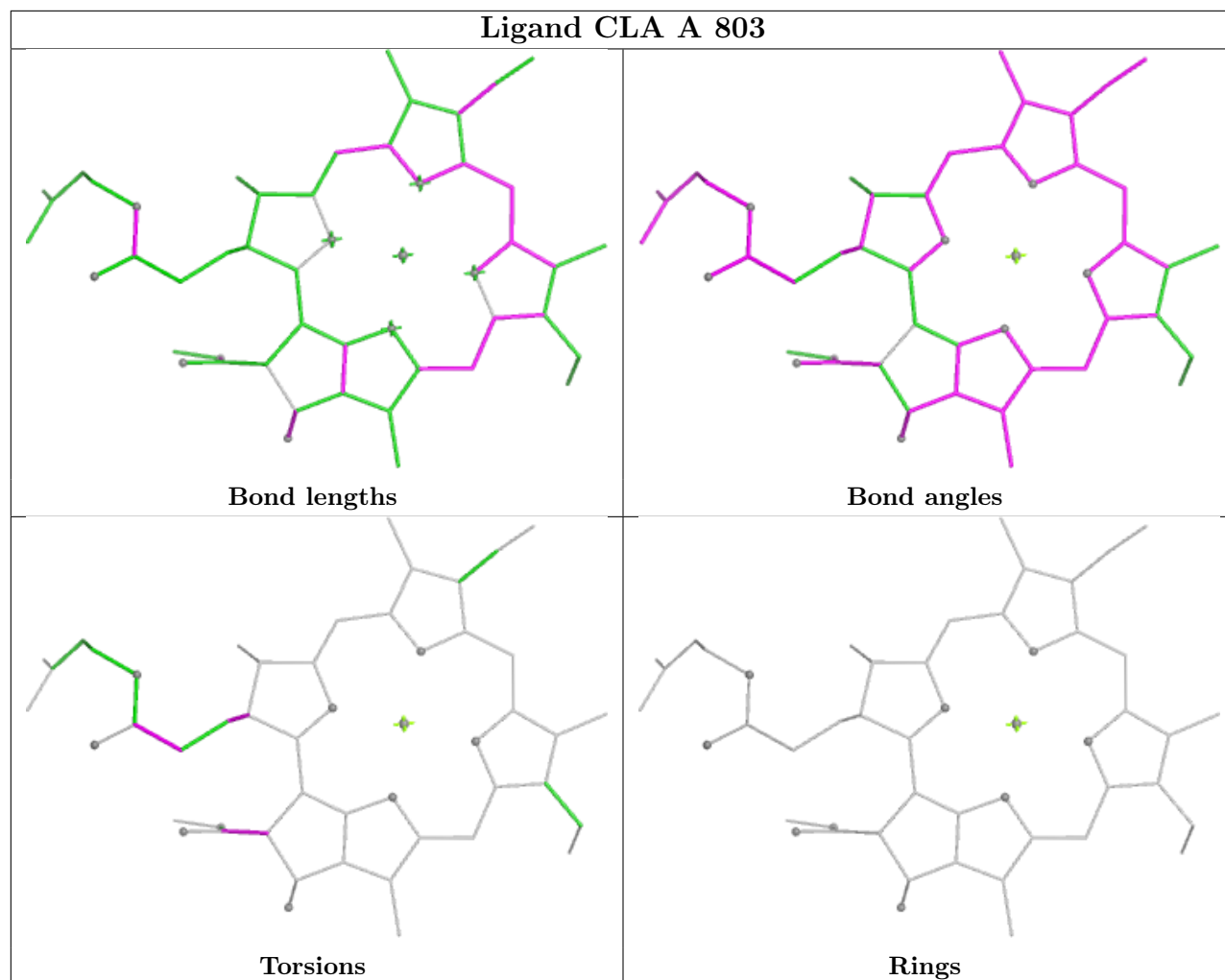


Rings

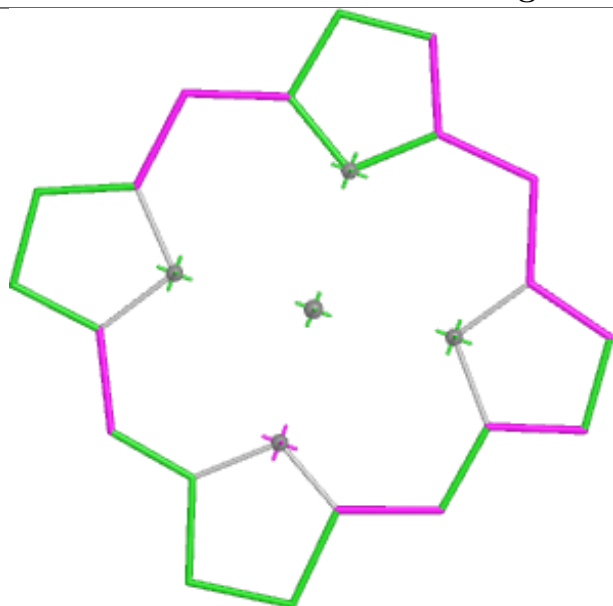
Ligand CLA 2 311



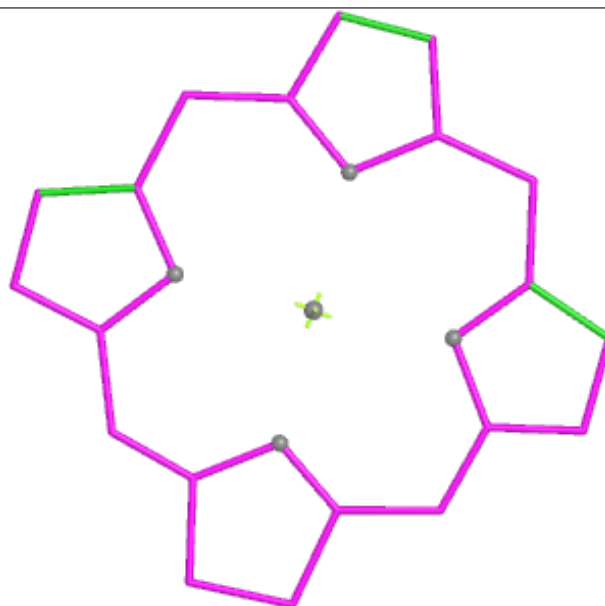
Ligand CLA A 803



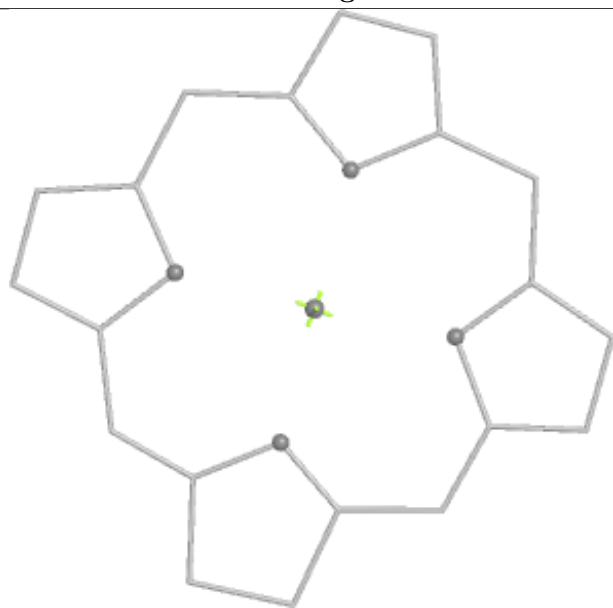
Ligand CLA 4 312



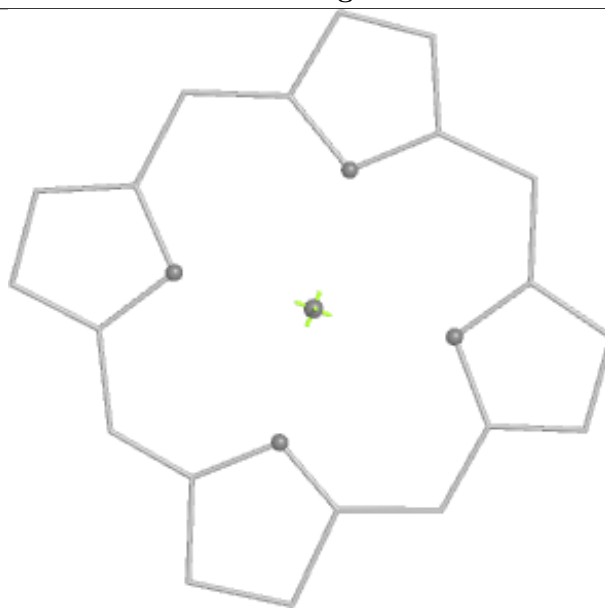
Bond lengths



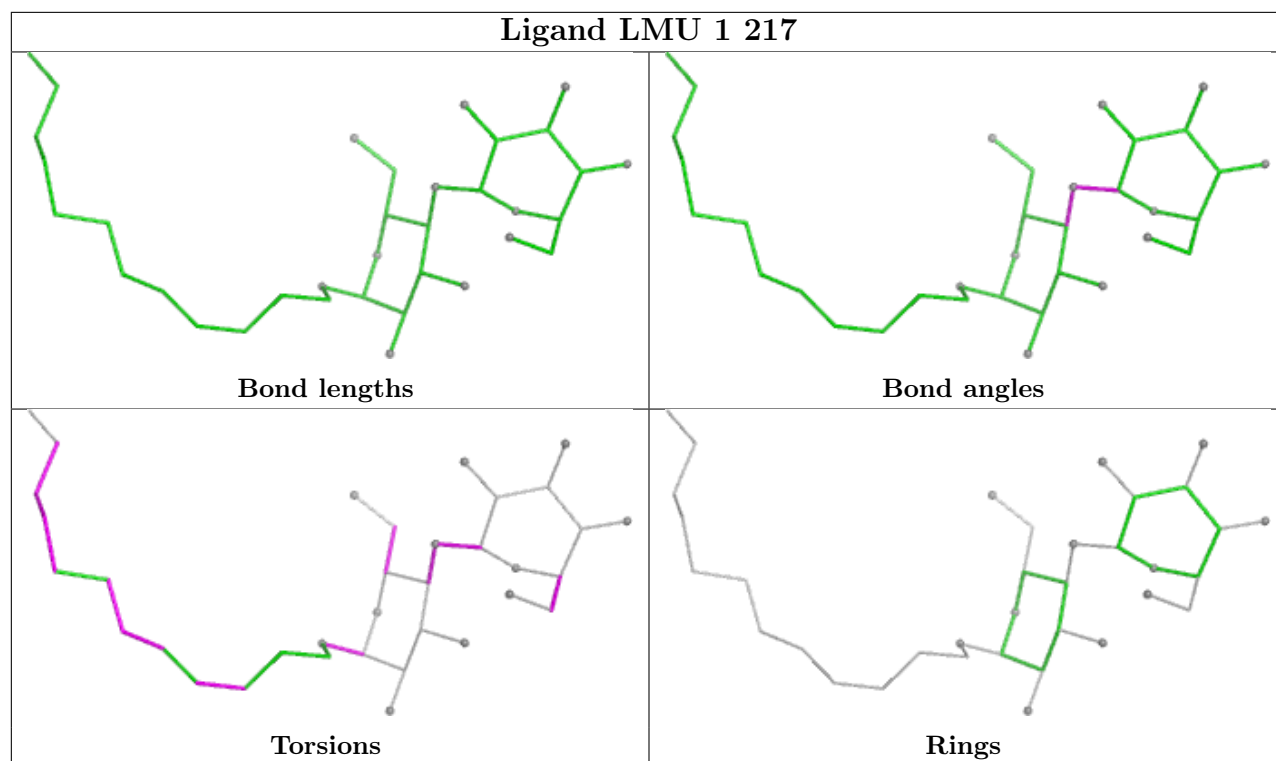
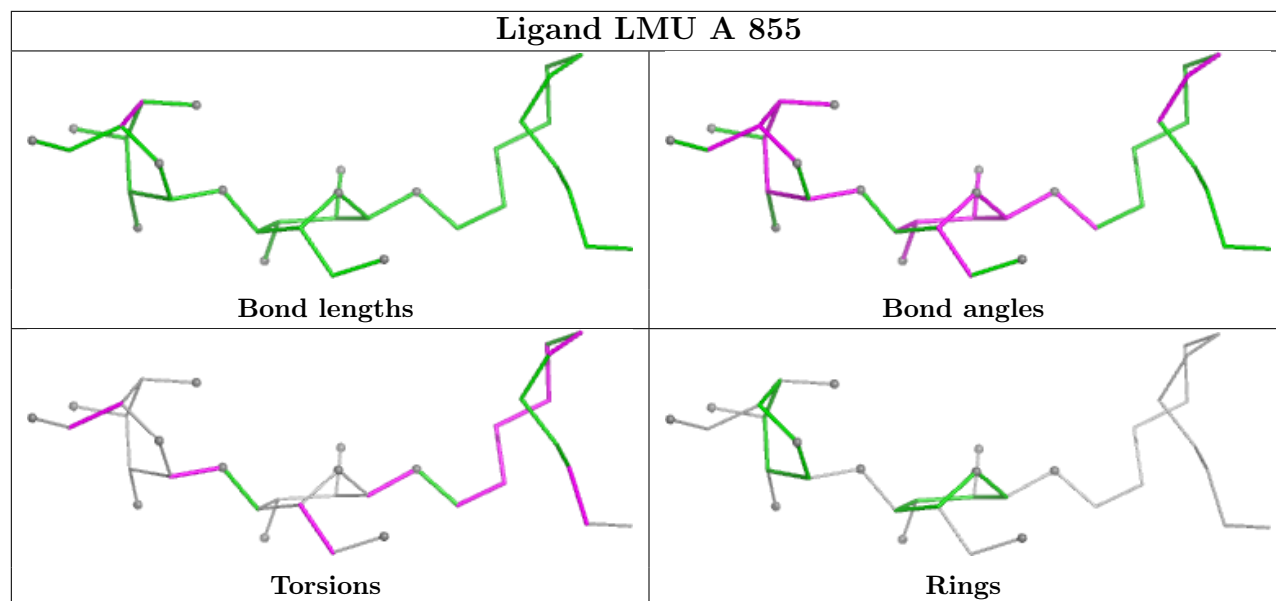
Bond angles

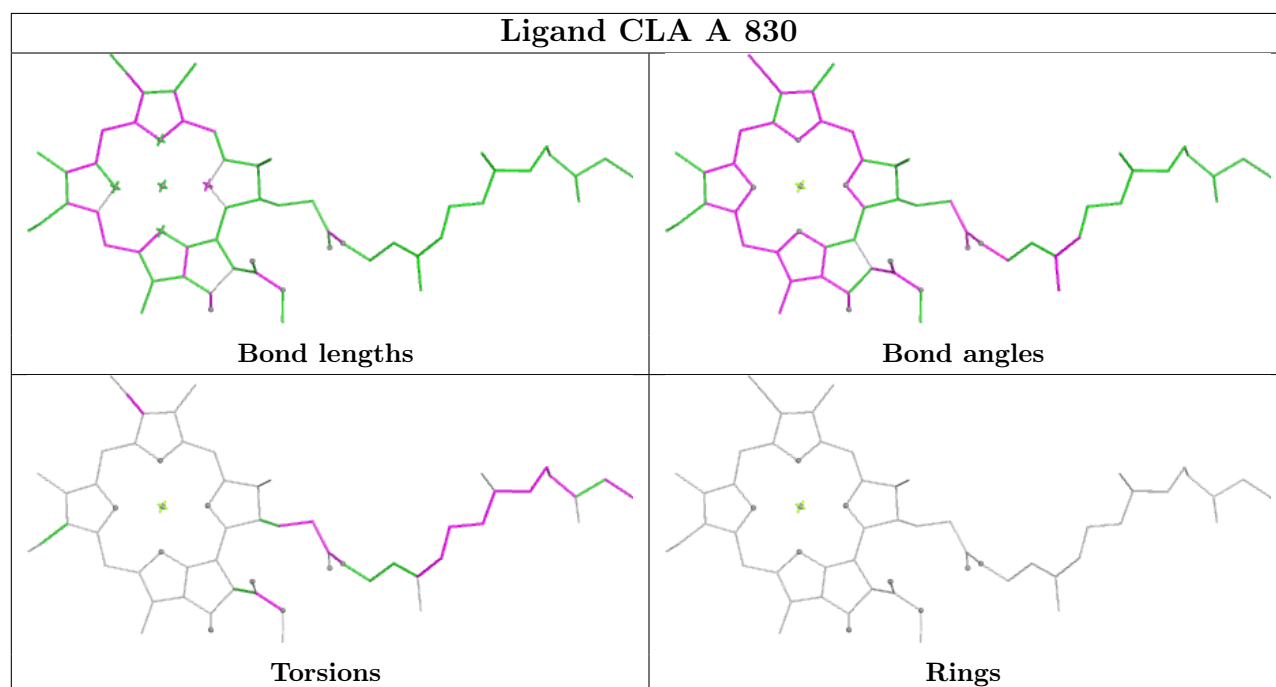
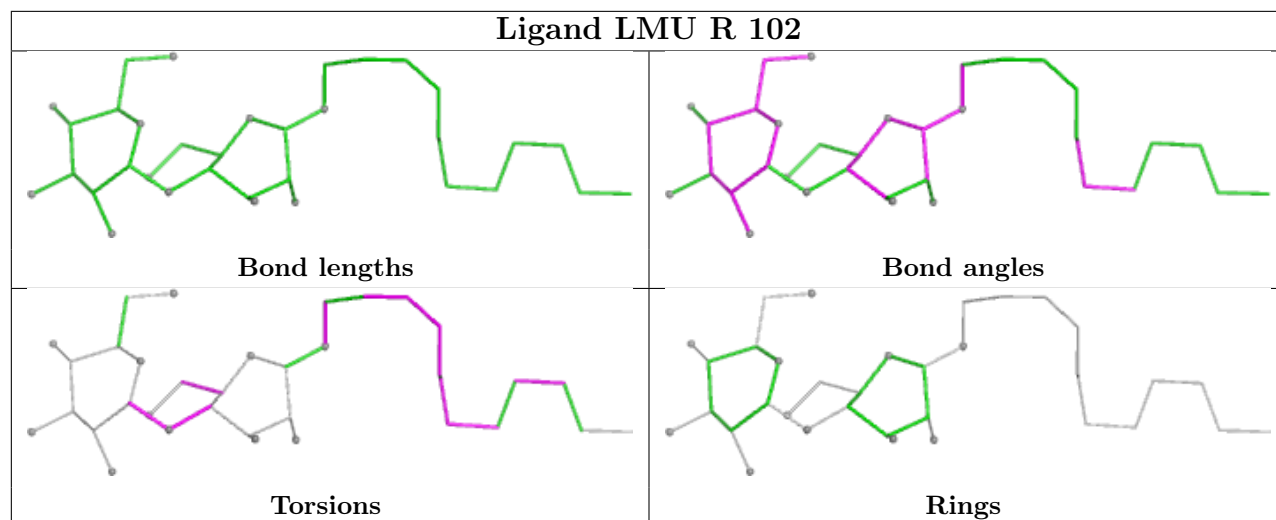


