wwPDB X-ray Structure Validation Summary Report (i)

Sep 11, 2026 – 12:25 am BST

PDB ID	:	5L8R / pdb_0000l8r
Title	:	The structure of plant photosystem I super-complex at 2.6 angstrom resolution.
Authors	:	Mazor, Y.; Borovikova, A.; Caspy, I.; Nelson, N.
Deposited on	:	2016-06-08
Resolution	:	2.60 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:

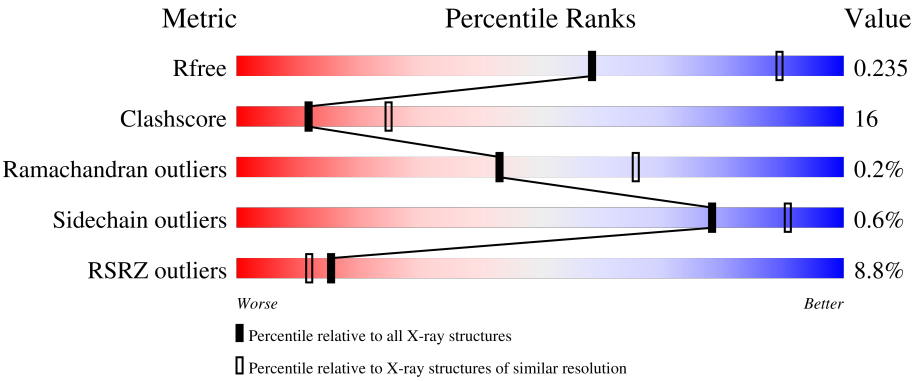
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.015 (Gargrove)
Density-Fitness	:	1.0.12
Ideal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

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.60 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	4008 (2.60-2.60)
Clashscore	190562	4347 (2.60-2.60)
Ramachandran outliers	187476	4277 (2.60-2.60)
Sidechain outliers	187428	4277 (2.60-2.60)
RSRZ outliers	180081	4008 (2.60-2.60)

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

Mol	Chain	Length	Quality of chain
1	1	193	19% 72% 28%
2	2	269	4% 55% 22% 23%
3	3	275	13% 60% 21% 20%
4	4	198	7% 74% 26%
5	A	758	6% 78% 19%

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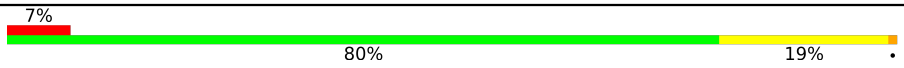
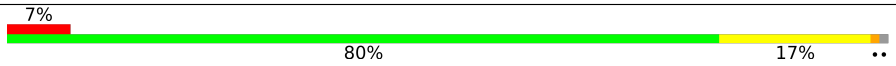
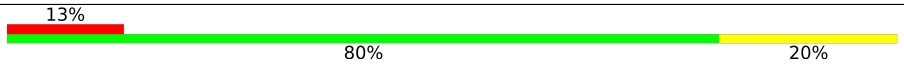
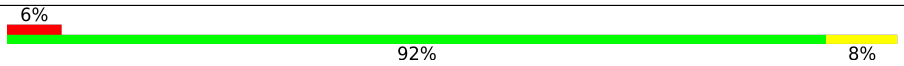
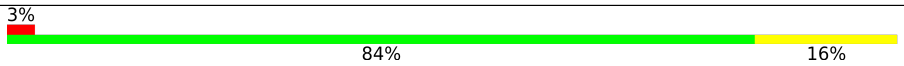
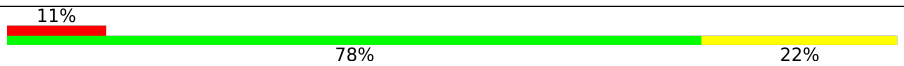
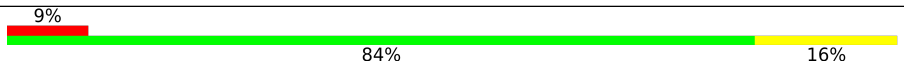
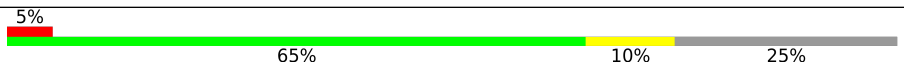
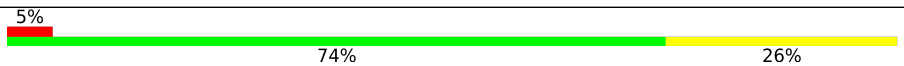
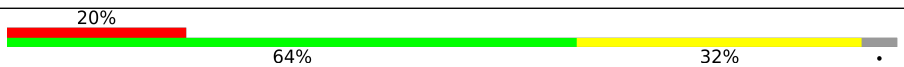
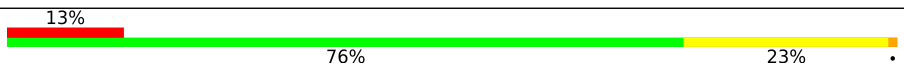
Mol	Chain	Length	Quality of chain
6	B	734	
7	C	81	
8	D	143	
9	E	66	
10	F	154	
11	G	97	
12	H	88	
13	I	40	
14	J	42	
15	K	80	
16	L	157	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
17	LUT	1	502	X	-	-	-
17	LUT	2	501	X	-	-	-
17	LUT	3	302	X	-	-	-
17	LUT	J	1109	X	-	-	-
20	CHL	1	514	X	-	-	-
20	CHL	1	521	X	-	-	-
20	CHL	2	516	X	-	-	-
20	CHL	2	526	X	-	-	-
20	CHL	4	316	X	-	-	-
23	XAT	4	303	X	-	-	-
28	SF4	C	102	-	-	X	-

2 Entry composition (i)

There are 31 unique types of molecules in this entry. The entry contains 37583 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 Lhca1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	1	193	Total	C	N	O	S	0	0	0
			1508	982	252	269	5			

- Molecule 2 is a protein called Chlorophyll a-b binding protein, chloroplastic.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	2	208	Total	C	N	O	S	0	0	0
			1620	1059	265	292	4			

- Molecule 3 is a protein called Chlorophyll a-b binding protein 3, chloroplastic.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	3	221	Total	C	N	O	S	0	0	0
			1699	1114	277	303	5			

- Molecule 4 is a protein called Chlorophyll a-b binding protein P4, chloroplastic.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	4	198	Total	C	N	O	S	0	0	0
			1559	1022	253	281	3			

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
4	89	LYS	ARG	conflict	UNP Q9SQL2
4	128	ASP	ALA	conflict	UNP Q9SQL2
4	149	PHE	SER	conflict	UNP Q9SQL2

- Molecule 5 is a protein called Photosystem I P700 chlorophyll a apoprotein A1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	A	743	Total	C	N	O	S	0	0	0
			5858	3839	998	1003	18			

There are 14 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	117	ARG	GLY	conflict	UNP P05310
A	176	ALA	GLY	conflict	UNP P05310
A	194	VAL	ALA	conflict	UNP P05310
A	220	GLY	ARG	conflict	UNP P05310
A	371	ILE	VAL	conflict	UNP P05310
A	374	HIS	GLN	conflict	UNP P05310
A	378	ALA	SER	conflict	UNP P05310
A	390	GLY	ALA	conflict	UNP P05310
A	509	THR	ALA	conflict	UNP P05310
A	522	SER	ALA	conflict	UNP P05310
A	525	GLY	ASN	conflict	UNP P05310
A	608	ALA	SER	conflict	UNP P05310
A	627	SER	THR	conflict	UNP P05310
A	639	GLY	ALA	conflict	UNP P05310

- 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
			5857	3848	998	997	14			

- Molecule 7 is a protein called Photosystem I iron-sulfur center.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	C	80	Total	C	N	O	S	0	0	0
			612	379	107	115	11			

- Molecule 8 is a protein called PsaD.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	D	143	Total	C	N	O	S	0	0	0
			1132	731	194	204	3			

- Molecule 9 is a protein called Putative uncharacterized protein.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
9	E	66	Total	C	N	O	0	0	0
			528	336	93	99			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	64	PRO	-	expression tag	UNP E1C9K6
E	65	PRO	-	expression tag	UNP E1C9K6
E	79	GLN	LYS	conflict	UNP E1C9K6
E	125	VAL	ILE	conflict	UNP E1C9K6
E	126	GLU	VAL	conflict	UNP E1C9K6
E	129	LYS	GLU	conflict	UNP E1C9K6

- Molecule 10 is a protein called Photosystem I reaction center subunit III.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	F	154	Total	C	N	O	S	0	0	0
			1213	786	210	215	2			

There are 7 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
F	80	ALA	SER	conflict	UNP A0A0M3KL12
F	87	ASP	GLU	conflict	UNP A0A0M3KL12
F	108	LEU	ILE	conflict	UNP A0A0M3KL12
F	111	PRO	ALA	conflict	UNP A0A0M3KL12
F	134	GLY	ALA	conflict	UNP A0A0M3KL12
F	188	ASP	GLU	conflict	UNP A0A0M3KL12
F	204	THR	SER	conflict	UNP A0A0M3KL12

- Molecule 11 is a protein called PsaG.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
11	G	97	Total	C	N	O	0	0	0
			757	492	125	140			

- Molecule 12 is a protein called Photosystem I reaction center subunit VI.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
12	H	88	Total	C	N	O	0	0	0
			673	442	106	125			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
H	60	LEU	ILE	conflict	UNP A0A0M3KL10
H	79	ASN	SER	conflict	UNP A0A0M3KL10
H	80	SER	PRO	conflict	UNP A0A0M3KL10
H	116	ALA	THR	conflict	UNP A0A0M3KL10
H	126	LYS	VAL	conflict	UNP A0A0M3KL10
H	134	GLN	LYS	conflict	UNP A0A0M3KL10
H	139	LEU	-	expression tag	UNP A0A0M3KL10
H	140	GLY	-	expression tag	UNP A0A0M3KL10

- 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
			232	159	37	35	1			

- 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	231	51	55	1			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
J	32	PHE	LEU	conflict	UNP D5MAL3

- Molecule 15 is a protein called Photosystem I reaction center subunit X psaK.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
15	K	77	Total	C	N	O	S	0	0	0
			515	326	86	100	3			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
K	85	ALA	VAL	conflict	UNP E1C9L3

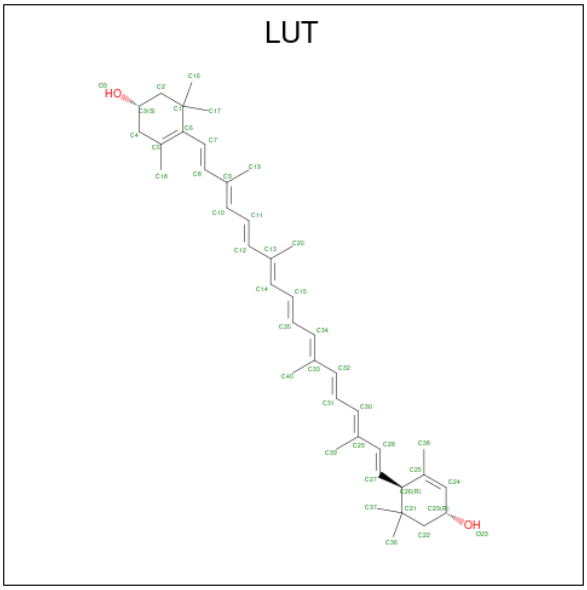
- Molecule 16 is a protein called Putative uncharacterized protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
16	L	157	Total	C	N	O	S	0	0	0
			1174	772	189	212	1			

There are 9 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
L	57	VAL	ILE	conflict	UNP E1C9L1
L	79	VAL	ILE	conflict	UNP E1C9L1
L	88	GLY	ALA	conflict	UNP E1C9L1
L	94	ASN	SER	conflict	UNP E1C9L1
L	108	PHE	TYR	conflict	UNP E1C9L1
L	143	ILE	LEU	conflict	UNP E1C9L1
L	157	ASP	ALA	conflict	UNP E1C9L1
L	172	GLN	GLU	conflict	UNP E1C9L1
L	201	PHE	TYR	conflict	UNP E1C9L1

- Molecule 17 is (3R,3'R,6S)-4,5-DIDEHYDRO-5,6-DIHYDRO-BETA,BETA-CAROTENE-3 ,3'-DIOL (CCD ID: LUT) (formula: $C_{40}H_{56}O_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
17	1	1	Total	C	O	0	0
			42	40	2		
17	1	1	Total	C	O	0	0
			42	40	2		
17	2	1	Total	C	O	0	0
			42	40	2		

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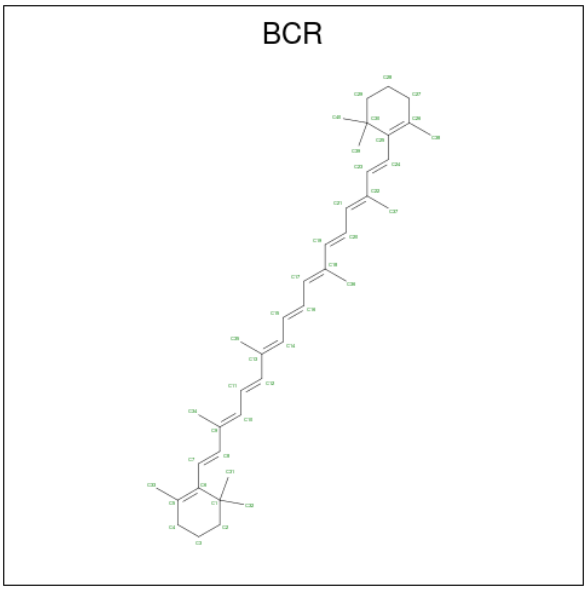
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
17	3	1	Total C O 42 40 2	0	0
17	3	1	Total C O 42 40 2	0	0
17	4	1	Total C O 42 40 2	0	0
17	J	1	Total C O 42 40 2	0	0

- Molecule 18 is BETA-CAROTENE (CCD ID: BCR) (formula: $C_{40}H_{56}$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
18	1	1	Total C 19 19	0	0
18	2	1	Total C 40 40	0	0
18	3	1	Total C 40 40	0	0
18	3	1	Total C 40 40	0	0
18	4	1	Total C 40 40	0	0
18	A	1	Total C 40 40	0	0
18	A	1	Total C 40 40	0	0

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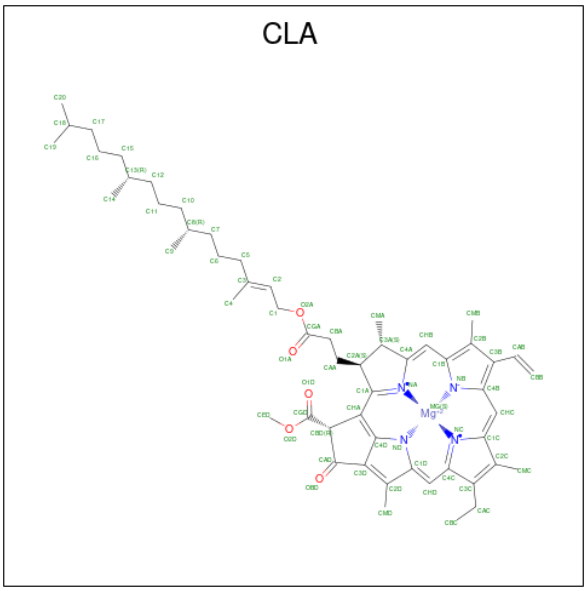
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
18	A	1	Total C 40 40	0	0
18	A	1	Total C 40 40	0	0
18	A	1	Total C 40 40	0	0
18	A	1	Total C 40 40	0	0
18	B	1	Total C 40 40	0	0
18	B	1	Total C 40 40	0	0
18	B	1	Total C 40 40	0	0
18	B	1	Total C 40 40	0	0
18	B	1	Total C 40 40	0	0
18	B	1	Total C 40 40	0	0
18	B	1	Total C 40 40	0	0
18	F	1	Total C 40 40	0	0
18	G	1	Total C 40 40	0	0
18	I	1	Total C 40 40	0	0
18	I	1	Total C 40 40	0	0
18	J	1	Total C 40 40	0	0
18	K	1	Total C 40 40	0	0
18	L	1	Total C 40 40	0	0
18	L	1	Total C 40 40	0	0
18	L	1	Total C 40 40	0	0

