wwPDB X-ray Structure Validation Summary Report (i)

Sep 10, 2026 – 05:29 pm BST

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

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) 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 (i)) were used in the production of this report:

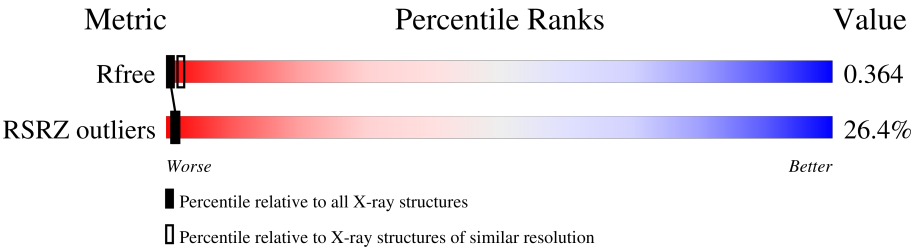
MolProbity	:	FAILED
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.015 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)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

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 3.30 Å.

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



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

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

2 Entry composition (i)

There are 26 unique types of molecules in this entry. The entry contains 36379 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called AT3G54890.

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

There are 2 discrepancies between the modelled and reference sequences:

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

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

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

There are 2 discrepancies between the modelled and reference sequences:

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

- Molecule 3 is a protein called LHCA3.

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

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

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

There is a discrepancy between the modelled and reference sequences:

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

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

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

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

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

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

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

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

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

There are 8 discrepancies between the modelled and reference sequences:

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

There is a discrepancy between the modelled and reference sequences:

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

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

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

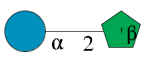
- Molecule 17 is a protein called PHOTOSYSTEM I-N SUBUNIT.

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

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

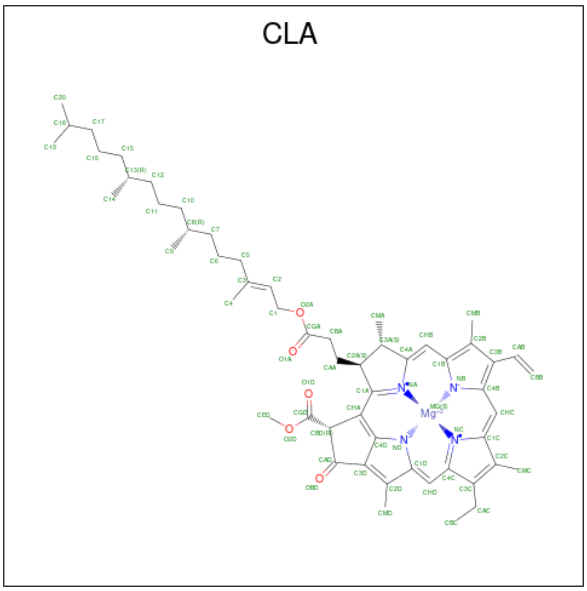
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
18	R	53	Total	C	N	O	0	0	0
			265	159	53	53			

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



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

- Molecule 20 is CHLOROPHYLL A (CCD ID: CLA) (formula: $C_{55}H_{72}MgN_4O_5$).



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

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

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

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
20	4	1	Total	C	Mg	N	O	0	0
			47	37	1	4	5		
20	A	1	Total	C	Mg	N	O	0	0
			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
			57	47	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
			55	45	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
			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
			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		
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		

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

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

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

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

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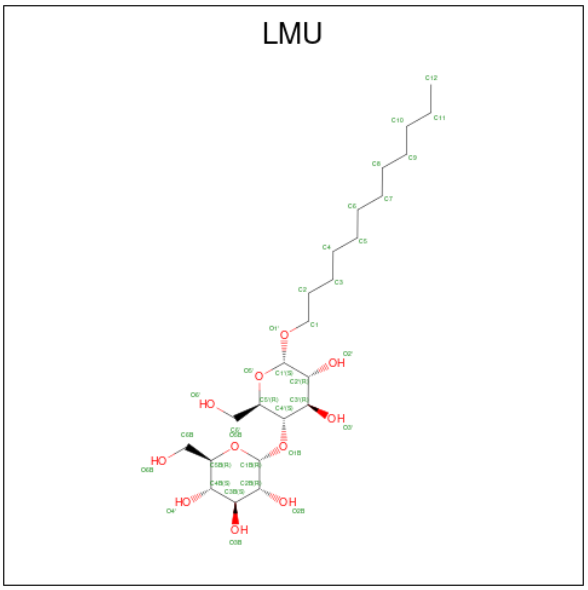
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
20	L	1	Total	C	Mg	N	O	0	0
			47	37	1	4	5		
20	L	1	Total	C	Mg	N	O	0	0
			50	40	1	4	5		
20	R	1	Total	C	Mg	N	O	0	0
			57	47	1	4	5		
20	R	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		

- Molecule 21 is DODECYL-ALPHA-D-MALTOSIDE (CCD ID: LMU) (formula: $C_{24}H_{46}O_{11}$).



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

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

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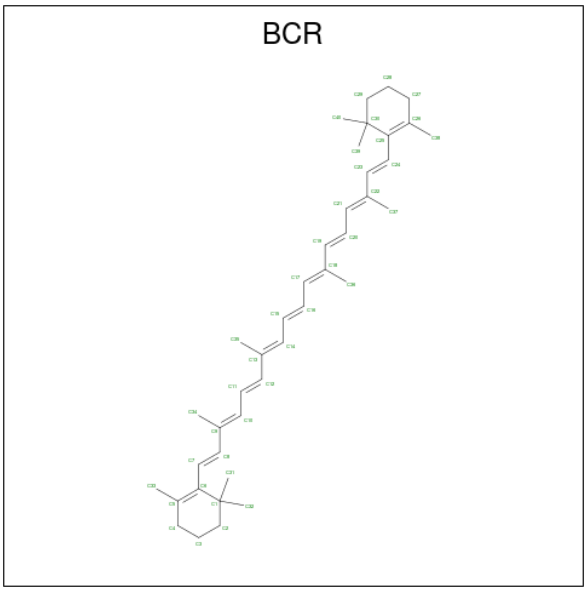
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
21	H	1	Total C O 35 24 11	0	0
21	H	1	Total C O 35 24 11	0	0
21	H	1	Total C O 35 24 11	0	0
21	H	1	Total C O 35 24 11	0	0
21	K	1	Total C O 35 24 11	0	0
21	K	1	Total C O 35 24 11	0	0
21	K	1	Total C O 35 24 11	0	0
21	L	1	Total C O 35 24 11	0	0
21	L	1	Total C O 35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

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



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

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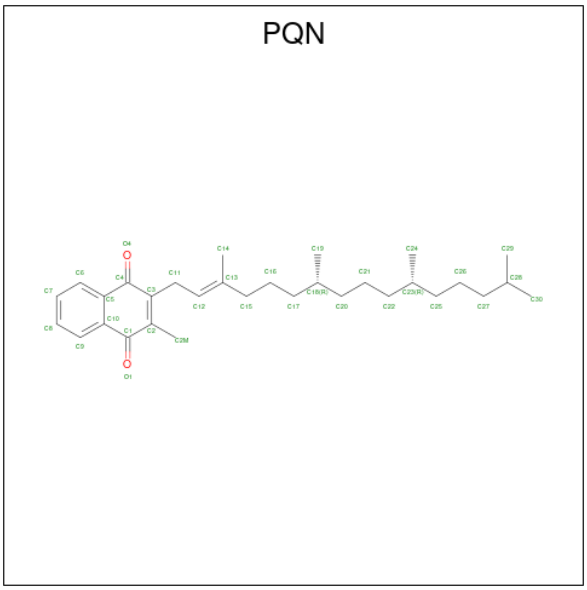
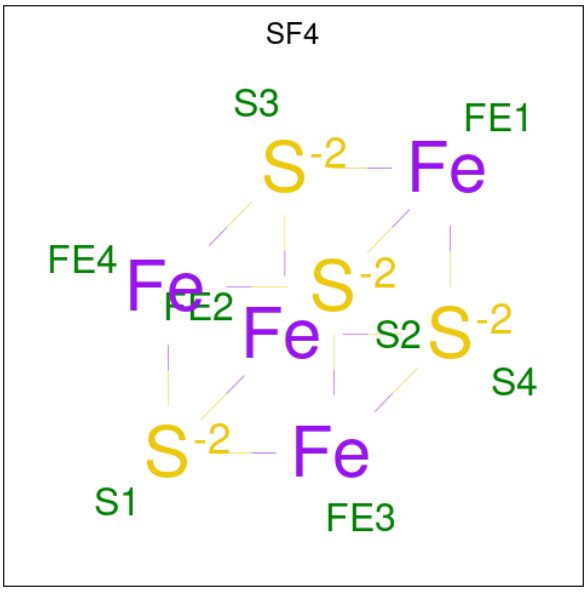
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
22	I	1	Total C 40 40	0	0
22	I	1	Total C 40 40	0	0
22	J	1	Total C 40 40	0	0
22	L	1	Total C 40 40	0	0

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



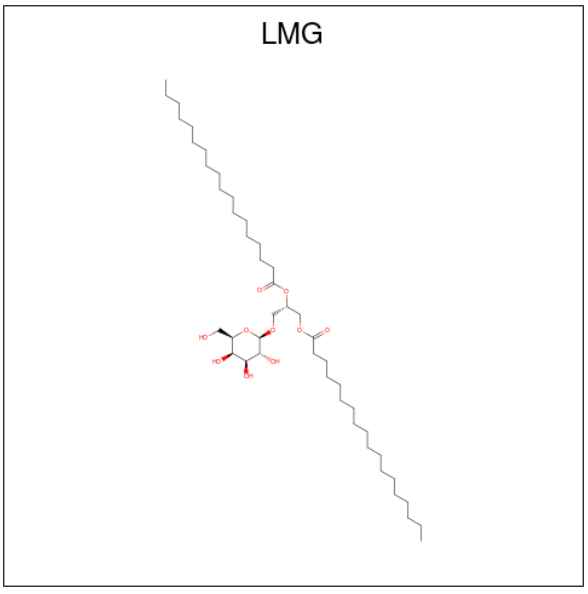
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
23	A	1	Total C O 33 31 2	0	0
23	B	1	Total C O 33 31 2	0	0

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



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

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



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

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

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

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

3 Data and refinement statistics (i)

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

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.11% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

4 Model quality

4.1 Standard geometry

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

4.2 Too-close contacts

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

4.3 Torsion angles

4.3.1 Protein backbone

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

4.3.2 Protein sidechains

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

4.3.3 RNA

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

4.4 Non-standard residues in protein, DNA, RNA chains

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

4.5 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	10,10,12	1.46	3 (30%)	14,14,17	3.31	10 (71%)
19	FRU	M	2	19	11,12,12	1.06	1 (9%)	10,18,18	2.33	3 (30%)
19	GLC	O	1	19	11,11,12	0.92	0	15,15,17	3.54	8 (53%)
19	FRU	O	2	19	11,12,12	1.08	1 (9%)	10,18,18	1.70	2 (20%)
19	GLC	P	1	19	11,11,12	0.99	0	15,15,17	2.44	3 (20%)
19	FRU	P	2	19	11,12,12	1.16	2 (18%)	10,18,18	0.96	0
19	GLC	Q	1	19	11,11,12	1.19	1 (9%)	15,15,17	2.20	5 (33%)
19	FRU	Q	2	19	11,12,12	1.00	1 (9%)	10,18,18	1.76	4 (40%)
19	GLC	S	1	19	11,11,12	0.44	0	15,15,17	1.12	2 (13%)
19	FRU	S	2	19,21	11,12,12	0.67	0	10,18,18	1.12	0
19	GLC	T	1	19	11,11,12	1.07	0	15,15,17	1.64	3 (20%)
19	FRU	T	2	19	11,12,12	2.01	4 (36%)	10,18,18	2.89	4 (40%)
19	GLC	U	1	19	11,11,12	1.06	1 (9%)	15,15,17	2.67	5 (33%)
19	FRU	U	2	19	11,12,12	0.96	0	10,18,18	1.53	2 (20%)
19	GLC	V	1	19	11,11,12	1.54	2 (18%)	15,15,17	1.98	5 (33%)
19	FRU	V	2	19	11,12,12	0.90	0	10,18,18	2.00	5 (50%)
19	GLC	W	1	19	11,11,12	1.30	1 (9%)	15,15,17	2.89	9 (60%)
19	FRU	W	2	19	11,12,12	1.17	2 (18%)	10,18,18	2.10	2 (20%)
19	GLC	X	1	19	11,11,12	1.22	1 (9%)	15,15,17	1.83	4 (26%)
19	FRU	X	2	19	11,12,12	1.56	2 (18%)	10,18,18	2.32	4 (40%)
19	GLC	Y	1	19	11,11,12	1.09	0	15,15,17	3.55	7 (46%)
19	FRU	Y	2	19	11,12,12	1.15	0	10,18,18	2.27	4 (40%)
19	GLC	Z	1	19	11,11,12	1.75	2 (18%)	15,15,17	4.50	8 (53%)
19	FRU	Z	2	19,21	11,12,12	1.06	1 (9%)	10,18,18	2.34	3 (30%)
19	GLC	a	1	19	11,11,12	1.06	1 (9%)	15,15,17	1.52	3 (20%)
19	FRU	a	2	19	11,12,12	1.07	0	10,18,18	2.15	3 (30%)

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

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

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

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	Z	1	GLC	O5-C1	-4.10	1.37	1.43
19	T	2	FRU	O5-C2	-3.74	1.37	1.43
19	T	2	FRU	C1-C2	-3.01	1.47	1.52
19	V	1	GLC	O5-C1	-2.83	1.39	1.43
19	X	2	FRU	O2-C2	-2.70	1.36	1.40

The worst 5 of 108 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
19	Z	1	GLC	C1-O5-C5	-11.46	96.66	112.19
19	M	1	GLC	C1-C2-C3	7.92	119.40	109.67
19	P	1	GLC	C1-O5-C5	7.71	122.64	112.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
19	Y	1	GLC	C1-O5-C5	7.50	122.35	112.19
19	Z	1	GLC	O5-C1-C2	-7.29	99.52	110.77

5 of 13 chirality outliers are listed below:

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

5 of 46 torsion outliers are listed below:

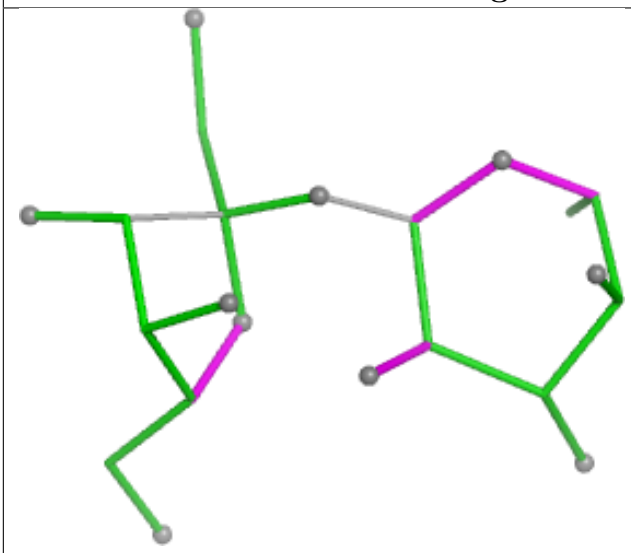
Mol	Chain	Res	Type	Atoms
19	O	2	FRU	O1-C1-C2-C3
19	O	2	FRU	O1-C1-C2-O2
19	Q	2	FRU	O1-C1-C2-C3
19	Q	2	FRU	O1-C1-C2-O2
19	Q	2	FRU	O1-C1-C2-O5

There are no ring outliers.

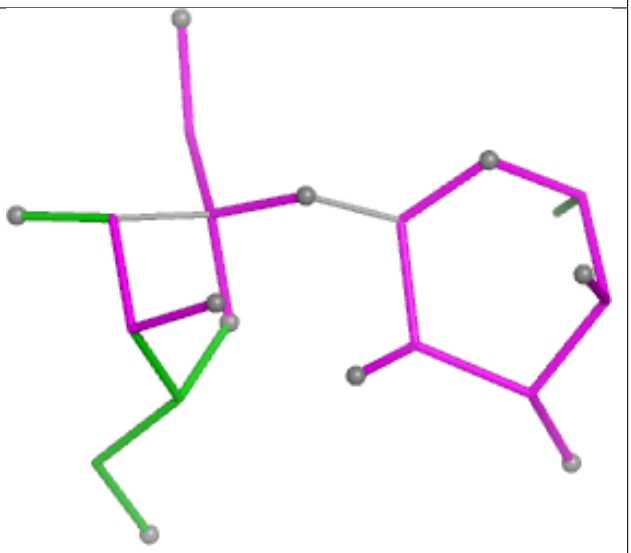
No monomer is involved in short contacts.

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

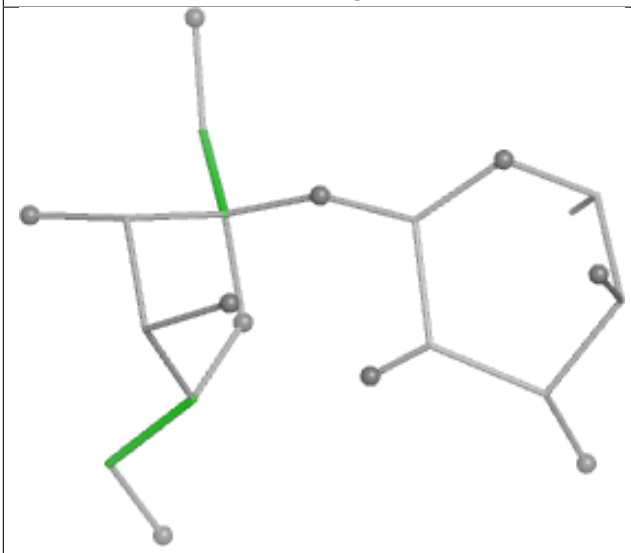
Oligosaccharide Chain M



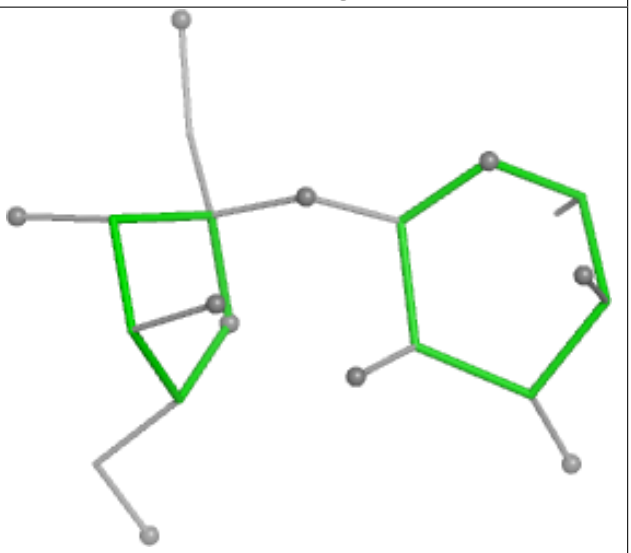
Bond lengths



Bond angles

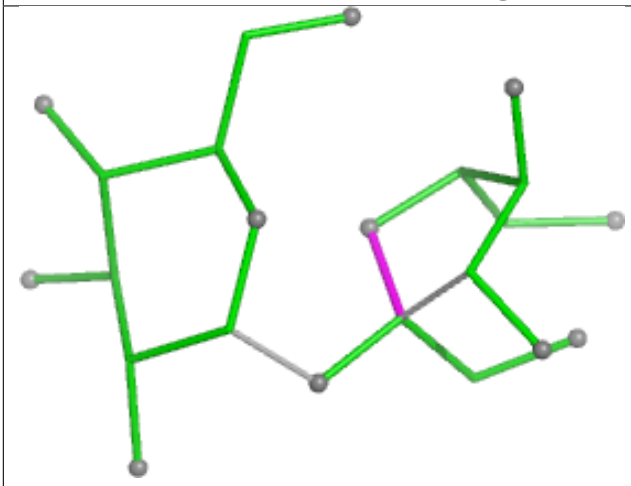


Torsions

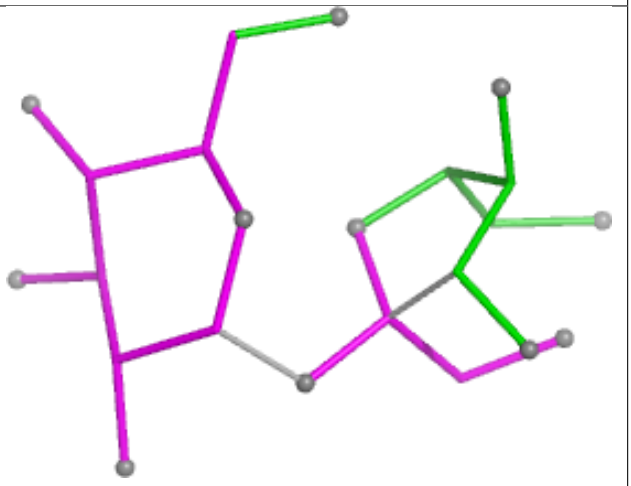


Rings

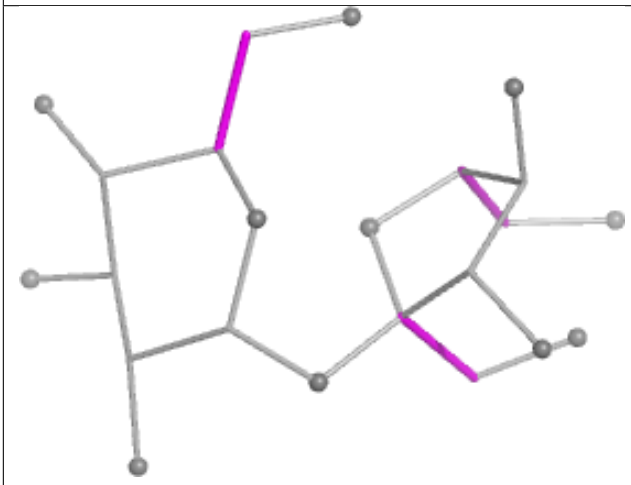
Oligosaccharide Chain O



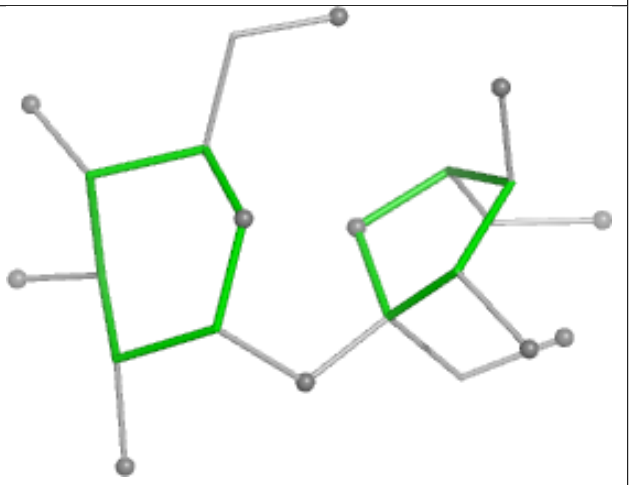
Bond lengths



Bond angles

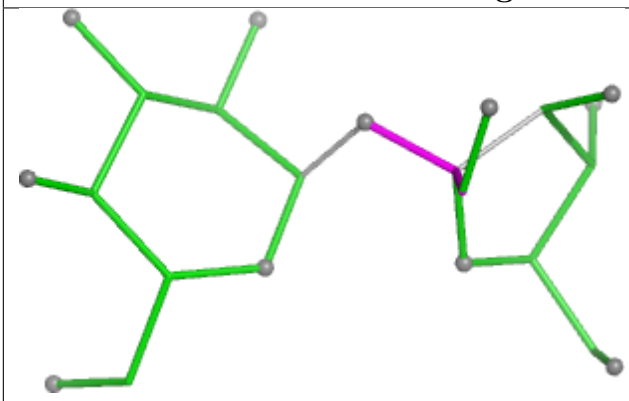


Torsions

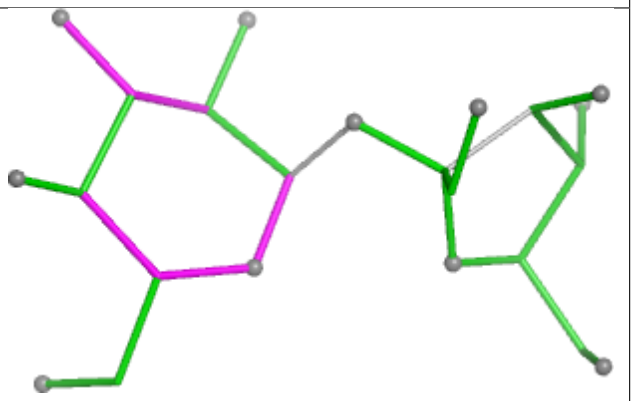


Rings

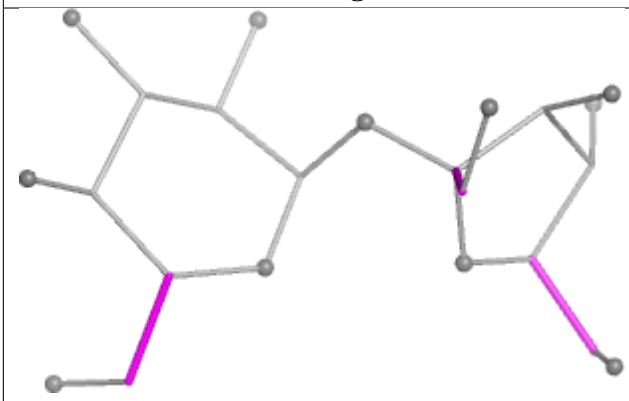
Oligosaccharide Chain P



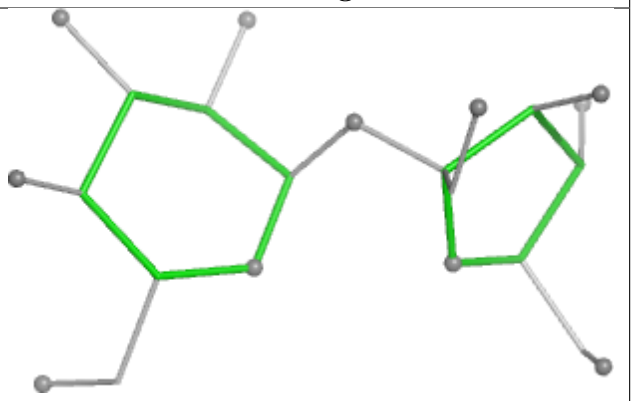
Bond lengths



Bond angles

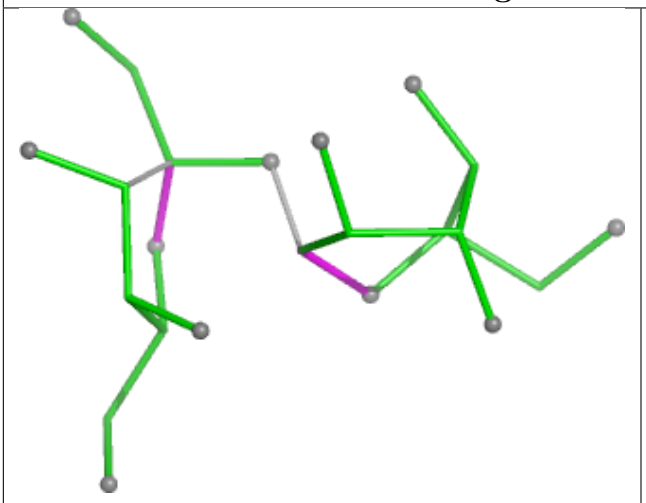


Torsions

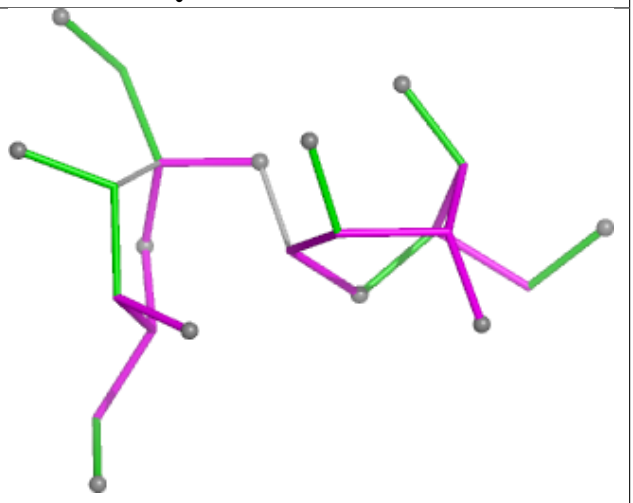


Rings

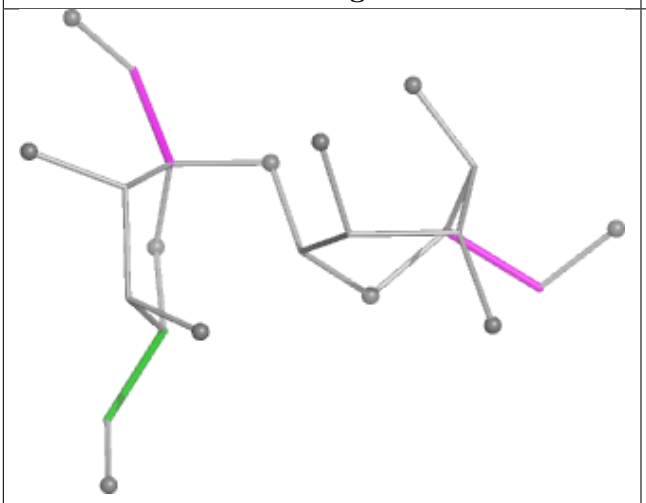
Oligosaccharide Chain Q



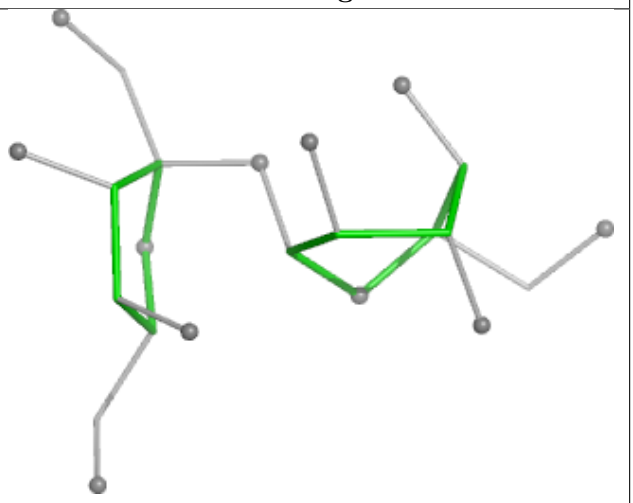
Bond lengths



Bond angles

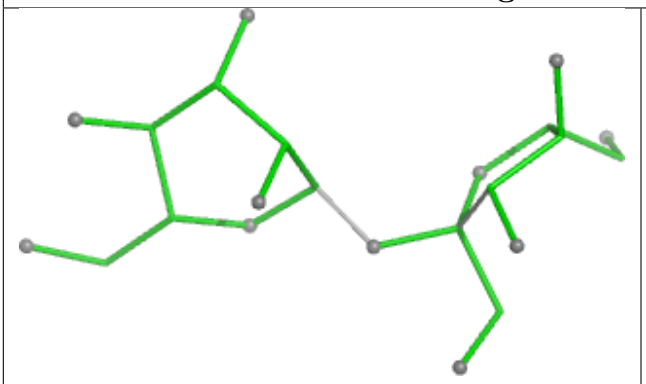


Torsions

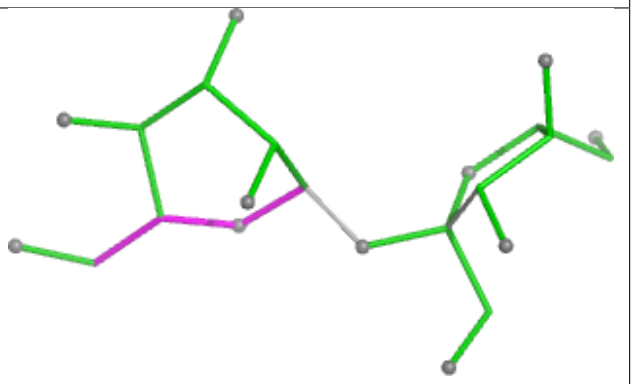


Rings

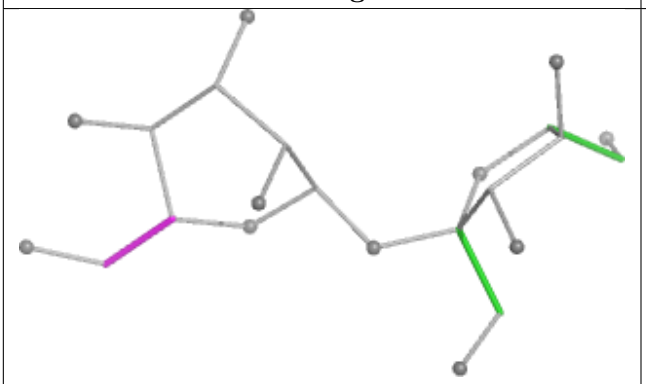
Oligosaccharide Chain S



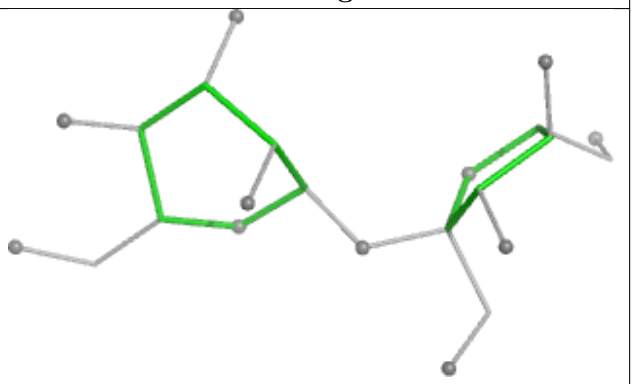
Bond lengths



Bond angles

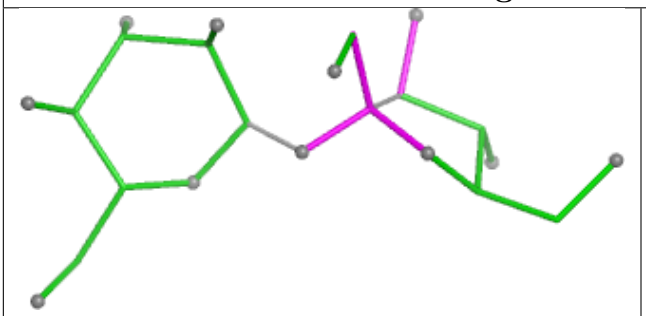


Torsions

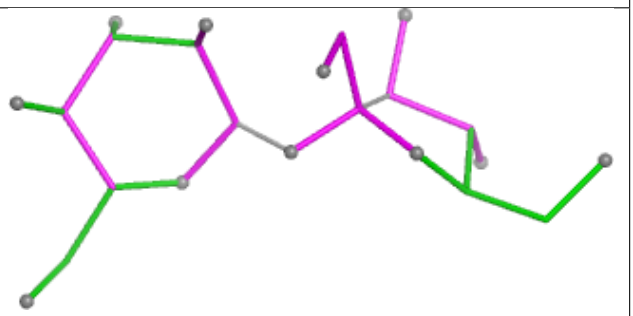


Rings

Oligosaccharide Chain T



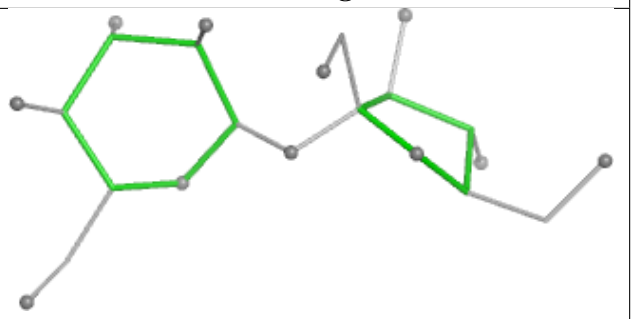
Bond lengths



Bond angles

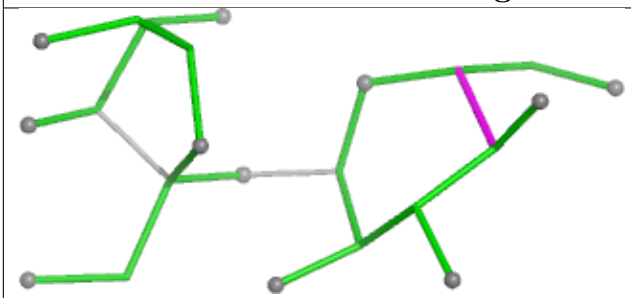


Torsions

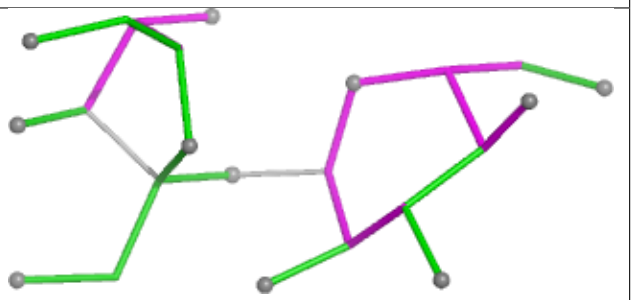


Rings

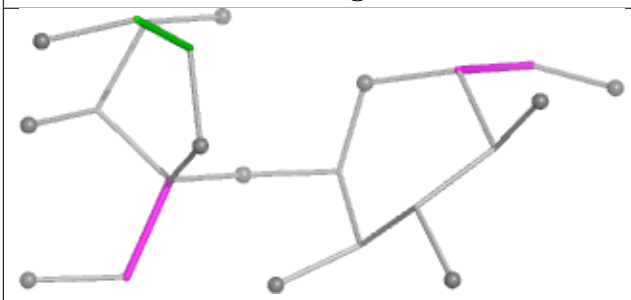
Oligosaccharide Chain U



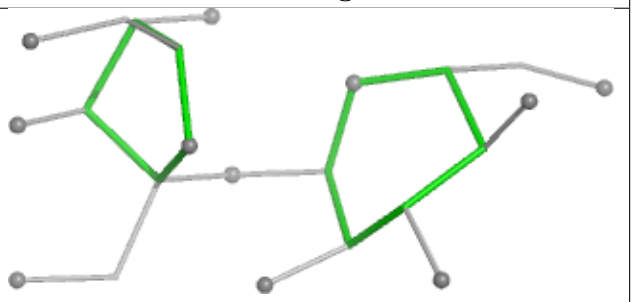
Bond lengths



Bond angles

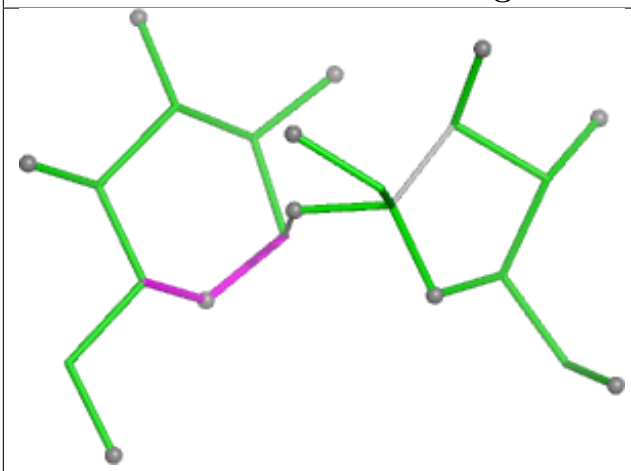


Torsions

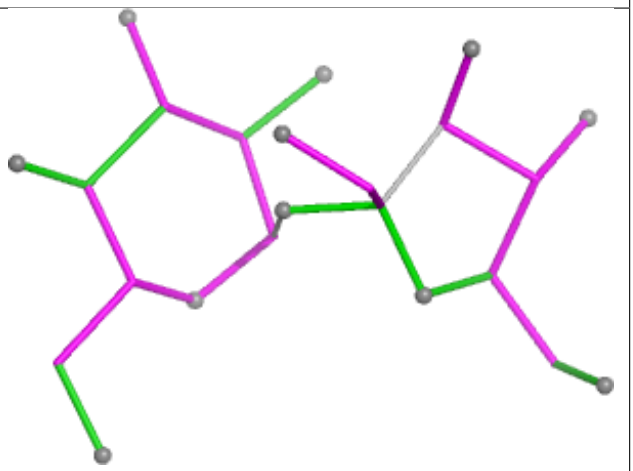


Rings

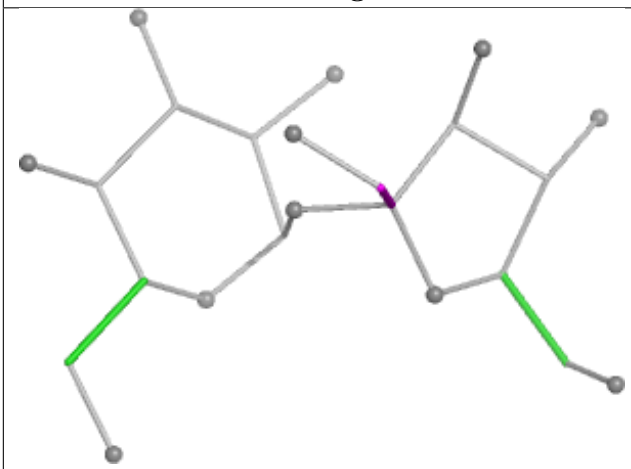
Oligosaccharide Chain V



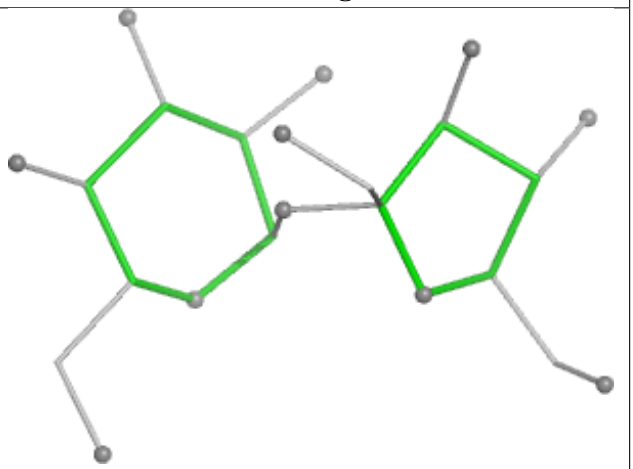
Bond lengths



Bond angles

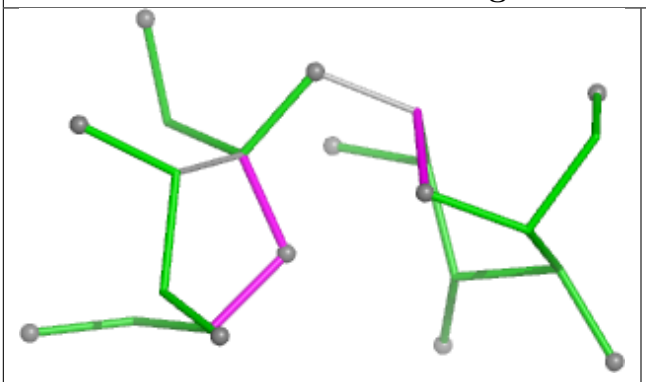


Torsions

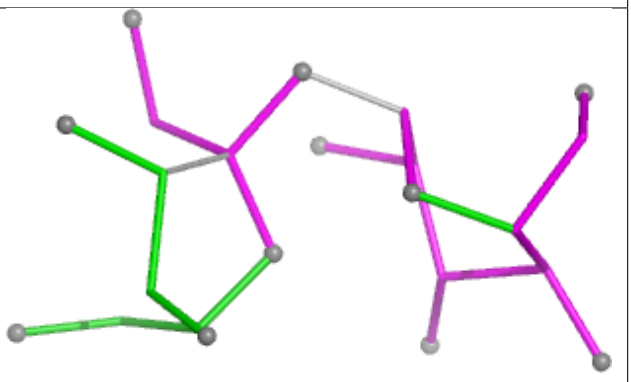


Rings

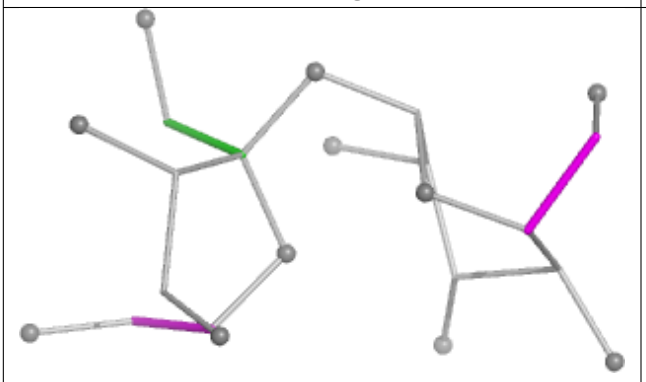
Oligosaccharide Chain W



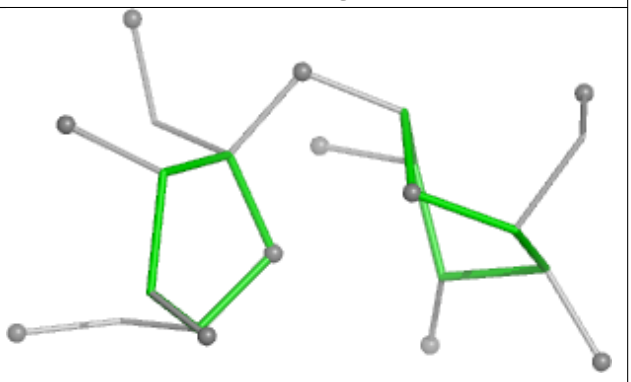
Bond lengths



Bond angles

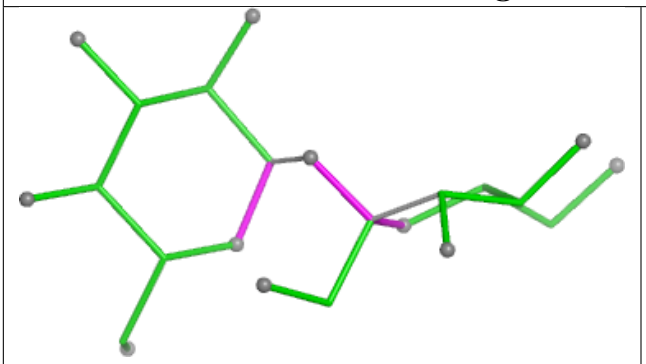


Torsions

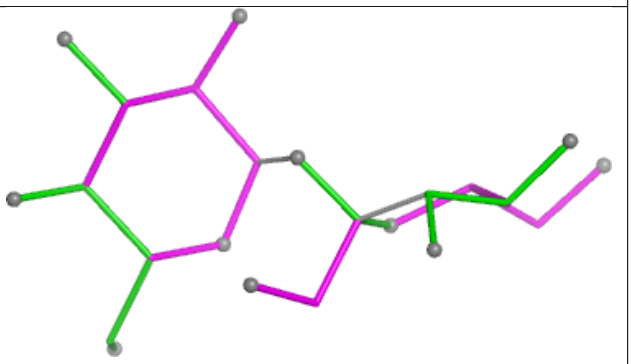


Rings

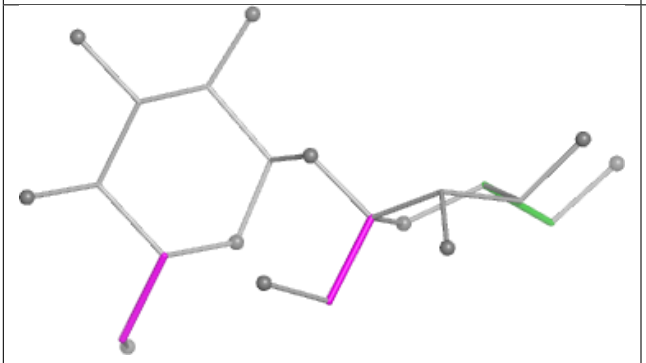
Oligosaccharide Chain X



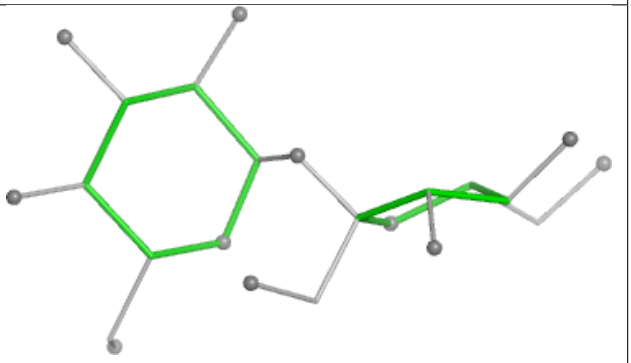
Bond lengths



Bond angles

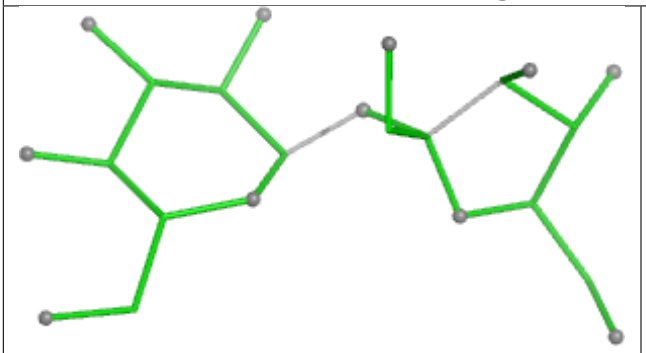


Torsions

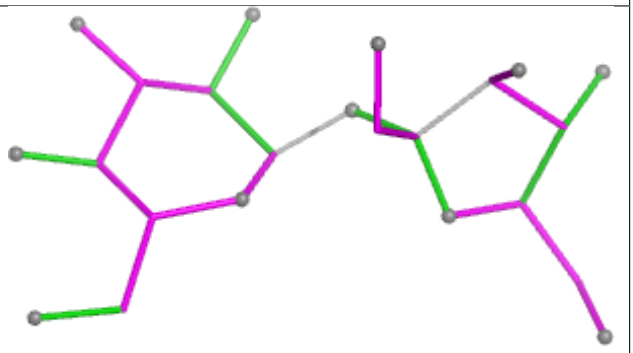


Rings

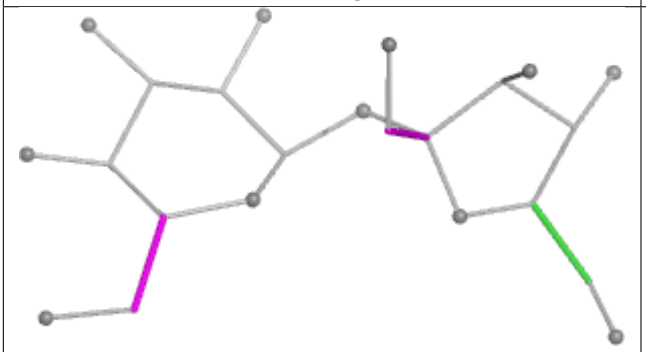
Oligosaccharide Chain Y



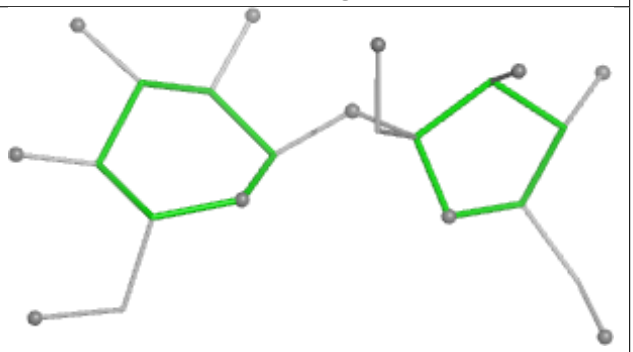
Bond lengths



Bond angles

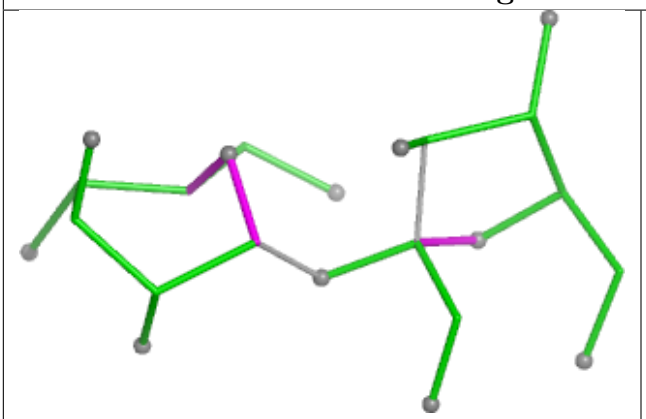


Torsions

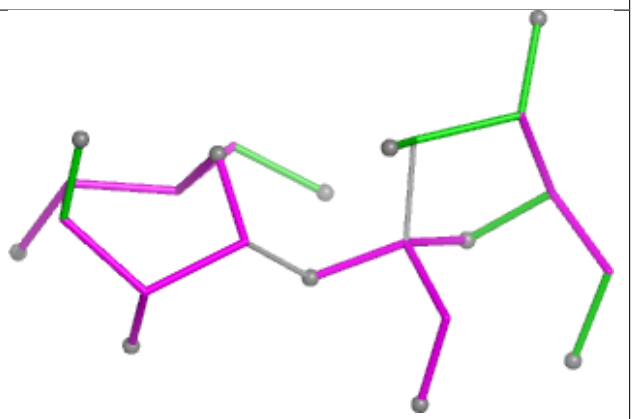


Rings

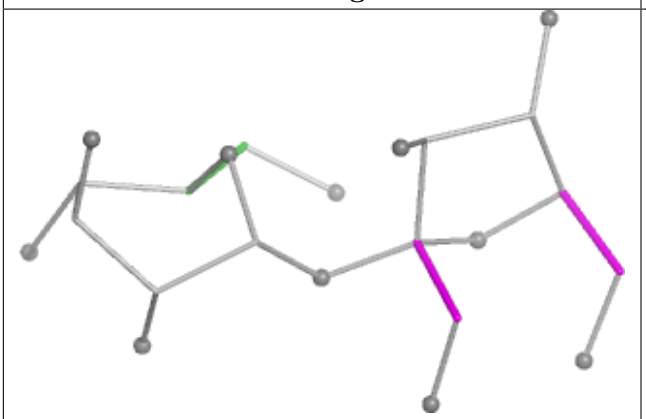
Oligosaccharide Chain Z



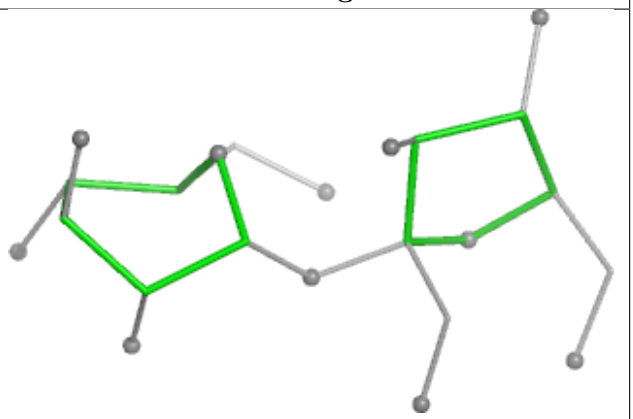
Bond lengths



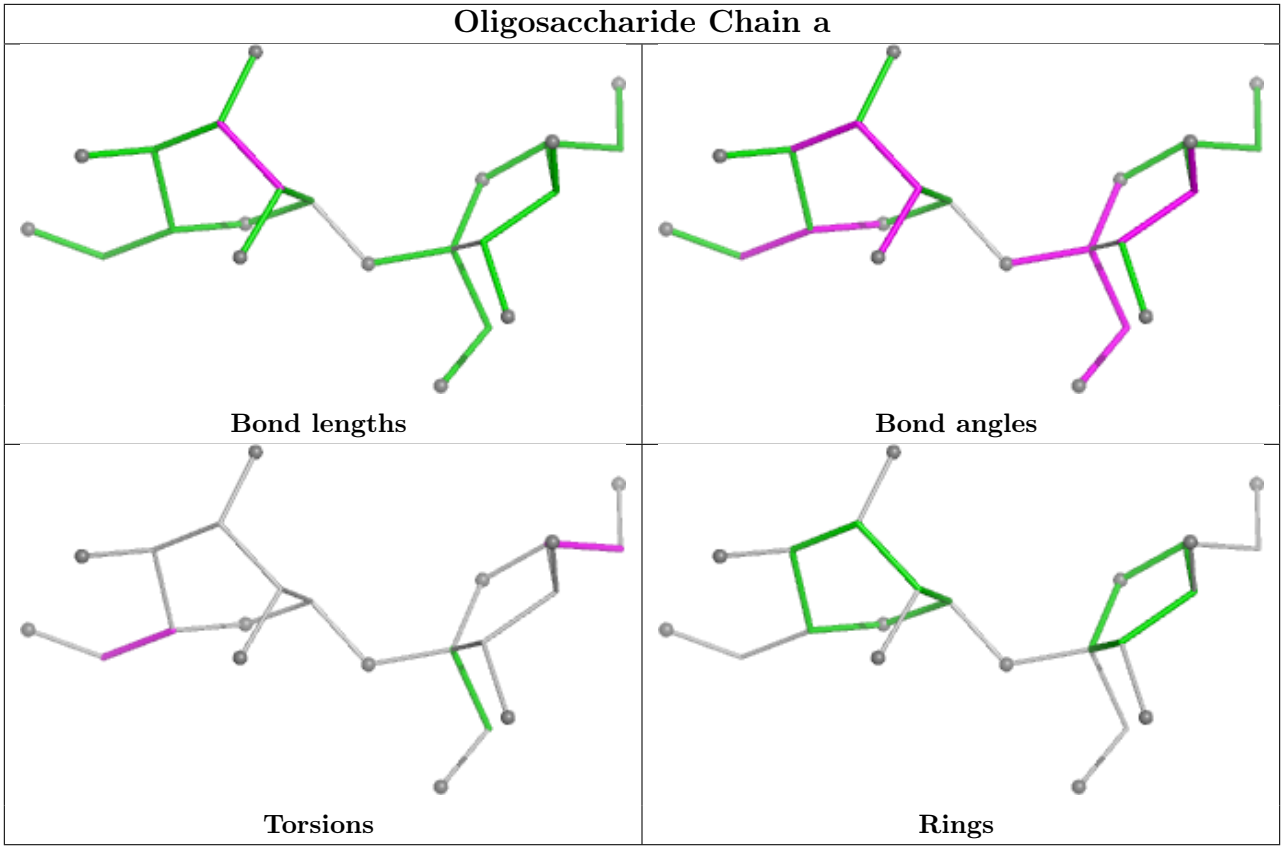
Bond angles



Torsions



Rings



4.6 Ligand geometry

Of 243 ligands modelled in this entry, 1 is unknown - leaving 242 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
22	BCR	B	850	20	41,41,41	3.29	19 (46%)	56,56,56	6.44	27 (48%)
20	CLA	A	808	-	49,53,73	2.70	13 (26%)	59,89,113	3.22	24 (40%)
20	CLA	4	318	-	56,60,73	2.45	13 (23%)	67,97,113	2.94	25 (37%)
20	CLA	4	317	-	26,32,73	2.36	9 (34%)	34,54,113	2.95	21 (61%)
21	LMU	A	845	-	36,36,36	0.94	0	47,47,47	1.38	7 (14%)
20	CLA	A	837	-	69,73,73	2.18	16 (23%)	83,113,113	2.67	24 (28%)
21	LMU	2	320	-	36,36,36	1.11	1 (2%)	47,47,47	1.34	3 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
22	BCR	A	840	-	41,41,41	1.93	4 (9%)	56,56,56	5.91	20 (35%)
23	PQN	B	840	-	34,34,34	1.66	2 (5%)	42,45,45	1.59	6 (14%)
20	CLA	1	204	-	50,54,73	2.65	14 (28%)	60,90,113	2.82	23 (38%)
21	LMU	R	101	-	36,36,36	0.41	0	47,47,47	1.75	12 (25%)
20	CLA	4	313	-	39,44,73	2.65	11 (28%)	52,78,113	3.51	26 (50%)
21	LMU	2	313	-	36,36,36	0.89	1 (2%)	47,47,47	0.92	2 (4%)
20	CLA	3	320	-	59,63,73	2.34	12 (20%)	71,101,113	2.98	26 (36%)
20	CLA	G	103	-	55,59,73	2.52	12 (21%)	66,96,113	2.93	27 (40%)
21	LMU	B	801	-	36,36,36	0.65	0	47,47,47	2.41	15 (31%)
21	LMU	R	103	-	36,36,36	0.70	0	47,47,47	2.16	16 (34%)
20	CLA	A	810	5	58,62,73	2.36	13 (22%)	69,99,113	2.64	23 (33%)
20	CLA	3	319	-	39,44,73	2.79	11 (28%)	52,78,113	3.36	22 (42%)
20	CLA	A	850	-	50,54,73	2.77	15 (30%)	63,90,113	3.90	36 (57%)
22	BCR	F	203	-	41,41,41	2.79	13 (31%)	56,56,56	6.08	31 (55%)
21	LMU	A	854	-	36,36,36	0.84	1 (2%)	47,47,47	1.58	8 (17%)
20	CLA	A	835	-	55,59,73	2.44	15 (27%)	66,96,113	2.97	24 (36%)
21	LMU	A	852	-	36,36,36	0.63	1 (2%)	47,47,47	1.89	11 (23%)
20	CLA	A	820	-	59,63,73	2.40	15 (25%)	71,101,113	2.88	24 (33%)
21	LMU	B	845	-	26,26,36	1.04	1 (3%)	37,37,47	1.42	6 (16%)
20	CLA	B	816	-	65,69,73	2.18	14 (21%)	78,108,113	2.84	28 (35%)
20	CLA	A	819	5	46,50,73	2.60	13 (28%)	55,85,113	3.36	23 (41%)
20	CLA	A	809	5	69,73,73	2.19	12 (17%)	83,113,113	3.06	30 (36%)
20	CLA	A	817	-	69,73,73	2.20	15 (21%)	83,113,113	2.64	24 (28%)
20	CLA	B	832	20	49,53,73	2.63	13 (26%)	59,89,113	3.18	23 (38%)
20	CLA	B	825	-	69,73,73	2.16	14 (20%)	83,113,113	2.87	31 (37%)
21	LMU	A	851	-	36,36,36	0.40	0	47,47,47	0.70	1 (2%)
21	LMU	R	102	-	36,36,36	0.76	0	47,47,47	2.07	14 (29%)
21	LMU	2	316	-	36,36,36	0.39	0	47,47,47	0.69	1 (2%)
22	BCR	A	842	-	41,41,41	1.94	4 (9%)	56,56,56	5.91	21 (37%)
20	CLA	B	849	-	69,73,73	2.27	15 (21%)	83,113,113	2.72	29 (34%)
20	CLA	4	305	-	59,63,73	2.31	12 (20%)	71,101,113	2.97	28 (39%)
20	CLA	4	310	-	59,63,73	2.42	12 (20%)	71,101,113	2.87	27 (38%)
20	CLA	2	309	-	26,32,73	2.37	9 (34%)	34,54,113	3.05	21 (61%)
20	CLA	K	107	6	69,73,73	2.21	12 (17%)	83,113,113	2.57	28 (33%)
22	BCR	I	103	-	41,41,41	2.67	8 (19%)	56,56,56	6.54	28 (50%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#|Z| > 2	Counts	RMSZ	#|Z| > 2
21	LMU	3	302	-	36,36,36	0.39	0	47,47,47	0.69	1 (2%)
20	CLA	B	819	6	59,63,73	2.49	16 (27%)	71,101,113	2.83	25 (35%)
22	BCR	G	102	-	41,41,41	1.95	4 (9%)	56,56,56	5.90	21 (37%)
20	CLA	B	848	-	69,73,73	2.14	14 (20%)	83,113,113	2.84	31 (37%)
20	CLA	L	208	-	54,58,73	2.64	19 (35%)	65,95,113	3.24	24 (36%)
22	BCR	F	202	-	41,41,41	1.94	3 (7%)	56,56,56	5.91	21 (37%)
24	SF4	A	856	5,6	0,12,12	-	-	-		
21	LMU	B	802	-	36,36,36	0.97	3 (8%)	47,47,47	2.46	13 (27%)
20	CLA	1	215	-	26,32,73	2.47	7 (26%)	34,54,113	3.50	21 (61%)
20	CLA	3	313	-	26,32,73	2.46	9 (34%)	34,54,113	3.04	20 (58%)
20	CLA	A	815	-	56,60,73	2.46	13 (23%)	67,97,113	3.03	27 (40%)
20	CLA	B	827	6	54,58,73	2.68	17 (31%)	65,95,113	2.76	27 (41%)
20	CLA	1	207	-	55,59,73	2.52	15 (27%)	66,96,113	3.42	31 (46%)
20	CLA	A	811	5	58,62,73	2.24	14 (24%)	69,99,113	2.77	27 (39%)
20	CLA	A	806	5	69,73,73	2.21	15 (21%)	83,113,113	2.96	32 (38%)
20	CLA	B	812	6	64,68,73	2.25	12 (18%)	77,107,113	2.65	26 (33%)
21	LMU	E	101	-	36,36,36	0.90	2 (5%)	47,47,47	3.08	22 (46%)
20	CLA	2	315	-	26,32,73	2.45	9 (34%)	34,54,113	2.93	21 (61%)
20	CLA	B	836	-	51,55,73	2.47	14 (27%)	61,91,113	2.97	25 (40%)
20	CLA	1	201	1	50,54,73	2.87	25 (50%)	60,90,113	4.21	37 (61%)
20	CLA	L	202	-	69,73,73	2.12	13 (18%)	83,113,113	2.81	29 (34%)
20	CLA	F	205	20	45,49,73	2.66	15 (33%)	54,84,113	3.19	21 (38%)
20	CLA	2	314	-	26,32,73	2.46	12 (46%)	34,54,113	3.16	23 (67%)
21	LMU	H	104	-	36,36,36	0.99	3 (8%)	47,47,47	2.76	19 (40%)
20	CLA	A	813	5	54,58,73	2.57	13 (24%)	65,95,113	2.81	27 (41%)
20	CLA	2	301	-	55,59,73	2.43	15 (27%)	66,96,113	2.97	24 (36%)
21	LMU	1	218	-	36,36,36	1.02	2 (5%)	47,47,47	2.25	13 (27%)
20	CLA	A	836	-	69,73,73	2.17	15 (21%)	83,113,113	2.67	24 (28%)
21	LMU	A	846	-	36,36,36	0.94	1 (2%)	47,47,47	1.65	10 (21%)
20	CLA	K	105	-	49,53,73	2.57	16 (32%)	59,89,113	3.06	21 (35%)
20	CLA	3	312	-	26,32,73	2.50	9 (34%)	34,54,113	3.07	21 (61%)
20	CLA	B	833	-	55,59,73	2.53	12 (21%)	66,96,113	2.99	26 (39%)
20	CLA	A	831	5	49,53,73	2.58	15 (30%)	59,89,113	3.07	21 (35%)
20	CLA	2	311	-	54,58,73	2.57	14 (25%)	65,95,113	3.05	26 (40%)
20	CLA	2	321	20	65,69,73	2.47	26 (40%)	78,108,113	3.05	32 (41%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
21	LMU	4	316	-	36,36,36	0.86	1 (2%)	47,47,47	1.18	3 (6%)
20	CLA	3	317	-	26,32,73	2.41	8 (30%)	34,54,113	3.01	21 (61%)
20	CLA	F	204	-	39,44,73	2.77	13 (33%)	52,78,113	3.29	27 (51%)
21	LMU	K	102	-	36,36,36	0.48	0	47,47,47	2.05	16 (34%)
22	BCR	B	843	-	41,41,41	1.95	4 (9%)	56,56,56	5.90	21 (37%)
21	LMU	R	104	-	36,36,36	0.97	2 (5%)	47,47,47	1.63	10 (21%)
20	CLA	1	209	-	39,44,73	3.58	23 (58%)	52,78,113	4.03	24 (46%)
20	CLA	3	307	-	26,32,73	2.37	9 (34%)	34,54,113	2.99	21 (61%)
20	CLA	3	306	-	26,32,73	2.40	9 (34%)	34,54,113	3.13	21 (61%)
20	CLA	1	212	-	65,69,73	2.36	21 (32%)	78,108,113	2.86	31 (39%)
20	CLA	B	807	6	69,73,73	2.15	15 (21%)	83,113,113	2.73	24 (28%)
20	CLA	B	828	6	54,58,73	2.34	11 (20%)	65,95,113	3.08	28 (43%)
21	LMU	2	318	-	36,36,36	1.12	1 (2%)	47,47,47	1.91	14 (29%)
20	CLA	A	812	5	49,53,73	2.63	12 (24%)	59,89,113	2.99	23 (38%)
20	CLA	B	803	6	49,53,73	2.62	16 (32%)	59,89,113	3.24	23 (38%)
21	LMU	K	104	20	36,36,36	0.75	0	47,47,47	2.27	12 (25%)
20	CLA	2	308	-	26,32,73	2.39	8 (30%)	34,54,113	3.10	21 (61%)
20	CLA	B	847	6	69,73,73	2.16	15 (21%)	83,113,113	2.88	35 (42%)
20	CLA	2	307	20	69,73,73	2.18	12 (17%)	83,113,113	2.78	28 (33%)
20	CLA	2	306	-	69,73,73	2.21	13 (18%)	83,113,113	2.82	26 (31%)
20	CLA	A	825	5	59,63,73	2.34	15 (25%)	71,101,113	2.83	27 (38%)
20	CLA	B	830	6	54,58,73	2.62	18 (33%)	65,95,113	3.19	27 (41%)
21	LMU	R	105	-	36,36,36	0.96	1 (2%)	47,47,47	1.58	10 (21%)
20	CLA	H	101	-	59,63,73	2.42	14 (23%)	71,101,113	3.00	30 (42%)
20	CLA	4	311	-	26,32,73	2.38	9 (34%)	34,54,113	3.15	21 (61%)
20	CLA	L	203	-	59,63,73	2.43	12 (20%)	71,101,113	2.79	27 (38%)
20	CLA	3	316	-	26,32,73	2.45	9 (34%)	34,54,113	3.26	22 (64%)
20	CLA	4	315	-	50,54,73	2.72	21 (42%)	60,90,113	3.17	25 (41%)
22	BCR	A	844	-	41,41,41	1.94	3 (7%)	56,56,56	5.91	21 (37%)
20	CLA	2	303	-	26,32,73	2.35	10 (38%)	34,54,113	3.07	21 (61%)
20	CLA	1	211	-	55,59,73	2.89	26 (47%)	66,96,113	4.07	31 (46%)
20	CLA	A	848	-	69,73,73	2.24	18 (26%)	83,113,113	2.72	25 (30%)
21	LMU	4	320	-	35,35,36	0.41	0	46,46,47	0.70	1 (2%)
21	LMU	1	216	-	36,36,36	0.40	0	47,47,47	0.69	1 (2%)
20	CLA	B	837	-	69,73,73	2.17	15 (21%)	83,113,113	2.89	28 (33%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
20	CLA	3	314	-	46,50,73	2.51	11 (23%)	55,85,113	3.19	26 (47%)
20	CLA	A	821	-	69,73,73	2.11	14 (20%)	83,113,113	2.62	25 (30%)
20	CLA	B	815	6	64,68,73	2.18	14 (21%)	77,107,113	2.77	28 (36%)
20	CLA	A	805	5	50,54,73	2.50	12 (24%)	60,90,113	2.95	25 (41%)
20	CLA	B	835	6	69,73,73	2.13	13 (18%)	83,113,113	2.72	24 (28%)
20	CLA	A	803	5	69,73,73	2.13	13 (18%)	83,113,113	2.81	29 (34%)
22	BCR	I	101	-	41,41,41	2.68	17 (41%)	56,56,56	5.37	31 (55%)
20	CLA	2	304	-	54,58,73	2.46	14 (25%)	65,95,113	2.74	24 (36%)
20	CLA	3	301	20	60,64,73	2.46	20 (33%)	72,102,113	2.95	27 (37%)
20	CLA	4	307	4	56,60,73	3.11	30 (53%)	67,97,113	3.75	41 (61%)
20	CLA	B	811	6	69,73,73	2.21	12 (17%)	83,113,113	2.54	27 (32%)
21	LMU	2	319	-	36,36,36	1.09	1 (2%)	47,47,47	1.28	6 (12%)
20	CLA	4	309	-	26,32,73	2.44	9 (34%)	34,54,113	3.21	20 (58%)
20	CLA	B	831	20	49,53,73	2.72	16 (32%)	59,89,113	3.10	23 (38%)
20	CLA	4	304	-	69,73,73	2.51	28 (40%)	83,113,113	3.51	39 (46%)
20	CLA	B	805	-	69,73,73	2.21	16 (23%)	83,113,113	3.08	36 (43%)
20	CLA	R	106	-	61,65,73	2.38	13 (21%)	73,103,113	2.94	28 (38%)
20	CLA	A	823	5,20	69,73,73	2.17	16 (23%)	83,113,113	2.68	24 (28%)
20	CLA	K	106	-	54,58,73	2.91	23 (42%)	65,95,113	3.30	29 (44%)
20	CLA	1	203	-	51,55,73	2.56	12 (23%)	61,91,113	3.29	27 (44%)
25	LMG	B	846	-	49,49,55	0.95	2 (4%)	57,57,63	1.01	3 (5%)
20	CLA	3	308	-	26,32,73	2.43	9 (34%)	34,54,113	3.29	21 (61%)
20	CLA	4	303	-	39,44,73	3.03	15 (38%)	52,78,113	3.61	23 (44%)
20	CLA	B	804	-	69,73,73	2.16	14 (20%)	83,113,113	3.07	35 (42%)
20	CLA	B	813	-	50,54,73	2.51	12 (24%)	60,90,113	2.98	23 (38%)
21	LMU	1	217	-	36,36,36	0.45	0	47,47,47	1.62	9 (19%)
21	LMU	4	322	20	36,36,36	0.85	1 (2%)	47,47,47	1.23	4 (8%)
20	CLA	A	826	5	69,73,73	2.18	16 (23%)	83,113,113	2.65	31 (37%)
21	LMU	R	109	-	36,36,36	1.16	2 (5%)	47,47,47	2.44	14 (29%)
20	CLA	L	201	5	69,73,73	2.23	15 (21%)	83,113,113	2.66	26 (31%)
20	CLA	B	829	6	69,73,73	2.28	17 (24%)	83,113,113	2.94	28 (33%)
22	BCR	3	311	-	41,41,41	2.06	5 (12%)	56,56,56	5.90	22 (39%)
20	CLA	B	822	-	62,66,73	2.29	16 (25%)	74,104,113	2.83	25 (33%)
21	LMU	L	210	-	36,36,36	0.99	3 (8%)	47,47,47	1.48	8 (17%)
21	LMU	F	201	-	35,35,36	1.21	5 (14%)	46,46,47	2.34	15 (32%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
20	CLA	A	814	-	69,73,73	2.28	19 (27%)	83,113,113	2.79	27 (32%)
20	CLA	H	109	16	54,58,73	2.48	12 (22%)	65,95,113	2.90	23 (35%)
20	CLA	L	204	-	59,63,73	2.95	25 (42%)	71,101,113	3.58	32 (45%)
20	CLA	4	314	4	26,32,73	2.36	9 (34%)	34,54,113	2.91	19 (55%)
20	CLA	A	804	-	61,65,73	2.34	15 (24%)	73,103,113	3.02	26 (35%)
20	CLA	H	110	-	59,63,73	2.38	12 (20%)	71,101,113	3.01	24 (33%)
24	SF4	C	103	7	0,12,12	-	-	-		
20	CLA	A	830	5,20	54,58,73	2.44	14 (25%)	65,95,113	2.93	26 (40%)
20	CLA	3	315	-	54,58,73	2.52	19 (35%)	65,95,113	3.22	29 (44%)
21	LMU	A	853	-	36,36,36	0.68	1 (2%)	47,47,47	1.97	17 (36%)
20	CLA	A	824	-	69,73,73	2.16	13 (18%)	83,113,113	2.76	30 (36%)
20	CLA	1	202	-	51,55,73	2.55	14 (27%)	61,91,113	3.08	23 (37%)
20	CLA	B	808	6	58,62,73	2.64	15 (25%)	73,100,113	2.86	30 (41%)
21	LMU	4	321	-	36,36,36	1.03	1 (2%)	47,47,47	1.41	8 (17%)
20	CLA	K	103	21	54,58,73	2.47	15 (27%)	65,95,113	2.99	24 (36%)
20	CLA	3	309	-	69,73,73	2.55	24 (34%)	83,113,113	3.16	30 (36%)
21	LMU	H	102	19	36,36,36	1.23	3 (8%)	47,47,47	3.10	22 (46%)
20	CLA	2	312	-	69,73,73	2.23	15 (21%)	83,113,113	2.72	27 (32%)
20	CLA	4	306	-	54,58,73	2.58	13 (24%)	65,95,113	2.76	21 (32%)
23	PQN	A	839	-	34,34,34	1.77	3 (8%)	42,45,45	1.49	6 (14%)
20	CLA	A	829	-	69,73,73	2.24	14 (20%)	83,113,113	3.00	32 (38%)
24	SF4	C	102	7	0,12,12	-	-	-		
20	CLA	1	213	-	26,32,73	2.46	9 (34%)	34,54,113	3.08	21 (61%)
22	BCR	B	844	-	41,41,41	1.93	3 (7%)	56,56,56	5.92	21 (37%)
20	CLA	4	312	-	26,32,73	2.57	8 (30%)	34,54,113	3.20	20 (58%)
21	LMU	C	101	-	36,36,36	0.94	1 (2%)	47,47,47	1.35	7 (14%)
20	CLA	2	302	-	60,64,73	2.38	15 (25%)	72,102,113	2.99	31 (43%)
20	CLA	A	807	5	59,63,73	2.33	12 (20%)	71,101,113	3.10	31 (43%)
20	CLA	1	214	-	55,59,73	2.96	25 (45%)	66,96,113	3.51	33 (50%)
20	CLA	1	205	-	39,44,73	2.94	12 (30%)	52,78,113	3.26	23 (44%)
20	CLA	B	817	-	54,58,73	2.41	13 (24%)	65,95,113	3.00	25 (38%)
20	CLA	A	857	-	26,32,73	2.35	11 (42%)	34,54,113	3.02	20 (58%)
20	CLA	1	206	-	65,69,73	2.28	15 (23%)	78,108,113	2.64	28 (35%)
20	CLA	I	102	-	64,68,73	2.30	15 (23%)	77,107,113	2.83	24 (31%)
20	CLA	A	849	-	69,73,73	2.35	16 (23%)	83,113,113	2.94	28 (33%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
20	CLA	J	103	20	59,63,73	2.50	21 (35%)	71,101,113	3.02	27 (38%)
21	LMU	G	101	-	36,36,36	0.99	2 (5%)	47,47,47	2.57	12 (25%)
20	CLA	4	308	-	26,32,73	2.45	9 (34%)	34,54,113	3.08	21 (61%)
20	CLA	4	319	21	51,55,73	2.54	16 (31%)	61,91,113	3.01	22 (36%)
20	CLA	A	801	-	54,58,73	2.37	14 (25%)	65,95,113	3.22	28 (43%)
20	CLA	3	305	-	26,32,73	2.42	9 (34%)	34,54,113	3.13	21 (61%)
20	CLA	1	208	-	26,32,73	2.33	9 (34%)	34,54,113	2.99	22 (64%)
20	CLA	L	207	16,22	51,55,73	2.46	13 (25%)	61,91,113	3.36	28 (45%)
20	CLA	B	838	-	69,73,73	2.12	14 (20%)	83,113,113	2.81	29 (34%)
21	LMU	K	101	-	36,36,36	0.62	0	47,47,47	1.90	13 (27%)
21	LMU	3	318	-	36,36,36	0.41	0	47,47,47	0.68	1 (2%)
20	CLA	R	107	-	69,73,73	2.27	12 (17%)	83,113,113	2.69	29 (34%)
20	CLA	B	818	-	50,54,73	2.50	13 (26%)	60,90,113	3.22	20 (33%)
20	CLA	H	108	-	59,63,73	2.41	12 (20%)	71,101,113	2.83	26 (36%)
21	LMU	H	103	-	36,36,36	0.91	1 (2%)	47,47,47	2.29	15 (31%)
20	CLA	A	833	5	69,73,73	2.18	15 (21%)	83,113,113	2.68	24 (28%)
20	CLA	4	302	-	59,63,73	2.36	15 (25%)	71,101,113	2.87	25 (35%)
20	CLA	A	855	-	69,73,73	2.18	15 (21%)	83,113,113	2.68	24 (28%)
20	CLA	2	317	-	69,73,73	2.16	16 (23%)	83,113,113	2.59	24 (28%)
20	CLA	3	304	-	26,32,73	2.43	12 (46%)	34,54,113	3.56	20 (58%)
20	CLA	J	102	-	65,69,73	2.23	15 (23%)	78,108,113	2.74	24 (30%)
21	LMU	H	105	19	36,36,36	0.76	0	47,47,47	2.25	17 (36%)
20	CLA	H	107	-	69,73,73	2.26	13 (18%)	83,113,113	2.90	29 (34%)
20	CLA	B	823	6	69,73,73	2.18	15 (21%)	83,113,113	2.68	24 (28%)
20	CLA	B	806	-	69,73,73	2.24	14 (20%)	83,113,113	2.83	29 (34%)
20	CLA	A	827	5	54,58,73	2.47	12 (22%)	65,95,113	3.09	30 (46%)
20	CLA	B	820	-	69,73,73	2.99	31 (44%)	83,113,113	2.96	29 (34%)
22	BCR	B	841	-	41,41,41	1.94	4 (9%)	56,56,56	5.90	21 (37%)
20	CLA	A	832	-	55,59,73	2.44	16 (29%)	66,96,113	2.98	24 (36%)
20	CLA	3	303	-	39,44,73	2.74	10 (25%)	52,78,113	3.06	20 (38%)
22	BCR	A	843	-	41,41,41	1.94	3 (7%)	56,56,56	5.91	21 (37%)
20	CLA	B	810	-	69,73,73	2.23	15 (21%)	83,113,113	2.55	26 (31%)
20	CLA	F	206	20	57,61,73	2.76	25 (43%)	68,98,113	2.83	28 (41%)
20	CLA	B	821	-	58,62,73	2.43	19 (32%)	69,99,113	2.87	31 (44%)
20	CLA	A	802	-	59,63,73	2.41	14 (23%)	71,101,113	2.86	27 (38%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
20	CLA	A	816	-	69,73,73	2.17	15 (21%)	83,113,113	2.66	28 (33%)
20	CLA	A	822	-	69,73,73	2.18	15 (21%)	83,113,113	2.68	24 (28%)
20	CLA	B	839	-	39,44,73	2.83	13 (33%)	52,78,113	3.37	27 (51%)
21	LMU	4	301	-	36,36,36	0.40	0	47,47,47	0.69	1 (2%)
20	CLA	1	210	1	39,44,73	2.82	11 (28%)	52,78,113	3.09	23 (44%)
21	LMU	L	205	-	36,36,36	0.70	2 (5%)	47,47,47	2.40	15 (31%)
20	CLA	3	310	-	69,73,73	2.17	15 (21%)	83,113,113	2.67	24 (28%)
22	BCR	B	842	-	41,41,41	1.87	5 (12%)	56,56,56	5.04	24 (42%)
20	CLA	B	809	6	59,63,73	2.28	15 (25%)	71,101,113	2.81	26 (36%)
22	BCR	J	101	-	41,41,41	1.93	4 (9%)	56,56,56	5.91	21 (37%)
20	CLA	2	305	-	26,32,73	2.44	12 (46%)	34,54,113	3.26	21 (61%)
20	CLA	2	310	2	54,58,73	2.46	13 (24%)	65,95,113	3.04	26 (40%)
20	CLA	B	814	-	63,67,73	2.31	14 (22%)	75,105,113	2.46	24 (32%)
20	CLA	B	826	6	69,73,73	2.19	17 (24%)	83,113,113	3.02	26 (31%)
20	CLA	A	838	-	54,58,73	2.53	15 (27%)	65,95,113	2.92	25 (38%)
21	LMU	R	108	-	36,36,36	0.39	0	47,47,47	0.69	1 (2%)
22	BCR	A	841	-	41,41,41	1.93	3 (7%)	56,56,56	5.91	21 (37%)
20	CLA	B	834	6	64,68,73	2.20	12 (18%)	77,107,113	3.00	22 (28%)
22	BCR	L	209	-	41,41,41	2.47	8 (19%)	56,56,56	5.72	20 (35%)
20	CLA	A	847	-	69,73,73	2.19	16 (23%)	83,113,113	2.85	27 (32%)
20	CLA	A	834	-	51,55,73	2.52	15 (29%)	61,91,113	3.02	22 (36%)
20	CLA	A	818	-	55,59,73	2.50	15 (27%)	66,96,113	2.96	23 (34%)
20	CLA	B	824	-	69,73,73	2.33	15 (21%)	83,113,113	2.91	28 (33%)
20	CLA	A	828	5	69,73,73	2.27	17 (24%)	83,113,113	2.73	25 (30%)
21	LMU	L	206	-	36,36,36	0.74	2 (5%)	47,47,47	1.89	17 (36%)

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
22	BCR	B	850	20	-	12/29/63/63	0/2/2/2
20	CLA	A	808	-	-	5/15/91/115	-
20	CLA	4	318	-	-	8/24/100/115	-
23	PQN	B	840	-	1/1/8/9	10/23/43/43	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
21	LMU	A	845	-	-	16/21/61/61	0/2/2/2
20	CLA	A	837	-	1/1/15/20	20/39/115/115	-
21	LMU	2	320	-	-	8/21/61/61	0/2/2/2
22	BCR	A	840	-	-	12/29/63/63	0/2/2/2
20	CLA	1	204	-	-	8/17/93/115	-
21	LMU	R	101	-	-	11/21/61/61	0/2/2/2
21	LMU	2	313	-	-	16/21/61/61	0/2/2/2
20	CLA	3	320	-	1/1/13/20	8/27/103/115	-
20	CLA	G	103	-	-	11/23/99/115	-
21	LMU	B	801	-	-	16/21/61/61	0/2/2/2
21	LMU	R	103	-	-	17/21/61/61	0/2/2/2
20	CLA	A	810	5	-	14/26/102/115	-
20	CLA	A	850	-	2/2/11/20	12/16/92/115	-
22	BCR	F	203	-	-	12/29/63/63	0/2/2/2
21	LMU	A	854	-	-	14/21/61/61	0/2/2/2
20	CLA	A	835	-	-	13/23/99/115	-
21	LMU	A	852	-	-	11/21/61/61	0/2/2/2
20	CLA	A	820	-	1/1/13/20	10/27/103/115	-
21	LMU	B	845	-	-	4/11/51/61	0/2/2/2
20	CLA	B	816	-	1/1/14/20	17/35/111/115	-
20	CLA	A	819	5	-	3/12/88/115	-
20	CLA	A	809	5	1/1/15/20	25/39/115/115	-
20	CLA	A	817	-	1/1/15/20	16/39/115/115	-
20	CLA	B	832	20	-	8/15/91/115	-
20	CLA	B	825	-	1/1/15/20	17/39/115/115	-
21	LMU	A	851	-	-	19/21/61/61	0/2/2/2
21	LMU	R	102	-	-	13/21/61/61	0/2/2/2
21	LMU	2	316	-	-	14/21/61/61	0/2/2/2
22	BCR	A	842	-	-	17/29/63/63	0/2/2/2
20	CLA	B	849	-	1/1/15/20	19/39/115/115	-
20	CLA	4	305	-	1/1/13/20	13/27/103/115	-
20	CLA	4	310	-	1/1/13/20	14/27/103/115	-
20	CLA	K	107	6	1/1/15/20	21/39/115/115	-
22	BCR	I	103	-	-	13/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
21	LMU	3	302	-	-	11/21/61/61	0/2/2/2
20	CLA	B	819	6	1/1/13/20	9/27/103/115	-
22	BCR	G	102	-	-	10/29/63/63	0/2/2/2
20	CLA	B	848	-	1/1/15/20	15/39/115/115	-
20	CLA	L	208	-	1/1/12/20	11/21/97/115	-
22	BCR	F	202	-	-	12/29/63/63	0/2/2/2
24	SF4	A	856	5,6	-	-	0/6/5/5
21	LMU	B	802	-	-	11/21/61/61	0/2/2/2
20	CLA	A	815	-	-	15/24/100/115	-
20	CLA	B	827	6	-	11/21/97/115	-
20	CLA	1	207	-	1/1/12/20	10/23/99/115	-
20	CLA	A	811	5	-	11/26/102/115	-
20	CLA	A	806	5	1/1/15/20	21/39/115/115	-
20	CLA	B	812	6	1/1/14/20	16/33/109/115	-
21	LMU	E	101	-	-	14/21/61/61	0/2/2/2
20	CLA	B	836	-	-	7/18/94/115	-
20	CLA	1	201	1	-	12/17/93/115	-
20	CLA	L	202	-	1/1/15/20	17/39/115/115	-
20	CLA	F	205	20	-	6/10/86/115	-
21	LMU	H	104	-	-	13/21/61/61	0/2/2/2
20	CLA	A	813	5	-	12/21/97/115	-
20	CLA	2	301	-	-	11/23/99/115	-
21	LMU	1	218	-	-	13/21/61/61	0/2/2/2
20	CLA	A	836	-	1/1/15/20	18/39/115/115	-
21	LMU	A	846	-	-	13/21/61/61	0/2/2/2
20	CLA	K	105	-	-	6/15/91/115	-
20	CLA	B	833	-	-	9/23/99/115	-
20	CLA	A	831	5	-	8/15/91/115	-
20	CLA	2	311	-	-	12/21/97/115	-
20	CLA	2	321	20	1/1/14/20	22/35/111/115	-
21	LMU	4	316	-	-	13/21/61/61	0/2/2/2
21	LMU	K	102	-	-	18/21/61/61	0/2/2/2
22	BCR	B	843	-	-	15/29/63/63	0/2/2/2
21	LMU	R	104	-	-	15/21/61/61	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
20	CLA	B	807	6	1/1/15/20	20/39/115/115	-
20	CLA	1	212	-	1/1/14/20	16/35/111/115	-
20	CLA	B	828	6	-	13/21/97/115	-
21	LMU	K	104	20	-	12/21/61/61	0/2/2/2
21	LMU	2	318	-	-	13/21/61/61	0/2/2/2
20	CLA	A	812	5	-	11/15/91/115	-
20	CLA	B	803	6	-	7/15/91/115	-
20	CLA	B	847	6	1/1/15/20	21/39/115/115	-
20	CLA	2	307	20	1/1/15/20	15/39/115/115	-
20	CLA	2	306	-	1/1/15/20	19/39/115/115	-
20	CLA	A	825	5	1/1/13/20	10/27/103/115	-
20	CLA	B	830	6	-	6/21/97/115	-
21	LMU	R	105	-	-	13/21/61/61	0/2/2/2
20	CLA	H	101	-	2/2/13/20	14/27/103/115	-
20	CLA	L	203	-	1/1/13/20	8/27/103/115	-
20	CLA	4	315	-	-	11/17/93/115	-
22	BCR	A	844	-	-	10/29/63/63	0/2/2/2
20	CLA	1	211	-	1/1/12/20	10/23/99/115	-
20	CLA	A	848	-	1/1/15/20	19/39/115/115	-
21	LMU	4	320	-	-	15/20/60/61	0/2/2/2
21	LMU	1	216	-	-	13/21/61/61	0/2/2/2
20	CLA	B	837	-	1/1/15/20	20/39/115/115	-
20	CLA	3	314	-	-	6/12/88/115	-
20	CLA	A	821	-	1/1/15/20	21/39/115/115	-
20	CLA	B	815	6	1/1/14/20	15/33/109/115	-
20	CLA	B	835	6	1/1/15/20	16/39/115/115	-
20	CLA	A	805	5	-	7/17/93/115	-
20	CLA	A	803	5	1/1/15/20	23/39/115/115	-
22	BCR	I	101	-	-	7/29/63/63	0/2/2/2
20	CLA	2	304	-	-	9/21/97/115	-
20	CLA	3	301	20	1/1/13/20	15/29/105/115	-
20	CLA	4	307	4	1/1/12/20	8/24/100/115	-
20	CLA	B	811	6	1/1/15/20	26/39/115/115	-
21	LMU	2	319	-	-	13/21/61/61	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
20	CLA	B	831	20	-	13/15/91/115	-
20	CLA	4	304	-	2/2/15/20	20/39/115/115	-
20	CLA	B	805	-	1/1/15/20	18/39/115/115	-
20	CLA	R	106	-	1/1/13/20	15/30/106/115	-
20	CLA	A	823	5,20	1/1/15/20	24/39/115/115	-
20	CLA	K	106	-	-	10/21/97/115	-
20	CLA	1	203	-	-	9/18/94/115	-
25	LMG	B	846	-	-	23/44/64/70	0/1/1/1
20	CLA	B	804	-	1/1/15/20	22/39/115/115	-
21	LMU	1	217	-	-	10/21/61/61	0/2/2/2
20	CLA	B	813	-	-	9/17/93/115	-
21	LMU	4	322	20	-	14/21/61/61	0/2/2/2
20	CLA	A	826	5	1/1/15/20	18/39/115/115	-
21	LMU	R	109	-	1/1/10/10	11/21/61/61	0/2/2/2
20	CLA	L	201	5	1/1/15/20	16/39/115/115	-
20	CLA	B	829	6	1/1/15/20	21/39/115/115	-
22	BCR	3	311	-	-	13/29/63/63	0/2/2/2
20	CLA	B	822	-	1/1/13/20	18/31/107/115	-
21	LMU	L	210	-	-	14/21/61/61	0/2/2/2
21	LMU	F	201	-	-	14/20/60/61	0/2/2/2
20	CLA	A	814	-	1/1/15/20	19/39/115/115	-
20	CLA	H	109	16	-	10/21/97/115	-
20	CLA	L	204	-	2/2/13/20	14/27/103/115	-
20	CLA	H	110	-	1/1/13/20	15/27/103/115	-
20	CLA	A	804	-	1/1/13/20	8/30/106/115	-
24	SF4	C	103	7	-	-	0/6/5/5
20	CLA	A	830	5,20	-	13/21/97/115	-
20	CLA	3	315	-	-	7/21/97/115	-
21	LMU	A	853	-	-	14/21/61/61	0/2/2/2
20	CLA	A	824	-	1/1/15/20	17/39/115/115	-
20	CLA	B	808	6	1/1/13/20	11/25/101/115	-
20	CLA	1	202	-	-	8/18/94/115	-
21	LMU	4	321	-	-	15/21/61/61	0/2/2/2
20	CLA	K	103	21	-	5/21/97/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
20	CLA	3	309	-	1/1/15/20	20/39/115/115	-
21	LMU	H	102	19	-	14/21/61/61	0/2/2/2
20	CLA	2	312	-	1/1/15/20	18/39/115/115	-
20	CLA	4	306	-	-	6/21/97/115	-
23	PQN	A	839	-	1/1/8/9	11/23/43/43	0/2/2/2
20	CLA	A	829	-	1/1/15/20	23/39/115/115	-
24	SF4	C	102	7	-	-	0/6/5/5
22	BCR	B	844	-	-	14/29/63/63	0/2/2/2
21	LMU	C	101	-	-	14/21/61/61	0/2/2/2
20	CLA	2	302	-	1/1/13/20	12/29/105/115	-
20	CLA	A	807	5	1/1/13/20	12/27/103/115	-
20	CLA	1	214	-	2/2/12/20	13/23/99/115	-
20	CLA	B	817	-	-	7/21/97/115	-
20	CLA	J	103	20	1/1/13/20	15/27/103/115	-
21	LMU	G	101	-	-	15/21/61/61	0/2/2/2
20	CLA	1	206	-	1/1/14/20	21/35/111/115	-
20	CLA	I	102	-	1/1/14/20	14/33/109/115	-
20	CLA	A	849	-	1/1/15/20	24/39/115/115	-
20	CLA	4	319	21	-	9/18/94/115	-
20	CLA	A	801	-	-	5/21/97/115	-
20	CLA	L	207	16,22	-	10/18/94/115	-
20	CLA	B	838	-	1/1/15/20	18/39/115/115	-
21	LMU	K	101	-	-	12/21/61/61	0/2/2/2
21	LMU	3	318	-	-	18/21/61/61	0/2/2/2
20	CLA	R	107	-	1/1/15/20	21/39/115/115	-
20	CLA	H	108	-	1/1/13/20	10/27/103/115	-
20	CLA	B	818	-	-	14/17/93/115	-
21	LMU	H	103	-	-	16/21/61/61	0/2/2/2
20	CLA	A	833	5	1/1/15/20	17/39/115/115	-
20	CLA	4	302	-	1/1/13/20	14/27/103/115	-
20	CLA	A	855	-	1/1/15/20	23/39/115/115	-
20	CLA	2	317	-	1/1/15/20	21/39/115/115	-
21	LMU	H	105	19	-	11/21/61/61	0/2/2/2
20	CLA	J	102	-	1/1/14/20	25/35/111/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
20	CLA	H	107	-	1/1/15/20	21/39/115/115	-
20	CLA	B	823	6	1/1/15/20	22/39/115/115	-
20	CLA	B	806	-	1/1/15/20	11/39/115/115	-
20	CLA	A	827	5	-	4/21/97/115	-
20	CLA	B	820	-	-	21/39/115/115	-
22	BCR	B	841	-	-	8/29/63/63	0/2/2/2
20	CLA	A	832	-	-	12/23/99/115	-
22	BCR	A	843	-	-	15/29/63/63	0/2/2/2
20	CLA	B	810	-	1/1/15/20	23/39/115/115	-
20	CLA	F	206	20	3/3/12/20	10/25/101/115	-
20	CLA	B	821	-	-	9/26/102/115	-
20	CLA	A	802	-	1/1/13/20	12/27/103/115	-
20	CLA	A	816	-	1/1/15/20	19/39/115/115	-
20	CLA	A	822	-	1/1/15/20	18/39/115/115	-
21	LMU	L	205	-	-	14/21/61/61	0/2/2/2
21	LMU	4	301	-	-	13/21/61/61	0/2/2/2
20	CLA	3	310	-	1/1/15/20	22/39/115/115	-
22	BCR	B	842	-	-	11/29/63/63	0/2/2/2
20	CLA	B	809	6	1/1/13/20	12/27/103/115	-
22	BCR	J	101	-	-	12/29/63/63	0/2/2/2
20	CLA	2	310	2	-	8/21/97/115	-
20	CLA	B	814	-	1/1/13/20	12/32/108/115	-
20	CLA	B	826	6	1/1/15/20	27/39/115/115	-
20	CLA	A	838	-	-	11/21/97/115	-
21	LMU	R	108	-	-	16/21/61/61	0/2/2/2
22	BCR	A	841	-	-	13/29/63/63	0/2/2/2
20	CLA	B	834	6	1/1/14/20	16/33/109/115	-
22	BCR	L	209	-	-	12/29/63/63	0/2/2/2
20	CLA	A	847	-	1/1/15/20	25/39/115/115	-
20	CLA	A	834	-	-	8/18/94/115	-
20	CLA	A	818	-	-	9/23/99/115	-
20	CLA	B	824	-	1/1/15/20	17/39/115/115	-
20	CLA	A	828	5	1/1/15/20	23/39/115/115	-
21	LMU	L	206	-	-	14/21/61/61	0/2/2/2

The worst 5 of 2661 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	B	850	BCR	C21-C22	-11.03	1.21	1.35
22	I	101	BCR	C21-C22	-10.00	1.22	1.35
22	B	850	BCR	C20-C21	-9.90	1.12	1.43
20	1	209	CLA	CAB-C3B	-9.65	1.30	1.50
22	F	203	BCR	C21-C22	-9.40	1.23	1.35

The worst 5 of 5347 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	B	844	BCR	C20-C21-C22	36.92	179.99	127.31
22	J	101	BCR	C20-C21-C22	36.90	179.97	127.31
22	A	842	BCR	C20-C21-C22	36.89	179.95	127.31
22	A	843	BCR	C20-C21-C22	36.88	179.95	127.31
22	A	841	BCR	C20-C21-C22	36.87	179.93	127.31

5 of 98 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
20	1	206	CLA	C8
20	1	207	CLA	C2A
20	1	211	CLA	CBD
20	1	212	CLA	C8
20	1	214	CLA	C3A

5 of 2841 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

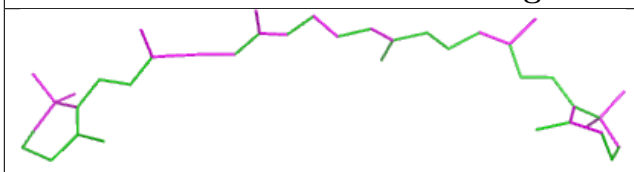
There are no ring outliers.

4 monomers are involved in 3 short contacts:

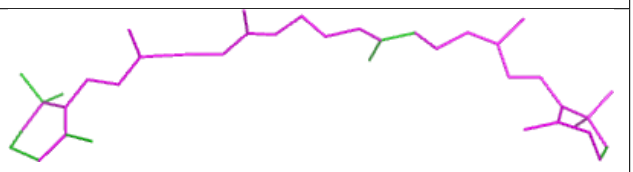
Mol	Chain	Res	Type	Clashes	Symm-Clashes
21	2	313	LMU	0	1
20	1	207	CLA	0	2
20	K	105	CLA	0	2
20	A	831	CLA	0	1

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 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.

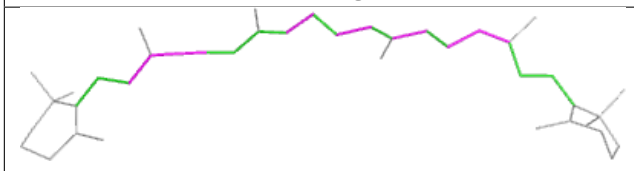
Ligand BCR B 850



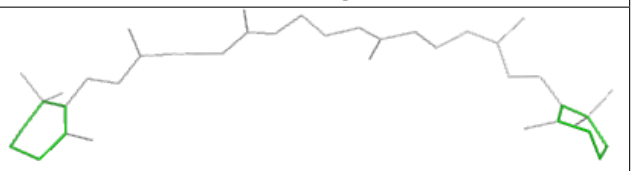
Bond lengths



Bond angles

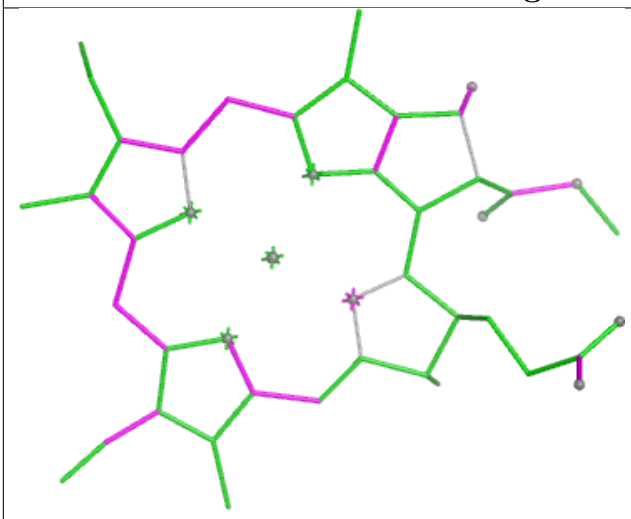


Torsions

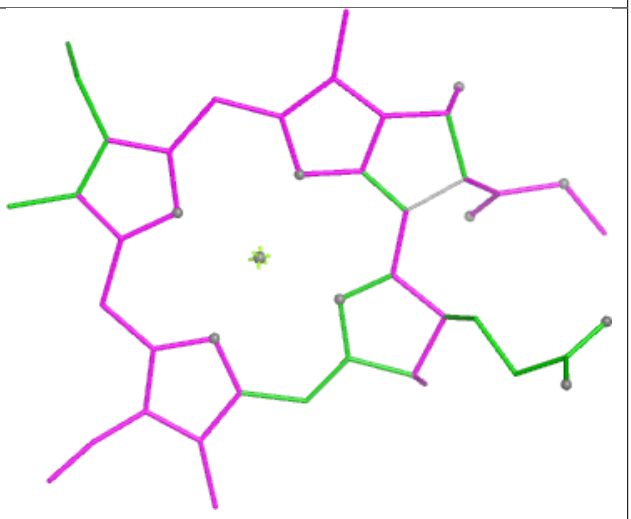


Rings

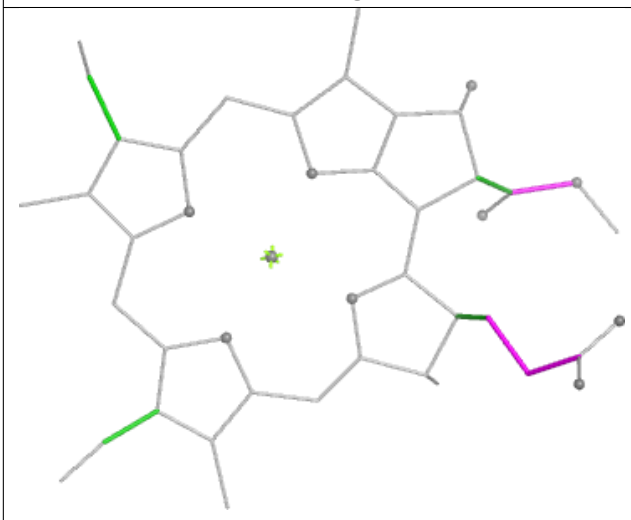
Ligand CLA A 808



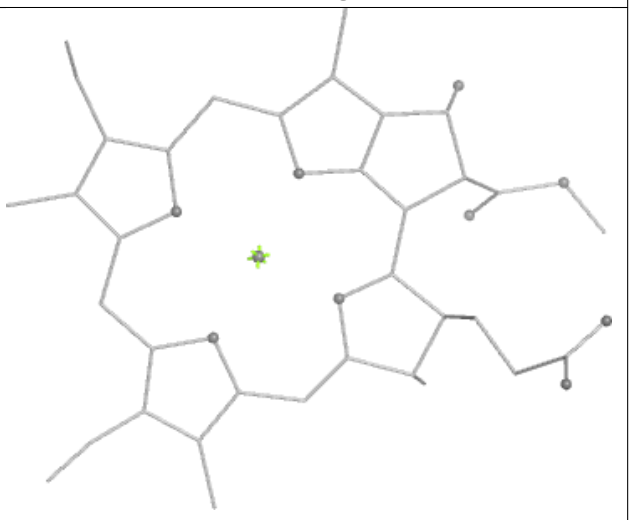
Bond lengths



Bond angles

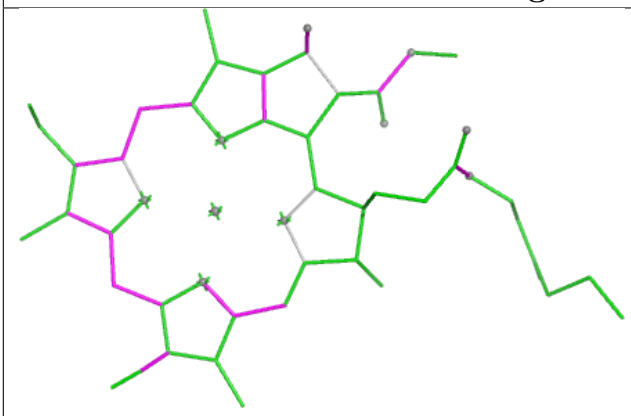


Torsions

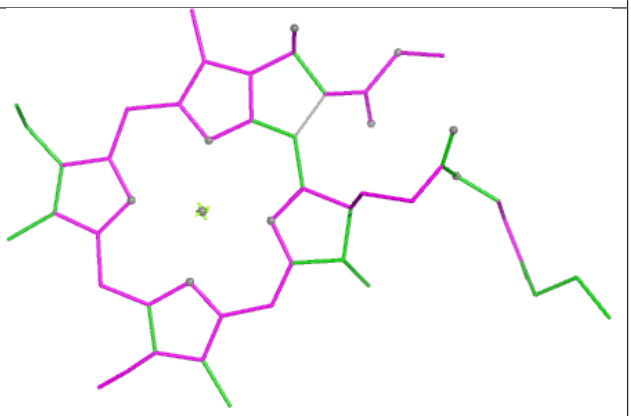


Rings

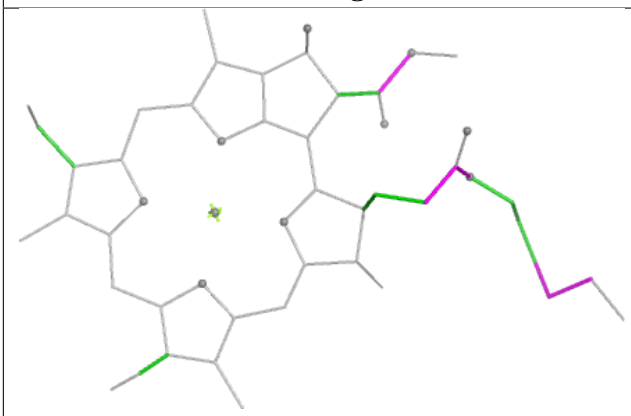
Ligand CLA 4 318



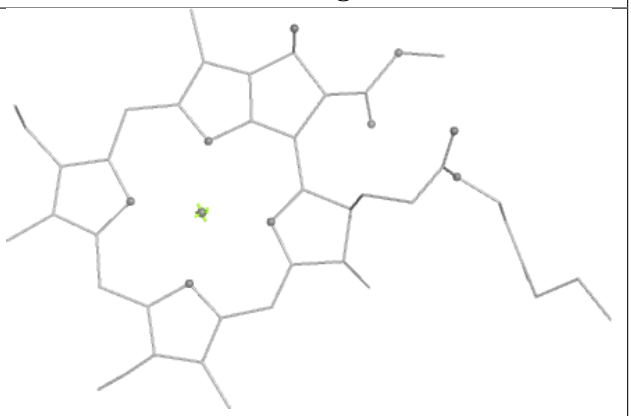
Bond lengths



Bond angles

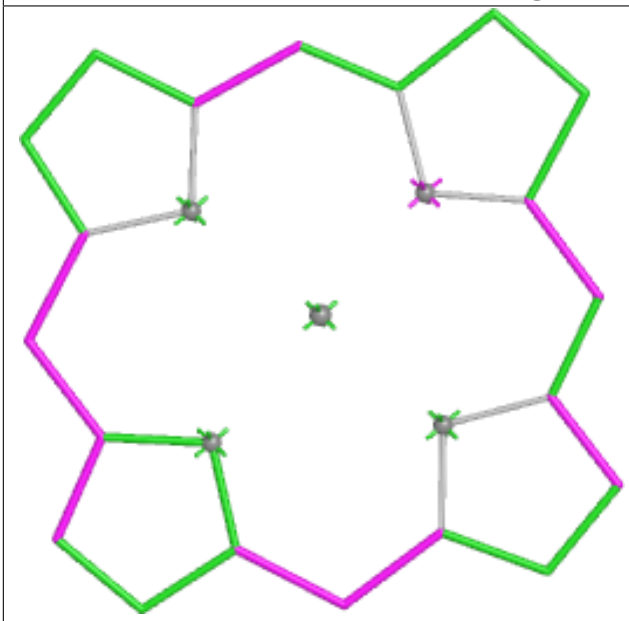


Torsions



Rings

Ligand CLA 4 317



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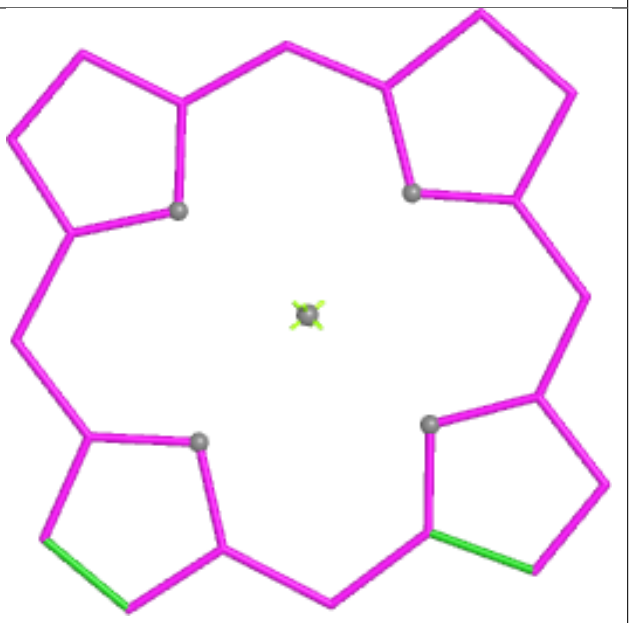
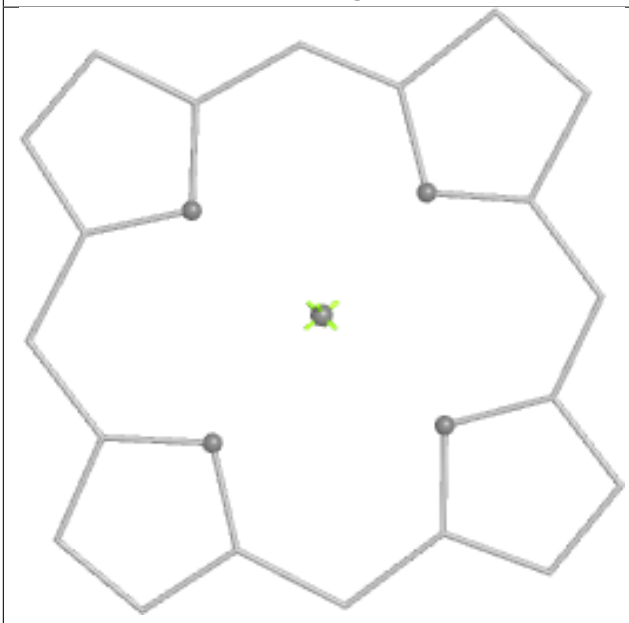


Bond angles



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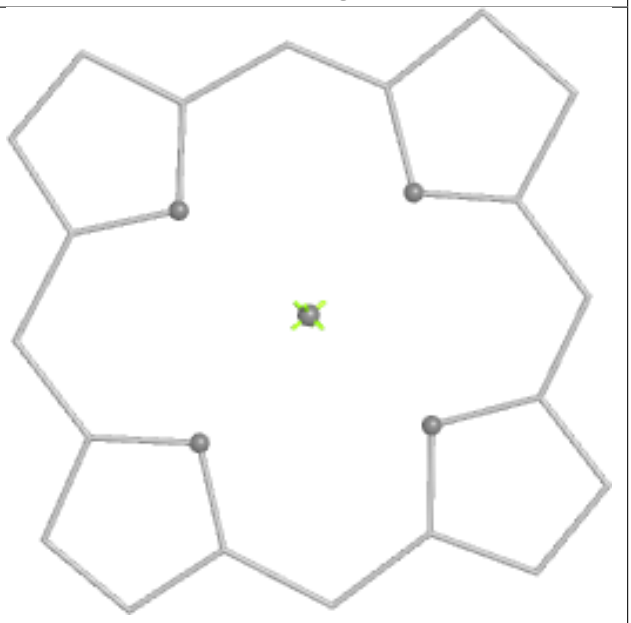
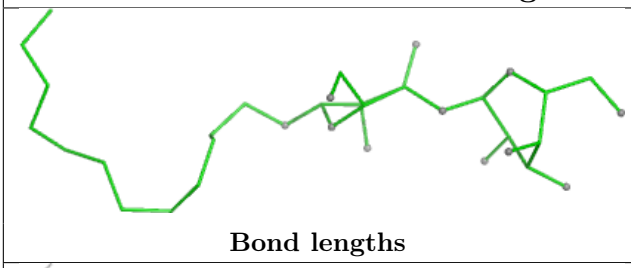


Rings

Ligand LMU A 845



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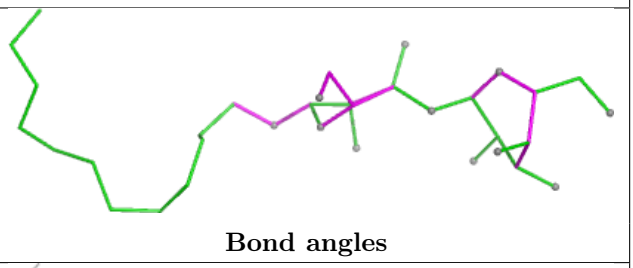
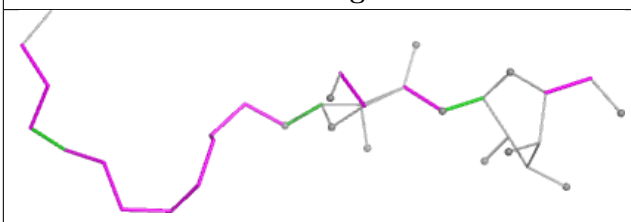


Bond angles



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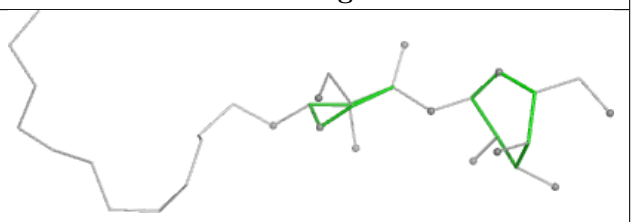
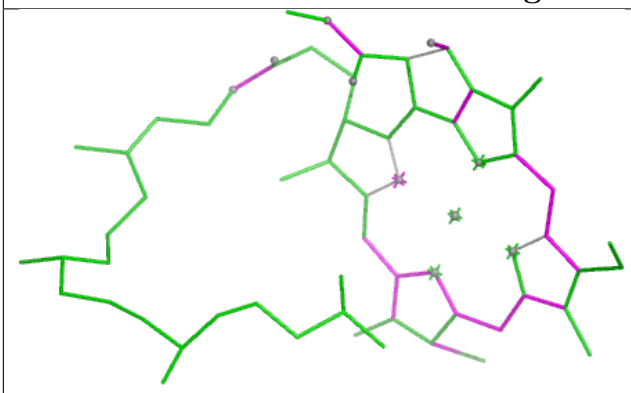


Rings

Ligand CLA A 837



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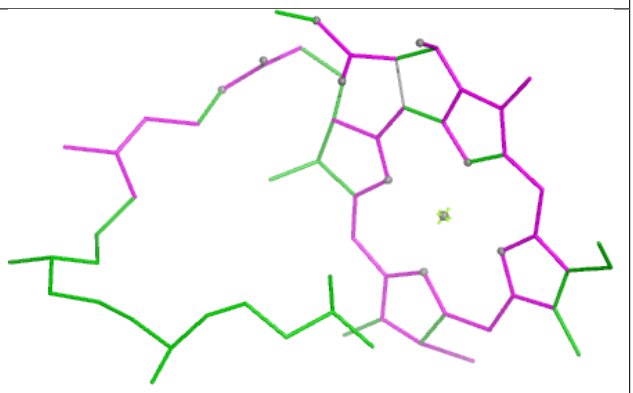
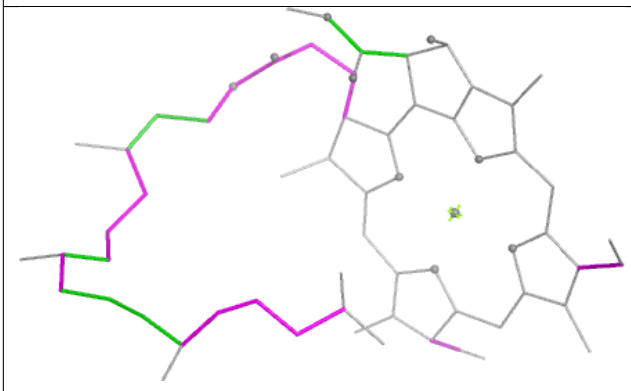


Bond angles



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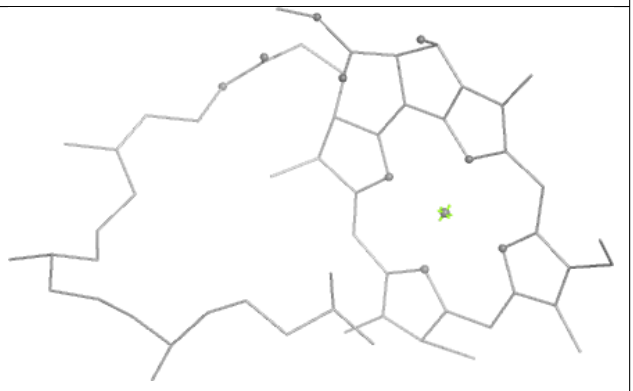
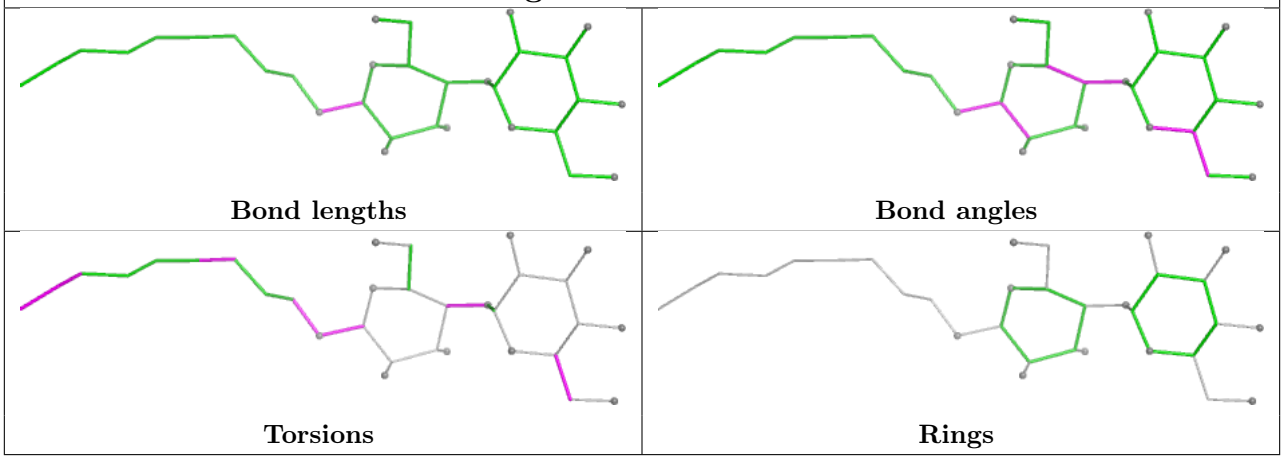
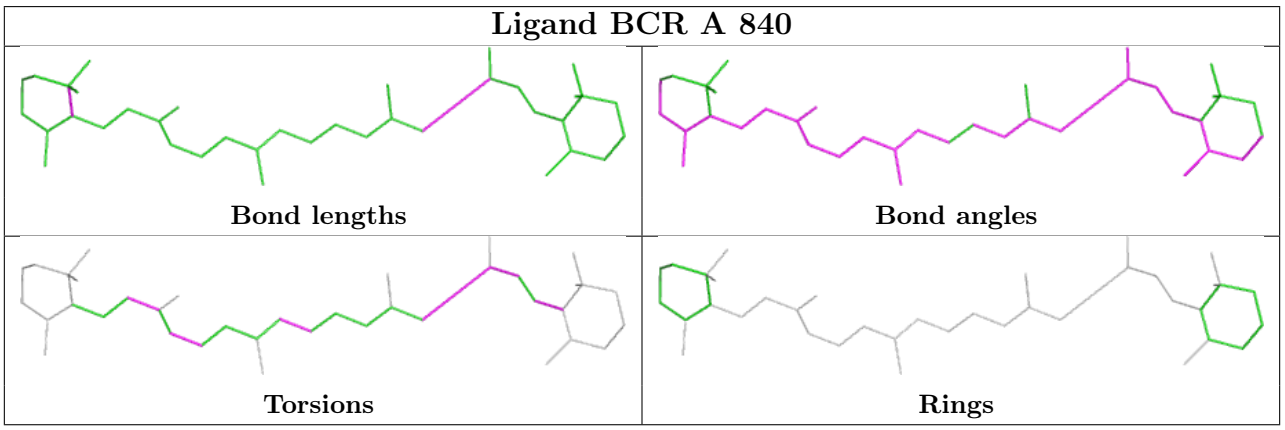


Rings

Ligand LMU 2 320



Ligand BCR A 840



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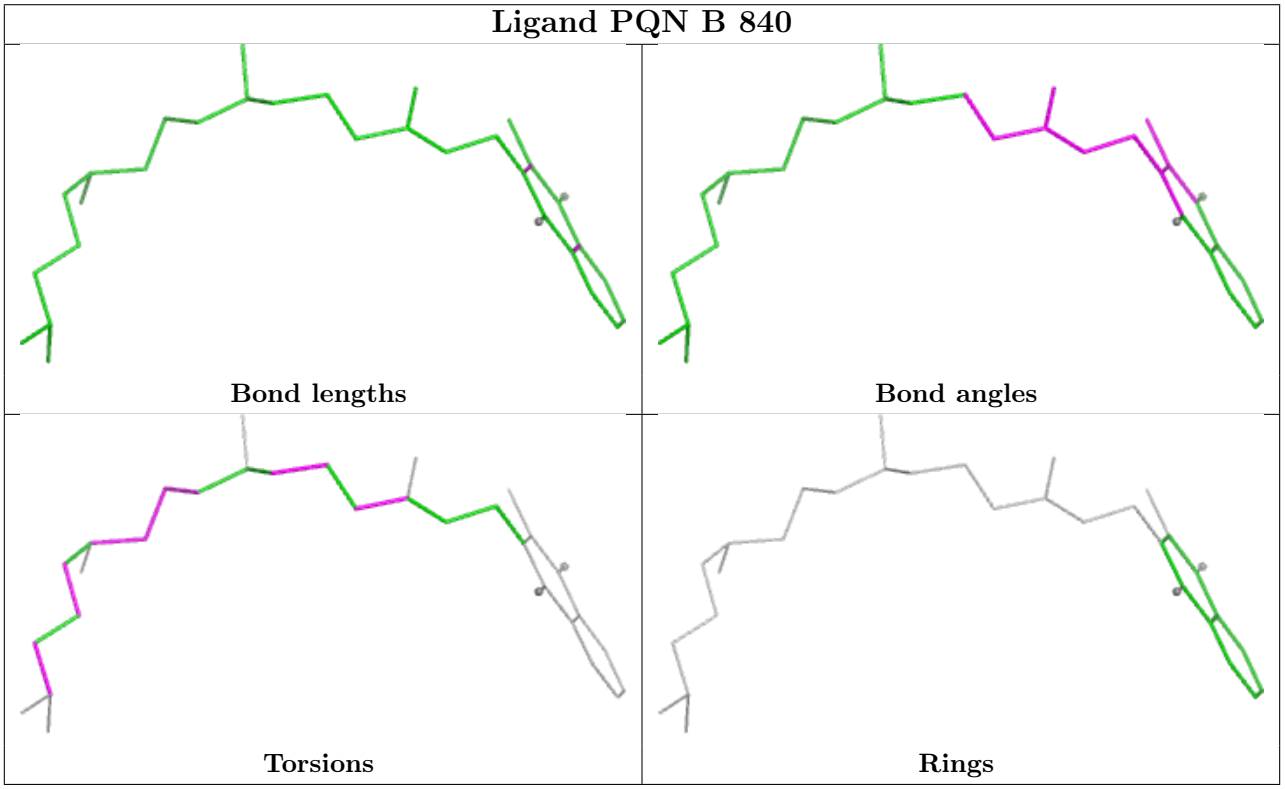
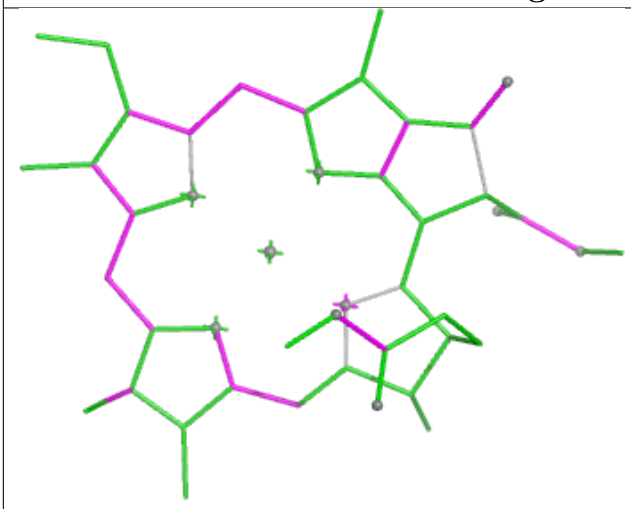
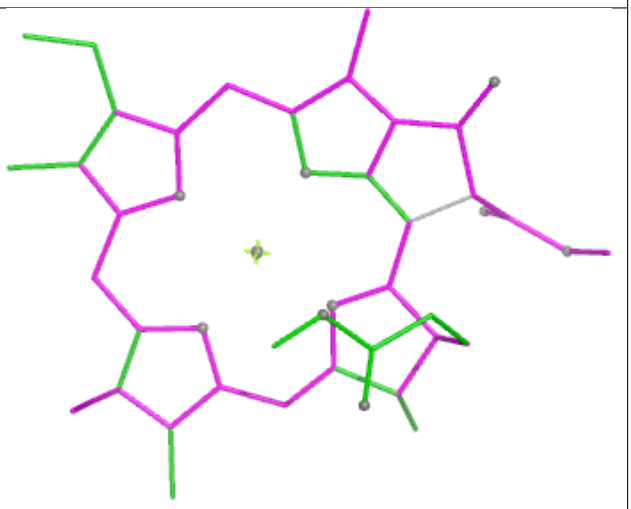


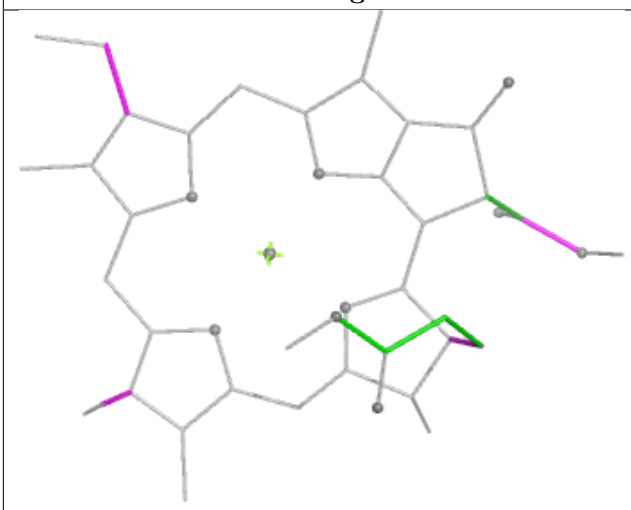
Ligand CLA 1 204



Bond lengths



Bond angles



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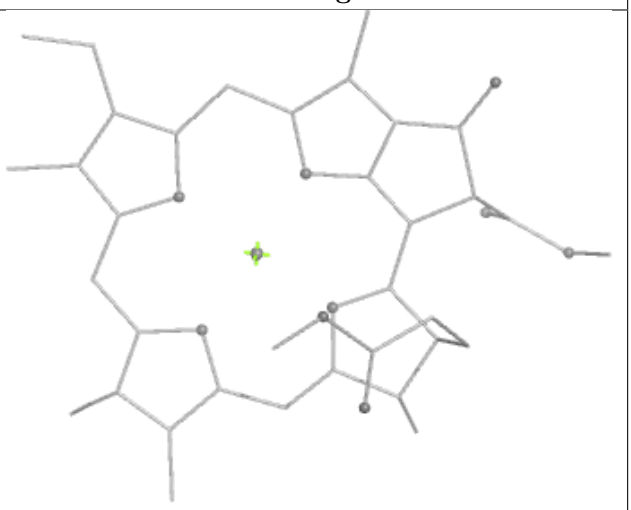
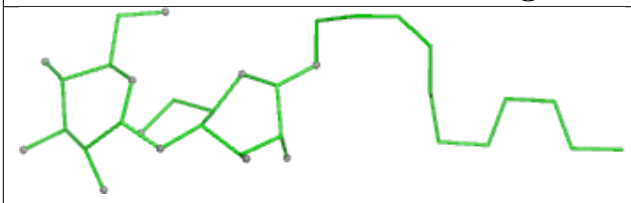


Rings

Ligand LMU R 101



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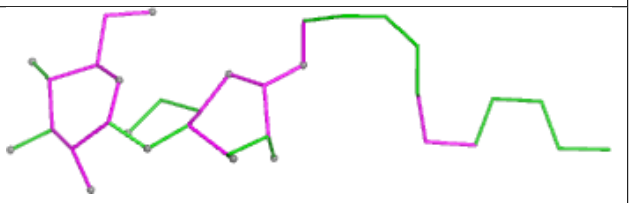
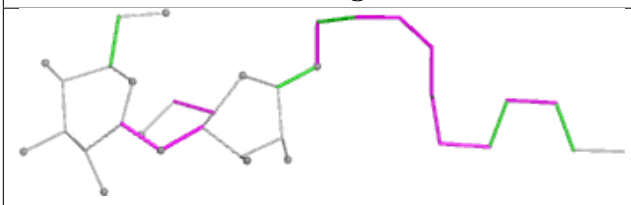
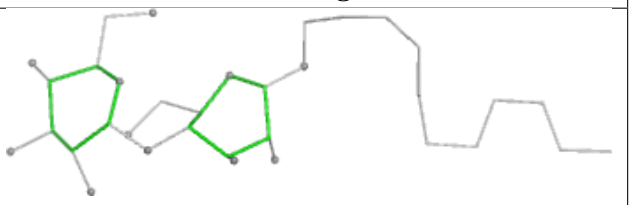


Bond angles

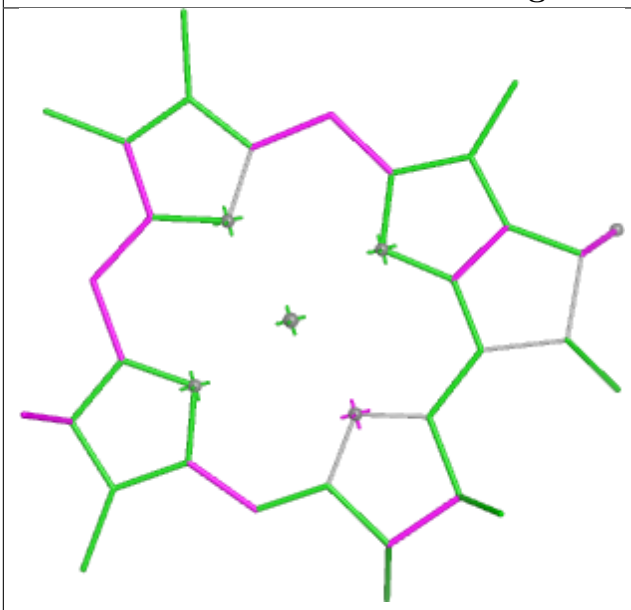


Torsions



Rings

Ligand CLA 4 313



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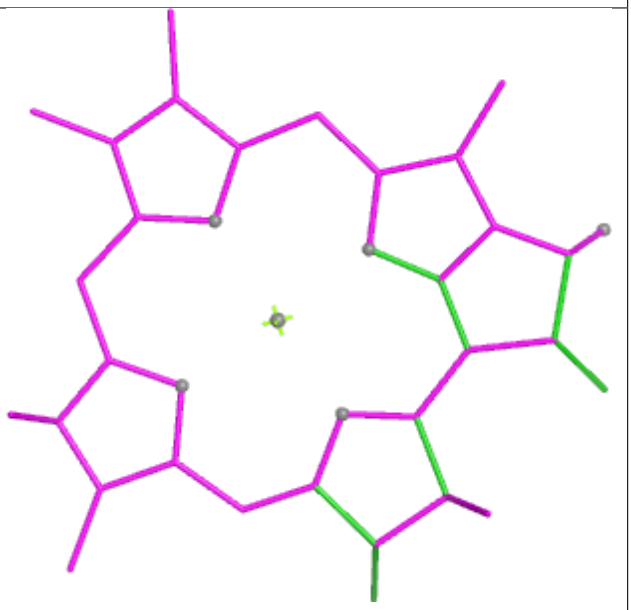
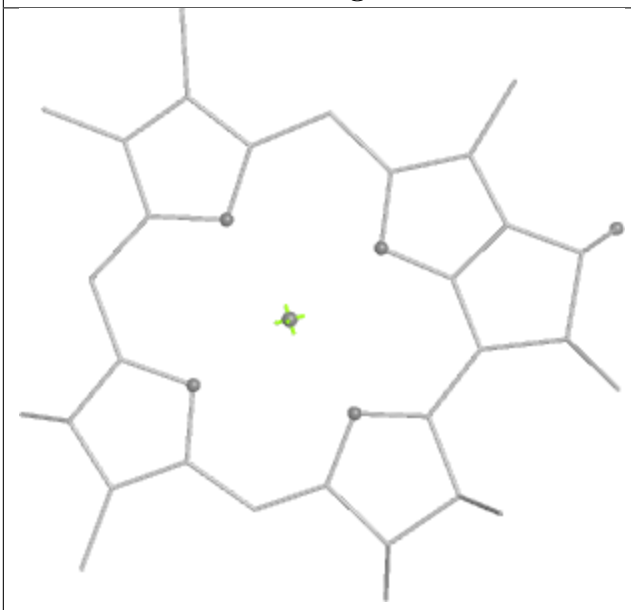


Bond angles



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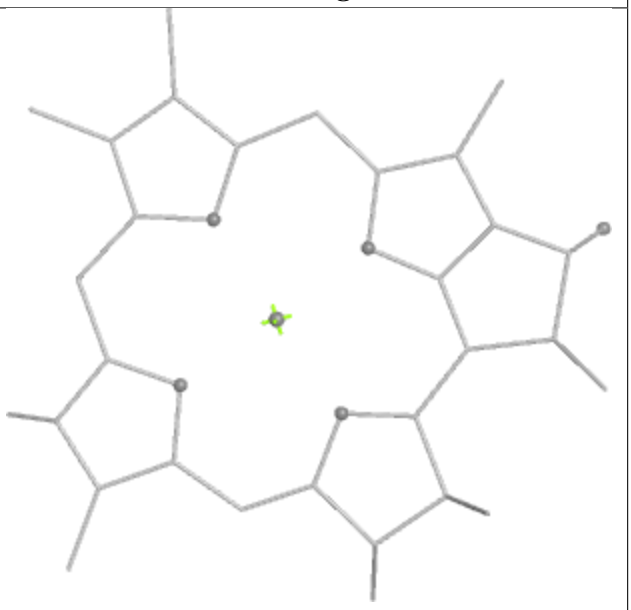
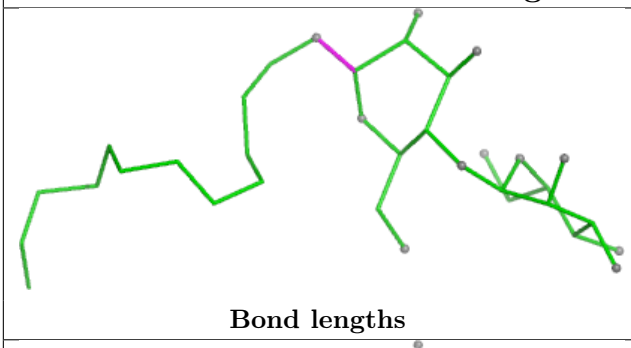
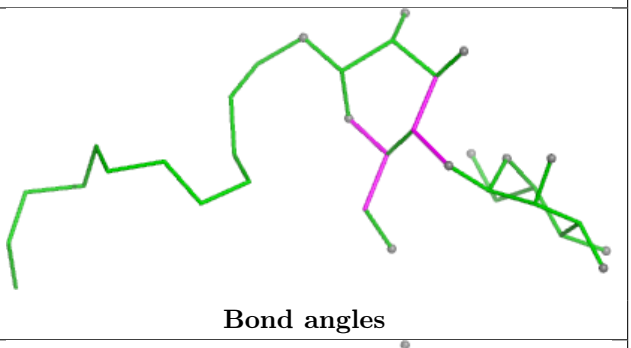


Rings

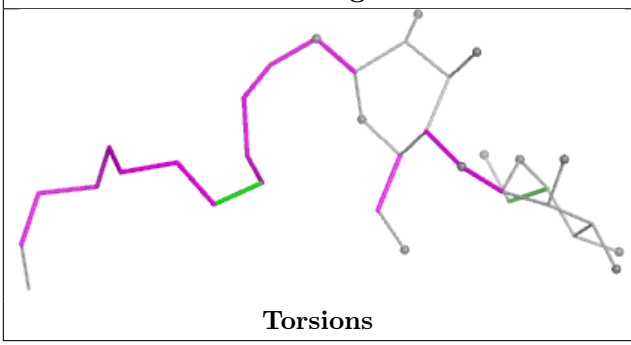
Ligand LMU 2 313



Bond lengths



Bond angles



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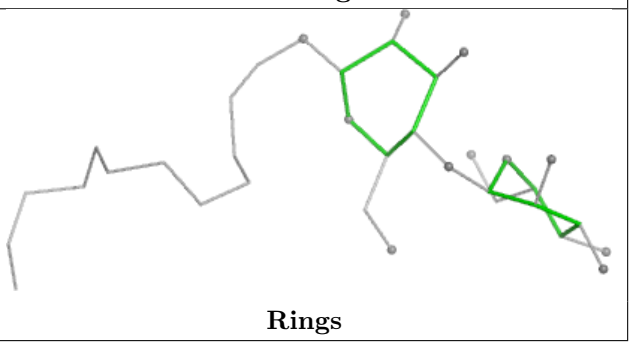
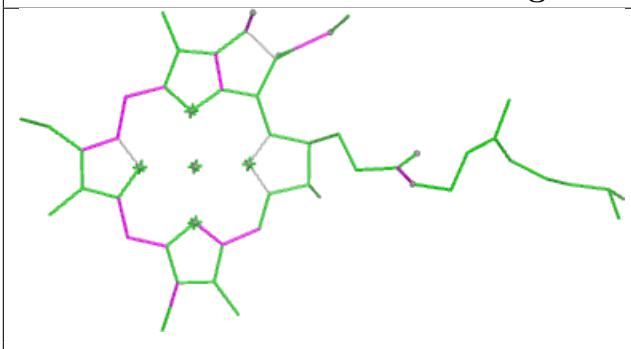


Rings

Ligand CLA 3 320



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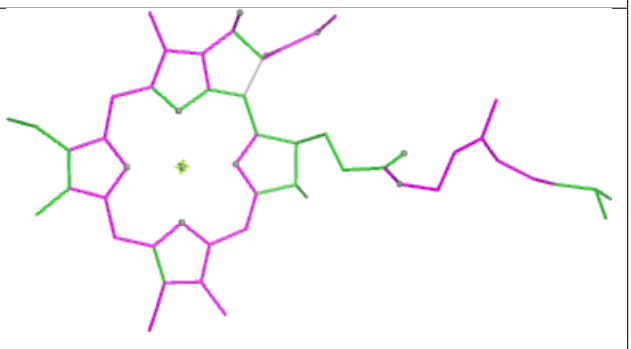
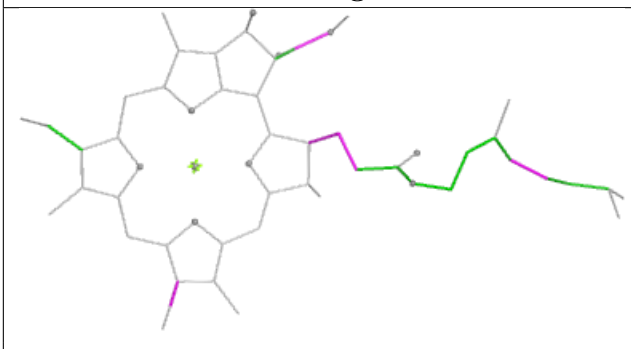


Bond angles



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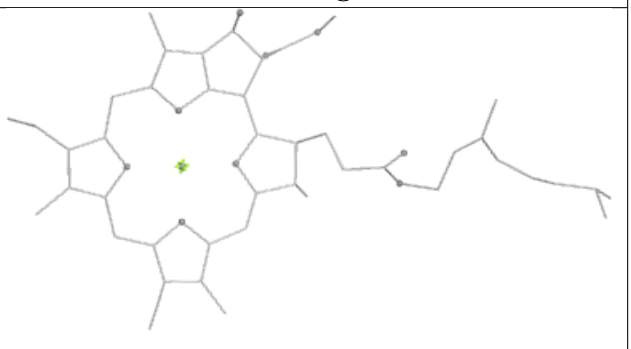
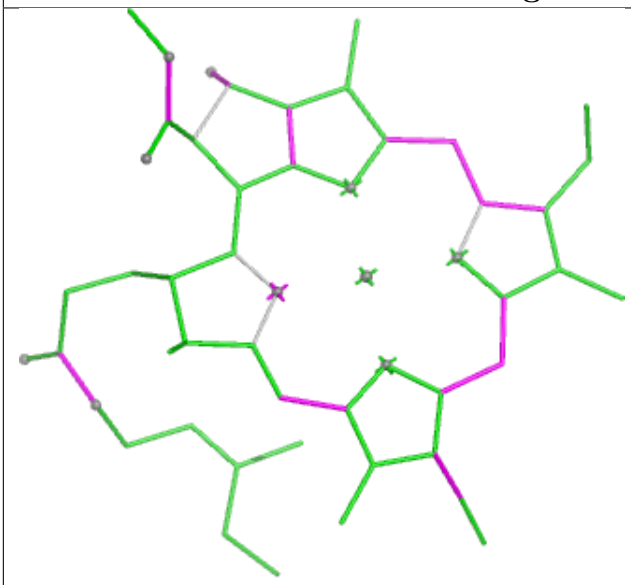
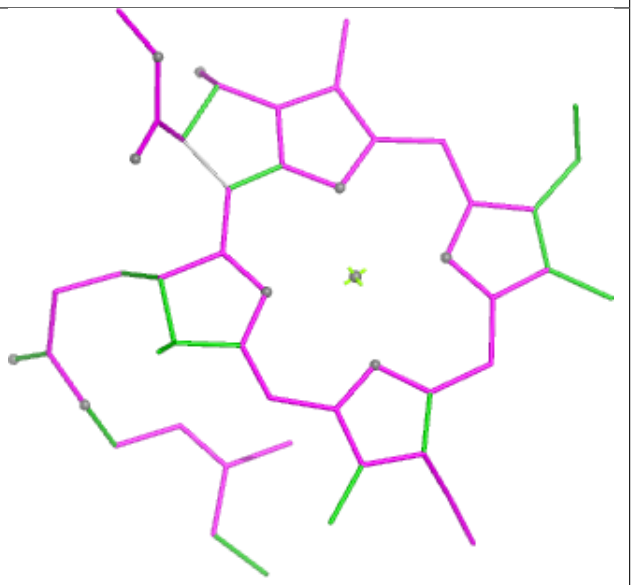


Rings

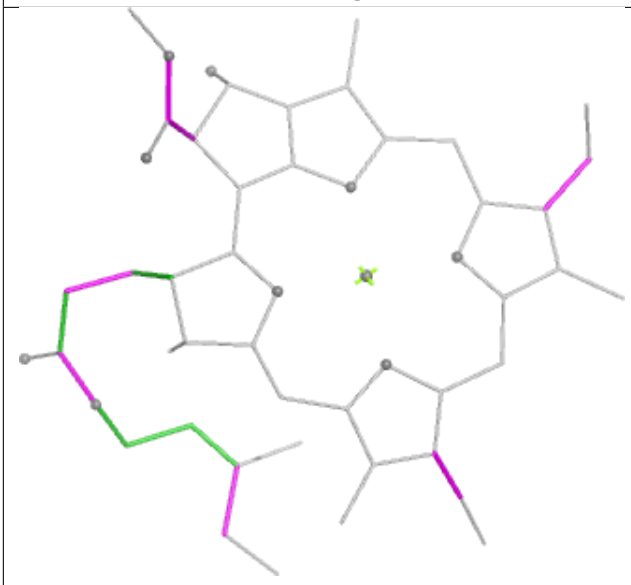
Ligand CLA G 103



Bond lengths



Bond angles



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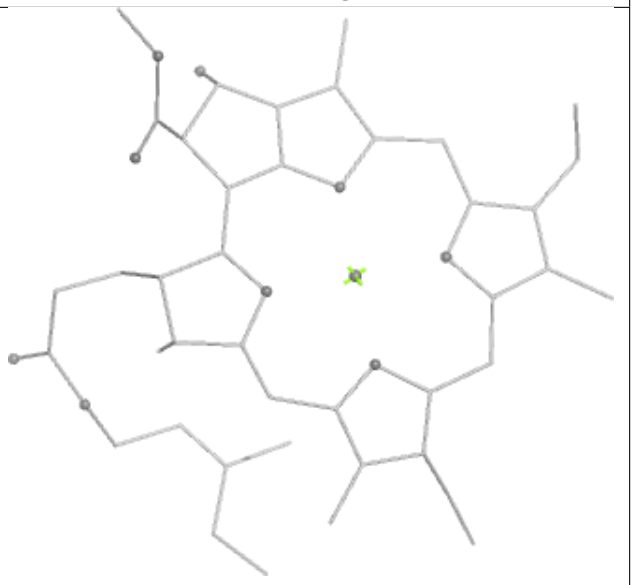
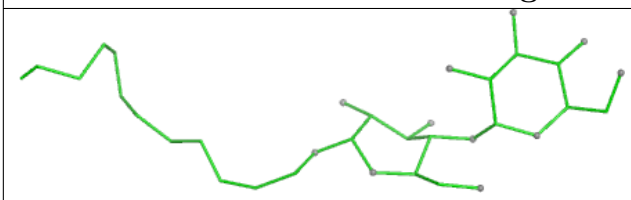
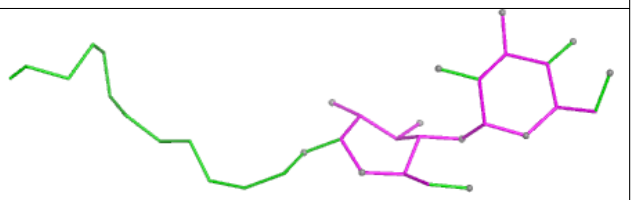


Rings

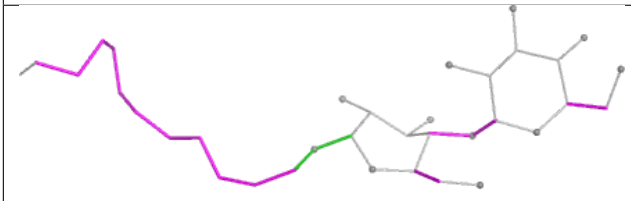
Ligand LMU B 801



Bond lengths



Bond angles



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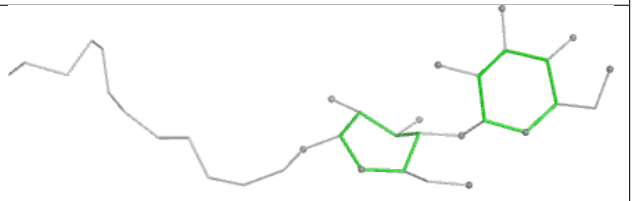
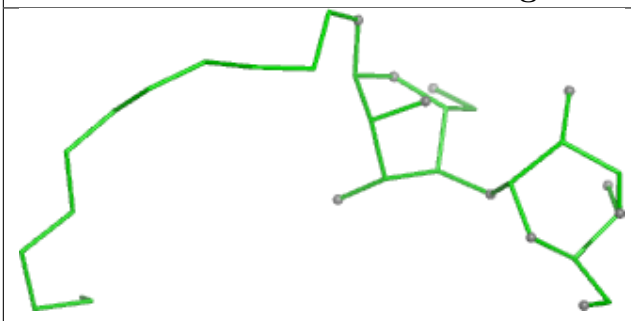


Rings

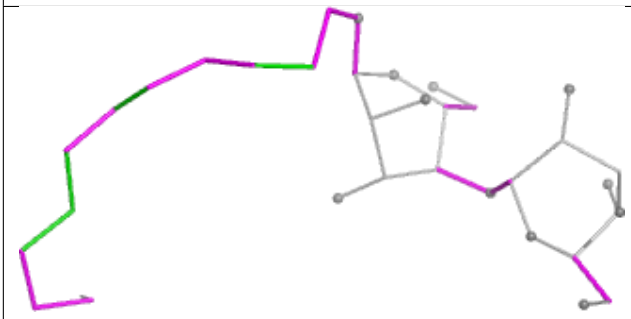
Ligand LMU R 103



Bond lengths



Bond angles



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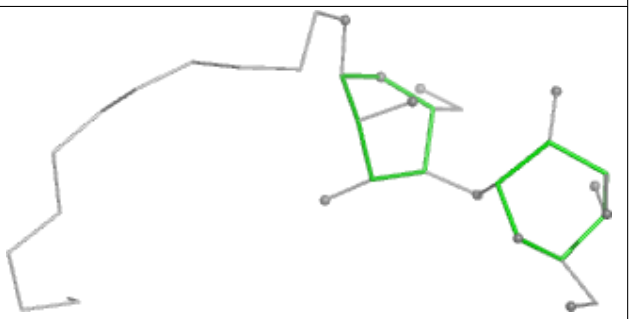
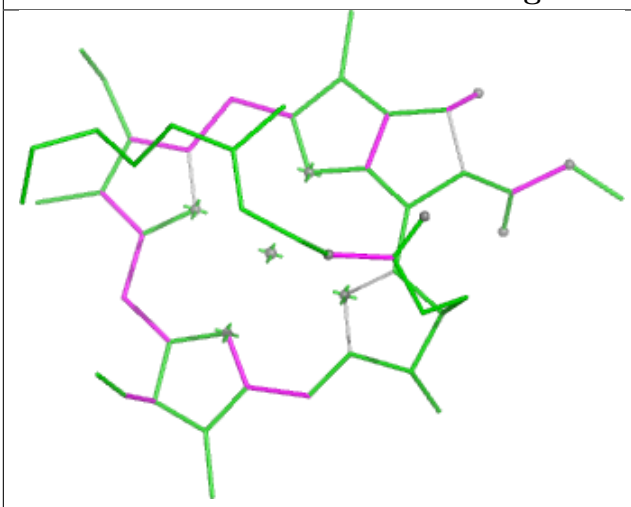
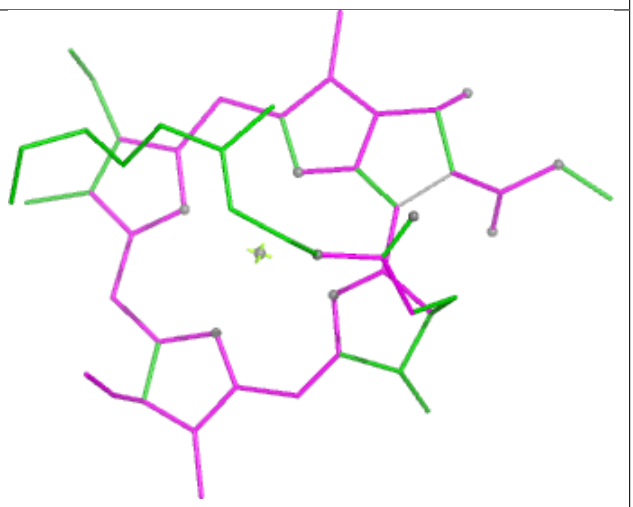


Rings

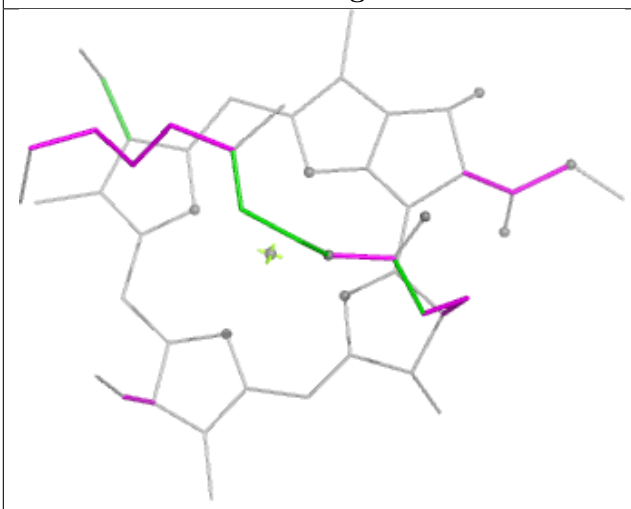
Ligand CLA A 810



Bond lengths



Bond angles



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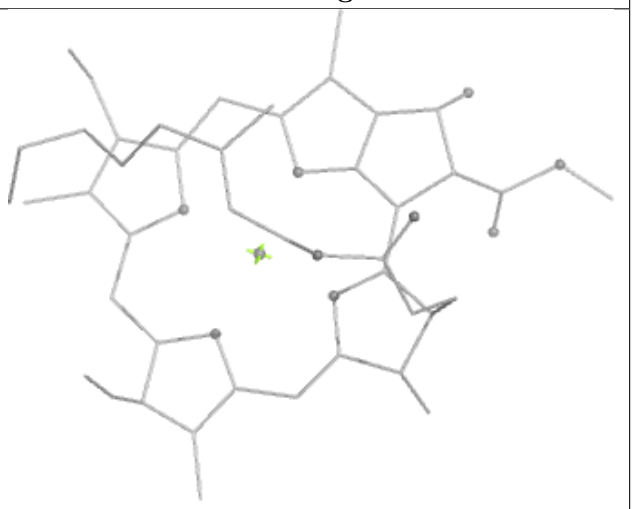
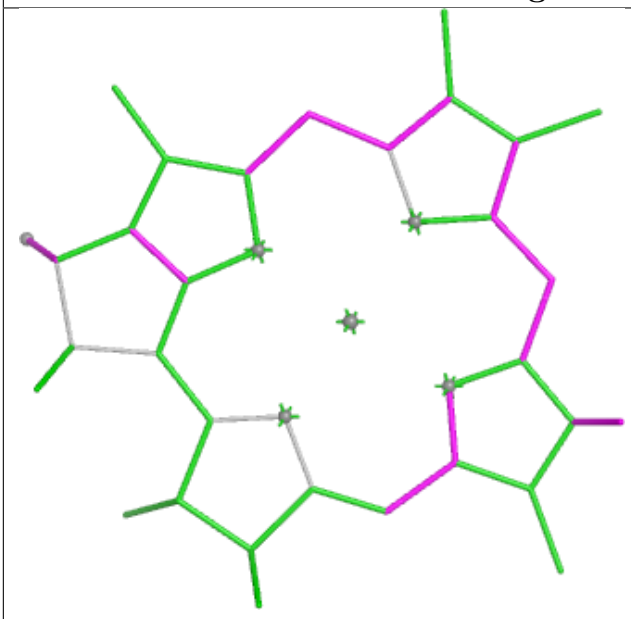
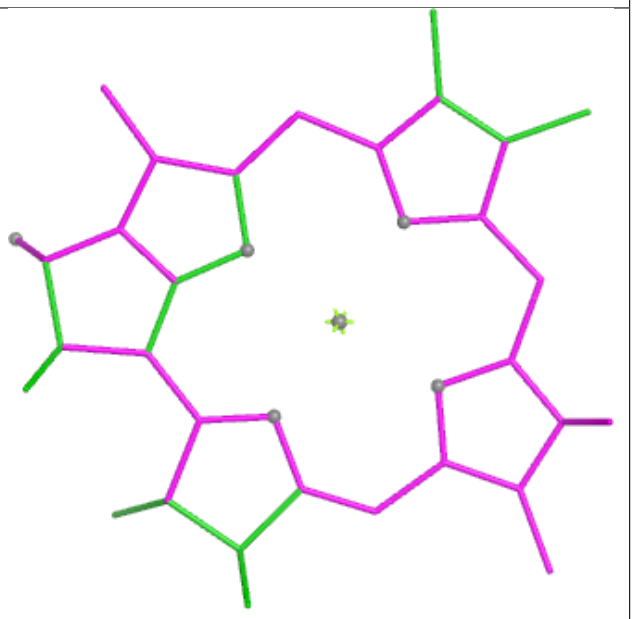


Rings

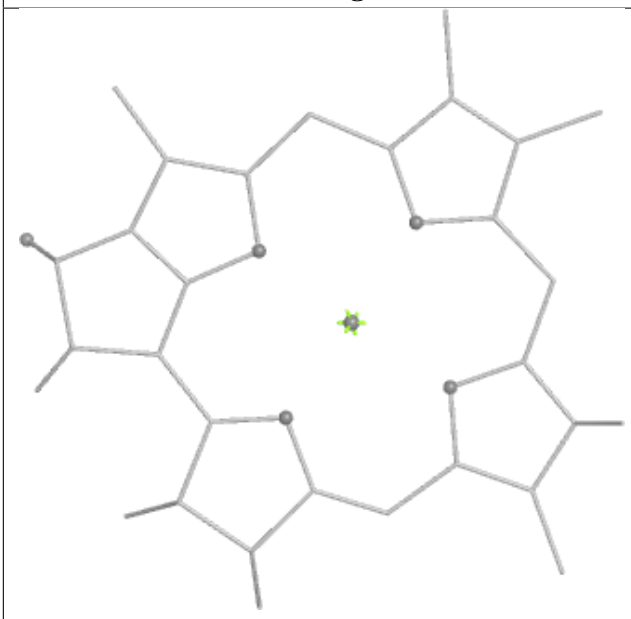
Ligand CLA 3 319



Bond lengths



Bond angles



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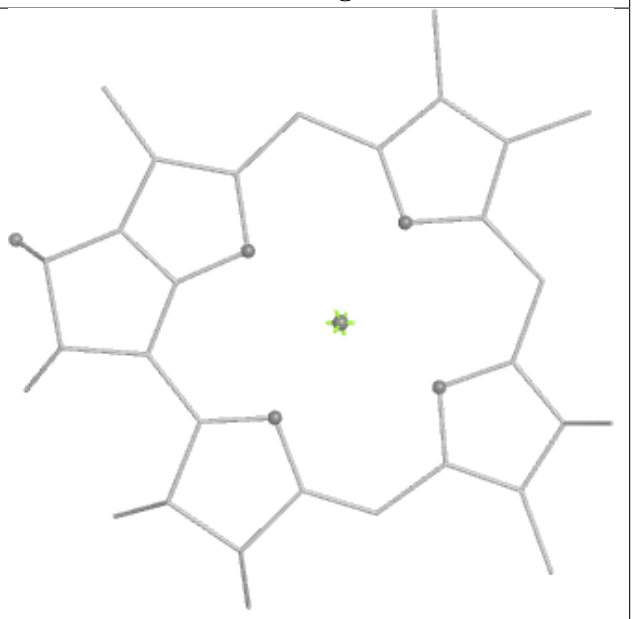
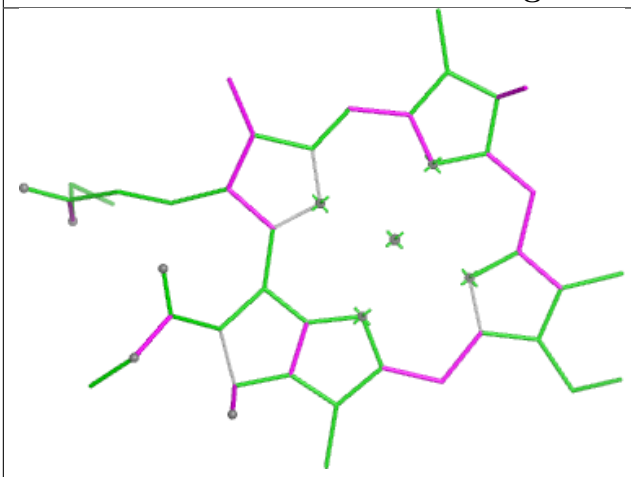
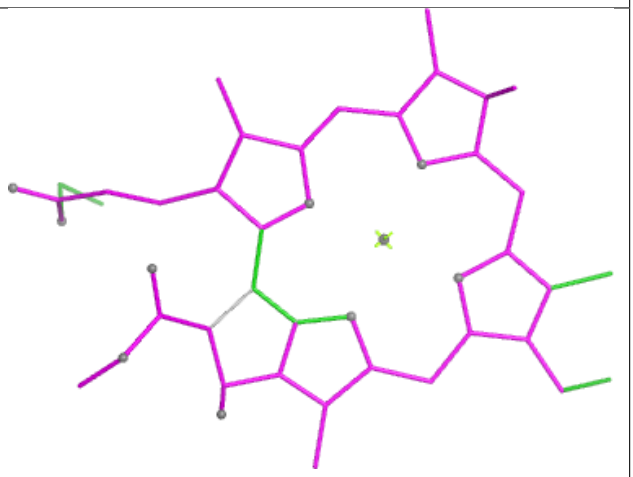


Rings

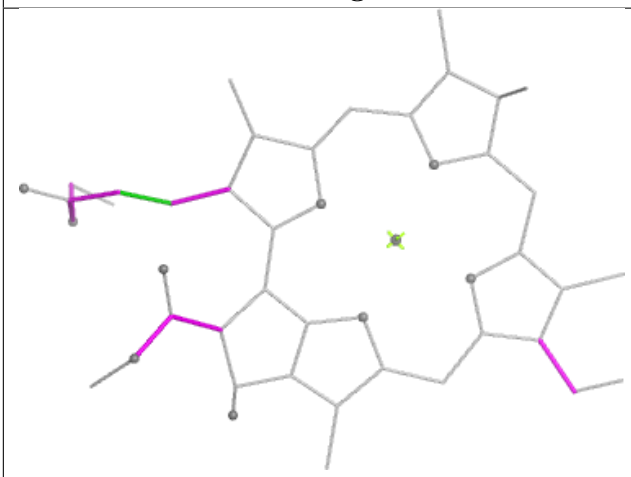
Ligand CLA A 850



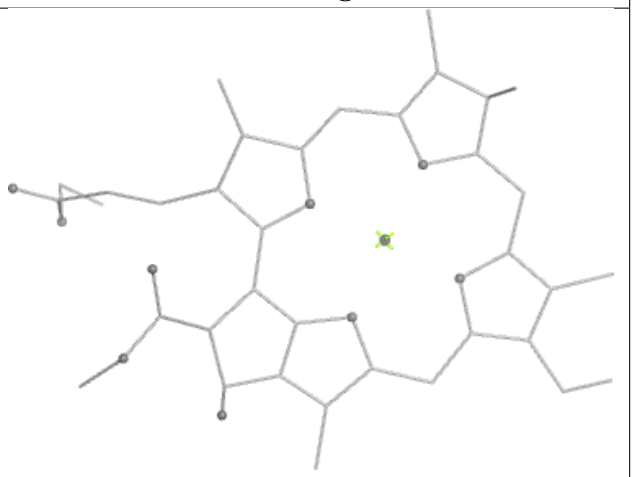
Bond lengths



Bond angles

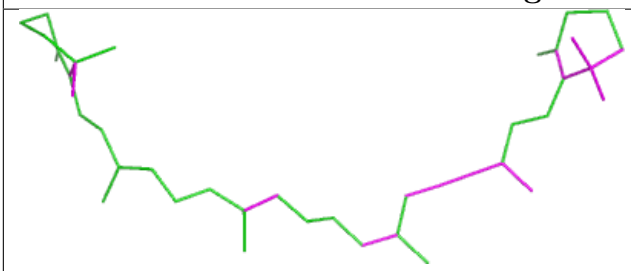


Torsions



Rings

Ligand BCR F 203



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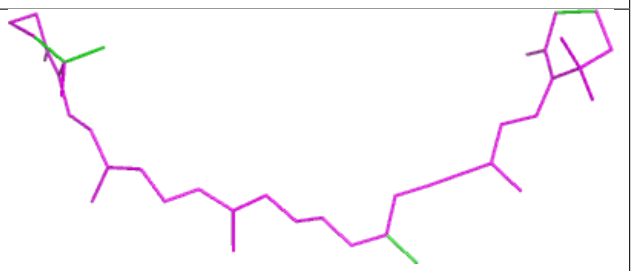

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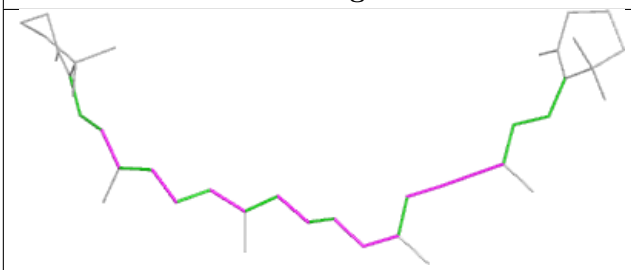

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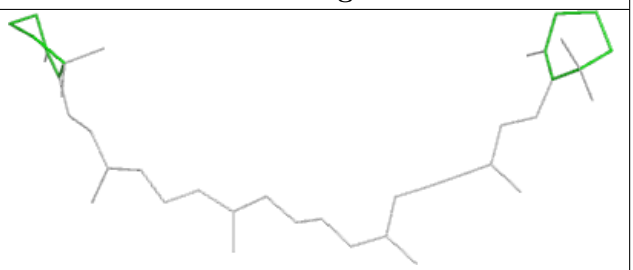
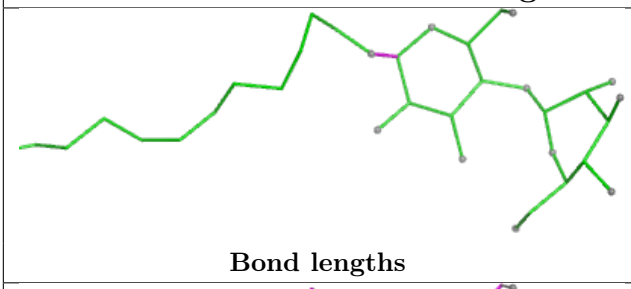


Rings

Ligand LMU A 854



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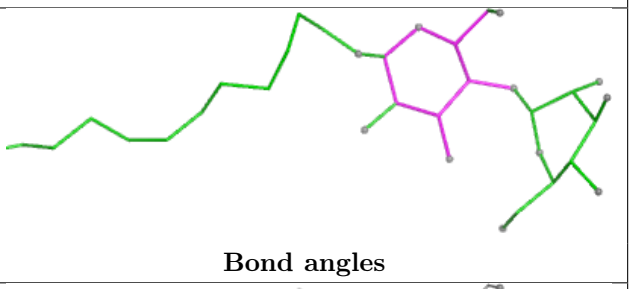
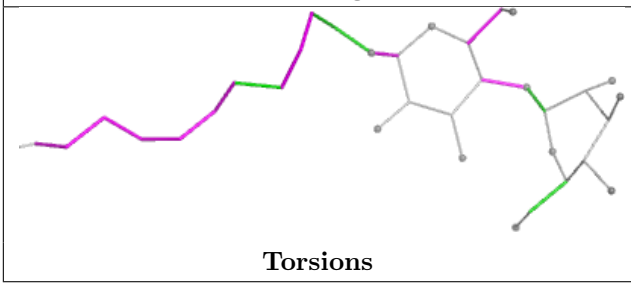
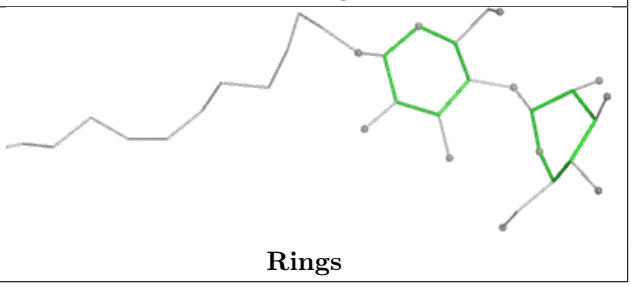


Bond angles

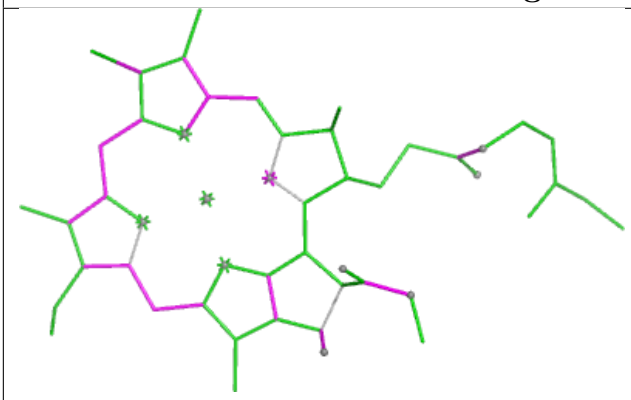


Torsions



Rings

Ligand CLA A 835



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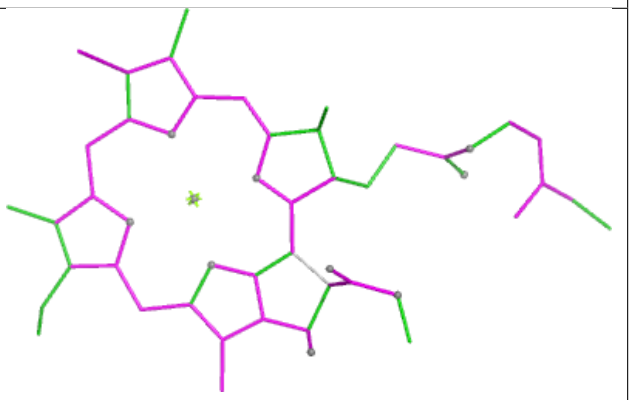
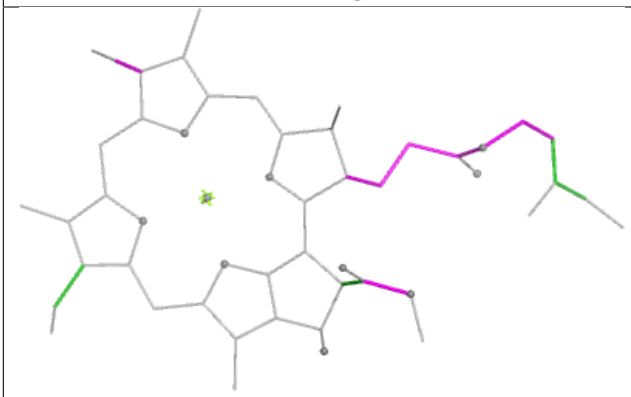
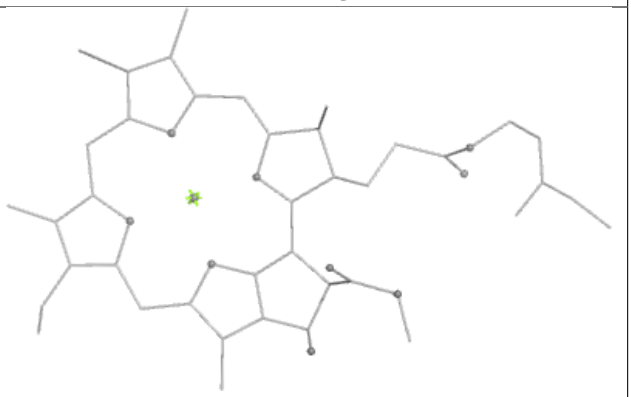