Torsions

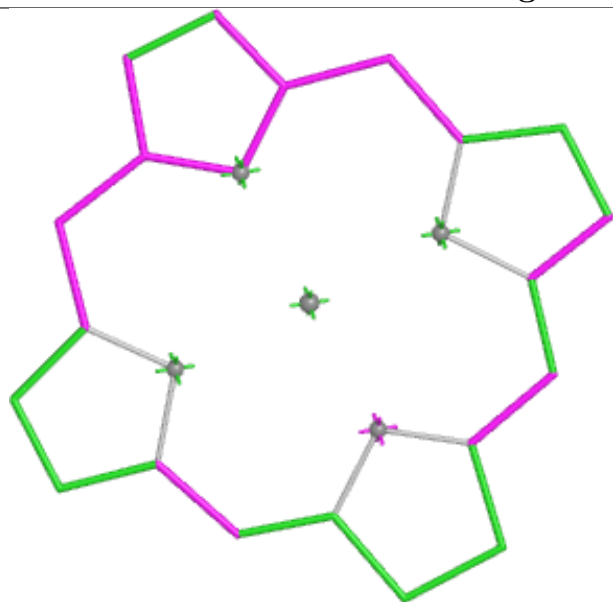


Rings

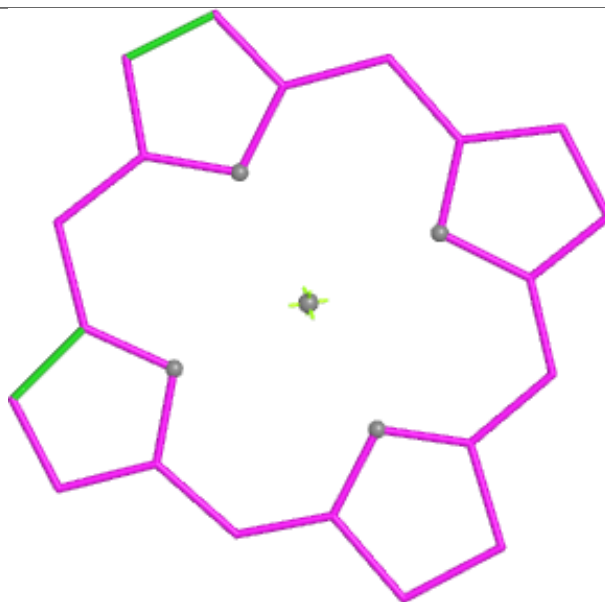




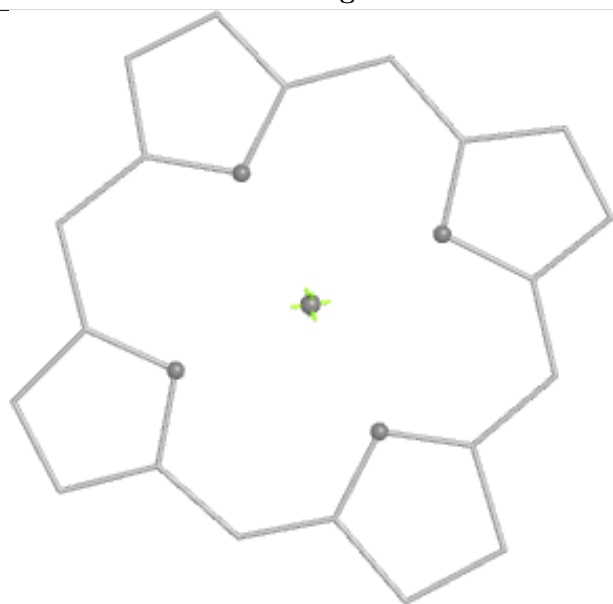
Ligand CLA 2 306



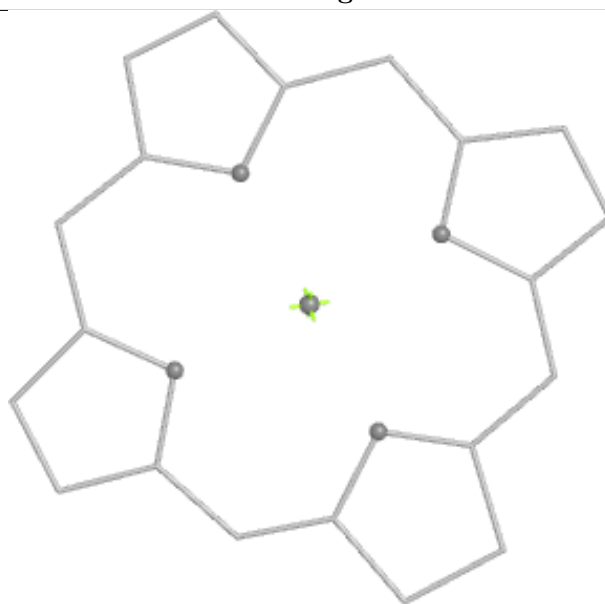
Bond lengths



Bond angles

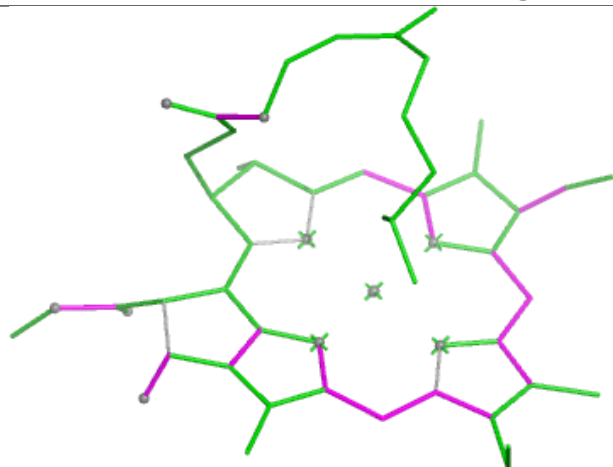


Torsions

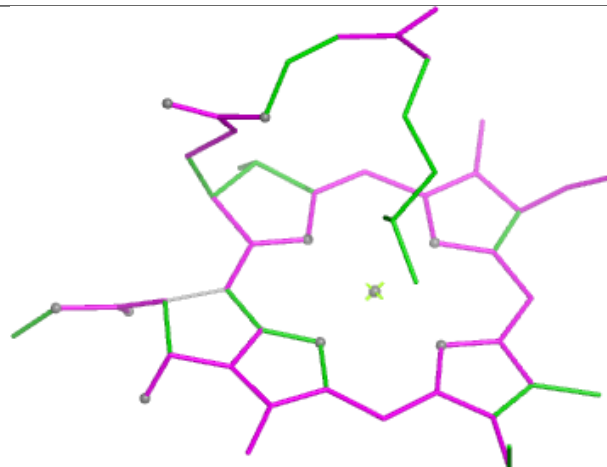


Rings

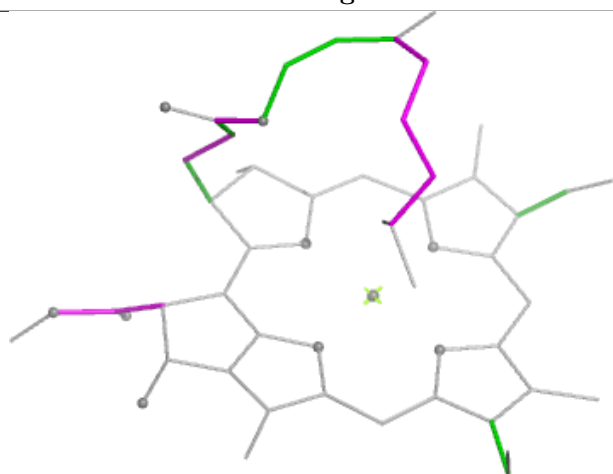
Ligand CLA B 810



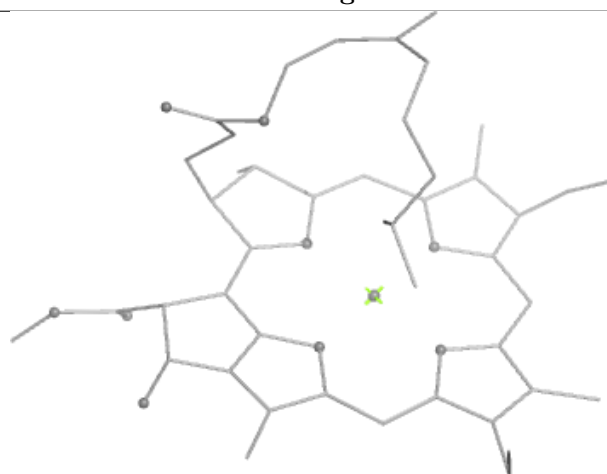
Bond lengths



Bond angles

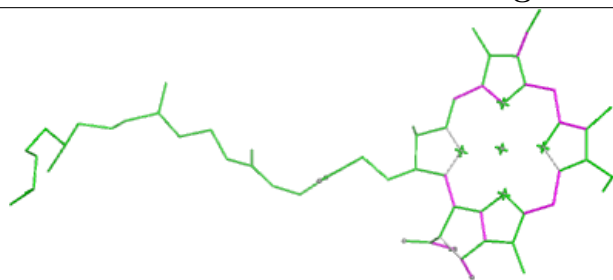


Torsions

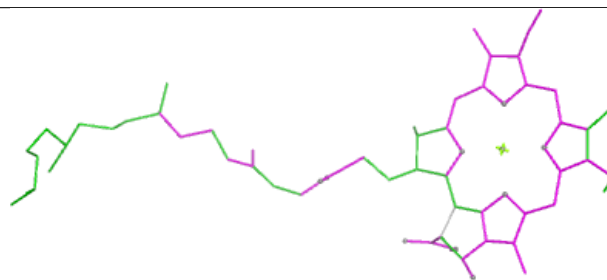


Rings

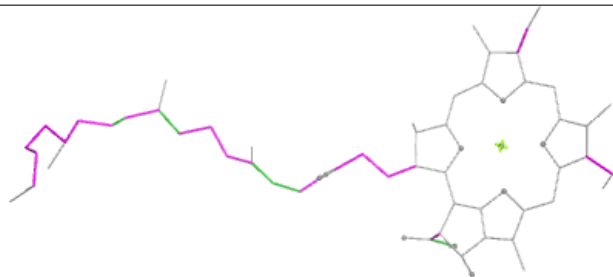
Ligand CLA A 805



Bond lengths



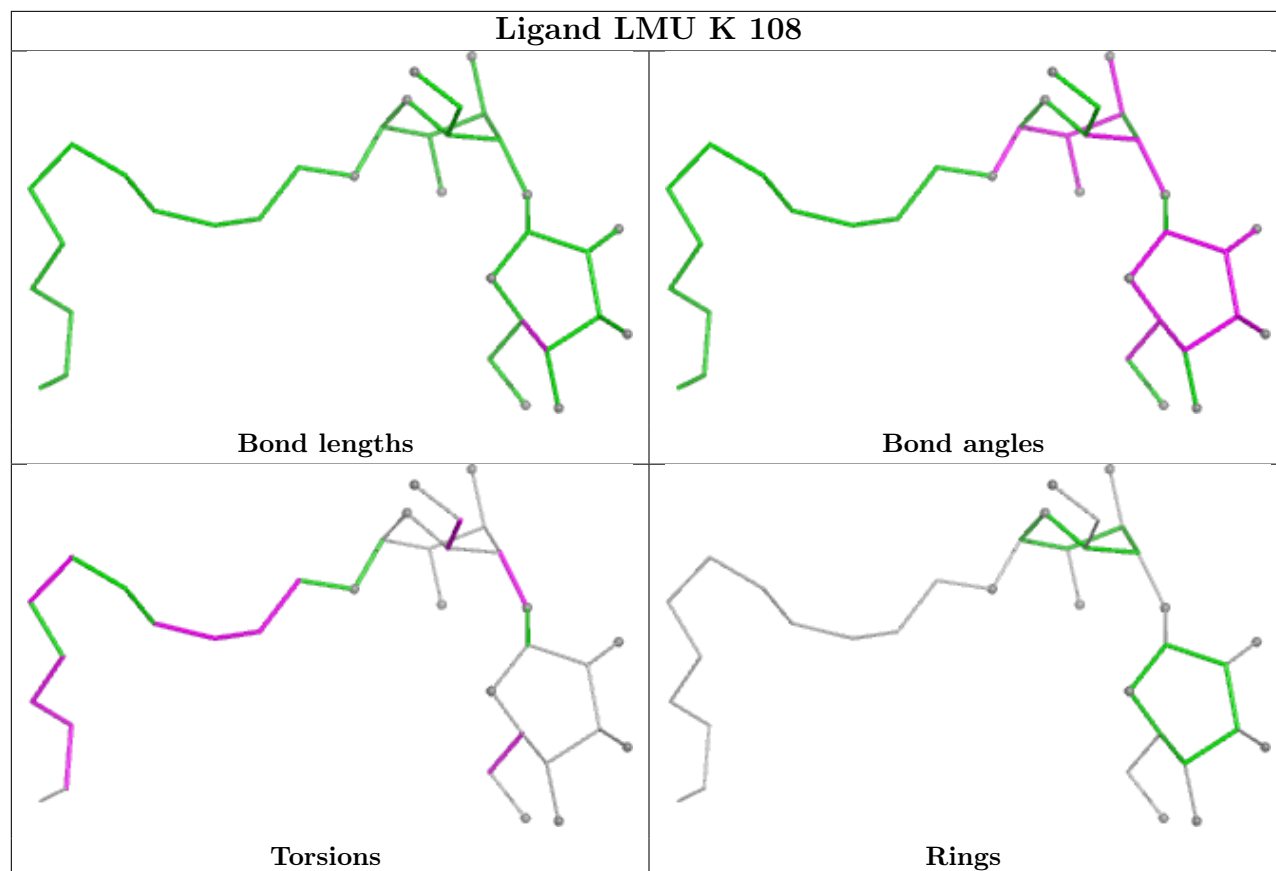
Bond angles



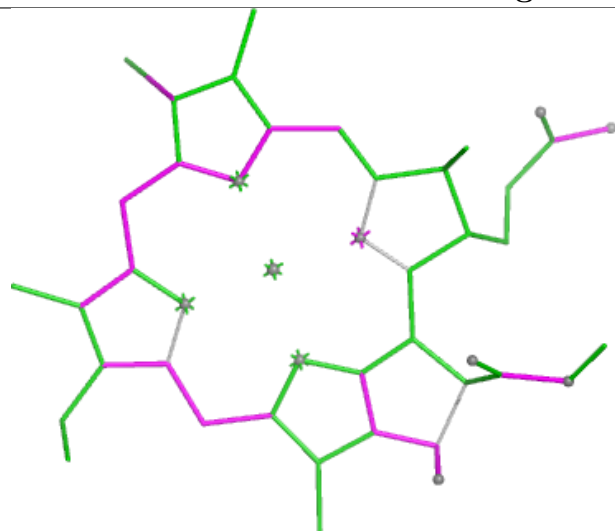
Torsions



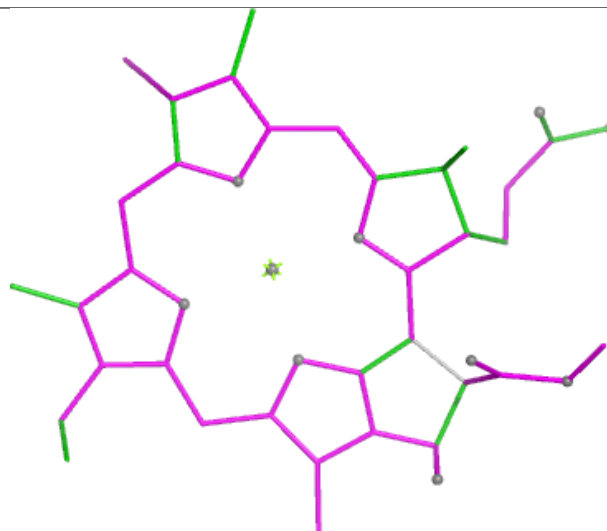
Rings



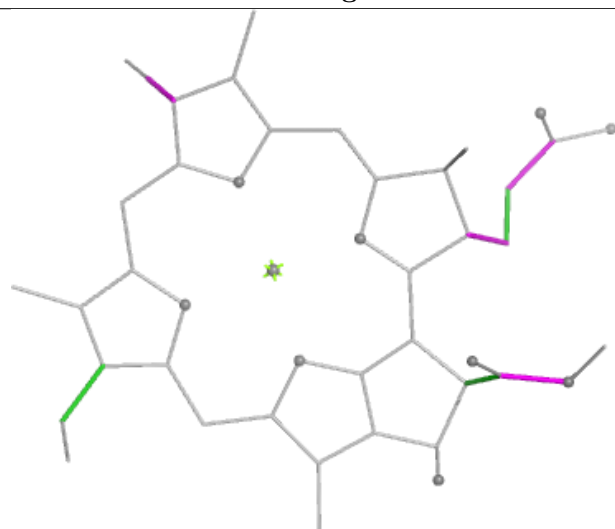
Ligand CLA A 833



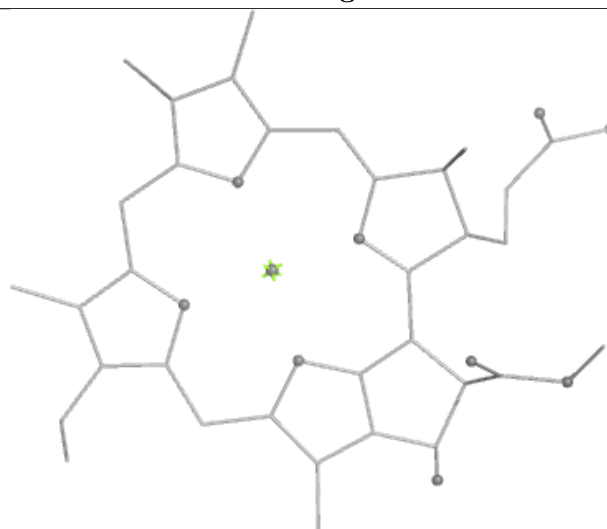
Bond lengths



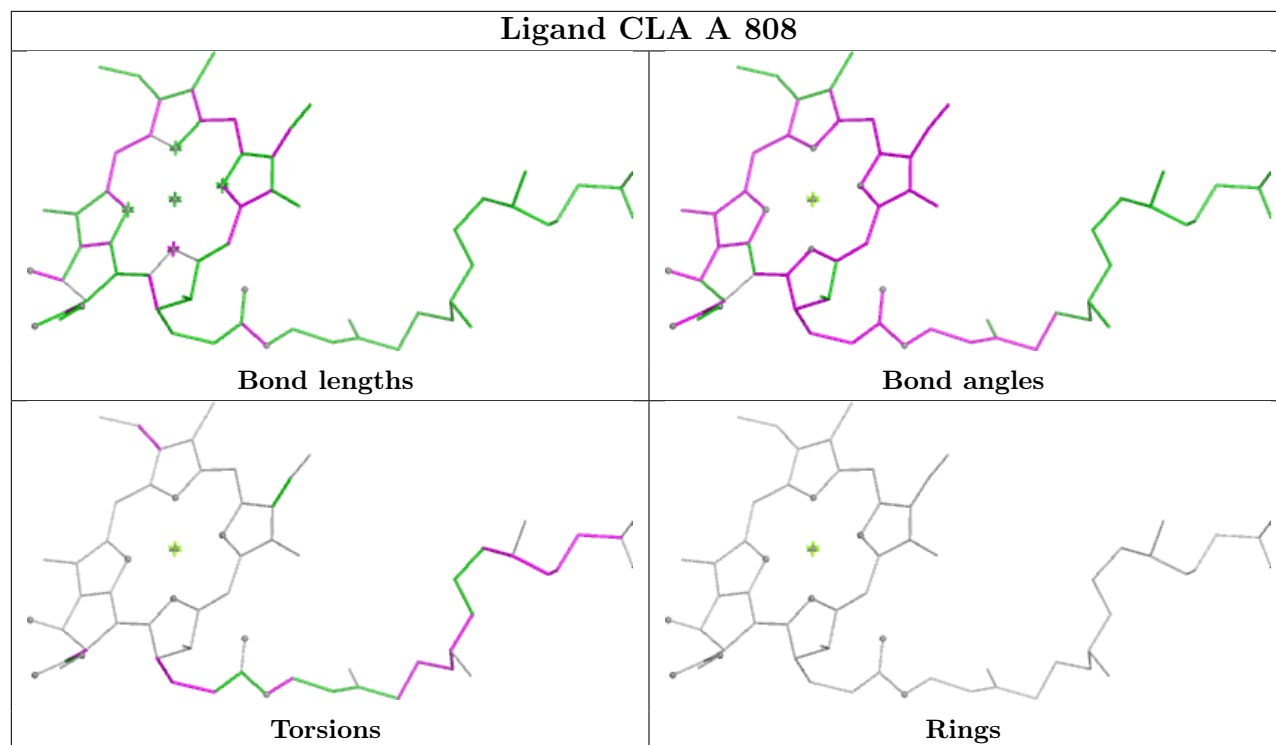
Bond angles



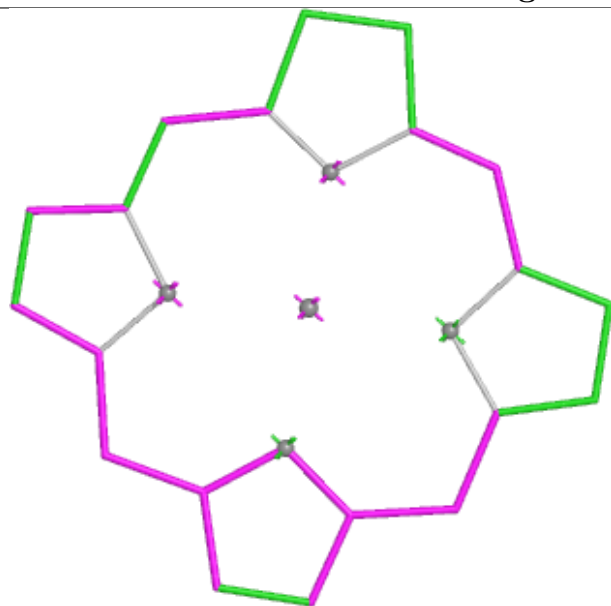
Torsions



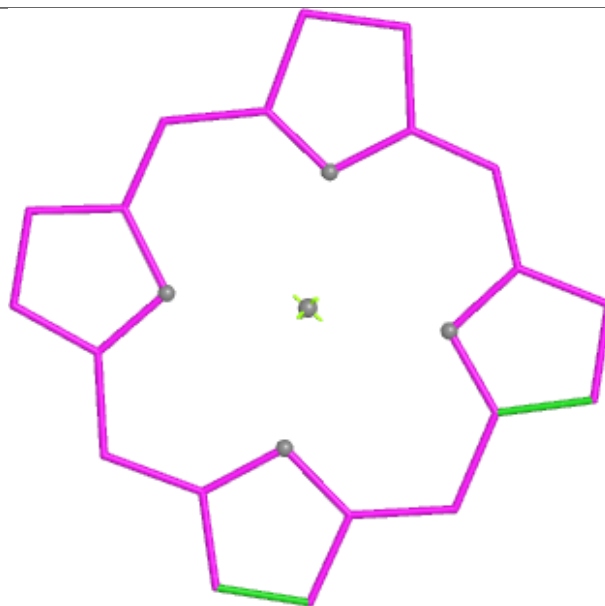
Rings



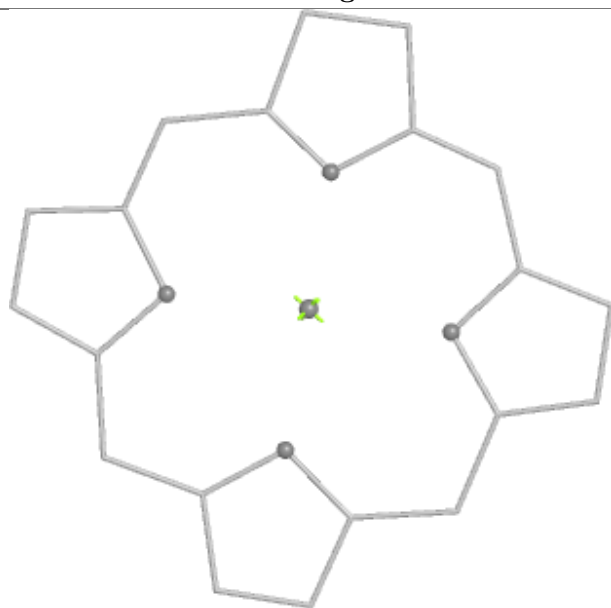
Ligand CLA 2 304



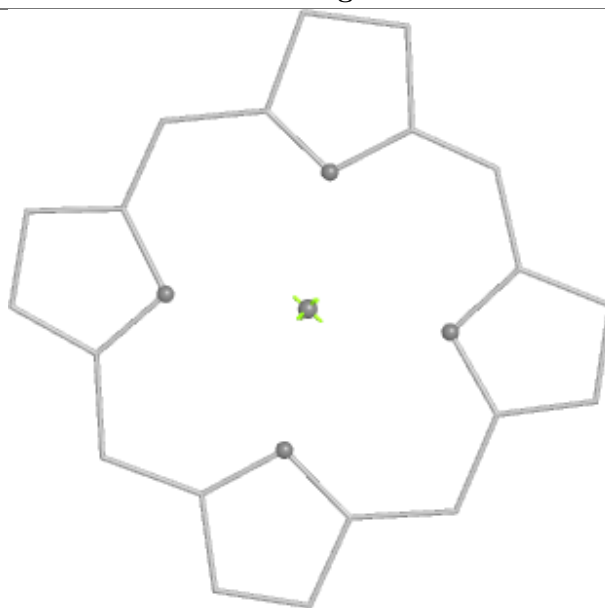
Bond lengths



Bond angles

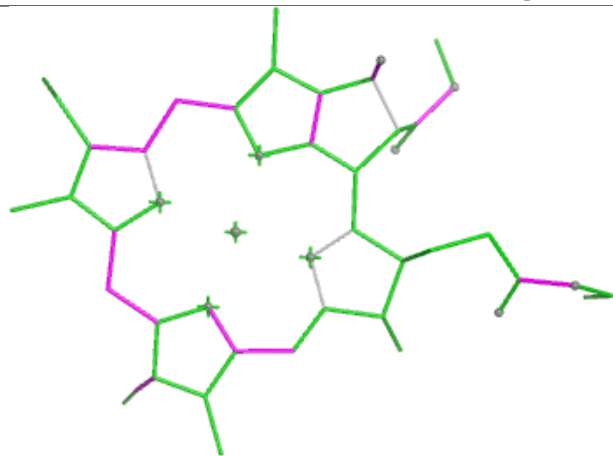


Torsions

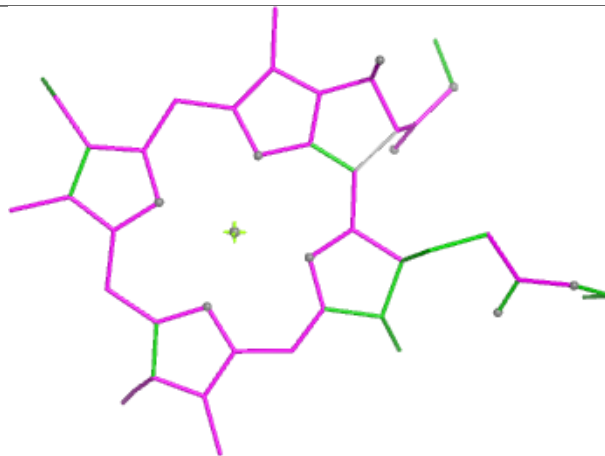


Rings

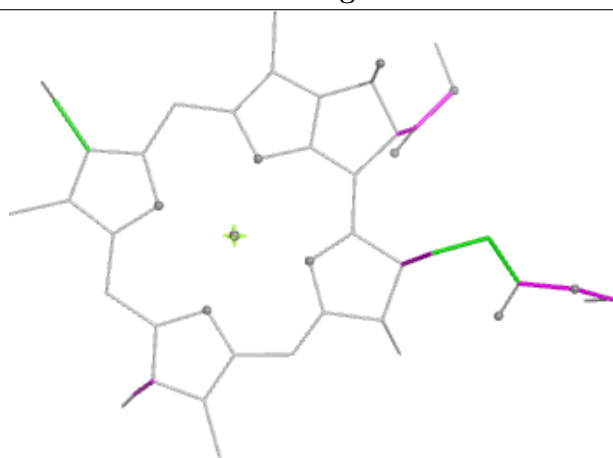
Ligand CLA 1 203



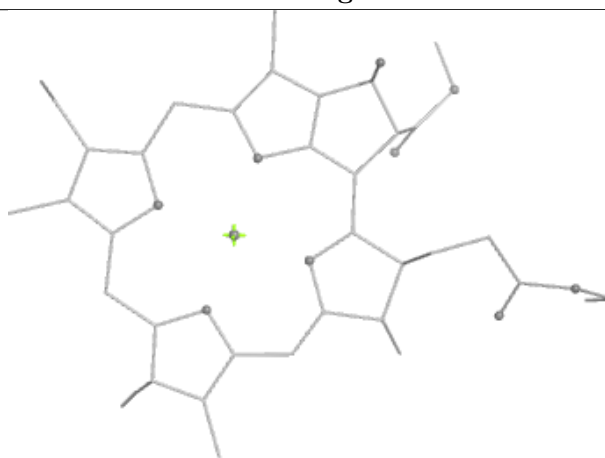
Bond lengths



Bond angles

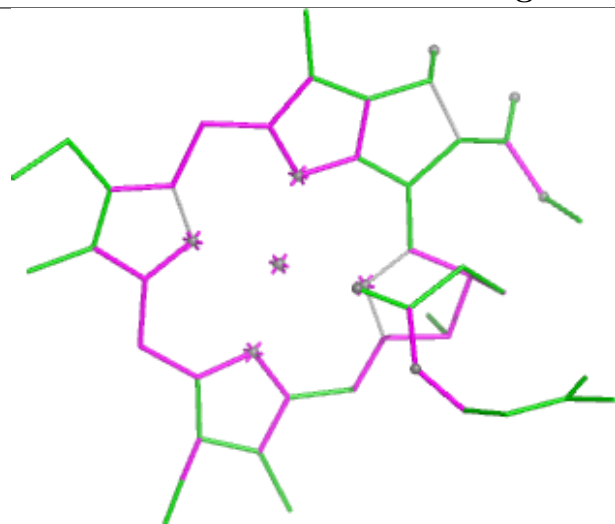


Torsions

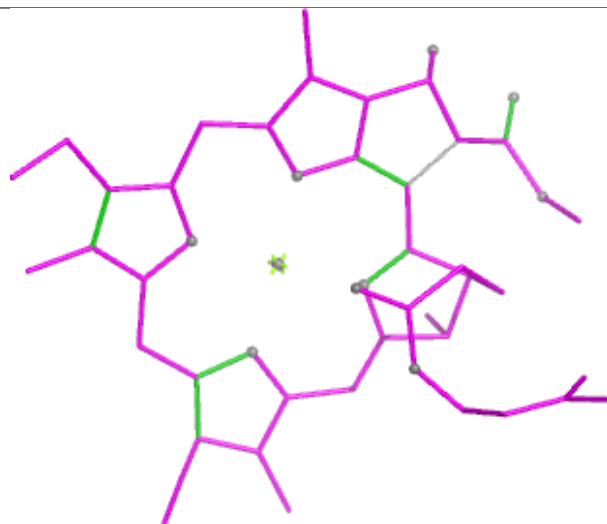


Rings

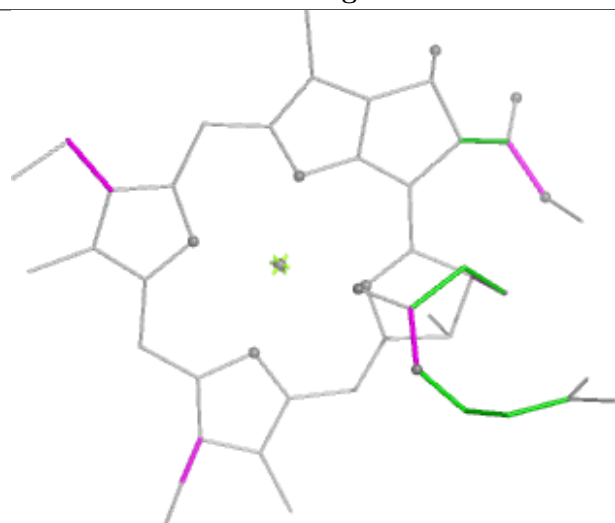
Ligand CLA A 815



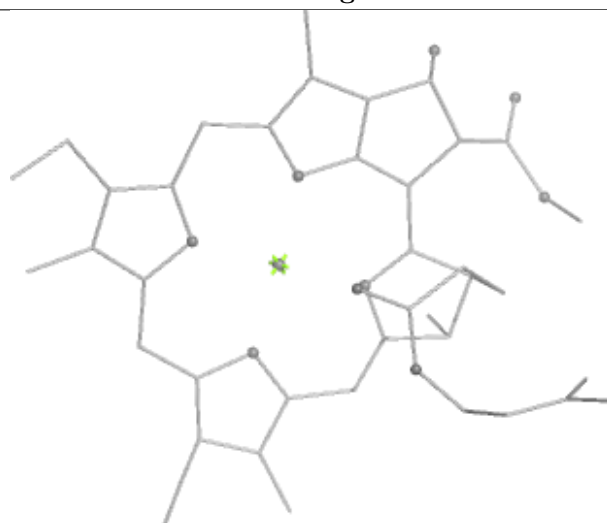
Bond lengths



Bond angles

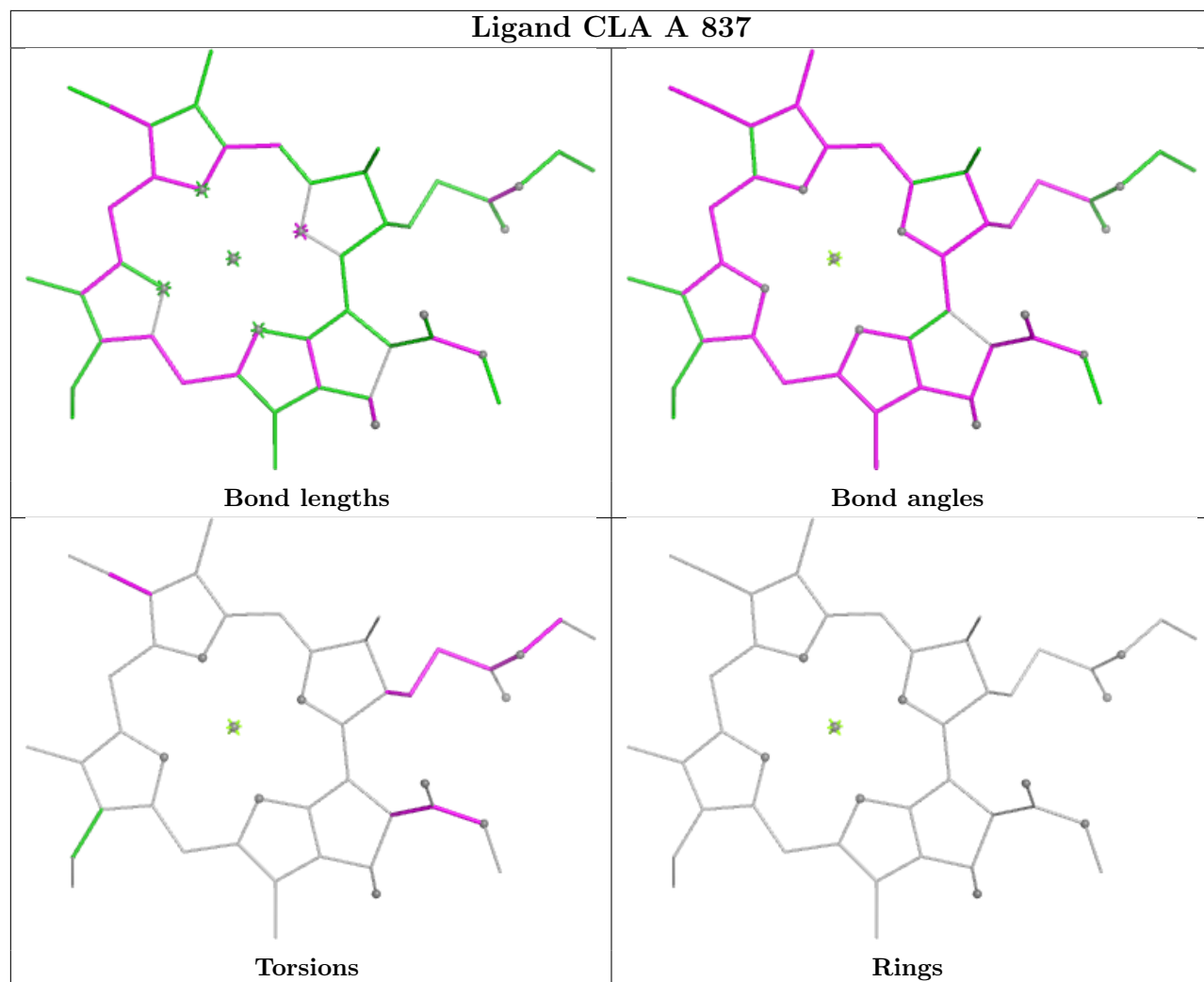


Torsions

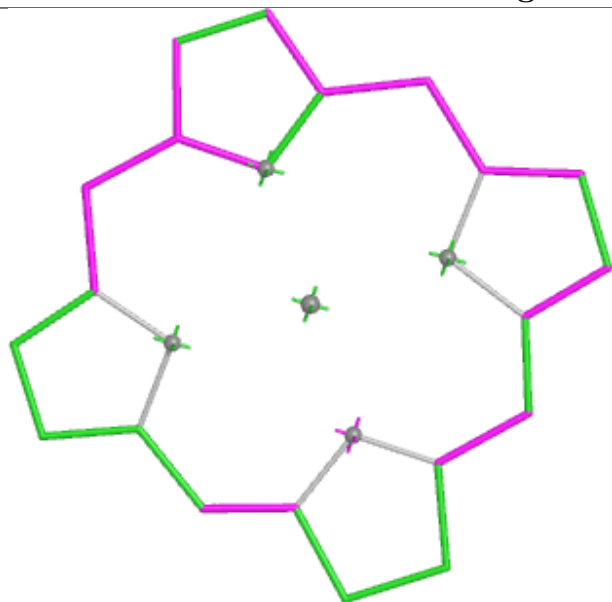


Rings

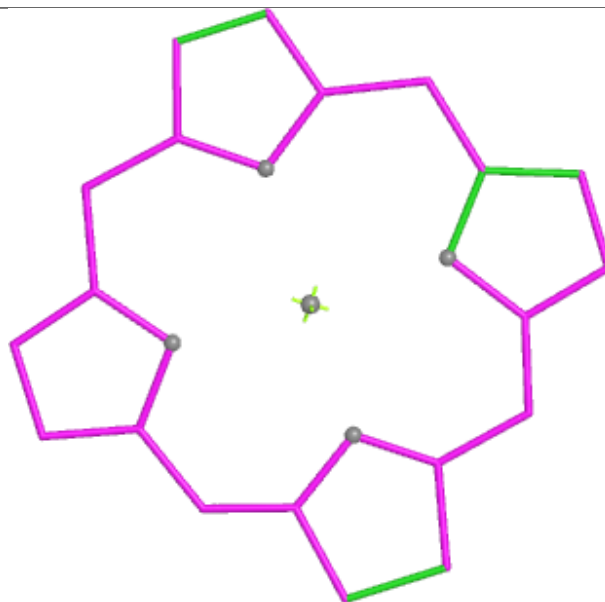
Ligand CLA A 837



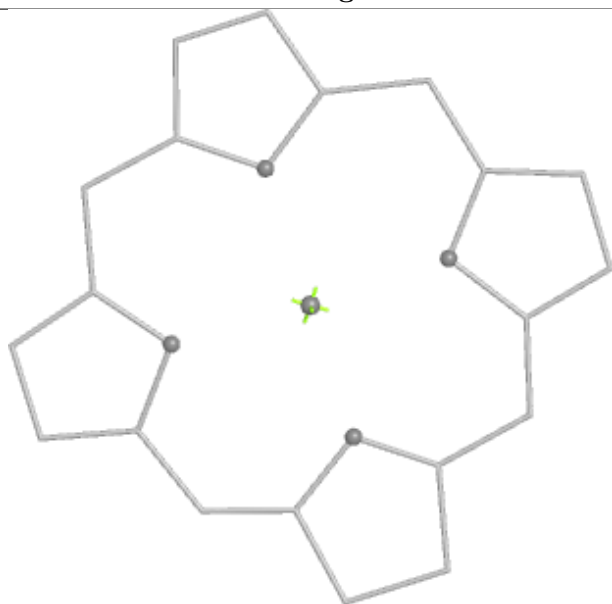
Ligand CLA 3 305



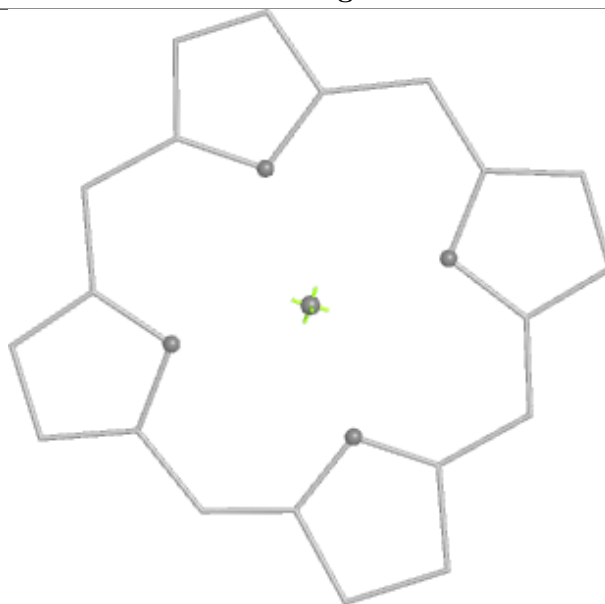
Bond lengths



Bond angles

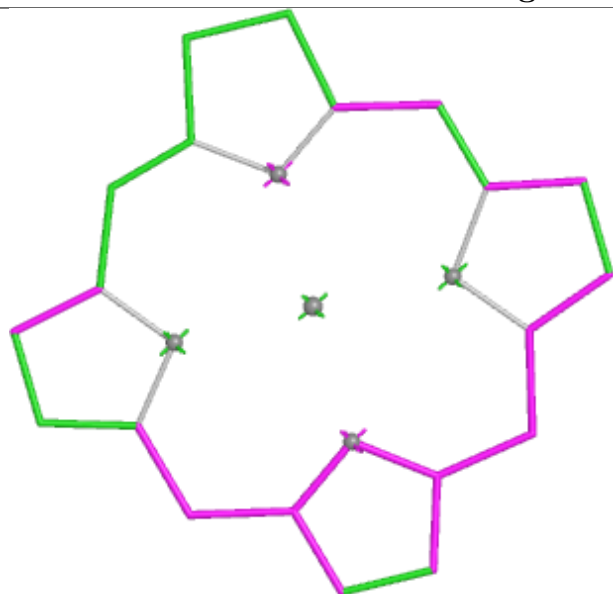


Torsions

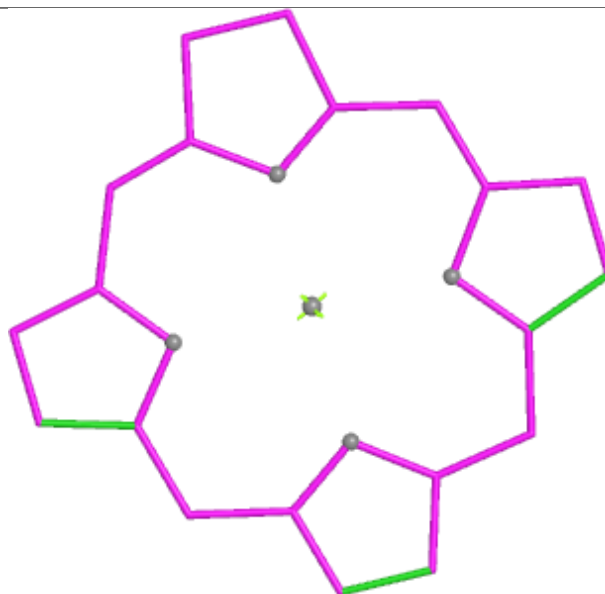


Rings

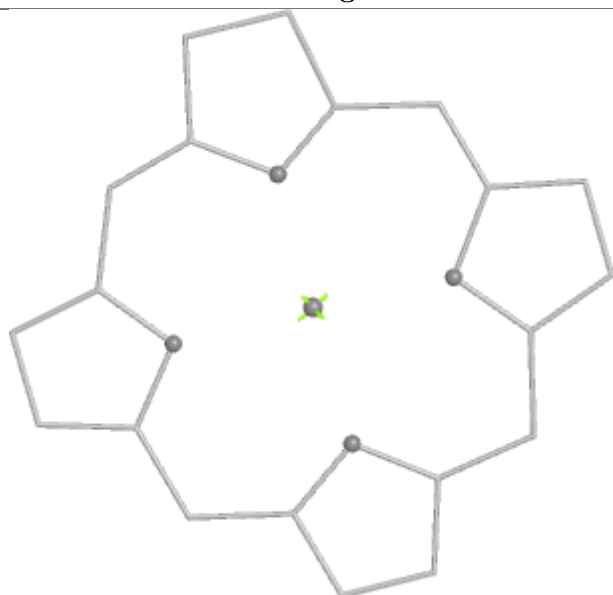
Ligand CLA 4 309



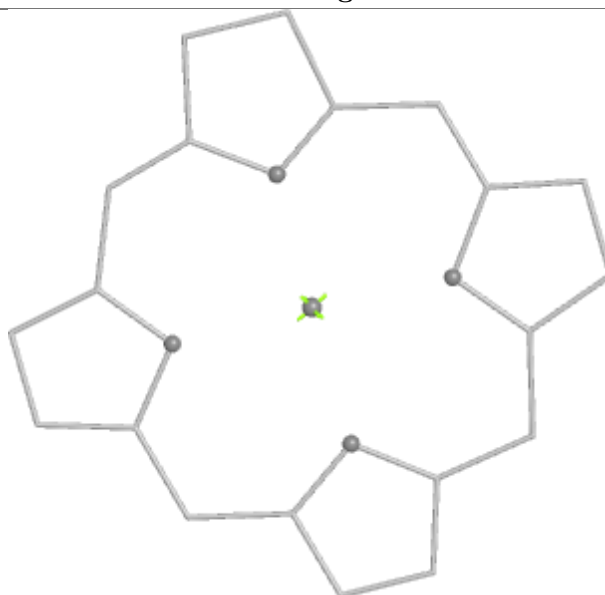
Bond lengths



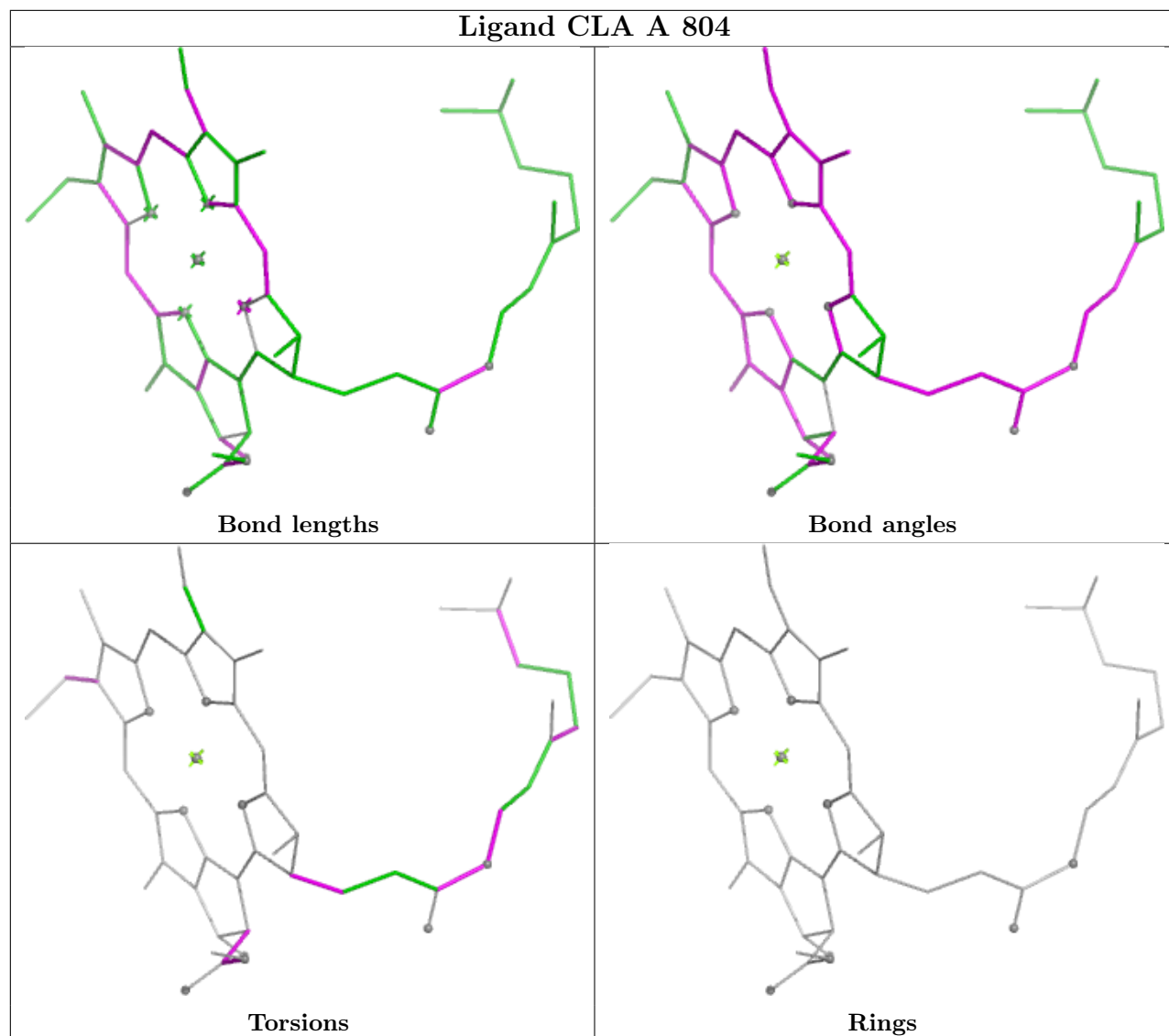
Bond angles



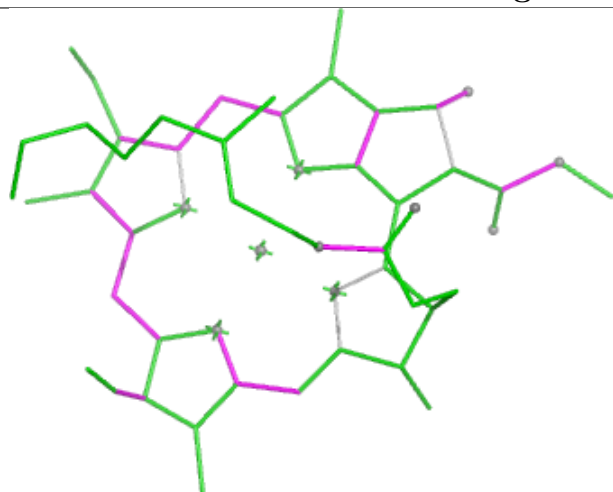
Torsions



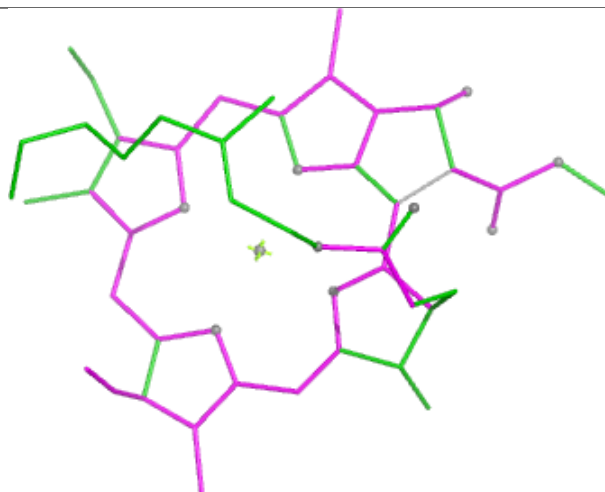
Rings



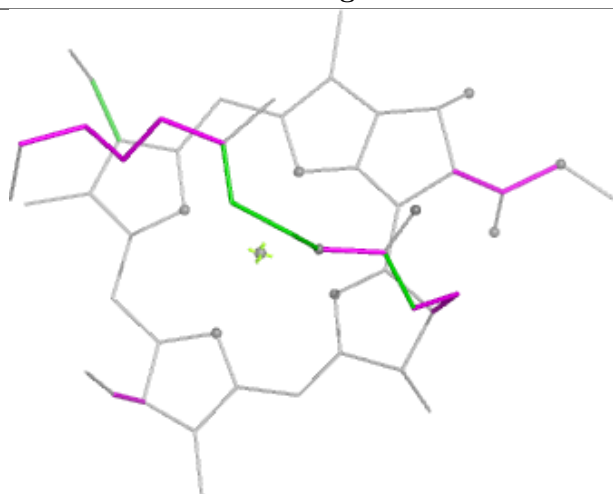
Ligand CLA A 812



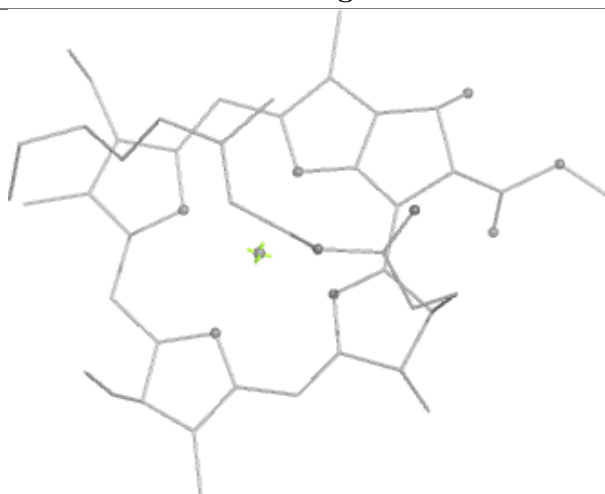
Bond lengths



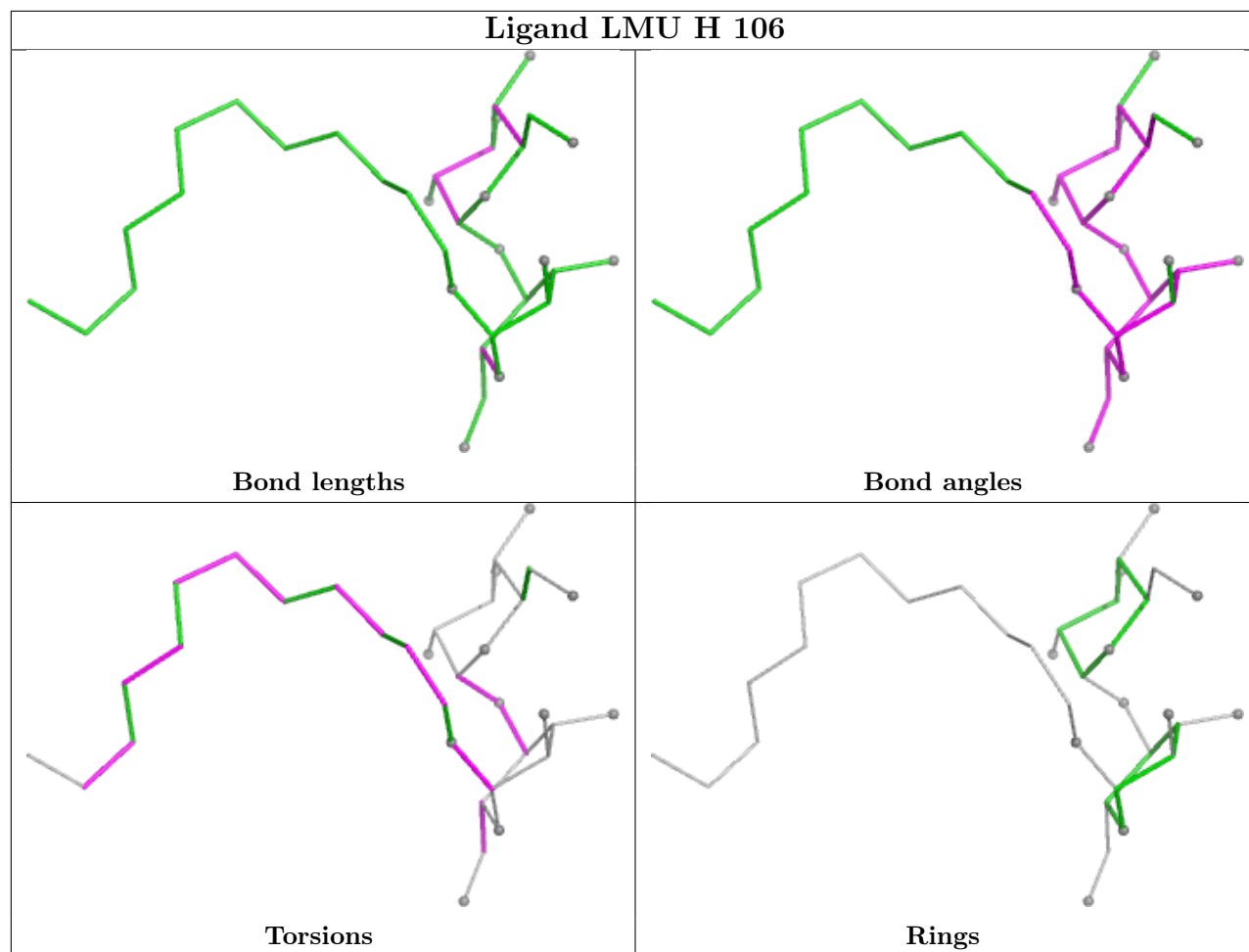
Bond angles

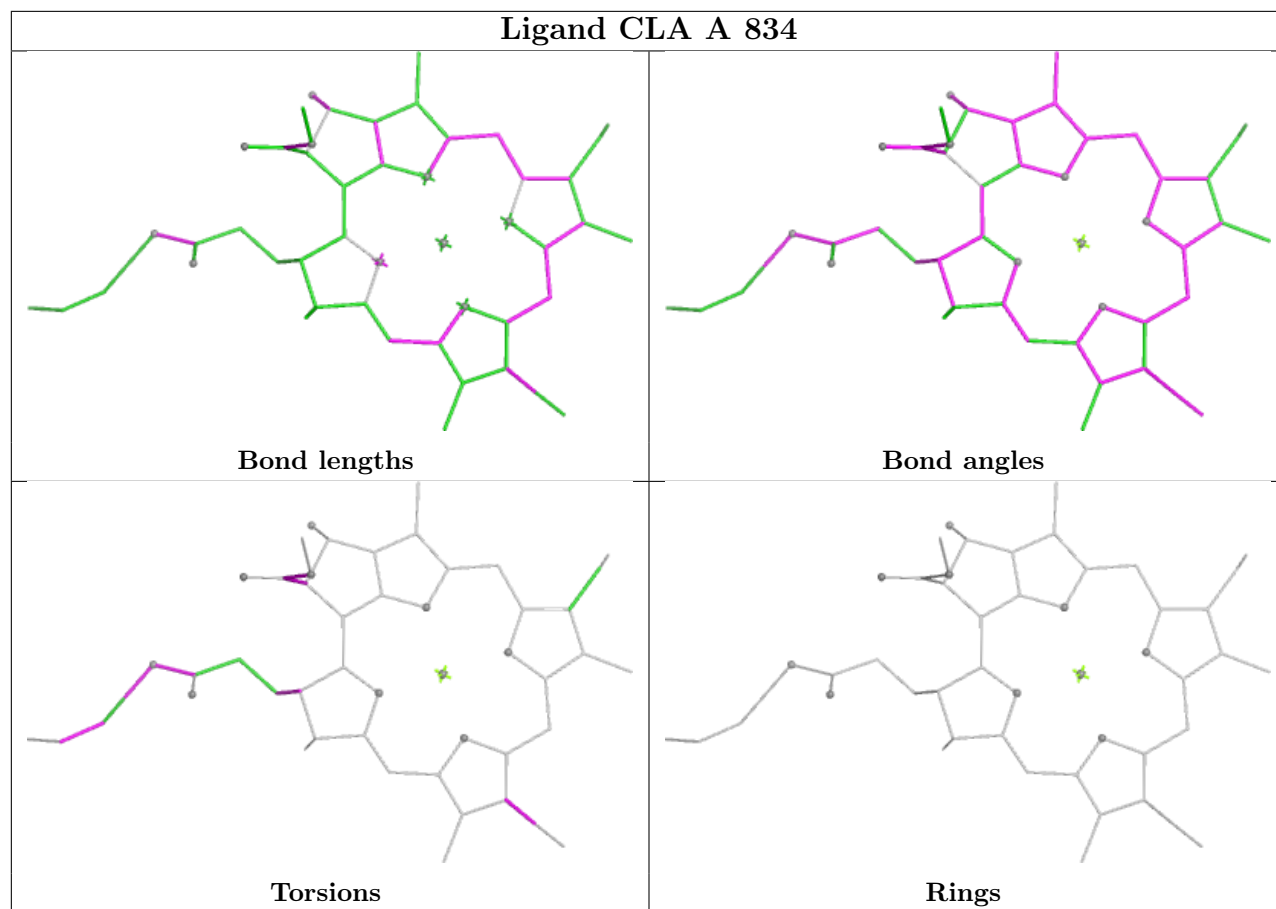


Torsions

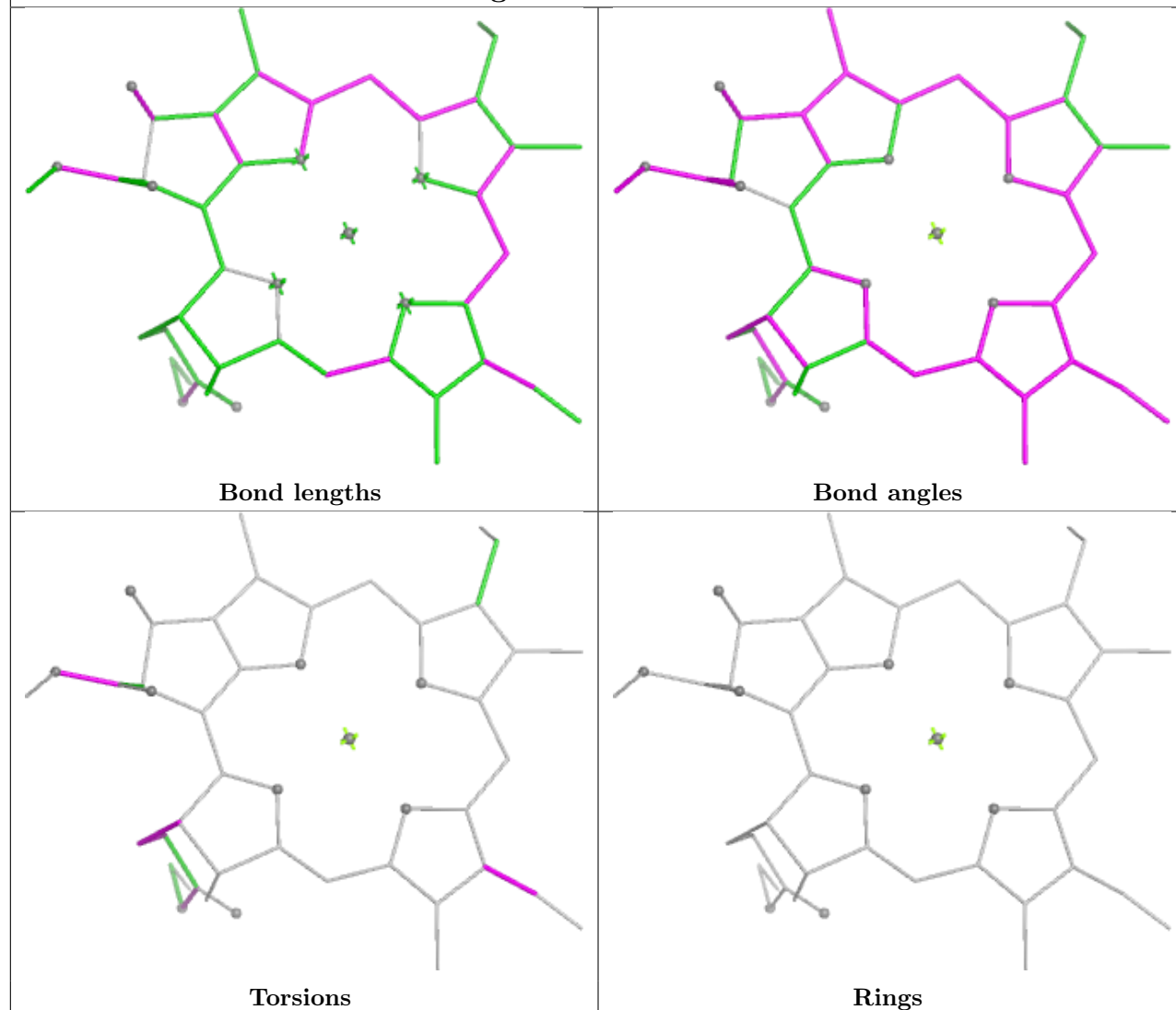


Rings

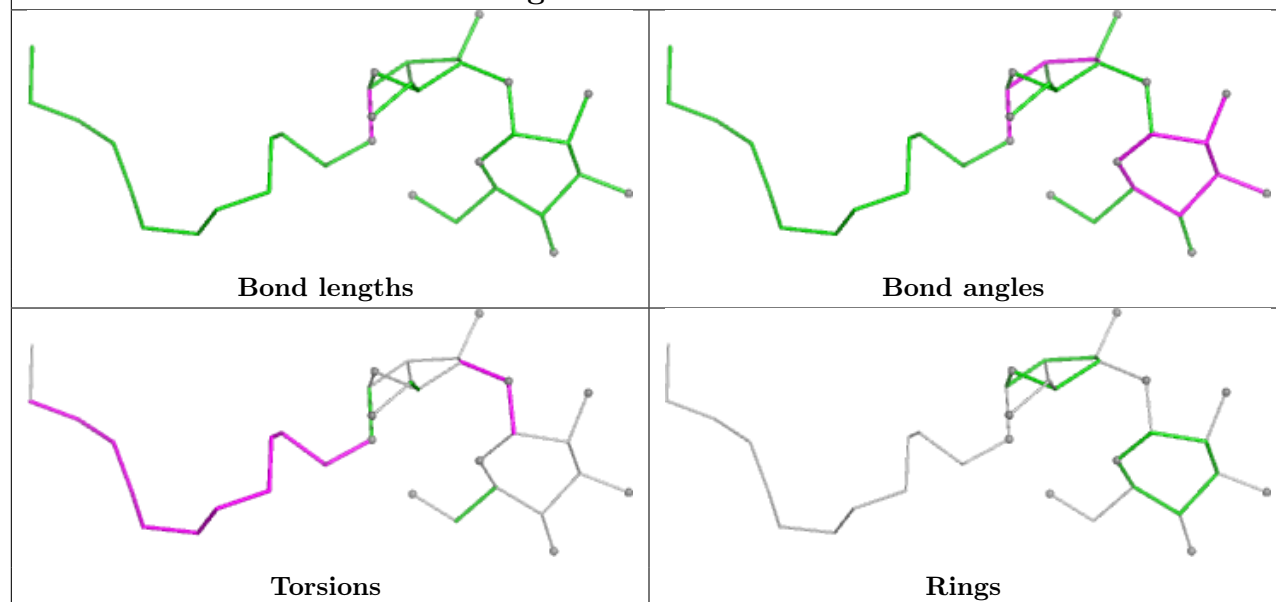


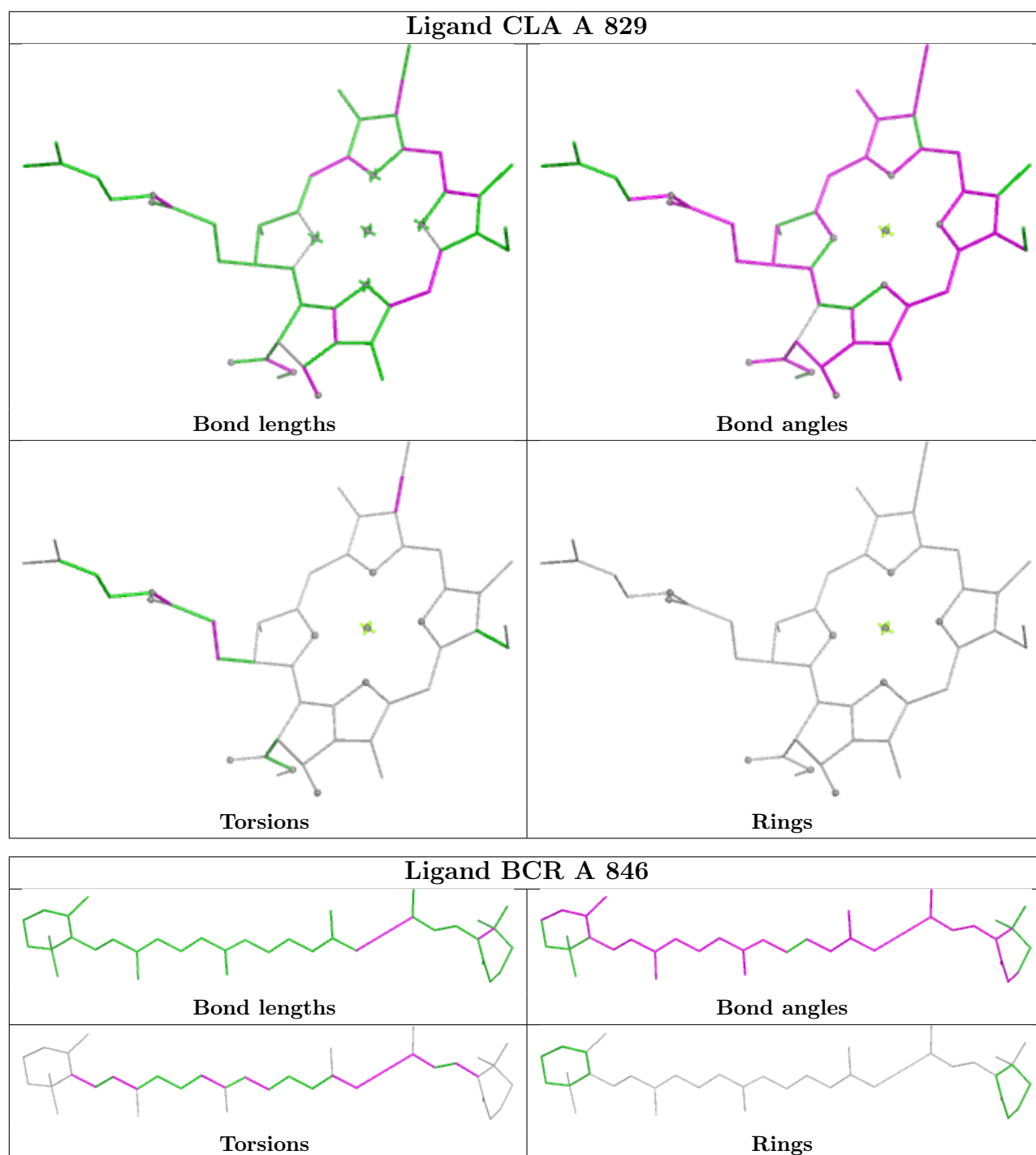


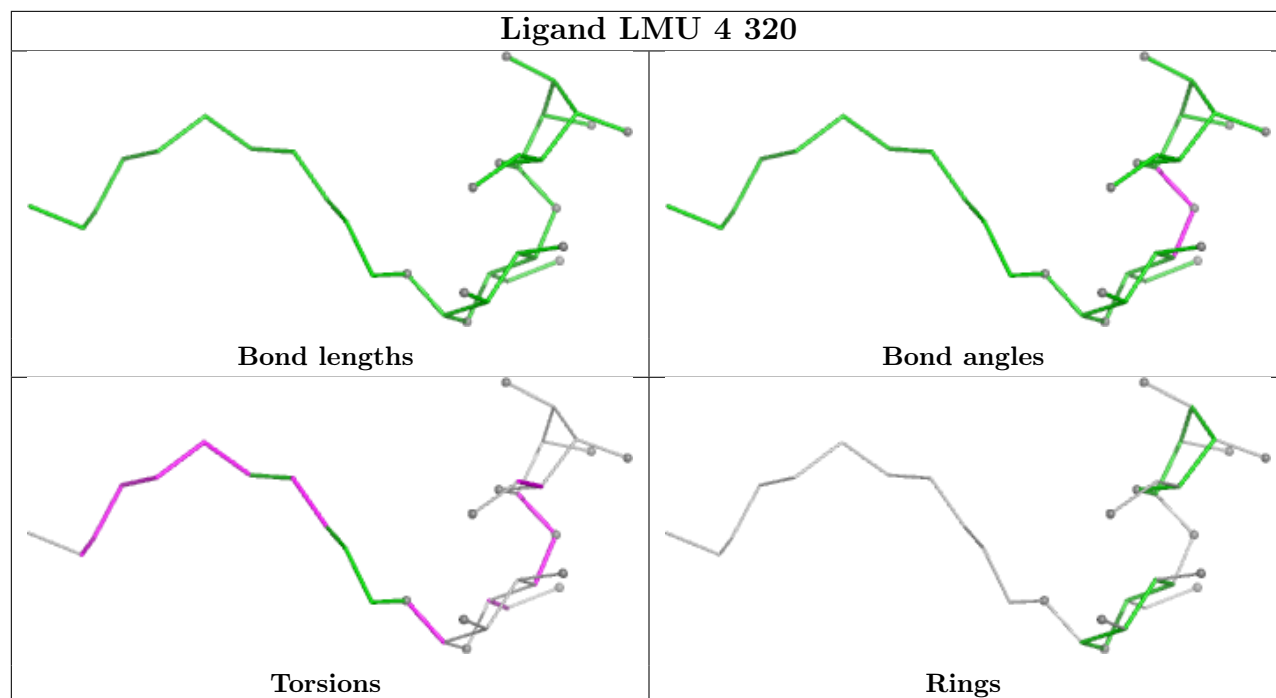
Ligand CLA B 837



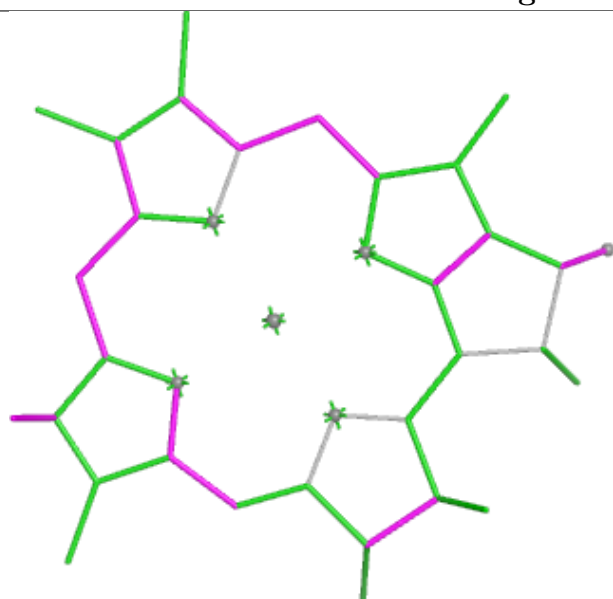
Ligand LMU A 849



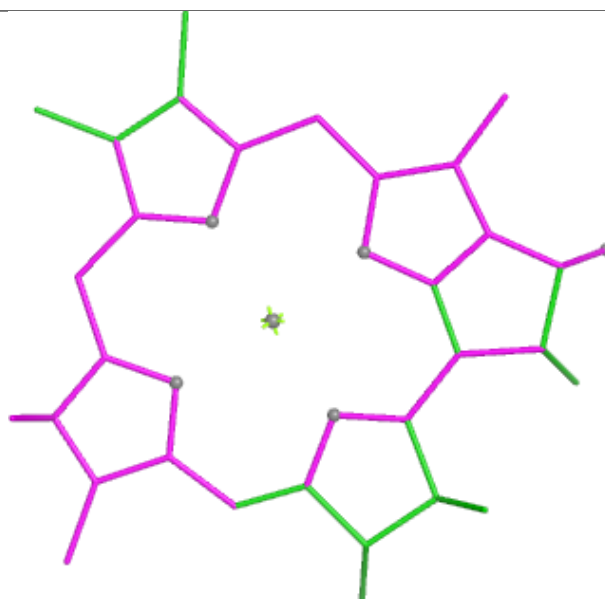




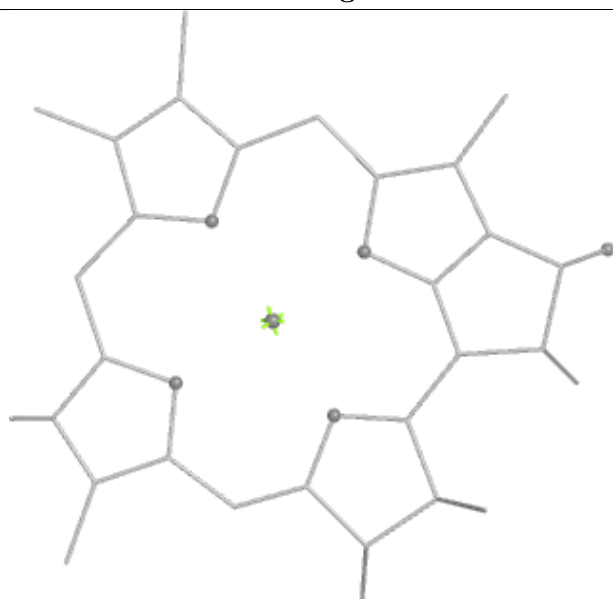
Ligand CLA 1 209



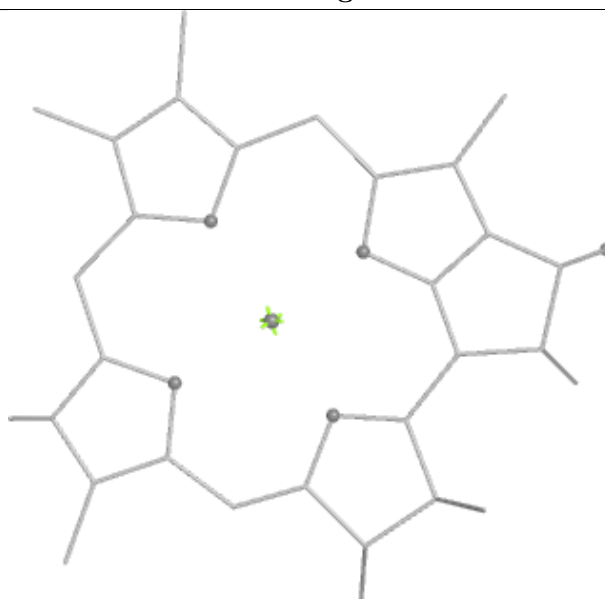
Bond lengths



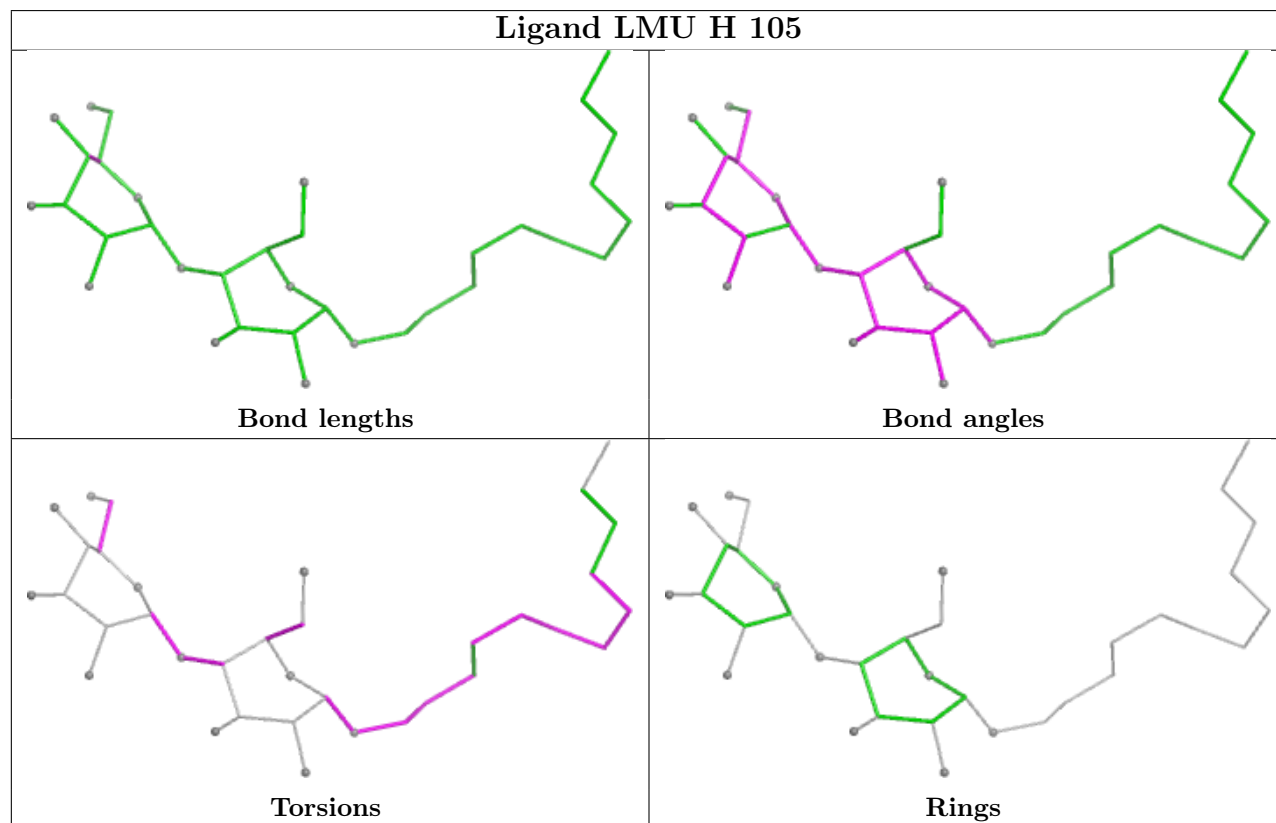
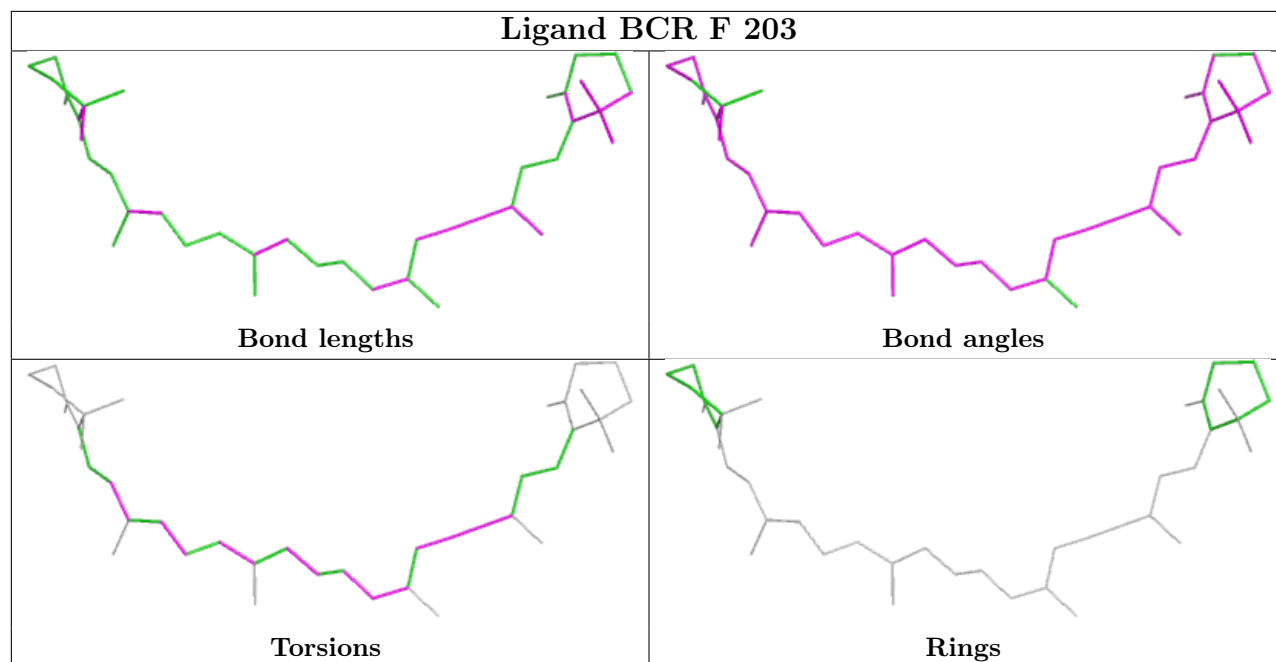
Bond angles

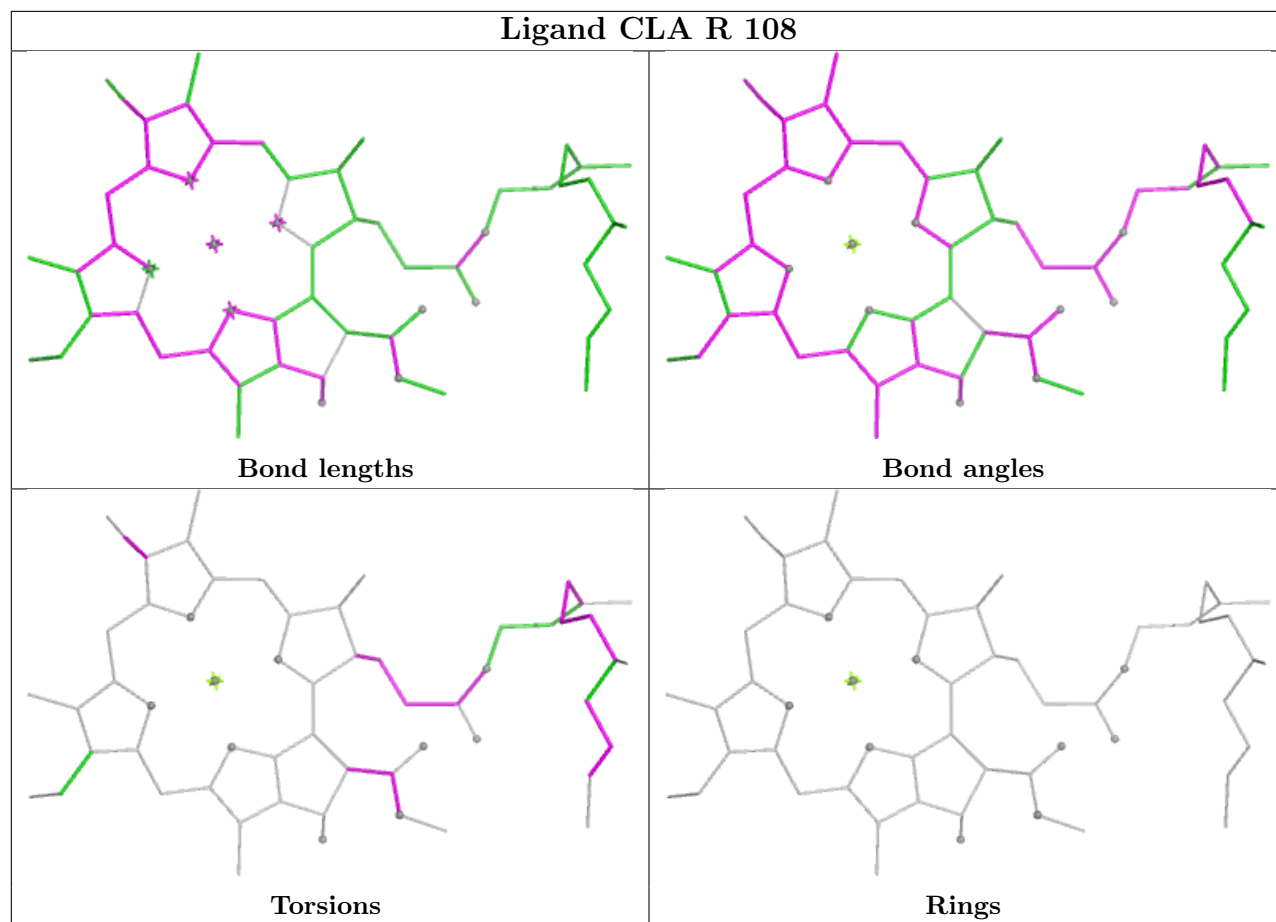


Torsions

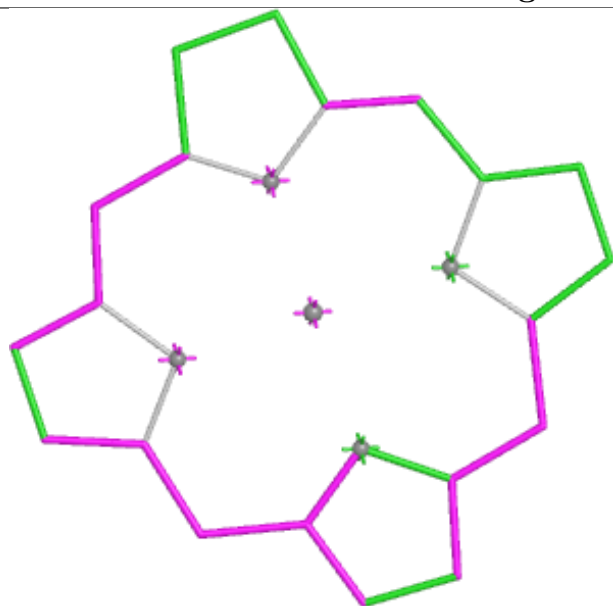


Rings

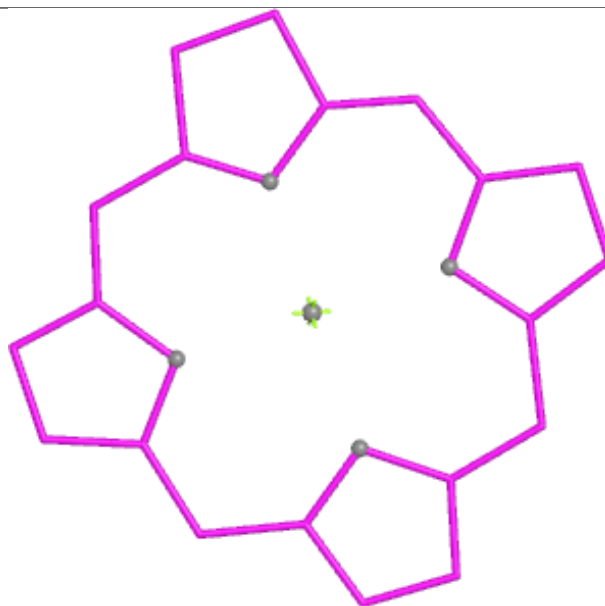




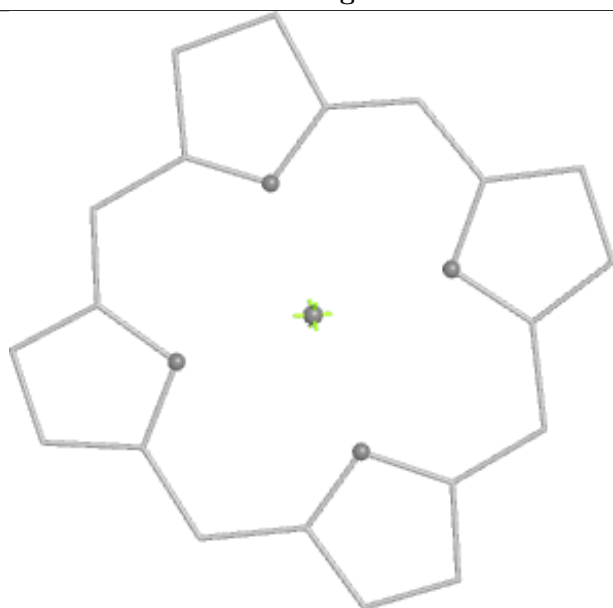
Ligand CLA 3 312



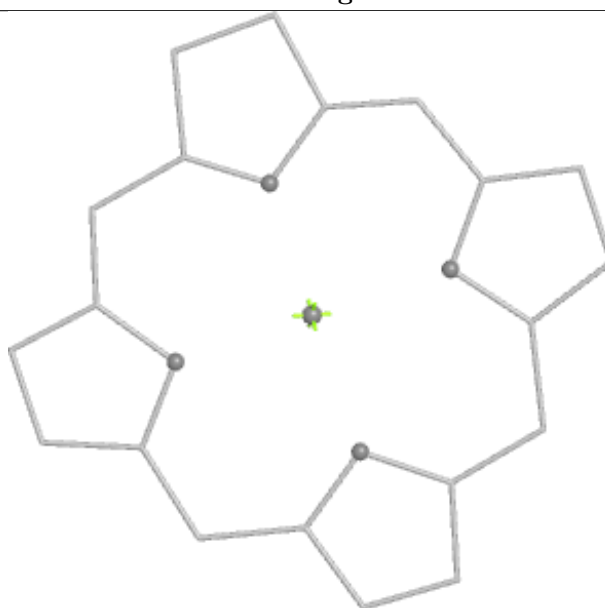
Bond lengths



Bond angles

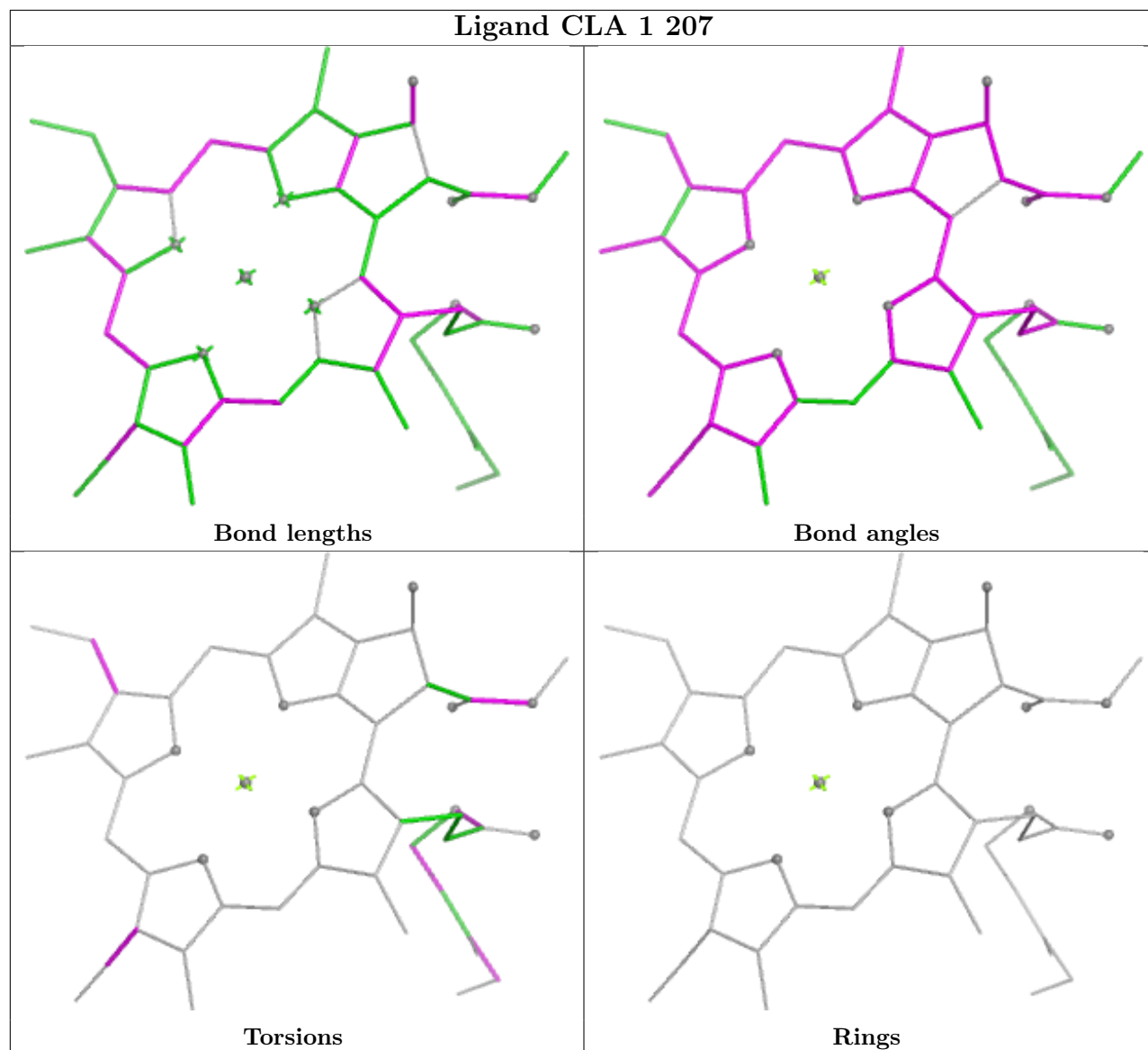


Torsions

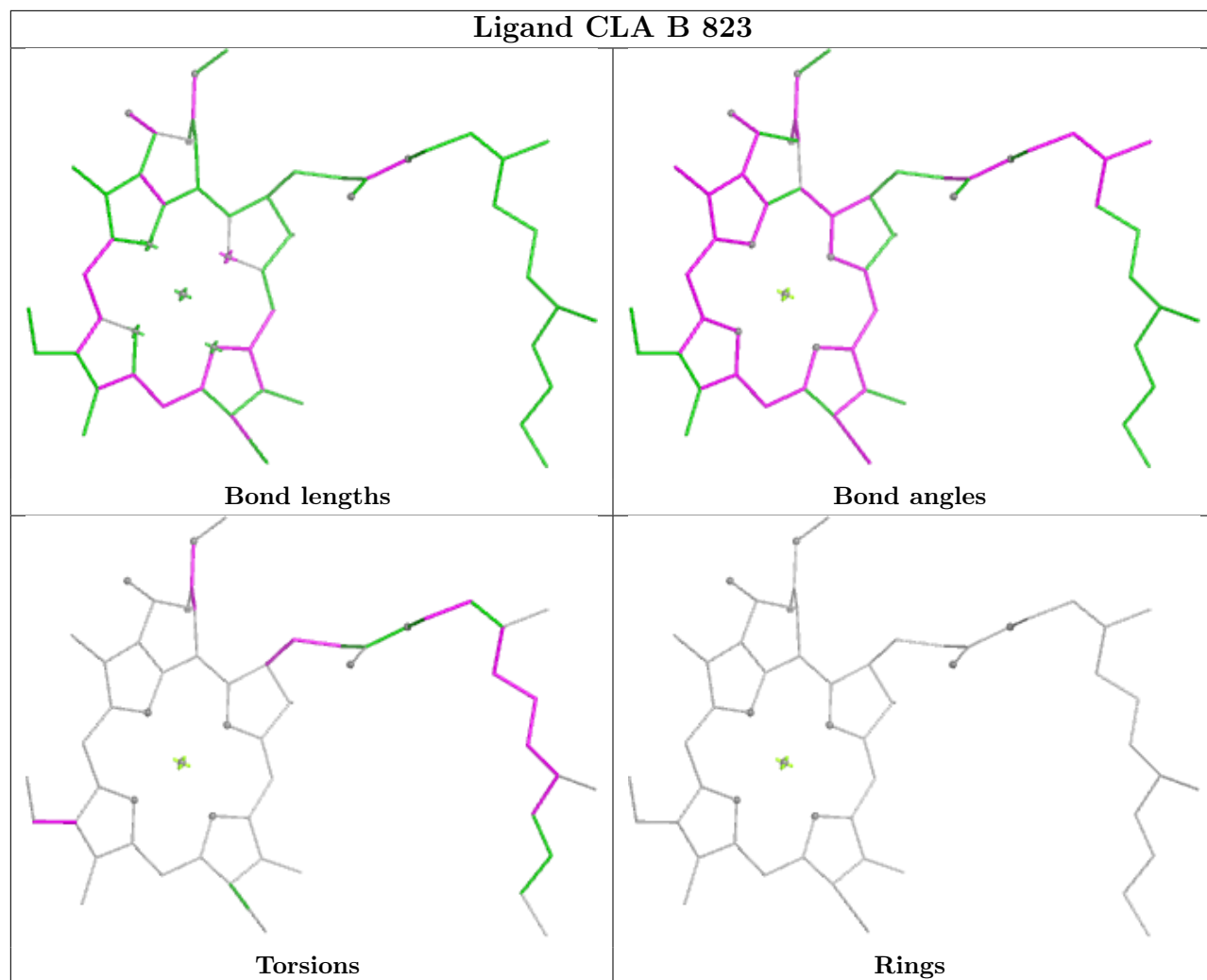


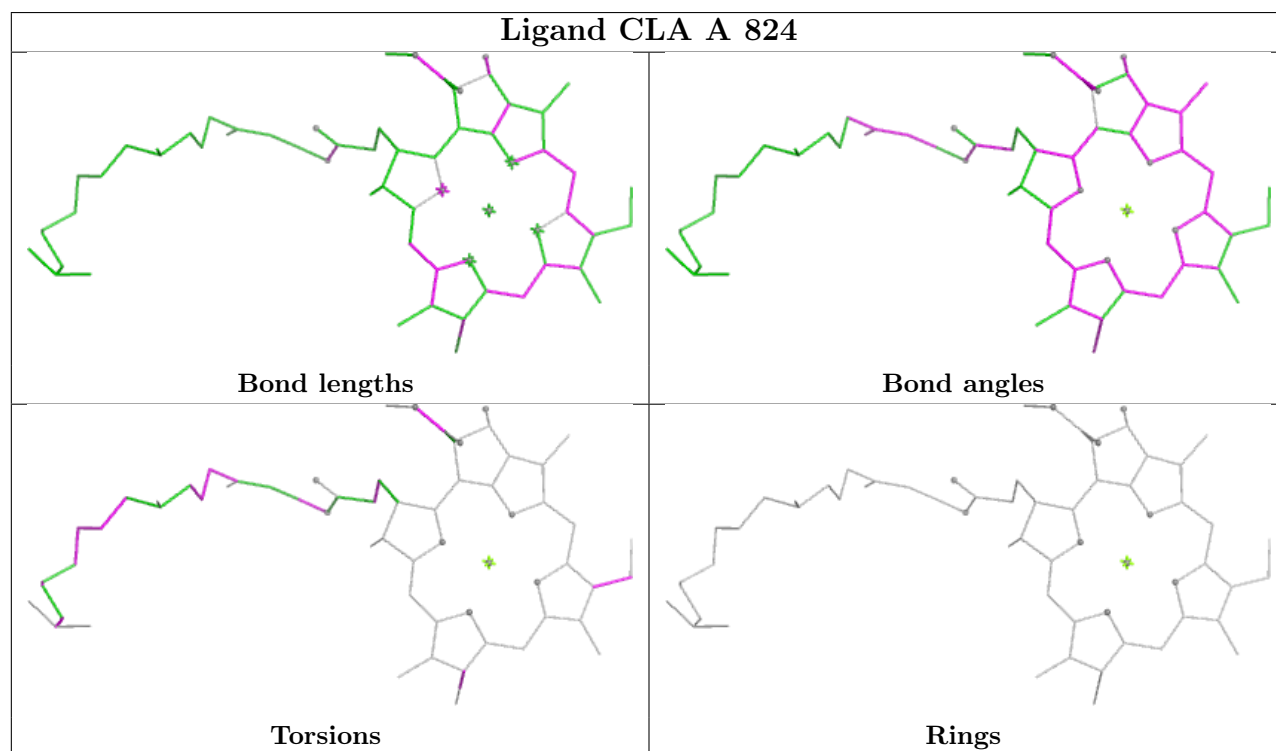
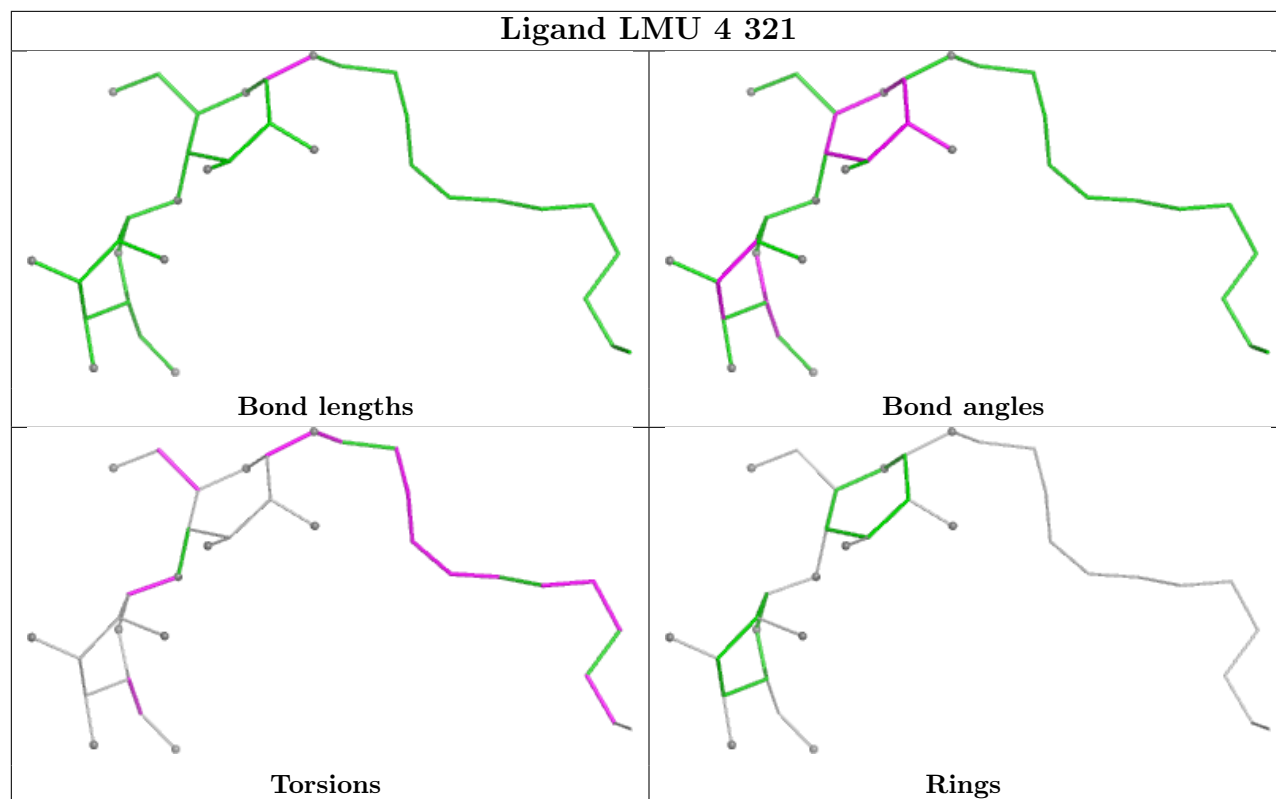
Rings

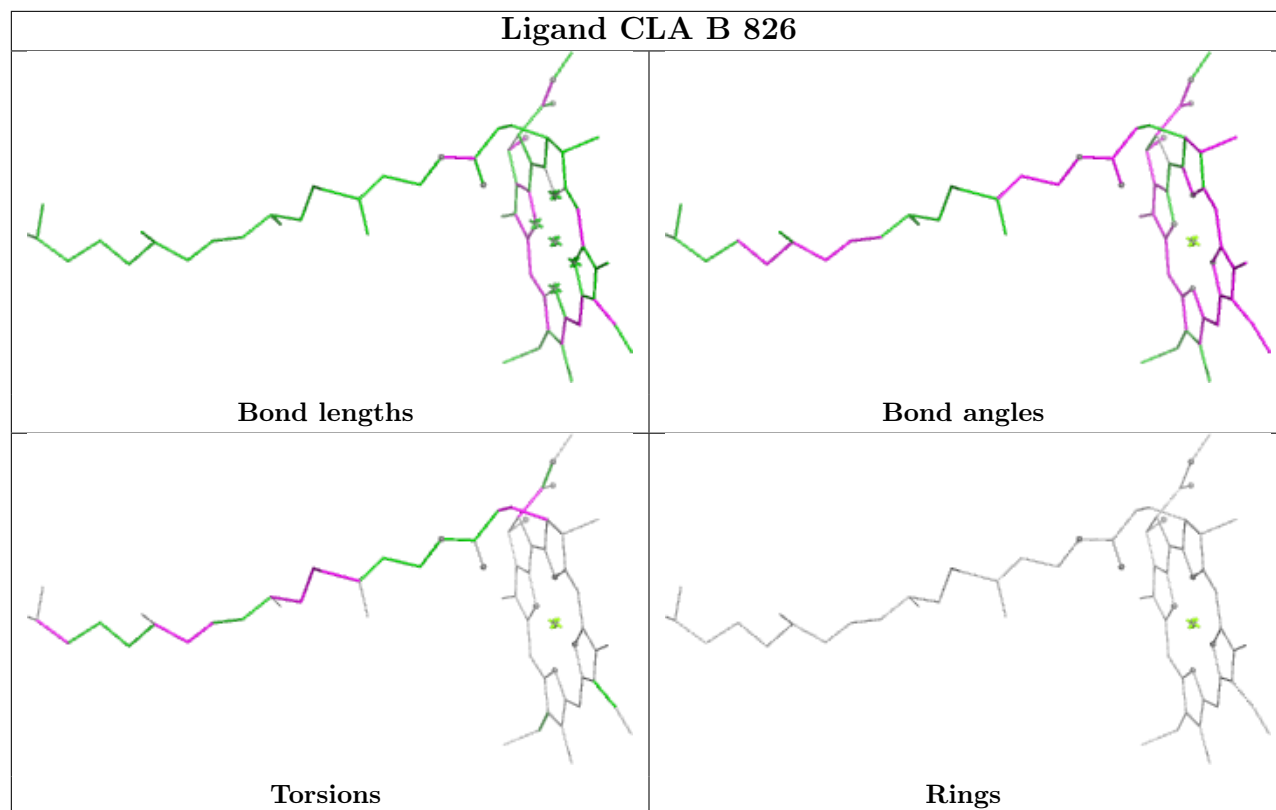
Ligand CLA 1 207

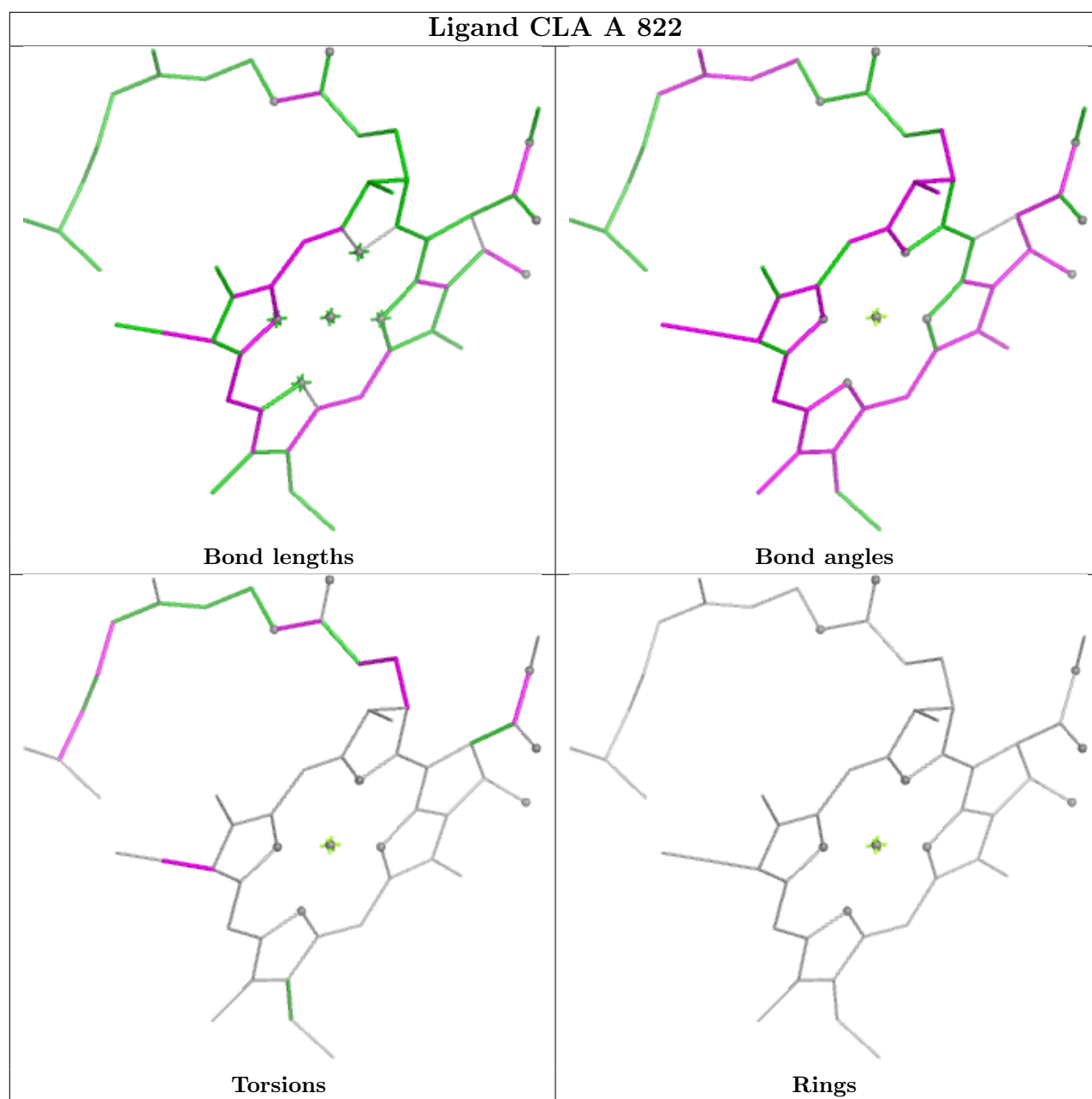


Ligand CLA B 823









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	164/241 (68%)	2.45	88 (53%) 0 0	32, 62, 71, 73	0
2	2	176/269 (65%)	1.64	53 (30%) 1 1	20, 20, 20, 20	0
3	3	160/276 (57%)	2.91	102 (63%) 0 0	49, 79, 110, 112	0
4	4	166/251 (66%)	1.60	49 (29%) 1 1	20, 20, 20, 20	0
5	A	730/758 (96%)	2.36	375 (51%) 0 1	20, 20, 20, 20	0
6	B	733/734 (99%)	2.27	373 (50%) 0 1	20, 20, 20, 20	0
7	C	81/81 (100%)	2.66	49 (60%) 0 0	20, 20, 20, 20	0
8	D	138/212 (65%)	1.90	53 (38%) 1 1	20, 20, 20, 20	0
9	E	65/143 (45%)	1.67	21 (32%) 1 1	20, 20, 20, 20	0
10	F	154/231 (66%)	1.70	45 (29%) 1 1	20, 20, 20, 20	0
11	G	95/167 (56%)	1.40	19 (20%) 3 3	20, 20, 20, 20	0
12	H	69/144 (47%)	1.35	14 (20%) 3 3	20, 20, 20, 20	0
13	I	30/40 (75%)	1.26	6 (20%) 3 3	20, 20, 20, 20	0
14	J	42/44 (95%)	1.68	14 (33%) 1 1	20, 20, 20, 20	0
15	K	84/131 (64%)	1.42	23 (27%) 1 2	20, 20, 20, 20	0
16	L	161/216 (74%)	1.94	67 (41%) 0 1	20, 20, 20, 20	0
17	N	85/170 (50%)	1.02	11 (12%) 7 6	20, 20, 20, 20	0
18	R	0/53	-	-	-	-
All	All	3133/4161 (75%)	2.08	1362 (43%) 0 1	20, 20, 65, 112	0

The worst 5 of 1362 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	3	61	ASN	14.3
5	A	752	ALA	14.1
6	B	491	ASN	11.7

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Mol	Chain	Res	Type	RSRZ
6	B	562	PRO	10.9
1	1	75	ALA	10.4

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

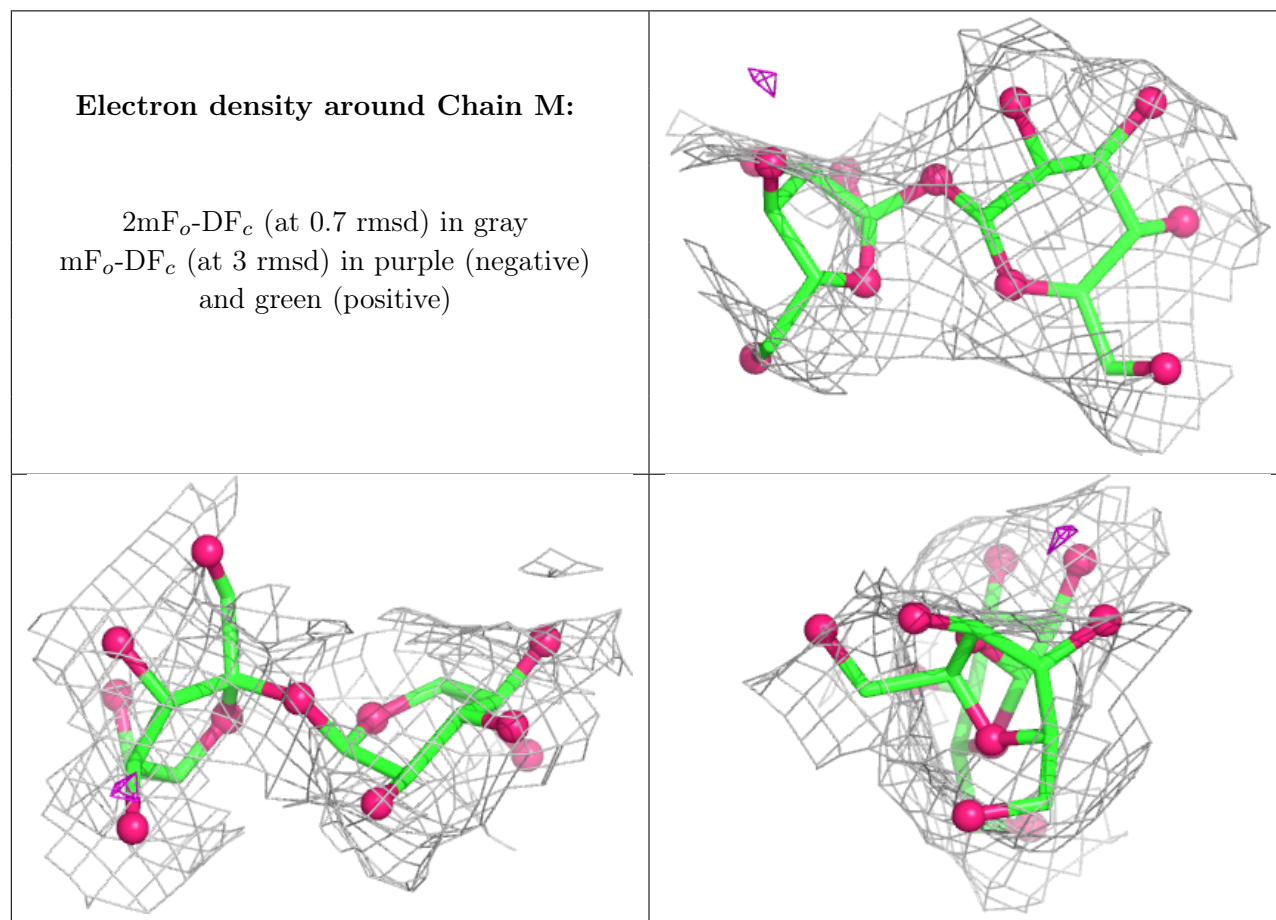
There are no non-standard protein/DNA/RNA residues in this entry.

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.

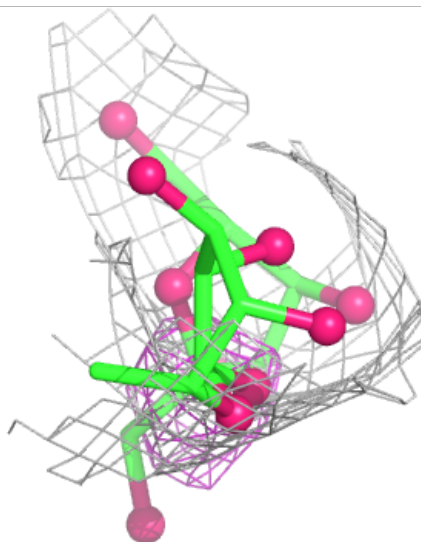
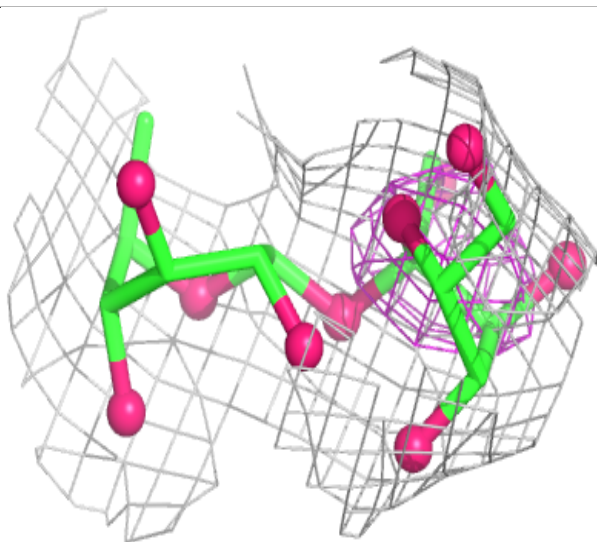
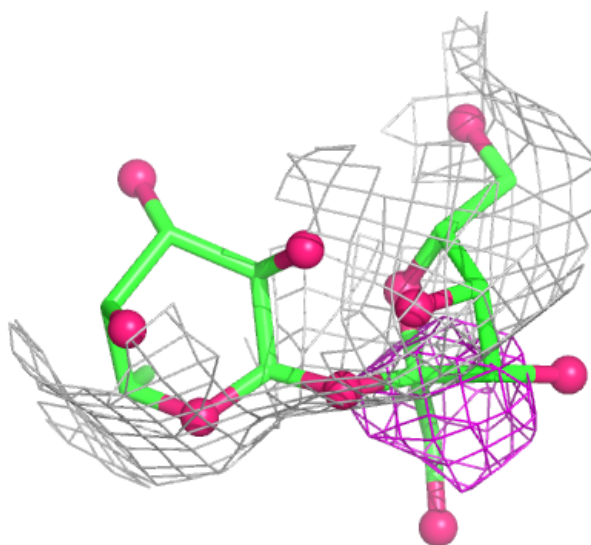
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
19	GLC	M	1	11/12	-	-	20,20,20,20	0
19	FRU	M	2	12/12	-	-	20,20,20,20	0
19	GLC	O	1	10/12	-	-	20,20,20,20	0
19	FRU	O	2	12/12	-	-	20,20,20,20	0
19	GLC	P	1	11/12	-	-	20,20,20,20	0
19	FRU	P	2	12/12	-	-	20,20,20,20	0
19	GLC	Q	1	11/12	-	-	20,20,20,20	0
19	FRU	Q	2	12/12	-	-	20,20,20,20	0
19	GLC	V	1	11/12	0.40	0.34	20,20,20,20	0
19	FRU	T	2	12/12	0.54	0.33	20,20,20,20	0
19	FRU	S	2	12/12	0.59	0.21	20,20,20,20	0
19	FRU	V	2	12/12	0.63	0.25	20,20,20,20	0
19	GLC	W	1	11/12	0.66	0.15	20,20,20,20	0
19	FRU	Y	2	12/12	0.67	0.13	20,20,20,20	0
19	FRU	Z	2	12/12	0.67	0.14	2,33,60,60	0
19	FRU	U	2	12/12	0.70	0.22	2,36,60,60	0
19	GLC	T	1	11/12	0.70	0.15	20,20,20,20	0
19	GLC	S	1	11/12	0.74	0.14	20,20,20,20	0
19	GLC	U	1	11/12	0.75	0.18	2,13,57,60	0
19	FRU	W	2	12/12	0.76	0.14	20,20,20,20	0
19	GLC	Z	1	11/12	0.77	0.10	2,57,60,60	0
19	GLC	X	1	11/12	0.83	0.10	20,20,20,20	0
19	GLC	Y	1	11/12	0.84	0.09	20,20,20,20	0
19	FRU	X	2	12/12	0.85	0.10	20,20,20,20	0
19	GLC	a	1	11/12	-	-	20,20,20,20	0
19	FRU	a	2	12/12	-	-	20,20,20,20	0

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



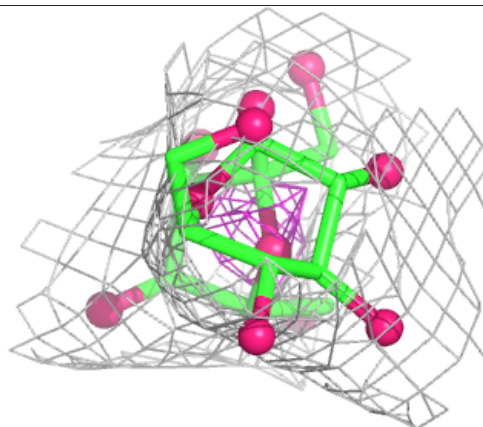
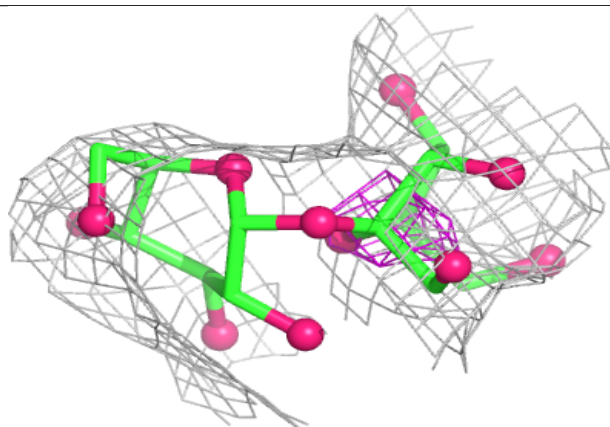
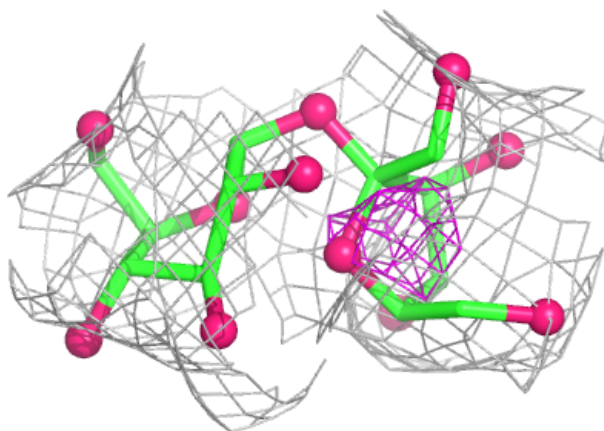
Electron density around Chain O:

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



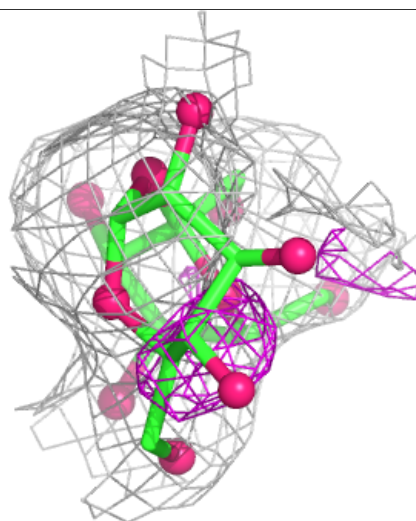
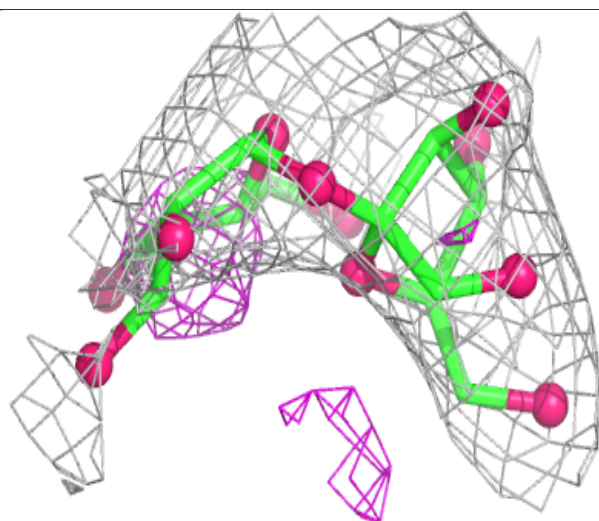
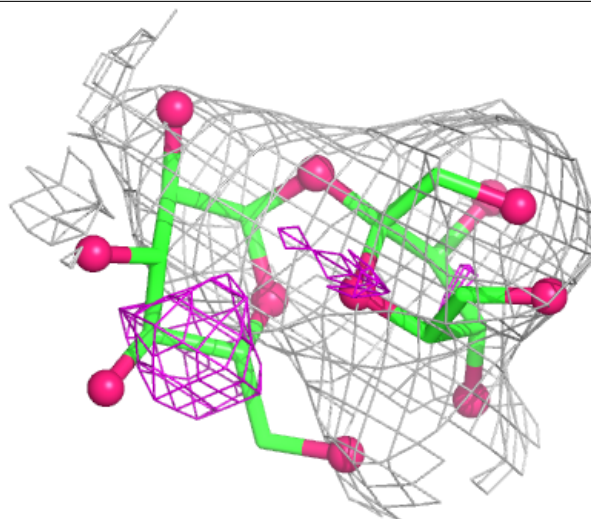
Electron density around Chain P:

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



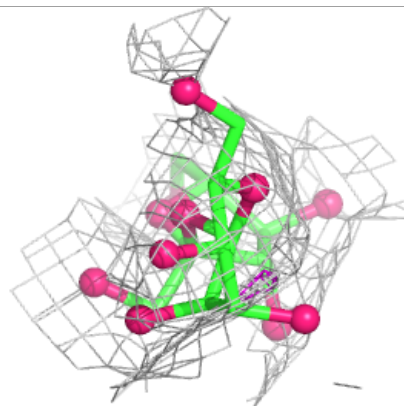
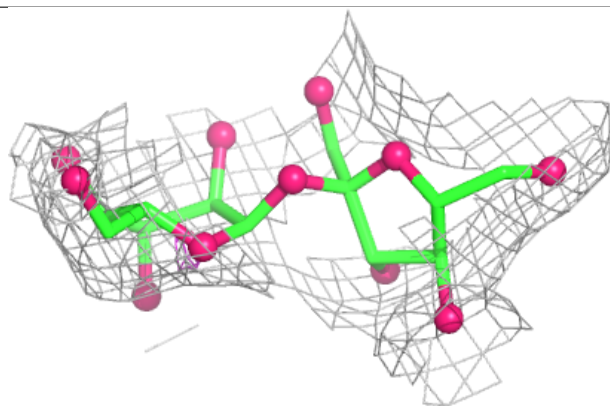
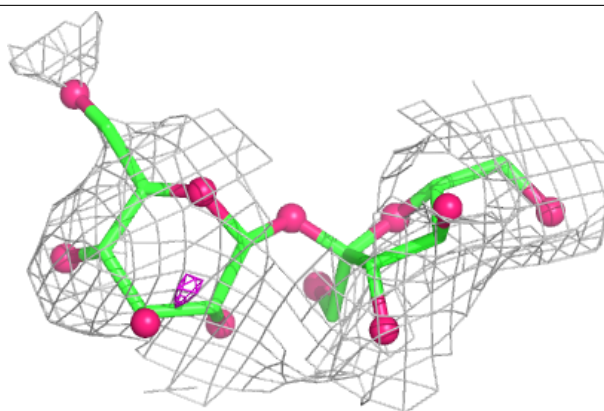
Electron density around Chain Q:

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

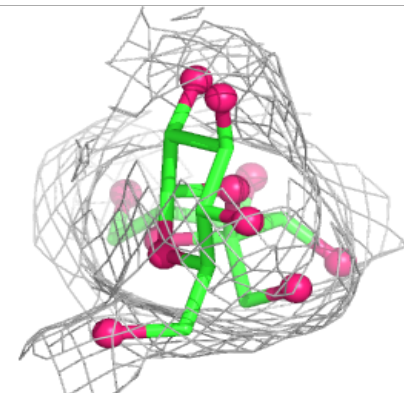
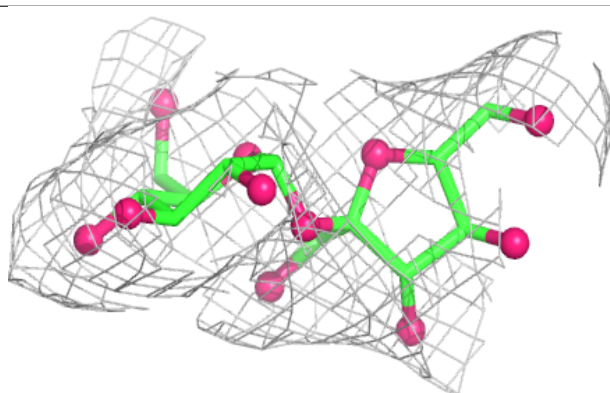
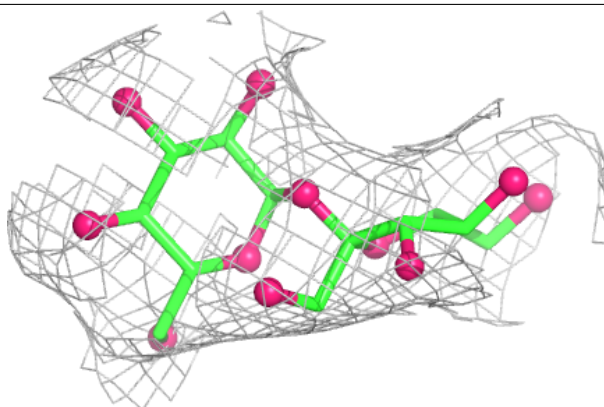


Electron density around Chain S:

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

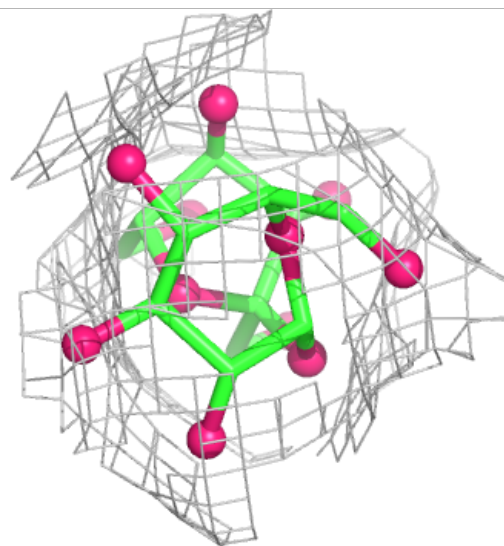
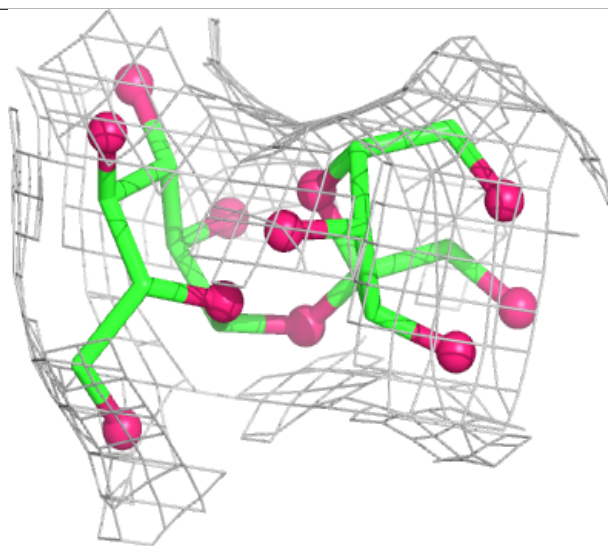
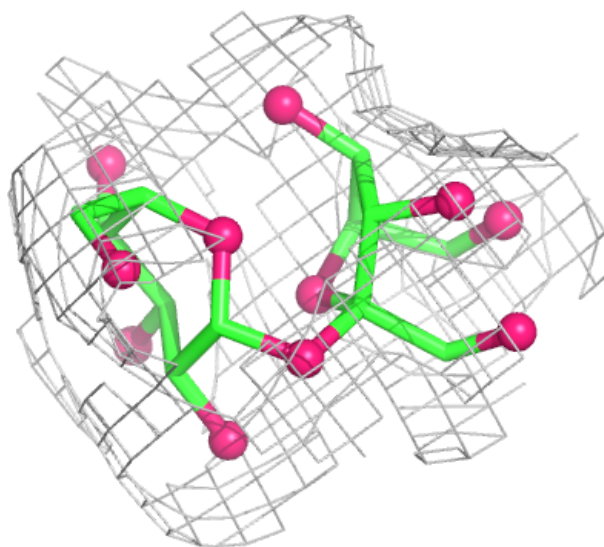
**Electron density around Chain T:**