- Molecule 19 is CHLOROPHYLL A (CCD ID: CLA) (formula: $C_{55}H_{72}MgN_4O_5$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
19	1	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
19	1	1	Total	C	Mg	N	O	0	0
			46	36	1	4	5		
19	1	1	Total	C	Mg	N	O	0	0
			55	45	1	4	5		
19	1	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
19	1	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
19	1	1	Total	C	Mg	N	O	0	0
			50	40	1	4	5		
19	1	1	Total	C	Mg	N	O	0	0
			46	36	1	4	5		
19	1	1	Total	C	Mg	N	O	0	0
			46	36	1	4	5		
19	1	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
19	1	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
19	1	1	Total	C	Mg	N	O	0	0
			60	50	1	4	5		
19	2	1	Total	C	Mg	N	O	0	0
			60	50	1	4	5		
19	2	1	Total	C	Mg	N	O	0	0
			52	42	1	4	5		
19	2	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
19	2	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
19	2	1	Total	C	Mg	N	O	0	0
			55	45	1	4	5		
19	2	1	Total	C	Mg	N	O	0	0
			50	40	1	4	5		
19	2	1	Total	C	Mg	N	O	0	0
			60	50	1	4	5		
19	2	1	Total	C	Mg	N	O	0	0
			50	40	1	4	5		
19	2	1	Total	C	Mg	N	O	0	0
			55	45	1	4	5		
19	3	1	Total	C	Mg	N	O	0	0
			55	45	1	4	5		
19	3	1	Total	C	Mg	N	O	0	0
			52	42	1	4	5		
19	3	1	Total	C	Mg	N	O	0	0
			55	45	1	4	5		
19	3	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
19	3	1	Total	C	Mg	N	O	0	0
			55	45	1	4	5		
19	3	1	Total	C	Mg	N	O	0	0
			50	40	1	4	5		
19	3	1	Total	C	Mg	N	O	0	0
			41	33	1	4	3		
19	3	1	Total	C	Mg	N	O	0	0
			48	38	1	4	5		
19	3	1	Total	C	Mg	N	O	0	0
			60	50	1	4	5		
19	3	1	Total	C	Mg	N	O	0	0
			50	40	1	4	5		
19	3	1	Total	C	Mg	N	O	0	0
			46	36	1	4	5		
19	3	1	Total	C	Mg	N	O	0	0
			46	36	1	4	5		
19	4	1	Total	C	Mg	N	O	0	0
			60	50	1	4	5		
19	4	1	Total	C	Mg	N	O	0	0
			50	40	1	4	5		
19	4	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
19	4	1	Total	C	Mg	N	O	0	0
			60	50	1	4	5		
19	4	1	Total	C	Mg	N	O	0	0
			60	50	1	4	5		
19	4	1	Total	C	Mg	N	O	0	0
			50	40	1	4	5		
19	4	1	Total	C	Mg	N	O	0	0
			60	50	1	4	5		
19	4	1	Total	C	Mg	N	O	0	0
			46	36	1	4	5		
19	4	1	Total	C	Mg	N	O	0	0
			50	40	1	4	5		
19	4	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
19	4	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
19	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
19	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
19	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
19	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
19	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
19	A	1	Total	C	Mg	N	O	0	0
			60	50	1	4	5		
19	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
19	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
19	A	1	Total	C	Mg	N	O	0	0
			50	40	1	4	5		
19	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
19	A	1	Total	C	Mg	N	O	0	0
			55	45	1	4	5		
19	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
19	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
19	A	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
19	A	1	Total	C	Mg	N	O	0	0
			46	36	1	4	5		
19	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
19	A	1	Total	C	Mg	N	O	0	0
			56	46	1	4	5		
19	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
19	A	1	Total	C	Mg	N	O	0	0
			50	40	1	4	5		
19	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
19	A	1	Total	C	Mg	N	O	0	0
			60	50	1	4	5		
19	A	1	Total	C	Mg	N	O	0	0
			60	50	1	4	5		
19	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
19	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
19	A	1	Total	C	Mg	N	O	0	0
			55	45	1	4	5		
19	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
19	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
19	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
19	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
19	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
19	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
19	A	1	Total	C	Mg	N	O	0	0
			55	45	1	4	5		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
19	A	1	Total	C	Mg	N	O	0	0
			51	41	1	4	5		
19	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
19	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
19	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
19	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
19	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
19	A	1	Total	C	Mg	N	O	0	0
			60	50	1	4	5		
19	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
19	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
19	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
19	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
19	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
19	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
19	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
19	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
19	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
19	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
19	B	1	Total	C	Mg	N	O	0	0
			60	50	1	4	5		
19	B	1	Total	C	Mg	N	O	0	0
			46	36	1	4	5		
19	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
19	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
19	B	1	Total	C	Mg	N	O	0	0
			55	45	1	4	5		
19	B	1	Total	C	Mg	N	O	0	0
			60	50	1	4	5		
19	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
19	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
19	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
19	B	1	Total	C	Mg	N	O	0	0
			46	36	1	4	5		
19	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
19	B	1	Total	C	Mg	N	O	0	0
			55	45	1	4	5		
19	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
19	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
19	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
19	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
19	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
19	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
19	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
19	B	1	Total	C	Mg	N	O	0	0
			60	50	1	4	5		
19	B	1	Total	C	Mg	N	O	0	0
			58	48	1	4	5		
19	B	1	Total	C	Mg	N	O	0	0
			60	50	1	4	5		
19	B	1	Total	C	Mg	N	O	0	0
			55	45	1	4	5		
19	B	1	Total	C	Mg	N	O	0	0
			55	45	1	4	5		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
19	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
19	B	1	Total	C	Mg	N	O	0	0
			50	40	1	4	5		
19	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
19	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
19	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
19	F	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
19	F	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
19	G	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
19	G	1	Total	C	Mg	N	O	0	0
			55	45	1	4	5		
19	G	1	Total	C	Mg	N	O	0	0
			46	36	1	4	5		
19	G	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
19	H	1	Total	C	Mg	N	O	0	0
			60	50	1	4	5		
19	J	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
19	J	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
19	J	1	Total	C	Mg	N	O	0	0
			50	40	1	4	5		
19	K	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
19	K	1	Total	C	Mg	N	O	0	0
			60	50	1	4	5		
19	K	1	Total	C	Mg	N		0	0
			27	22	1	4			
19	K	1	Total	C	Mg	N		0	0
			27	22	1	4			
19	L	1	Total	C	Mg	N	O	0	0
			55	45	1	4	5		
19	L	1	Total	C	Mg	N	O	0	0
			50	40	1	4	5		

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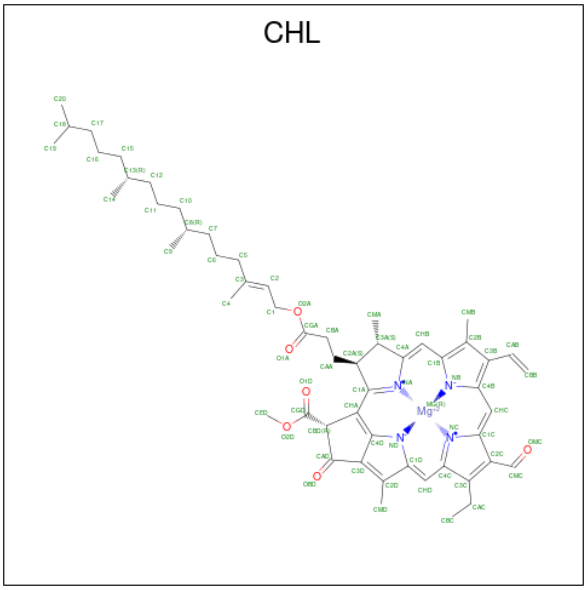
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
19	L	1	Total	C	Mg	N	O	0	0
			60	50	1	4	5		
19	L	1	Total	C	Mg	N	O	0	0
			50	40	1	4	5		

- Molecule 20 is CHLOROPHYLL B (CCD ID: CHL) (formula: $C_{55}H_{70}MgN_4O_6$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
20	1	1	Total	C	Mg	N	O	0	0
			47	36	1	4	6		
20	1	1	Total	C	Mg	N	O	0	0
			61	50	1	4	6		
20	1	1	Total	C	Mg	N	O	0	0
			56	45	1	4	6		
20	2	1	Total	C	Mg	N	O	0	0
			47	36	1	4	6		
20	2	1	Total	C	Mg	N	O	0	0
			48	37	1	4	6		
20	2	1	Total	C	Mg	N	O	0	0
			46	35	1	4	6		
20	2	1	Total	C	Mg	N	O	0	0
			56	45	1	4	6		
20	2	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		
20	3	1	Total	C	Mg	N	O	0	0
			47	36	1	4	6		

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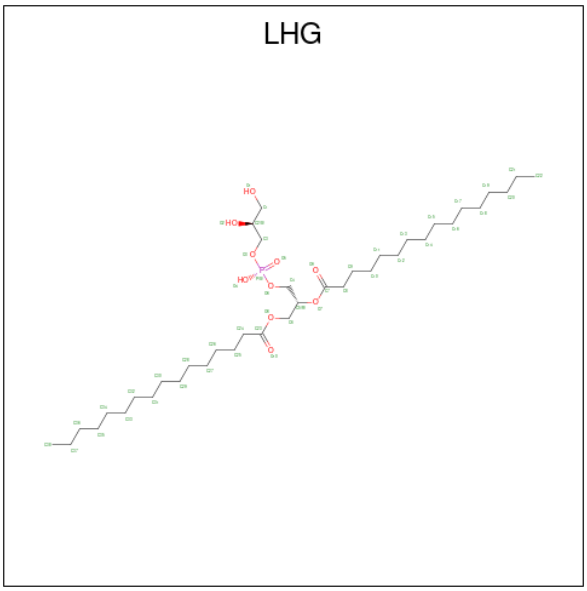
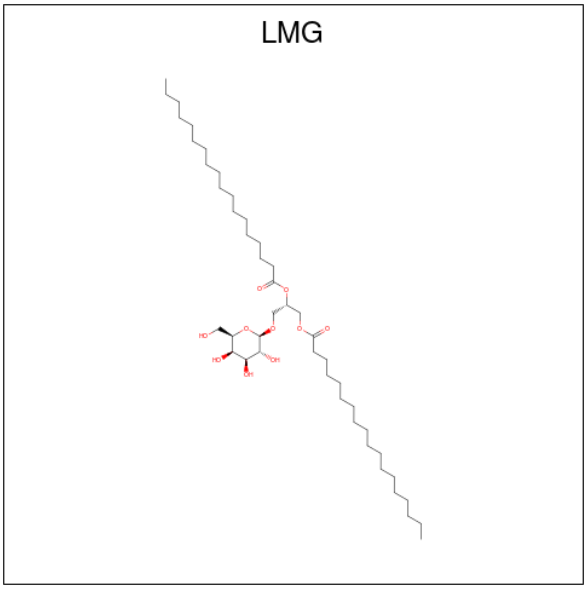
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
20	4	1	Total	C	Mg	N	O	0	0
			47	36	1	4	6		
20	4	1	Total	C	Mg	N	O	0	0
			51	40	1	4	6		
20	4	1	Total	C	Mg	N	O	0	0
			61	50	1	4	6		
20	4	1	Total	C	Mg	N	O	0	0
			43	34	1	4	4		

- Molecule 21 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (CCD ID: LHG) (formula: $C_{38}H_{75}O_{10}P$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
21	1	1	Total	C	O	P	0	0
			49	38	10	1		
21	1	1	Total	C	O	P	0	0
			42	31	10	1		
21	2	1	Total	C	O	P	0	0
			35	24	10	1		
21	A	1	Total	C	O	P	0	0
			40	29	10	1		
21	A	1	Total	C	O	P	0	0
			49	38	10	1		
21	B	1	Total	C	O	P	0	0
			21	10	10	1		
21	B	1	Total	C	O	P	0	0
			49	38	10	1		

- Molecule 22 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (CCD ID: LMG) (formula: $C_{45}H_{86}O_{10}$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
22	1	1	Total C O 46 36 10	0	0
22	1	1	Total C O 13 7 6	0	0
22	2	1	Total C O 25 15 10	0	0
22	2	1	Total C O 36 26 10	0	0
22	2	1	Total C O 13 7 6	0	0
22	2	1	Total C O 13 7 6	0	0
22	2	1	Total C O 13 7 6	0	0
22	2	1	Total C O 13 7 6	0	0
22	2	1	Total C O 13 7 6	0	0
22	4	1	Total C O 13 7 6	0	0
22	4	1	Total C O 45 35 10	0	0
22	A	1	Total C O 50 40 10	0	0

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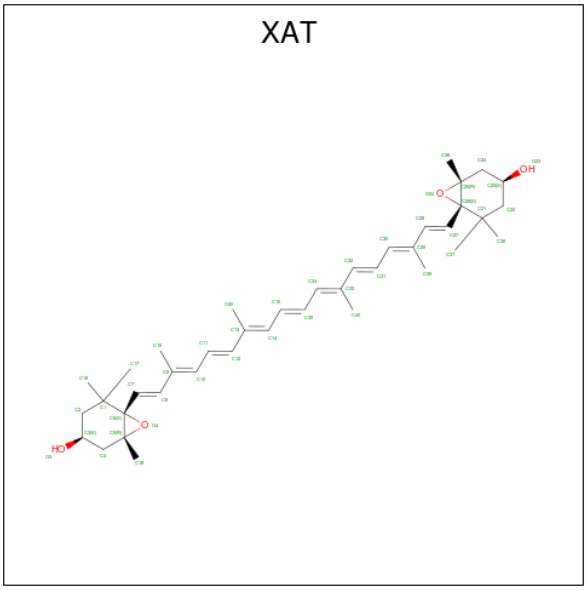
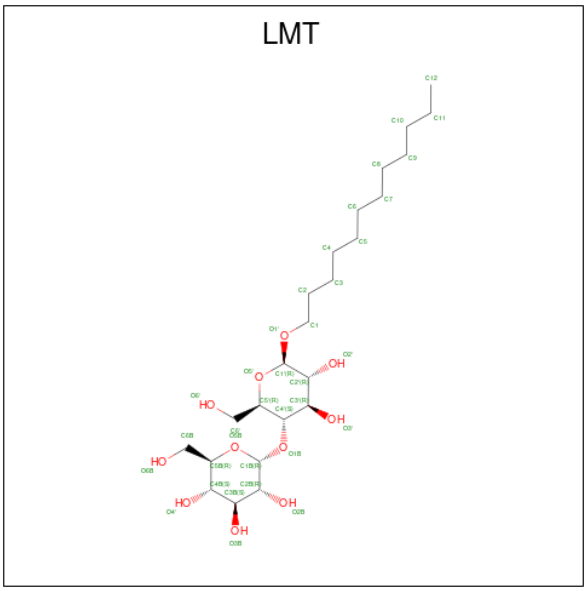
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
22	B	1	Total C O 35 25 10	0	0
22	B	1	Total C O 33 23 10	0	0
22	F	1	Total C O 47 37 10	0	0
22	F	1	Total C O 36 26 10	0	0
22	G	1	Total C O 50 40 10	0	0
22	G	1	Total C O 25 15 10	0	0
22	J	1	Total C O 30 20 10	0	0
22	J	1	Total C O 34 24 10	0	0

- Molecule 23 is (3S,5R,6S,3'S,5'R,6'S)-5,6,5',6'-DIEPOXY-5,6,5',6'- TETRAHYDRO-BETA ,BETA-CAROTENE-3,3'-DIOL (CCD ID: XAT) (formula: $C_{40}H_{56}O_4$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
23	2	1	Total C O 44 40 4	0	0
23	4	1	Total C O 44 40 4	0	0

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

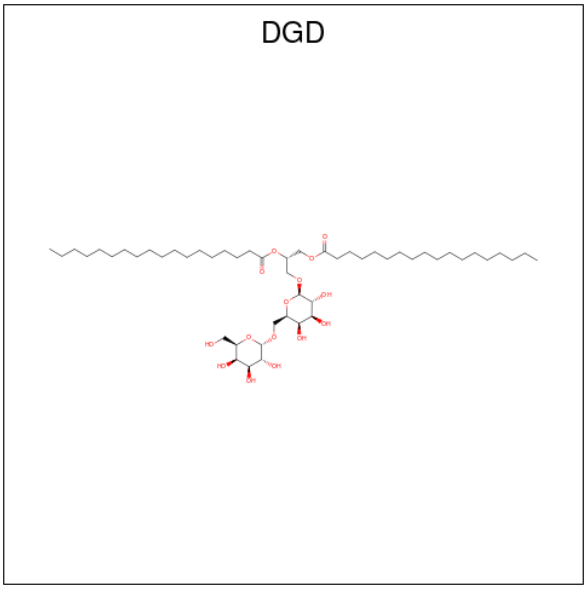


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
24	2	1	Total C O 35 24 11	0	0
24	3	1	Total C O 31 20 11	0	0
24	4	1	Total C O 35 24 11	0	0
24	A	1	Total C O 35 24 11	0	0
24	B	1	Total C O 35 24 11	0	0
24	B	1	Total C O 32 21 11	0	0
24	B	1	Total C O 31 20 11	0	0
24	G	1	Total C O 35 24 11	0	0
24	G	1	Total C O 31 20 11	0	0
24	J	1	Total C O 25 14 11	0	0

- Molecule 25 is CALCIUM ION (CCD ID: CA) (formula: Ca).

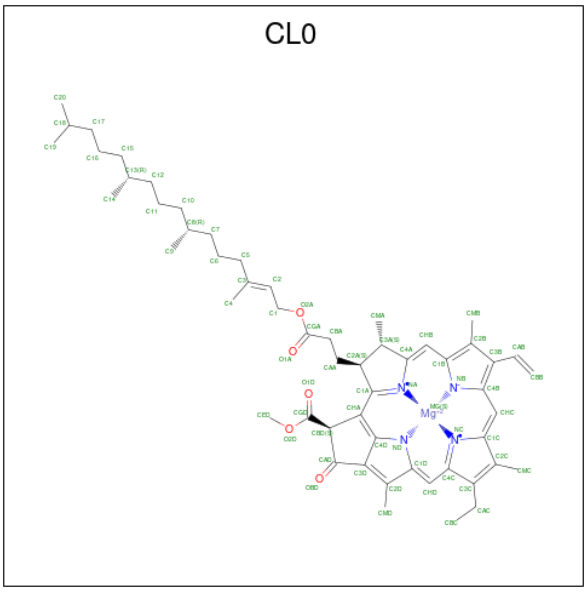
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
25	3	1	Total Ca 1 1	0	0
25	B	1	Total Ca 1 1	0	0

- Molecule 26 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (CCD ID: DGD) (formula: $C_{51}H_{96}O_{15}$).