Bond angles

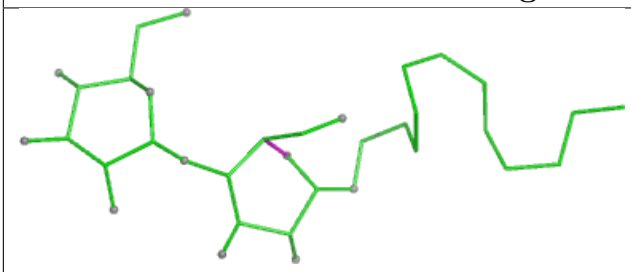


Torsions

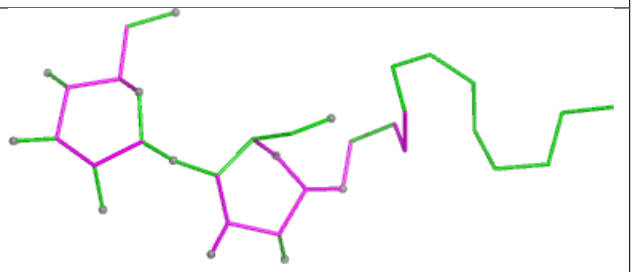


Rings

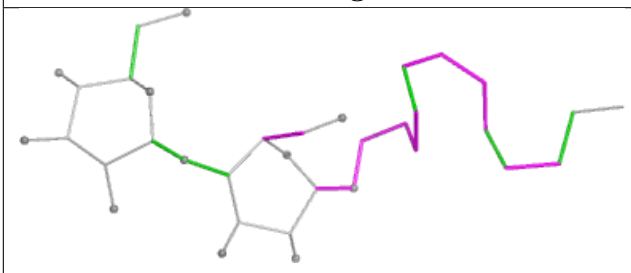
Ligand LMU A 852



Bond lengths



Bond angles



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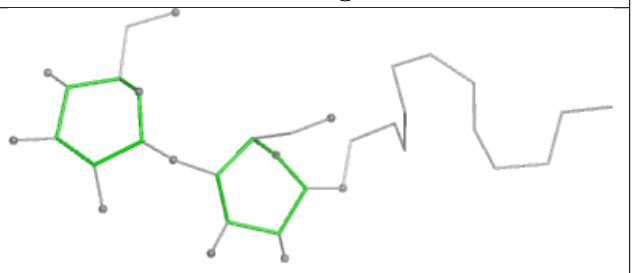
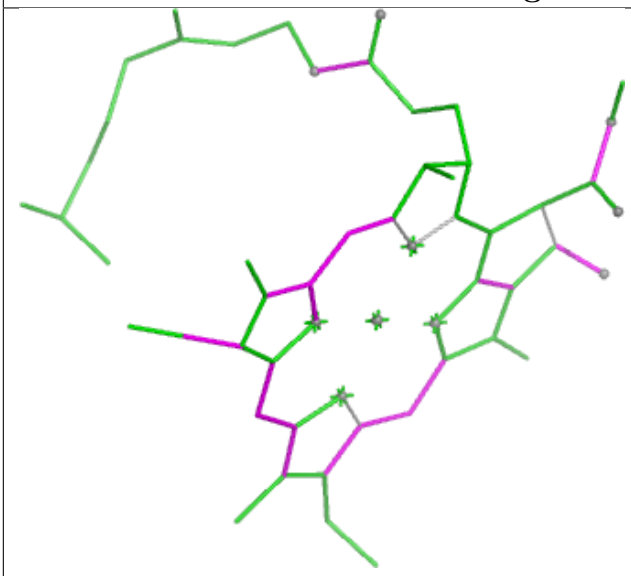


Rings

Ligand CLA A 820



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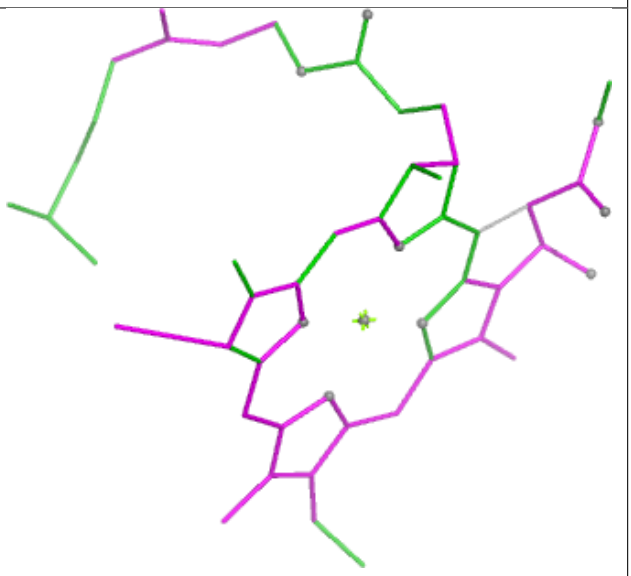
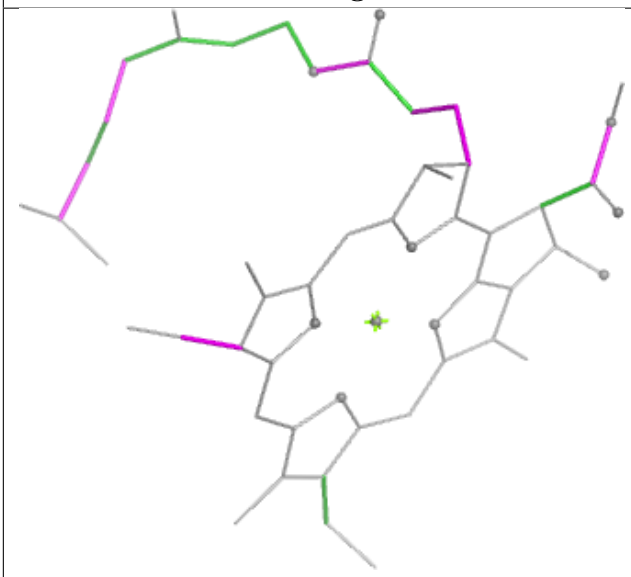


Bond angles

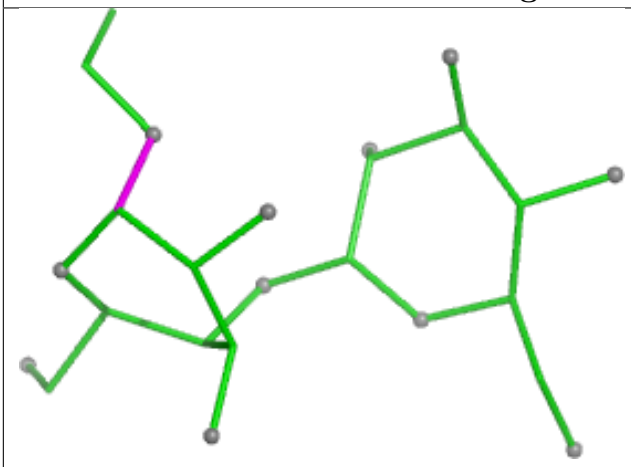


Torsions



Rings

Ligand LMU B 845



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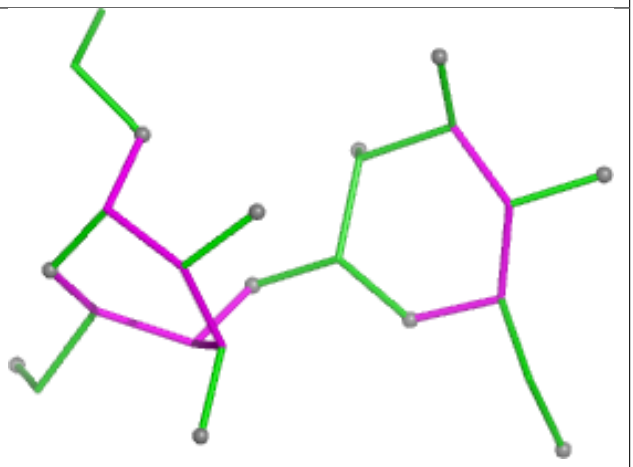
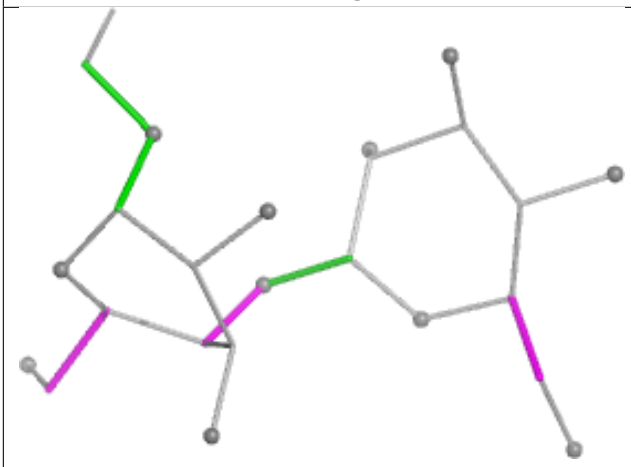


Bond angles



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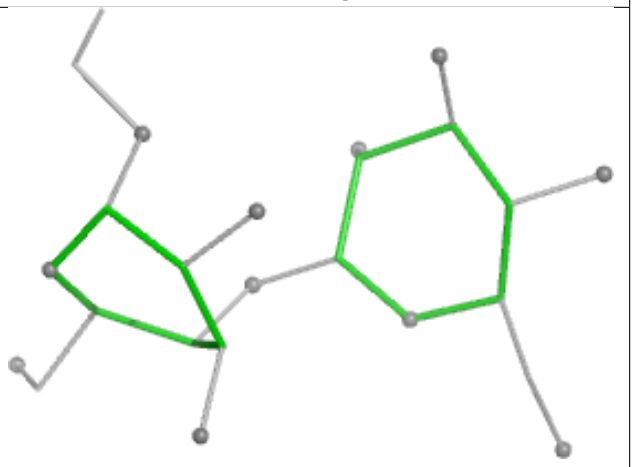
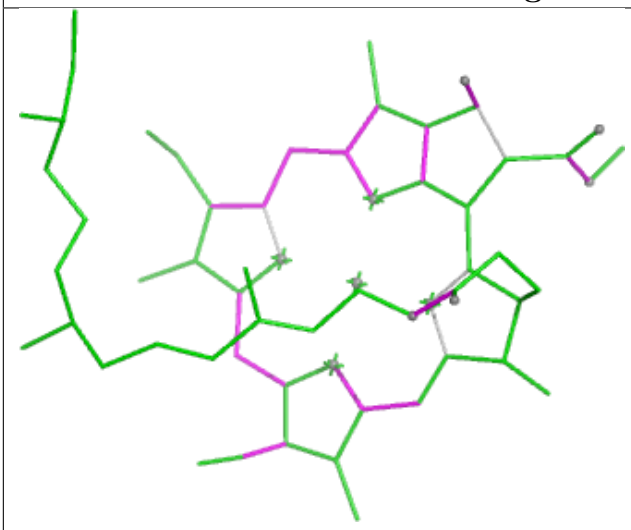
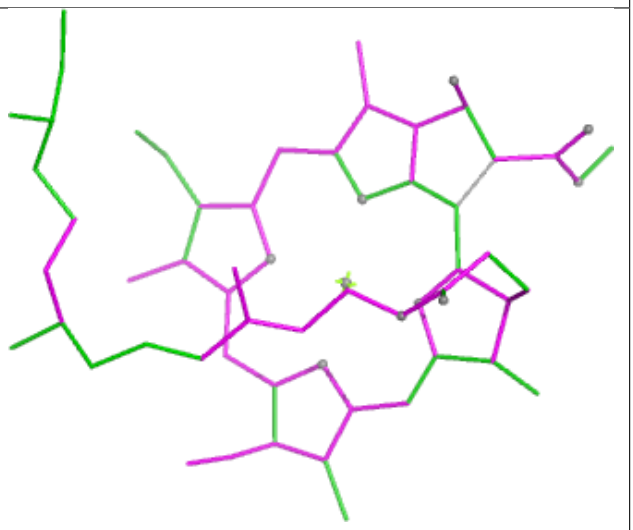


Rings

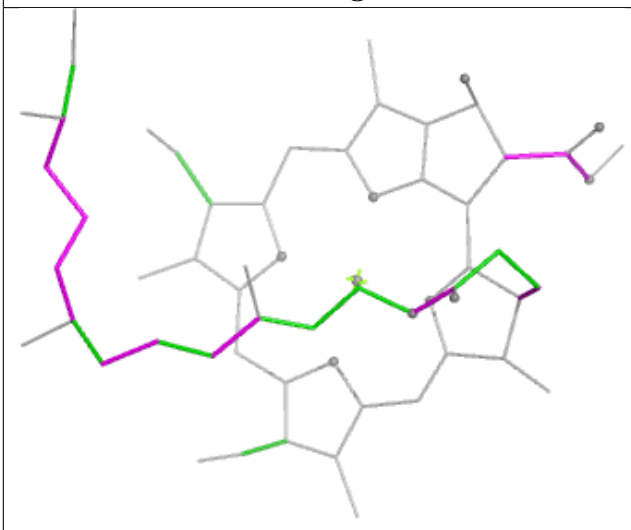
Ligand CLA B 816



Bond lengths



Bond angles



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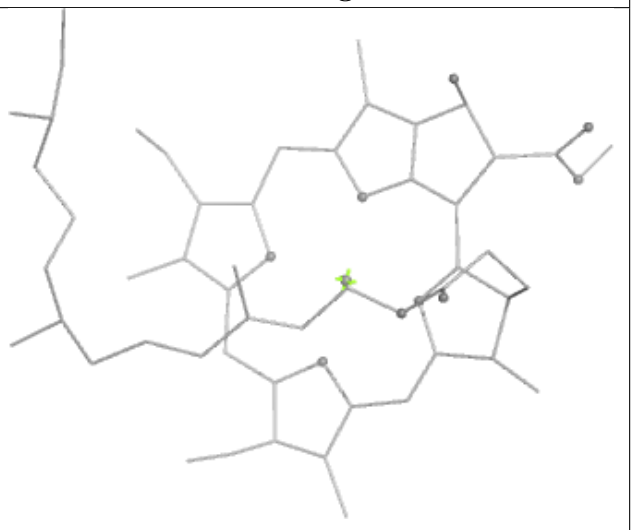
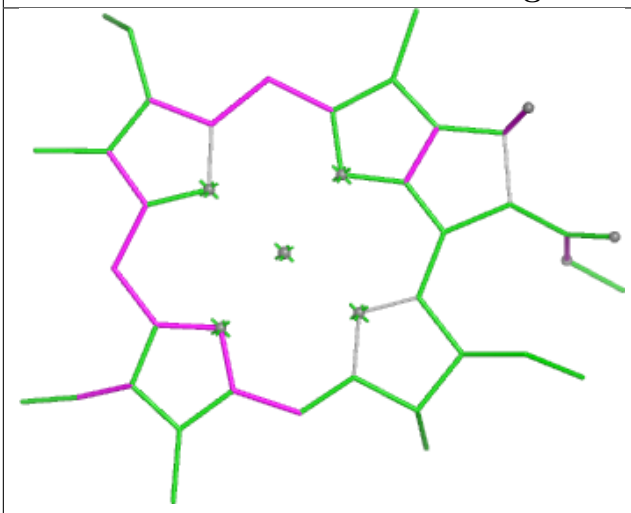


Rings

Ligand CLA A 819



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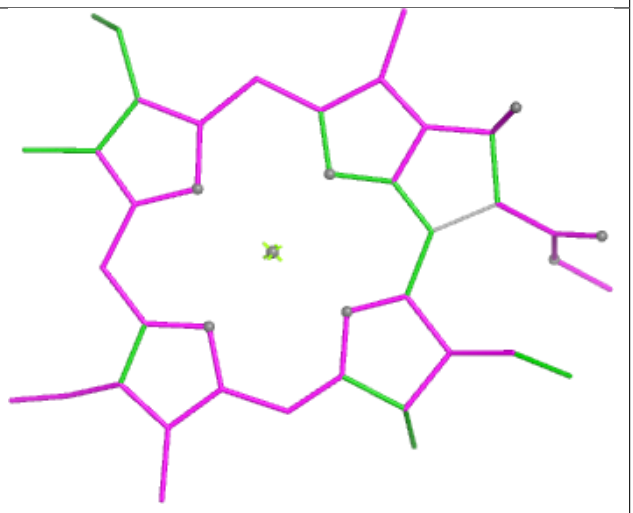
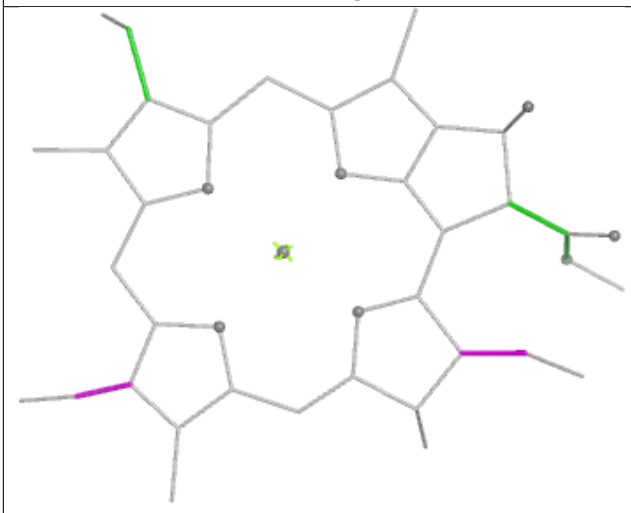


Bond angles



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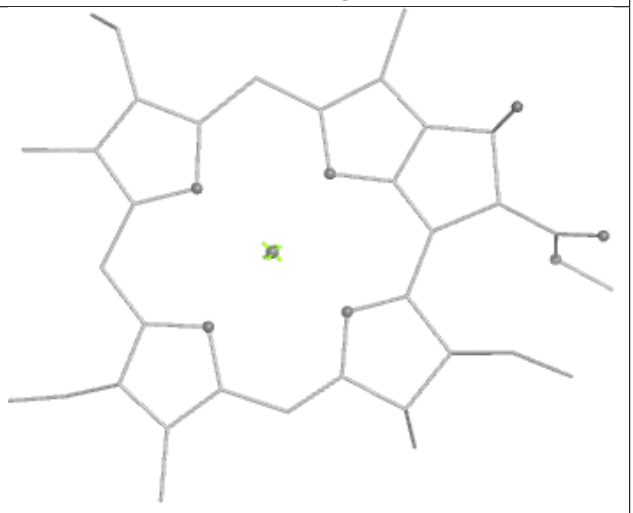
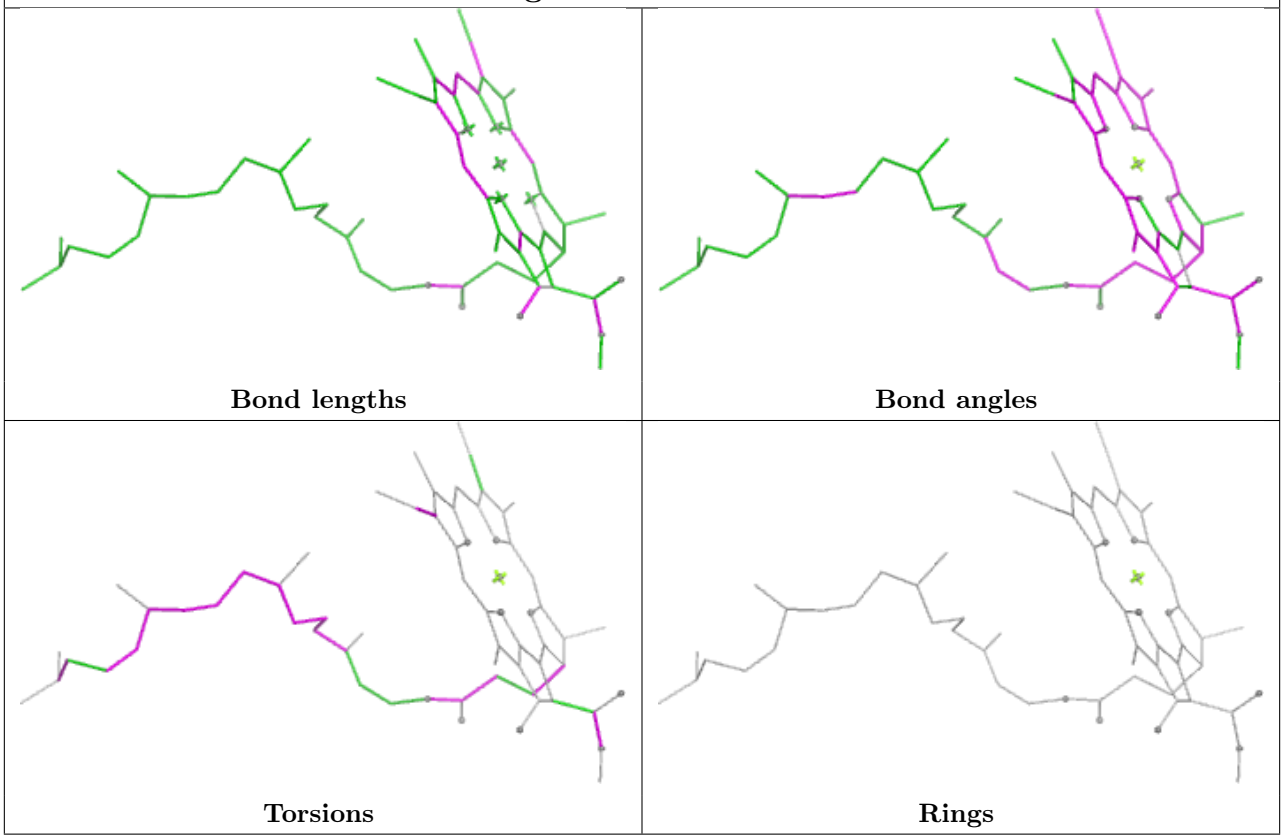
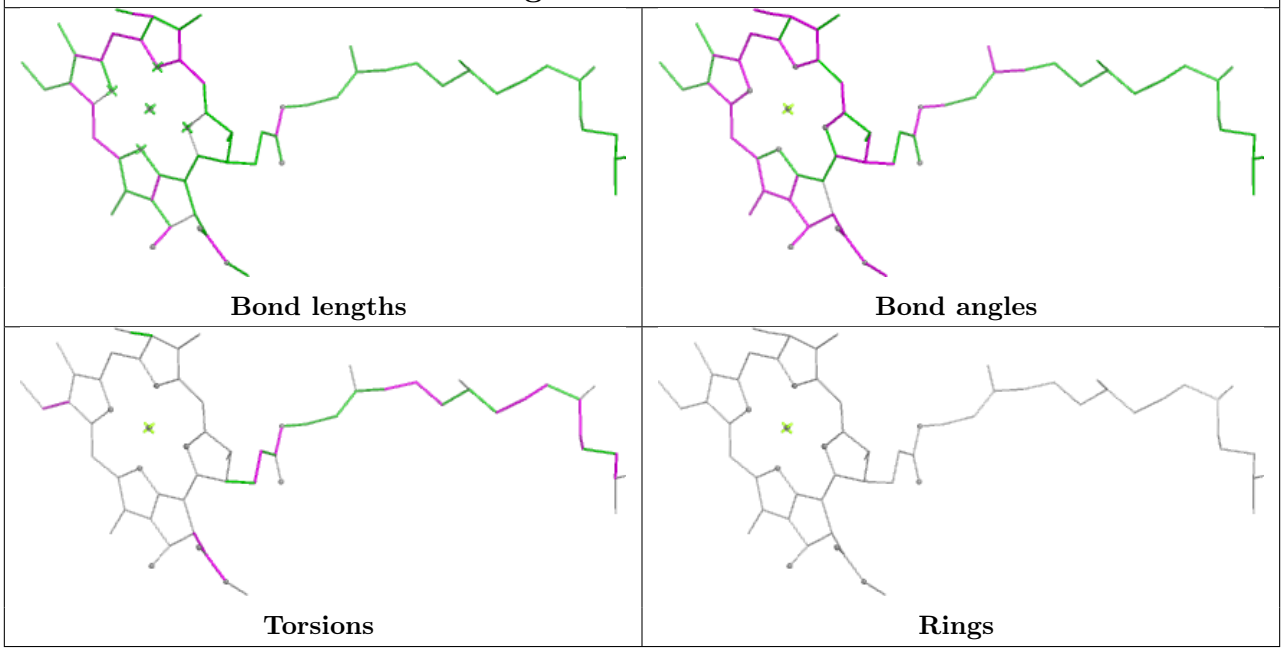


Rings

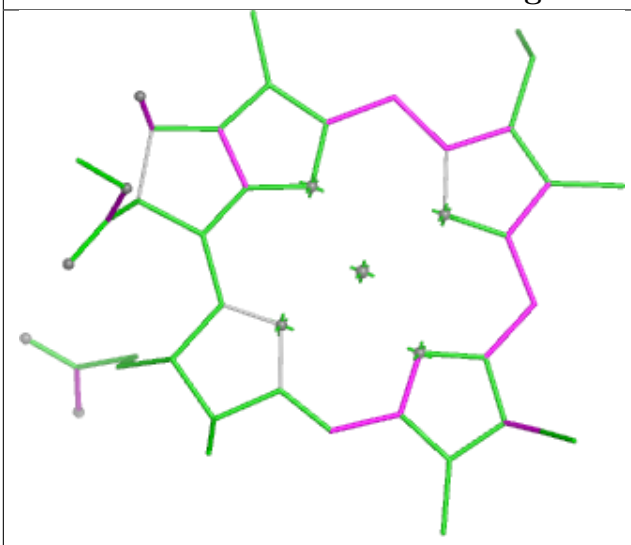
Ligand CLA A 809



Ligand CLA A 817



Ligand CLA B 832



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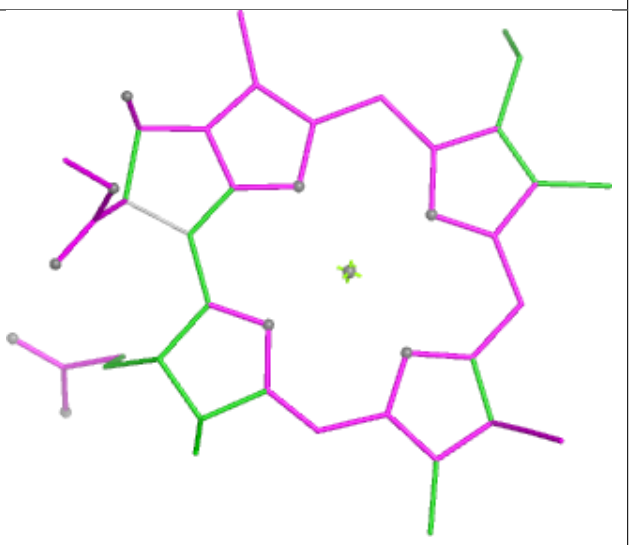
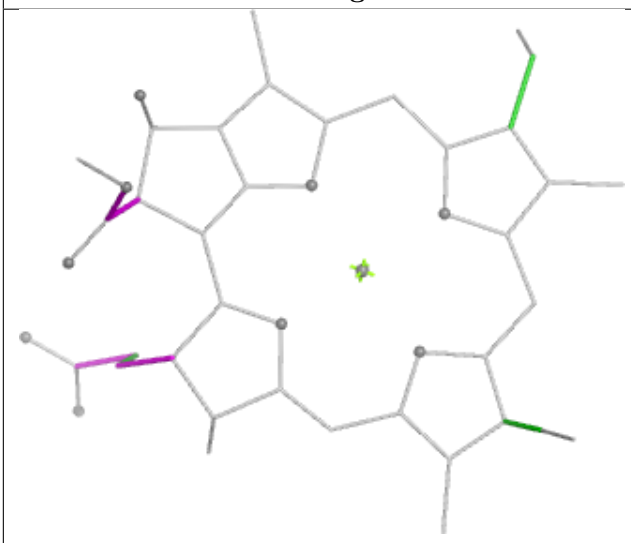
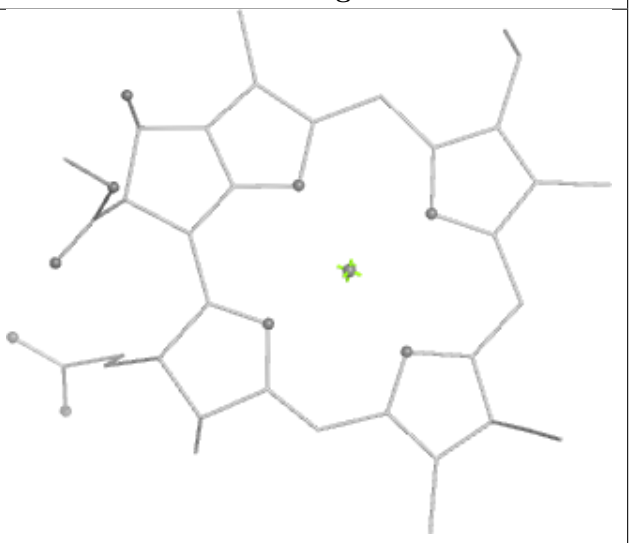


Bond angles

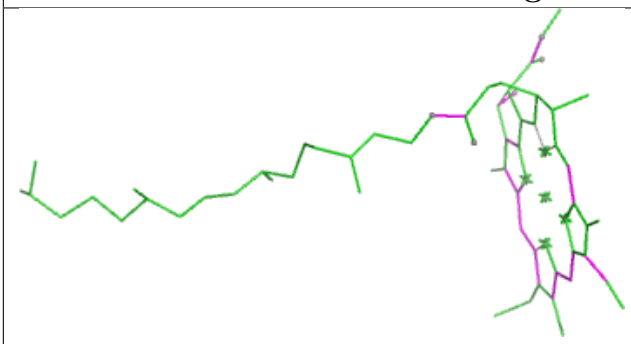


Torsions



Rings

Ligand CLA B 825



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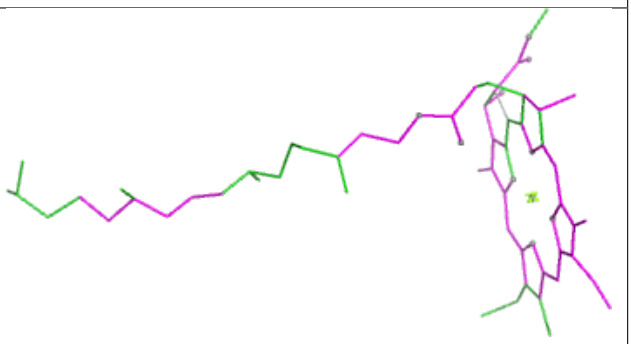
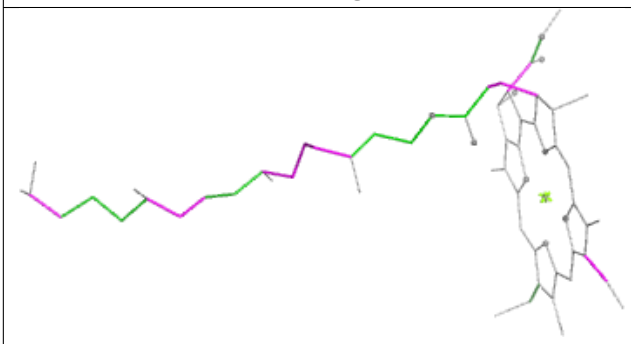


Bond angles



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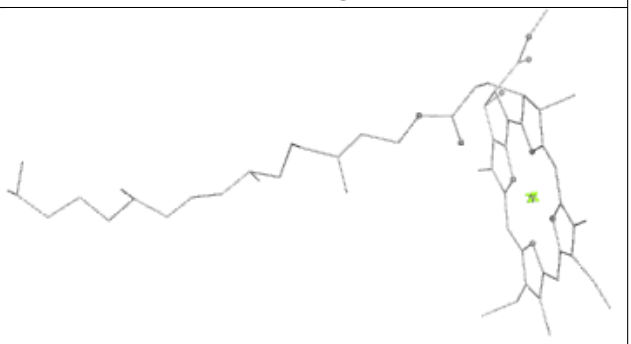
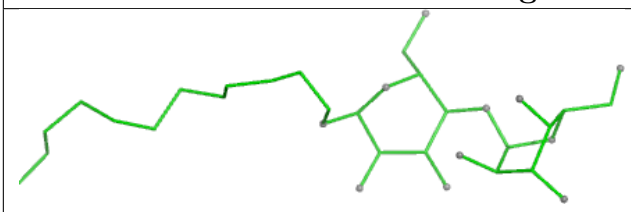


Rings

Ligand LMU A 851



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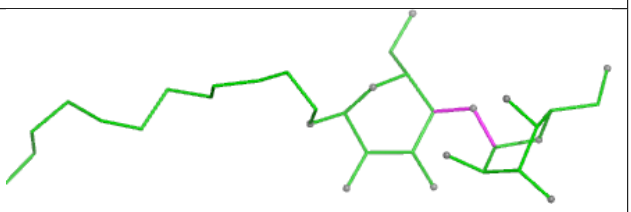
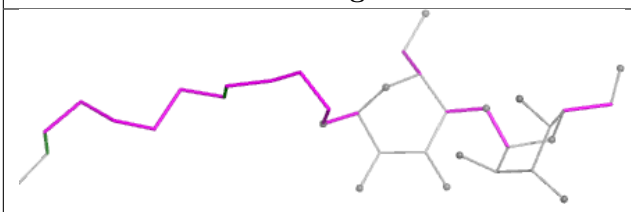
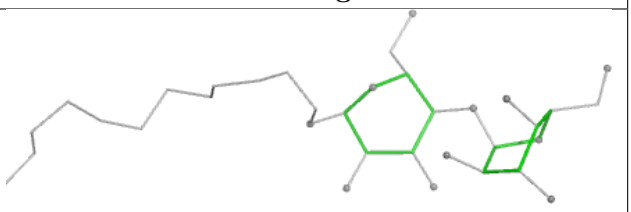


Bond angles

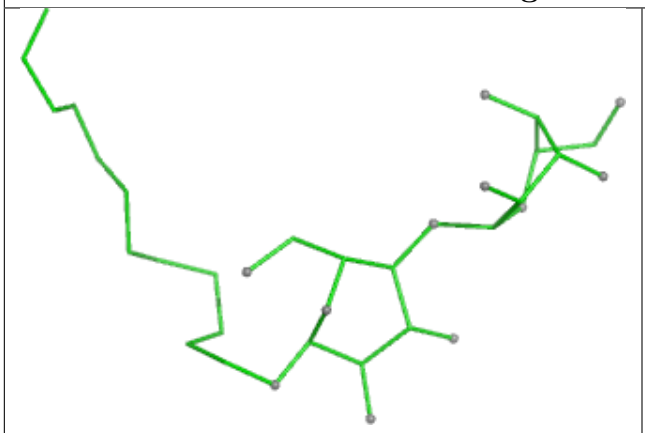


Torsions

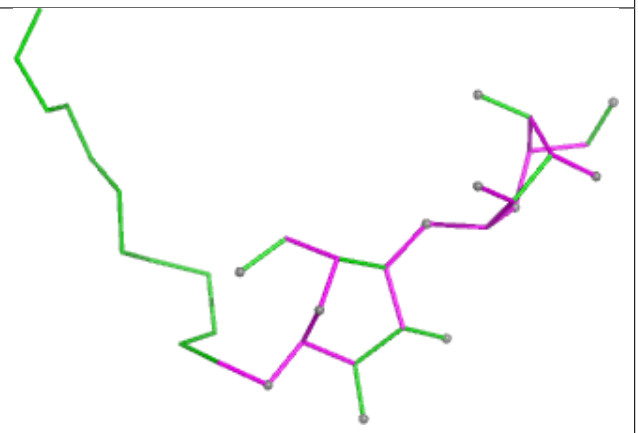


Rings

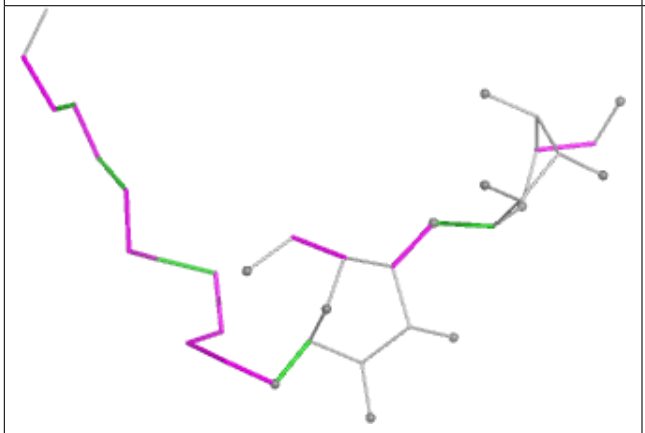
Ligand LMU R 102



Bond lengths



Bond angles



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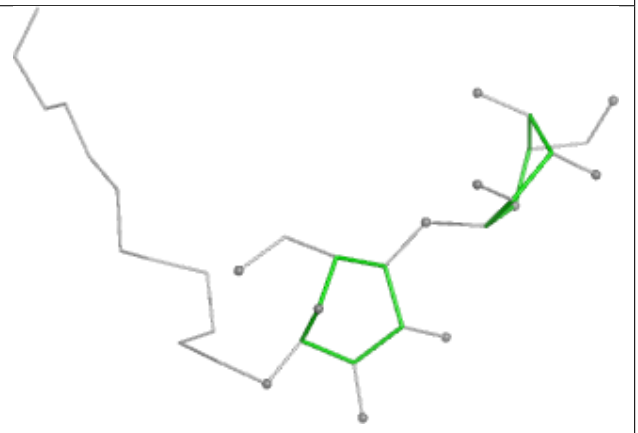
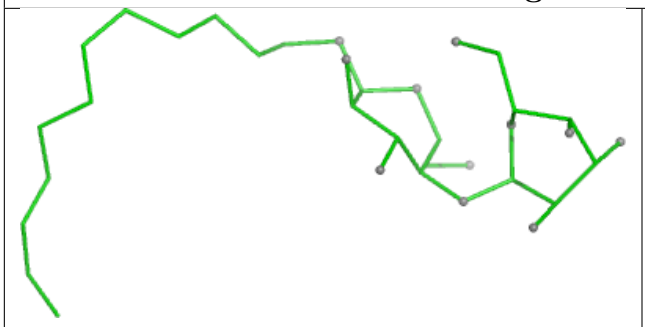
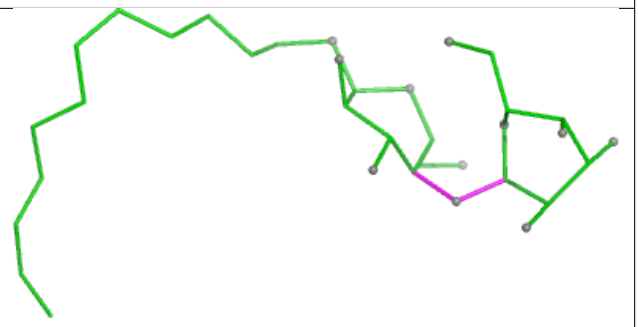


Rings

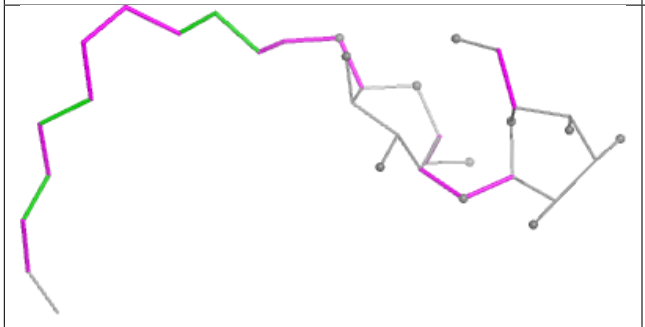
Ligand LMU 2 316



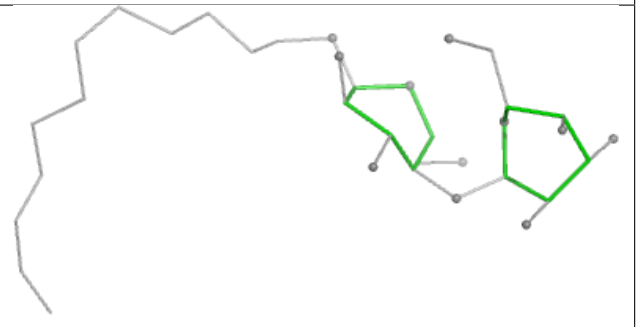
Bond lengths



Bond angles

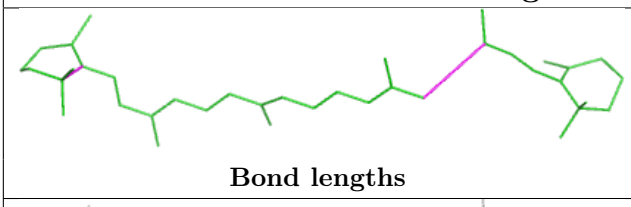


Torsions

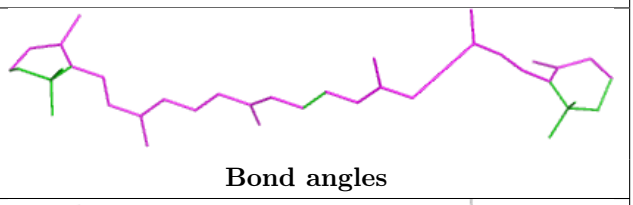


Rings

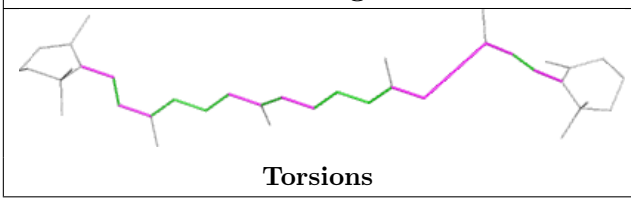
Ligand BCR A 842



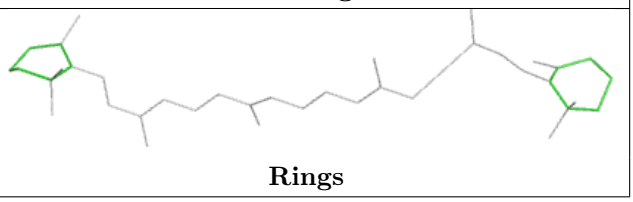
Bond lengths



Bond angles

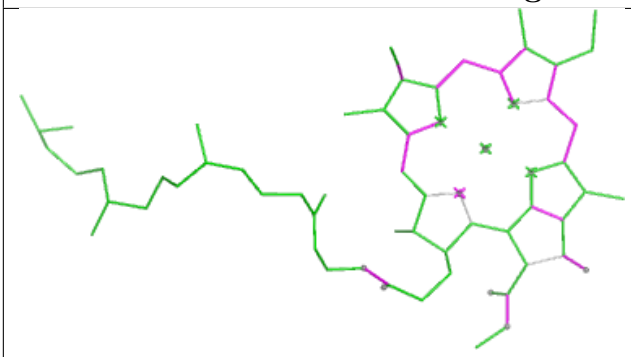


Torsions

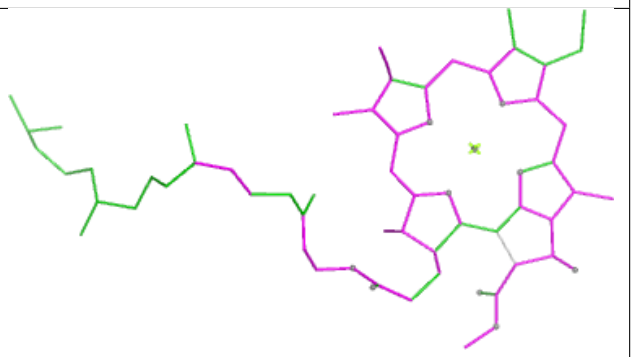


Rings

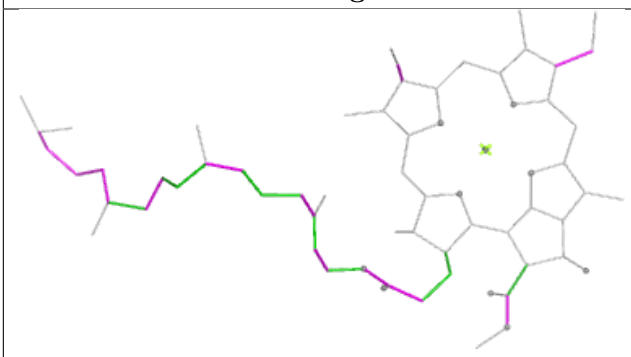
Ligand CLA B 849



Bond lengths



Bond angles

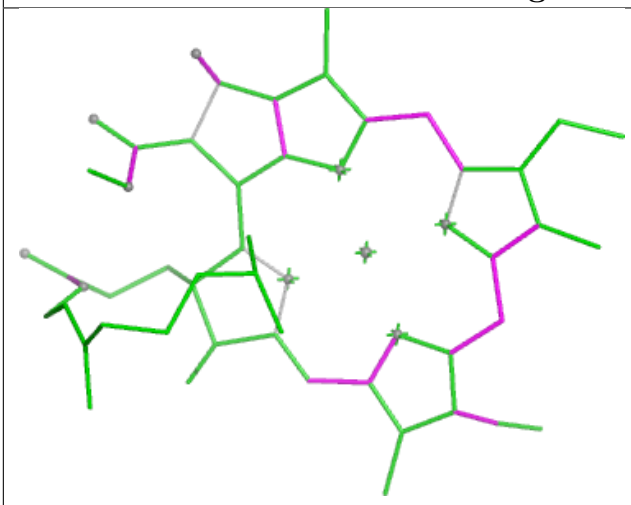


Torsions



Rings

Ligand CLA 4 305



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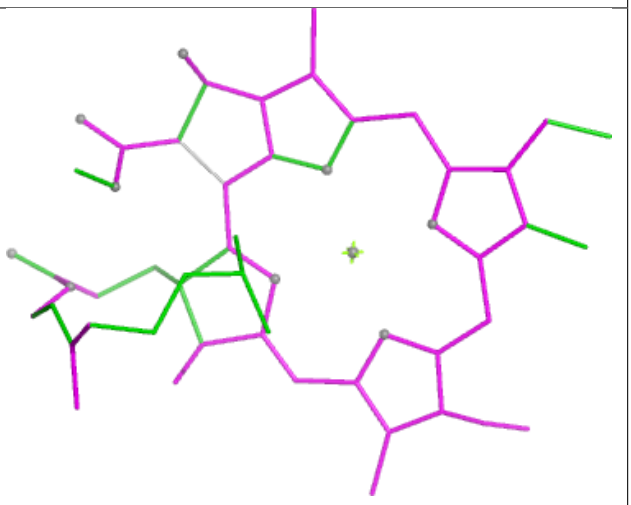
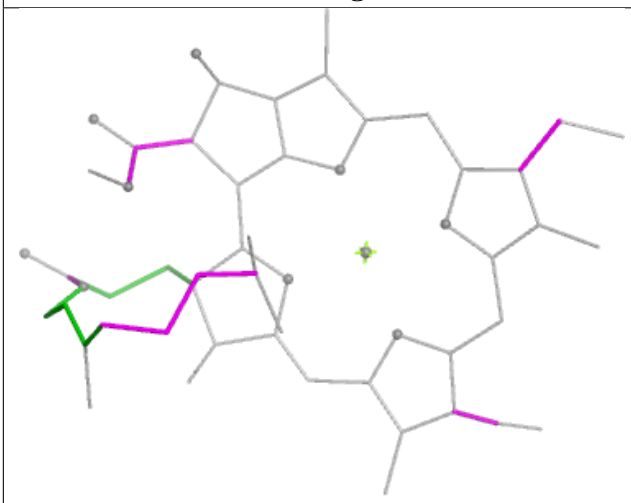


Bond angles



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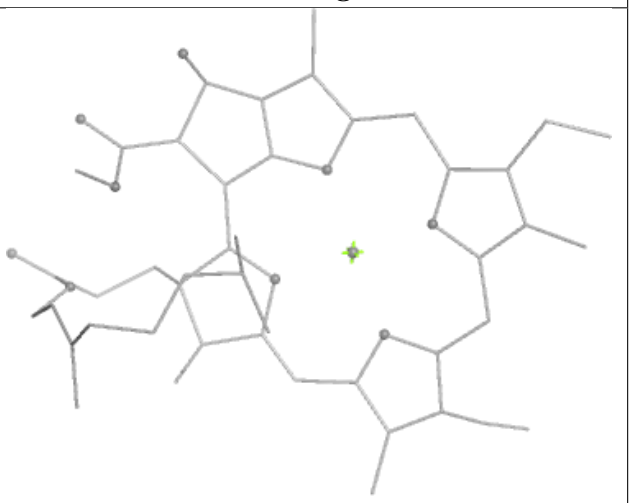
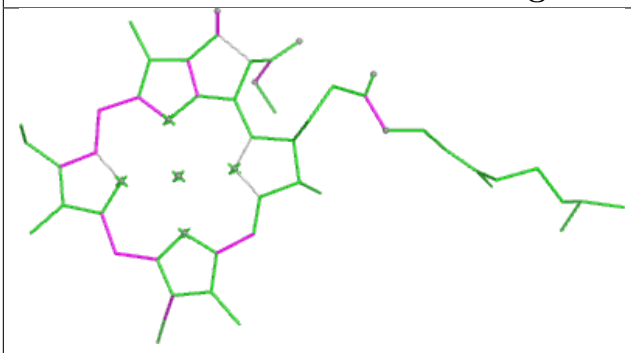


Rings

Ligand CLA 4 310



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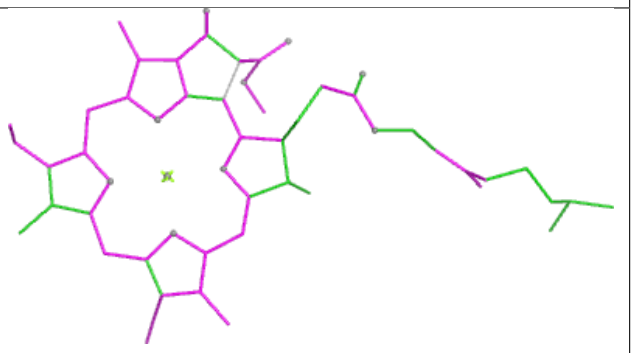
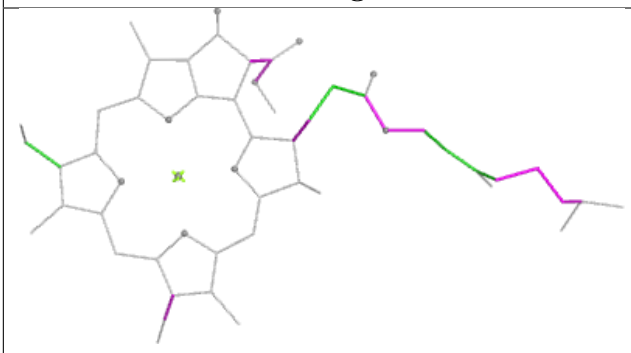


Bond angles



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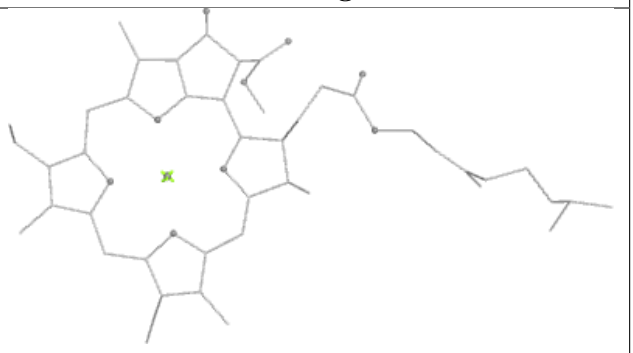
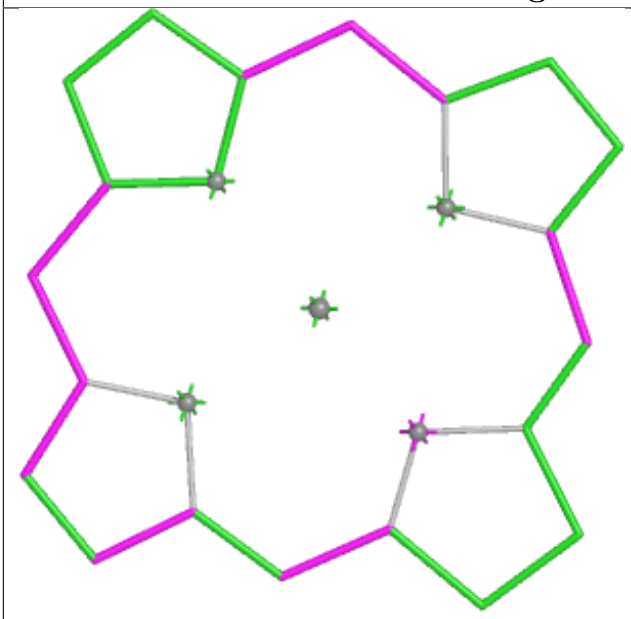


Rings

Ligand CLA 2 309



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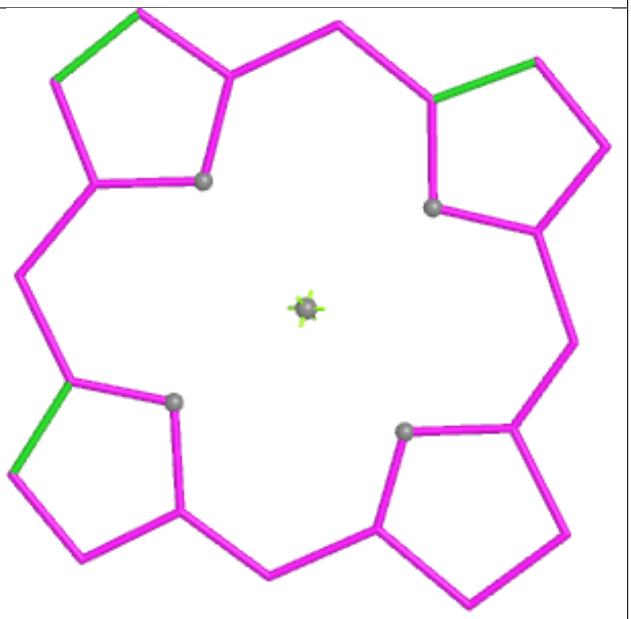
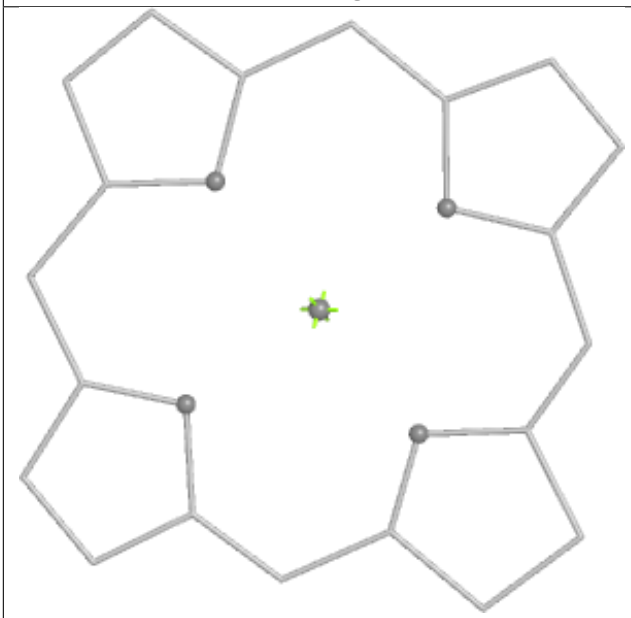


Bond angles



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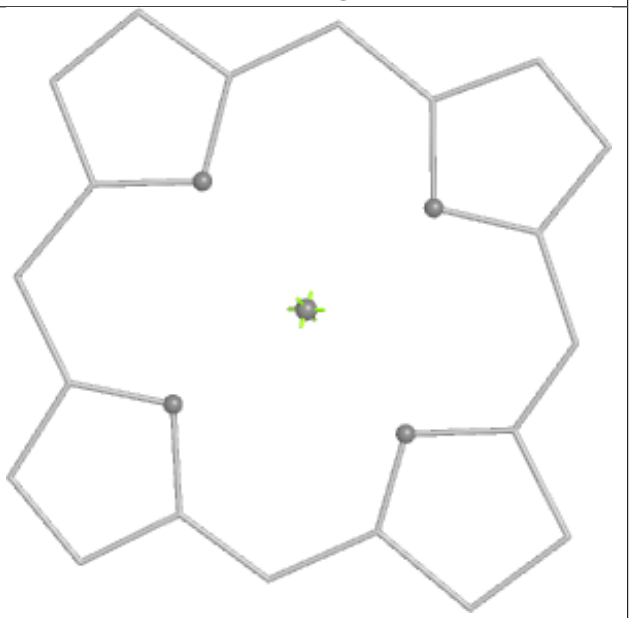
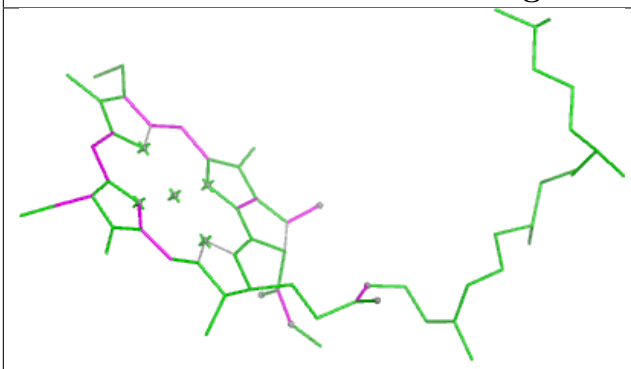


Rings

Ligand CLA K 107



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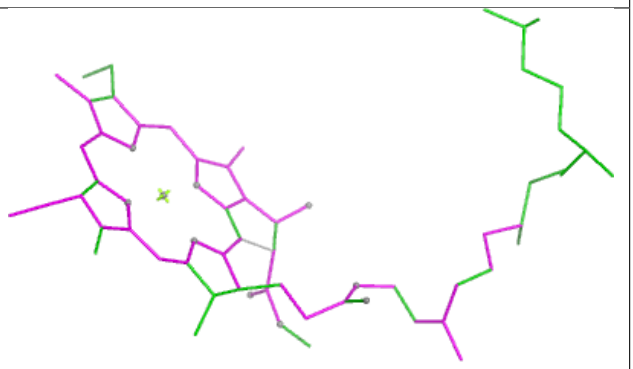
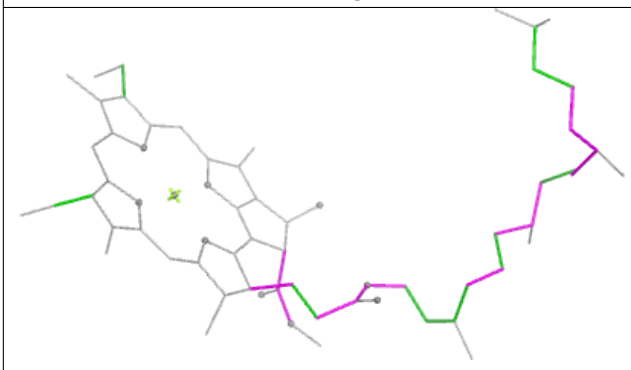


Bond angles



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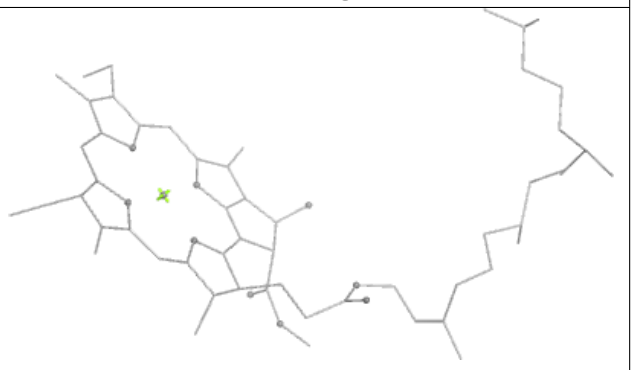
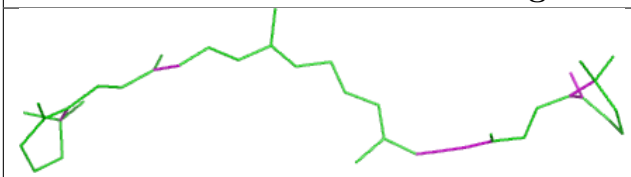


Rings

Ligand BCR I 103



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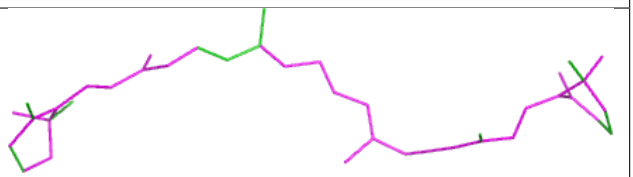
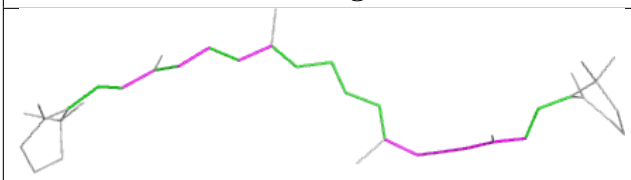


Bond angles



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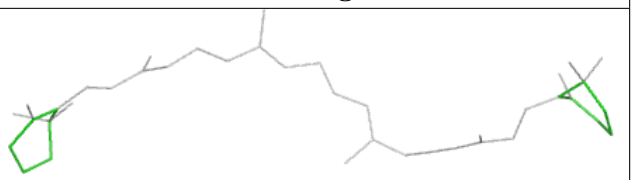
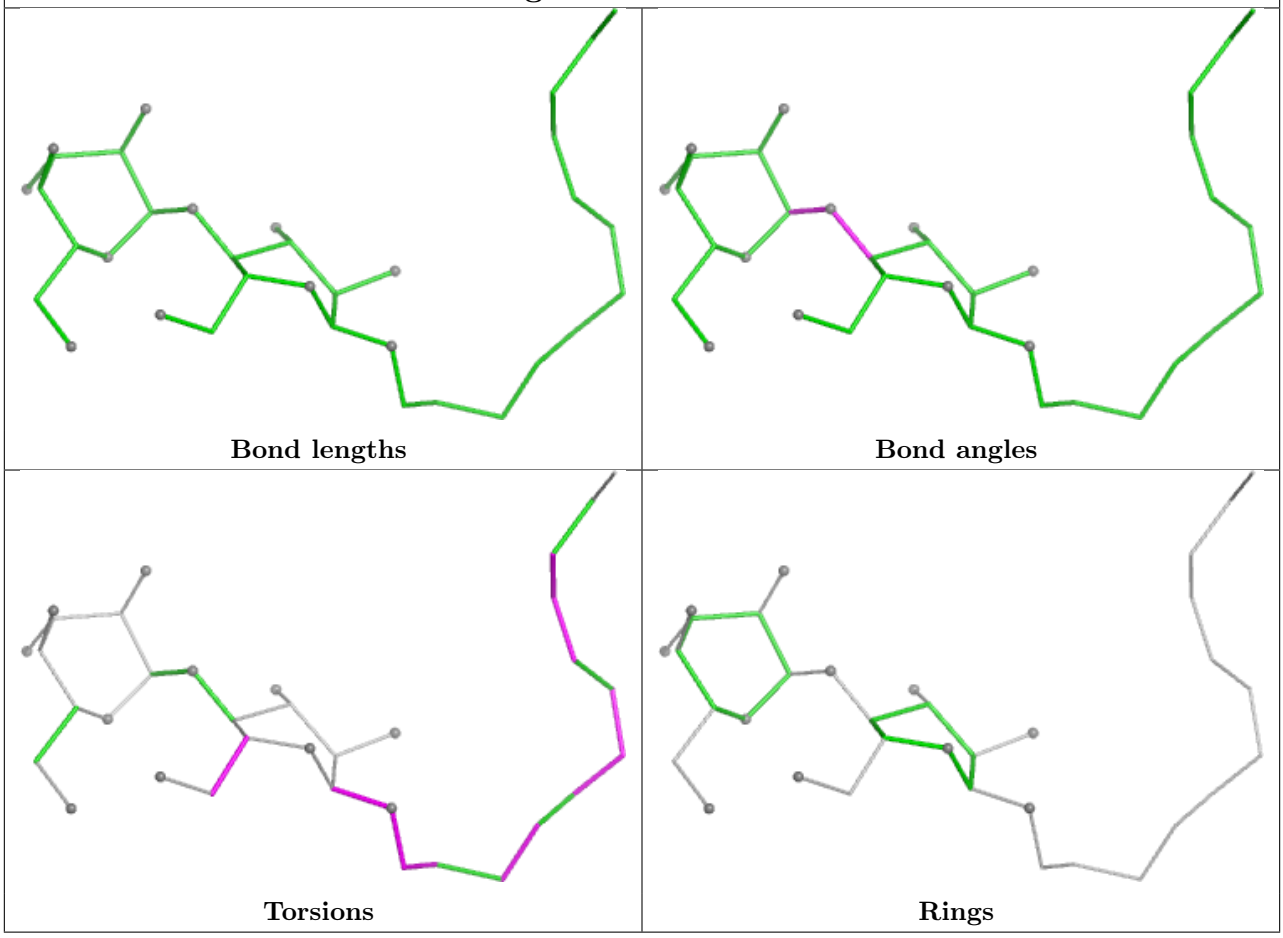
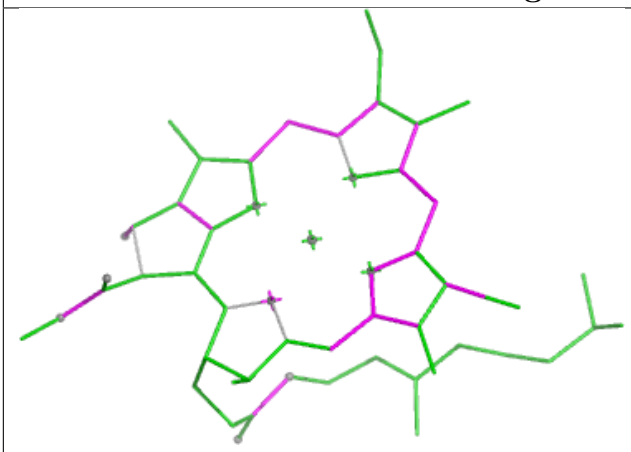


Rings

Ligand LMU 3 302



Ligand CLA B 819



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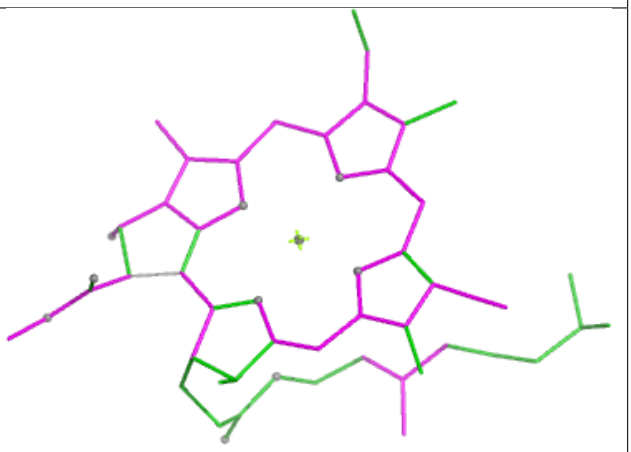
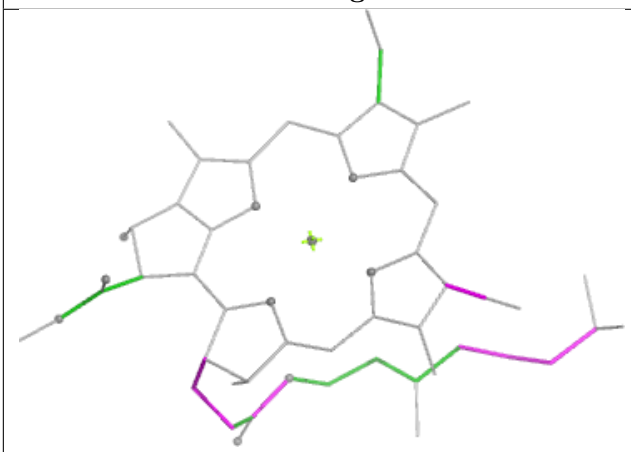


Bond angles

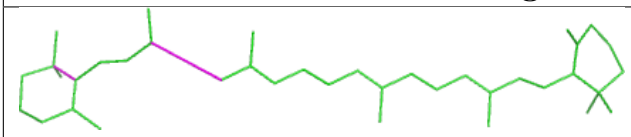


Torsions



Rings

Ligand BCR G 102



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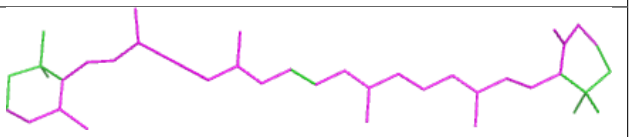
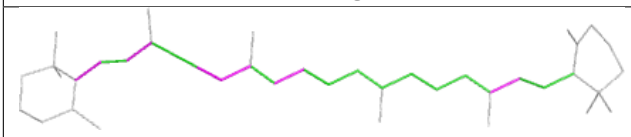


Bond angles



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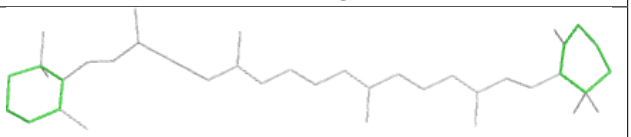
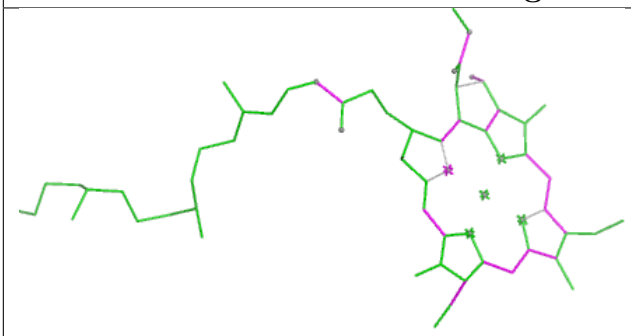


Rings

Ligand CLA B 848



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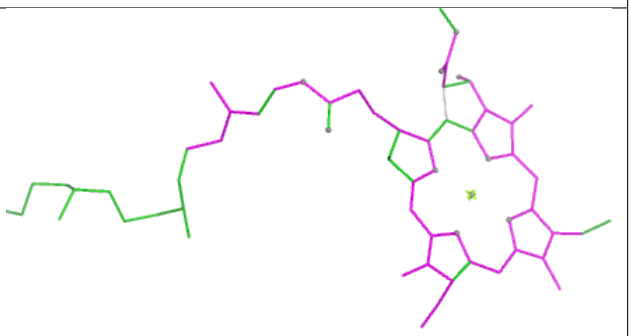
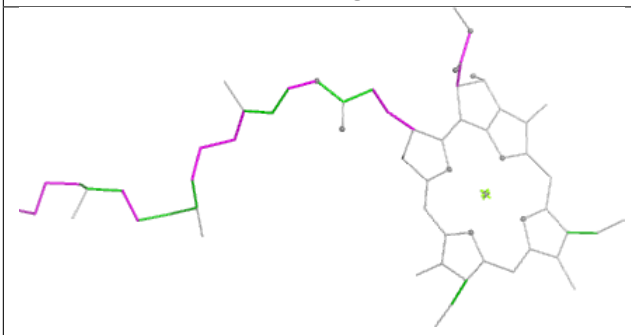


Bond angles

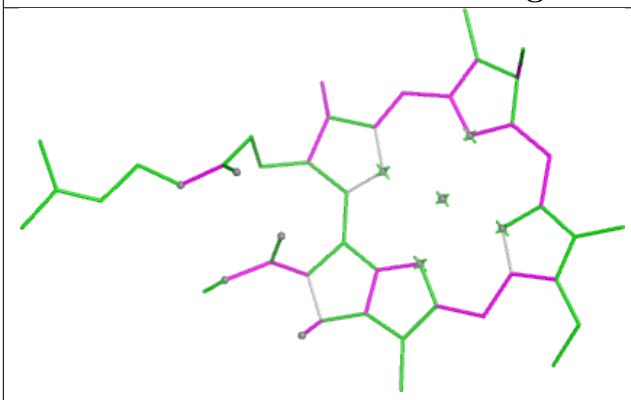


Torsions



Rings

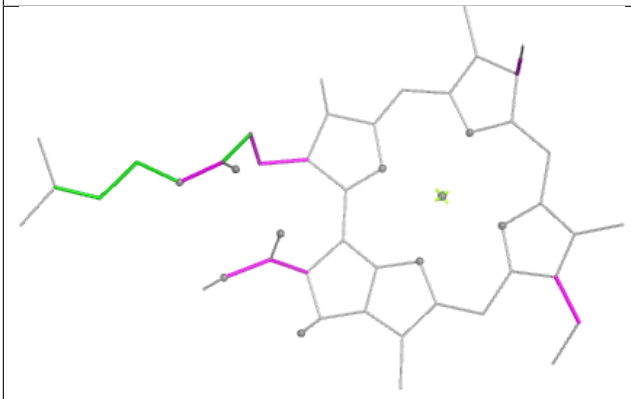
Ligand CLA L 208



Bond lengths



Bond angles



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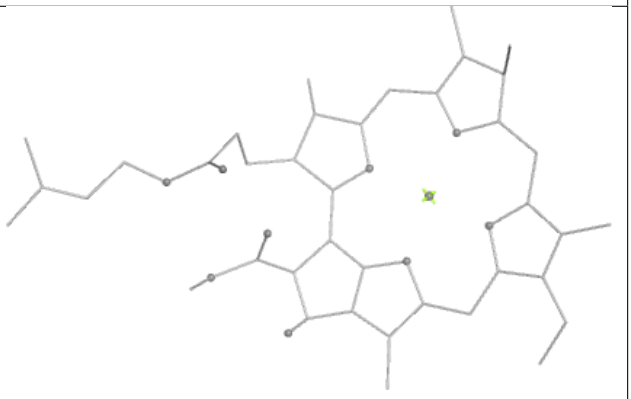
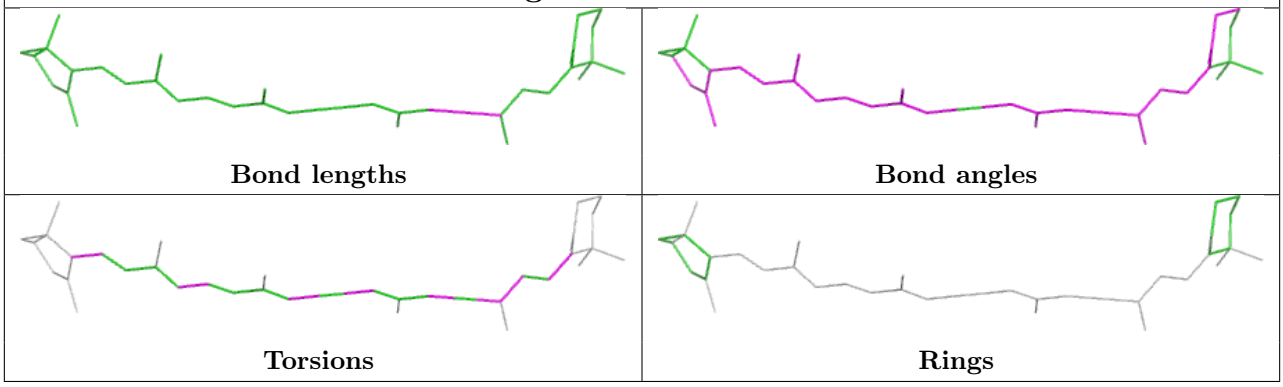
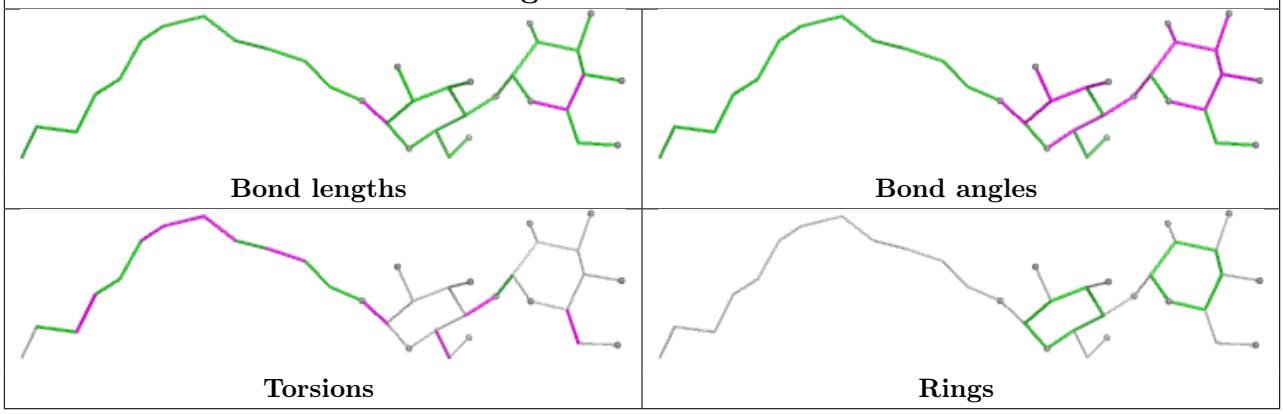


Rings

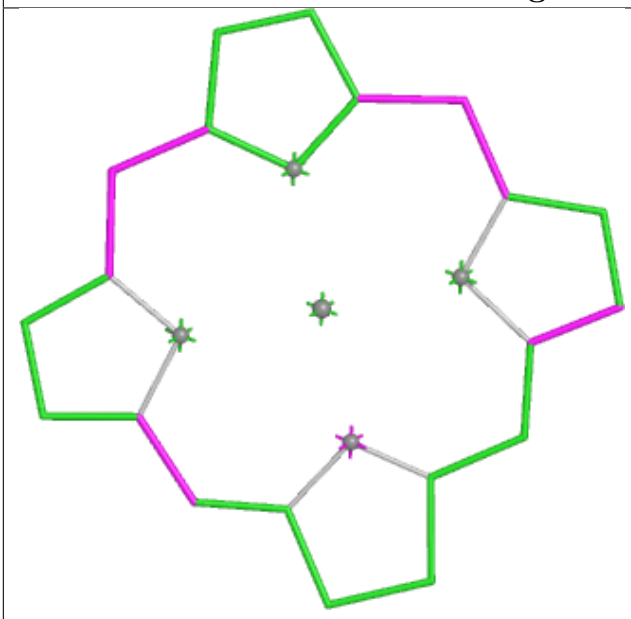
Ligand BCR F 202



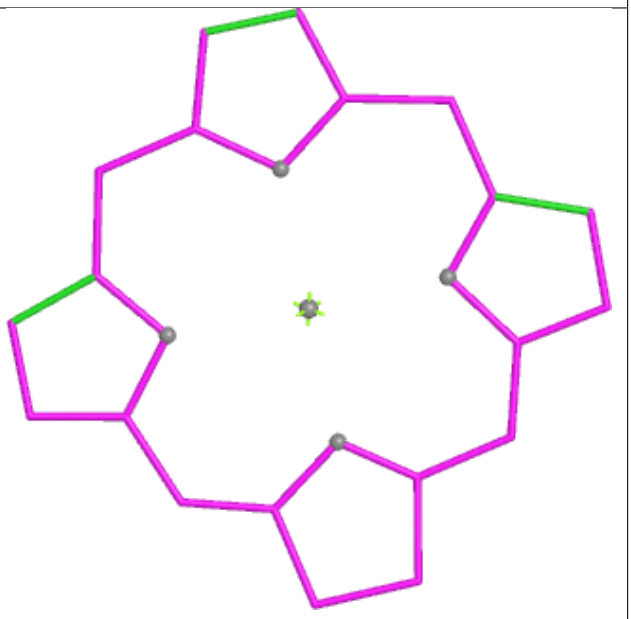
Ligand LMU B 802



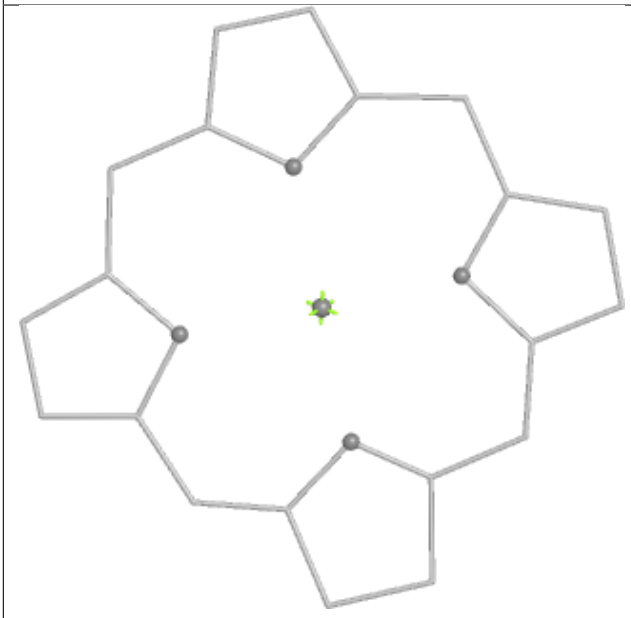
Ligand CLA 1 215



Bond lengths



Bond angles



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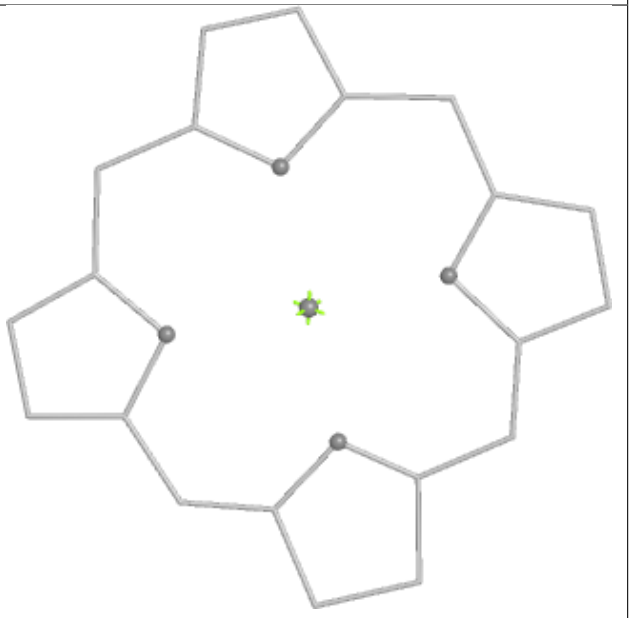
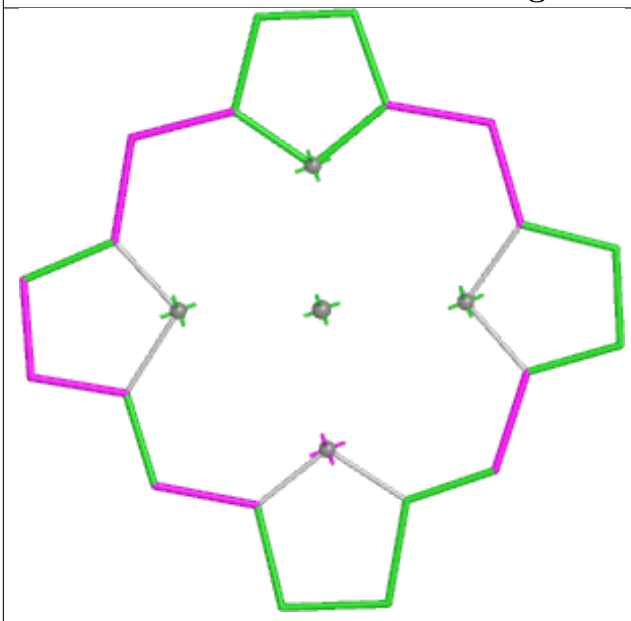


Rings

Ligand CLA 3 313



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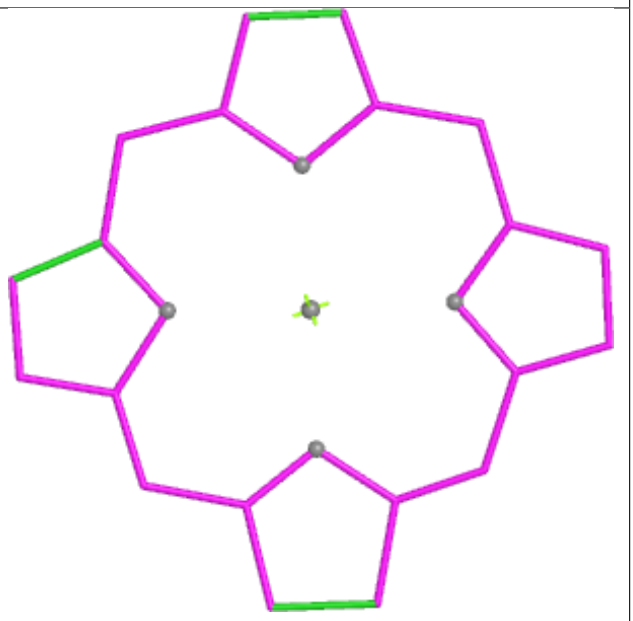
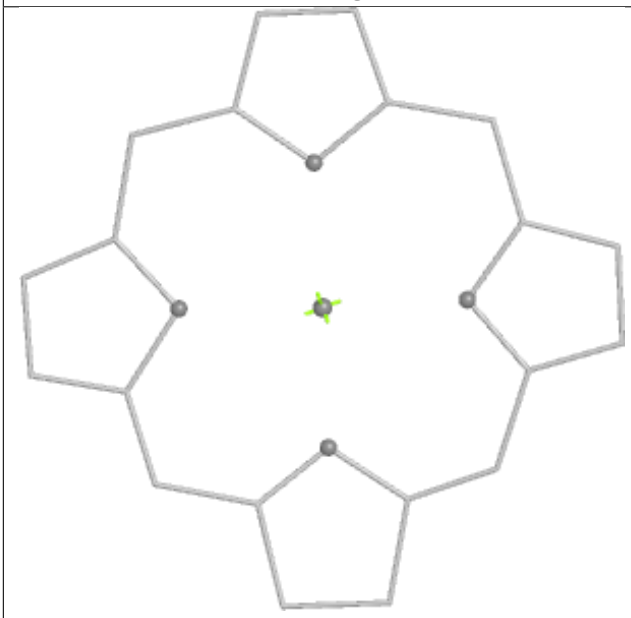


Bond angles



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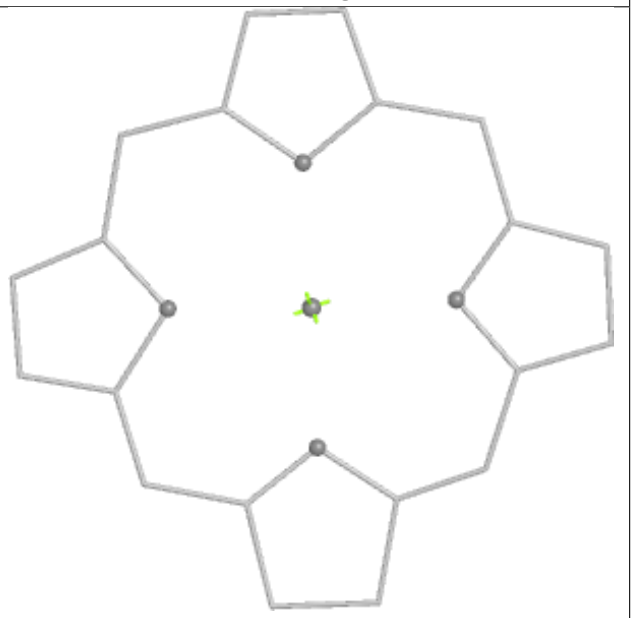
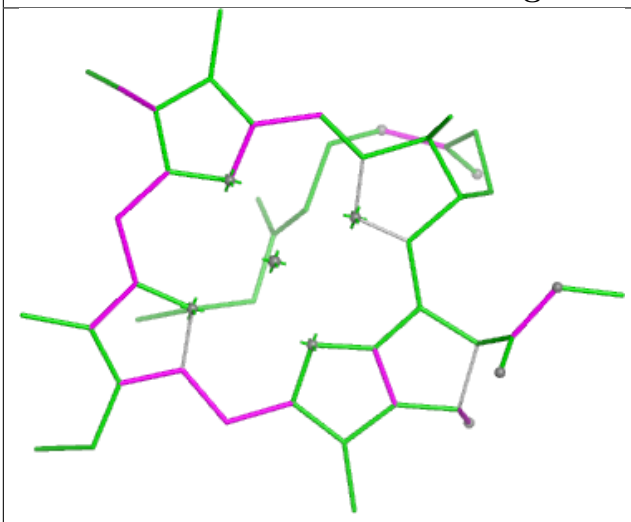
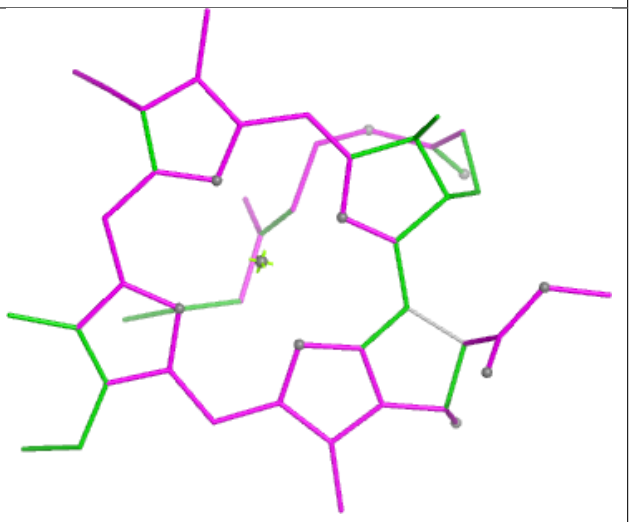


Rings

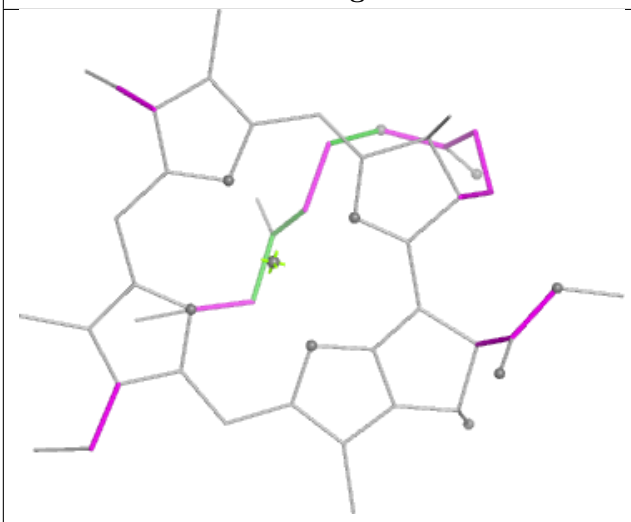
Ligand CLA A 815



Bond lengths



Bond angles



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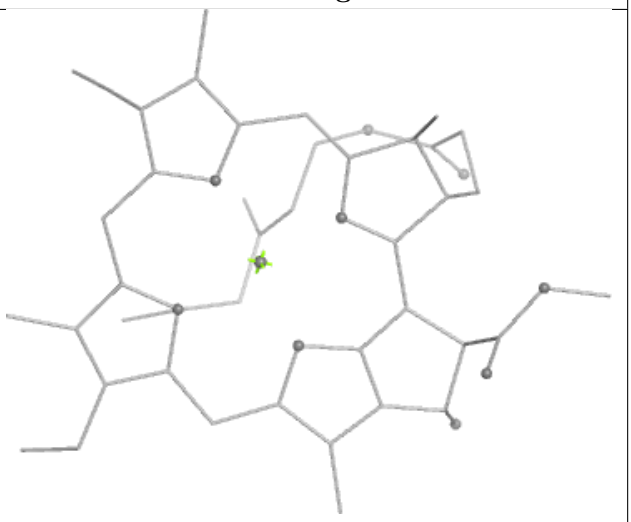
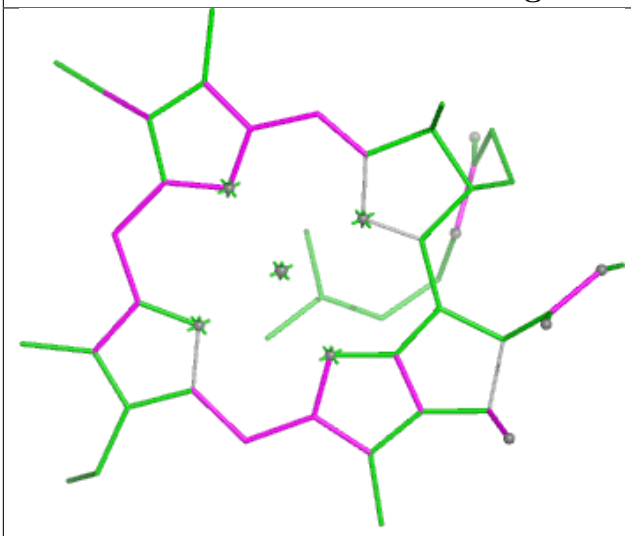
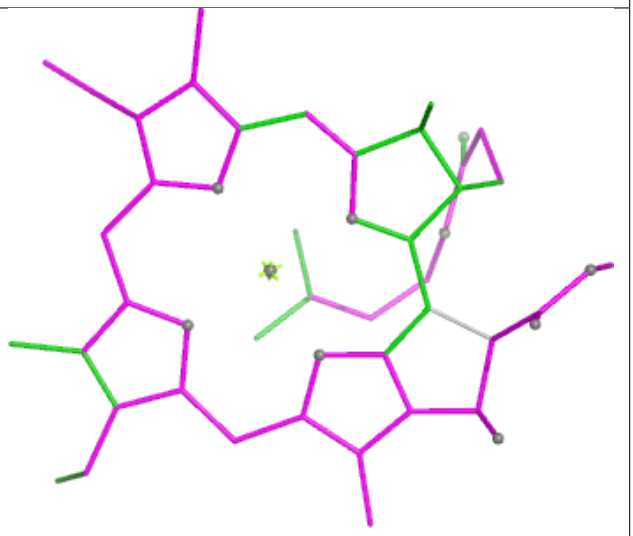


Rings

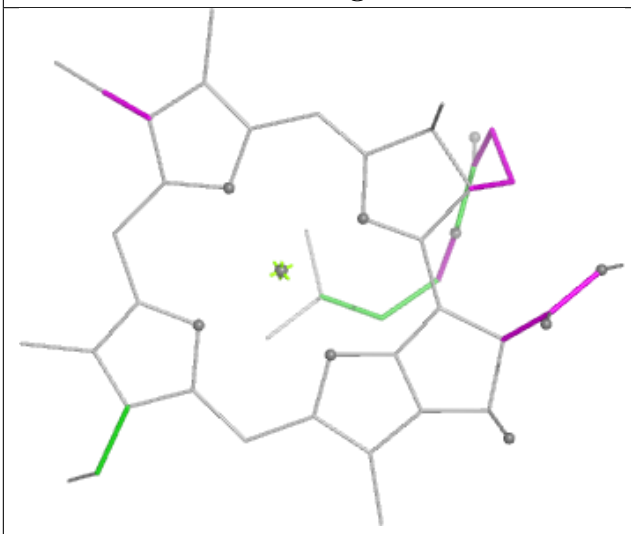
Ligand CLA B 827



Bond lengths



Bond angles



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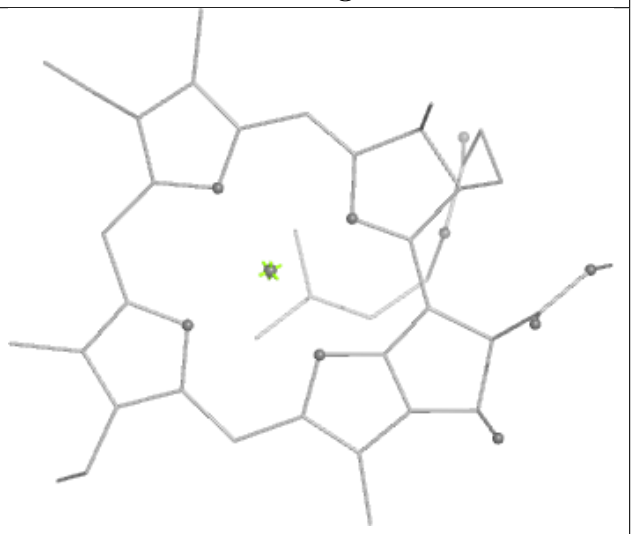
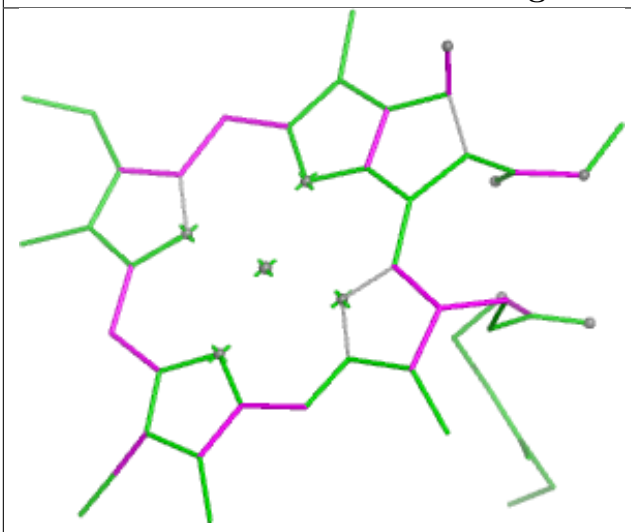
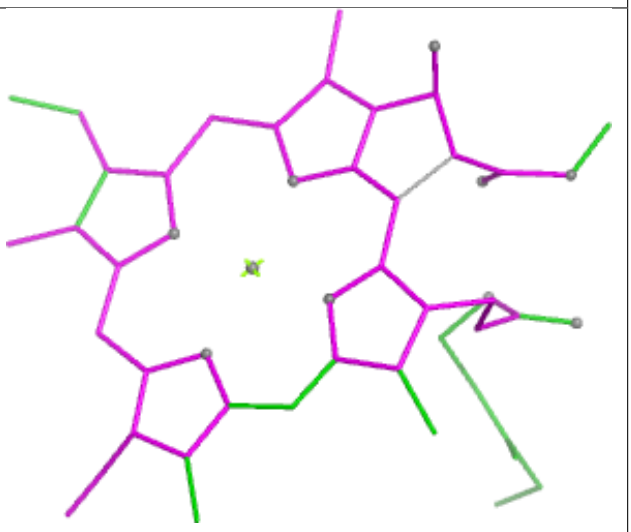


Rings

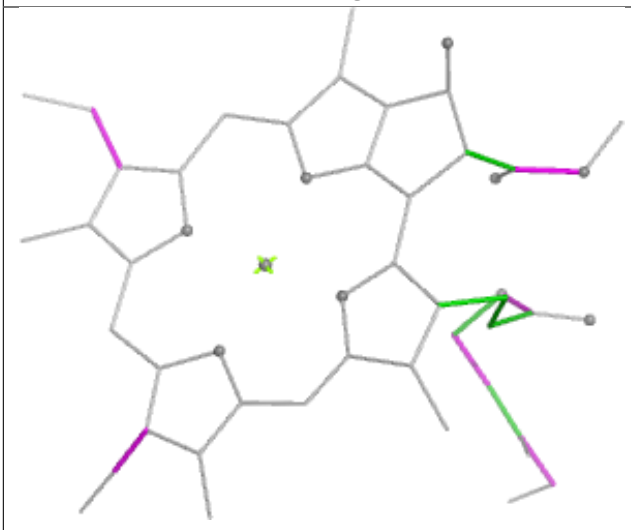
Ligand CLA 1 207



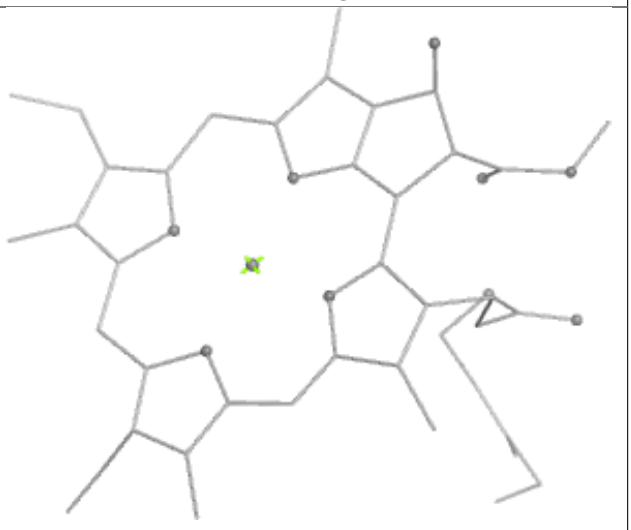
Bond lengths



Bond angles



Torsions

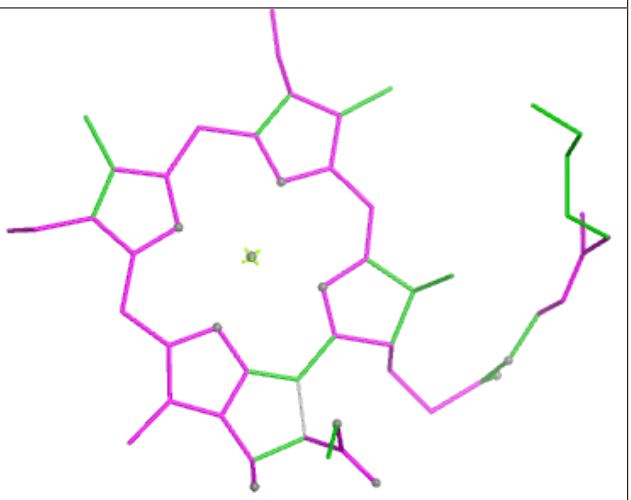


Rings

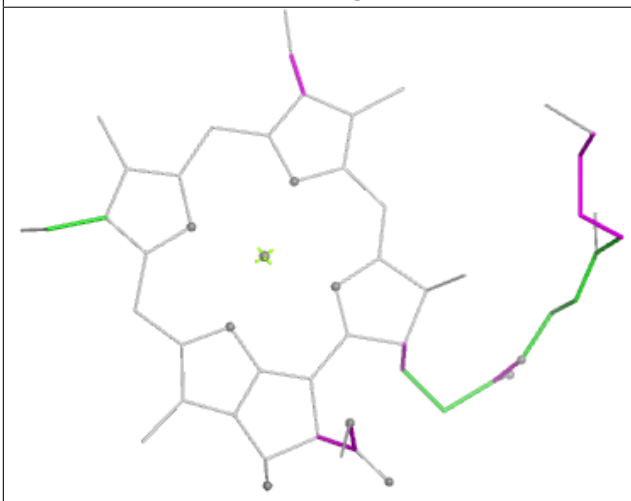
Ligand CLA A 811



Bond lengths



Bond angles



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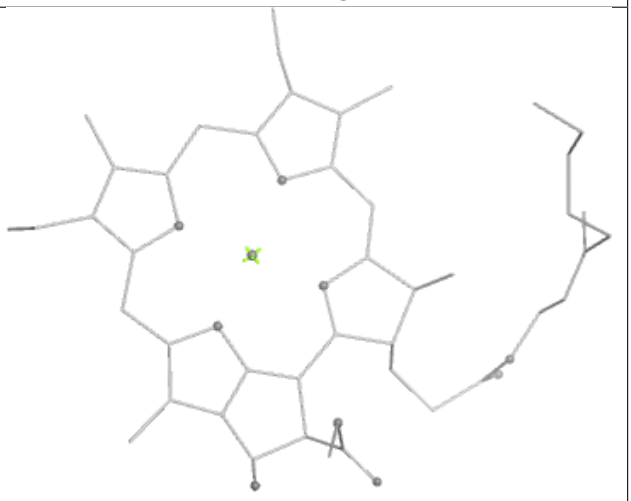
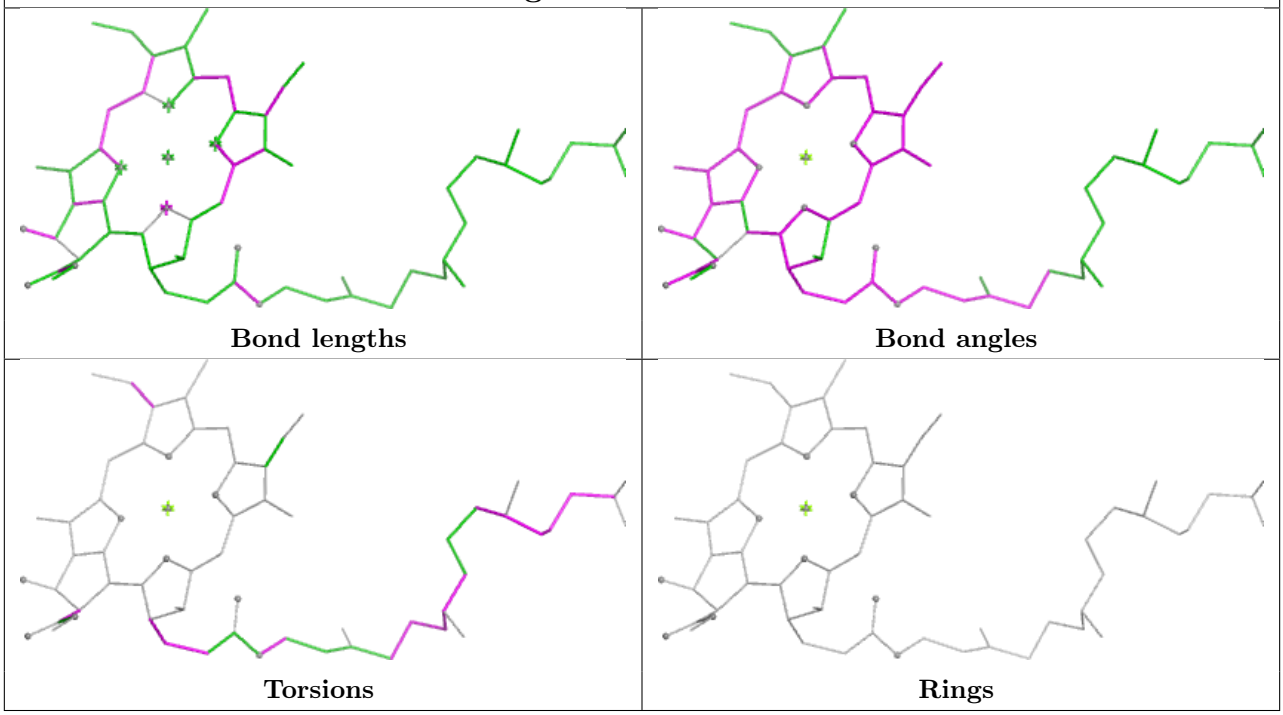
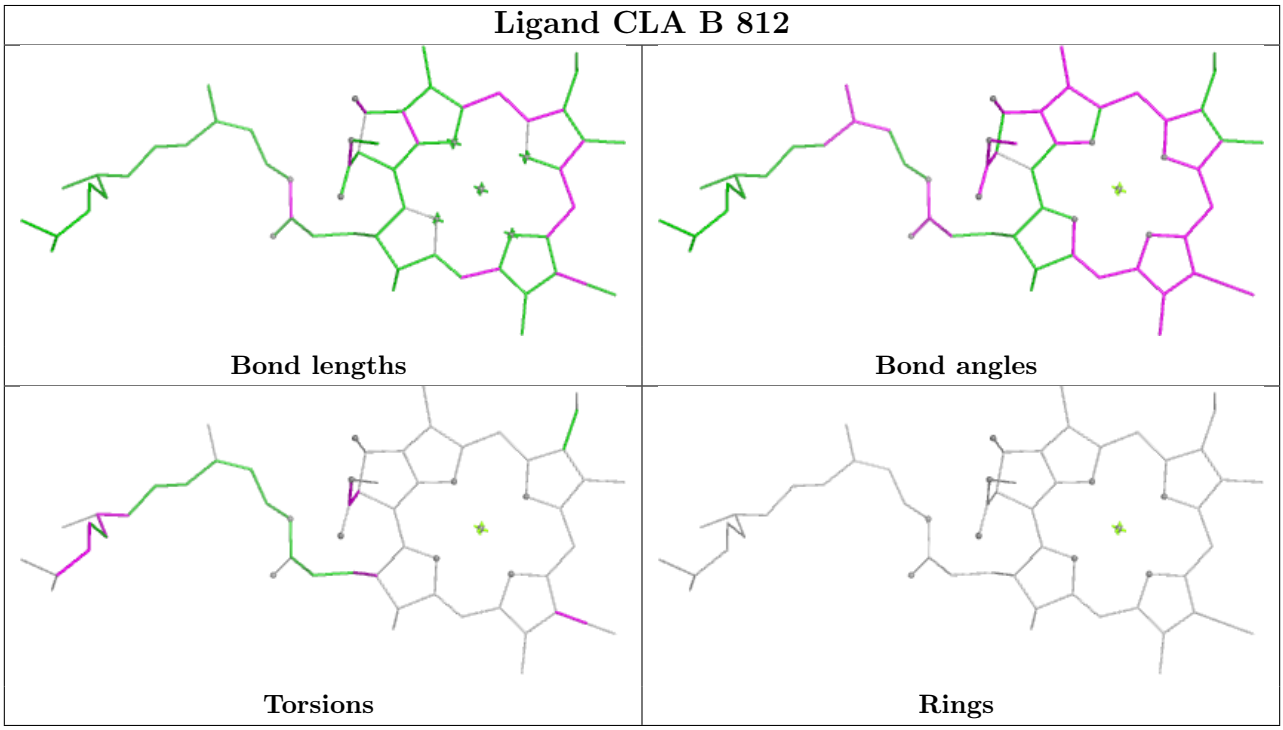


Rings

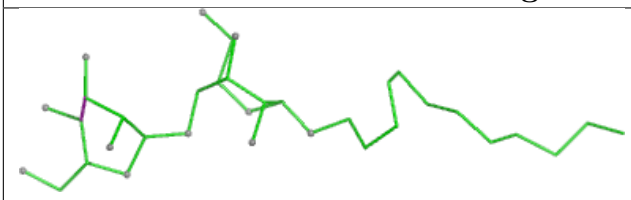
Ligand CLA A 806



Ligand CLA B 812



Ligand LMU E 101



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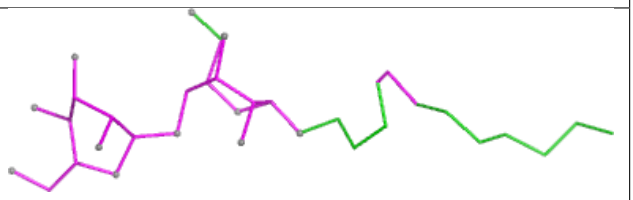
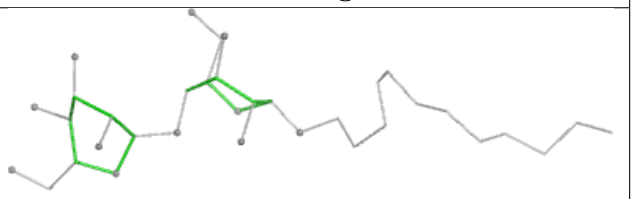


Bond angles

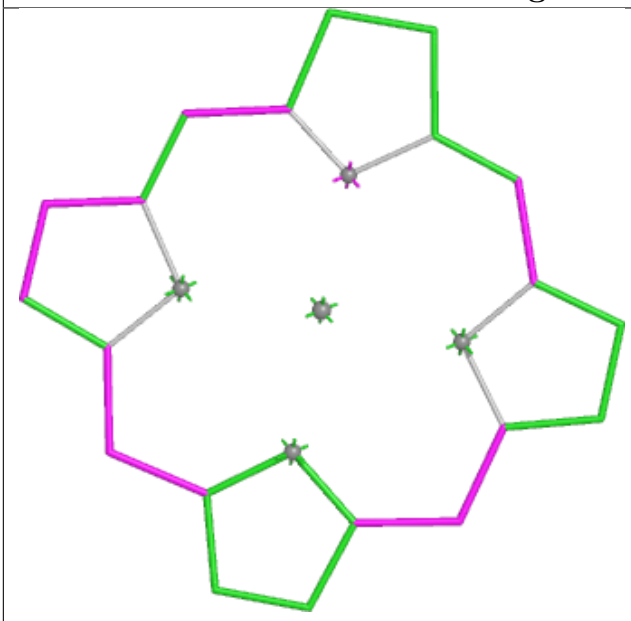


Torsions



Rings

Ligand CLA 2 315



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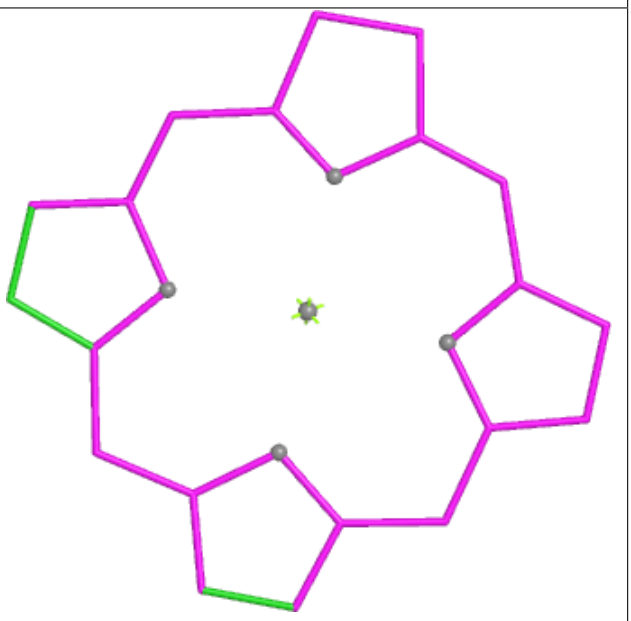
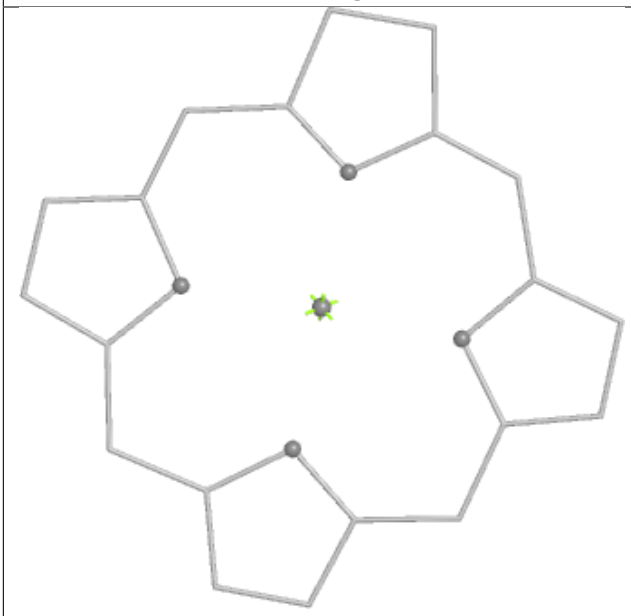


Bond angles



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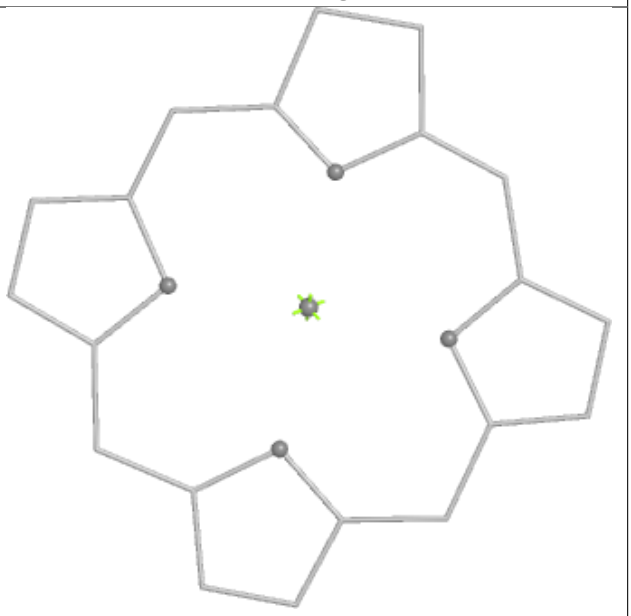
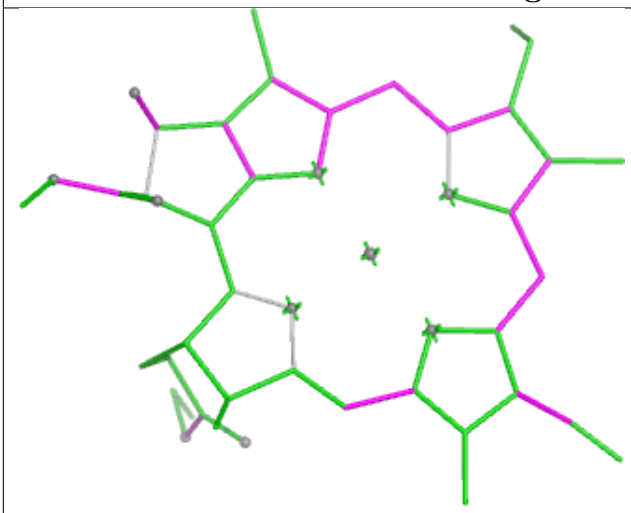


Rings

Ligand CLA B 836



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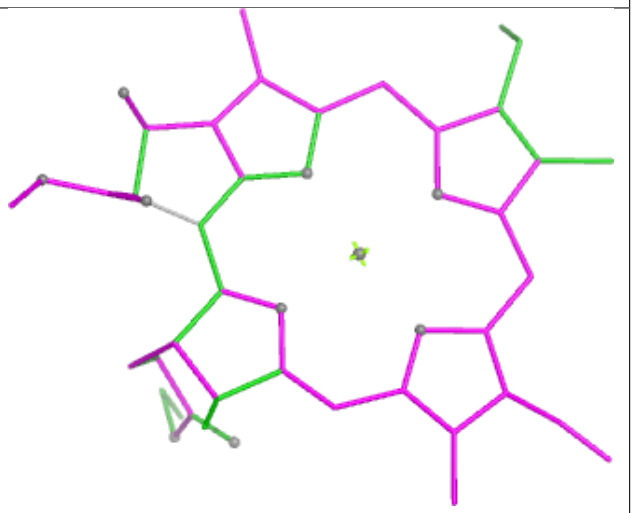

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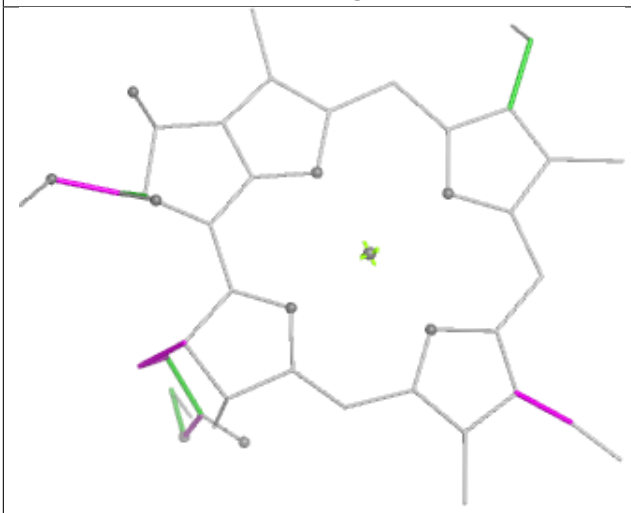

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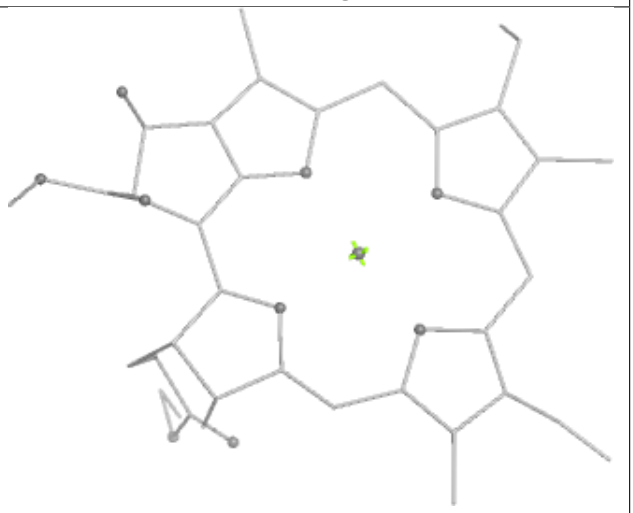
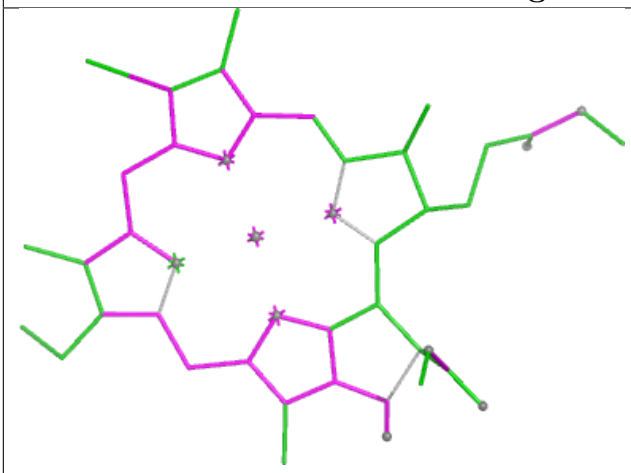


Rings

Ligand CLA 1 201



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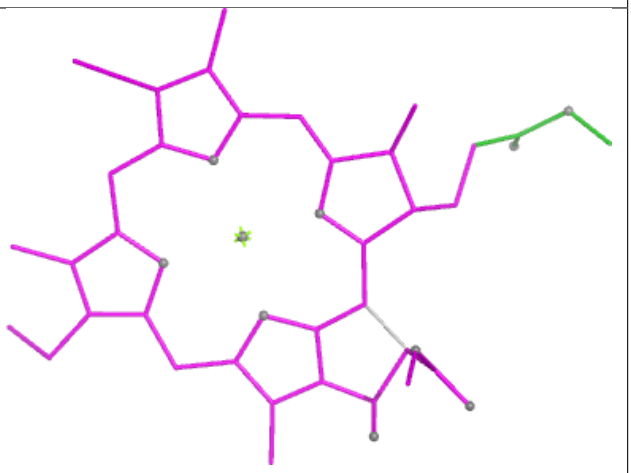

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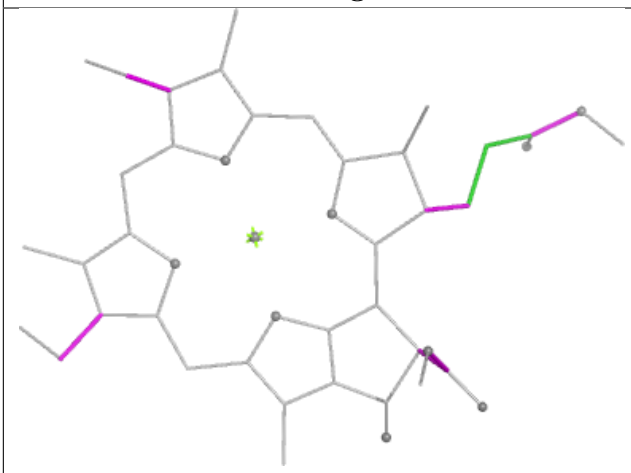

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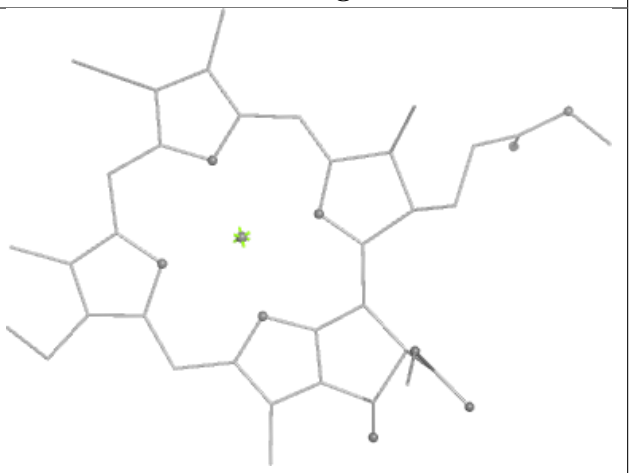
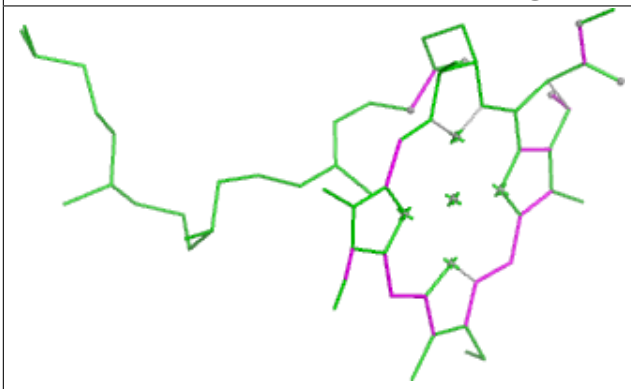


Rings

Ligand CLA L 202



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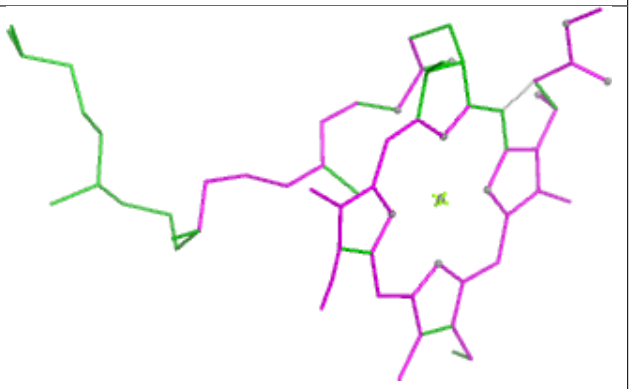
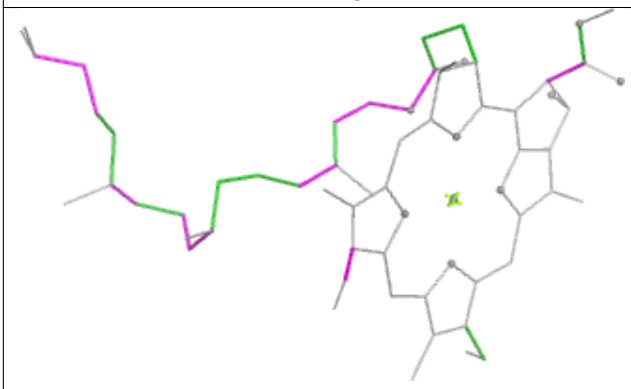


Bond angles



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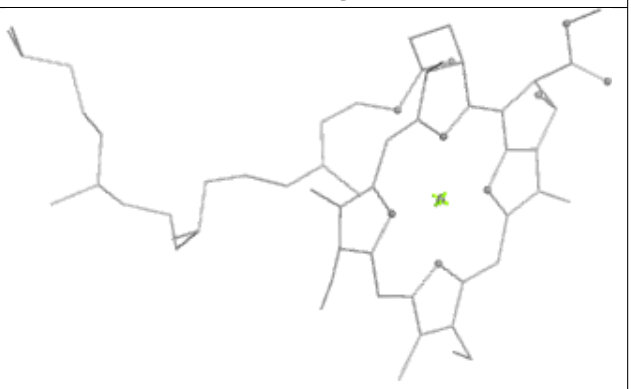
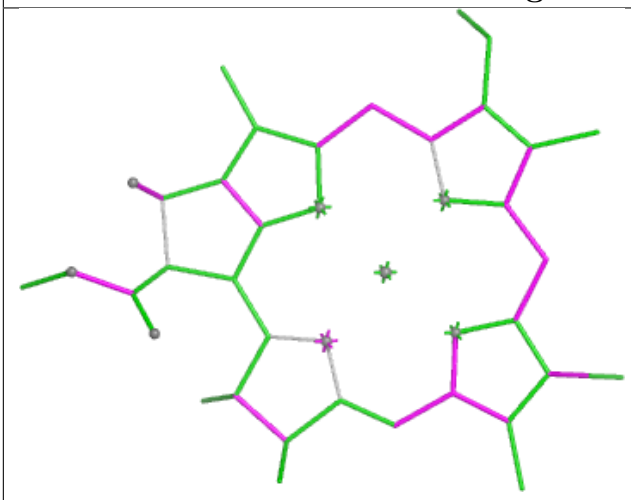


Rings

Ligand CLA F 205



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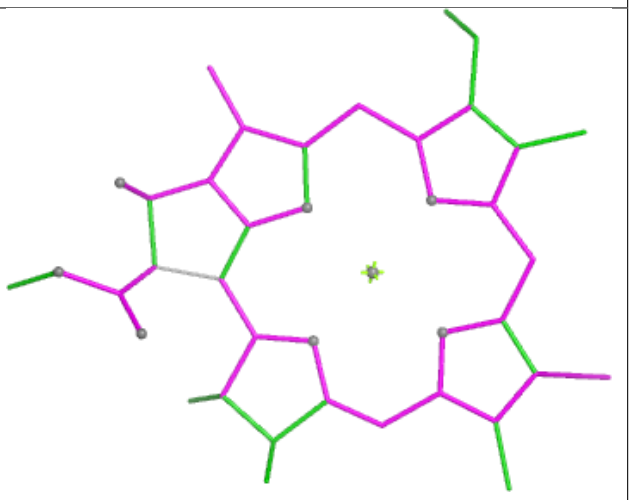
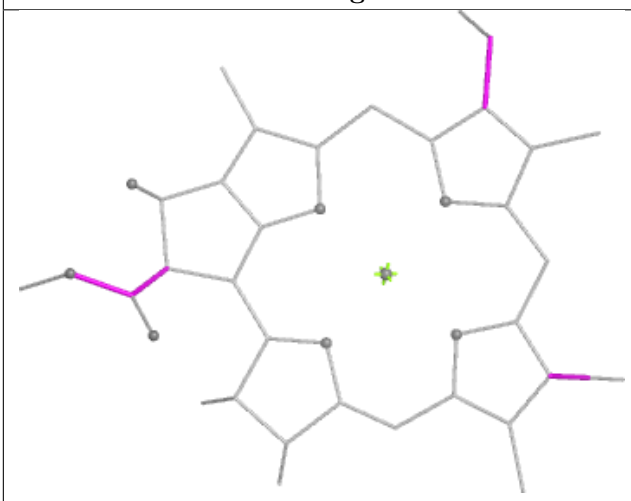


Bond angles



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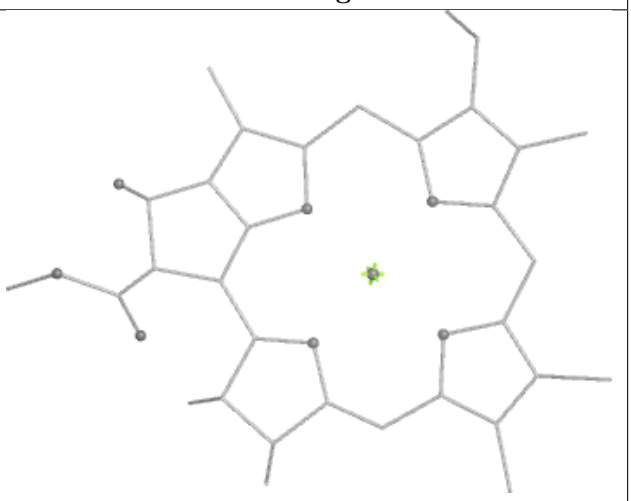
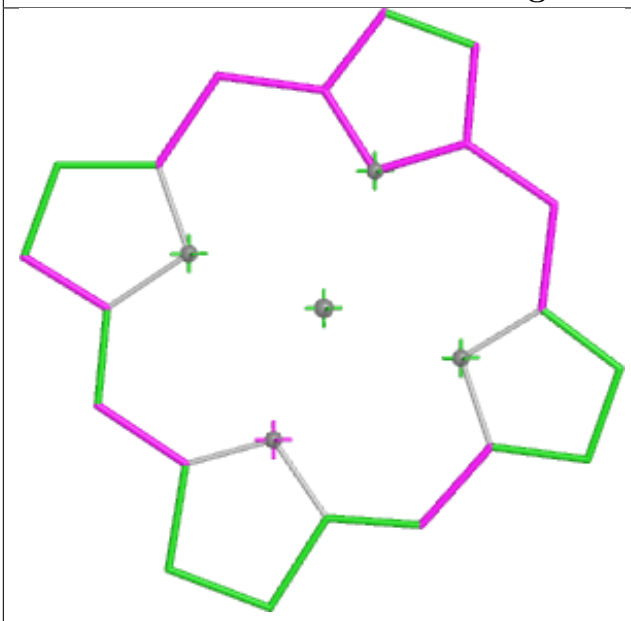


Rings

Ligand CLA 2 314



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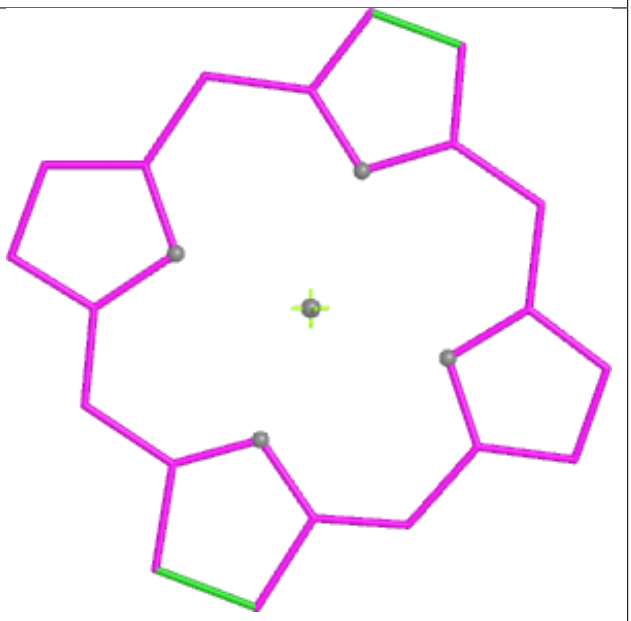
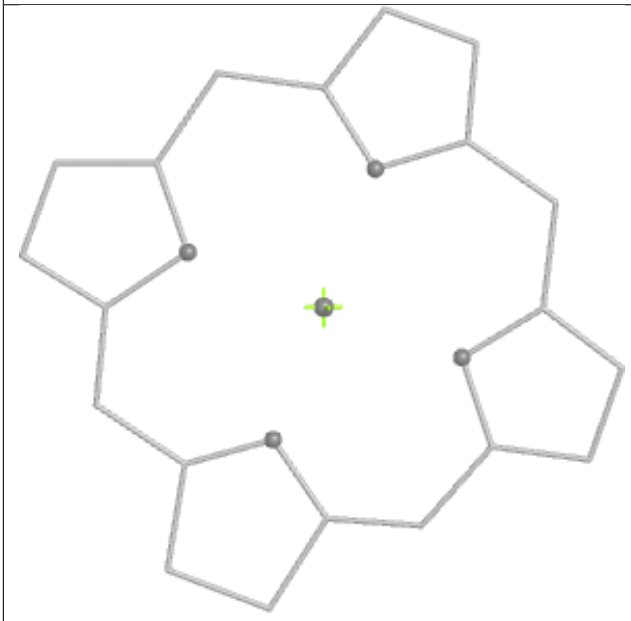


Bond angles



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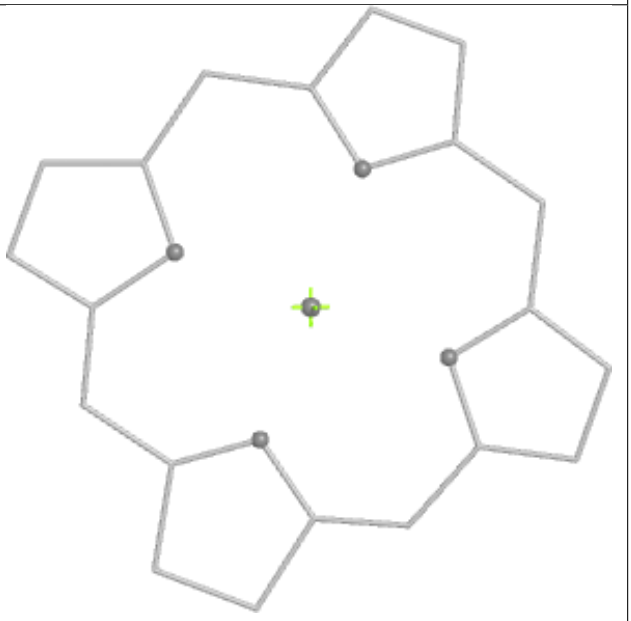
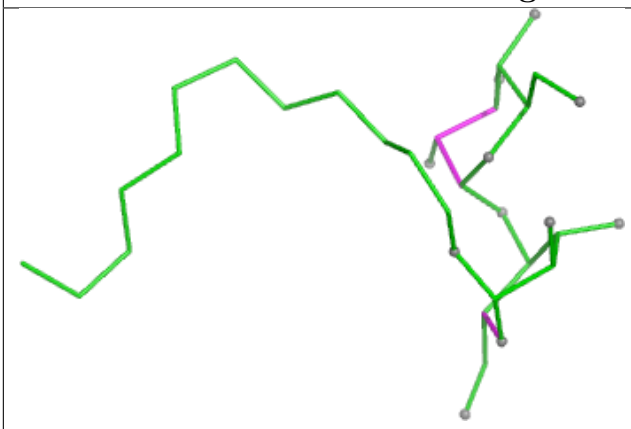


Rings

Ligand LMU H 104



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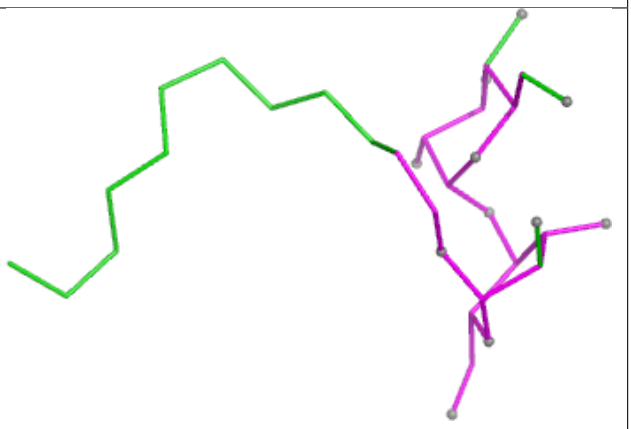
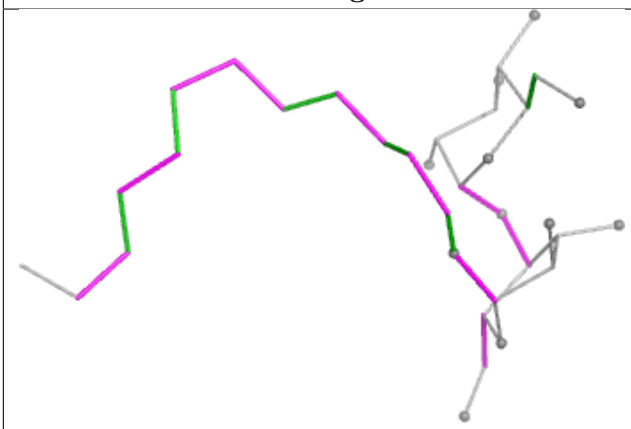


Bond angles



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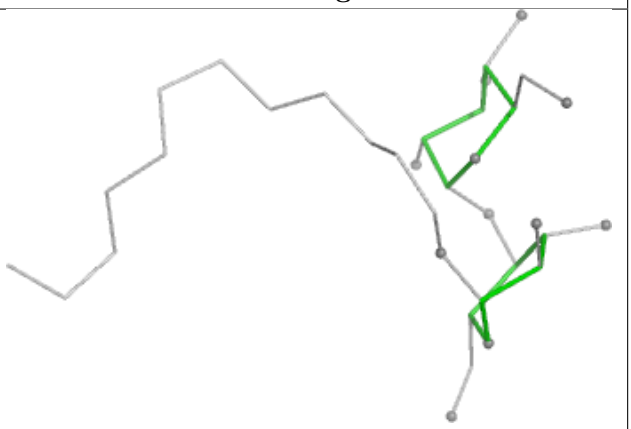
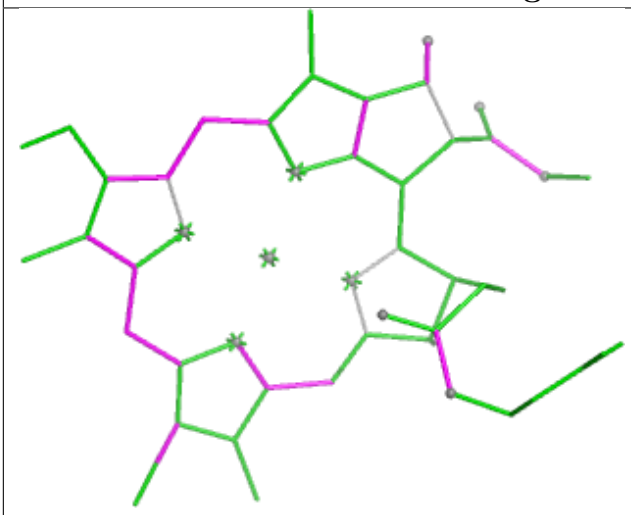


Rings

Ligand CLA A 813



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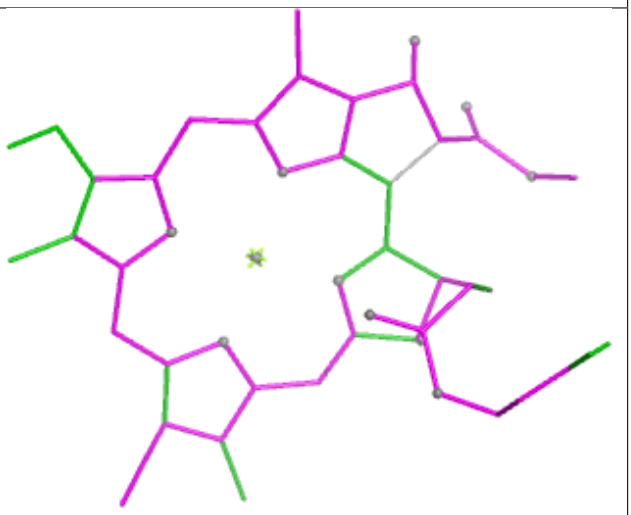
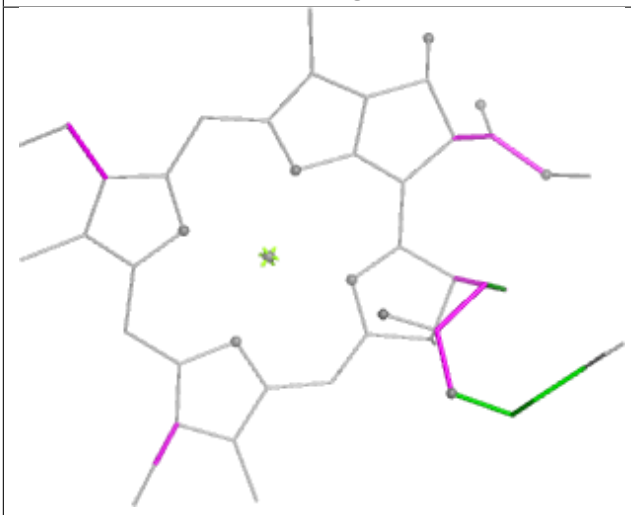


Bond angles



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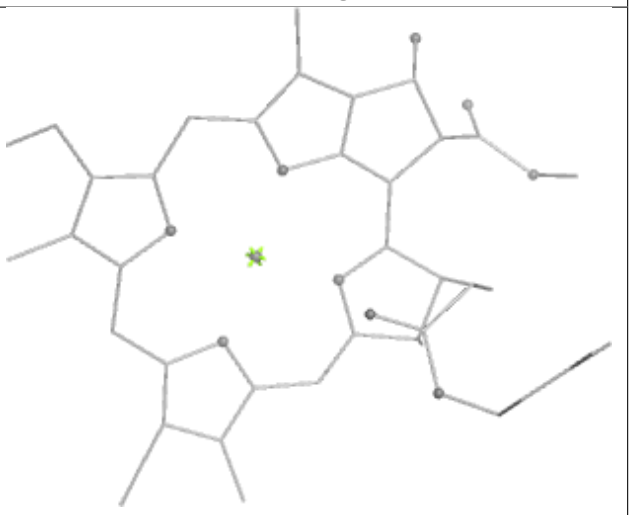
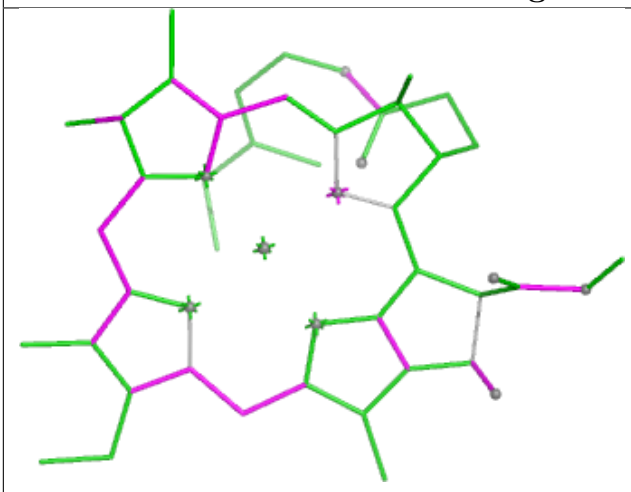


Rings

Ligand CLA 2 301



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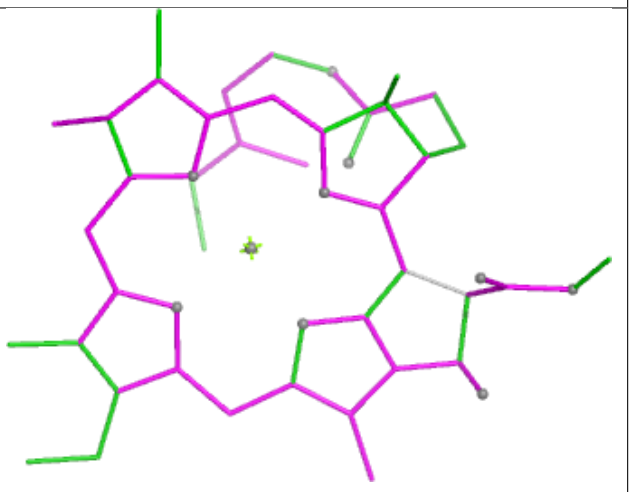
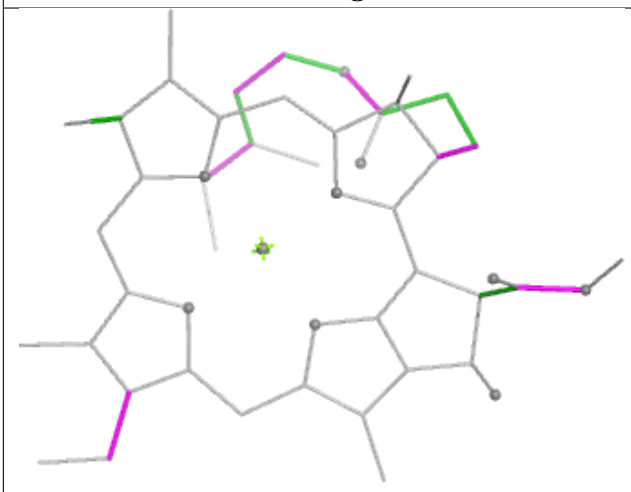


Bond angles



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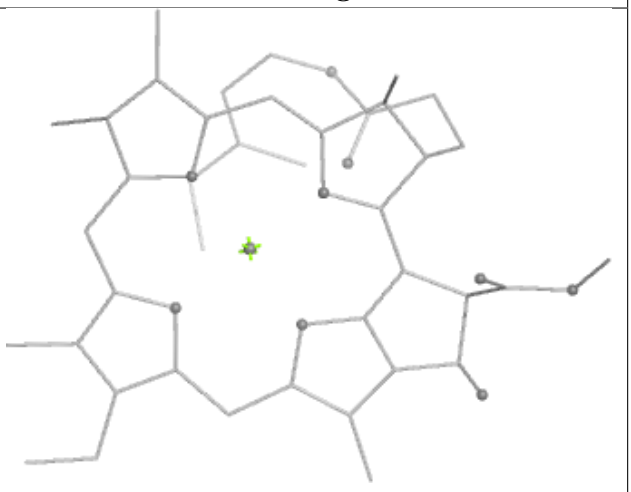
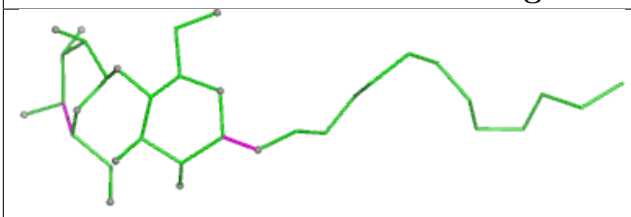


Rings

Ligand LMU 1 218



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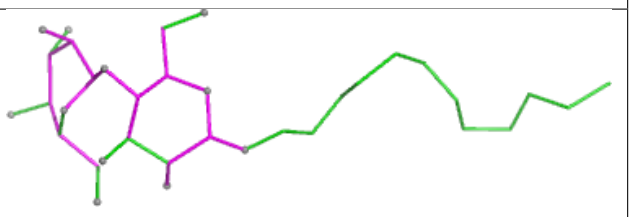
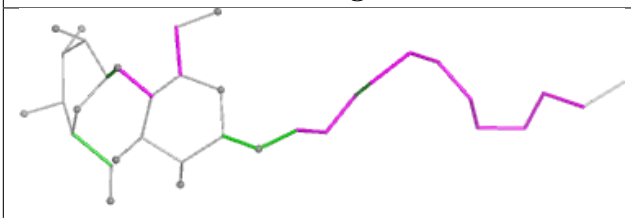


Bond angles



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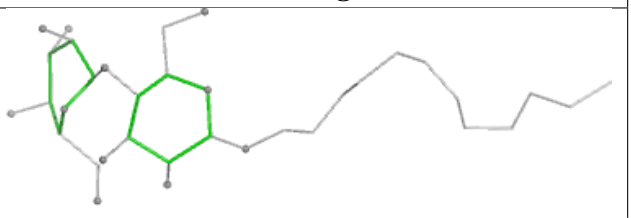
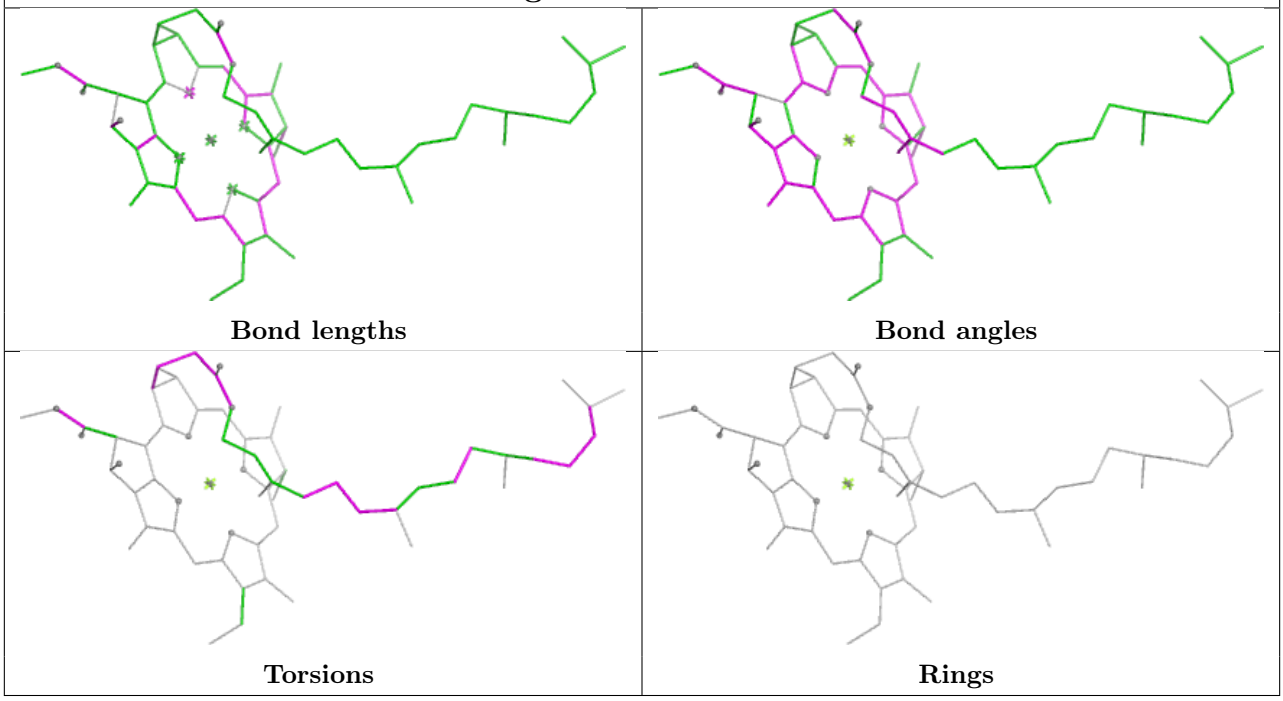
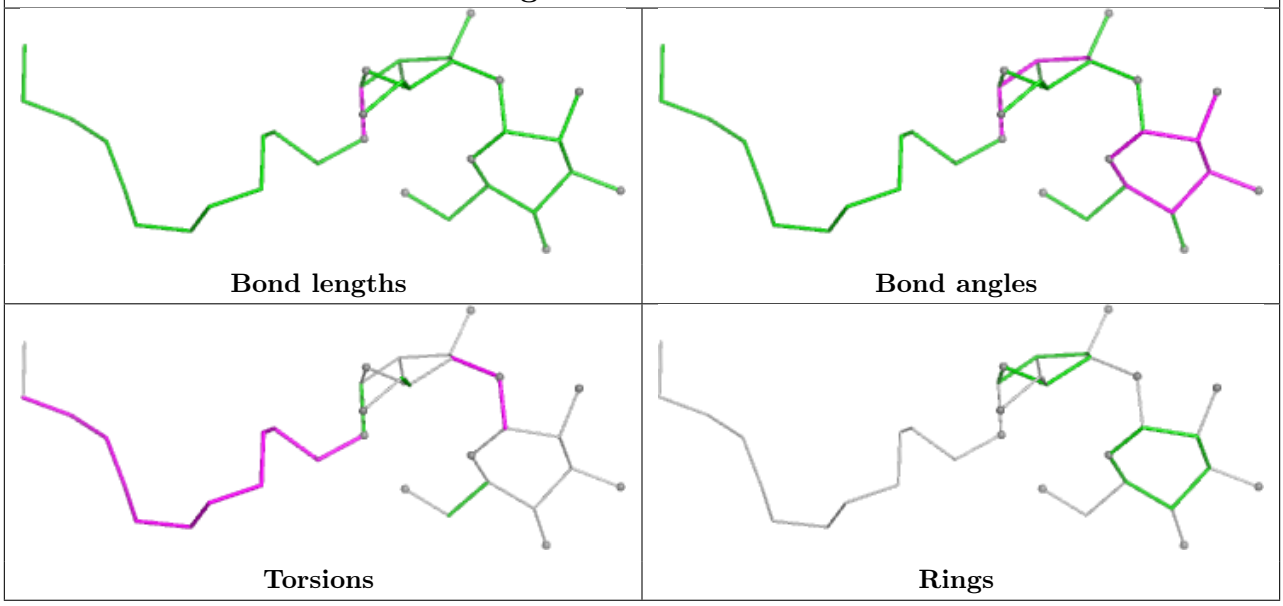


Rings

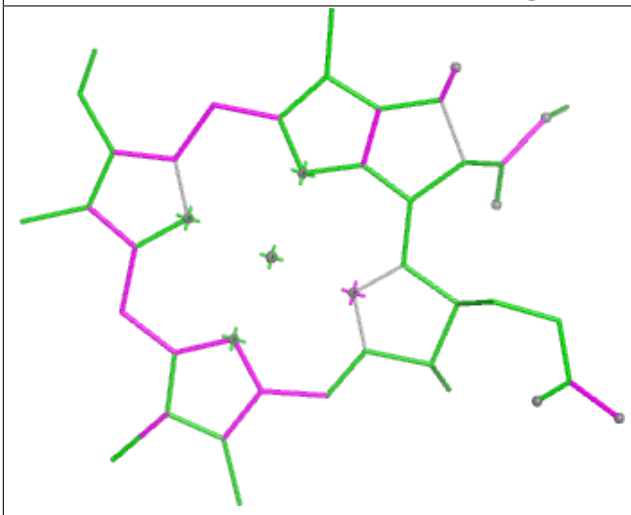
Ligand CLA A 836



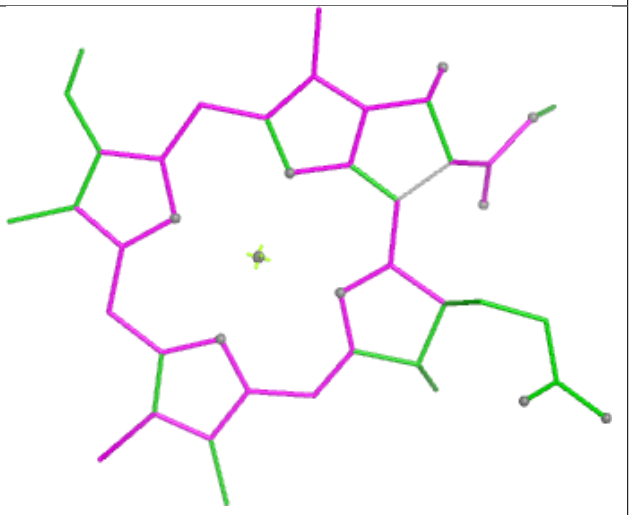
Ligand LMU A 846



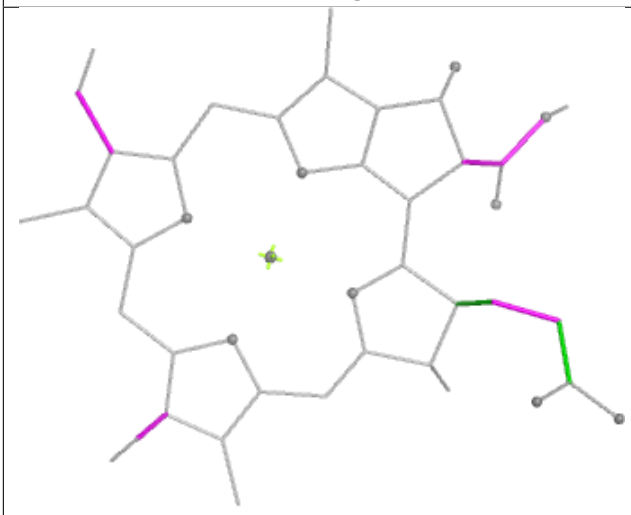
Ligand CLA K 105



Bond lengths



Bond angles



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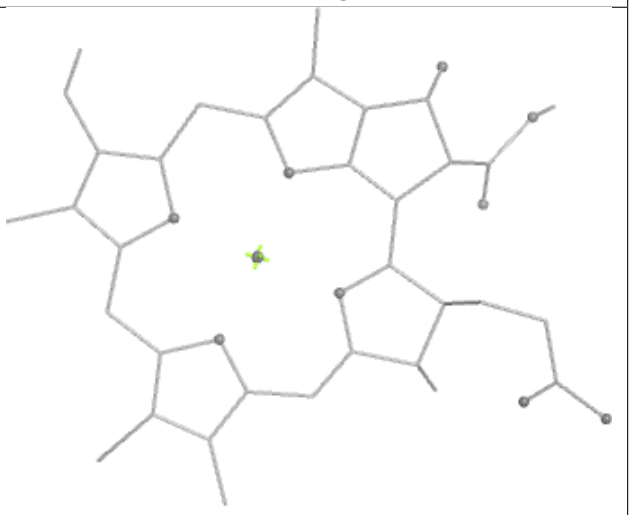
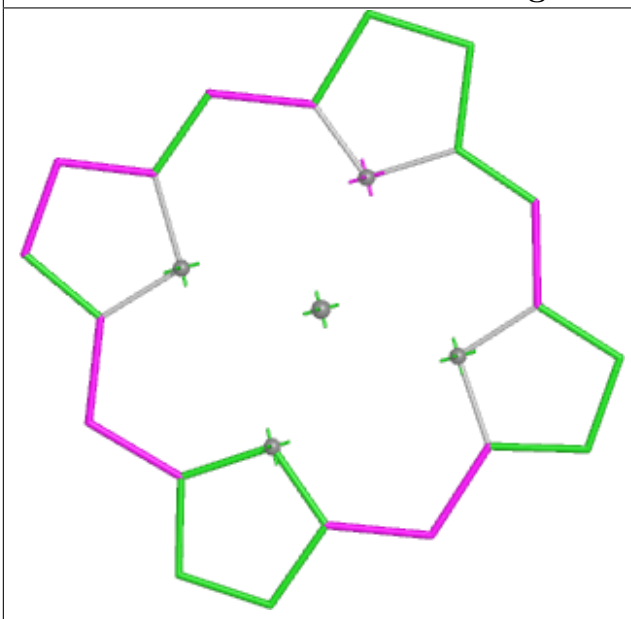
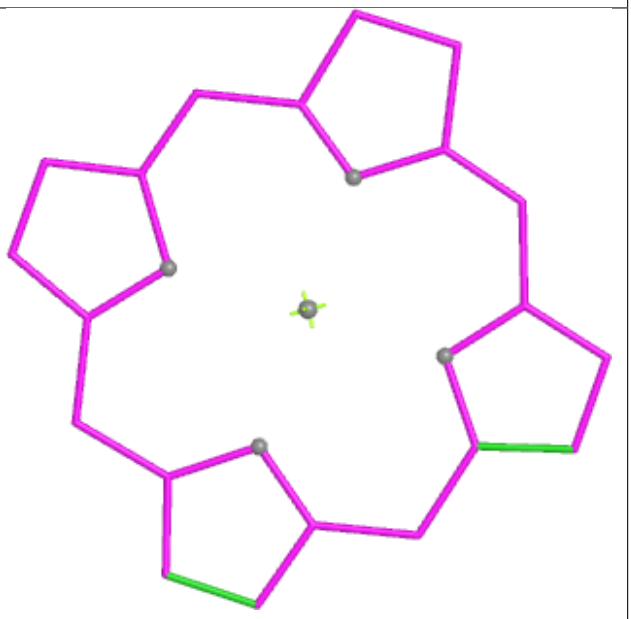


Rings

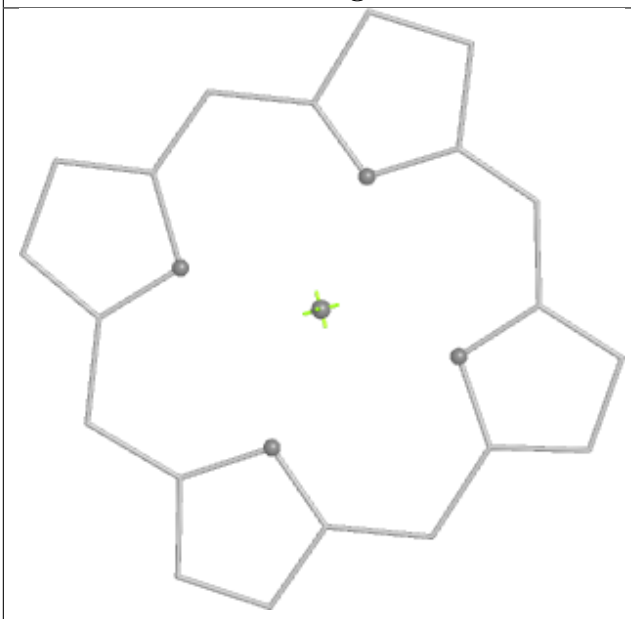
Ligand CLA 3 312



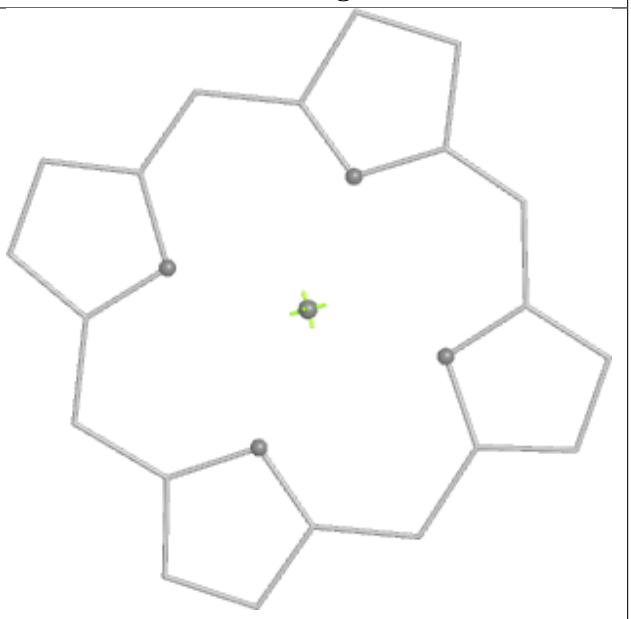
Bond lengths



Bond angles

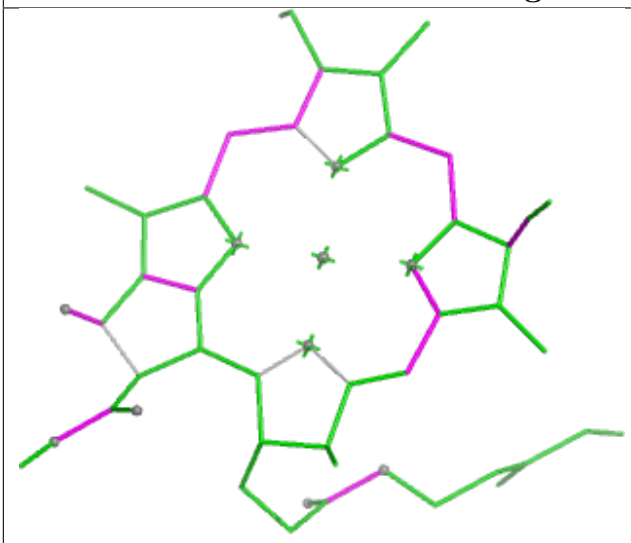


Torsions



Rings

Ligand CLA B 833



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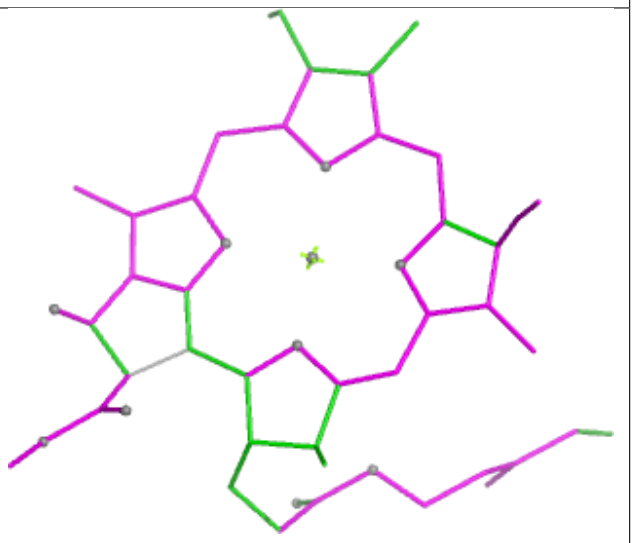
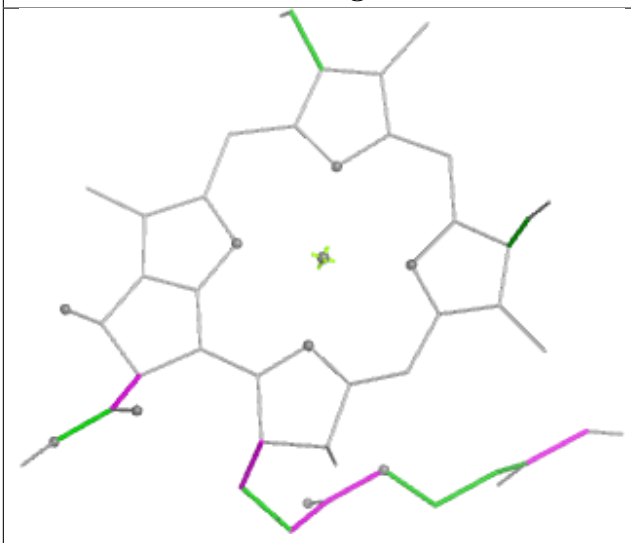


Bond angles



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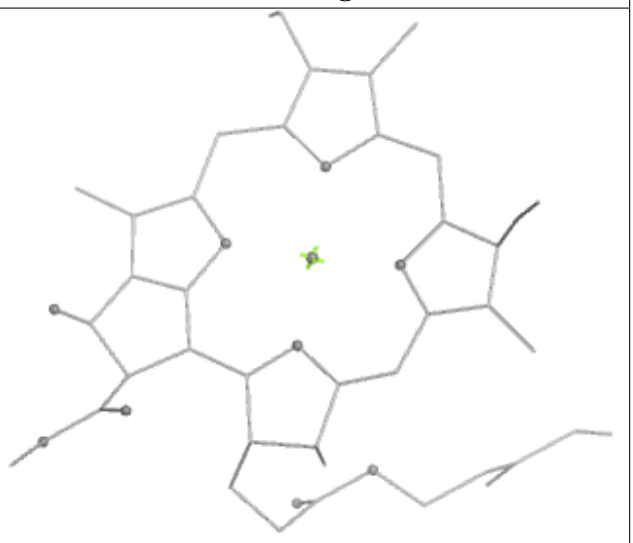
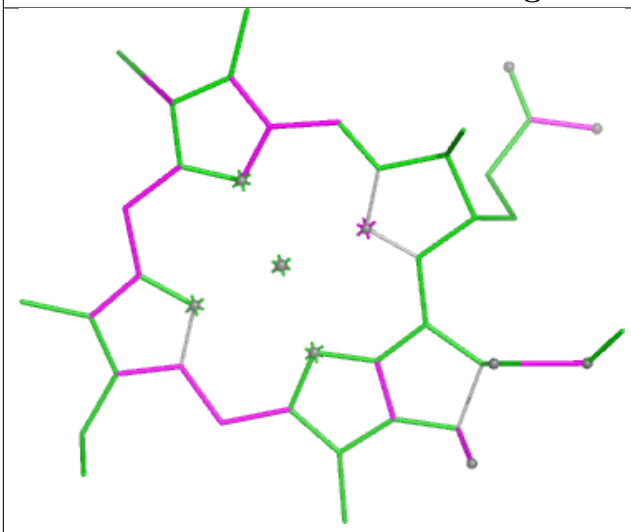


Rings

Ligand CLA A 831



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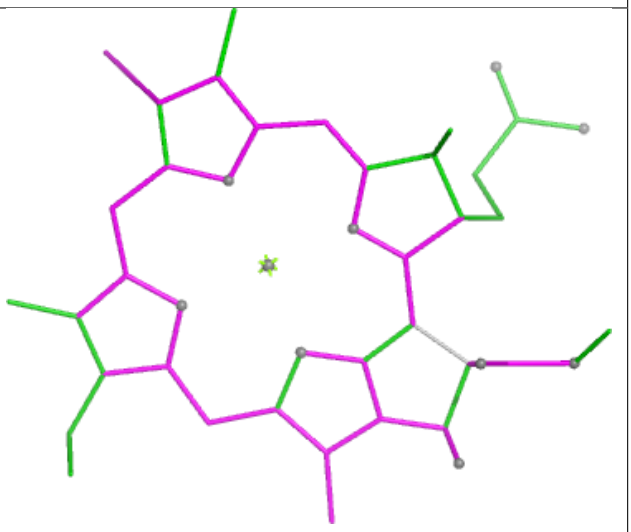
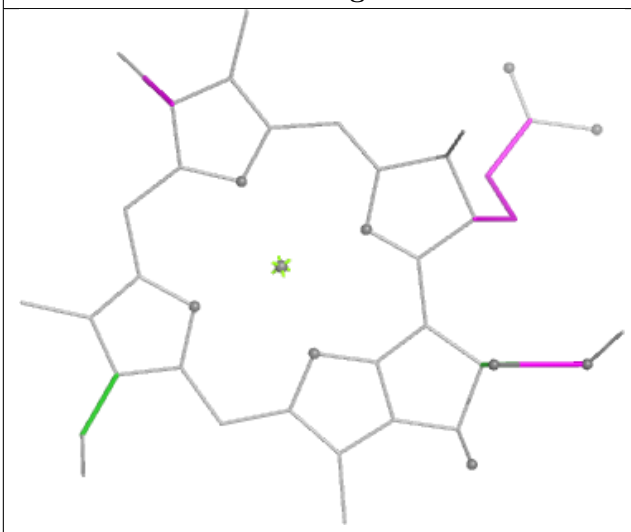


Bond angles



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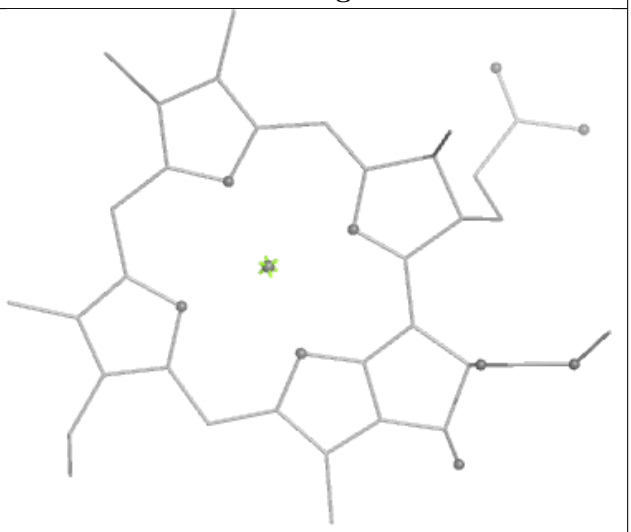
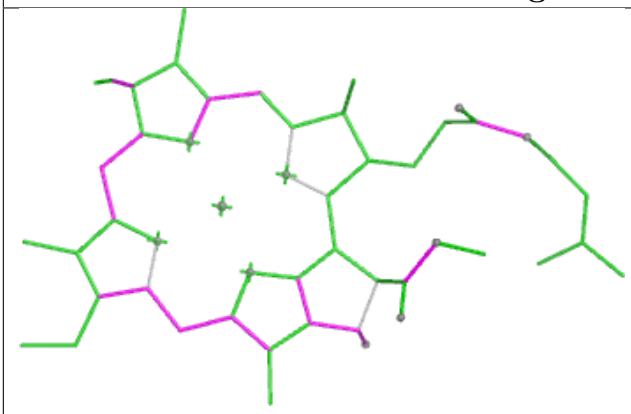


Rings

Ligand CLA 2 311



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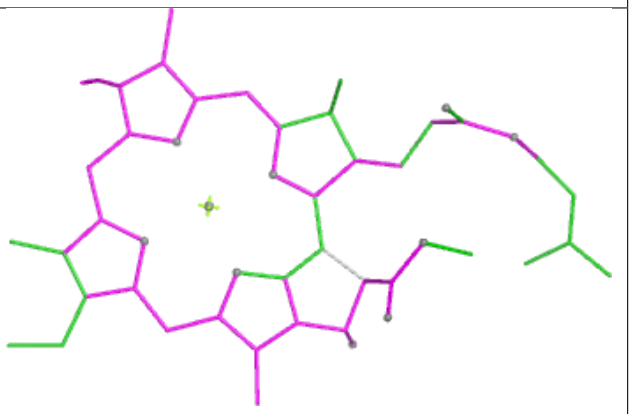
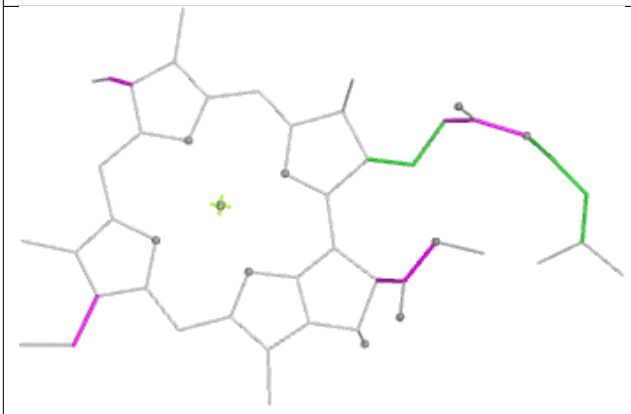