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



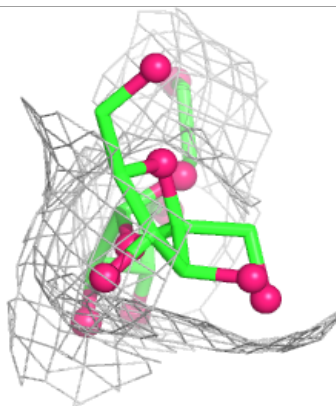
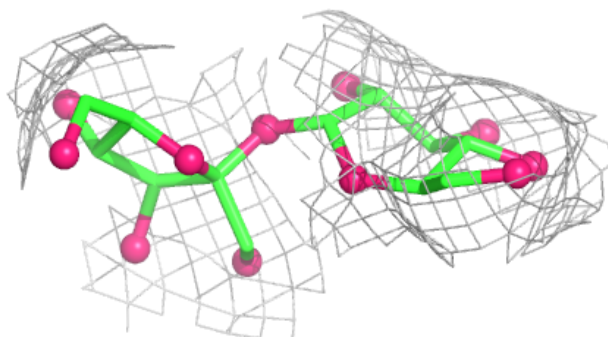
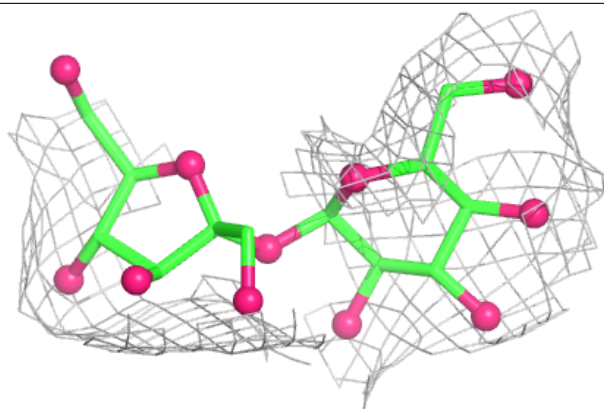
Electron density around Chain U:

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

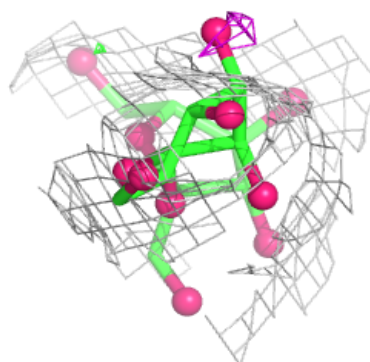
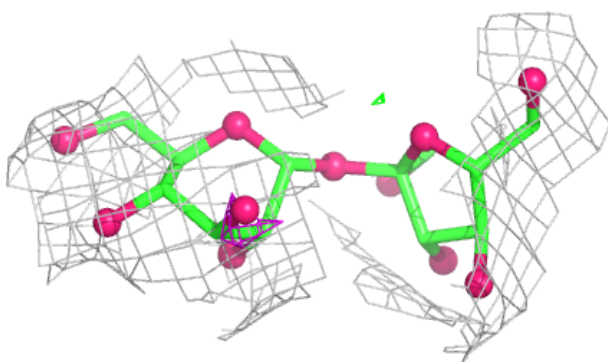
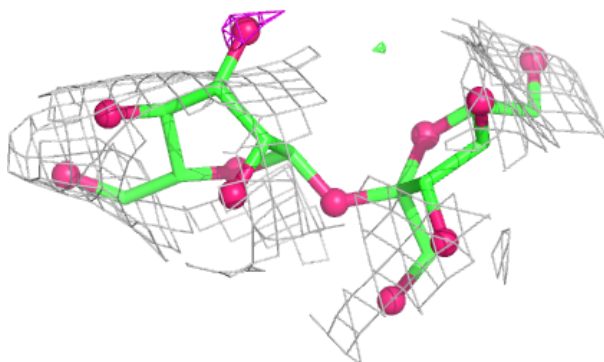


Electron density around Chain V:

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

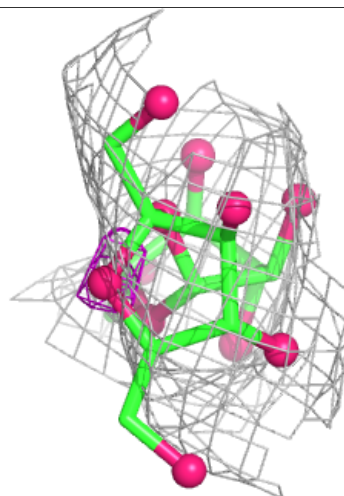
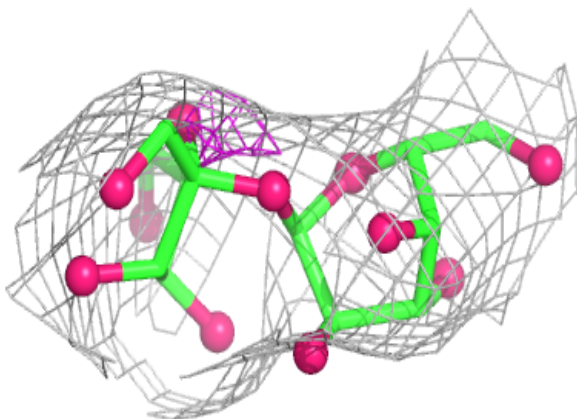
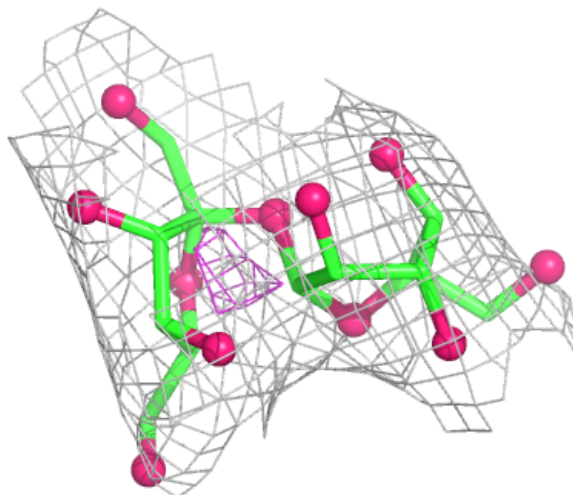
**Electron density around Chain W:**

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



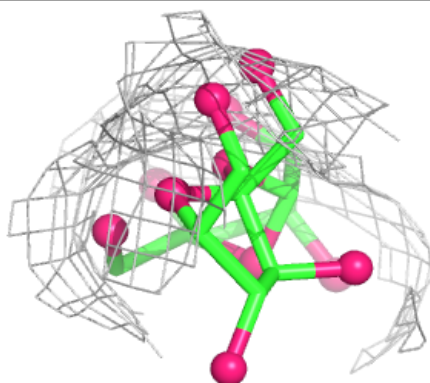
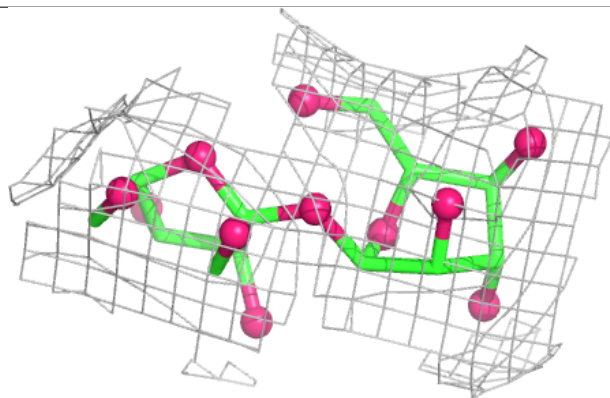
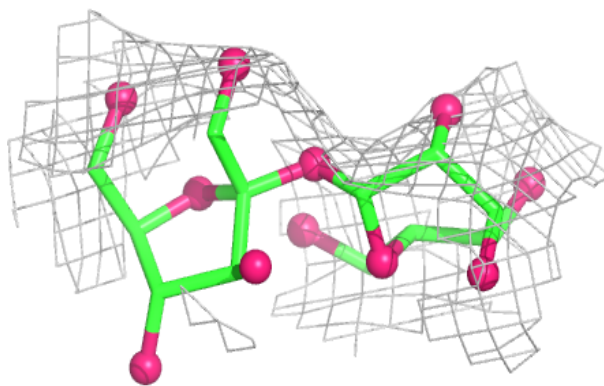
Electron density around Chain X:

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



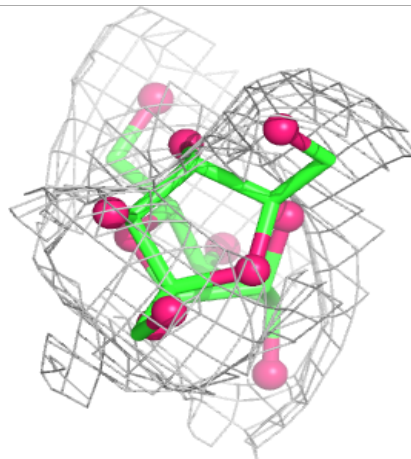
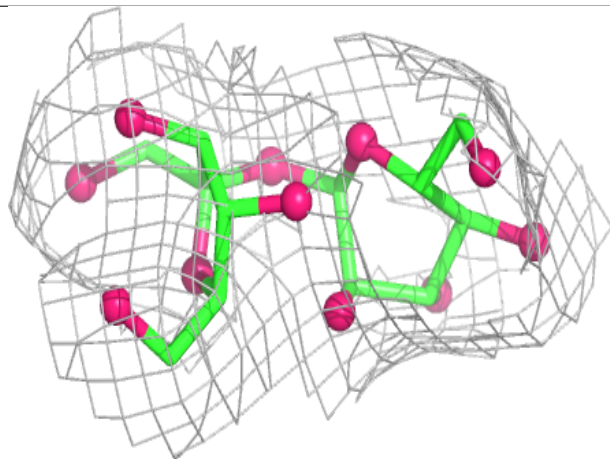
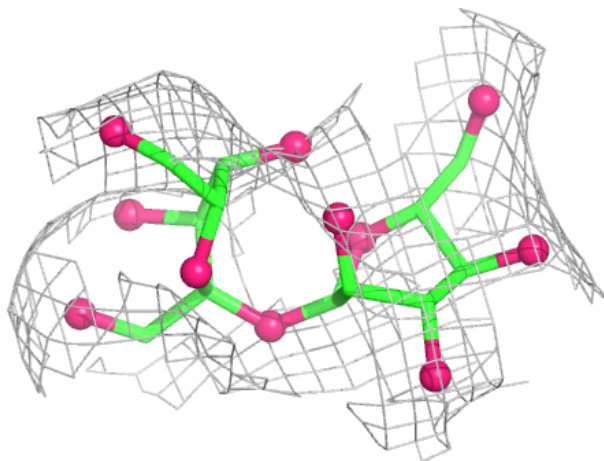
Electron density around Chain Y:

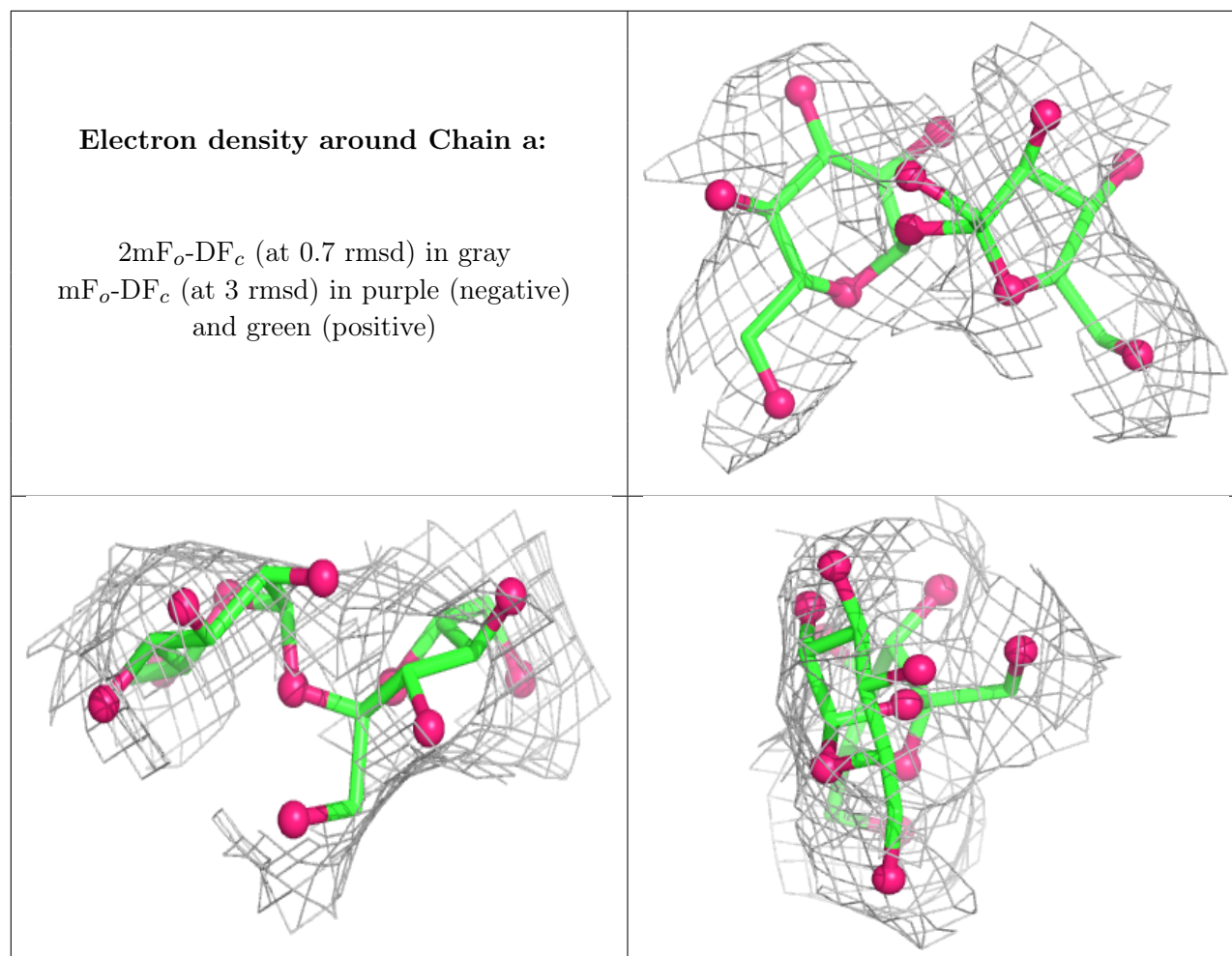
$2mF_o - DF_c$ (at 0.7 rmsd) in gray
 $mF_o - DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around Chain Z:

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





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	1	218	35/35	0.43	0.19	20,20,20,20	0
21	LMU	R	102	35/35	0.45	0.19	20,20,20,20	0
21	LMU	H	108	35/35	0.47	0.18	2,41,60,60	0
20	CLA	3	310	25/65	0.47	0.20	20,20,20,20	0
21	LMU	A	853	35/35	0.49	0.19	20,20,20,20	0
21	LMU	4	301	35/35	0.50	0.17	20,20,20,20	0
20	CLA	B	834	51/65	0.50	0.20	20,20,20,20	0
20	CLA	3	306	25/65	0.51	0.20	20,20,20,20	0
21	LMU	L	204	35/35	0.51	0.17	20,20,20,20	0
20	CLA	2	308	65/65	0.51	0.18	20,20,20,20	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
21	LMU	1	220	35/35	0.53	0.17	2,51,60,60	0
20	CLA	4	308	36/65	0.53	0.17	20,20,20,20	0
22	BCR	A	843	40/40	0.53	0.23	20,20,20,20	0
20	CLA	K	103	65/65	0.54	0.17	20,20,20,20	0
20	CLA	B	813	60/65	0.54	0.21	20,20,20,20	0
21	LMU	R	106	35/35	0.54	0.17	20,20,20,20	0
22	BCR	3	314	40/40	0.54	0.21	20,20,20,20	0
20	CLA	H	103	55/65	0.54	0.18	20,20,20,20	0
22	BCR	J	102	40/40	0.54	0.22	20,20,20,20	0
20	CLA	2	302	51/65	0.55	0.20	20,20,20,20	0
20	CLA	2	320	61/65	0.55	0.18	20,20,20,20	0
20	CLA	4	302	55/65	0.55	0.19	20,20,20,20	0
20	CLA	4	306	50/65	0.55	0.21	20,20,20,20	0
20	CLA	B	833	45/65	0.56	0.18	20,20,20,20	0
20	CLA	4	305	55/65	0.56	0.18	20,20,20,20	0
20	CLA	A	810	45/65	0.56	0.21	20,20,20,20	0
20	CLA	A	839	65/65	0.56	0.18	20,20,20,20	0
20	CLA	3	311	65/65	0.56	0.19	20,20,20,20	0
22	BCR	L	208	40/40	0.56	0.27	20,20,20,20	0
20	CLA	3	301	36/65	0.57	0.19	20,20,20,20	0
21	LMU	B	801	35/35	0.57	0.17	20,20,20,20	0
20	CLA	H	102	55/65	0.57	0.19	20,20,20,20	0
21	LMU	1	213	35/35	0.57	0.17	2,45,60,60	0
21	LMU	4	317	35/35	0.57	0.16	20,20,20,20	0
20	CLA	L	201	55/65	0.58	0.18	20,20,20,20	0
22	BCR	A	845	40/40	0.58	0.26	20,20,20,20	0
20	CLA	3	308	42/65	0.59	0.18	20,20,20,20	0
21	LMU	D	201	35/35	0.59	0.16	2,30,60,60	0
20	CLA	1	211	25/65	0.59	0.20	20,20,20,20	0
21	LMU	K	108	35/35	0.59	0.15	20,20,20,20	0
20	CLA	K	102	50/65	0.59	0.18	20,20,20,20	0
21	LMU	R	101	35/35	0.59	0.16	20,20,20,20	0
21	LMU	2	313	35/35	0.59	0.17	20,20,20,20	0
21	LMU	2	316	35/35	0.59	0.17	20,20,20,20	0
21	LMU	2	319	35/35	0.59	0.19	20,20,20,20	0
21	LMU	3	320	35/35	0.59	0.17	20,20,20,20	0
20	CLA	2	306	25/65	0.59	0.17	20,20,20,20	0
20	CLA	K	107	50/65	0.59	0.17	20,20,20,20	0
20	CLA	3	307	25/65	0.59	0.20	20,20,20,20	0
21	LMU	H	105	35/35	0.60	0.15	20,20,20,20	0
20	CLA	3	313	65/65	0.60	0.16	20,20,20,20	0
20	CLA	J	103	61/65	0.60	0.17	20,20,20,20	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
21	LMU	F	201	34/35	0.61	0.15	20,20,20,20	0
21	LMU	K	106	35/35	0.61	0.15	2,38,60,60	0
20	CLA	H	101	55/65	0.61	0.16	20,20,20,20	0
21	LMU	R	104	35/35	0.62	0.16	20,20,20,20	0
20	CLA	3	305	25/65	0.62	0.15	20,20,20,20	0
20	CLA	4	304	65/65	0.62	0.17	20,20,20,20	0
21	LMU	2	317	35/35	0.62	0.16	20,20,20,20	0
21	LMU	A	848	35/35	0.62	0.17	20,20,20,20	0
20	CLA	A	820	51/65	0.62	0.19	20,20,20,20	0
21	LMU	R	103	35/35	0.62	0.16	20,20,20,20	0
20	CLA	4	311	55/65	0.63	0.19	20,20,20,20	0
20	CLA	A	801	46/65	0.63	0.17	20,20,20,20	0
20	CLA	2	301	25/65	0.63	0.16	20,20,20,20	0
20	CLA	A	814	45/65	0.63	0.21	20,20,20,20	0
20	CLA	1	210	51/65	0.63	0.18	20,20,20,20	0
21	LMU	H	107	35/35	0.63	0.15	20,20,20,20	0
21	LMU	1	217	35/35	0.63	0.16	20,20,20,20	0
20	CLA	A	823	65/65	0.63	0.27	20,20,20,20	0
20	CLA	1	201	46/65	0.63	0.15	20,20,20,20	0
21	LMU	A	849	35/35	0.63	0.17	20,20,20,20	0
20	CLA	4	318	52/65	0.64	0.15	20,20,20,20	0
20	CLA	A	819	65/65	0.64	0.22	20,20,20,20	0
20	CLA	B	814	46/65	0.64	0.24	20,20,20,20	0
20	CLA	3	302	50/65	0.64	0.20	20,20,20,20	0
20	CLA	K	101	45/65	0.64	0.15	20,20,20,20	0
22	BCR	I	103	40/40	0.64	0.18	20,20,20,20	0
20	CLA	1	215	61/65	0.64	0.15	2,35,60,60	0
20	CLA	B	840	36/65	0.64	0.16	20,20,20,20	0
20	CLA	2	307	65/65	0.65	0.17	20,20,20,20	0
22	BCR	B	846	40/40	0.65	0.26	20,20,20,20	0
20	CLA	3	317	65/65	0.65	0.19	20,20,20,20	0
20	CLA	A	811	65/65	0.65	0.23	20,20,20,20	0
20	CLA	3	309	25/65	0.65	0.18	20,20,20,20	0
25	LMG	B	848	49/55	0.65	0.24	20,20,20,20	0
26	UNL	H	110	23/-	0.65	0.16	20,20,20,20	0
20	CLA	3	318	25/65	0.66	0.17	20,20,20,20	0
21	LMU	N	101	35/35	0.66	0.15	2,39,60,60	0
23	PQN	A	842	33/33	0.66	0.35	20,20,20,20	0
20	CLA	R	108	58/65	0.66	0.16	20,20,20,20	0
20	CLA	A	806	55/65	0.66	0.25	20,20,20,20	0
20	CLA	A	852	65/65	0.67	0.25	20,20,20,20	0
22	BCR	B	844	40/40	0.67	0.24	20,20,20,20	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
21	LMU	H	104	35/35	0.67	0.14	20,20,20,20	0
20	CLA	F	205	41/65	0.67	0.15	20,20,20,20	0
20	CLA	3	316	50/65	0.67	0.14	20,20,20,20	0
20	CLA	A	818	65/65	0.67	0.25	20,20,20,20	0
20	CLA	B	823	58/65	0.67	0.24	20,20,20,20	0
20	CLA	A	829	50/65	0.67	0.21	20,20,20,20	0
20	CLA	2	303	65/65	0.67	0.20	20,20,20,20	0
20	CLA	3	319	25/65	0.68	0.16	20,20,20,20	0
20	CLA	R	107	57/65	0.68	0.16	20,20,20,20	0
21	LMU	C	101	35/35	0.68	0.14	20,20,20,20	0
21	LMU	L	209	35/35	0.68	0.16	20,20,20,20	0
20	CLA	1	207	51/65	0.68	0.14	20,20,20,20	0
20	CLA	2	310	25/65	0.68	0.20	20,20,20,20	0
20	CLA	A	817	52/65	0.68	0.23	20,20,20,20	0
20	CLA	A	840	50/65	0.68	0.16	20,20,20,20	0
20	CLA	A	805	65/65	0.68	0.25	20,20,20,20	0
20	CLA	4	310	25/65	0.68	0.16	20,20,20,20	0
21	LMU	R	109	35/35	0.68	0.15	20,20,20,20	0
21	LMU	4	320	34/35	0.69	0.15	20,20,20,20	0
21	LMU	4	322	35/35	0.69	0.14	20,20,20,20	0
20	CLA	2	312	50/65	0.69	0.21	20,20,20,20	0
20	CLA	A	825	65/65	0.69	0.21	20,20,20,20	0
20	CLA	A	812	54/65	0.69	0.18	20,20,20,20	0
21	LMU	A	856	35/35	0.69	0.15	20,20,20,20	0
21	LMU	K	104	35/35	0.69	0.14	20,20,20,20	0
21	LMU	K	105	35/35	0.69	0.14	20,20,20,20	0
20	CLA	4	319	47/65	0.69	0.16	20,20,20,20	0
20	CLA	A	816	54/65	0.69	0.19	20,20,20,20	0
20	CLA	B	803	65/65	0.70	0.30	20,20,20,20	0
21	LMU	1	219	35/35	0.70	0.14	20,20,20,20	0
20	CLA	F	204	36/65	0.70	0.26	20,20,20,20	0
20	CLA	A	828	65/65	0.70	0.23	20,20,20,20	0
21	LMU	A	854	35/35	0.70	0.13	20,20,20,20	0
22	BCR	A	847	40/40	0.70	0.27	20,20,20,20	0
20	CLA	A	807	46/65	0.70	0.17	20,20,20,20	0
20	CLA	L	203	55/65	0.70	0.17	20,20,20,20	0
22	BCR	F	203	40/40	0.70	0.20	20,20,20,20	0
21	LMU	B	847	35/35	0.70	0.15	2,35,60,60	0
20	CLA	L	207	50/65	0.70	0.18	20,20,20,20	0
20	CLA	A	821	42/65	0.70	0.16	20,20,20,20	0
20	CLA	B	824	65/65	0.70	0.23	20,20,20,20	0
20	CLA	2	315	65/65	0.70	0.18	20,20,20,20	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
20	CLA	A	804	55/65	0.70	0.21	20,20,20,20	0
21	LMU	2	318	35/35	0.71	0.12	20,20,20,20	0
21	LMU	3	321	35/35	0.71	0.13	20,20,20,20	0
22	BCR	A	844	40/40	0.71	0.22	20,20,20,20	0
22	BCR	B	852	40/40	0.71	0.22	20,20,20,20	0
22	BCR	F	202	40/40	0.71	0.29	20,20,20,20	0
20	CLA	3	312	25/65	0.71	0.18	20,20,20,20	0
20	CLA	A	851	65/65	0.72	0.27	20,20,20,20	0
21	LMU	B	802	35/35	0.72	0.14	20,20,20,20	0
20	CLA	A	802	25/65	0.72	0.15	20,20,20,20	0
21	LMU	R	105	35/35	0.72	0.13	20,20,20,20	0
20	CLA	A	826	65/65	0.72	0.29	20,20,20,20	0
22	BCR	B	845	40/40	0.72	0.27	20,20,20,20	0
20	CLA	H	109	60/65	0.72	0.20	20,20,20,20	0
20	CLA	F	206	53/65	0.72	0.14	20,20,20,20	0
20	CLA	4	307	52/65	0.73	0.15	20,20,20,20	0
20	CLA	B	829	50/65	0.73	0.21	20,20,20,20	0
20	CLA	G	102	51/65	0.73	0.15	20,20,20,20	0
20	CLA	B	809	54/65	0.73	0.21	20,20,20,20	0
20	CLA	1	203	47/65	0.73	0.16	20,20,20,20	0
20	CLA	2	305	50/65	0.73	0.16	20,20,20,20	0
20	CLA	A	833	45/65	0.73	0.18	20,20,20,20	0
20	CLA	J	101	48/65	0.73	0.14	20,20,20,20	0
20	CLA	A	815	50/65	0.74	0.19	20,20,20,20	0
20	CLA	B	838	65/65	0.74	0.27	20,20,20,20	0
20	CLA	B	819	46/65	0.74	0.17	20,20,20,20	0
20	CLA	B	831	50/65	0.74	0.23	20,20,20,20	0
21	LMU	4	321	35/35	0.74	0.13	20,20,20,20	0
20	CLA	B	832	45/65	0.74	0.18	20,20,20,20	0
20	CLA	H	111	50/65	0.74	0.18	20,20,20,20	0
20	CLA	A	803	50/65	0.74	0.19	20,20,20,20	0
21	LMU	E	101	35/35	0.74	0.12	20,20,20,20	0
20	CLA	A	822	55/65	0.75	0.24	20,20,20,20	0
20	CLA	A	835	65/65	0.75	0.22	20,20,20,20	0
20	CLA	4	316	46/65	0.75	0.12	20,20,20,20	0
20	CLA	A	813	54/65	0.75	0.21	20,20,20,20	0
20	CLA	A	841	65/65	0.75	0.23	20,20,20,20	0
20	CLA	4	309	25/65	0.75	0.15	20,20,20,20	0
20	CLA	B	830	65/65	0.75	0.21	20,20,20,20	0
20	CLA	3	303	25/65	0.75	0.13	20,20,20,20	0
20	CLA	3	315	25/65	0.75	0.13	20,20,20,20	0
20	CLA	L	202	65/65	0.75	0.24	20,20,20,20	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
20	CLA	A	830	65/65	0.75	0.20	20,20,20,20	0
22	BCR	B	843	40/40	0.75	0.20	20,20,20,20	0
20	CLA	2	304	25/65	0.76	0.16	20,20,20,20	0
20	CLA	B	835	60/65	0.76	0.23	20,20,20,20	0
20	CLA	1	216	25/65	0.76	0.15	20,20,20,20	0
20	CLA	B	804	45/65	0.76	0.20	20,20,20,20	0
20	CLA	1	205	25/65	0.76	0.13	20,20,20,20	0
20	CLA	B	812	65/65	0.76	0.19	20,20,20,20	0
20	CLA	1	212	25/65	0.76	0.12	20,20,20,20	0
20	CLA	1	206	61/65	0.76	0.15	20,20,20,20	0
20	CLA	B	815	59/65	0.76	0.21	20,20,20,20	0
21	LMU	L	205	35/35	0.77	0.13	20,20,20,20	0
20	CLA	B	817	61/65	0.77	0.21	20,20,20,20	0
20	CLA	B	808	65/65	0.77	0.22	20,20,20,20	0
20	CLA	A	832	50/65	0.77	0.19	20,20,20,20	0
20	CLA	A	827	55/65	0.77	0.22	20,20,20,20	0
22	BCR	A	846	40/40	0.77	0.23	20,20,20,20	0
20	CLA	1	202	57/65	0.77	0.14	2,38,60,60	0
20	CLA	A	809	52/65	0.77	0.21	20,20,20,20	0
21	LMU	A	855	35/35	0.77	0.12	20,20,20,20	0
20	CLA	2	311	50/65	0.77	0.15	20,20,20,20	0
20	CLA	B	822	54/65	0.78	0.22	20,20,20,20	0
20	CLA	1	204	46/65	0.78	0.15	20,20,20,20	0
20	CLA	3	304	36/65	0.78	0.14	20,20,20,20	0
21	LMU	G	101	35/35	0.78	0.11	20,20,20,20	0
20	CLA	A	824	65/65	0.78	0.18	20,20,20,20	0
20	CLA	B	849	65/65	0.78	0.28	20,20,20,20	0
20	CLA	B	850	65/65	0.78	0.25	20,20,20,20	0
22	BCR	B	842	40/40	0.79	0.19	20,20,20,20	0
21	LMU	H	106	35/35	0.79	0.11	20,20,20,20	0
20	CLA	A	850	65/65	0.79	0.27	20,20,20,20	0
20	CLA	B	821	65/65	0.79	0.17	20,20,20,20	0
20	CLA	1	214	25/65	0.79	0.15	20,20,20,20	0
20	CLA	A	836	47/65	0.79	0.23	20,20,20,20	0
20	CLA	A	837	47/65	0.79	0.21	20,20,20,20	0
20	CLA	B	805	60/65	0.80	0.23	20,20,20,20	0
20	CLA	B	806	65/65	0.80	0.23	20,20,20,20	0
20	CLA	B	851	65/65	0.80	0.24	20,20,20,20	0
20	CLA	4	314	36/65	0.80	0.17	20,20,20,20	0
22	BCR	I	101	40/40	0.80	0.18	20,20,20,20	0
20	CLA	I	102	60/65	0.80	0.17	20,20,20,20	0
20	CLA	L	206	47/65	0.80	0.21	20,20,20,20	0

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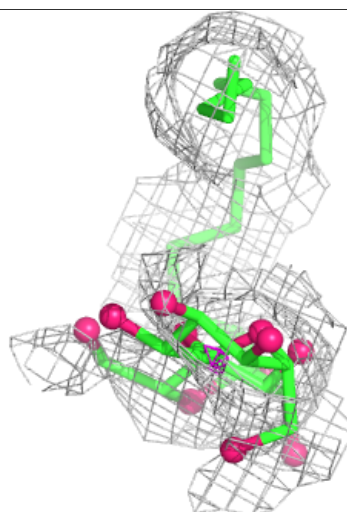
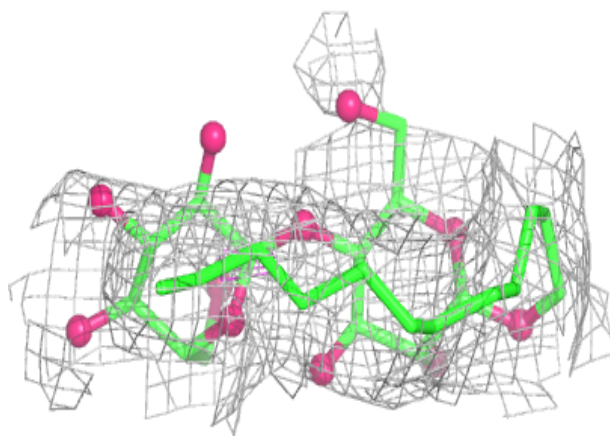
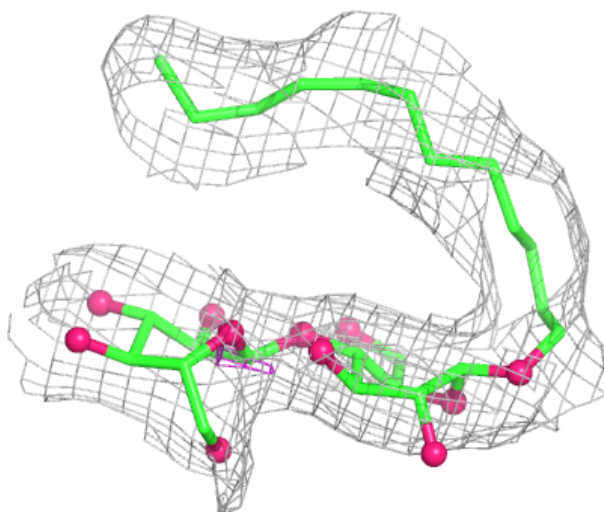
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
20	CLA	2	314	25/65	0.80	0.14	20,20,20,20	0
20	CLA	B	827	65/65	0.80	0.24	20,20,20,20	0
20	CLA	B	810	55/65	0.80	0.16	20,20,20,20	0
20	CLA	B	811	58/65	0.80	0.16	20,20,20,20	0
20	CLA	A	831	55/65	0.81	0.22	20,20,20,20	0
20	CLA	B	820	55/65	0.81	0.17	20,20,20,20	0
20	CLA	4	313	25/65	0.81	0.16	20,20,20,20	0
20	CLA	A	808	65/65	0.81	0.24	20,20,20,20	0
20	CLA	4	312	25/65	0.81	0.19	20,20,20,20	0
20	CLA	4	315	25/65	0.81	0.12	20,20,20,20	0
20	CLA	1	209	36/65	0.82	0.14	20,20,20,20	0
20	CLA	B	825	65/65	0.82	0.23	20,20,20,20	0
20	CLA	B	826	65/65	0.82	0.21	20,20,20,20	0
20	CLA	4	303	36/65	0.82	0.17	20,20,20,20	0
20	CLA	B	828	50/65	0.82	0.16	20,20,20,20	0
20	CLA	A	834	49/65	0.82	0.19	20,20,20,20	0
20	CLA	A	838	65/65	0.82	0.18	20,20,20,20	0
23	PQN	B	841	33/33	0.83	0.20	20,20,20,20	0
20	CLA	2	309	25/65	0.83	0.14	20,20,20,20	0
20	CLA	B	836	65/65	0.83	0.20	20,20,20,20	0
20	CLA	1	208	25/65	0.84	0.11	20,20,20,20	0
20	CLA	B	818	50/65	0.84	0.20	20,20,20,20	0
20	CLA	B	816	60/65	0.84	0.23	20,20,20,20	0
20	CLA	B	839	65/65	0.84	0.22	20,20,20,20	0
20	CLA	B	807	65/65	0.86	0.22	20,20,20,20	0
20	CLA	B	837	47/65	0.87	0.19	20,20,20,20	0
24	SF4	C	102	8/8	0.88	0.13	20,20,20,20	0
24	SF4	C	103	8/8	0.90	0.11	20,20,20,20	0
24	SF4	A	857	8/8	0.93	0.09	20,20,20,20	0

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

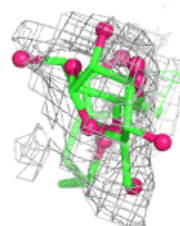
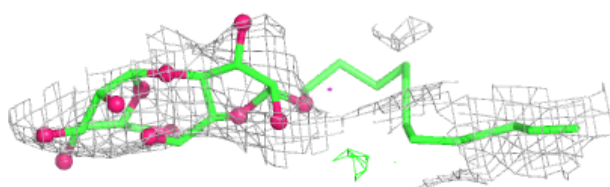
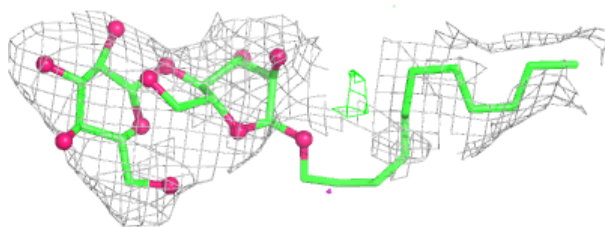
Electron density around LMU 1 218:

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

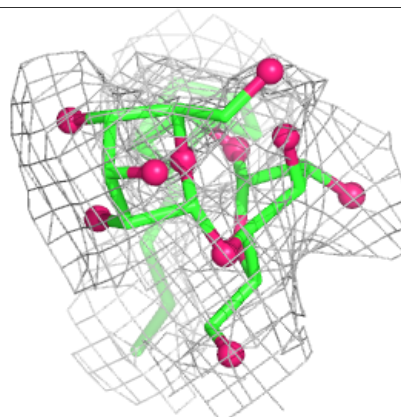
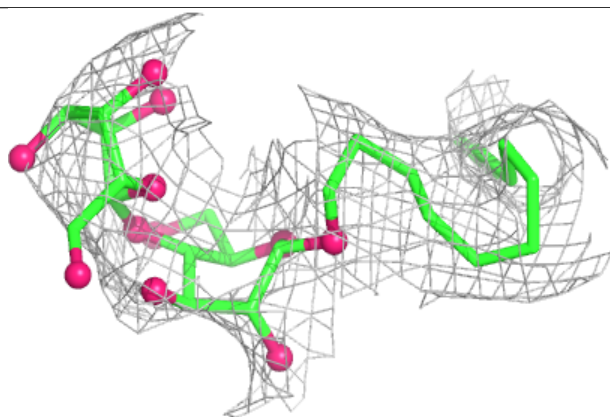
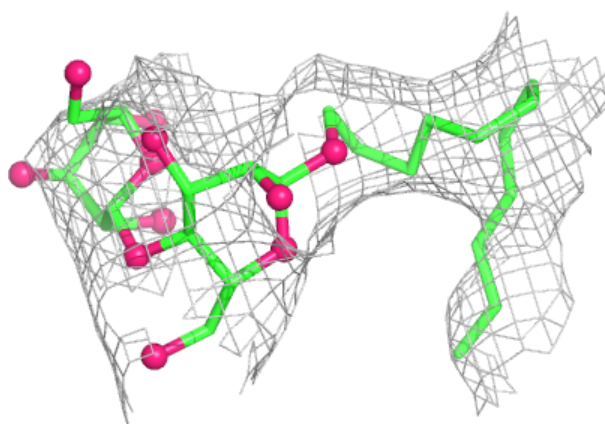


Electron density around LMU R 102:

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

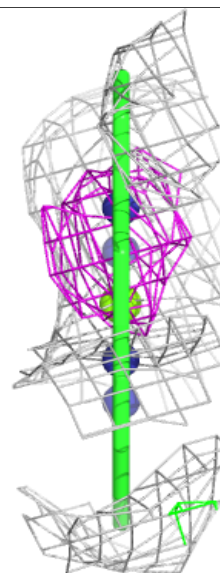
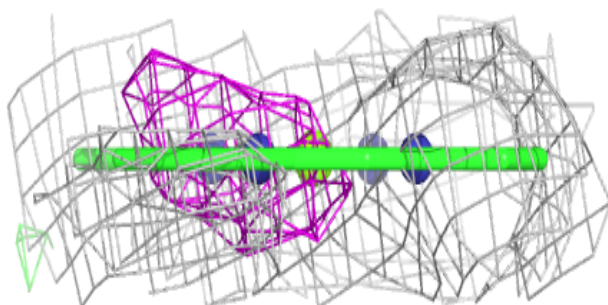
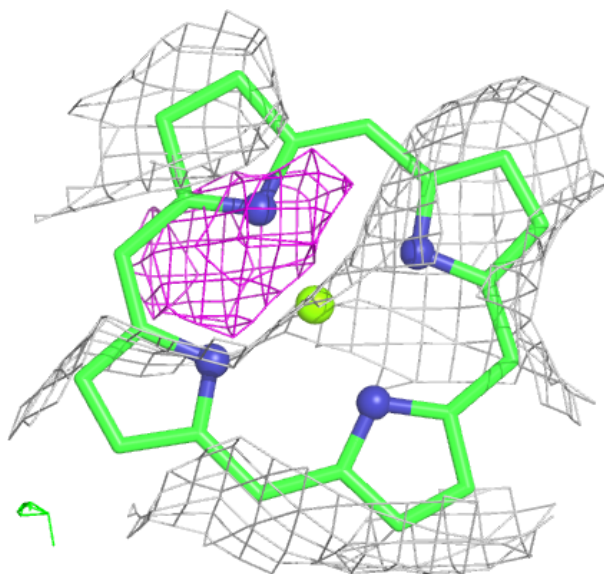
**Electron density around LMU H 108:**

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



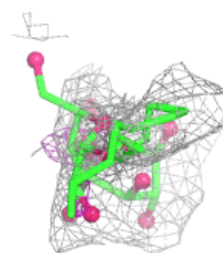
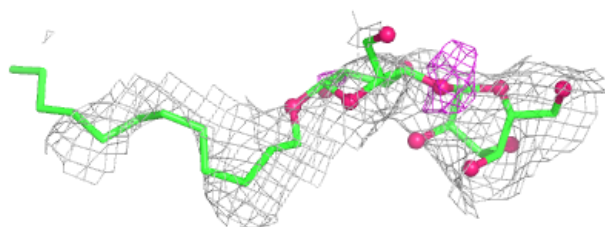
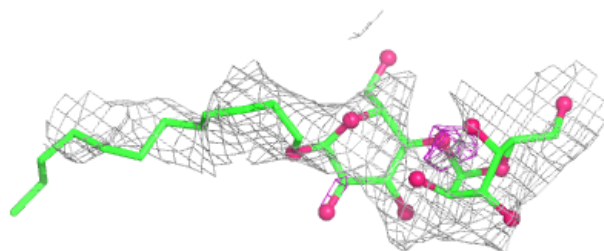
Electron density around CLA 3 310:

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

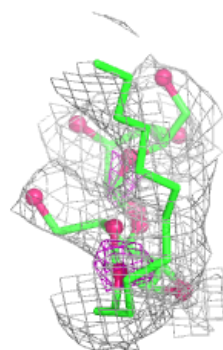
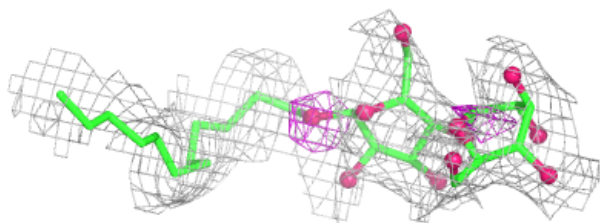
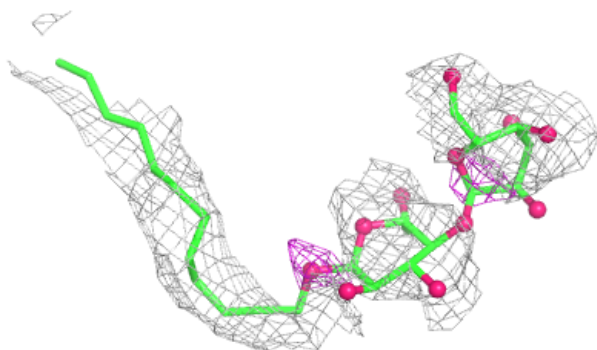


Electron density around LMU A 853:

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

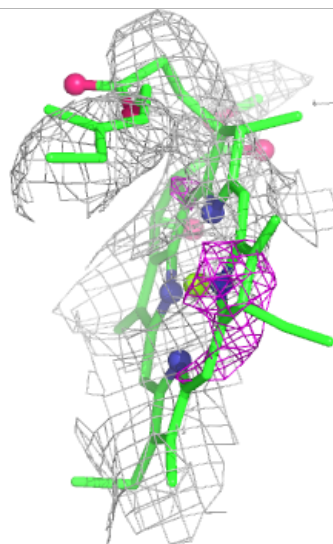
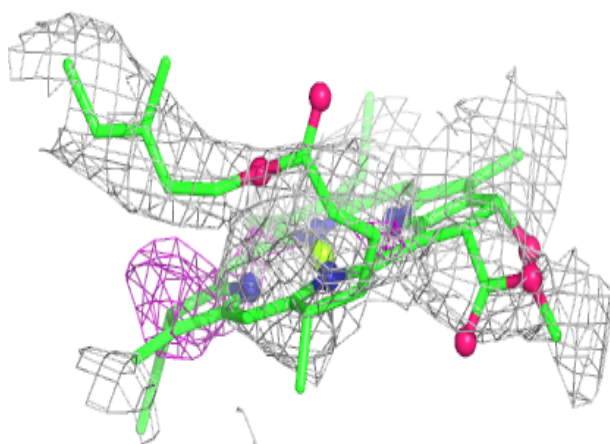
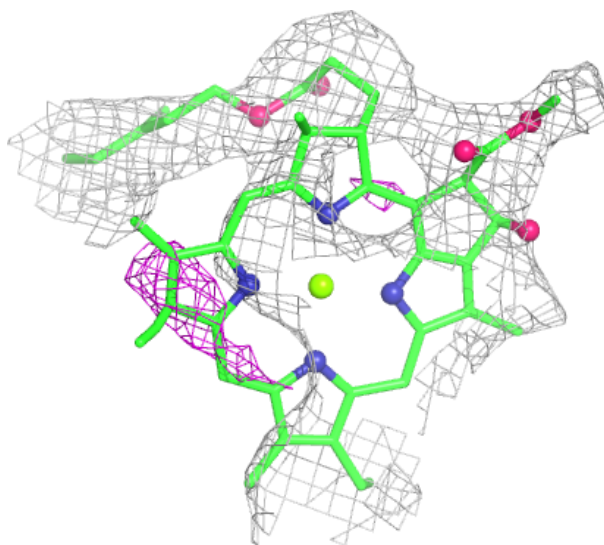
**Electron density around LMU 4 301:**

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



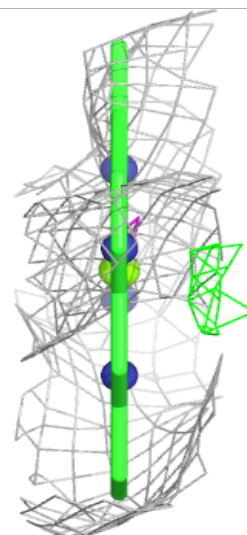
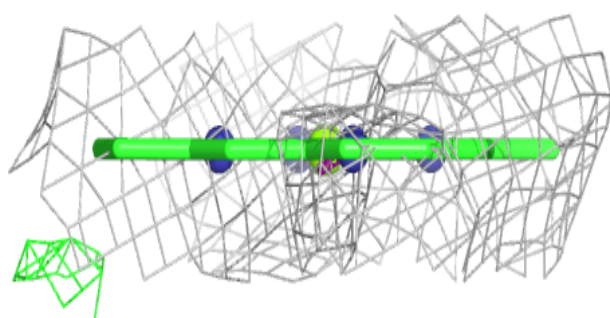
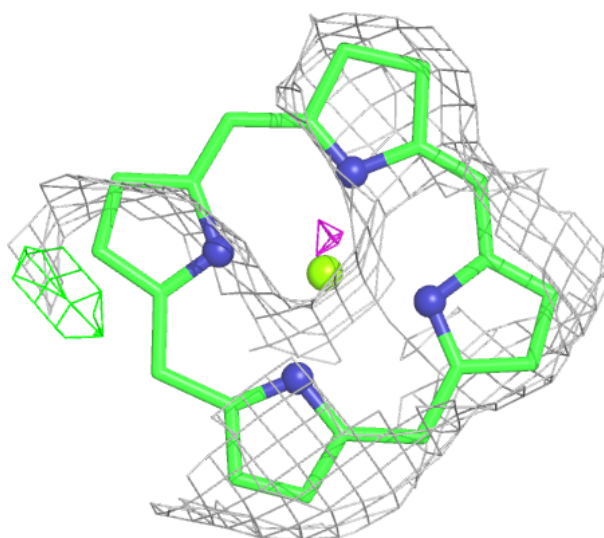
Electron density around CLA B 834:

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



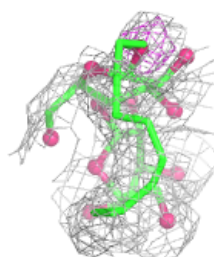
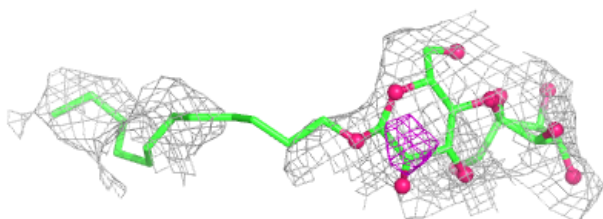
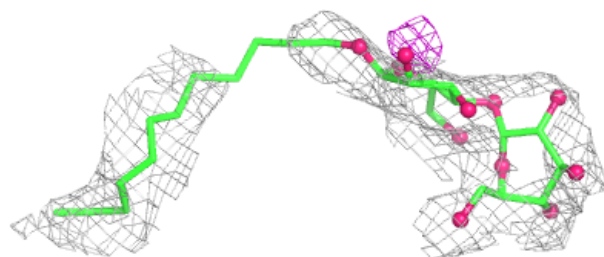
Electron density around CLA 3 306:

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

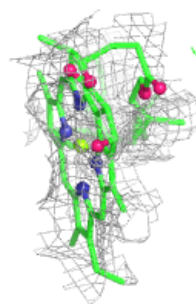
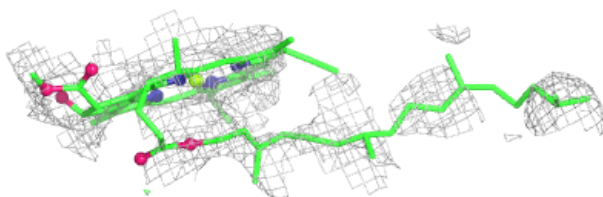
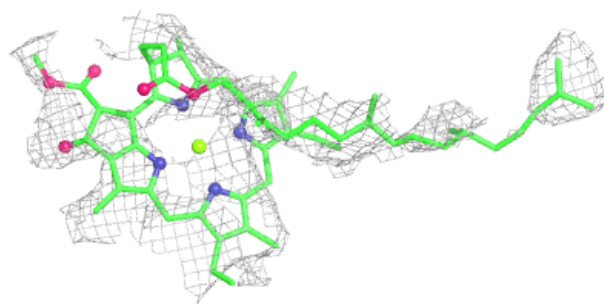


Electron density around LMU L 204:

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

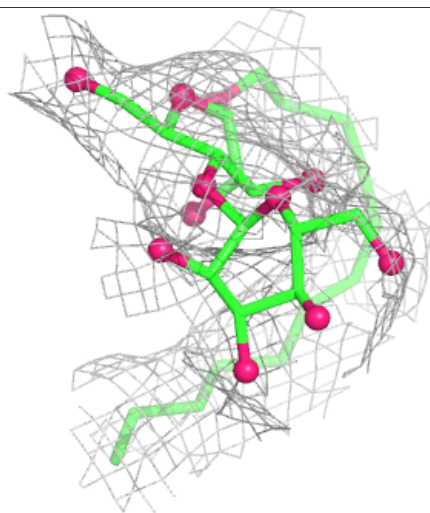
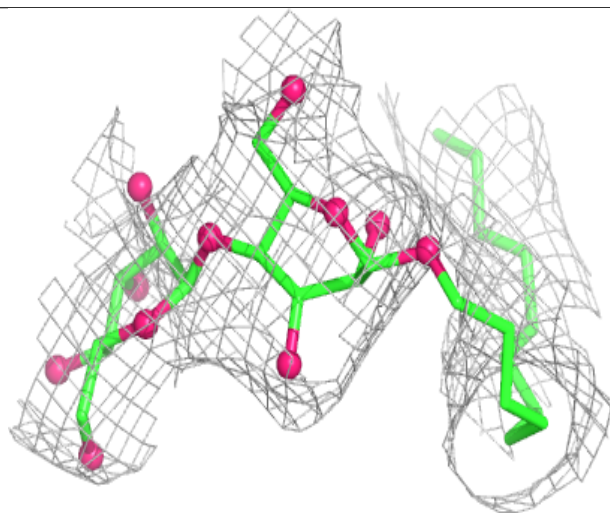
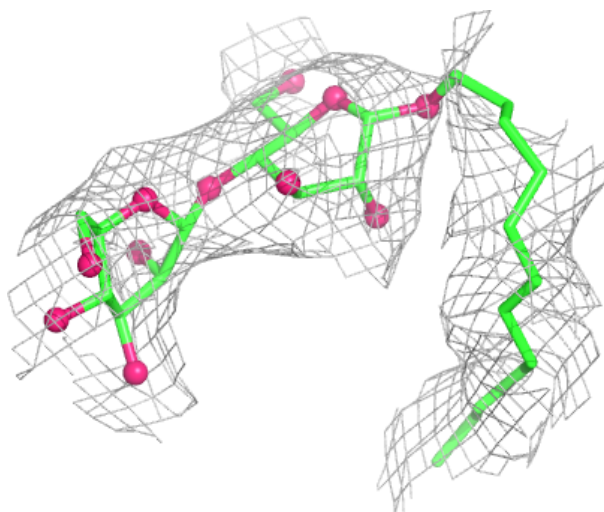
**Electron density around CLA 2 308:**

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



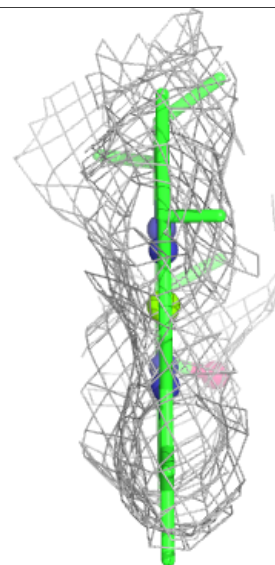
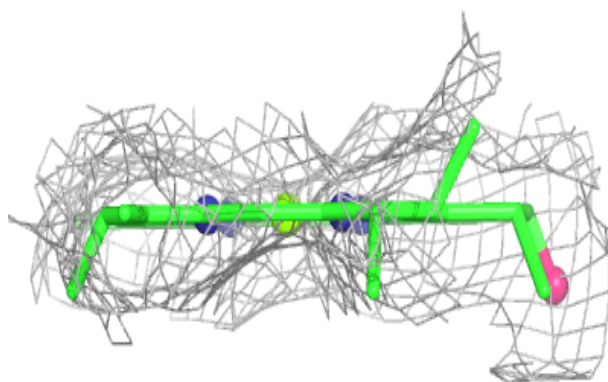
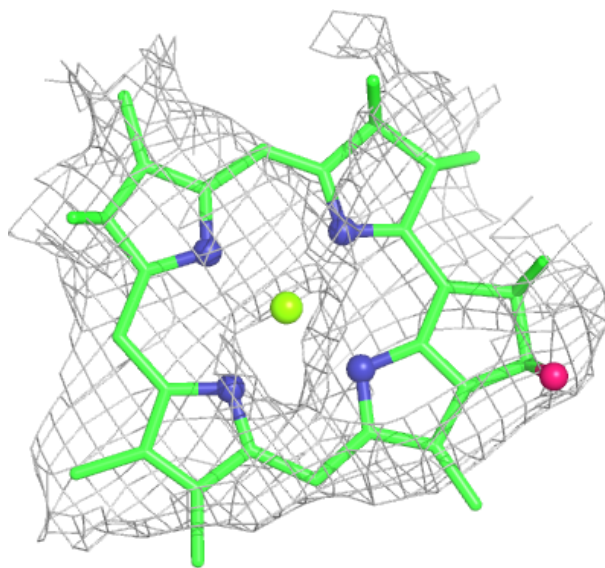
Electron density around LMU 1 220:

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



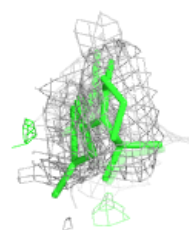
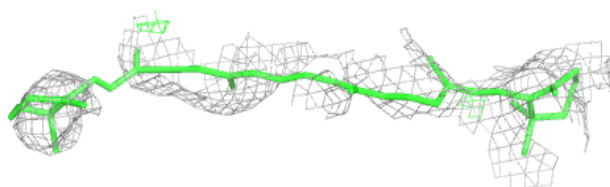
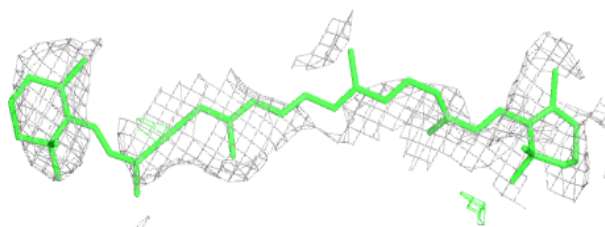
Electron density around CLA 4 308:

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

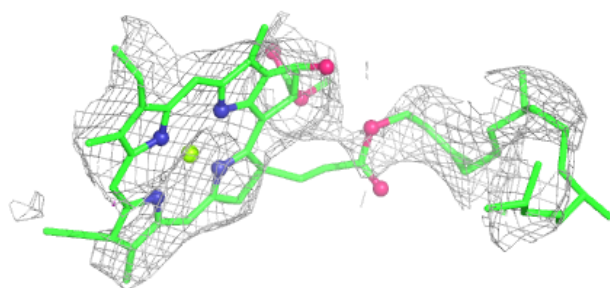
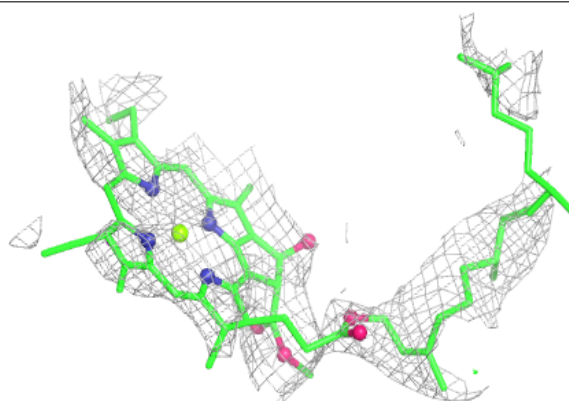


Electron density around BCR A 843:

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

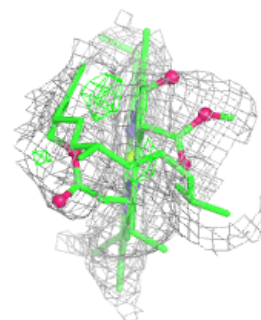
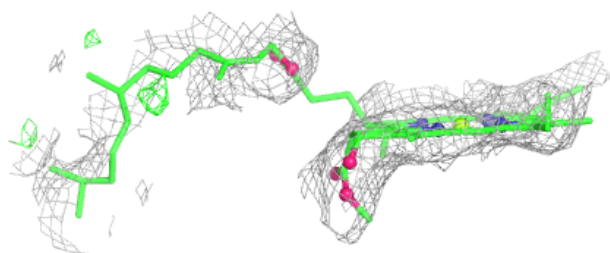
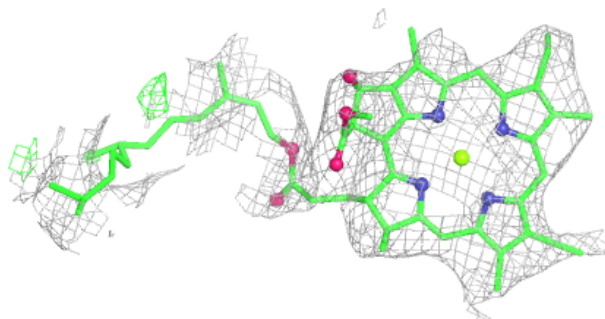
**Electron density around CLA K 103:**

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

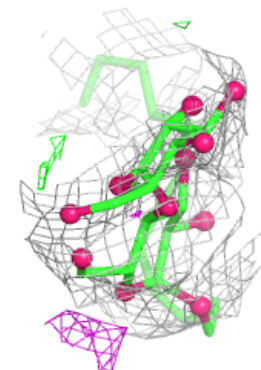
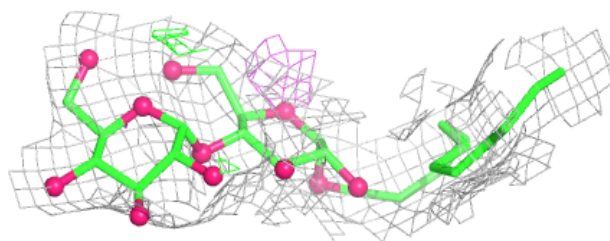


Electron density around CLA B 813:

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

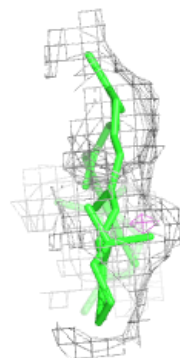
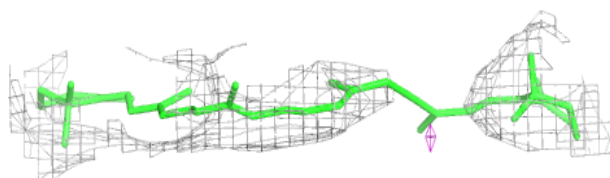
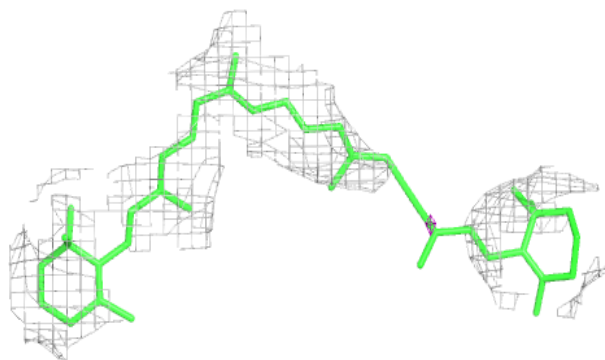
**Electron density around LMU R 106:**

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



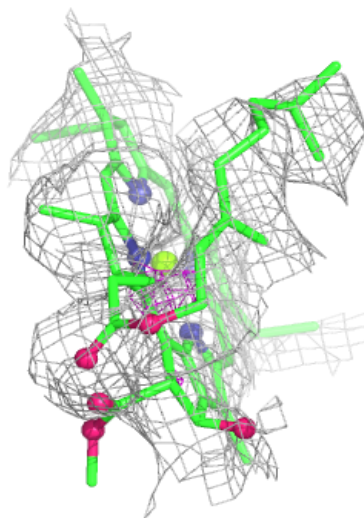
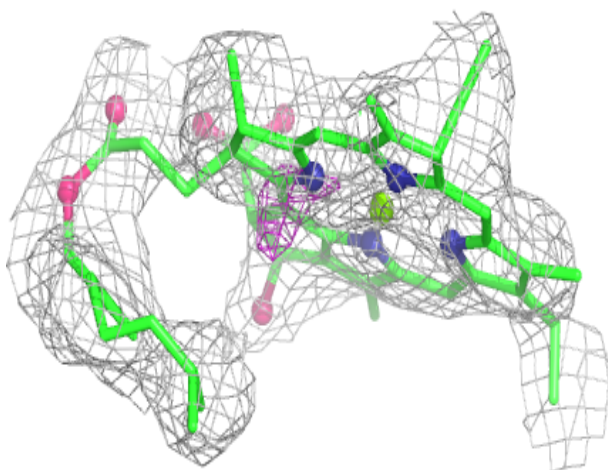
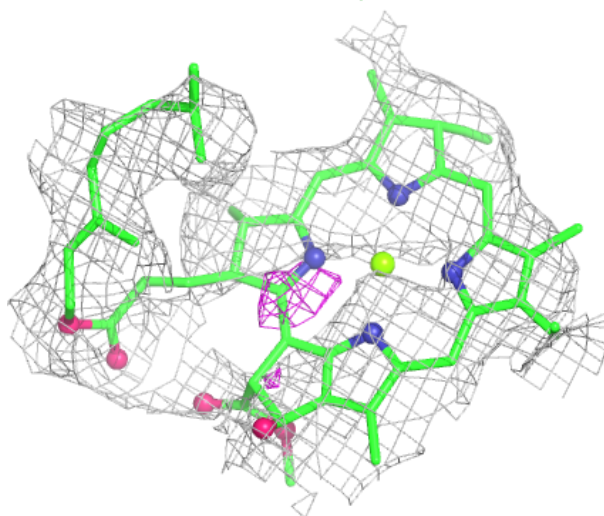
Electron density around BCR 3 314:

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



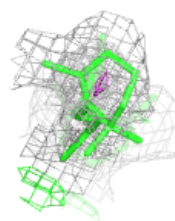
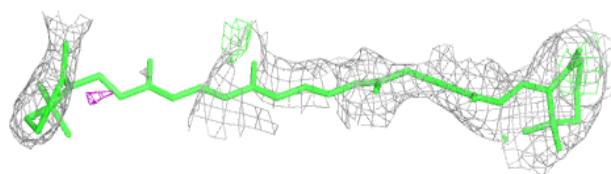
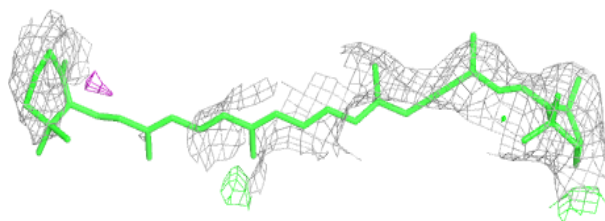
Electron density around CLA H 103:

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



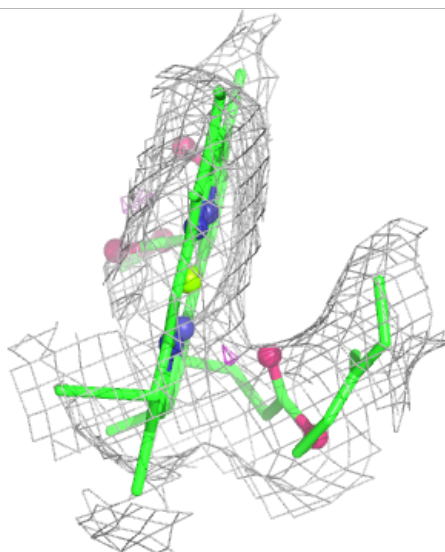
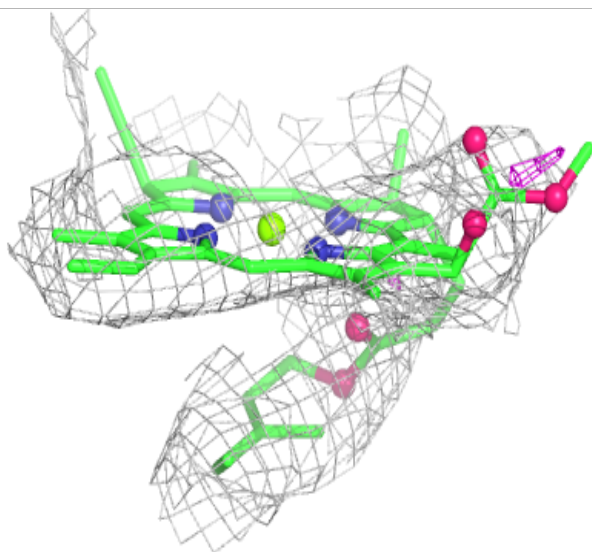
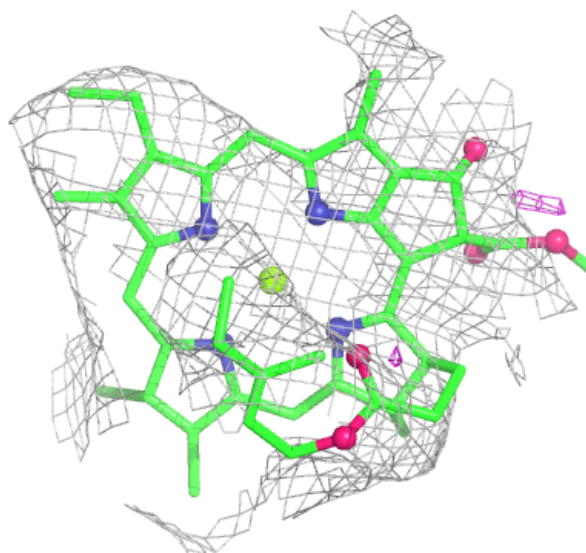
Electron density around BCR J 102:

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



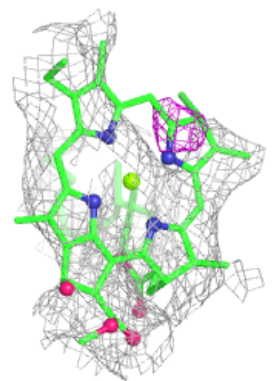
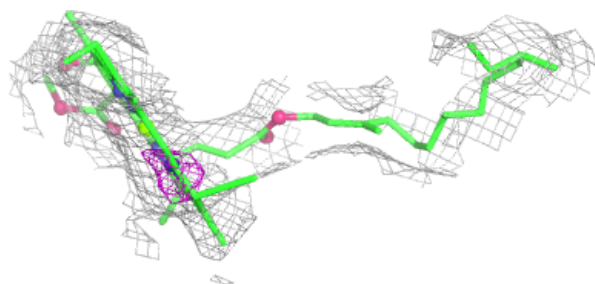
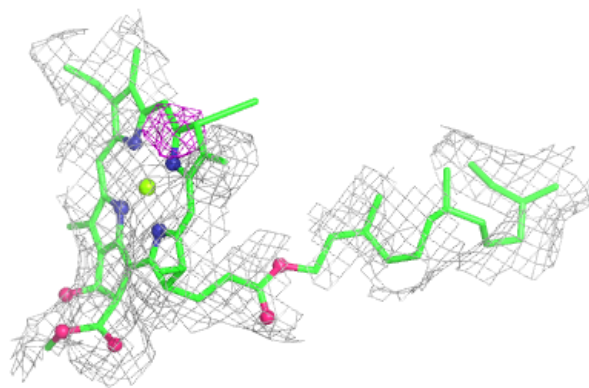
Electron density around CLA 2 302:

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



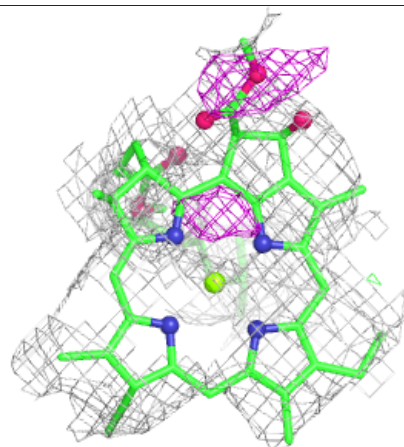
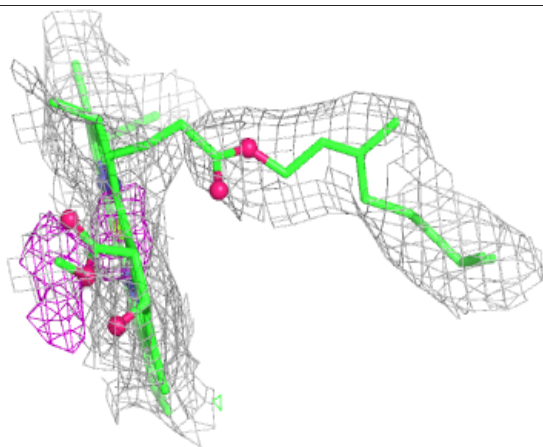
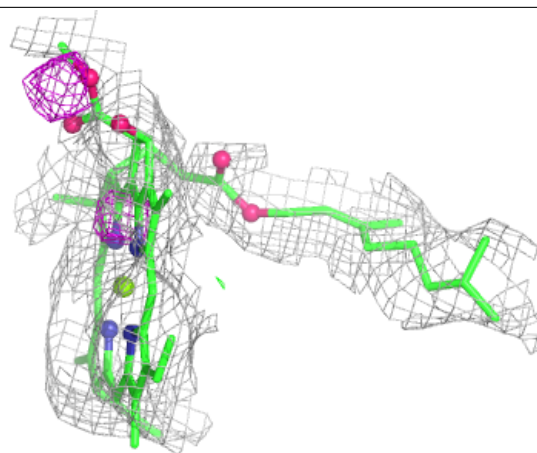
Electron density around CLA 2 320:

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



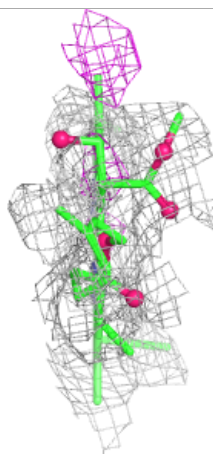
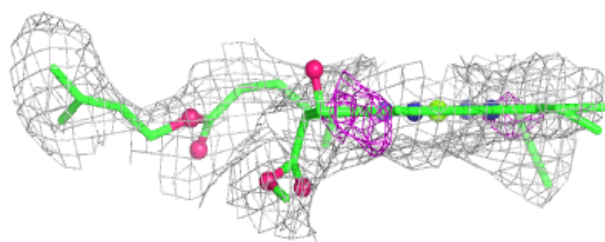
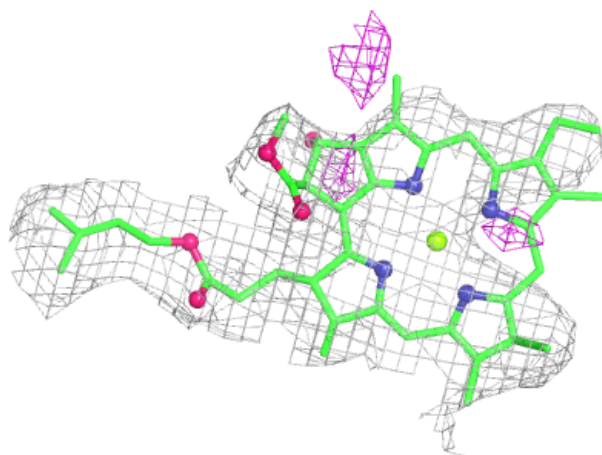
Electron density around CLA 4 302:

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



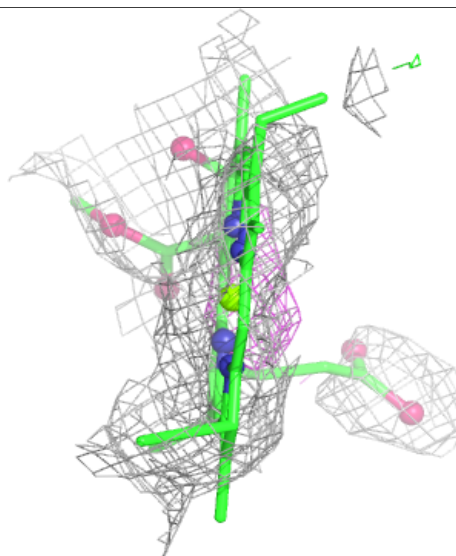
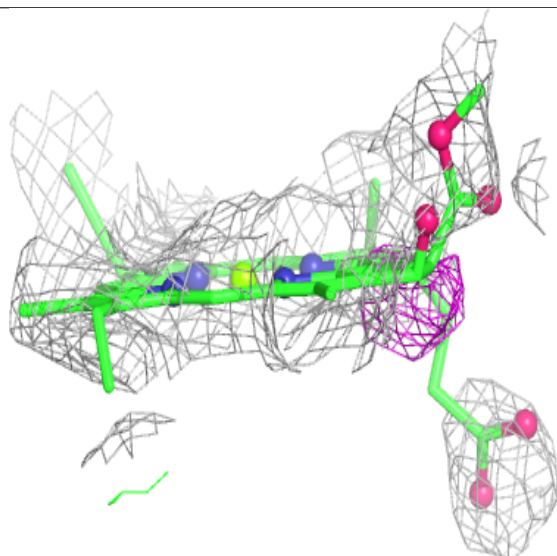
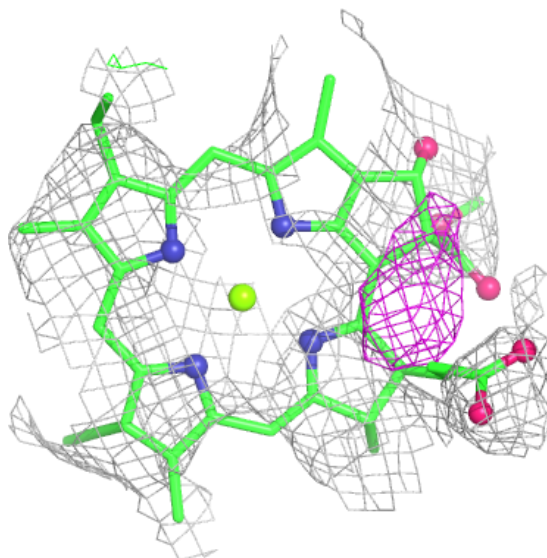
Electron density around CLA 4 306:

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



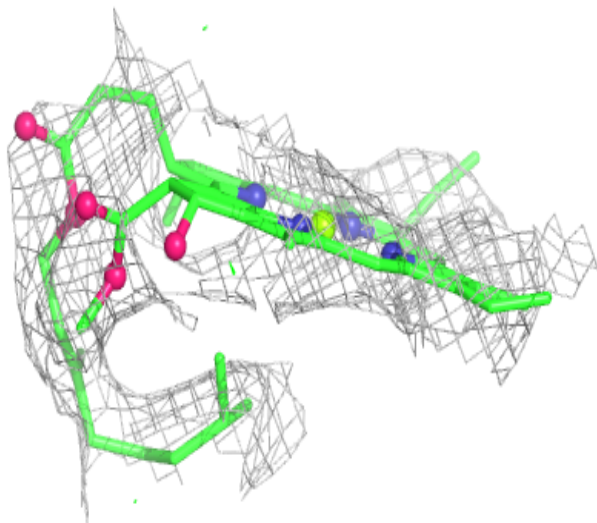
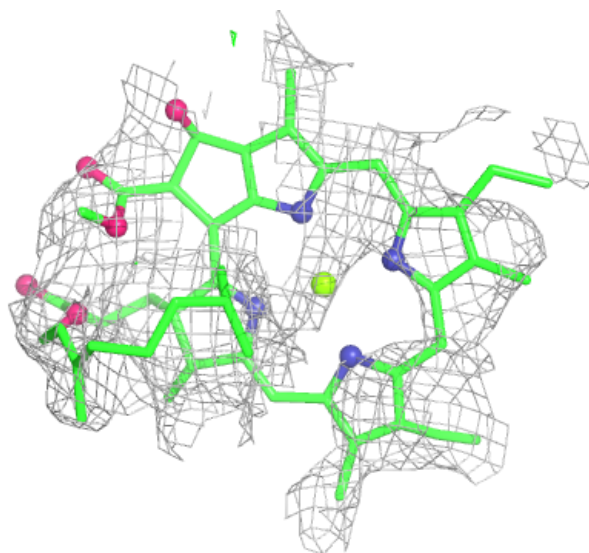
Electron density around CLA B 833:

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



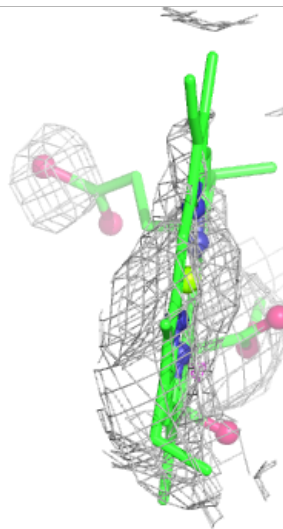
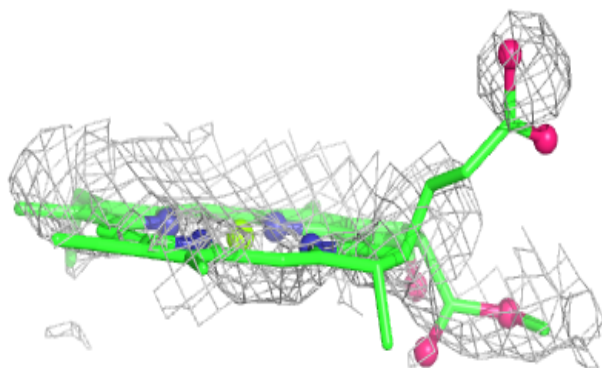
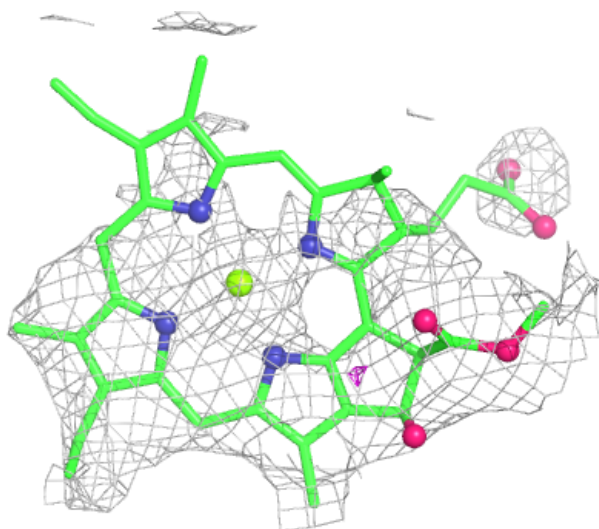
Electron density around CLA 4 305:

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



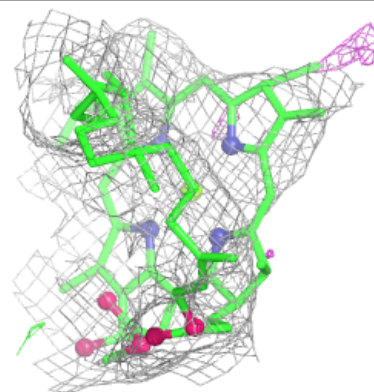
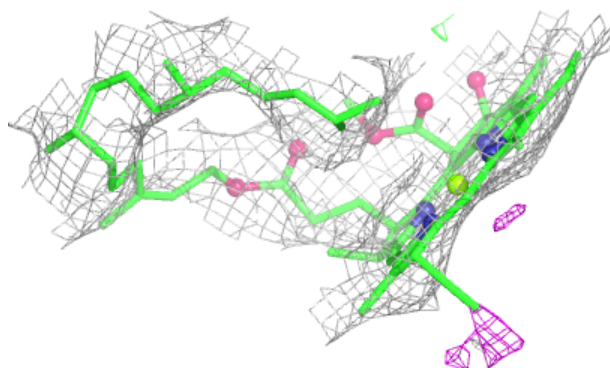
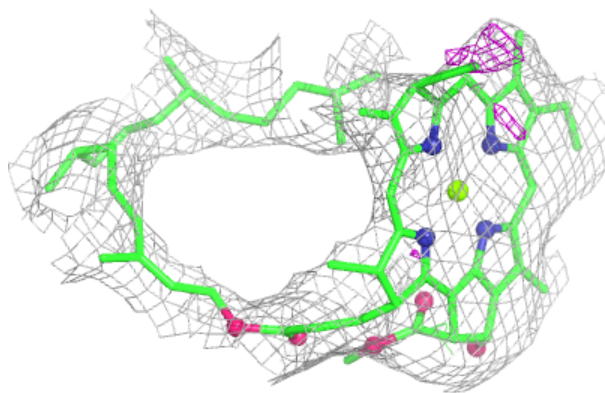
Electron density around CLA A 810:

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

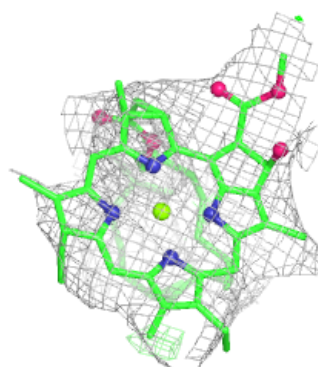
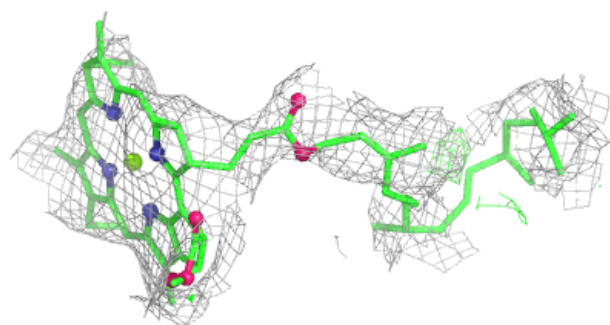
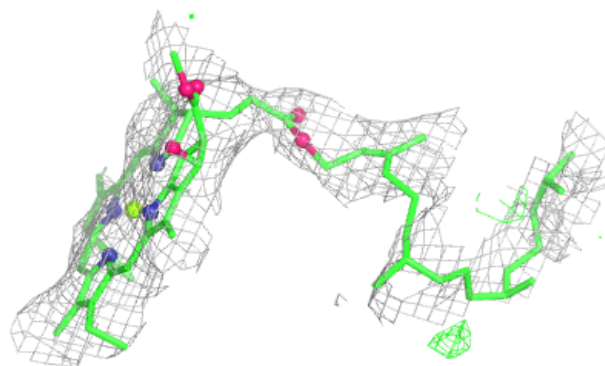


Electron density around CLA A 839:

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

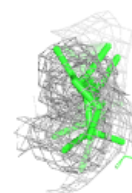
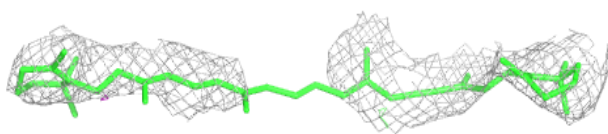
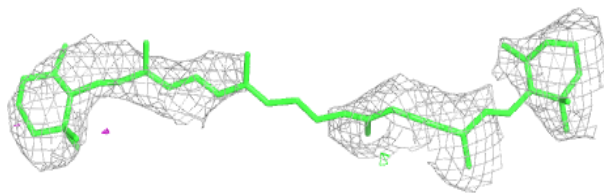
**Electron density around CLA 3 311:**

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



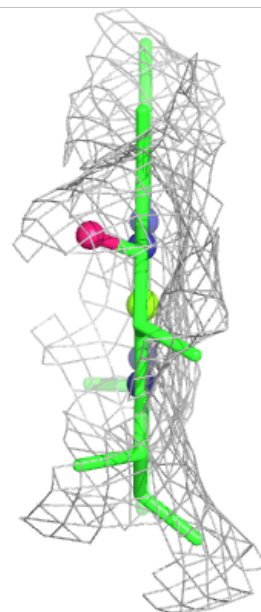
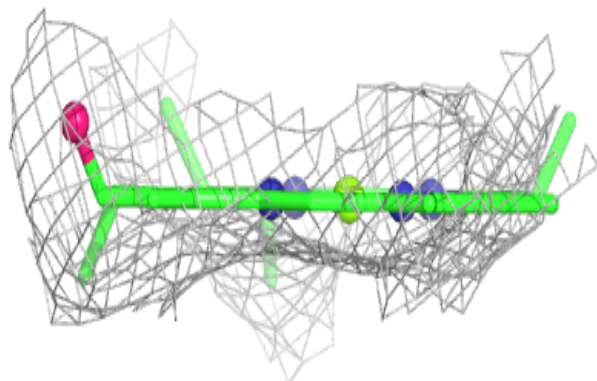
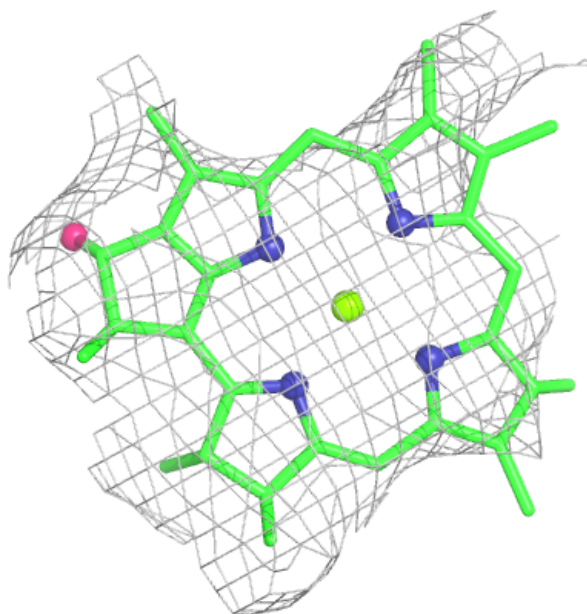
Electron density around BCR L 208:

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



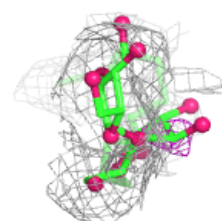
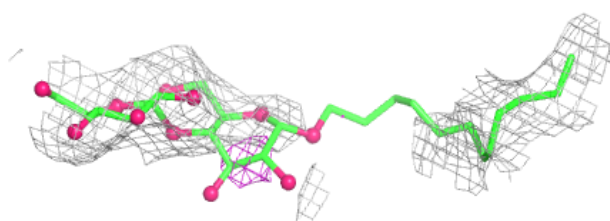
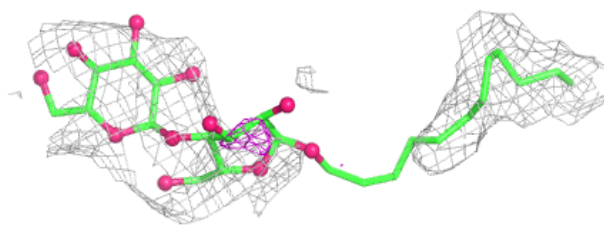
Electron density around CLA 3 301:

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

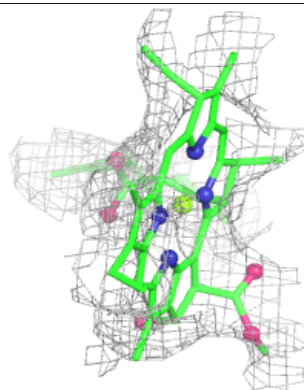
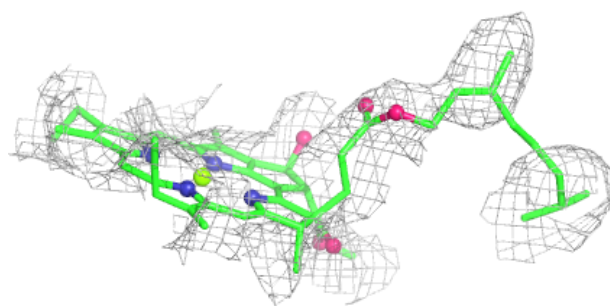
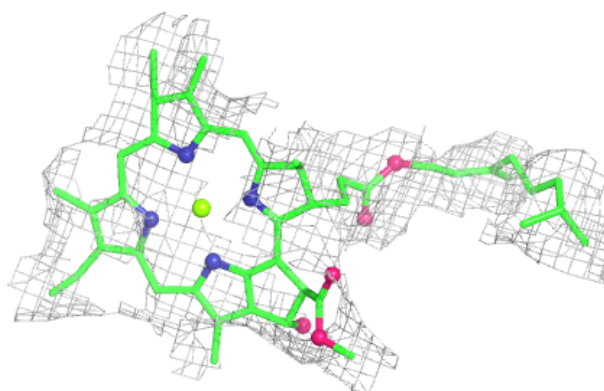


Electron density around LMU B 801:

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

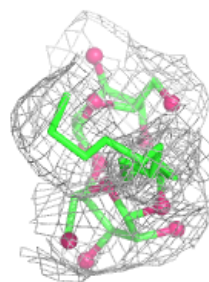
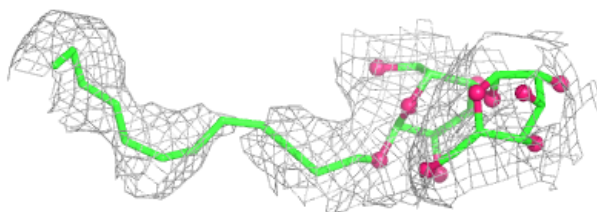
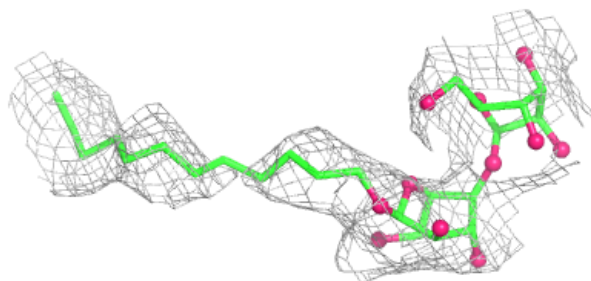
**Electron density around CLA H 102:**

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

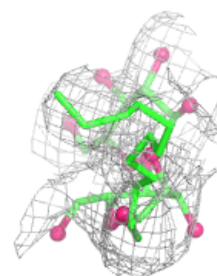
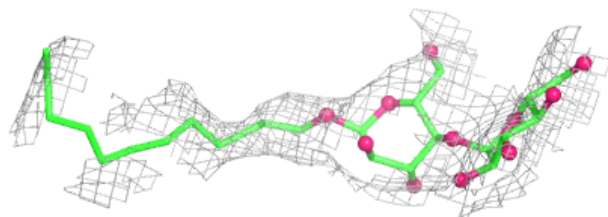
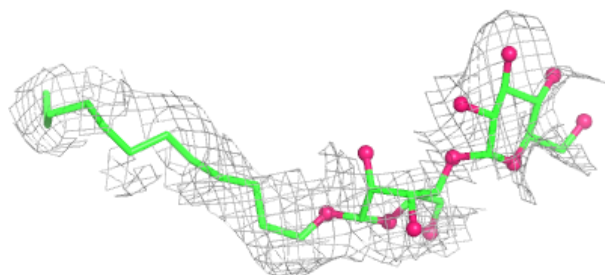


Electron density around LMU 1 213:

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

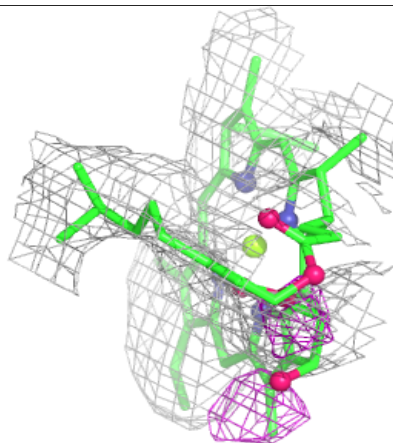
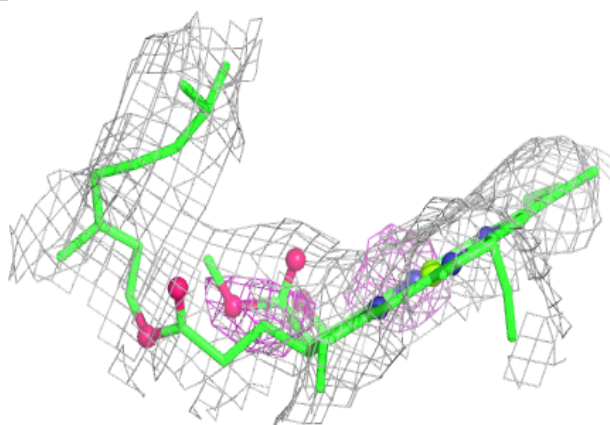
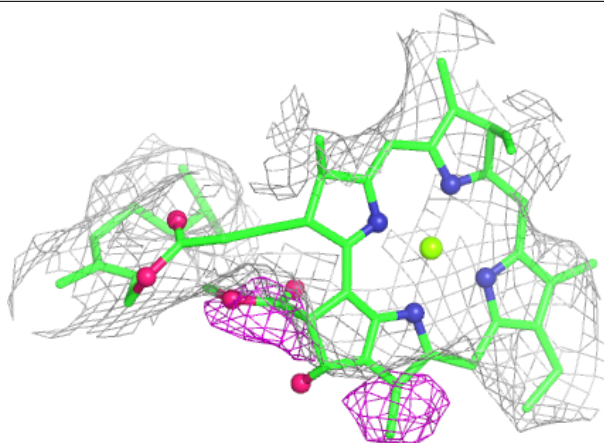
**Electron density around LMU 4 317:**

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

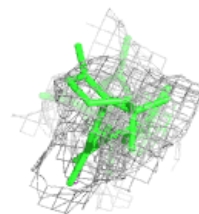
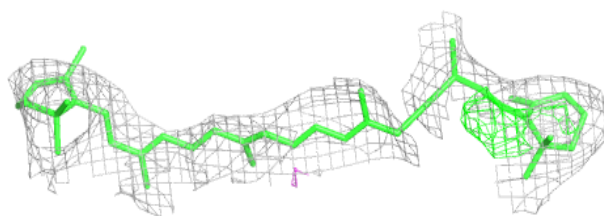


Electron density around CLA L 201:

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

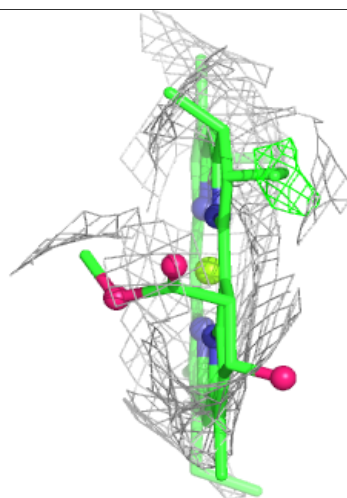
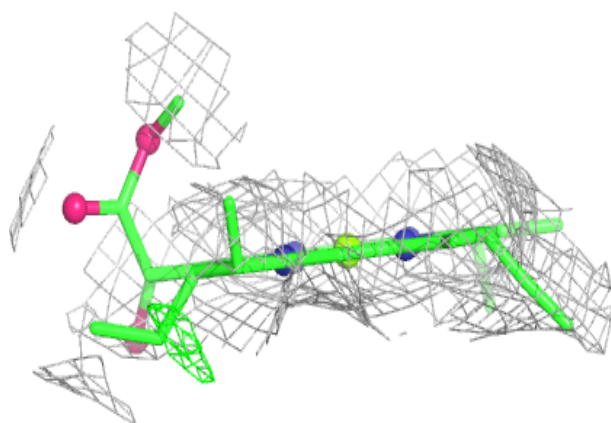
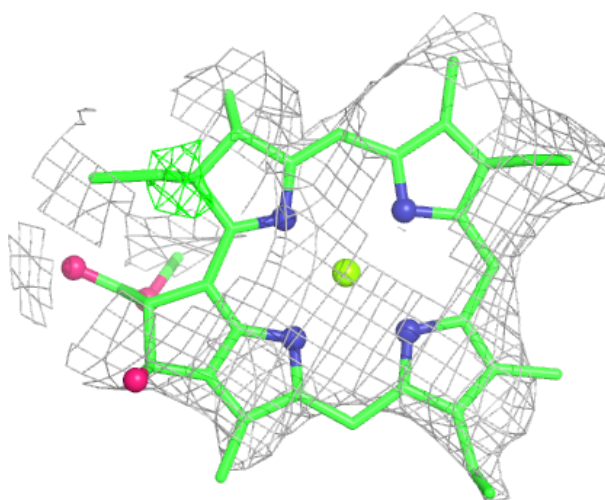
**Electron density around BCR A 845:**

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



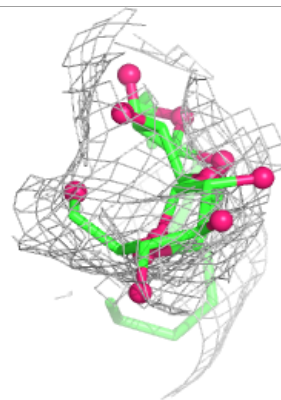
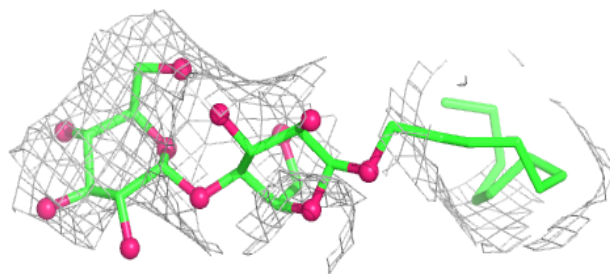
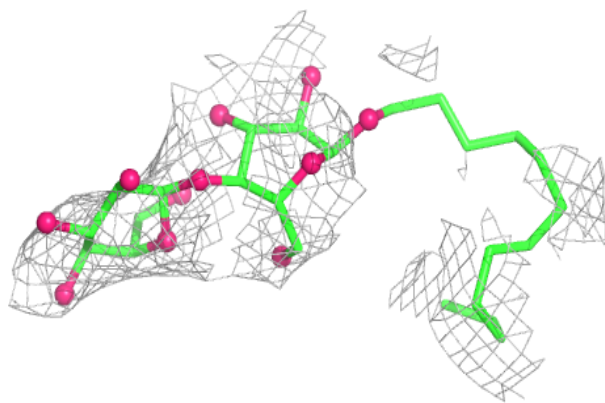
Electron density around CLA 3 308:

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



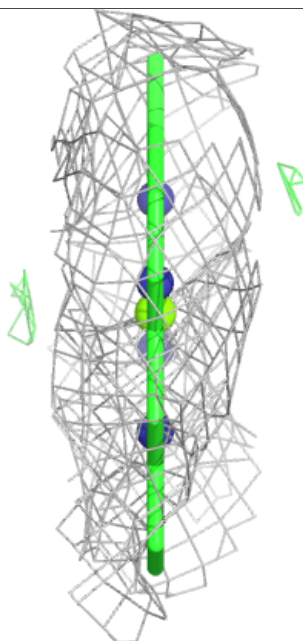
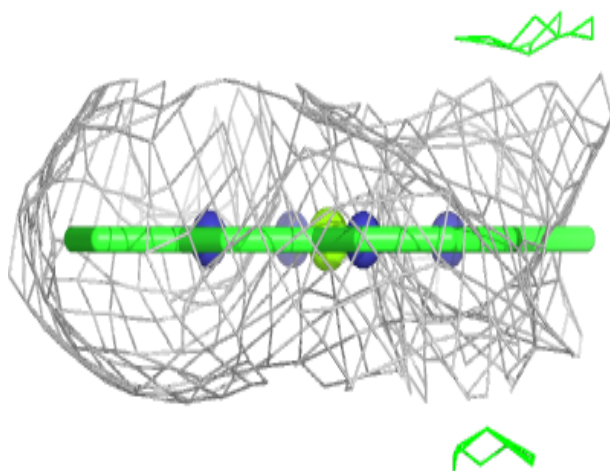
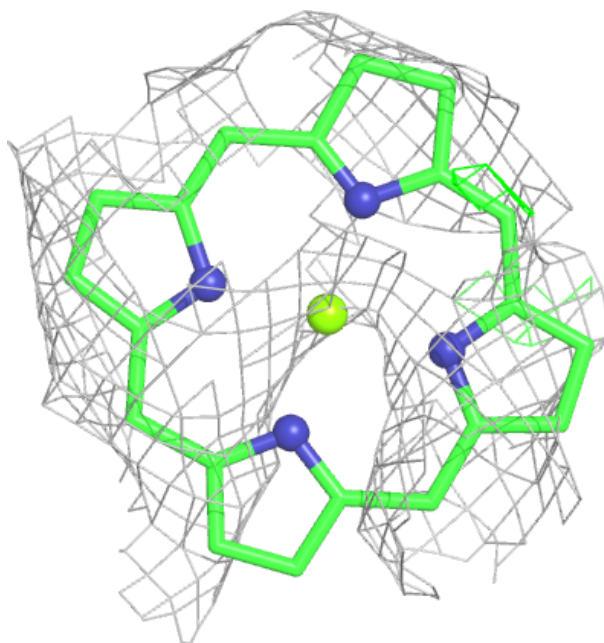
Electron density around LMU D 201:

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



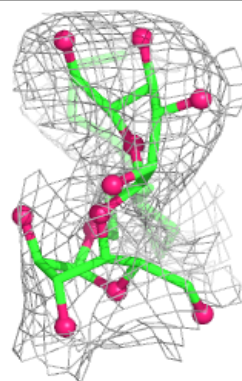
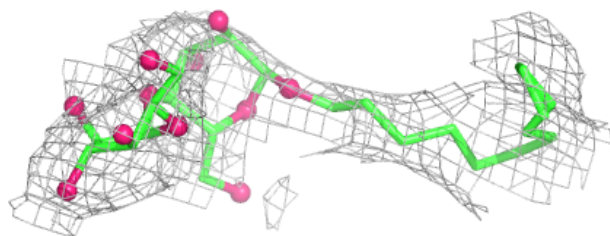
Electron density around CLA 1 211:

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



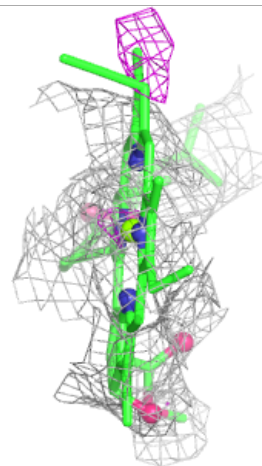
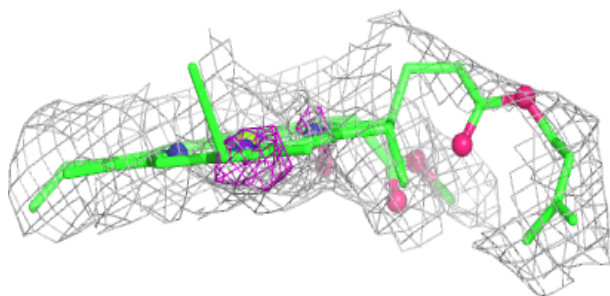
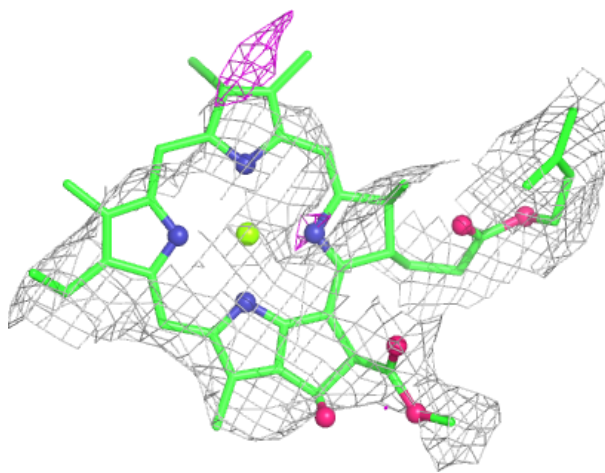
Electron density around LMU K 108:

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



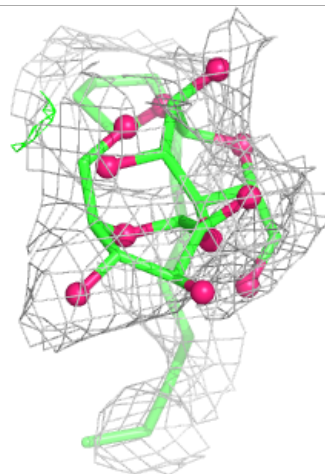
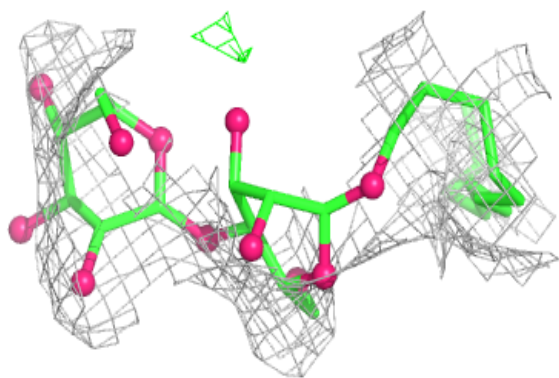
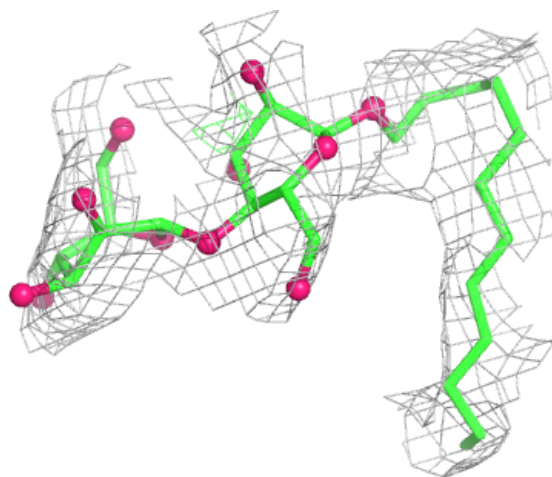
Electron density around CLA K 102:

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



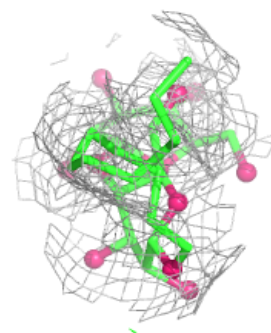
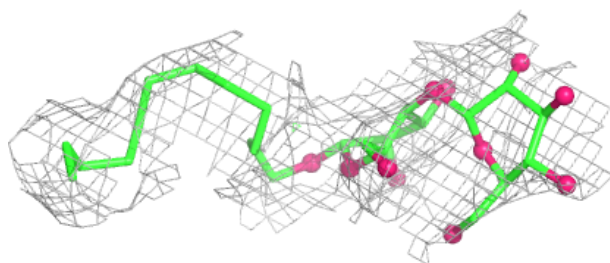
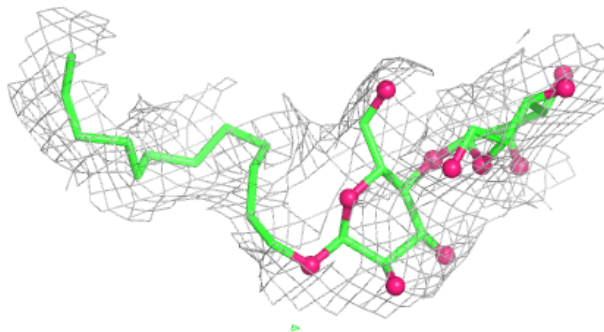
Electron density around LMU R 101:

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

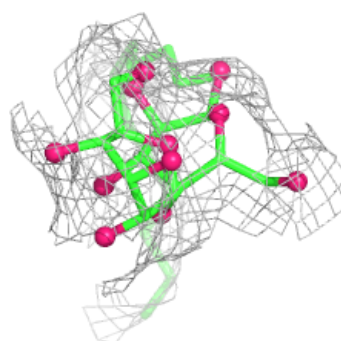
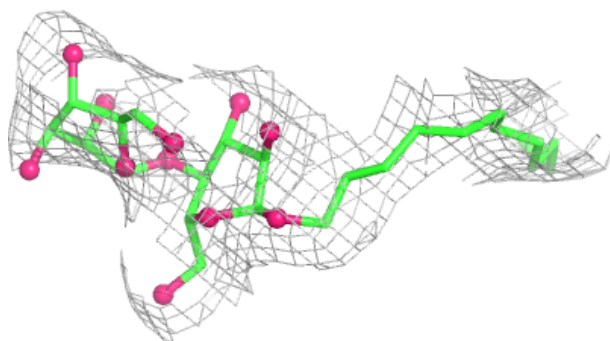
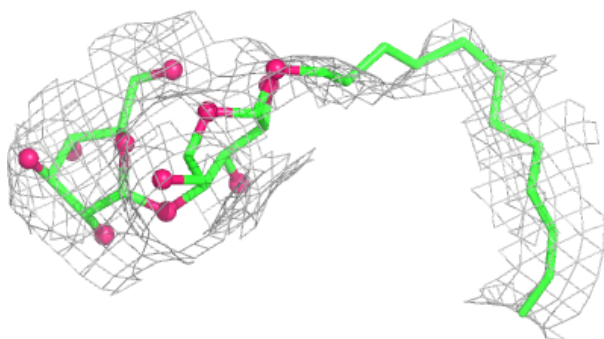


Electron density around LMU 2 313:

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

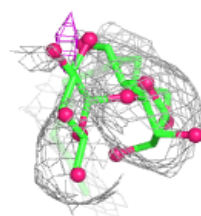
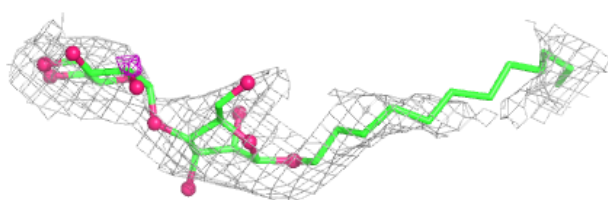
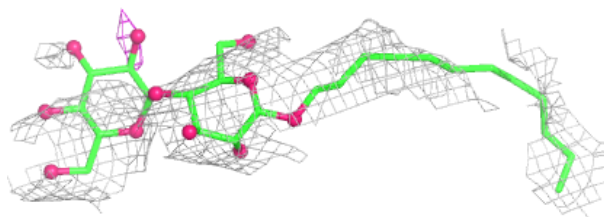
**Electron density around LMU 2 316:**

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

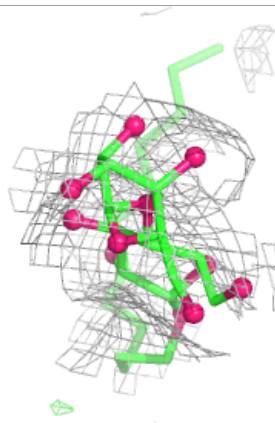
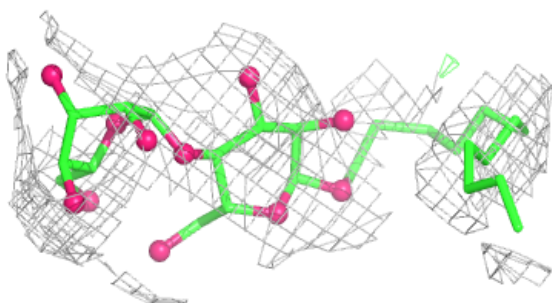
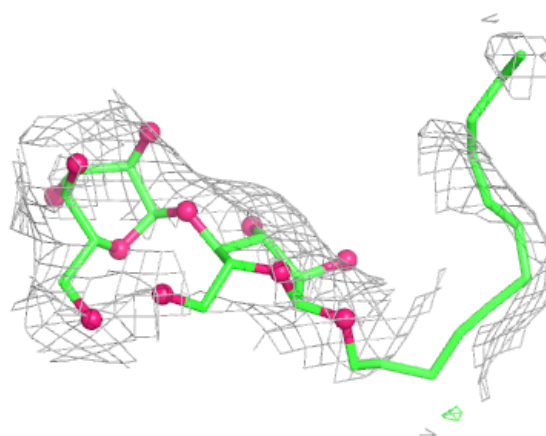


Electron density around LMU 2 319:

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

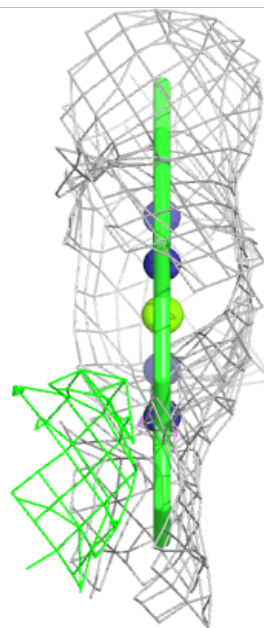
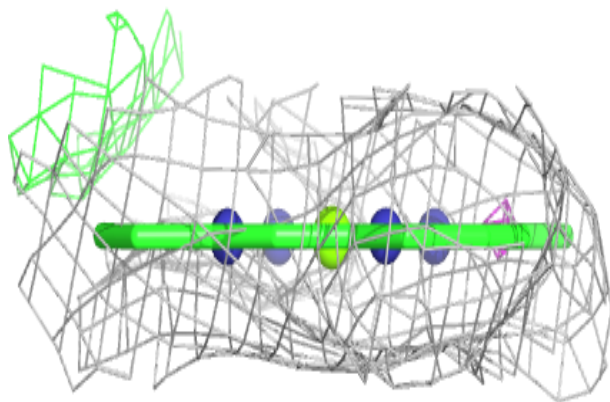
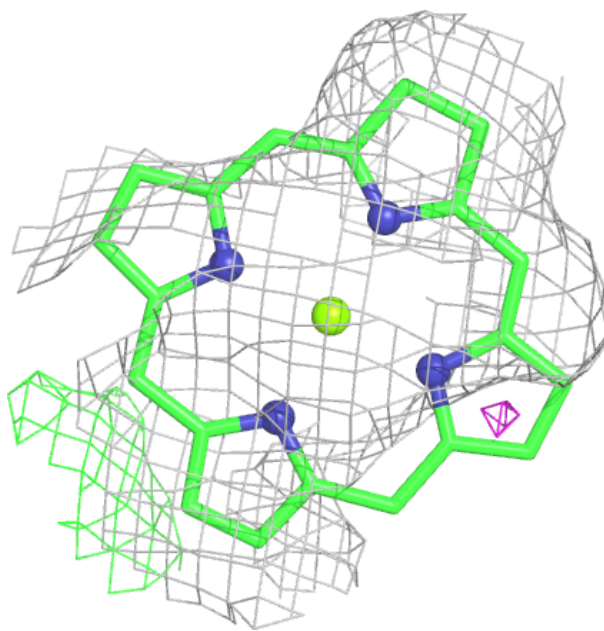
**Electron density around LMU 3 320:**

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



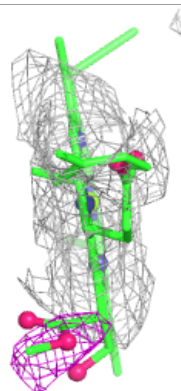
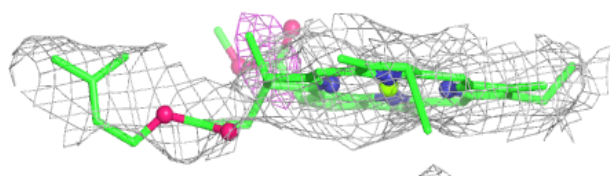
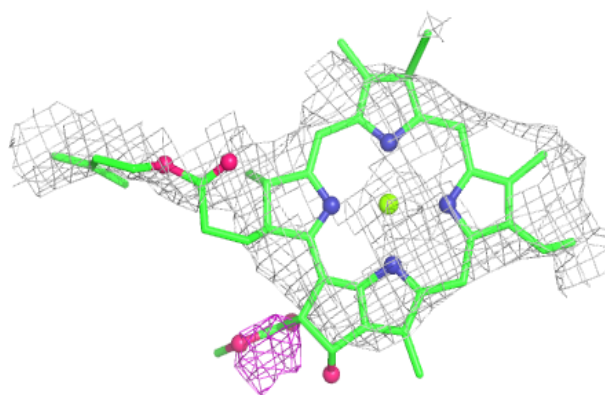
Electron density around CLA 2 306:

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



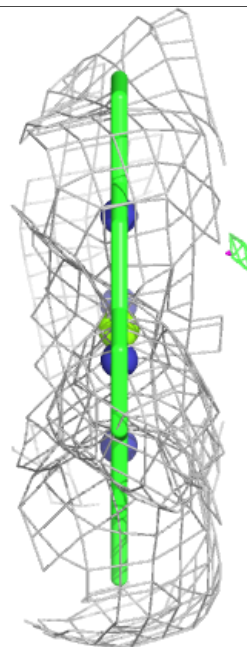
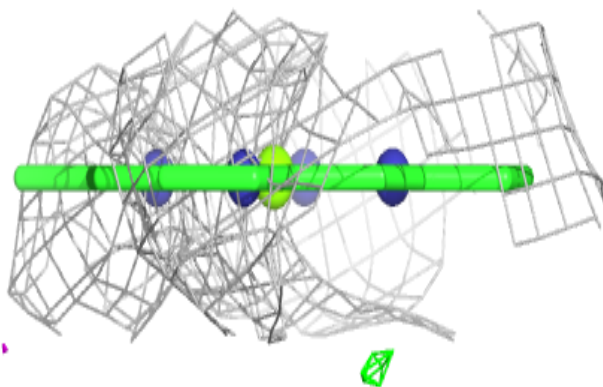
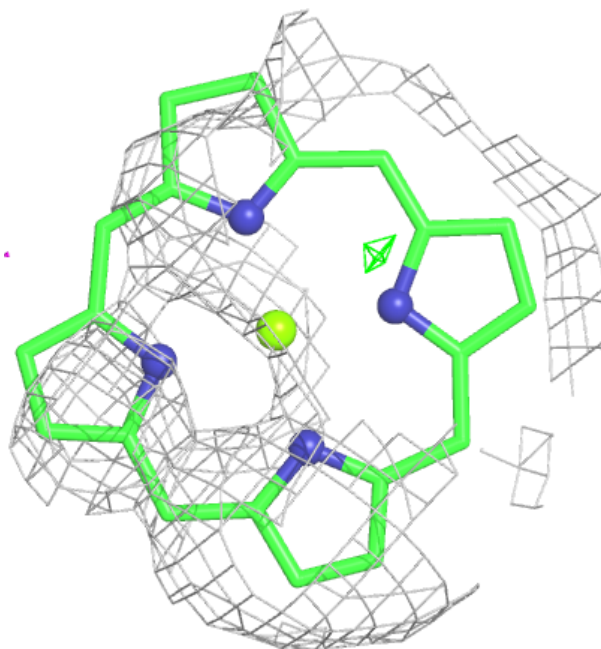
Electron density around CLA K 107:

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



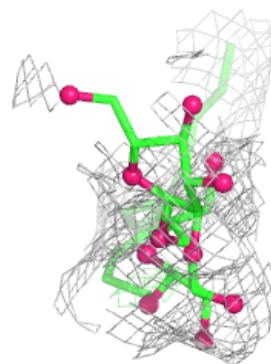
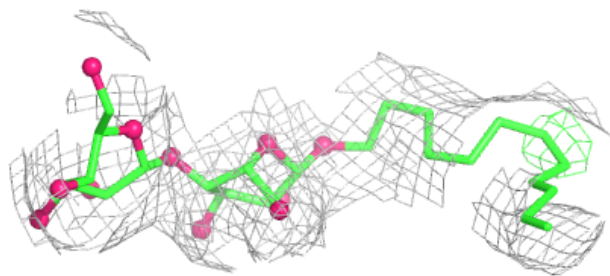
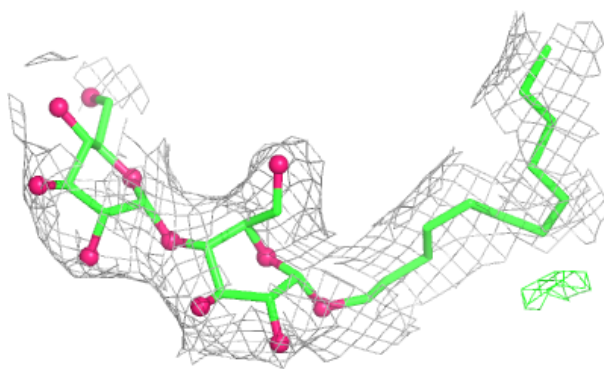
Electron density around CLA 3 307:

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



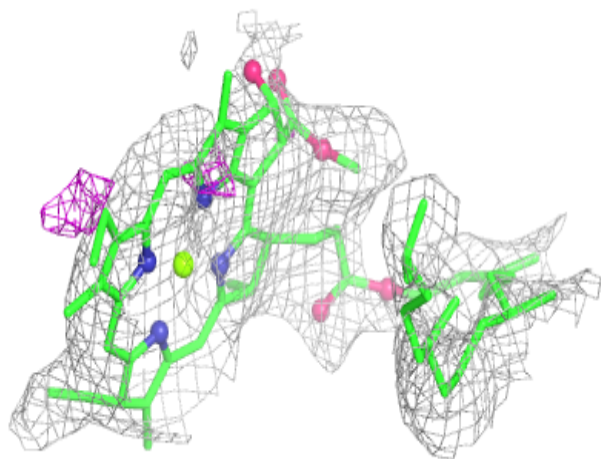
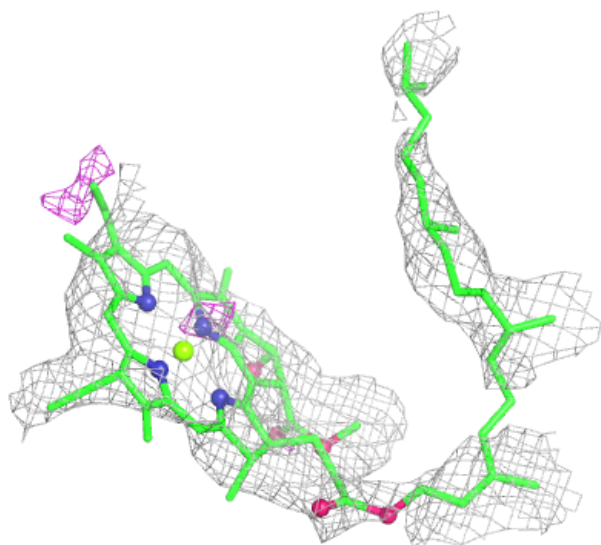
Electron density around LMU H 105:

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



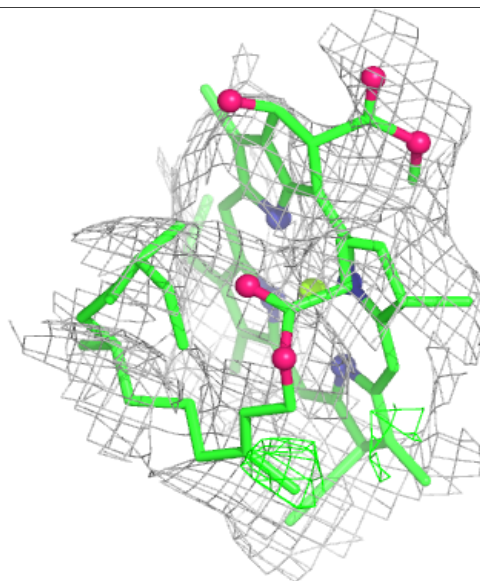
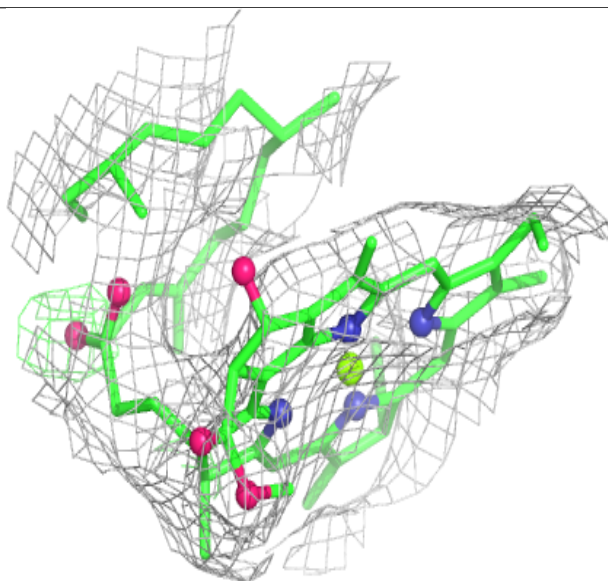
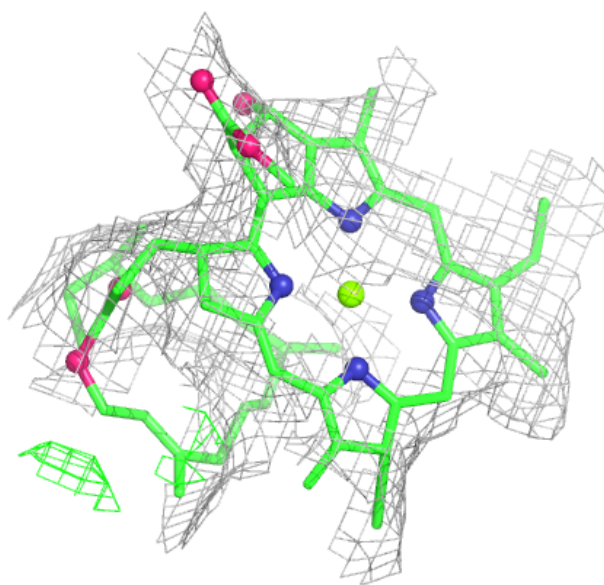
Electron density around CLA 3 313:

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



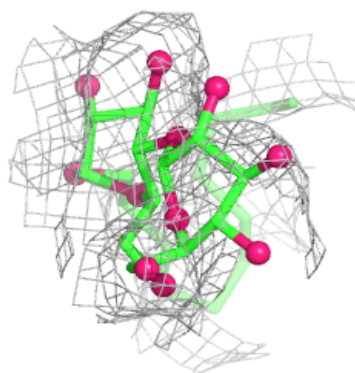
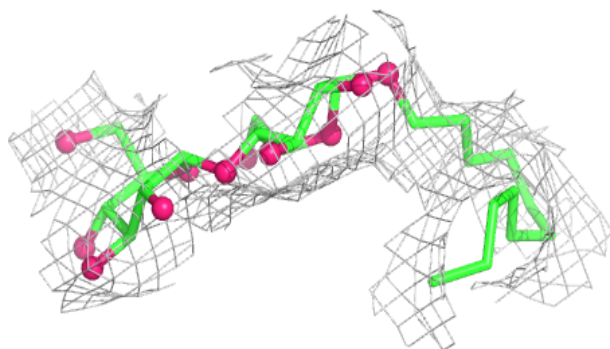
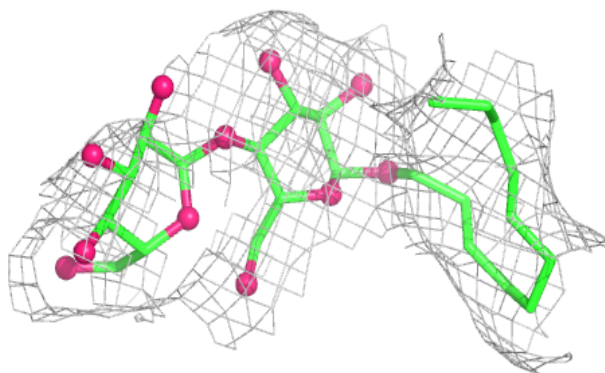
Electron density around CLA J 103:

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

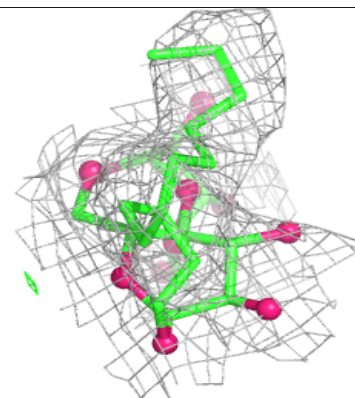
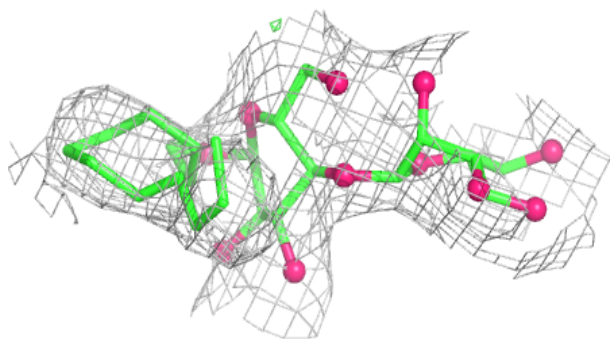
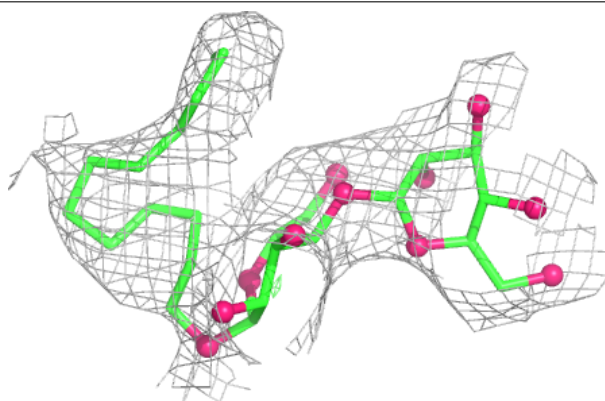


Electron density around LMU F 201:

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

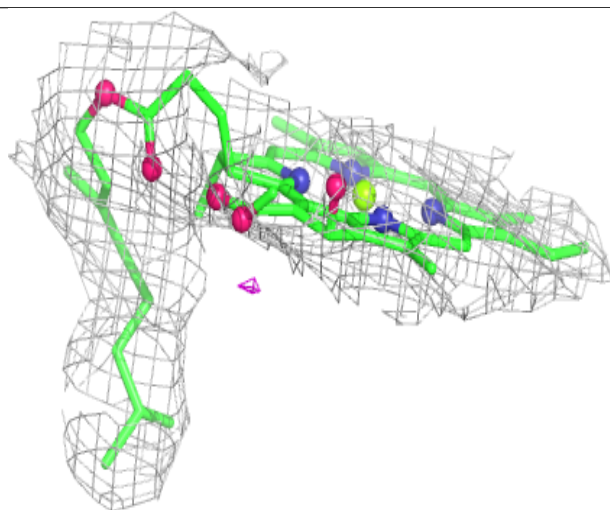
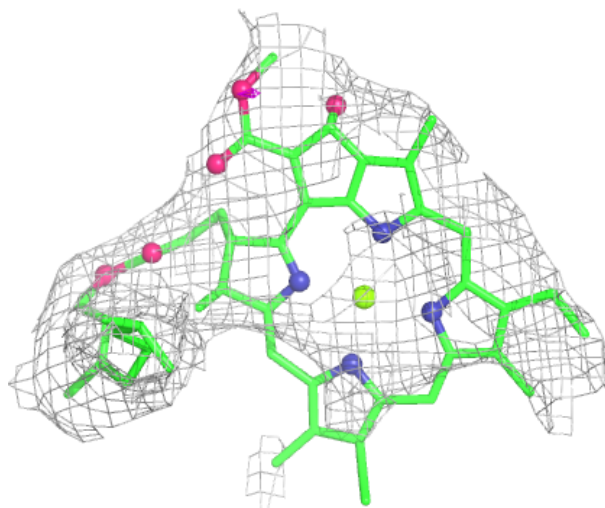
**Electron density around LMU K 106:**

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



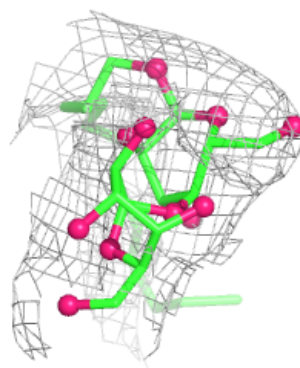
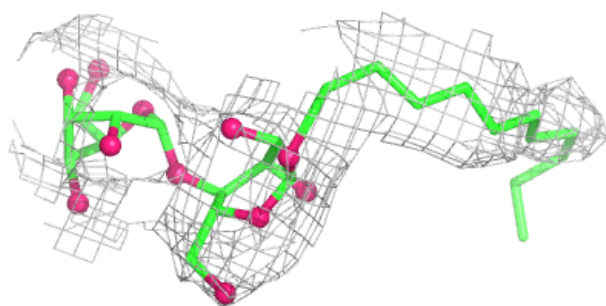
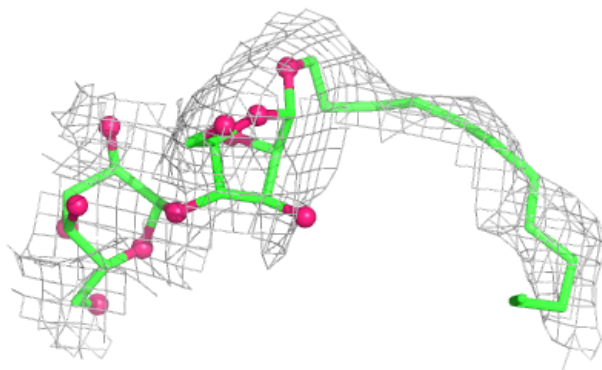
Electron density around CLA H 101:

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



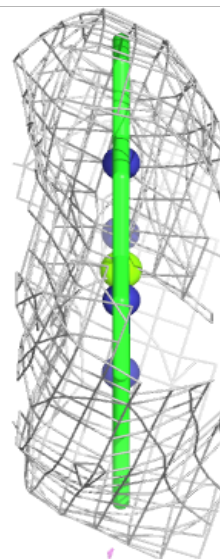
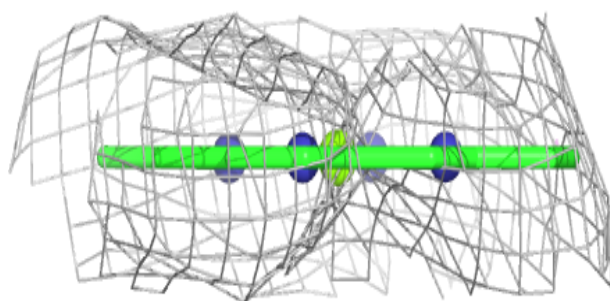
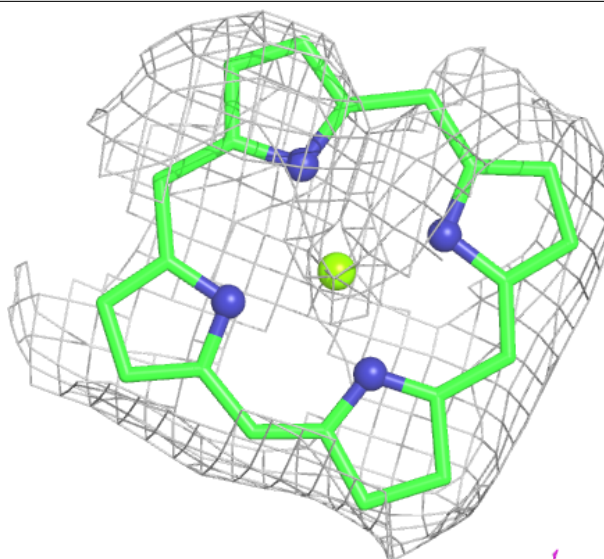
Electron density around LMU R 104:

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



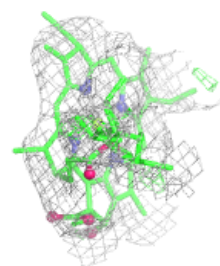
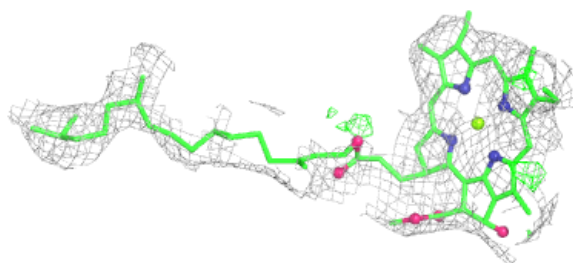
Electron density around CLA 3 305:

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

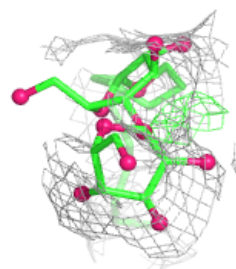
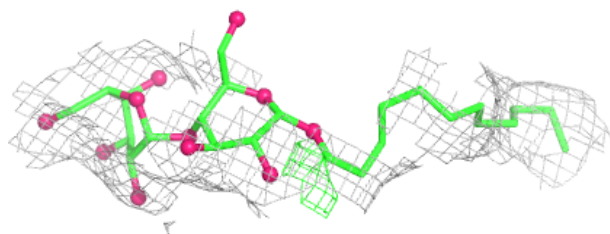
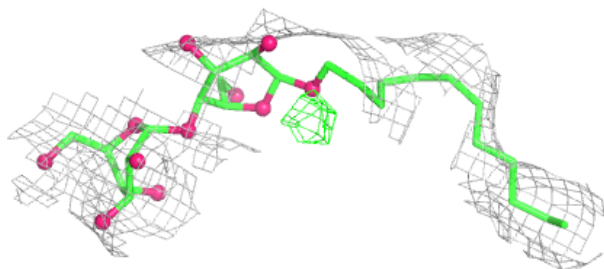


Electron density around CLA 4 304:

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

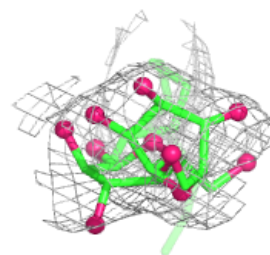
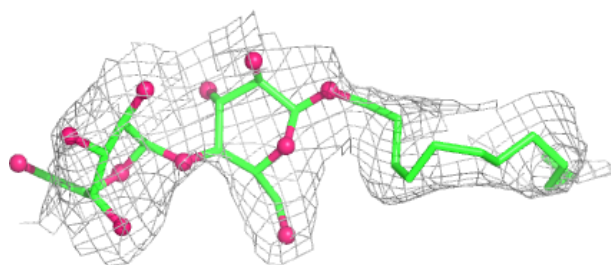
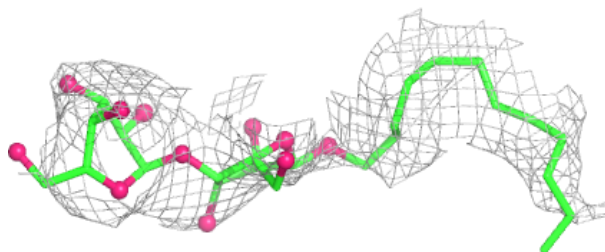
**Electron density around LMU 2 317:**

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



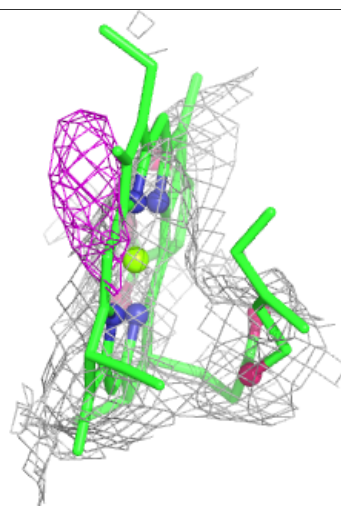
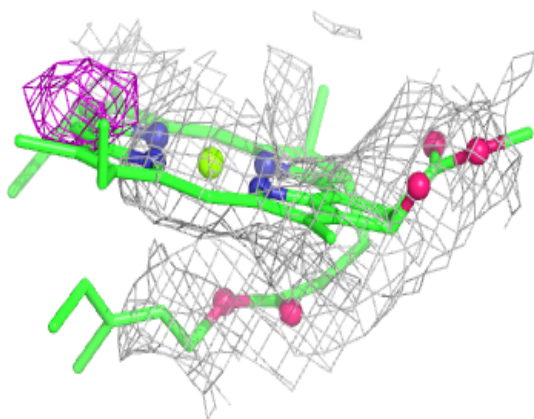
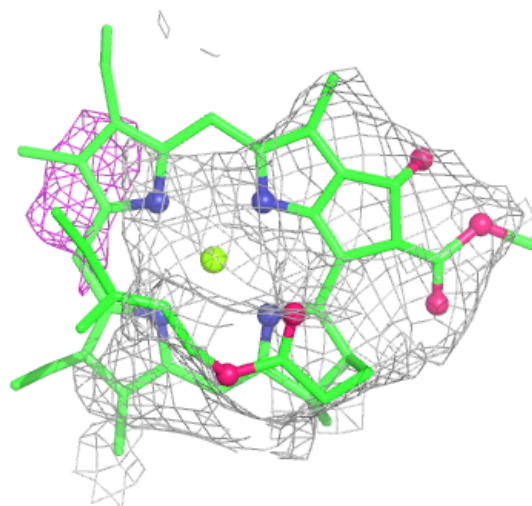
Electron density around LMU A 848:

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



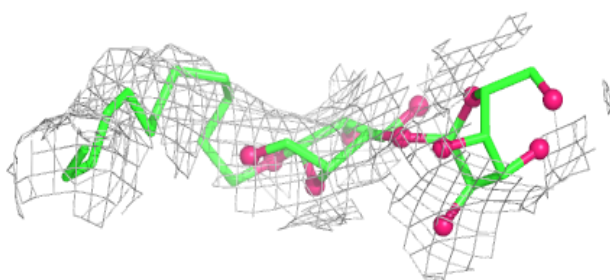
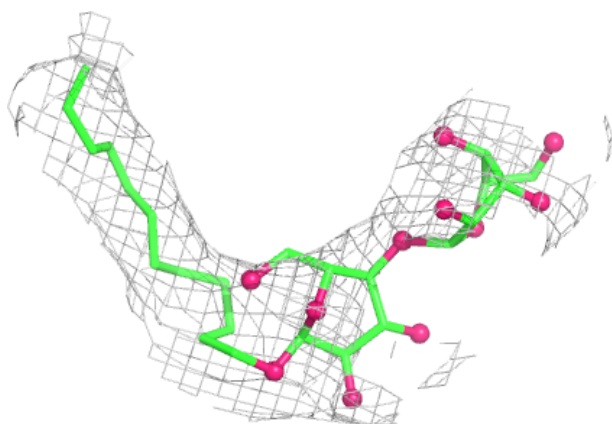
Electron density around CLA A 820:

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

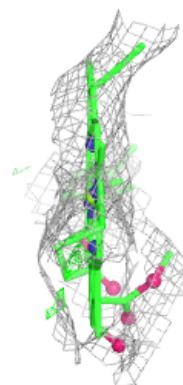
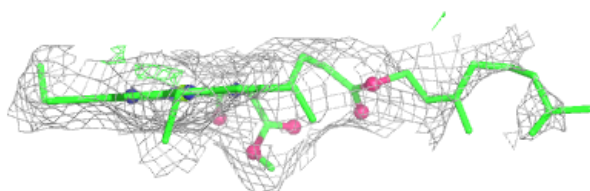
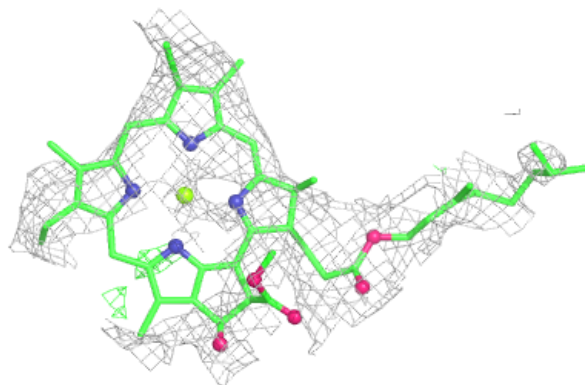


Electron density around LMU R 103:

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

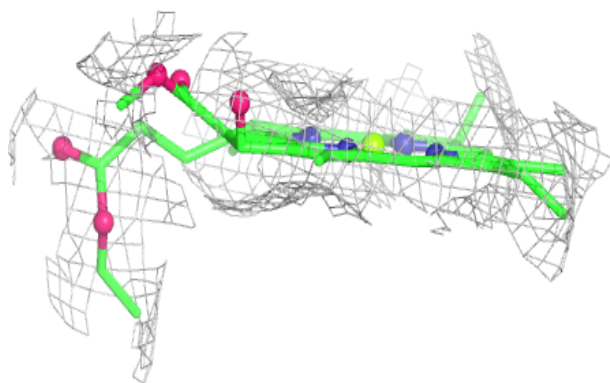
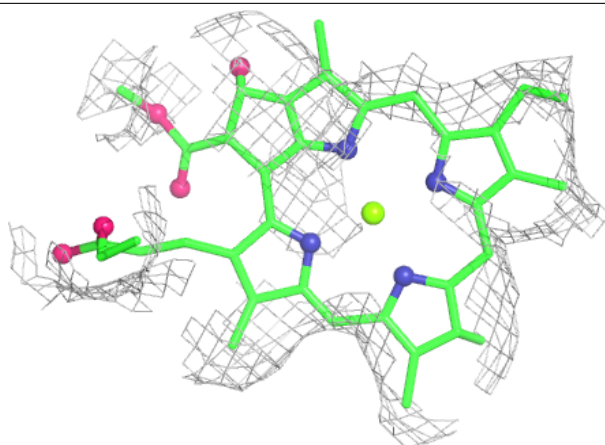
**Electron density around CLA 4 311:**

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



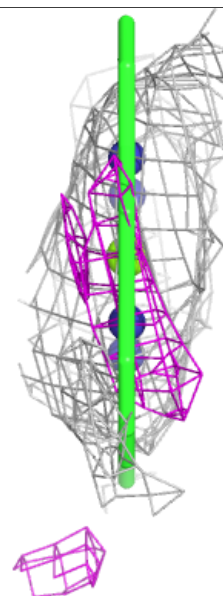
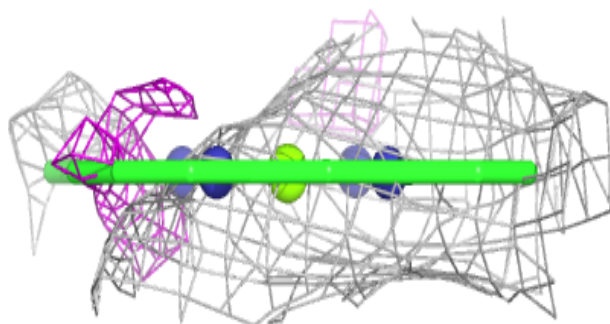
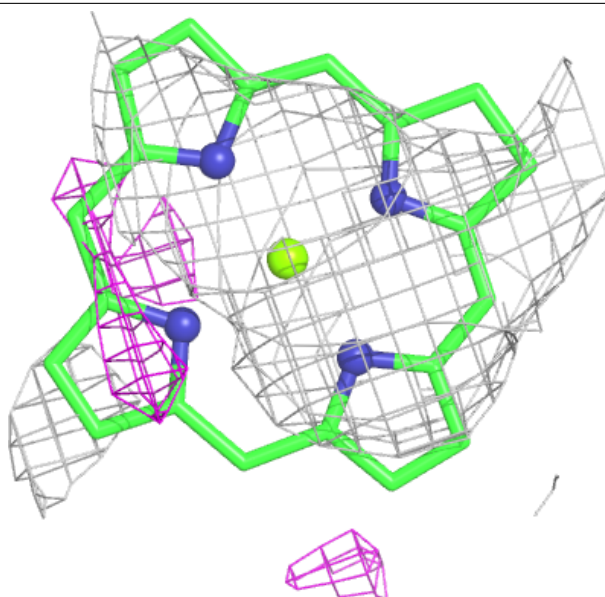
Electron density around CLA A 801:

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



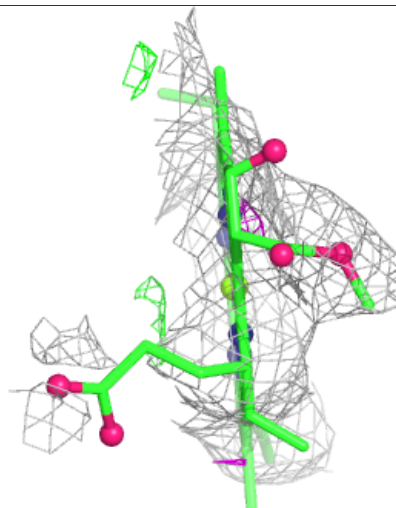
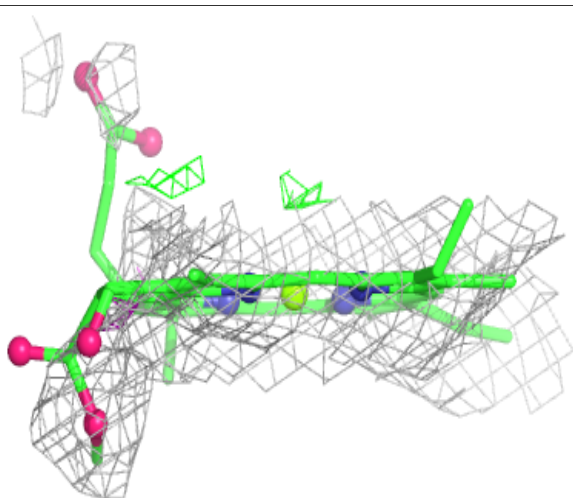
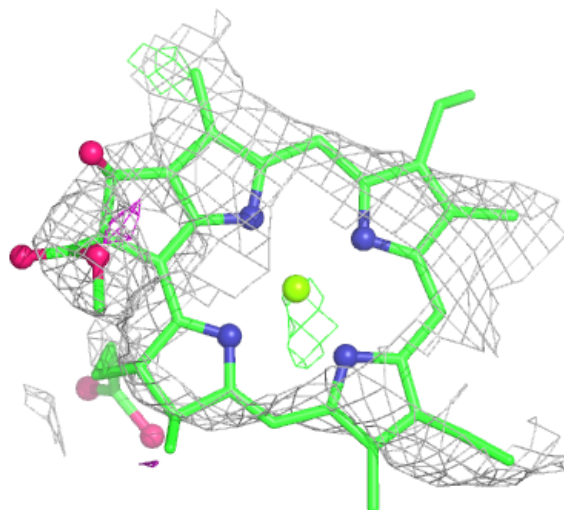
Electron density around CLA 2 301:

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



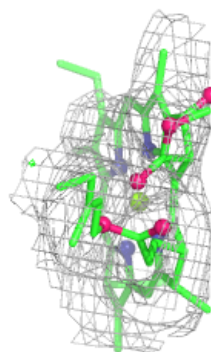
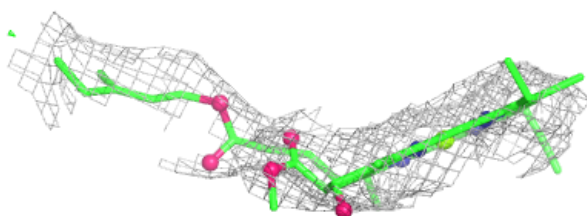
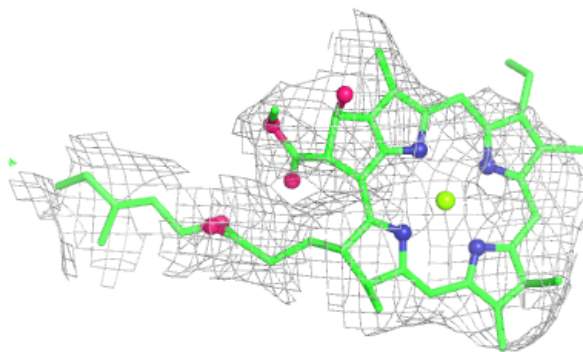
Electron density around CLA A 814:

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

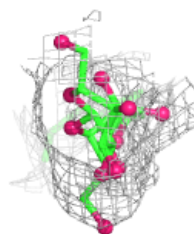
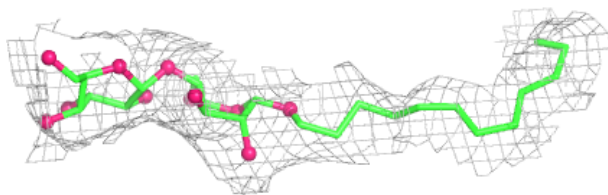


Electron density around CLA 1 210:

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

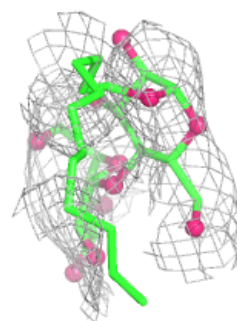
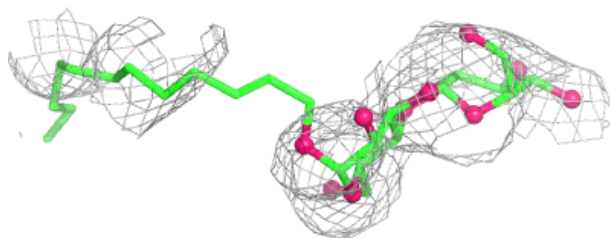
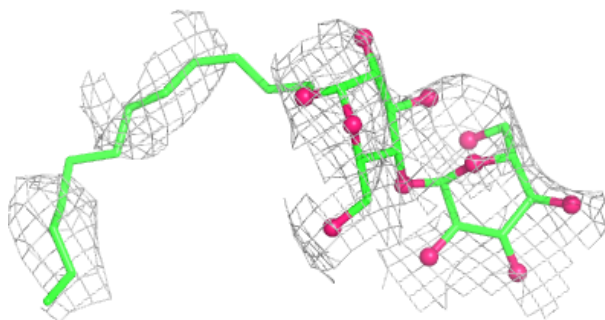
**Electron density around LMU H 107:**