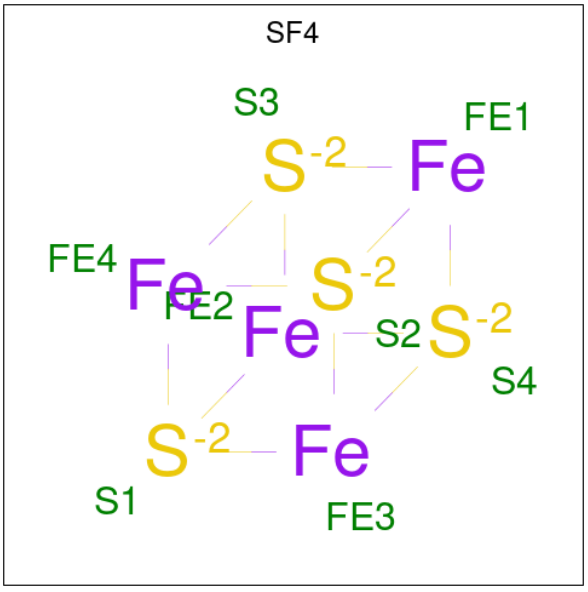
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
26	4	1	Total C O 51 36 15	0	0
26	B	1	Total C O 41 26 15	0	0
26	B	1	Total C O 61 46 15	0	0
26	G	1	Total C O 47 32 15	0	0
26	J	1	Total C O 58 43 15	0	0

- Molecule 27 is CHLOROPHYLL A ISOMER (CCD ID: CL0) (formula: $C_{55}H_{72}MgN_4O_5$).



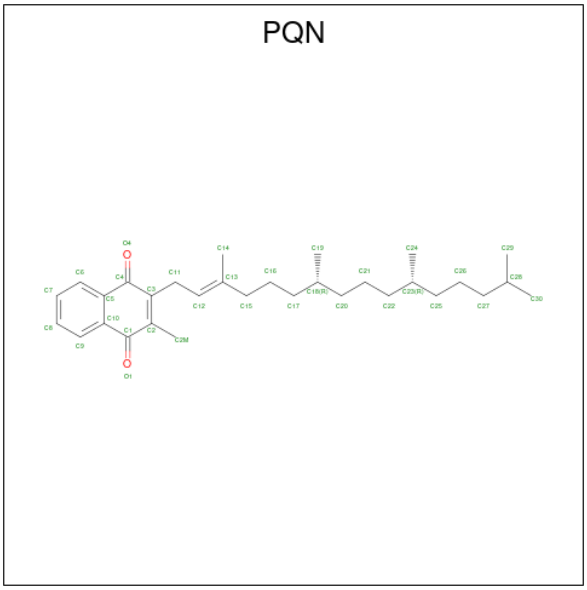
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
27	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		

- Molecule 28 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe_4S_4).



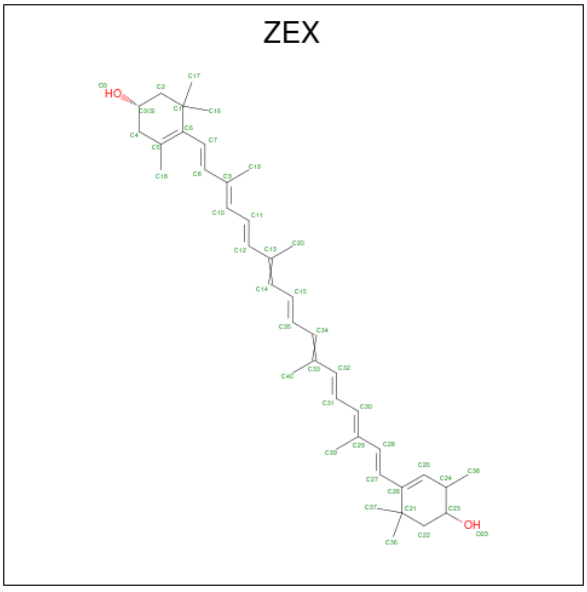
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
28	A	1	Total	Fe	S		0	0
			8	4	4			
28	C	1	Total	Fe	S		0	0
			8	4	4			
28	C	1	Total	Fe	S		0	0
			8	4	4			

- Molecule 29 is PHYLLOQUINONE (CCD ID: PQN) (formula: $C_{31}H_{46}O_2$).



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

- Molecule 30 is (1R,2S)-4-{(1E,3E,5E,7E,9E,11E,13E,15E,17E)-18-[(4S)-4-hydroxy-2,6,6-trimethylcyclohex-1-en-1-yl]-3,7,12,16-tetramethyloctadeca-1,3,5,7,9,11,13,15,17-nonaen-1-yl}-2,5,5-trimethylcyclohex-3-en-1-ol (CCD ID: ZEX) (formula: $C_{40}H_{56}O_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
30	F	1	Total	C	O	0	0
			42	40	2		

- Molecule 31 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
31	2	7	Total	O	0	0
			7	7		
31	3	3	Total	O	0	0
			3	3		
31	4	13	Total	O	0	0
			13	13		
31	A	49	Total	O	0	0
			49	49		
31	B	73	Total	O	0	0
			73	73		
31	C	19	Total	O	0	0
			19	19		
31	D	14	Total	O	0	0
			14	14		
31	E	10	Total	O	0	0
			10	10		
31	F	9	Total	O	0	0
			9	9		
31	G	3	Total	O	0	0
			3	3		
31	H	1	Total	O	0	0
			1	1		
31	J	4	Total	O	0	0
			4	4		
31	L	4	Total	O	0	0
			4	4		

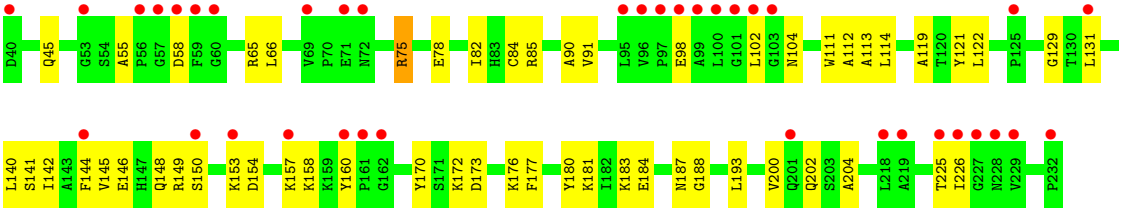
3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: Lhca1

Chain 1:

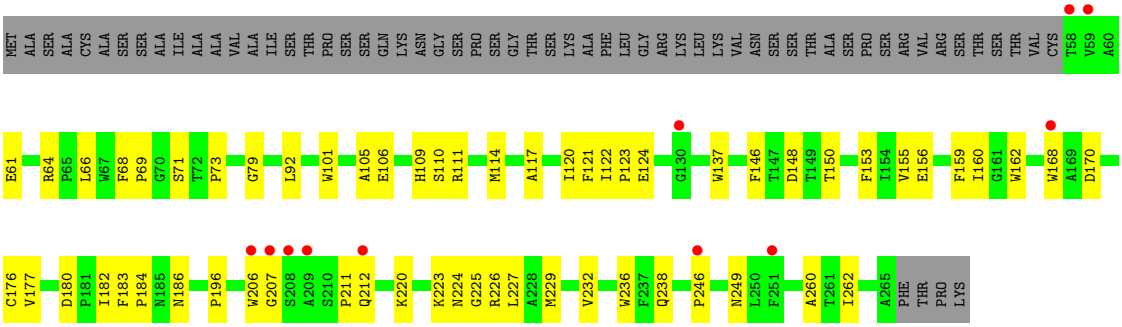




• Molecule 2: Chlorophyll a-b binding protein, chloroplastic

Chain 2:

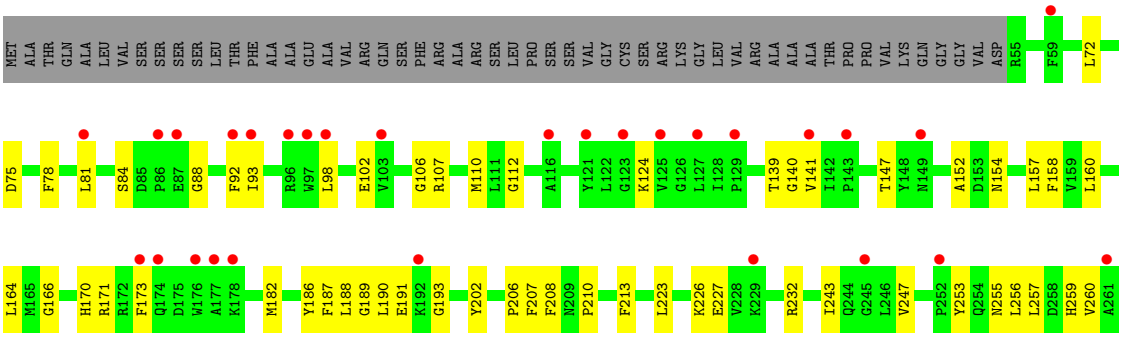


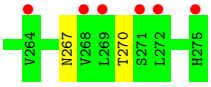


• Molecule 3: Chlorophyll a-b binding protein 3, chloroplastic

Chain 3:



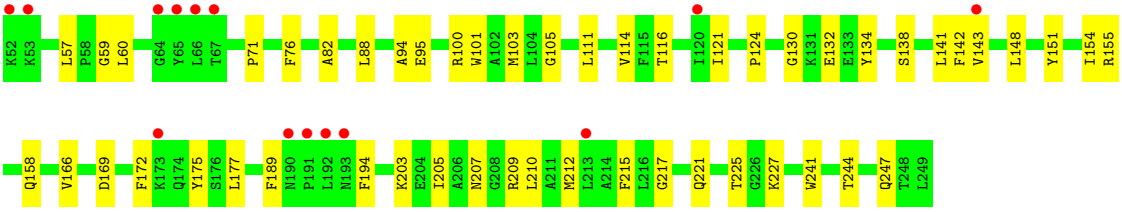




• Molecule 4: Chlorophyll a-b binding protein P4, chloroplastic

Chain 4:

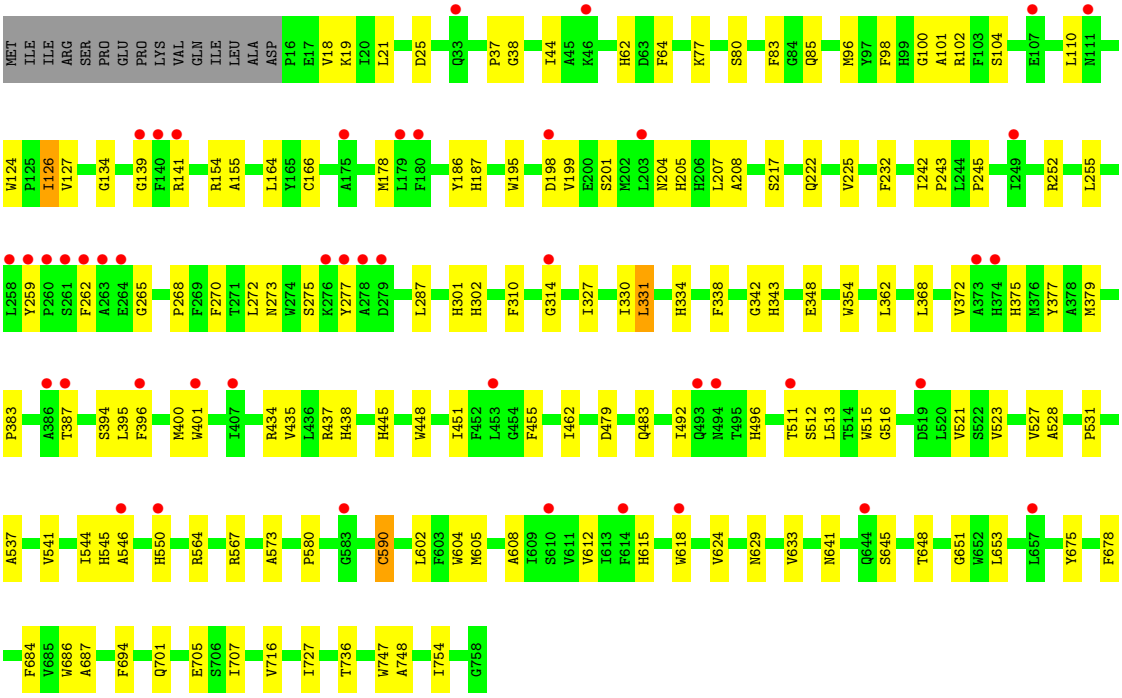




• Molecule 5: Photosystem I P700 chlorophyll a apoprotein A1

Chain A:

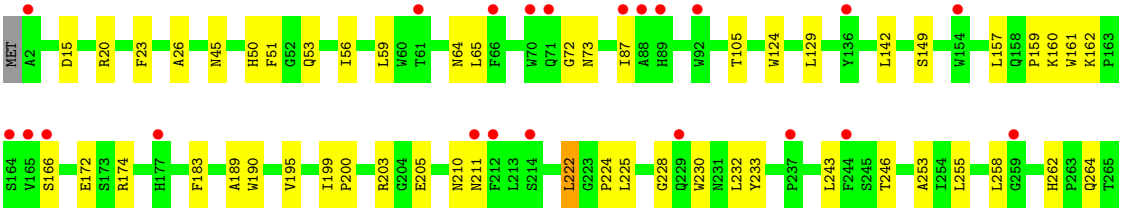


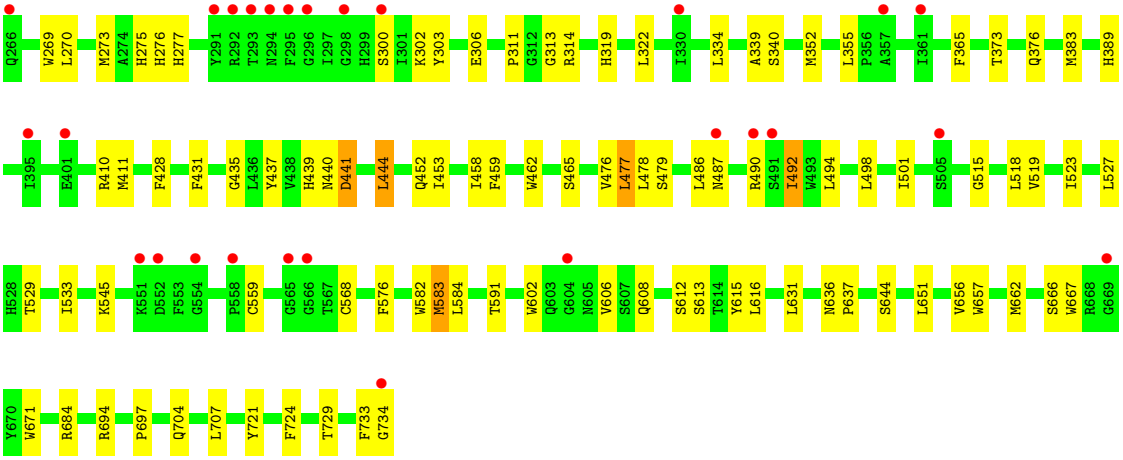


• Molecule 6: Photosystem I P700 chlorophyll a apoprotein A2

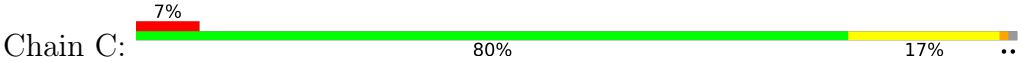
Chain B:

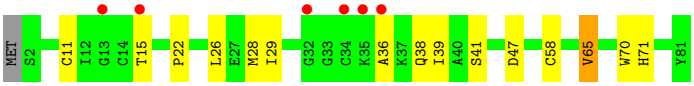




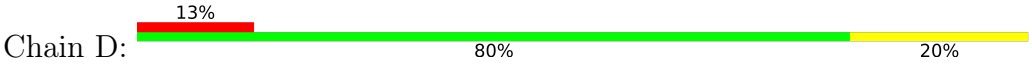


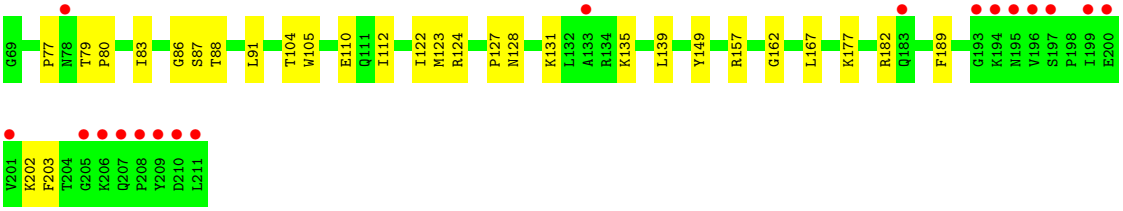
• Molecule 7: Photosystem I iron-sulfur center



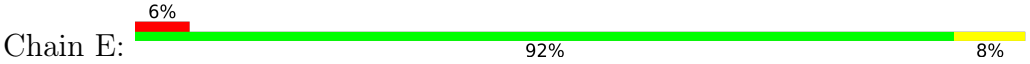


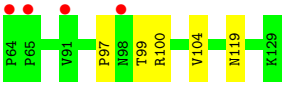
• Molecule 8: PsaD



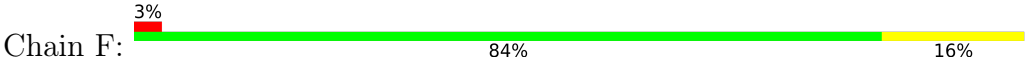


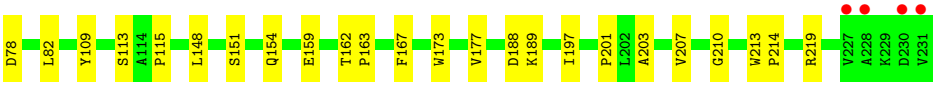
• Molecule 9: Putative uncharacterized protein