Bond angles

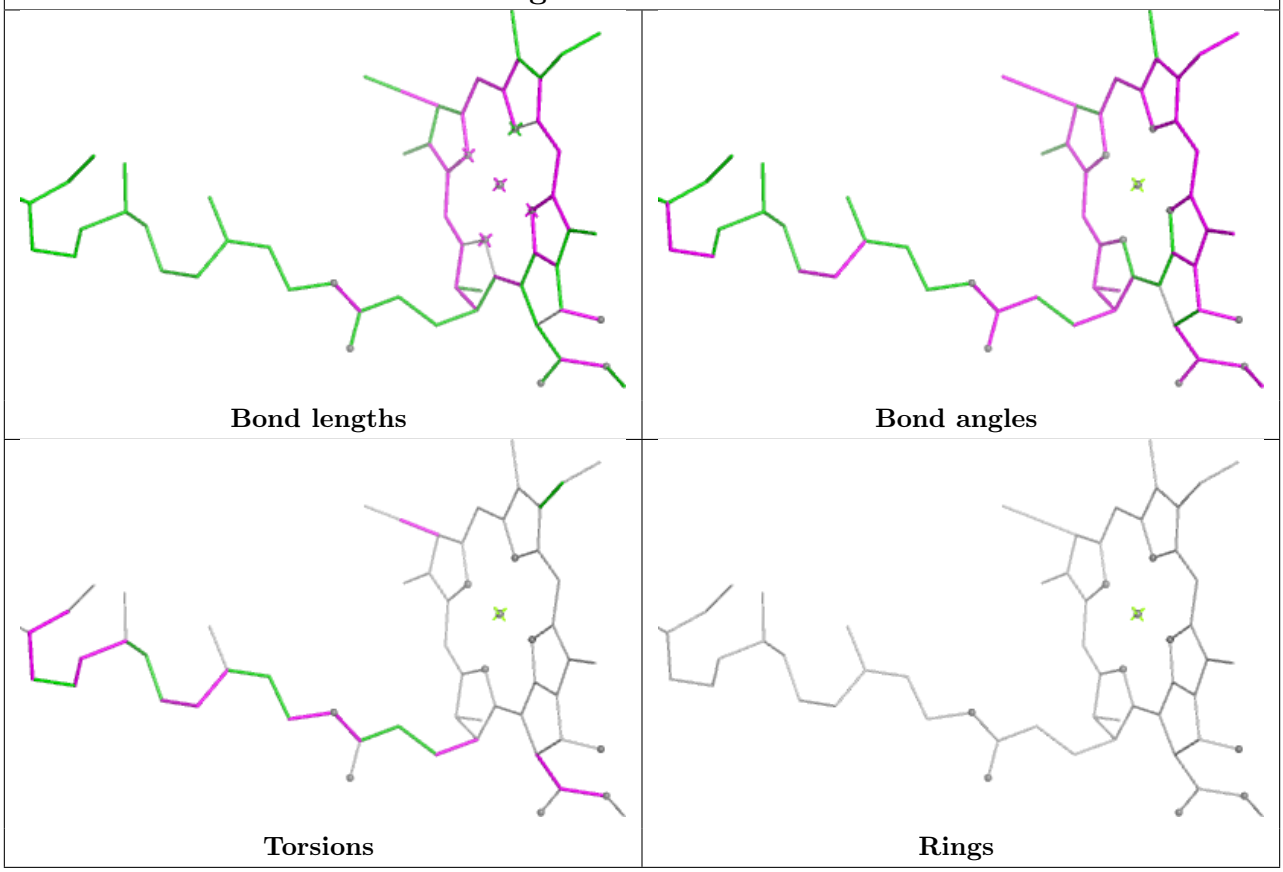


Torsions

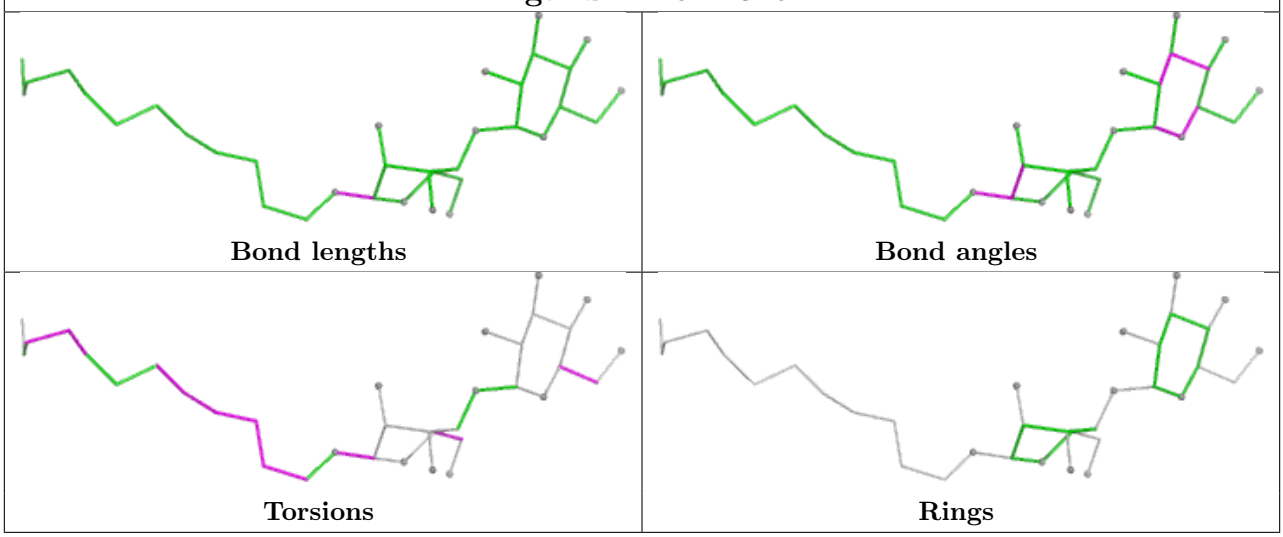


Rings

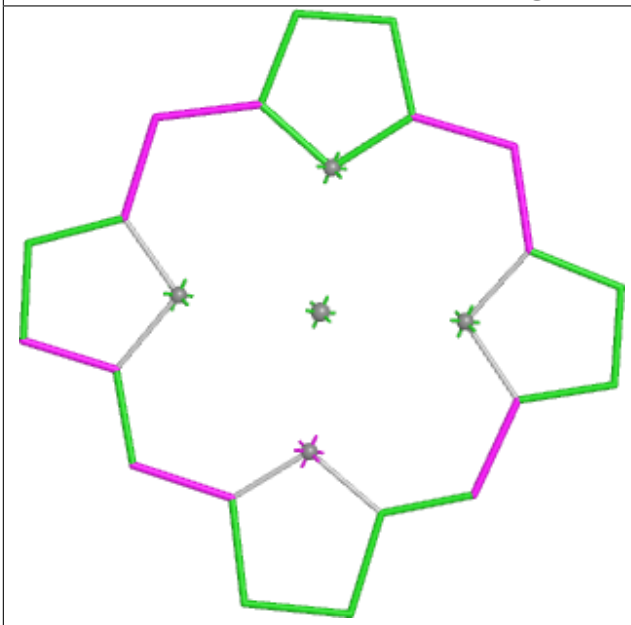
Ligand CLA 2 321



Ligand LMU 4 316



Ligand CLA 3 317



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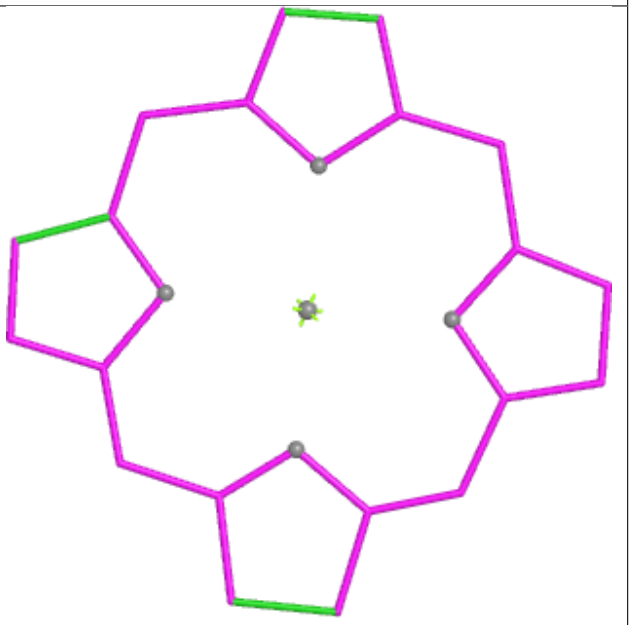
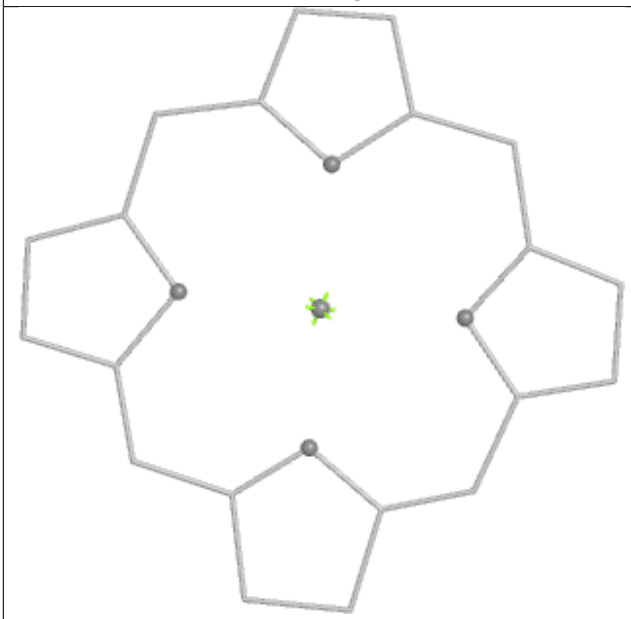


Bond angles



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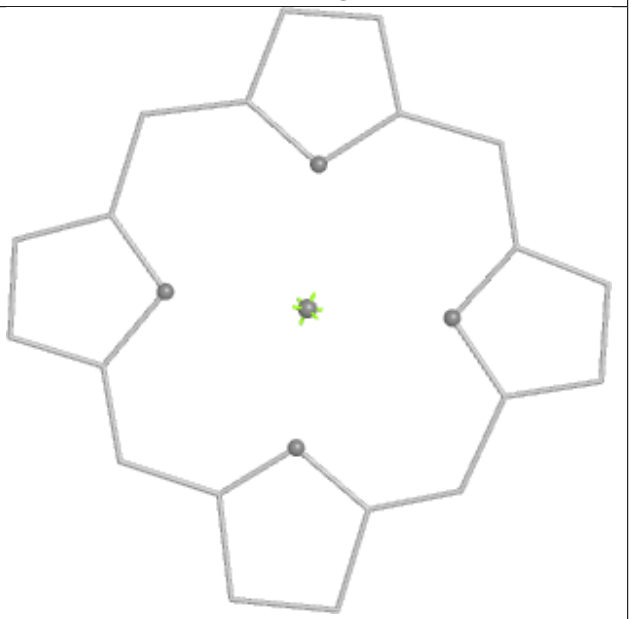
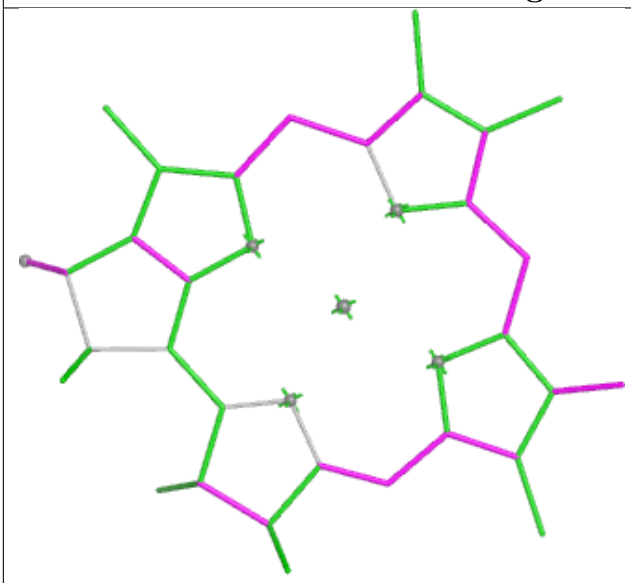


Rings

Ligand CLA F 204



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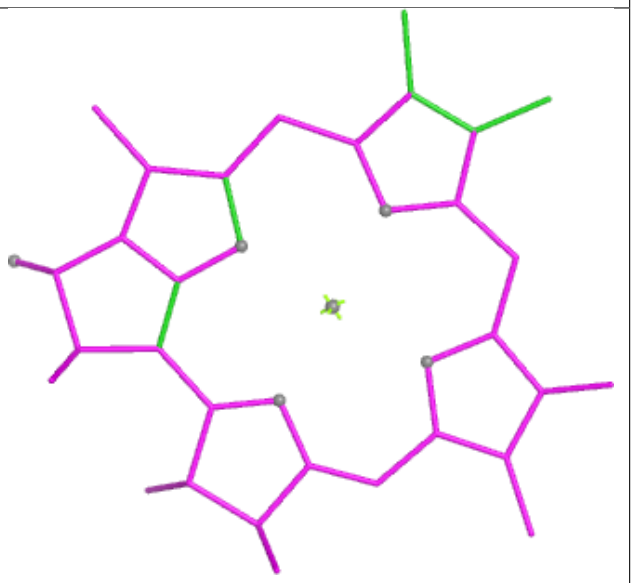
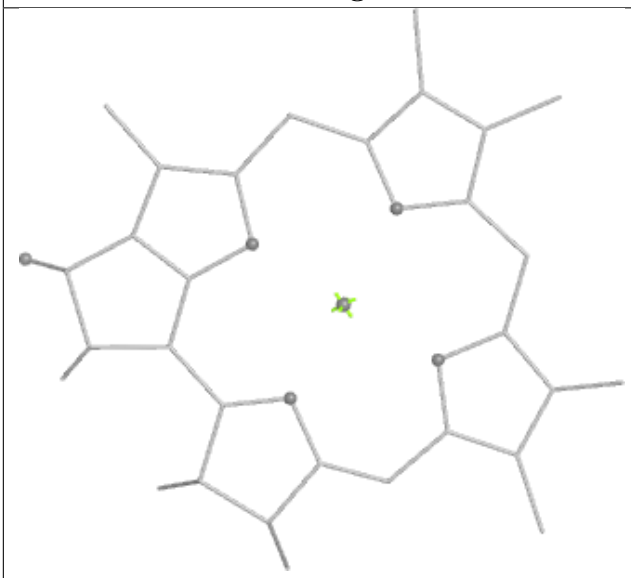


Bond angles



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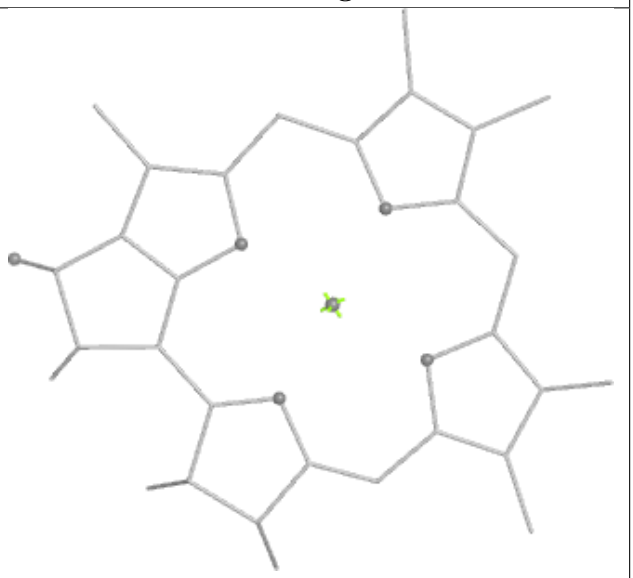
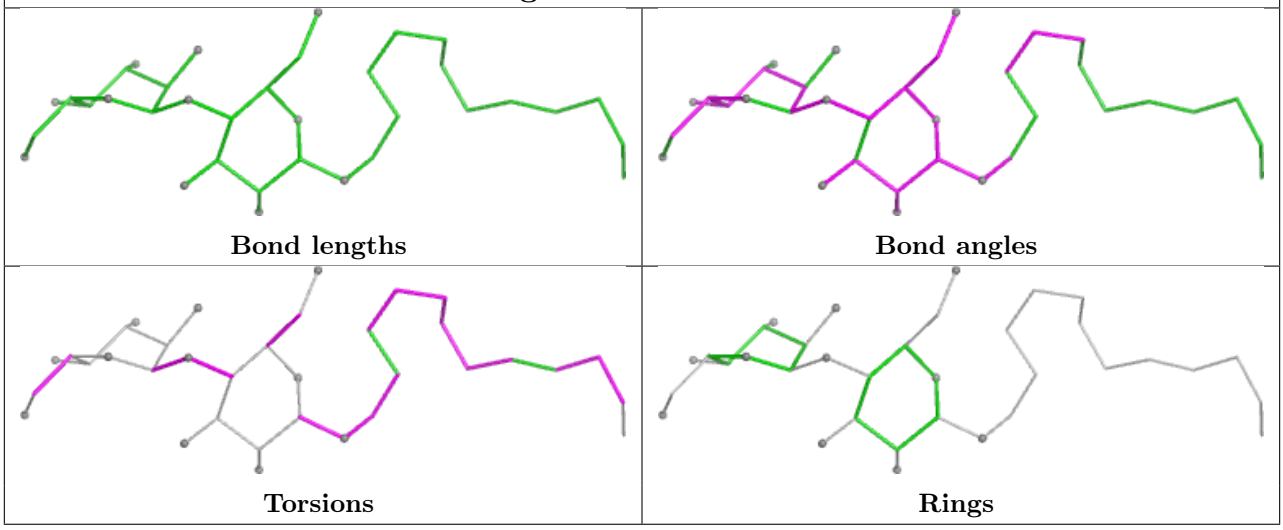
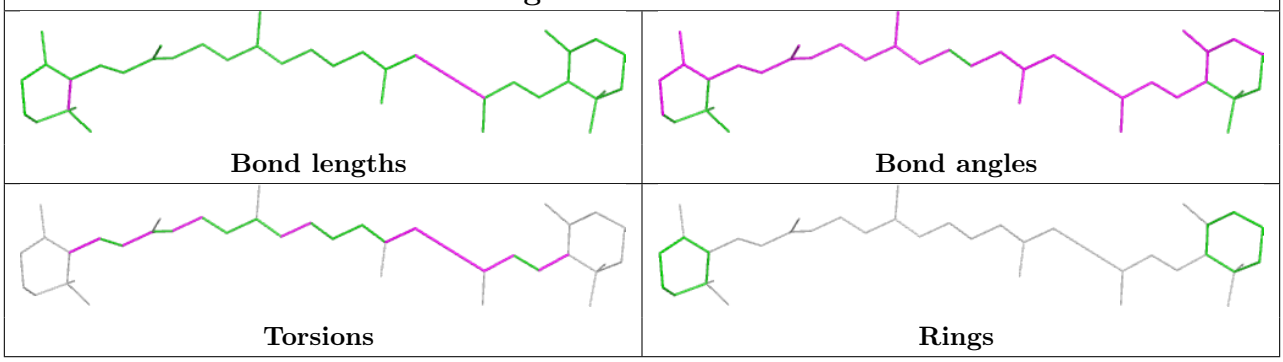


Rings

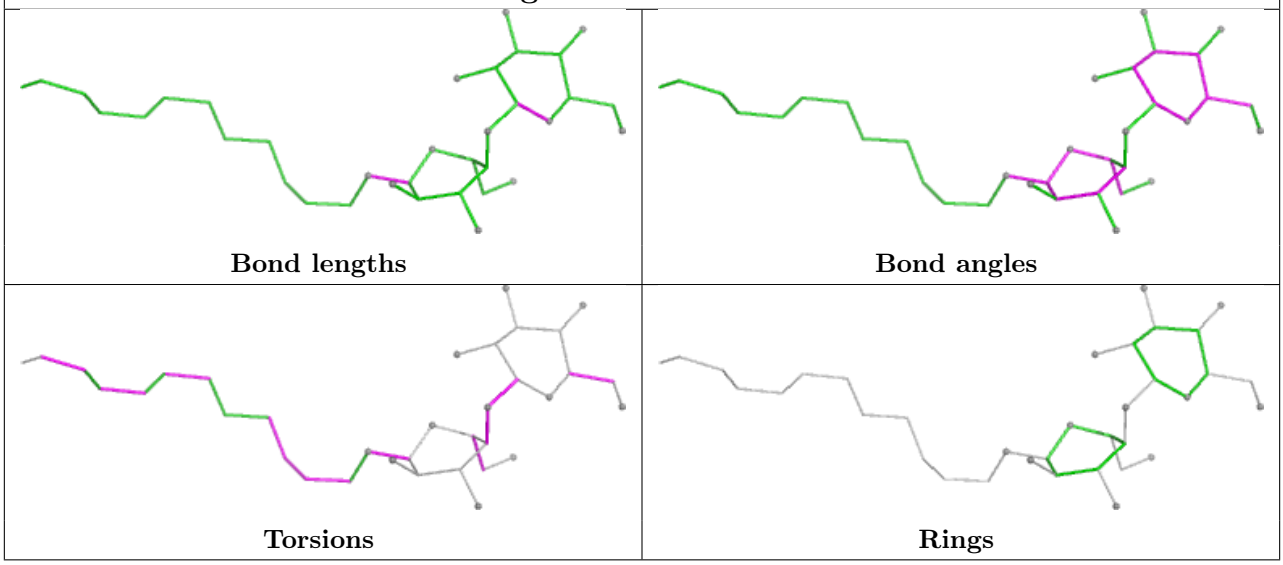
Ligand LMU K 102



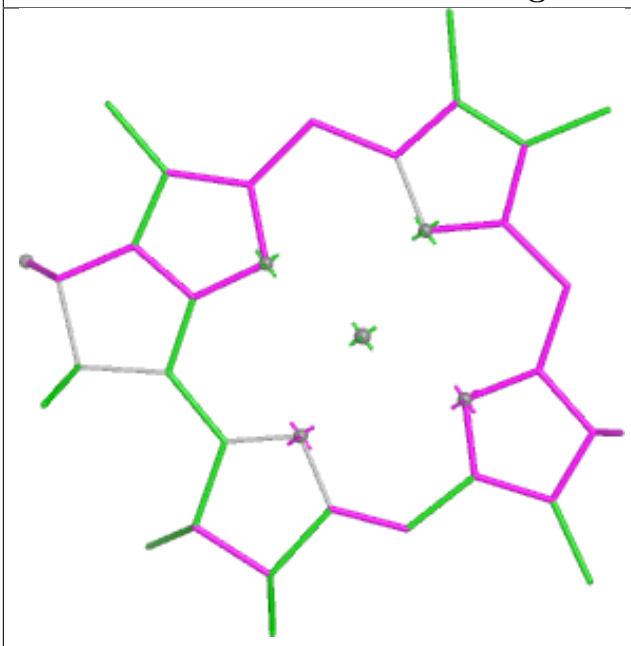
Ligand BCR B 843



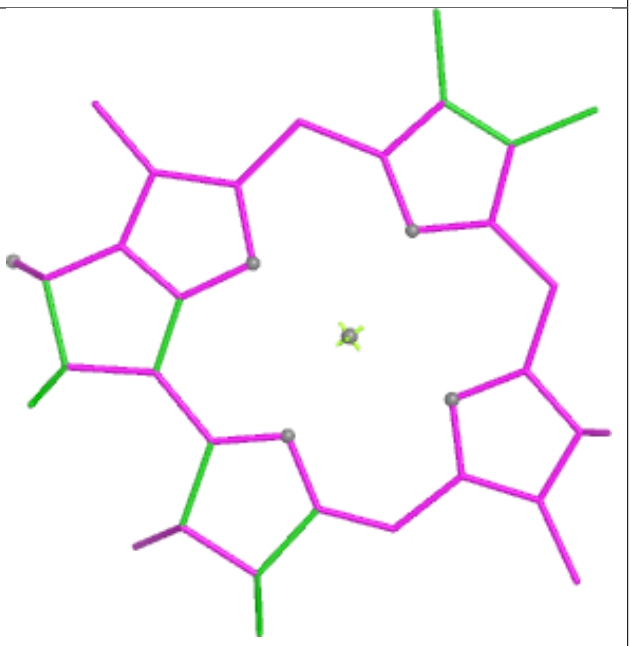
Ligand LMU R 104



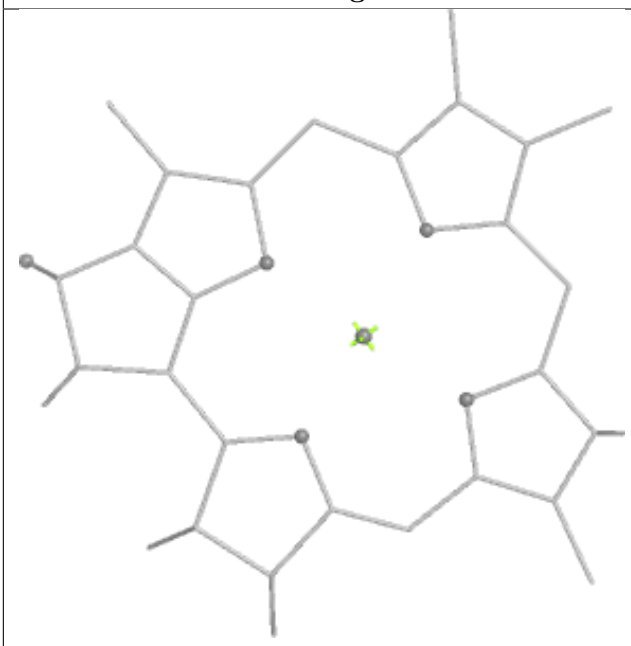
Ligand CLA 1 209



Bond lengths



Bond angles



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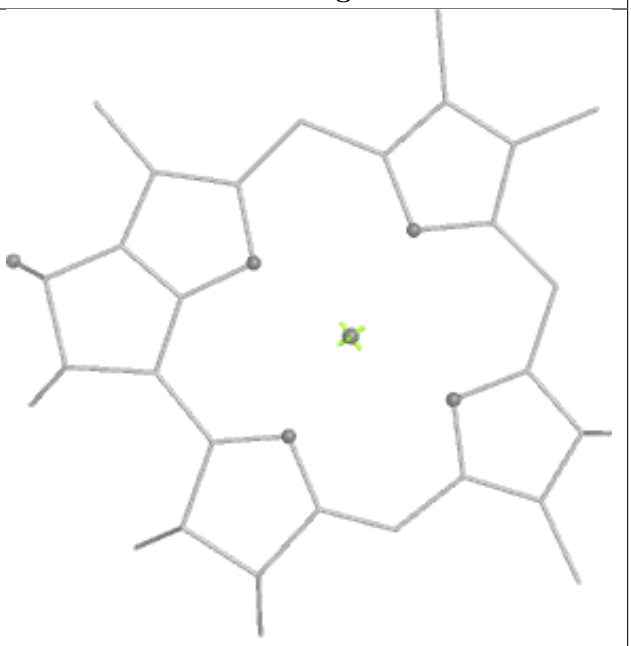
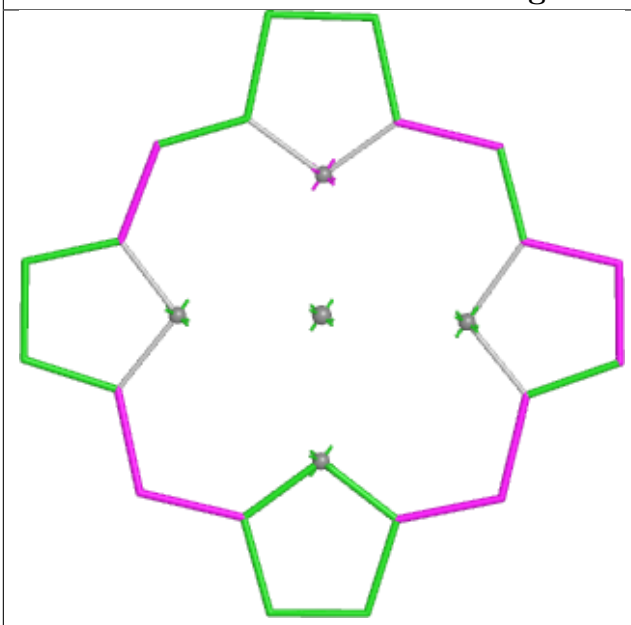


Rings

Ligand CLA 3 307



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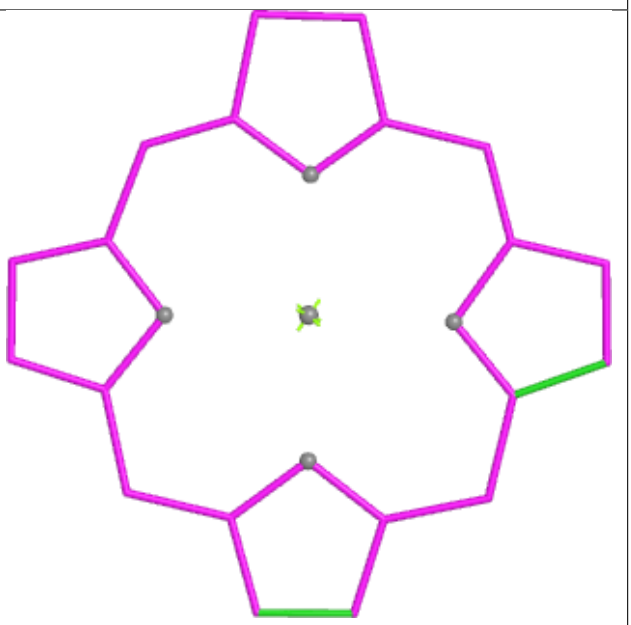
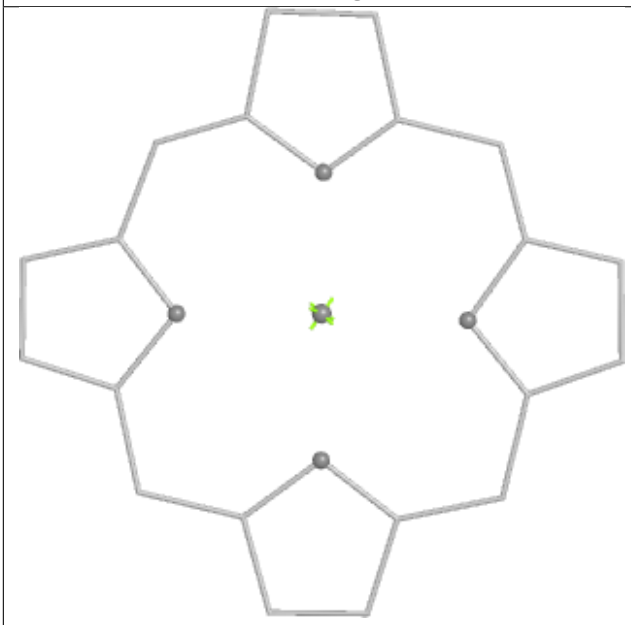


Bond angles



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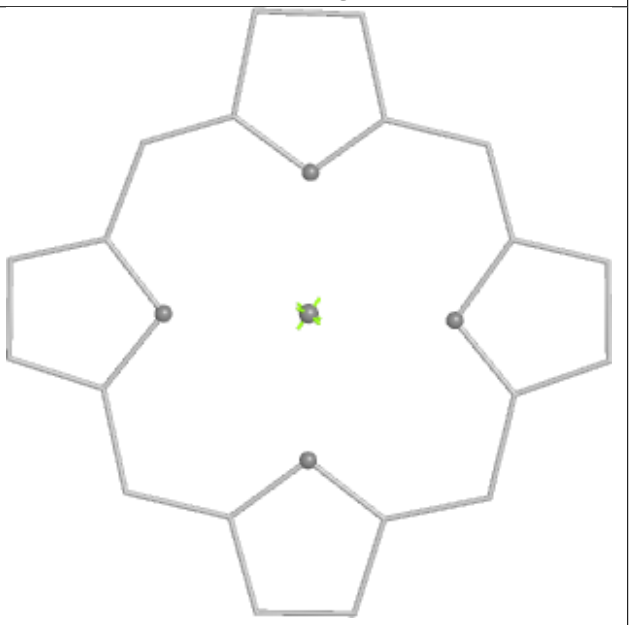
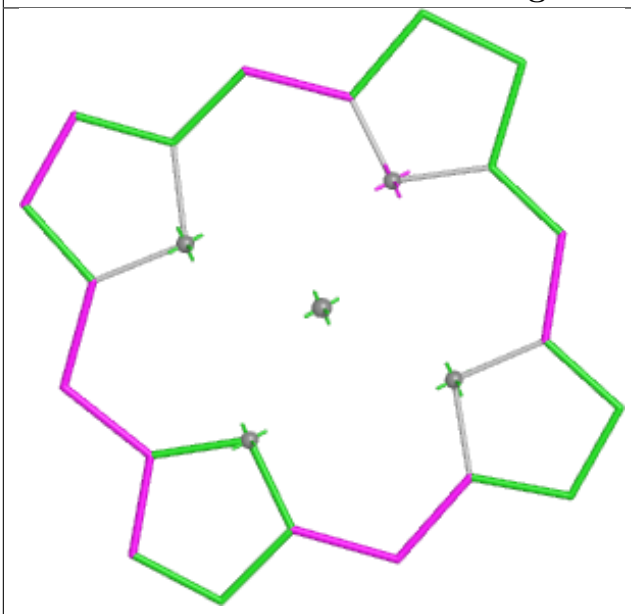
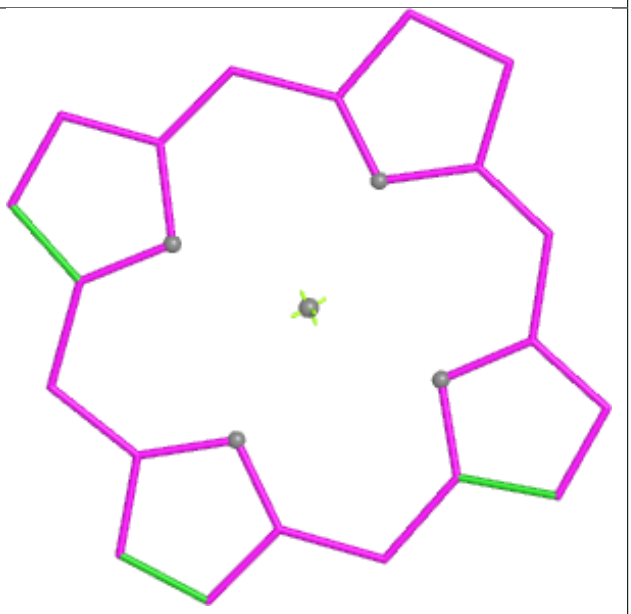


Rings

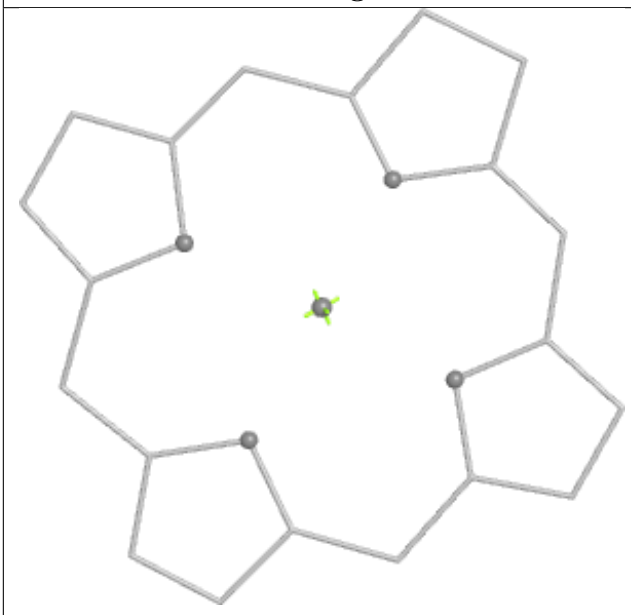
Ligand CLA 3 306



Bond lengths



Bond angles



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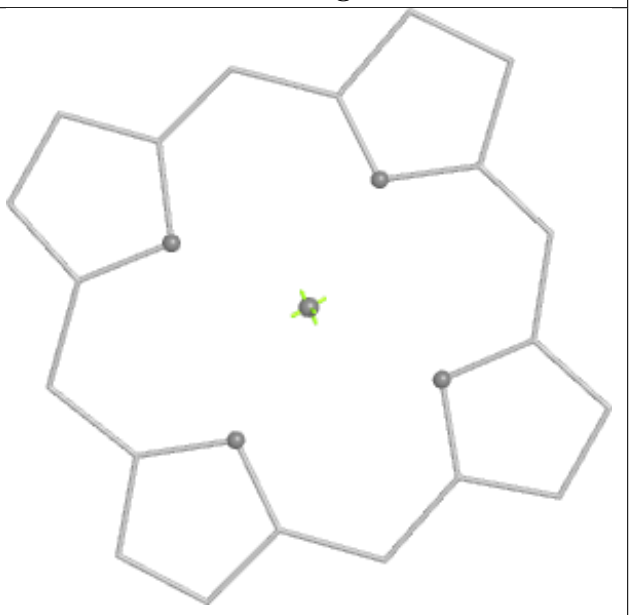
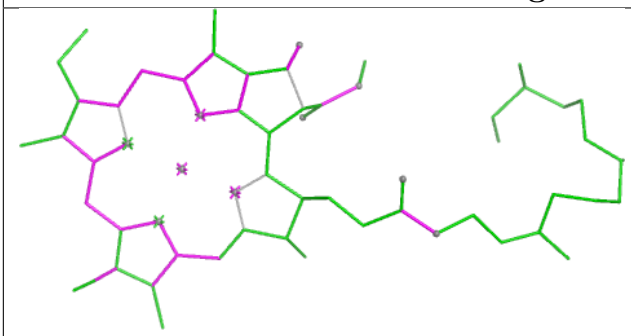


Rings

Ligand CLA 1 212



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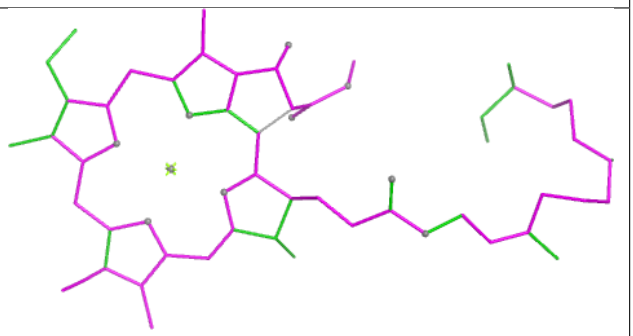
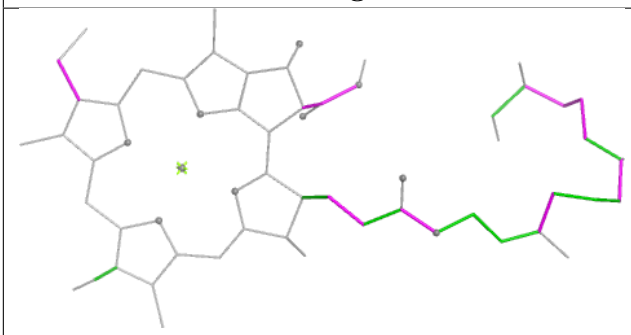


Bond angles



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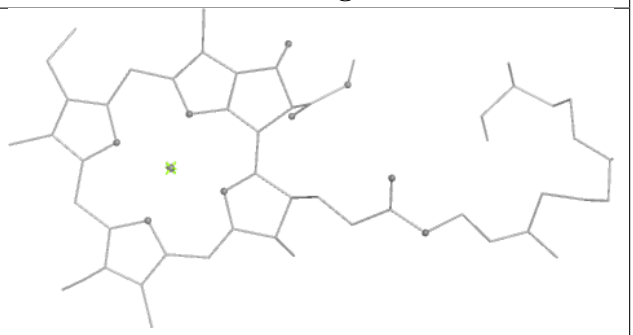
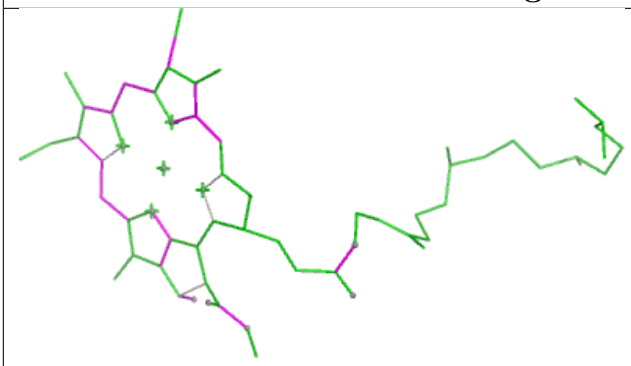


Rings

Ligand CLA B 807



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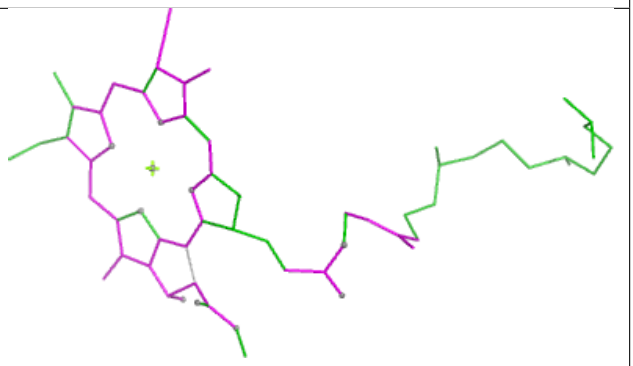
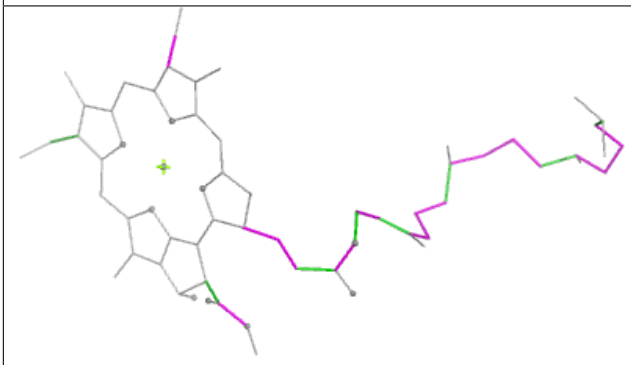


Bond angles



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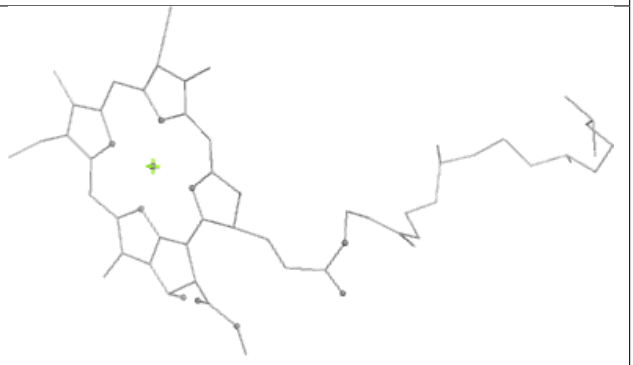
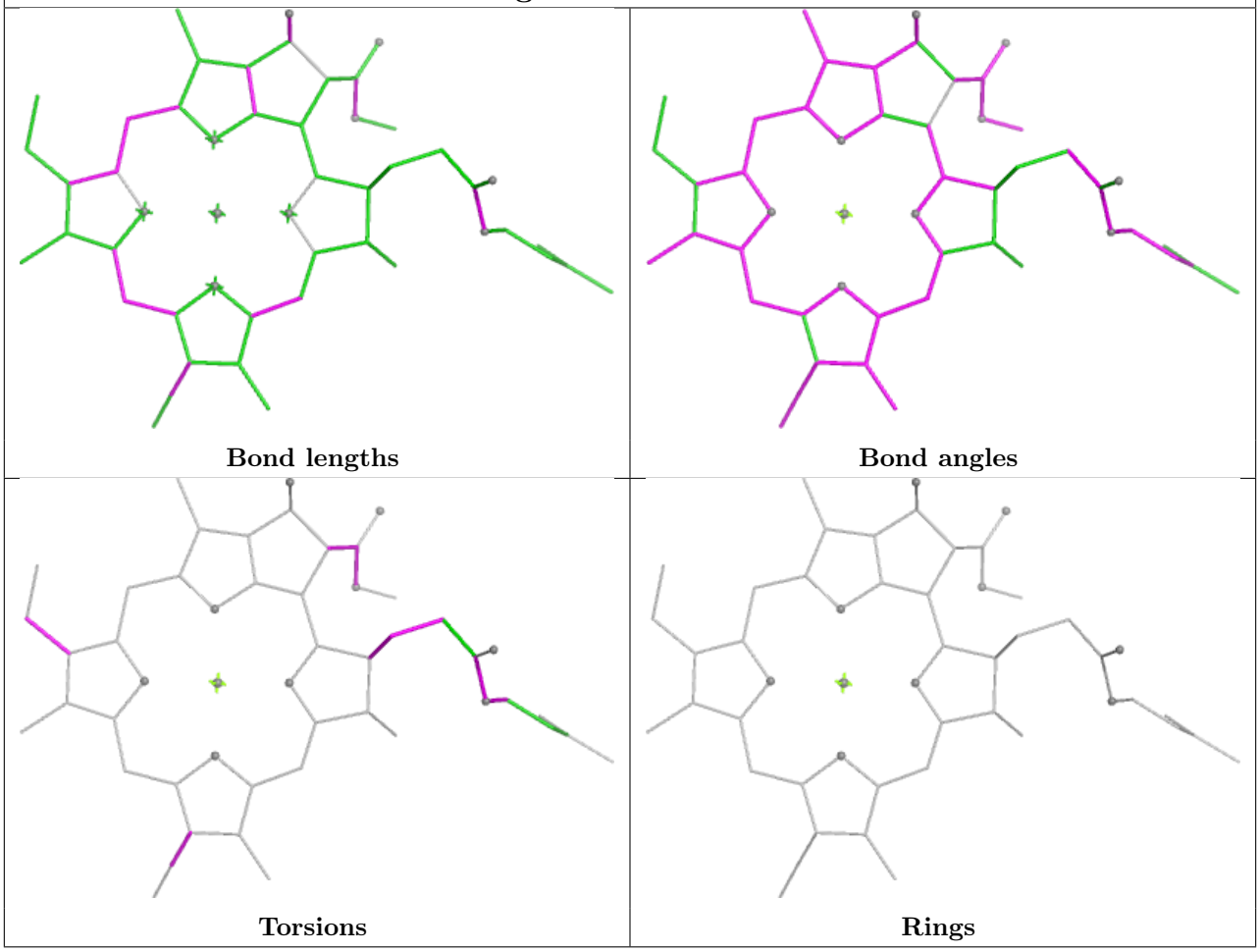
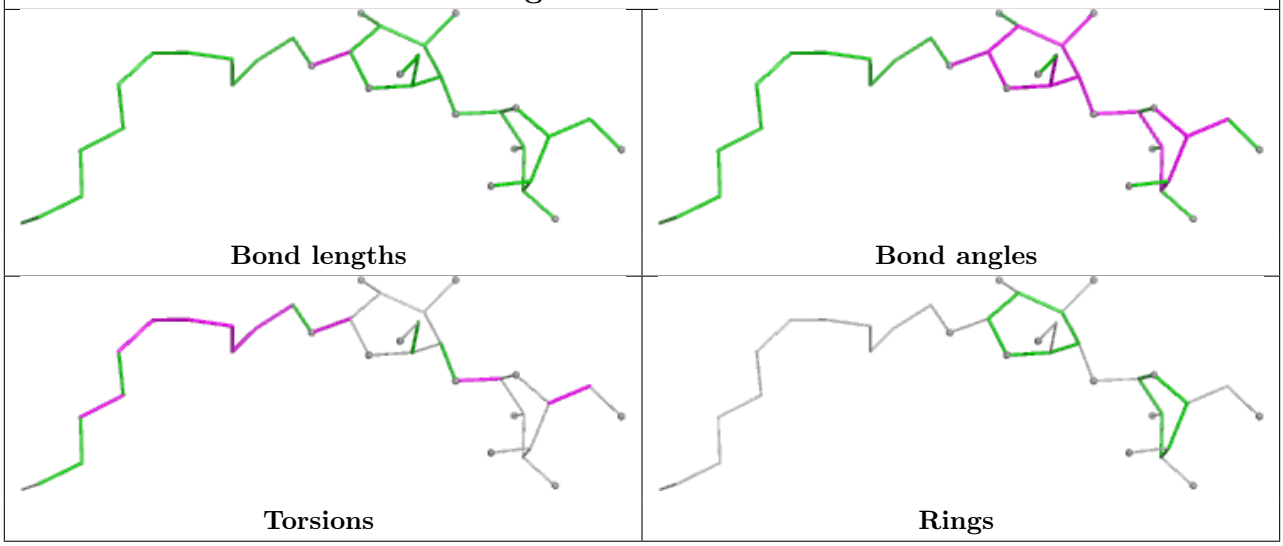


Rings

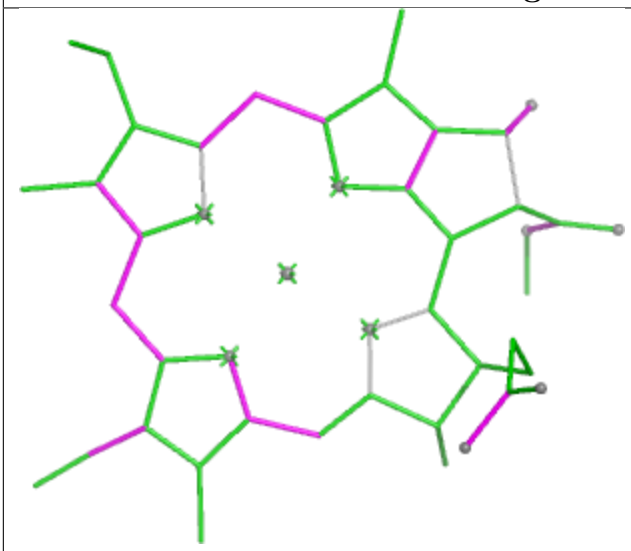
Ligand CLA B 828



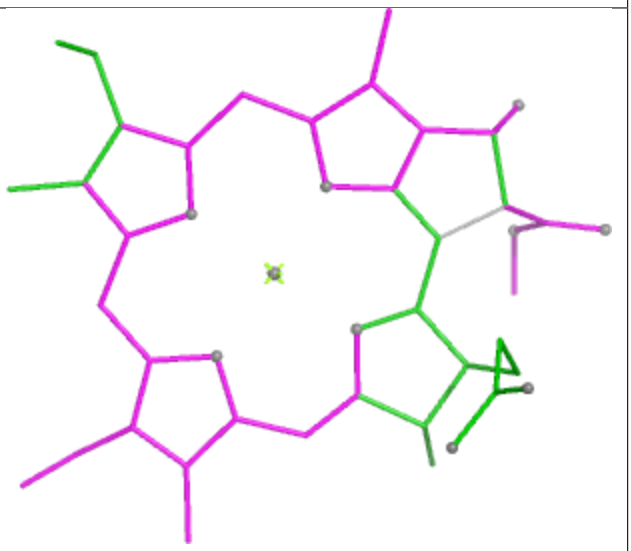
Ligand LMU 2 318



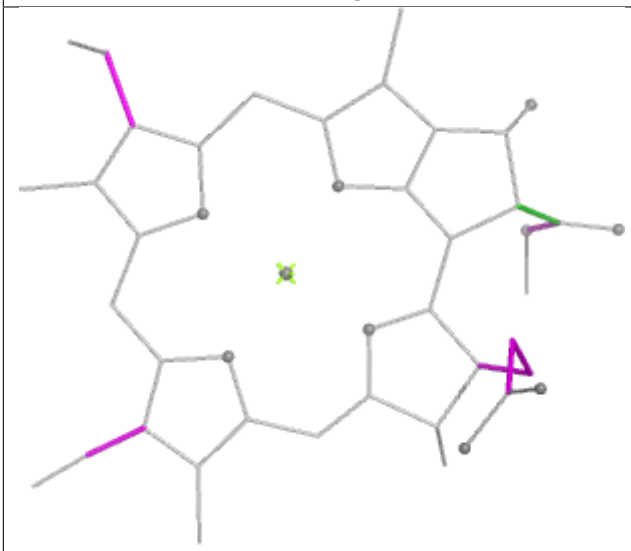
Ligand CLA A 812



Bond lengths



Bond angles



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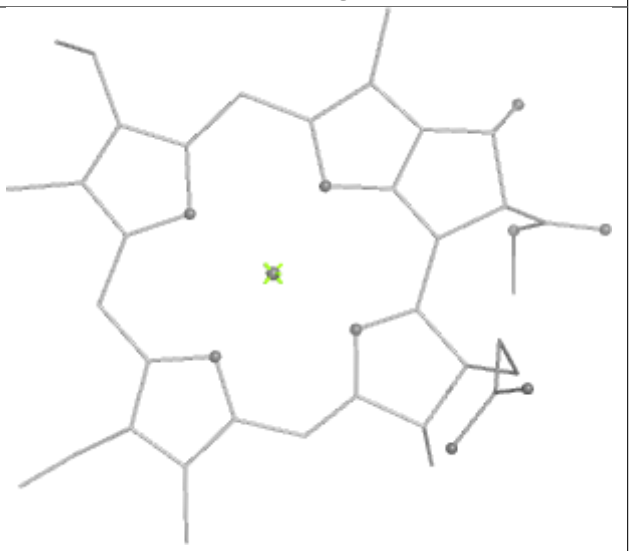
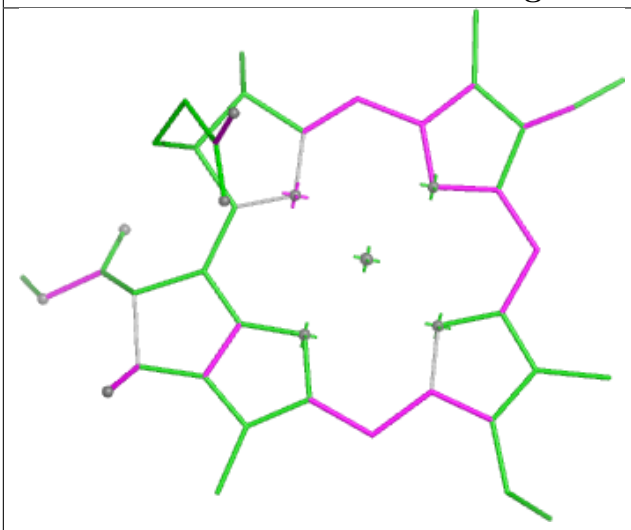


Rings

Ligand CLA B 803



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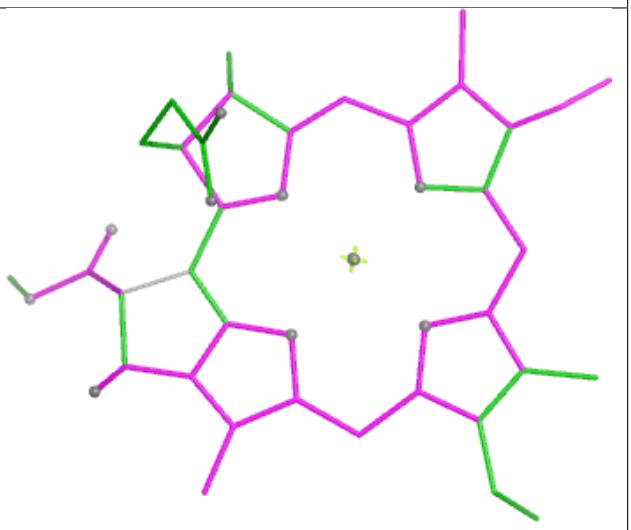
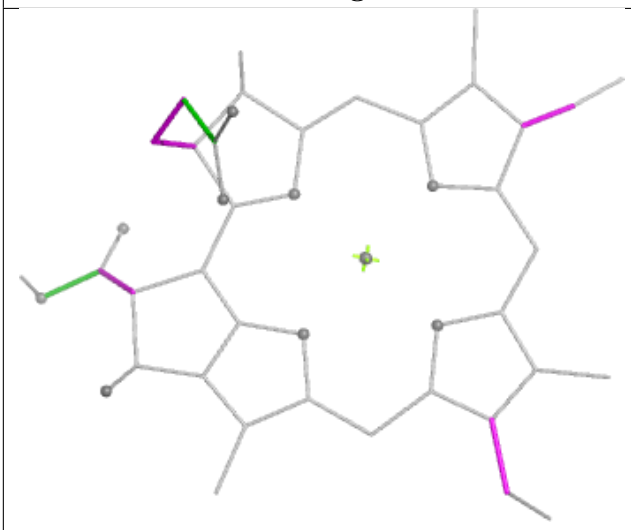


Bond angles



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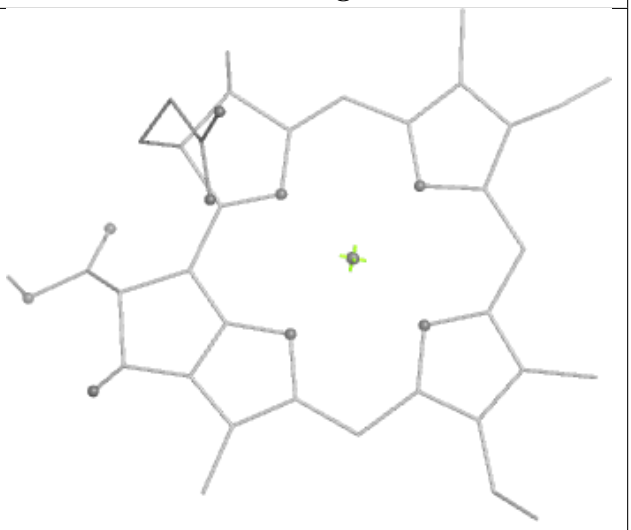
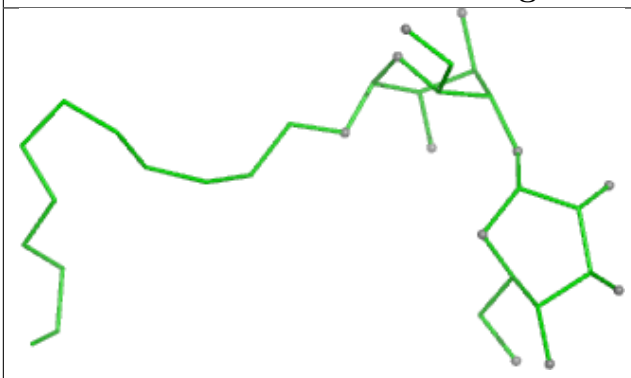
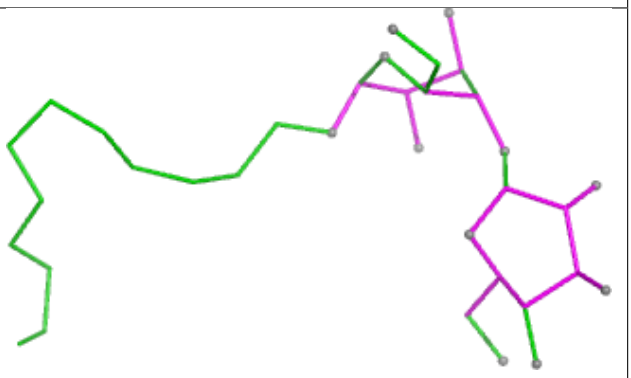


Rings

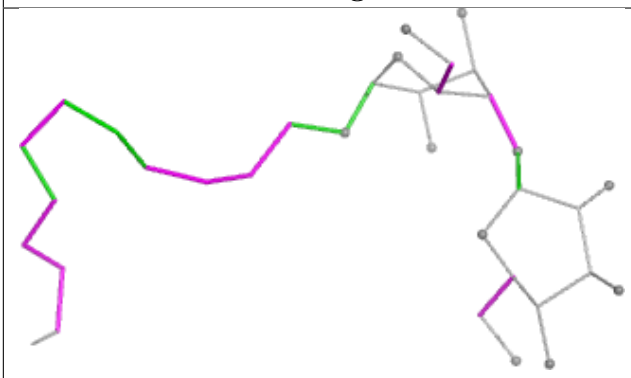
Ligand LMU K 104



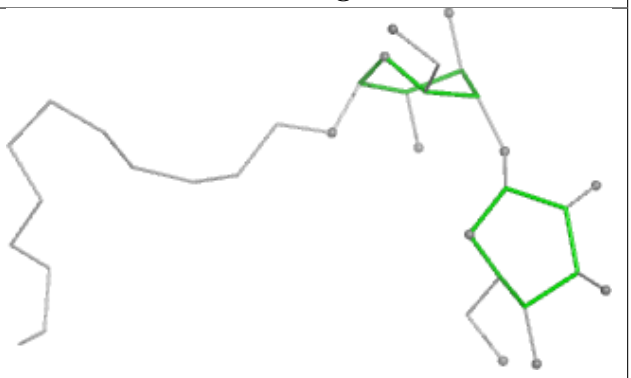
Bond lengths



Bond angles

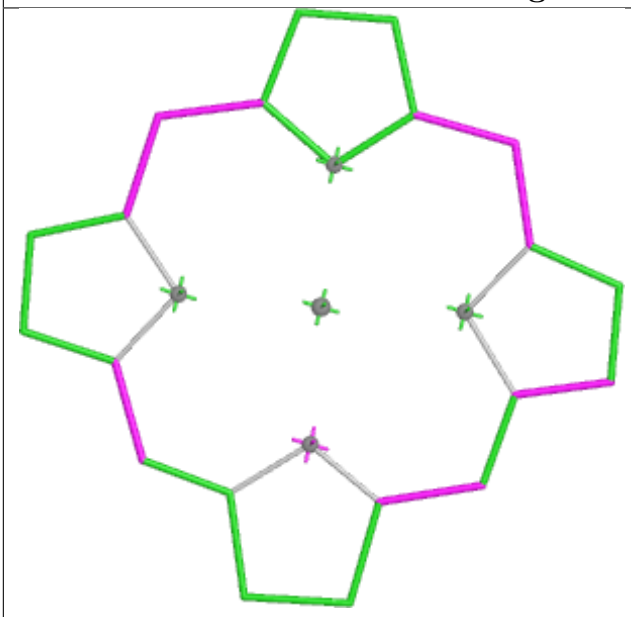


Torsions



Rings

Ligand CLA 2 308



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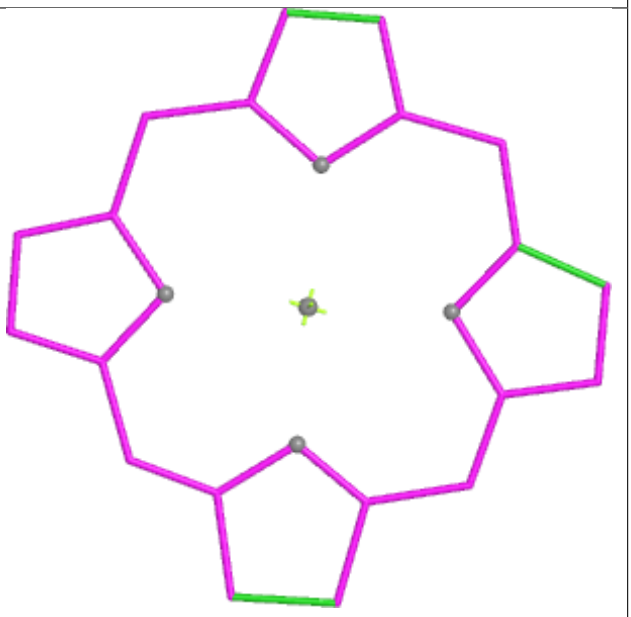
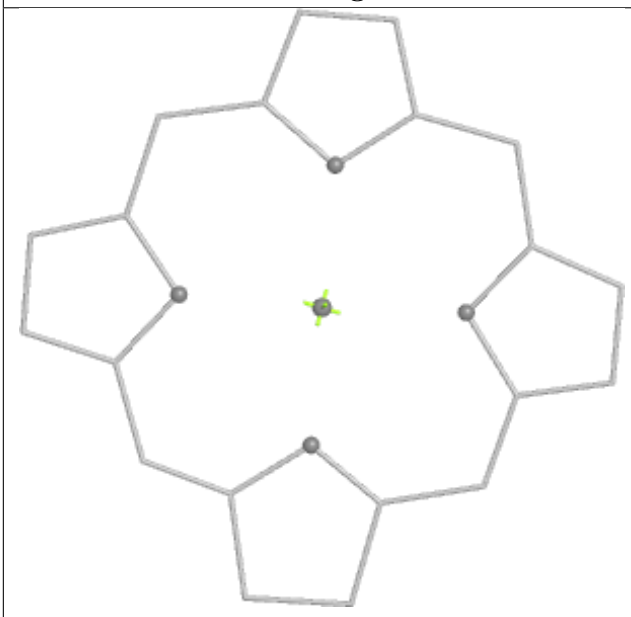


Bond angles



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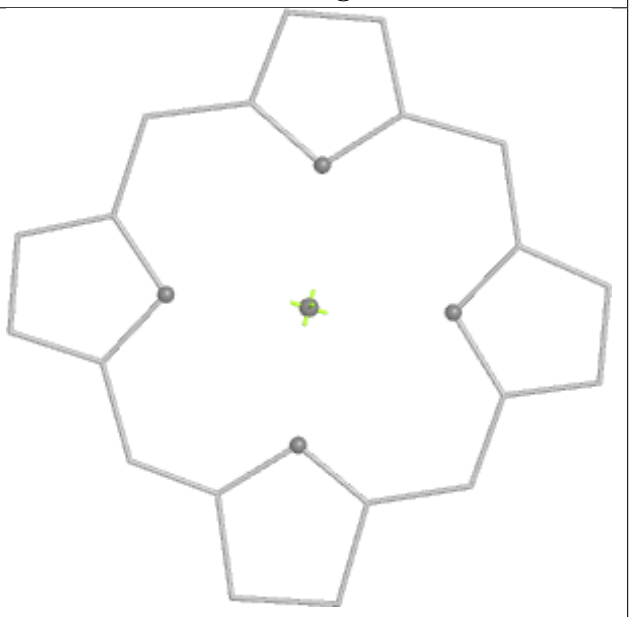
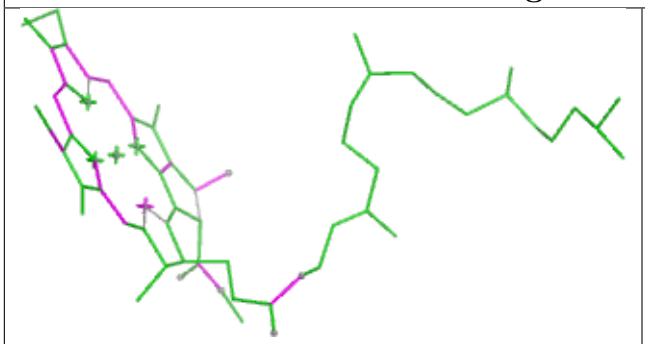


Rings

Ligand CLA B 847



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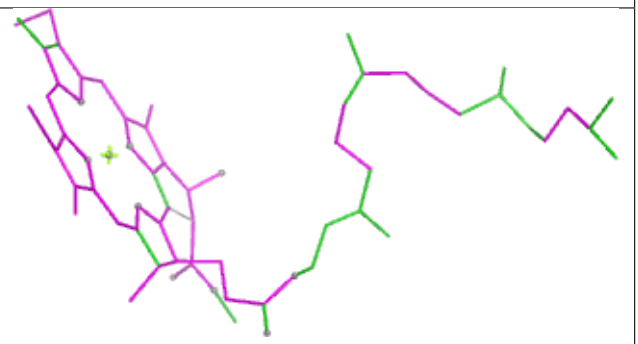
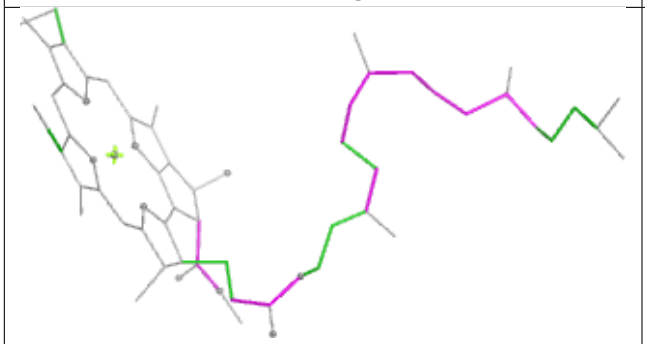


Bond angles



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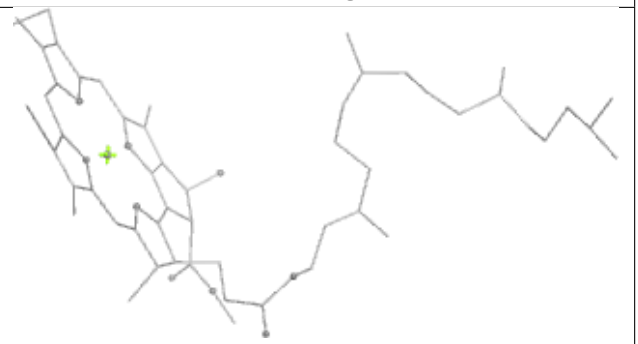
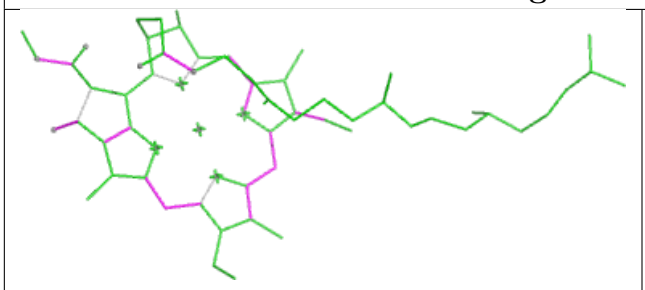


Rings

Ligand CLA 2 307



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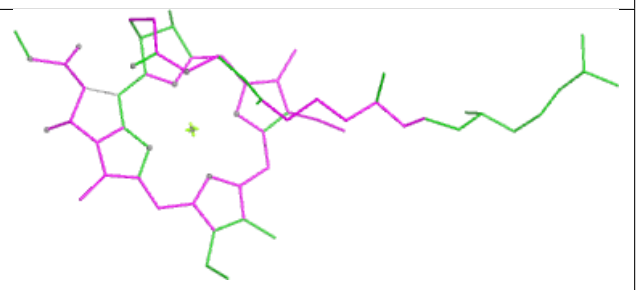

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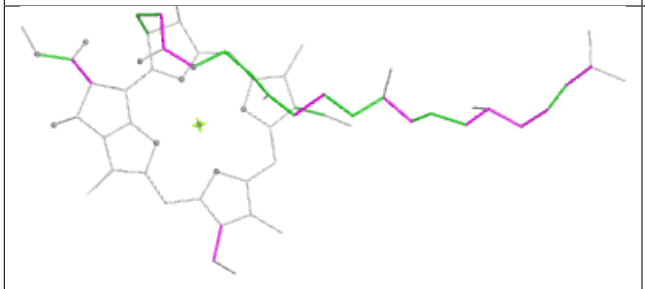

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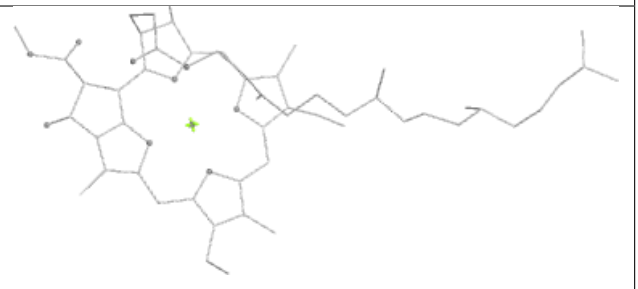
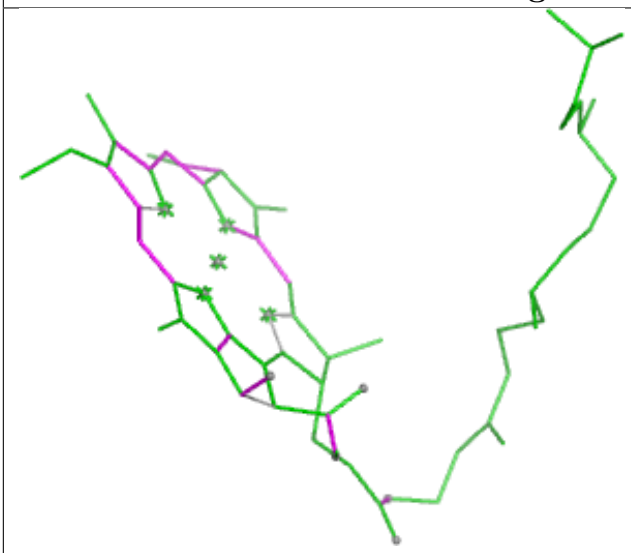


Rings

Ligand CLA 2 306



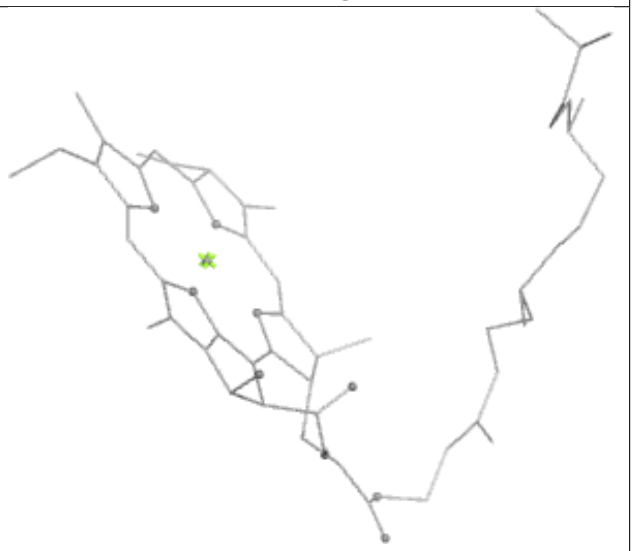
Bond lengths



Bond angles

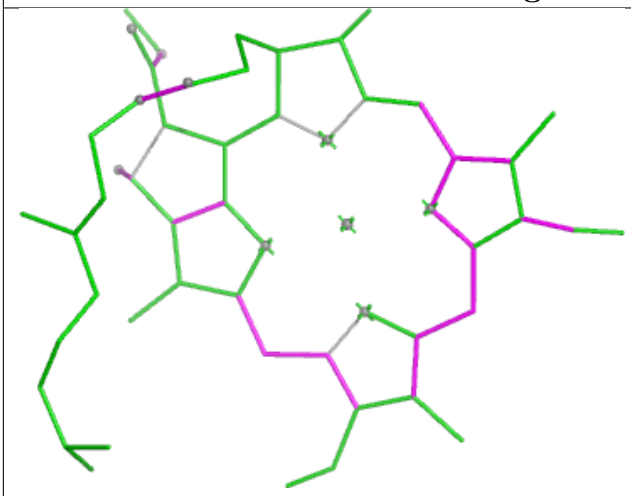


Torsions



Rings

Ligand CLA A 825



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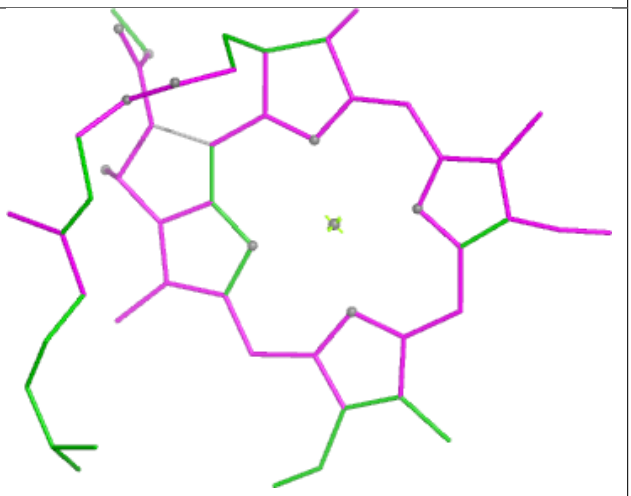
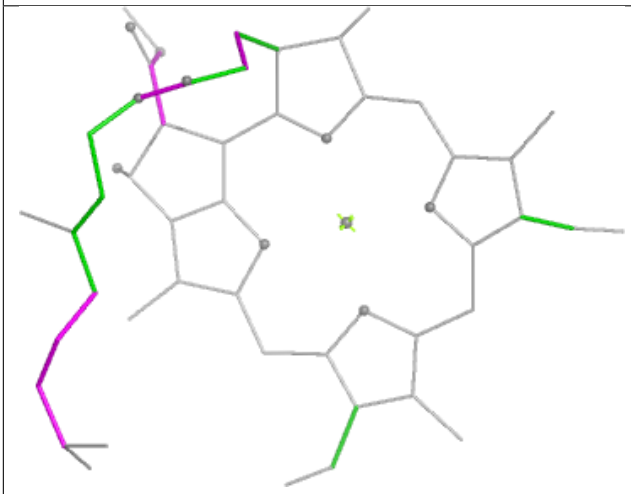


Bond angles



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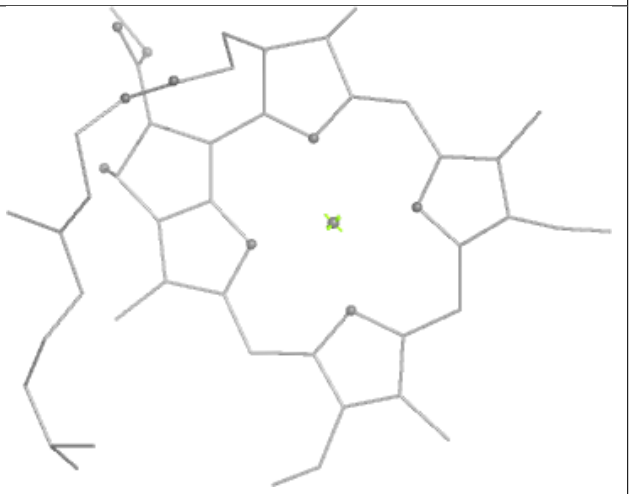
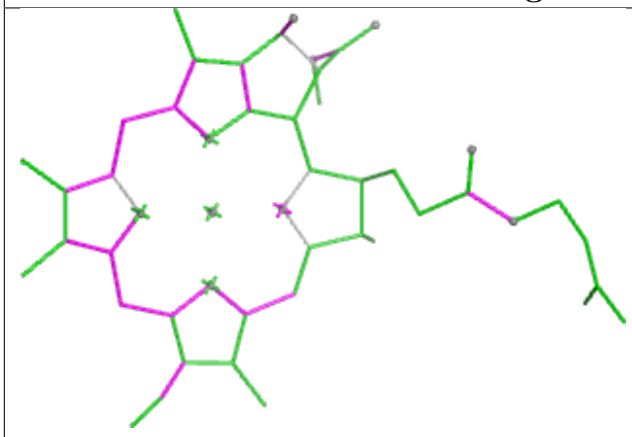


Rings

Ligand CLA B 830



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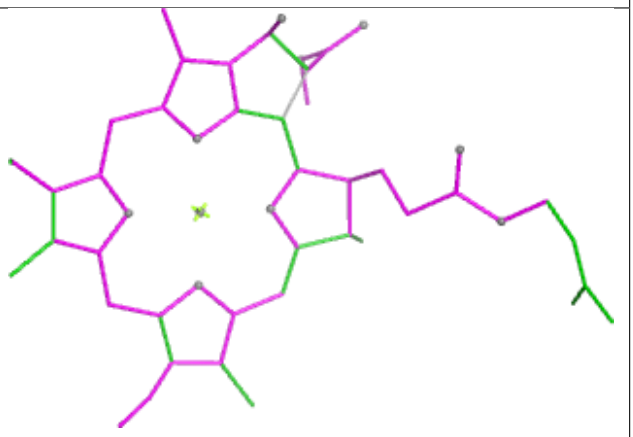
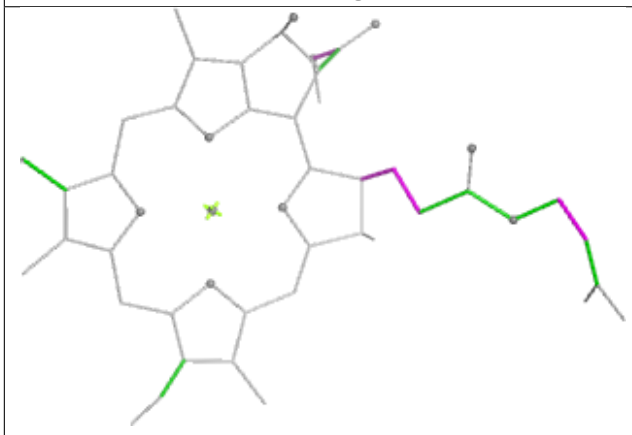


Bond angles



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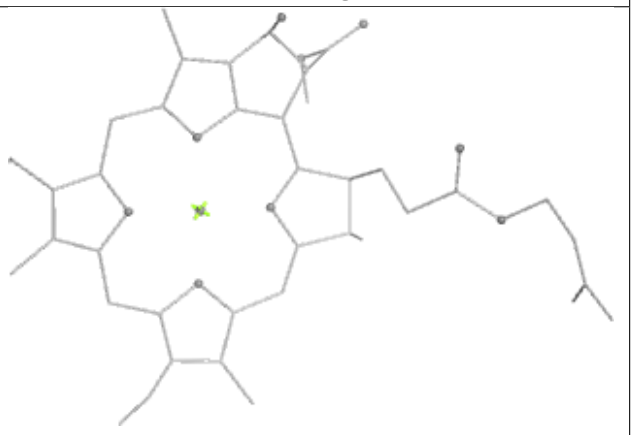
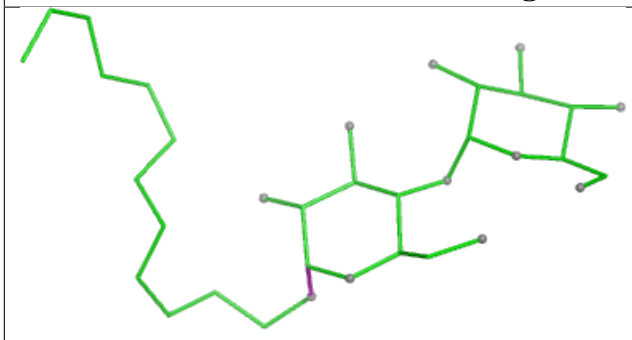


Rings

Ligand LMU R 105



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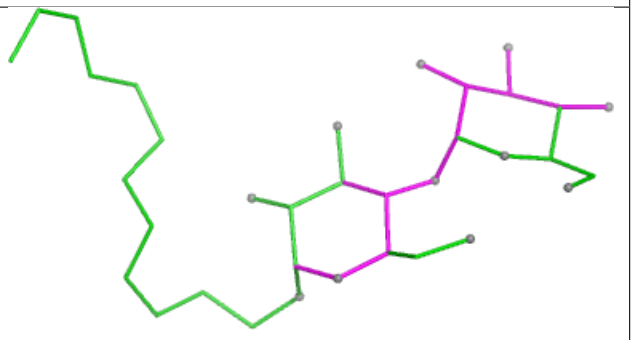
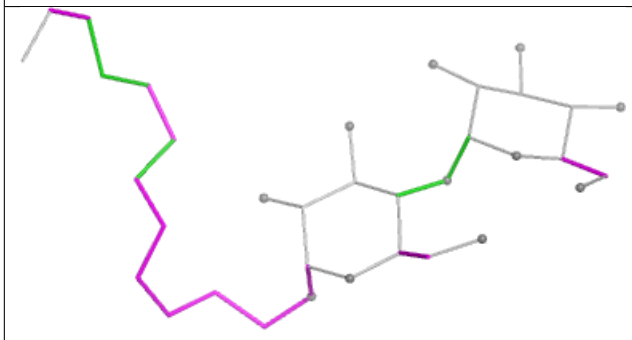


Bond angles



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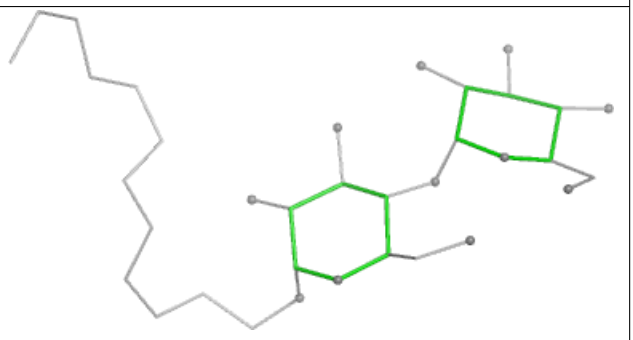
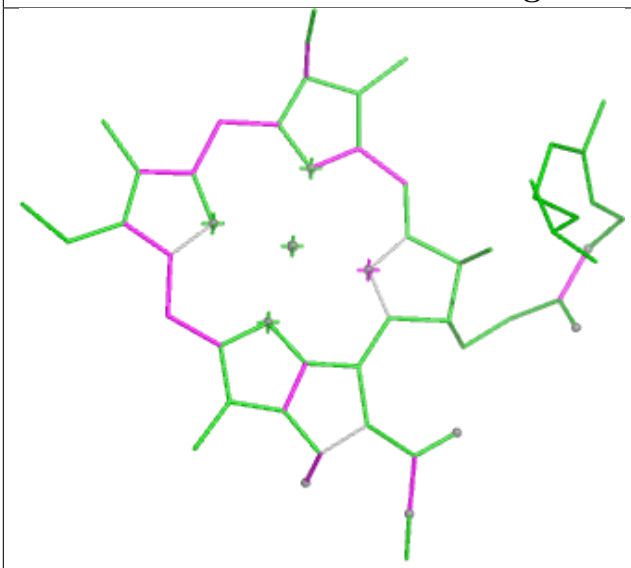


Rings

Ligand CLA H 101



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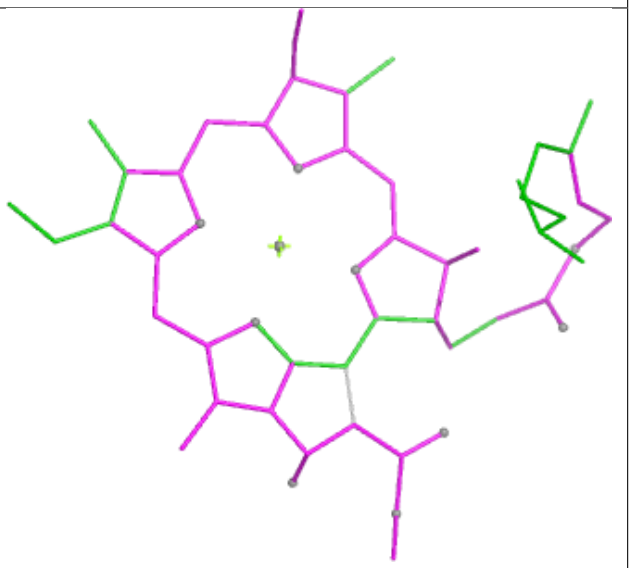
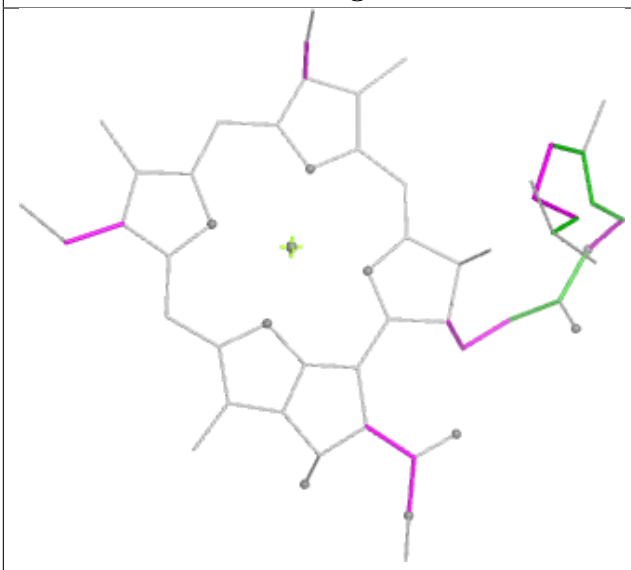


Bond angles



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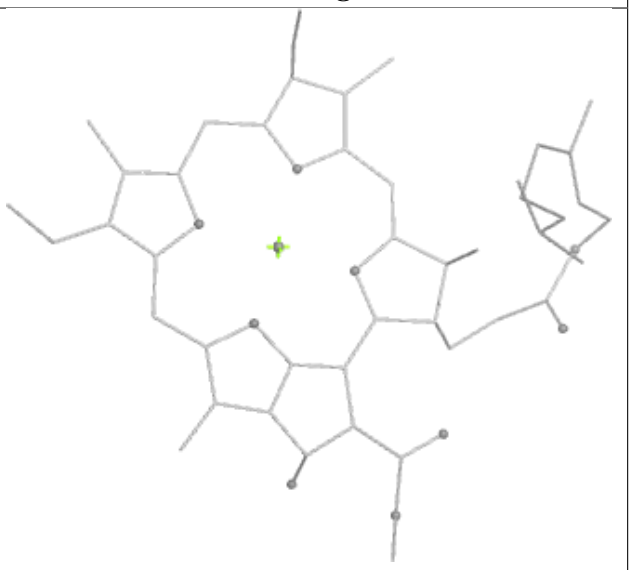
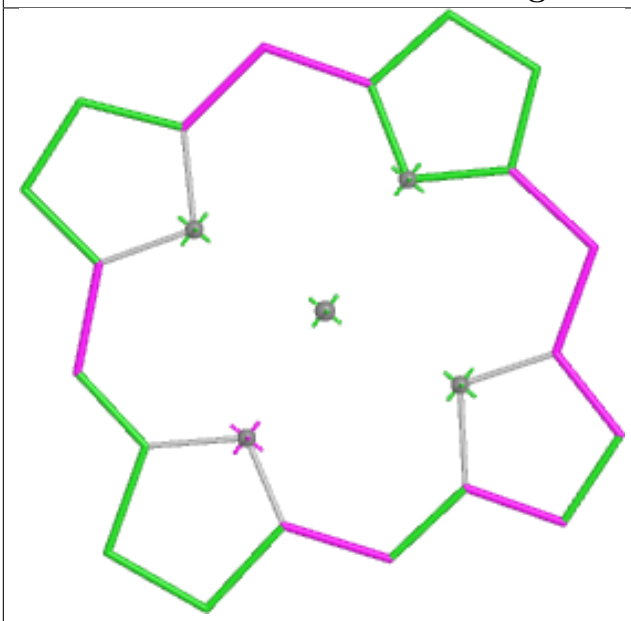


Rings

Ligand CLA 4 311



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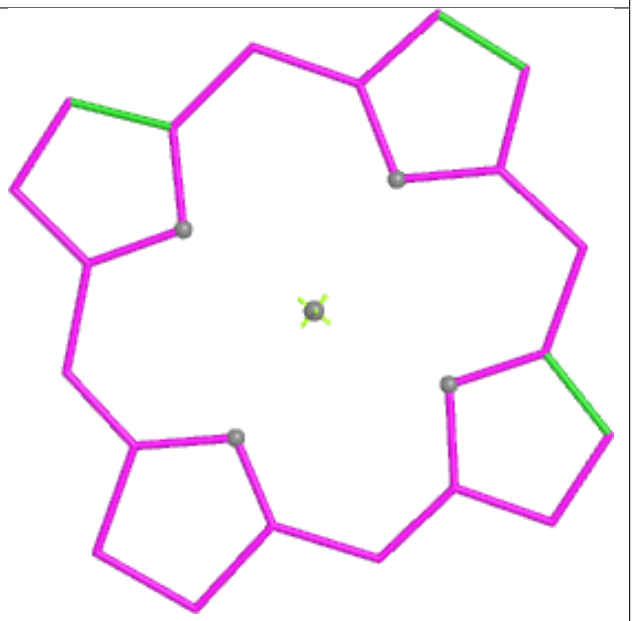
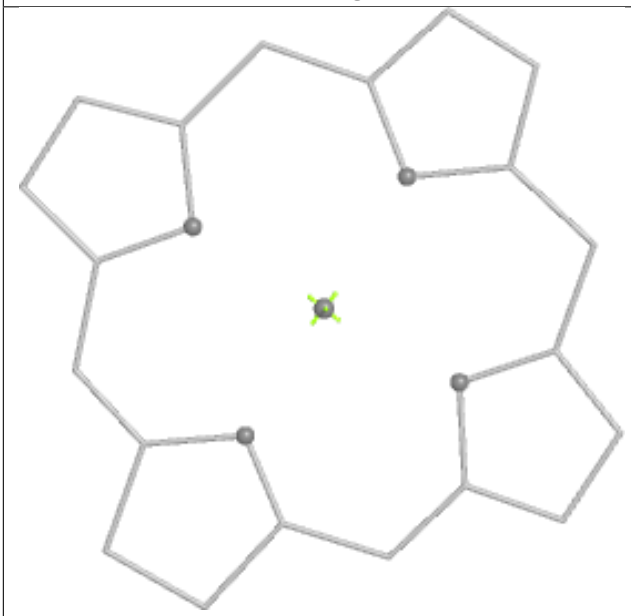


Bond angles



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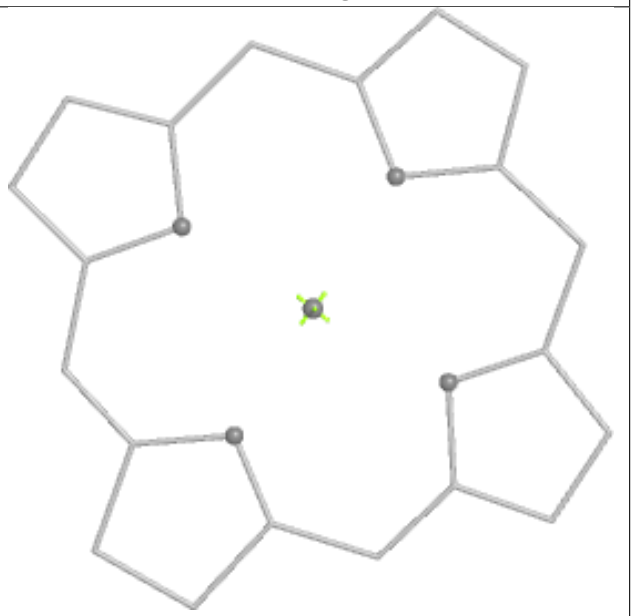
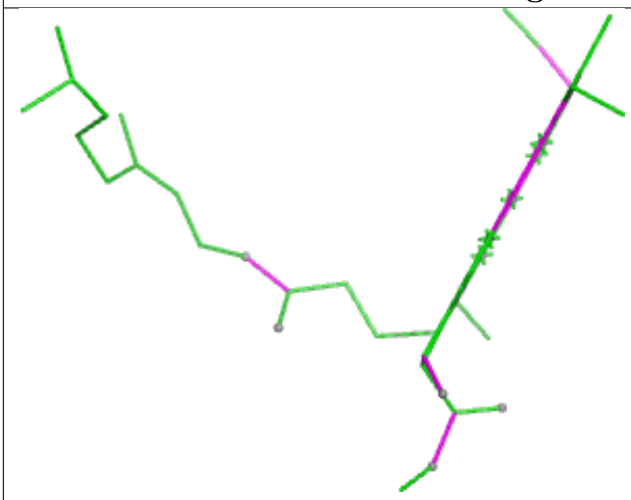


Rings

Ligand CLA L 203



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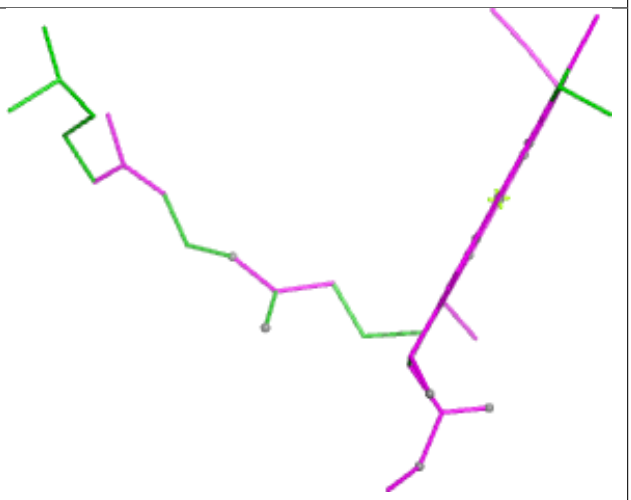
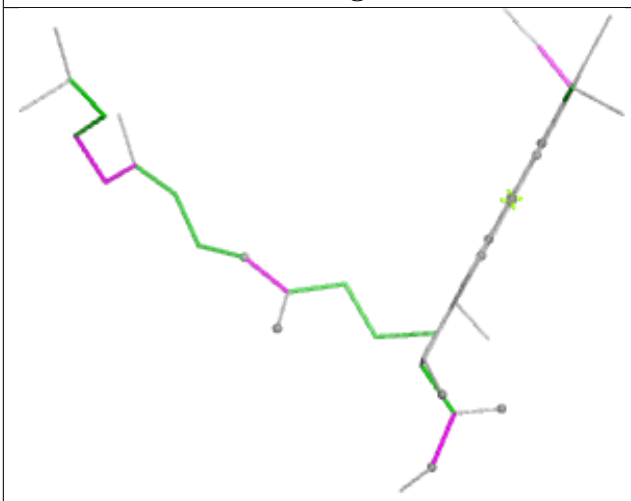


Bond angles

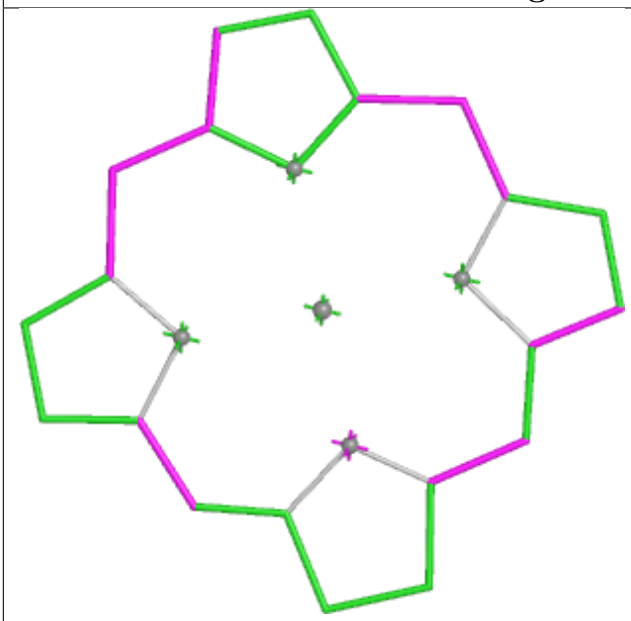


Torsions



Rings

Ligand CLA 3 316



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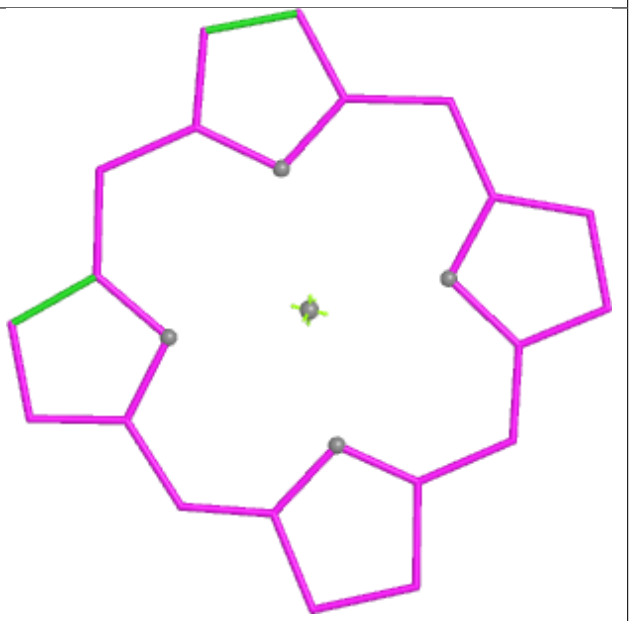
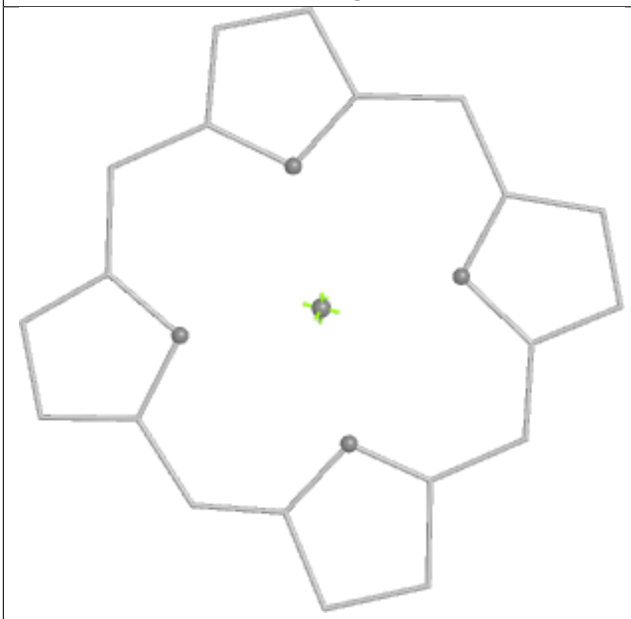


Bond angles



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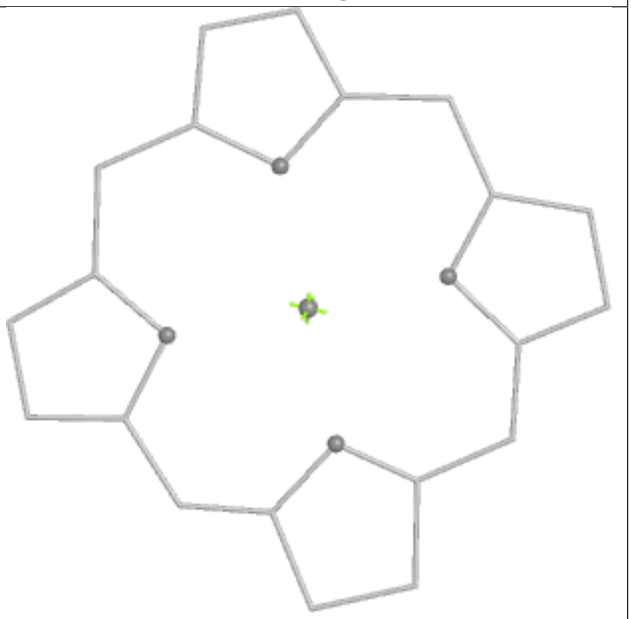
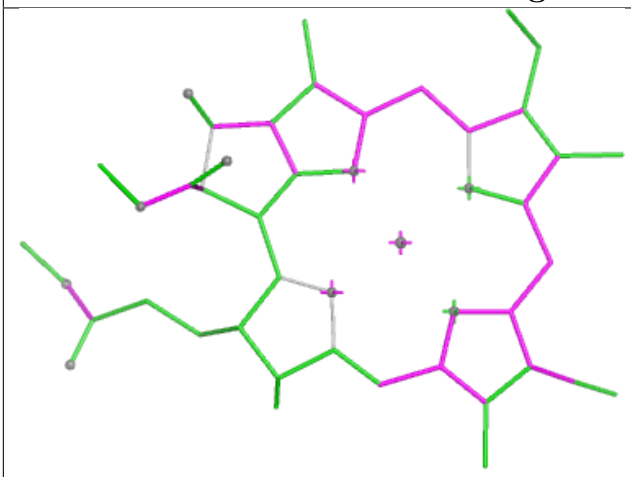


Rings

Ligand CLA 4 315



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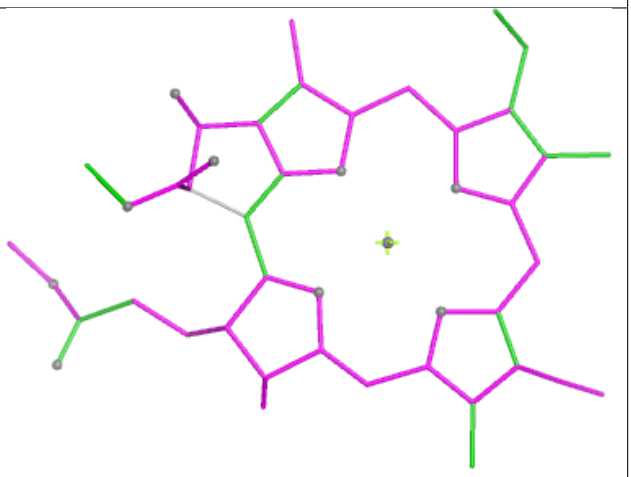
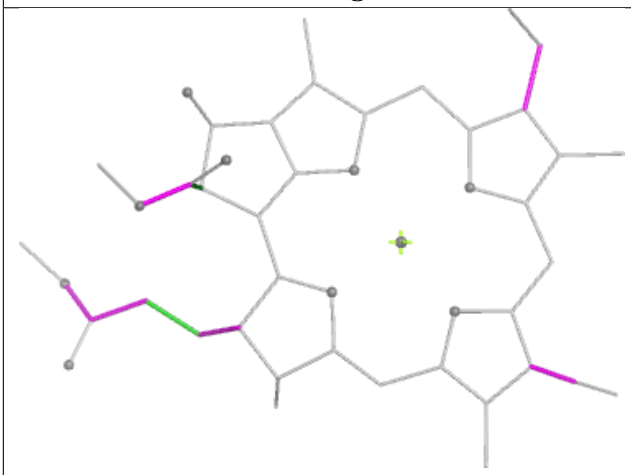


Bond angles



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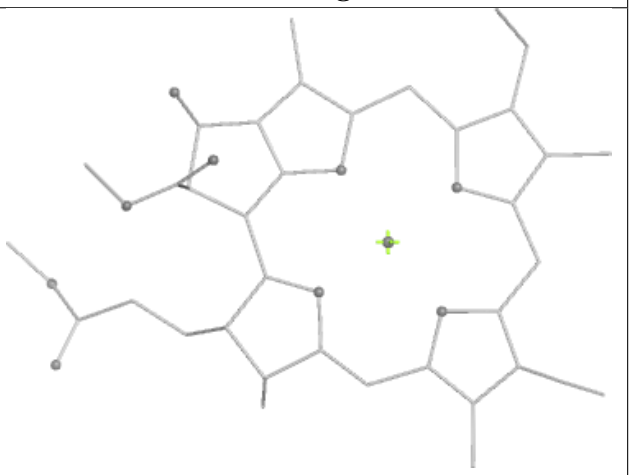
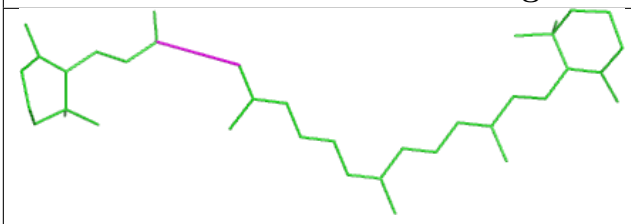


Rings

Ligand BCR A 844



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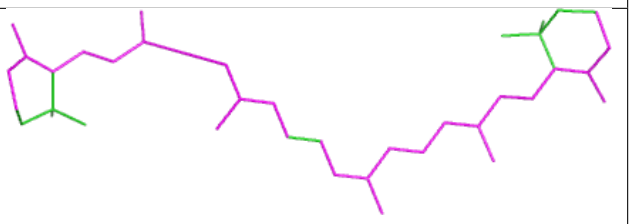
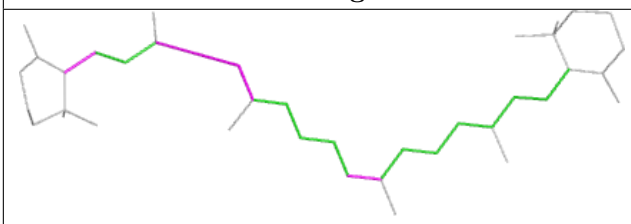


Bond angles



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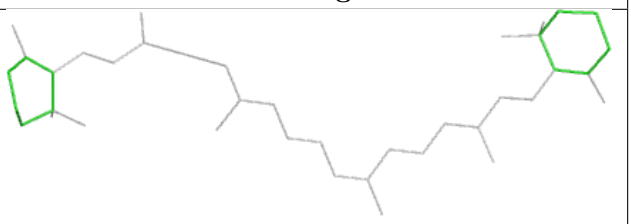
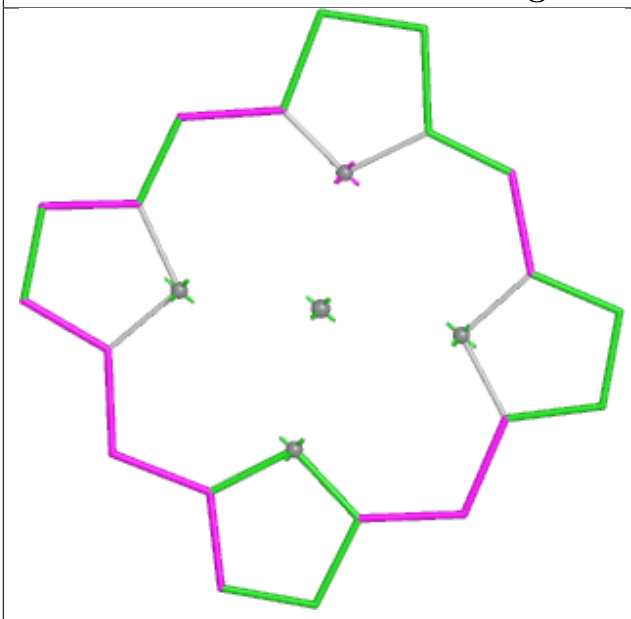
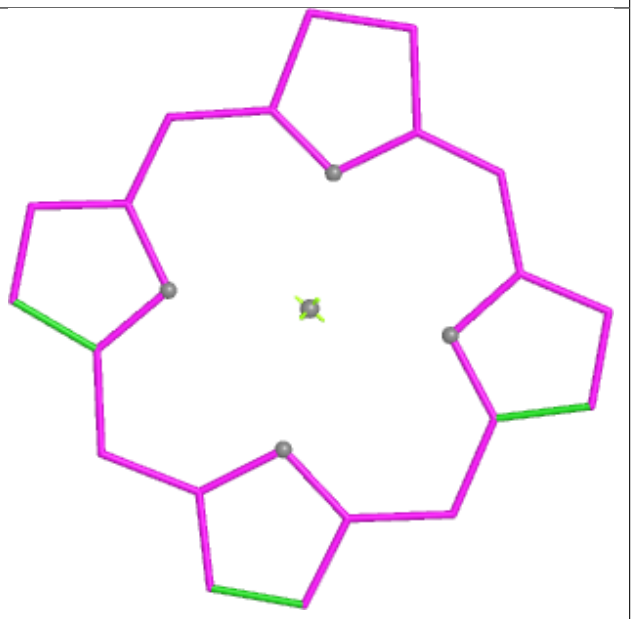


Rings

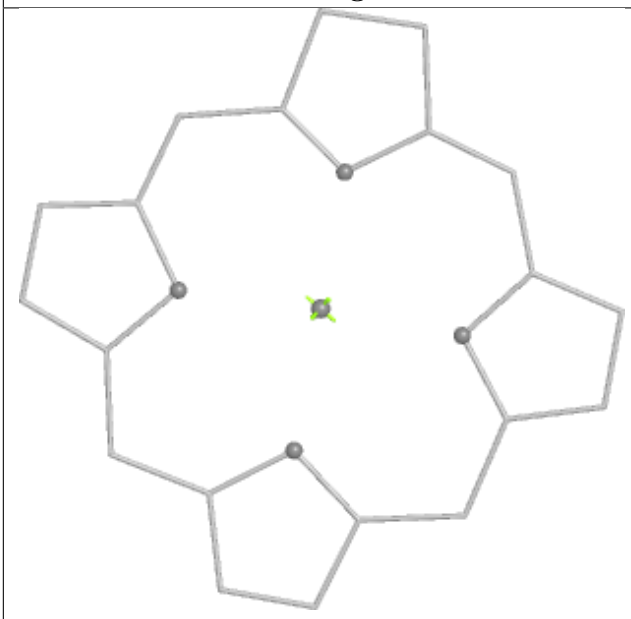
Ligand CLA 2 303



Bond lengths



Bond angles



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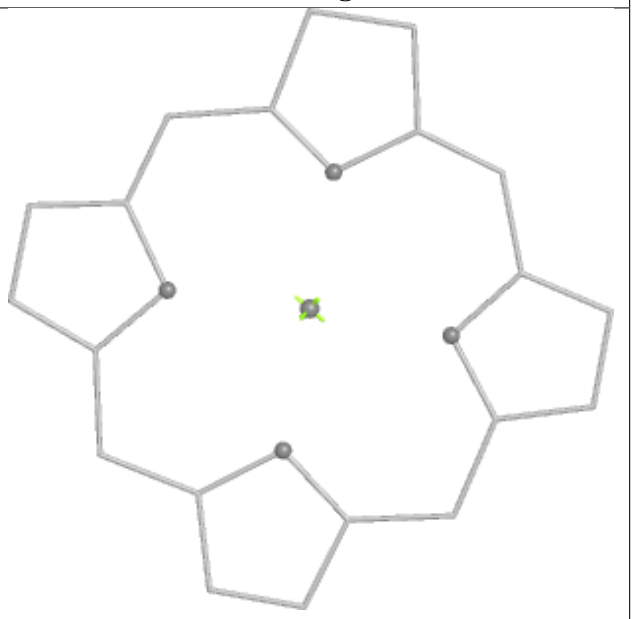
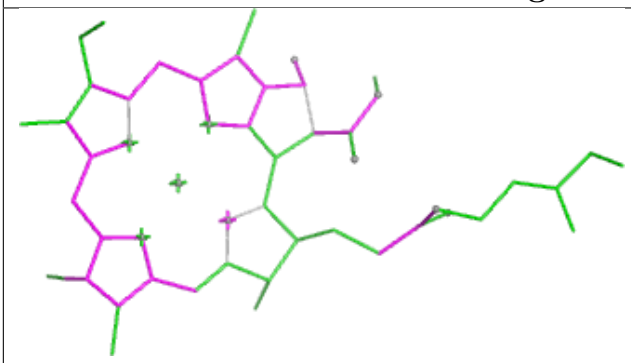


Rings

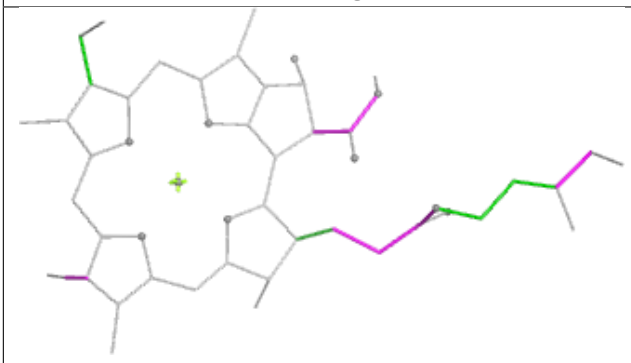
Ligand CLA 1 211



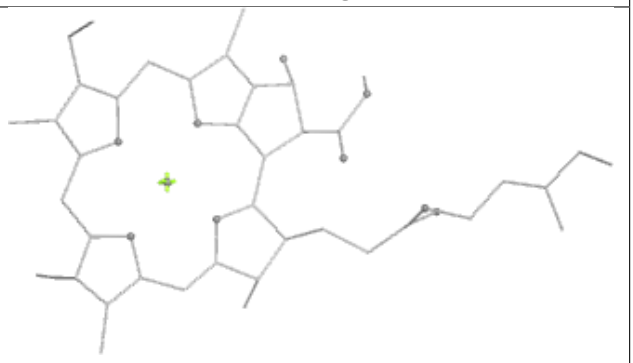
Bond lengths



Bond angles

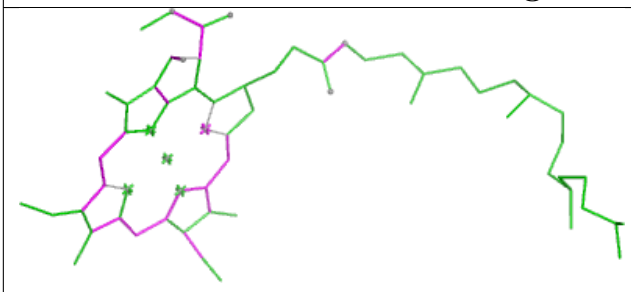


Torsions

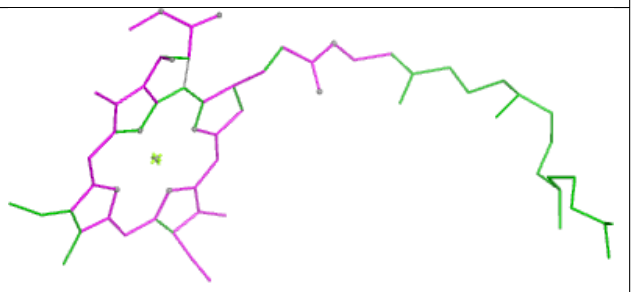


Rings

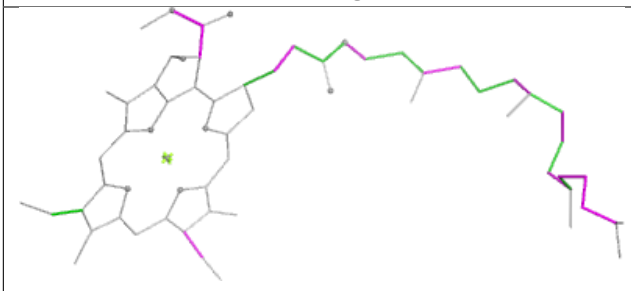
Ligand CLA A 848



Bond lengths



Bond angles



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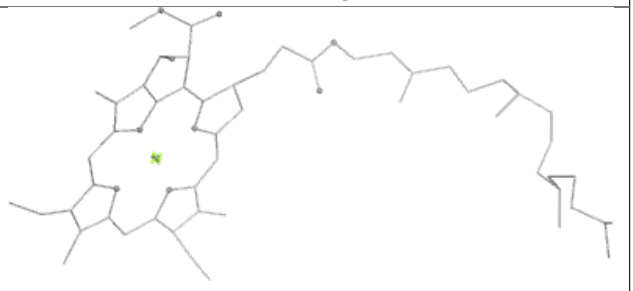
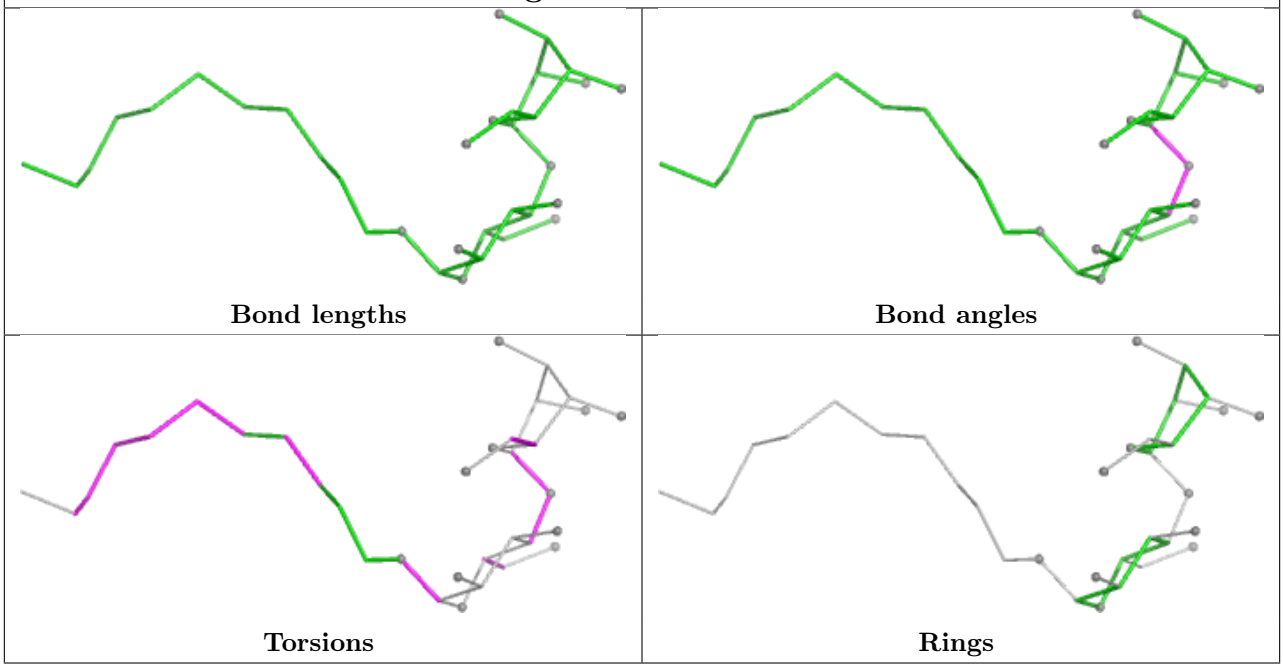


Rings

Ligand LMU 4 320



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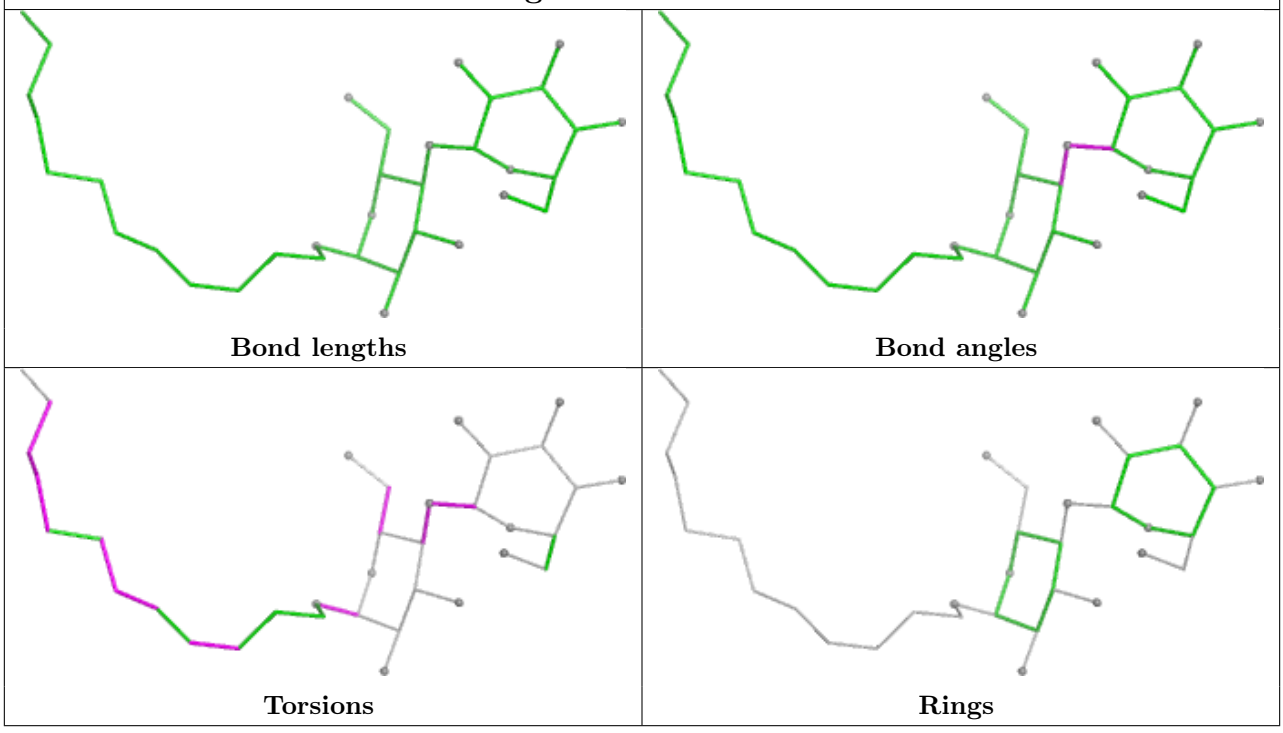
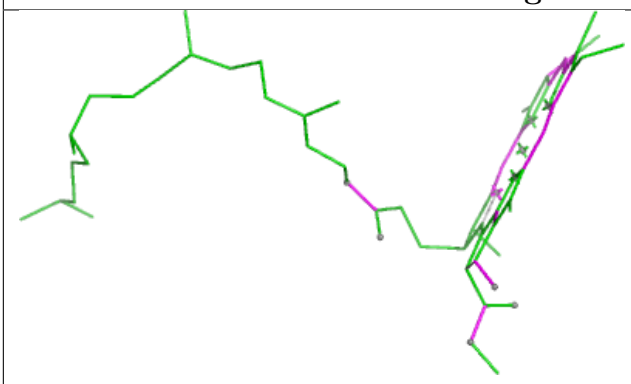


Ligand CLA B 837



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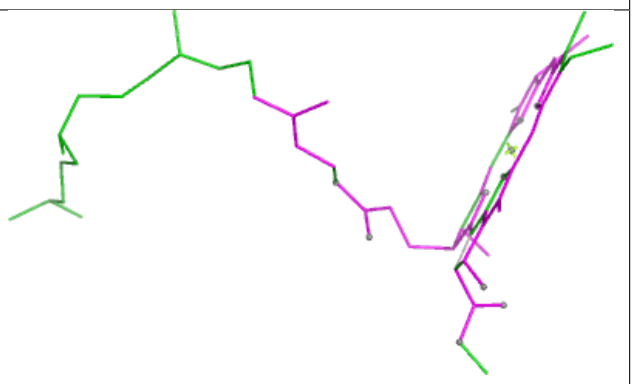
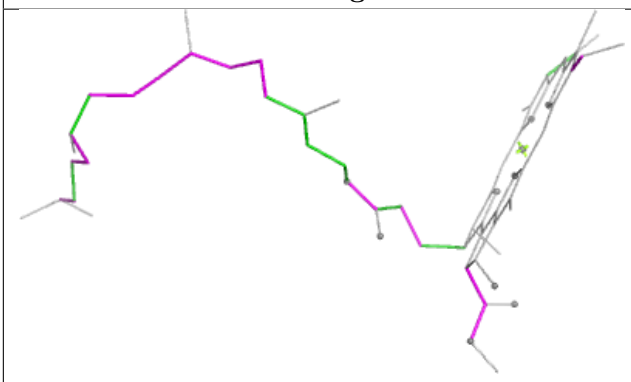


Bond angles



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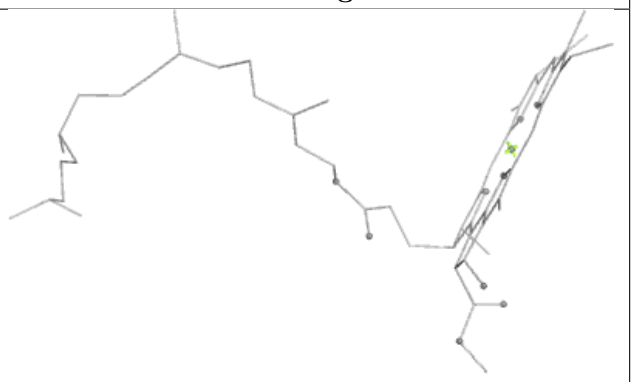
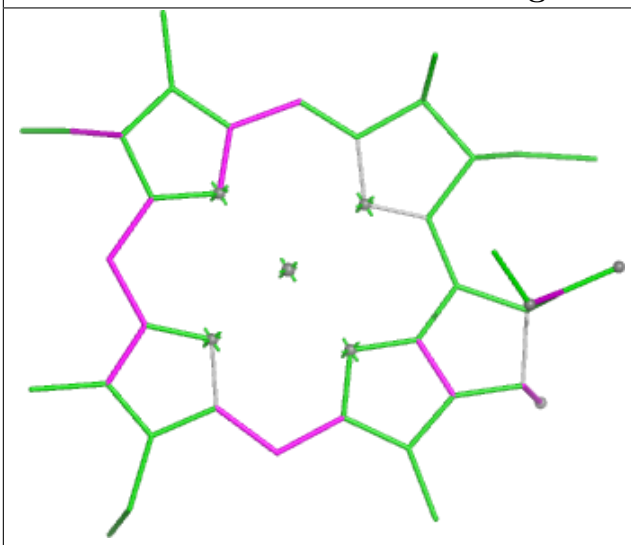


Rings

Ligand CLA 3 314



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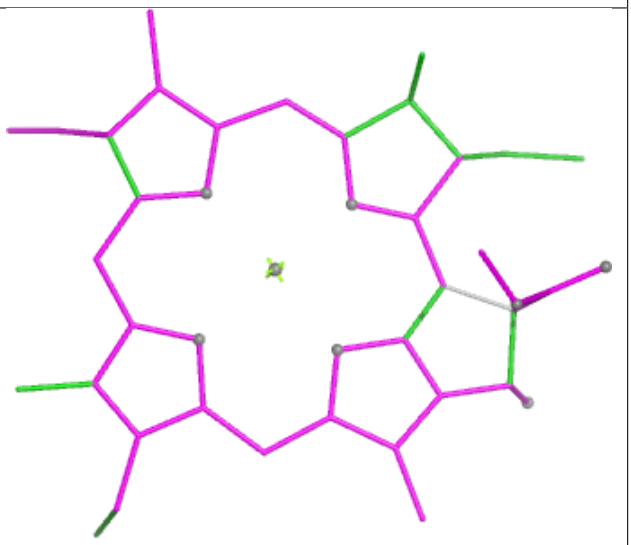
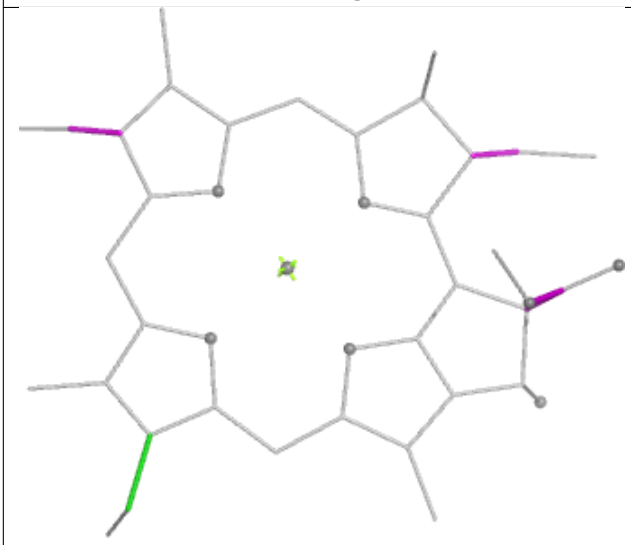


Bond angles



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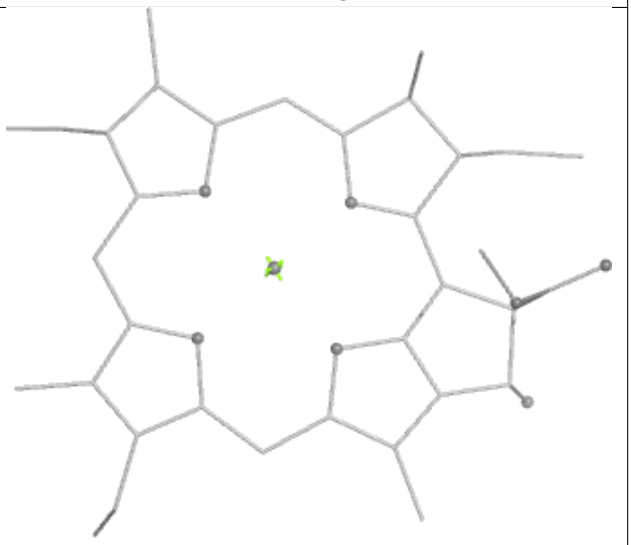
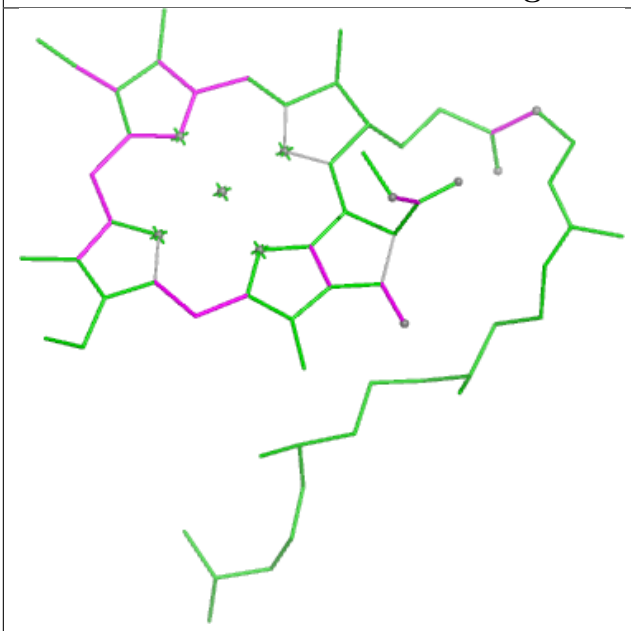


Rings

Ligand CLA A 821



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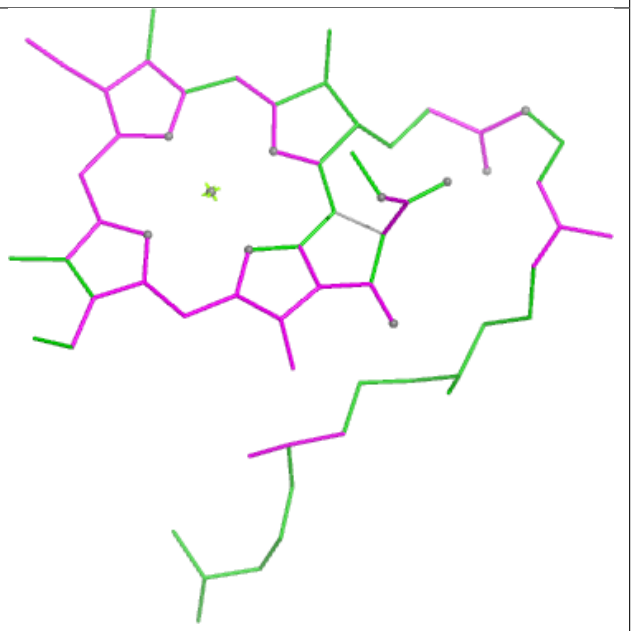
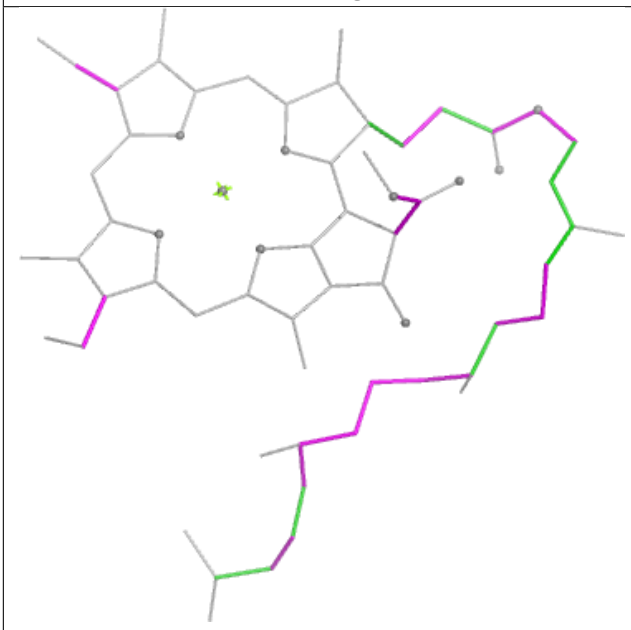


Bond angles



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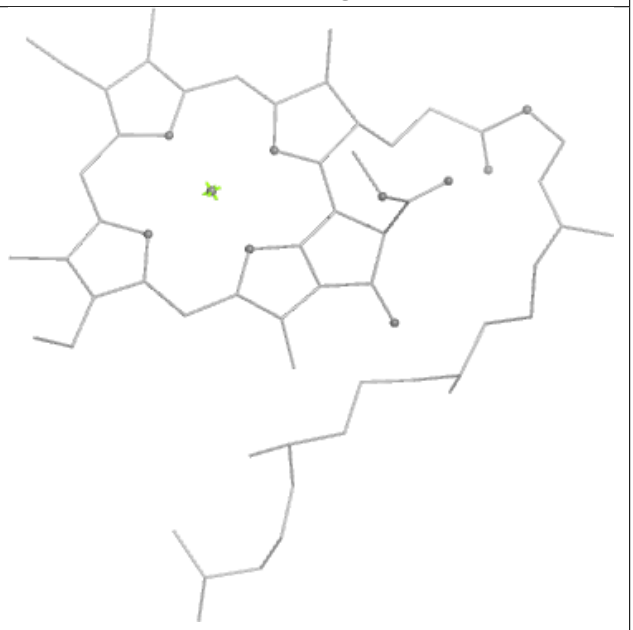
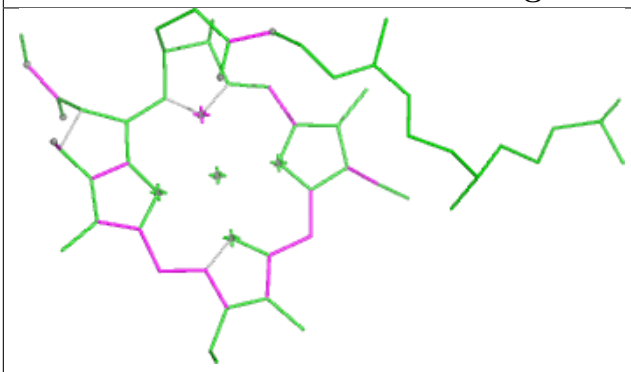


Rings

Ligand CLA B 815



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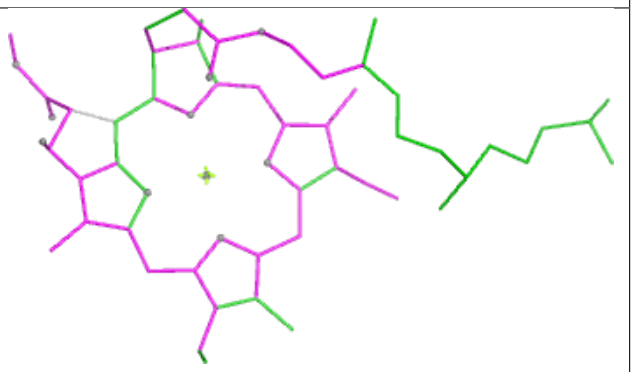

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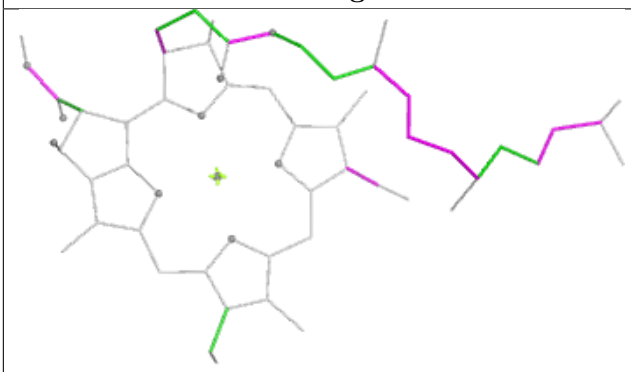

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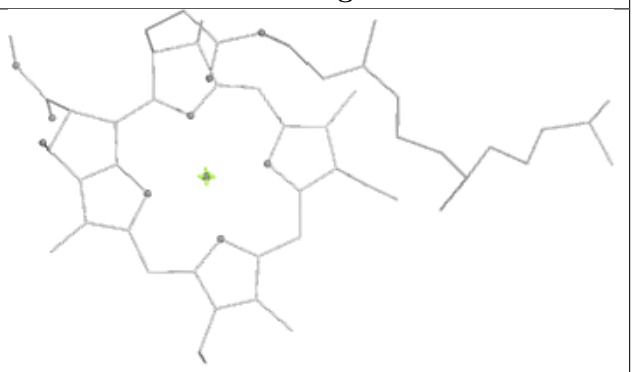
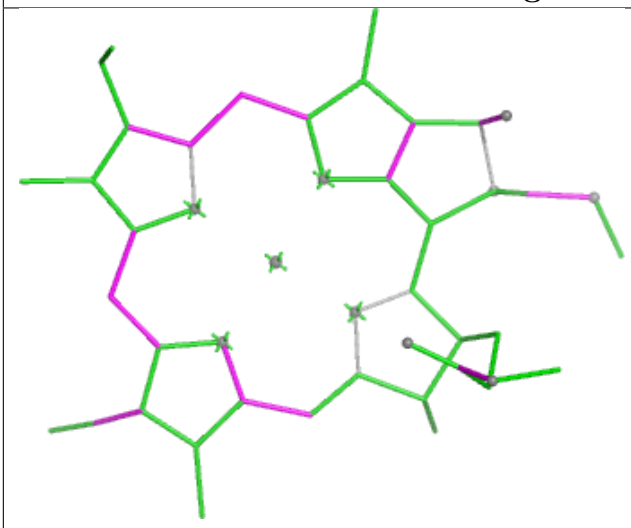


Rings

Ligand CLA A 805



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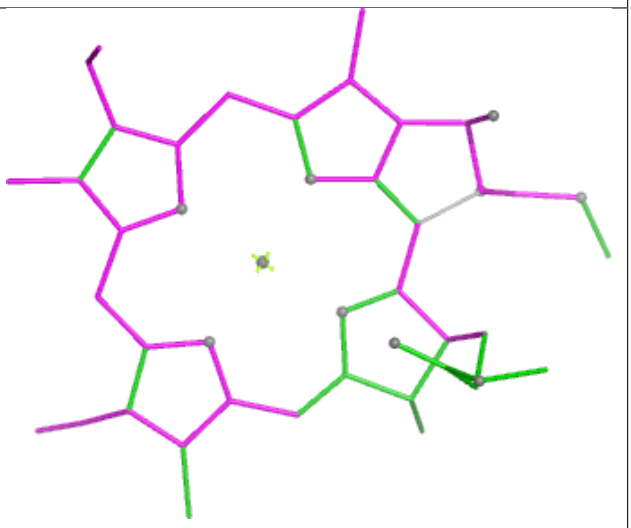
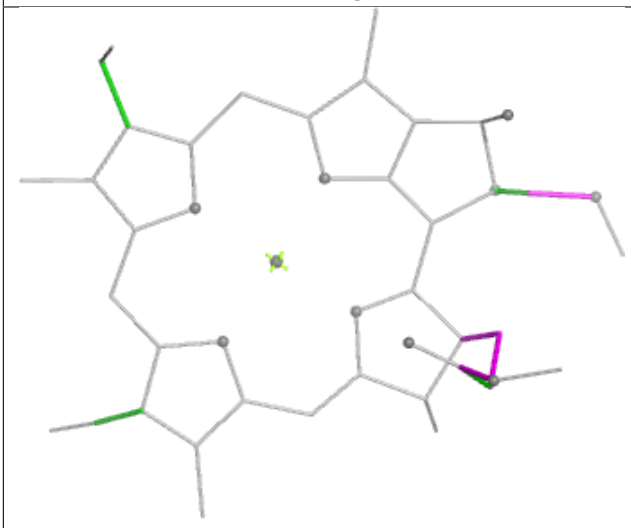


Bond angles



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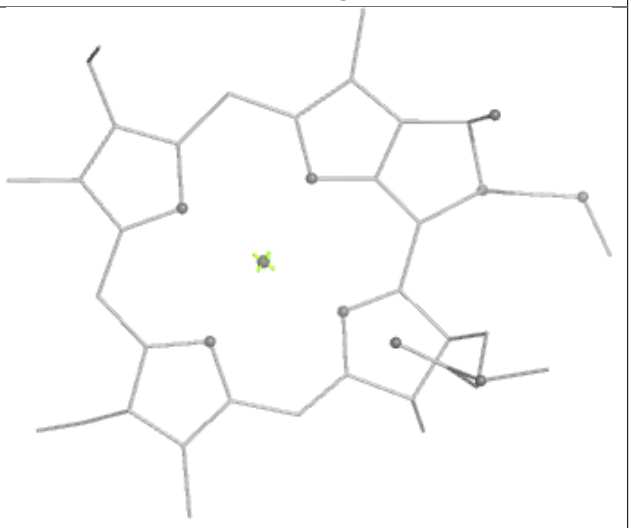
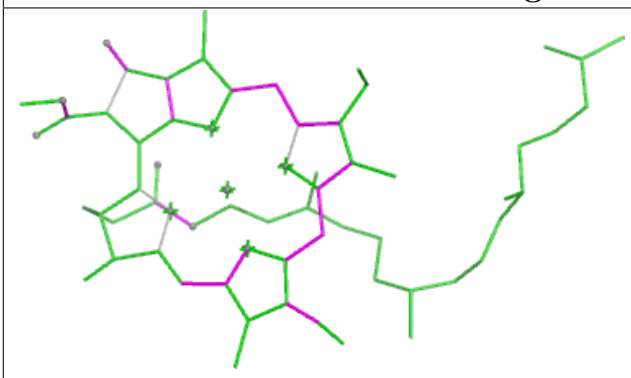


Rings

Ligand CLA B 835



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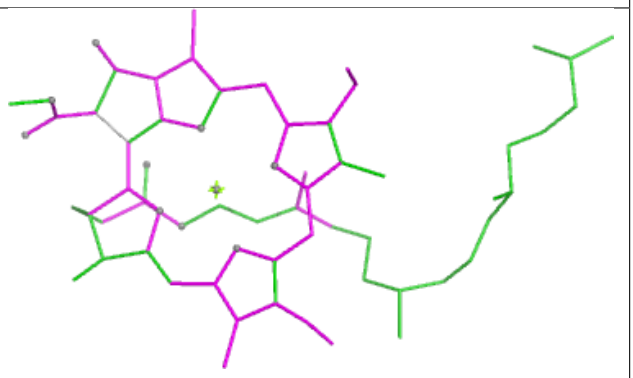
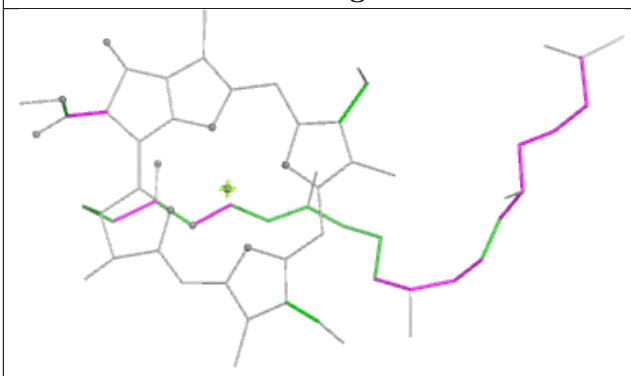


Bond angles



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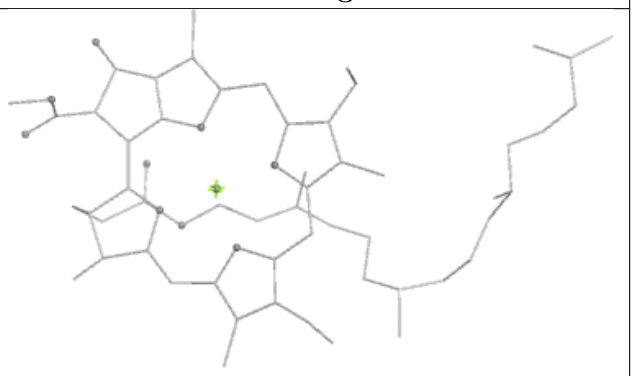
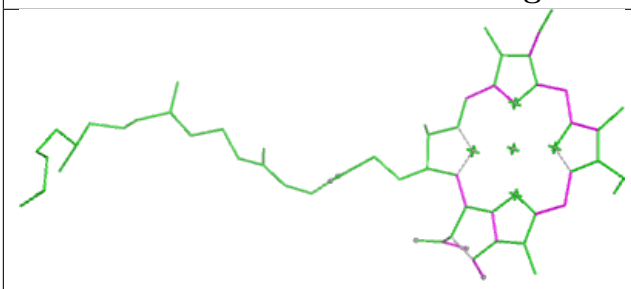


Rings

Ligand CLA A 803



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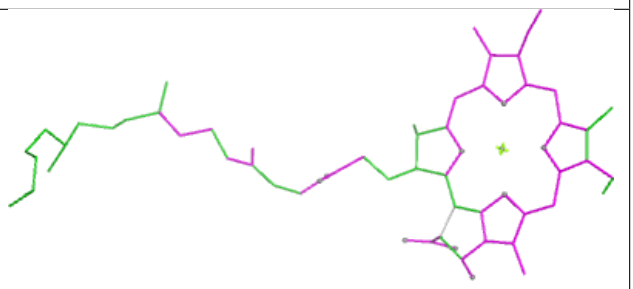
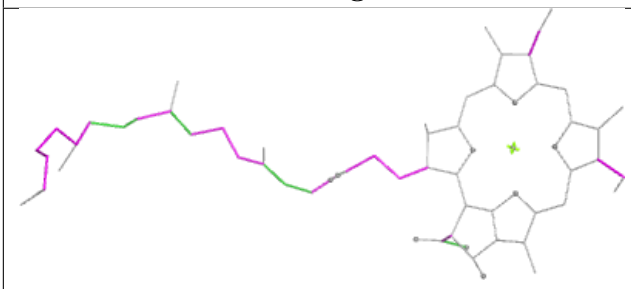


Bond angles



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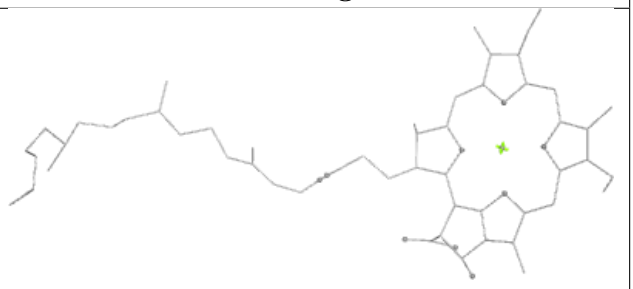
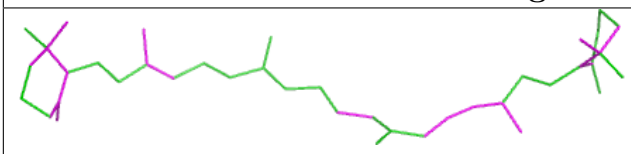


Rings

Ligand BCR I 101



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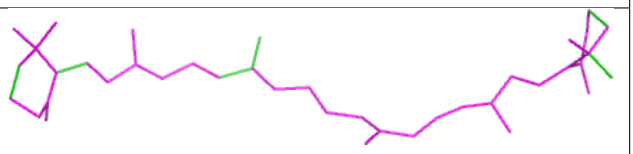
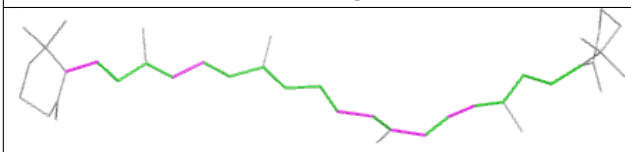


Bond angles



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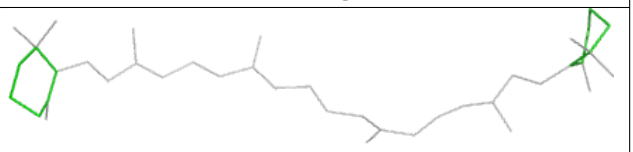
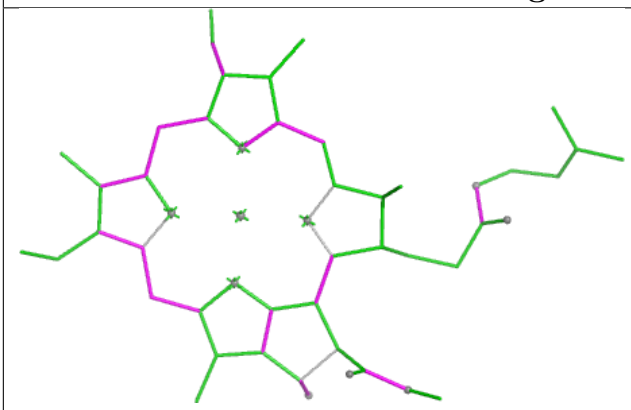


Rings

Ligand CLA 2 304



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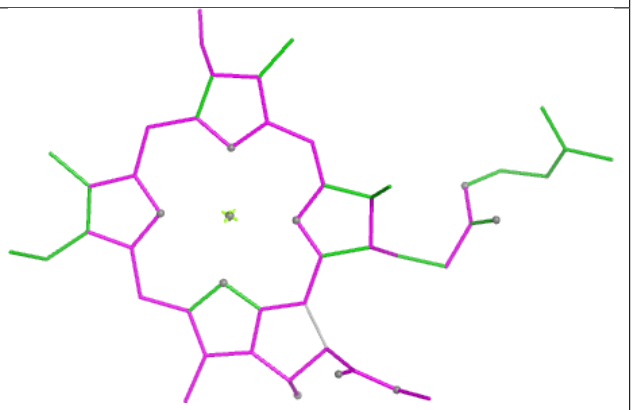
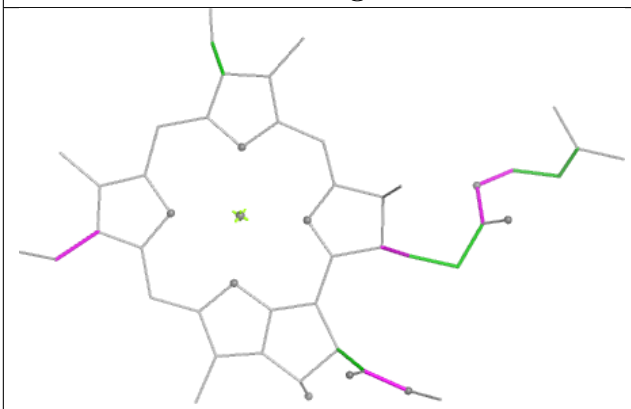


Bond angles



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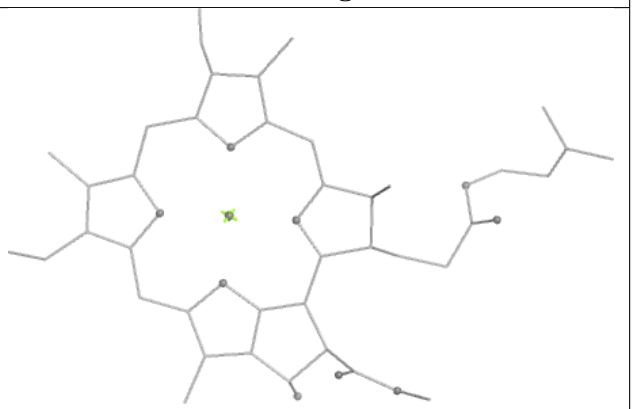
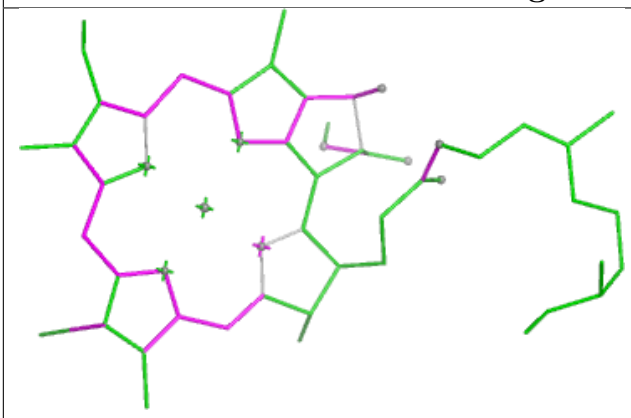


Rings

Ligand CLA 3 301



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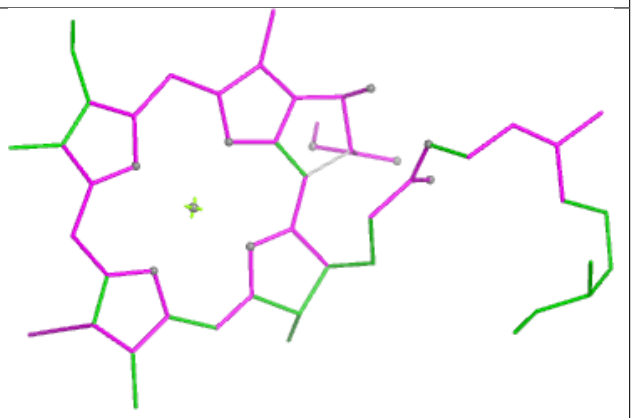

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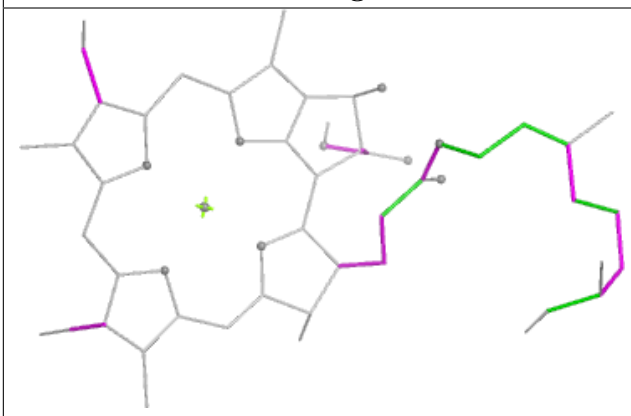

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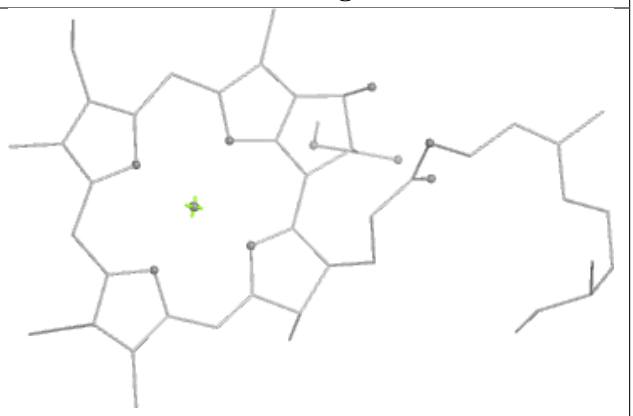
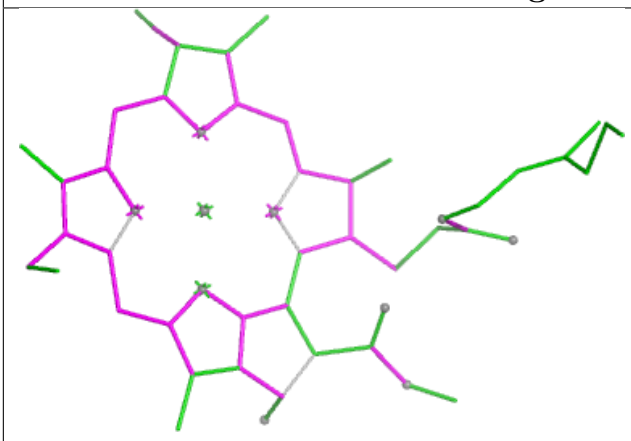


Rings

Ligand CLA 4 307



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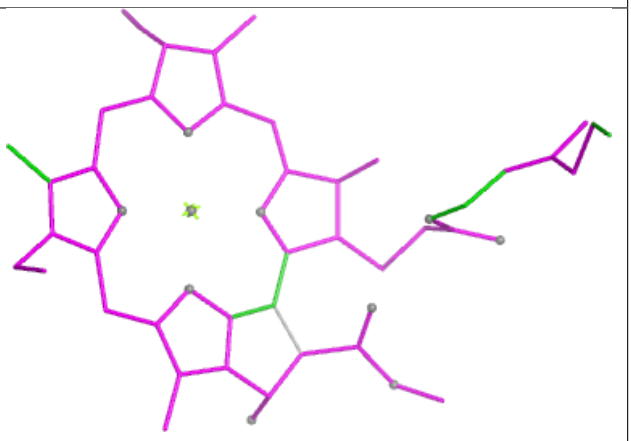
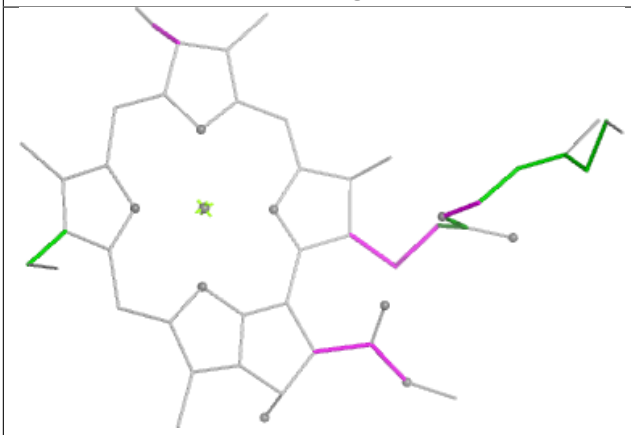


Bond angles



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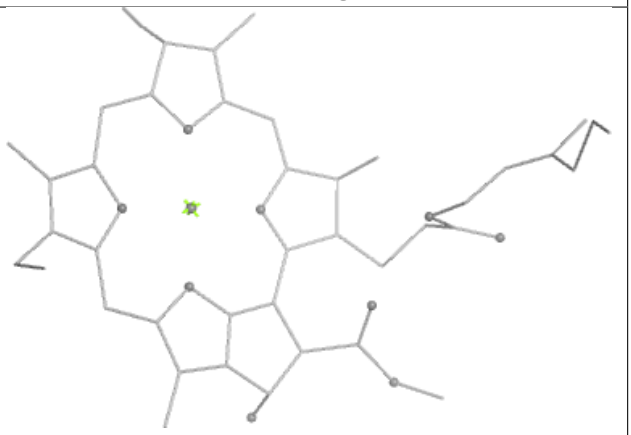
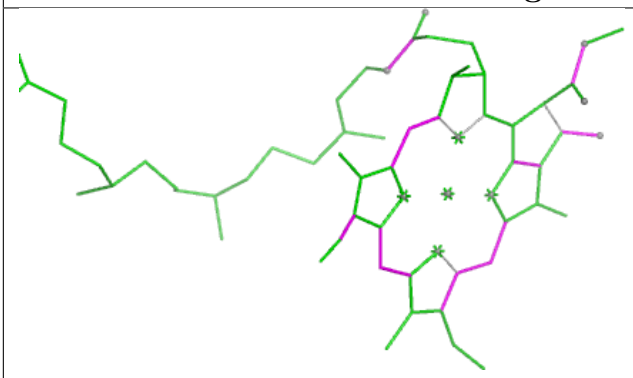


Rings

Ligand CLA B 811



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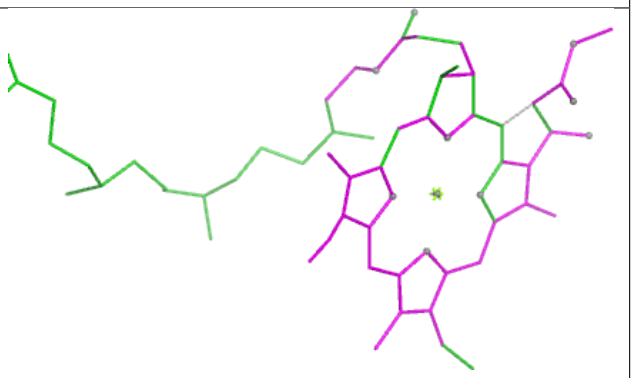
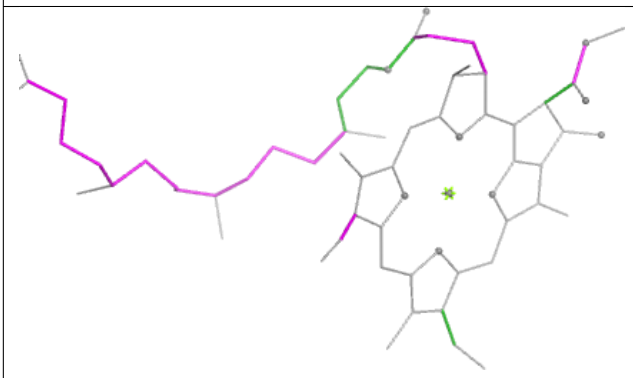


Bond angles



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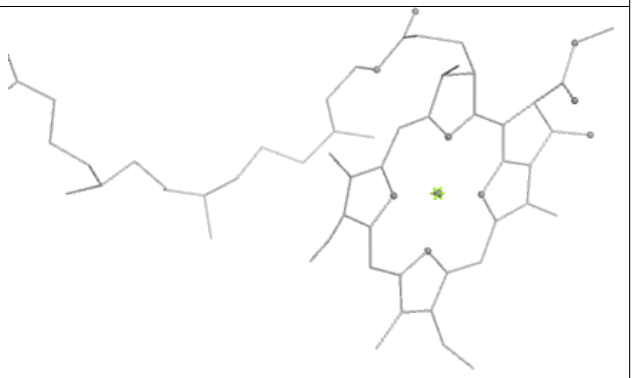
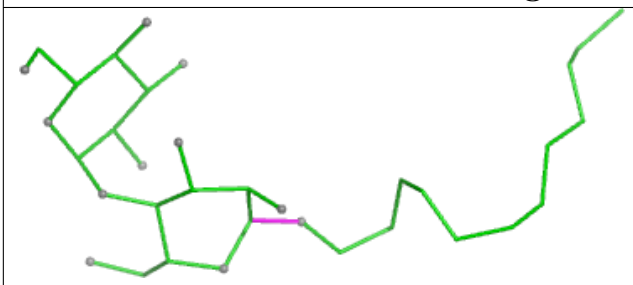
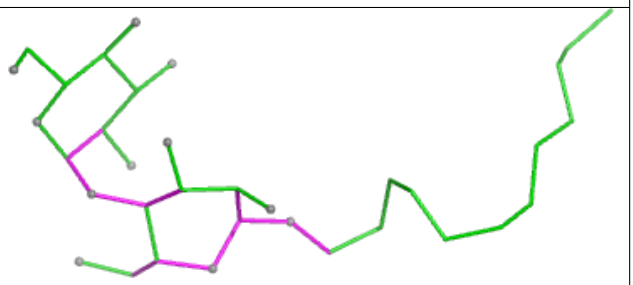


Rings

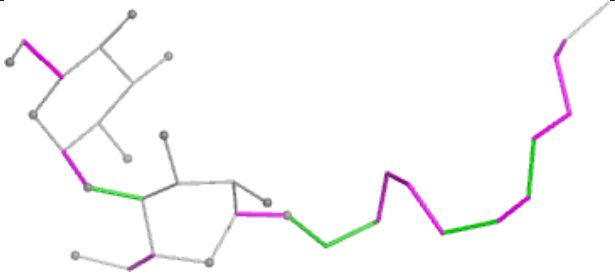
Ligand LMU 2 319



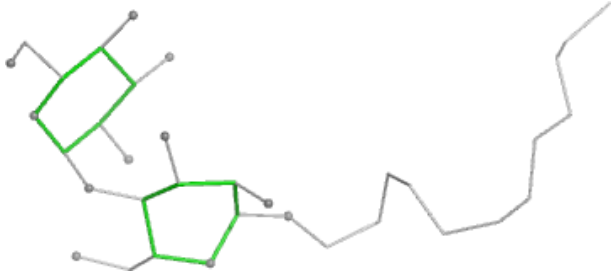
Bond lengths



Bond angles

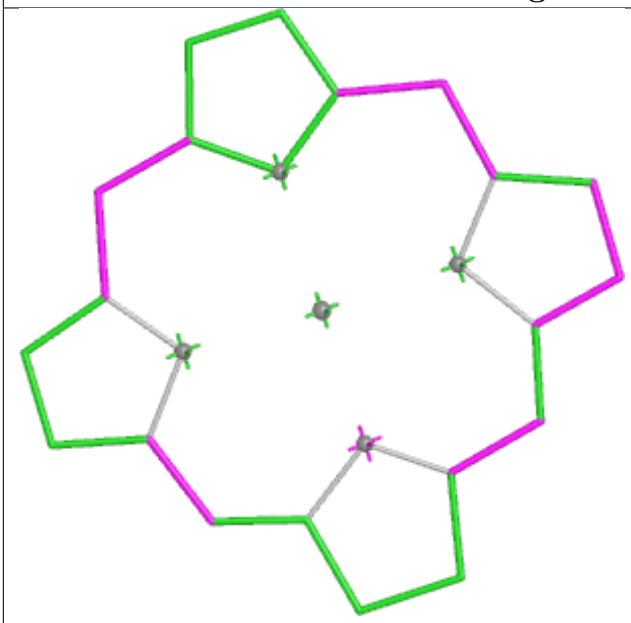


Torsions



Rings

Ligand CLA 4 309



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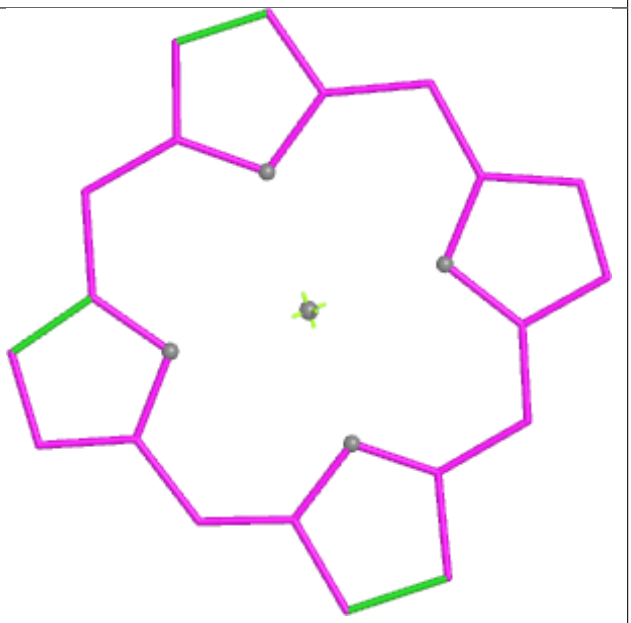
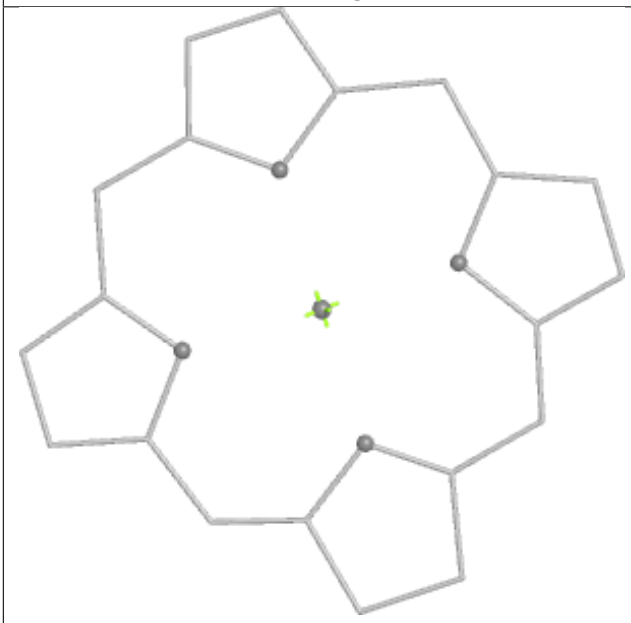


Bond angles



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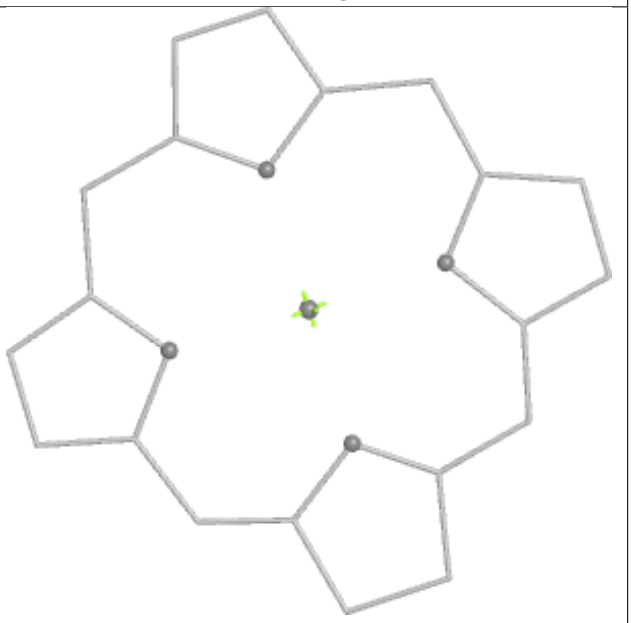
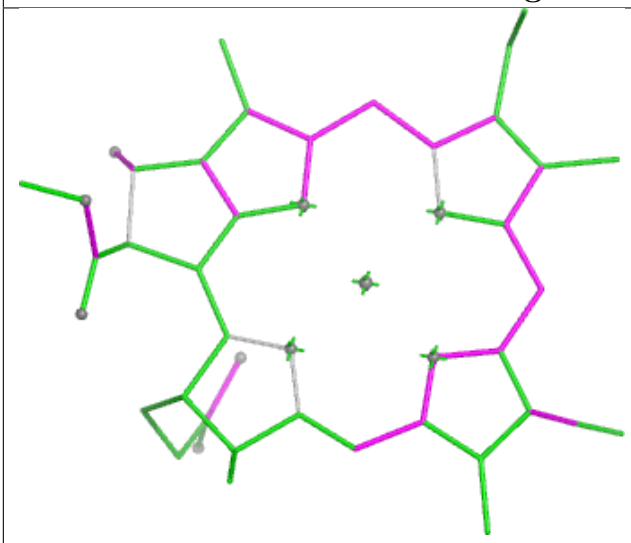


Rings

Ligand CLA B 831



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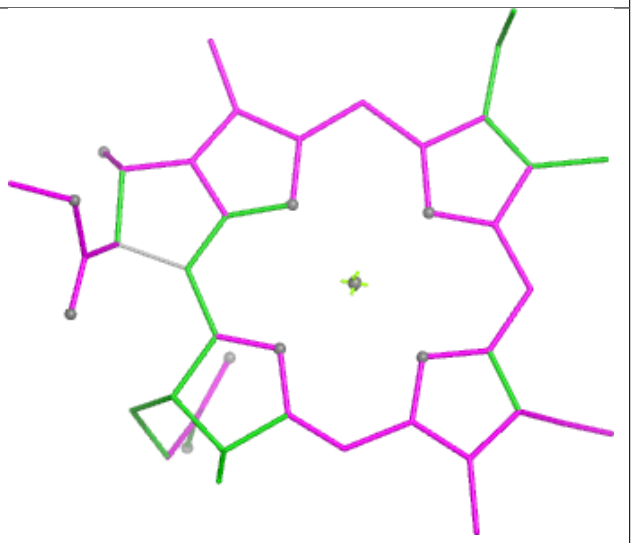

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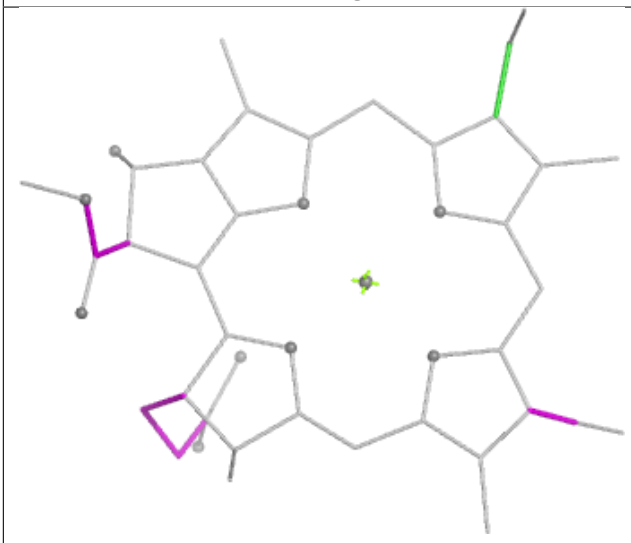

