



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 6, 2026 – 07:43 PM UTC

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

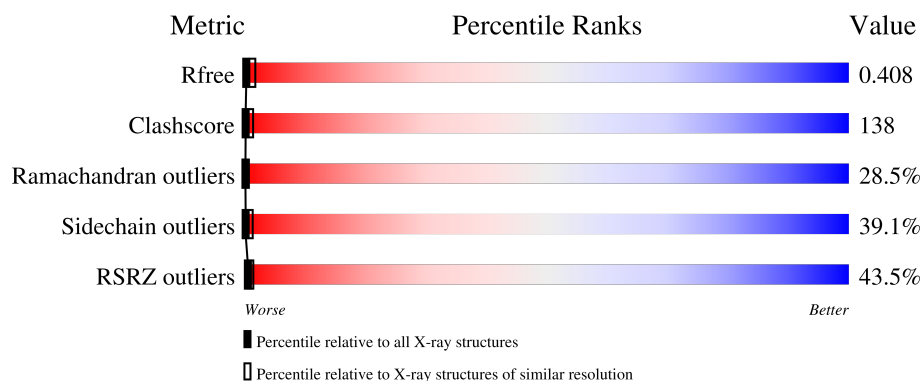
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.49 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% .

Continued on next page...

Continued from previous page...

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	

Continued on next page...

Continued from previous page...

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	201	X	-	-	-
20	CLA	1	202	X	-	X	-
20	CLA	1	203	X	-	-	-
20	CLA	1	204	X	-	-	-
20	CLA	1	205	X	-	-	-
20	CLA	1	206	X	-	-	-
20	CLA	1	207	X	-	-	-
20	CLA	1	208	X	-	-	-
20	CLA	1	209	X	-	-	-
20	CLA	1	210	X	-	-	-
20	CLA	1	211	X	-	-	-
20	CLA	1	212	X	-	-	-
20	CLA	1	214	X	-	-	-
20	CLA	1	215	X	-	X	-
20	CLA	1	216	X	-	-	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
20	CLA	2	301	X	-	-	-
20	CLA	2	302	X	-	-	-
20	CLA	2	303	X	-	-	-
20	CLA	2	304	X	-	-	-
20	CLA	2	305	X	-	-	-
20	CLA	2	306	X	-	-	-
20	CLA	2	307	X	-	-	-
20	CLA	2	308	X	-	-	-
20	CLA	2	309	X	-	-	-
20	CLA	2	310	X	-	-	-
20	CLA	2	311	X	-	-	-
20	CLA	2	312	X	-	-	-
20	CLA	2	314	X	-	-	-
20	CLA	2	315	X	-	-	-
20	CLA	2	320	X	-	X	-
20	CLA	3	301	X	-	-	-
20	CLA	3	302	X	-	X	-
20	CLA	3	303	X	-	-	-
20	CLA	3	304	X	-	-	-
20	CLA	3	305	X	-	-	-
20	CLA	3	306	X	-	-	-
20	CLA	3	307	X	-	-	-
20	CLA	3	308	X	-	-	-
20	CLA	3	309	X	-	-	-
20	CLA	3	310	X	-	-	-
20	CLA	3	311	X	-	-	-
20	CLA	3	312	X	-	-	-
20	CLA	3	313	X	-	X	-
20	CLA	3	315	X	-	-	-
20	CLA	3	316	X	-	-	-
20	CLA	3	317	X	-	-	-
20	CLA	3	318	X	-	-	-
20	CLA	3	319	X	-	-	-
20	CLA	4	302	X	-	X	-
20	CLA	4	303	X	-	-	-
20	CLA	4	304	X	-	X	-
20	CLA	4	305	X	-	-	-
20	CLA	4	306	X	-	-	-
20	CLA	4	307	X	-	-	-
20	CLA	4	308	X	-	-	-
20	CLA	4	309	X	-	-	-
20	CLA	4	310	X	-	-	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
20	CLA	4	311	X	-	-	-
20	CLA	4	312	X	-	-	-
20	CLA	4	313	X	-	-	-
20	CLA	4	314	X	-	-	-
20	CLA	4	315	X	-	-	-
20	CLA	4	316	X	-	-	-
20	CLA	4	318	X	-	-	-
20	CLA	4	319	X	-	-	-
20	CLA	A	801	X	-	-	-
20	CLA	A	802	X	-	-	-
20	CLA	A	803	X	-	-	-
20	CLA	A	804	X	-	X	-
20	CLA	A	805	X	-	X	-
20	CLA	A	806	X	-	-	-
20	CLA	A	807	X	-	X	-
20	CLA	A	808	X	-	X	-
20	CLA	A	809	X	-	X	-
20	CLA	A	810	X	-	-	-
20	CLA	A	811	X	-	X	-
20	CLA	A	812	X	-	-	-
20	CLA	A	813	X	-	-	-
20	CLA	A	814	X	-	X	-
20	CLA	A	815	X	-	X	-
20	CLA	A	816	X	-	X	-
20	CLA	A	817	X	-	-	-
20	CLA	A	818	X	-	X	-
20	CLA	A	819	X	-	X	-
20	CLA	A	820	X	-	-	-
20	CLA	A	821	X	-	-	-
20	CLA	A	822	X	-	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	829	X	-	-	-
20	CLA	A	830	X	-	X	-
20	CLA	A	831	X	-	-	-
20	CLA	A	832	X	-	-	-
20	CLA	A	833	X	-	-	-
20	CLA	A	834	X	-	-	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
20	CLA	A	835	X	-	-	-
20	CLA	A	836	X	-	-	-
20	CLA	A	837	X	-	-	-
20	CLA	A	838	X	-	X	-
20	CLA	A	839	X	-	X	-
20	CLA	A	840	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	804	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	-	-	-
20	CLA	B	813	X	-	-	-
20	CLA	B	814	X	-	-	-
20	CLA	B	815	X	-	-	-
20	CLA	B	816	X	-	-	-
20	CLA	B	817	X	-	-	-
20	CLA	B	818	X	-	-	-
20	CLA	B	819	X	-	-	-
20	CLA	B	820	X	-	-	-
20	CLA	B	821	X	-	X	-
20	CLA	B	822	X	-	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	828	X	-	-	-
20	CLA	B	829	X	-	-	-
20	CLA	B	830	X	-	X	-
20	CLA	B	831	X	-	-	-
20	CLA	B	832	X	-	-	-
20	CLA	B	833	X	-	X	-
20	CLA	B	834	X	-	-	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
20	CLA	B	835	X	-	-	-
20	CLA	B	836	X	-	X	-
20	CLA	B	837	X	-	X	-
20	CLA	B	838	X	-	X	-
20	CLA	B	839	X	-	X	-
20	CLA	B	840	X	-	-	-
20	CLA	B	849	X	-	X	-
20	CLA	B	850	X	-	X	-
20	CLA	B	851	X	-	X	-
20	CLA	F	204	X	-	-	-
20	CLA	F	205	X	-	-	-
20	CLA	F	206	X	-	-	-
20	CLA	G	102	X	-	-	-
20	CLA	H	101	X	-	X	-
20	CLA	H	102	X	-	-	-
20	CLA	H	103	X	-	-	-
20	CLA	H	109	X	-	-	-
20	CLA	H	111	X	-	-	-
20	CLA	I	102	X	-	-	-
20	CLA	J	101	X	-	X	-
20	CLA	J	103	X	-	X	-
20	CLA	K	101	X	-	-	-
20	CLA	K	102	X	-	-	-
20	CLA	K	103	X	-	-	-
20	CLA	K	107	X	-	X	-
20	CLA	L	201	X	-	X	-
20	CLA	L	202	X	-	X	-
20	CLA	L	203	X	-	-	-
20	CLA	L	206	X	-	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	-
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	-	-	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
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

Continued on next page...

Continued from previous page...

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			

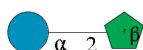
- Molecule 17 is a protein called PHOTOSYSTEM I-N SUBUNIT.

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.

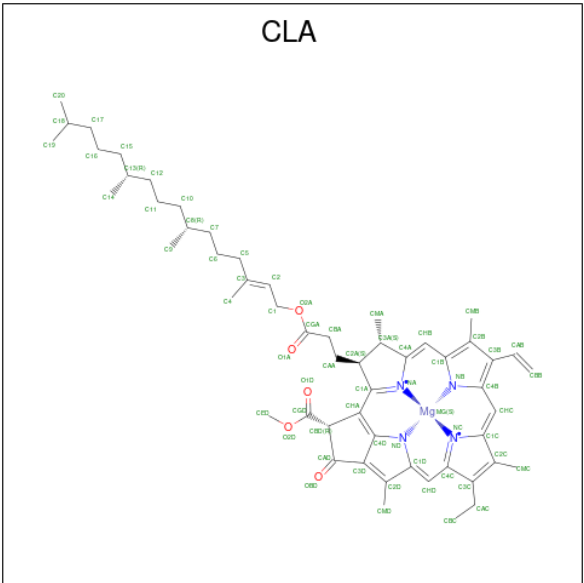
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
18	R	53	Total	C	N	O	0	0	0
			265	159	53	53			

- 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		

Continued on next page...

Continued from previous page...

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		

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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		

Continued on next page...

Continued from previous page...

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		

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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		

Continued on next page...

Continued from previous page...

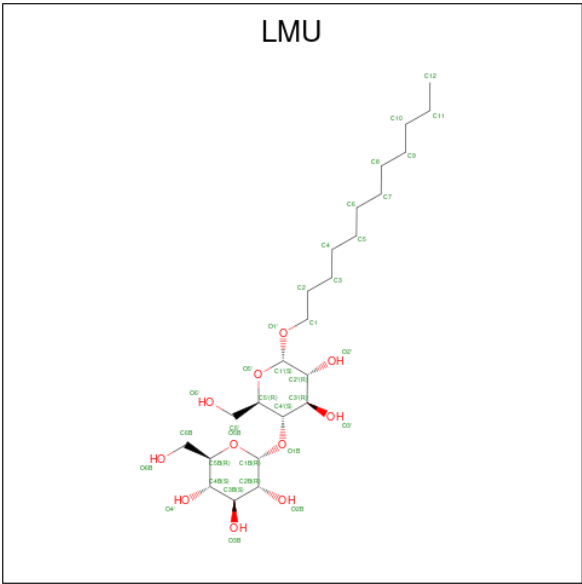
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
20	B	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
20	B	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
20	F	1	Total 36	C 30	Mg 1	N 4	O 1	0	0
20	F	1	Total 41	C 33	Mg 1	N 4	O 3	0	0
20	F	1	Total 53	C 43	Mg 1	N 4	O 5	0	0
20	G	1	Total 51	C 41	Mg 1	N 4	O 5	0	0
20	H	1	Total 55	C 45	Mg 1	N 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

Continued on next page...

Continued from previous page...

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		

Continued on next page...

Continued from previous page...

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		

Continued on next page...

Continued from previous page...

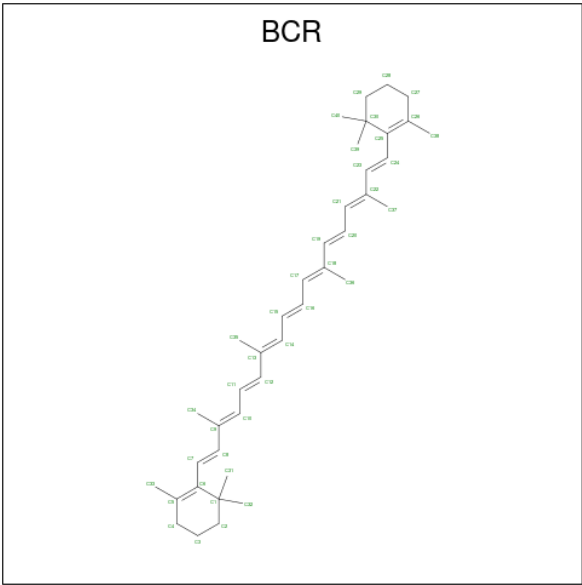
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
21	E	1	Total	C	O	0	0
			35	24	11		
21	F	1	Total	C	O	0	0
			34	23	11		
21	G	1	Total	C	O	0	0
			35	24	11		
21	H	1	Total	C	O	0	0
			35	24	11		
21	H	1	Total	C	O	0	0
			35	24	11		
21	H	1	Total	C	O	0	0
			35	24	11		
21	H	1	Total	C	O	0	0
			35	24	11		
21	K	1	Total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

Continued on next page...

Continued from previous page...

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).



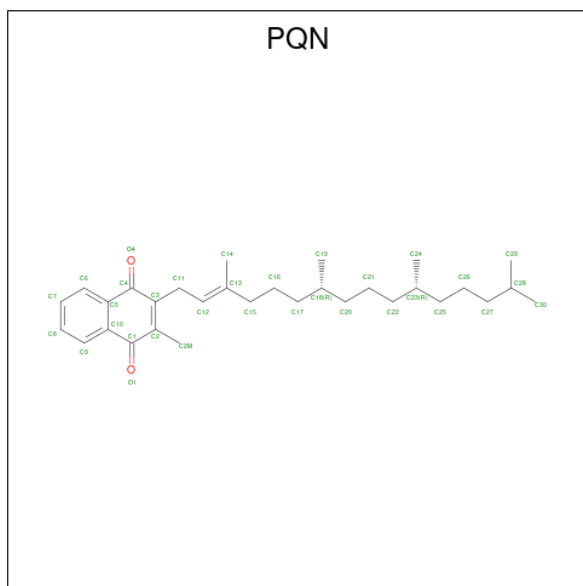
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
22	3	1	Total	C	0	0
			40	40		
22	A	1	Total	C	0	0
			40	40		
22	A	1	Total	C	0	0
			40	40		
22	A	1	Total	C	0	0
			40	40		
22	A	1	Total	C	0	0
			40	40		
22	A	1	Total	C	0	0
			40	40		
22	B	1	Total	C	0	0
			40	40		
22	B	1	Total	C	0	0
			40	40		
22	B	1	Total	C	0	0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

Continued on next page...

Continued from previous page...

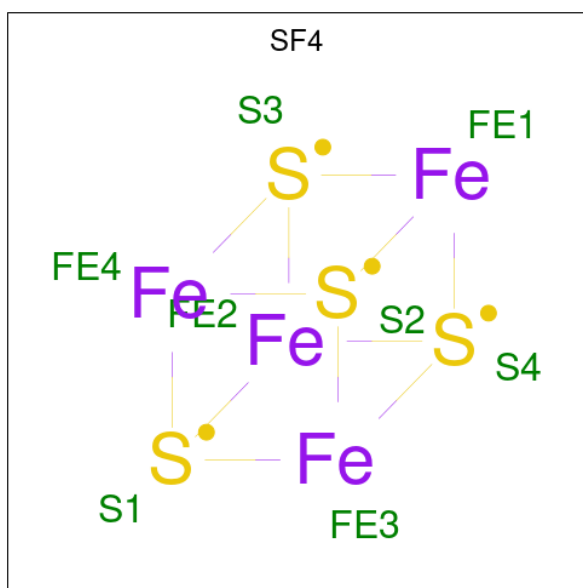
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
22	B	1	Total C 40 40	0	0
22	B	1	Total C 40 40	0	0
22	B	1	Total C 40 40	0	0
22	F	1	Total C 40 40	0	0
22	F	1	Total C 40 40	0	0
22	I	1	Total C 40 40	0	0
22	I	1	Total C 40 40	0	0
22	J	1	Total C 40 40	0	0
22	L	1	Total C 40 40	0	0

- Molecule 23 is PHYLLOQUINONE (CCD ID: PQN) (formula: C₃₁H₄₆O₂).



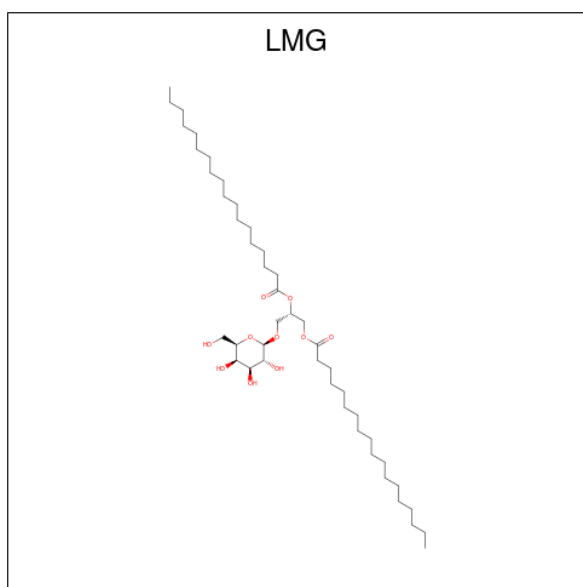
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
23	A	1	Total C O 33 31 2	0	0
23	B	1	Total C O 33 31 2	0	0

- 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		

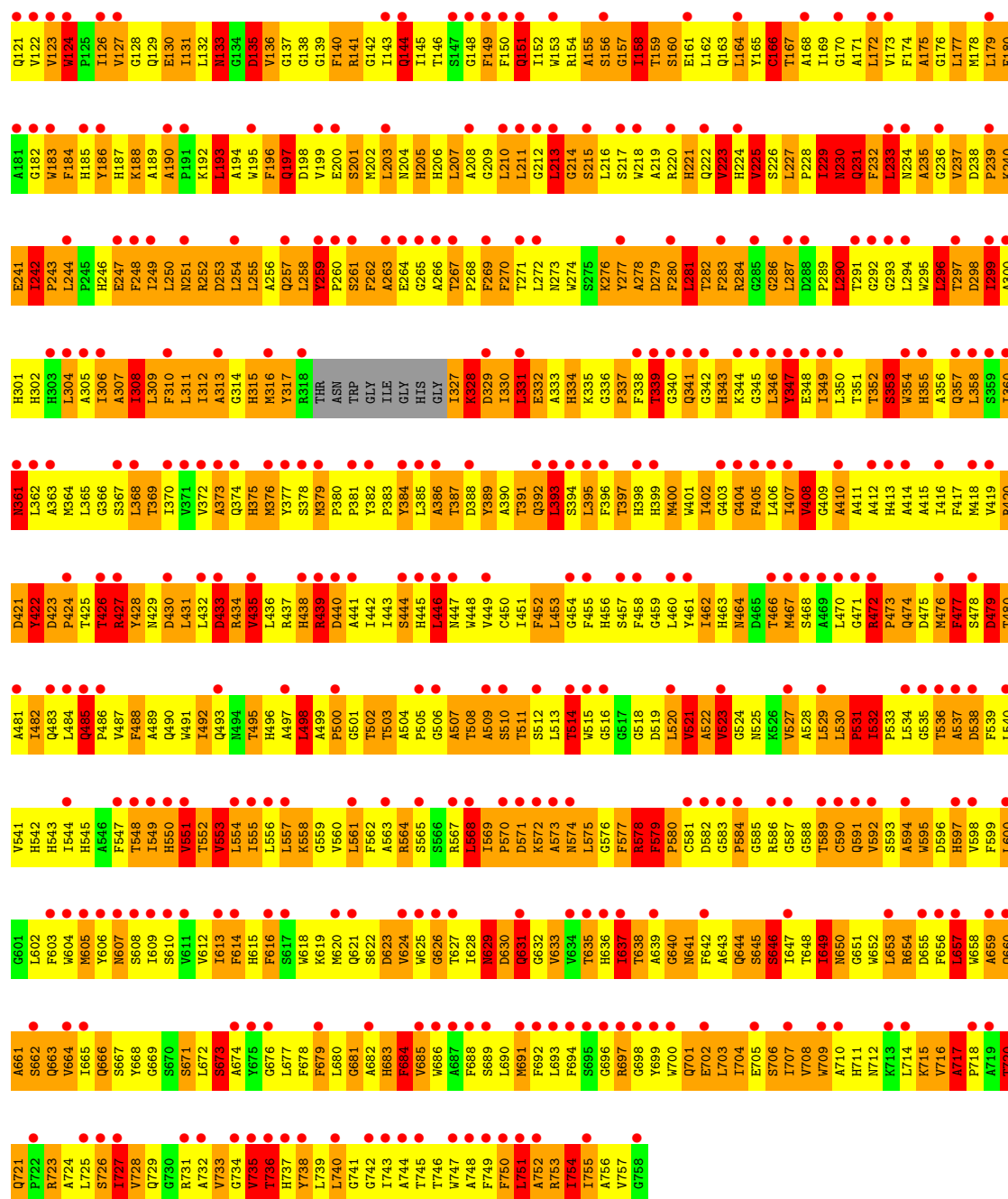
- Molecule 25 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (CCD ID: LMG) (formula: $\text{C}_{45}\text{H}_{86}\text{O}_{10}$).

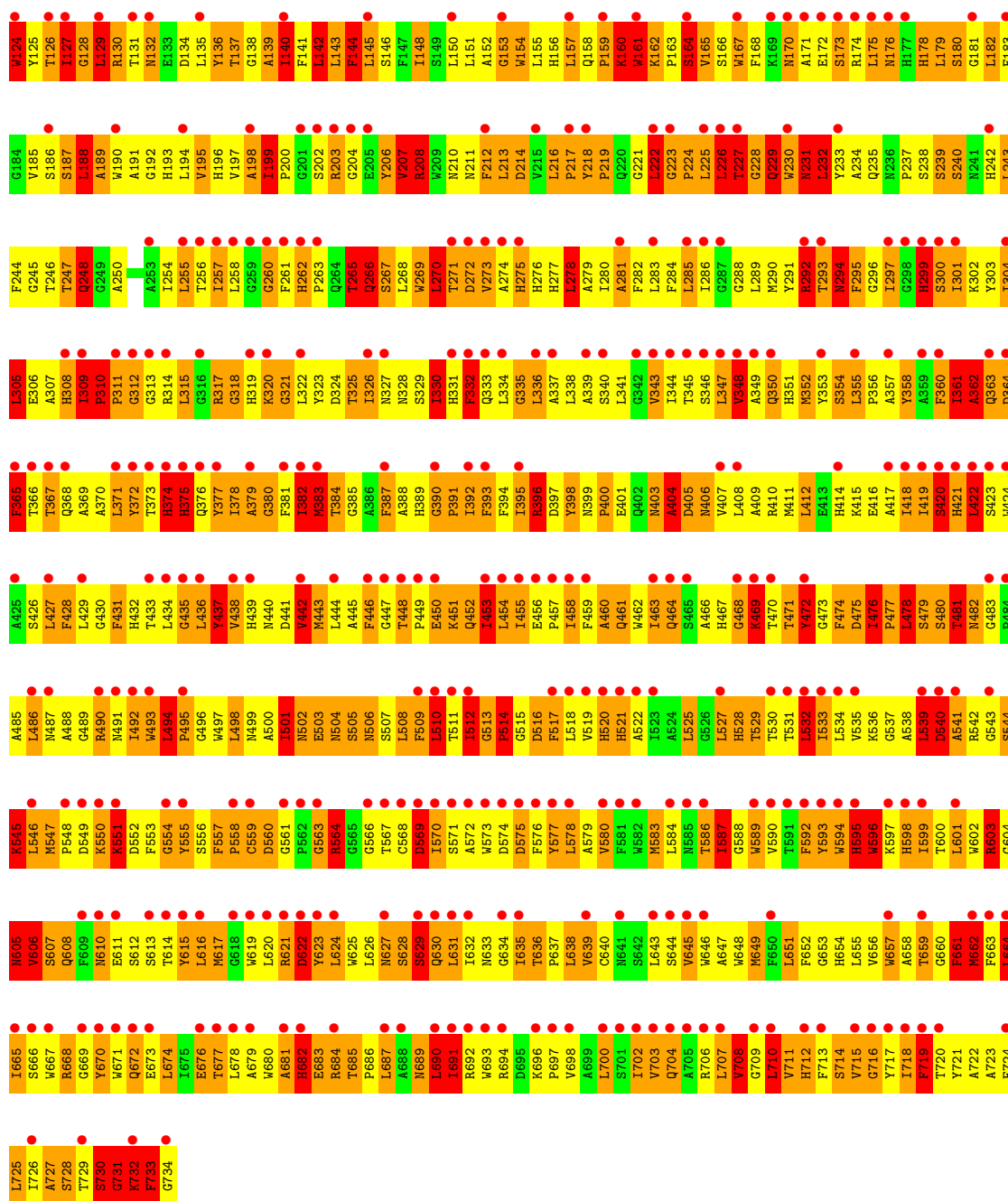


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
25	B	1	Total	C	O	0	0
			49	39	10		

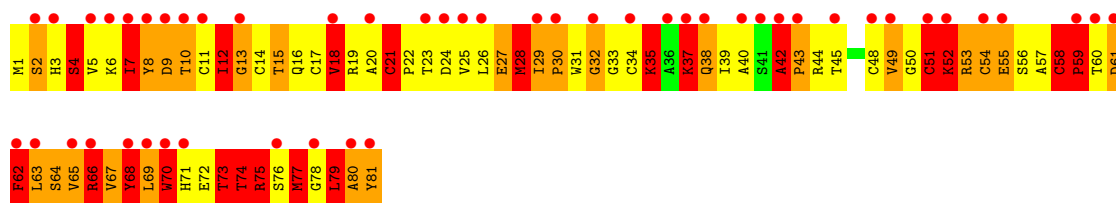
- Molecule 26 is UNKNOWN LIGAND (CCD ID: UNL) (formula:).

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

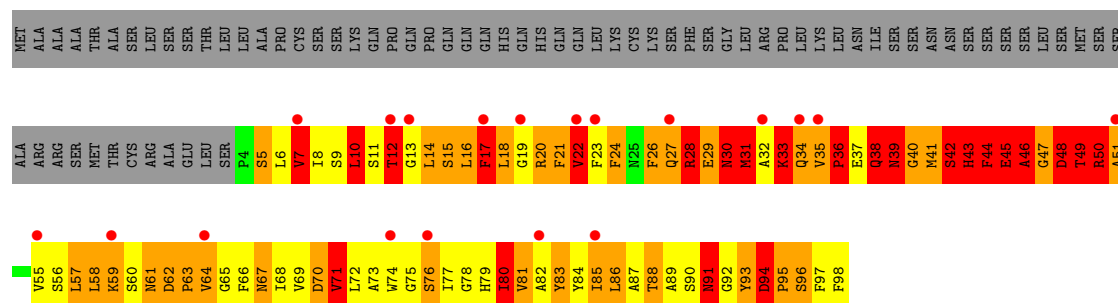




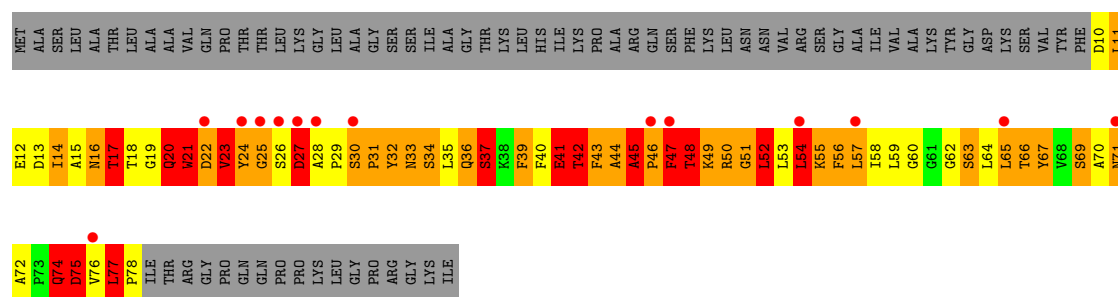
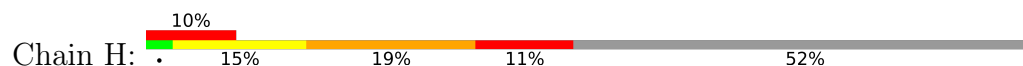
• Molecule 7: PHOTOSYSTEM I IRON-SULFUR CENTER



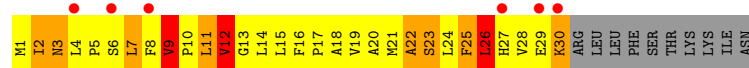
• Molecule 8: PHOTOSYSTEM I REACTION CENTER SUBUNIT II, CHLOROPLASTIC



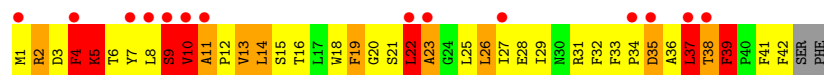
• Molecule 12: PHOTOSYSTEM I REACTION CENTER SUBUNIT VI, CHLOROPLASTIC



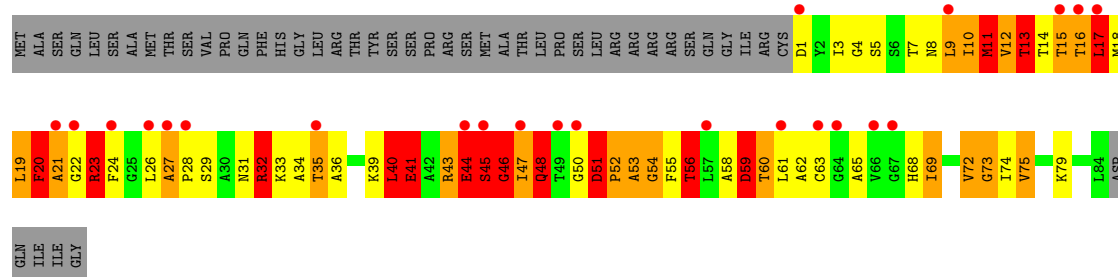
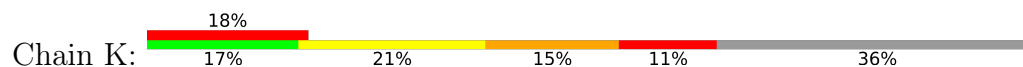
• Molecule 13: PHOTOSYSTEM I REACTION CENTER SUBUNIT VIII



• Molecule 14: PHOTOSYSTEM I REACTION CENTER SUBUNIT IX



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



WORLD WIDE
PDB
PROTEIN DATA BANK

- 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: PQN, CLA, GLC, LMG, BCR, UNL, SF4, FRU, LMU

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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	5
21	A	210	0	276	85	0
21	B	105	0	138	45	30
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	5
22	3	40	0	54	19	28
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

Continued on next page...

Continued from previous page...

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	69

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 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 69 symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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	0.85	0	15,15,17	2.41	3 (20%)
19	FRU	M	2	19	11,12,12	1.04	1 (9%)	10,18,18	0.98	0
19	GLC	O	1	19	10,10,12	1.50	3 (30%)	14,14,17	3.00	9 (64%)
19	FRU	O	2	19	11,12,12	1.12	1 (9%)	10,18,18	2.28	3 (30%)
19	GLC	P	1	19	11,11,12	1.47	2 (18%)	15,15,17	2.73	8 (53%)
19	FRU	P	2	19	11,12,12	1.36	2 (18%)	10,18,18	2.10	2 (20%)
19	GLC	Q	1	19	11,11,12	1.00	0	15,15,17	3.29	8 (53%)
19	FRU	Q	2	19	11,12,12	1.30	1 (9%)	10,18,18	1.71	2 (20%)
19	GLC	S	1	19	11,11,12	1.17	1 (9%)	15,15,17	1.43	2 (13%)
19	FRU	S	2	19	11,12,12	2.09	4 (36%)	10,18,18	2.72	4 (40%)
19	GLC	T	1	19	11,11,12	1.32	1 (9%)	15,15,17	1.62	3 (20%)
19	FRU	T	2	19	11,12,12	1.72	2 (18%)	10,18,18	2.34	4 (40%)
19	GLC	U	1	19	11,11,12	1.33	1 (9%)	15,15,17	1.42	2 (13%)
19	FRU	U	2	19	11,12,12	1.26	1 (9%)	10,18,18	1.61	2 (20%)
19	GLC	V	1	19	11,11,12	1.13	1 (9%)	15,15,17	3.26	6 (40%)
19	FRU	V	2	19	11,12,12	1.15	0	10,18,18	2.25	4 (40%)
19	GLC	W	1	19	11,11,12	1.12	1 (9%)	15,15,17	1.41	3 (20%)
19	FRU	W	2	19	11,12,12	1.24	1 (9%)	10,18,18	2.18	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	1.25	1 (9%)	15,15,17	2.05	4 (26%)
19	FRU	X	2	19	11,12,12	1.16	1 (9%)	10,18,18	1.83	4 (40%)
19	GLC	Y	1	19	11,11,12	1.89	2 (18%)	15,15,17	4.21	8 (53%)
19	FRU	Y	2	19	11,12,12	1.13	1 (9%)	10,18,18	2.38	3 (30%)
19	GLC	Z	1	19	11,11,12	1.05	0	15,15,17	1.84	5 (33%)
19	FRU	Z	2	19	11,12,12	0.70	0	10,18,18	1.70	4 (40%)
19	GLC	a	1	19	11,11,12	1.69	2 (18%)	15,15,17	1.89	5 (33%)
19	FRU	a	2	19	11,12,12	1.07	0	10,18,18	1.99	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	3/5/24/24	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	19	1/1/4/4	3/5/24/24	0/1/1/1

Continued on next page...

Continued from previous page...

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	2/5/24/24	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 30 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	Y	1	GLC	O5-C1	-4.55	1.36	1.43
19	S	2	FRU	O5-C2	-3.66	1.37	1.43
19	U	2	FRU	O5-C2	-3.39	1.38	1.43
19	Q	2	FRU	O5-C2	-3.24	1.38	1.43
19	T	2	FRU	O5-C2	-3.20	1.38	1.43

The worst 5 of 106 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	Y	1	GLC	C1-O5-C5	-11.33	97.00	112.19
19	M	1	GLC	C1-O5-C5	8.01	122.92	112.19
19	V	1	GLC	C1-O5-C5	7.55	122.31	112.19
19	S	2	FRU	O1-C1-C2	-6.55	97.18	111.67
19	O	1	GLC	C1-C2-C3	6.50	119.11	109.64

5 of 13 chirality outliers are listed below:

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

5 of 52 torsion outliers are listed below:

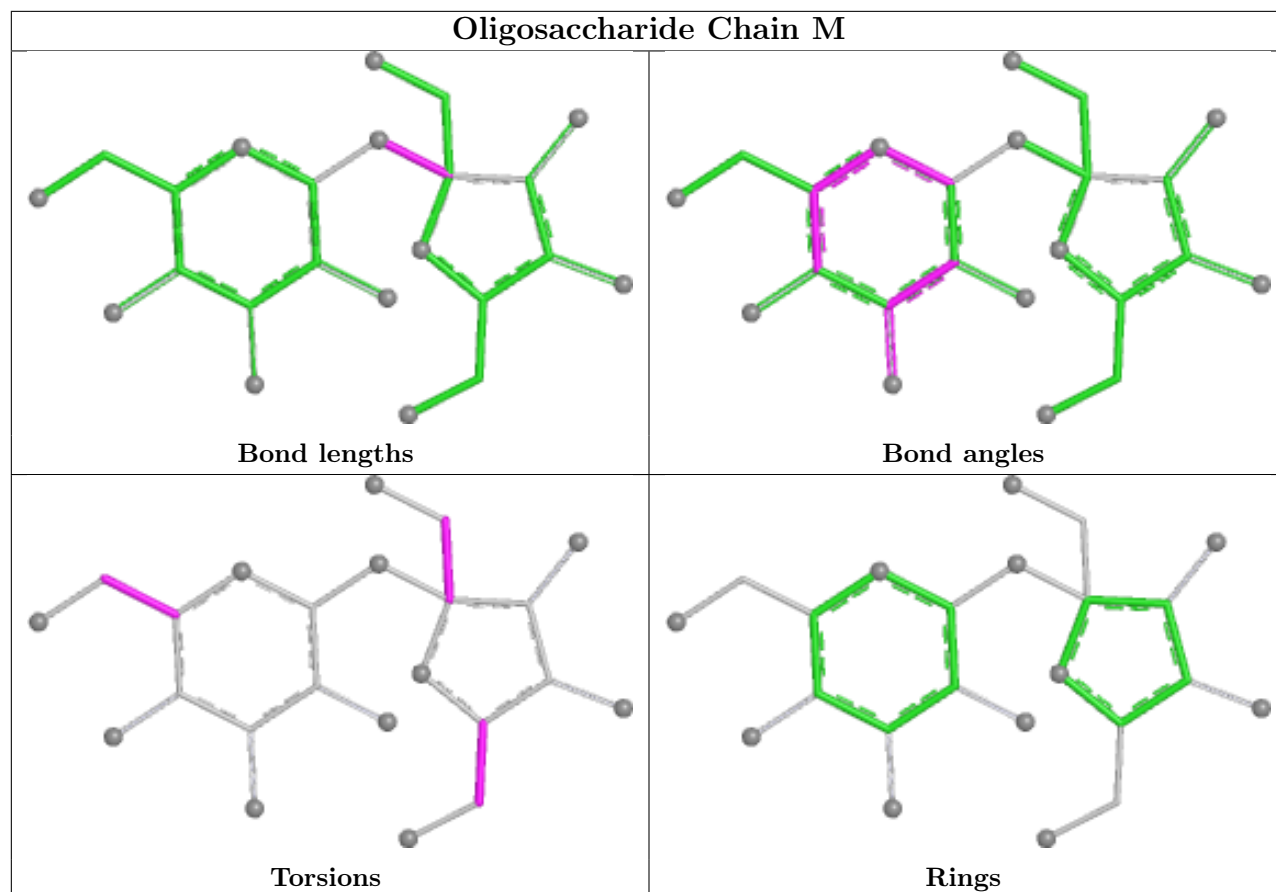
Mol	Chain	Res	Type	Atoms
19	Q	2	FRU	O1-C1-C2-C3
19	Q	2	FRU	O1-C1-C2-O2
19	U	2	FRU	O1-C1-C2-C3
19	U	2	FRU	O1-C1-C2-O2
19	U	2	FRU	C4-C5-C6-O6

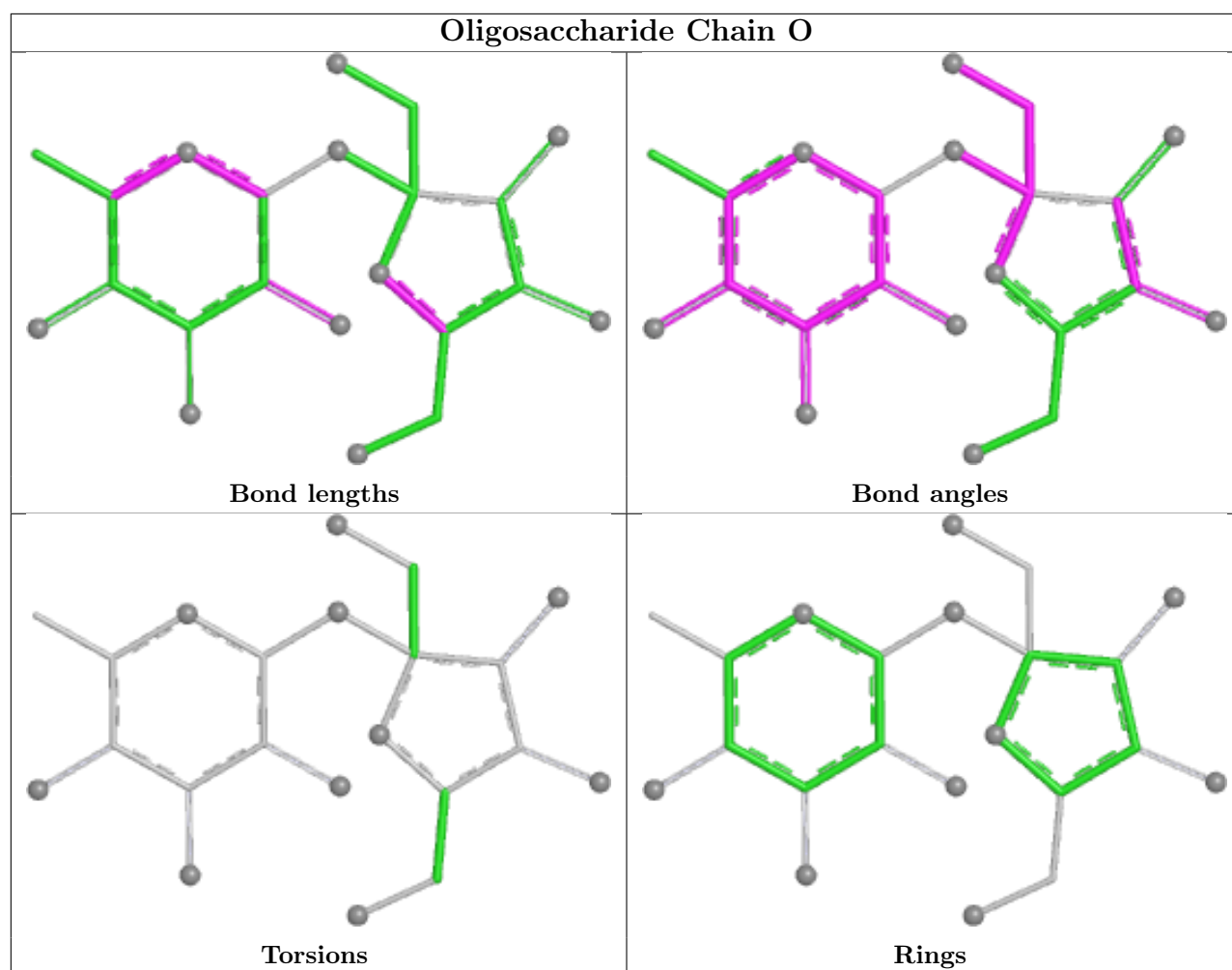
There are no ring outliers.

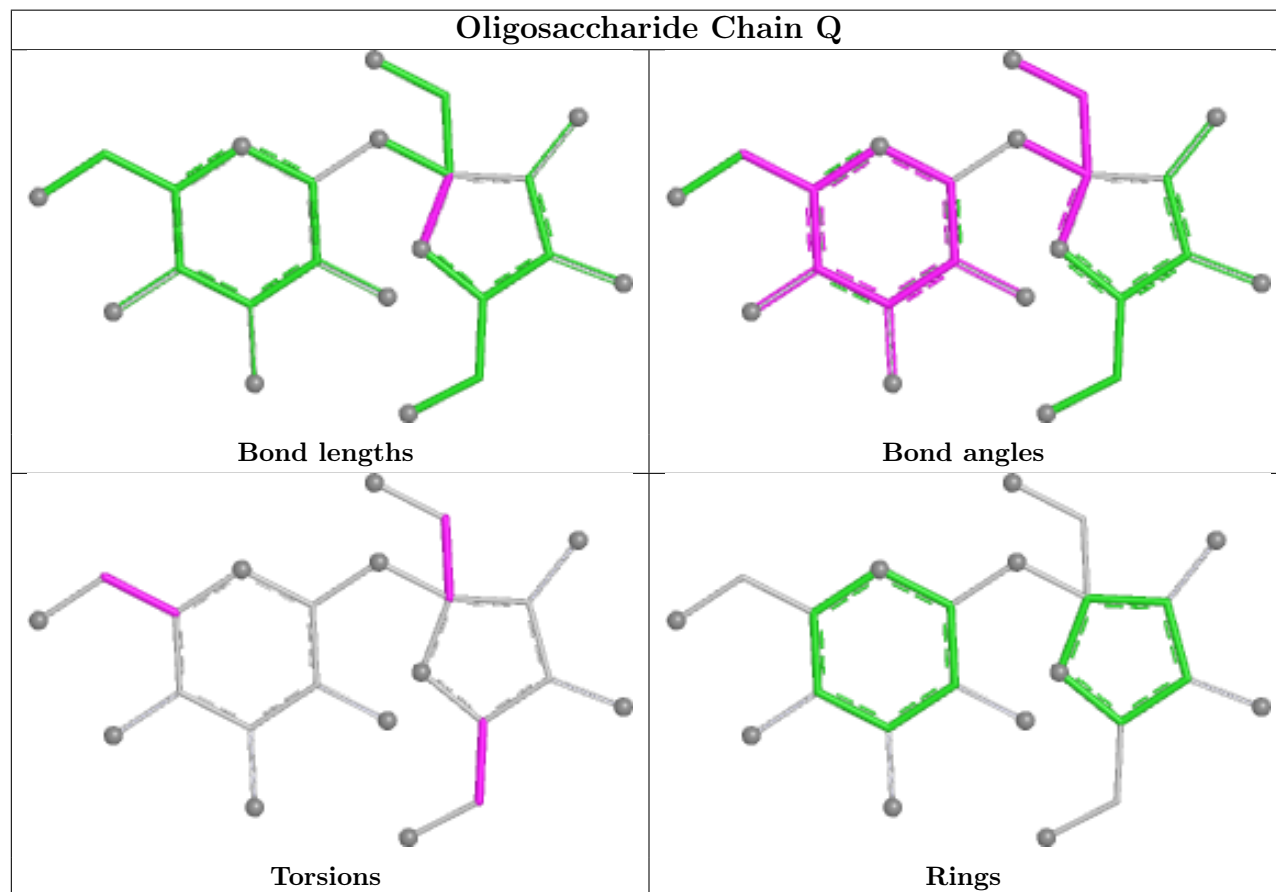
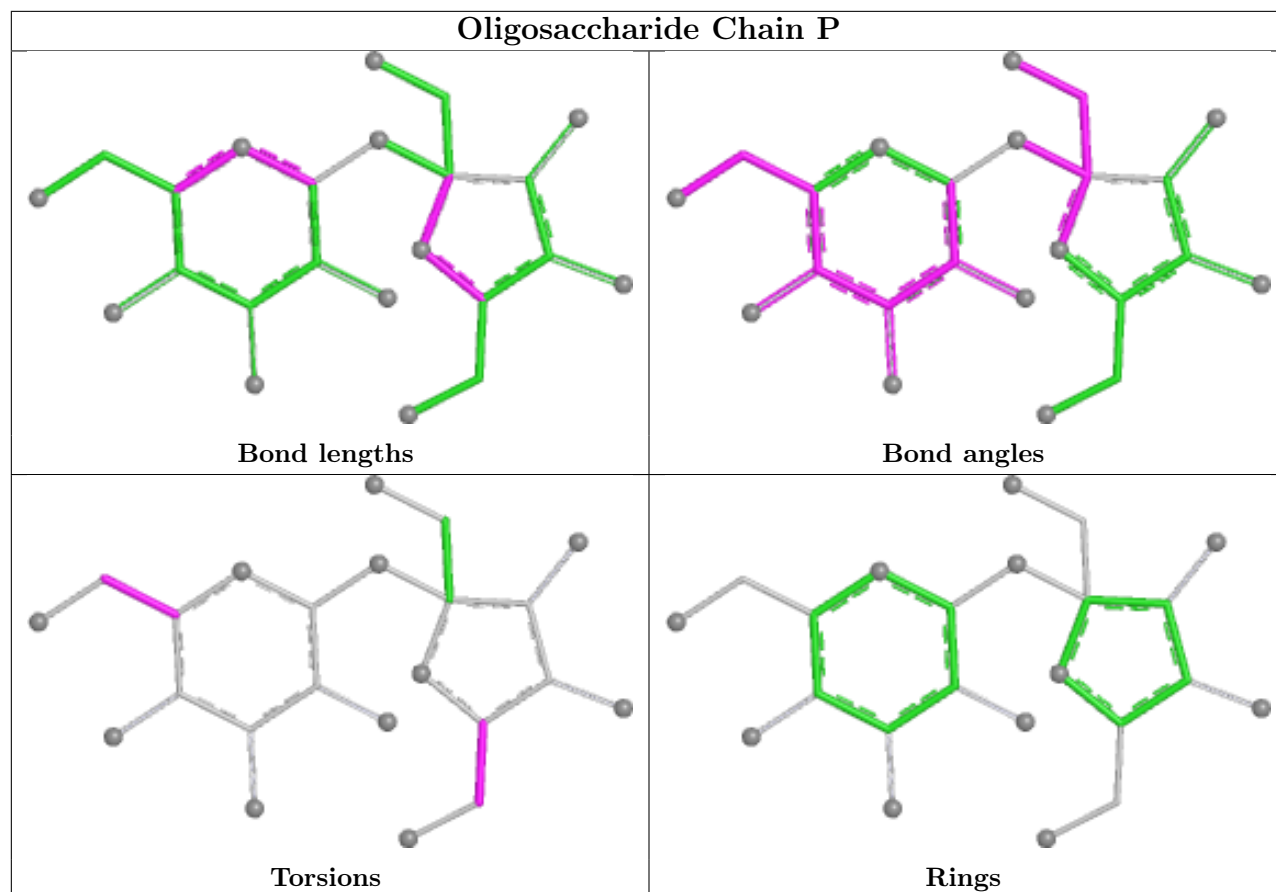
24 monomers are involved in 128 short contacts:

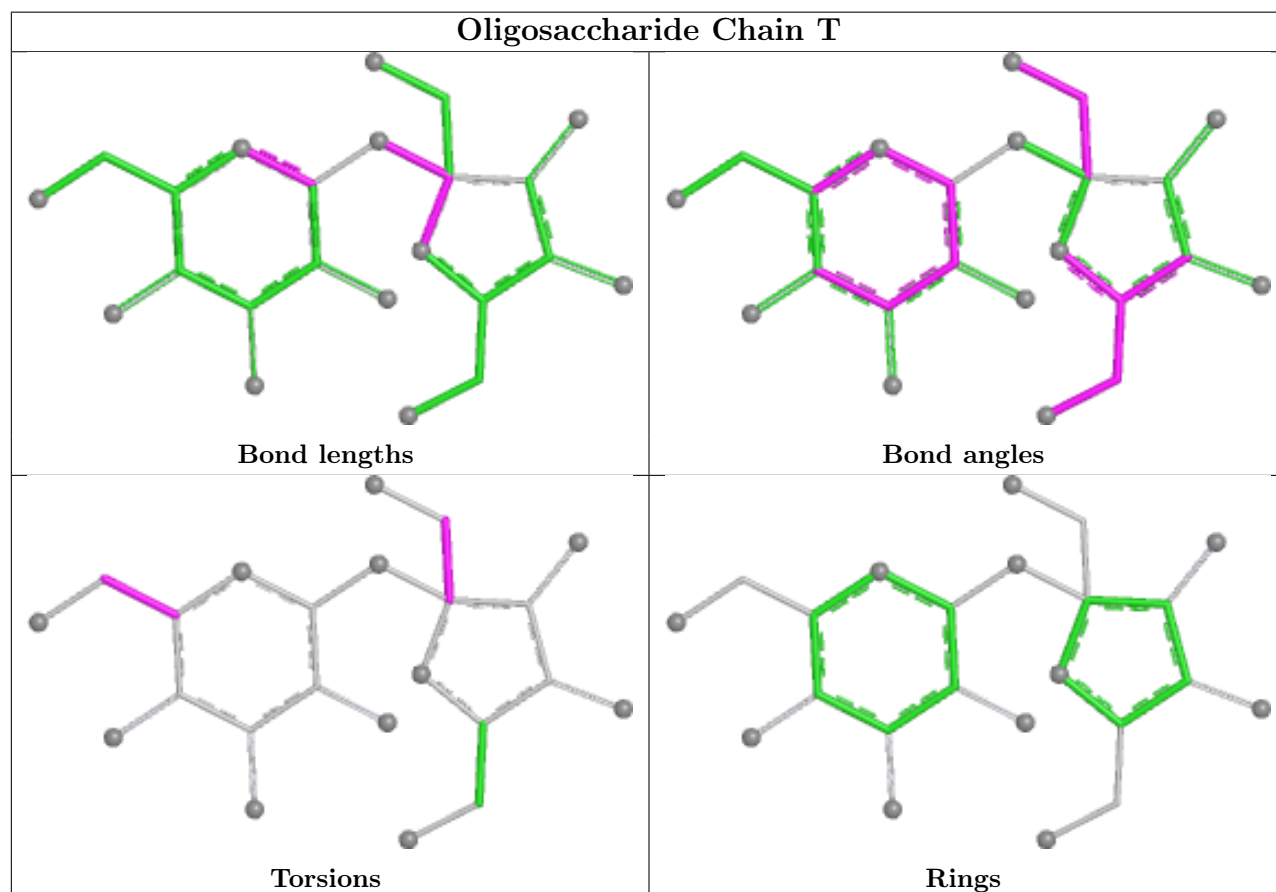
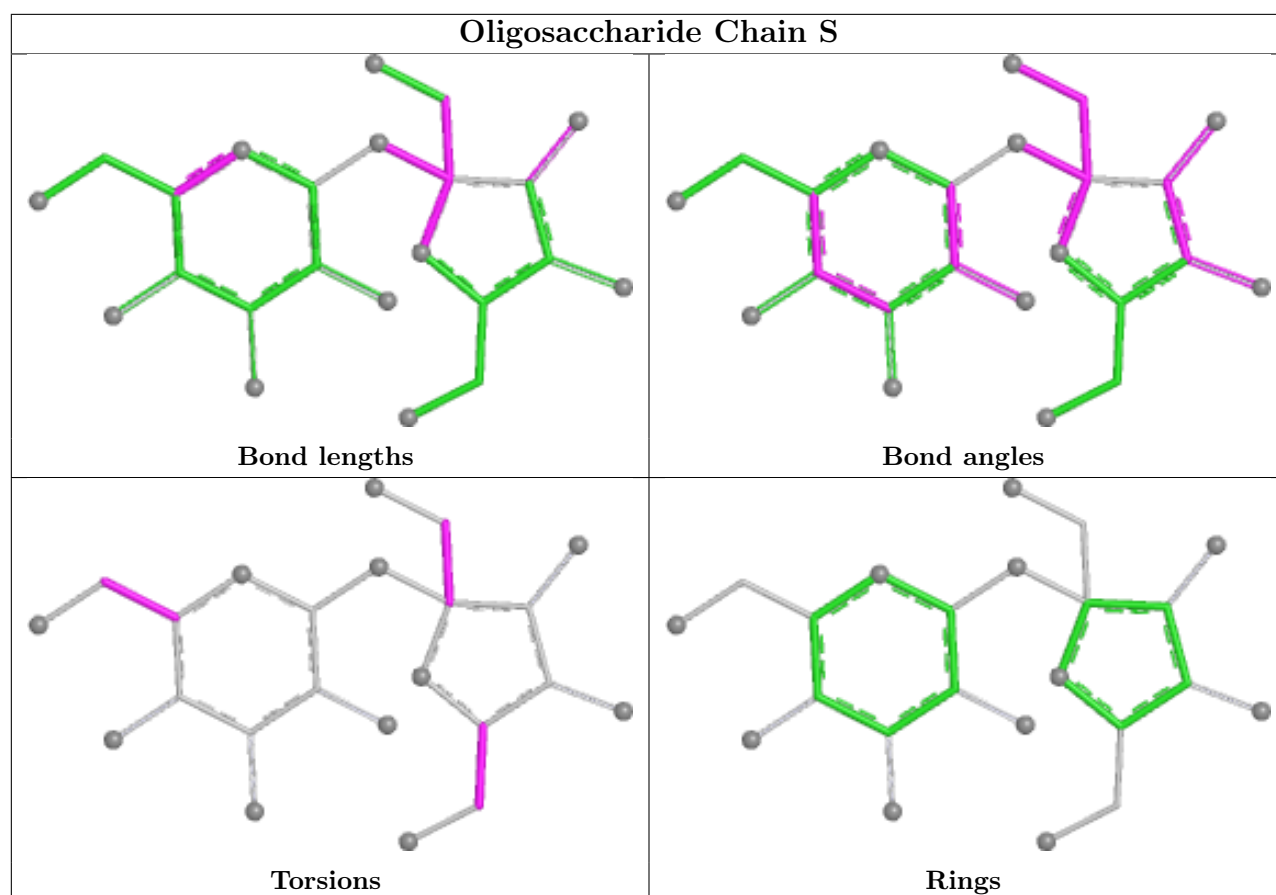
Mol	Chain	Res	Type	Clashes	Symm-Clashes
19	X	1	GLC	11	0
19	S	1	GLC	5	0
19	Y	2	FRU	17	0
19	O	2	FRU	6	0
19	X	2	FRU	9	0
19	W	2	FRU	3	0
19	P	2	FRU	15	0
19	S	2	FRU	6	0
19	Y	1	GLC	7	0
19	P	1	GLC	10	0
19	V	2	FRU	2	0
19	a	2	FRU	4	0
19	W	1	GLC	2	0
19	T	2	FRU	6	0
19	Q	2	FRU	14	0
19	O	1	GLC	10	0
19	T	1	GLC	6	0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

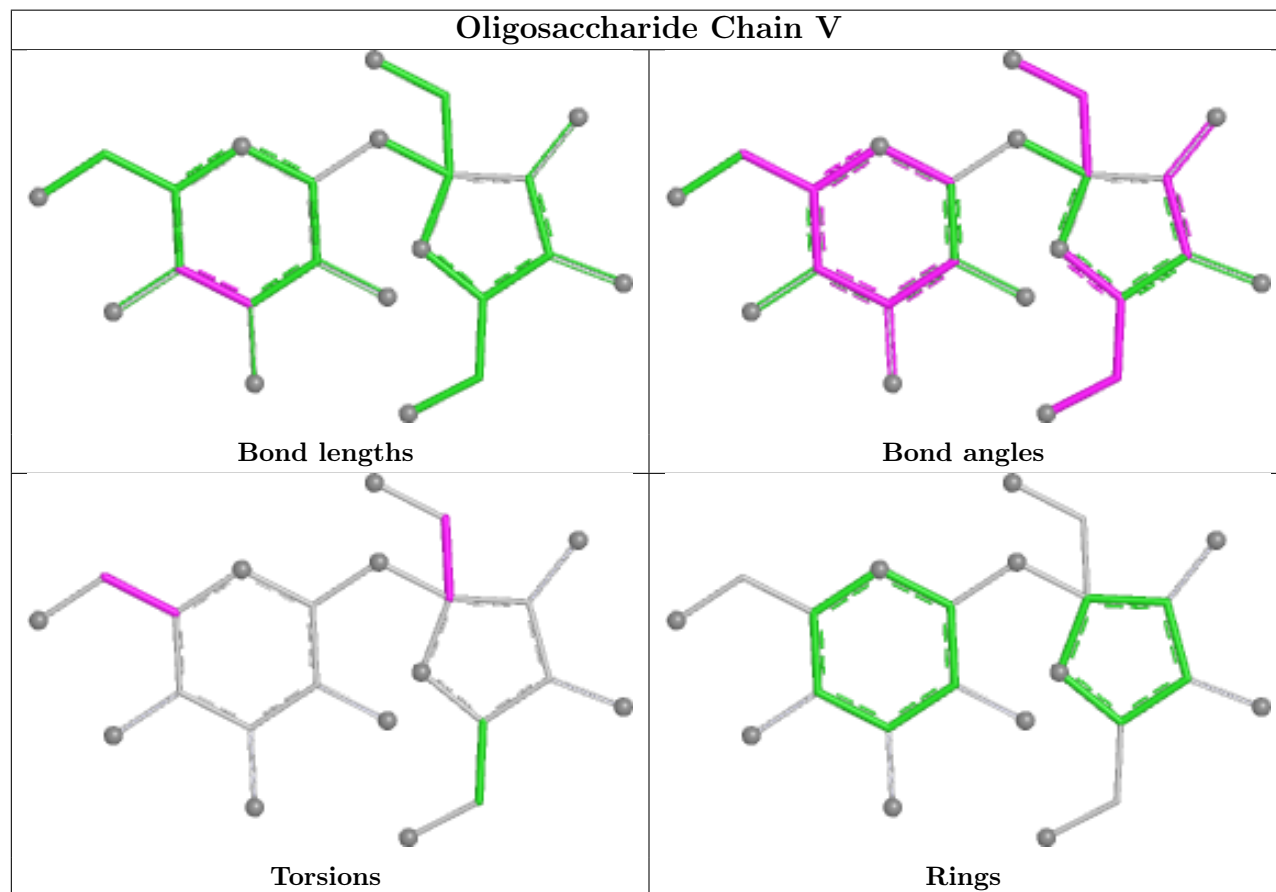
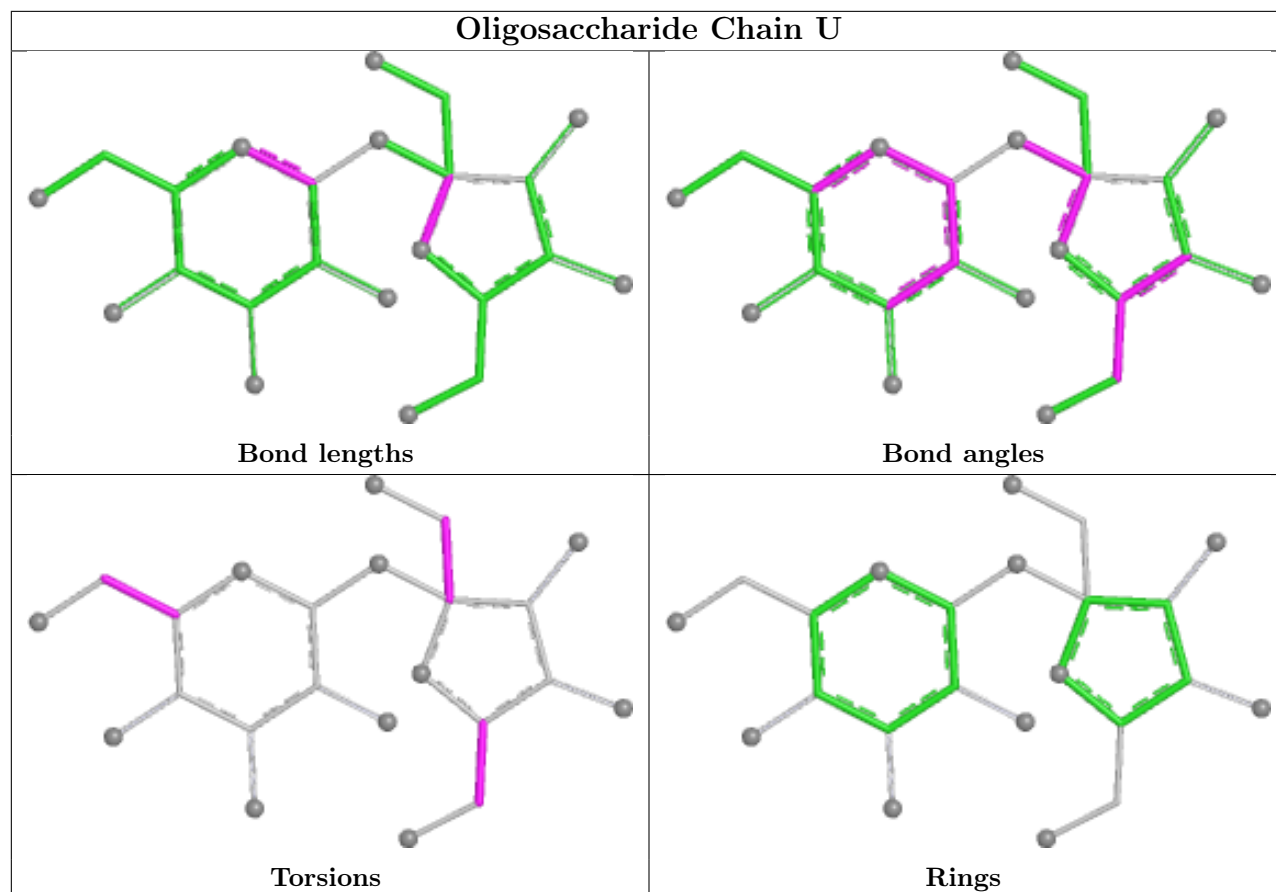
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

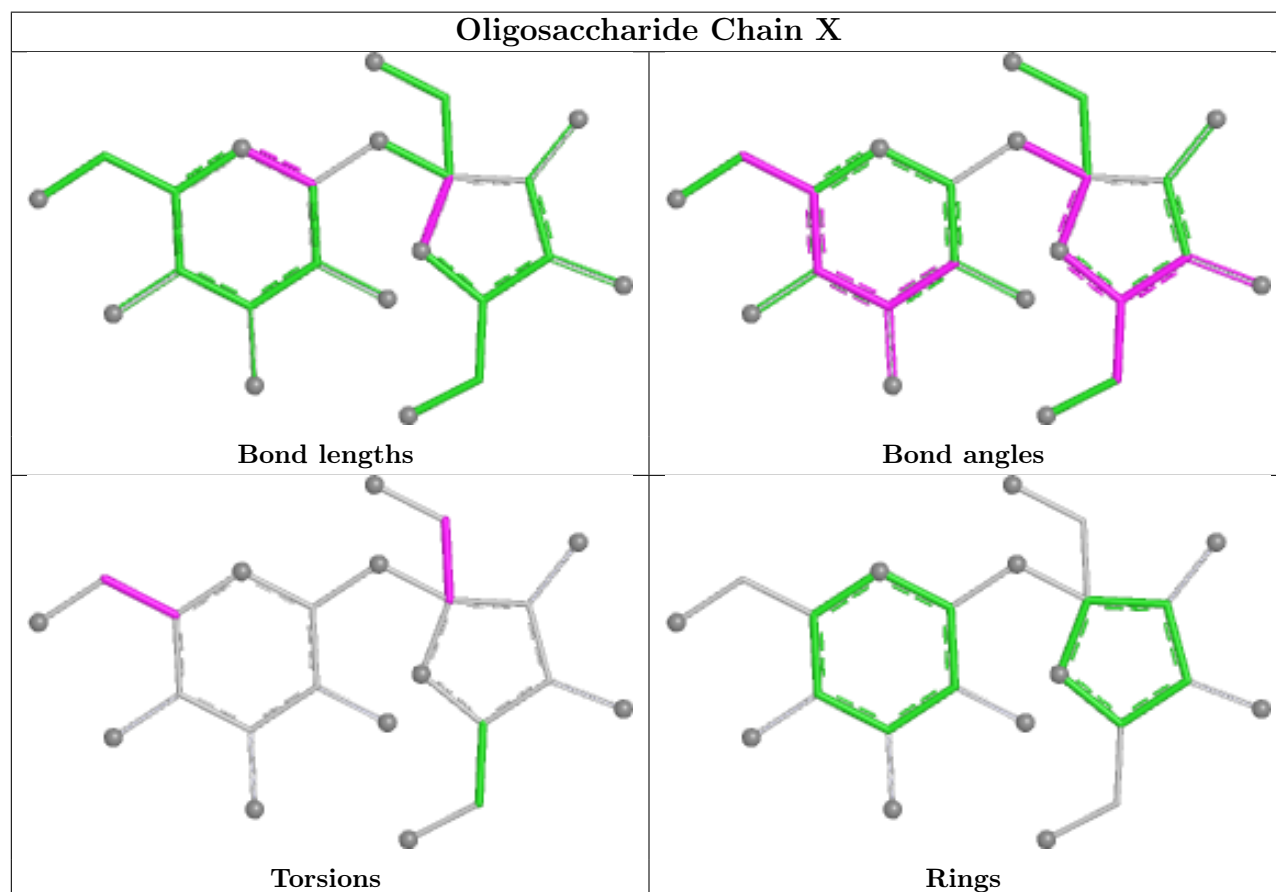
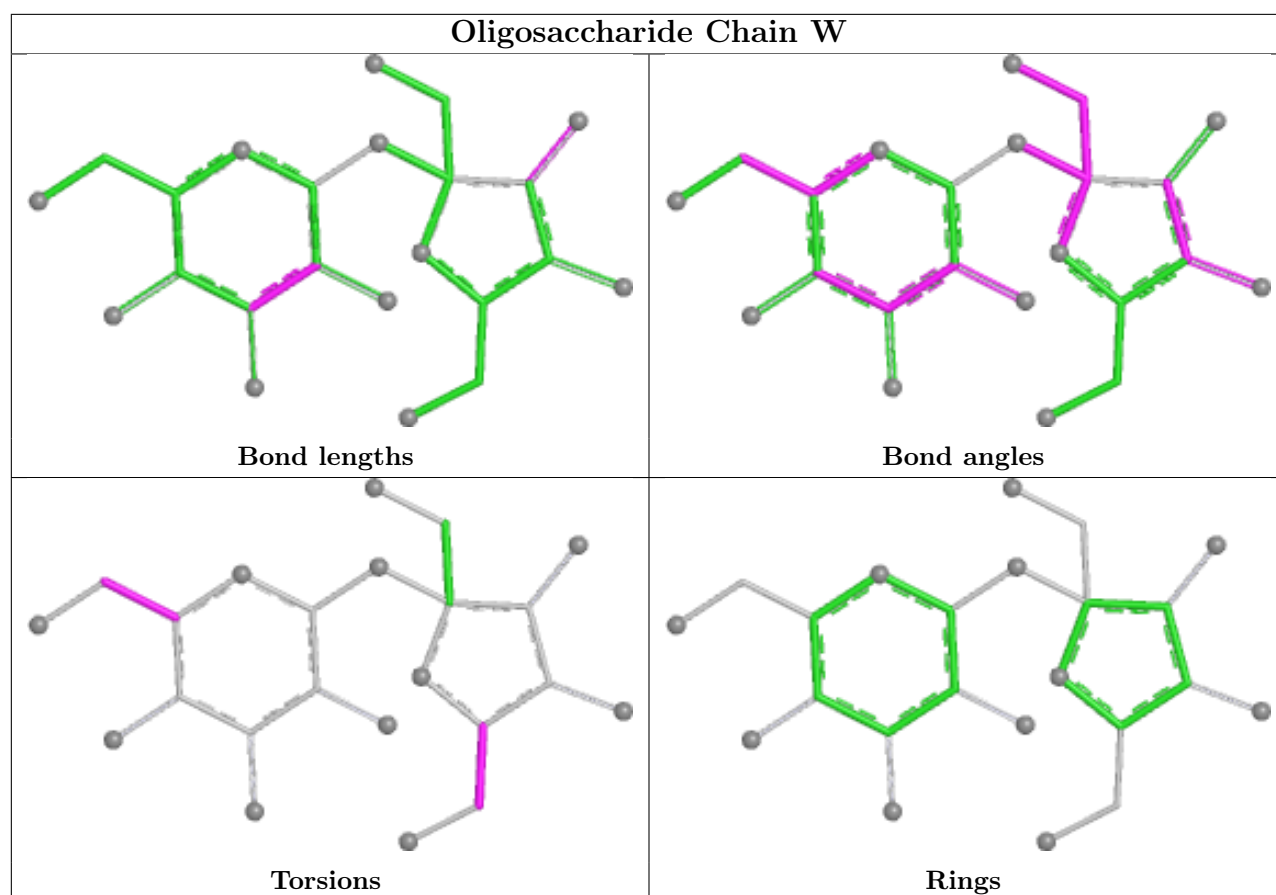


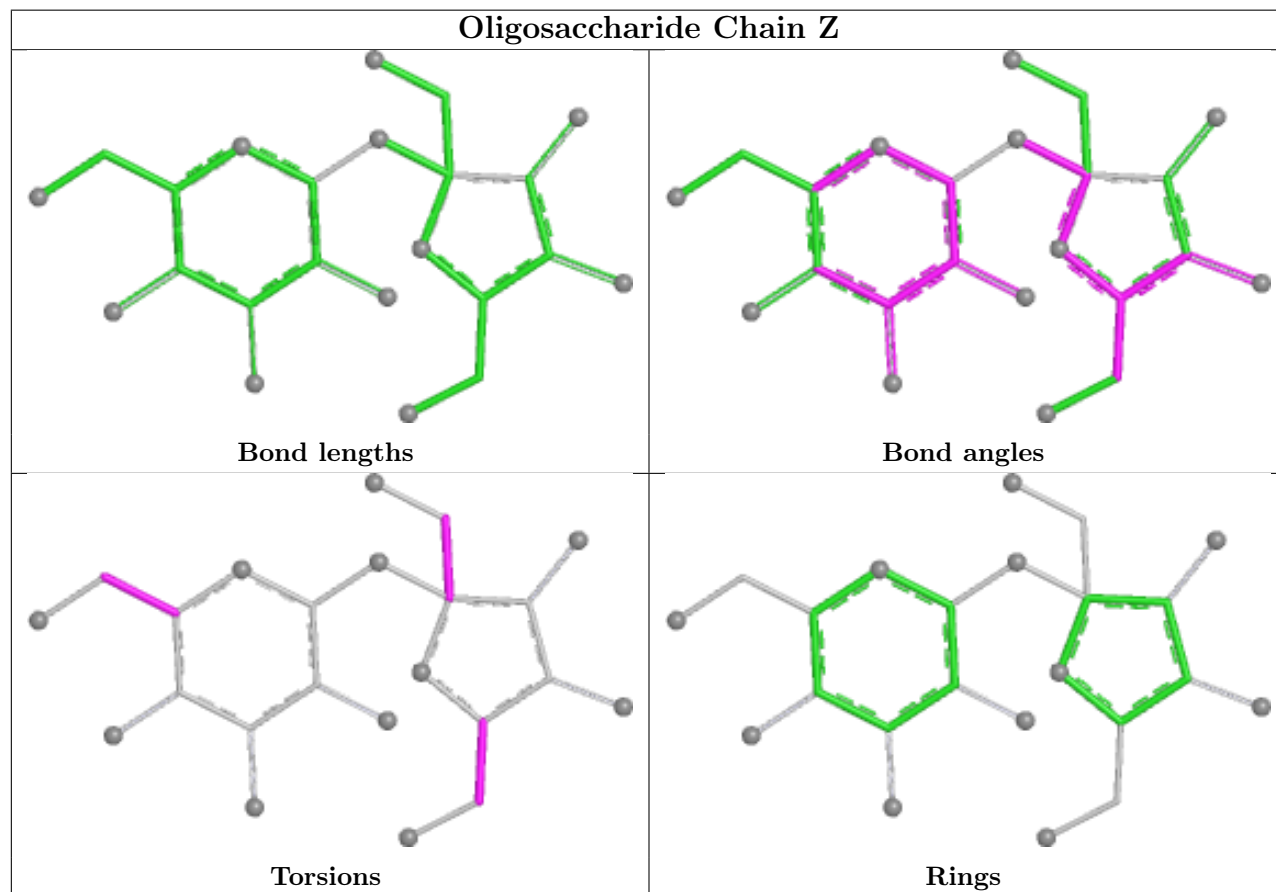
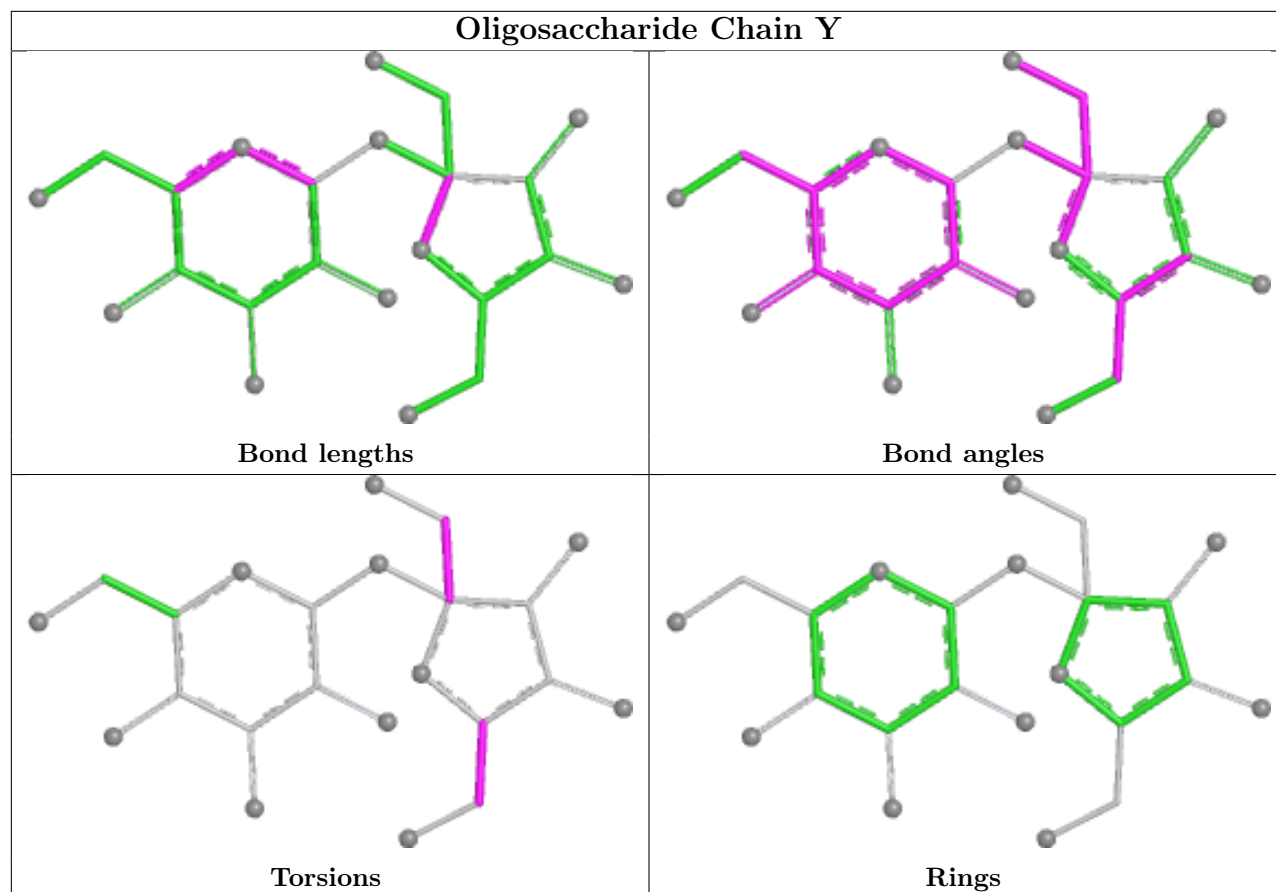


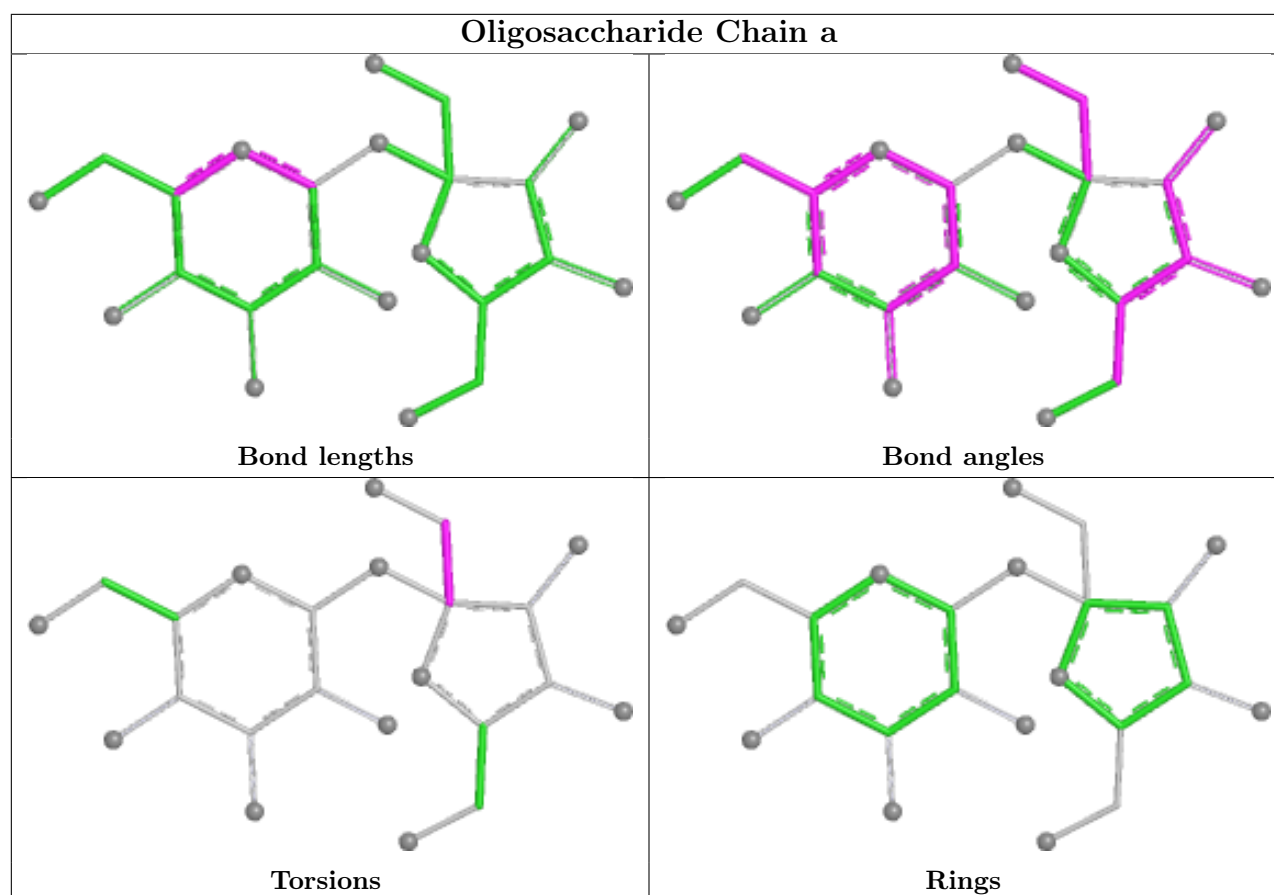












5.6 Ligand geometry [i](#)

Of 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	1	205	-	24,32,73	2.48	11 (45%)	31,54,113	3.49	20 (64%)
20	CLA	A	819	-	69,73,73	2.17	15 (21%)	82,113,113	2.59	24 (29%)
20	CLA	A	851	-	69,73,73	2.21	18 (26%)	82,113,113	2.62	26 (31%)
21	LMU	R	109	-	36,36,36	0.37	0	47,47,47	0.71	1 (2%)
21	LMU	1	213	-	36,36,36	0.80	0	47,47,47	2.15	16 (34%)
23	PQN	A	842	-	34,34,34	1.77	3 (8%)	43,45,45	1.51	8 (18%)
20	CLA	2	310	-	24,32,73	2.33	8 (33%)	31,54,113	2.81	17 (54%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
20	CLA	4	312	-	24,32,73	2.35	10 (41%)	31,54,113	3.04	20 (64%)
20	CLA	1	201	-	50,54,73	2.88	27 (54%)	59,90,113	4.07	37 (62%)
20	CLA	B	816	-	64,68,73	2.19	13 (20%)	76,107,113	2.69	29 (38%)
20	CLA	A	826	-	69,73,73	2.15	13 (18%)	82,113,113	2.69	29 (35%)
20	CLA	4	309	-	24,32,73	2.73	12 (50%)	31,54,113	3.50	19 (61%)
20	CLA	2	314	-	24,32,73	2.42	7 (29%)	31,54,113	2.71	17 (54%)
22	BCR	F	202	-	41,41,41	1.73	4 (9%)	56,56,56	6.04	17 (30%)
22	BCR	I	103	-	41,41,41	2.58	10 (24%)	56,56,56	6.70	31 (55%)
20	CLA	B	811	-	62,66,73	2.67	25 (40%)	73,104,113	3.38	28 (38%)
20	CLA	B	807	-	69,73,73	2.25	16 (23%)	82,113,113	2.80	28 (34%)
20	CLA	A	815	-	54,58,73	3.09	26 (48%)	64,95,113	3.65	35 (54%)
24	SF4	A	857	5,6	0,12,12	-	-	-	-	-
20	CLA	3	317	-	69,73,73	2.14	16 (23%)	82,113,113	2.47	22 (26%)
21	LMU	A	856	-	36,36,36	0.78	1 (2%)	47,47,47	1.64	8 (17%)
20	CLA	B	803	-	69,73,73	2.20	16 (23%)	82,113,113	2.65	31 (37%)
20	CLA	4	306	-	54,58,73	2.89	22 (40%)	64,95,113	3.22	23 (35%)
21	LMU	4	322	-	36,36,36	0.75	1 (2%)	47,47,47	1.28	4 (8%)
20	CLA	4	313	-	24,32,73	2.52	7 (29%)	31,54,113	2.90	21 (67%)
20	CLA	4	319	-	51,55,73	2.51	16 (31%)	60,91,113	2.96	21 (35%)
20	CLA	A	823	-	69,73,73	2.09	15 (21%)	82,113,113	2.52	24 (29%)
20	CLA	B	834	-	55,59,73	2.50	13 (23%)	64,96,113	2.97	26 (40%)
21	LMU	N	101	-	36,36,36	0.55	1 (2%)	47,47,47	2.07	14 (29%)
22	BCR	A	844	-	41,41,41	1.73	4 (9%)	56,56,56	6.09	18 (32%)
20	CLA	A	803	-	54,58,73	2.41	15 (27%)	64,95,113	3.28	28 (43%)
20	CLA	A	852	-	69,73,73	2.34	16 (23%)	82,113,113	2.86	27 (32%)
20	CLA	B	813	-	64,68,73	2.24	13 (20%)	76,107,113	2.62	27 (35%)
20	CLA	B	831	-	54,58,73	2.57	18 (33%)	64,95,113	3.11	27 (42%)
20	CLA	B	832	20	49,53,73	2.74	17 (34%)	58,89,113	3.07	21 (36%)
21	LMU	B	801	-	36,36,36	0.66	0	47,47,47	2.46	16 (34%)
20	CLA	H	109	-	64,68,73	2.35	14 (21%)	76,107,113	2.93	28 (36%)
20	CLA	2	303	-	69,73,73	2.22	16 (23%)	82,113,113	2.71	31 (37%)
20	CLA	A	836	-	51,55,73	2.48	14 (27%)	60,91,113	2.66	24 (40%)
20	CLA	2	309	-	24,32,73	2.40	8 (33%)	31,54,113	2.99	19 (61%)
20	CLA	1	202	-	61,65,73	2.73	28 (45%)	72,103,113	3.40	33 (45%)
20	CLA	F	205	-	45,49,73	2.70	15 (33%)	54,84,113	3.12	24 (44%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
20	CLA	3	313	-	69,73,73	2.61	27 (39%)	82,113,113	3.17	28 (34%)
20	CLA	A	818	-	69,73,73	2.17	16 (23%)	82,113,113	2.63	32 (39%)
21	LMU	2	319	-	36,36,36	1.05	1 (2%)	47,47,47	1.41	4 (8%)
20	CLA	1	209	1	38,44,73	2.87	12 (31%)	52,78,113	3.08	22 (42%)
20	CLA	B	822	-	58,62,73	2.42	19 (32%)	68,99,113	2.76	28 (41%)
20	CLA	2	312	-	54,58,73	2.56	13 (24%)	64,95,113	3.01	24 (37%)
20	CLA	1	211	-	24,32,73	2.44	7 (29%)	31,54,113	2.94	18 (58%)
20	CLA	1	216	-	24,32,73	2.34	14 (58%)	31,54,113	2.81	18 (58%)
20	CLA	A	840	-	54,58,73	2.51	15 (27%)	64,95,113	2.85	24 (37%)
21	LMU	B	802	-	36,36,36	1.01	4 (11%)	47,47,47	2.49	13 (27%)
20	CLA	B	825	-	69,73,73	2.34	16 (23%)	82,113,113	2.84	26 (31%)
21	LMU	F	201	-	35,35,36	1.29	4 (11%)	46,46,47	2.39	15 (32%)
20	CLA	B	818	-	54,58,73	2.41	14 (25%)	64,95,113	2.91	23 (35%)
20	CLA	4	314	-	38,44,73	2.76	12 (31%)	52,78,113	3.47	26 (50%)
21	LMU	K	104	-	36,36,36	0.66	1 (2%)	47,47,47	1.91	14 (29%)
20	CLA	4	307	-	56,60,73	3.19	28 (50%)	65,97,113	3.84	40 (61%)
20	CLA	4	308	-	38,44,73	2.98	15 (39%)	52,78,113	3.29	22 (42%)
22	BCR	B	846	-	41,41,41	1.80	4 (9%)	56,56,56	6.09	17 (30%)
21	LMU	4	321	-	36,36,36	0.95	1 (2%)	47,47,47	1.41	8 (17%)
20	CLA	A	830	-	69,73,73	2.27	16 (23%)	82,113,113	2.65	24 (29%)
20	CLA	1	208	-	24,32,73	2.64	11 (45%)	31,54,113	3.27	19 (61%)
20	CLA	2	307	-	69,73,73	2.51	27 (39%)	82,113,113	2.93	31 (37%)
20	CLA	A	806	-	59,63,73	2.36	14 (23%)	70,101,113	2.99	29 (41%)
20	CLA	B	814	-	50,54,73	2.50	12 (24%)	59,90,113	2.95	23 (38%)
20	CLA	H	101	-	59,63,73	2.67	24 (40%)	70,101,113	3.30	34 (48%)
20	CLA	L	207	-	54,58,73	2.61	19 (35%)	64,95,113	3.21	25 (39%)
20	CLA	1	204	-	50,54,73	2.62	16 (32%)	59,90,113	2.82	23 (38%)
25	LMG	B	848	-	49,49,55	0.97	2 (4%)	57,57,63	1.03	4 (7%)
20	CLA	B	839	-	69,73,73	2.10	17 (24%)	82,113,113	2.80	30 (36%)
21	LMU	1	218	-	36,36,36	0.43	0	47,47,47	1.64	9 (19%)
20	CLA	3	305	-	24,32,73	2.48	11 (45%)	31,54,113	3.33	20 (64%)
21	LMU	A	849	-	36,36,36	0.86	1 (2%)	47,47,47	1.68	10 (21%)
22	BCR	F	203	-	41,41,41	2.66	13 (31%)	56,56,56	6.23	31 (55%)
20	CLA	2	302	-	55,59,73	2.47	16 (29%)	64,96,113	2.95	24 (37%)
21	LMU	R	104	-	36,36,36	0.75	0	47,47,47	2.19	18 (38%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
20	CLA	4	302	-	59,63,73	2.40	17 (28%)	70,101,113	2.90	27 (38%)
20	CLA	A	813	-	58,62,73	2.26	16 (27%)	68,99,113	2.78	25 (36%)
20	CLA	3	310	-	24,32,73	2.42	10 (41%)	31,54,113	3.34	21 (67%)
20	CLA	A	831	-	59,63,73	2.41	15 (25%)	70,101,113	3.14	32 (45%)
21	LMU	4	317	-	36,36,36	0.75	1 (2%)	47,47,47	1.15	3 (6%)
21	LMU	H	107	-	36,36,36	0.75	0	47,47,47	2.25	14 (29%)
20	CLA	B	828	-	54,58,73	2.68	16 (29%)	64,95,113	2.67	30 (46%)
20	CLA	A	810	-	49,53,73	2.68	16 (32%)	58,89,113	3.20	25 (43%)
20	CLA	2	315	-	69,73,73	2.21	15 (21%)	82,113,113	2.72	25 (30%)
20	CLA	4	303	-	38,44,73	3.10	16 (42%)	52,78,113	3.56	23 (44%)
22	BCR	B	842	-	41,41,41	1.73	5 (12%)	56,56,56	6.04	18 (32%)
20	CLA	I	102	-	64,68,73	2.28	15 (23%)	76,107,113	2.84	23 (30%)
20	CLA	A	822	-	59,63,73	2.38	16 (27%)	70,101,113	2.85	25 (35%)
20	CLA	A	801	-	50,54,73	2.76	16 (32%)	61,90,113	3.90	34 (55%)
22	BCR	I	101	-	41,41,41	2.50	17 (41%)	56,56,56	5.48	31 (55%)
20	CLA	A	835	-	69,73,73	2.25	16 (23%)	82,113,113	2.90	28 (34%)
20	CLA	K	107	-	54,58,73	2.50	16 (29%)	64,95,113	2.92	23 (35%)
20	CLA	2	306	-	24,32,73	2.43	12 (50%)	31,54,113	3.20	20 (64%)
20	CLA	3	302	-	54,58,73	3.08	23 (42%)	64,95,113	3.03	27 (42%)
20	CLA	B	821	-	69,73,73	3.00	29 (42%)	82,113,113	2.97	28 (34%)
21	LMU	3	321	-	36,36,36	0.70	0	47,47,47	1.92	11 (23%)
20	CLA	4	304	-	69,73,73	2.49	29 (42%)	82,113,113	3.57	37 (45%)
20	CLA	J	101	-	52,56,73	2.52	17 (32%)	61,92,113	3.02	24 (39%)
22	BCR	B	843	-	41,41,41	1.81	5 (12%)	56,56,56	6.07	19 (33%)
20	CLA	B	838	-	69,73,73	2.18	14 (20%)	82,113,113	2.86	31 (37%)
20	CLA	4	315	-	24,32,73	2.35	8 (33%)	31,54,113	2.65	18 (58%)
21	LMU	K	105	-	36,36,36	0.53	0	47,47,47	2.06	14 (29%)
20	CLA	K	102	-	54,58,73	2.92	26 (48%)	64,95,113	3.24	28 (43%)
20	CLA	2	308	-	69,73,73	2.17	12 (17%)	82,113,113	2.70	29 (35%)
20	CLA	A	814	-	49,53,73	2.64	15 (30%)	58,89,113	2.94	25 (43%)
21	LMU	2	313	-	36,36,36	0.82	1 (2%)	47,47,47	0.93	2 (4%)
20	CLA	3	303	-	24,32,73	2.58	13 (54%)	31,54,113	3.00	18 (58%)
20	CLA	A	839	-	69,73,73	2.52	20 (28%)	82,113,113	3.45	35 (42%)
20	CLA	A	850	-	69,73,73	2.23	17 (24%)	82,113,113	2.84	27 (32%)
20	CLA	B	805	-	64,68,73	2.25	14 (21%)	76,107,113	3.15	32 (42%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
20	CLA	B	812	-	69,73,73	2.20	14 (20%)	82,113,113	2.52	29 (35%)
22	BCR	B	845	-	41,41,41	1.86	5 (12%)	56,56,56	6.08	21 (37%)
20	CLA	B	809	-	58,62,73	2.64	15 (25%)	71,100,113	2.77	28 (39%)
20	CLA	B	817	-	65,69,73	2.18	16 (24%)	77,108,113	2.83	28 (36%)
20	CLA	R	108	-	62,66,73	2.62	25 (40%)	73,104,113	3.11	31 (42%)
20	CLA	A	808	5	69,73,73	2.24	17 (24%)	82,113,113	2.98	33 (40%)
20	CLA	B	823	-	62,66,73	2.31	16 (25%)	73,104,113	2.83	25 (34%)
20	CLA	A	828	-	69,73,73	2.17	16 (23%)	82,113,113	2.64	29 (35%)
20	CLA	B	833	20	49,53,73	2.63	14 (28%)	58,89,113	3.11	22 (37%)
20	CLA	4	305	-	59,63,73	2.27	14 (23%)	70,101,113	2.89	27 (38%)
20	CLA	3	312	-	24,32,73	2.77	12 (50%)	31,54,113	3.72	20 (64%)
20	CLA	2	311	2	54,58,73	2.44	13 (24%)	64,95,113	2.95	25 (39%)
21	LMU	B	847	-	36,36,36	0.99	1 (2%)	47,47,47	2.39	17 (36%)
22	BCR	J	102	-	41,41,41	1.66	4 (9%)	56,56,56	6.07	19 (33%)
21	LMU	R	105	-	36,36,36	0.86	1 (2%)	47,47,47	1.65	11 (23%)
20	CLA	B	806	-	69,73,73	2.19	16 (23%)	82,113,113	3.02	35 (42%)
20	CLA	A	841	-	69,73,73	2.10	15 (21%)	82,113,113	2.82	30 (36%)
21	LMU	C	101	-	36,36,36	0.85	1 (2%)	47,47,47	1.38	7 (14%)
20	CLA	4	311	-	59,63,73	2.39	13 (22%)	70,101,113	2.84	28 (40%)
20	CLA	4	316	-	50,54,73	2.80	23 (46%)	59,90,113	3.14	25 (42%)
21	LMU	H	104	-	36,36,36	1.12	3 (8%)	47,47,47	3.11	22 (46%)
20	CLA	1	206	-	65,69,73	2.25	15 (23%)	77,108,113	2.57	27 (35%)
20	CLA	B	849	-	69,73,73	2.19	16 (23%)	82,113,113	2.77	35 (42%)
20	CLA	G	102	-	55,59,73	2.65	23 (41%)	64,96,113	3.35	31 (48%)
20	CLA	H	111	16	54,58,73	2.47	15 (27%)	64,95,113	2.89	24 (37%)
21	LMU	A	848	-	36,36,36	0.86	0	47,47,47	1.42	6 (12%)
21	LMU	1	217	-	36,36,36	0.38	0	47,47,47	0.71	1 (2%)
20	CLA	A	812	-	58,62,73	2.35	13 (22%)	68,99,113	2.57	23 (33%)
21	LMU	4	301	-	36,36,36	0.41	0	47,47,47	0.73	1 (2%)
20	CLA	A	809	-	56,60,73	2.36	15 (26%)	65,97,113	3.08	31 (47%)
20	CLA	3	319	-	24,32,73	2.47	8 (33%)	31,54,113	3.05	17 (54%)
21	LMU	2	317	-	36,36,36	1.06	1 (2%)	47,47,47	1.95	15 (31%)
20	CLA	B	850	-	69,73,73	2.12	15 (21%)	82,113,113	2.80	31 (37%)
20	CLA	H	102	-	59,63,73	2.40	15 (25%)	70,101,113	2.81	25 (35%)
22	BCR	A	843	-	41,41,41	1.66	4 (9%)	56,56,56	6.05	19 (33%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
20	CLA	A	838	-	69,73,73	2.26	17 (24%)	82,113,113	2.77	33 (40%)
20	CLA	B	829	-	54,58,73	2.31	13 (24%)	64,95,113	2.97	28 (43%)
20	CLA	1	203	-	51,55,73	2.57	12 (23%)	60,91,113	3.23	24 (40%)
21	LMU	K	106	-	36,36,36	0.46	0	47,47,47	2.20	16 (34%)
20	CLA	B	808	6	69,73,73	2.15	18 (26%)	82,113,113	2.69	24 (29%)
20	CLA	3	308	-	46,50,73	2.52	12 (26%)	53,85,113	3.19	27 (50%)
21	LMU	R	102	-	36,36,36	0.43	0	47,47,47	1.75	12 (25%)
21	LMU	G	101	-	36,36,36	1.01	3 (8%)	47,47,47	2.61	13 (27%)
20	CLA	3	316	-	54,58,73	2.55	12 (22%)	64,95,113	2.60	23 (35%)
20	CLA	A	807	-	50,54,73	3.06	27 (54%)	59,90,113	3.40	28 (47%)
21	LMU	1	219	-	36,36,36	1.02	2 (5%)	47,47,47	2.29	13 (27%)
20	CLA	A	805	-	69,73,73	2.11	12 (17%)	82,113,113	2.74	30 (36%)
22	BCR	A	845	-	41,41,41	1.75	5 (12%)	56,56,56	6.07	20 (35%)
21	LMU	R	106	-	36,36,36	0.88	1 (2%)	47,47,47	1.58	10 (21%)
20	CLA	A	817	-	56,60,73	2.46	15 (26%)	65,97,113	3.02	26 (40%)
20	CLA	B	804	-	49,53,73	2.63	18 (36%)	58,89,113	3.09	21 (36%)
22	BCR	A	847	-	41,41,41	1.79	5 (12%)	56,56,56	6.08	20 (35%)
23	PQN	B	841	-	34,34,34	1.71	3 (8%)	43,45,45	1.61	7 (16%)
20	CLA	A	816	-	58,62,73	2.73	24 (41%)	68,99,113	3.03	25 (36%)
20	CLA	3	311	-	69,73,73	2.53	26 (37%)	82,113,113	3.21	29 (35%)
20	CLA	B	840	-	38,44,73	2.87	13 (34%)	52,78,113	3.42	29 (55%)
20	CLA	3	318	-	24,32,73	2.78	13 (54%)	31,54,113	3.37	20 (64%)
21	LMU	A	853	-	36,36,36	0.41	0	47,47,47	0.74	1 (2%)
20	CLA	A	832	-	54,58,73	2.43	15 (27%)	64,95,113	2.86	25 (39%)
20	CLA	2	304	-	24,32,73	2.55	15 (62%)	31,54,113	3.18	20 (64%)
20	CLA	3	301	-	38,44,73	2.73	10 (26%)	52,78,113	3.43	27 (51%)
21	LMU	1	220	-	36,36,36	0.59	1 (2%)	47,47,47	1.36	6 (12%)
20	CLA	2	320	-	65,69,73	2.45	24 (36%)	77,108,113	2.96	32 (41%)
20	CLA	L	203	-	59,63,73	2.39	12 (20%)	70,101,113	2.72	28 (40%)
20	CLA	1	215	-	65,69,73	2.43	24 (36%)	77,108,113	3.42	35 (45%)
20	CLA	A	834	-	53,57,73	2.53	15 (28%)	61,93,113	2.92	26 (42%)
20	CLA	1	214	-	24,32,73	2.30	8 (33%)	31,54,113	2.77	19 (61%)
20	CLA	2	305	-	54,58,73	2.44	15 (27%)	64,95,113	2.71	26 (40%)
20	CLA	F	206	-	57,61,73	2.74	23 (40%)	67,98,113	2.82	25 (37%)
20	CLA	J	103	-	65,69,73	2.25	16 (24%)	77,108,113	2.77	24 (31%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
20	CLA	K	101	-	49,53,73	2.60	16 (32%)	58,89,113	3.10	22 (37%)
20	CLA	2	301	-	24,32,73	2.57	14 (58%)	31,54,113	3.11	17 (54%)
20	CLA	L	201	-	59,63,73	2.90	24 (40%)	70,101,113	3.57	31 (44%)
24	SF4	C	102	7	0,12,12	-	-	-		
20	CLA	A	829	-	54,58,73	2.47	12 (22%)	64,95,113	3.01	28 (43%)
24	SF4	C	103	7	0,12,12	-	-	-		
20	CLA	B	824	-	69,73,73	2.22	18 (26%)	82,113,113	2.61	21 (25%)
20	CLA	A	837	-	51,55,73	2.59	16 (31%)	60,91,113	3.25	27 (45%)
20	CLA	1	212	-	24,32,73	2.50	8 (33%)	31,54,113	3.31	19 (61%)
21	LMU	R	103	-	36,36,36	0.77	0	47,47,47	2.07	14 (29%)
21	LMU	3	320	-	36,36,36	0.40	0	47,47,47	0.72	1 (2%)
20	CLA	A	802	-	24,32,73	2.54	11 (45%)	31,54,113	3.56	18 (58%)
20	CLA	B	810	-	59,63,73	2.28	14 (23%)	70,101,113	2.72	28 (40%)
21	LMU	E	101	-	36,36,36	0.92	2 (5%)	47,47,47	3.09	25 (53%)
21	LMU	L	204	-	36,36,36	0.69	2 (5%)	47,47,47	2.43	14 (29%)
20	CLA	B	827	-	69,73,73	2.22	19 (27%)	82,113,113	2.93	25 (30%)
22	BCR	A	846	-	41,41,41	1.80	5 (12%)	56,56,56	6.07	19 (33%)
20	CLA	A	804	-	59,63,73	2.41	15 (25%)	70,101,113	2.84	27 (38%)
20	CLA	R	107	-	61,65,73	2.35	13 (21%)	72,103,113	2.90	27 (37%)
20	CLA	3	307	-	24,32,73	2.35	10 (41%)	31,54,113	3.01	18 (58%)
22	BCR	B	852	-	41,41,41	2.89	20 (48%)	56,56,56	6.59	26 (46%)
20	CLA	A	820	-	55,59,73	2.49	16 (29%)	64,96,113	2.94	22 (34%)
20	CLA	B	835	-	64,68,73	2.18	13 (20%)	76,107,113	2.97	21 (27%)
20	CLA	B	819	-	50,54,73	2.46	13 (26%)	59,90,113	3.18	20 (33%)
20	CLA	A	827	-	59,63,73	2.32	16 (27%)	70,101,113	2.78	26 (37%)
20	CLA	B	851	-	69,73,73	2.23	16 (23%)	82,113,113	2.64	29 (35%)
21	LMU	D	201	-	36,36,36	0.40	0	47,47,47	0.70	1 (2%)
20	CLA	4	310	-	24,32,73	2.45	14 (58%)	31,54,113	2.87	16 (51%)
22	BCR	L	208	-	41,41,41	2.26	11 (26%)	56,56,56	5.86	20 (35%)
20	CLA	H	103	-	59,63,73	2.35	14 (23%)	70,101,113	3.00	28 (40%)
20	CLA	L	202	-	69,73,73	2.21	14 (20%)	82,113,113	2.56	26 (31%)
20	CLA	B	830	-	69,73,73	2.26	18 (26%)	82,113,113	2.93	29 (35%)
20	CLA	K	103	-	69,73,73	2.20	12 (17%)	82,113,113	2.52	26 (31%)
21	LMU	L	205	-	36,36,36	0.79	2 (5%)	47,47,47	1.91	17 (36%)
20	CLA	3	304	-	38,44,73	2.79	11 (28%)	52,78,113	3.01	21 (40%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
20	CLA	A	811	-	69,73,73	2.18	12 (17%)	82,113,113	3.03	31 (37%)
20	CLA	F	204	-	38,44,73	2.80	12 (31%)	52,78,113	3.22	27 (51%)
20	CLA	B	826	-	69,73,73	2.17	15 (21%)	82,113,113	2.81	30 (36%)
21	LMU	H	105	-	36,36,36	0.96	1 (2%)	47,47,47	2.35	16 (34%)
20	CLA	B	837	-	51,55,73	2.45	14 (27%)	60,91,113	2.95	26 (43%)
21	LMU	R	101	-	36,36,36	1.03	2 (5%)	47,47,47	2.46	14 (29%)
21	LMU	A	855	-	36,36,36	0.77	1 (2%)	47,47,47	1.95	18 (38%)
21	LMU	H	108	-	36,36,36	1.02	3 (8%)	47,47,47	2.80	19 (40%)
22	BCR	B	844	-	41,41,41	1.70	4 (9%)	56,56,56	5.16	24 (42%)
21	LMU	K	108	-	36,36,36	0.78	1 (2%)	47,47,47	2.28	12 (25%)
20	CLA	A	833	5	49,53,73	2.54	16 (32%)	58,89,113	3.49	27 (46%)
20	CLA	B	815	-	63,67,73	2.28	16 (25%)	74,105,113	2.36	21 (28%)
20	CLA	3	309	-	24,32,73	2.34	9 (37%)	31,54,113	2.78	18 (58%)
22	BCR	3	314	-	41,41,41	1.80	5 (12%)	56,56,56	6.04	22 (39%)
20	CLA	3	315	-	24,32,73	2.52	9 (37%)	31,54,113	2.91	19 (61%)
21	LMU	4	320	-	35,35,36	0.30	0	46,46,47	0.72	1 (2%)
21	LMU	2	318	-	36,36,36	1.01	1 (2%)	47,47,47	1.31	6 (12%)
20	CLA	1	207	-	55,59,73	2.51	15 (27%)	64,96,113	3.43	30 (46%)
20	CLA	A	821	5	46,50,73	2.56	13 (28%)	53,85,113	3.29	24 (45%)
20	CLA	A	824	-	69,73,73	2.19	16 (23%)	82,113,113	2.64	24 (29%)
20	CLA	A	825	-	69,73,73	2.21	16 (23%)	82,113,113	2.66	23 (28%)
20	CLA	B	820	-	59,63,73	2.45	15 (25%)	70,101,113	2.77	23 (32%)
20	CLA	L	206	-	51,55,73	2.44	12 (23%)	60,91,113	3.31	27 (45%)
20	CLA	1	210	-	55,59,73	2.88	24 (43%)	64,96,113	4.15	31 (48%)
20	CLA	4	318	-	56,60,73	2.85	21 (37%)	65,97,113	3.65	28 (43%)
20	CLA	3	306	-	24,32,73	2.37	10 (41%)	31,54,113	3.03	18 (58%)
21	LMU	L	209	-	36,36,36	0.86	1 (2%)	47,47,47	1.51	9 (19%)
21	LMU	A	854	-	36,36,36	0.68	1 (2%)	47,47,47	1.90	11 (23%)
21	LMU	H	106	-	36,36,36	1.03	4 (11%)	47,47,47	2.75	19 (40%)
20	CLA	B	836	-	69,73,73	2.11	15 (21%)	82,113,113	2.67	25 (30%)
21	LMU	2	316	-	36,36,36	0.39	0	47,47,47	0.72	1 (2%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
20	CLA	1	205	-	1/1/4/20	-	-
20	CLA	A	819	-	2/2/15/20	13/39/115/115	-
20	CLA	A	851	-	2/2/15/20	17/39/115/115	-
21	LMU	R	109	-	-	16/21/61/61	0/2/2/2
21	LMU	1	213	-	-	13/21/61/61	0/2/2/2
23	PQN	A	842	-	1/1/8/9	11/23/43/43	0/2/2/2
20	CLA	2	310	-	1/1/4/20	-	-
20	CLA	4	312	-	1/1/4/20	-	-
20	CLA	1	201	-	1/1/11/20	12/17/93/115	-
20	CLA	B	816	-	2/2/14/20	15/33/109/115	-
20	CLA	A	826	-	2/2/15/20	18/39/115/115	-
20	CLA	4	309	-	1/1/4/20	-	-
20	CLA	2	314	-	1/1/4/20	-	-
22	BCR	F	202	-	-	12/29/63/63	0/2/2/2
22	BCR	I	103	-	-	13/29/63/63	0/2/2/2
20	CLA	B	811	-	2/2/13/20	16/31/107/115	-
20	CLA	B	807	-	2/2/15/20	12/39/115/115	-
20	CLA	A	815	-	1/1/12/20	9/21/97/115	-
24	SF4	A	857	5,6	-	-	0/6/5/5
20	CLA	3	317	-	2/2/15/20	20/39/115/115	-
21	LMU	A	856	-	-	14/21/61/61	0/2/2/2
20	CLA	B	803	-	2/2/15/20	19/39/115/115	-
20	CLA	4	306	-	1/1/12/20	9/21/97/115	-
21	LMU	4	322	-	-	14/21/61/61	0/2/2/2
20	CLA	4	313	-	1/1/4/20	-	-
20	CLA	4	319	-	1/1/11/20	10/18/94/115	-
20	CLA	A	823	-	2/2/15/20	20/39/115/115	-
20	CLA	B	834	-	1/1/12/20	8/23/99/115	-
21	LMU	N	101	-	-	16/21/61/61	0/2/2/2
22	BCR	A	844	-	-	12/29/63/63	0/2/2/2
20	CLA	A	803	-	1/1/12/20	4/21/97/115	-
20	CLA	A	852	-	2/2/15/20	22/39/115/115	-
20	CLA	B	813	-	2/2/14/20	11/33/109/115	-
20	CLA	B	831	-	1/1/12/20	8/21/97/115	-
20	CLA	B	832	20	1/1/11/20	11/15/91/115	-
21	LMU	B	801	-	-	16/21/61/61	0/2/2/2

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
20	CLA	H	109	-	2/2/14/20	14/33/109/115	-
20	CLA	2	303	-	2/2/15/20	18/39/115/115	-
20	CLA	A	836	-	1/1/11/20	8/18/94/115	-
20	CLA	2	309	-	1/1/4/20	-	-
20	CLA	1	202	-	2/2/13/20	16/30/106/115	-
20	CLA	F	205	-	1/1/10/20	5/10/86/115	-
20	CLA	3	313	-	2/2/15/20	17/39/115/115	-
20	CLA	A	818	-	2/2/15/20	18/39/115/115	-
21	LMU	2	319	-	-	8/21/61/61	0/2/2/2
20	CLA	1	209	1	1/1/9/20	-	-
20	CLA	B	822	-	1/1/12/20	8/26/102/115	-
20	CLA	2	312	-	1/1/12/20	9/21/97/115	-
20	CLA	1	211	-	1/1/4/20	-	-
20	CLA	1	216	-	1/1/4/20	-	-
20	CLA	A	840	-	1/1/12/20	10/21/97/115	-
21	LMU	B	802	-	-	11/21/61/61	0/2/2/2
20	CLA	B	825	-	2/2/15/20	17/39/115/115	-
21	LMU	F	201	-	-	14/20/60/61	0/2/2/2
20	CLA	B	818	-	1/1/12/20	7/21/97/115	-
20	CLA	4	314	-	1/1/9/20	-	-
21	LMU	K	104	-	-	12/21/61/61	0/2/2/2
20	CLA	4	307	-	2/2/12/20	7/24/100/115	-
20	CLA	4	308	-	1/1/9/20	-	-
22	BCR	B	846	-	-	12/29/63/63	0/2/2/2
21	LMU	4	321	-	-	15/21/61/61	0/2/2/2
20	CLA	A	830	-	2/2/15/20	20/39/115/115	-
20	CLA	1	208	-	1/1/4/20	-	-
20	CLA	2	307	-	2/2/15/20	21/39/115/115	-
20	CLA	A	806	-	2/2/13/20	8/27/103/115	-
20	CLA	B	814	-	1/1/11/20	9/17/93/115	-
20	CLA	H	101	-	2/2/13/20	17/27/103/115	-
20	CLA	L	207	-	2/2/12/20	10/21/97/115	-
20	CLA	1	204	-	1/1/11/20	8/17/93/115	-
25	LMG	B	848	-	-	23/44/64/70	0/1/1/1
20	CLA	B	839	-	2/2/15/20	16/39/115/115	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
21	LMU	1	218	-	-	10/21/61/61	0/2/2/2
20	CLA	3	305	-	1/1/4/20	-	-
21	LMU	A	849	-	-	13/21/61/61	0/2/2/2
22	BCR	F	203	-	-	12/29/63/63	0/2/2/2
20	CLA	2	302	-	1/1/12/20	12/23/99/115	-
21	LMU	R	104	-	-	17/21/61/61	0/2/2/2
20	CLA	4	302	-	2/2/13/20	15/27/103/115	-
20	CLA	A	813	-	1/1/12/20	11/26/102/115	-
20	CLA	3	310	-	1/1/4/20	-	-
20	CLA	A	831	-	2/2/13/20	15/27/103/115	-
21	LMU	4	317	-	-	13/21/61/61	0/2/2/2
21	LMU	H	107	-	-	12/21/61/61	0/2/2/2
20	CLA	B	828	-	1/1/12/20	8/21/97/115	-
20	CLA	A	810	-	1/1/11/20	4/15/91/115	-
20	CLA	2	315	-	2/2/15/20	18/39/115/115	-
20	CLA	4	303	-	1/1/9/20	-	-
22	BCR	B	842	-	-	13/29/63/63	0/2/2/2
20	CLA	I	102	-	2/2/14/20	12/33/109/115	-
20	CLA	A	822	-	2/2/13/20	10/27/103/115	-
20	CLA	A	801	-	3/3/11/20	12/16/92/115	-
22	BCR	I	101	-	-	7/29/63/63	0/2/2/2
20	CLA	A	835	-	2/2/15/20	17/39/115/115	-
20	CLA	K	107	-	1/1/12/20	6/21/97/115	-
20	CLA	2	306	-	1/1/4/20	-	-
20	CLA	3	302	-	1/1/12/20	4/21/97/115	-
20	CLA	B	821	-	1/1/15/20	18/39/115/115	-
21	LMU	3	321	-	-	17/21/61/61	0/2/2/2
20	CLA	4	304	-	3/3/15/20	18/39/115/115	-
20	CLA	J	101	-	1/1/11/20	12/19/95/115	-
22	BCR	B	843	-	-	7/29/63/63	0/2/2/2
20	CLA	B	838	-	2/2/15/20	17/39/115/115	-
20	CLA	4	315	-	1/1/4/20	-	-
21	LMU	K	105	-	-	18/21/61/61	0/2/2/2
20	CLA	K	102	-	1/1/12/20	9/21/97/115	-
20	CLA	2	308	-	2/2/15/20	14/39/115/115	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
20	CLA	A	814	-	1/1/11/20	13/15/91/115	-
21	LMU	2	313	-	-	16/21/61/61	0/2/2/2
20	CLA	3	303	-	1/1/4/20	-	-
20	CLA	A	839	-	2/2/15/20	21/39/115/115	-
20	CLA	A	850	-	2/2/15/20	21/39/115/115	-
20	CLA	B	805	-	2/2/14/20	17/33/109/115	-
20	CLA	B	812	-	2/2/15/20	25/39/115/115	-
22	BCR	B	845	-	-	12/29/63/63	0/2/2/2
20	CLA	B	809	-	2/2/13/20	11/25/101/115	-
20	CLA	B	817	-	2/2/14/20	17/35/111/115	-
20	CLA	R	108	-	2/2/13/20	16/31/107/115	-
20	CLA	A	808	5	2/2/15/20	19/39/115/115	-
20	CLA	B	823	-	2/2/13/20	15/31/107/115	-
20	CLA	A	828	-	2/2/15/20	17/39/115/115	-
20	CLA	B	833	20	1/1/11/20	7/15/91/115	-
20	CLA	4	305	-	2/2/13/20	13/27/103/115	-
20	CLA	3	312	-	1/1/4/20	-	-
20	CLA	2	311	2	1/1/12/20	5/21/97/115	-
21	LMU	B	847	-	-	10/21/61/61	0/2/2/2
22	BCR	J	102	-	-	12/29/63/63	0/2/2/2
21	LMU	R	105	-	-	15/21/61/61	0/2/2/2
20	CLA	B	806	-	2/2/15/20	20/39/115/115	-
20	CLA	A	841	-	2/2/15/20	14/39/115/115	-
21	LMU	C	101	-	-	14/21/61/61	0/2/2/2
20	CLA	4	311	-	2/2/13/20	14/27/103/115	-
20	CLA	4	316	-	1/1/11/20	10/17/93/115	-
21	LMU	H	104	-	-	14/21/61/61	0/2/2/2
20	CLA	1	206	-	2/2/14/20	21/35/111/115	-
20	CLA	B	849	-	2/2/15/20	16/39/115/115	-
20	CLA	G	102	-	1/1/12/20	9/23/99/115	-
20	CLA	H	111	16	1/1/12/20	10/21/97/115	-
21	LMU	A	848	-	-	16/21/61/61	0/2/2/2
21	LMU	1	217	-	-	14/21/61/61	0/2/2/2
20	CLA	A	812	-	1/1/12/20	13/26/102/115	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
21	LMU	4	301	-	-	13/21/61/61	0/2/2/2
20	CLA	A	809	-	1/1/12/20	11/24/100/115	-
20	CLA	3	319	-	1/1/4/20	-	-
21	LMU	2	317	-	-	13/21/61/61	0/2/2/2
20	CLA	B	850	-	2/2/15/20	16/39/115/115	-
20	CLA	H	102	-	2/2/13/20	10/27/103/115	-
22	BCR	A	843	-	-	11/29/63/63	0/2/2/2
20	CLA	A	838	-	2/2/15/20	18/39/115/115	-
20	CLA	B	829	-	1/1/12/20	13/21/97/115	-
20	CLA	1	203	-	1/1/11/20	8/18/94/115	-
21	LMU	K	106	-	-	15/21/61/61	0/2/2/2
20	CLA	B	808	6	2/2/15/20	20/39/115/115	-
20	CLA	3	308	-	1/1/10/20	5/12/88/115	-
21	LMU	R	102	-	-	11/21/61/61	0/2/2/2
21	LMU	G	101	-	-	14/21/61/61	0/2/2/2
20	CLA	3	316	-	1/1/12/20	9/21/97/115	-
20	CLA	A	807	-	1/1/11/20	7/17/93/115	-
21	LMU	1	219	-	-	13/21/61/61	0/2/2/2
20	CLA	A	805	-	2/2/15/20	22/39/115/115	-
22	BCR	A	845	-	-	14/29/63/63	0/2/2/2
21	LMU	R	106	-	-	13/21/61/61	0/2/2/2
20	CLA	A	817	-	1/1/12/20	11/24/100/115	-
20	CLA	B	804	-	1/1/11/20	6/15/91/115	-
23	PQN	B	841	-	1/1/8/9	10/23/43/43	0/2/2/2
22	BCR	A	847	-	-	10/29/63/63	0/2/2/2
20	CLA	A	816	-	1/1/12/20	13/26/102/115	-
20	CLA	3	311	-	2/2/15/20	24/39/115/115	-
20	CLA	B	840	-	1/1/9/20	-	-
20	CLA	3	318	-	1/1/4/20	-	-
21	LMU	A	853	-	-	19/21/61/61	0/2/2/2
20	CLA	A	832	-	1/1/12/20	13/21/97/115	-
20	CLA	2	304	-	1/1/4/20	-	-
20	CLA	3	301	-	1/1/9/20	-	-
21	LMU	1	220	-	-	13/21/61/61	0/2/2/2
20	CLA	2	320	-	2/2/14/20	20/35/111/115	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
20	CLA	L	203	-	2/2/13/20	8/27/103/115	-
20	CLA	1	215	-	2/2/14/20	22/35/111/115	-
20	CLA	A	834	-	1/1/11/20	10/20/96/115	-
20	CLA	1	214	-	1/1/4/20	-	-
20	CLA	2	305	-	1/1/12/20	9/21/97/115	-
20	CLA	F	206	-	4/4/12/20	11/25/101/115	-
20	CLA	J	103	-	2/2/14/20	25/35/111/115	-
20	CLA	K	101	-	1/1/11/20	4/15/91/115	-
20	CLA	2	301	-	1/1/4/20	-	-
20	CLA	L	201	-	3/3/13/20	14/27/103/115	-
24	SF4	C	102	7	-	-	0/6/5/5
20	CLA	A	829	-	1/1/12/20	4/21/97/115	-
24	SF4	C	103	7	-	-	0/6/5/5
20	CLA	B	824	-	2/2/15/20	21/39/115/115	-
20	CLA	A	837	-	1/1/11/20	11/18/94/115	-
20	CLA	1	212	-	1/1/4/20	-	-
21	LMU	R	103	-	-	13/21/61/61	0/2/2/2
21	LMU	3	320	-	-	11/21/61/61	0/2/2/2
20	CLA	A	802	-	1/1/4/20	-	-
20	CLA	B	810	-	2/2/13/20	10/27/103/115	-
21	LMU	E	101	-	-	14/21/61/61	0/2/2/2
21	LMU	L	204	-	-	15/21/61/61	0/2/2/2
20	CLA	B	827	-	2/2/15/20	25/39/115/115	-
22	BCR	A	846	-	-	17/29/63/63	0/2/2/2
20	CLA	A	804	-	2/2/13/20	11/27/103/115	-
20	CLA	R	107	-	2/2/13/20	15/30/106/115	-
20	CLA	3	307	-	1/1/4/20	-	-
22	BCR	B	852	-	-	12/29/63/63	0/2/2/2
20	CLA	A	820	-	1/1/12/20	9/23/99/115	-
20	CLA	B	835	-	2/2/14/20	17/33/109/115	-
20	CLA	B	819	-	1/1/11/20	14/17/93/115	-
20	CLA	A	827	-	2/2/13/20	10/27/103/115	-
20	CLA	B	851	-	2/2/15/20	18/39/115/115	-
21	LMU	D	201	-	-	14/21/61/61	0/2/2/2
20	CLA	4	310	-	1/1/4/20	-	-
22	BCR	L	208	-	-	10/29/63/63	0/2/2/2

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
20	CLA	H	103	-	2/2/13/20	15/27/103/115	-
20	CLA	L	202	-	2/2/15/20	14/39/115/115	-
20	CLA	B	830	-	2/2/15/20	21/39/115/115	-
20	CLA	K	103	-	2/2/15/20	19/39/115/115	-
21	LMU	L	205	-	-	14/21/61/61	0/2/2/2
20	CLA	3	304	-	1/1/9/20	-	-
20	CLA	A	811	-	2/2/15/20	24/39/115/115	-
20	CLA	F	204	-	1/1/9/20	-	-
20	CLA	B	826	-	2/2/15/20	14/39/115/115	-
21	LMU	H	105	-	-	17/21/61/61	0/2/2/2
20	CLA	B	837	-	1/1/11/20	7/18/94/115	-
21	LMU	R	101	-	1/1/10/10	11/21/61/61	0/2/2/2
21	LMU	A	855	-	-	14/21/61/61	0/2/2/2
21	LMU	H	108	-	-	14/21/61/61	0/2/2/2
22	BCR	B	844	-	-	11/29/63/63	0/2/2/2
21	LMU	K	108	-	-	12/21/61/61	0/2/2/2
20	CLA	A	833	5	1/1/11/20	7/15/91/115	-
20	CLA	B	815	-	2/2/13/20	12/32/108/115	-
20	CLA	3	309	-	1/1/4/20	-	-
22	BCR	3	314	-	-	13/29/63/63	0/2/2/2
20	CLA	3	315	-	1/1/4/20	-	-
21	LMU	4	320	-	-	15/20/60/61	0/2/2/2
21	LMU	2	318	-	-	13/21/61/61	0/2/2/2
20	CLA	1	207	-	2/2/12/20	9/23/99/115	-
20	CLA	A	821	5	1/1/10/20	3/12/88/115	-
20	CLA	A	824	-	2/2/15/20	18/39/115/115	-
20	CLA	A	825	-	2/2/15/20	22/39/115/115	-
20	CLA	B	820	-	2/2/13/20	9/27/103/115	-
20	CLA	L	206	-	1/1/11/20	11/18/94/115	-
20	CLA	1	210	-	2/2/12/20	10/23/99/115	-
20	CLA	4	318	-	1/1/12/20	10/24/100/115	-
20	CLA	3	306	-	1/1/4/20	-	-
21	LMU	L	209	-	-	14/21/61/61	0/2/2/2
21	LMU	A	854	-	-	11/21/61/61	0/2/2/2
21	LMU	H	106	-	-	13/21/61/61	0/2/2/2

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
20	CLA	B	836	-	2/2/15/20	13/39/115/115	-
21	LMU	2	316	-	-	14/21/61/61	0/2/2/2

The worst 5 of 2900 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	B	852	BCR	C20-C21	-10.03	1.12	1.43
22	L	208	BCR	C20-C21	-8.78	1.15	1.43
20	B	821	CLA	C4C-C3C	-8.67	1.30	1.45
22	F	203	BCR	C20-C21	-8.58	1.16	1.43
22	I	101	BCR	C20-C21	-8.36	1.17	1.43

The worst 5 of 5410 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	A	846	BCR	C20-C21-C22	37.56	179.96	127.28
22	J	102	BCR	C20-C21-C22	37.56	179.96	127.28
22	B	846	BCR	C20-C21-C22	37.54	179.93	127.28
22	A	845	BCR	C20-C21-C22	37.53	179.91	127.28
22	A	844	BCR	C20-C21-C22	37.51	179.89	127.28

5 of 264 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
20	1	201	CLA	ND
20	1	202	CLA	ND
20	1	202	CLA	C8
20	1	203	CLA	ND
20	1	204	CLA	ND

5 of 2780 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 3651 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
20	A	819	CLA	45	0
20	A	851	CLA	35	0
21	R	109	LMU	20	5
21	1	213	LMU	8	0
23	A	842	PQN	9	0
20	4	312	CLA	4	0
20	1	201	CLA	14	0
20	B	816	CLA	16	0
20	A	826	CLA	60	0
20	4	309	CLA	1	0
22	F	202	BCR	31	0
22	I	103	BCR	46	0
20	B	811	CLA	29	0
20	B	807	CLA	23	0
20	A	815	CLA	45	0
24	A	857	SF4	19	0
20	3	317	CLA	18	0
20	B	803	CLA	28	0
20	4	306	CLA	10	0
21	4	322	LMU	2	0
20	4	313	CLA	5	0
20	4	319	CLA	11	0
20	A	823	CLA	17	0
20	B	834	CLA	4	0
21	N	101	LMU	35	0
22	A	844	BCR	24	0
20	A	803	CLA	13	0
20	A	852	CLA	27	0
20	B	813	CLA	13	0
20	B	831	CLA	18	0
20	B	832	CLA	20	0
21	B	801	LMU	13	0
20	H	109	CLA	17	0
20	2	303	CLA	12	0
20	A	836	CLA	16	0
20	2	309	CLA	1	0
20	1	202	CLA	39	0
20	F	205	CLA	13	0
20	3	313	CLA	27	0
20	A	818	CLA	28	0
21	2	319	LMU	0	2
20	1	209	CLA	11	0
20	B	822	CLA	25	0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
20	2	312	CLA	11	0
20	1	211	CLA	6	0
20	A	840	CLA	9	0
21	B	802	LMU	4	0
20	B	825	CLA	24	0
21	F	201	LMU	19	0
20	B	818	CLA	8	0
20	4	314	CLA	8	0
21	K	104	LMU	8	0
20	4	307	CLA	17	0
20	4	308	CLA	2	0
22	B	846	BCR	53	0
21	4	321	LMU	2	0
20	A	830	CLA	38	0
20	2	307	CLA	18	0
20	A	806	CLA	17	0
20	B	814	CLA	20	0
20	H	101	CLA	36	0
20	L	207	CLA	12	0
20	1	204	CLA	7	0
25	B	848	LMG	29	0
20	B	839	CLA	25	0
21	1	218	LMU	8	0
20	3	305	CLA	1	0
21	A	849	LMU	4	0
22	F	203	BCR	42	0
20	2	302	CLA	15	0
21	R	104	LMU	10	0
20	4	302	CLA	28	0
20	A	813	CLA	19	0
20	3	310	CLA	7	0
20	A	831	CLA	15	0
21	4	317	LMU	4	0
21	H	107	LMU	11	0
20	B	828	CLA	13	0
20	A	810	CLA	5	0
20	2	315	CLA	6	0
20	4	303	CLA	3	0
22	B	842	BCR	9	0
20	I	102	CLA	10	0
20	A	822	CLA	34	0
20	A	801	CLA	8	0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
22	I	101	BCR	19	0
20	A	835	CLA	17	0
20	K	107	CLA	24	0
20	3	302	CLA	26	0
20	B	821	CLA	41	0
21	3	321	LMU	8	0
20	4	304	CLA	22	0
20	J	101	CLA	27	0
22	B	843	BCR	18	0
20	B	838	CLA	25	0
20	4	315	CLA	3	0
21	K	105	LMU	35	0
20	K	102	CLA	10	0
20	2	308	CLA	8	0
20	A	814	CLA	34	0
21	2	313	LMU	3	1
20	A	839	CLA	43	0
20	A	850	CLA	18	0
20	B	805	CLA	17	0
20	B	812	CLA	20	0
22	B	845	BCR	33	0
20	B	809	CLA	5	0
20	B	817	CLA	17	0
20	R	108	CLA	12	0
20	A	808	CLA	26	0
20	B	823	CLA	64	0
20	A	828	CLA	14	0
20	B	833	CLA	22	0
20	4	305	CLA	20	0
20	2	311	CLA	18	0
21	B	847	LMU	28	30
22	J	102	BCR	42	0
20	B	806	CLA	17	0
20	A	841	CLA	29	0
20	4	311	CLA	17	0
20	4	316	CLA	6	0
21	H	104	LMU	20	0
20	1	206	CLA	15	0
20	B	849	CLA	21	0
20	G	102	CLA	19	0
20	H	111	CLA	9	0
21	A	848	LMU	3	0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
21	1	217	LMU	9	0
20	A	812	CLA	2	0
21	4	301	LMU	7	0
20	A	809	CLA	26	0
21	2	317	LMU	6	0
20	B	850	CLA	40	0
20	H	102	CLA	15	0
22	A	843	BCR	46	0
20	A	838	CLA	39	0
20	B	829	CLA	13	0
20	1	203	CLA	13	0
21	K	106	LMU	47	0
20	B	808	CLA	19	0
20	3	308	CLA	2	0
21	R	102	LMU	21	0
21	G	101	LMU	19	0
20	3	316	CLA	2	0
20	A	807	CLA	31	0
21	1	219	LMU	20	0
20	A	805	CLA	25	0
22	A	845	BCR	45	0
21	R	106	LMU	2	0
20	A	817	CLA	10	0
20	B	804	CLA	7	0
22	A	847	BCR	63	0
23	B	841	PQN	31	0
20	A	816	CLA	35	0
20	3	311	CLA	20	0
20	B	840	CLA	2	0
21	A	853	LMU	9	0
20	A	832	CLA	16	0
20	2	304	CLA	5	0
20	2	320	CLA	34	0
20	L	203	CLA	19	0
20	1	215	CLA	54	0
20	A	834	CLA	12	0
20	2	305	CLA	12	0
20	F	206	CLA	15	0
20	J	103	CLA	27	0
20	K	101	CLA	19	1
20	L	201	CLA	35	0
24	C	102	SF4	4	0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
20	A	829	CLA	6	0
24	C	103	SF4	4	0
20	B	824	CLA	50	0
20	A	837	CLA	17	0
21	R	103	LMU	25	0
21	3	320	LMU	4	0
20	B	810	CLA	19	0
21	E	101	LMU	30	0
21	L	204	LMU	3	0
20	B	827	CLA	30	0
22	A	846	BCR	35	0
20	A	804	CLA	28	0
20	R	107	CLA	10	0
20	3	307	CLA	16	0
22	B	852	BCR	13	0
20	A	820	CLA	15	0
20	B	835	CLA	12	0
20	B	819	CLA	17	0
20	A	827	CLA	22	0
20	B	851	CLA	48	0
21	D	201	LMU	12	0
20	4	310	CLA	3	0
22	L	208	BCR	51	0
20	H	103	CLA	3	0
20	L	202	CLA	23	0
20	B	830	CLA	27	0
20	K	103	CLA	3	0
21	L	205	LMU	4	0
20	3	304	CLA	14	0
20	A	811	CLA	22	0
20	F	204	CLA	2	0
20	B	826	CLA	33	0
21	H	105	LMU	12	0
20	B	837	CLA	26	0
21	R	101	LMU	6	0
21	A	855	LMU	27	0
21	H	108	LMU	37	0
22	B	844	BCR	18	0
21	K	108	LMU	6	0
20	A	833	CLA	18	1
20	B	815	CLA	20	0
20	3	309	CLA	5	0

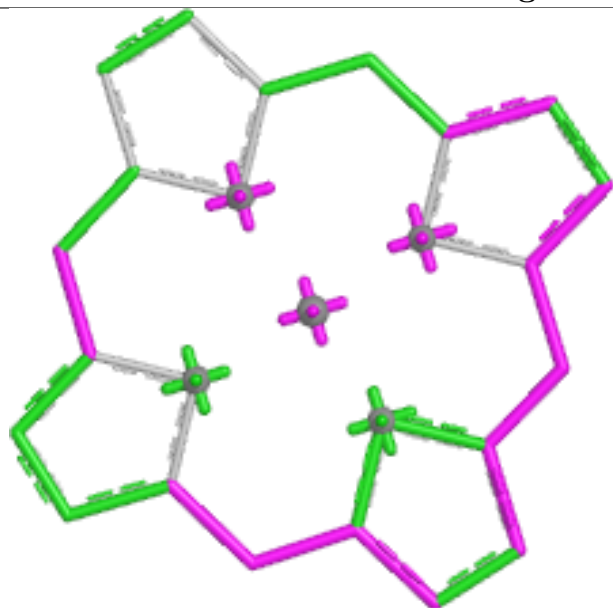
Continued on next page...

Continued from previous page...

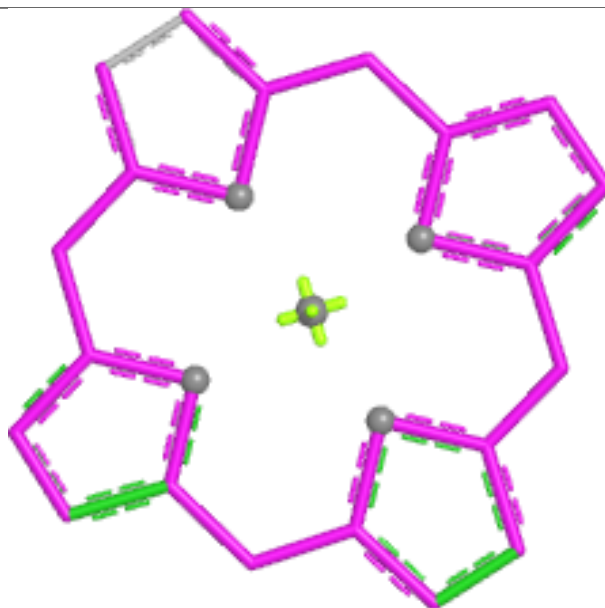
Mol	Chain	Res	Type	Clashes	Symm-Clashes
22	3	314	BCR	19	28
21	4	320	LMU	8	5
21	2	318	LMU	4	0
20	1	207	CLA	6	1
20	A	821	CLA	10	0
20	A	824	CLA	84	0
20	A	825	CLA	76	0
20	B	820	CLA	14	0
20	L	206	CLA	21	0
20	1	210	CLA	8	0
20	4	318	CLA	19	0
20	3	306	CLA	3	0
21	L	209	LMU	3	0
21	A	854	LMU	42	0
21	H	106	LMU	29	0
20	B	836	CLA	43	0
21	2	316	LMU	12	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.