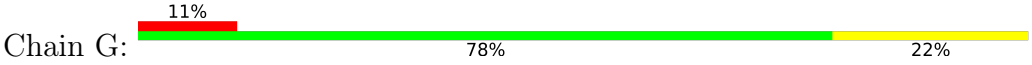


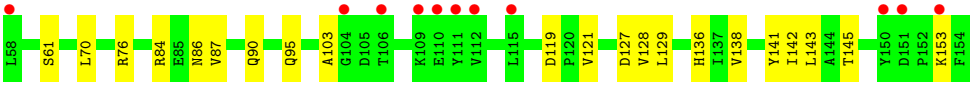
• Molecule 10: Photosystem I reaction center subunit III



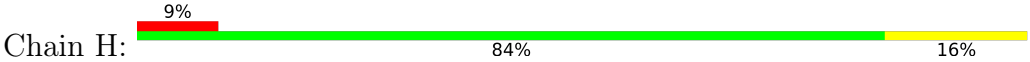


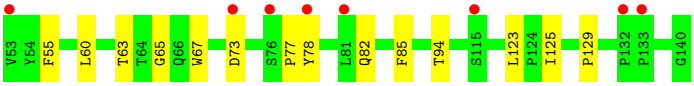
• Molecule 11: PsaG





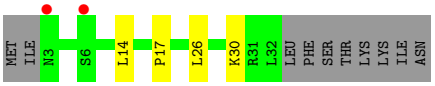
• Molecule 12: Photosystem I reaction center subunit VI





• Molecule 13: Photosystem I reaction center subunit VIII





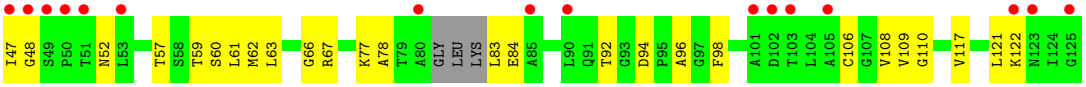
• Molecule 14: Photosystem I reaction center subunit IX



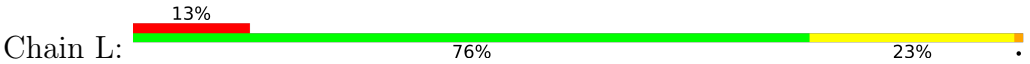


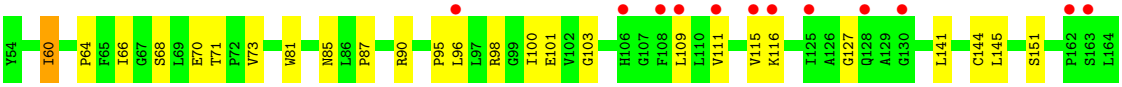
• Molecule 15: Photosystem I reaction center subunit X psaK

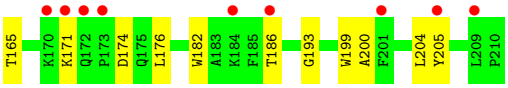




• Molecule 16: Putative uncharacterized protein







4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	189.61Å 200.99Å 212.94Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	39.91 – 2.60 39.91 – 2.60	Depositor EDS
% Data completeness (in resolution range)	99.7 (39.91-2.60) 93.4 (39.91-2.60)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.54 (at 2.61Å)	Xtriage
Refinement program	PHENIX (1.10.1_2155: ???)	Depositor
R, R_{free}	0.210 , 0.232 0.213 , 0.235	Depositor DCC
R_{free} test set	4925 reflections (1.73%)	wwPDB-VP
Wilson B-factor (Å^2)	60.7	Xtriage
Anisotropy	0.292	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.24 , 51.1	EDS
L-test for twinning[2]	$< \|L\| > = 0.45$, $< L^2 > = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	37583	wwPDB-VP
Average B, all atoms (Å^2)	100.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.75% 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.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: LMG, CA, ZEX, CLA, SF4, PQN, BCR, CHL, CL0, XAT, LHG, DGD, LMT, LUT

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| > 5$	RMSZ	$\#\|Z\| > 5$
1	1	0.15	0/1558	0.32	0/2125
2	2	0.16	0/1679	0.35	0/2302
3	3	0.15	0/1753	0.34	0/2382
4	4	0.17	0/1608	0.33	0/2191
5	A	0.17	0/6057	0.37	0/8264
6	B	0.18	0/6069	0.37	0/8286
7	C	0.21	0/625	0.44	0/846
8	D	0.18	0/1163	0.43	0/1572
9	E	0.13	0/540	0.36	0/734
10	F	0.17	0/1241	0.36	0/1679
11	G	0.12	0/776	0.31	0/1054
12	H	0.15	0/693	0.36	0/942
13	I	0.14	0/238	0.32	0/324
14	J	0.25	0/349	0.40	0/476
15	K	0.12	0/520	0.30	0/707
16	L	0.14	0/1207	0.33	0/1651
All	All	0.17	0/26076	0.36	0/35535

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	1	1508	0	1489	56	0
2	2	1620	0	1557	56	0
3	3	1699	0	1648	65	0
4	4	1559	0	1527	51	0
5	A	5858	0	5719	145	0
6	B	5857	0	5653	135	0
7	C	612	0	592	11	0
8	D	1132	0	1141	21	0
9	E	528	0	528	3	0
10	F	1213	0	1241	19	0
11	G	757	0	743	21	0
12	H	673	0	667	13	0
13	I	232	0	253	2	0
14	J	338	0	345	16	0
15	K	515	0	513	23	0
16	L	1174	0	1183	34	0
17	1	84	0	110	11	0
17	2	42	0	55	7	0
17	3	84	0	110	20	0
17	4	42	0	55	3	0
17	J	42	0	55	8	0
18	1	19	0	24	4	0
18	2	40	0	55	11	0
18	3	80	0	109	12	0
18	4	40	0	55	9	0
18	A	240	0	329	20	0
18	B	280	0	384	27	0
18	F	40	0	55	1	0
18	G	40	0	55	3	0
18	I	80	0	110	11	0
18	J	40	0	55	4	0
18	K	40	0	55	7	0
18	L	120	0	165	6	0
19	1	608	0	563	50	0
19	2	512	0	479	32	0
19	3	623	0	526	59	0
19	4	631	0	599	53	0
19	A	2653	0	2772	218	0
19	B	2350	0	2461	178	0
19	F	130	0	144	10	0
19	G	231	0	225	24	0
19	H	60	0	59	2	0
19	J	160	0	143	23	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
19	K	159	0	96	10	0
19	L	215	0	185	8	0
20	1	164	0	134	20	0
20	2	263	0	210	30	0
20	3	47	0	30	9	0
20	4	202	0	150	18	0
21	1	91	0	131	18	0
21	2	35	0	40	9	0
21	A	89	0	127	9	0
21	B	70	0	86	8	0
22	1	59	0	76	4	0
22	2	126	0	117	10	0
22	4	58	0	71	4	0
22	A	50	0	73	4	0
22	B	68	0	76	6	0
22	F	83	0	109	10	0
22	G	75	0	90	6	0
22	J	64	0	68	3	0
23	2	44	0	56	4	0
23	4	44	0	56	9	0
24	2	35	0	46	0	0
24	3	31	0	34	2	0
24	4	35	0	45	2	0
24	A	35	0	46	3	0
24	B	98	0	114	8	0
24	G	66	0	80	5	0
24	J	25	0	23	1	0
25	3	1	0	0	0	0
25	B	1	0	0	0	0
26	4	51	0	60	6	0
26	B	102	0	123	14	0
26	G	47	0	52	1	0
26	J	58	0	77	6	0
27	A	65	0	72	6	0
28	A	8	0	0	1	0
28	C	16	0	0	2	0
29	A	33	0	46	3	0
29	B	33	0	46	8	0
30	F	42	0	56	5	0
31	2	7	0	0	0	0
31	3	3	0	0	0	0
31	4	13	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
31	A	49	0	0	1	0
31	B	73	0	0	2	0
31	C	19	0	0	0	0
31	D	14	0	0	0	0
31	E	10	0	0	0	0
31	F	9	0	0	2	0
31	G	3	0	0	1	0
31	H	1	0	0	0	0
31	J	4	0	0	0	0
31	L	4	0	0	1	0
All	All	37583	0	37507	1186	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 16.

The worst 5 of 1186 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:4:302:LUT:H373	19:4:304:CLA:H11	1.35	1.07
19:A:832:CLA:HBB1	19:A:833:CLA:H2	1.48	0.95
17:3:301:LUT:H32	19:3:305:CLA:HBB1	1.45	0.94
19:J:1105:CLA:HHC	19:J:1105:CLA:HBB1	1.55	0.86
5:A:379:MET:HE1	19:A:827:CLA:HAB	1.59	0.84

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	1	191/193 (99%)	184 (96%)	6 (3%)	1 (0%)	24	46
2	2	206/269 (77%)	196 (95%)	9 (4%)	1 (0%)	24	46

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	3	219/275 (80%)	207 (94%)	12 (6%)	0	100	100
4	4	196/198 (99%)	194 (99%)	2 (1%)	0	100	100
5	A	741/758 (98%)	710 (96%)	30 (4%)	1 (0%)	48	70
6	B	731/734 (100%)	710 (97%)	18 (2%)	3 (0%)	30	51
7	C	78/81 (96%)	76 (97%)	2 (3%)	0	100	100
8	D	141/143 (99%)	135 (96%)	6 (4%)	0	100	100
9	E	64/66 (97%)	60 (94%)	4 (6%)	0	100	100
10	F	152/154 (99%)	149 (98%)	3 (2%)	0	100	100
11	G	95/97 (98%)	93 (98%)	2 (2%)	0	100	100
12	H	86/88 (98%)	81 (94%)	5 (6%)	0	100	100
13	I	28/40 (70%)	27 (96%)	1 (4%)	0	100	100
14	J	40/42 (95%)	37 (92%)	3 (8%)	0	100	100
15	K	73/80 (91%)	67 (92%)	6 (8%)	0	100	100
16	L	155/157 (99%)	149 (96%)	6 (4%)	0	100	100
All	All	3196/3375 (95%)	3075 (96%)	115 (4%)	6 (0%)	43	66

5 of 6 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	1	172	LYS
6	B	222	LEU
6	B	559	CYS
2	2	260	ALA
6	B	492	ILE

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	1	158/158 (100%)	156 (99%)	2 (1%)	61	82
2	2	167/216 (77%)	167 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
3	3	169/213 (79%)	169 (100%)	0	100 100
4	4	164/164 (100%)	164 (100%)	0	100 100
5	A	604/618 (98%)	599 (99%)	5 (1%)	73 88
6	B	598/599 (100%)	591 (99%)	7 (1%)	63 83
7	C	69/70 (99%)	68 (99%)	1 (1%)	59 81
8	D	122/122 (100%)	122 (100%)	0	100 100
9	E	58/58 (100%)	58 (100%)	0	100 100
10	F	126/127 (99%)	126 (100%)	0	100 100
11	G	82/82 (100%)	81 (99%)	1 (1%)	63 83
12	H	71/71 (100%)	71 (100%)	0	100 100
13	I	26/36 (72%)	26 (100%)	0	100 100
14	J	35/35 (100%)	35 (100%)	0	100 100
15	K	51/58 (88%)	51 (100%)	0	100 100
16	L	124/124 (100%)	123 (99%)	1 (1%)	73 88
All	All	2624/2751 (95%)	2607 (99%)	17 (1%)	78 91

5 of 17 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
7	C	65	VAL
16	L	60	ILE
6	B	157	LEU
6	B	441	ASP
6	B	444	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 33 such sidechains are listed below:

Mol	Chain	Res	Type
9	E	119	ASN
10	F	193	GLN
15	K	52	ASN
5	A	303	HIS
5	A	301	HIS

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 242 ligands modelled in this entry, 2 are monoatomic - leaving 240 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	$\#\|Z\| > 2$
19	CLA	A	819	-	69,73,73	1.36	7 (10%)	83,113,113	1.75	14 (16%)
19	CLA	2	505	2	56,60,73	1.53	9 (16%)	67,97,113	1.96	15 (22%)
19	CLA	3	306	-	56,60,73	1.53	7 (12%)	67,97,113	1.94	14 (20%)
22	LMG	A	847	-	50,50,55	1.03	5 (10%)	58,58,63	0.98	2 (3%)
19	CLA	A	822	5	64,68,73	1.45	7 (10%)	77,107,113	1.83	15 (19%)
19	CLA	B	815	6	69,73,73	1.37	6 (8%)	83,113,113	1.82	13 (15%)
19	CLA	3	312	3	52,56,73	1.59	8 (15%)	62,92,113	2.03	15 (24%)
20	CHL	2	516	2	60,64,74	0.81	1 (1%)	68,102,114	1.35	11 (16%)
19	CLA	1	504	1	69,73,73	1.38	7 (10%)	83,113,113	1.81	16 (19%)
28	SF4	C	102	7	0,12,12	-	-	-		
18	BCR	B	851	-	41,41,41	0.66	0	56,56,56	2.67	15 (26%)
19	CLA	B	804	-	69,73,73	1.39	7 (10%)	83,113,113	1.89	16 (19%)
18	BCR	F	306	-	41,41,41	0.65	0	56,56,56	3.05	8 (14%)
17	LUT	3	301	-	42,43,43	2.41	1 (2%)	51,60,60	1.68	7 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
17	LUT	1	502	-	42,43,43	2.37	1 (2%)	51,60,60	1.81	9 (17%)
22	LMG	F	305	-	36,36,55	0.72	1 (2%)	44,44,63	1.10	2 (4%)
19	CLA	B	827	6	69,73,73	1.35	8 (11%)	83,113,113	1.81	12 (14%)
18	BCR	A	850	-	41,41,41	0.64	0	56,56,56	3.20	14 (25%)
19	CLA	K	1002	-	64,68,73	1.44	8 (12%)	77,107,113	1.85	16 (20%)
24	LMT	2	523	-	36,36,36	1.13	5 (13%)	47,47,47	1.00	2 (4%)
21	LHG	B	842	19	20,20,48	0.59	0	23,26,54	1.55	3 (13%)
19	CLA	1	516	1	64,68,73	1.44	7 (10%)	77,107,113	1.85	16 (20%)
19	CLA	B	811	6	69,73,73	1.39	8 (11%)	83,113,113	1.79	15 (18%)
19	CLA	L	305	31	54,58,73	1.57	9 (16%)	65,95,113	1.91	15 (23%)
19	CLA	4	306	4	69,73,73	1.39	7 (10%)	83,113,113	1.80	16 (19%)
19	CLA	4	315	4	69,73,73	1.38	7 (10%)	83,113,113	1.78	15 (18%)
21	LHG	A	853	-	48,48,48	0.40	0	51,54,54	1.04	3 (5%)
22	LMG	2	522	-	13,13,55	0.58	0	18,18,63	0.63	0
18	BCR	A	852	-	41,41,41	0.63	0	56,56,56	2.90	14 (25%)
19	CLA	2	510	21	64,68,73	1.44	8 (12%)	77,107,113	1.83	13 (16%)
19	CLA	A	803	31	69,73,73	1.36	8 (11%)	83,113,113	1.81	13 (15%)
18	BCR	3	303	-	41,41,41	0.65	0	56,56,56	3.22	12 (21%)
19	CLA	A	837	-	69,73,73	1.38	8 (11%)	83,113,113	1.74	14 (16%)
19	CLA	B	820	31	69,73,73	1.38	8 (11%)	83,113,113	1.67	14 (16%)
24	LMT	G	209	-	32,32,36	1.23	6 (18%)	43,43,47	0.97	1 (2%)
19	CLA	3	313	3	64,68,73	1.42	7 (10%)	77,107,113	1.82	15 (19%)
20	CHL	4	316	-	65,69,74	0.86	2 (3%)	74,108,114	1.42	12 (16%)
19	CLA	A	827	5	69,73,73	1.37	8 (11%)	83,113,113	1.79	15 (18%)
19	CLA	1	506	-	59,63,73	1.47	8 (13%)	71,101,113	1.95	14 (19%)
19	CLA	A	825	31	69,73,73	1.41	9 (13%)	83,113,113	1.84	15 (18%)
19	CLA	A	839	5	69,73,73	1.36	6 (8%)	83,113,113	1.69	12 (14%)
18	BCR	B	856	-	41,41,41	0.66	0	56,56,56	3.05	13 (23%)
20	CHL	4	314	31	55,59,74	0.93	2 (3%)	62,96,114	1.82	14 (22%)
19	CLA	A	821	-	69,73,73	1.36	6 (8%)	83,113,113	1.68	15 (18%)
19	CLA	B	813	6	50,54,73	1.62	7 (14%)	60,90,113	1.97	14 (23%)
19	CLA	B	826	6	69,73,73	1.39	9 (13%)	83,113,113	1.78	14 (16%)
19	CLA	G	201	6	69,73,73	1.37	7 (10%)	83,113,113	1.85	17 (20%)
22	LMG	B	844	-	35,35,55	0.74	1 (2%)	43,43,63	1.08	3 (6%)
19	CLA	G	202	11	59,63,73	1.50	8 (13%)	71,101,113	1.89	15 (21%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
18	BCR	2	503	-	41,41,41	0.86	0	56,56,56	3.25	14 (25%)
19	CLA	B	805	6	69,73,73	1.37	7 (10%)	83,113,113	1.76	13 (15%)
19	CLA	A	814	-	69,73,73	1.38	8 (11%)	83,113,113	1.83	16 (19%)
20	CHL	1	521	1	60,64,74	0.84	1 (1%)	68,102,114	1.33	9 (13%)
19	CLA	A	829	5	69,73,73	1.35	8 (11%)	83,113,113	1.76	13 (15%)
19	CLA	B	819	6	69,73,73	1.34	6 (8%)	83,113,113	1.82	15 (18%)
19	CLA	2	511	2	54,58,73	1.54	7 (12%)	65,95,113	2.02	15 (23%)
19	CLA	A	804	5	69,73,73	1.35	8 (11%)	83,113,113	1.83	14 (16%)
28	SF4	A	843	5,6	0,12,12	-	-	-		
29	PQN	B	841	-	34,34,34	0.37	0	42,45,45	1.14	3 (7%)
20	CHL	2	526	2	70,74,74	0.78	1 (1%)	80,114,114	1.26	12 (15%)
17	LUT	2	501	-	42,43,43	2.35	1 (2%)	51,60,60	1.78	9 (17%)
19	CLA	B	836	6	69,73,73	1.37	6 (8%)	83,113,113	1.71	13 (15%)
24	LMT	4	320	-	36,36,36	1.15	4 (11%)	47,47,47	0.95	3 (6%)
19	CLA	A	812	5	59,63,73	1.49	7 (11%)	71,101,113	1.89	16 (22%)
22	LMG	4	321	-	13,13,55	0.57	0	18,18,63	0.68	0
19	CLA	L	304	16	64,68,73	1.41	6 (9%)	77,107,113	1.87	13 (16%)
19	CLA	4	312	4	54,58,73	1.54	7 (12%)	65,95,113	1.98	17 (26%)
24	LMT	J	1107	-	26,26,36	1.34	5 (19%)	37,37,47	1.08	2 (5%)
18	BCR	4	301	-	41,41,41	0.65	0	56,56,56	3.34	15 (26%)
20	CHL	1	512	-	51,55,74	0.86	1 (1%)	57,91,114	1.53	12 (21%)
19	CLA	3	315	3	54,58,73	1.53	6 (11%)	65,95,113	1.97	13 (20%)
18	BCR	B	853	-	41,41,41	0.63	0	56,56,56	3.06	13 (23%)
19	CLA	A	854	31	69,73,73	1.35	7 (10%)	83,113,113	1.81	16 (19%)
18	BCR	G	205	-	41,41,41	0.73	0	56,56,56	3.09	11 (19%)
18	BCR	J	1108	-	41,41,41	0.60	0	56,56,56	2.87	15 (26%)
18	BCR	A	849	-	41,41,41	0.63	0	56,56,56	3.28	16 (28%)
19	CLA	J	1101	5	69,73,73	1.36	6 (8%)	83,113,113	1.88	16 (19%)
19	CLA	B	803	6	69,73,73	1.37	6 (8%)	83,113,113	1.75	12 (14%)
19	CLA	B	828	6	69,73,73	1.35	8 (11%)	83,113,113	1.77	11 (13%)
19	CLA	J	1102	31	49,53,73	1.60	7 (14%)	59,89,113	1.99	12 (20%)
26	DGD	4	319	-	52,52,67	0.73	2 (3%)	66,66,81	1.44	9 (13%)
21	LHG	A	845	19	39,39,48	0.42	0	42,45,54	1.25	4 (9%)
17	LUT	3	302	-	42,43,43	2.31	1 (2%)	51,60,60	1.61	13 (25%)
19	CLA	B	817	6	64,68,73	1.44	8 (12%)	77,107,113	1.88	14 (18%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
19	CLA	A	831	5	69,73,73	1.37	6 (8%)	83,113,113	1.76	15 (18%)
19	CLA	A	809	5	69,73,73	1.35	7 (10%)	83,113,113	1.80	15 (18%)
19	CLA	A	813	5	69,73,73	1.35	7 (10%)	83,113,113	1.83	15 (18%)
20	CHL	3	314	-	51,55,74	0.91	1 (1%)	57,91,114	1.60	12 (21%)
18	BCR	A	848	-	41,41,41	0.63	0	56,56,56	3.27	18 (32%)
19	CLA	B	821	6	50,54,73	1.61	7 (14%)	60,90,113	1.96	13 (21%)
19	CLA	K	1001	-	49,53,73	1.63	8 (16%)	59,89,113	2.01	14 (23%)
19	CLA	A	828	5	69,73,73	1.36	7 (10%)	83,113,113	1.86	13 (15%)
19	CLA	A	808	5	69,73,73	1.36	6 (8%)	83,113,113	1.83	13 (15%)
21	LHG	1	520	-	41,41,48	0.45	0	44,47,54	1.15	4 (9%)
22	LMG	J	1104	-	34,34,55	0.46	0	42,42,63	1.23	5 (11%)
26	DGD	B	801	-	42,42,67	0.61	0	56,56,81	1.16	6 (10%)
19	CLA	G	203	11	50,54,73	1.62	8 (16%)	60,90,113	1.91	12 (20%)
19	CLA	4	309	-	54,58,73	1.52	7 (12%)	65,95,113	2.04	17 (26%)
19	CLA	4	305	4	54,58,73	1.58	8 (14%)	65,95,113	2.01	18 (27%)
19	CLA	3	305	-	59,63,73	1.48	8 (13%)	71,101,113	2.02	16 (22%)
18	BCR	L	306	-	41,41,41	0.67	0	56,56,56	3.01	13 (23%)
19	CLA	1	507	1	69,73,73	1.38	7 (10%)	83,113,113	1.82	15 (18%)
22	LMG	4	322	-	45,45,55	0.93	3 (6%)	53,53,63	1.08	4 (7%)
18	BCR	A	851	-	41,41,41	0.66	0	56,56,56	3.23	14 (25%)
19	CLA	B	824	31	69,73,73	1.37	8 (11%)	83,113,113	1.90	14 (16%)
19	CLA	B	829	6	69,73,73	1.40	7 (10%)	83,113,113	1.70	13 (15%)
19	CLA	2	508	-	59,63,73	1.45	7 (11%)	71,101,113	1.96	15 (21%)
19	CLA	A	807	5	64,68,73	1.45	7 (10%)	77,107,113	1.83	14 (18%)
19	CLA	A	840	31	69,73,73	1.35	7 (10%)	83,113,113	1.79	14 (16%)
19	CLA	B	822	6	69,73,73	1.38	8 (11%)	83,113,113	1.79	15 (18%)
22	LMG	J	1103	-	30,30,55	0.51	0	38,38,63	1.08	2 (5%)
19	CLA	B	816	6	59,63,73	1.49	8 (13%)	71,101,113	1.91	13 (18%)
18	BCR	3	304	-	41,41,41	0.69	0	56,56,56	3.40	14 (25%)
30	ZEX	F	301	-	42,43,43	0.73	0	55,60,60	1.76	11 (20%)
19	CLA	A	818	5	60,64,73	1.48	9 (15%)	72,102,113	1.86	14 (19%)
19	CLA	B	808	6	69,73,73	1.39	7 (10%)	83,113,113	1.74	14 (16%)
19	CLA	2	504	2	64,68,73	1.42	7 (10%)	77,107,113	1.94	15 (19%)
19	CLA	B	834	31	59,63,73	1.49	8 (13%)	71,101,113	1.85	15 (21%)
19	CLA	F	303	10	69,73,73	1.36	6 (8%)	83,113,113	1.78	14 (16%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
19	CLA	B	837	6	54,58,73	1.53	8 (14%)	65,95,113	1.91	14 (21%)
24	LMT	B	846	-	36,36,36	1.14	6 (16%)	47,47,47	1.04	3 (6%)
23	XAT	4	303	-	39,47,47	0.64	0	54,74,74	2.45	13 (24%)
21	LHG	2	517	19	34,34,48	0.46	0	37,40,54	1.07	2 (5%)
19	CLA	2	509	-	54,58,73	1.54	6 (11%)	65,95,113	1.89	13 (20%)
19	CLA	1	510	-	50,54,73	1.65	7 (14%)	60,90,113	2.25	15 (25%)
19	CLA	1	505	1	50,54,73	1.60	8 (16%)	60,90,113	1.95	13 (21%)
19	CLA	A	816	-	50,54,73	1.60	7 (14%)	60,90,113	1.97	12 (20%)
19	CLA	A	841	5	69,73,73	1.38	8 (11%)	83,113,113	1.73	14 (16%)
24	LMT	G	208	-	36,36,36	1.15	5 (13%)	47,47,47	0.98	2 (4%)
19	CLA	B	809	6	69,73,73	1.38	8 (11%)	83,113,113	1.73	14 (16%)
17	LUT	4	302	-	42,43,43	2.46	1 (2%)	51,60,60	1.92	12 (23%)
19	CLA	B	810	6	69,73,73	1.37	7 (10%)	83,113,113	1.79	13 (15%)
27	CL0	A	801	5	69,73,73	1.58	10 (14%)	83,113,113	2.16	18 (21%)
19	CLA	A	834	-	69,73,73	1.35	6 (8%)	83,113,113	1.76	14 (16%)
19	CLA	3	308	-	69,73,73	1.38	7 (10%)	83,113,113	1.83	16 (19%)
19	CLA	A	823	5	64,68,73	1.44	8 (12%)	77,107,113	1.80	15 (19%)
17	LUT	J	1109	-	42,43,43	2.28	1 (2%)	51,60,60	1.94	9 (17%)
19	CLA	3	310	31	54,58,73	1.52	7 (12%)	65,95,113	2.15	13 (20%)
19	CLA	1	513	-	69,73,73	1.36	7 (10%)	83,113,113	1.79	15 (18%)
18	BCR	B	852	-	41,41,41	0.61	0	56,56,56	2.95	14 (25%)
19	CLA	1	515	-	49,53,73	1.65	9 (18%)	59,89,113	1.84	12 (20%)
19	CLA	B	818	6	69,73,73	1.38	9 (13%)	83,113,113	1.73	16 (19%)
19	CLA	2	506	-	69,73,73	1.38	8 (11%)	83,113,113	1.87	16 (19%)
19	CLA	2	514	2	59,63,73	1.48	7 (11%)	71,101,113	1.90	13 (18%)
19	CLA	A	811	5	69,73,73	1.37	8 (11%)	83,113,113	1.82	15 (18%)
19	CLA	4	318	-	69,73,73	1.35	7 (10%)	83,113,113	1.81	14 (16%)
19	CLA	A	836	5	55,59,73	1.54	7 (12%)	66,96,113	1.95	15 (22%)
24	LMT	3	318	-	32,32,36	1.17	5 (15%)	43,43,47	1.19	5 (11%)
24	LMT	B	855	-	32,32,36	1.25	6 (18%)	43,43,47	0.97	2 (4%)
22	LMG	2	518	-	25,25,55	0.59	0	33,33,63	1.13	3 (9%)
19	CLA	B	838	31	69,73,73	1.38	7 (10%)	83,113,113	1.77	15 (18%)
20	CHL	2	513	-	52,56,74	0.89	1 (1%)	58,92,114	1.38	9 (15%)
24	LMT	A	846	-	36,36,36	1.14	5 (13%)	47,47,47	1.13	2 (4%)
19	CLA	L	303	16	54,58,73	1.54	7 (12%)	65,95,113	1.97	14 (21%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
20	CHL	4	317	4	47,51,74	0.95	1 (2%)	52,86,114	1.65	12 (23%)
19	CLA	A	835	5	59,63,73	1.51	9 (15%)	71,101,113	1.87	16 (22%)
19	CLA	3	307	-	59,63,73	1.49	7 (11%)	71,101,113	2.00	18 (25%)
24	LMT	B	847	-	33,33,36	1.22	5 (15%)	44,44,47	0.96	1 (2%)
19	CLA	B	833	-	64,68,73	1.41	8 (12%)	77,107,113	1.79	12 (15%)
18	BCR	B	802	-	41,41,41	0.68	0	56,56,56	4.02	18 (32%)
18	BCR	L	302	-	41,41,41	0.84	0	56,56,56	3.17	15 (26%)
19	CLA	K	1004	-	28,35,73	2.09	9 (32%)	32,60,113	2.10	7 (21%)
19	CLA	A	855	-	69,73,73	1.35	8 (11%)	83,113,113	1.80	15 (18%)
18	BCR	L	307	-	41,41,41	0.69	0	56,56,56	3.34	11 (19%)
22	LMG	2	524	-	13,13,55	0.56	0	18,18,63	0.81	0
19	CLA	B	840	21	69,73,73	1.37	6 (8%)	83,113,113	1.76	13 (15%)
18	BCR	I	102	-	41,41,41	0.65	0	56,56,56	3.13	13 (23%)
19	CLA	A	806	5	69,73,73	1.36	7 (10%)	83,113,113	1.77	14 (16%)
19	CLA	A	838	-	69,73,73	1.38	7 (10%)	83,113,113	1.77	15 (18%)
19	CLA	1	509	-	54,58,73	1.55	7 (12%)	65,95,113	1.97	17 (26%)
22	LMG	B	845	-	33,33,55	0.57	1 (3%)	41,41,63	1.24	5 (12%)
19	CLA	K	1003	-	28,35,73	2.09	9 (32%)	32,60,113	2.21	8 (25%)
18	BCR	A	856	-	41,41,41	0.67	0	56,56,56	3.27	15 (26%)
19	CLA	A	833	5	69,73,73	1.37	8 (11%)	83,113,113	1.78	15 (18%)
19	CLA	G	204	31	69,73,73	1.36	9 (13%)	83,113,113	1.84	15 (18%)
20	CHL	2	512	-	51,55,74	1.13	3 (5%)	57,91,114	1.72	12 (21%)
26	DGD	J	1106	-	59,59,67	0.92	4 (6%)	73,73,81	1.06	5 (6%)
18	BCR	1	503	-	19,19,41	0.66	0	26,26,56	3.15	7 (26%)
18	BCR	B	850	-	41,41,41	0.66	0	56,56,56	3.01	11 (19%)
19	CLA	B	823	6	59,63,73	1.49	8 (13%)	71,101,113	1.90	12 (16%)
28	SF4	C	101	7	0,12,12	-	-	-		
20	CHL	2	515	-	50,54,74	0.91	1 (2%)	56,90,114	1.38	12 (21%)
19	CLA	B	812	6	64,68,73	1.44	7 (10%)	77,107,113	1.77	13 (16%)
26	DGD	G	207	-	48,48,67	0.59	1 (2%)	62,62,81	1.07	3 (4%)
19	CLA	B	806	6	69,73,73	1.35	5 (7%)	83,113,113	1.76	14 (16%)
22	LMG	G	206	-	50,50,55	1.05	4 (8%)	58,58,63	1.07	3 (5%)
19	CLA	A	830	5	69,73,73	1.36	7 (10%)	83,113,113	1.76	14 (16%)
19	CLA	3	316	-	50,54,73	1.62	9 (18%)	60,90,113	1.97	14 (23%)
19	CLA	A	824	5	69,73,73	1.37	7 (10%)	83,113,113	1.73	14 (16%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
18	BCR	B	849	-	41,41,41	0.79	0	56,56,56	3.73	20 (35%)
19	CLA	A	832	5	69,73,73	1.38	6 (8%)	83,113,113	1.75	13 (15%)
19	CLA	A	815	5	49,53,73	1.64	8 (16%)	59,89,113	1.91	14 (23%)
22	LMG	2	521	-	13,13,55	0.59	0	18,18,63	0.75	0
19	CLA	4	310	-	64,68,73	1.44	9 (14%)	77,107,113	1.82	13 (16%)
19	CLA	B	839	6	69,73,73	1.38	6 (8%)	83,113,113	1.77	14 (16%)
19	CLA	H	1000	-	64,68,73	1.44	8 (12%)	77,107,113	1.85	15 (19%)
22	LMG	1	519	-	13,13,55	0.56	0	18,18,63	0.89	1 (5%)
19	CLA	A	842	21	64,68,73	1.42	8 (12%)	77,107,113	1.87	14 (18%)
19	CLA	B	835	6	59,63,73	1.47	7 (11%)	71,101,113	1.85	13 (18%)
19	CLA	L	301	-	59,63,73	1.49	7 (11%)	71,101,113	1.92	15 (21%)
19	CLA	1	511	1	50,54,73	1.60	6 (12%)	60,90,113	1.93	13 (21%)
26	DGD	B	854	-	62,62,67	0.97	5 (8%)	76,76,81	1.00	3 (3%)
19	CLA	4	311	4	50,54,73	1.60	6 (12%)	60,90,113	1.97	12 (20%)
19	CLA	F	302	6	69,73,73	1.40	8 (11%)	83,113,113	1.78	15 (18%)
19	CLA	B	825	31	69,73,73	1.37	7 (10%)	83,113,113	1.86	17 (20%)
19	CLA	3	311	-	45,49,73	1.71	8 (17%)	54,84,113	2.03	15 (27%)
22	LMG	F	304	-	47,47,55	0.97	4 (8%)	55,55,63	1.09	2 (3%)
29	PQN	A	844	-	34,34,34	0.39	0	42,45,45	1.25	5 (11%)
19	CLA	B	807	6	69,73,73	1.36	6 (8%)	83,113,113	1.77	13 (15%)
19	CLA	B	814	6	69,73,73	1.38	8 (11%)	83,113,113	1.77	15 (18%)
17	LUT	1	501	-	42,43,43	2.39	1 (2%)	51,60,60	1.69	10 (19%)
19	CLA	B	832	6	62,66,73	1.44	6 (9%)	74,104,113	1.91	16 (21%)
19	CLA	3	309	-	59,63,73	1.51	8 (13%)	71,101,113	1.91	16 (22%)
19	CLA	J	1105	-	54,58,73	1.56	7 (12%)	65,95,113	2.20	18 (27%)
22	LMG	2	520	-	13,13,55	0.59	0	18,18,63	0.87	1 (5%)
20	CHL	1	514	1	65,69,74	0.80	1 (1%)	74,108,114	1.37	12 (16%)
23	XAT	2	502	-	39,47,47	0.62	0	54,74,74	1.72	11 (20%)
19	CLA	2	507	2	69,73,73	1.38	6 (8%)	83,113,113	1.85	14 (16%)
19	CLA	B	830	6	69,73,73	1.37	10 (14%)	83,113,113	1.75	14 (16%)
19	CLA	3	317	3	50,54,73	1.62	8 (16%)	60,90,113	1.92	13 (21%)
18	BCR	K	1005	-	41,41,41	0.67	0	56,56,56	3.18	13 (23%)
18	BCR	I	101	-	41,41,41	0.73	0	56,56,56	3.50	16 (28%)
19	CLA	A	817	-	69,73,73	1.37	6 (8%)	83,113,113	1.71	13 (15%)
19	CLA	4	308	4	64,68,73	1.40	6 (9%)	77,107,113	1.96	14 (18%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
19	CLA	A	810	5	54,58,73	1.56	9 (16%)	65,95,113	2.02	13 (20%)
22	LMG	1	518	-	46,46,55	0.92	3 (6%)	54,54,63	1.04	2 (3%)
21	LHG	B	843	-	48,48,48	0.40	0	51,54,54	1.01	2 (3%)
19	CLA	B	831	6	64,68,73	1.42	8 (12%)	77,107,113	1.77	13 (16%)
19	CLA	1	508	1	69,73,73	1.37	8 (11%)	83,113,113	1.80	14 (16%)
19	CLA	4	307	4	64,68,73	1.42	7 (10%)	77,107,113	1.88	16 (20%)
19	CLA	4	304	4	64,68,73	1.44	7 (10%)	77,107,113	2.03	18 (23%)
21	LHG	1	517	-	48,48,48	0.41	0	51,54,54	1.09	4 (7%)
19	CLA	A	826	31	59,63,73	1.48	7 (11%)	71,101,113	1.90	15 (21%)
20	CHL	4	313	-	51,55,74	0.92	2 (3%)	57,91,114	1.48	11 (19%)
22	LMG	G	210	-	25,25,55	0.54	0	33,33,63	1.29	4 (12%)
19	CLA	A	820	-	54,58,73	1.56	8 (14%)	65,95,113	1.95	14 (21%)
22	LMG	2	525	-	13,13,55	0.62	0	18,18,63	0.70	0
22	LMG	2	519	-	36,36,55	0.66	1 (2%)	44,44,63	1.24	7 (15%)
19	CLA	A	802	-	69,73,73	1.34	8 (11%)	83,113,113	1.79	18 (21%)
19	CLA	A	805	5	69,73,73	1.37	8 (11%)	83,113,113	1.79	12 (14%)