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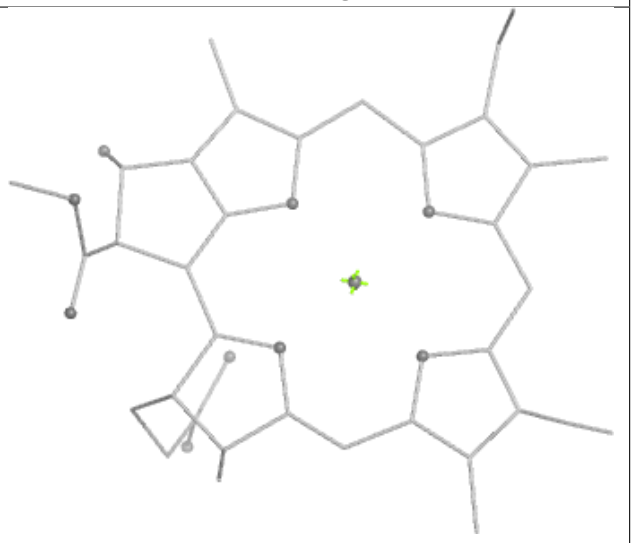
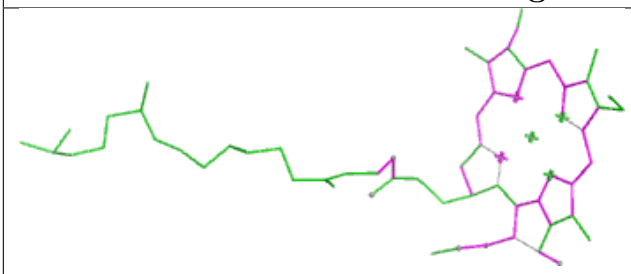


Rings

Ligand CLA 4 304



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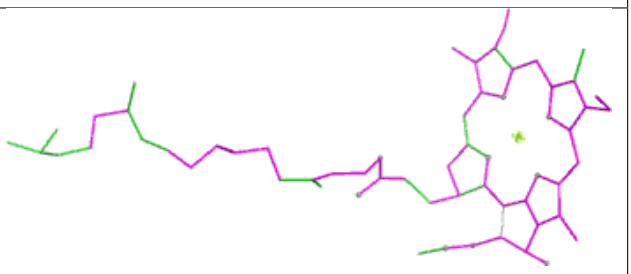
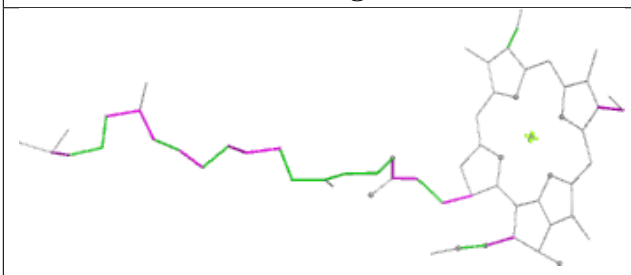


Bond angles



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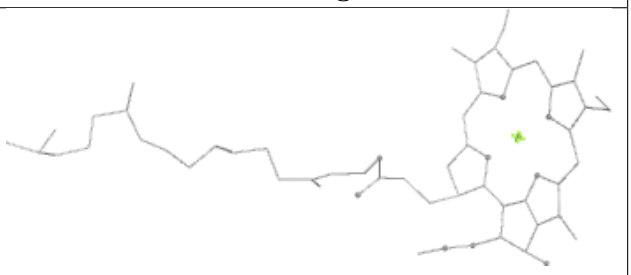
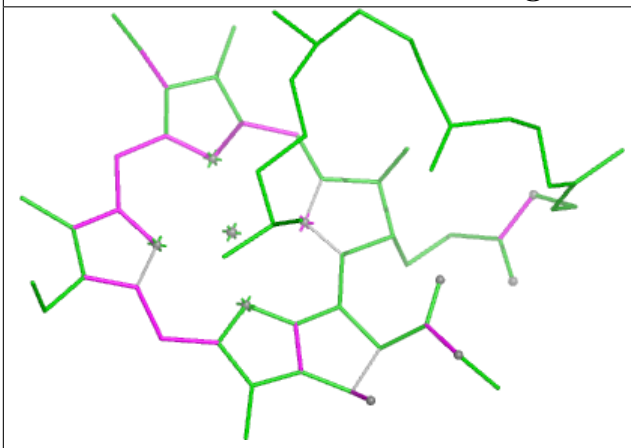


Rings

Ligand CLA B 805



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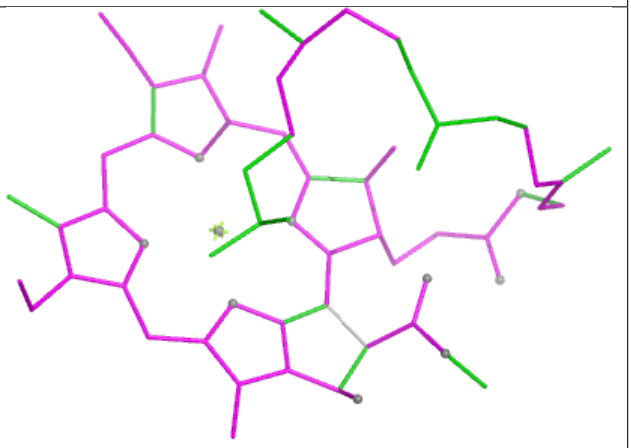

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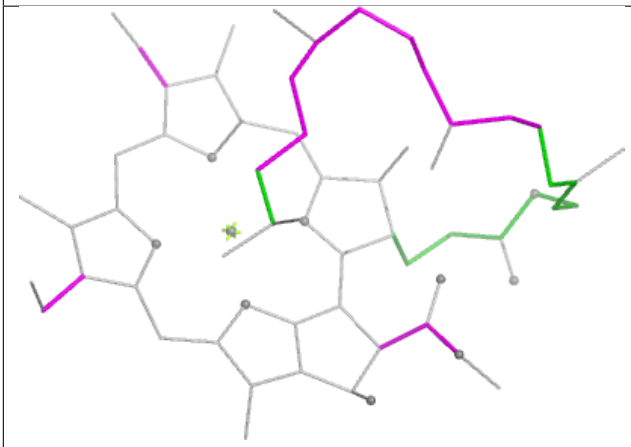

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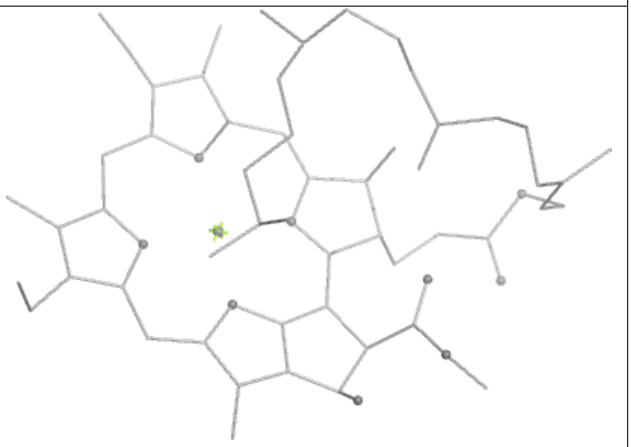
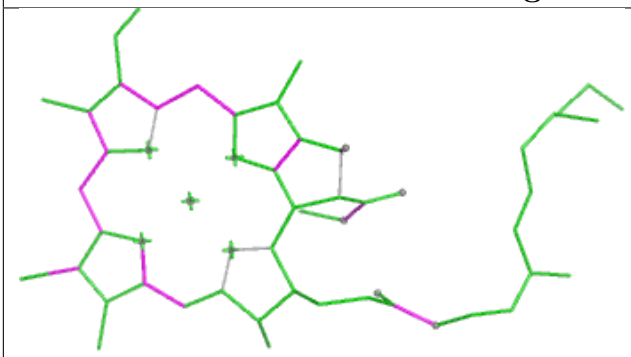


Rings

Ligand CLA R 106



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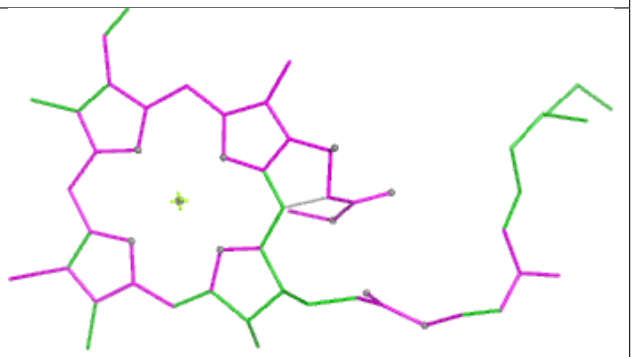

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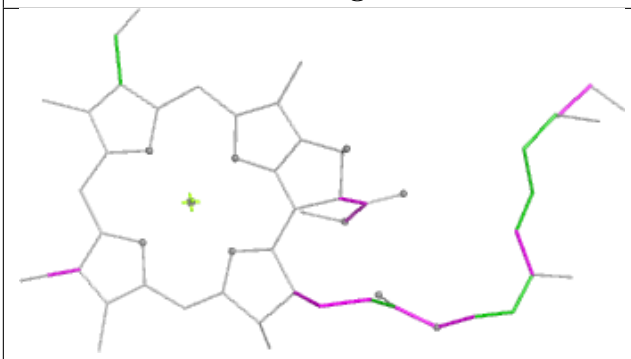

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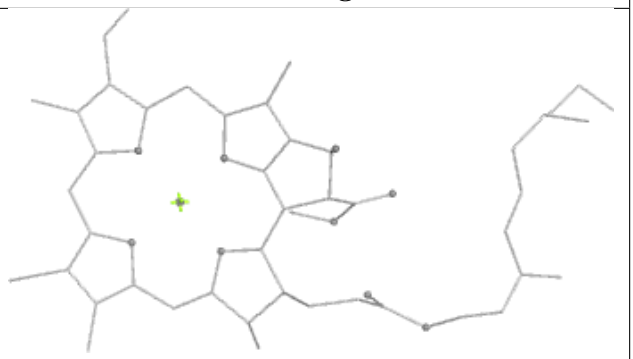
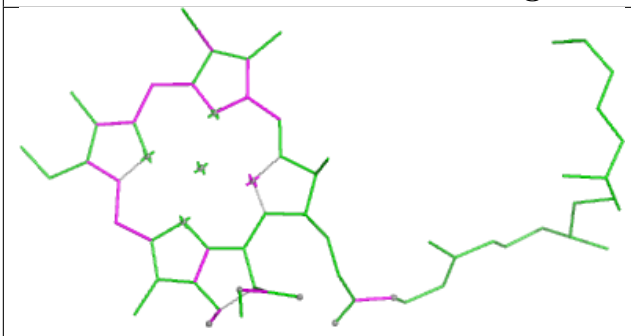


Rings

Ligand CLA A 823



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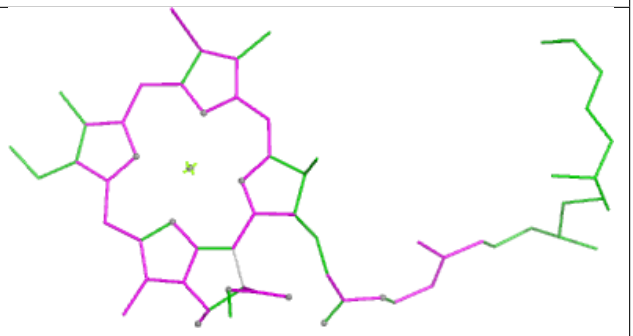
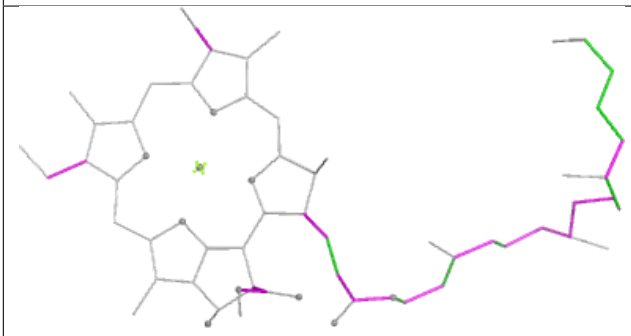


Bond angles



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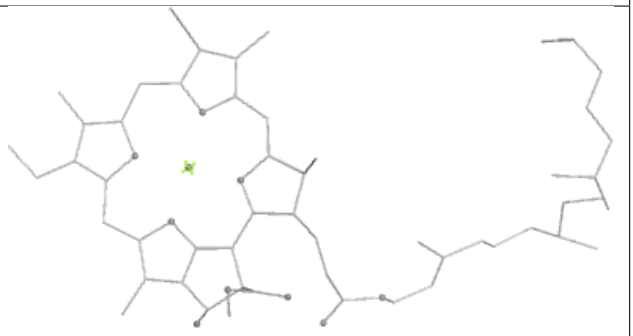
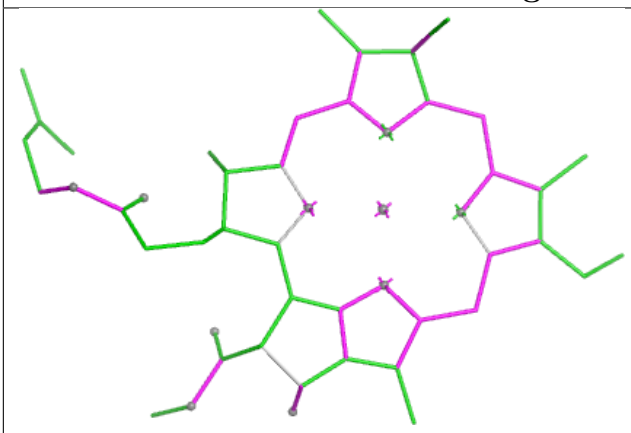


Rings

Ligand CLA K 106



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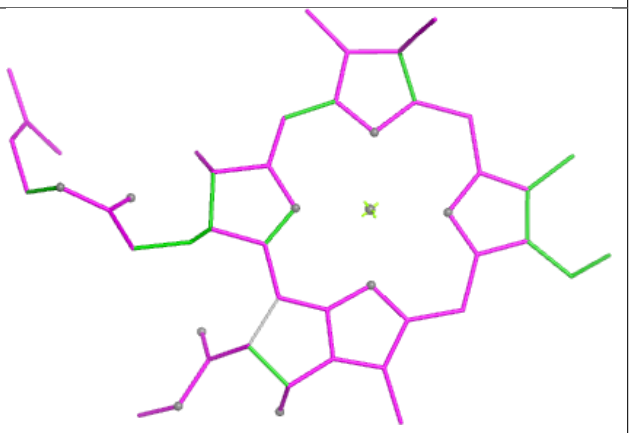
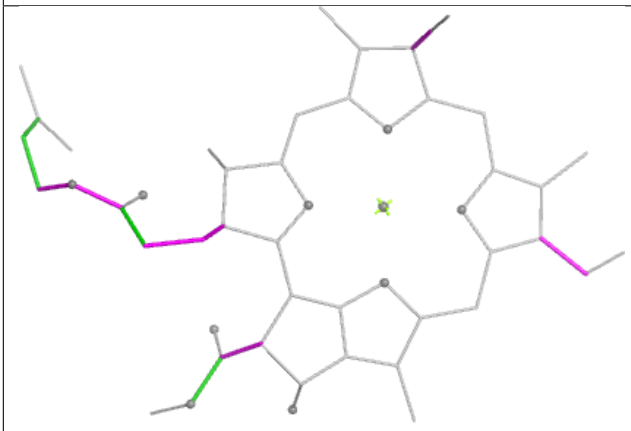


Bond angles



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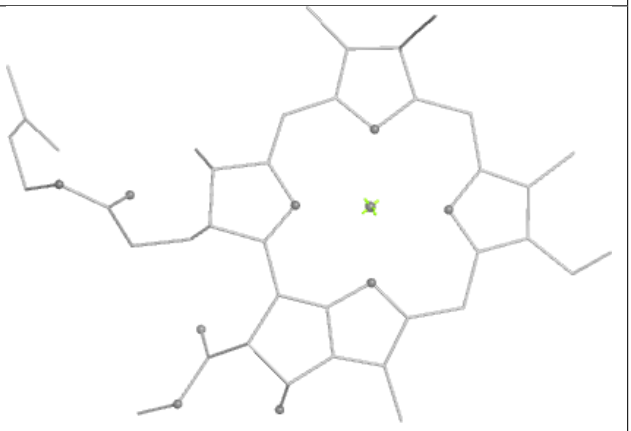
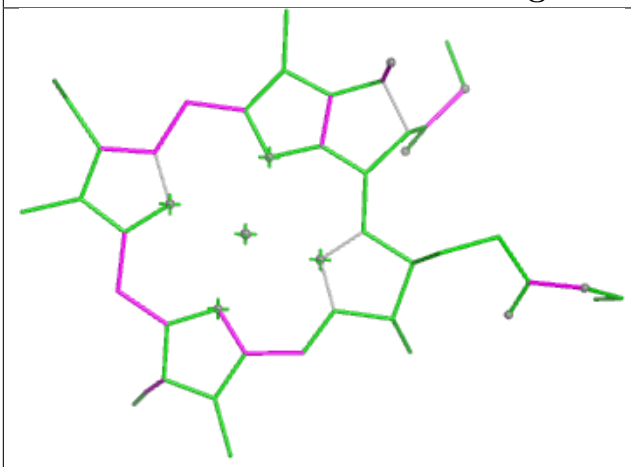


Rings

Ligand CLA 1 203



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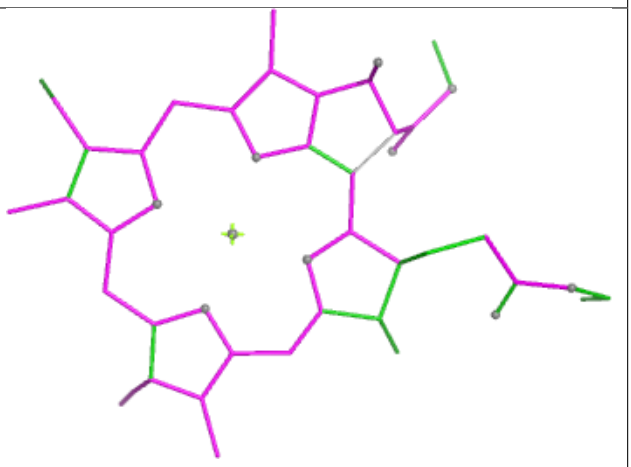
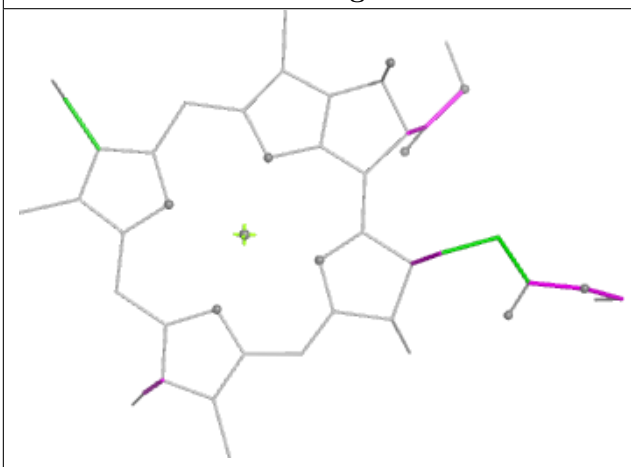


Bond angles



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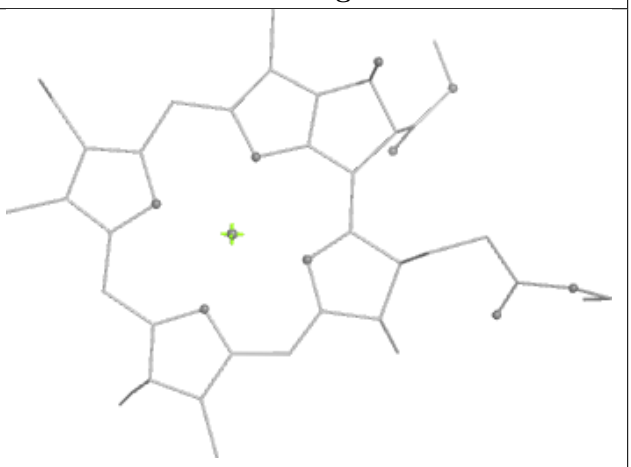
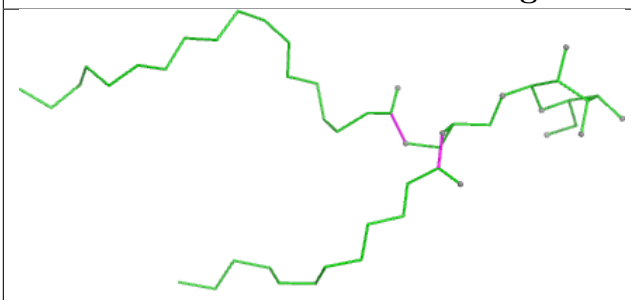


Rings

Ligand LMG B 846



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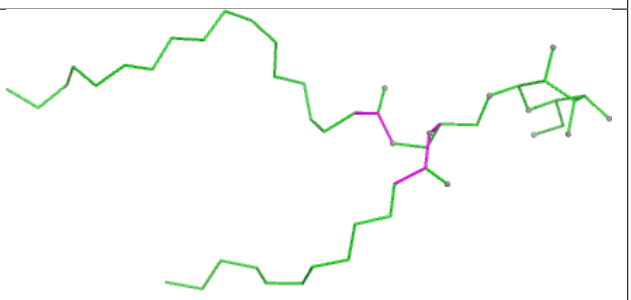
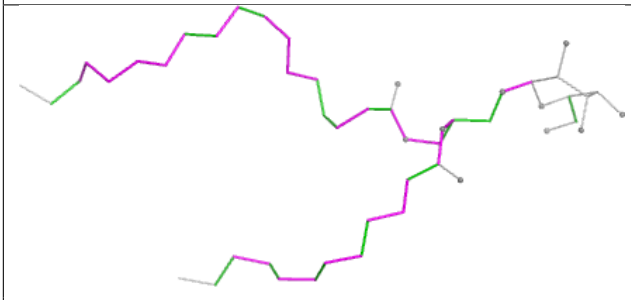


Bond angles



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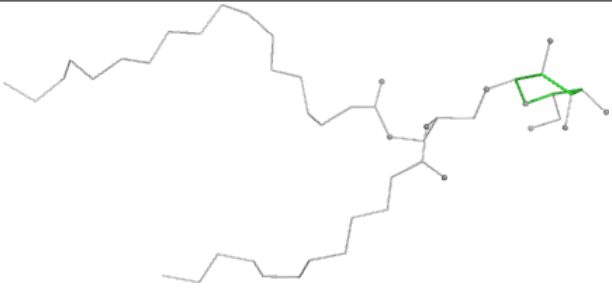
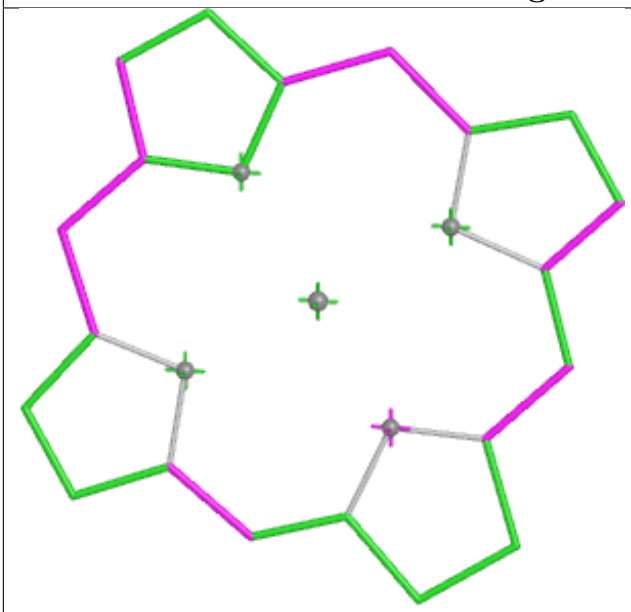


Rings

Ligand CLA 3 308



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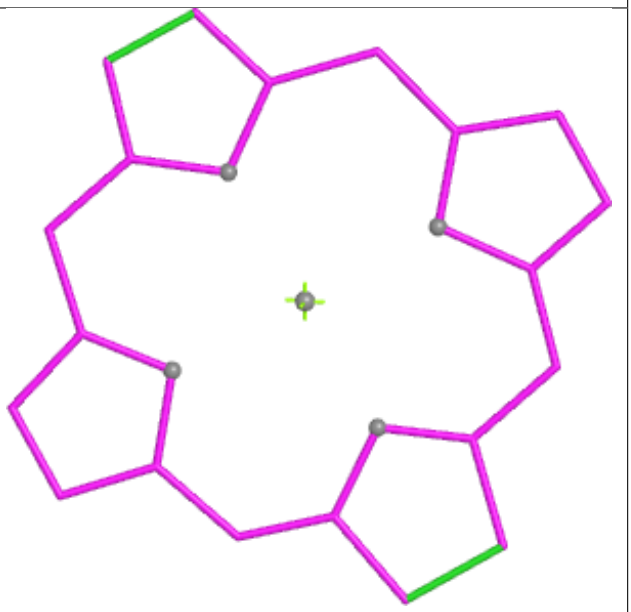
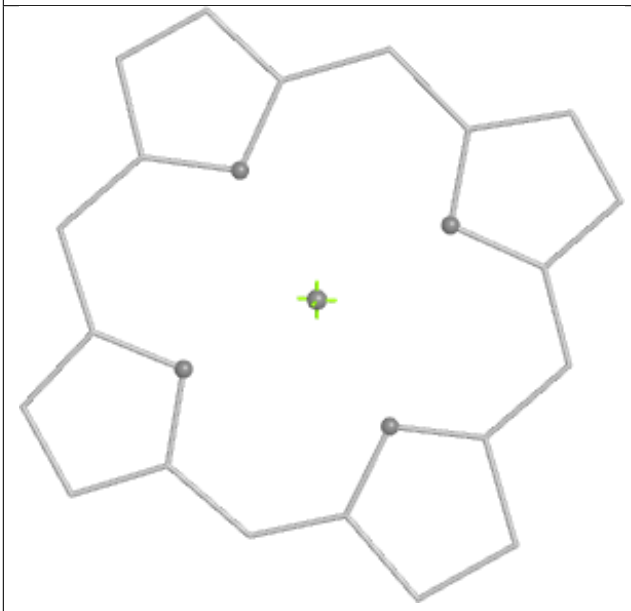


Bond angles



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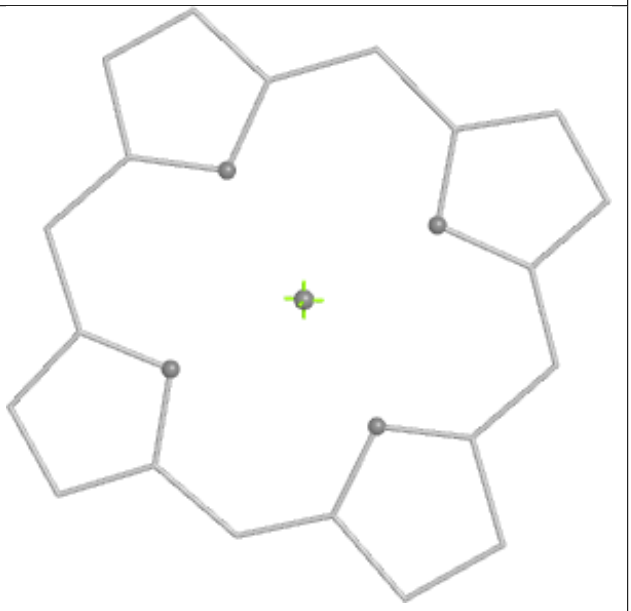
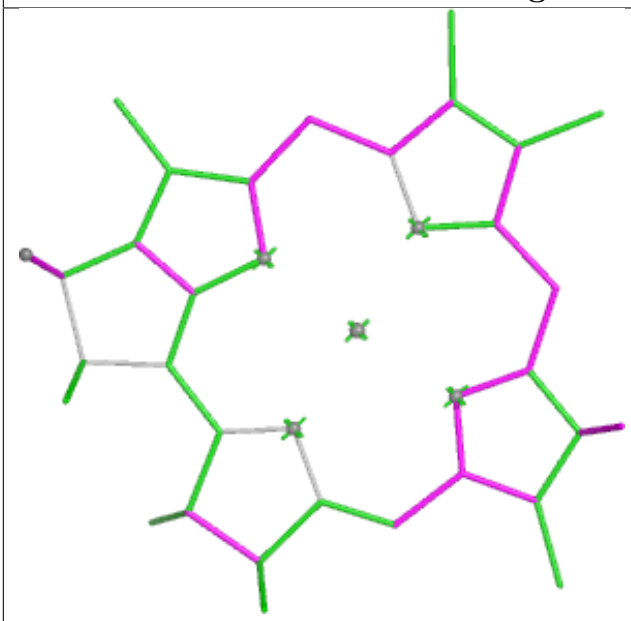


Rings

Ligand CLA 4 303



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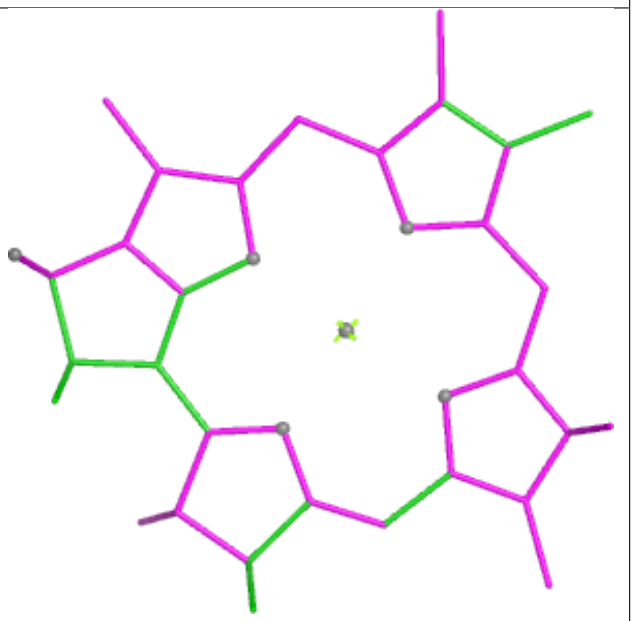

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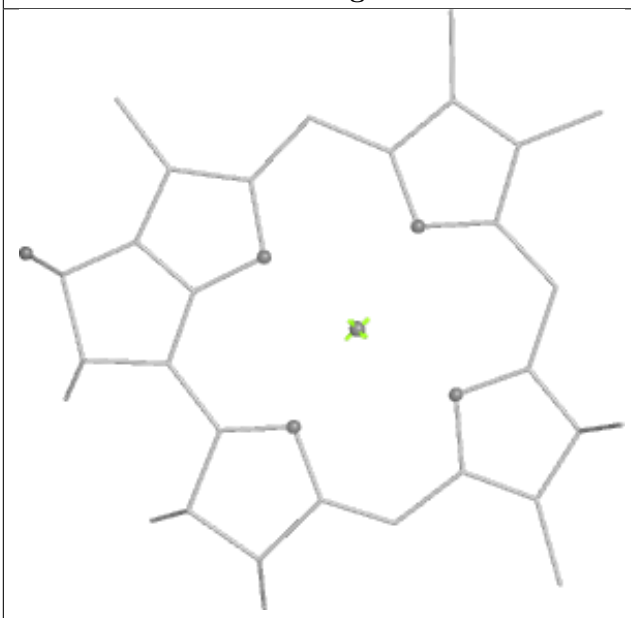

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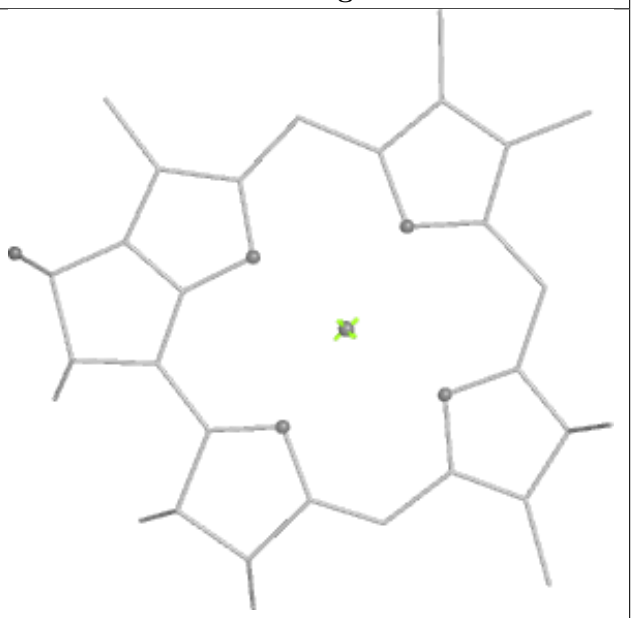
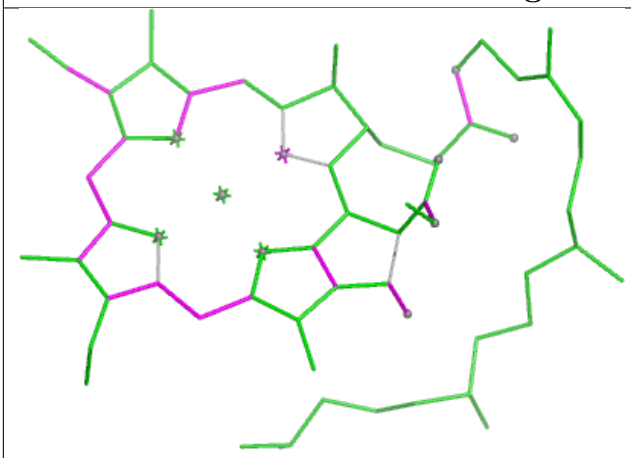


Rings

Ligand CLA B 804



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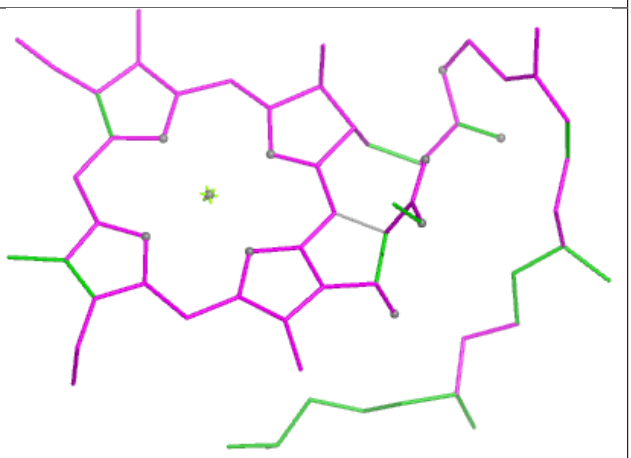
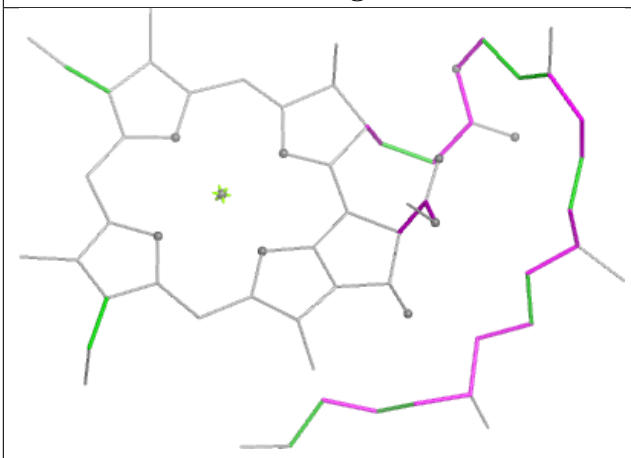


Bond angles



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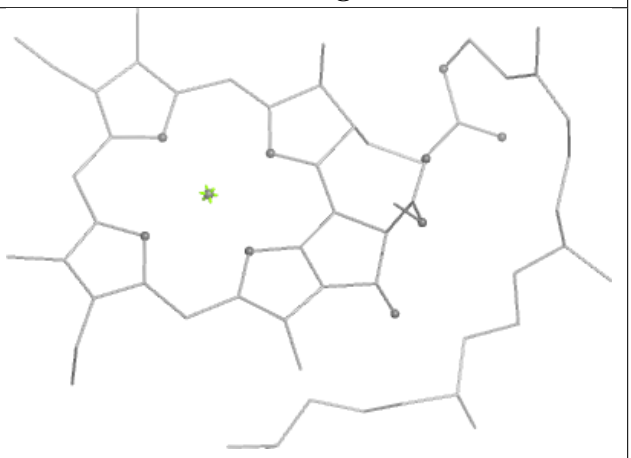
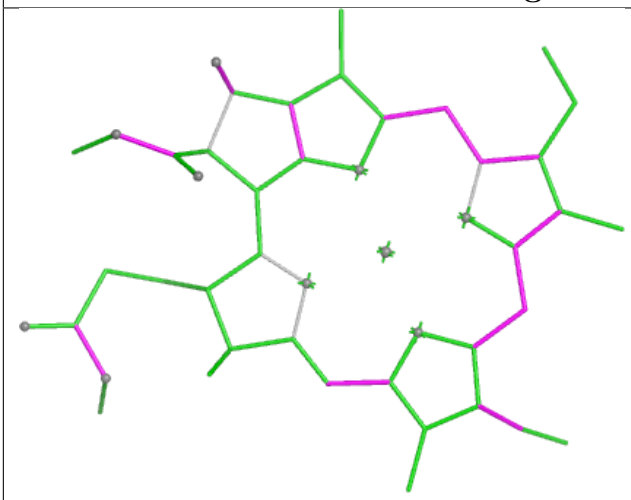
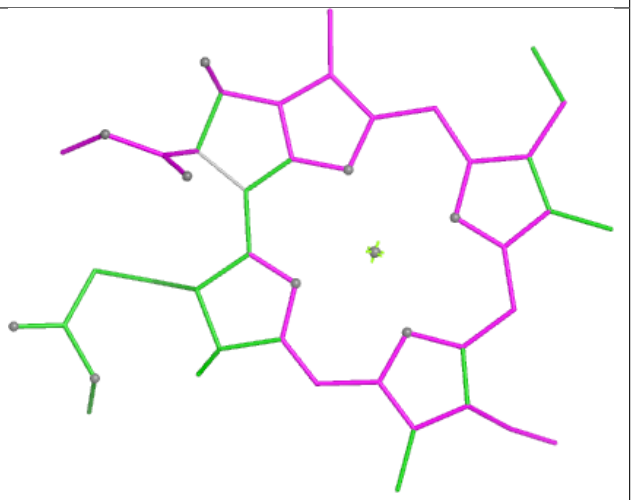


Rings

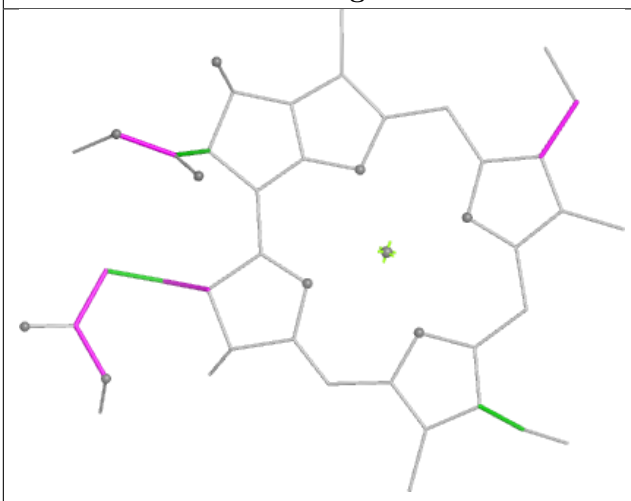
Ligand CLA B 813



Bond lengths



Bond angles



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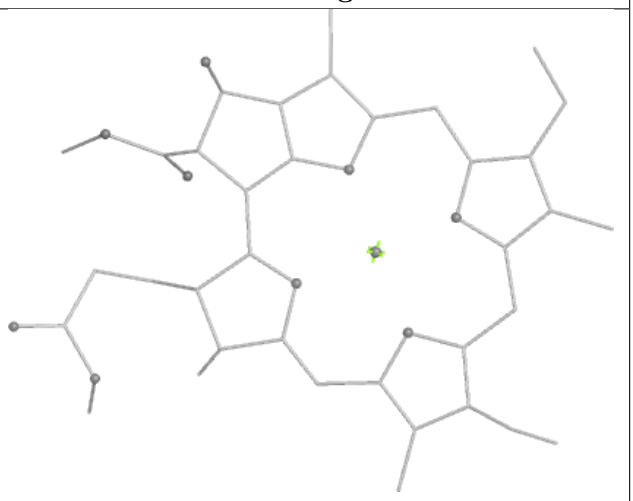


Rings

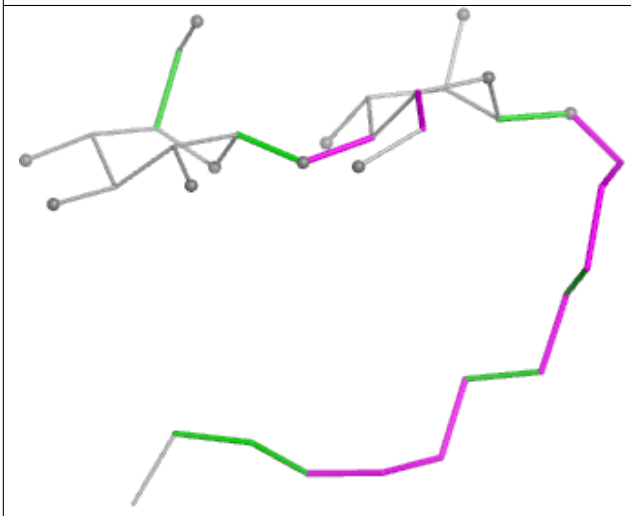
Ligand LMU 1 217



Bond lengths



Bond angles



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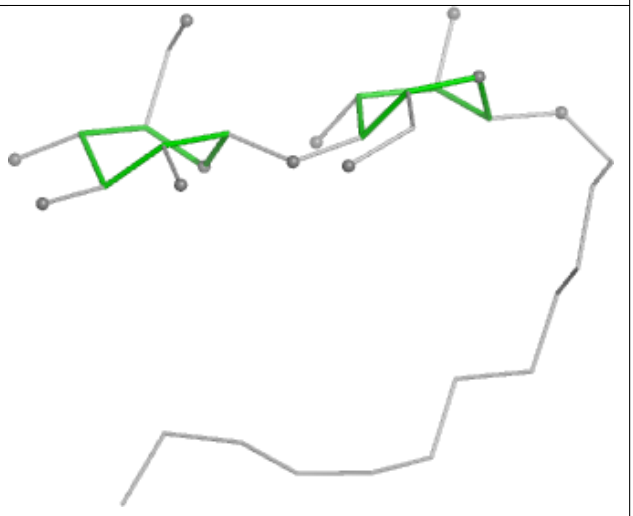
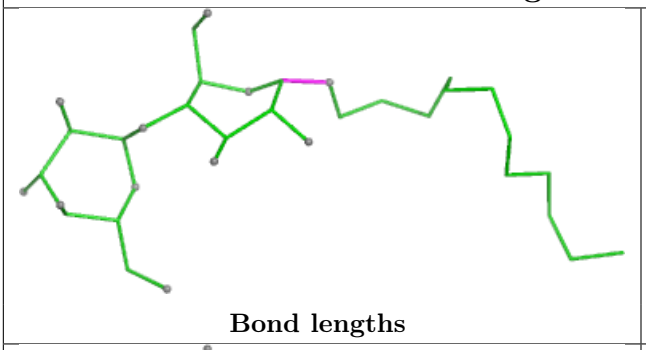
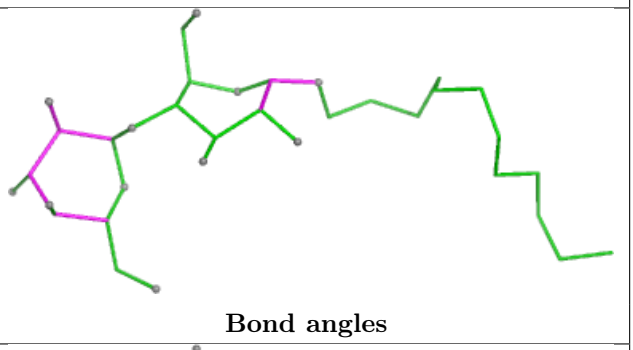


Rings

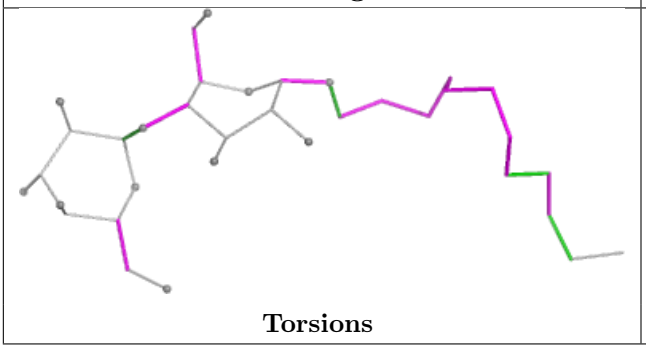
Ligand LMU 4 322



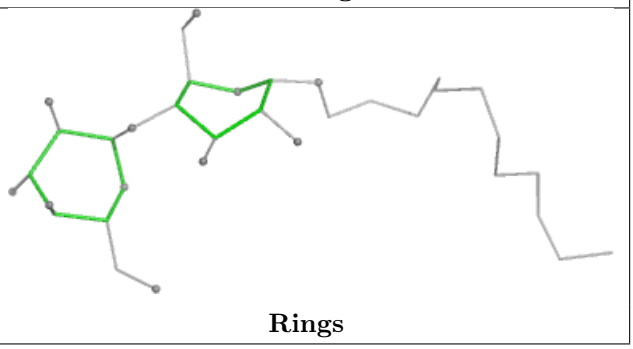
Bond lengths



Bond angles

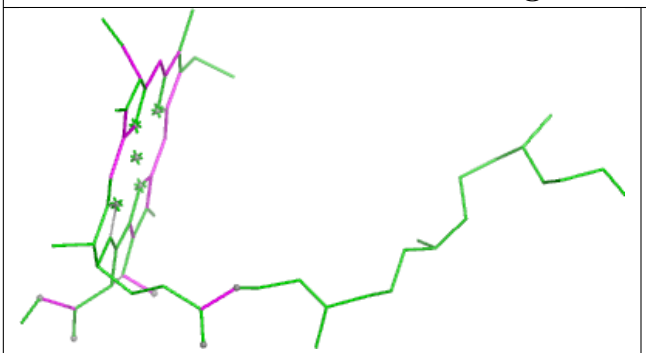


Torsions

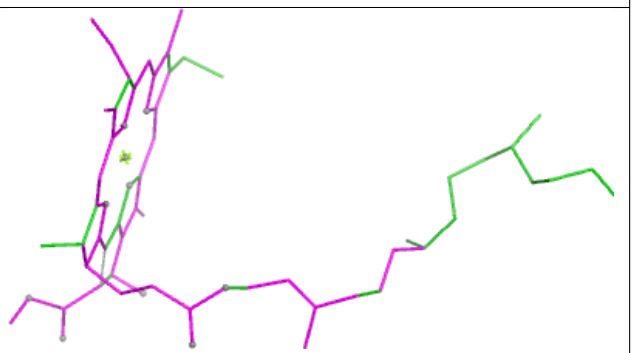


Rings

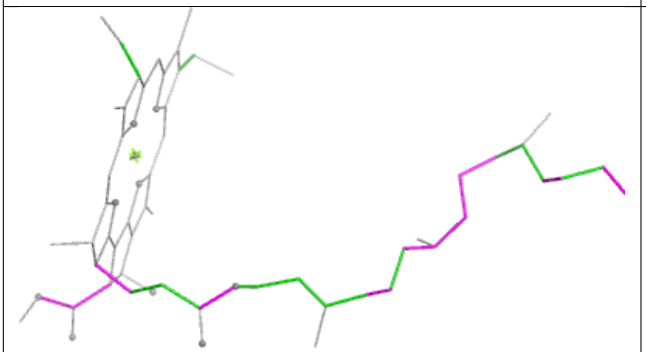
Ligand CLA A 826



Bond lengths



Bond angles



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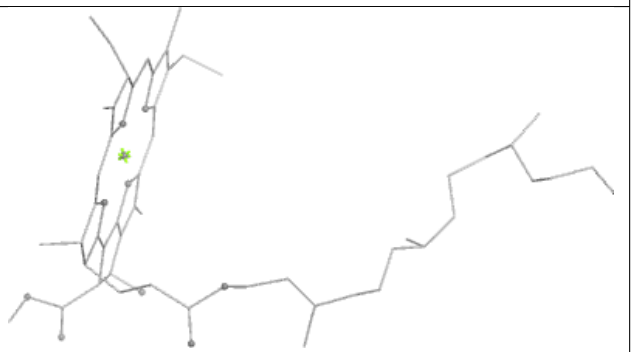
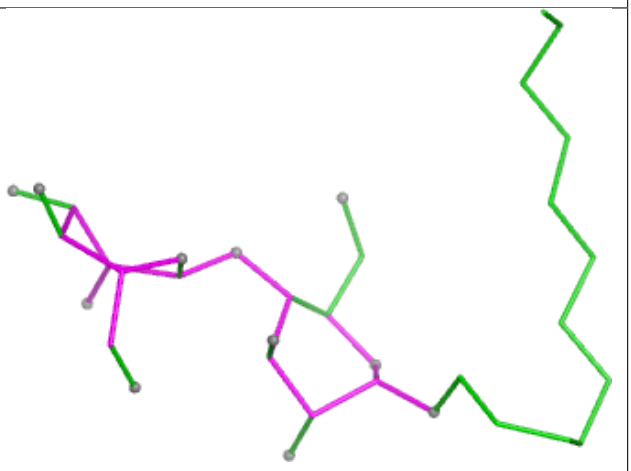


Rings

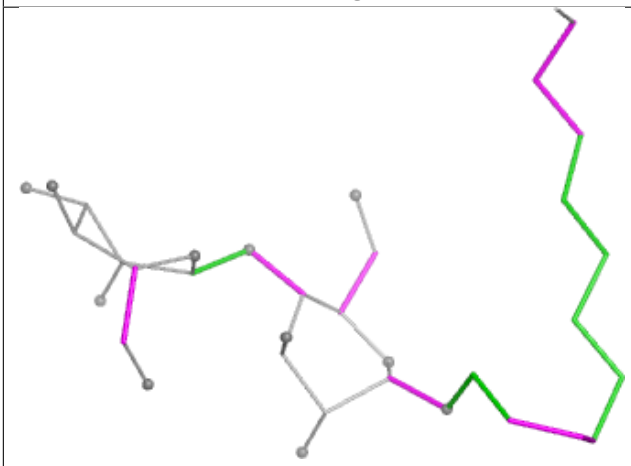
Ligand LMU R 109



Bond lengths



Bond angles



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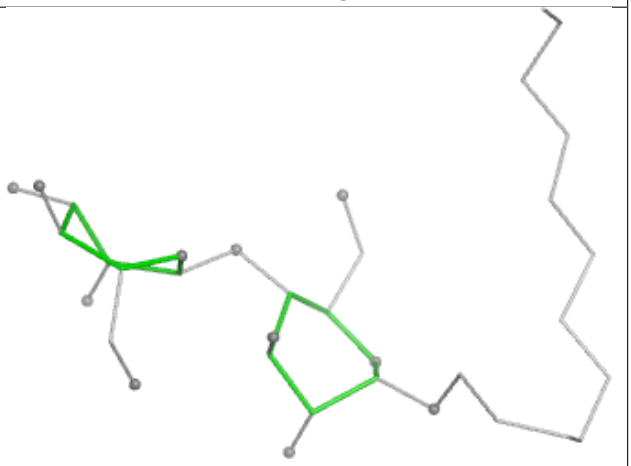
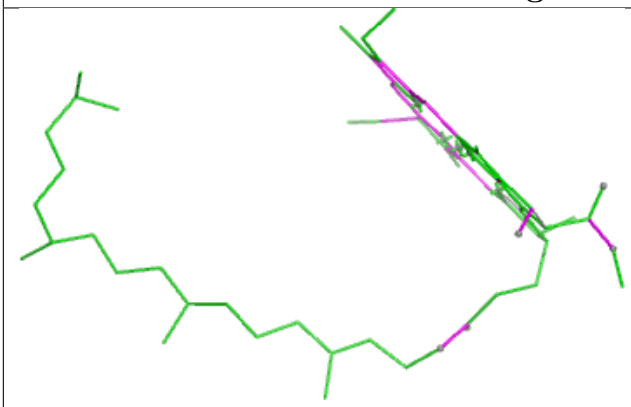


Rings

Ligand CLA L 201



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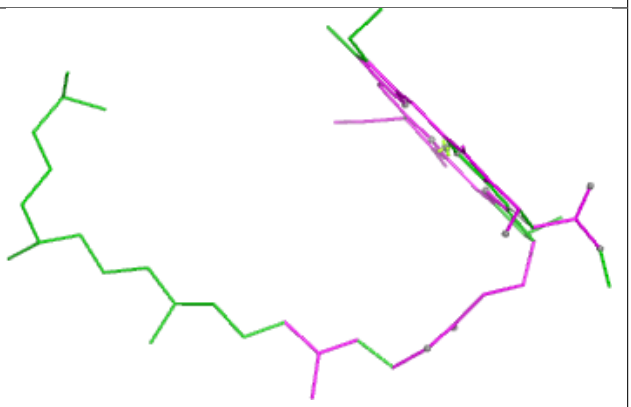
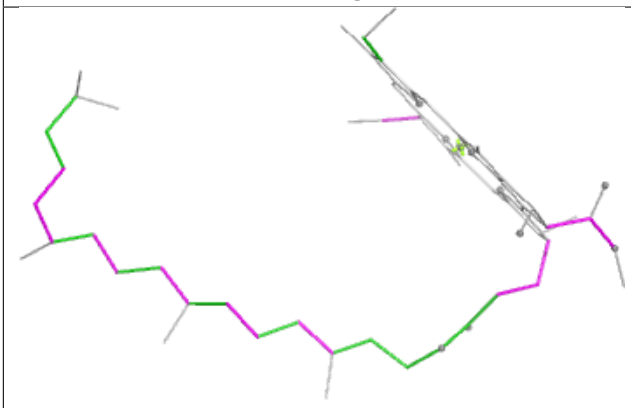


Bond angles

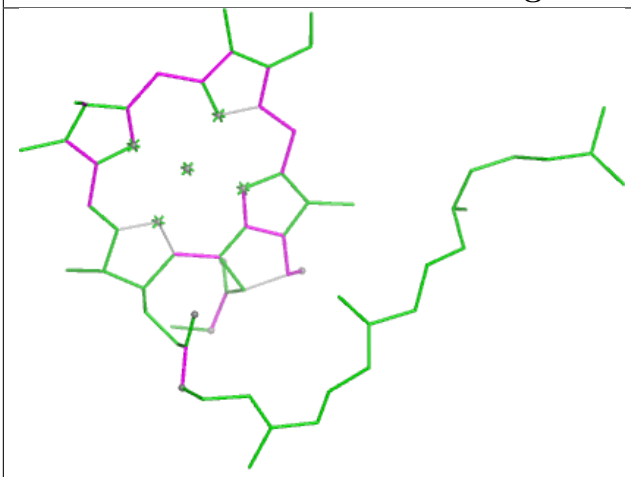


Torsions

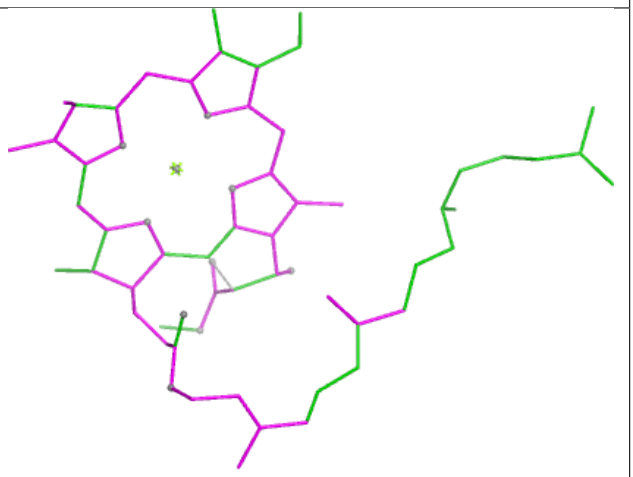


Rings

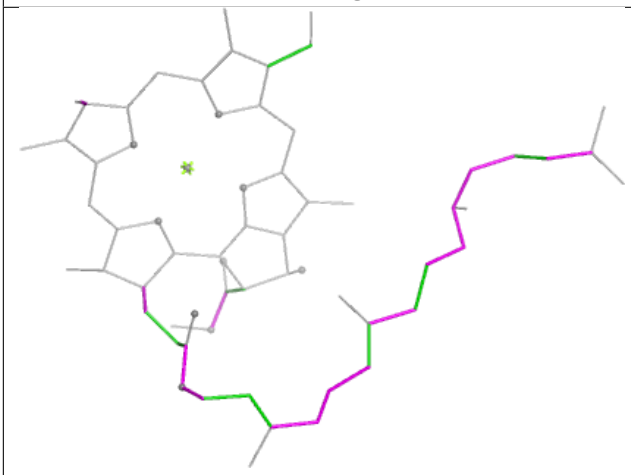
Ligand CLA B 829



Bond lengths



Bond angles



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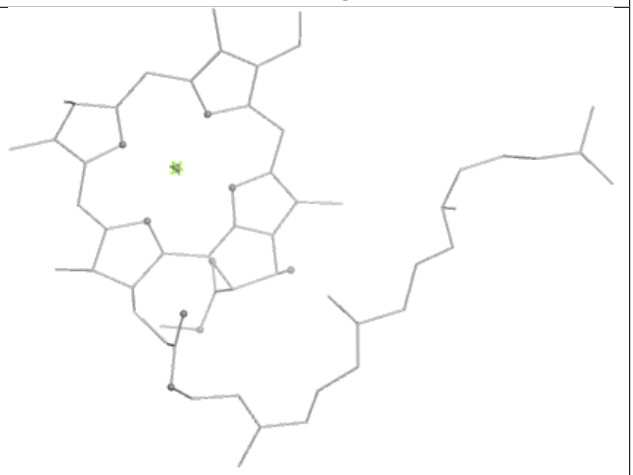
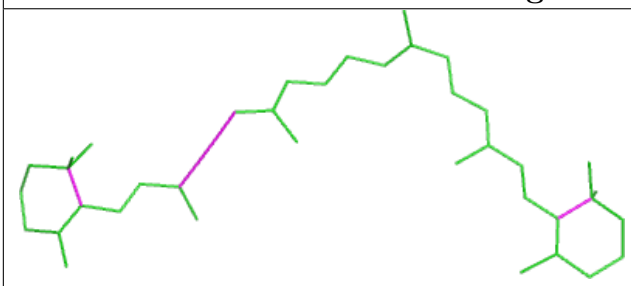


Rings

Ligand BCR 3 311



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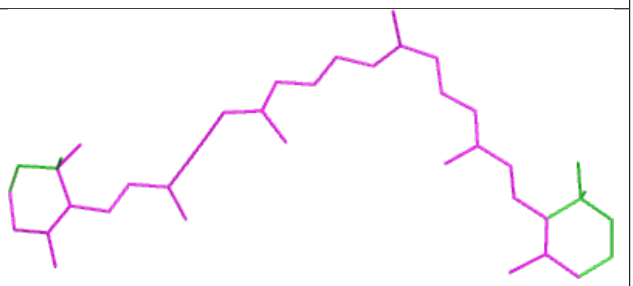
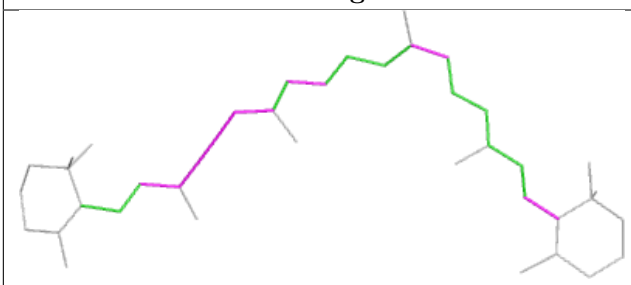


Bond angles



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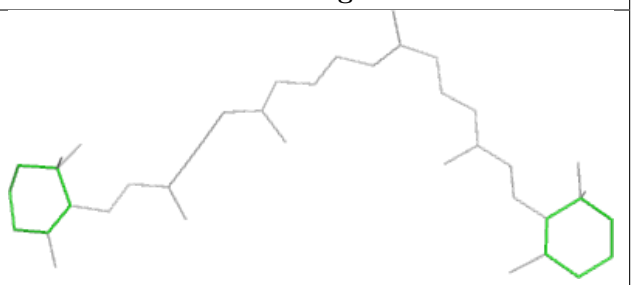
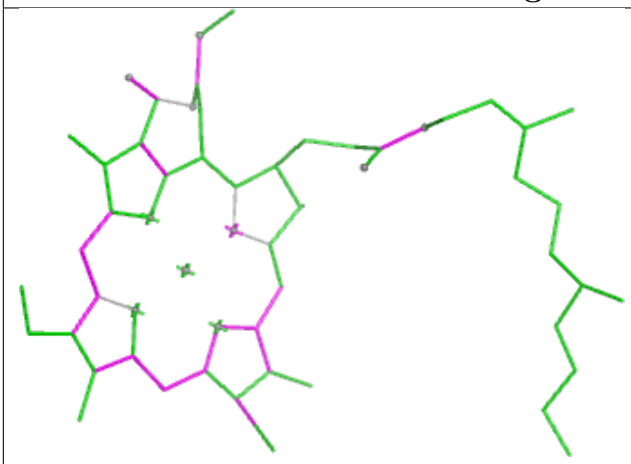
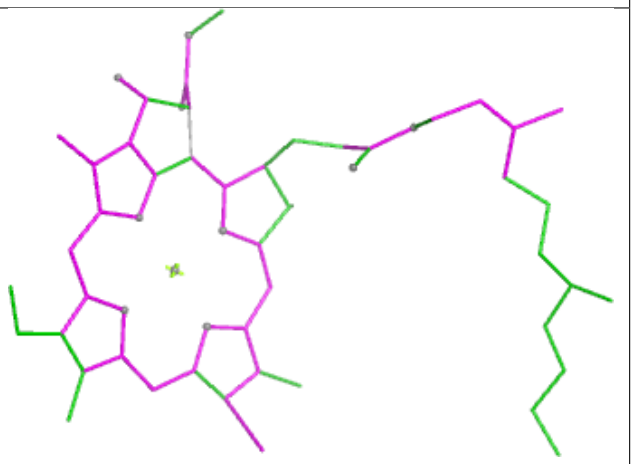


Rings

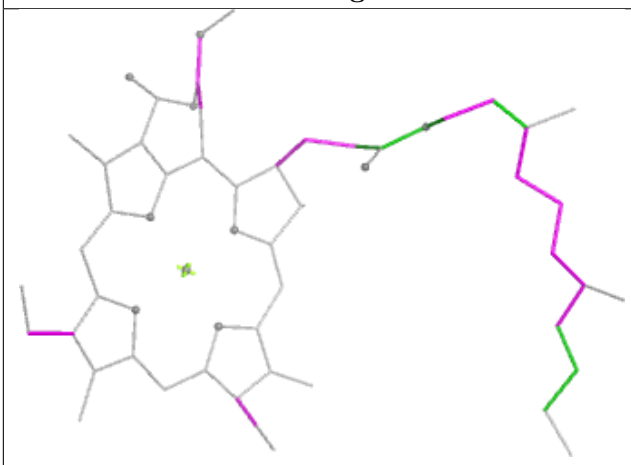
Ligand CLA B 822



Bond lengths



Bond angles



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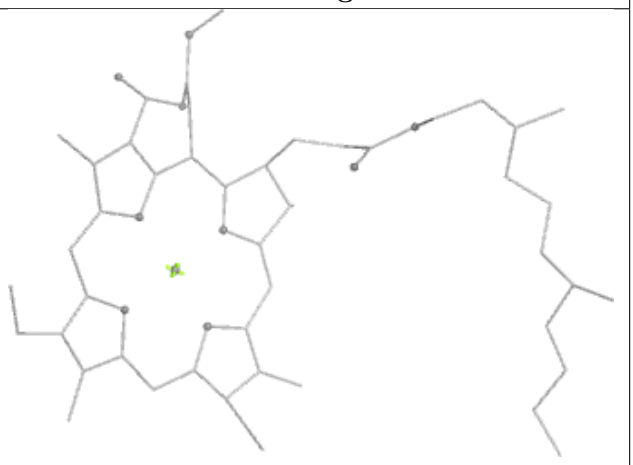
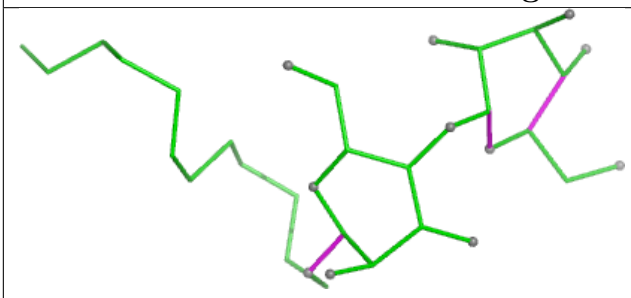


Rings

Ligand LMU L 210



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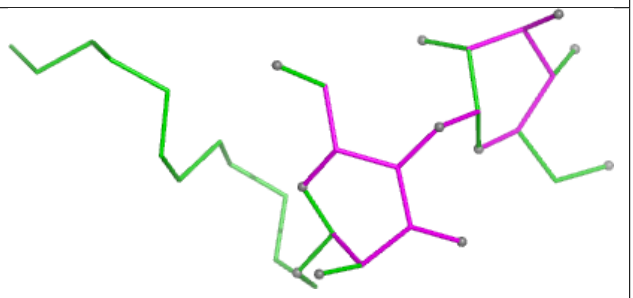
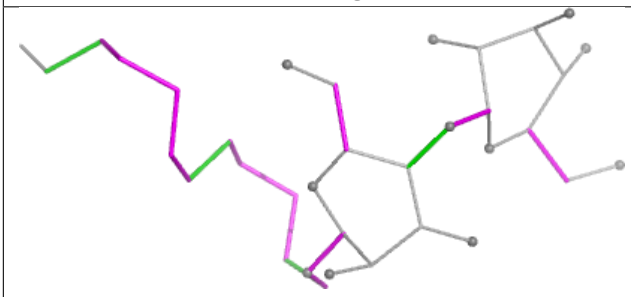


Bond angles



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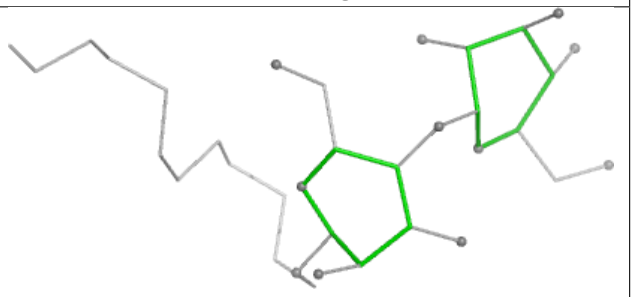
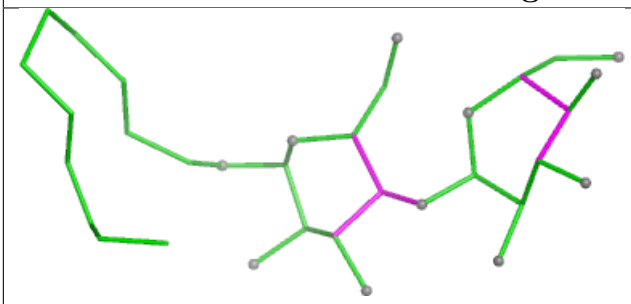


Rings

Ligand LMU F 201



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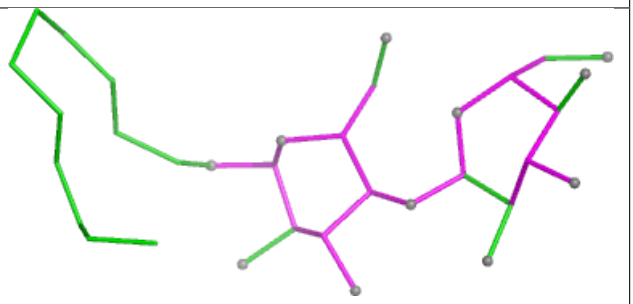
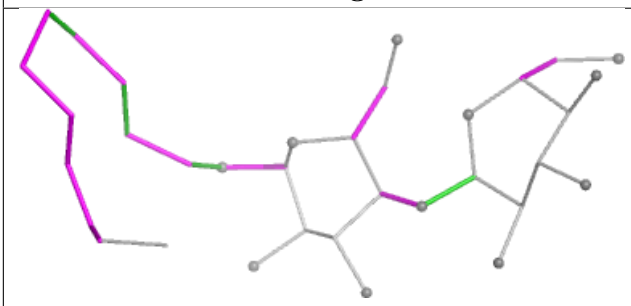


Bond angles



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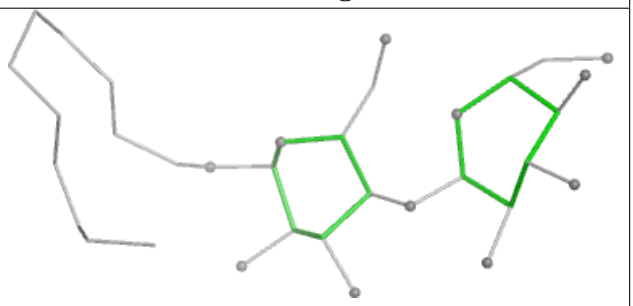
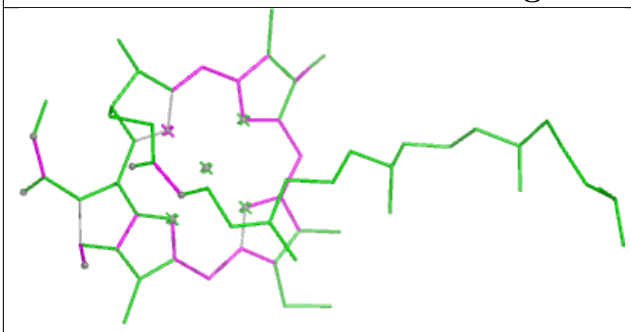


Rings

Ligand CLA A 814



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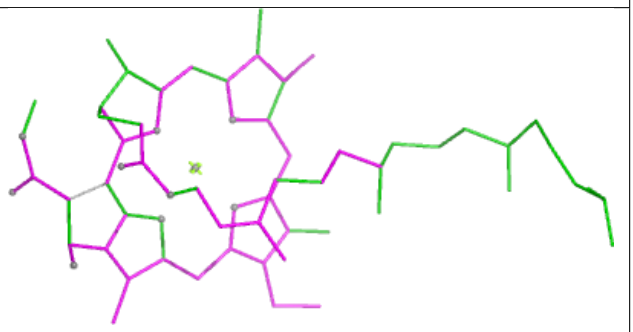
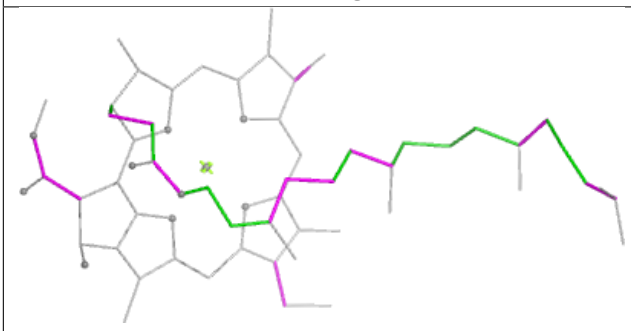


Bond angles



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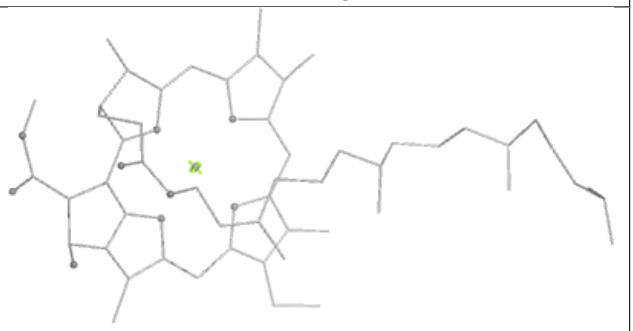
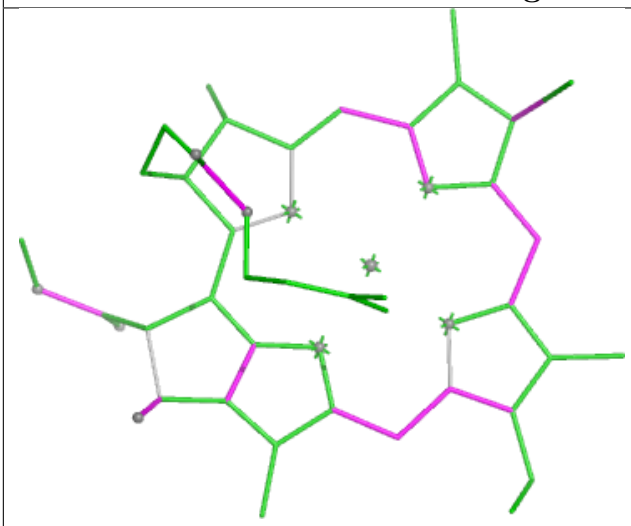


Rings

Ligand CLA H 109



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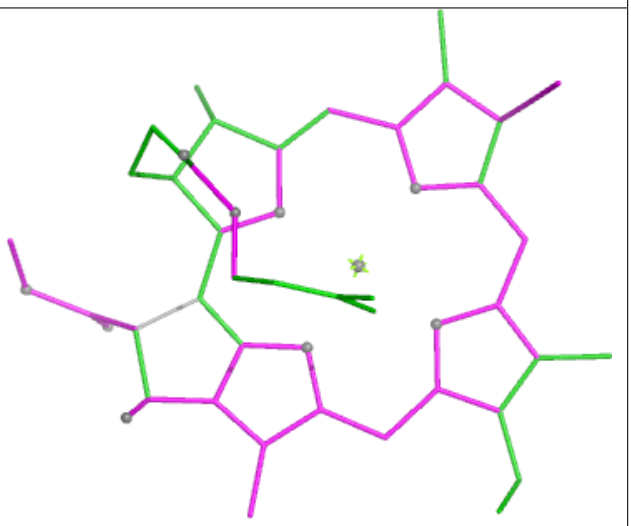
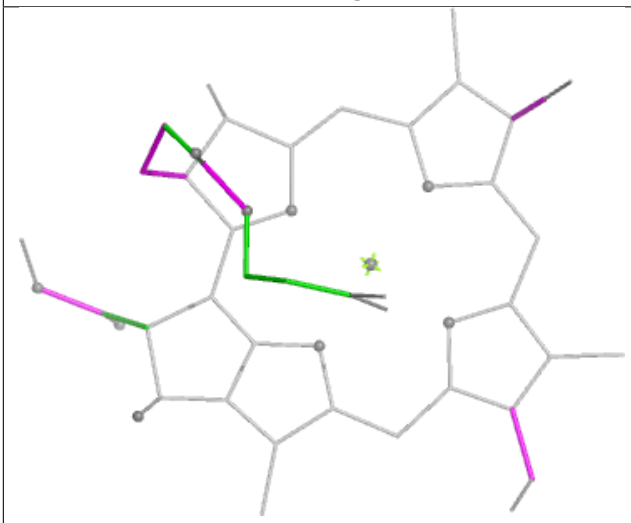


Bond angles



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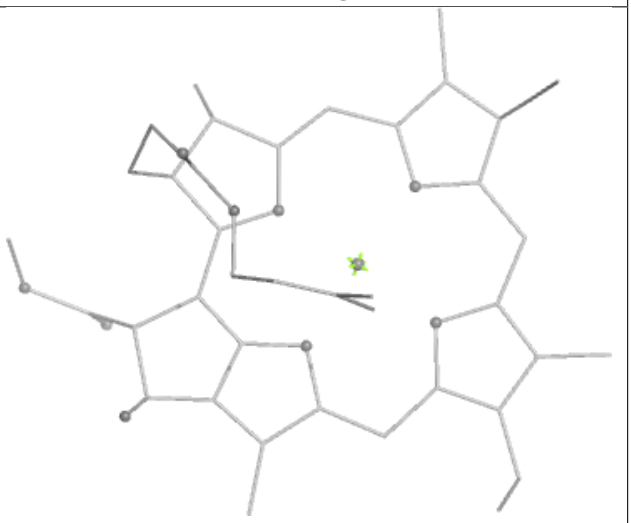
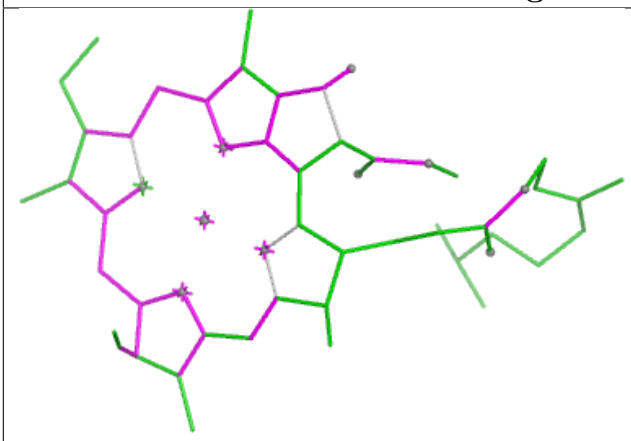


Rings

Ligand CLA L 204



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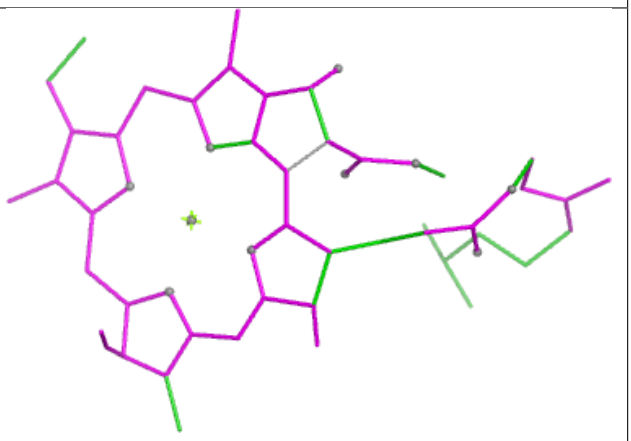
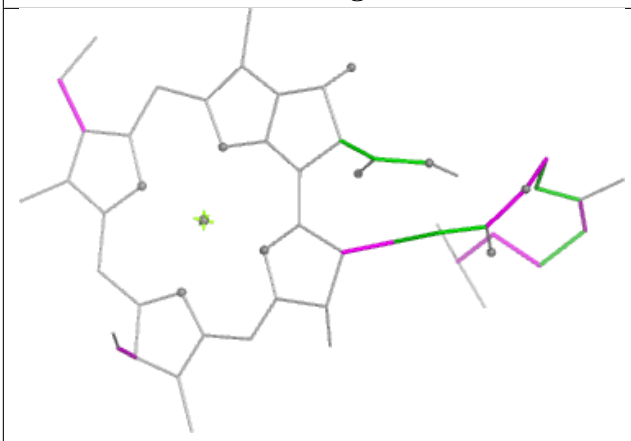


Bond angles

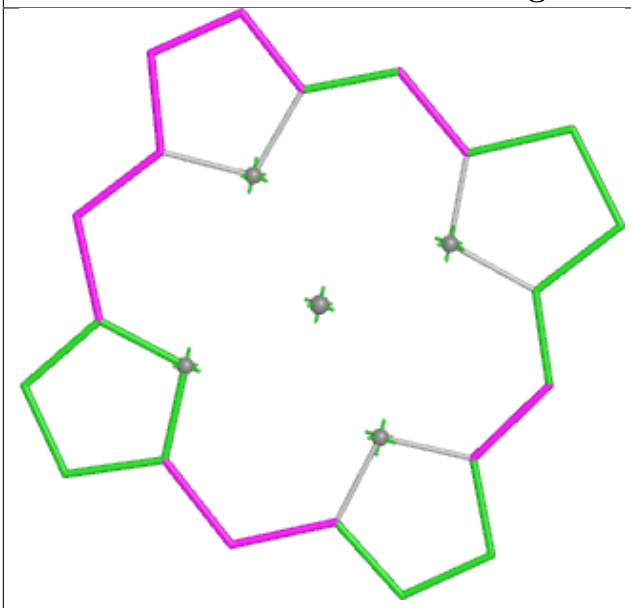


Torsions



Rings

Ligand CLA 4 314



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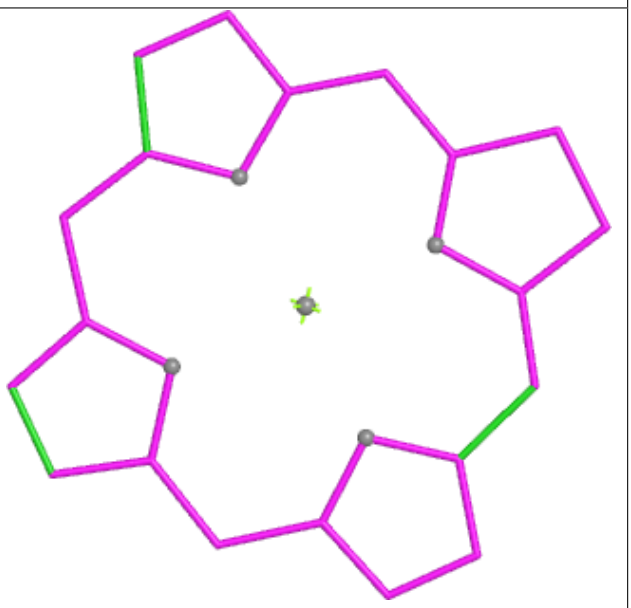
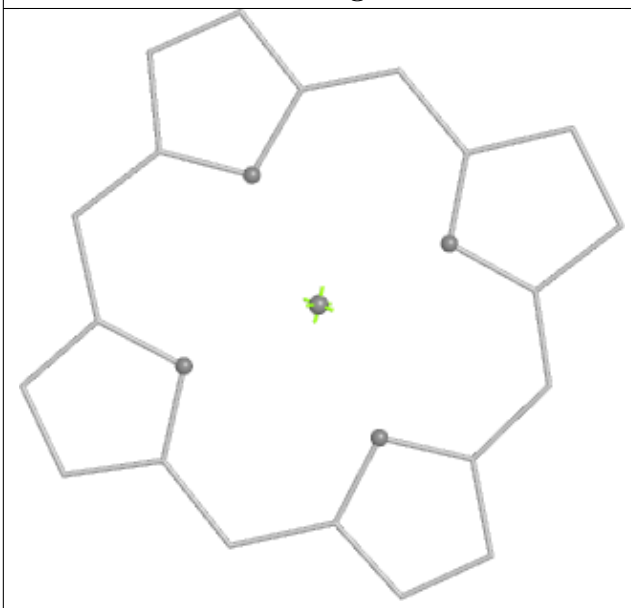


Bond angles



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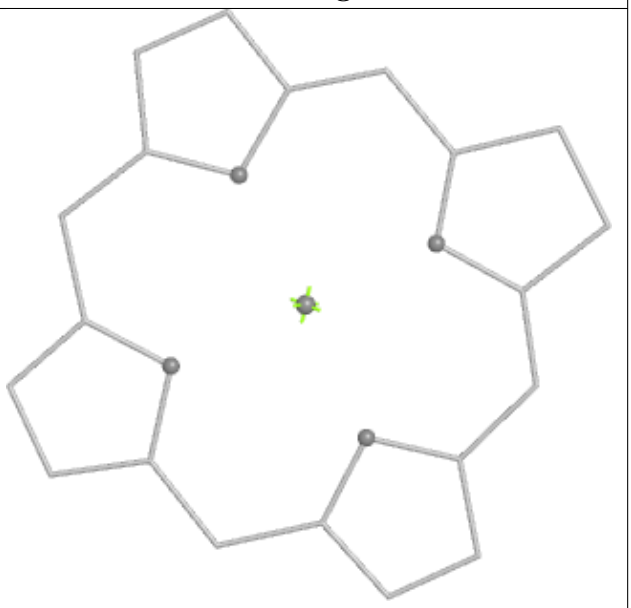
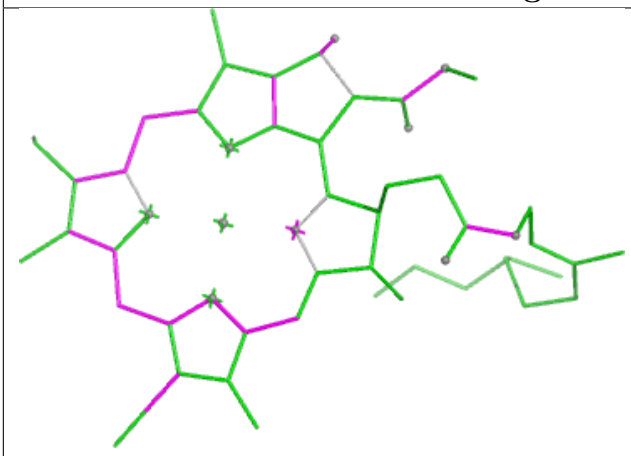


Rings

Ligand CLA A 804



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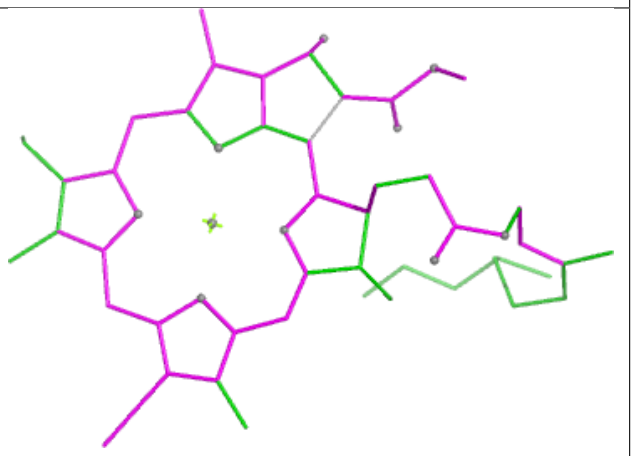
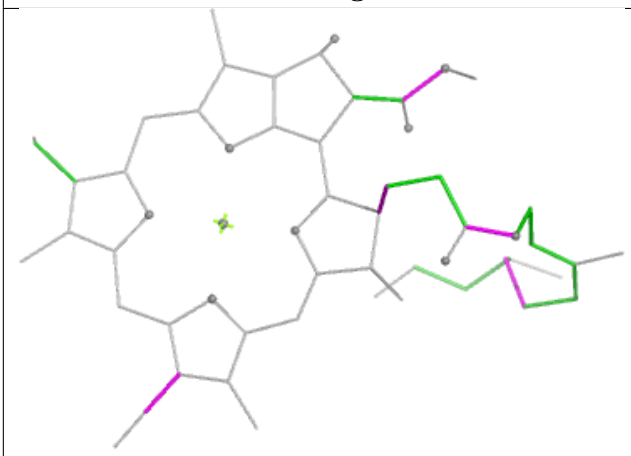


Bond angles



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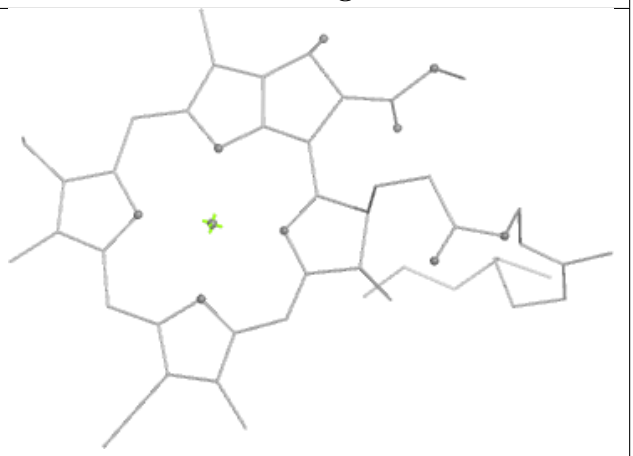
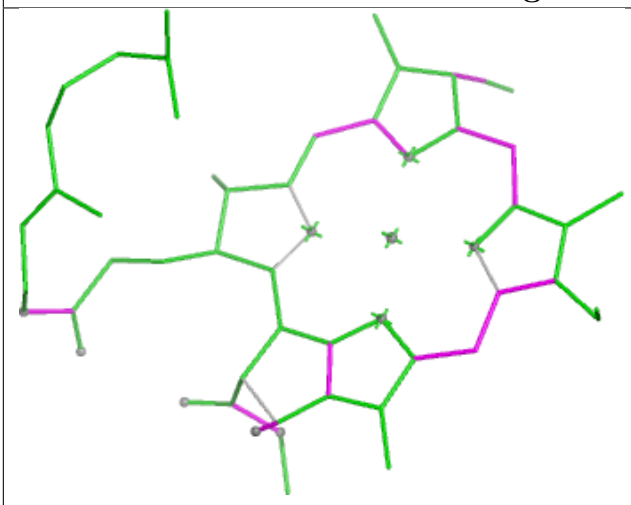


Rings

Ligand CLA H 110



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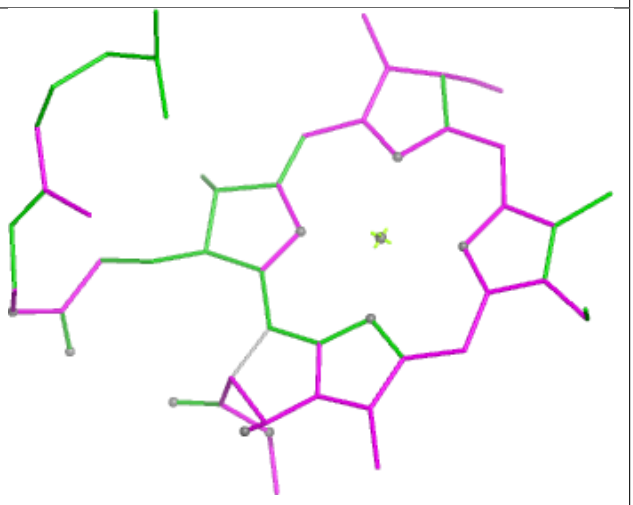
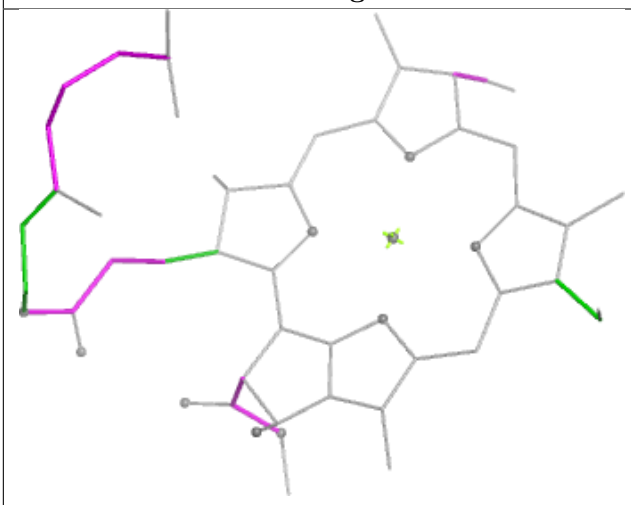


Bond angles



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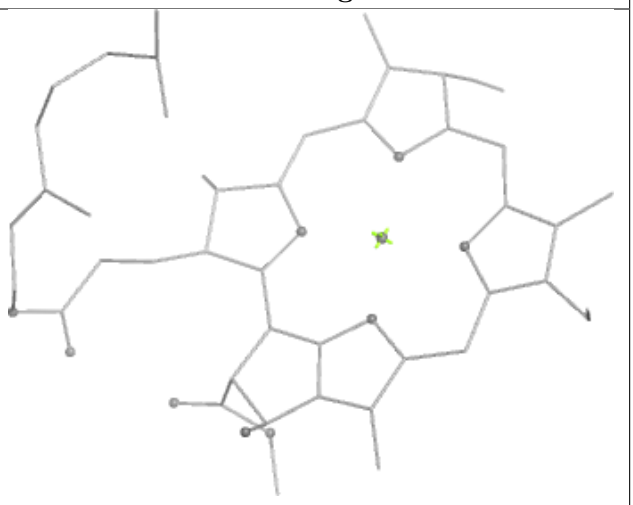
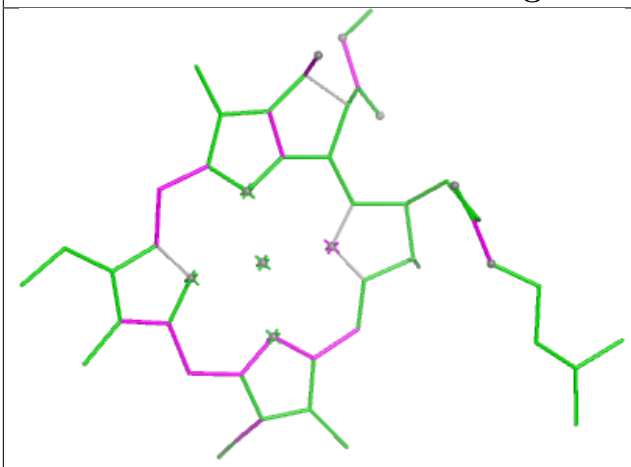
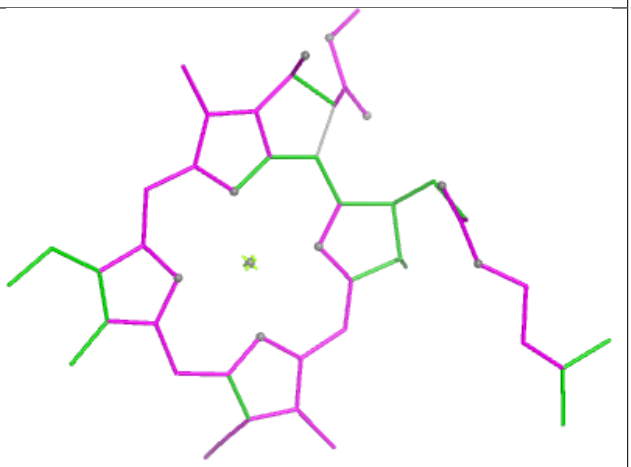


Rings

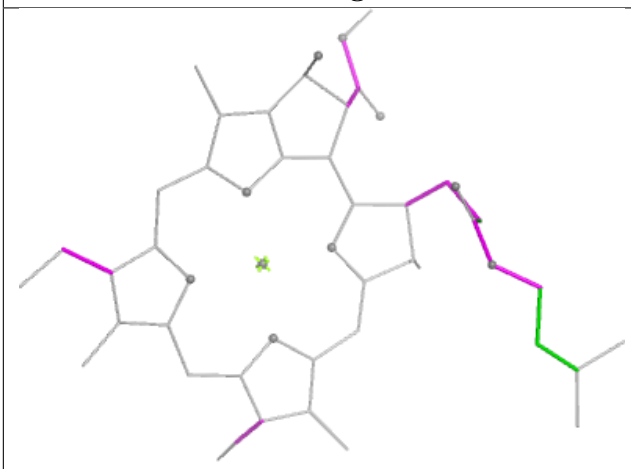
Ligand CLA A 830



Bond lengths



Bond angles



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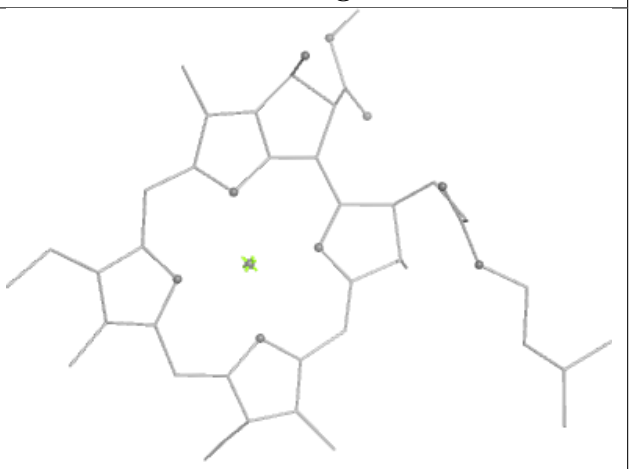
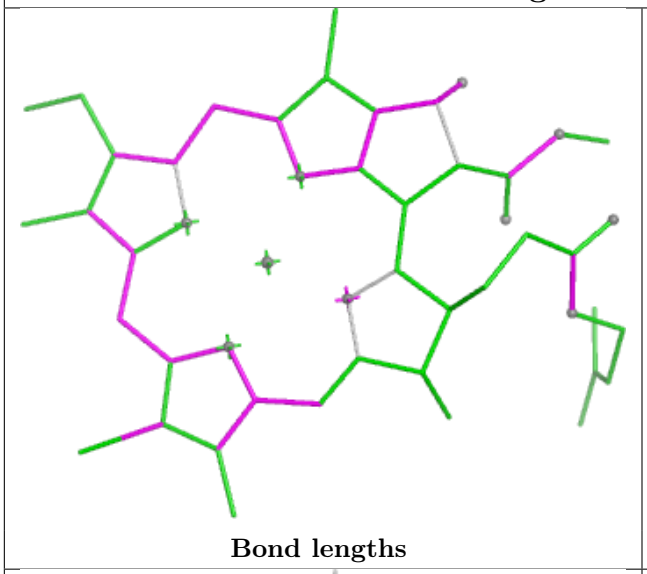
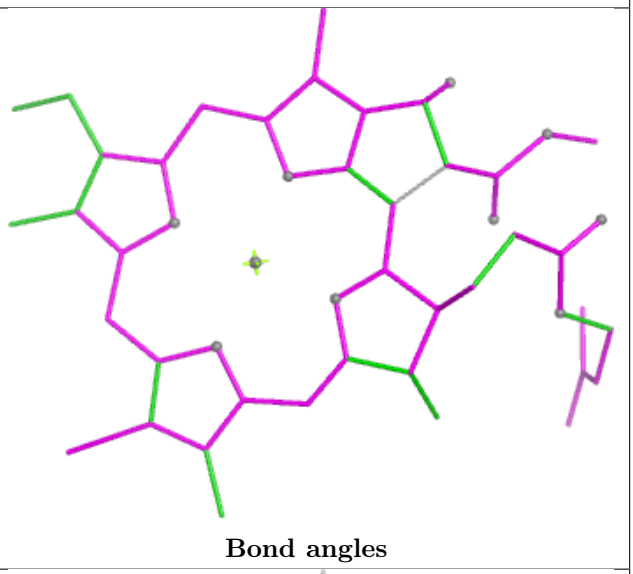


Rings

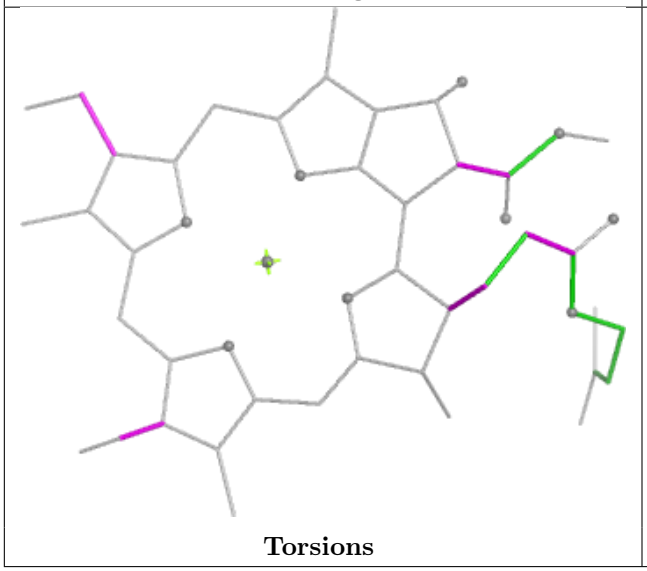
Ligand CLA 3 315



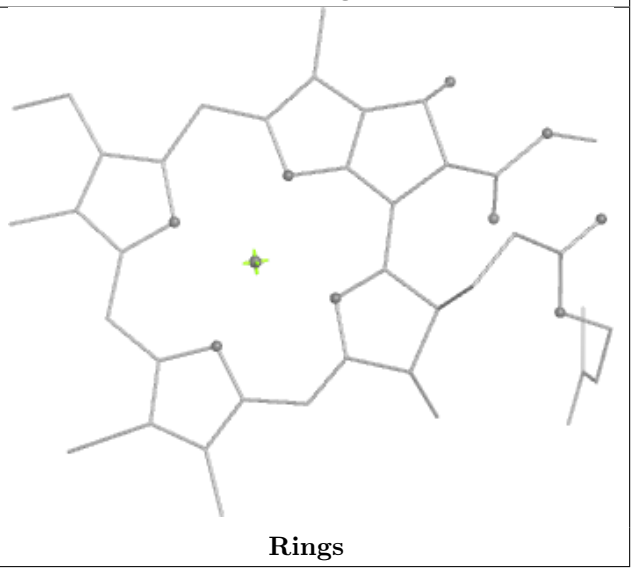
Bond lengths



Bond angles

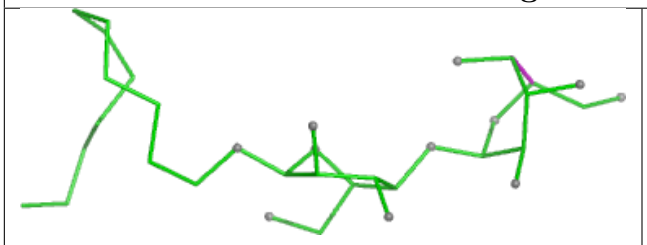


Torsions



Rings

Ligand LMU A 853



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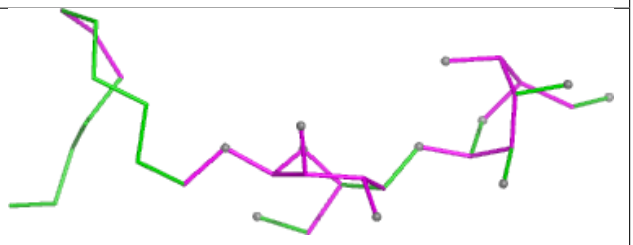

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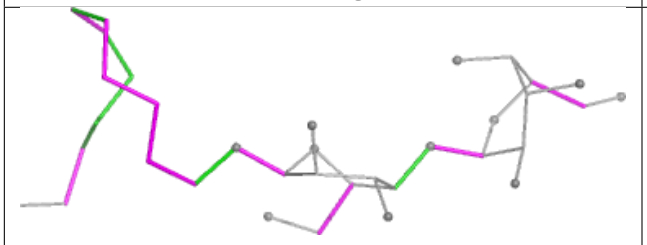

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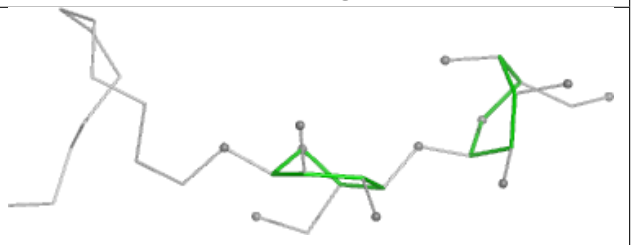
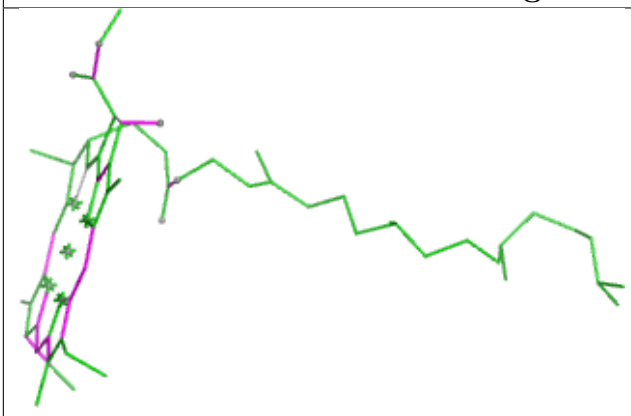


Rings

Ligand CLA A 824



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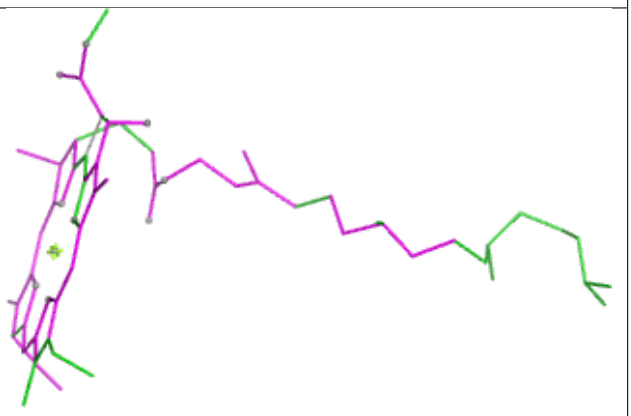
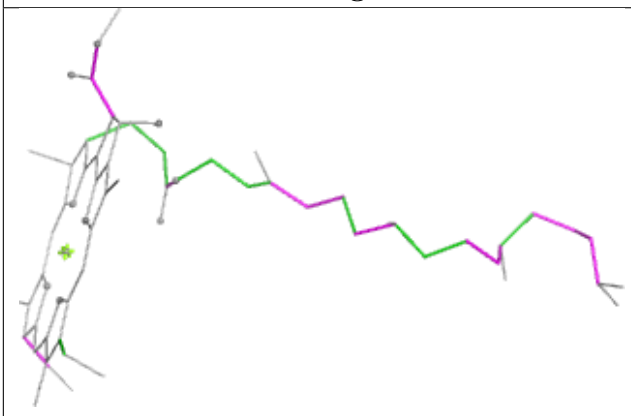


Bond angles



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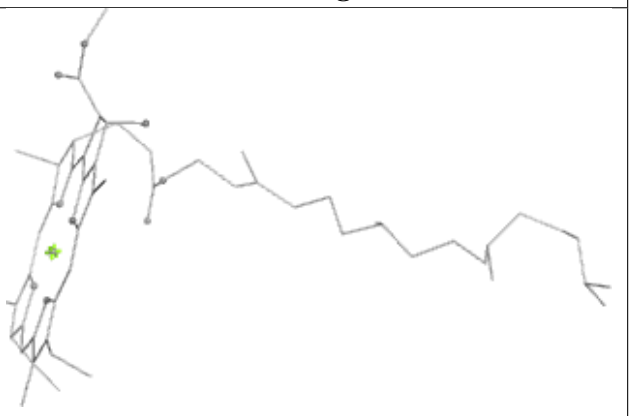
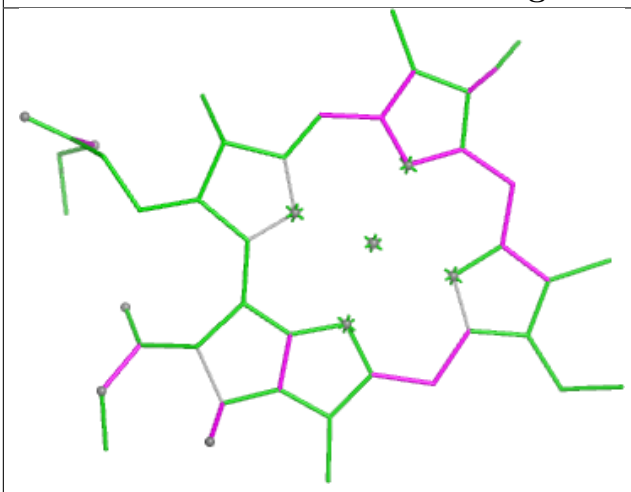


Rings

Ligand CLA 1 202



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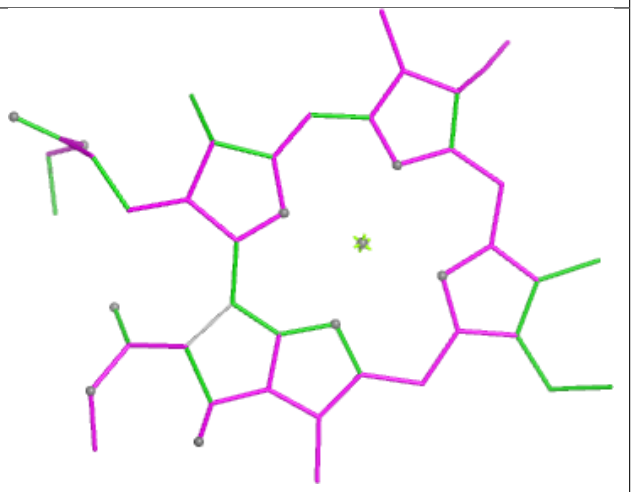

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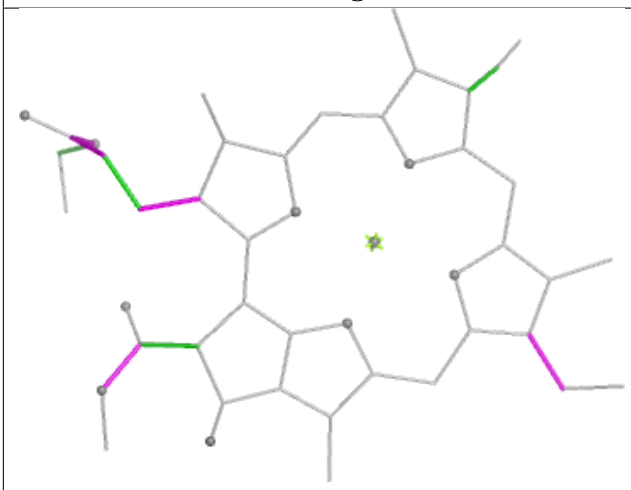

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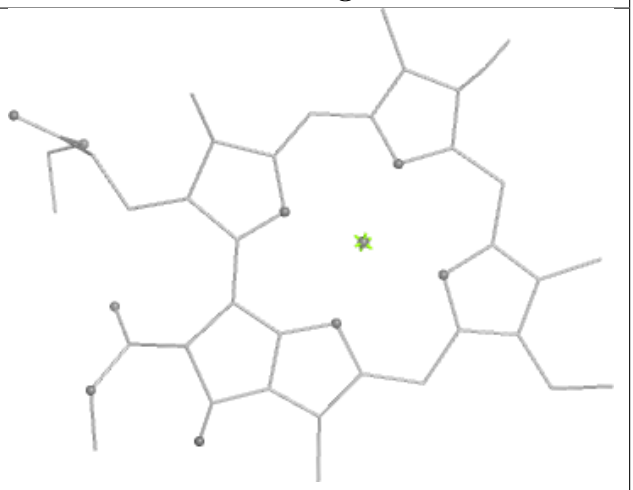
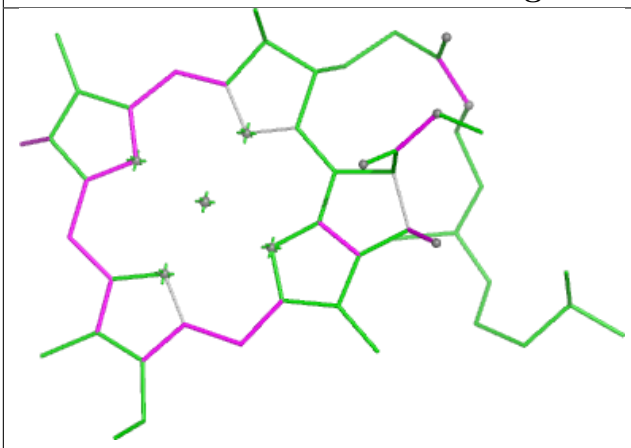


Rings

Ligand CLA B 808



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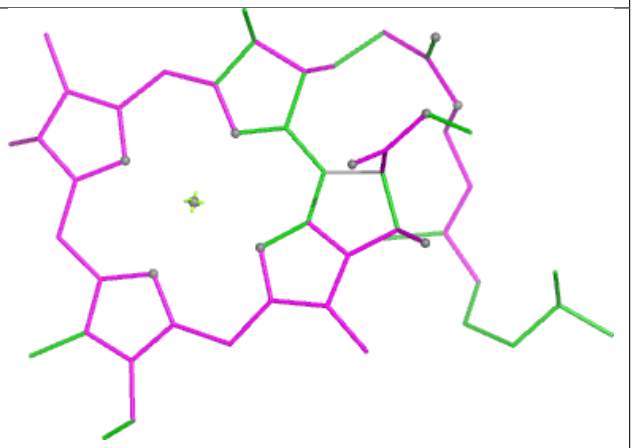

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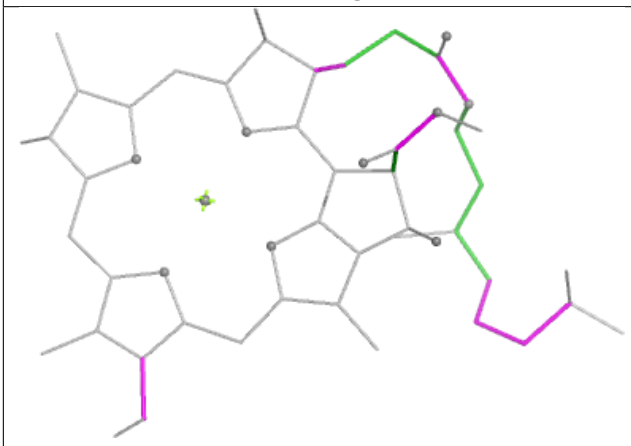

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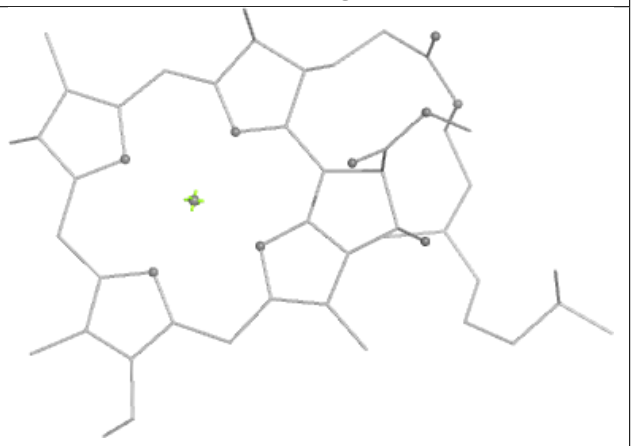
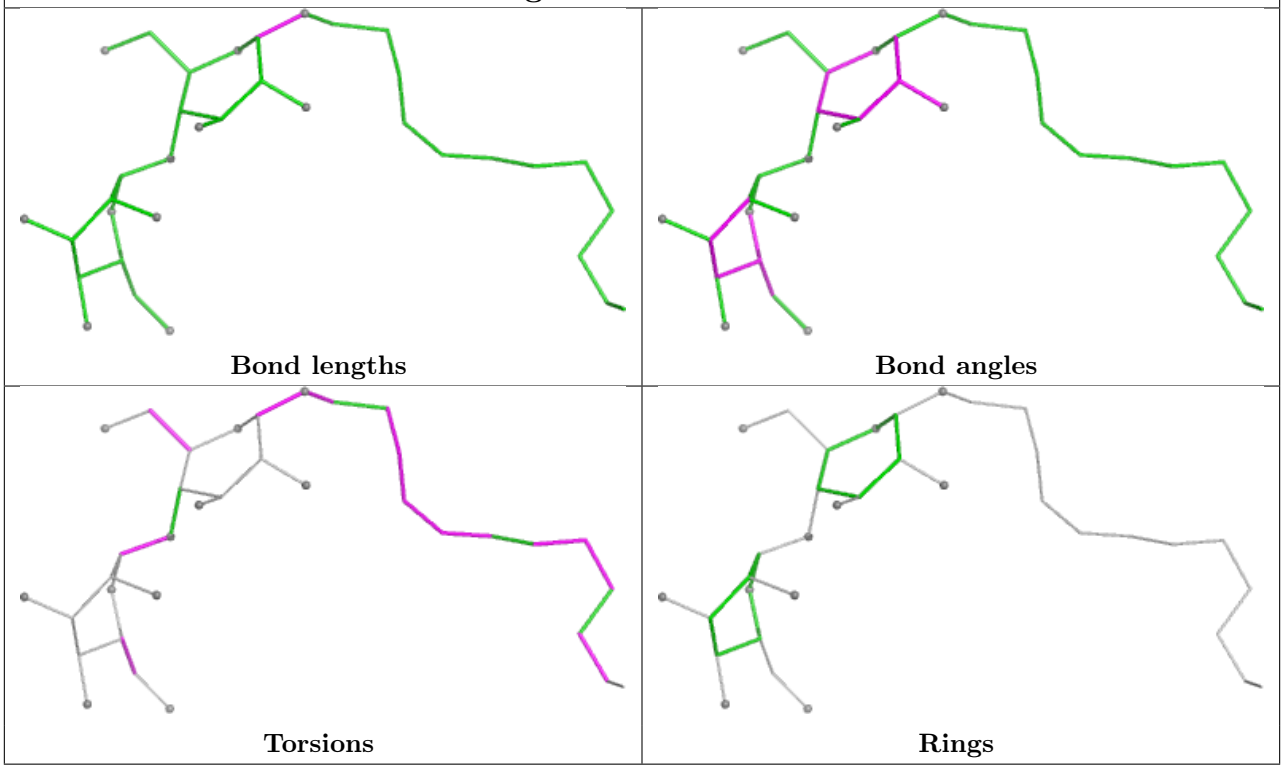


Rings

Ligand LMU 4 321



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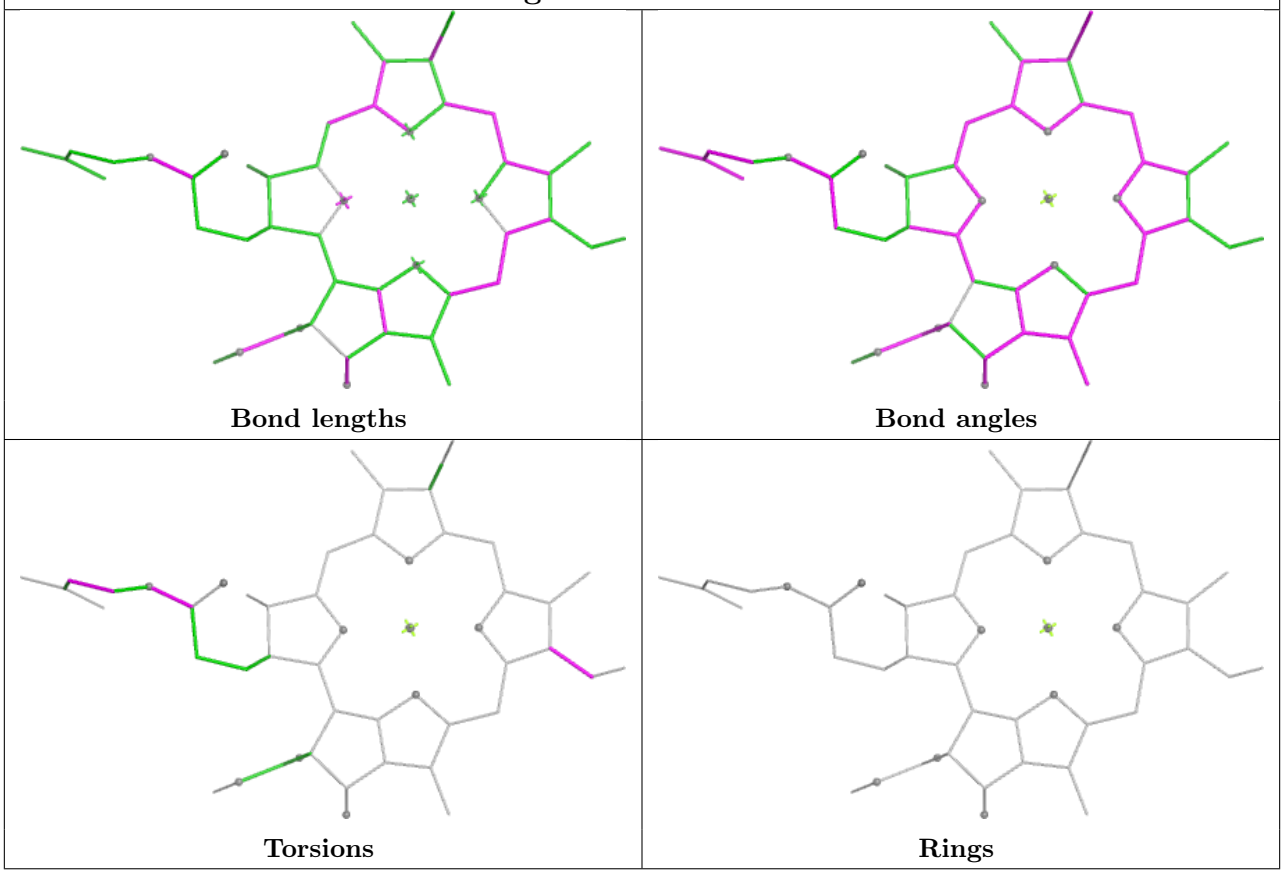

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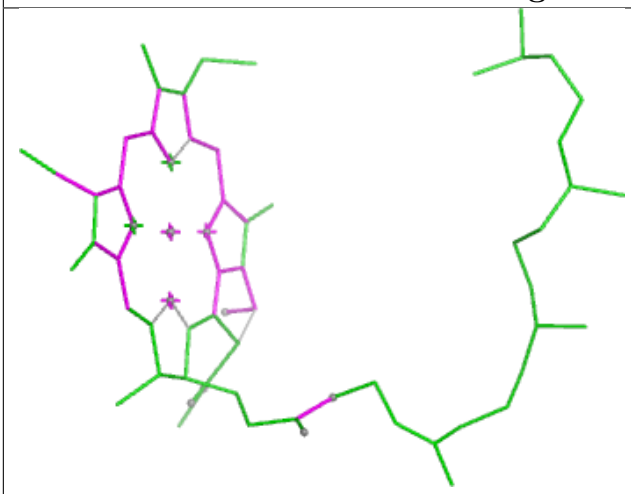

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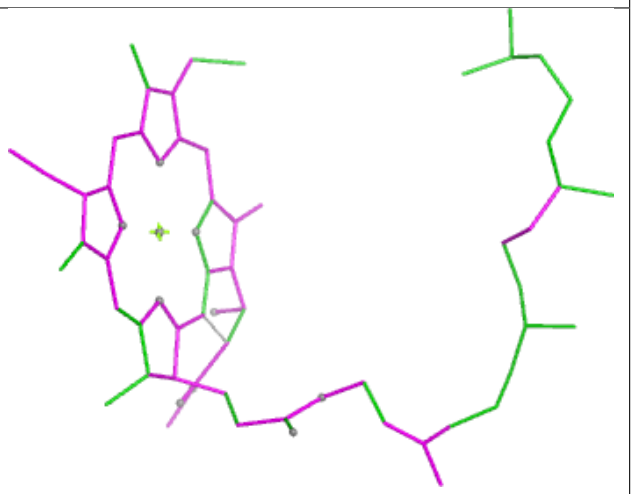
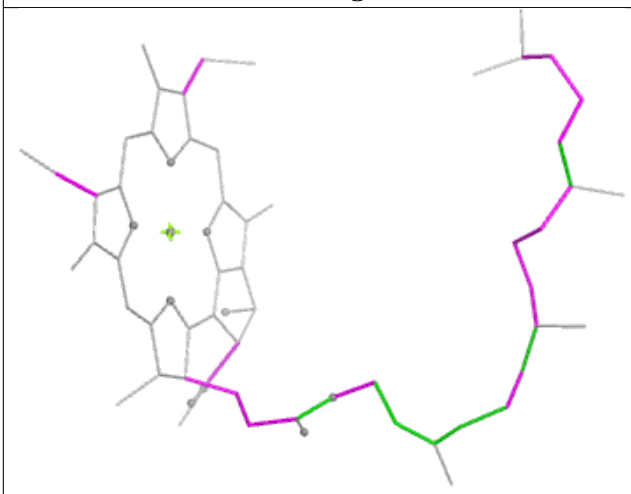


Bond angles



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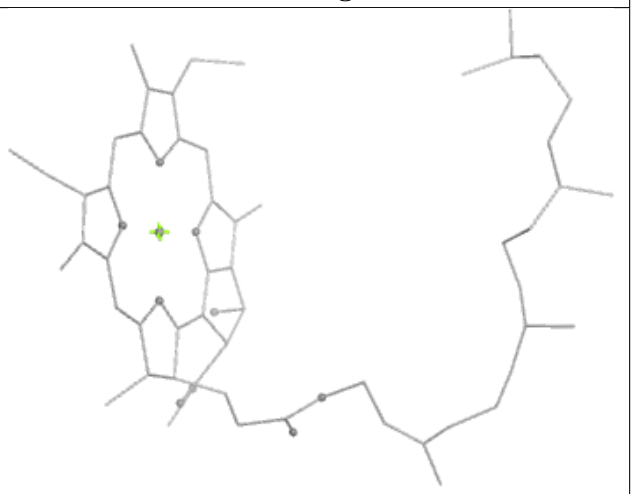
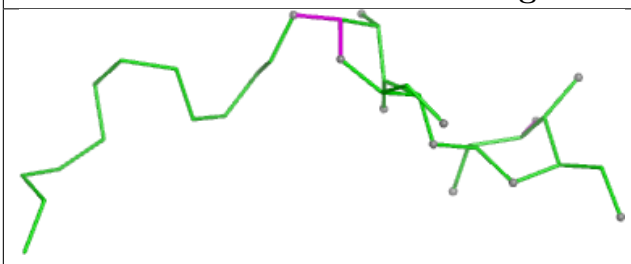


Rings

Ligand LMU H 102



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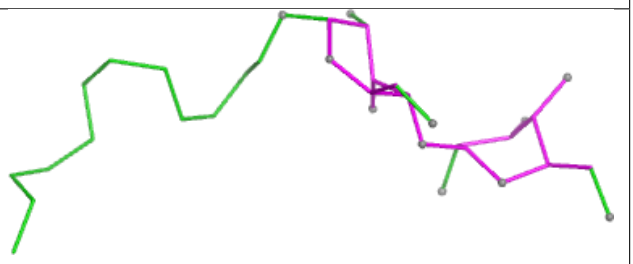
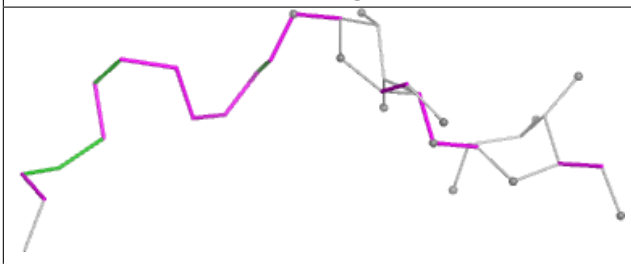


Bond angles



Torsions



Rings

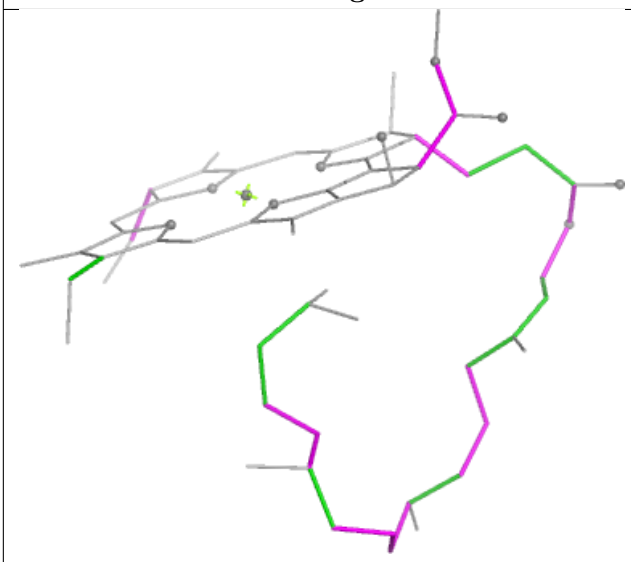
Ligand CLA 2 312



Bond lengths



Bond angles

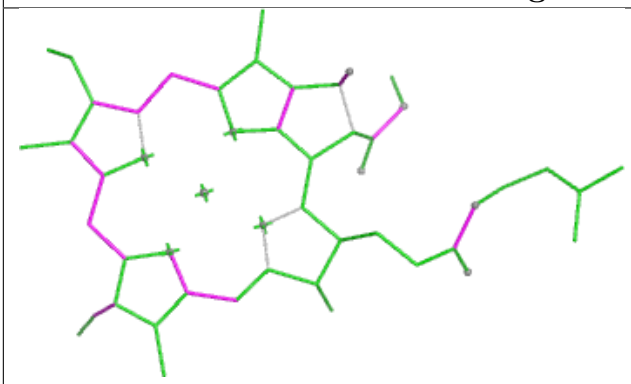


Torsions



Rings

Ligand CLA 4 306



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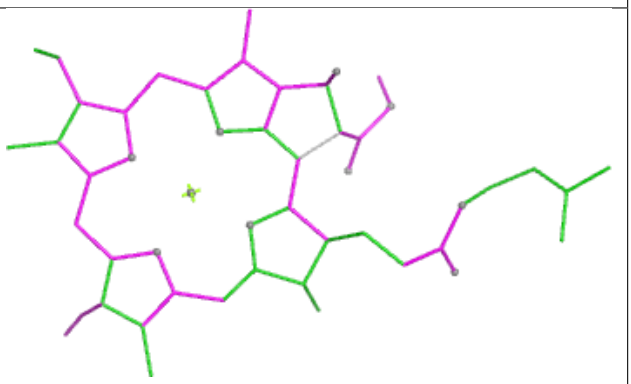
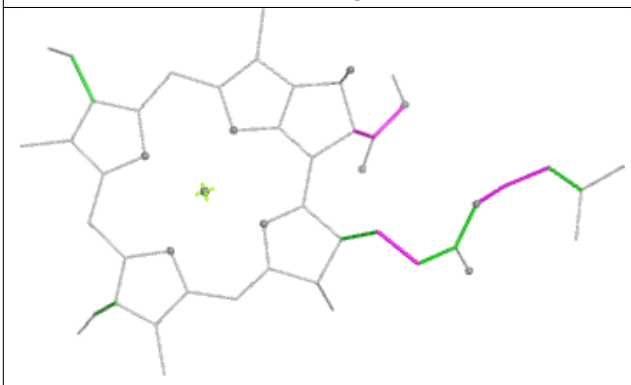


Bond angles



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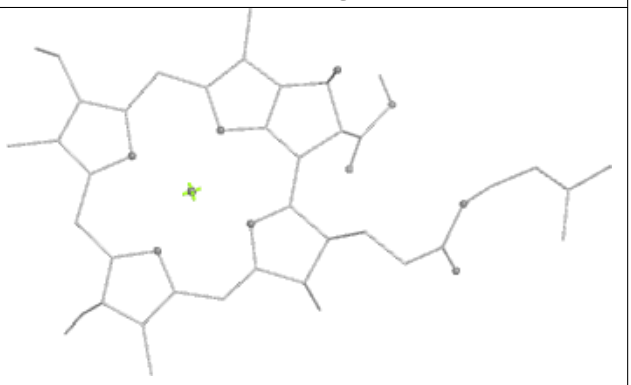
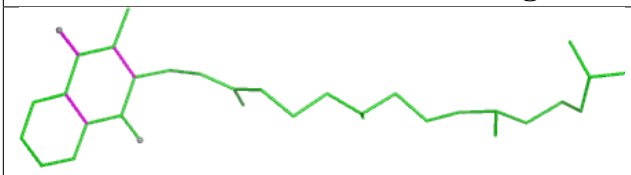


Rings

Ligand PQN A 839



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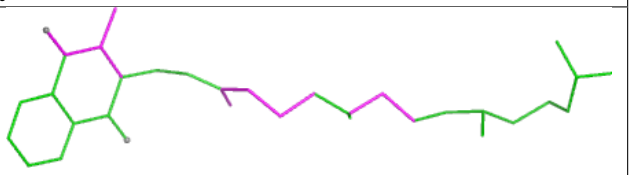
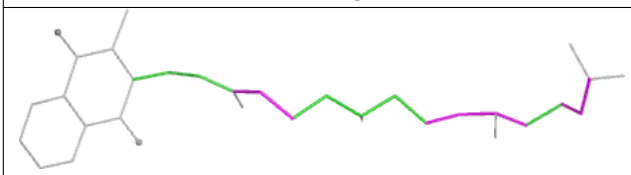


Bond angles



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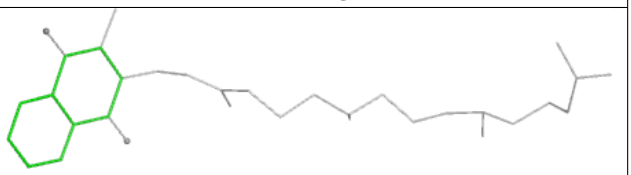

Rings

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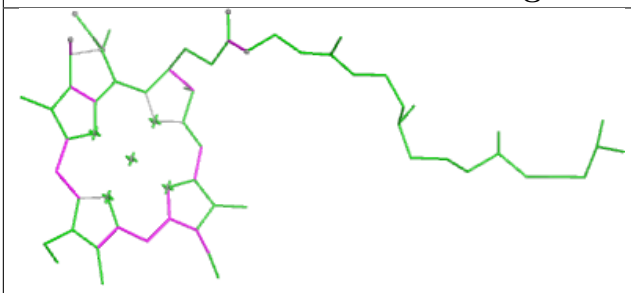

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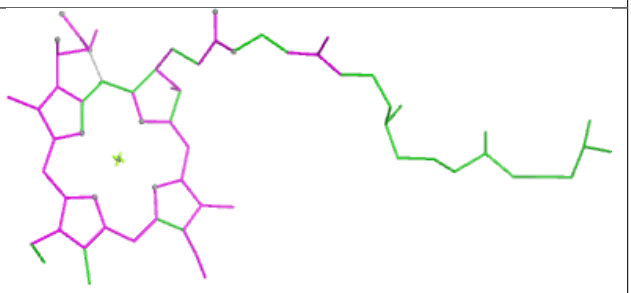
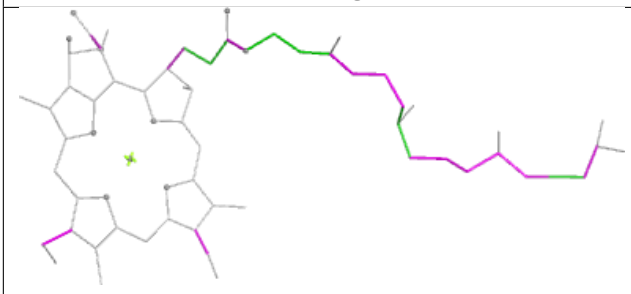


Bond angles



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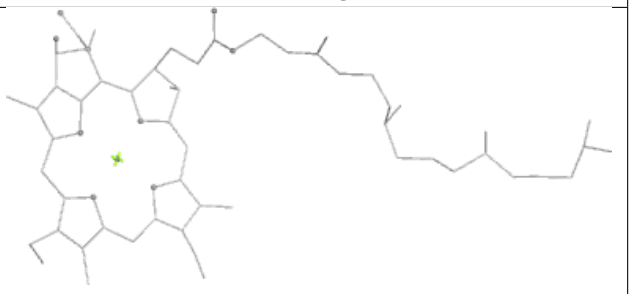
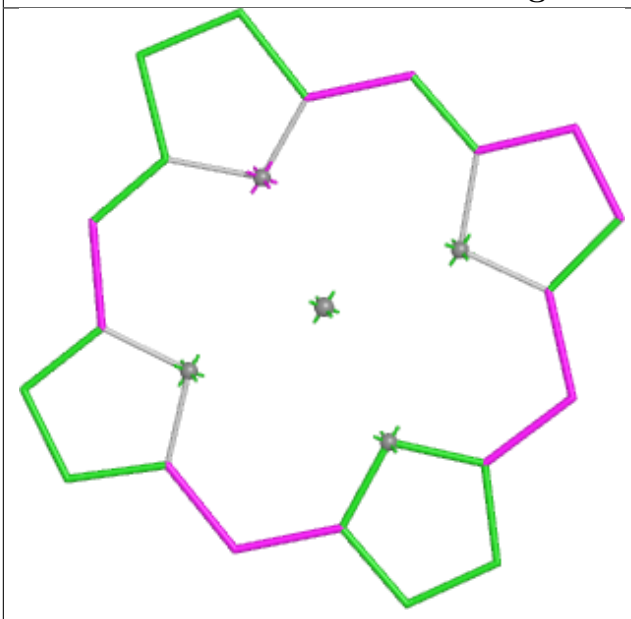


Rings

Ligand CLA 1 213



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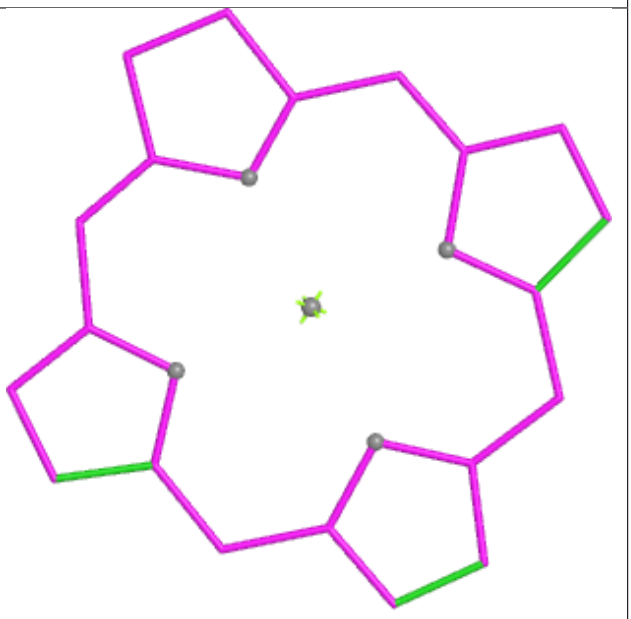
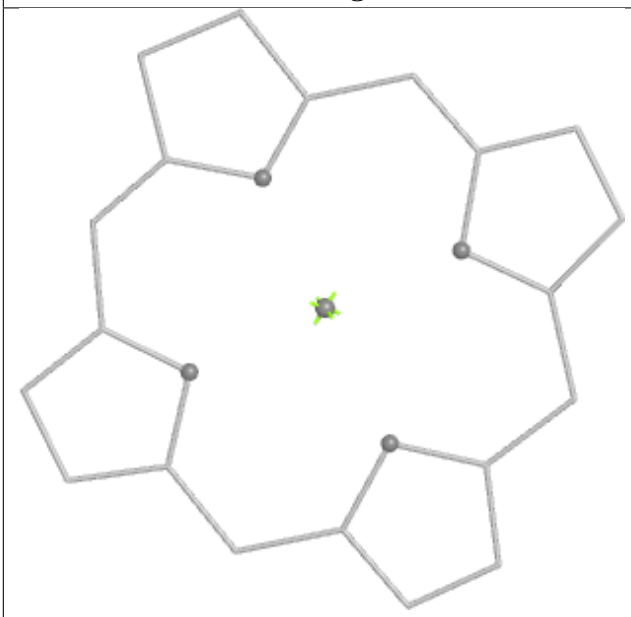


Bond angles



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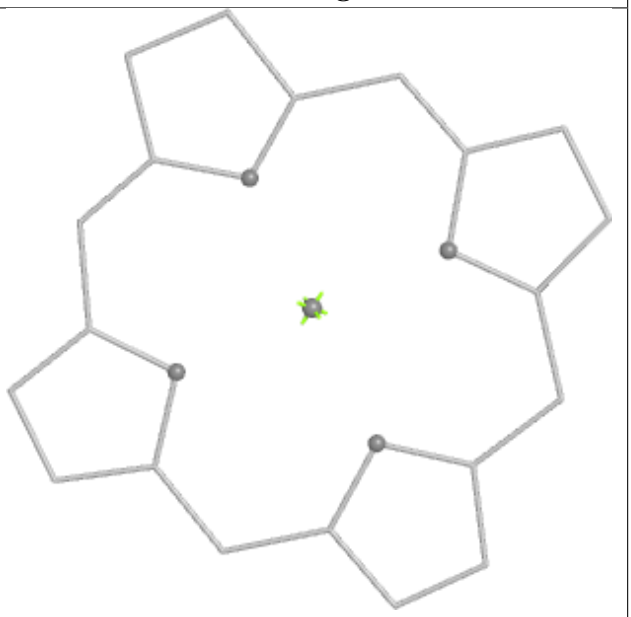
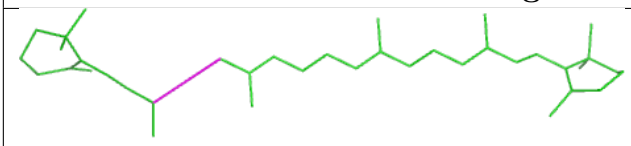


Rings

Ligand BCR B 844



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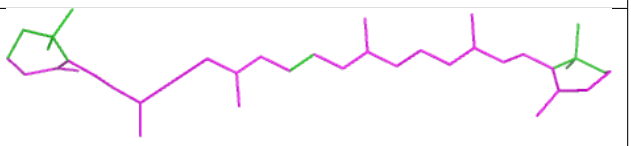
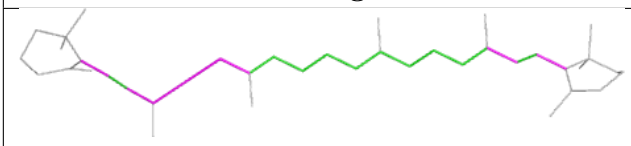


Bond angles



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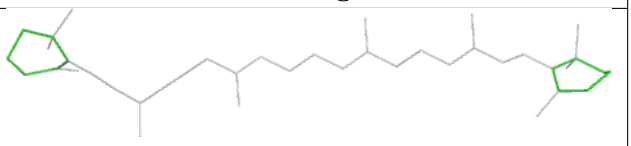
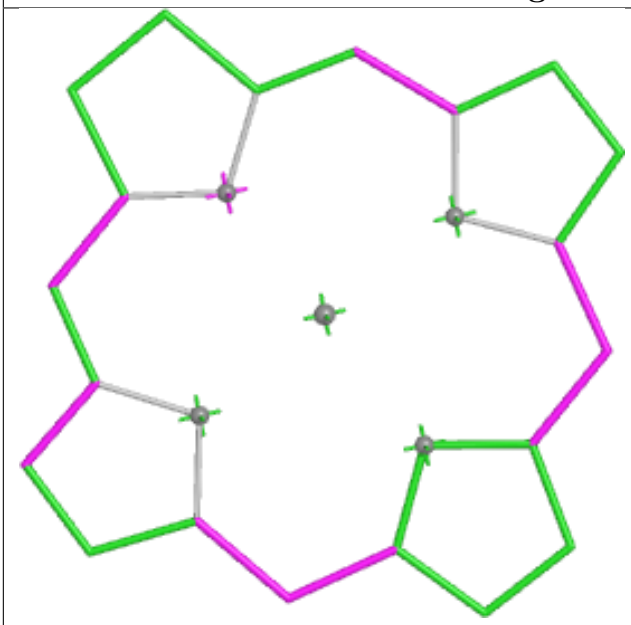


Rings

Ligand CLA 4 312



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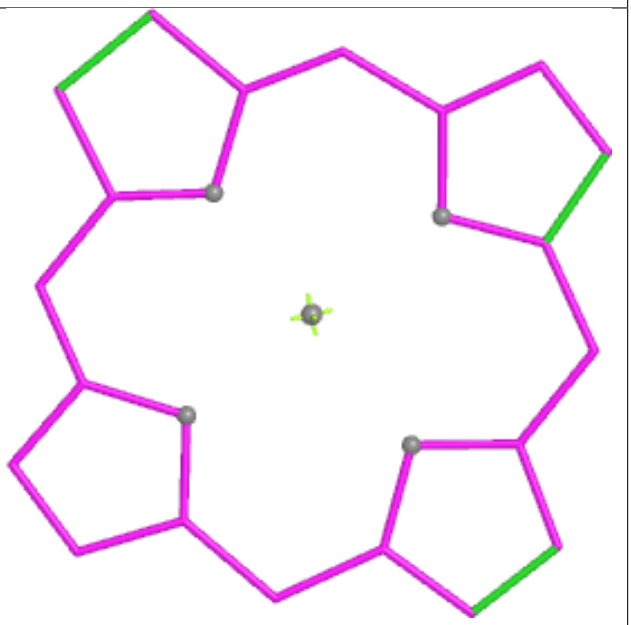
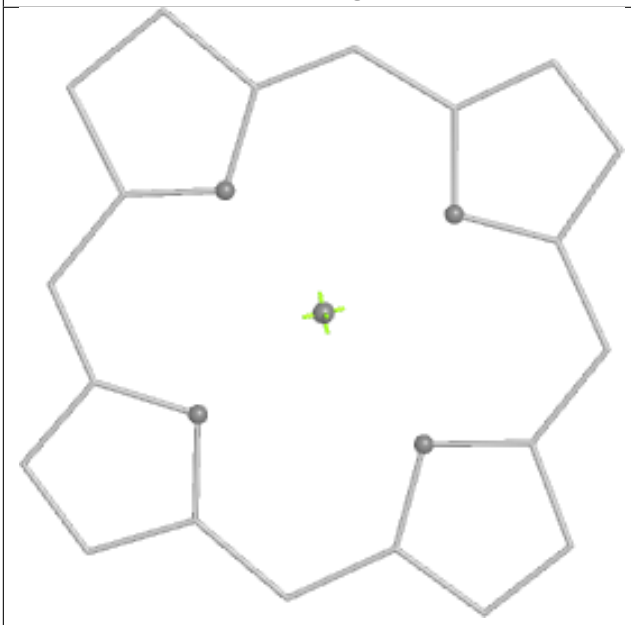


Bond angles



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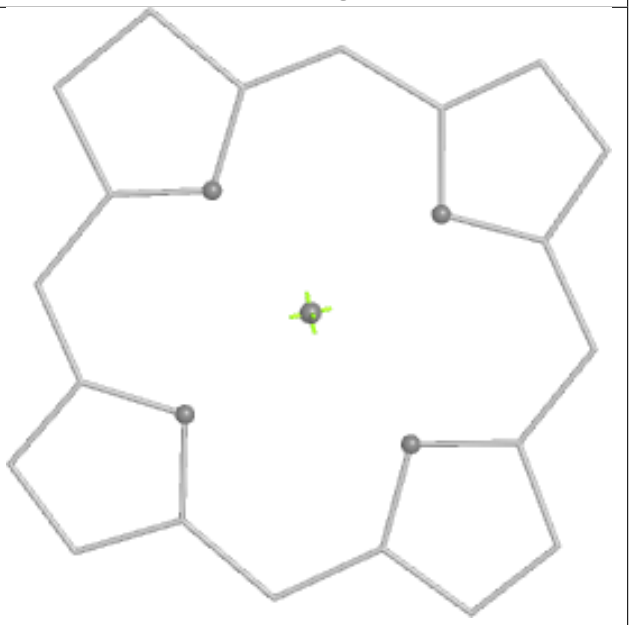
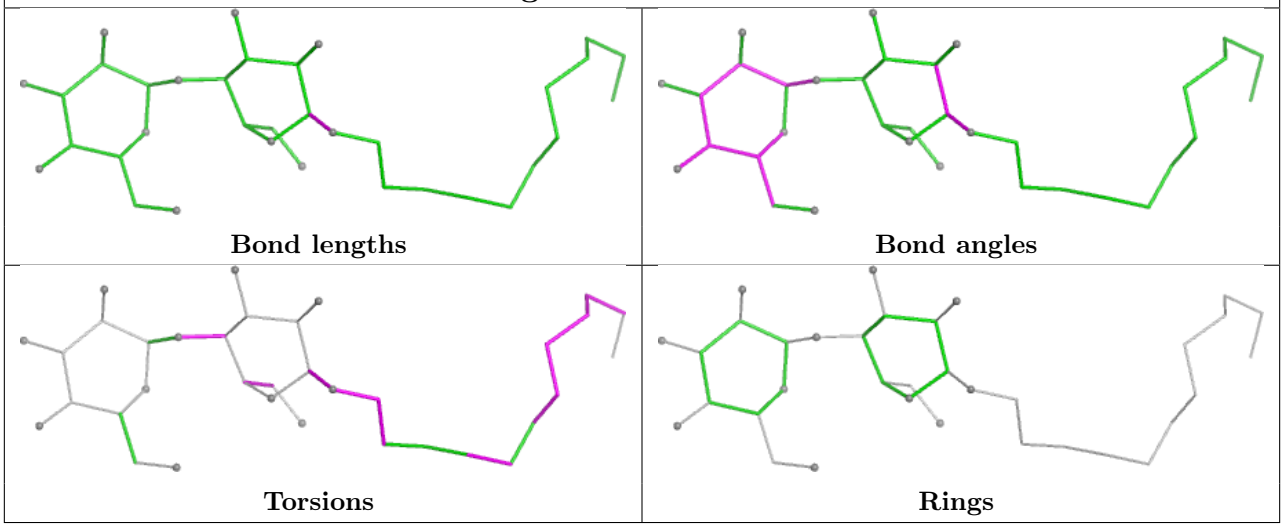
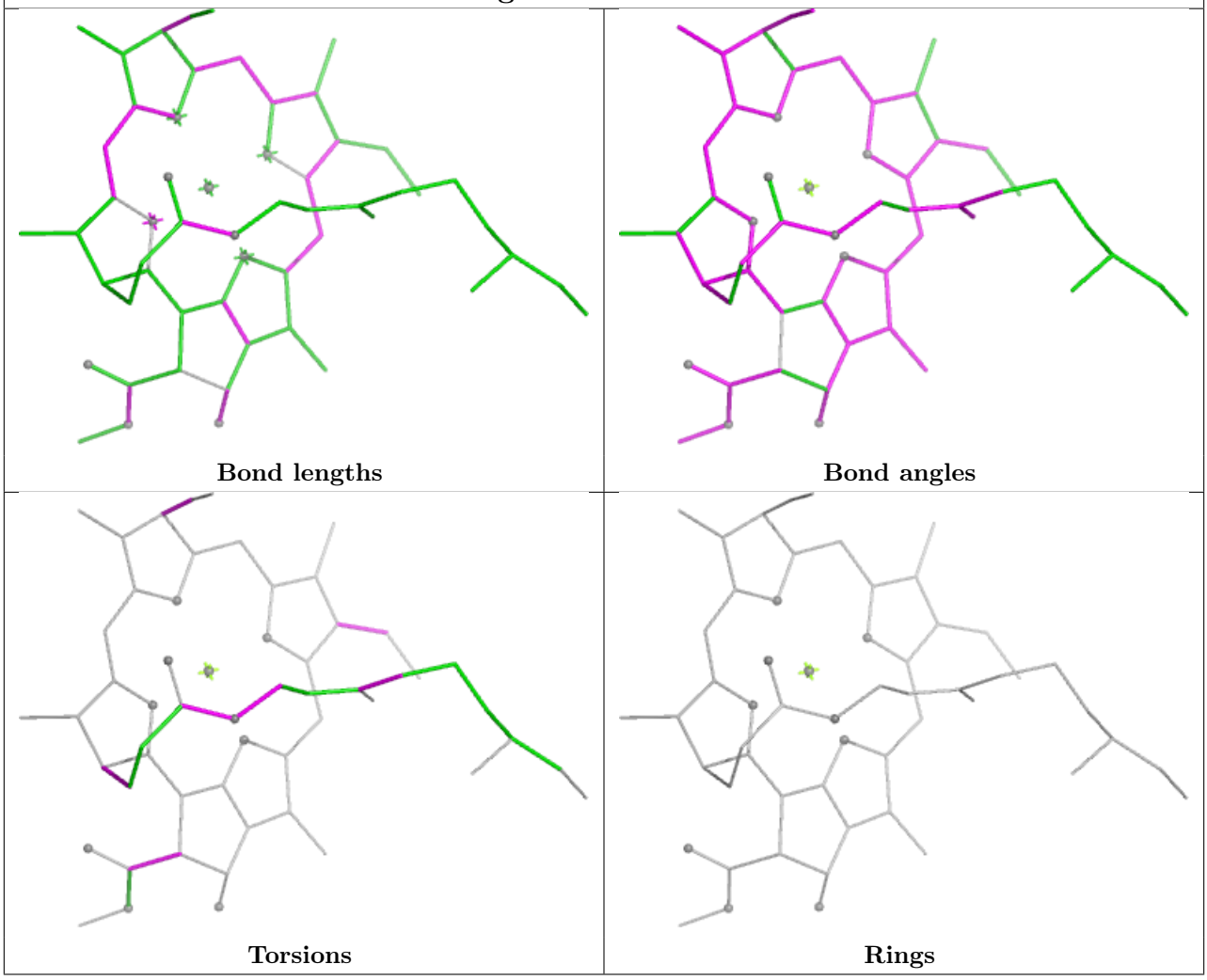


Rings

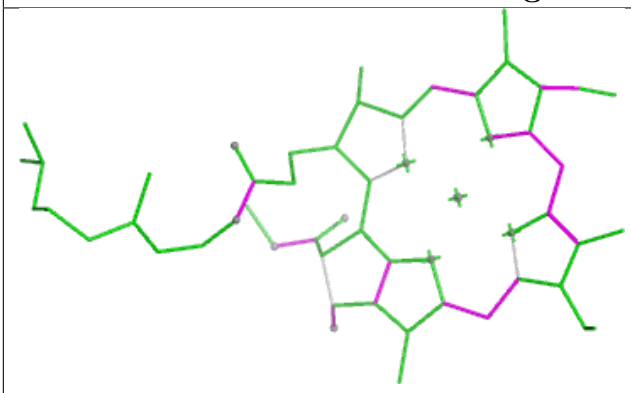
Ligand LMU C 101



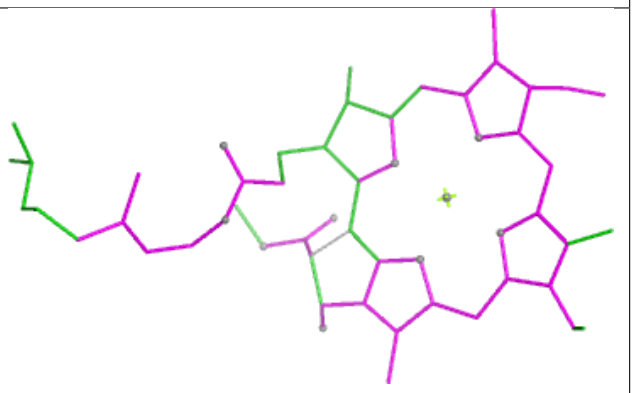
Ligand CLA 2 302



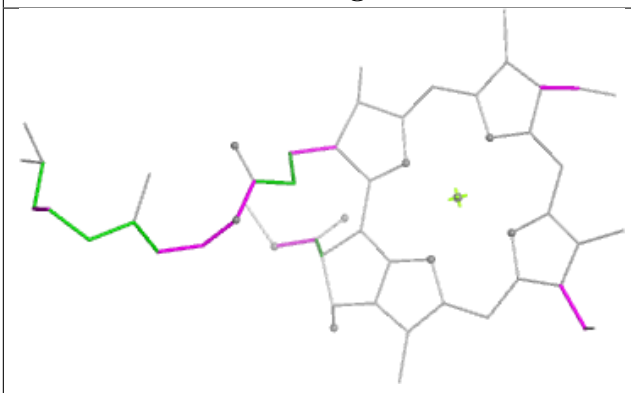
Ligand CLA A 807



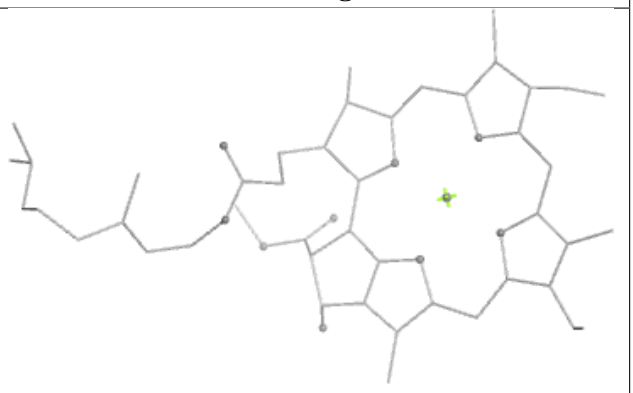
Bond lengths



Bond angles

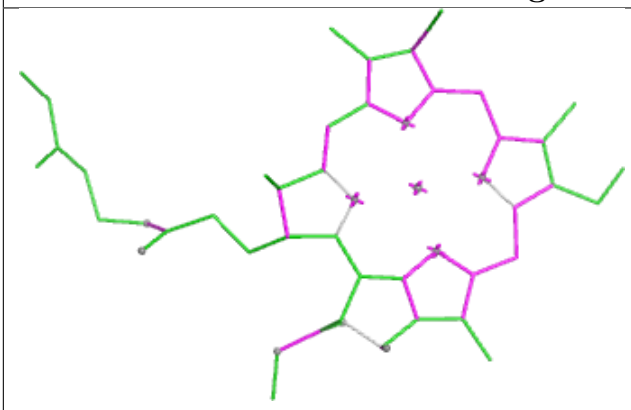


Torsions

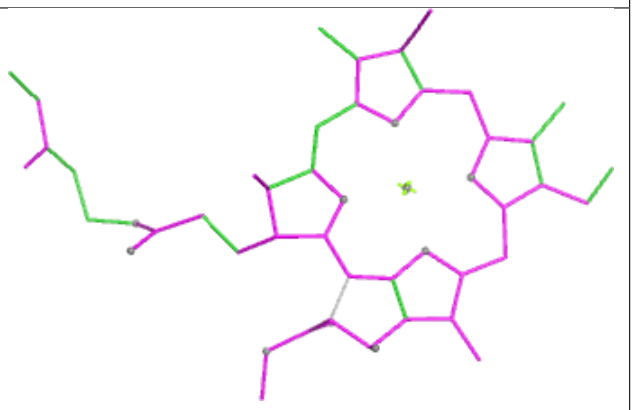


Rings

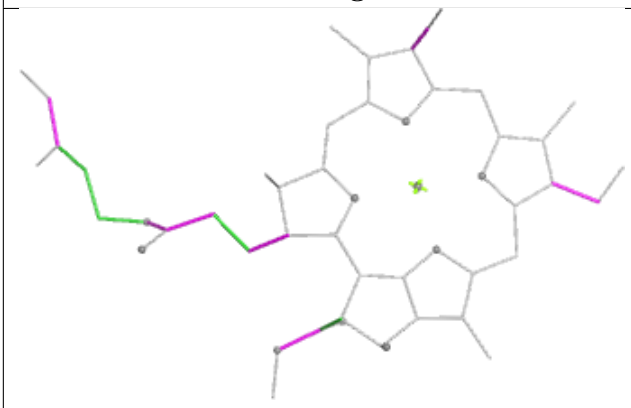
Ligand CLA 1 214



Bond lengths



Bond angles



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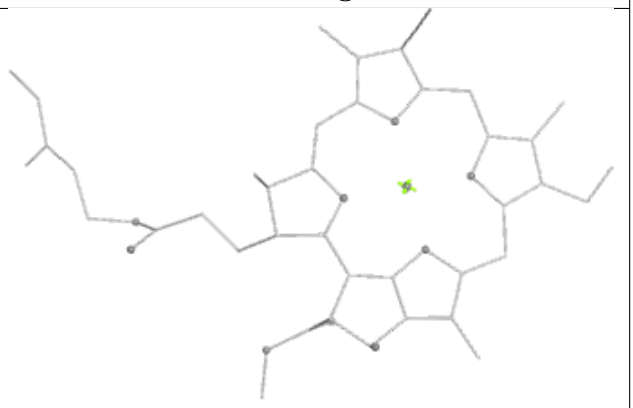
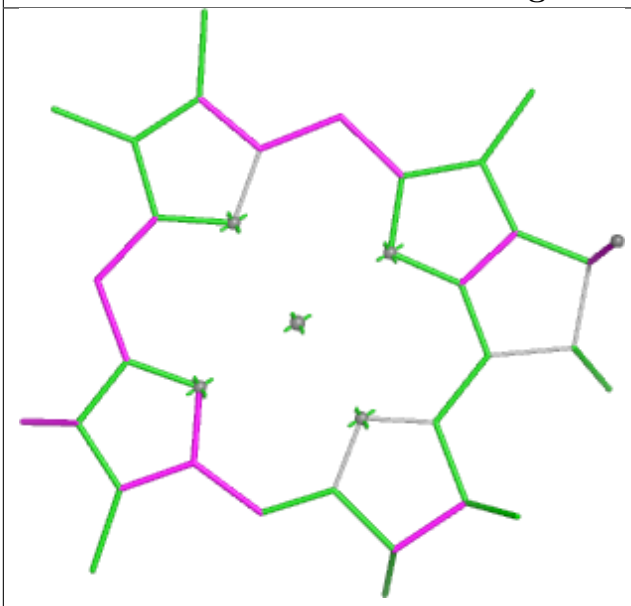


Rings

Ligand CLA 1 205



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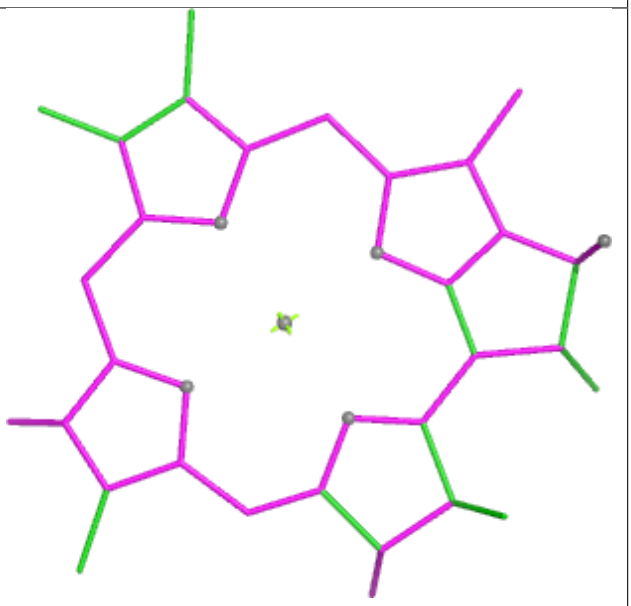
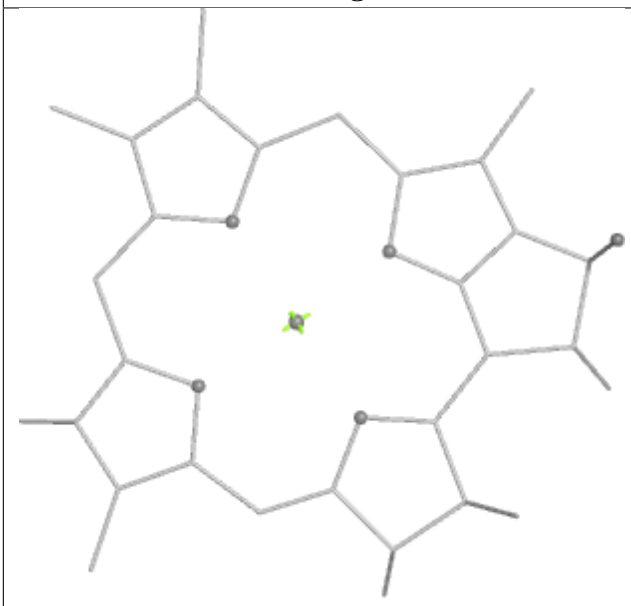


Bond angles



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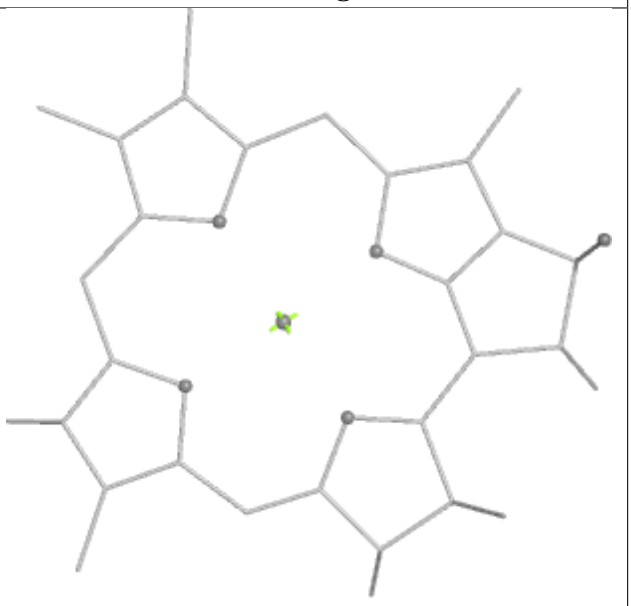
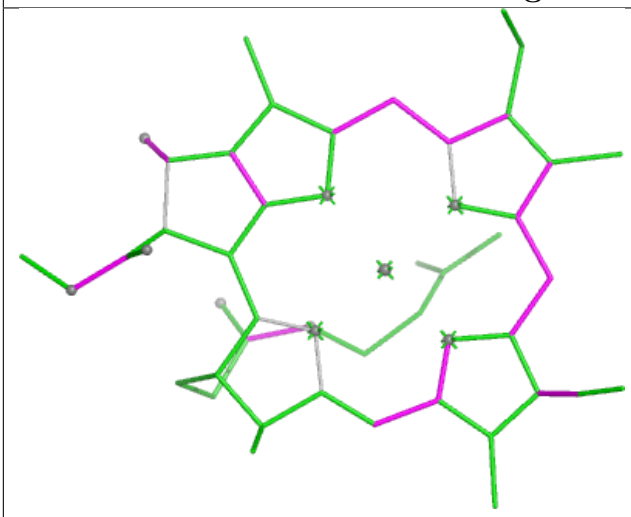


Rings

Ligand CLA B 817



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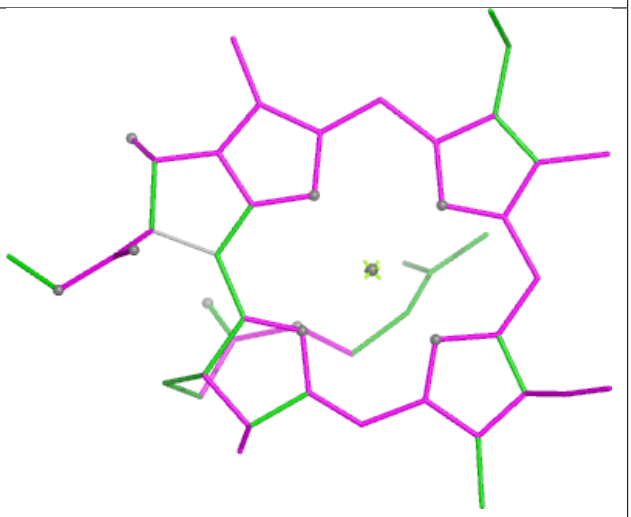
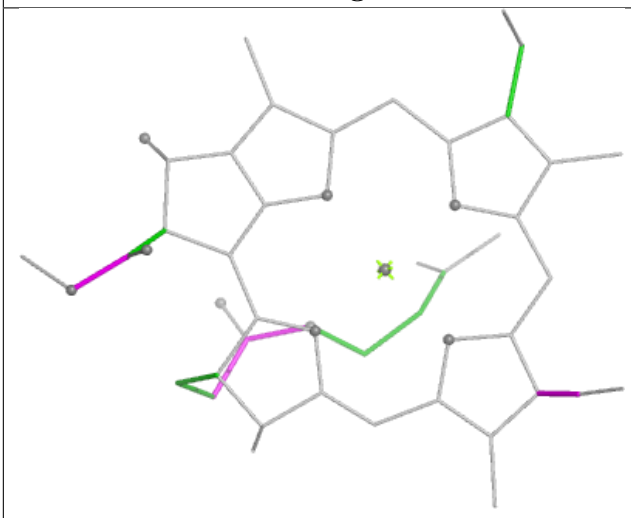


Bond angles



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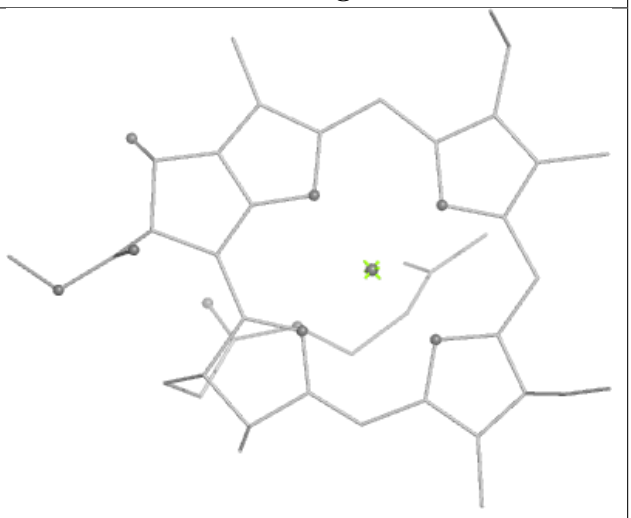
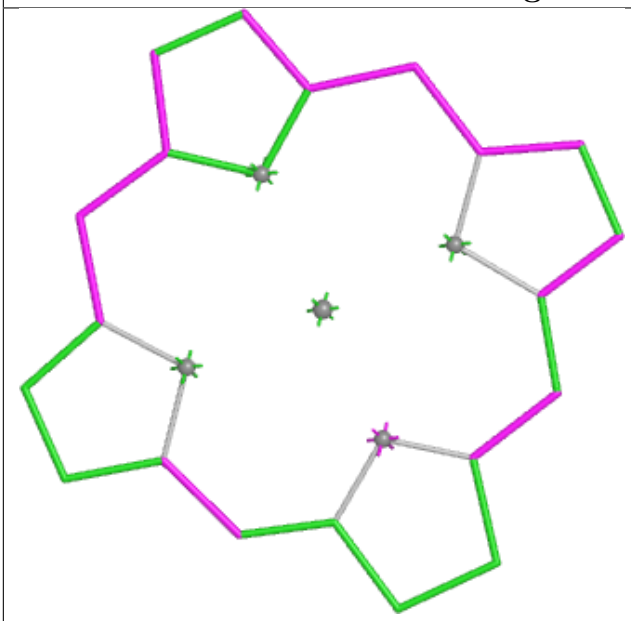


Rings

Ligand CLA A 857



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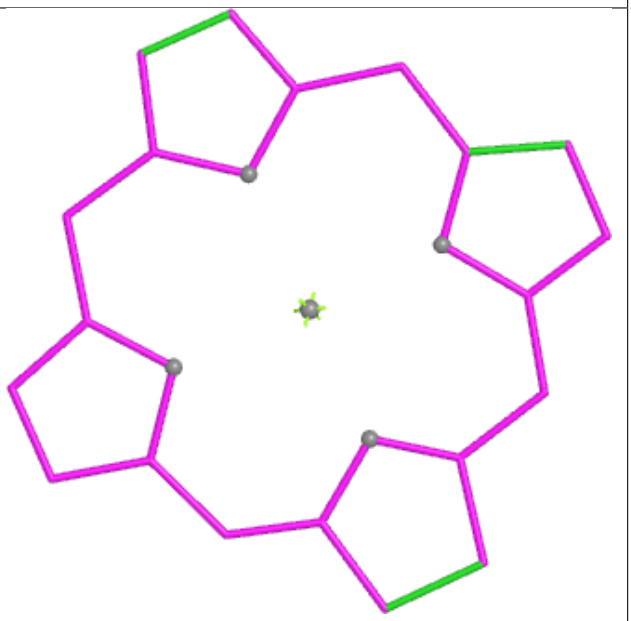

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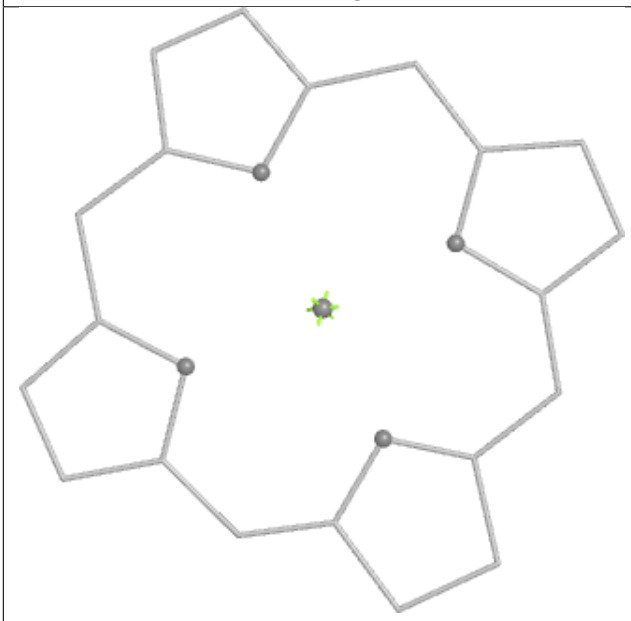

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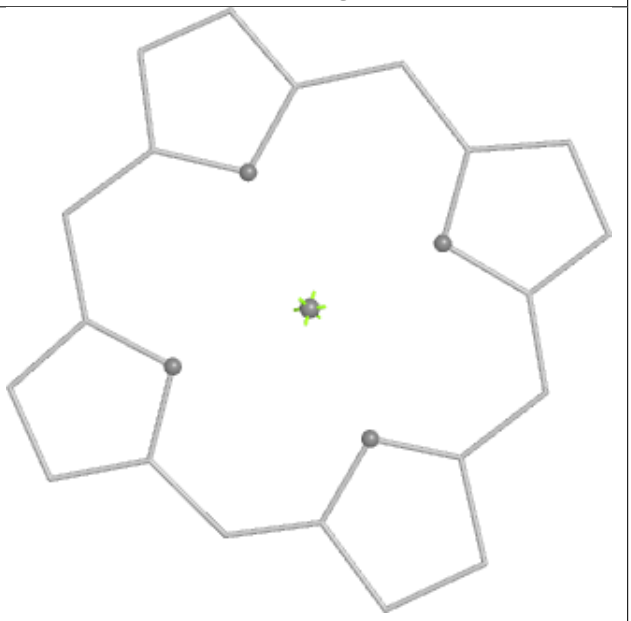
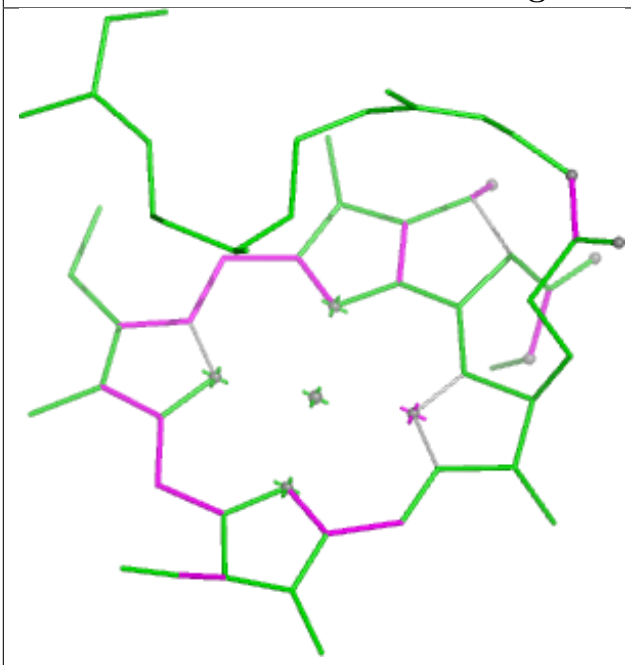