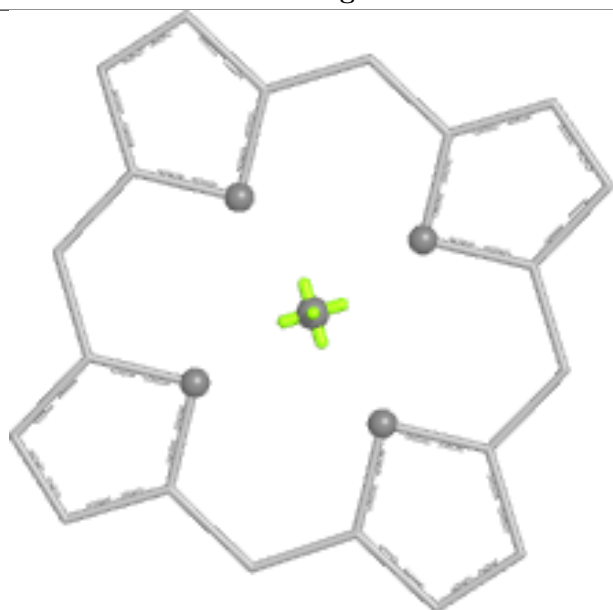
Ligand CLA 1 205



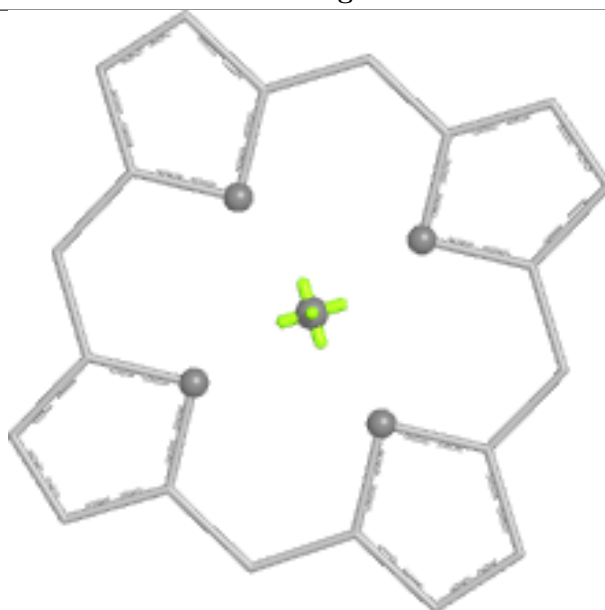
Bond lengths



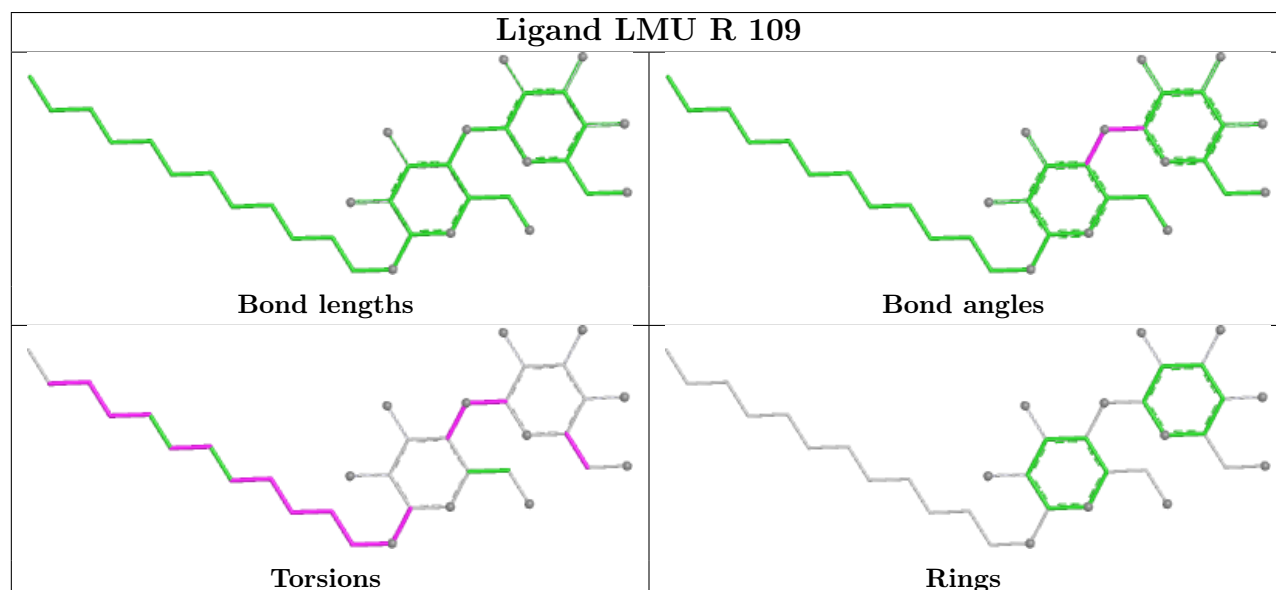
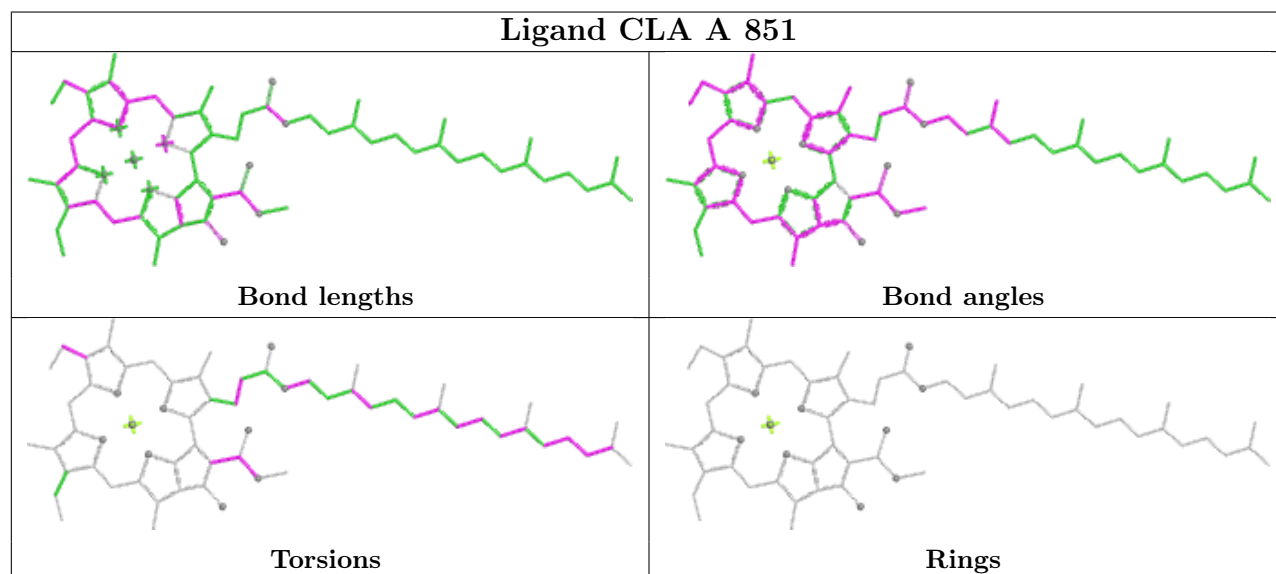
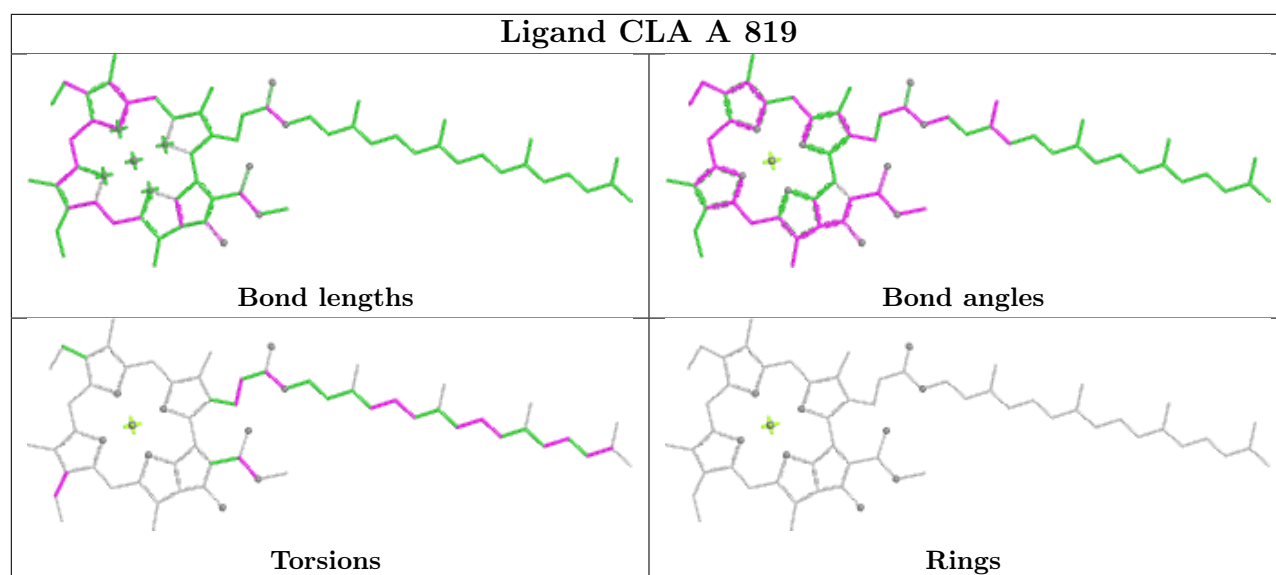
Bond angles

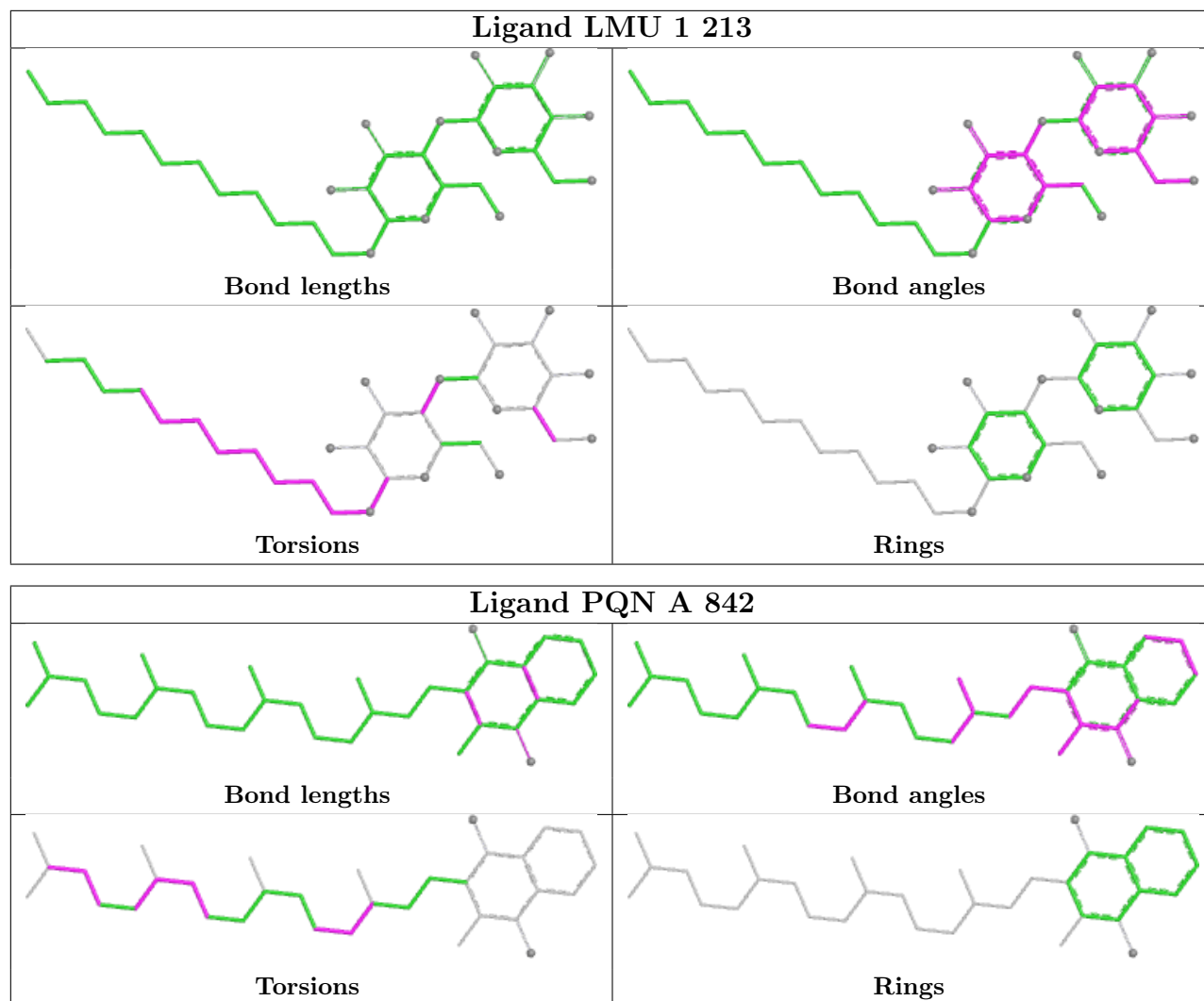


Torsions

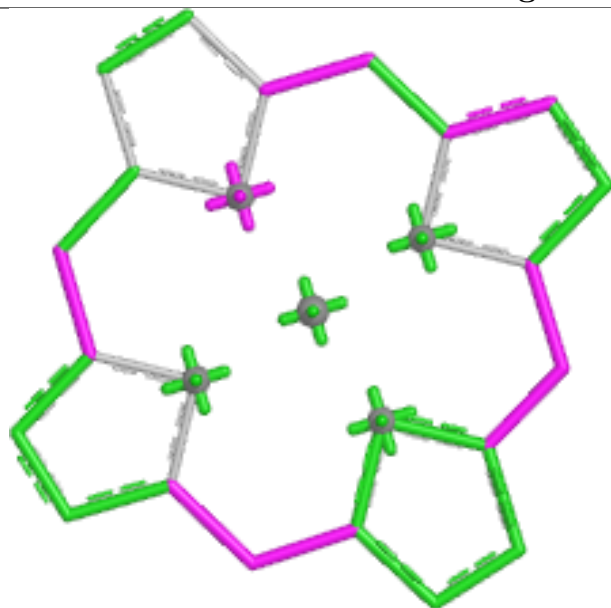


Rings

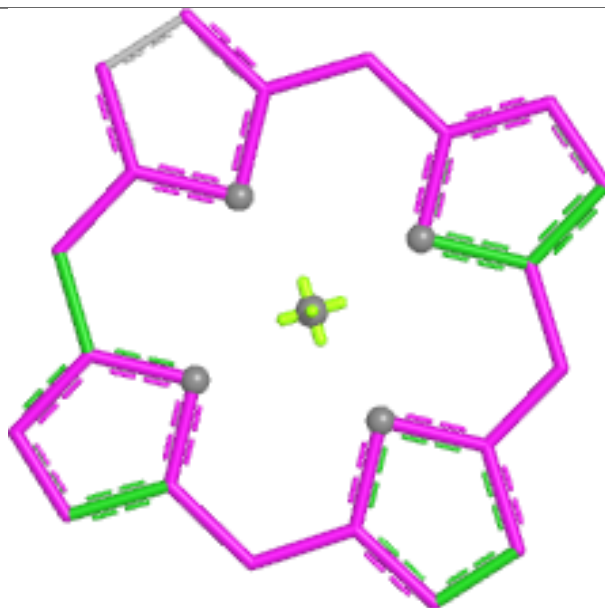




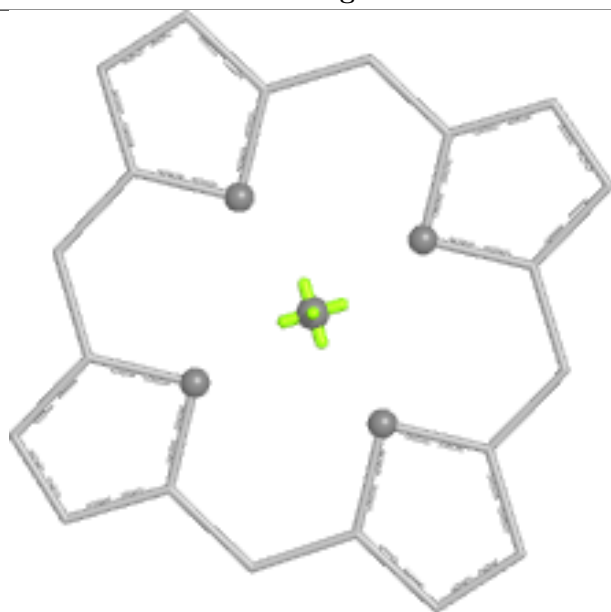
Ligand CLA 2 310



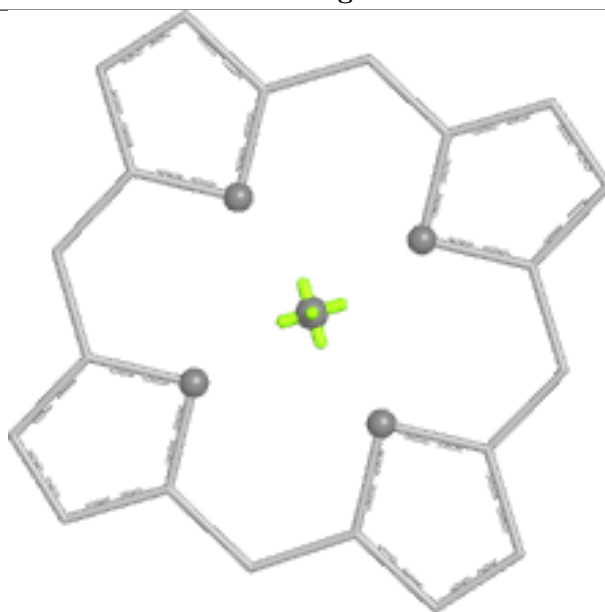
Bond lengths



Bond angles

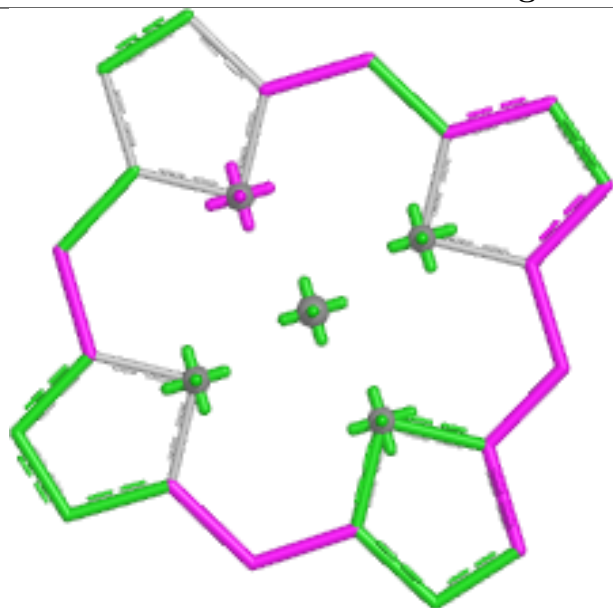


Torsions

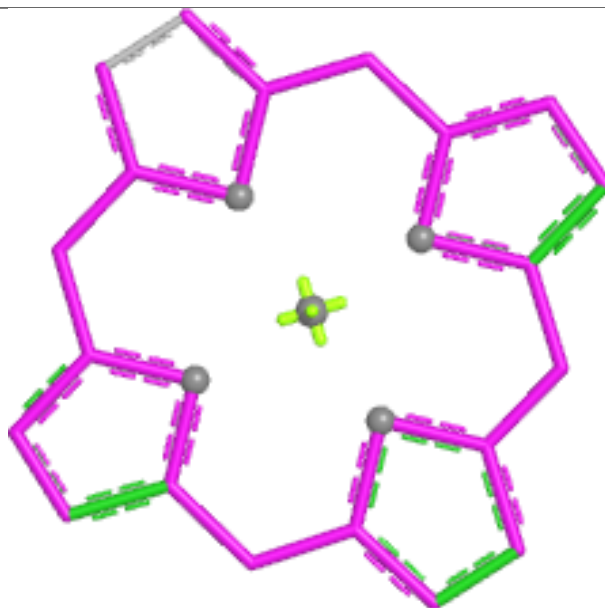


Rings

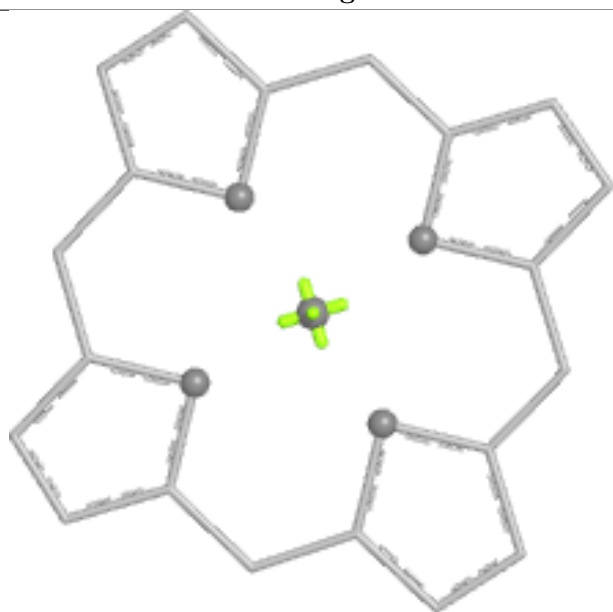
Ligand CLA 4 312



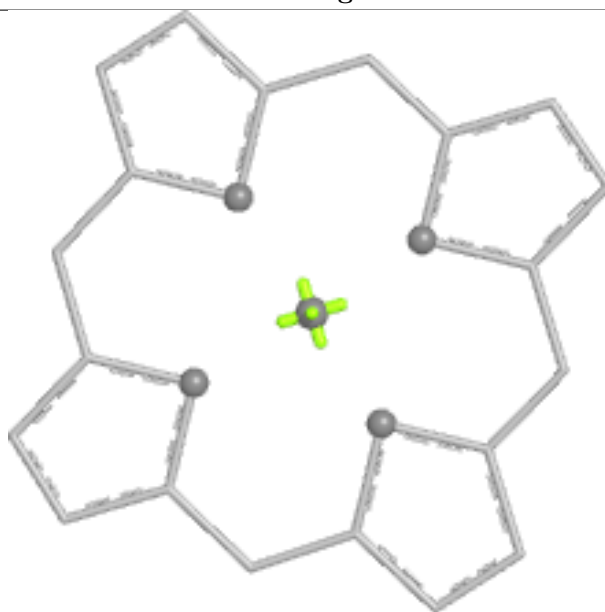
Bond lengths



Bond angles

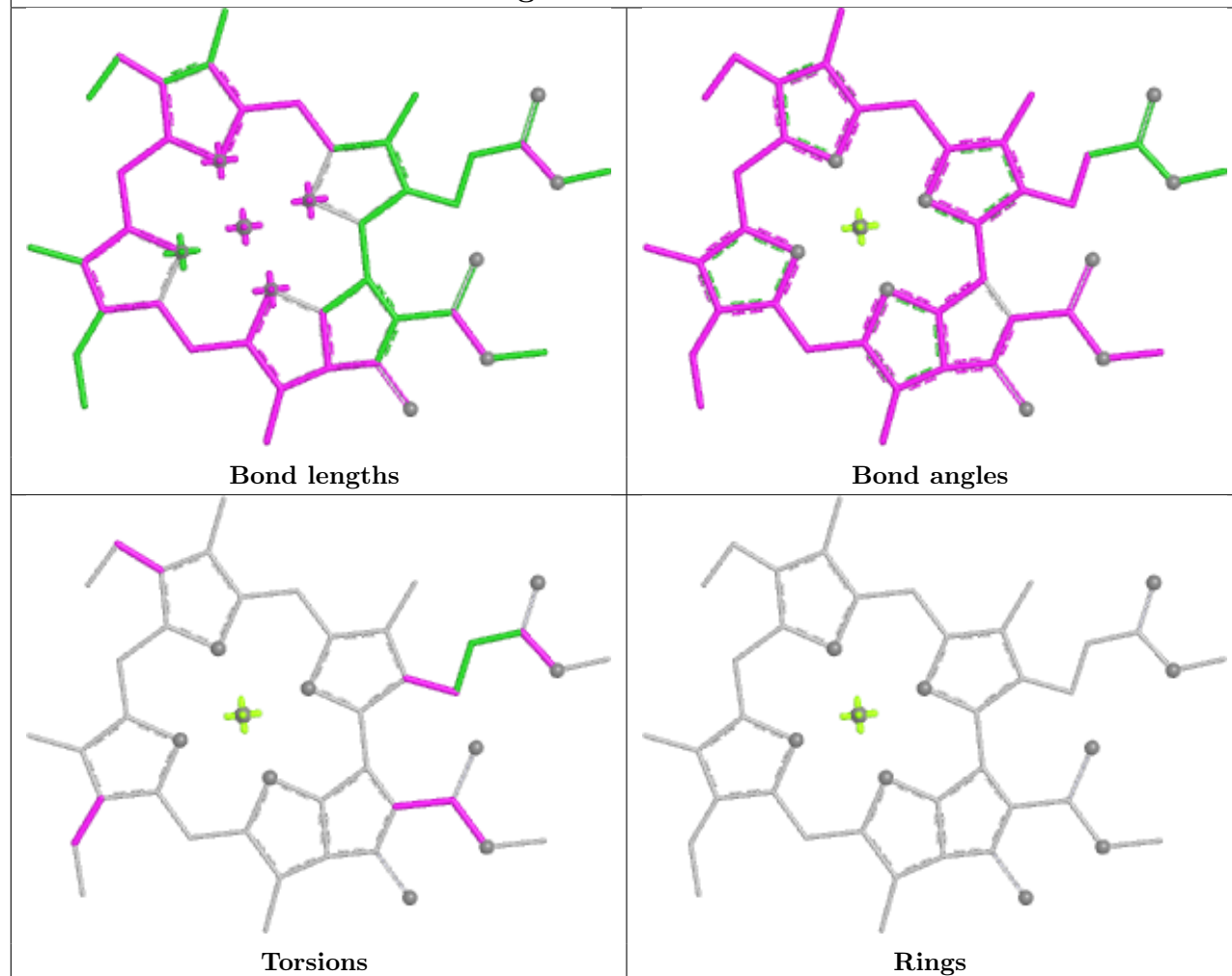


Torsions

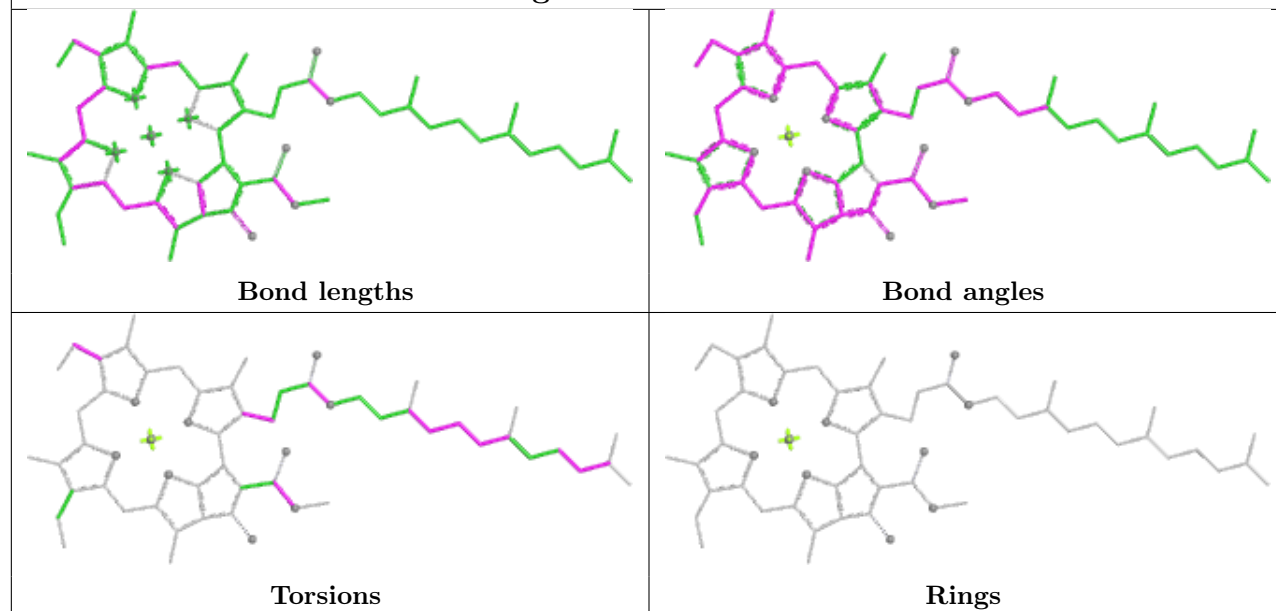


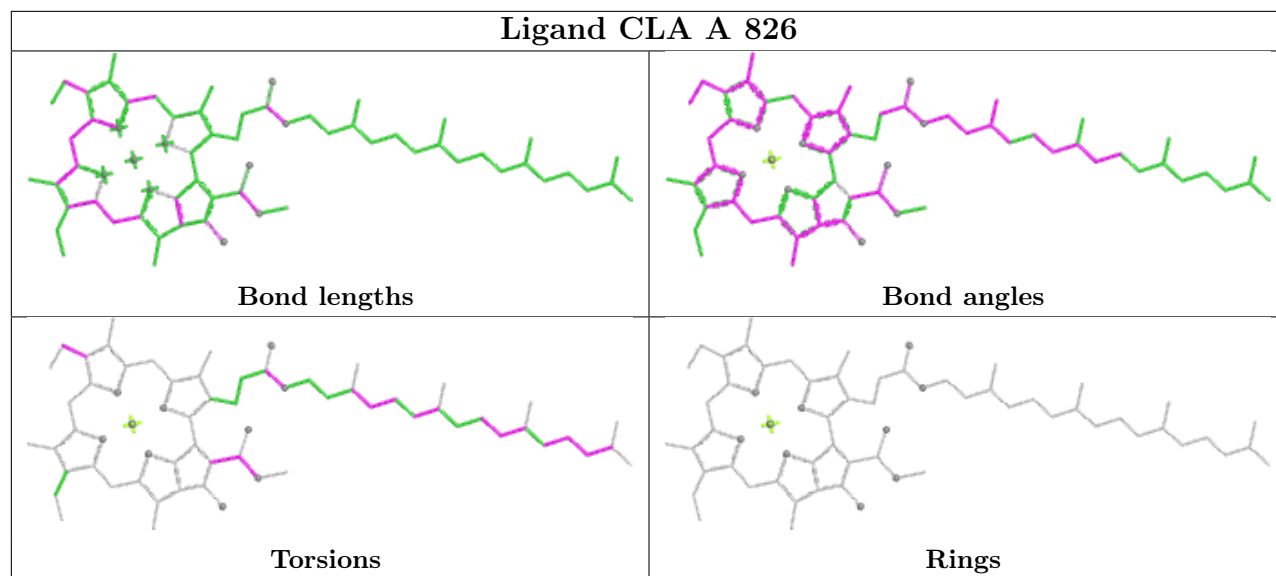
Rings

Ligand CLA 1 201

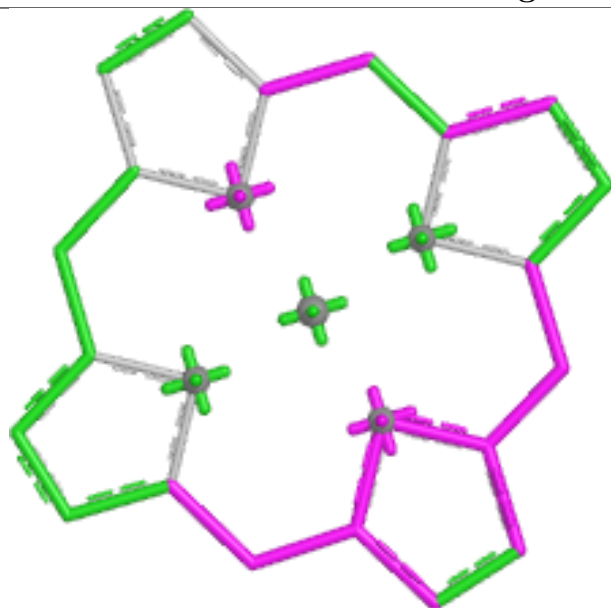


Ligand CLA B 816

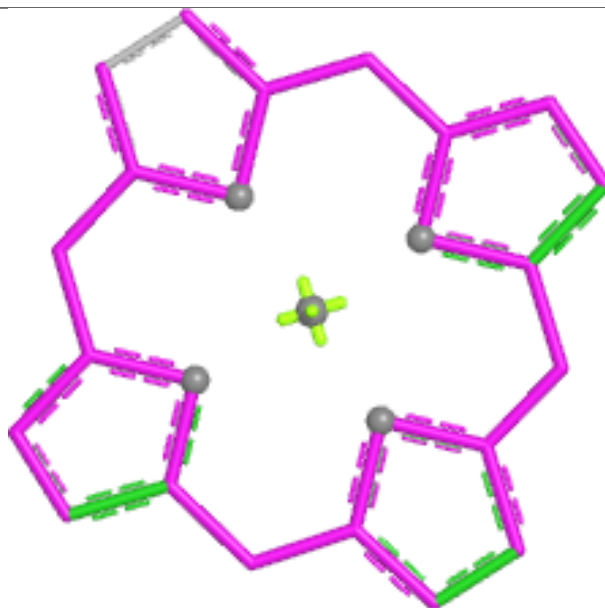




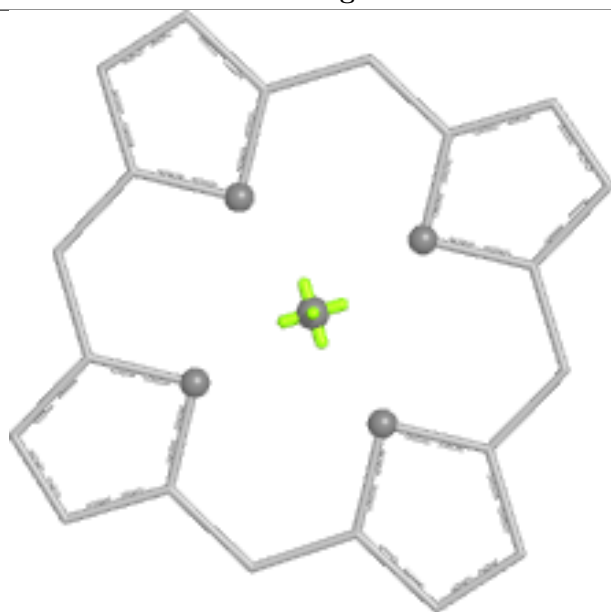
Ligand CLA 4 309



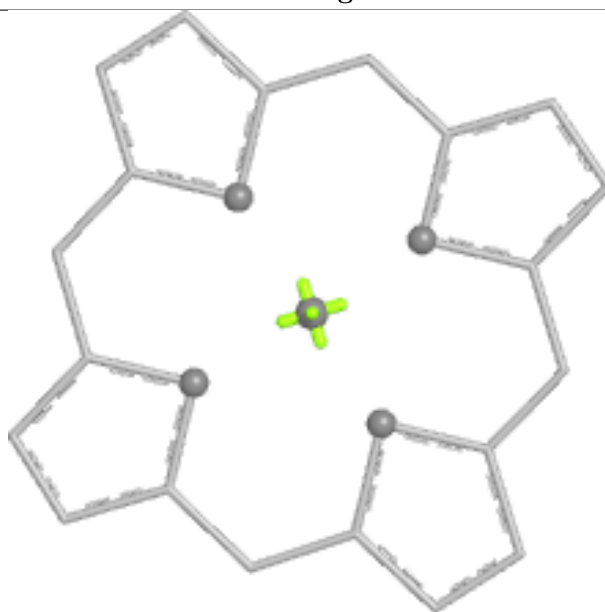
Bond lengths



Bond angles

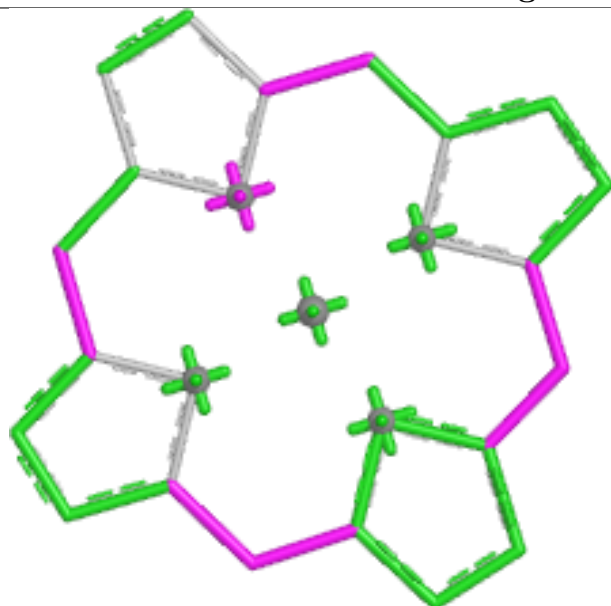


Torsions

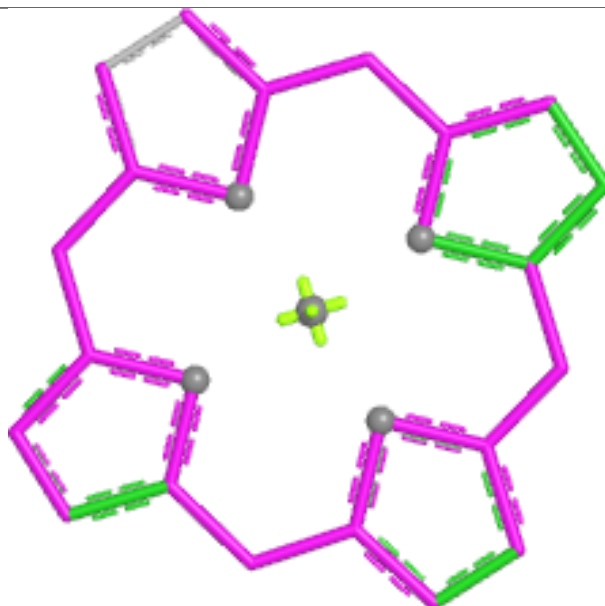


Rings

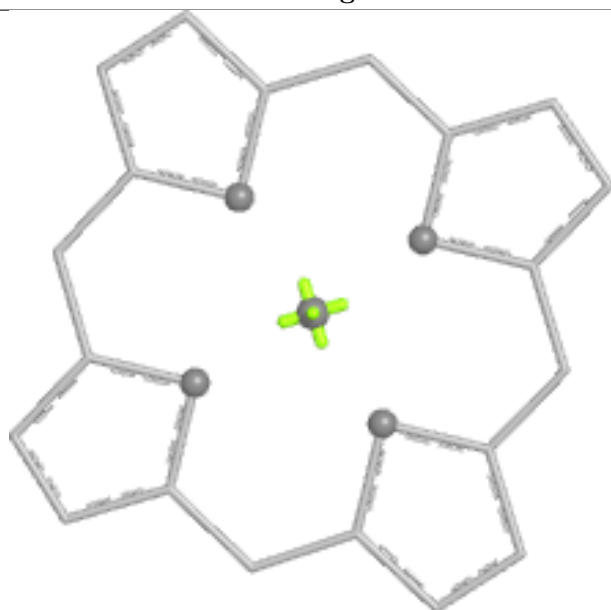
Ligand CLA 2 314



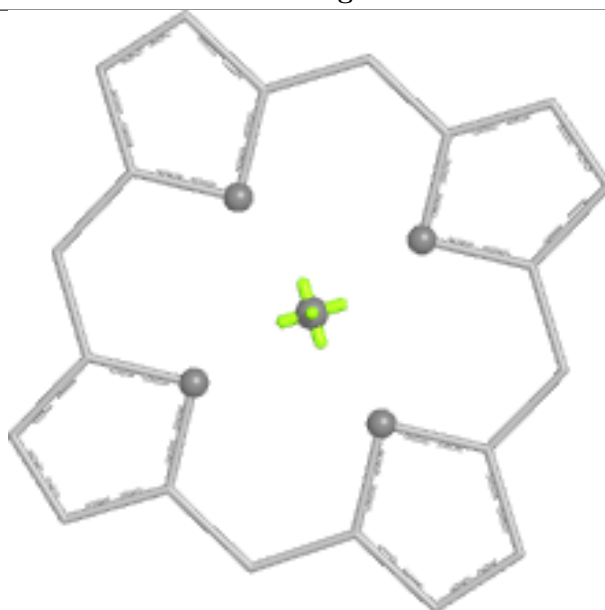
Bond lengths



Bond angles

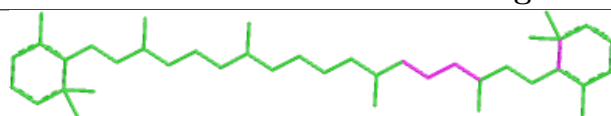


Torsions

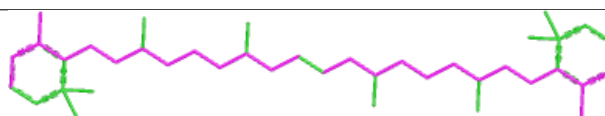


Rings

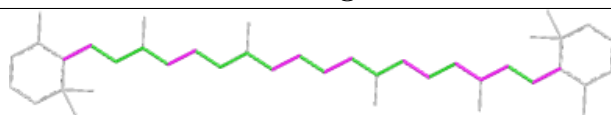
Ligand BCR F 202



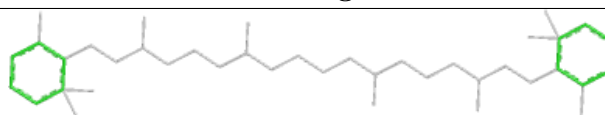
Bond lengths



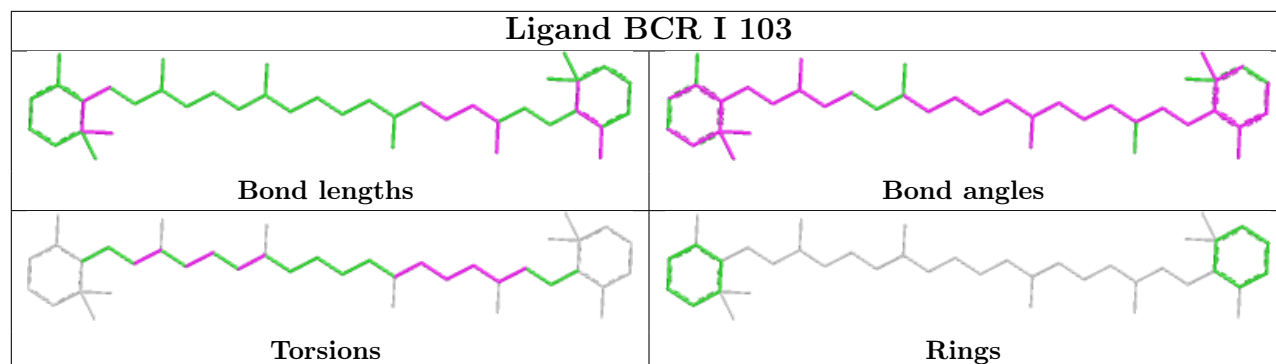
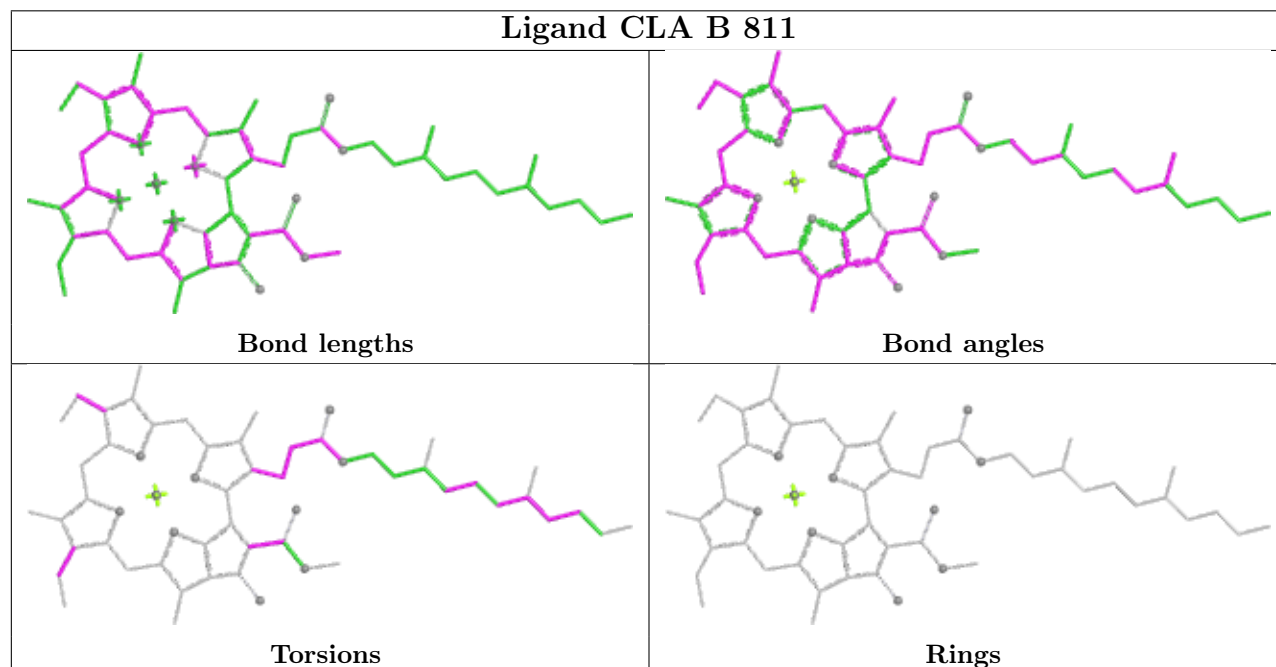
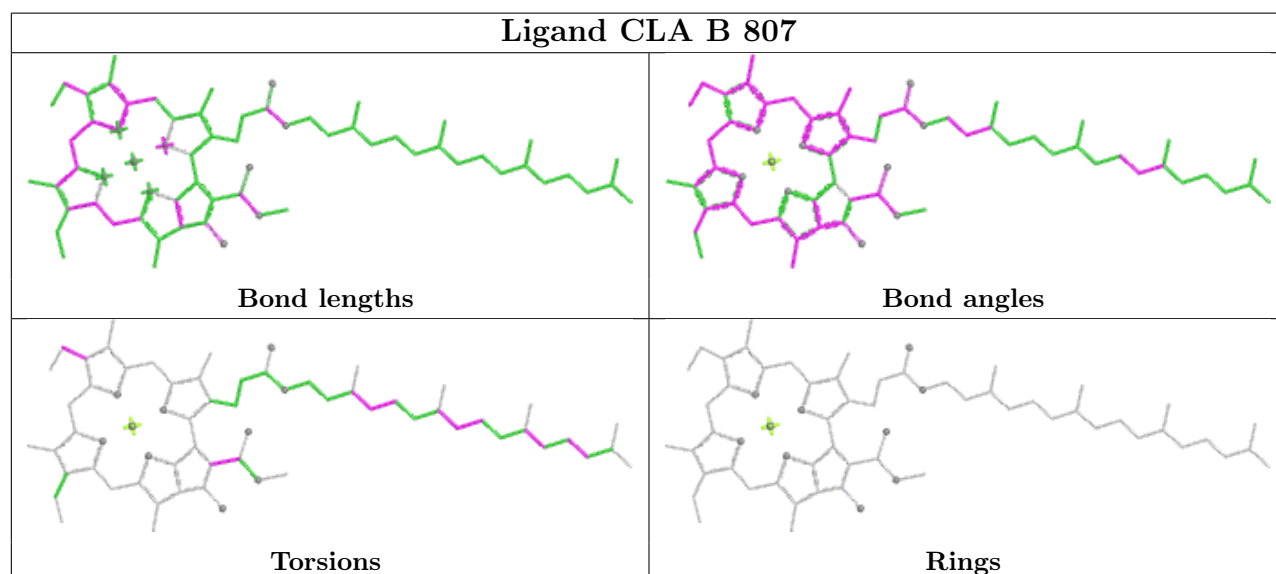
Bond angles

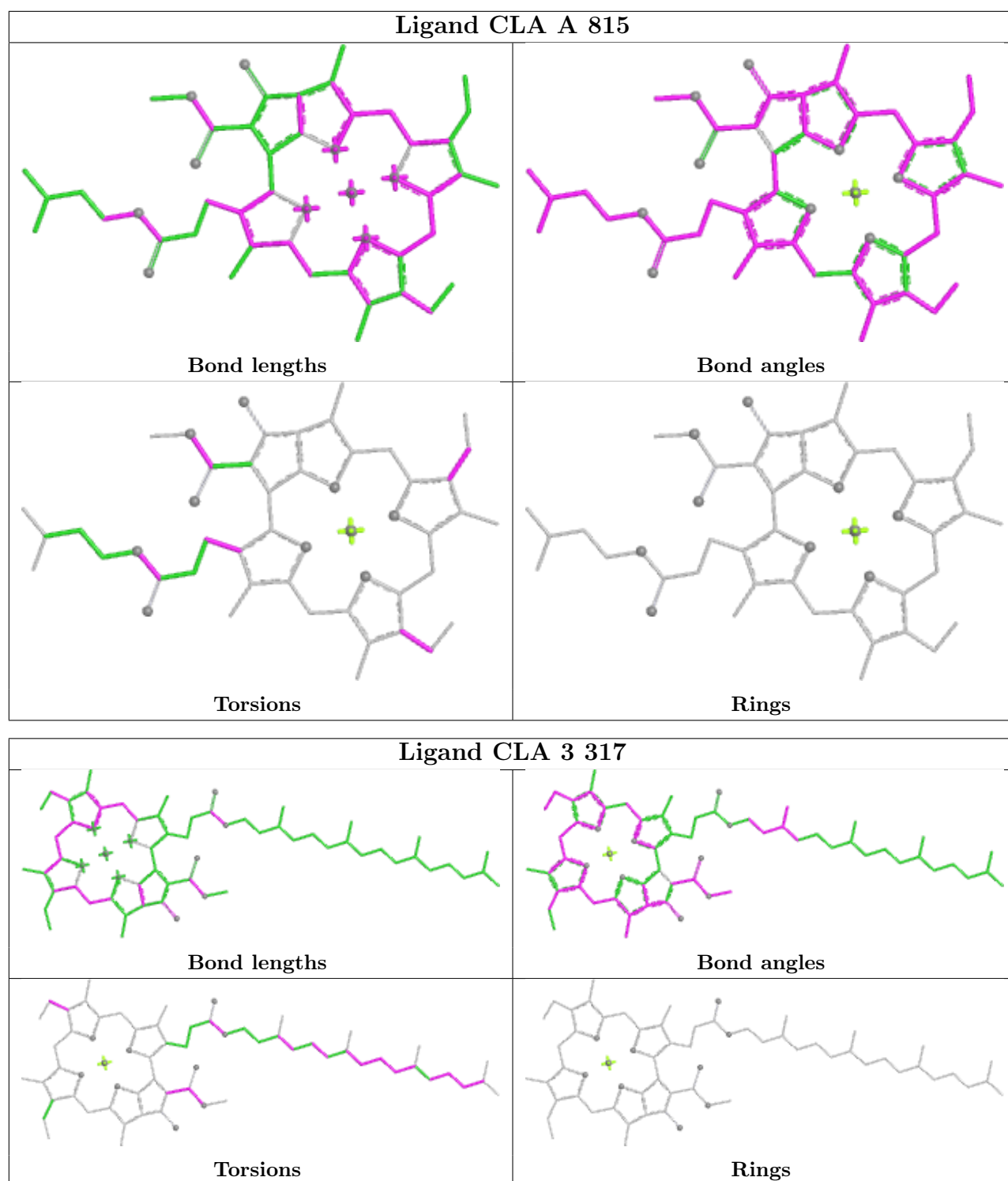


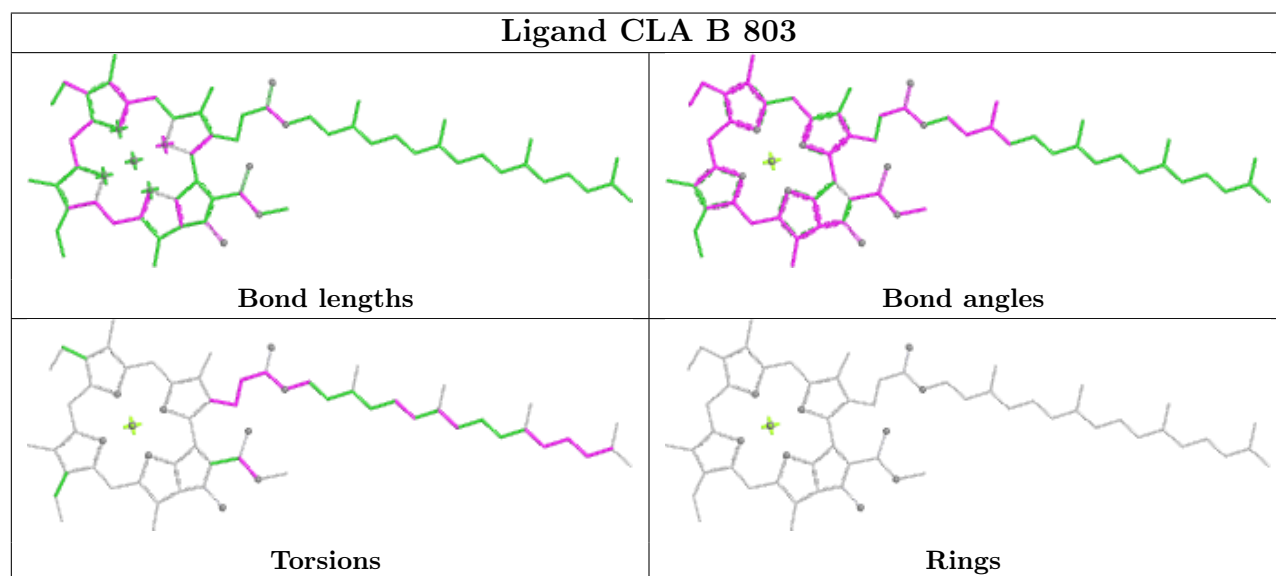
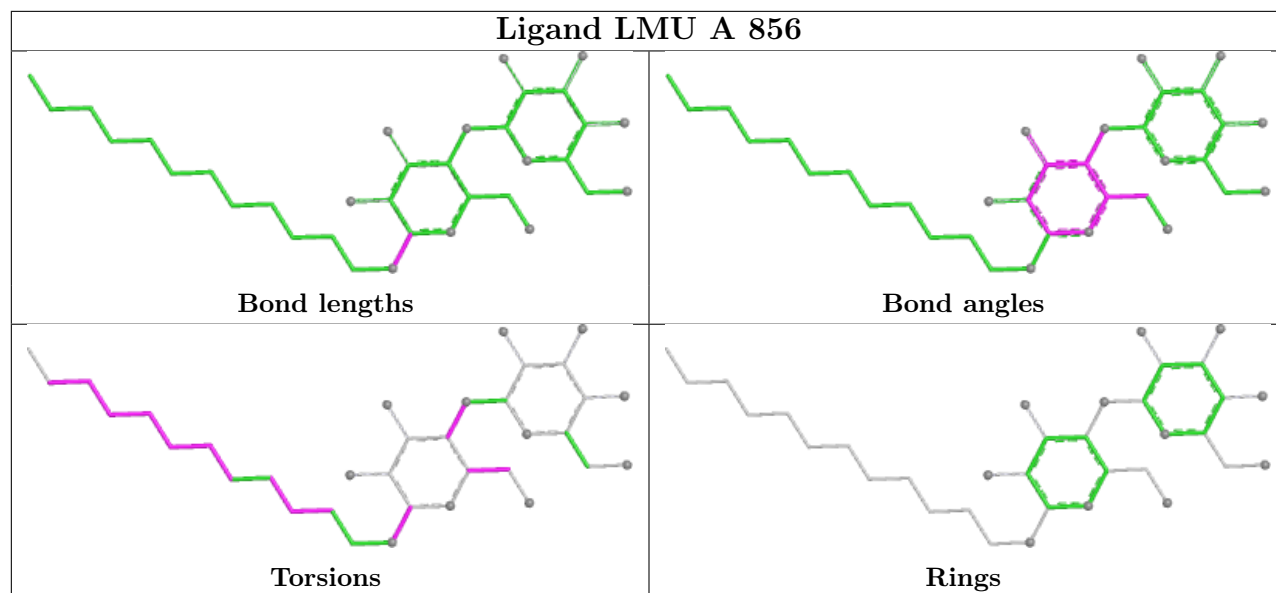
Torsions



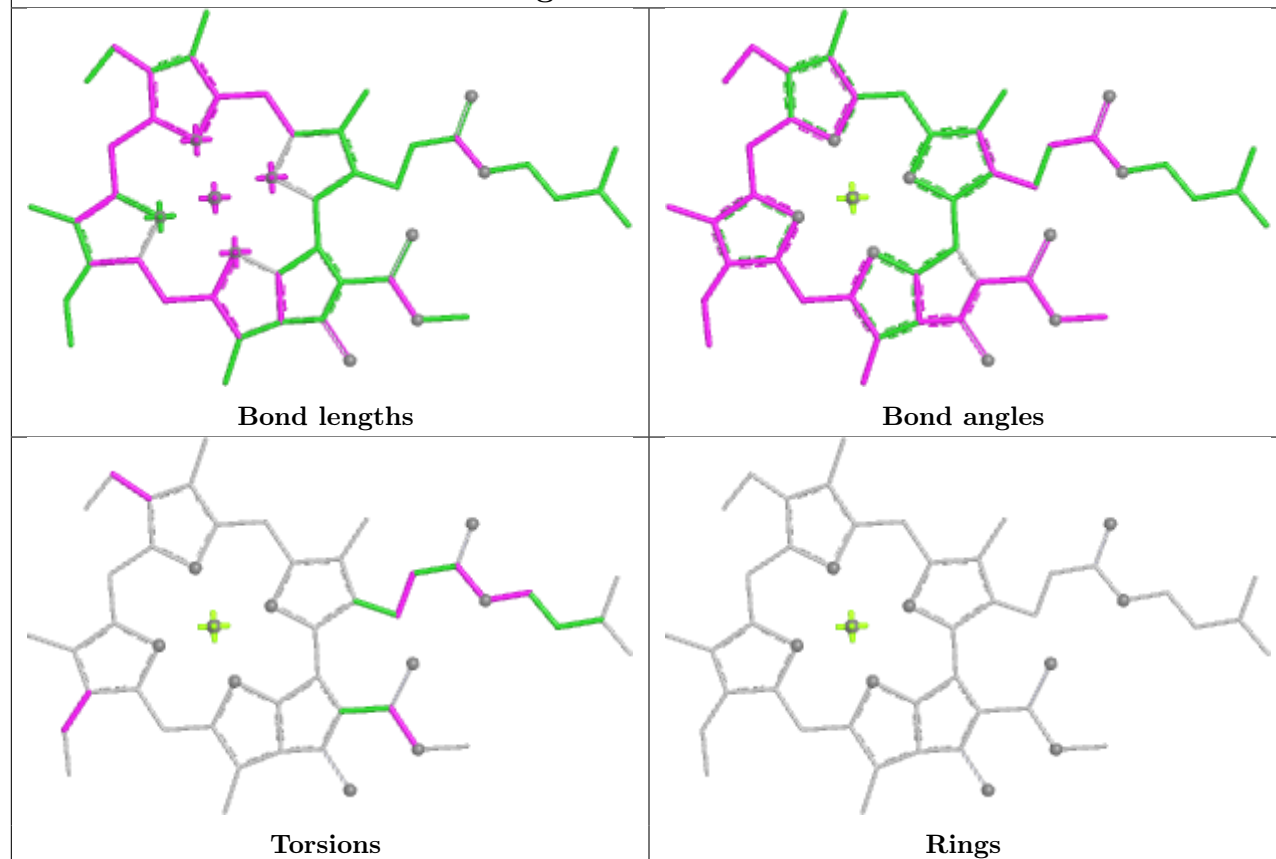
Rings

Ligand BCR I 103**Ligand CLA B 811****Ligand CLA B 807**

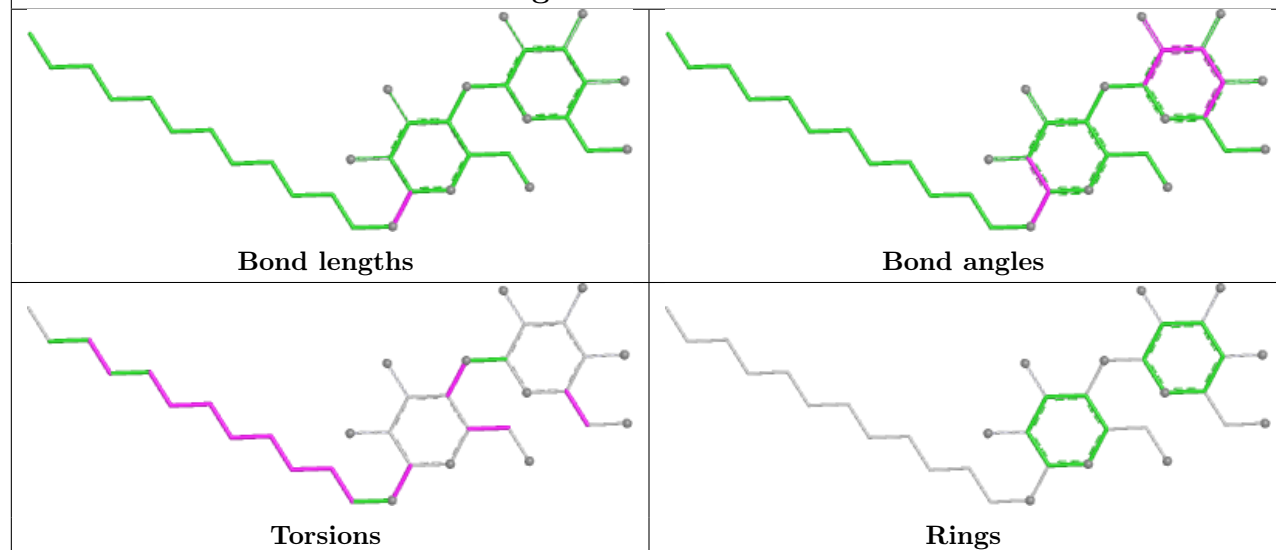




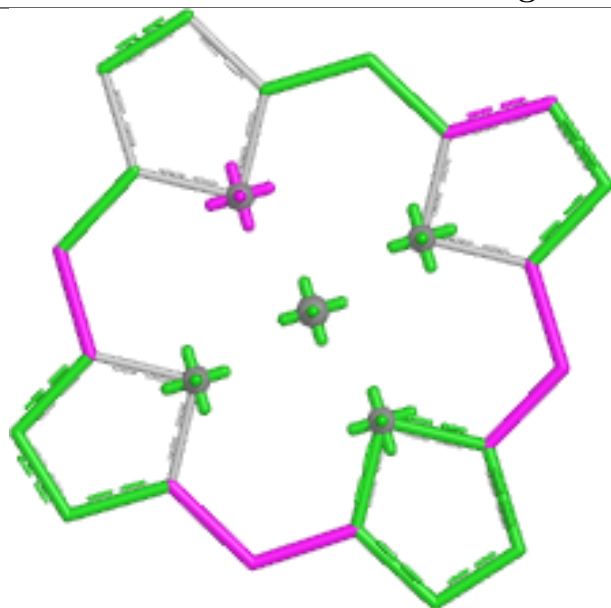
Ligand CLA 4 306



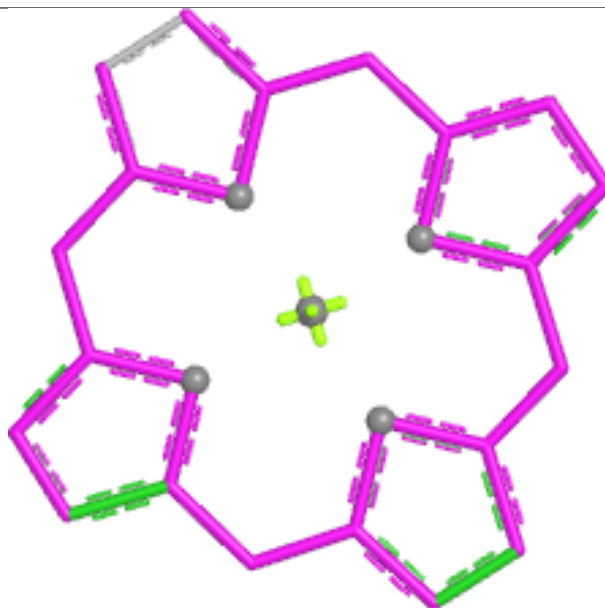
Ligand LMU 4 322



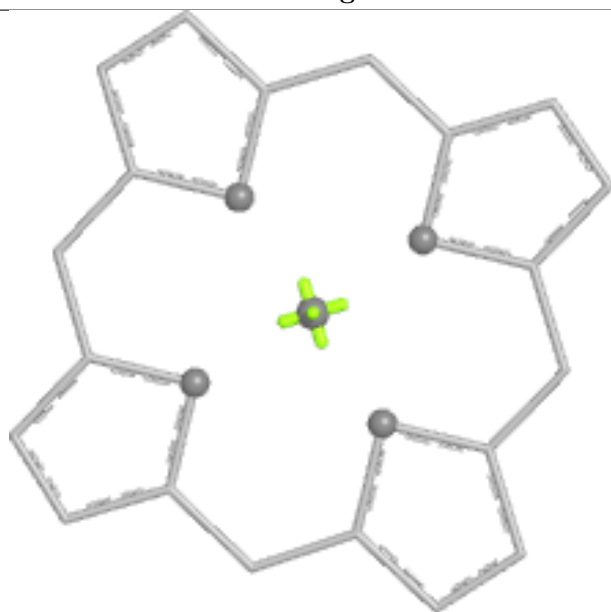
Ligand CLA 4 313



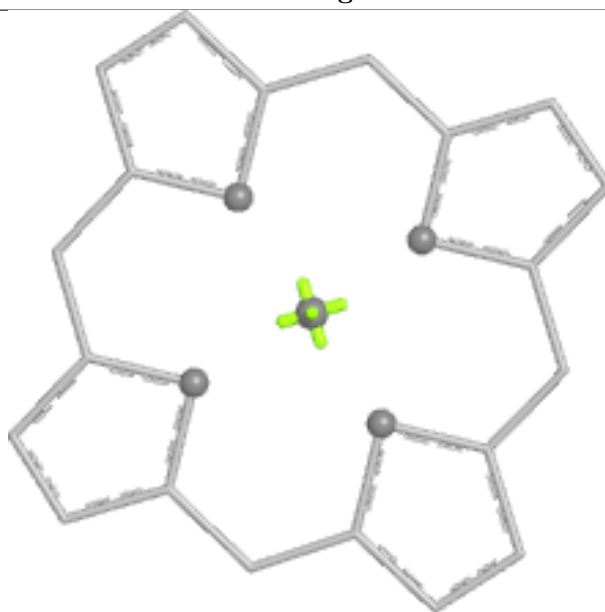
Bond lengths



Bond angles

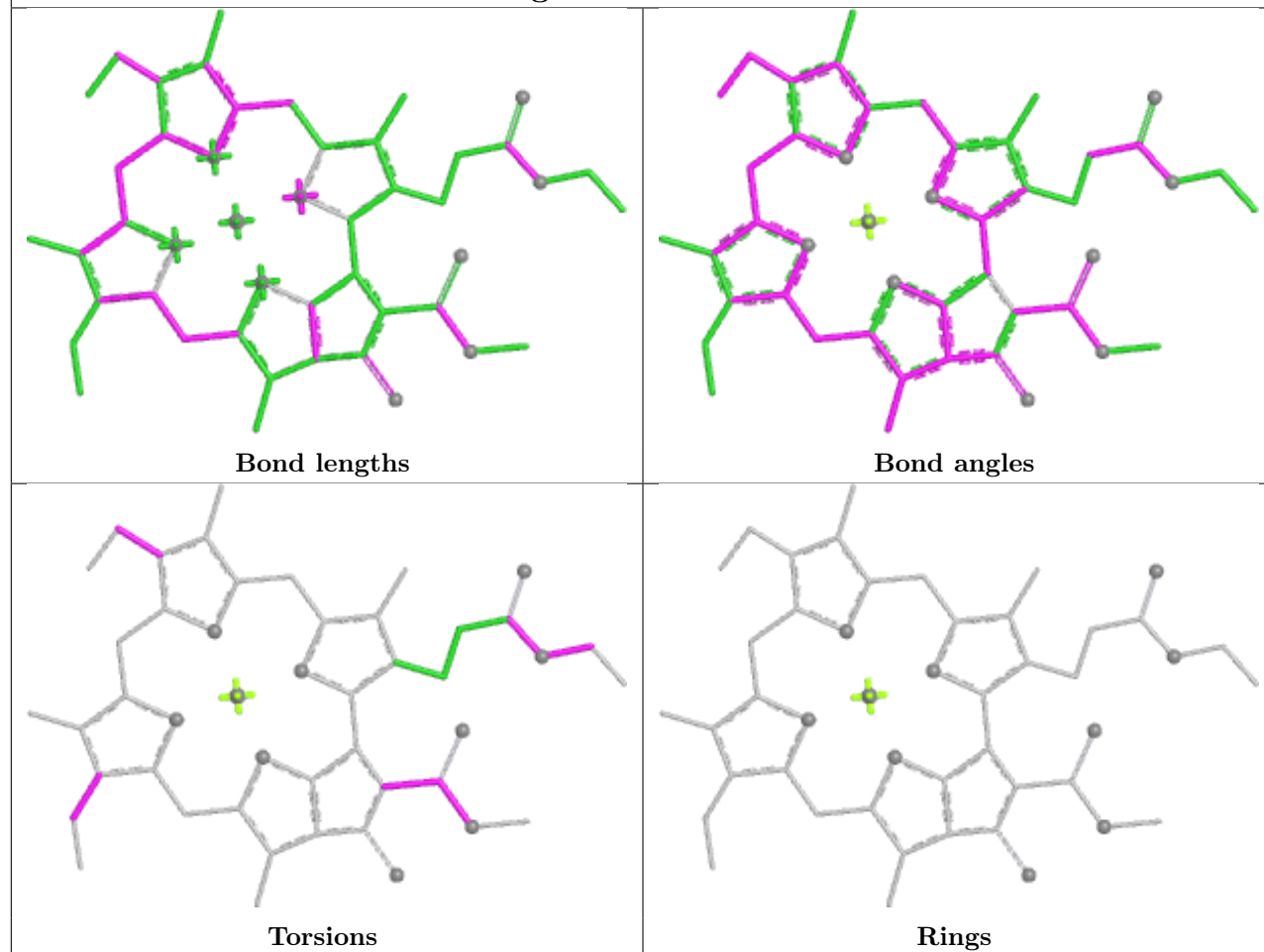


Torsions

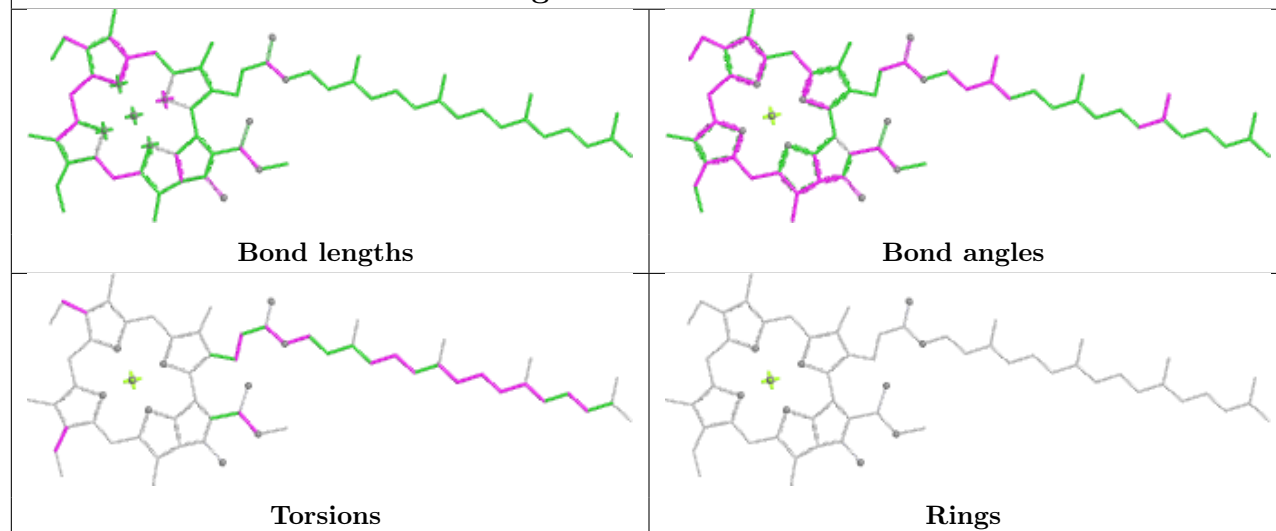


Rings

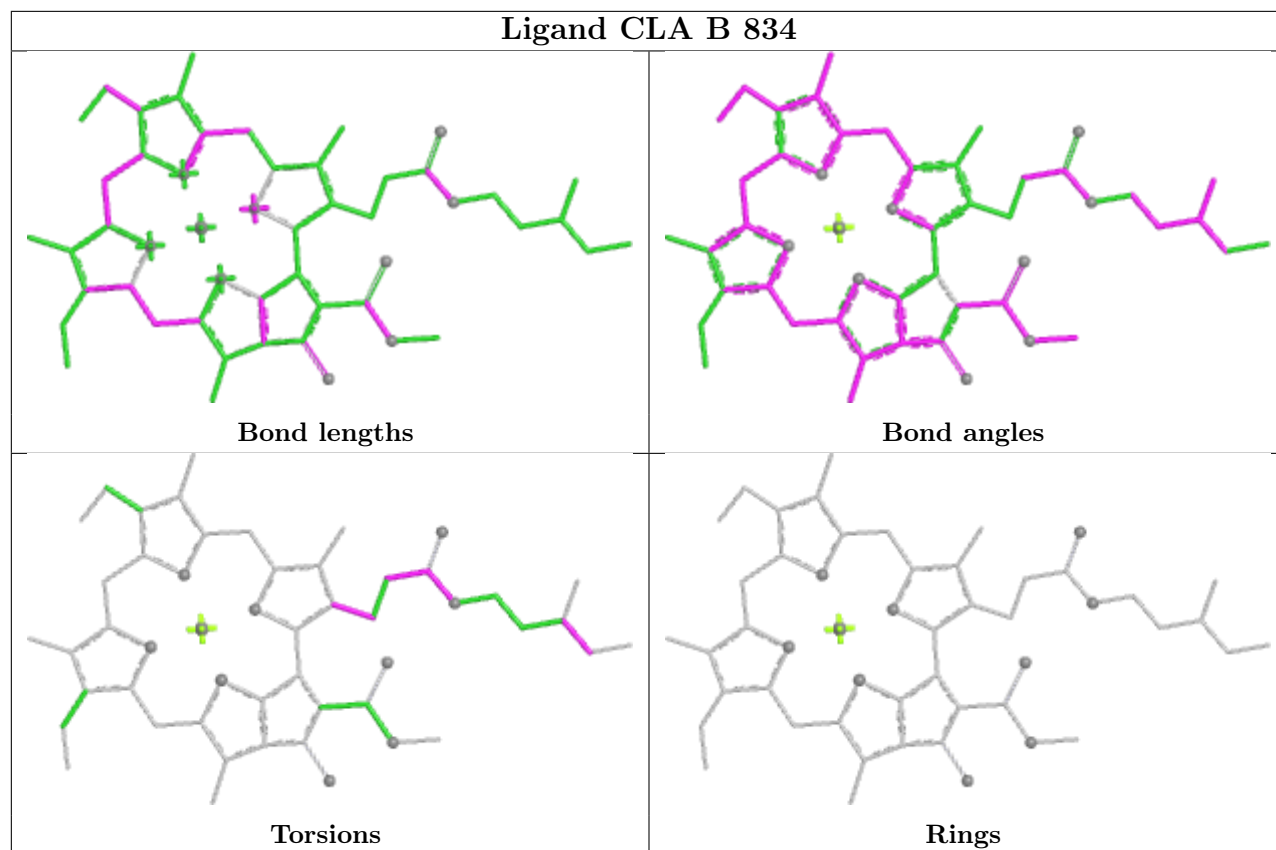
Ligand CLA 4 319



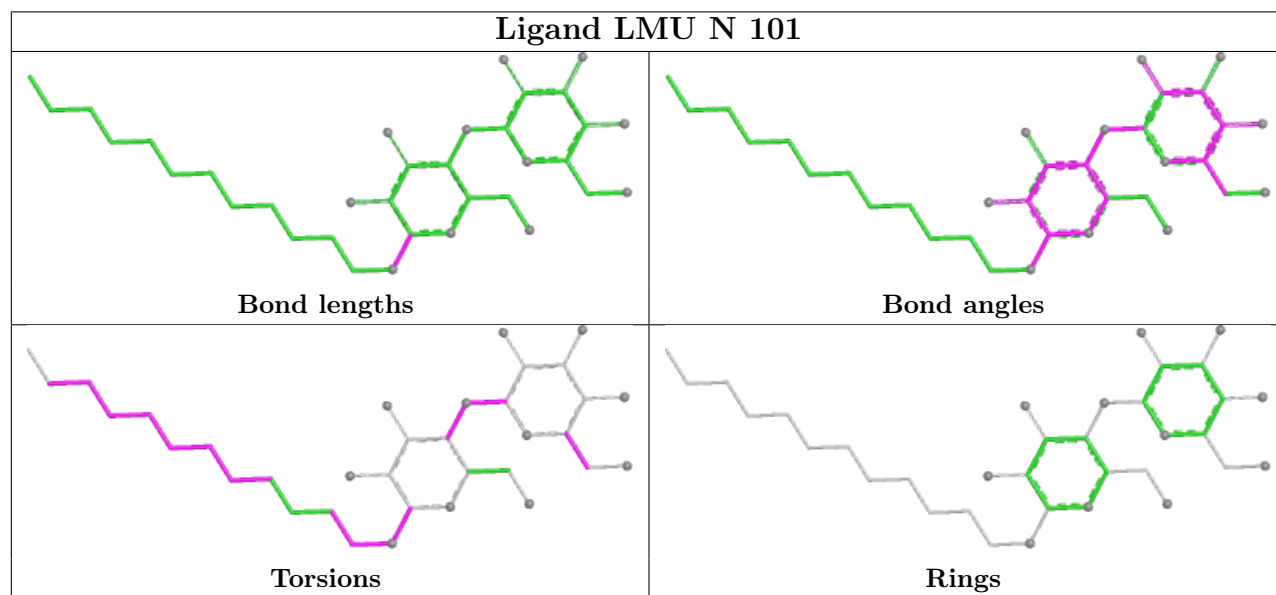
Ligand CLA A 823

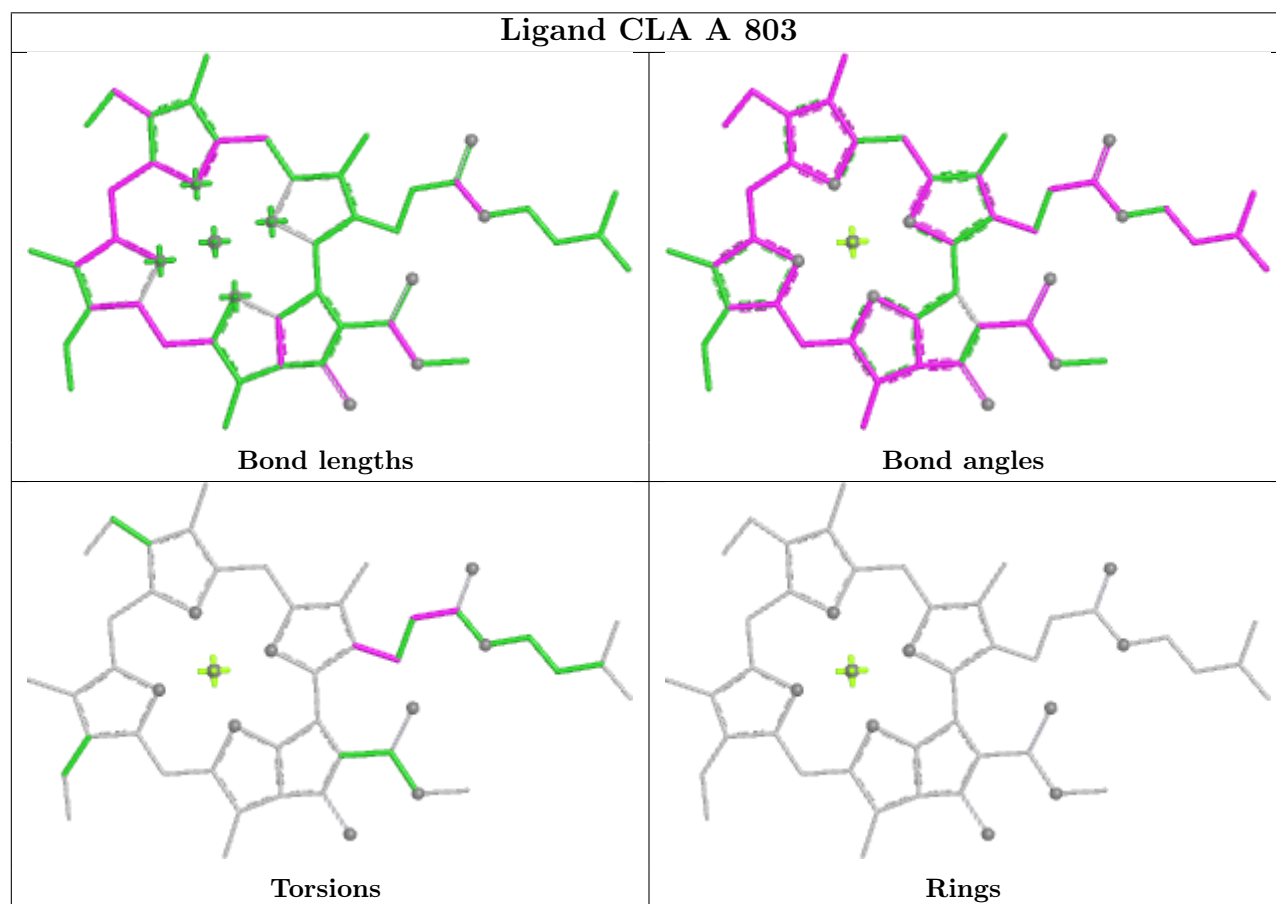
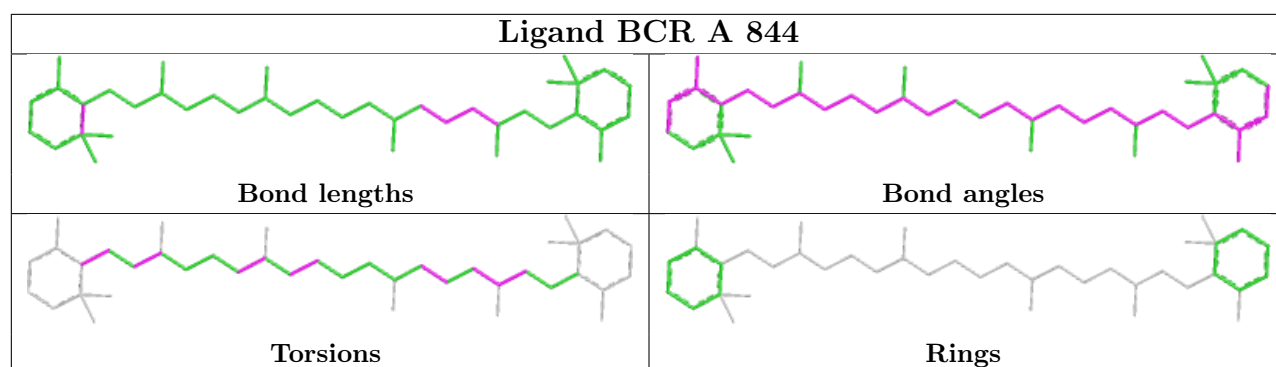


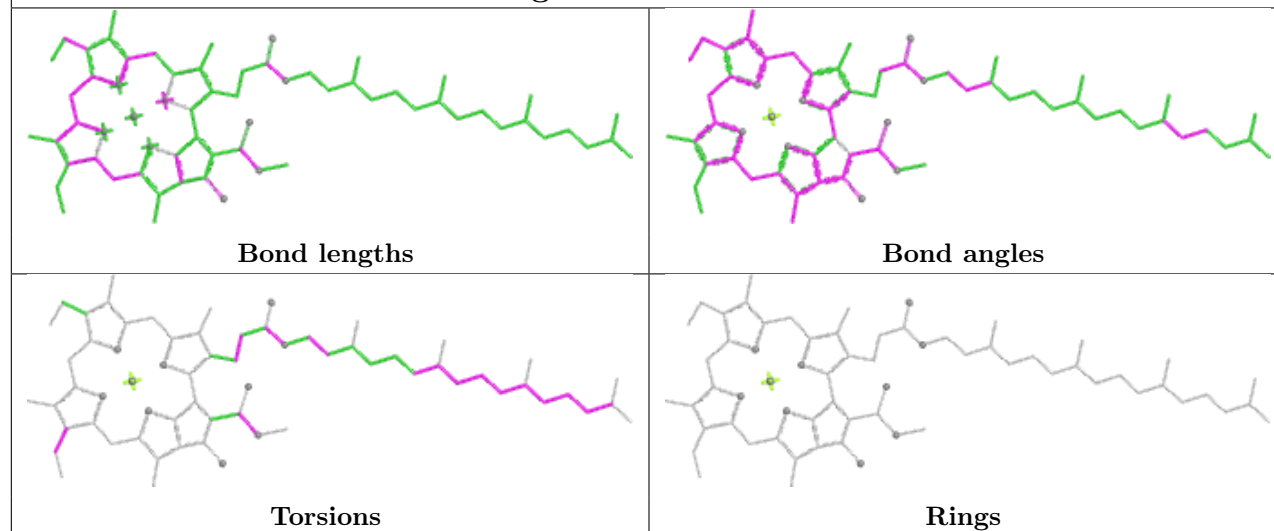
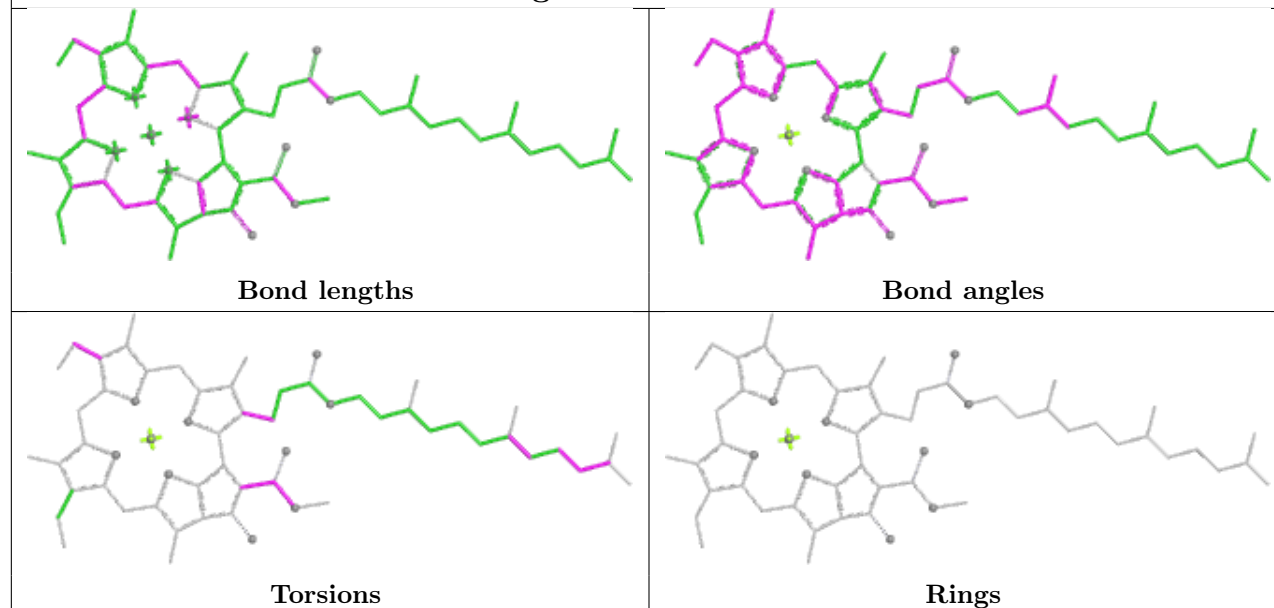
Ligand CLA B 834

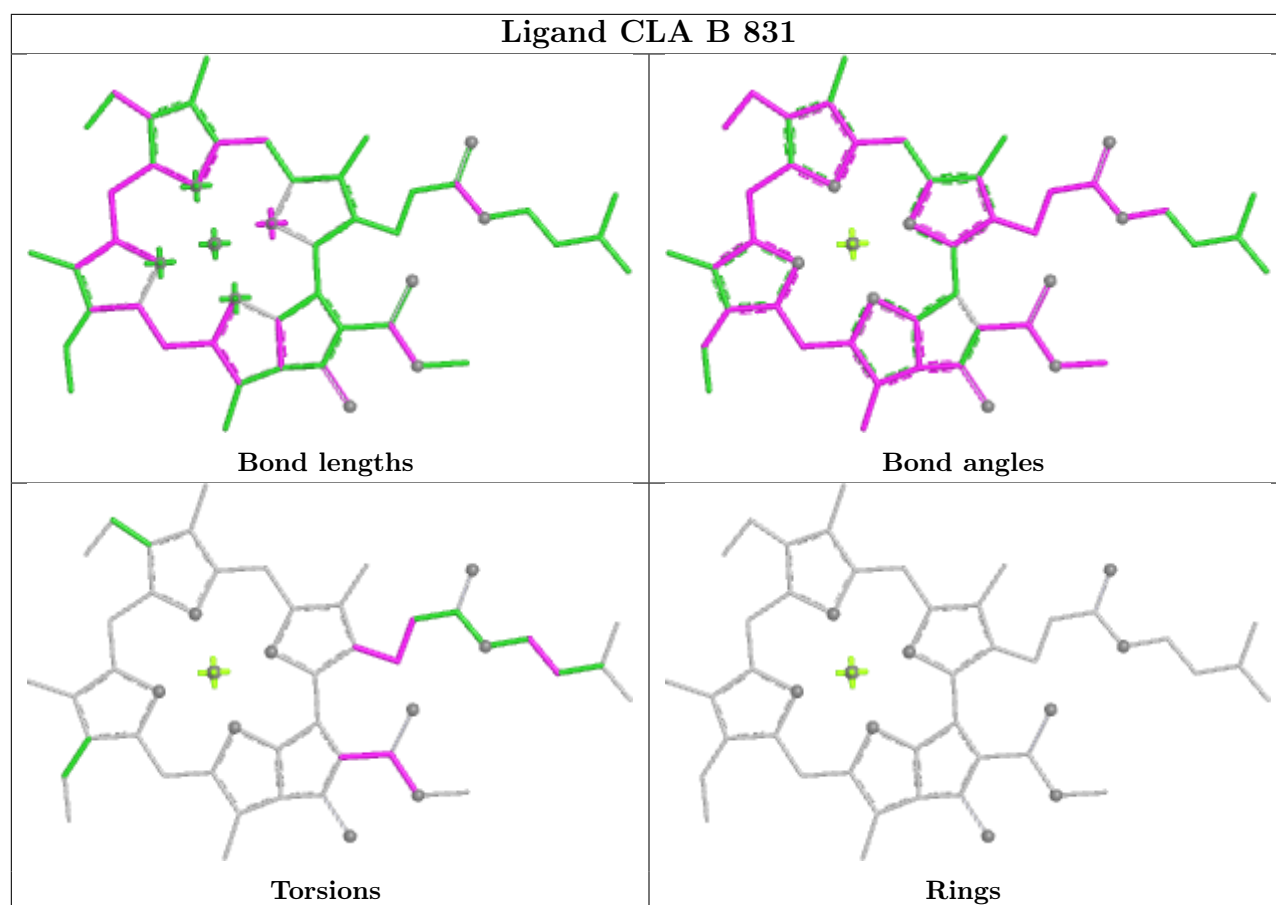


Ligand LMU N 101

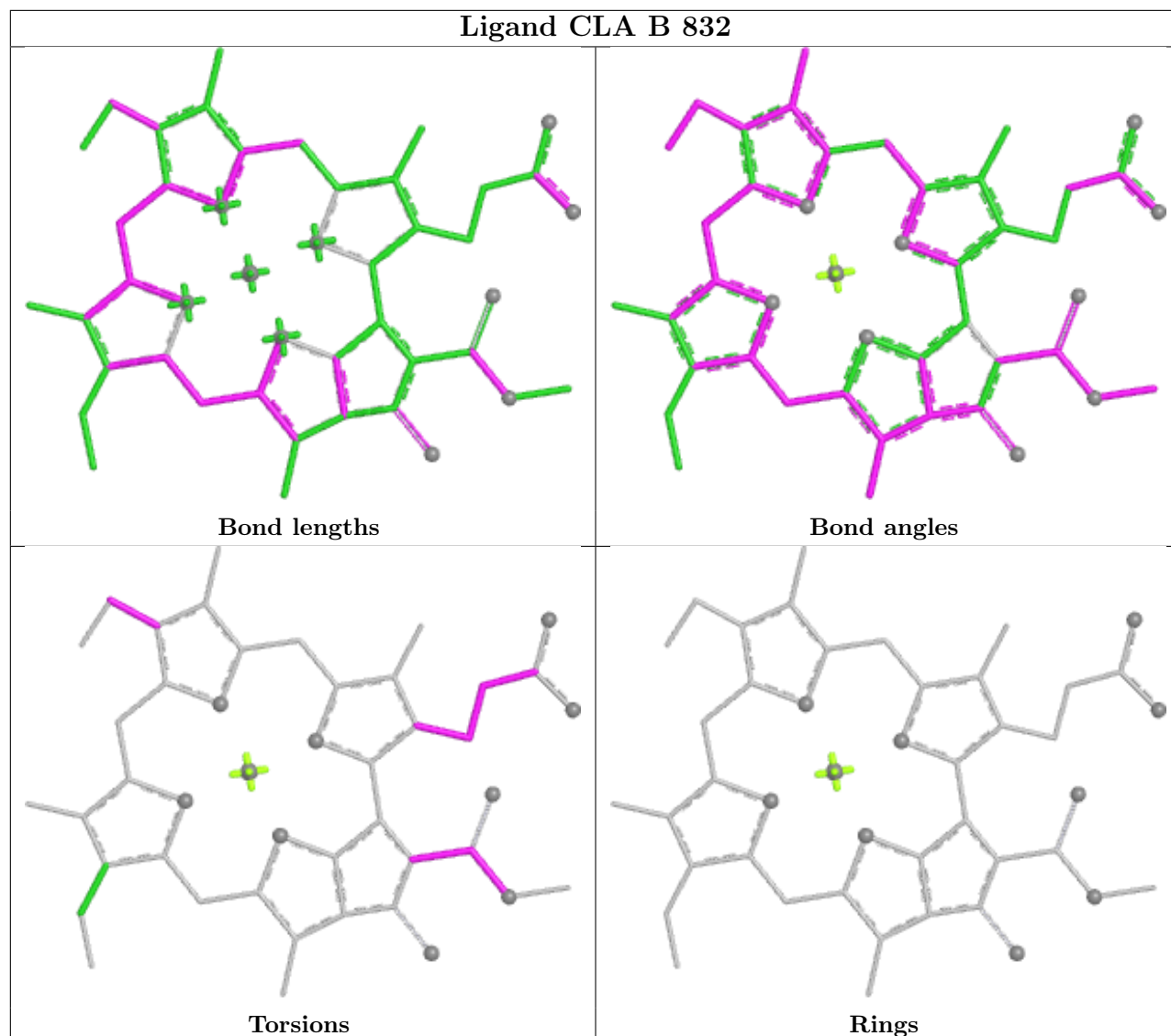




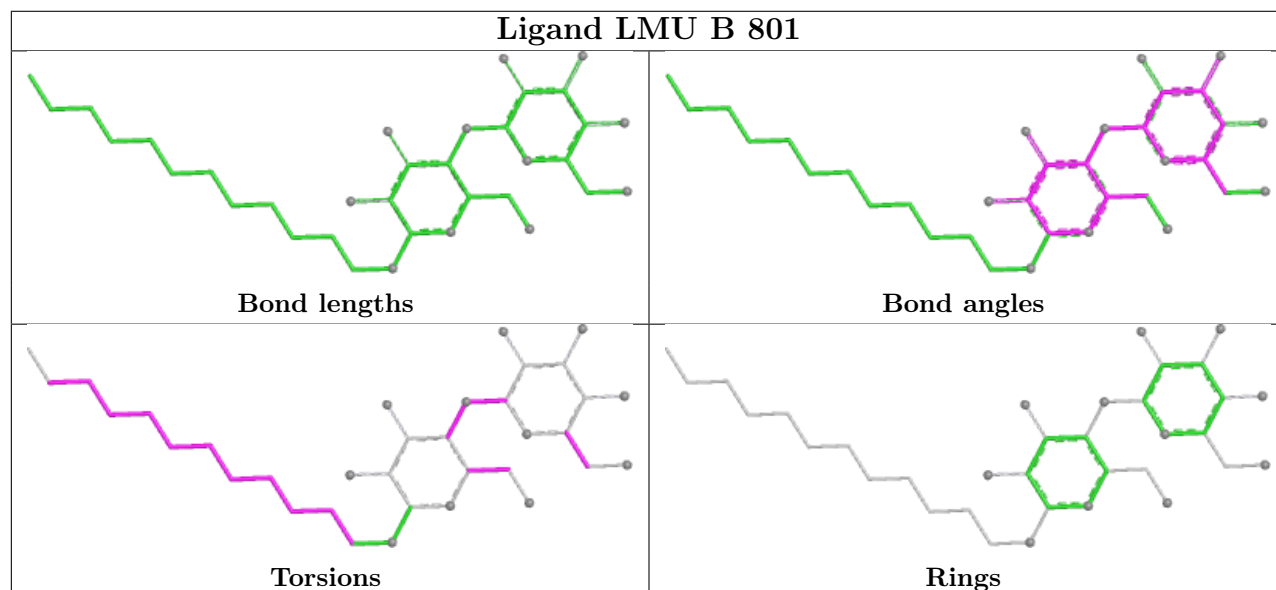
Ligand CLA A 852**Ligand CLA B 813**



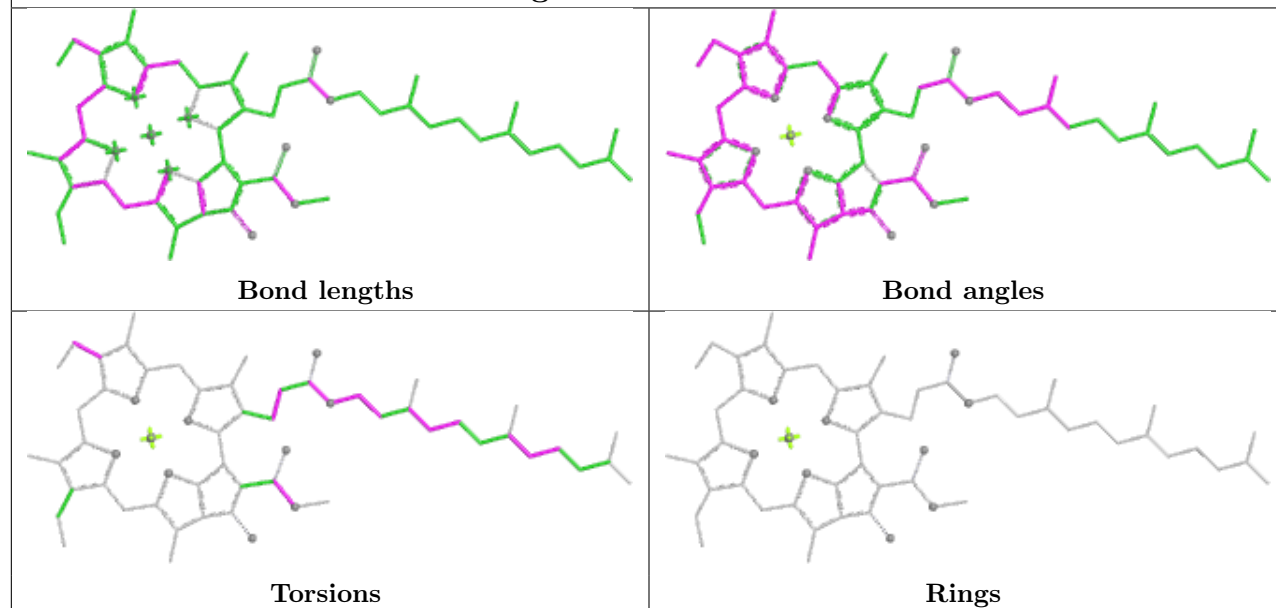
Ligand CLA B 832



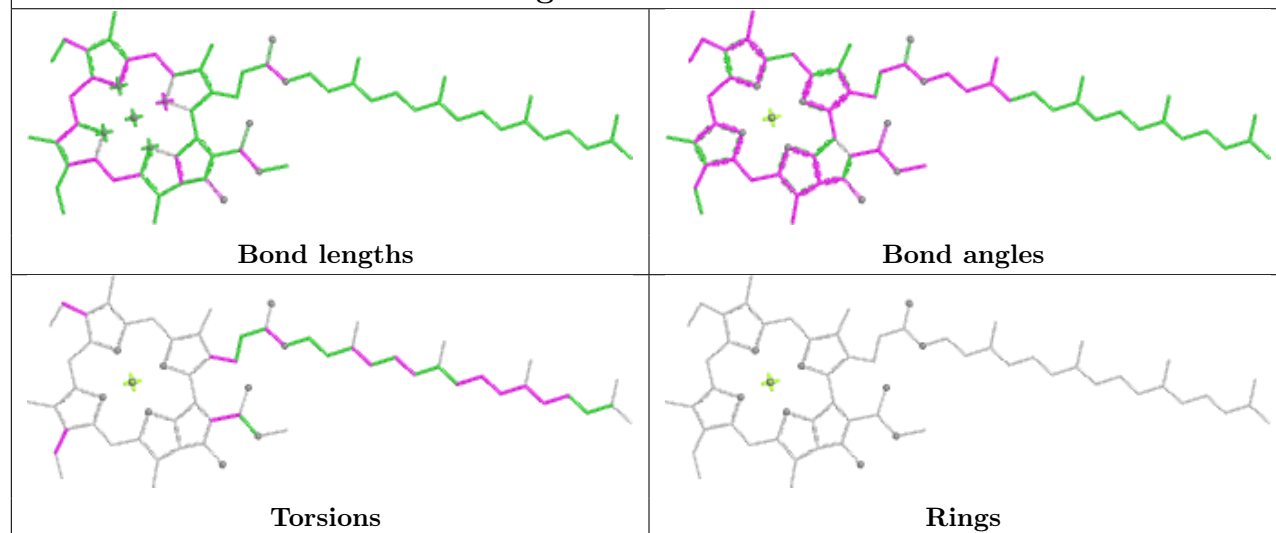
Ligand LMU B 801



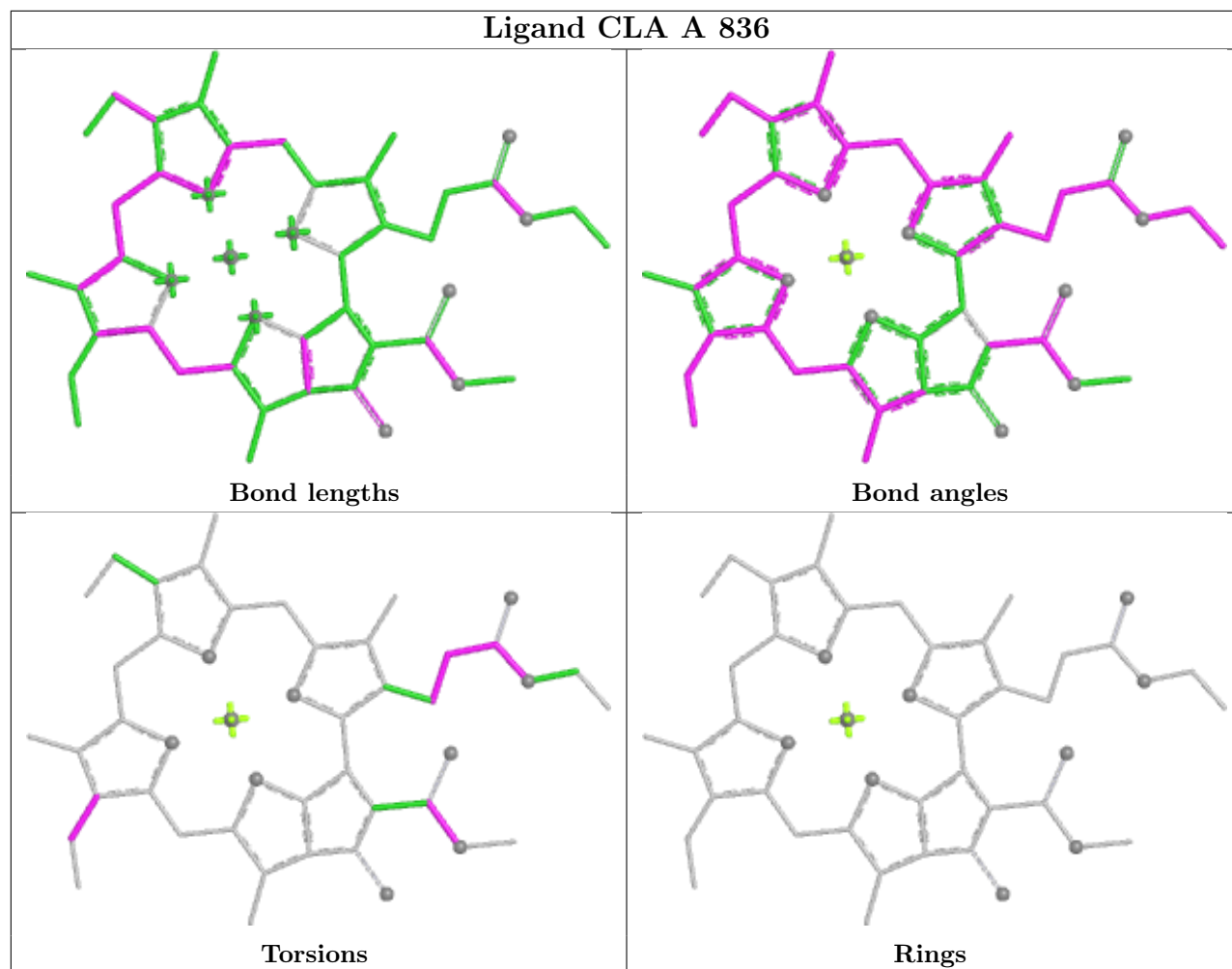
Ligand CLA H 109



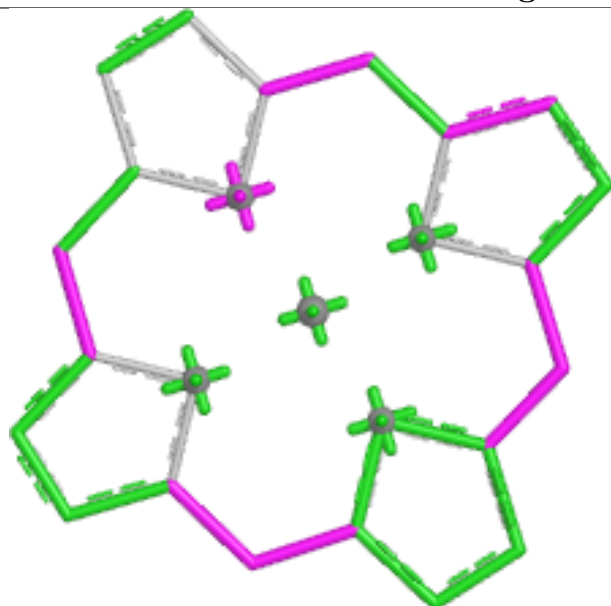
Ligand CLA 2 303



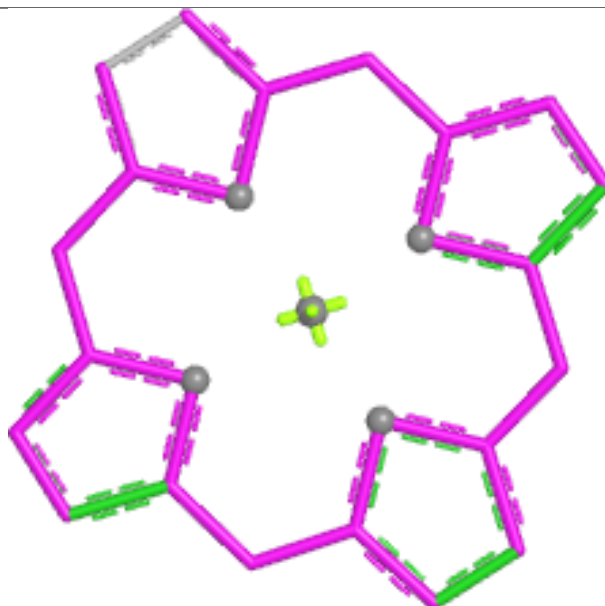
Ligand CLA A 836



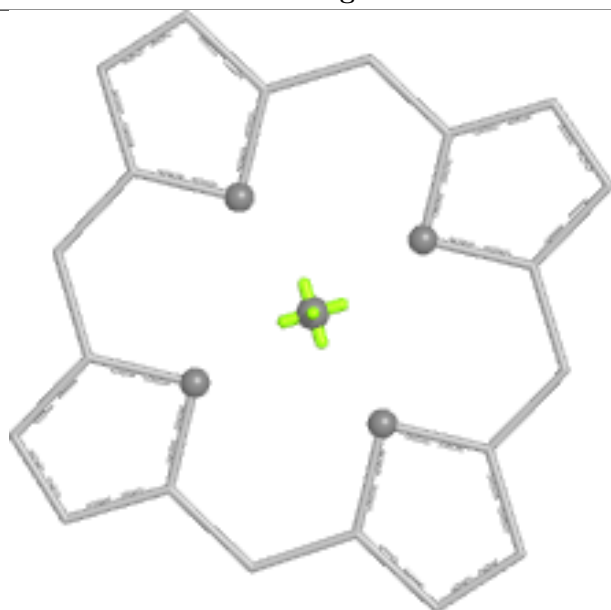
Ligand CLA 2 309



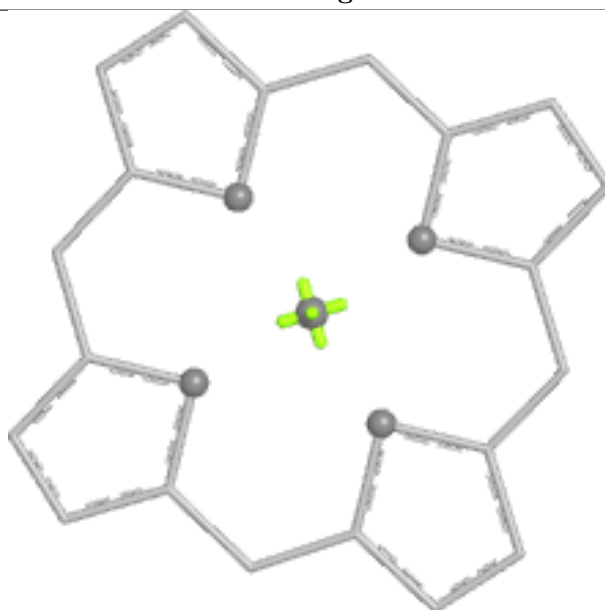
Bond lengths



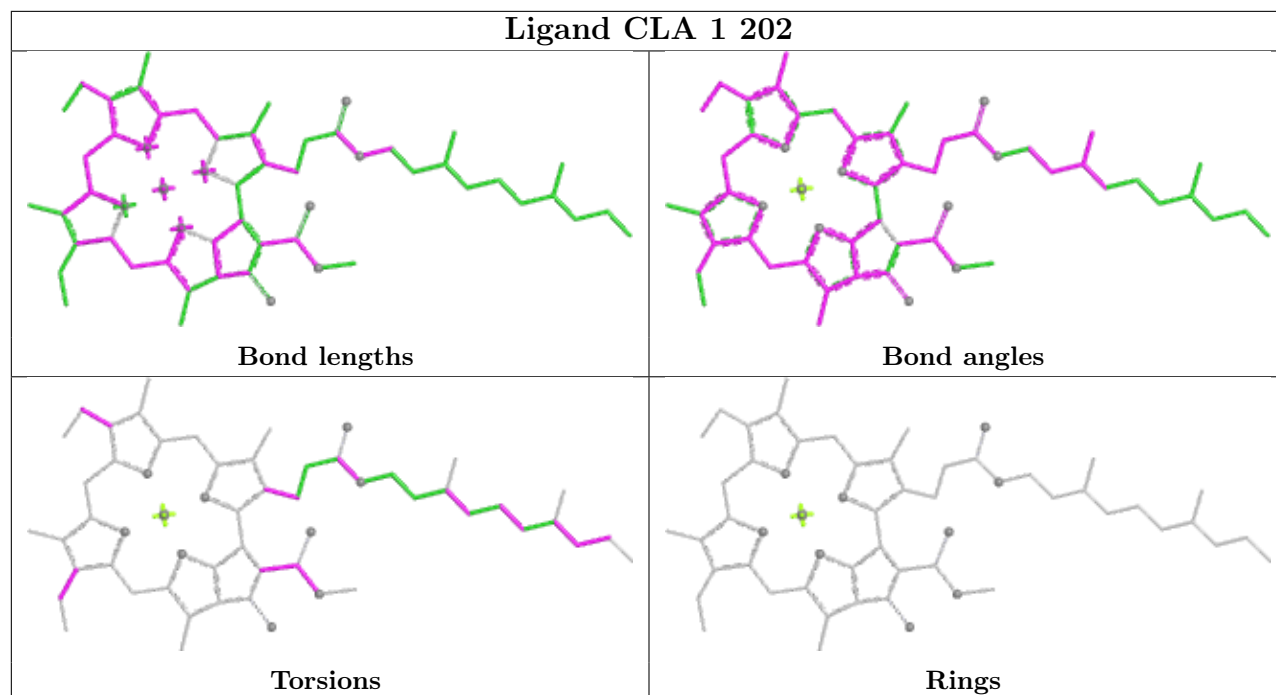
Bond angles



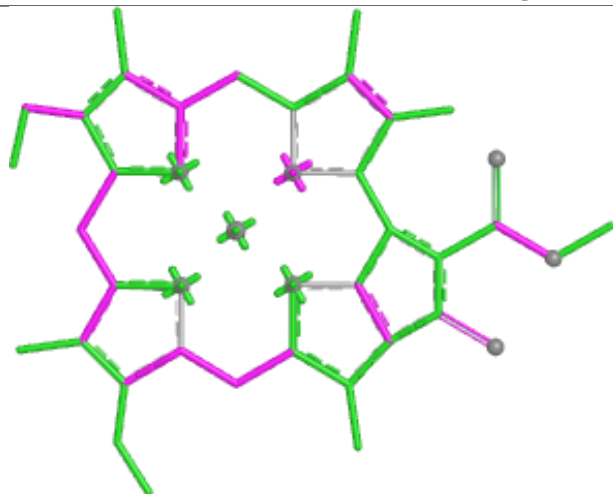
Torsions



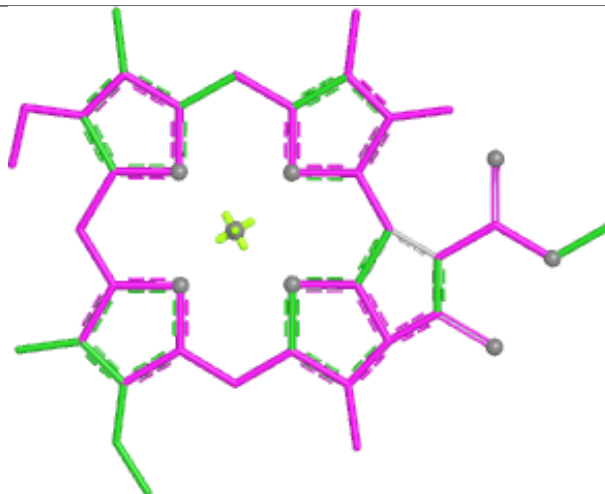
Rings



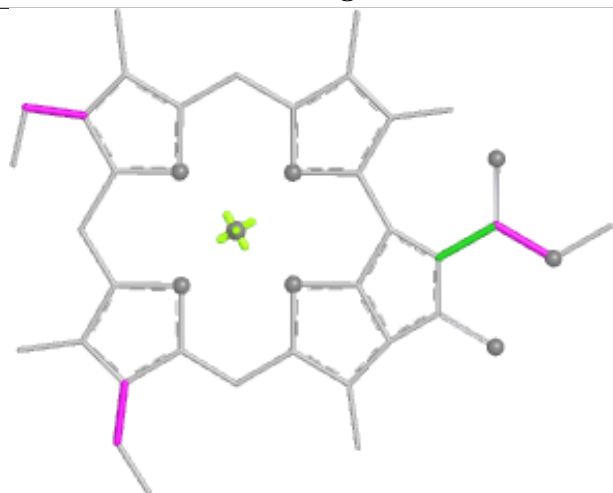
Ligand CLA F 205



Bond lengths



Bond angles

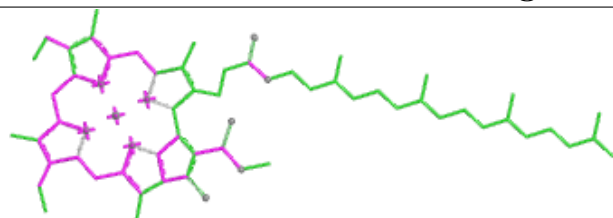


Torsions

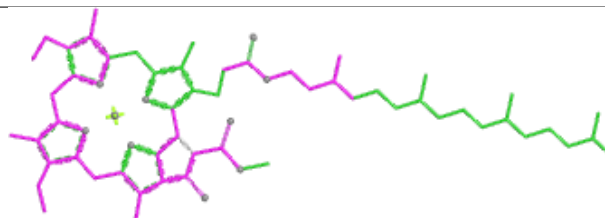


Rings

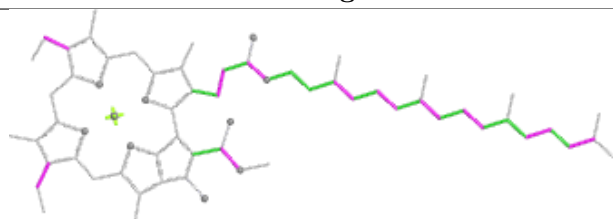
Ligand CLA 3 313



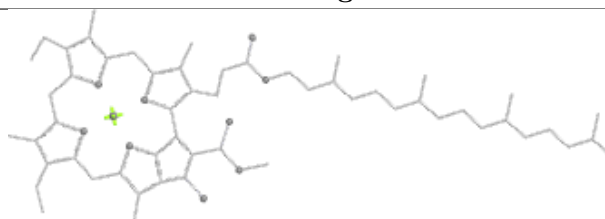
Bond lengths



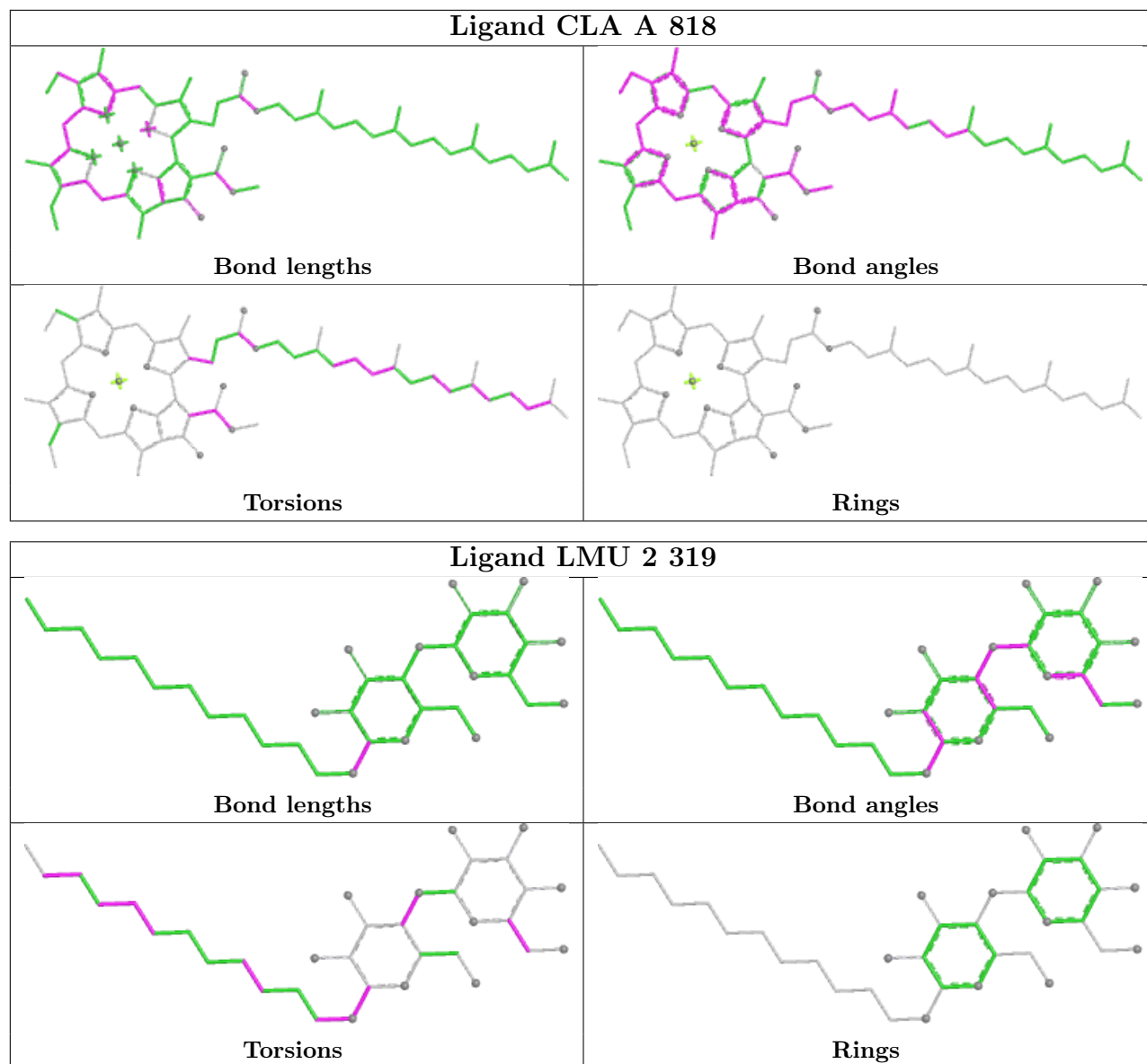
Bond angles



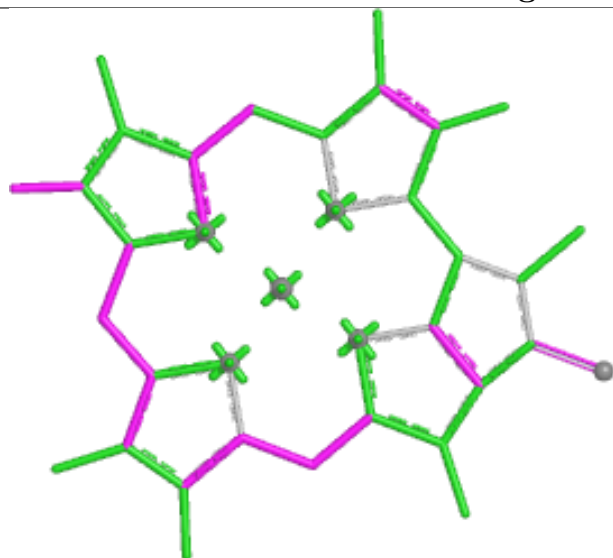
Torsions



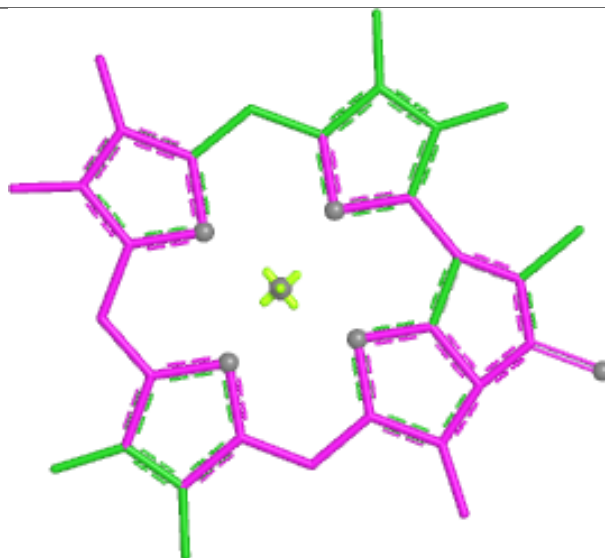
Rings



Ligand CLA 1 209



Bond lengths



Bond angles

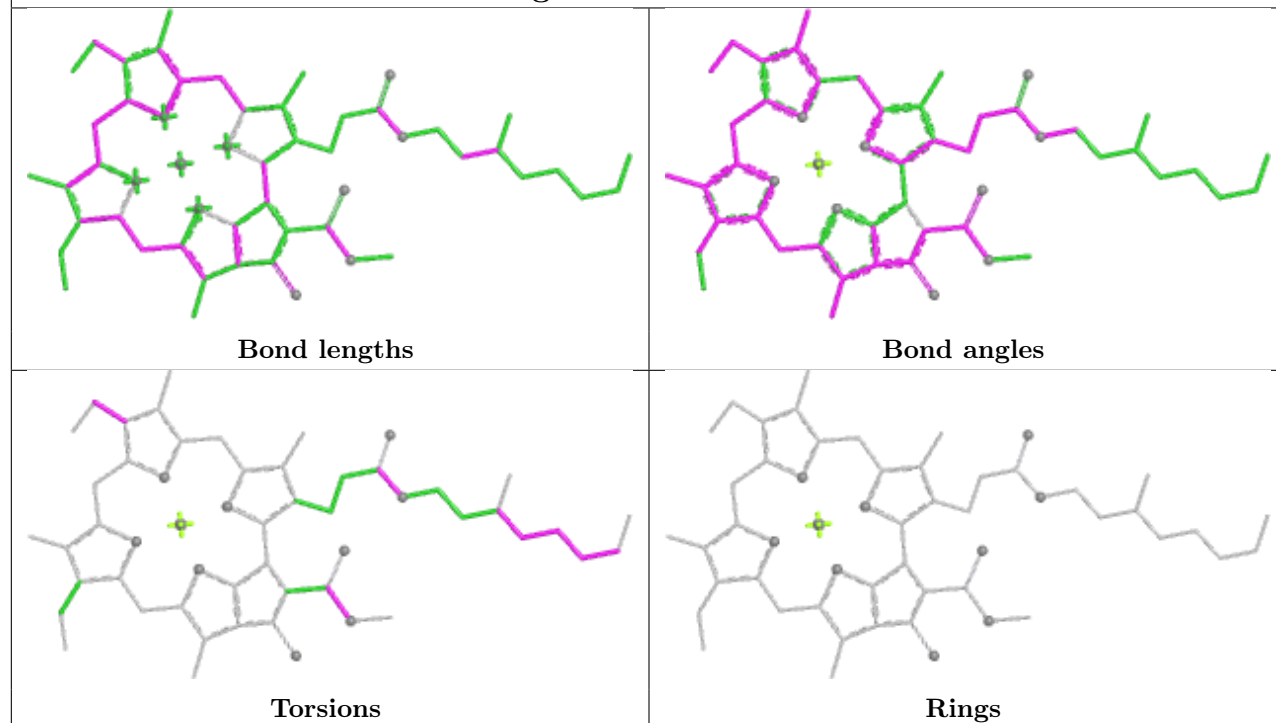


Torsions

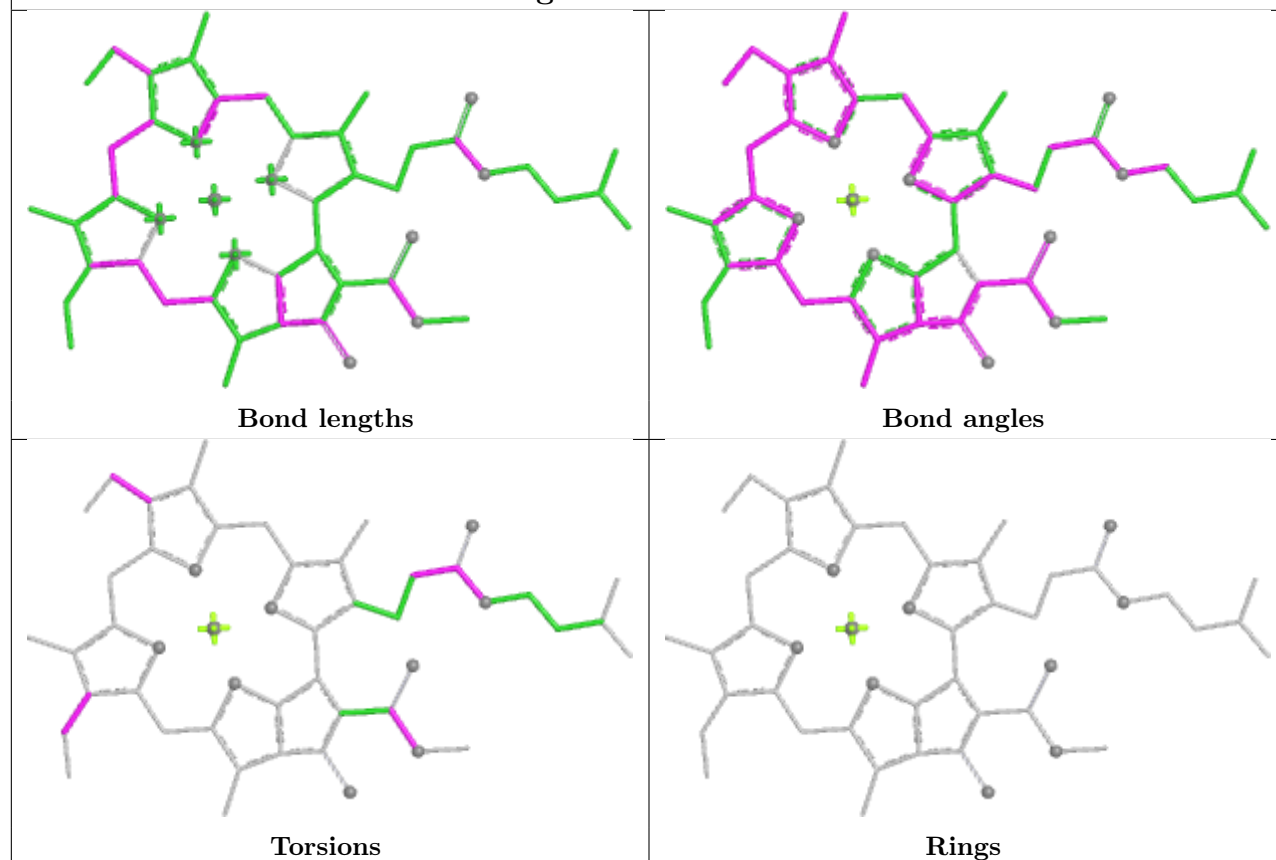


Rings

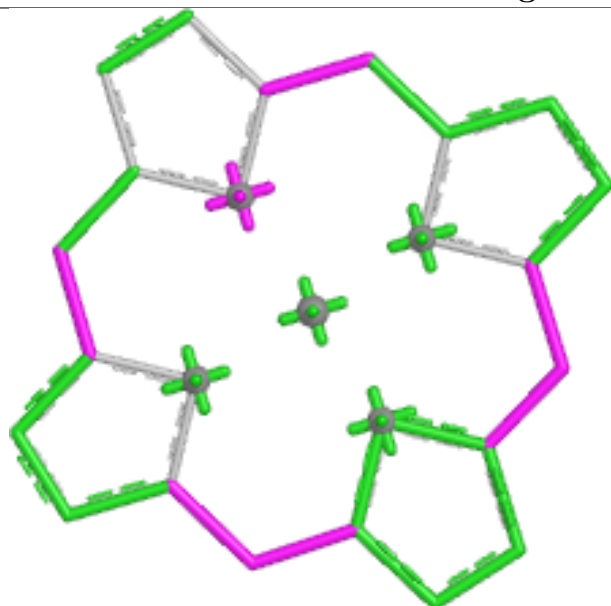
Ligand CLA B 822



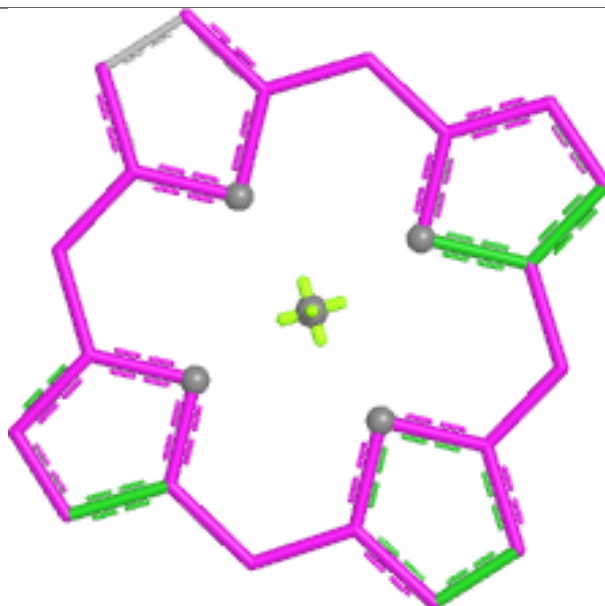
Ligand CLA 2 312



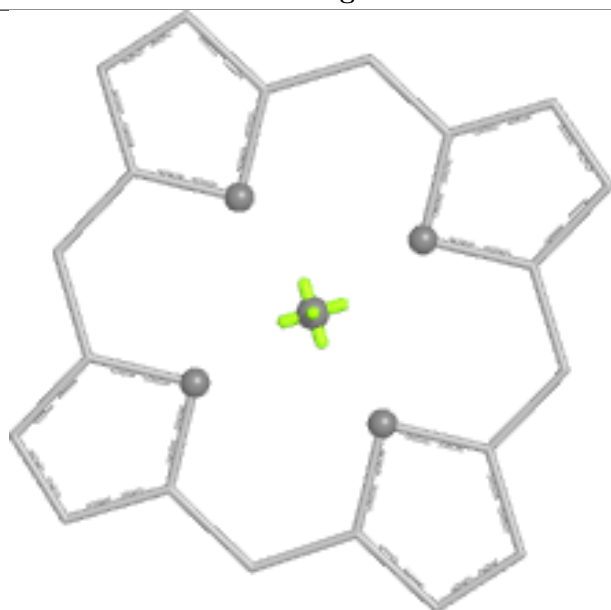
Ligand CLA 1 211



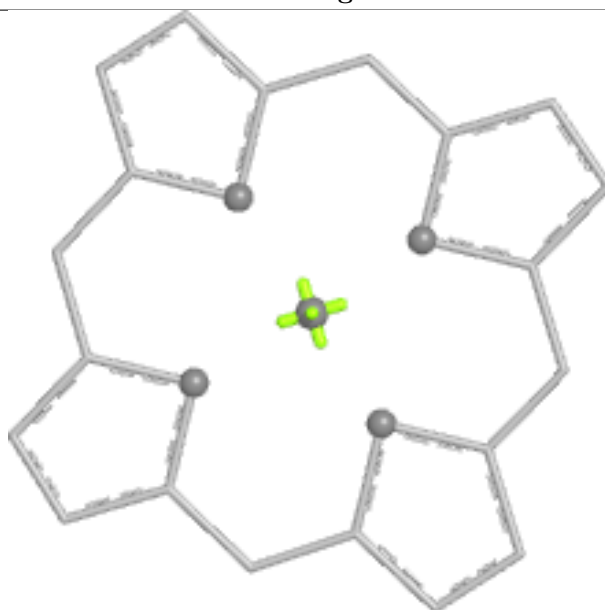
Bond lengths



Bond angles

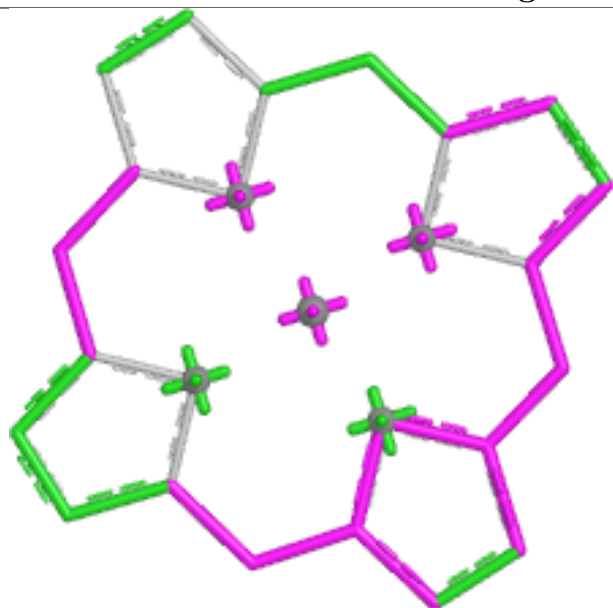


Torsions

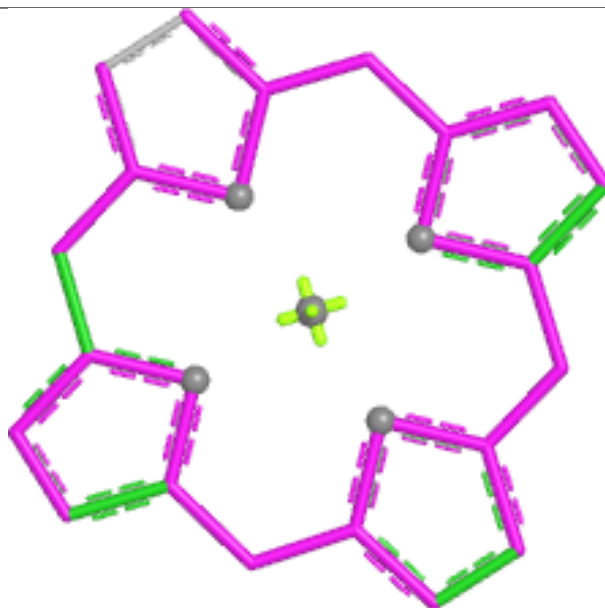


Rings

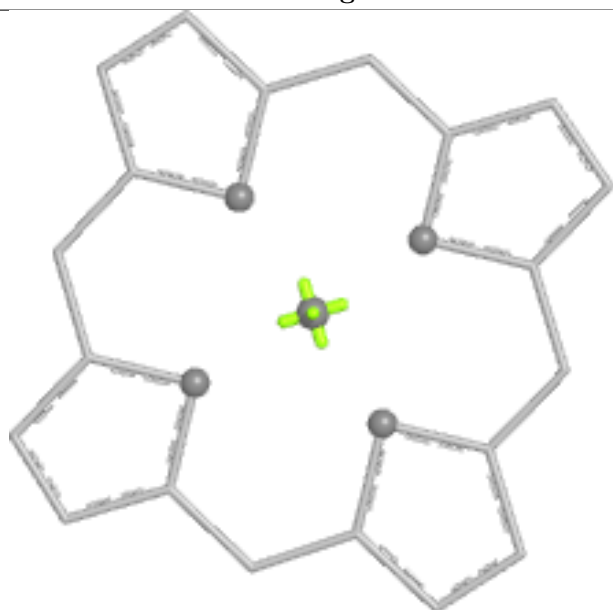
Ligand CLA 1 216



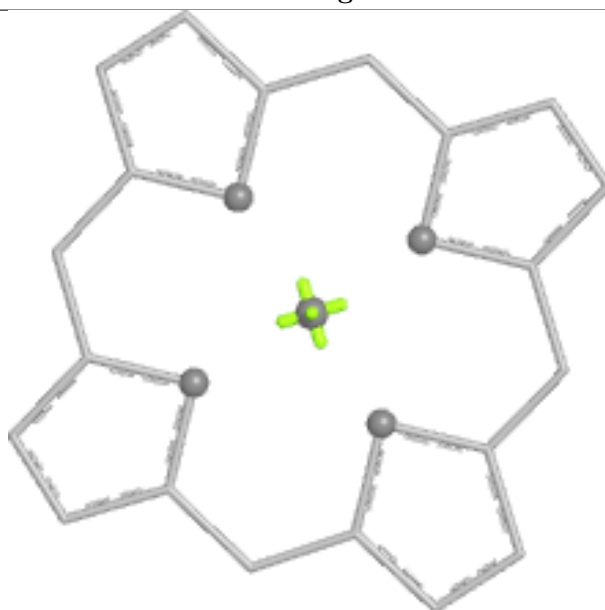
Bond lengths



Bond angles

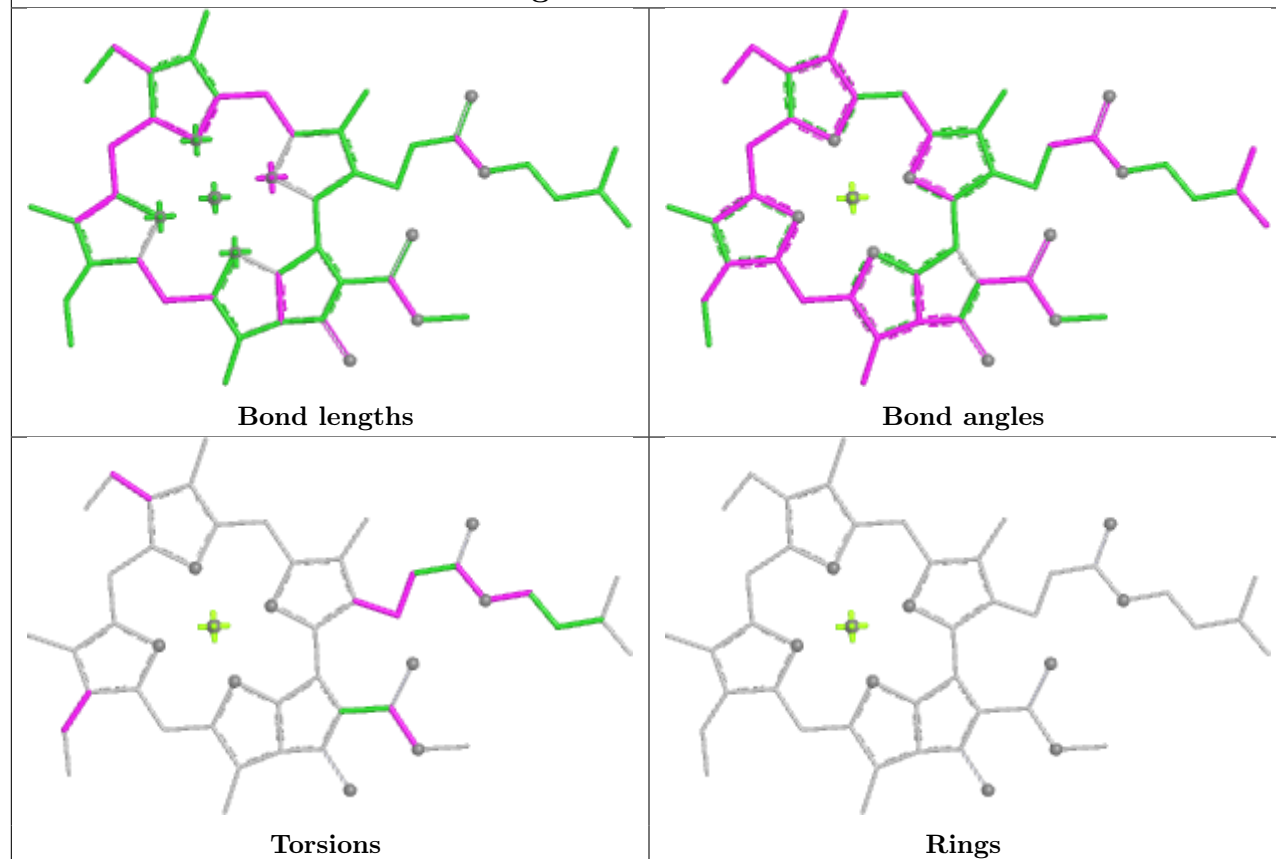


Torsions

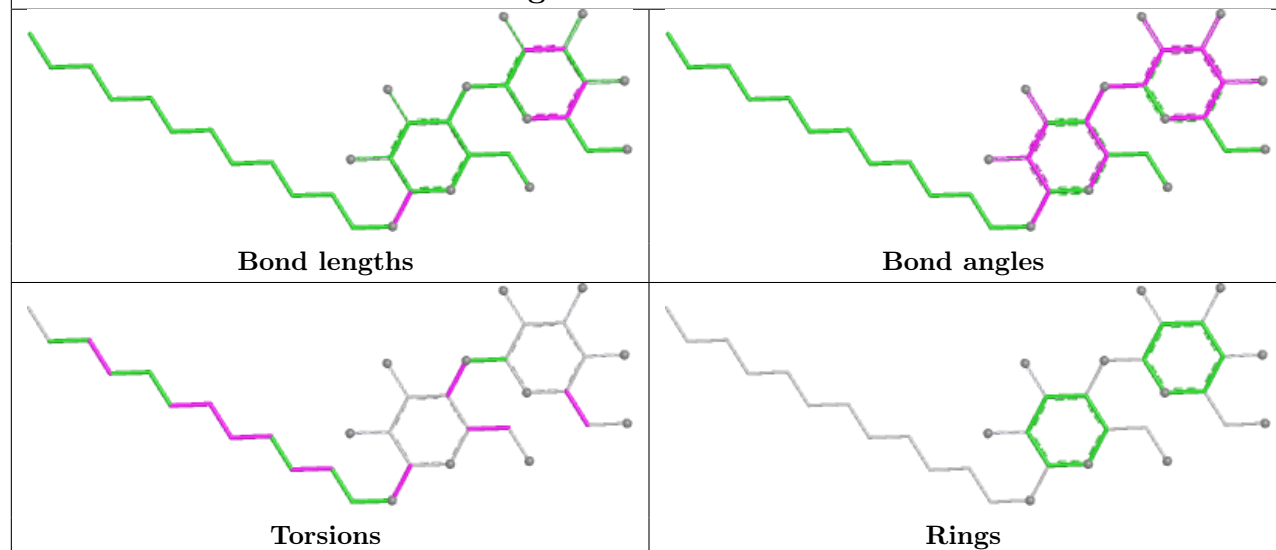


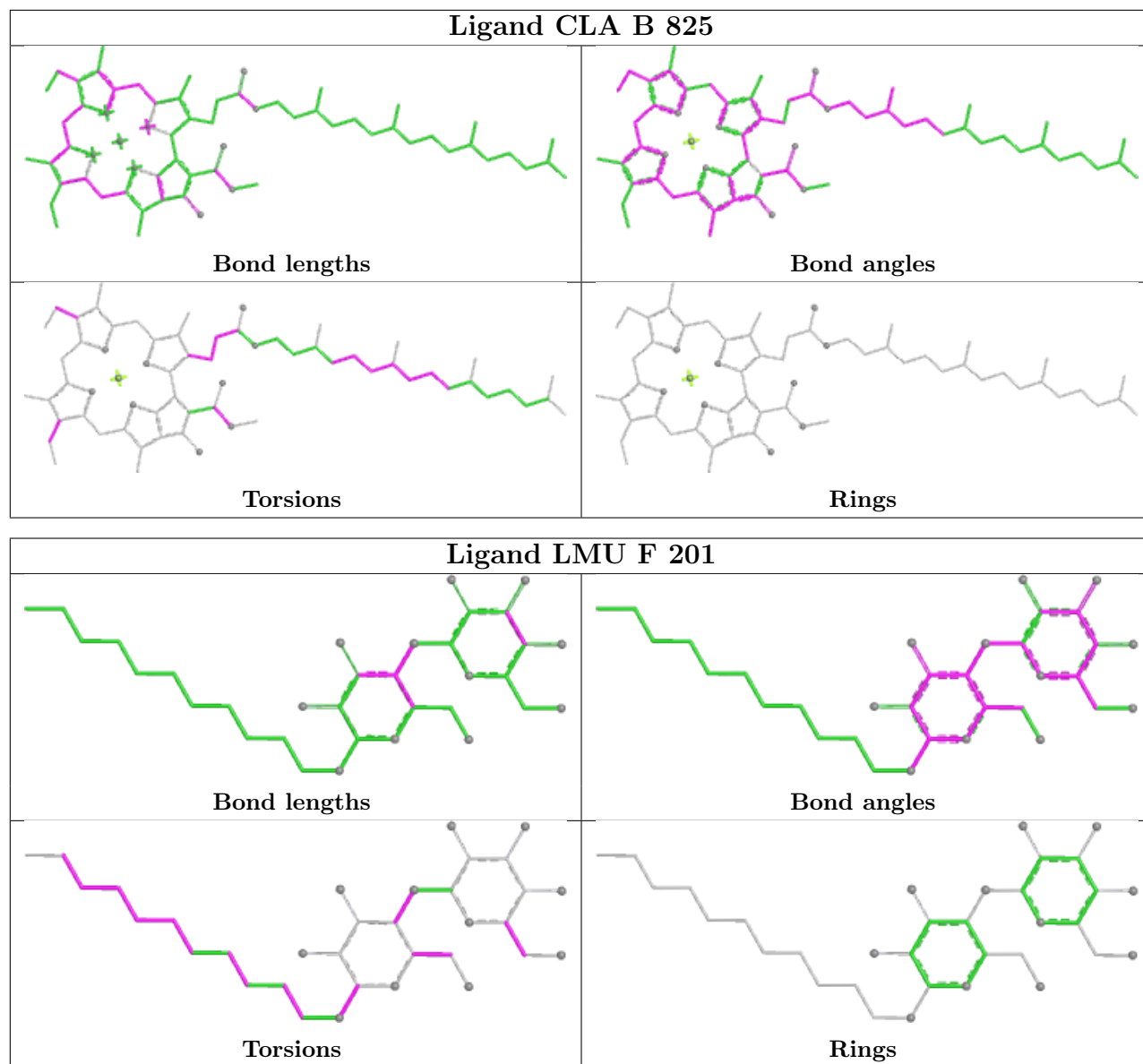
Rings

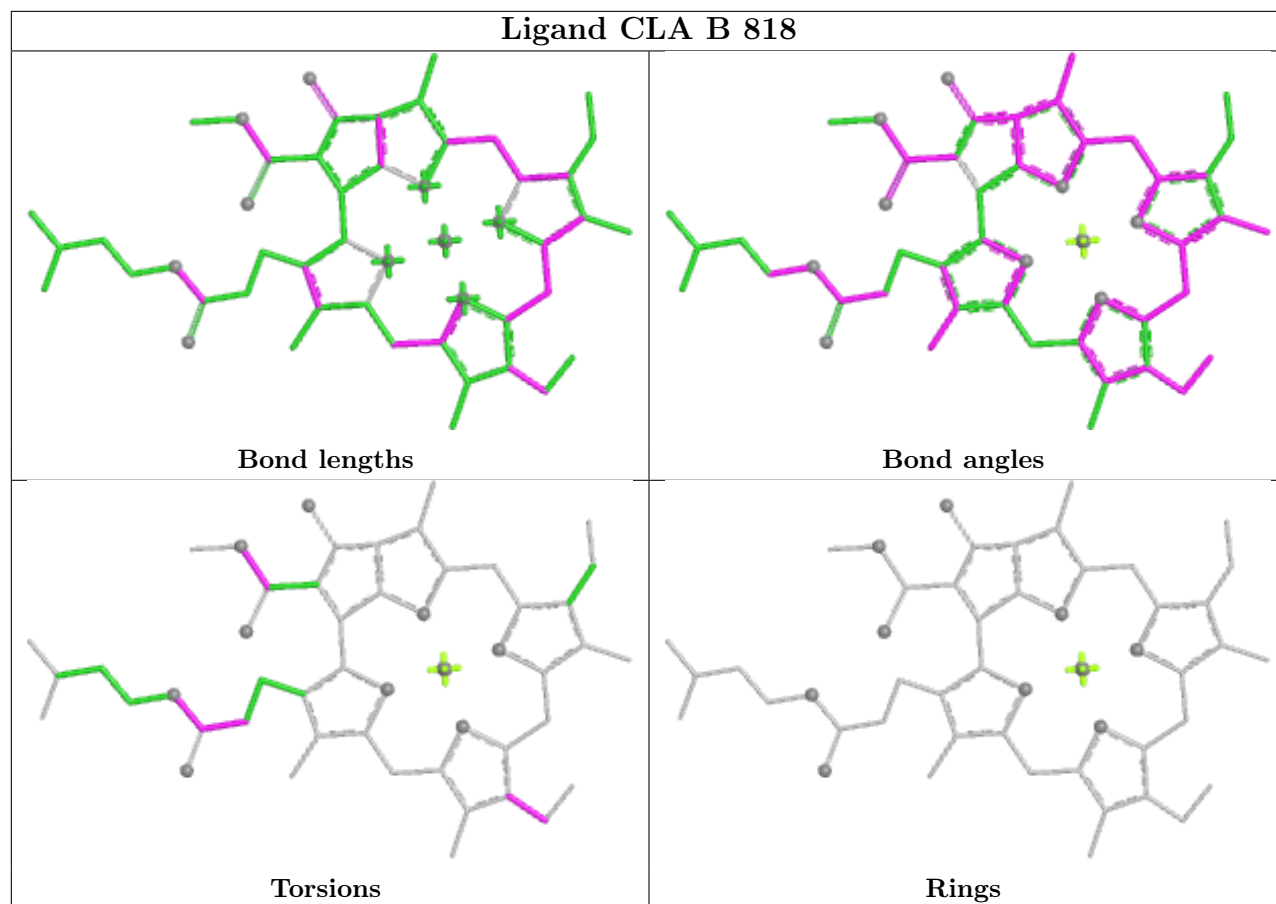
Ligand CLA A 840



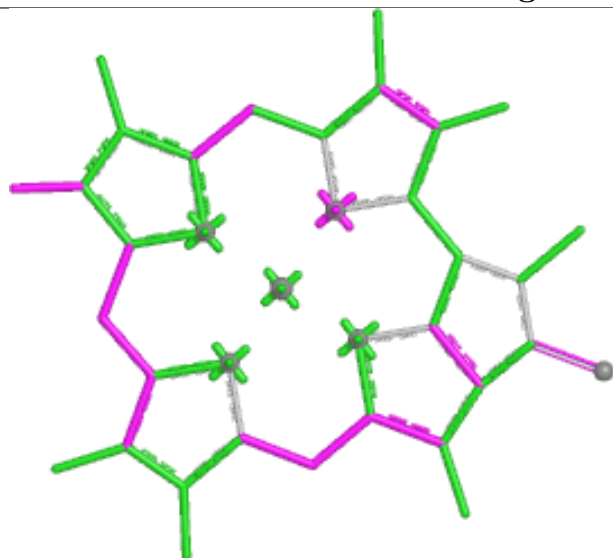
Ligand LMU B 802



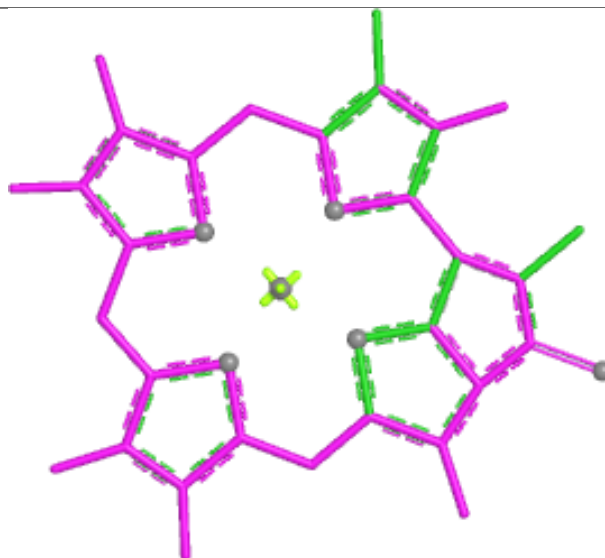




Ligand CLA 4 314



Bond lengths



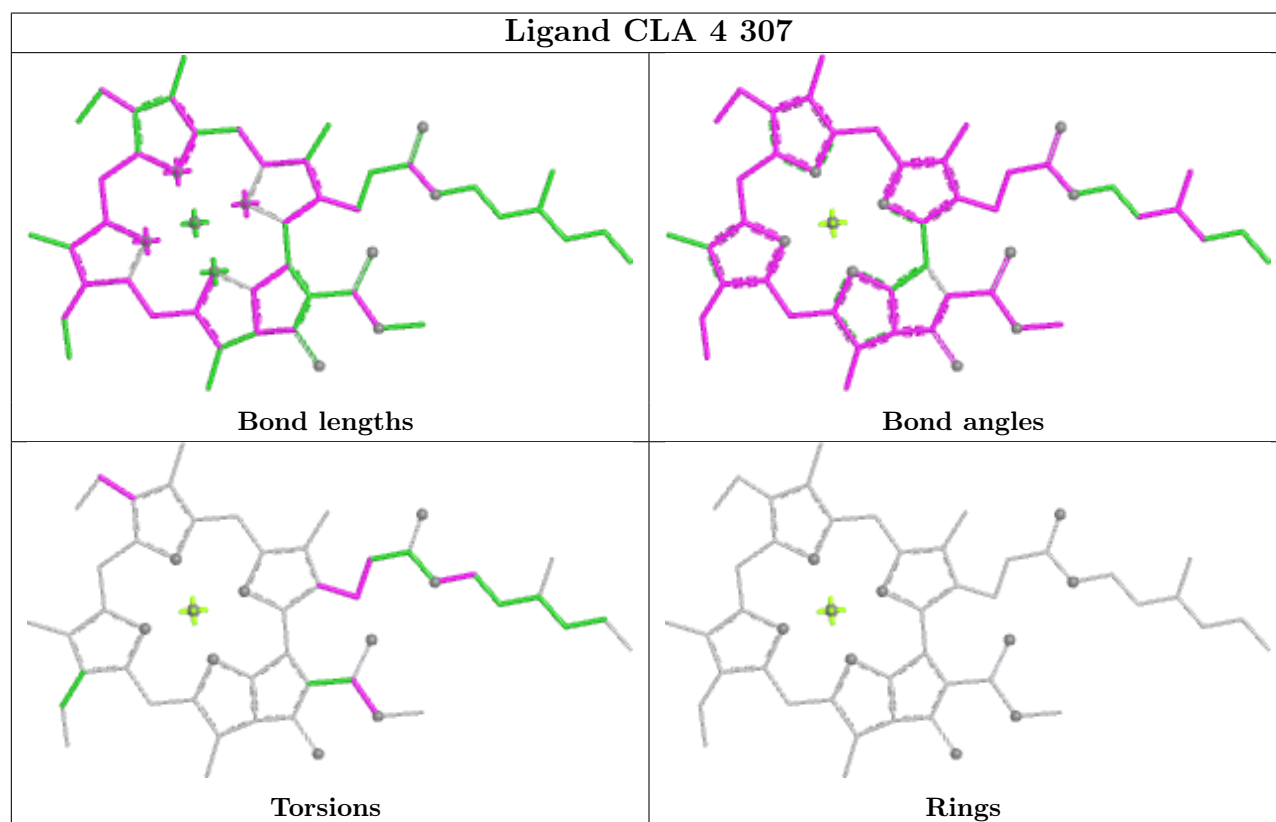
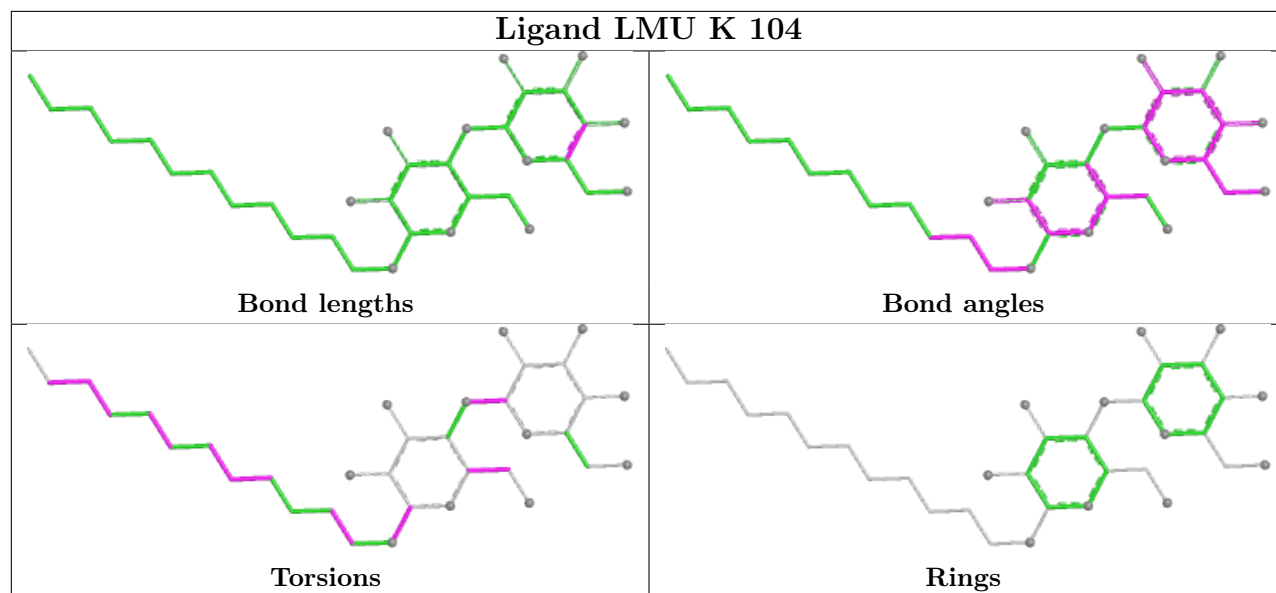
Bond angles



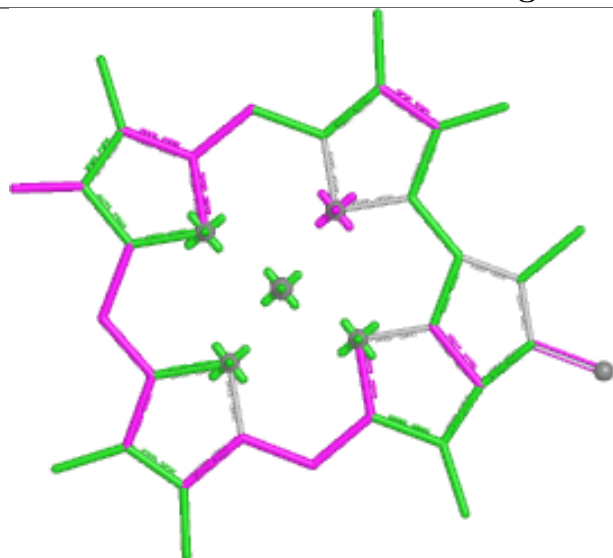
Torsions



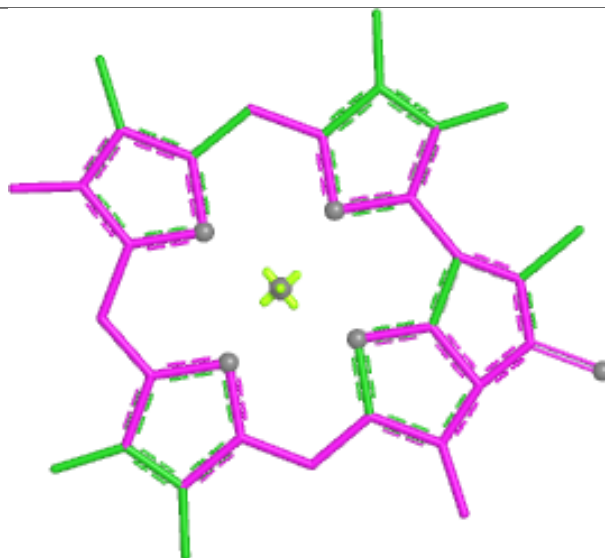
Rings



Ligand CLA 4 308



Bond lengths



Bond angles

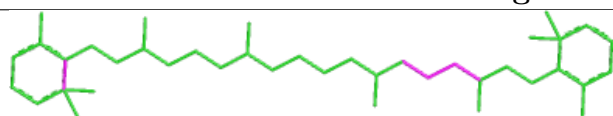


Torsions

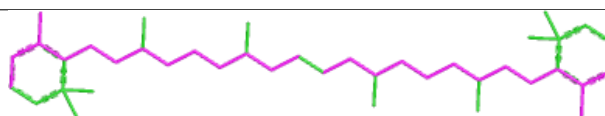


Rings

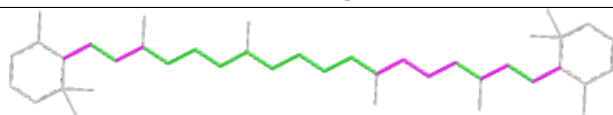
Ligand BCR B 846



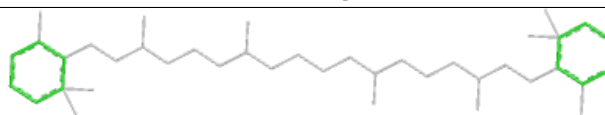
Bond lengths



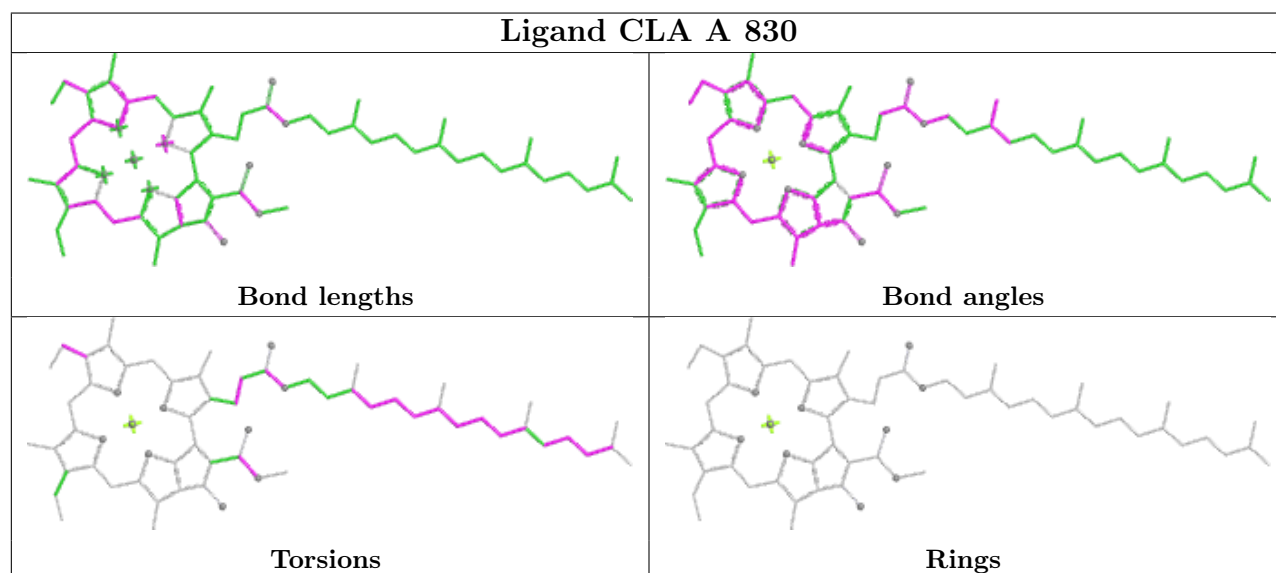
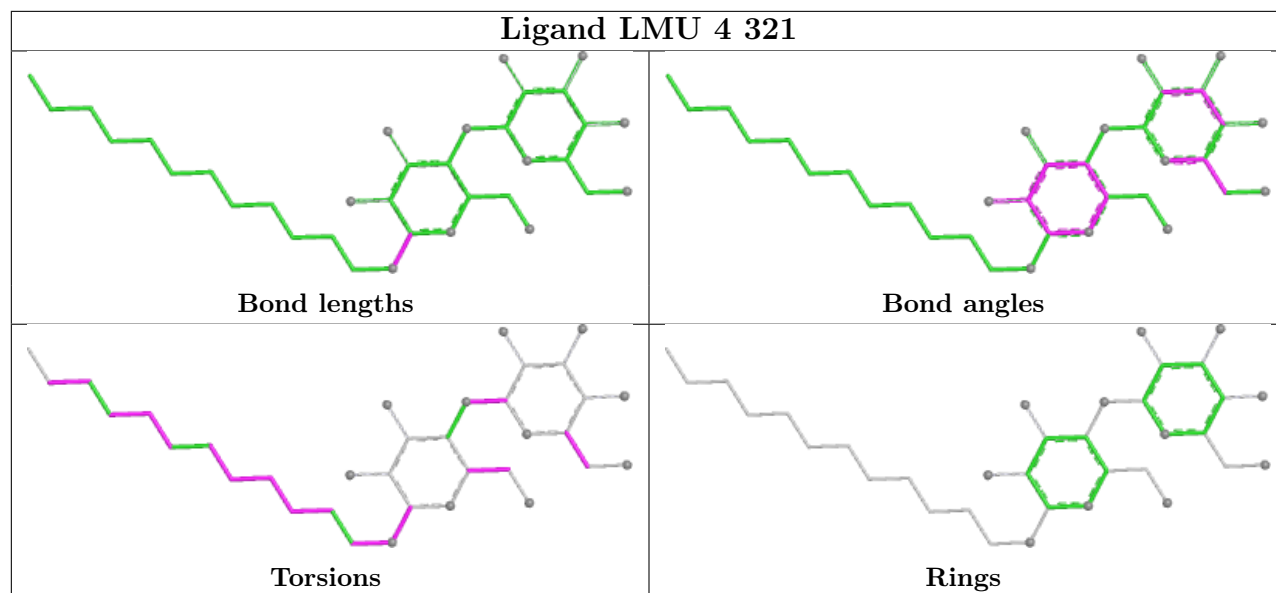
Bond angles



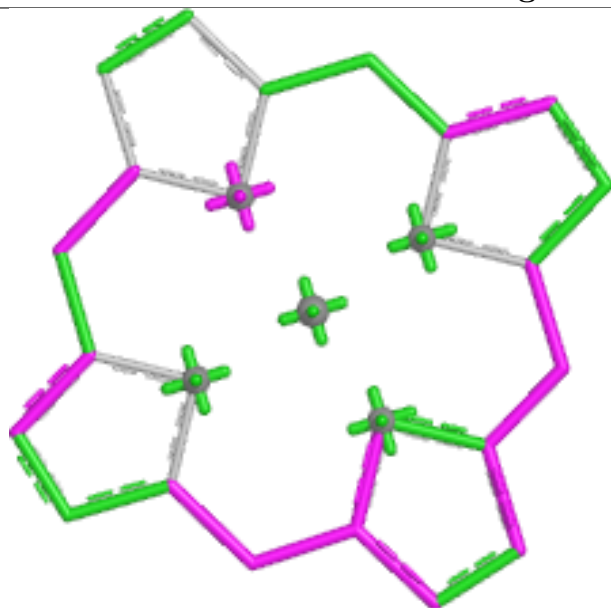
Torsions



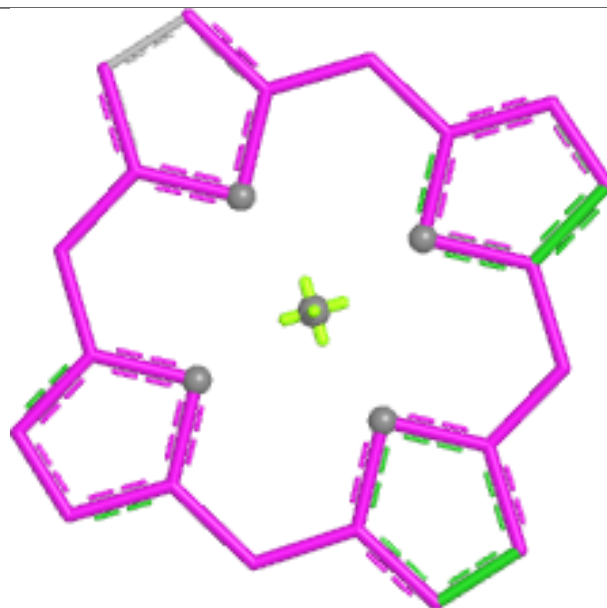
Rings



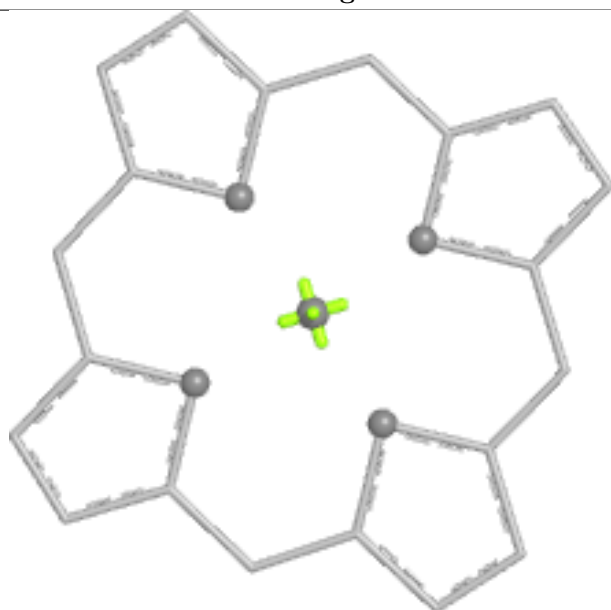
Ligand CLA 1 208



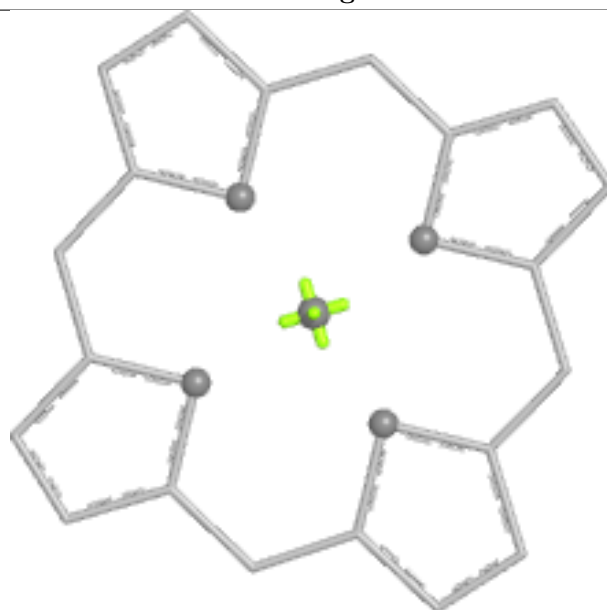
Bond lengths



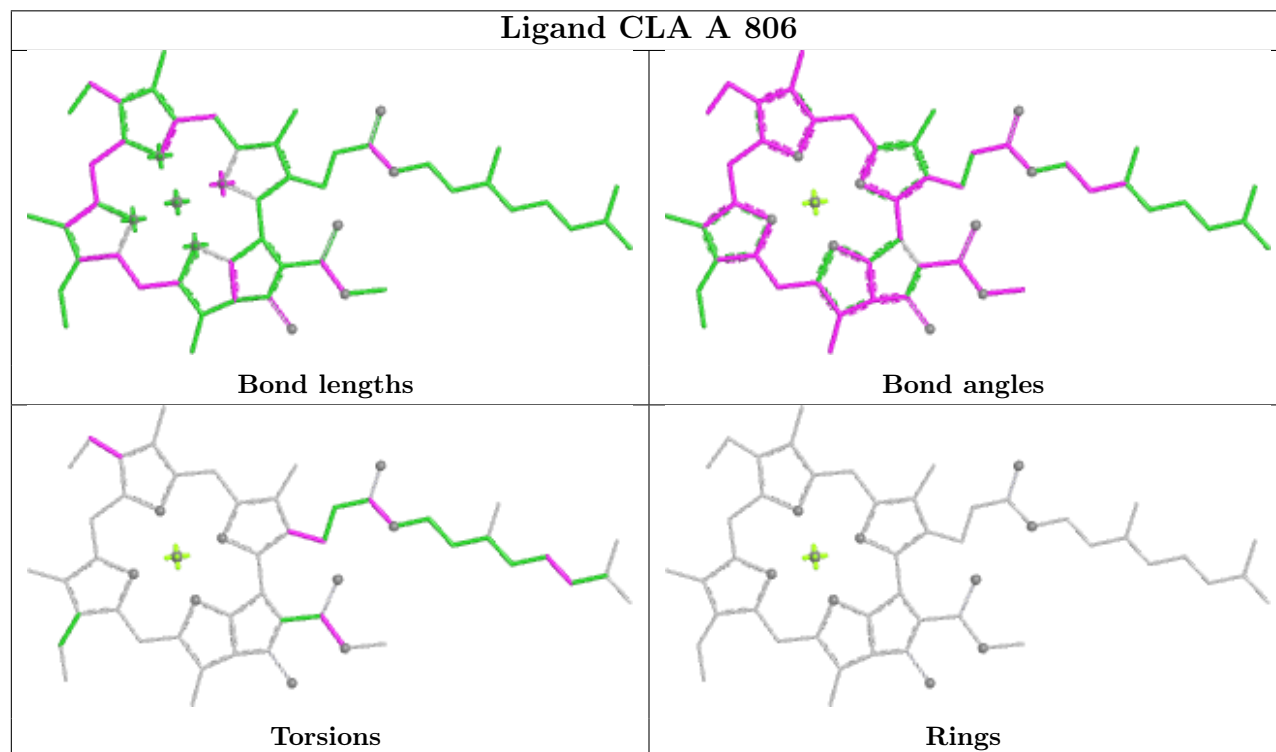
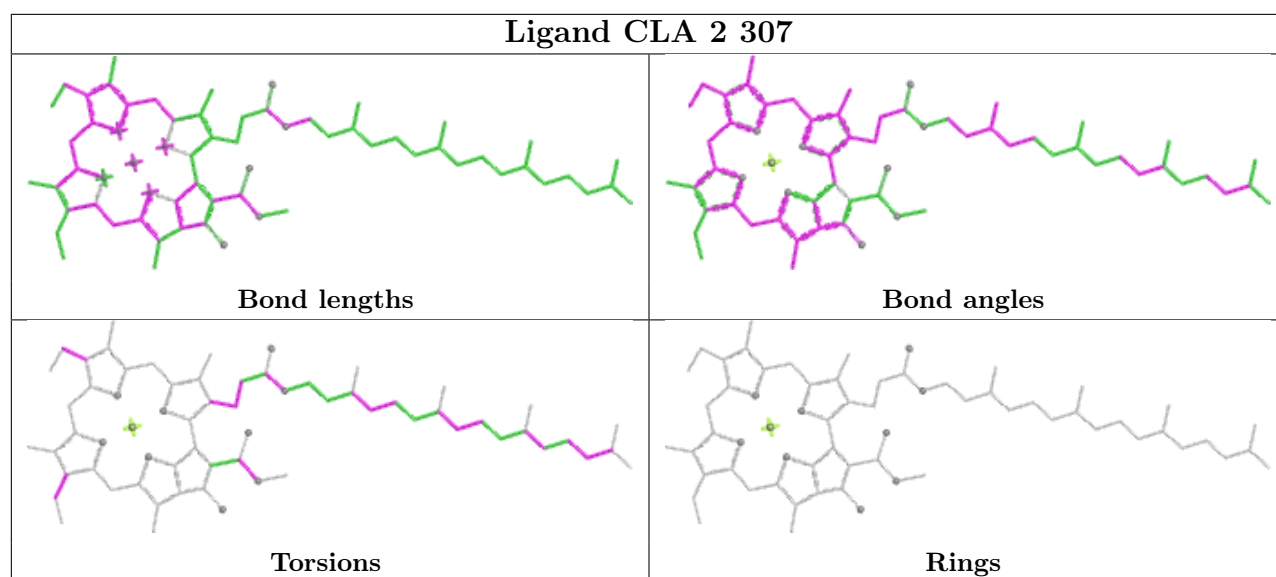
Bond angles