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	CLA	A	819	-	-	16/39/115/115	-
19	CLA	2	505	2	-	8/24/100/115	-
19	CLA	3	306	-	-	8/24/100/115	-
22	LMG	A	847	-	-	15/45/65/70	0/1/1/1
19	CLA	A	822	5	-	14/33/109/115	-
19	CLA	B	815	6	-	10/39/115/115	-
19	CLA	3	312	3	-	8/19/95/115	-
20	CHL	2	516	2	1/1/13/21	7/29/105/117	-
19	CLA	1	504	1	-	14/39/115/115	-
28	SF4	C	102	7	-	-	0/6/5/5
18	BCR	B	851	-	-	11/29/63/63	0/2/2/2
19	CLA	B	804	-	-	13/39/115/115	-
18	BCR	F	306	-	-	8/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
17	LUT	3	301	-	-	3/29/67/67	0/2/2/2
17	LUT	1	502	-	1/1/12/27	9/29/67/67	0/2/2/2
22	LMG	F	305	-	-	10/31/51/70	0/1/1/1
19	CLA	B	827	6	-	20/39/115/115	-
18	BCR	A	850	-	-	5/29/63/63	0/2/2/2
19	CLA	K	1002	-	-	21/33/109/115	-
24	LMT	2	523	-	-	10/21/61/61	0/2/2/2
21	LHG	B	842	19	-	12/23/23/53	-
19	CLA	1	516	1	-	13/33/109/115	-
19	CLA	B	811	6	-	17/39/115/115	-
19	CLA	L	305	31	-	10/21/97/115	-
19	CLA	4	306	4	-	16/39/115/115	-
19	CLA	4	315	4	-	15/39/115/115	-
21	LHG	A	853	-	-	30/53/53/53	-
22	LMG	2	522	-	-	4/4/24/70	0/1/1/1
18	BCR	A	852	-	-	12/29/63/63	0/2/2/2
19	CLA	2	510	21	-	15/33/109/115	-
19	CLA	A	803	31	-	8/39/115/115	-
18	BCR	3	303	-	-	12/29/63/63	0/2/2/2
19	CLA	A	837	-	-	9/39/115/115	-
19	CLA	B	820	31	-	18/39/115/115	-
24	LMT	G	209	-	-	13/17/57/61	0/2/2/2
19	CLA	3	313	3	-	16/33/109/115	-
20	CHL	4	316	-	1/1/14/21	8/35/111/117	-
19	CLA	A	827	5	-	16/39/115/115	-
19	CLA	1	506	-	-	9/27/103/115	-
19	CLA	A	825	31	-	14/39/115/115	-
19	CLA	A	839	5	-	14/39/115/115	-
18	BCR	B	856	-	-	13/29/63/63	0/2/2/2
20	CHL	4	314	31	-	4/23/99/117	-
19	CLA	A	821	-	-	17/39/115/115	-
19	CLA	B	813	6	-	3/17/93/115	-
19	CLA	B	826	6	-	6/39/115/115	-
19	CLA	G	201	6	-	20/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	LMG	B	844	-	-	11/30/50/70	0/1/1/1
19	CLA	G	202	11	-	13/27/103/115	-
18	BCR	2	503	-	-	11/29/63/63	0/2/2/2
19	CLA	B	805	6	-	21/39/115/115	-
19	CLA	A	814	-	-	16/39/115/115	-
20	CHL	1	521	1	1/1/13/21	7/29/105/117	-
19	CLA	A	829	5	-	19/39/115/115	-
19	CLA	B	819	6	-	18/39/115/115	-
19	CLA	2	511	2	-	12/21/97/115	-
19	CLA	A	804	5	-	24/39/115/115	-
29	PQN	B	841	-	-	12/23/43/43	0/2/2/2
28	SF4	A	843	5,6	-	-	0/6/5/5
20	CHL	2	526	2	1/1/15/21	10/41/117/117	-
17	LUT	2	501	-	1/1/12/27	5/29/67/67	0/2/2/2
19	CLA	B	836	6	-	11/39/115/115	-
24	LMT	4	320	-	-	4/21/61/61	0/2/2/2
19	CLA	A	812	5	-	11/27/103/115	-
22	LMG	4	321	-	-	0/4/24/70	0/1/1/1
19	CLA	L	304	16	-	12/33/109/115	-
19	CLA	4	312	4	-	8/21/97/115	-
24	LMT	J	1107	-	-	7/11/51/61	0/2/2/2
18	BCR	4	301	-	-	13/29/63/63	0/2/2/2
20	CHL	1	512	-	-	3/19/95/117	-
19	CLA	3	315	3	-	7/21/97/115	-
18	BCR	B	853	-	-	10/29/63/63	0/2/2/2
19	CLA	A	854	31	-	16/39/115/115	-
18	BCR	G	205	-	-	11/29/63/63	0/2/2/2
18	BCR	J	1108	-	-	9/29/63/63	0/2/2/2
18	BCR	A	849	-	-	11/29/63/63	0/2/2/2
19	CLA	J	1101	5	-	13/39/115/115	-
19	CLA	B	803	6	-	8/39/115/115	-
19	CLA	B	828	6	-	18/39/115/115	-
19	CLA	J	1102	31	-	2/15/91/115	-
26	DGD	4	319	-	-	17/40/80/95	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
21	LHG	A	845	19	-	27/44/44/53	-
17	LUT	3	302	-	1/1/12/27	8/29/67/67	0/2/2/2
19	CLA	B	817	6	-	9/33/109/115	-
19	CLA	A	831	5	-	13/39/115/115	-
19	CLA	A	809	5	-	17/39/115/115	-
19	CLA	A	813	5	-	11/39/115/115	-
20	CHL	3	314	-	-	4/19/95/117	-
18	BCR	A	848	-	-	10/29/63/63	0/2/2/2
19	CLA	B	821	6	-	9/17/93/115	-
19	CLA	K	1001	-	-	10/15/91/115	-
19	CLA	A	828	5	-	22/39/115/115	-
19	CLA	A	808	5	-	19/39/115/115	-
21	LHG	1	520	-	-	26/46/46/53	-
22	LMG	J	1104	-	-	12/29/49/70	0/1/1/1
26	DGD	B	801	-	-	21/30/70/95	0/2/2/2
19	CLA	G	203	11	-	6/17/93/115	-
19	CLA	4	309	-	-	12/21/97/115	-
19	CLA	4	305	4	-	7/21/97/115	-
19	CLA	3	305	-	-	18/27/103/115	-
18	BCR	L	306	-	-	8/29/63/63	0/2/2/2
19	CLA	1	507	1	-	14/39/115/115	-
22	LMG	4	322	-	-	13/40/60/70	0/1/1/1
18	BCR	A	851	-	-	12/29/63/63	0/2/2/2
19	CLA	B	824	31	-	15/39/115/115	-
19	CLA	B	829	6	-	20/39/115/115	-
19	CLA	2	508	-	-	7/27/103/115	-
19	CLA	A	807	5	-	17/33/109/115	-
19	CLA	A	840	31	-	16/39/115/115	-
19	CLA	B	822	6	-	20/39/115/115	-
22	LMG	J	1103	-	-	4/25/45/70	0/1/1/1
19	CLA	B	816	6	-	8/27/103/115	-
18	BCR	3	304	-	-	16/29/63/63	0/2/2/2
30	ZEX	F	301	-	-	3/29/67/67	0/2/2/2
19	CLA	A	818	5	-	15/29/105/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
19	CLA	B	808	6	-	21/39/115/115	-
19	CLA	2	504	2	-	9/33/109/115	-
19	CLA	B	834	31	-	12/27/103/115	-
19	CLA	F	303	10	-	20/39/115/115	-
19	CLA	B	837	6	-	5/21/97/115	-
24	LMT	B	846	-	-	11/21/61/61	0/2/2/2
23	XAT	4	303	-	2/2/12/26	0/31/93/93	0/4/4/4
21	LHG	2	517	19	-	15/39/39/53	-
19	CLA	2	509	-	-	11/21/97/115	-
19	CLA	1	510	-	-	7/17/93/115	-
19	CLA	1	505	1	-	6/17/93/115	-
19	CLA	A	816	-	-	8/17/93/115	-
19	CLA	A	841	5	-	6/39/115/115	-
24	LMT	G	208	-	-	9/21/61/61	0/2/2/2
19	CLA	B	809	6	-	10/39/115/115	-
17	LUT	4	302	-	-	3/29/67/67	0/2/2/2
19	CLA	B	810	6	-	12/39/115/115	-
27	CL0	A	801	5	-	7/39/115/115	-
19	CLA	A	834	-	-	19/39/115/115	-
19	CLA	3	308	-	-	22/39/115/115	-
19	CLA	A	823	5	-	15/33/109/115	-
17	LUT	J	1109	-	1/1/12/27	6/29/67/67	0/2/2/2
19	CLA	3	310	31	-	8/21/97/115	-
19	CLA	1	513	-	-	17/39/115/115	-
18	BCR	B	852	-	-	11/29/63/63	0/2/2/2
19	CLA	1	515	-	-	7/15/91/115	-
19	CLA	B	818	6	-	18/39/115/115	-
19	CLA	2	506	-	-	14/39/115/115	-
19	CLA	2	514	2	-	7/27/103/115	-
19	CLA	A	811	5	-	17/39/115/115	-
19	CLA	4	318	-	-	13/39/115/115	-
19	CLA	A	836	5	-	9/23/99/115	-
24	LMT	3	318	-	-	4/17/57/61	0/2/2/2
24	LMT	B	855	-	-	4/17/57/61	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	LMG	2	518	-	-	6/20/40/70	0/1/1/1
19	CLA	B	838	31	-	13/39/115/115	-
20	CHL	2	513	-	-	1/20/96/117	-
24	LMT	A	846	-	-	8/21/61/61	0/2/2/2
19	CLA	L	303	16	-	9/21/97/115	-
20	CHL	4	317	4	-	2/14/90/117	-
19	CLA	A	835	5	-	10/27/103/115	-
19	CLA	3	307	-	-	13/27/103/115	-
24	LMT	B	847	-	-	6/18/58/61	0/2/2/2
19	CLA	B	833	-	-	10/33/109/115	-
18	BCR	B	802	-	-	5/29/63/63	0/2/2/2
18	BCR	L	302	-	-	6/29/63/63	0/2/2/2
22	LMG	2	524	-	-	1/4/24/70	0/1/1/1
19	CLA	A	855	-	-	19/39/115/115	-
18	BCR	L	307	-	-	11/29/63/63	0/2/2/2
19	CLA	B	840	21	-	18/39/115/115	-
18	BCR	I	102	-	-	14/29/63/63	0/2/2/2
19	CLA	A	806	5	-	21/39/115/115	-
19	CLA	A	838	-	-	14/39/115/115	-
19	CLA	1	509	-	-	8/21/97/115	-
22	LMG	B	845	-	-	13/28/48/70	0/1/1/1
18	BCR	A	856	-	-	13/29/63/63	0/2/2/2
19	CLA	A	833	5	-	20/39/115/115	-
19	CLA	G	204	31	-	20/39/115/115	-
20	CHL	2	512	-	-	2/19/95/117	-
26	DGD	J	1106	-	-	14/47/87/95	0/2/2/2
18	BCR	1	503	-	-	7/11/28/63	0/1/1/2
18	BCR	B	850	-	-	10/29/63/63	0/2/2/2
19	CLA	B	823	6	-	15/27/103/115	-
28	SF4	C	101	7	-	-	0/6/5/5
20	CHL	2	515	-	-	4/17/93/117	-
19	CLA	B	812	6	-	13/33/109/115	-
26	DGD	G	207	-	-	10/36/76/95	0/2/2/2
19	CLA	B	806	6	-	18/39/115/115	-
22	LMG	G	206	-	-	18/45/65/70	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
19	CLA	A	830	5	-	16/39/115/115	-
19	CLA	3	316	-	-	11/17/93/115	-
19	CLA	A	824	5	-	18/39/115/115	-
18	BCR	B	849	-	-	10/29/63/63	0/2/2/2
19	CLA	A	832	5	-	13/39/115/115	-
19	CLA	A	815	5	-	7/15/91/115	-
22	LMG	2	521	-	-	0/4/24/70	0/1/1/1
19	CLA	4	310	-	-	13/33/109/115	-
19	CLA	B	839	6	-	20/39/115/115	-
19	CLA	H	1000	-	-	10/33/109/115	-
22	LMG	1	519	-	-	1/4/24/70	0/1/1/1
19	CLA	A	842	21	-	13/33/109/115	-
19	CLA	B	835	6	-	12/27/103/115	-
19	CLA	L	301	-	-	8/27/103/115	-
19	CLA	1	511	1	-	9/17/93/115	-
26	DGD	B	854	-	-	19/50/90/95	0/2/2/2
19	CLA	4	311	4	-	7/17/93/115	-
19	CLA	F	302	6	-	13/39/115/115	-
19	CLA	B	825	31	-	22/39/115/115	-
19	CLA	3	311	-	-	7/10/86/115	-
22	LMG	F	304	-	-	11/42/62/70	0/1/1/1
29	PQN	A	844	-	-	7/23/43/43	0/2/2/2
19	CLA	B	807	6	-	13/39/115/115	-
19	CLA	B	814	6	-	18/39/115/115	-
17	LUT	1	501	-	-	3/29/67/67	0/2/2/2
19	CLA	B	832	6	-	11/31/107/115	-
19	CLA	3	309	-	-	11/27/103/115	-
19	CLA	J	1105	-	-	10/21/97/115	-
22	LMG	2	520	-	-	0/4/24/70	0/1/1/1
20	CHL	1	514	1	1/1/14/21	11/35/111/117	-
23	XAT	2	502	-	-	5/31/93/93	0/4/4/4
19	CLA	2	507	2	-	13/39/115/115	-
19	CLA	B	830	6	-	13/39/115/115	-
19	CLA	3	317	3	-	6/17/93/115	-
18	BCR	K	1005	-	-	12/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
18	BCR	I	101	-	-	11/29/63/63	0/2/2/2
19	CLA	A	817	-	-	18/39/115/115	-
19	CLA	4	308	4	-	13/33/109/115	-
19	CLA	A	810	5	-	8/21/97/115	-
22	LMG	1	518	-	-	12/41/61/70	0/1/1/1
21	LHG	B	843	-	-	28/53/53/53	-
19	CLA	B	831	6	-	17/33/109/115	-
19	CLA	1	508	1	-	22/39/115/115	-
19	CLA	4	307	4	-	13/33/109/115	-
19	CLA	4	304	4	-	10/33/109/115	-
21	LHG	1	517	-	-	28/53/53/53	-
19	CLA	A	826	31	-	11/27/103/115	-
20	CHL	4	313	-	-	0/19/95/117	-
22	LMG	G	210	-	-	10/20/40/70	0/1/1/1
19	CLA	A	820	-	-	10/21/97/115	-
22	LMG	2	525	-	-	0/4/24/70	0/1/1/1
22	LMG	2	519	-	-	17/31/51/70	0/1/1/1
19	CLA	A	802	-	-	19/39/115/115	-
19	CLA	A	805	5	-	28/39/115/115	-

The worst 5 of 1169 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	4	302	LUT	C24-C25	14.95	1.51	1.33
17	3	301	LUT	C24-C25	14.77	1.51	1.33
17	1	501	LUT	C24-C25	14.56	1.51	1.33
17	1	502	LUT	C24-C25	14.52	1.51	1.33
17	2	501	LUT	C24-C25	14.34	1.51	1.33

The worst 5 of 2796 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
18	B	802	BCR	C16-C15-C14	18.74	161.87	123.47
18	I	101	BCR	C16-C15-C14	15.15	154.50	123.47
18	B	849	BCR	C21-C20-C19	14.35	168.01	123.22
18	3	304	BCR	C16-C15-C14	13.99	152.13	123.47
18	3	304	BCR	C21-C20-C19	13.99	166.87	123.22

5 of 11 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
17	1	502	LUT	C26
17	2	501	LUT	C26
17	3	302	LUT	C26
17	J	1109	LUT	C26
20	1	514	CHL	C8

5 of 2756 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
17	1	502	LUT	C21-C26-C27-C28
17	1	502	LUT	C27-C28-C29-C30
17	1	502	LUT	C27-C28-C29-C39
17	1	502	LUT	C31-C32-C33-C40
17	2	501	LUT	C1-C6-C7-C8

There are no ring outliers.