Rings

Ligand CLA 1 206



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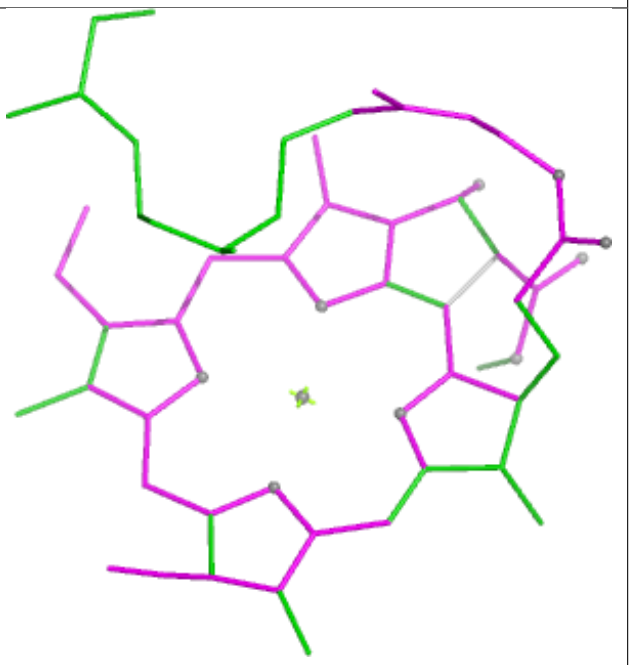
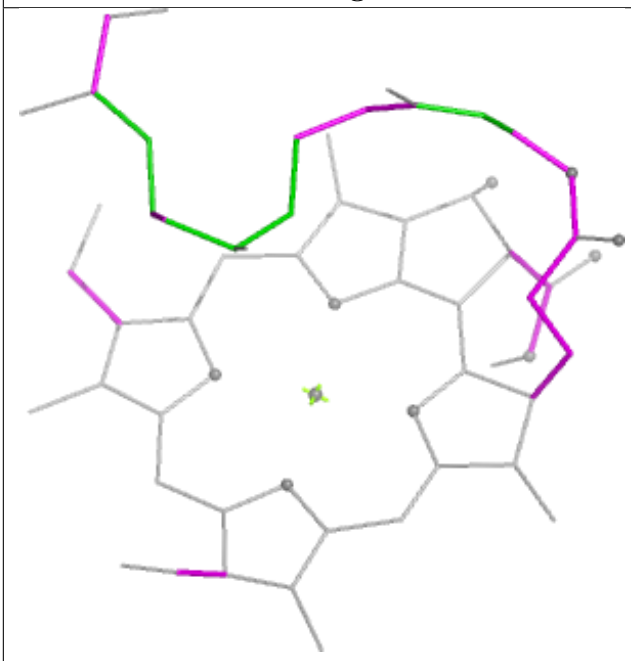


Bond angles



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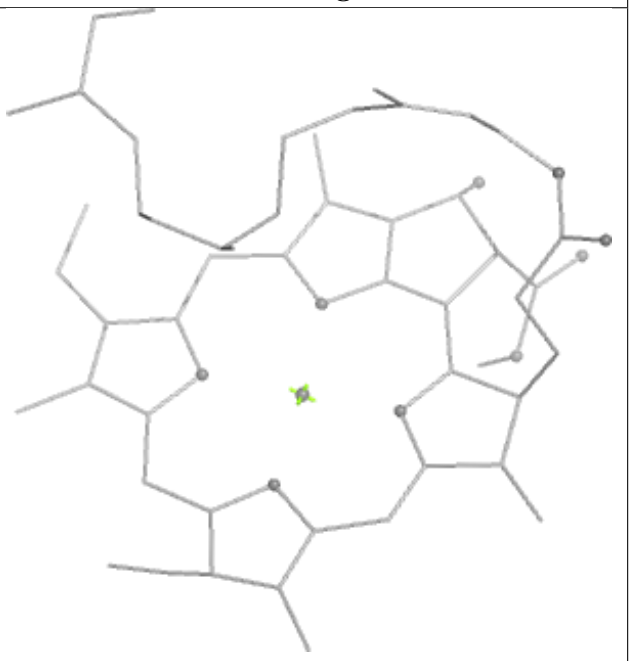
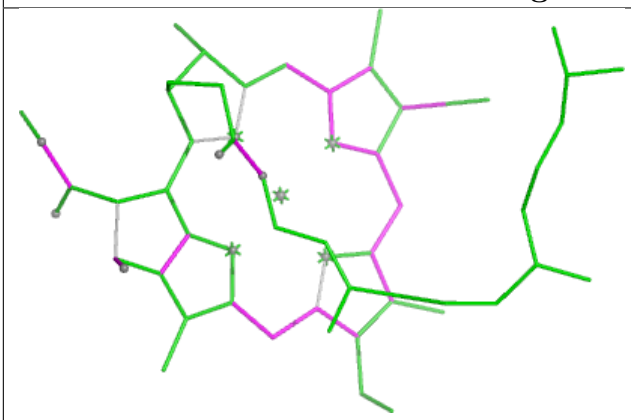


Rings

Ligand CLA I 102



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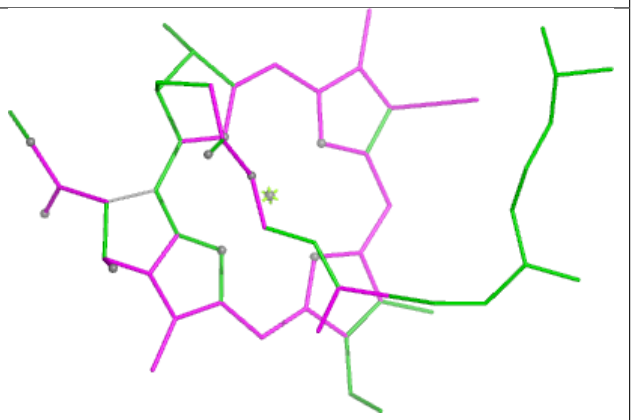
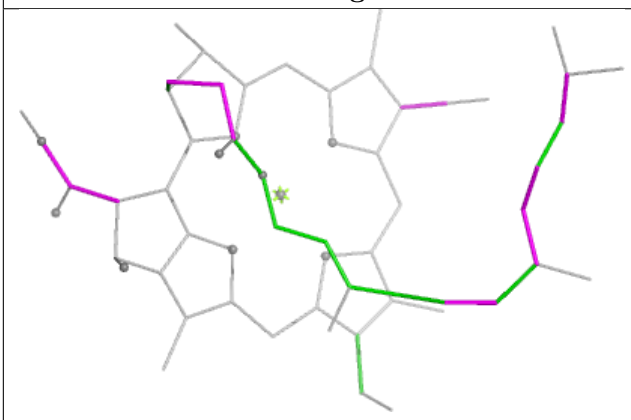


Bond angles



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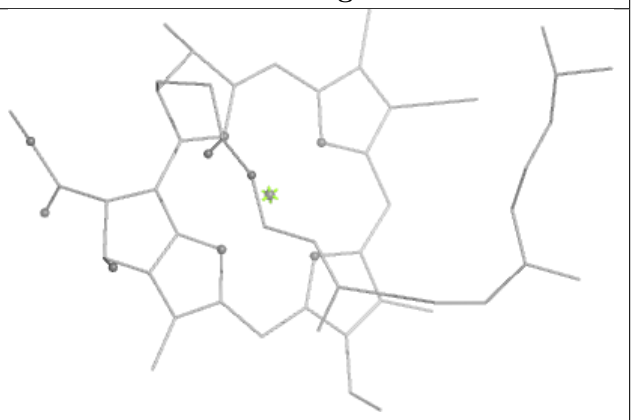
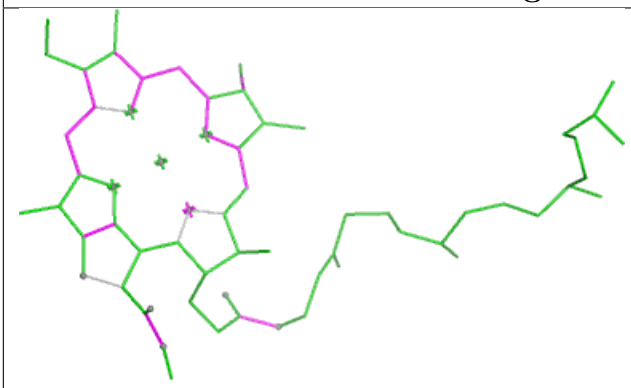


Rings

Ligand CLA A 849



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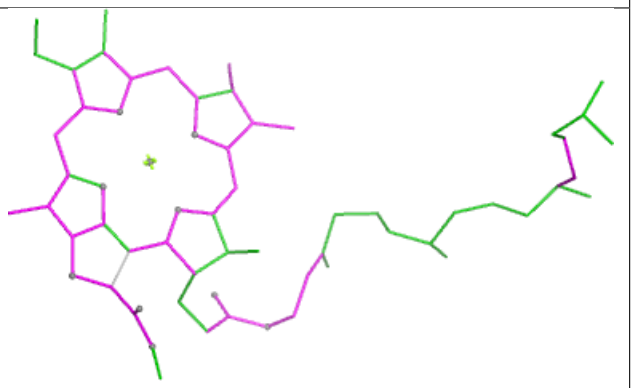

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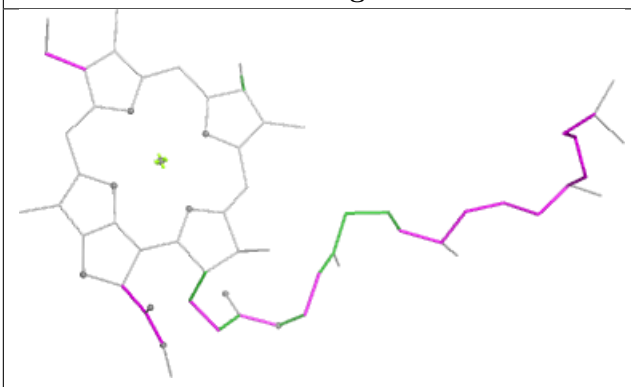

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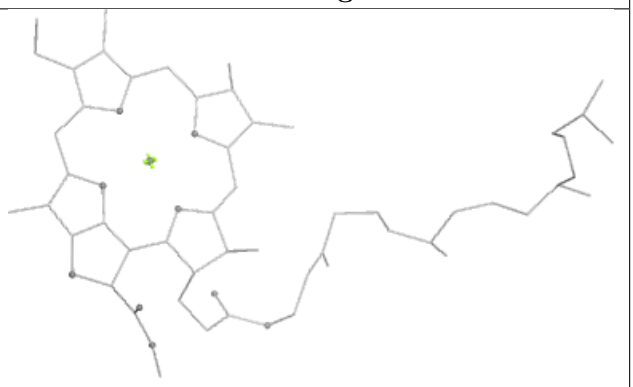
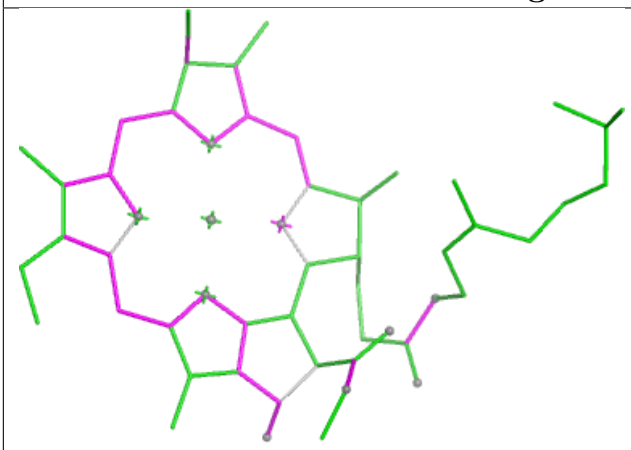


Rings

Ligand CLA J 103



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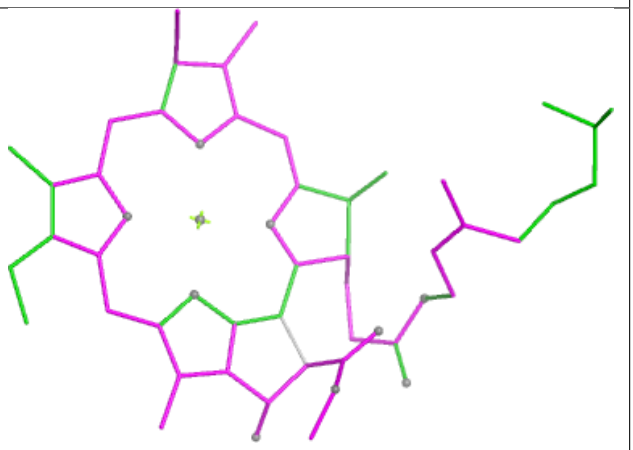

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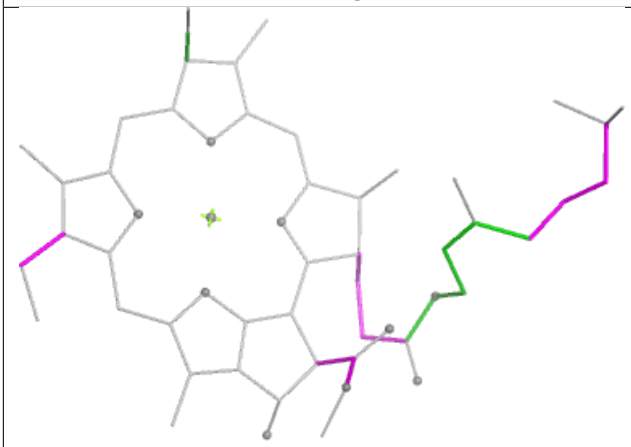

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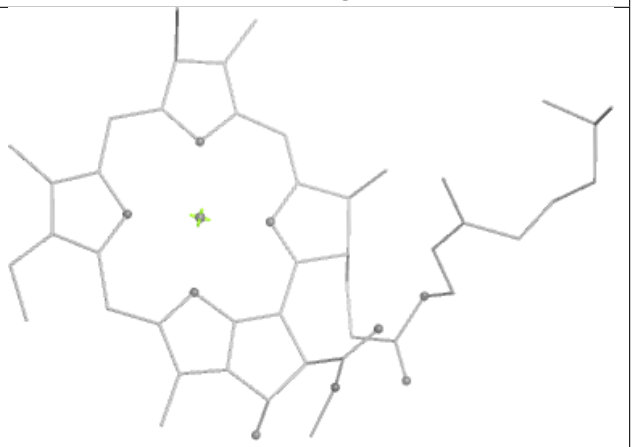
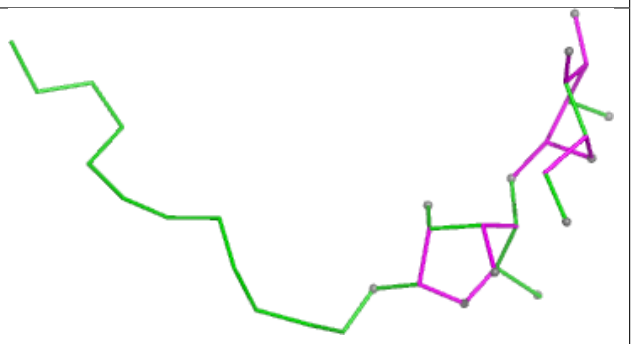


Rings

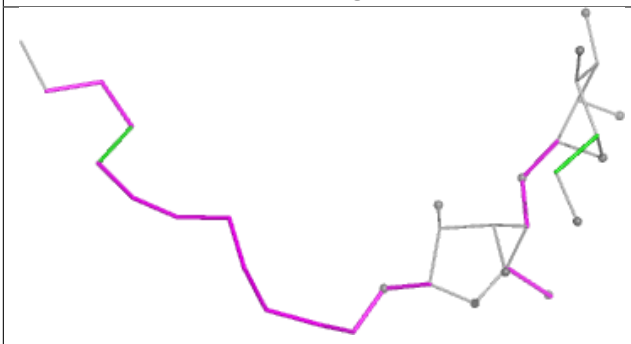
Ligand LMU G 101



Bond lengths



Bond angles



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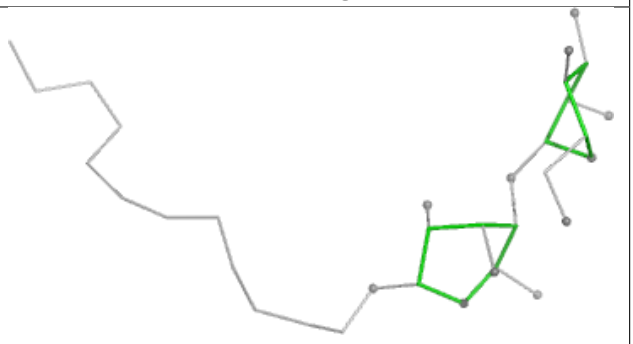
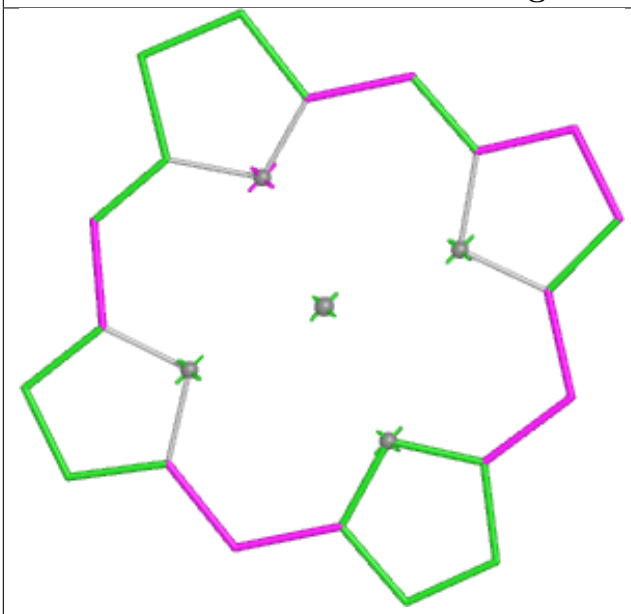


Rings

Ligand CLA 4 308



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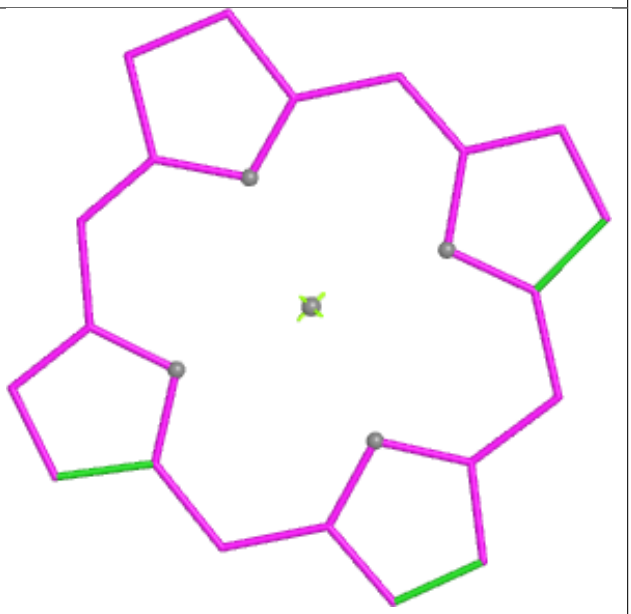
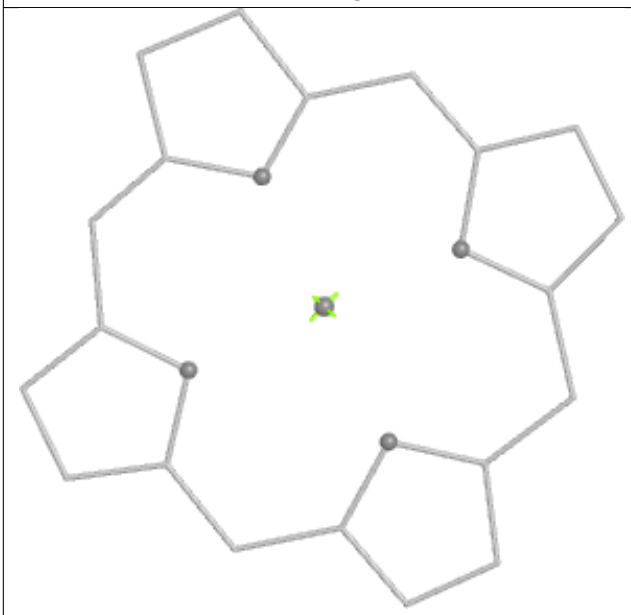


Bond angles



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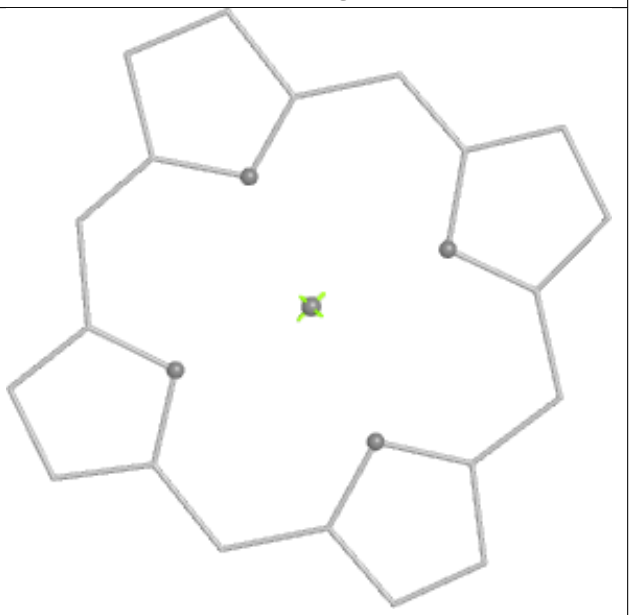
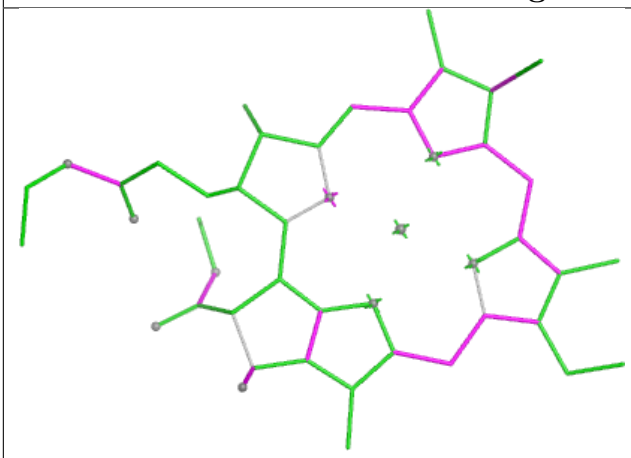


Rings

Ligand CLA 4 319



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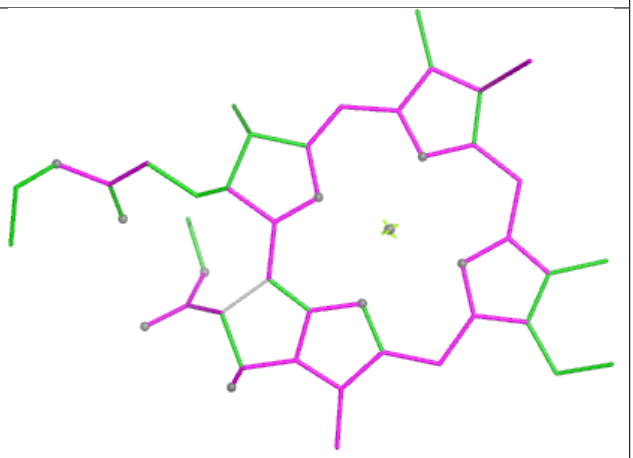
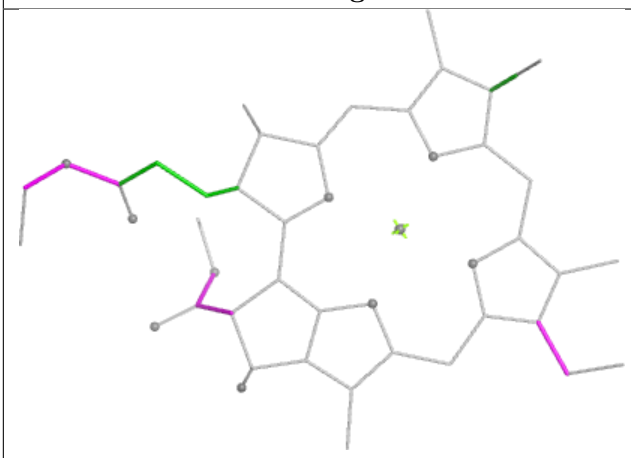


Bond angles



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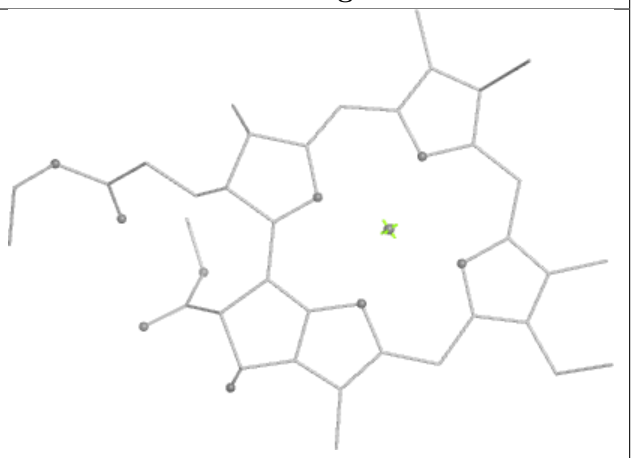
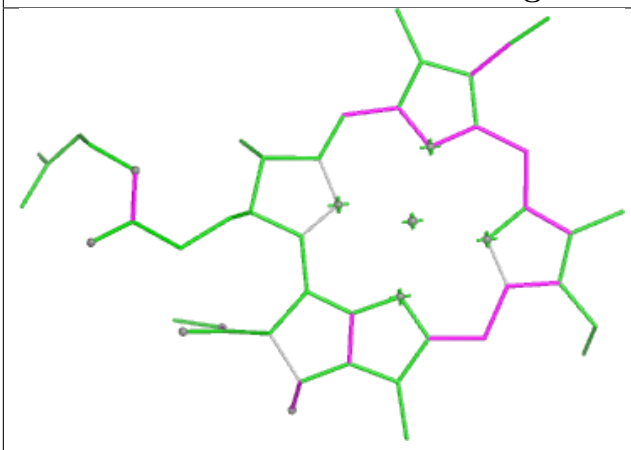


Rings

Ligand CLA A 801



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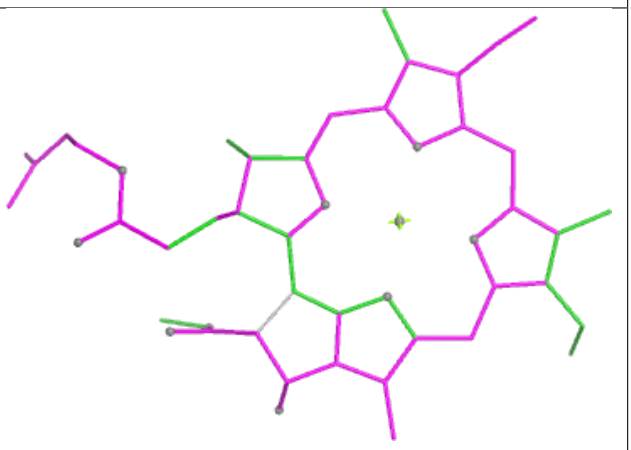

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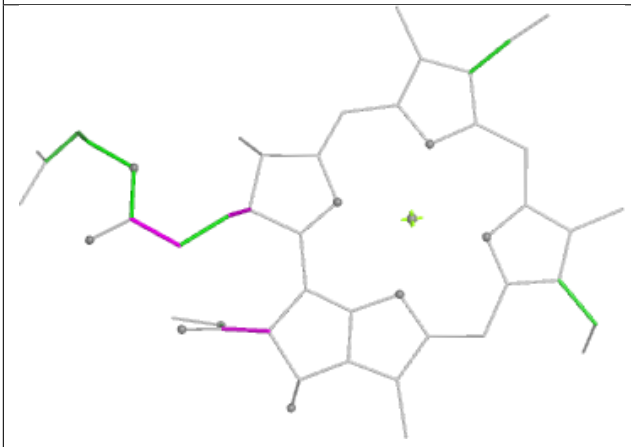

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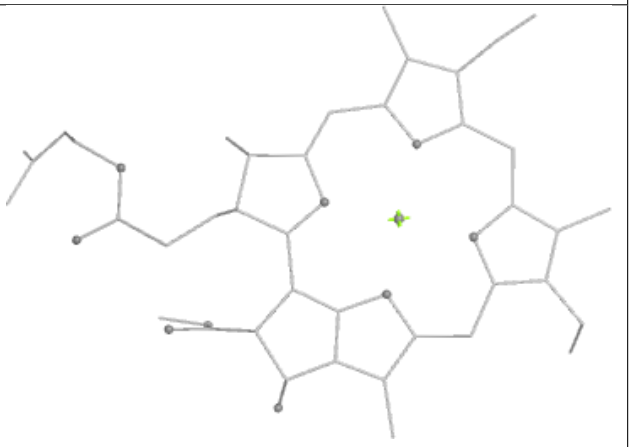
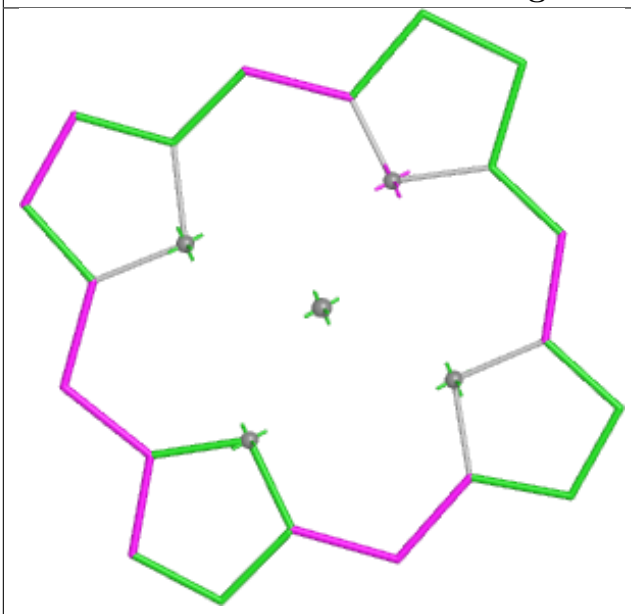


Rings

Ligand CLA 3 305



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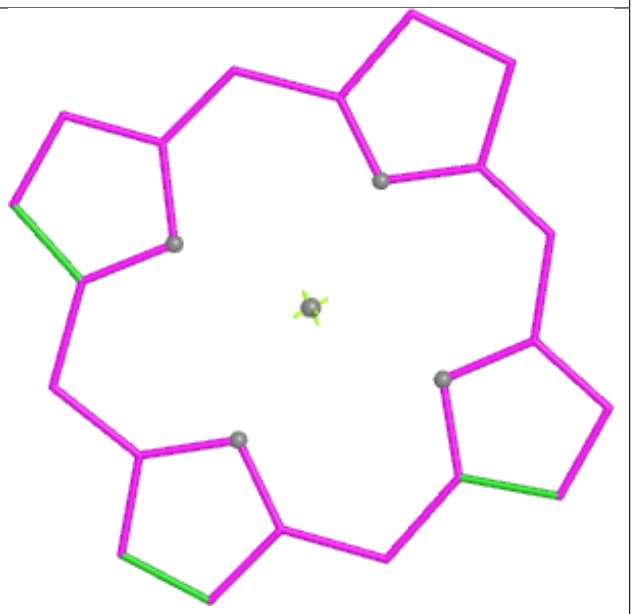
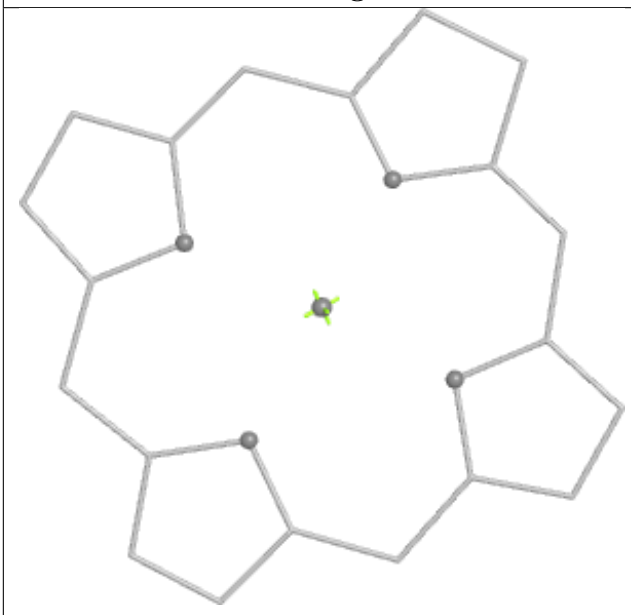


Bond angles



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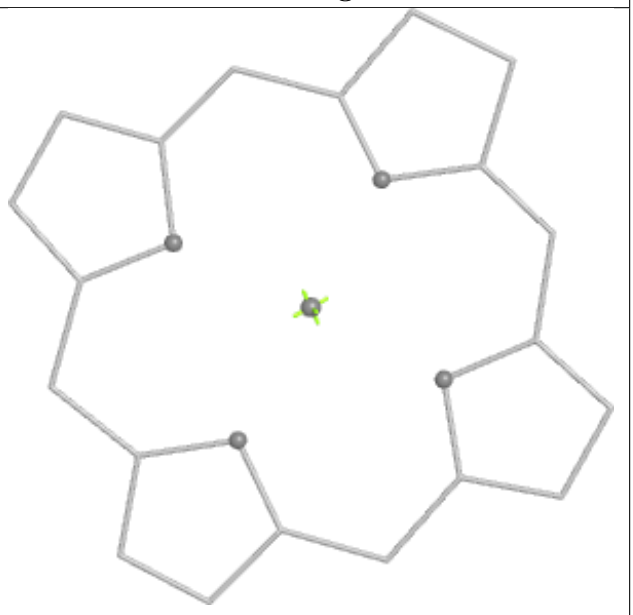
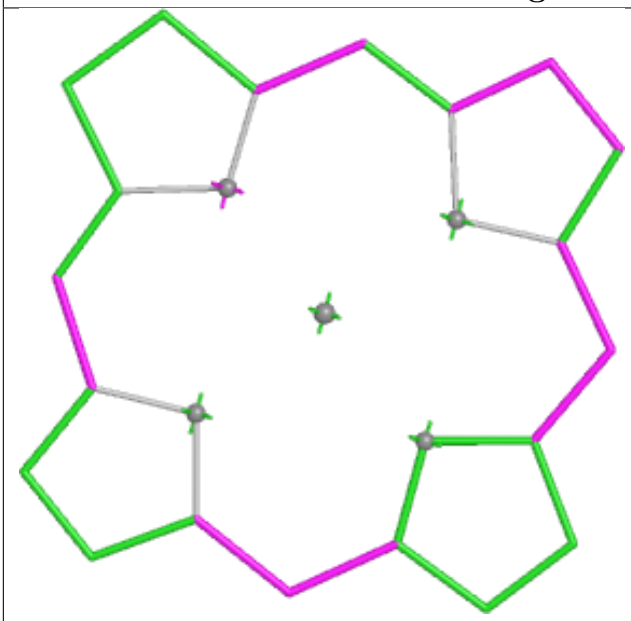


Rings

Ligand CLA 1 208



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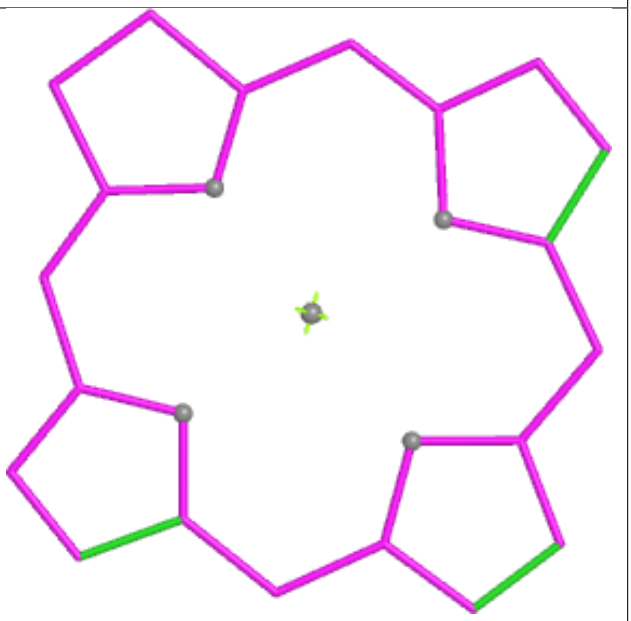
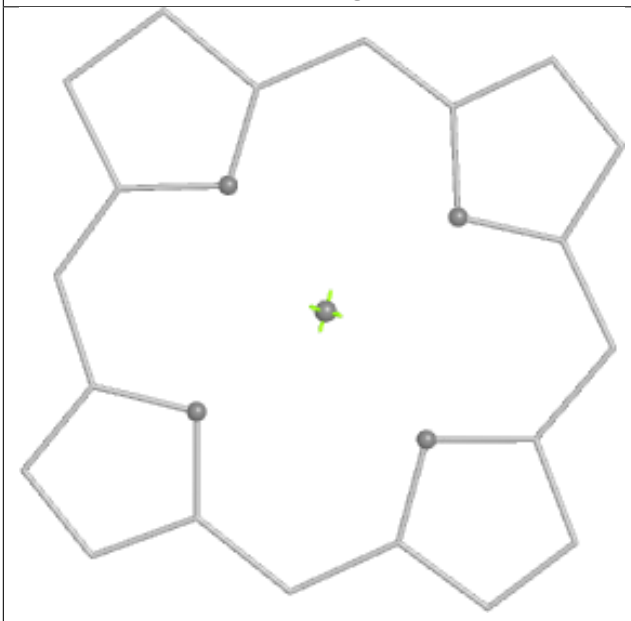


Bond angles



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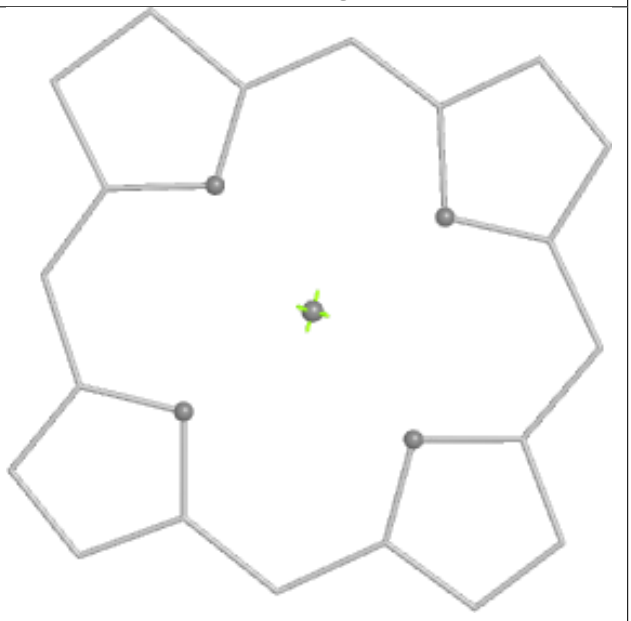


Rings

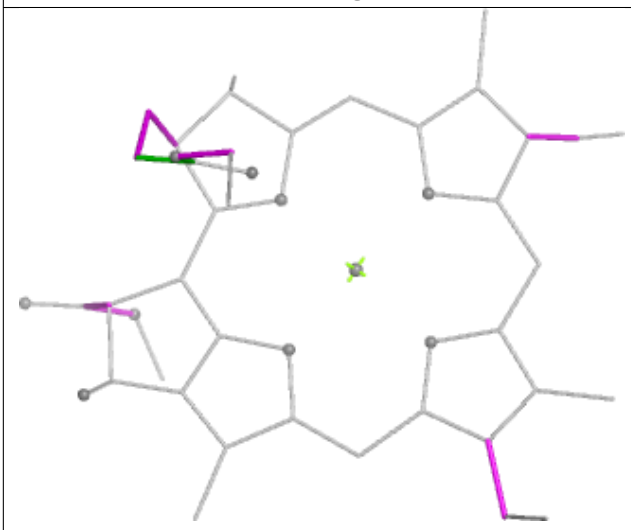
Ligand CLA L 207



Bond lengths



Bond angles



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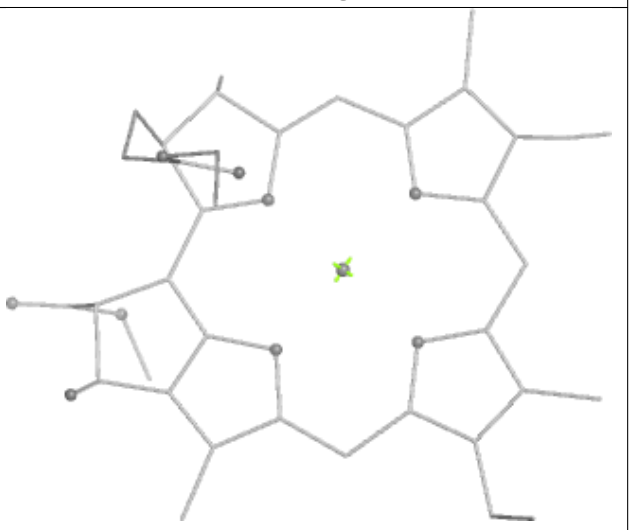
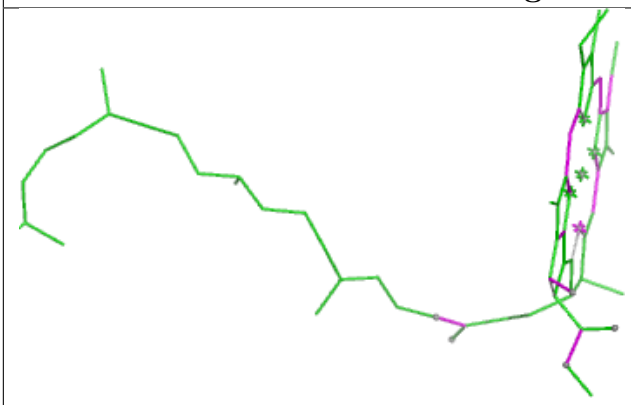


Rings

Ligand CLA B 838



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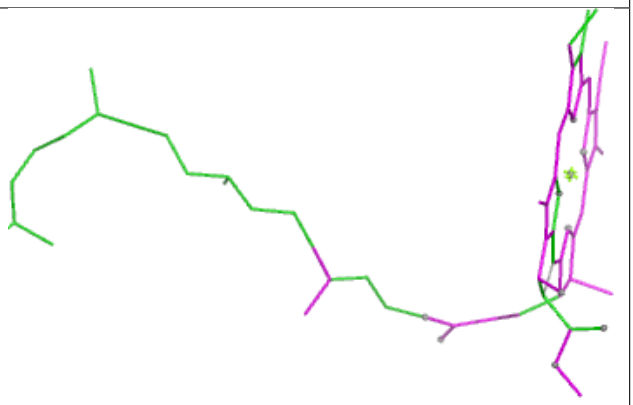
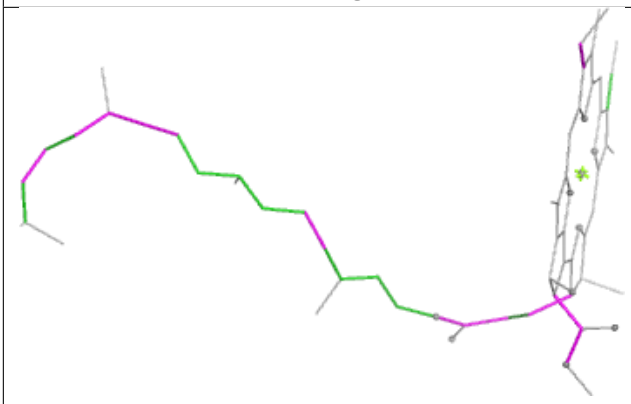
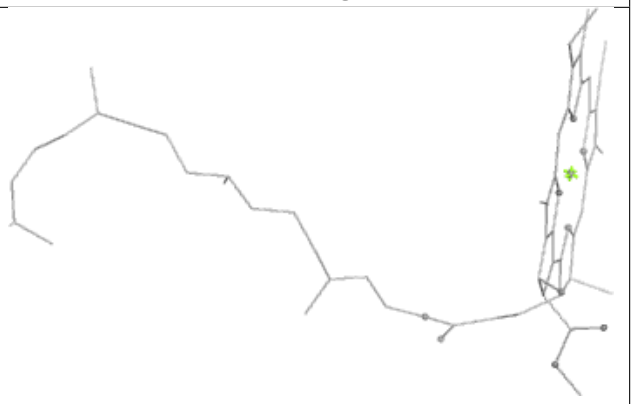


Bond angles

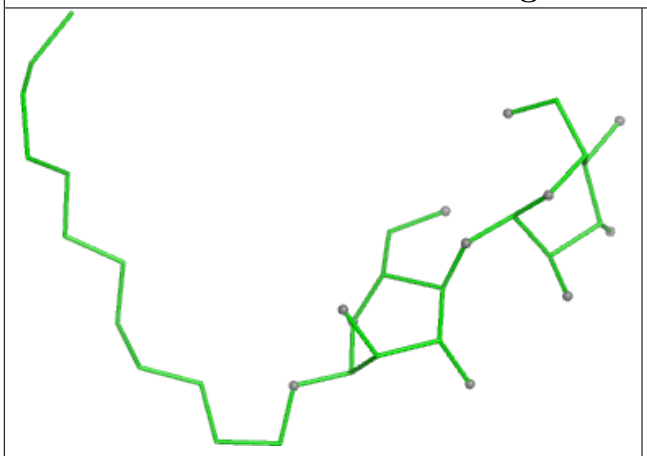


Torsions



Rings

Ligand LMU K 101



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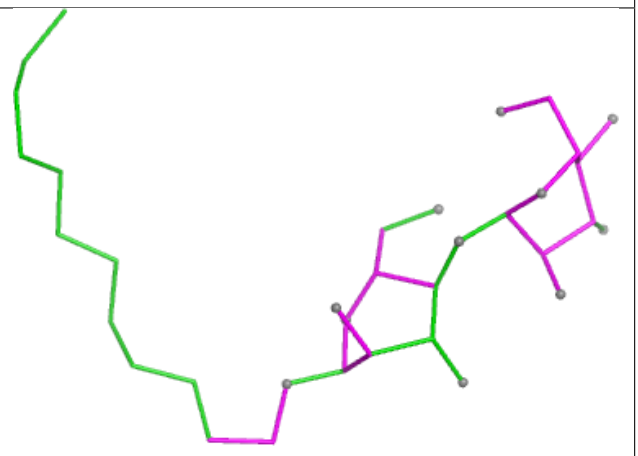

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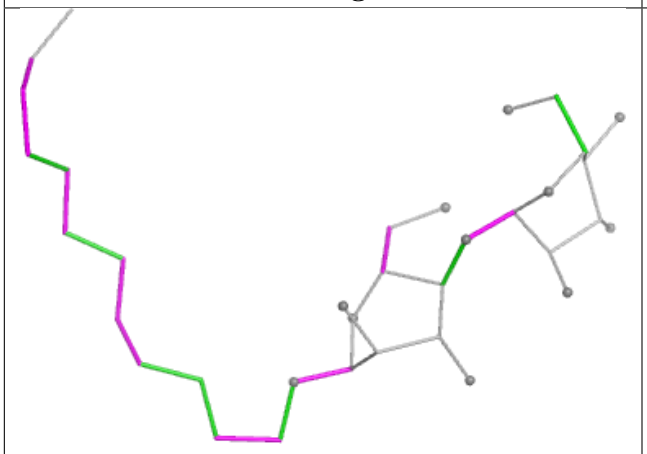

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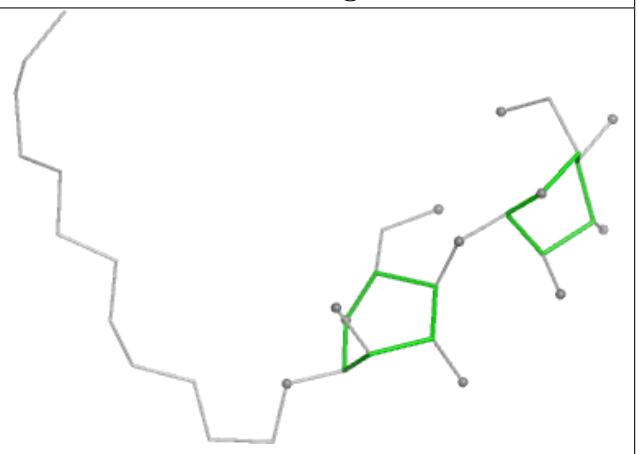
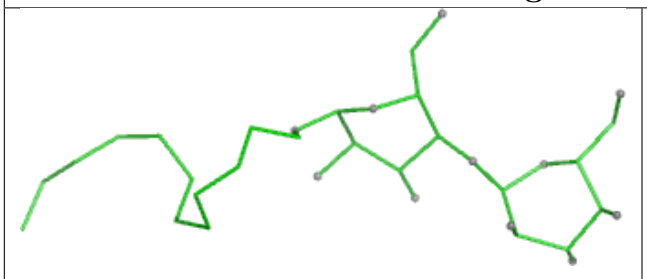


Rings

Ligand LMU 3 318



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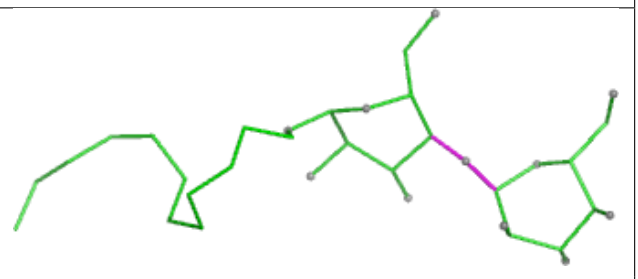

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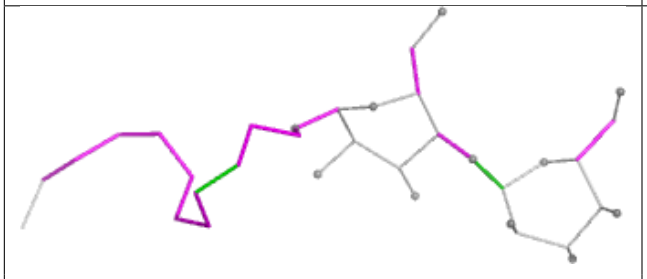

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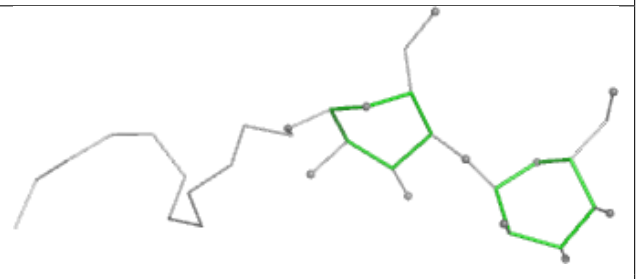
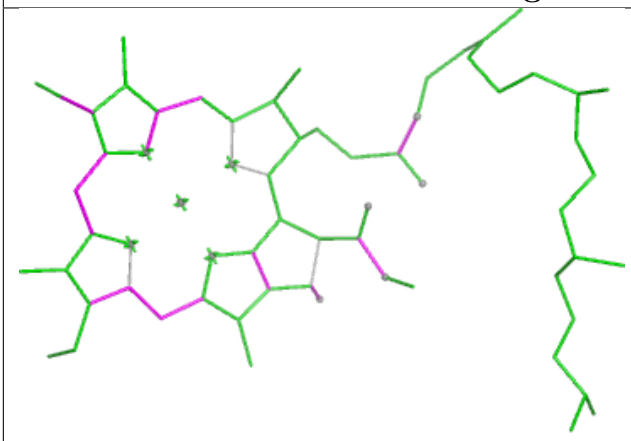


Rings

Ligand CLA R 107



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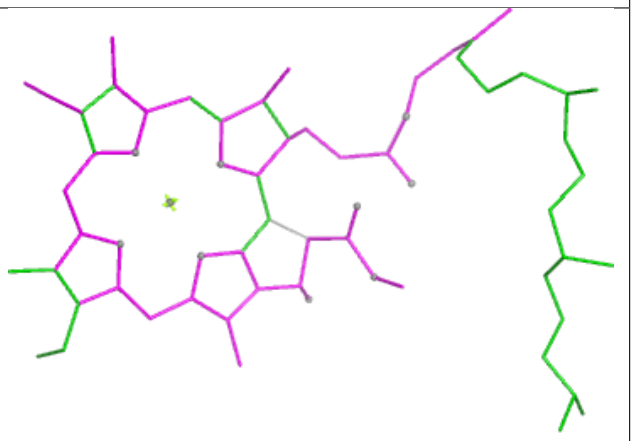

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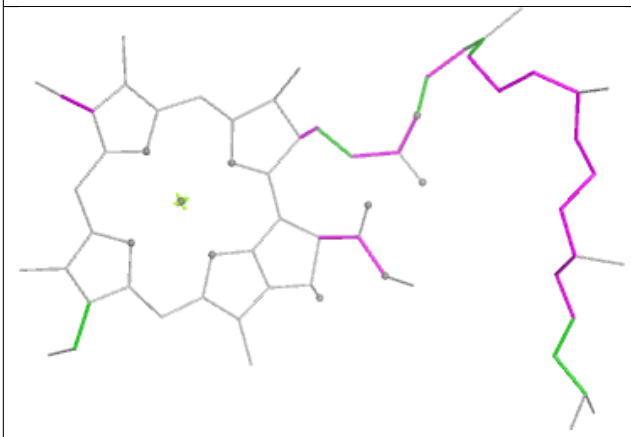

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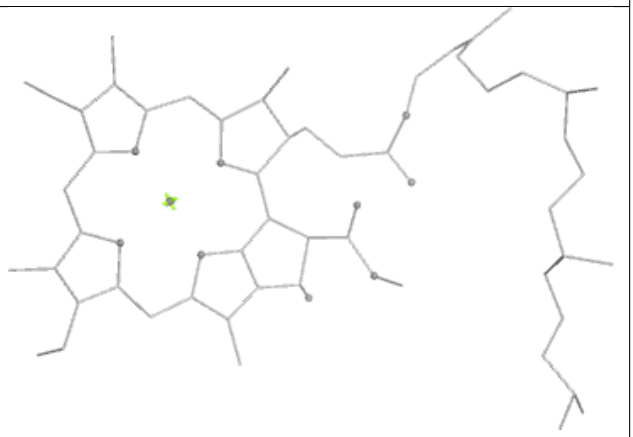
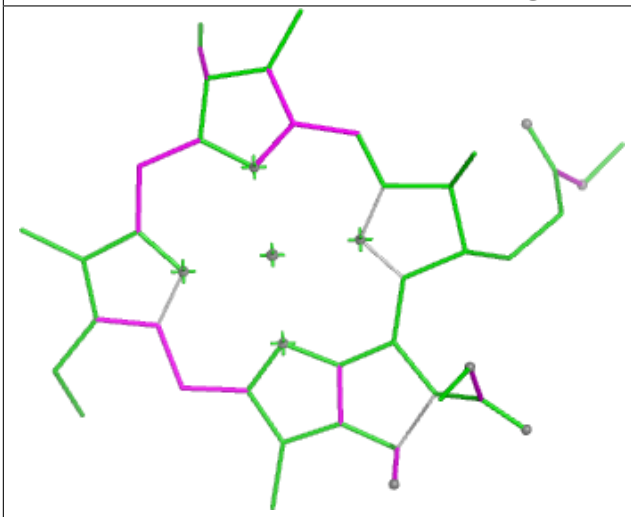


Rings

Ligand CLA B 818



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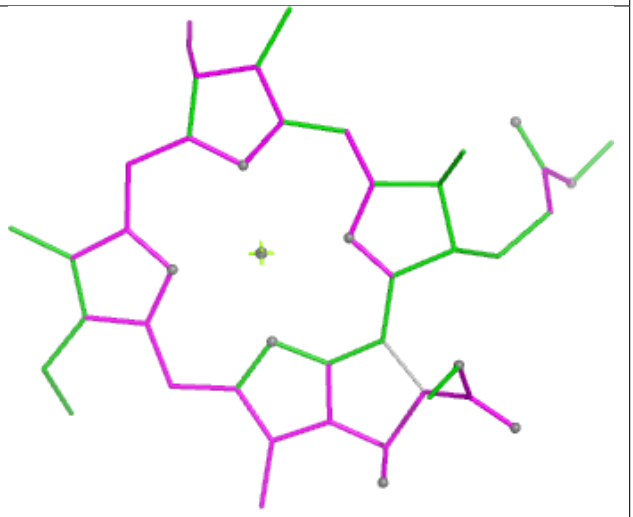

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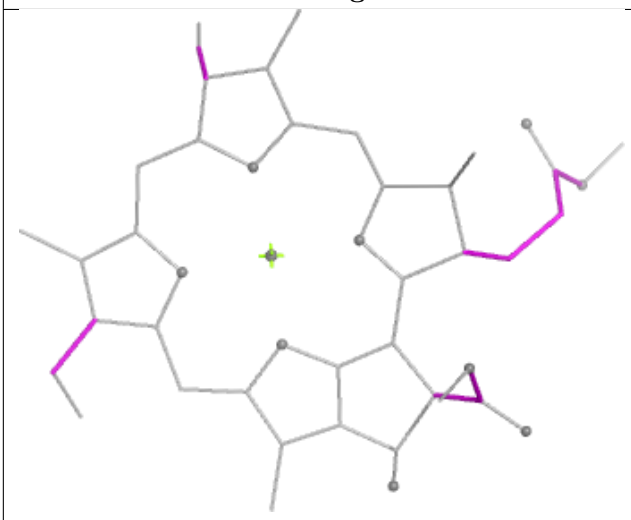

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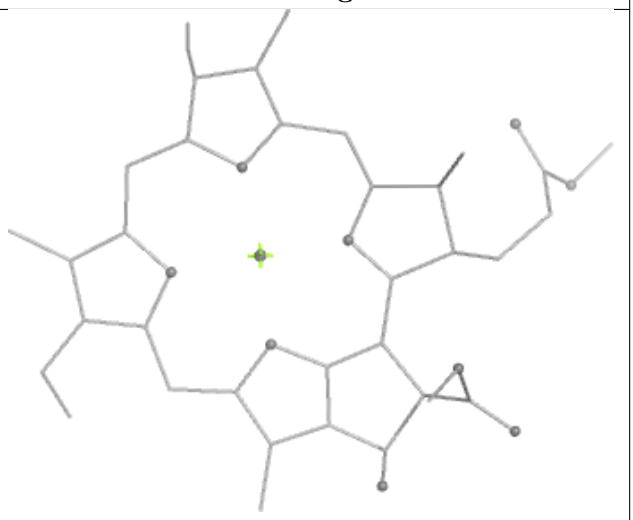
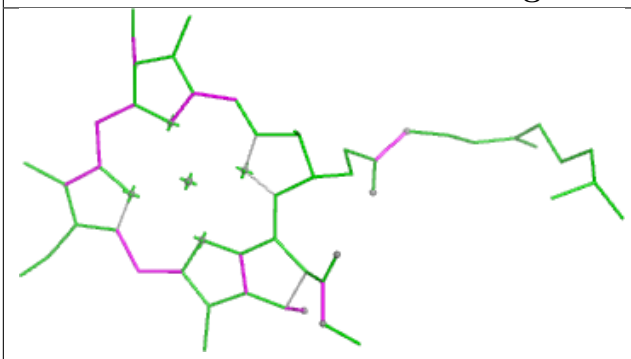


Rings

Ligand CLA H 108



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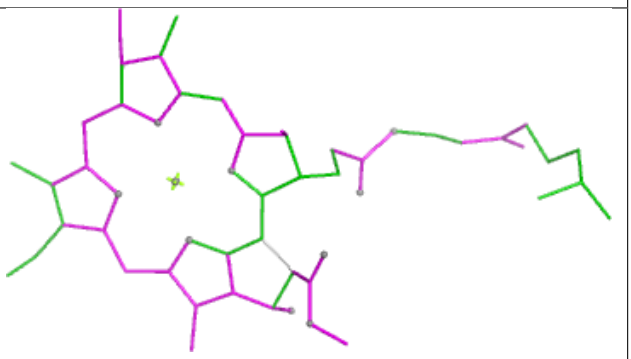

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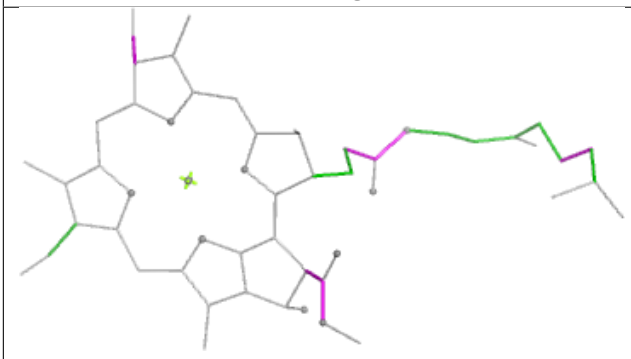

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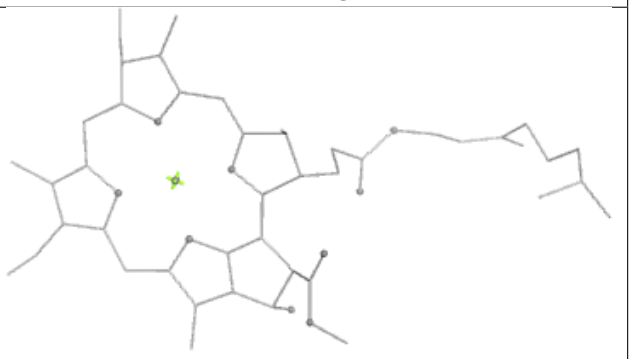
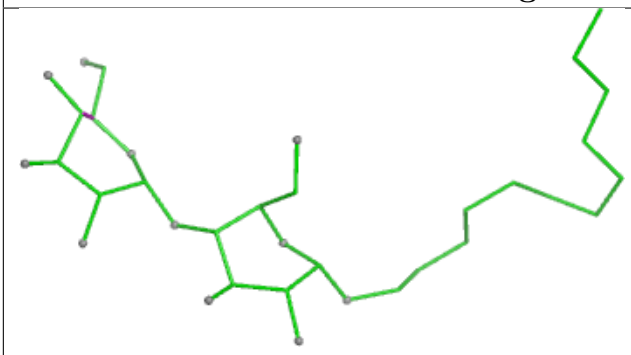


Rings

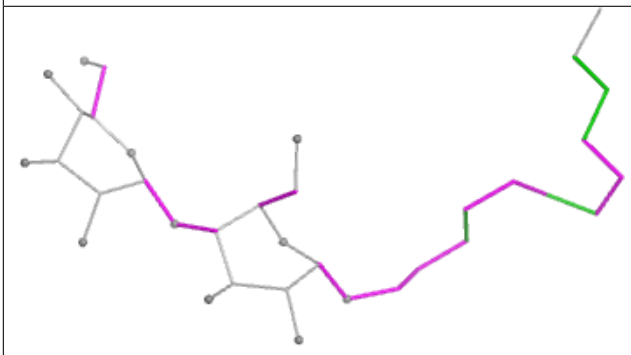
Ligand LMU H 103



Bond lengths



Bond angles



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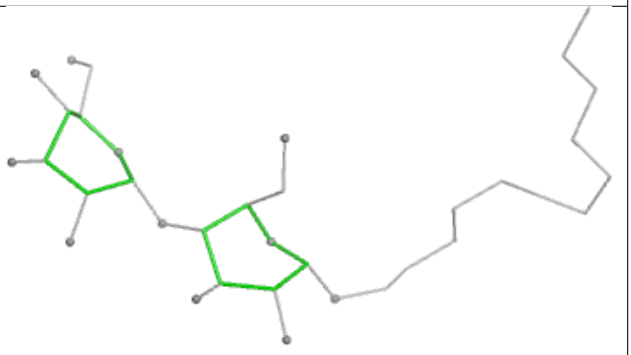
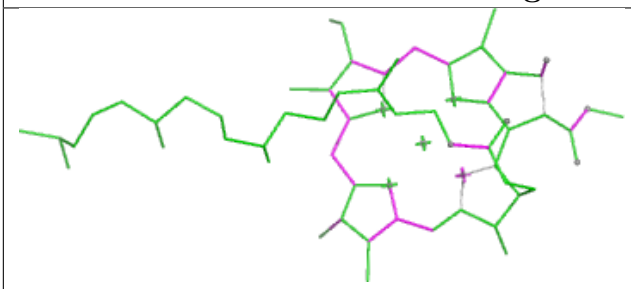


Rings

Ligand CLA A 833



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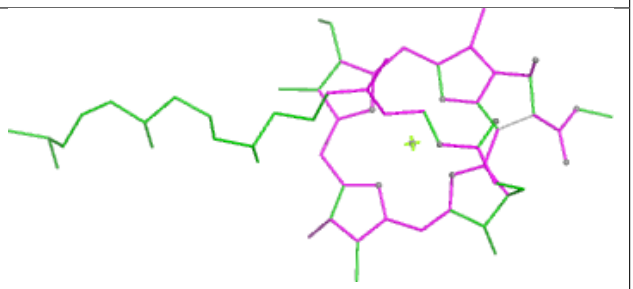
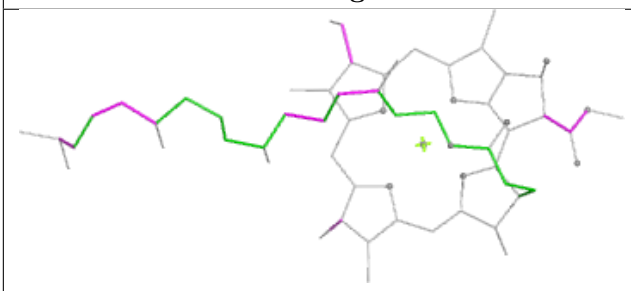


Bond angles



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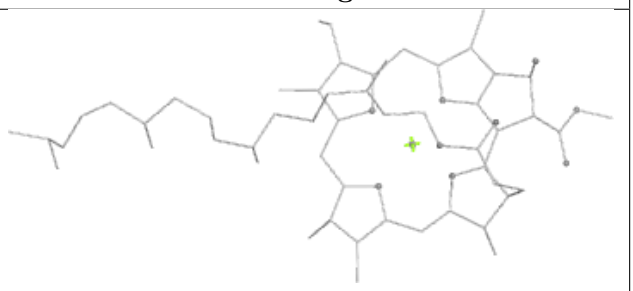
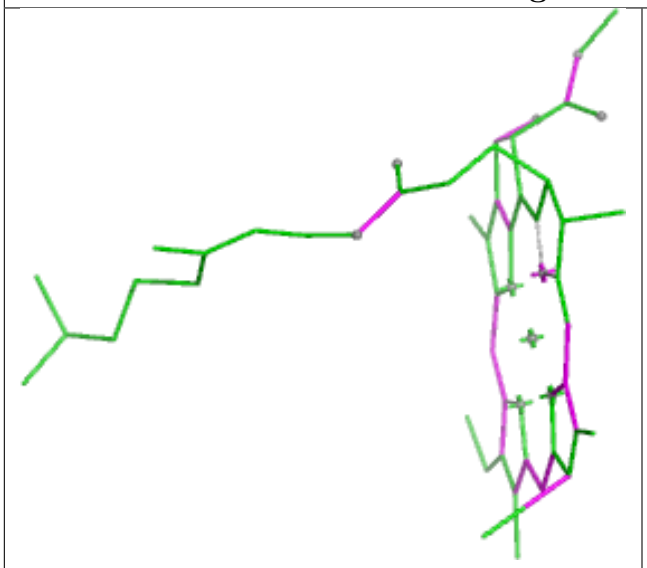


Rings

Ligand CLA 4 302



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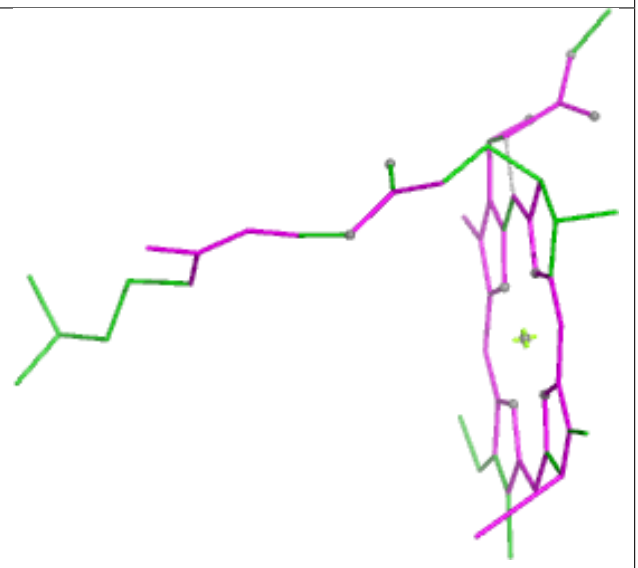


Bond angles

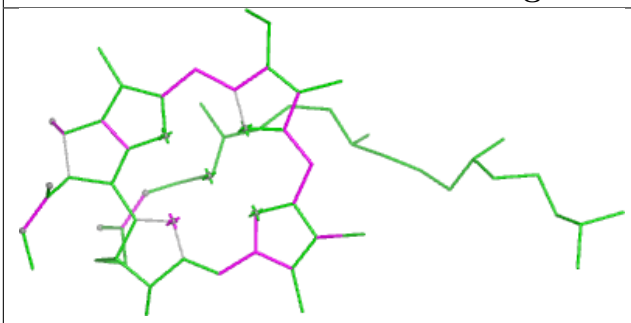


Torsions



Rings

Ligand CLA A 855



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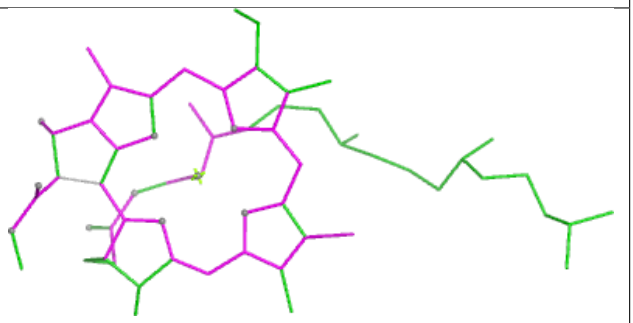
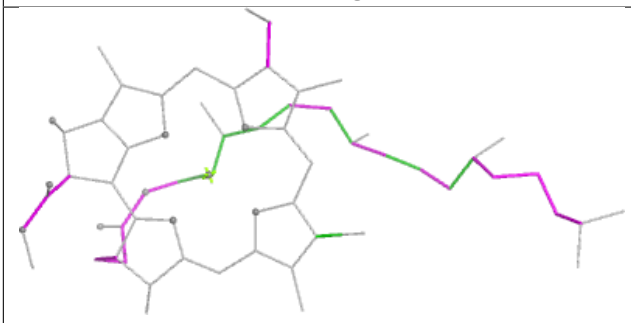


Bond angles



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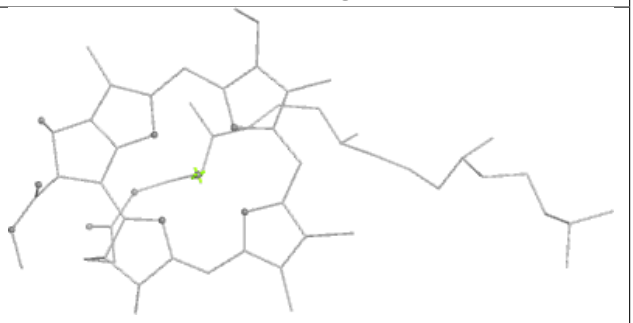
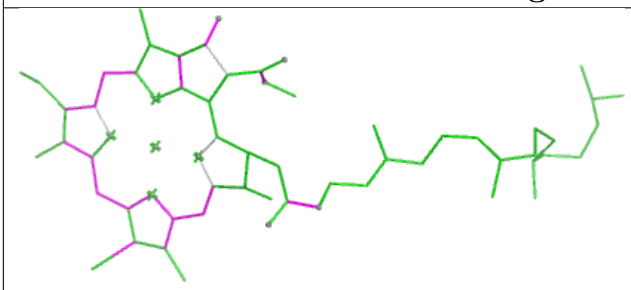


Rings

Ligand CLA 2 317



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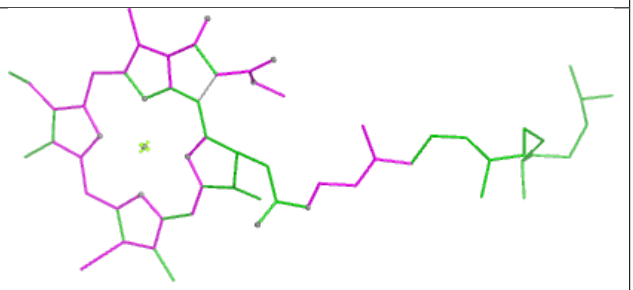

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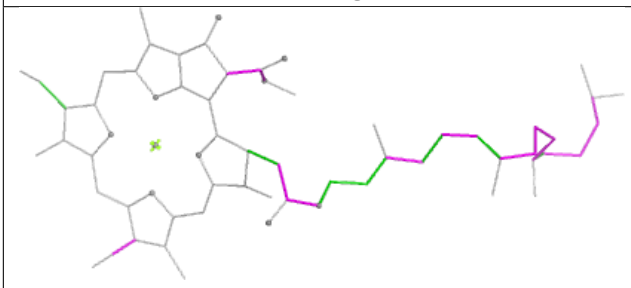

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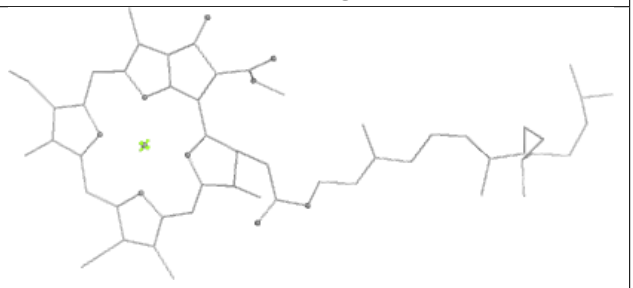
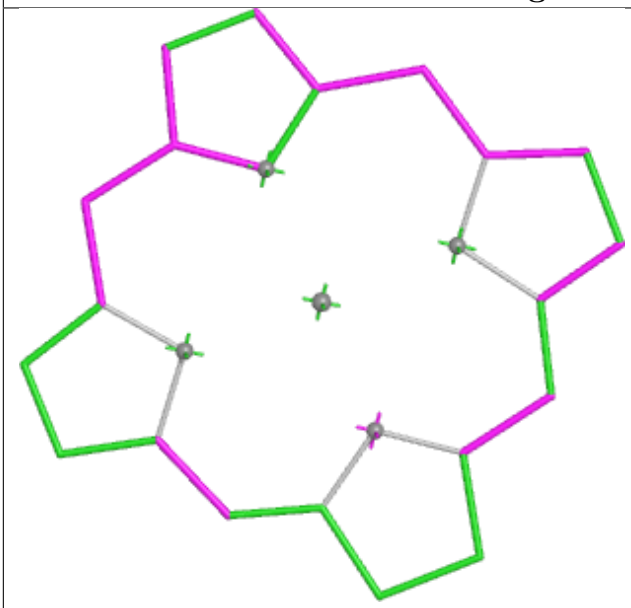


Rings

Ligand CLA 3 304



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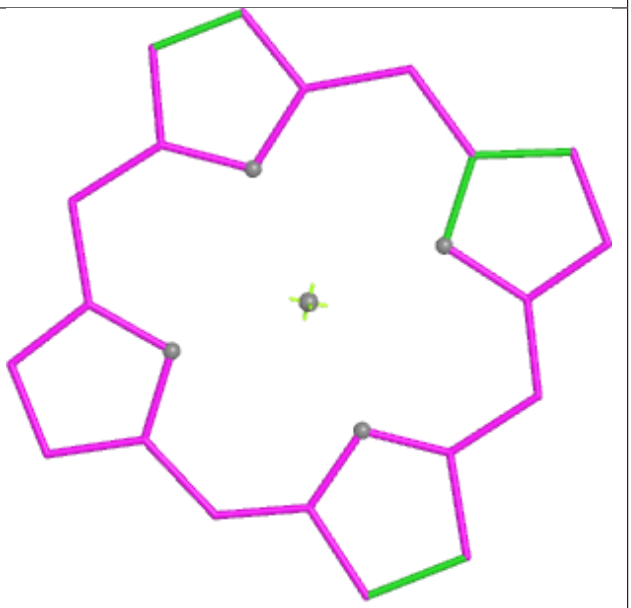

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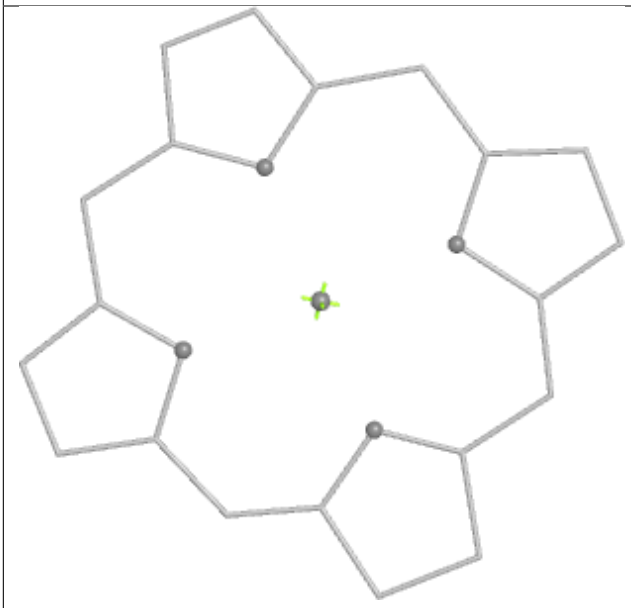

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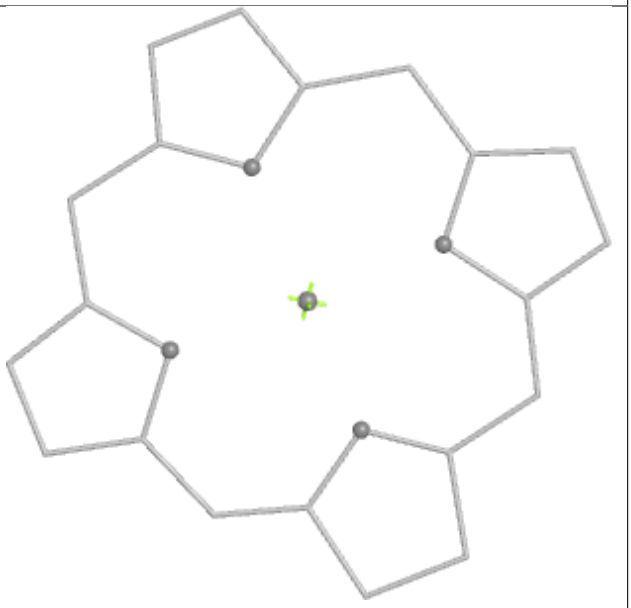
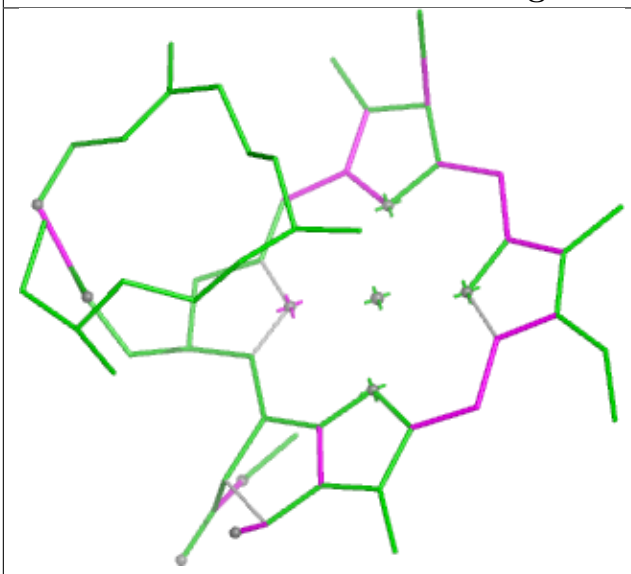


Rings

Ligand CLA J 102



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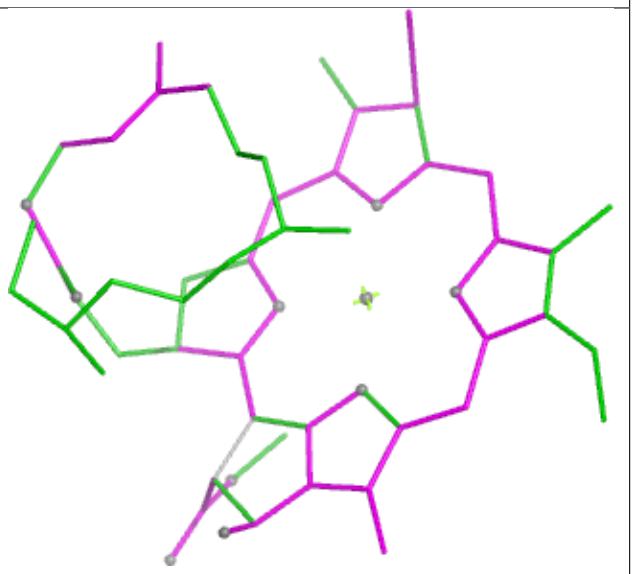
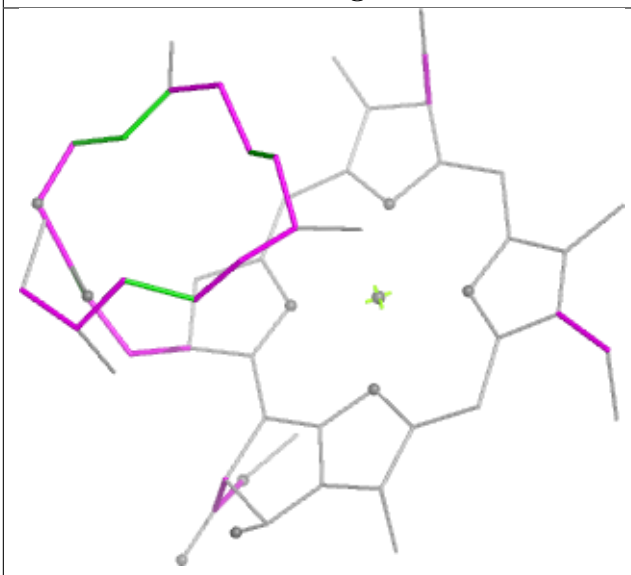


Bond angles



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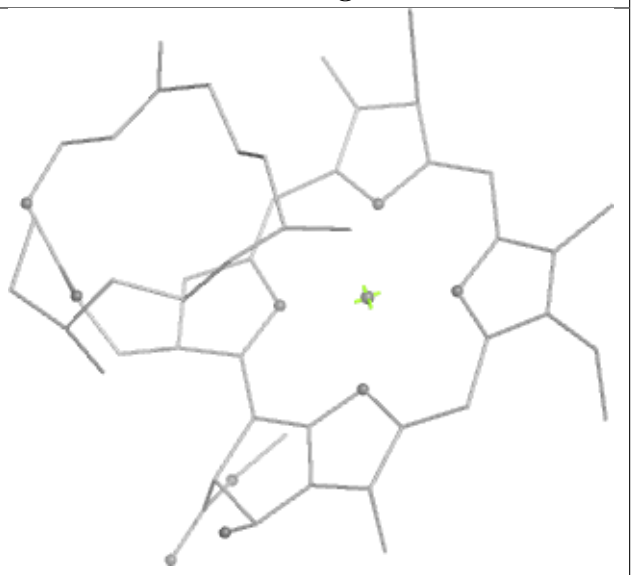
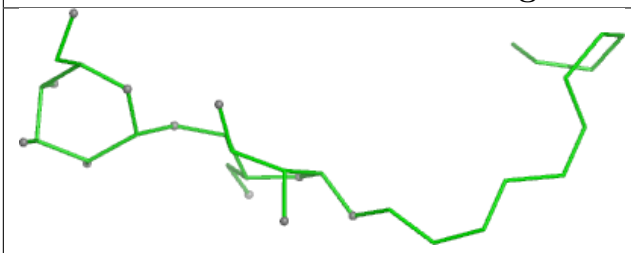


Rings

Ligand LMU H 105



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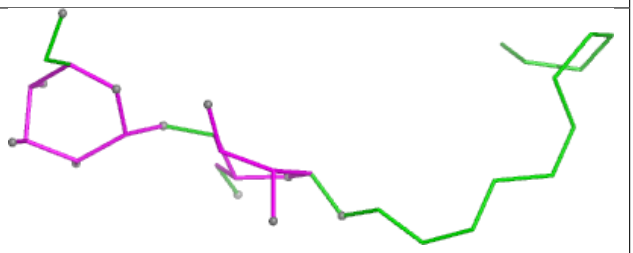
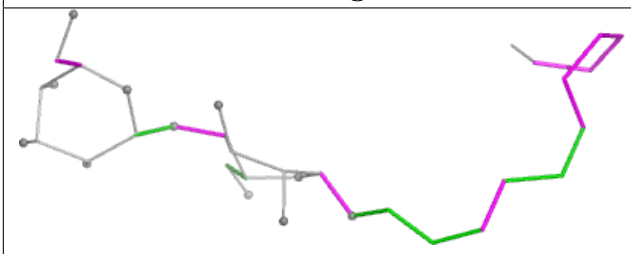


Bond angles



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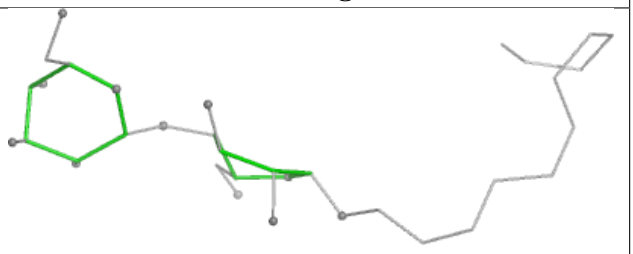
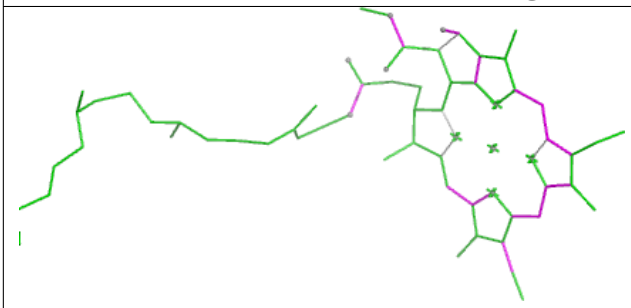


Rings

Ligand CLA H 107



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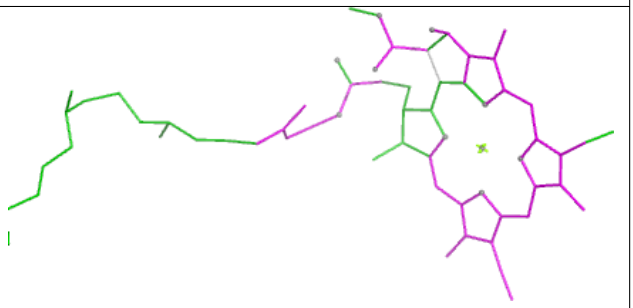
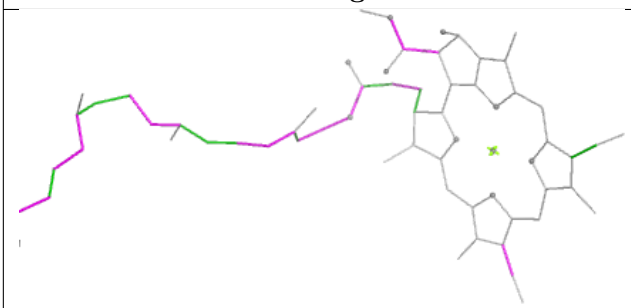


Bond angles

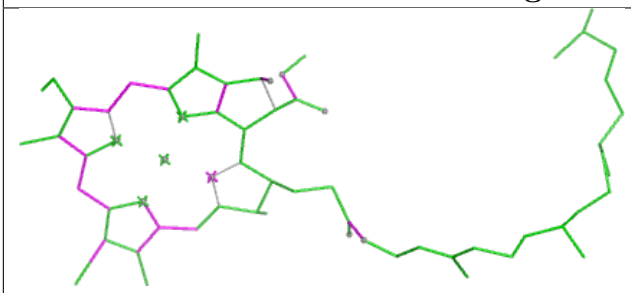


Torsions



Rings

Ligand CLA B 823



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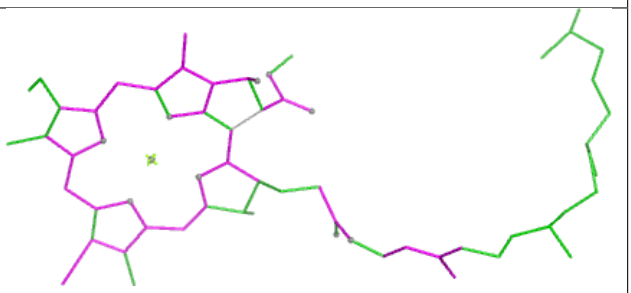
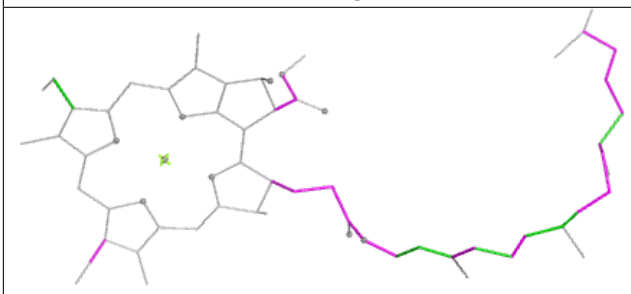
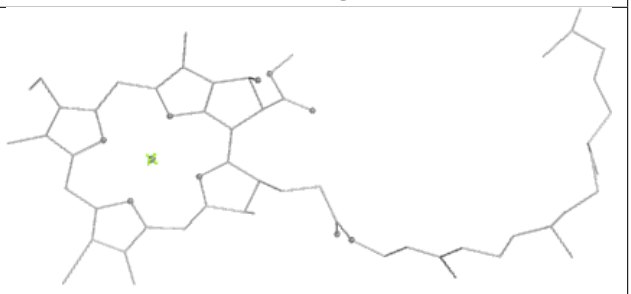


Bond angles

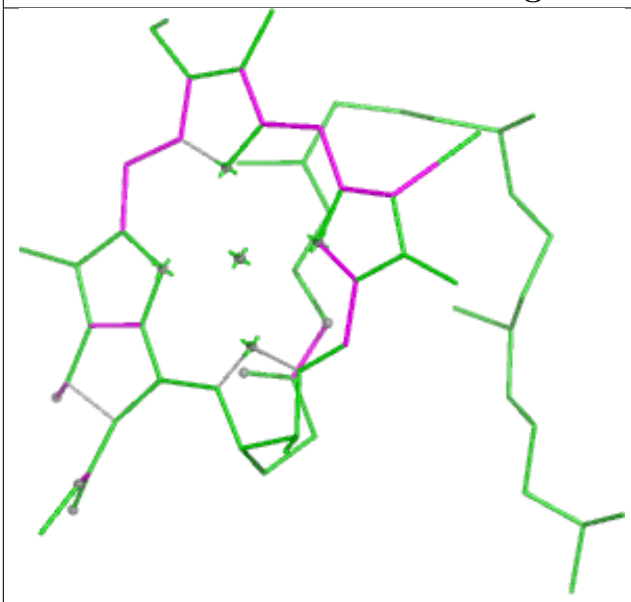


Torsions

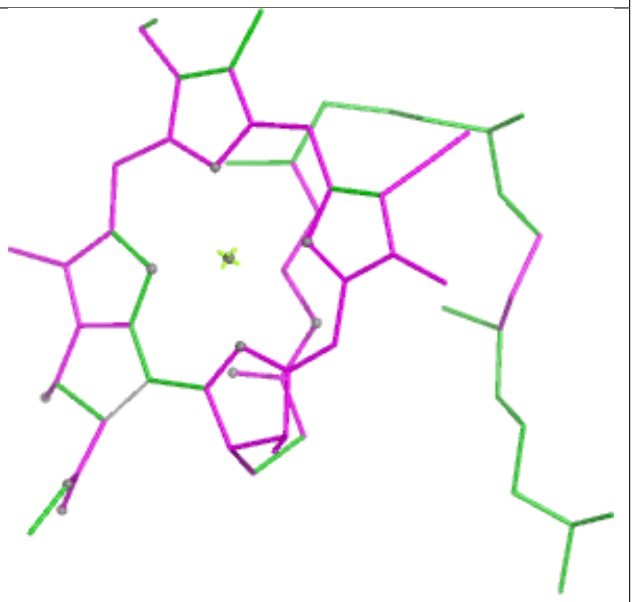


Rings

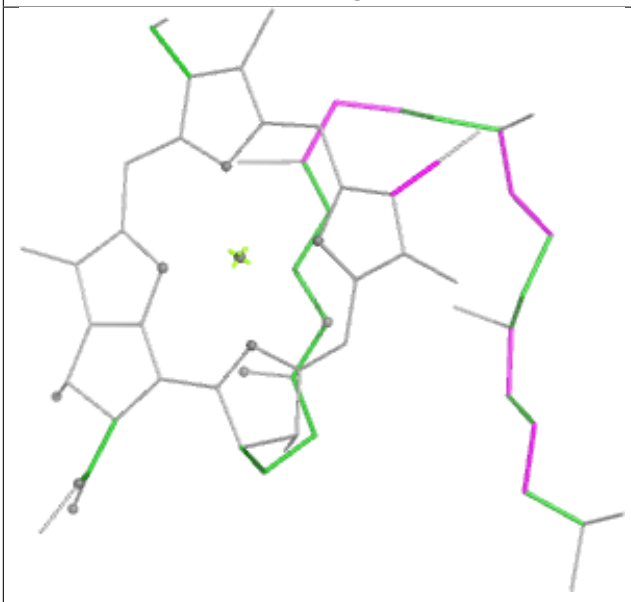
Ligand CLA B 806



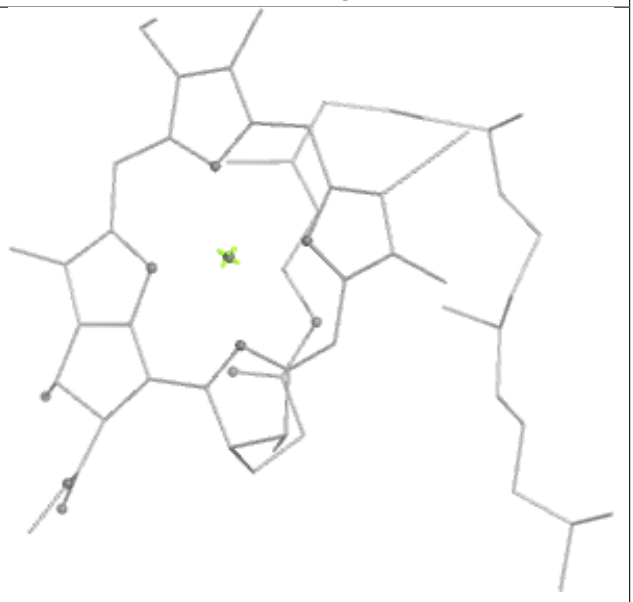
Bond lengths



Bond angles

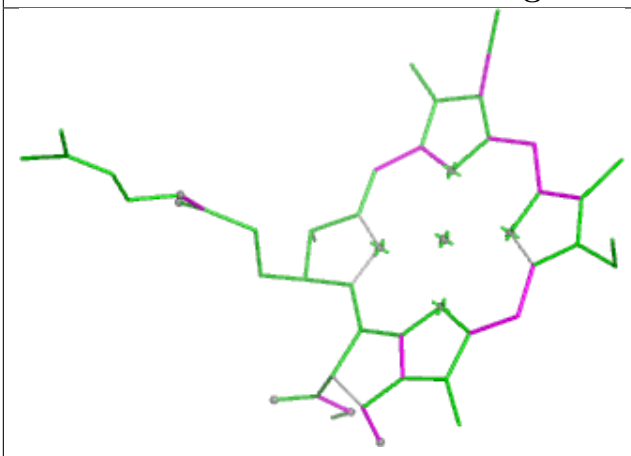


Torsions



Rings

Ligand CLA A 827



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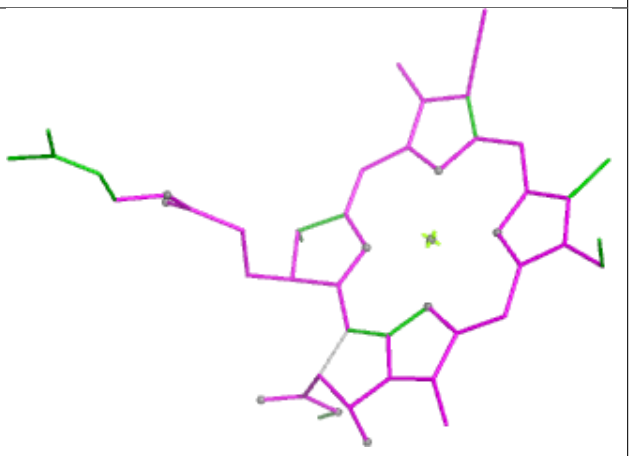
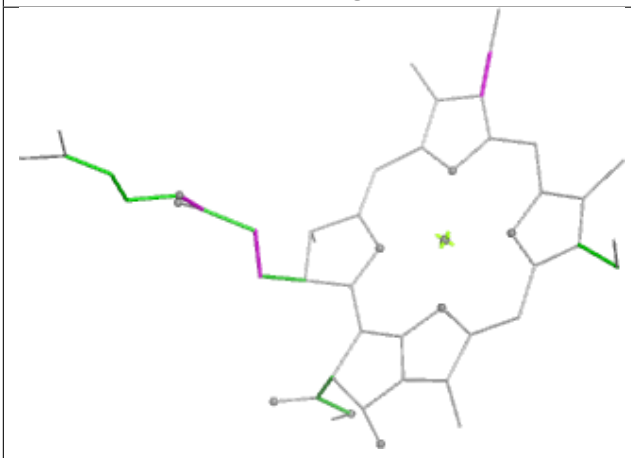


Bond angles

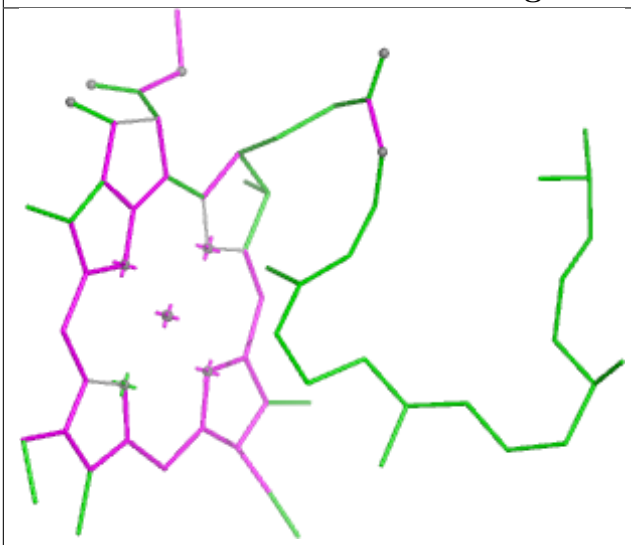


Torsions



Rings

Ligand CLA B 820



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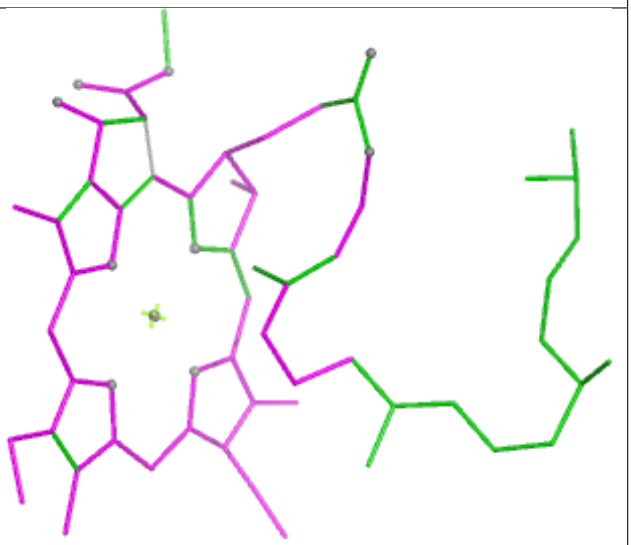
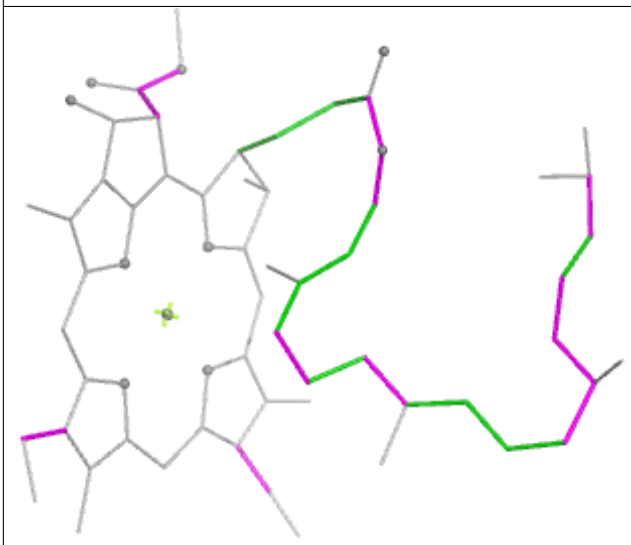


Bond angles



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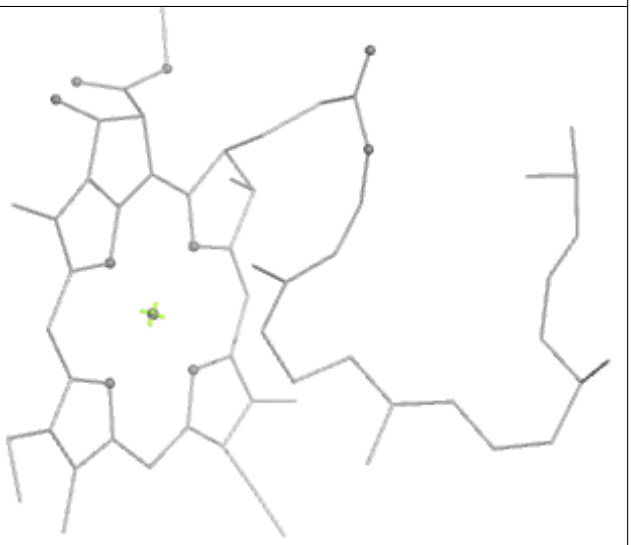
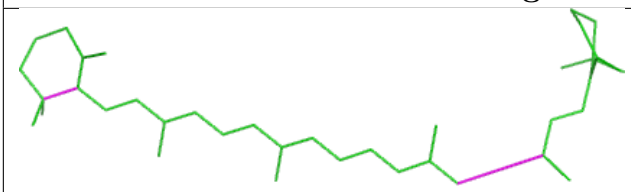


Rings

Ligand BCR B 841



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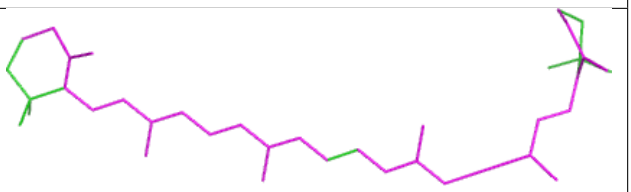
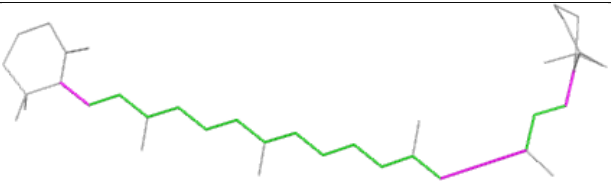


Bond angles



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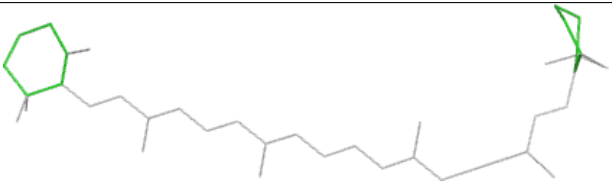
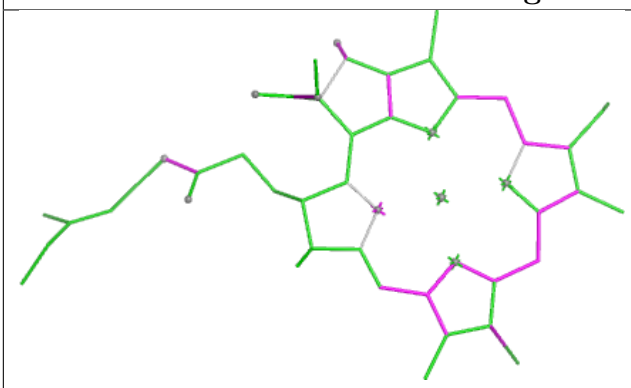


Rings

Ligand CLA A 832



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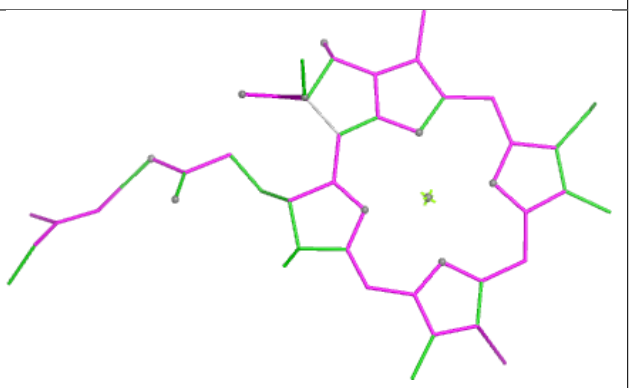
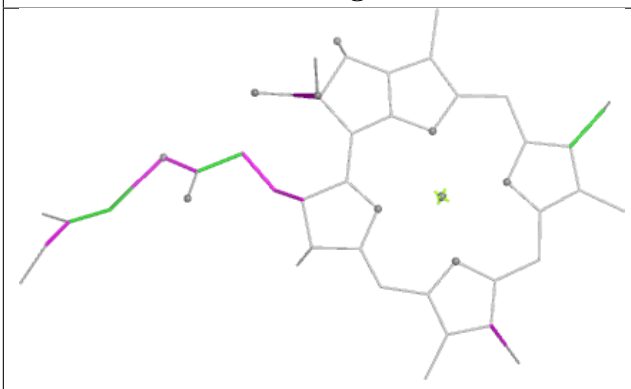


Bond angles



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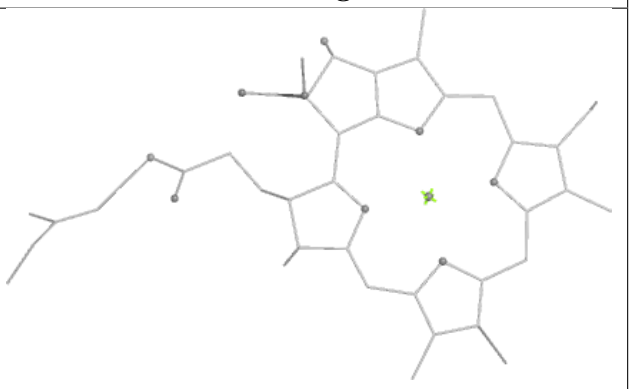
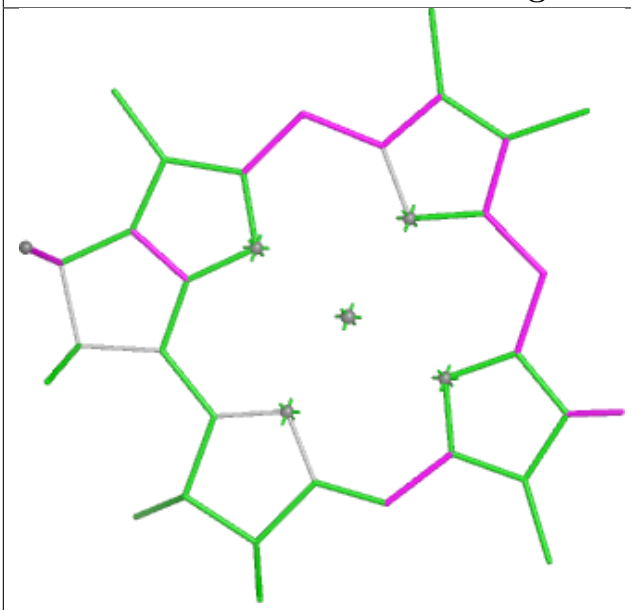


Rings

Ligand CLA 3 303



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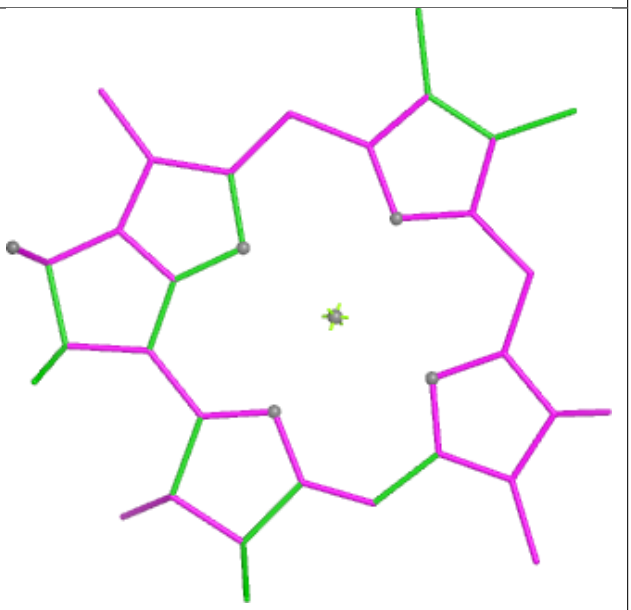
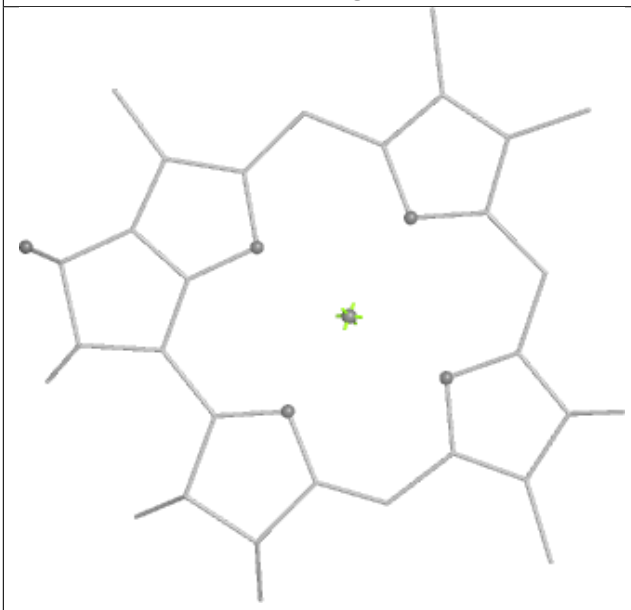


Bond angles



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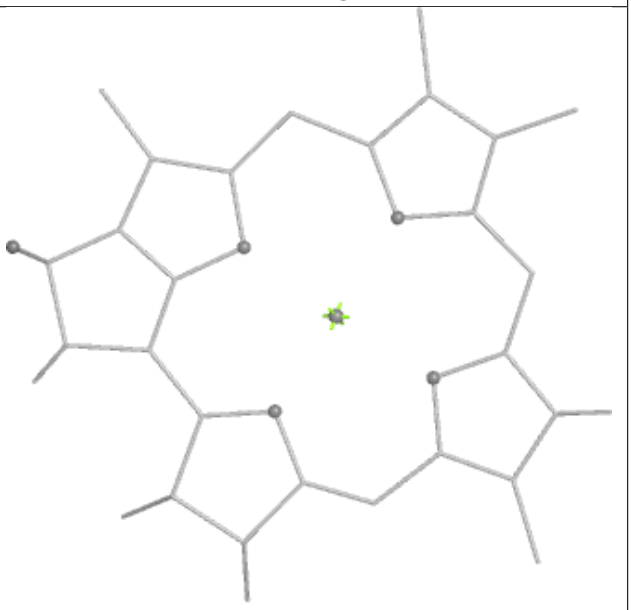
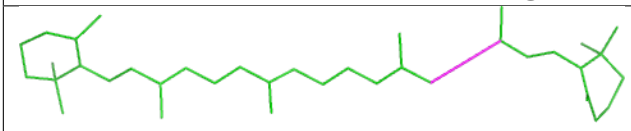


Rings

Ligand BCR A 843



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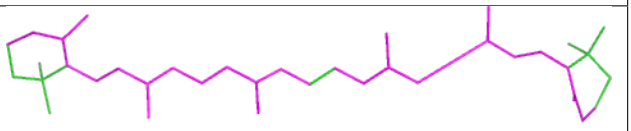
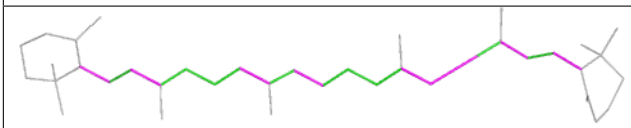


Bond angles



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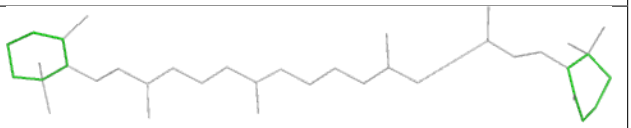
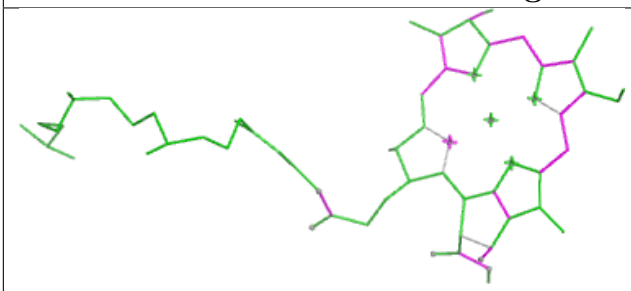


Rings

Ligand CLA B 810



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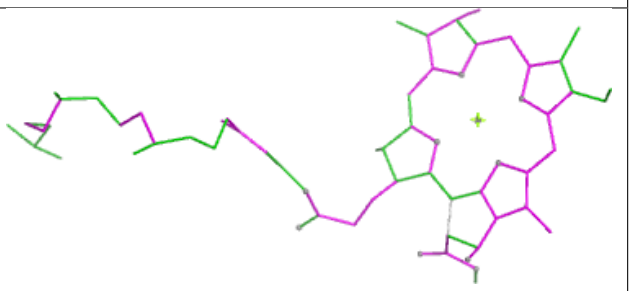
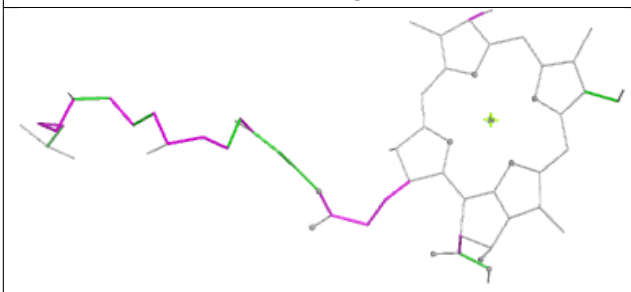


Bond angles



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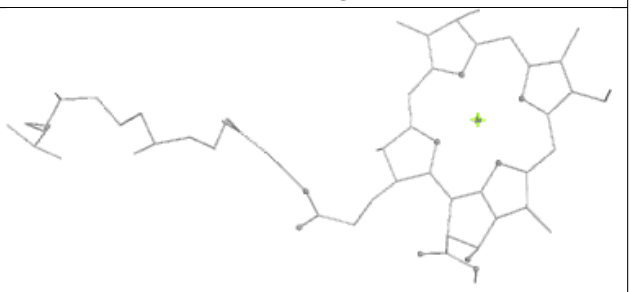
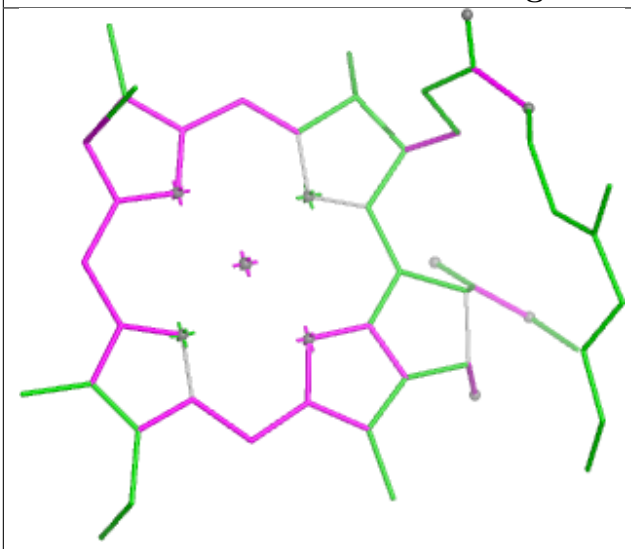


Rings

Ligand CLA F 206



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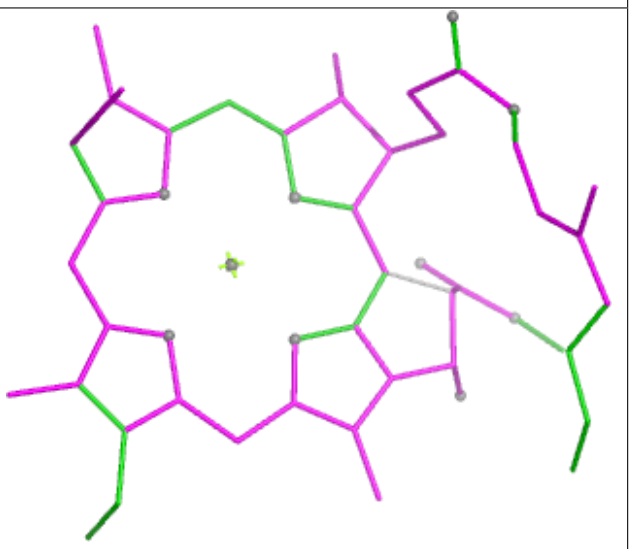
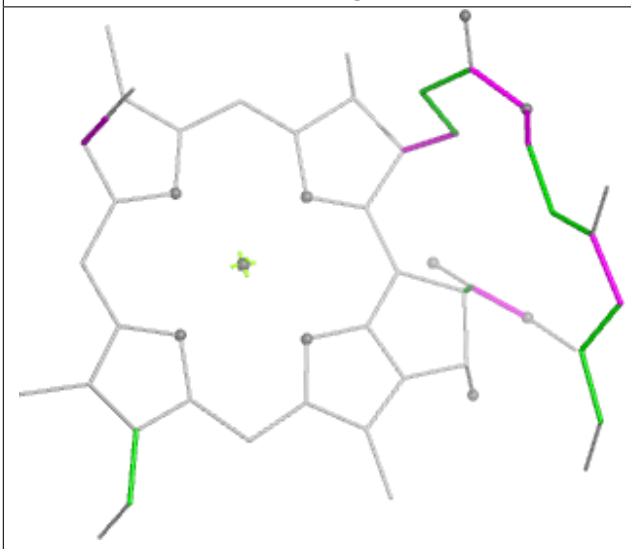


Bond angles



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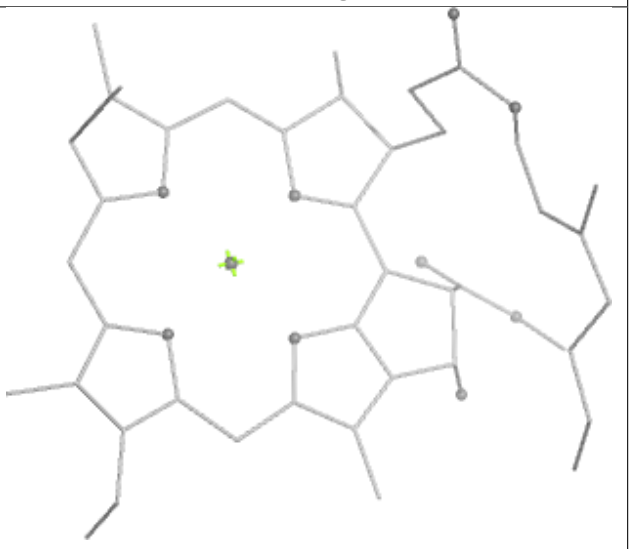
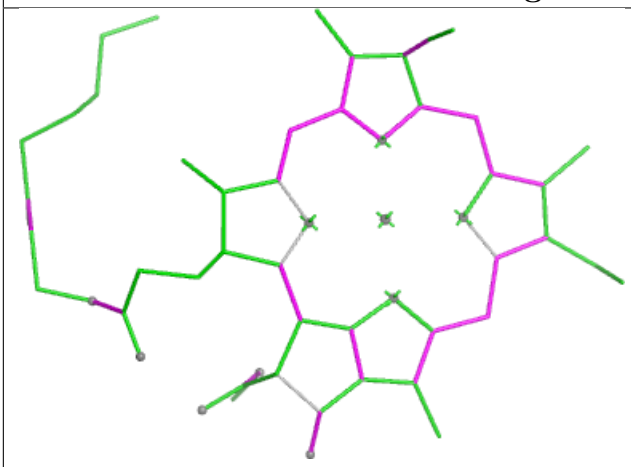


Rings

Ligand CLA B 821



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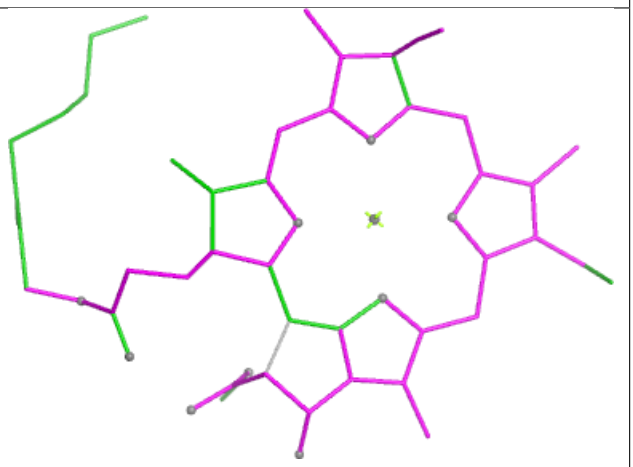
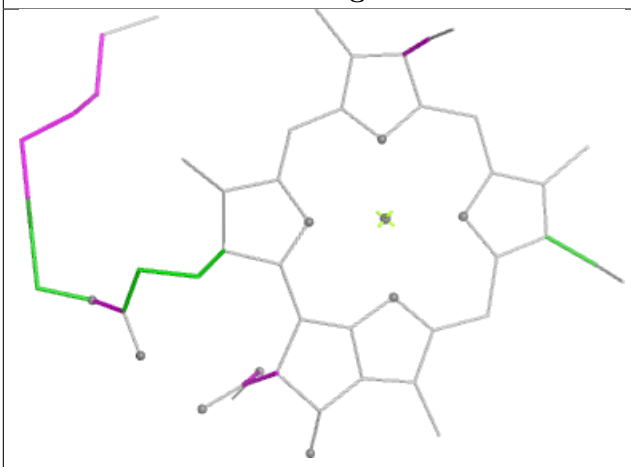


Bond angles



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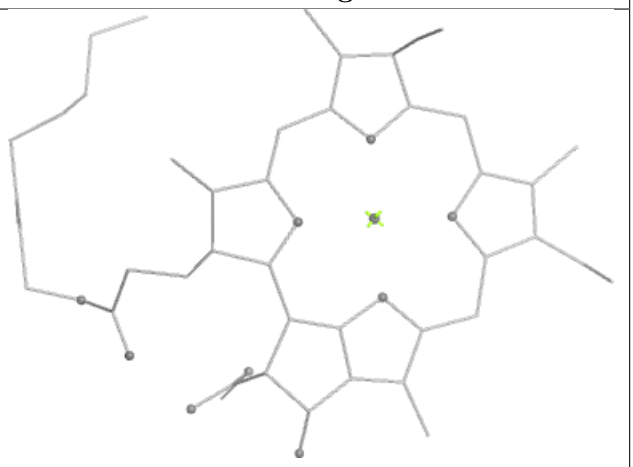
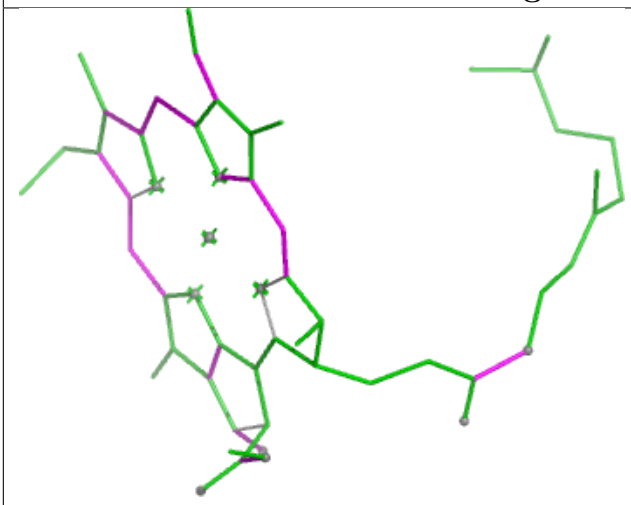


Rings

Ligand CLA A 802



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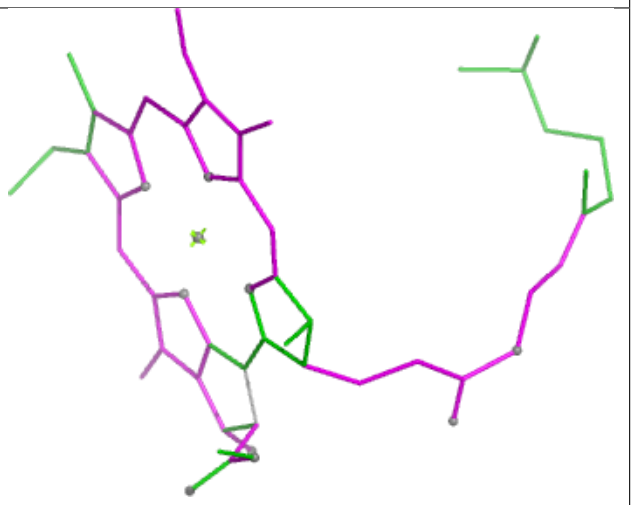
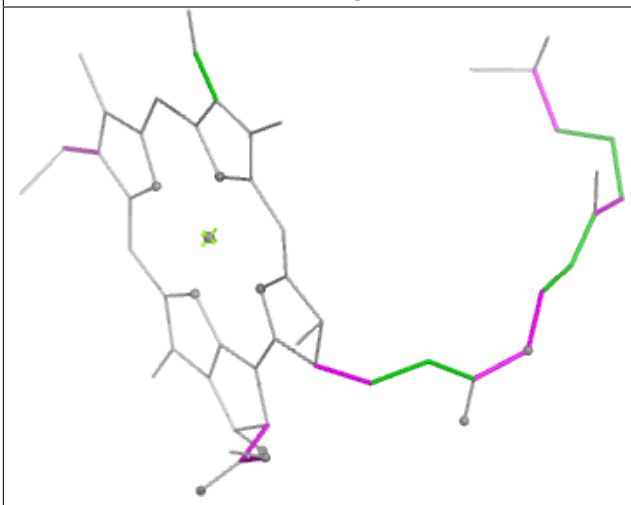


Bond angles



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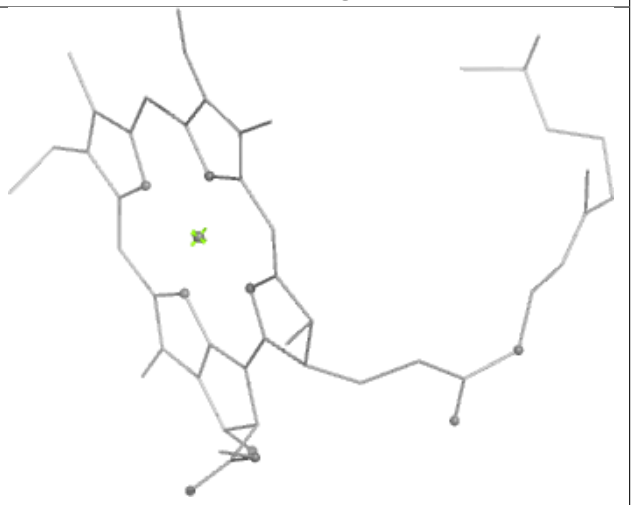
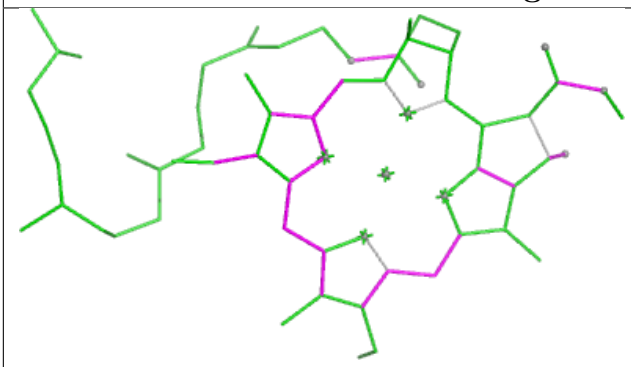


Rings

Ligand CLA A 816



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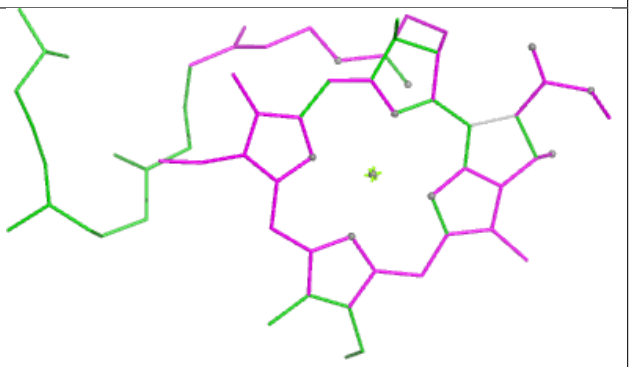
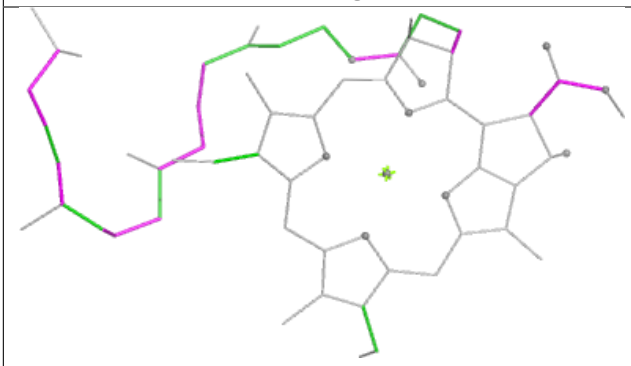


Bond angles



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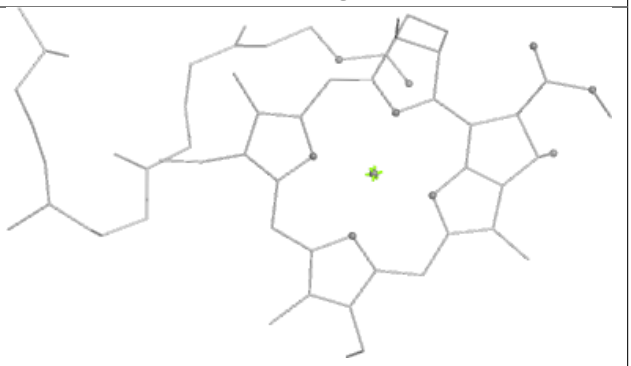
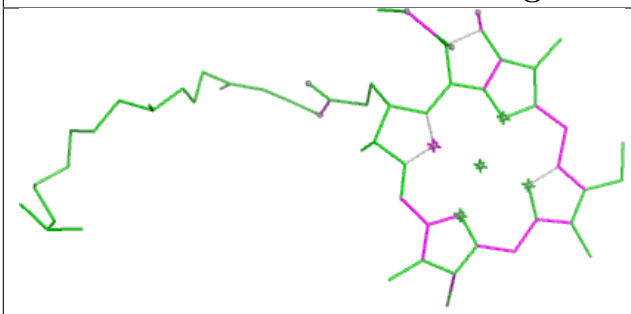


Rings

Ligand CLA A 822



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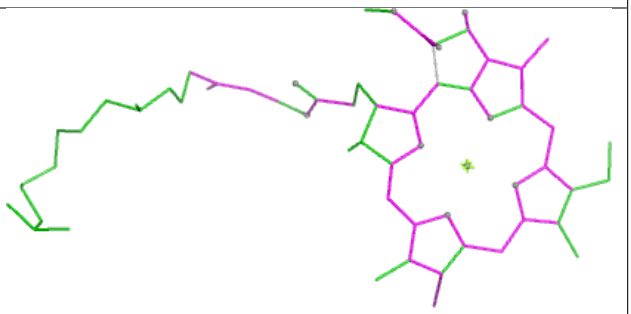
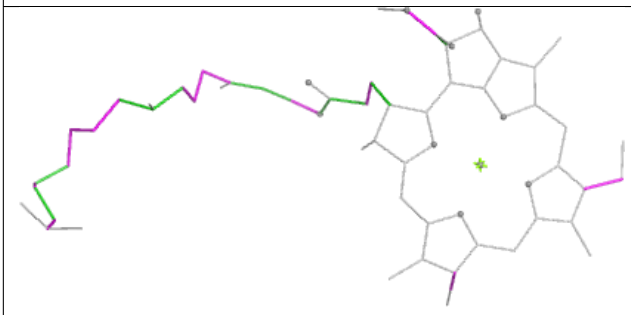


Bond angles

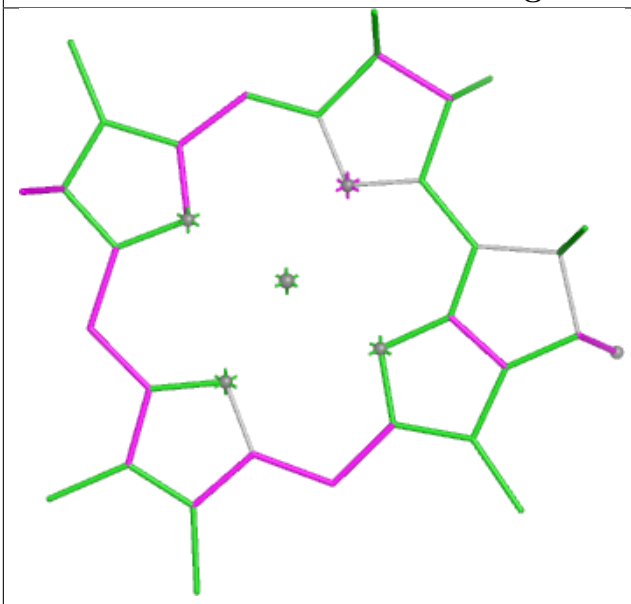


Torsions



Rings

Ligand CLA B 839



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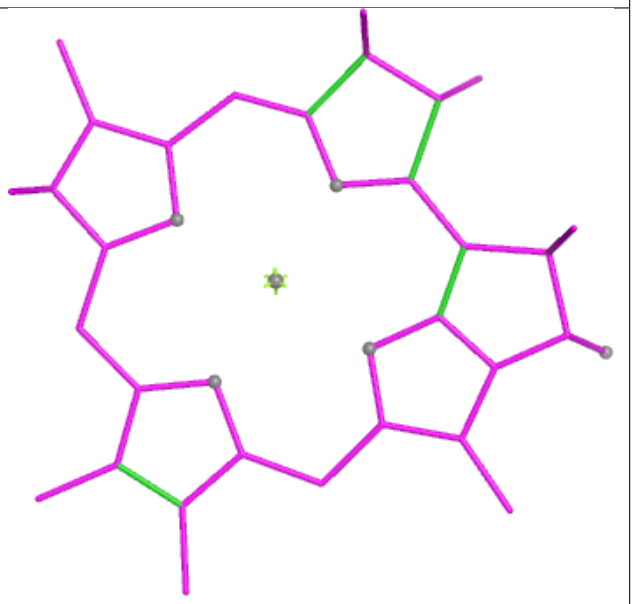
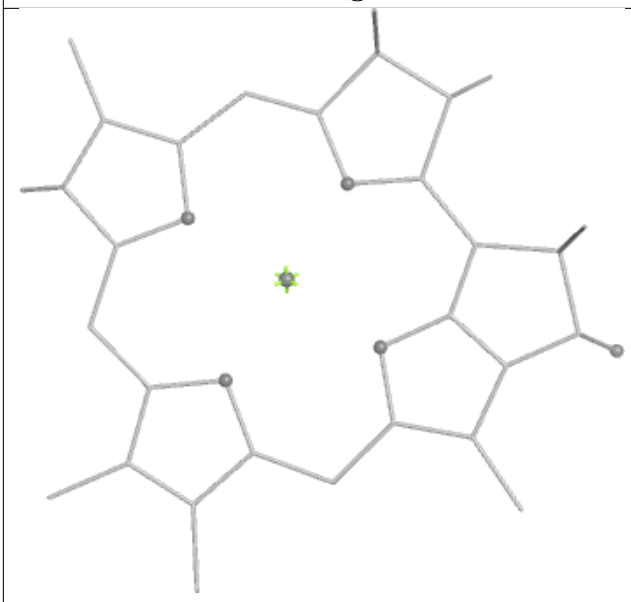


Bond angles



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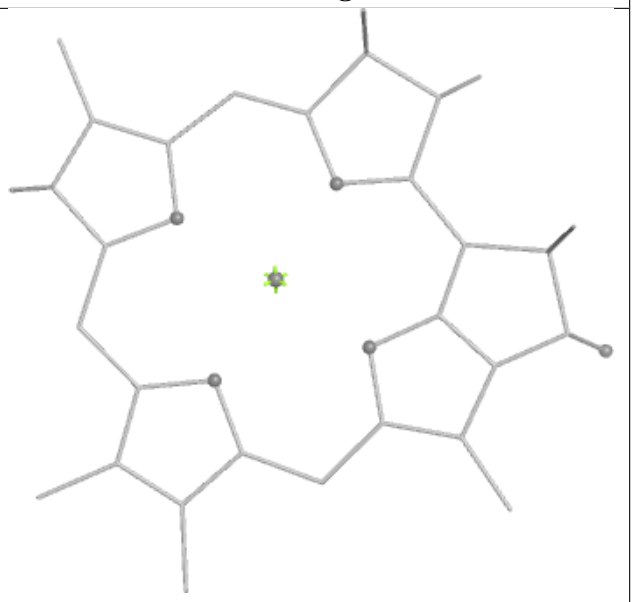
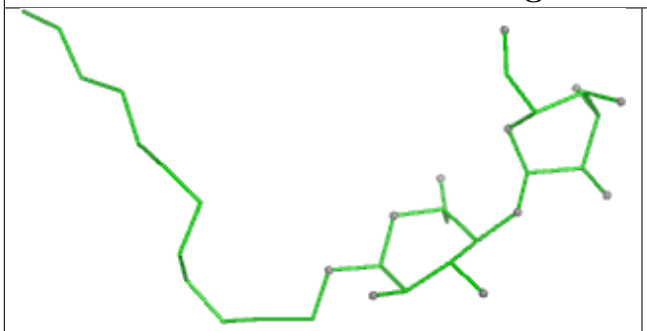


Rings

Ligand LMU 4 301



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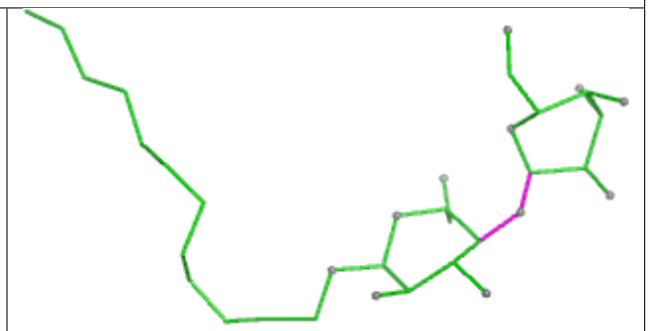
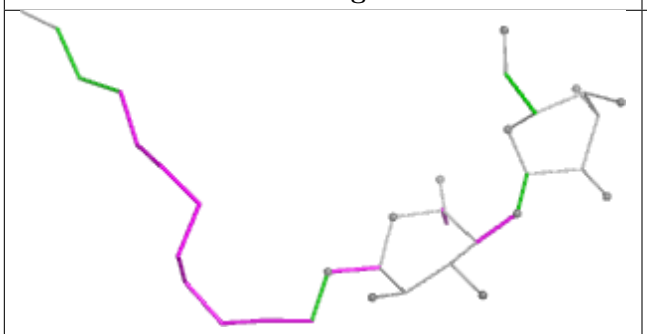
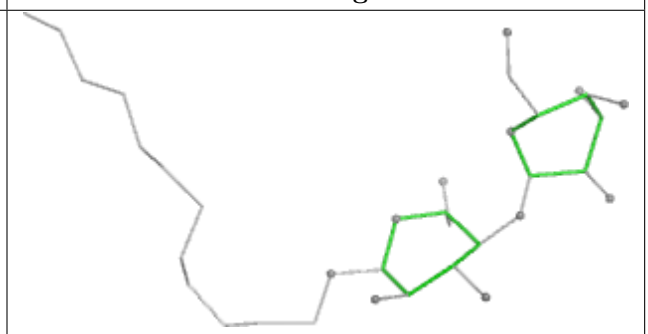


Bond angles

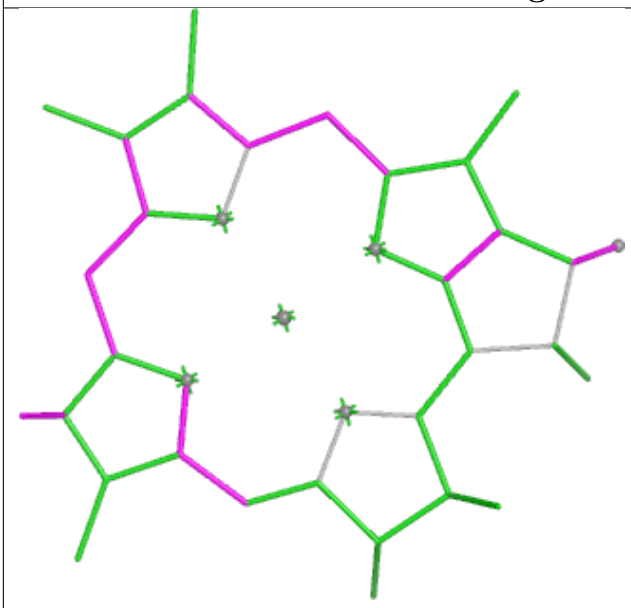


Torsions

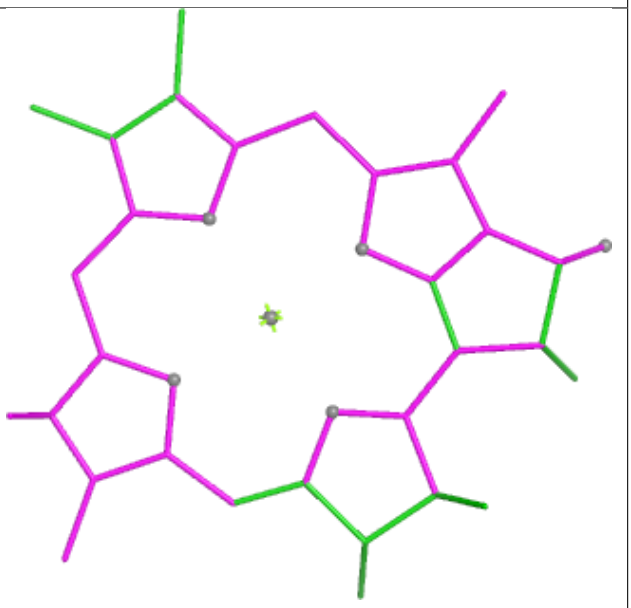


Rings

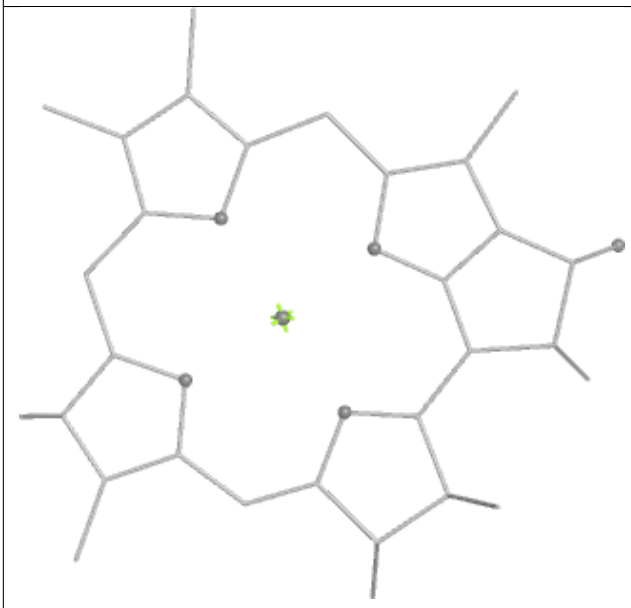
Ligand CLA 1 210



Bond lengths



Bond angles



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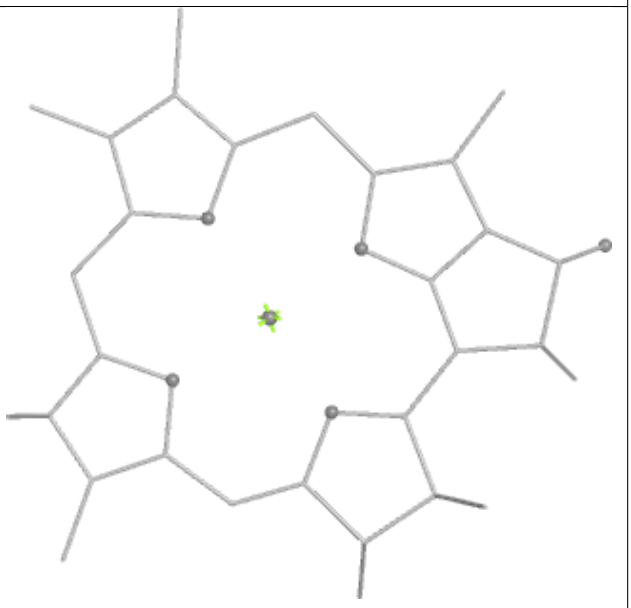
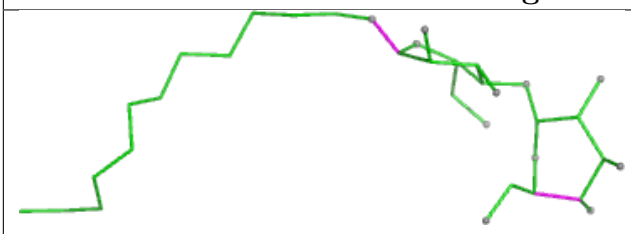


Rings

Ligand LMU L 205



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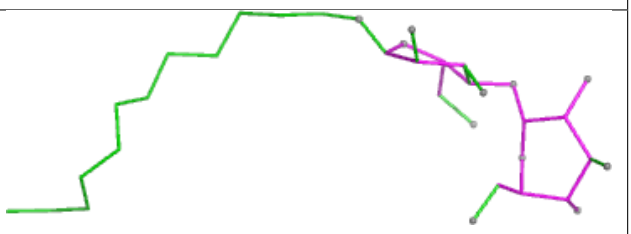
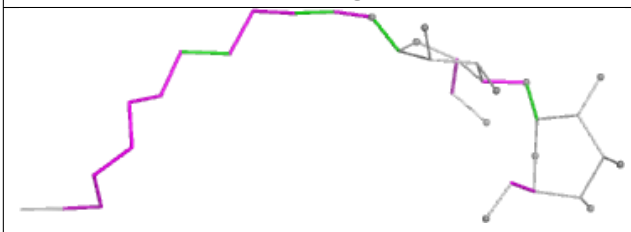


Bond angles



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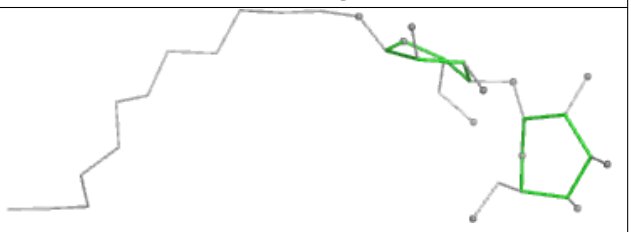
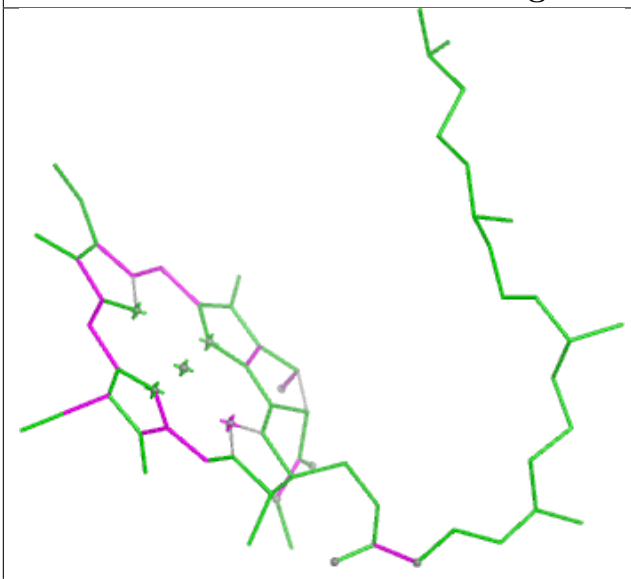


Rings

Ligand CLA 3 310



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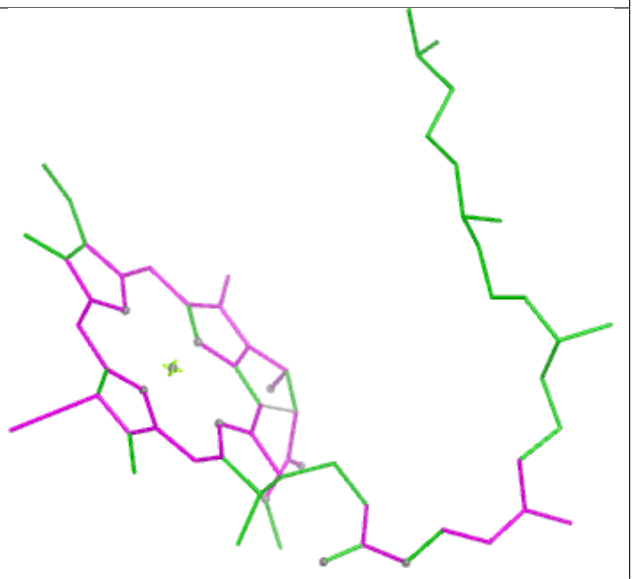
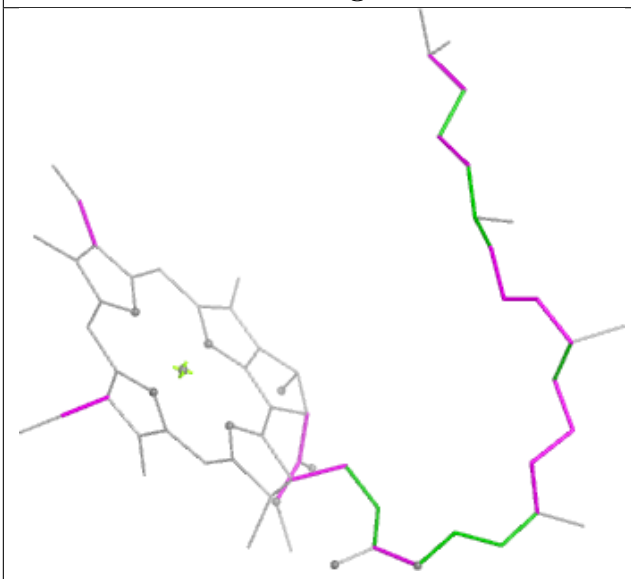


Bond angles



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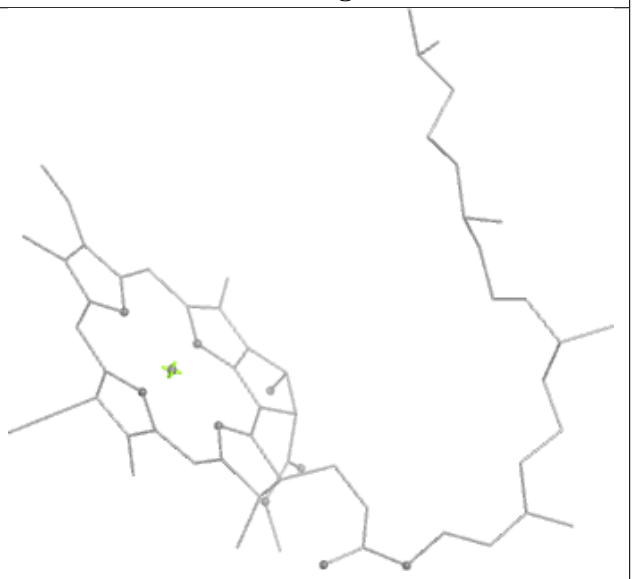
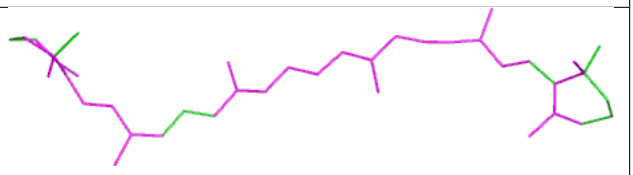


Rings

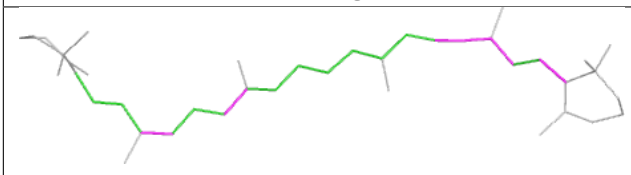
Ligand BCR B 842



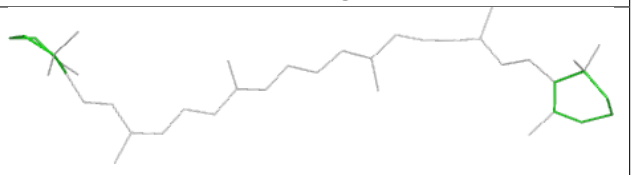
Bond lengths



Bond angles

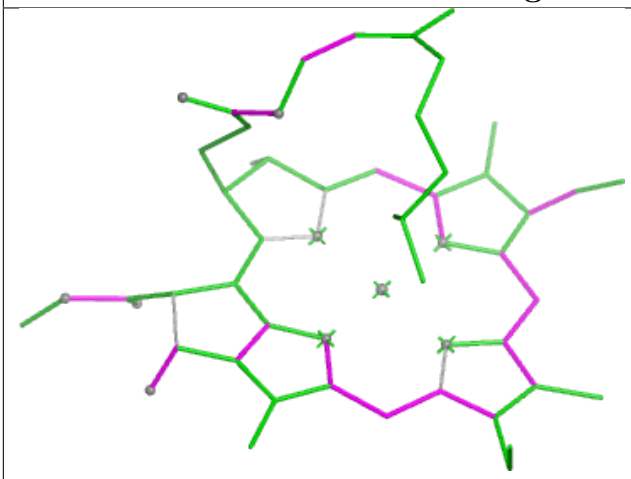


Torsions

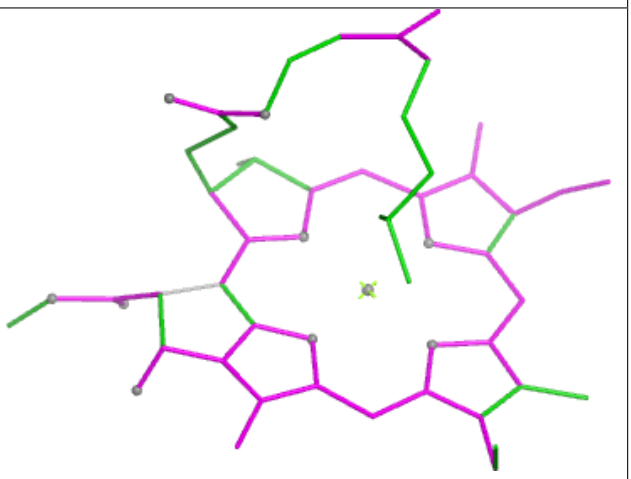


Rings

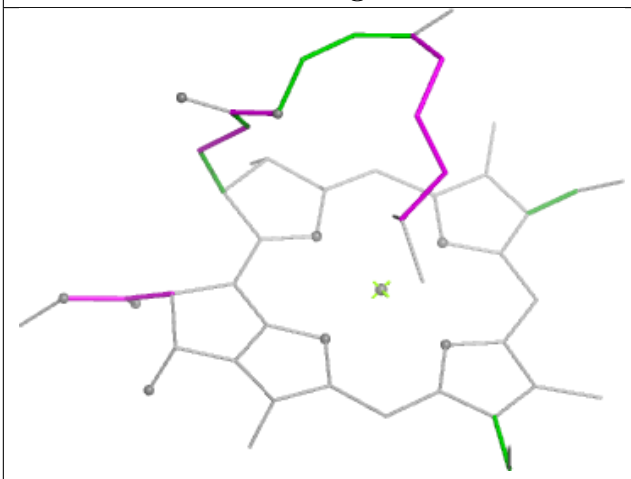
Ligand CLA B 809



Bond lengths



Bond angles



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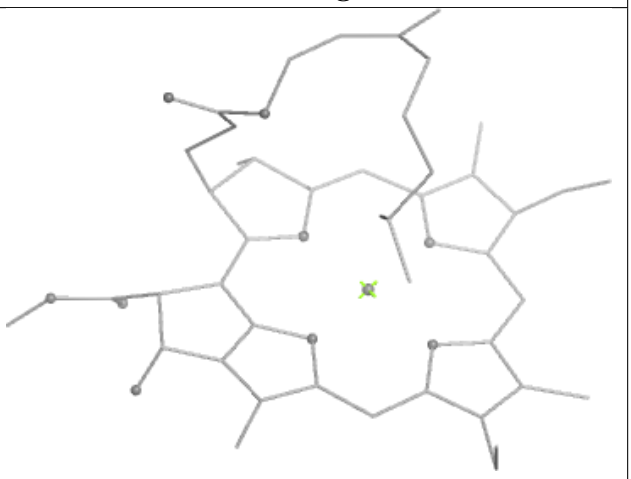
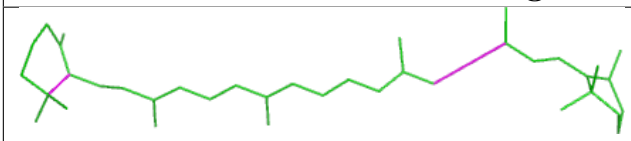
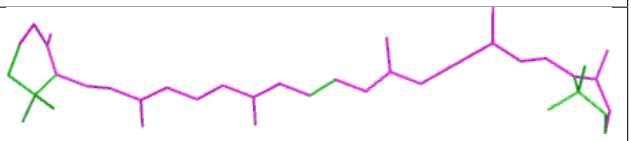


Rings

Ligand BCR J 101



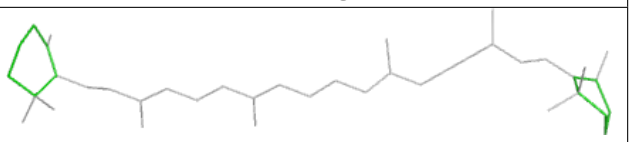
Bond lengths



Bond angles

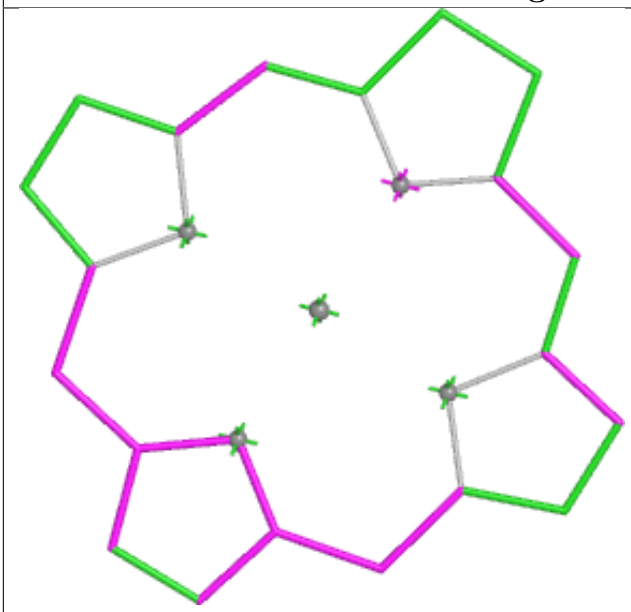


Torsions



Rings

Ligand CLA 2 305



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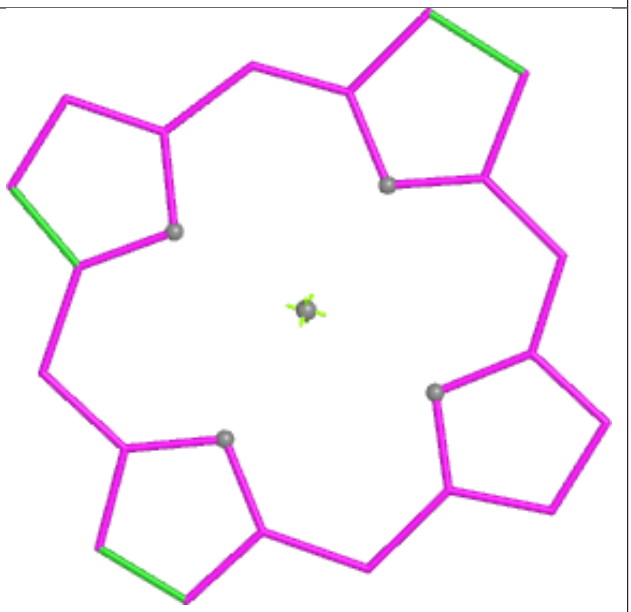
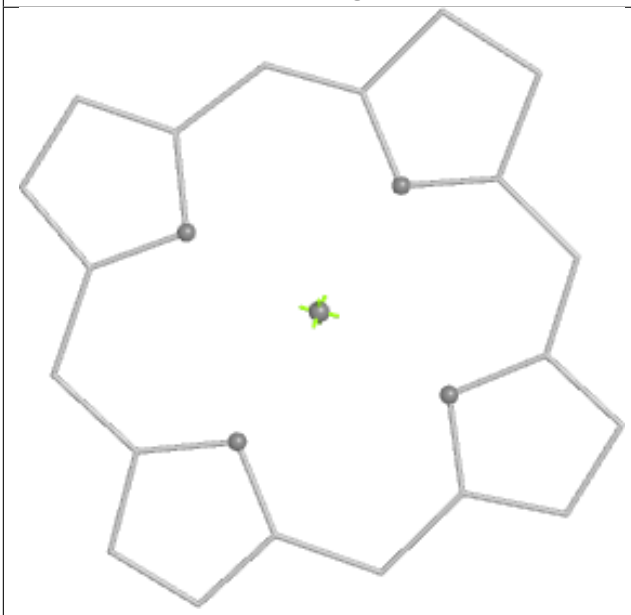


Bond angles



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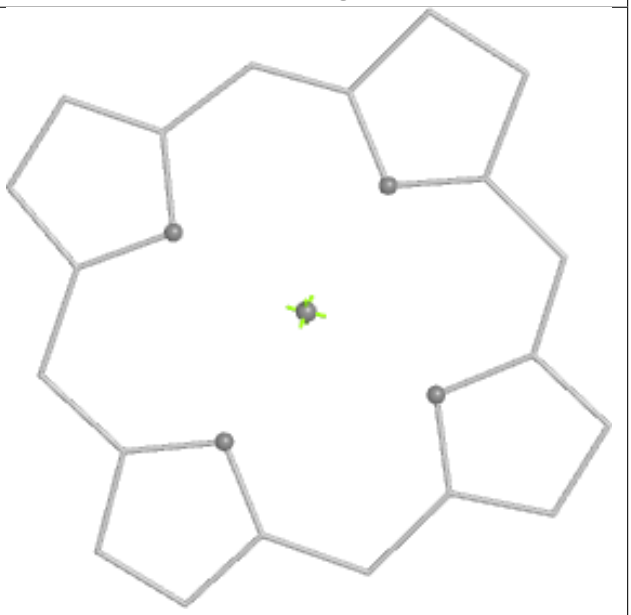
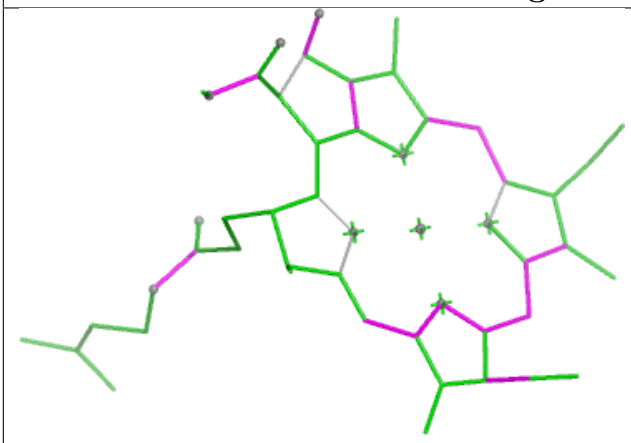
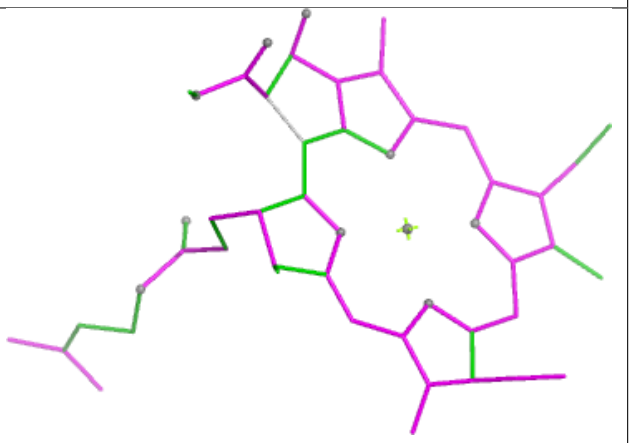


Rings

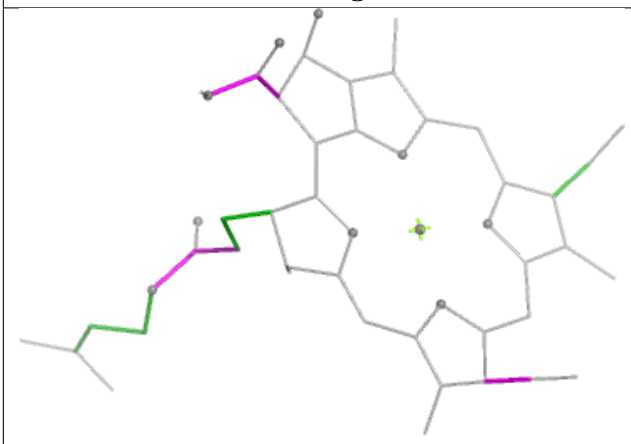
Ligand CLA 2 310



Bond lengths



Bond angles



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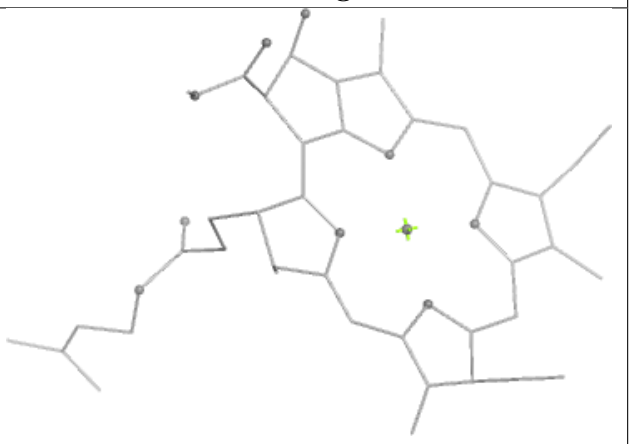
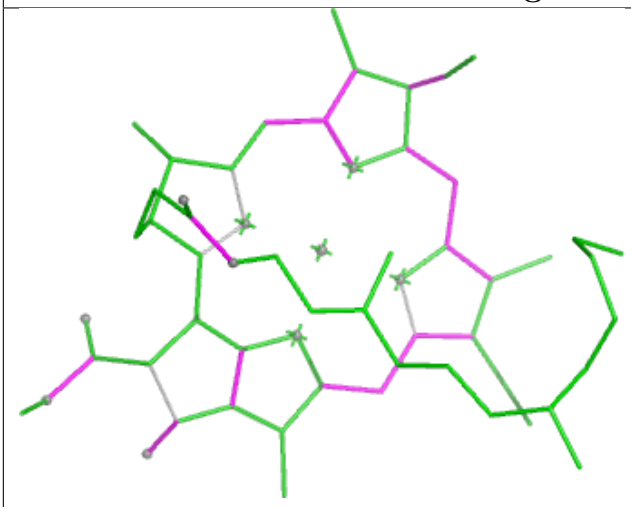


Rings

Ligand CLA B 814



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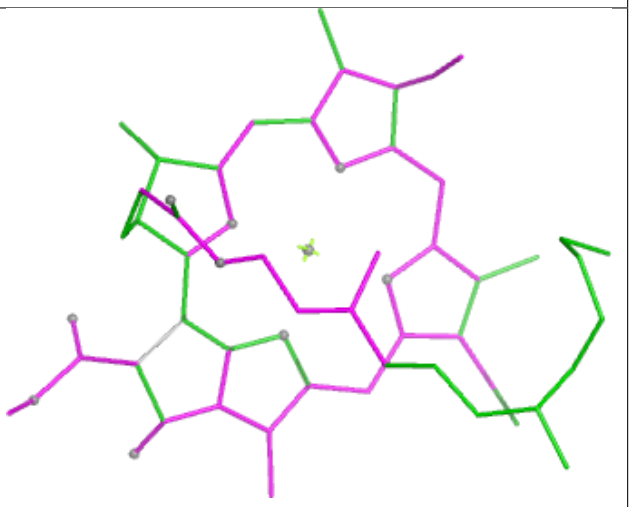
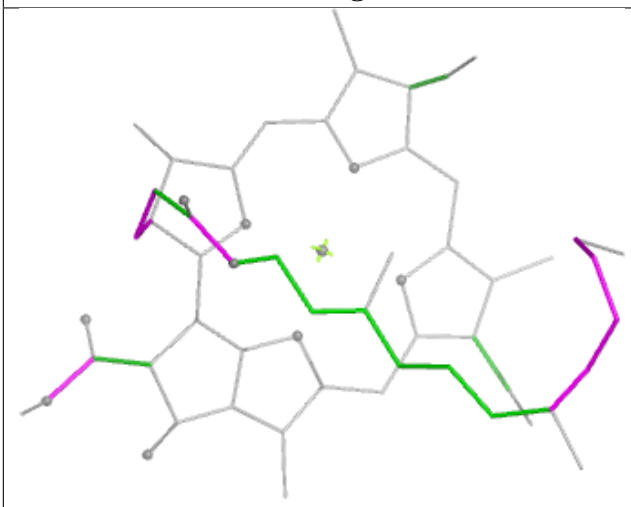
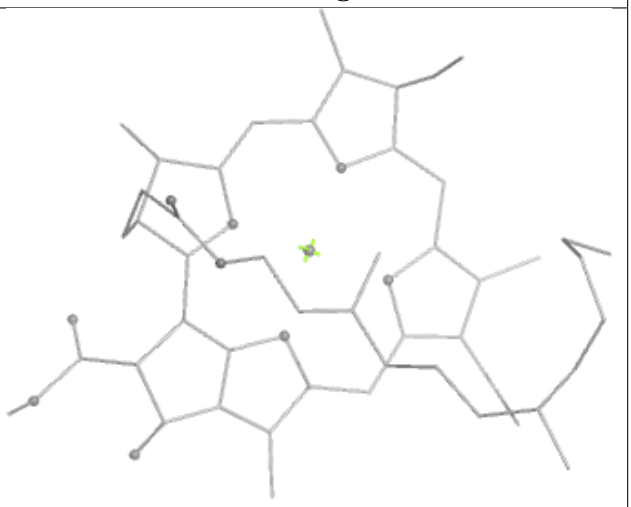


Bond angles

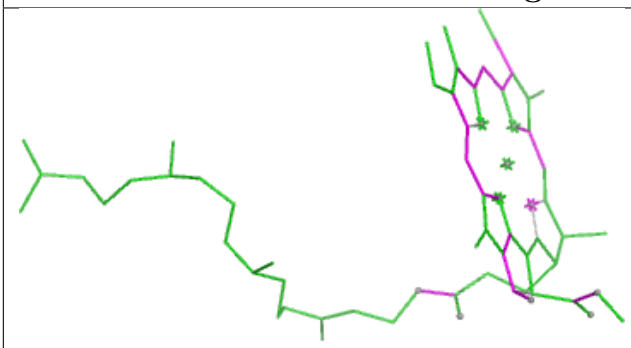


Torsions



Rings

Ligand CLA B 826



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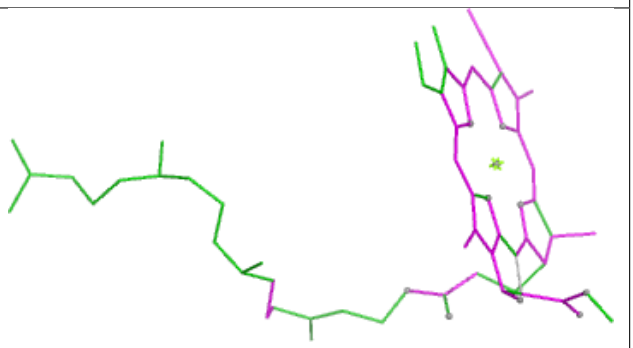
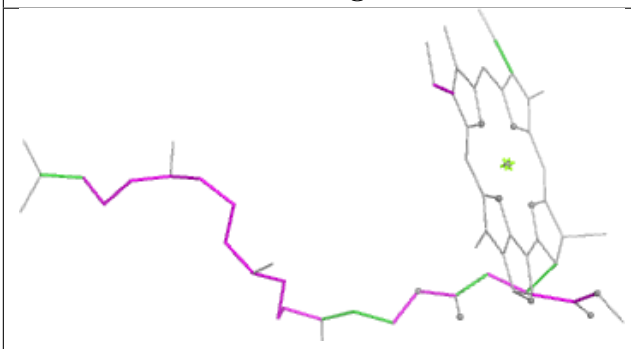


Bond angles

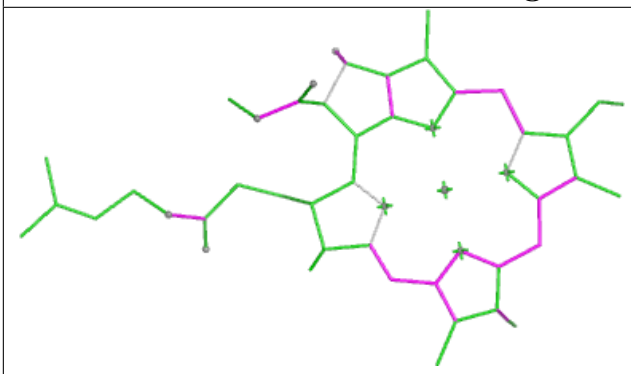


Torsions



Rings

Ligand CLA A 838



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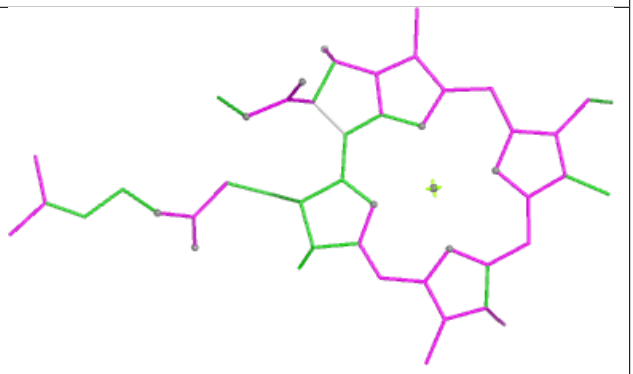
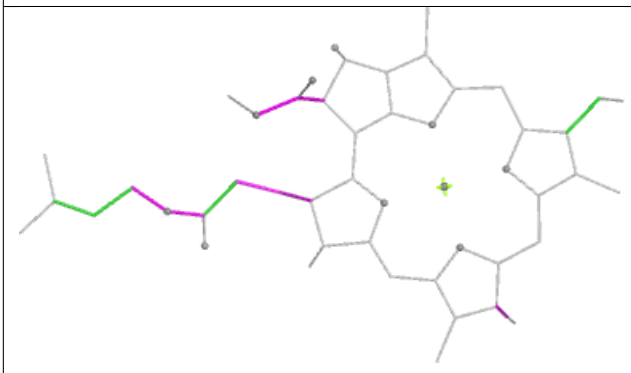