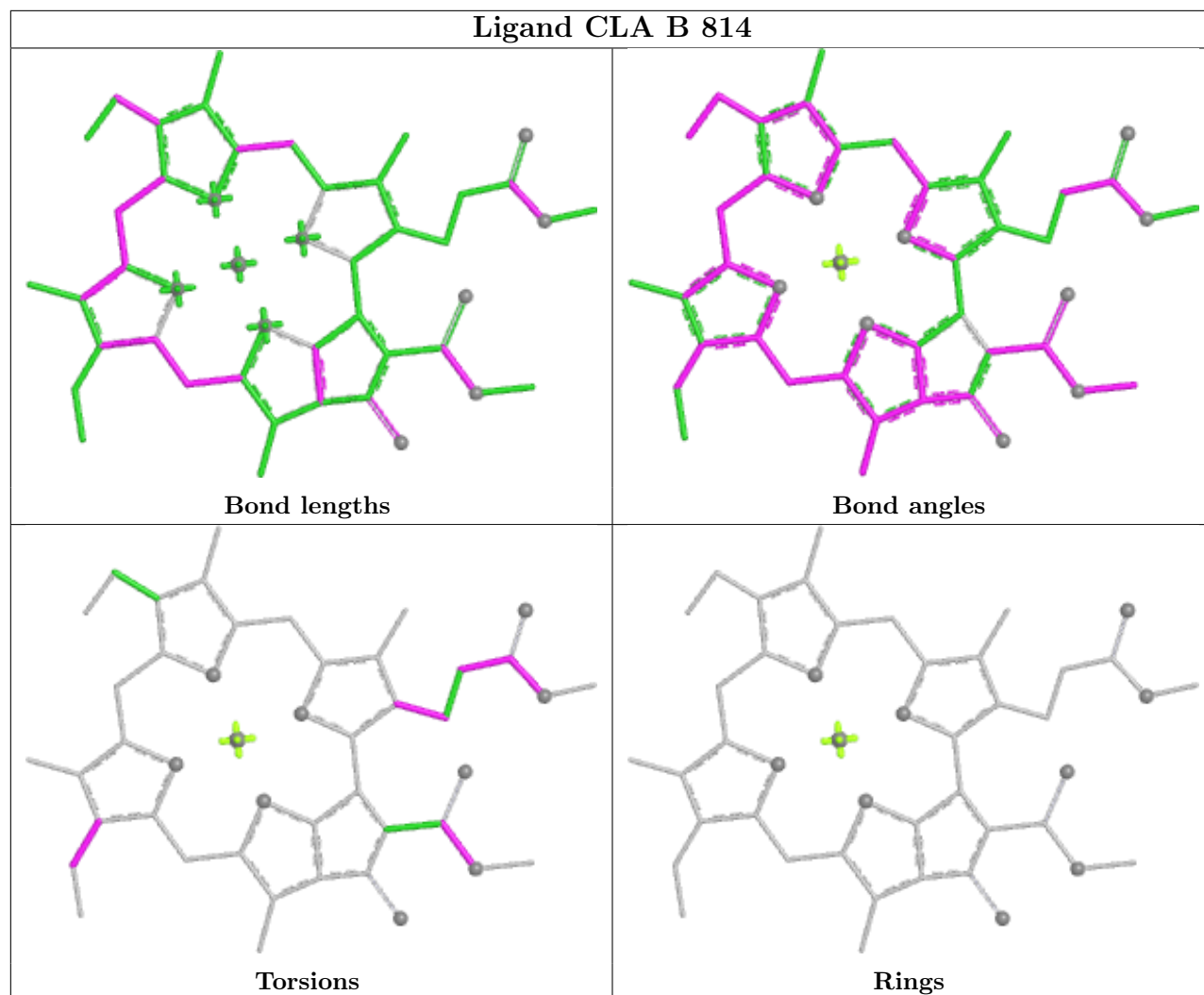
Torsions



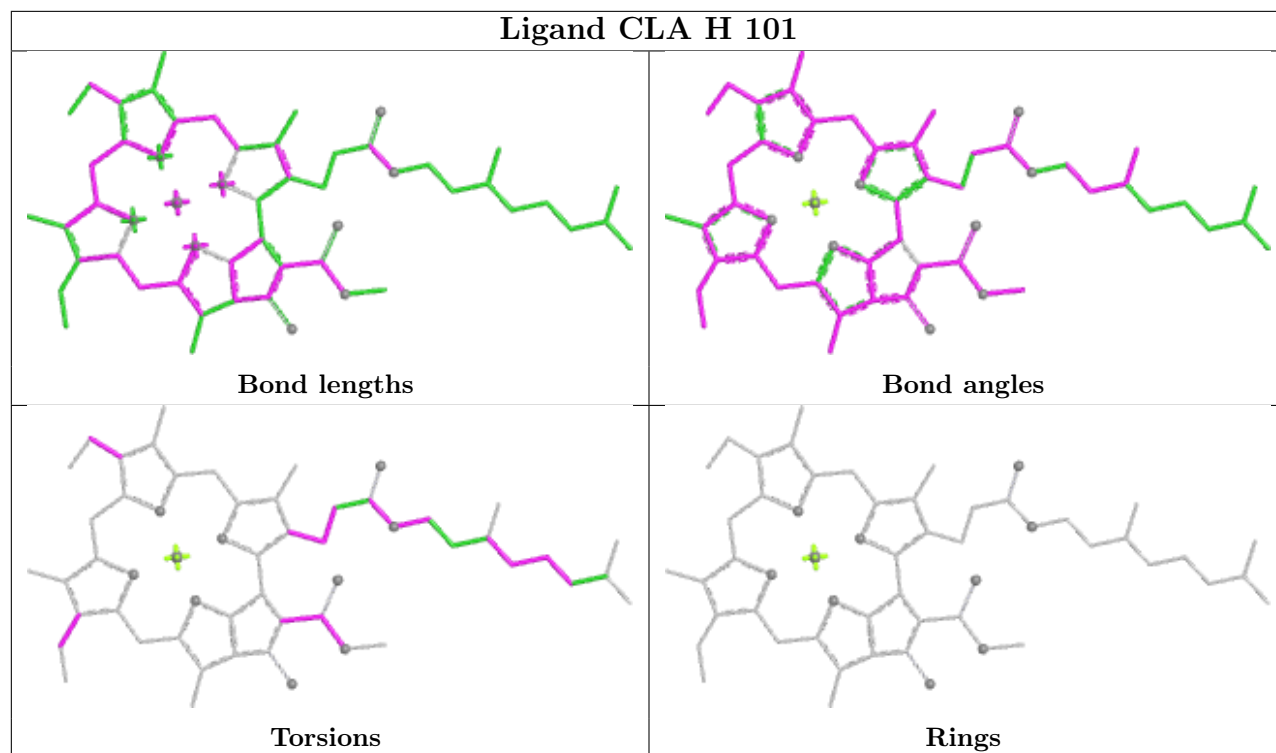
Rings



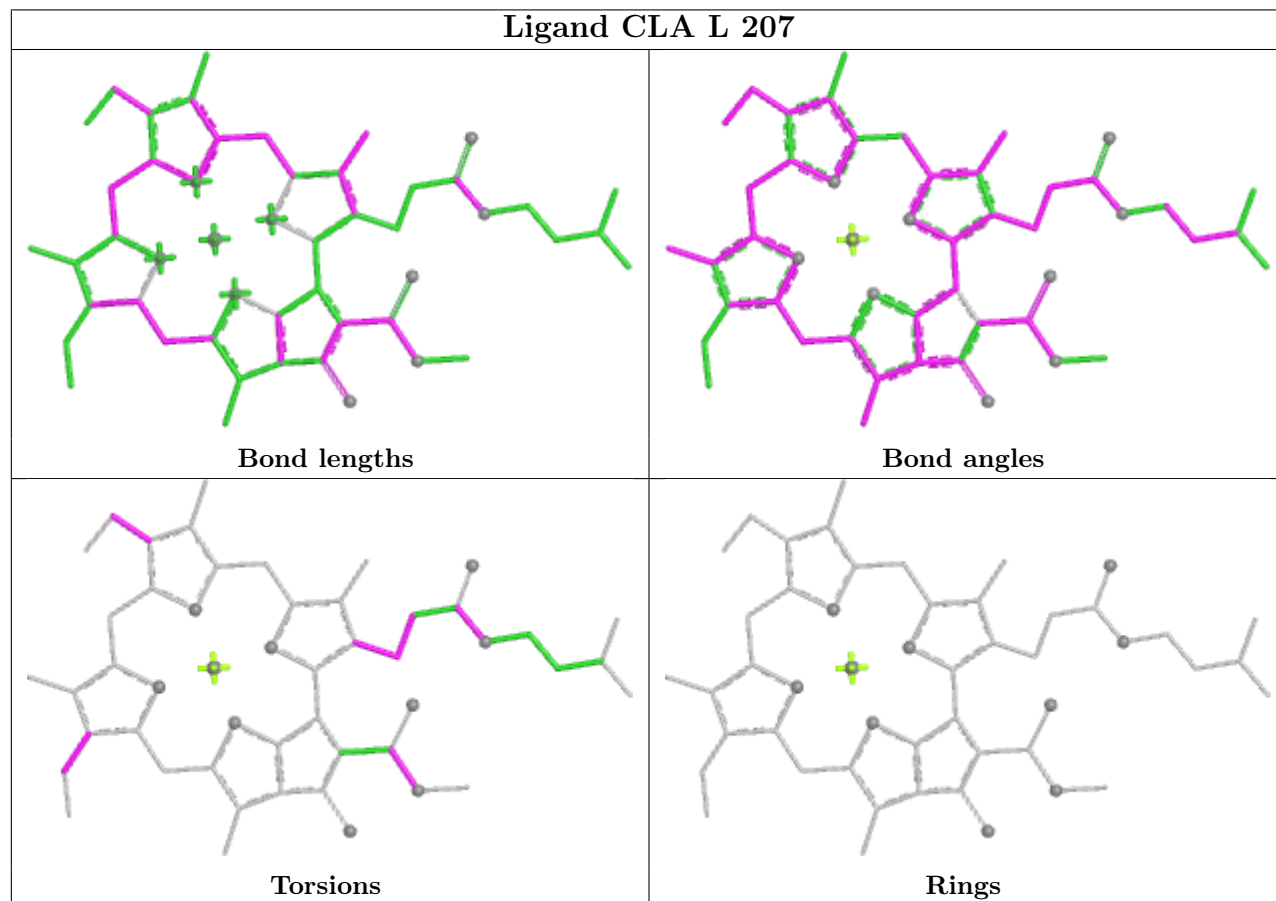
Ligand CLA B 814



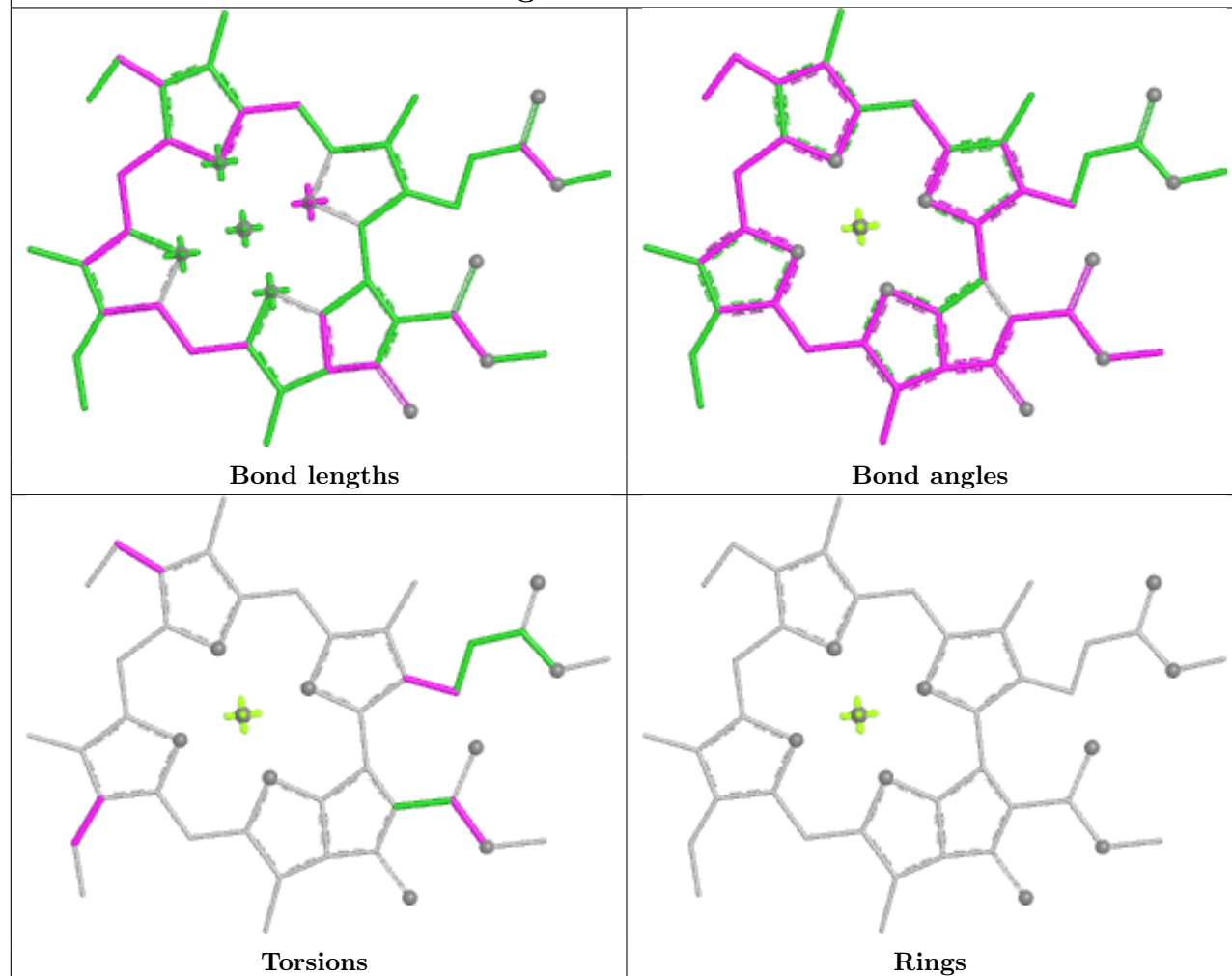
Ligand CLA H 101



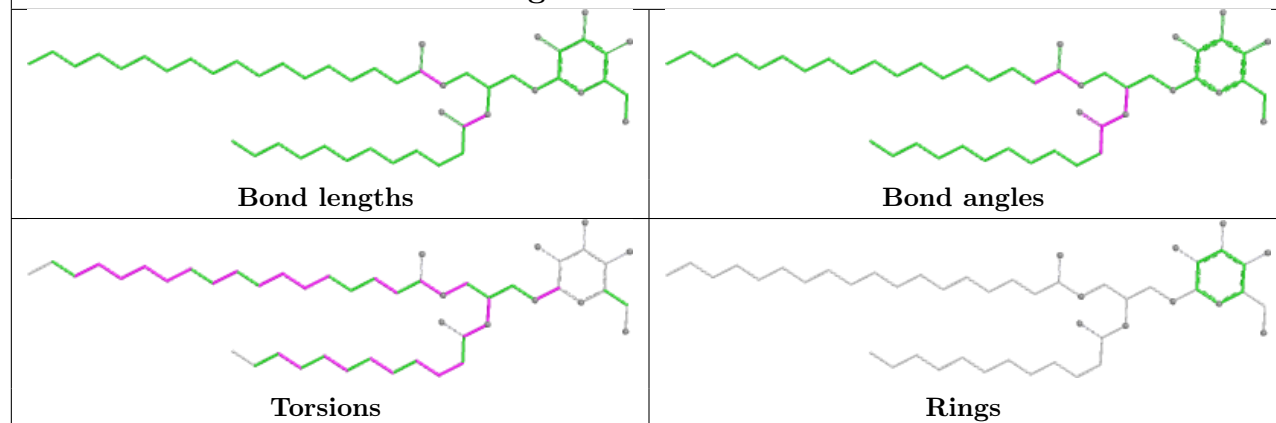
Ligand CLA L 207

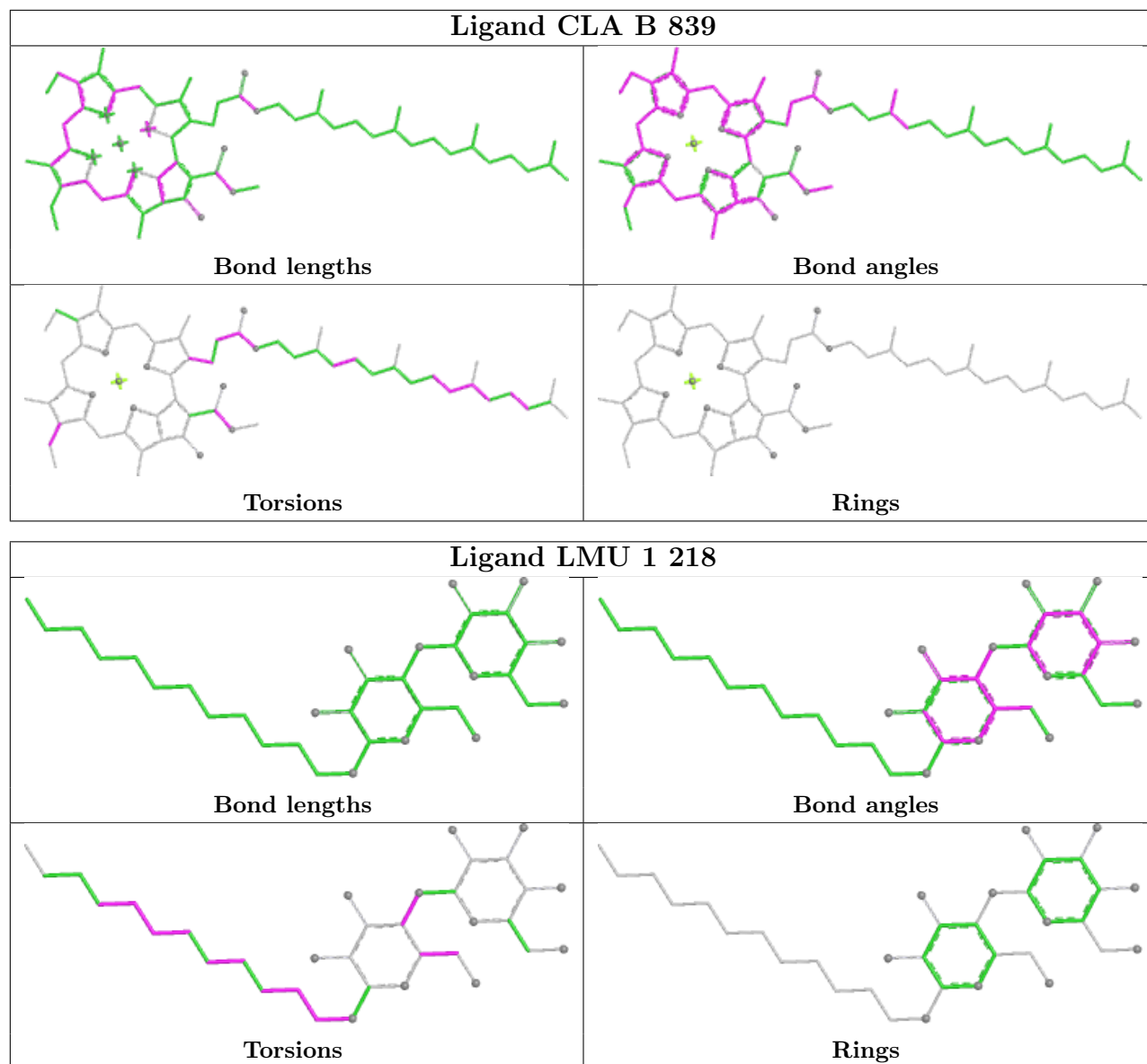


Ligand CLA 1 204

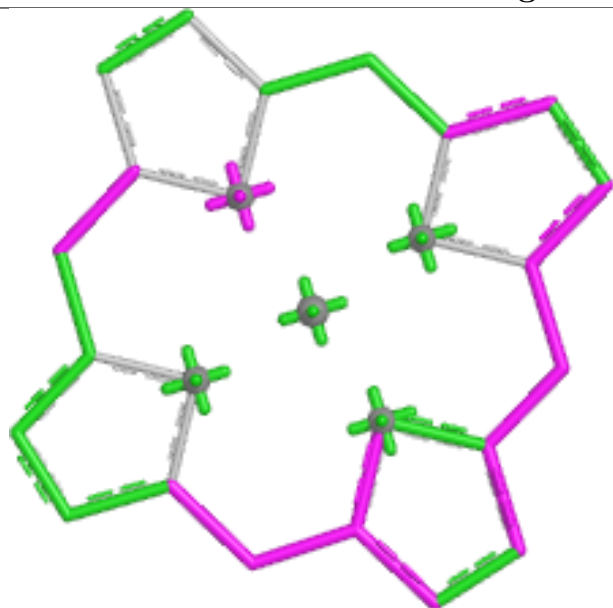


Ligand LMG B 848

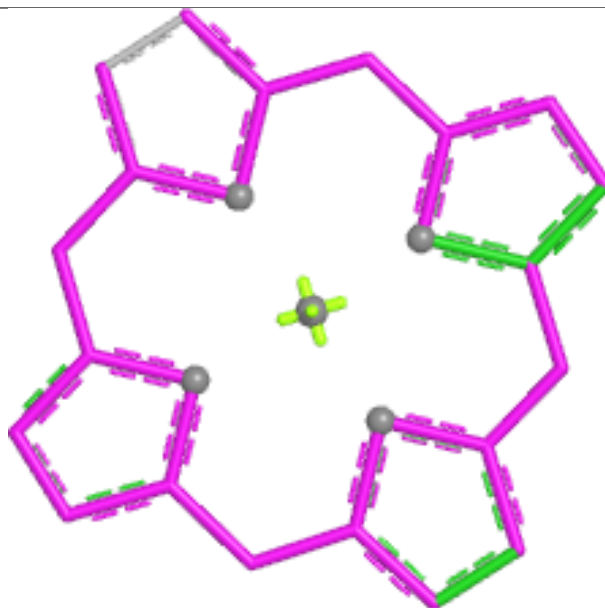




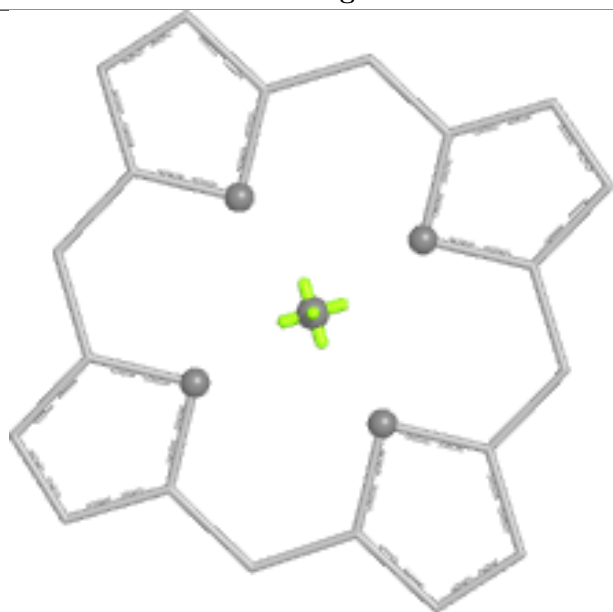
Ligand CLA 3 305



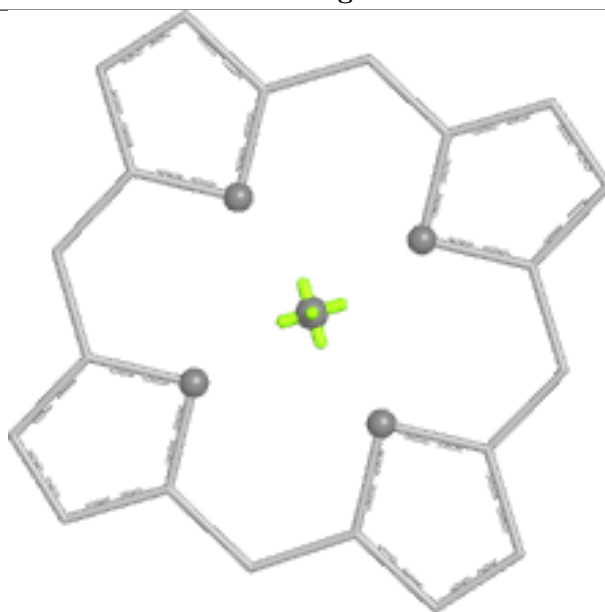
Bond lengths



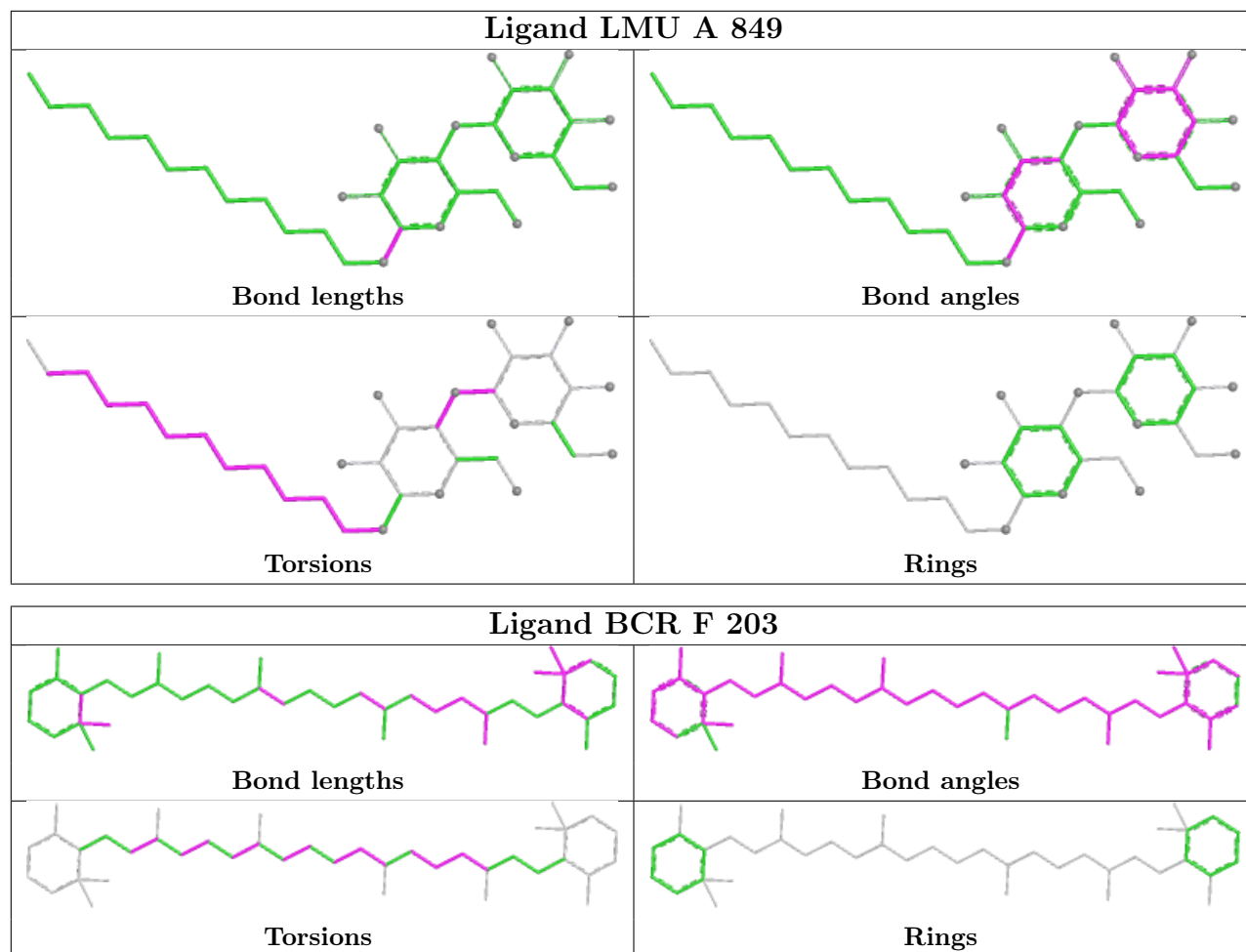
Bond angles



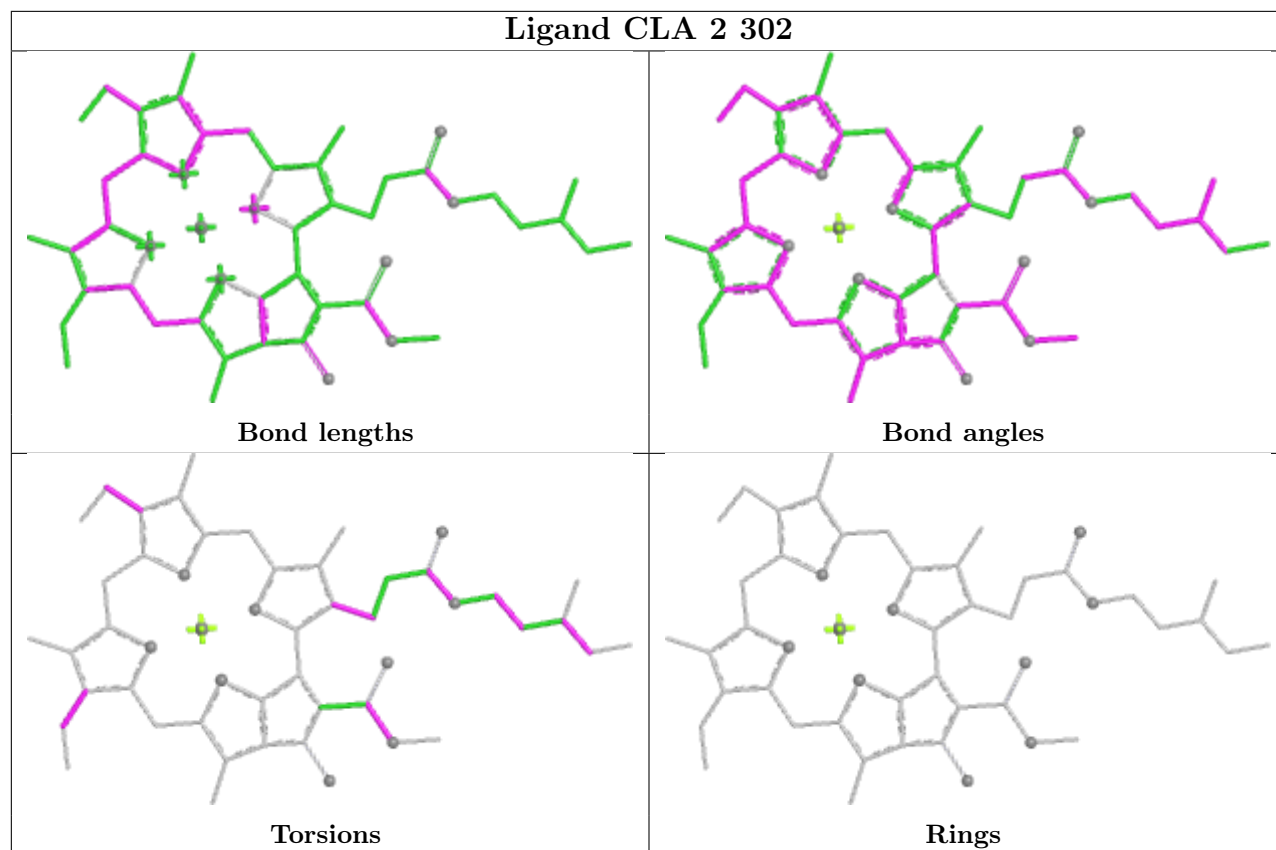
Torsions



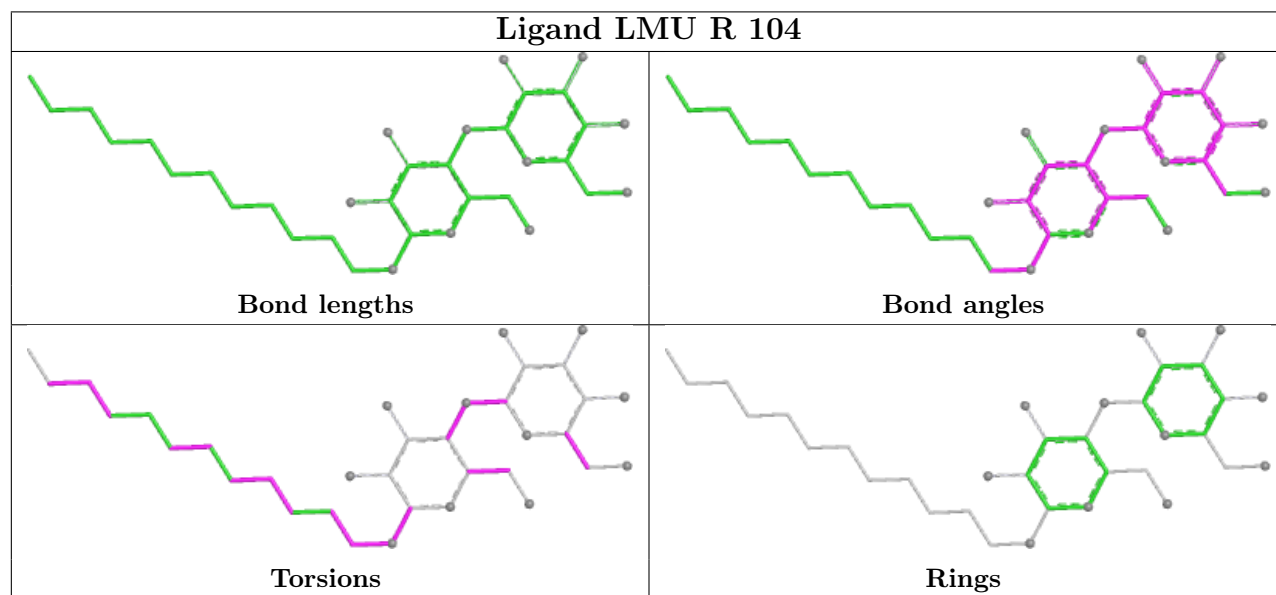
Rings

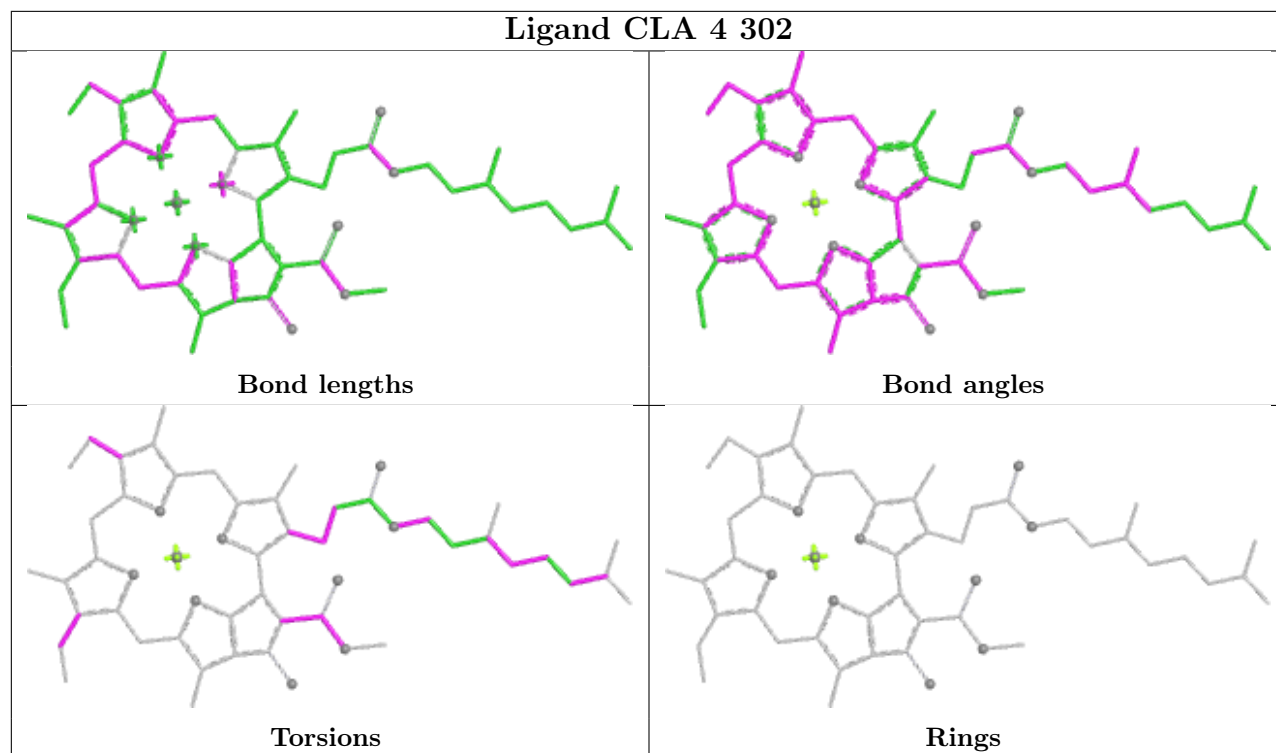
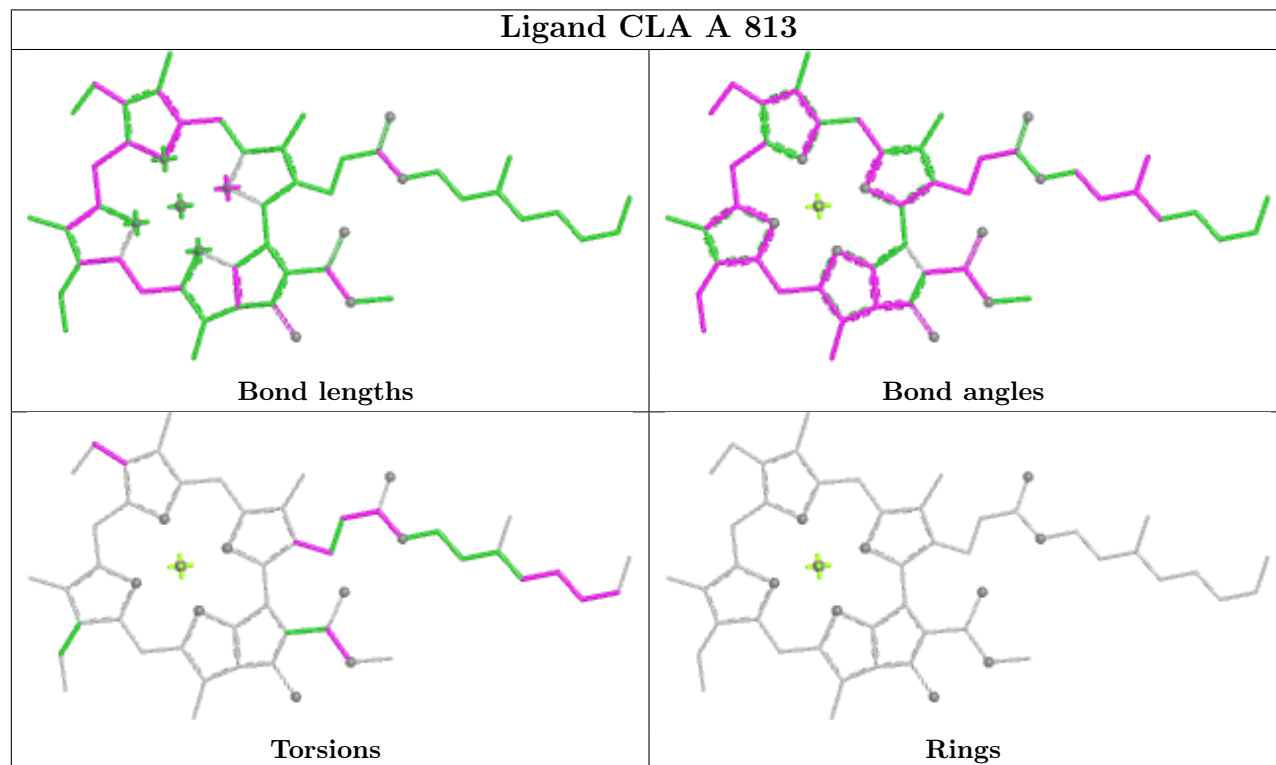


Ligand CLA 2 302

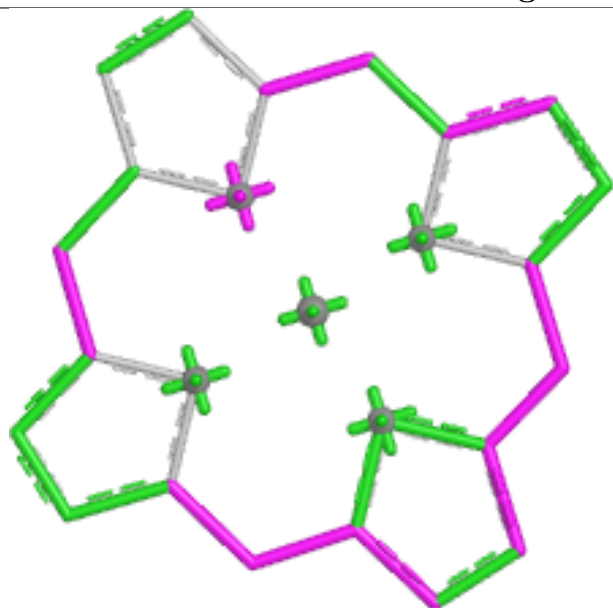


Ligand LMU R 104

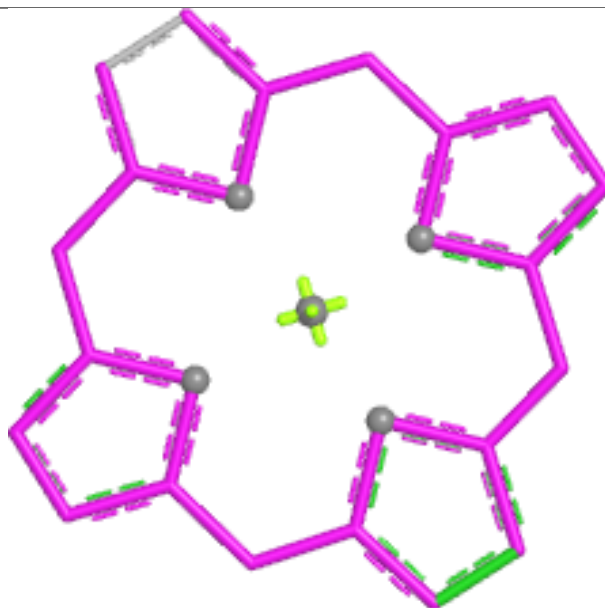


Ligand CLA 4 302**Ligand CLA A 813**

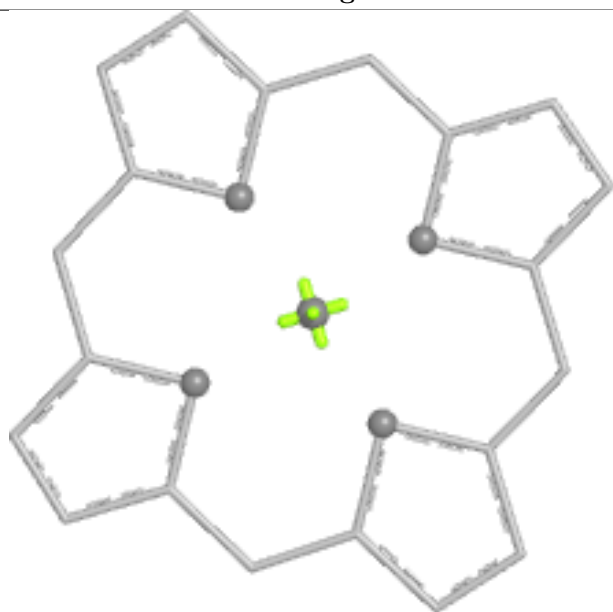
Ligand CLA 3 310



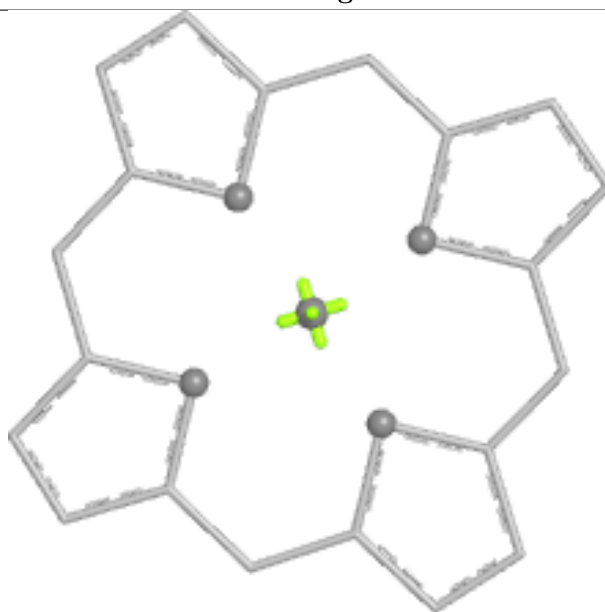
Bond lengths



Bond angles

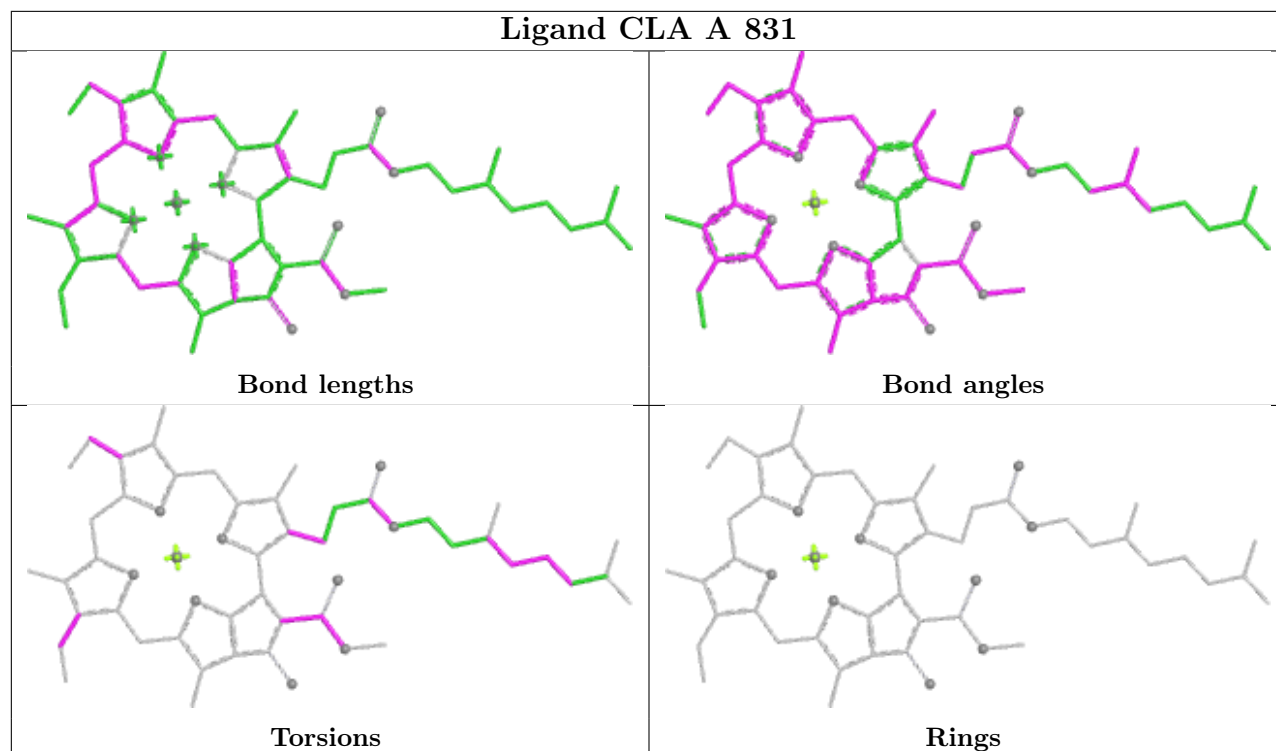


Torsions

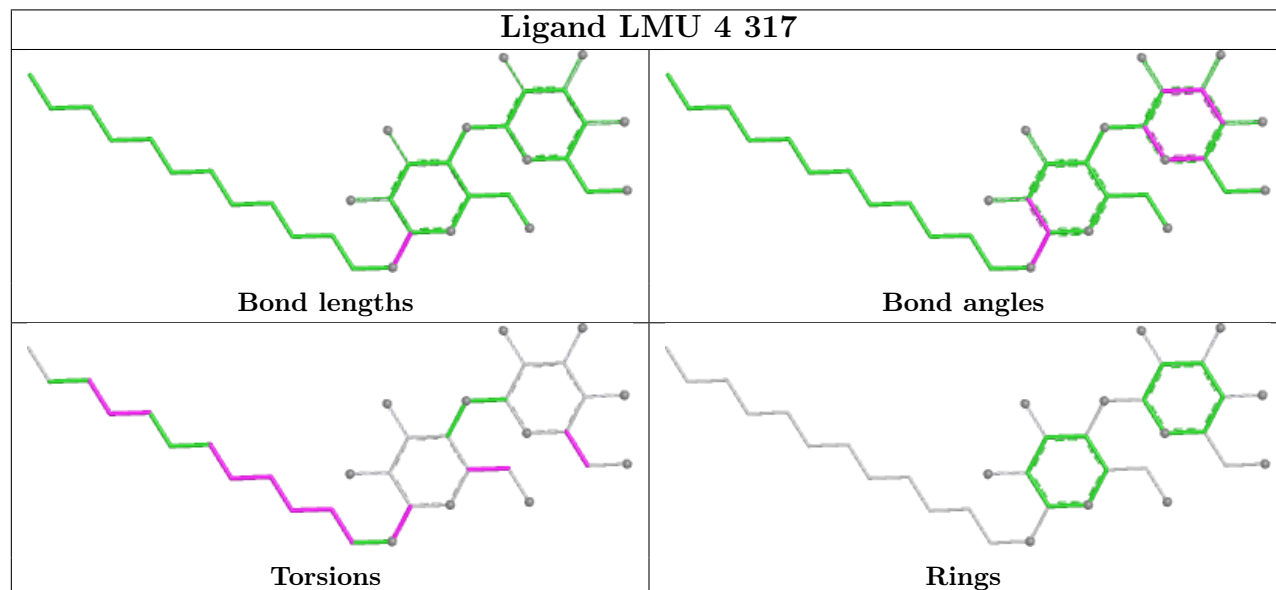


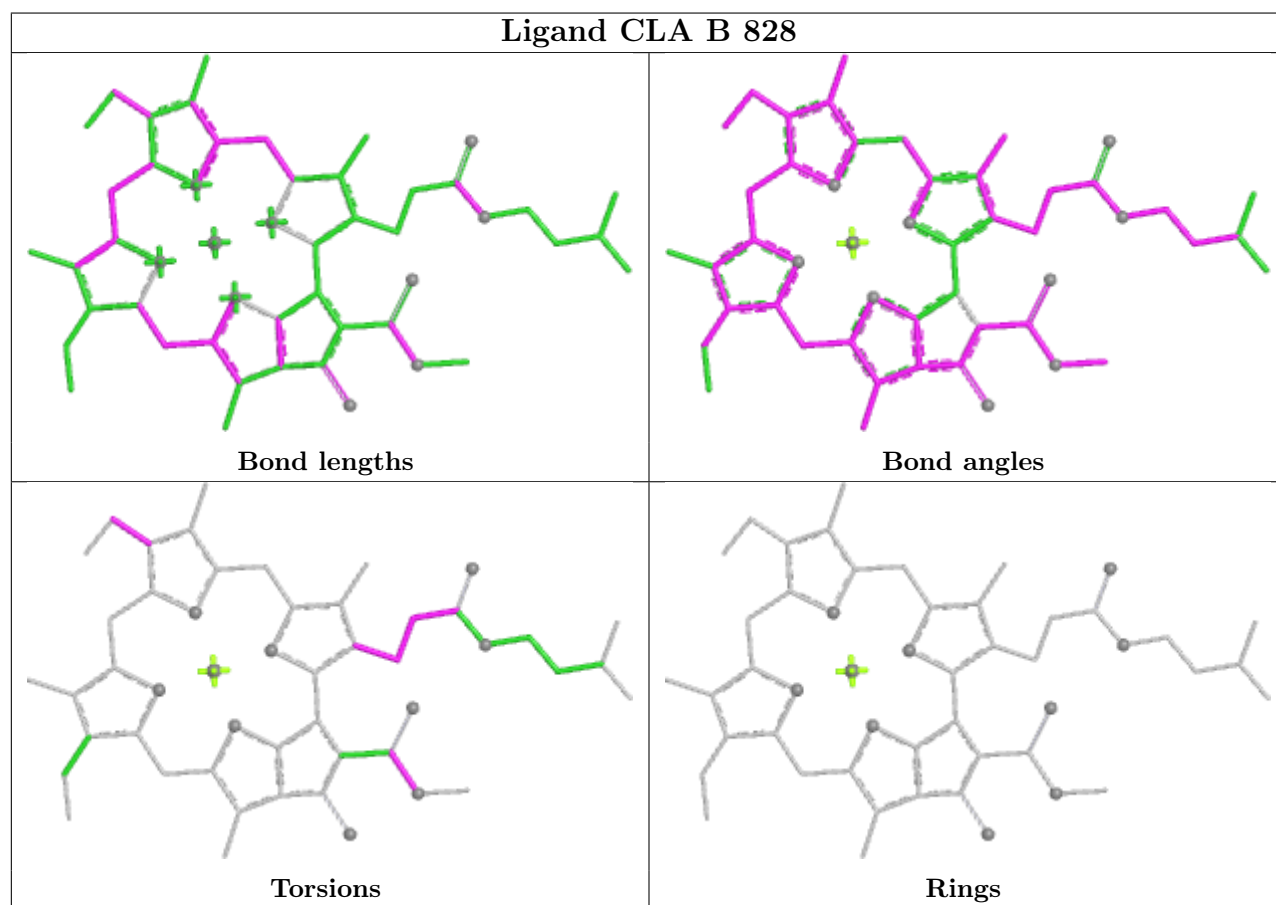
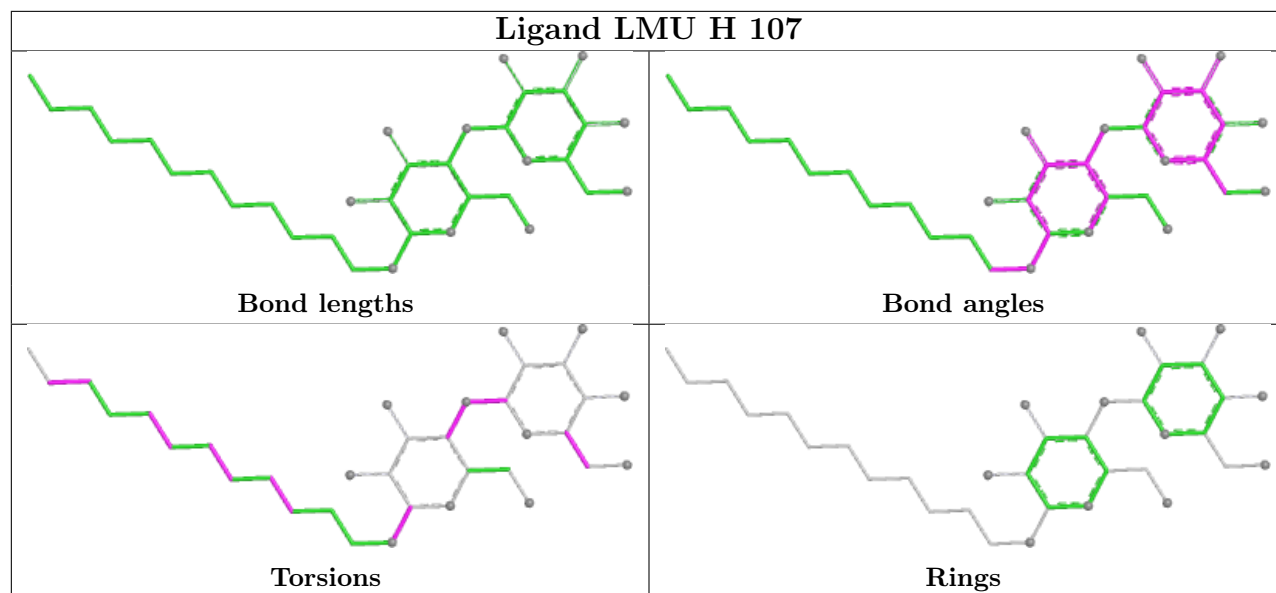
Rings

Ligand CLA A 831

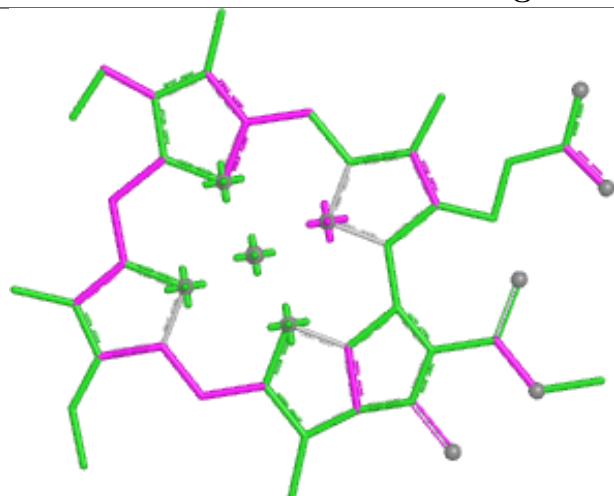


Ligand LMU 4 317

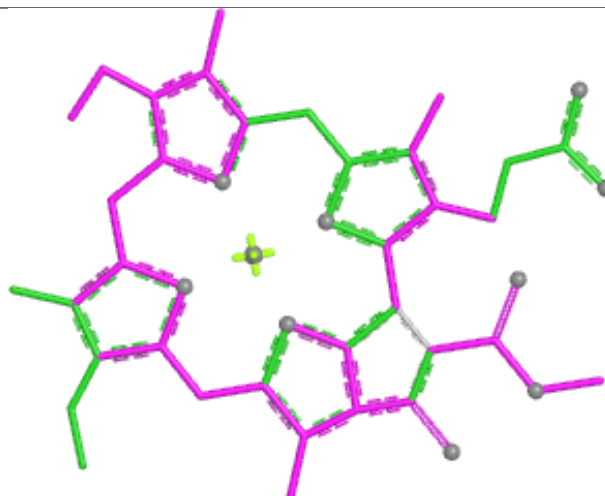




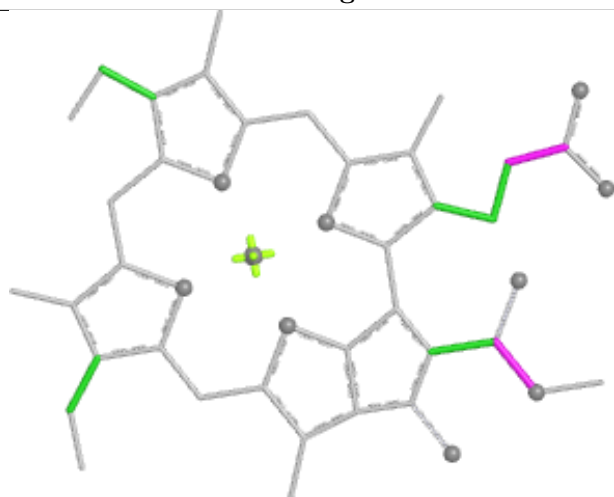
Ligand CLA A 810



Bond lengths



Bond angles

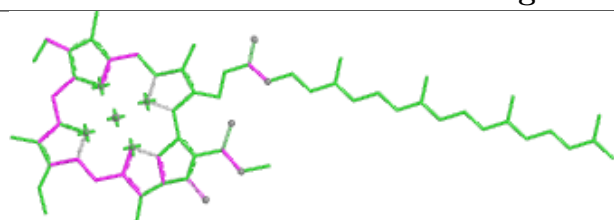


Torsions

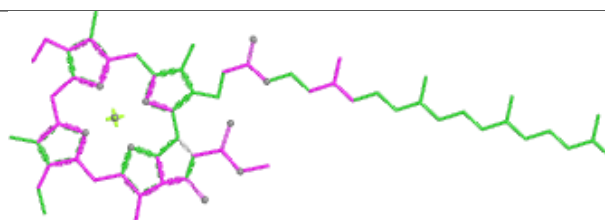


Rings

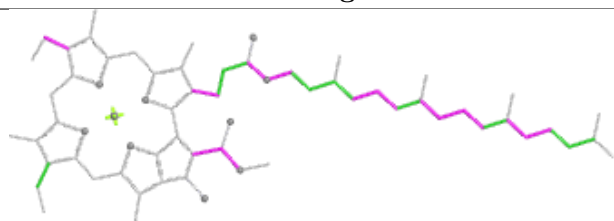
Ligand CLA 2 315



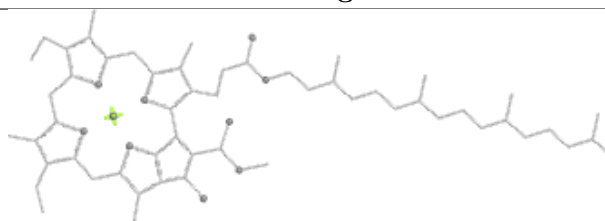
Bond lengths



Bond angles

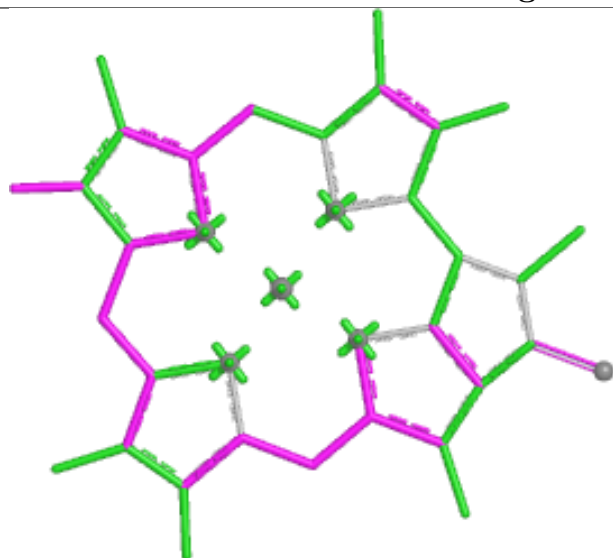


Torsions

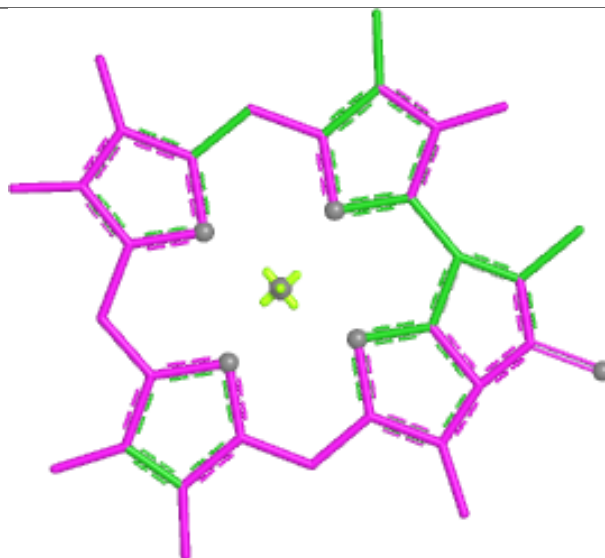


Rings

Ligand CLA 4 303



Bond lengths



Bond angles

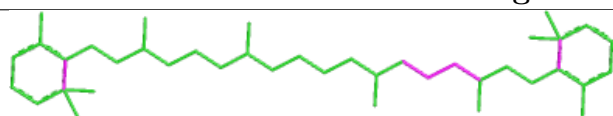


Torsions

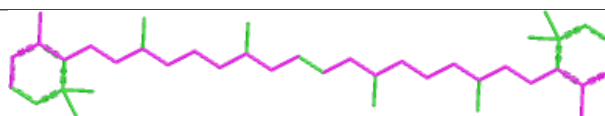


Rings

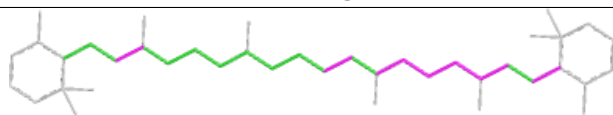
Ligand BCR B 842



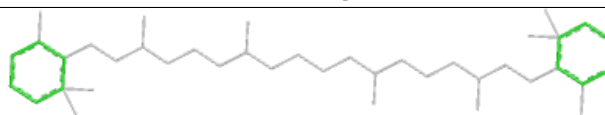
Bond lengths



Bond angles

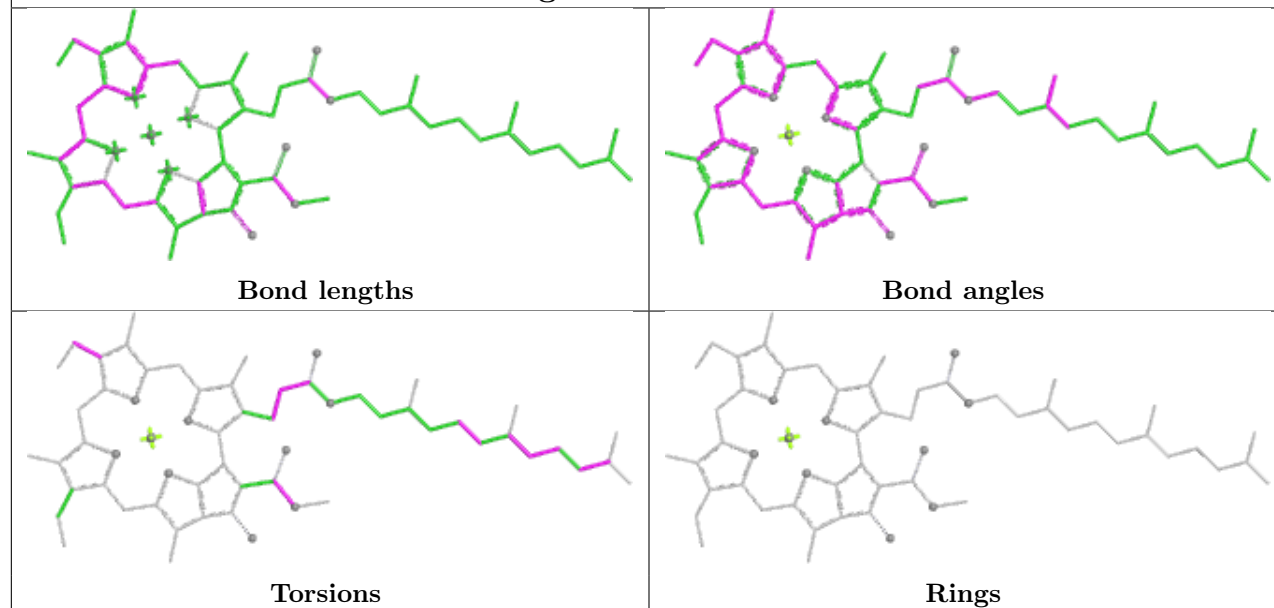


Torsions

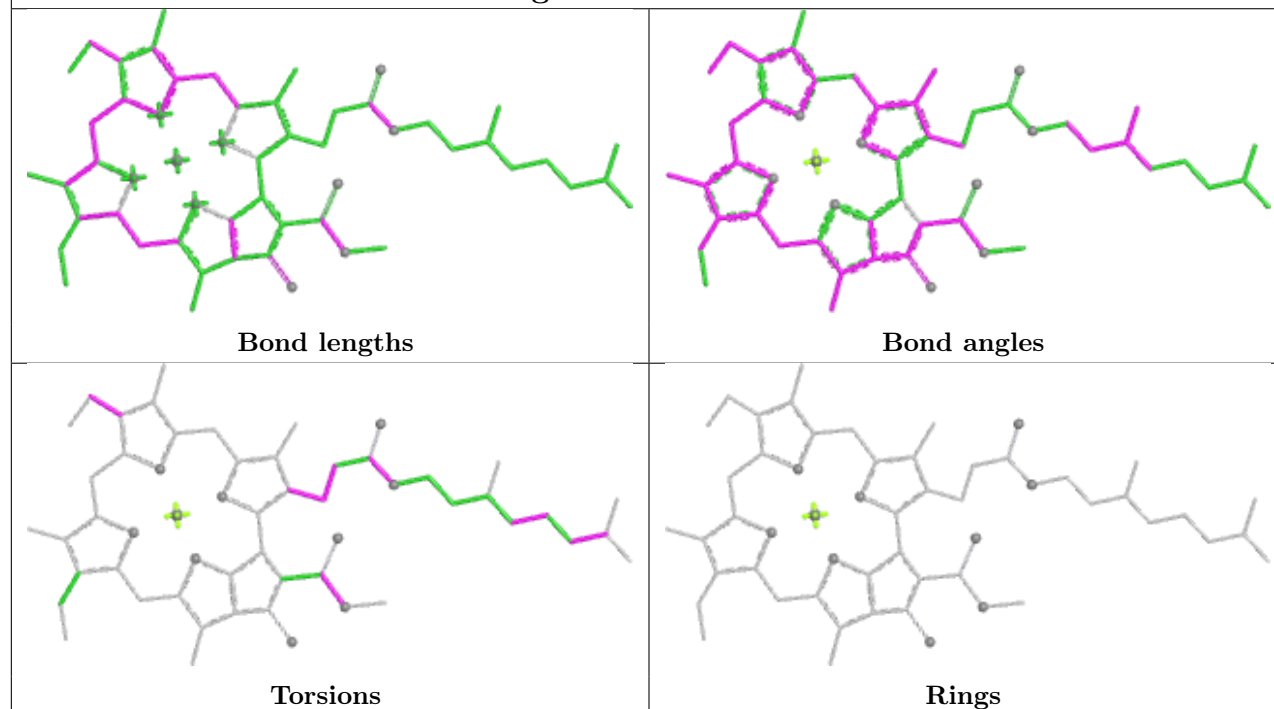


Rings

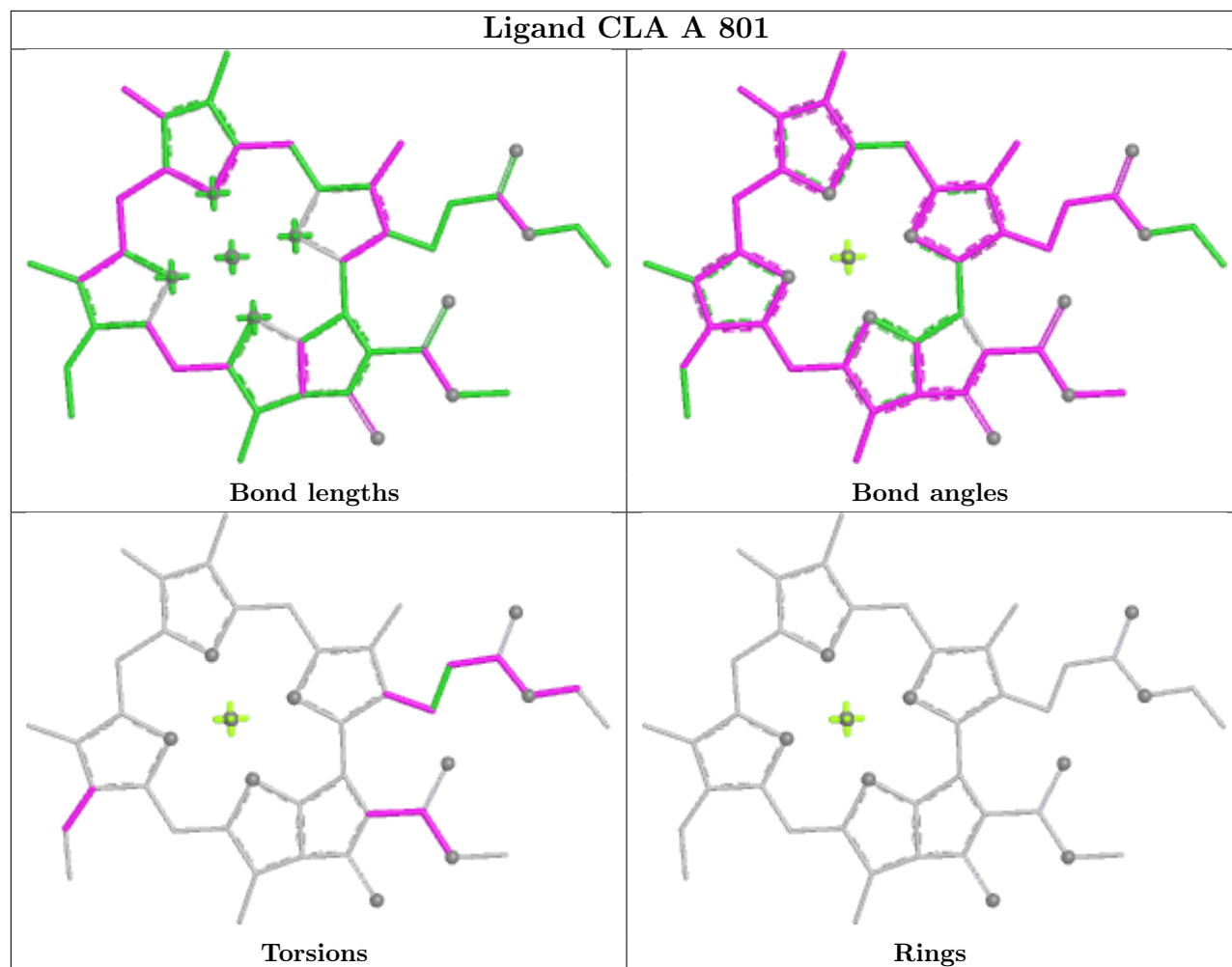
Ligand CLA I 102



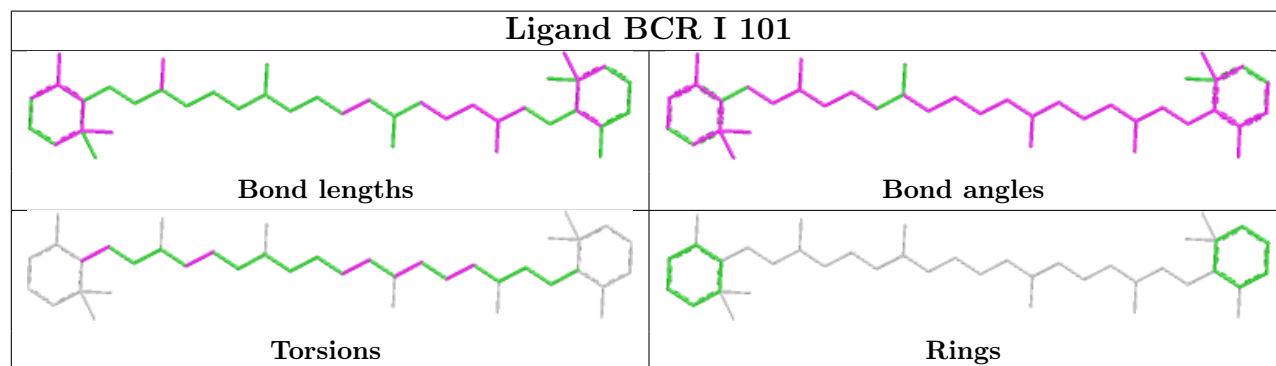
Ligand CLA A 822



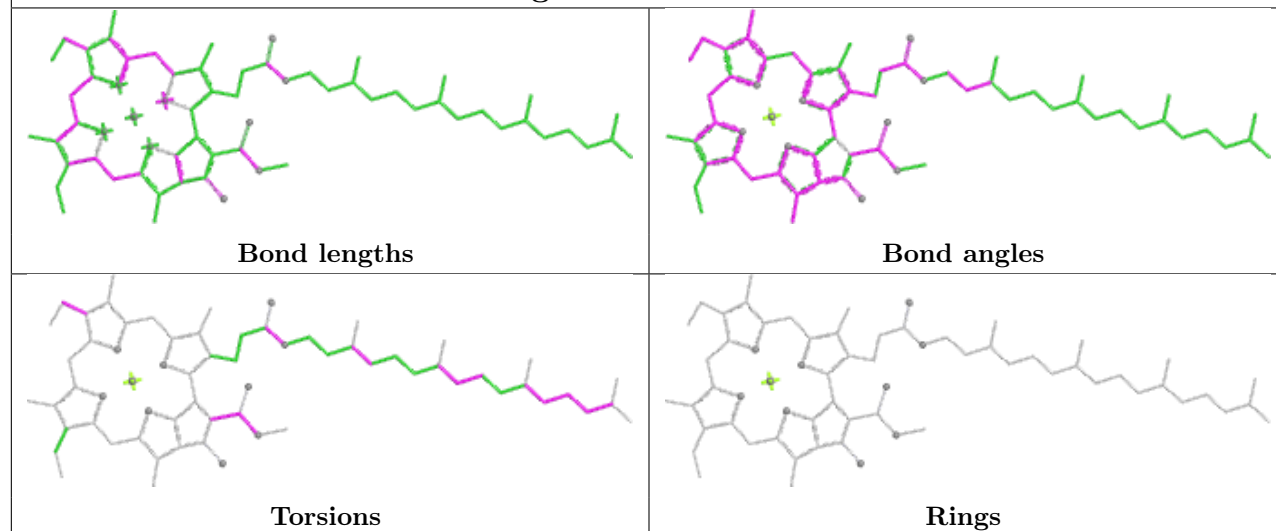
Ligand CLA A 801



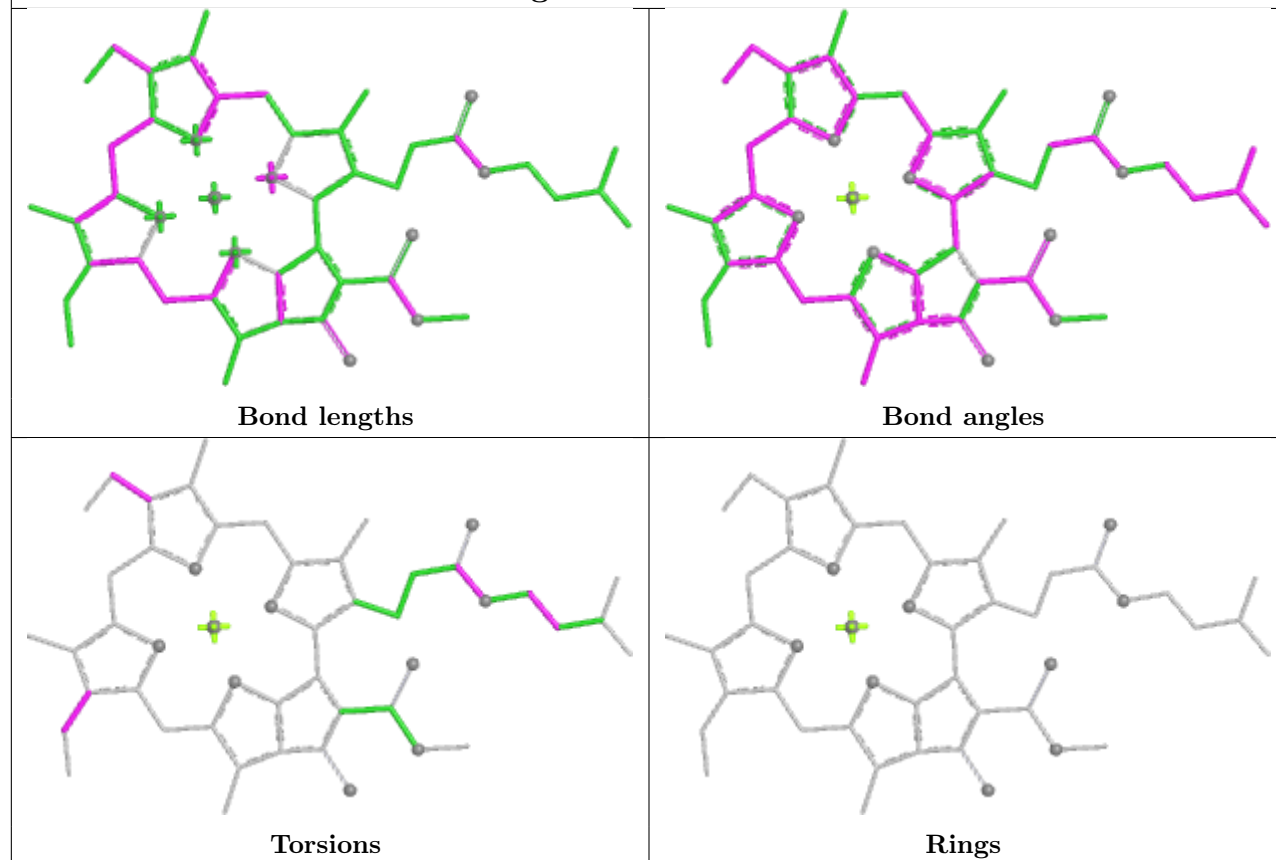
Ligand BCR I 101



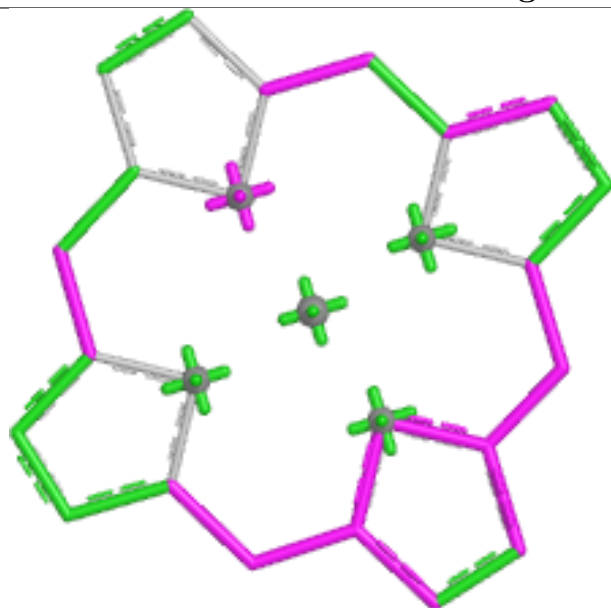
Ligand CLA A 835



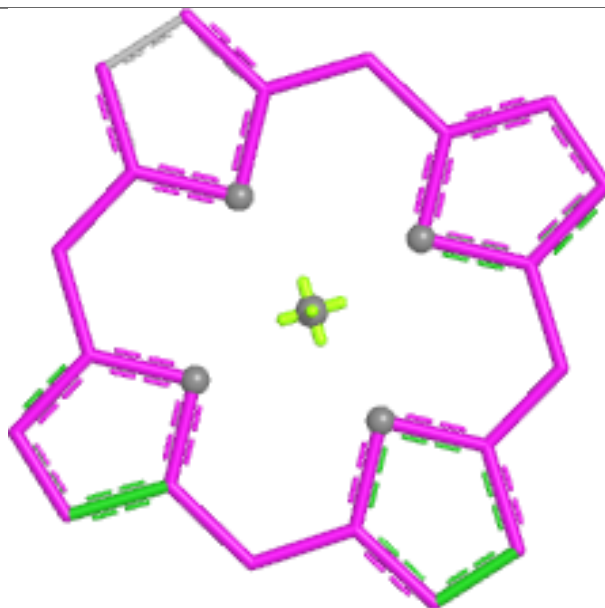
Ligand CLA K 107



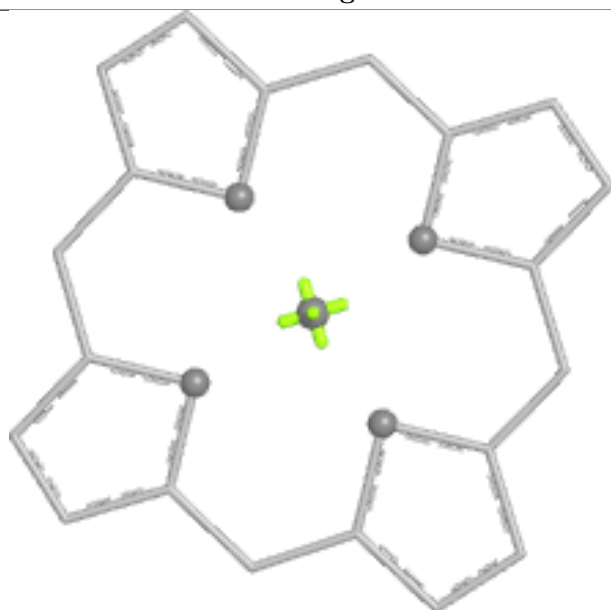
Ligand CLA 2 306



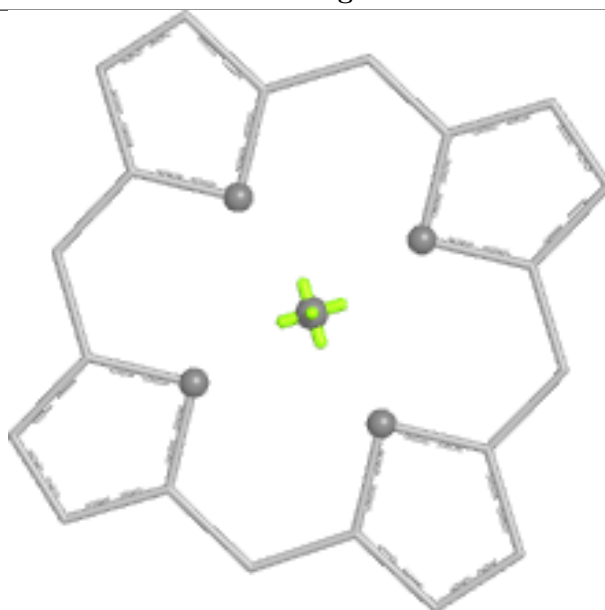
Bond lengths



Bond angles

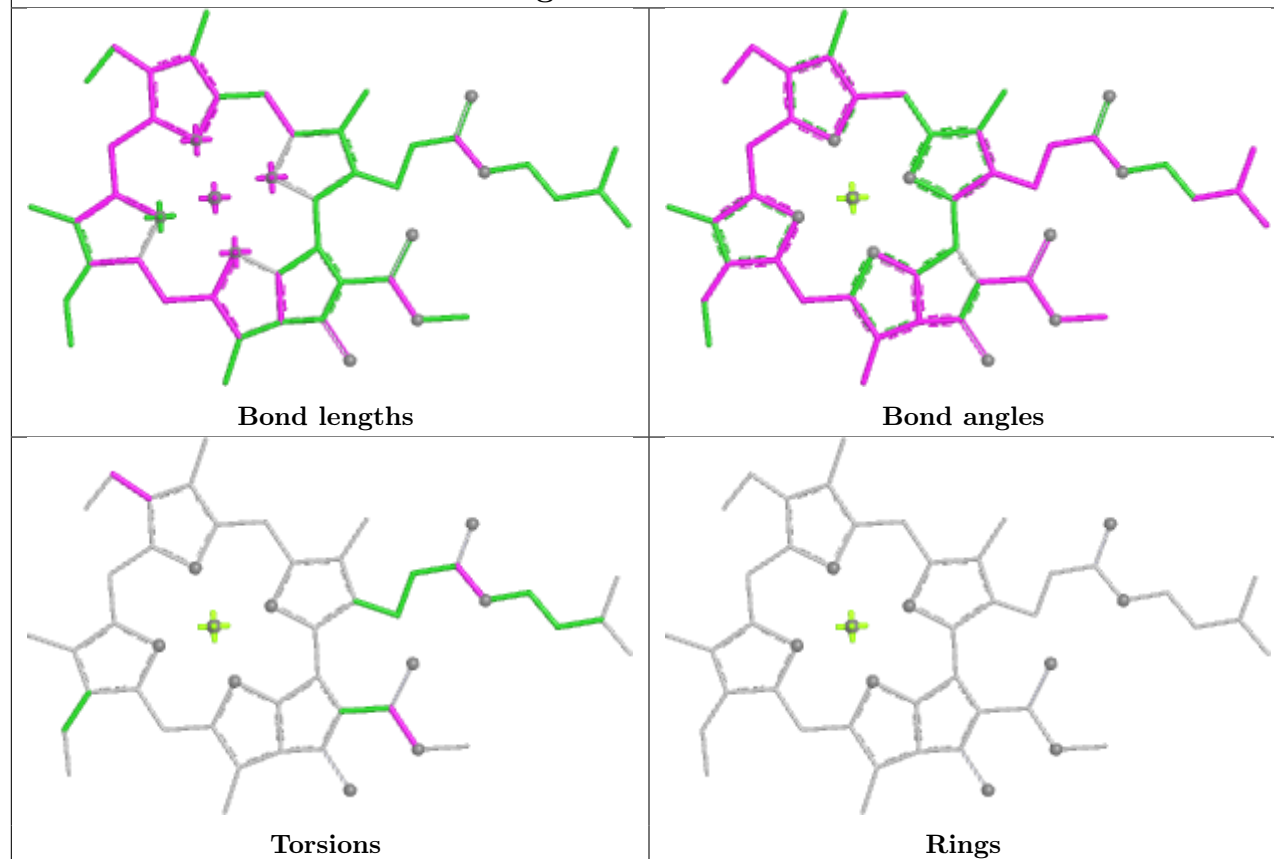


Torsions

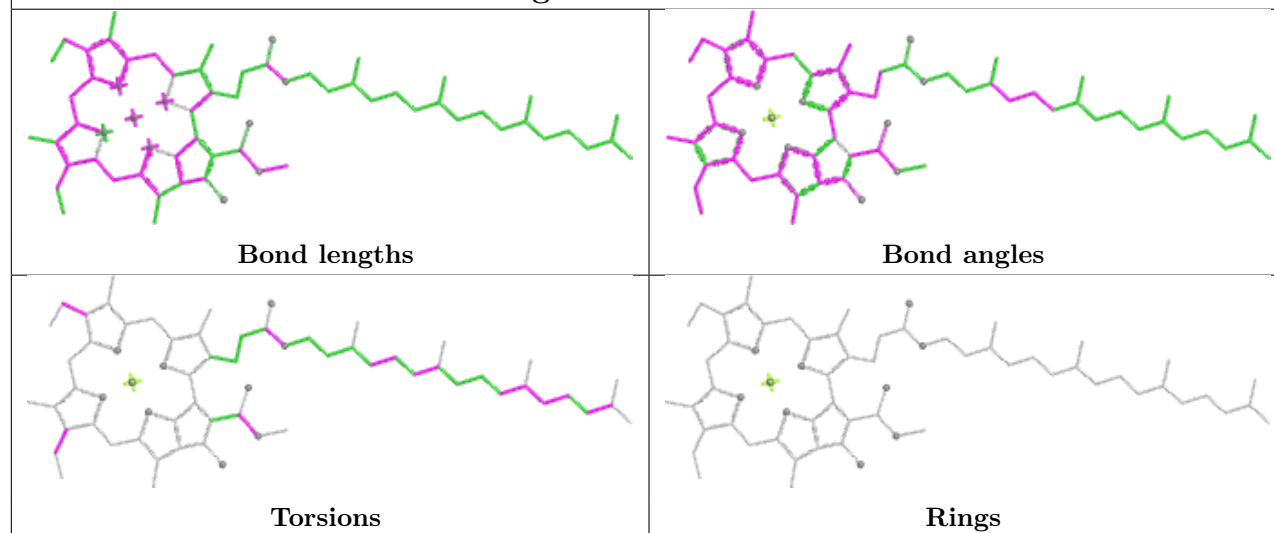


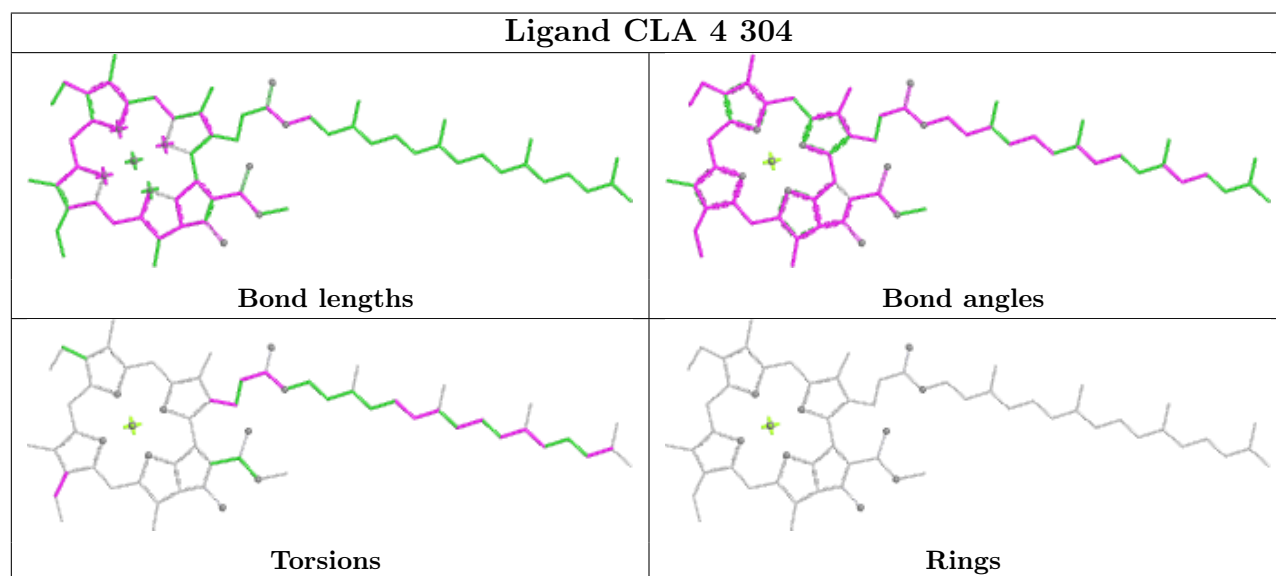
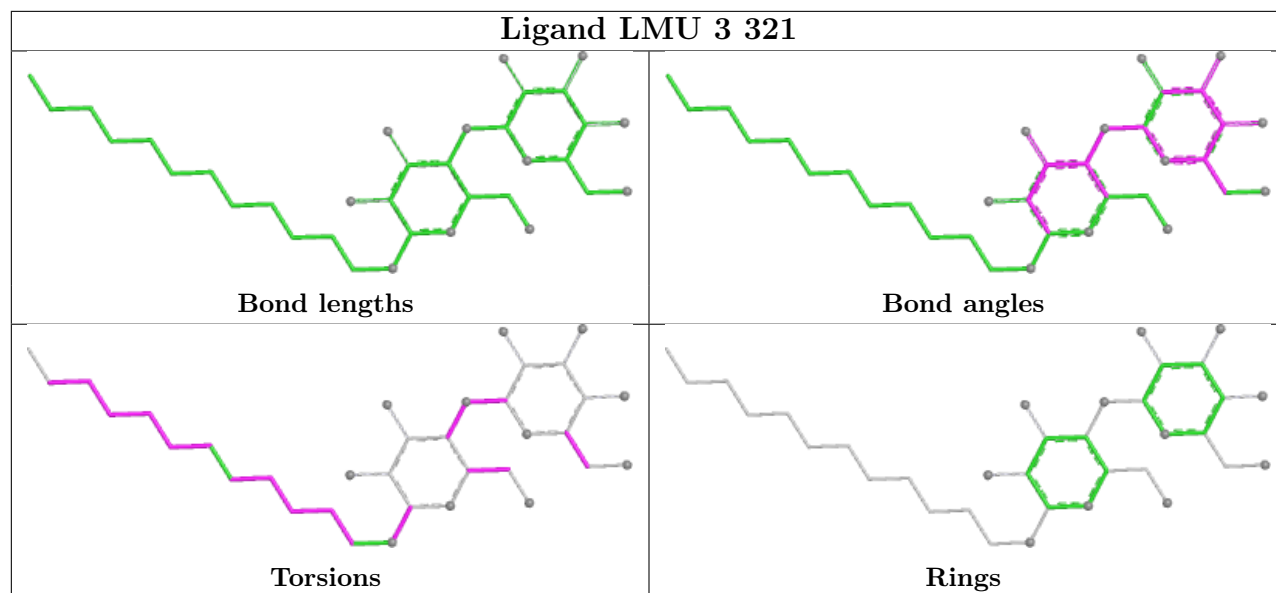
Rings

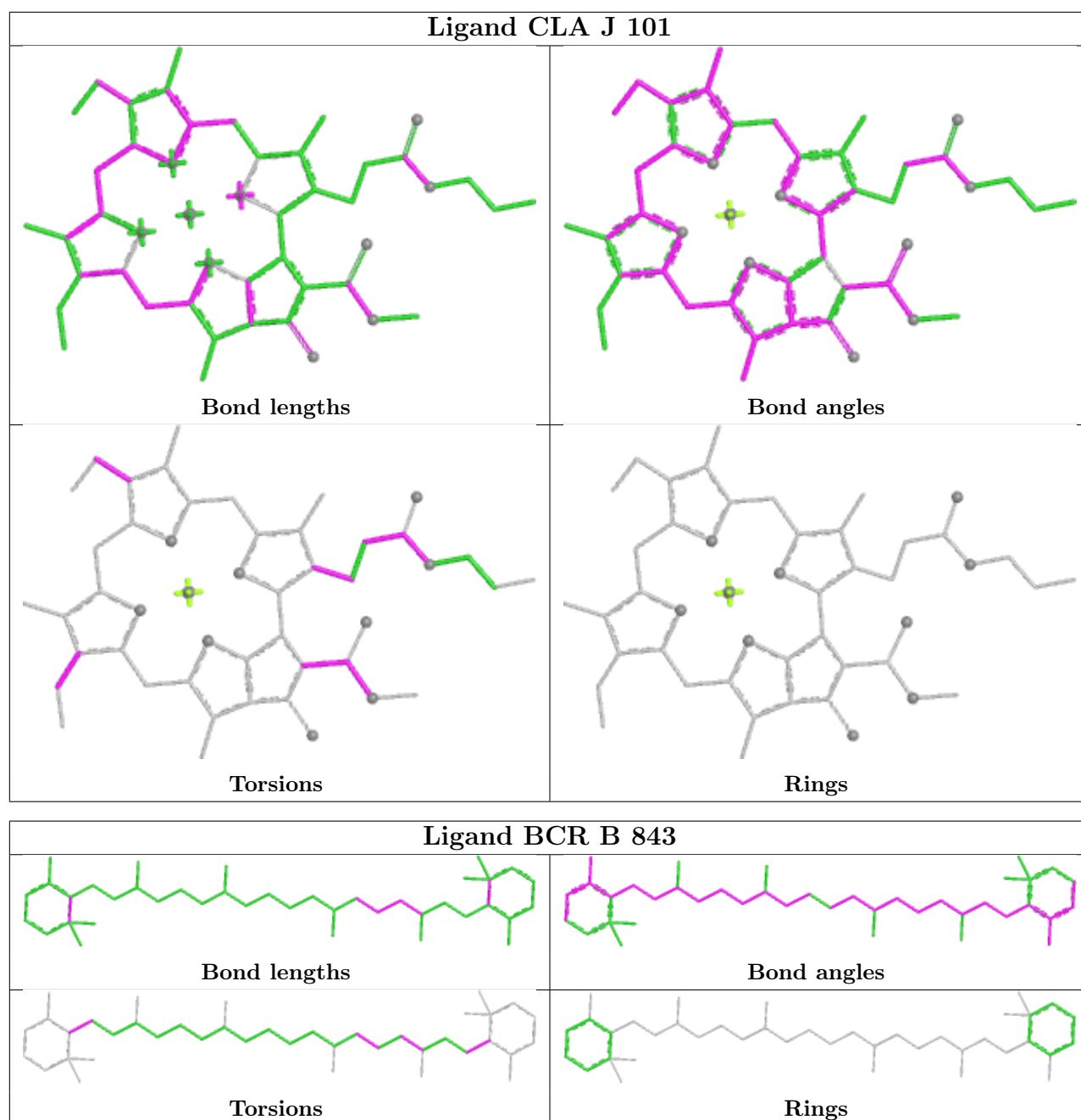
Ligand CLA 3 302

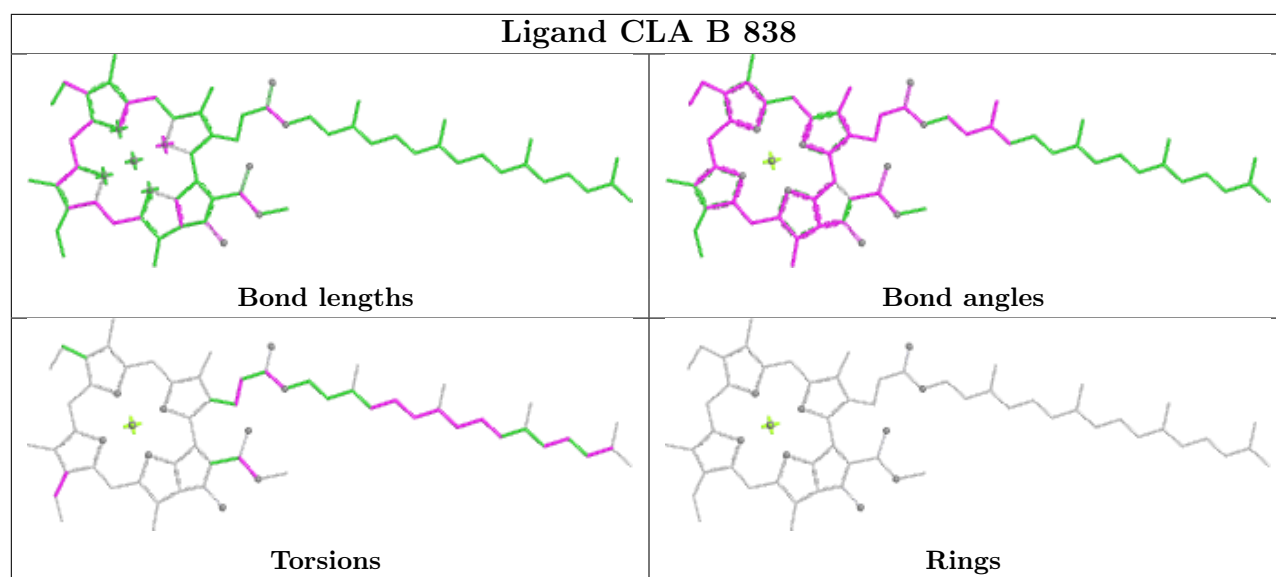


Ligand CLA B 821

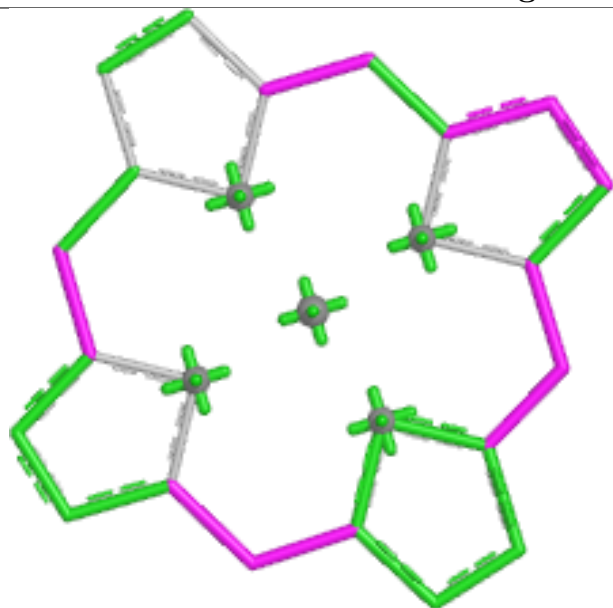




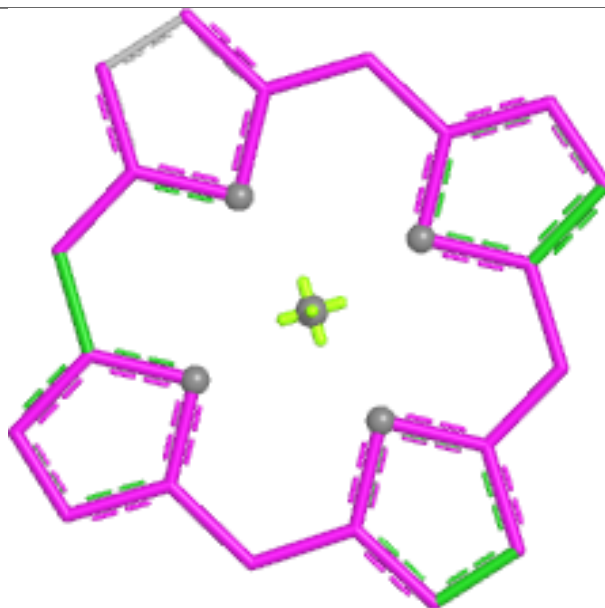




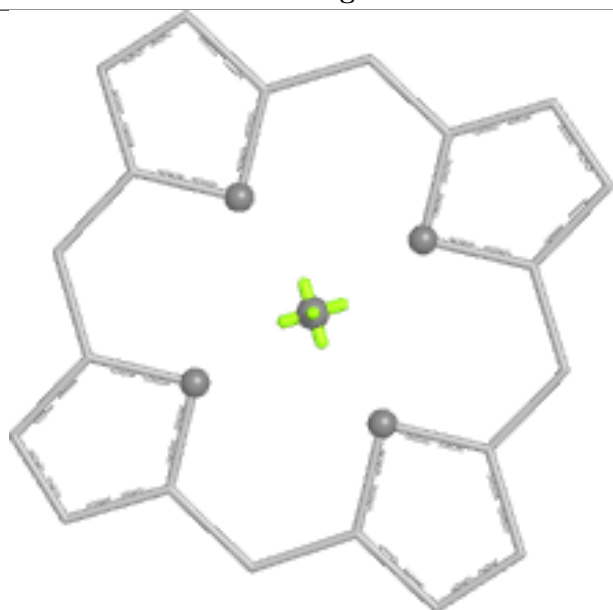
Ligand CLA 4 315



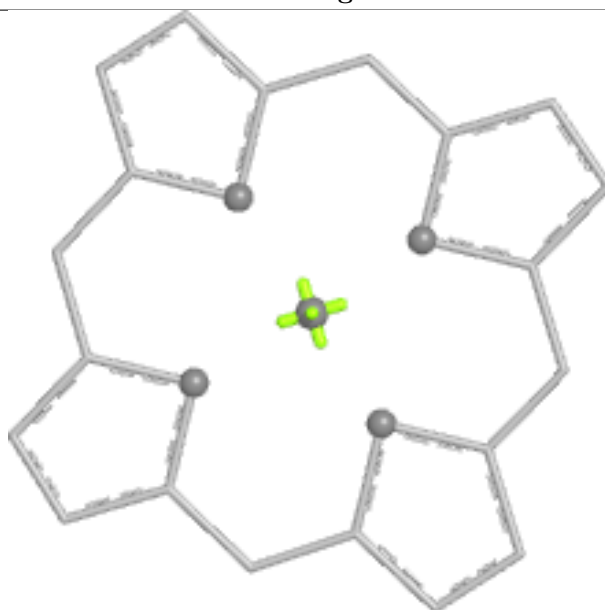
Bond lengths



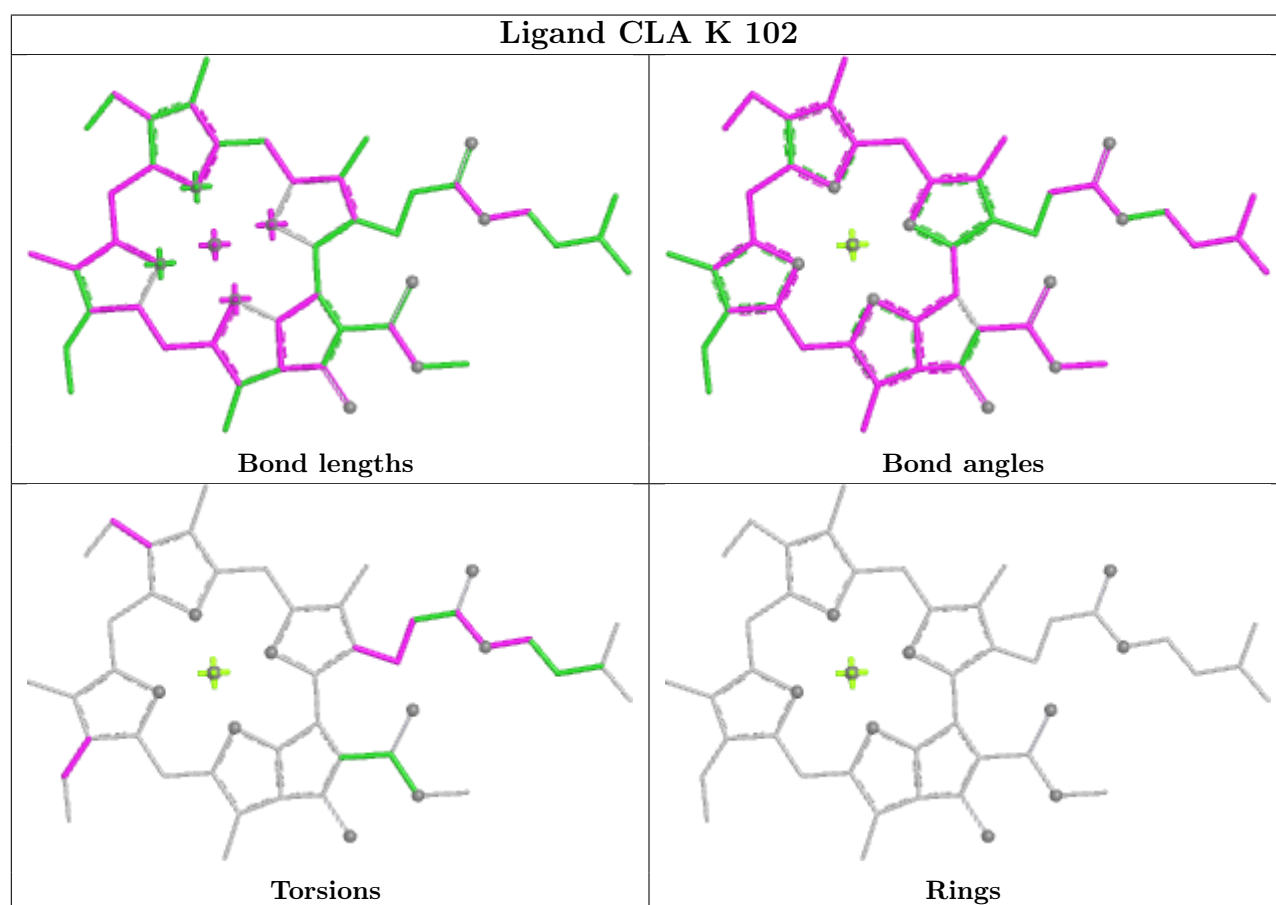
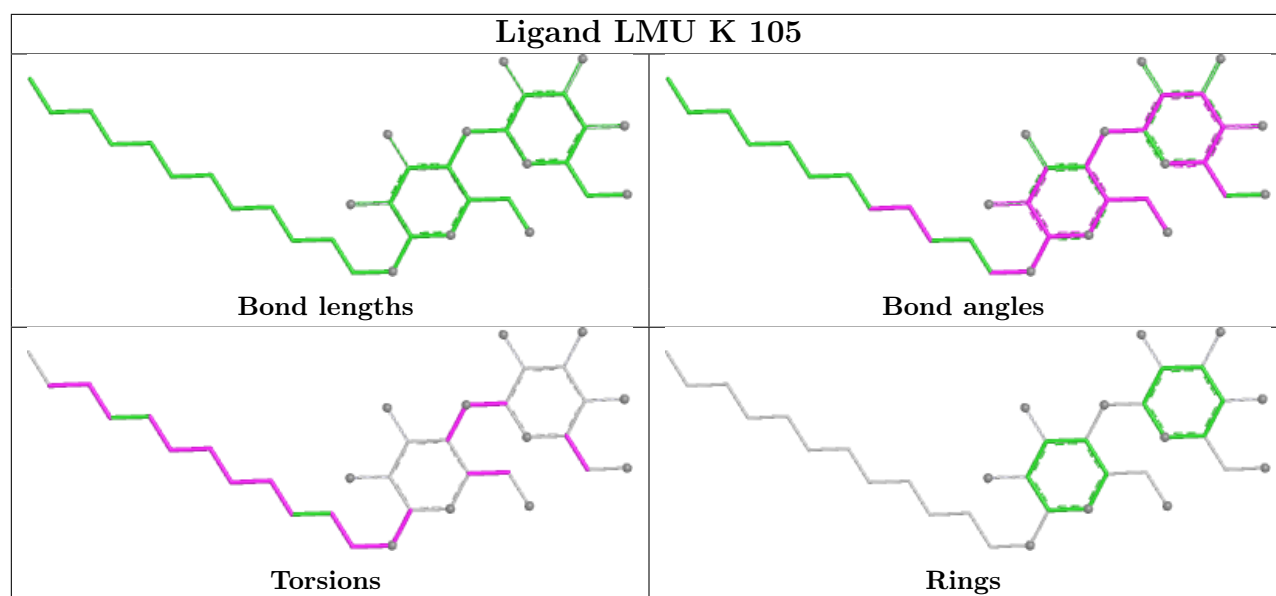
Bond angles



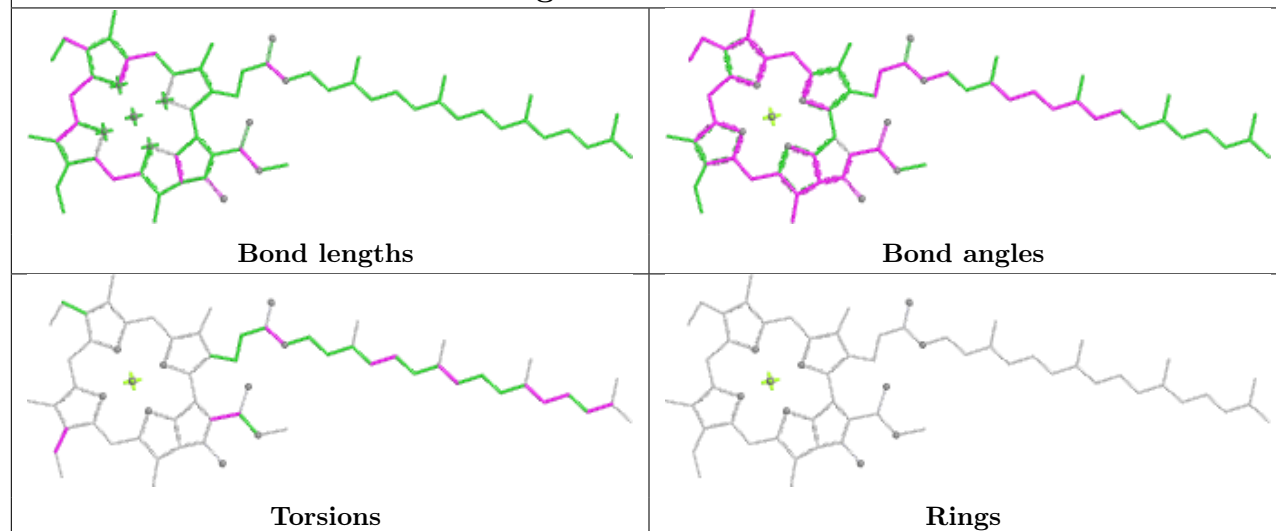
Torsions



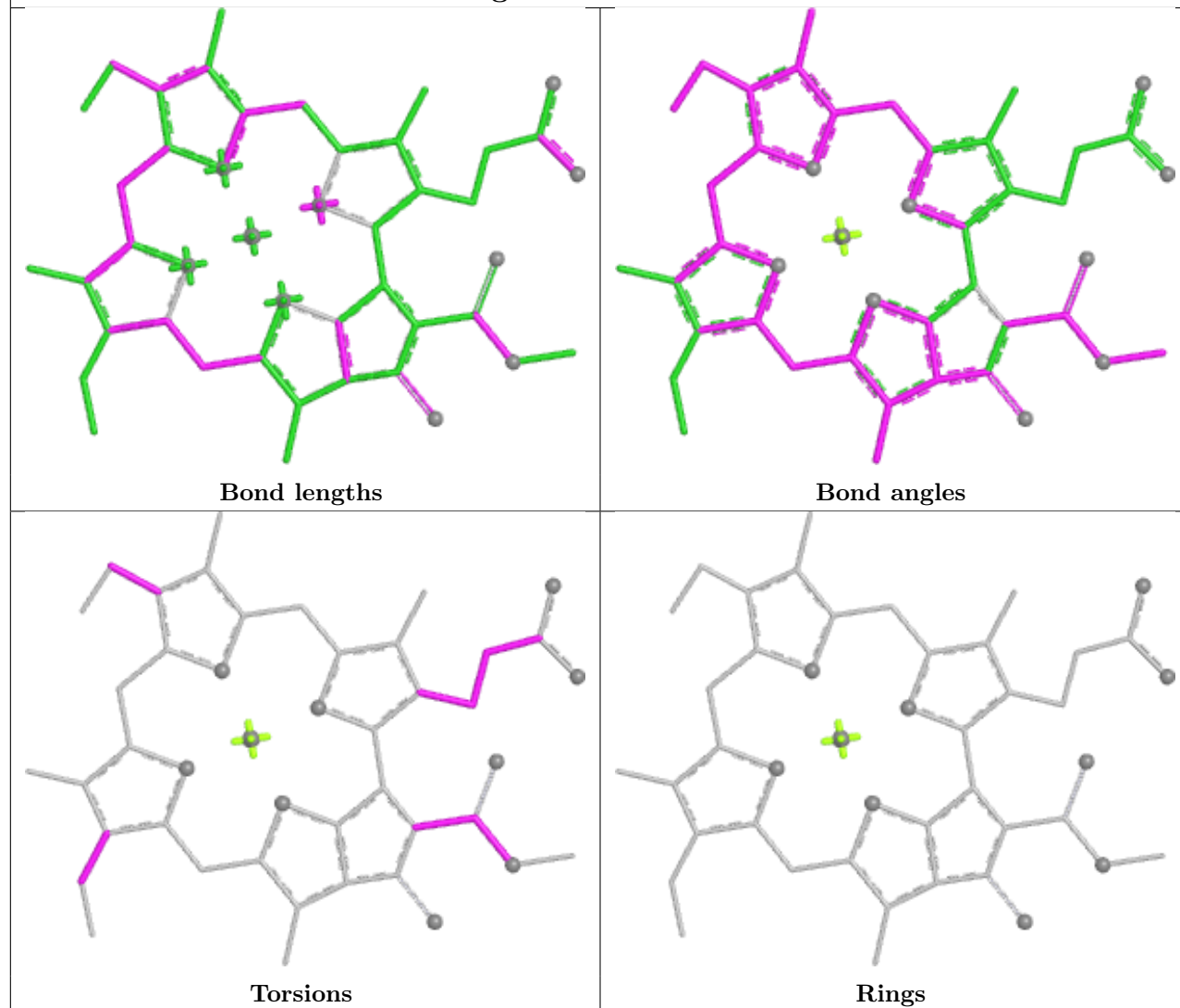
Rings

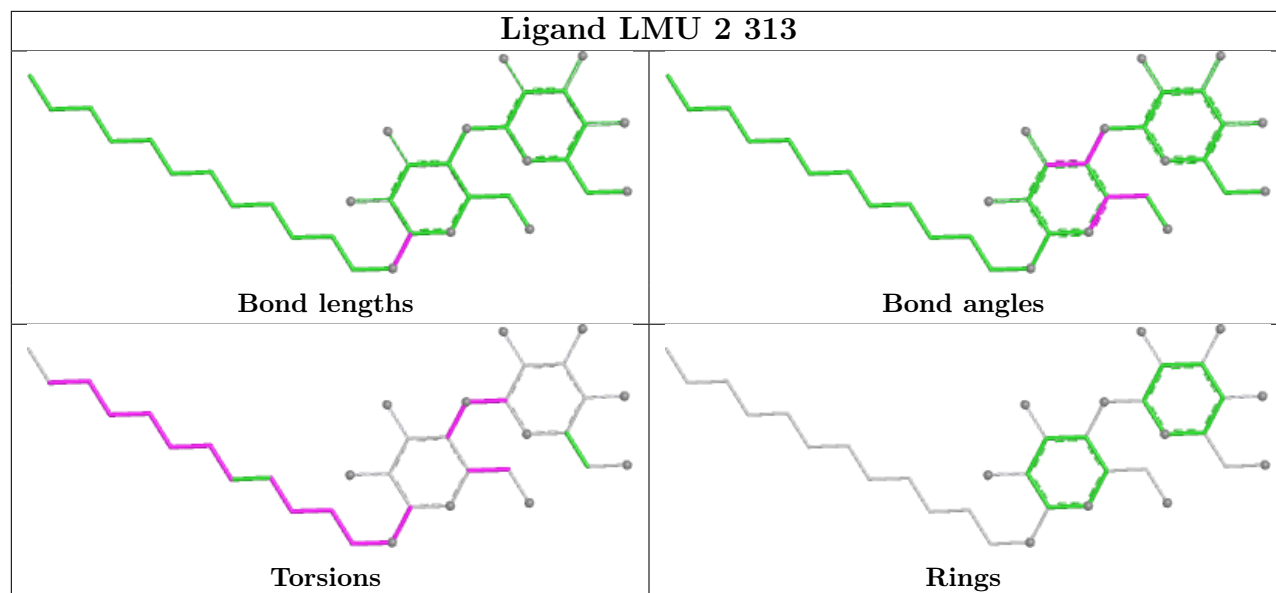


Ligand CLA 2 308

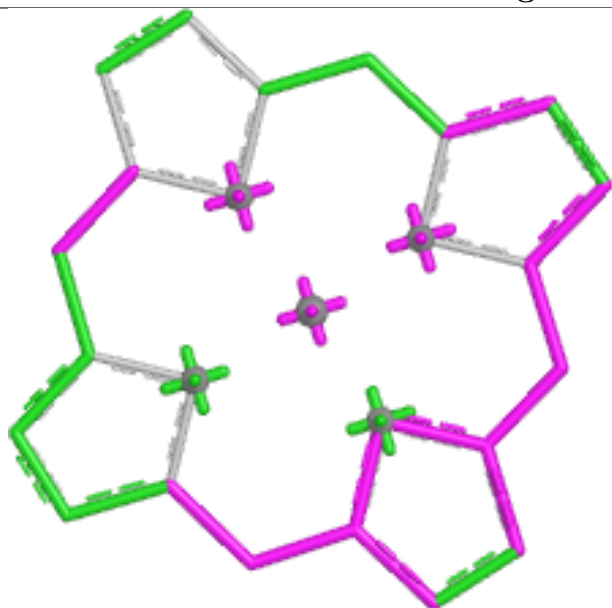


Ligand CLA A 814

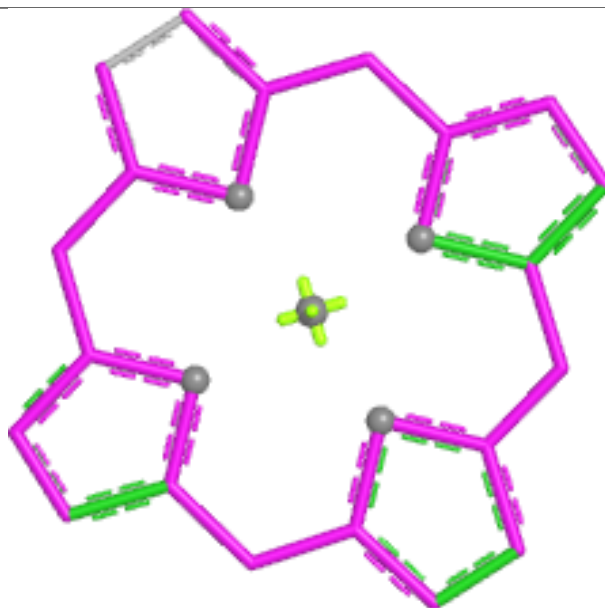




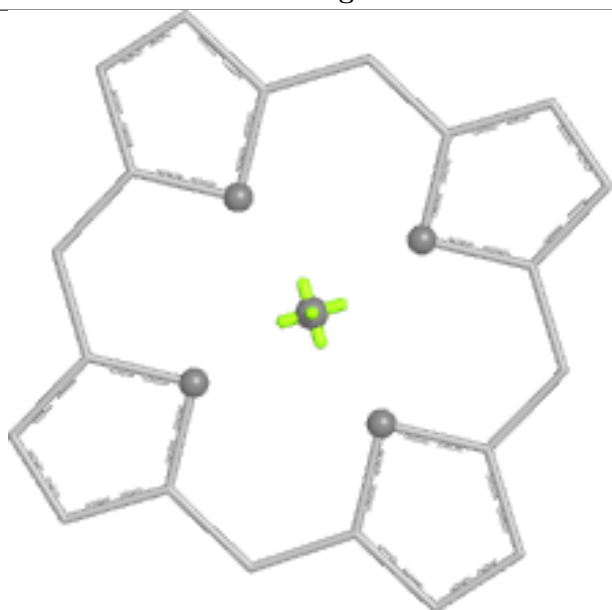
Ligand CLA 3 303



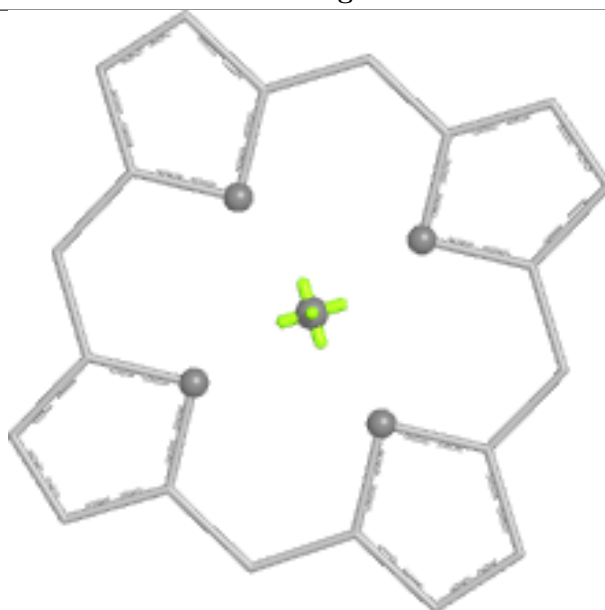
Bond lengths



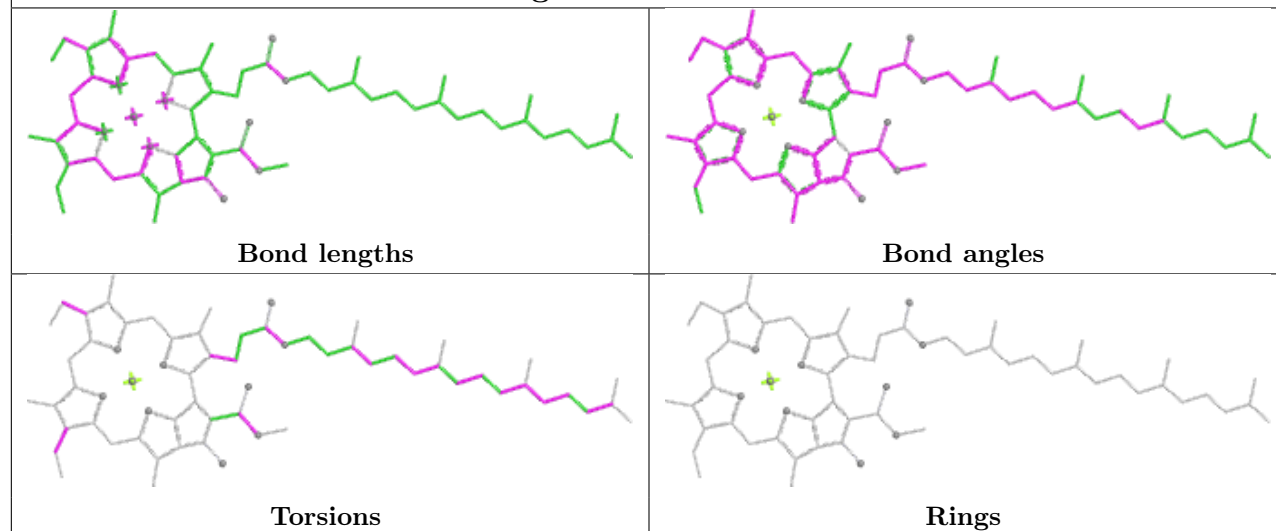
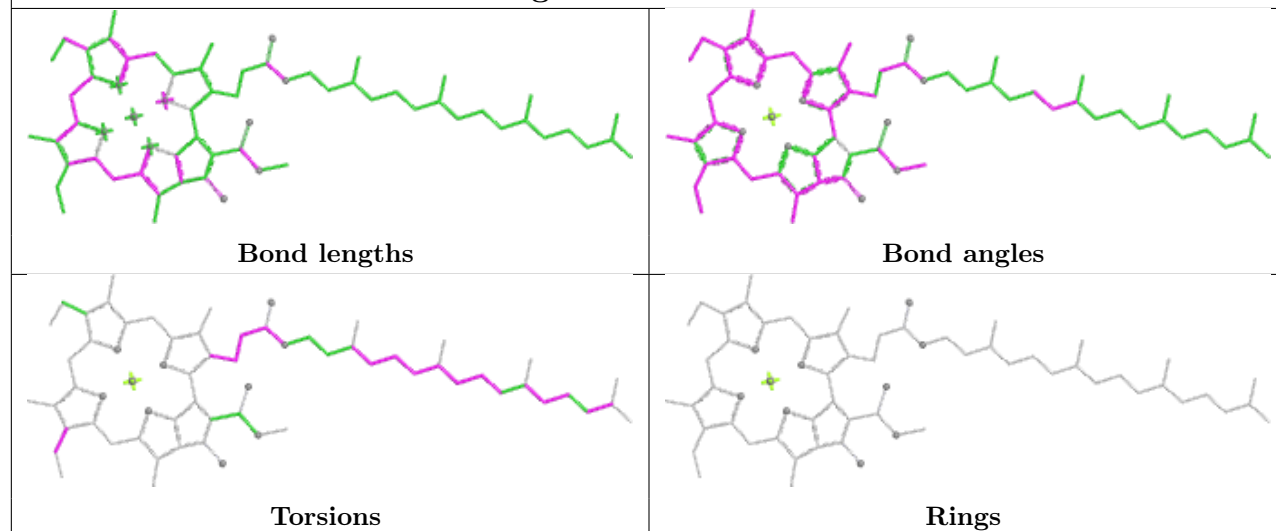
Bond angles

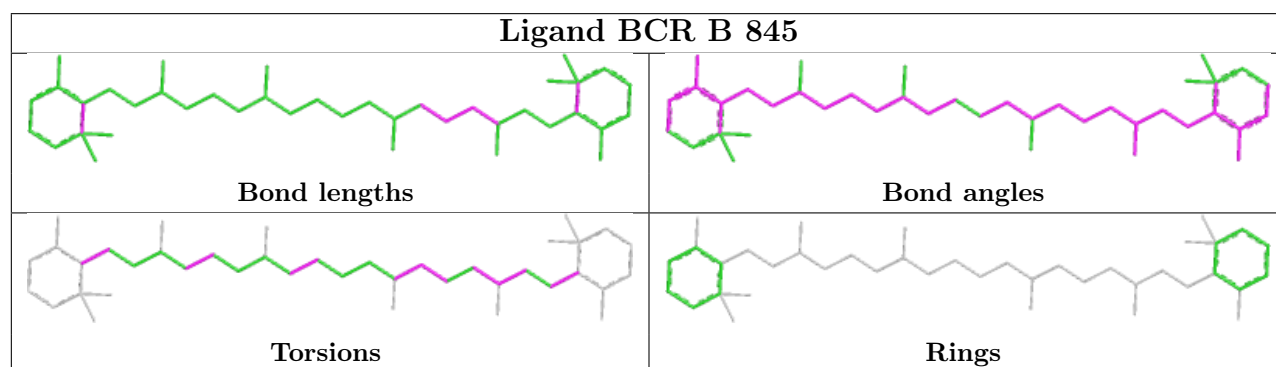
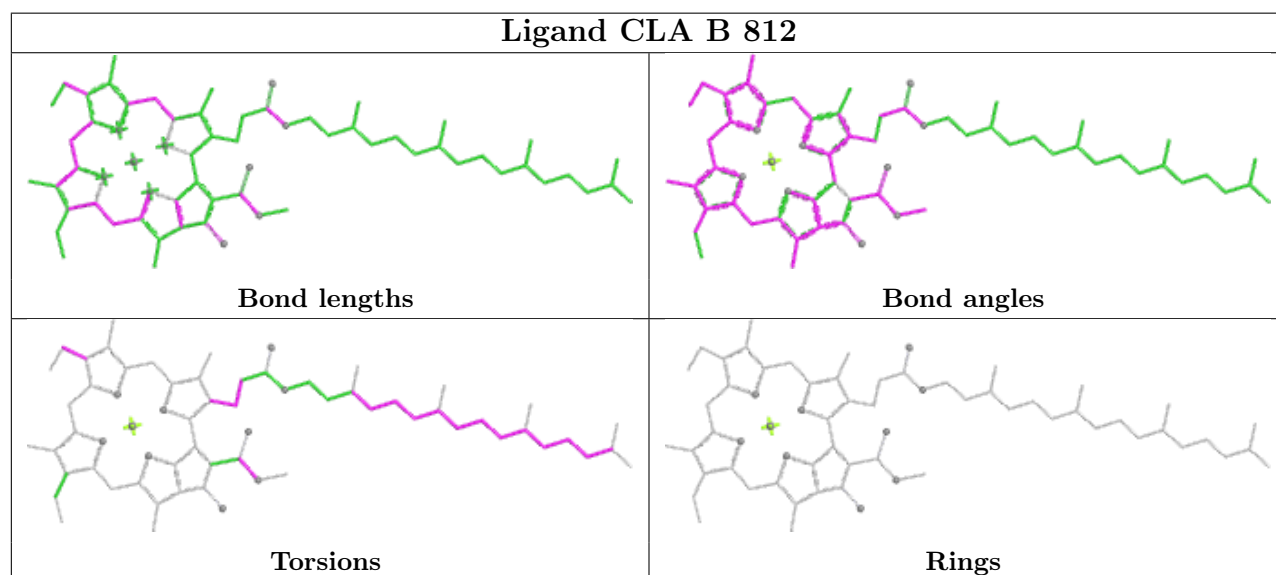
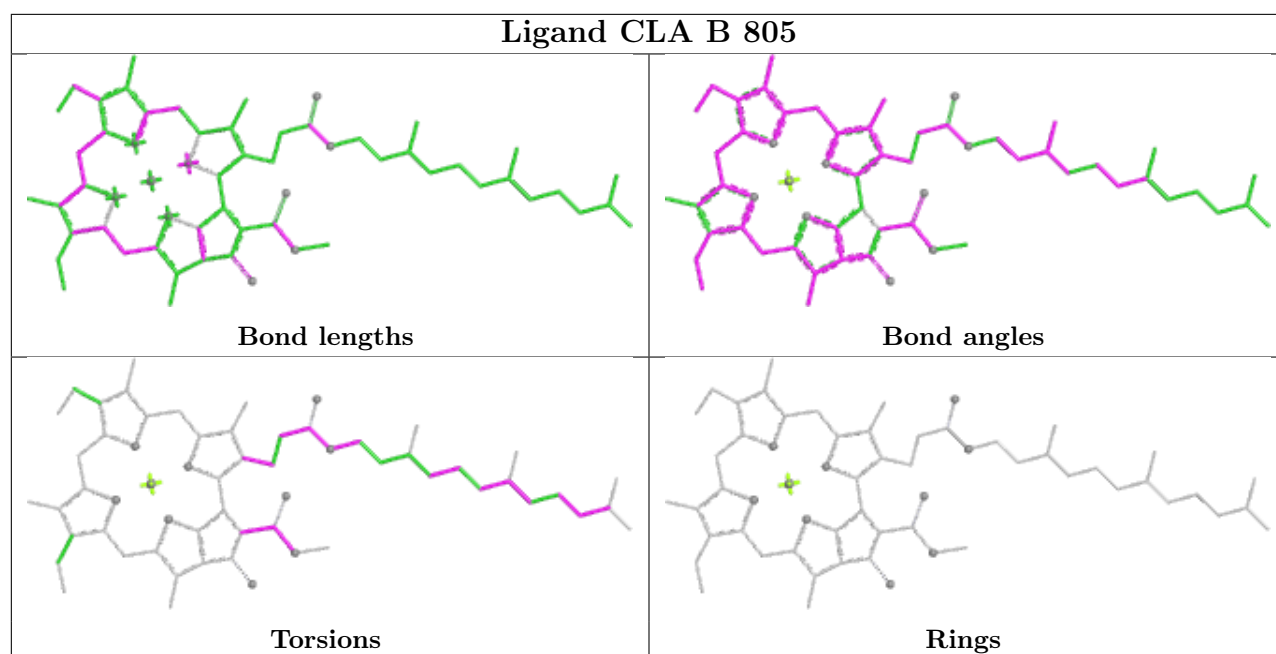