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



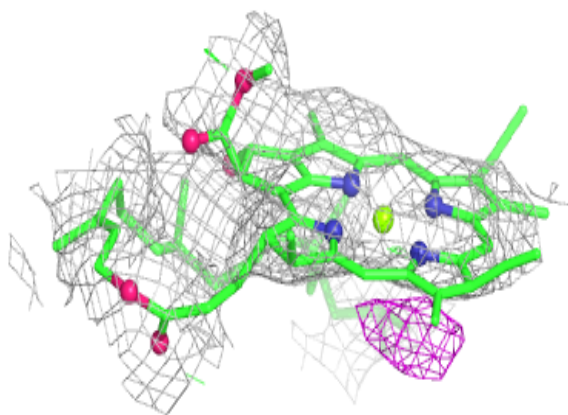
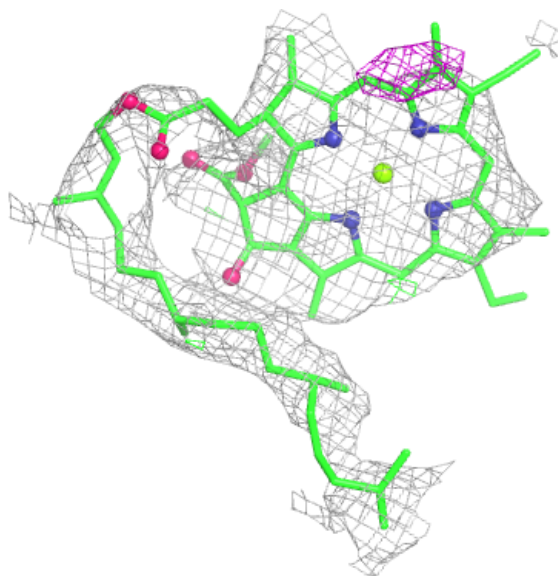
Electron density around LMU 1 217:

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



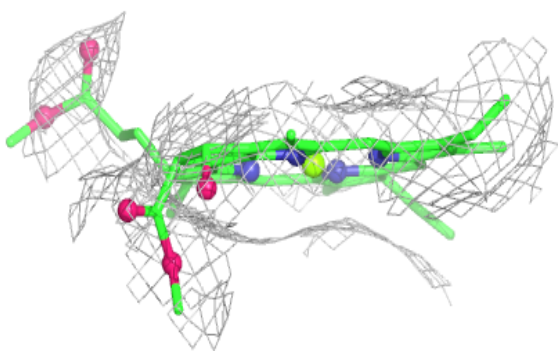
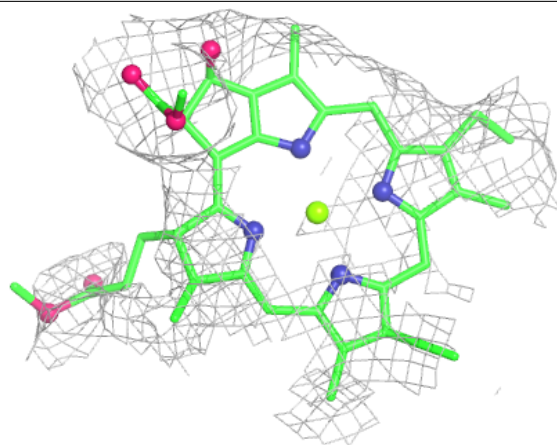
Electron density around CLA A 823:

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

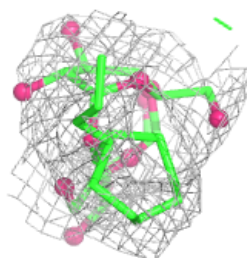
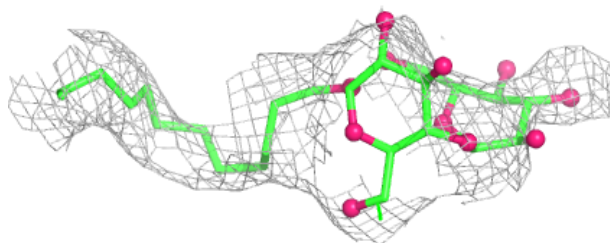
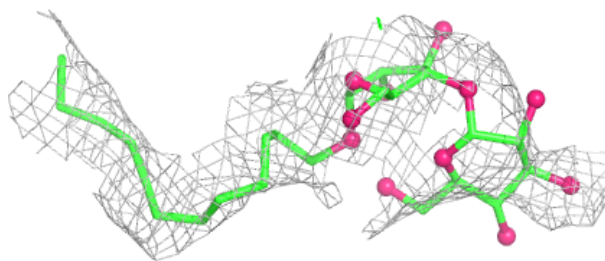


Electron density around CLA 1 201:

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

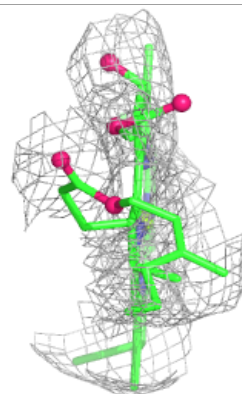
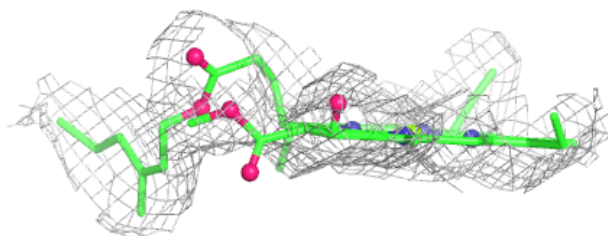
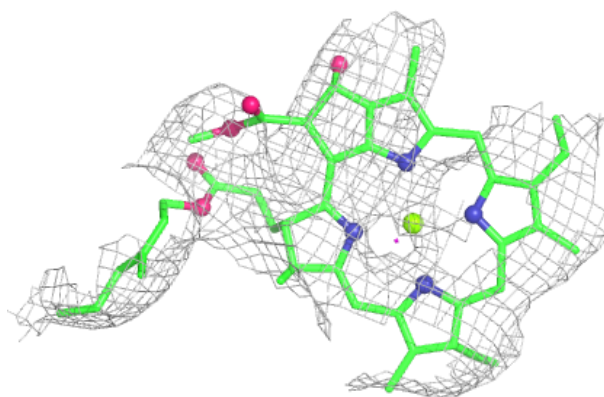
**Electron density around LMU A 849:**

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

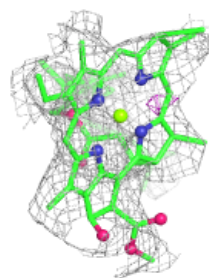
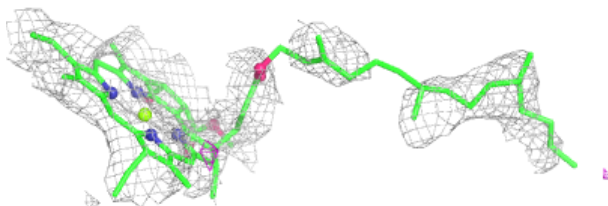
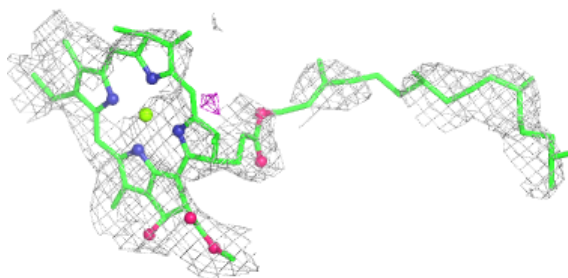


Electron density around CLA 4 318:

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

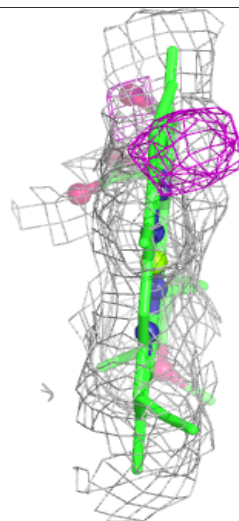
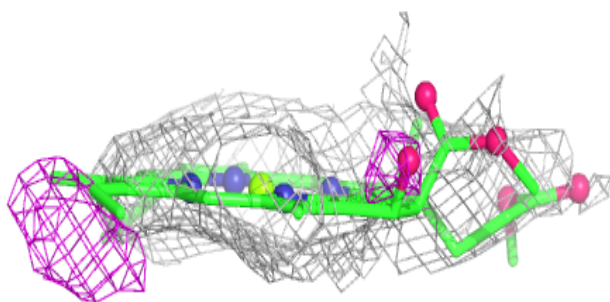
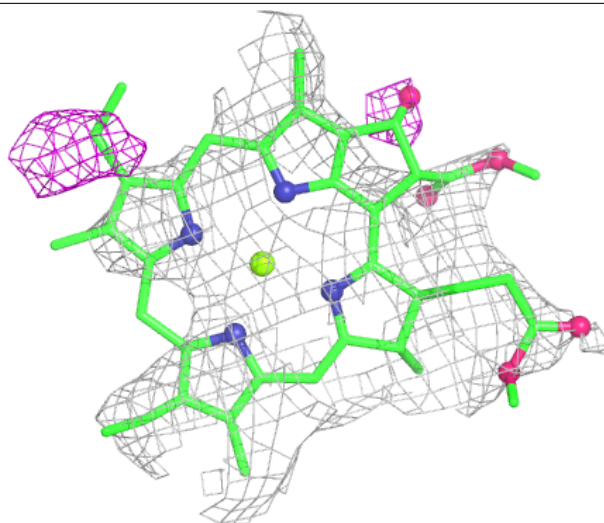
**Electron density around CLA A 819:**

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



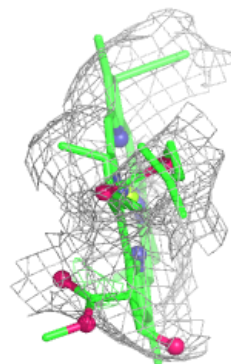
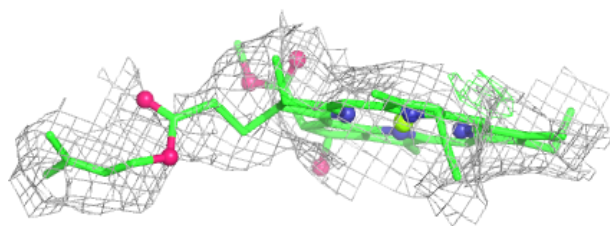
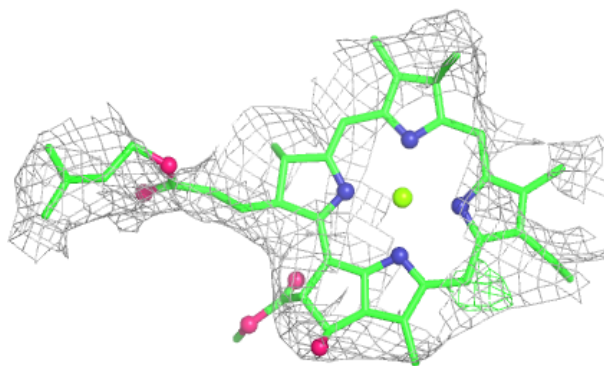
Electron density around CLA B 814:

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



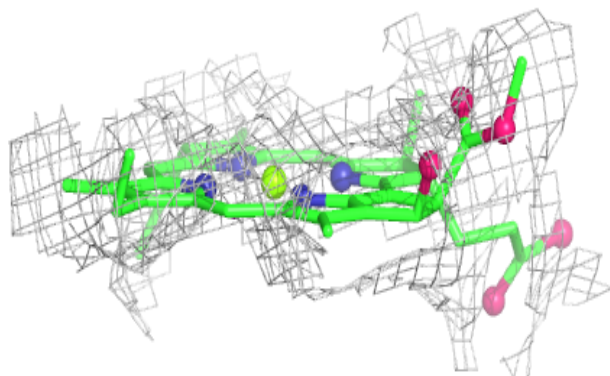
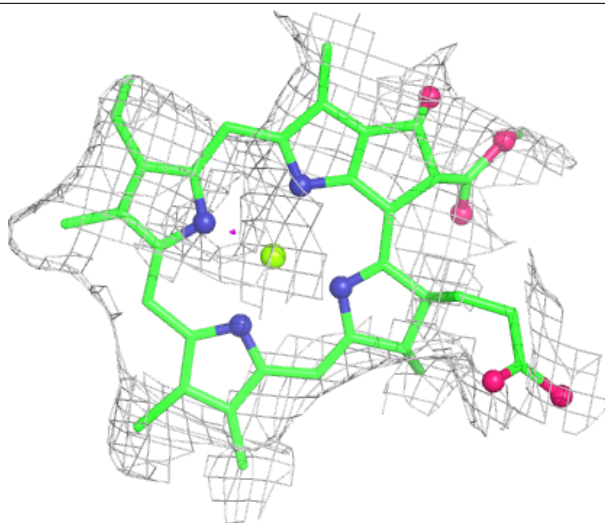
Electron density around CLA 3 302:

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



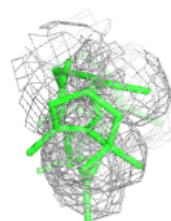
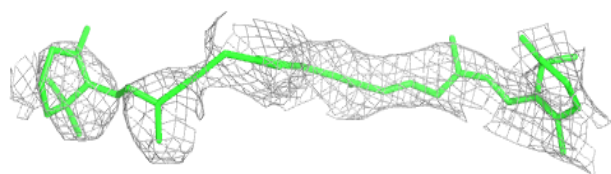
Electron density around CLA K 101:

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

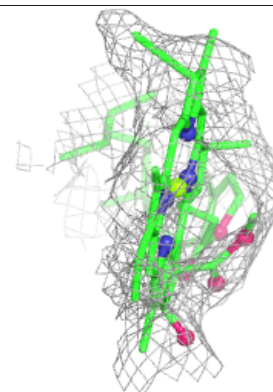
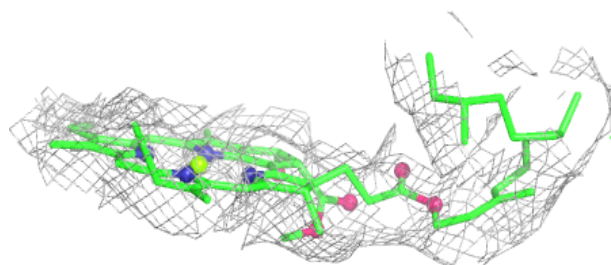
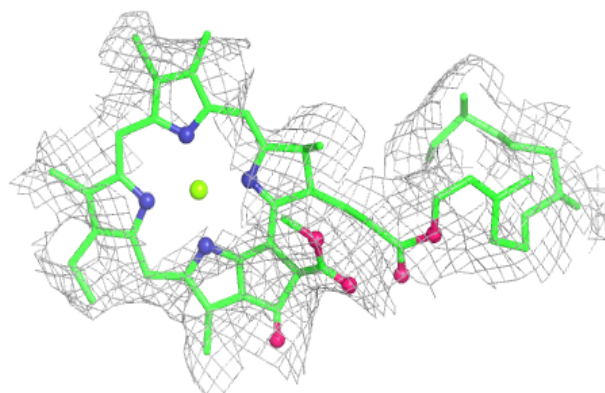


Electron density around BCR I 103:

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

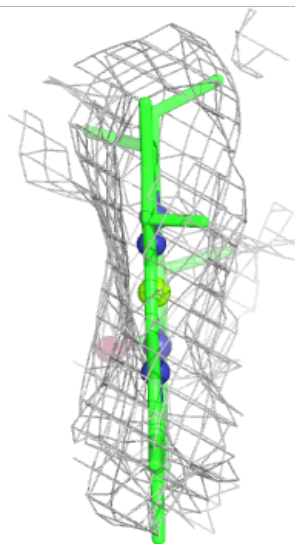
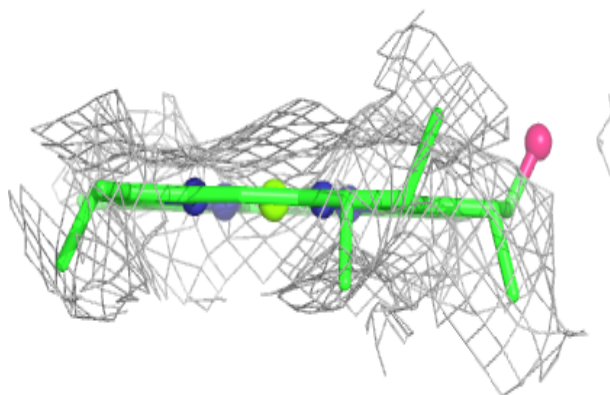
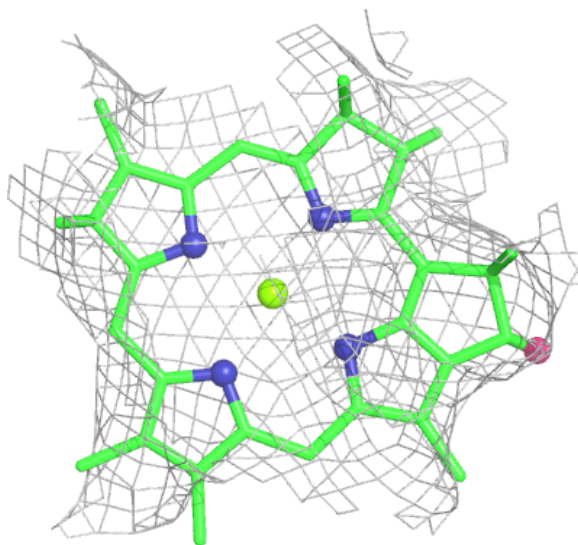
**Electron density around CLA 1 215:**

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



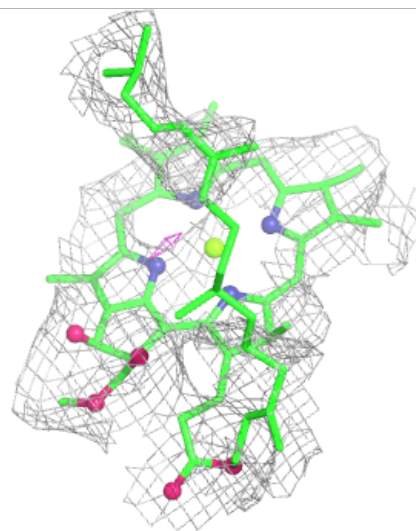
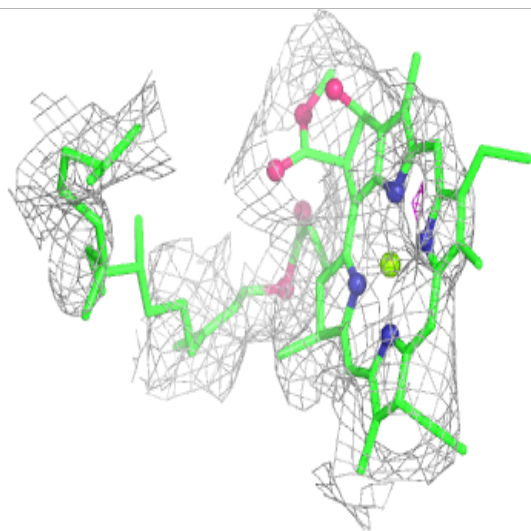
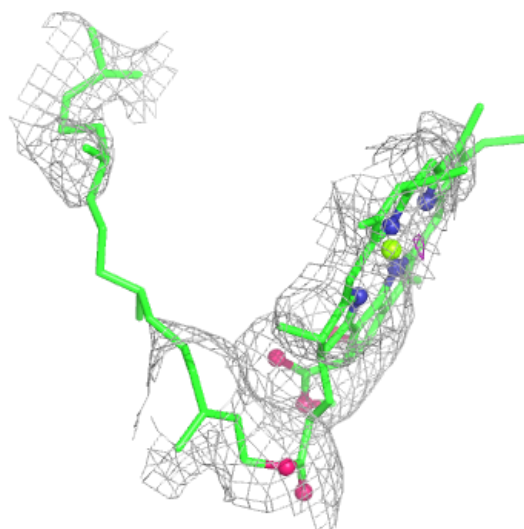
Electron density around CLA B 840:

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



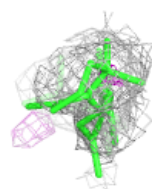
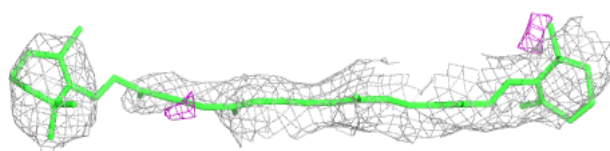
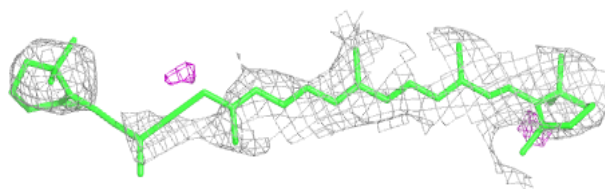
Electron density around CLA 2 307:

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

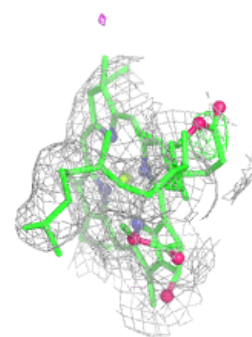
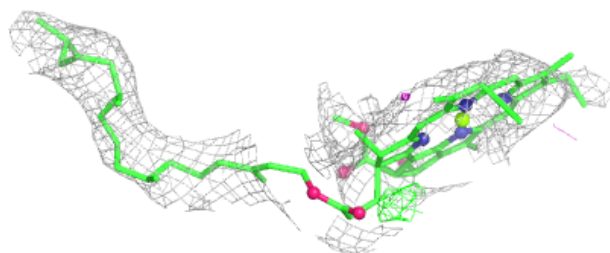
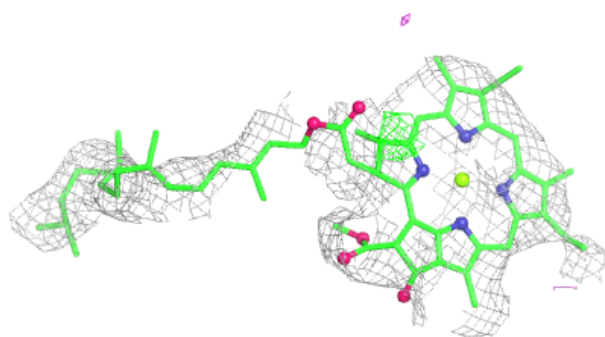


Electron density around BCR B 846:

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

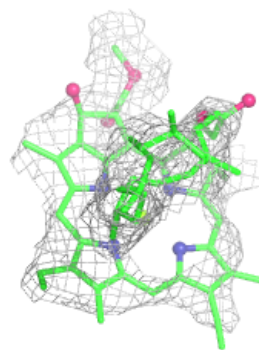
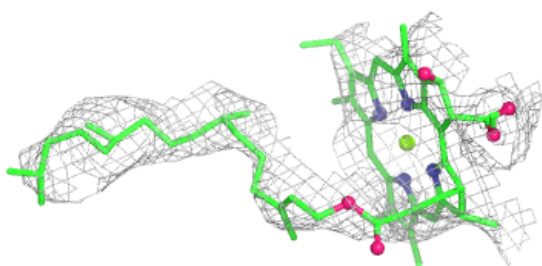
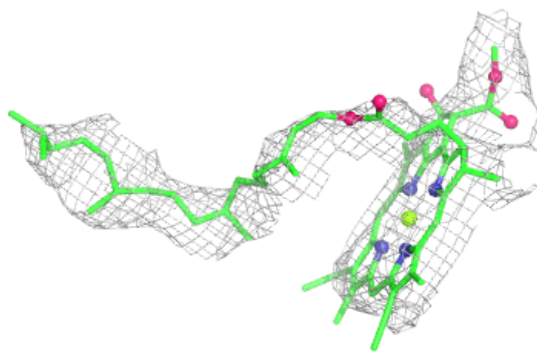
**Electron density around CLA 3 317:**

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



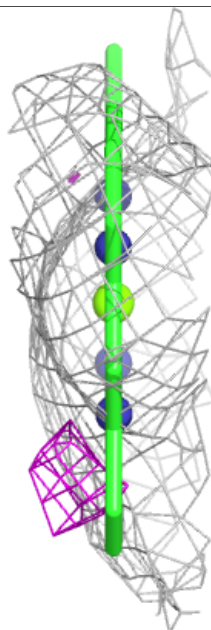
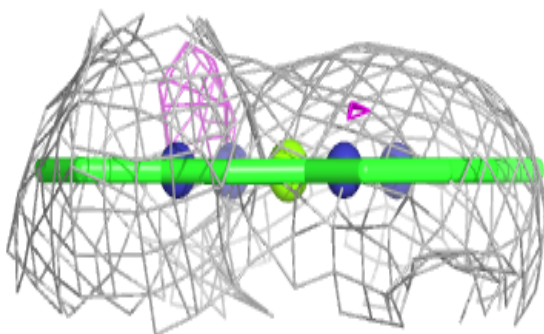
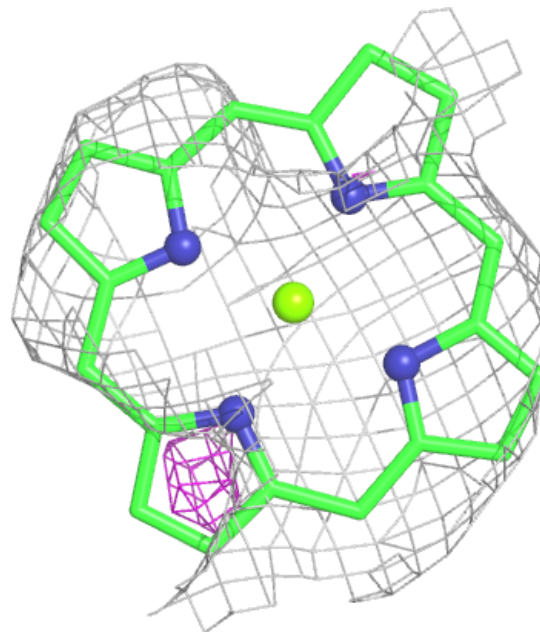
Electron density around CLA A 811:

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



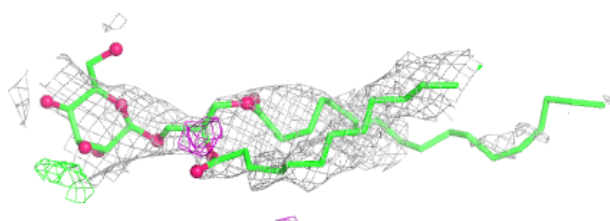
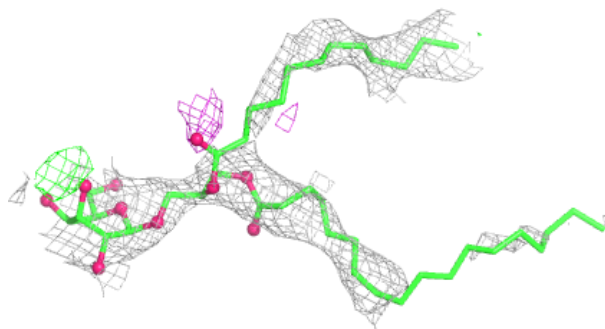
Electron density around CLA 3 309:

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



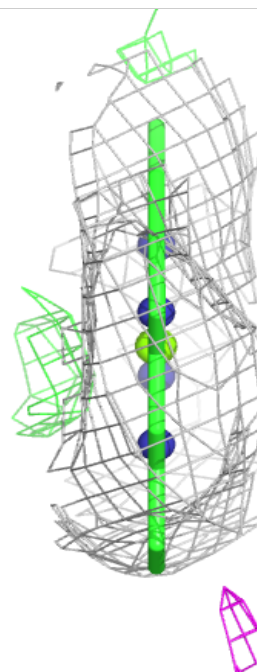
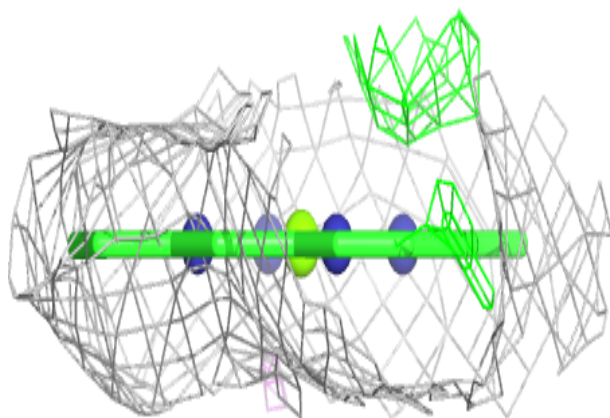
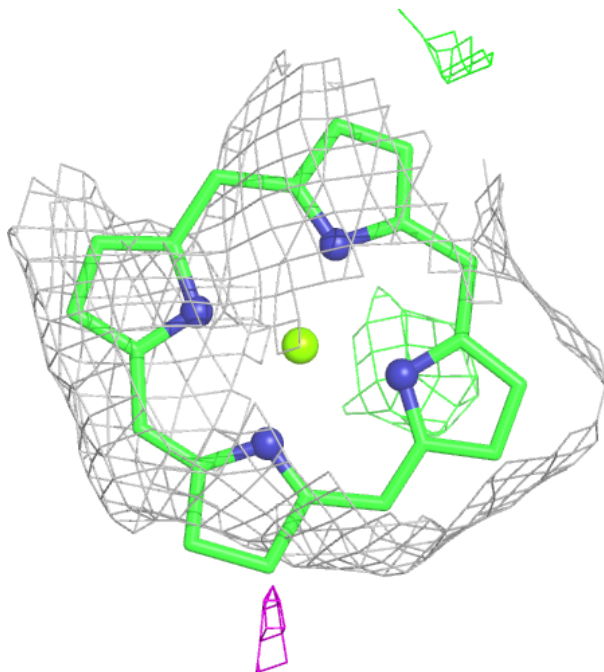
Electron density around LMG B 848:

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



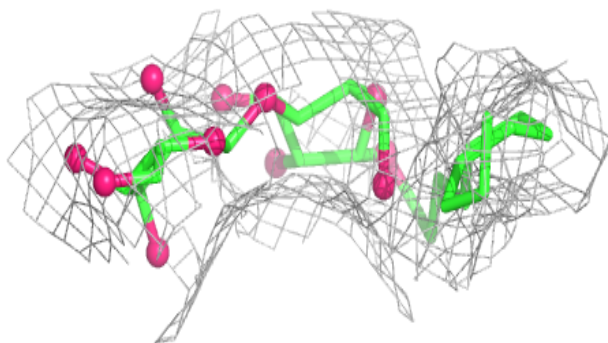
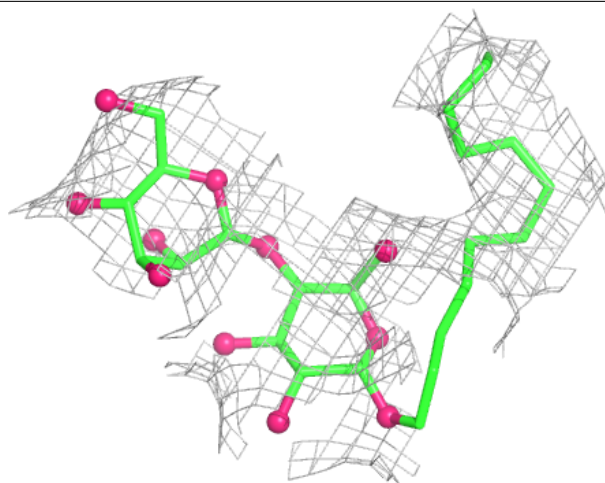
Electron density around CLA 3 318:

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



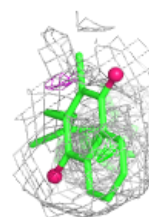
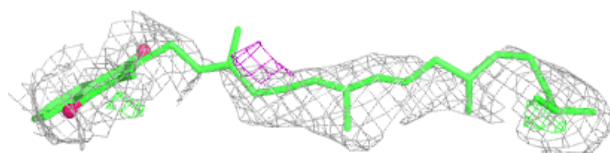
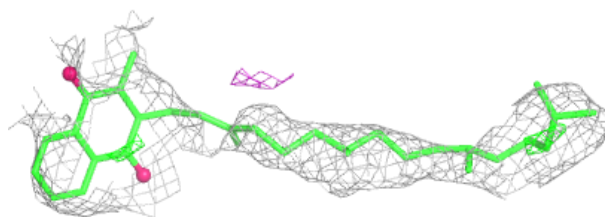
Electron density around LMU N 101:

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

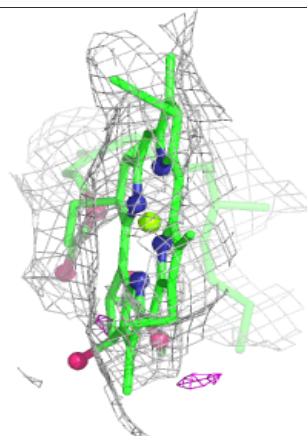
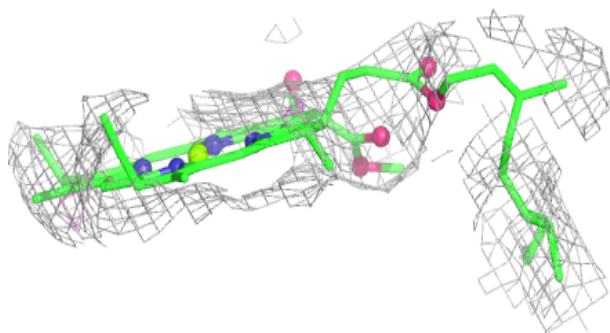
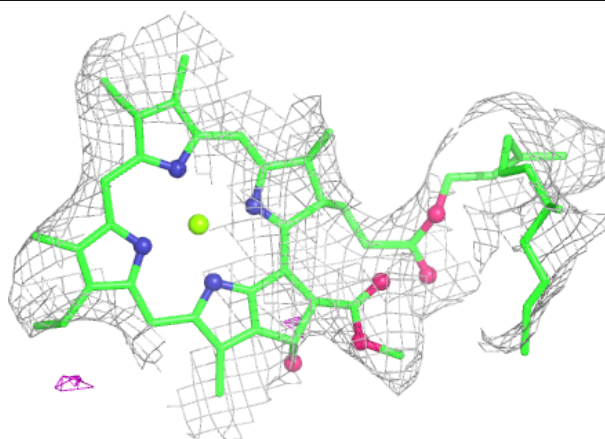


Electron density around PQN A 842:

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

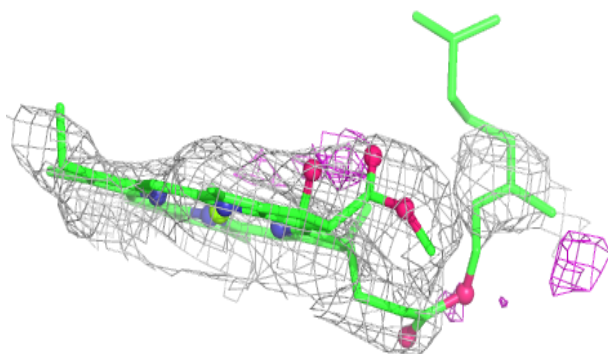
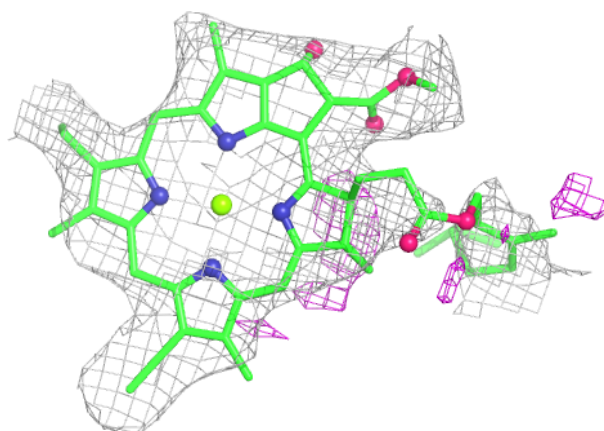
**Electron density around CLA R 108:**

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

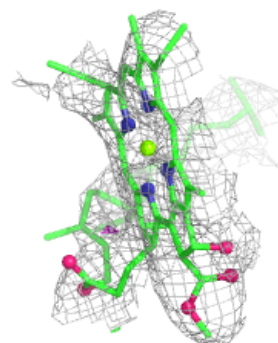
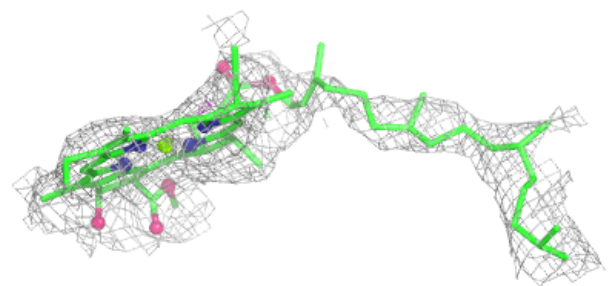
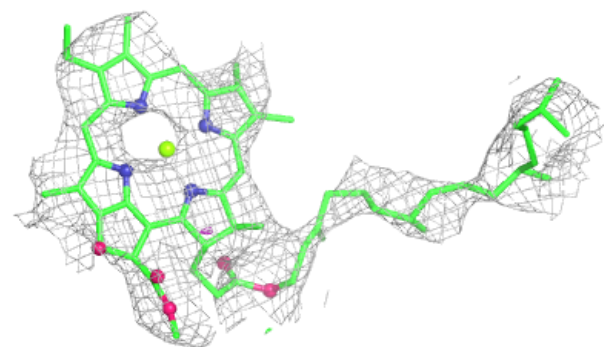


Electron density around CLA A 806:

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

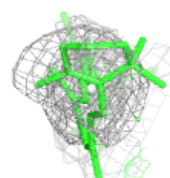
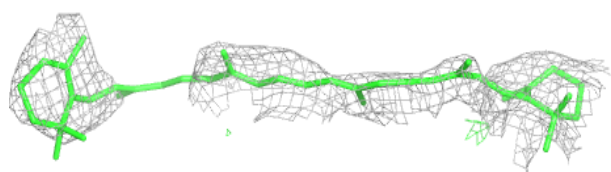
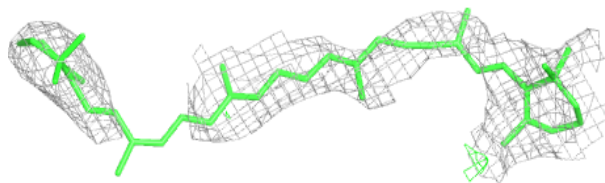
**Electron density around CLA A 852:**

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

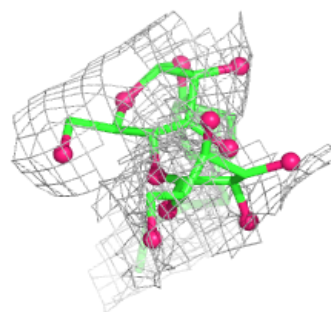
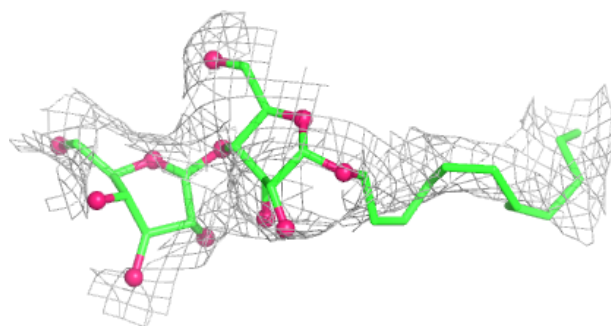
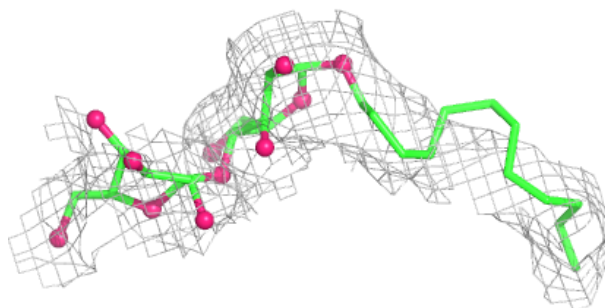


Electron density around BCR B 844:

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

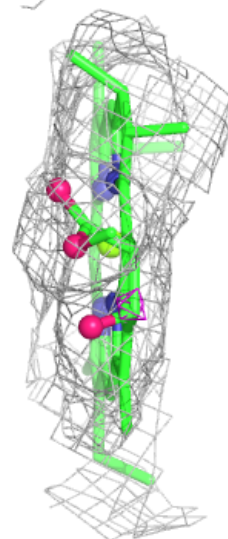
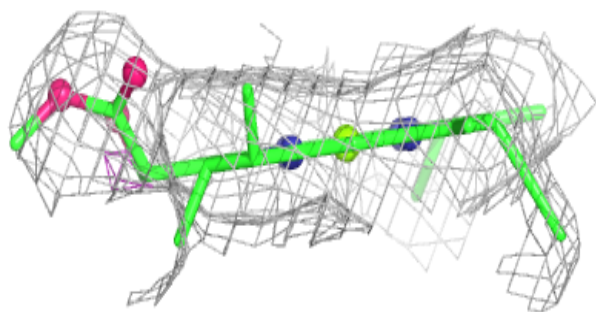
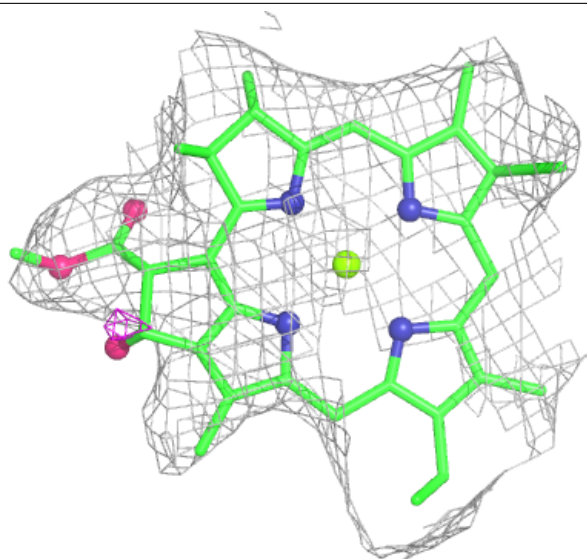
**Electron density around LMU H 104:**

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



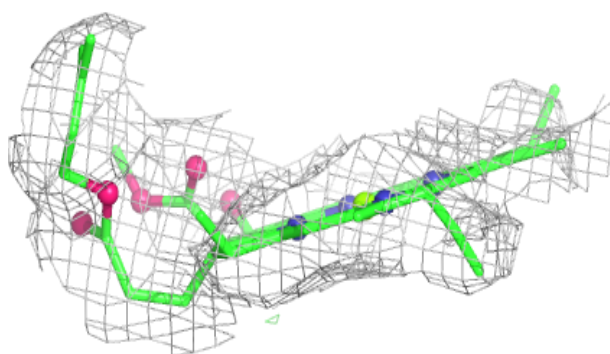
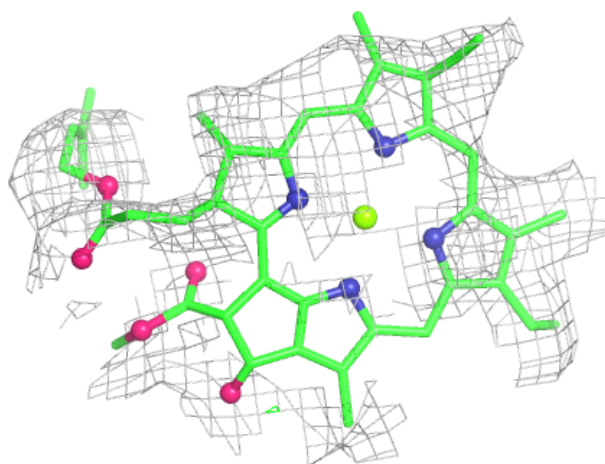
Electron density around CLA F 205:

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



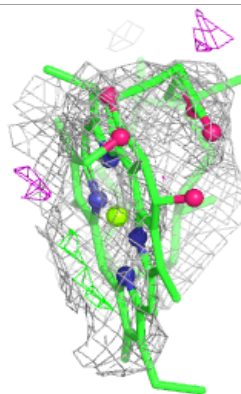
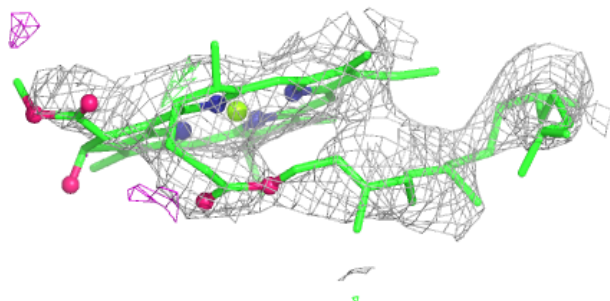
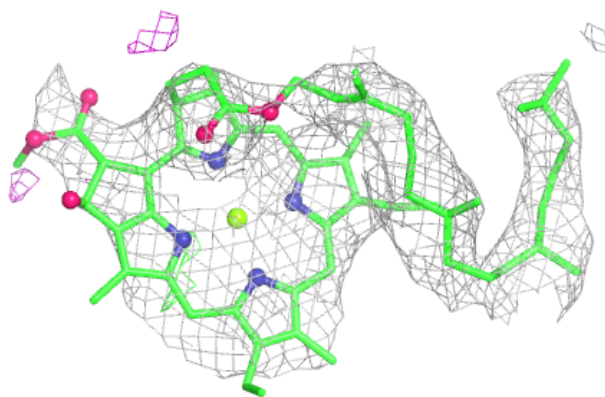
Electron density around CLA 3 316:

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



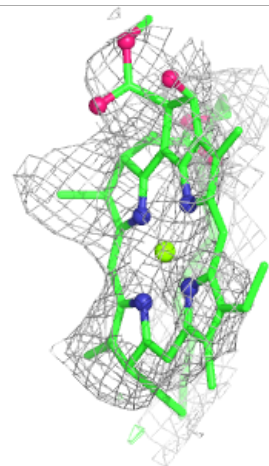
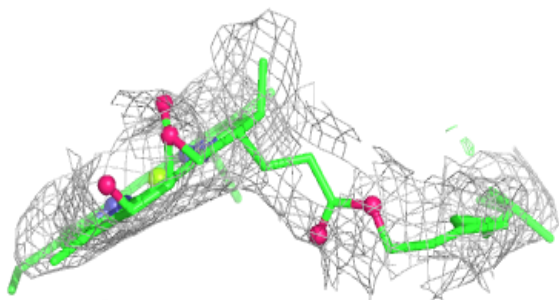
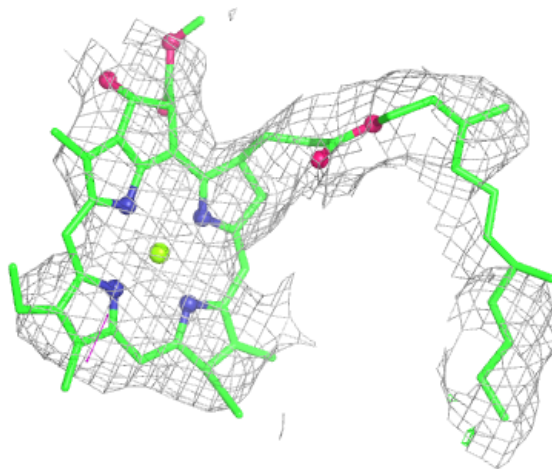
Electron density around CLA A 818:

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



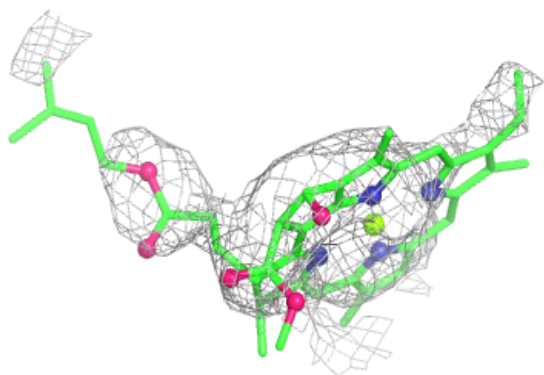
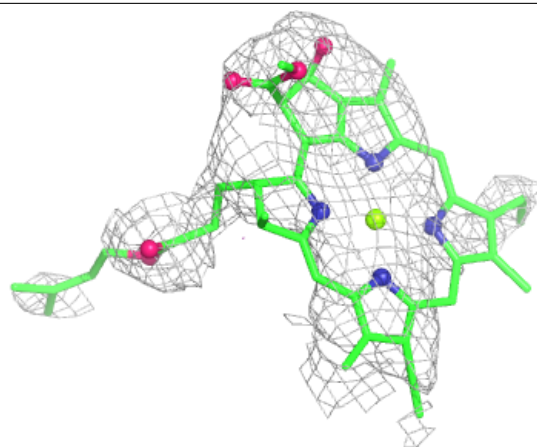
Electron density around CLA B 823:

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



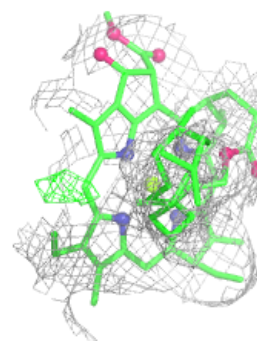
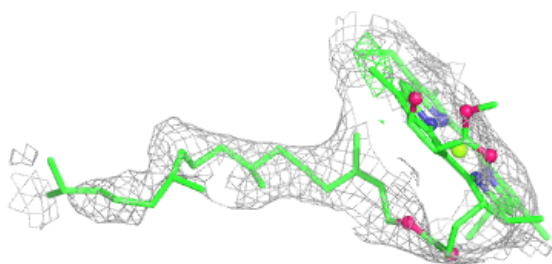
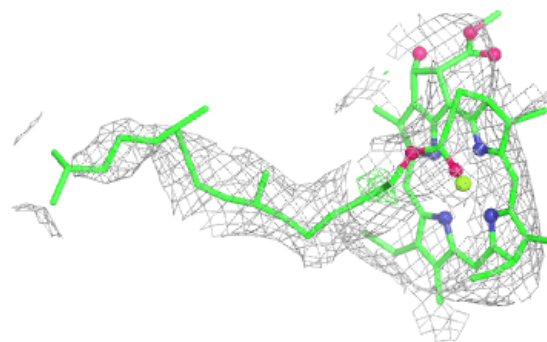
Electron density around CLA A 829:

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



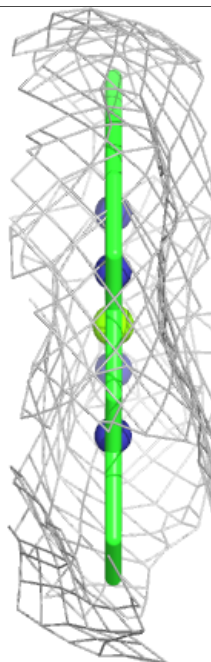
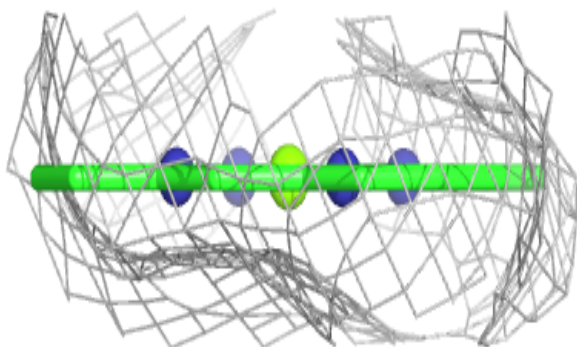
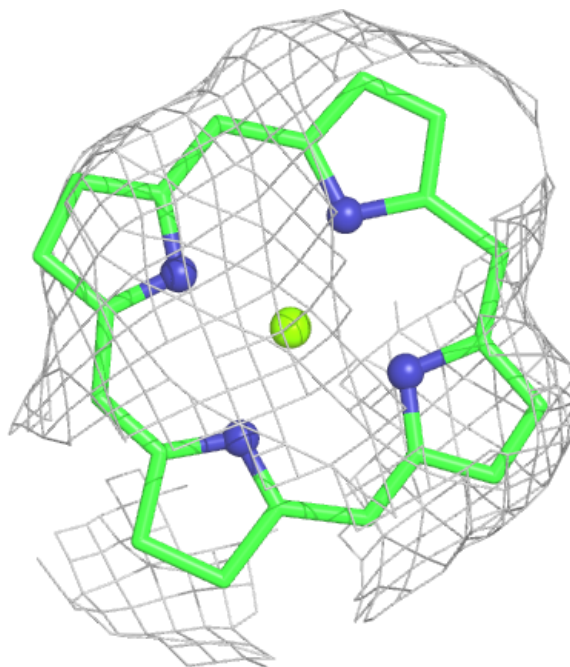
Electron density around CLA 2 303:

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



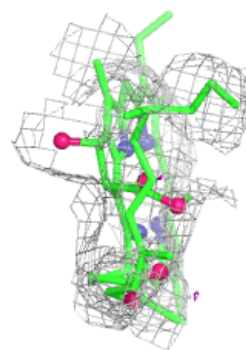
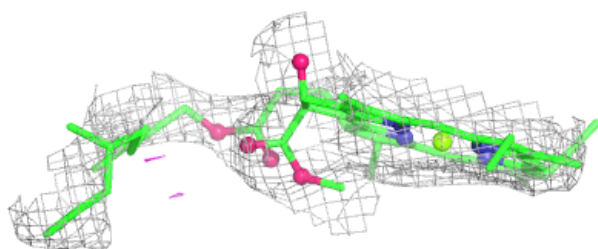
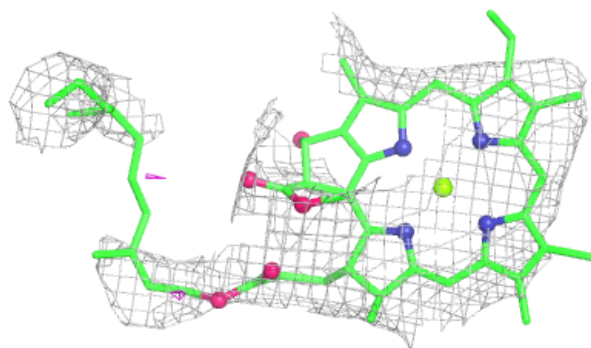
Electron density around CLA 3 319:

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

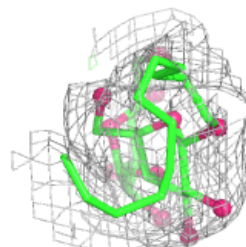
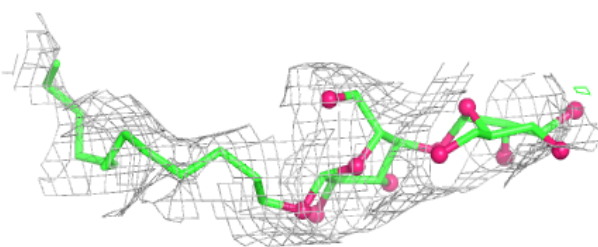
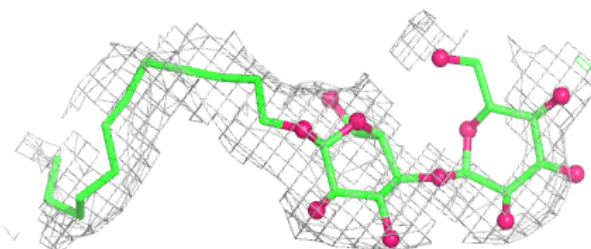


Electron density around CLA R 107:

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

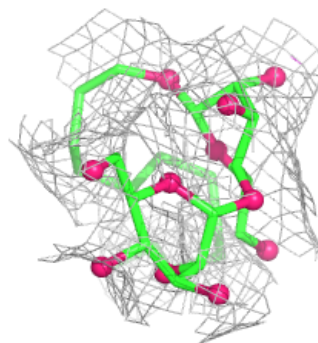
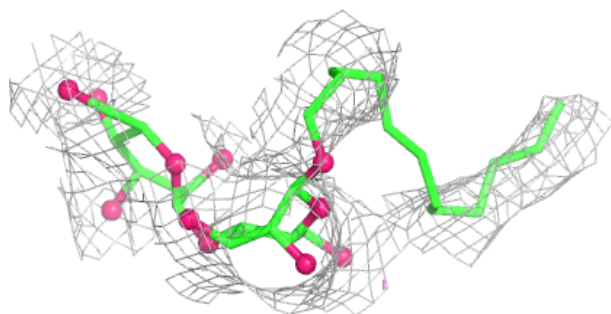
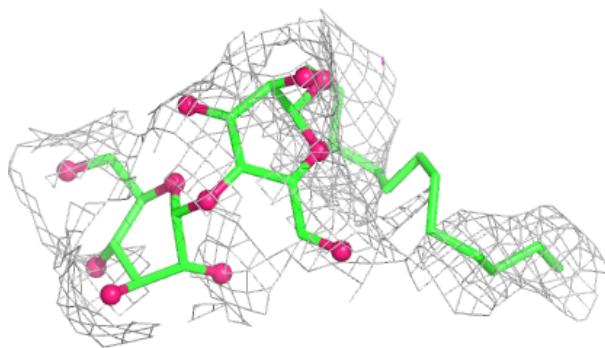
**Electron density around LMU C 101:**

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



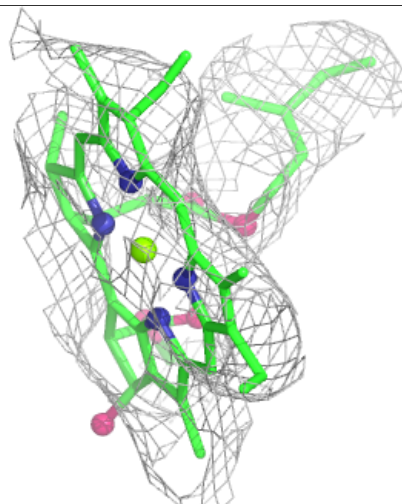
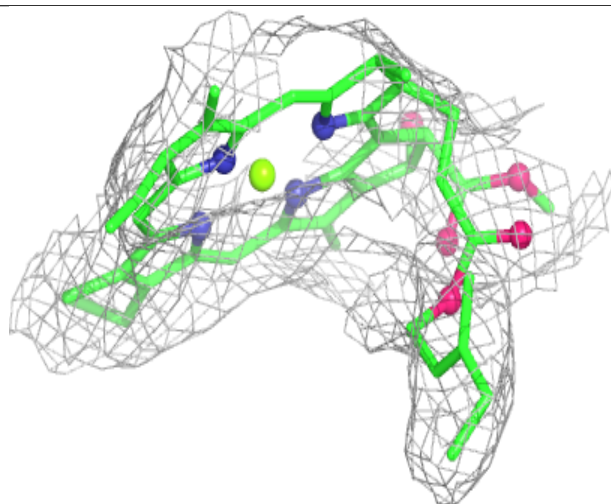
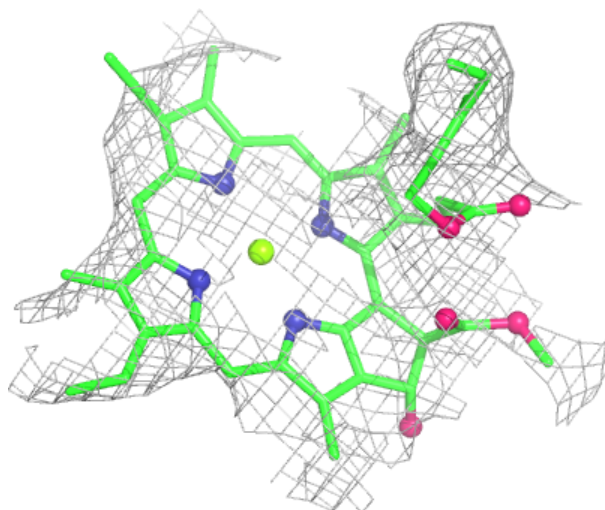
Electron density around LMU L 209:

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



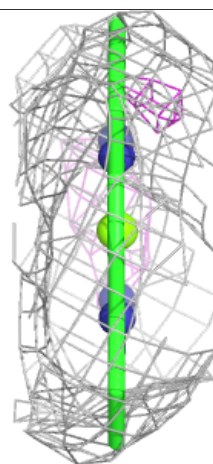
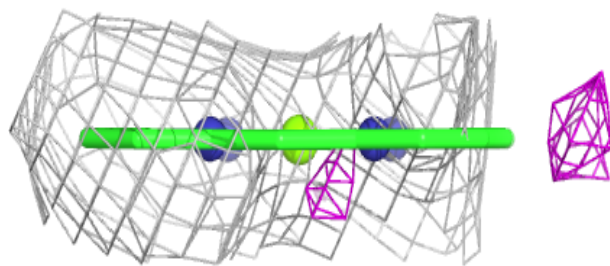
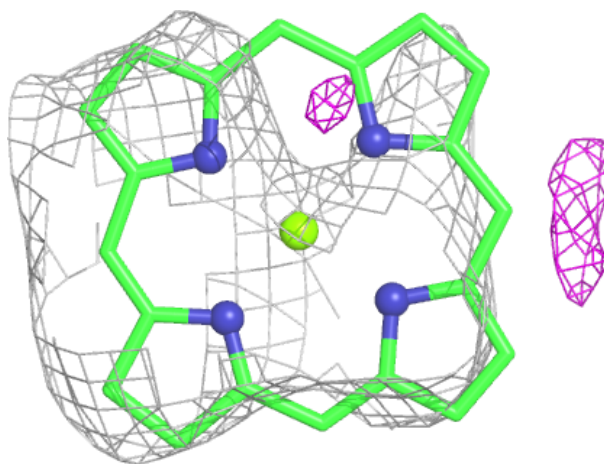
Electron density around CLA 1 207:

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



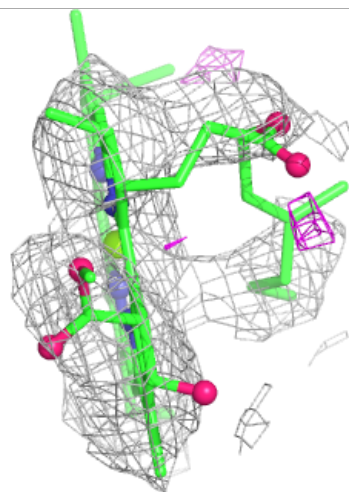
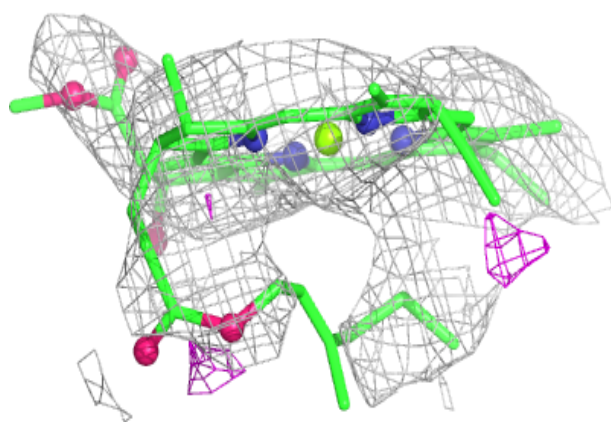
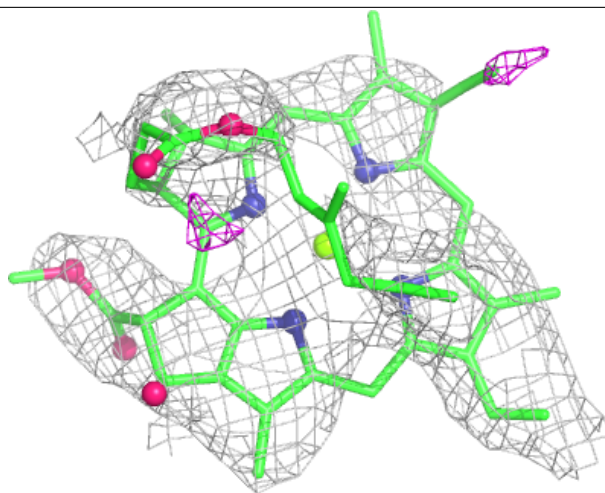
Electron density around CLA 2 310:

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



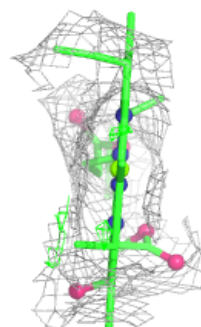
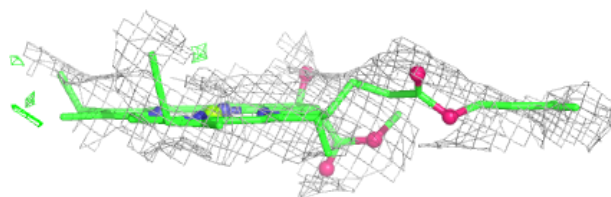
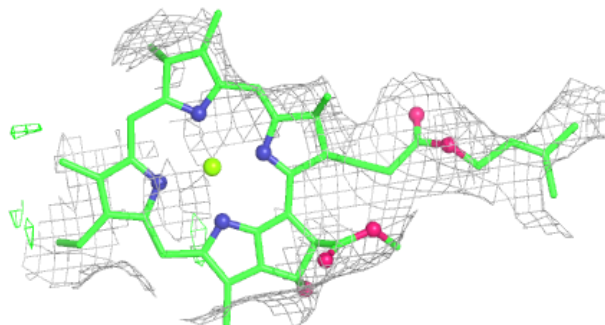
Electron density around CLA A 817:

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

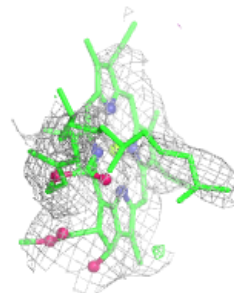
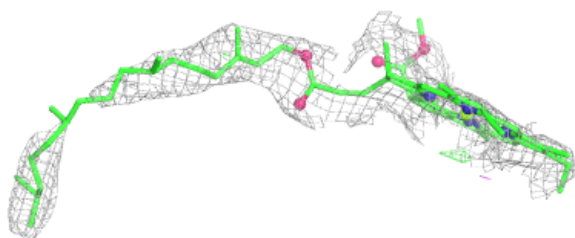
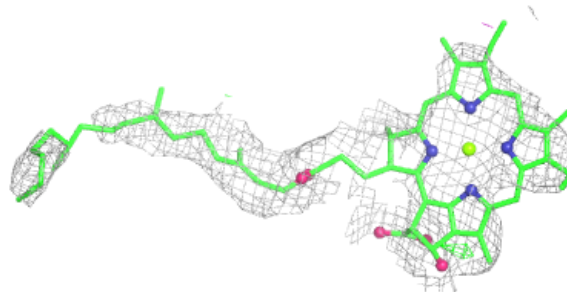


Electron density around CLA A 840:

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

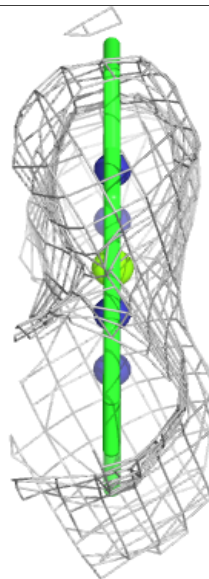
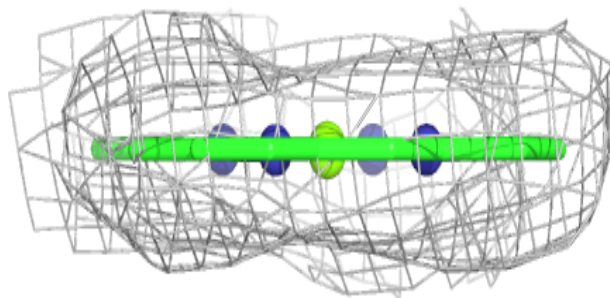
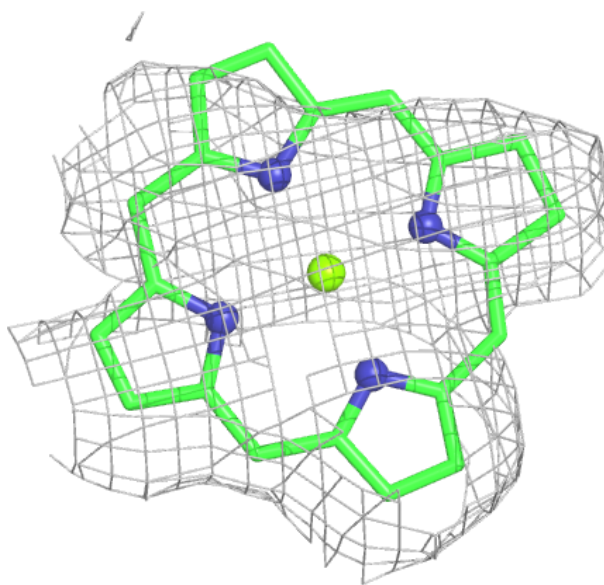
**Electron density around CLA A 805:**

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



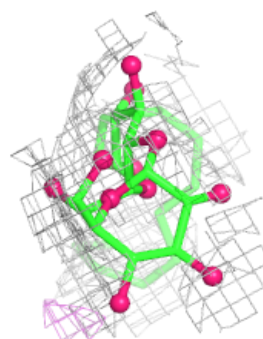
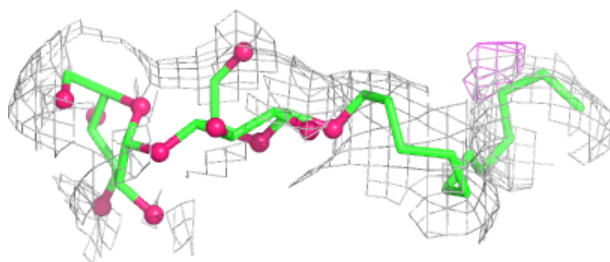
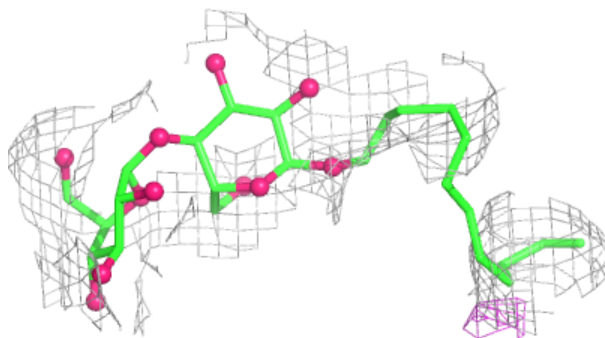
Electron density around CLA 4 310:

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

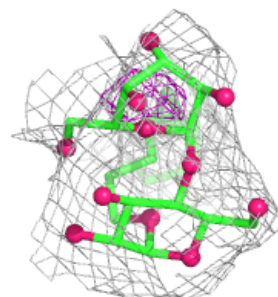
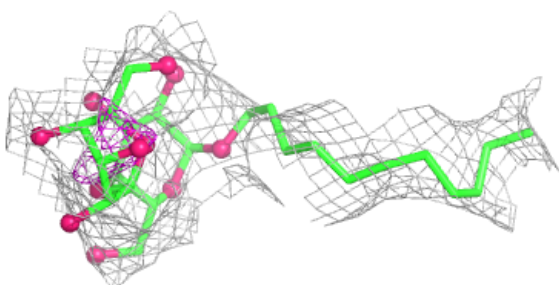
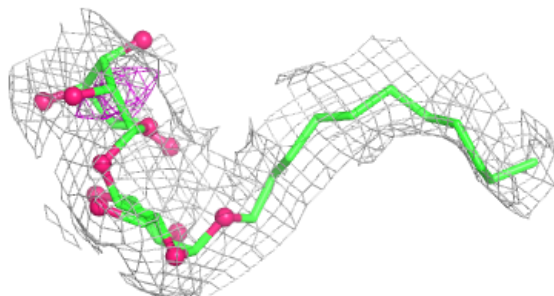


Electron density around LMU R 109:

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

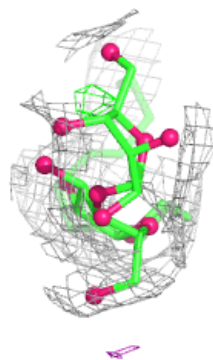
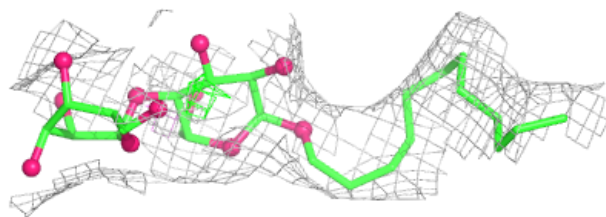
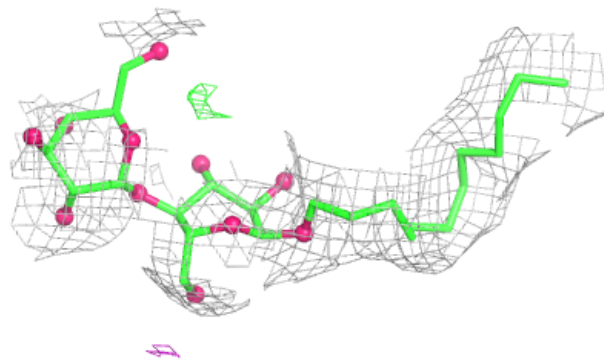
**Electron density around LMU 4 320:**

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



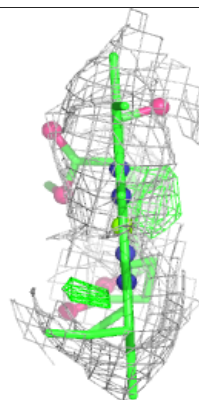
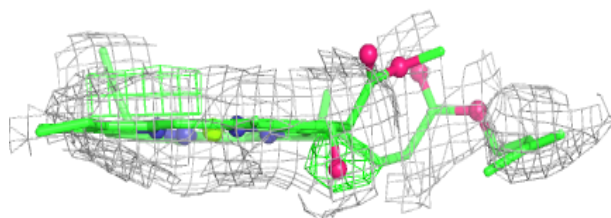
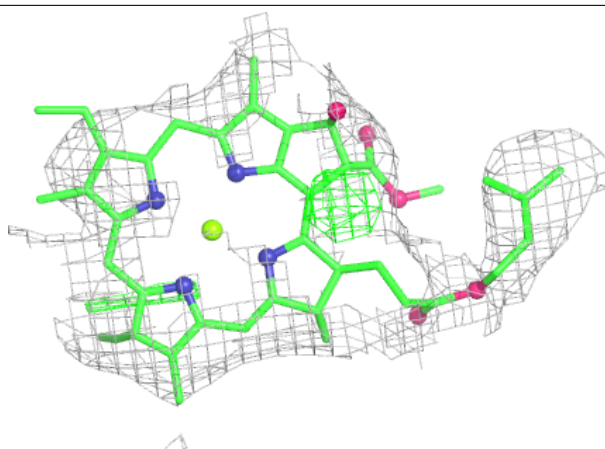
Electron density around LMU 4 322:

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

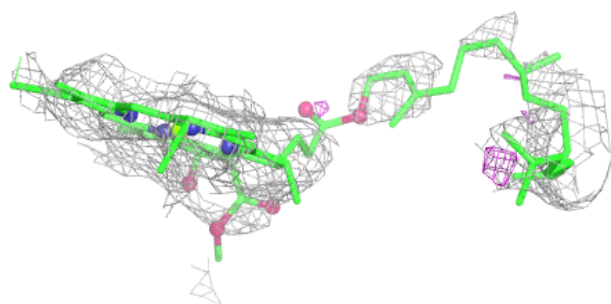
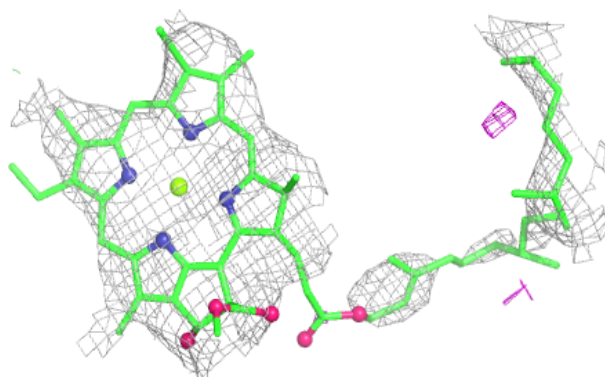


Electron density around CLA 2 312:

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

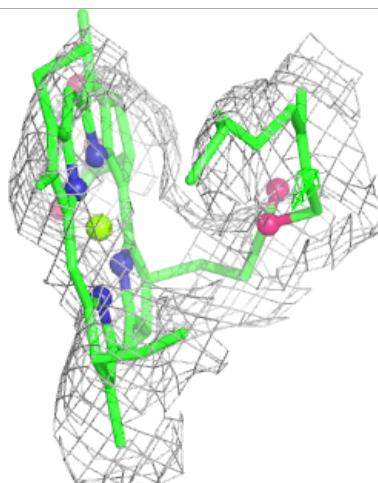
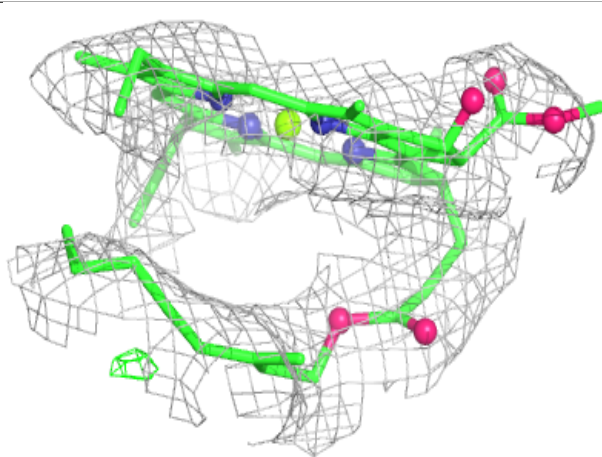
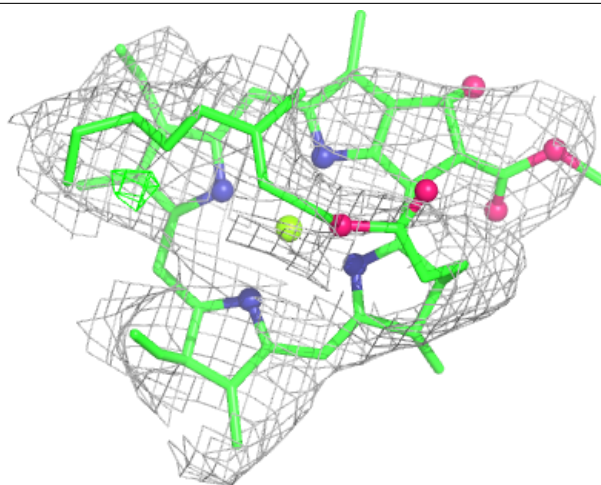
**Electron density around CLA A 825:**