Bond angles



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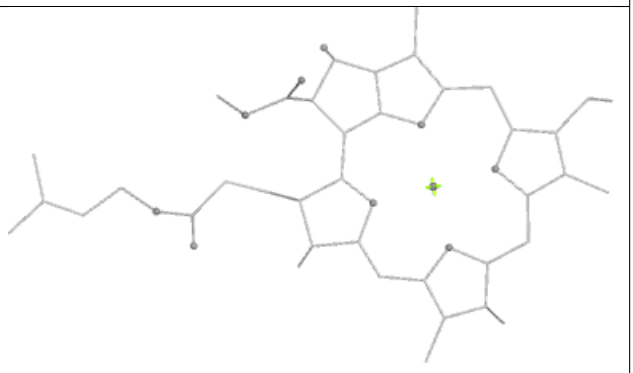
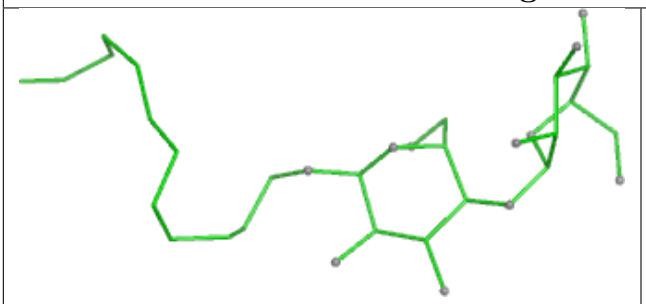


Rings

Ligand LMU R 108



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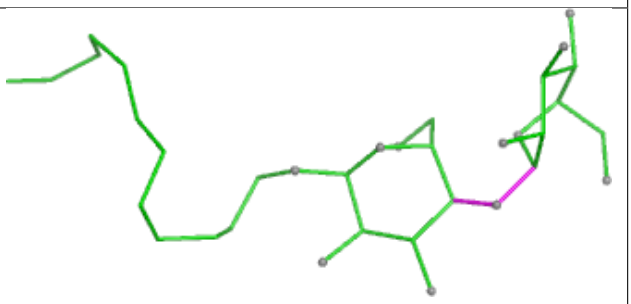
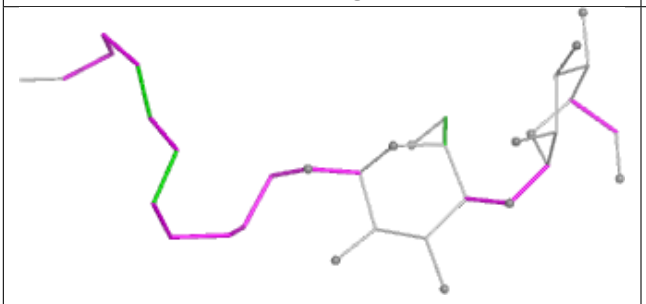


Bond angles



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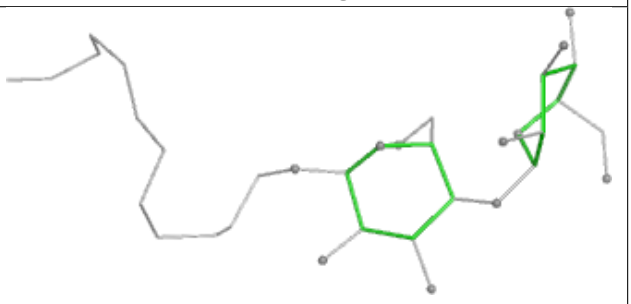
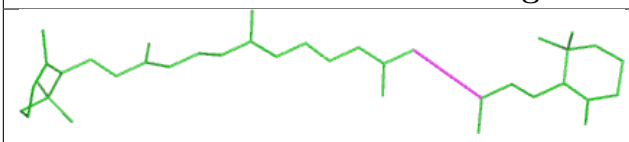


Rings

Ligand BCR A 841



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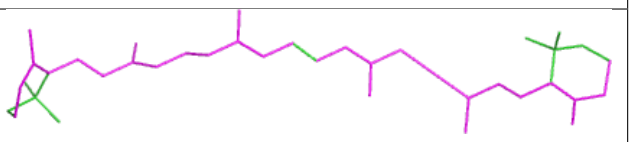
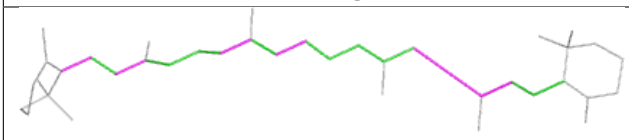


Bond angles



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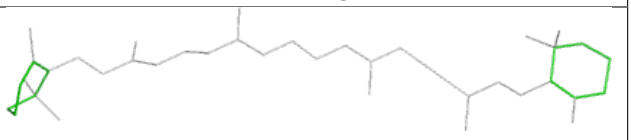
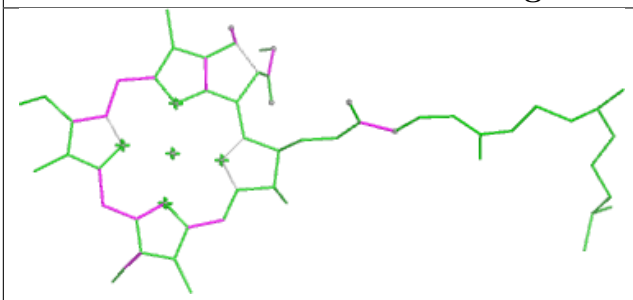
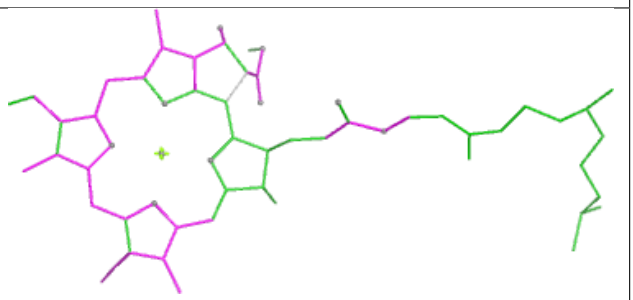


Rings

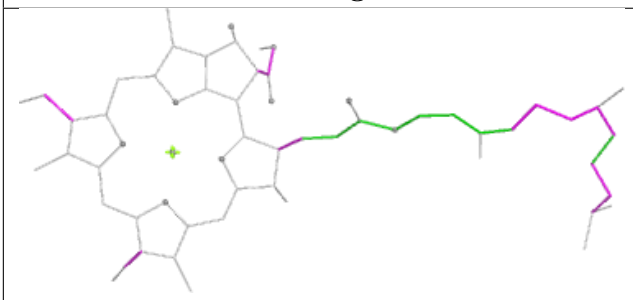
Ligand CLA B 834



Bond lengths



Bond angles



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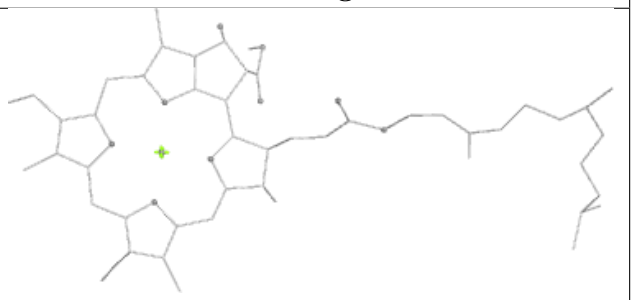
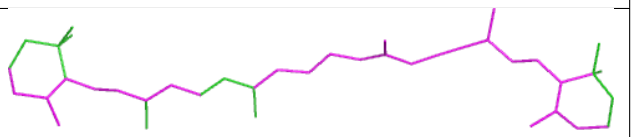


Rings

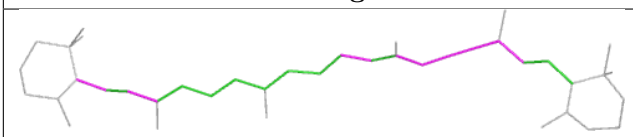
Ligand BCR L 209



Bond lengths



Bond angles



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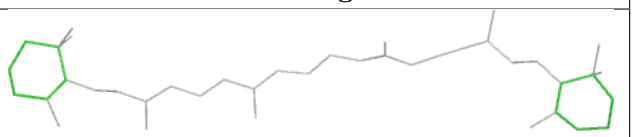
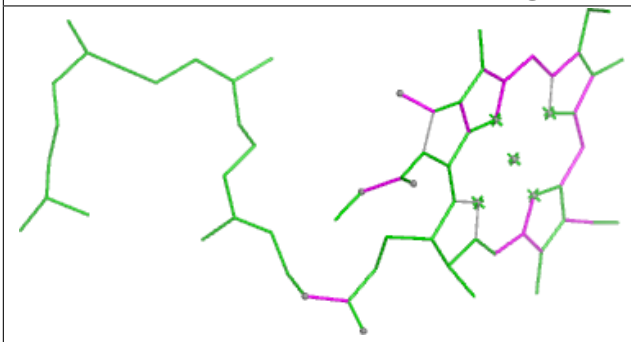
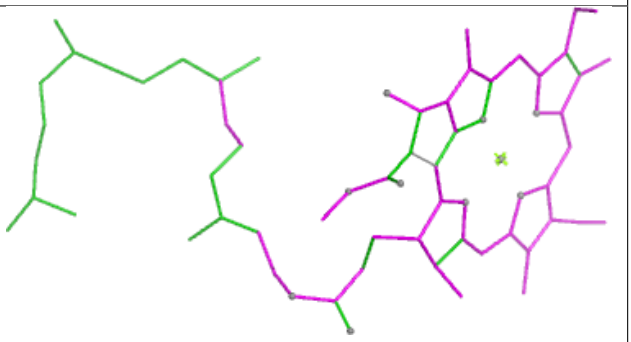


Rings

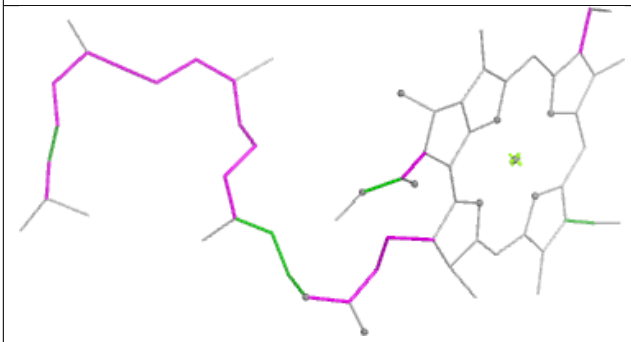
Ligand CLA A 847



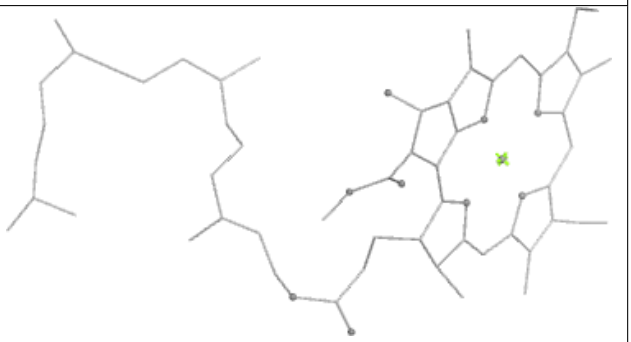
Bond lengths



Bond angles

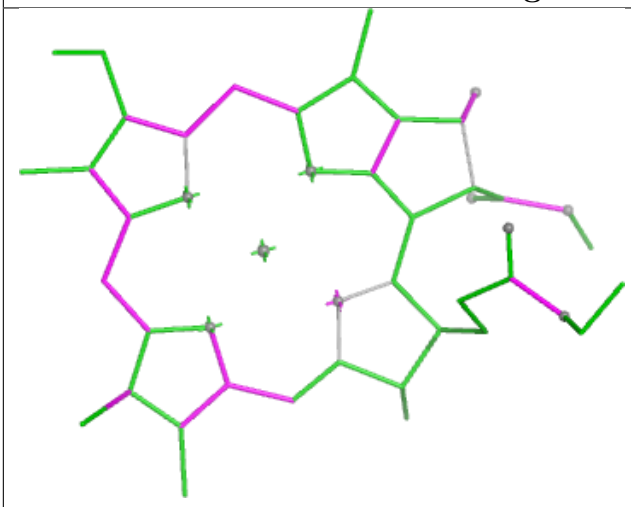


Torsions

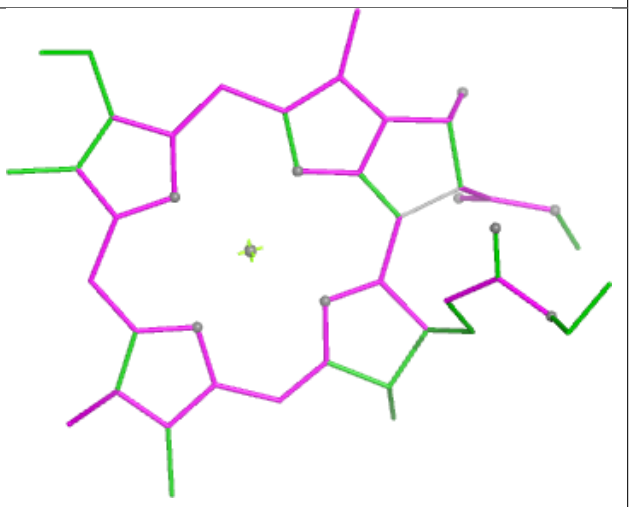


Rings

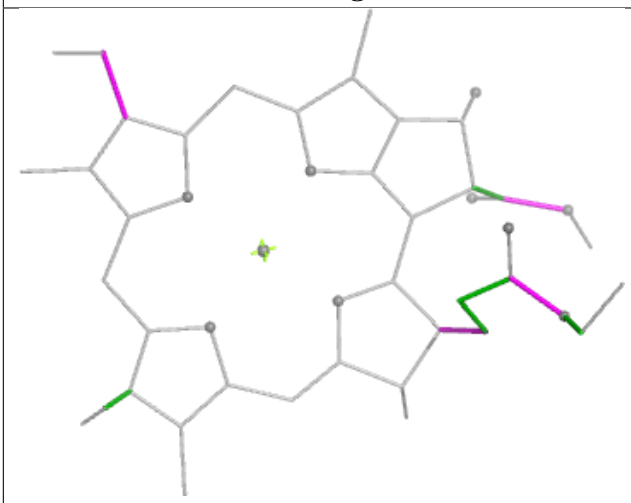
Ligand CLA A 834



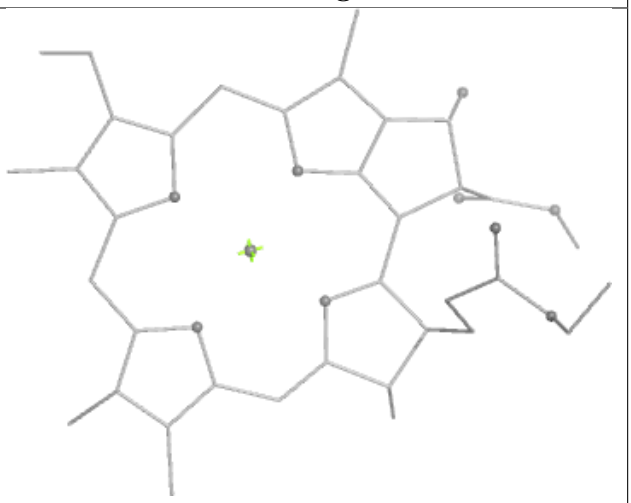
Bond lengths



Bond angles

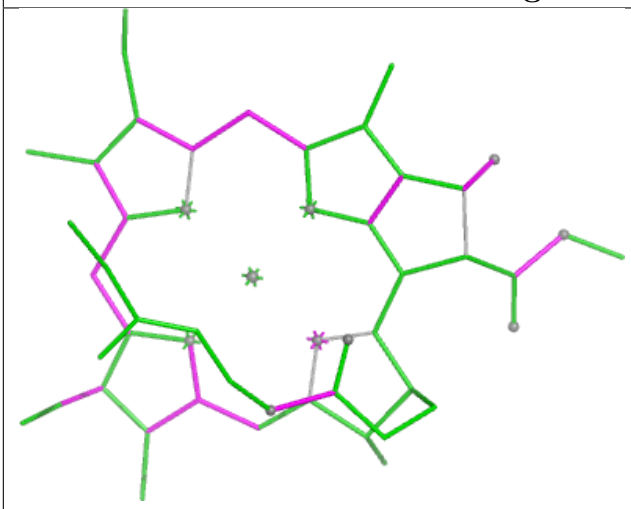


Torsions

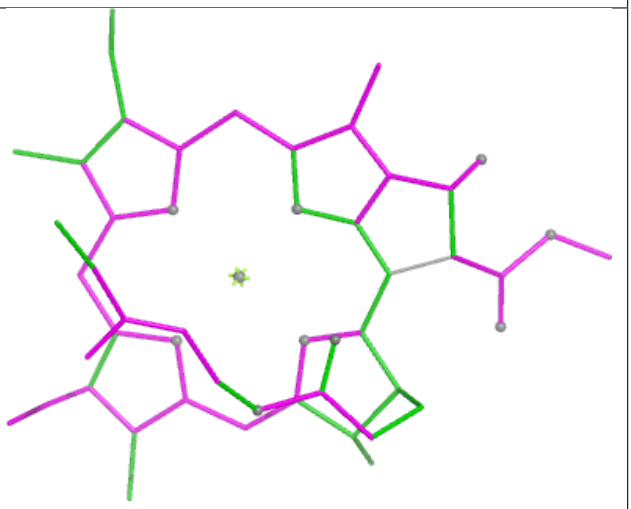


Rings

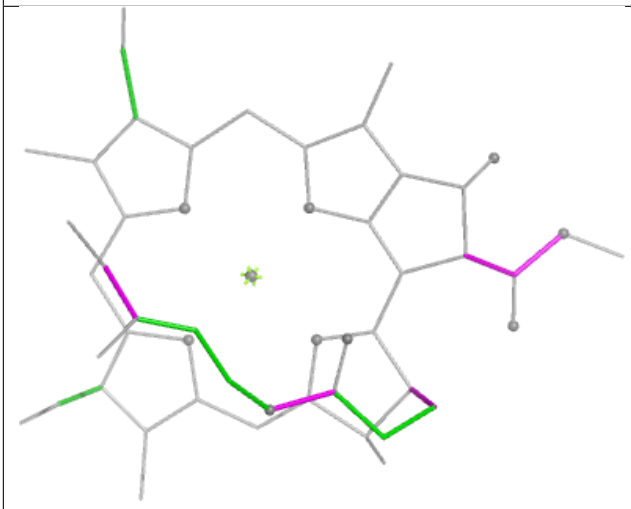
Ligand CLA A 818



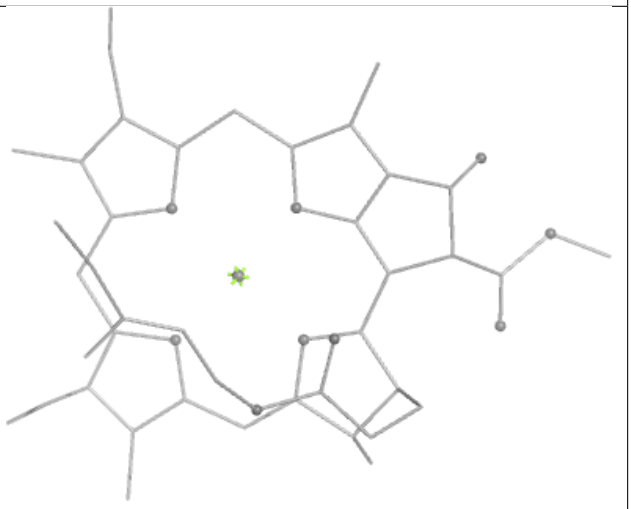
Bond lengths



Bond angles

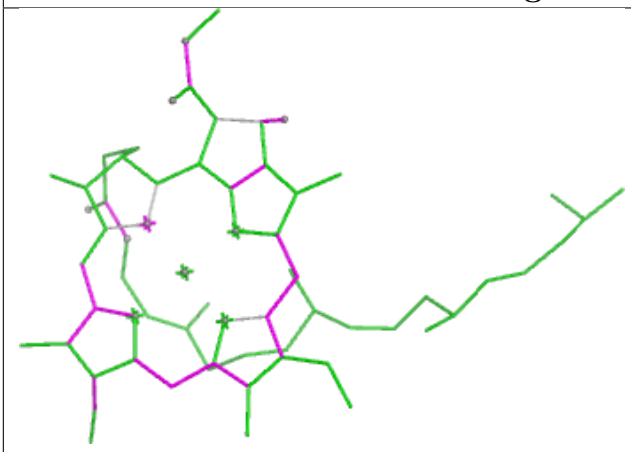


Torsions

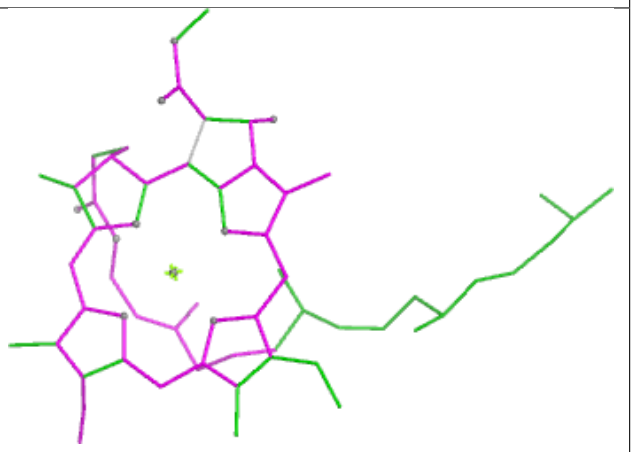


Rings

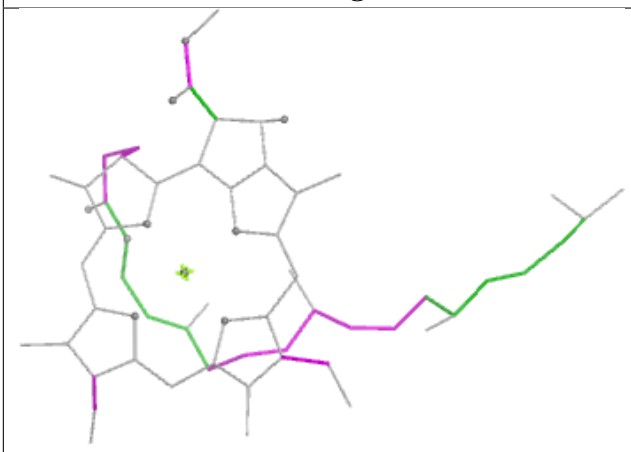
Ligand CLA B 824



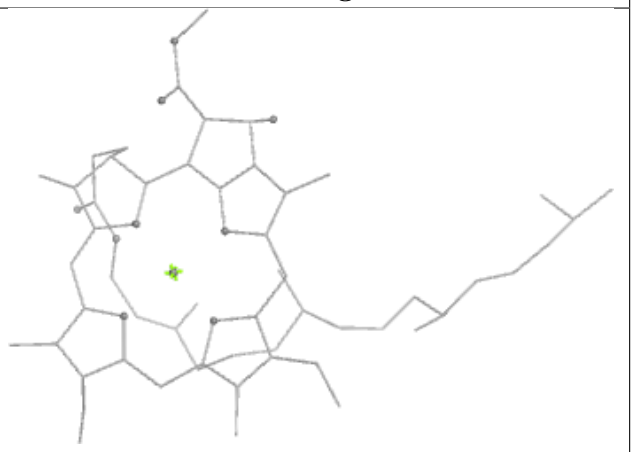
Bond lengths



Bond angles

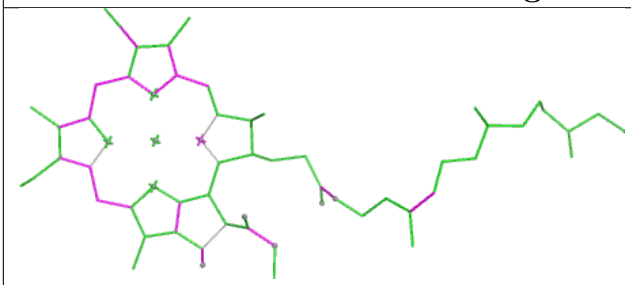


Torsions

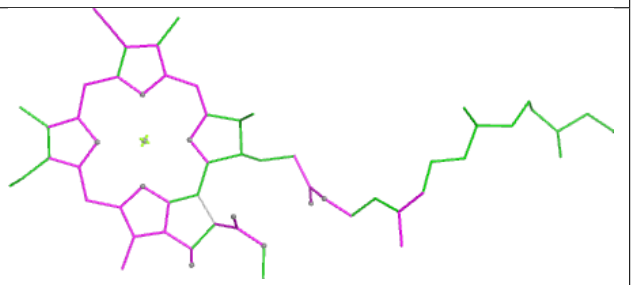


Rings

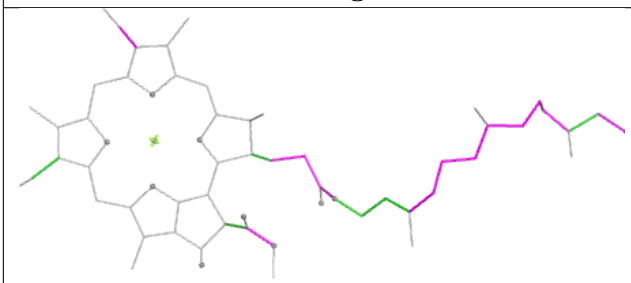
Ligand CLA A 828



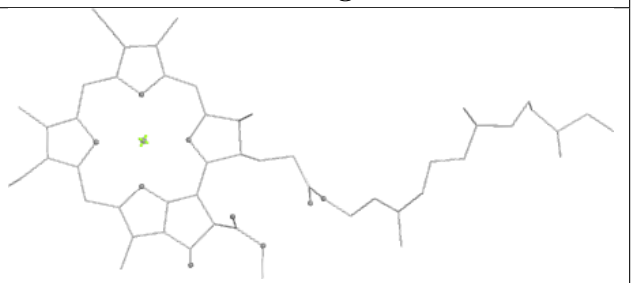
Bond lengths



Bond angles

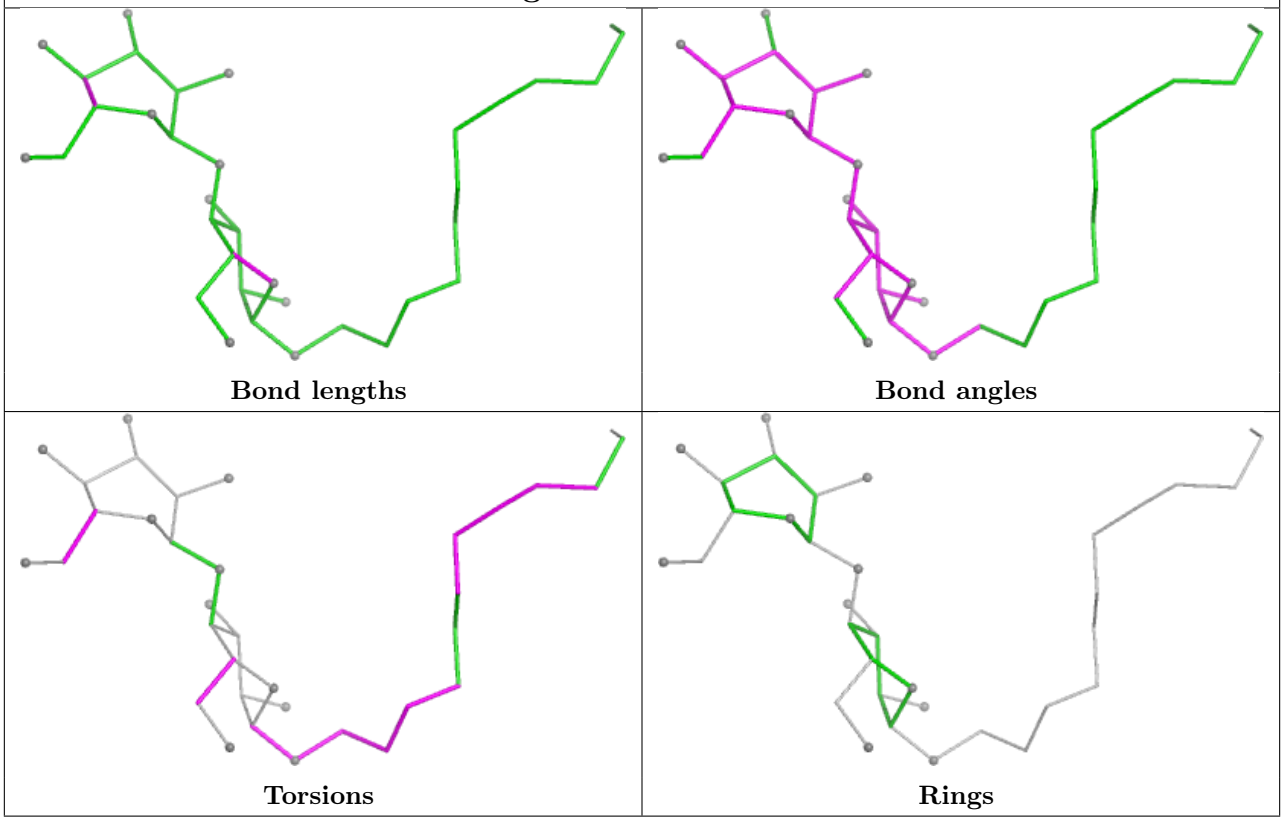


Torsions



Rings

Ligand LMU L 206



4.7 Other polymers (i)

There are no such residues in this entry.

4.8 Polymer linkage issues (i)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
5	A	1

All chain breaks are listed below:

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

5 Fit of model and data

5.1 Protein, DNA and RNA chains

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

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

The worst 5 of 827 RSRZ outliers are listed below:

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

Continued on next page...

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

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

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

5.3 Carbohydrates (i)

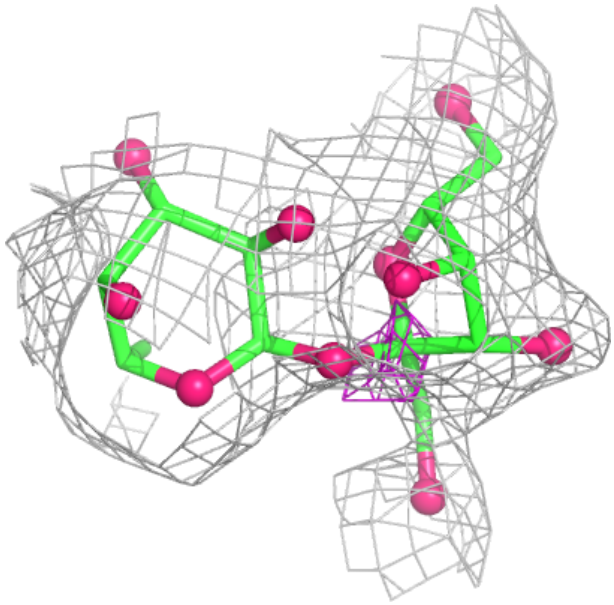
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

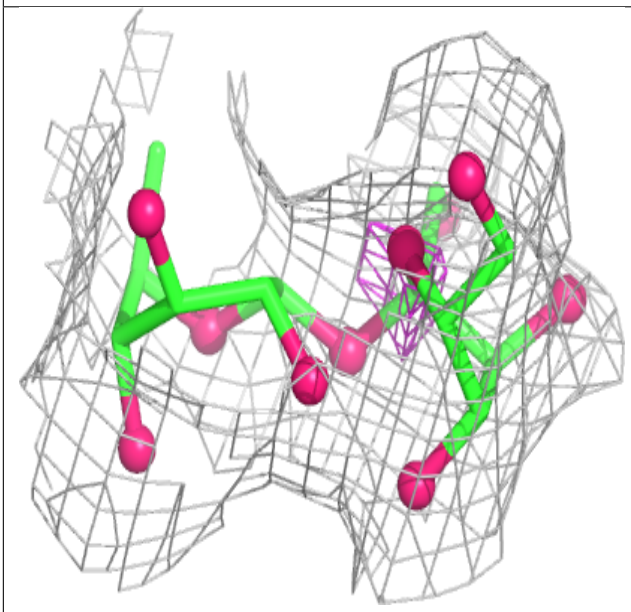
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
19	GLC	M	1	10/12	-	-	20,20,20,20	0
19	FRU	M	2	12/12	-	-	20,20,20,20	0
19	GLC	O	1	11/12	-	-	20,20,20,20	0
19	FRU	O	2	12/12	-	-	20,20,20,20	0
19	GLC	P	1	11/12	-	-	20,20,20,20	0
19	FRU	P	2	12/12	-	-	20,20,20,20	0
19	GLC	Q	1	11/12	-	-	20,20,20,20	0
19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

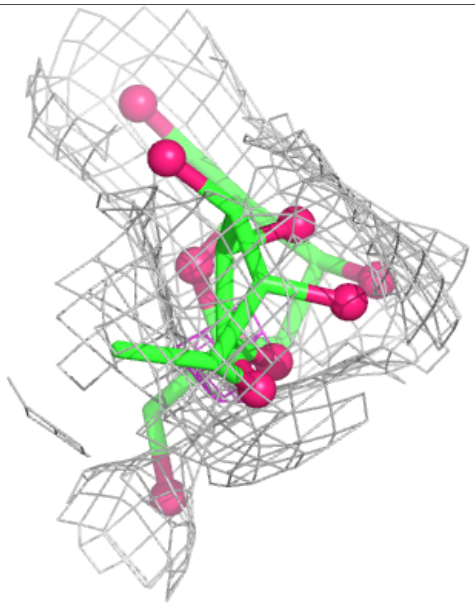
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around Chain M:

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

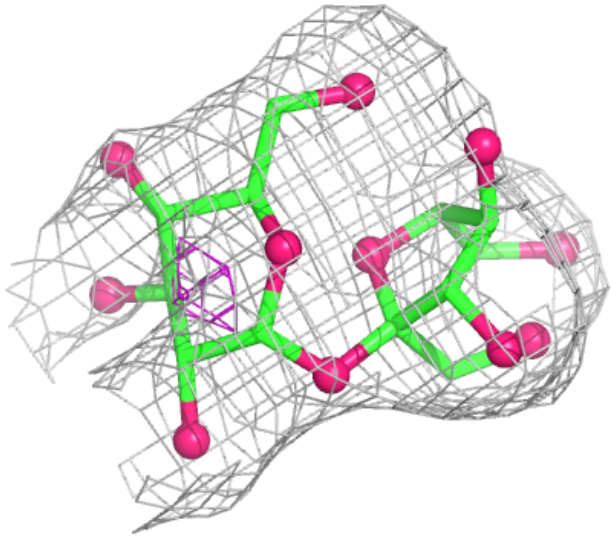


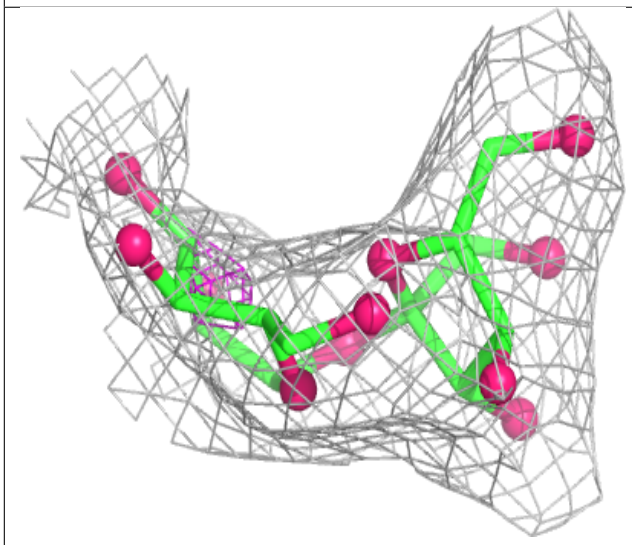


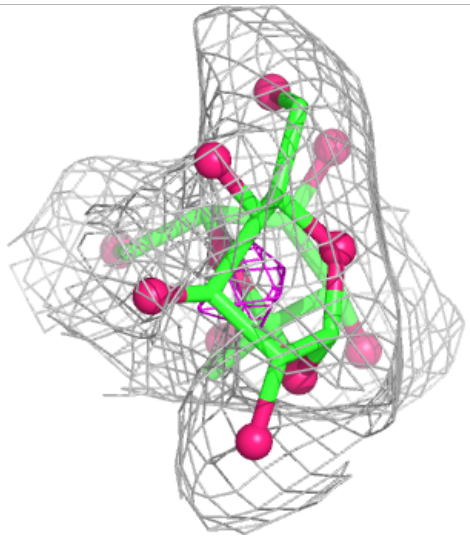


Electron density around Chain O:

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

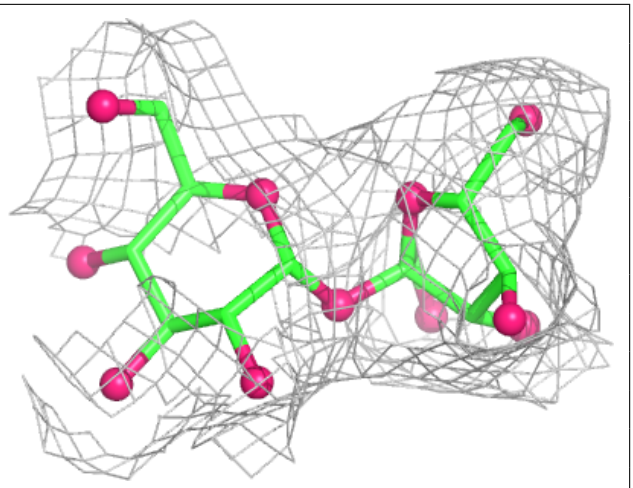


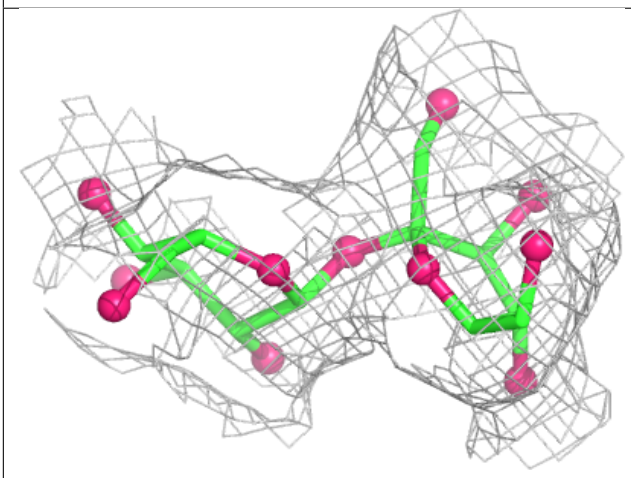


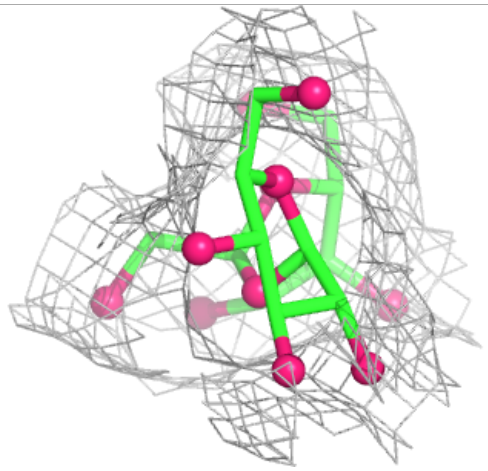


Electron density around Chain P:

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

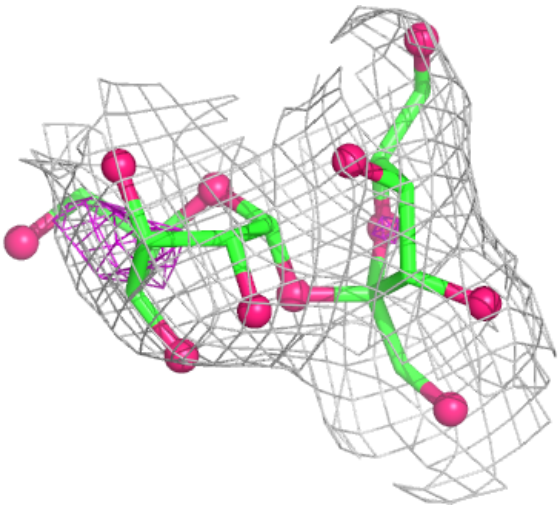


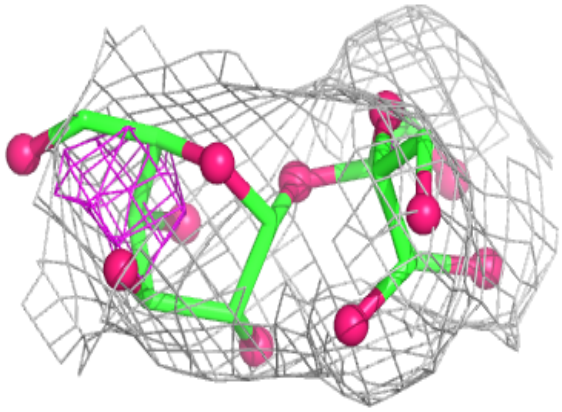


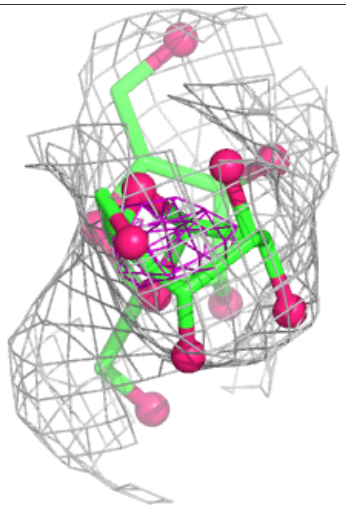


Electron density around Chain Q:

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

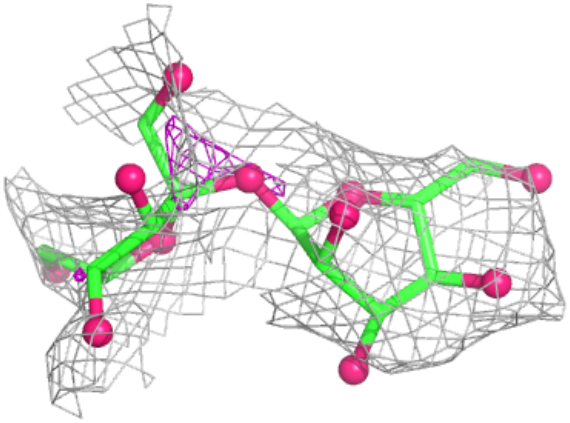


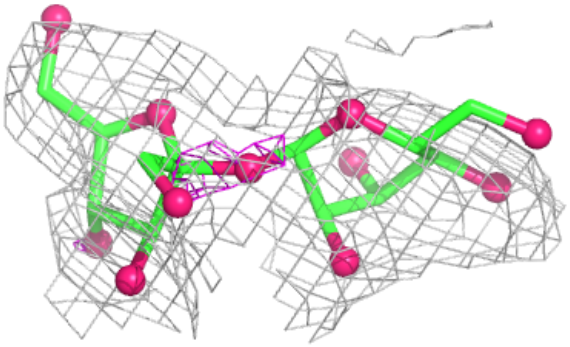


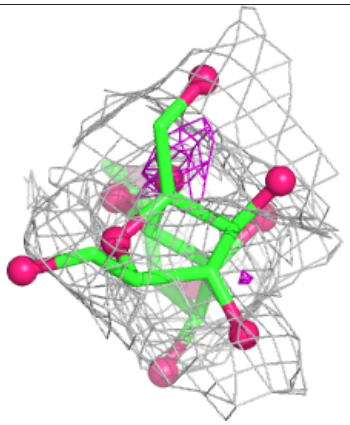


Electron density around Chain S:

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

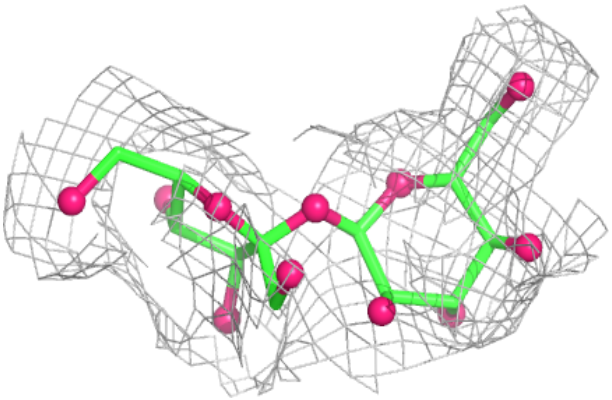


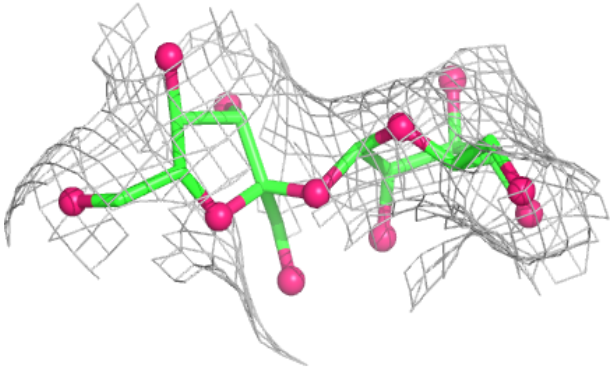


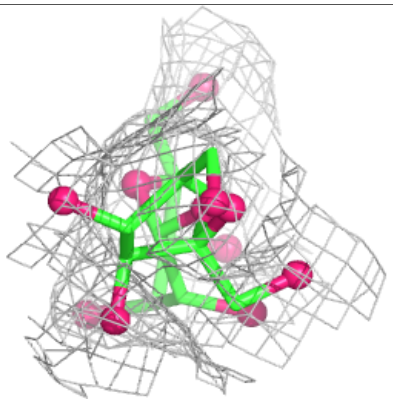


Electron density around Chain T:

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

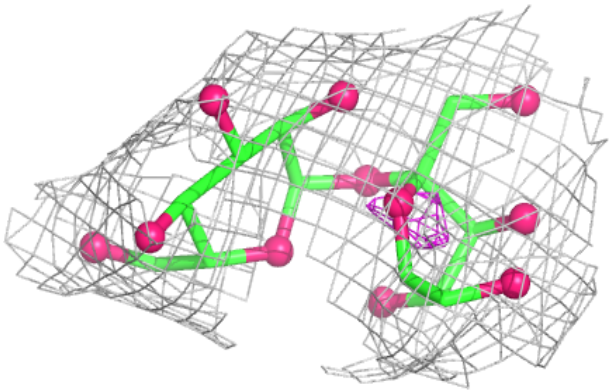


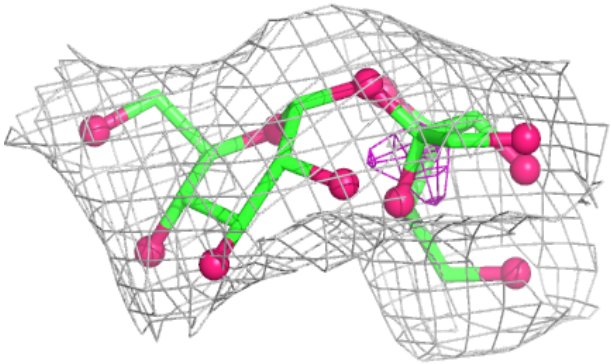


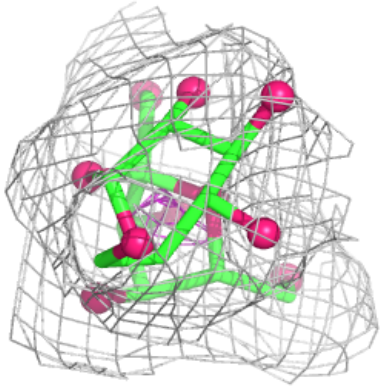


Electron density around Chain U:

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

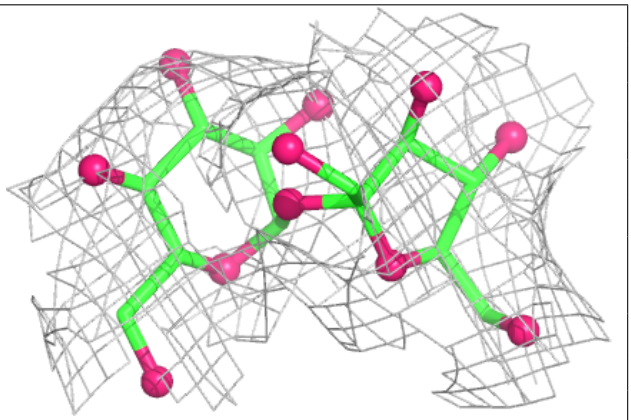


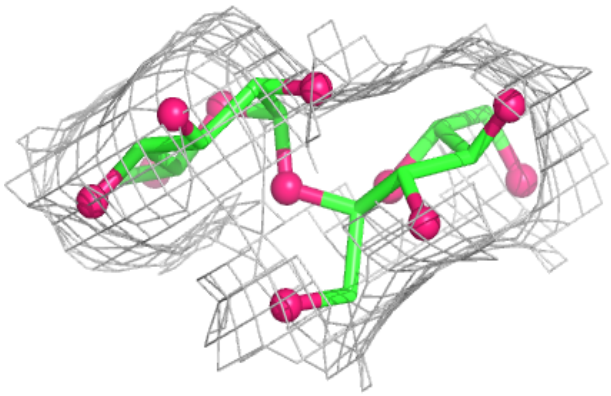


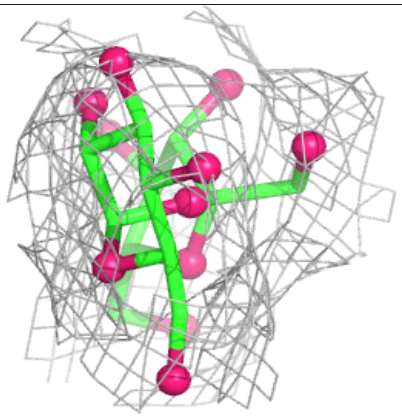


Electron density around Chain V:

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

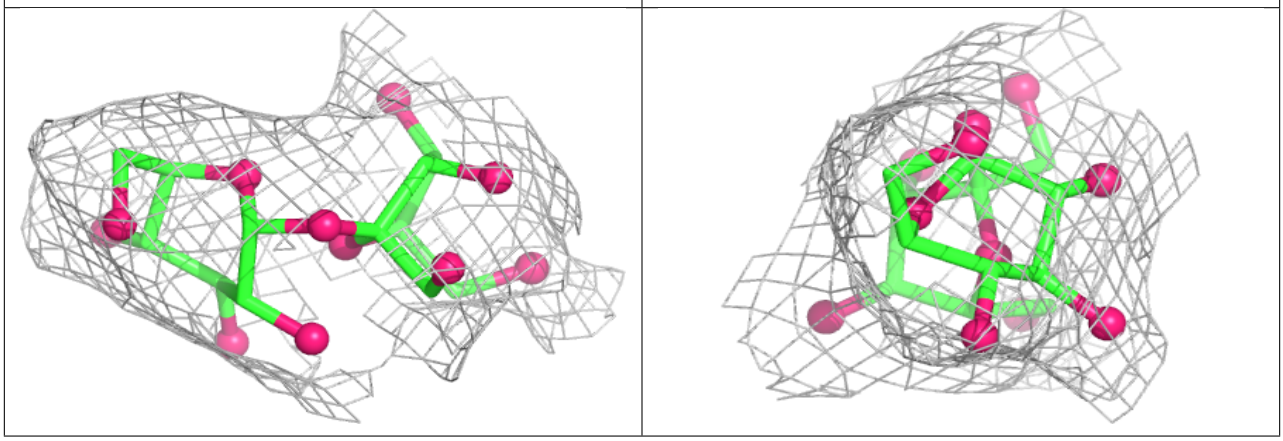






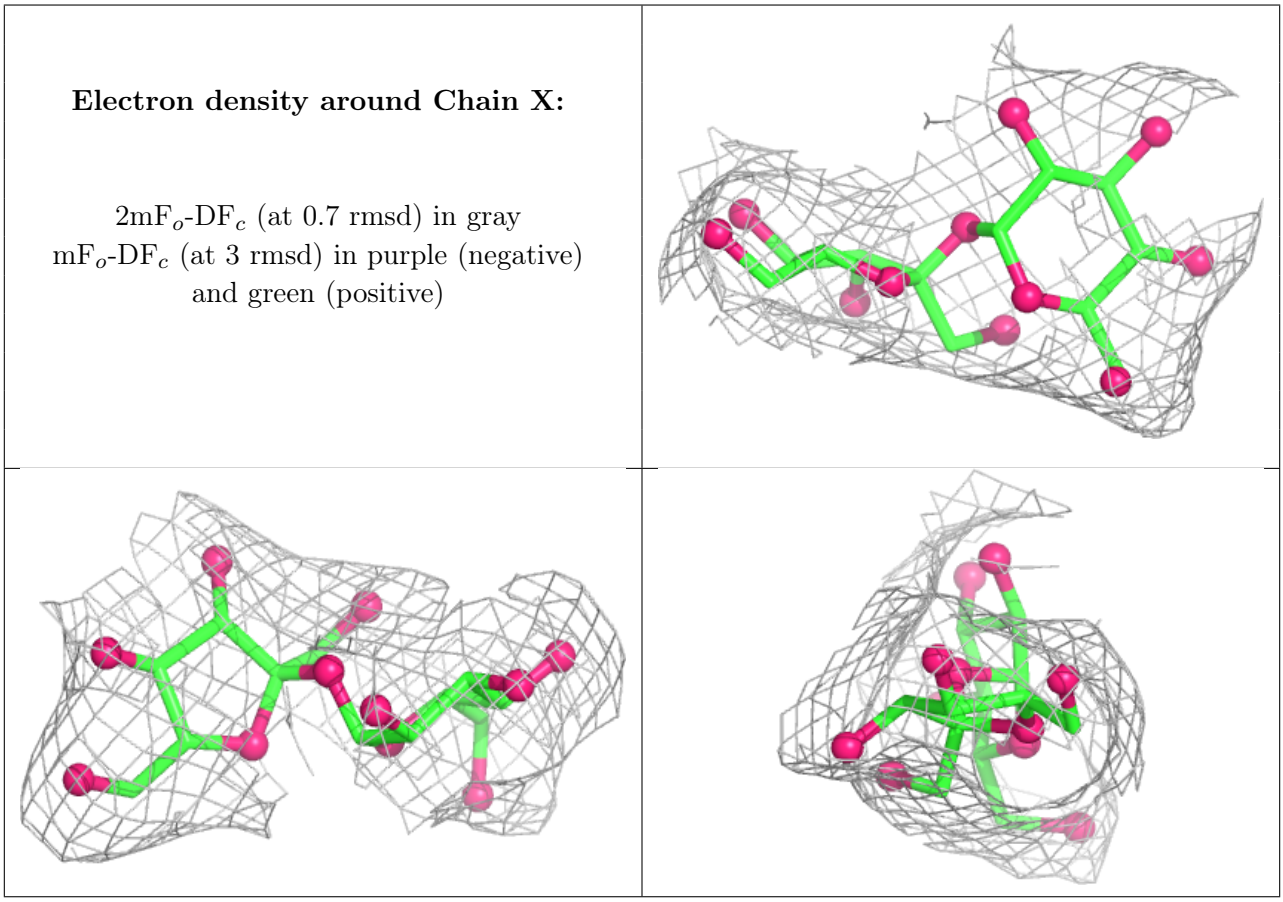
Electron density around Chain W:

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



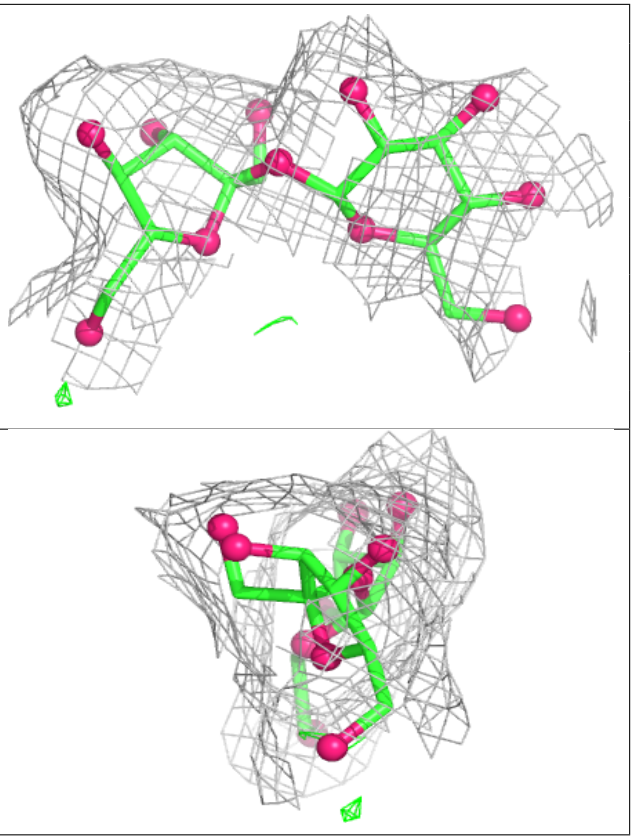
Electron density around Chain X:

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



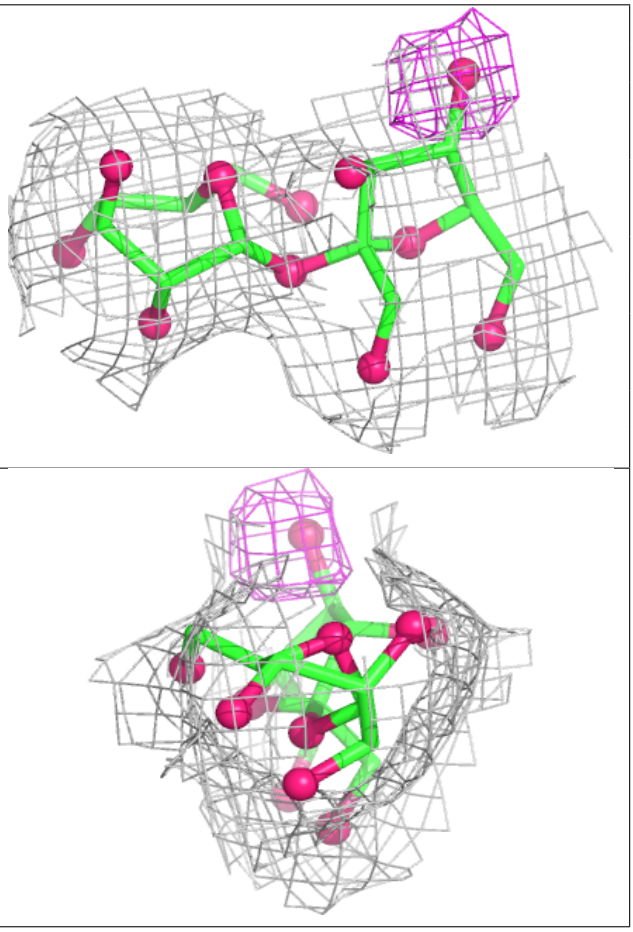
Electron density around Chain Y:

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



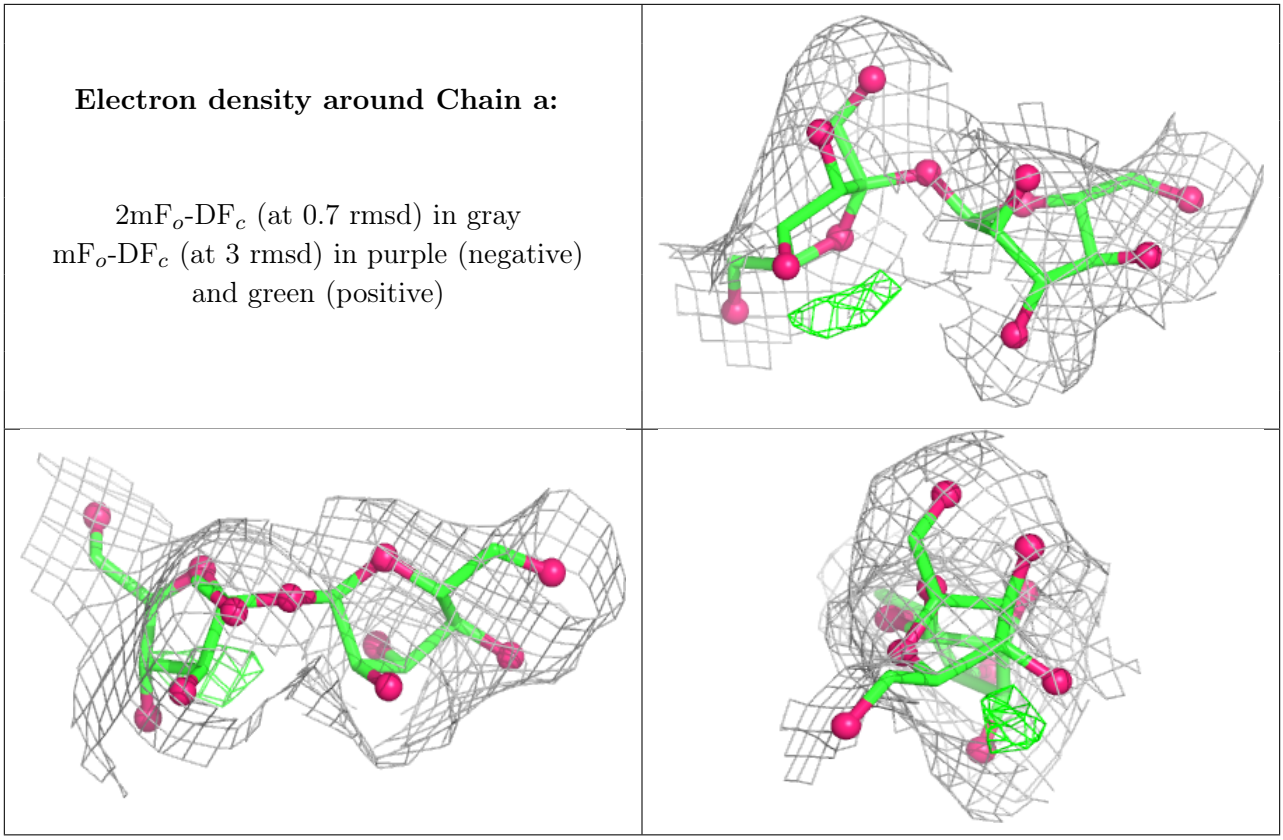
Electron density around Chain Z:

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



Electron density around Chain a:

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



5.4 Ligands

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
20	CLA	A	857	25/65	0.43	0.17	5,42,60,60	0
22	BCR	A	840	40/40	0.50	0.24	20,20,20,20	0
21	LMU	1	217	35/35	0.57	0.16	20,20,20,20	0
20	CLA	H	110	55/65	0.58	0.17	20,20,20,20	0
20	CLA	3	308	25/65	0.58	0.19	20,20,20,20	0
20	CLA	1	213	25/65	0.58	0.22	20,20,20,20	0
20	CLA	2	307	65/65	0.59	0.18	20,20,20,20	0
22	BCR	J	101	40/40	0.59	0.22	20,20,20,20	0
21	LMU	E	101	35/35	0.60	0.18	20,20,20,20	0
20	CLA	H	108	55/65	0.61	0.16	20,20,20,20	0
22	BCR	3	311	40/40	0.61	0.19	20,20,20,20	0
20	CLA	4	317	25/65	0.61	0.17	20,20,20,20	0
20	CLA	2	301	51/65	0.61	0.20	20,20,20,20	0
20	CLA	A	837	65/65	0.62	0.17	20,20,20,20	0

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

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

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

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

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

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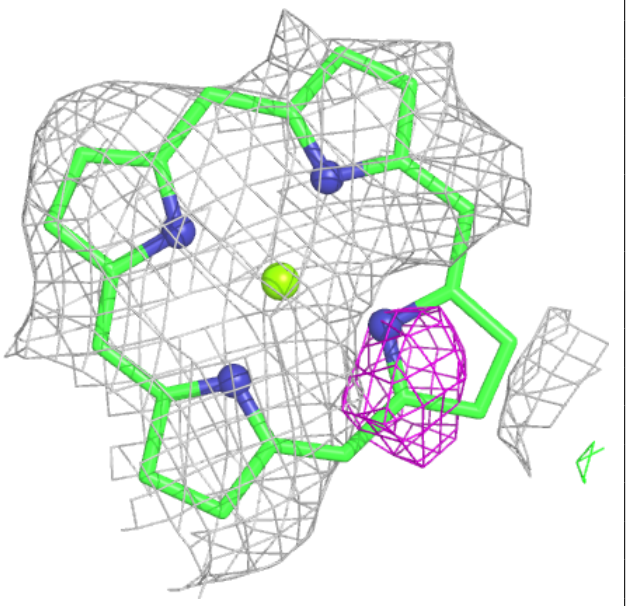
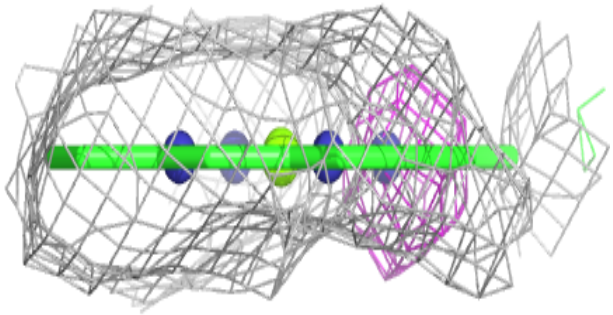
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
26	UNL	H	106	23/-	0.86	0.09	20,20,20,20	0
20	CLA	B	824	65/65	0.87	0.18	20,20,20,20	0
20	CLA	A	834	47/65	0.87	0.17	20,20,20,20	0
20	CLA	B	838	65/65	0.87	0.17	20,20,20,20	0
20	CLA	B	821	54/65	0.87	0.18	20,20,20,20	0
20	CLA	B	847	65/65	0.87	0.20	20,20,20,20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

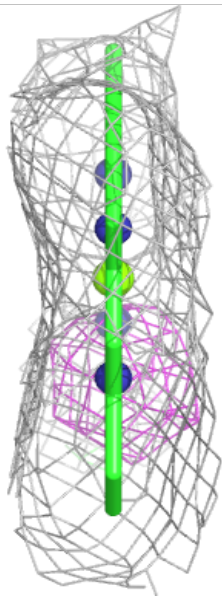
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around CLA A 857:

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

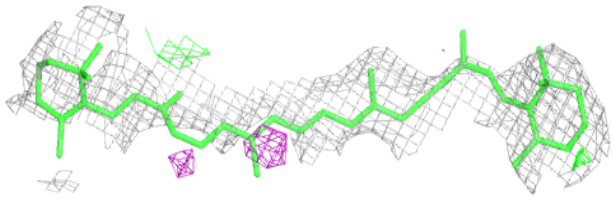


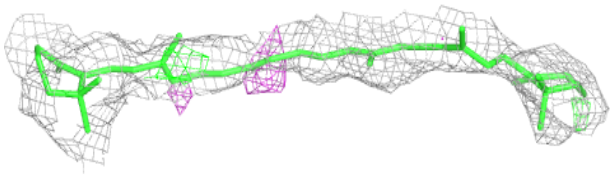


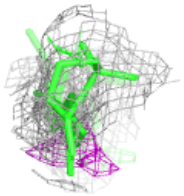


Electron density around BCR A 840:

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

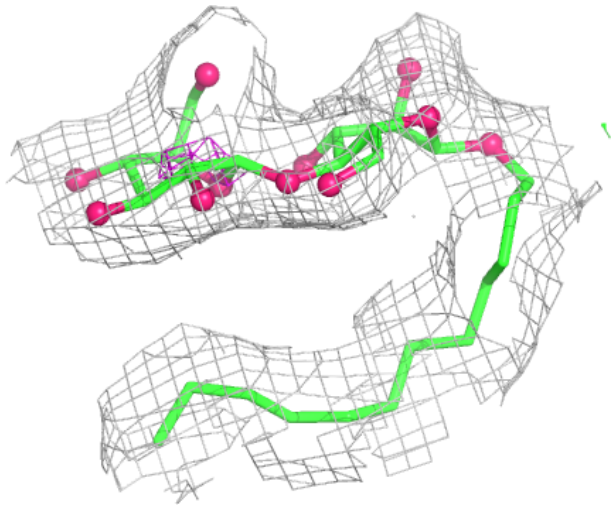


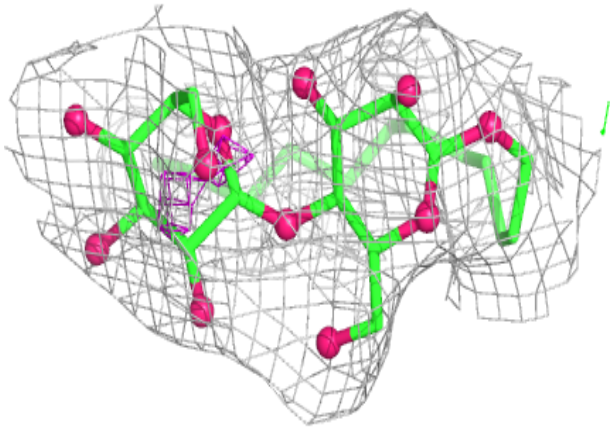




Electron density around LMU 1 217:

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

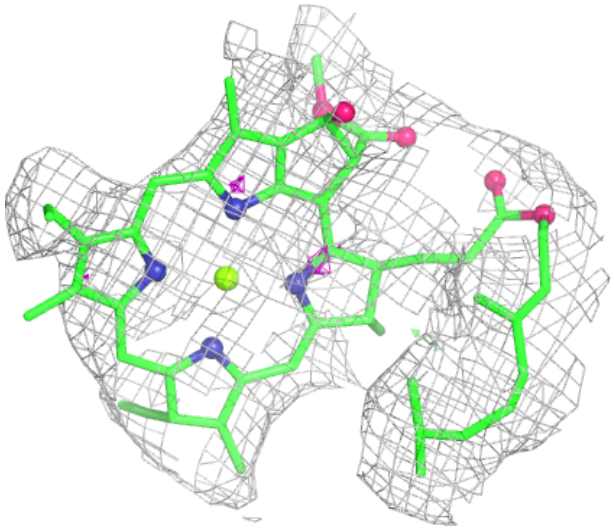


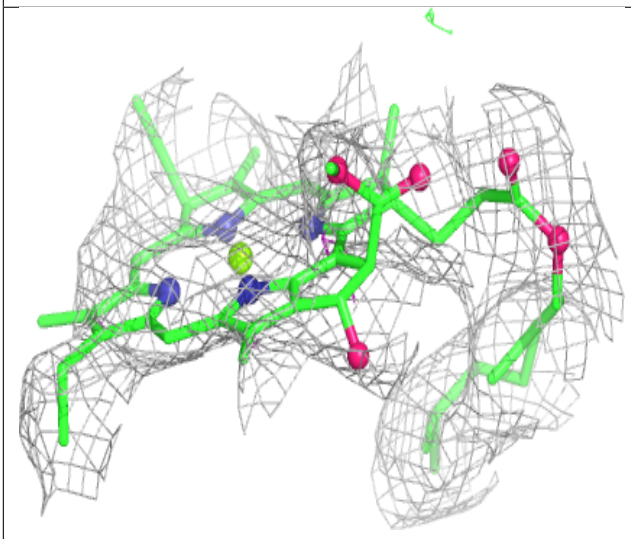


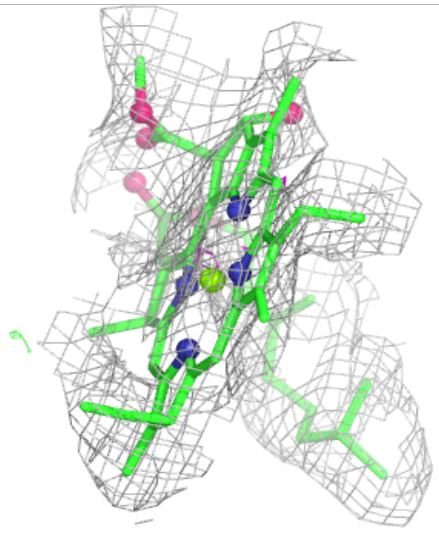


Electron density around CLA H 110:

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

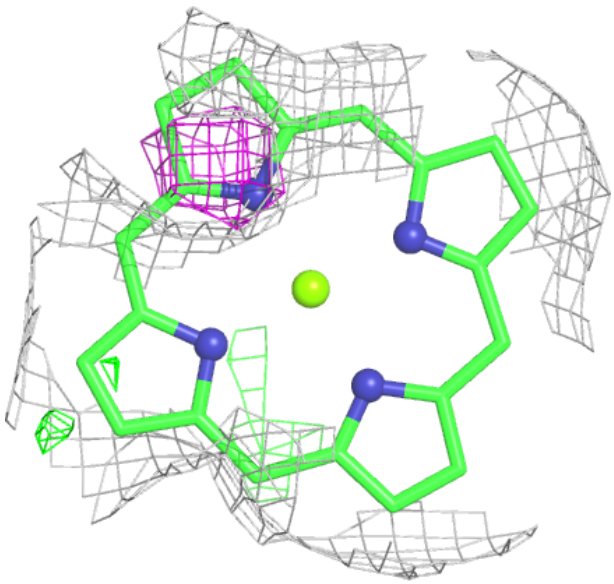


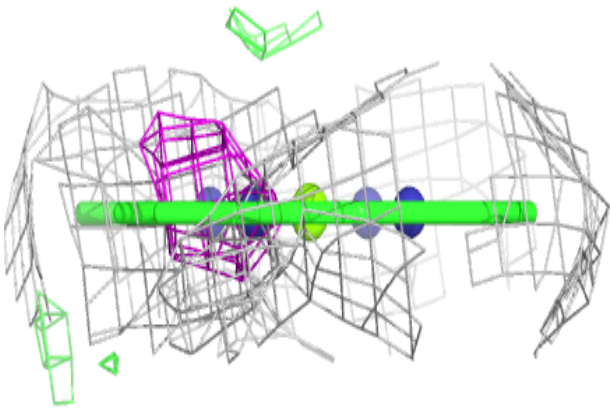


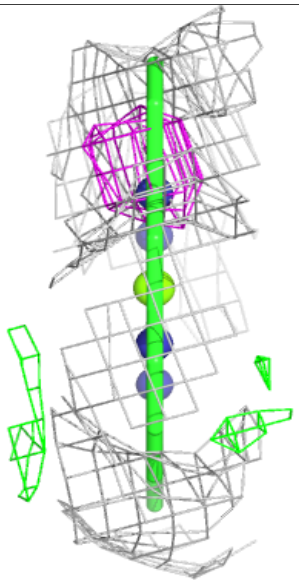


Electron density around CLA 3 308:

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

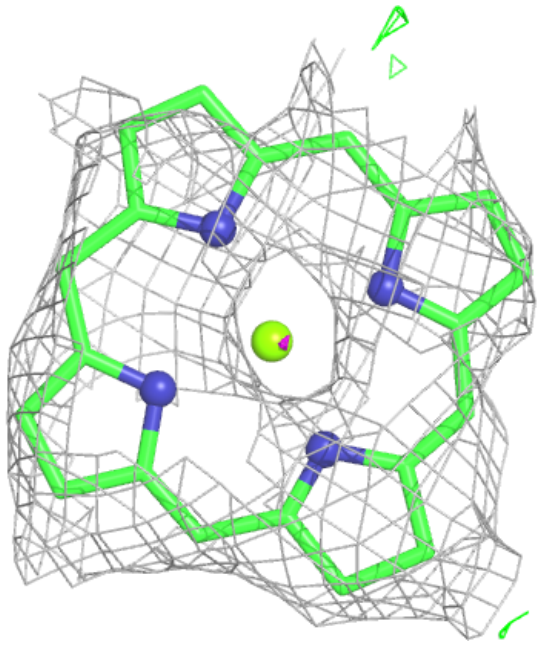


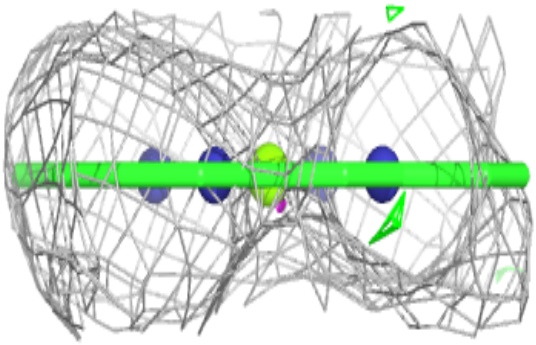


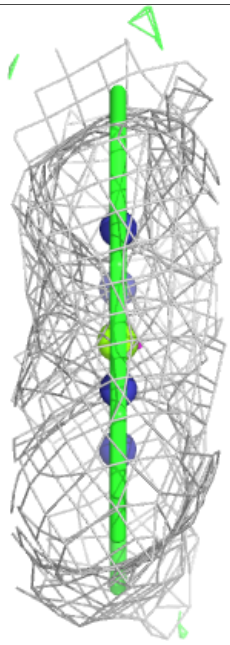


Electron density around CLA 1 213:

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

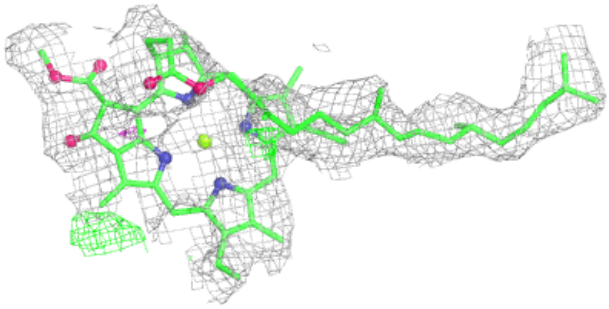


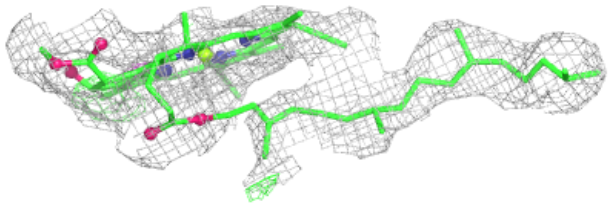


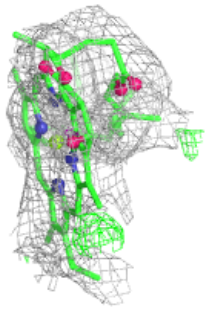


Electron density around CLA 2 307:

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

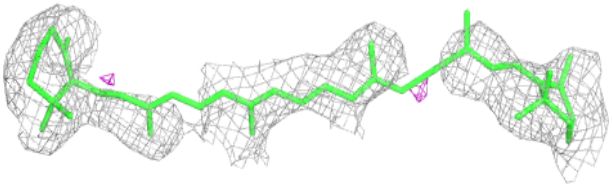


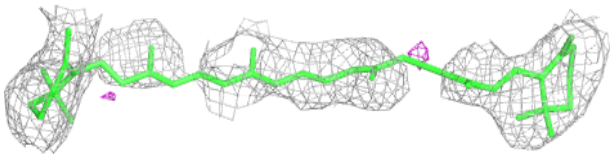


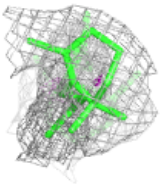


Electron density around BCR J 101:

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

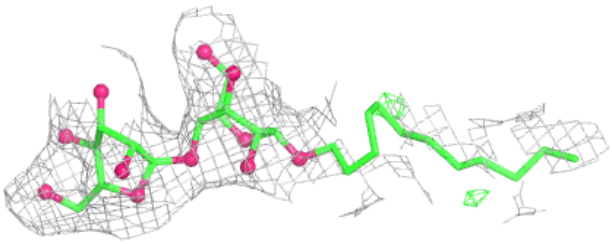


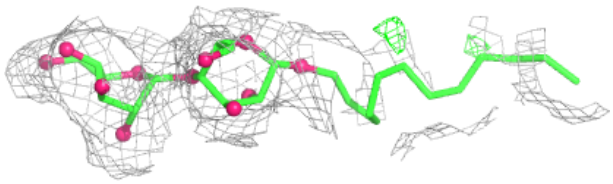


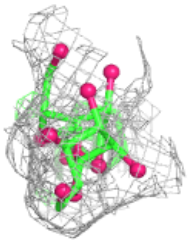


Electron density around LMU E 101:

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

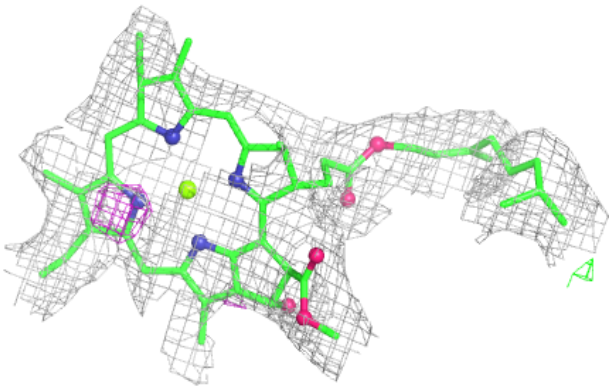


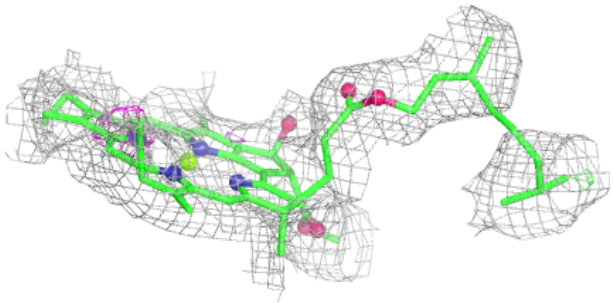


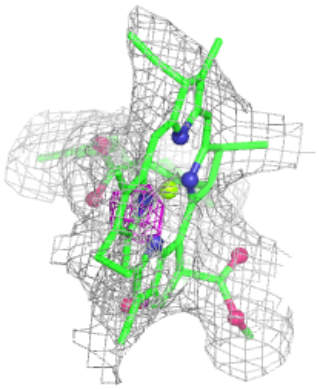


Electron density around CLA H 108:

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



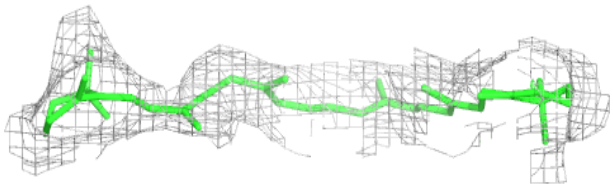




Electron density around BCR 3 311:

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

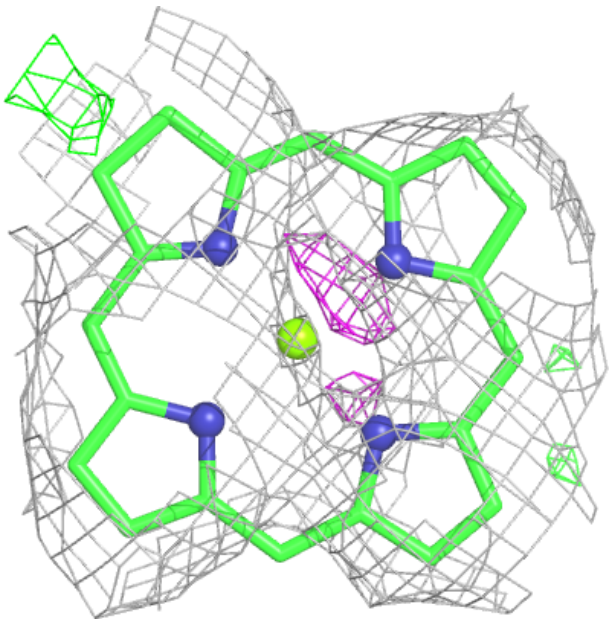


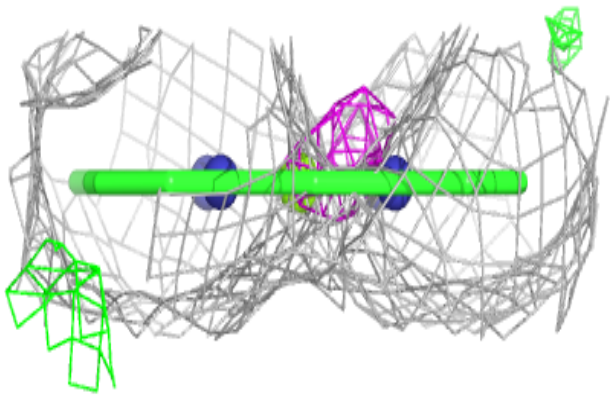


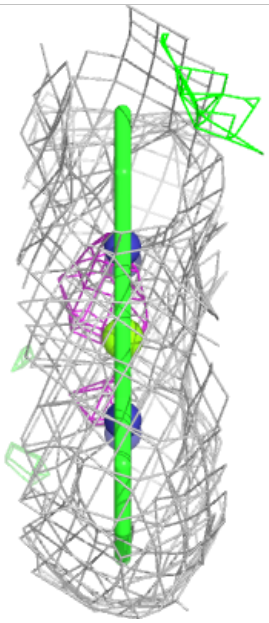


Electron density around CLA 4 317:

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

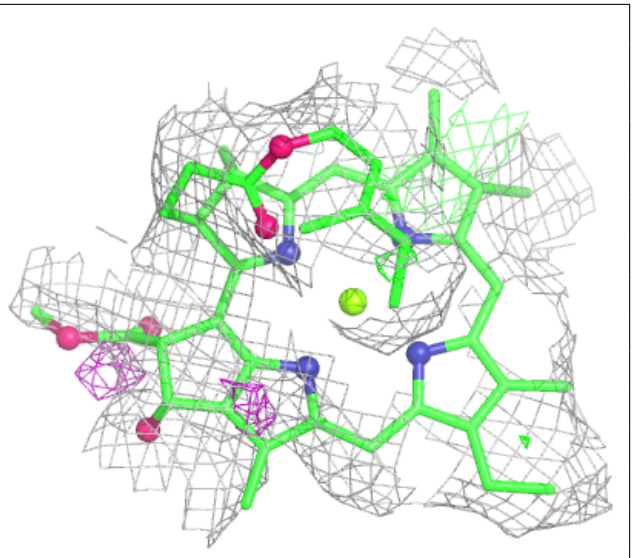


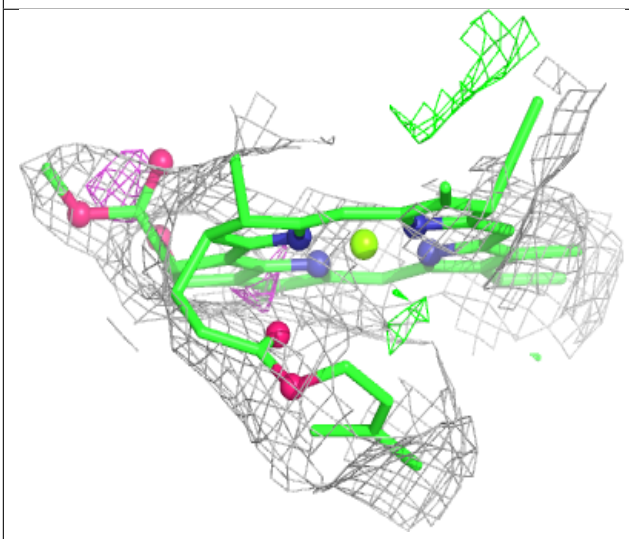


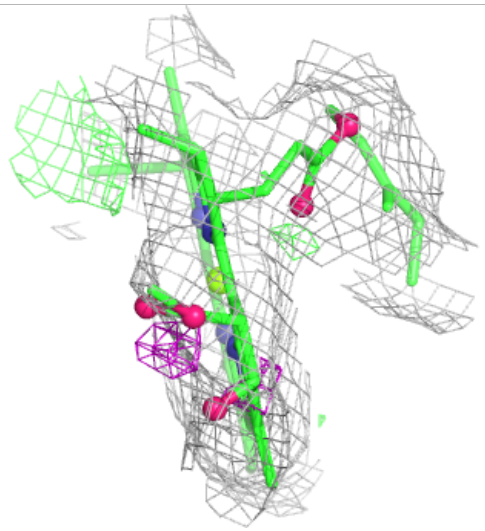


Electron density around CLA 2 301:

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

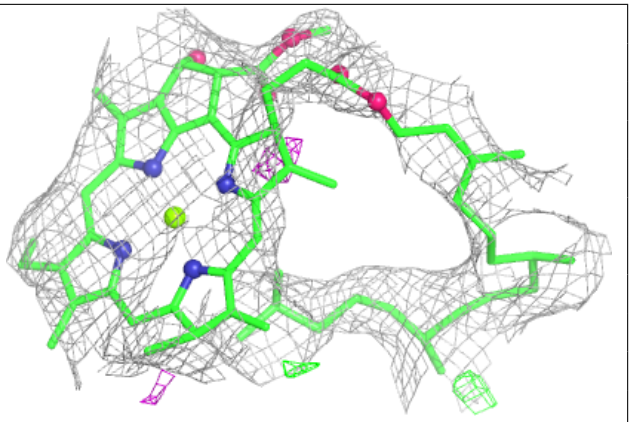


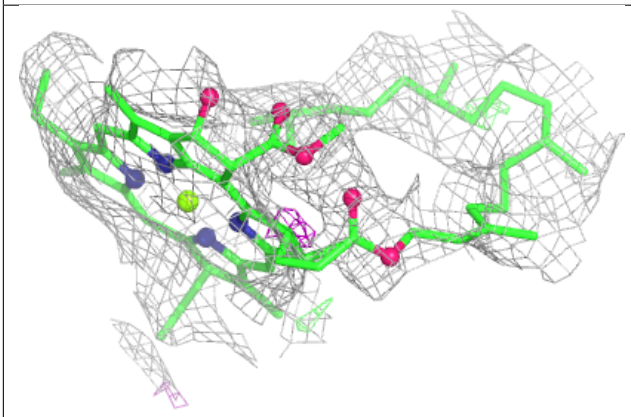


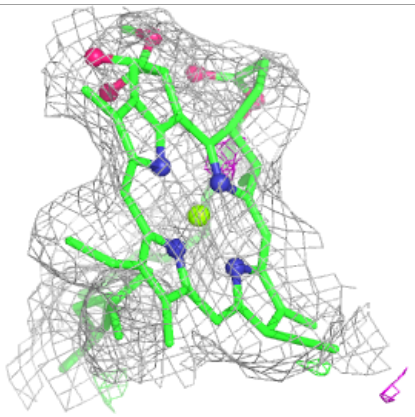


Electron density around CLA A 837:

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

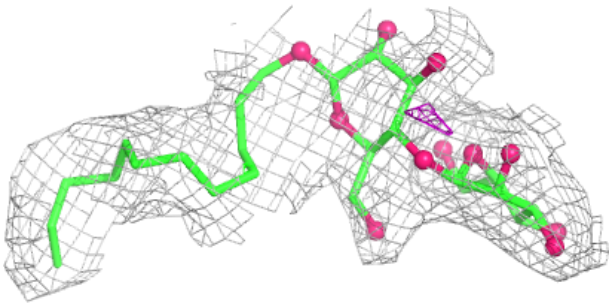


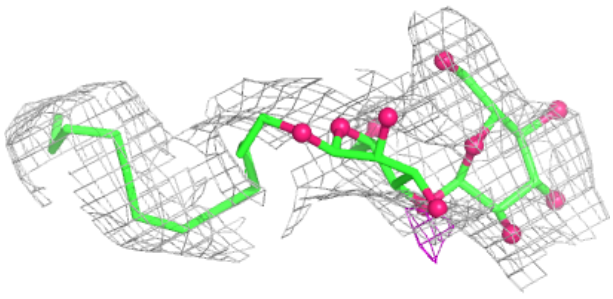


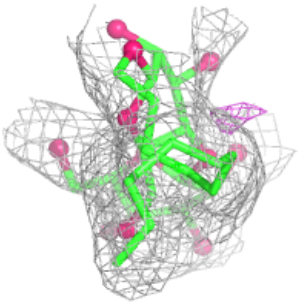


Electron density around LMU 2 313:

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

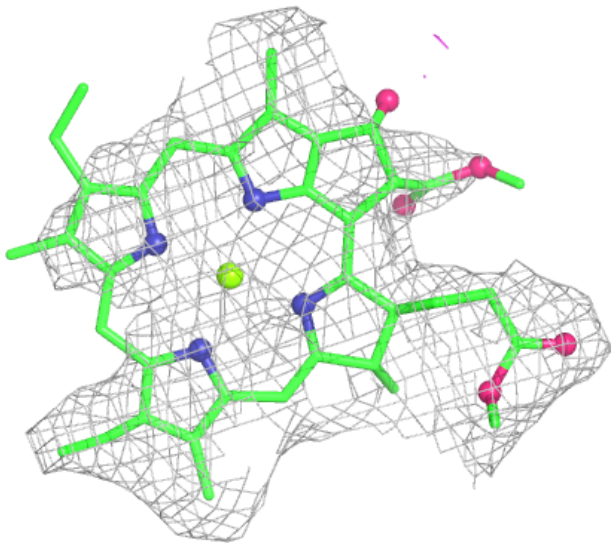


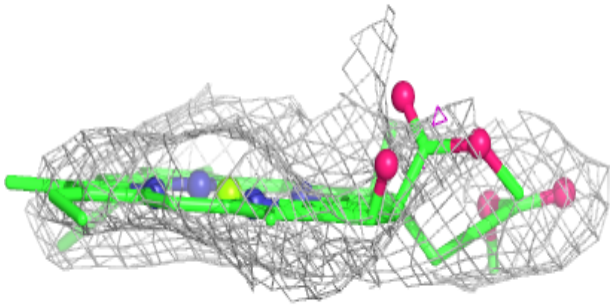


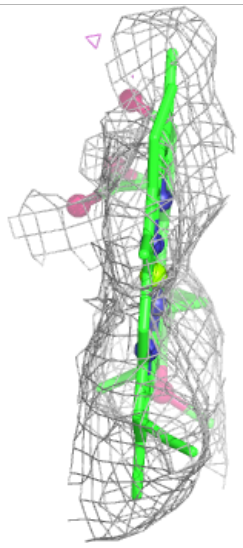


Electron density around CLA B 813:

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

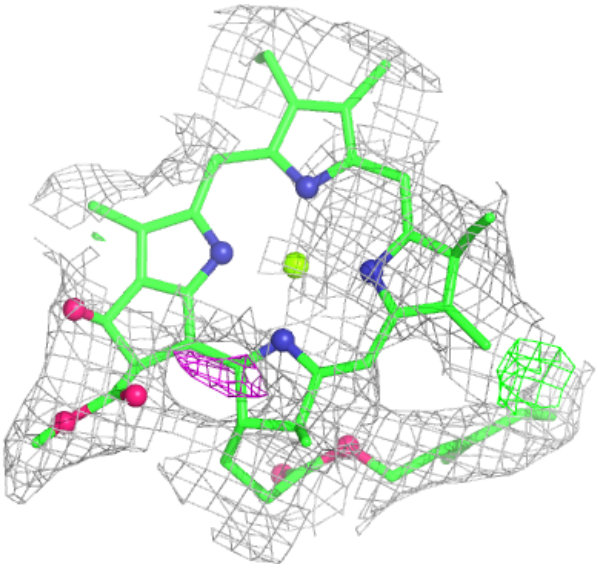


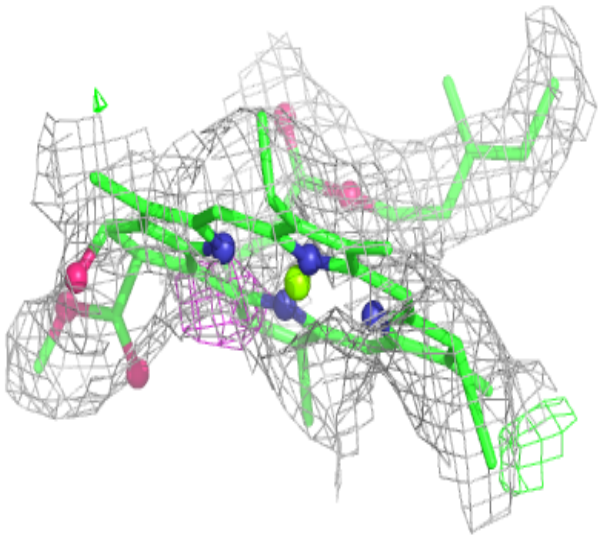




Electron density around CLA B 833:

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

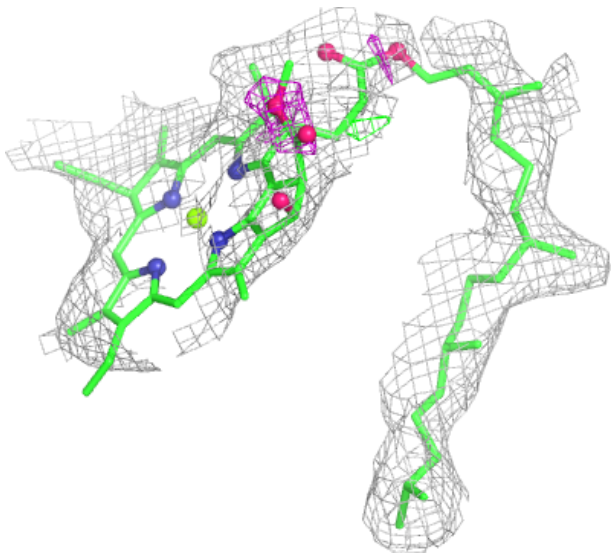


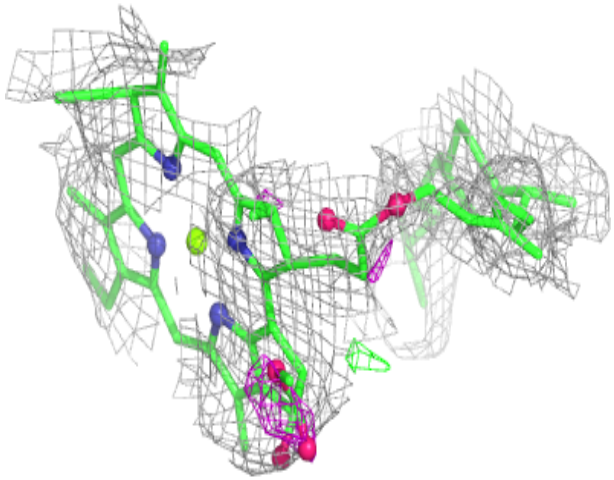


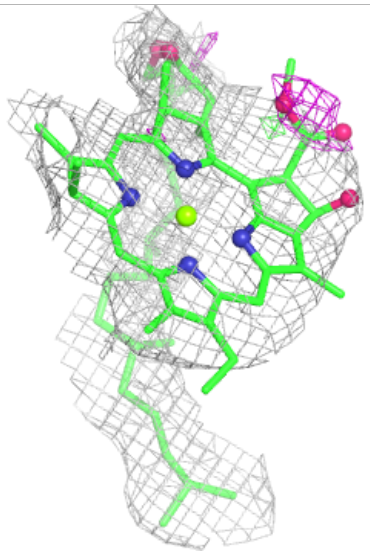


Electron density around CLA 3 310:

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

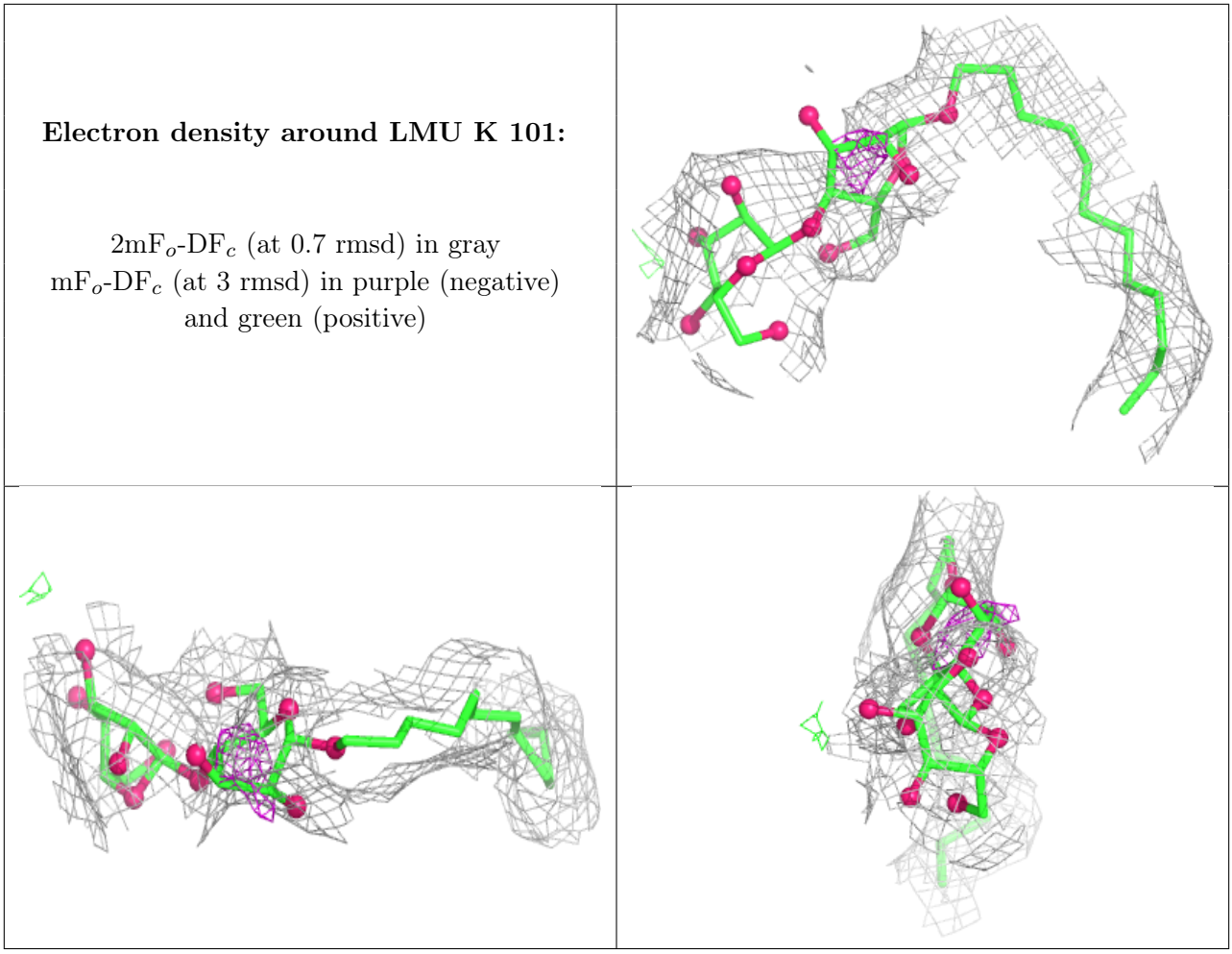






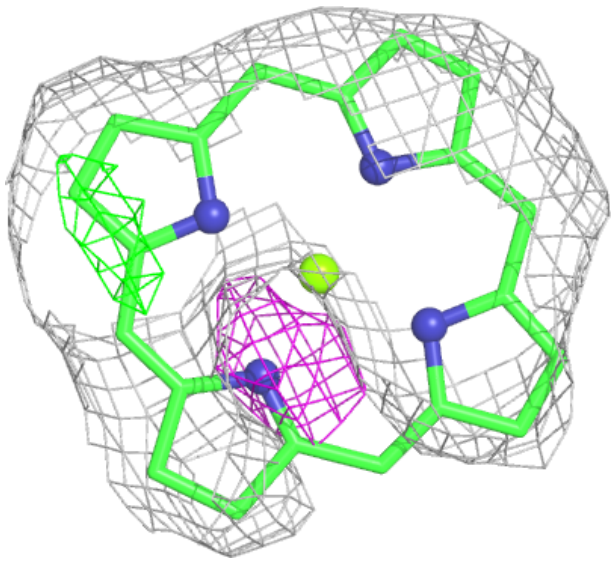
Electron density around LMU K 101:

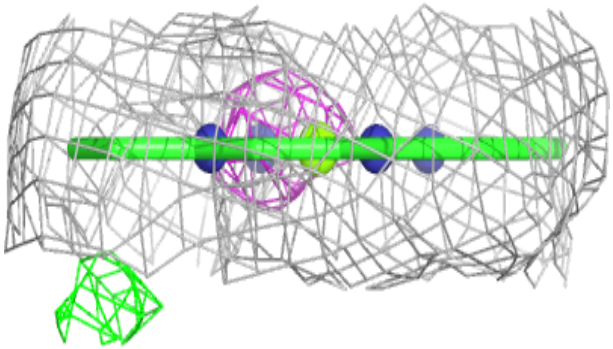
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

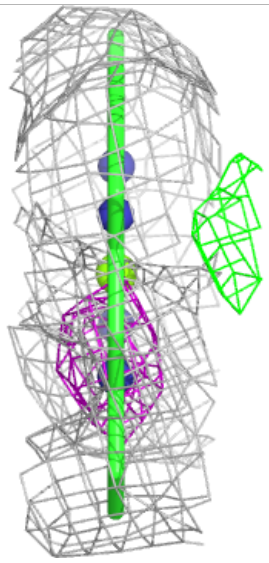


Electron density around CLA 3 305:

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

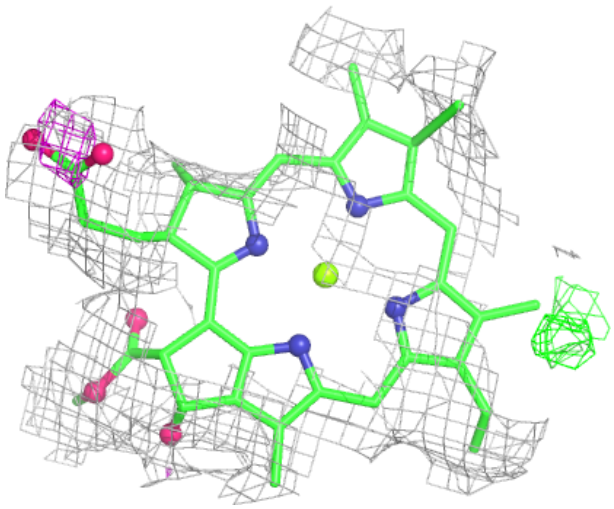


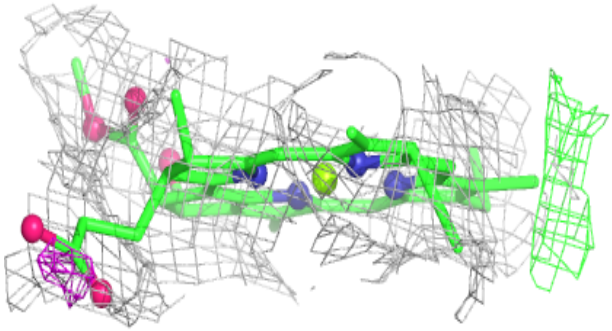




Electron density around CLA K 105:

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

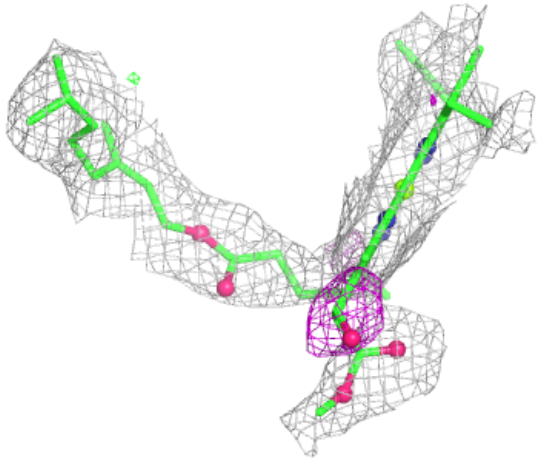


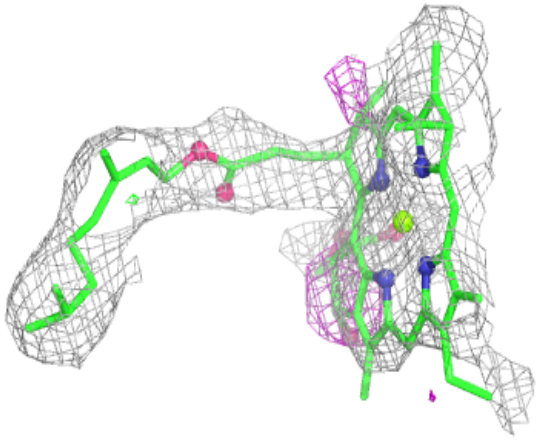


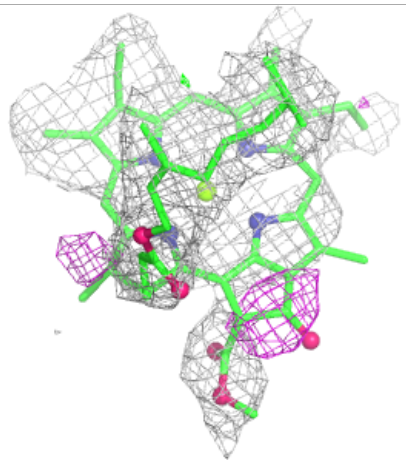


Electron density around CLA L 203:

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

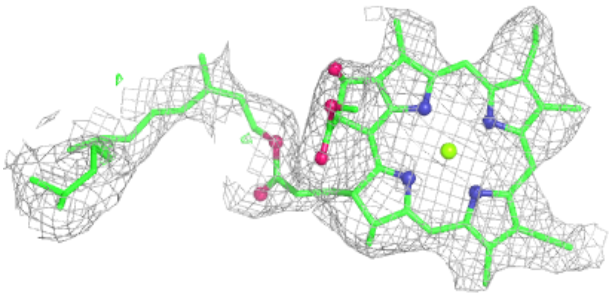


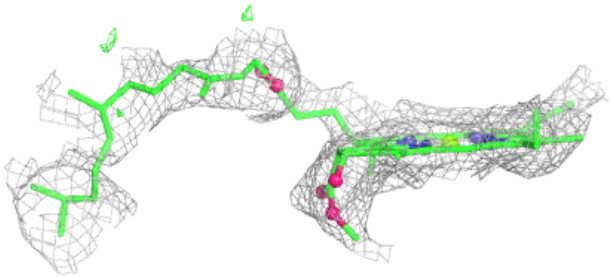


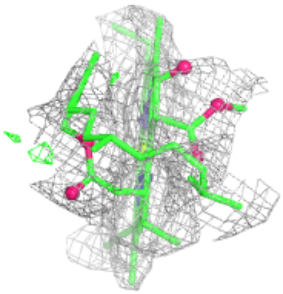


Electron density around CLA B 812:

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

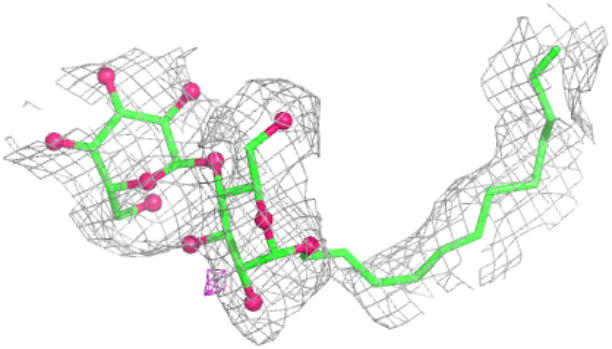


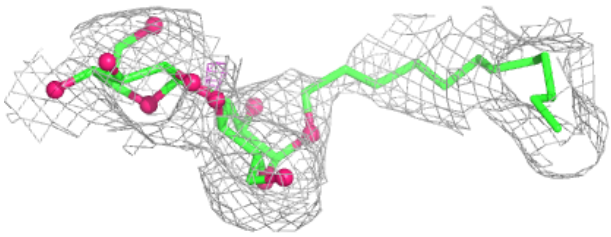


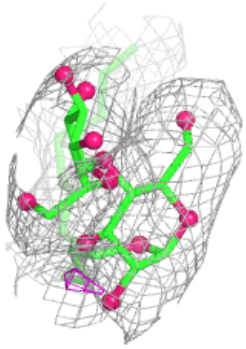


Electron density around LMU 1 216:

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

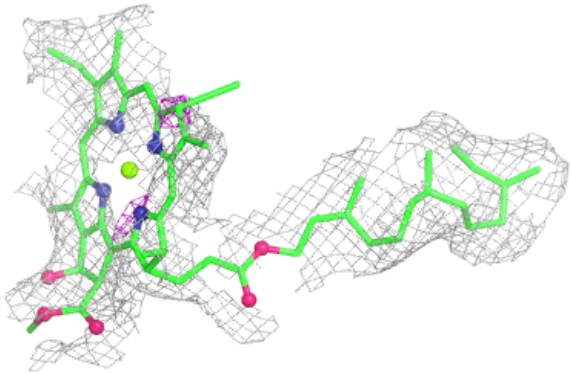


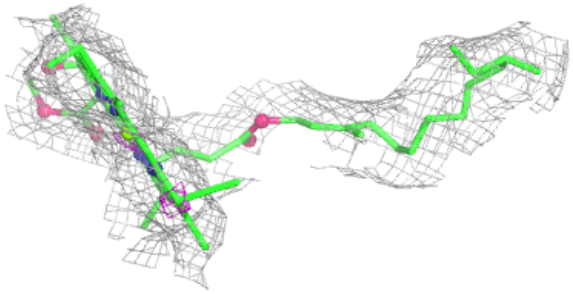


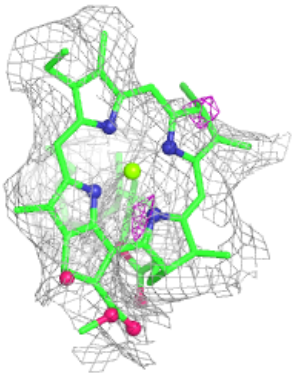


Electron density around CLA 2 321:

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

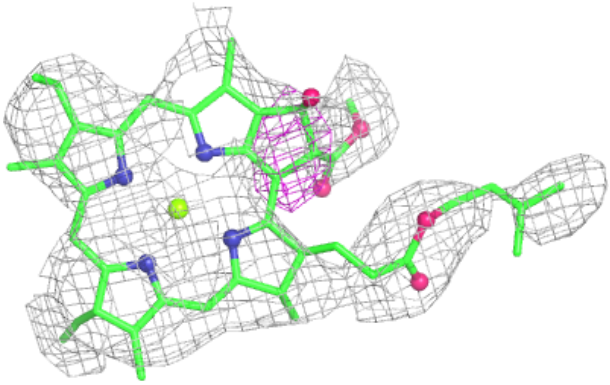


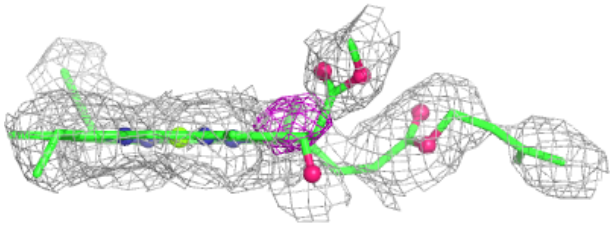


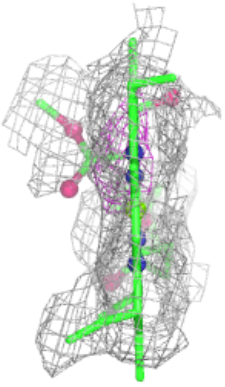


Electron density around CLA 4 306:

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

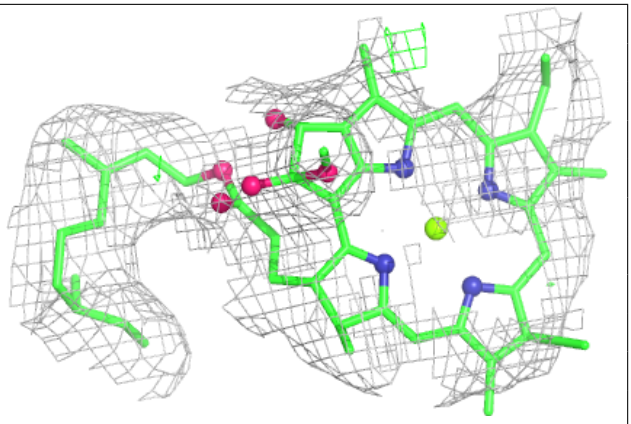


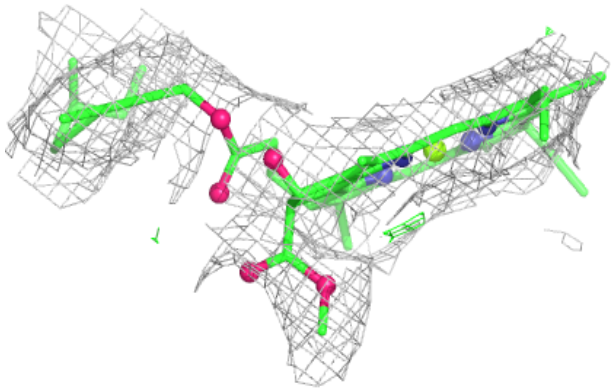




Electron density around CLA 3 301:

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

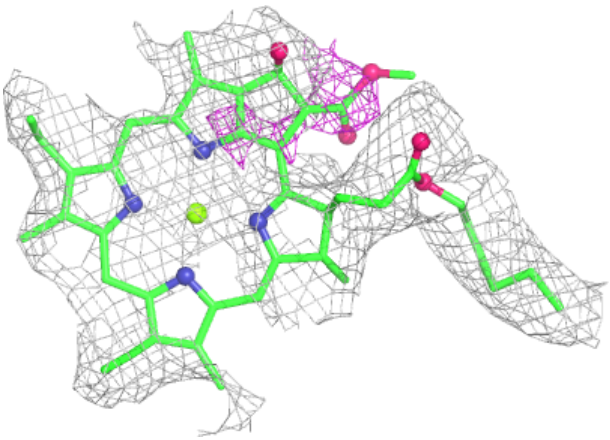


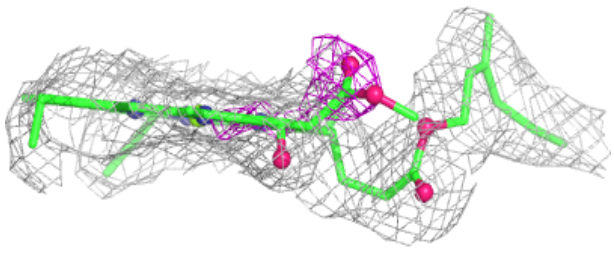


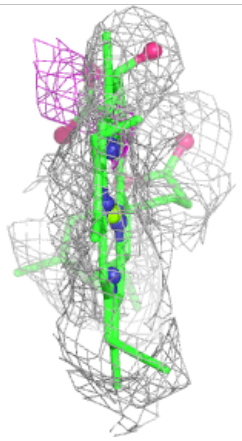


Electron density around CLA 4 318:

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

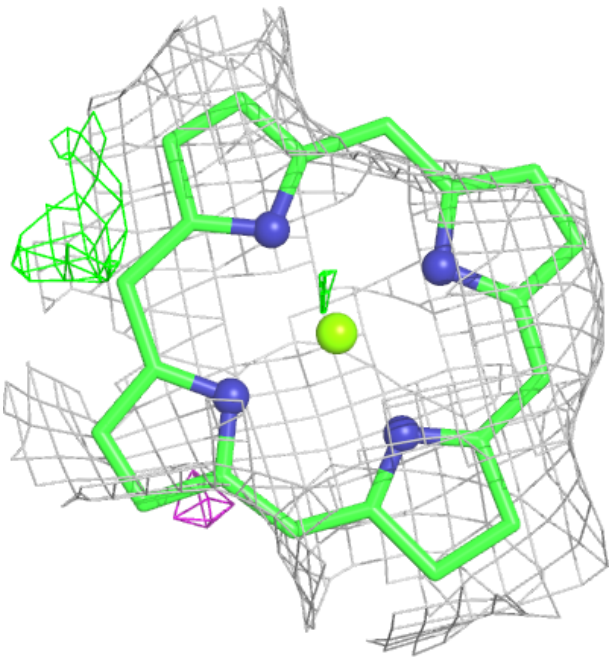


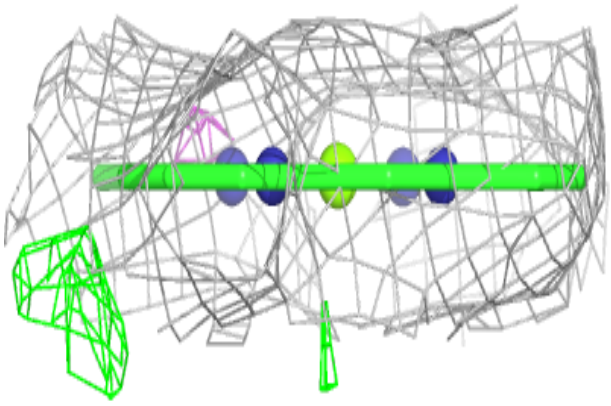


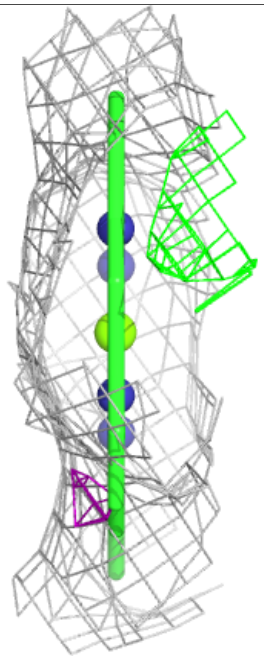


Electron density around CLA 2 305:

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

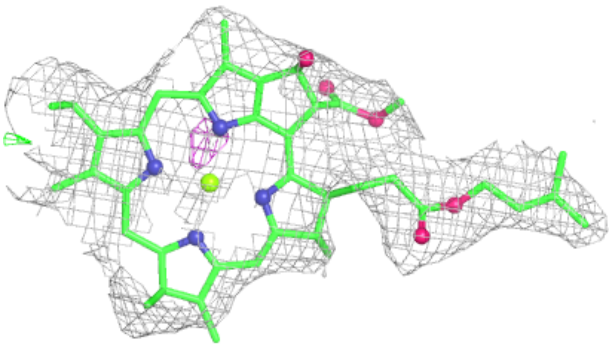


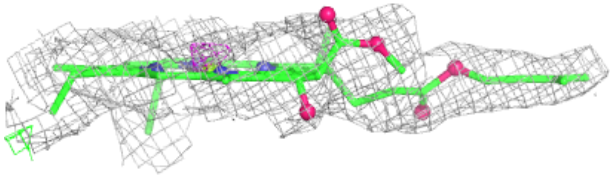


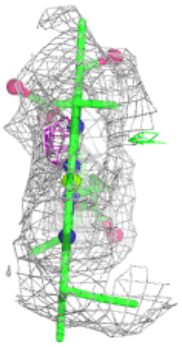


Electron density around CLA A 838:

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

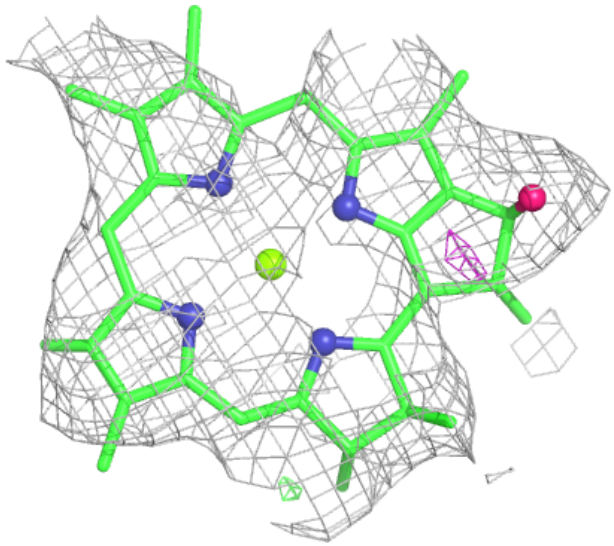


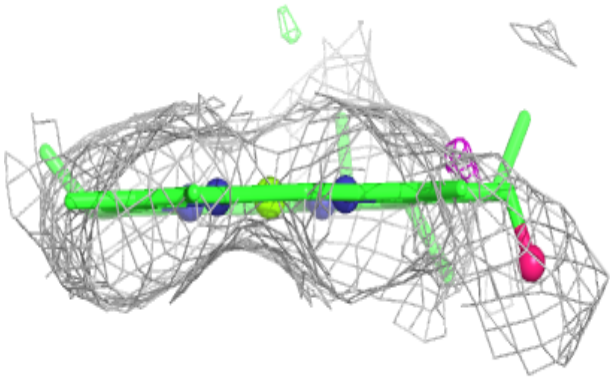


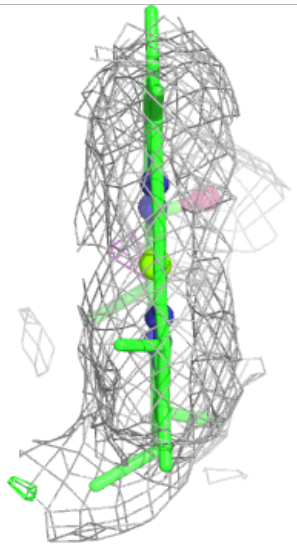


Electron density around CLA 1 205:

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

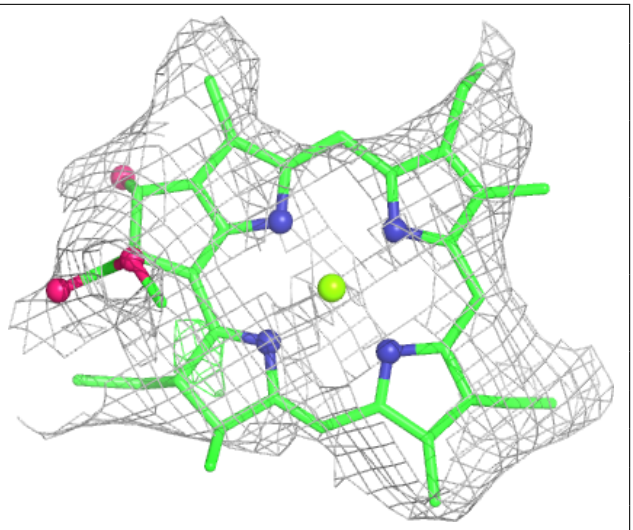


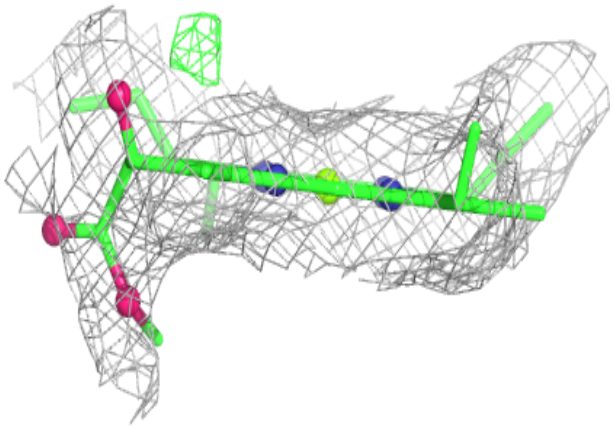


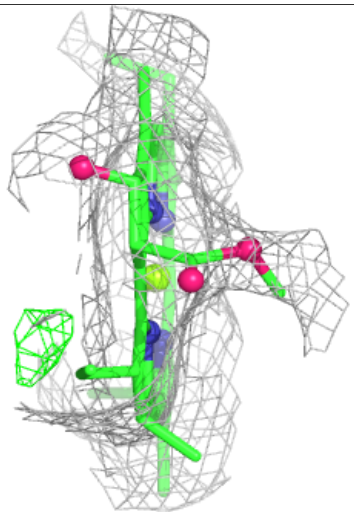


Electron density around CLA 3 314:

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

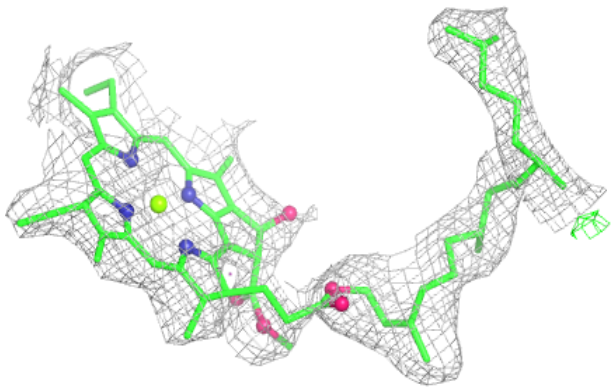


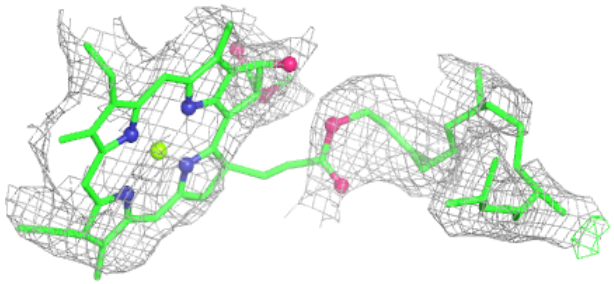


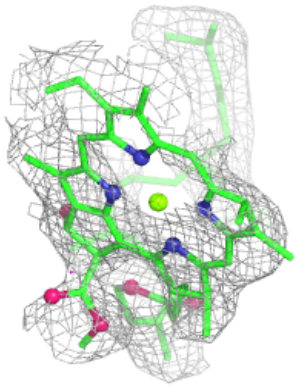


Electron density around CLA K 107:

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

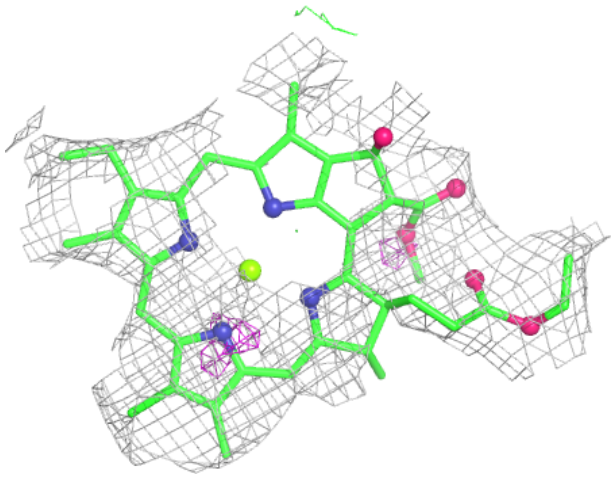


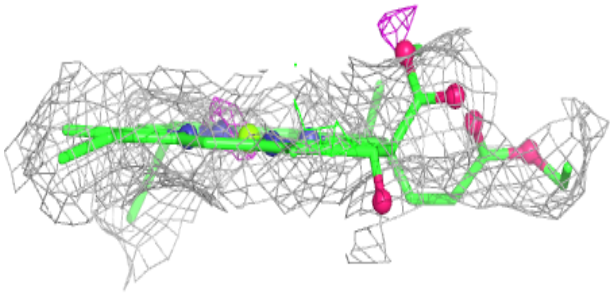


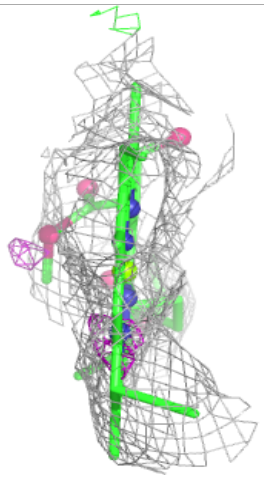


Electron density around CLA 4 319:

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

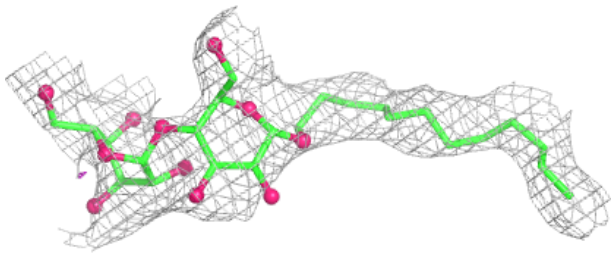


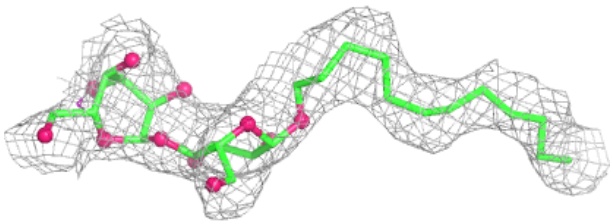


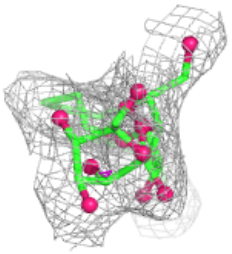


Electron density around LMU A 851:

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

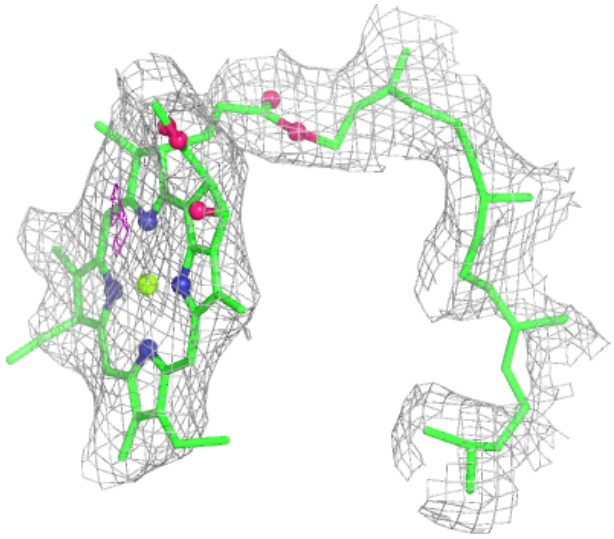


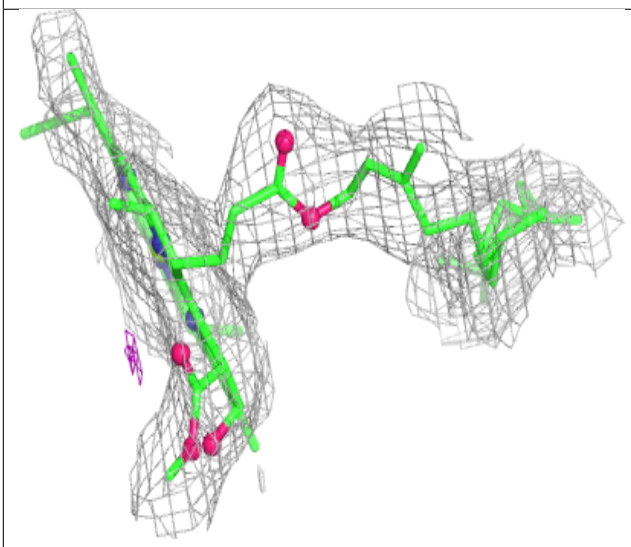


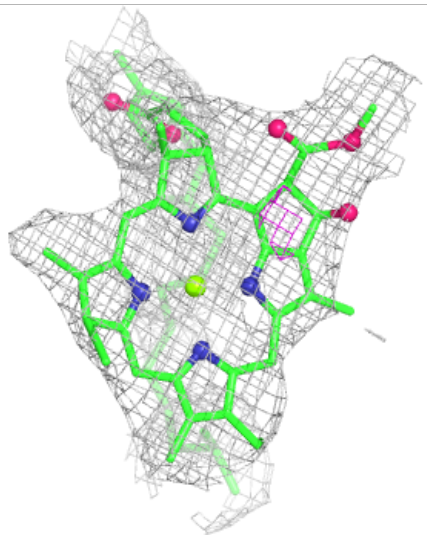


Electron density around CLA 3 309:

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

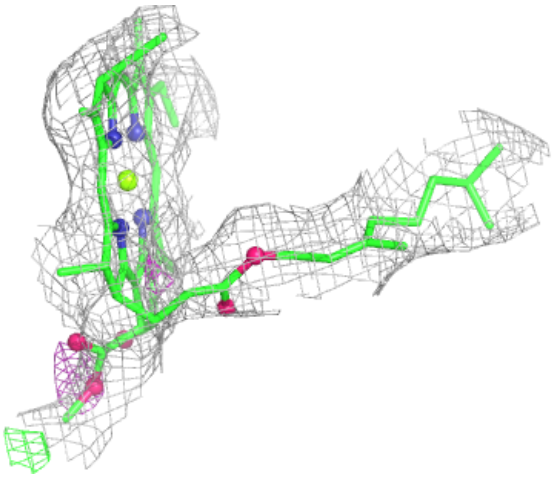


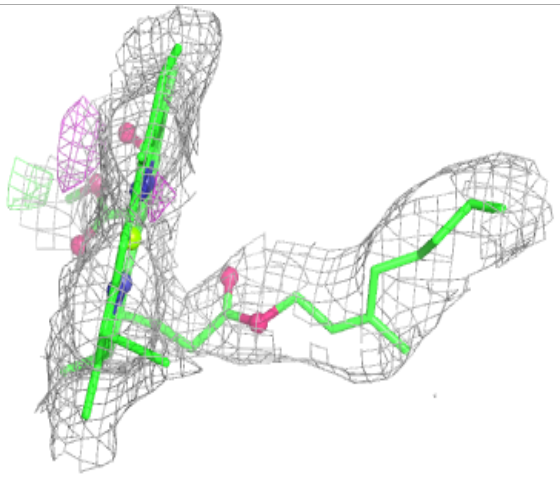


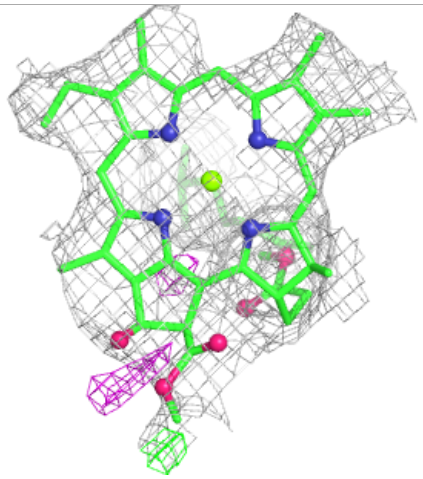


Electron density around CLA 4 302:

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

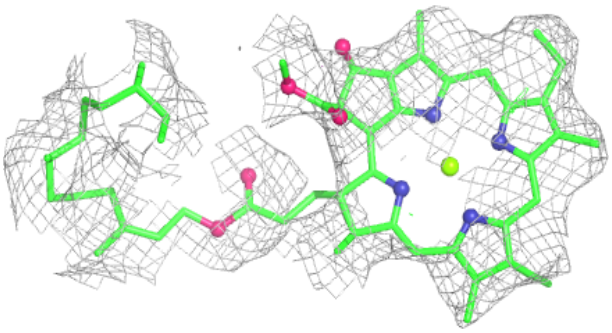


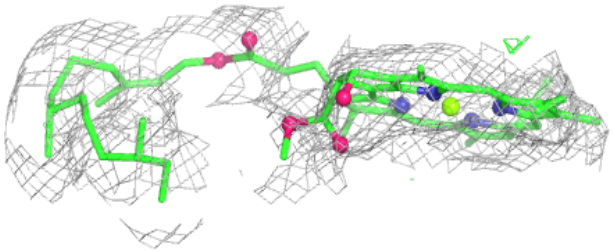


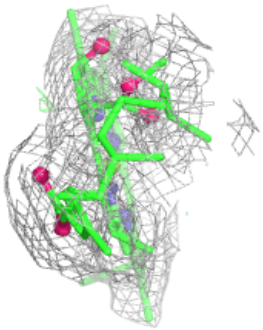


Electron density around CLA 1 212:

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

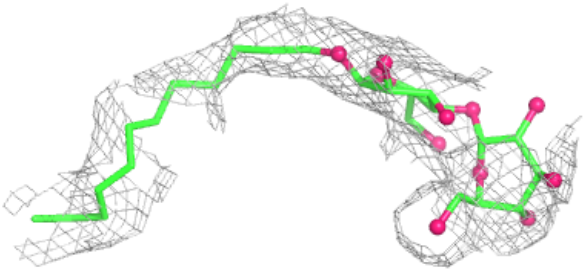






Electron density around LMU L 205:

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

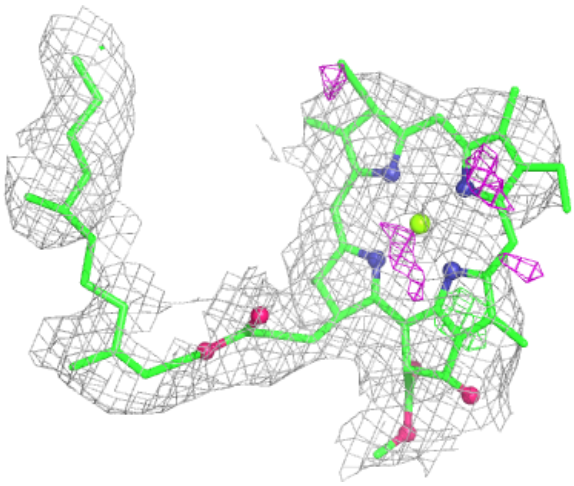


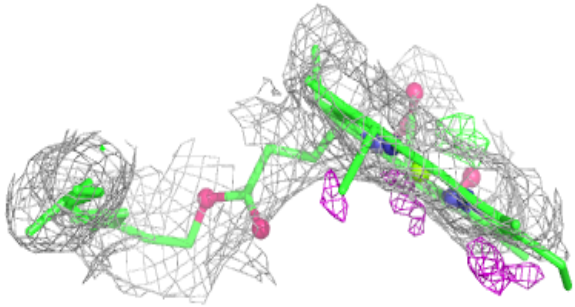


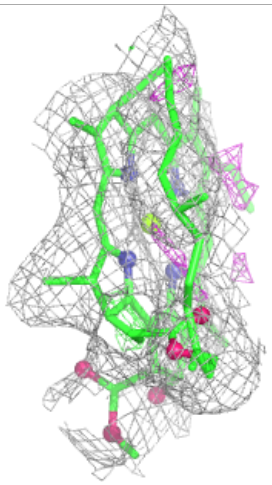


Electron density around CLA B 822:

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

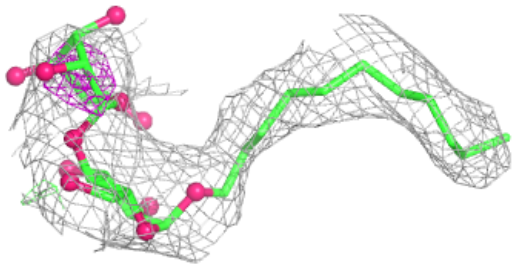


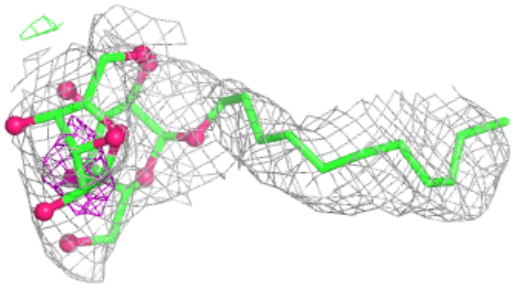


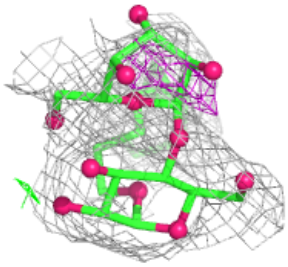


Electron density around LMU 4 320:

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

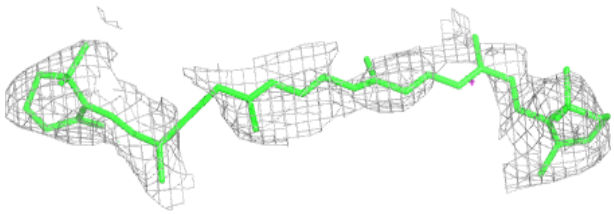


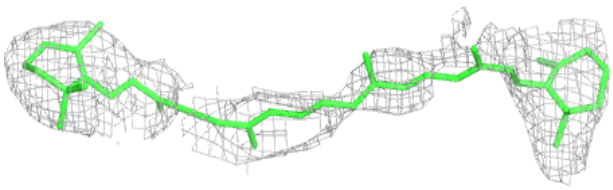




Electron density around BCR A 842:

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

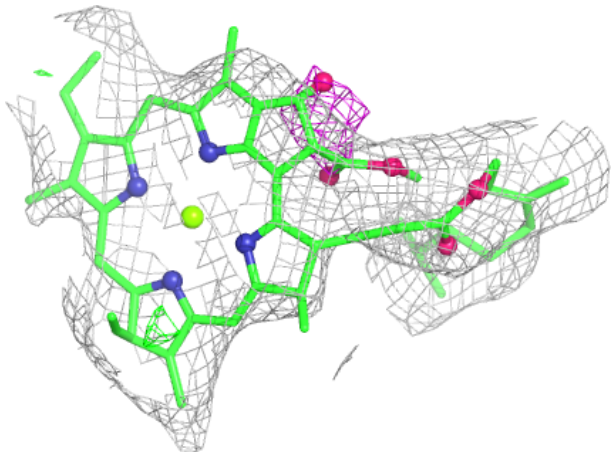


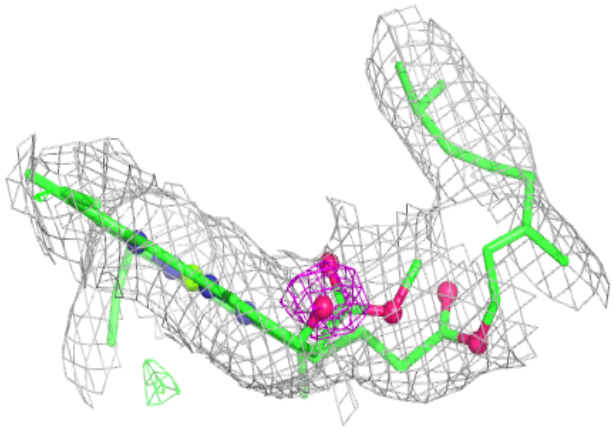


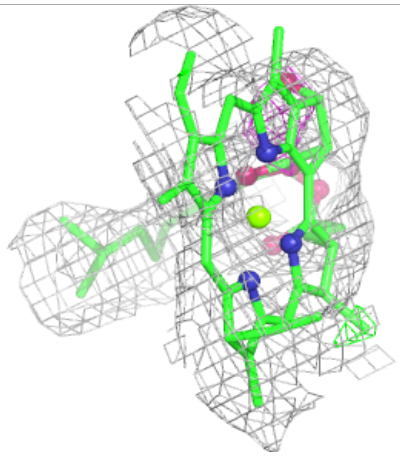


Electron density around CLA L 204:

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

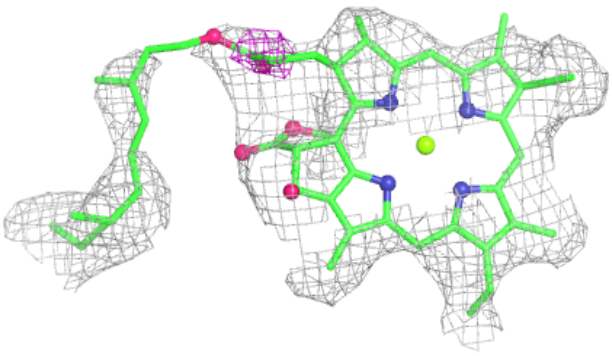


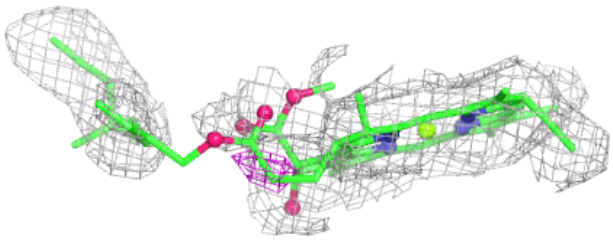




Electron density around CLA R 106:

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

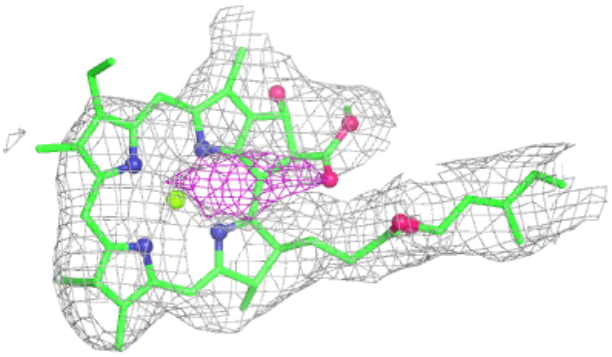


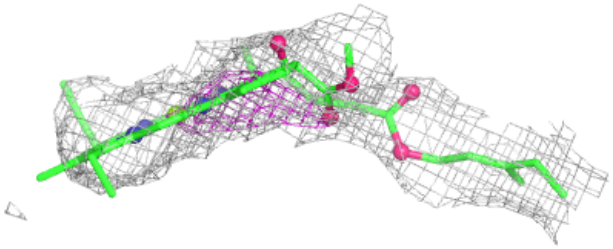


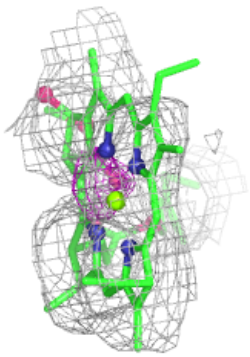


Electron density around CLA 1 211:

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

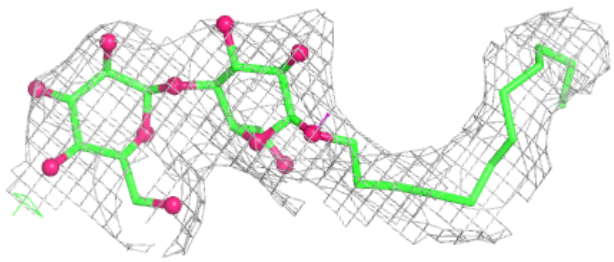


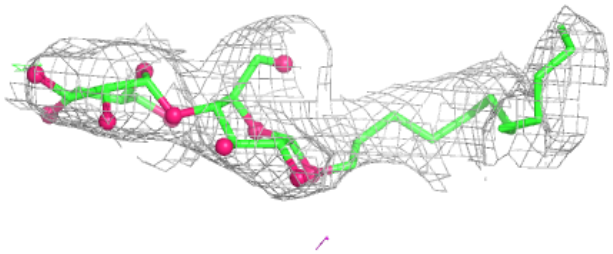


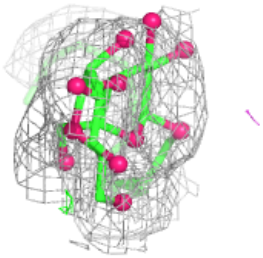


Electron density around LMU C 101:

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

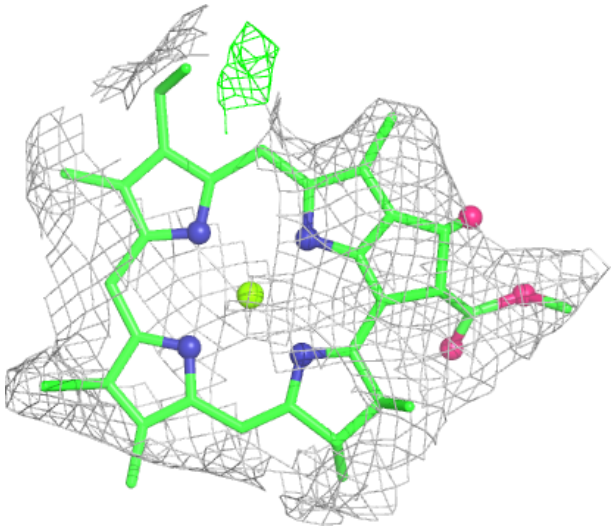


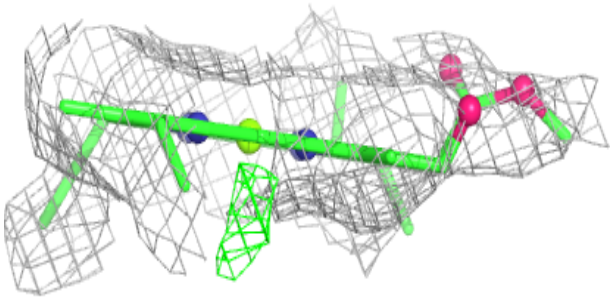


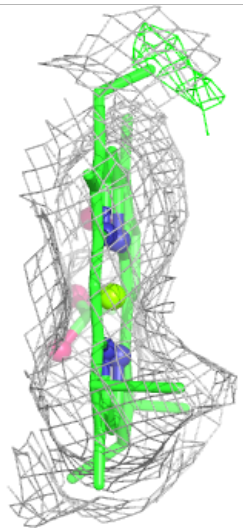


Electron density around CLA F 205:

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

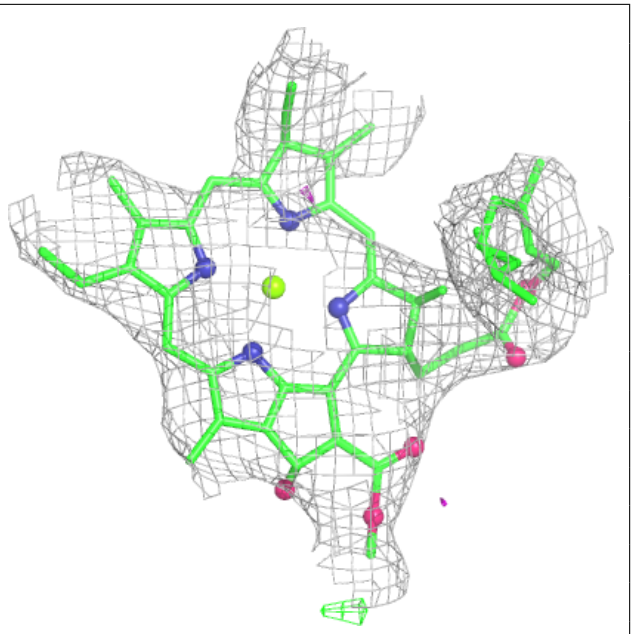


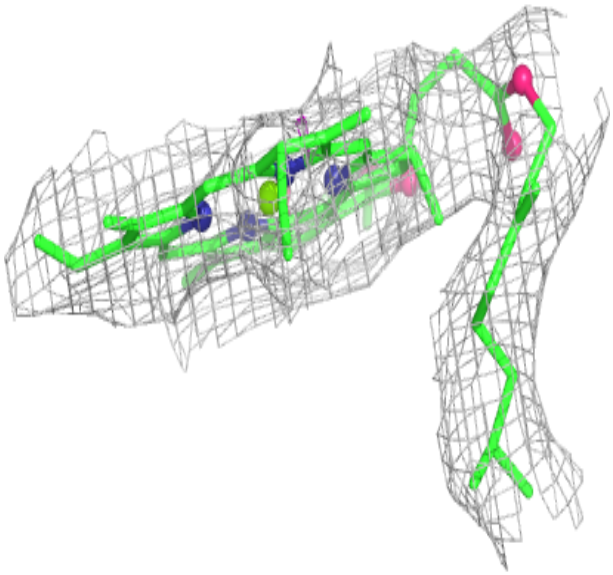


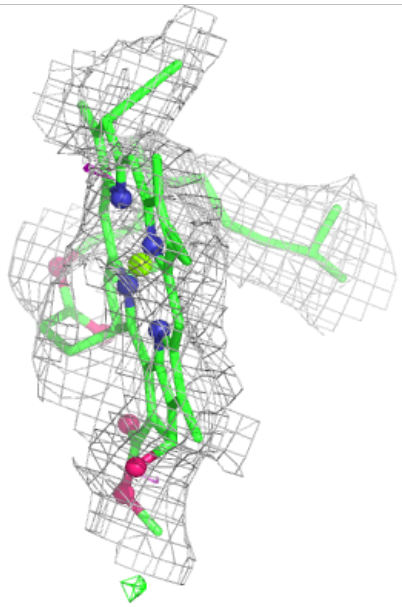


Electron density around CLA H 101:

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

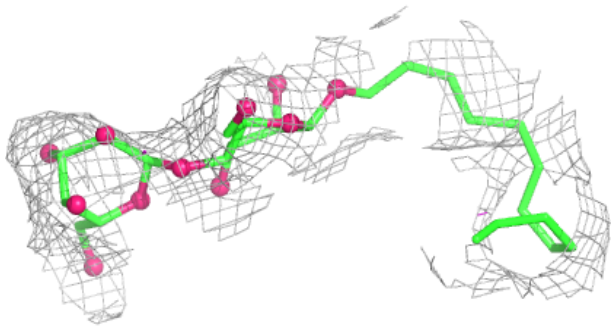


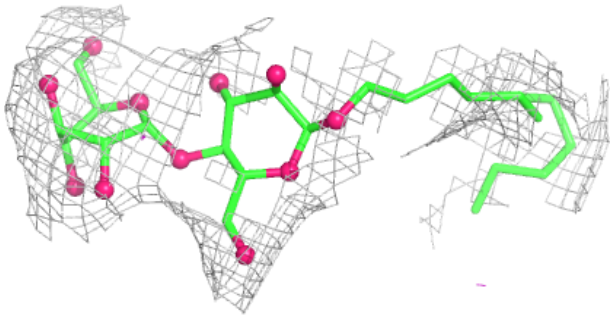


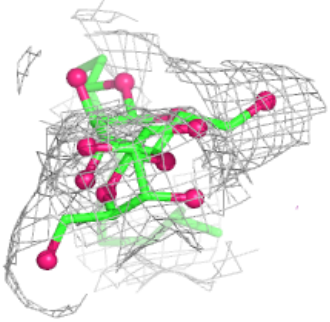


Electron density around LMU H 105:

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

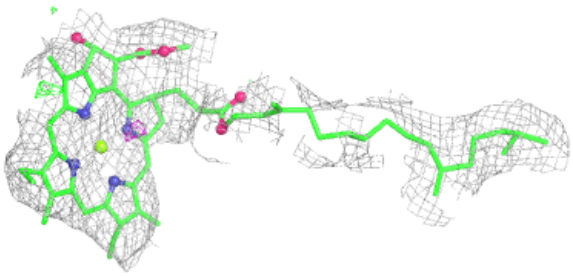


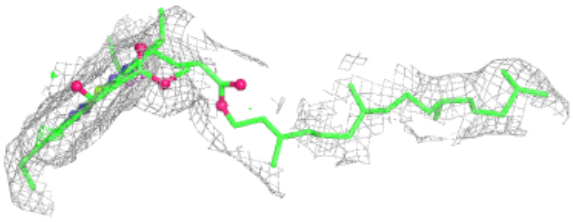




Electron density around CLA 4 304:

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

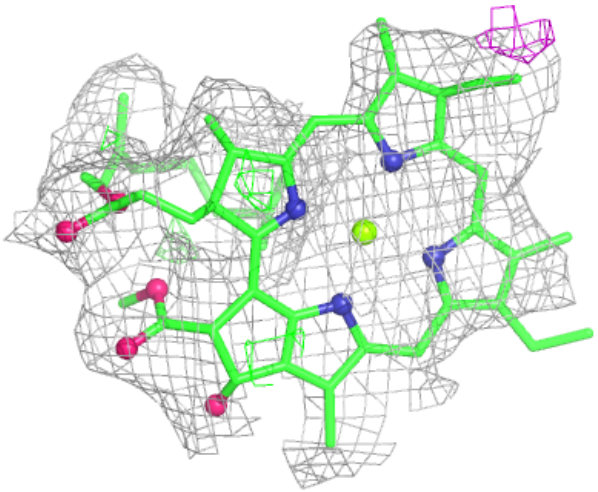


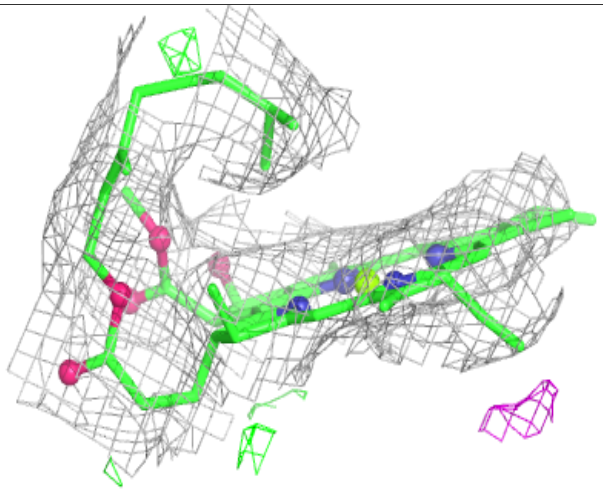


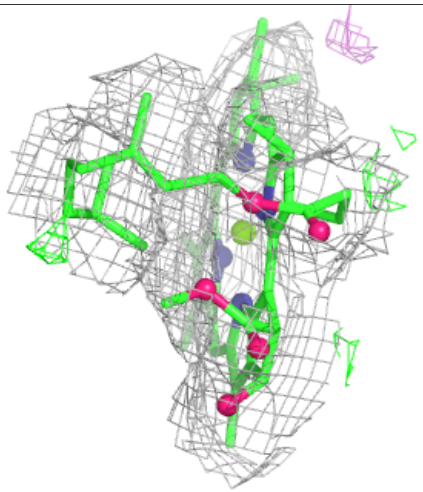


Electron density around CLA 4 305:

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

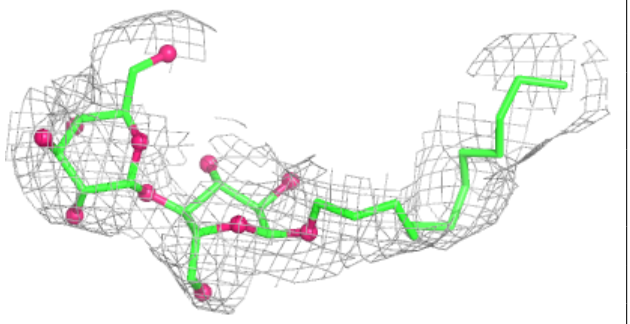


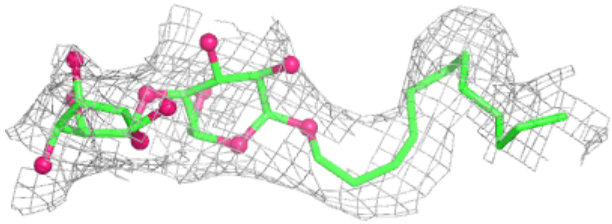


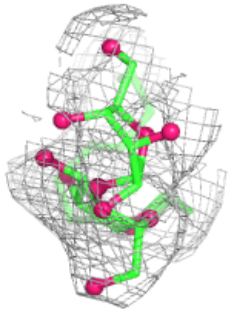


Electron density around LMU 4 322:

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

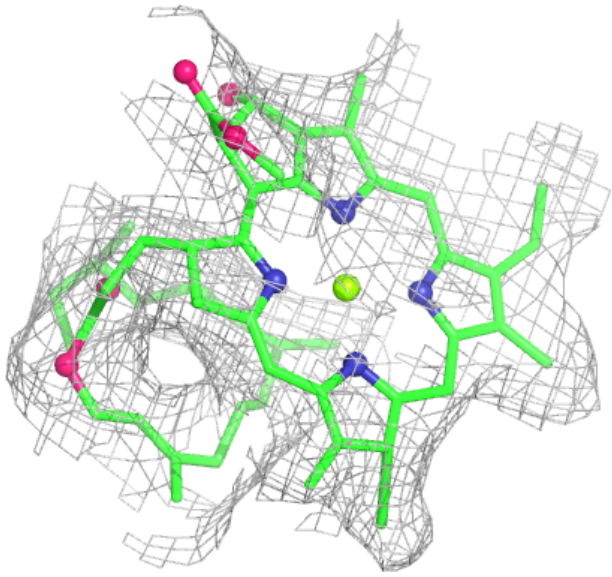


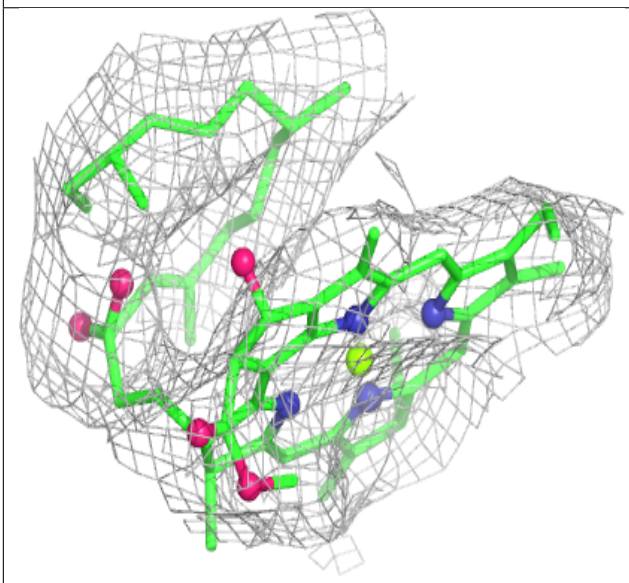


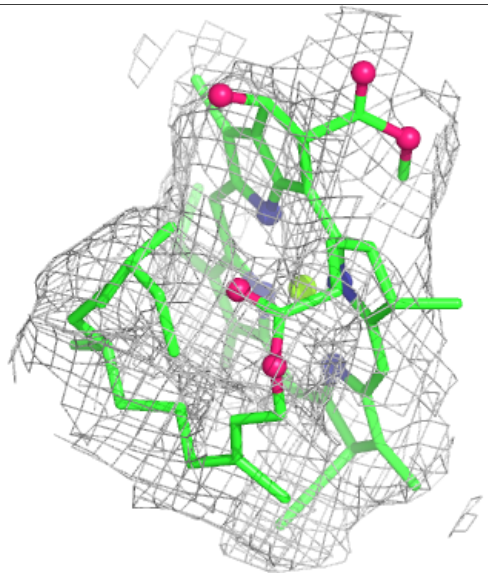


Electron density around CLA J 102:

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

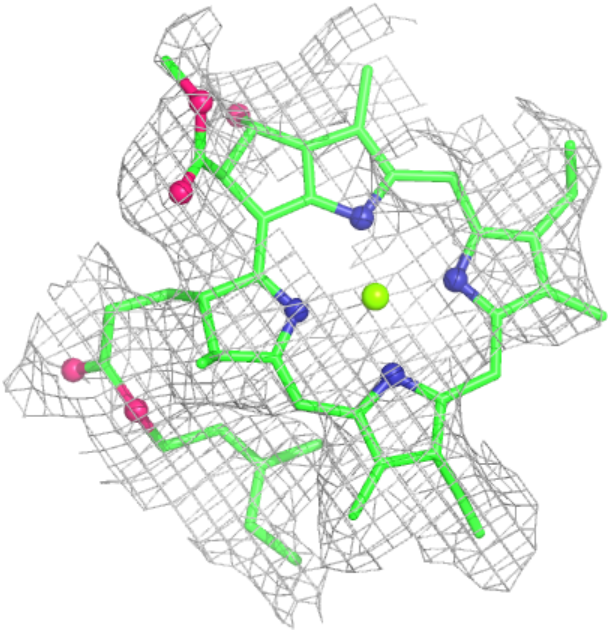


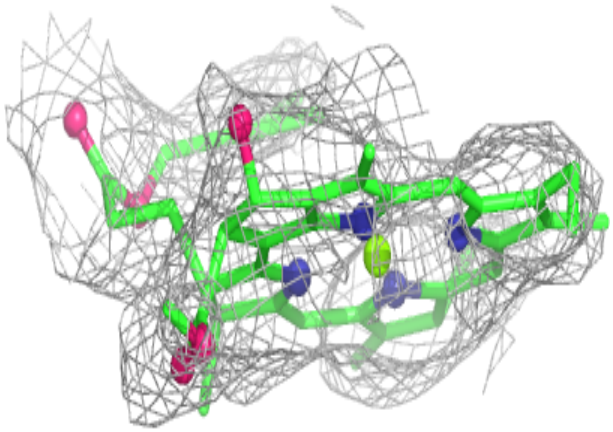


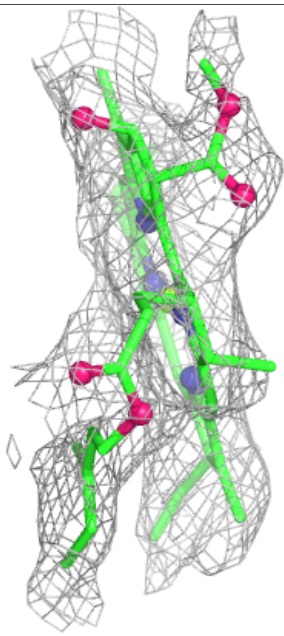


Electron density around CLA G 103:

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

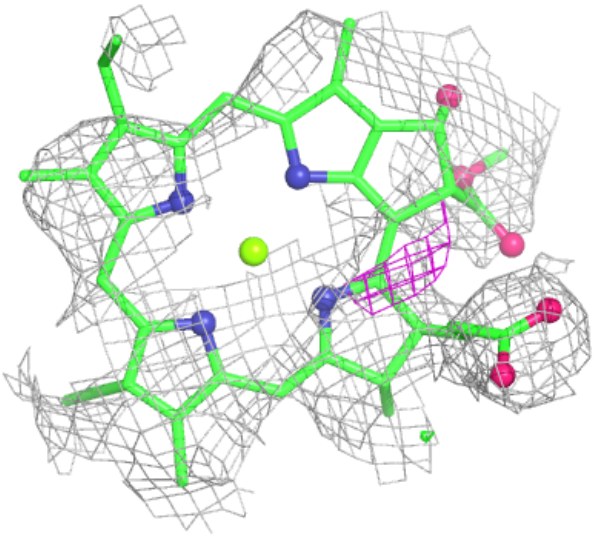


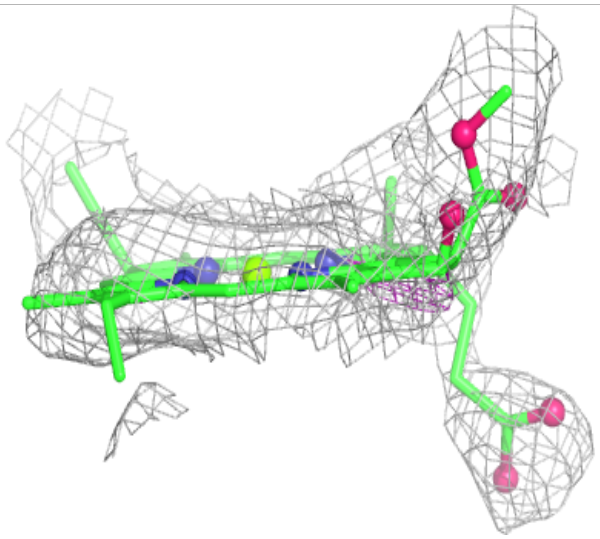


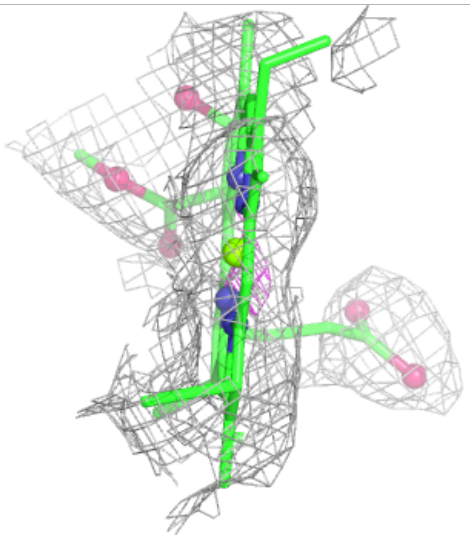


Electron density around CLA B 832:

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

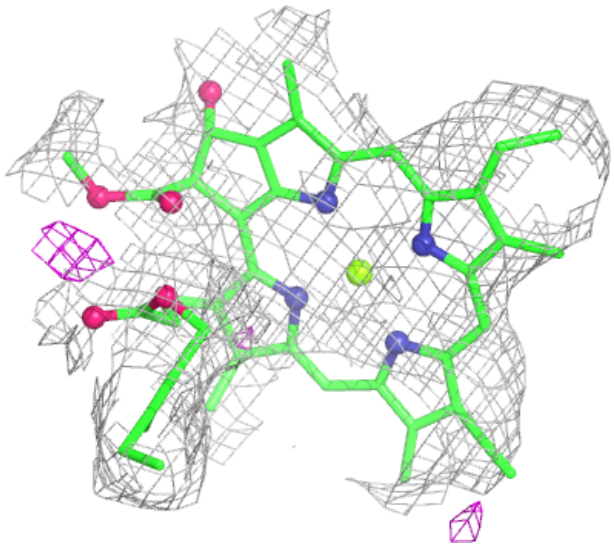


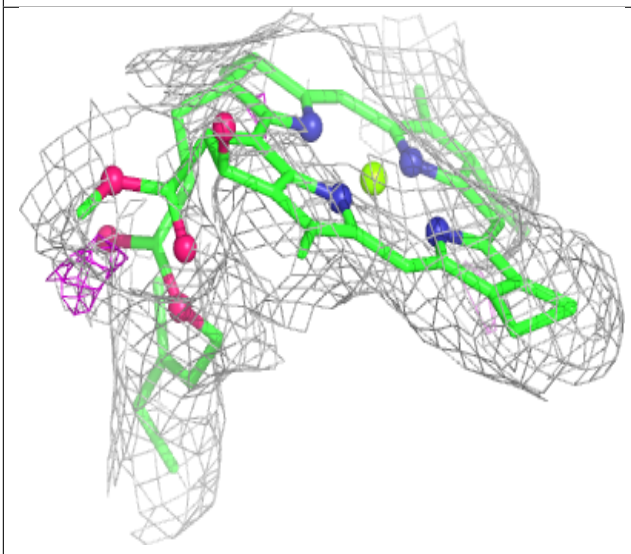




Electron density around CLA 1 207:

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

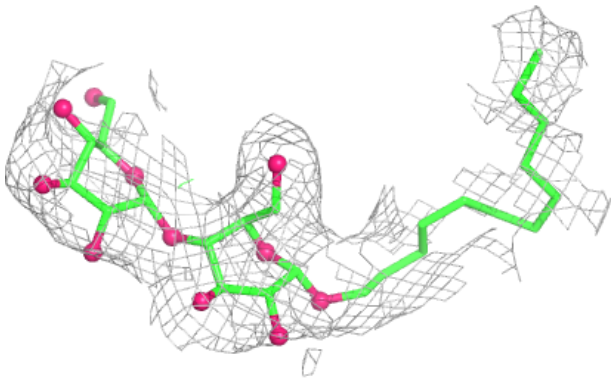


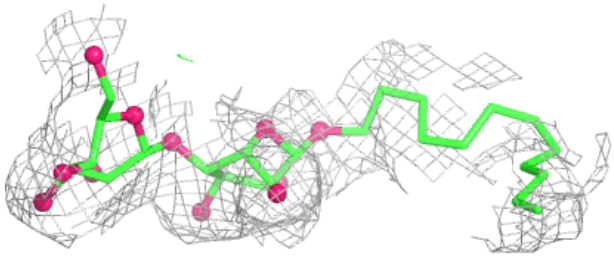


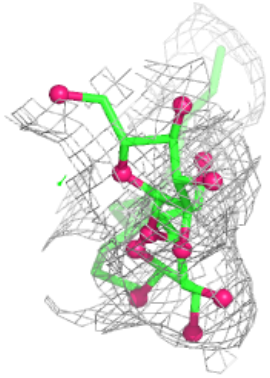


Electron density around LMU H 103:

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

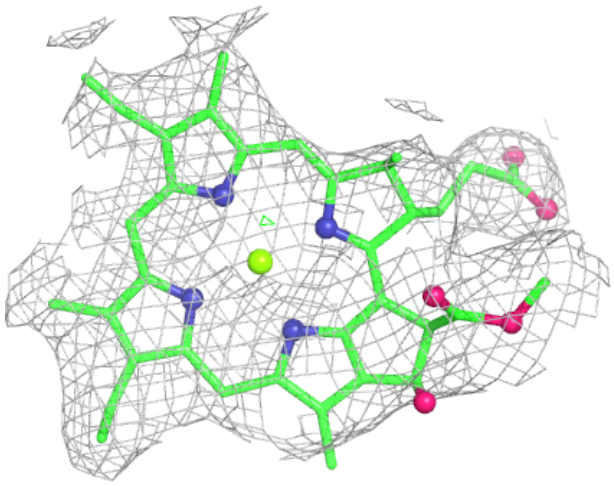


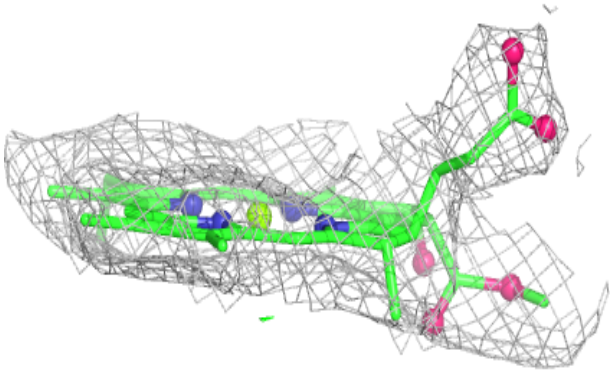


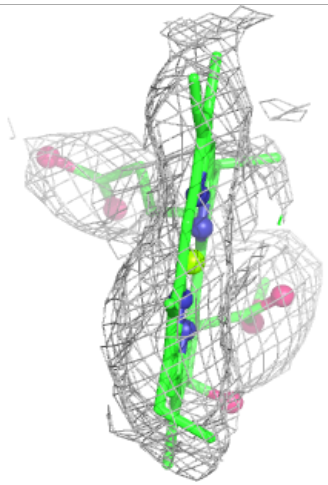


Electron density around CLA A 808:

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

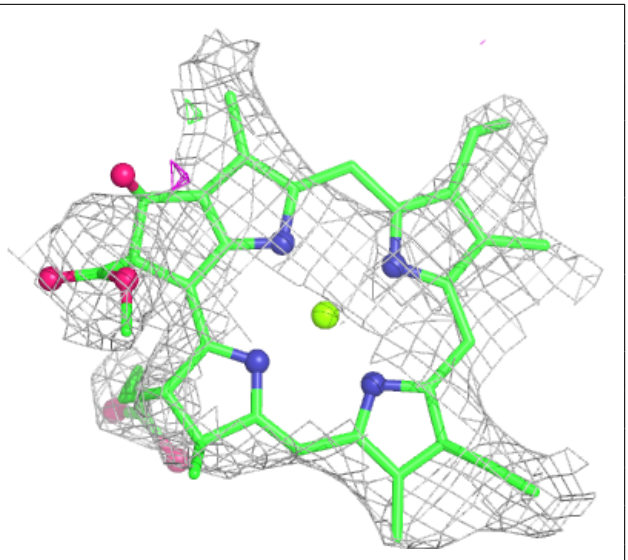


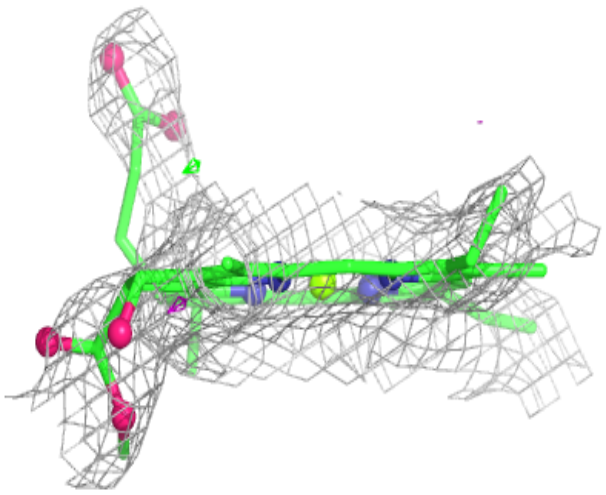


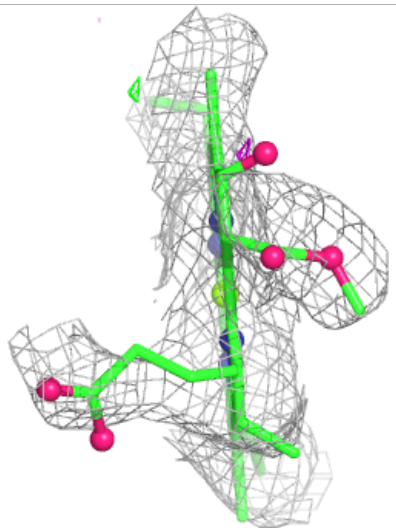


Electron density around CLA A 812:

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

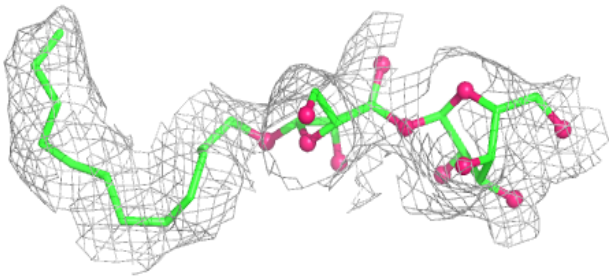


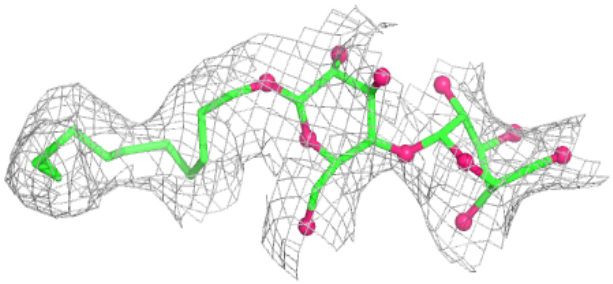


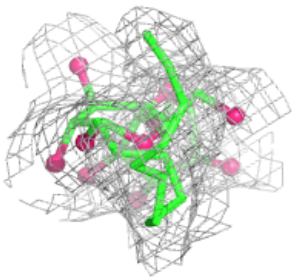


Electron density around LMU A 845:

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

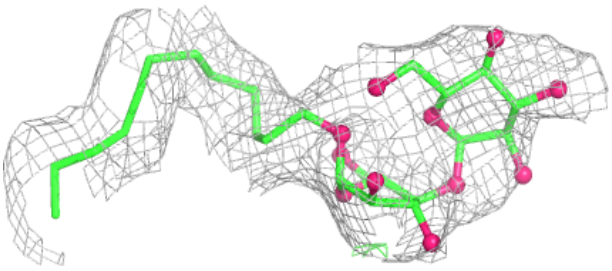


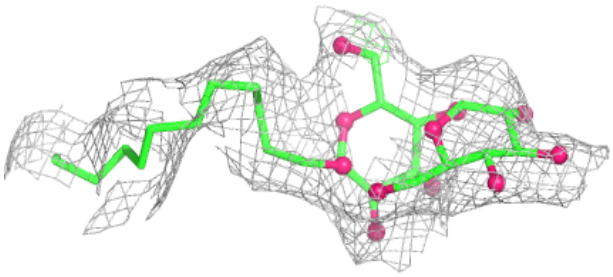


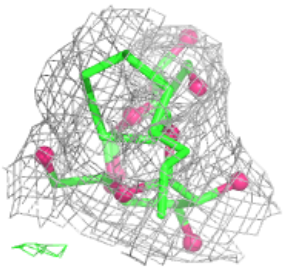


Electron density around LMU A 846:

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

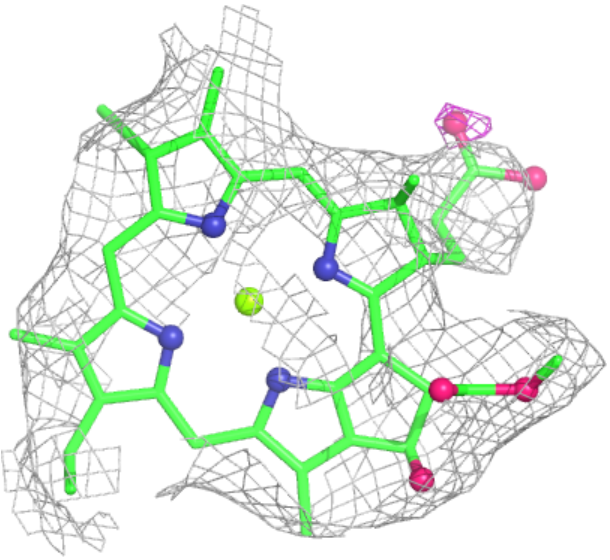


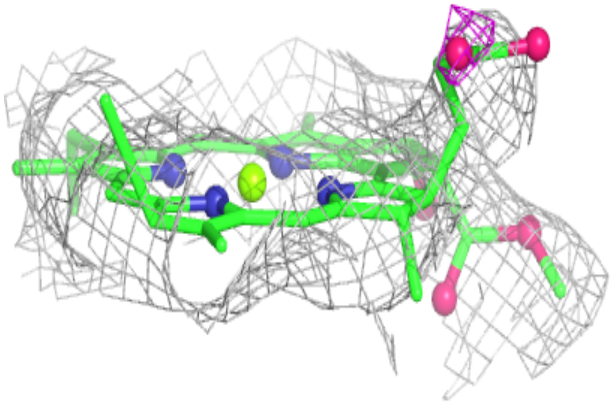


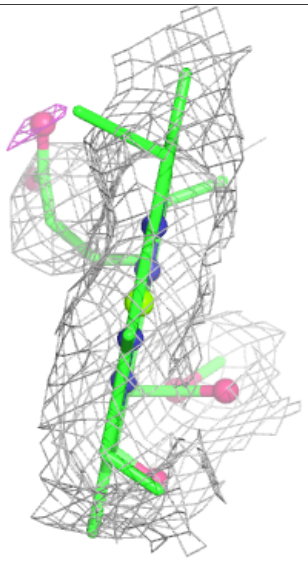


Electron density around CLA A 831:

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

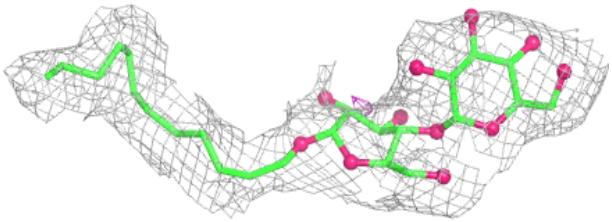


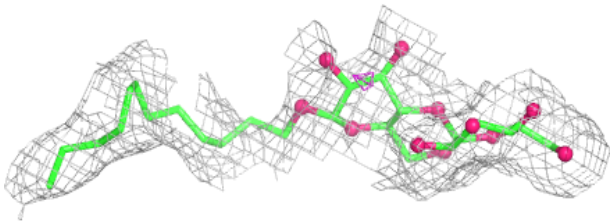


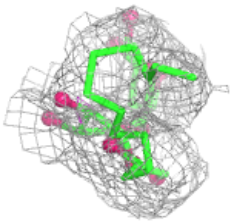


Electron density around LMU B 801:

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

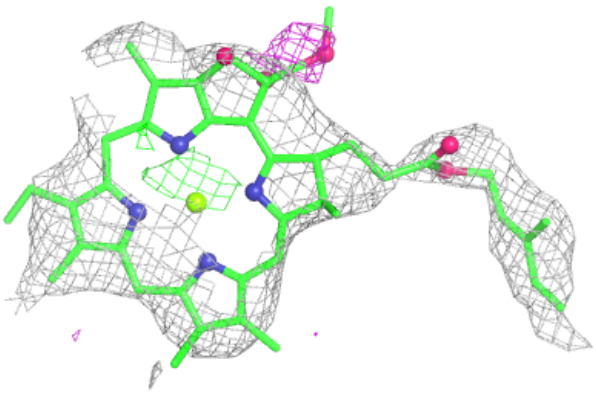


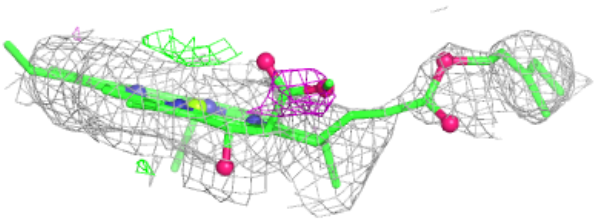


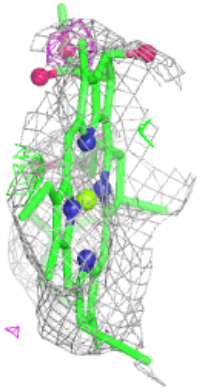


Electron density around CLA 1 214:

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

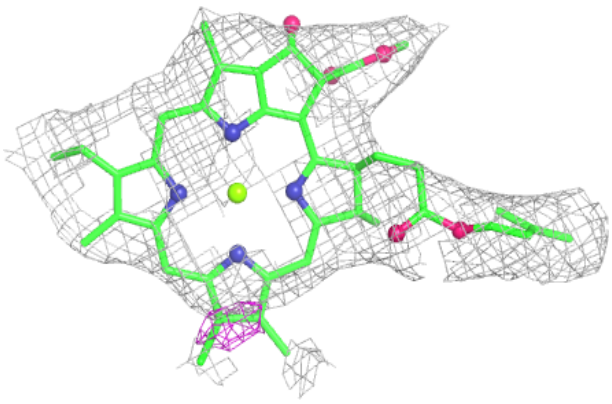


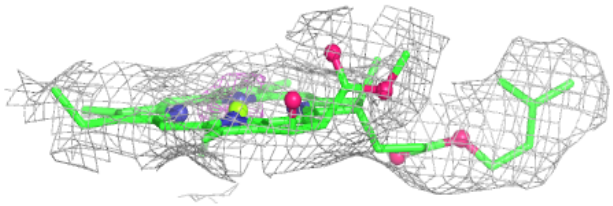


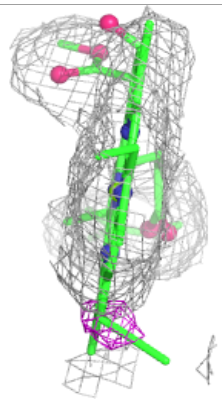


Electron density around CLA K 103:

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

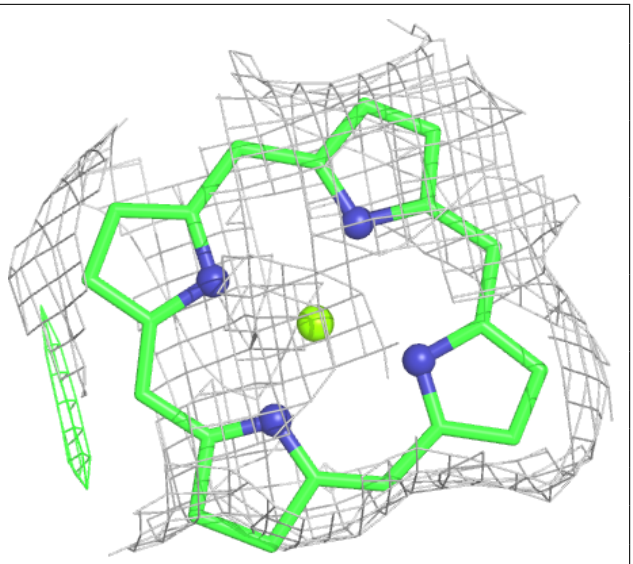


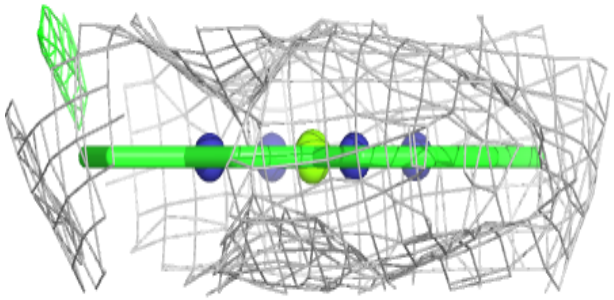


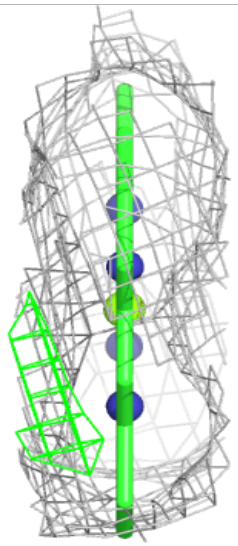


Electron density around CLA 3 304:

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

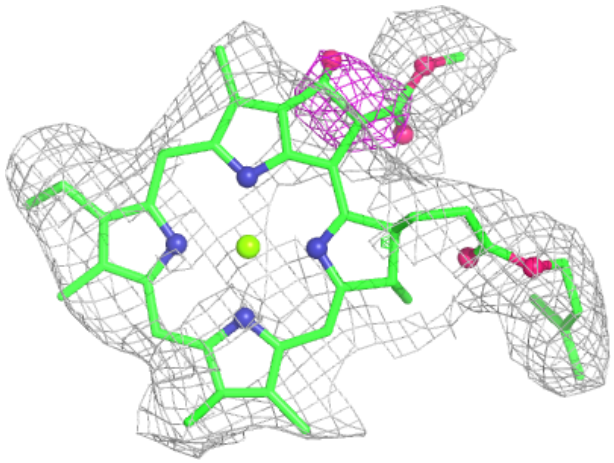


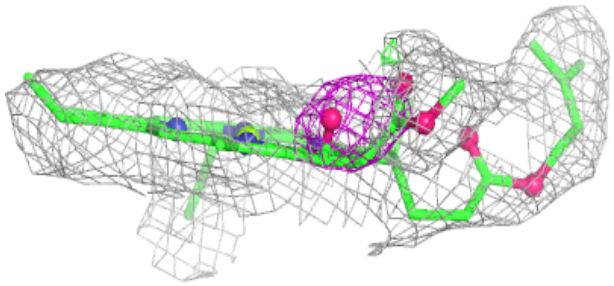


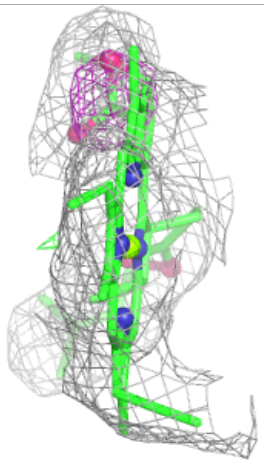


Electron density around CLA K 106:

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

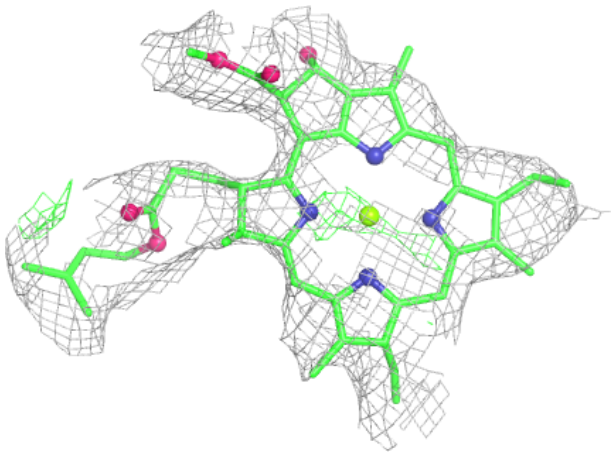


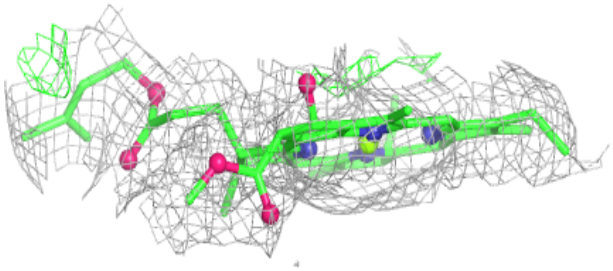


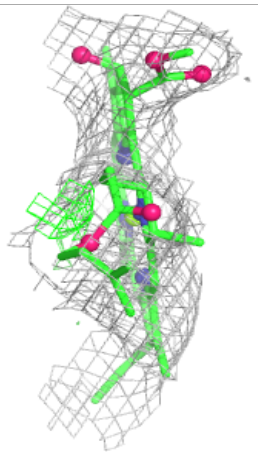


Electron density around CLA 2 304:

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

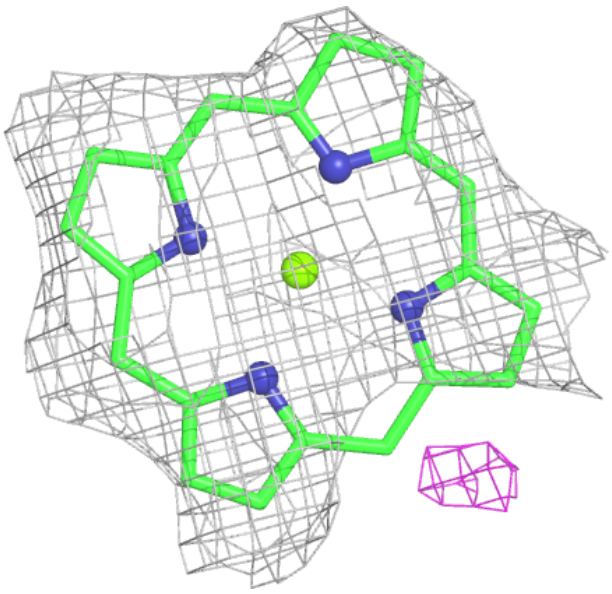


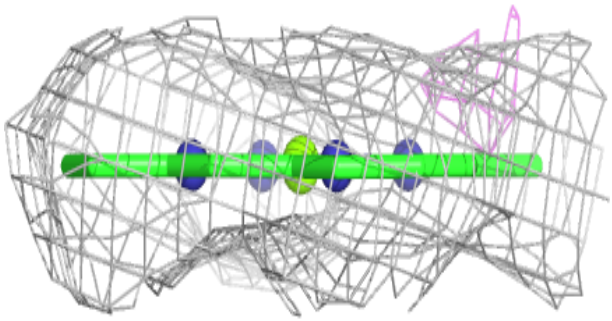


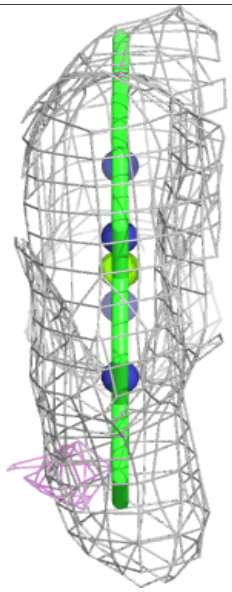


Electron density around CLA 3 312:

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

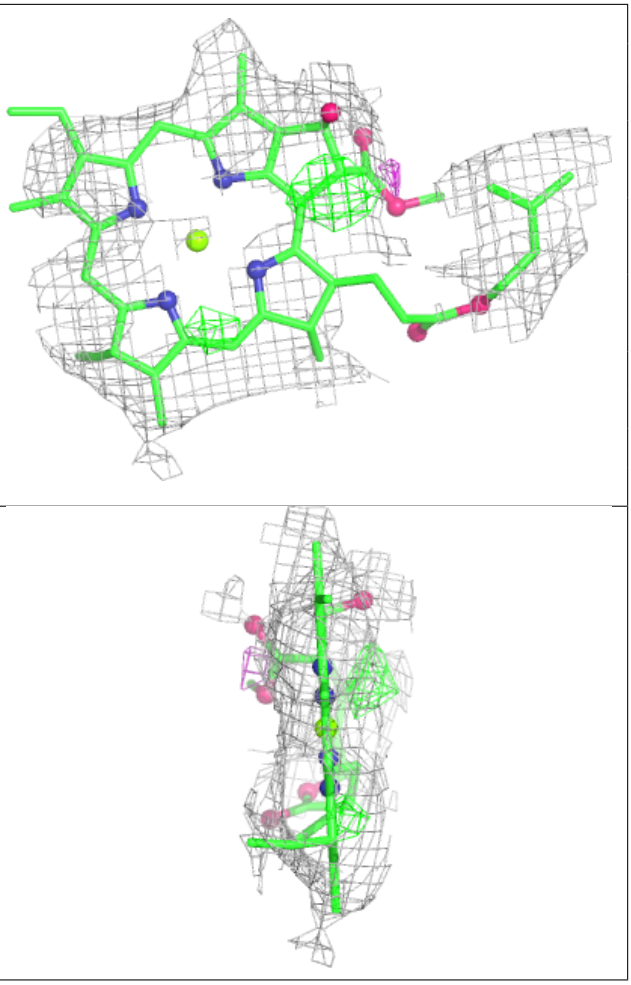


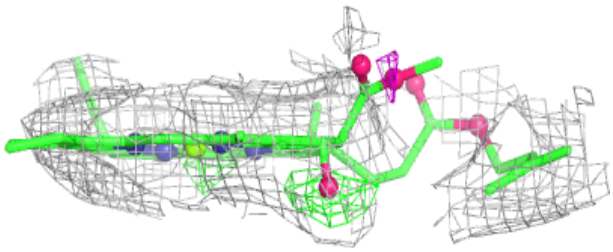




Electron density around CLA 2 311:

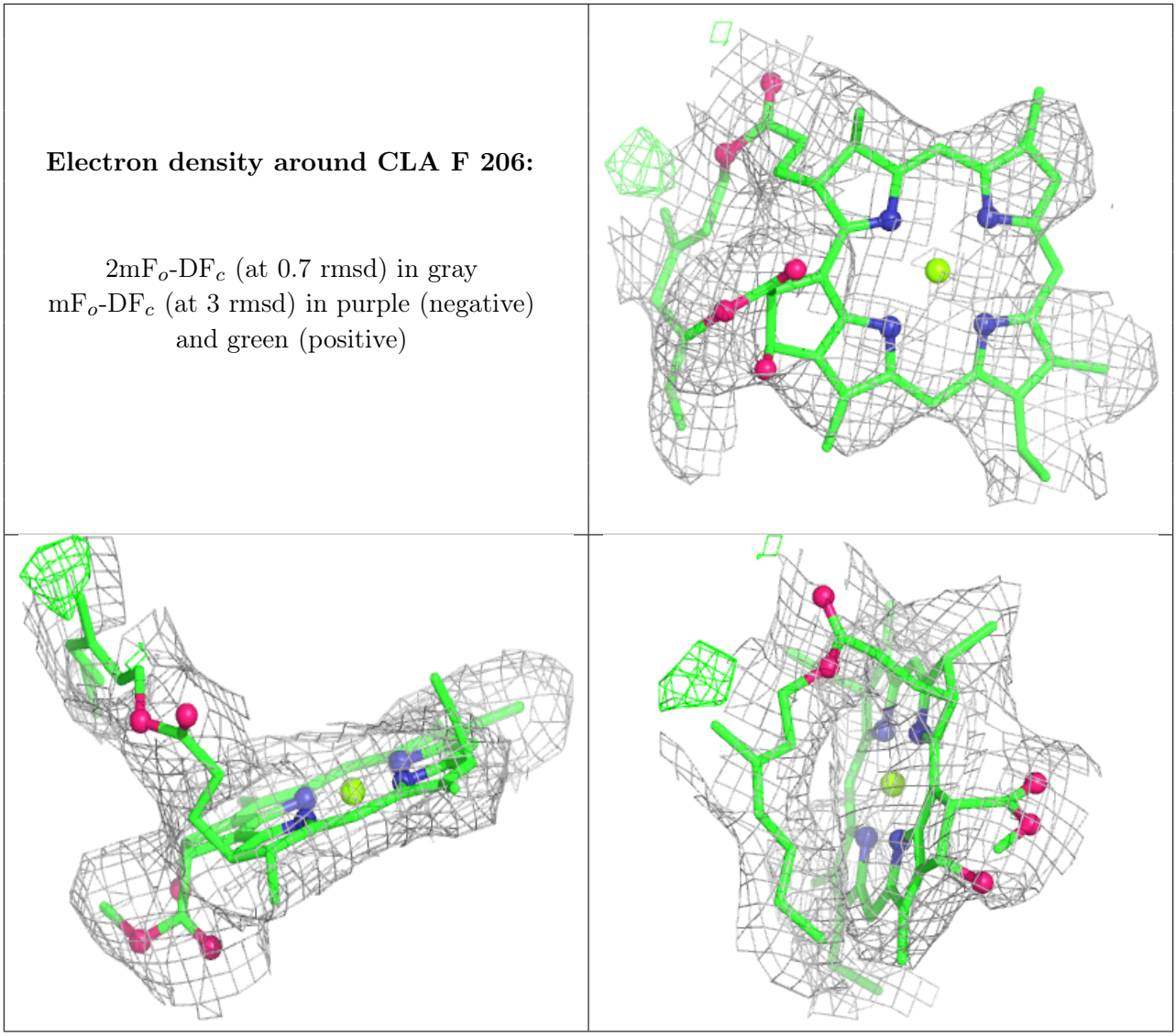
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)





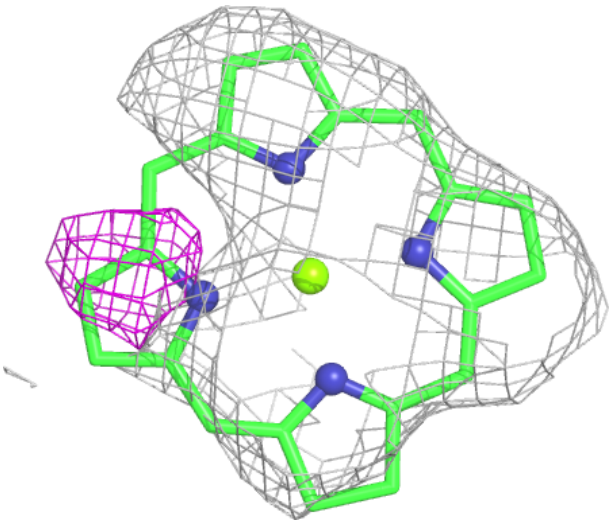
Electron density around CLA F 206:

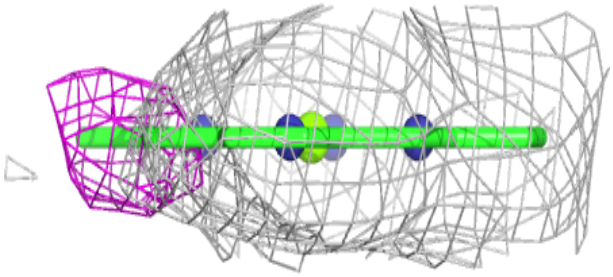
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

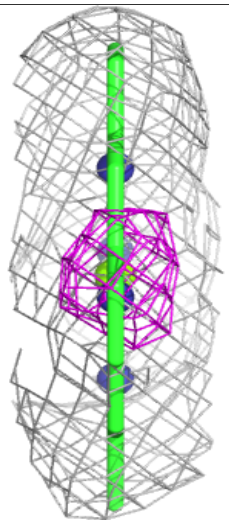


Electron density around CLA 3 316:

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

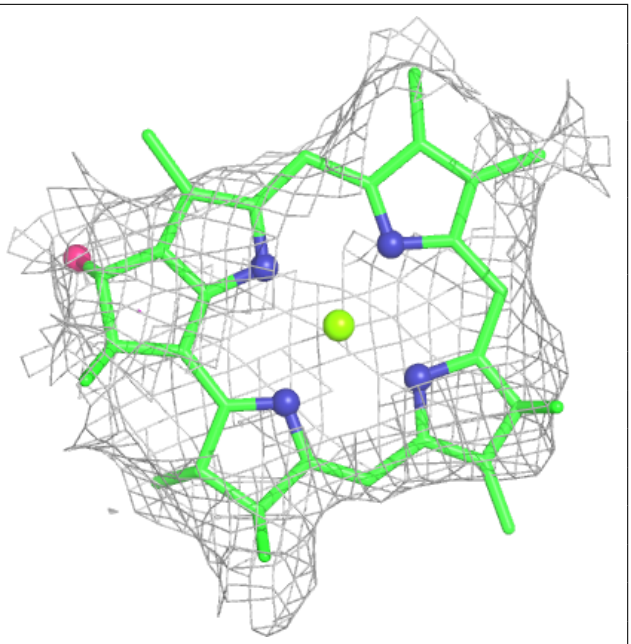


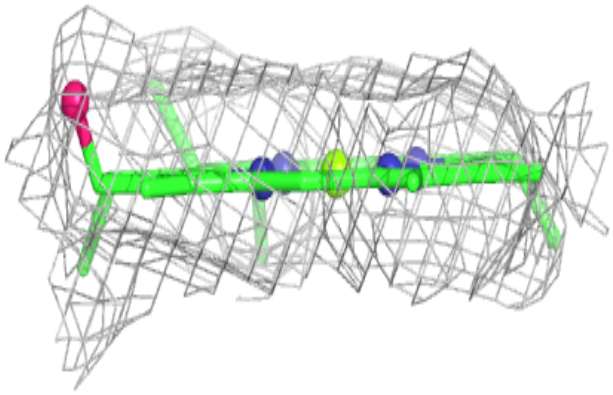


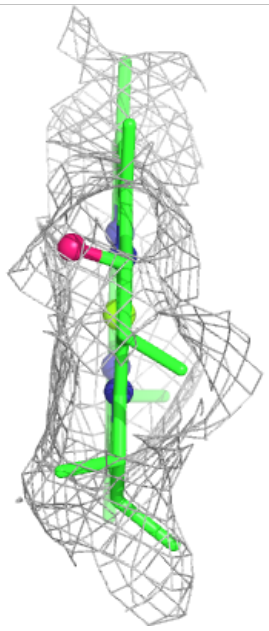


Electron density around CLA 3 319:

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

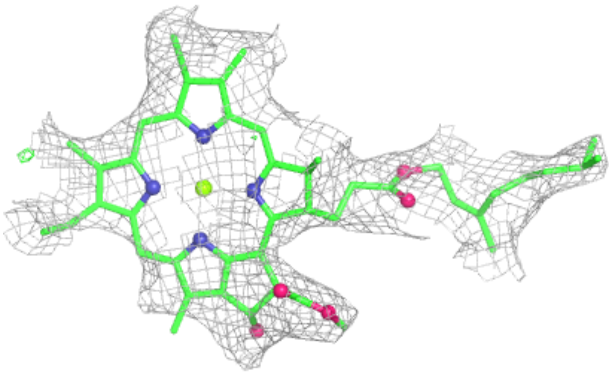


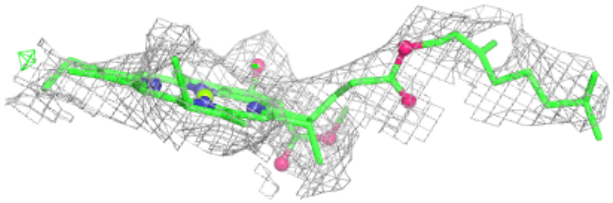


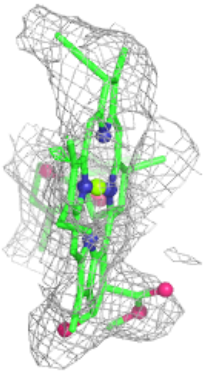


Electron density around CLA 3 320:

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

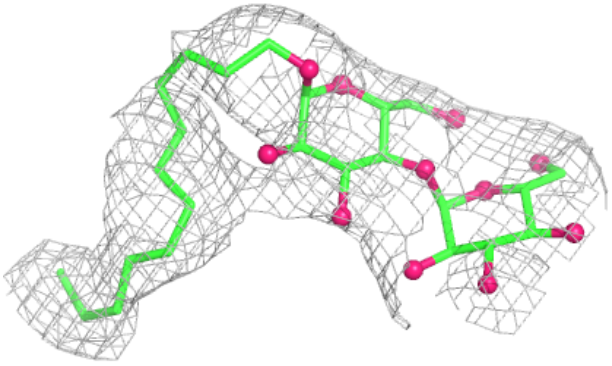


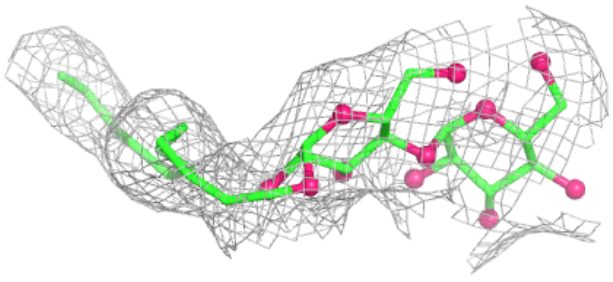




Electron density around LMU R 105:

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

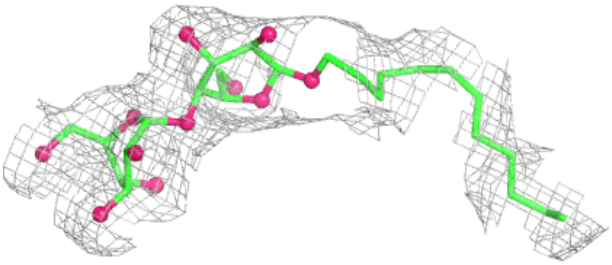


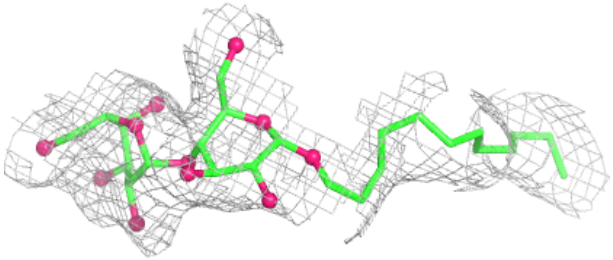


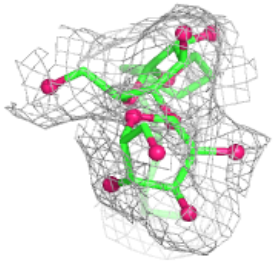


Electron density around LMU 2 318:

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

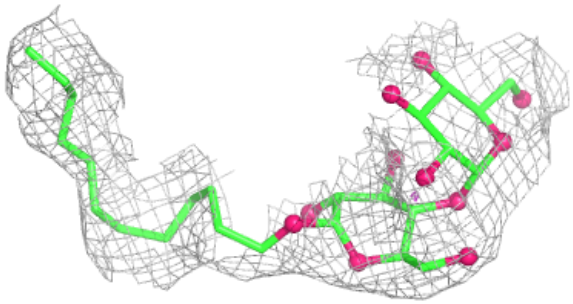


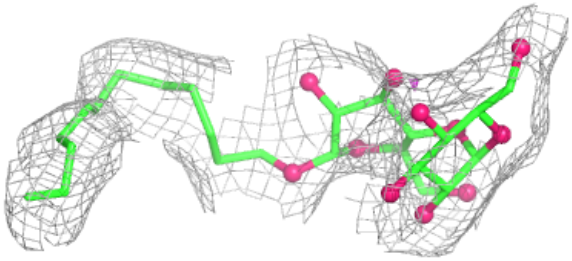


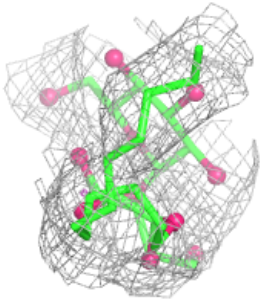


Electron density around LMU 2 319:

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

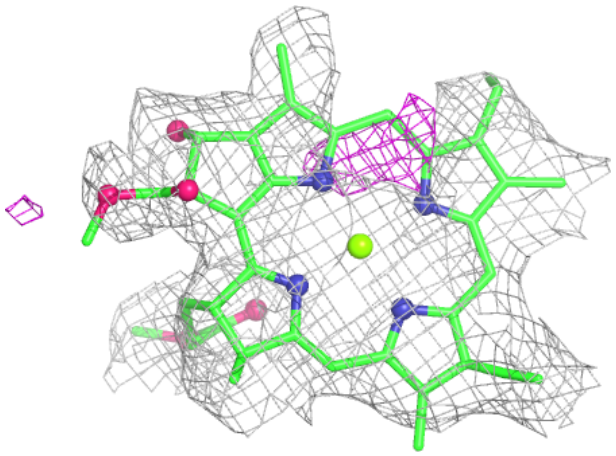


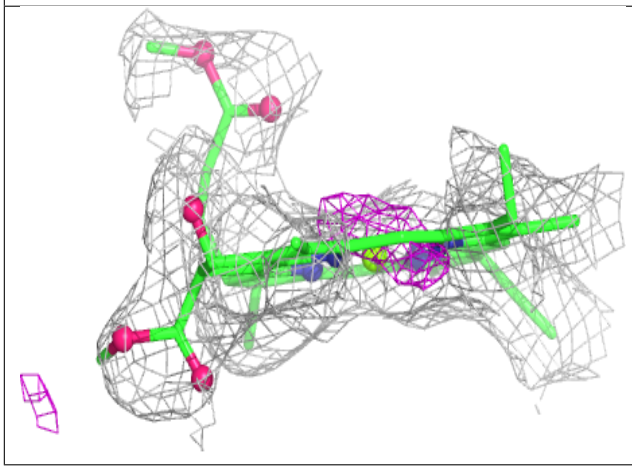


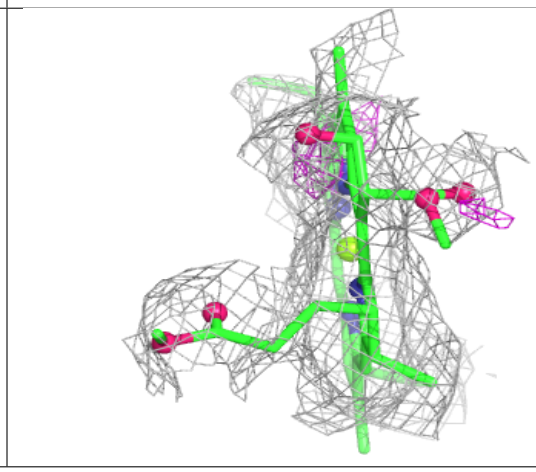


Electron density around CLA A 805:

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

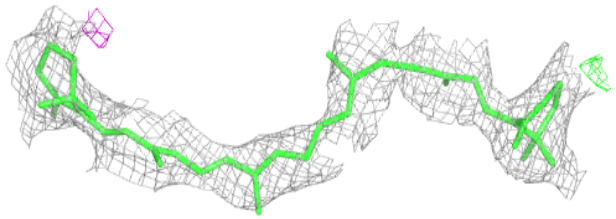


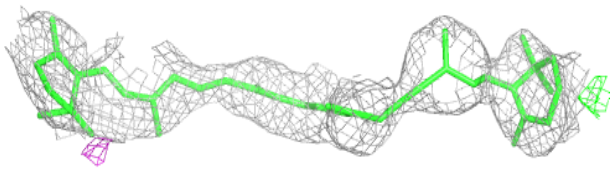


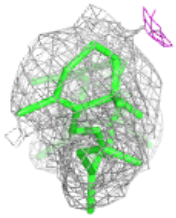


Electron density around BCR I 103:

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

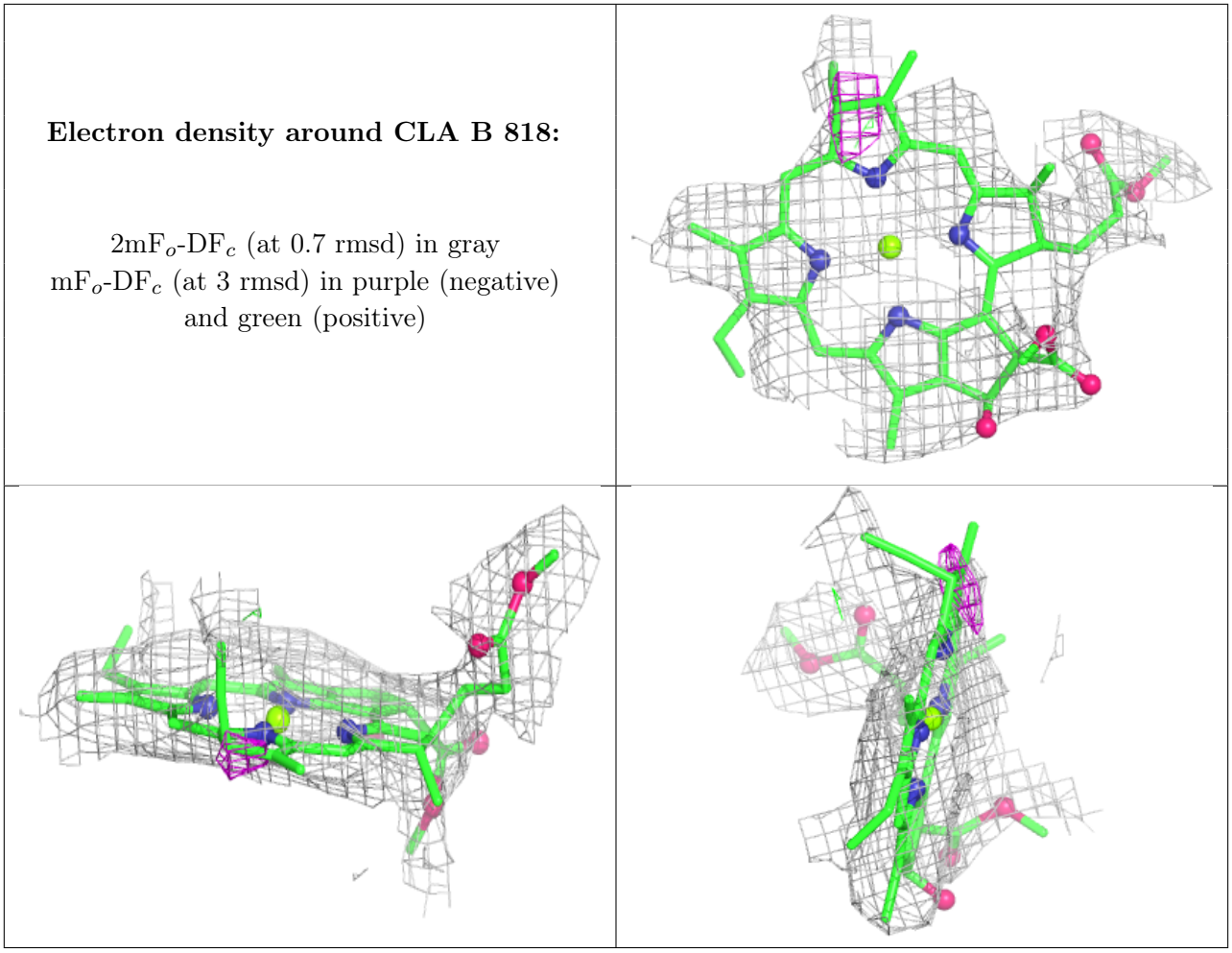






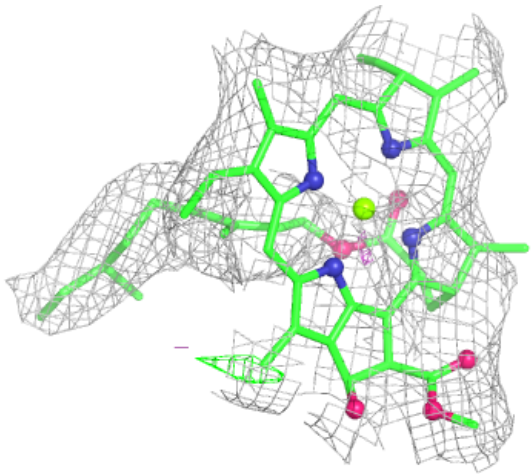
Electron density around CLA B 818:

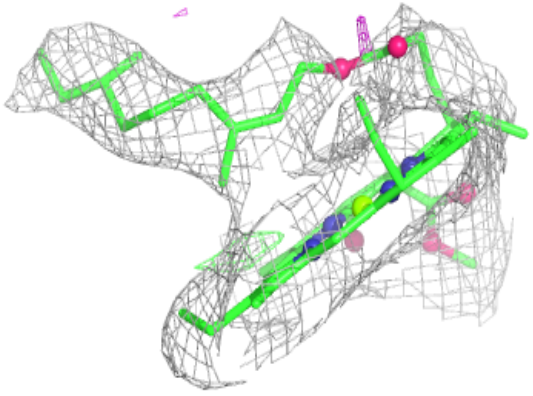
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

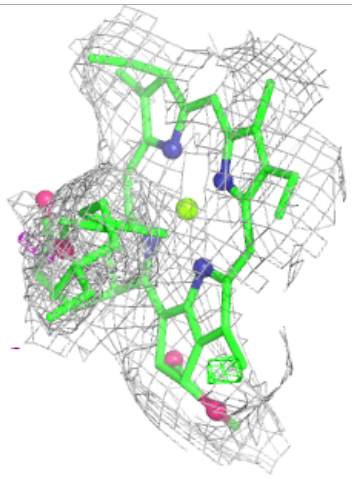


Electron density around CLA 2 302:

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

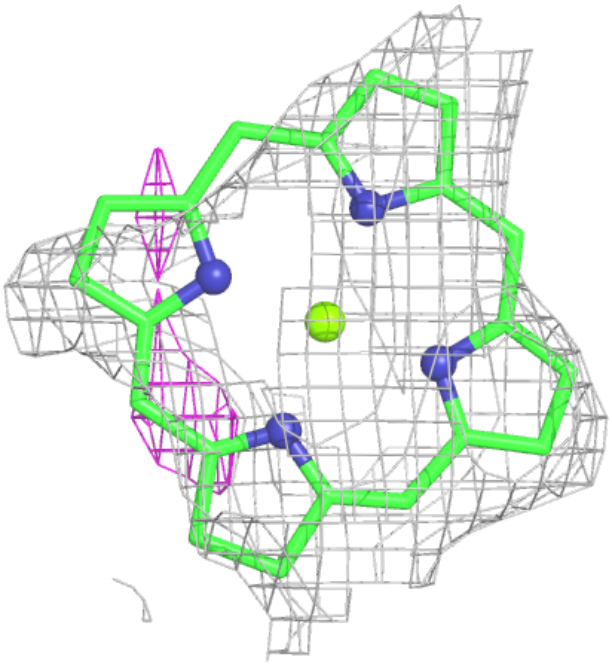


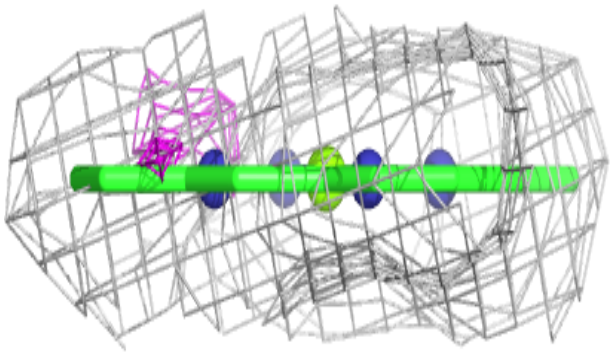


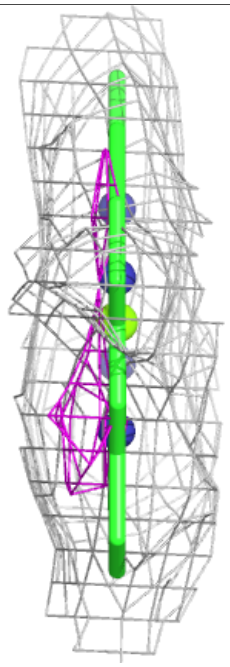


Electron density around CLA 2 314:

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

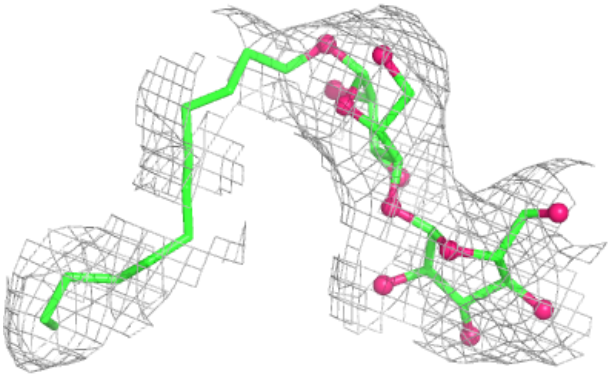


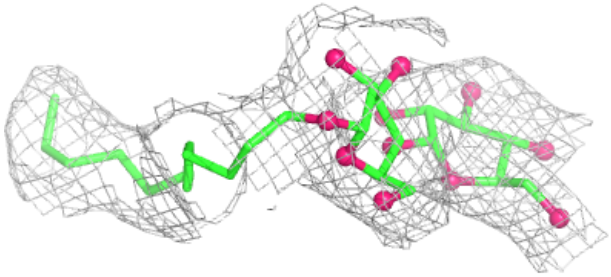




Electron density around LMU L 206:

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

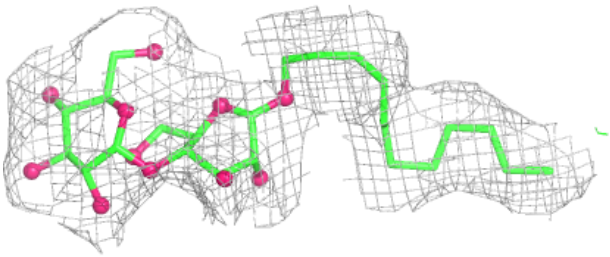


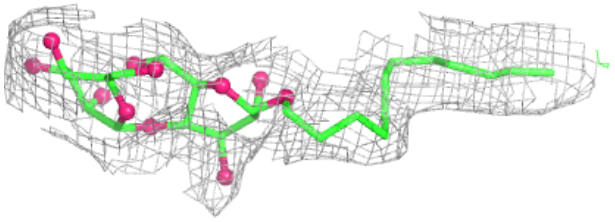


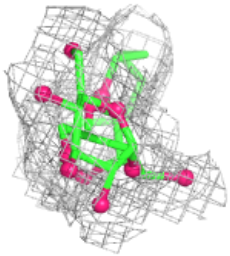


Electron density around LMU R 101:

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

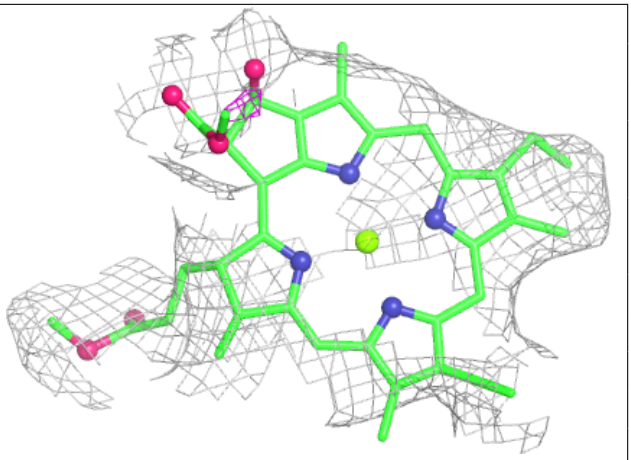


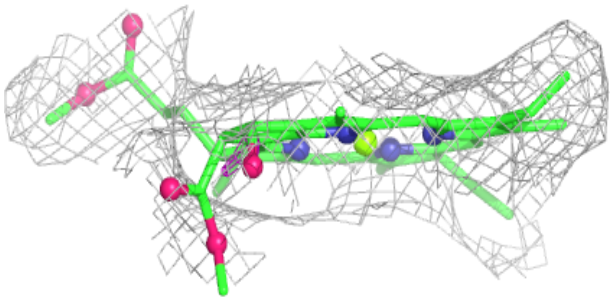




Electron density around CLA 1 201:

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

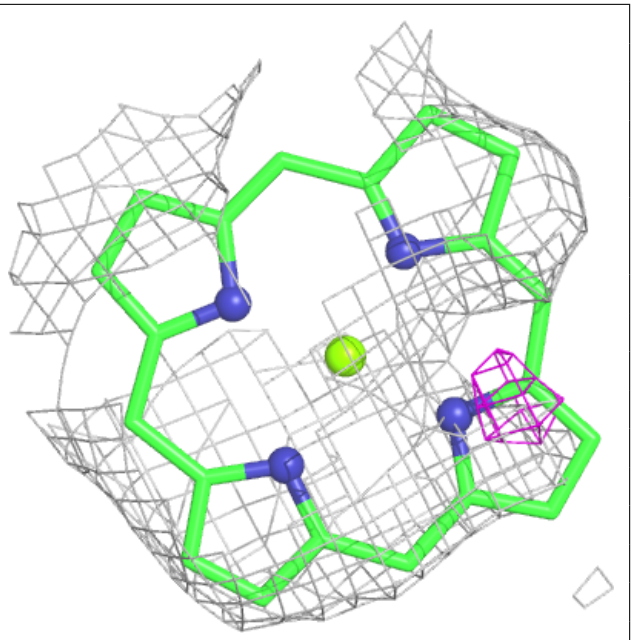


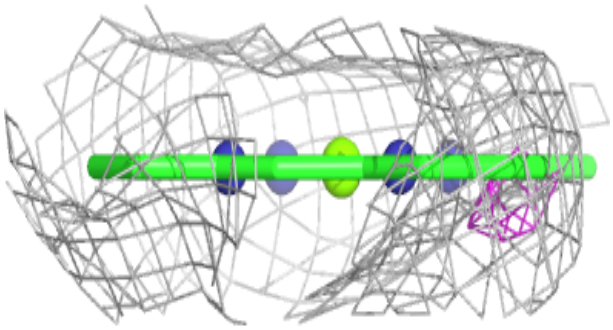


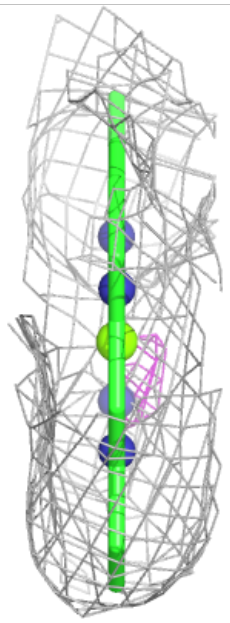


Electron density around CLA 3 306:

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

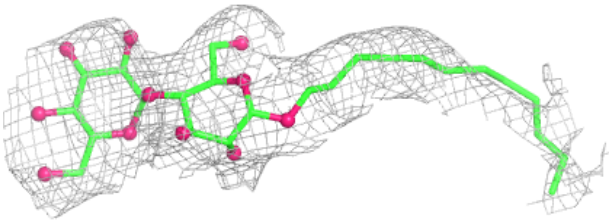


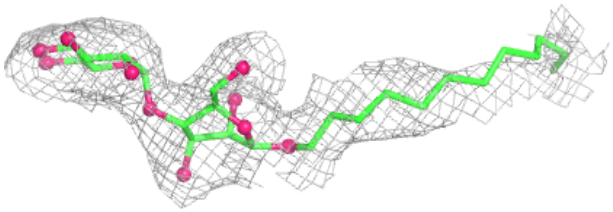


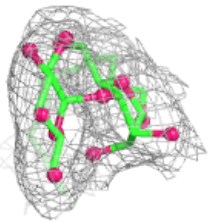


Electron density around LMU 2 320:

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



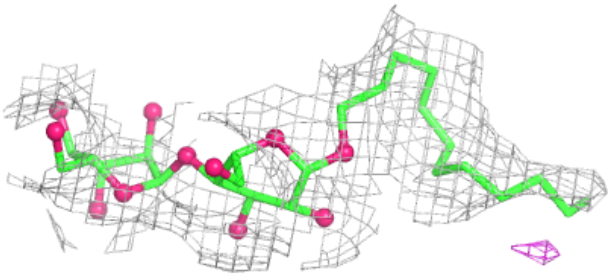


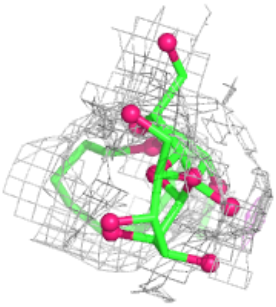


Electron density around LMU 3 318:

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

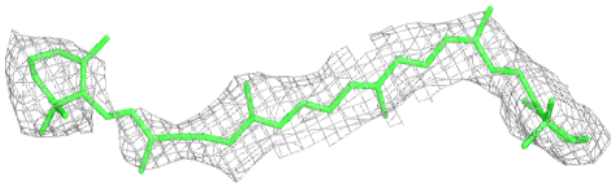


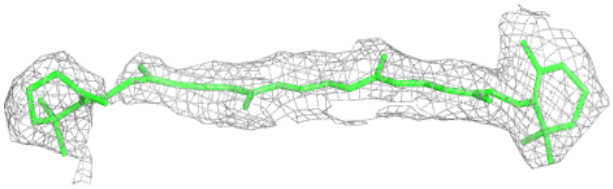


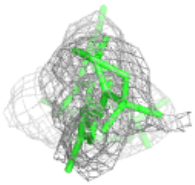


Electron density around BCR B 842:

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

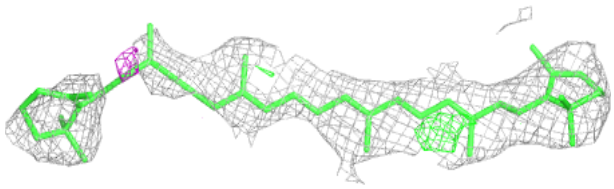


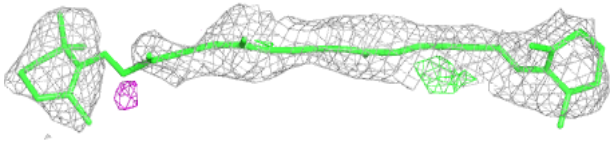


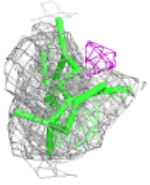


Electron density around BCR B 844:

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

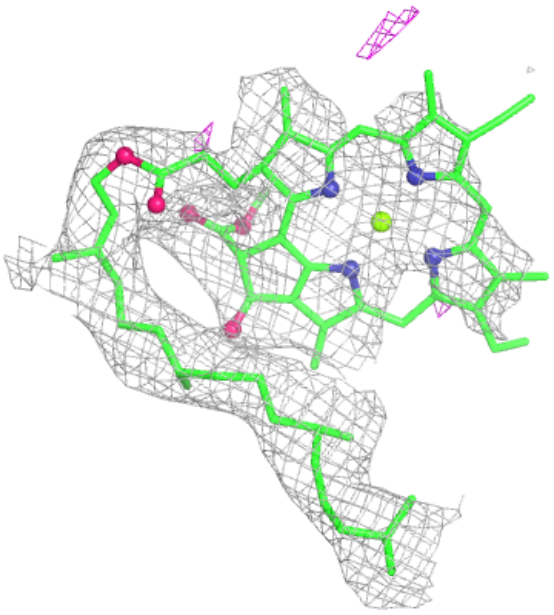


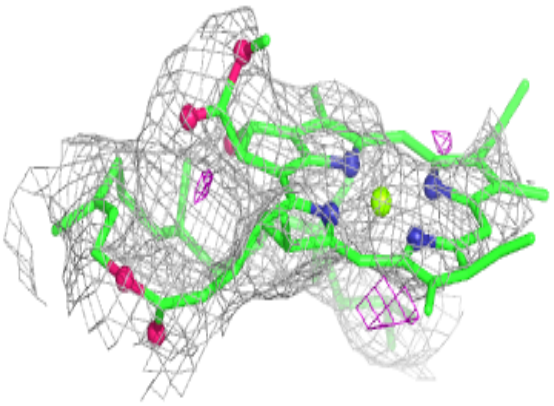




Electron density around CLA A 821:

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

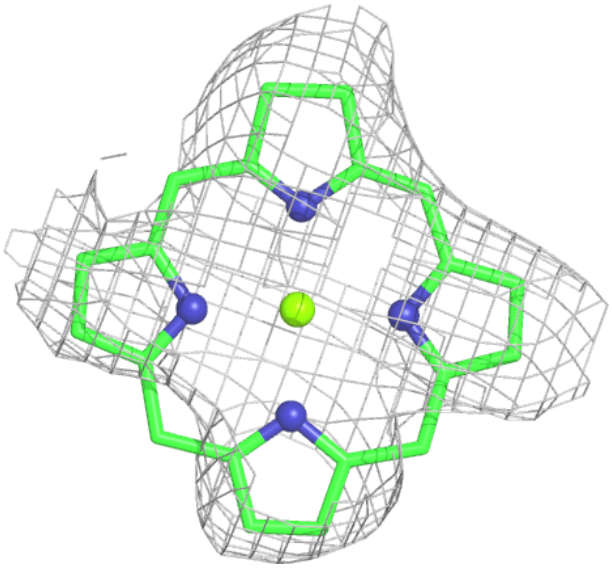


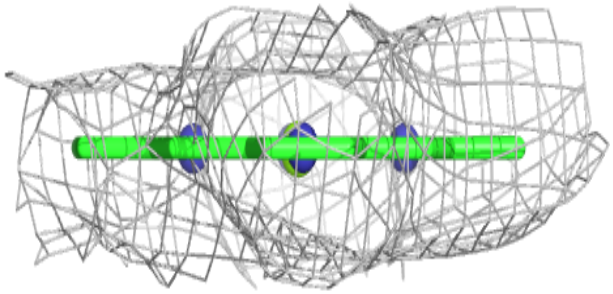


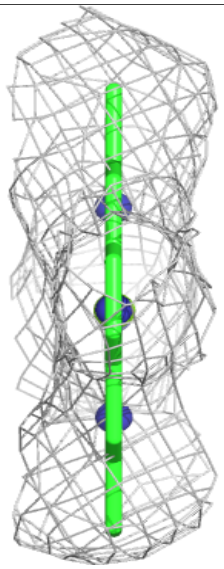


Electron density around CLA 3 313:

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



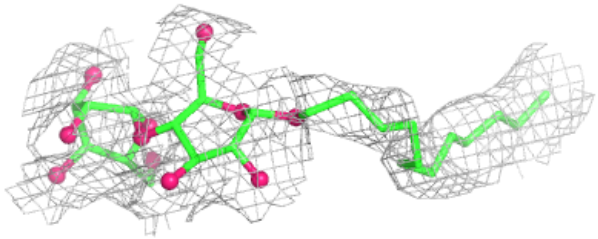




Electron density around LMU 4 301:

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

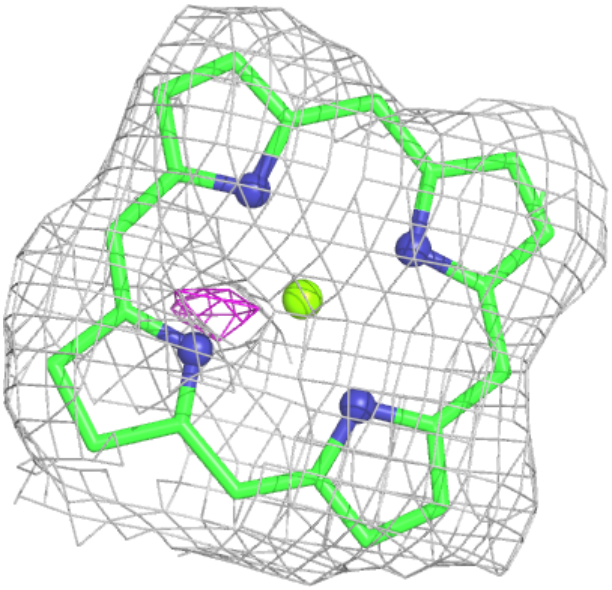


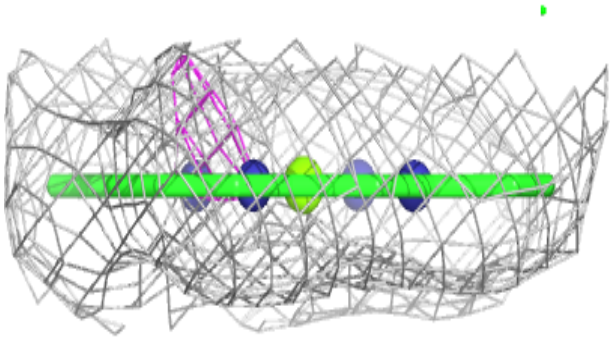


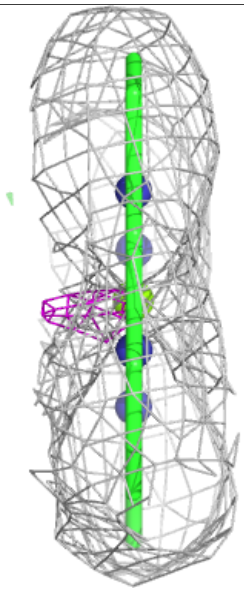


Electron density around CLA 4 314:

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

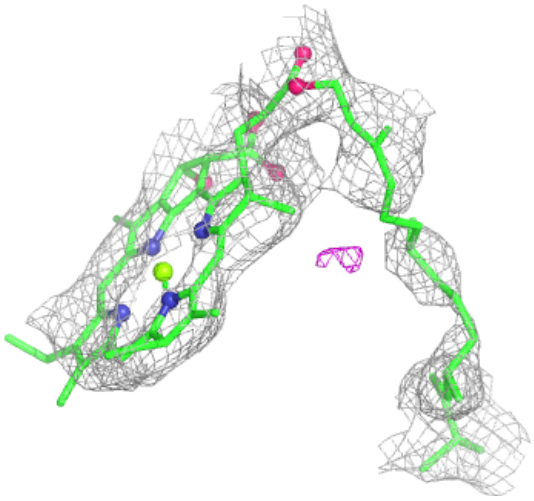


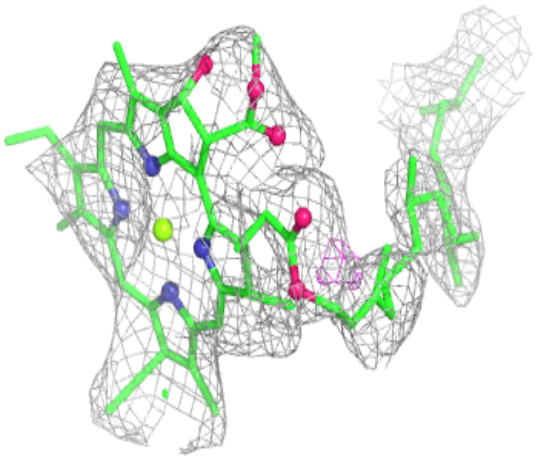


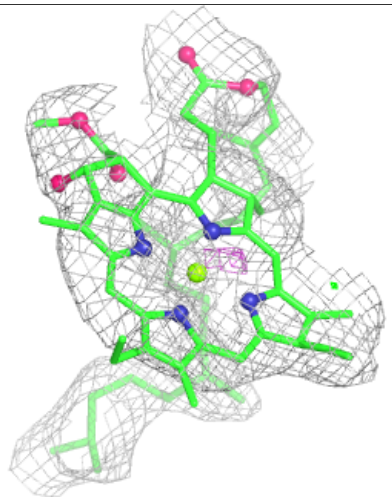


Electron density around CLA 2 306:

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

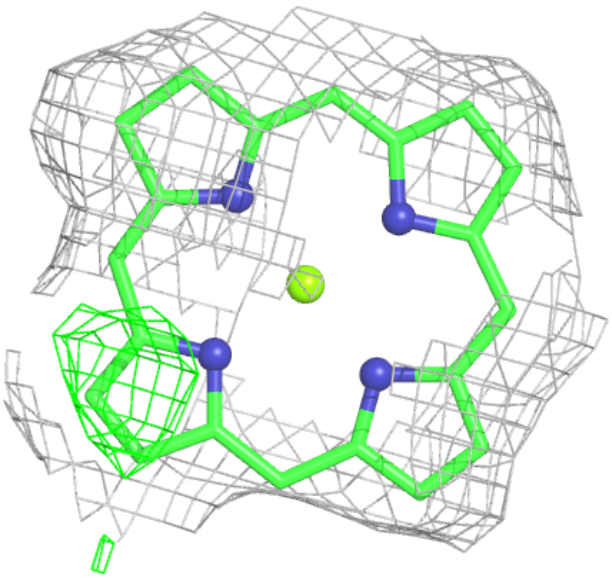


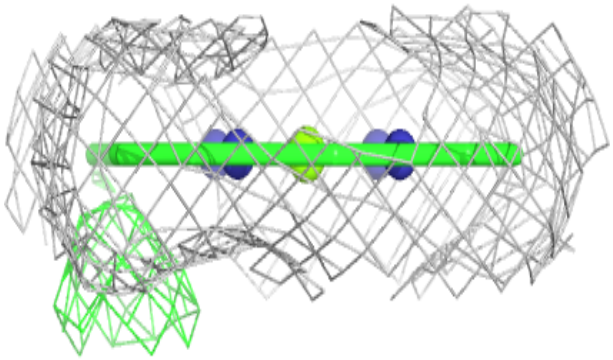


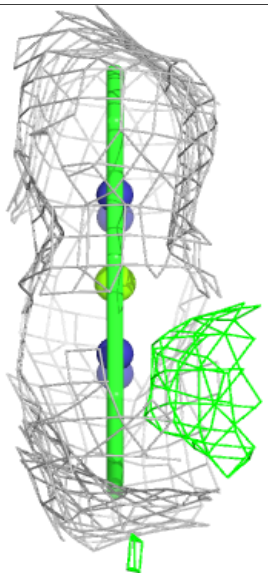


Electron density around CLA 1 208:

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

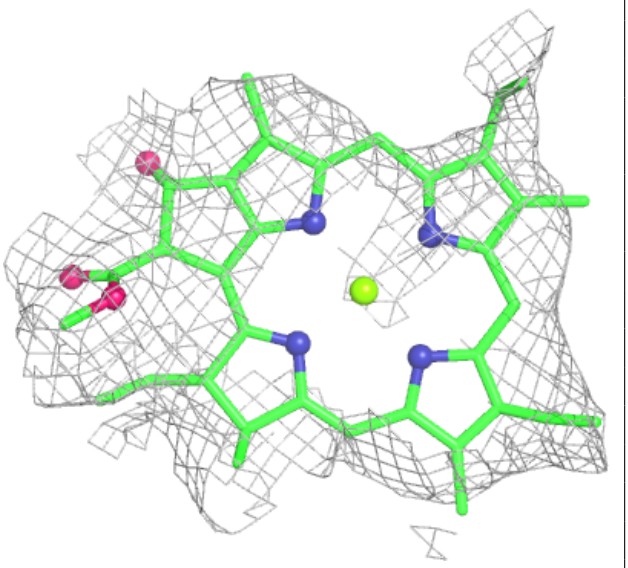


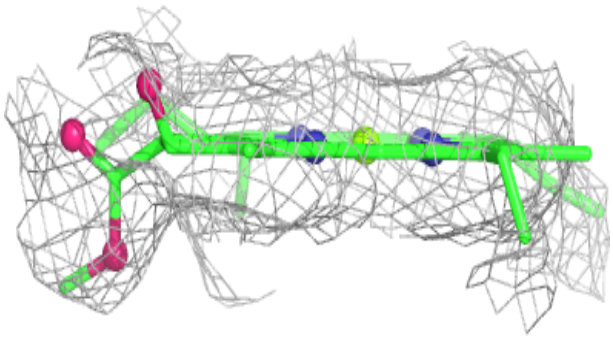


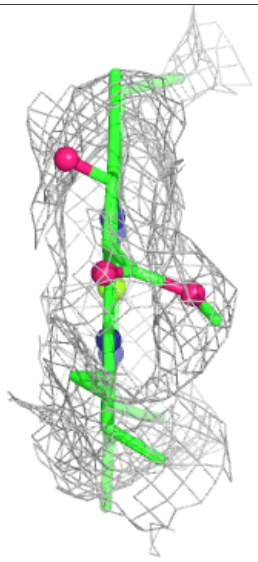


Electron density around CLA A 819:

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



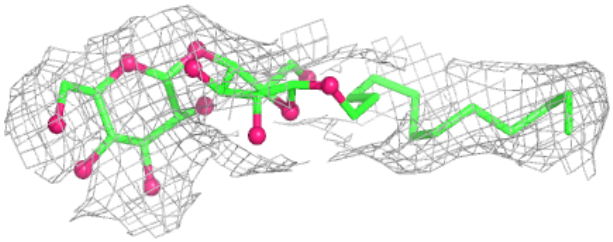


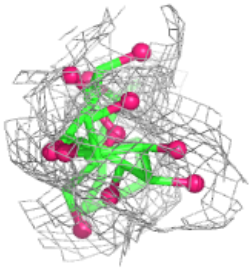


Electron density around LMU K 102:

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

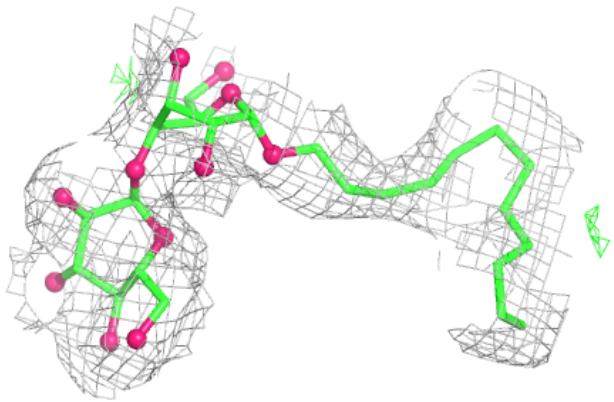


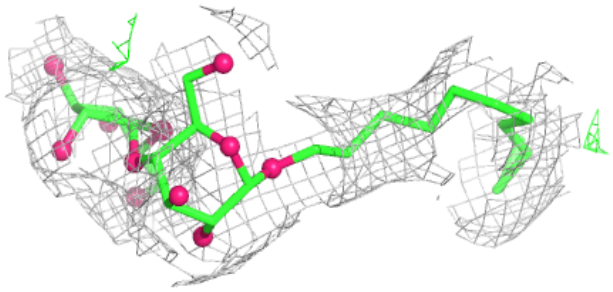


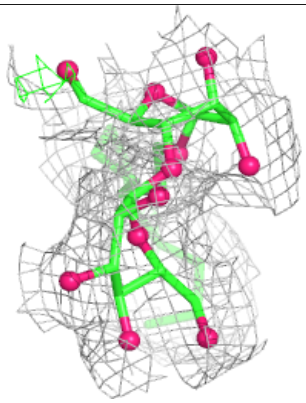


Electron density around LMU K 104:

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

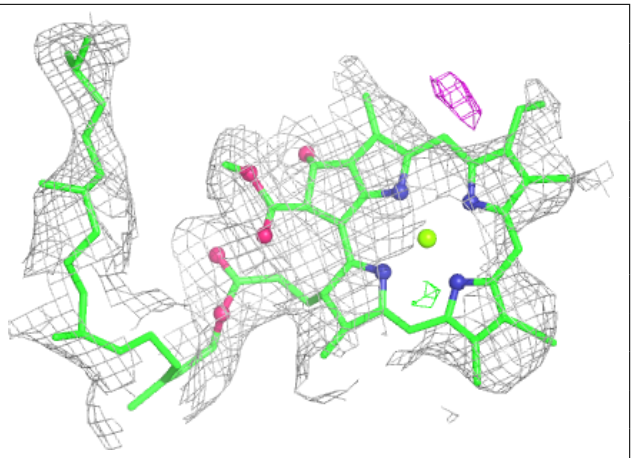


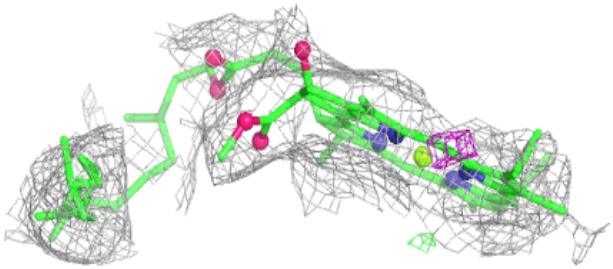




Electron density around CLA R 107:

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

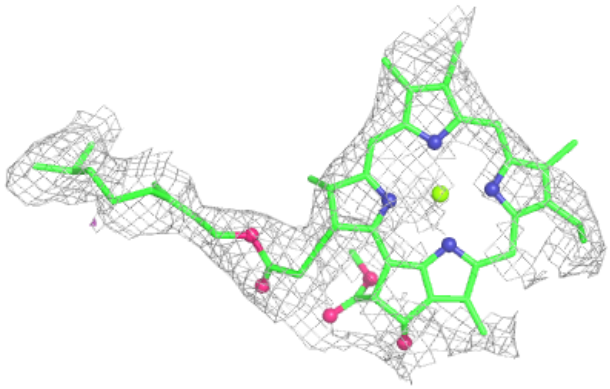


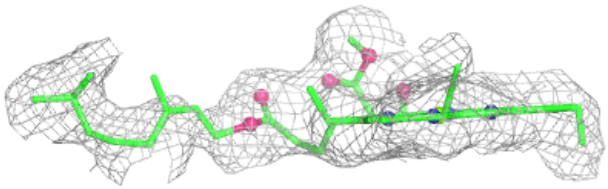


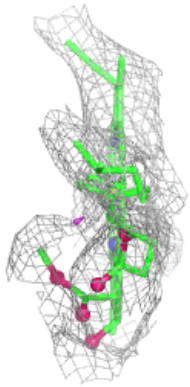


Electron density around CLA 4 310:

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

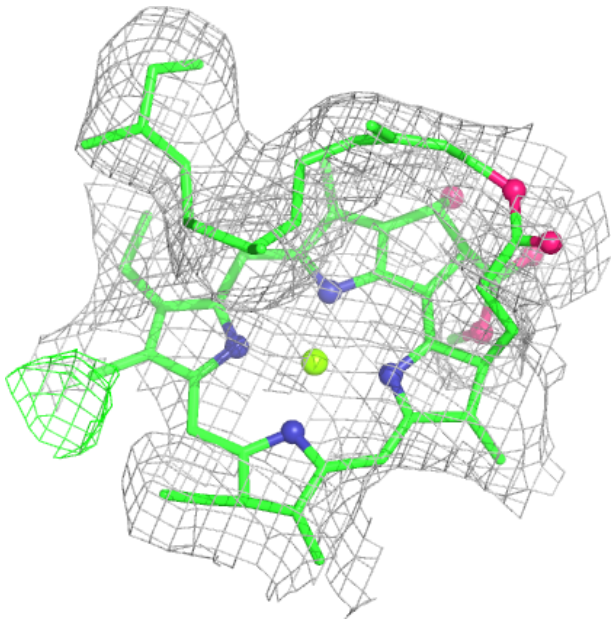


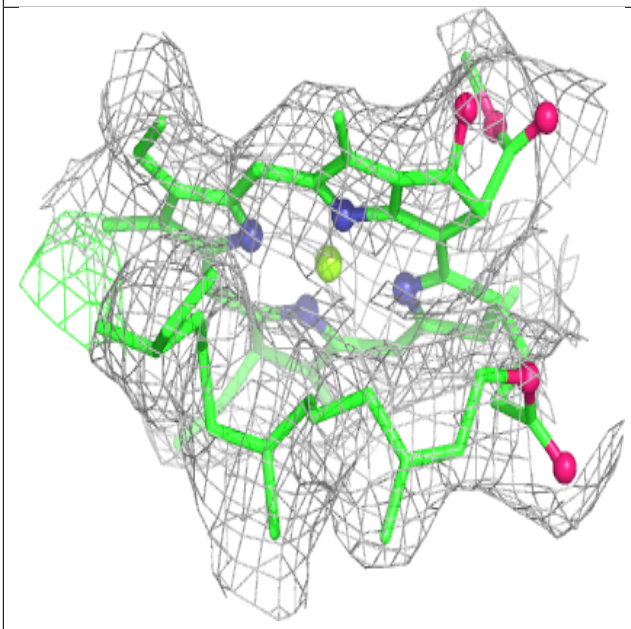


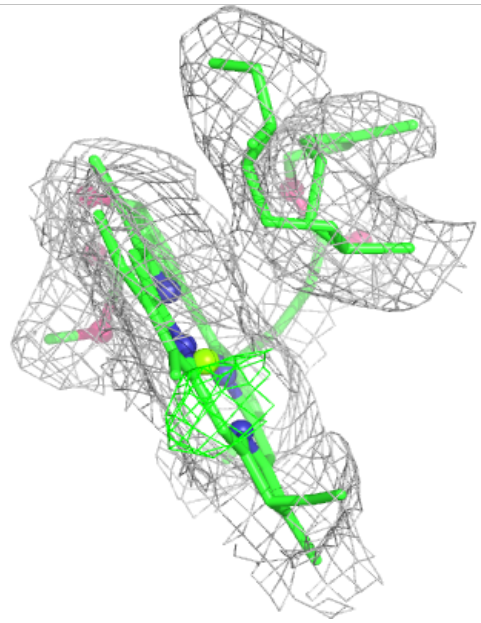


Electron density around CLA 1 206:

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

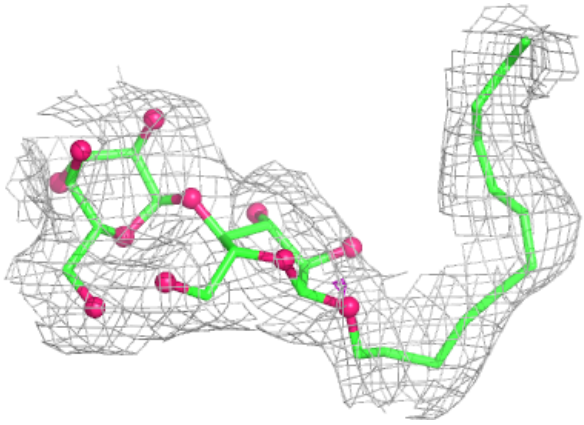


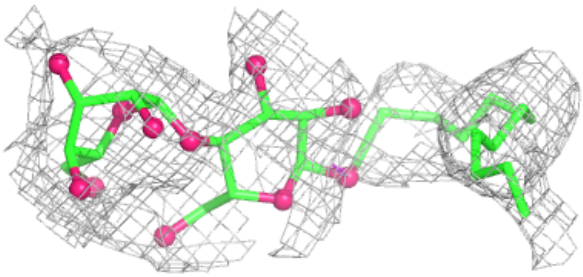


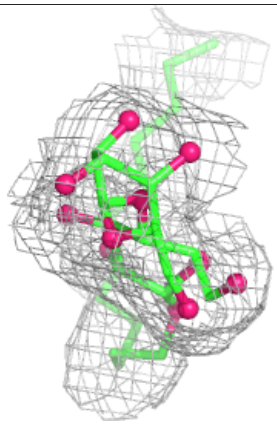


Electron density around LMU 3 302:

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

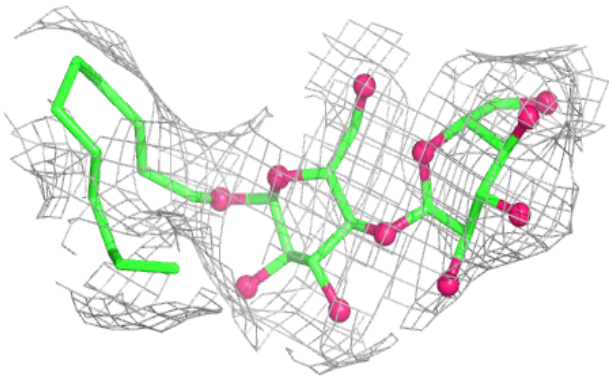


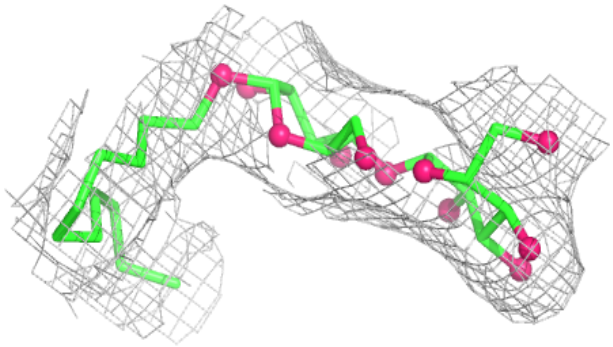


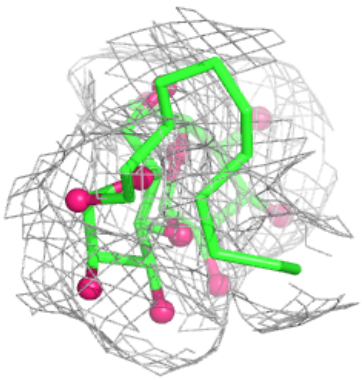


Electron density around LMU F 201:

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

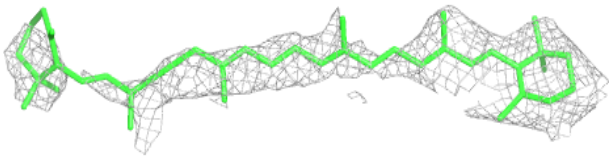


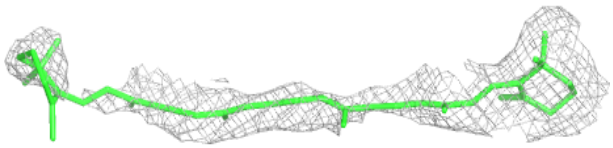


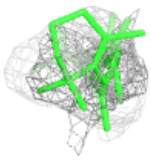


Electron density around BCR A 843:

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

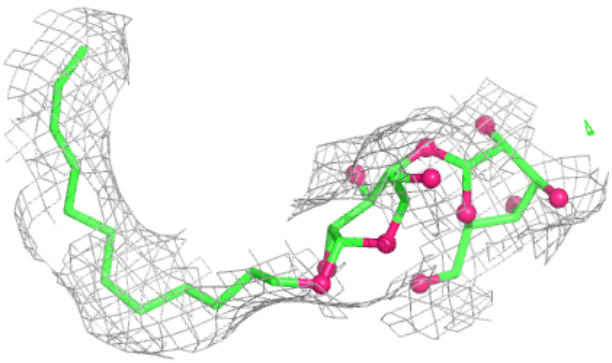


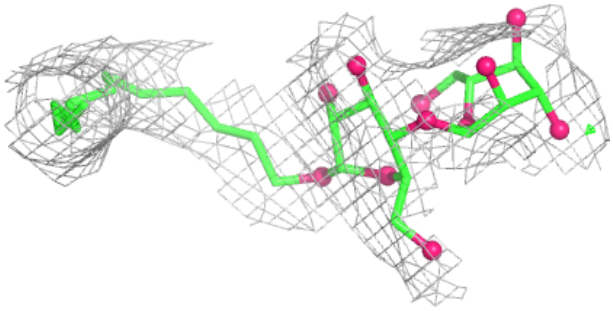




Electron density around LMU 2 316:

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

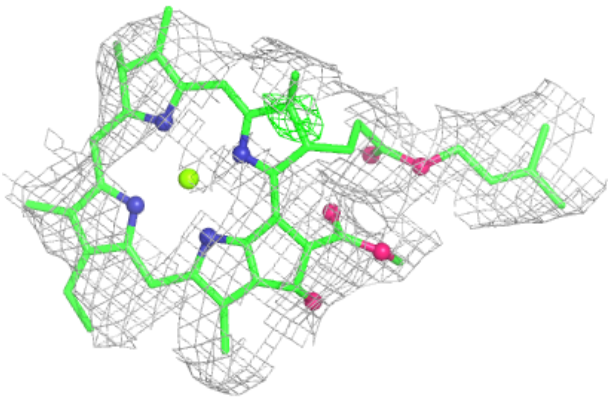


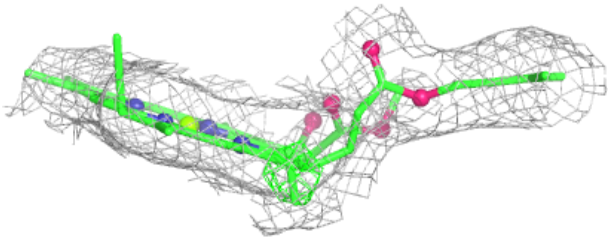


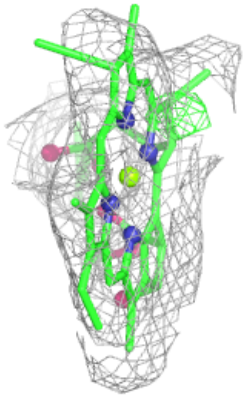


Electron density around CLA L 208:

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

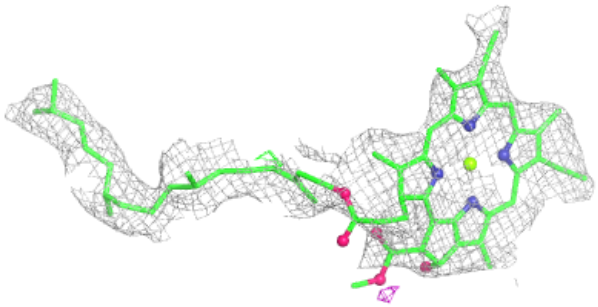


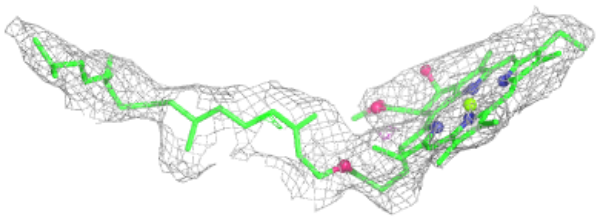


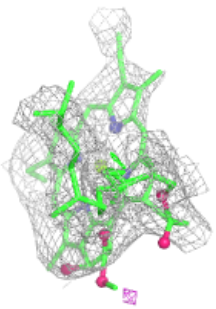


Electron density around CLA H 107:

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

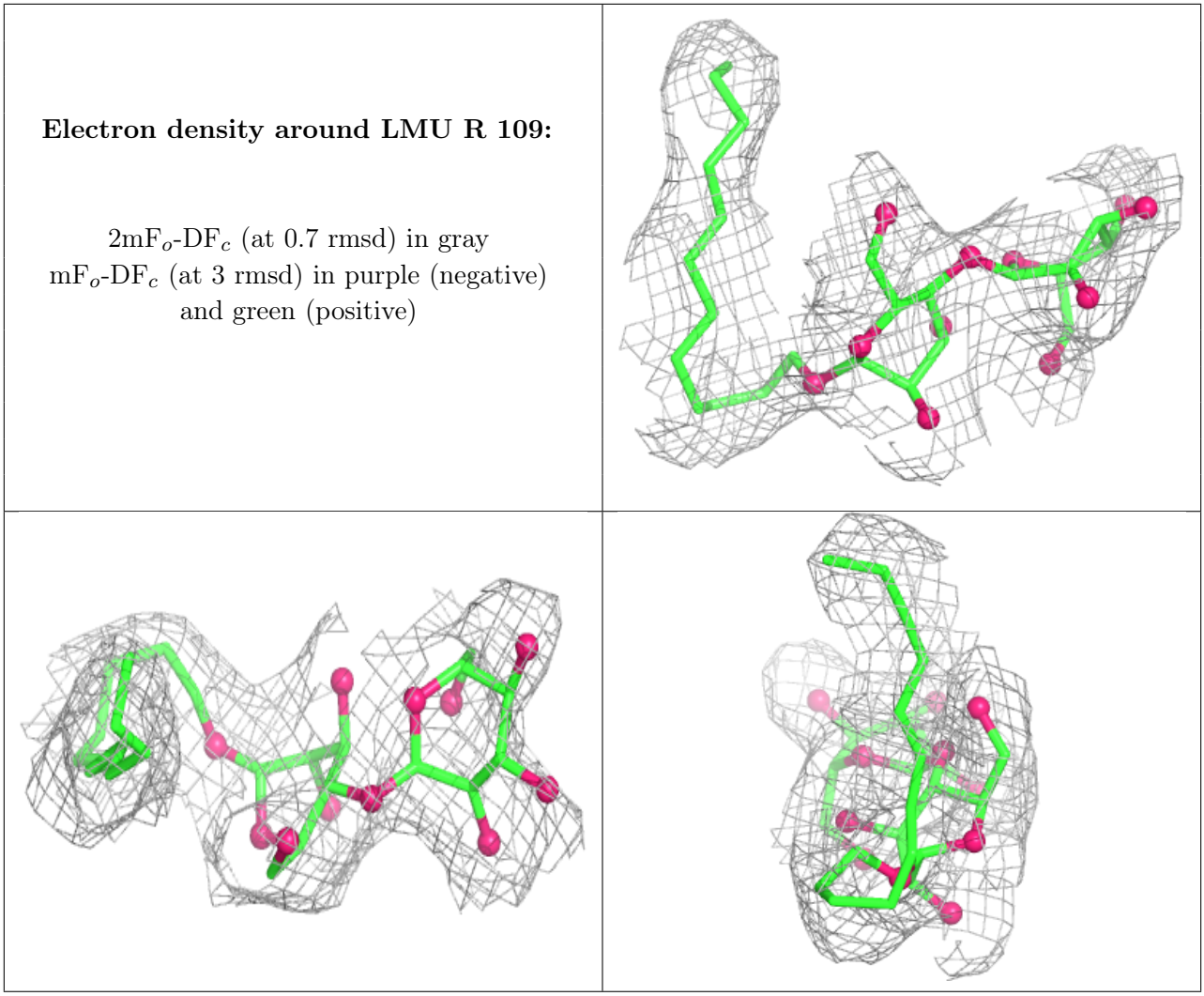






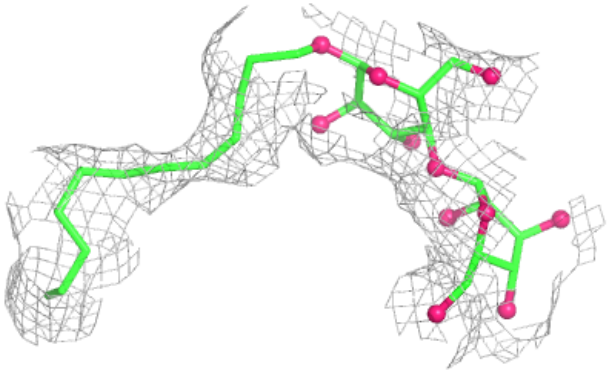
Electron density around LMU R 109:

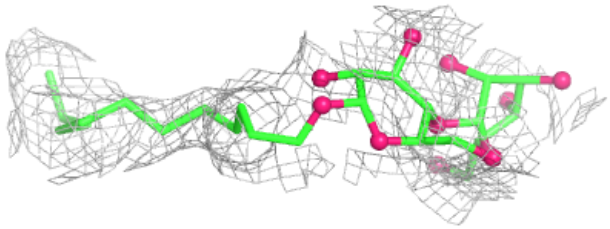
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

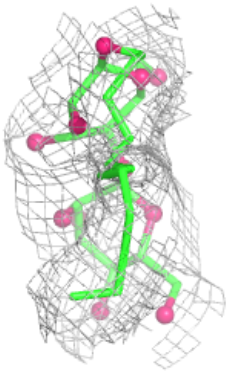


Electron density around LMU 4 321:

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

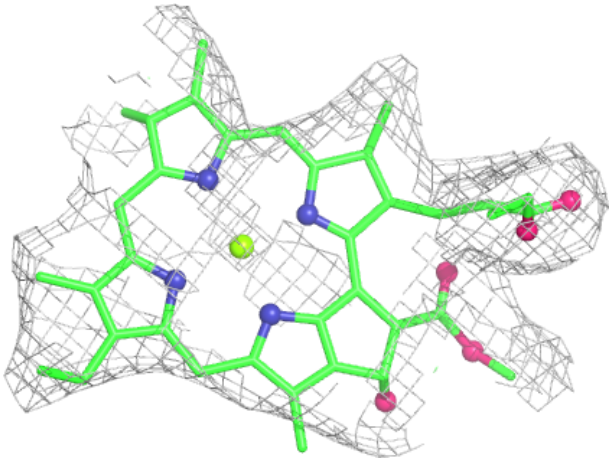


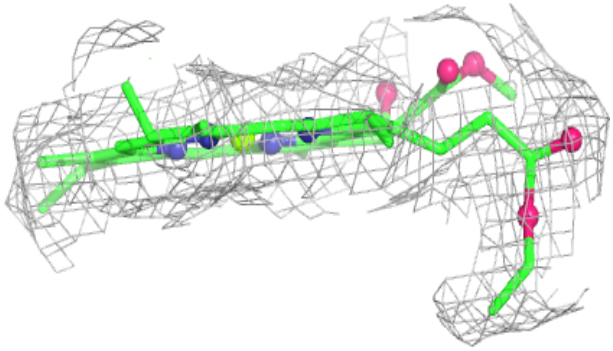


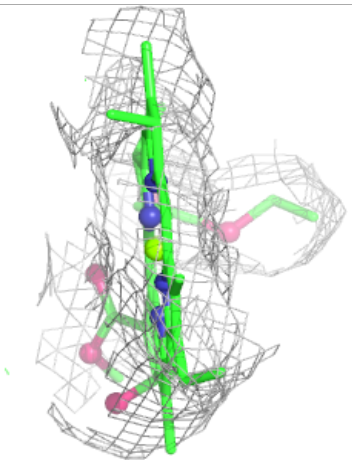


Electron density around CLA A 850:

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

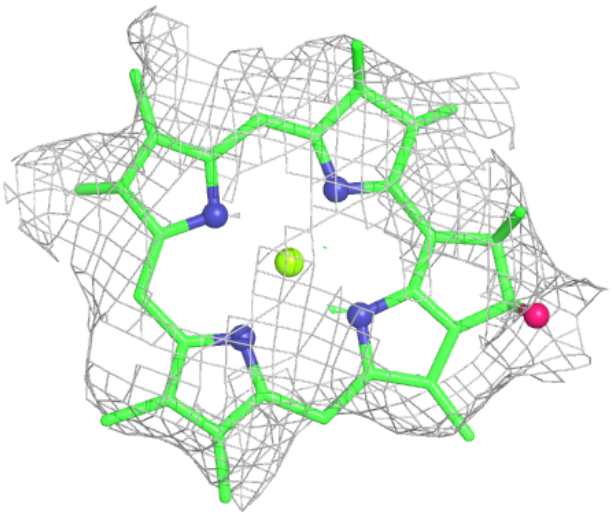


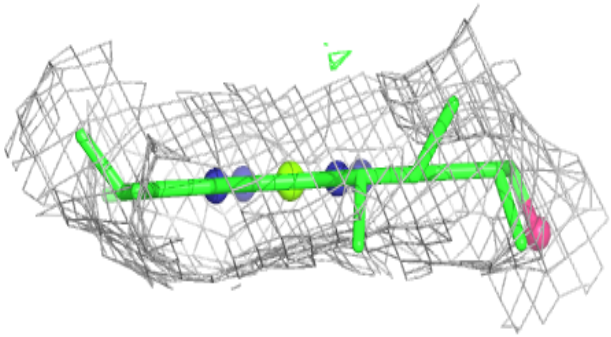


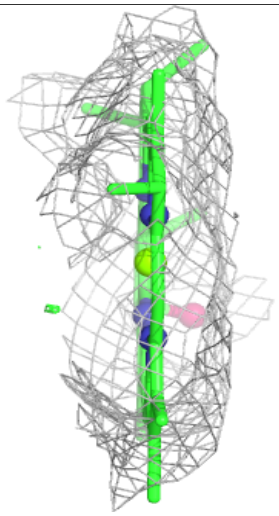


Electron density around CLA 3 303:

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

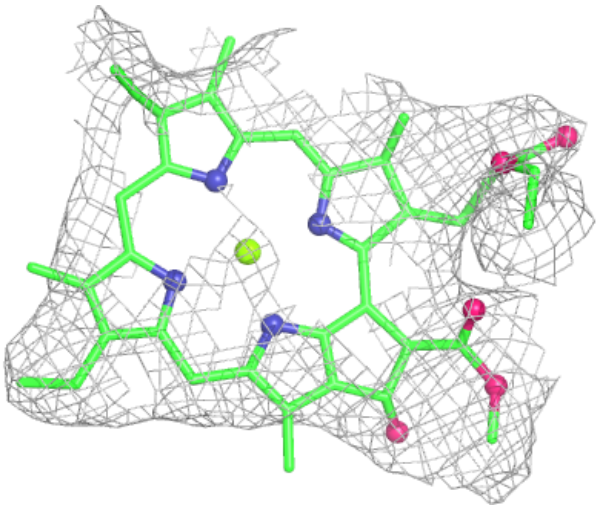


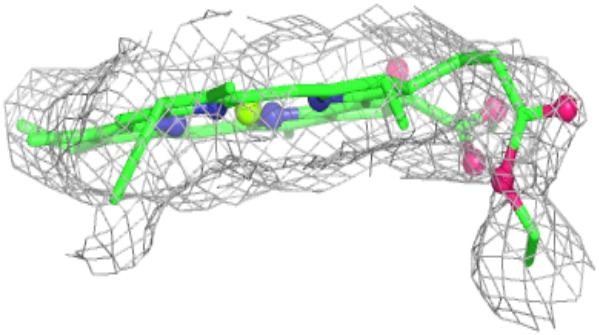


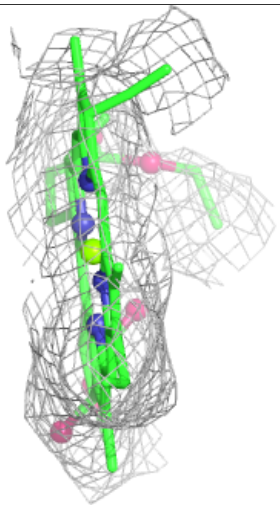


Electron density around CLA 1 202:

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

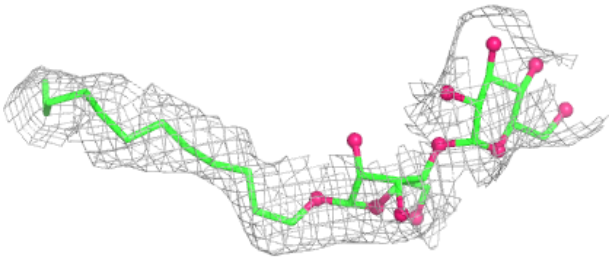


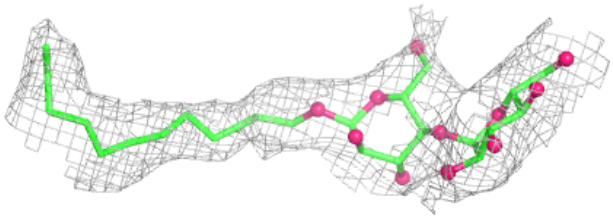


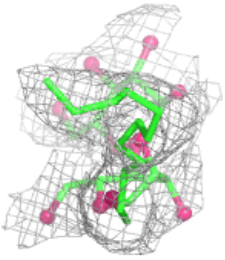


Electron density around LMU 4 316:

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

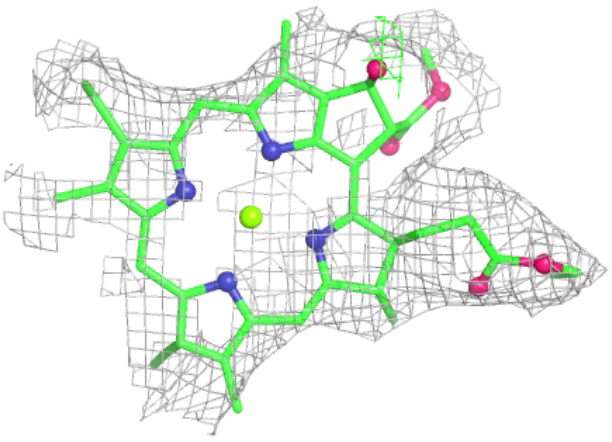


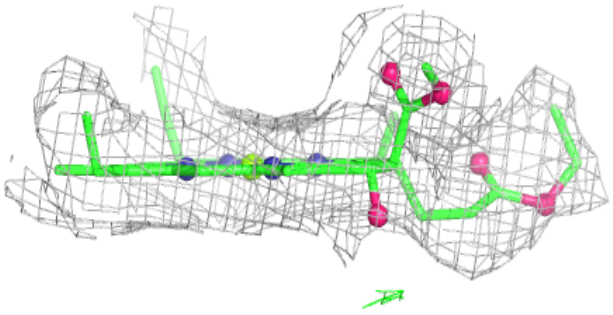


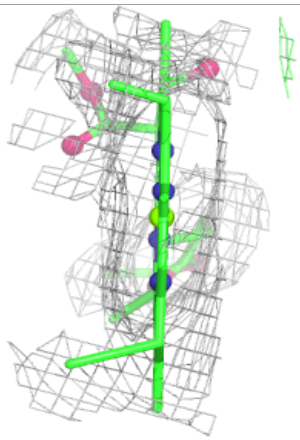


Electron density around CLA 1 203:

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

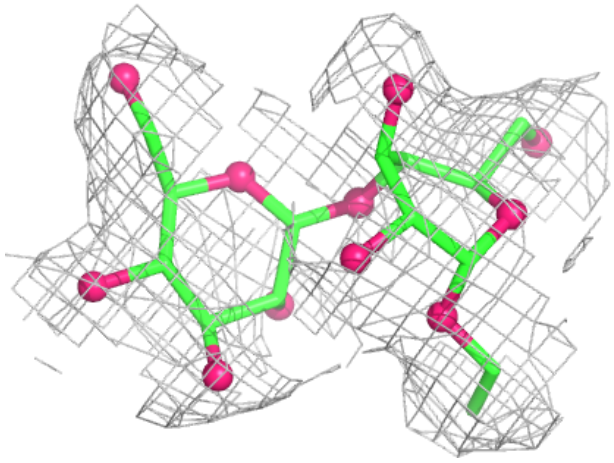


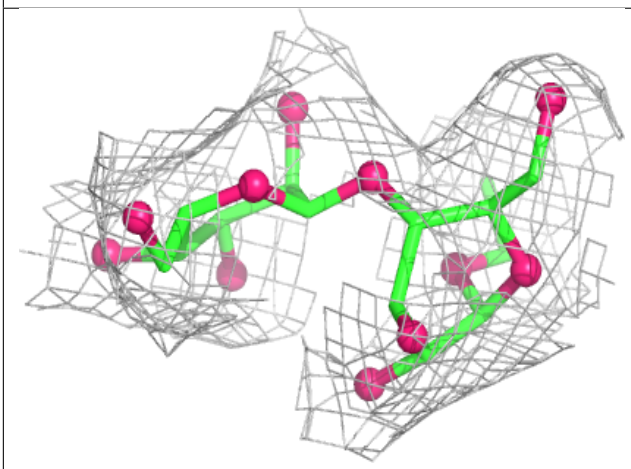


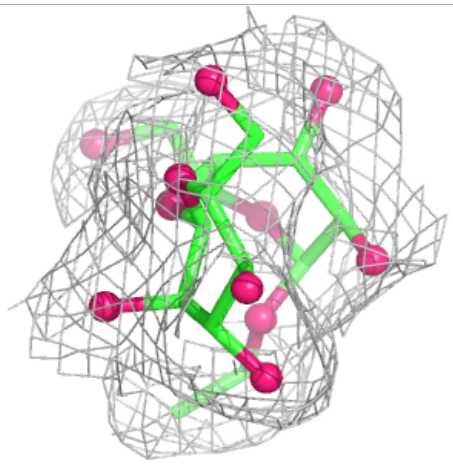


Electron density around LMU B 845:

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

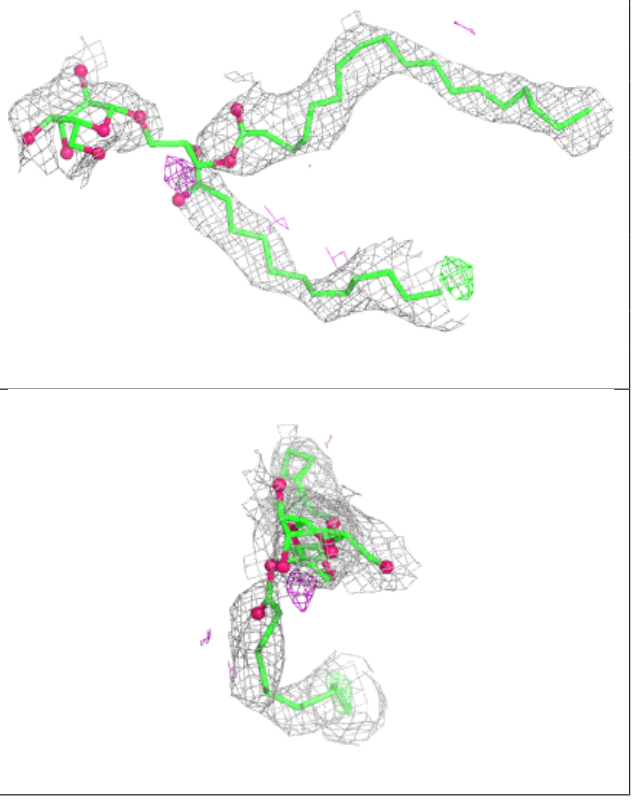






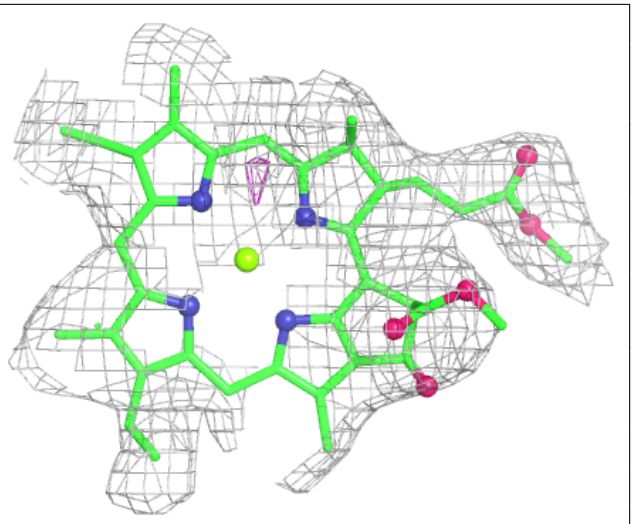
Electron density around LMG B 846:

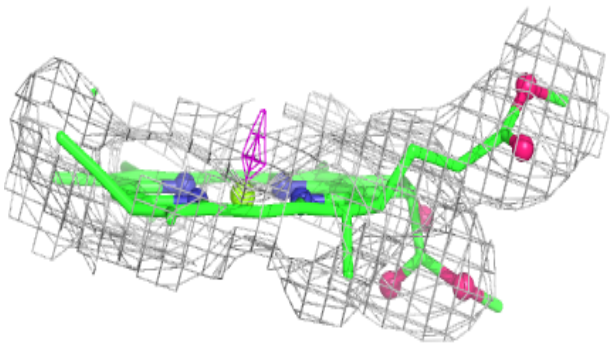
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

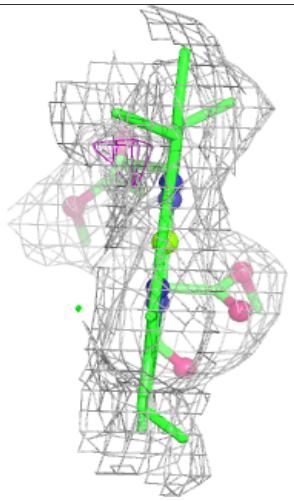


Electron density around CLA 4 315:

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

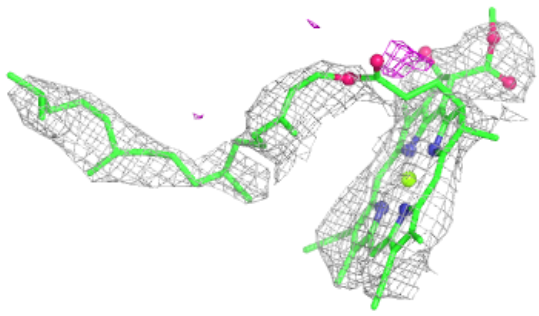


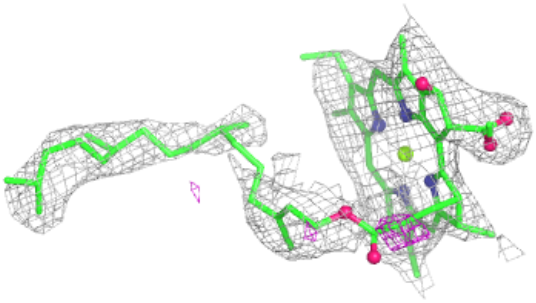


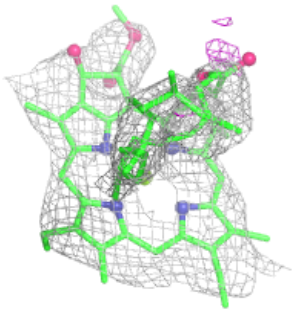


Electron density around CLA A 809:

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

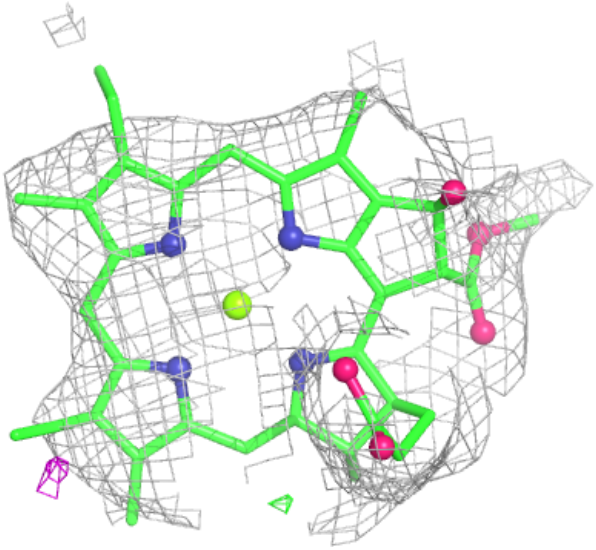


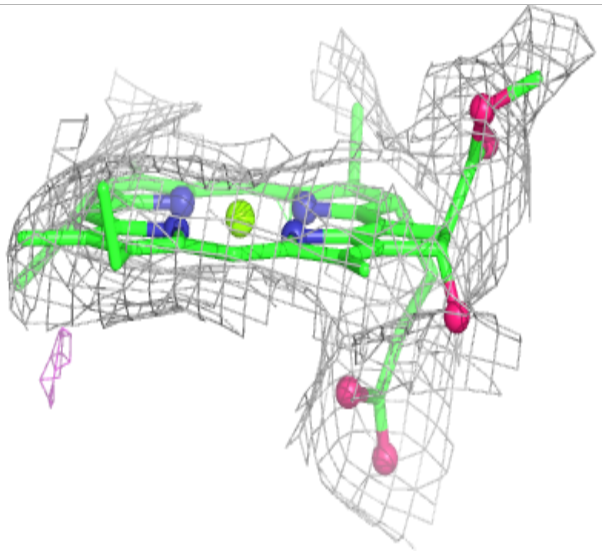


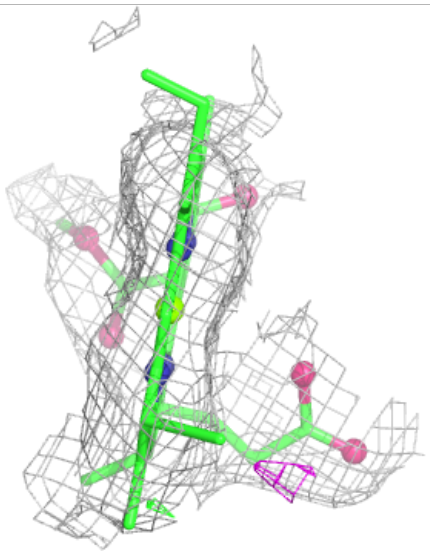


Electron density around CLA B 831:

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

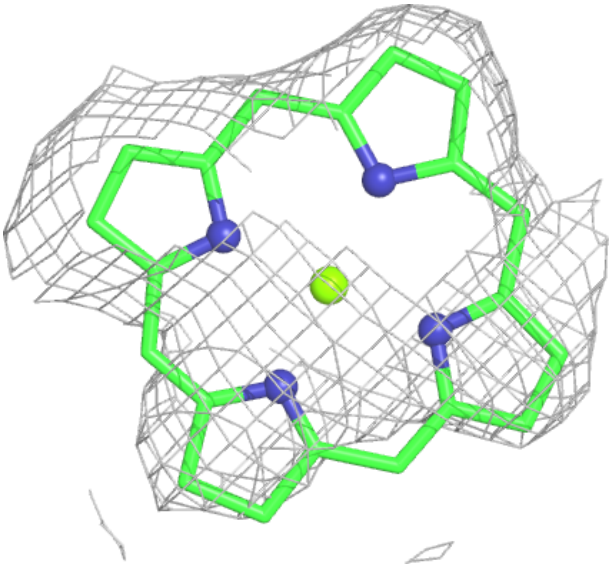


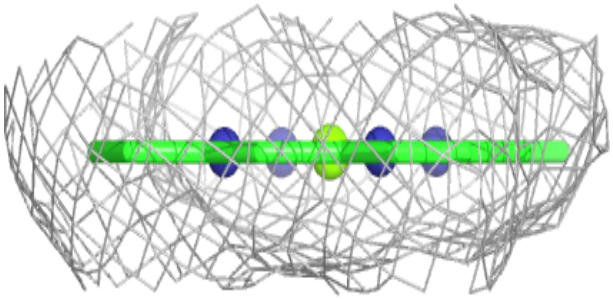


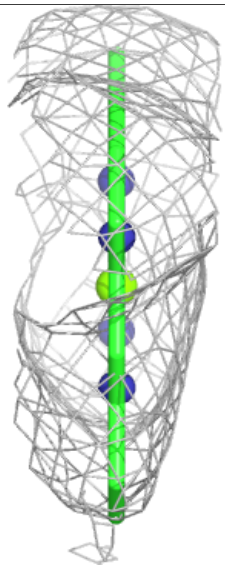


Electron density around CLA 4 308:

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

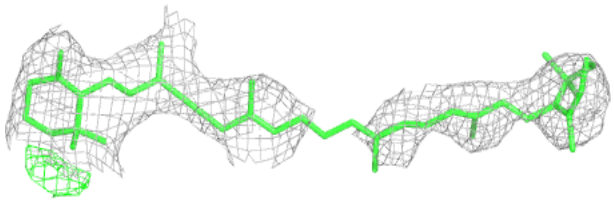


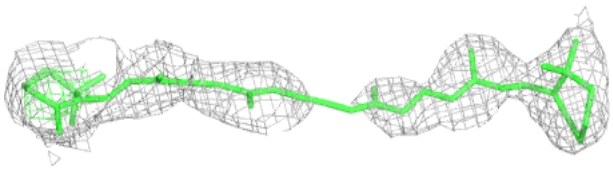


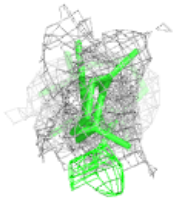


Electron density around BCR A 841:

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

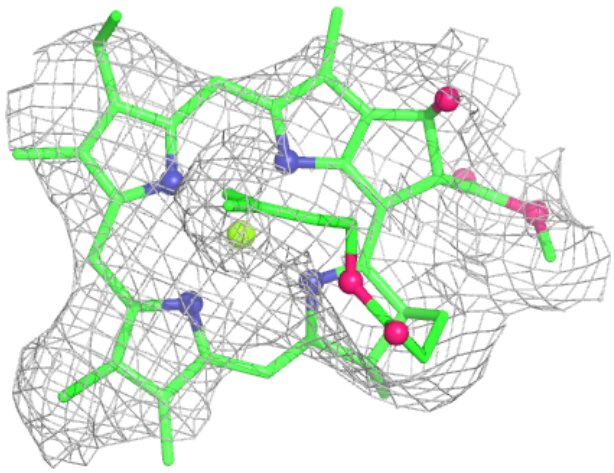


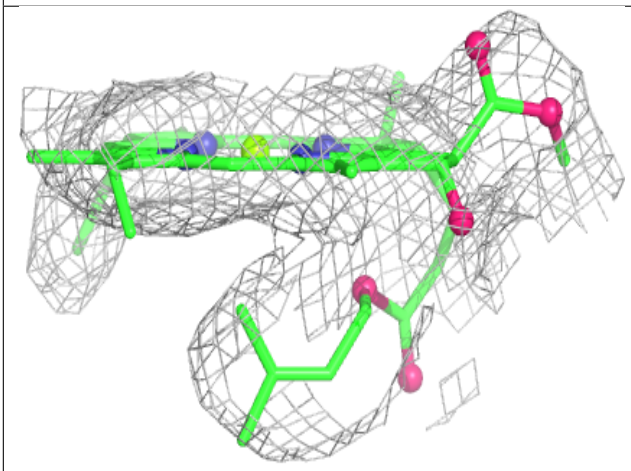


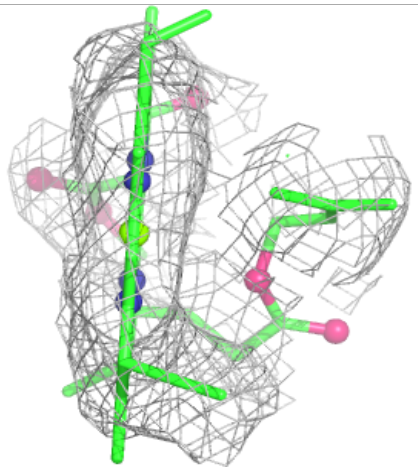


Electron density around CLA H 109:

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

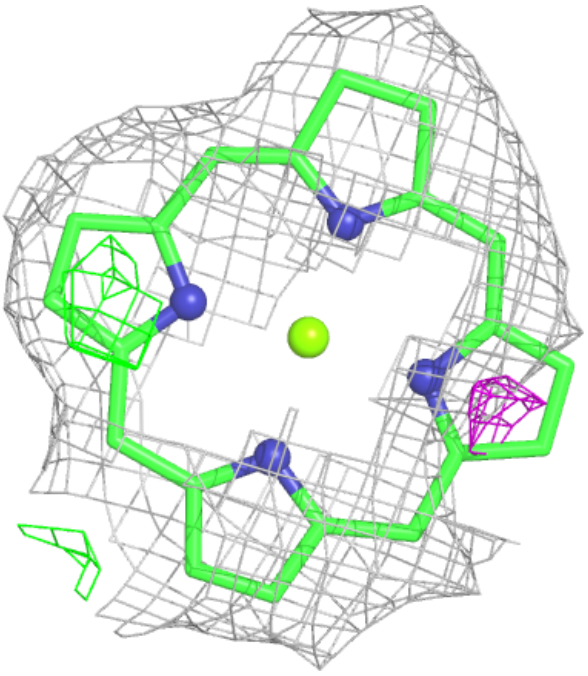


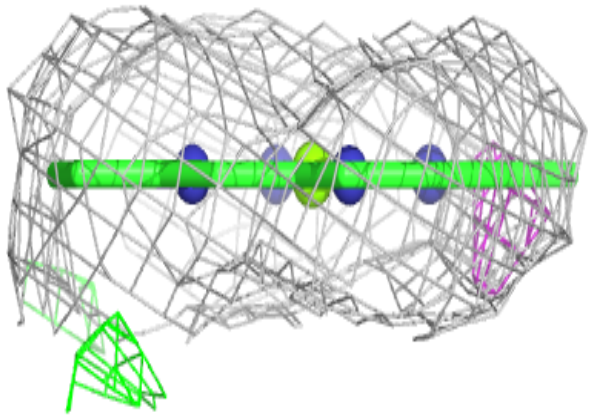


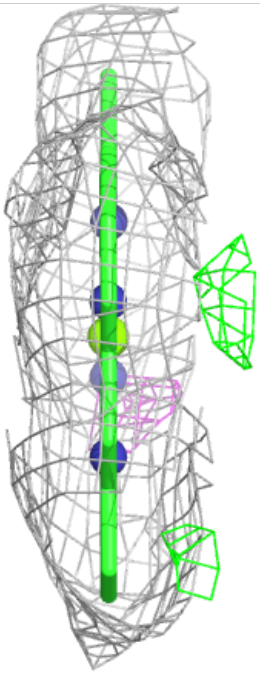


Electron density around CLA 4 309:

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

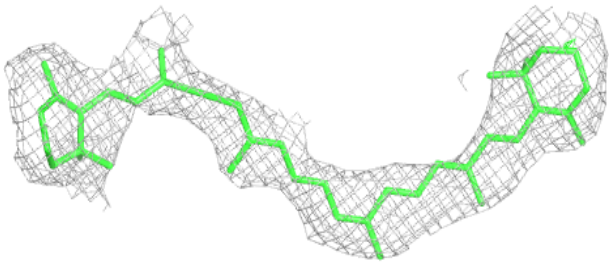


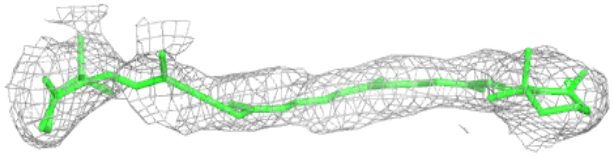


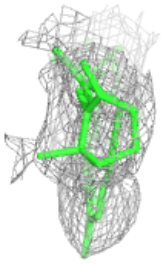


Electron density around BCR A 844:

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

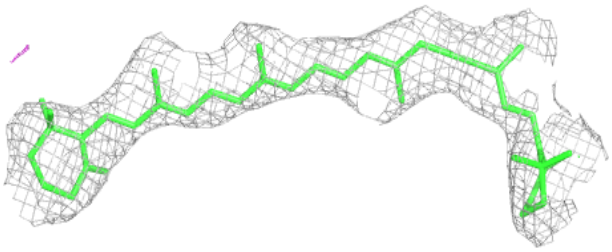


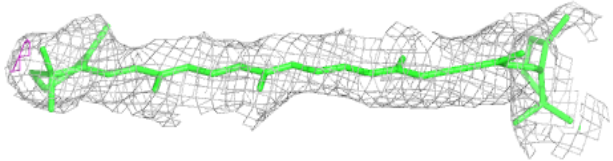


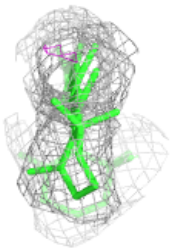


Electron density around BCR B 841:

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

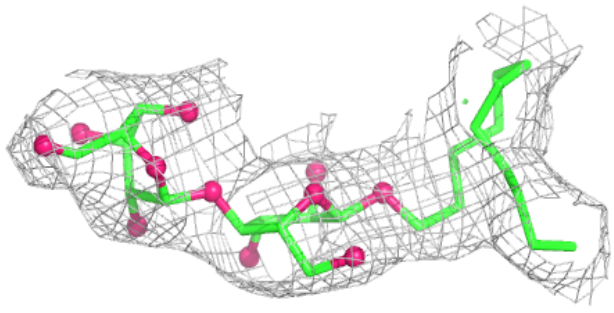


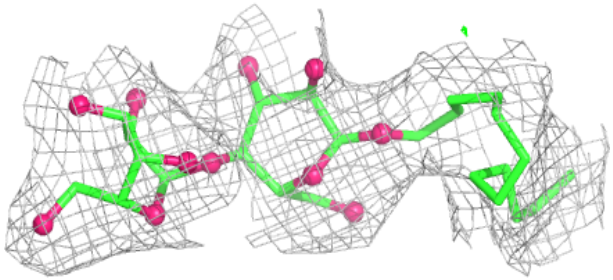


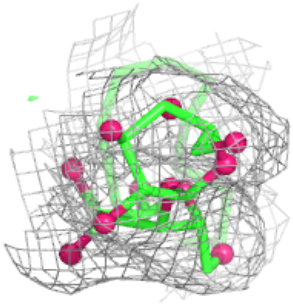


Electron density around LMU A 853:

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

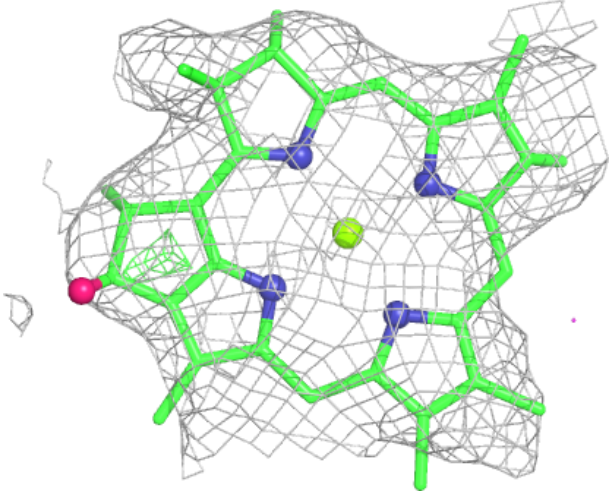


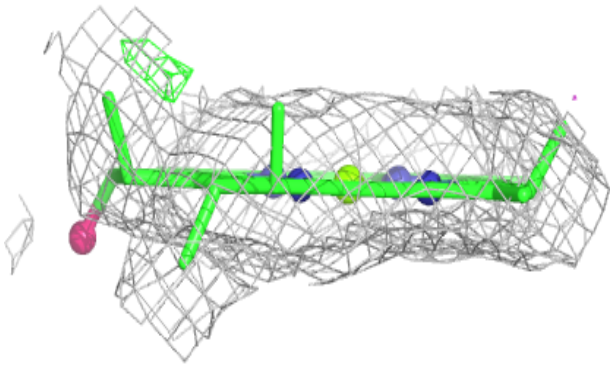


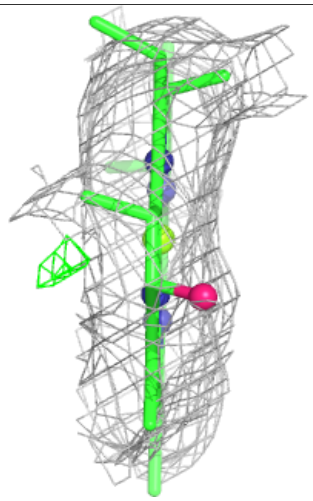


Electron density around CLA B 839:

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

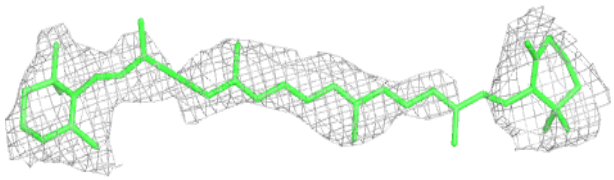


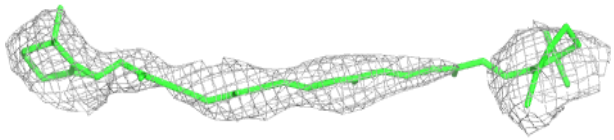


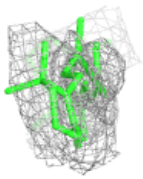


Electron density around BCR G 102:

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

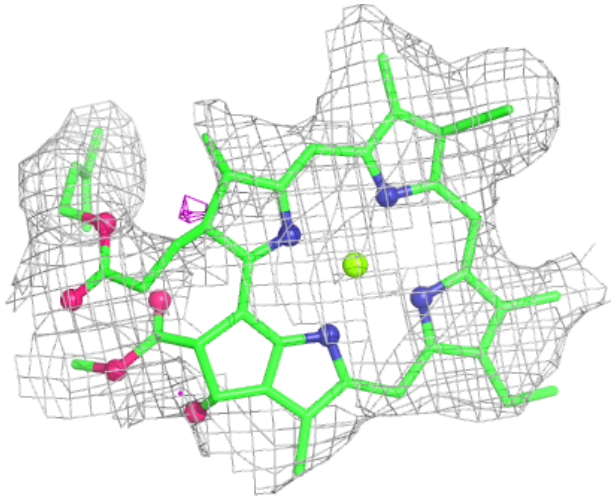


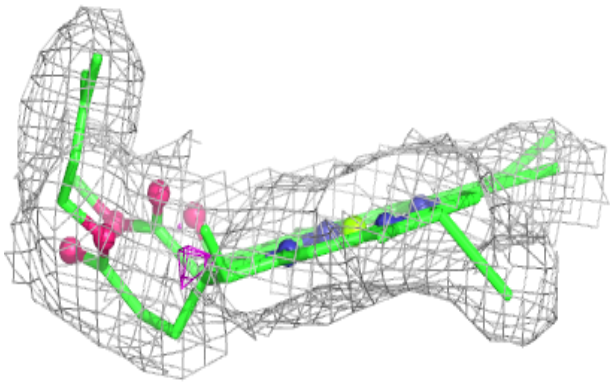


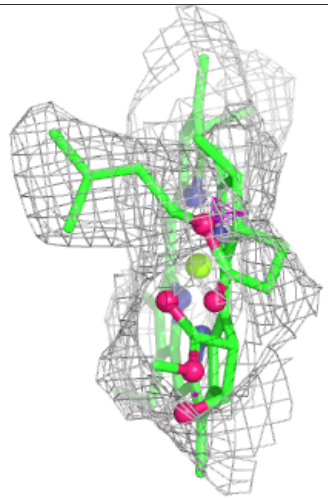


Electron density around CLA 3 315:

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

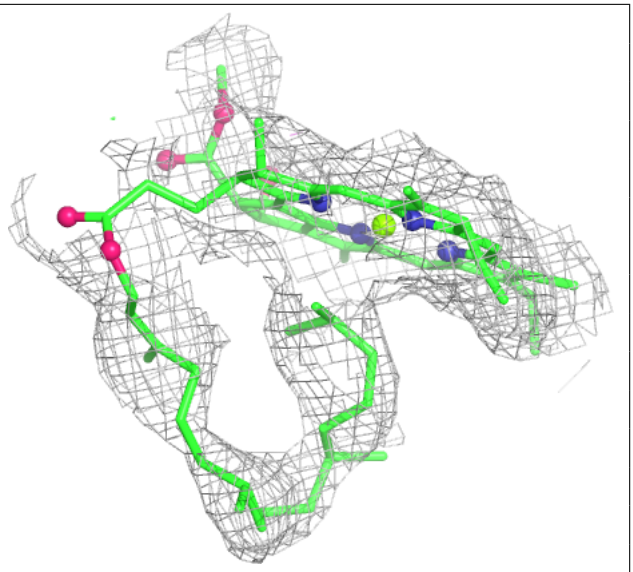


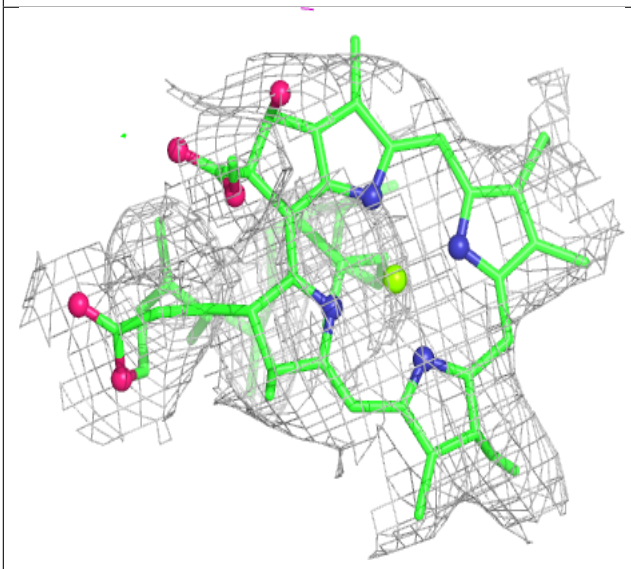


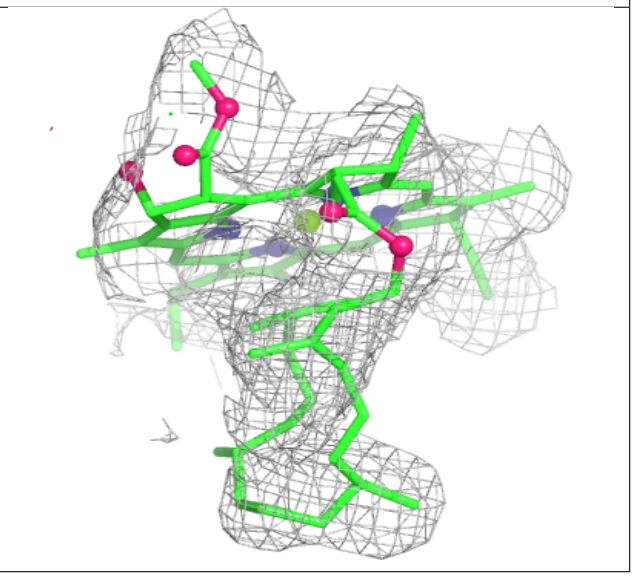


Electron density around CLA 2 312:

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

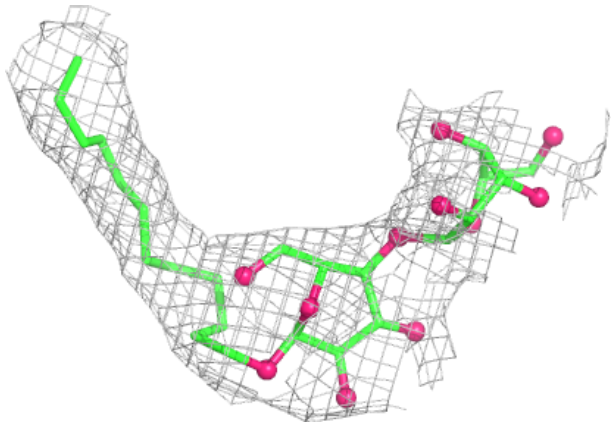


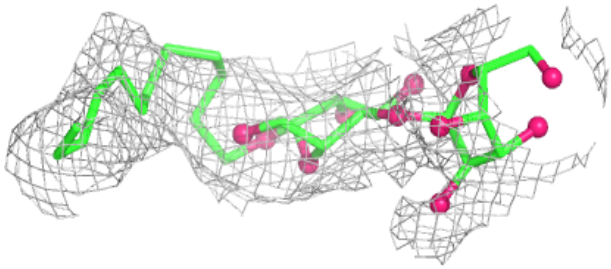




Electron density around LMU R 102:

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

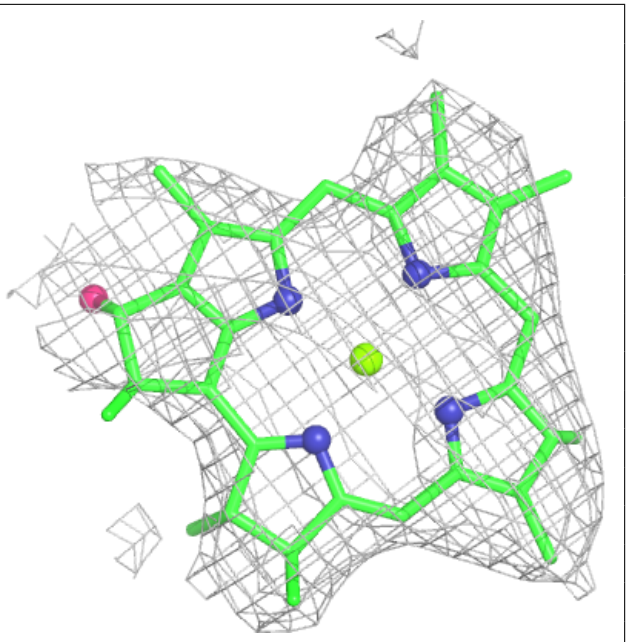


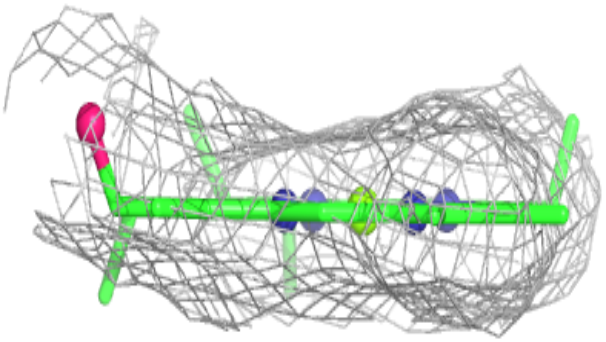


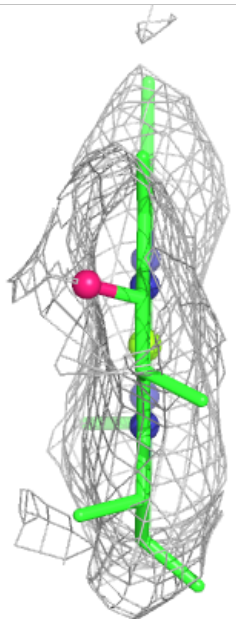


Electron density around CLA 1 209:

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

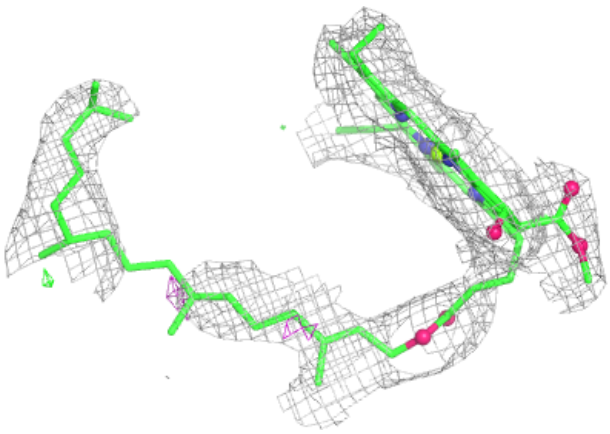


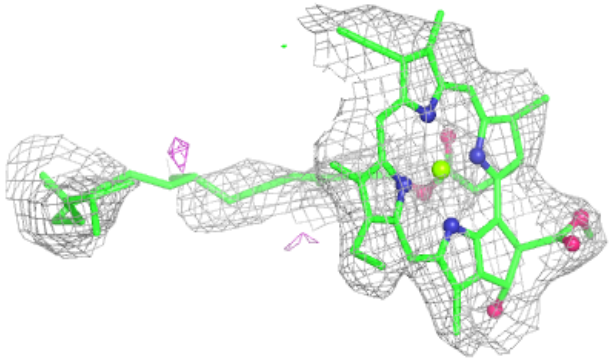


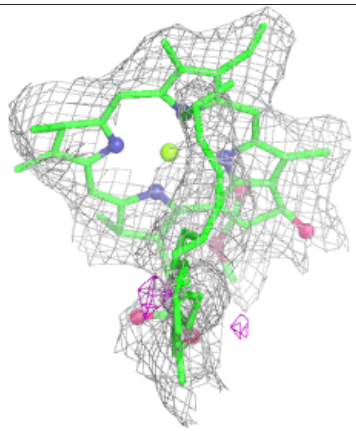


Electron density around CLA L 201:

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

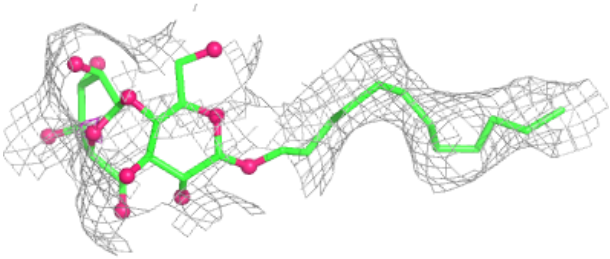


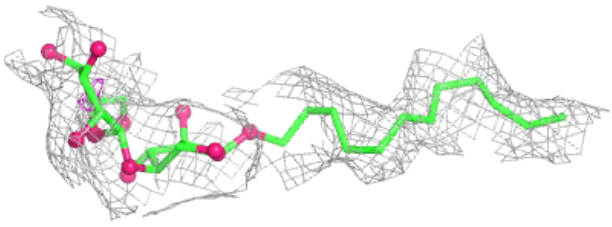


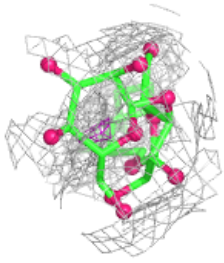


Electron density around LMU 1 218:

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

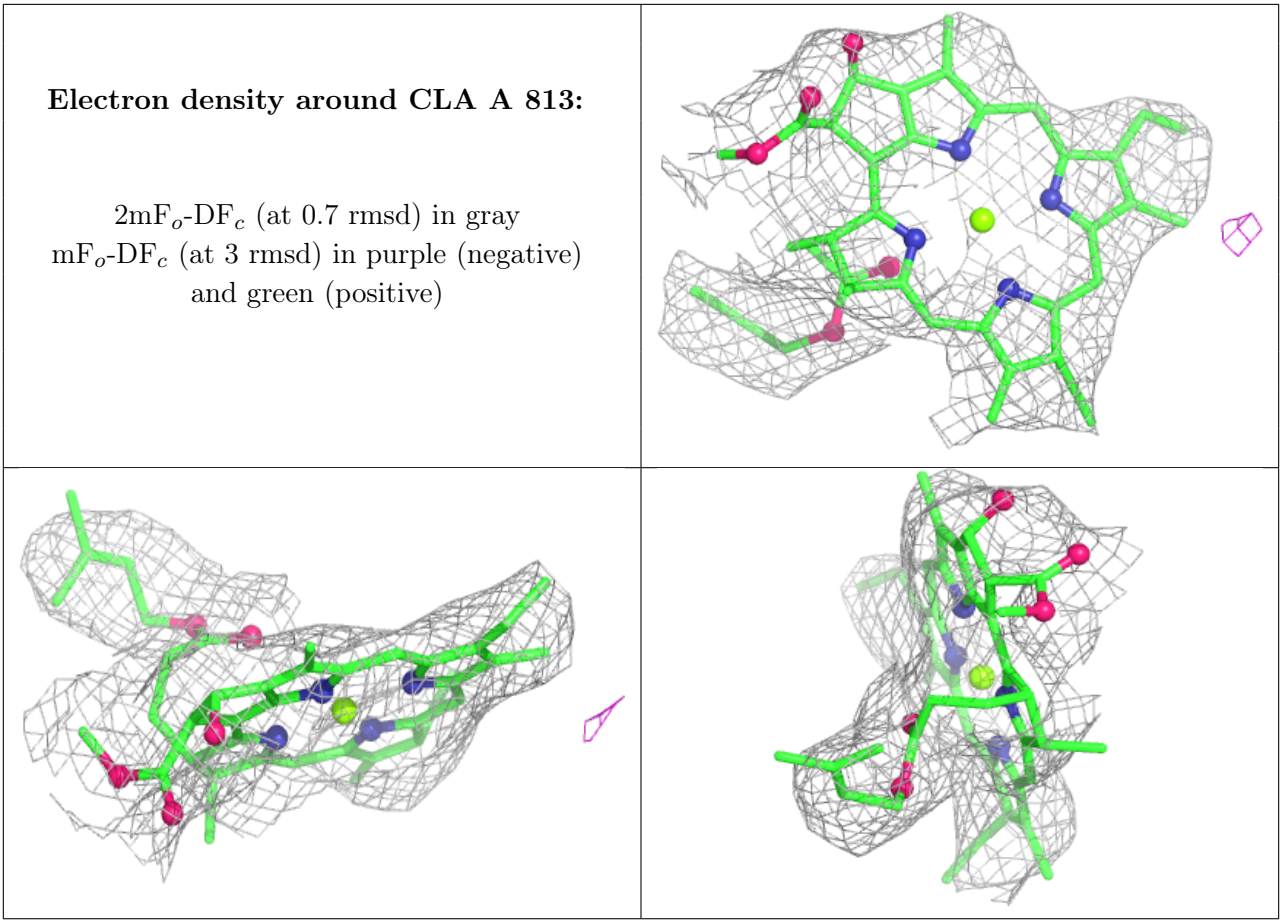






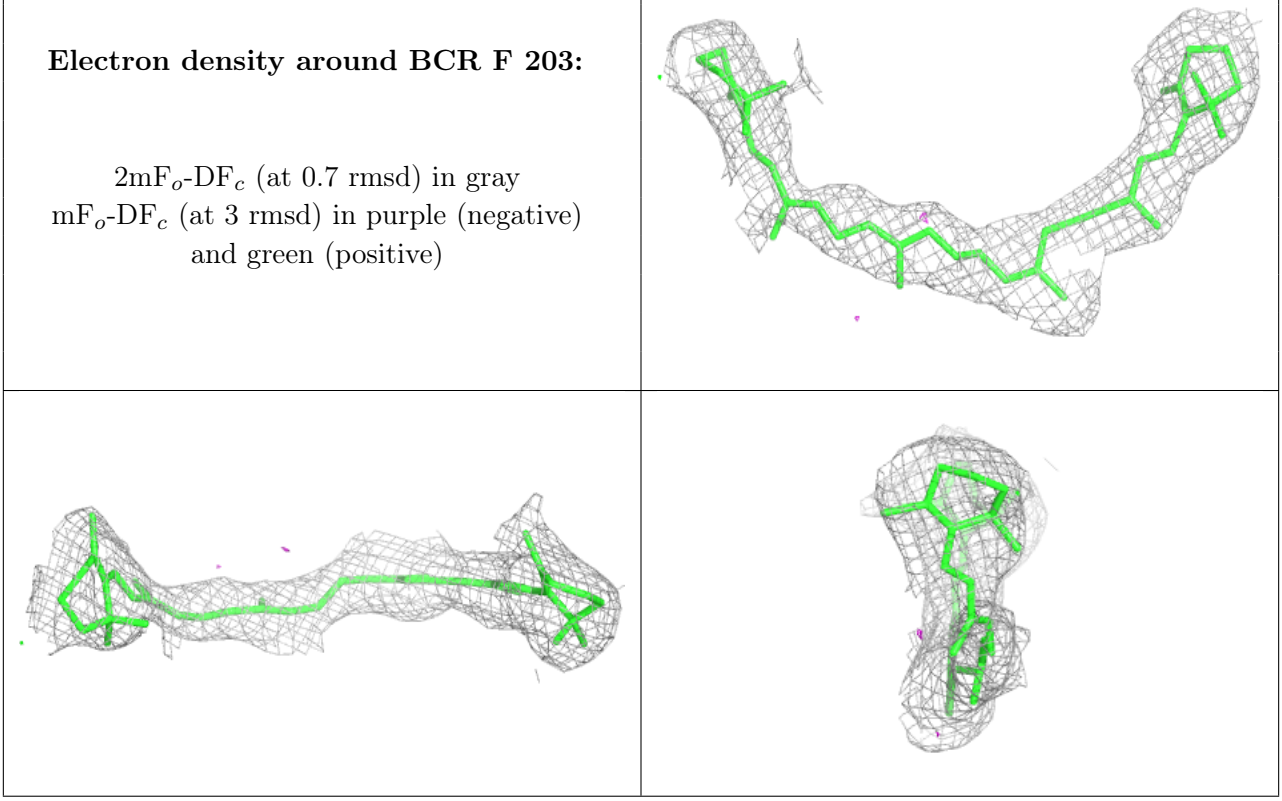
Electron density around CLA A 813:

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



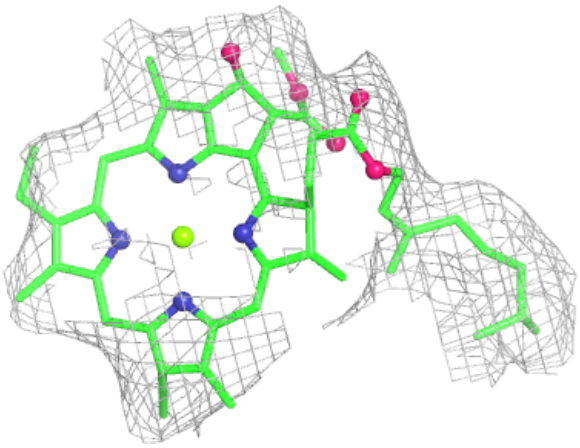
Electron density around BCR F 203:

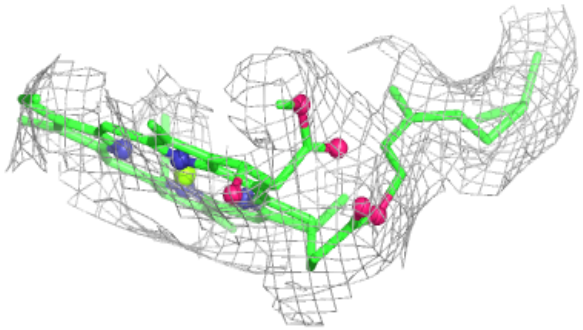
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

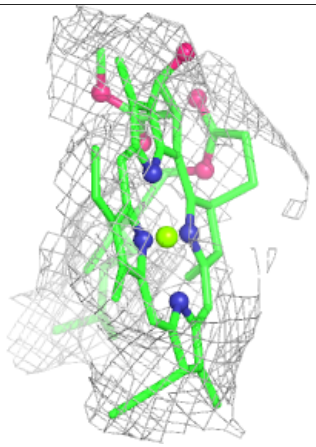


Electron density around CLA J 103:

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

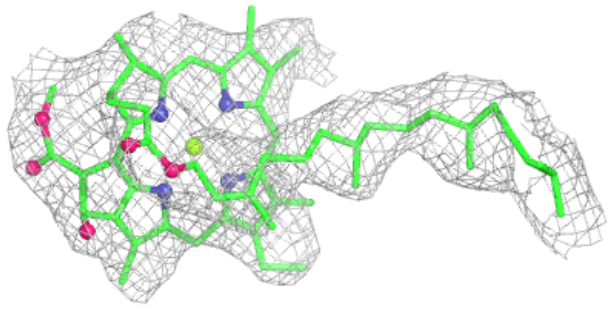


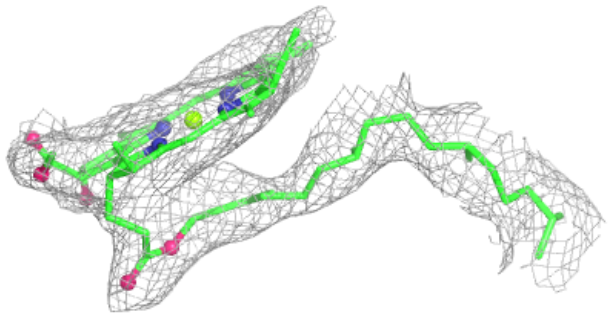


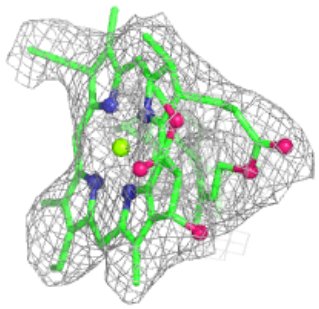


Electron density around CLA A 814:

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

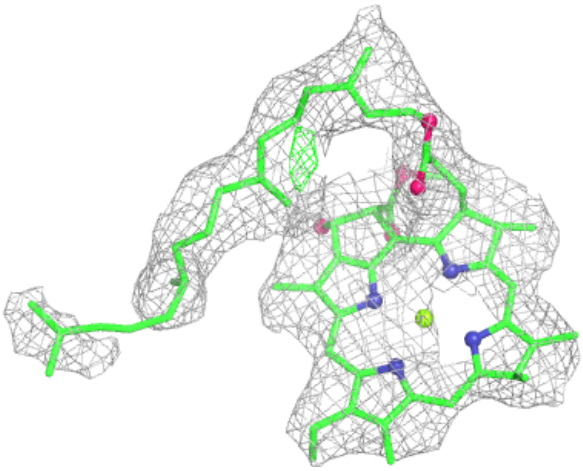


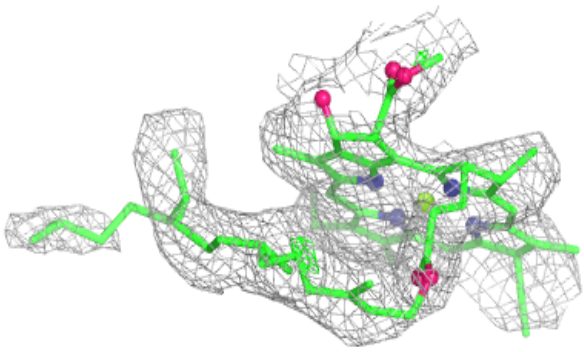




Electron density around CLA B 829:

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

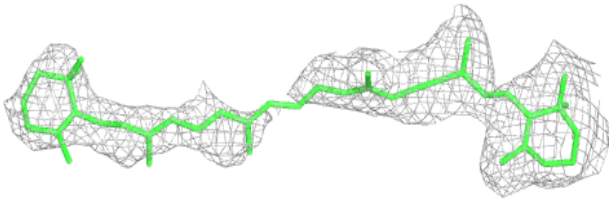


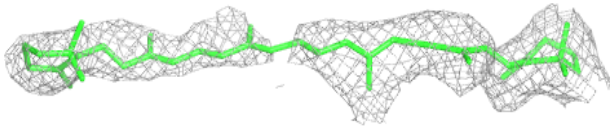


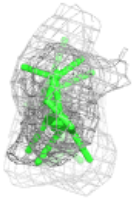


Electron density around BCR L 209:

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

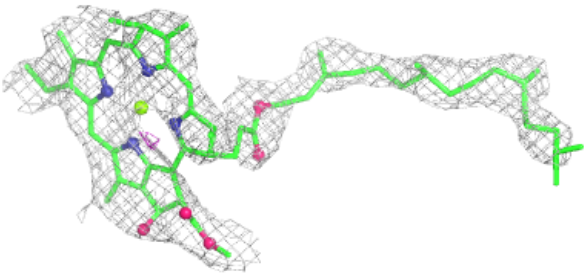


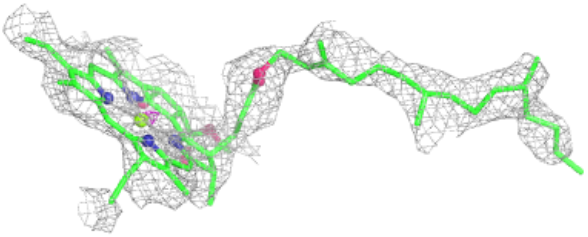


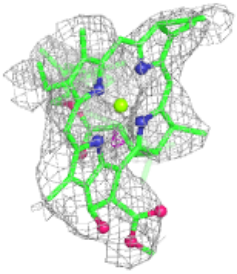


Electron density around CLA A 817:

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

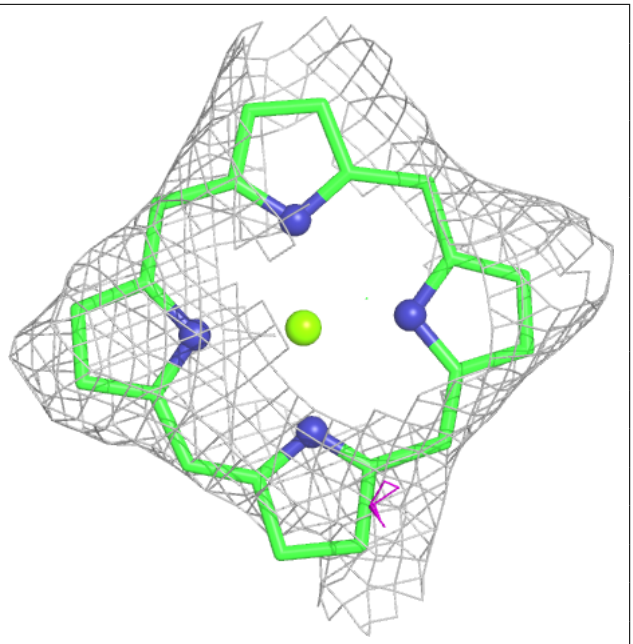


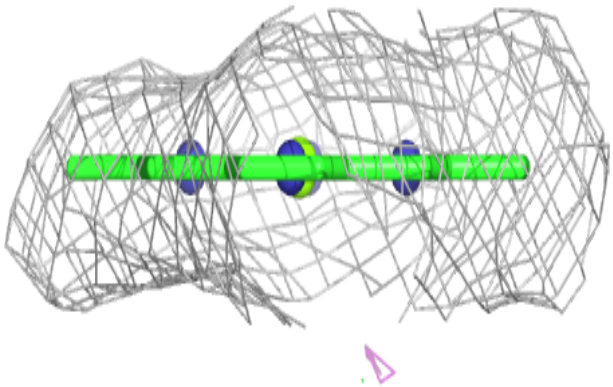


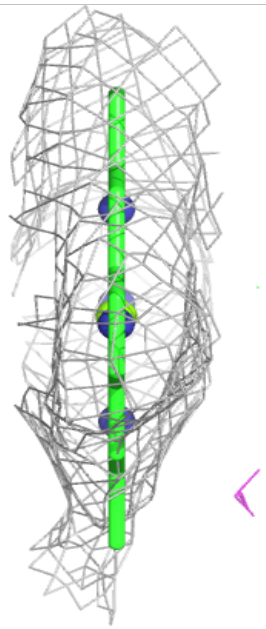


Electron density around CLA 3 317:

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

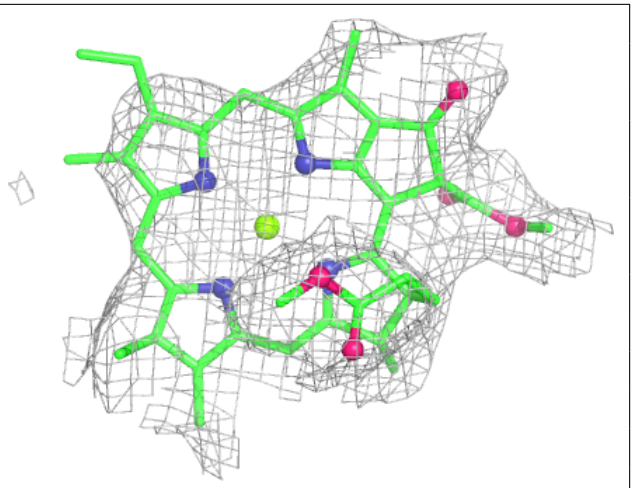


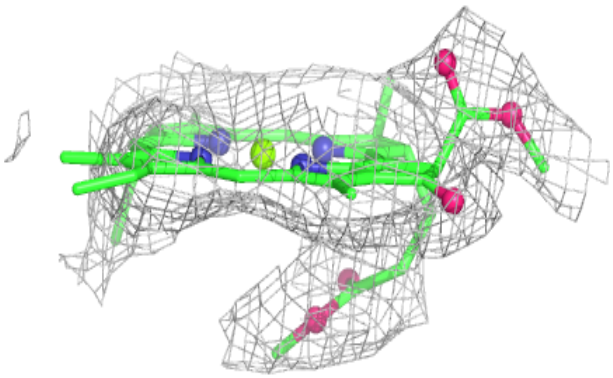


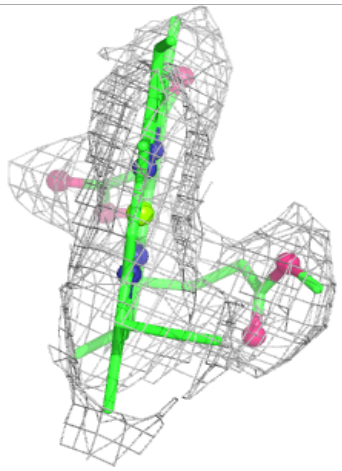


Electron density around CLA 1 204:

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

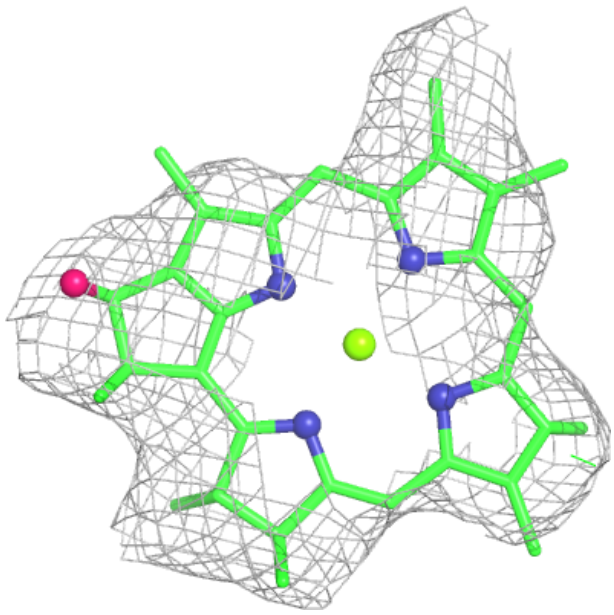


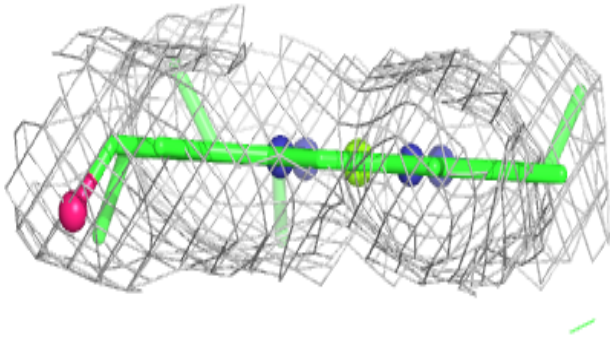


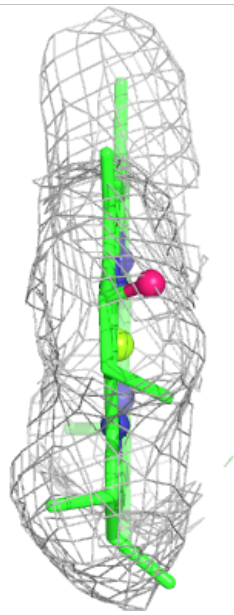


Electron density around CLA 1 210:

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

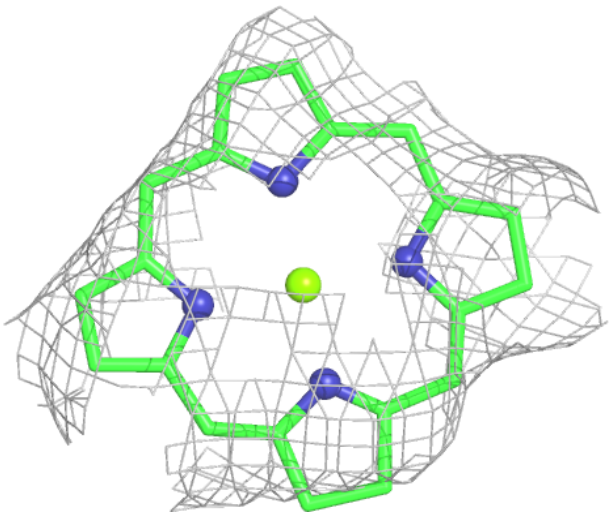


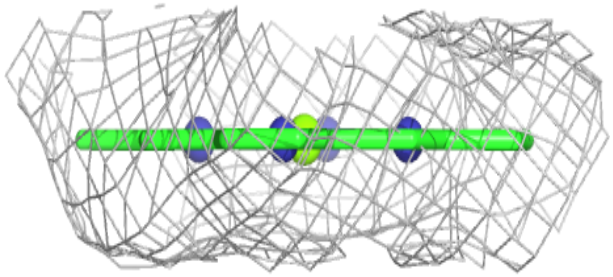


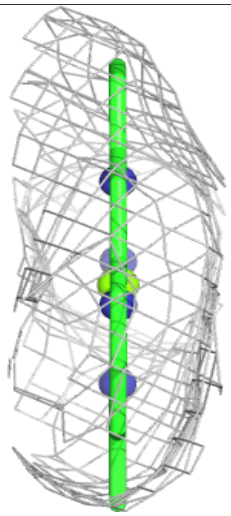


Electron density around CLA 1 215:

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

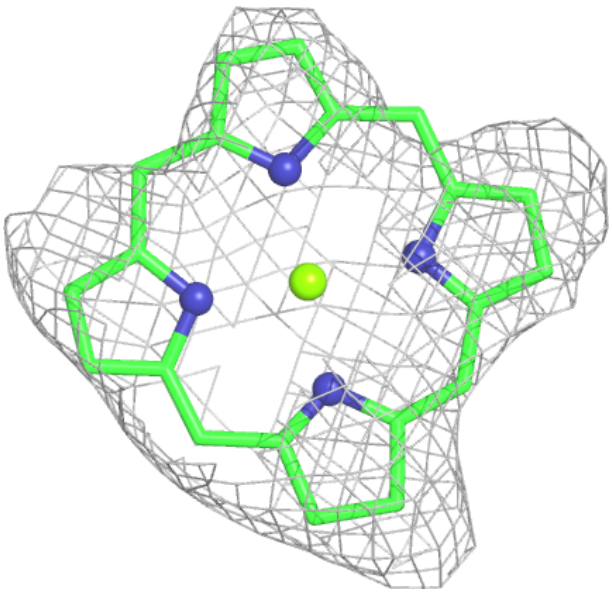


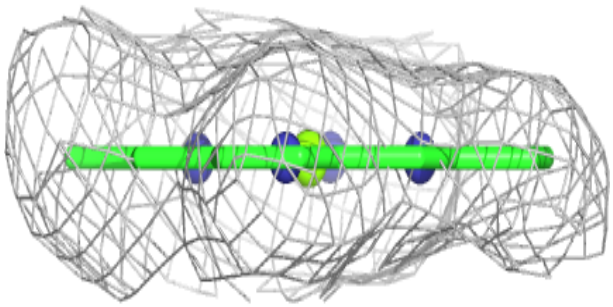


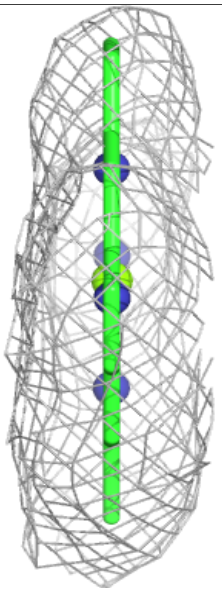


Electron density around CLA 2 315:

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

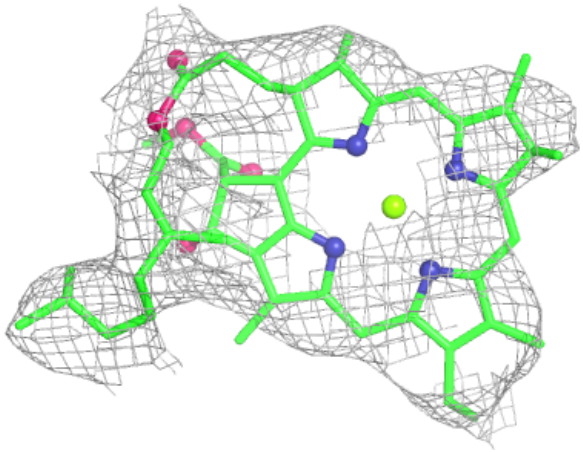


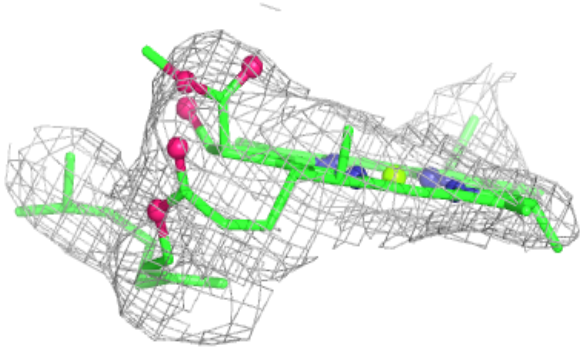


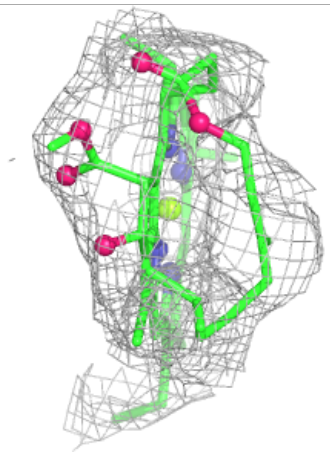


Electron density around CLA B 808:

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

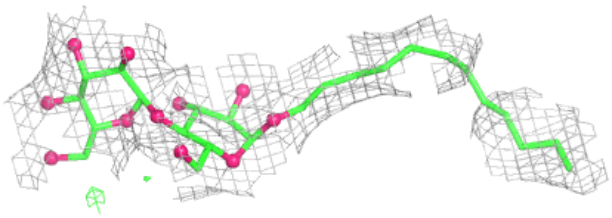


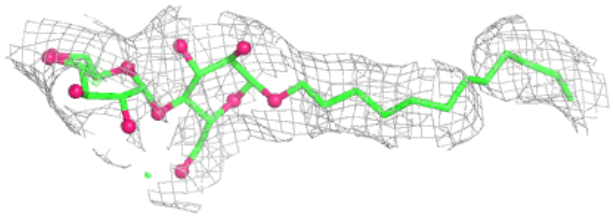


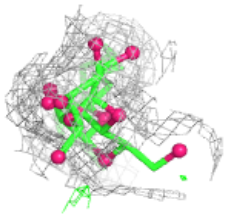


Electron density around LMU B 802:

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

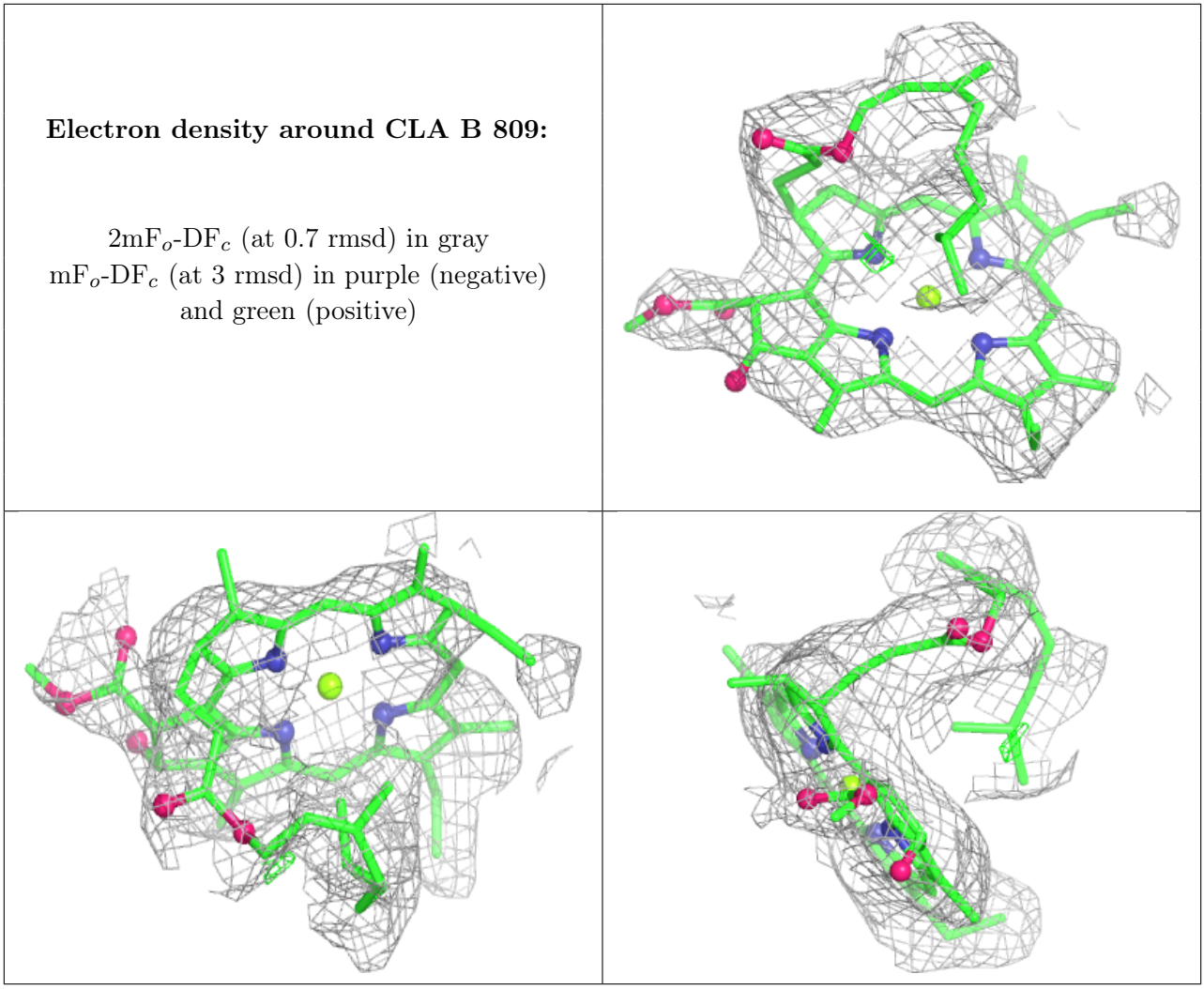






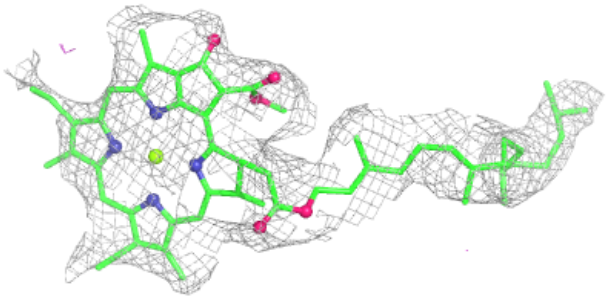
Electron density around CLA B 809:

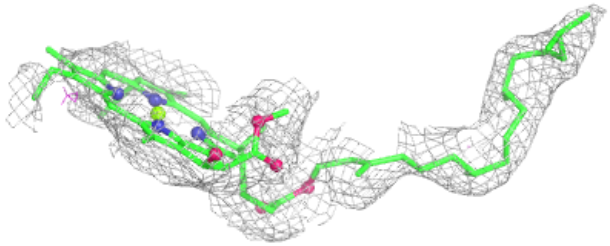
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

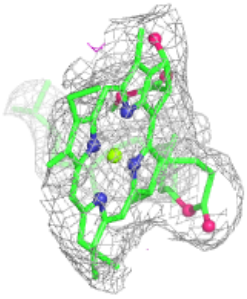


Electron density around CLA 2 317:

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

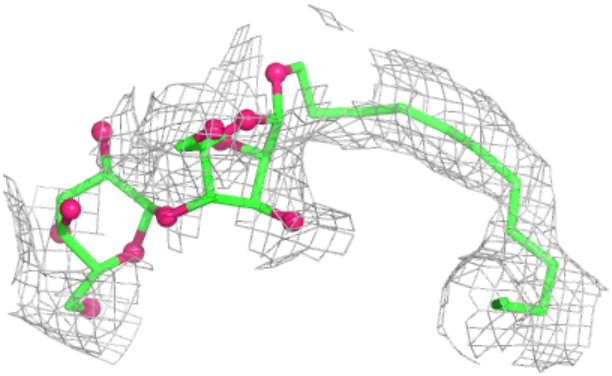


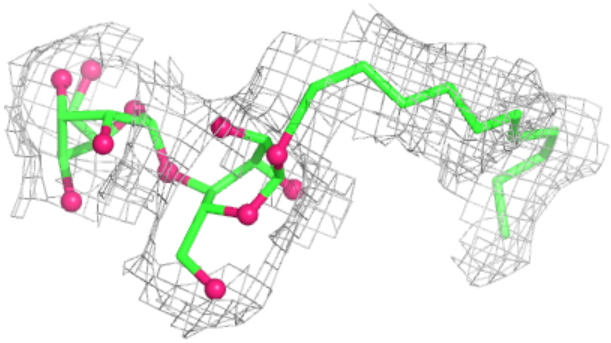


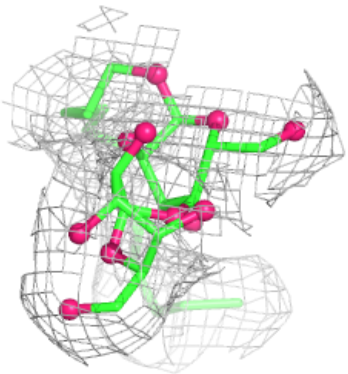


Electron density around LMU R 103:

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

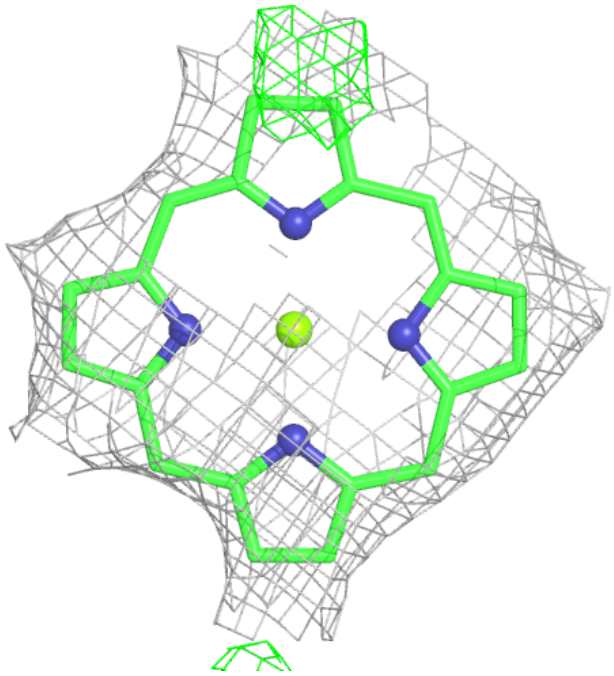


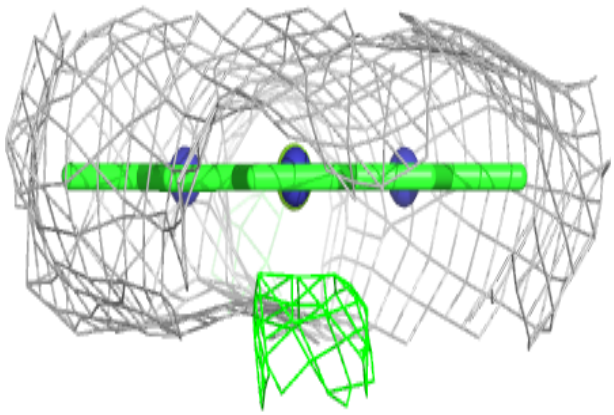


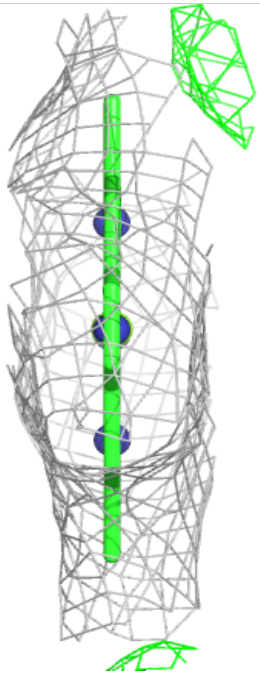


Electron density around CLA 3 307:

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

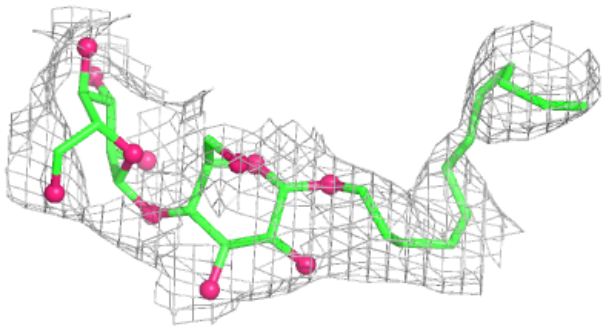


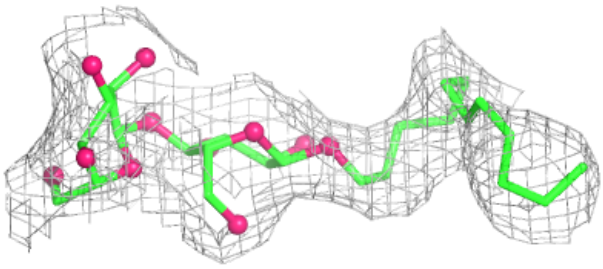


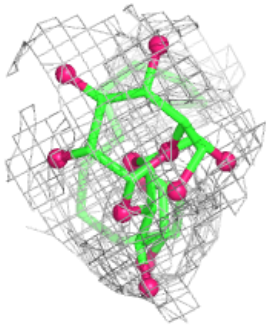


Electron density around LMU R 108:

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

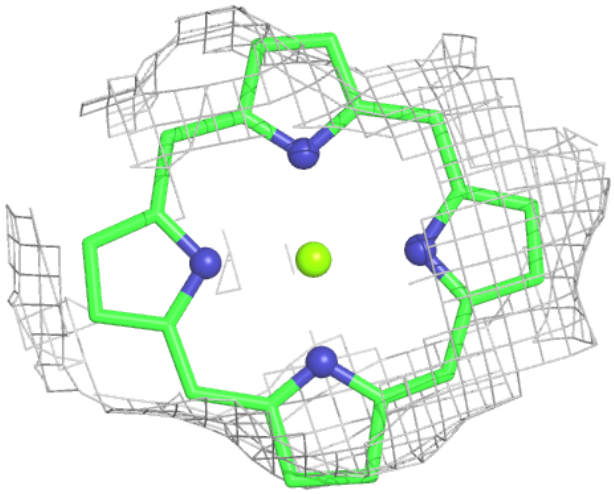


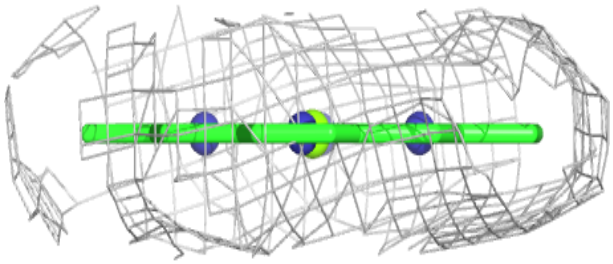


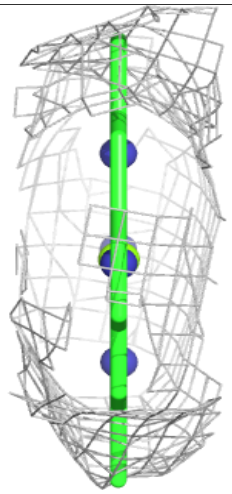


Electron density around CLA 2 308:

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

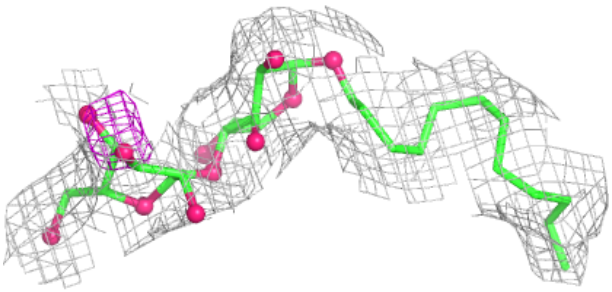


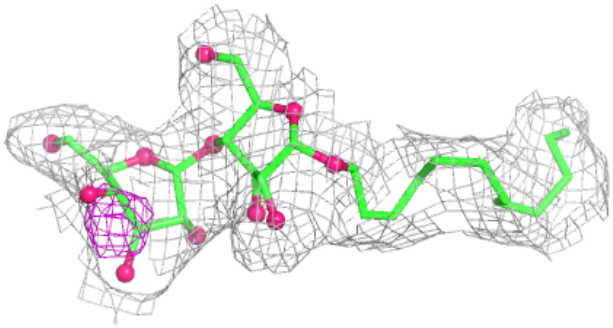


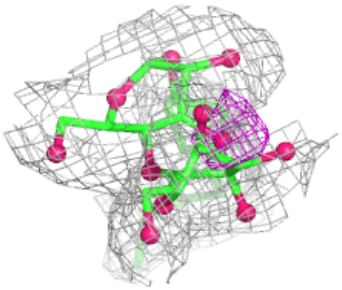


Electron density around LMU H 102:

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

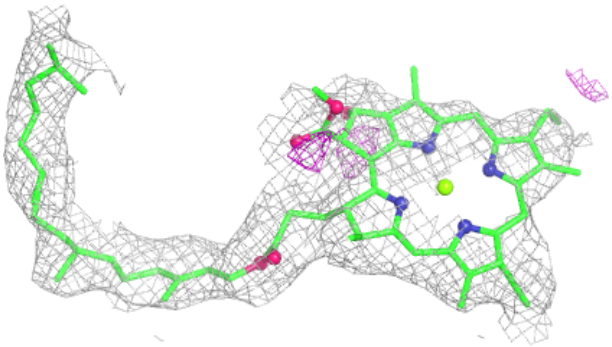


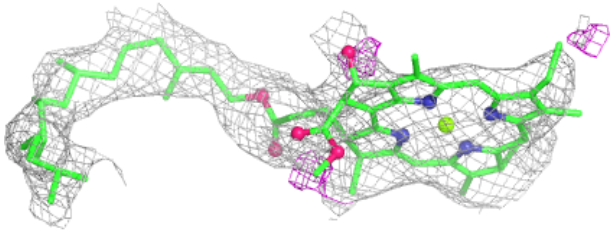




Electron density around CLA B 823:

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

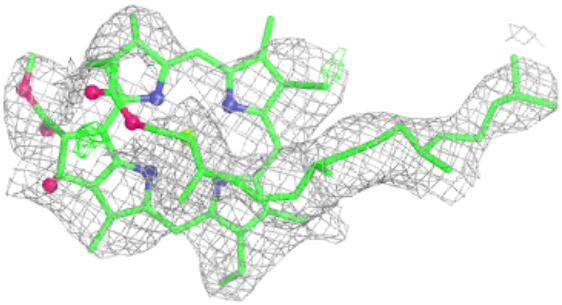


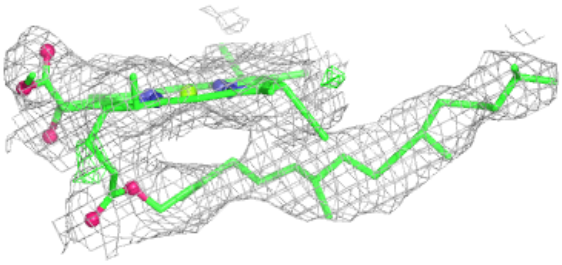


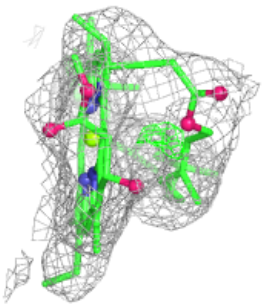


Electron density around CLA A 855:

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



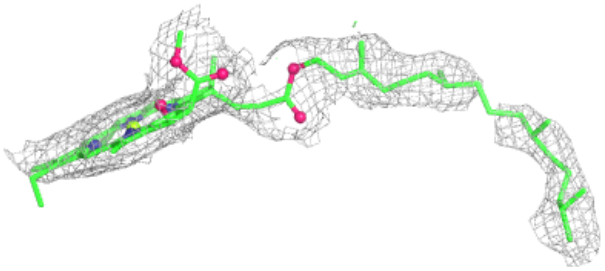


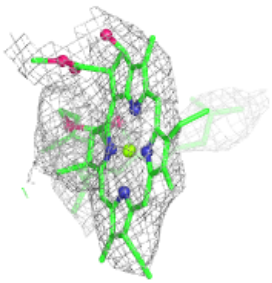


Electron density around CLA A 803:

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

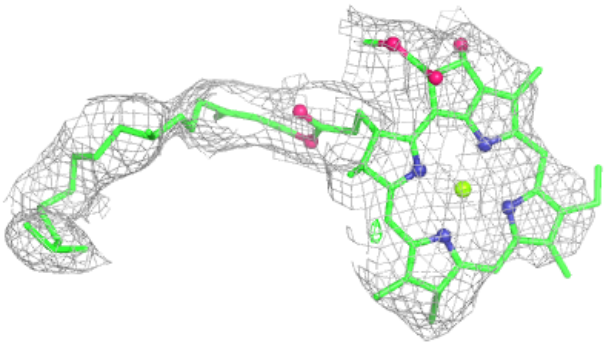






Electron density around CLA A 822:

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

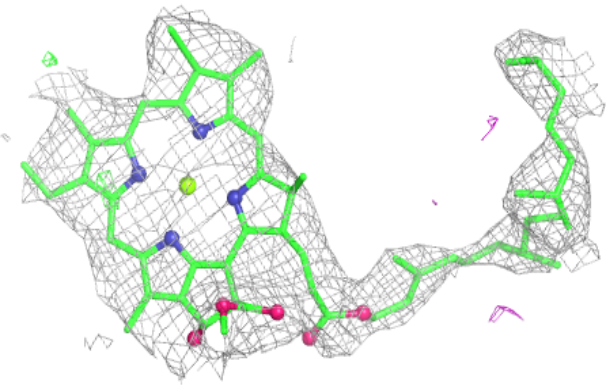


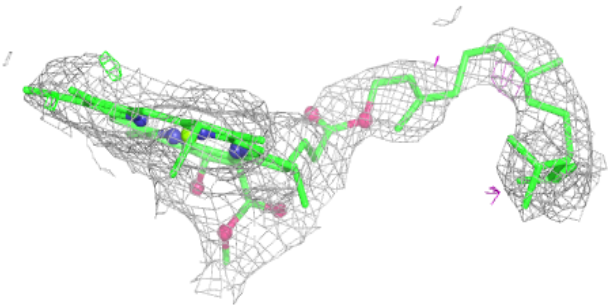


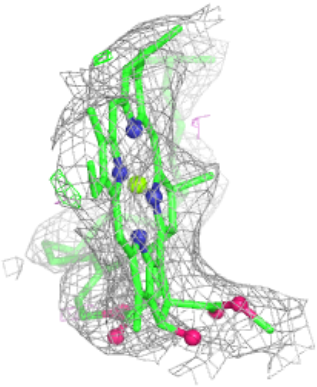


Electron density around CLA A 823:

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

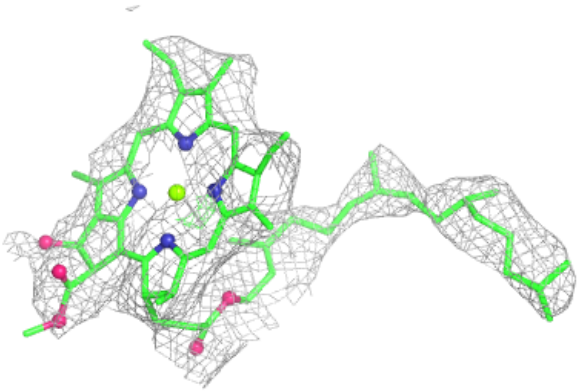


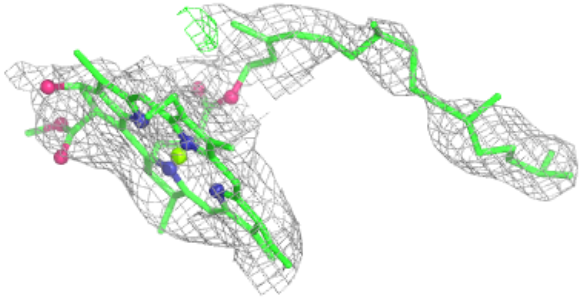


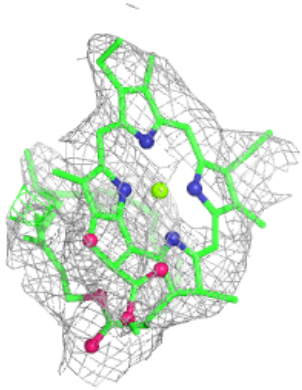


Electron density around CLA B 811:

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

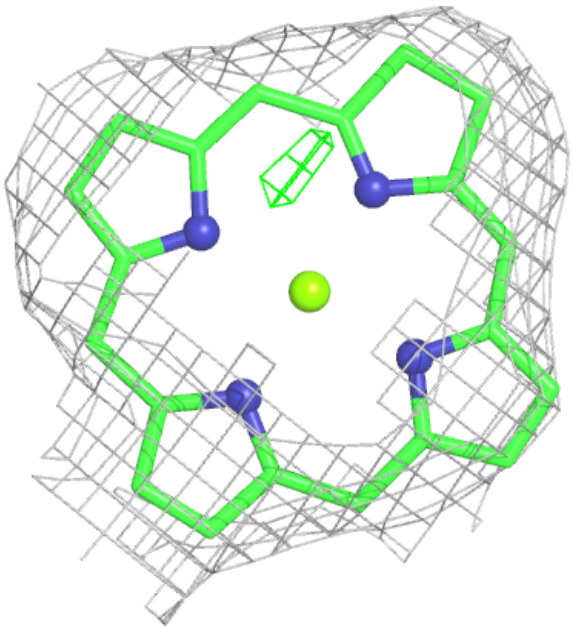


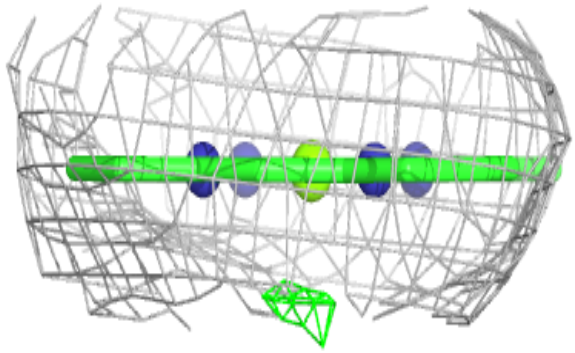


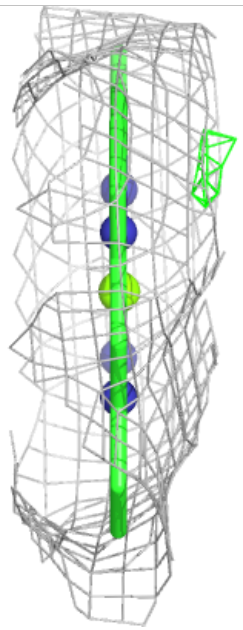


Electron density around CLA 4 311:

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

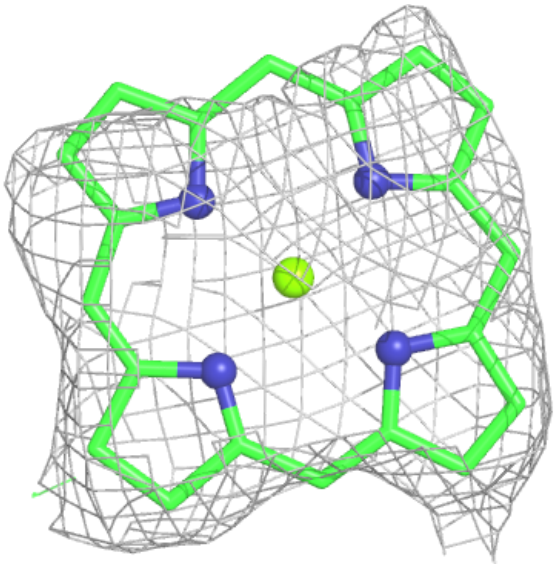


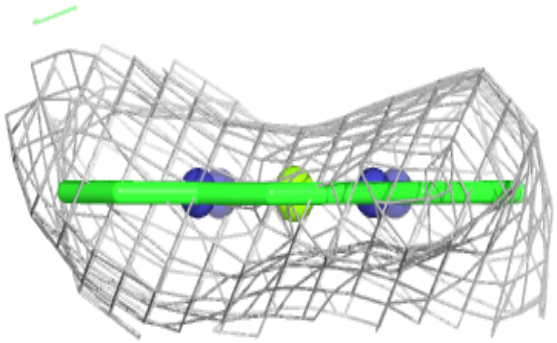


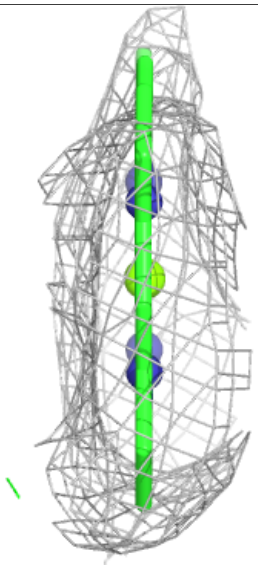


Electron density around CLA 2 309:

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

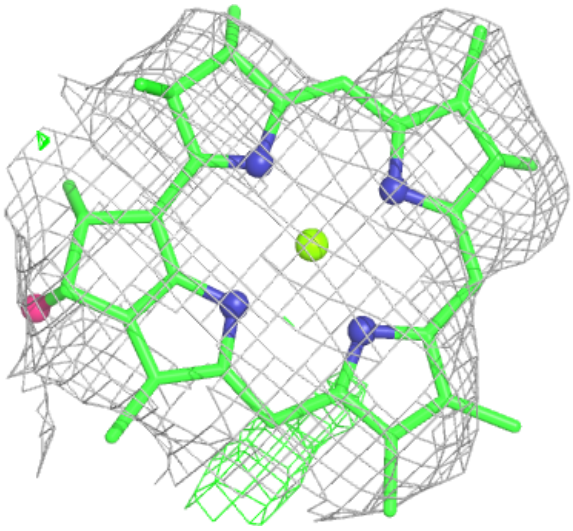


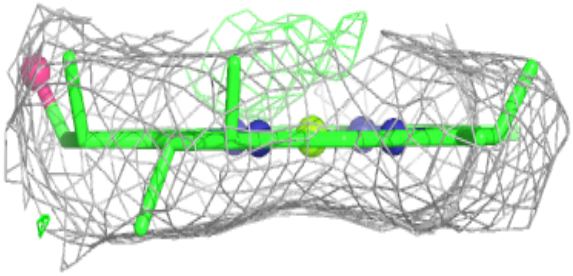


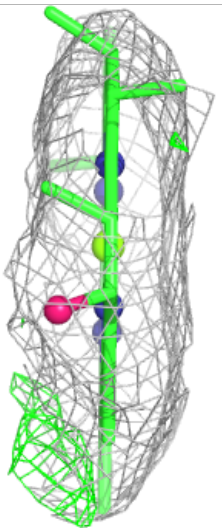


Electron density around CLA 4 303:

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

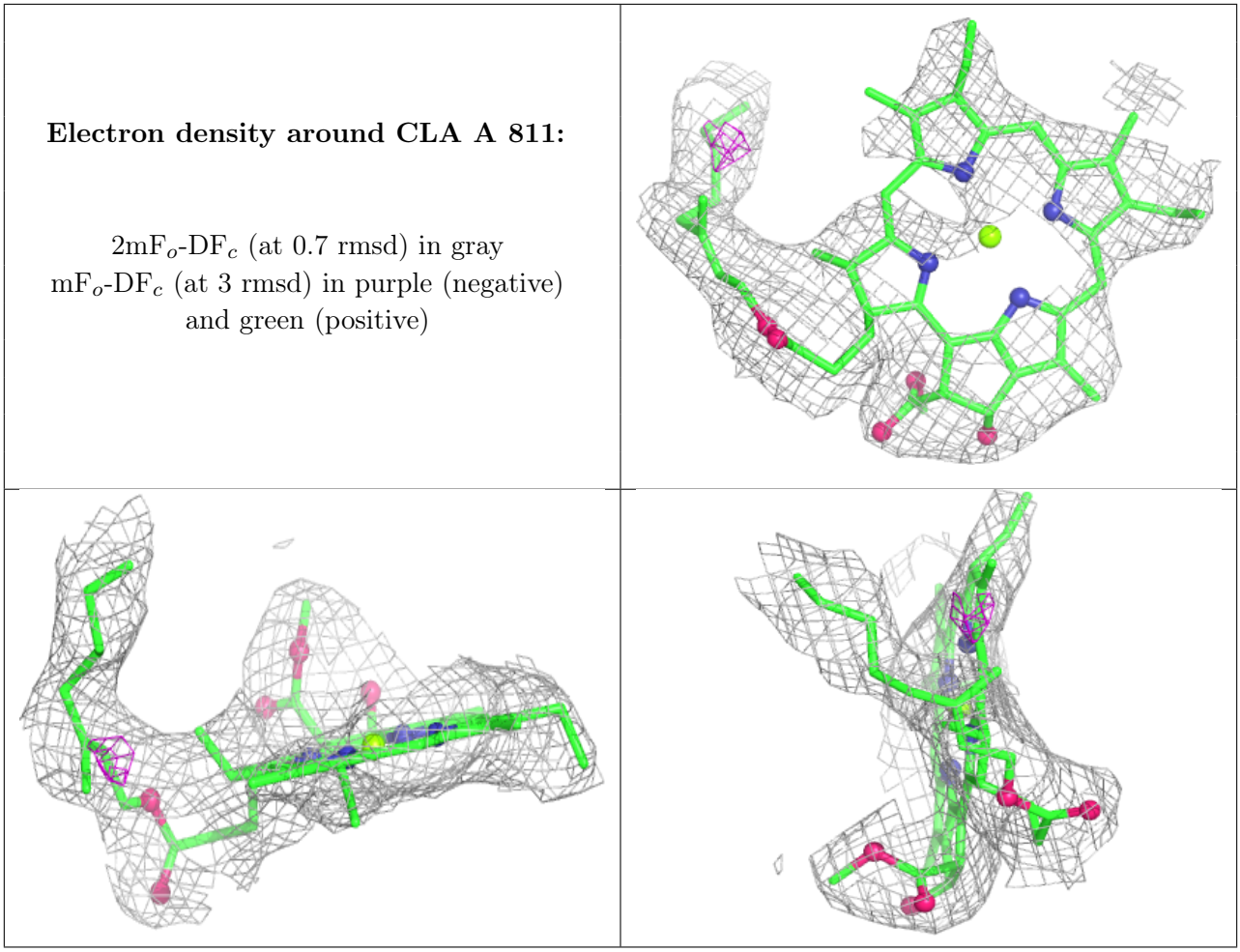






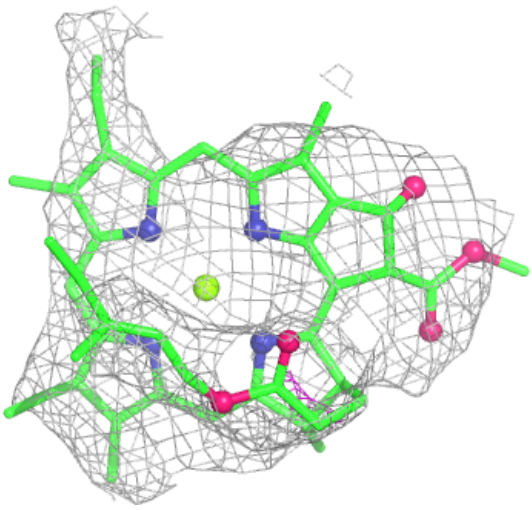
Electron density around CLA A 811:

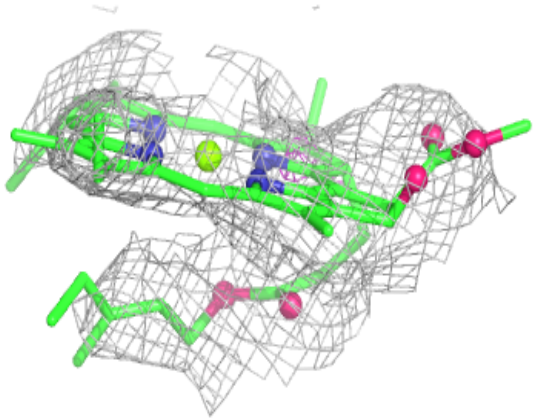
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

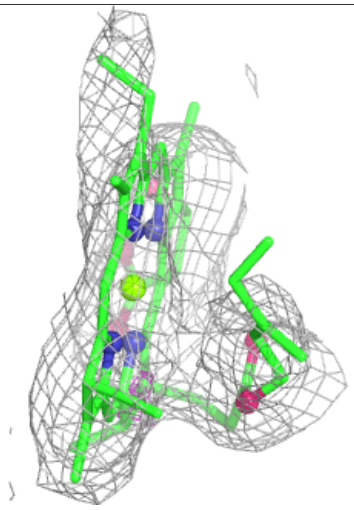


Electron density around CLA A 818:

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

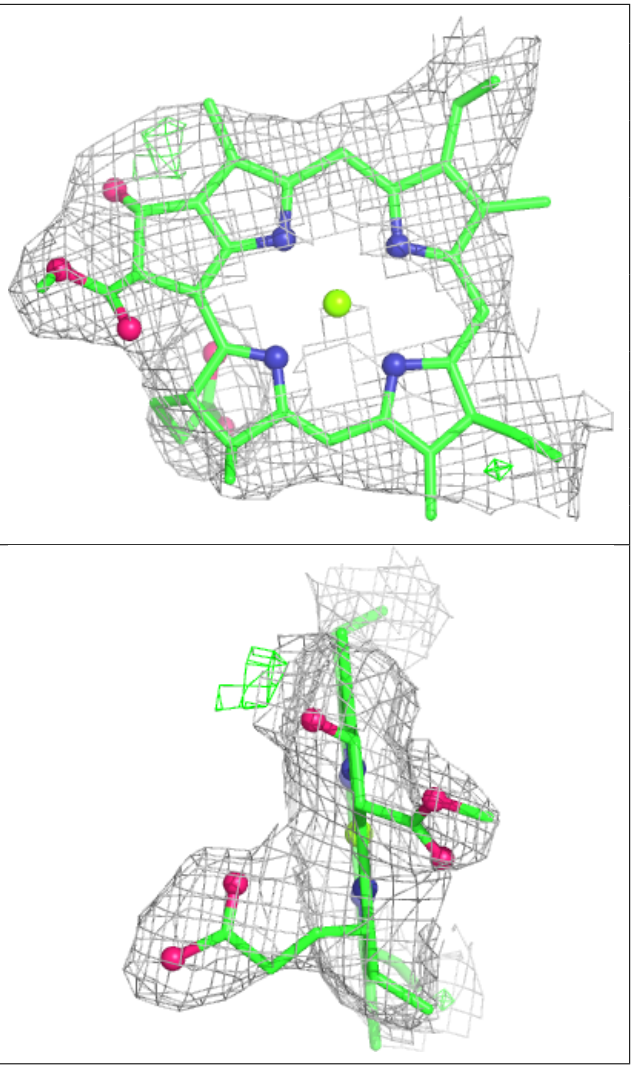






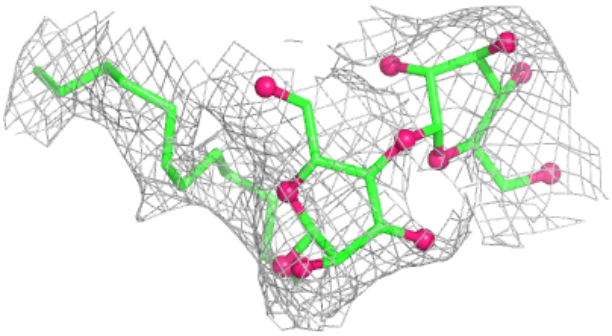
Electron density around CLA B 803:

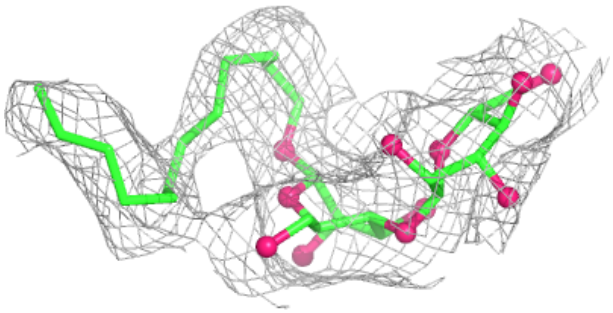
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

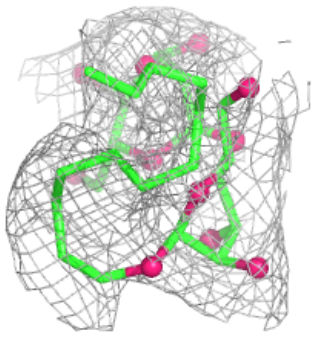


Electron density around LMU L 210:

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

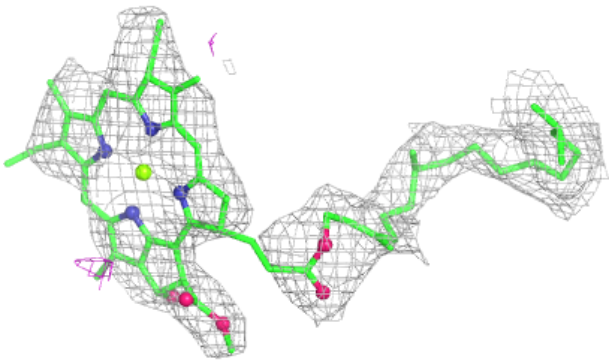


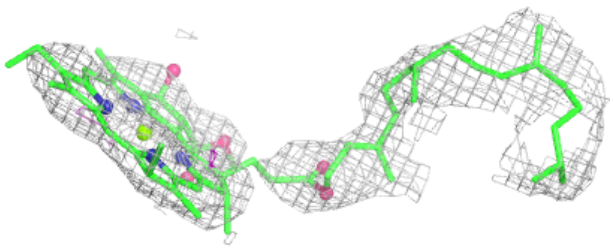


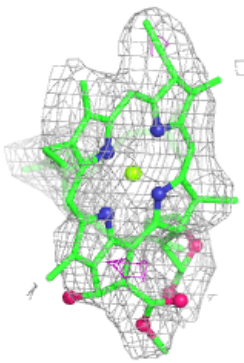


Electron density around CLA B 807:

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

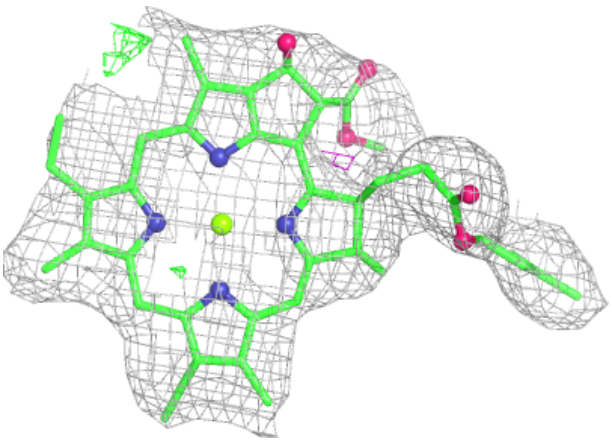


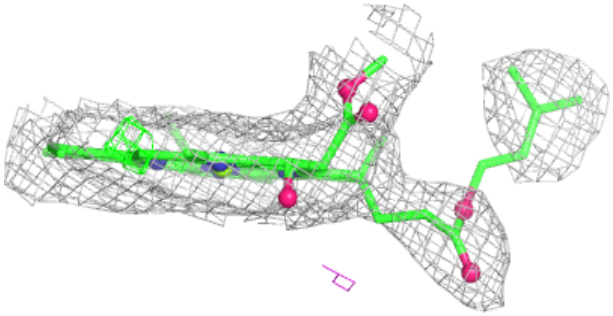




Electron density around CLA B 828:

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

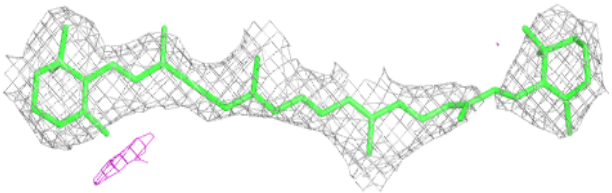


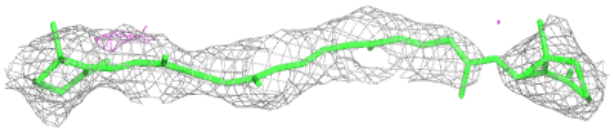


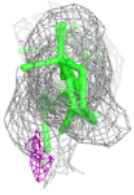


Electron density around BCR B 843:

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

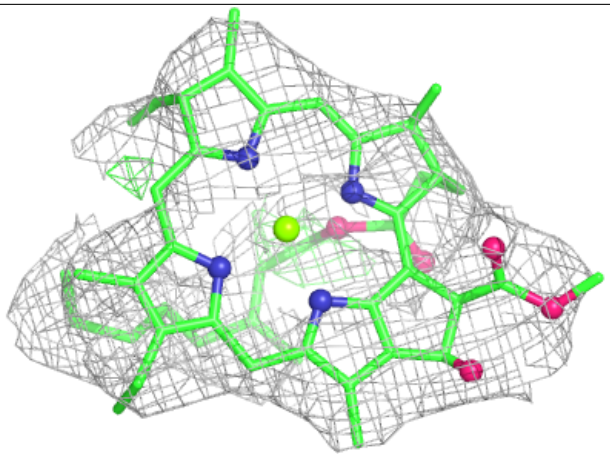


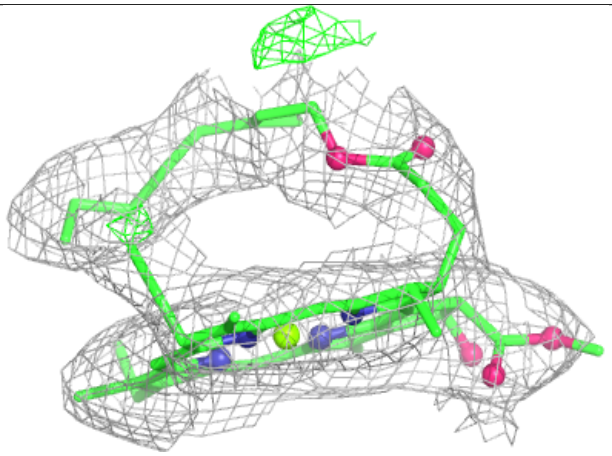


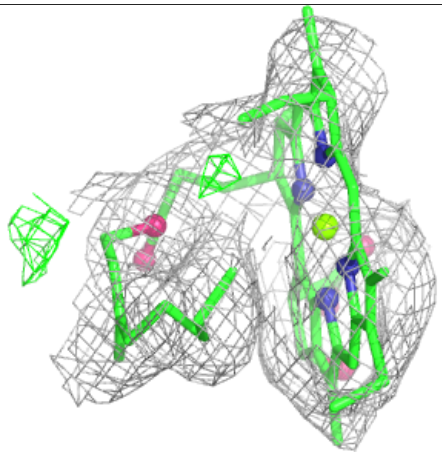


Electron density around CLA A 810:

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

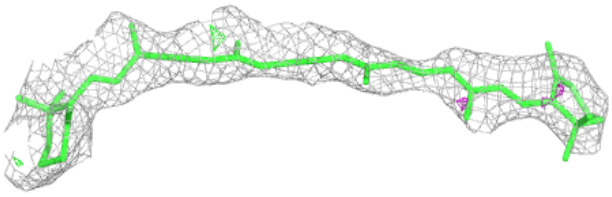


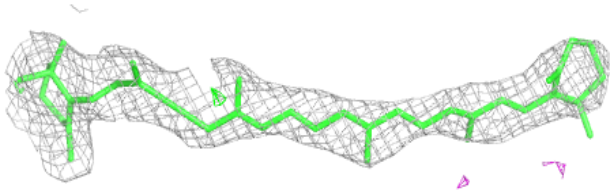


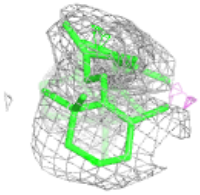


Electron density around BCR F 202:

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

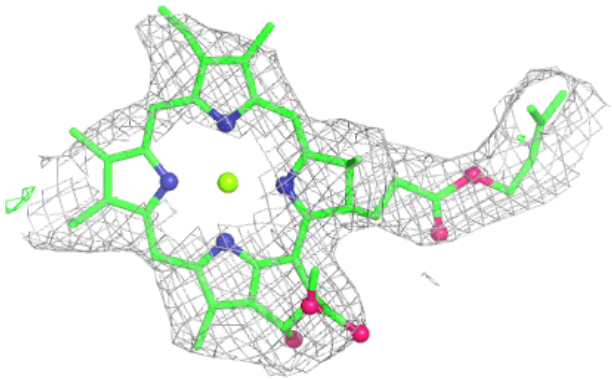


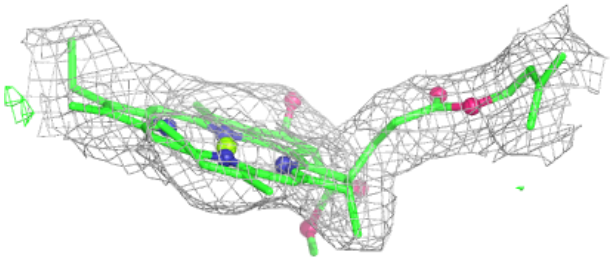


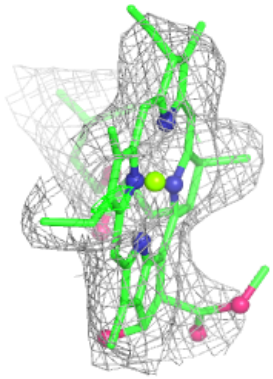


Electron density around CLA B 830:

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

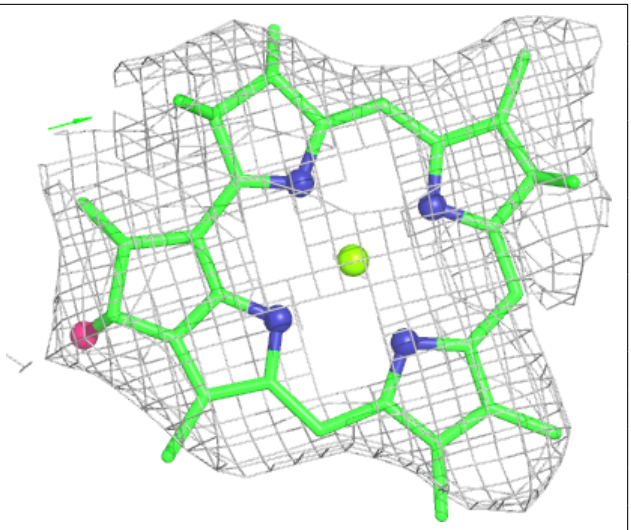


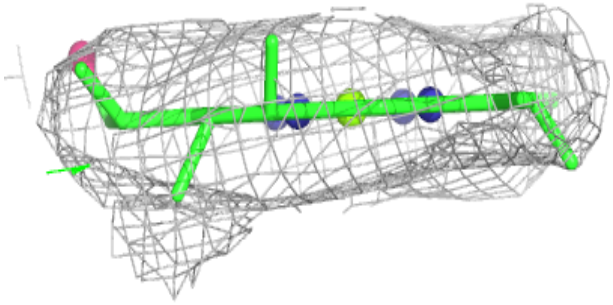


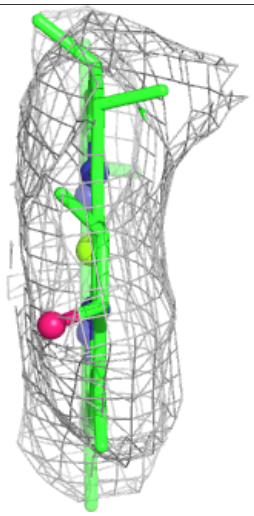


Electron density around CLA 4 313:

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

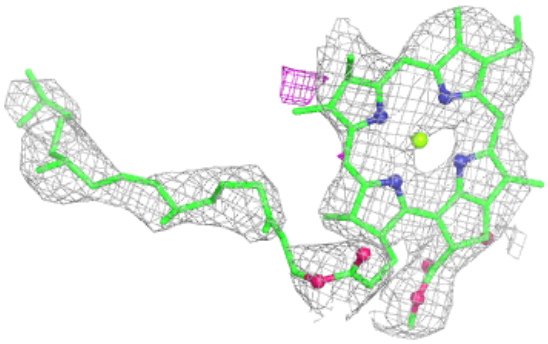


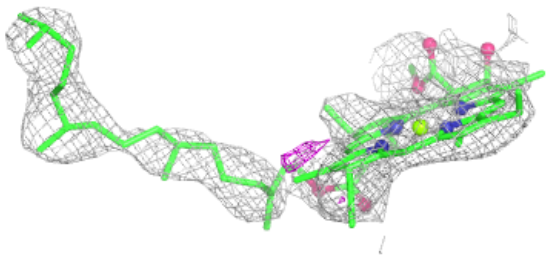


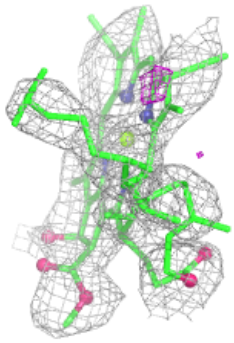


Electron density around CLA A 849:

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

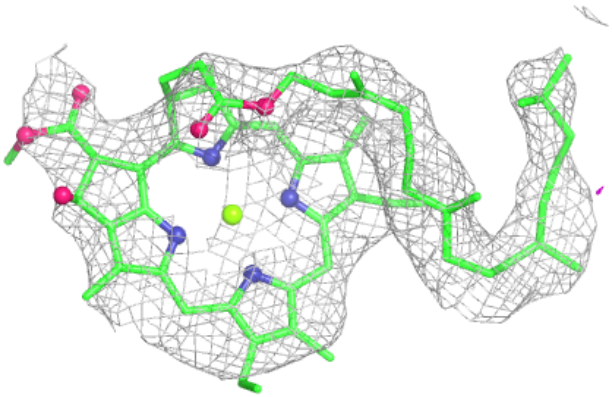


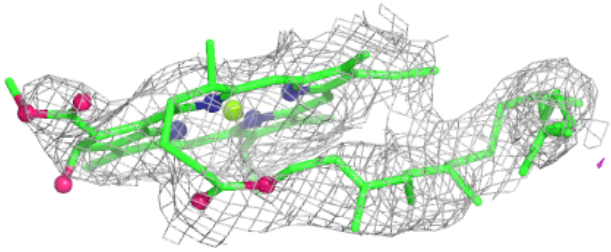


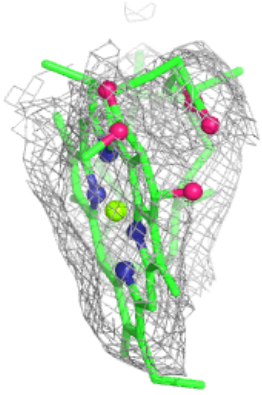


Electron density around CLA A 816:

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

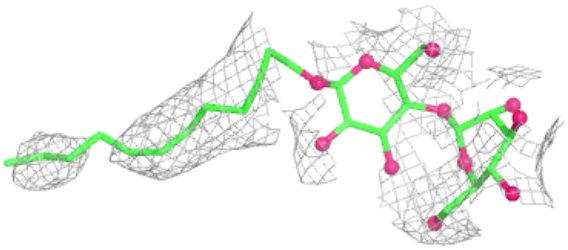


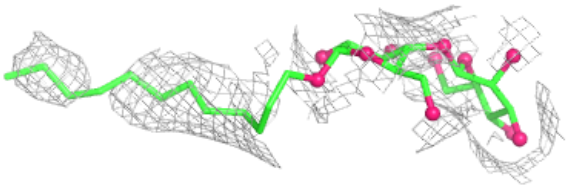


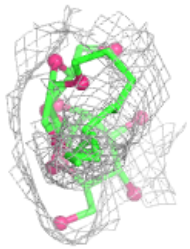


Electron density around LMU A 854:

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

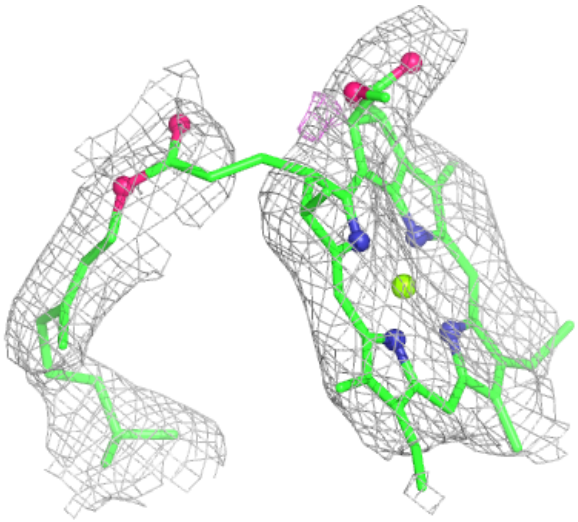


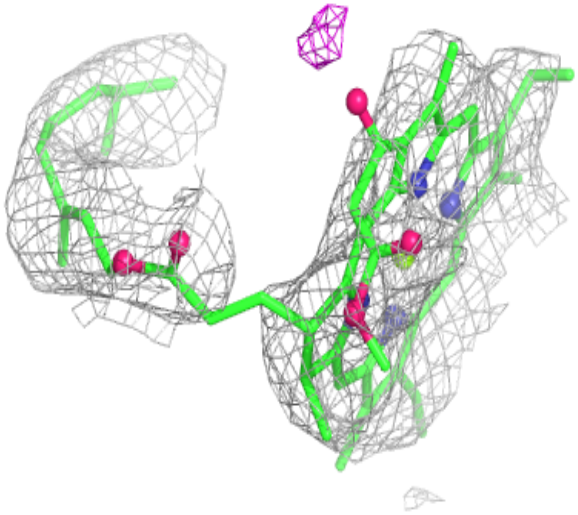


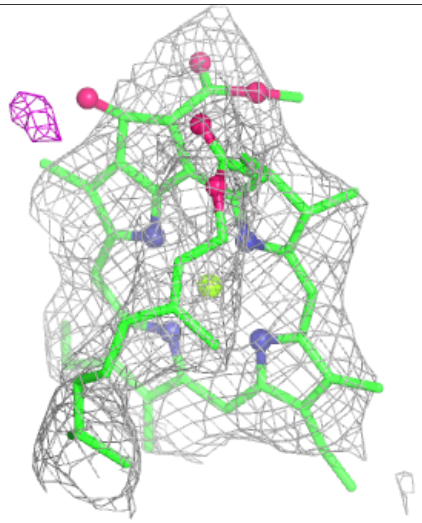


Electron density around CLA A 802:

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

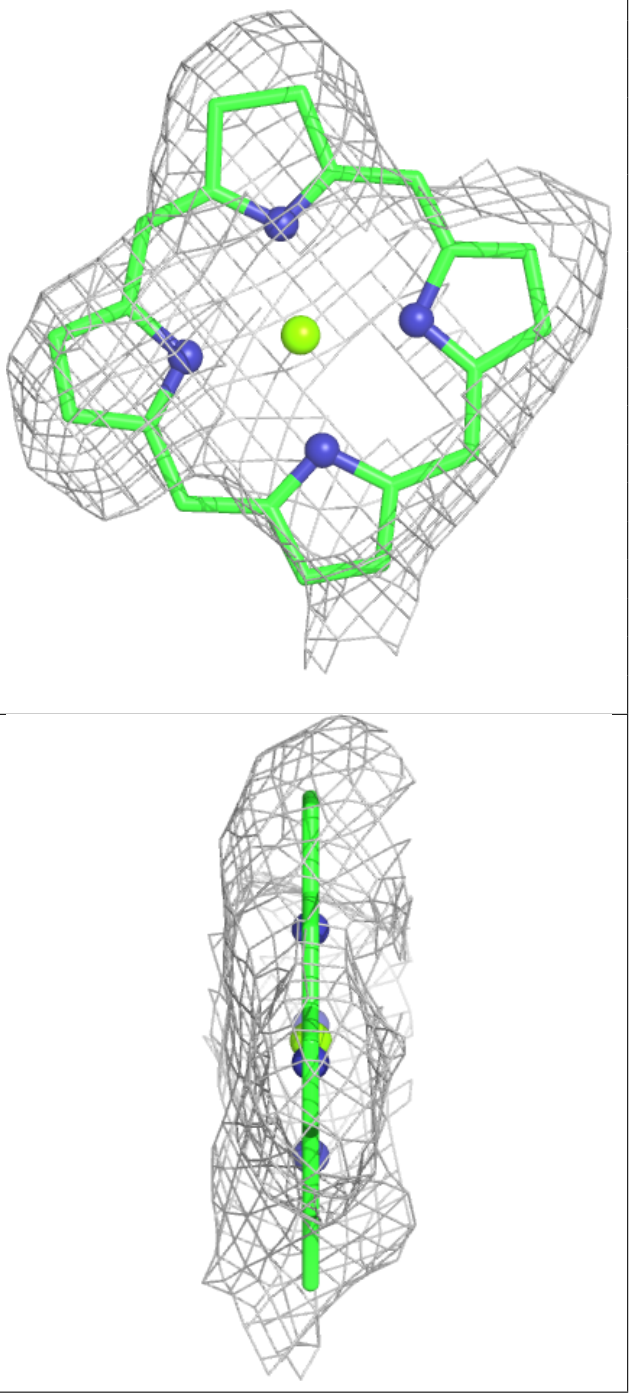






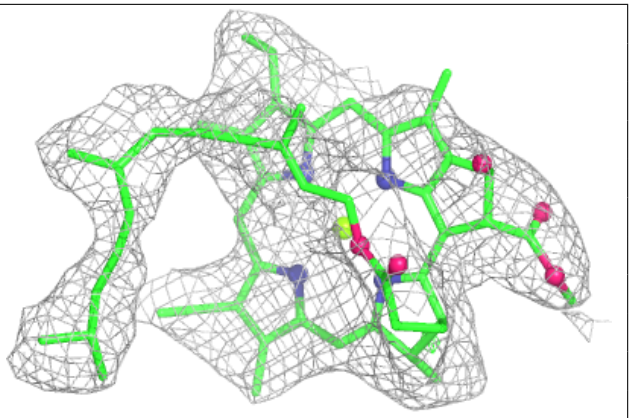
Electron density around CLA 2 303:

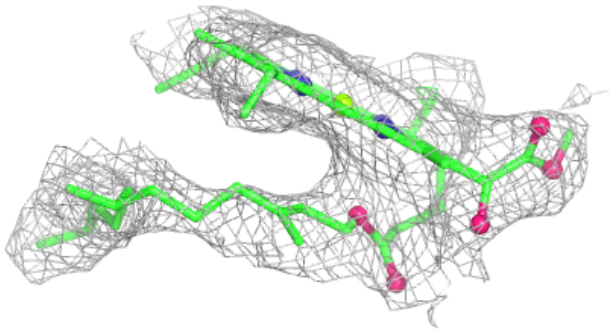
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



Electron density around CLA I 102:

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

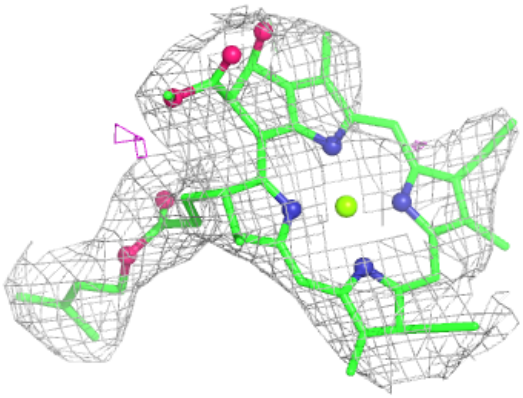


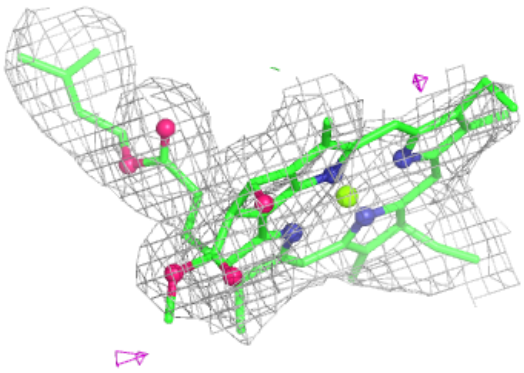


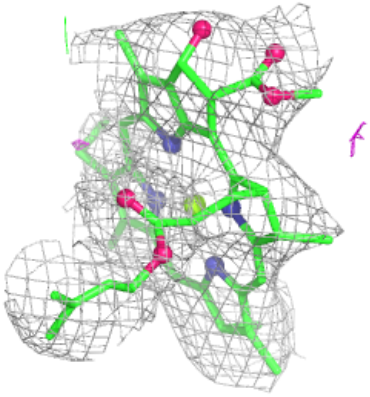


Electron density around CLA 2 310:

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

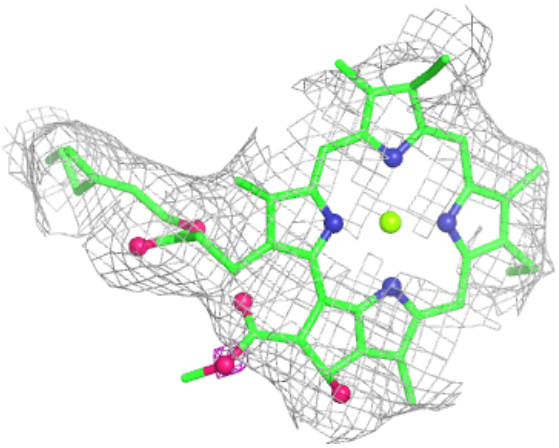


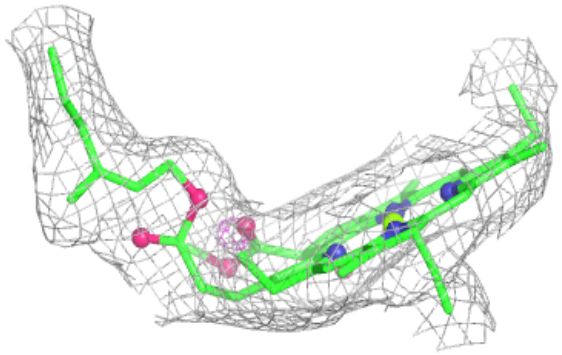


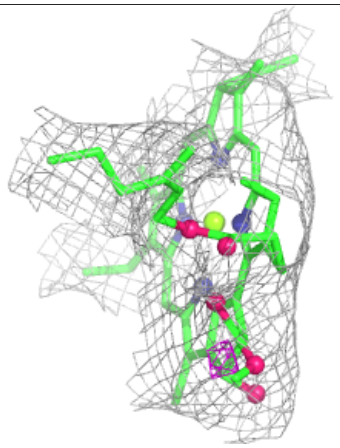


Electron density around CLA 4 307:

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

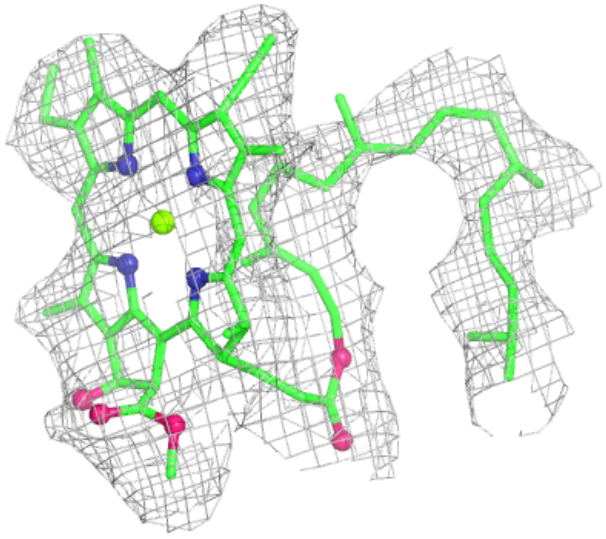


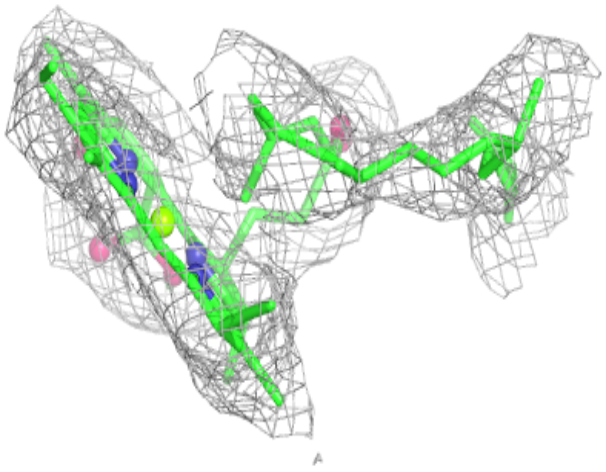


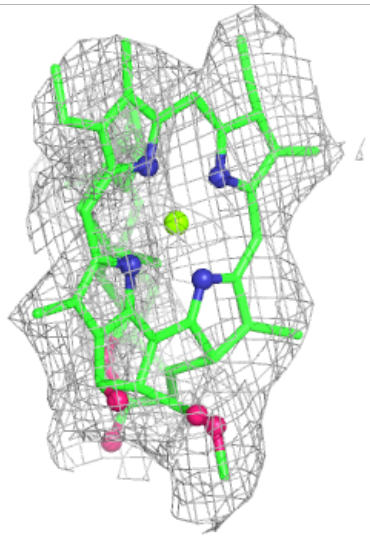


Electron density around CLA B 820:

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

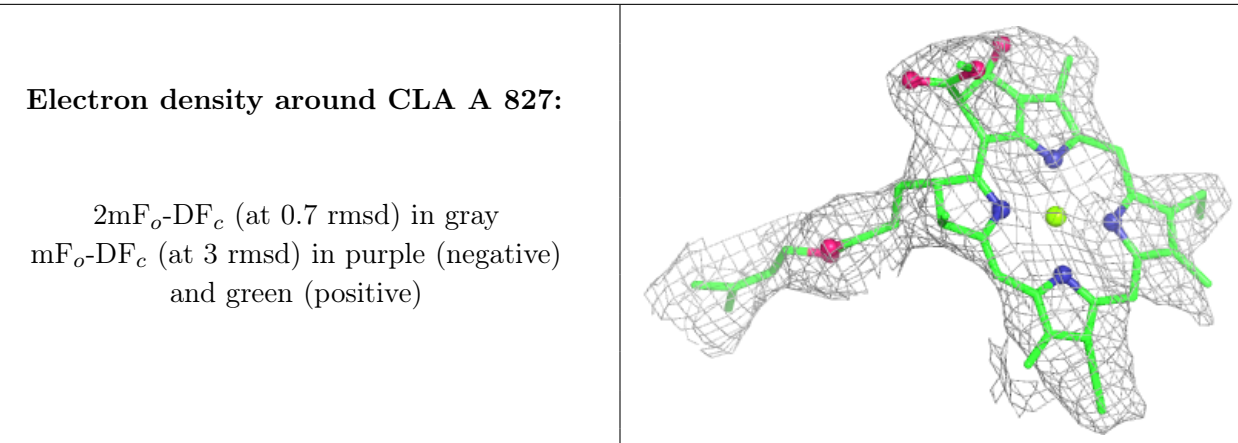






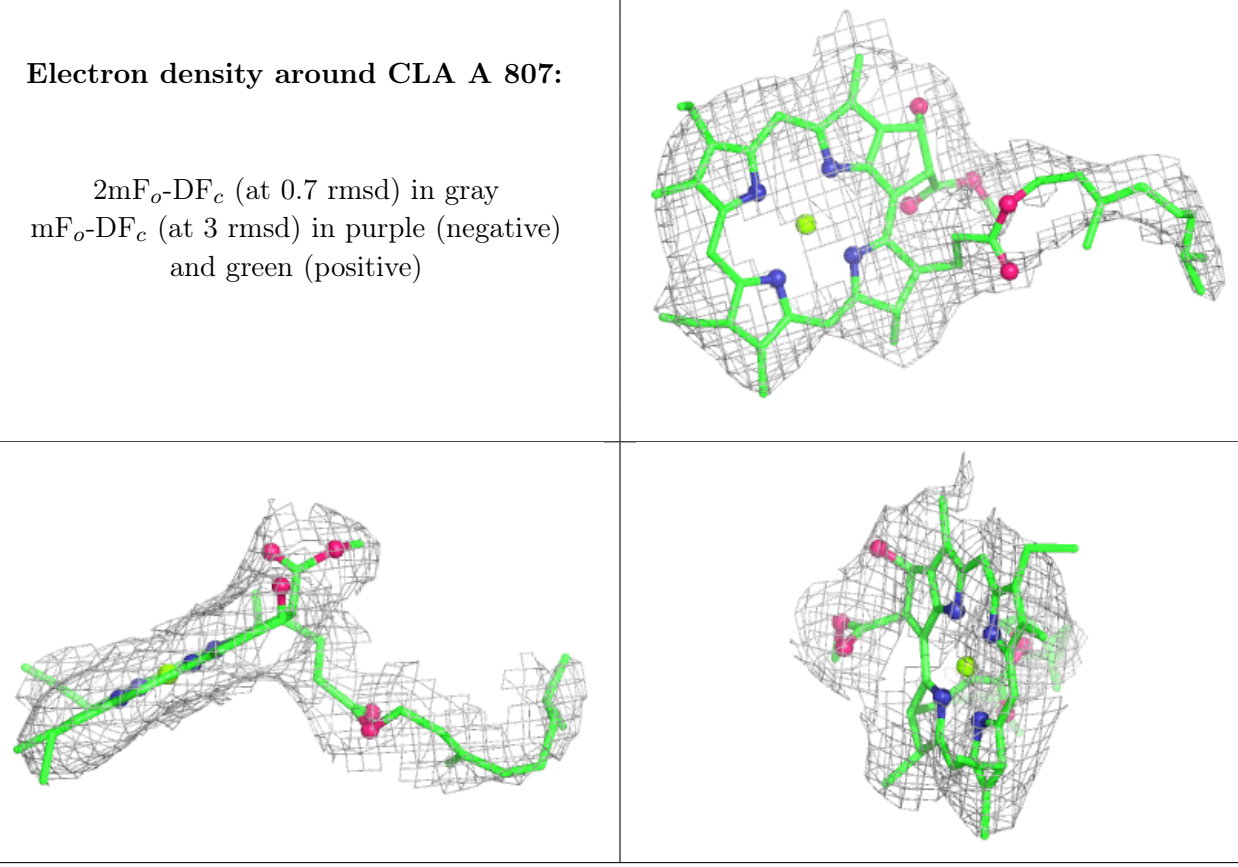
Electron density around CLA A 827:

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



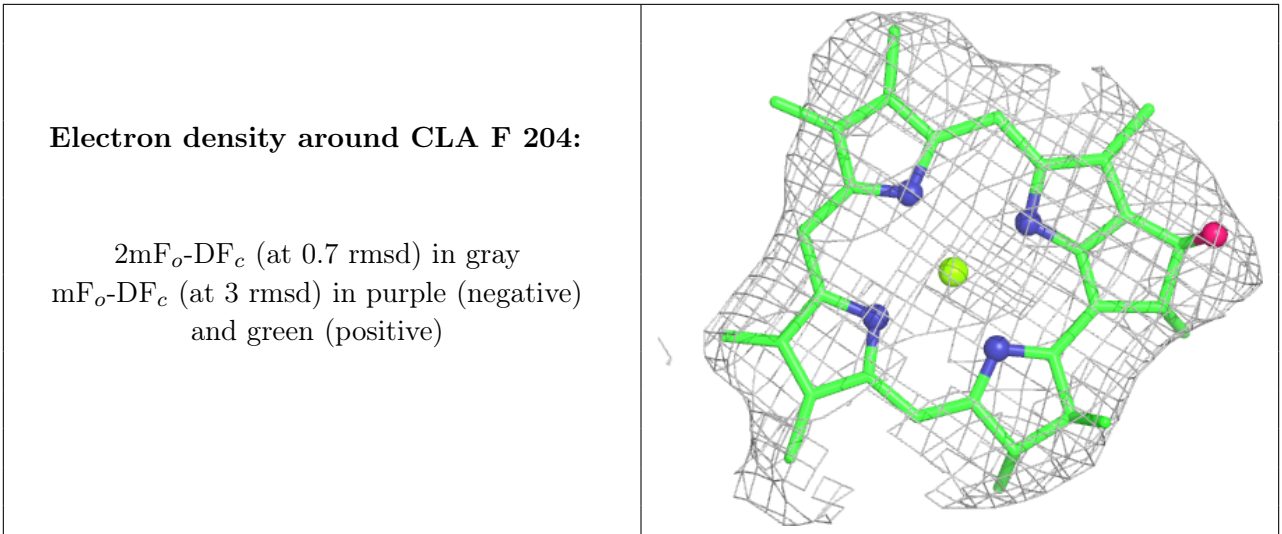
Electron density around CLA A 807:

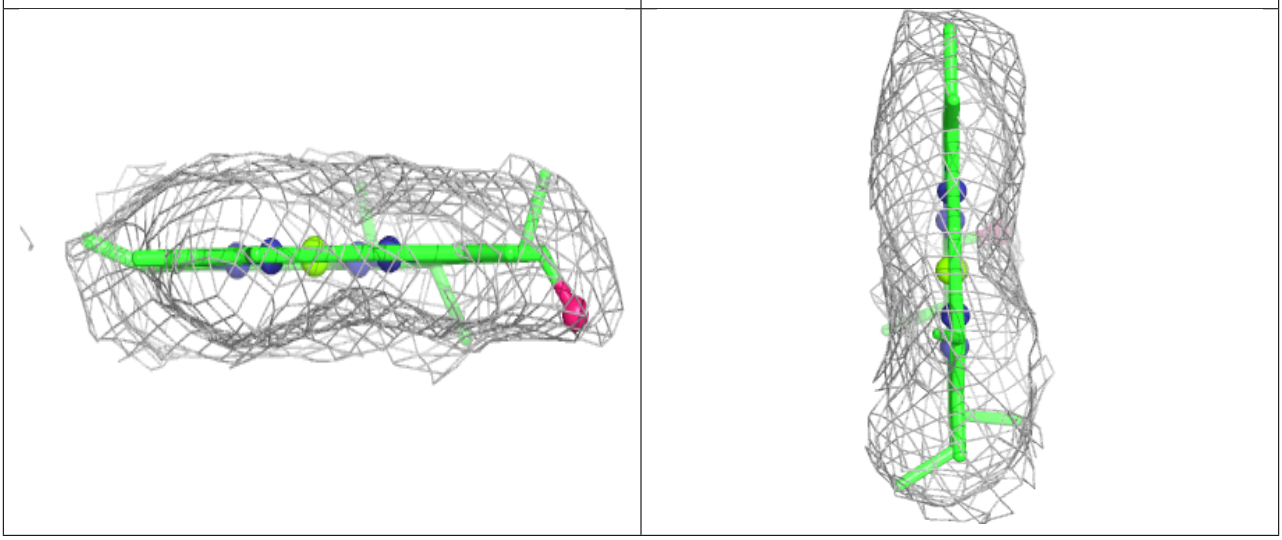
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



Electron density around CLA F 204:

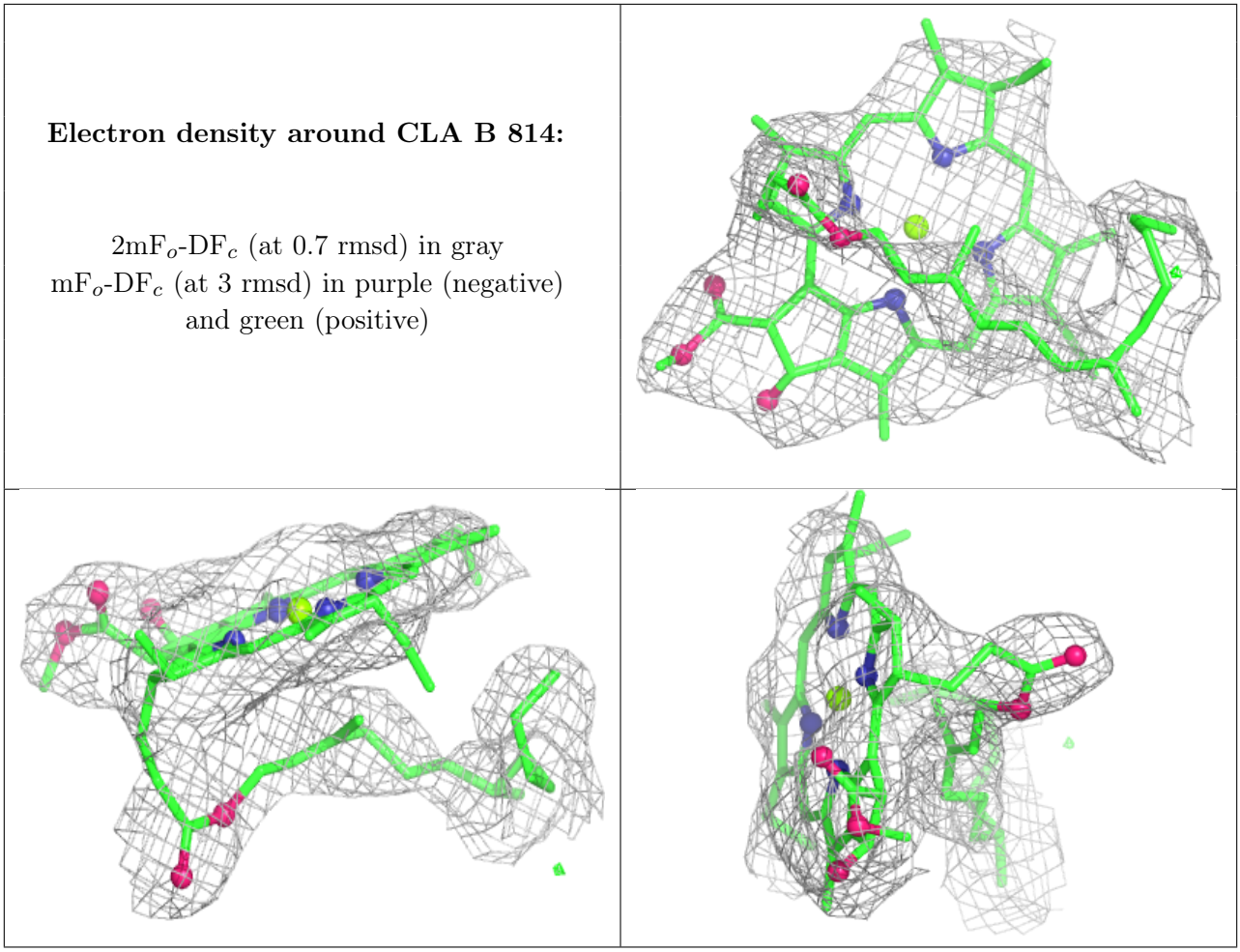
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)





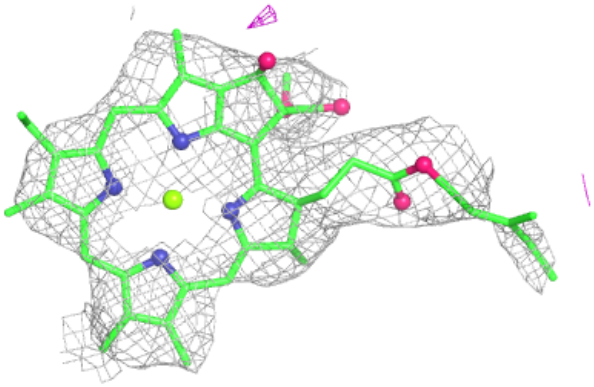
Electron density around CLA B 814:

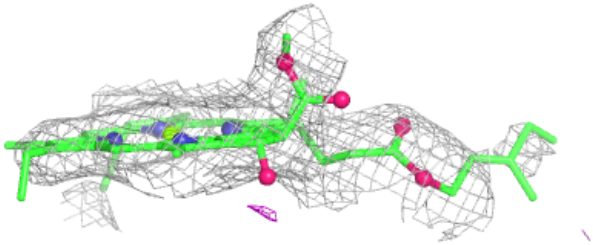
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



Electron density around CLA A 832:

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

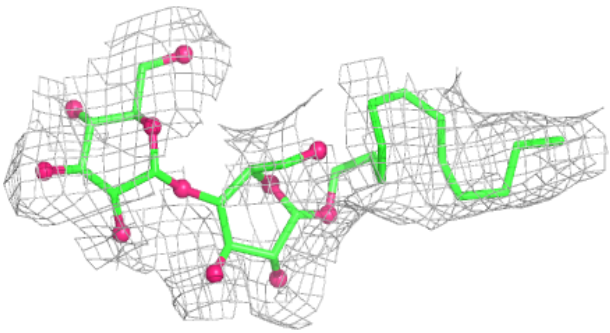


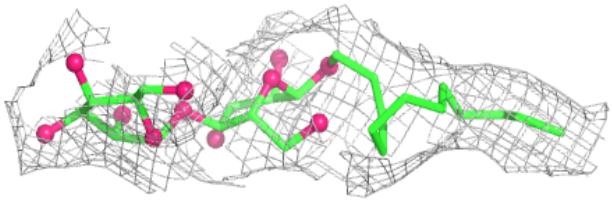


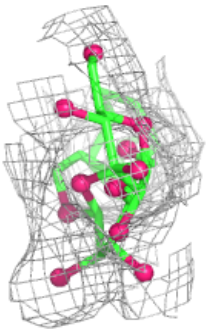


Electron density around LMU A 852:

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

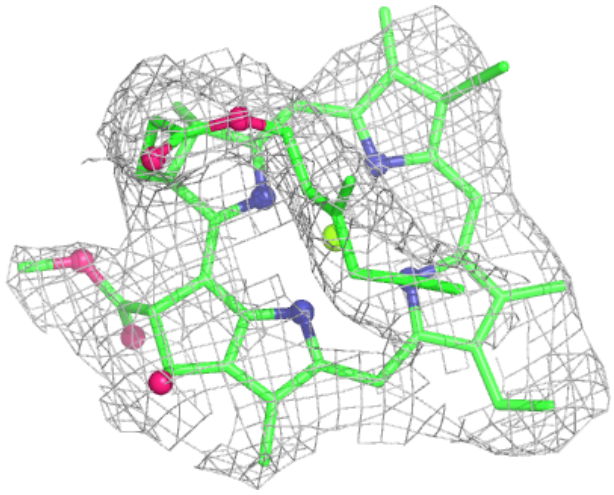


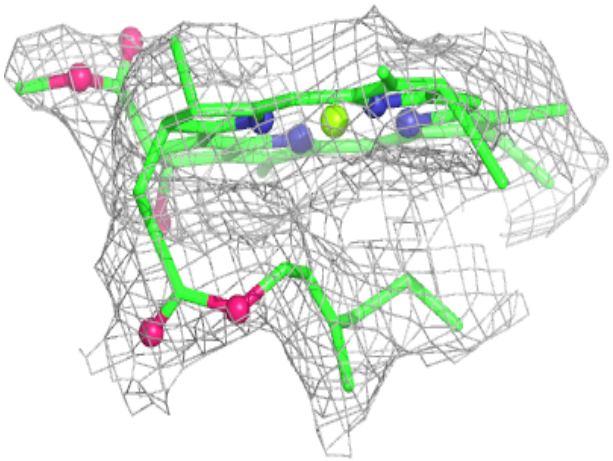




Electron density around CLA A 815:

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

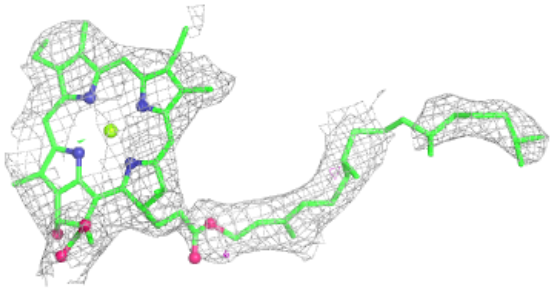


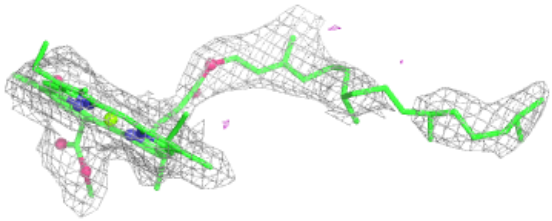


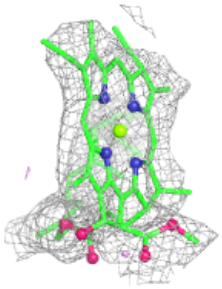


Electron density around CLA A 829:

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

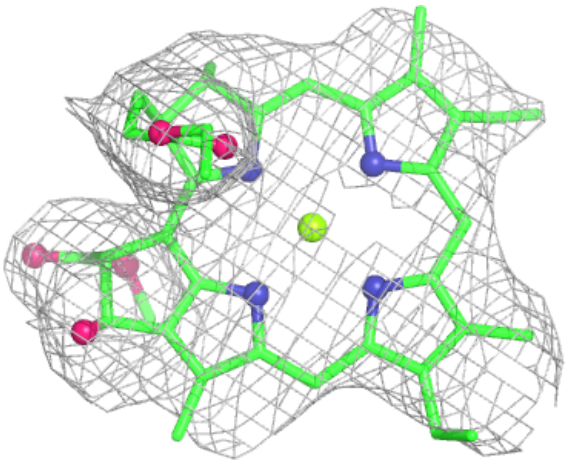


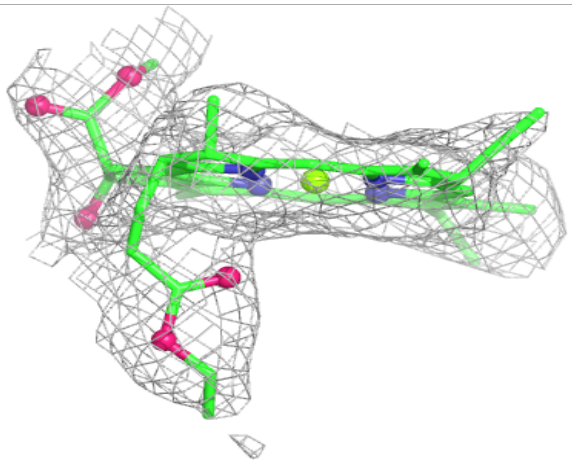


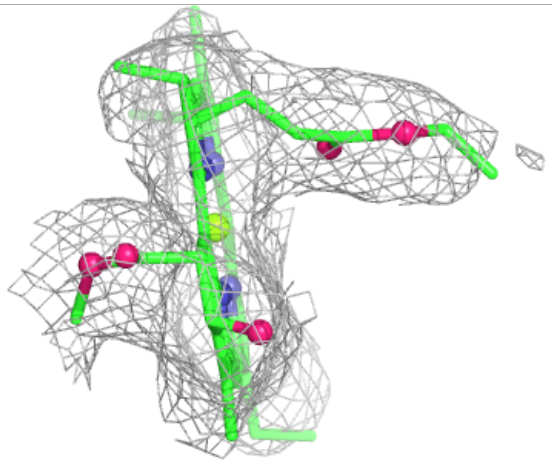


Electron density around CLA L 207:

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

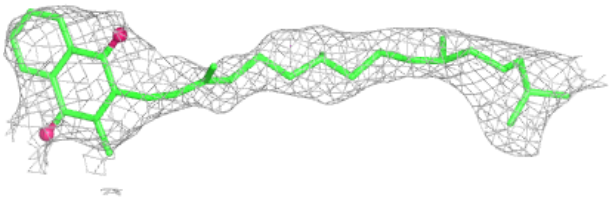


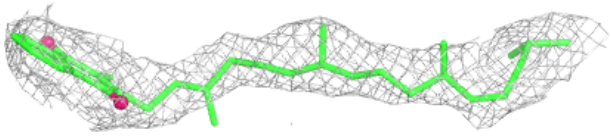


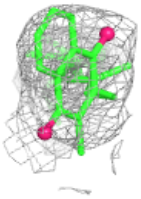


Electron density around PQN A 839:

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

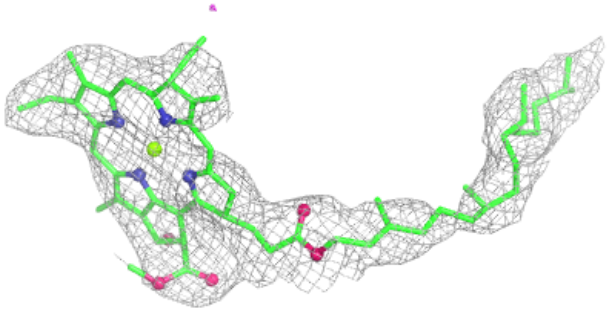


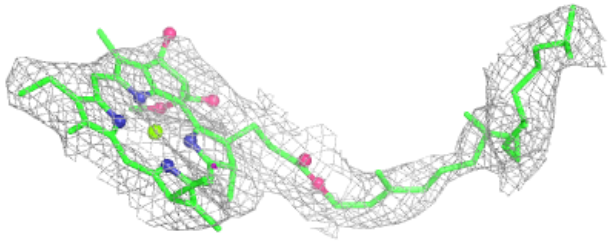


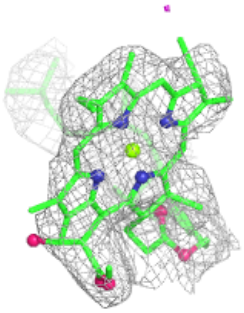


Electron density around CLA A 848:

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

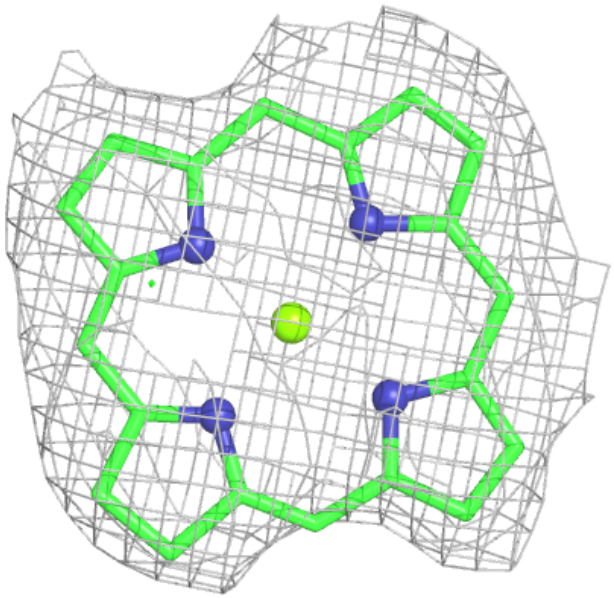


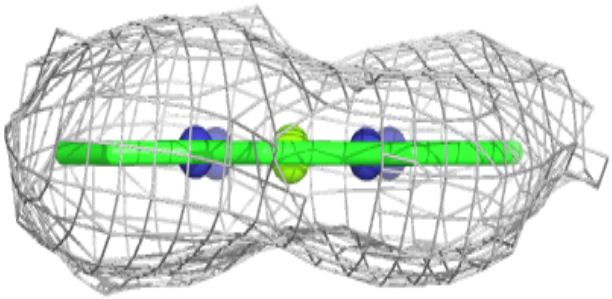


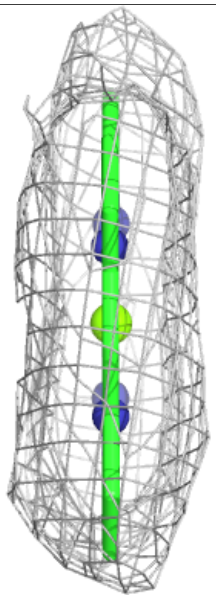


Electron density around CLA 4 312:

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

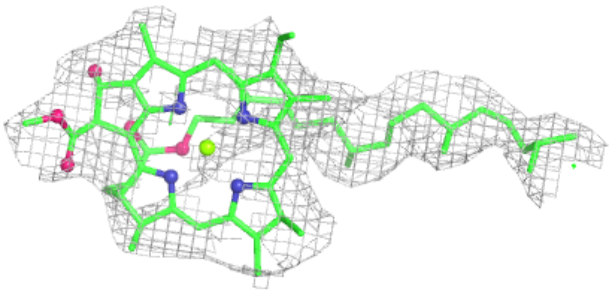


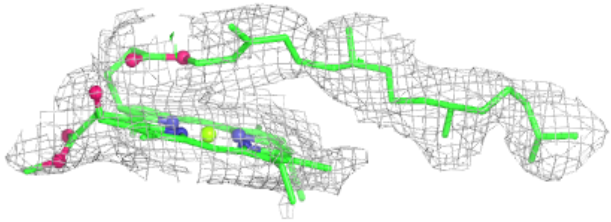


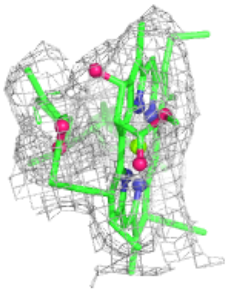


Electron density around CLA A 833:

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

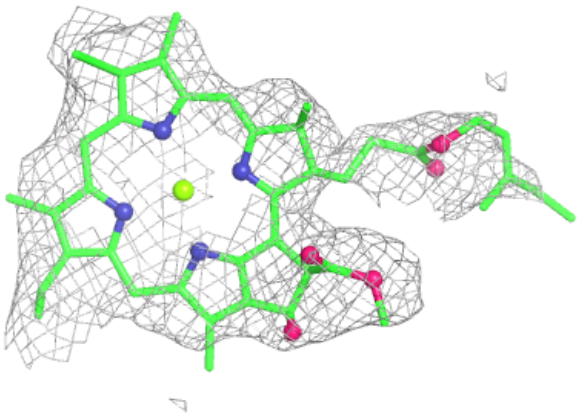


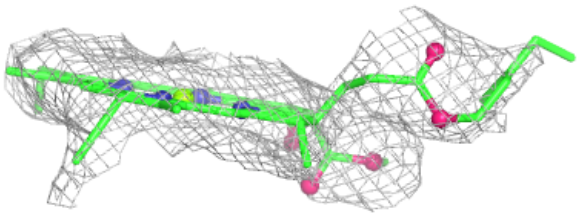


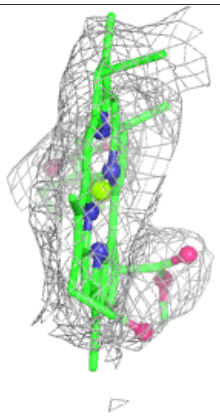


Electron density around CLA A 835:

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



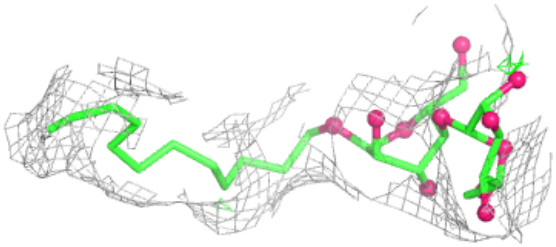


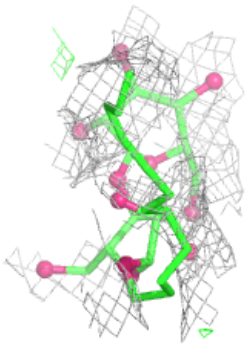


Electron density around LMU G 101:

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

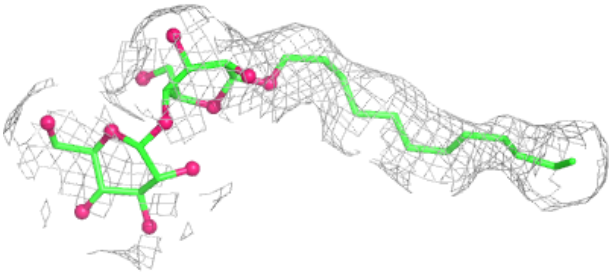


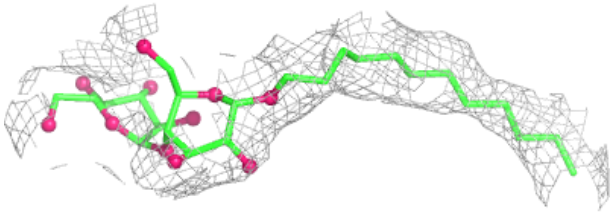


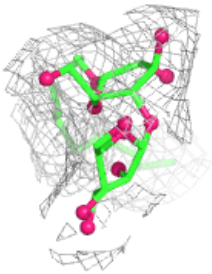


Electron density around LMU R 104:

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

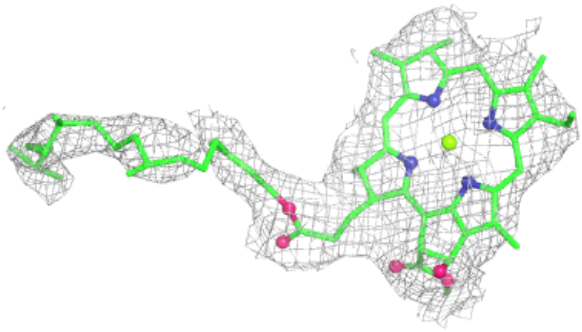


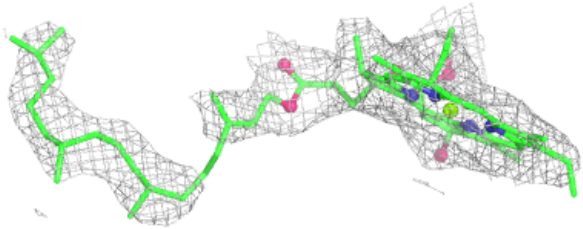


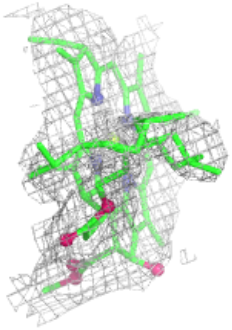


Electron density around CLA B 810:

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

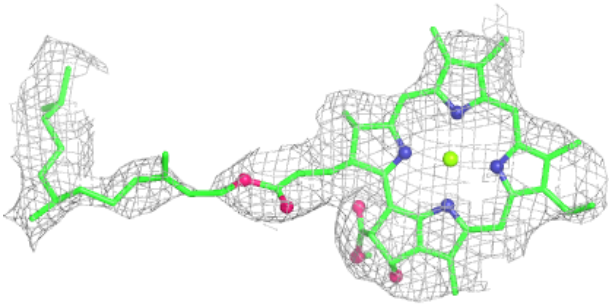


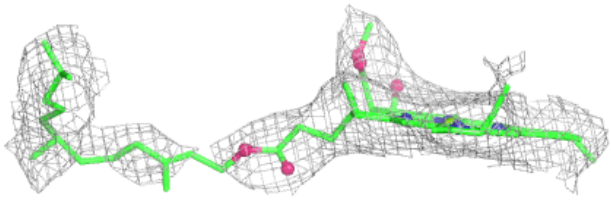


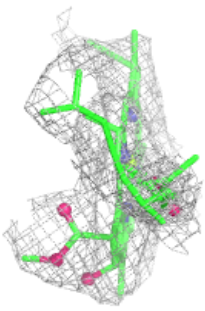


Electron density around CLA B 834:

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

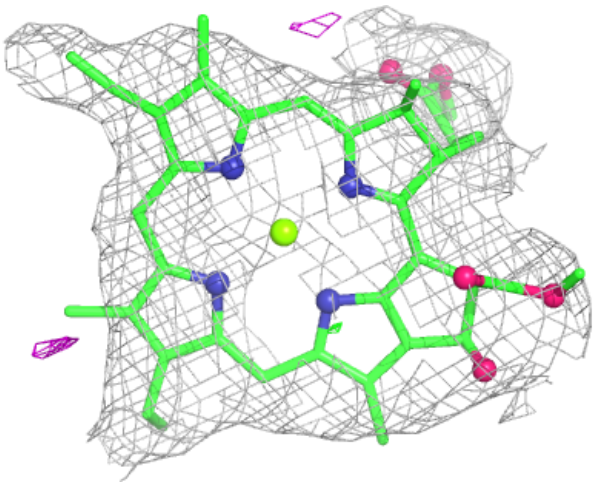


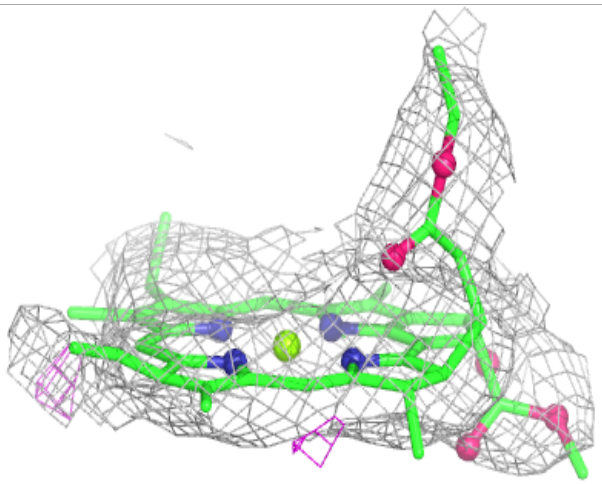


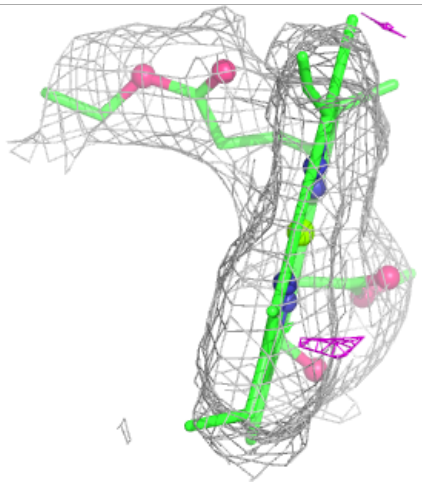


Electron density around CLA B 836:

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

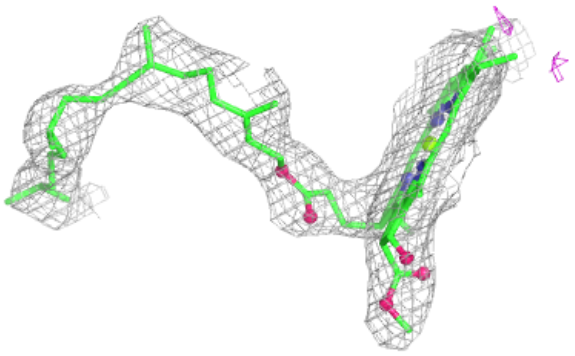


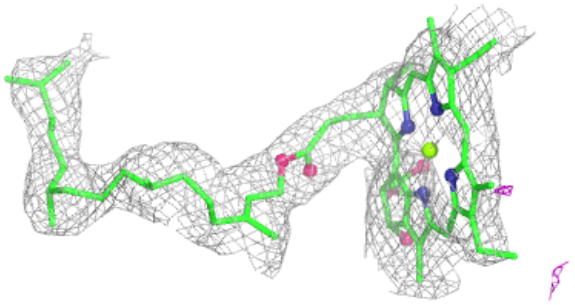


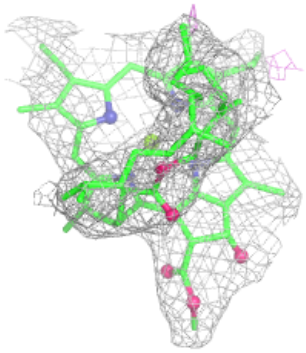


Electron density around CLA B 837:

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

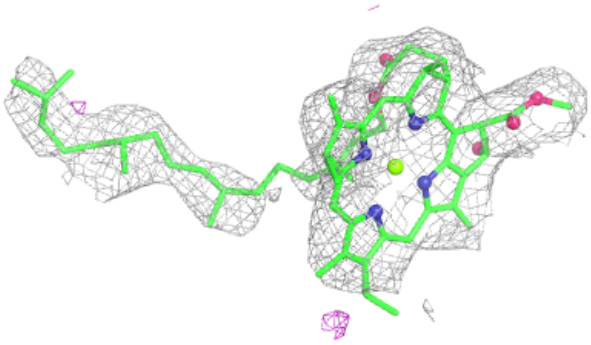


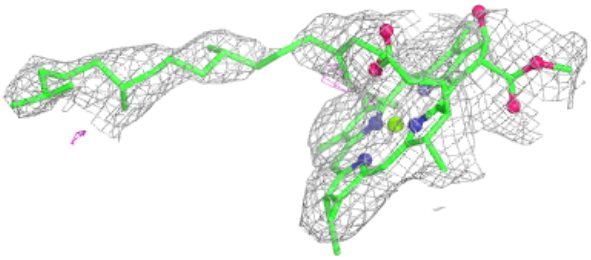


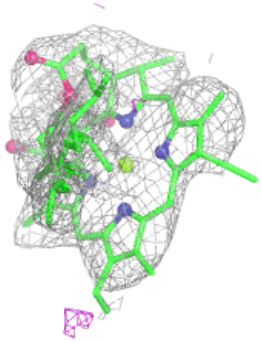


Electron density around CLA A 836:

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

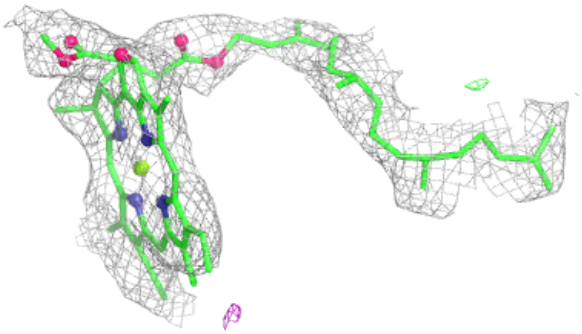


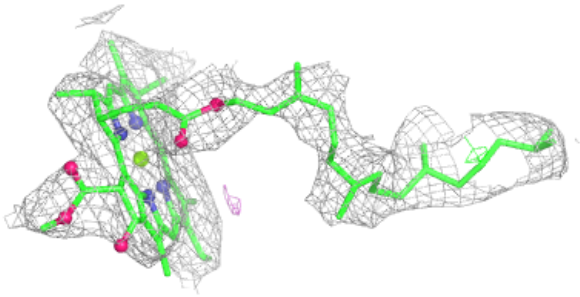


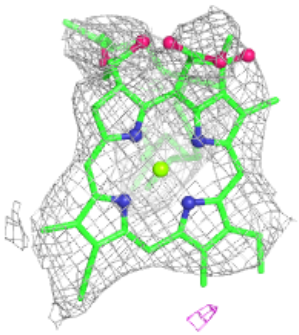


Electron density around CLA B 826:

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

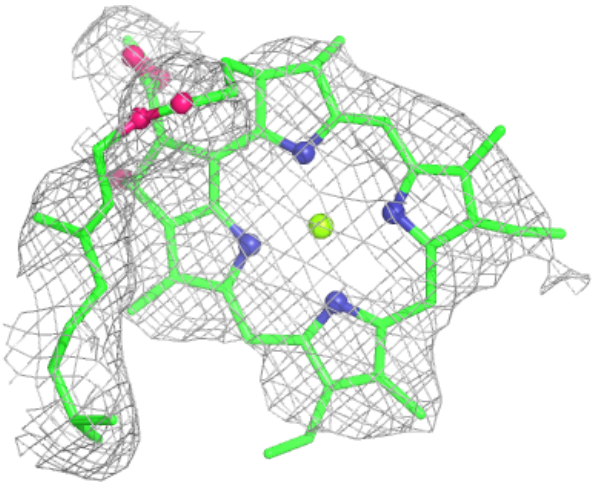


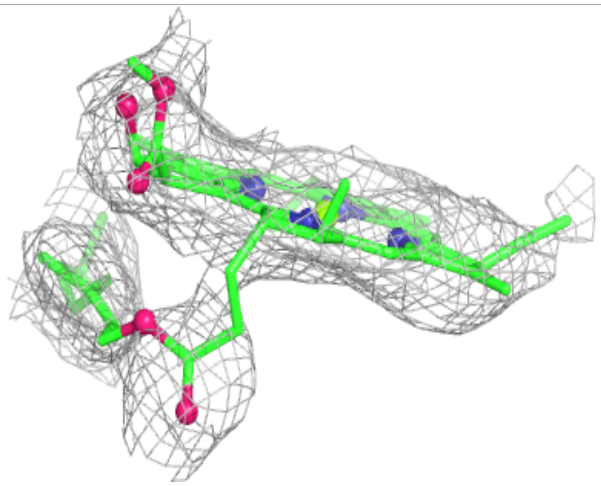


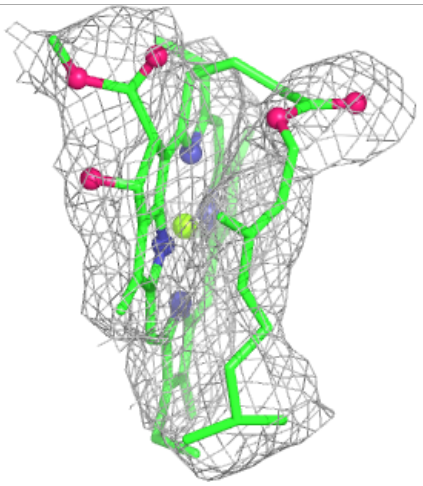


Electron density around CLA A 825:

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

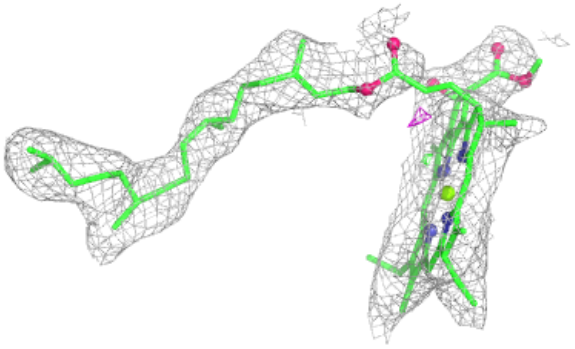


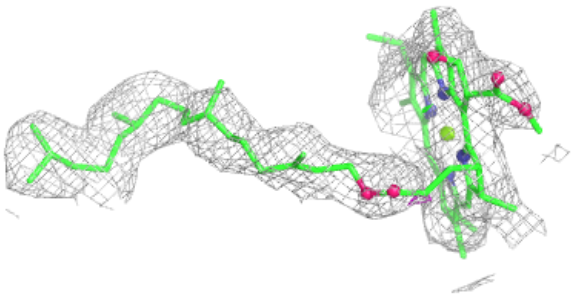


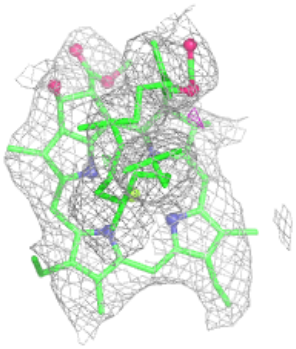


Electron density around CLA A 826:

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

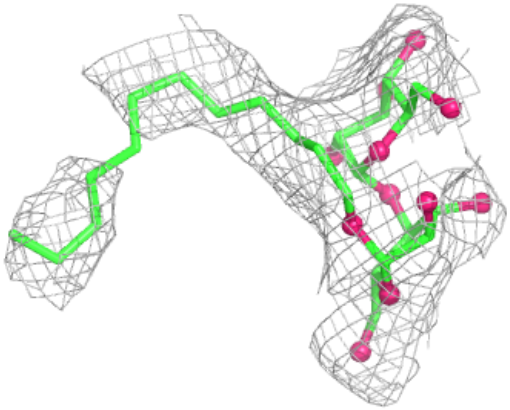


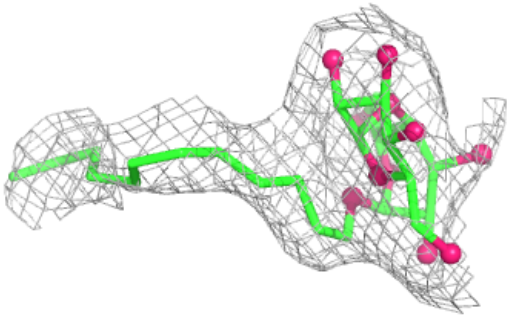


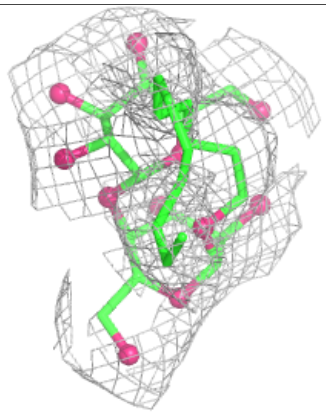


Electron density around LMU H 104:

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

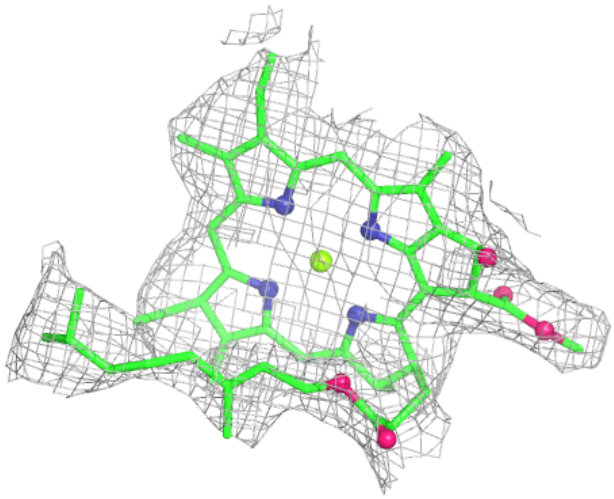


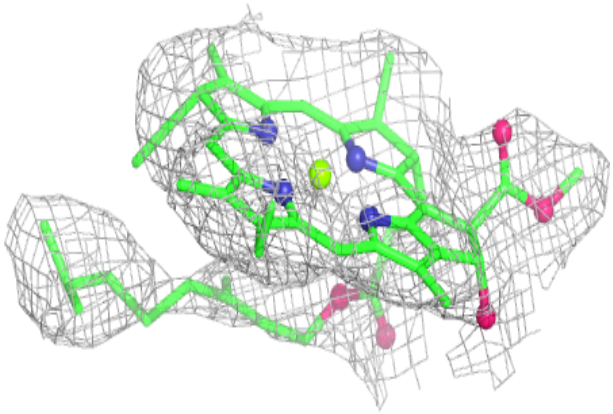




Electron density around CLA B 819:

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

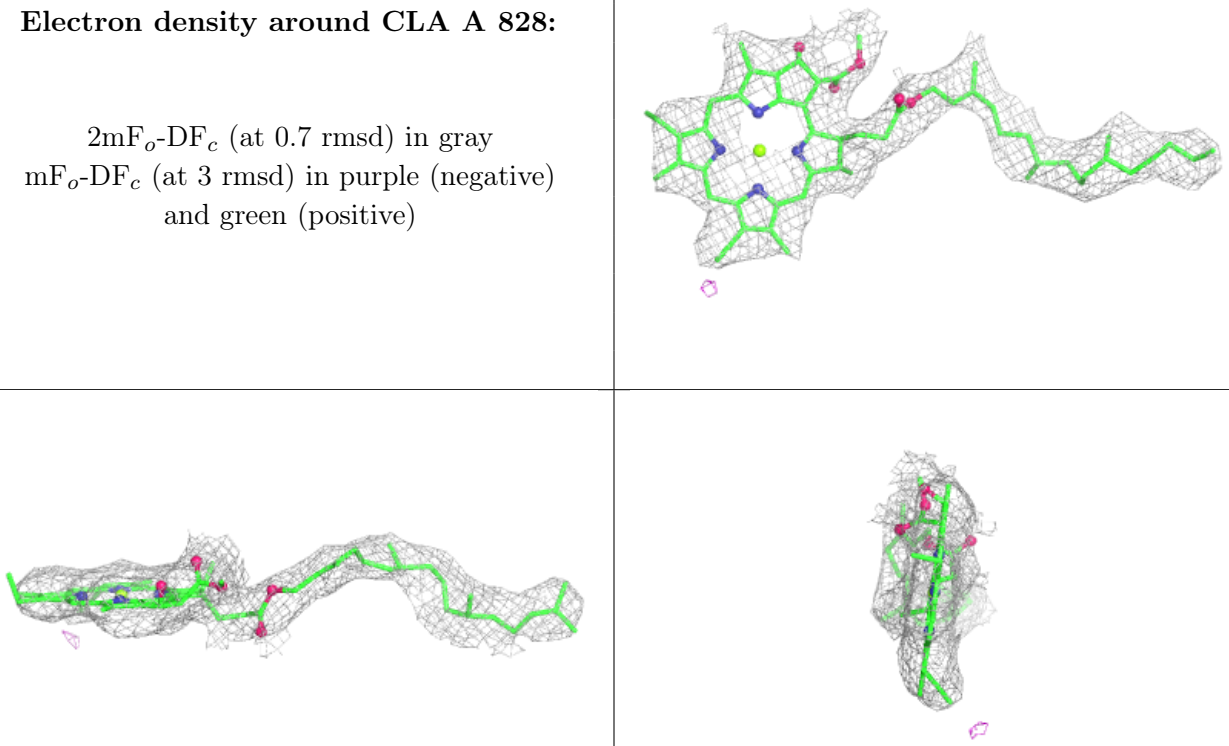






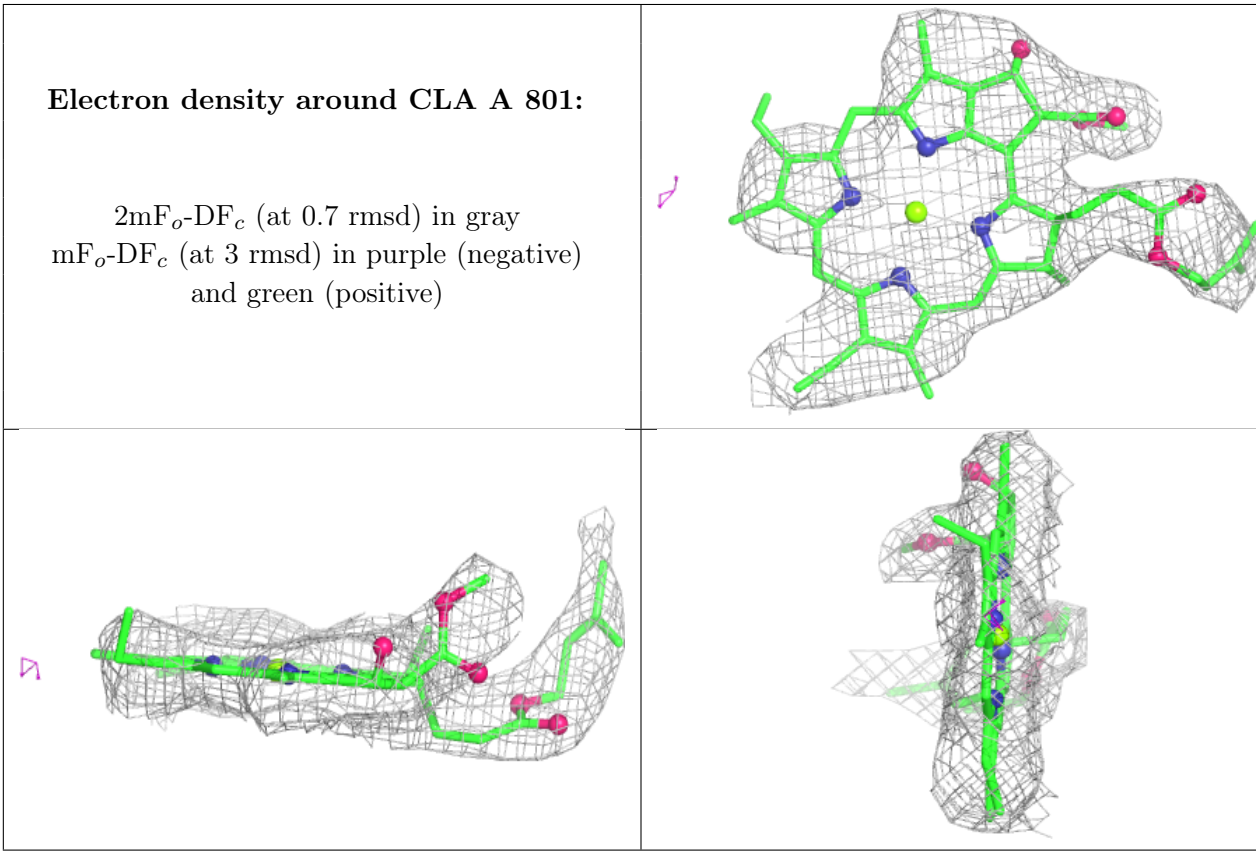
Electron density around CLA A 828:

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



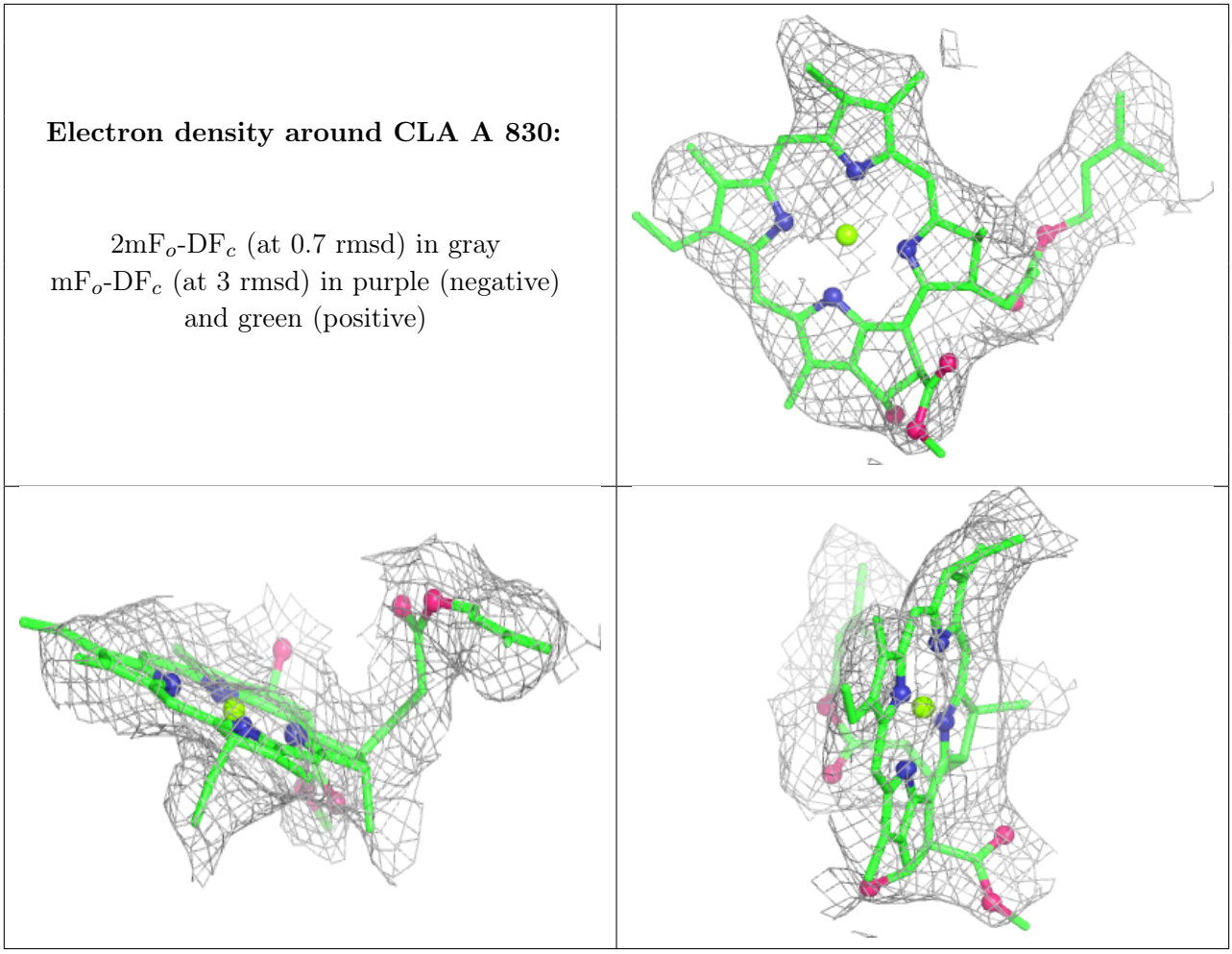
Electron density around CLA A 801:

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



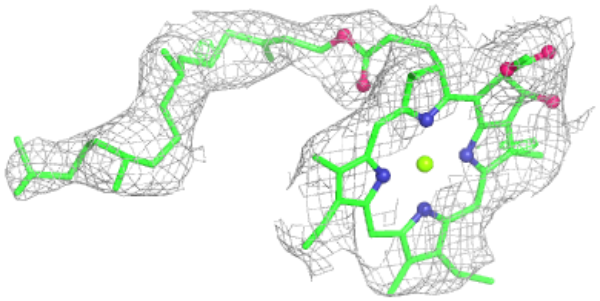
Electron density around CLA A 830:

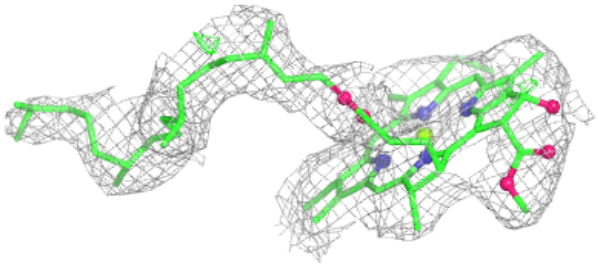
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

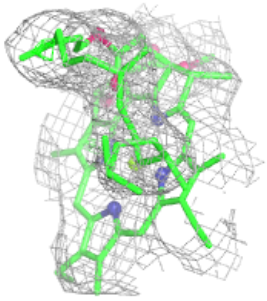


Electron density around CLA A 806:

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

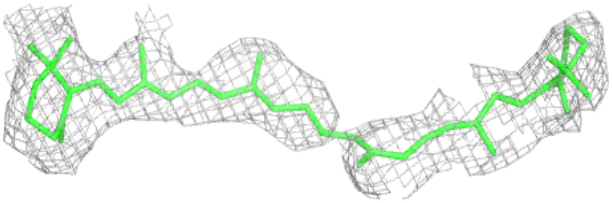


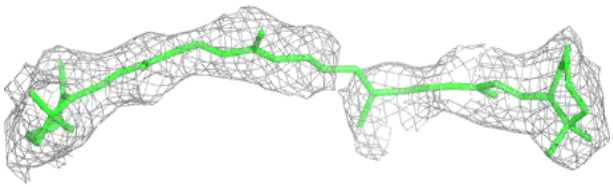


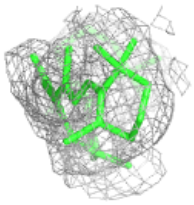


Electron density around BCR I 101:

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

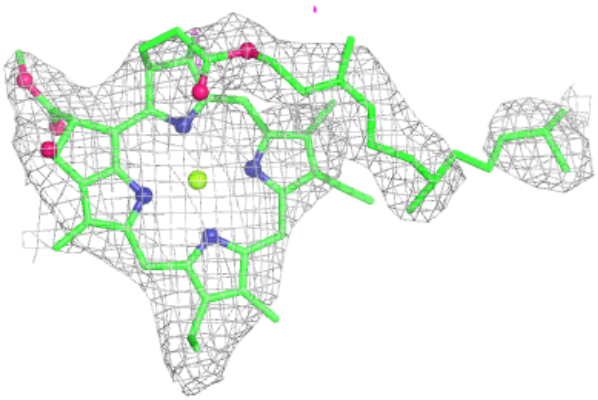


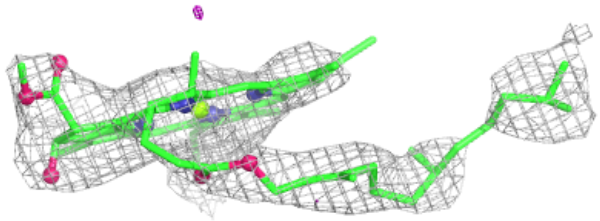




Electron density around CLA B 815:

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

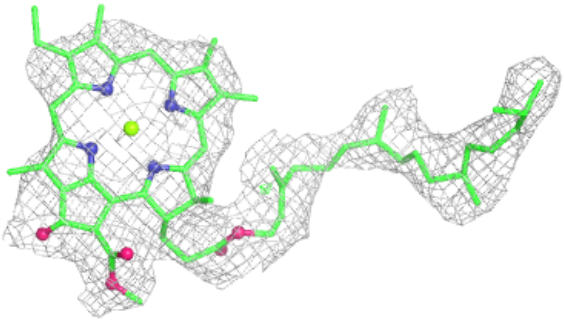


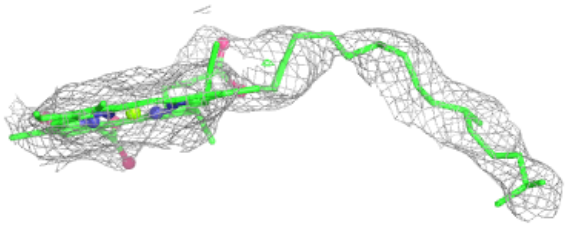


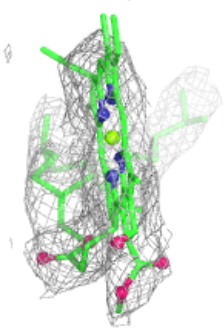


Electron density around CLA B 849:

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

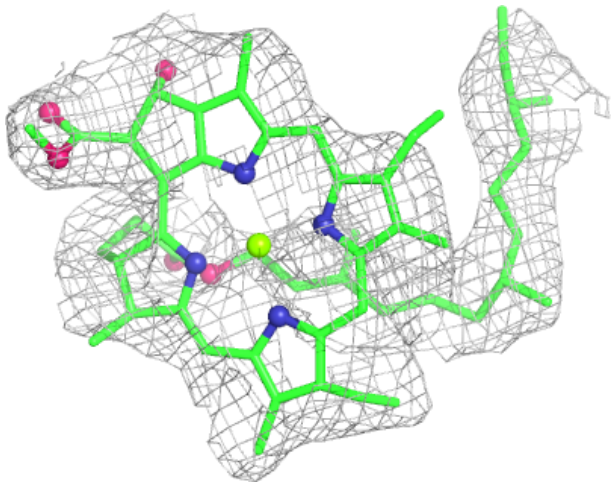


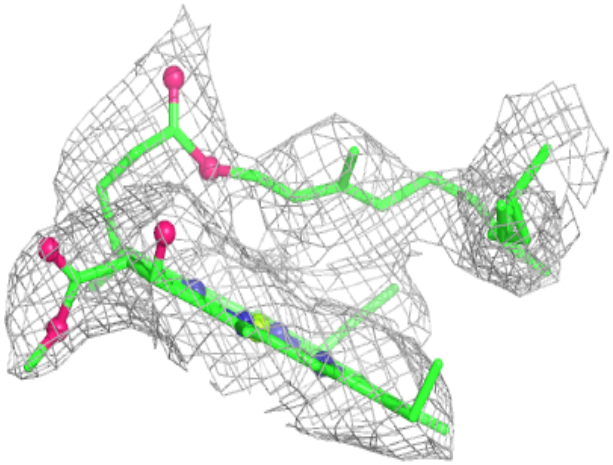


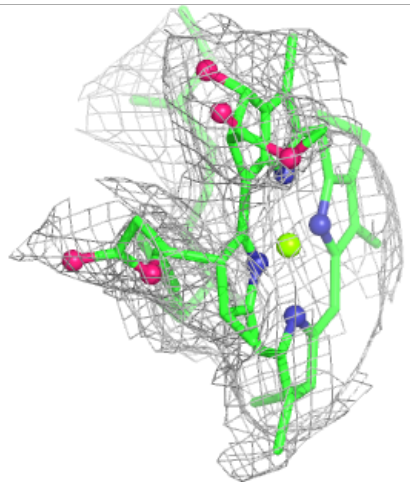


Electron density around CLA B 816:

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

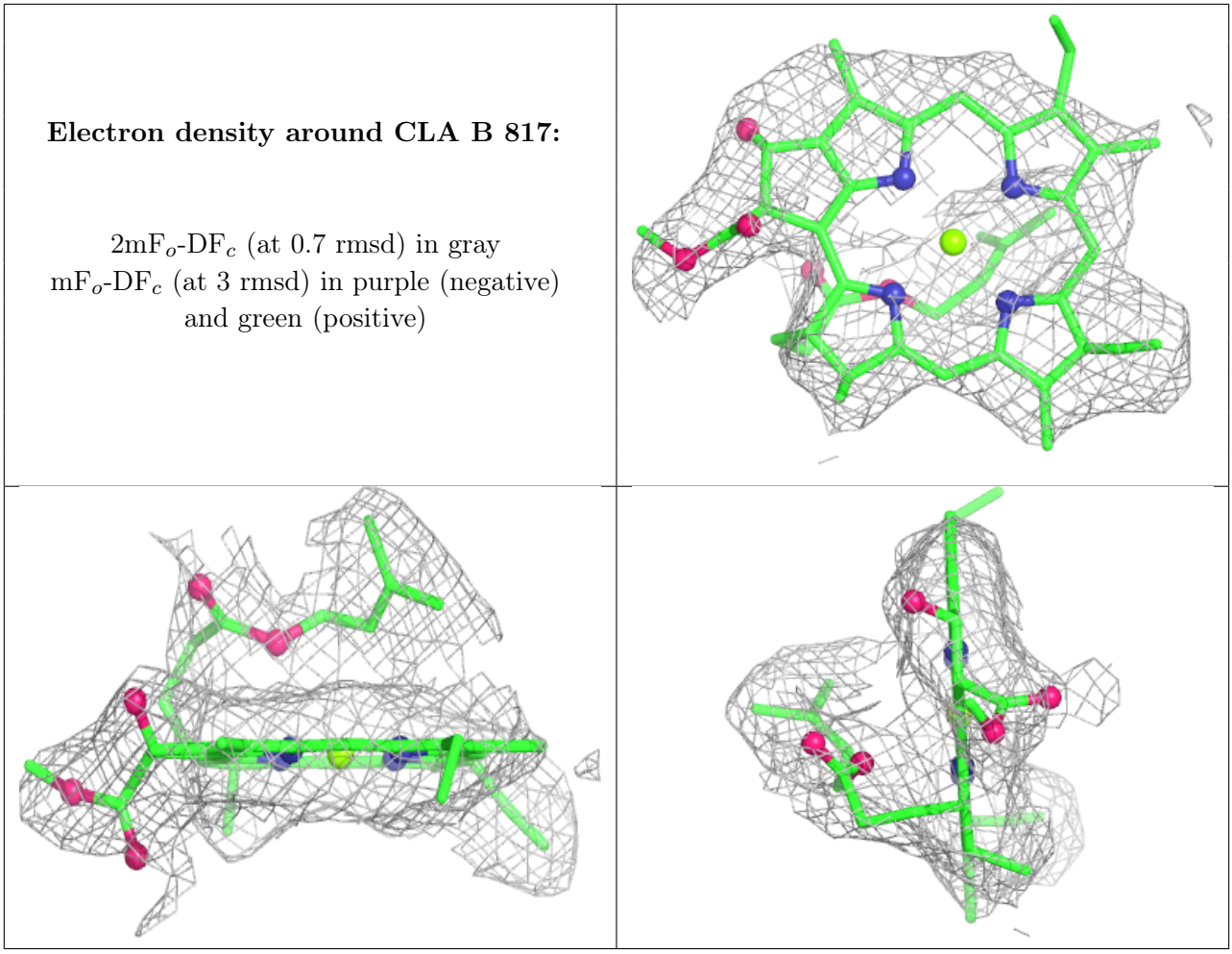






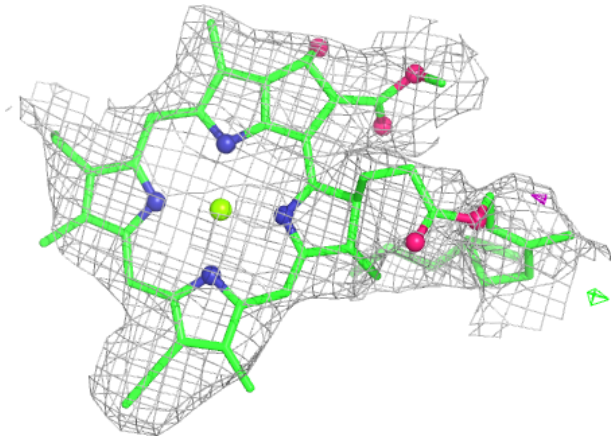
Electron density around CLA B 817:

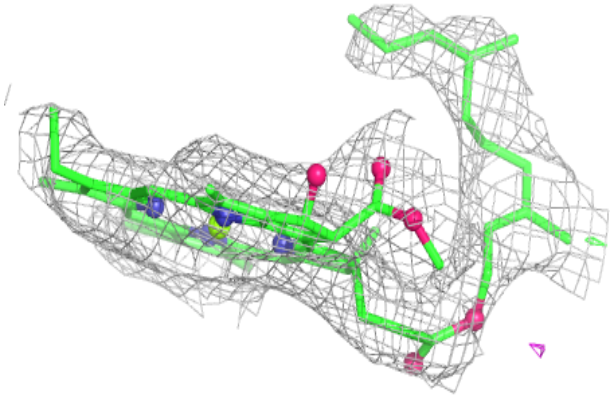
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

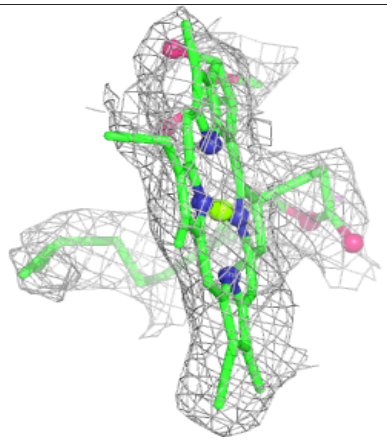


Electron density around CLA A 804:

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

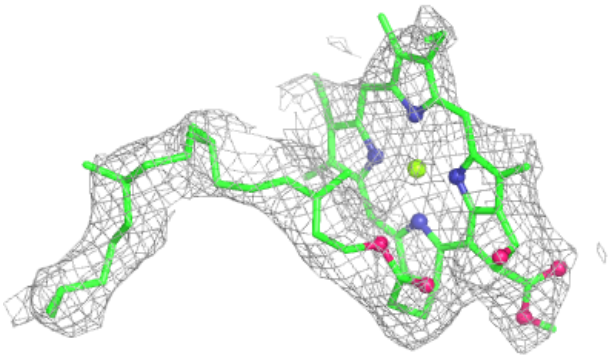


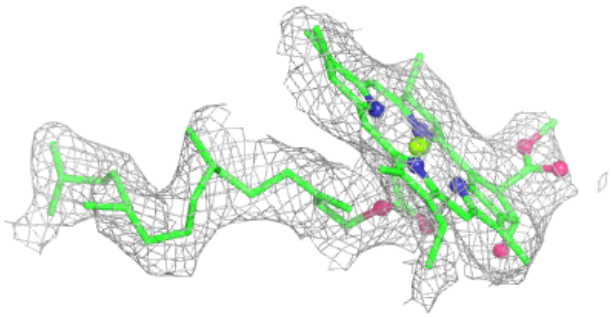


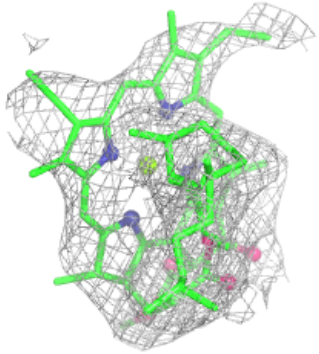


Electron density around CLA L 202:

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

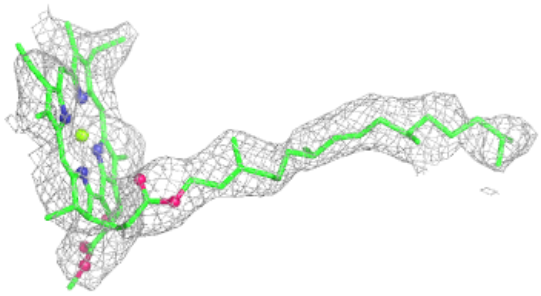


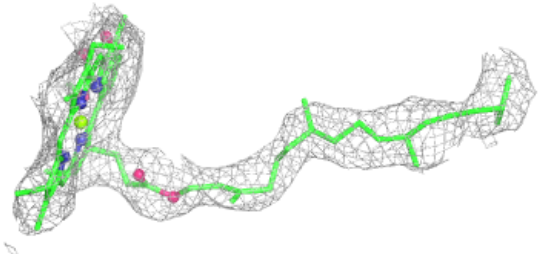


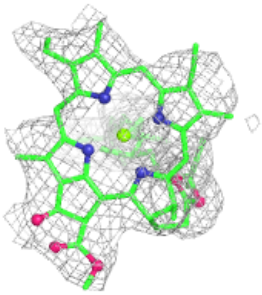


Electron density around CLA B 825:

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

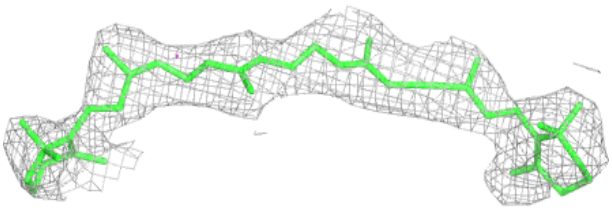


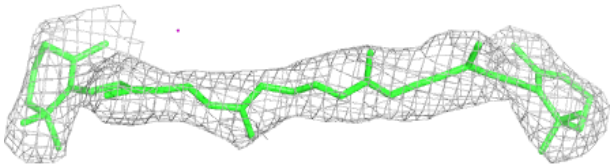


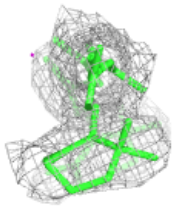


Electron density around BCR B 850:

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

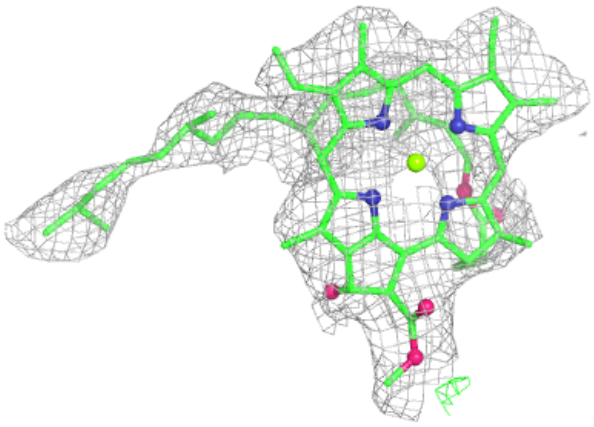


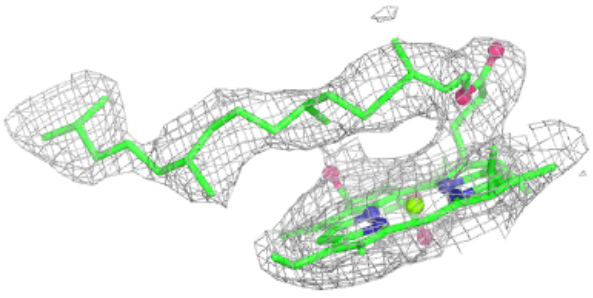




Electron density around CLA B 824:

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

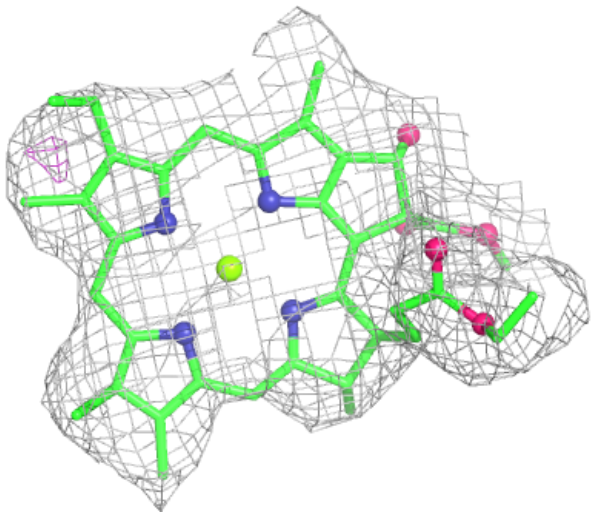


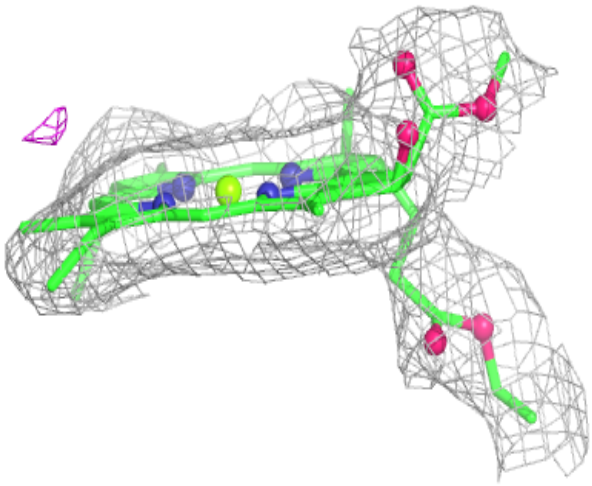


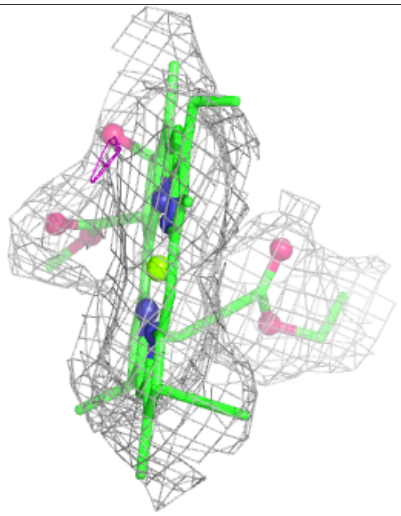


Electron density around CLA A 834:

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

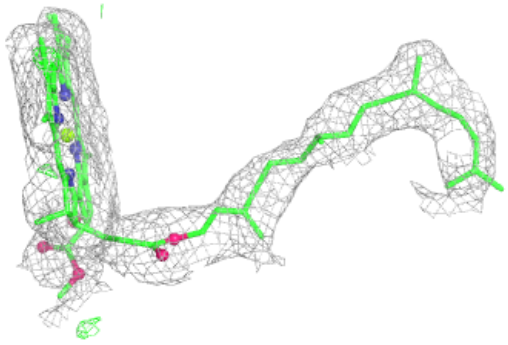


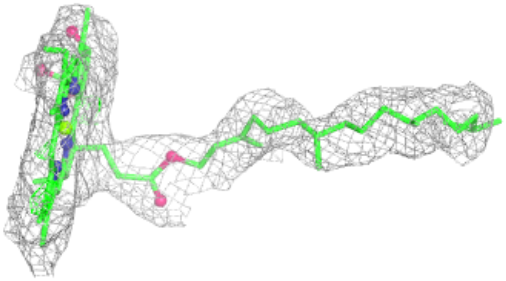


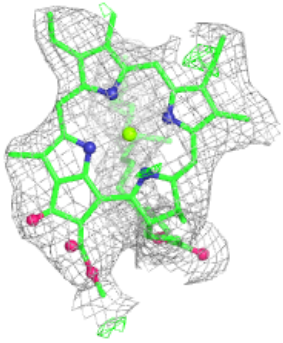


Electron density around CLA B 838:

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

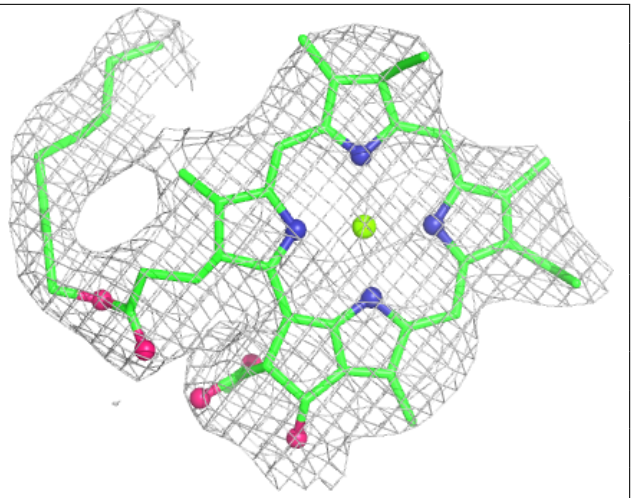


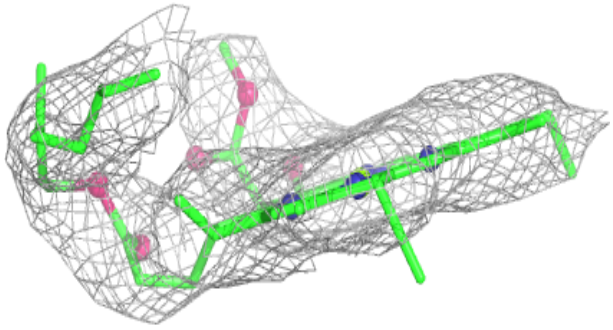


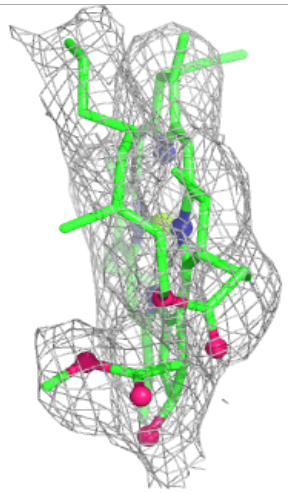


Electron density around CLA B 821:

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

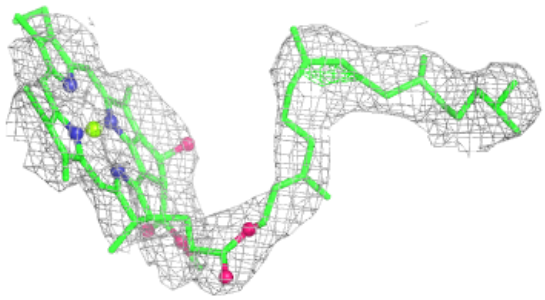


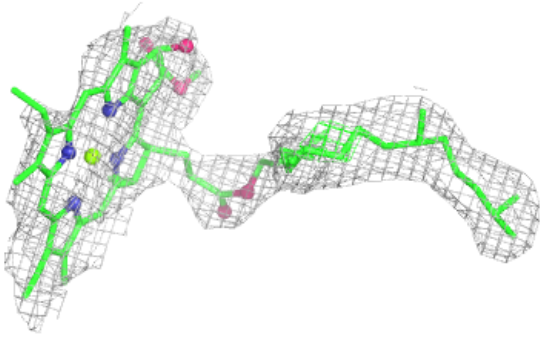


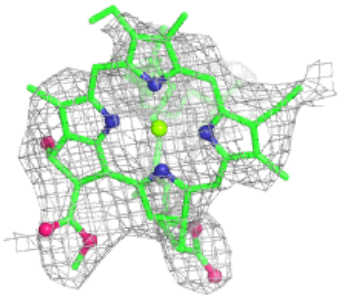


Electron density around CLA B 847:

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

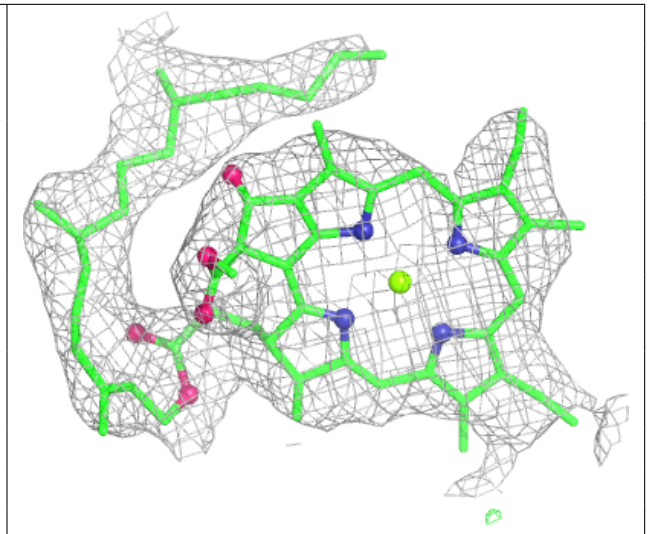


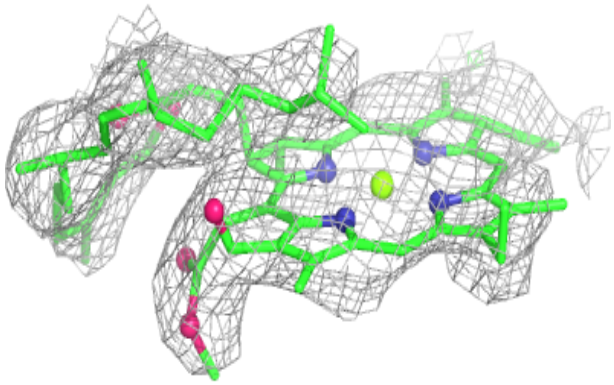


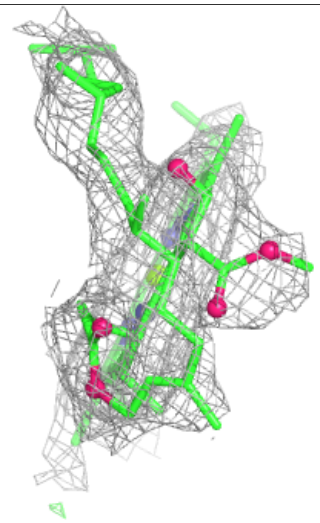


Electron density around CLA B 804:

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

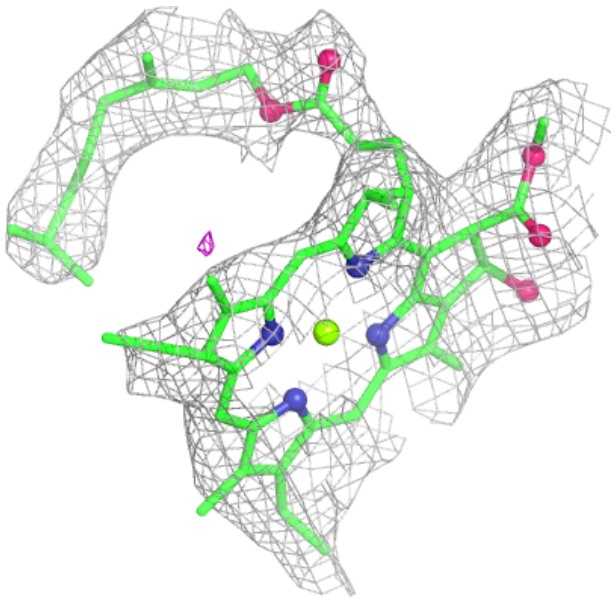


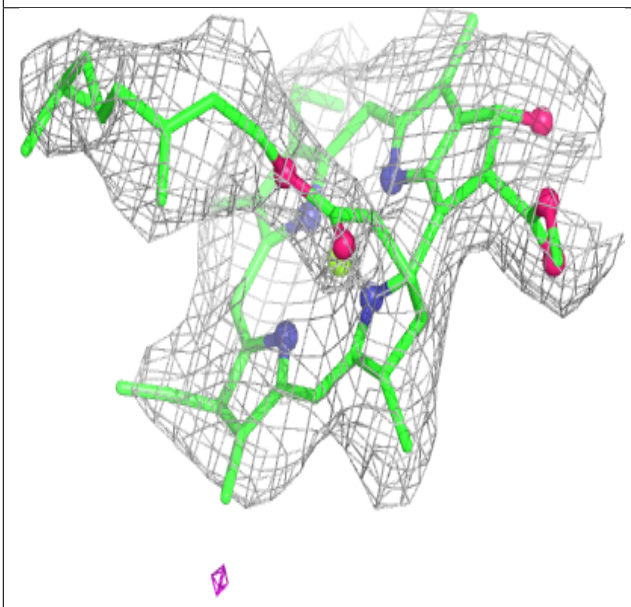


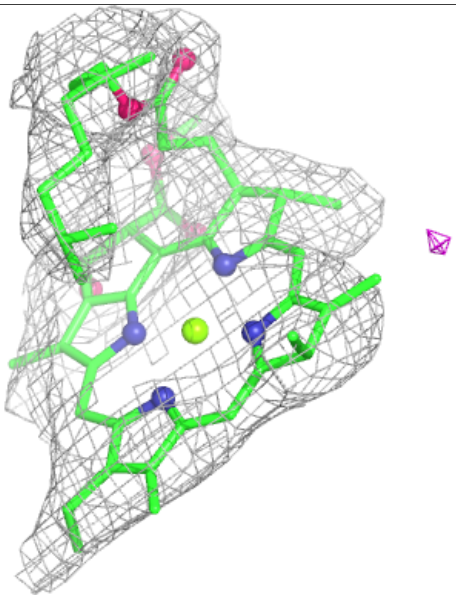


Electron density around CLA A 820:

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

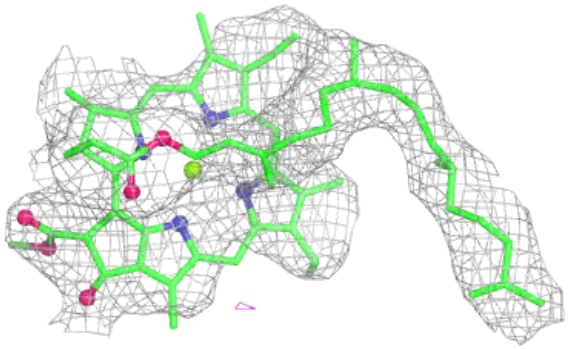


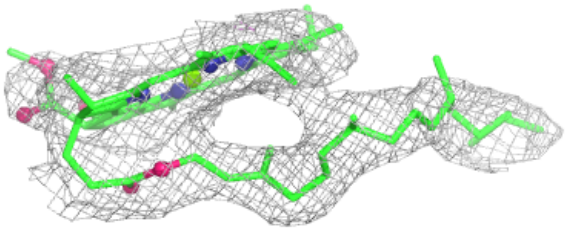


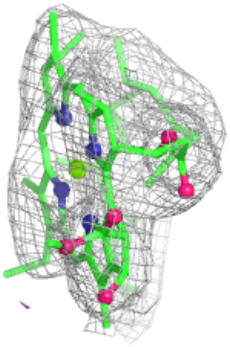


Electron density around CLA B 835:

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

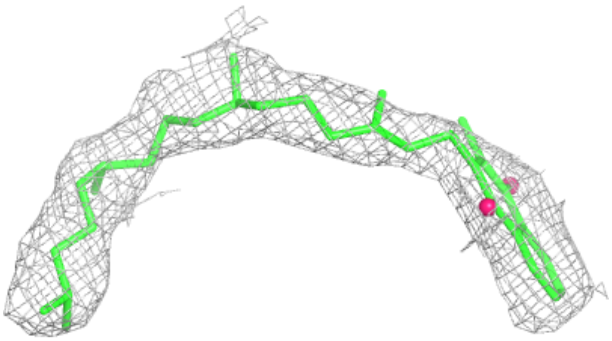


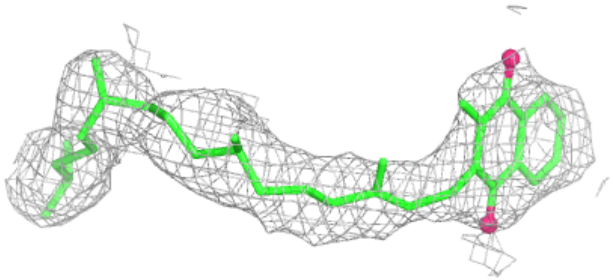




Electron density around PQN B 840:

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

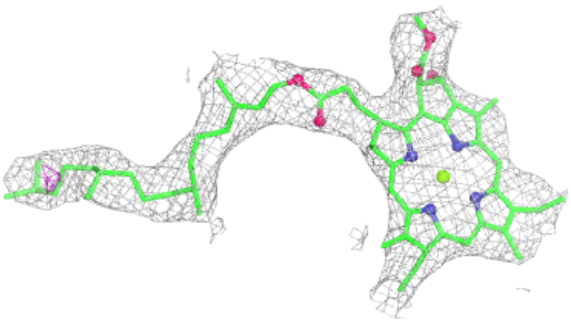


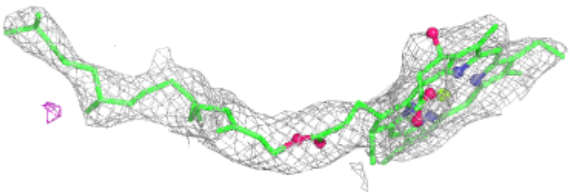


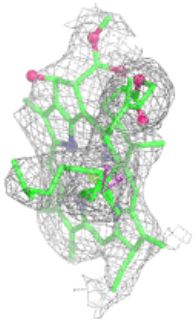


Electron density around CLA B 848:

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

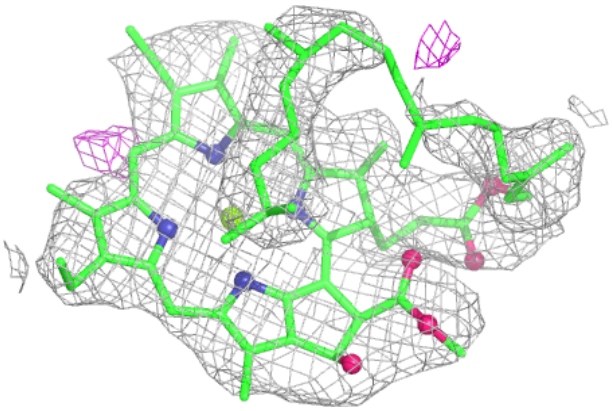


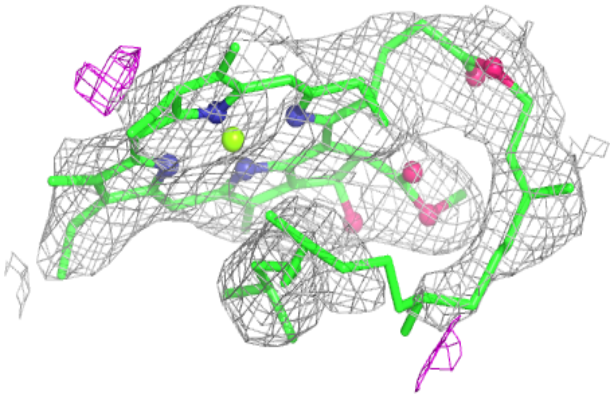


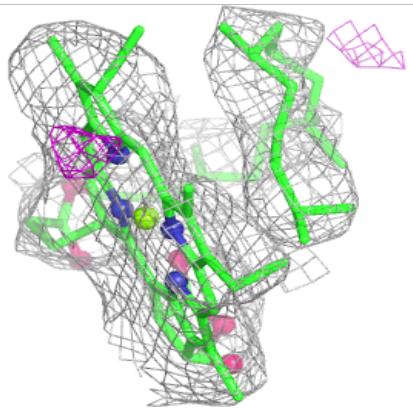


Electron density around CLA B 805:

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

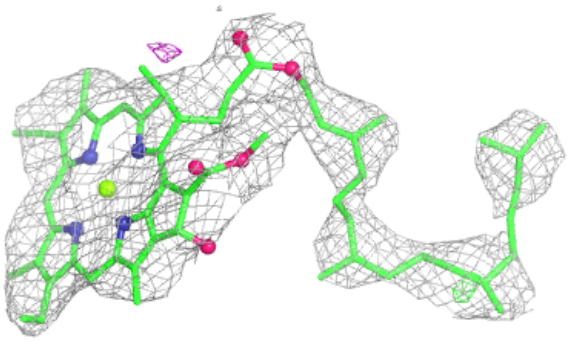


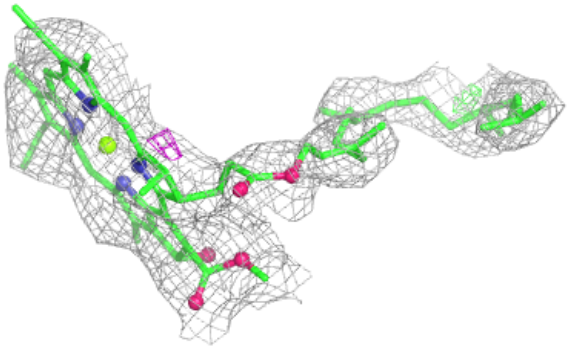


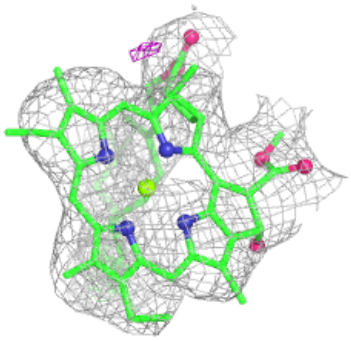


Electron density around CLA A 847:

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

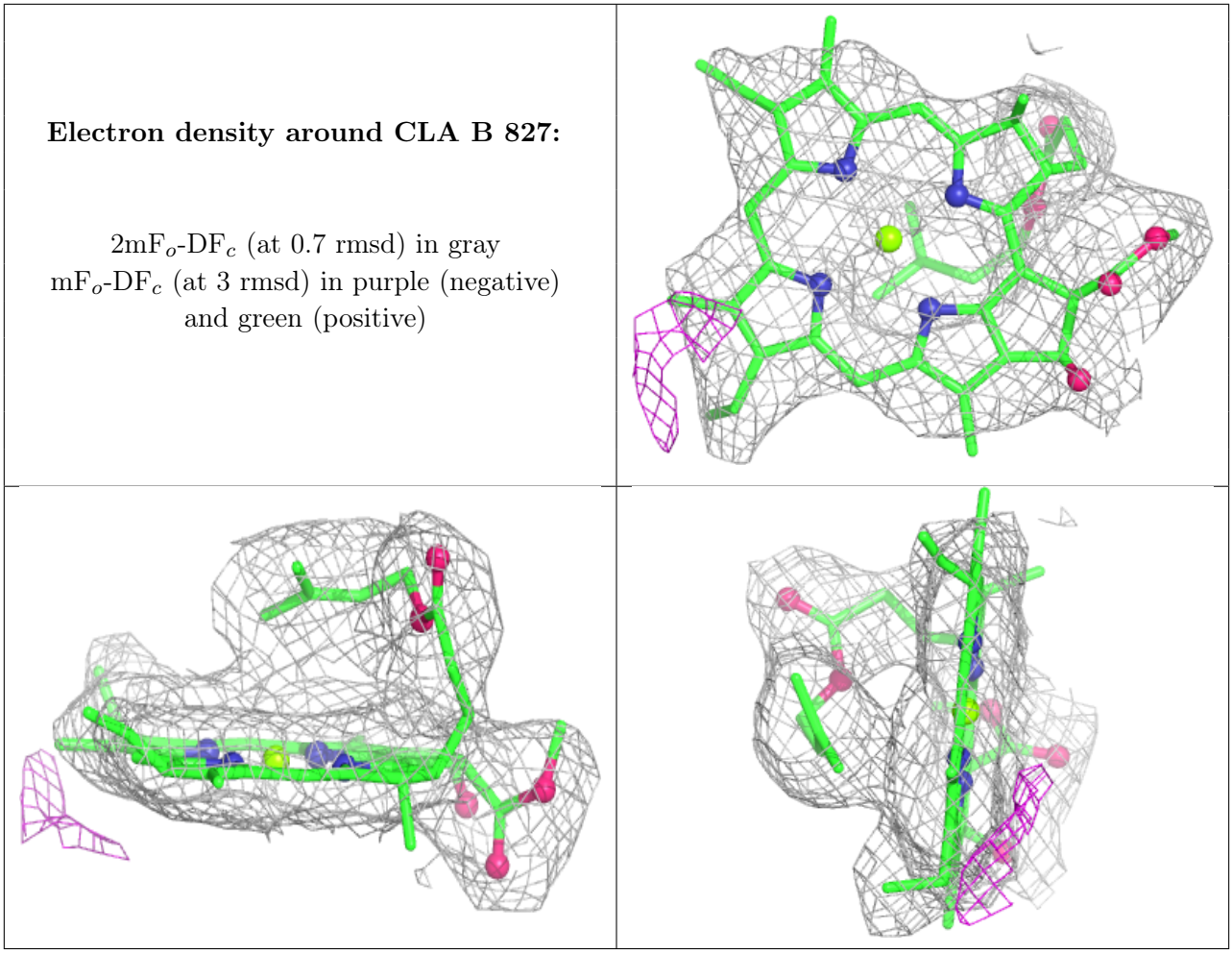






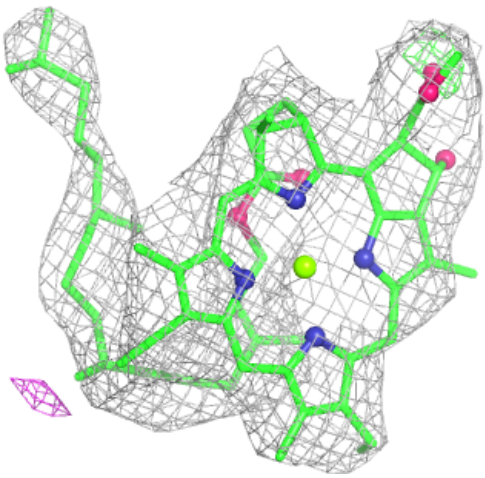
Electron density around CLA B 827:

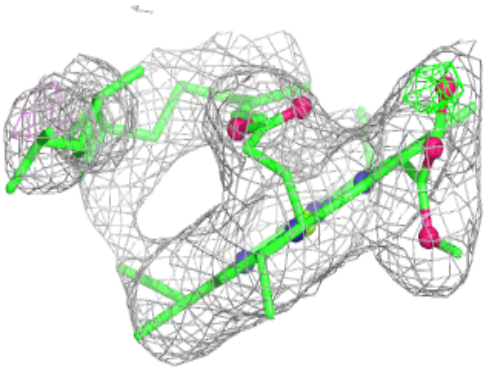
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

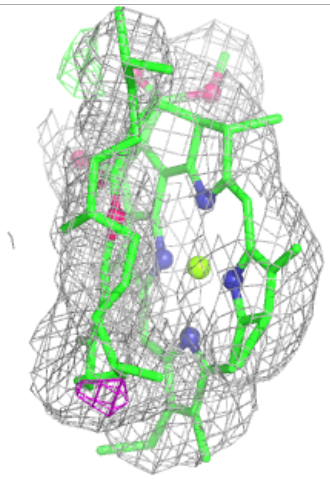


Electron density around CLA B 806:

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

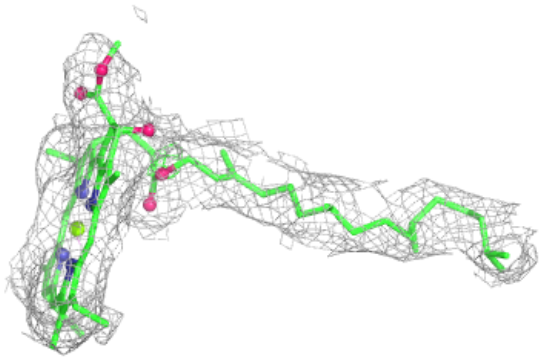


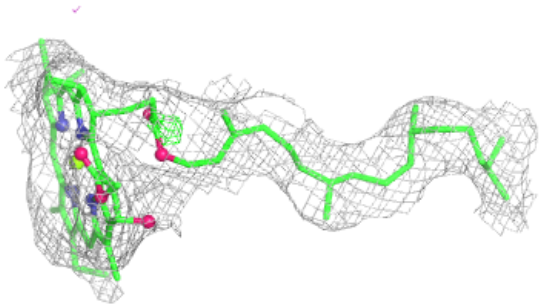


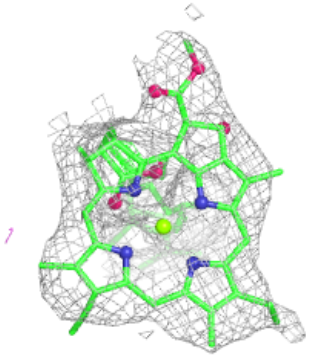


Electron density around CLA A 824:

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







5.5 Other polymers

There are no such residues in this entry.