229 monomers are involved in 878 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
19	A	819	CLA	7	0
19	2	505	CLA	1	0
19	3	306	CLA	9	0
22	A	847	LMG	4	0
19	A	822	CLA	4	0
19	B	815	CLA	4	0
20	2	516	CHL	3	0
19	1	504	CLA	10	0
28	C	102	SF4	2	0
18	B	851	BCR	4	0
19	B	804	CLA	4	0
18	F	306	BCR	1	0
17	3	301	LUT	11	0
17	1	502	LUT	5	0
22	F	305	LMG	2	0
19	B	827	CLA	2	0
18	A	850	BCR	5	0
19	K	1002	CLA	1	0
21	B	842	LHG	2	0
19	1	516	CLA	4	0
19	B	811	CLA	5	0
19	L	305	CLA	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
19	4	306	CLA	5	0
19	4	315	CLA	3	0
21	A	853	LHG	3	0
18	A	852	BCR	6	0
19	2	510	CLA	4	0
19	A	803	CLA	5	0
18	3	303	BCR	8	0
19	A	837	CLA	5	0
19	B	820	CLA	5	0
24	G	209	LMT	1	0
19	3	313	CLA	3	0
20	4	316	CHL	8	0
19	A	827	CLA	8	0
19	A	825	CLA	8	0
19	A	839	CLA	6	0
18	B	856	BCR	6	0
20	4	314	CHL	6	0
19	A	821	CLA	9	0
19	B	813	CLA	1	0
19	B	826	CLA	6	0
19	G	201	CLA	6	0
22	B	844	LMG	4	0
19	G	202	CLA	3	0
18	2	503	BCR	11	0
19	B	805	CLA	7	0
19	A	814	CLA	2	0
20	1	521	CHL	7	0
19	A	829	CLA	4	0
19	B	819	CLA	12	0
19	2	511	CLA	4	0
19	A	804	CLA	5	0
28	A	843	SF4	1	0
29	B	841	PQN	8	0
20	2	526	CHL	10	0
17	2	501	LUT	7	0
19	B	836	CLA	5	0
24	4	320	LMT	2	0
19	A	812	CLA	6	0
19	L	304	CLA	3	0
19	4	312	CLA	2	0
24	J	1107	LMT	1	0
18	4	301	BCR	9	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
20	1	512	CHL	4	0
19	3	315	CLA	4	0
18	B	853	BCR	6	0
19	A	854	CLA	8	0
18	G	205	BCR	3	0
18	J	1108	BCR	4	0
18	A	849	BCR	1	0
19	J	1101	CLA	11	0
19	B	803	CLA	5	0
19	B	828	CLA	2	0
19	J	1102	CLA	5	0
26	4	319	DGD	6	0
21	A	845	LHG	6	0
17	3	302	LUT	9	0
19	B	817	CLA	3	0
19	A	831	CLA	4	0
19	A	809	CLA	9	0
19	A	813	CLA	8	0
20	3	314	CHL	9	0
18	A	848	BCR	1	0
19	B	821	CLA	1	0
19	K	1001	CLA	6	0
19	A	828	CLA	8	0
19	A	808	CLA	6	0
21	1	520	LHG	11	0
22	J	1104	LMG	2	0
26	B	801	DGD	5	0
19	G	203	CLA	3	0
19	4	309	CLA	9	0
19	4	305	CLA	4	0
19	3	305	CLA	18	0
18	L	306	BCR	2	0
19	1	507	CLA	5	0
22	4	322	LMG	4	0
18	A	851	BCR	4	0
19	B	824	CLA	3	0
19	B	829	CLA	10	0
19	2	508	CLA	5	0
19	A	807	CLA	4	0
19	A	840	CLA	3	0
19	B	822	CLA	5	0
22	J	1103	LMG	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
19	B	816	CLA	4	0
18	3	304	BCR	4	0
30	F	301	ZEX	5	0
19	A	818	CLA	8	0
19	B	808	CLA	6	0
19	2	504	CLA	6	0
19	B	834	CLA	7	0
19	F	303	CLA	6	0
19	B	837	CLA	6	0
24	B	846	LMT	3	0
23	4	303	XAT	9	0
21	2	517	LHG	9	0
19	2	509	CLA	1	0
19	1	510	CLA	8	0
19	1	505	CLA	3	0
19	A	816	CLA	1	0
19	A	841	CLA	8	0
24	G	208	LMT	4	0
19	B	809	CLA	5	0
17	4	302	LUT	3	0
19	B	810	CLA	3	0
27	A	801	CL0	6	0
19	A	834	CLA	6	0
19	3	308	CLA	12	0
19	A	823	CLA	3	0
17	J	1109	LUT	8	0
19	3	310	CLA	7	0
19	1	513	CLA	2	0
18	B	852	BCR	4	0
19	1	515	CLA	4	0
19	B	818	CLA	5	0
19	2	506	CLA	6	0
19	2	514	CLA	3	0
19	A	811	CLA	10	0
19	4	318	CLA	10	0
19	A	836	CLA	3	0
24	3	318	LMT	2	0
24	B	855	LMT	3	0
22	2	518	LMG	2	0
19	B	838	CLA	9	0
20	2	513	CHL	7	0
24	A	846	LMT	3	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
19	L	303	CLA	2	0
20	4	317	CHL	5	0
19	A	835	CLA	2	0
19	3	307	CLA	5	0
24	B	847	LMT	2	0
19	B	833	CLA	6	0
18	B	802	BCR	4	0
18	L	302	BCR	3	0
19	K	1004	CLA	2	0
19	A	855	CLA	8	0
18	L	307	BCR	1	0
22	2	524	LMG	1	0
19	B	840	CLA	14	0
18	I	102	BCR	5	0
19	A	806	CLA	6	0
19	A	838	CLA	4	0
19	1	509	CLA	3	0
22	B	845	LMG	2	0
19	K	1003	CLA	1	0
18	A	856	BCR	3	0
19	A	833	CLA	7	0
19	G	204	CLA	13	0
20	2	512	CHL	8	0
26	J	1106	DGD	6	0
18	1	503	BCR	4	0
18	B	850	BCR	2	0
19	B	823	CLA	9	0
20	2	515	CHL	4	0
19	B	812	CLA	6	0
26	G	207	DGD	1	0
19	B	806	CLA	7	0
22	G	206	LMG	5	0
19	A	830	CLA	8	0
19	3	316	CLA	4	0
19	A	824	CLA	12	0
18	B	849	BCR	1	0
19	A	832	CLA	6	0
19	A	815	CLA	1	0
19	4	310	CLA	5	0
19	B	839	CLA	6	0
19	H	1000	CLA	2	0
19	A	842	CLA	8	0

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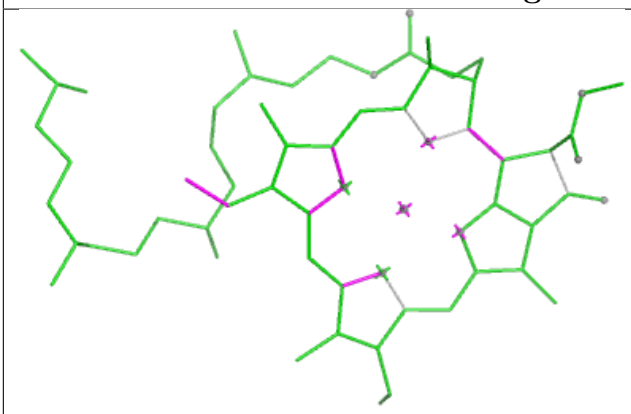
Mol	Chain	Res	Type	Clashes	Symm-Clashes
19	B	835	CLA	4	0
19	L	301	CLA	2	0
19	1	511	CLA	1	0
26	B	854	DGD	9	0
19	4	311	CLA	4	0
19	F	302	CLA	4	0
19	B	825	CLA	9	0
22	F	304	LMG	8	0
29	A	844	PQN	3	0
19	B	807	CLA	3	0
19	B	814	CLA	4	0
17	1	501	LUT	6	0
19	B	832	CLA	7	0
19	3	309	CLA	2	0
19	J	1105	CLA	7	0
20	1	514	CHL	9	0
23	2	502	XAT	4	0
19	2	507	CLA	4	0
19	B	830	CLA	10	0
19	3	317	CLA	3	0
18	K	1005	BCR	7	0
18	I	101	BCR	6	0
19	A	817	CLA	3	0
19	4	308	CLA	3	0
19	A	810	CLA	3	0
22	1	518	LMG	4	0
21	B	843	LHG	6	0
19	B	831	CLA	1	0
19	1	508	CLA	13	0
19	4	307	CLA	7	0
19	4	304	CLA	6	0
21	1	517	LHG	7	0
19	A	826	CLA	3	0
20	4	313	CHL	1	0
22	G	210	LMG	1	0
19	A	820	CLA	2	0
22	2	519	LMG	7	0
19	A	802	CLA	11	0
19	A	805	CLA	10	0

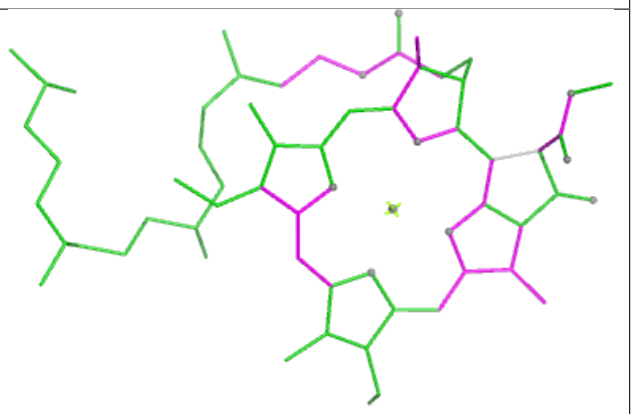
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will

also be included. For torsion angles, if less 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.

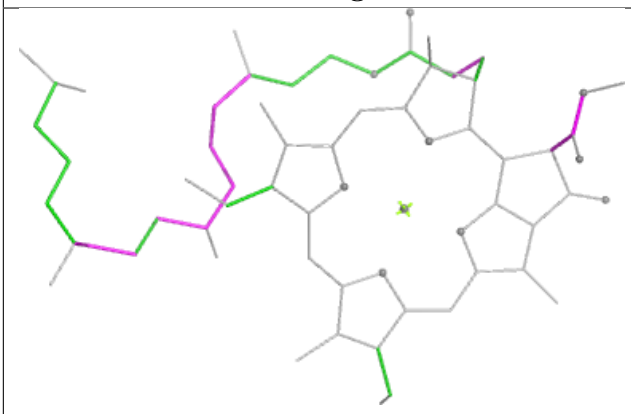
Ligand CLA A 819



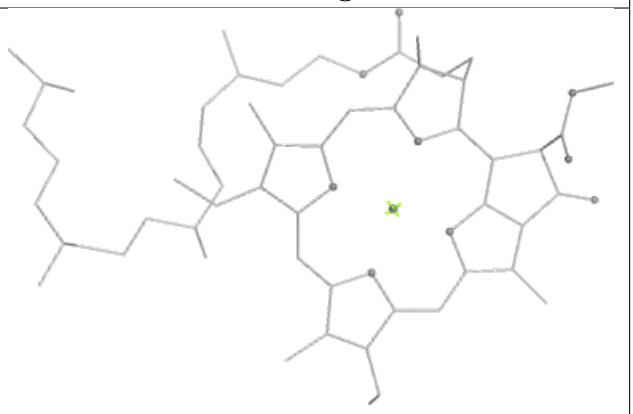
Bond lengths



Bond angles

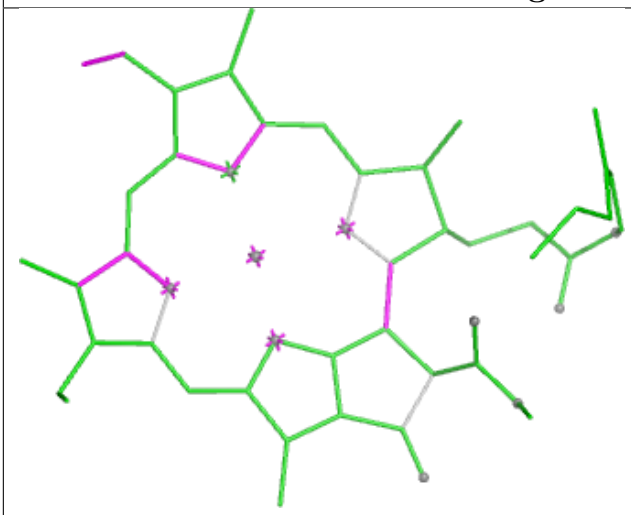


Torsions



Rings

Ligand CLA 2 505



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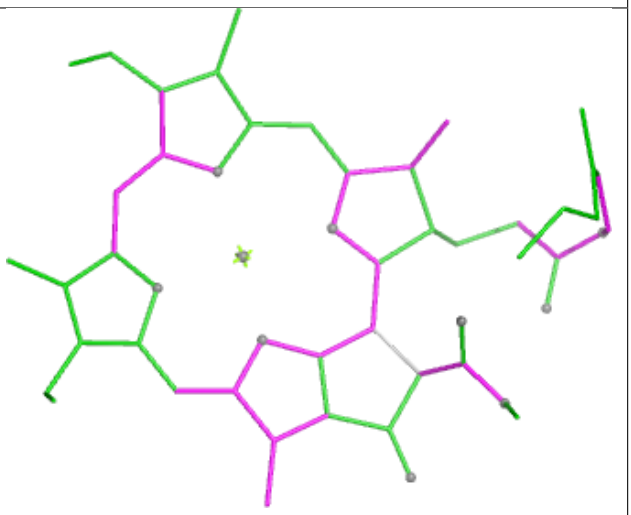
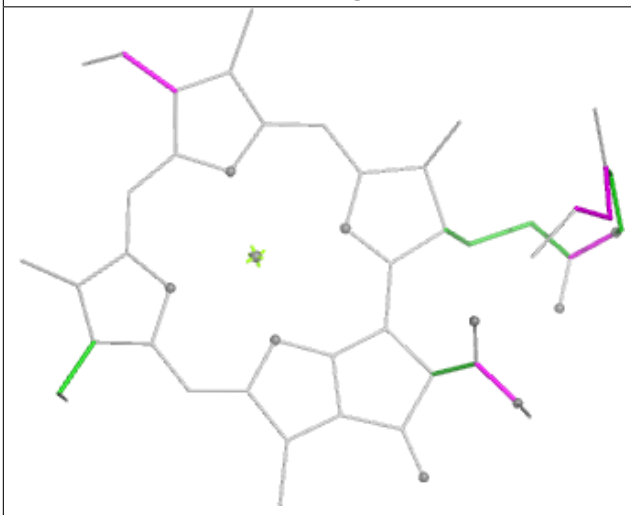


Bond angles



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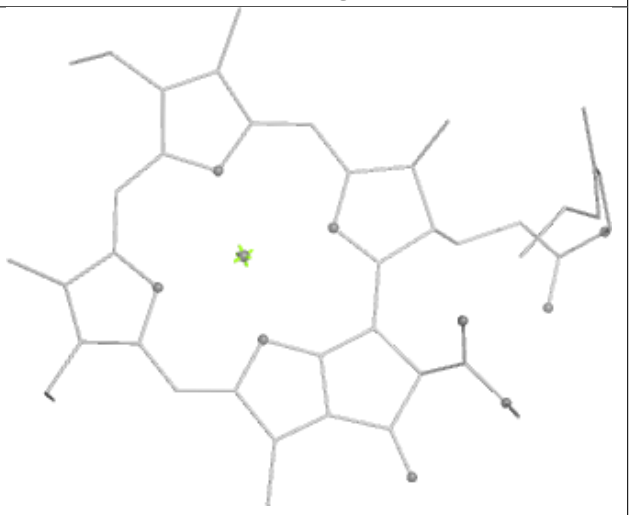
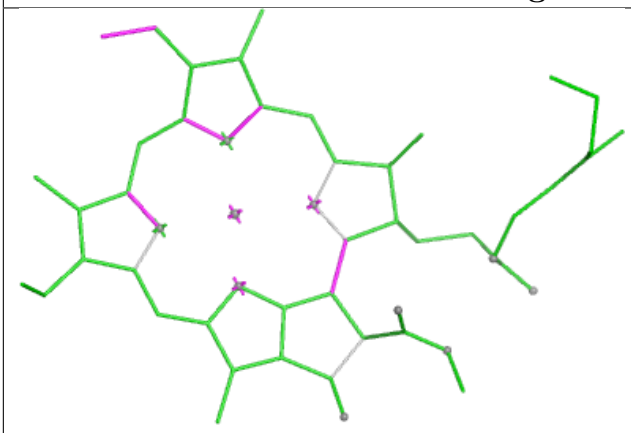
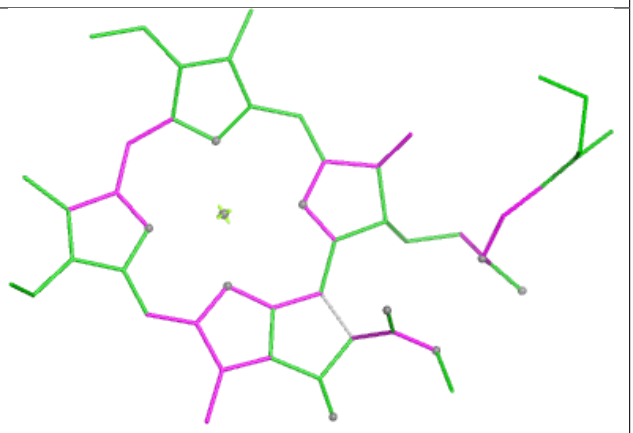