Torsions

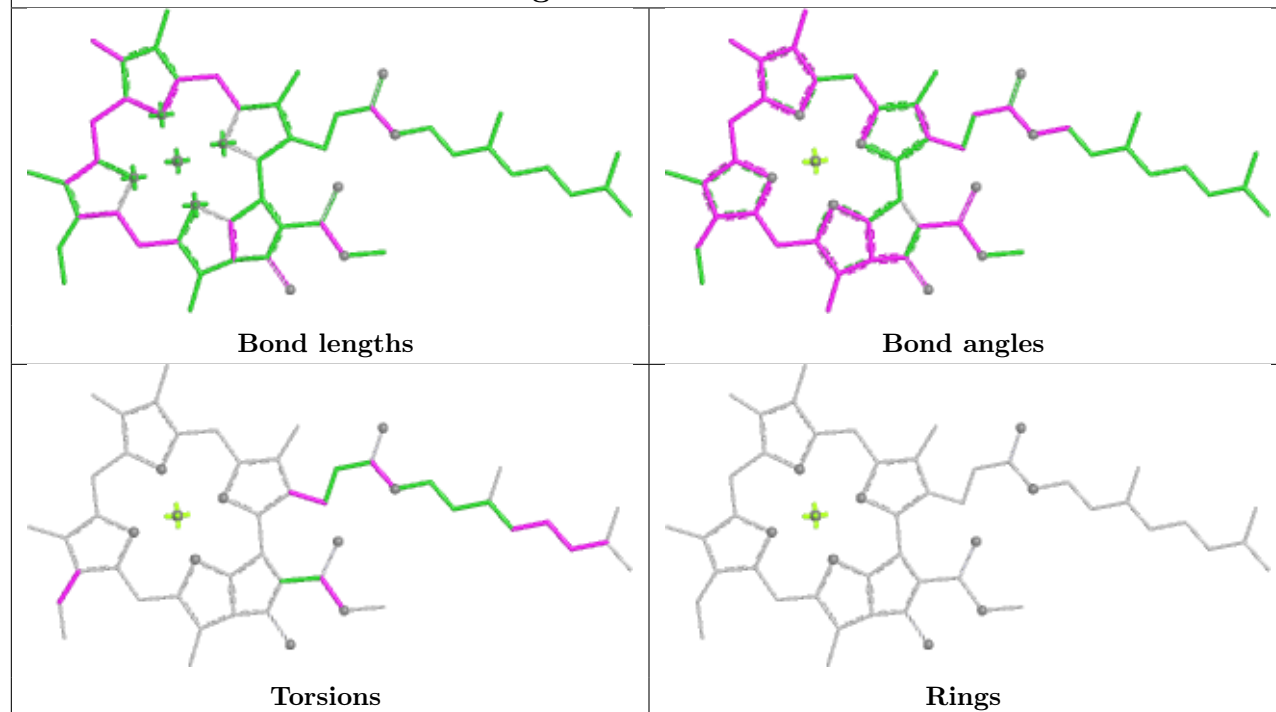


Rings

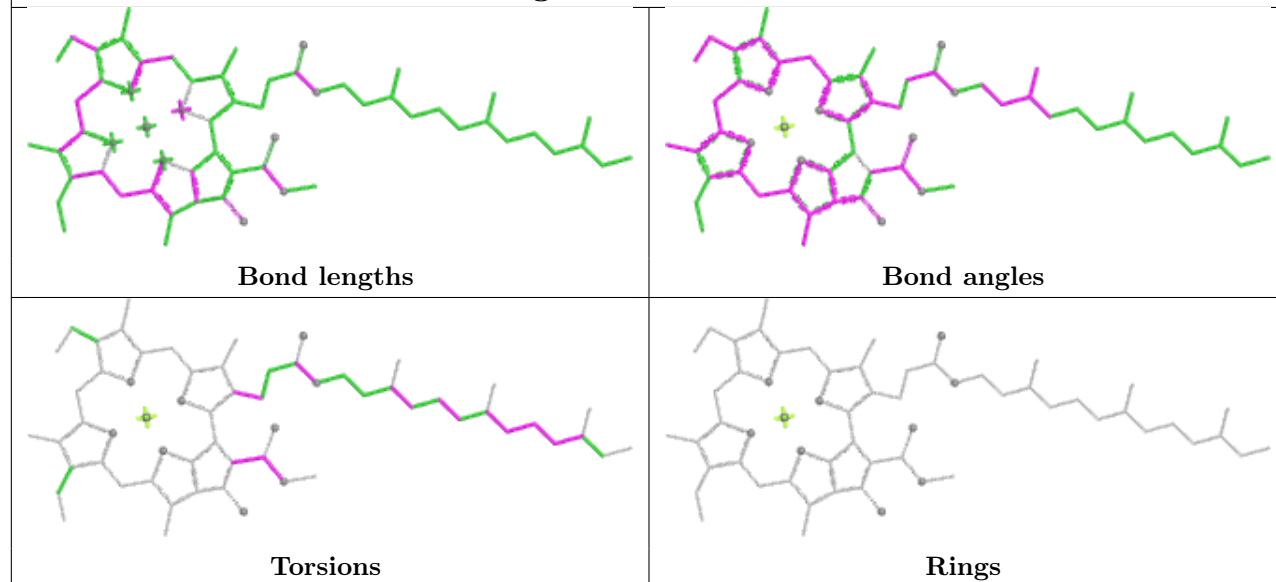
Ligand CLA A 839**Ligand CLA A 850**



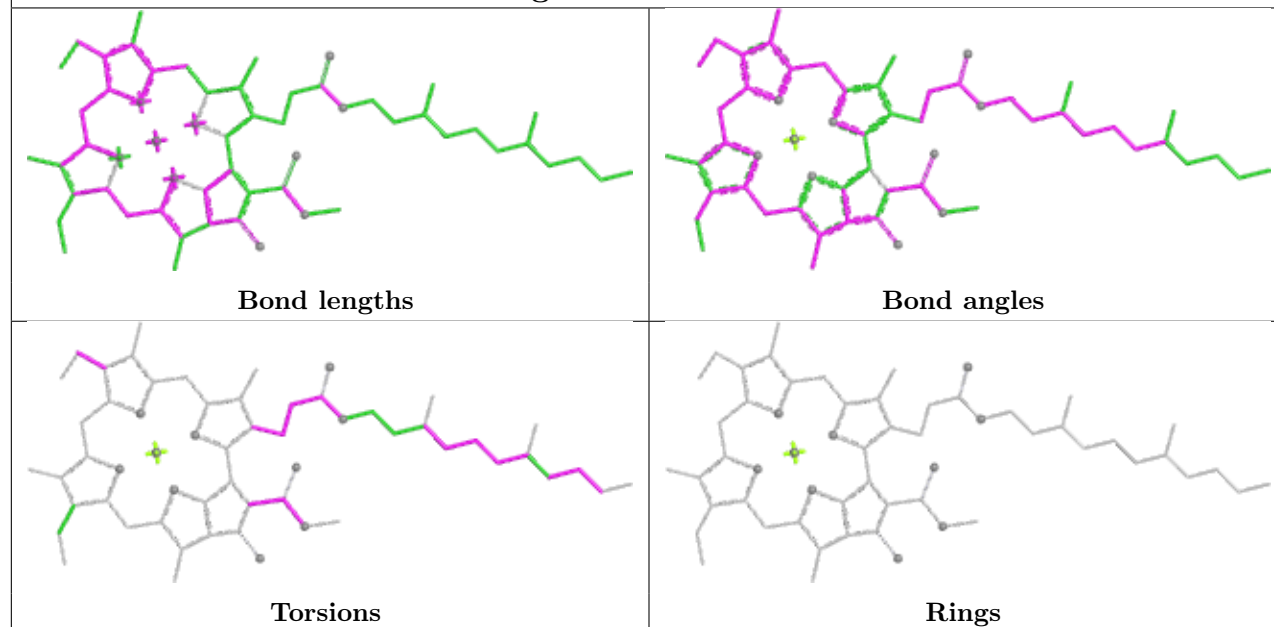
Ligand CLA B 809



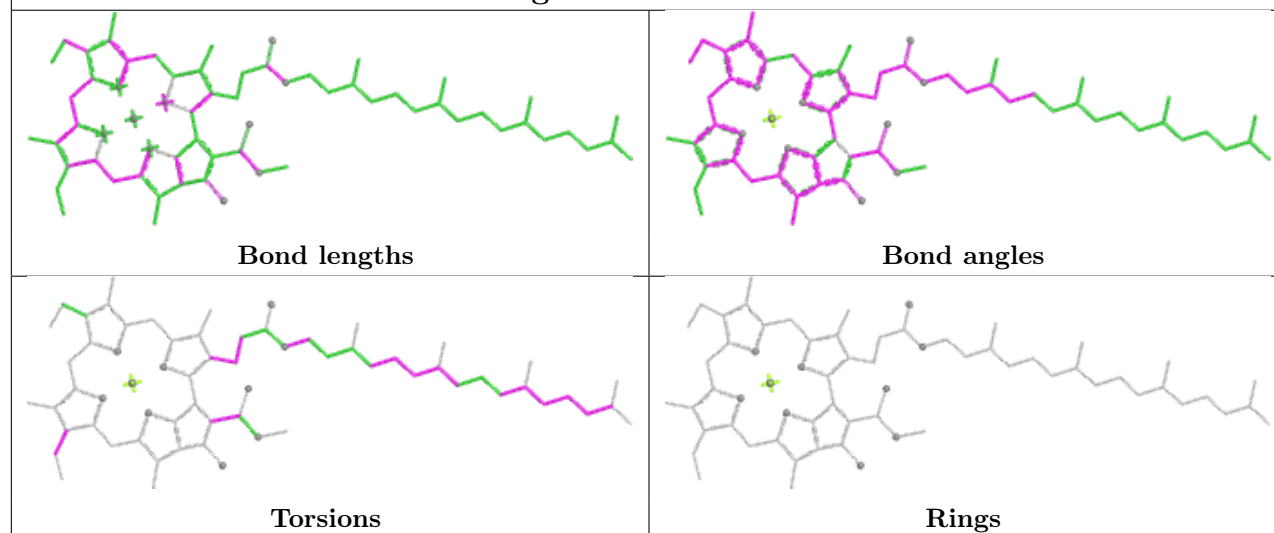
Ligand CLA B 817

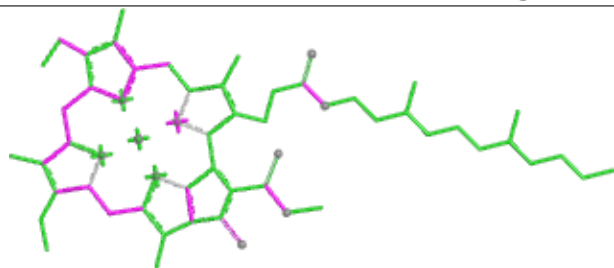


Ligand CLA R 108

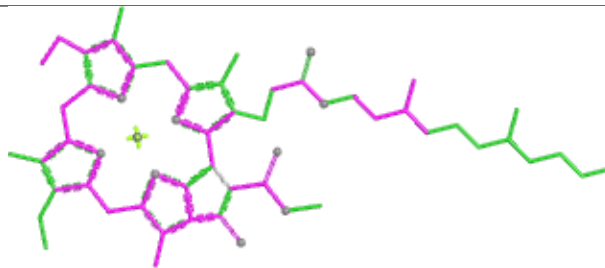


Ligand CLA A 808

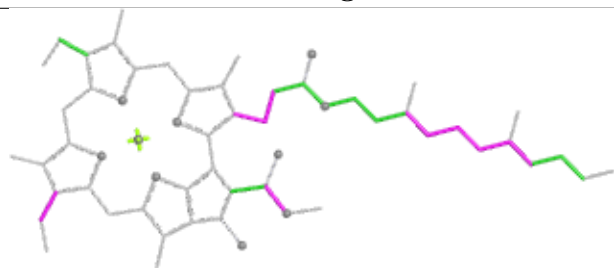


Ligand CLA B 823

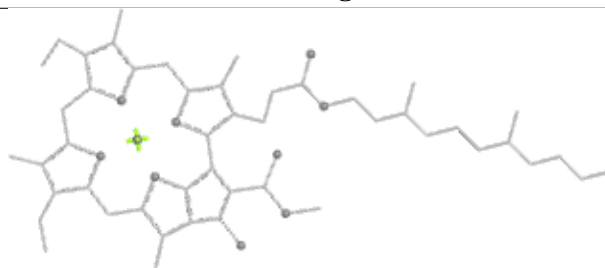
Bond lengths



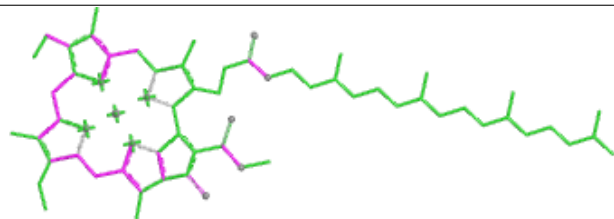
Bond angles



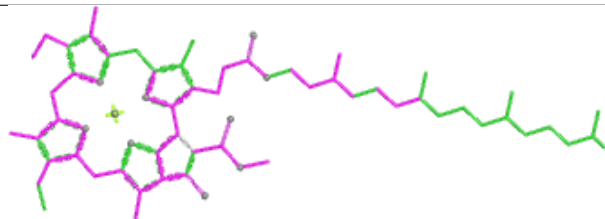
Torsions



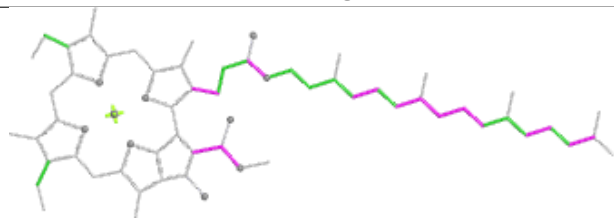
Rings

Ligand CLA A 828

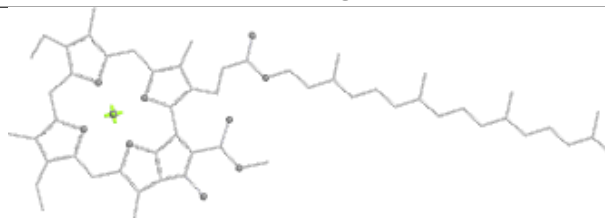
Bond lengths



Bond angles

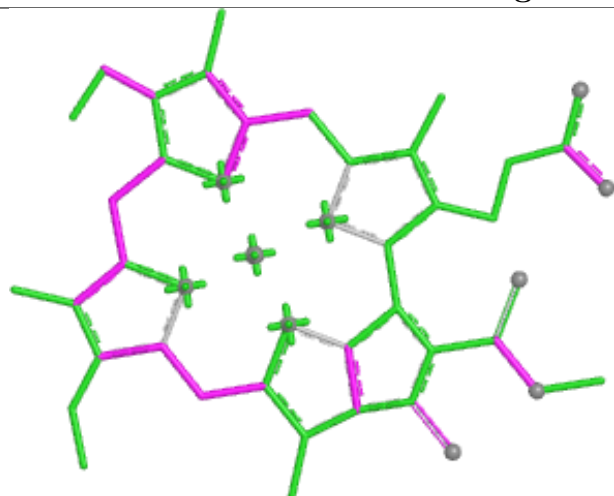


Torsions

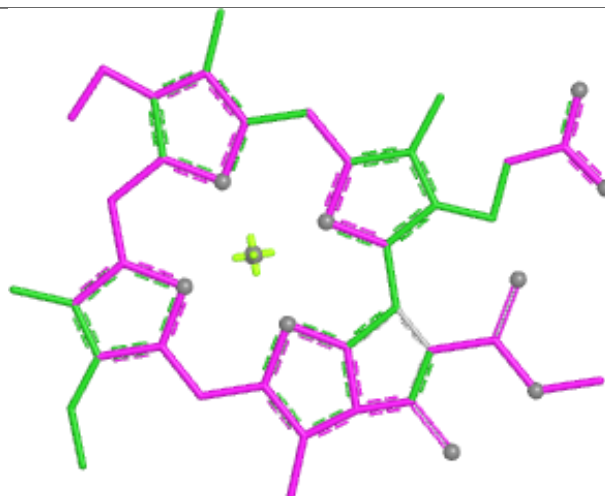


Rings

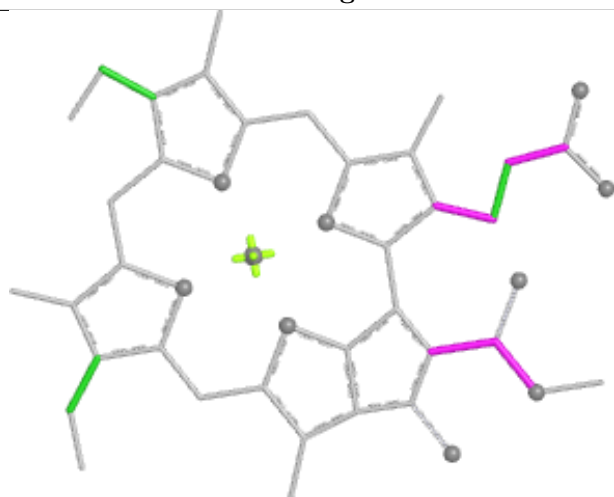
Ligand CLA B 833



Bond lengths



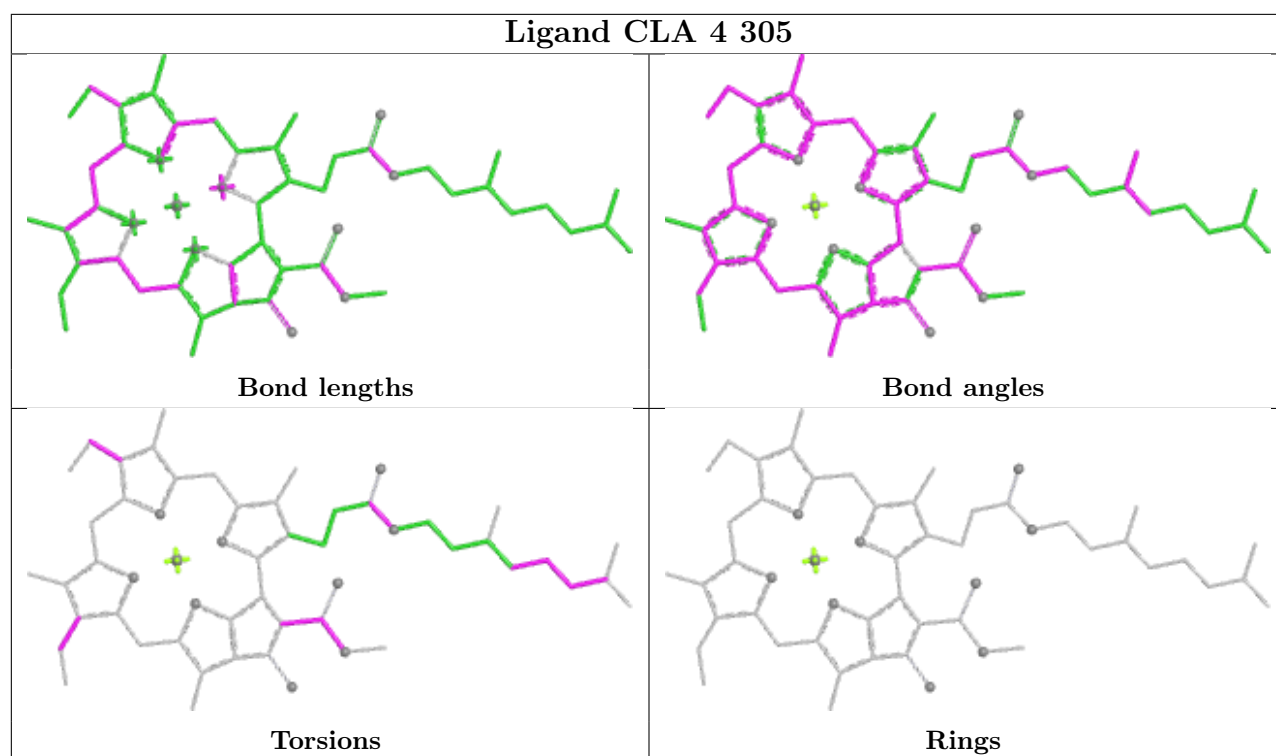
Bond angles



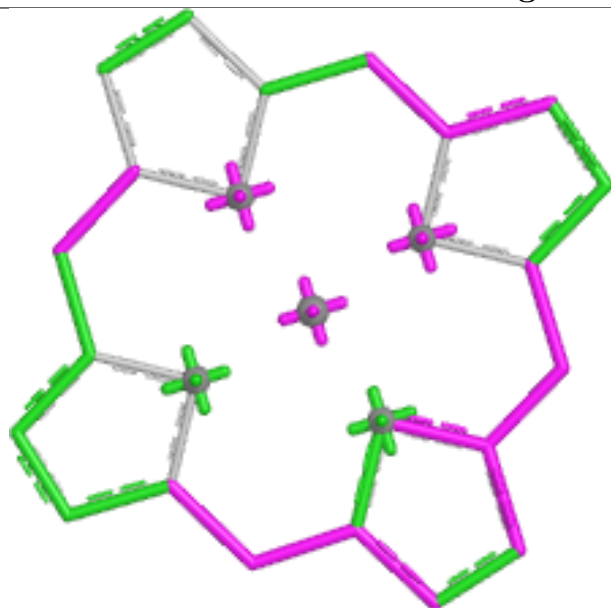
Torsions



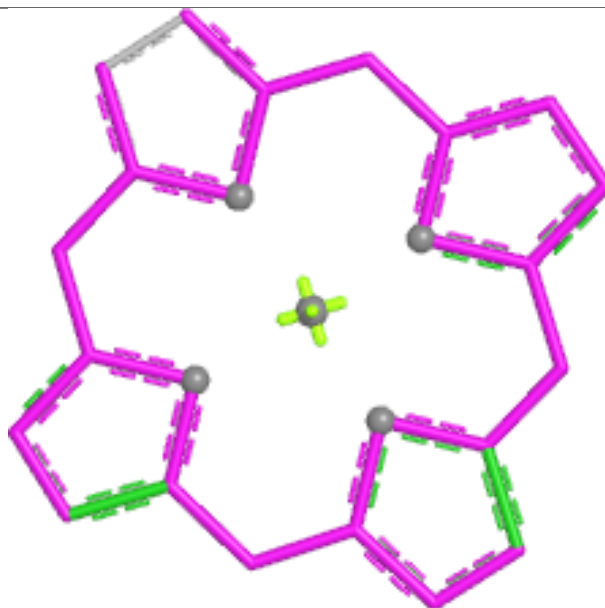
Rings



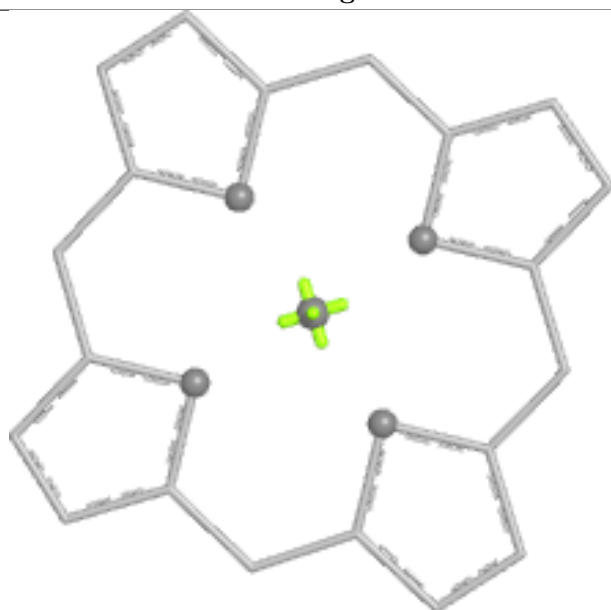
Ligand CLA 3 312



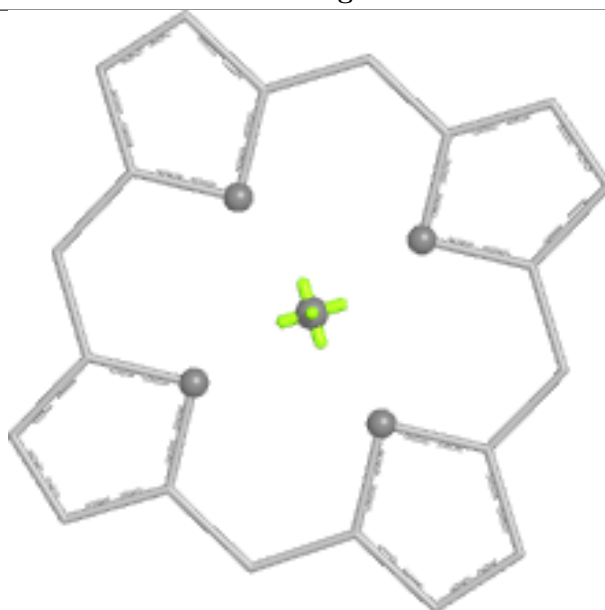
Bond lengths



Bond angles

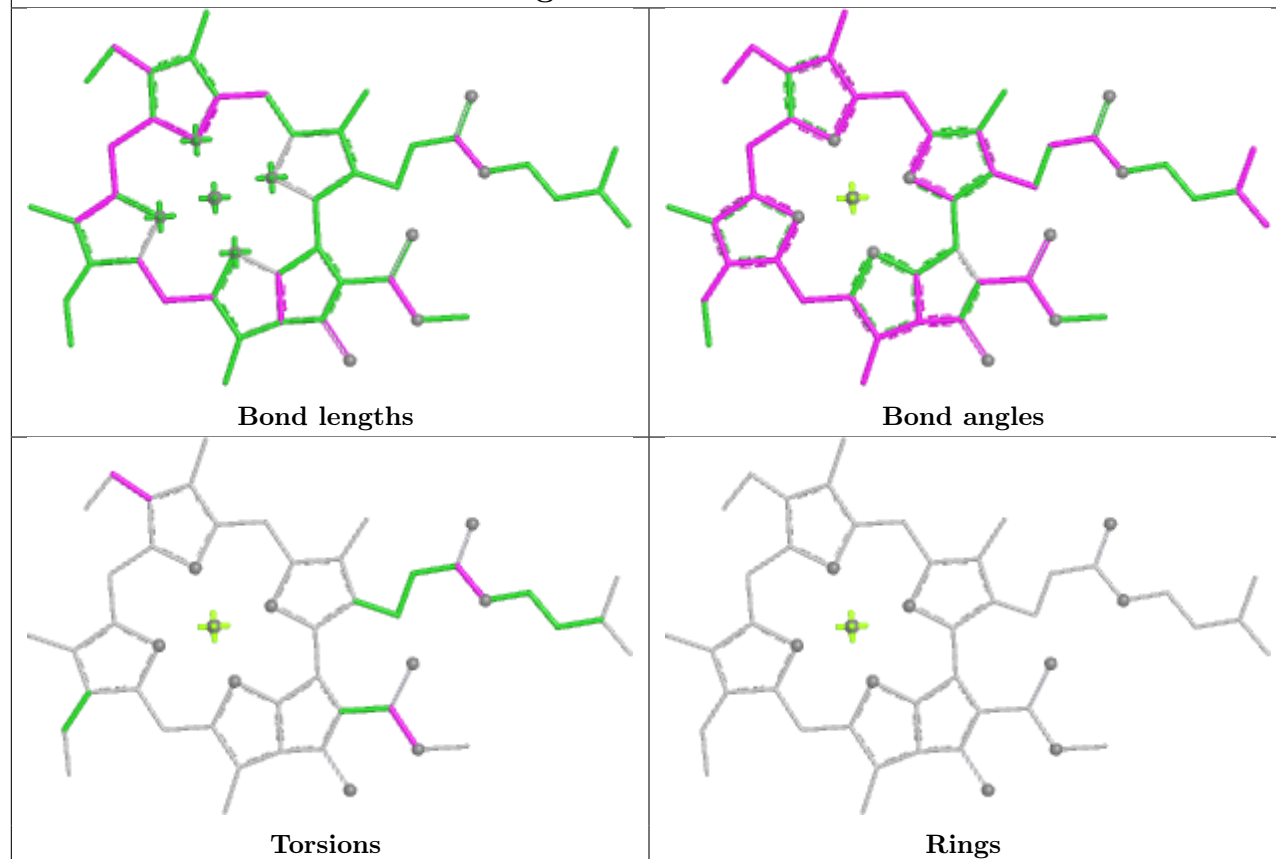


Torsions

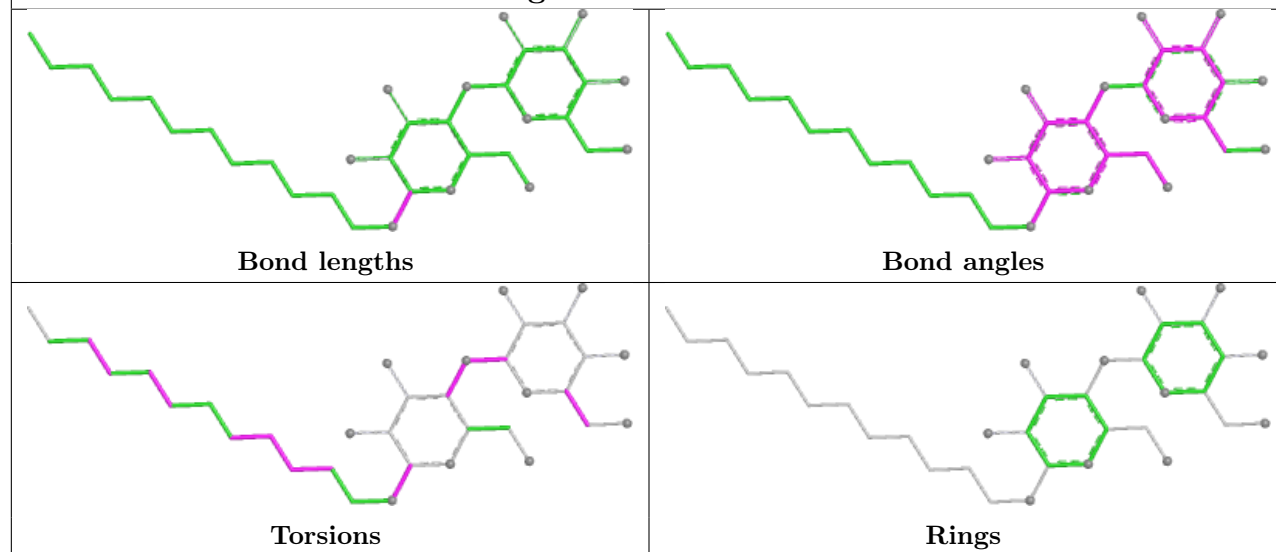


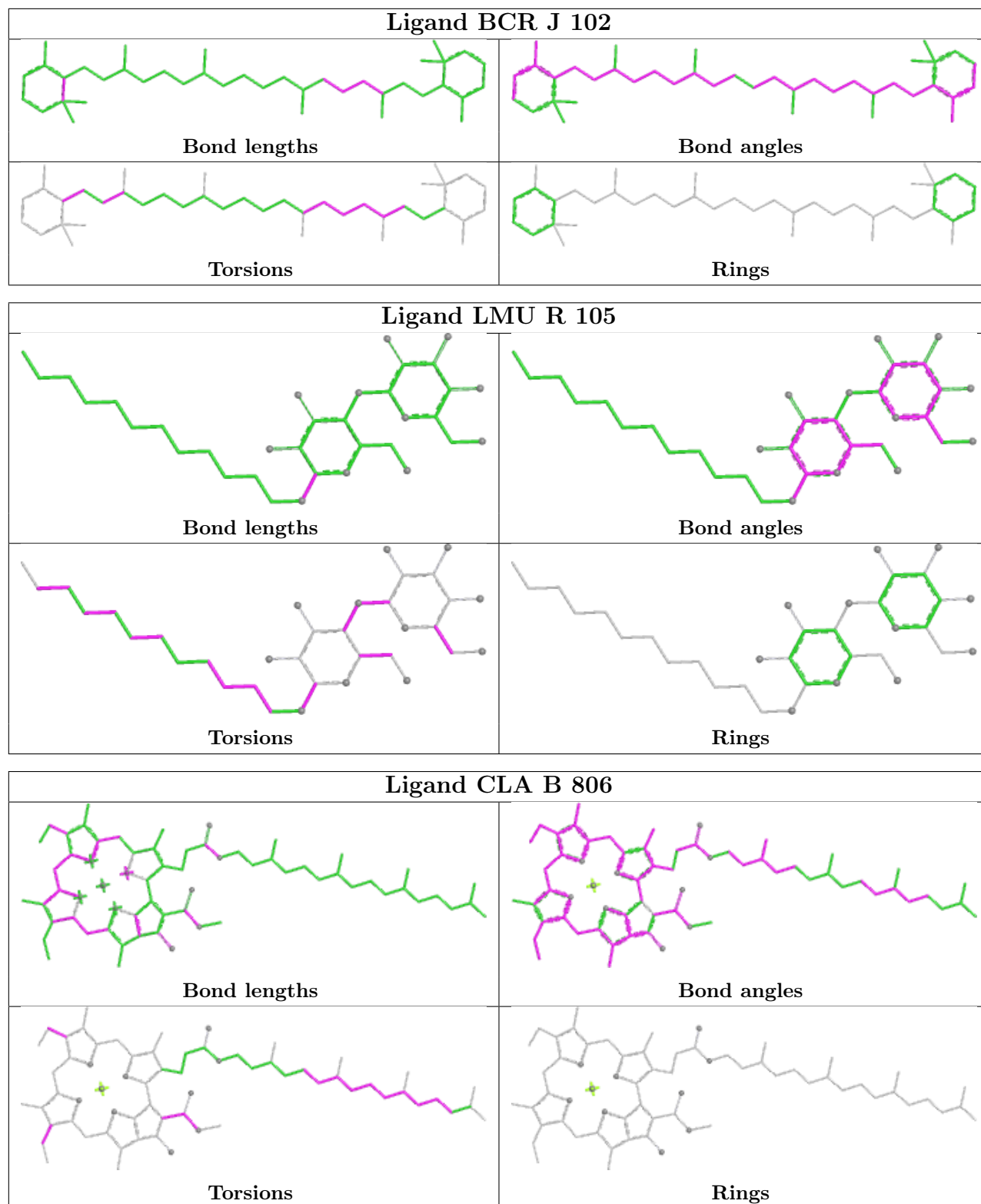
Rings

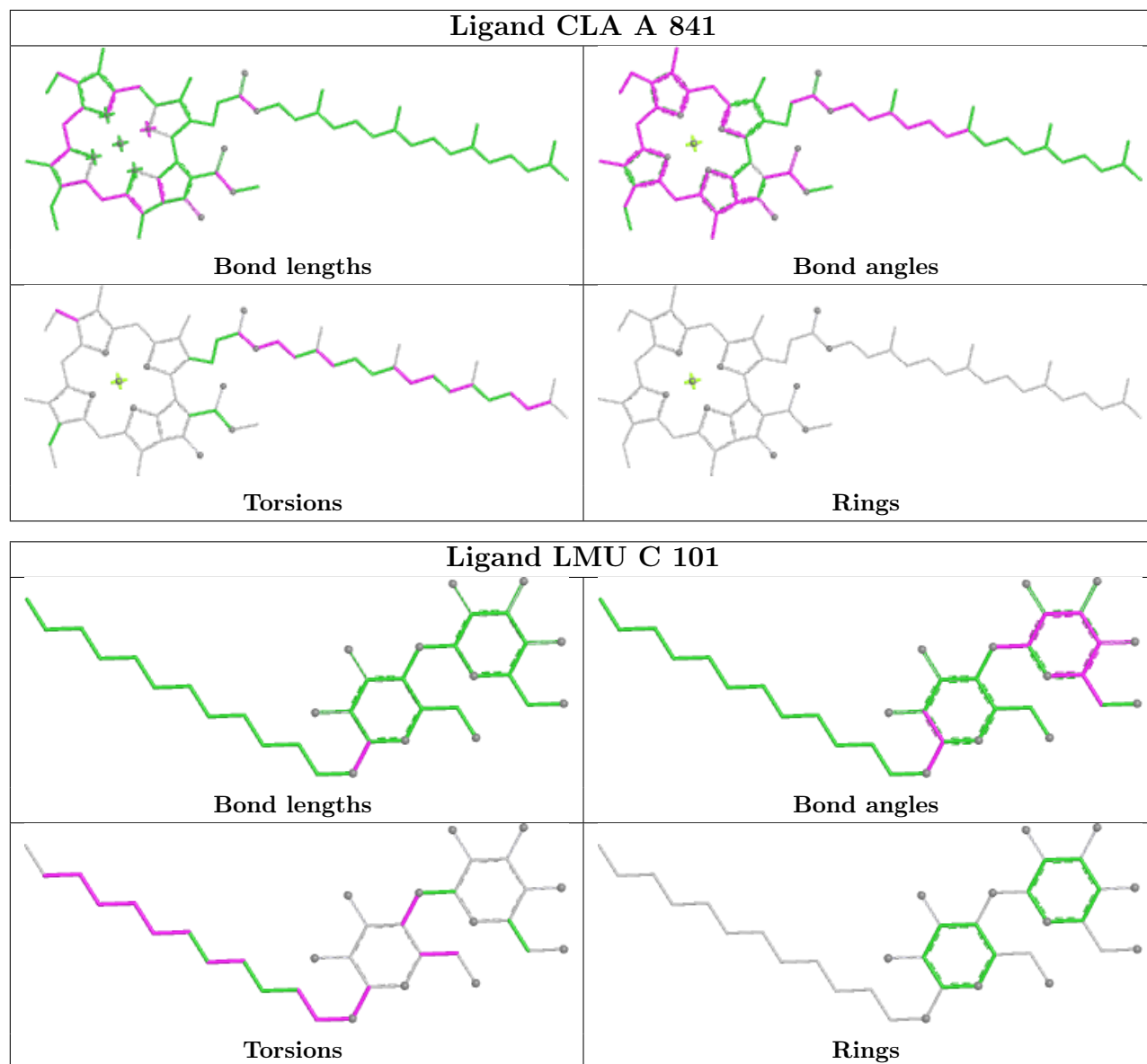
Ligand CLA 2 311

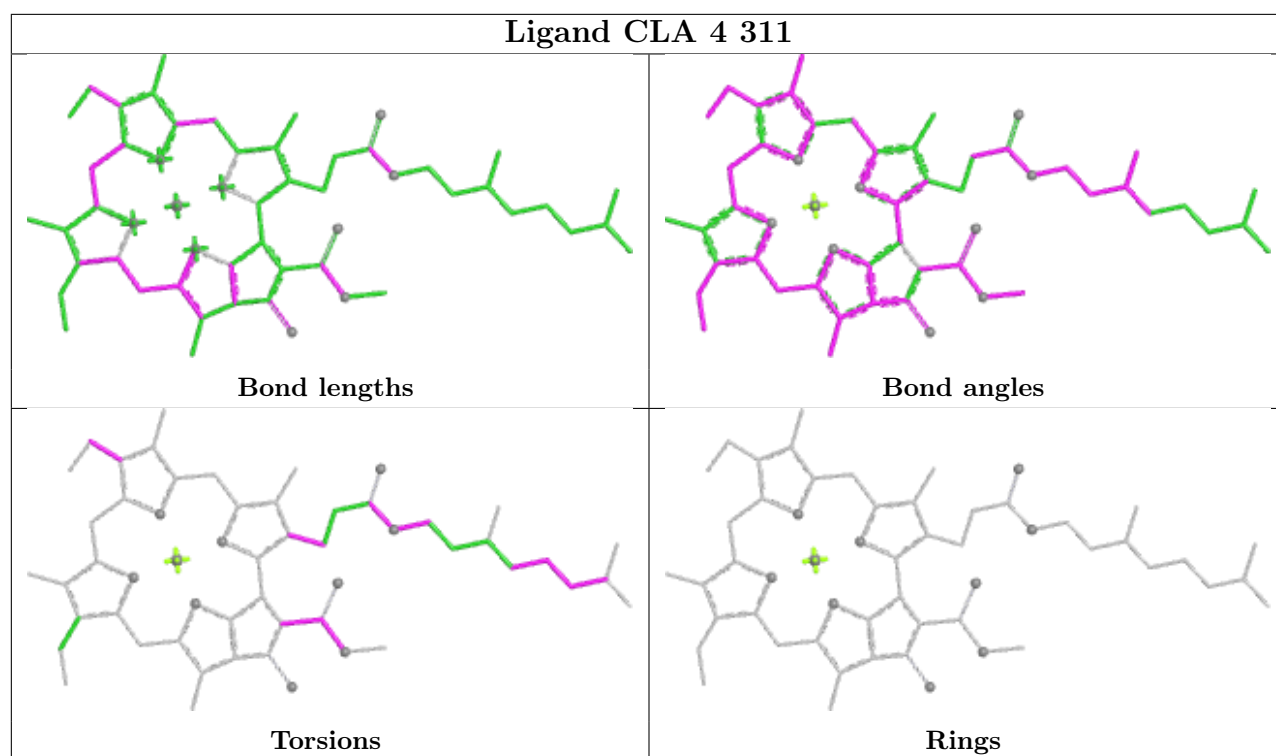


Ligand LMU B 847

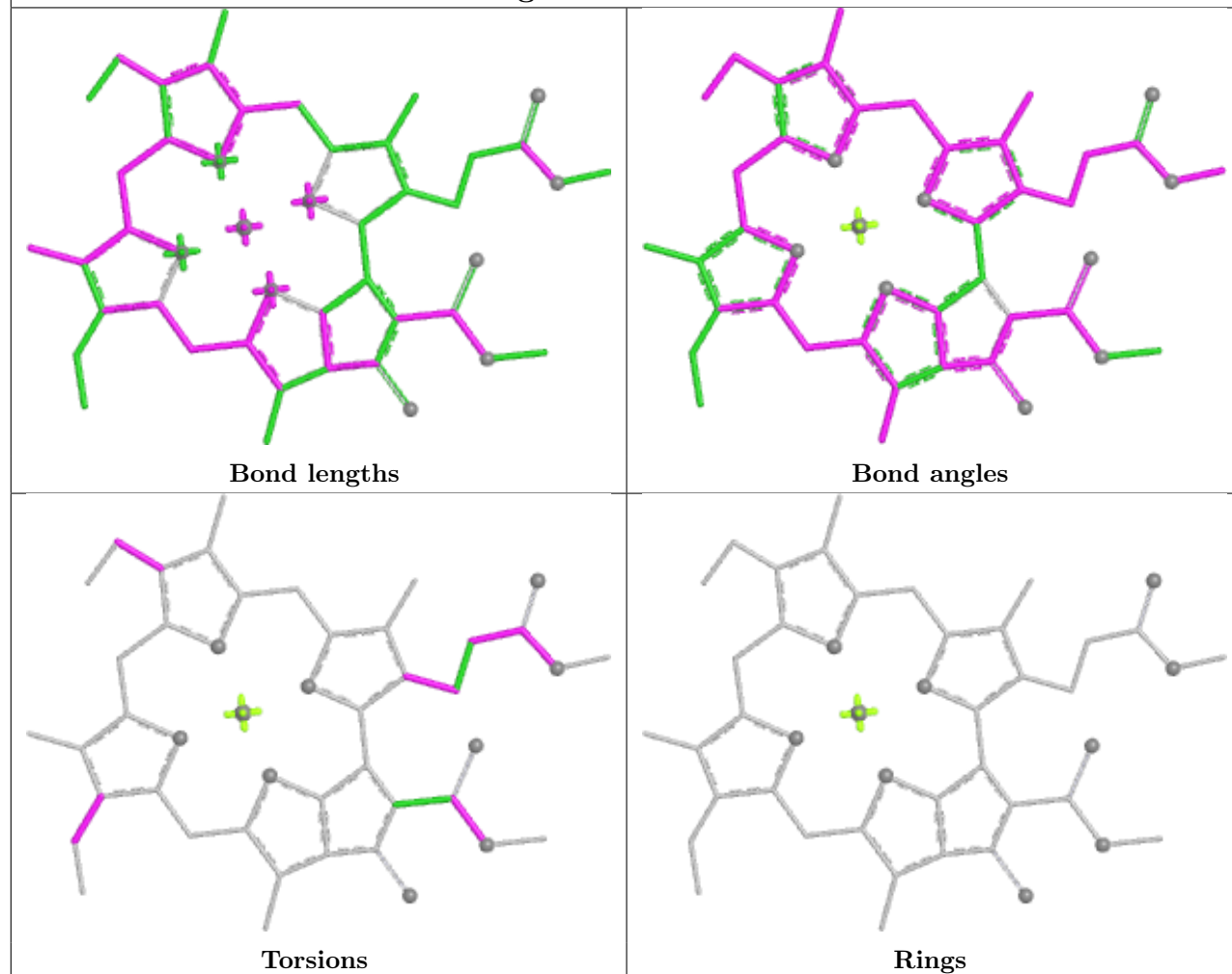




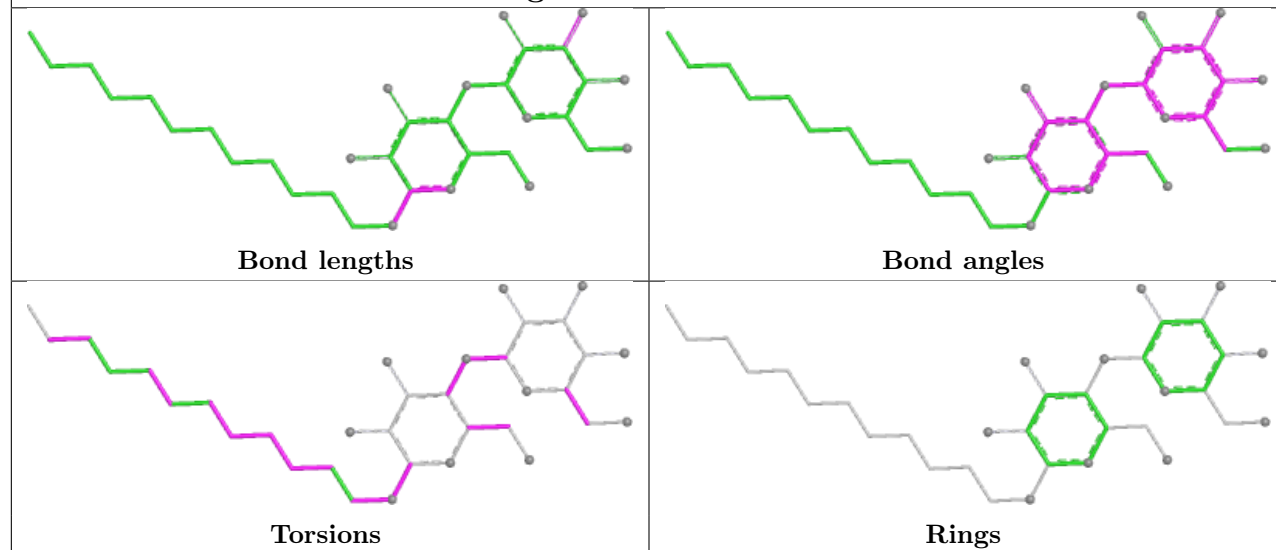


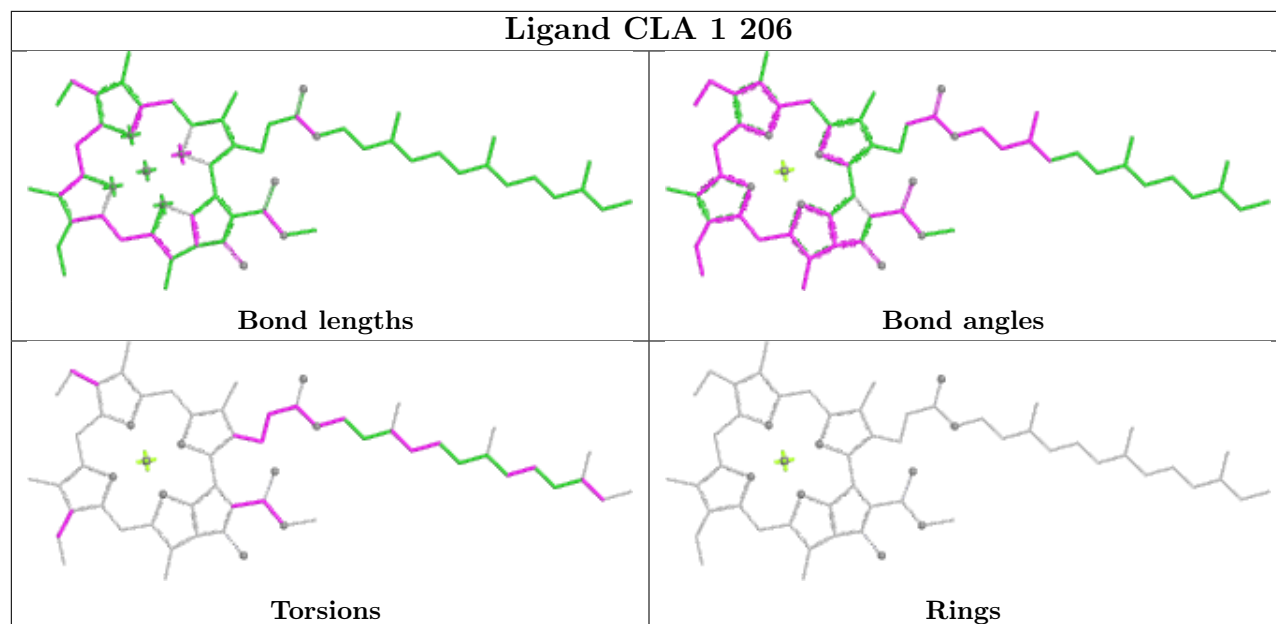
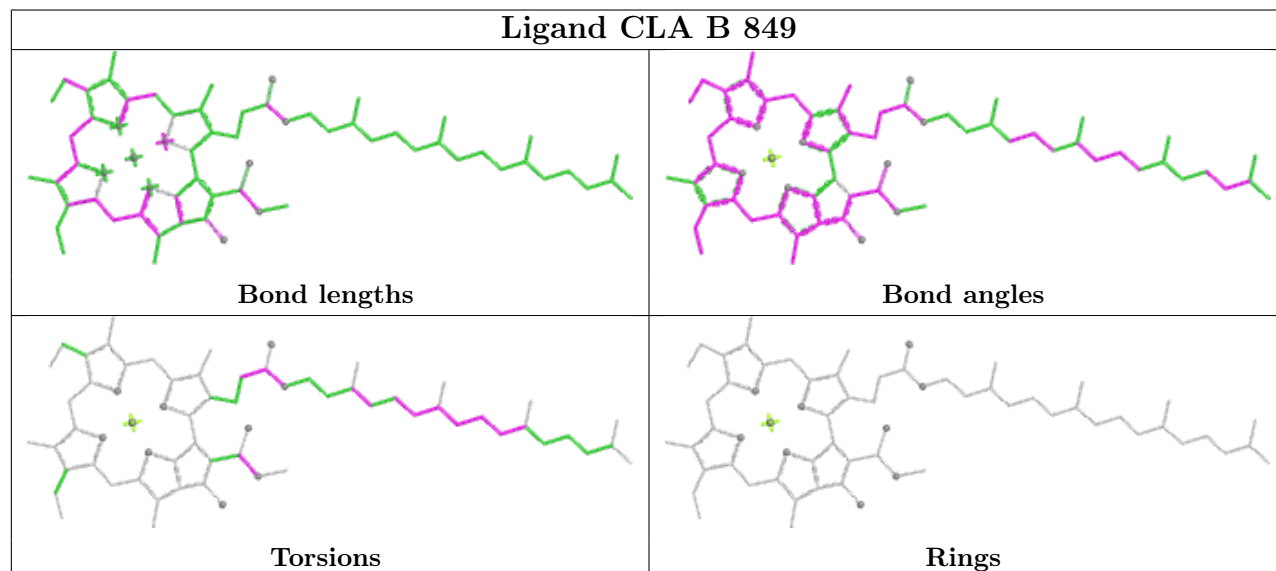


Ligand CLA 4 316

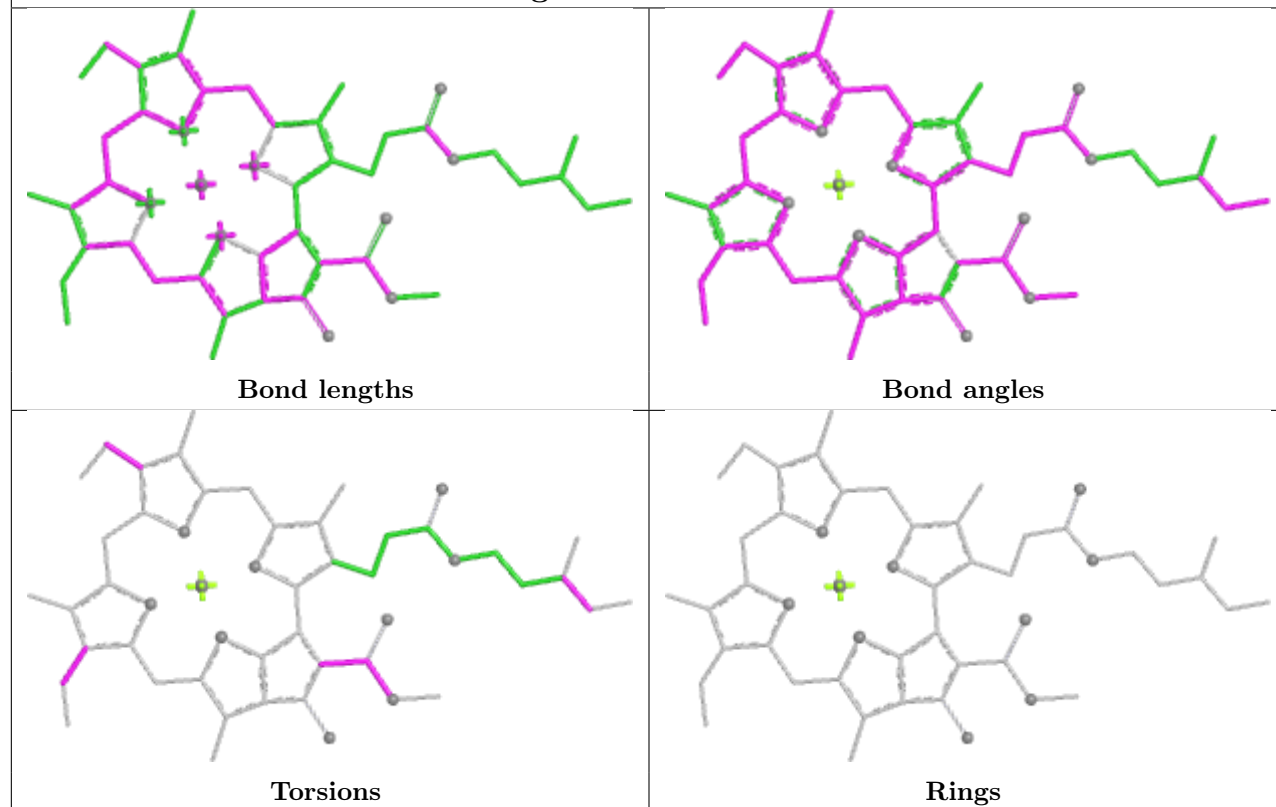


Ligand LMU H 104

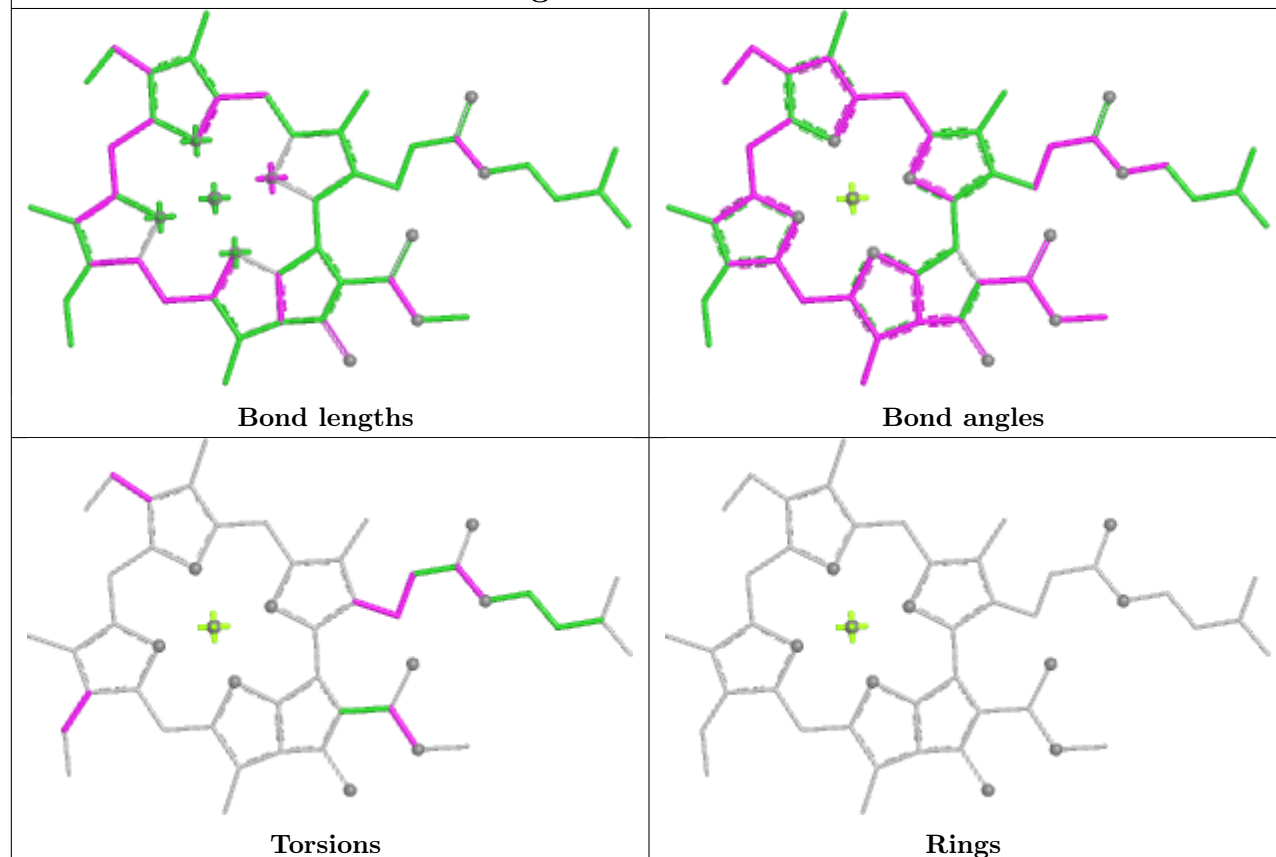


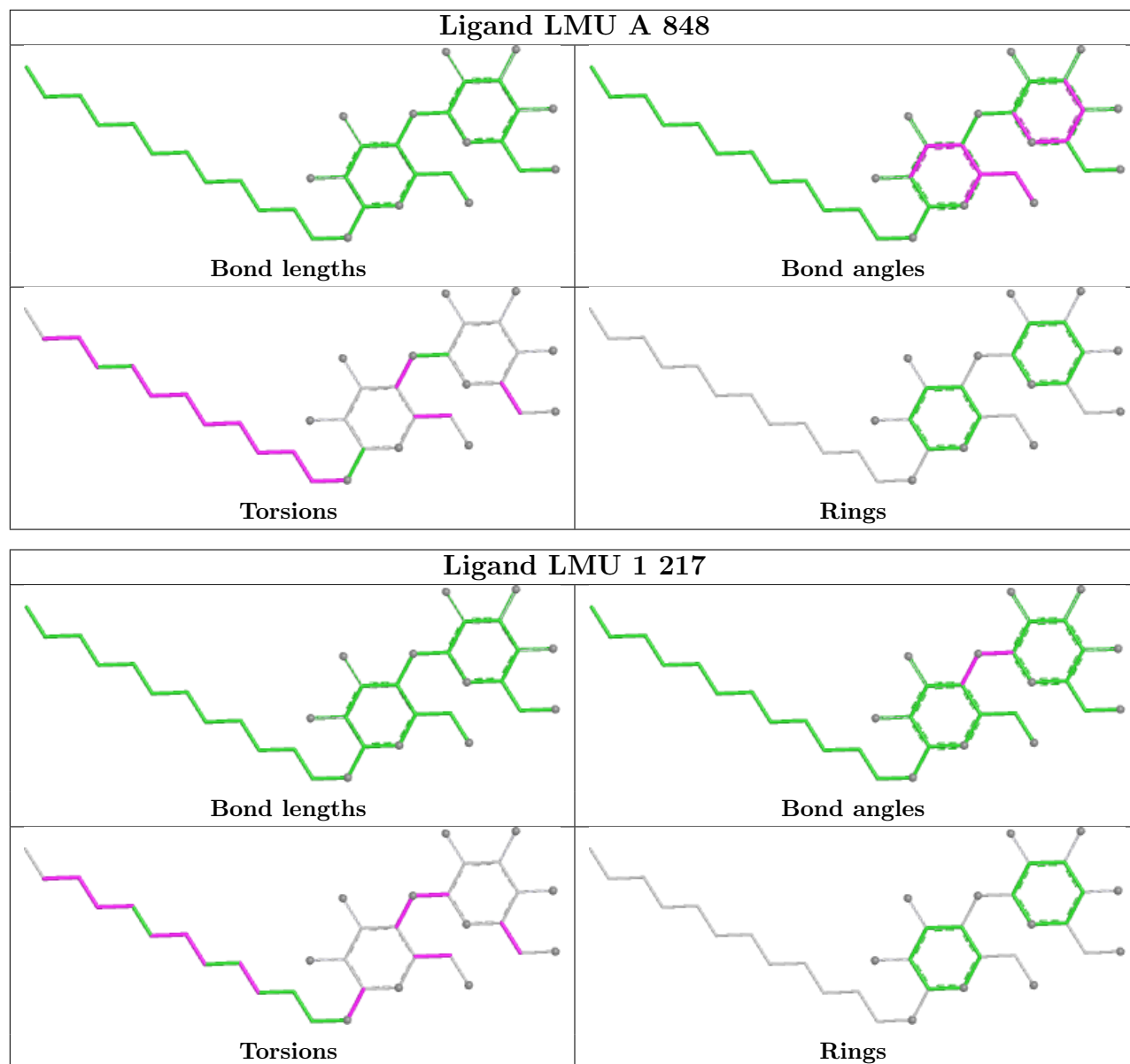
Ligand CLA 1 206**Ligand CLA B 849**

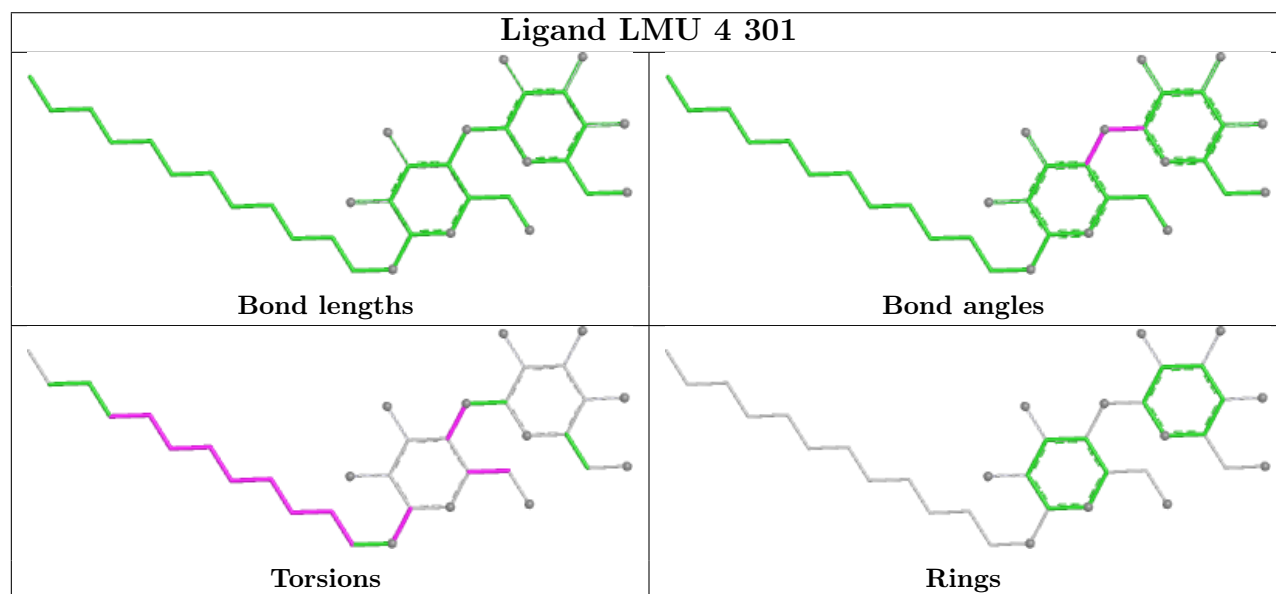
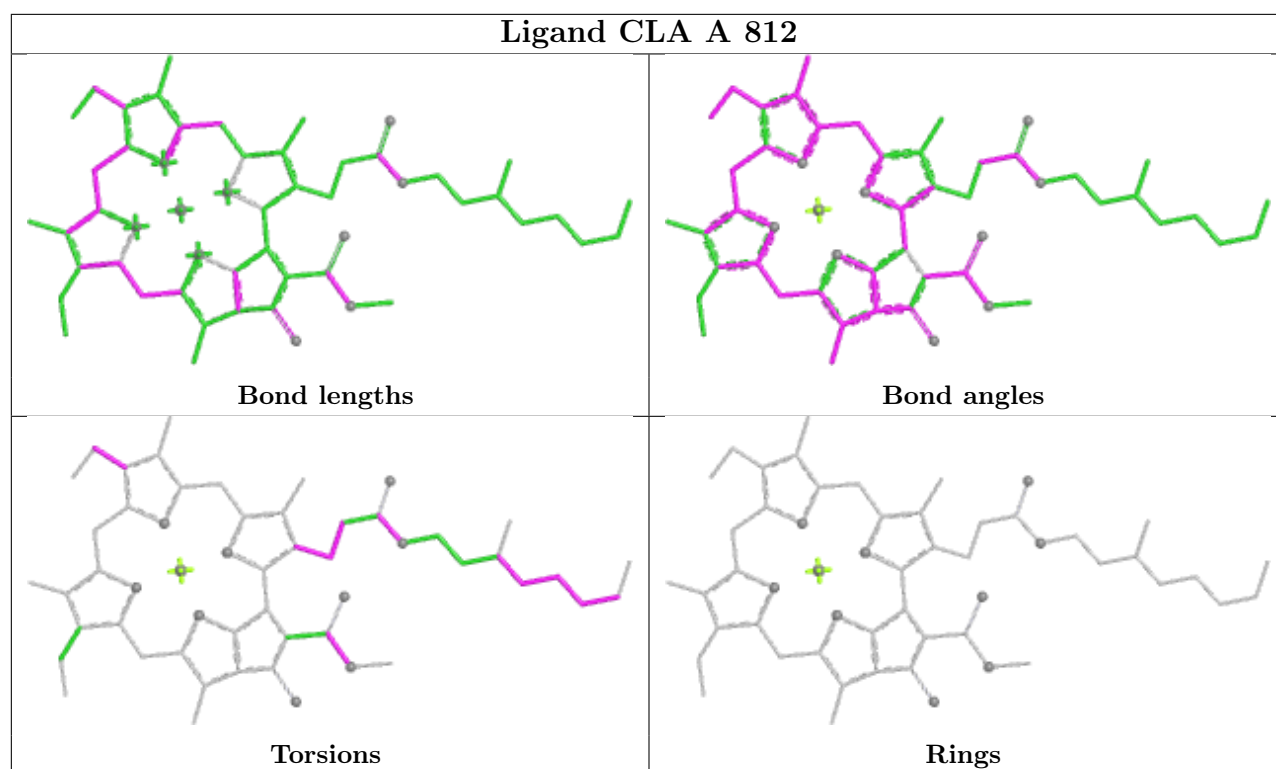
Ligand CLA G 102



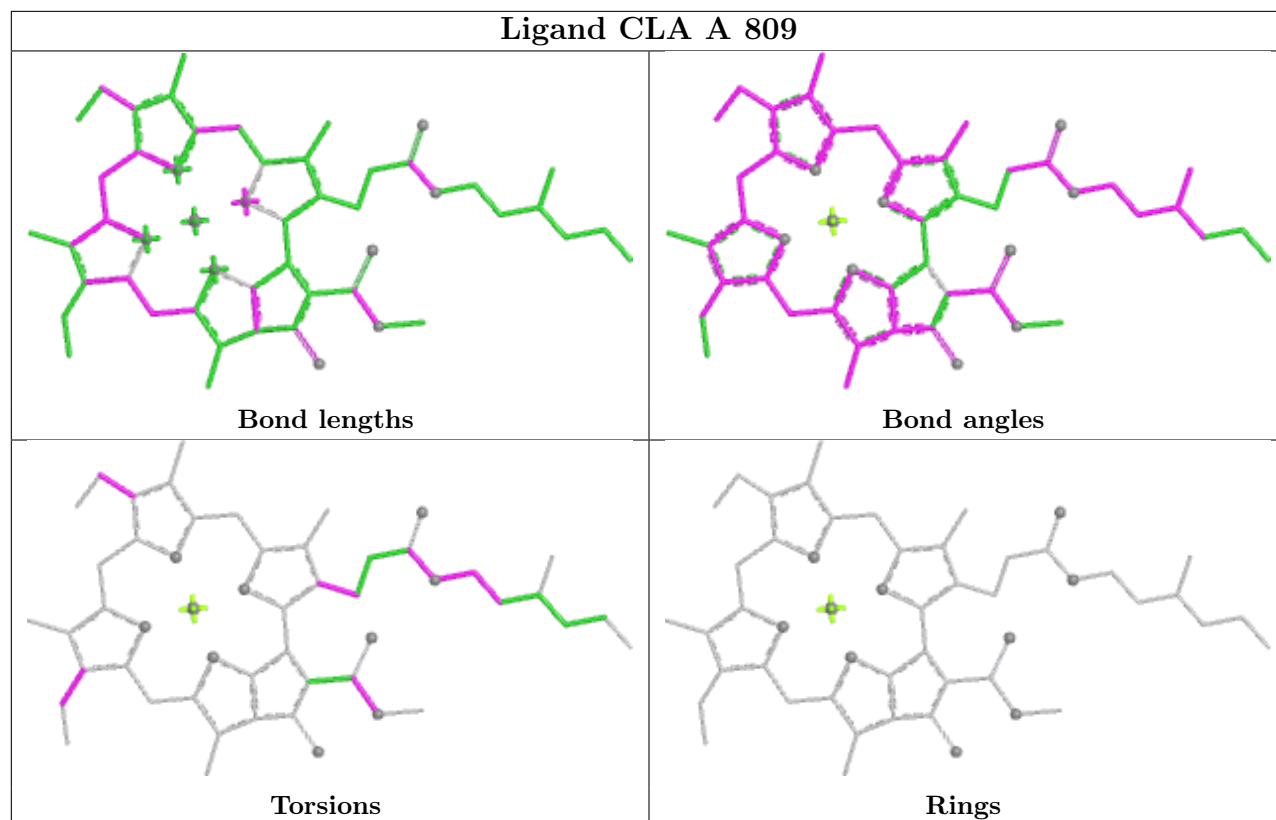
Ligand CLA H 111



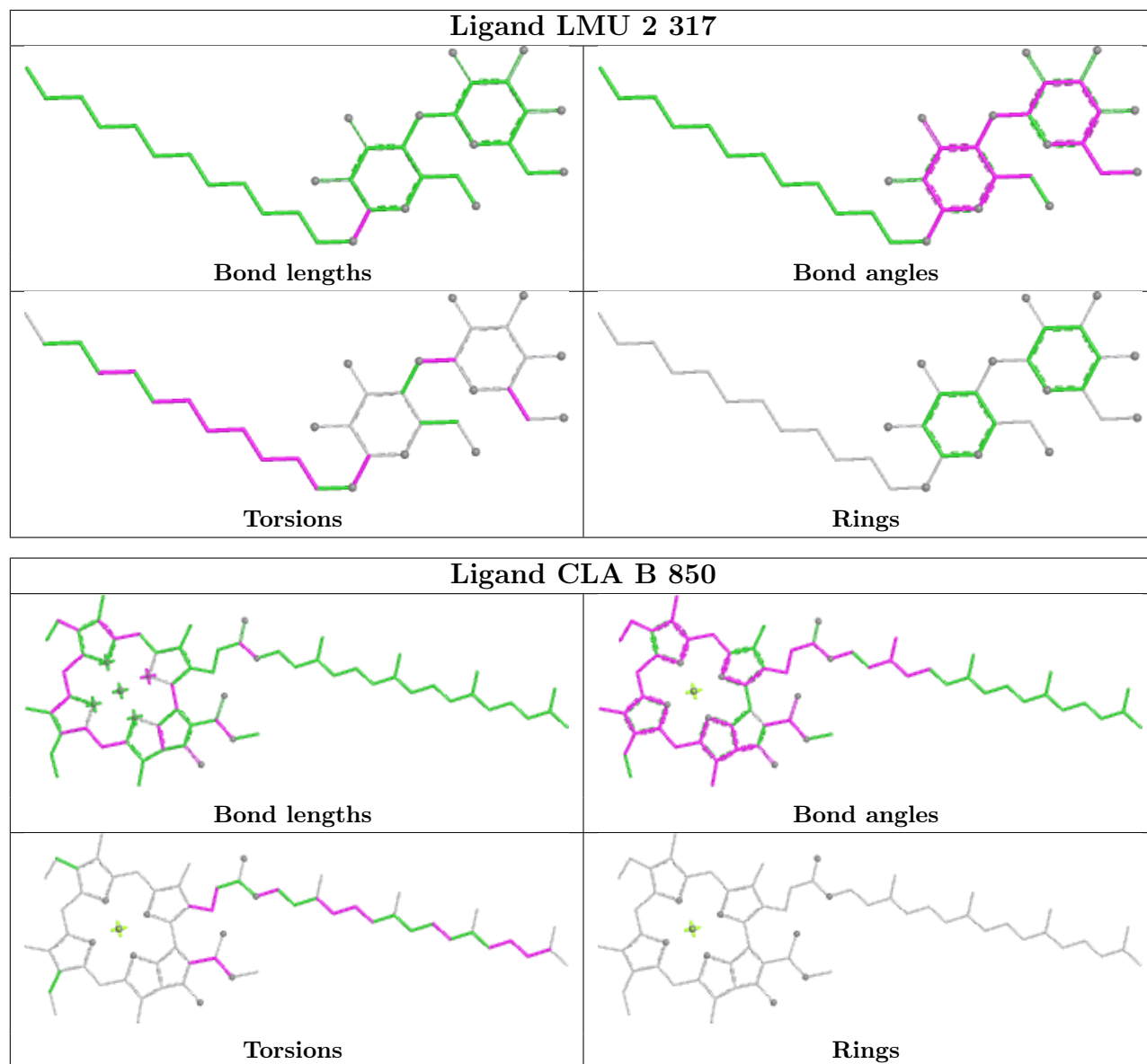


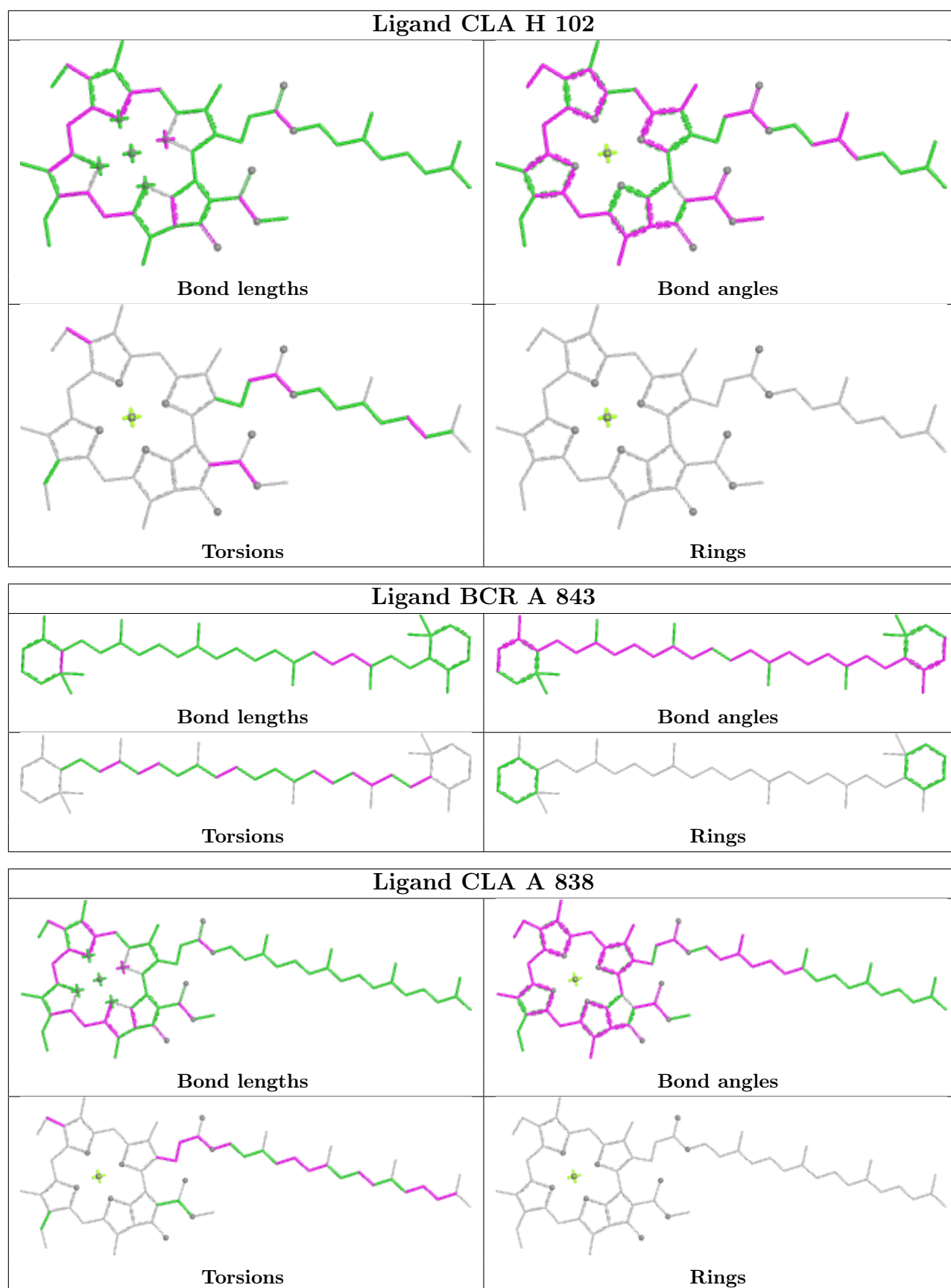


Ligand CLA A 809

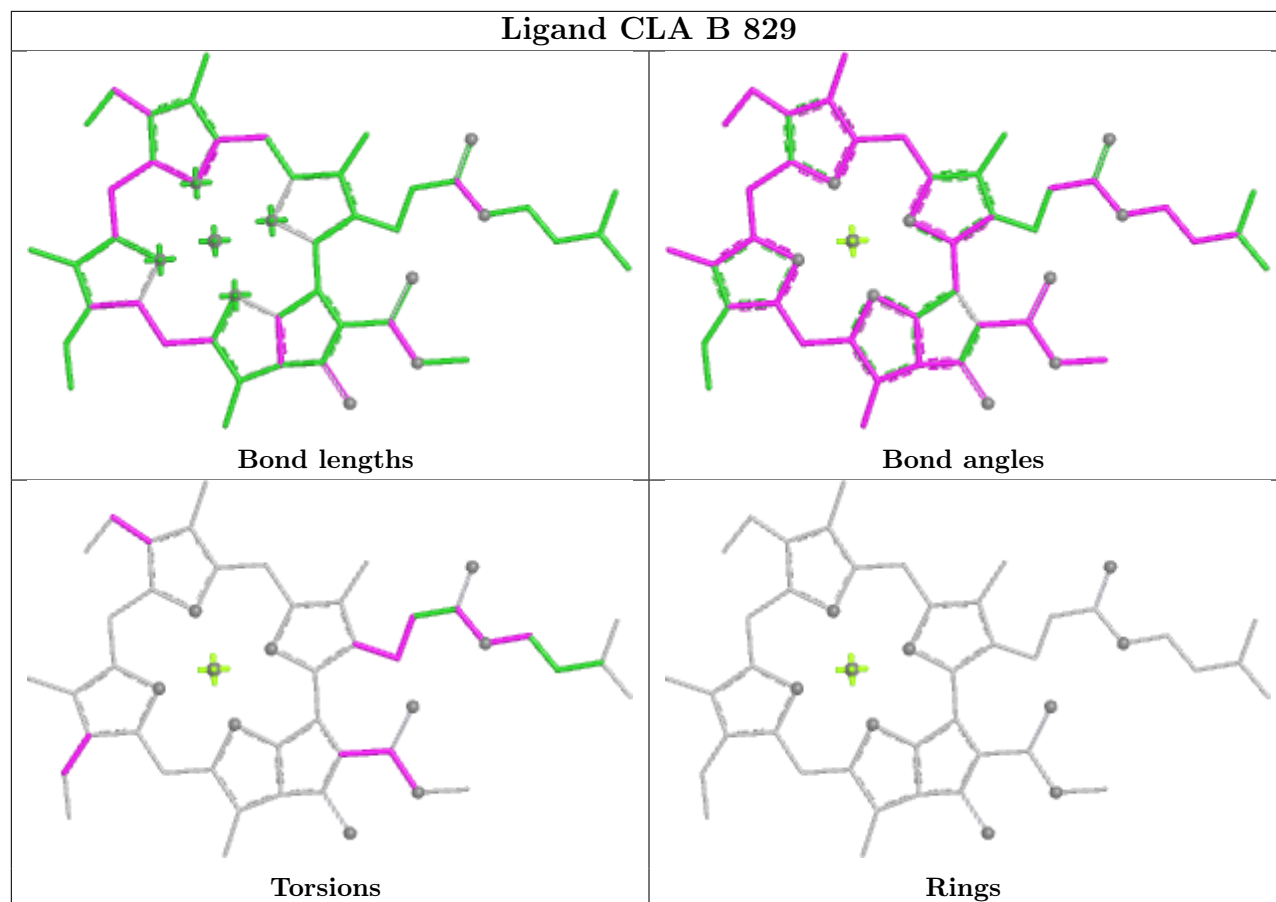


Ligand CLA 3 319	
Bond lengths	Bond angles
Torsions	Rings

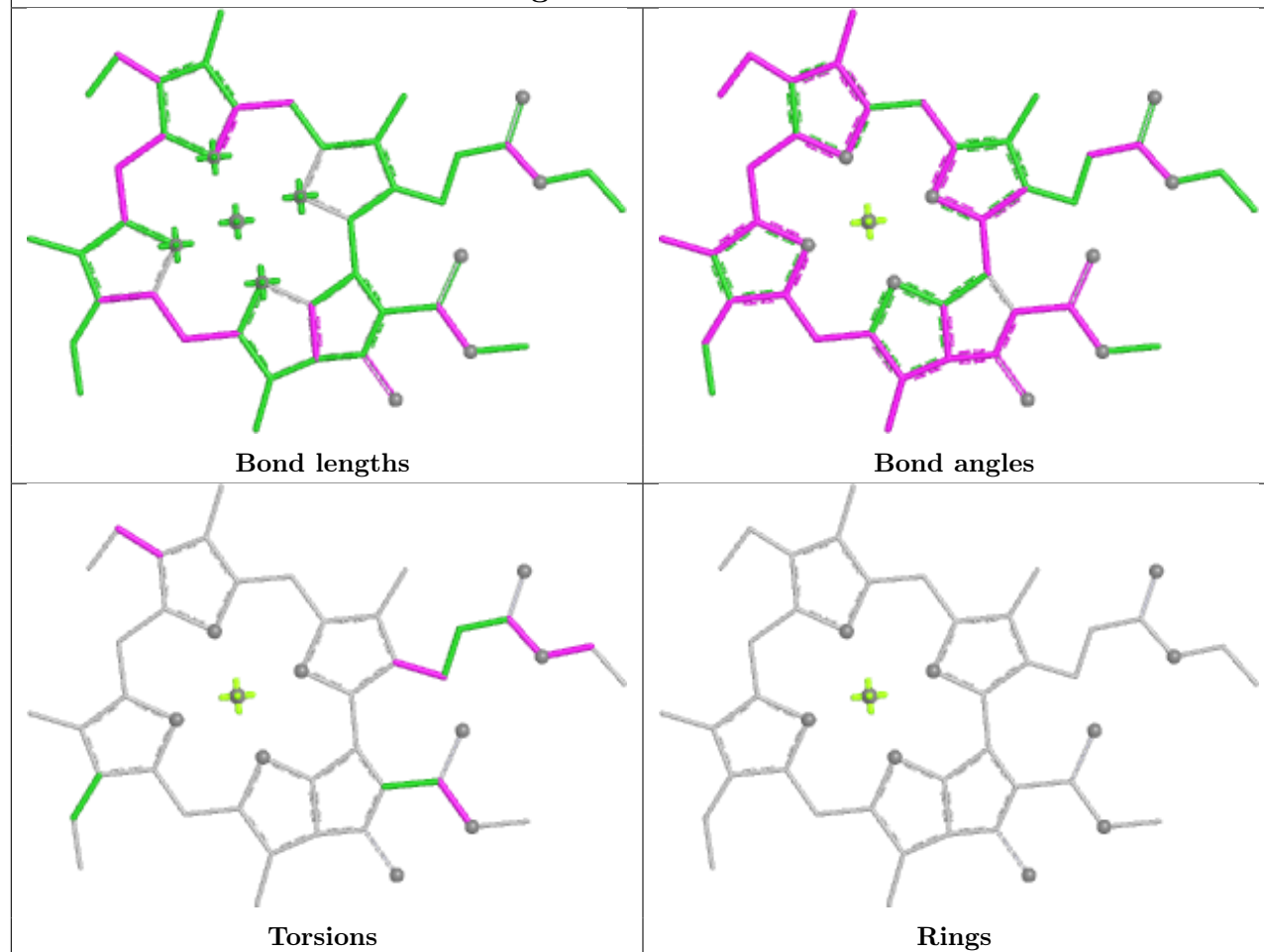




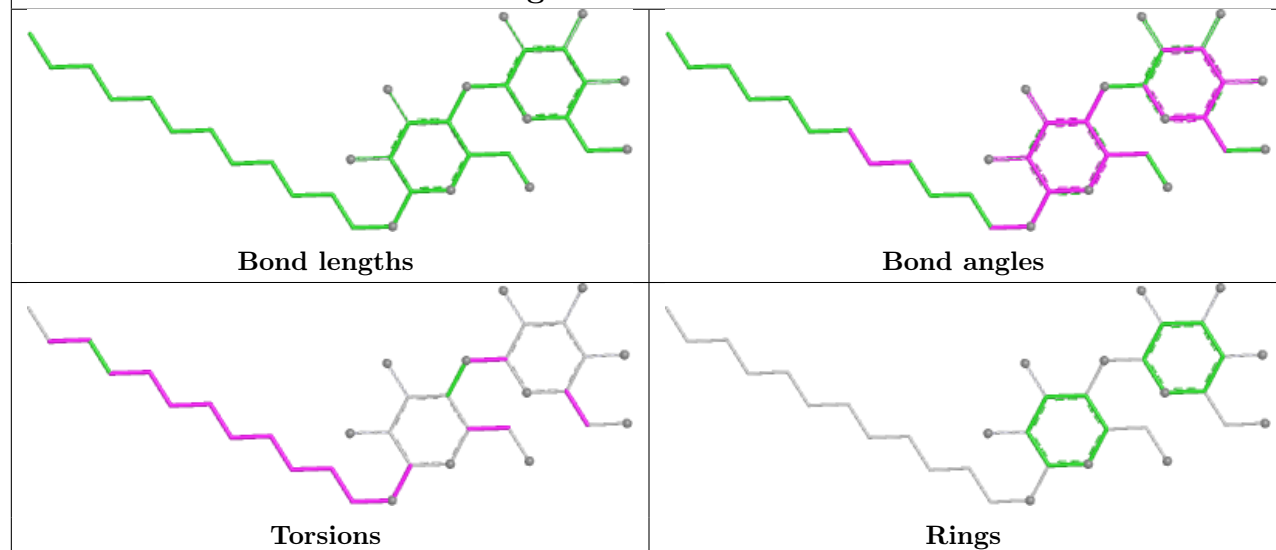
Ligand CLA B 829



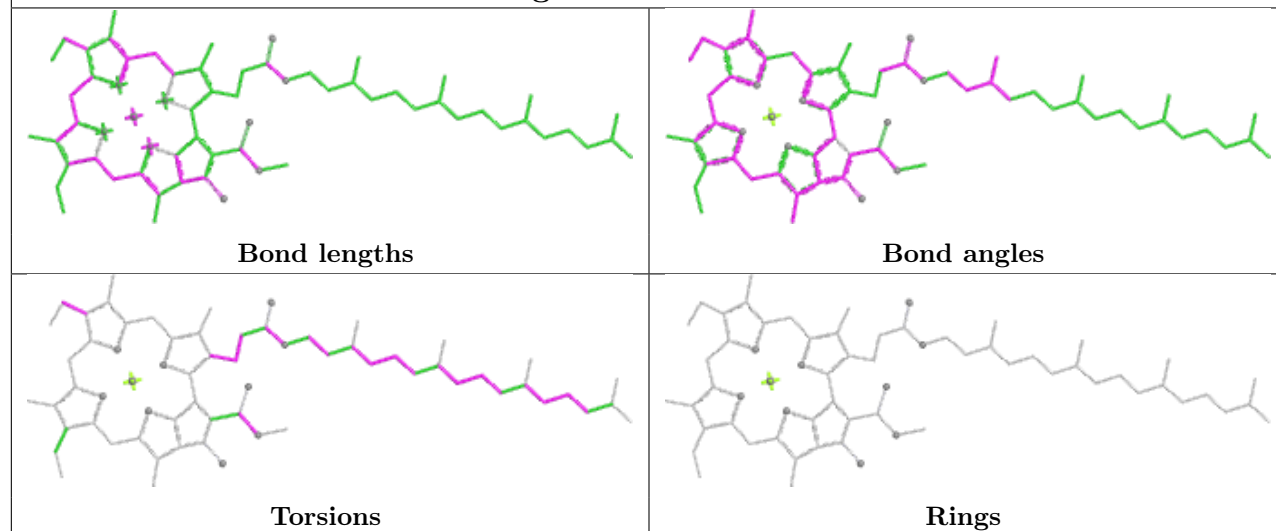
Ligand CLA 1 203



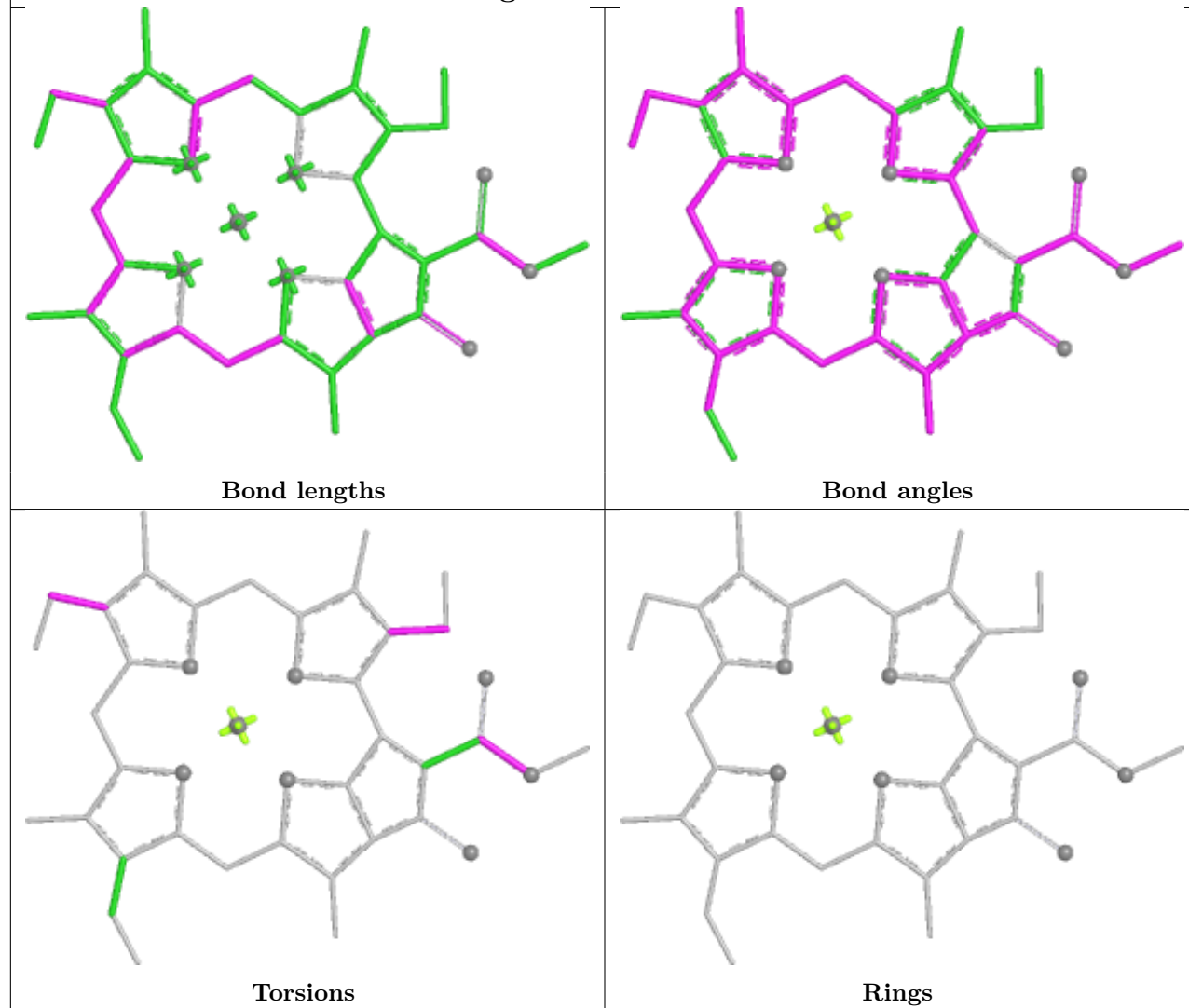
Ligand LMU K 106

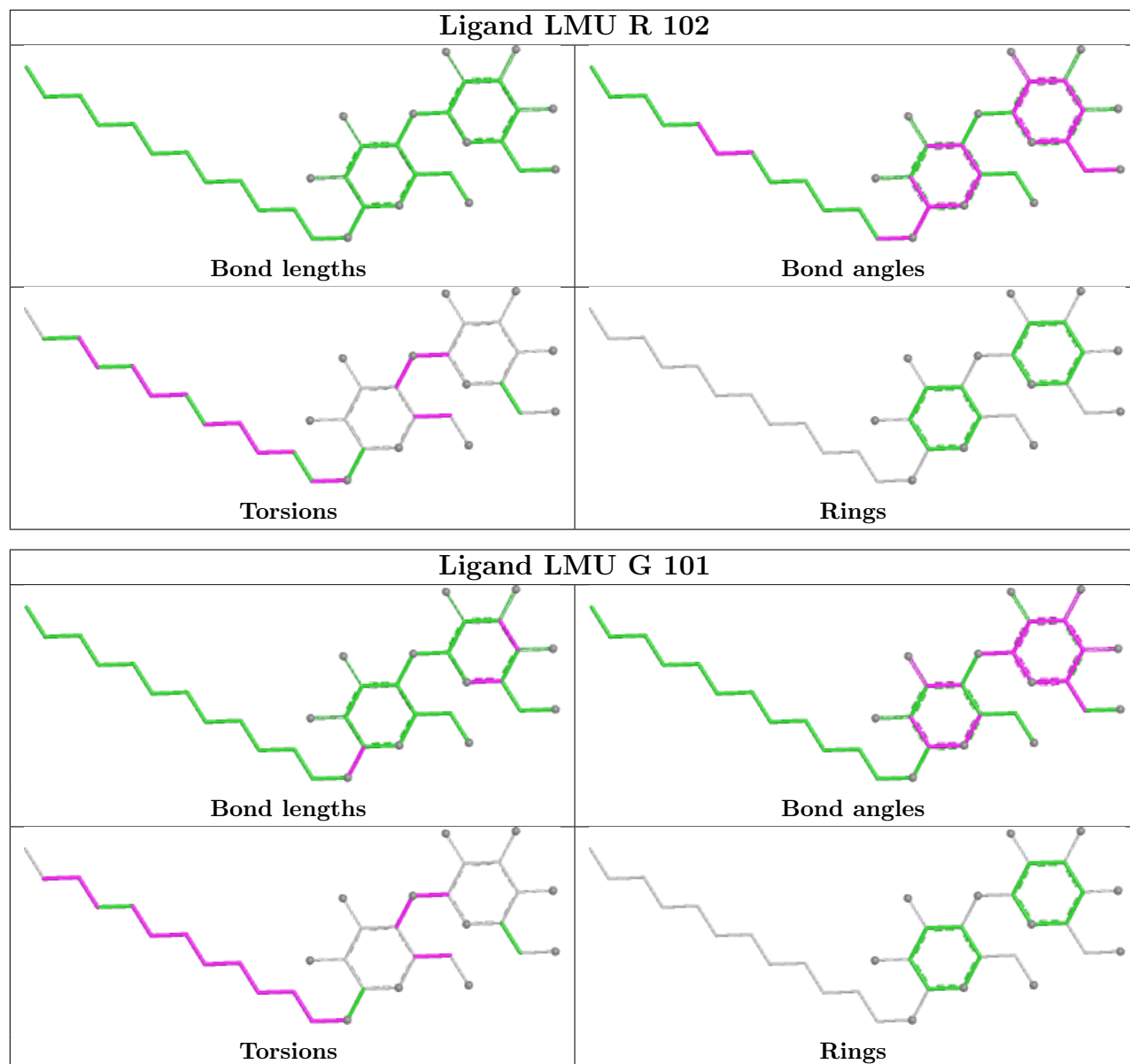


Ligand CLA B 808

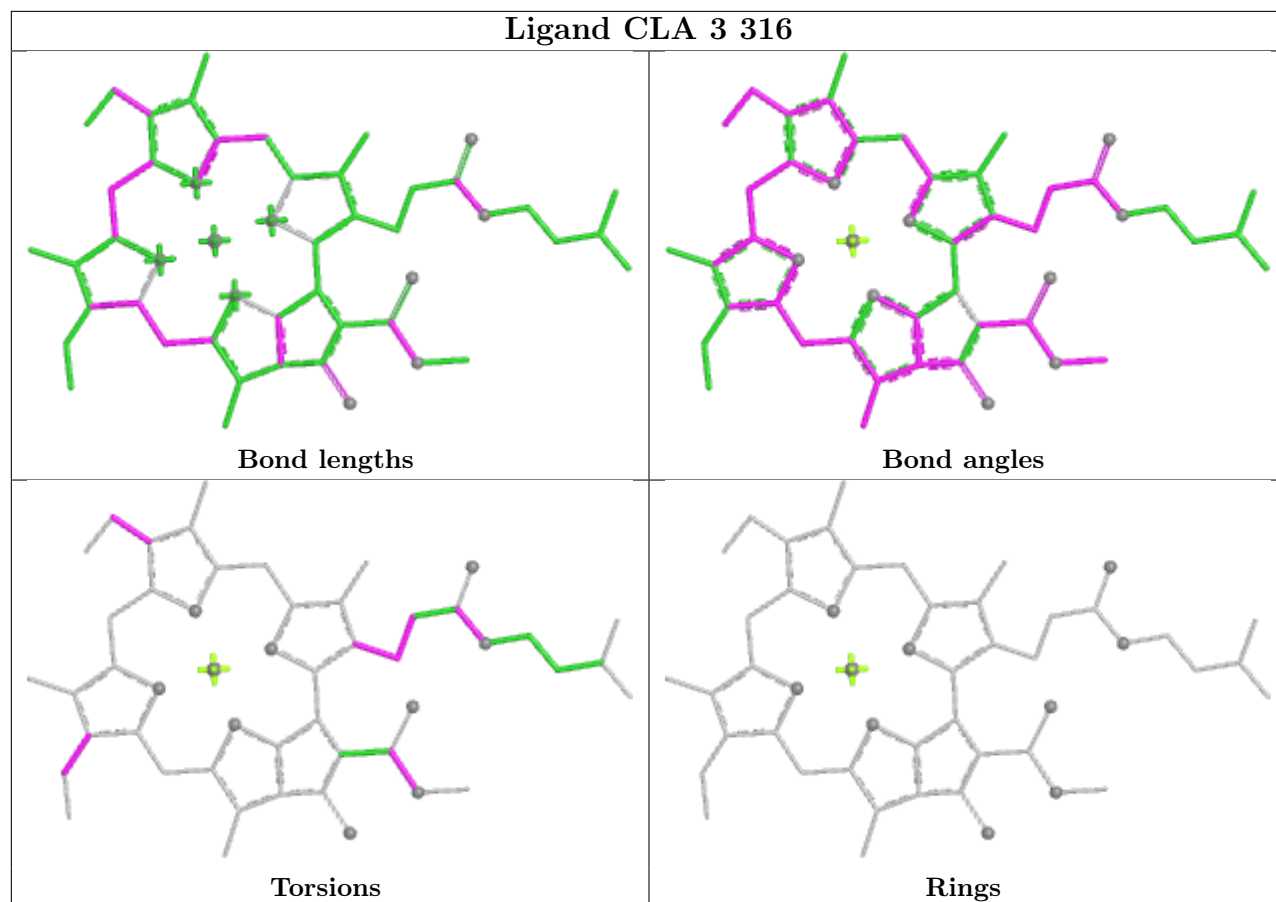


Ligand CLA 3 308

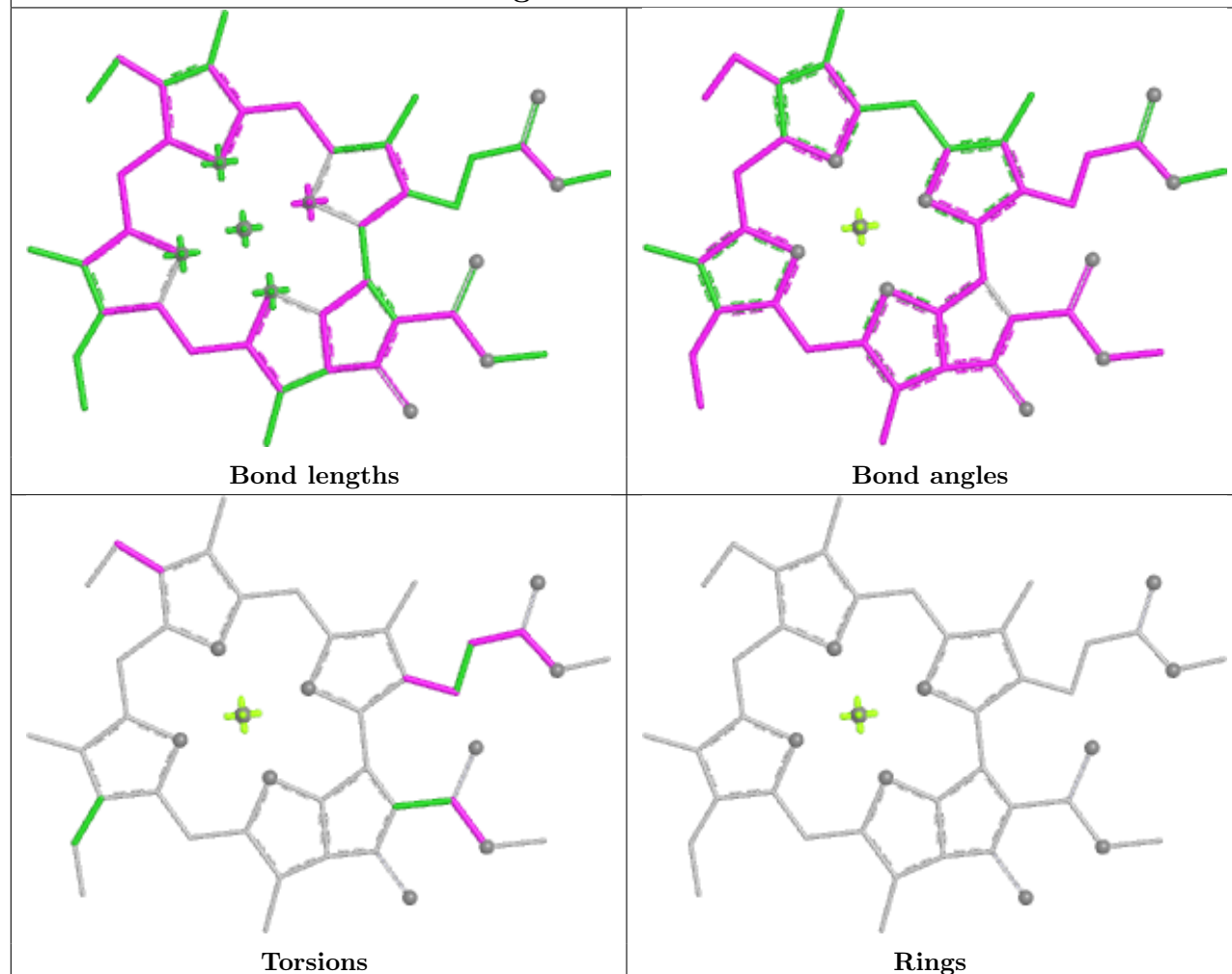




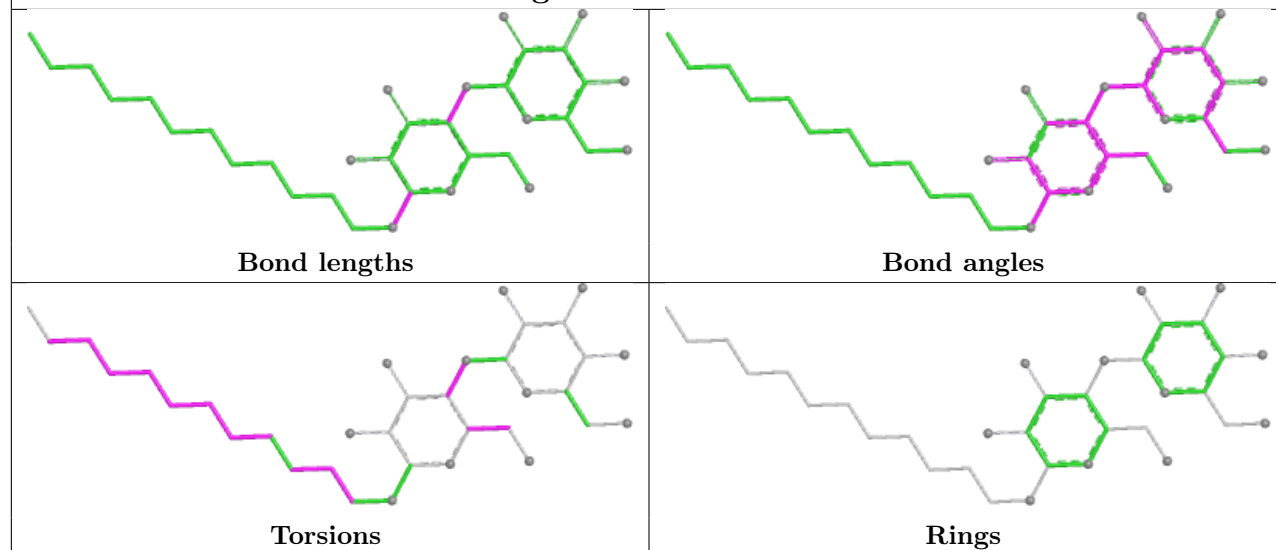
Ligand CLA 3 316

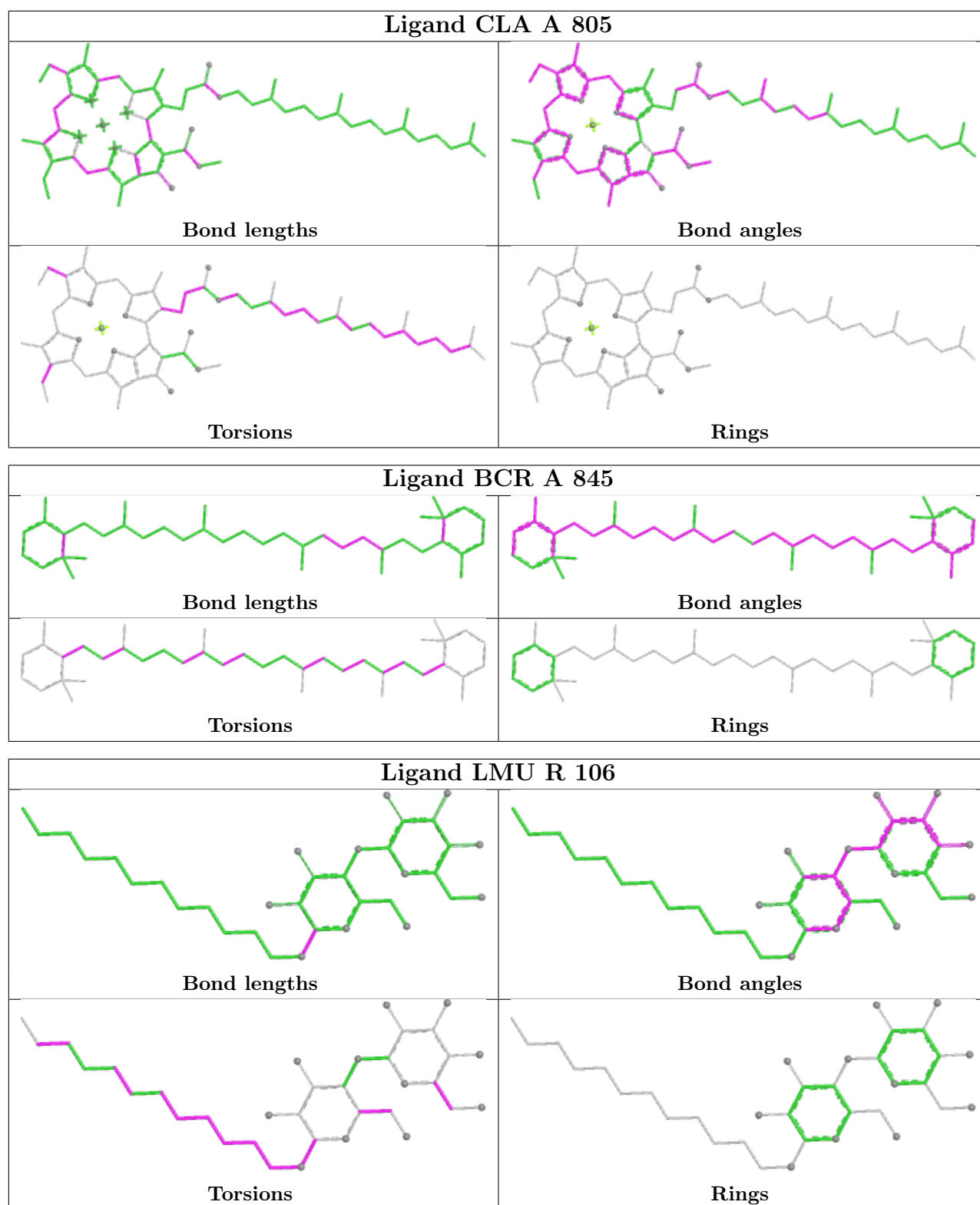


Ligand CLA A 807

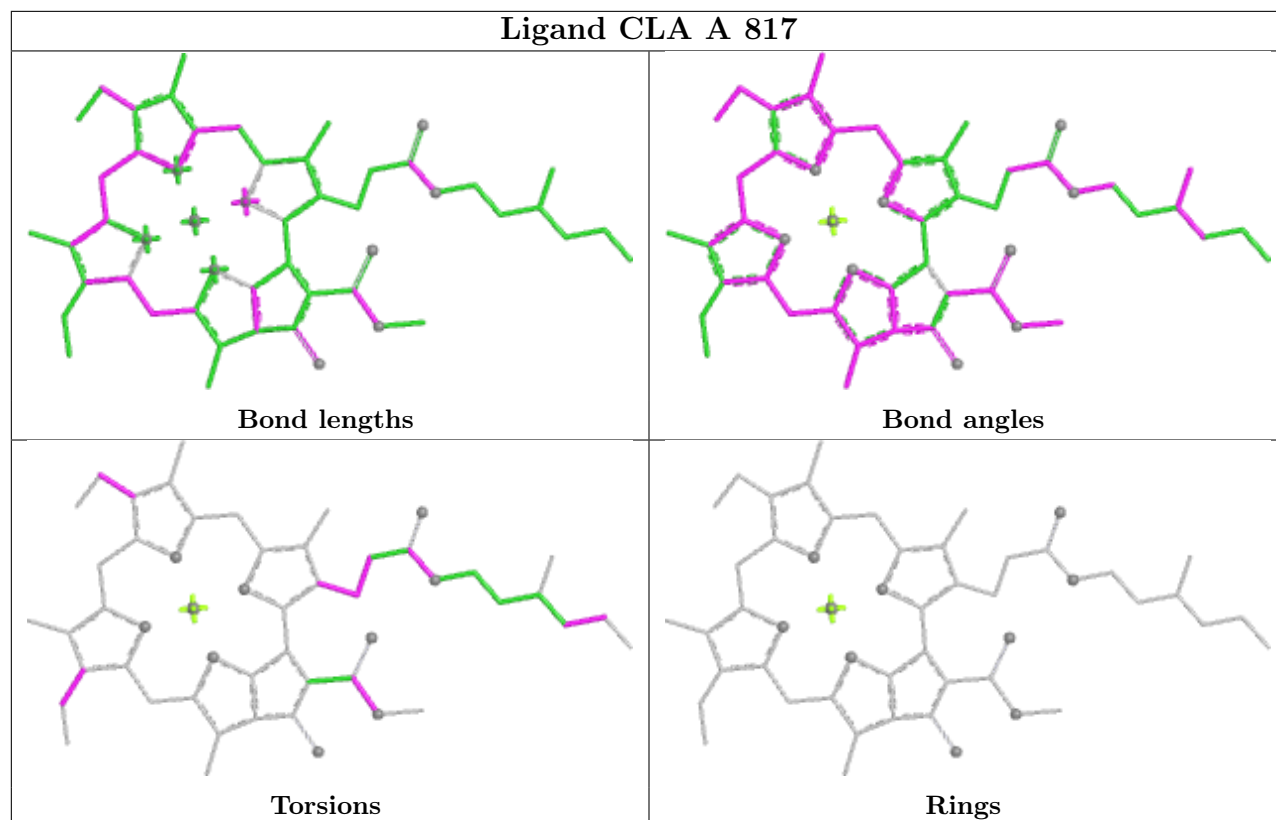


Ligand LMU 1 219

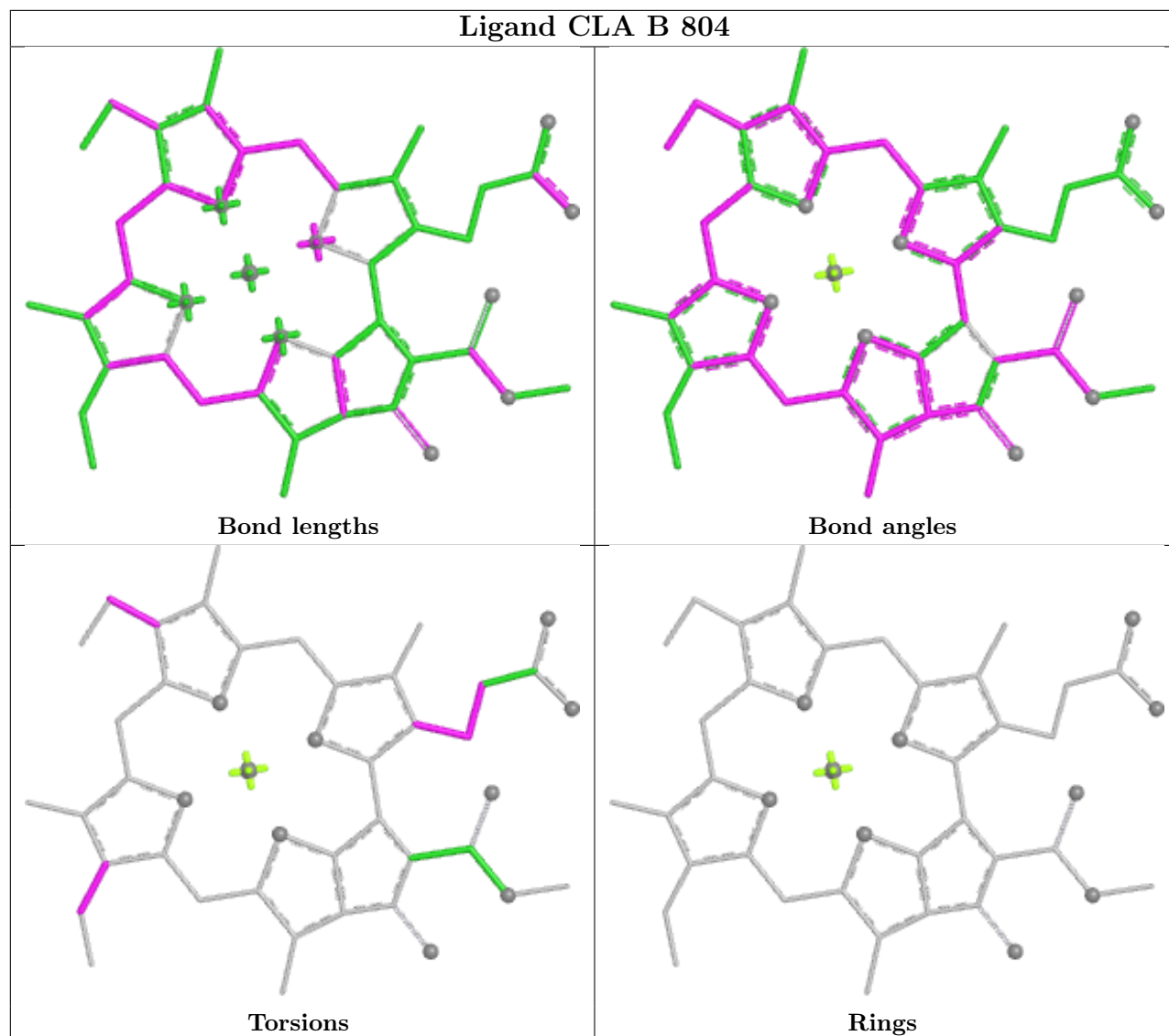




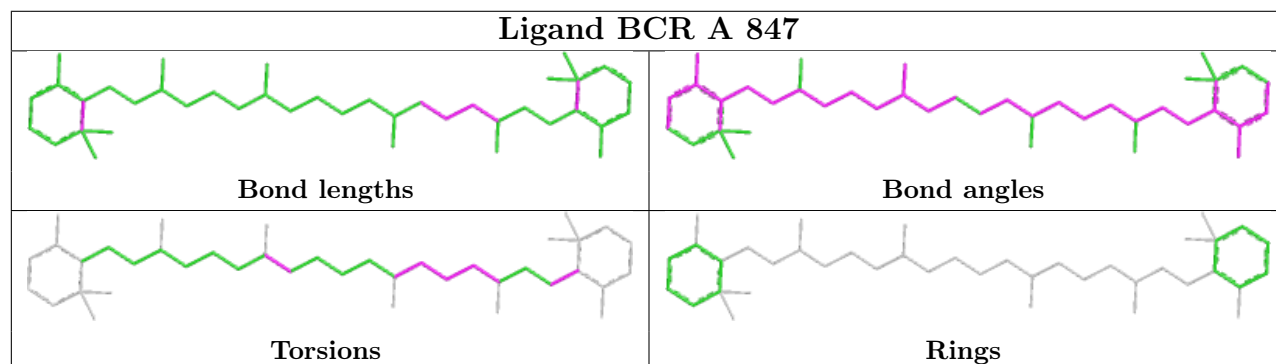
Ligand CLA A 817

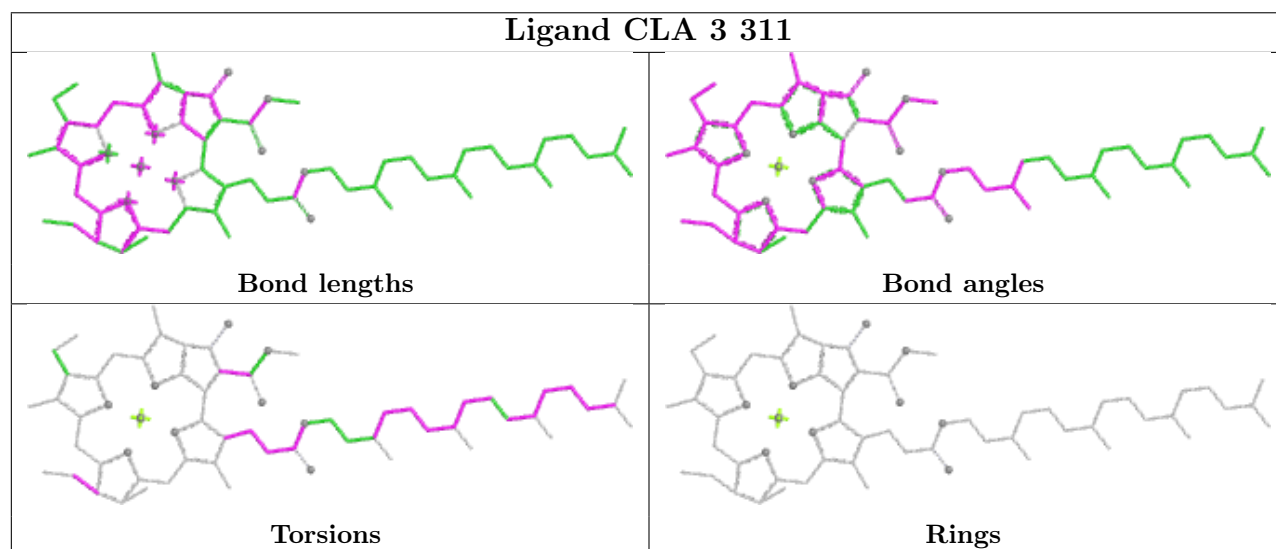
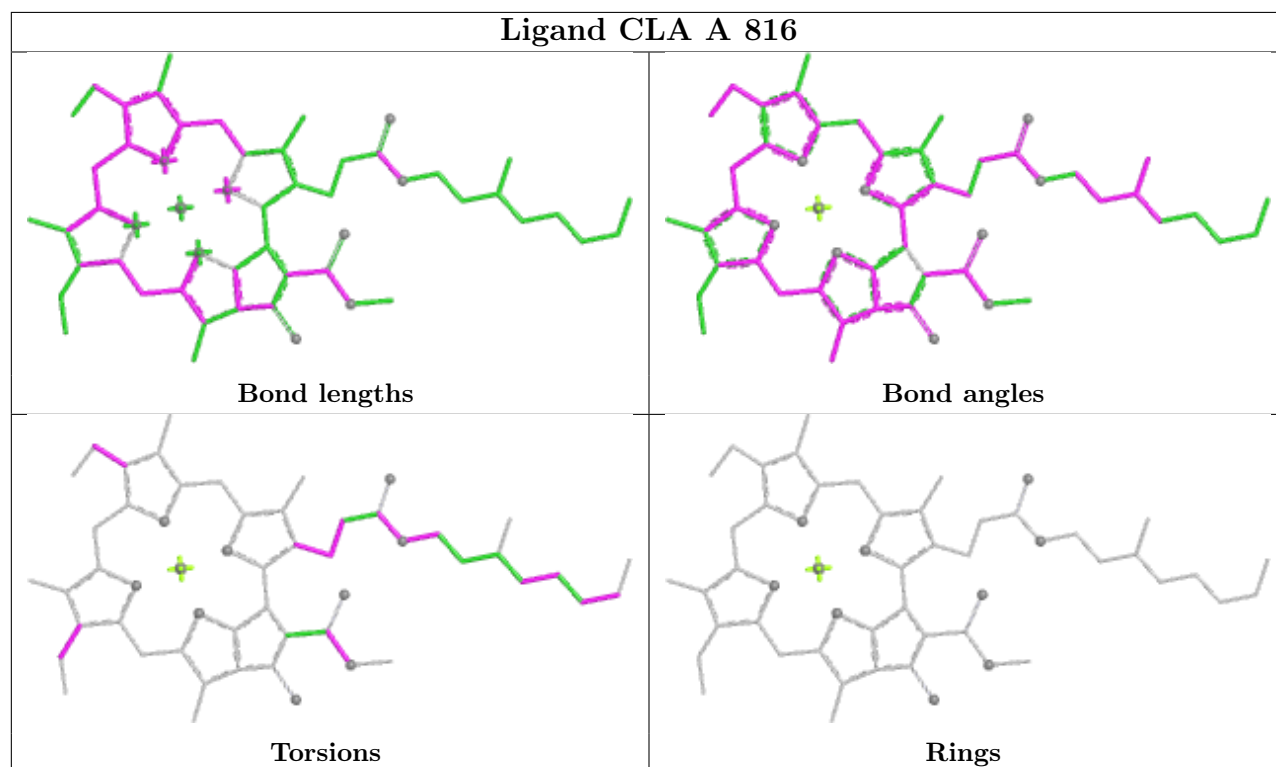
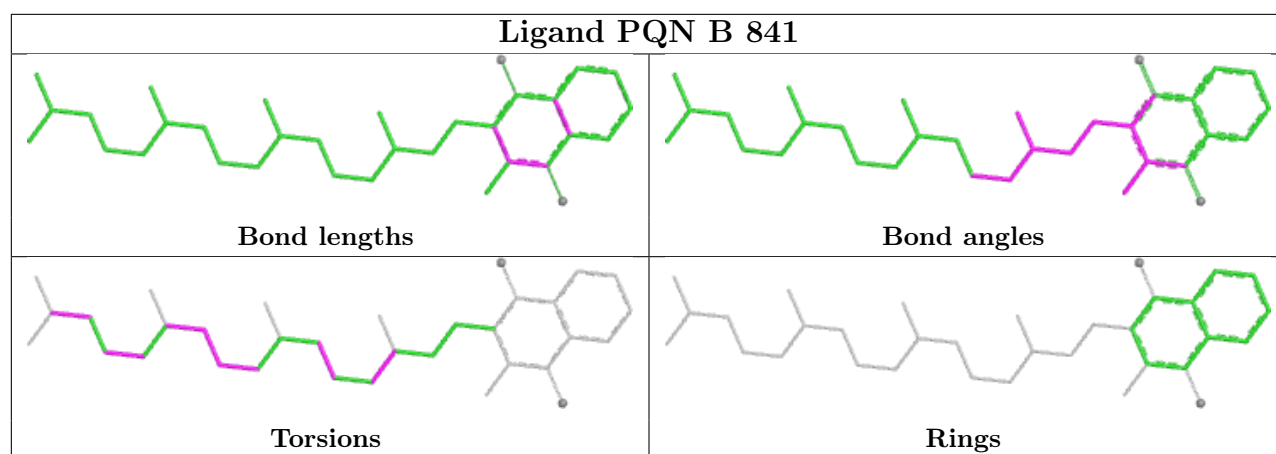


Ligand CLA B 804

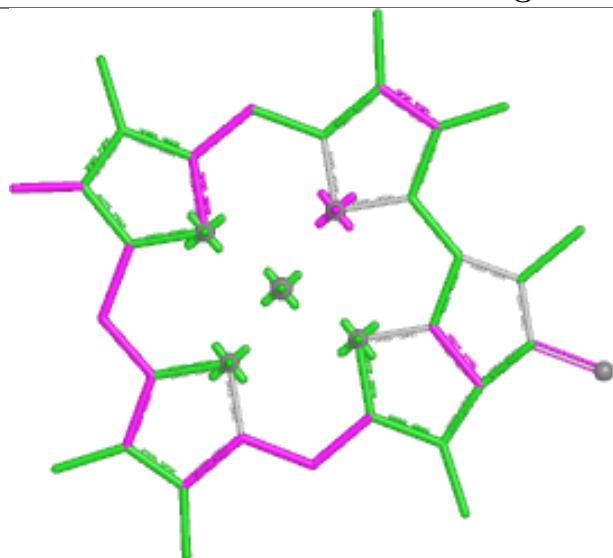


Ligand BCR A 847

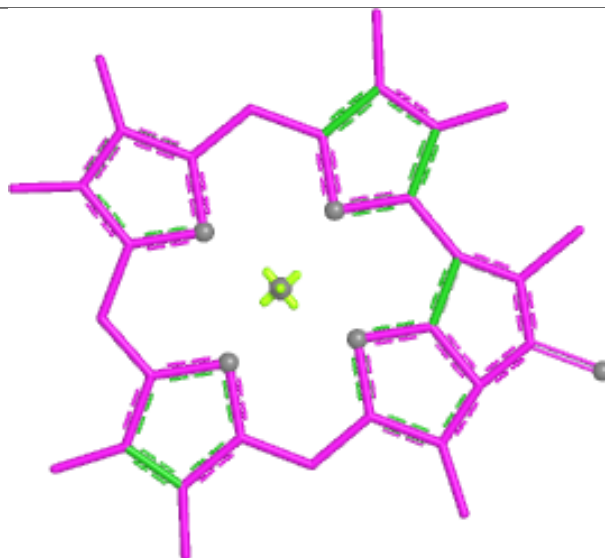




Ligand CLA B 840



Bond lengths



Bond angles

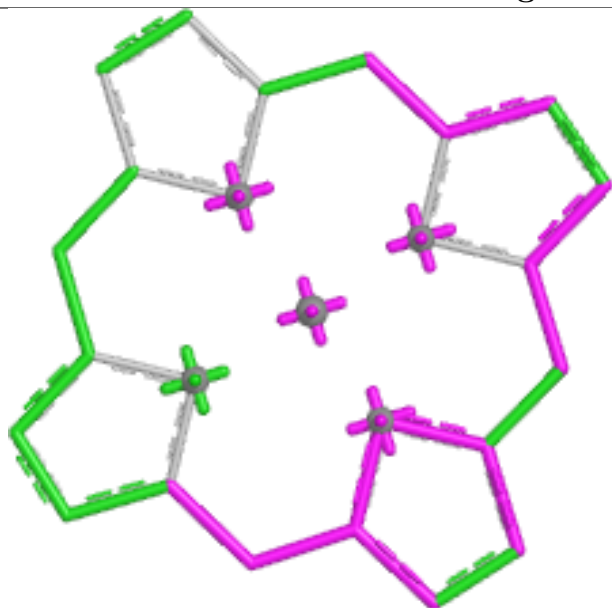


Torsions

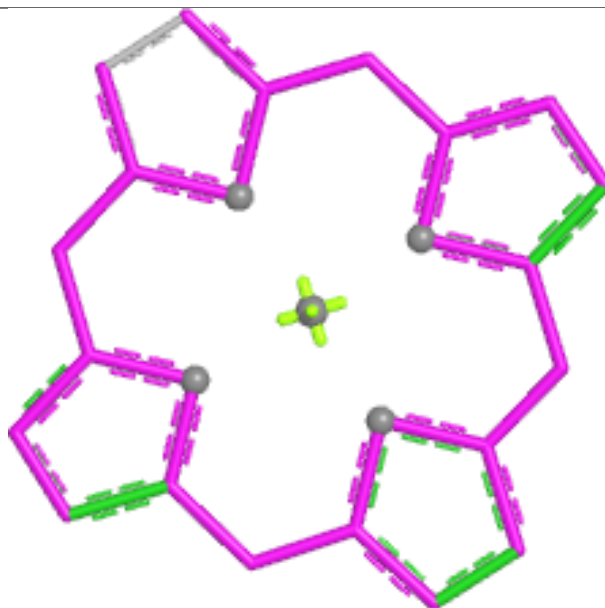


Rings

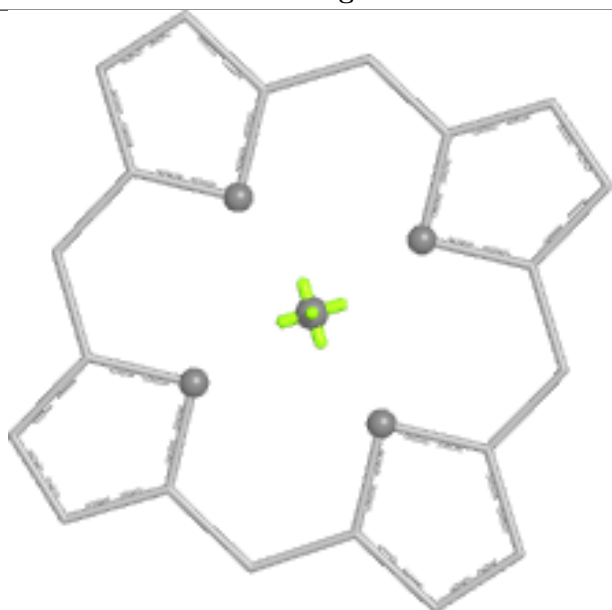
Ligand CLA 3 318



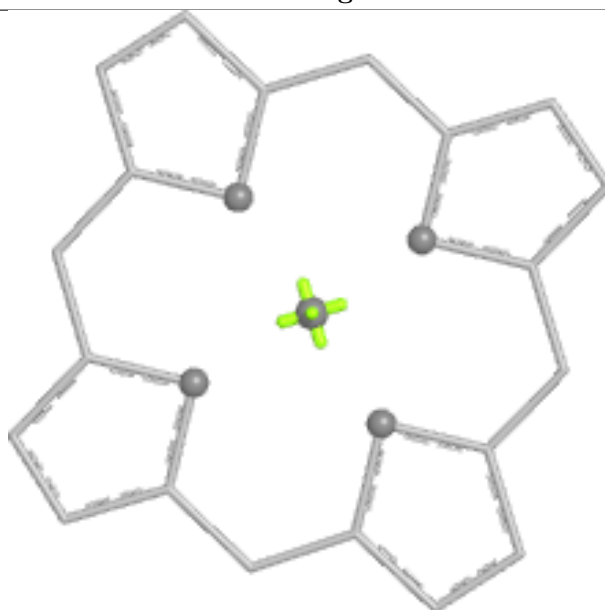
Bond lengths



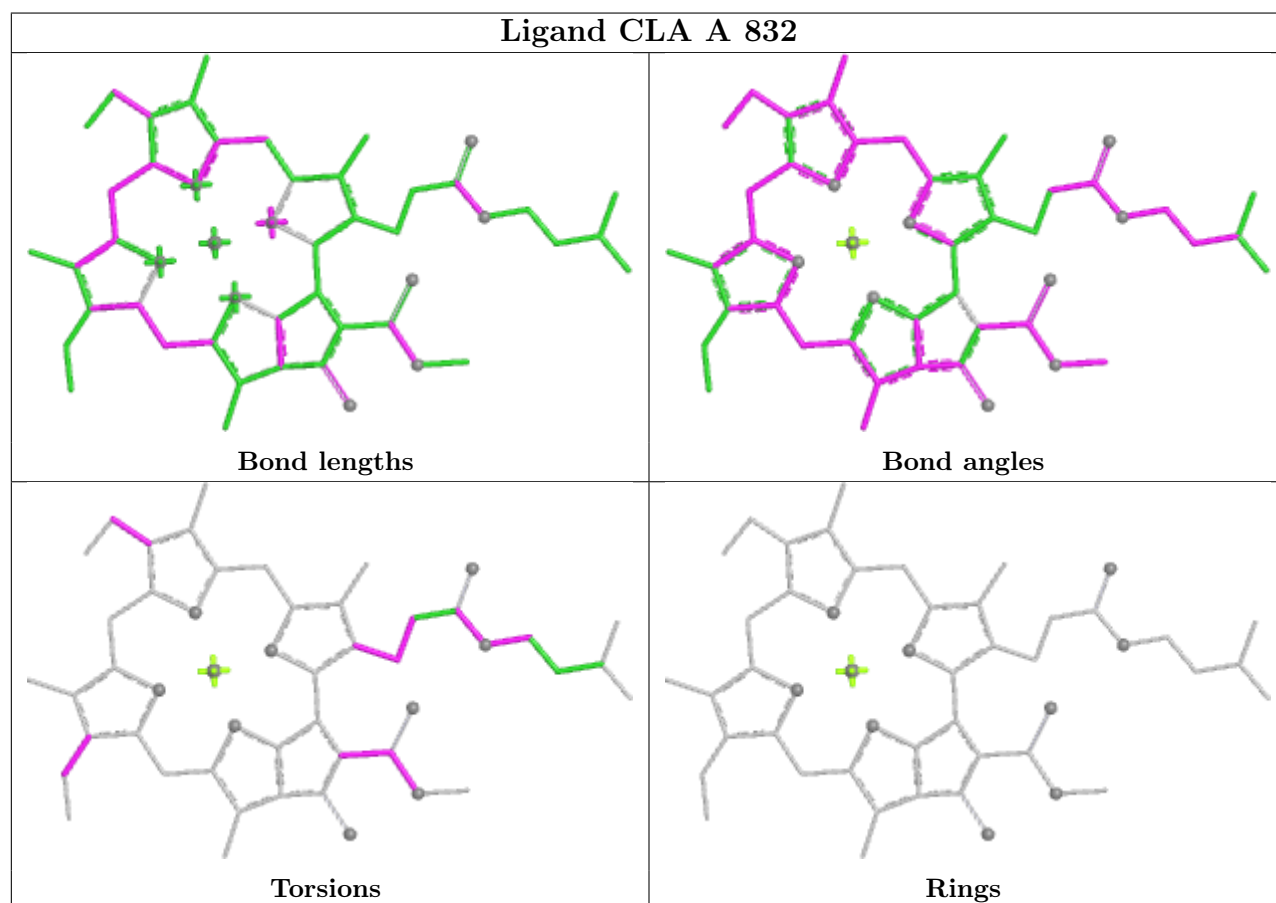
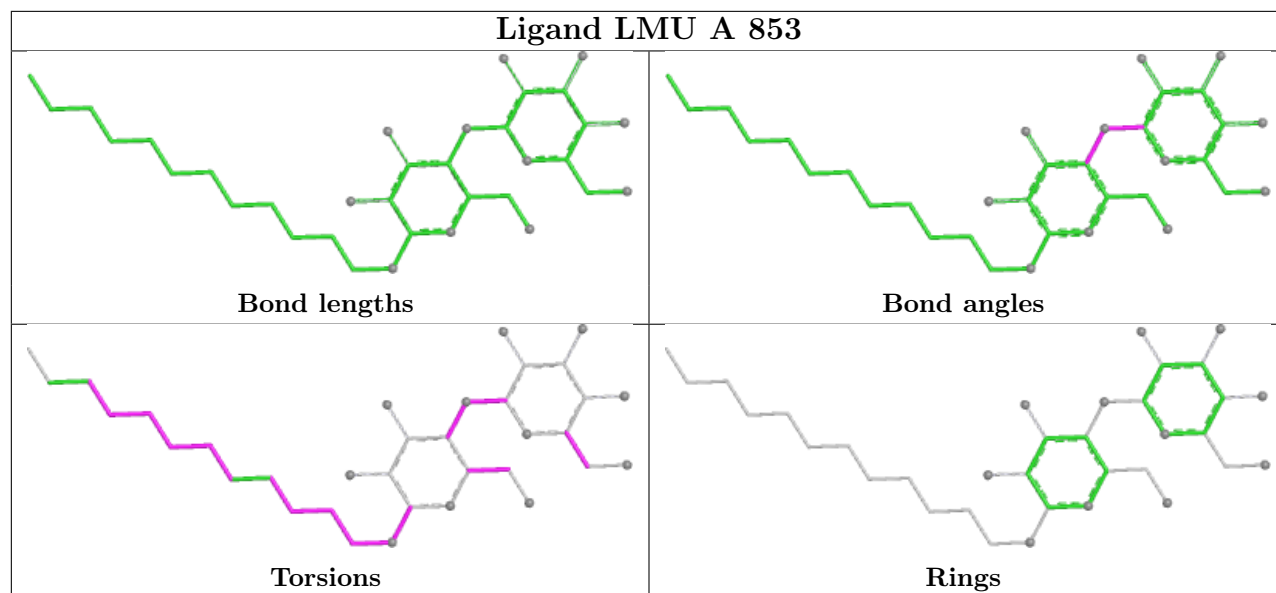
Bond angles



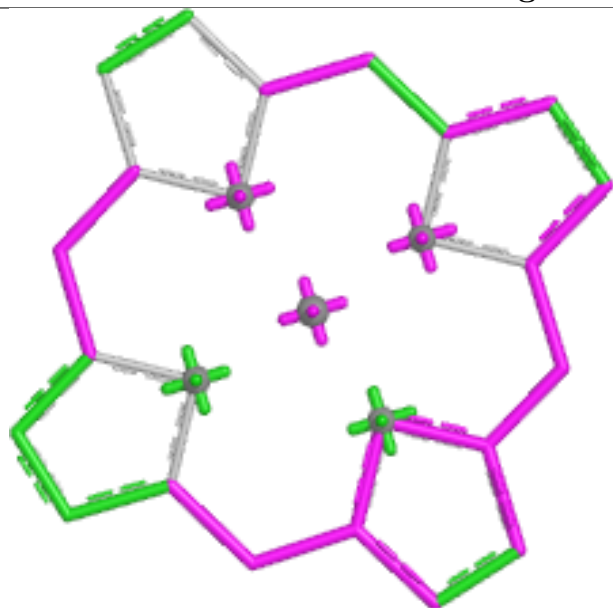
Torsions



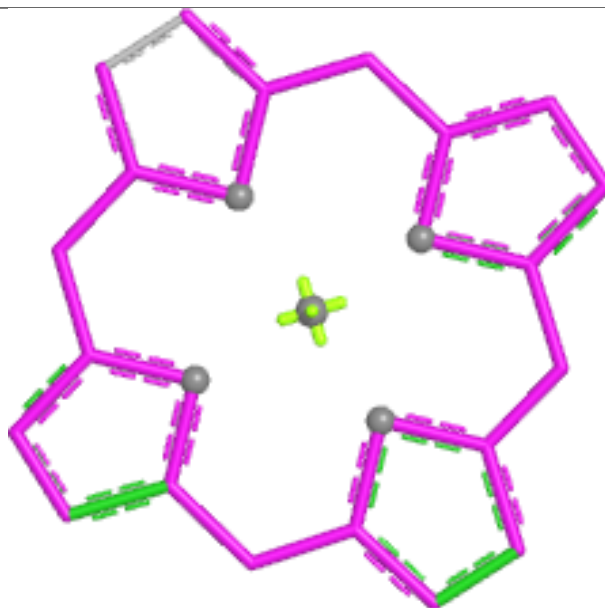
Rings



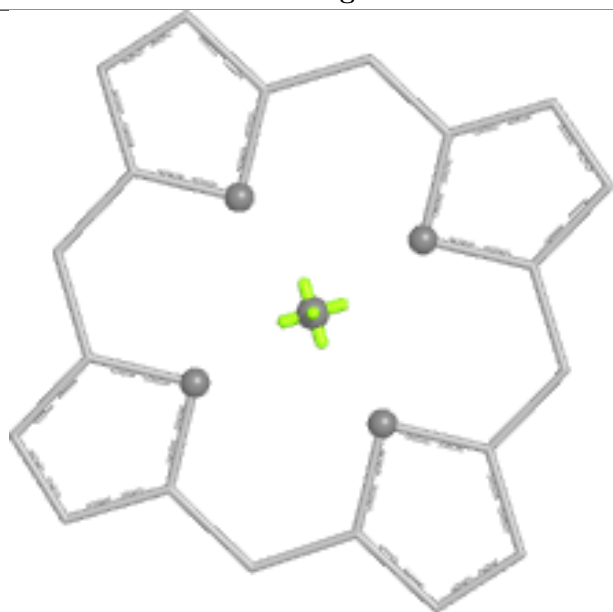
Ligand CLA 2 304



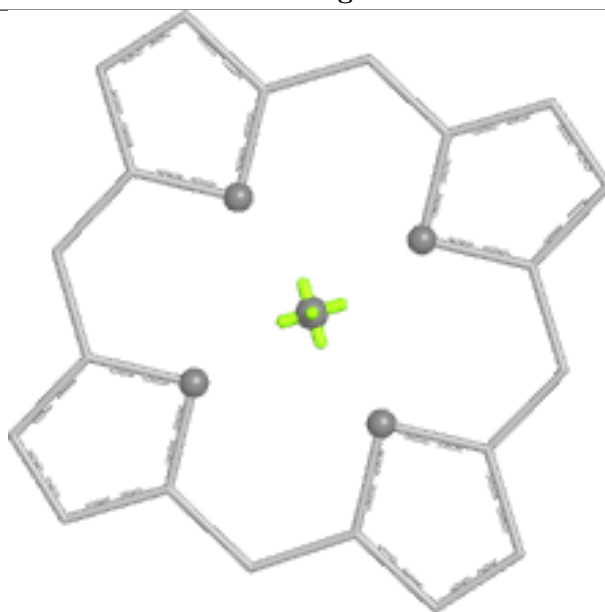
Bond lengths



Bond angles

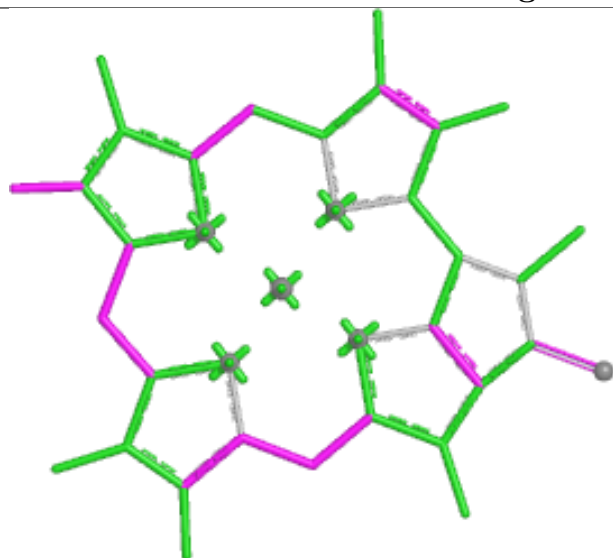


Torsions

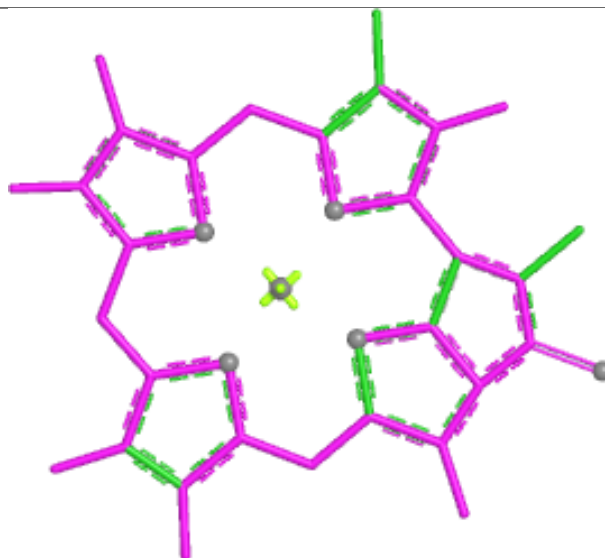


Rings

Ligand CLA 3 301



Bond lengths



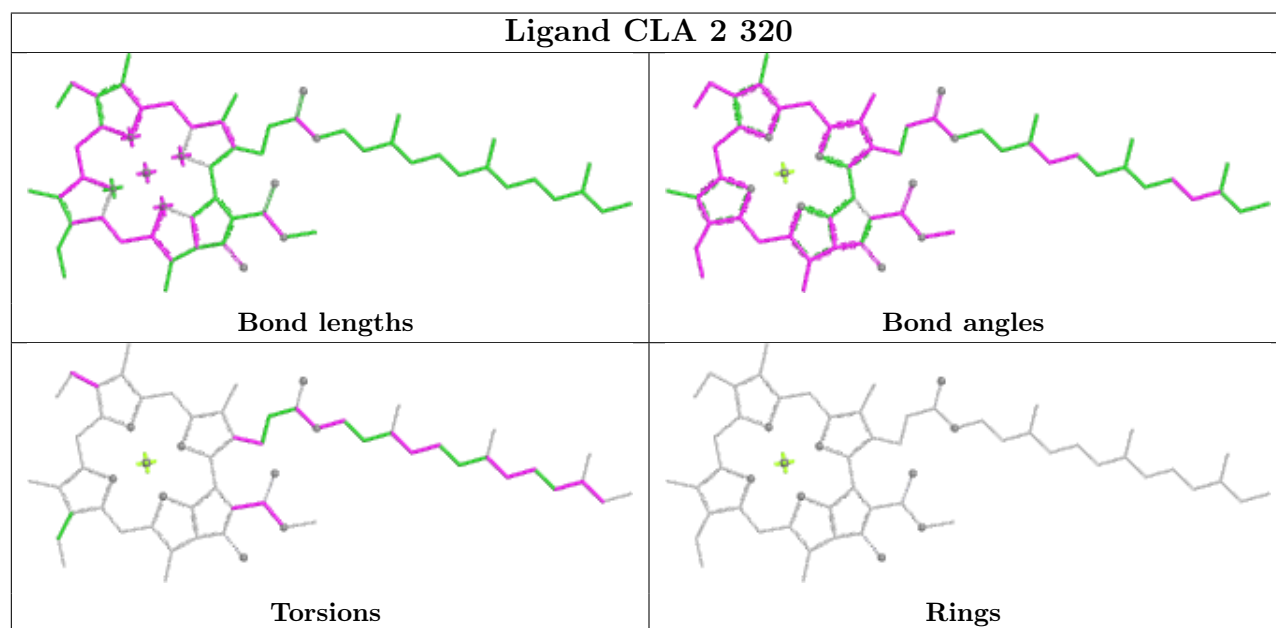
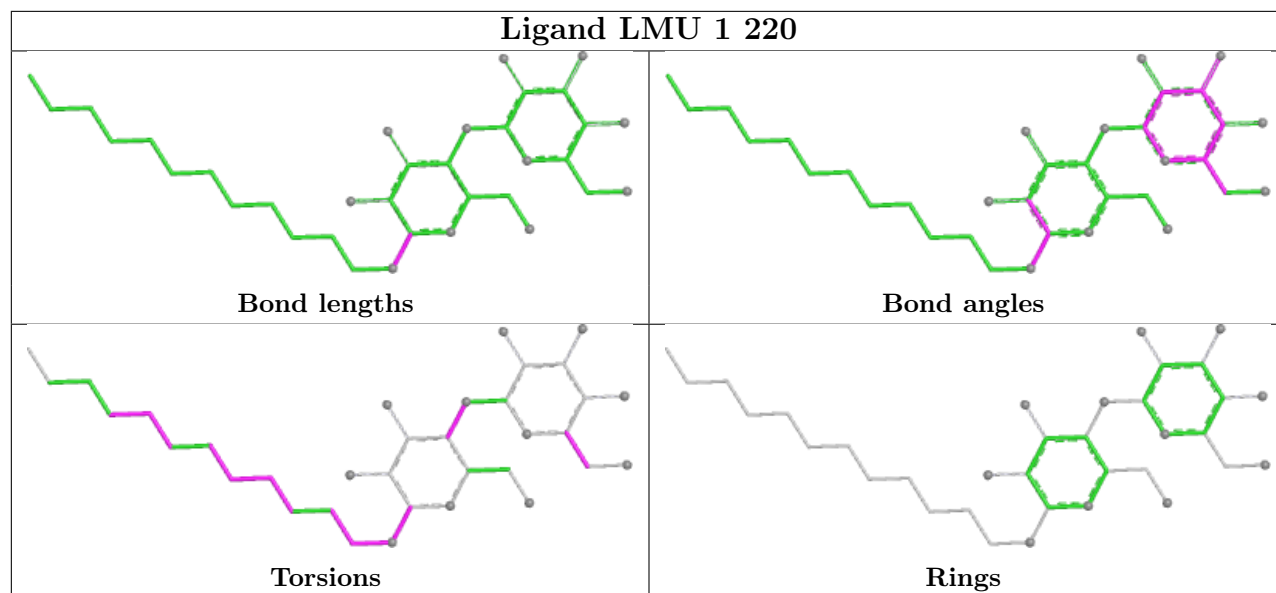
Bond angles



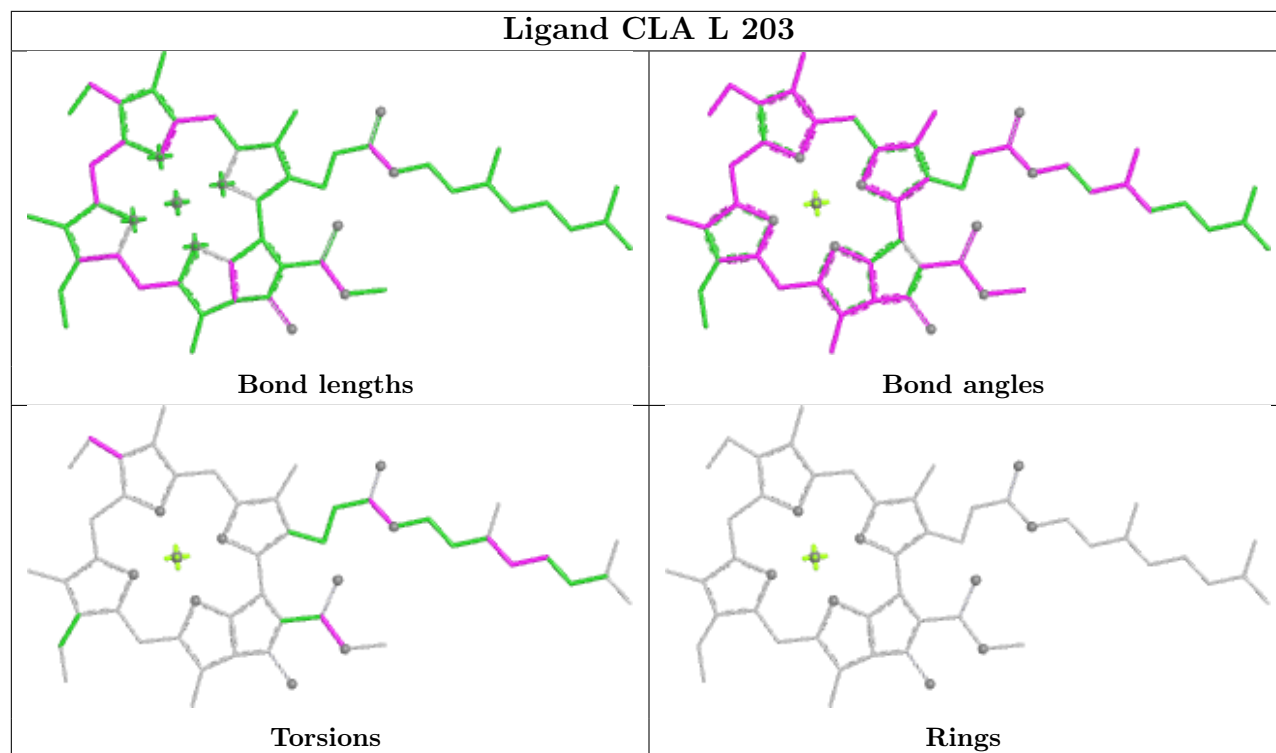
Torsions



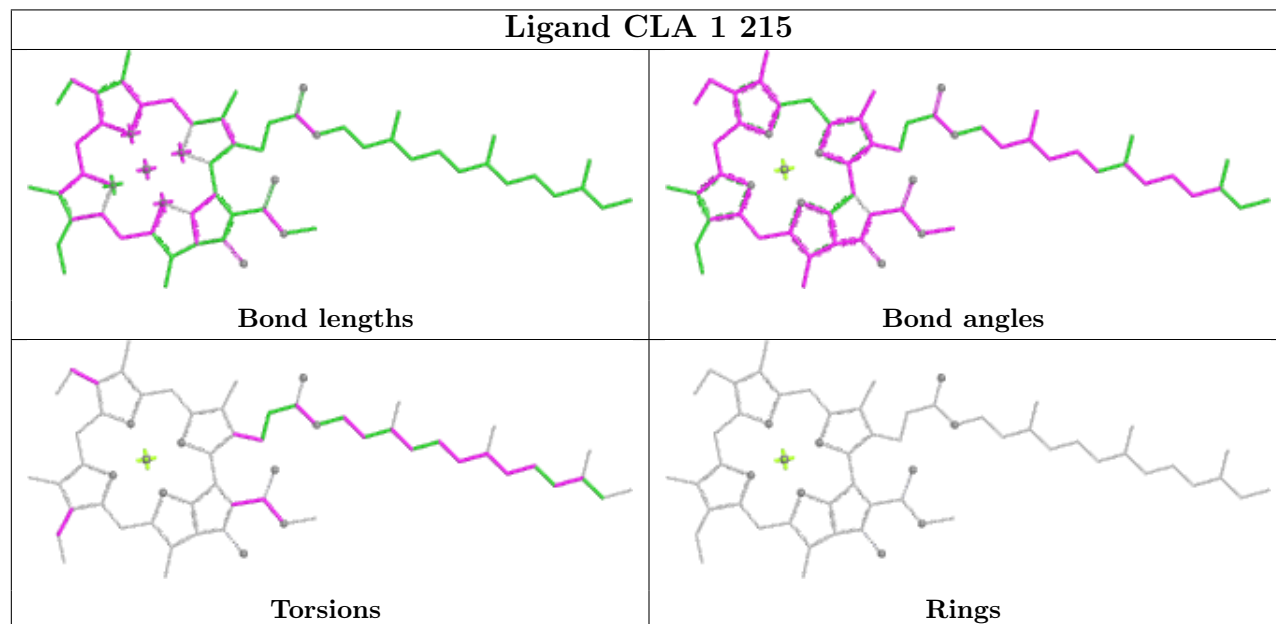
Rings



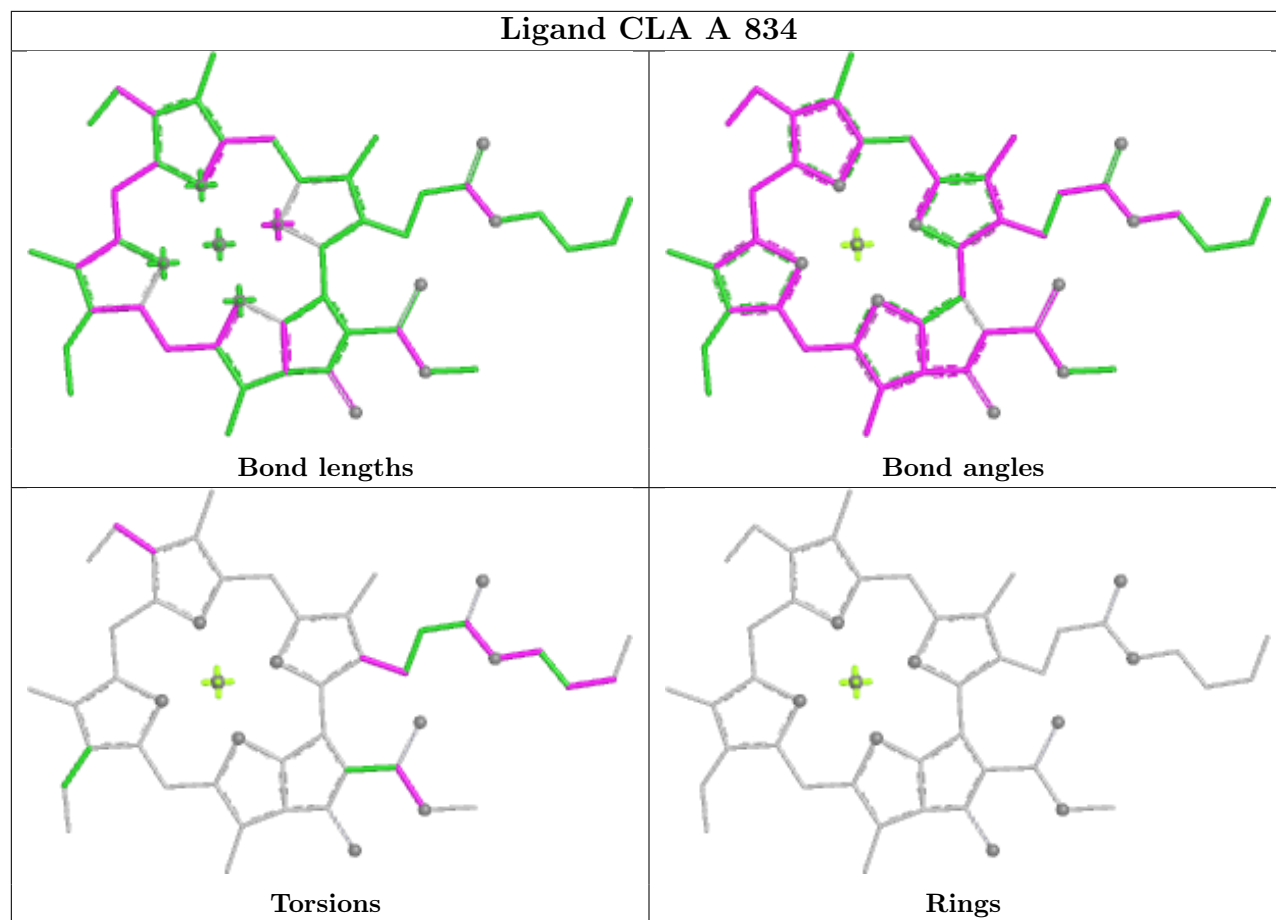
Ligand CLA L 203



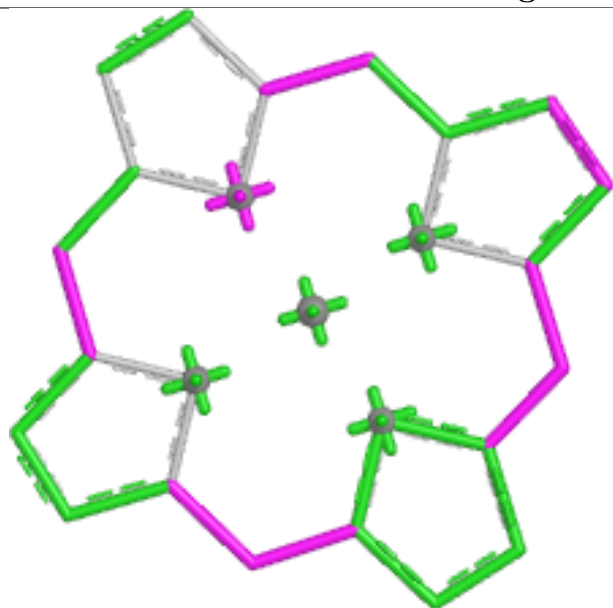
Ligand CLA 1 215



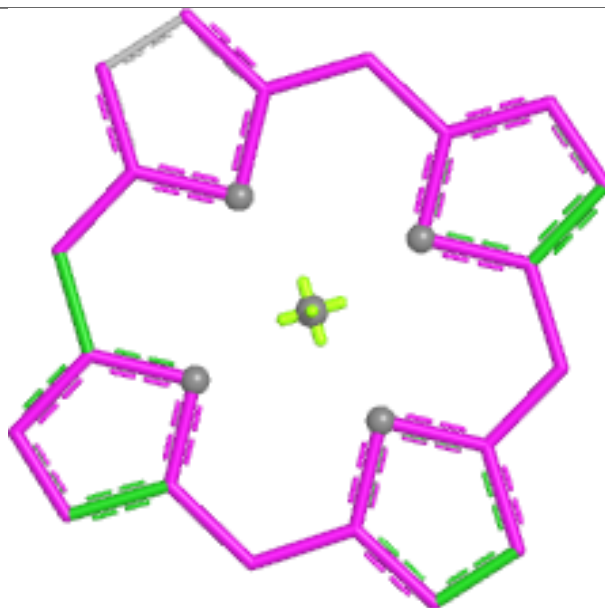
Ligand CLA A 834



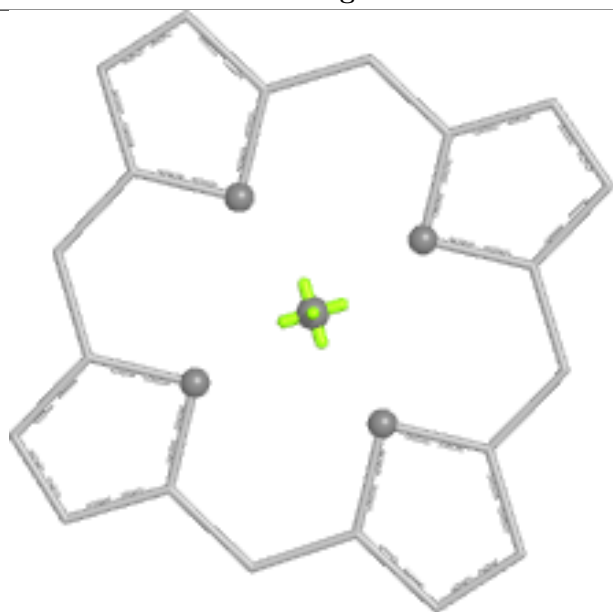
Ligand CLA 1 214



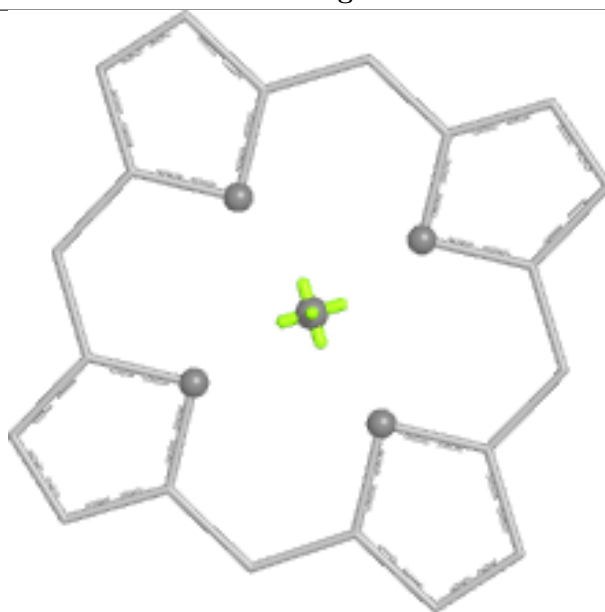
Bond lengths



Bond angles

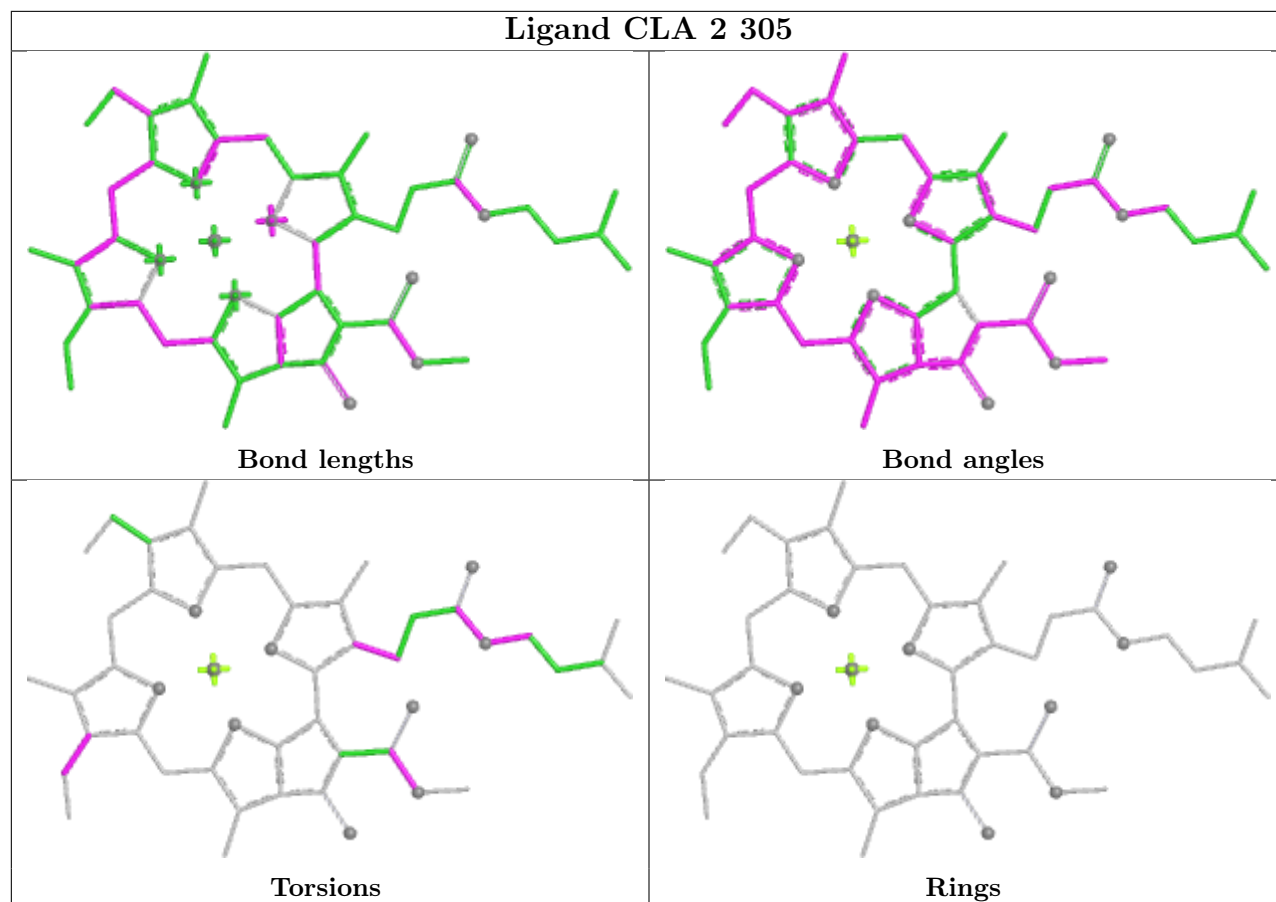


Torsions

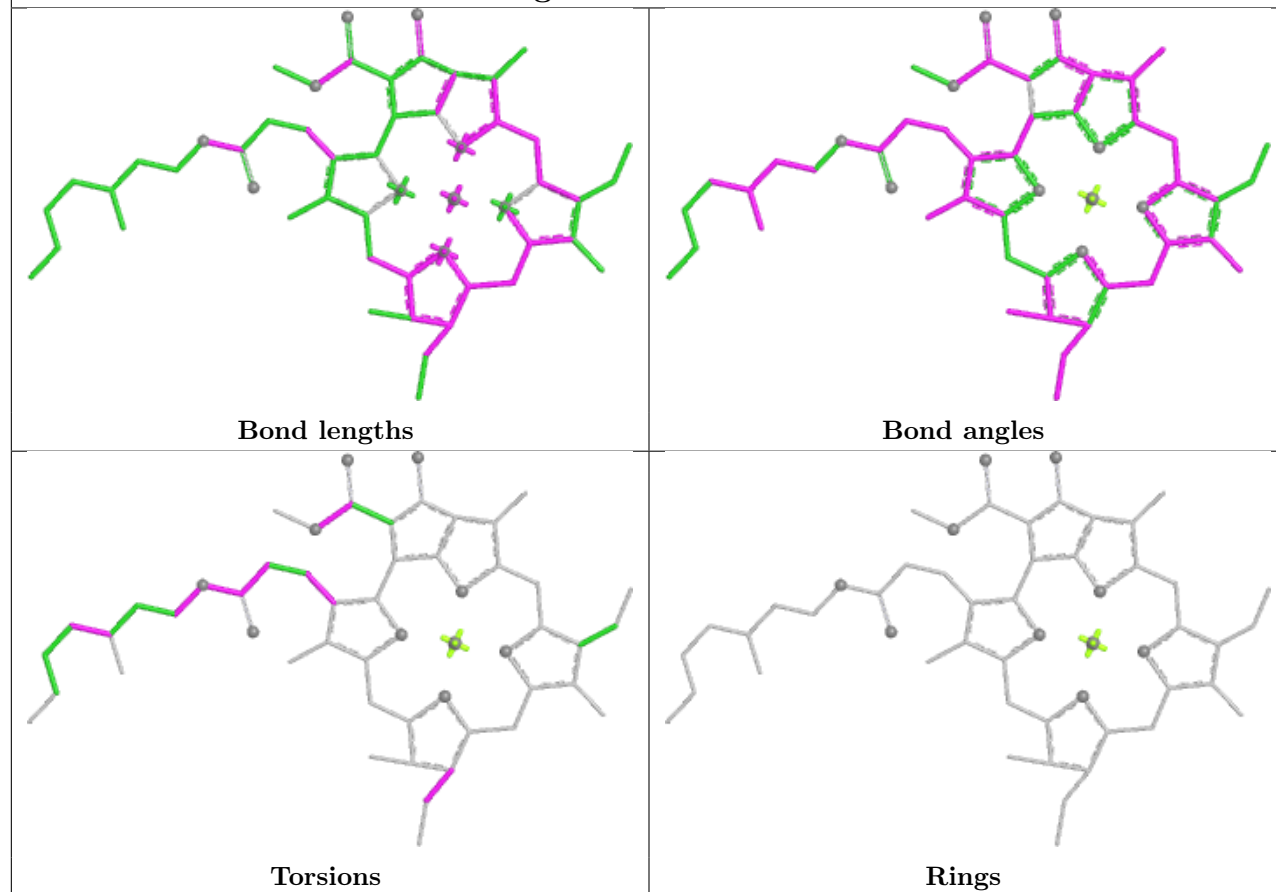


Rings

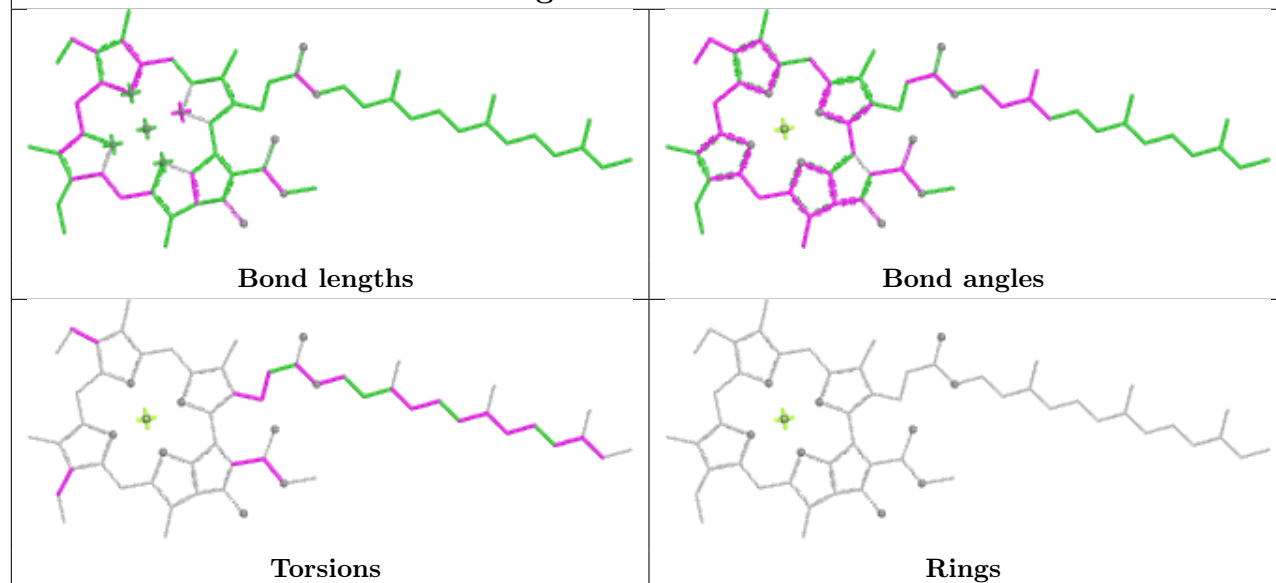
Ligand CLA 2 305



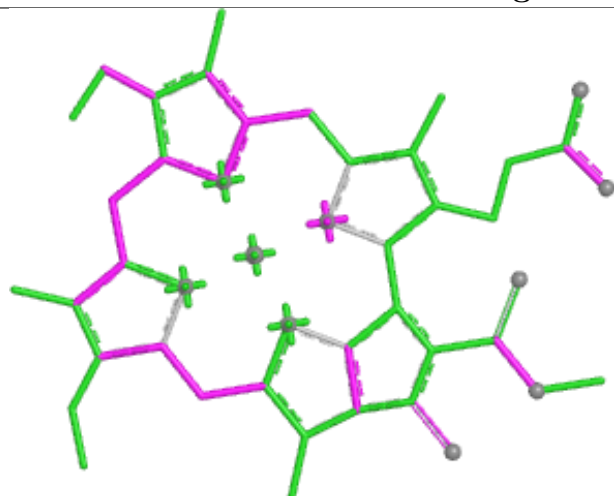
Ligand CLA F 206



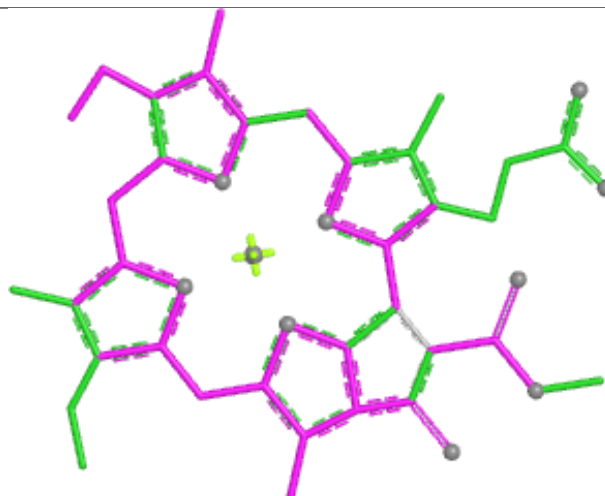
Ligand CLA J 103



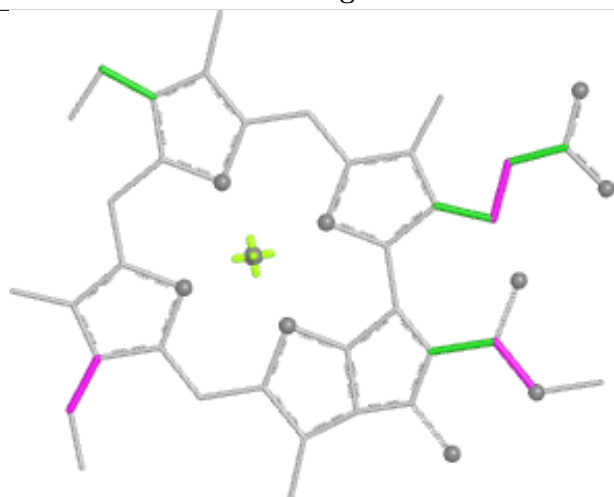
Ligand CLA K 101



Bond lengths



Bond angles

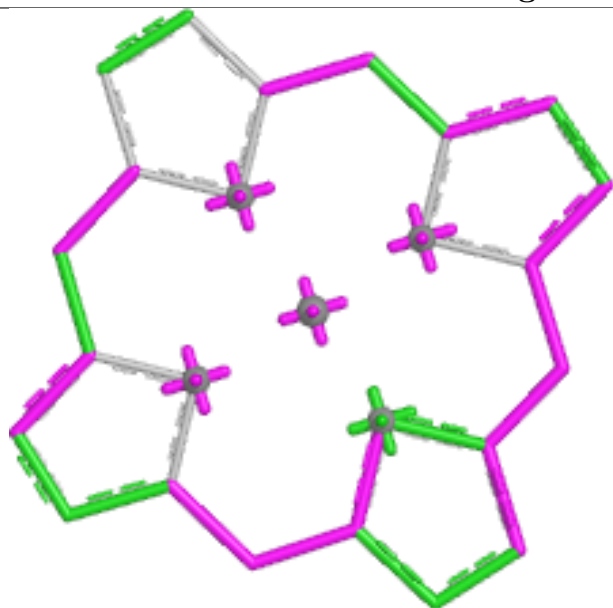


Torsions

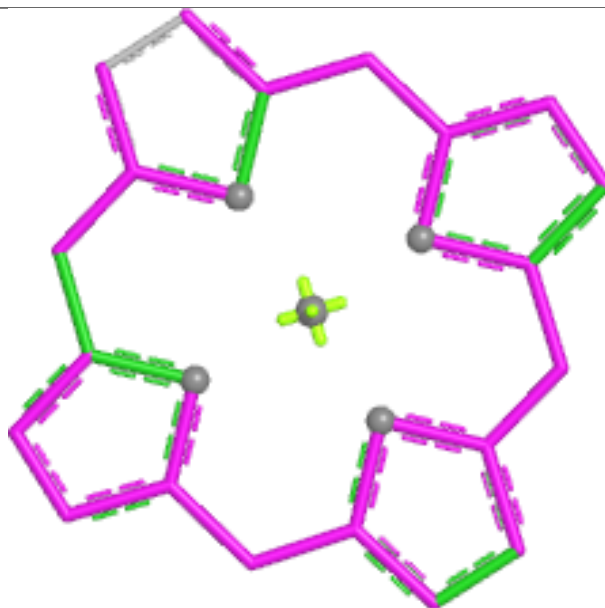


Rings

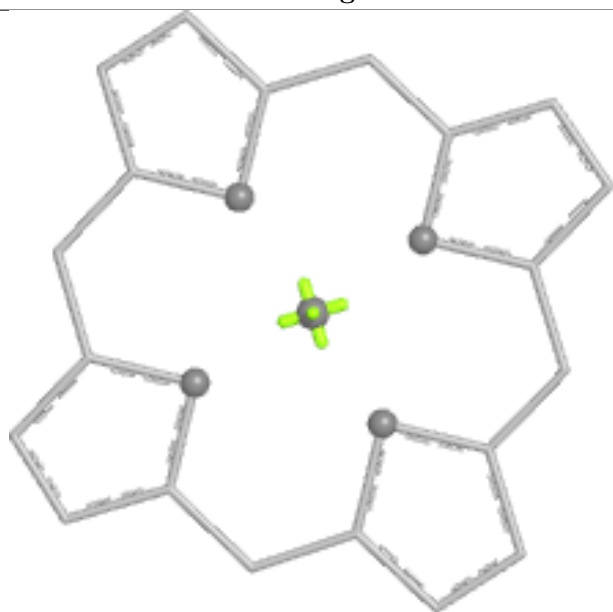
Ligand CLA 2 301



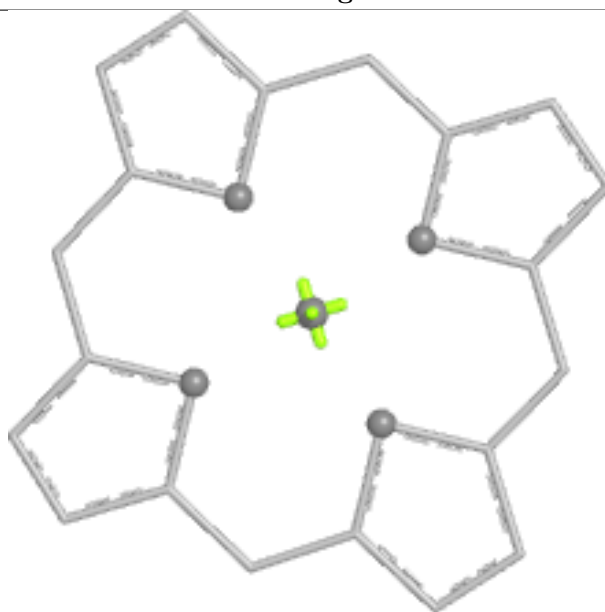
Bond lengths



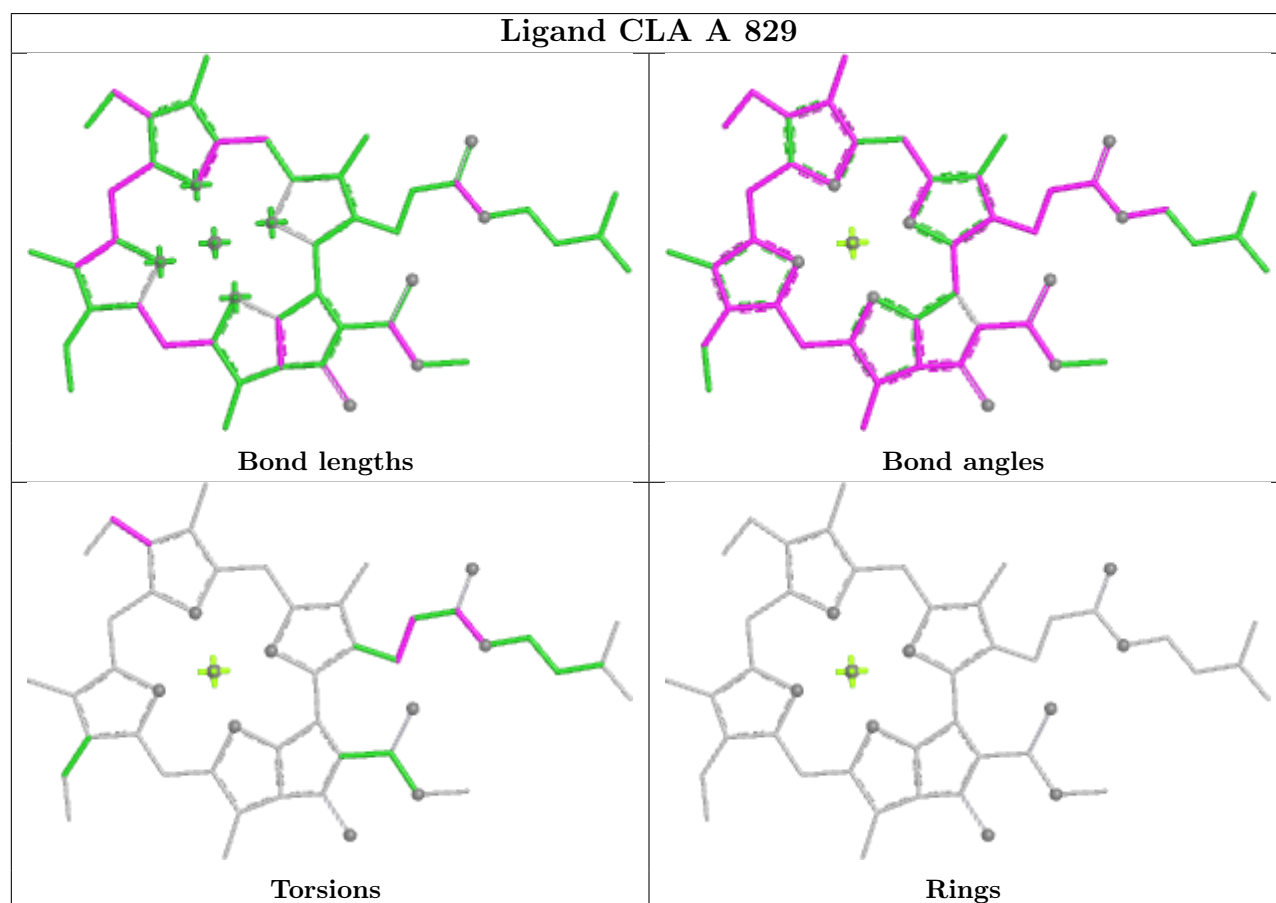
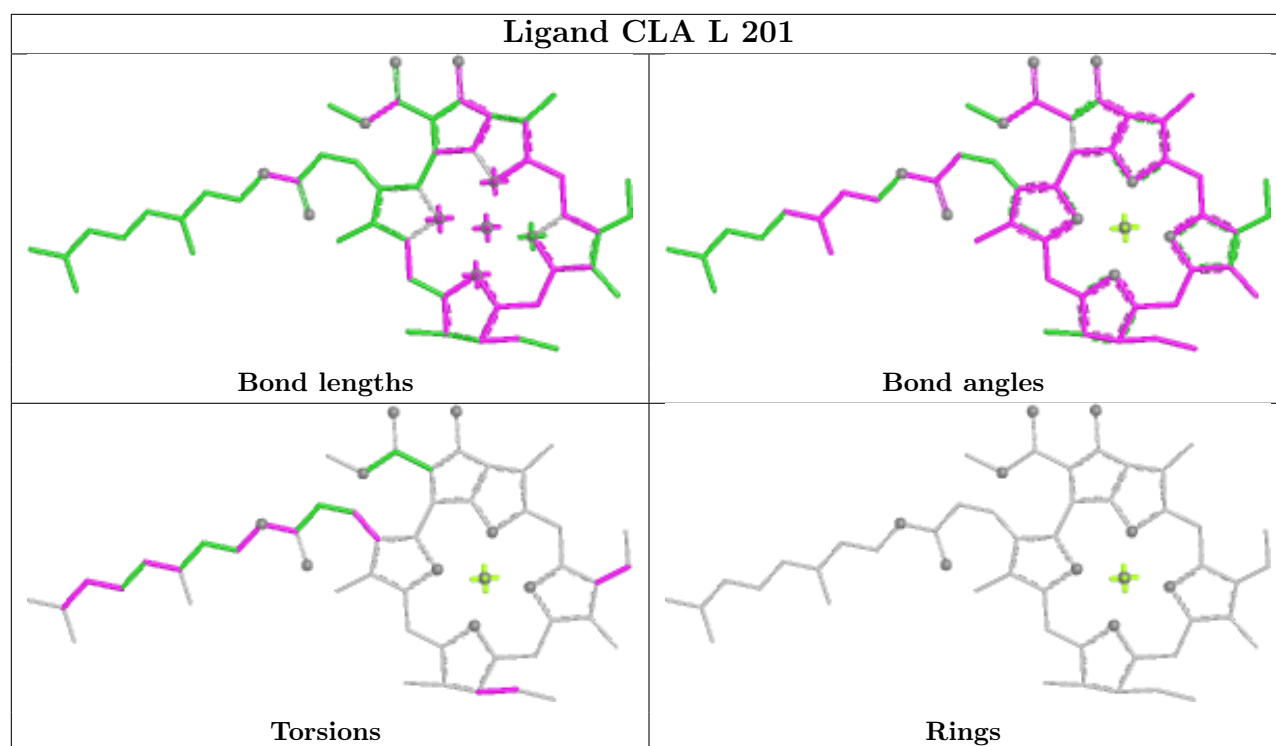
Bond angles