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



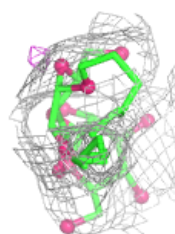
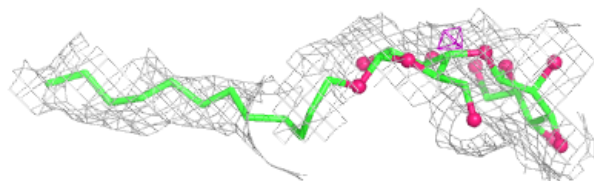
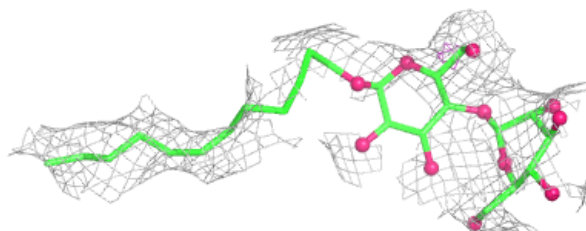
Electron density around CLA A 812:

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



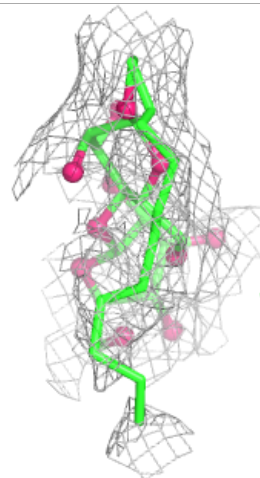
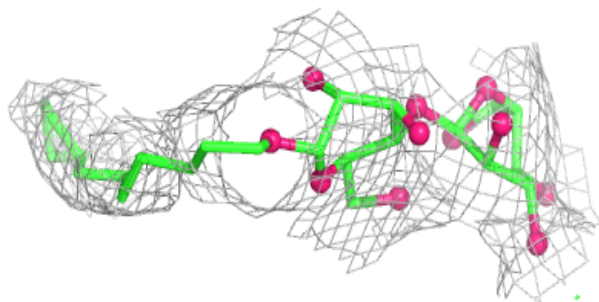
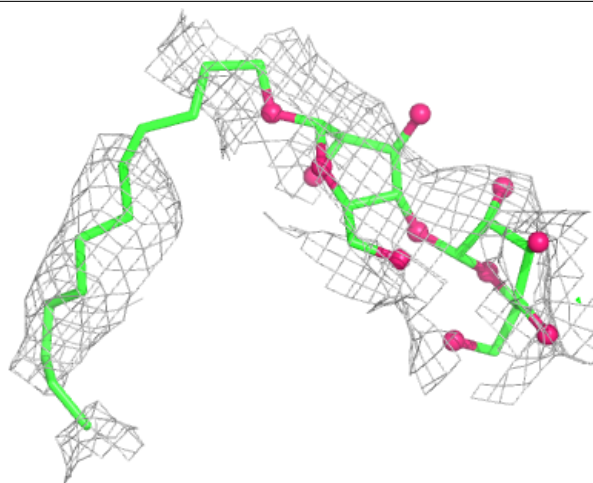
Electron density around LMU A 856:

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



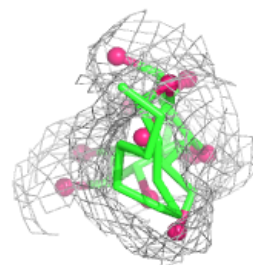
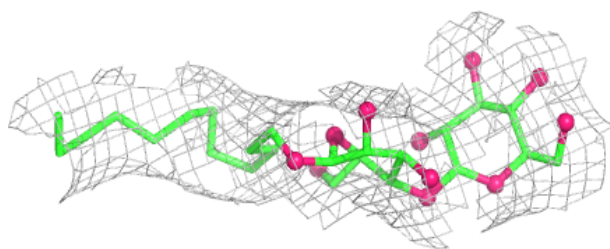
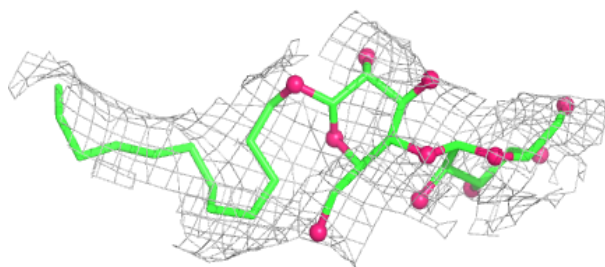
Electron density around LMU K 104:

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



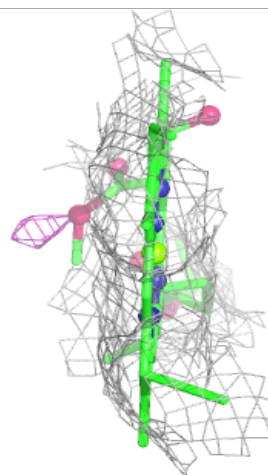
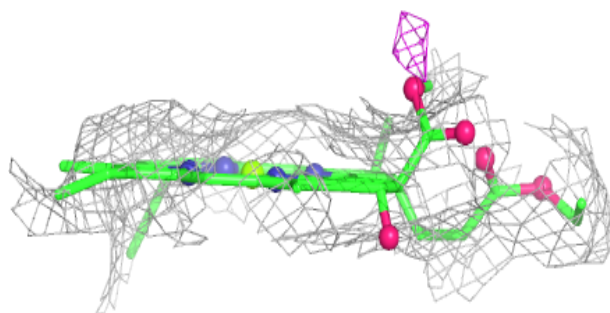
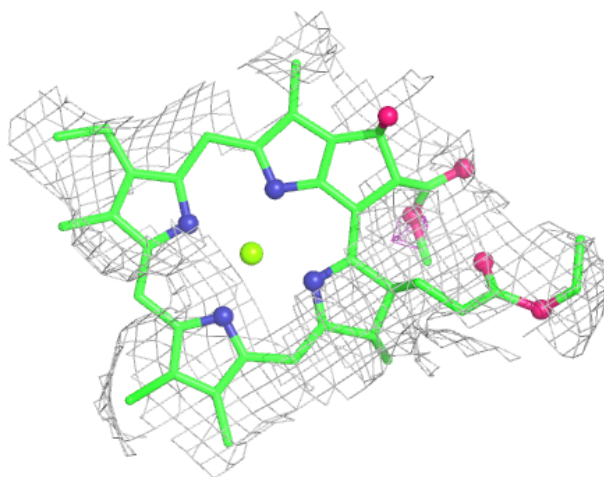
Electron density around LMU K 105:

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



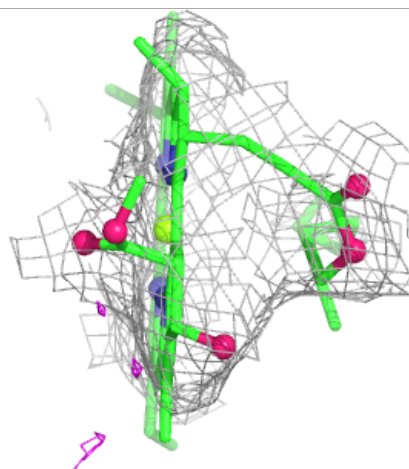
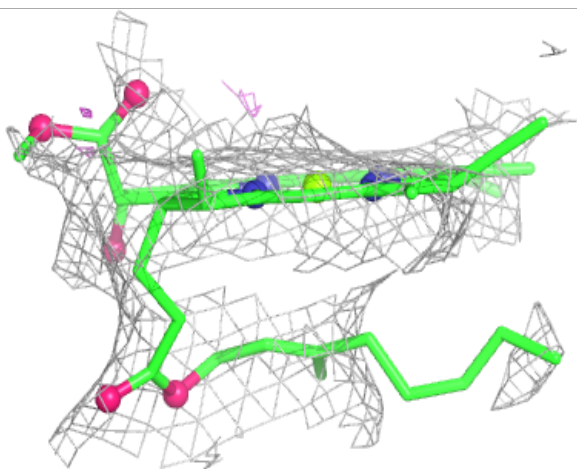
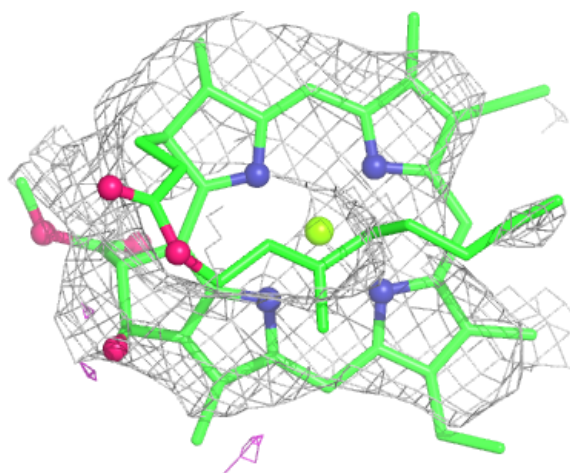
Electron density around CLA 4 319:

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



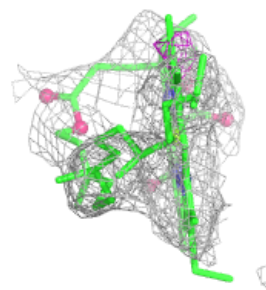
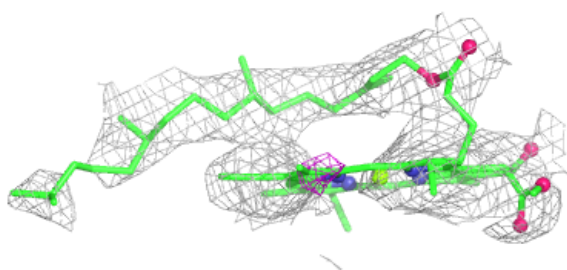
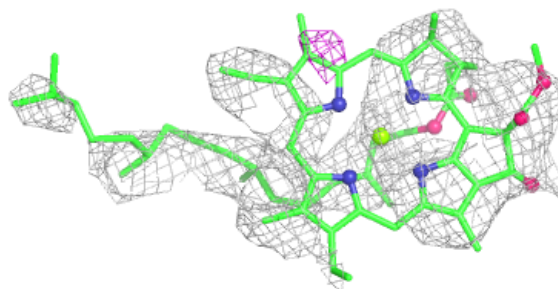
Electron density around CLA A 816:

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

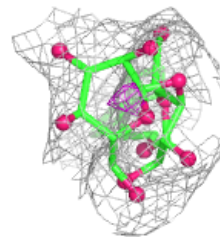
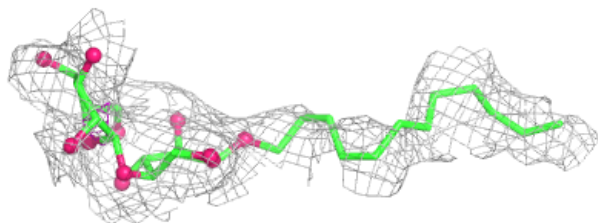
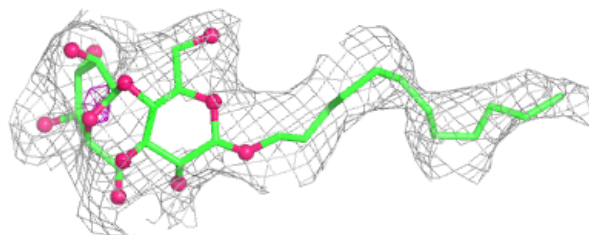


Electron density around CLA B 803:

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

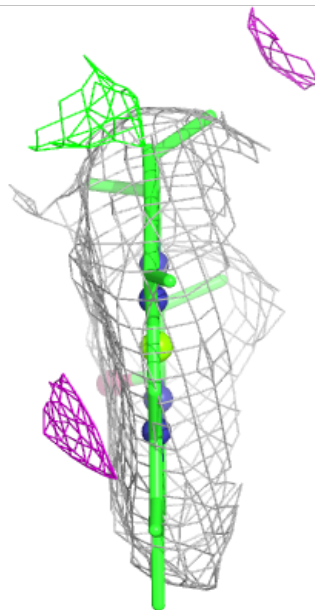
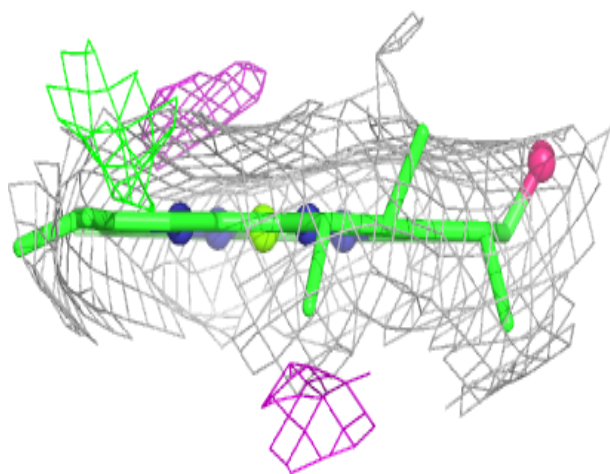
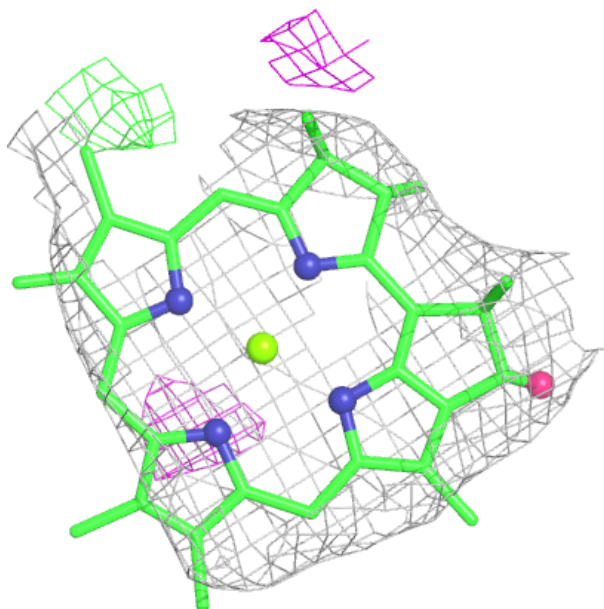
**Electron density around LMU 1 219:**

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



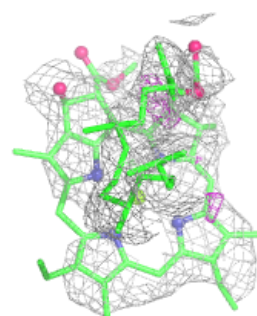
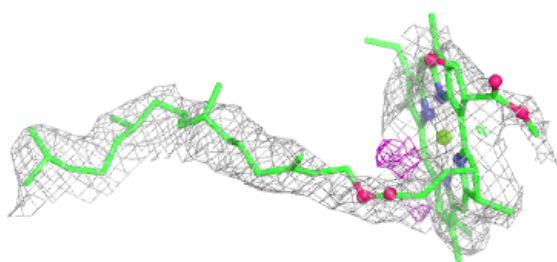
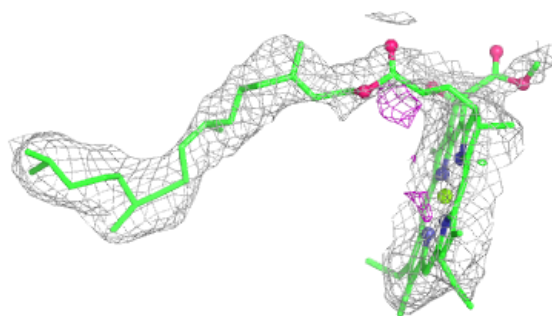
Electron density around CLA F 204:

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

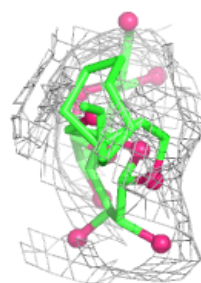
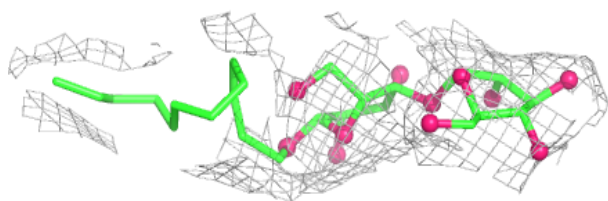
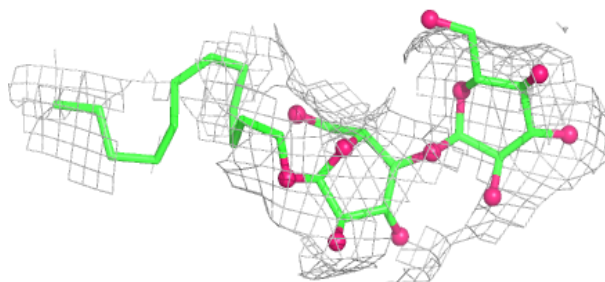


Electron density around CLA A 828:

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

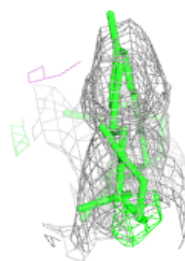
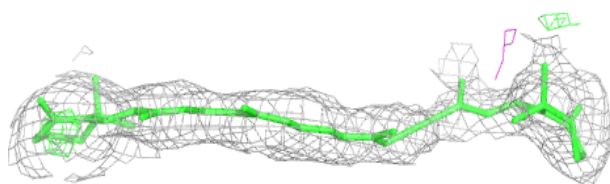
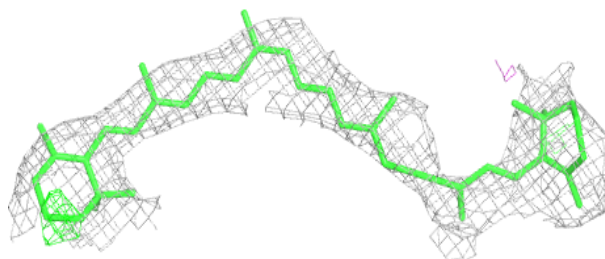
**Electron density around LMU A 854:**

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

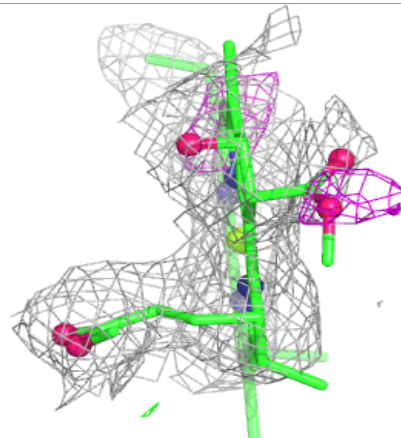
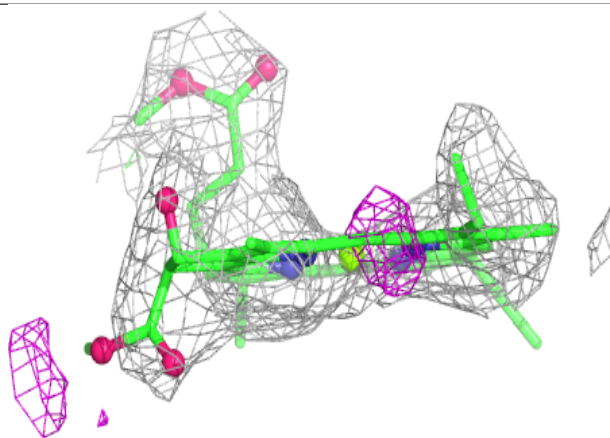
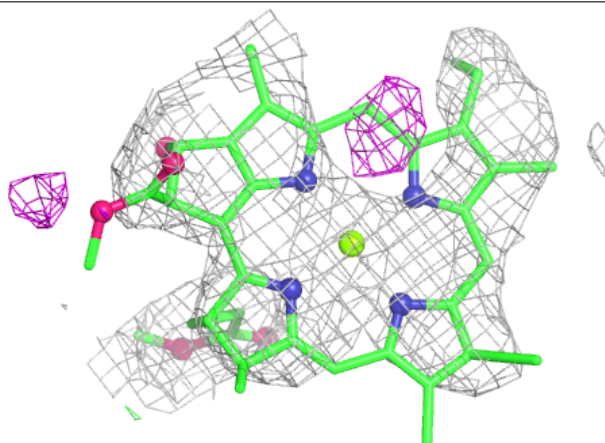


Electron density around BCR A 847:

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

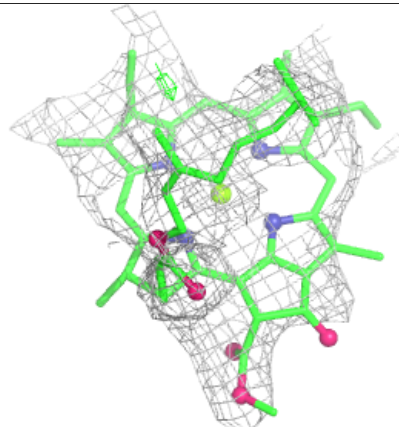
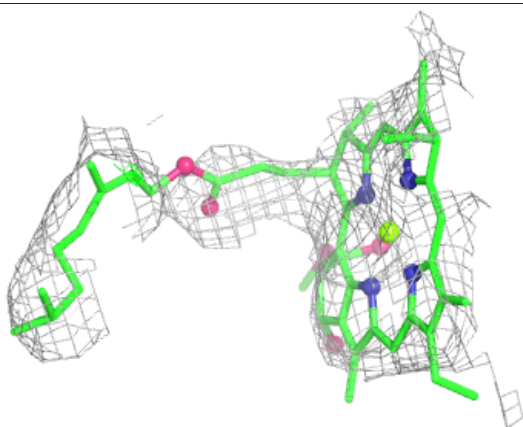
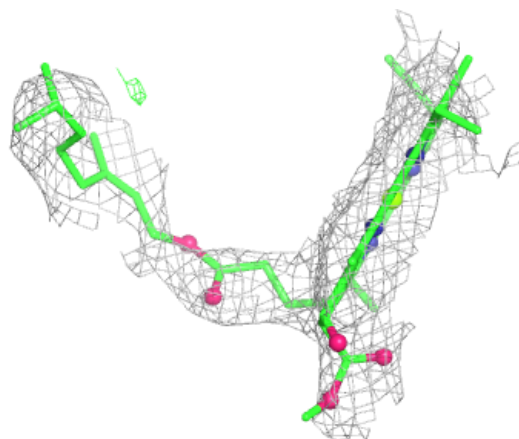
**Electron density around CLA A 807:**

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

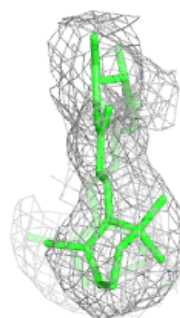
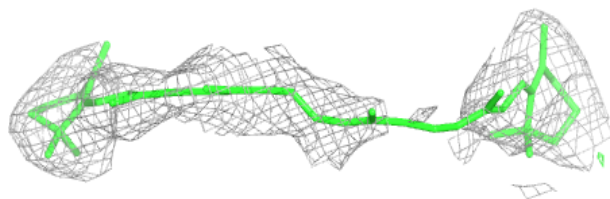
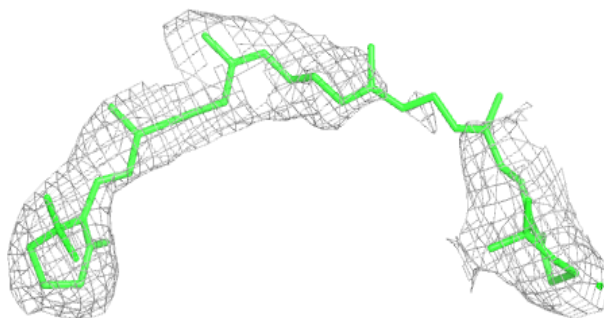


Electron density around CLA L 203:

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

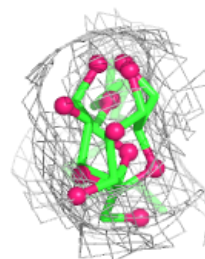
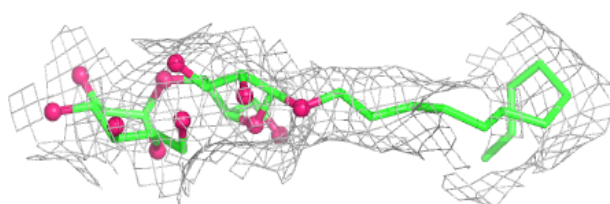
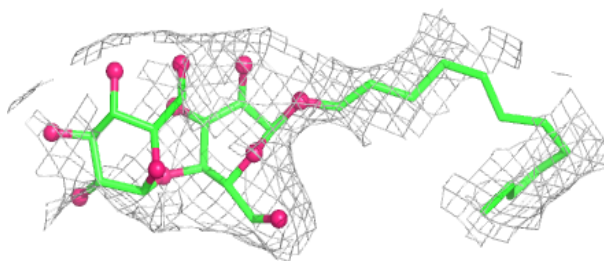
**Electron density around BCR F 203:**

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

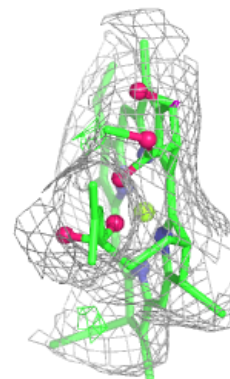
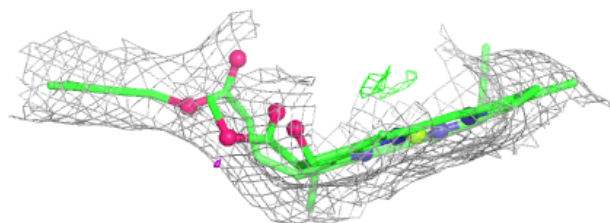
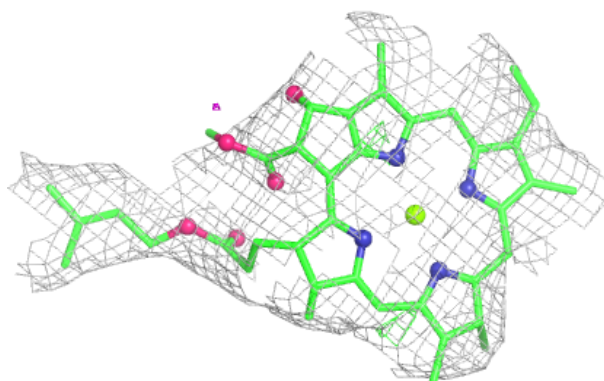


Electron density around LMU B 847:

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

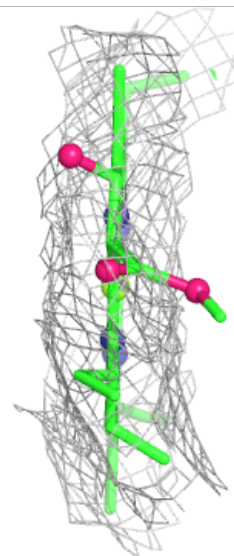
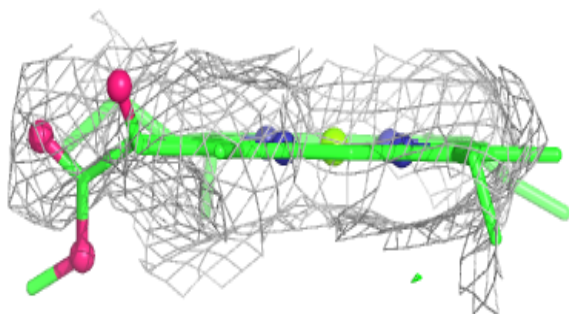
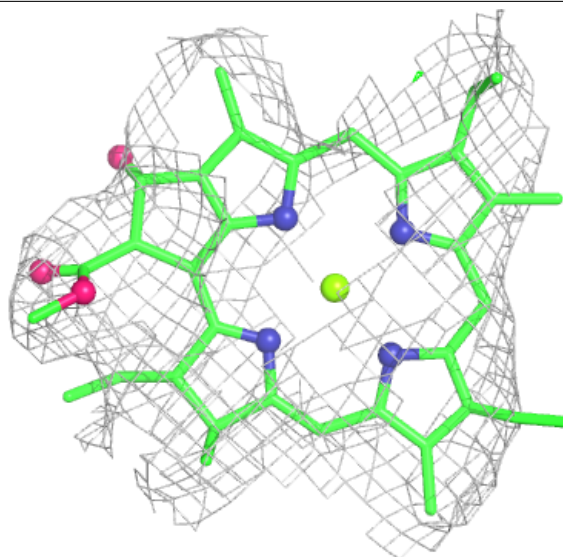
**Electron density around CLA L 207:**

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



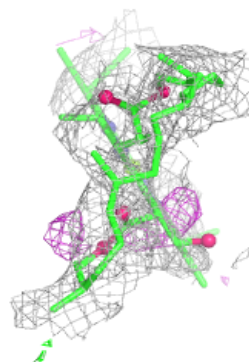
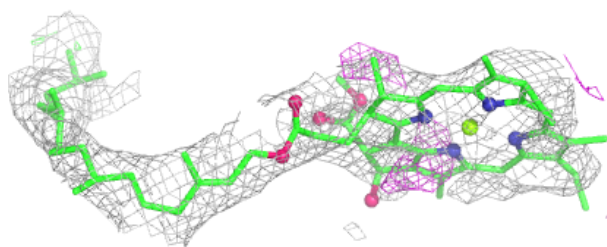
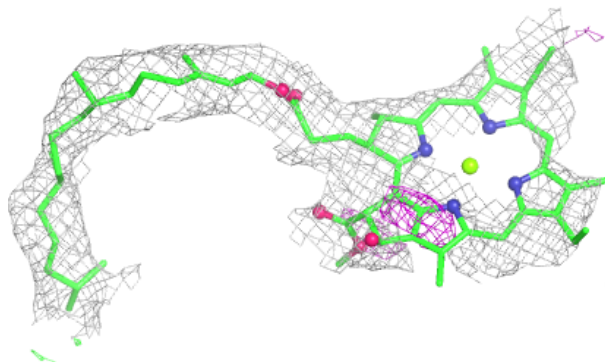
Electron density around CLA A 821:

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



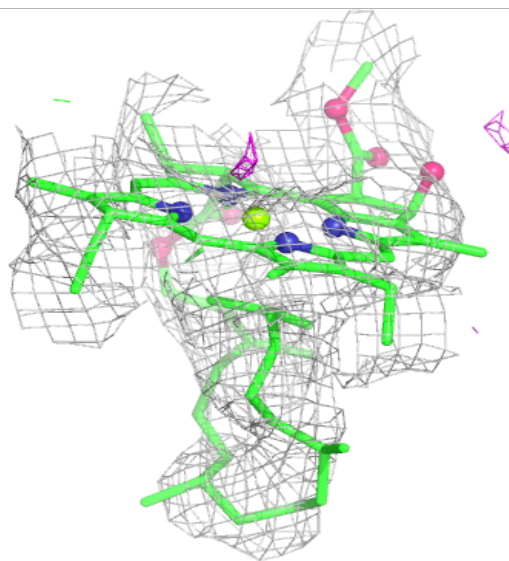
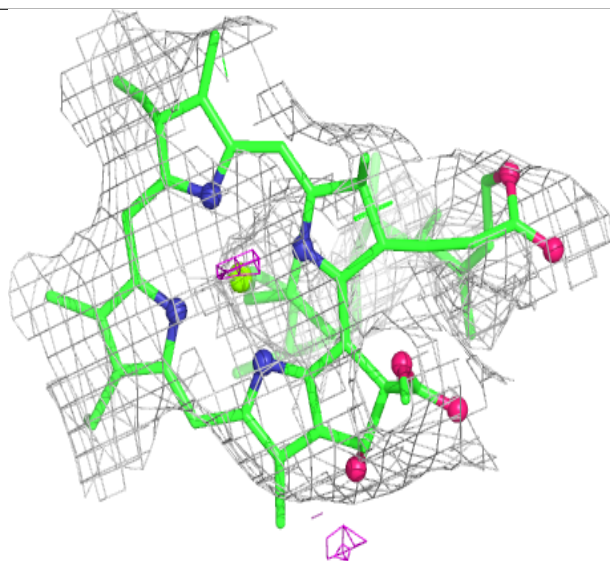
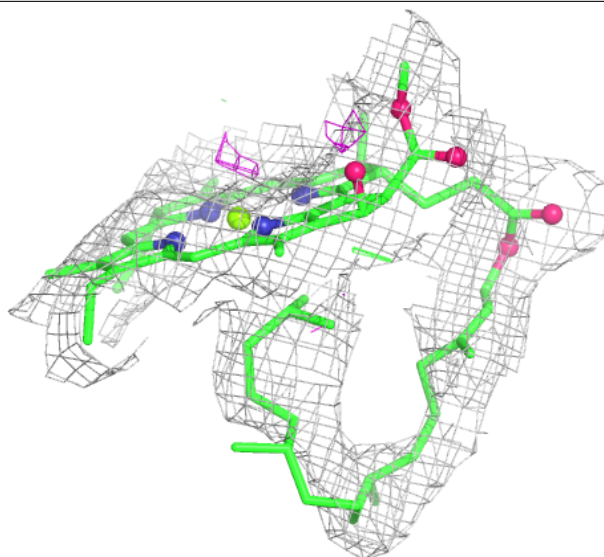
Electron density around CLA B 824:

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



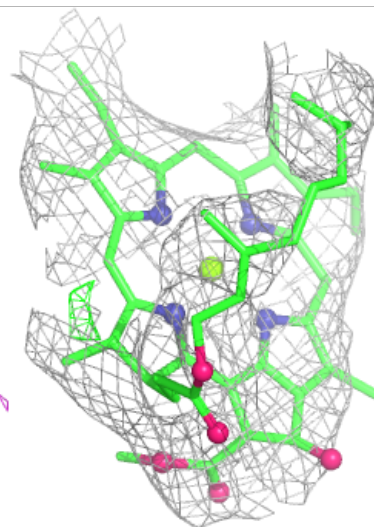
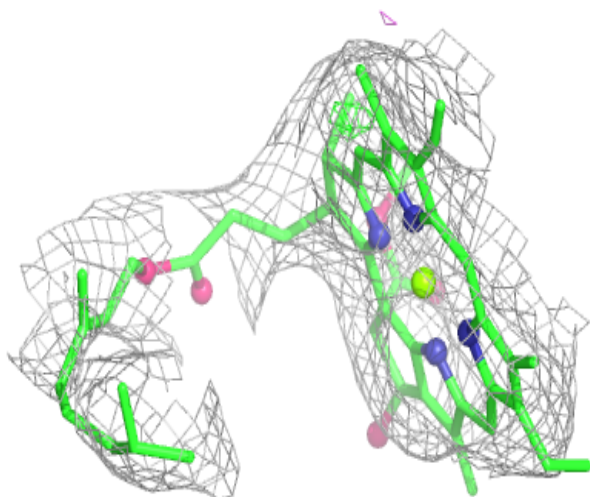
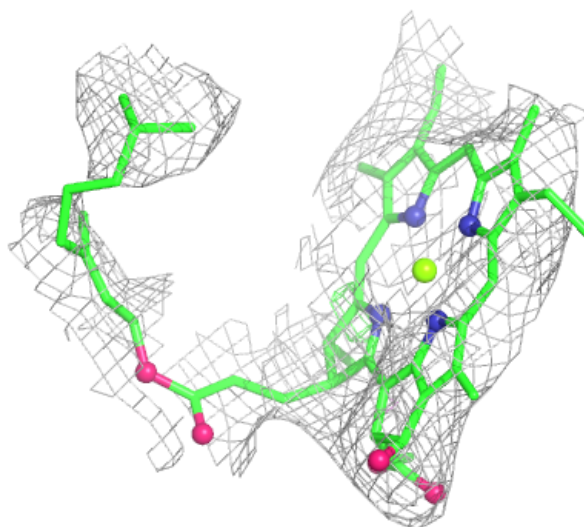
Electron density around CLA 2 315:

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



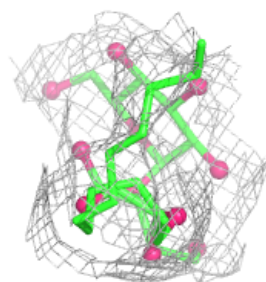
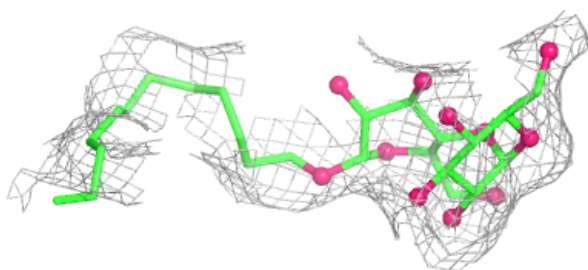
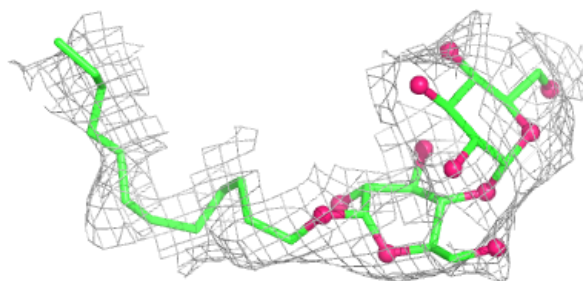
Electron density around CLA A 804:

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

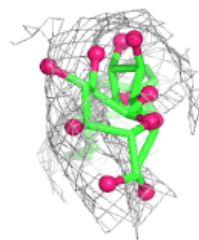
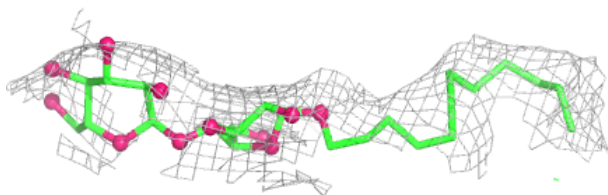
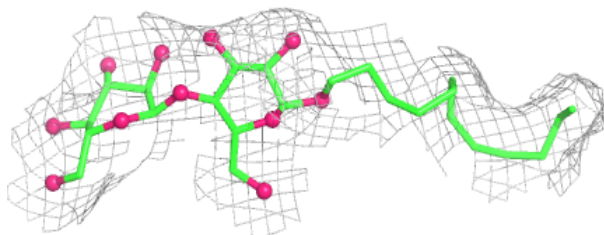


Electron density around LMU 2 318:

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

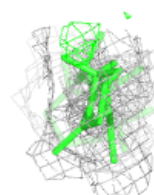
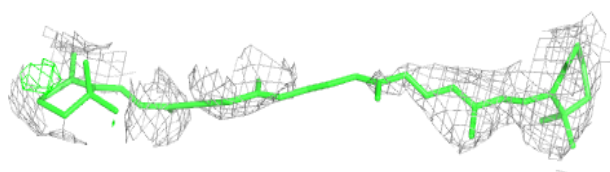
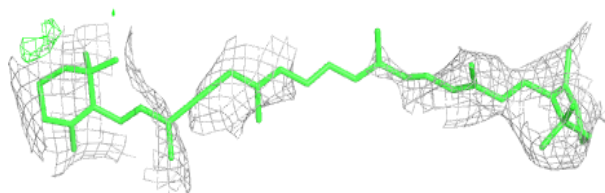
**Electron density around LMU 3 321:**

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

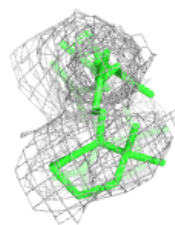
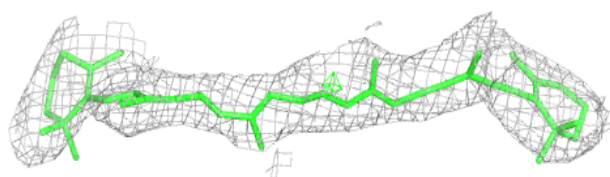
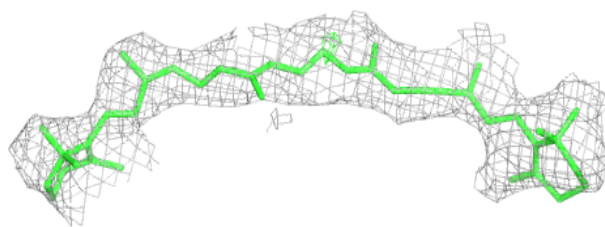


Electron density around BCR A 844:

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

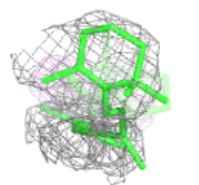
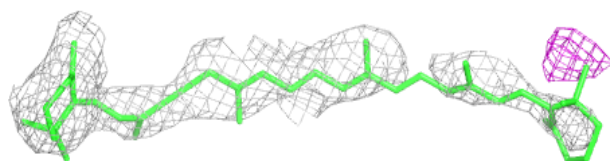
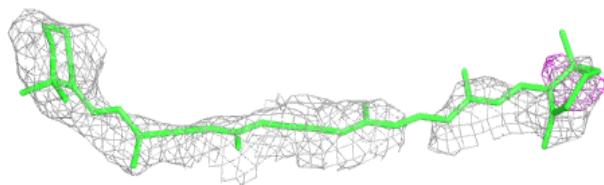
**Electron density around BCR B 852:**

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



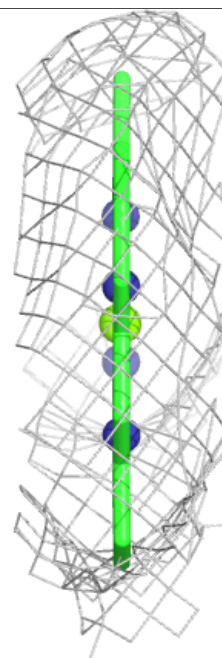
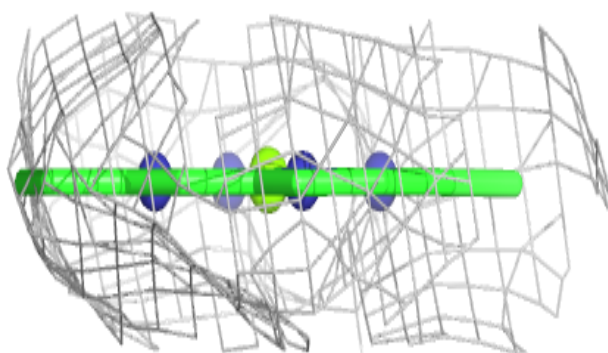
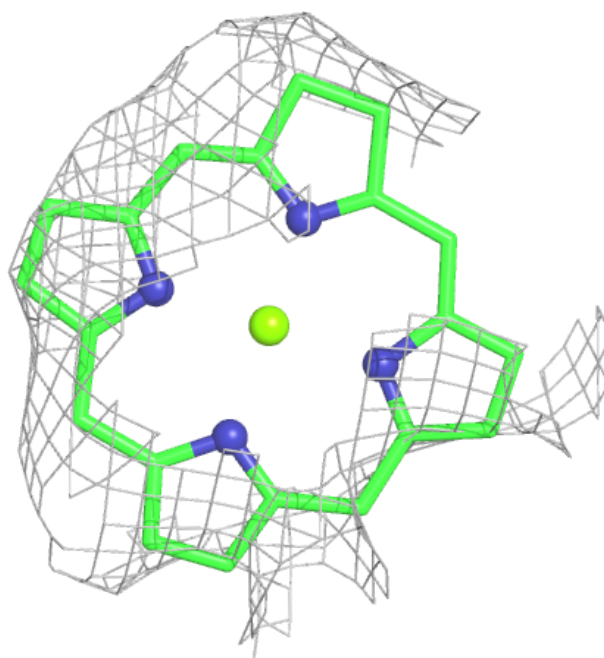
Electron density around BCR F 202:

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



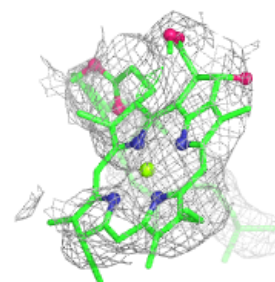
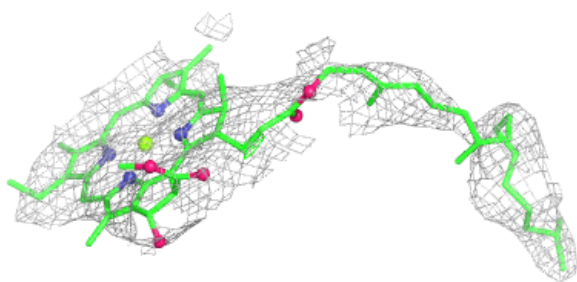
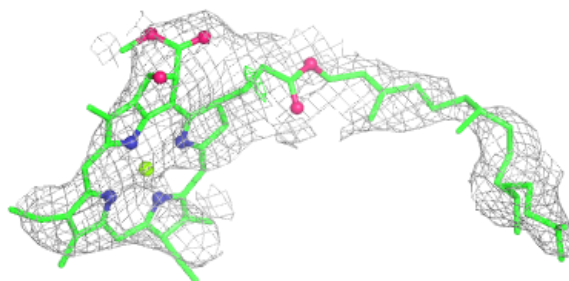
Electron density around CLA 3 312:

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

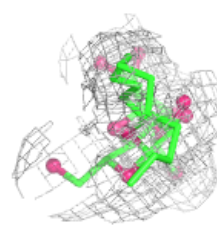
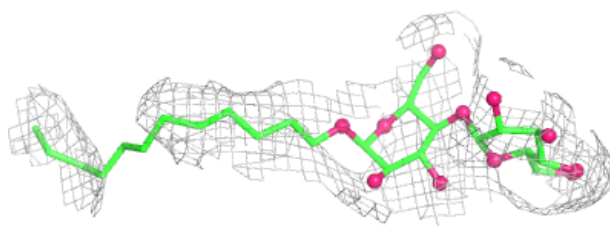
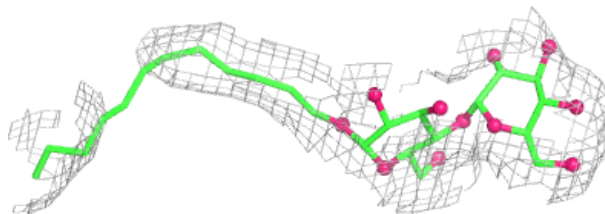


Electron density around CLA A 851:

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

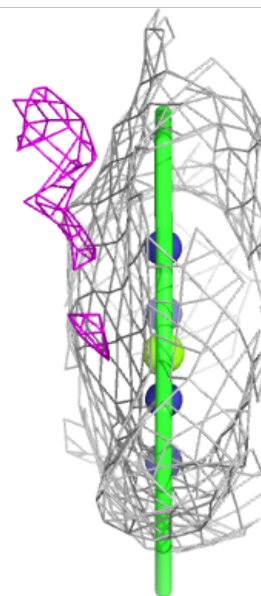
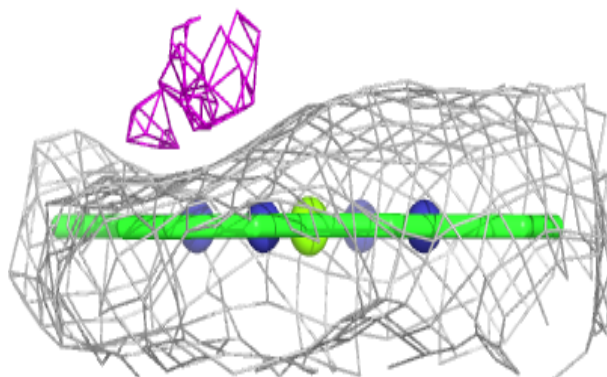
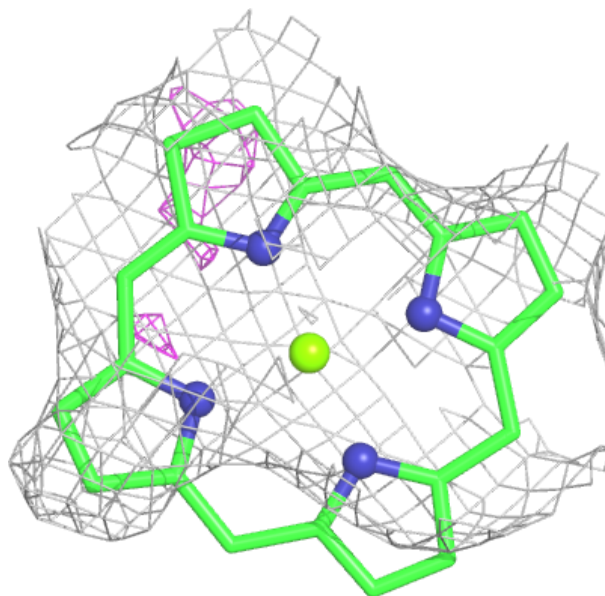
**Electron density around LMU B 802:**

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



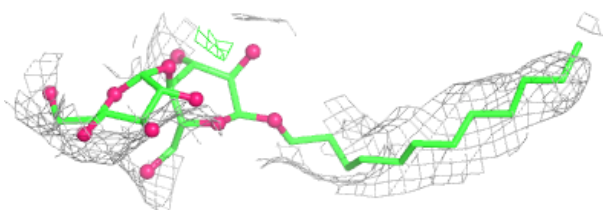
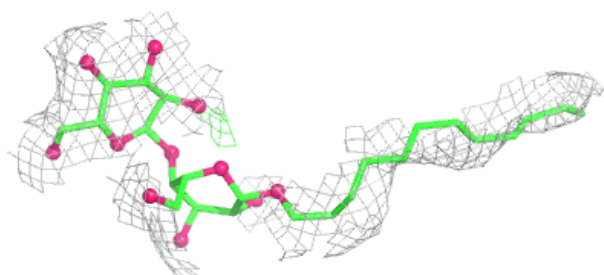
Electron density around CLA A 802:

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

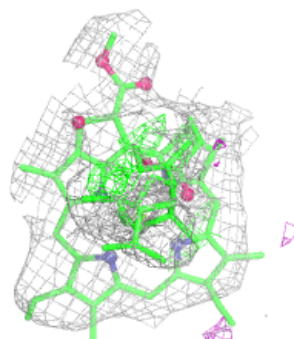
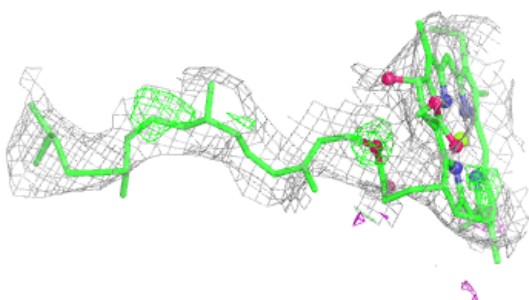
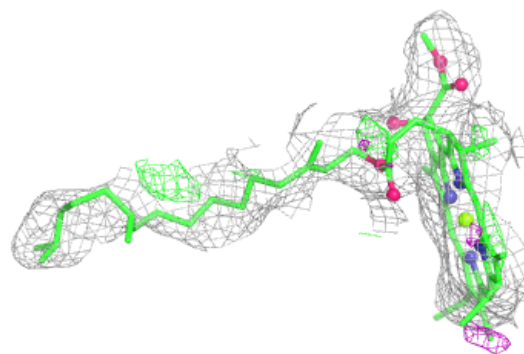


Electron density around LMU R 105:

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

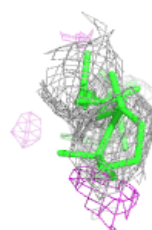
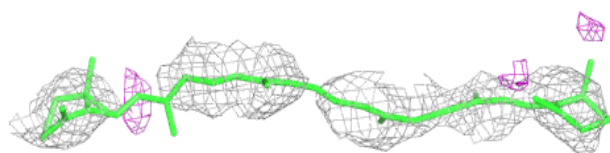
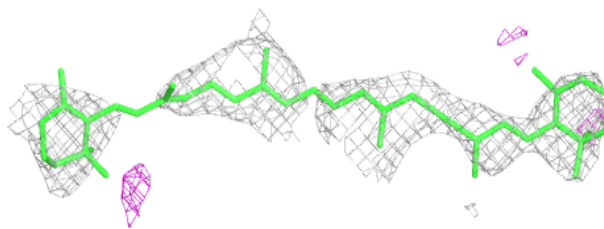
**Electron density around CLA A 826:**

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

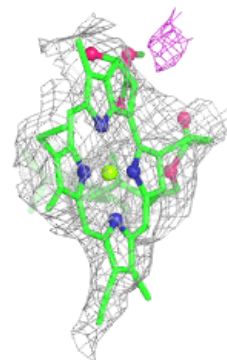
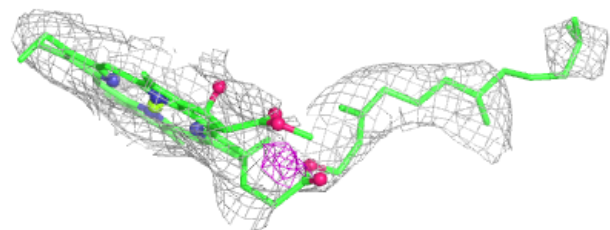
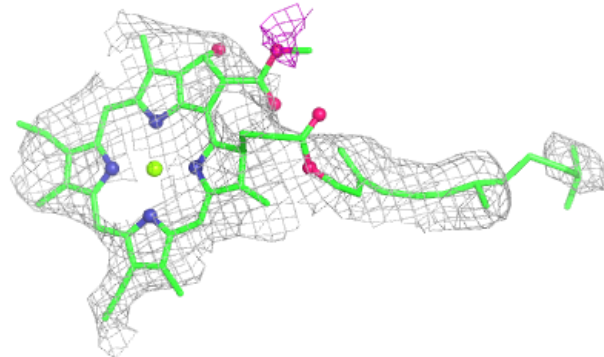


Electron density around BCR B 845:

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

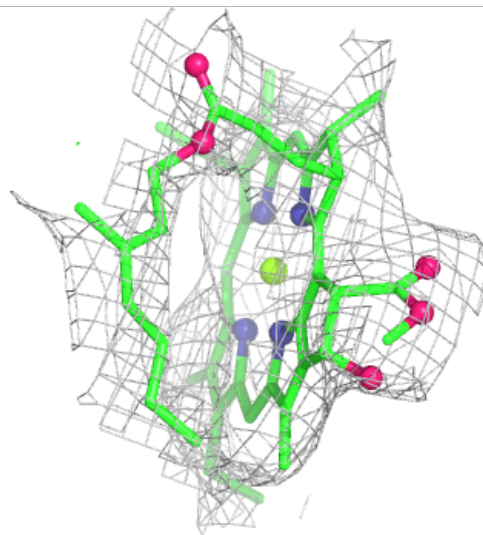
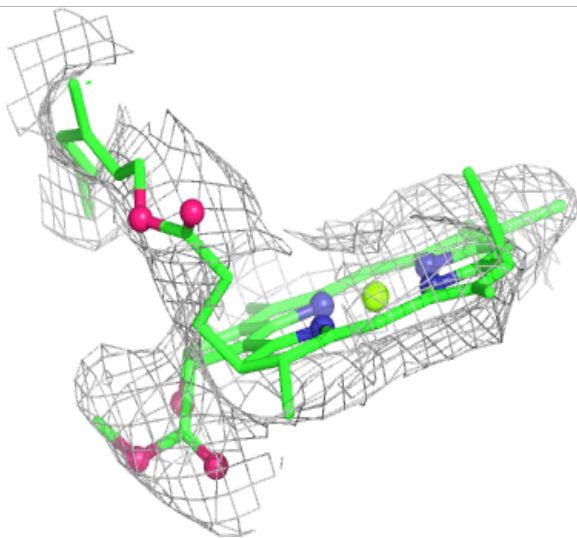
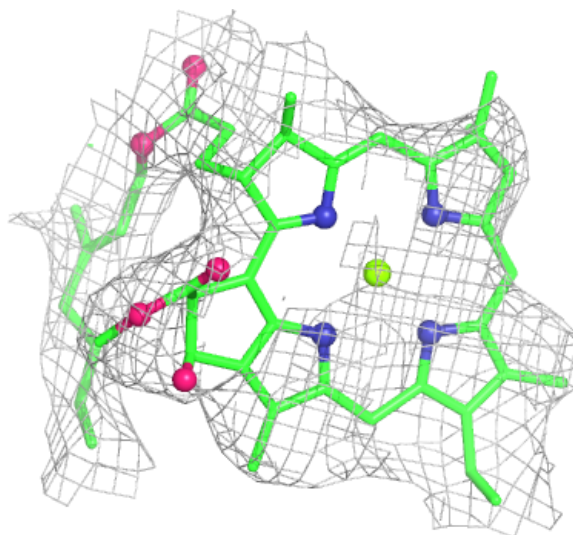
**Electron density around CLA H 109:**

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



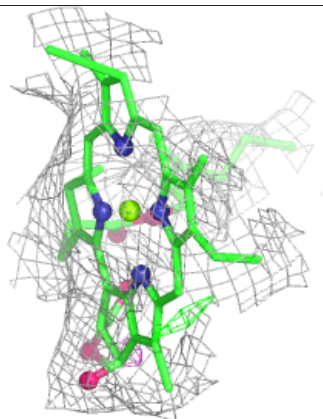
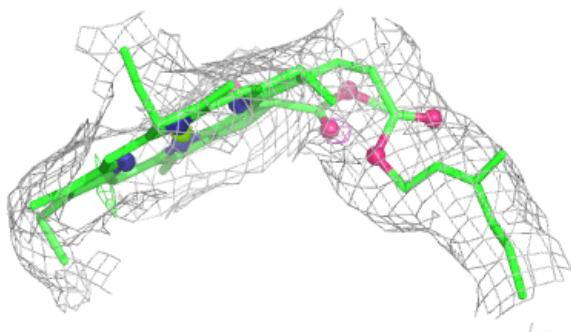
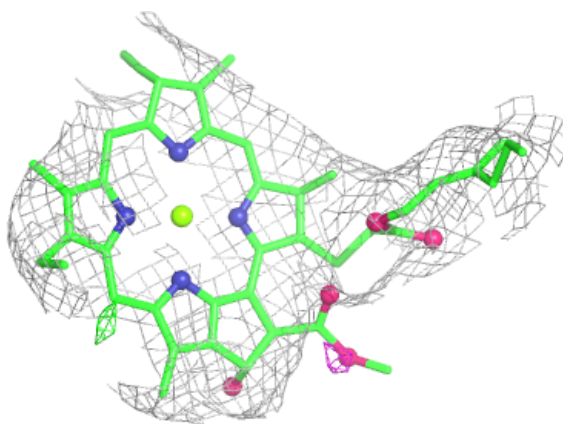
Electron density around CLA F 206:

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



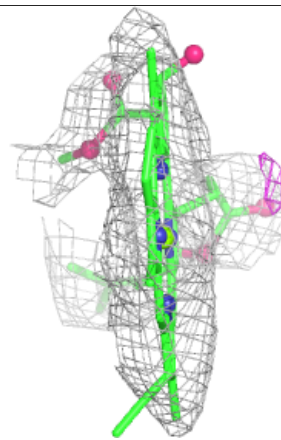
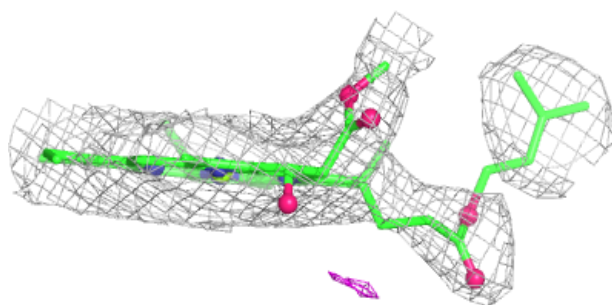
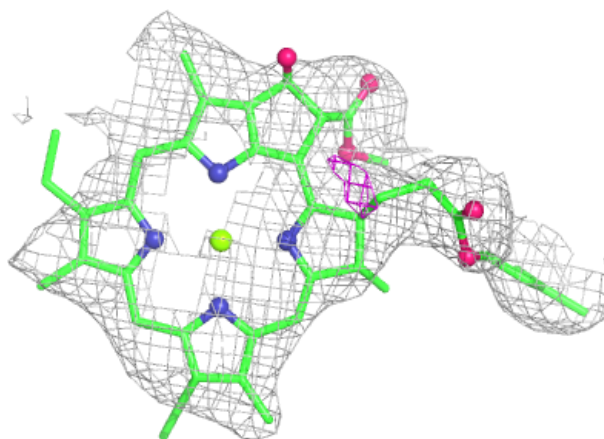
Electron density around CLA 4 307:

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



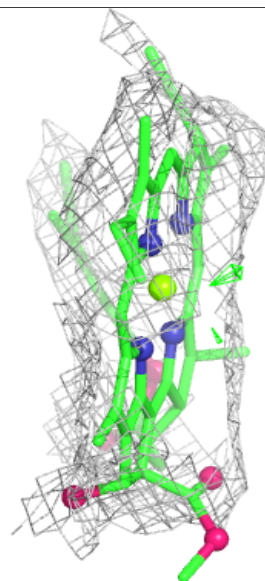
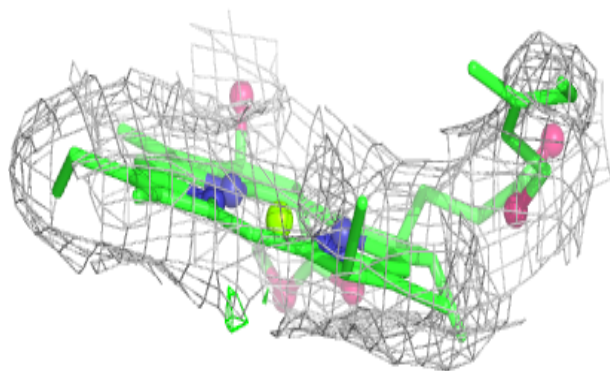
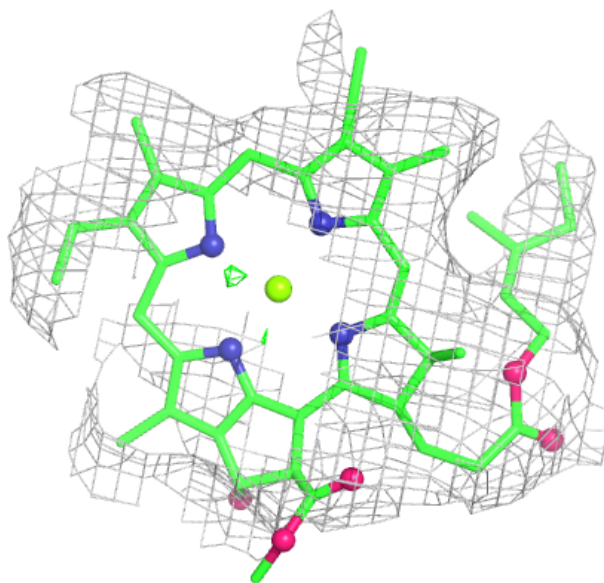
Electron density around CLA B 829:

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



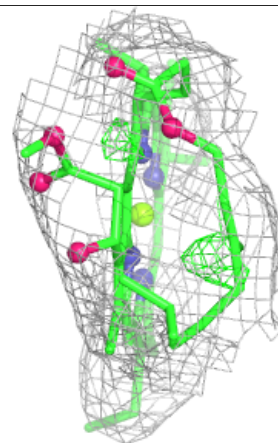
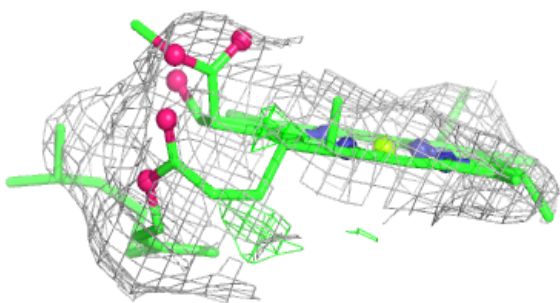
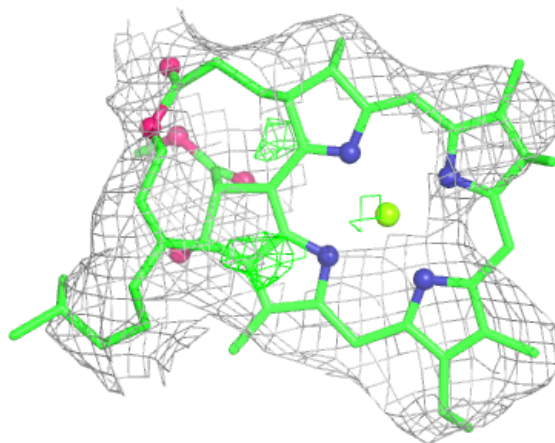
Electron density around CLA G 102:

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



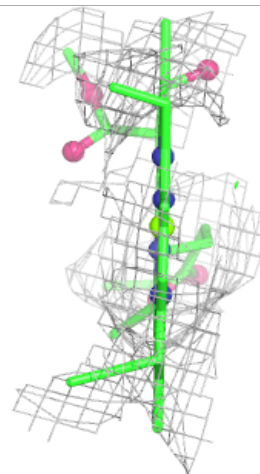
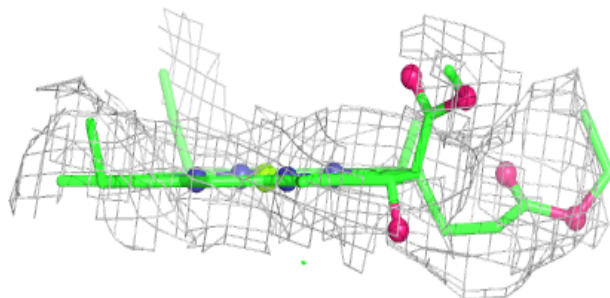
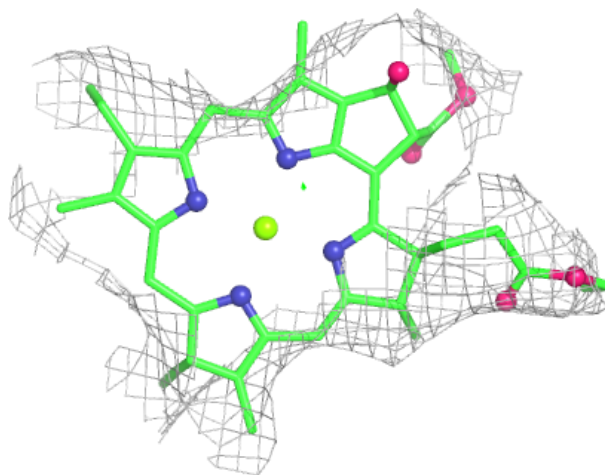
Electron density around CLA B 809:

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



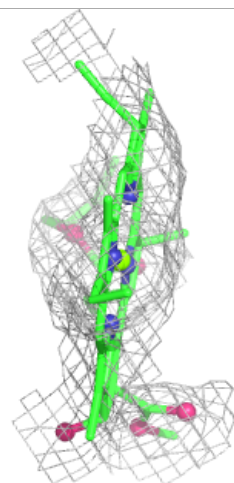
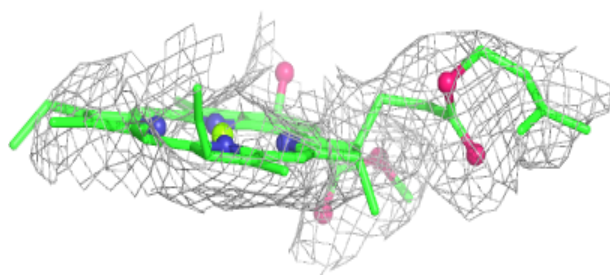
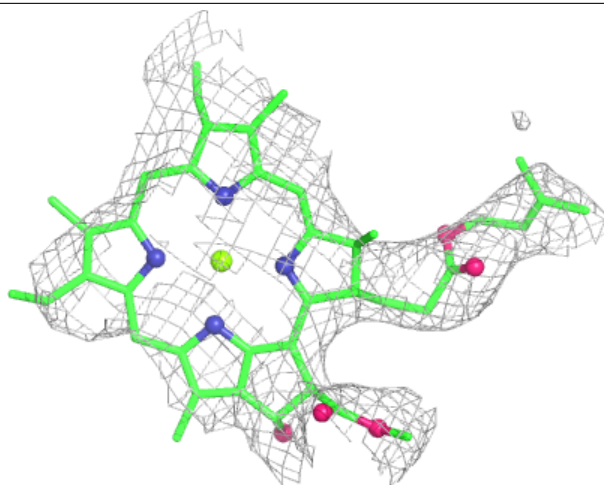
Electron density around CLA 1 203:

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



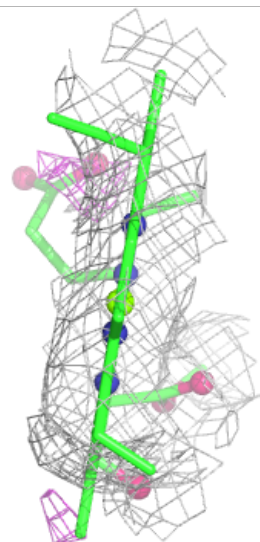
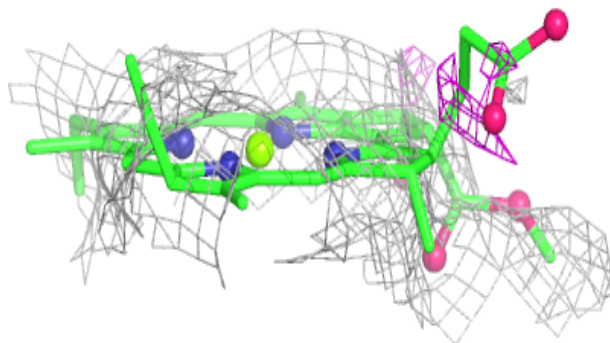
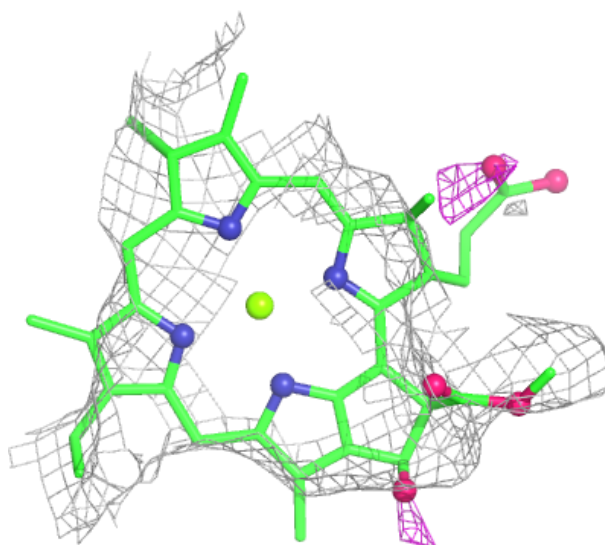
Electron density around CLA 2 305:

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



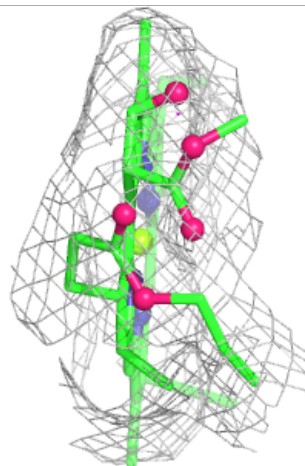
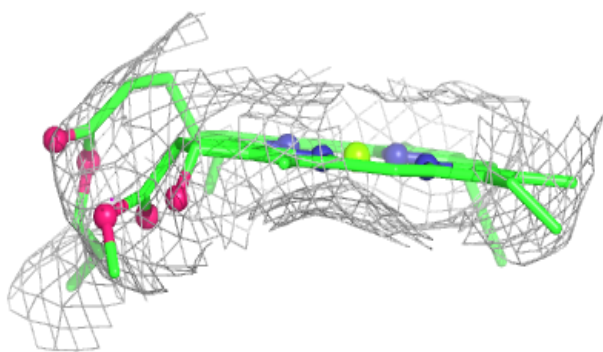
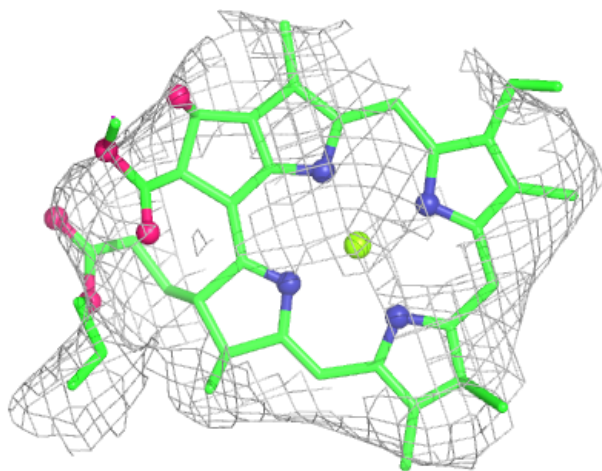
Electron density around CLA A 833:

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



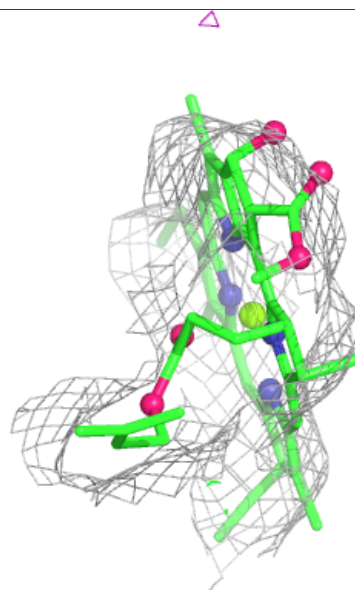
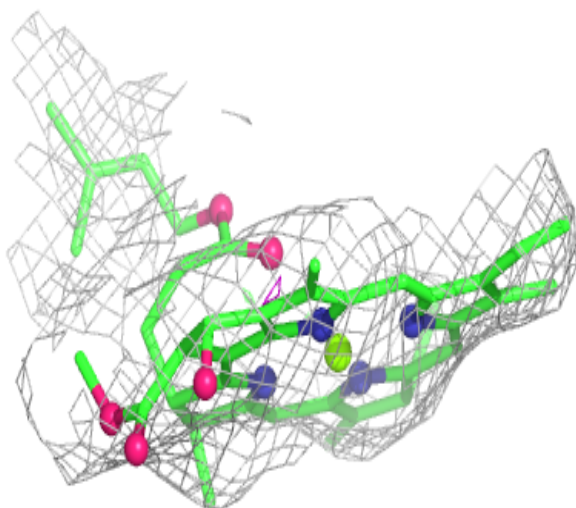
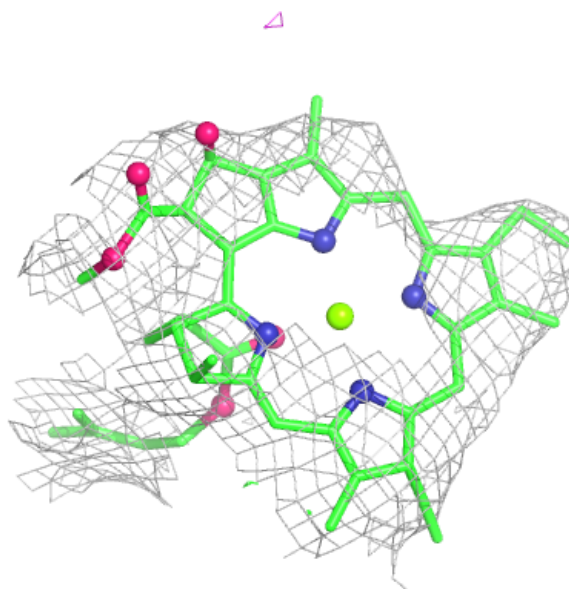
Electron density around CLA J 101:

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



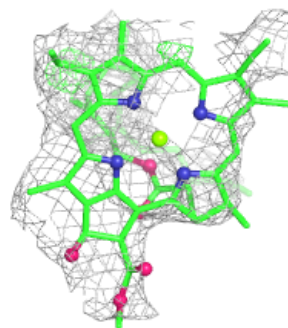
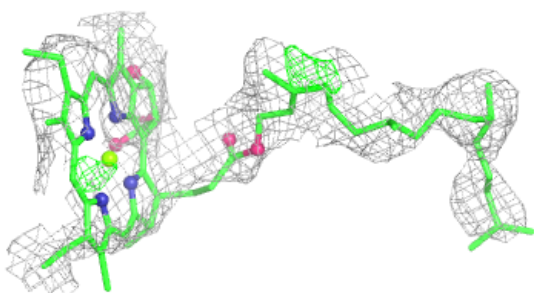
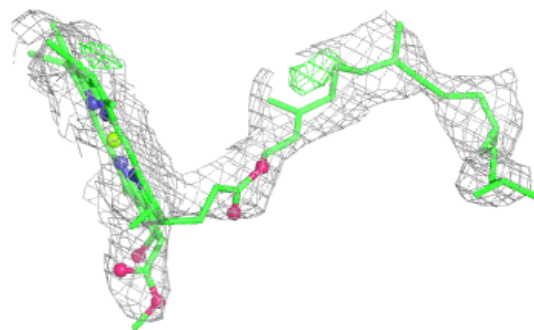
Electron density around CLA A 815:

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



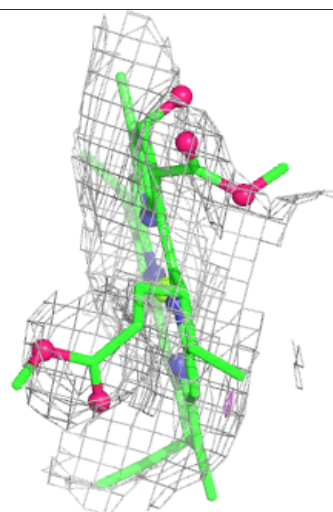
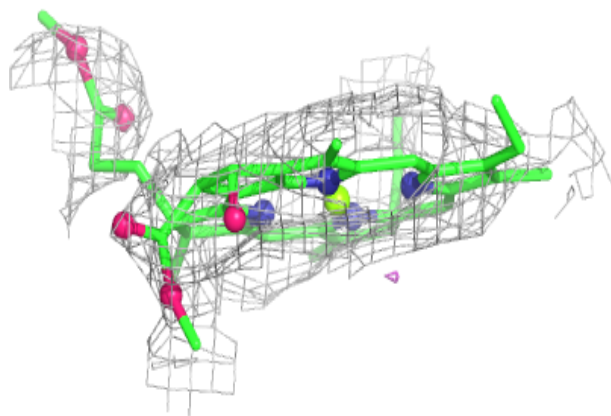
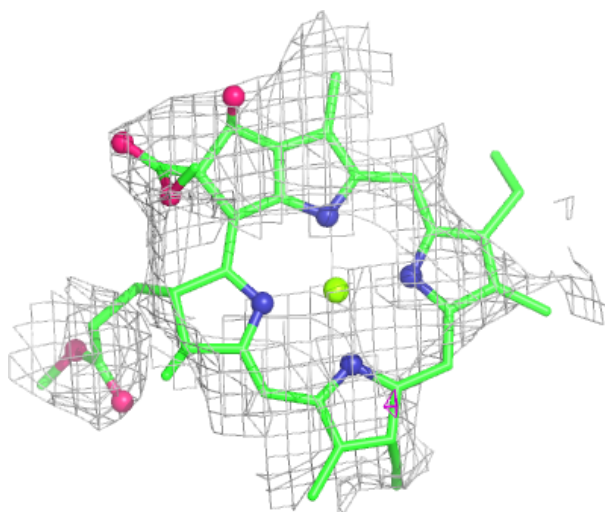
Electron density around CLA B 838:

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



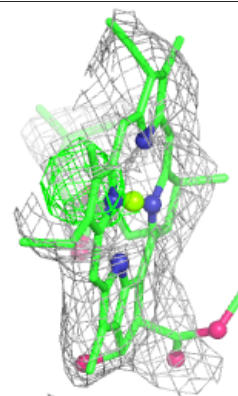
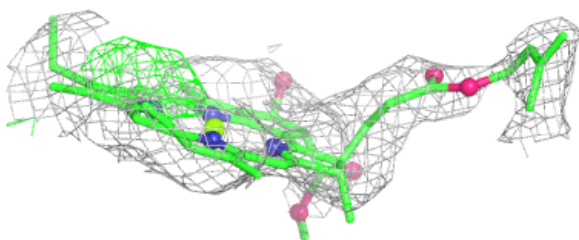
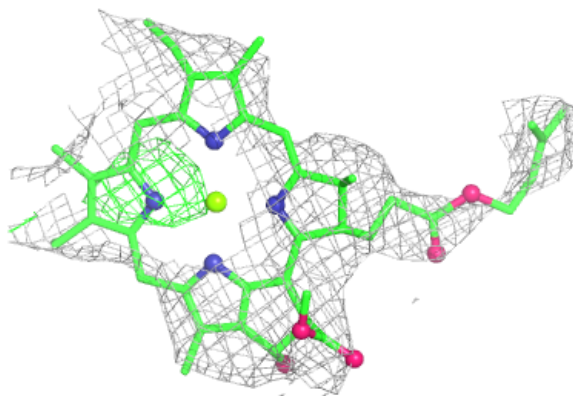
Electron density around CLA B 819:

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

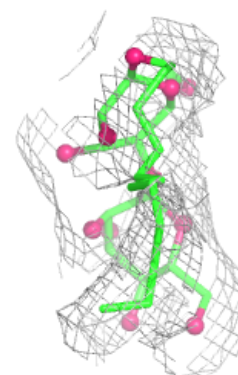
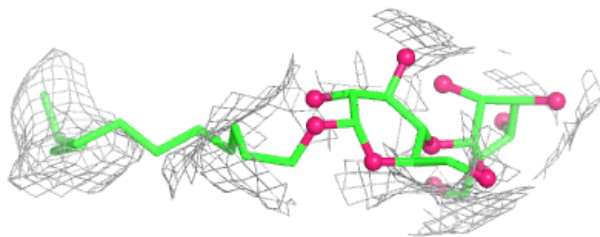
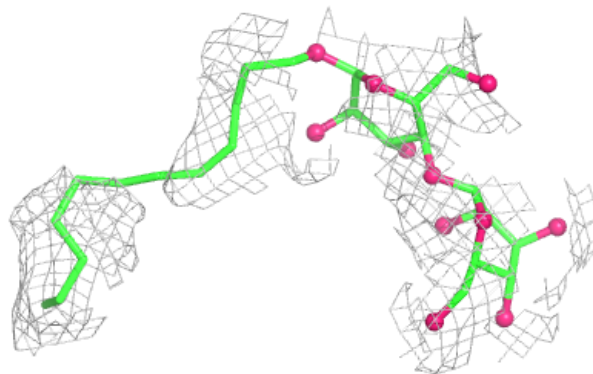


Electron density around CLA B 831:

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

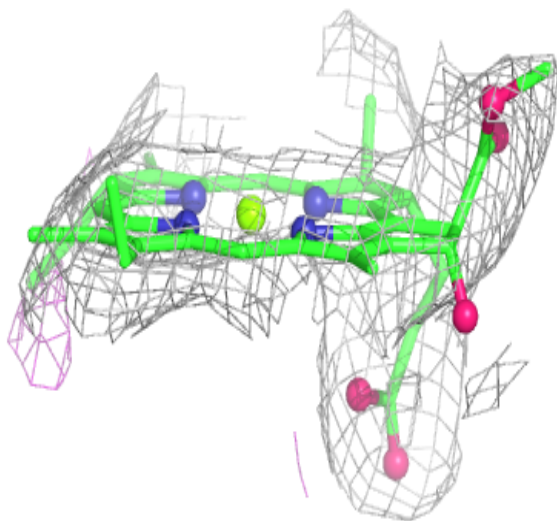
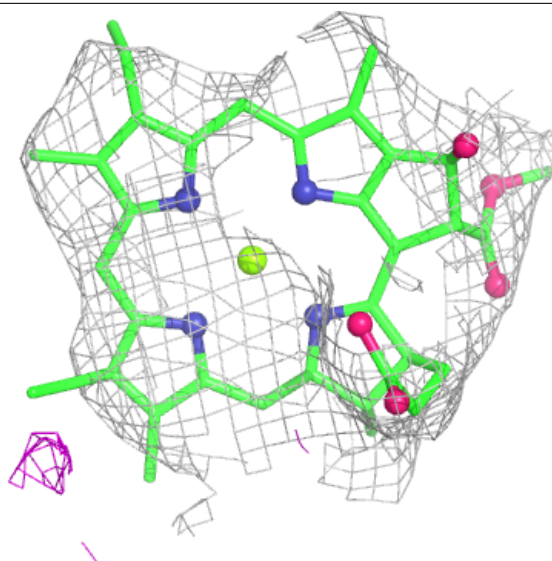
**Electron density around LMU 4 321:**

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



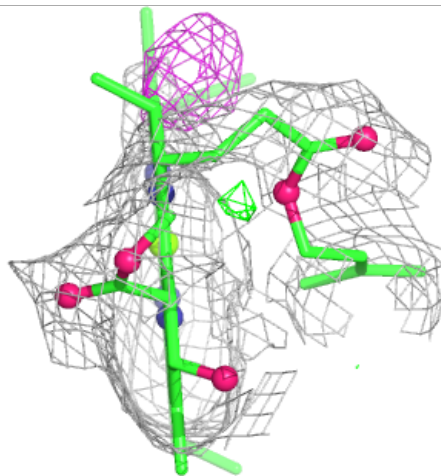
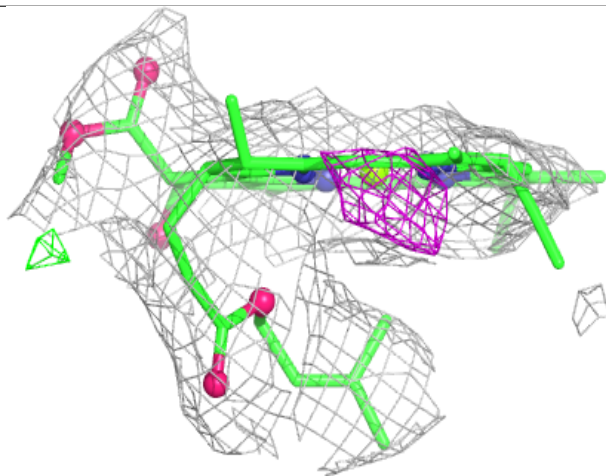
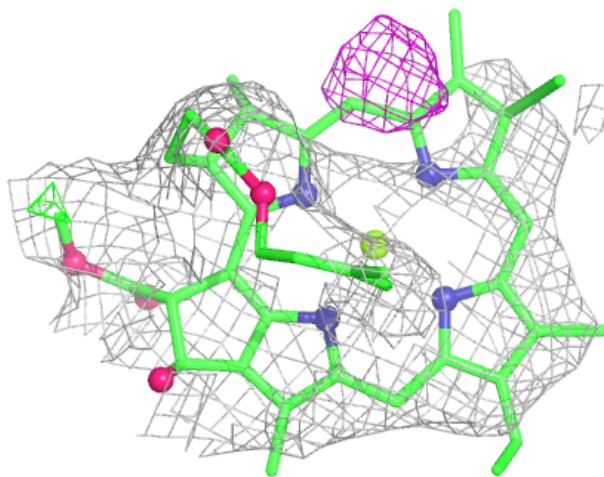
Electron density around CLA B 832:

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



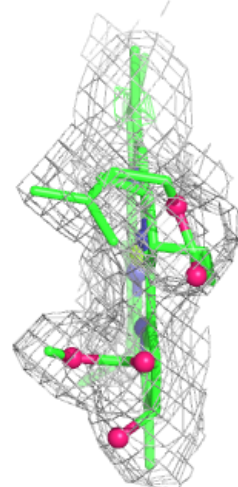
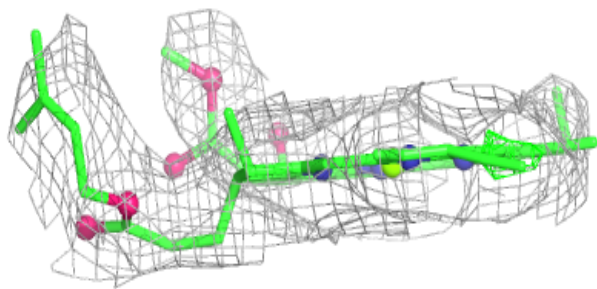
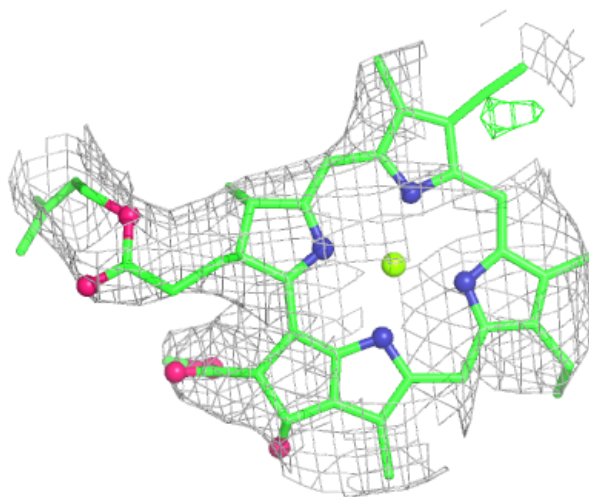
Electron density around CLA H 111:

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



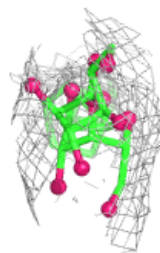
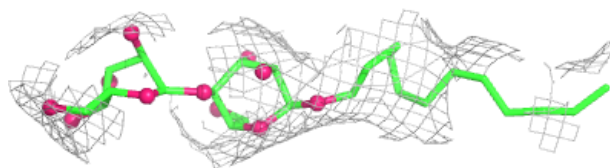
Electron density around CLA A 803:

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



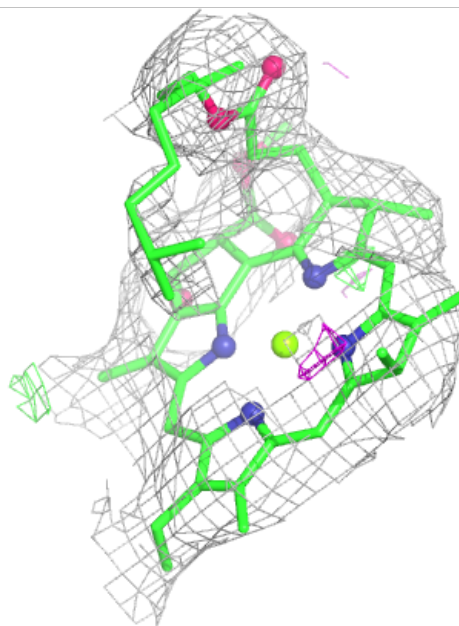
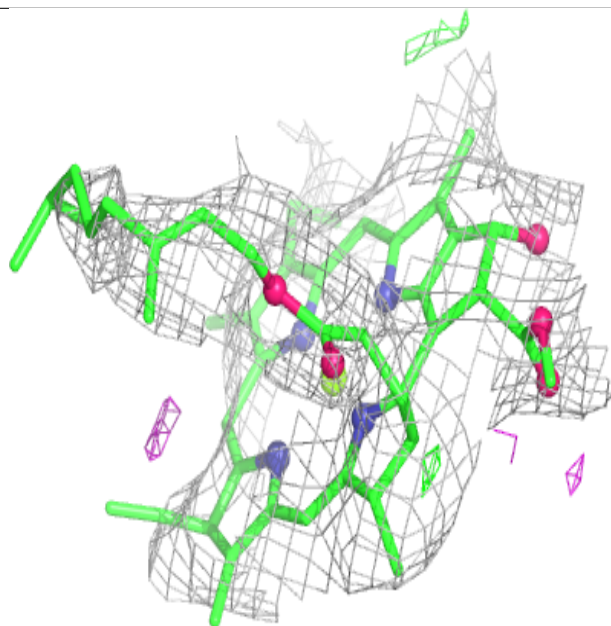
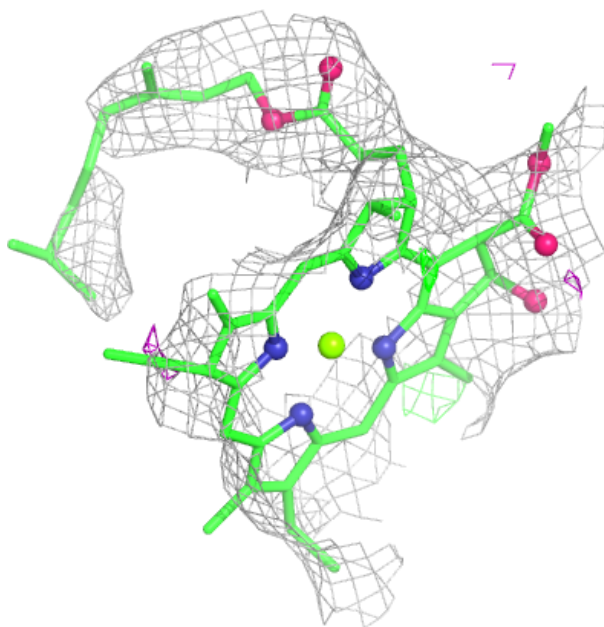
Electron density around LMU E 101:

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



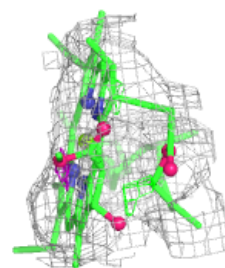
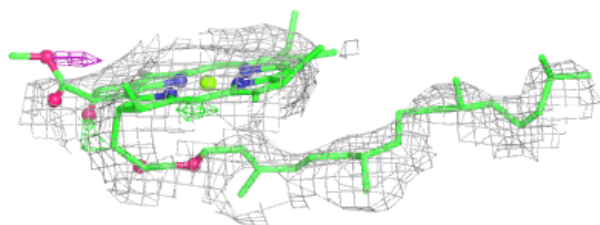
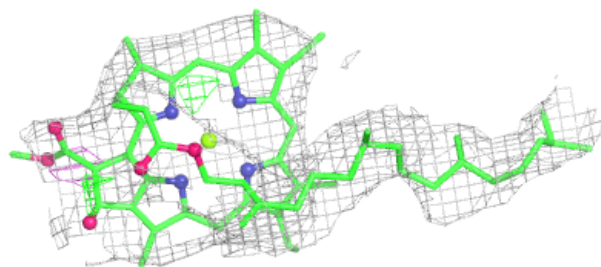
Electron density around CLA A 822:

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



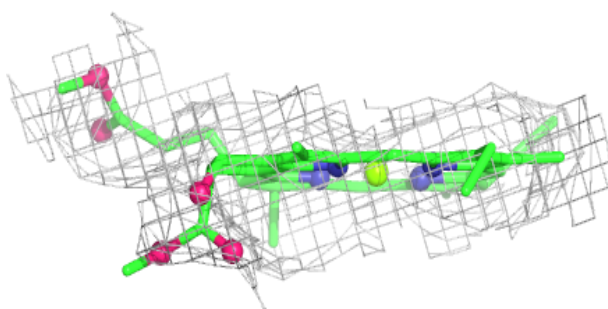
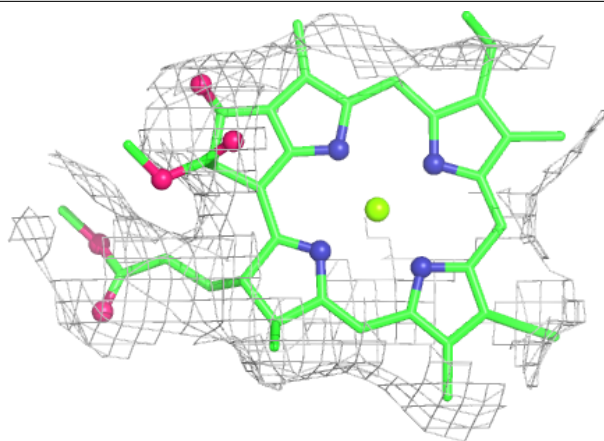
Electron density around CLA A 835:

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



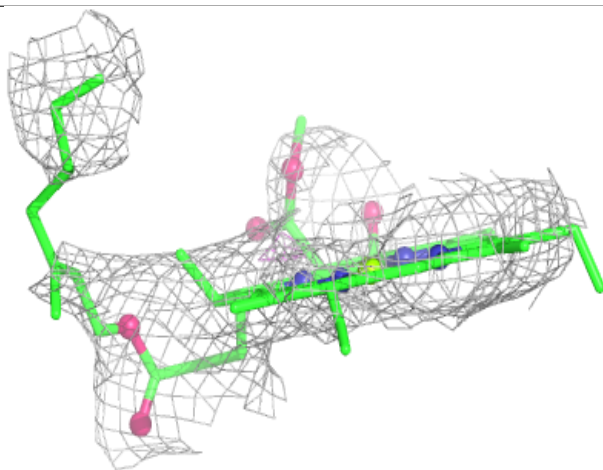
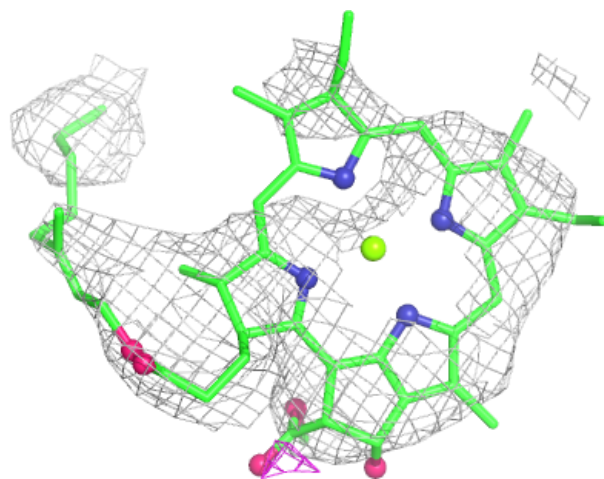
Electron density around CLA 4 316:

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



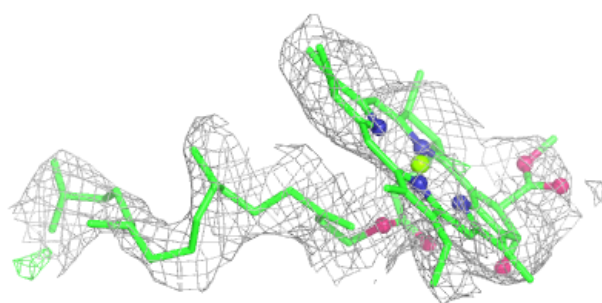
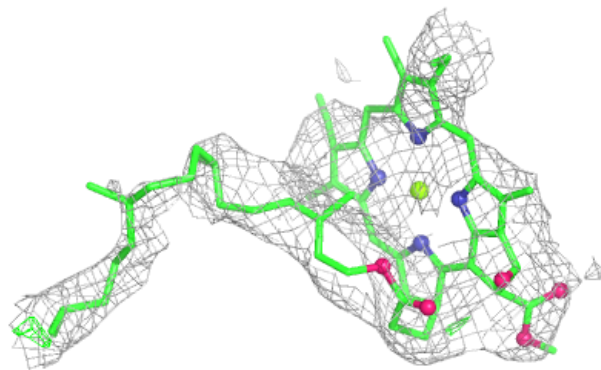
Electron density around CLA A 813:

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



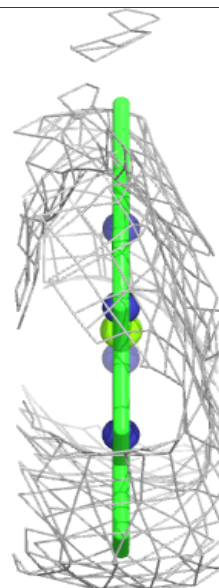
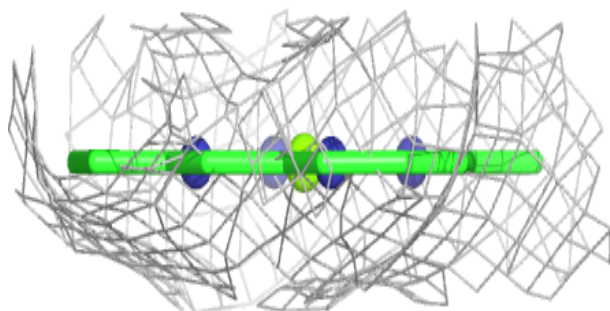
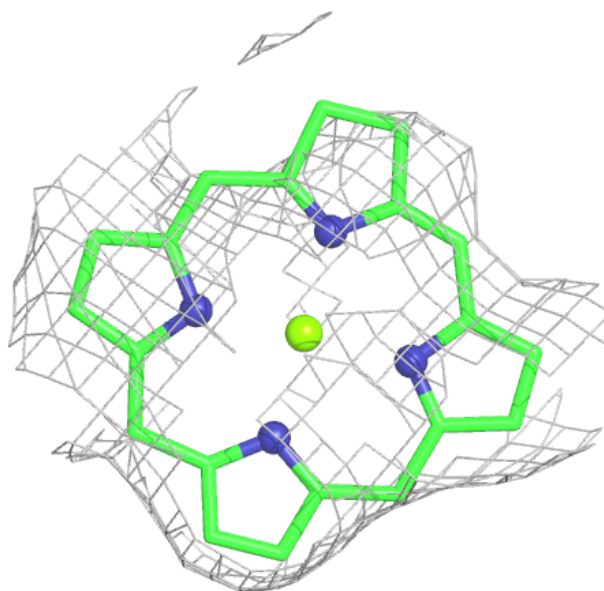
Electron density around CLA A 841:

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



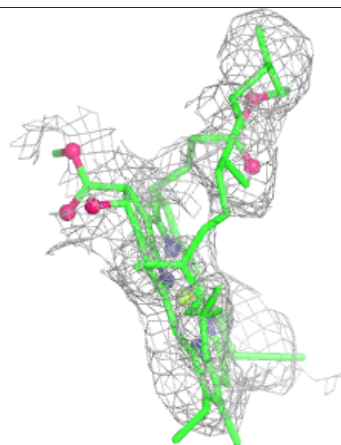
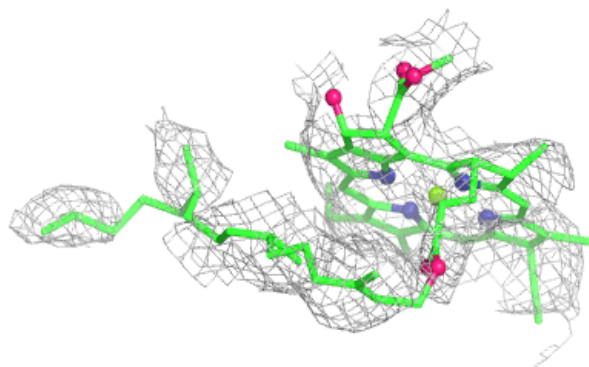
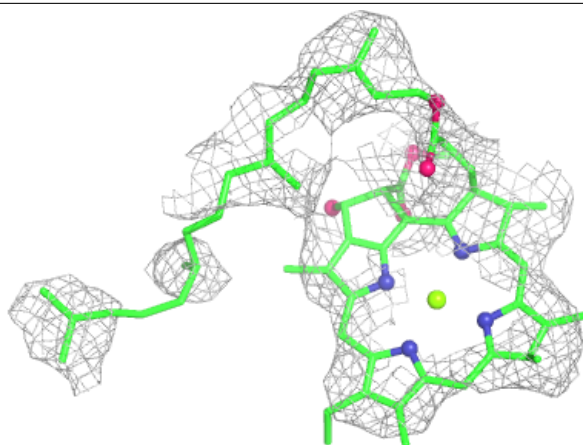
Electron density around CLA 4 309:

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



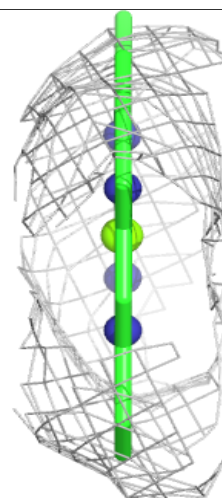
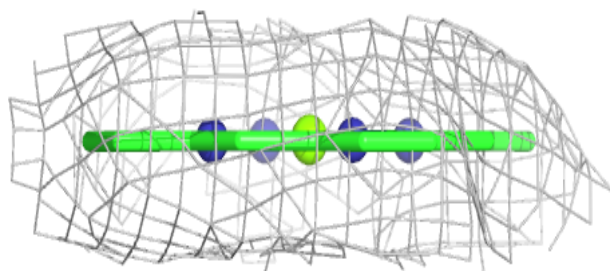
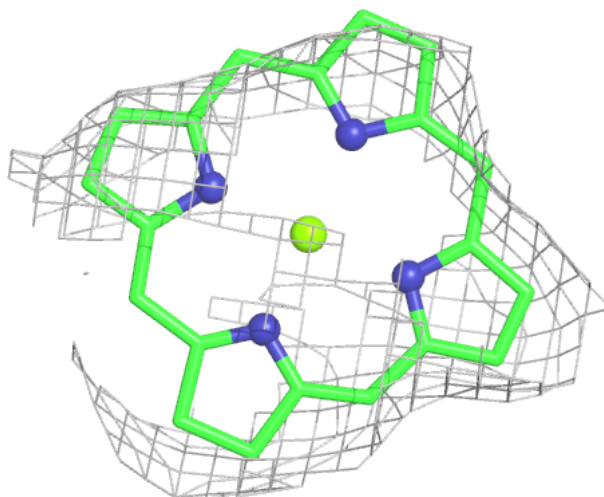
Electron density around CLA B 830:

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



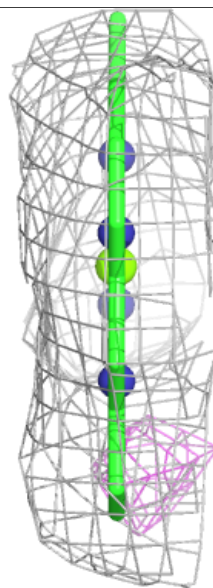
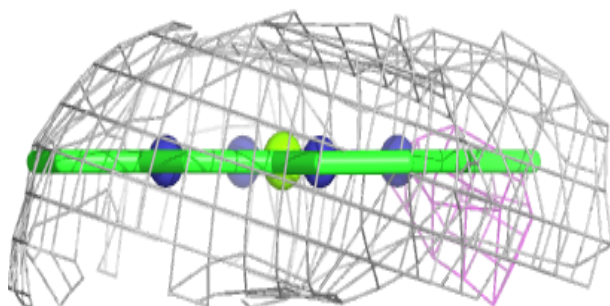
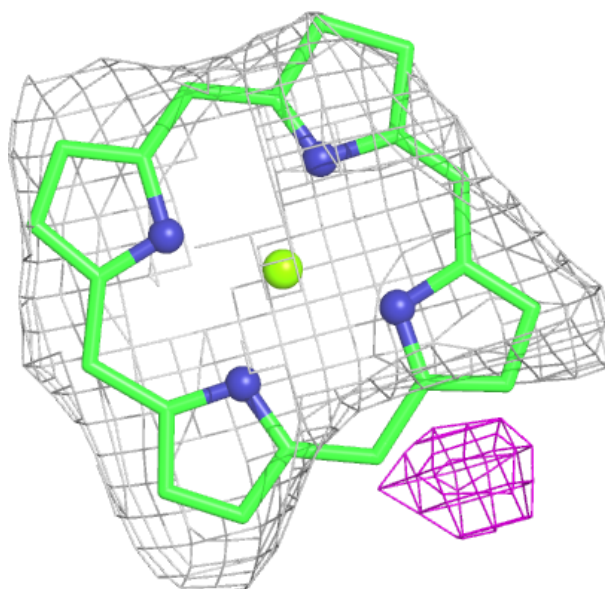
Electron density around CLA 3 303:

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



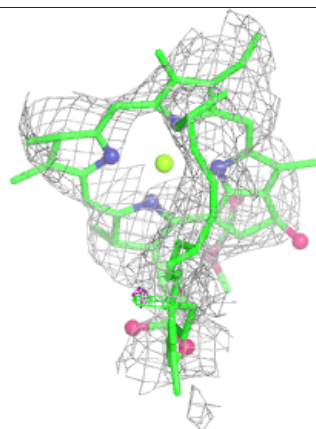
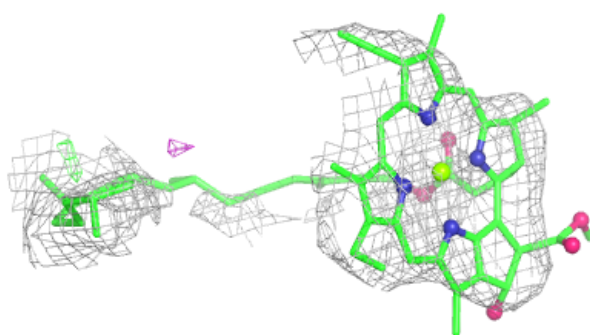
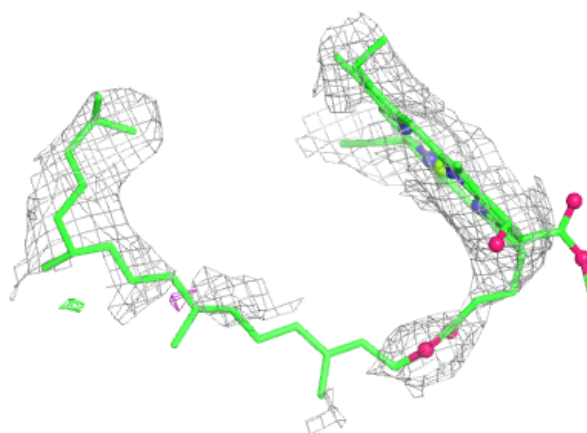
Electron density around CLA 3 315:

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

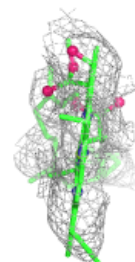
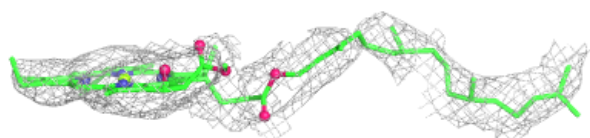
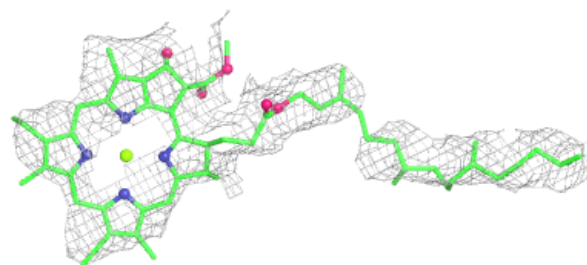


Electron density around CLA L 202:

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

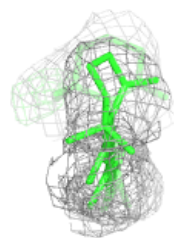
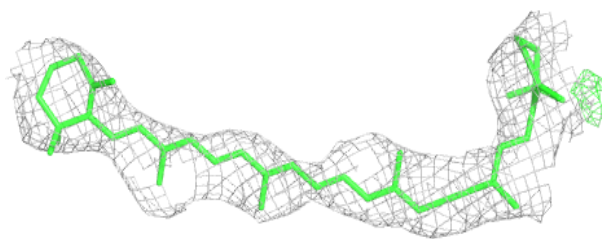
**Electron density around CLA A 830:**

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



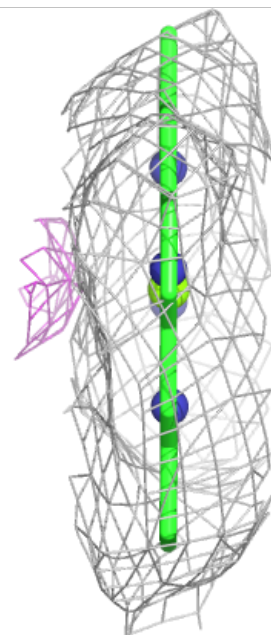
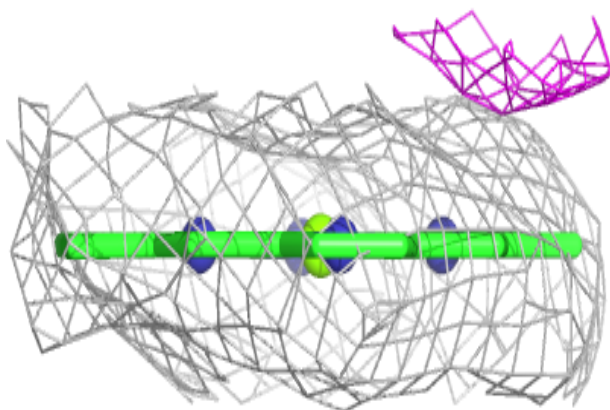
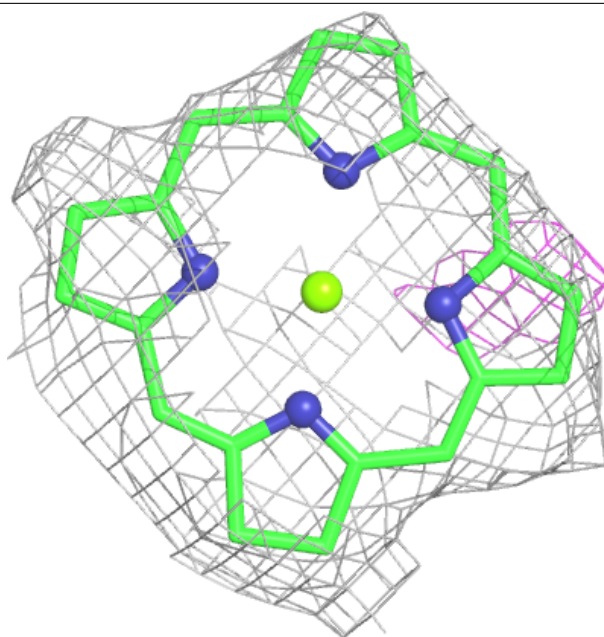
Electron density around BCR B 843:

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



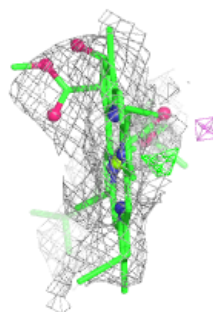
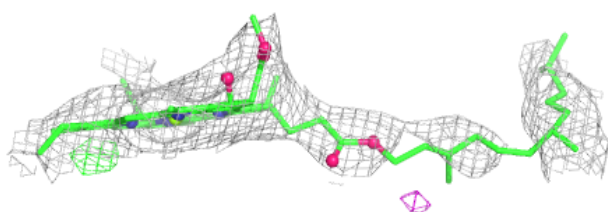
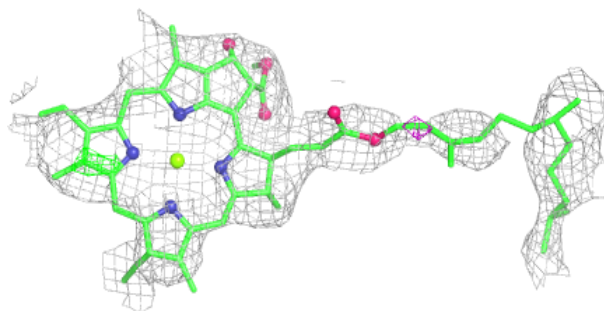
Electron density around CLA 2 304:

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



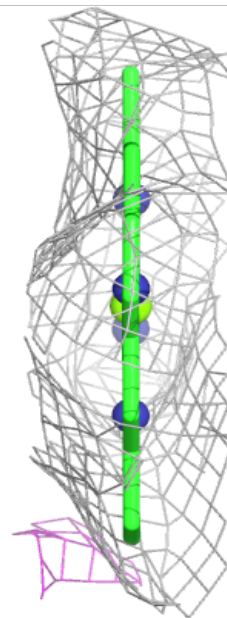
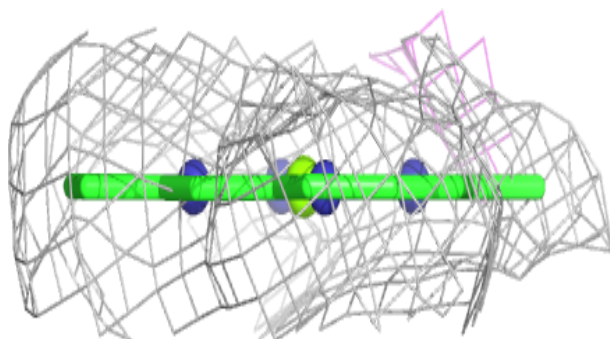
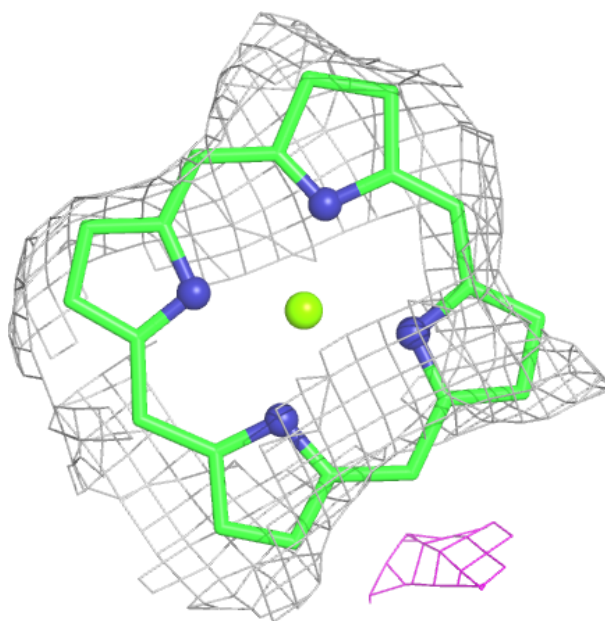
Electron density around CLA B 835:

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



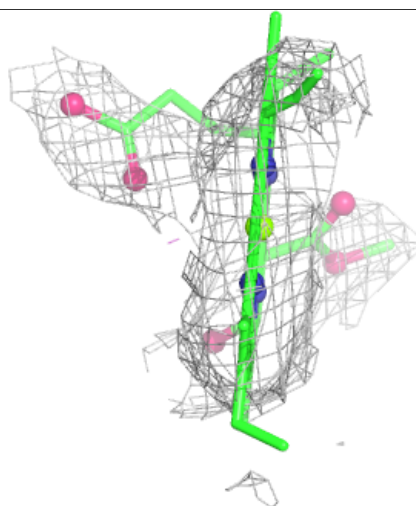
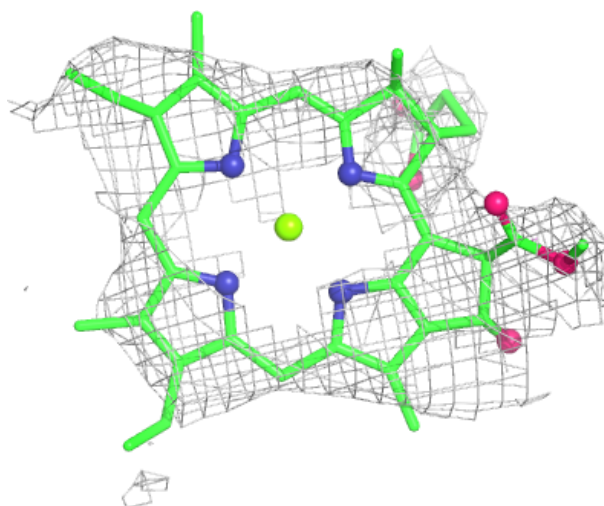
Electron density around CLA 1 216:

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



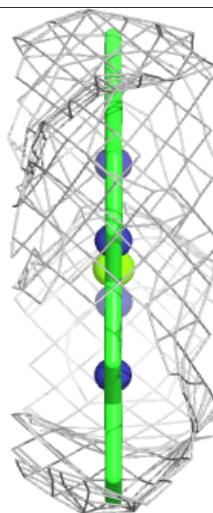
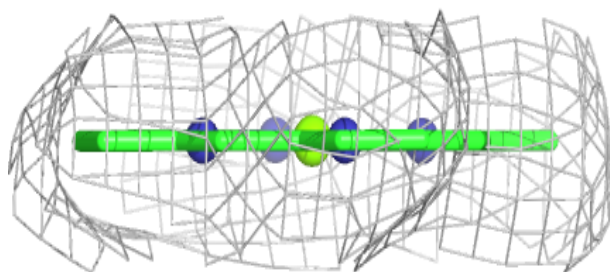
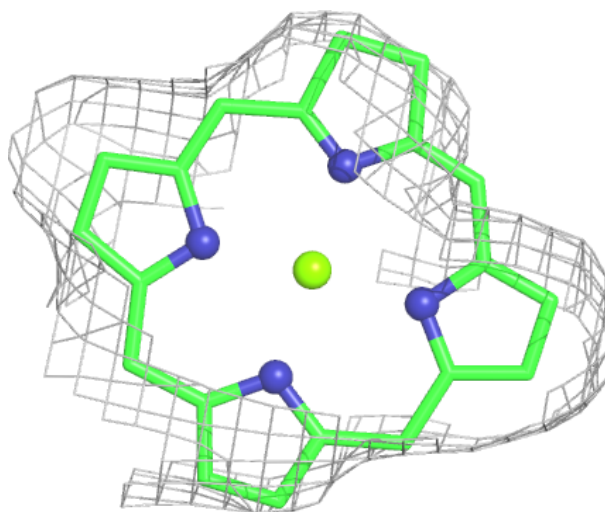
Electron density around CLA B 804:

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



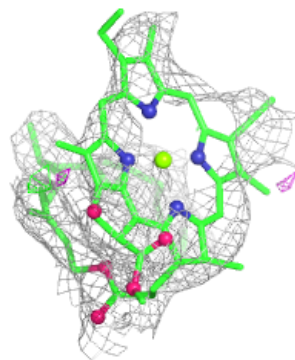
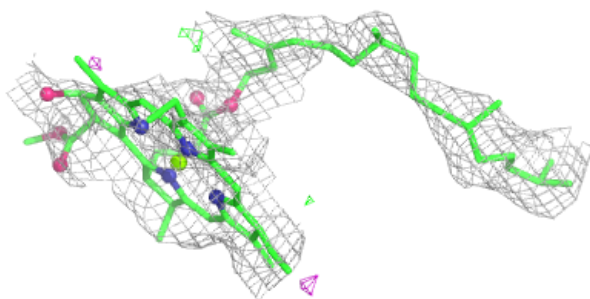
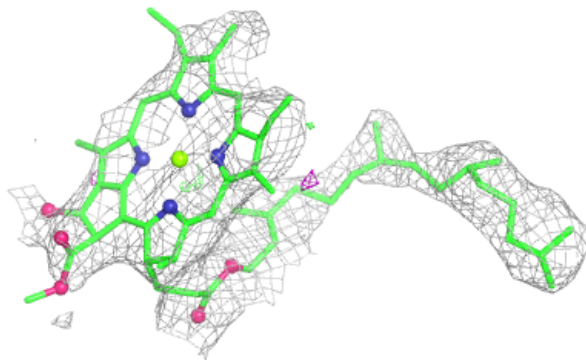
Electron density around CLA 1 205:

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



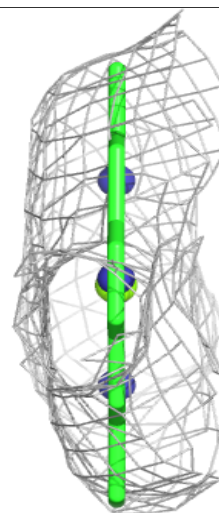
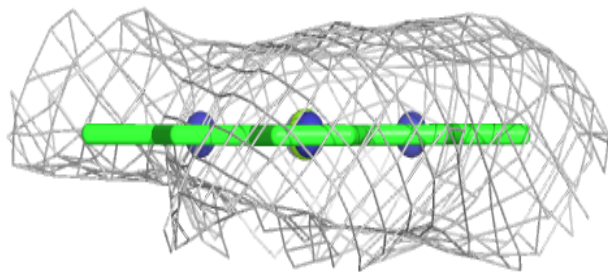
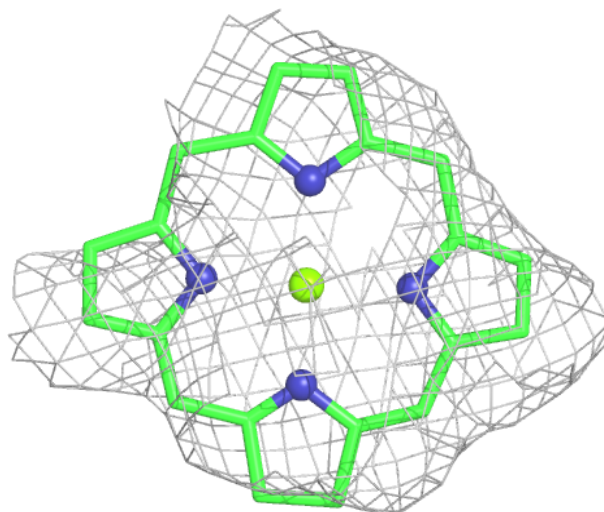
Electron density around CLA B 812:

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



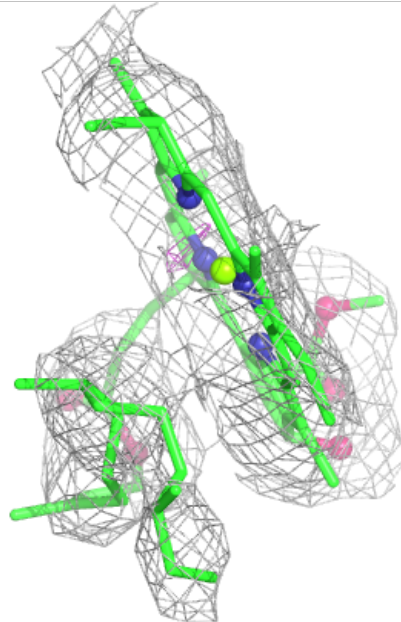
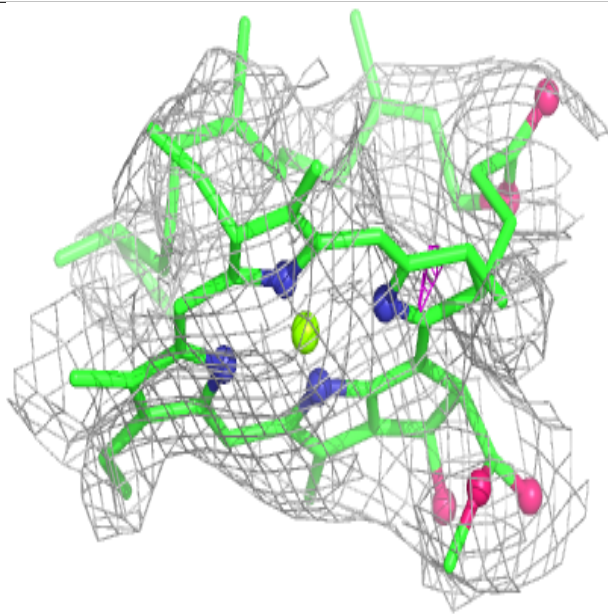
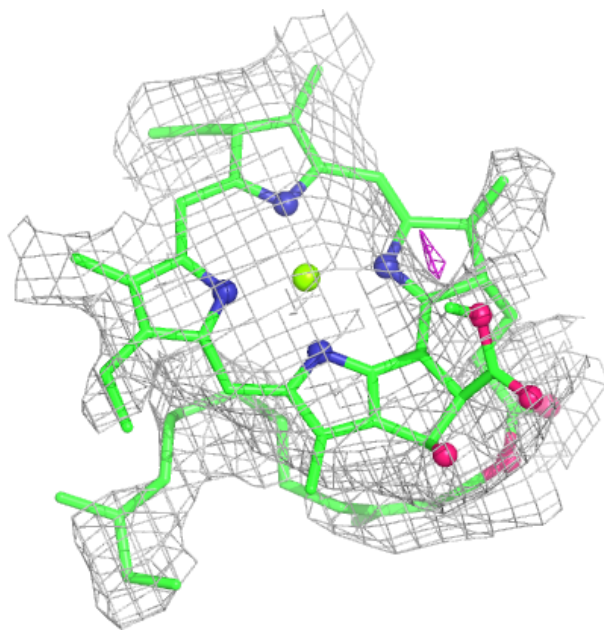
Electron density around CLA 1 212:

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



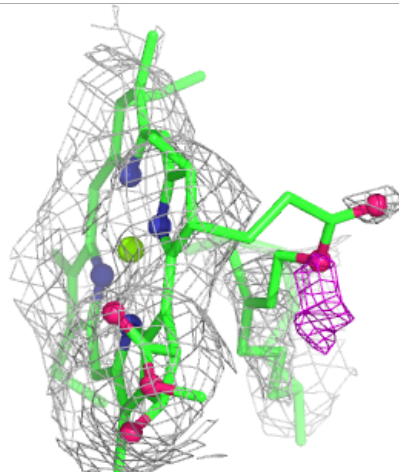
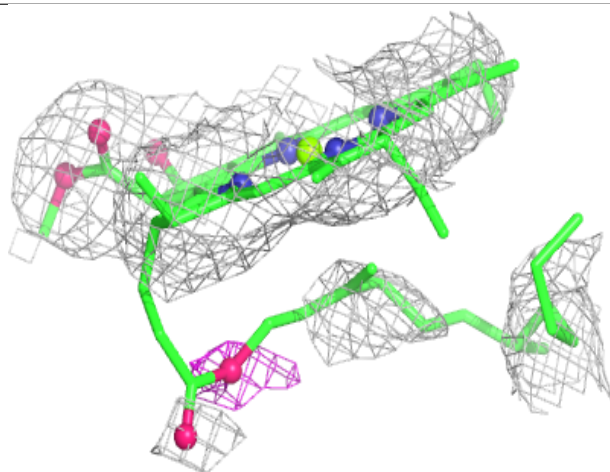
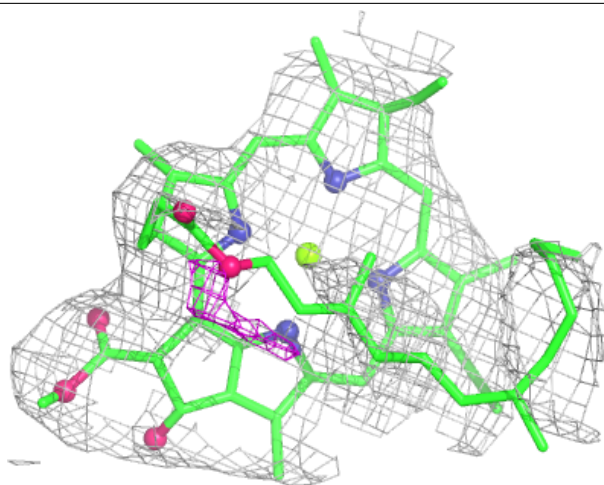
Electron density around CLA 1 206:

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



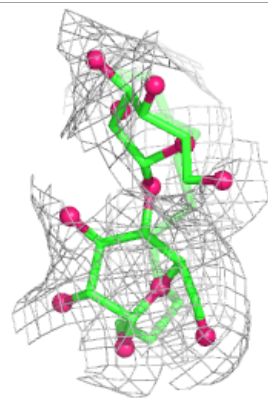
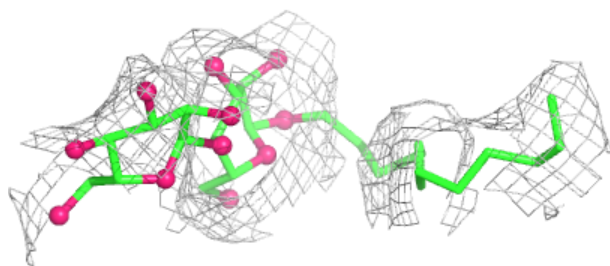
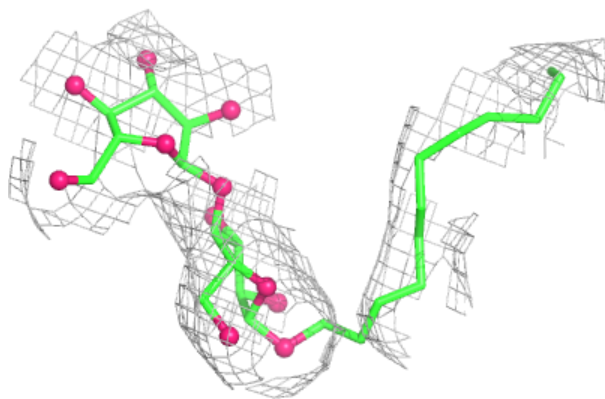
Electron density around CLA B 815:

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



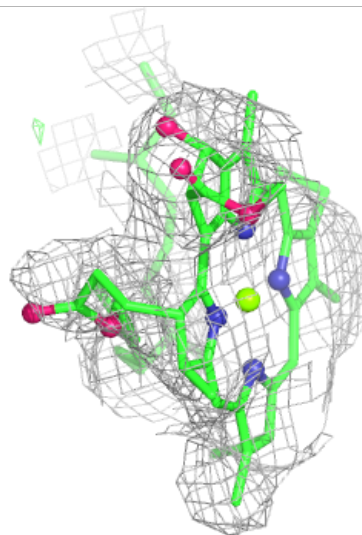
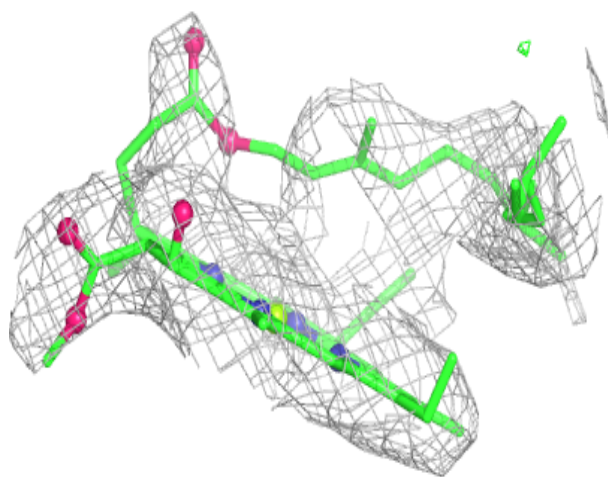
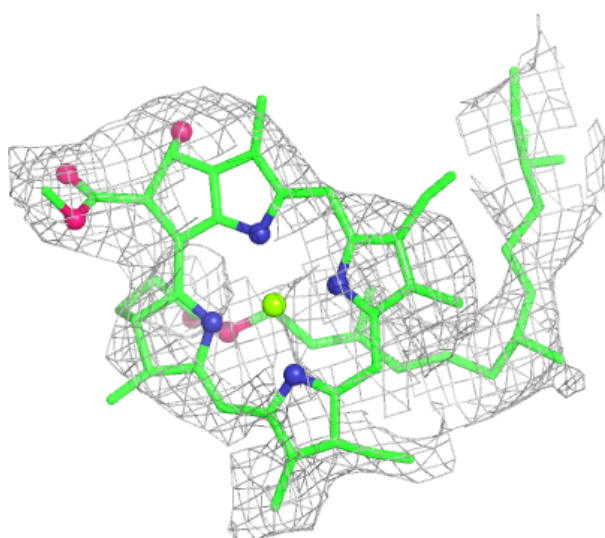
Electron density around LMU L 205:

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



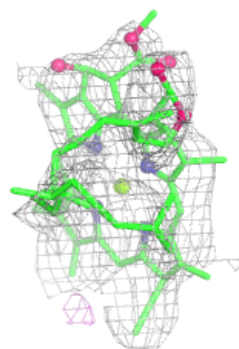
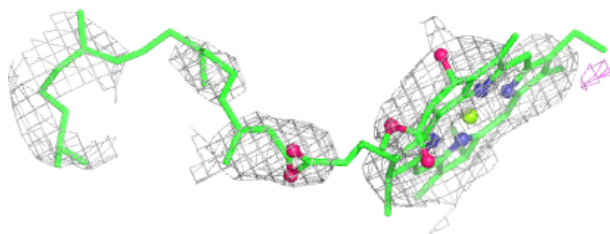
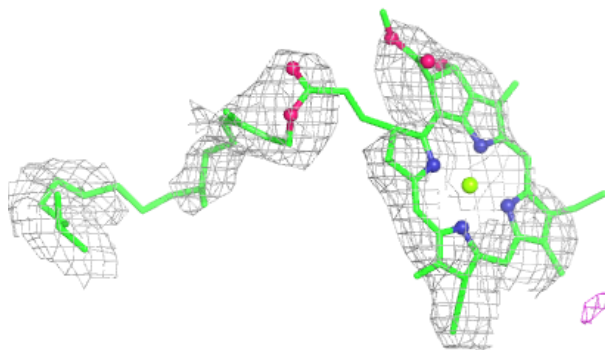
Electron density around CLA B 817:

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



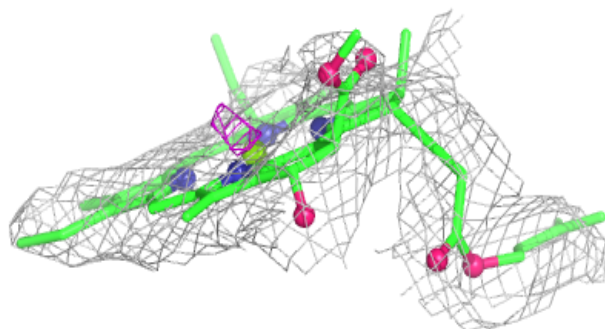
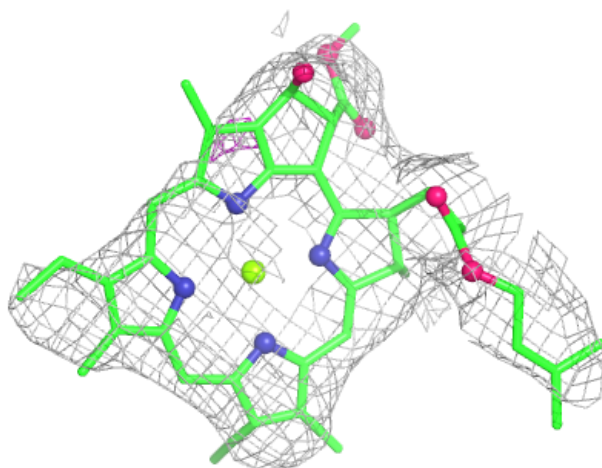
Electron density around CLA B 808:

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



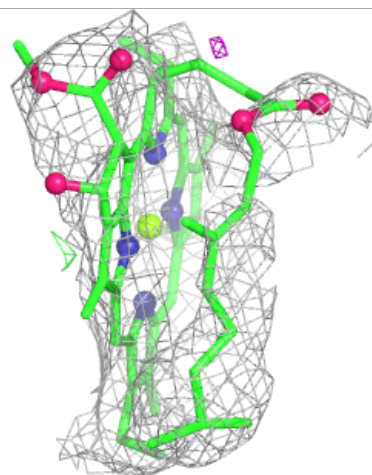
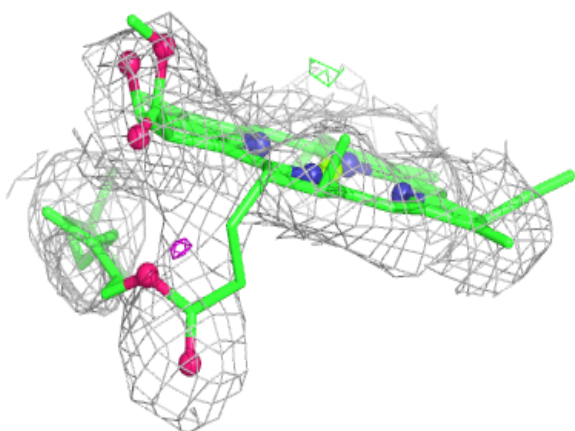
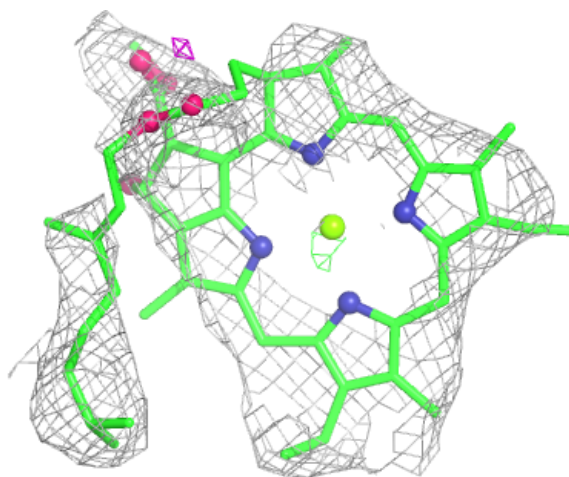
Electron density around CLA A 832:

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



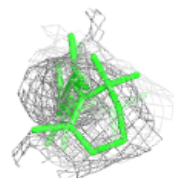
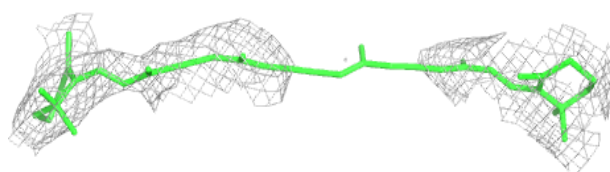
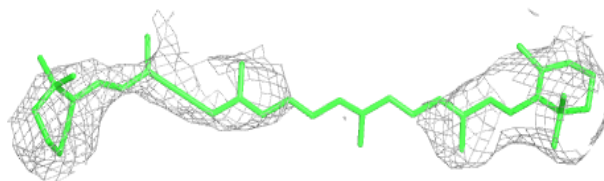
Electron density around CLA A 827:

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

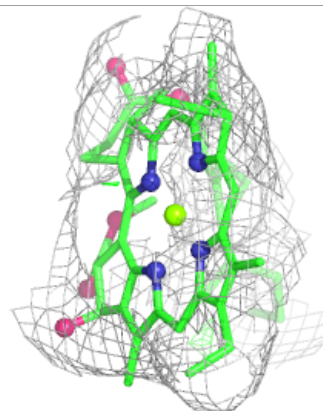
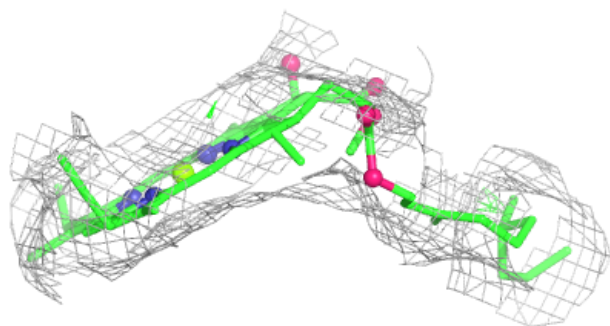
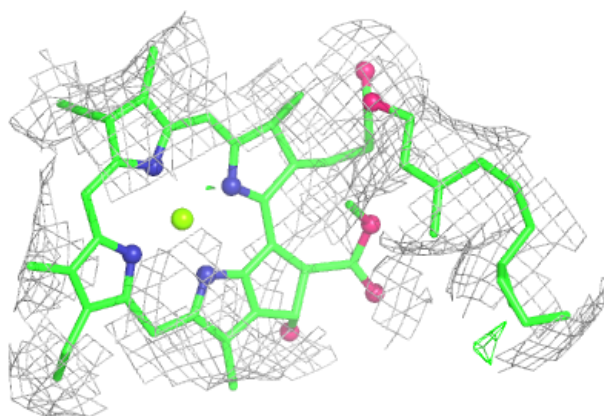


Electron density around BCR A 846:

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

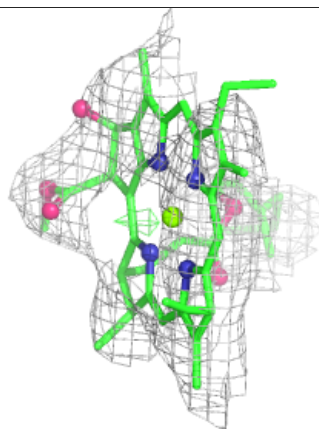
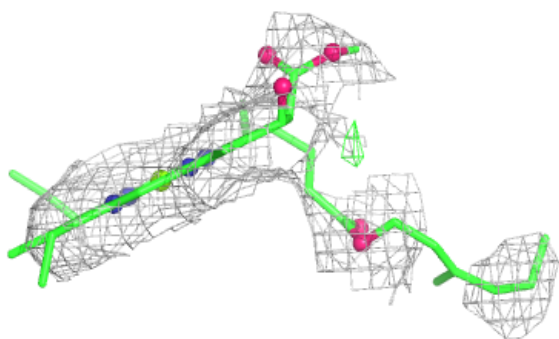
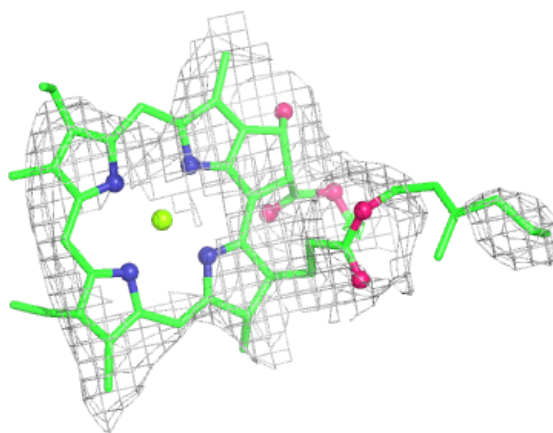
**Electron density around CLA 1 202:**

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

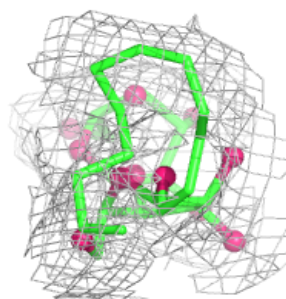
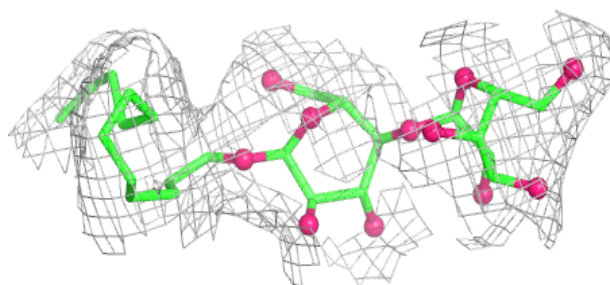
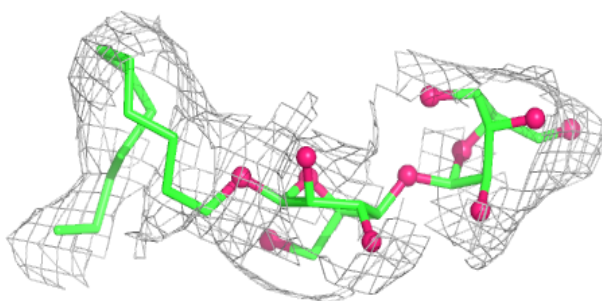


Electron density around CLA A 809:

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

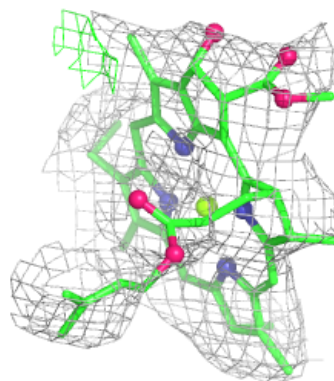
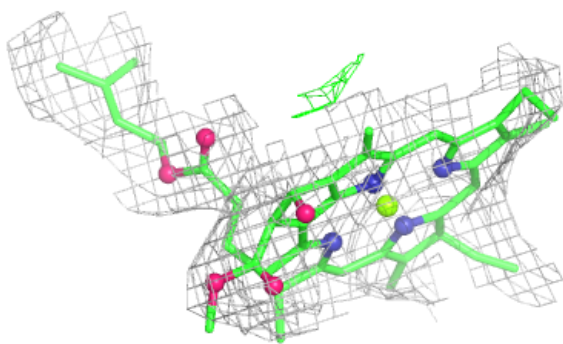
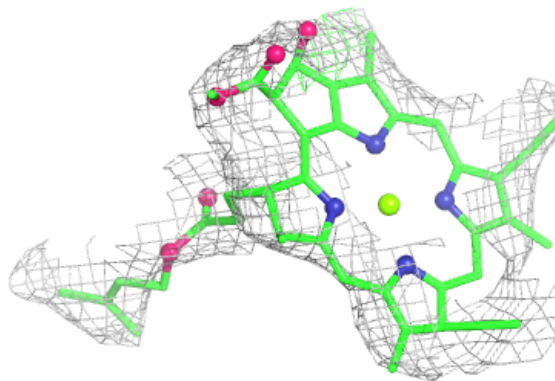
**Electron density around LMU A 855:**

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



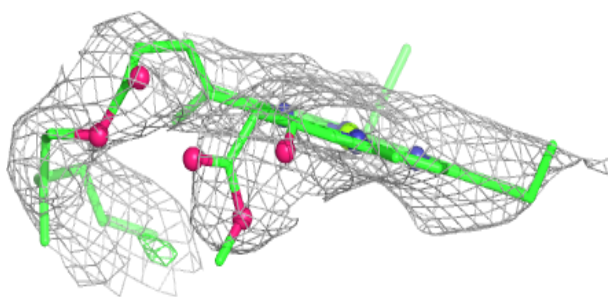
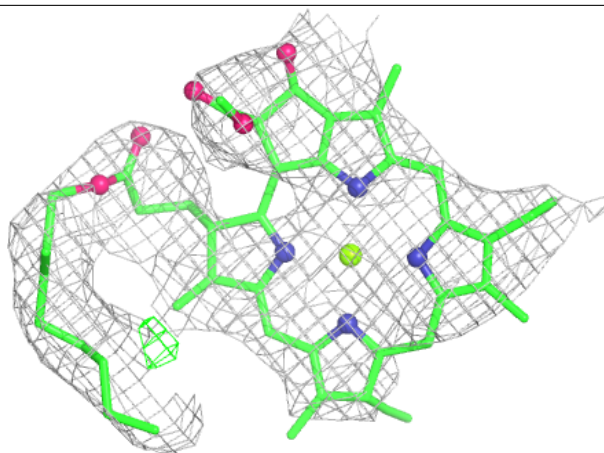
Electron density around CLA 2 311:

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



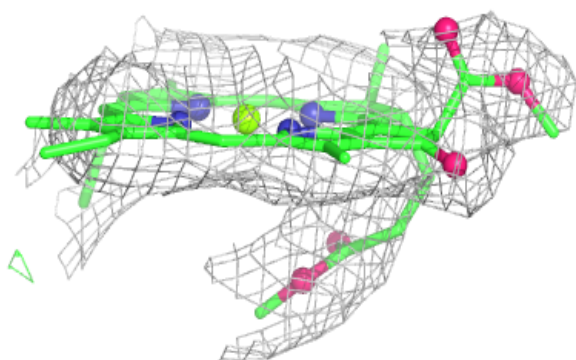
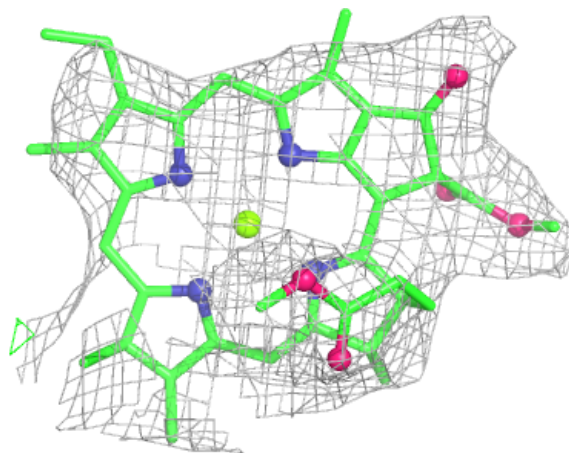
Electron density around CLA B 822:

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



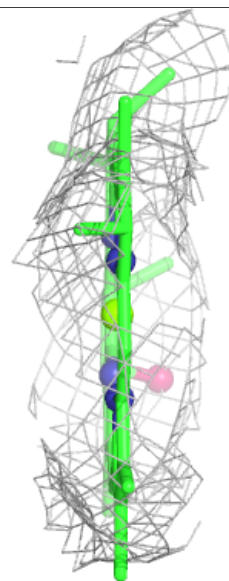
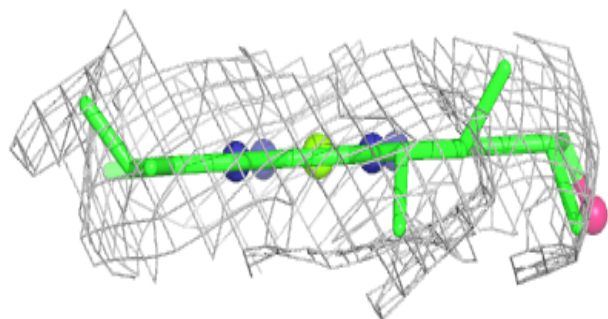
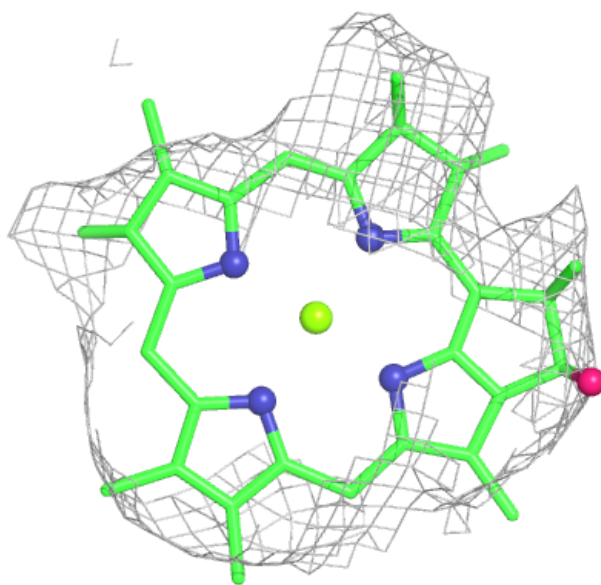
Electron density around CLA 1 204:

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



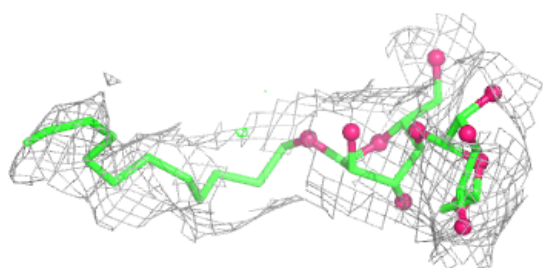
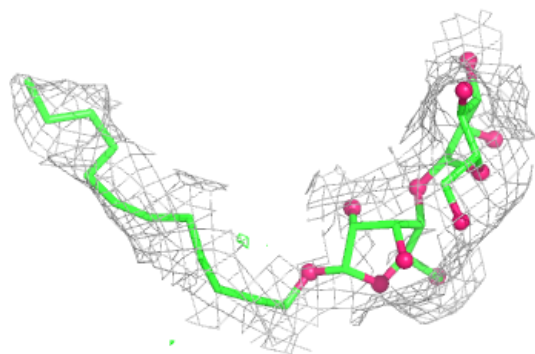
Electron density around CLA 3 304:

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

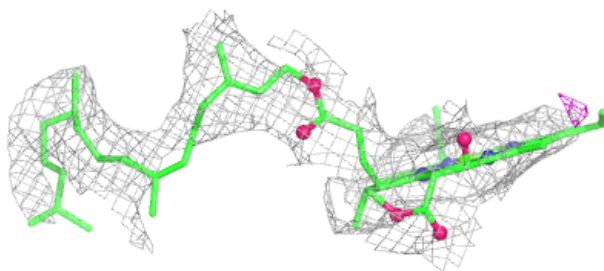
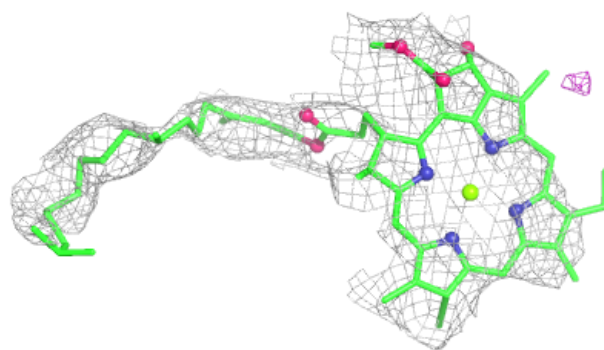