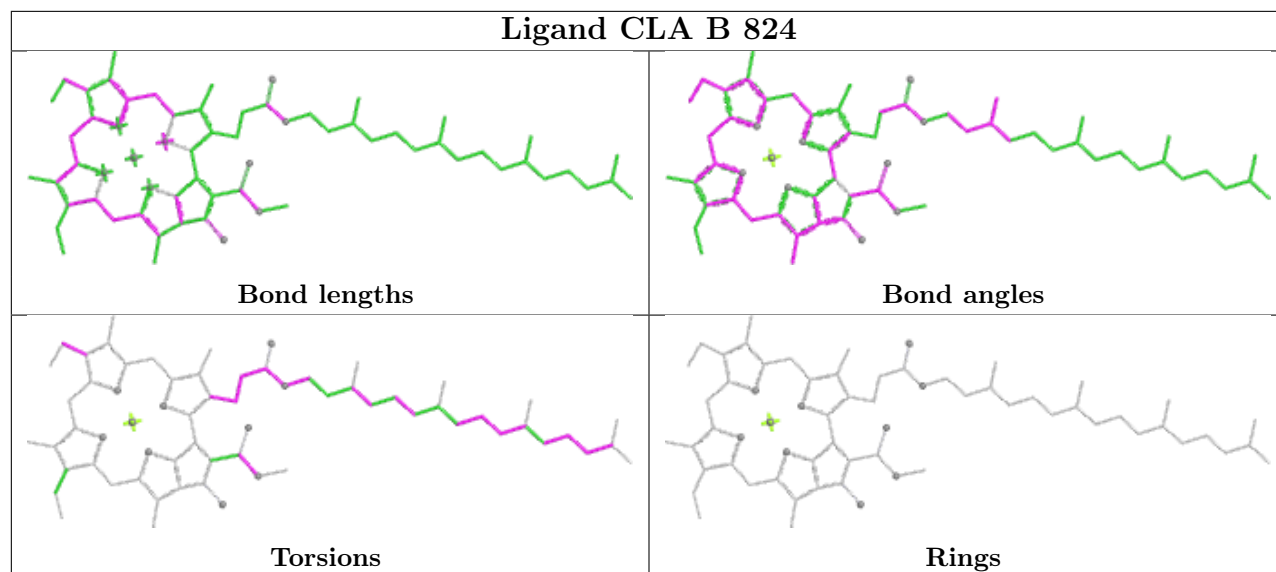
Torsions



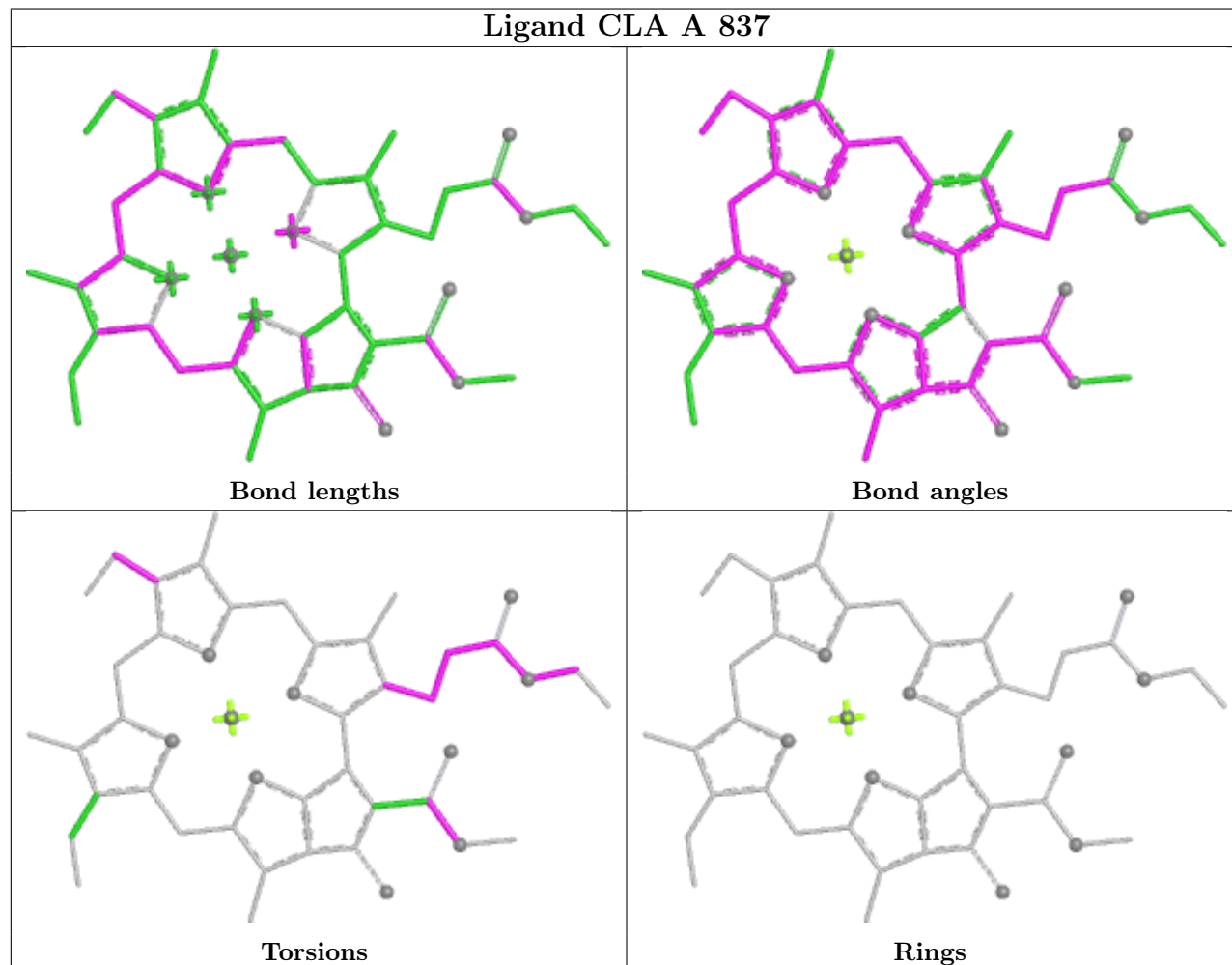
Rings



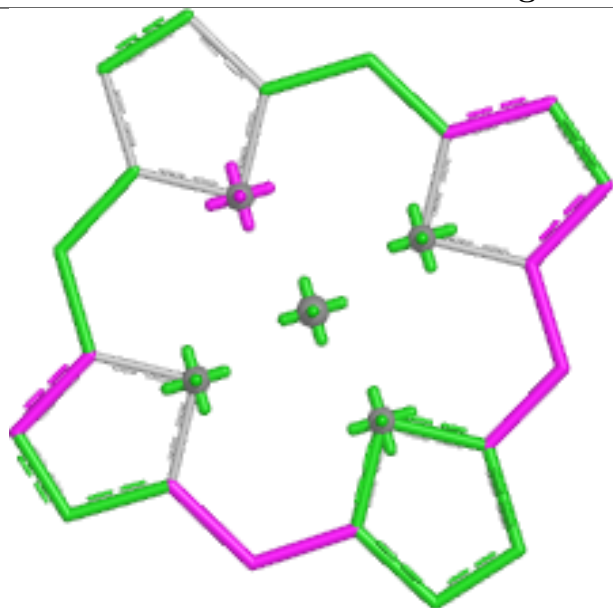
Ligand CLA B 824



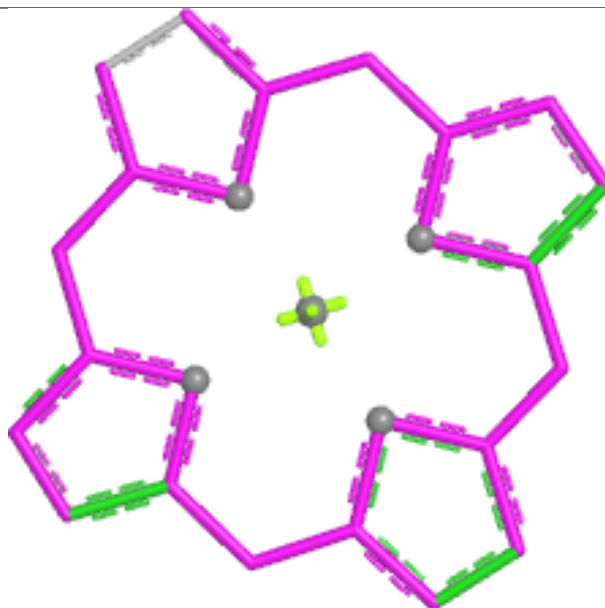
Ligand CLA A 837



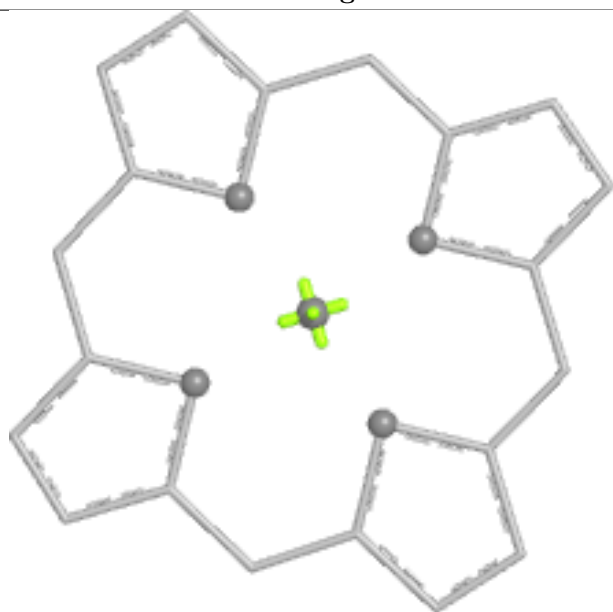
Ligand CLA 1 212



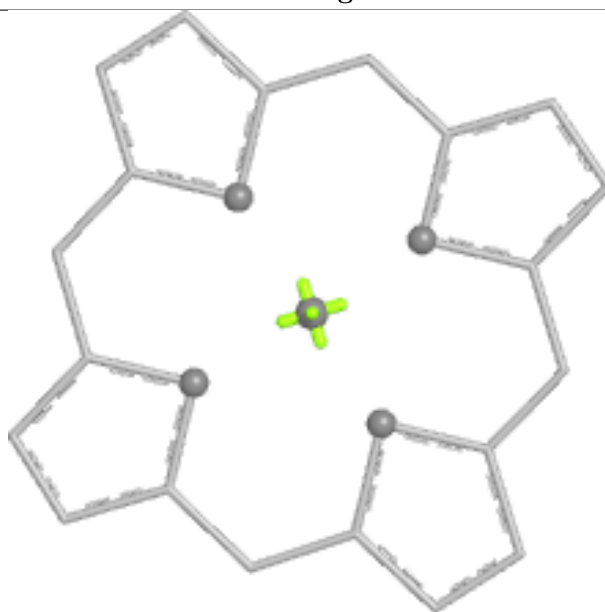
Bond lengths



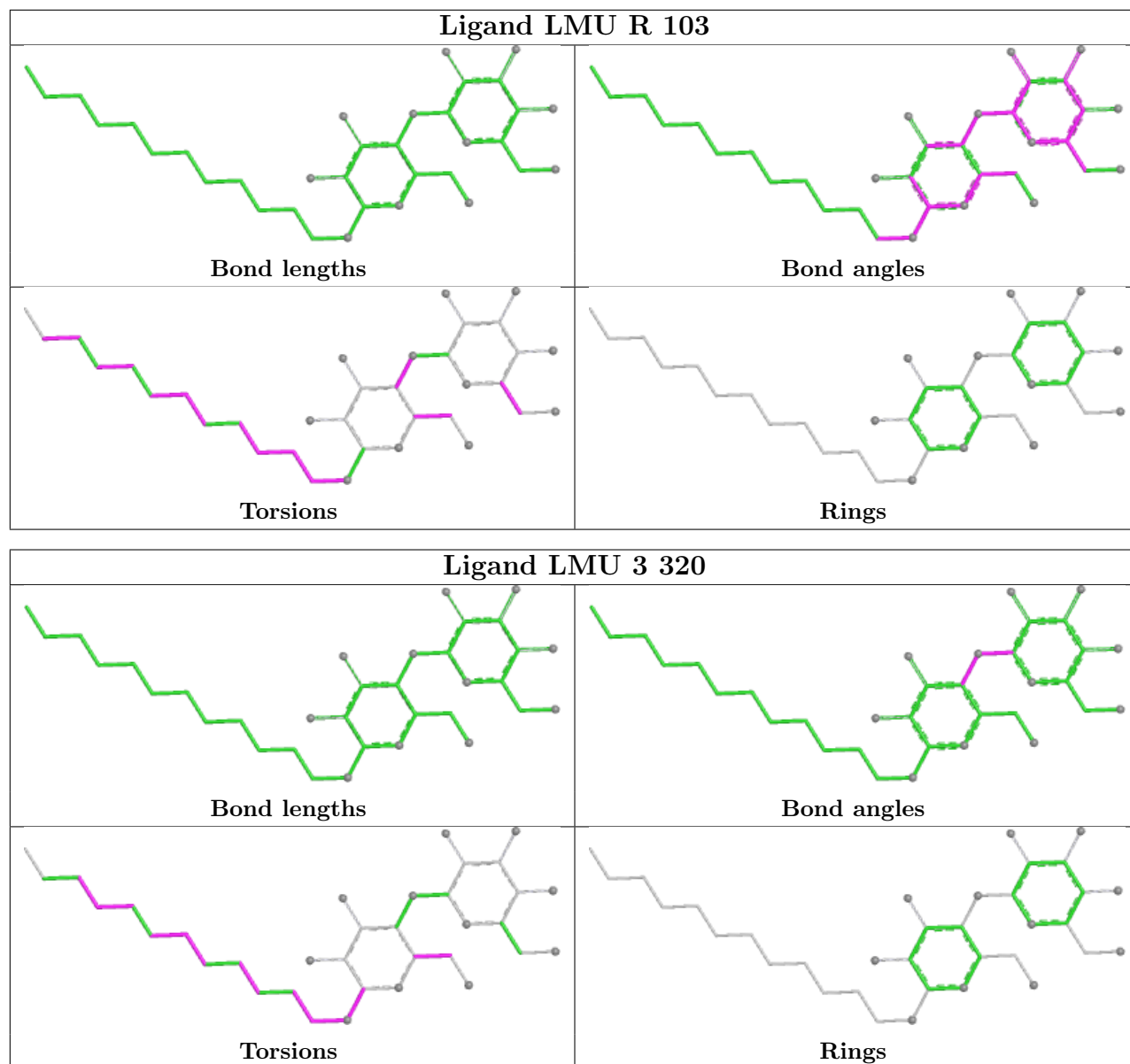
Bond angles



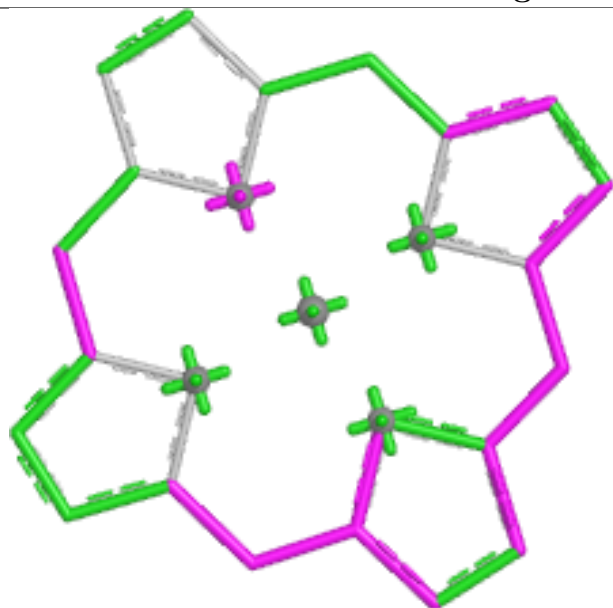
Torsions



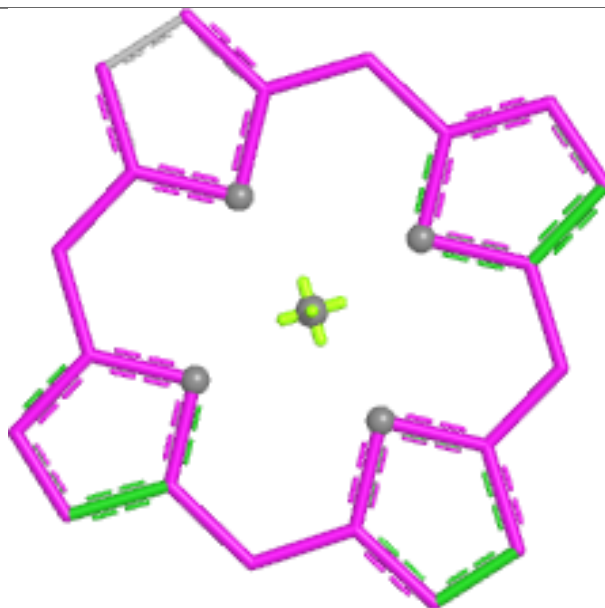
Rings



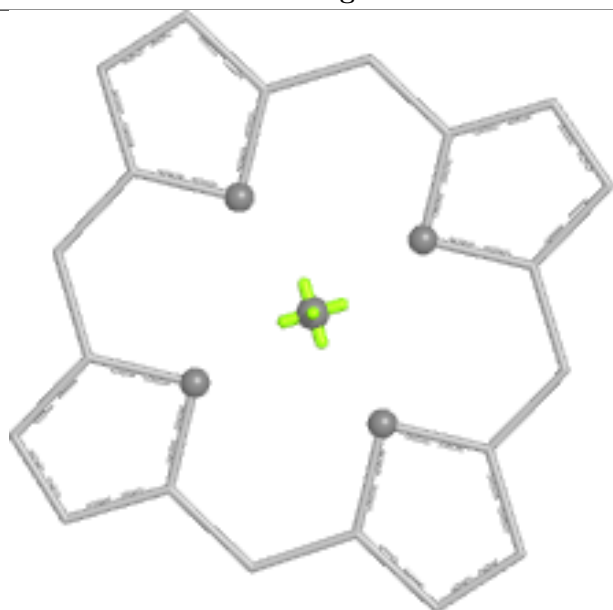
Ligand CLA A 802



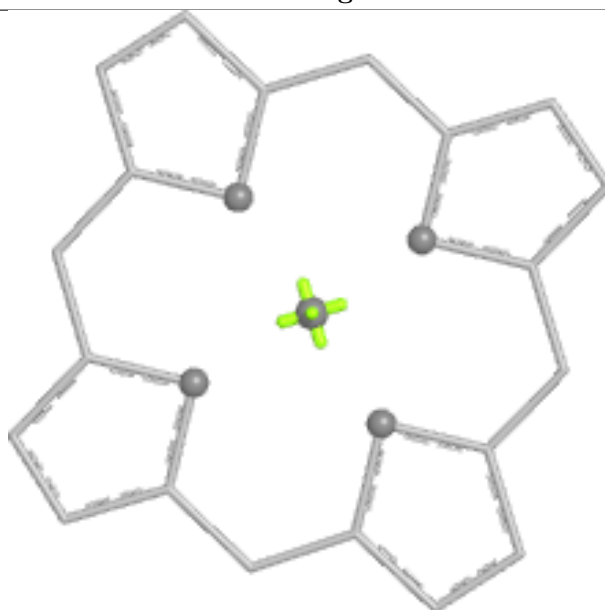
Bond lengths



Bond angles

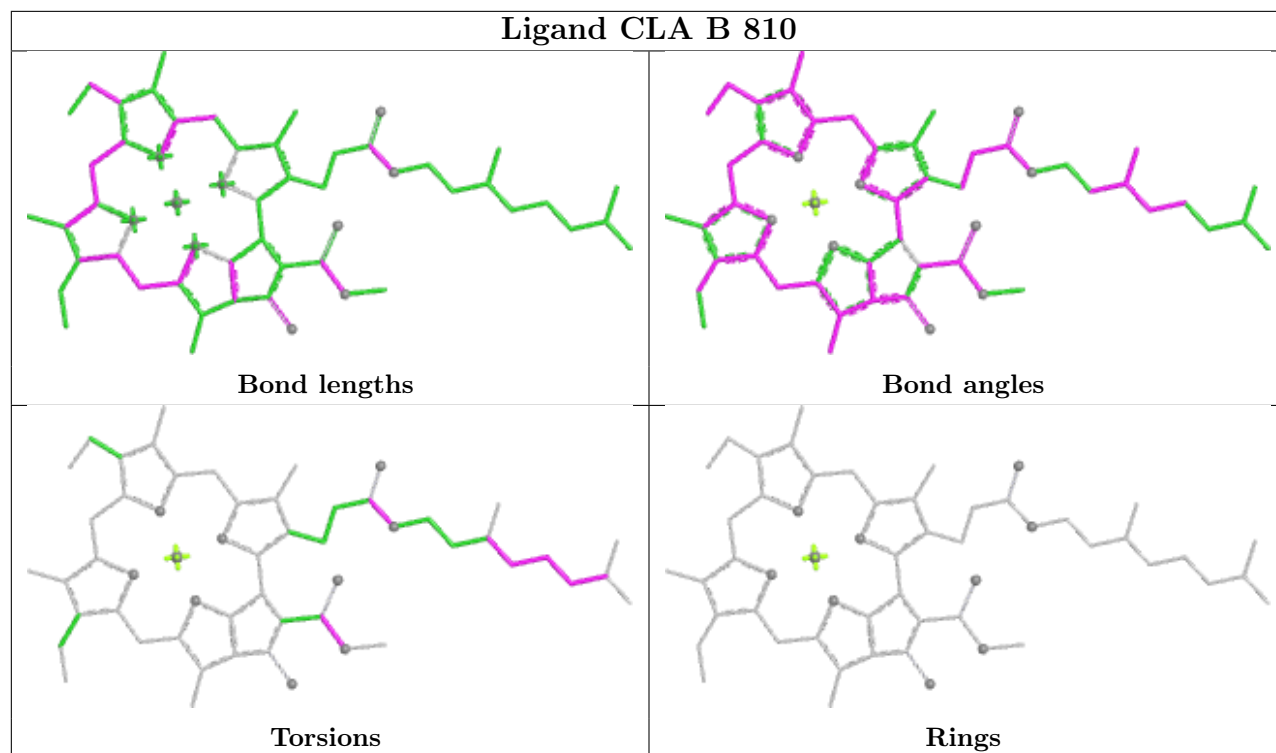


Torsions

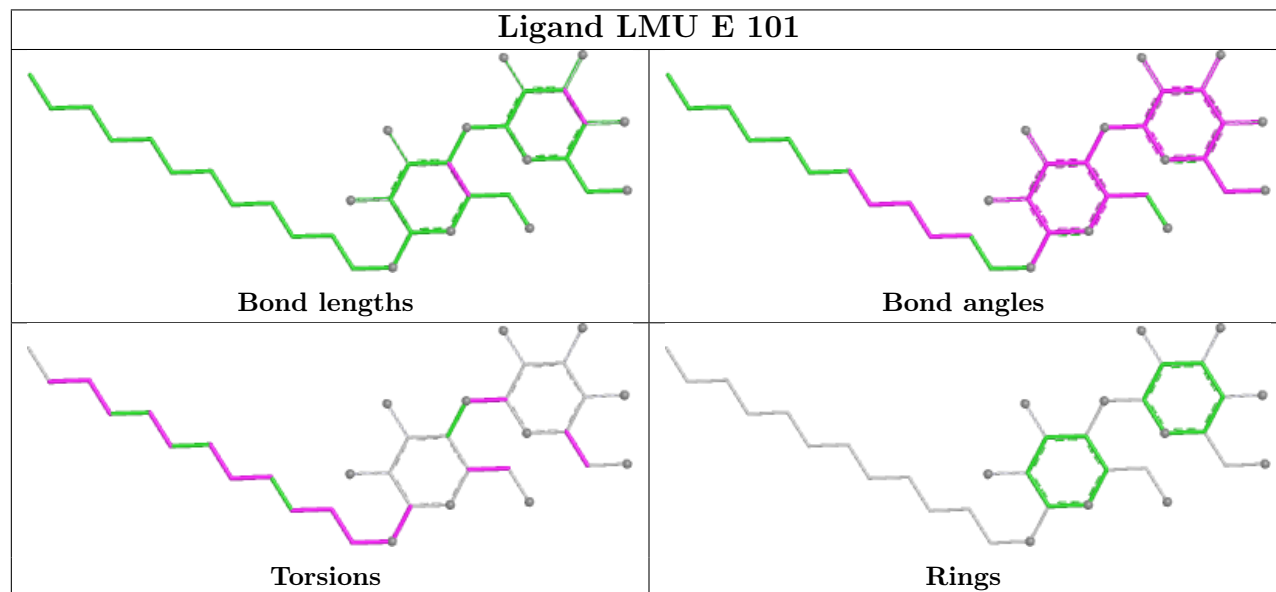


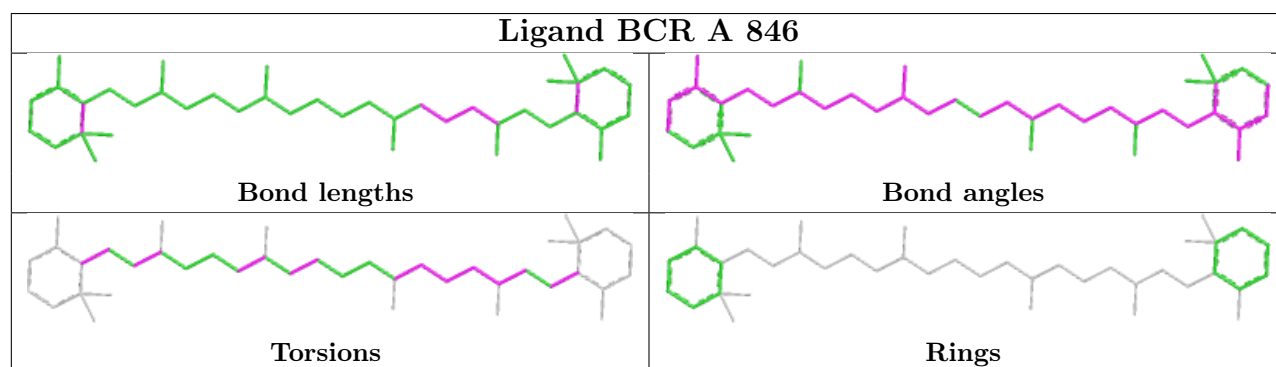
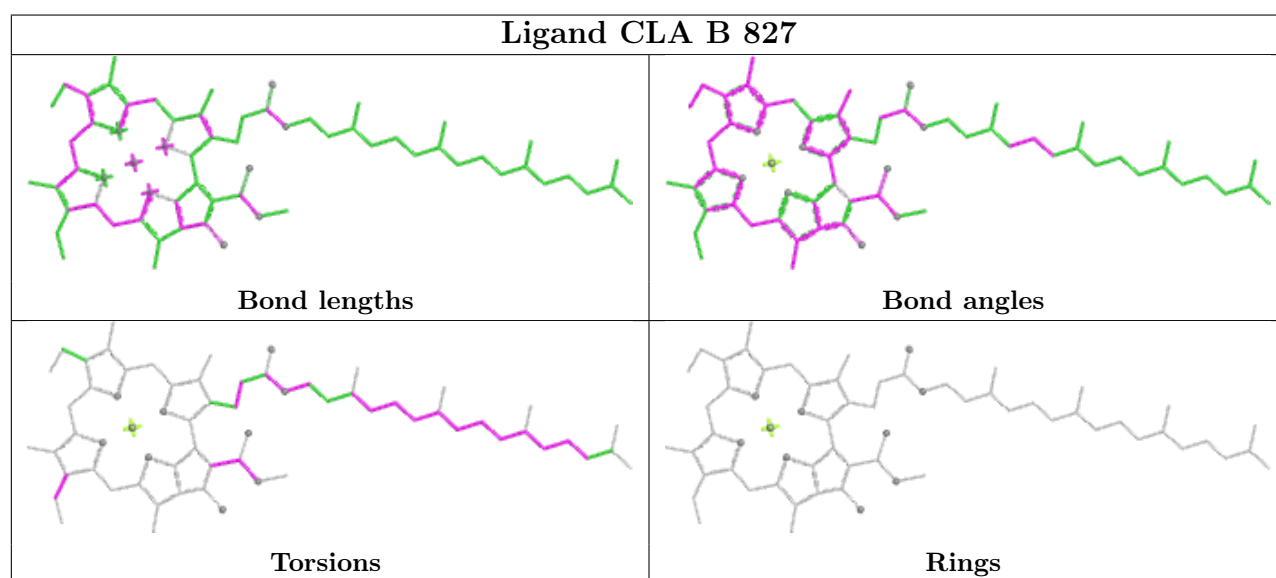
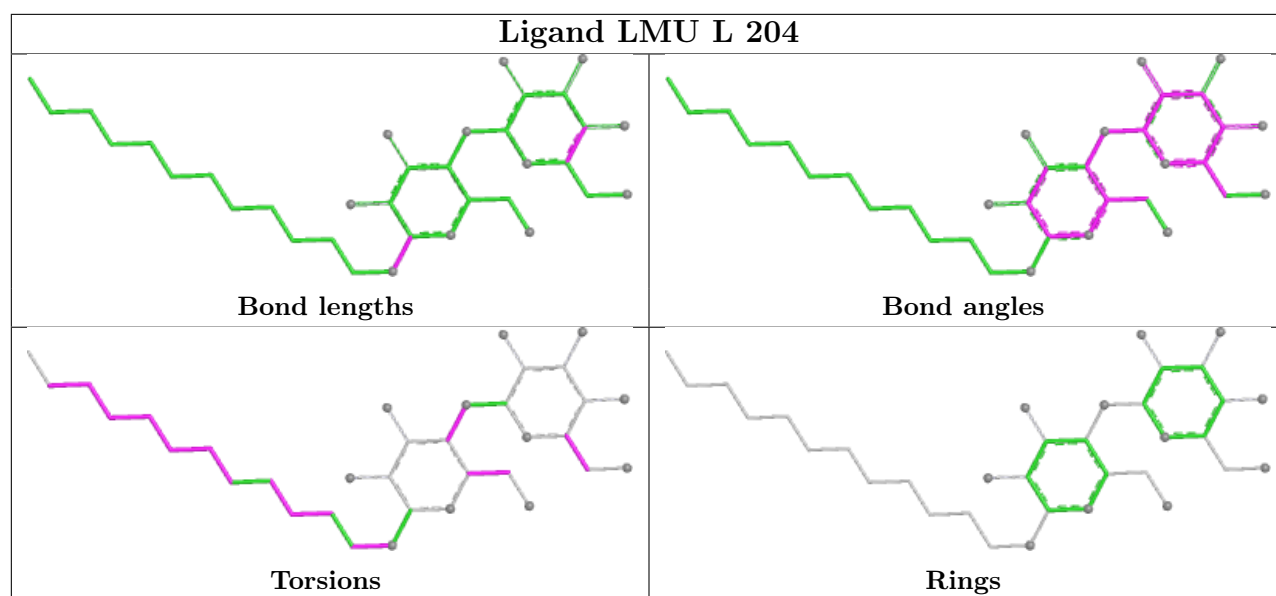
Rings

Ligand CLA B 810

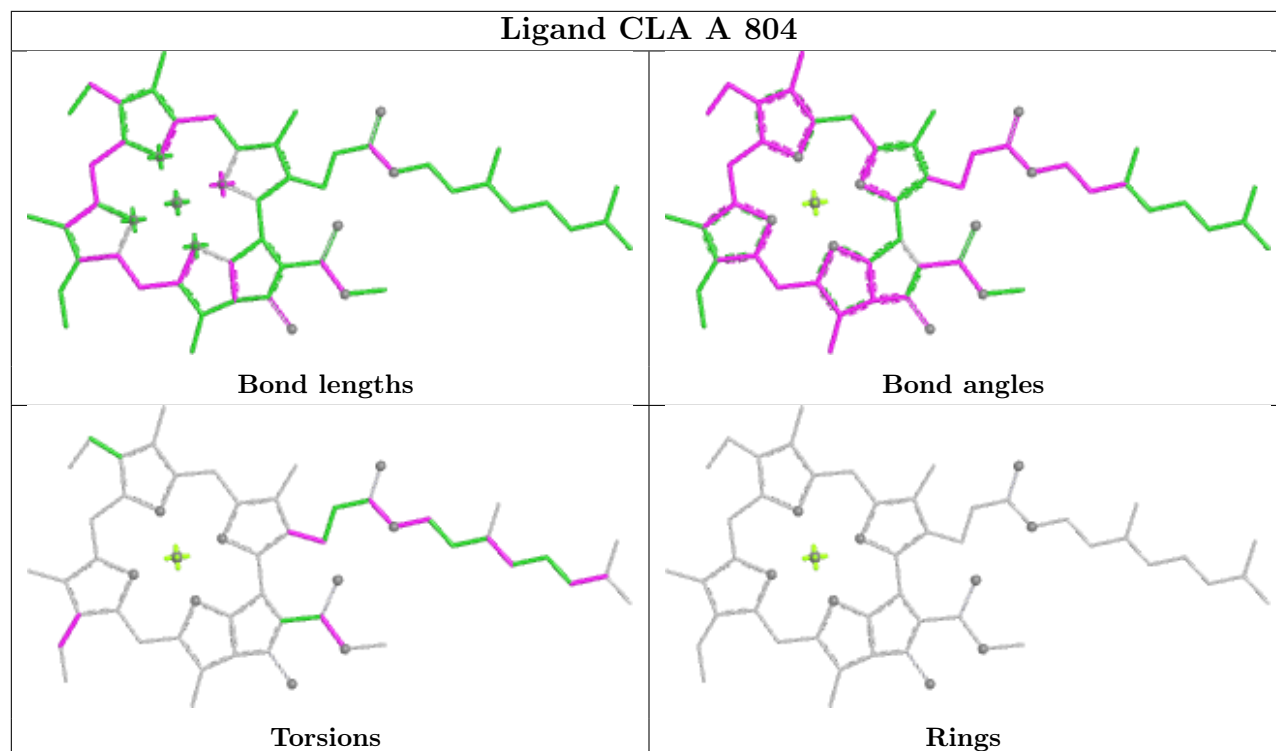


Ligand LMU E 101

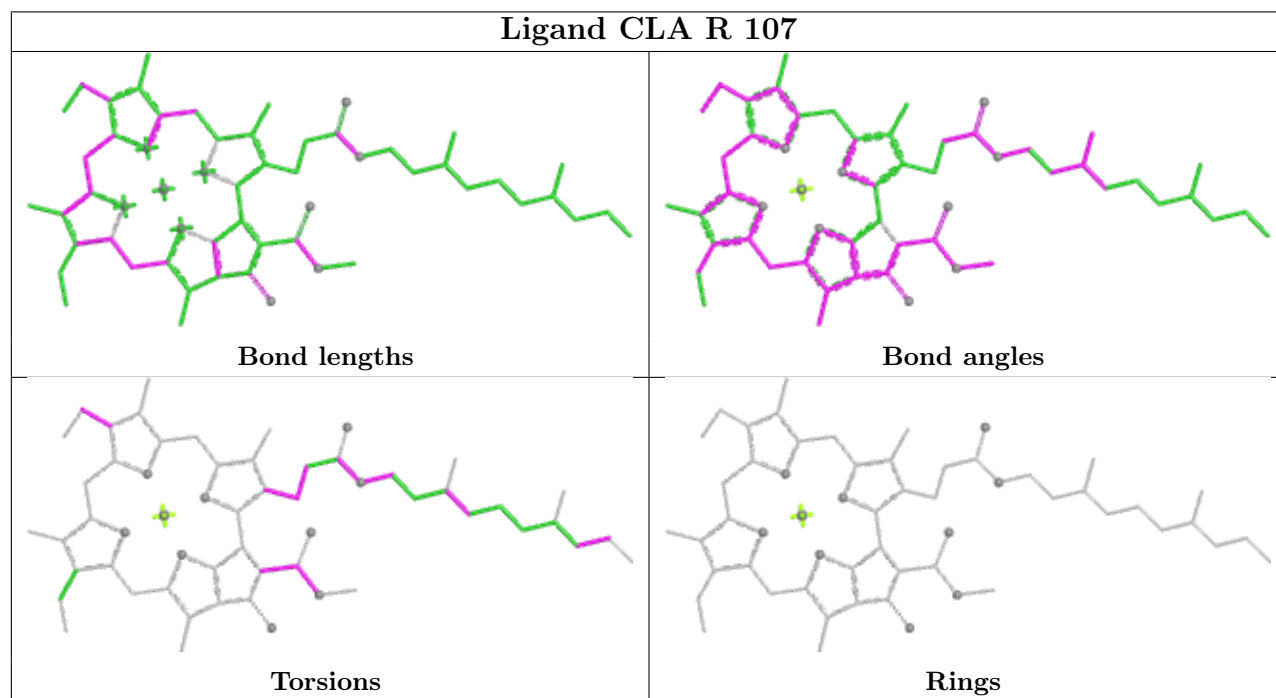




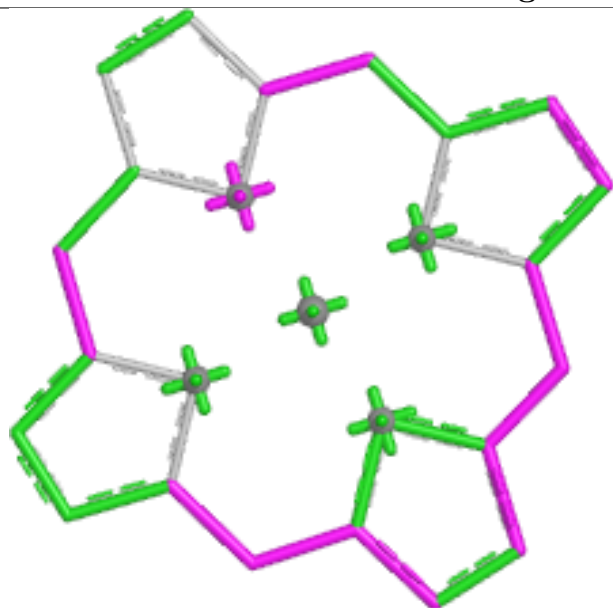
Ligand CLA A 804



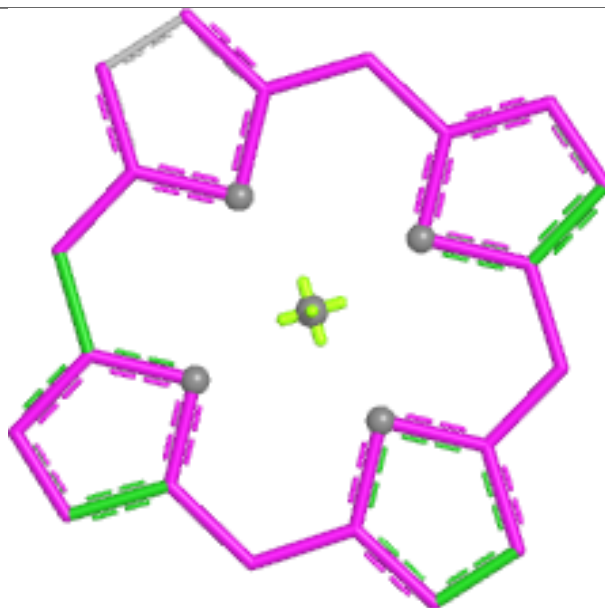
Ligand CLA R 107



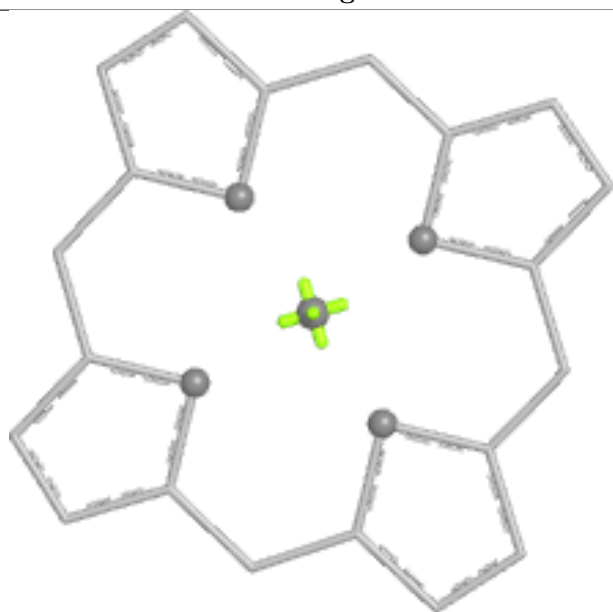
Ligand CLA 3 307



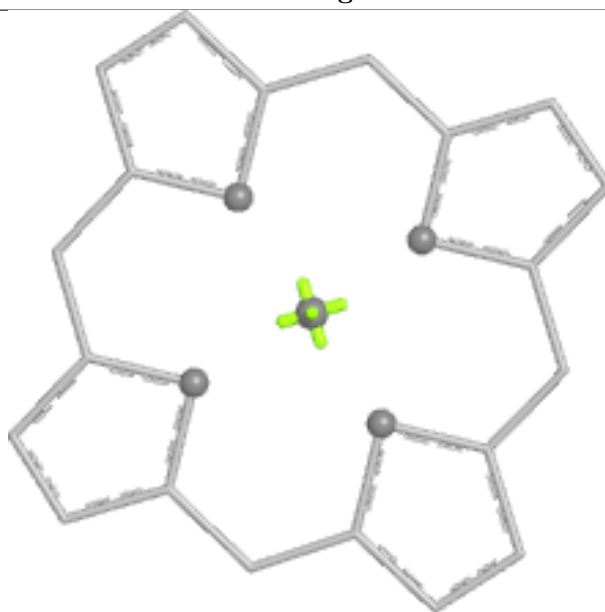
Bond lengths



Bond angles

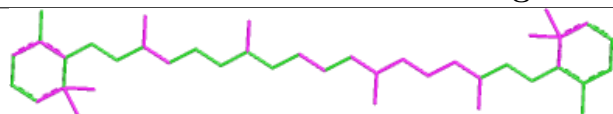


Torsions

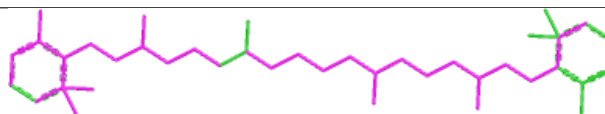


Rings

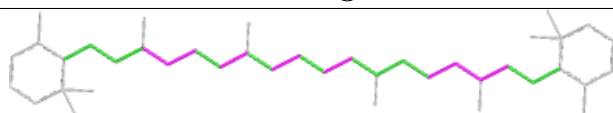
Ligand BCR B 852



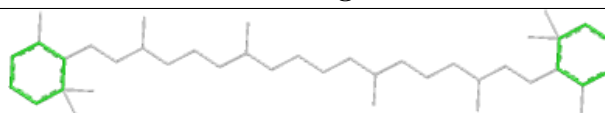
Bond lengths



Bond angles

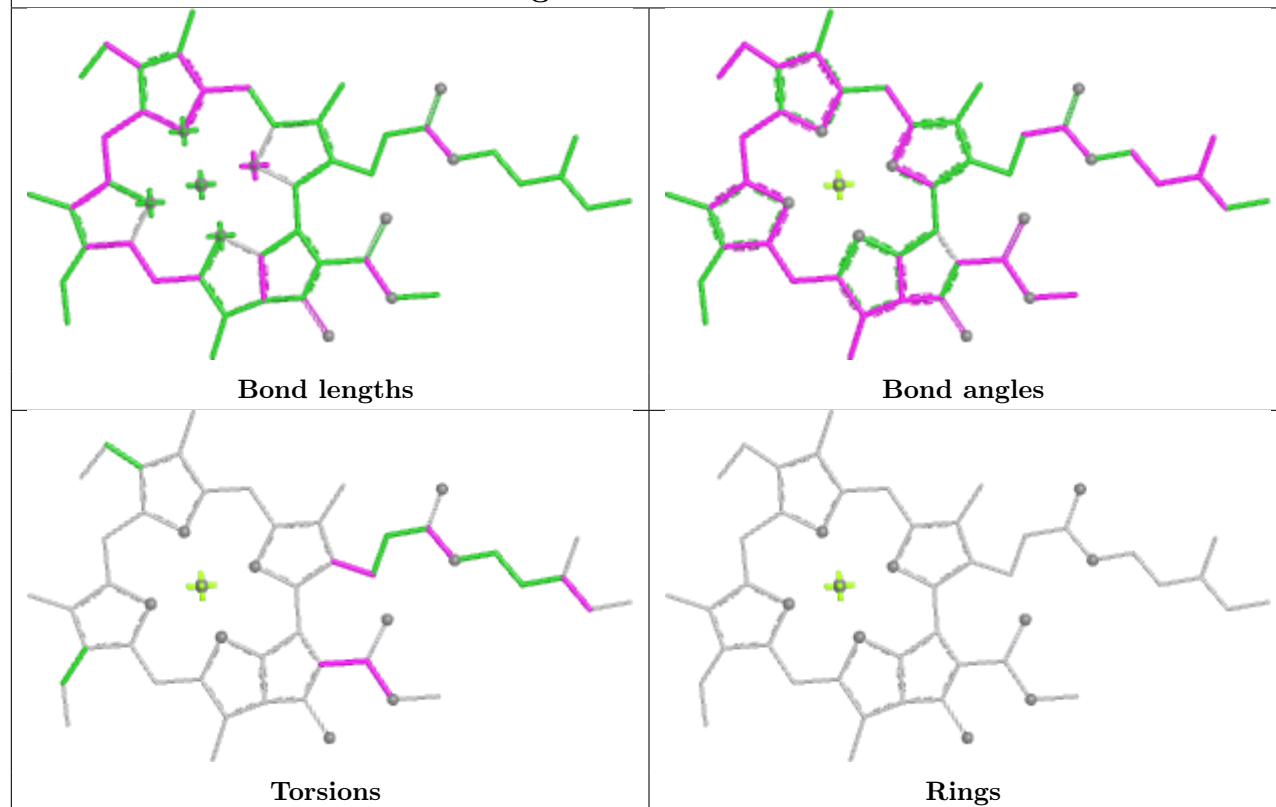


Torsions

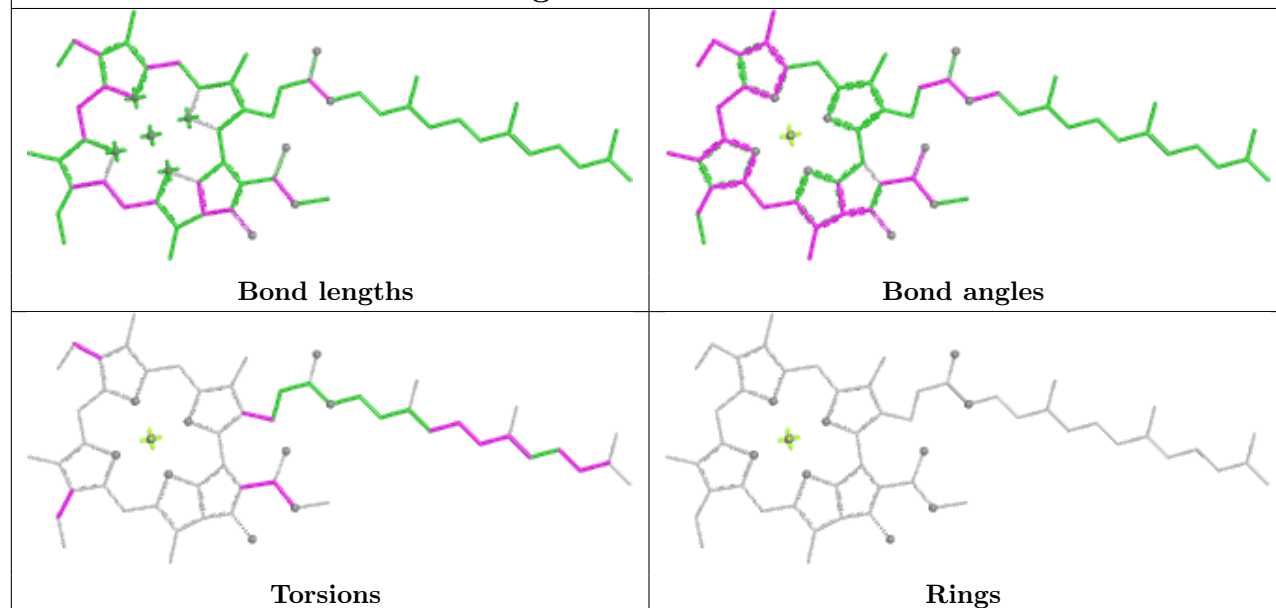


Rings

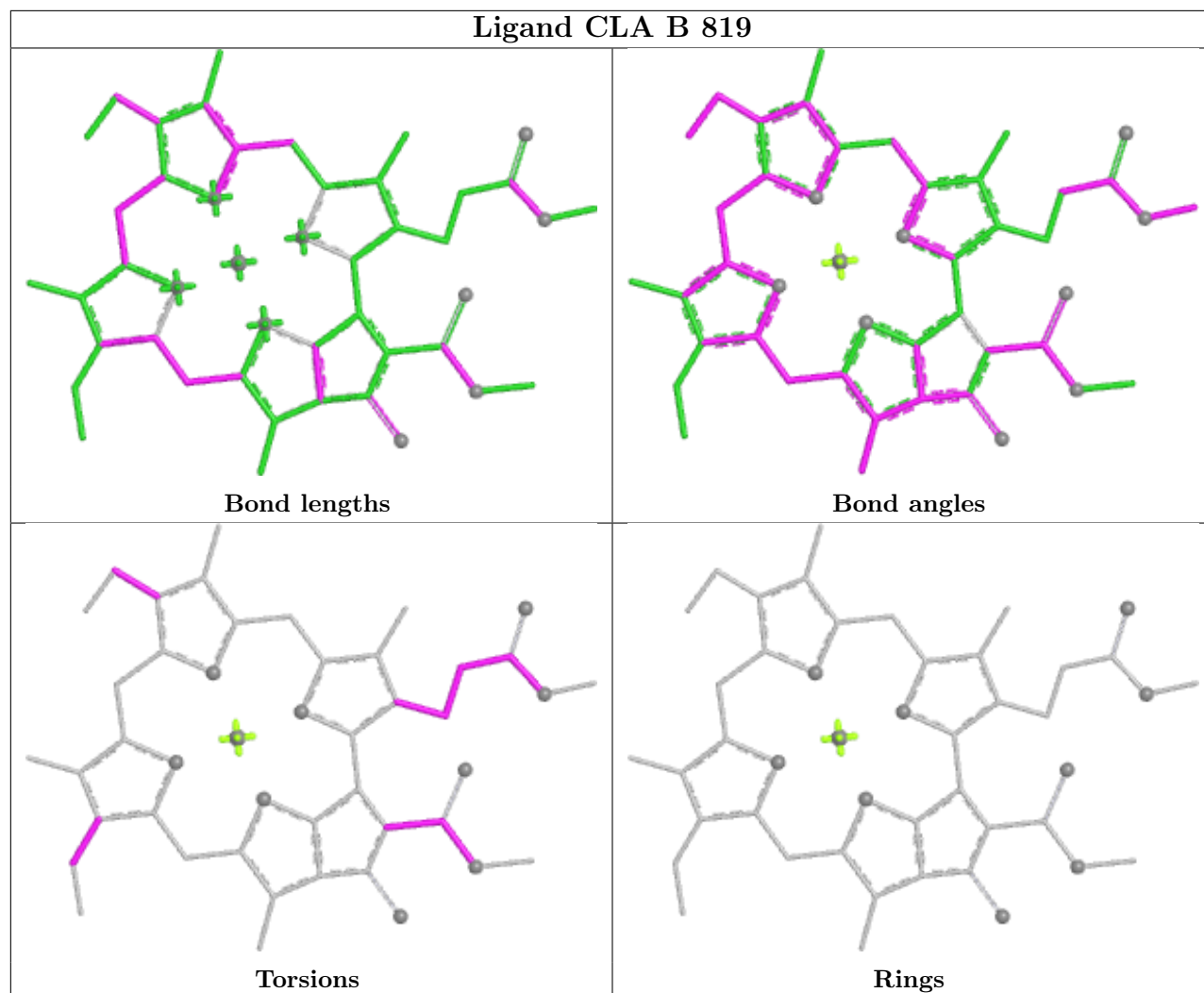
Ligand CLA A 820



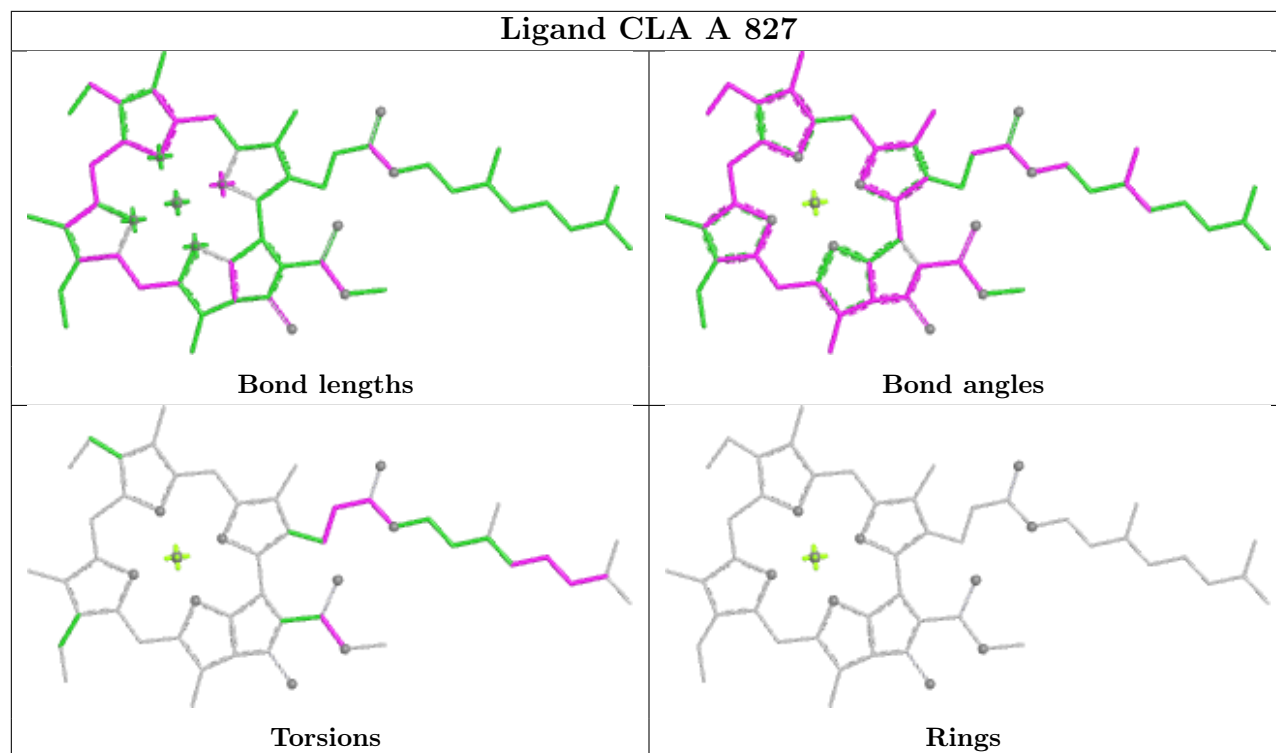
Ligand CLA B 835



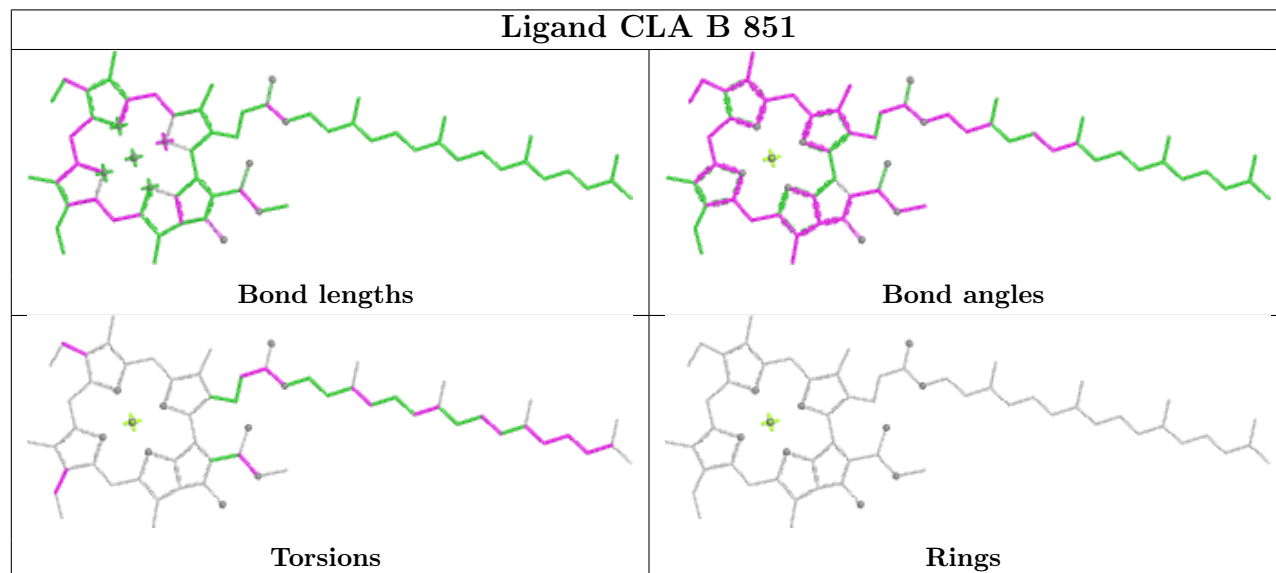
Ligand CLA B 819

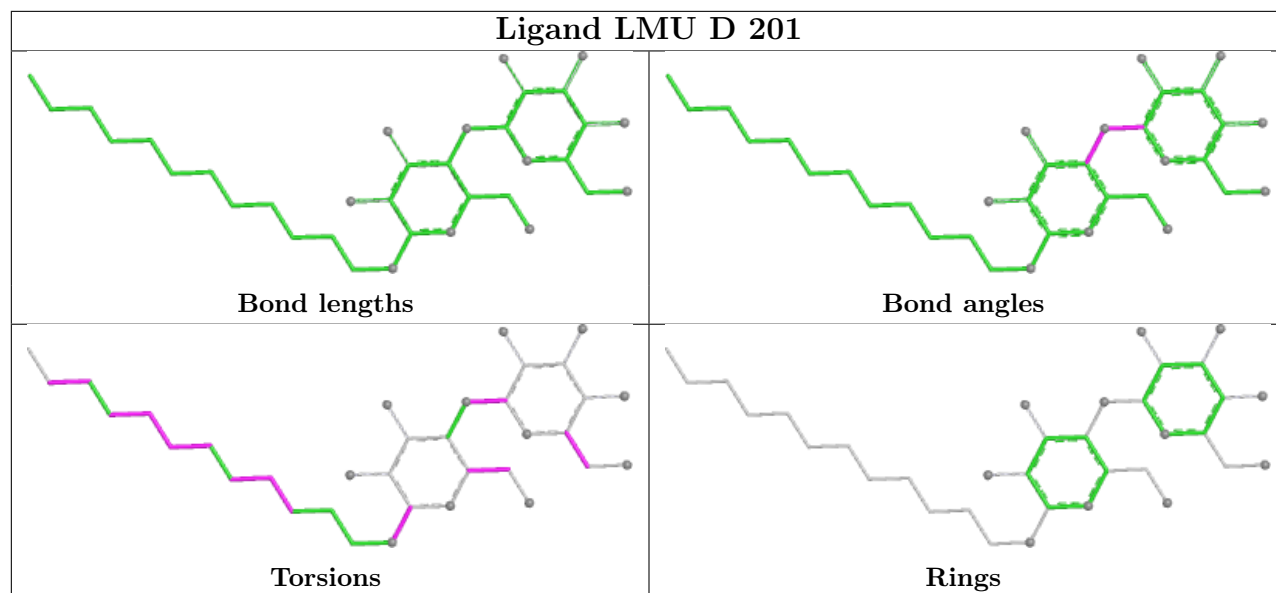


Ligand CLA A 827

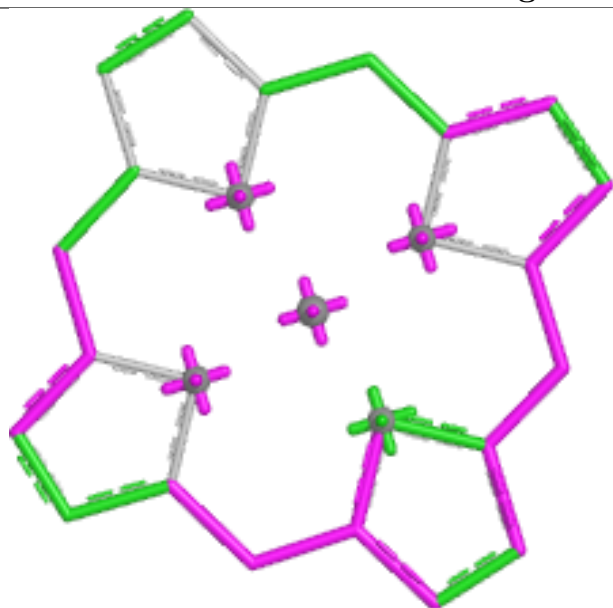


Ligand CLA B 851

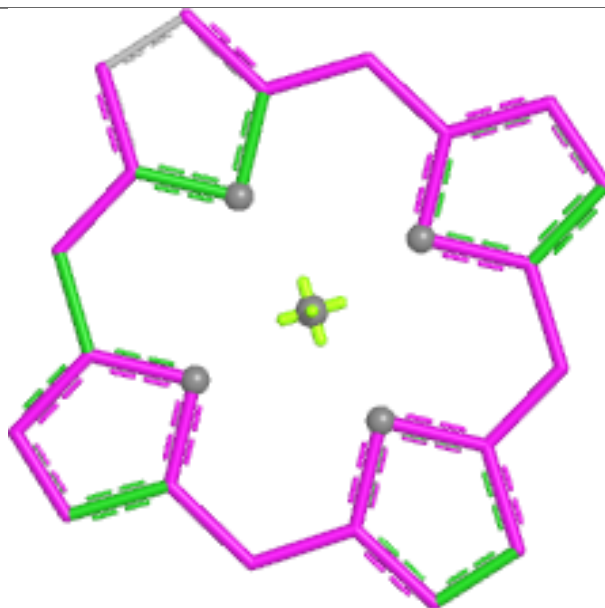




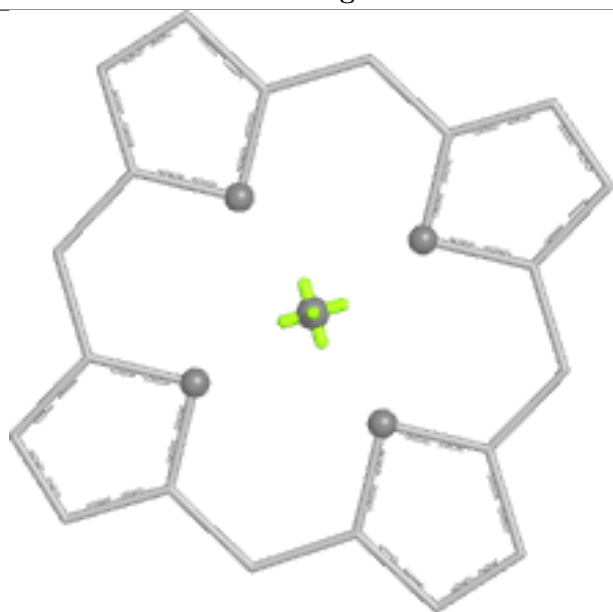
Ligand CLA 4 310



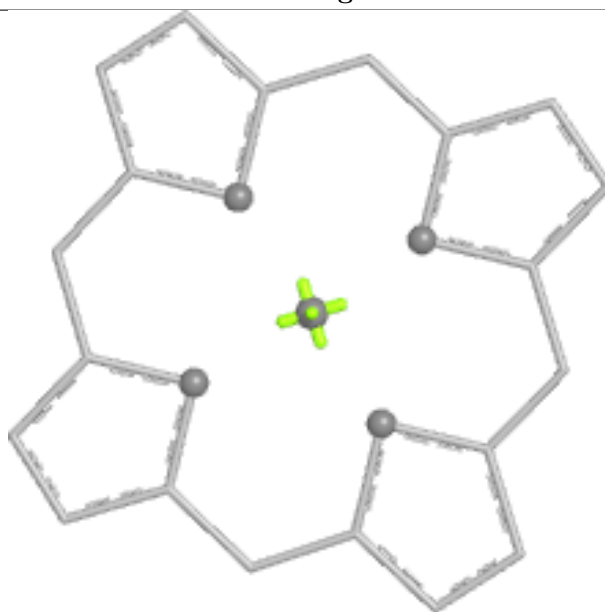
Bond lengths



Bond angles

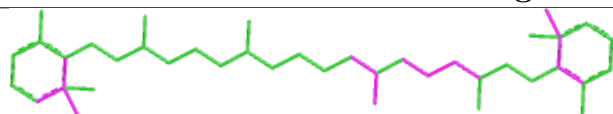


Torsions

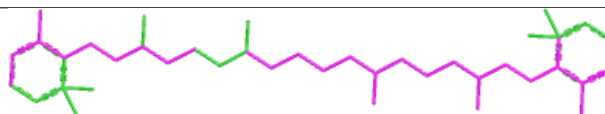


Rings

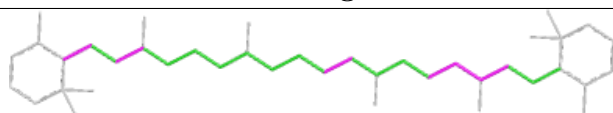
Ligand BCR L 208



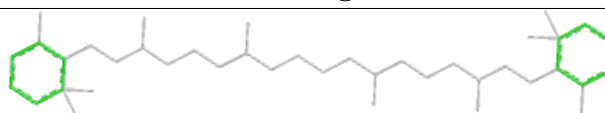
Bond lengths



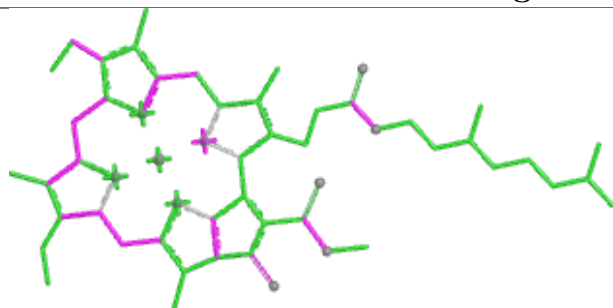
Bond angles



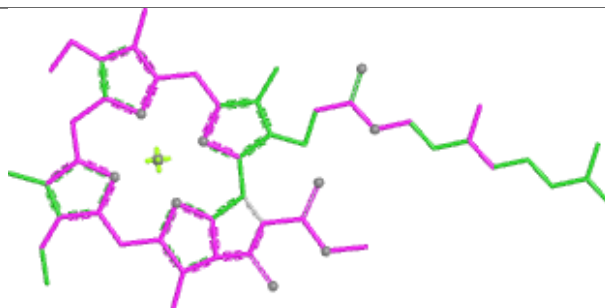
Torsions



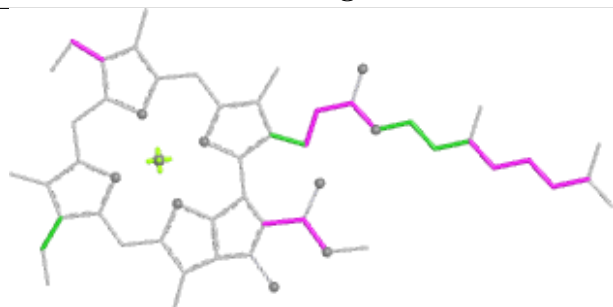
Rings

Ligand CLA H 103

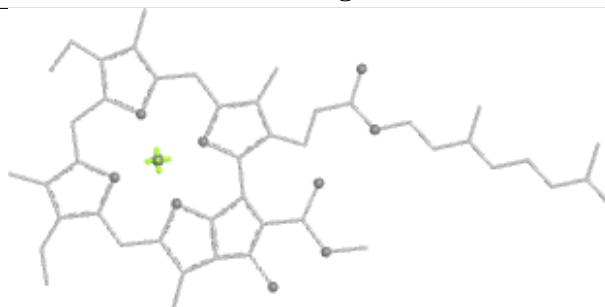
Bond lengths



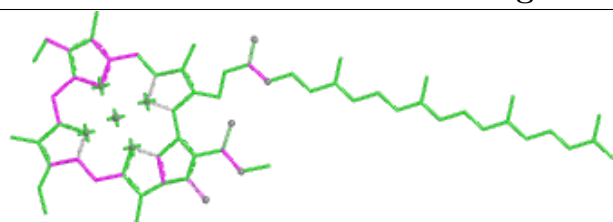
Bond angles



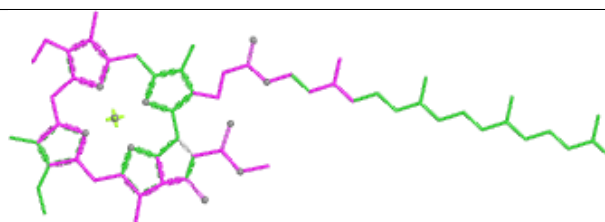
Torsions



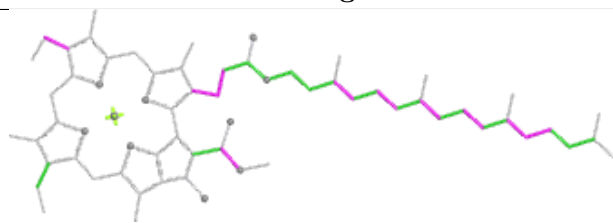
Rings

Ligand CLA L 202

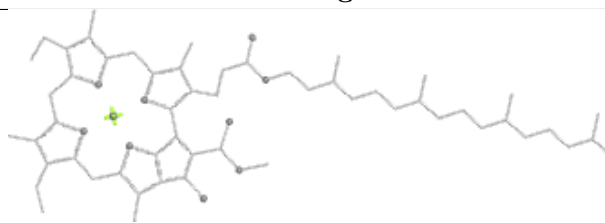
Bond lengths



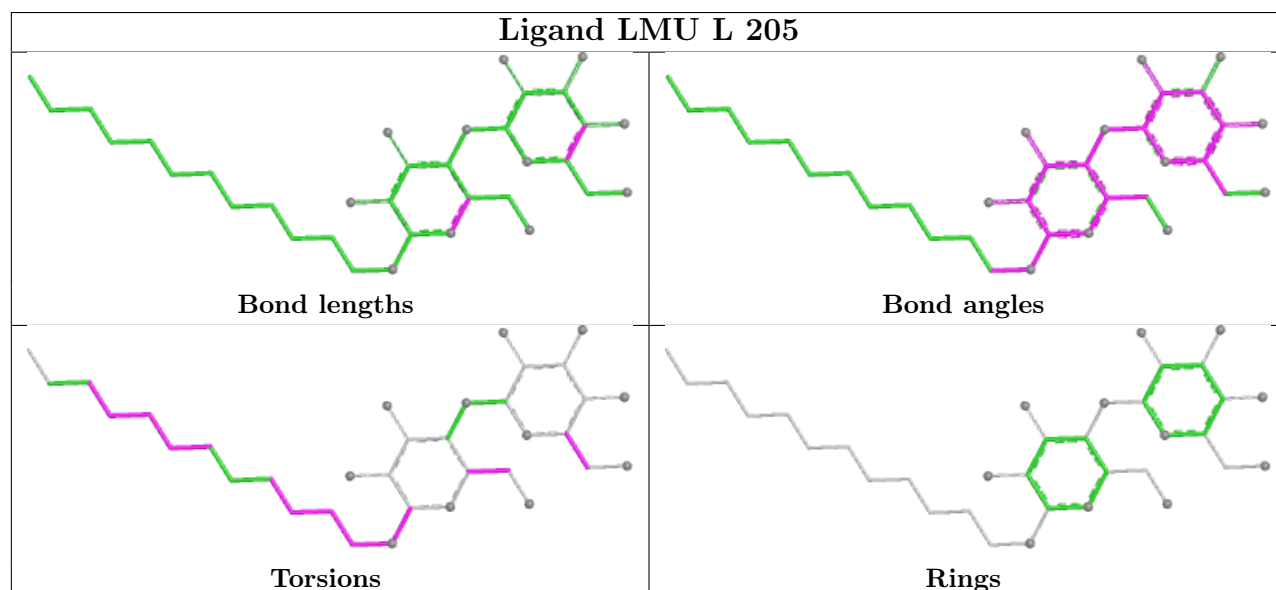
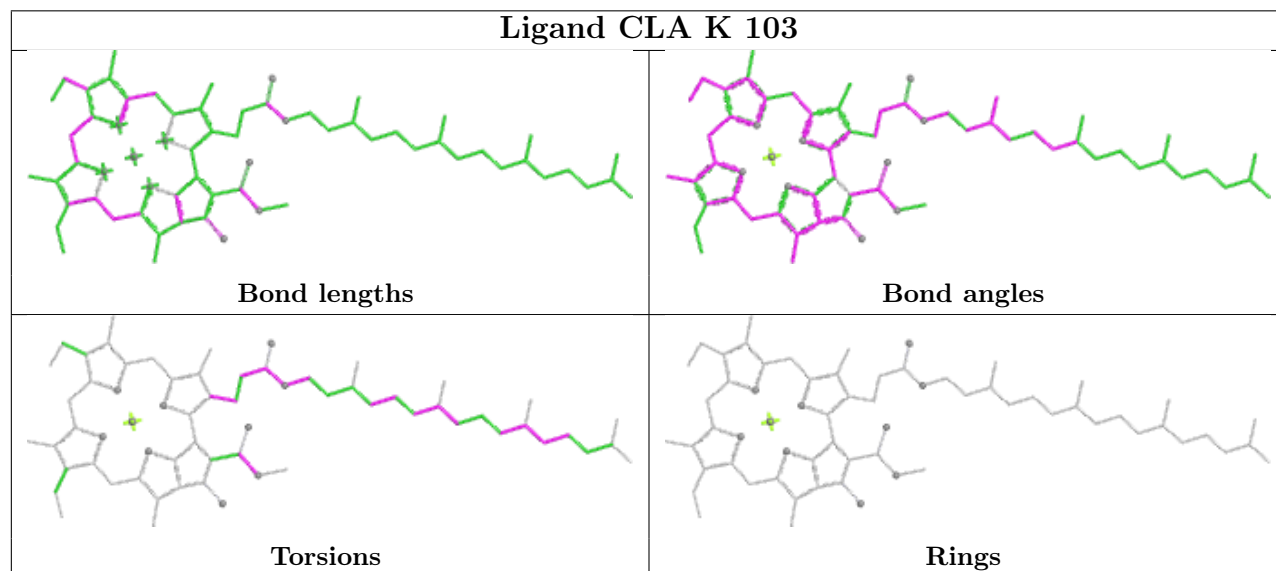
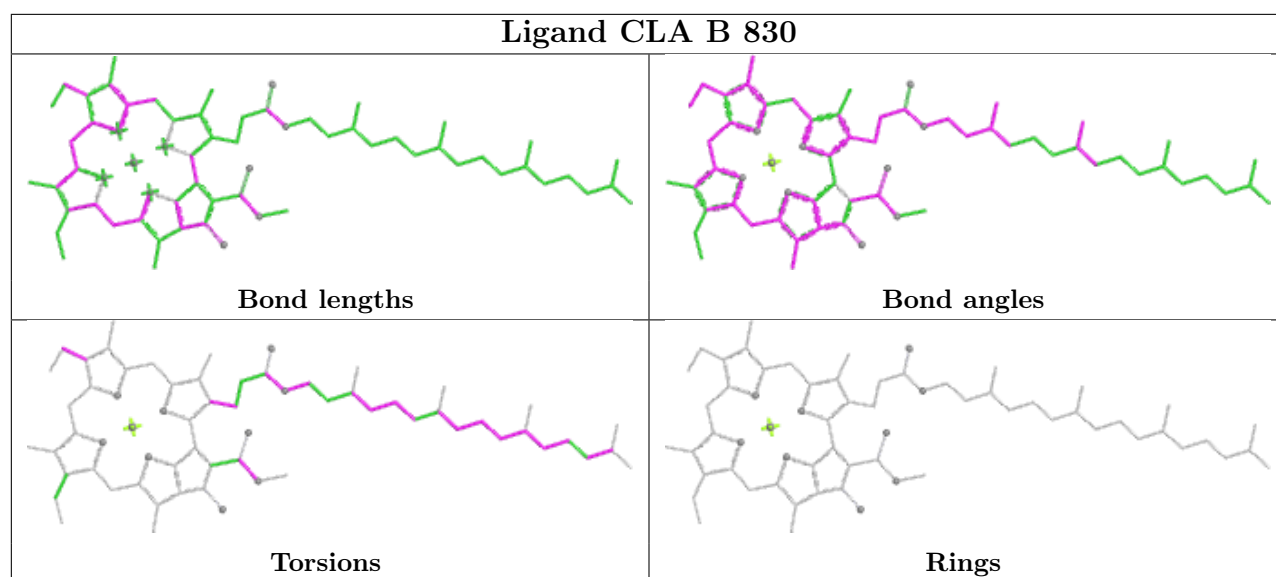
Bond angles



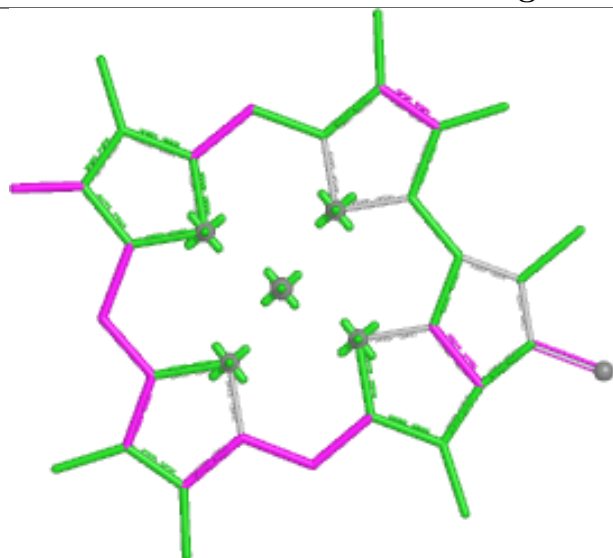
Torsions



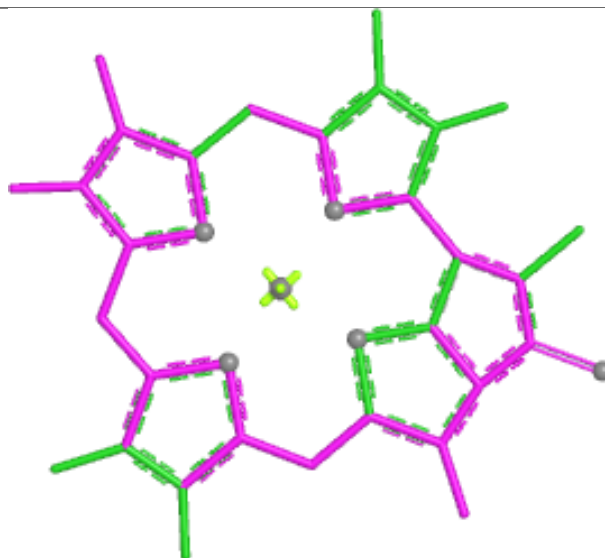
Rings



Ligand CLA 3 304



Bond lengths



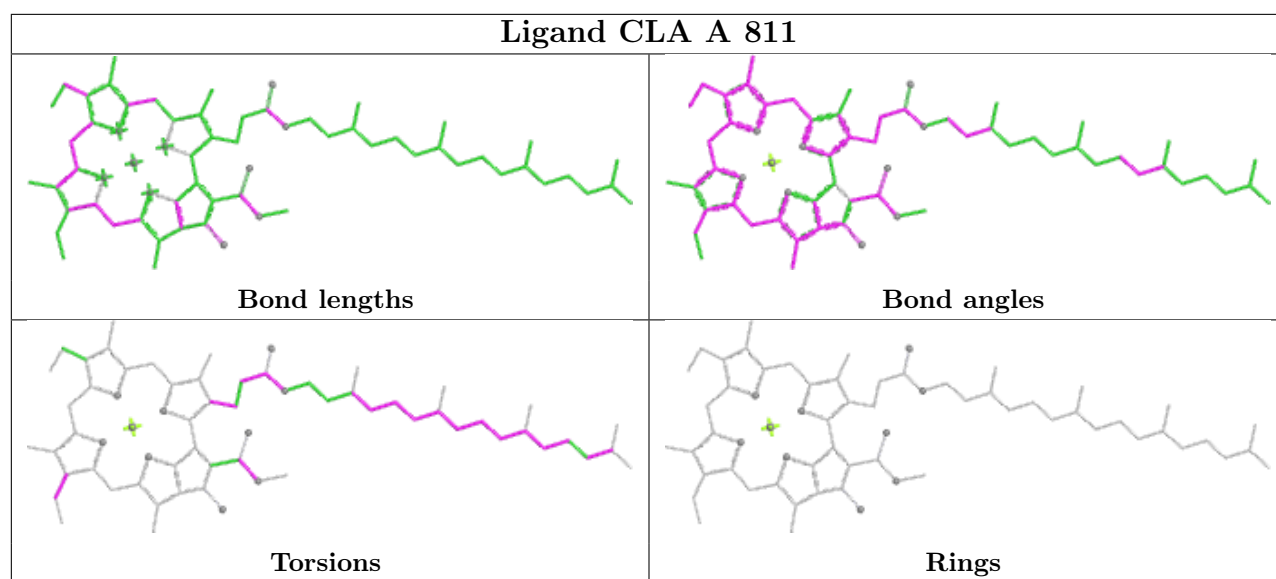
Bond angles



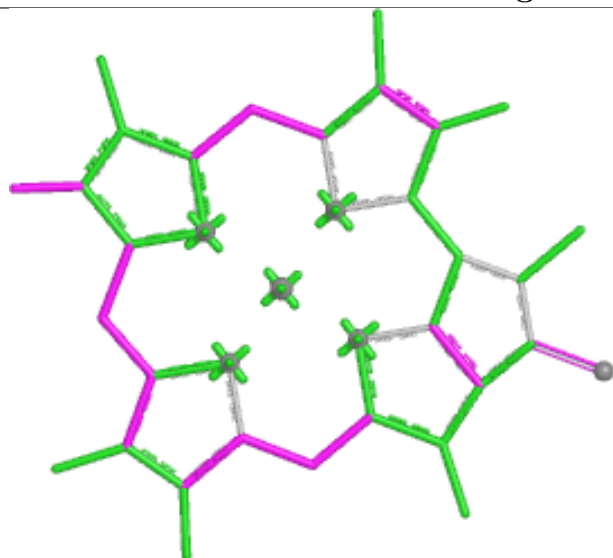
Torsions



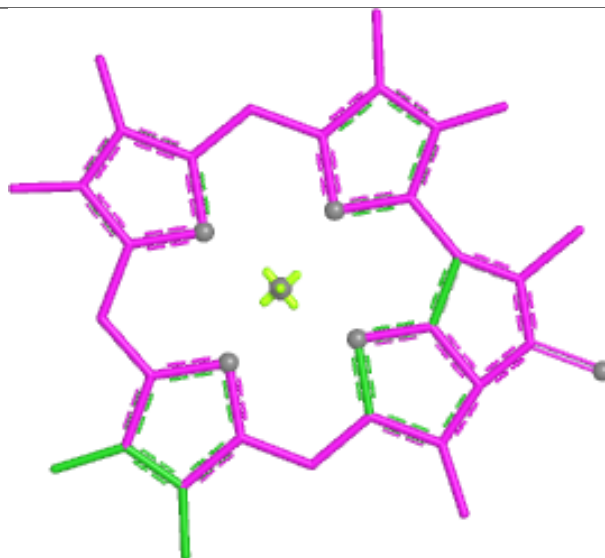
Rings



Ligand CLA F 204



Bond lengths



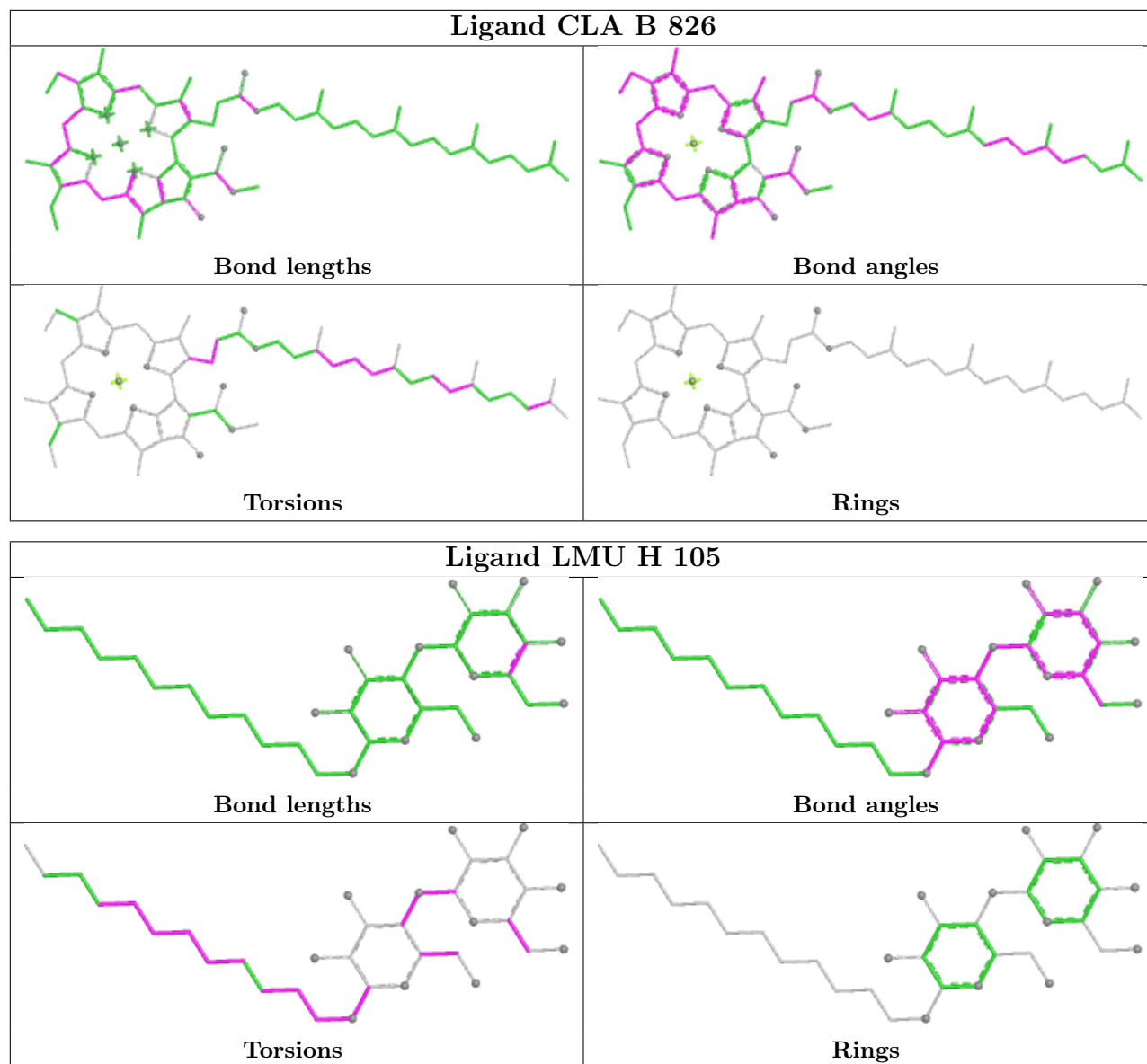
Bond angles



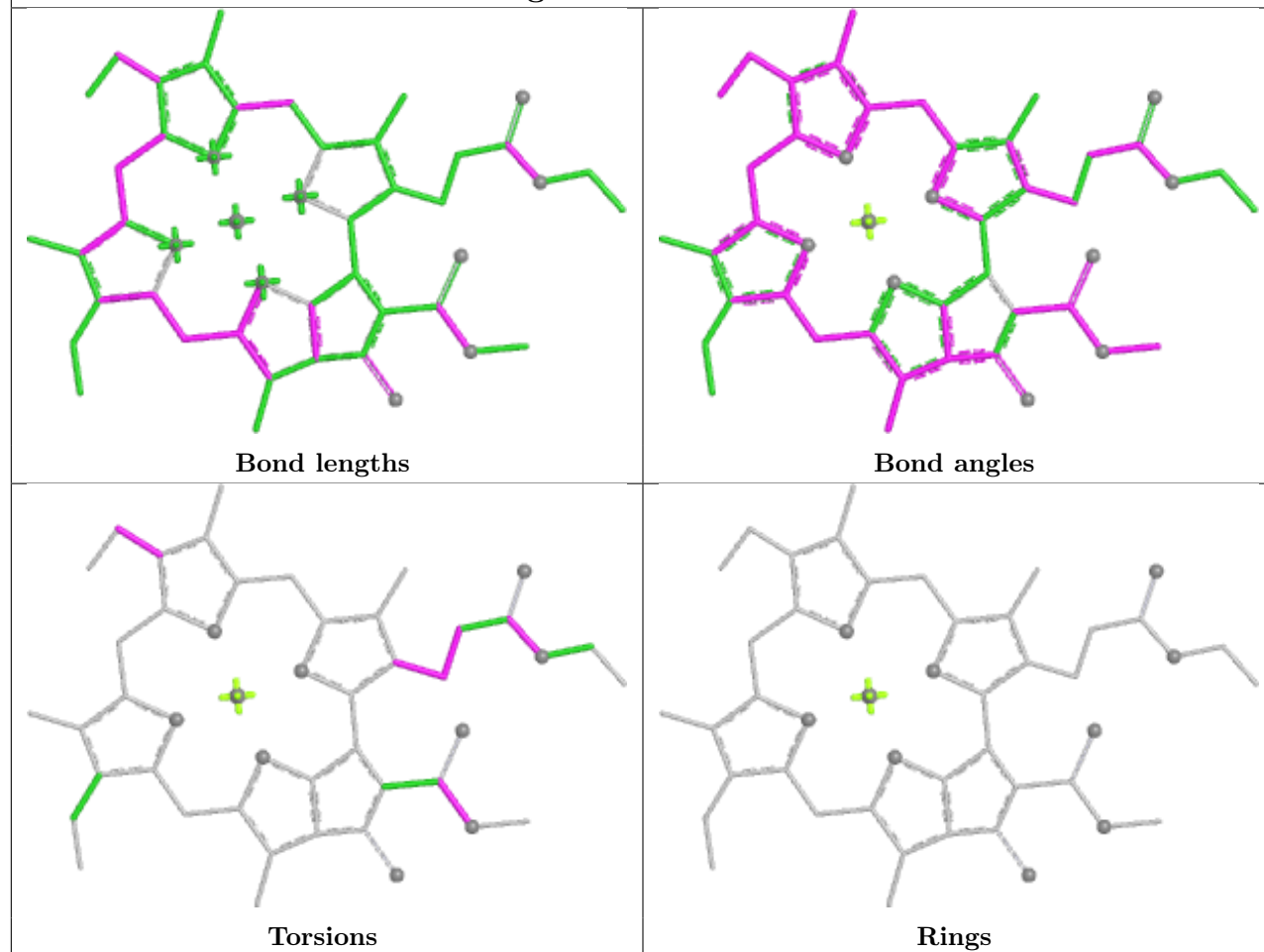
Torsions



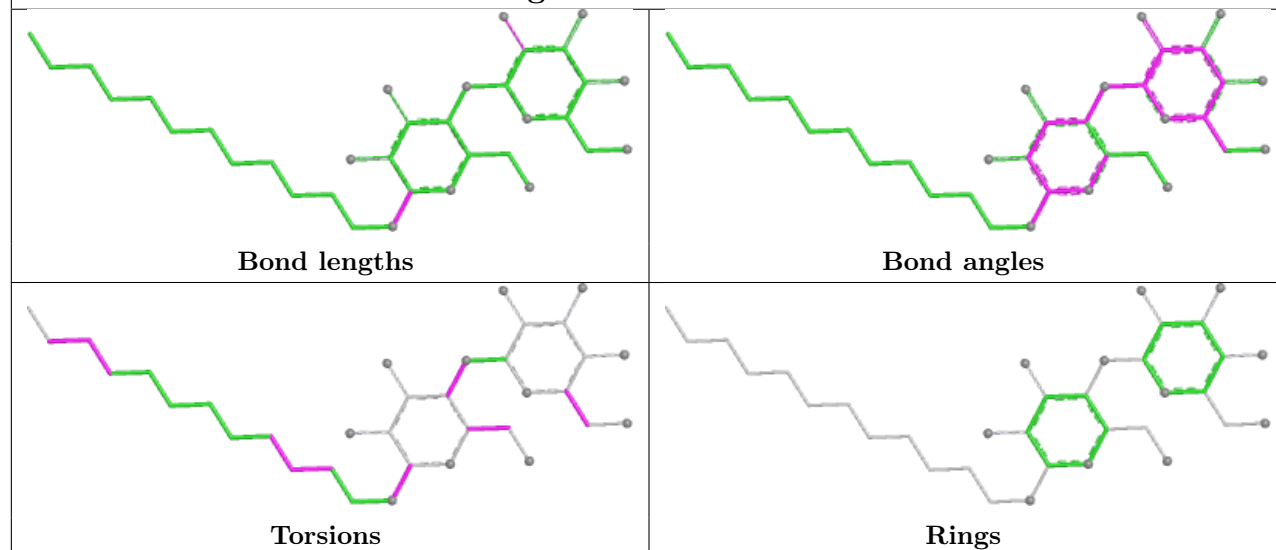
Rings

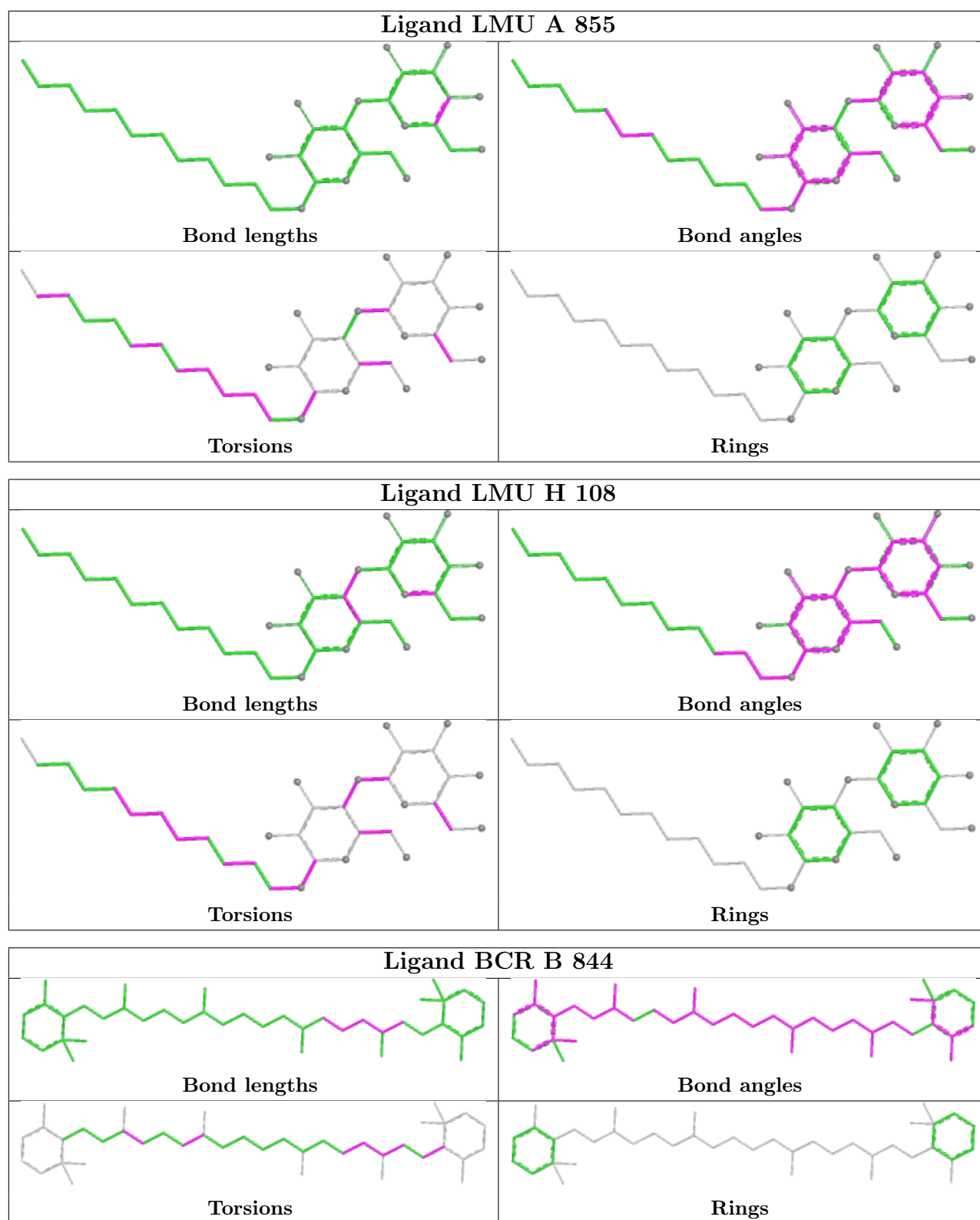


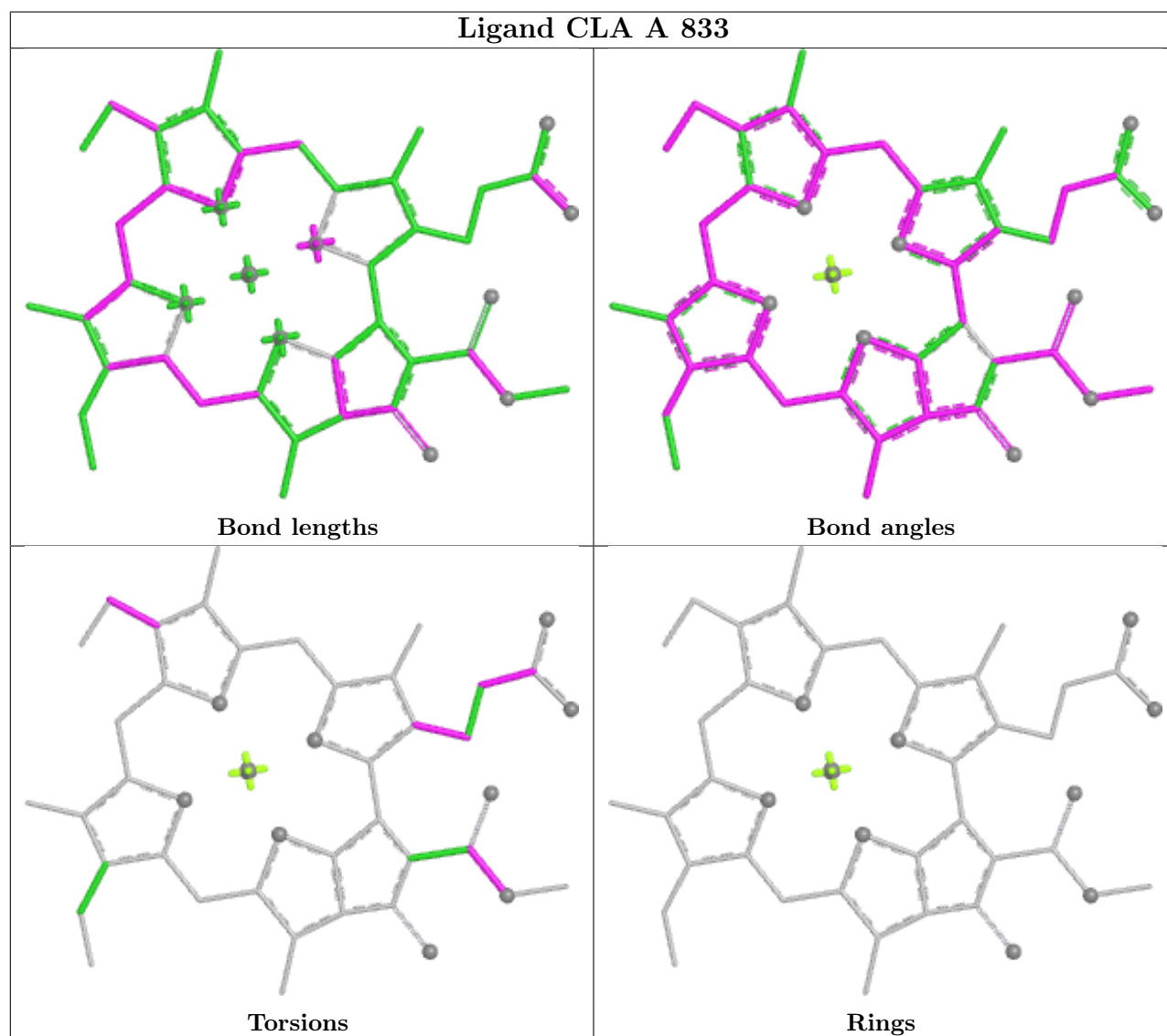
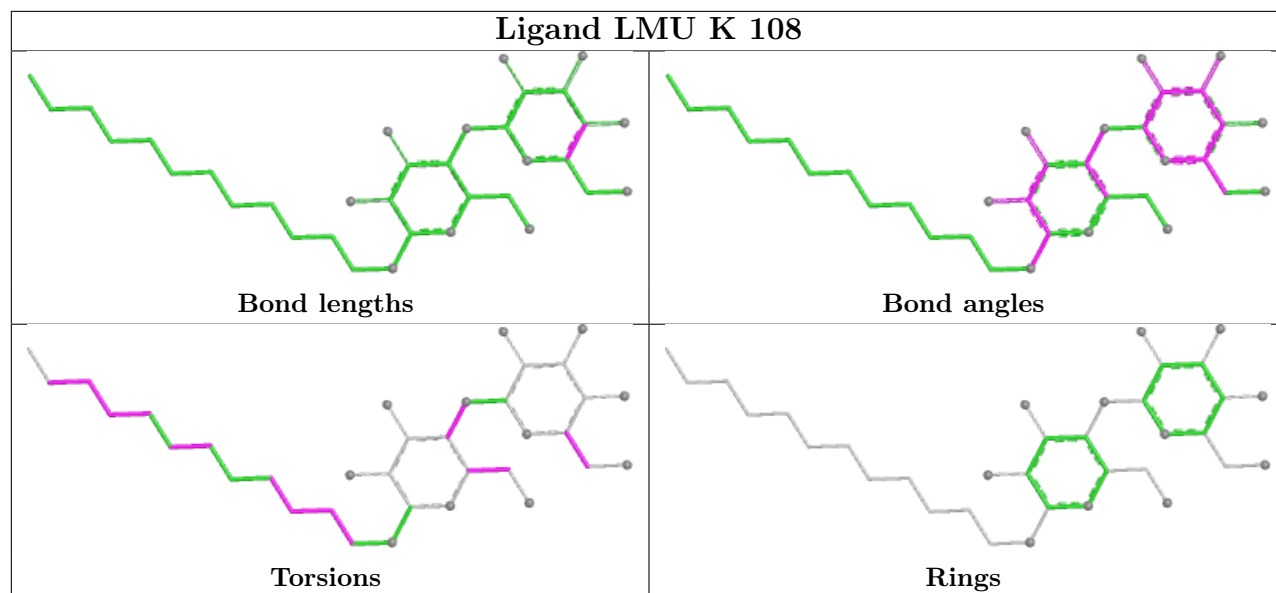
Ligand CLA B 837

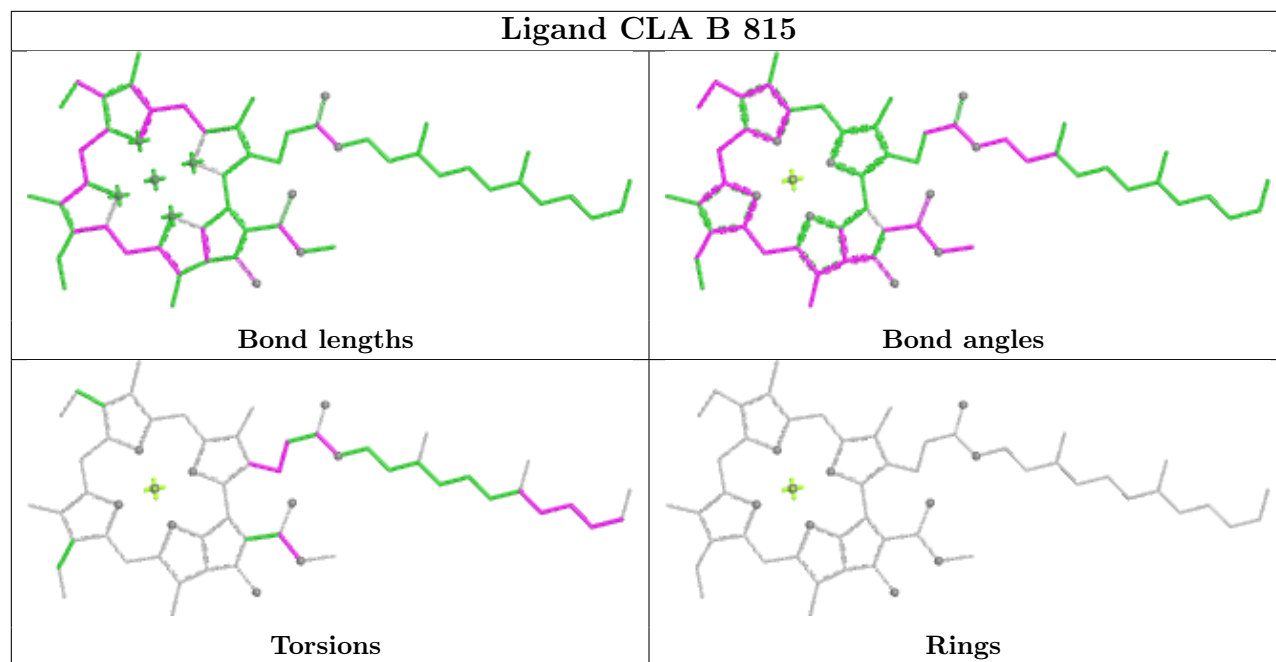


Ligand LMU R 101

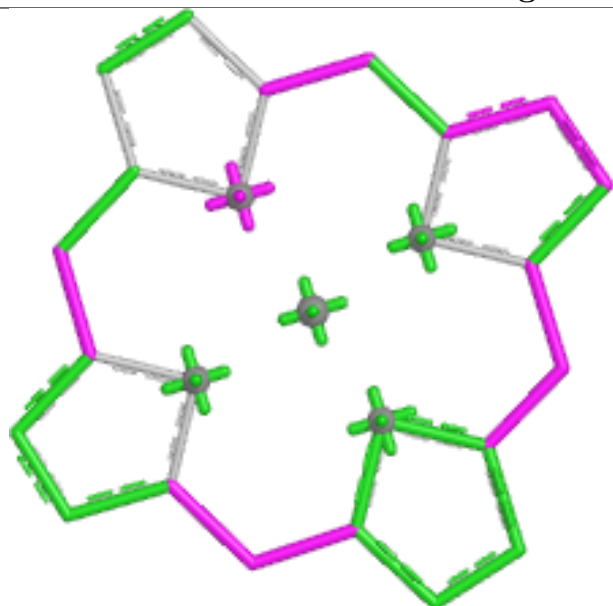




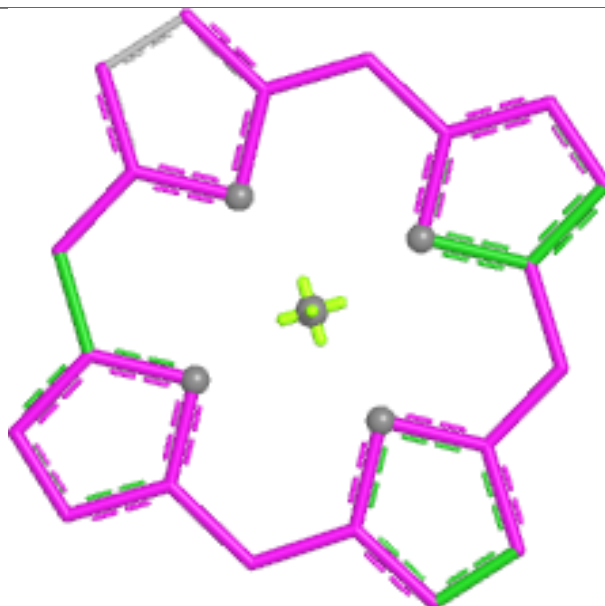




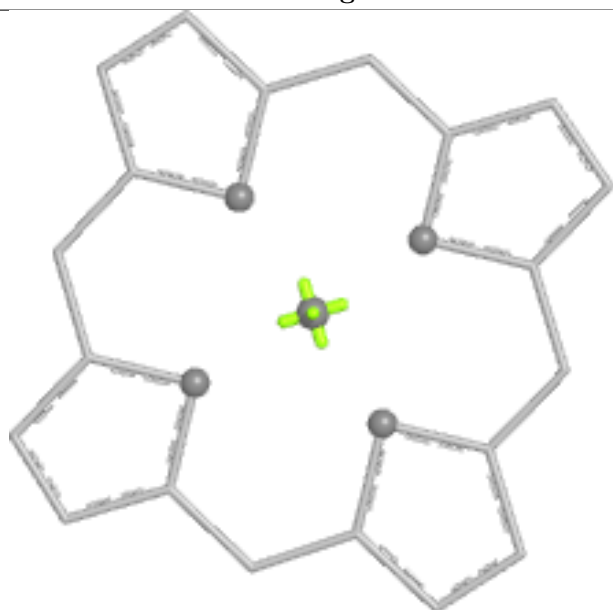
Ligand CLA 3 309



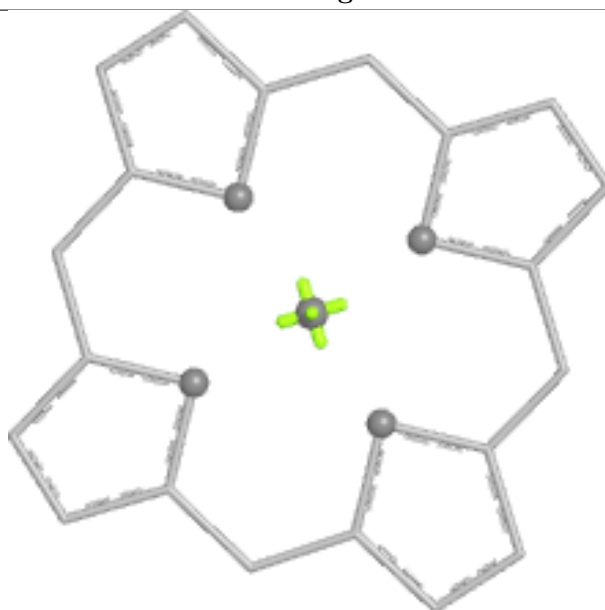
Bond lengths



Bond angles

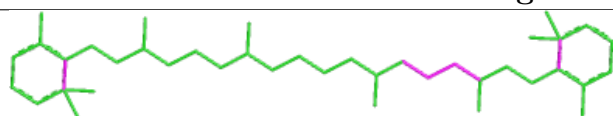


Torsions

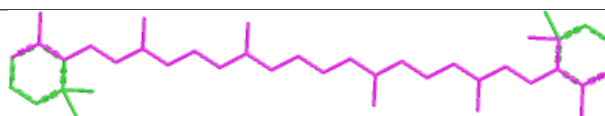


Rings

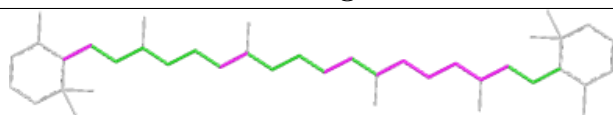
Ligand BCR 3 314



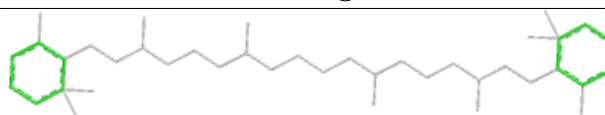
Bond lengths



Bond angles

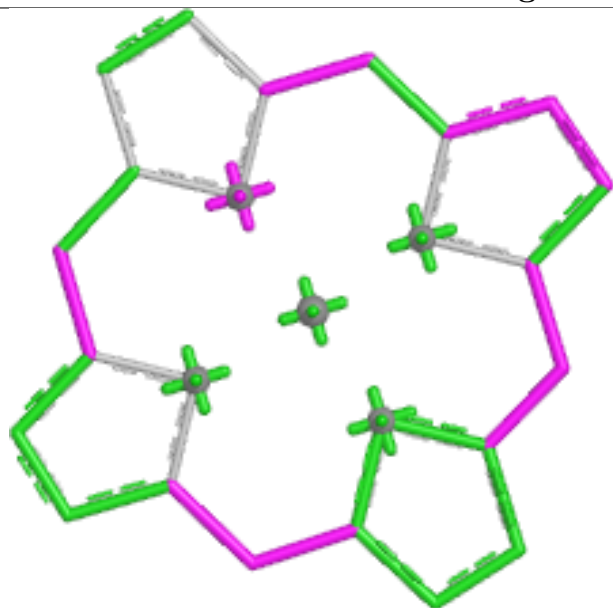


Torsions

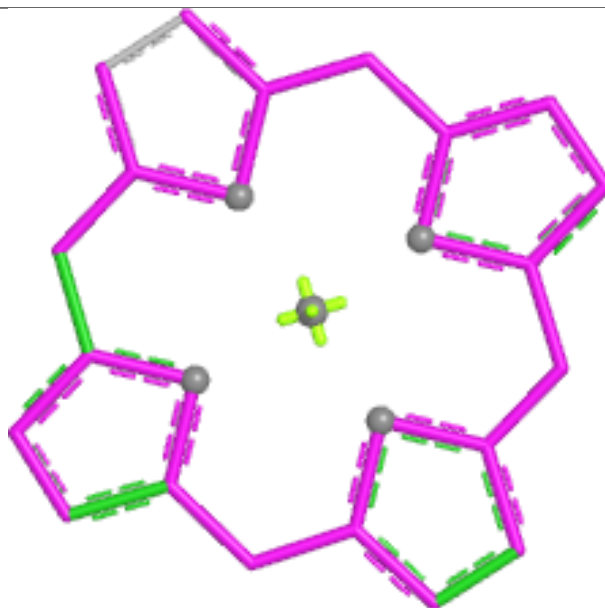


Rings

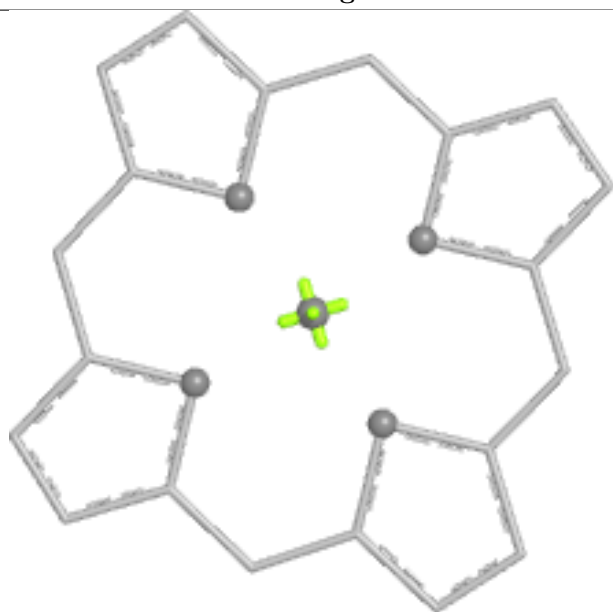
Ligand CLA 3 315



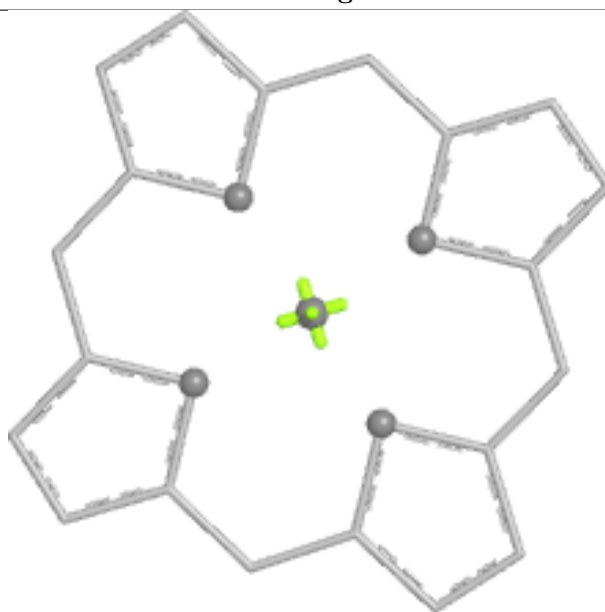
Bond lengths



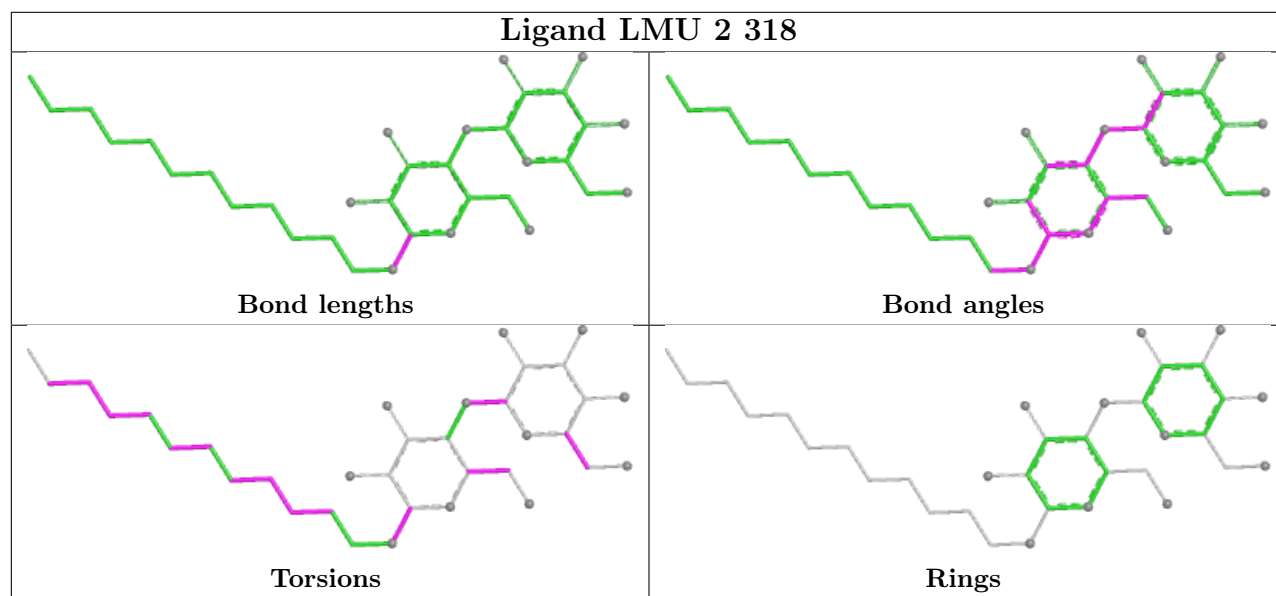
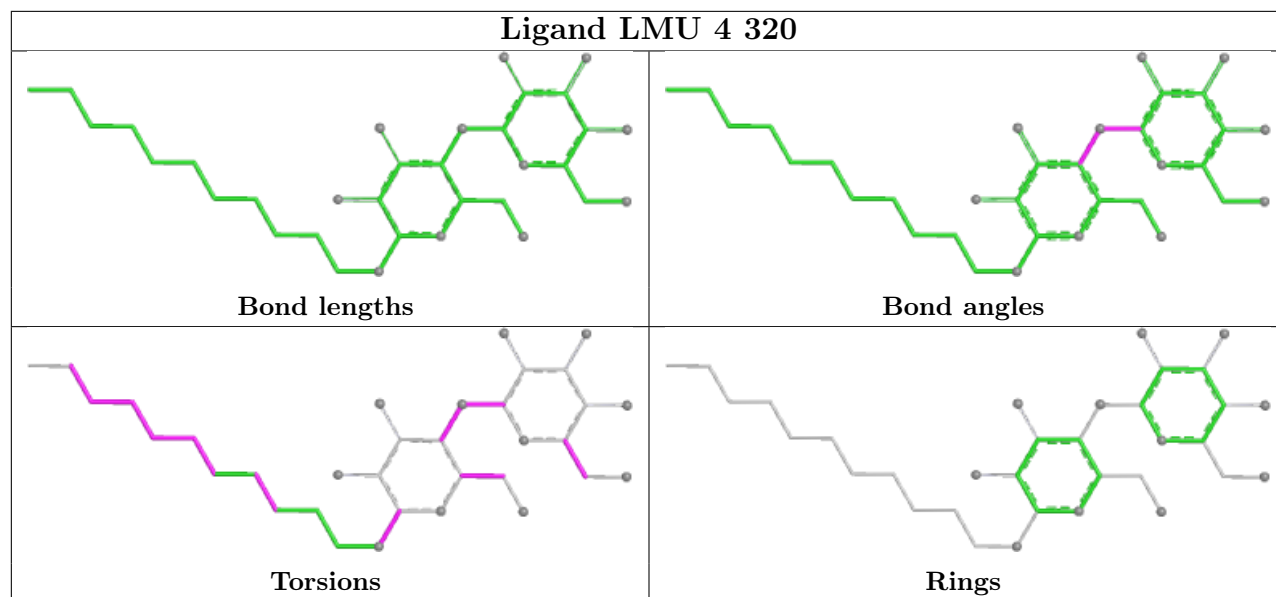
Bond angles



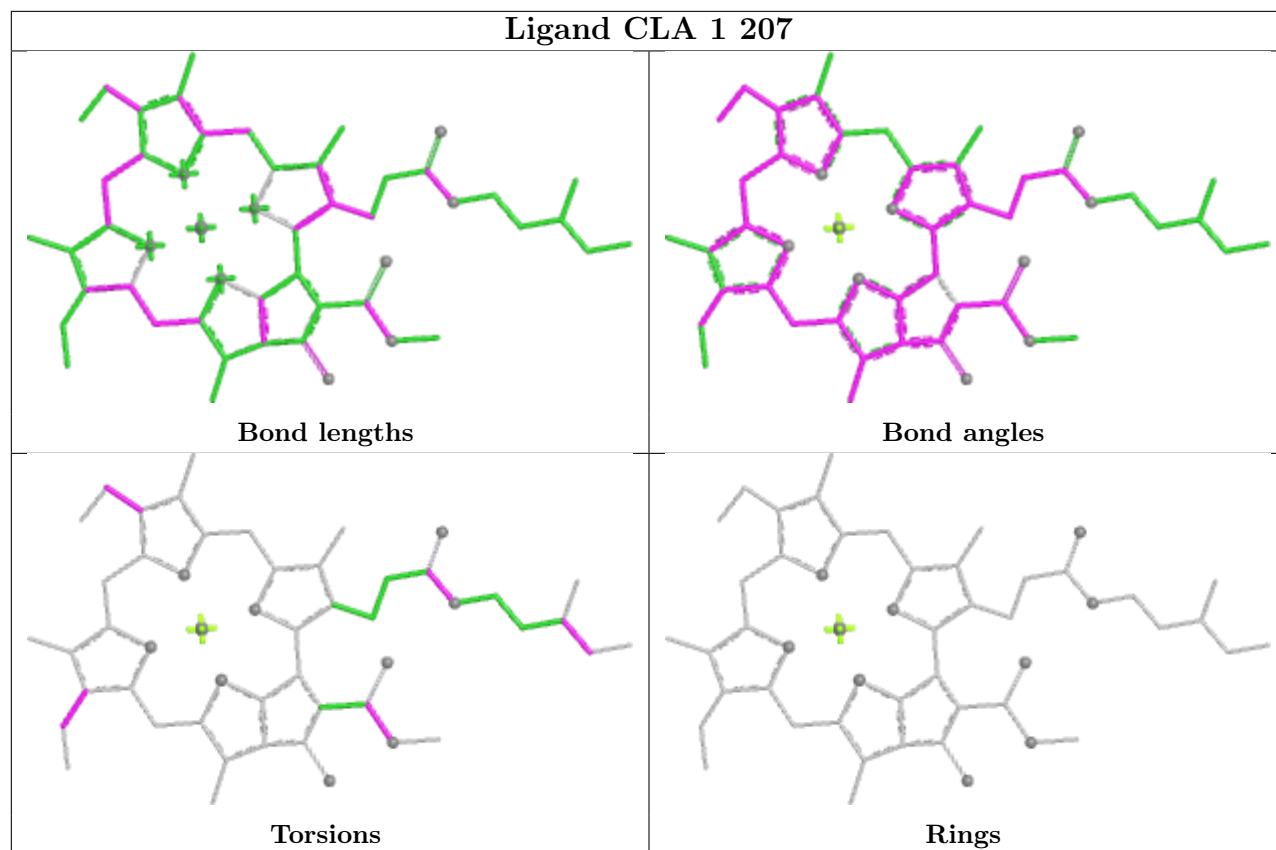
Torsions



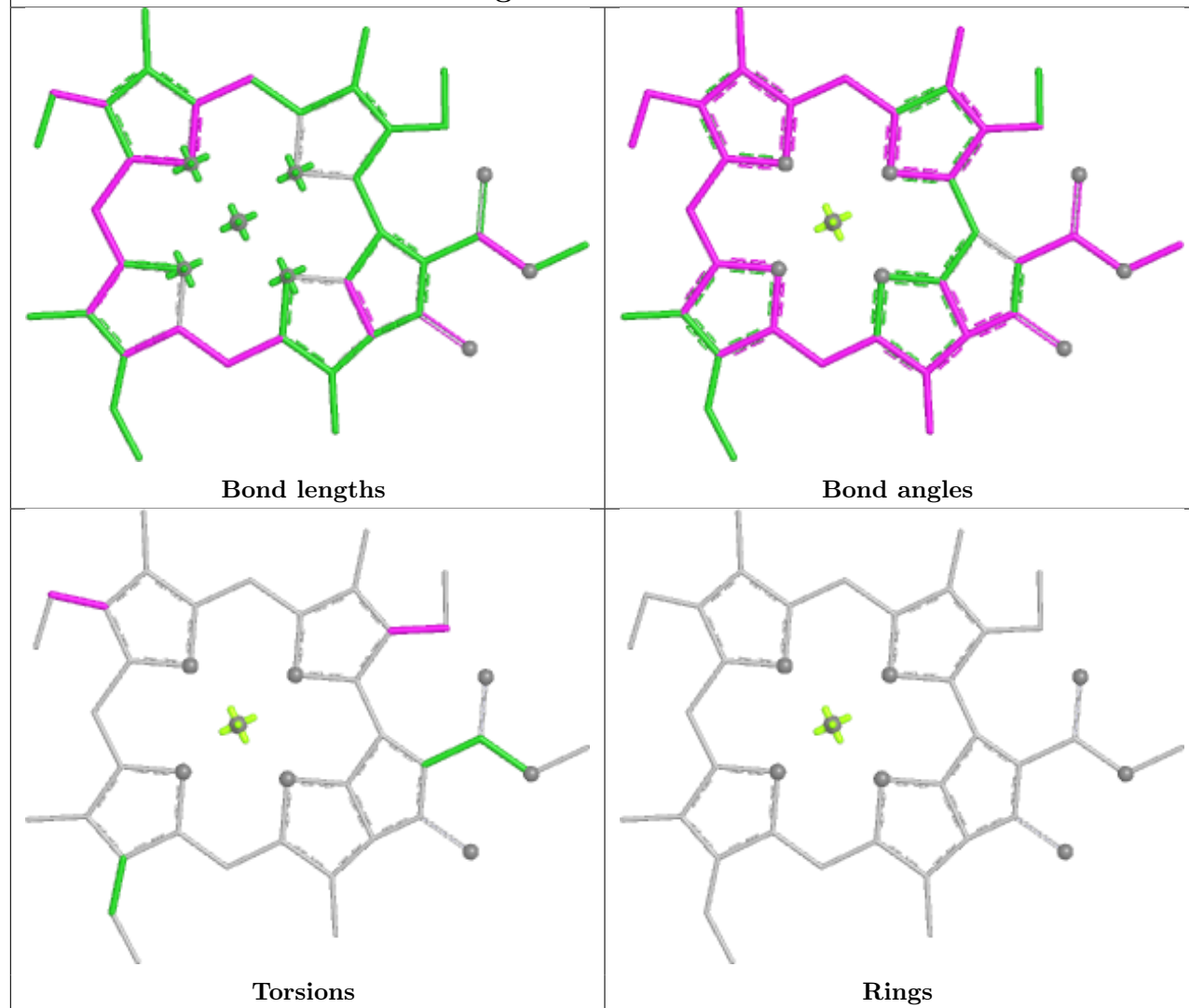
Rings



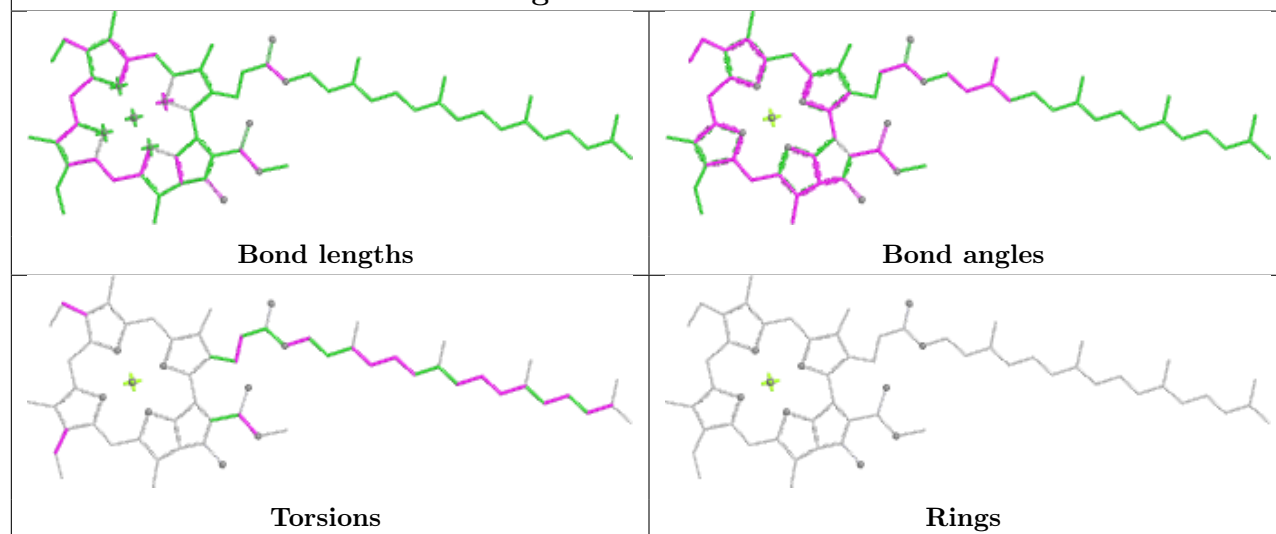
Ligand CLA 1 207

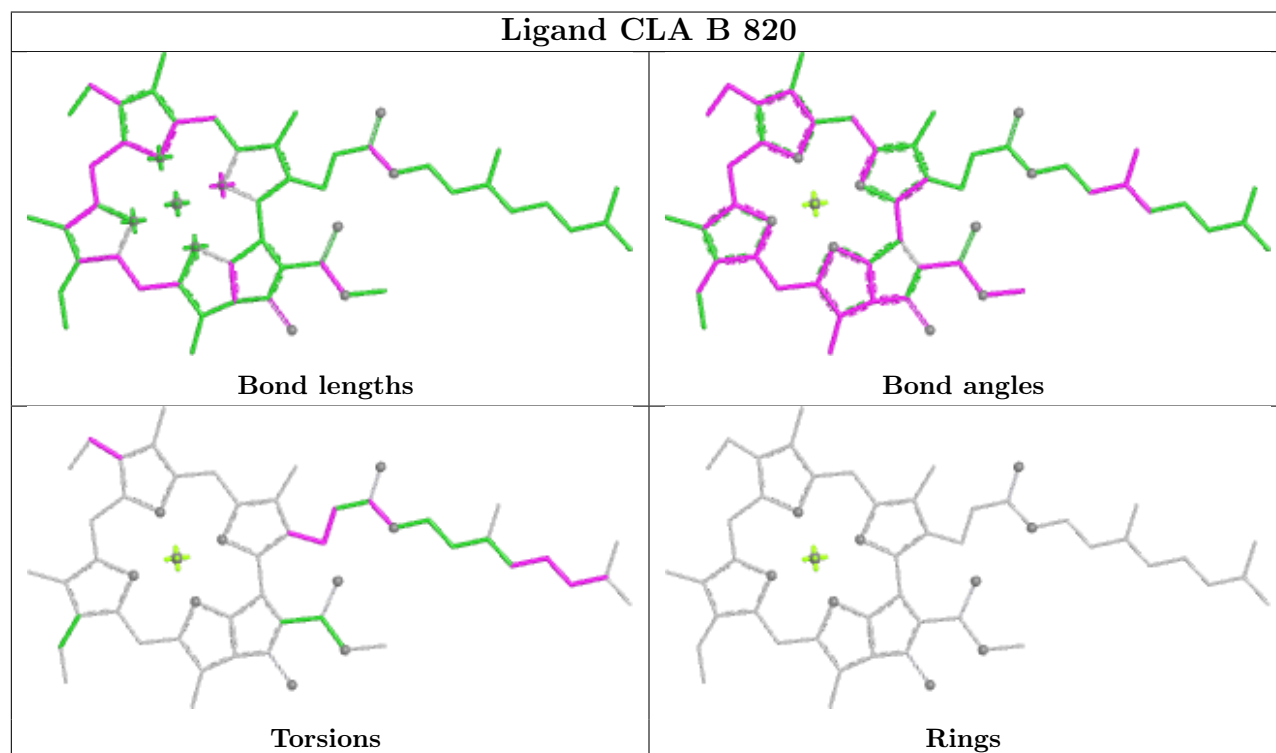
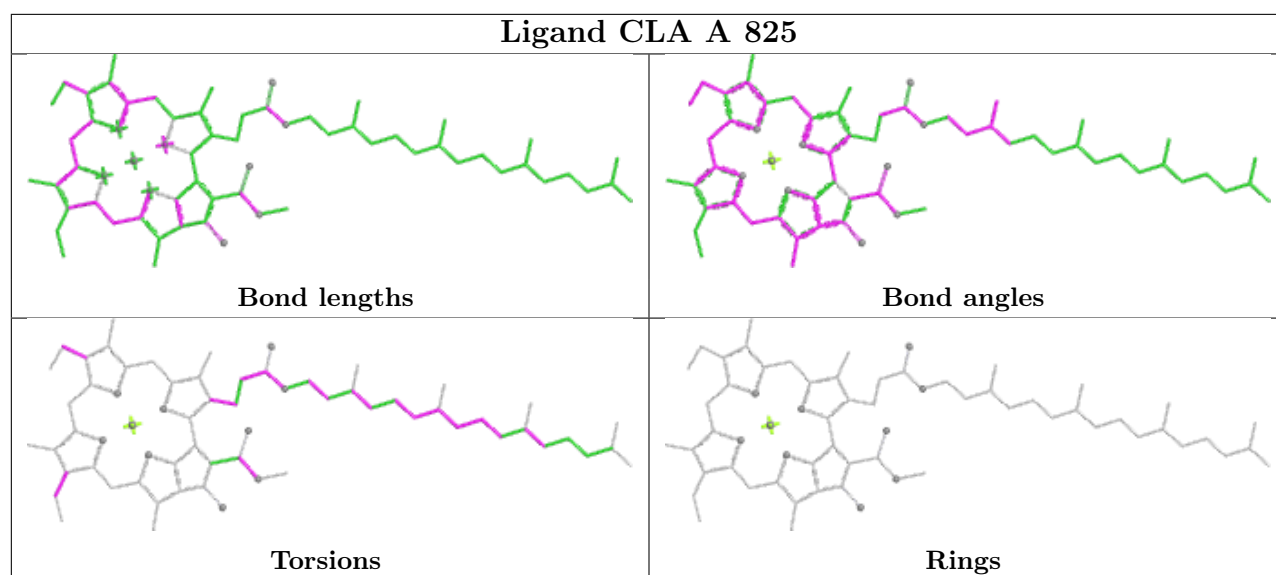


Ligand CLA A 821

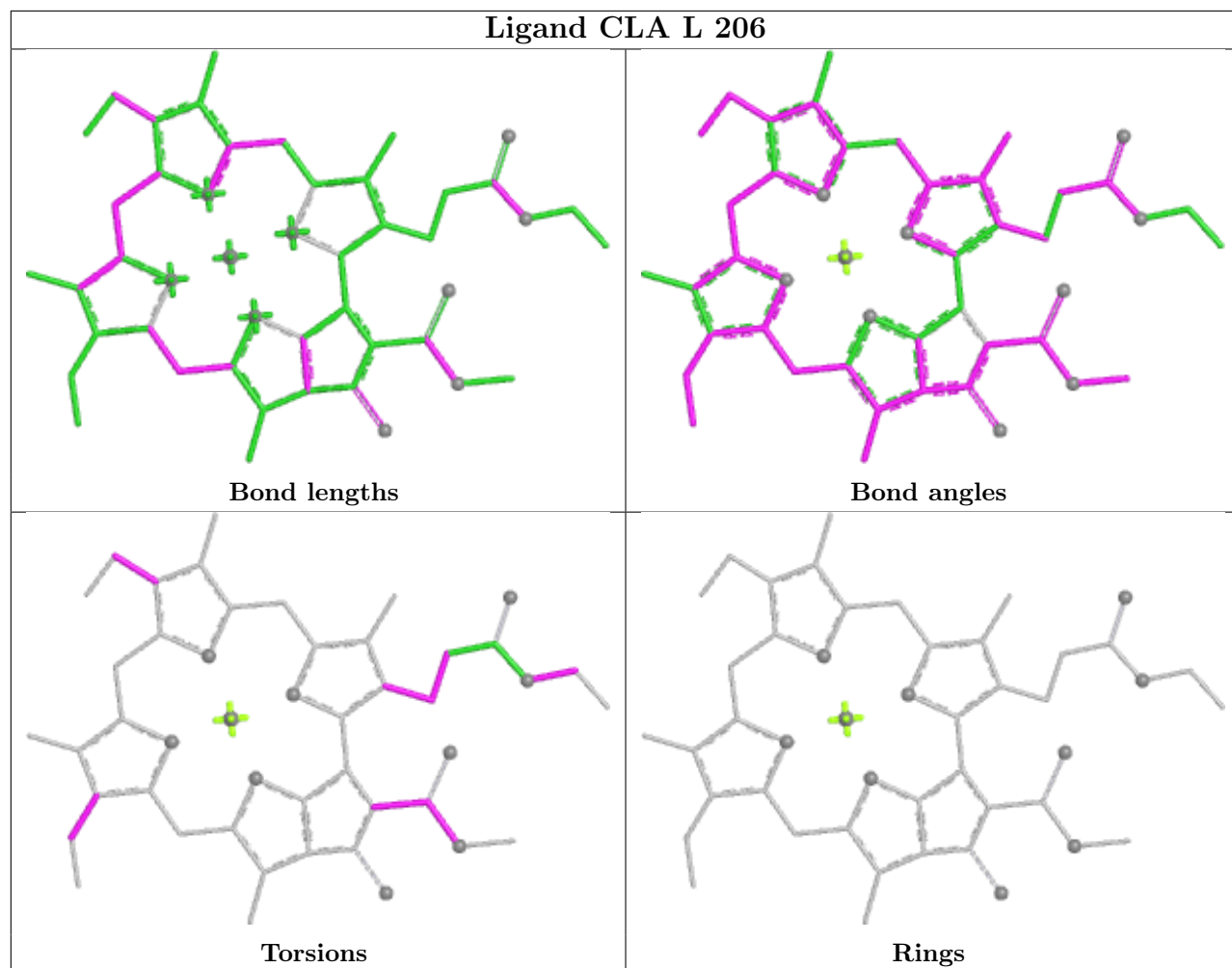


Ligand CLA A 824

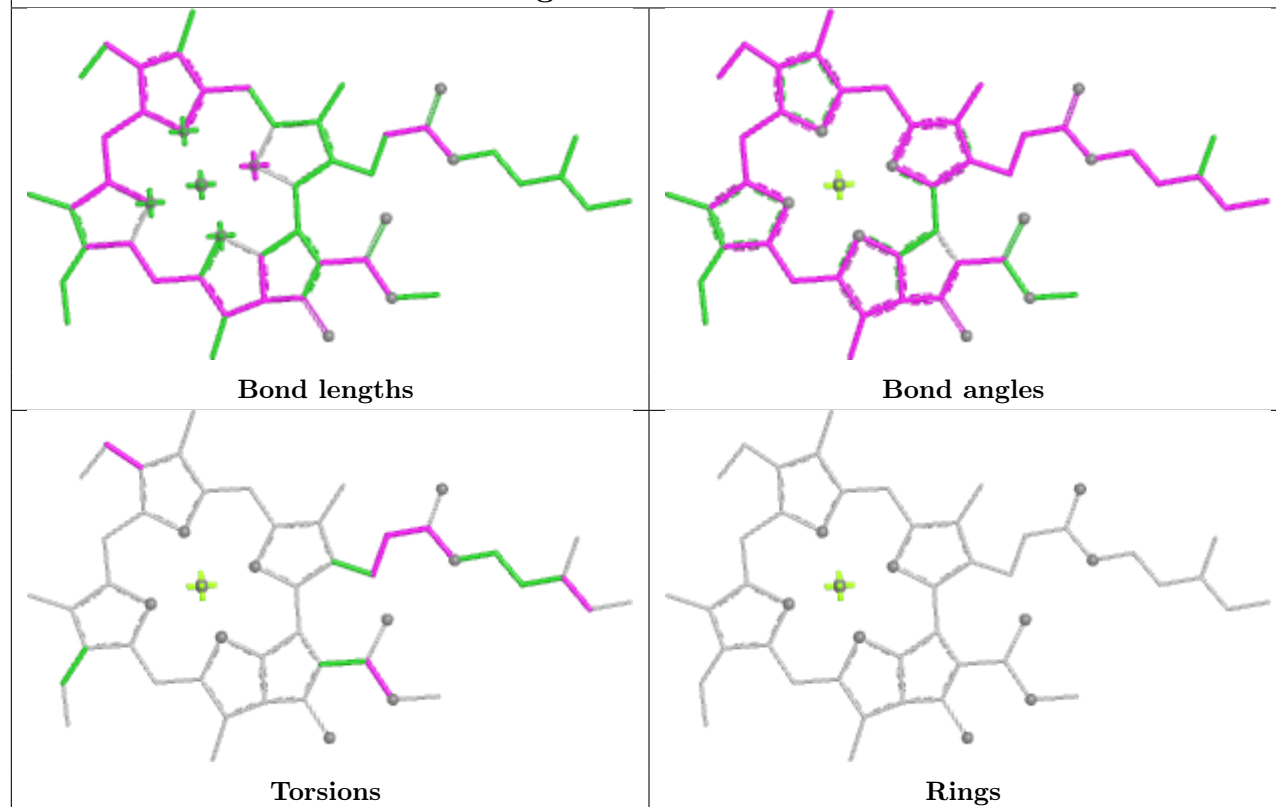




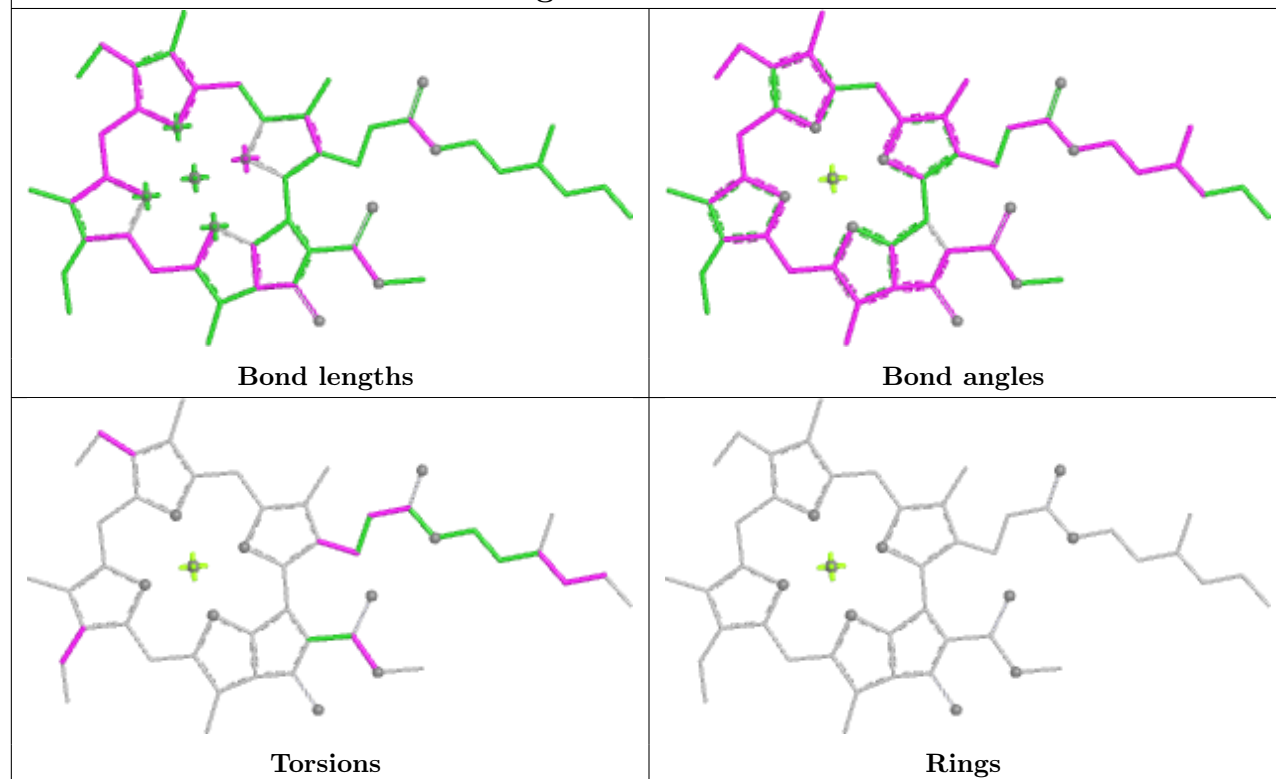
Ligand CLA L 206



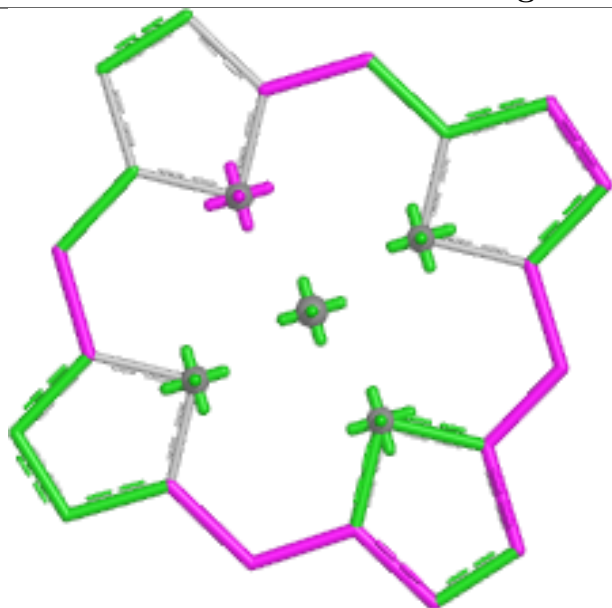
Ligand CLA 1 210



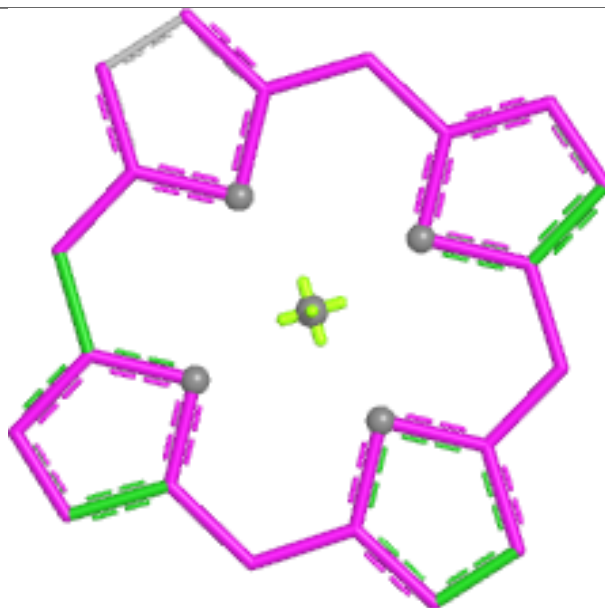
Ligand CLA 4 318



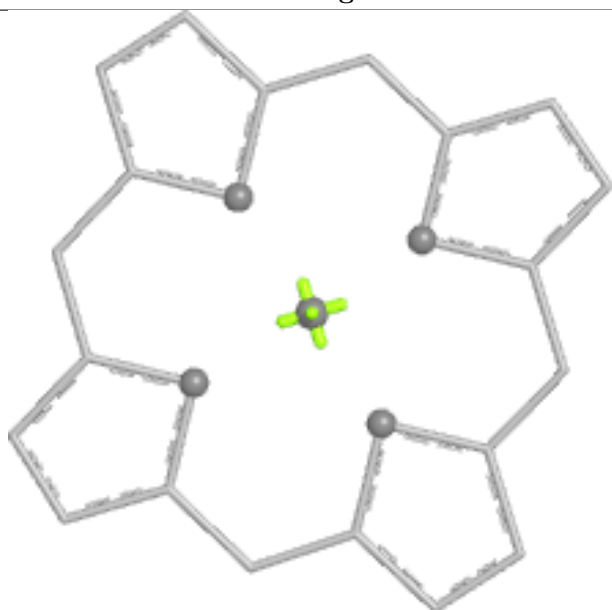
Ligand CLA 3 306



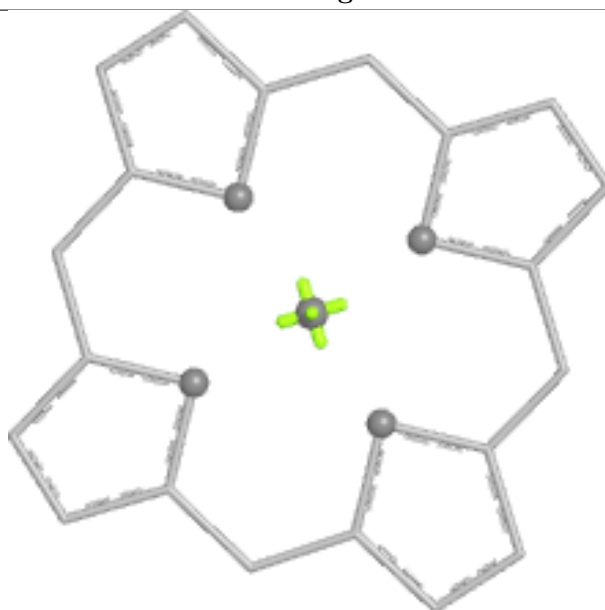
Bond lengths



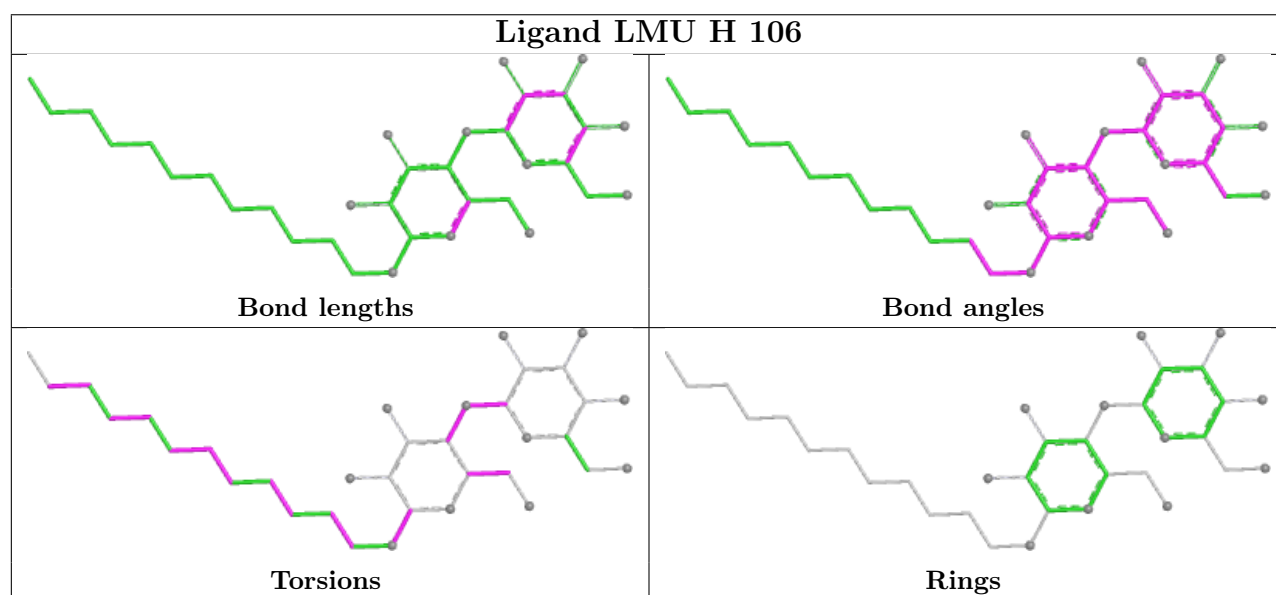
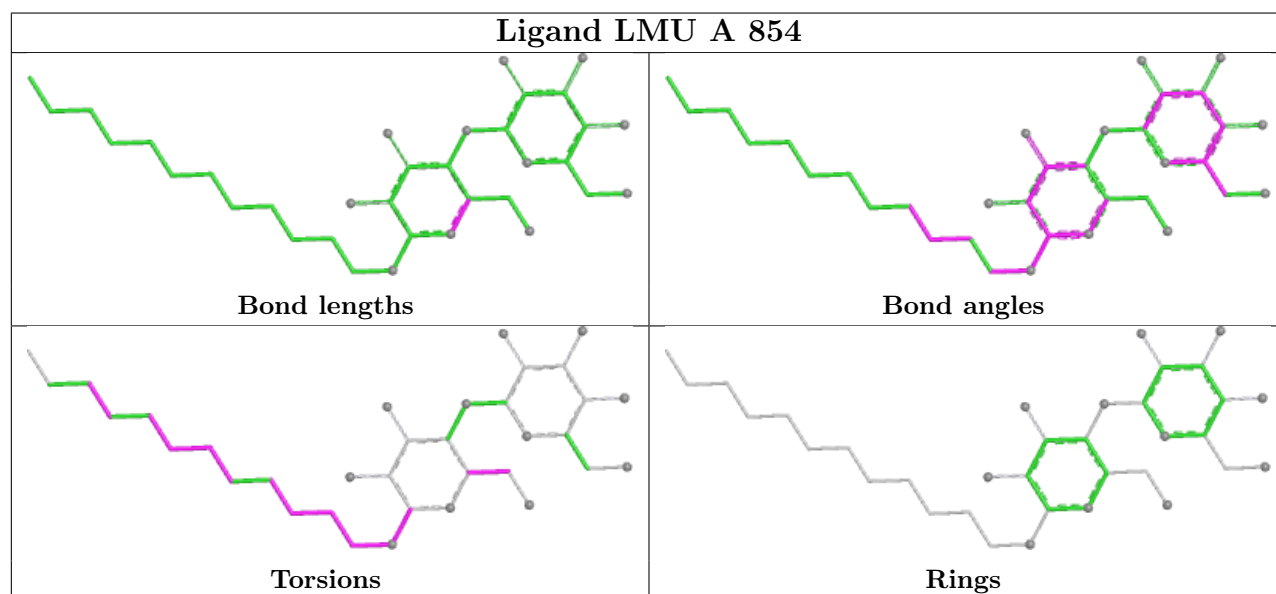
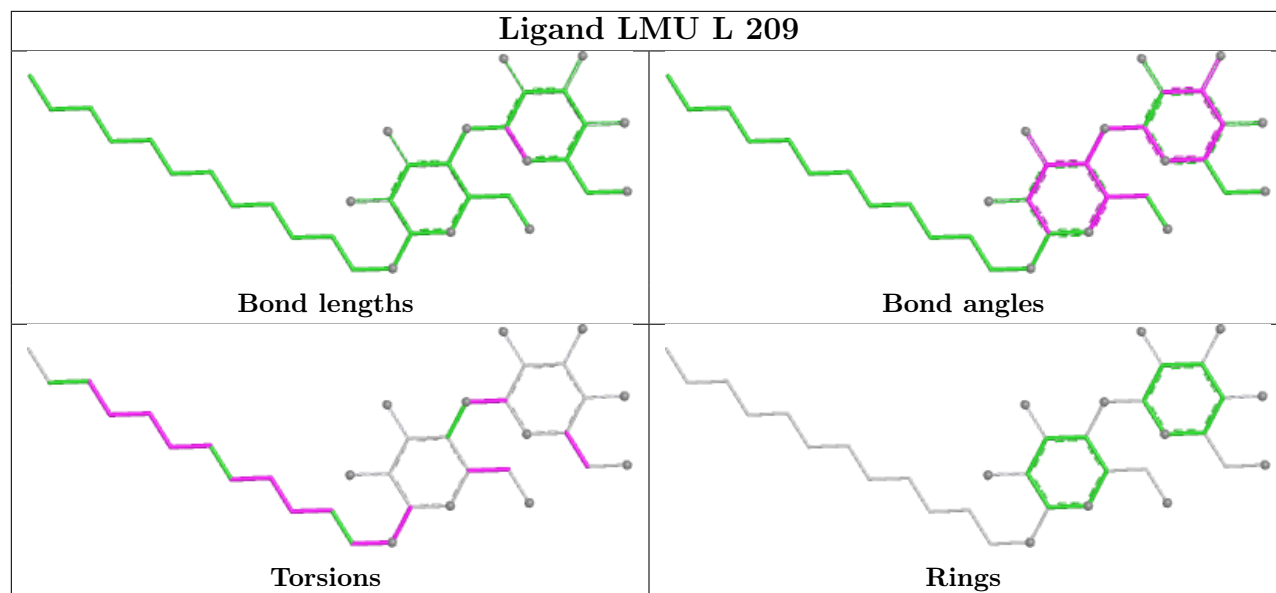
Bond angles

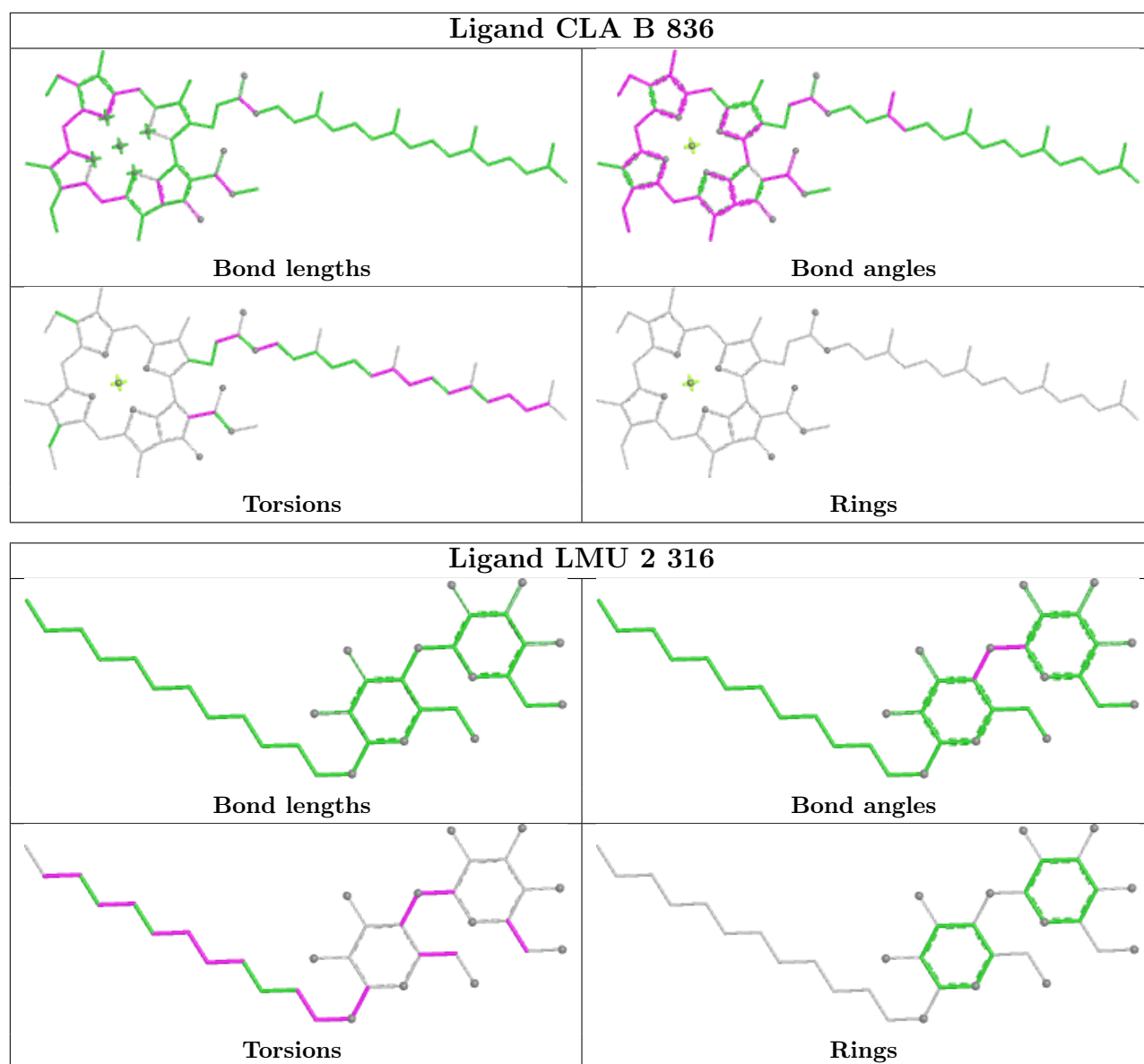


Torsions



Rings





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	1	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

Continued on next page...

Continued from previous page...

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](#)

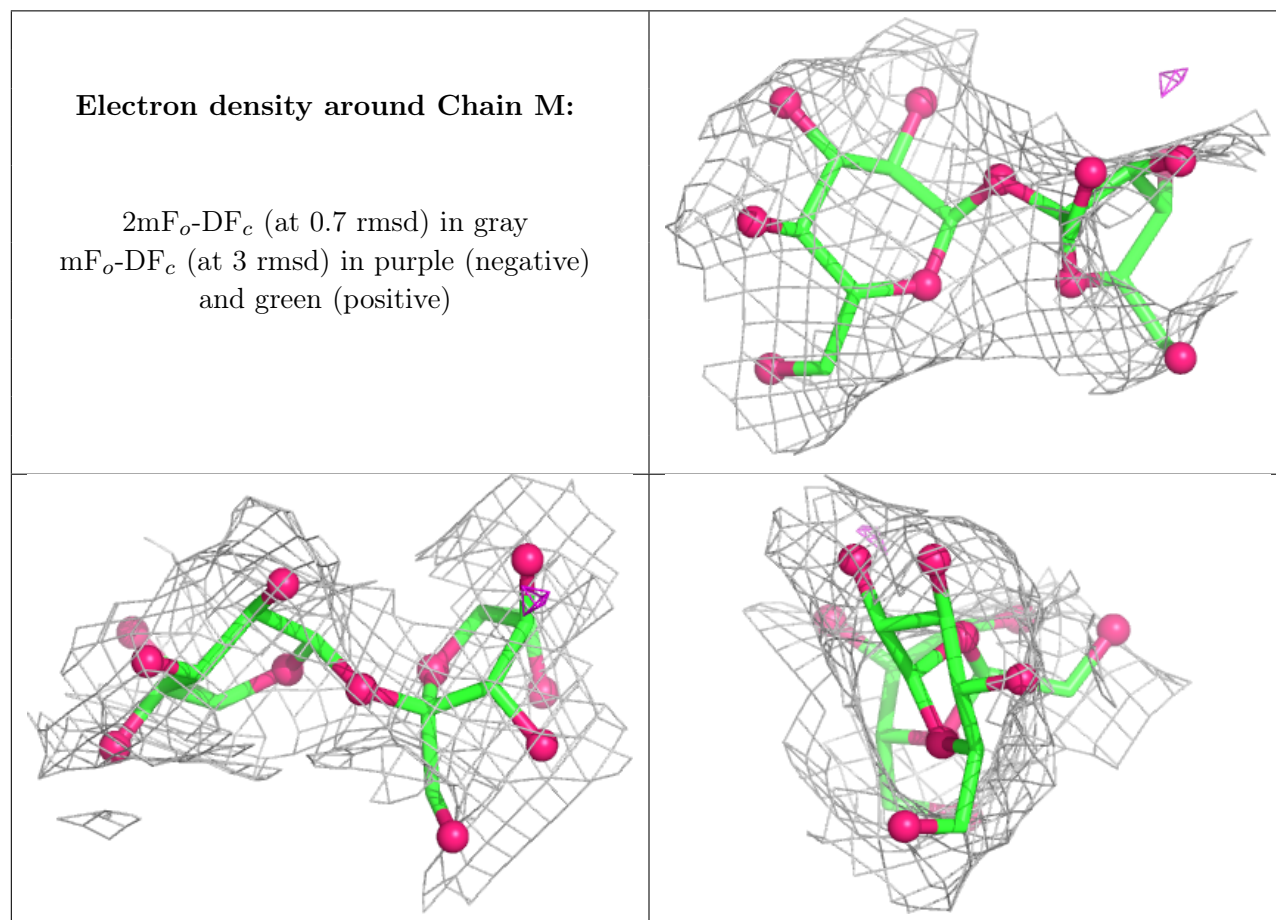
There are no non-standard protein/DNA/RNA residues in this entry.

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.

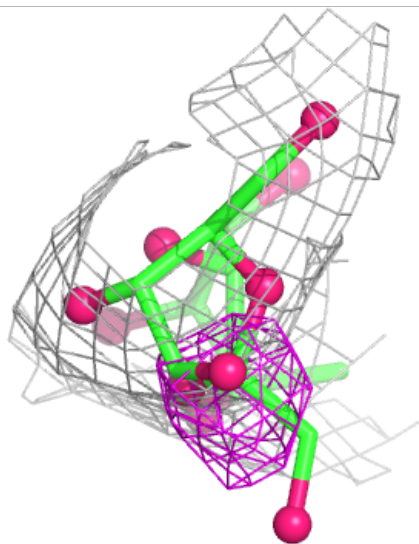
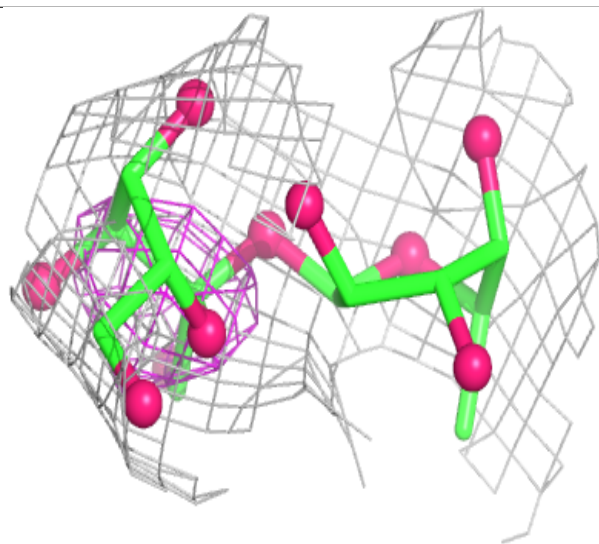
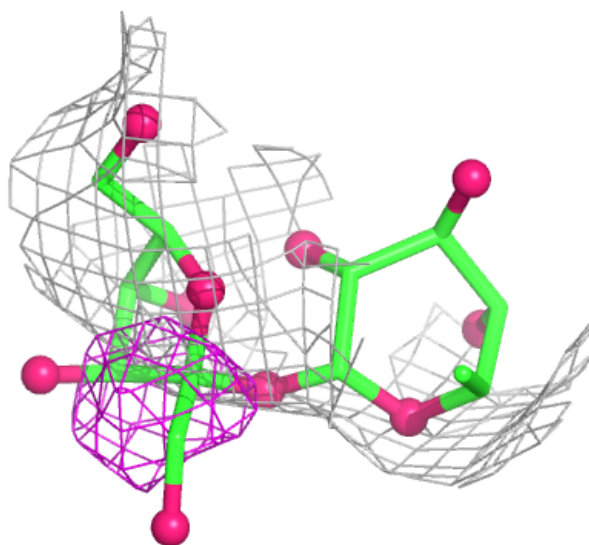
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
19	GLC	M	1	11/12	-	-	20,20,20,20	0
19	FRU	M	2	12/12	-	-	20,20,20,20	0
19	GLC	O	1	10/12	-	-	20,20,20,20	0
19	FRU	O	2	12/12	-	-	20,20,20,20	0
19	GLC	P	1	11/12	-	-	20,20,20,20	0
19	FRU	P	2	12/12	-	-	20,20,20,20	0
19	GLC	Q	1	11/12	-	-	20,20,20,20	0
19	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.



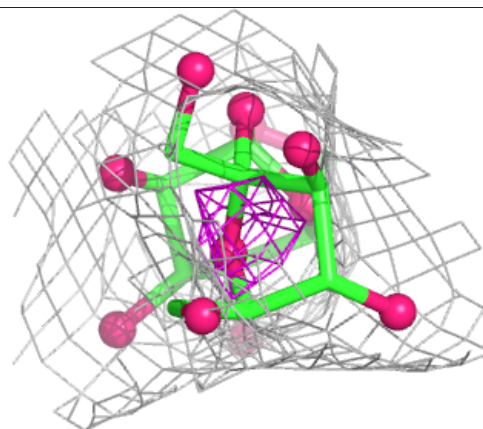
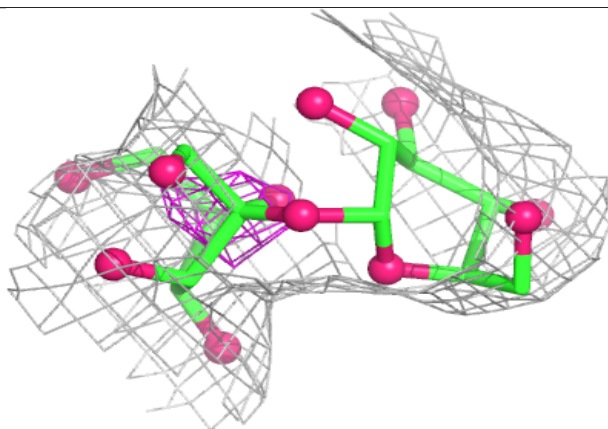
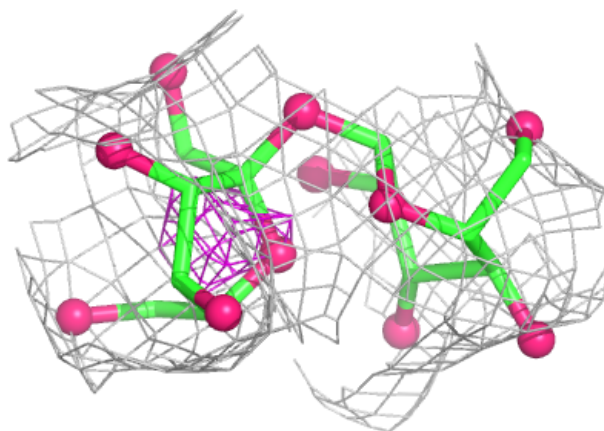
Electron density around Chain O:

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



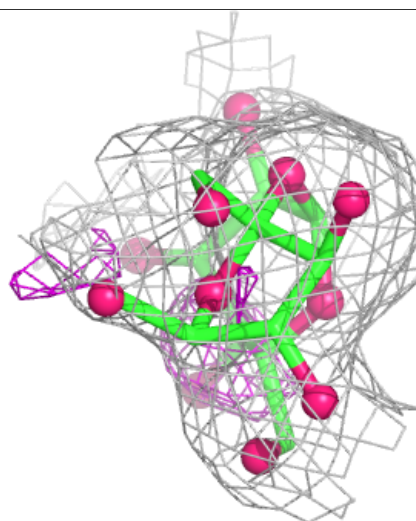
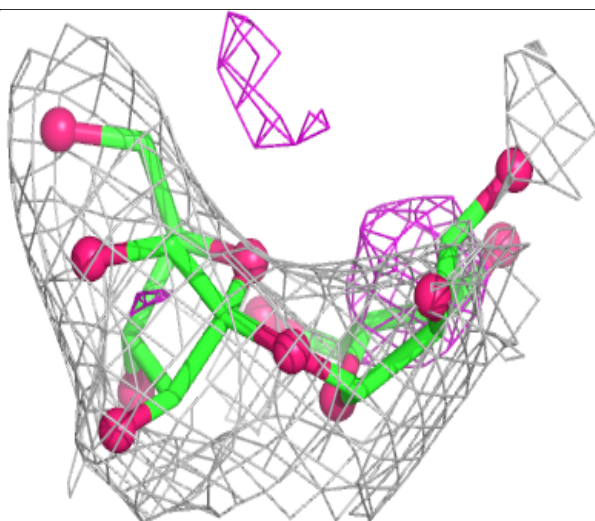
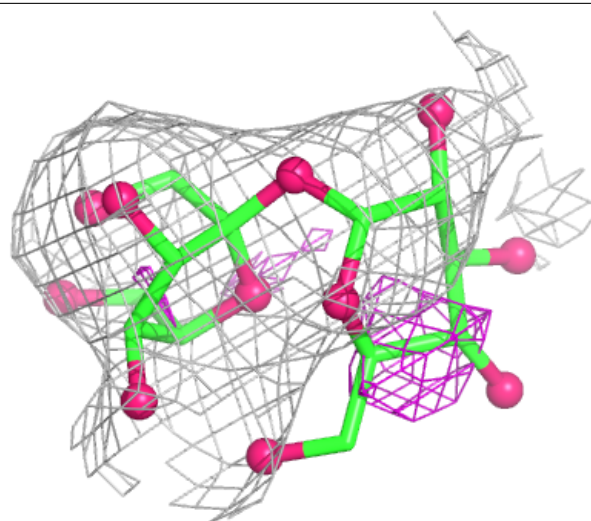
Electron density around Chain P:

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



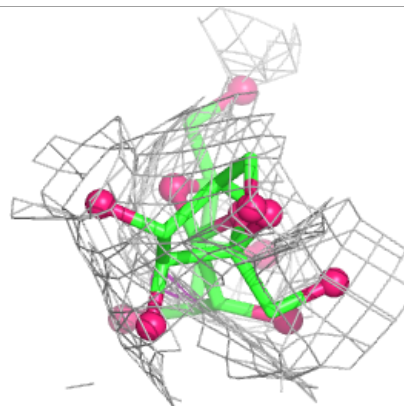
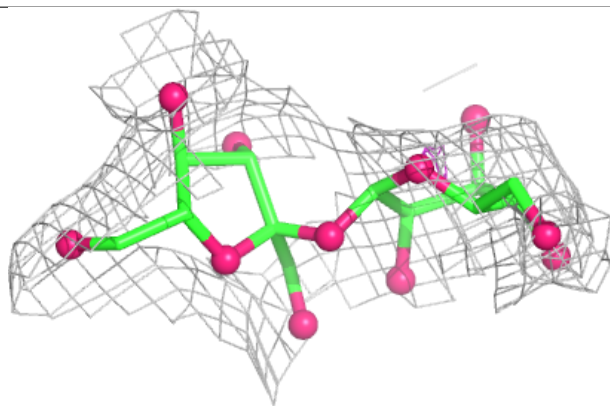
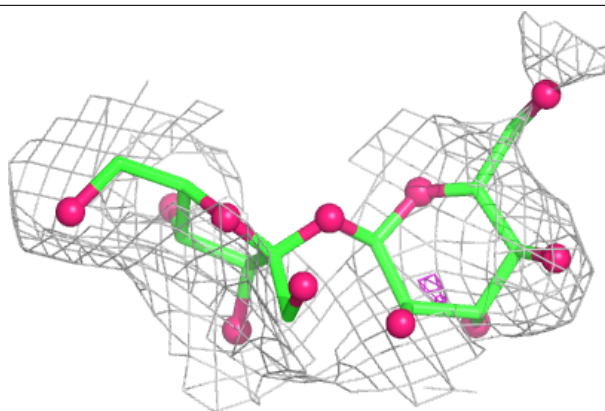
Electron density around Chain Q:

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

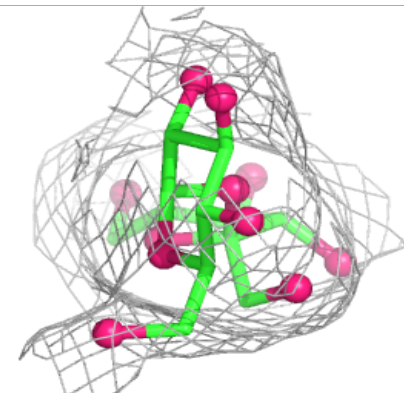
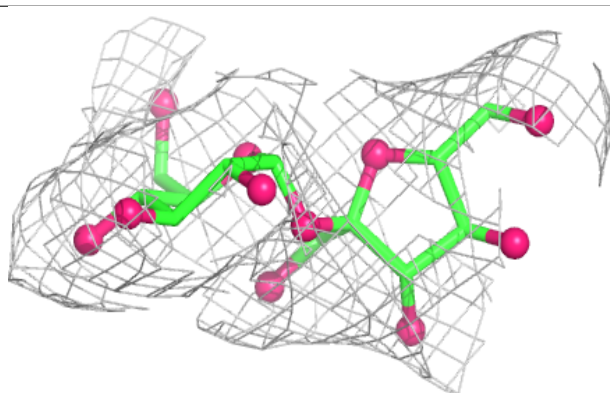
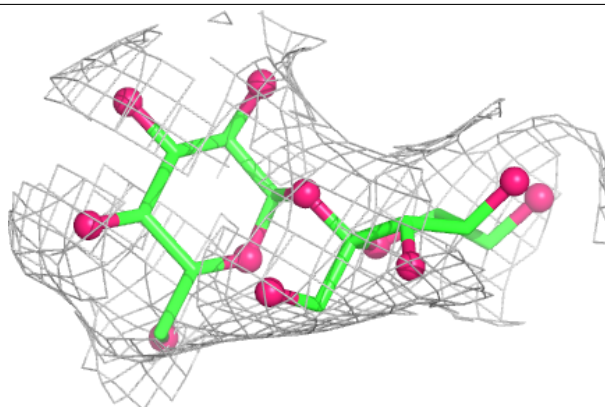


Electron density around Chain S:

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

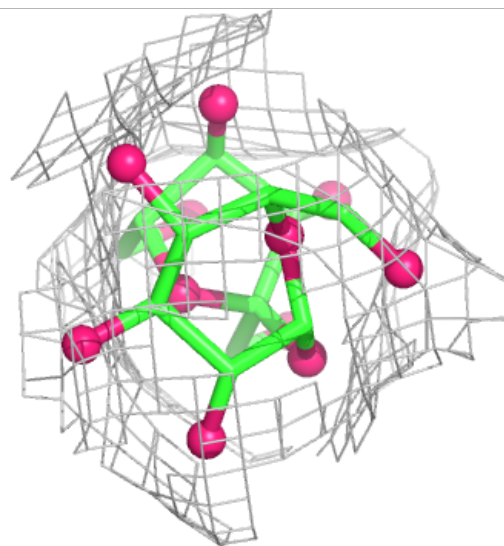
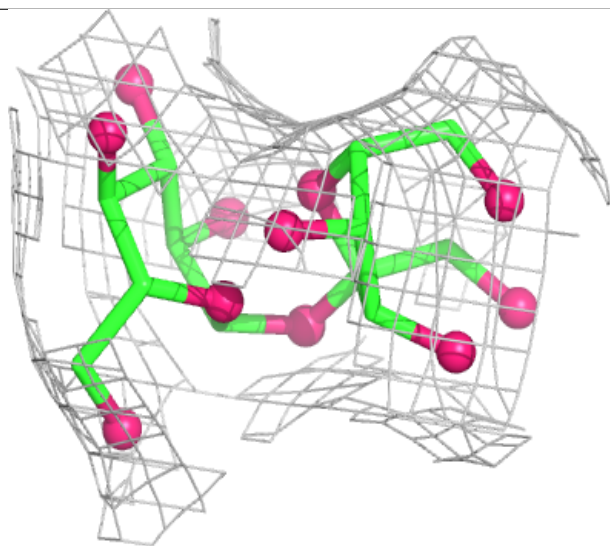
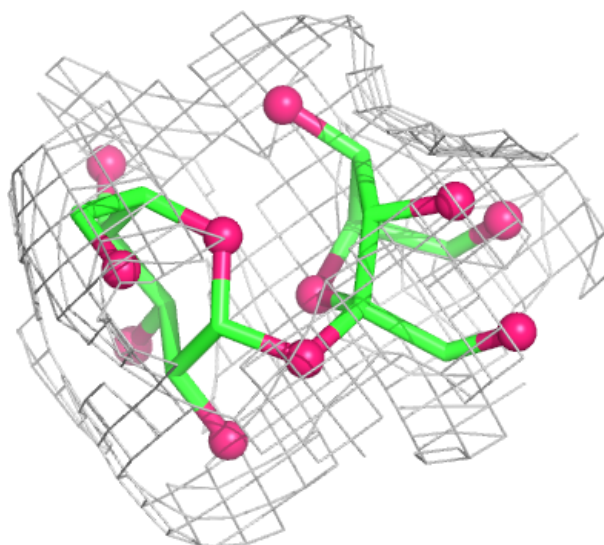
**Electron density around Chain T:**

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



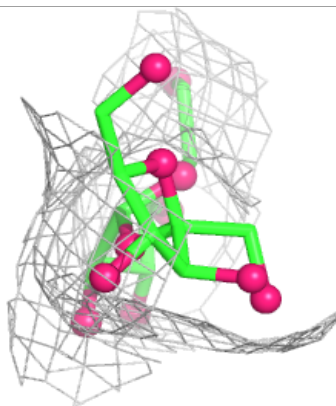
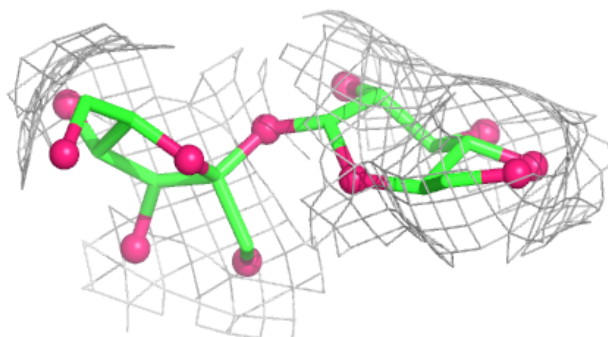
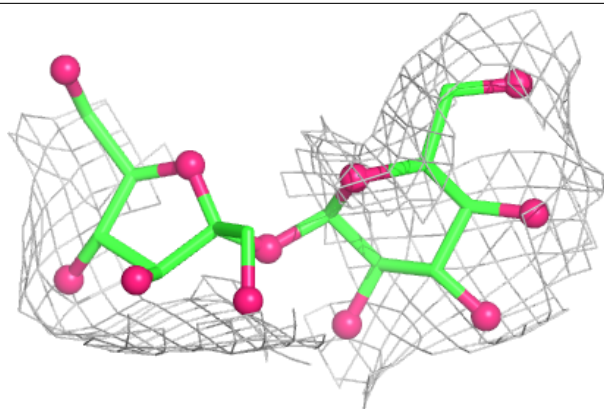
Electron density around Chain U:

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

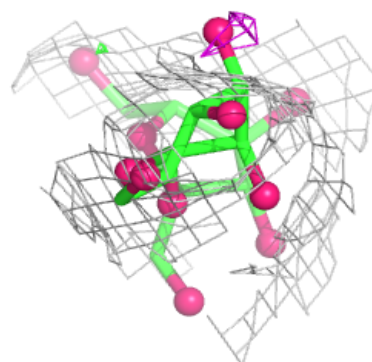
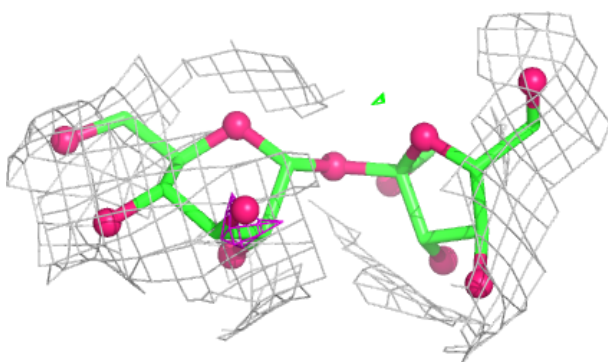
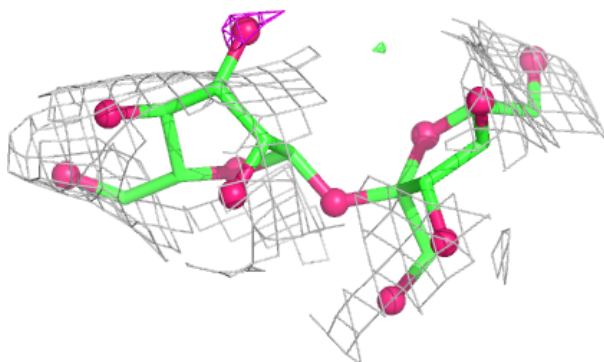


Electron density around Chain V:

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

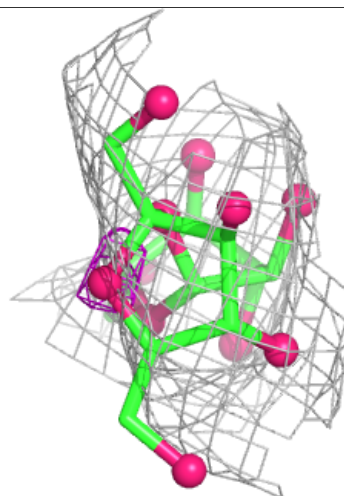
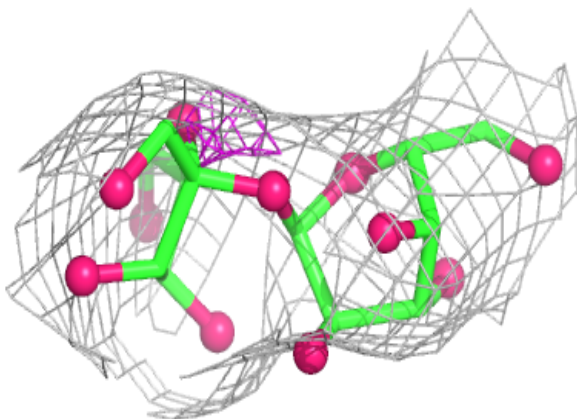
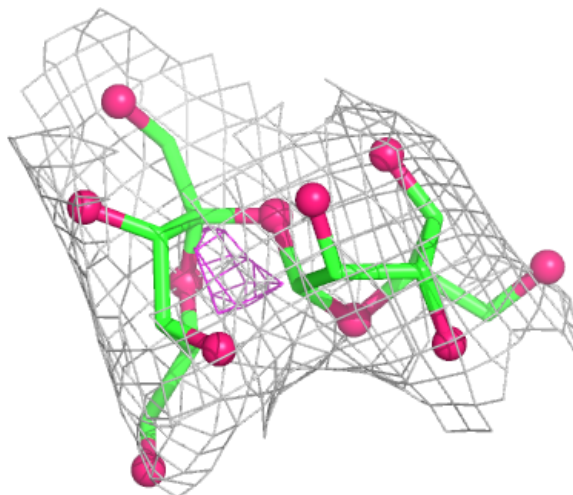
**Electron density around Chain W:**

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



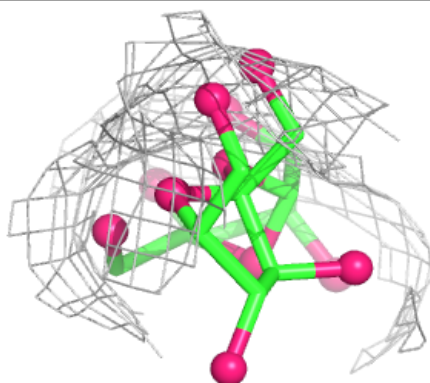
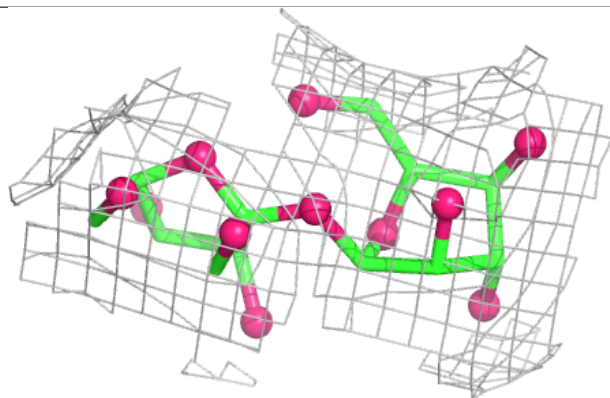
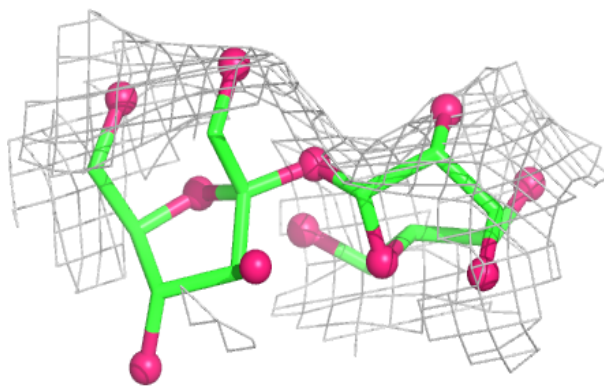
Electron density around Chain X:

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



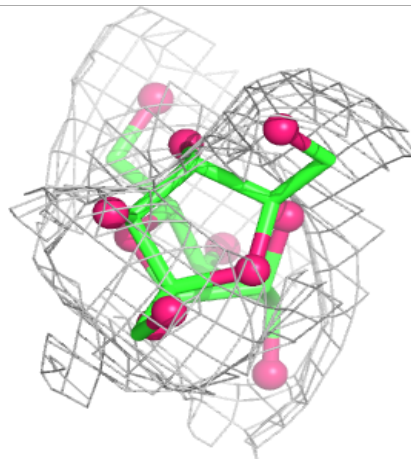
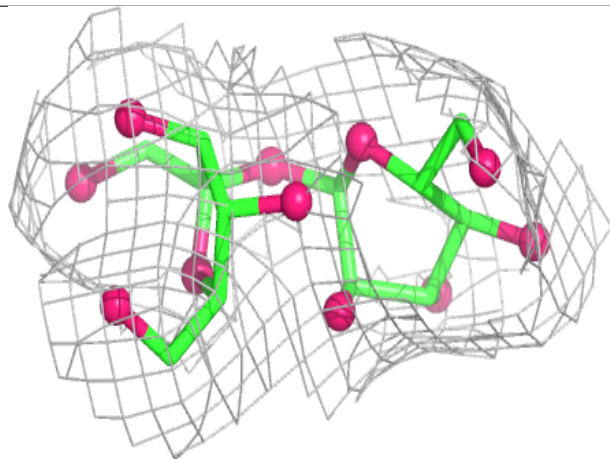
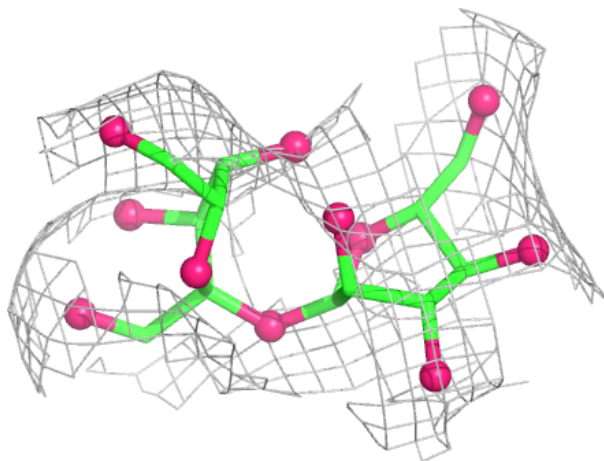
Electron density around Chain Y:

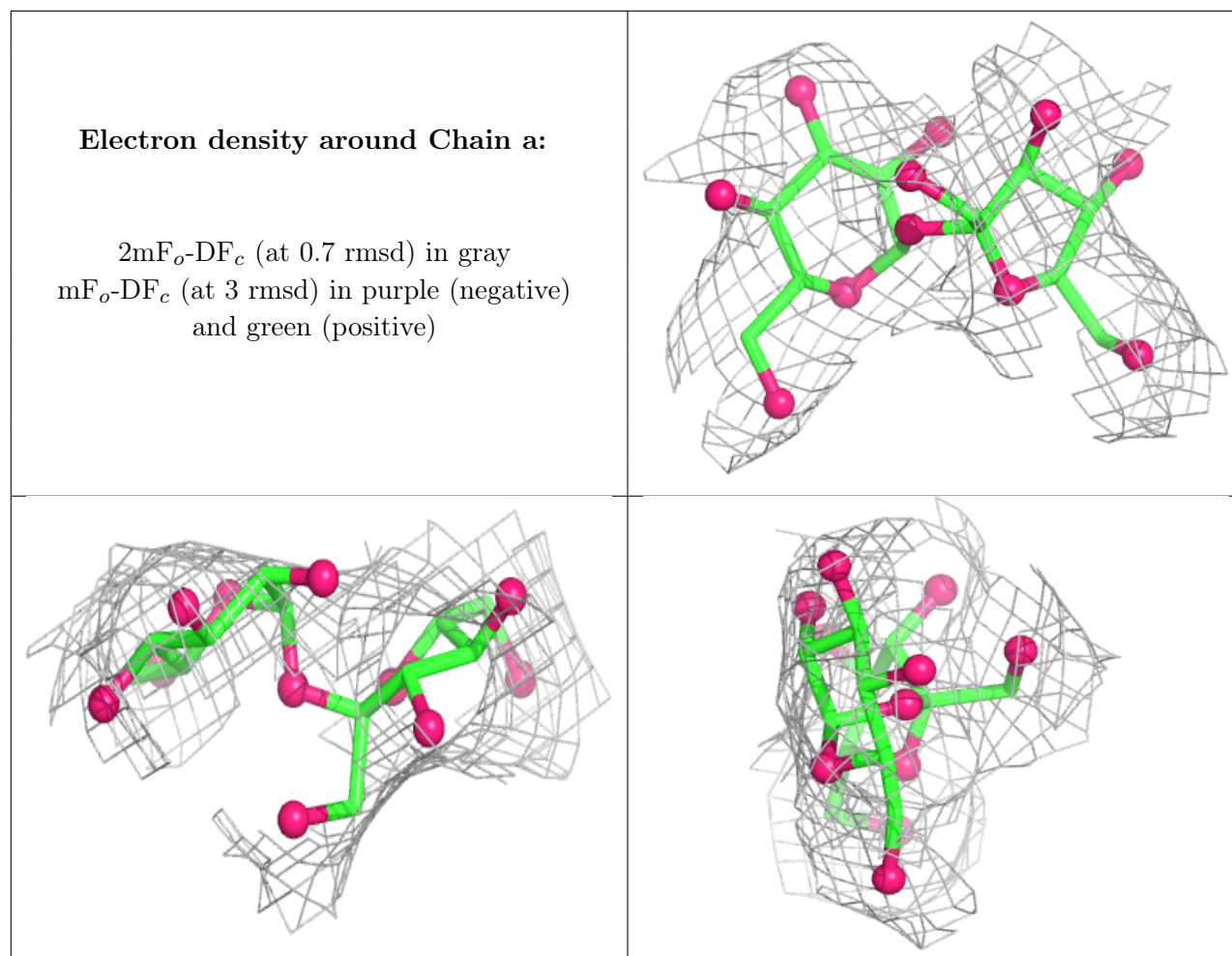
$2mF_o - DF_c$ (at 0.7 rmsd) in gray
 $mF_o - DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)



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(Å 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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

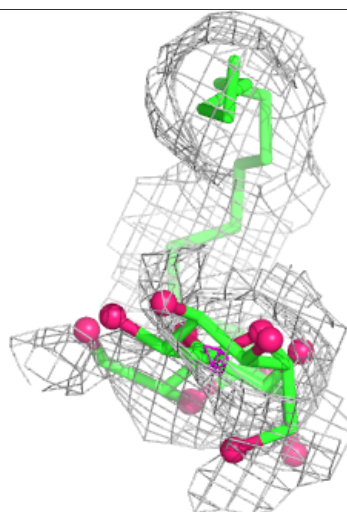
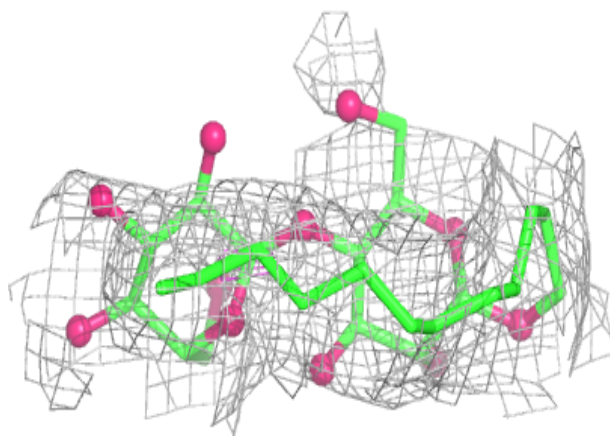
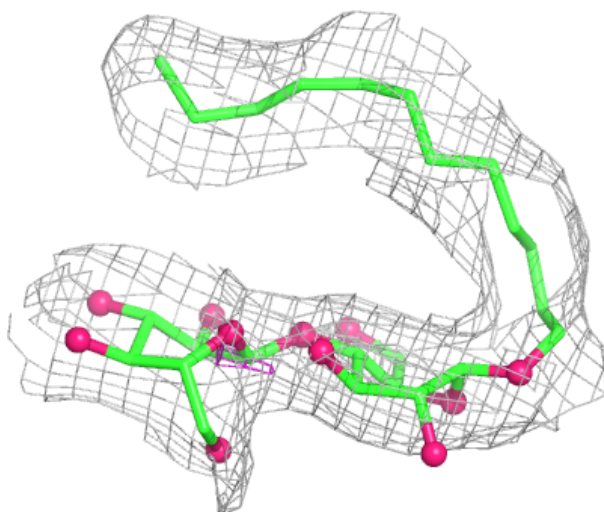
Continued from previous page...

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.

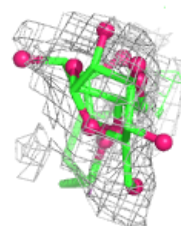
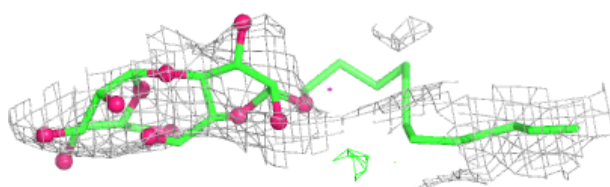
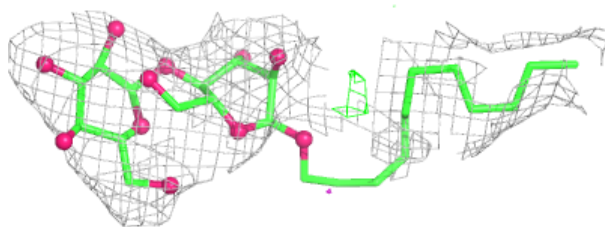
Electron density around LMU 1 218:

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

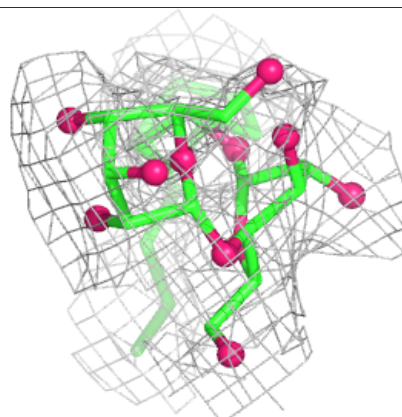
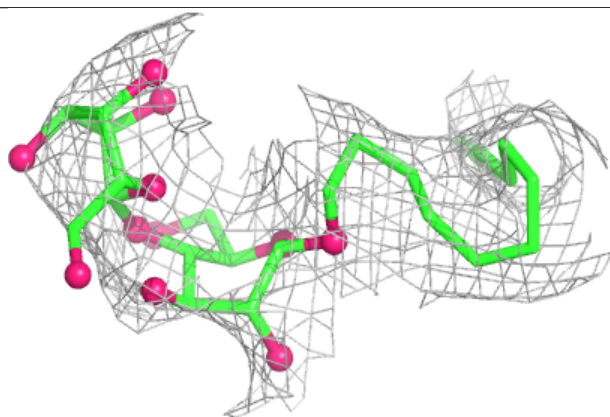
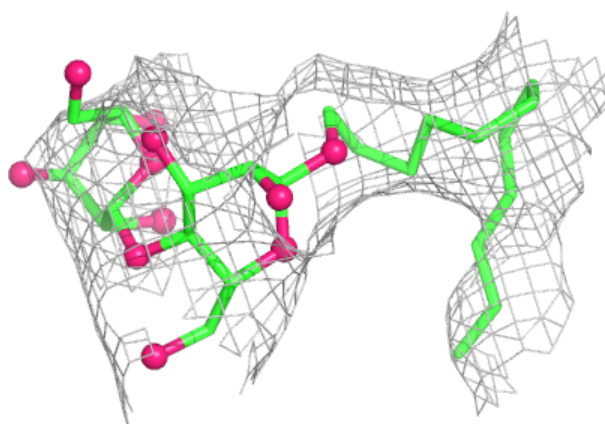


Electron density around LMU R 102:

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

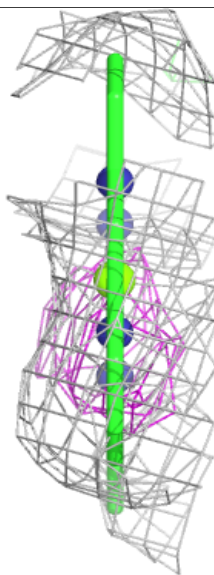
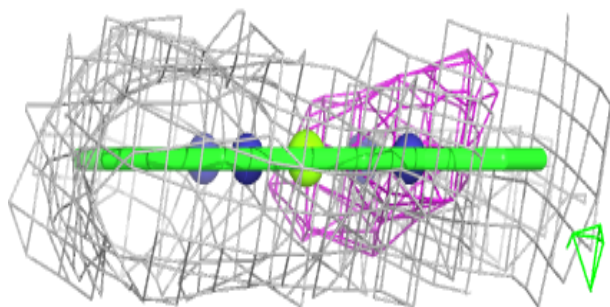
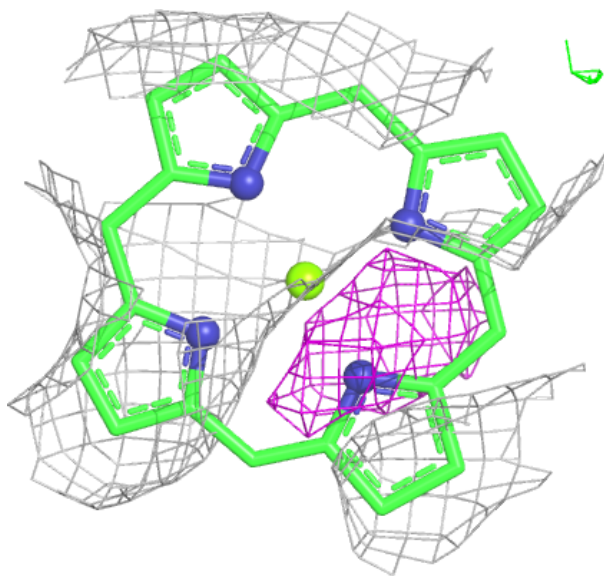
**Electron density around LMU H 108:**

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



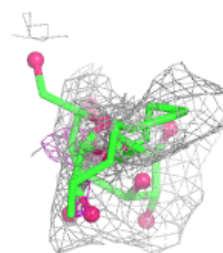
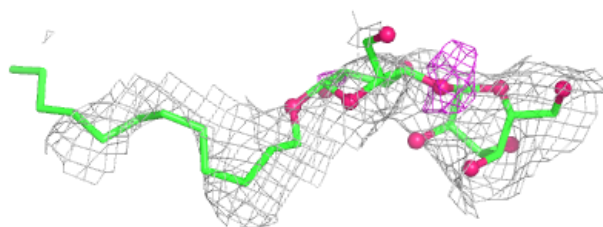
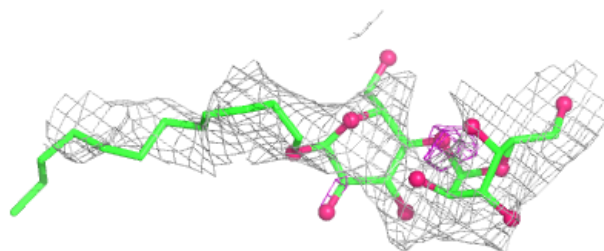
Electron density around CLA 3 310:

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

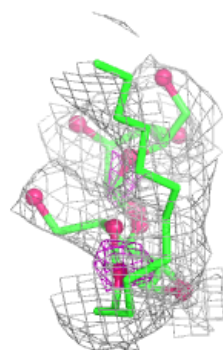
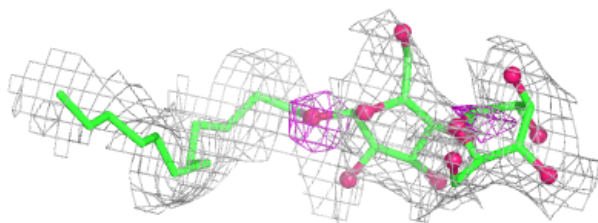
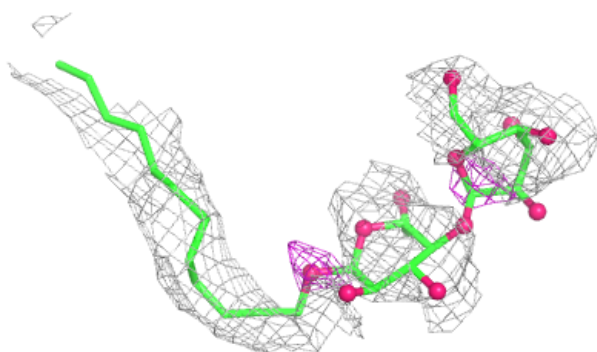


Electron density around LMU A 853:

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

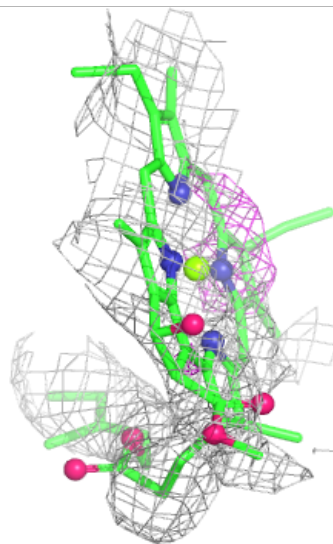
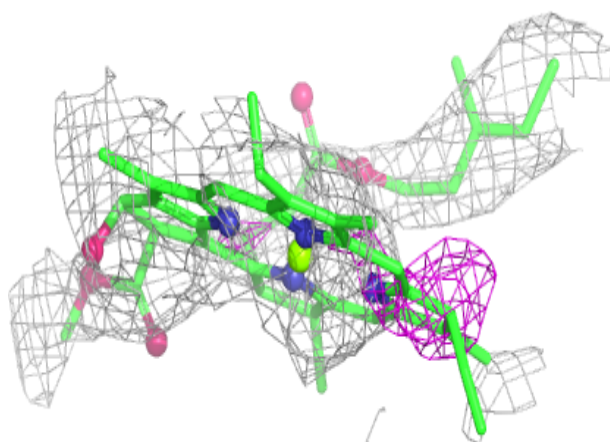
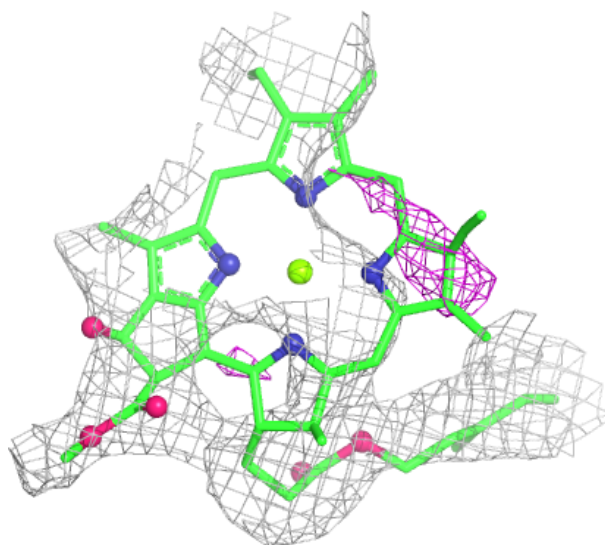
**Electron density around LMU 4 301:**

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



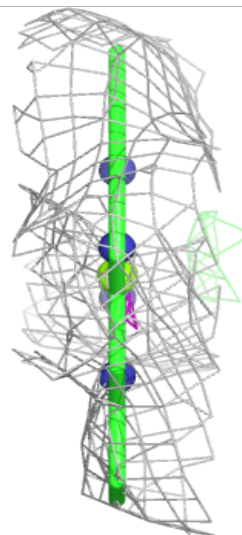
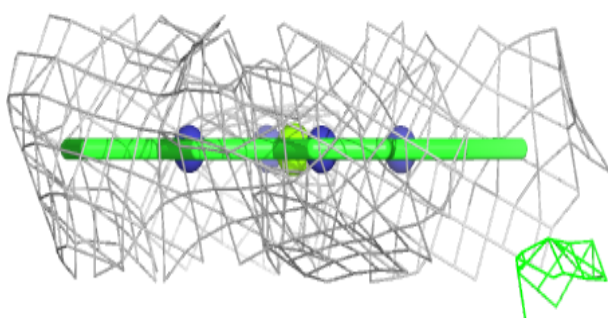
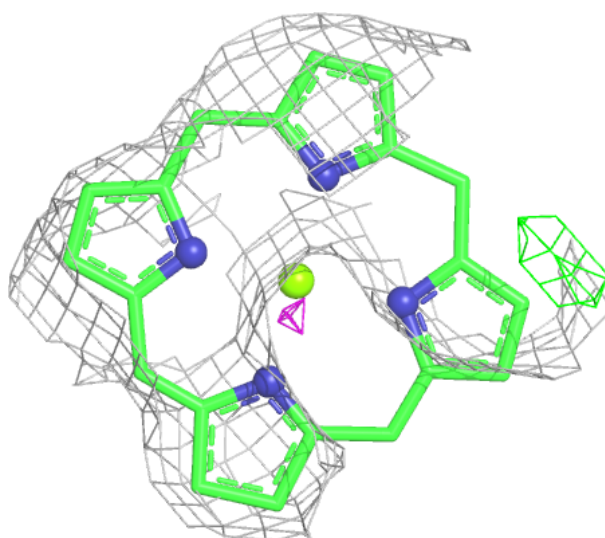
Electron density around CLA B 834:

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



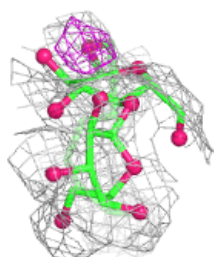
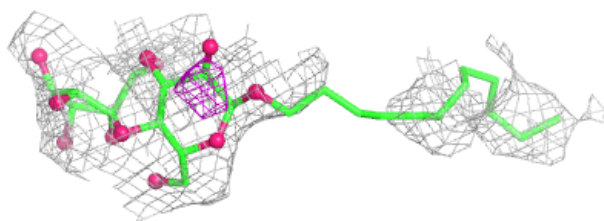
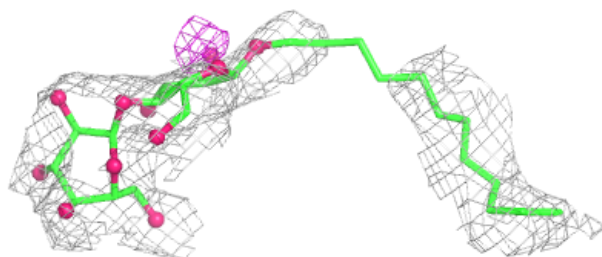
Electron density around CLA 3 306:

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

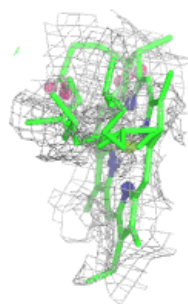
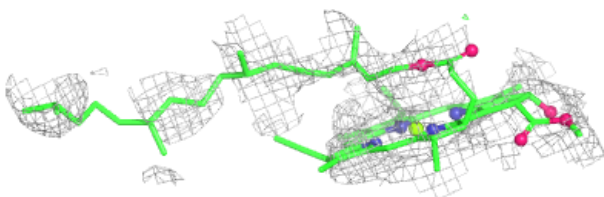
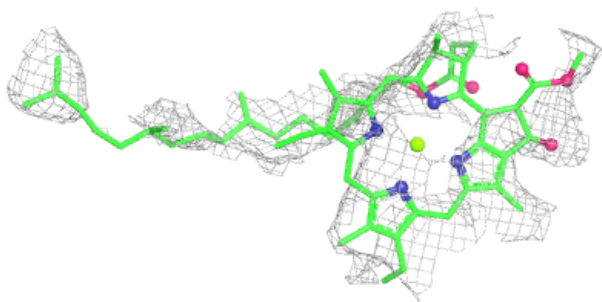


Electron density around LMU L 204:

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

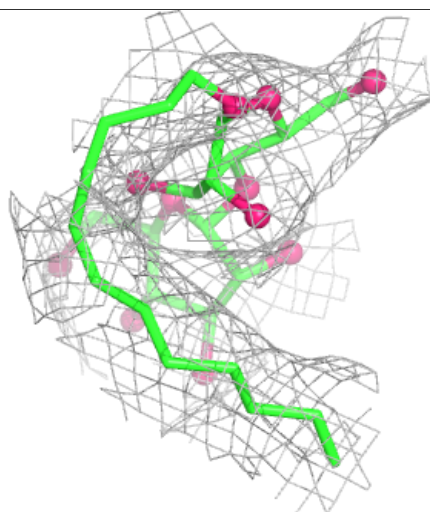
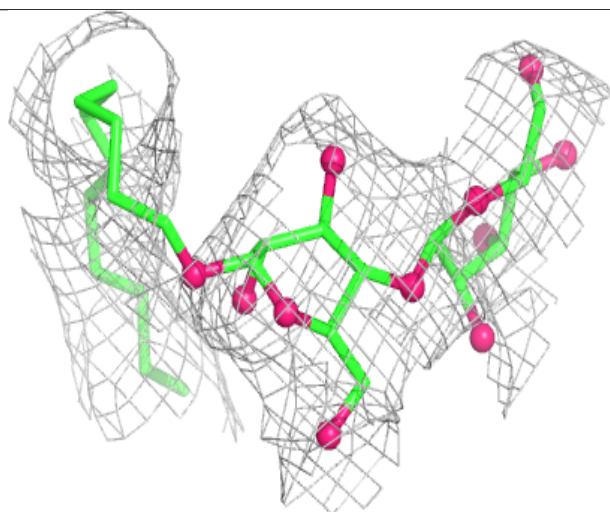
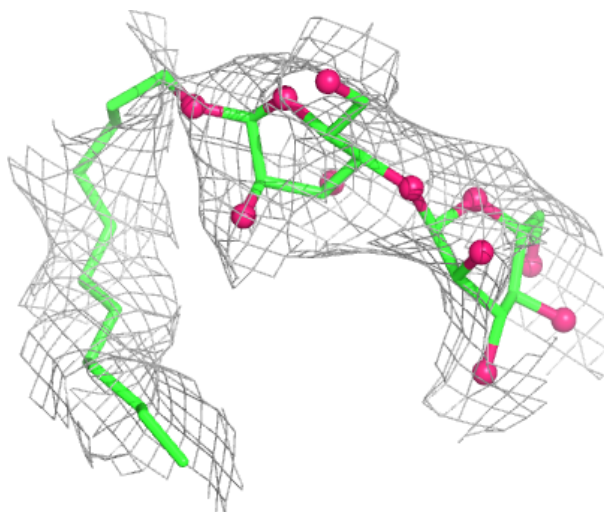
**Electron density around CLA 2 308:**

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



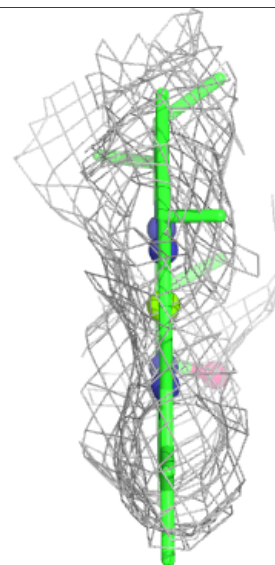
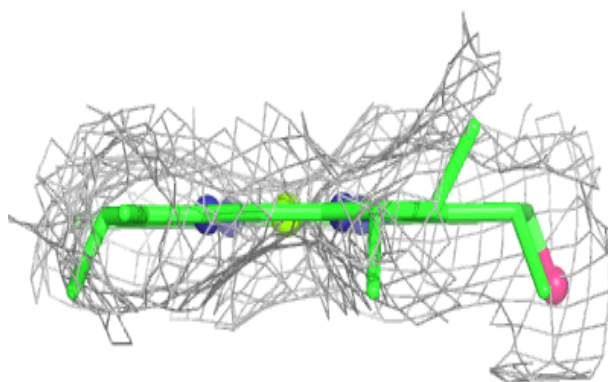
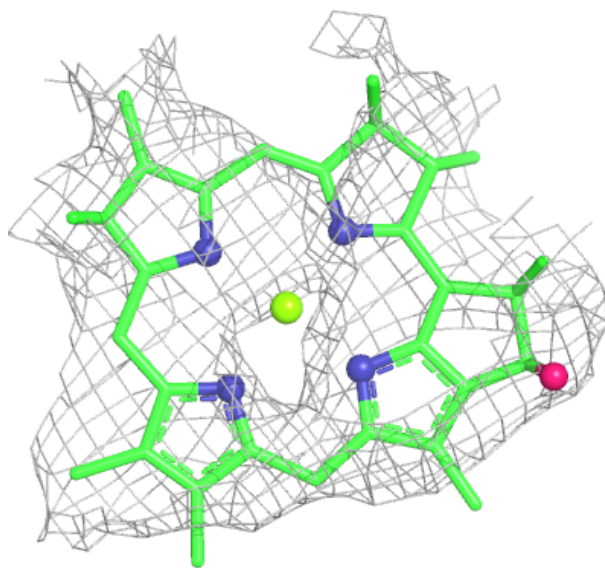
Electron density around LMU 1 220:

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



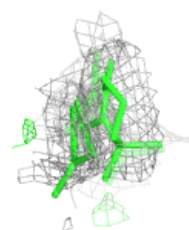
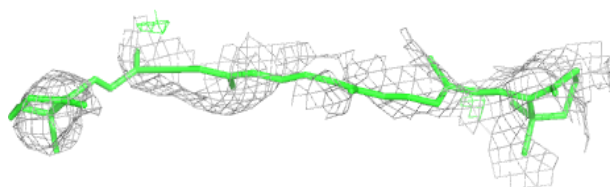
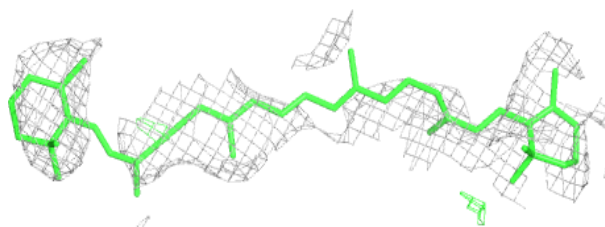
Electron density around CLA 4 308:

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

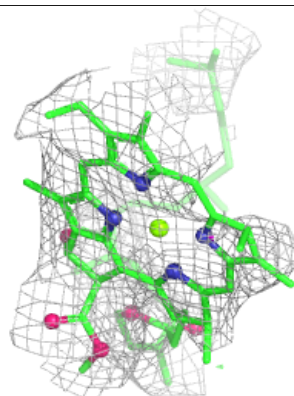
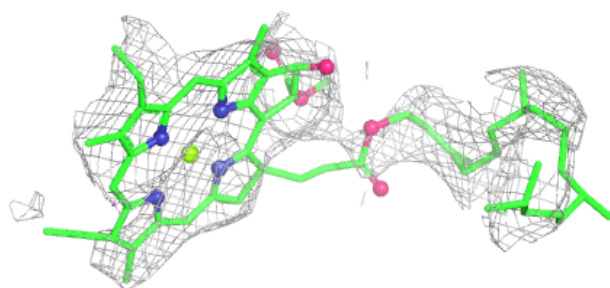
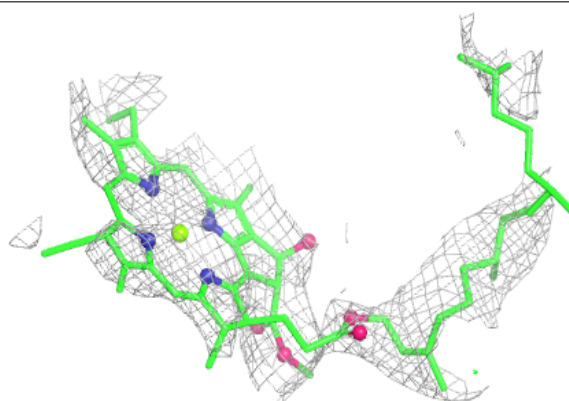


Electron density around BCR A 843:

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

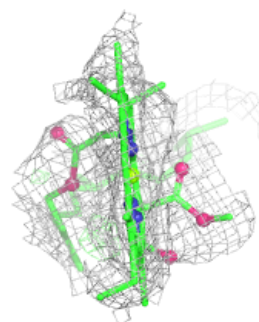
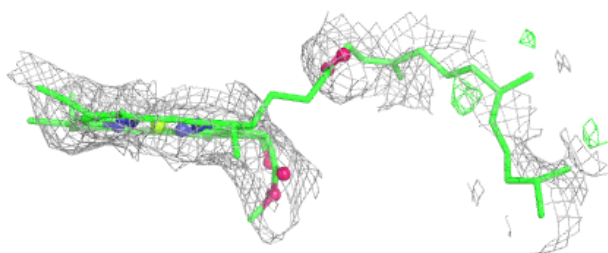
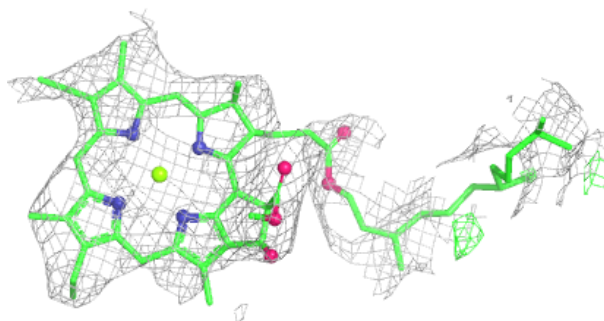
**Electron density around CLA K 103:**

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

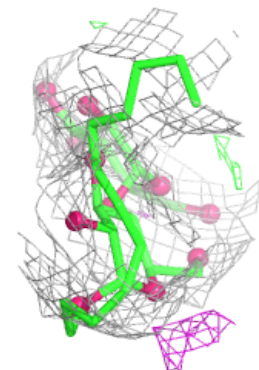
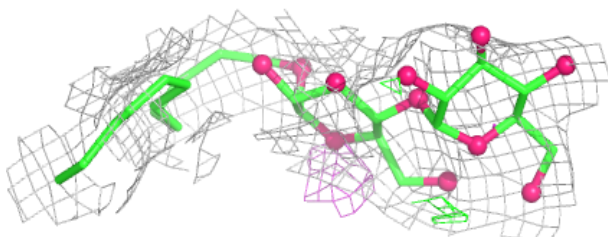
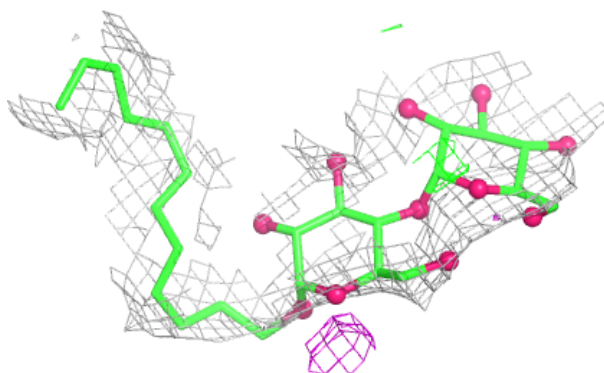


Electron density around CLA B 813:

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

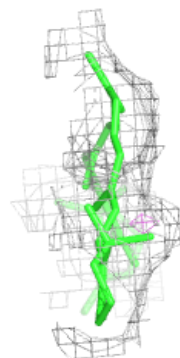
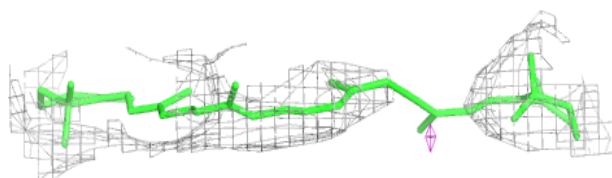
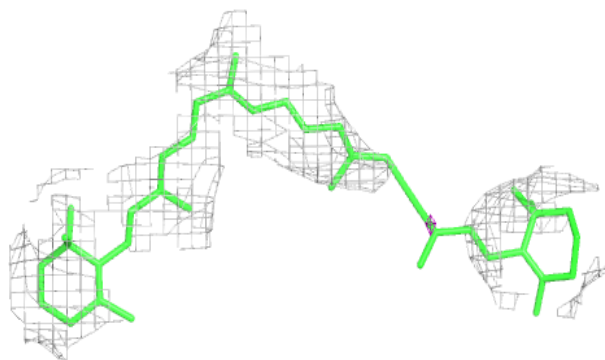
**Electron density around LMU R 106:**

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



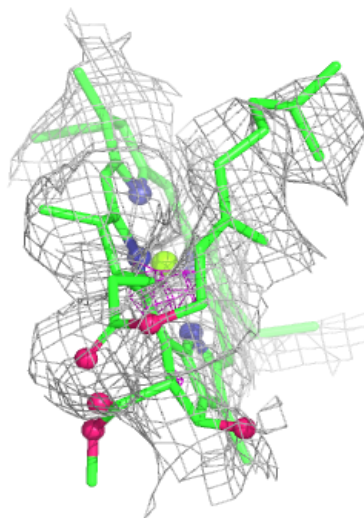
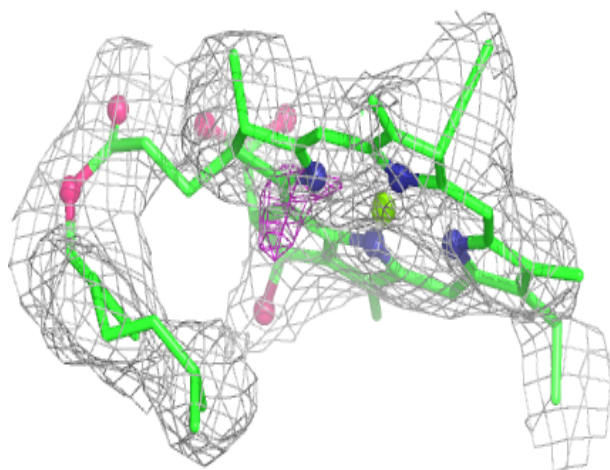
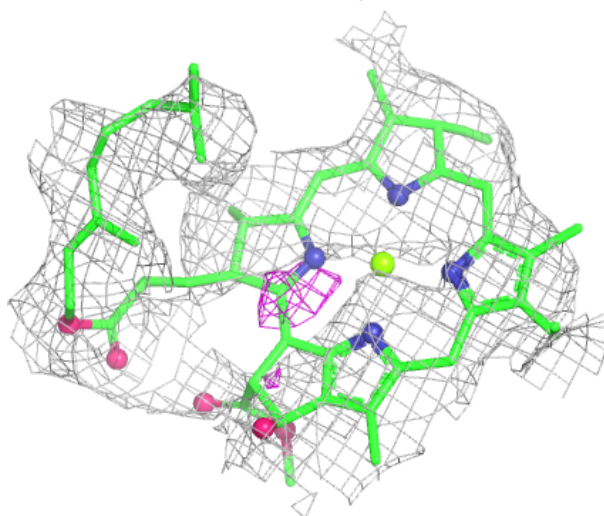
Electron density around BCR 3 314:

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



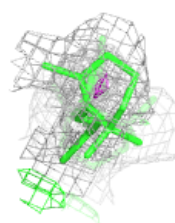
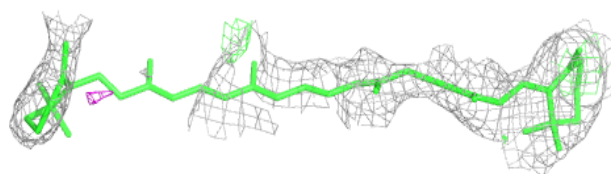
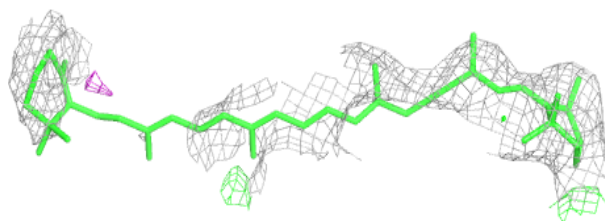
Electron density around CLA H 103:

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



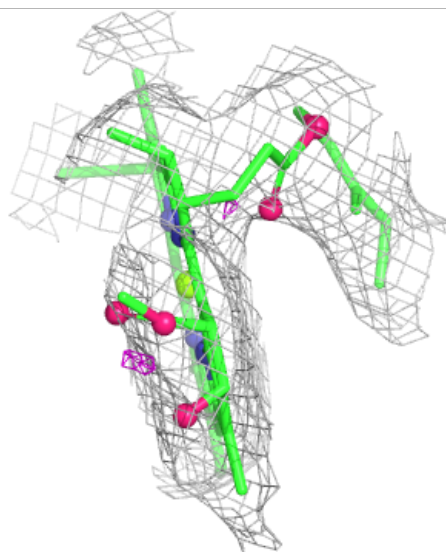
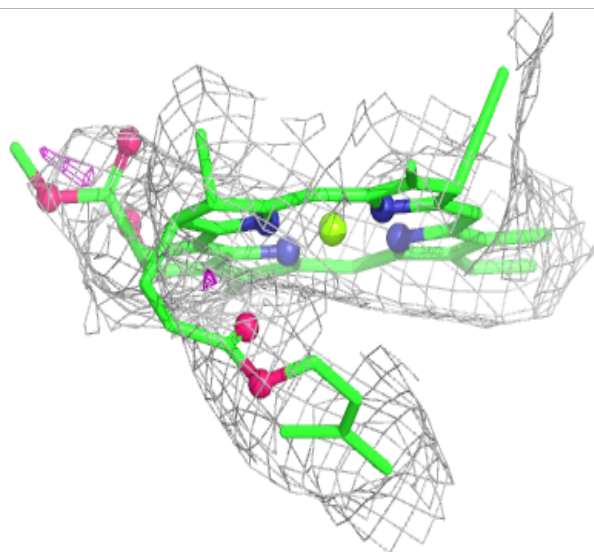
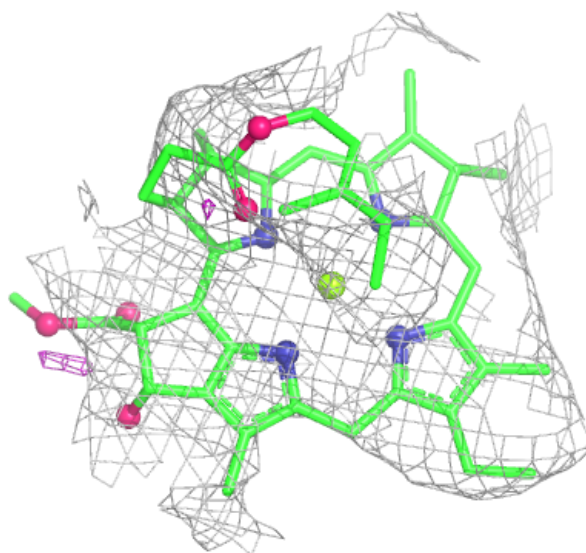
Electron density around BCR J 102:

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



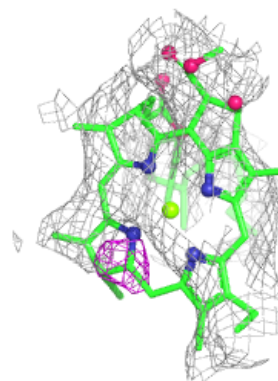
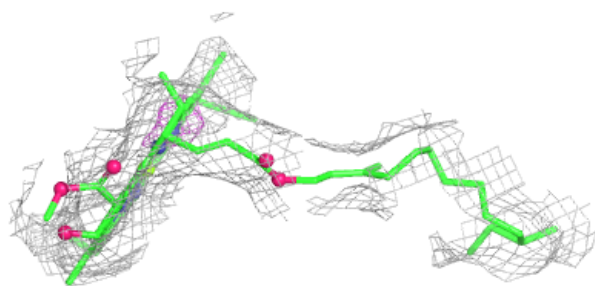
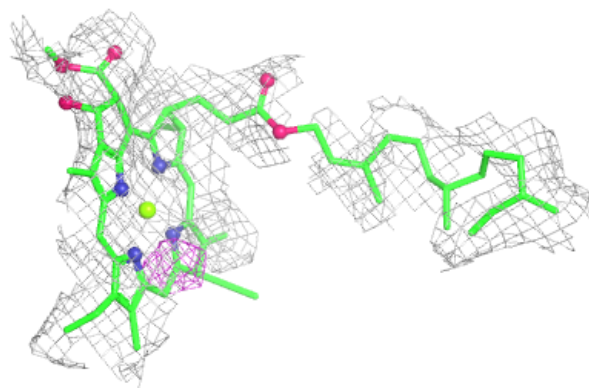
Electron density around CLA 2 302:

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



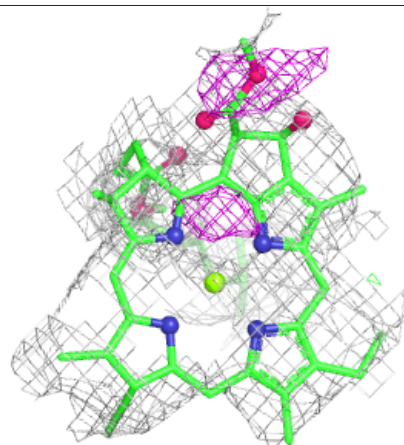
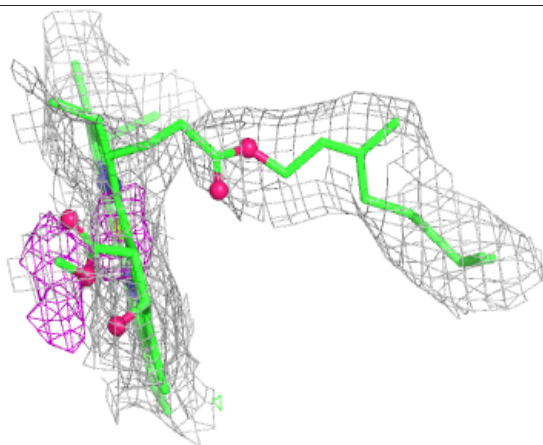
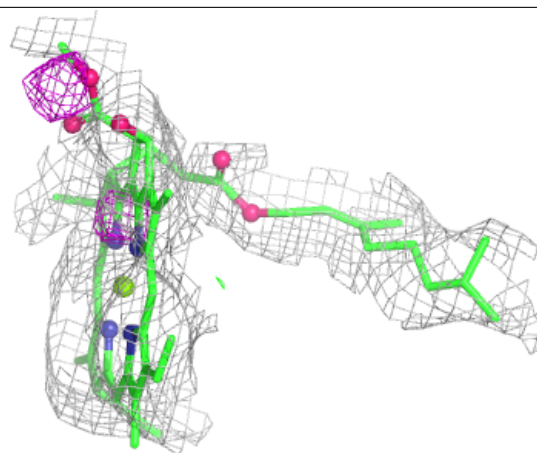
Electron density around CLA 2 320:

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



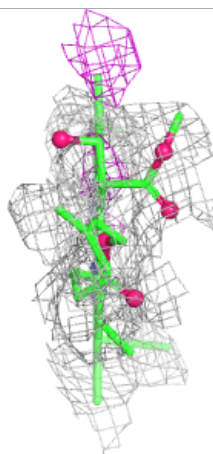
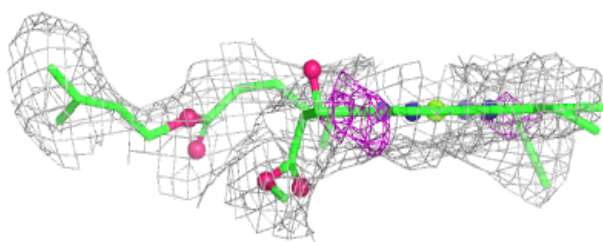
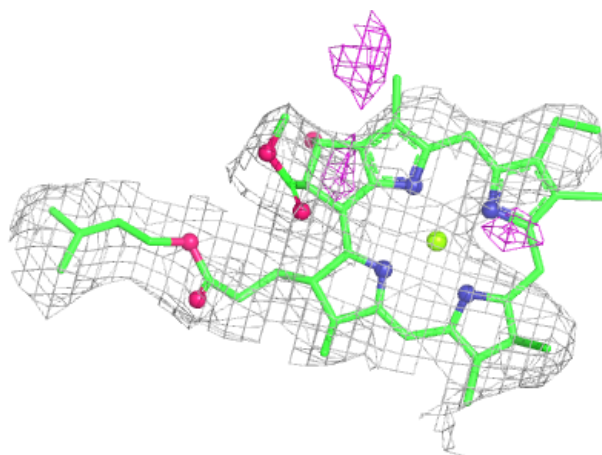
Electron density around CLA 4 302:

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



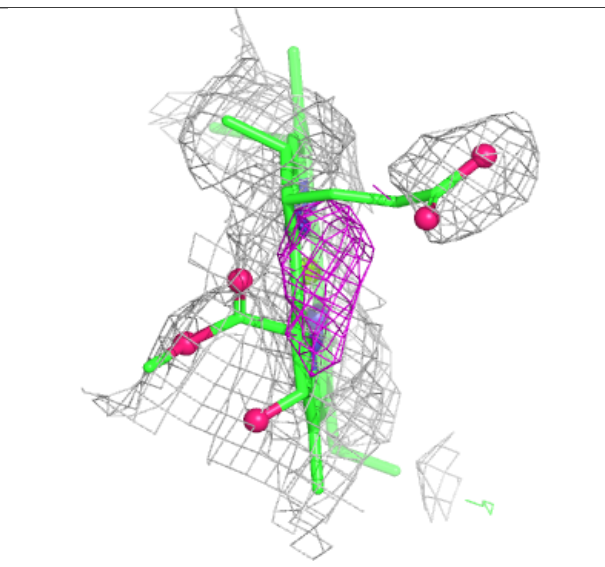
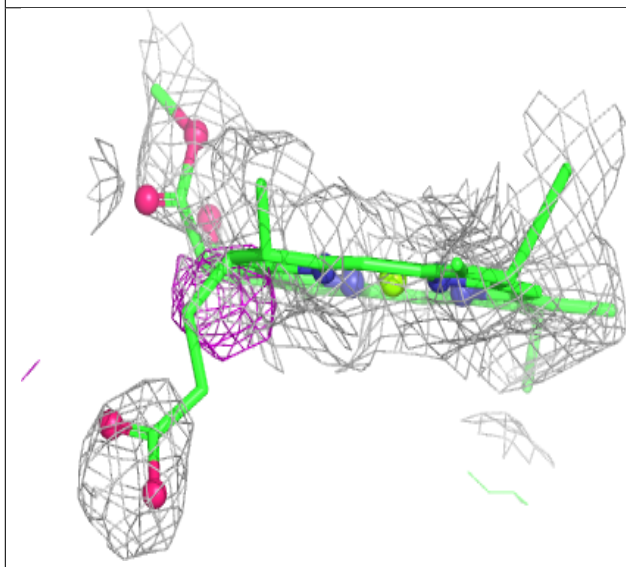
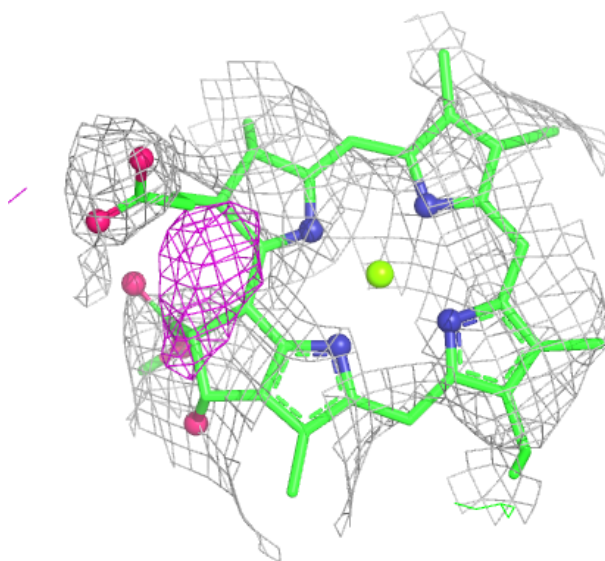
Electron density around CLA 4 306:

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



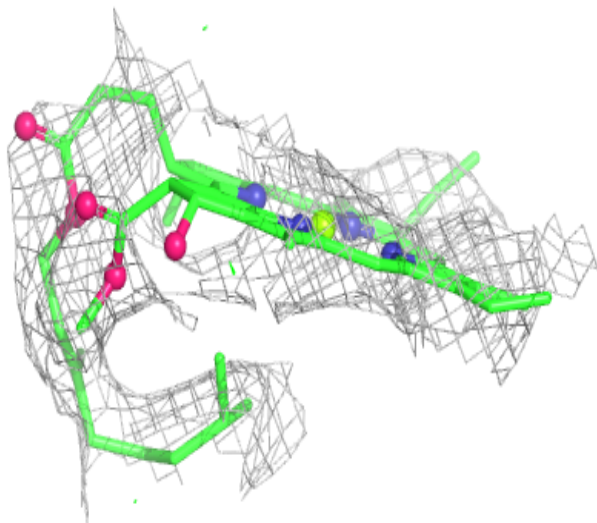
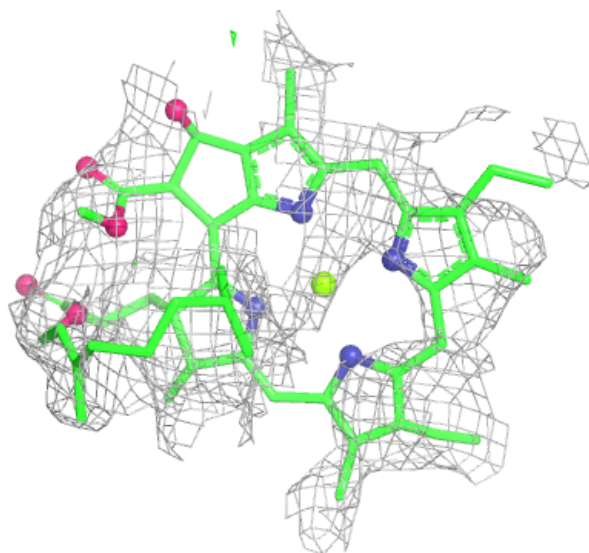
Electron density around CLA B 833:

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



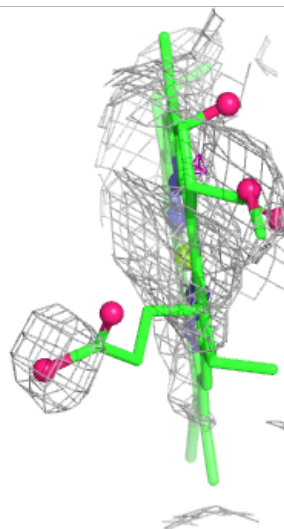
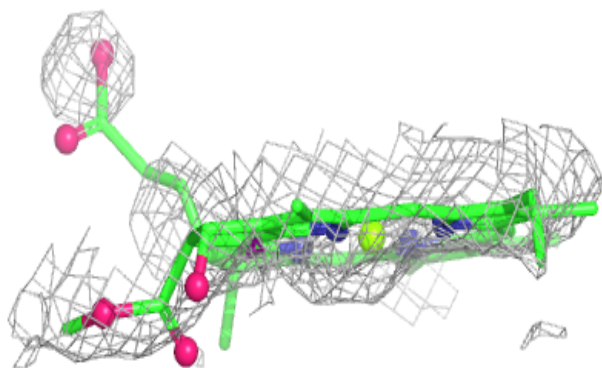
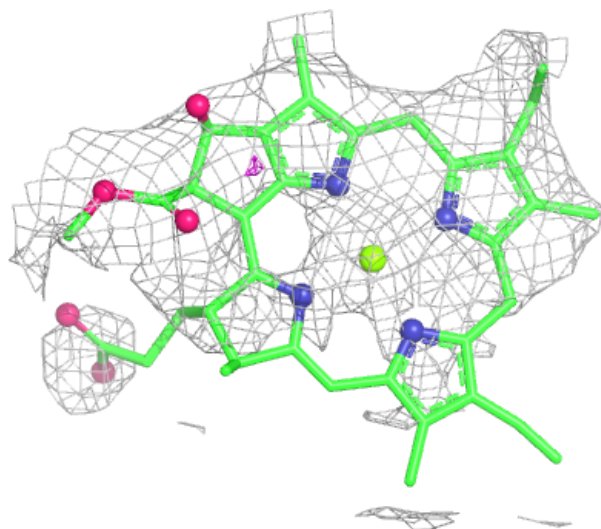
Electron density around CLA 4 305:

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



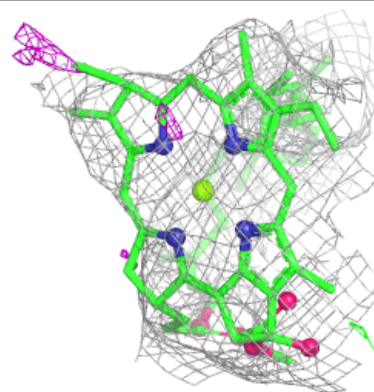
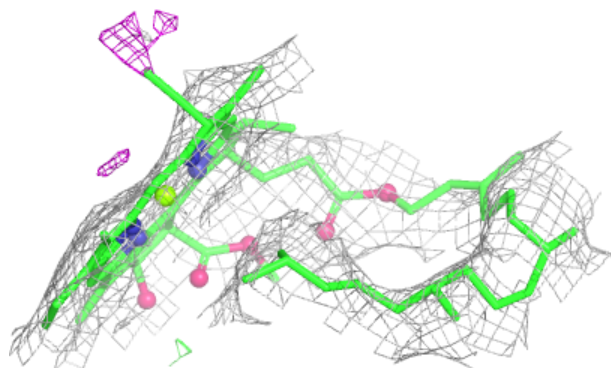
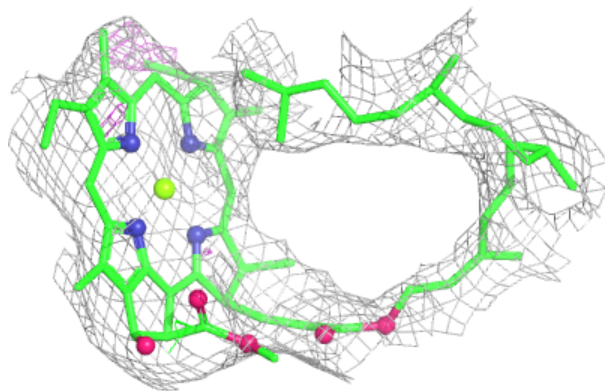
Electron density around CLA A 810:

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

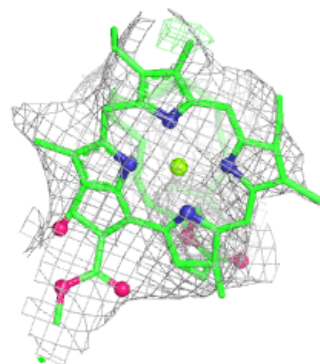
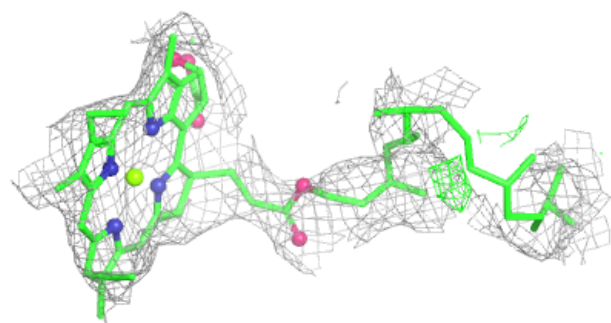
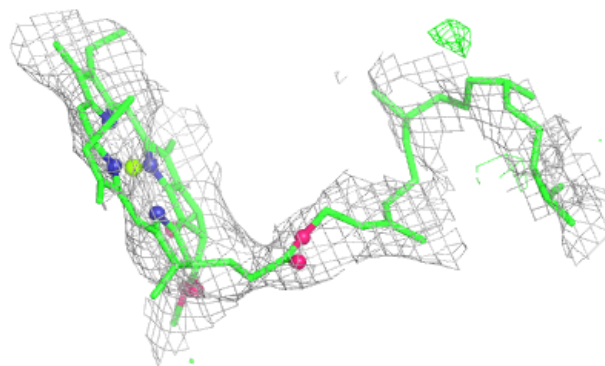


Electron density around CLA A 839:

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

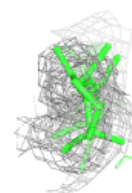
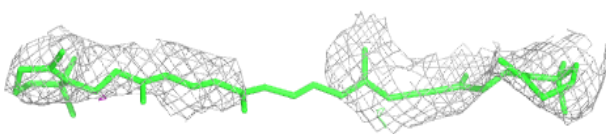
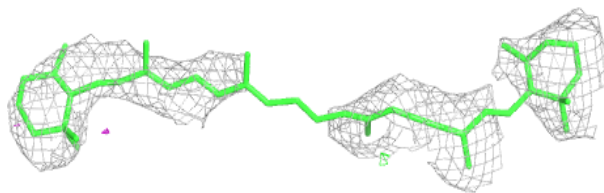
**Electron density around CLA 3 311:**

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



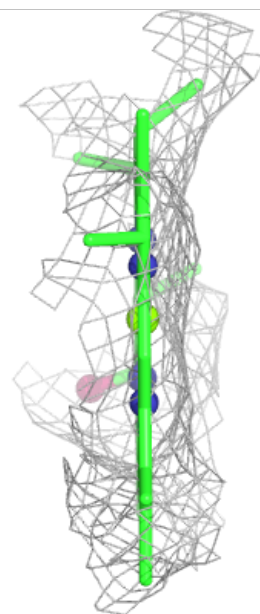
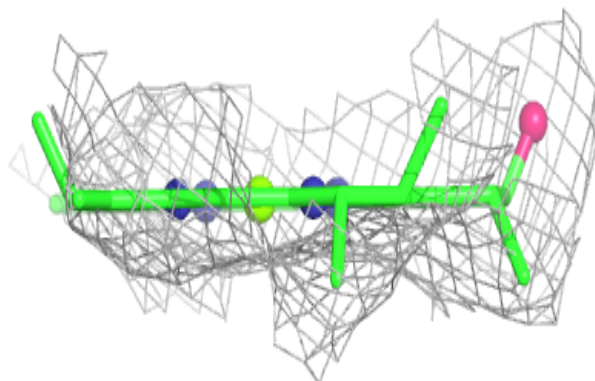
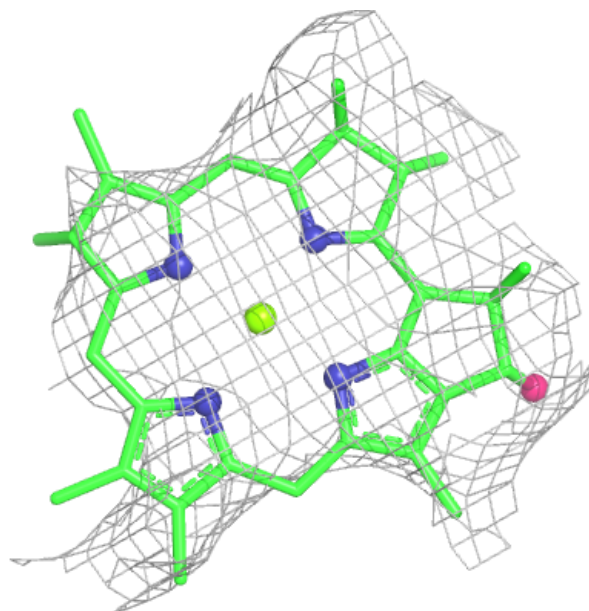
Electron density around BCR L 208:

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



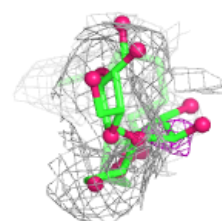
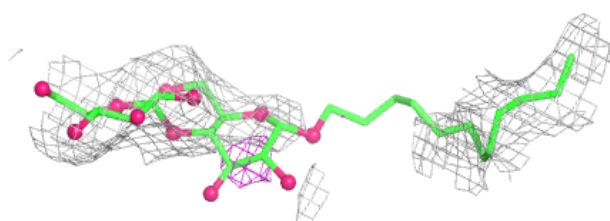
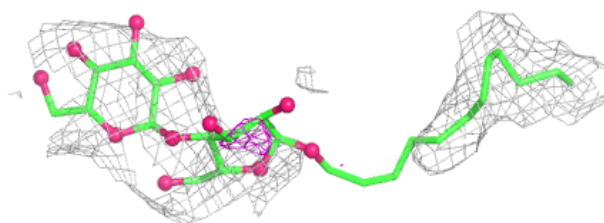
Electron density around CLA 3 301:

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

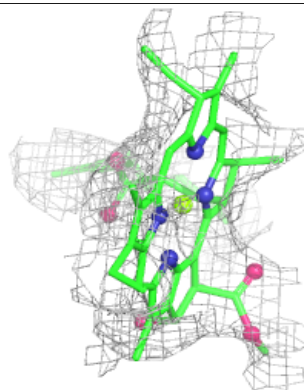
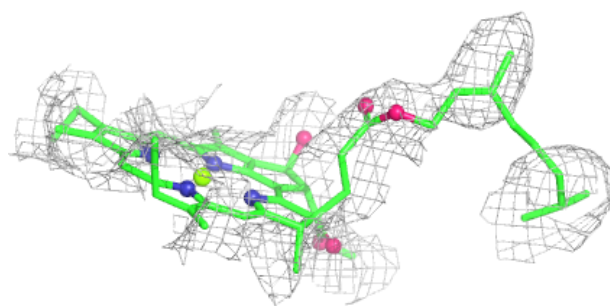
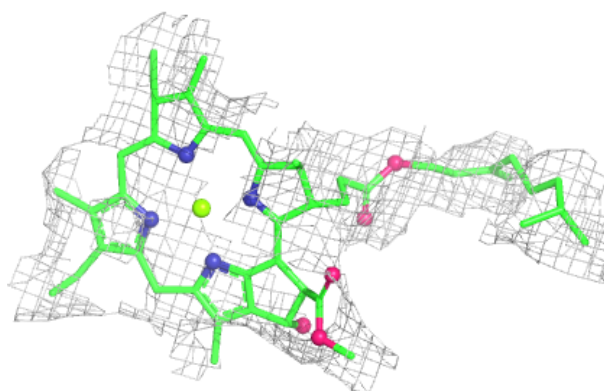


Electron density around LMU B 801:

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

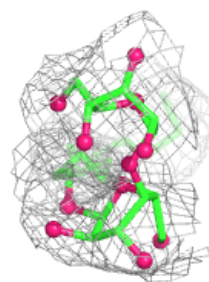
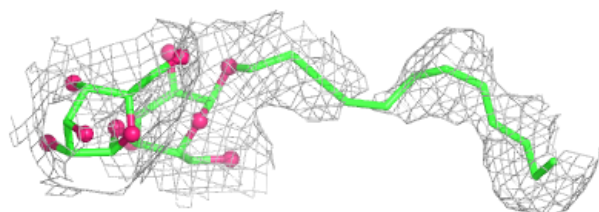
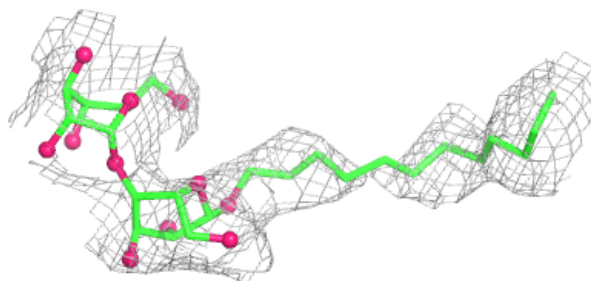
**Electron density around CLA H 102:**

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

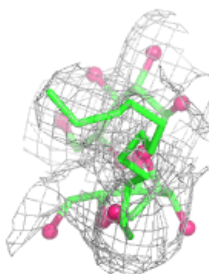
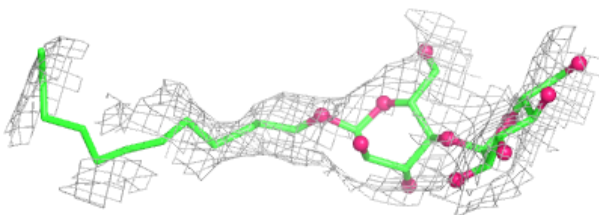
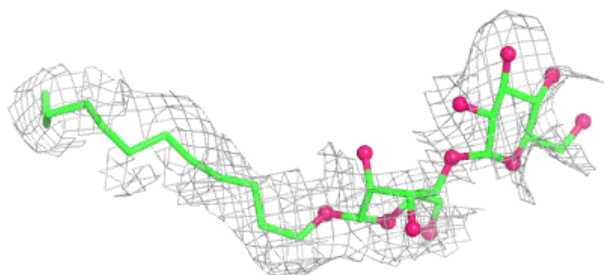


Electron density around LMU 1 213:

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

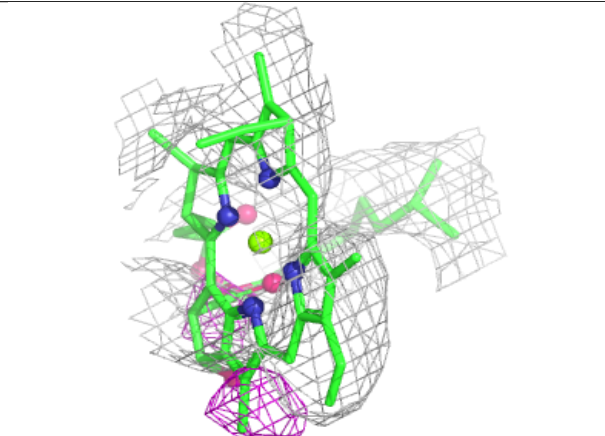
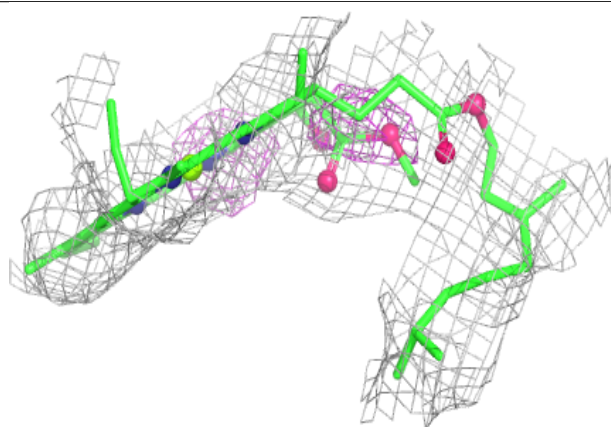
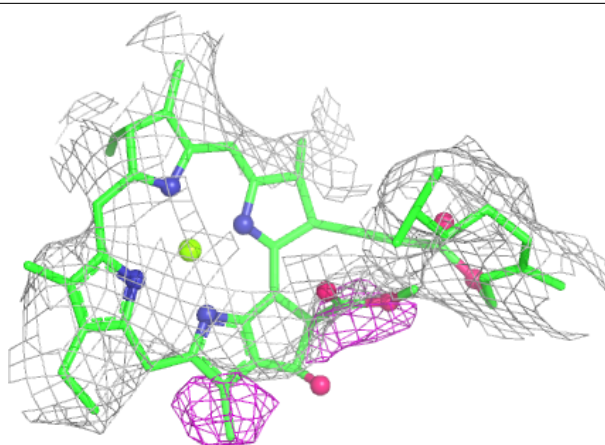
**Electron density around LMU 4 317:**

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

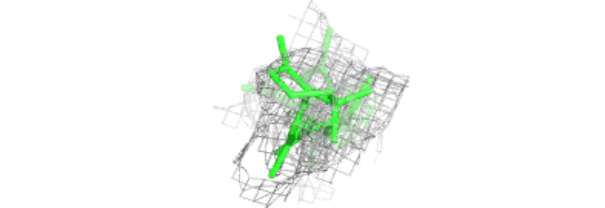
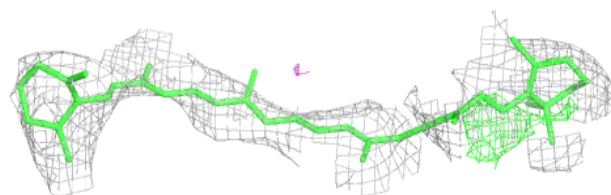
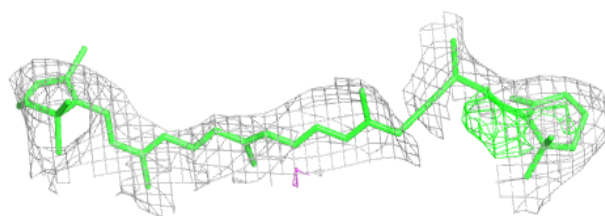


Electron density around CLA L 201:

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

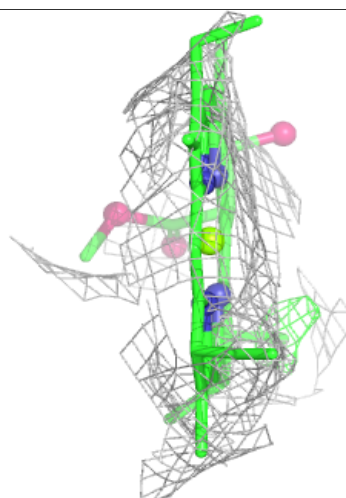
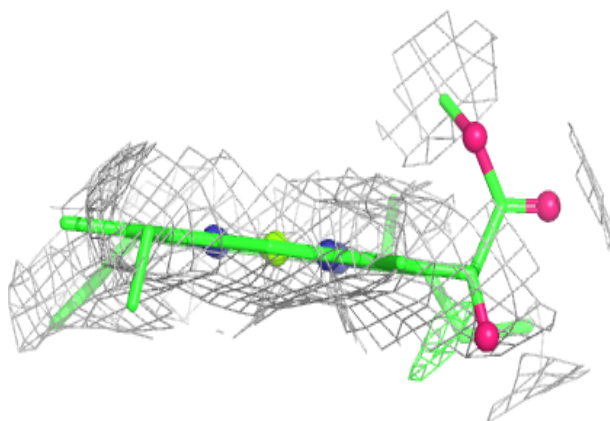
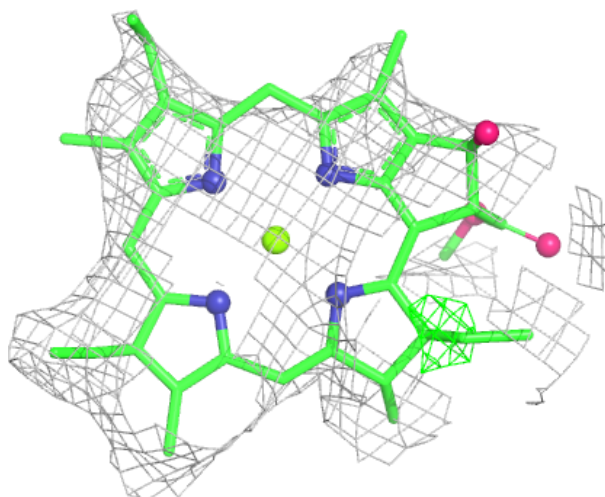
**Electron density around BCR A 845:**

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



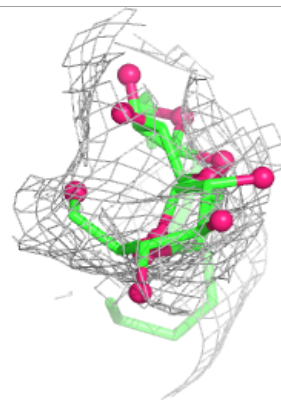
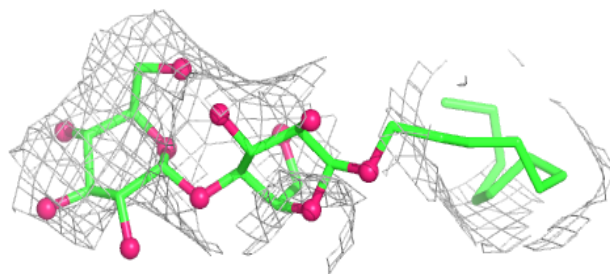
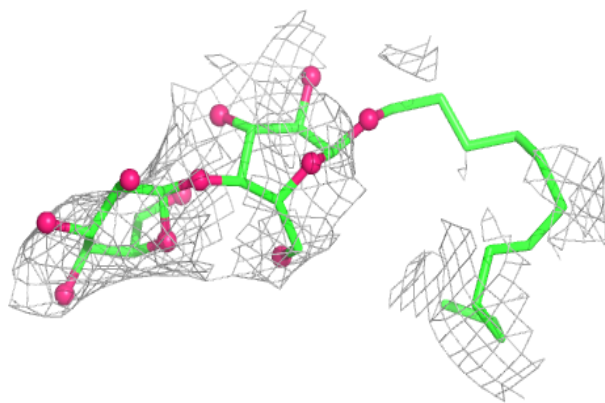
Electron density around CLA 3 308:

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



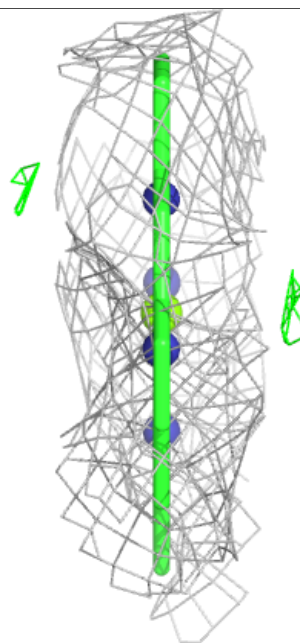
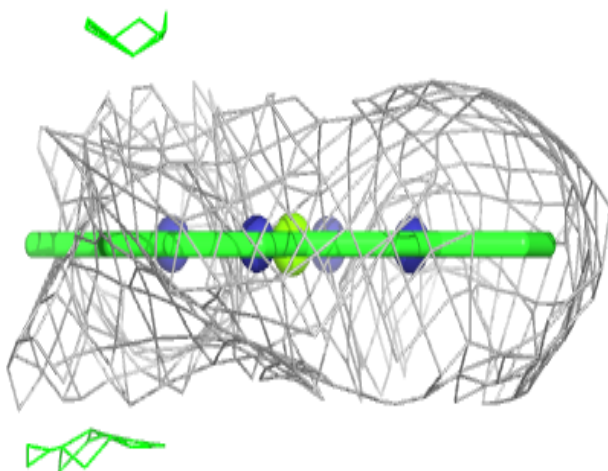
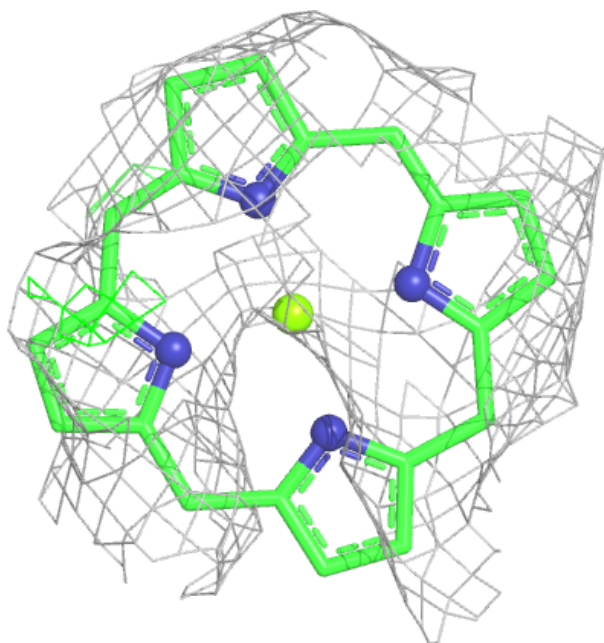
Electron density around LMU D 201:

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



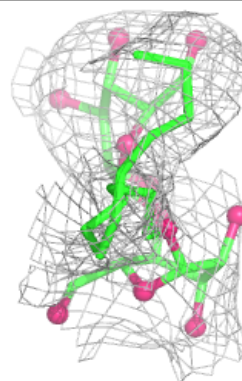
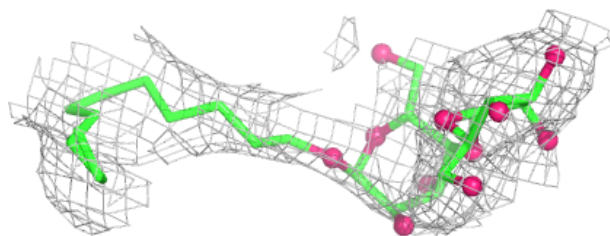
Electron density around CLA 1 211:

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



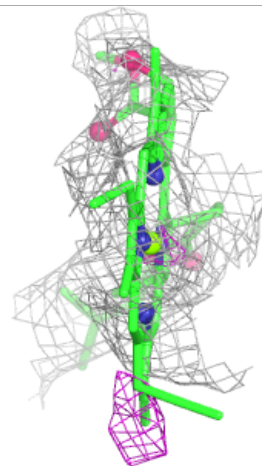
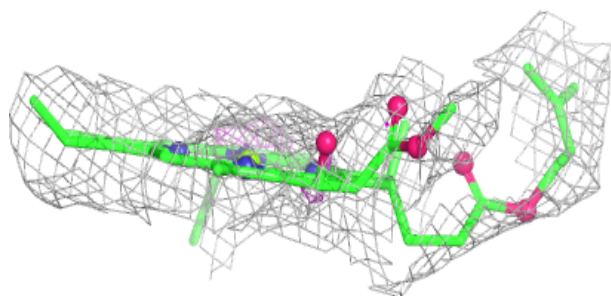
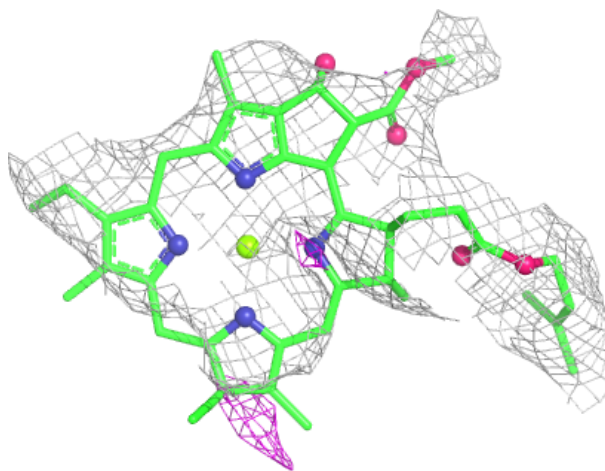
Electron density around LMU K 108:

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



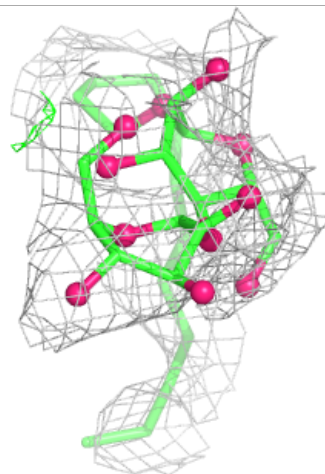
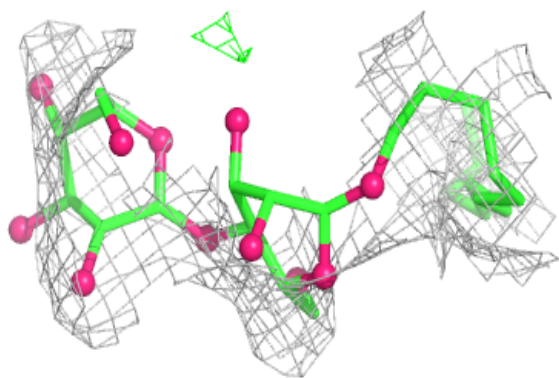
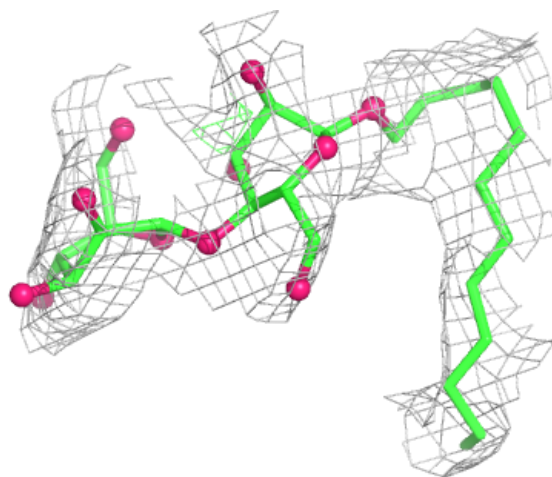
Electron density around CLA K 102:

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



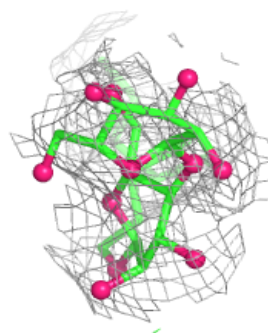
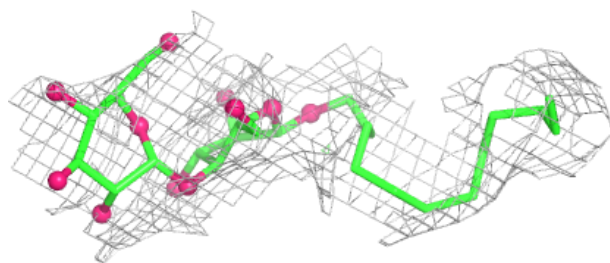
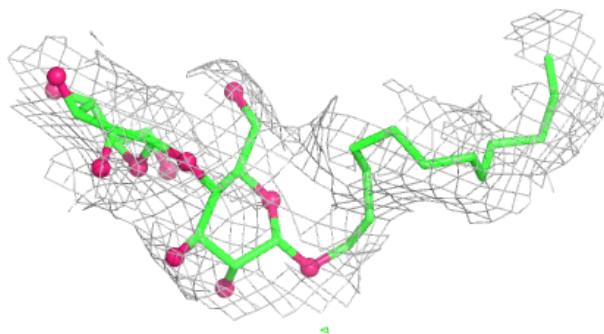
Electron density around LMU R 101:

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

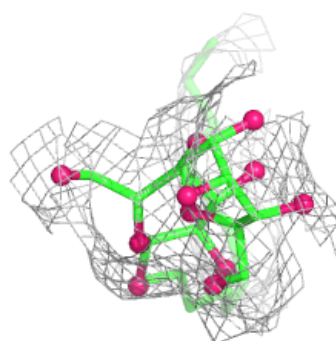
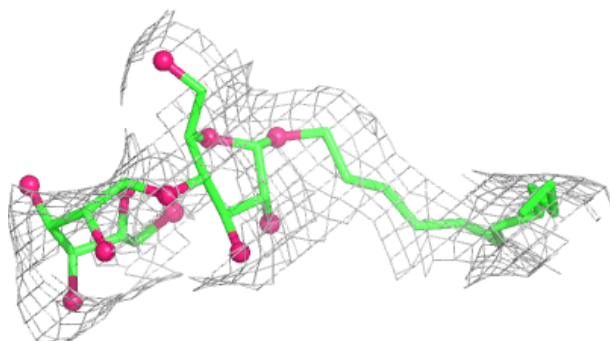
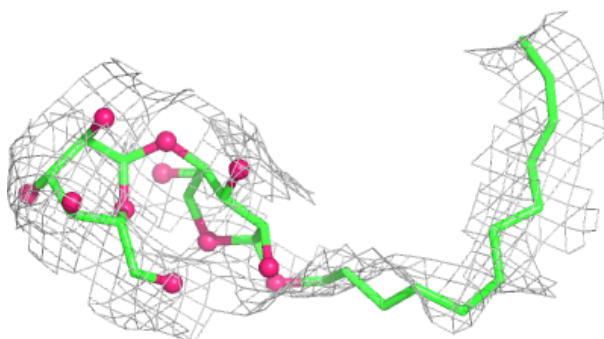


Electron density around LMU 2 313:

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

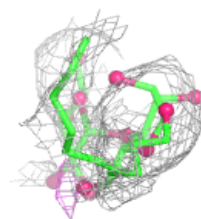
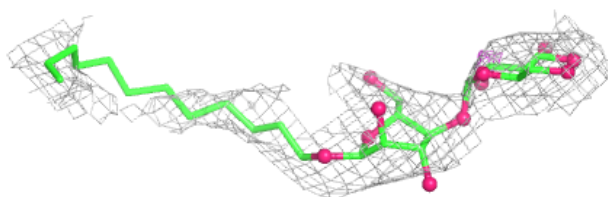
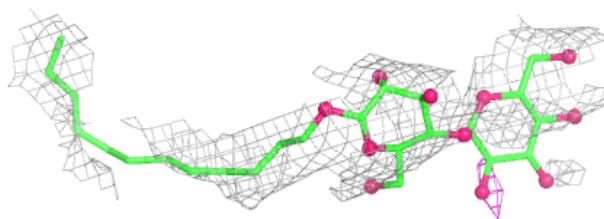
**Electron density around LMU 2 316:**

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

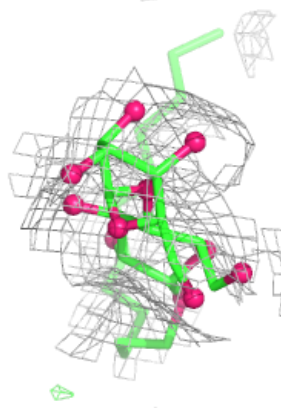
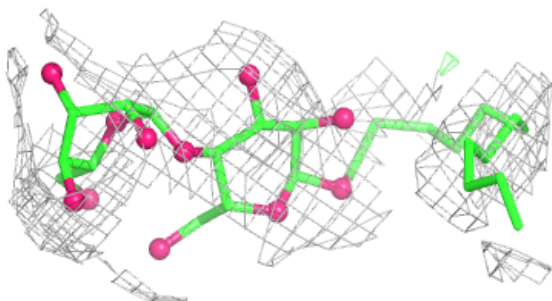
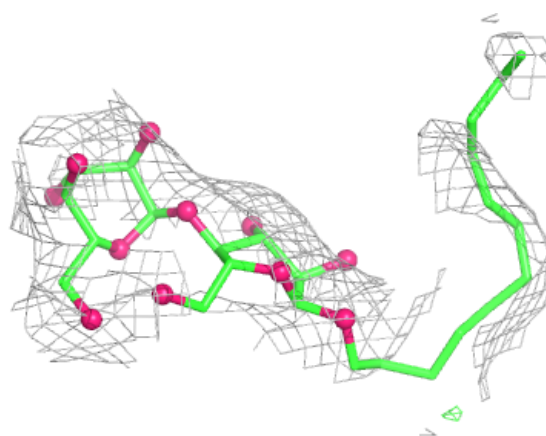


Electron density around LMU 2 319:

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

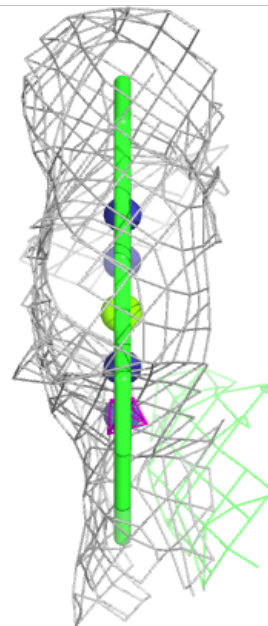
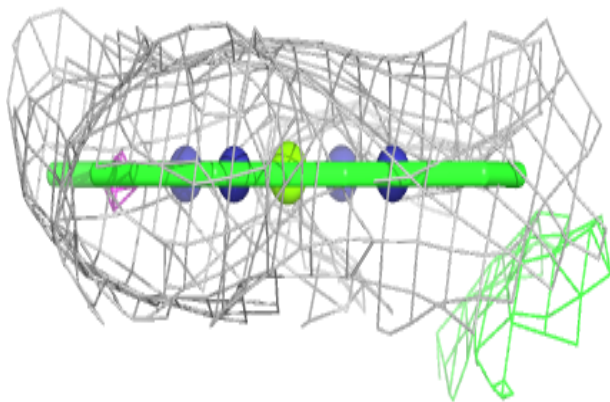
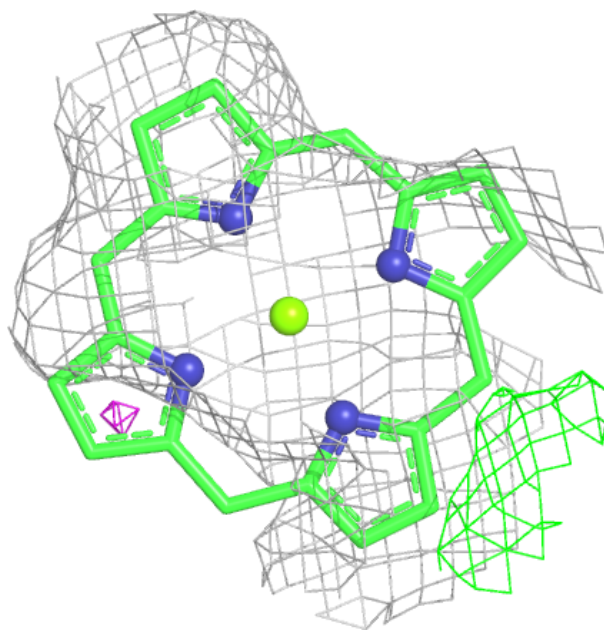
**Electron density around LMU 3 320:**

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



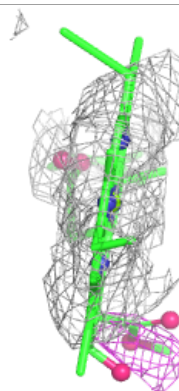
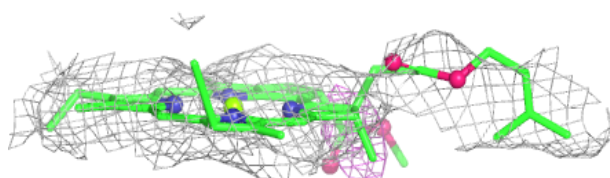
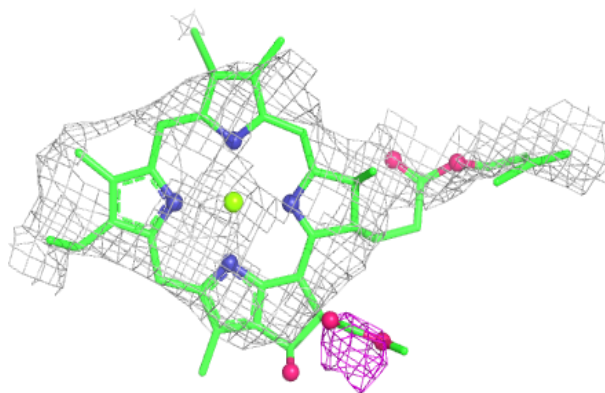
Electron density around CLA 2 306:

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



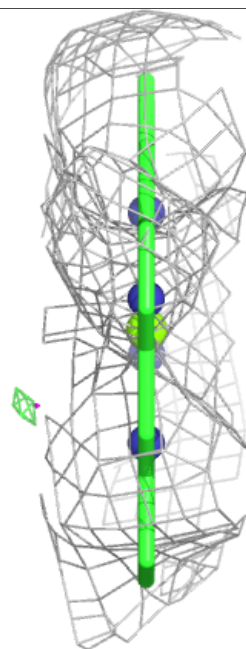
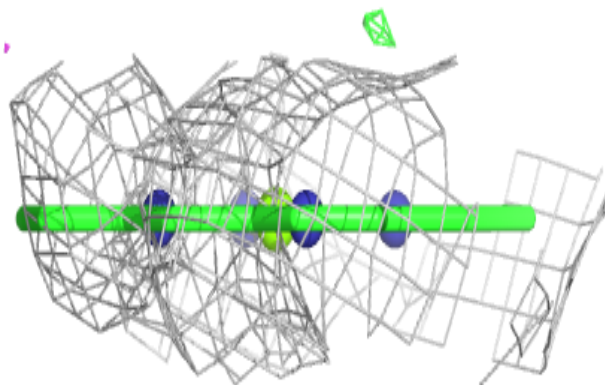
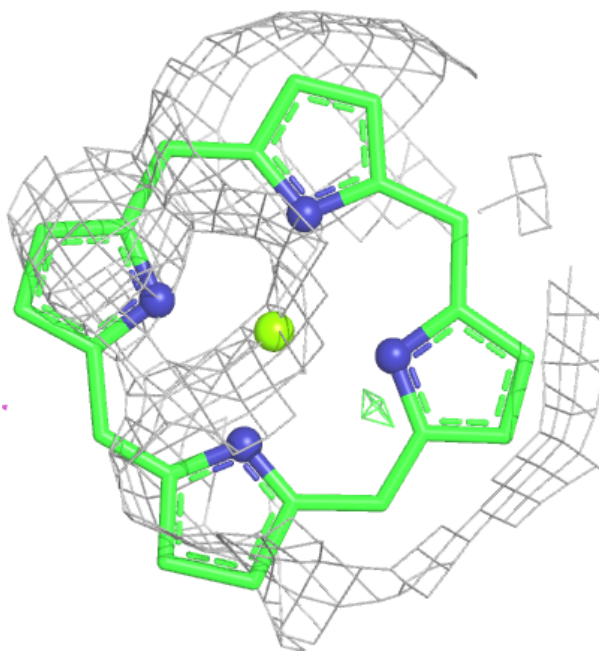
Electron density around CLA K 107:

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



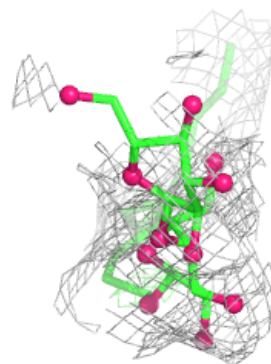
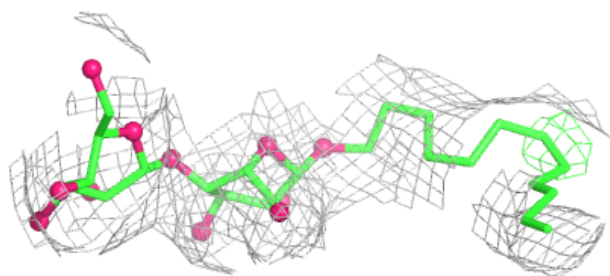
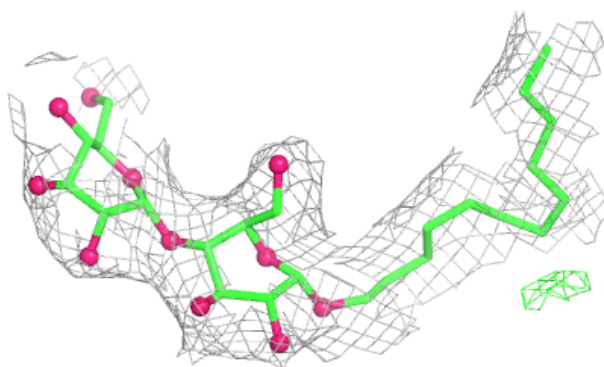
Electron density around CLA 3 307:

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



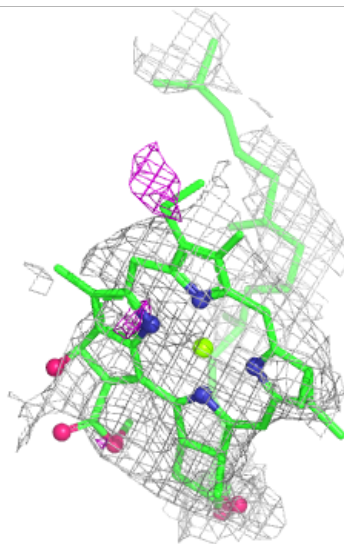
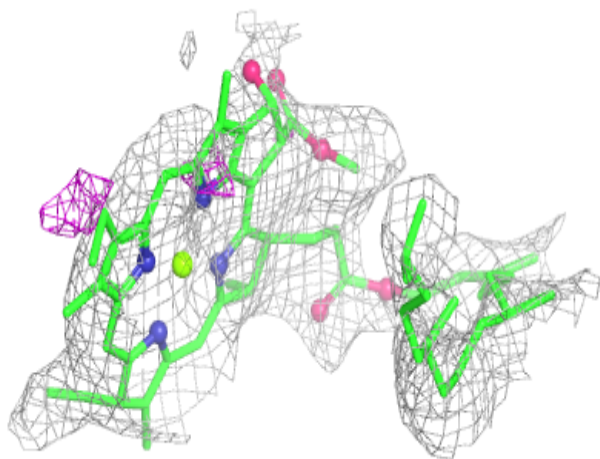
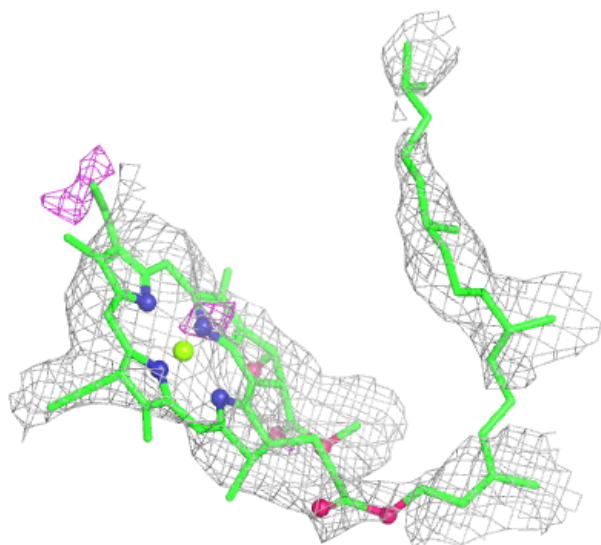
Electron density around LMU H 105:

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



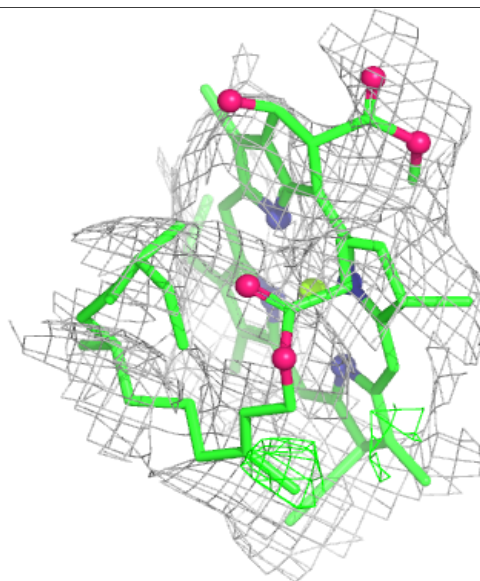
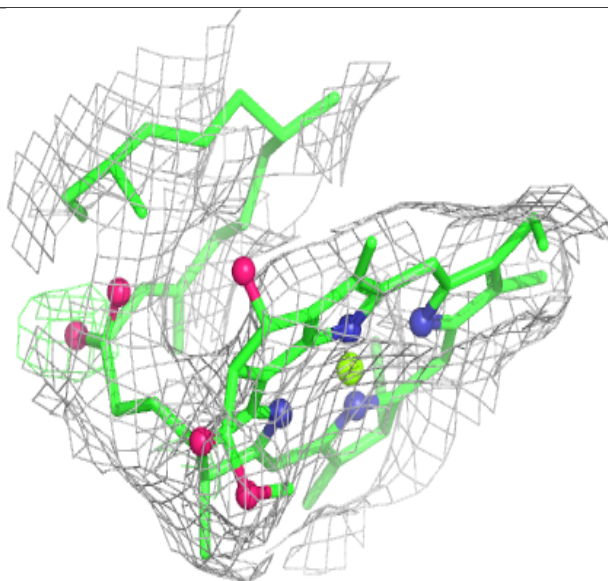
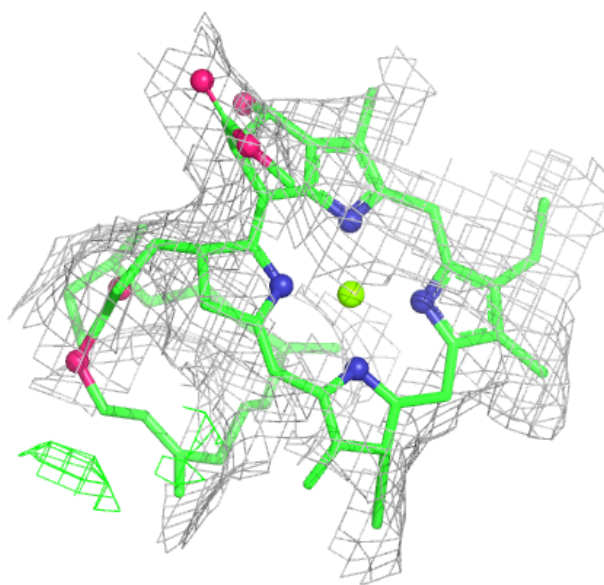
Electron density around CLA 3 313:

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



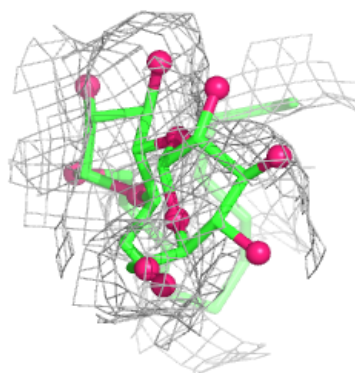
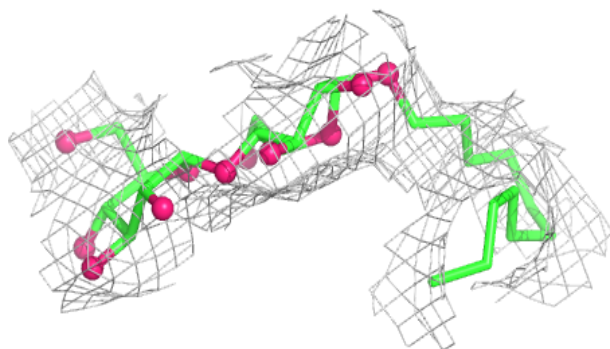
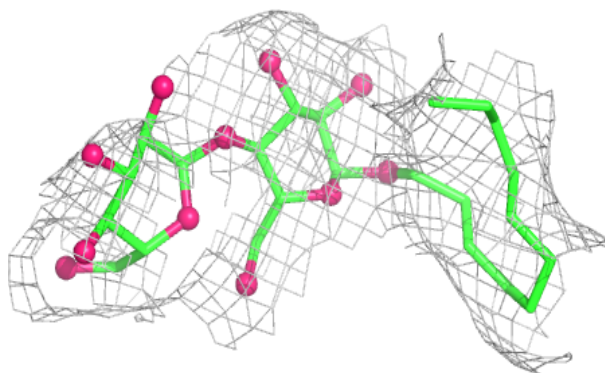
Electron density around CLA J 103:

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

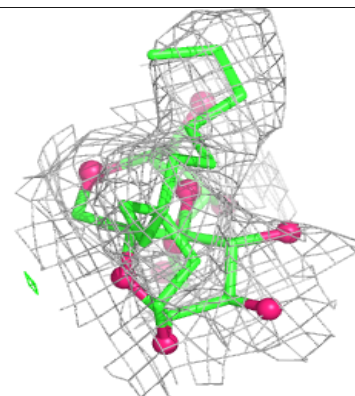
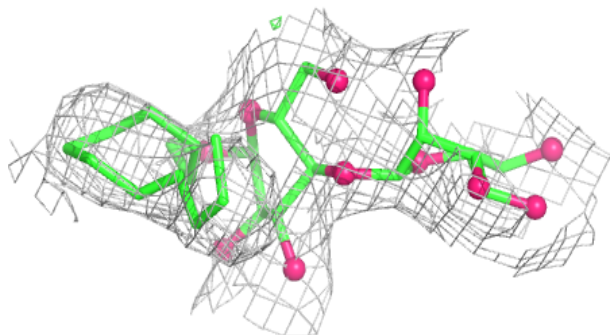
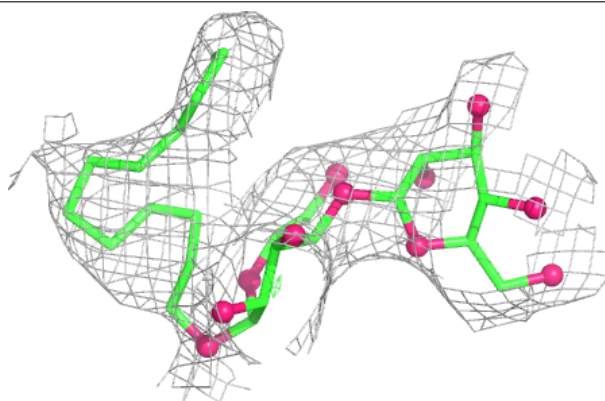


Electron density around LMU F 201:

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

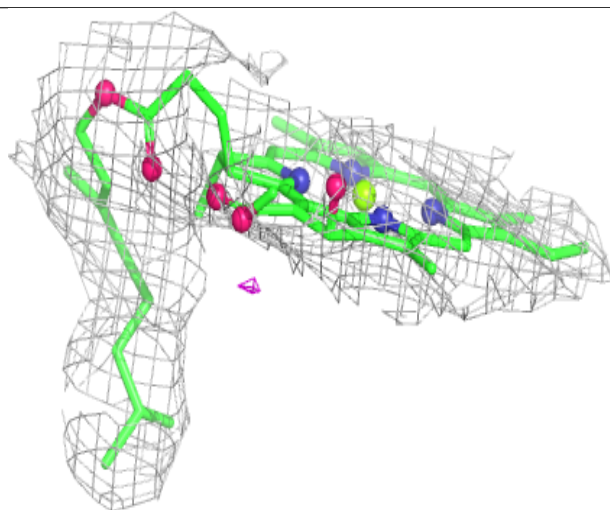
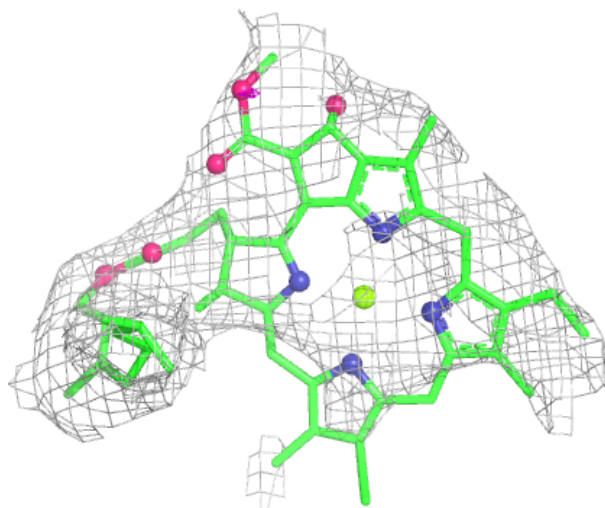
**Electron density around LMU K 106:**

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



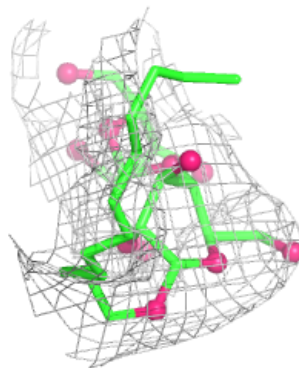
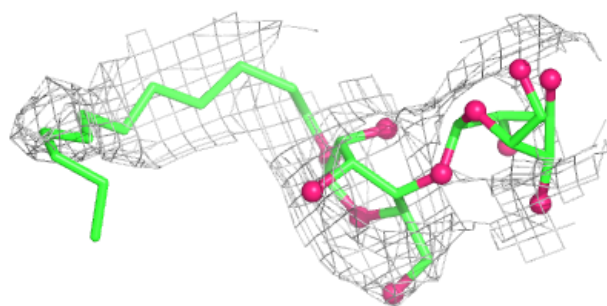
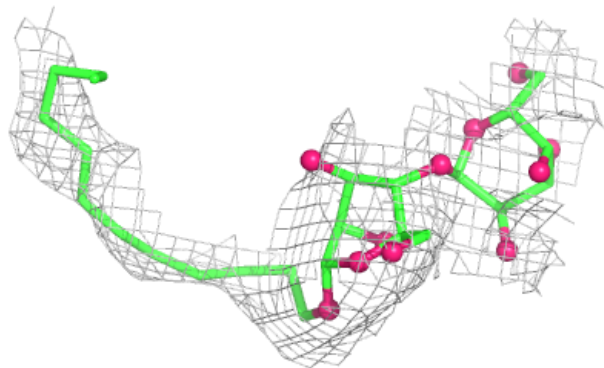
Electron density around CLA H 101:

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



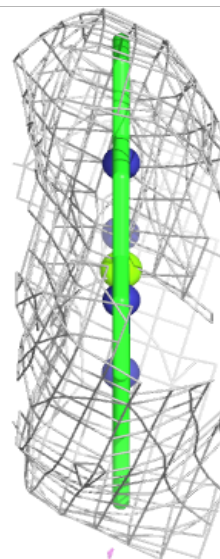
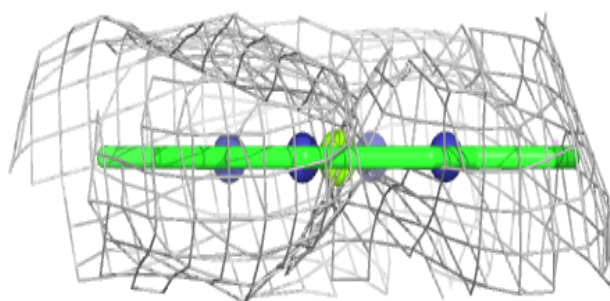
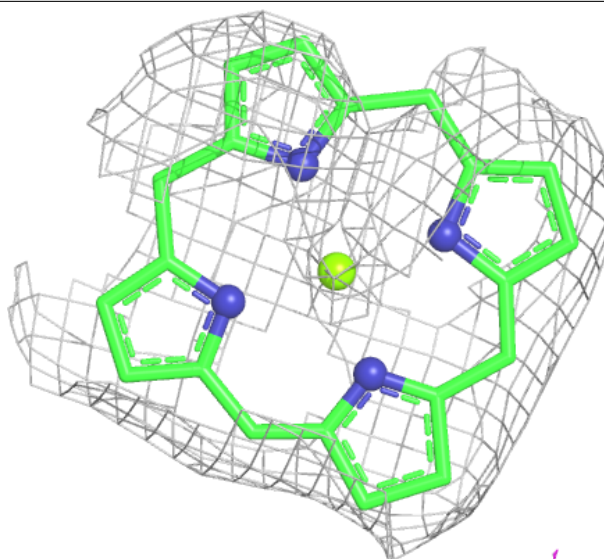
Electron density around LMU R 104:

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



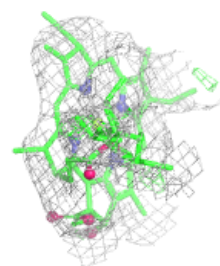
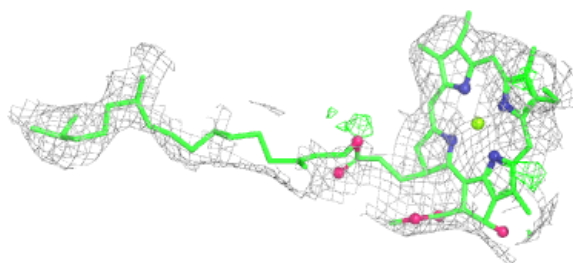
Electron density around CLA 3 305:

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

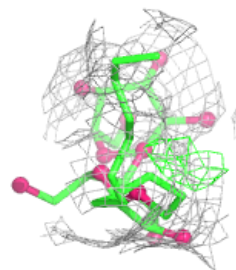
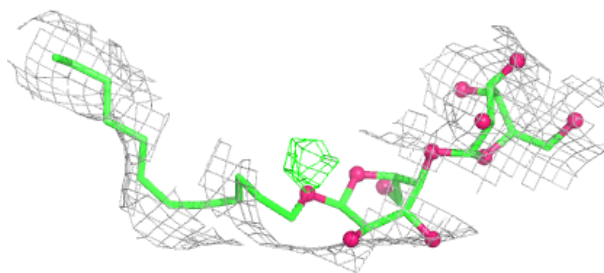


Electron density around CLA 4 304:

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

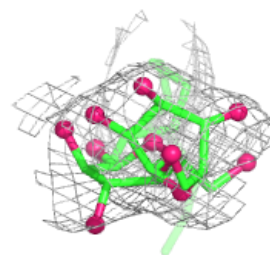
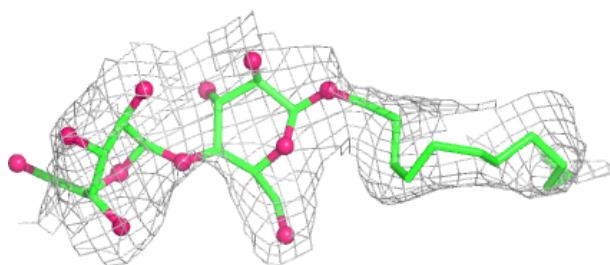
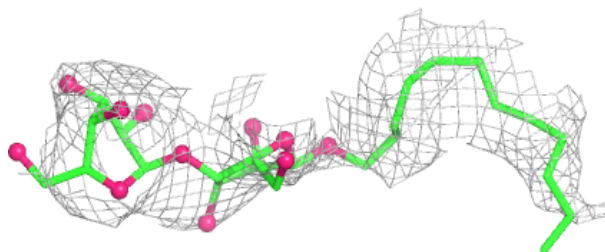
**Electron density around LMU 2 317:**

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



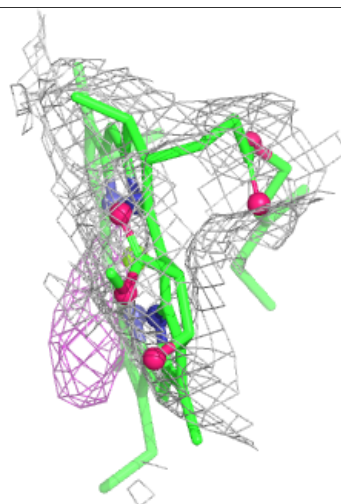
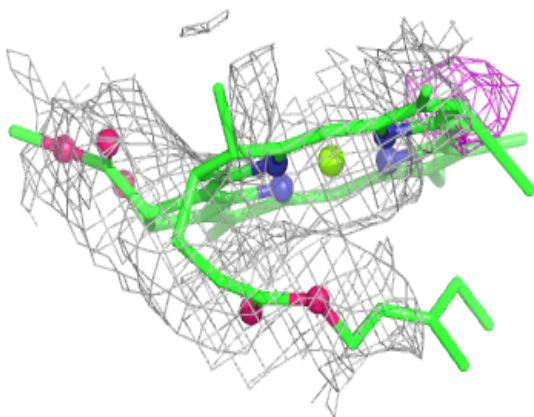
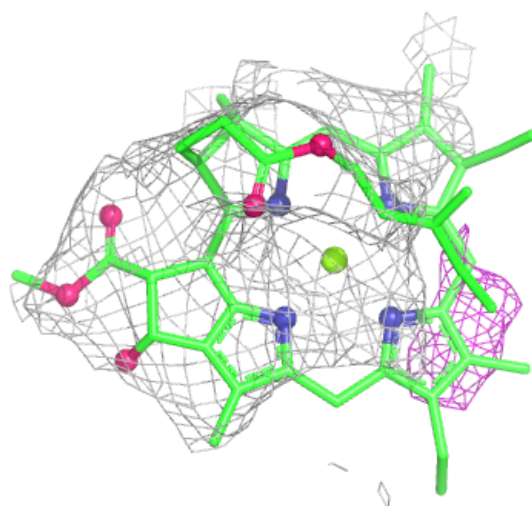
Electron density around LMU A 848:

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



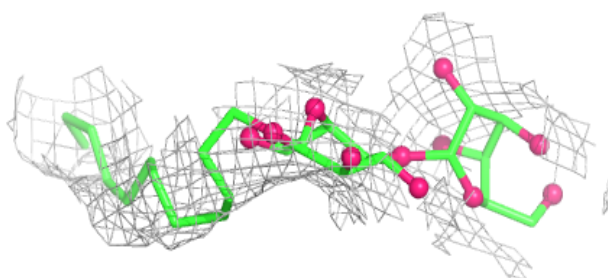
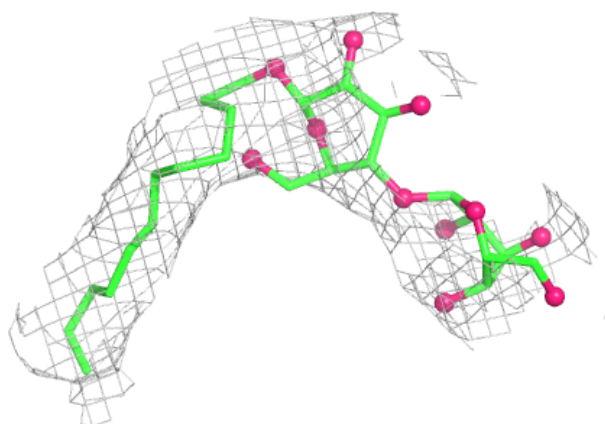
Electron density around CLA A 820:

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

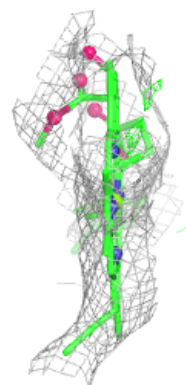
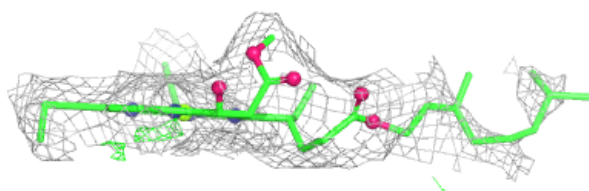
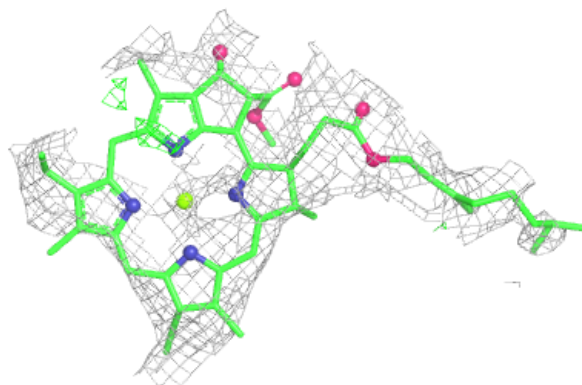


Electron density around LMU R 103:

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

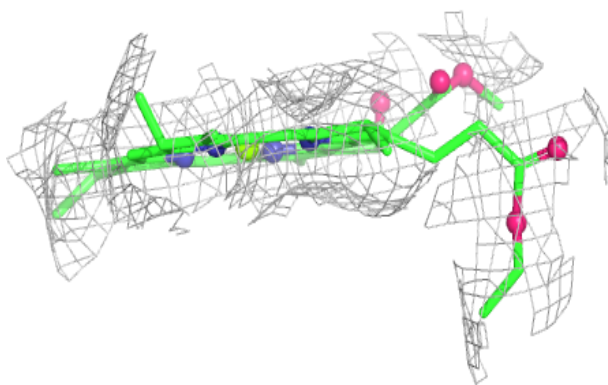
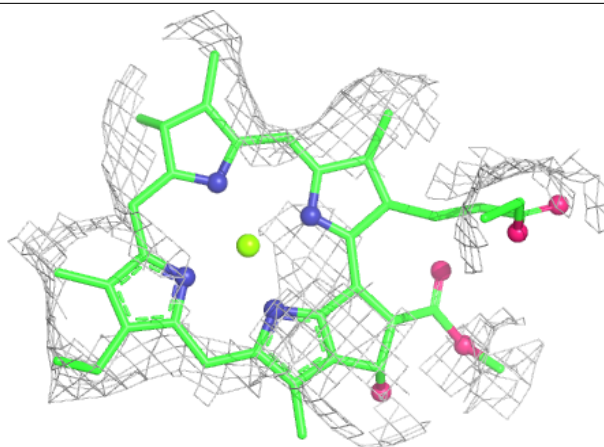
**Electron density around CLA 4 311:**