Electron density around LMU G 101:

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

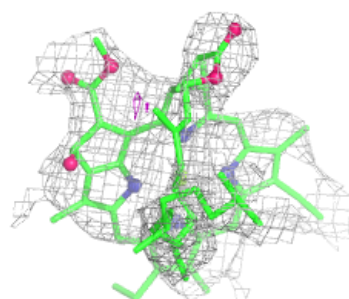
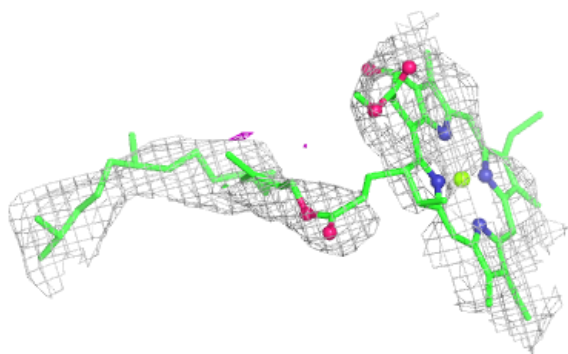
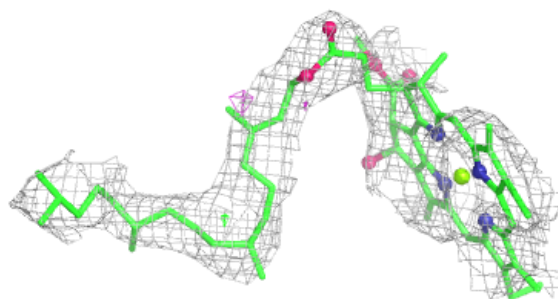
**Electron density around CLA A 824:**

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

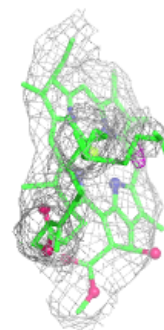
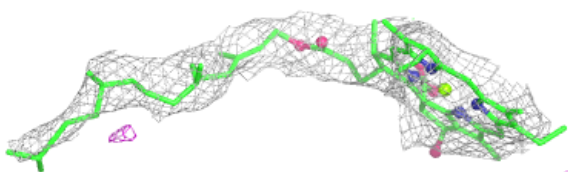
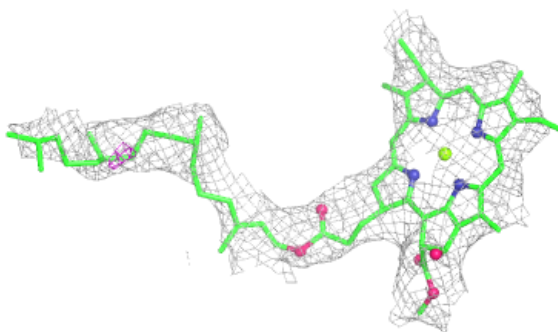


Electron density around CLA B 849:

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

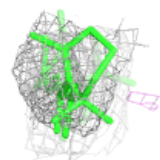
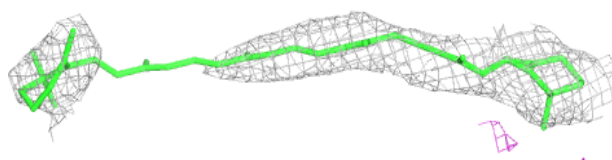
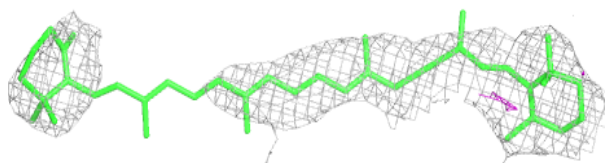
**Electron density around CLA B 850:**

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

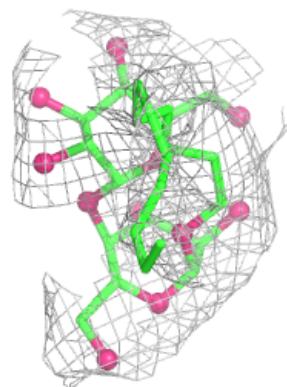
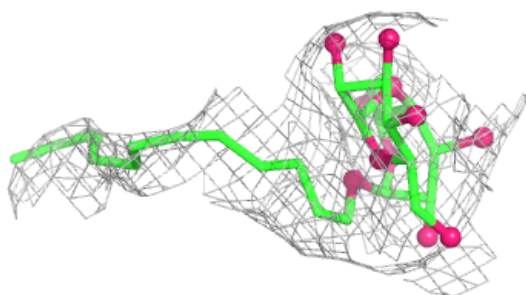
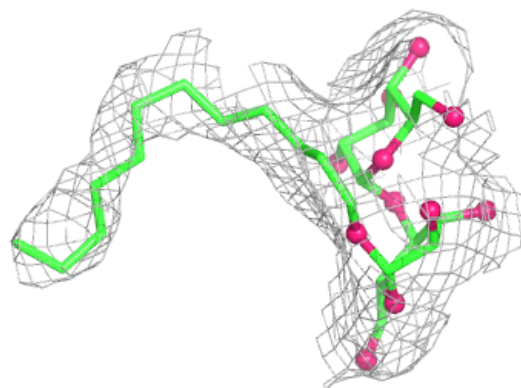


Electron density around BCR B 842:

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

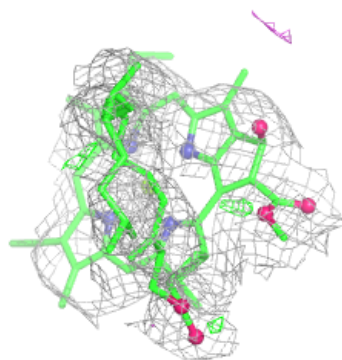
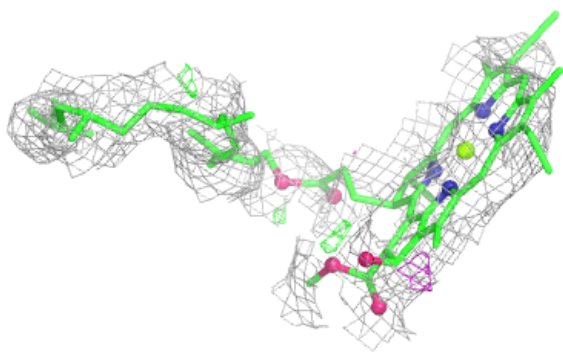
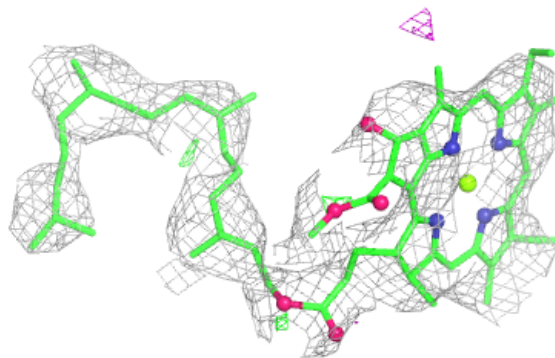
**Electron density around LMU H 106:**

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



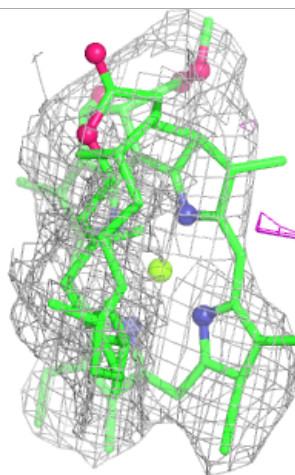
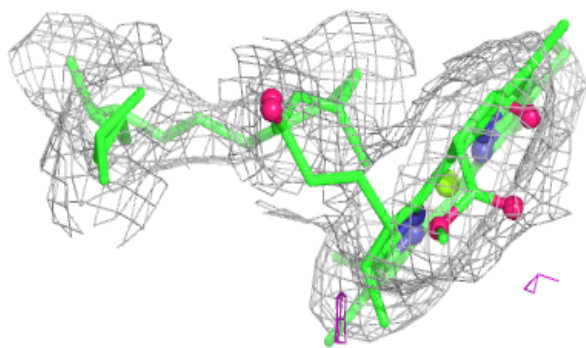
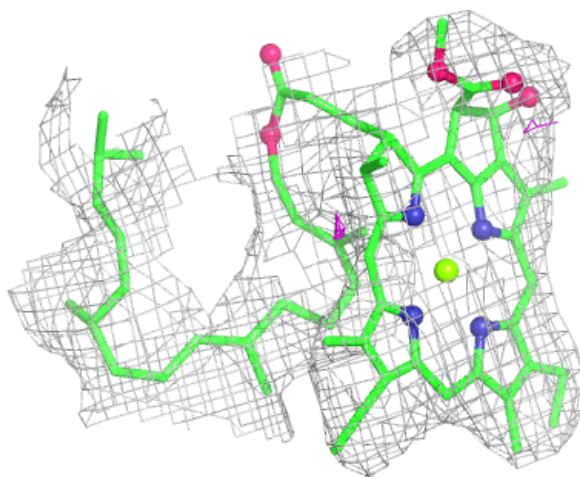
Electron density around CLA A 850:

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



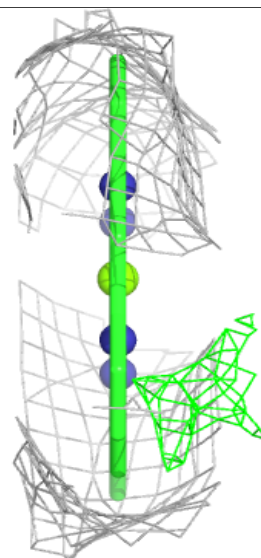
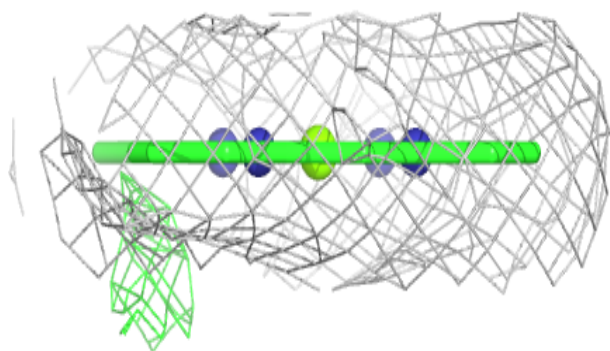
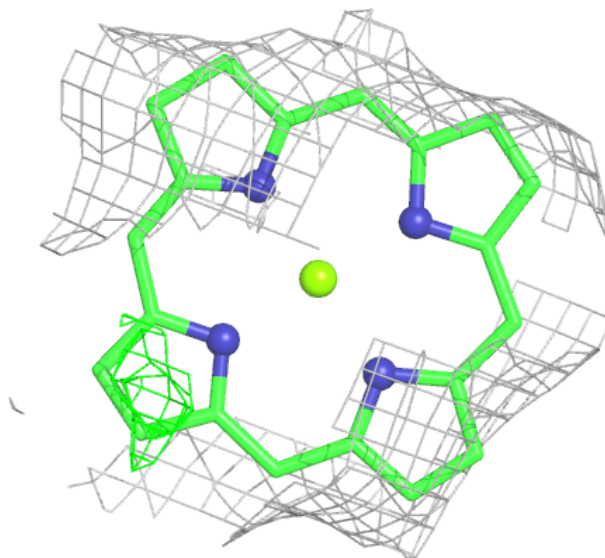
Electron density around CLA B 821:

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



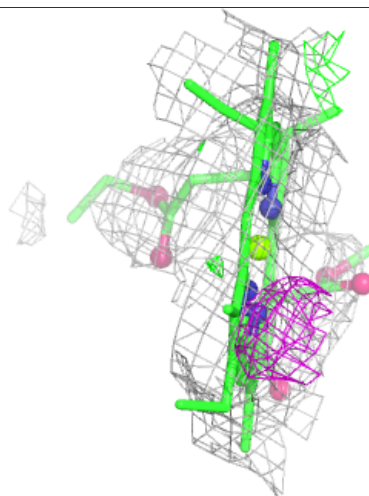
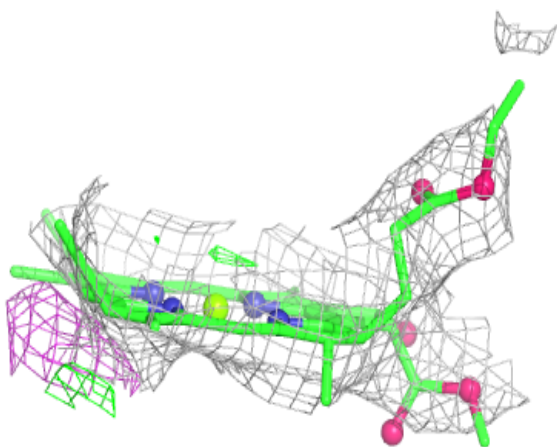
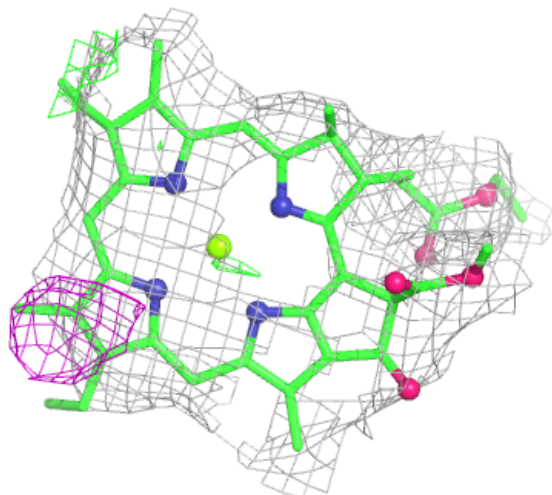
Electron density around CLA 1 214:

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



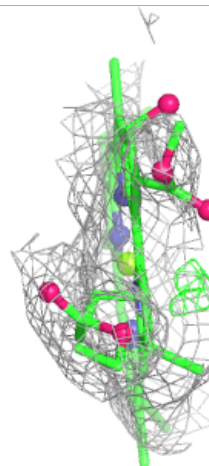
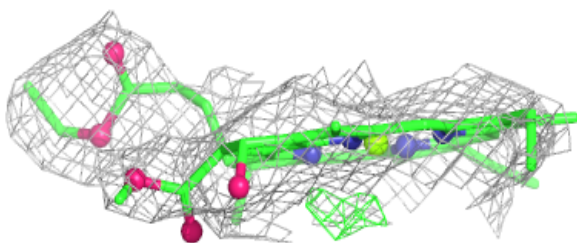
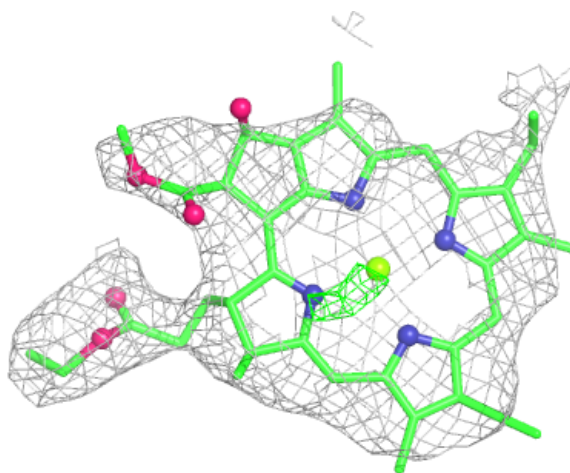
Electron density around CLA A 836:

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



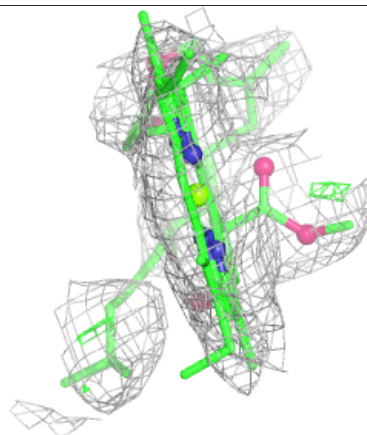
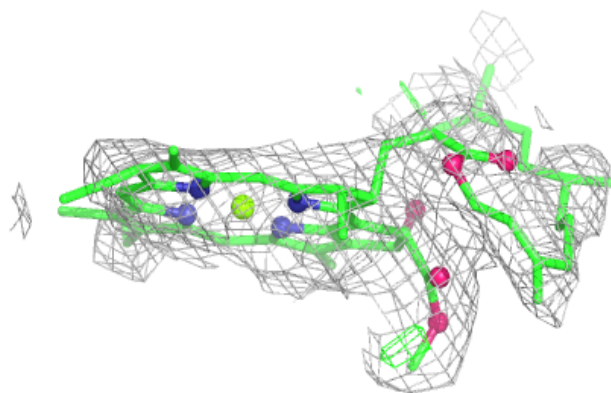
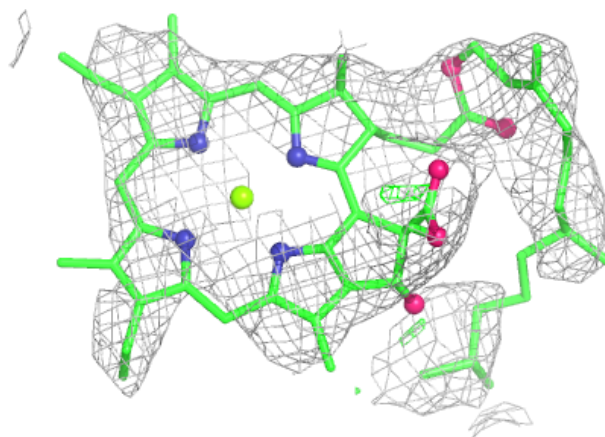
Electron density around CLA A 837:

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



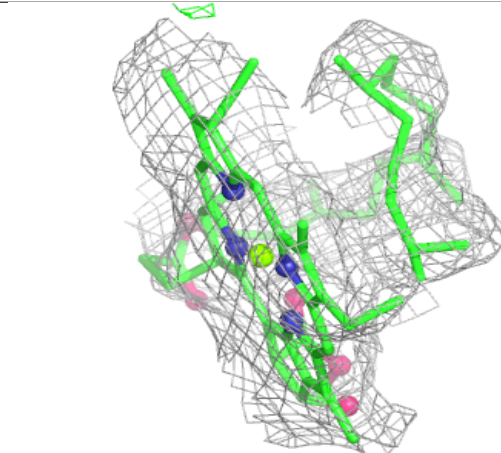
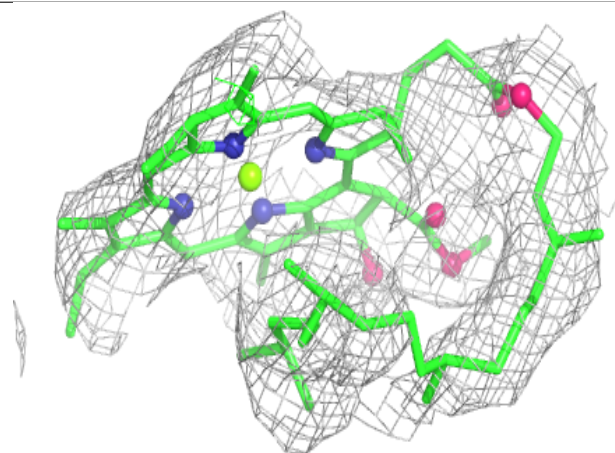
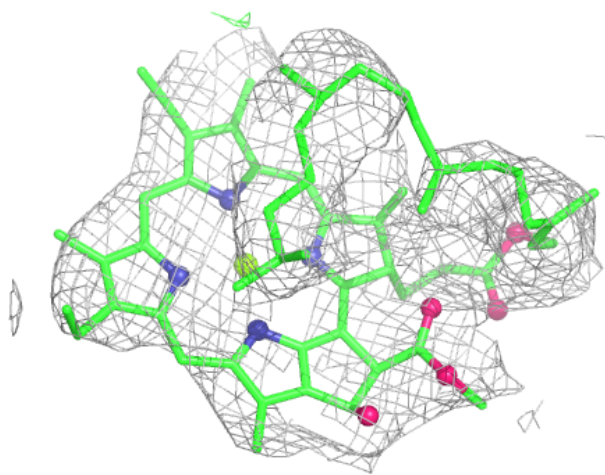
Electron density around CLA B 805:

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



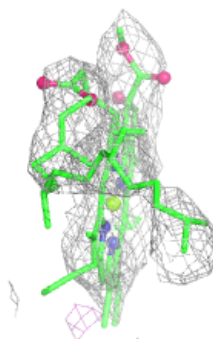
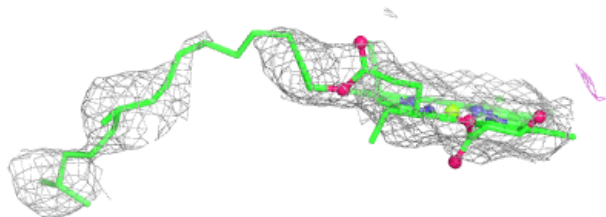
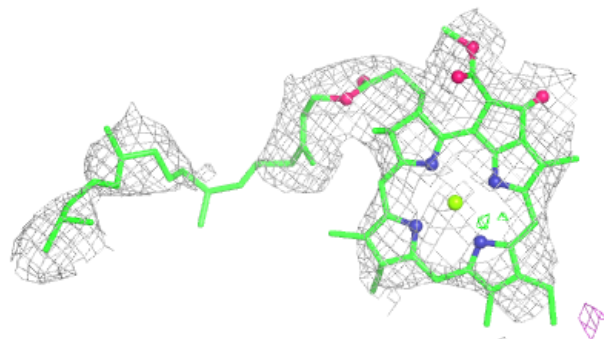
Electron density around CLA B 806:

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



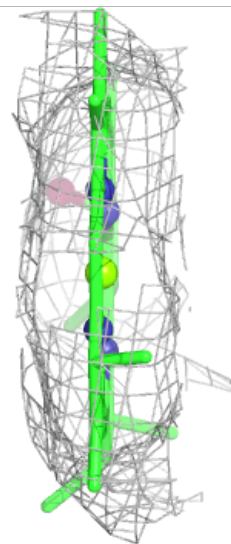
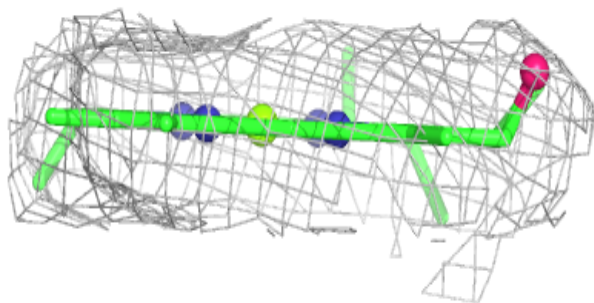
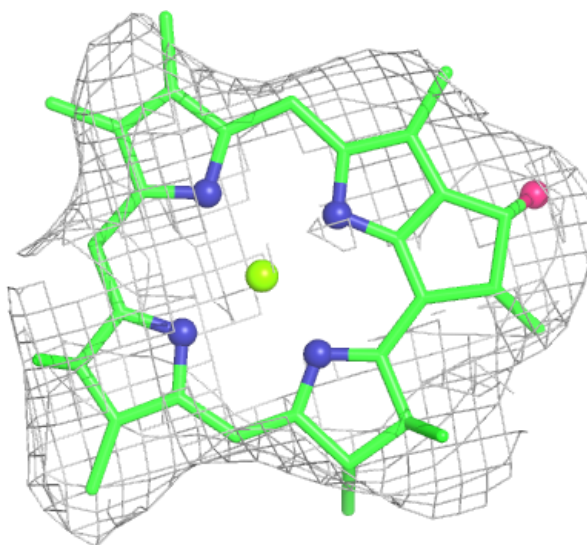
Electron density around CLA B 851:

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



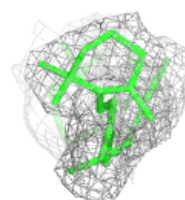
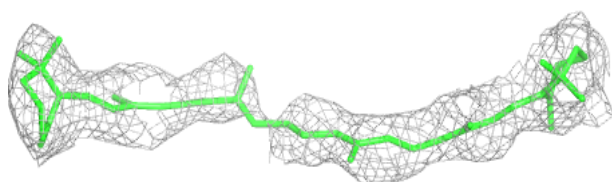
Electron density around CLA 4 314:

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

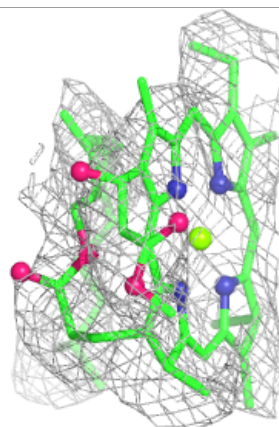
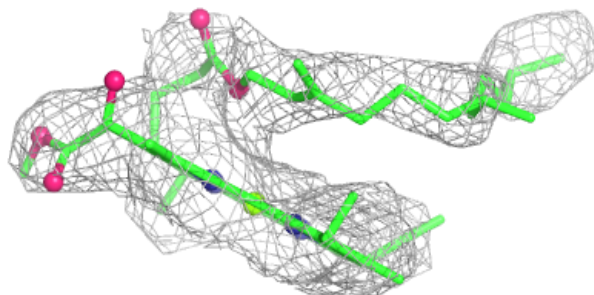
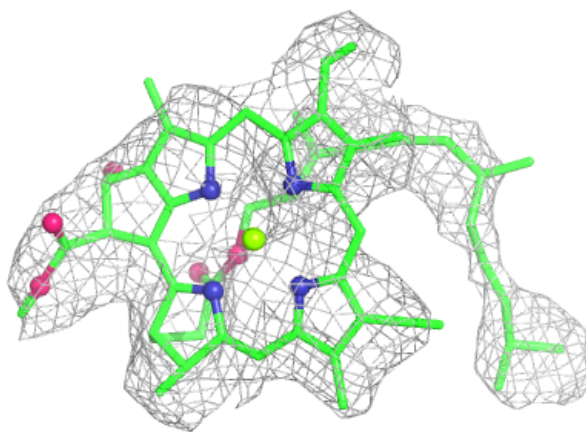


Electron density around BCR I 101:

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

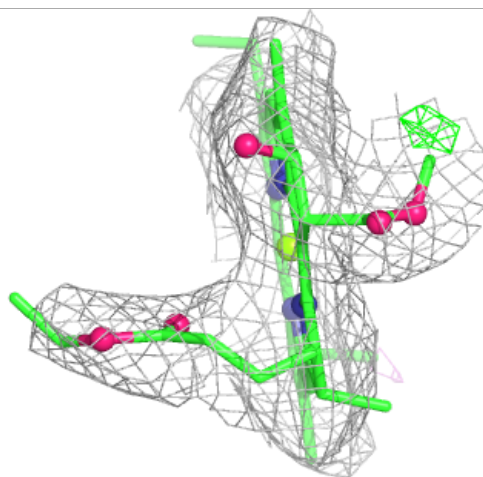
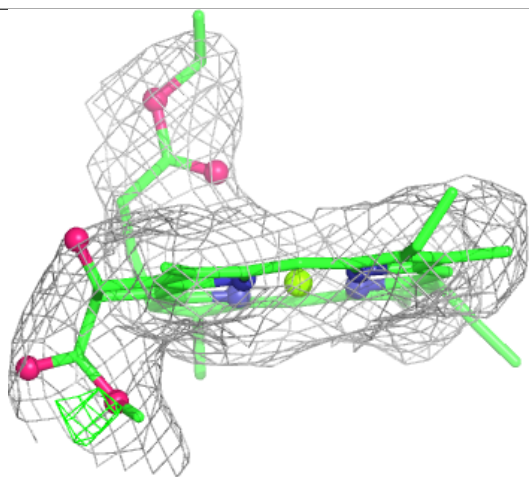
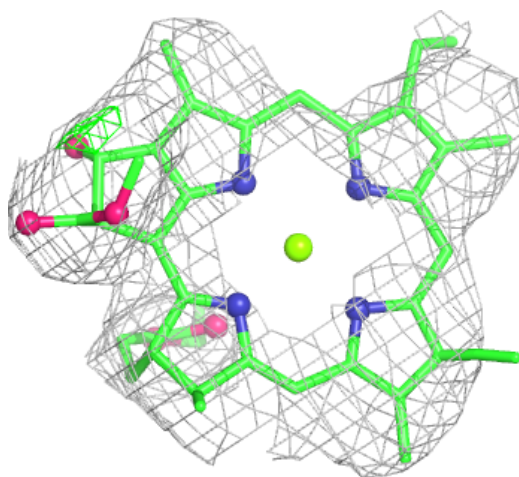
**Electron density around CLA I 102:**

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



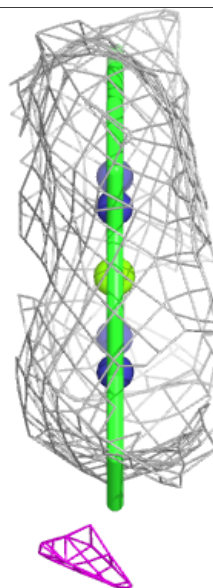
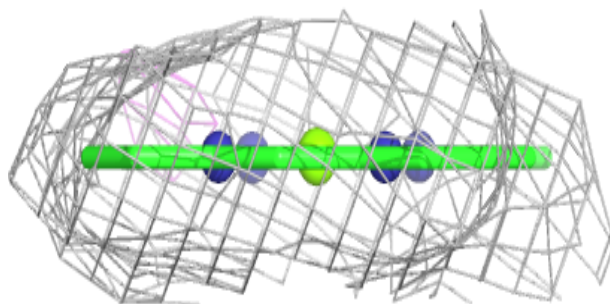
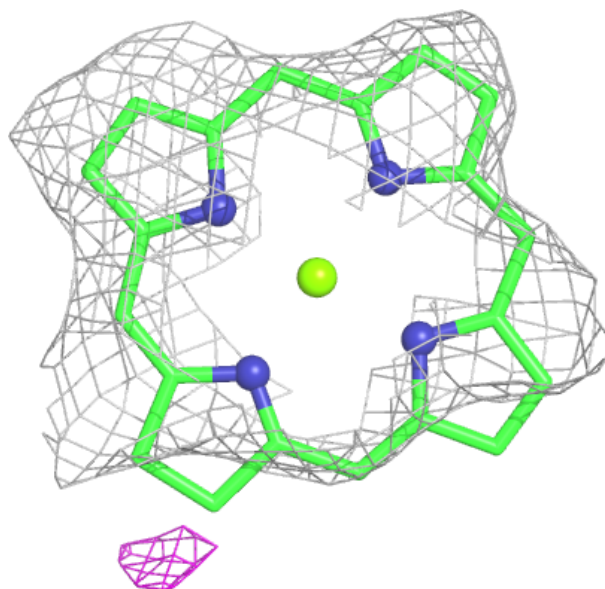
Electron density around CLA L 206:

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



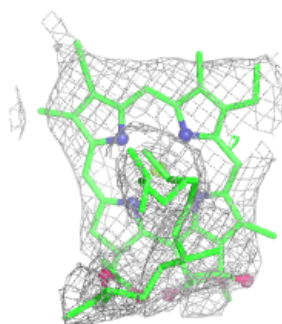
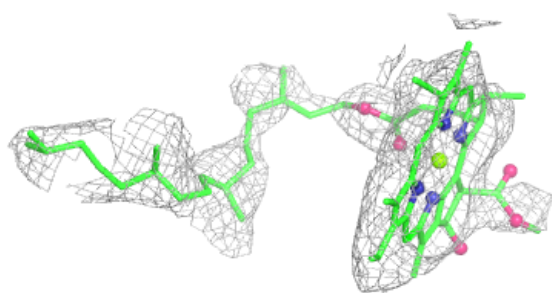
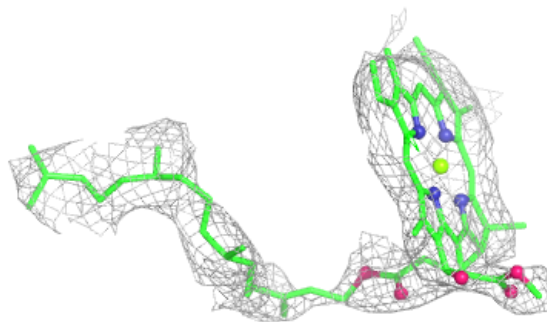
Electron density around CLA 2 314:

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



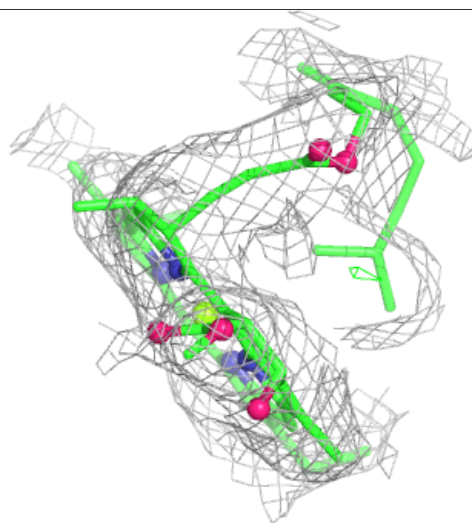
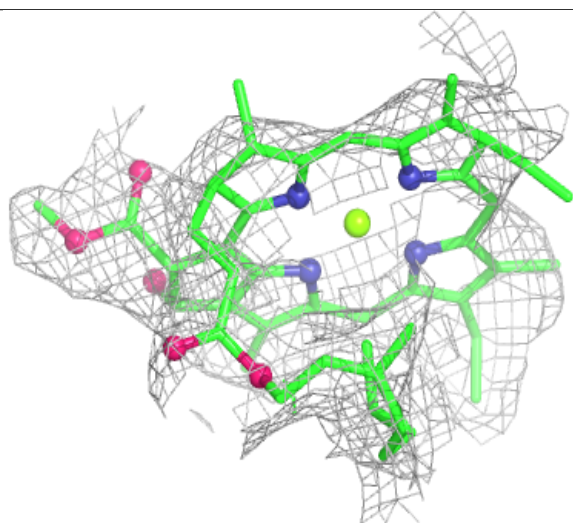
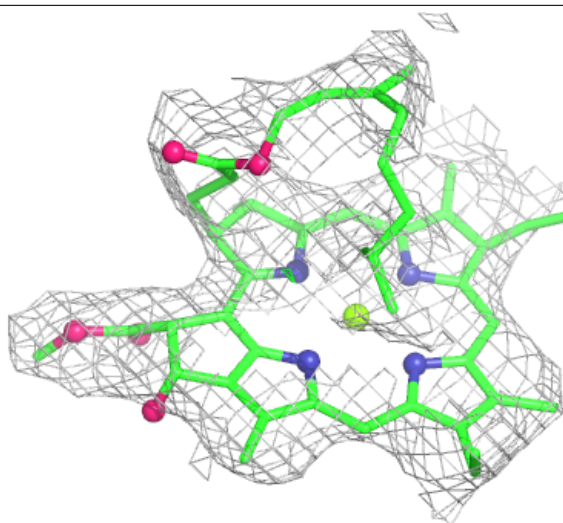
Electron density around CLA B 827:

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



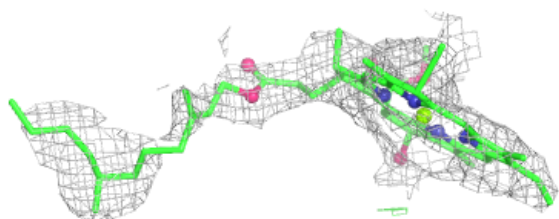
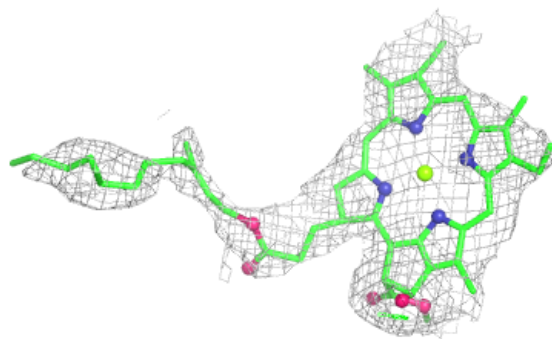
Electron density around CLA B 810:

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



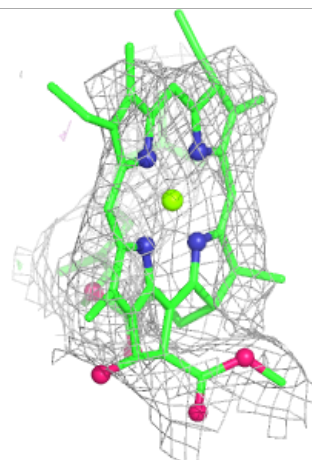
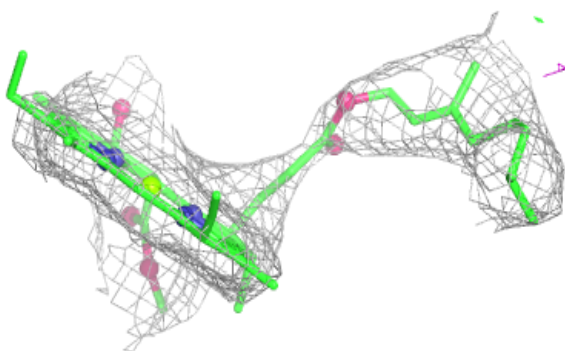
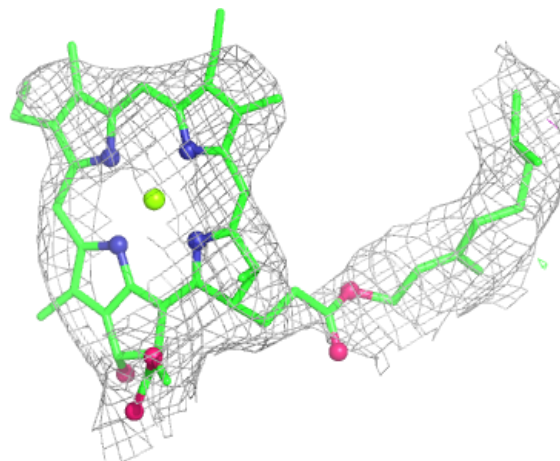
Electron density around CLA B 811:

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



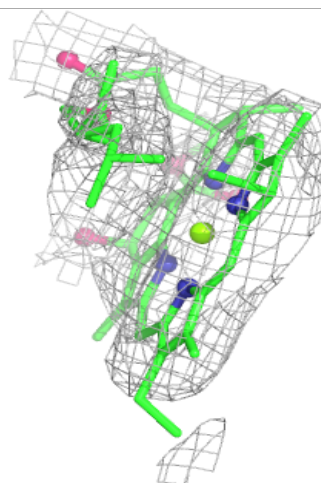
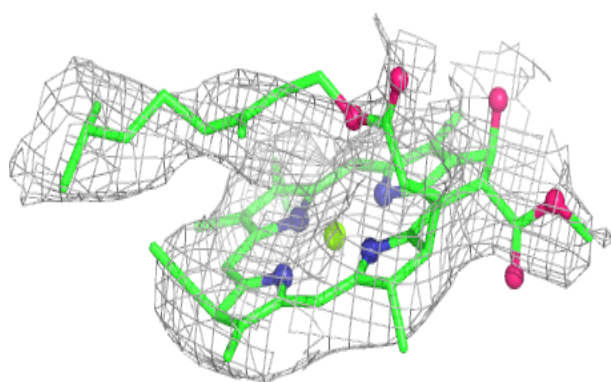
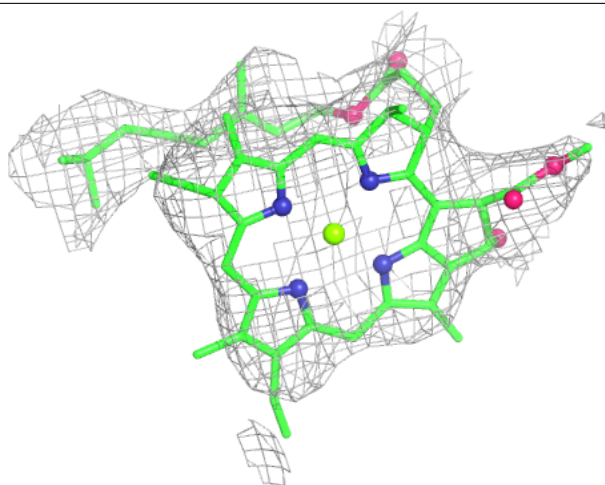
Electron density around CLA A 831:

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



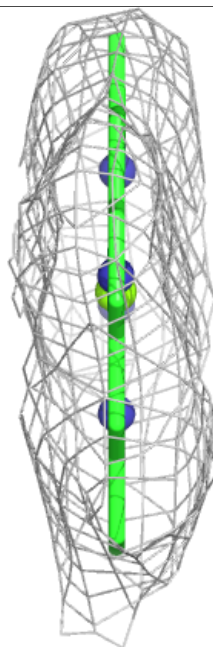
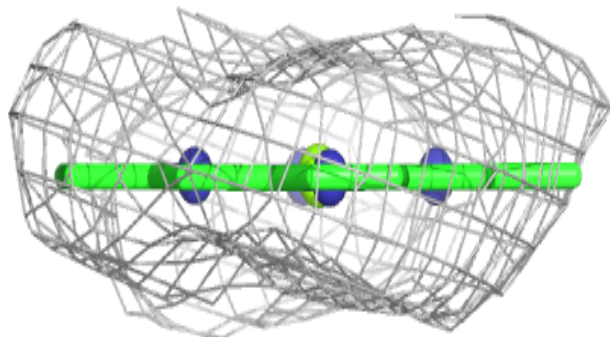
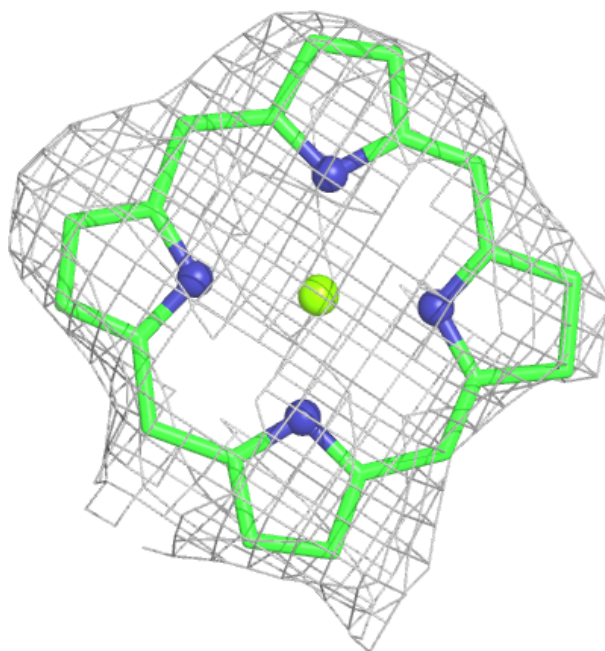
Electron density around CLA B 820:

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



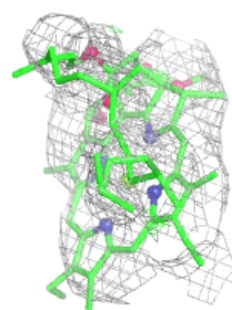
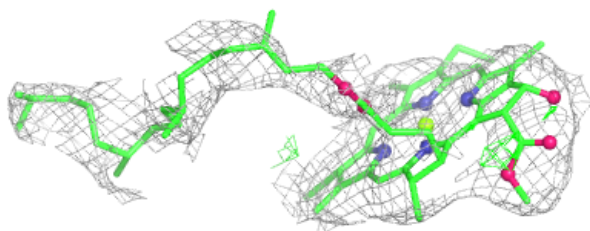
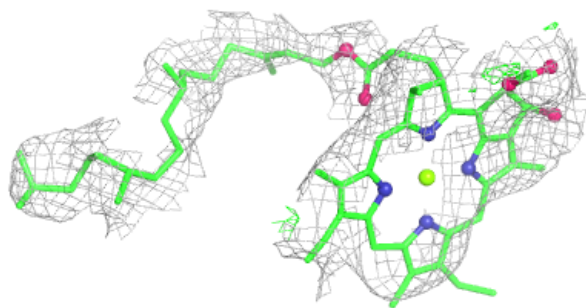
Electron density around CLA 4 313:

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



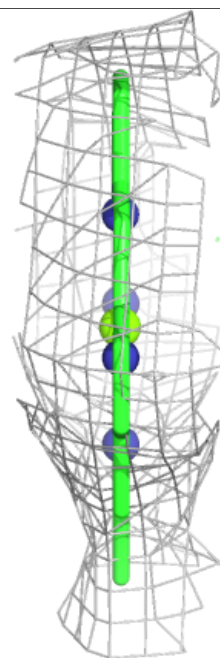
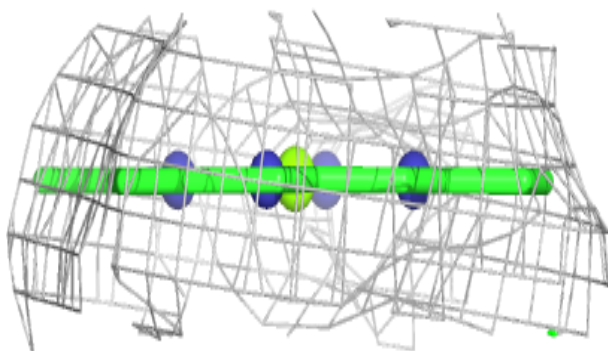
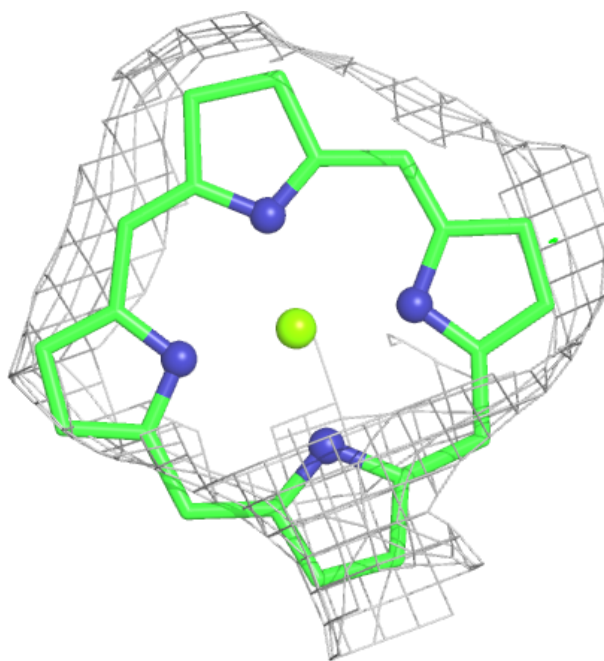
Electron density around CLA A 808:

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



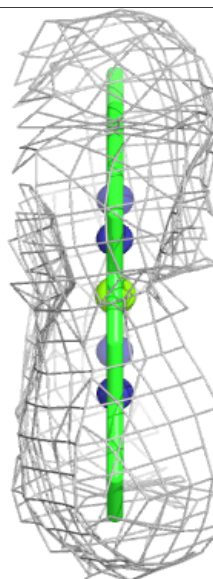
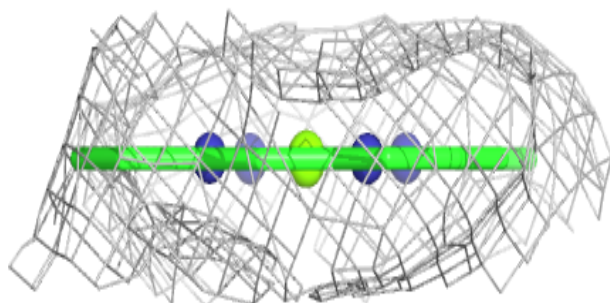
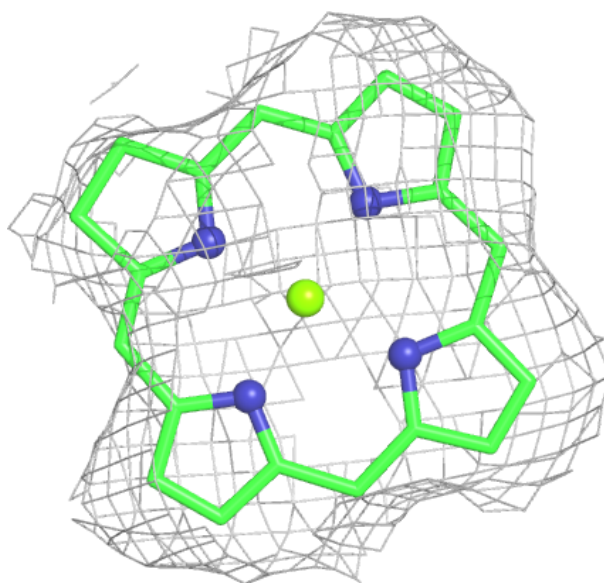
Electron density around CLA 4 312:

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



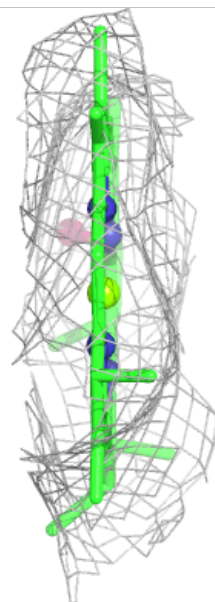
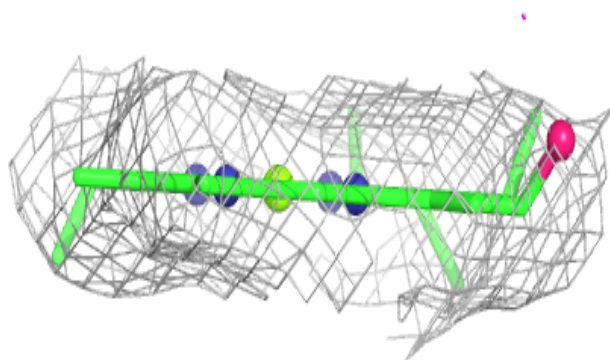
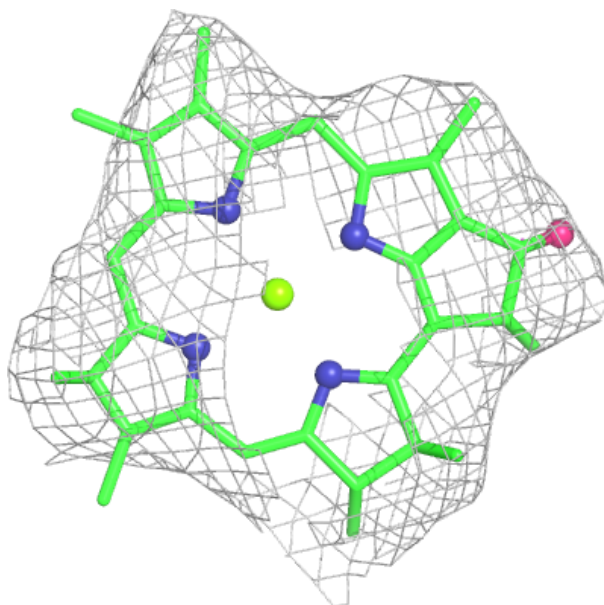
Electron density around CLA 4 315:

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



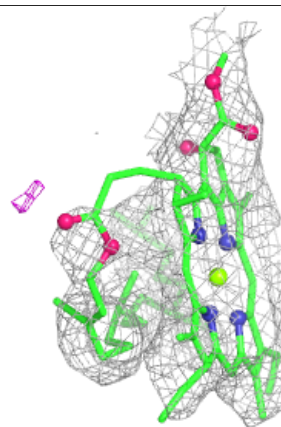
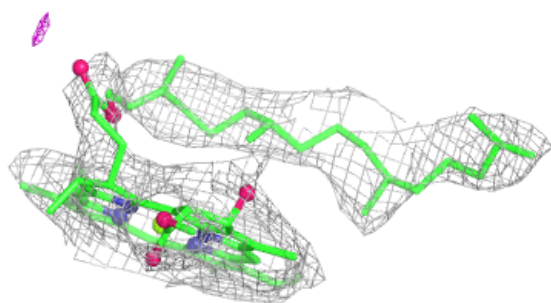
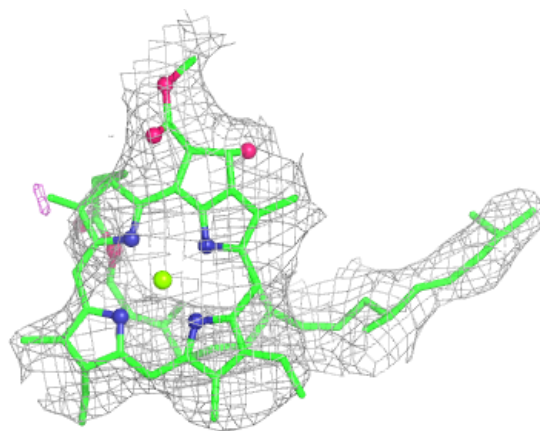
Electron density around CLA 1 209:

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

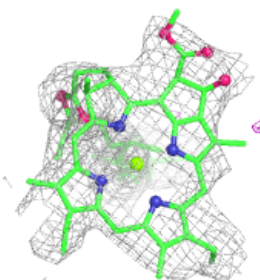
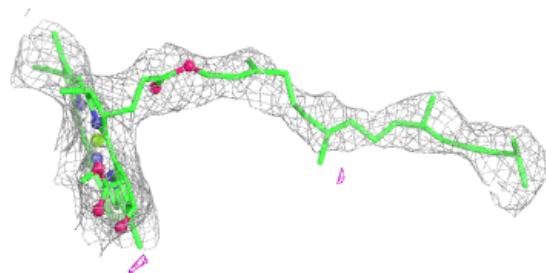
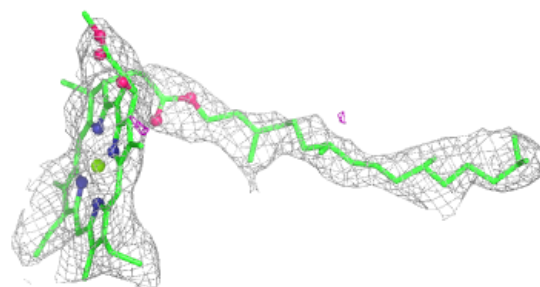


Electron density around CLA B 825:

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

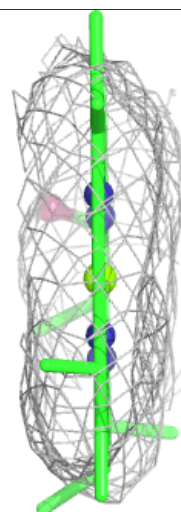
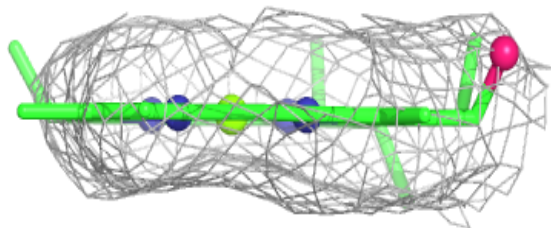
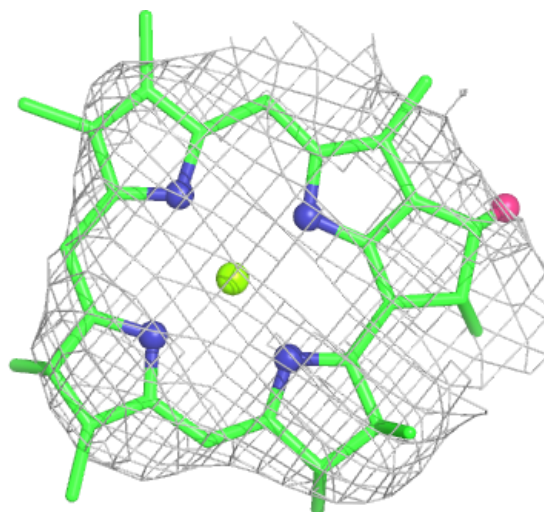
**Electron density around CLA B 826:**

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



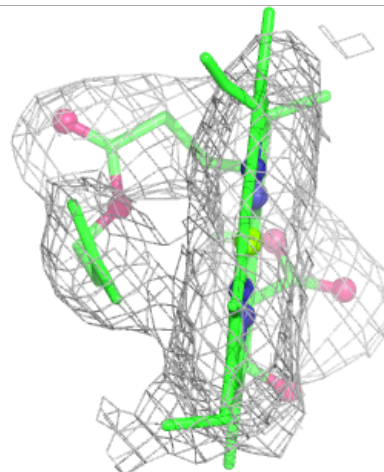
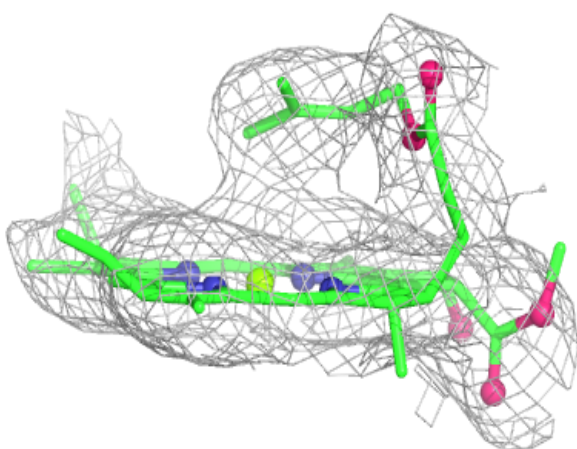
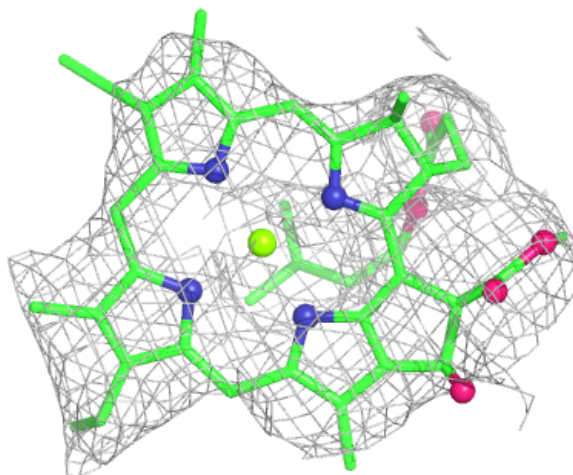
Electron density around CLA 4 303:

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



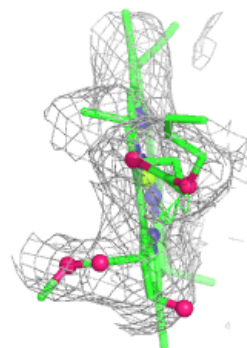
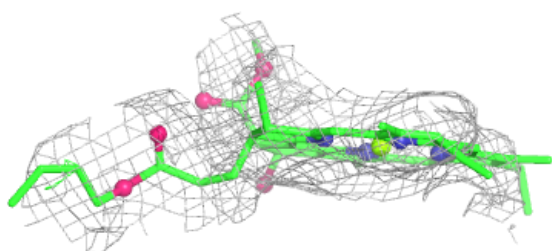
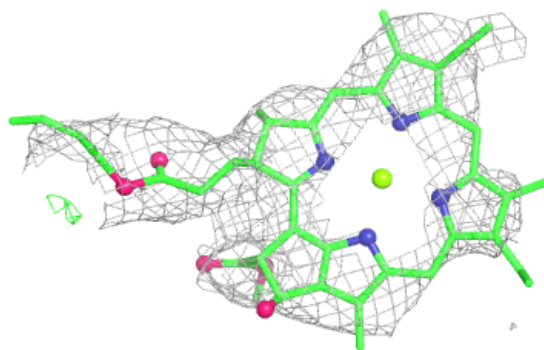
Electron density around CLA B 828:

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

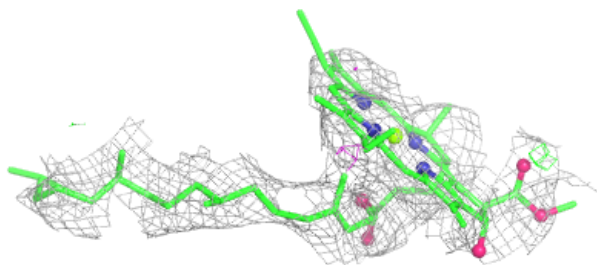
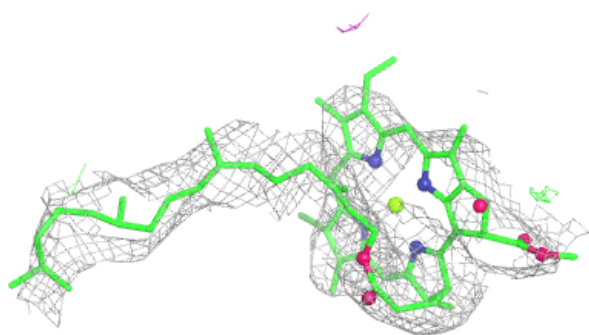


Electron density around CLA A 834:

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

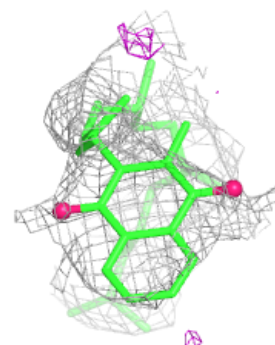
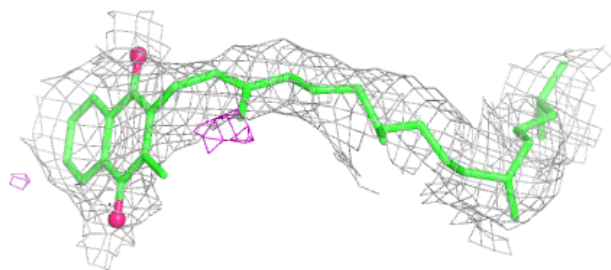
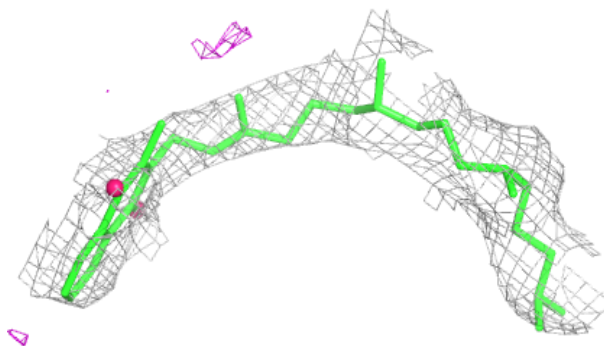
**Electron density around CLA A 838:**

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



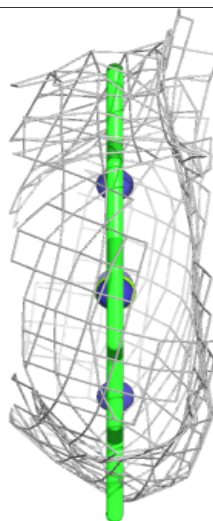
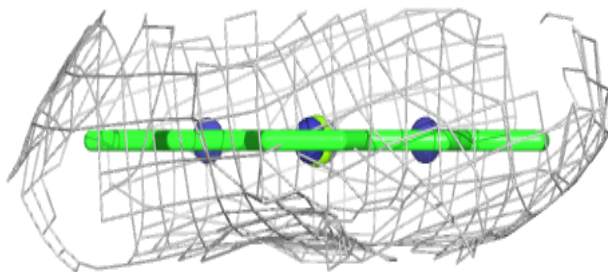
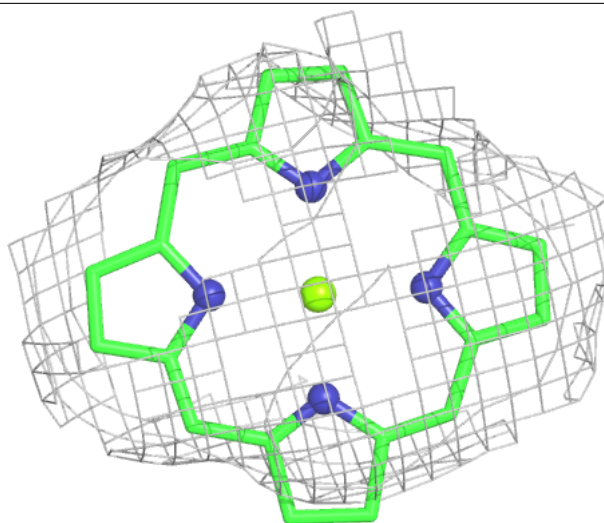
Electron density around PQN B 841:

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



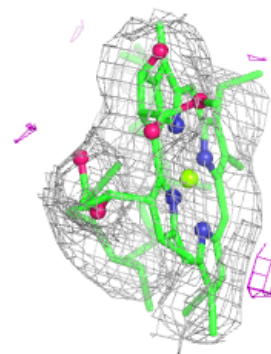
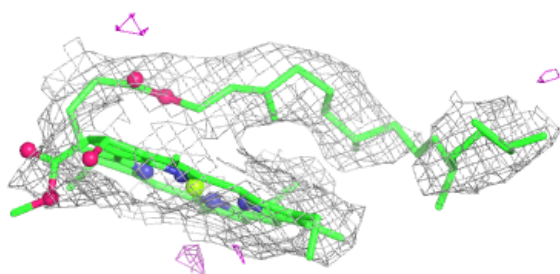
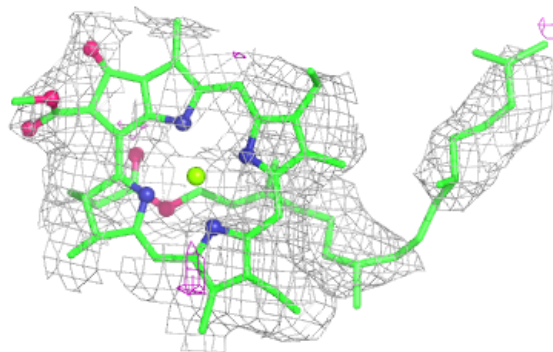
Electron density around CLA 2 309:

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



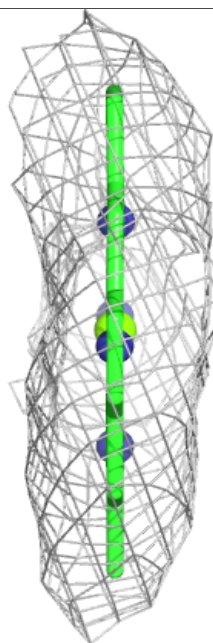
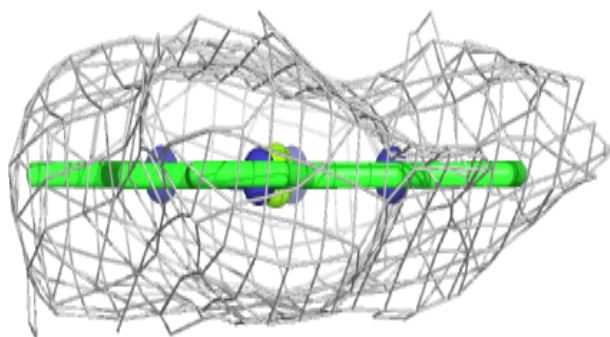
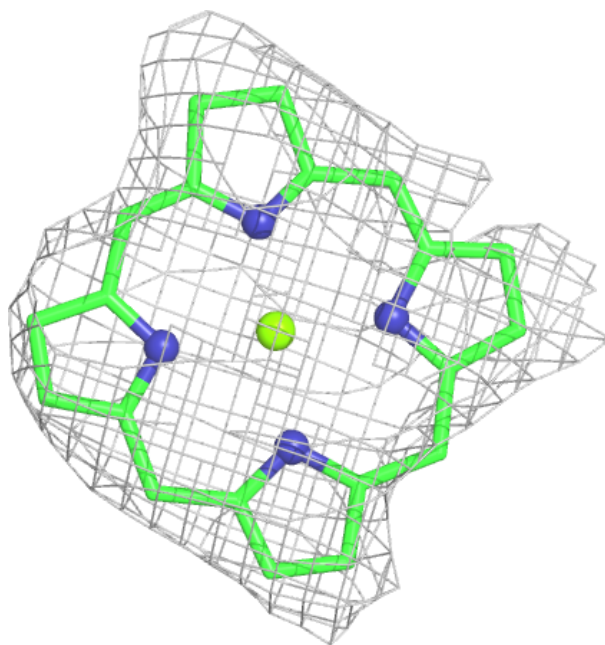
Electron density around CLA B 836:

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



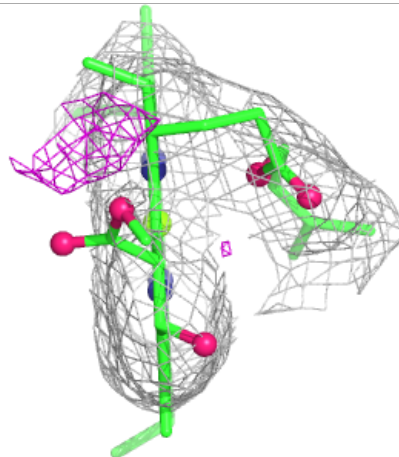
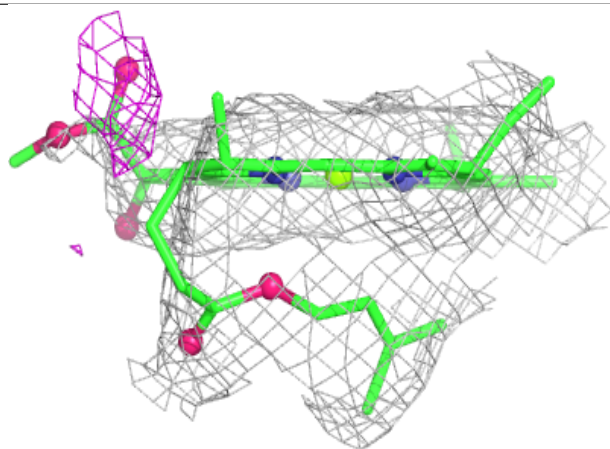
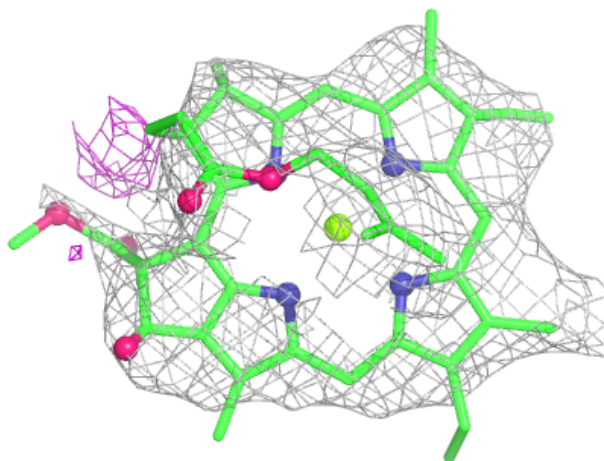
Electron density around CLA 1 208:

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



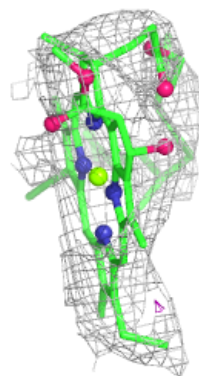
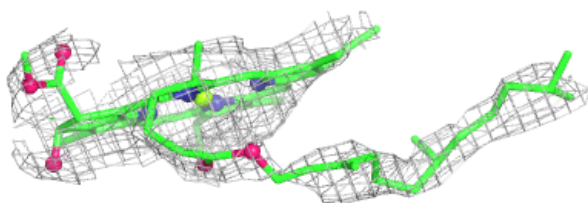
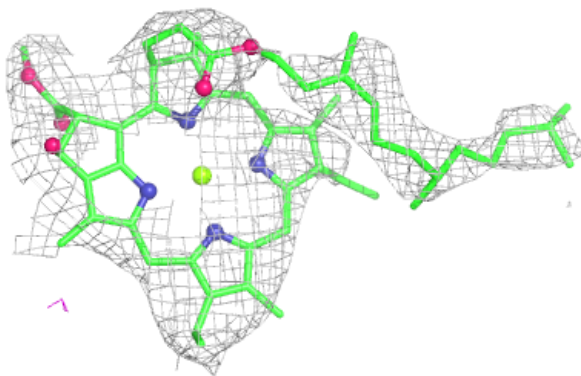
Electron density around CLA B 818:

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

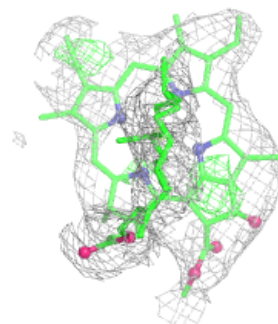
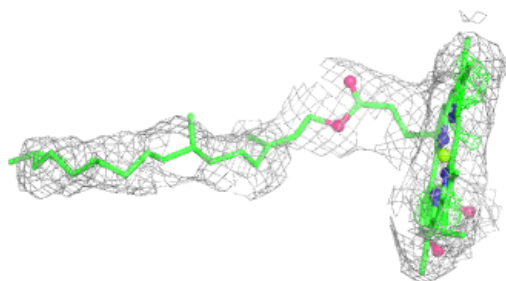
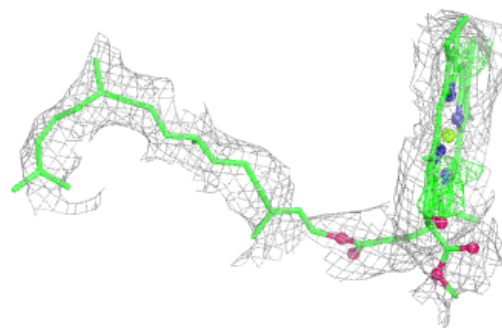


Electron density around CLA B 816:

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

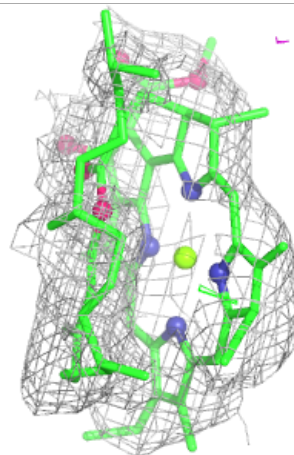
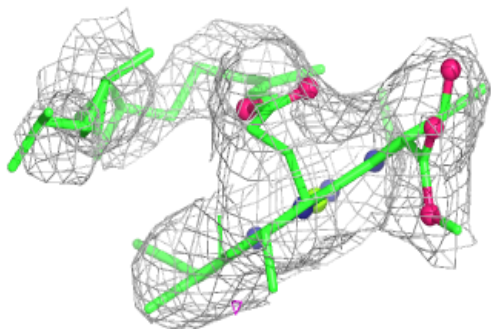
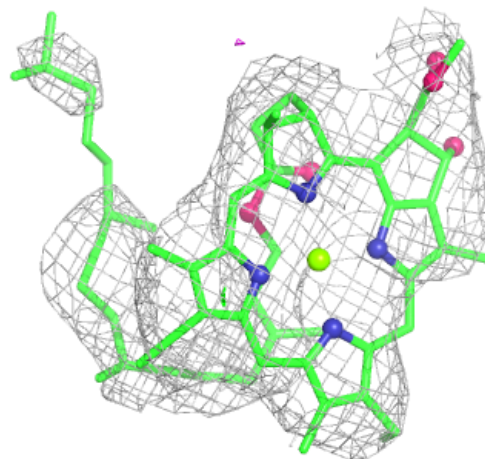
**Electron density around CLA B 839:**

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



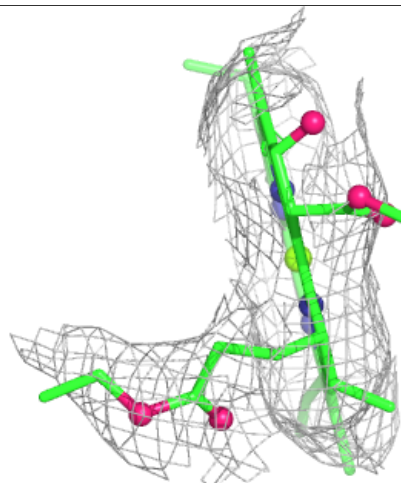
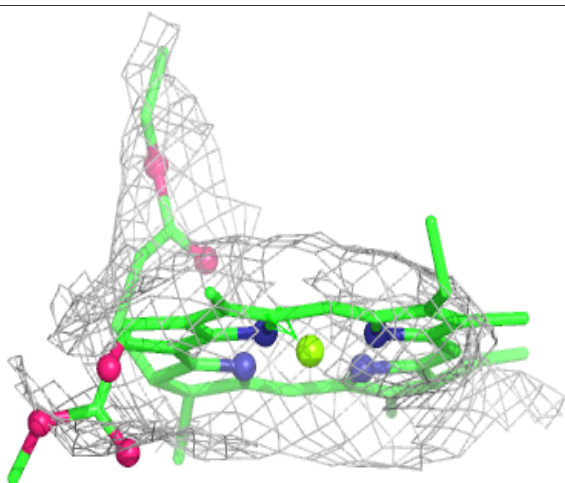
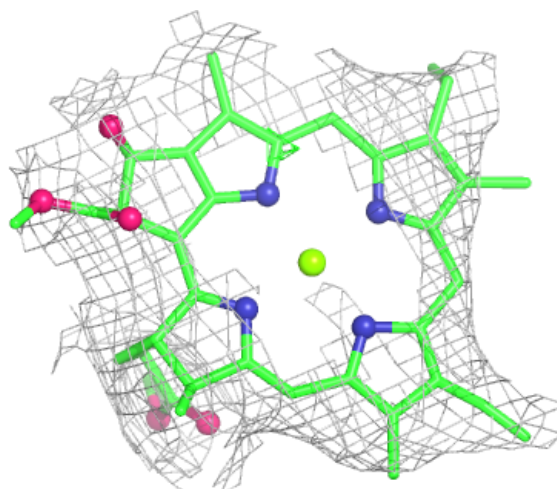
Electron density around CLA B 807:

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



Electron density around CLA B 837:

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



6.5 Other polymers [i](#)

There are no such residues in this entry.