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



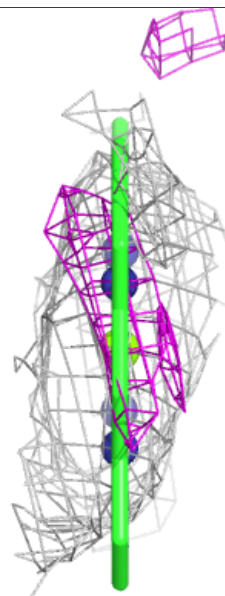
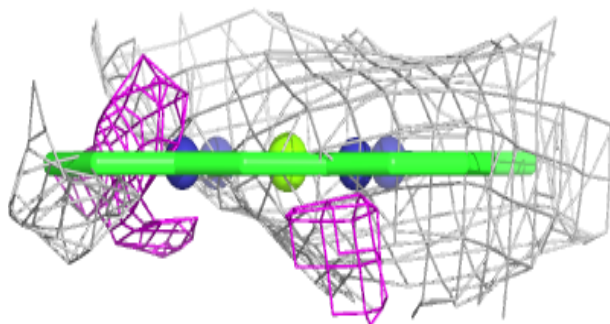
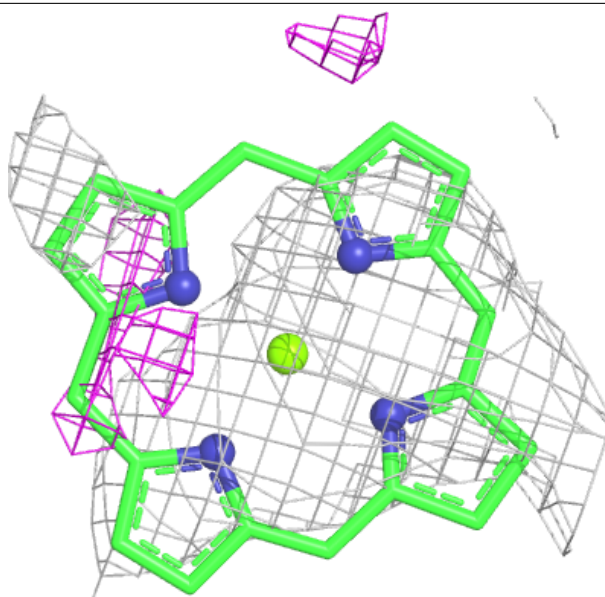
Electron density around CLA A 801:

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



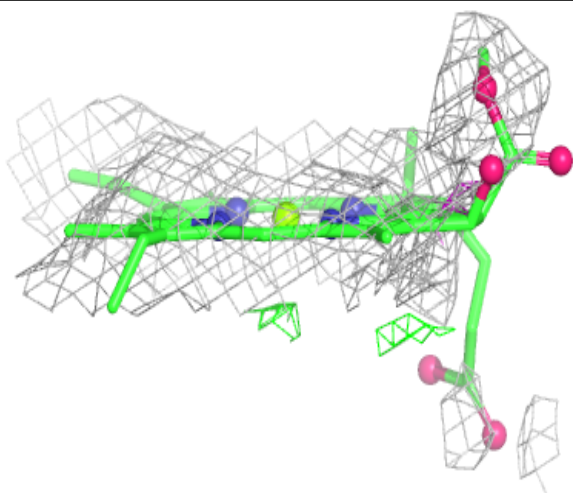
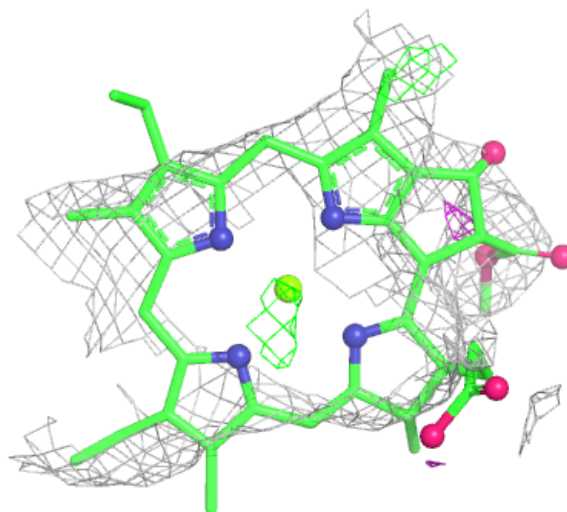
Electron density around CLA 2 301:

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



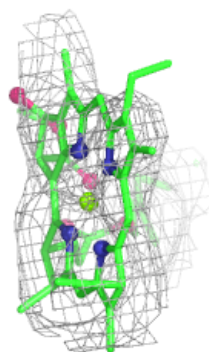
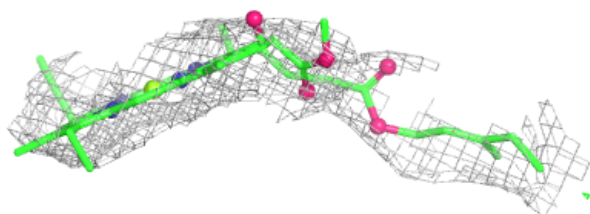
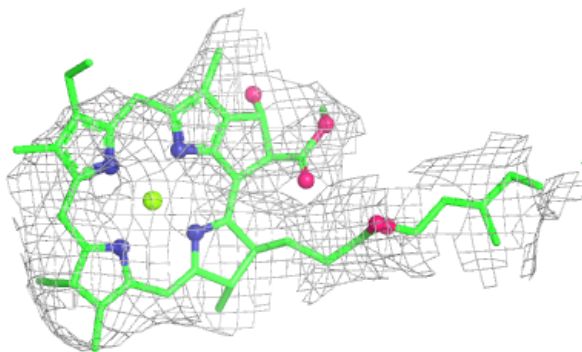
Electron density around CLA A 814:

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

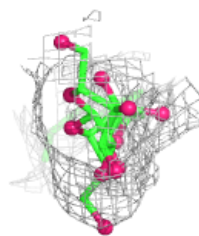
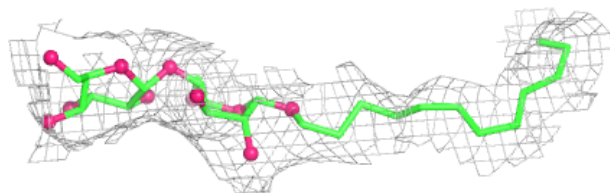


Electron density around CLA 1 210:

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

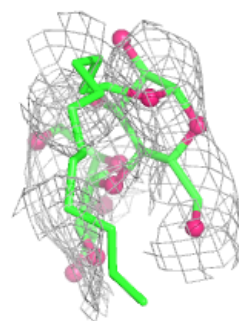
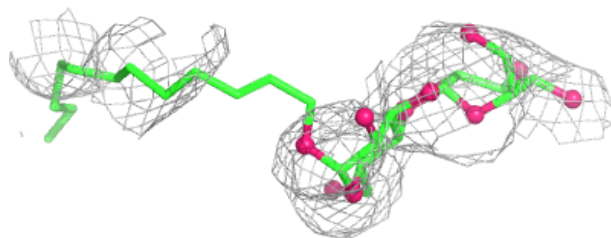
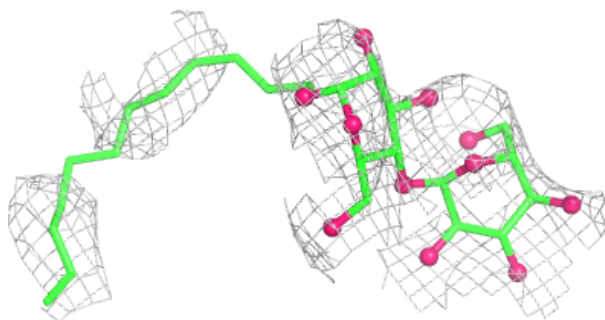
**Electron density around LMU H 107:**

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



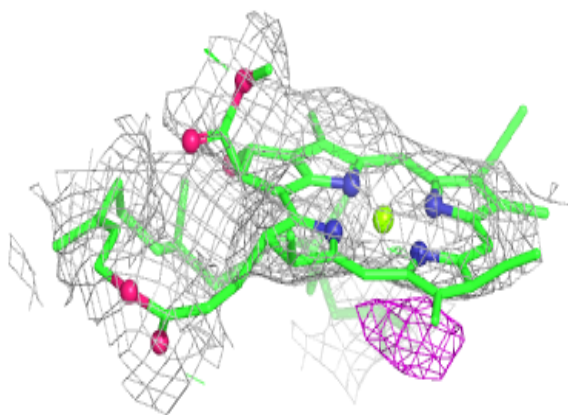
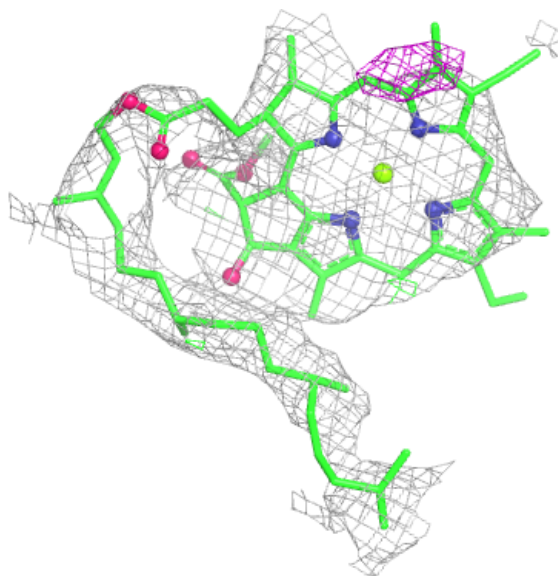
Electron density around LMU 1 217:

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



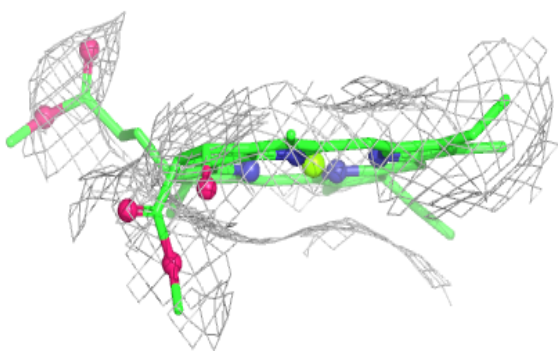
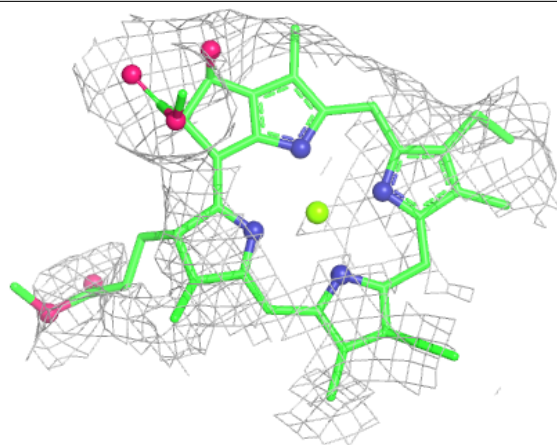
Electron density around CLA A 823:

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

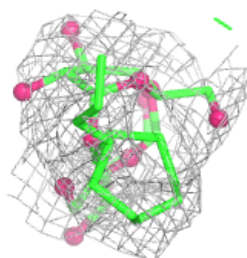
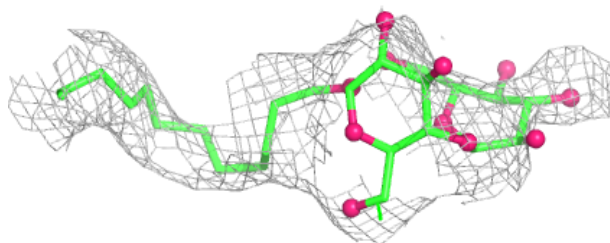
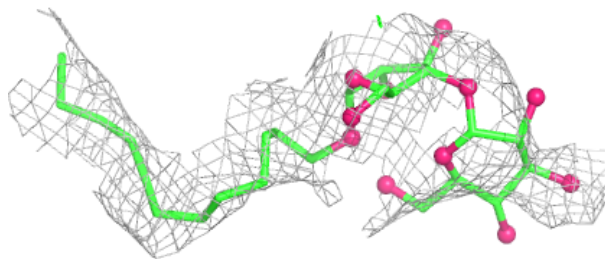


Electron density around CLA 1 201:

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

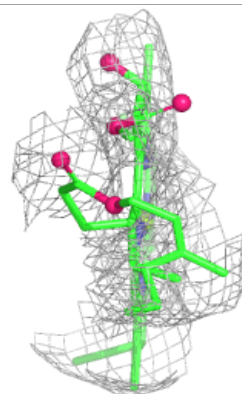
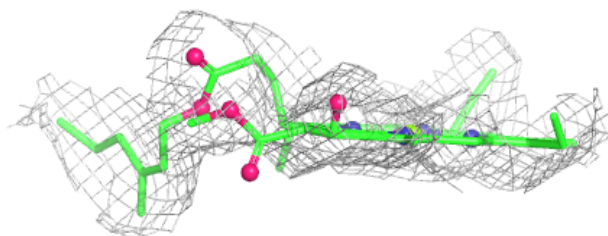
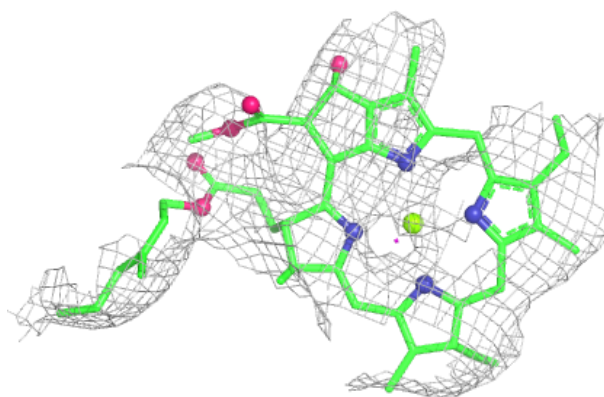
**Electron density around LMU A 849:**

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

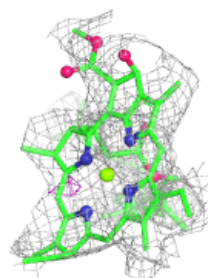
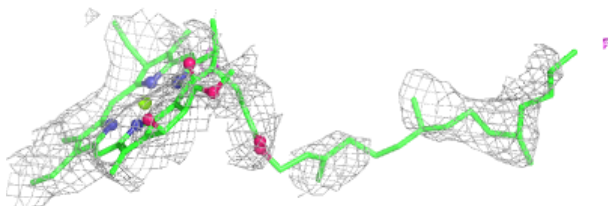
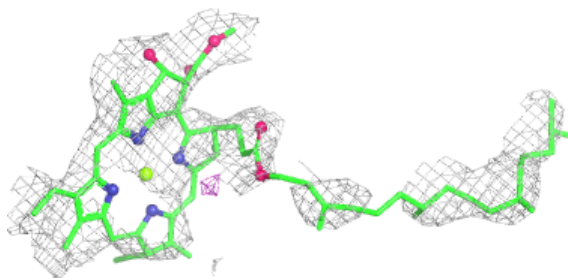


Electron density around CLA 4 318:

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

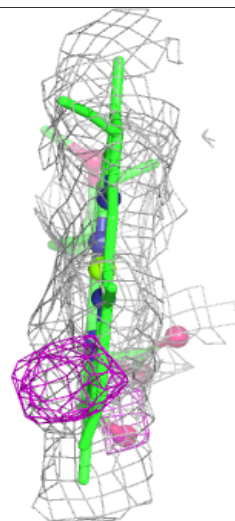
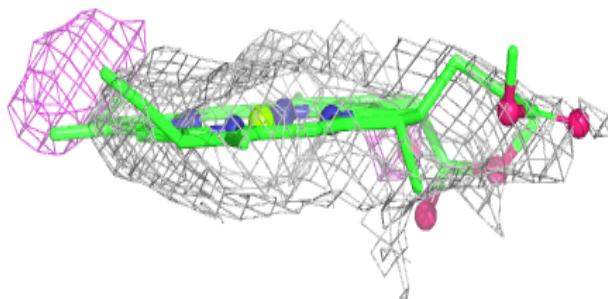
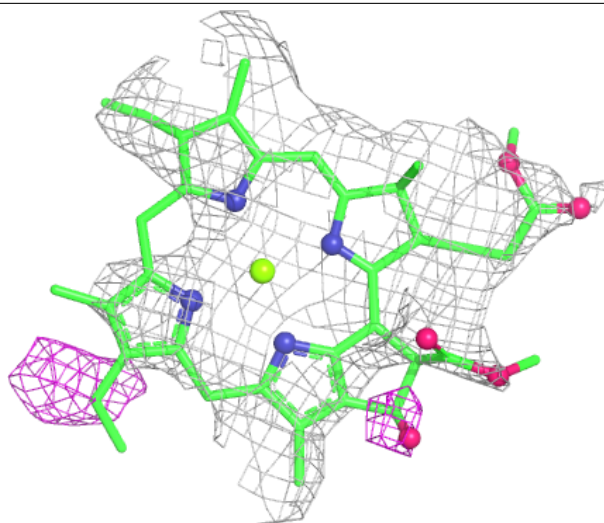
**Electron density around CLA A 819:**

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



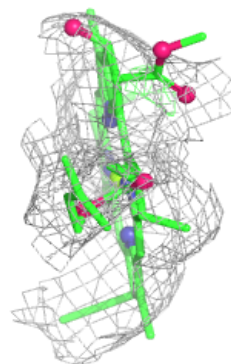
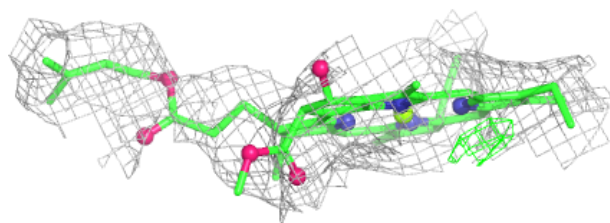
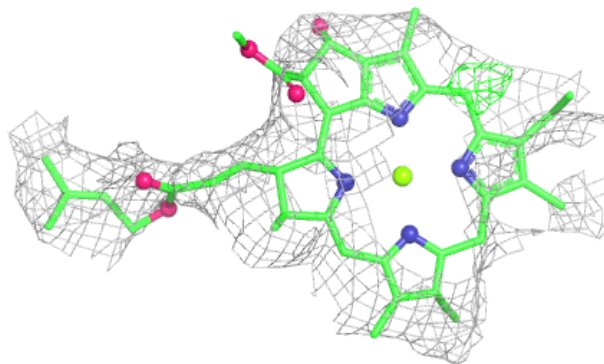
Electron density around CLA B 814:

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



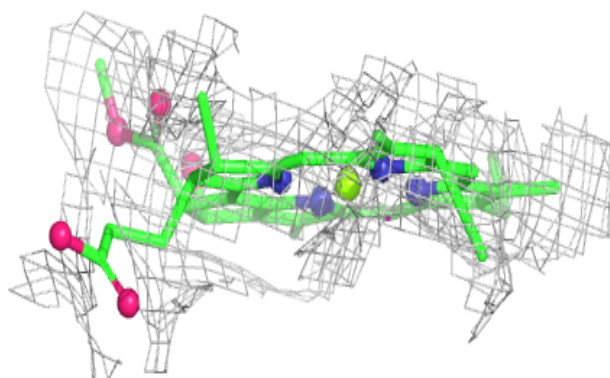
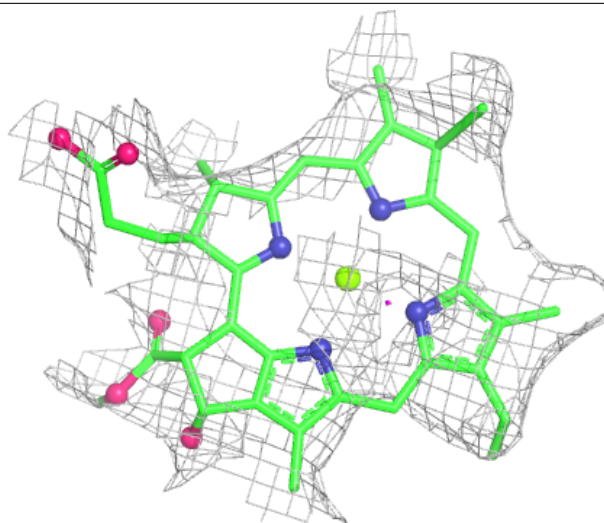
Electron density around CLA 3 302:

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



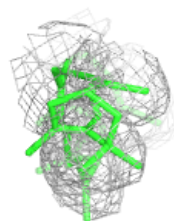
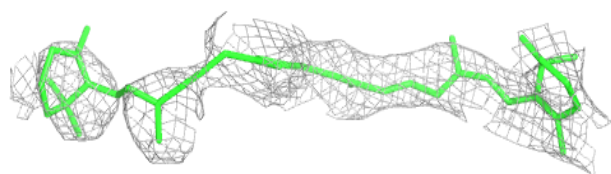
Electron density around CLA K 101:

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

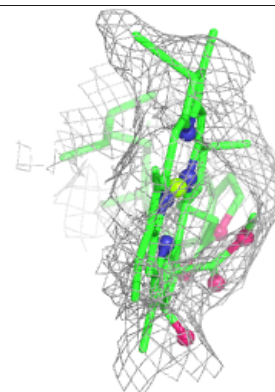
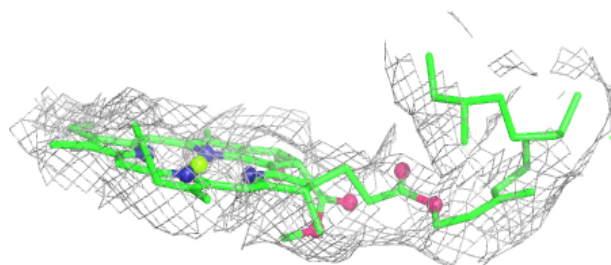
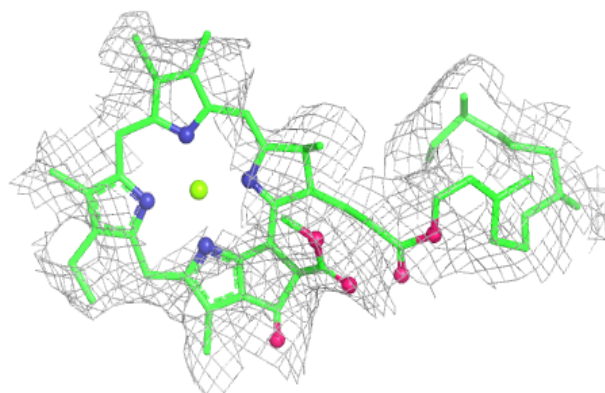


Electron density around BCR I 103:

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

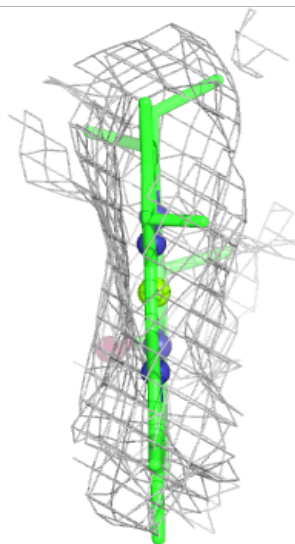
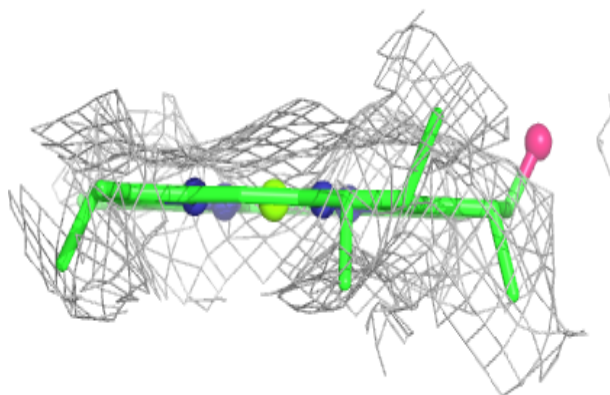
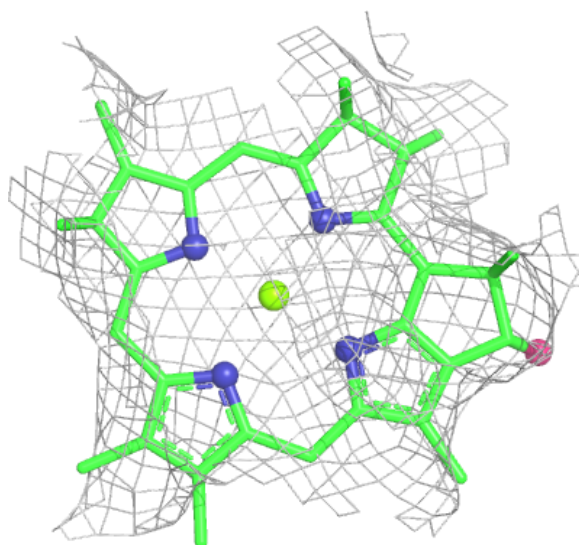
**Electron density around CLA 1 215:**

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



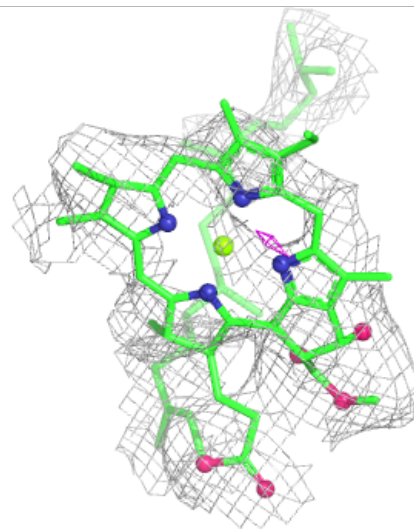
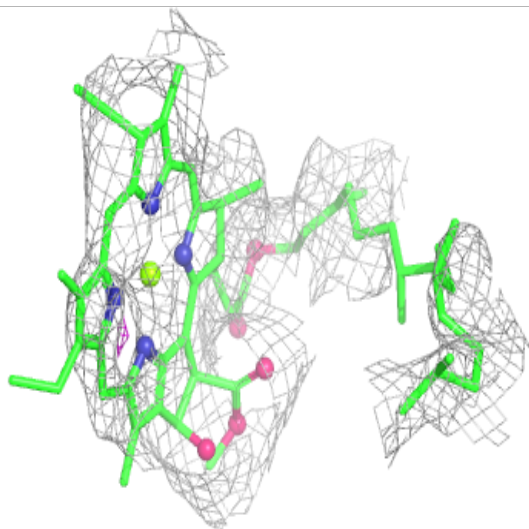
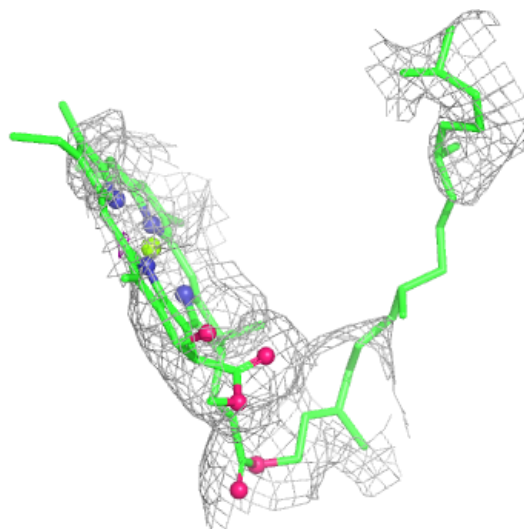
Electron density around CLA B 840:

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



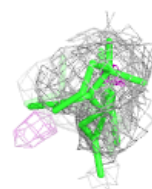
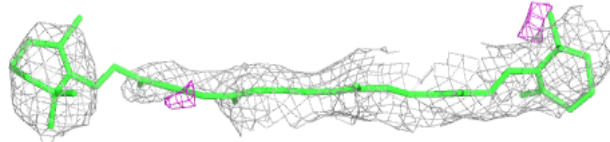
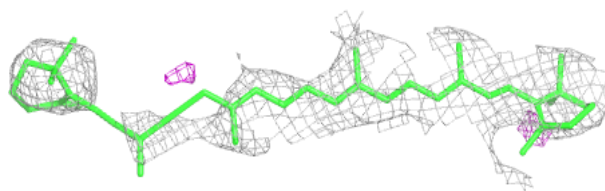
Electron density around CLA 2 307:

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

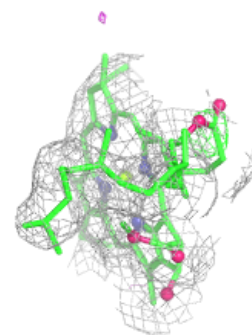
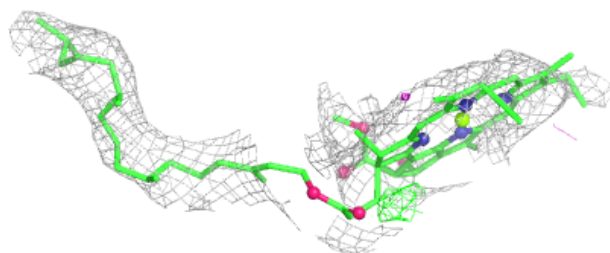
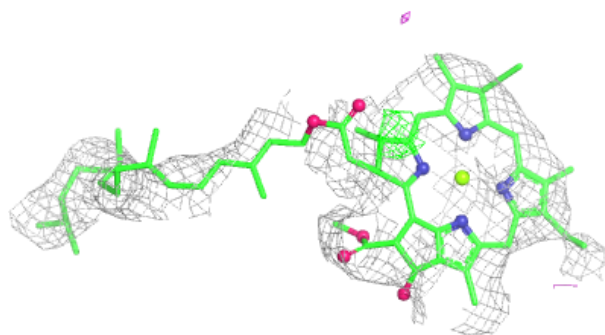


Electron density around BCR B 846:

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

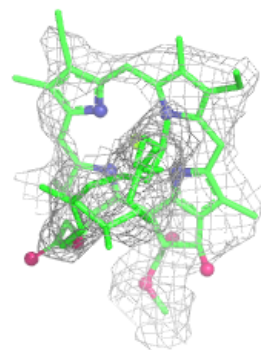
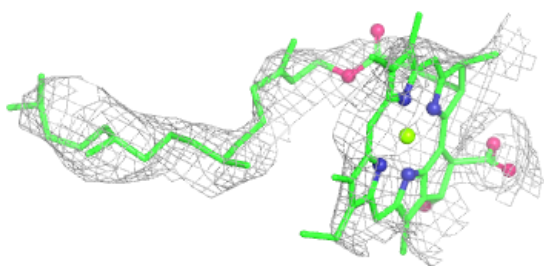
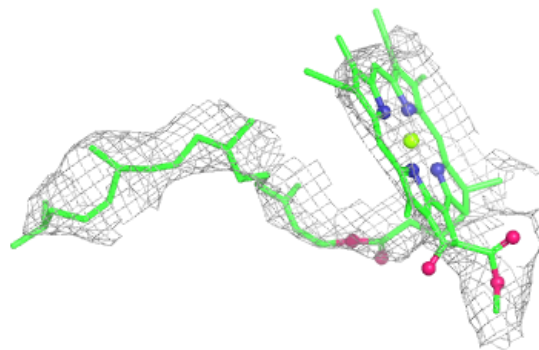
**Electron density around CLA 3 317:**

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



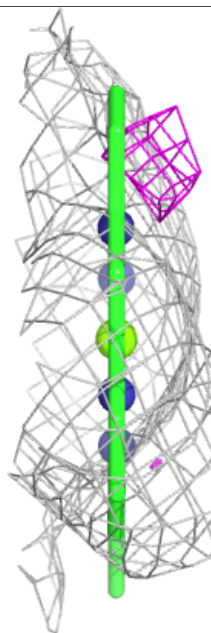
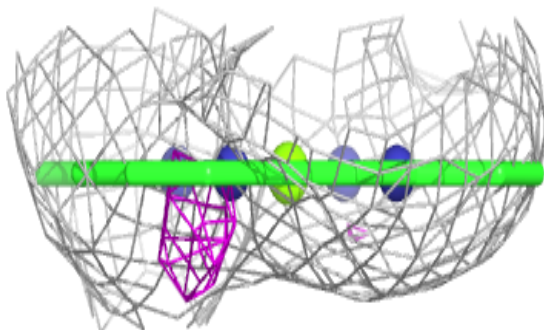
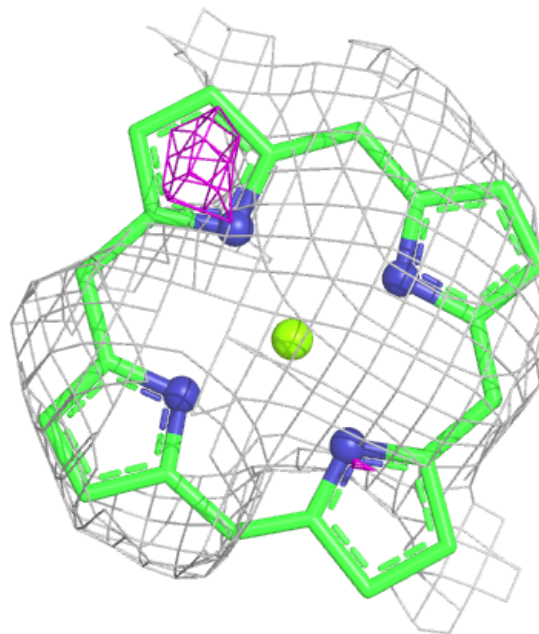
Electron density around CLA A 811:

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



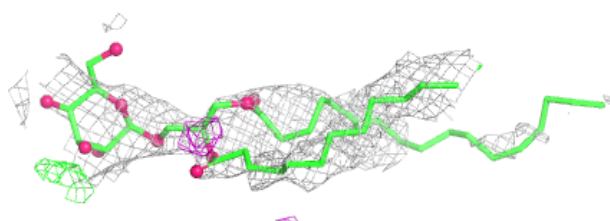
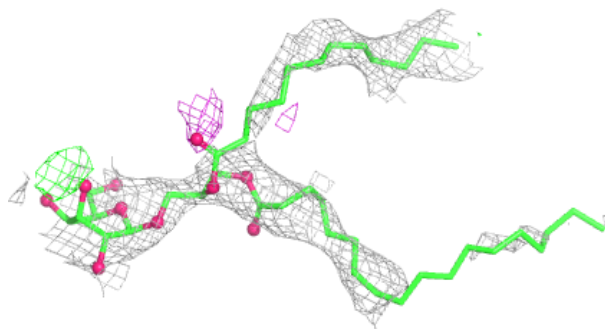
Electron density around CLA 3 309:

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



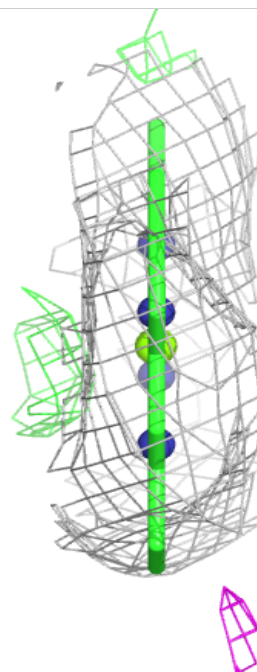
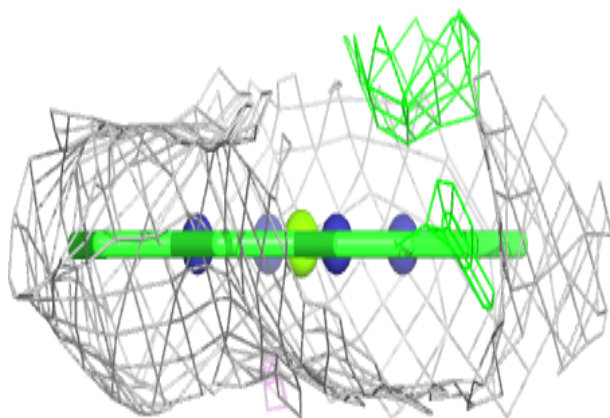
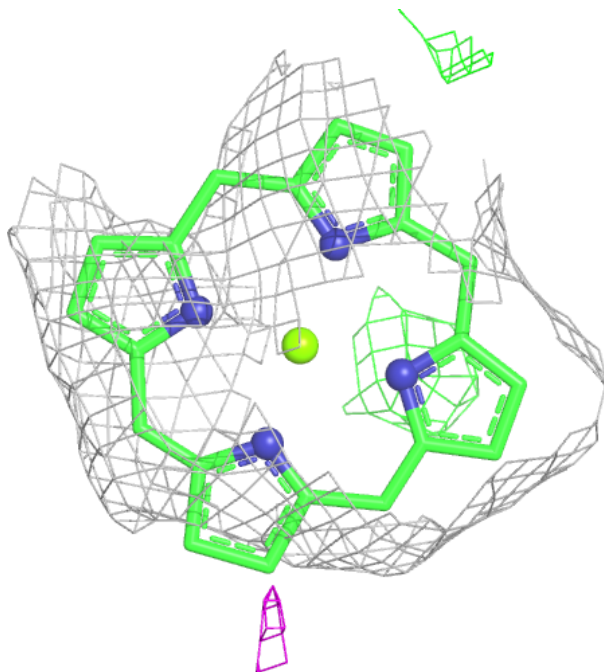
Electron density around LMG B 848:

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



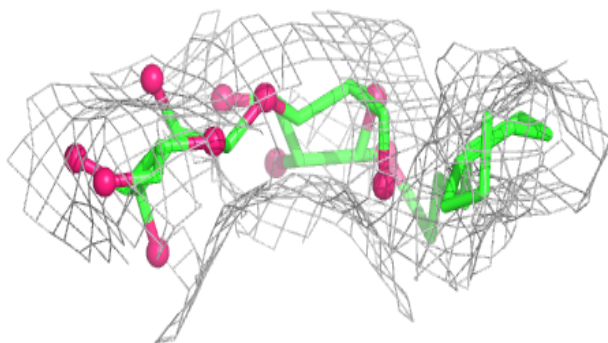
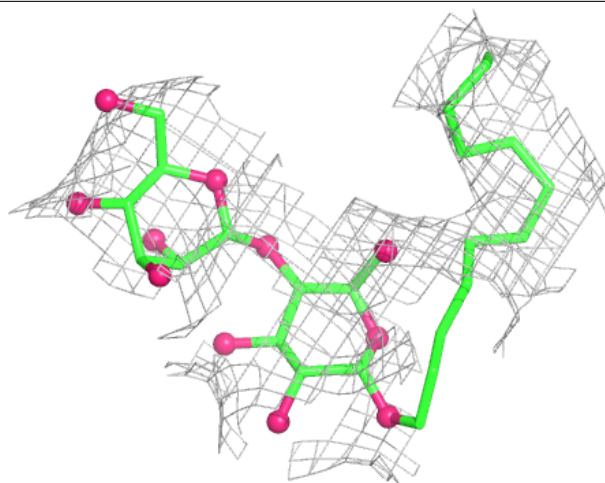
Electron density around CLA 3 318:

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



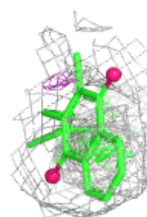
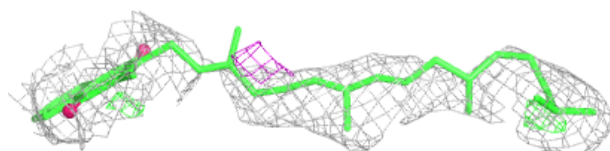
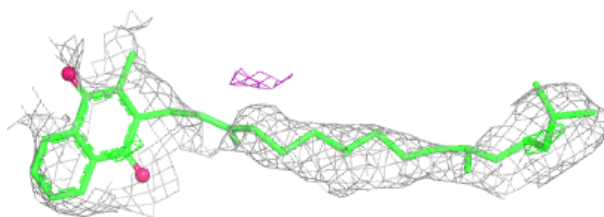
Electron density around LMU N 101:

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

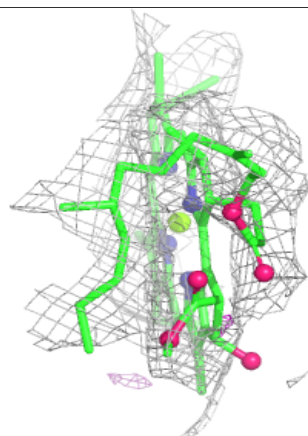
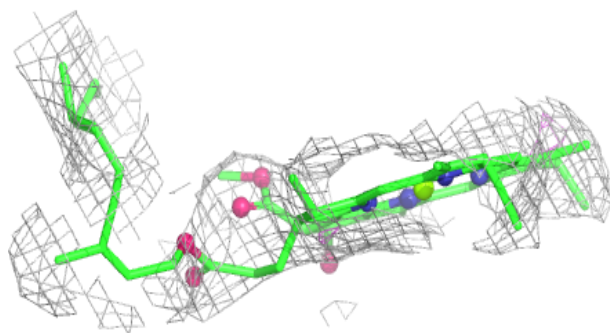
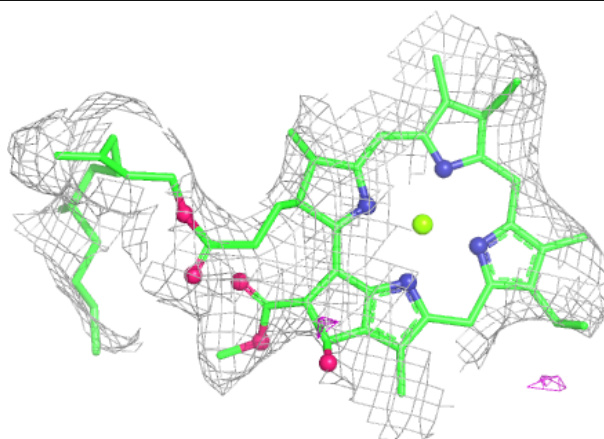


Electron density around PQN A 842:

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

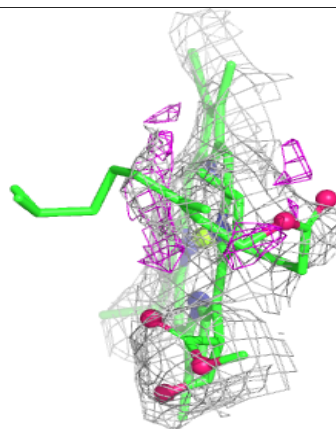
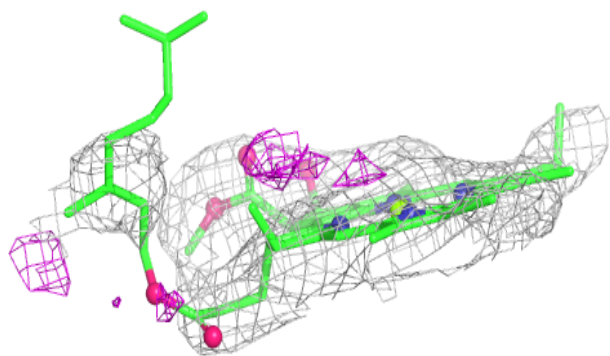
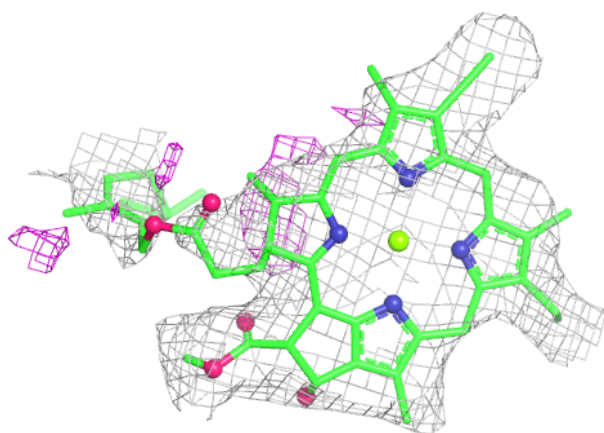
**Electron density around CLA R 108:**

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

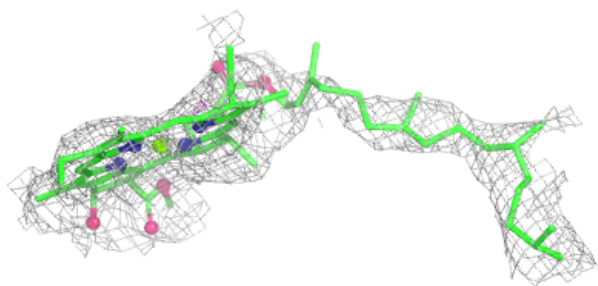
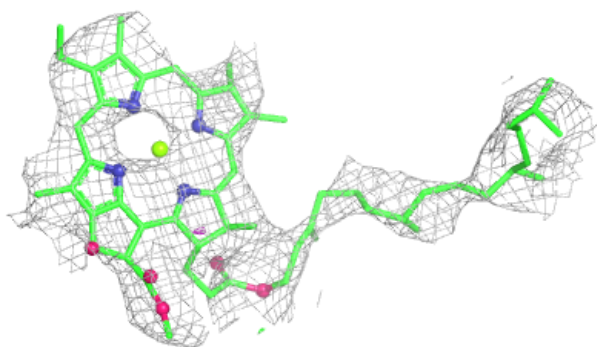


Electron density around CLA A 806:

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

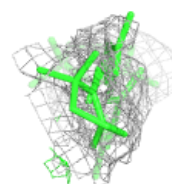
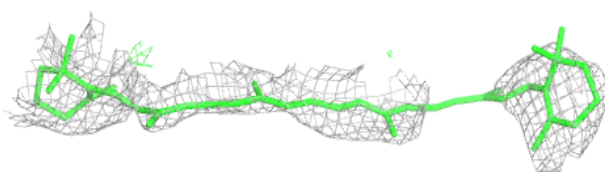
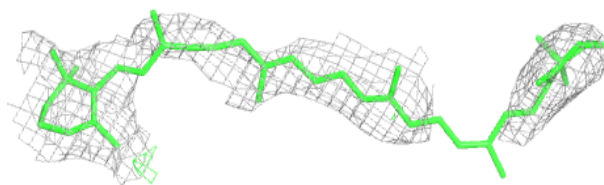
**Electron density around CLA A 852:**

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

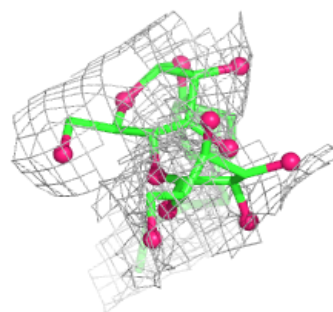
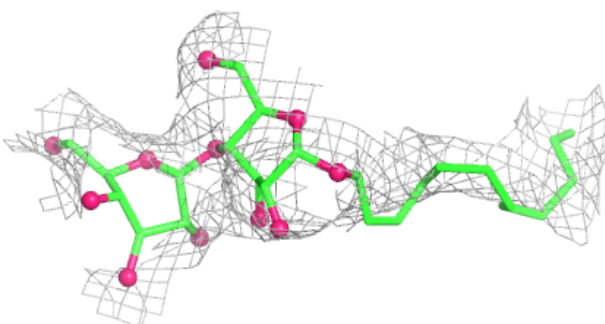
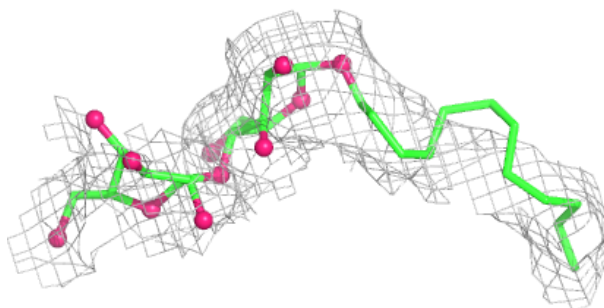


Electron density around BCR B 844:

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

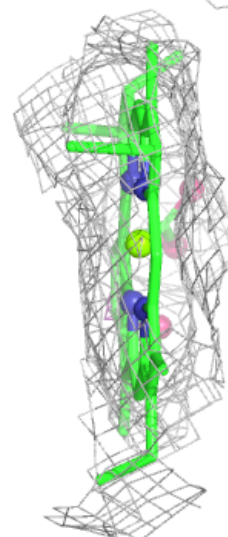
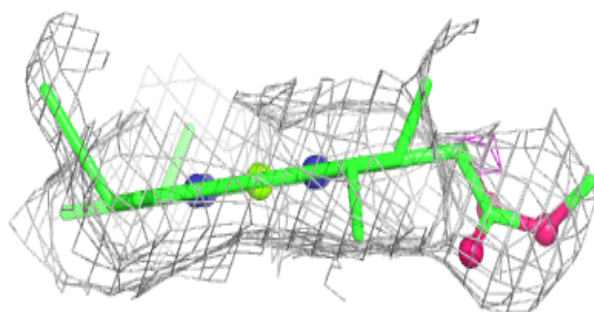
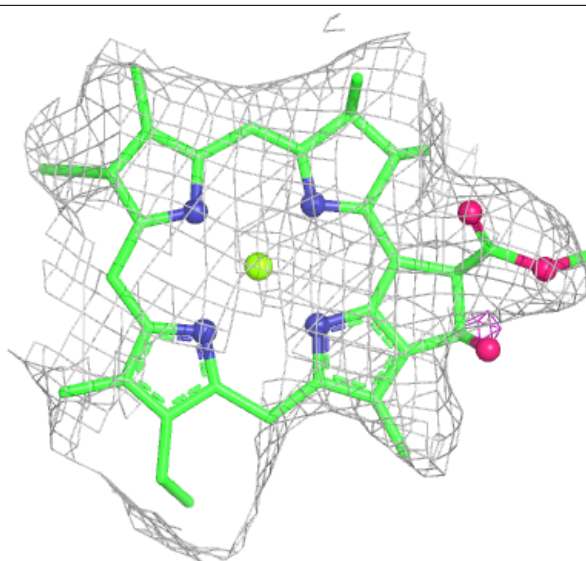
**Electron density around LMU H 104:**

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



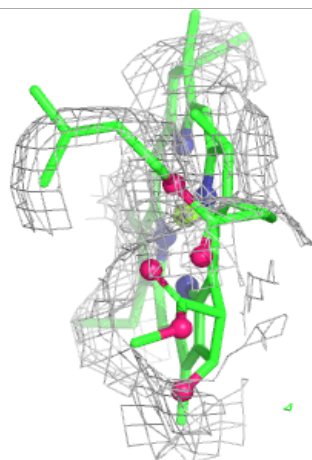
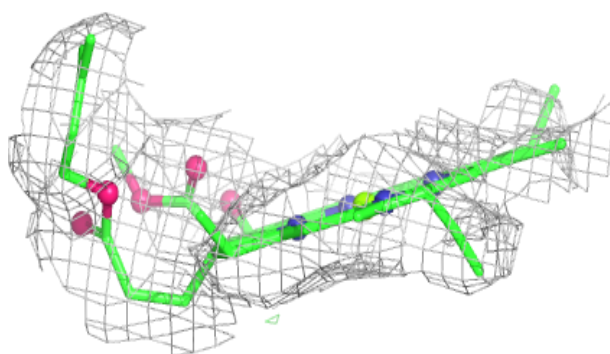
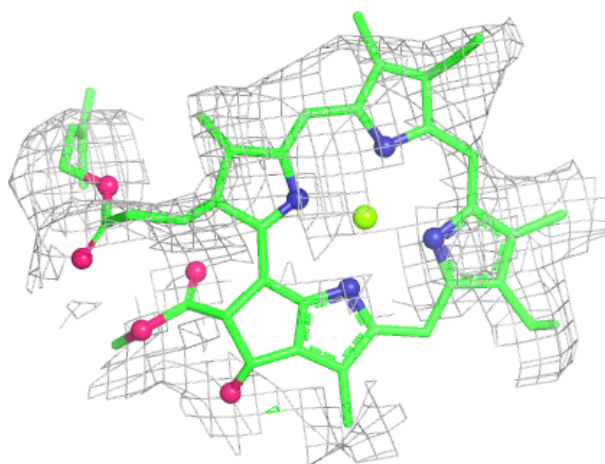
Electron density around CLA F 205:

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



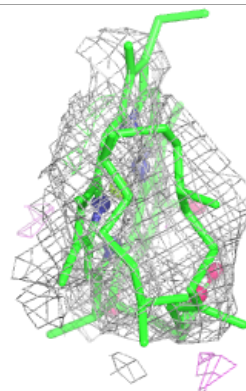
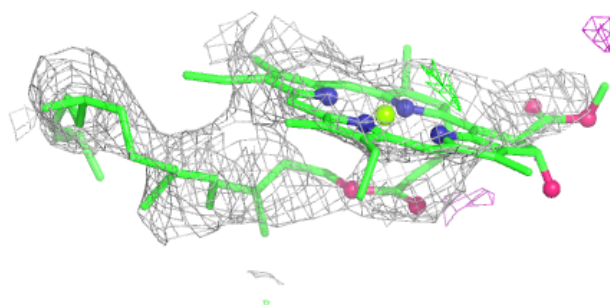
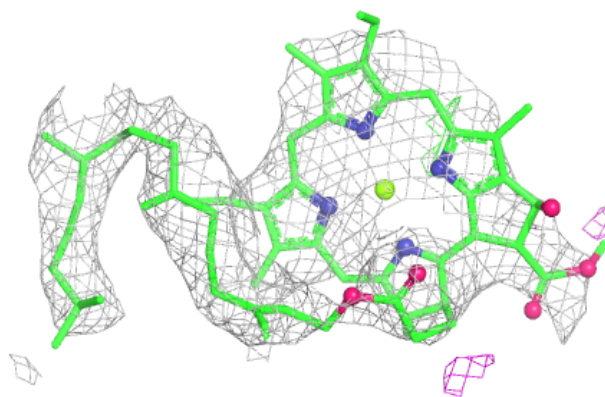
Electron density around CLA 3 316:

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



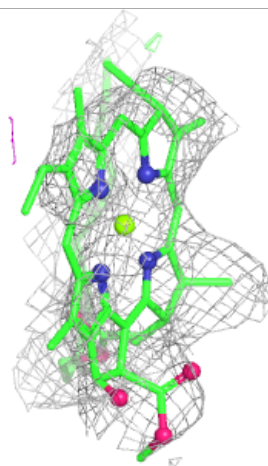
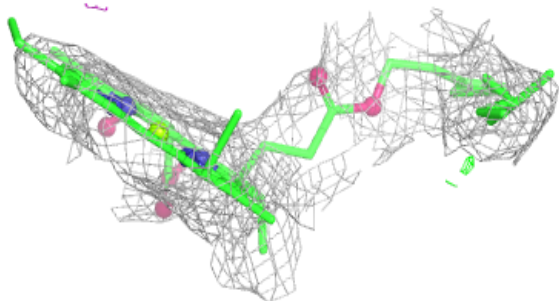
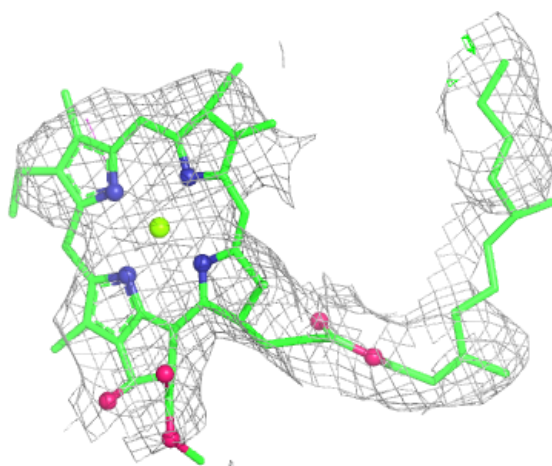
Electron density around CLA A 818:

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



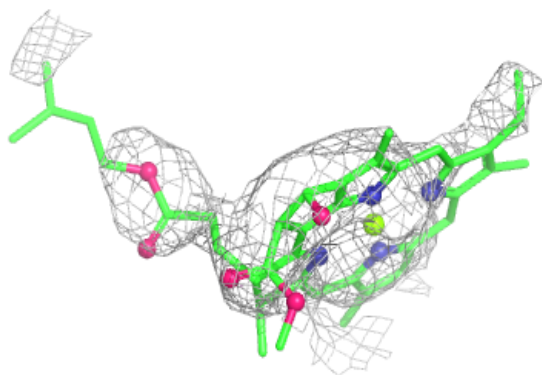
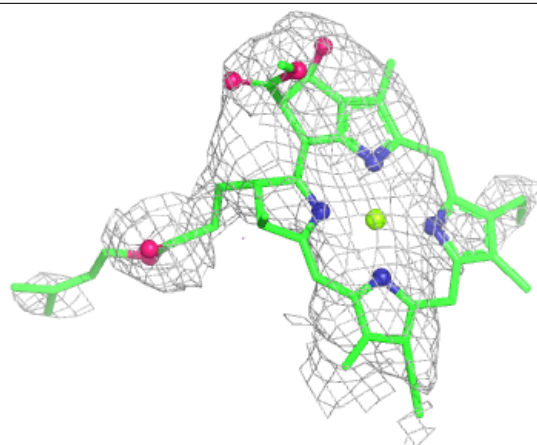
Electron density around CLA B 823:

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



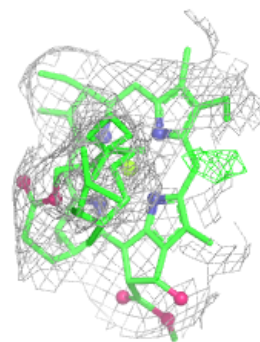
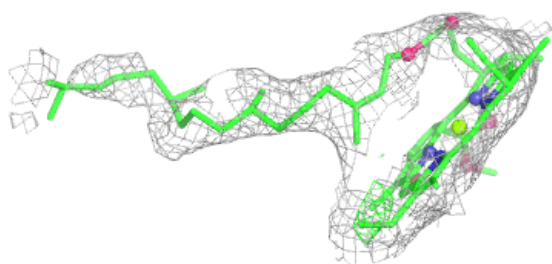
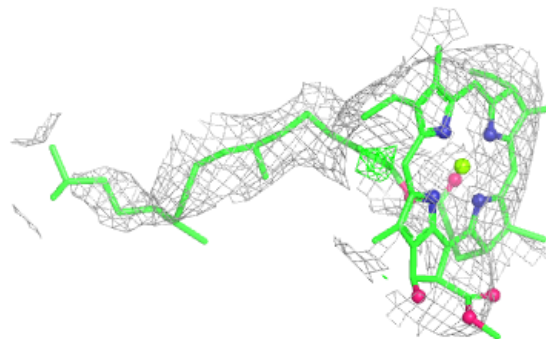
Electron density around CLA A 829:

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



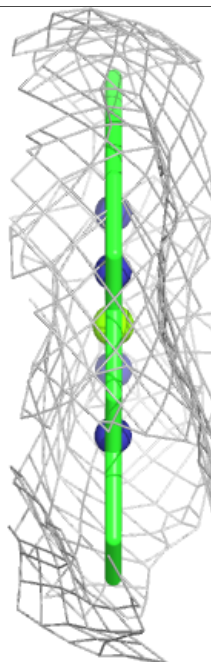
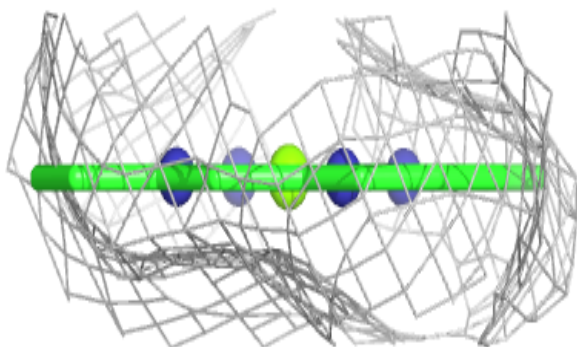
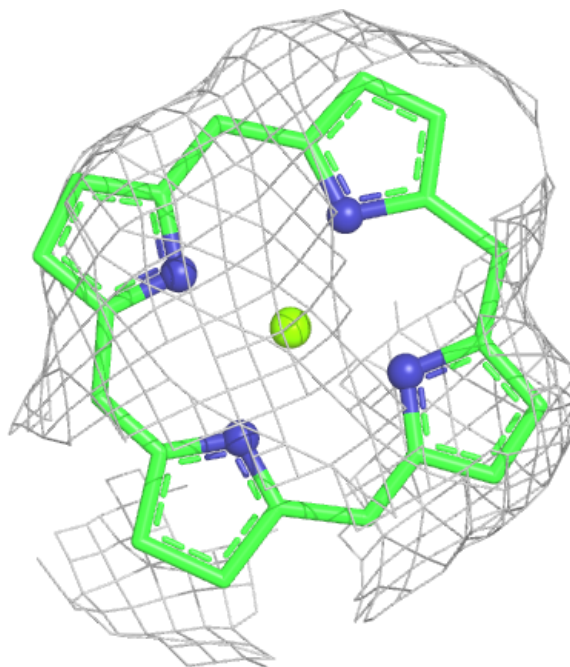
Electron density around CLA 2 303:

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



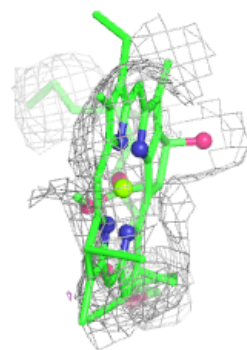
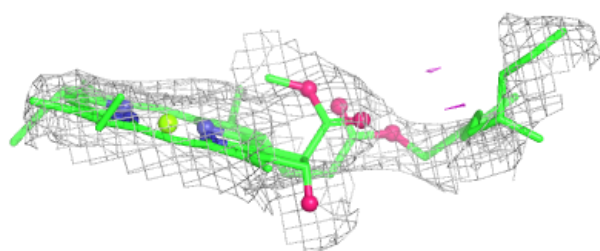
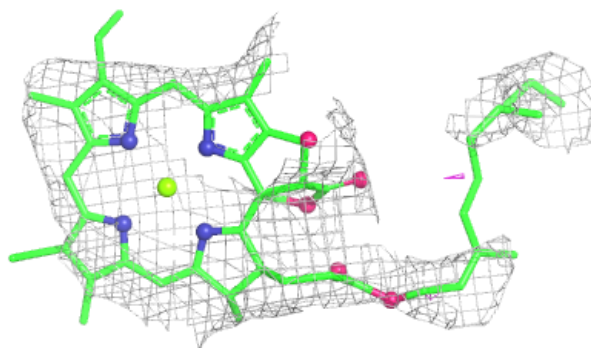
Electron density around CLA 3 319:

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

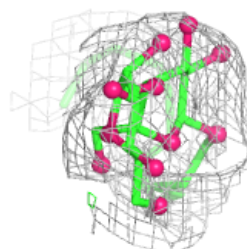
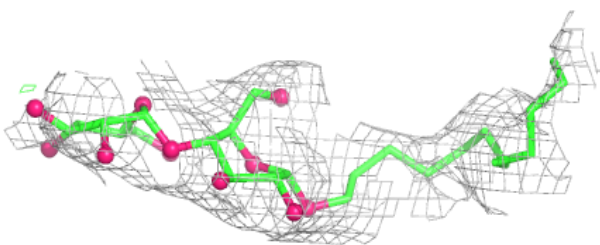
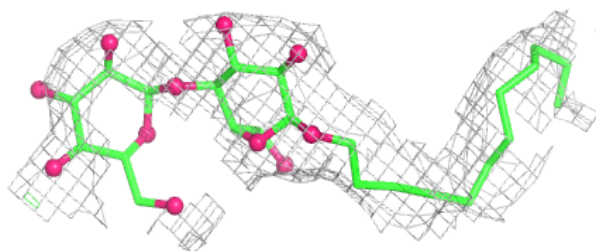


Electron density around CLA R 107:

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

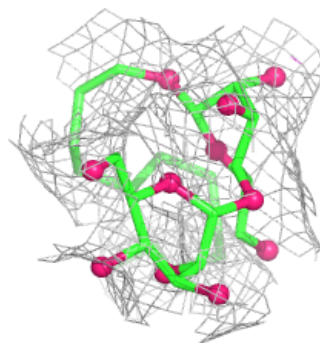
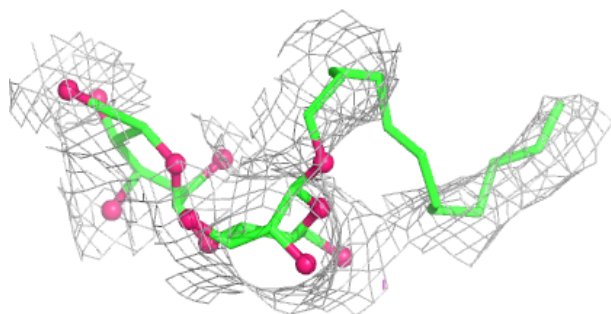
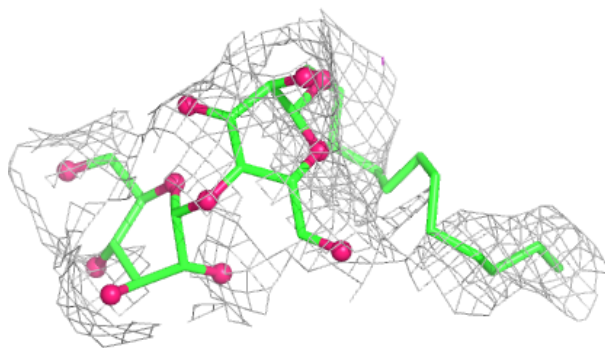
**Electron density around LMU C 101:**

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



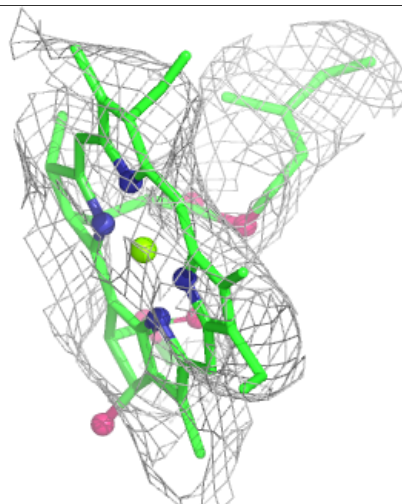
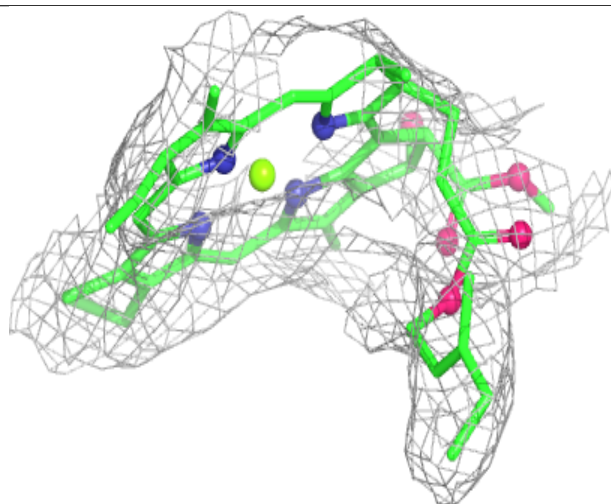
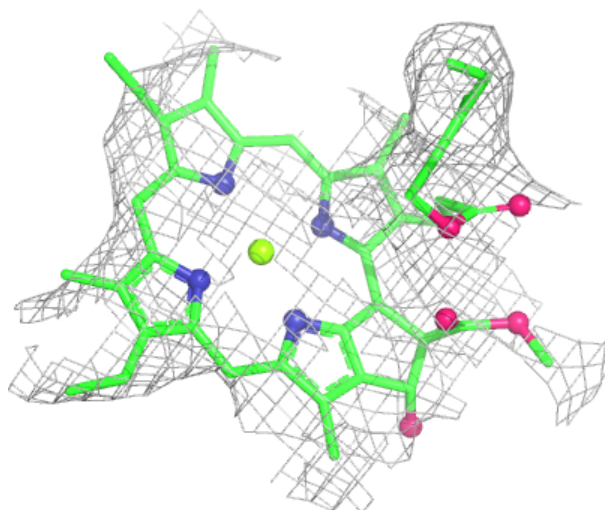
Electron density around LMU L 209:

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



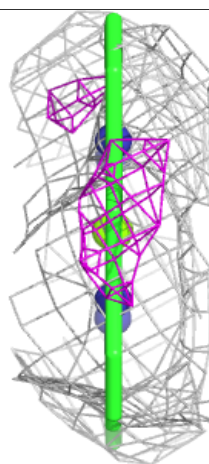
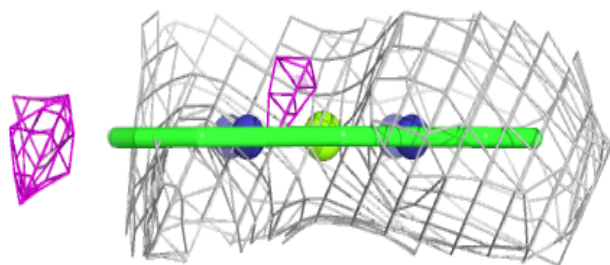
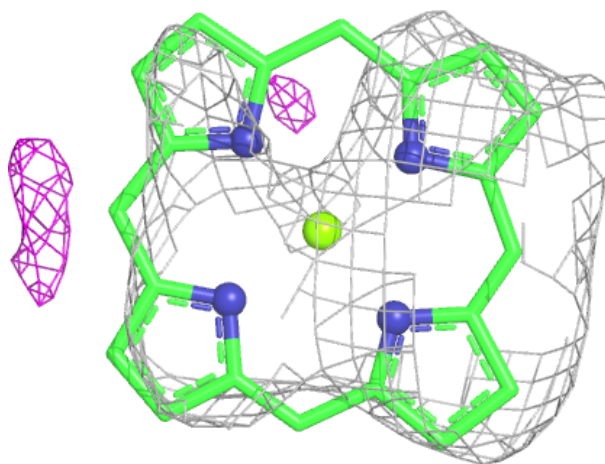
Electron density around CLA 1 207:

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



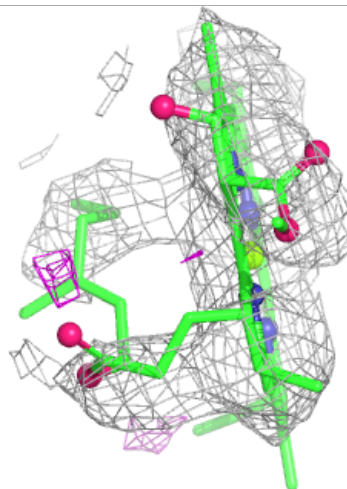
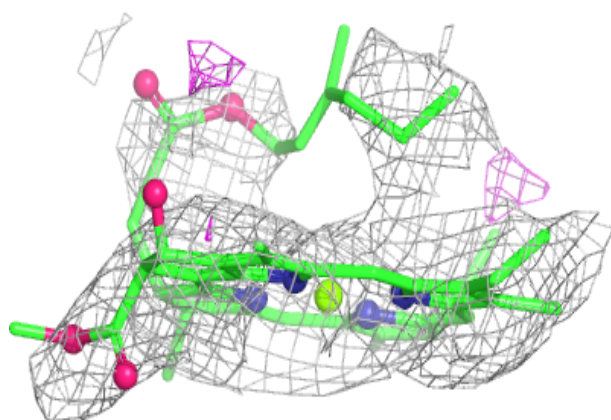
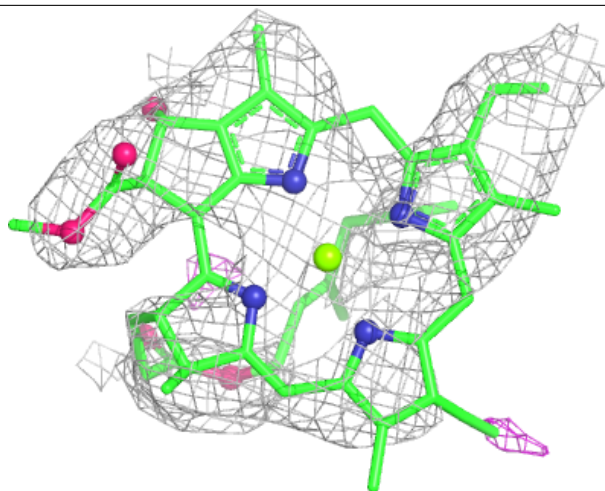
Electron density around CLA 2 310:

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



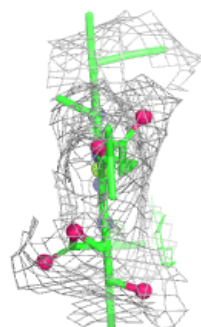
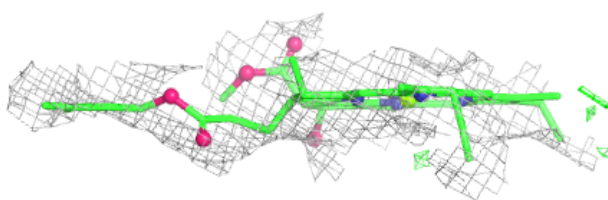
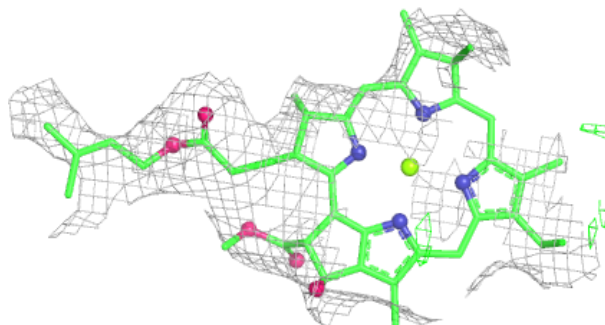
Electron density around CLA A 817:

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

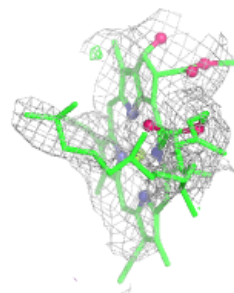
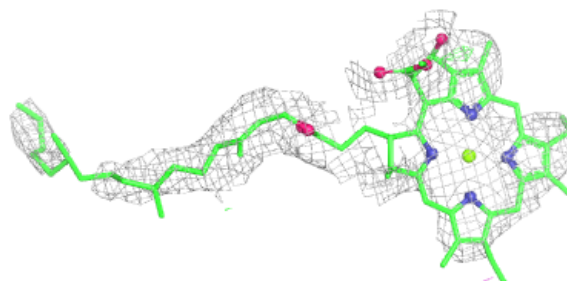


Electron density around CLA A 840:

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

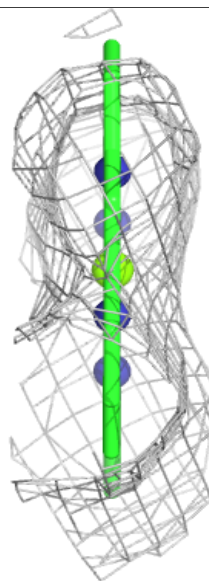
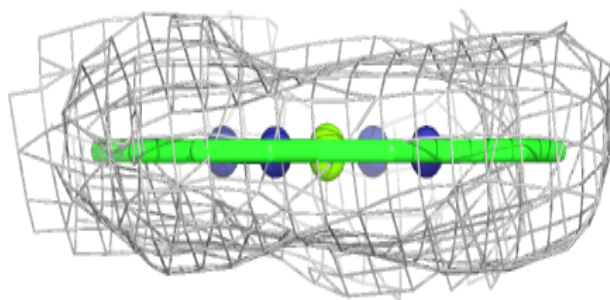
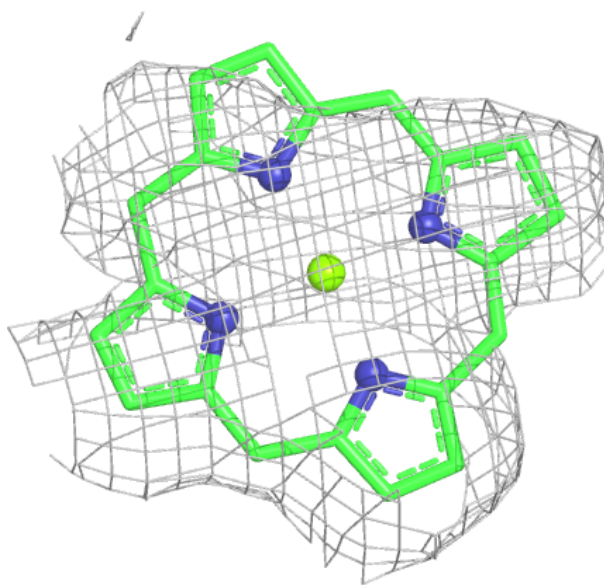
**Electron density around CLA A 805:**

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



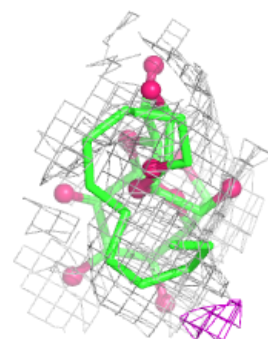
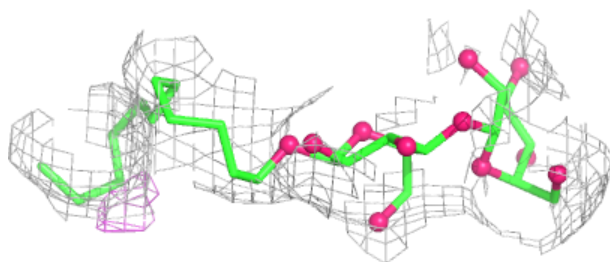
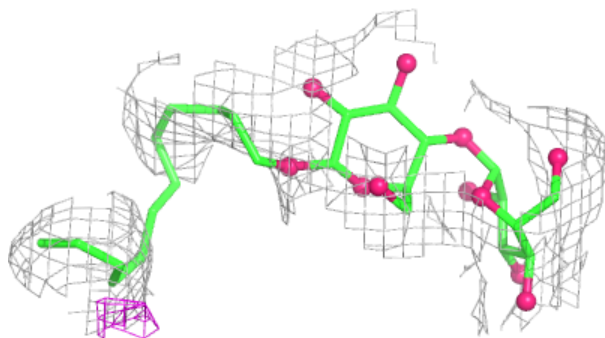
Electron density around CLA 4 310:

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

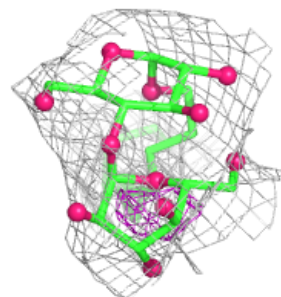
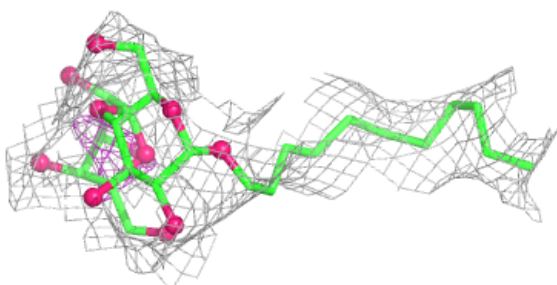
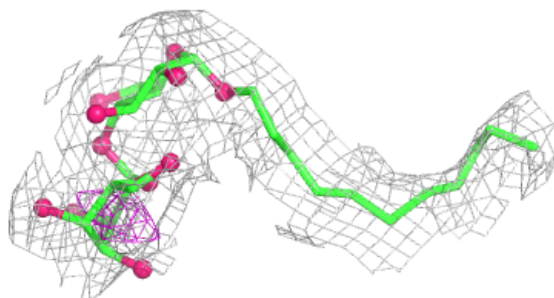


Electron density around LMU R 109:

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

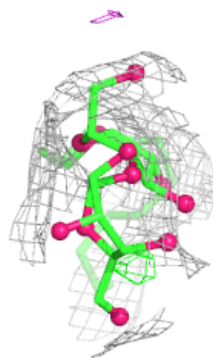
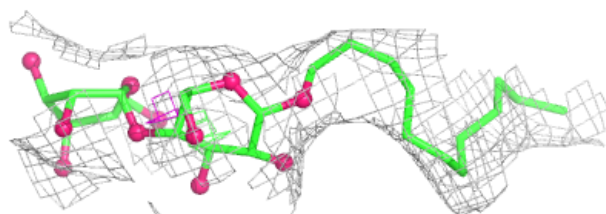
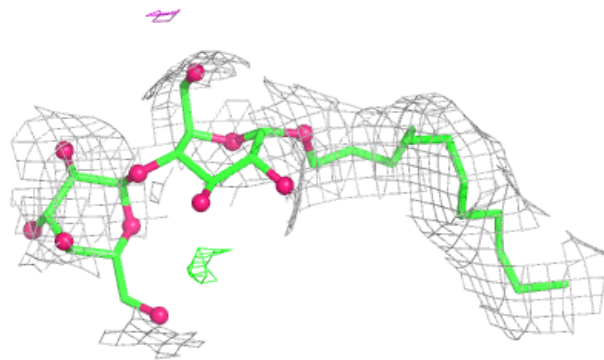
**Electron density around LMU 4 320:**

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



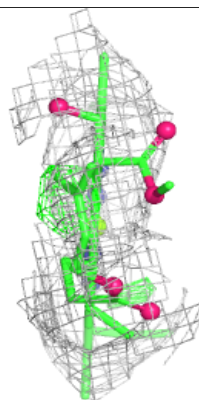
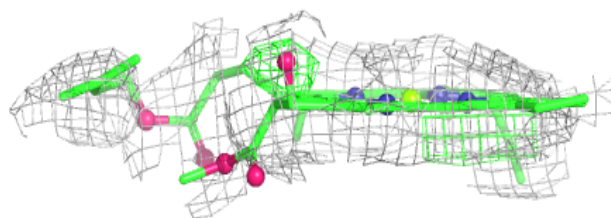
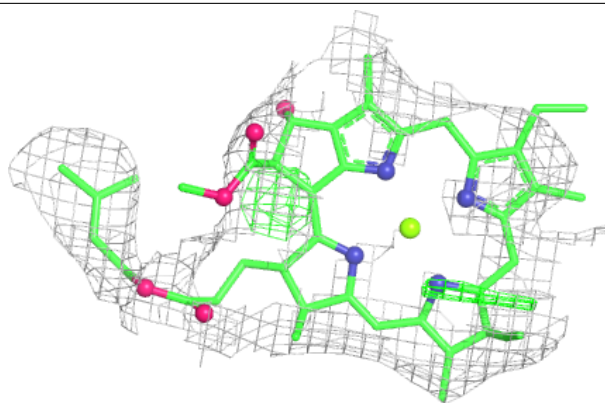
Electron density around LMU 4 322:

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

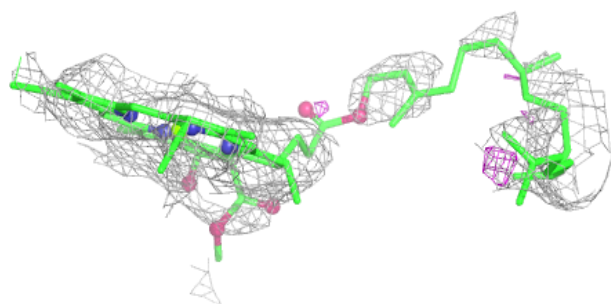
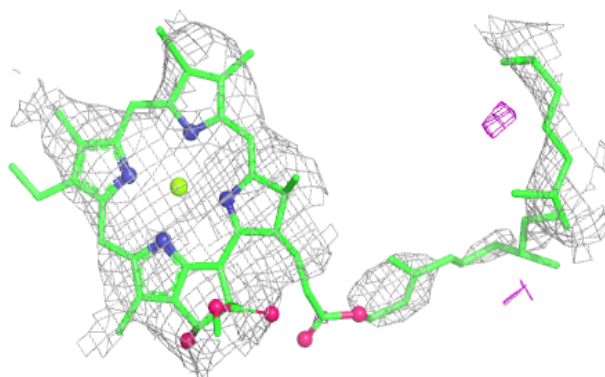


Electron density around CLA 2 312:

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

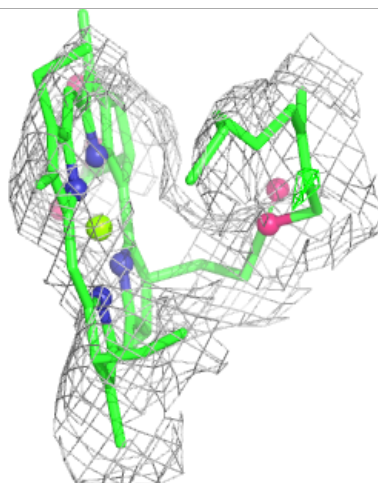
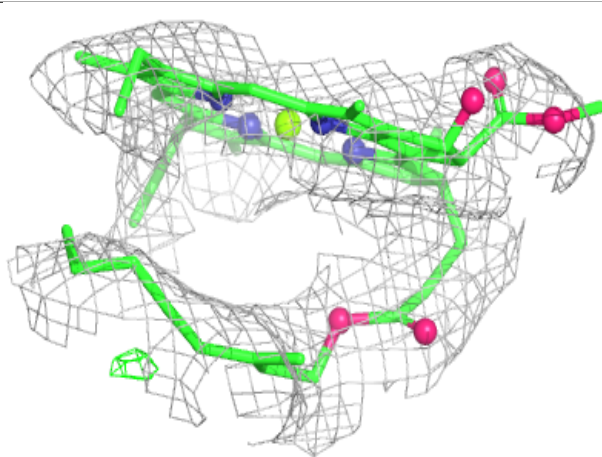
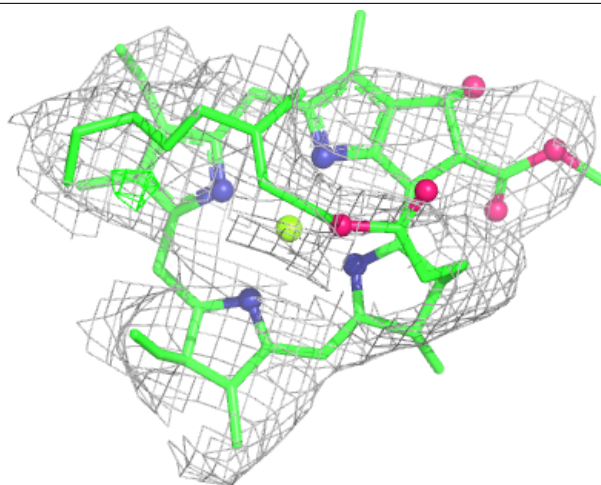
**Electron density around CLA A 825:**

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



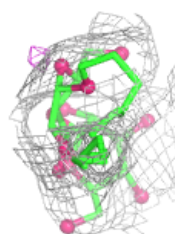
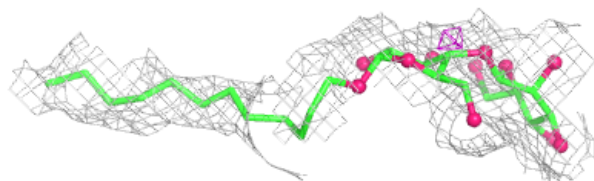
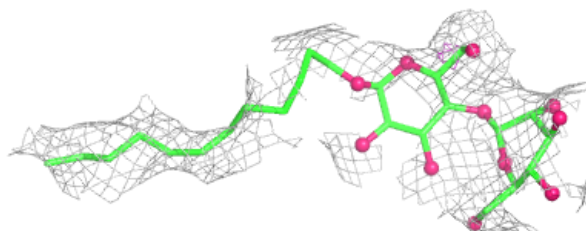
Electron density around CLA A 812:

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



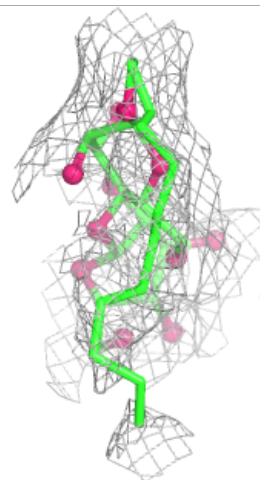
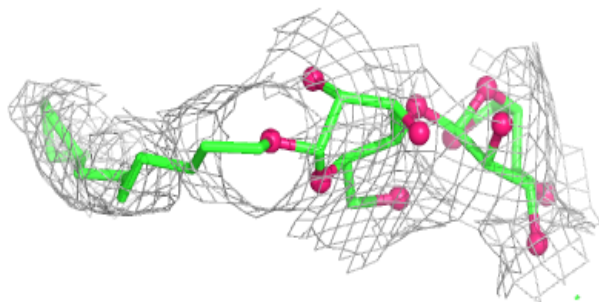
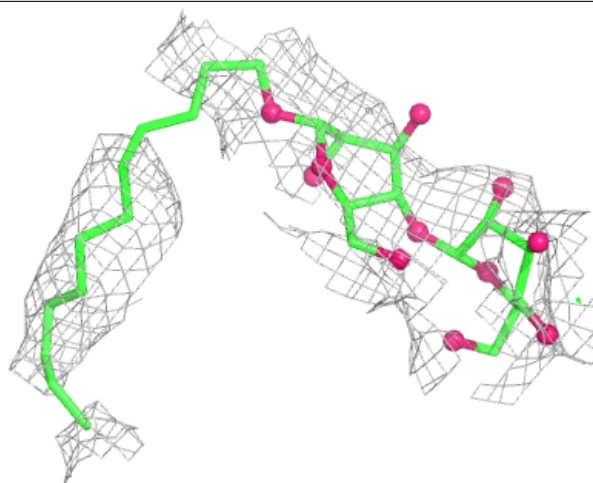
Electron density around LMU A 856:

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



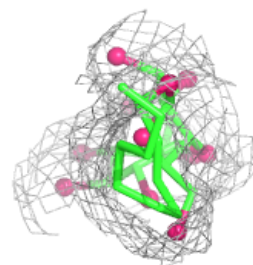
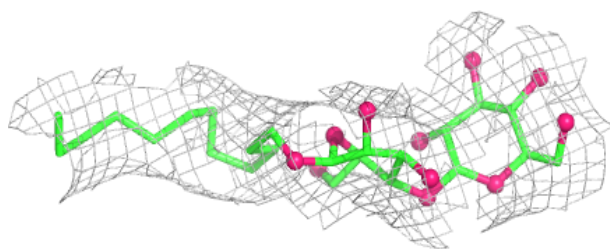
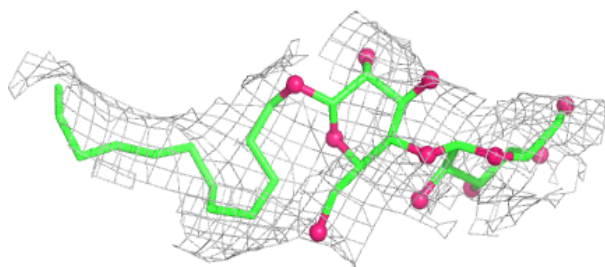
Electron density around LMU K 104:

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



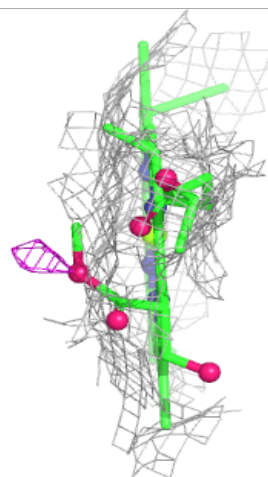
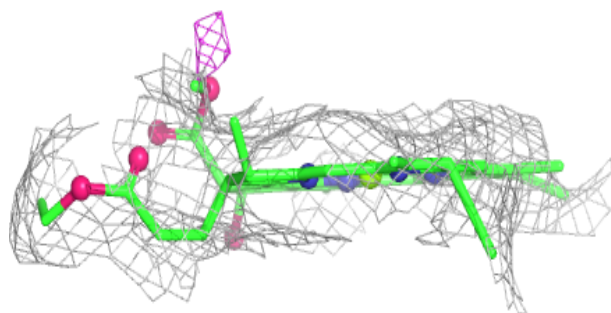
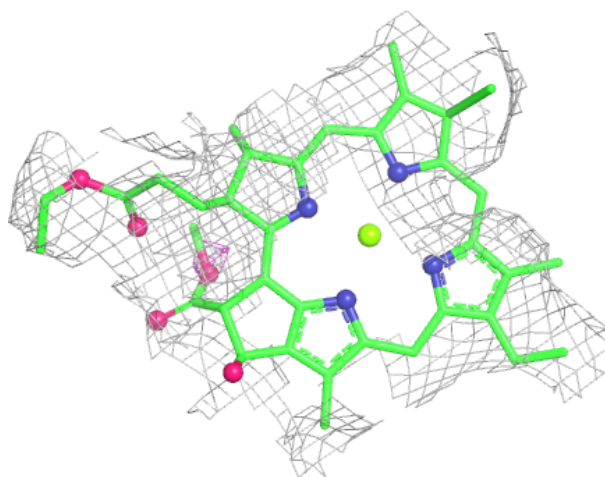
Electron density around LMU K 105:

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



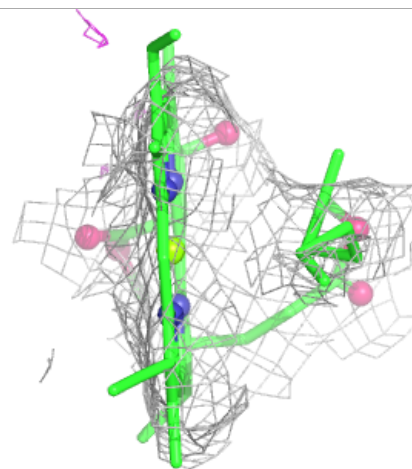
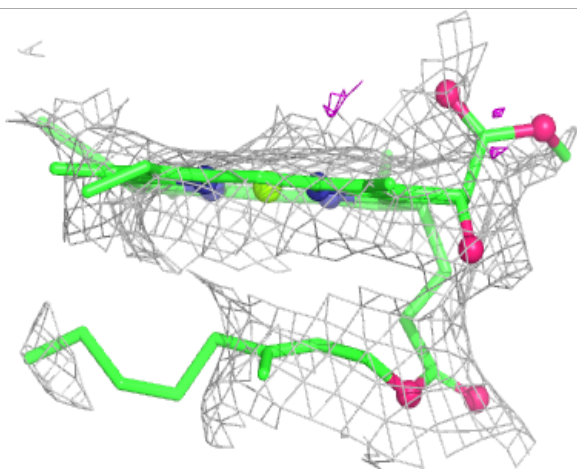
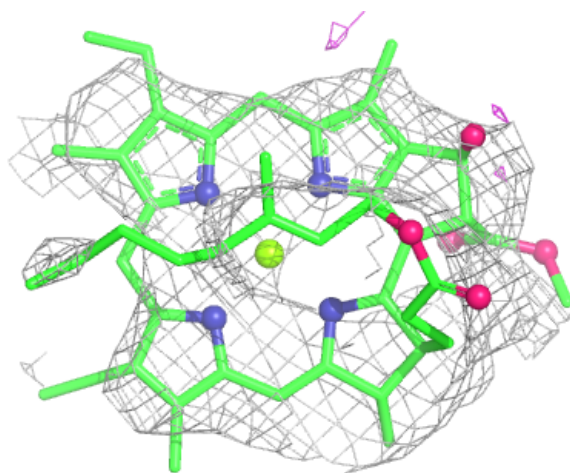
Electron density around CLA 4 319:

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



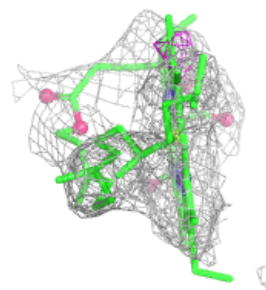
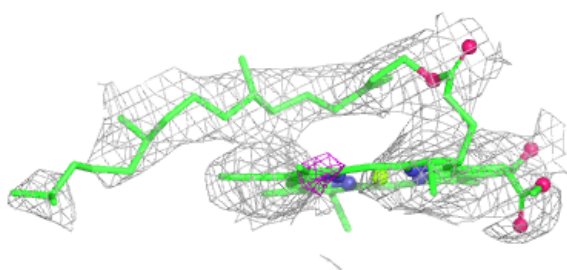
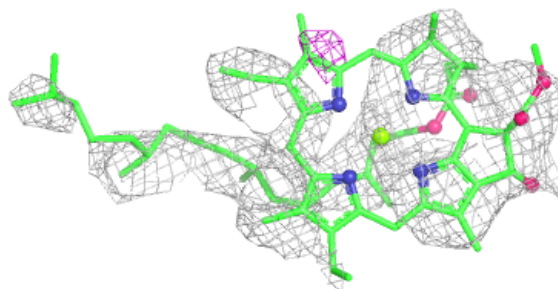
Electron density around CLA A 816:

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

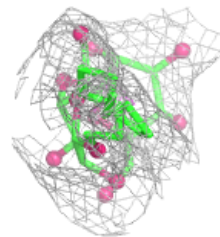
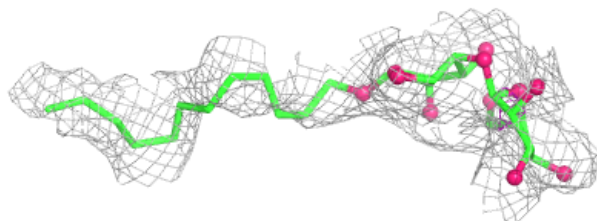
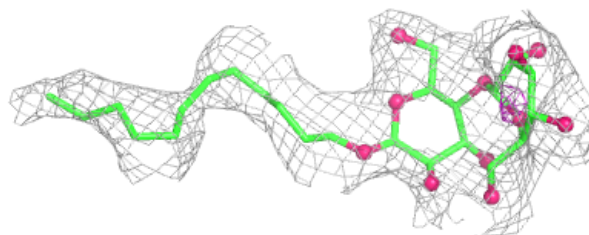


Electron density around CLA B 803:

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

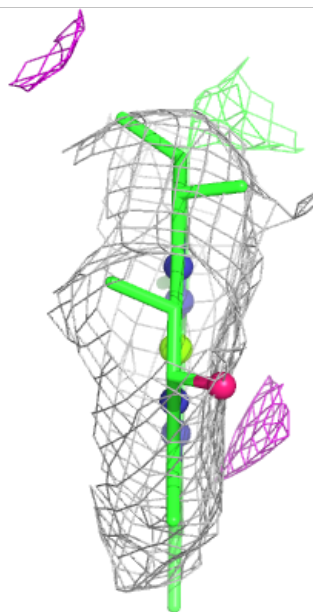
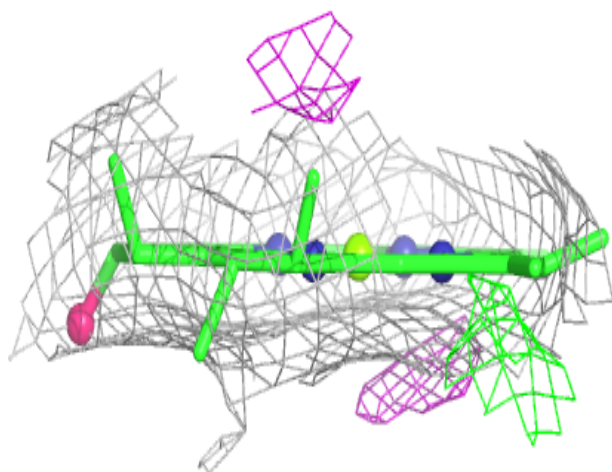
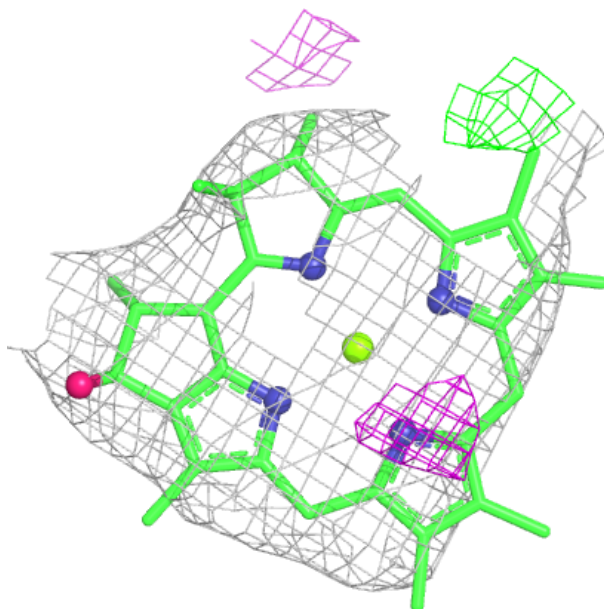
**Electron density around LMU 1 219:**

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



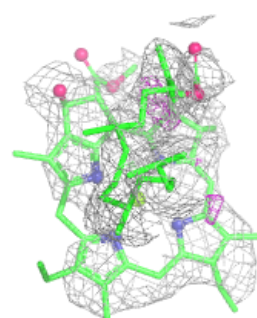
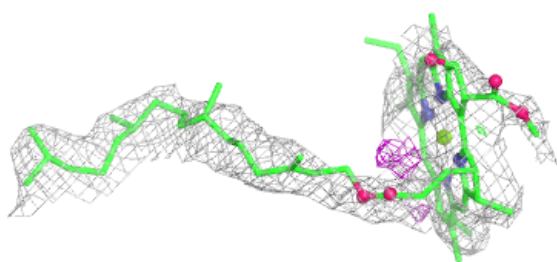
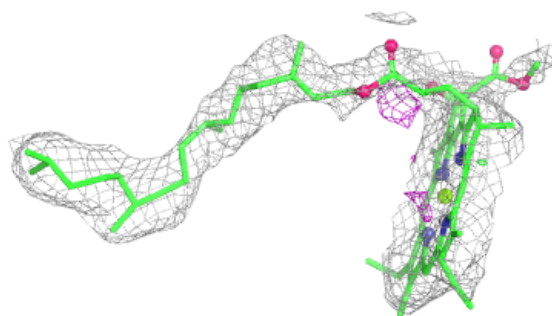
Electron density around CLA F 204:

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

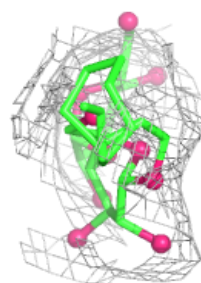
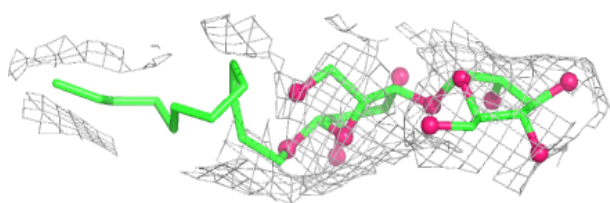
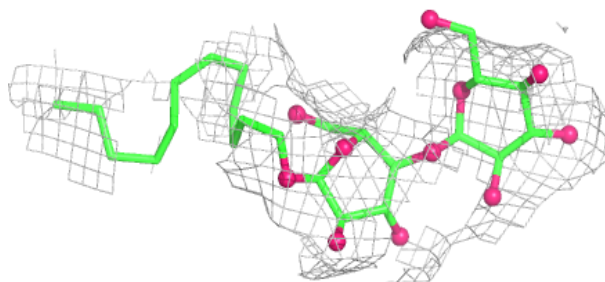


Electron density around CLA A 828:

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

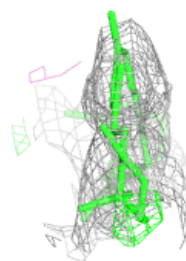
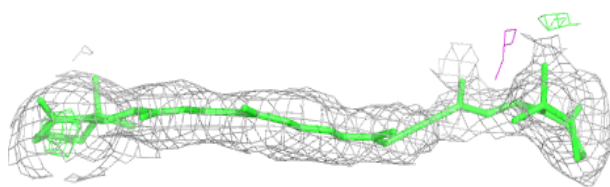
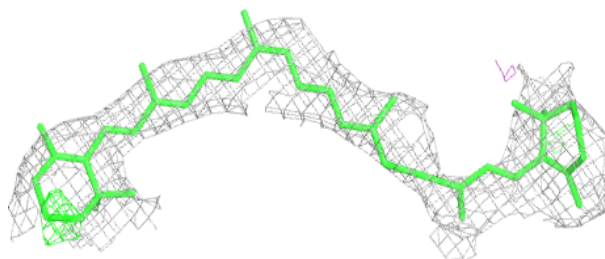
**Electron density around LMU A 854:**

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

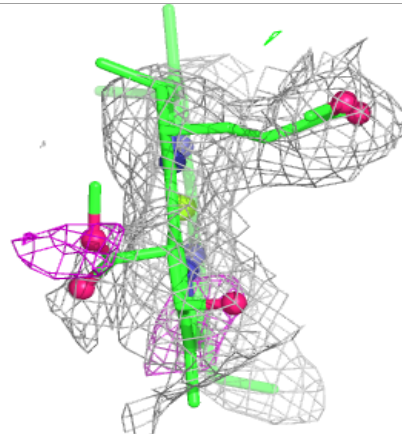
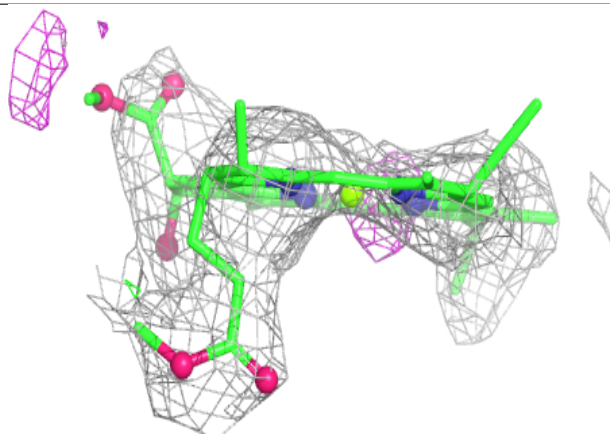
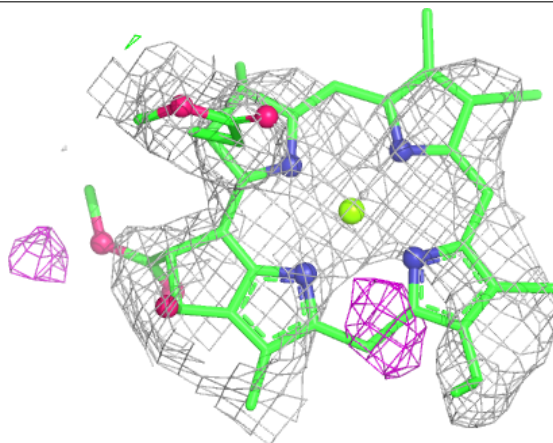


Electron density around BCR A 847:

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

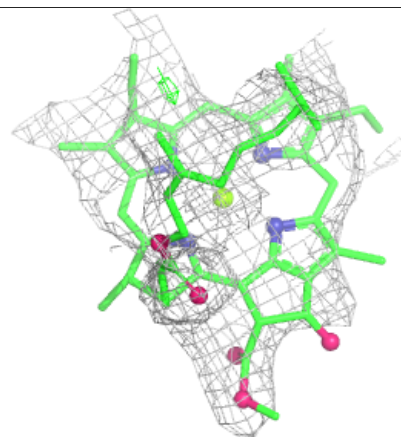
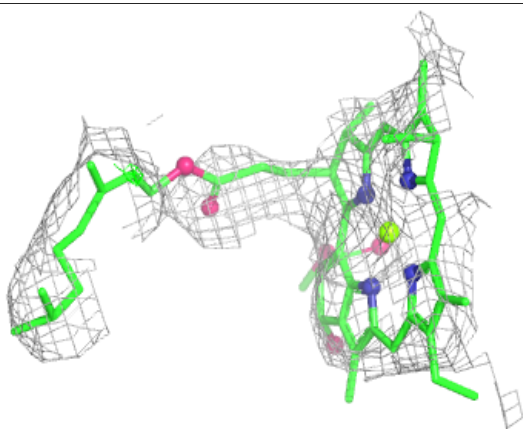
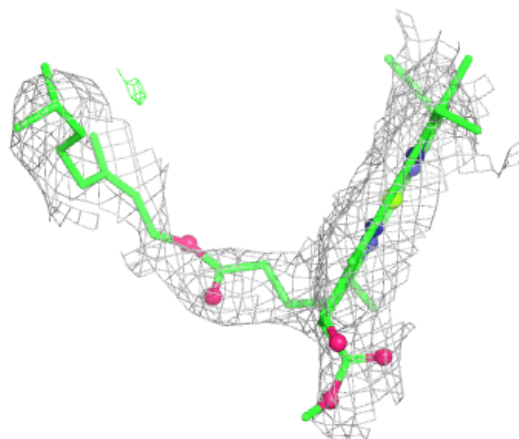
**Electron density around CLA A 807:**

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

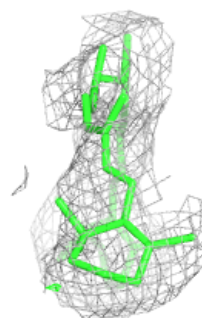
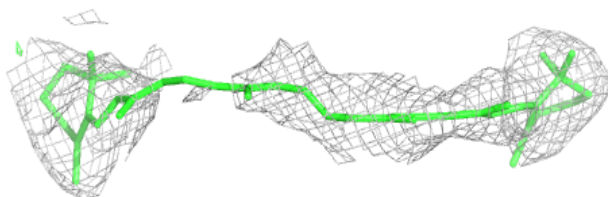
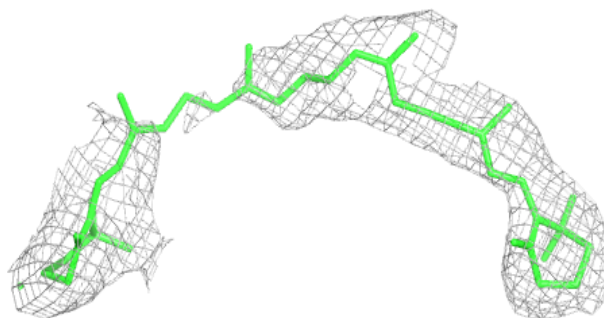


Electron density around CLA L 203:

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

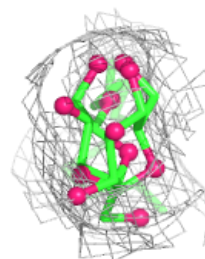
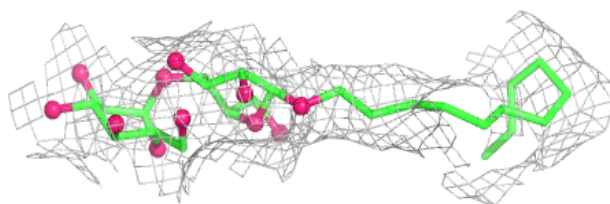
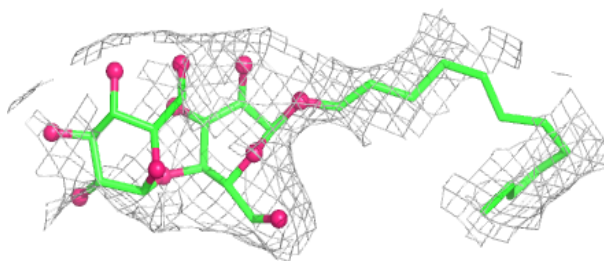
**Electron density around BCR F 203:**

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

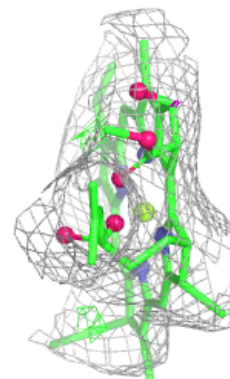
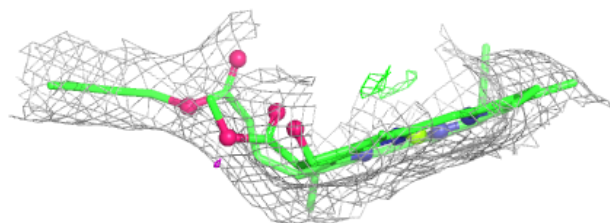
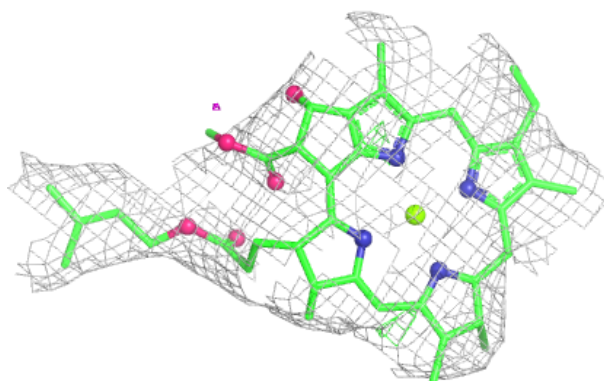


Electron density around LMU B 847:

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

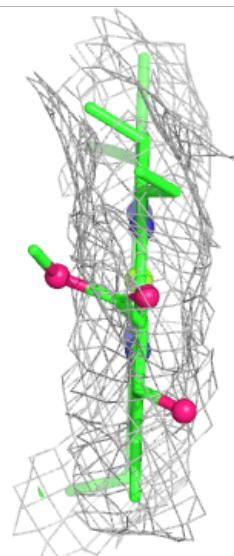
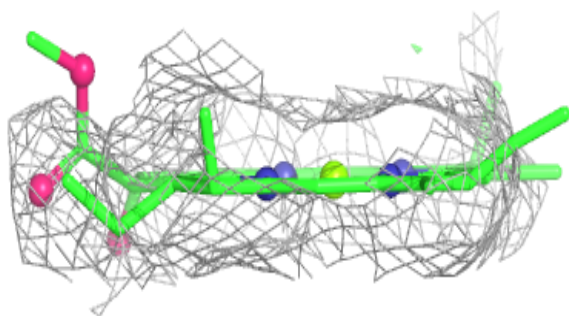
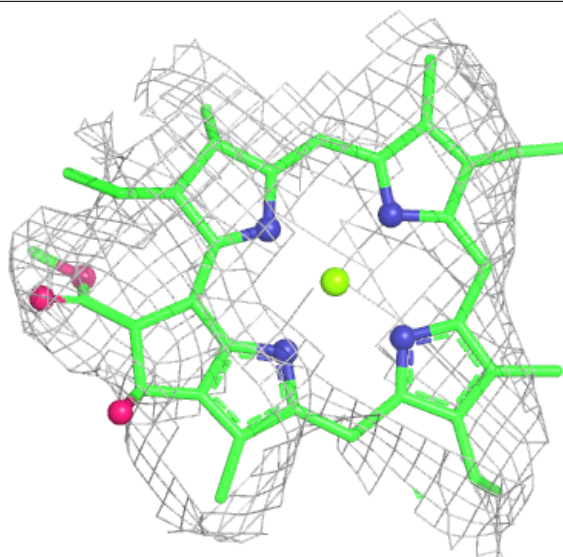
**Electron density around CLA L 207:**

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



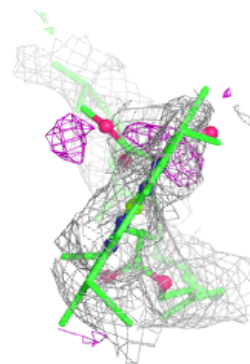
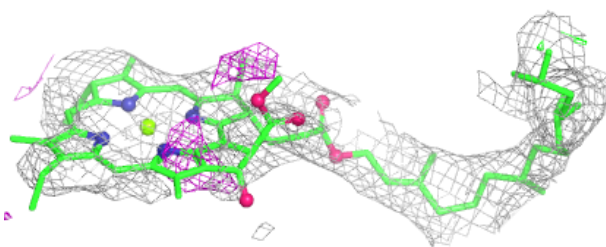
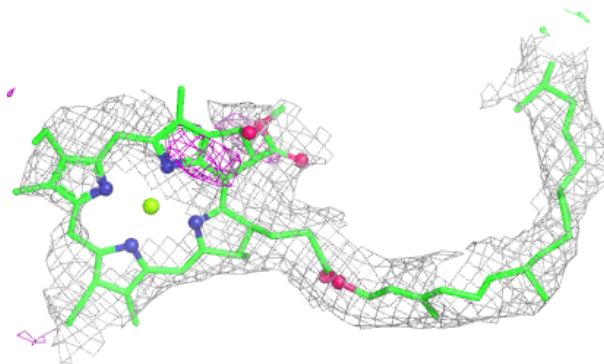
Electron density around CLA A 821:

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



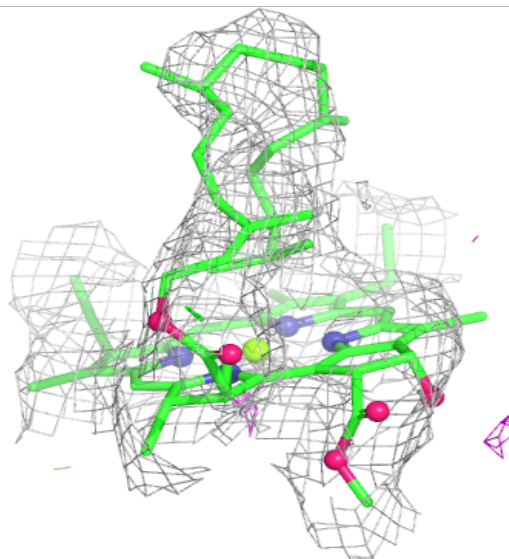
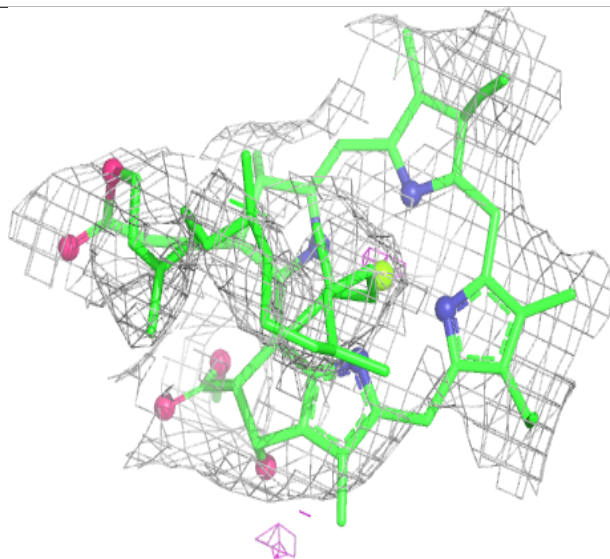
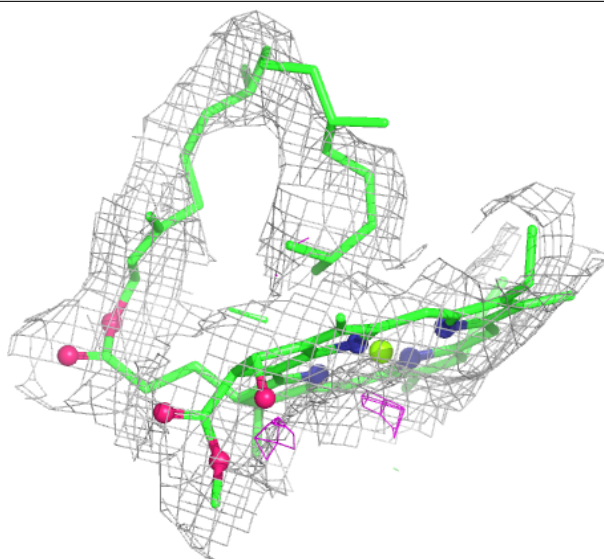
Electron density around CLA B 824:

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



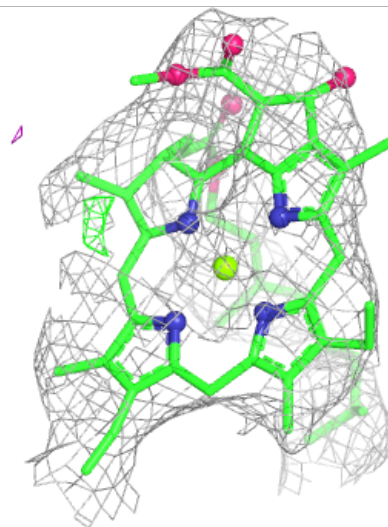
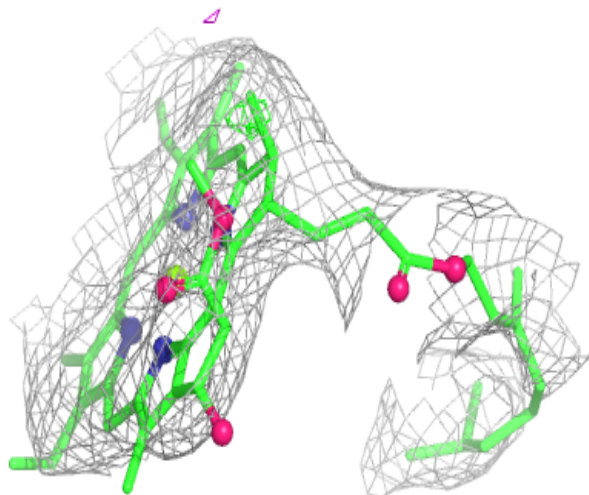
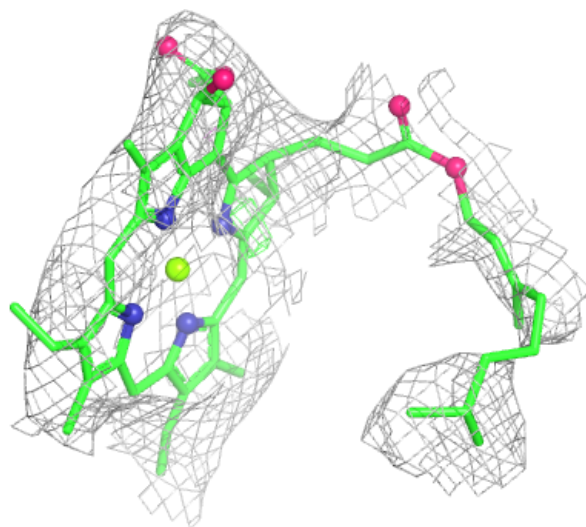
Electron density around CLA 2 315:

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



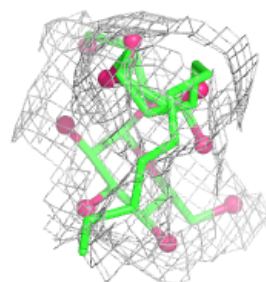
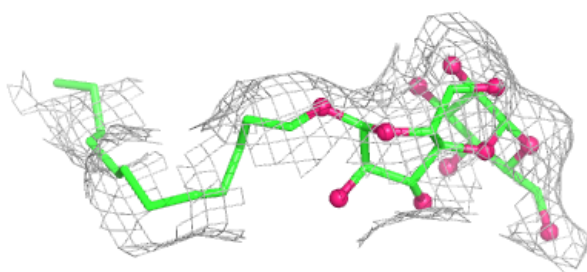
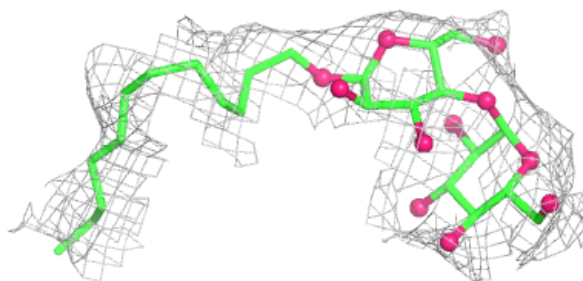
Electron density around CLA A 804:

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

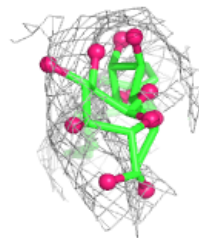
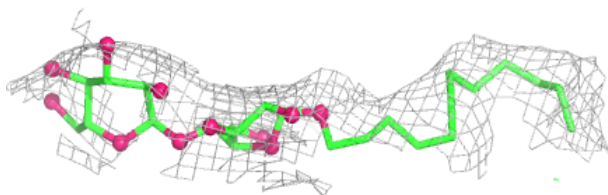
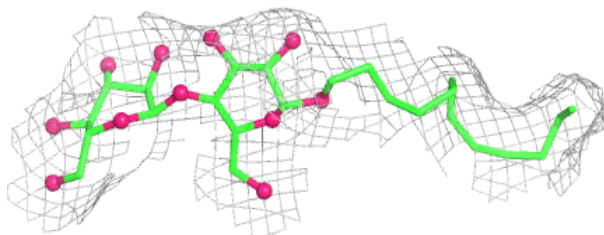


Electron density around LMU 2 318:

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

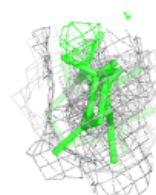
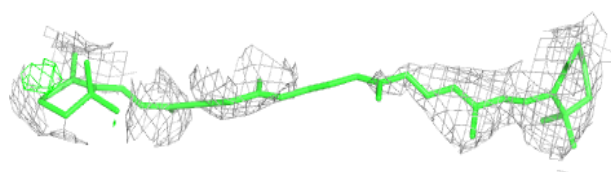
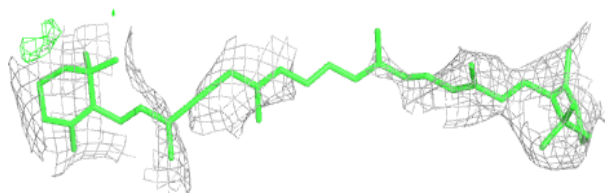
**Electron density around LMU 3 321:**

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

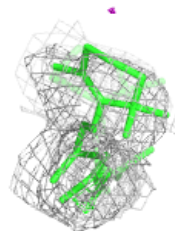
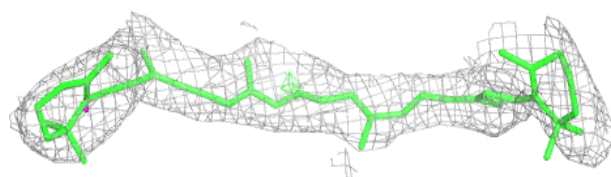
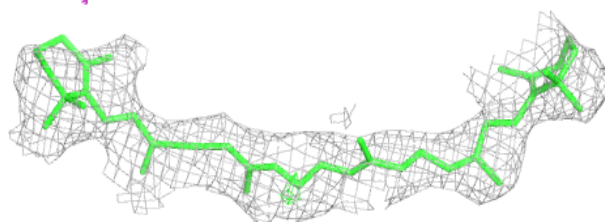


Electron density around BCR A 844:

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

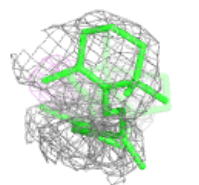
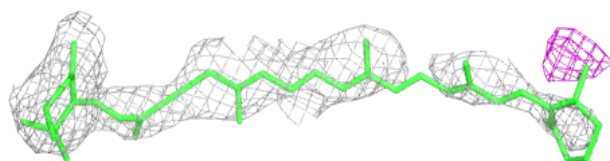
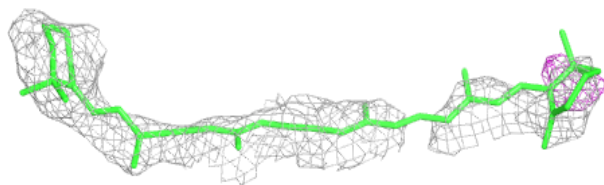
**Electron density around BCR B 852:**

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



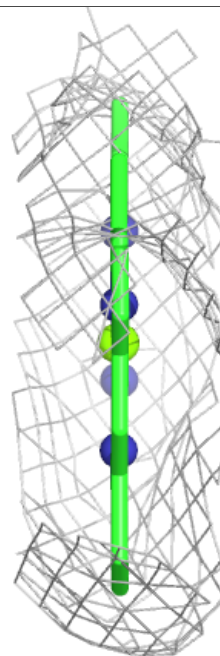
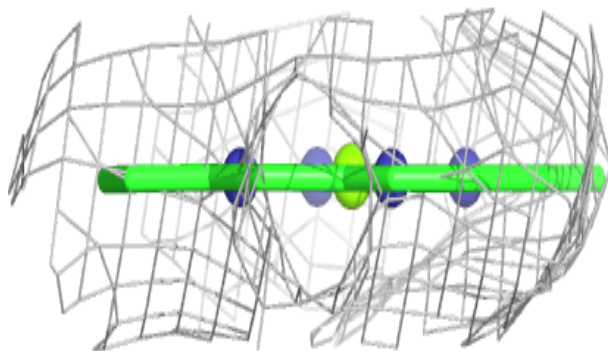
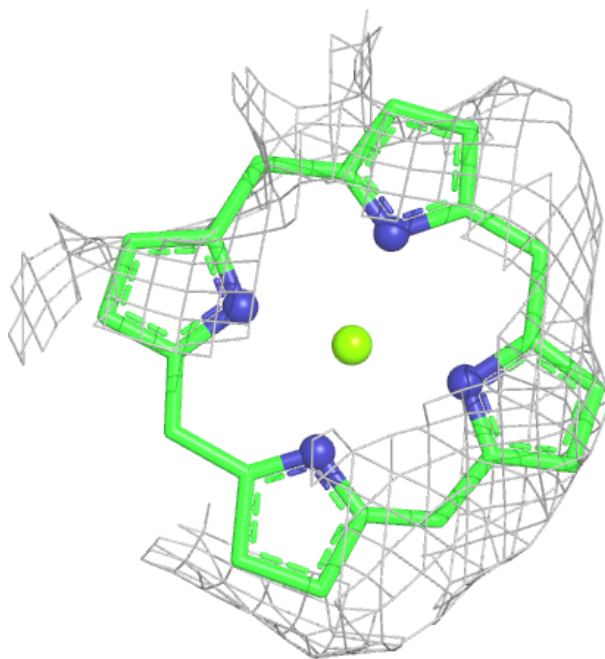
Electron density around BCR F 202:

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



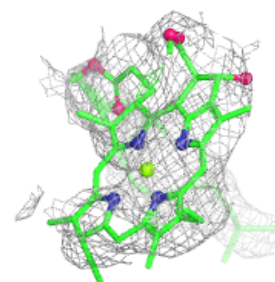
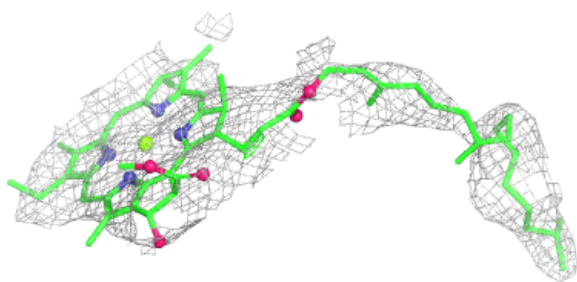
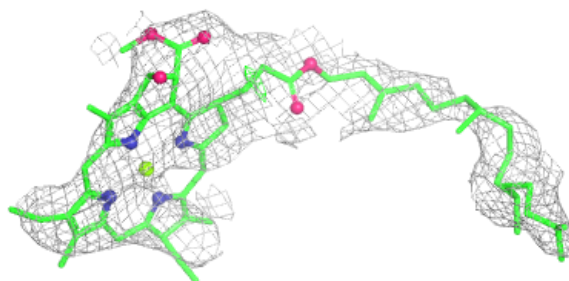
Electron density around CLA 3 312:

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

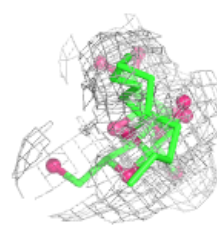
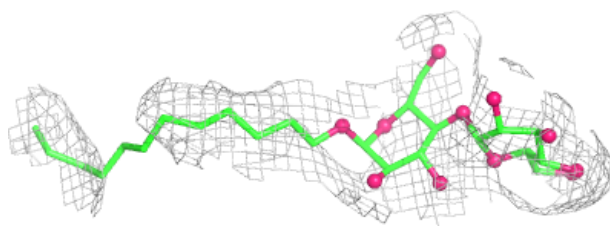
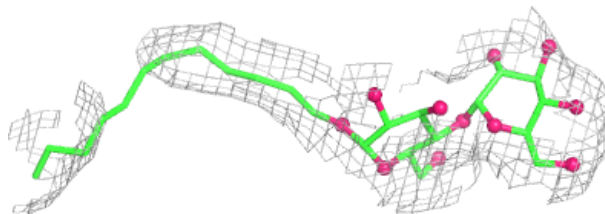


Electron density around CLA A 851:

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

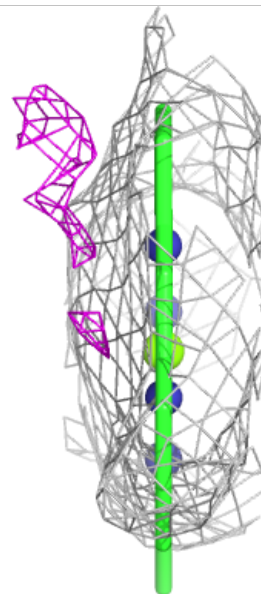
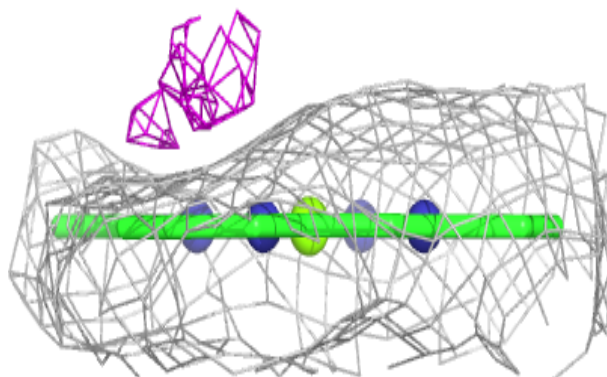
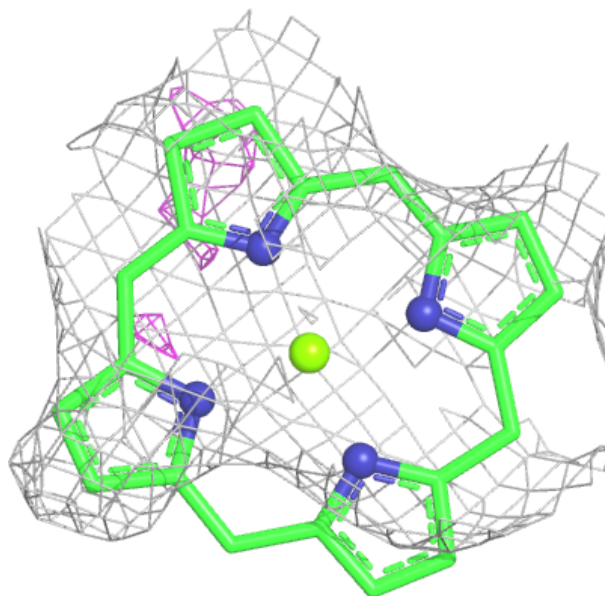
**Electron density around LMU B 802:**

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



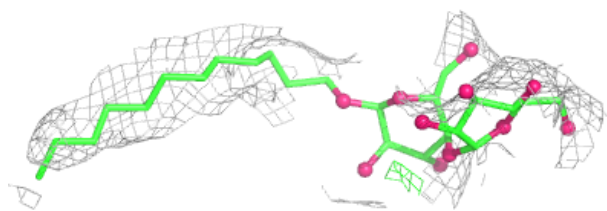
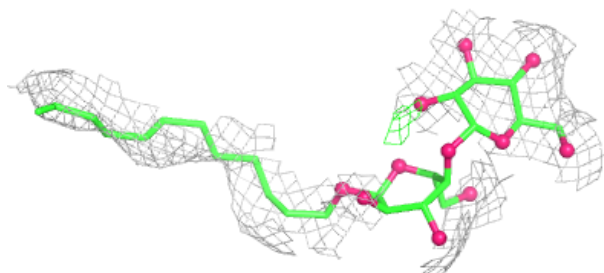
Electron density around CLA A 802:

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

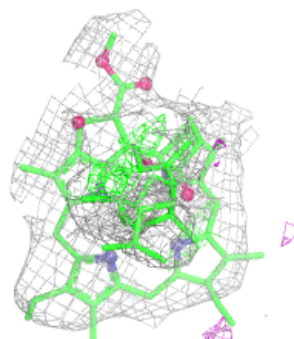
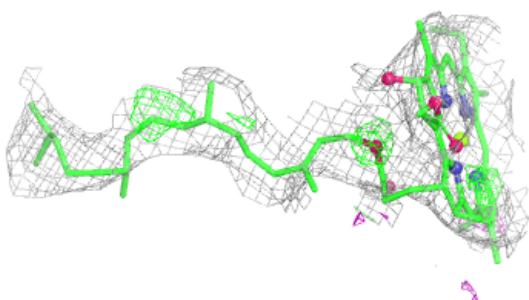
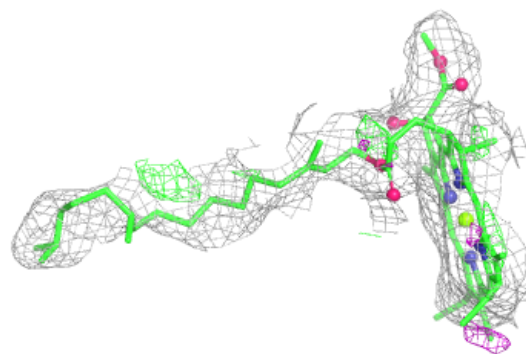


Electron density around LMU R 105:

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

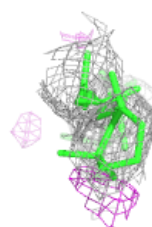
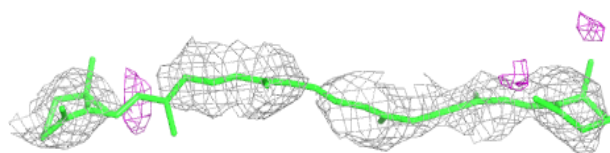
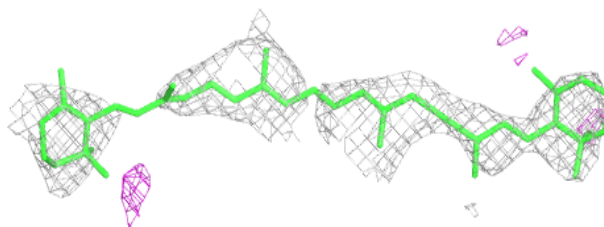
**Electron density around CLA A 826:**

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

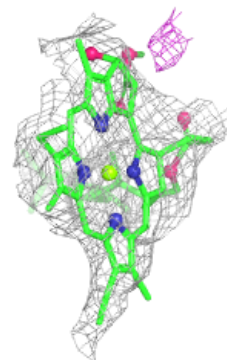
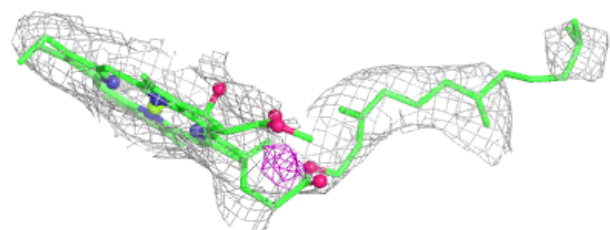
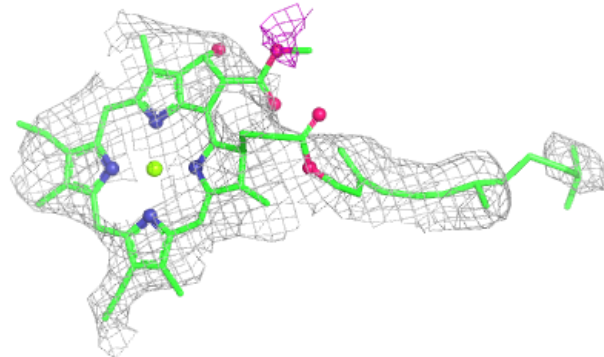


Electron density around BCR B 845:

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

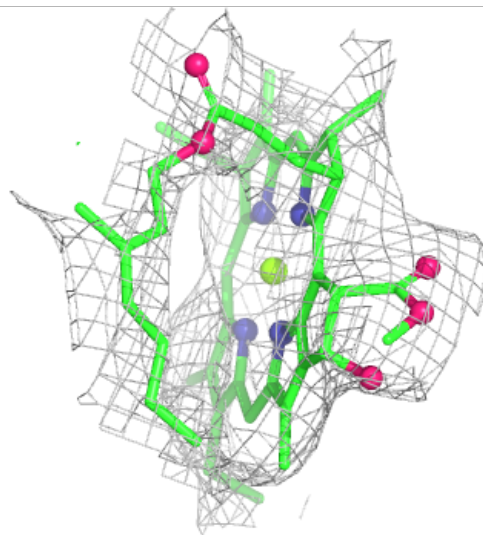
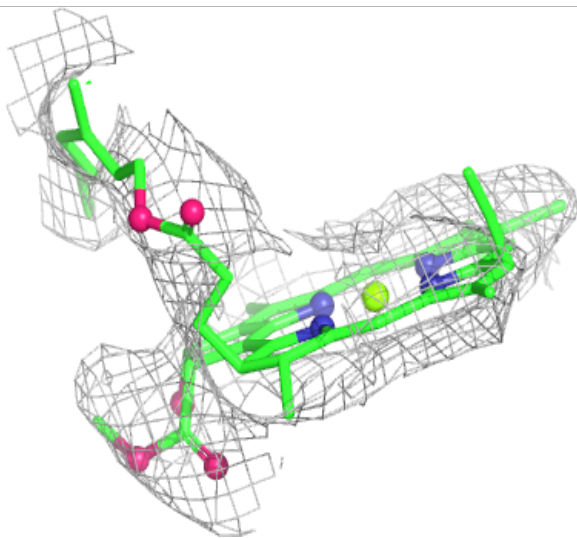
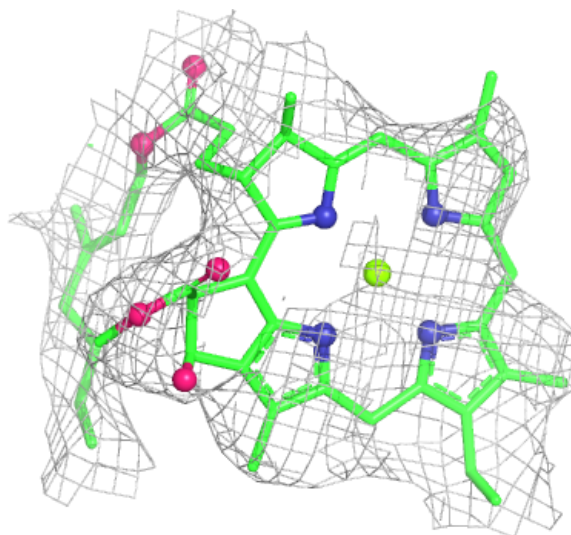
**Electron density around CLA H 109:**

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



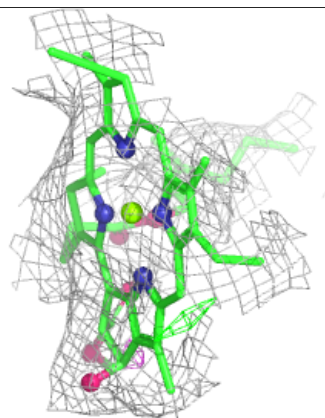
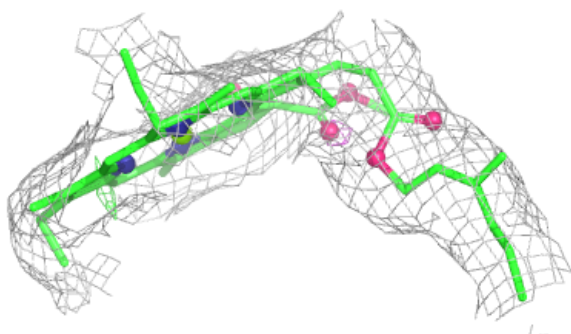
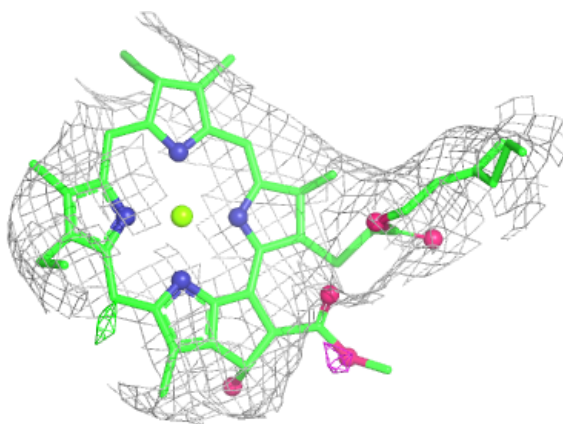
Electron density around CLA F 206:

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



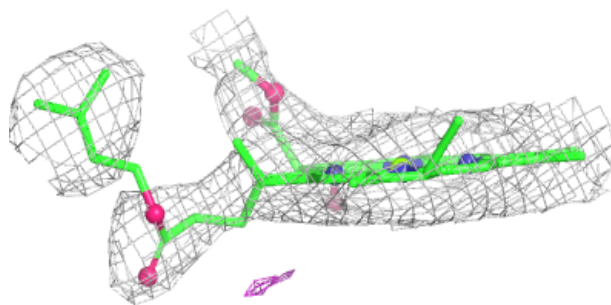
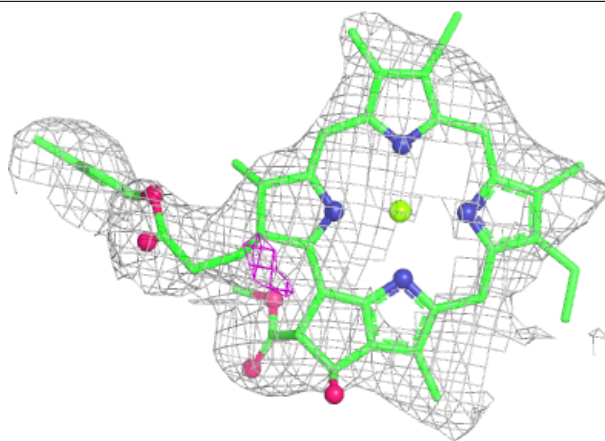
Electron density around CLA 4 307:

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



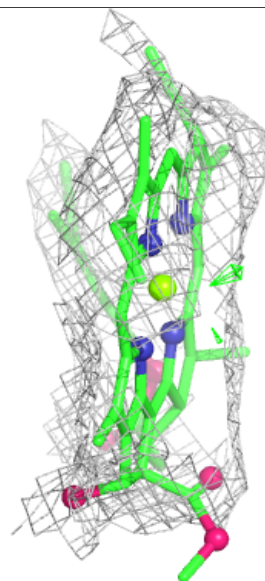
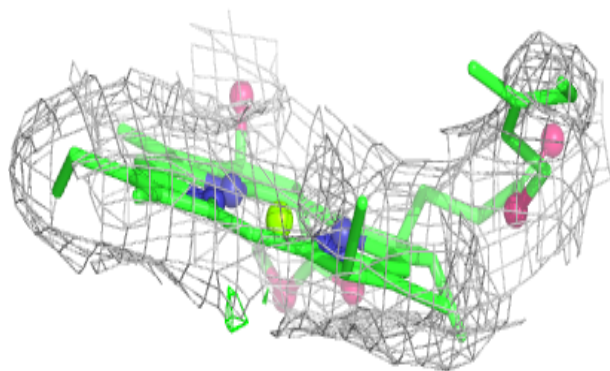
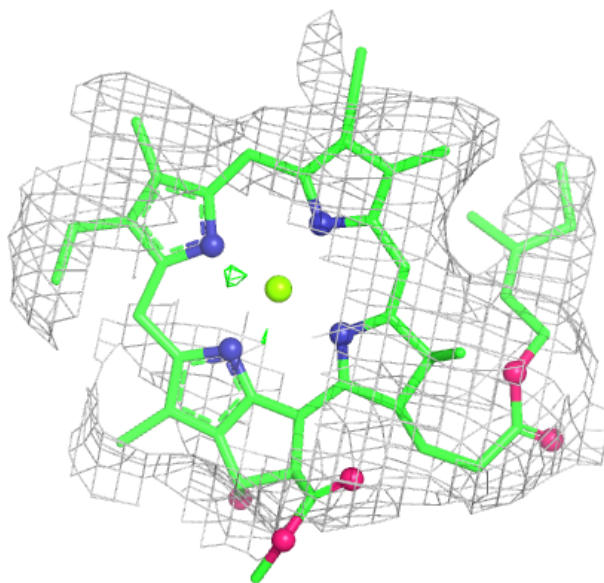
Electron density around CLA B 829:

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



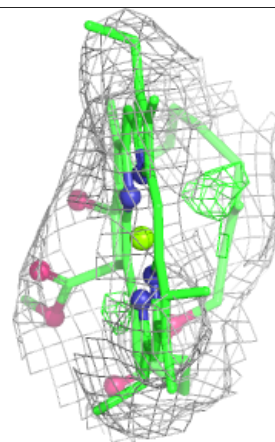
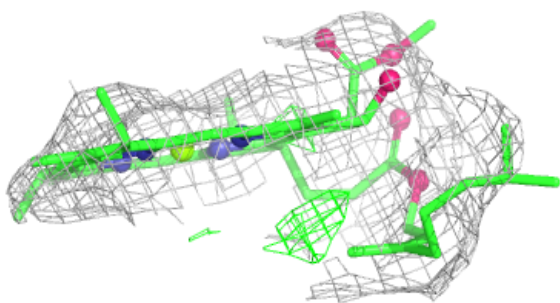
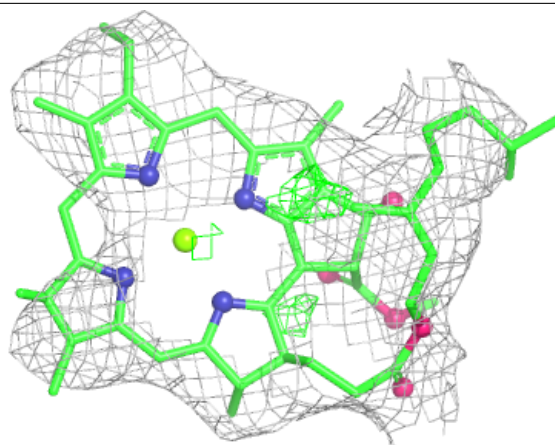
Electron density around CLA G 102:

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



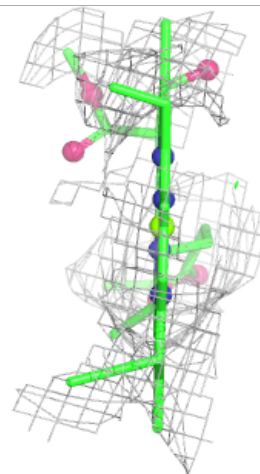
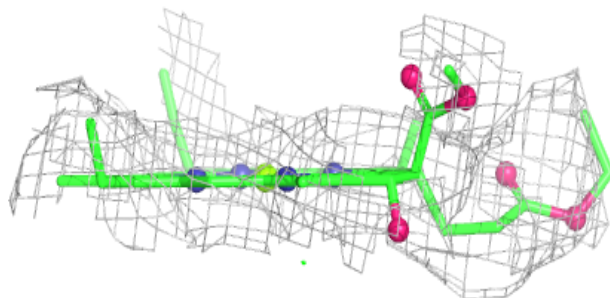
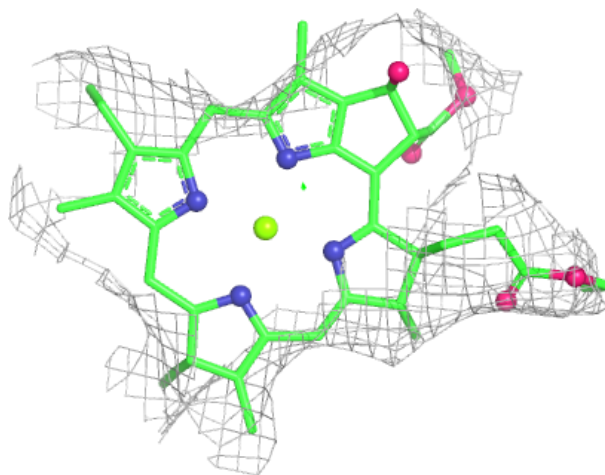
Electron density around CLA B 809:

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



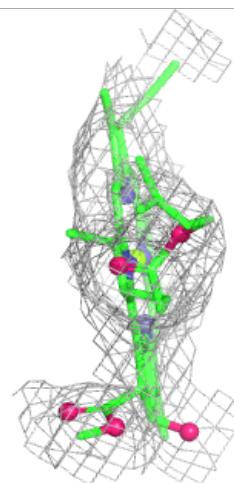
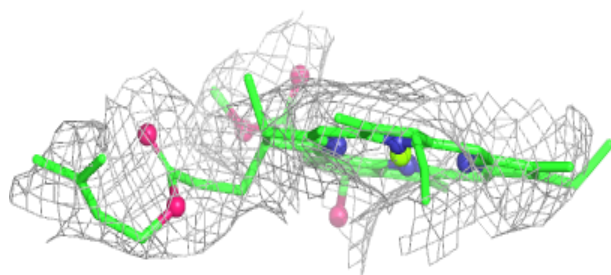
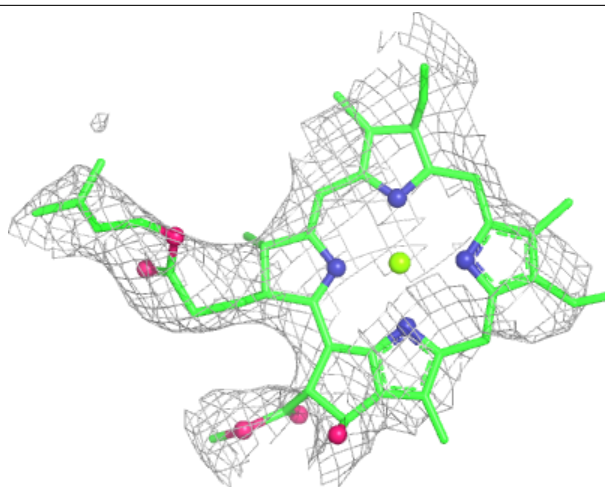
Electron density around CLA 1 203:

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



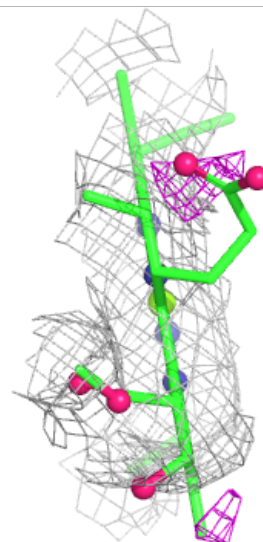
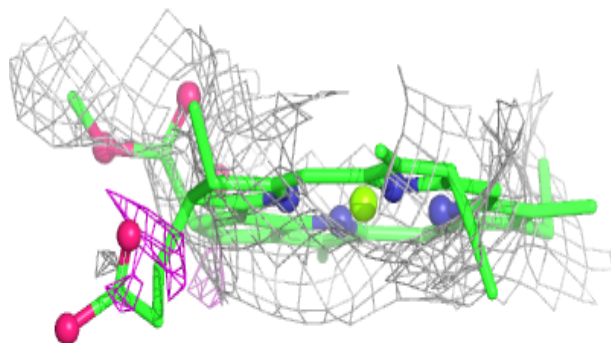
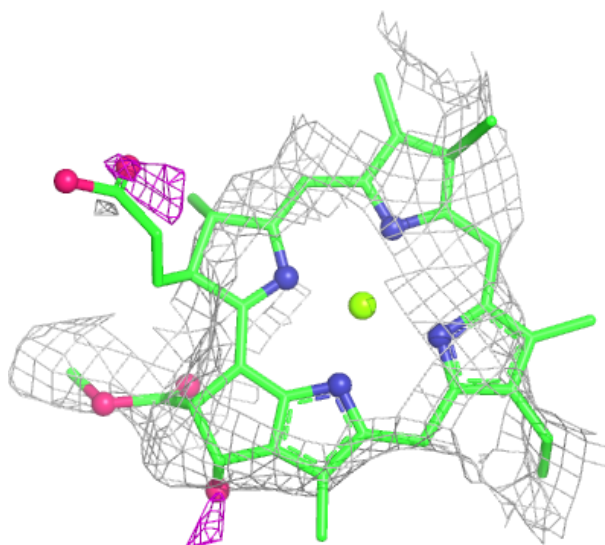
Electron density around CLA 2 305:

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



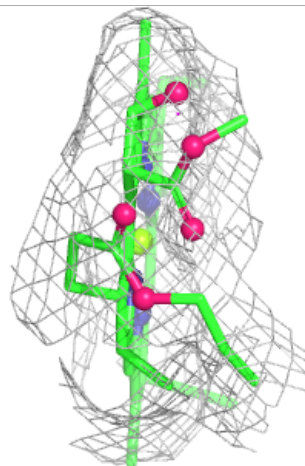
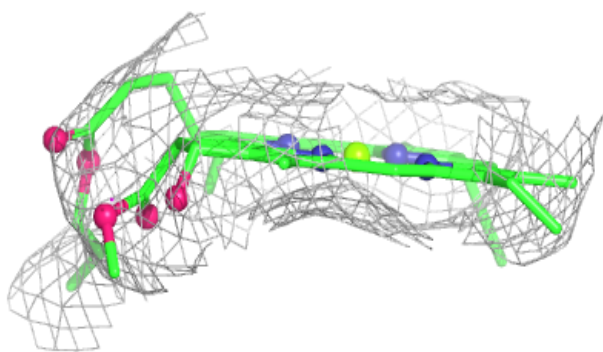
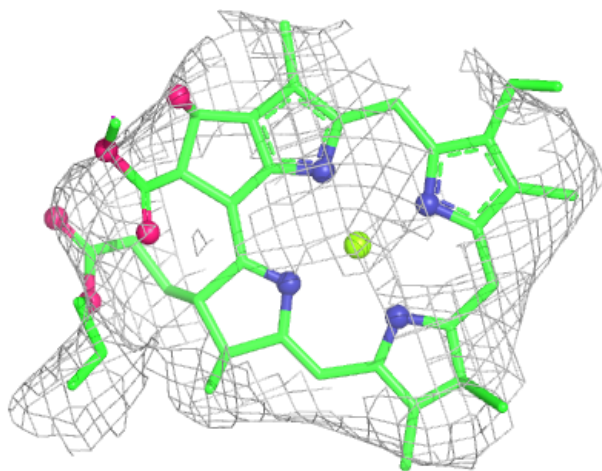
Electron density around CLA A 833:

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



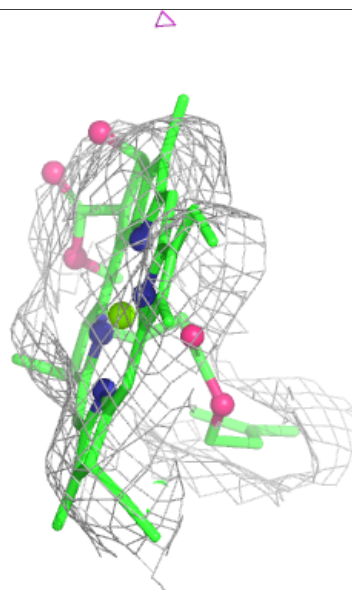
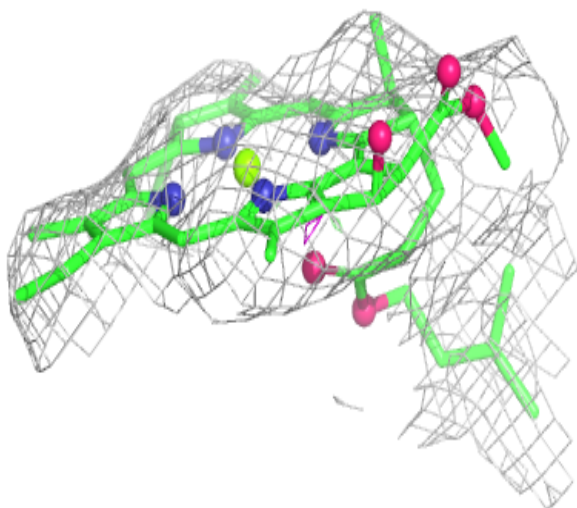
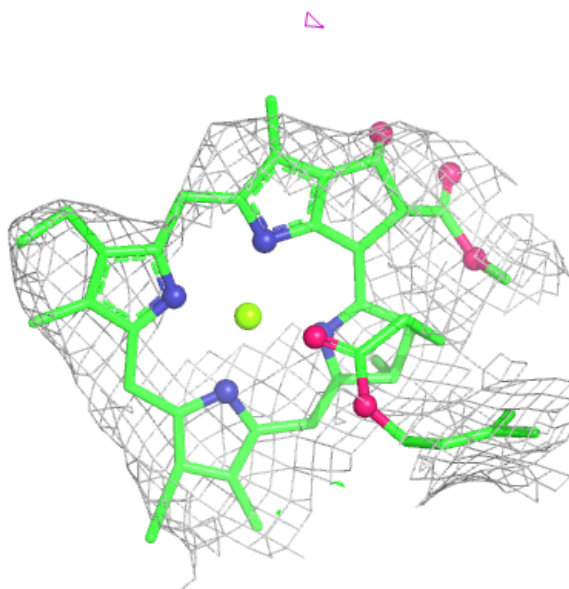
Electron density around CLA J 101:

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



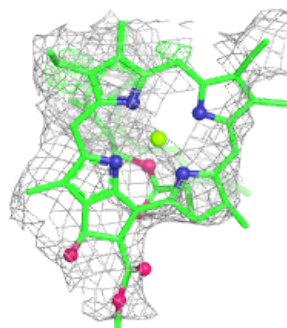
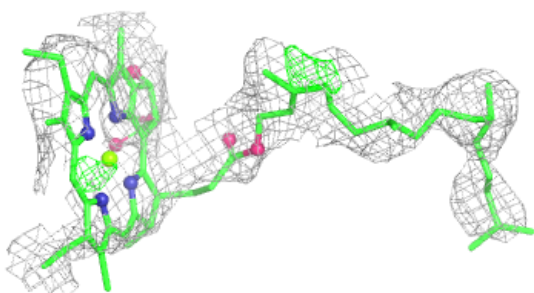
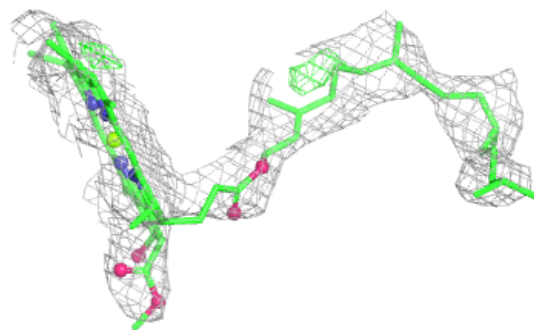
Electron density around CLA A 815:

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



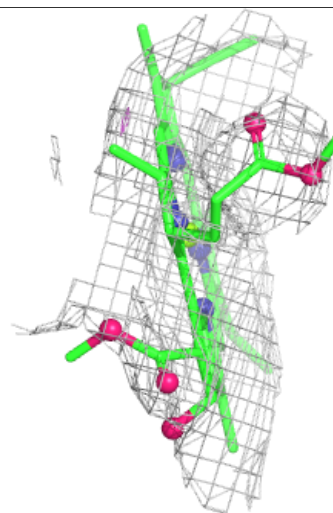
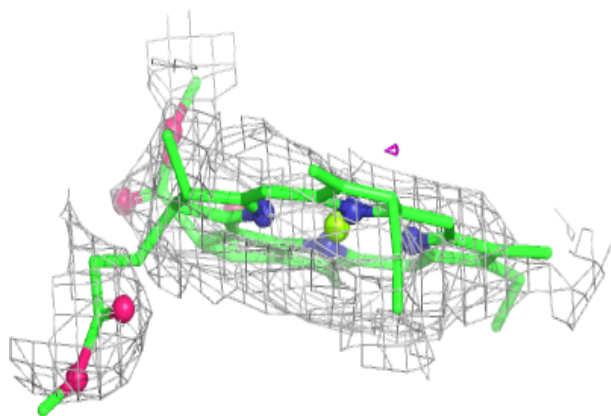
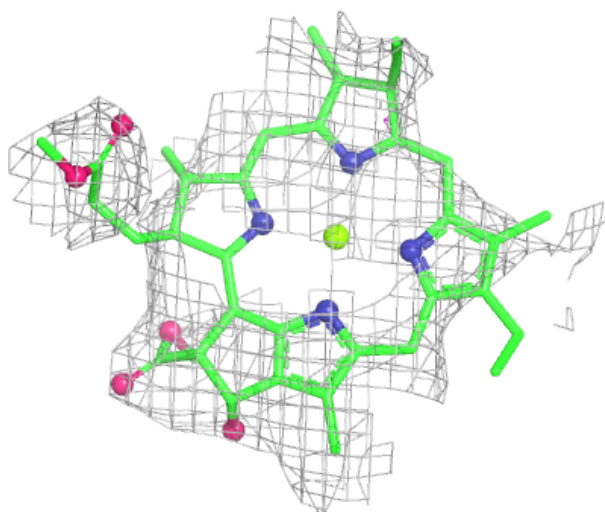
Electron density around CLA B 838:

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



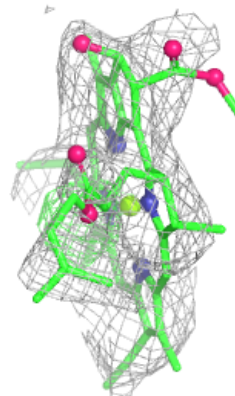
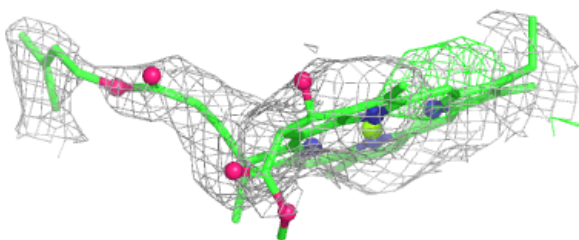
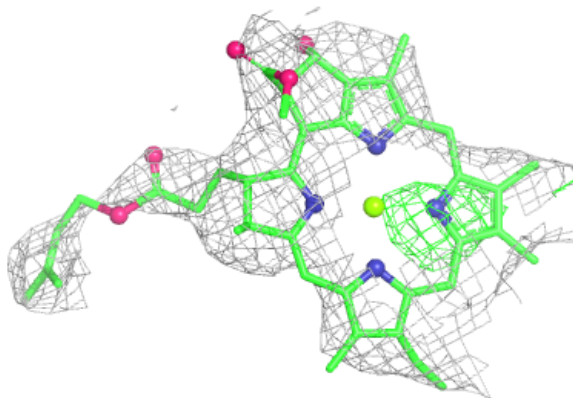
Electron density around CLA B 819:

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

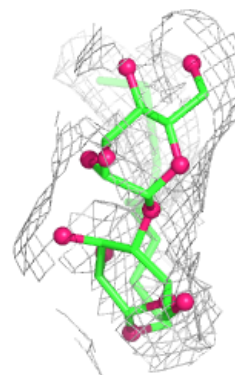
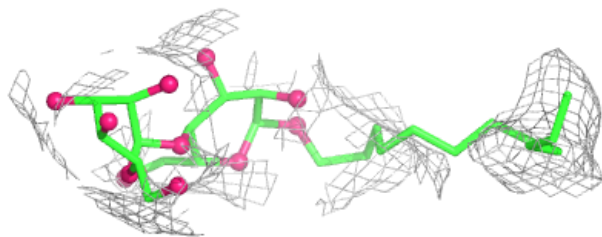


Electron density around CLA B 831:

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

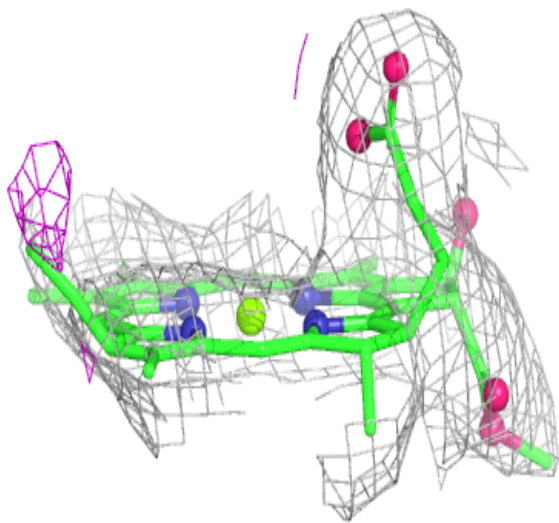
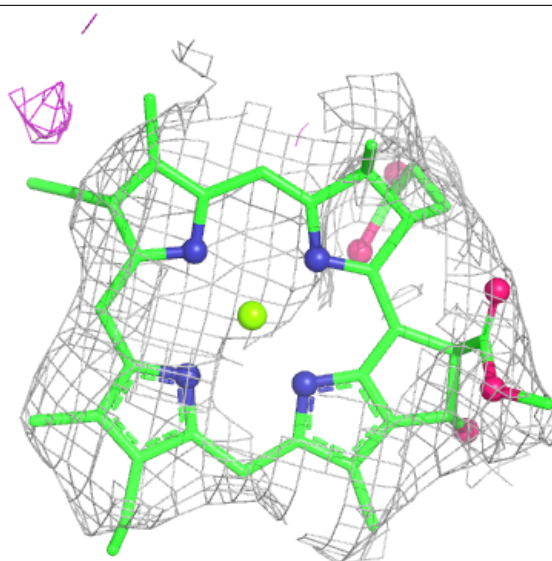
**Electron density around LMU 4 321:**

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



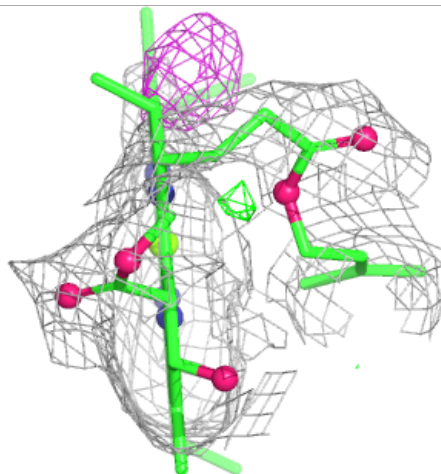
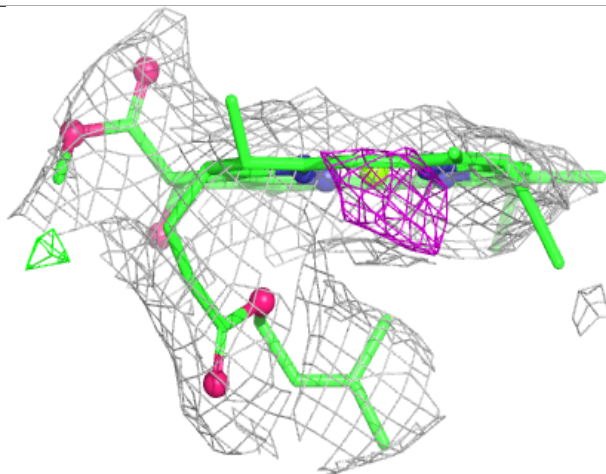
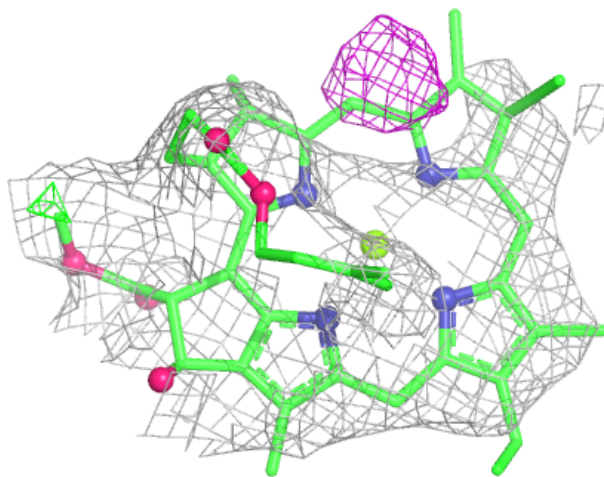
Electron density around CLA B 832:

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



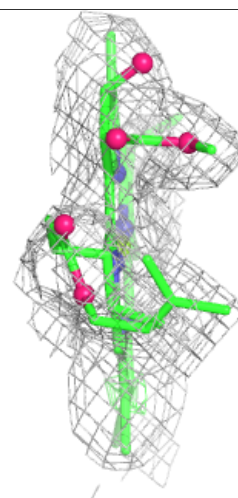
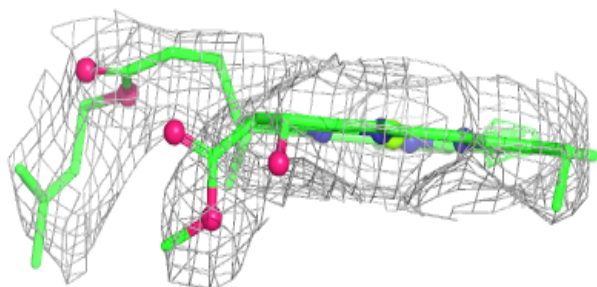
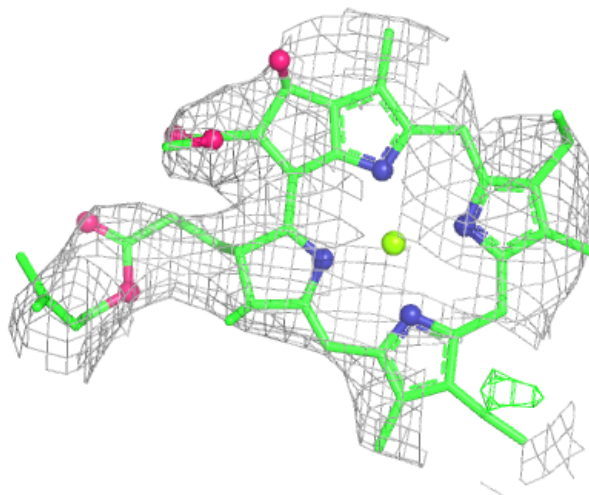
Electron density around CLA H 111:

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



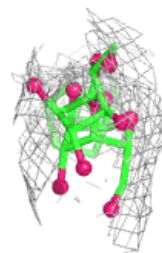
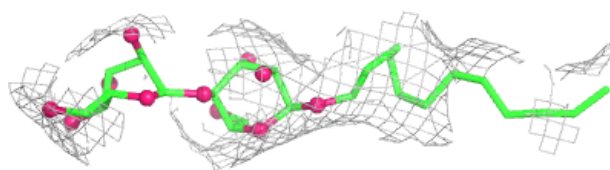
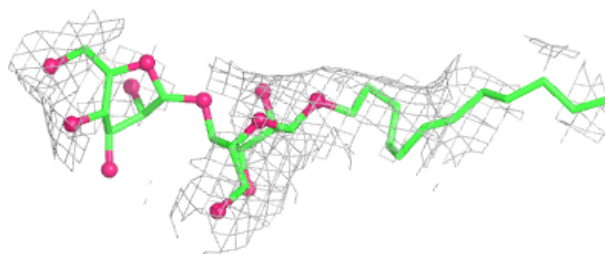
Electron density around CLA A 803:

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



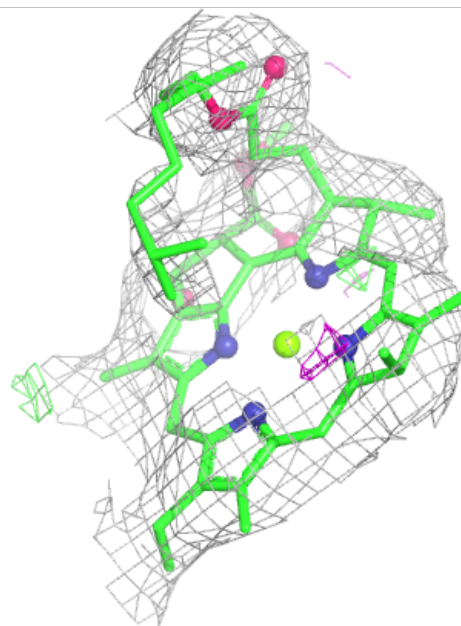
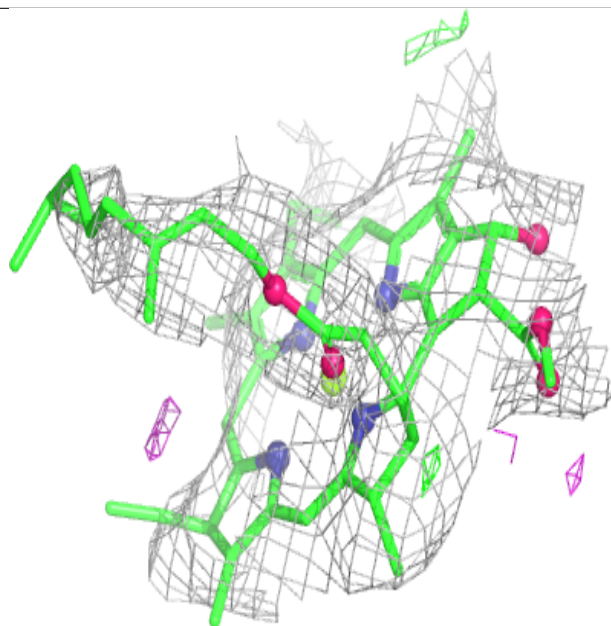
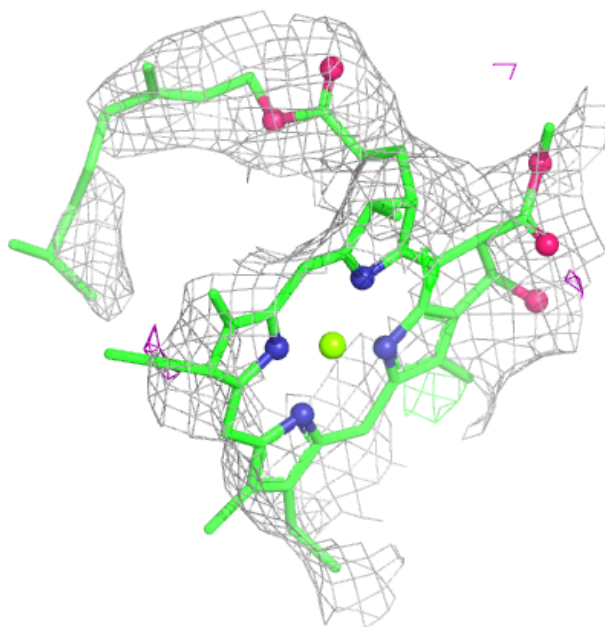
Electron density around LMU E 101:

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



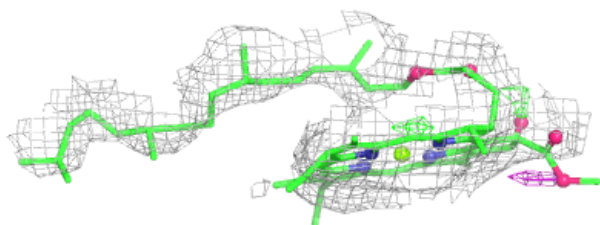
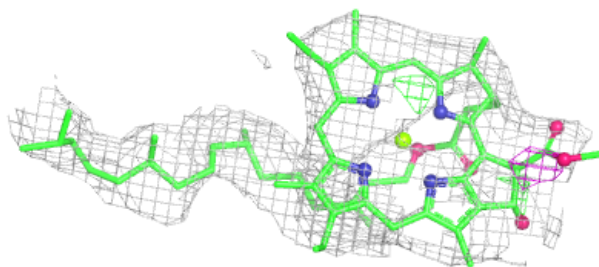
Electron density around CLA A 822:

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



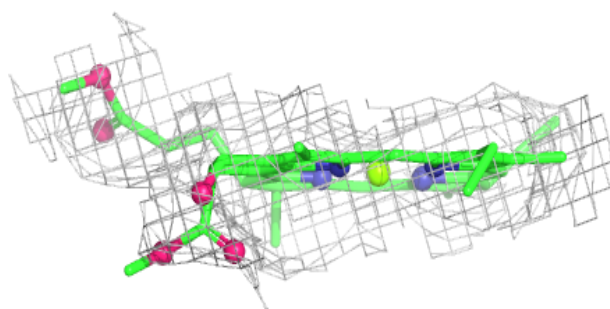
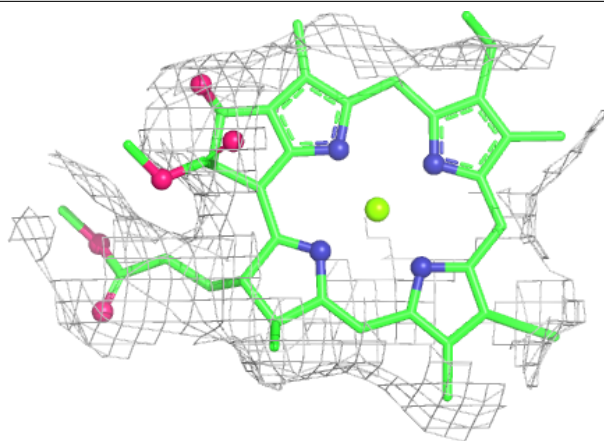
Electron density around CLA A 835:

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



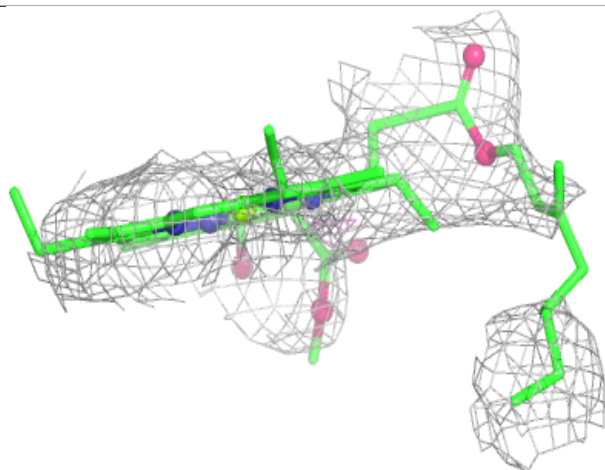
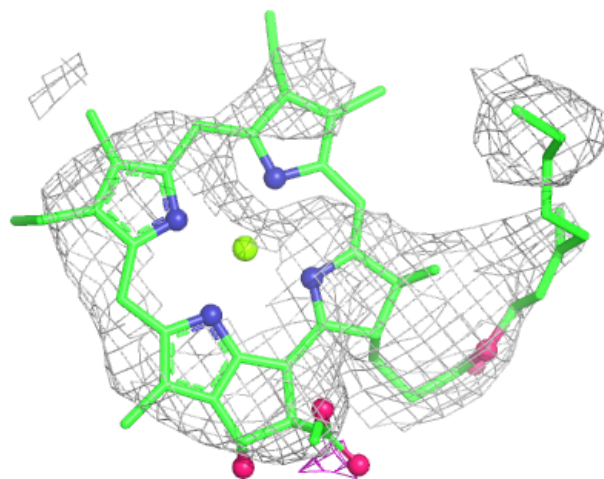
Electron density around CLA 4 316:

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



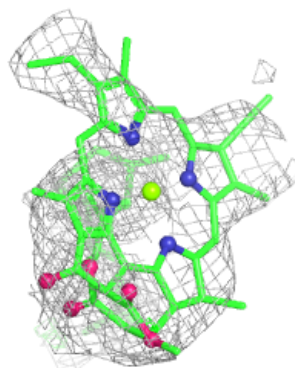
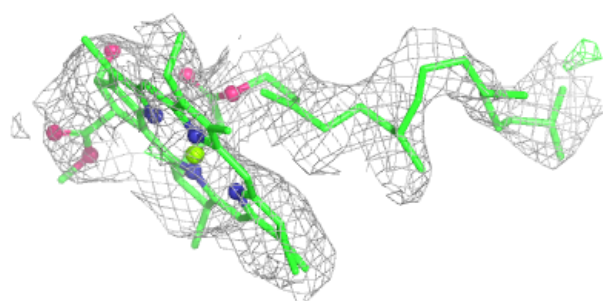
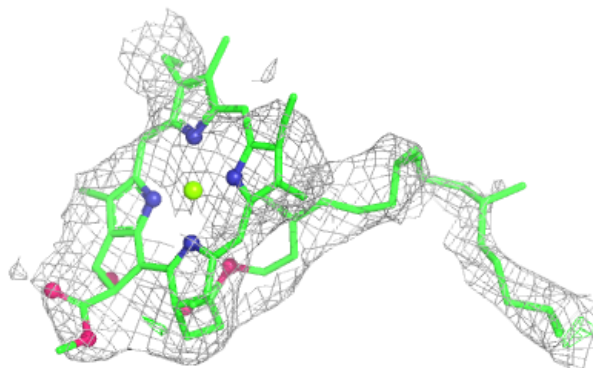
Electron density around CLA A 813:

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



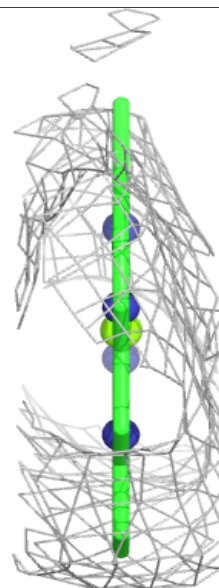
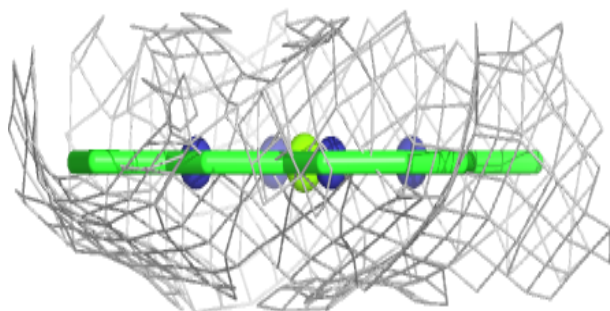
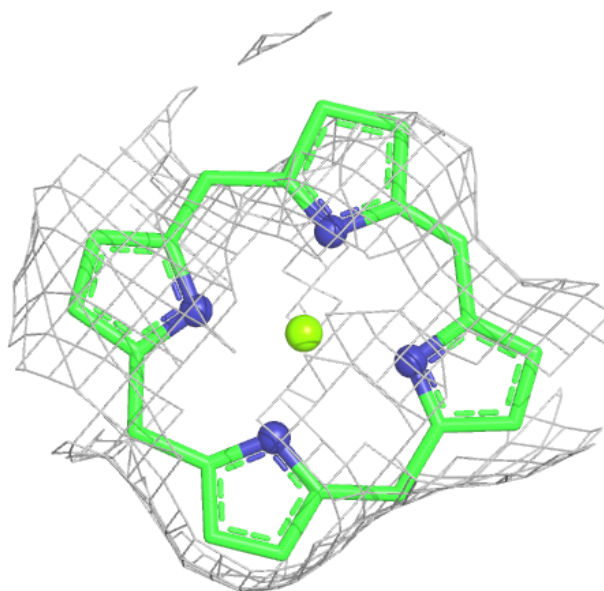
Electron density around CLA A 841:

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



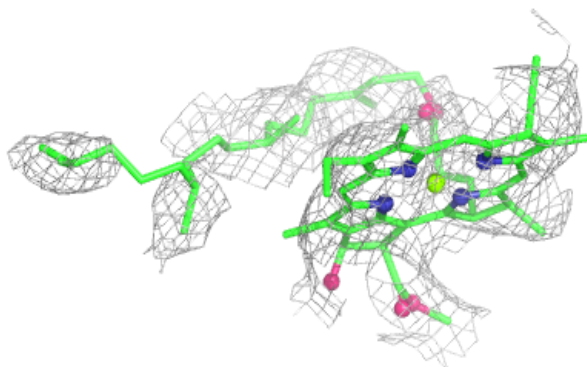
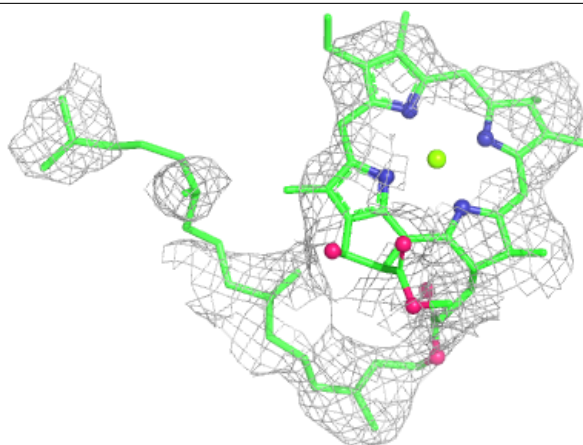
Electron density around CLA 4 309:

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



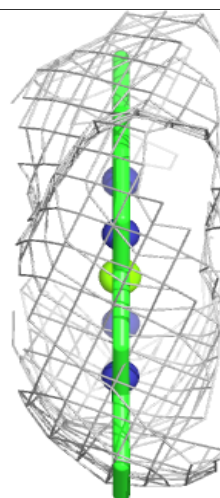
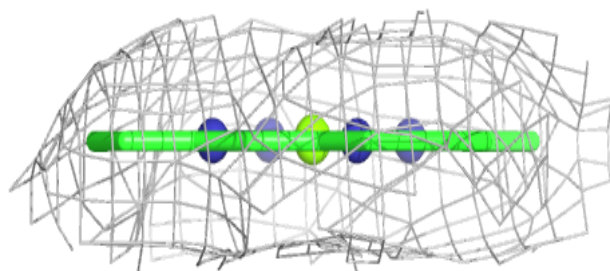
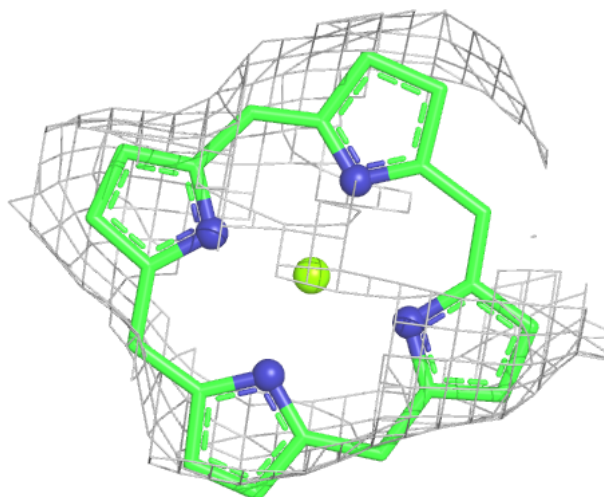
Electron density around CLA B 830:

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



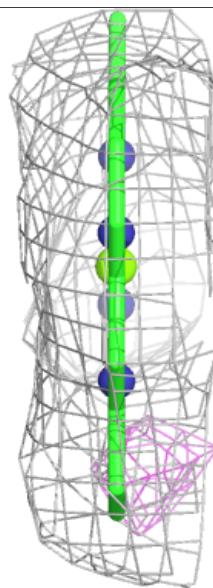
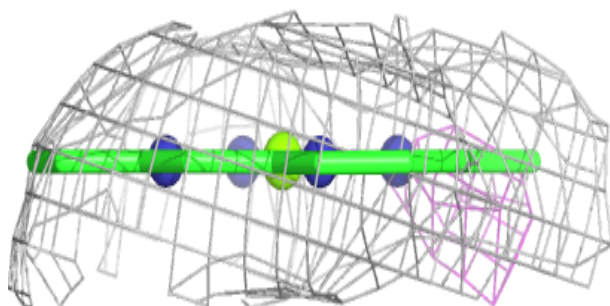
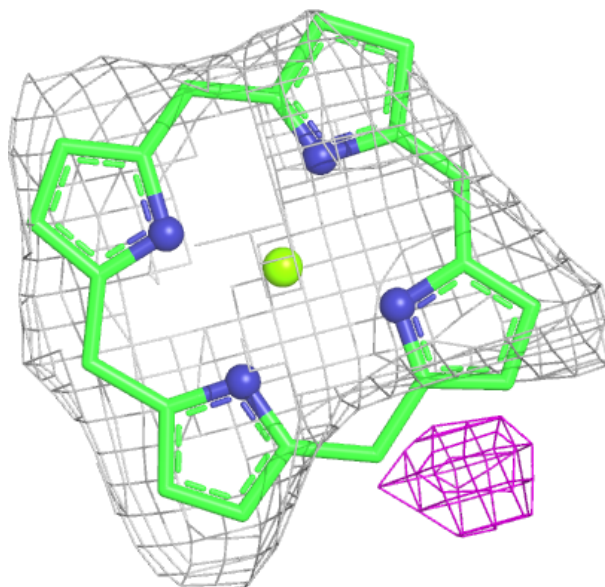
Electron density around CLA 3 303:

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



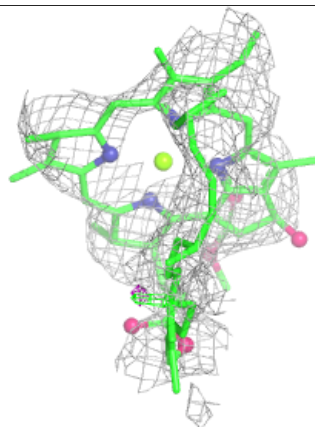
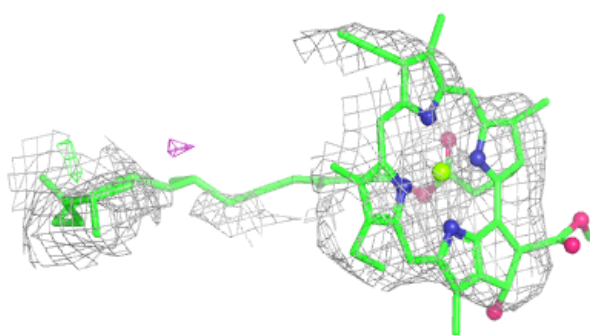
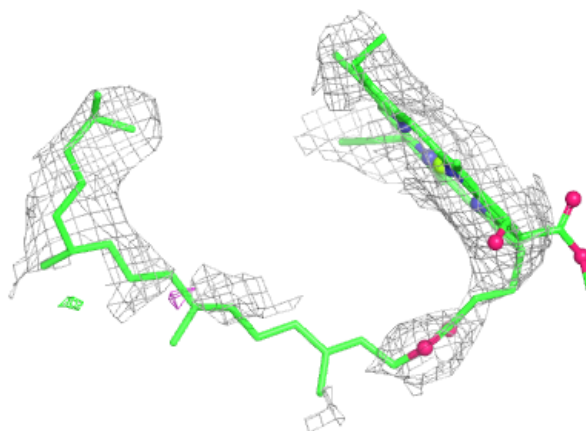
Electron density around CLA 3 315:

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

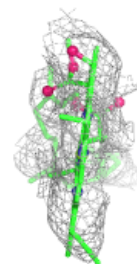
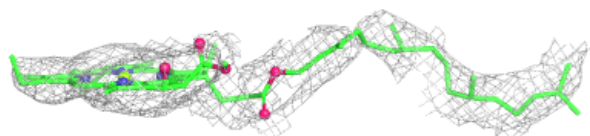
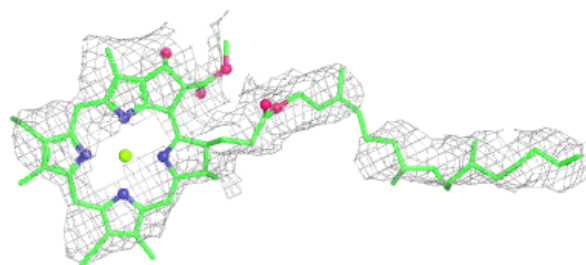


Electron density around CLA L 202:

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

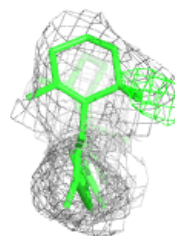
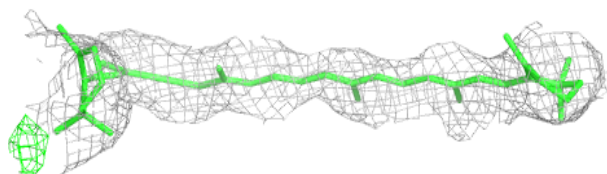
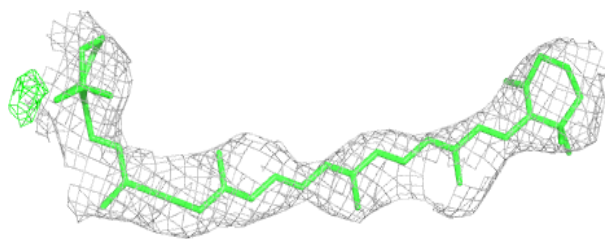
**Electron density around CLA A 830:**

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



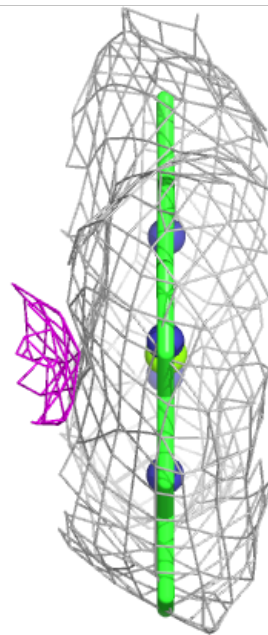
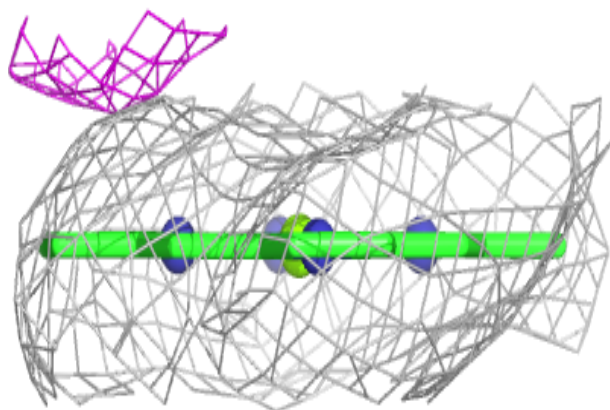
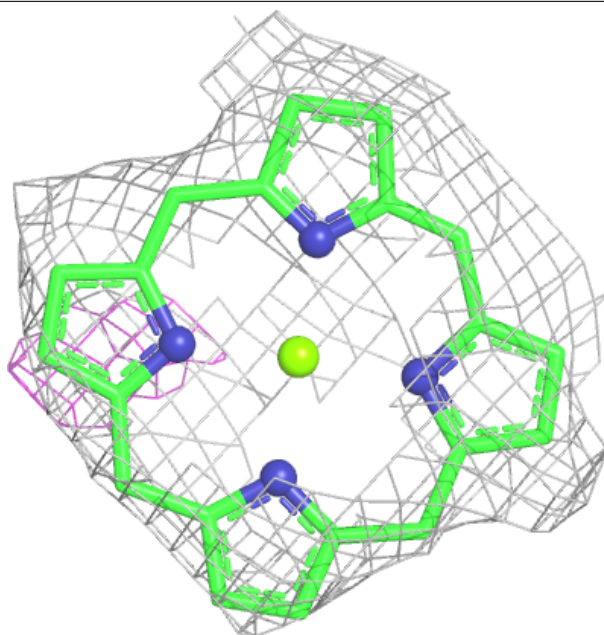
Electron density around BCR B 843:

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



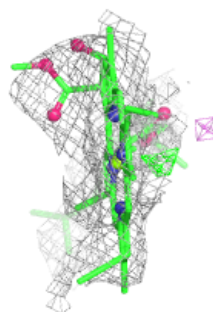
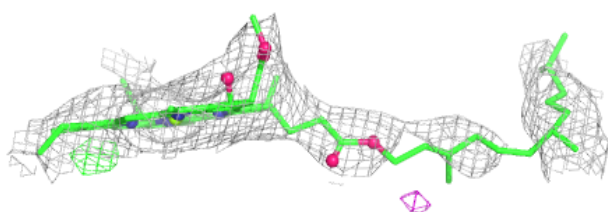
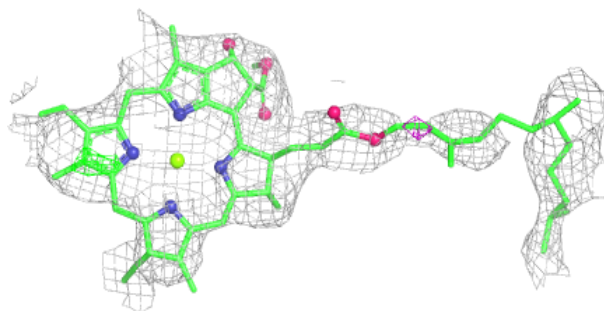
Electron density around CLA 2 304:

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



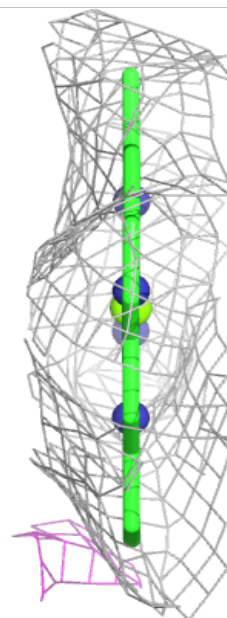
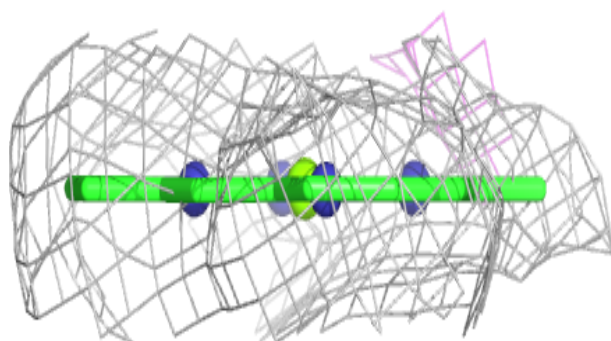
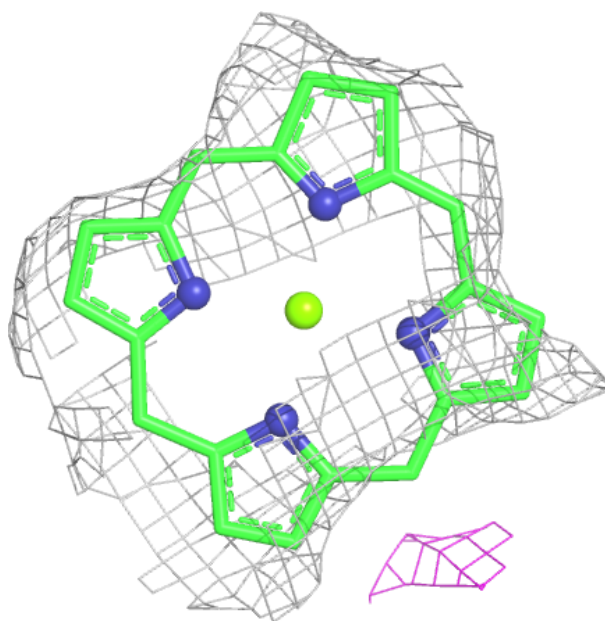
Electron density around CLA B 835:

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



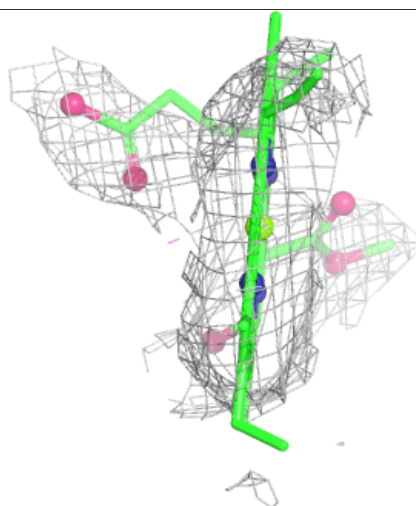
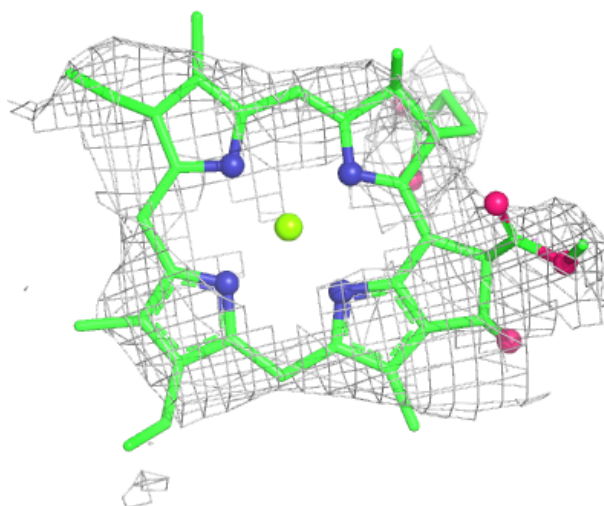
Electron density around CLA 1 216:

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



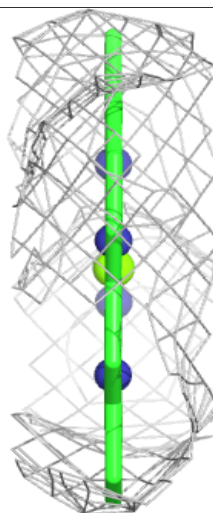
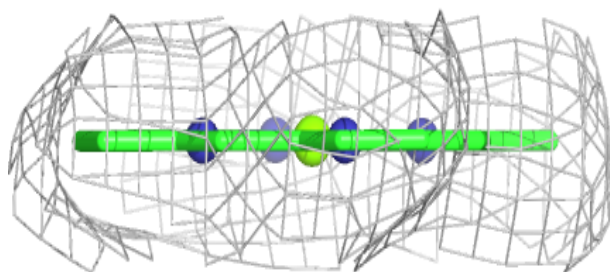
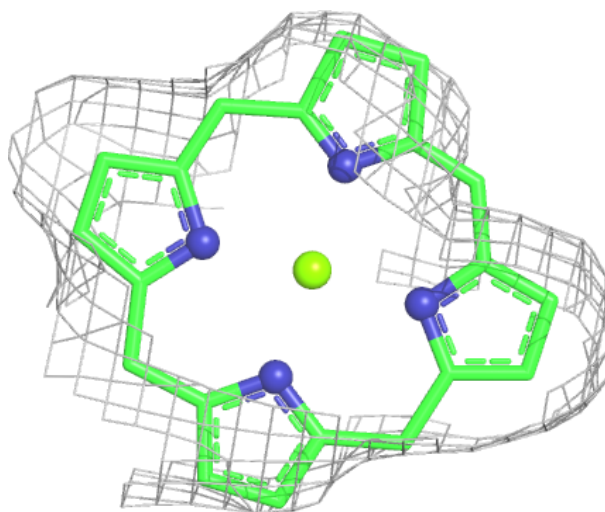
Electron density around CLA B 804:

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



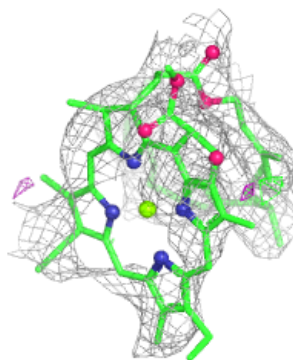
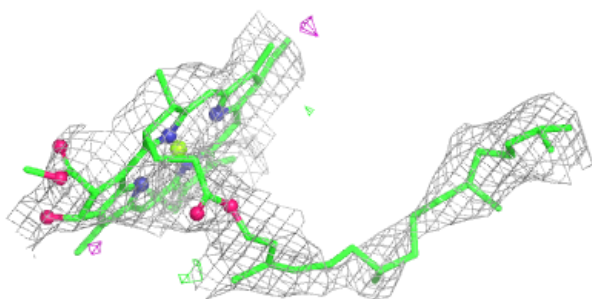
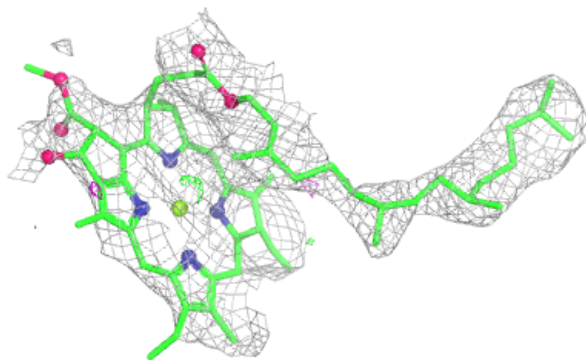
Electron density around CLA 1 205:

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



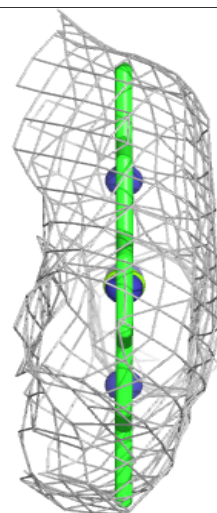
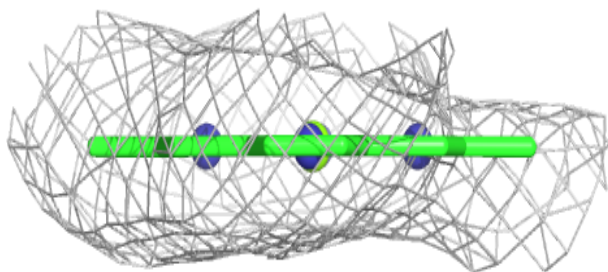
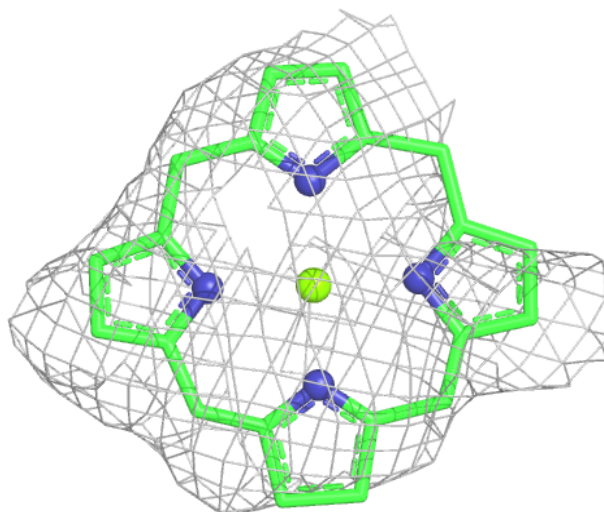
Electron density around CLA B 812:

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



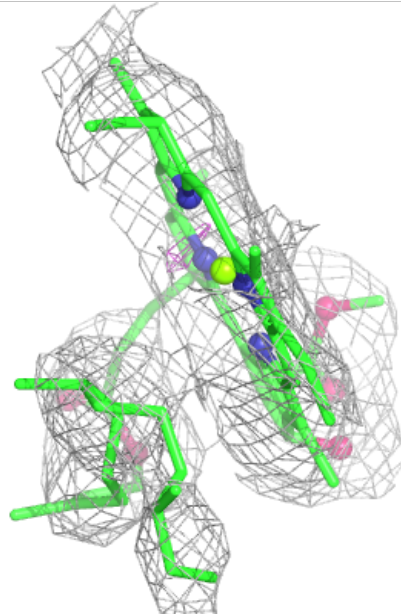
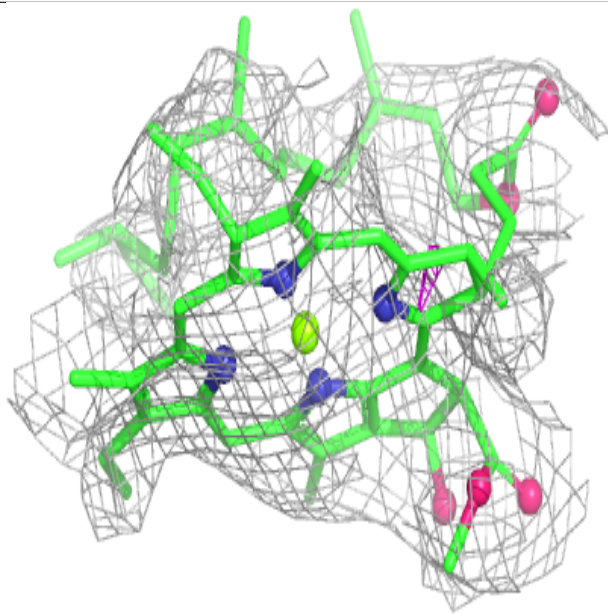
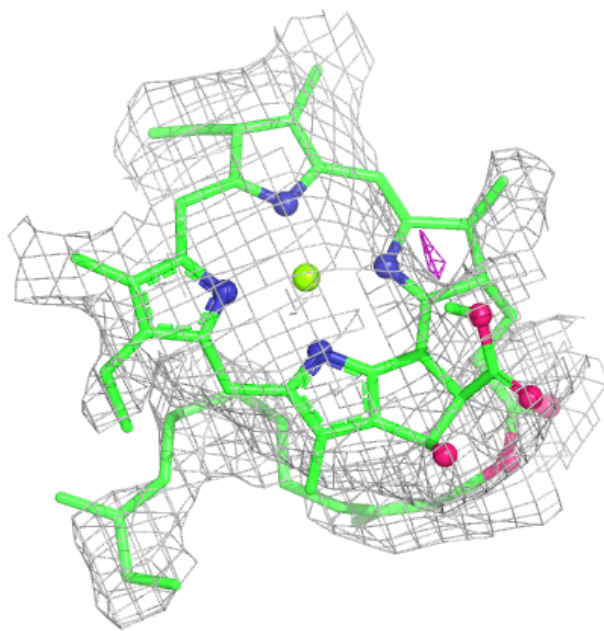
Electron density around CLA 1 212:

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



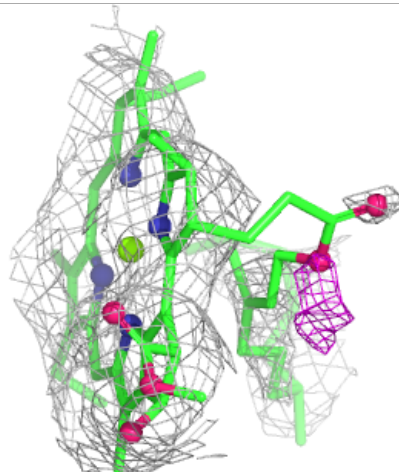
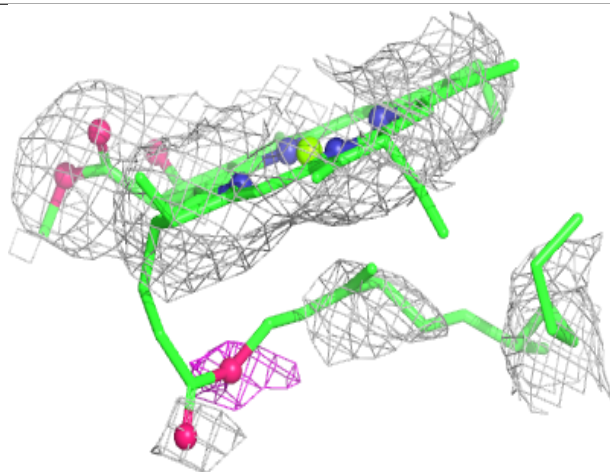
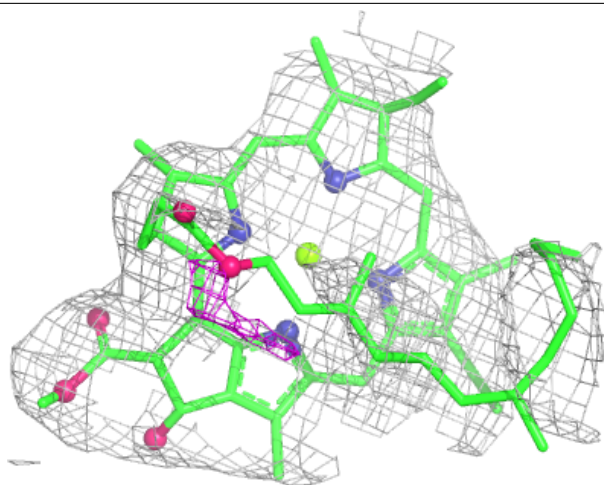
Electron density around CLA 1 206:

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



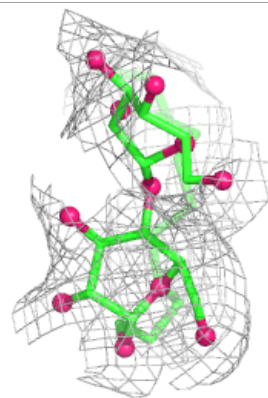
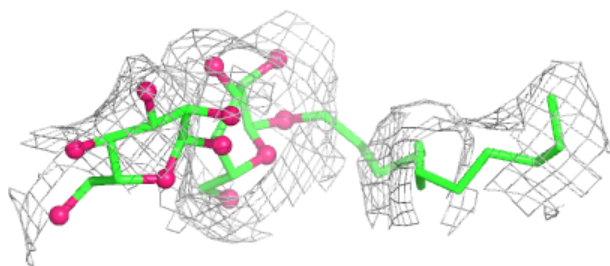
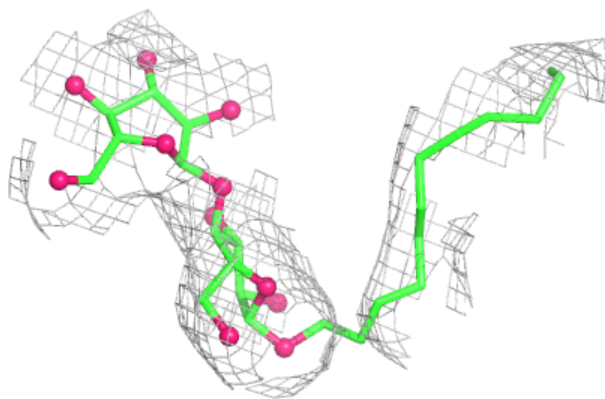
Electron density around CLA B 815:

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



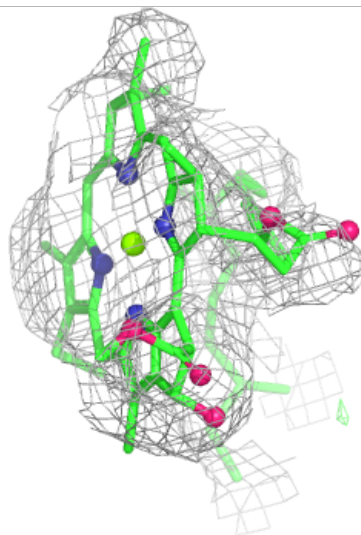
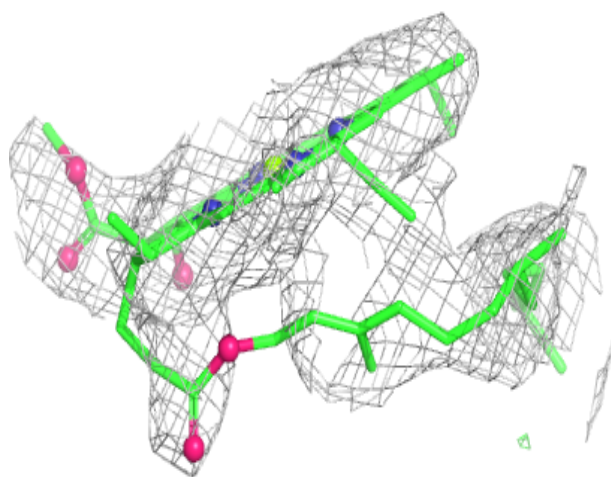
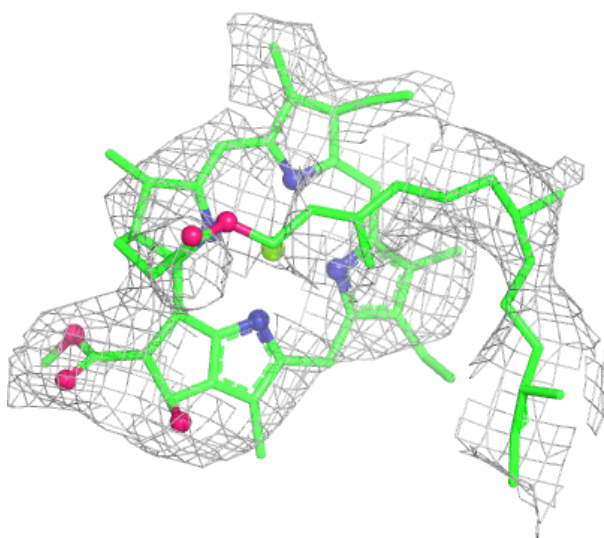
Electron density around LMU L 205:

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



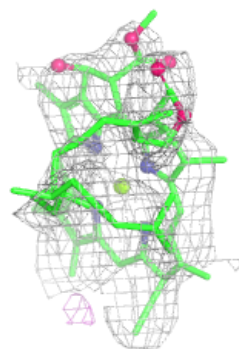
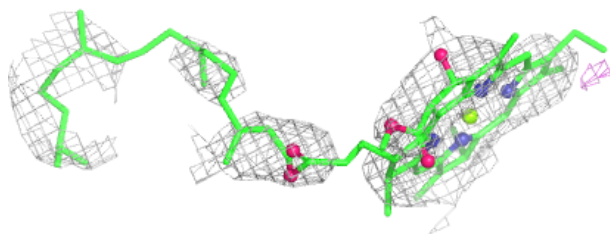
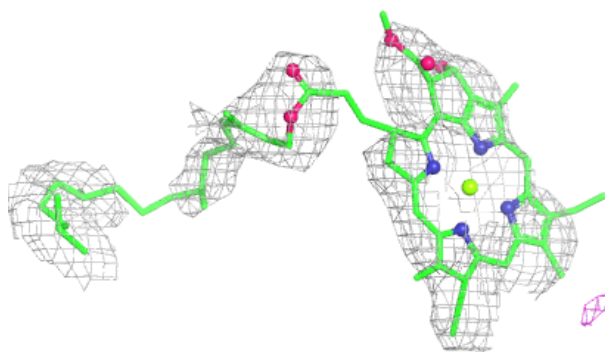
Electron density around CLA B 817:

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



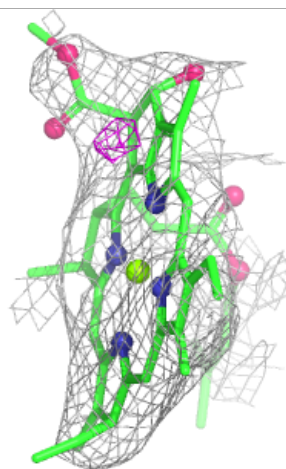
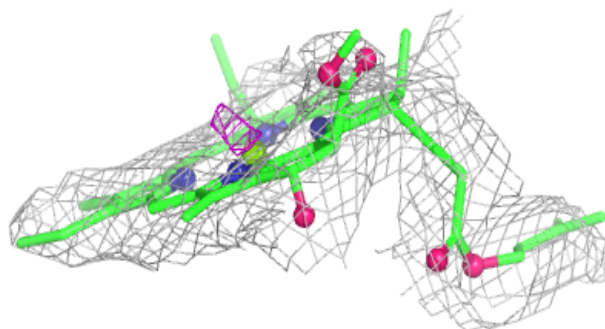
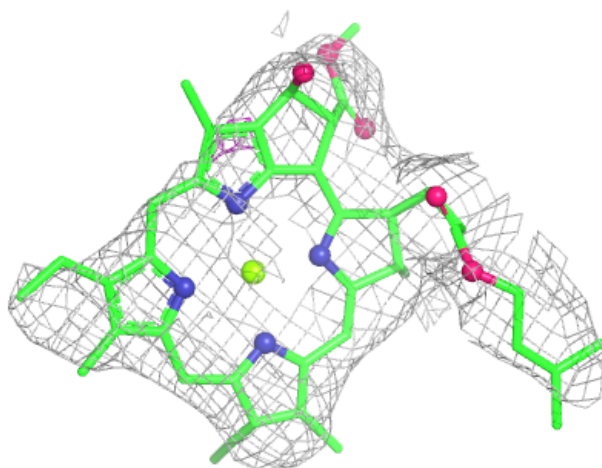
Electron density around CLA B 808:

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



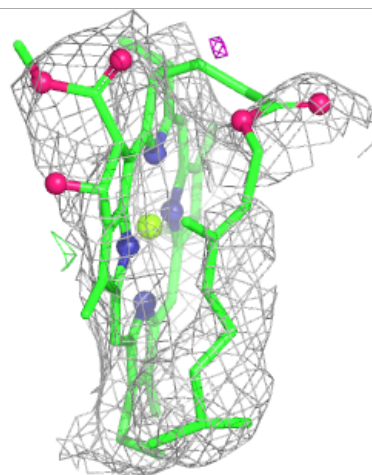
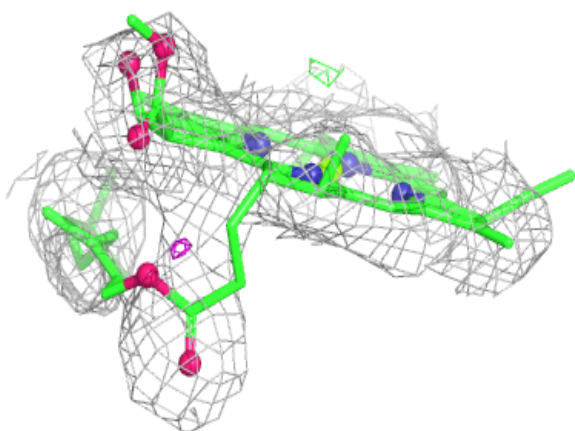
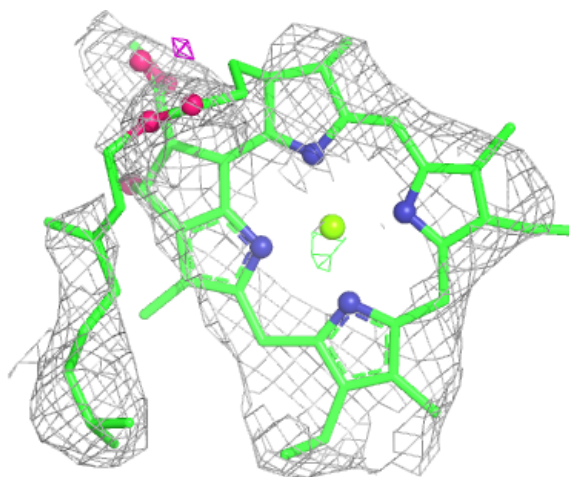
Electron density around CLA A 832:

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



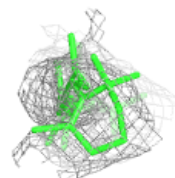
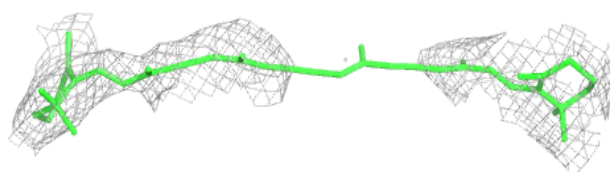
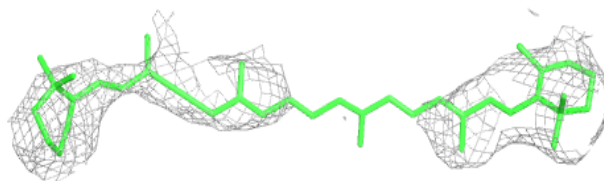
Electron density around CLA A 827:

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

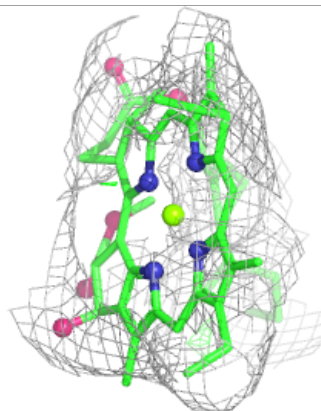
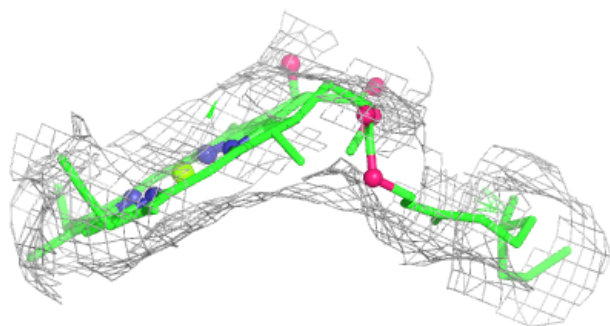
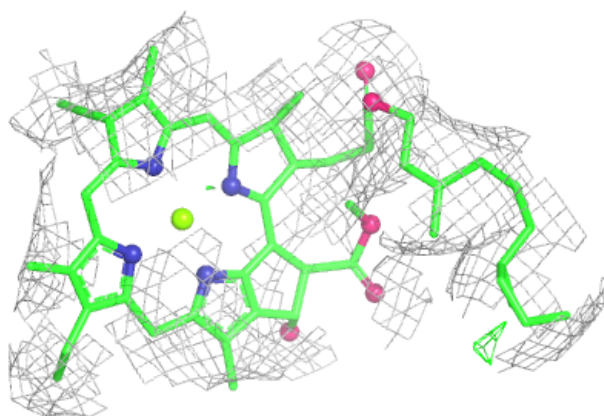


Electron density around BCR A 846:

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

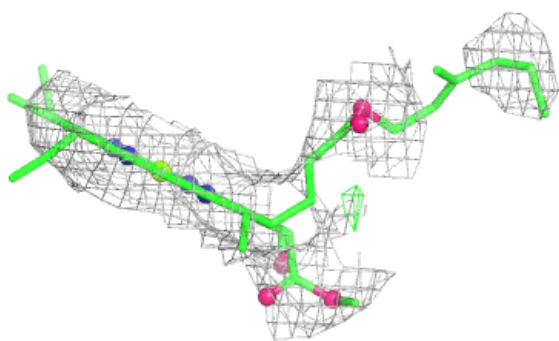
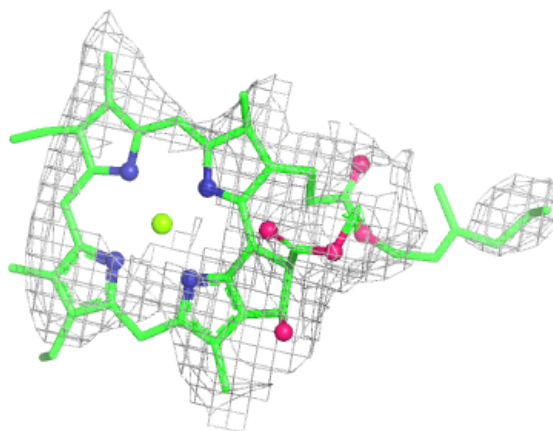
**Electron density around CLA 1 202:**

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

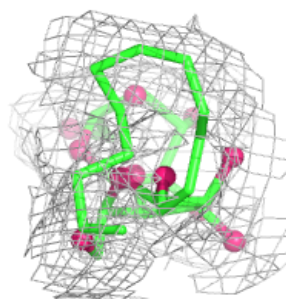
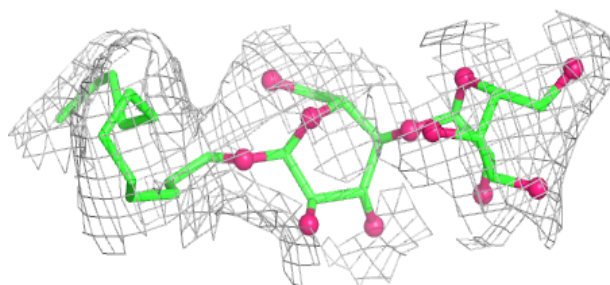
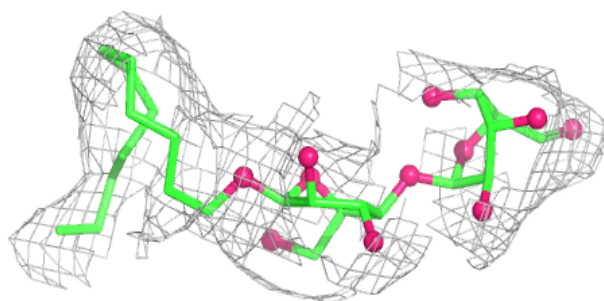


Electron density around CLA A 809:

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

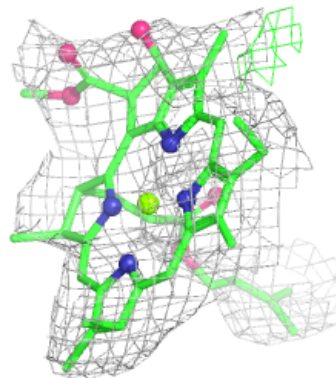
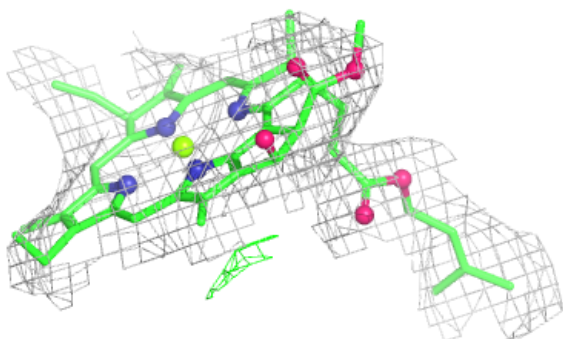
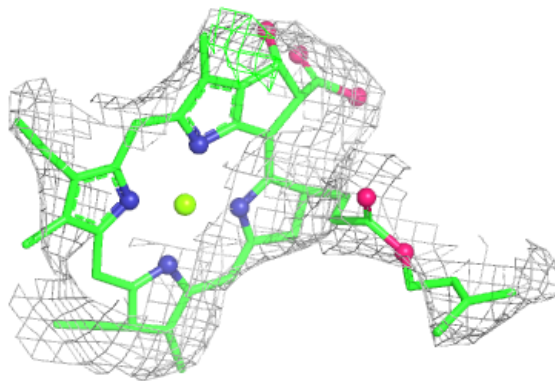
**Electron density around LMU A 855:**

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



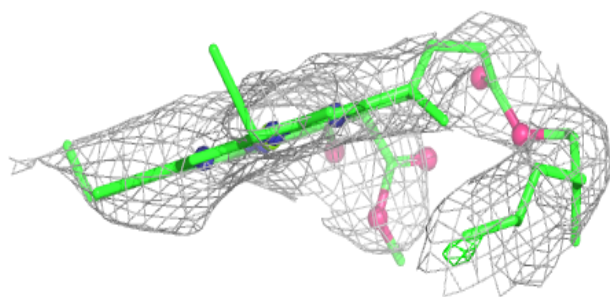
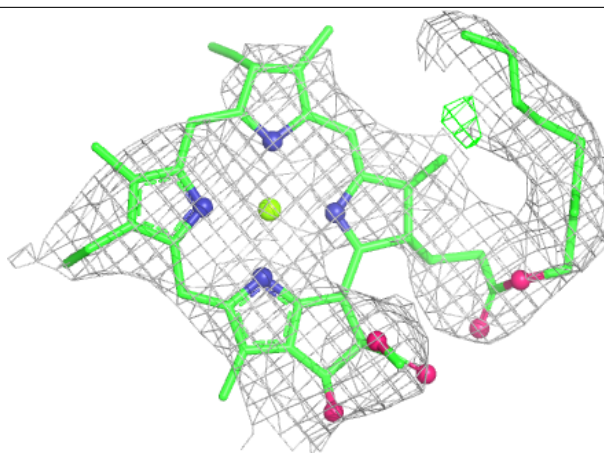
Electron density around CLA 2 311:

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



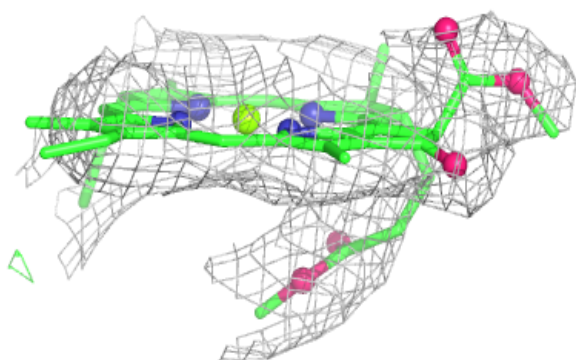
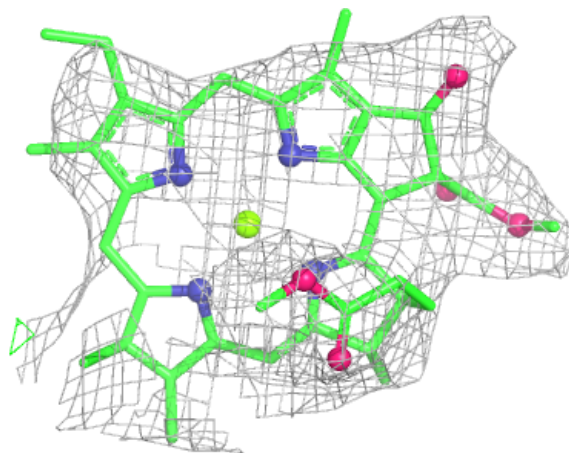
Electron density around CLA B 822:

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



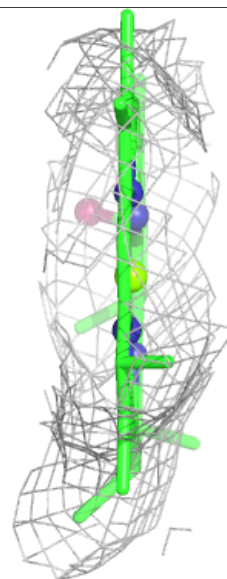
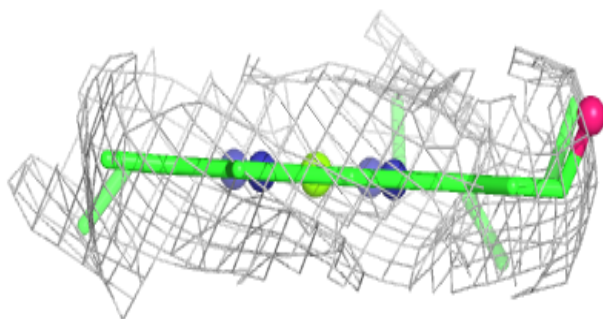
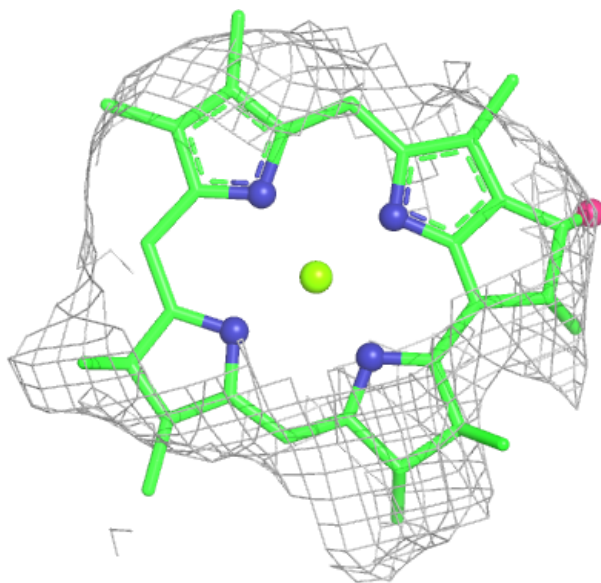
Electron density around CLA 1 204:

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



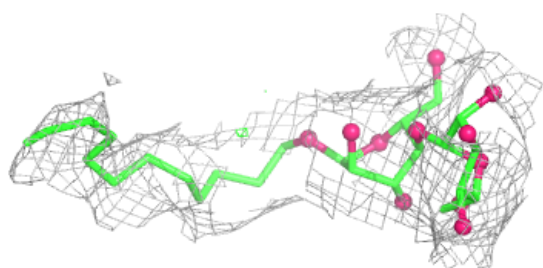
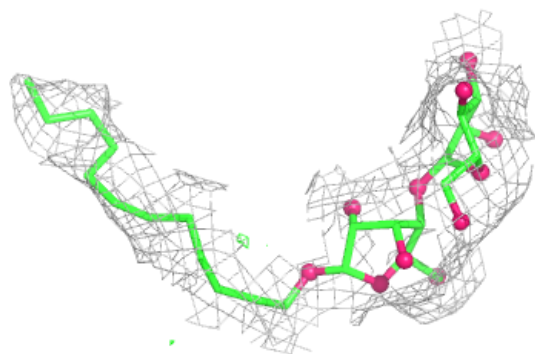
Electron density around CLA 3 304:

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

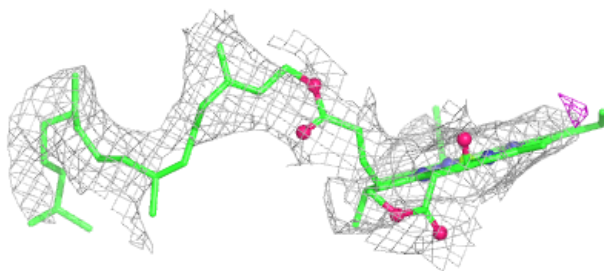
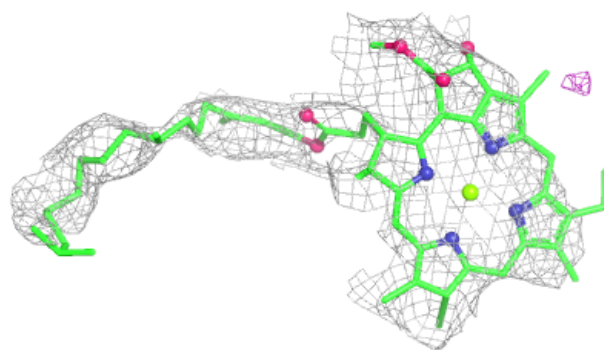


Electron density around LMU G 101:

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

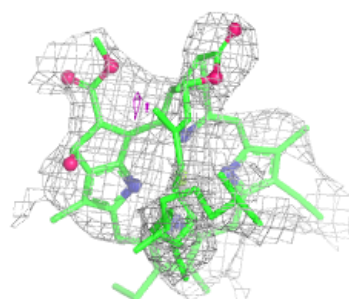
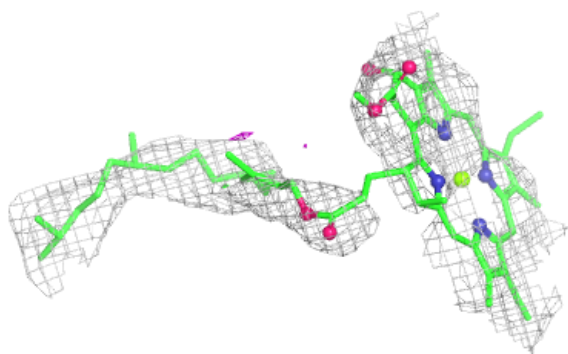
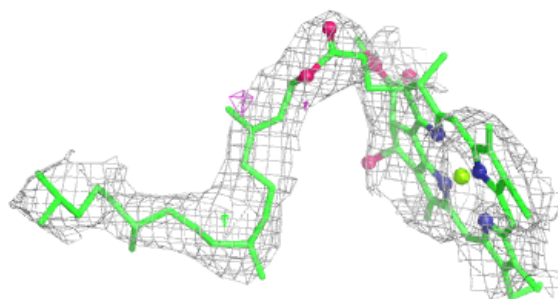
**Electron density around CLA A 824:**

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

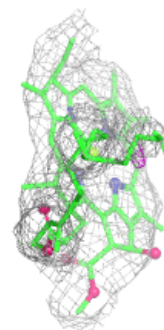
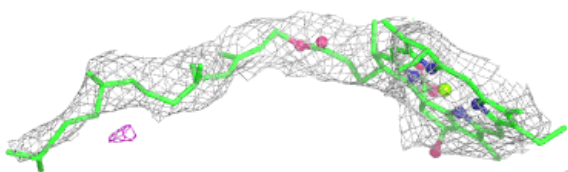
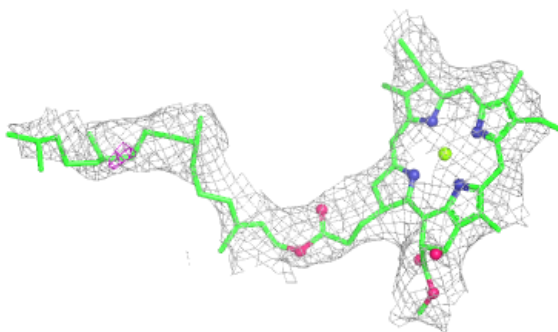


Electron density around CLA B 849:

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

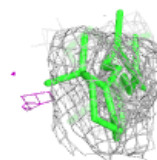
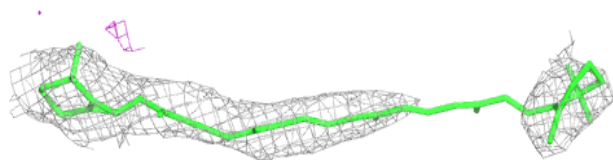
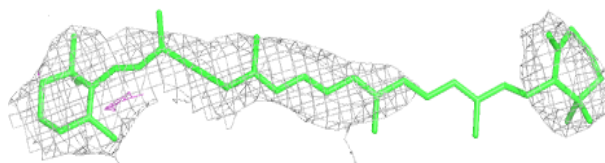
**Electron density around CLA B 850:**

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

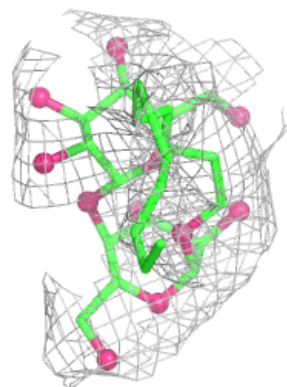
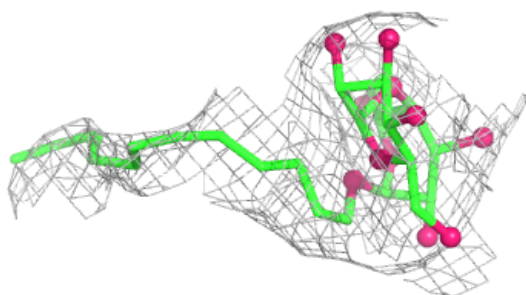
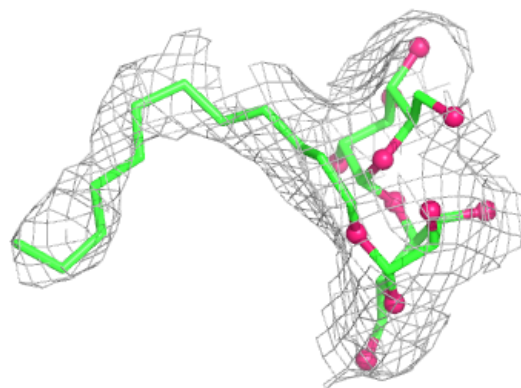


Electron density around BCR B 842:

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

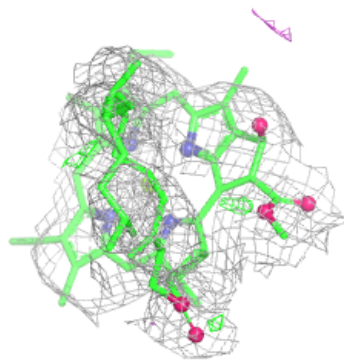
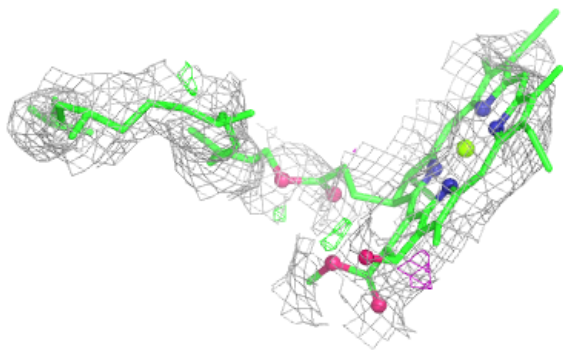
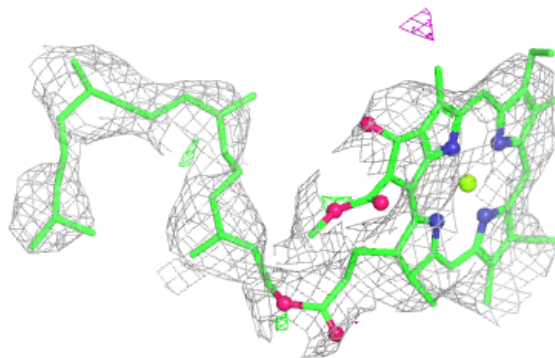
**Electron density around LMU H 106:**

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



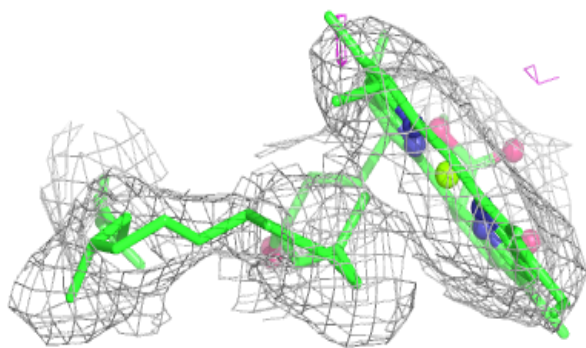
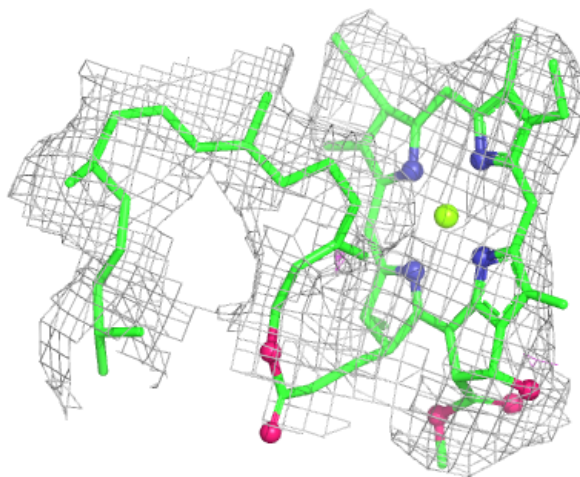
Electron density around CLA A 850:

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



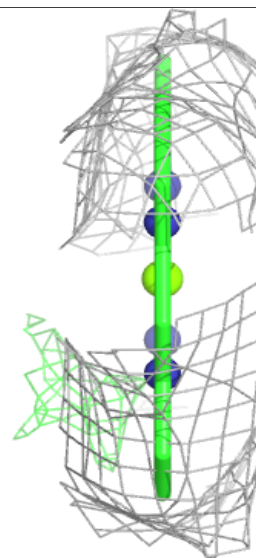
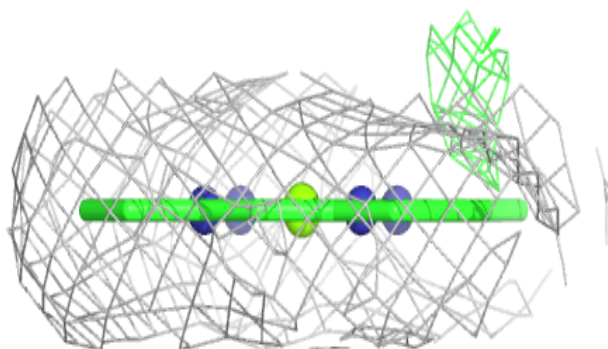
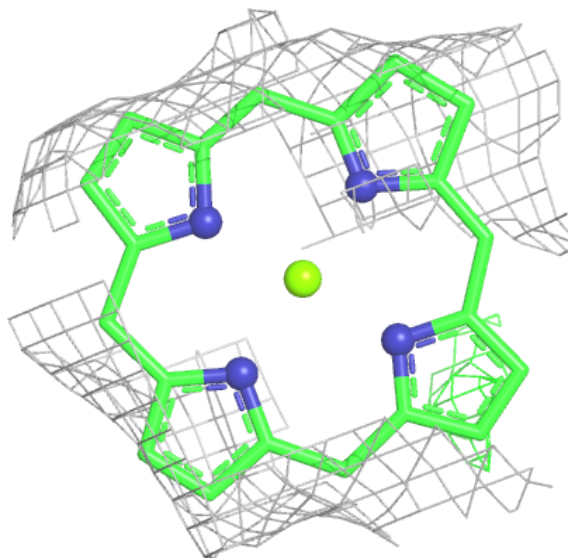
Electron density around CLA B 821:

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



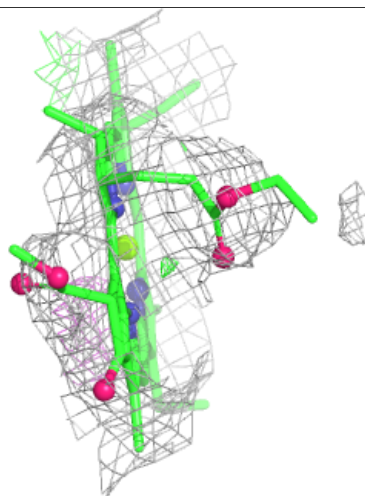
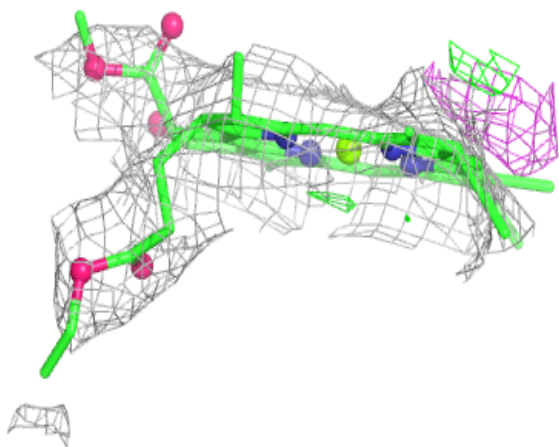
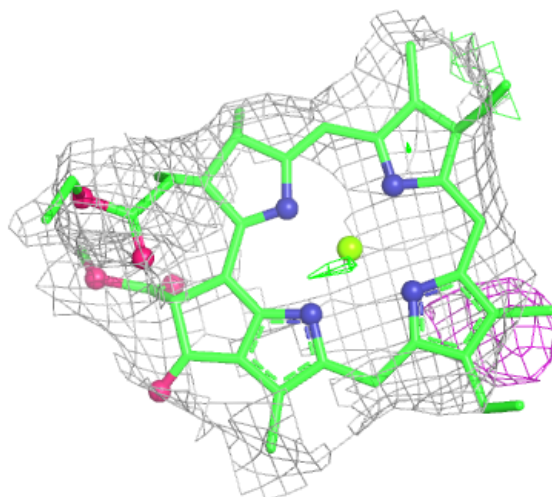
Electron density around CLA 1 214:

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



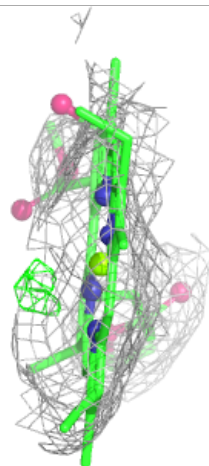
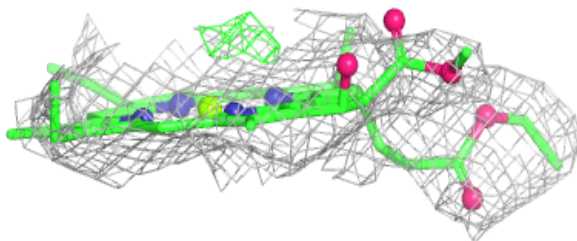
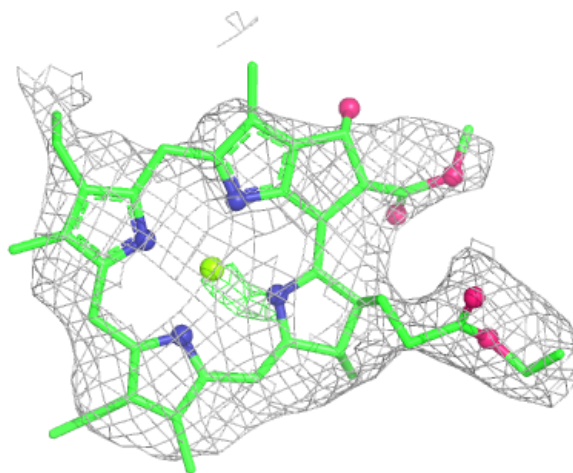
Electron density around CLA A 836:

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



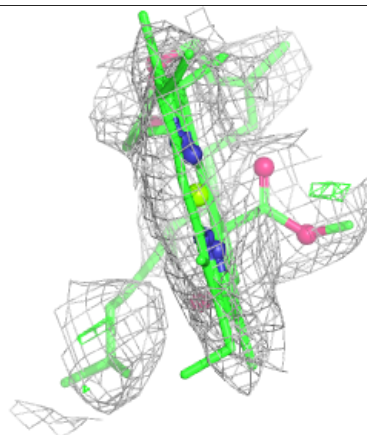
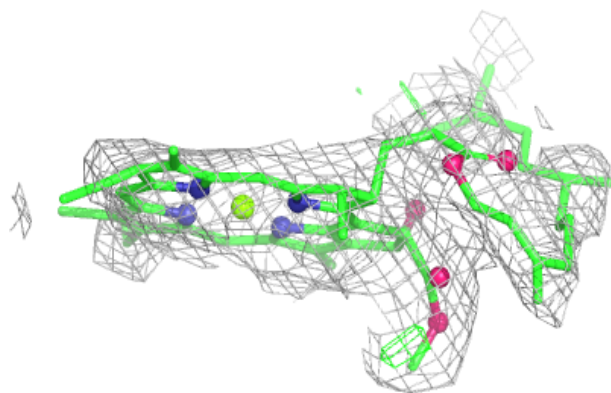
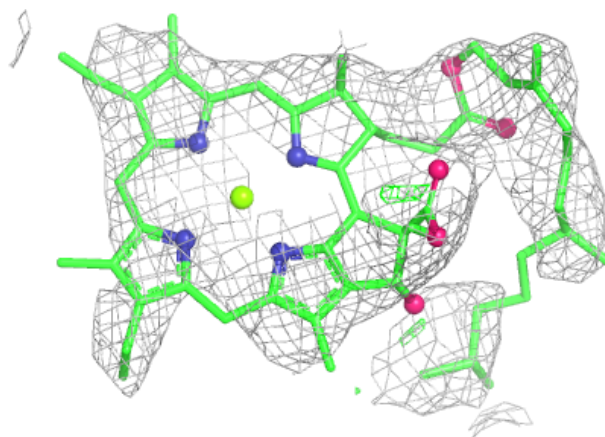
Electron density around CLA A 837:

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



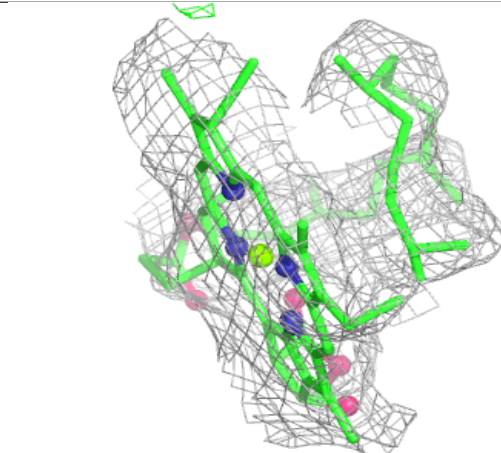
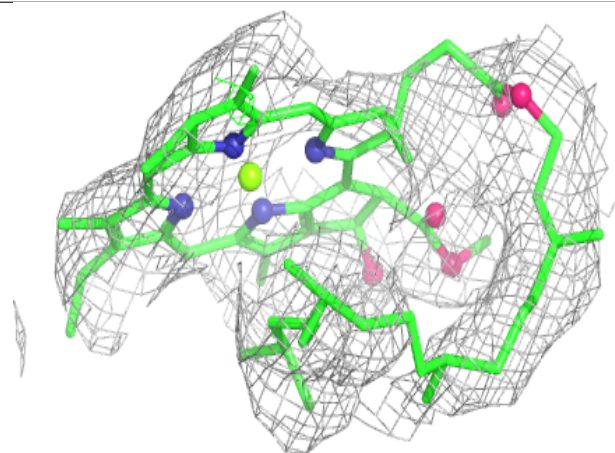
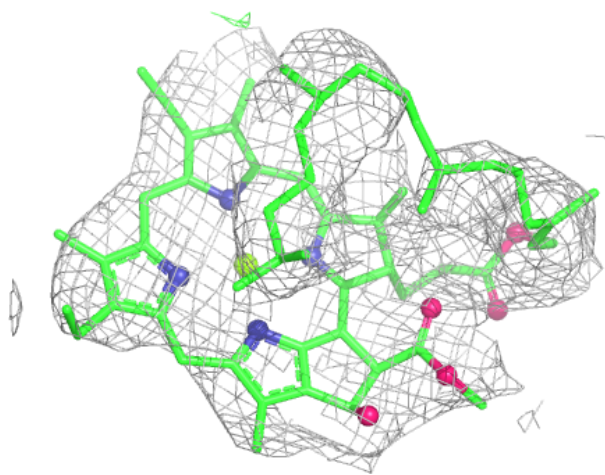
Electron density around CLA B 805:

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



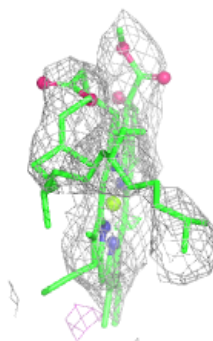
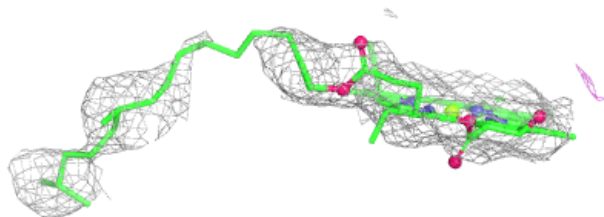
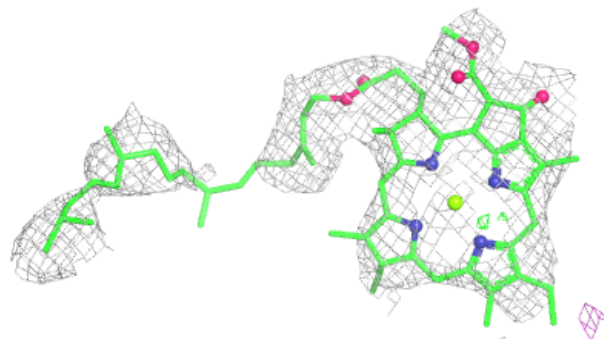
Electron density around CLA B 806:

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



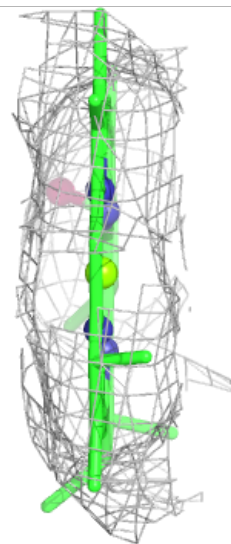
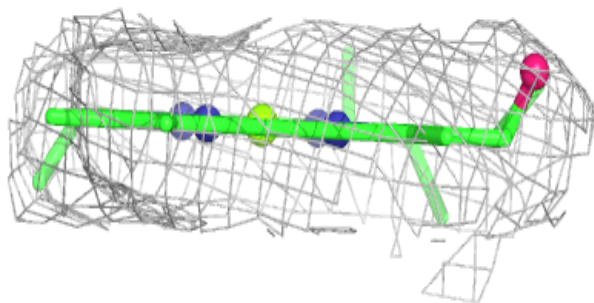
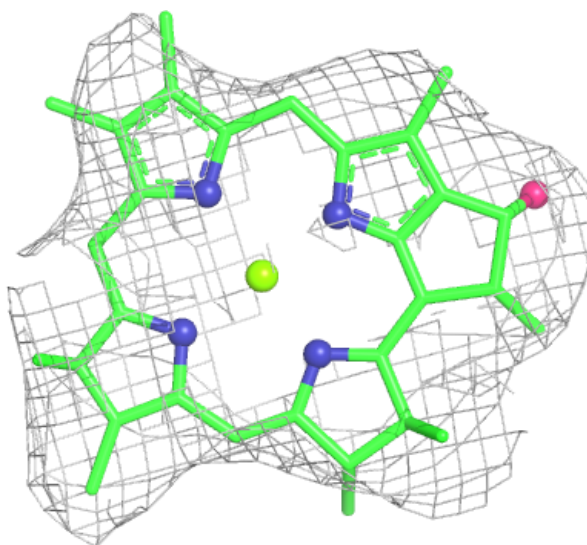
Electron density around CLA B 851:

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



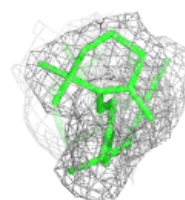
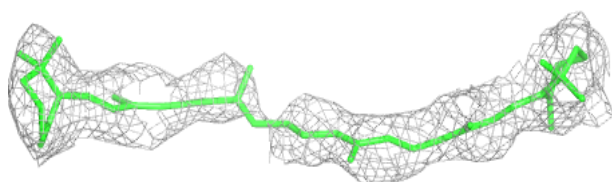
Electron density around CLA 4 314:

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

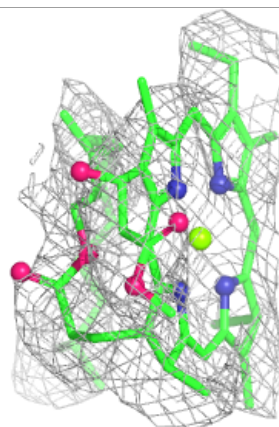
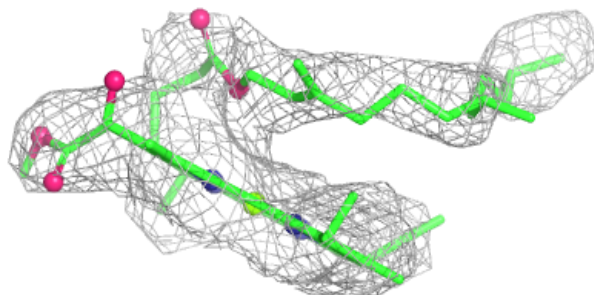
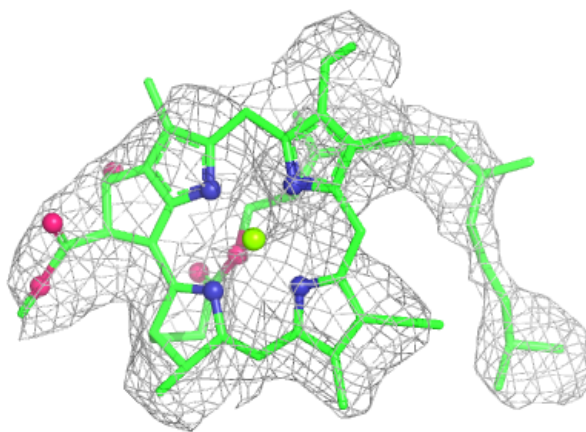


Electron density around BCR I 101:

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

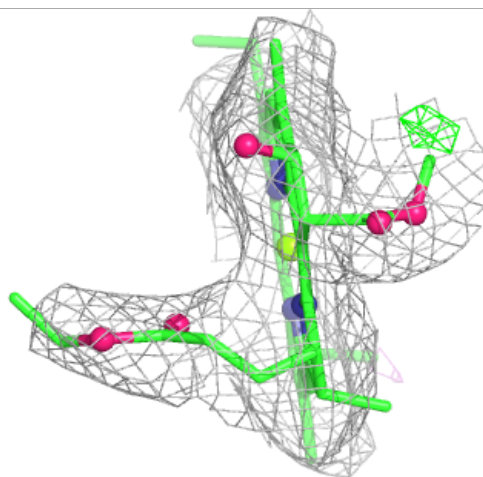
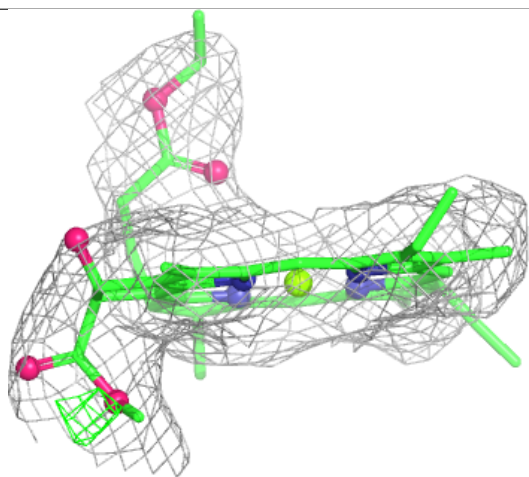
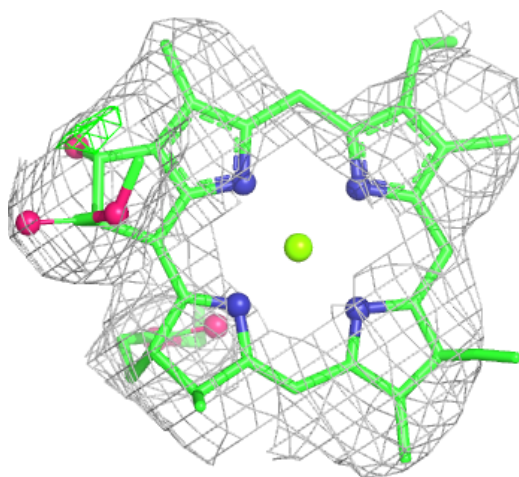
**Electron density around CLA I 102:**

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



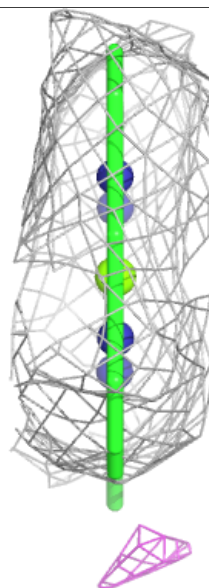
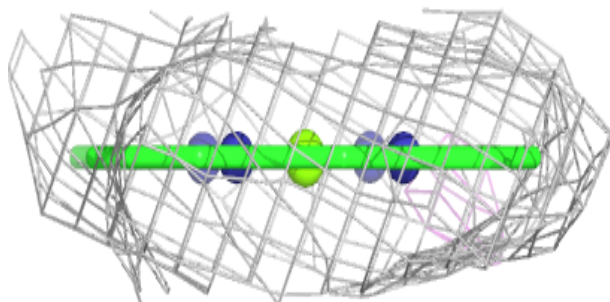
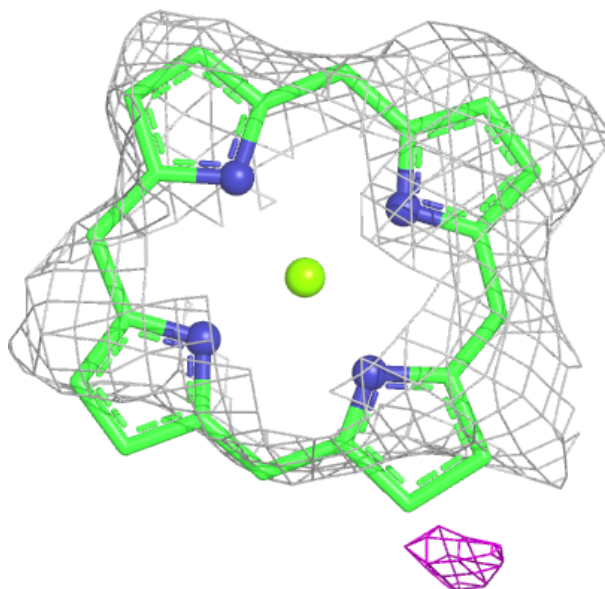
Electron density around CLA L 206:

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



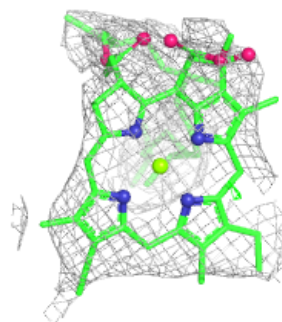
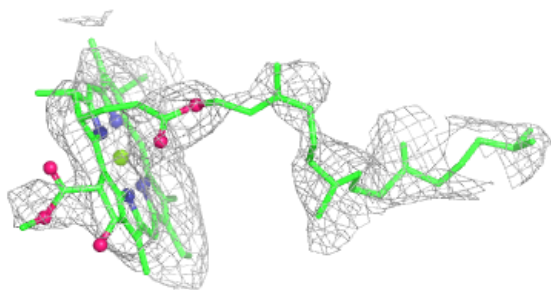
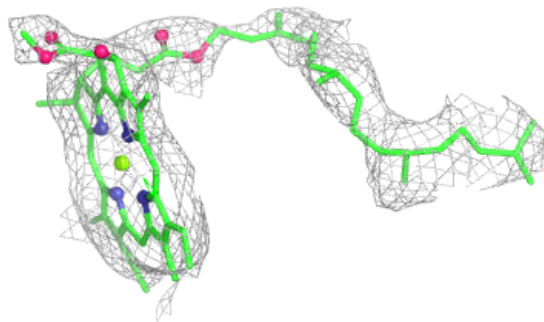
Electron density around CLA 2 314:

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



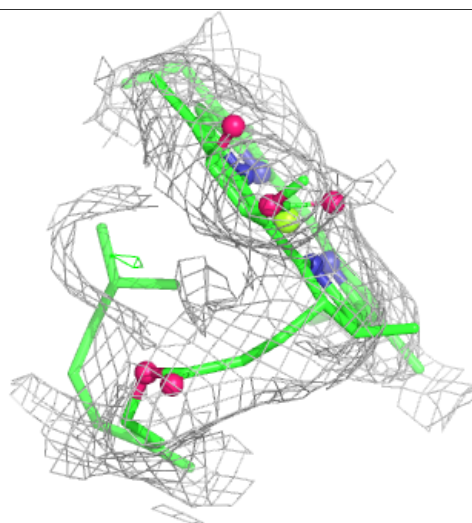
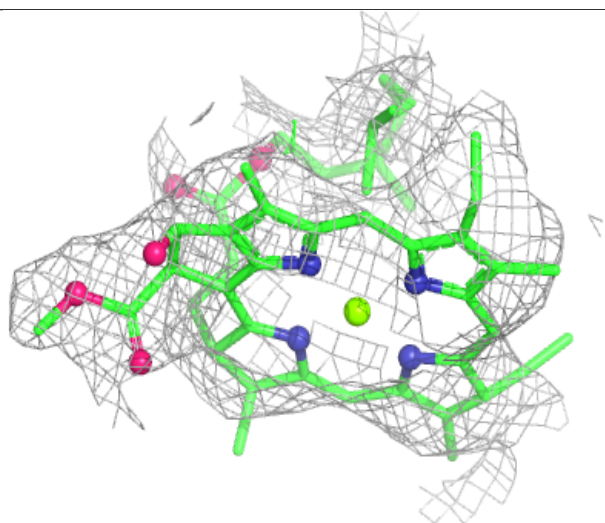
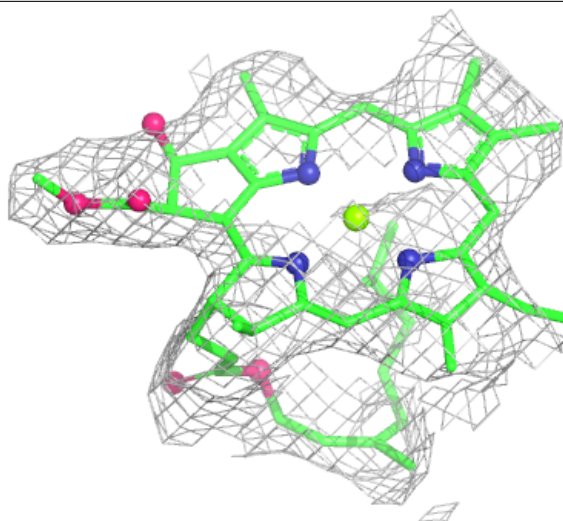
Electron density around CLA B 827:

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



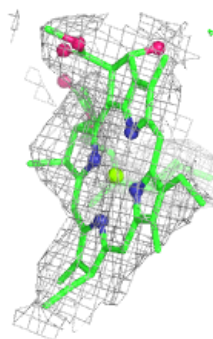
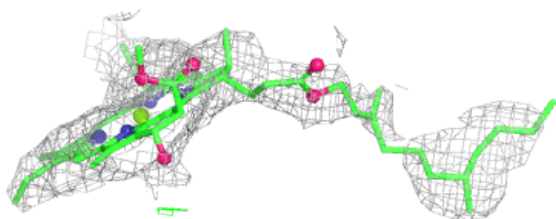
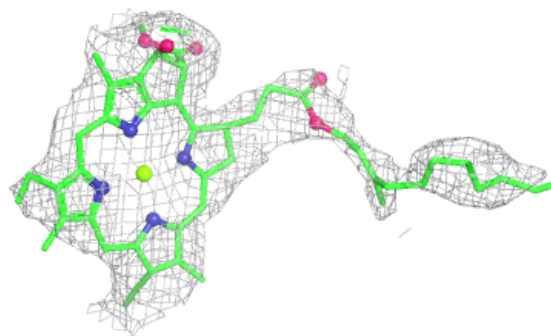
Electron density around CLA B 810:

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



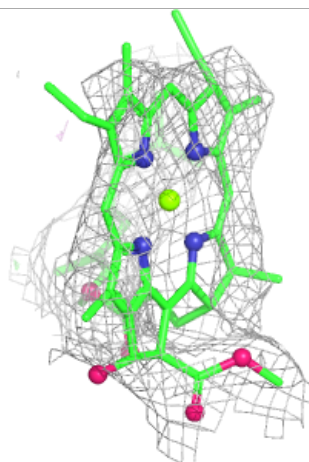
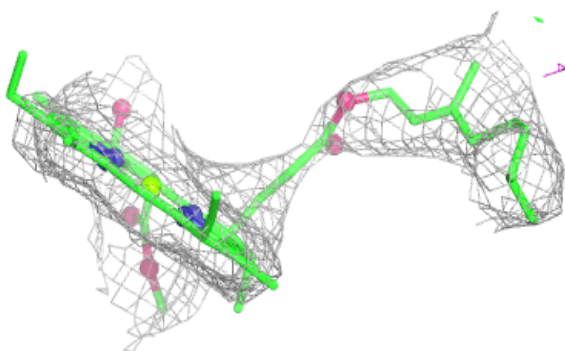
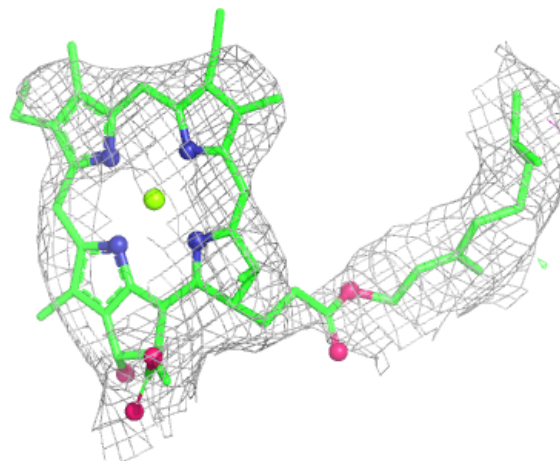
Electron density around CLA B 811:

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



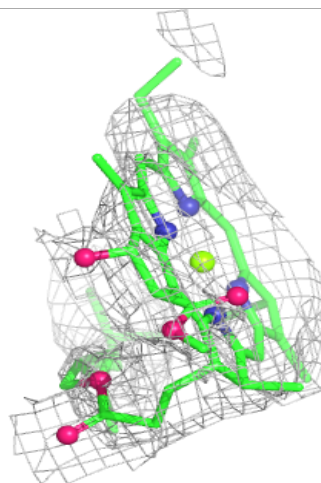
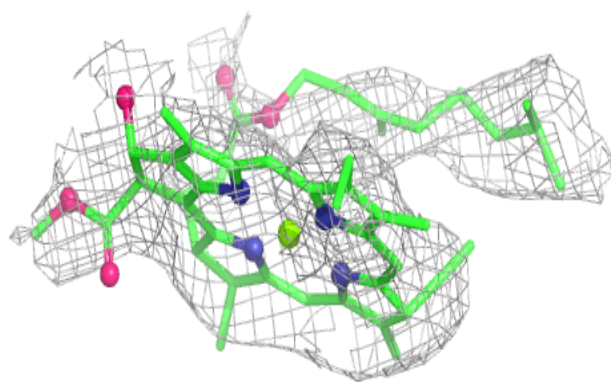
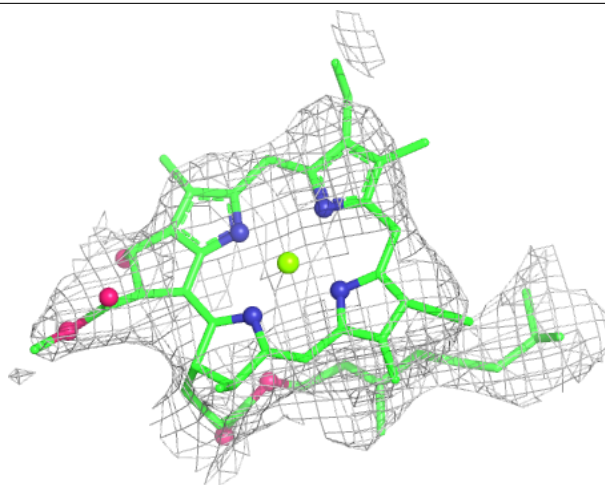
Electron density around CLA A 831:

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



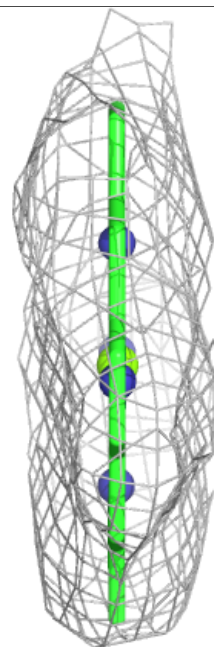
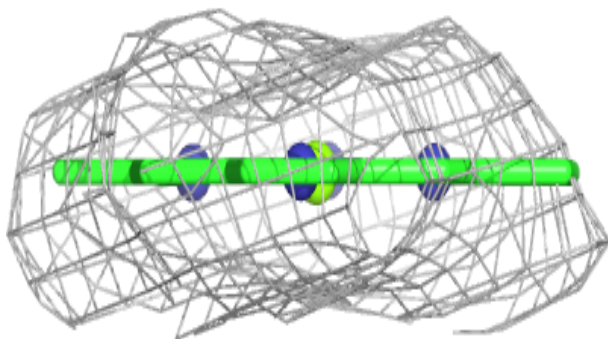
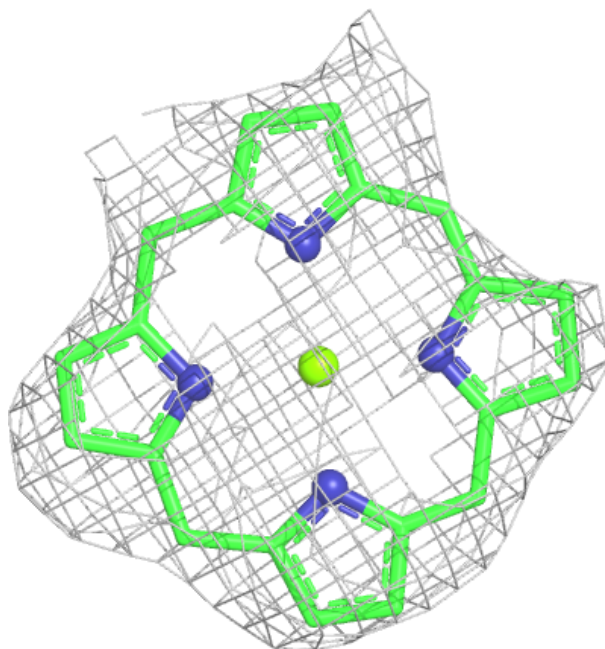
Electron density around CLA B 820:

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



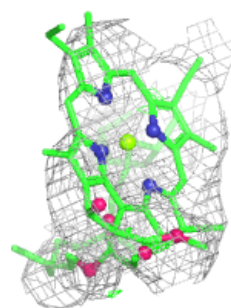
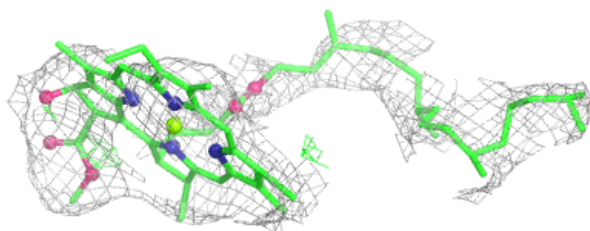
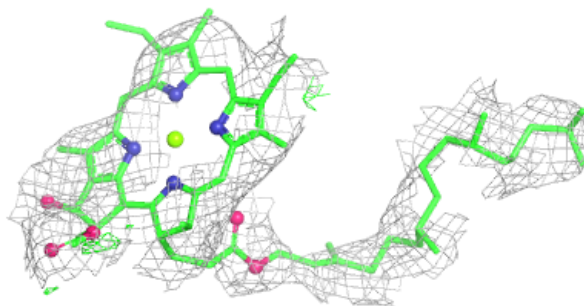
Electron density around CLA 4 313:

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



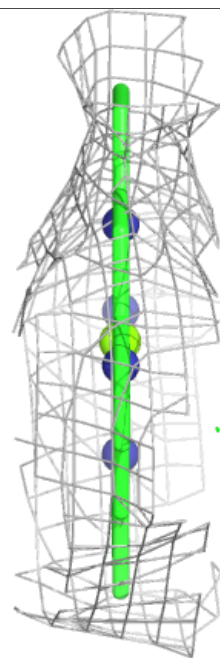
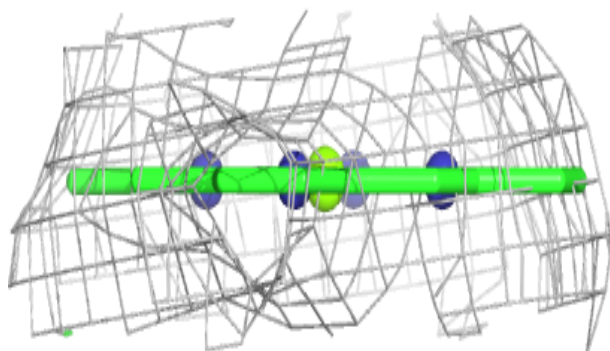
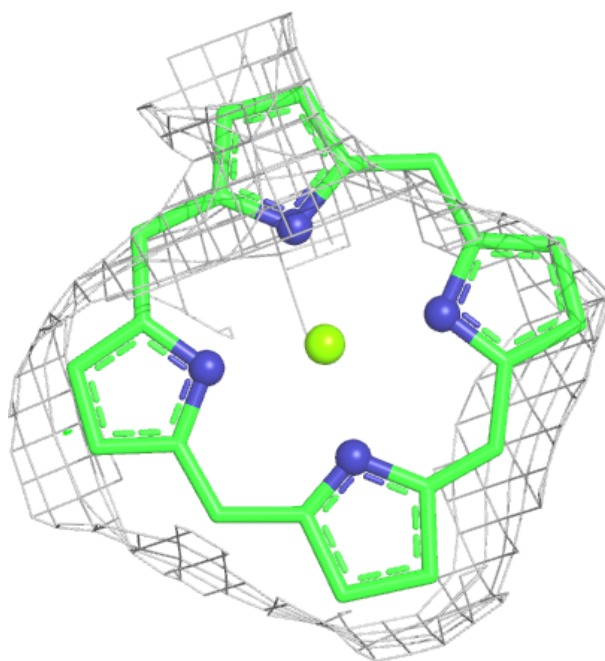
Electron density around CLA A 808:

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



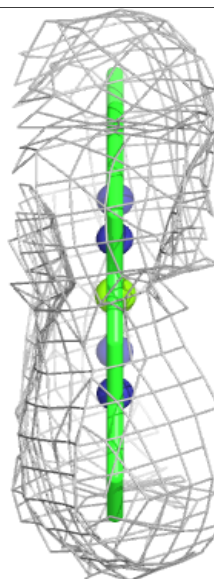
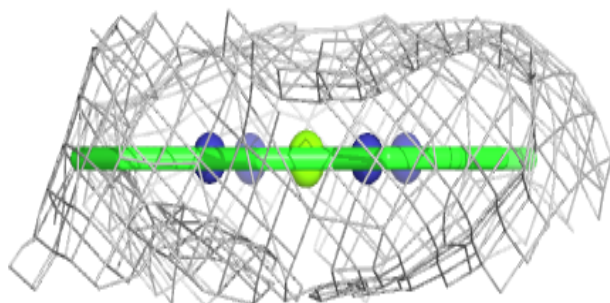
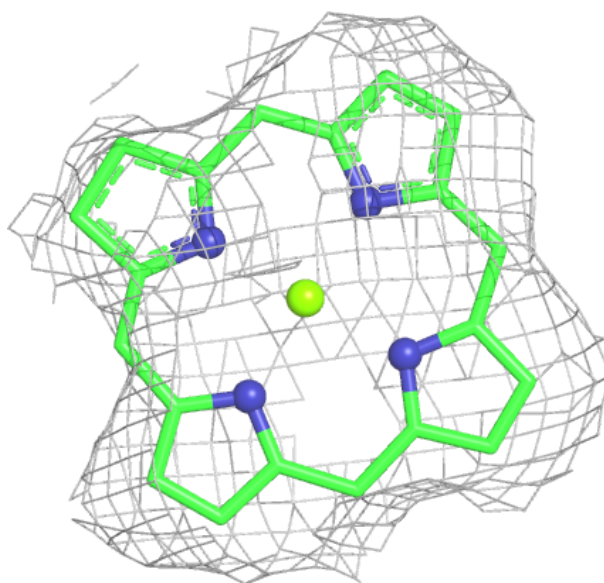
Electron density around CLA 4 312:

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



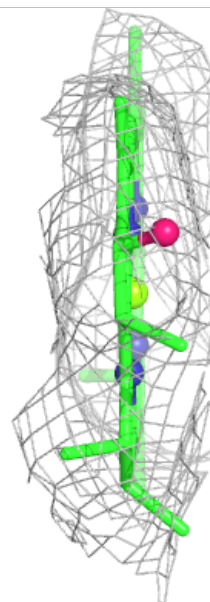
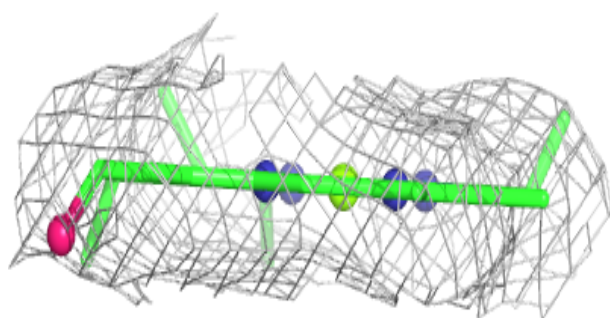
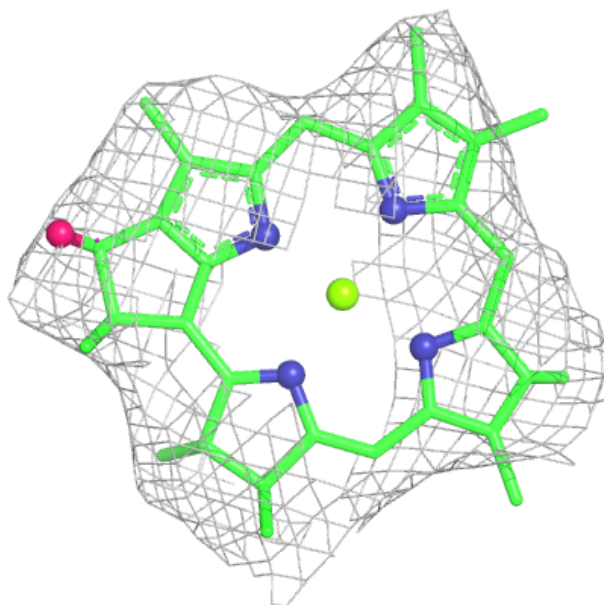
Electron density around CLA 4 315:

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



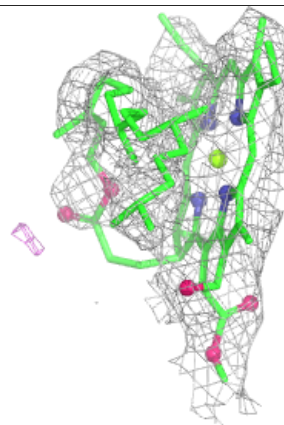
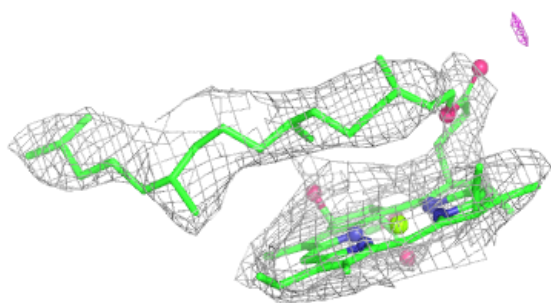
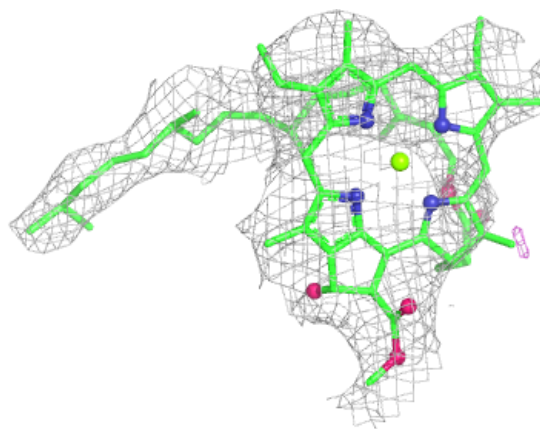
Electron density around CLA 1 209:

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

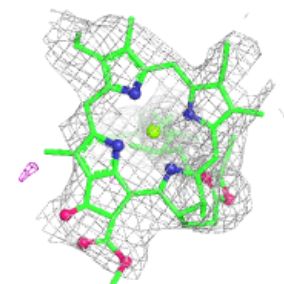
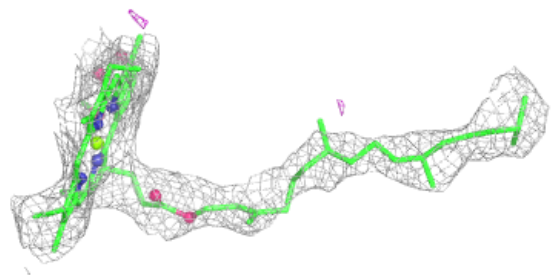
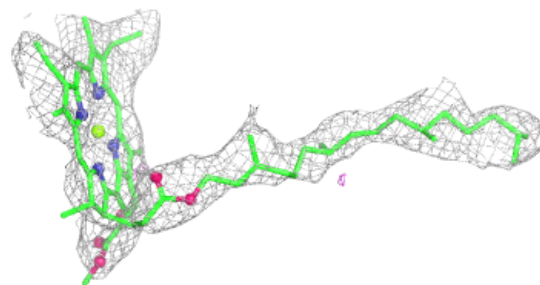


Electron density around CLA B 825:

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

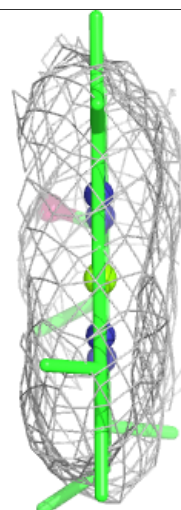
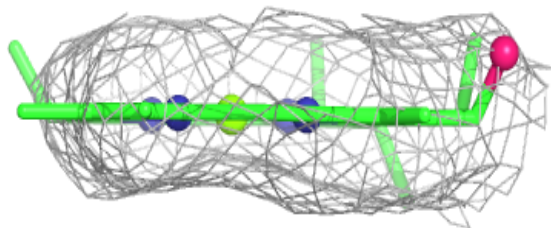
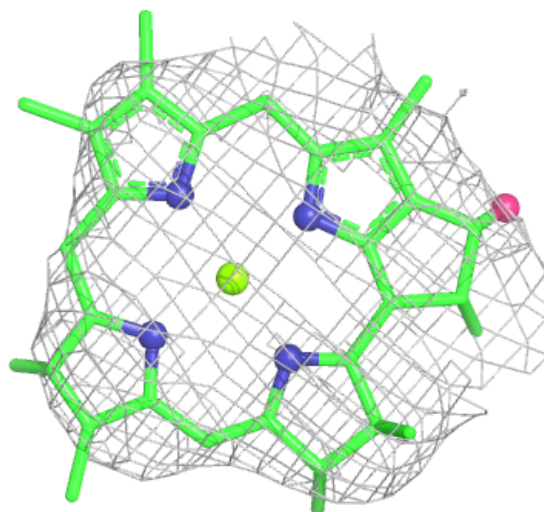
**Electron density around CLA B 826:**

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



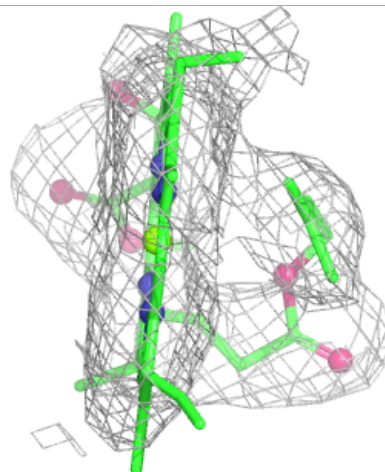
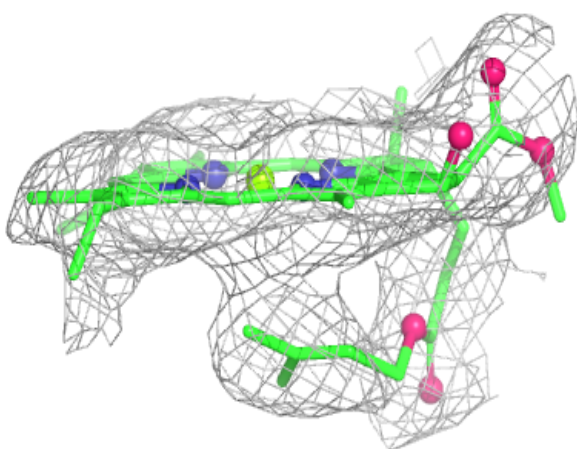
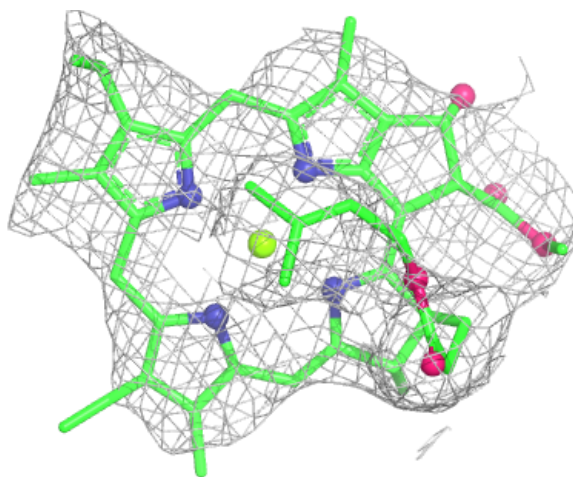
Electron density around CLA 4 303:

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



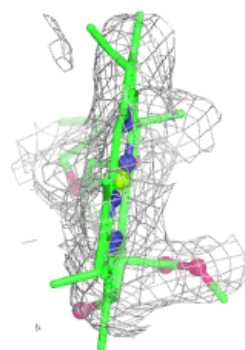
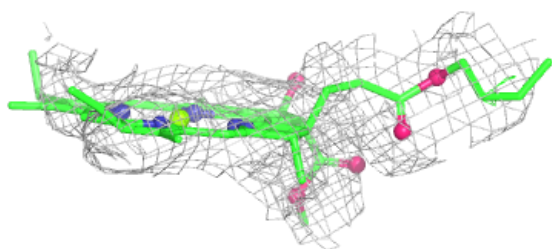
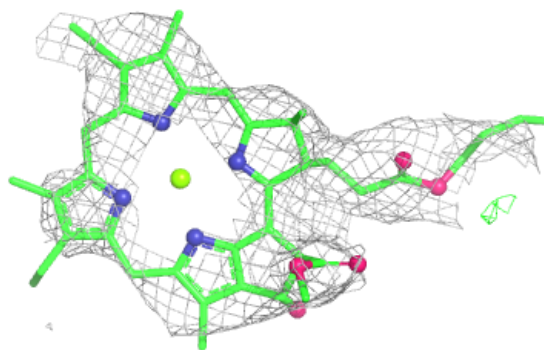
Electron density around CLA B 828:

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

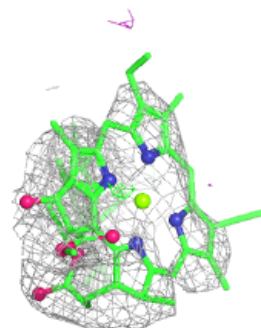
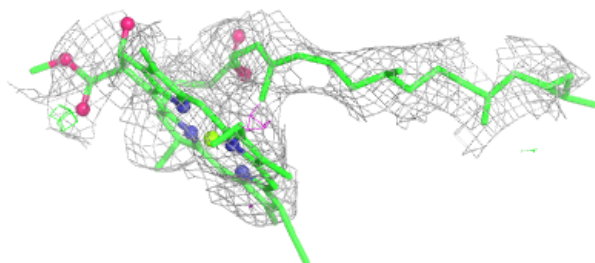
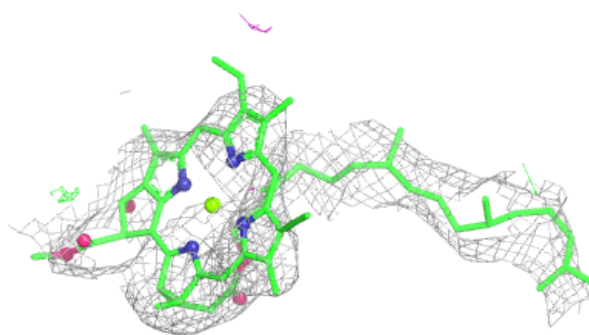


Electron density around CLA A 834:

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

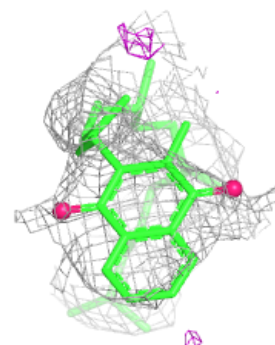
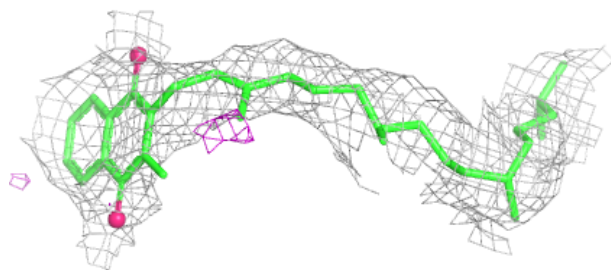
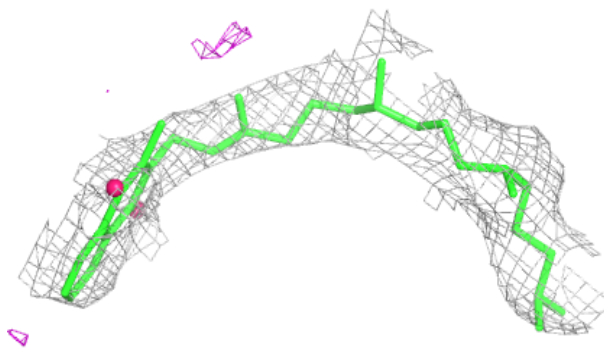
**Electron density around CLA A 838:**

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



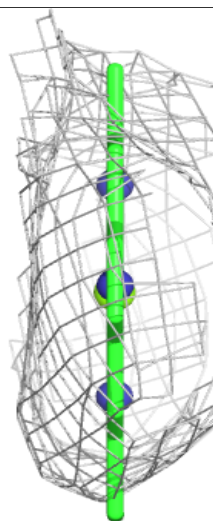
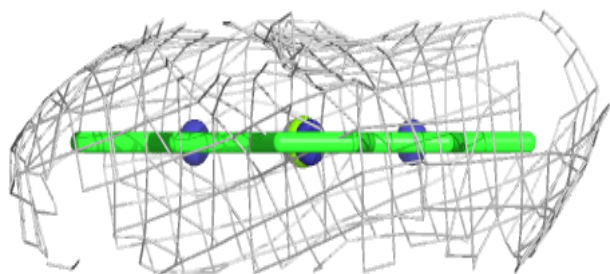
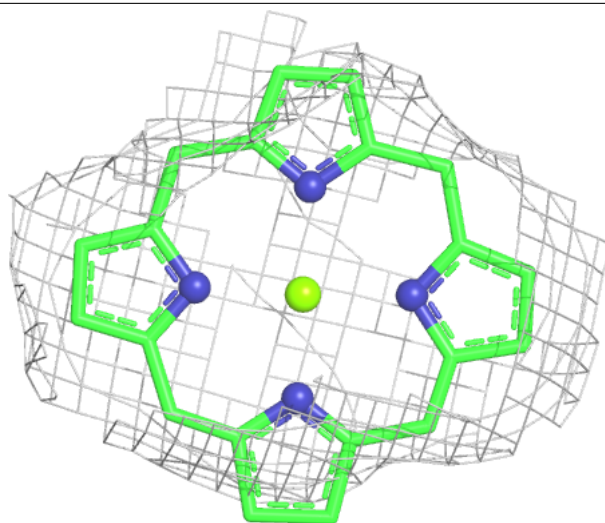
Electron density around PQN B 841:

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



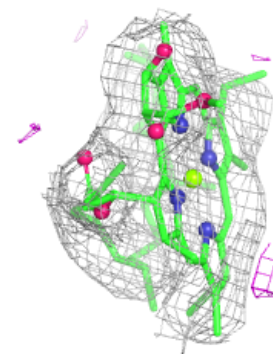
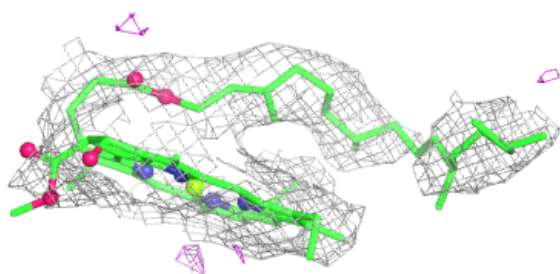
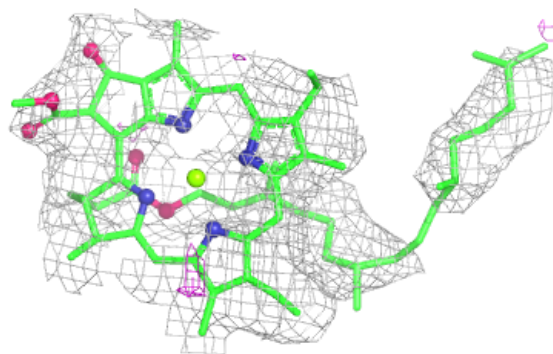
Electron density around CLA 2 309:

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



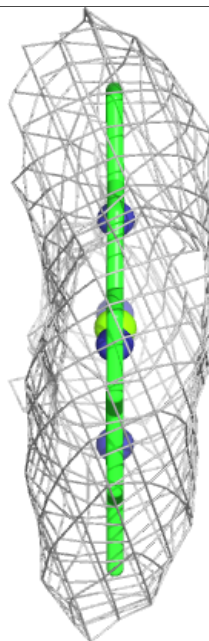
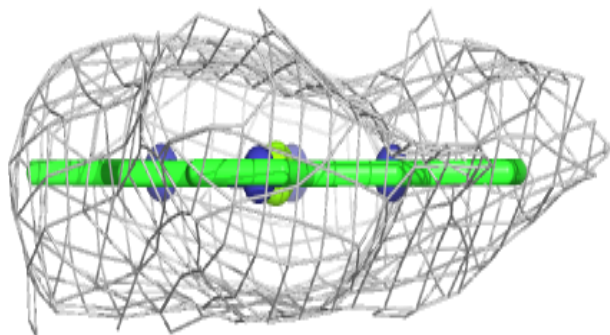
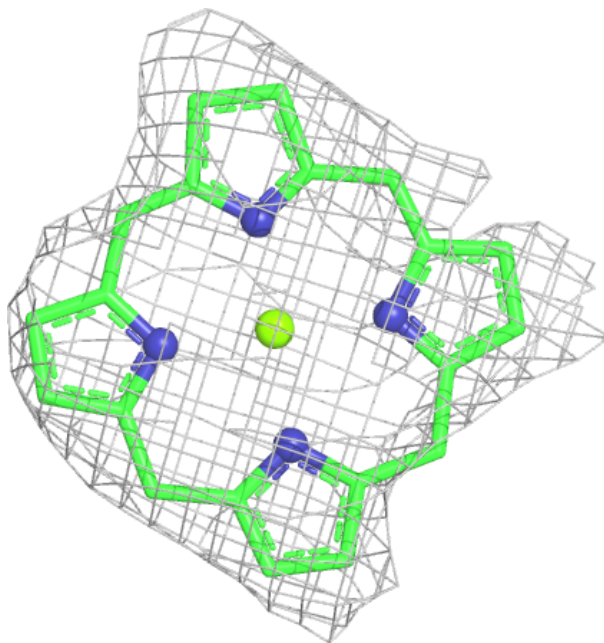
Electron density around CLA B 836:

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



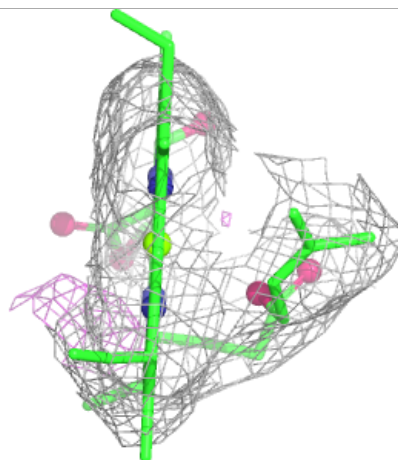
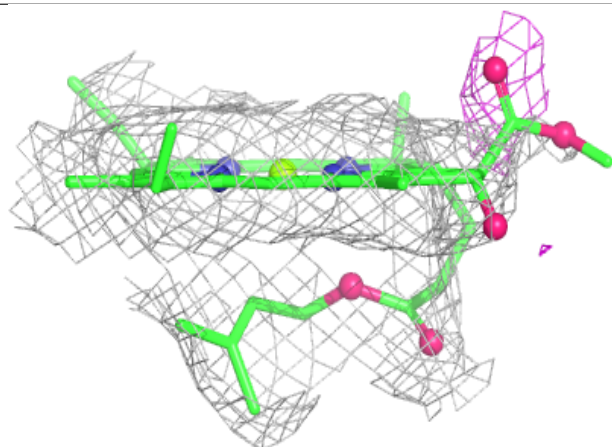
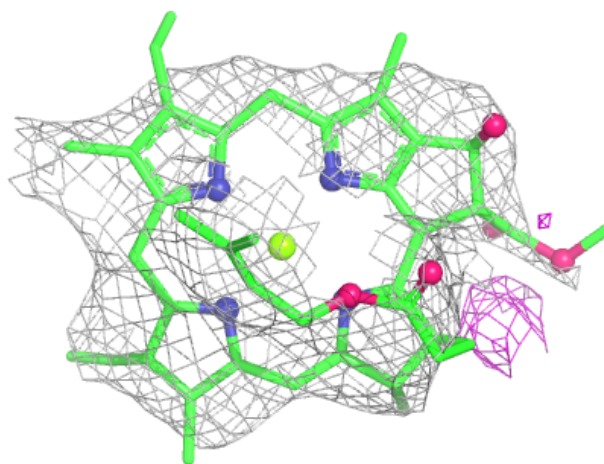
Electron density around CLA 1 208:

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



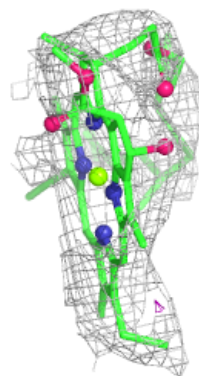
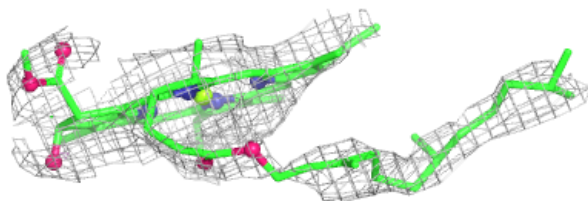
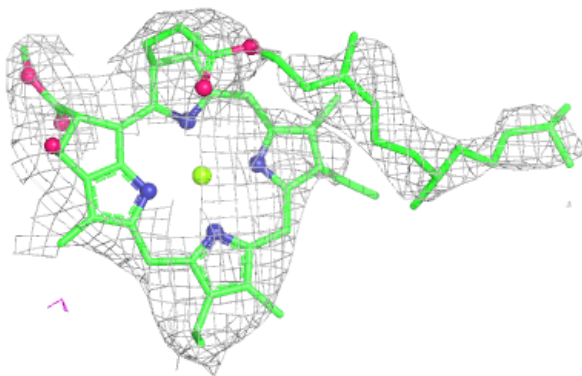
Electron density around CLA B 818:

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

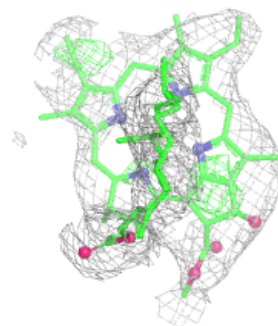
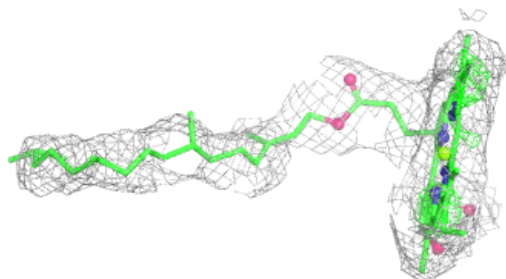
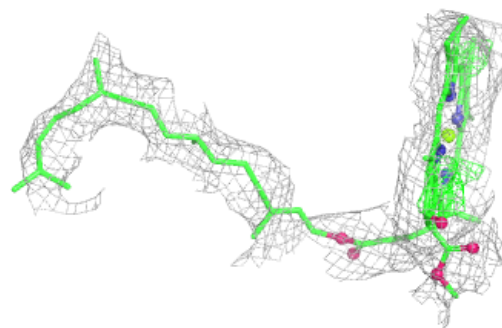


Electron density around CLA B 816:

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

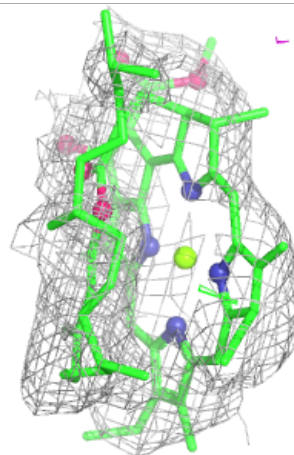
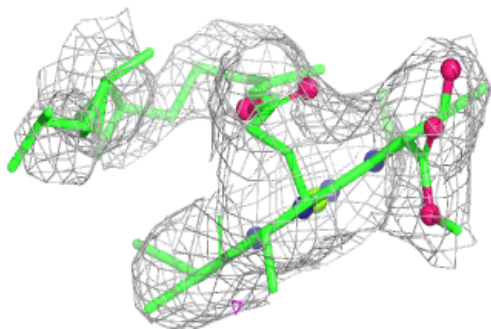
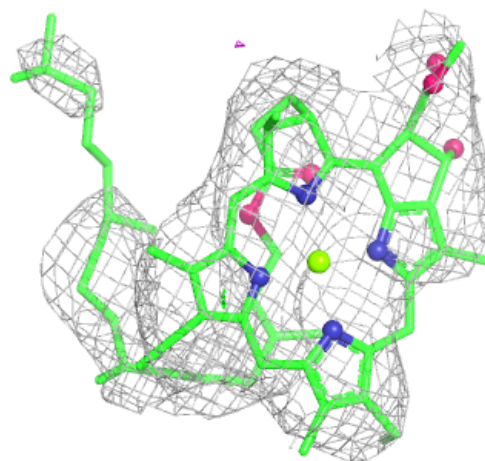
**Electron density around CLA B 839:**

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



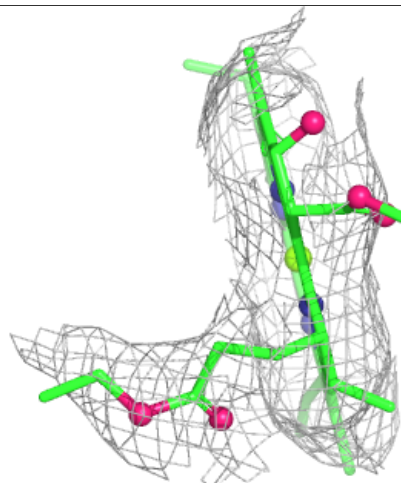
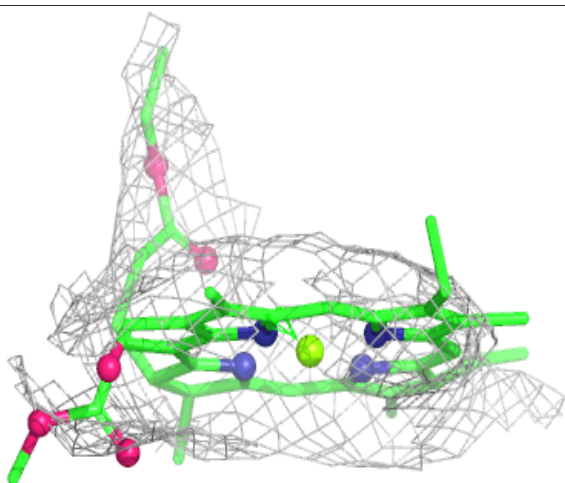
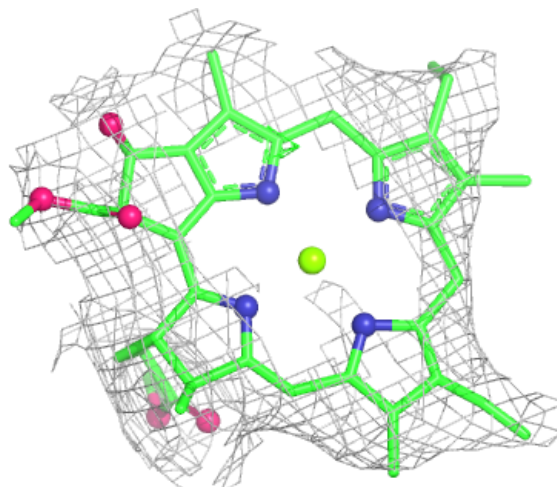
Electron density around CLA B 807:

$2mF_o-DF_c$ (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.