Rings

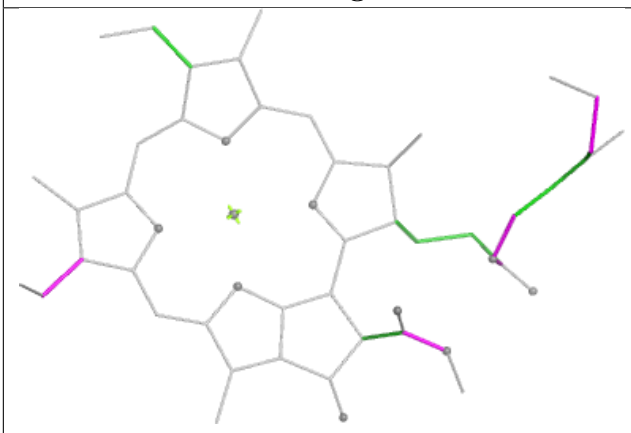
Ligand CLA 3 306



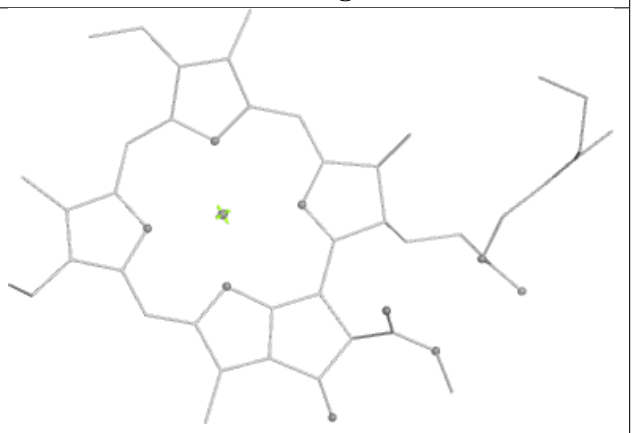
Bond lengths



Bond angles

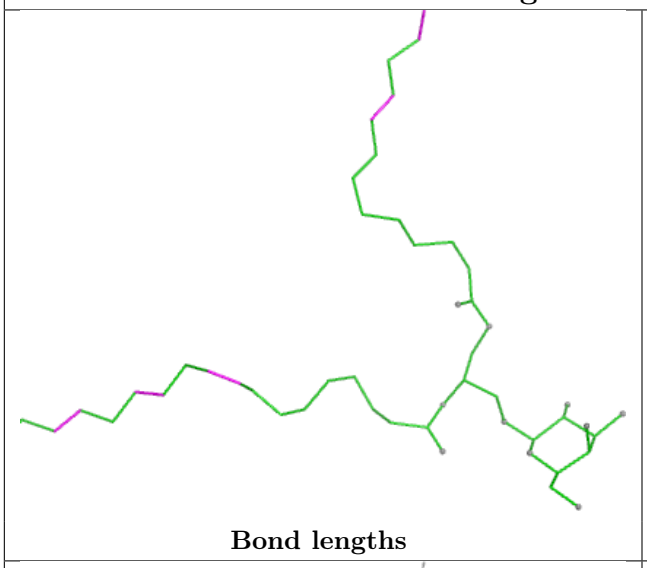


Torsions



Rings

Ligand LMG A 847



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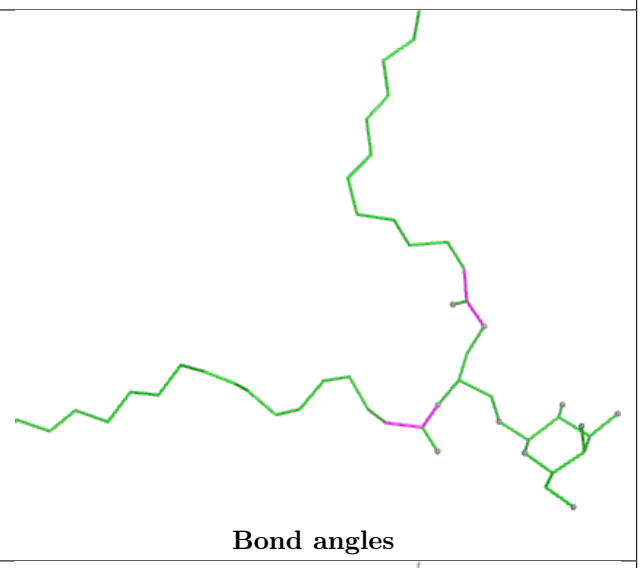
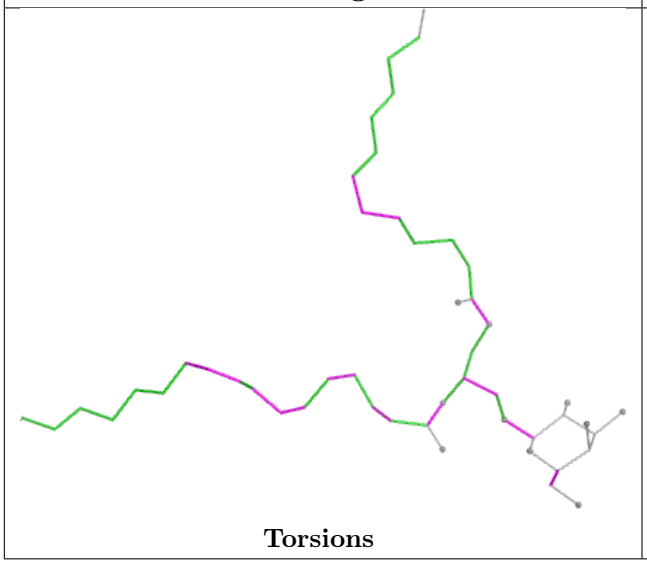
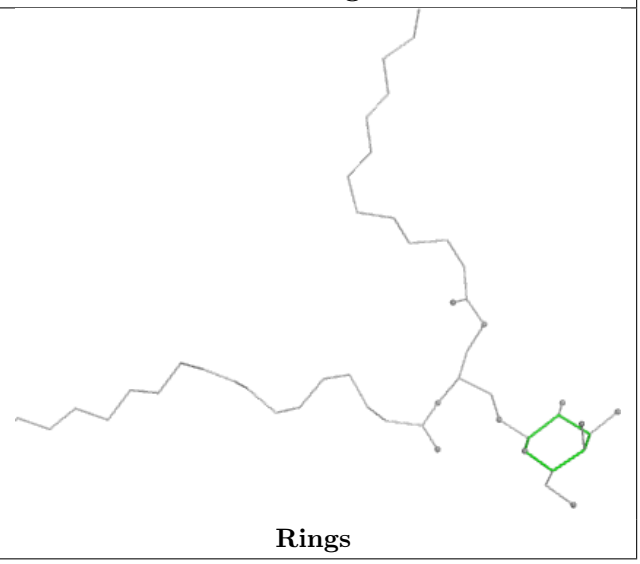


Bond angles

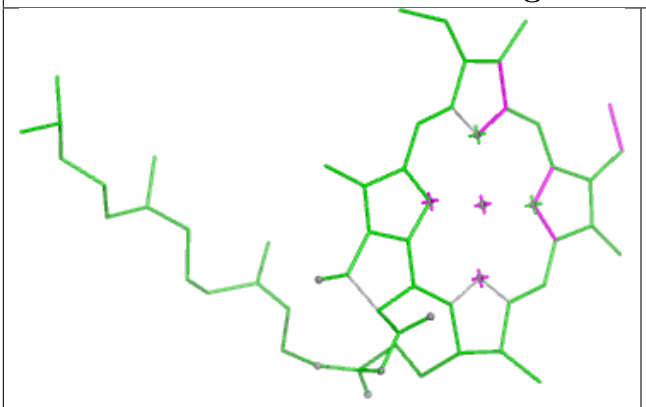


Torsions

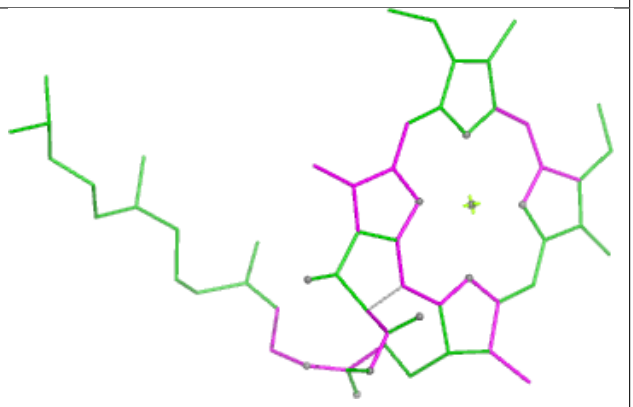


Rings

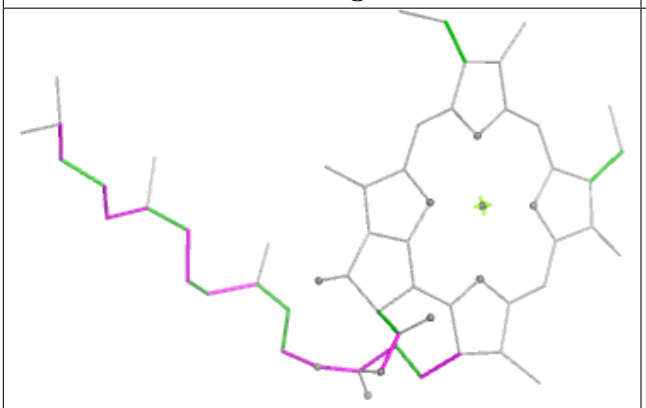
Ligand CLA A 822



Bond lengths



Bond angles

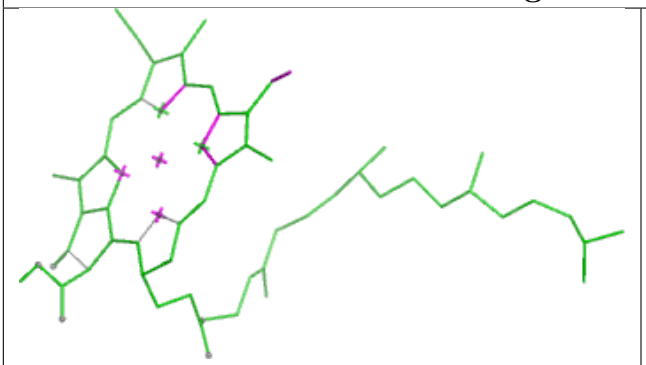


Torsions

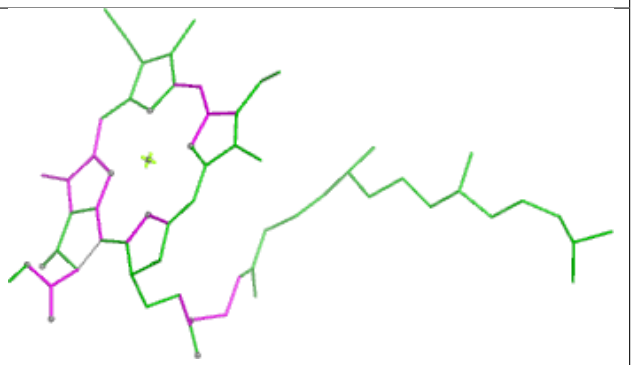


Rings

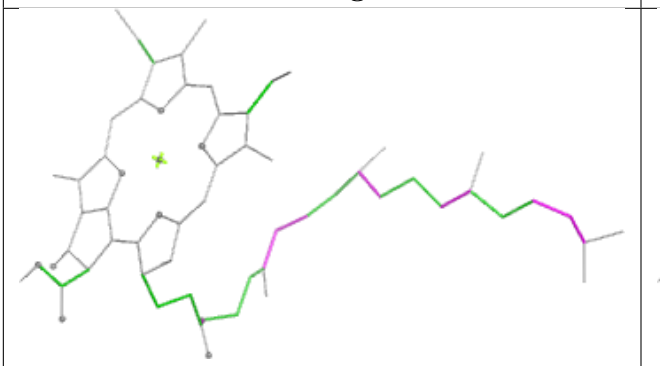
Ligand CLA B 815



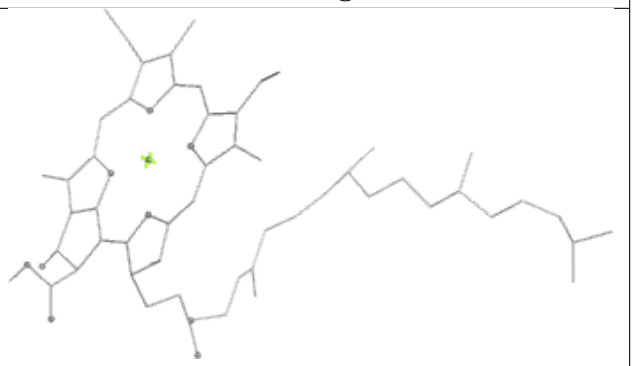
Bond lengths



Bond angles

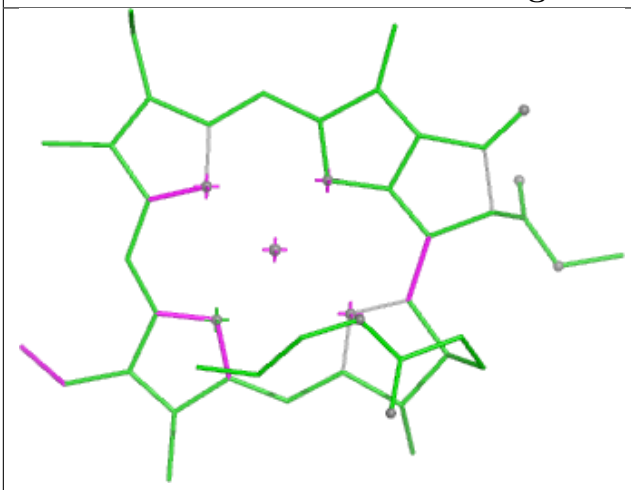


Torsions

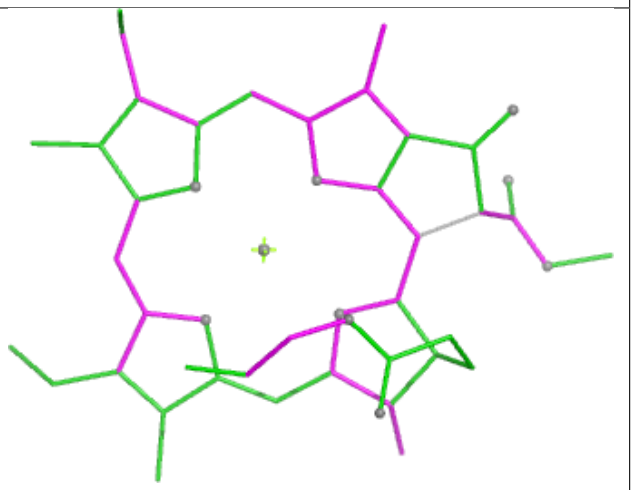


Rings

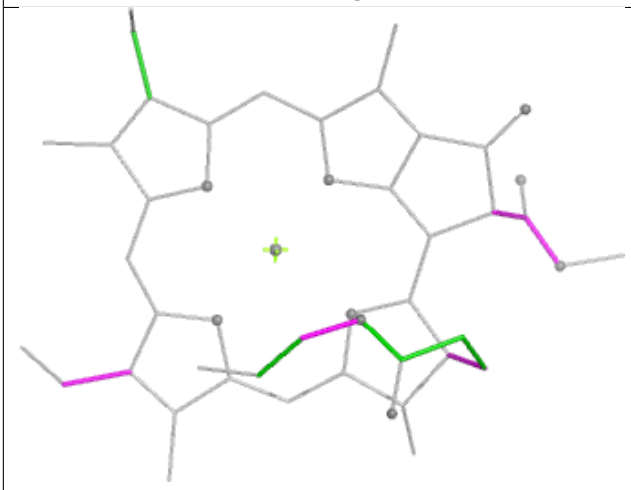
Ligand CLA 3 312



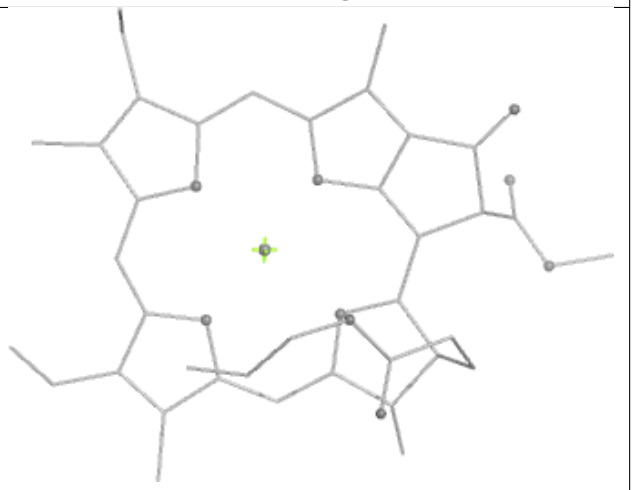
Bond lengths



Bond angles

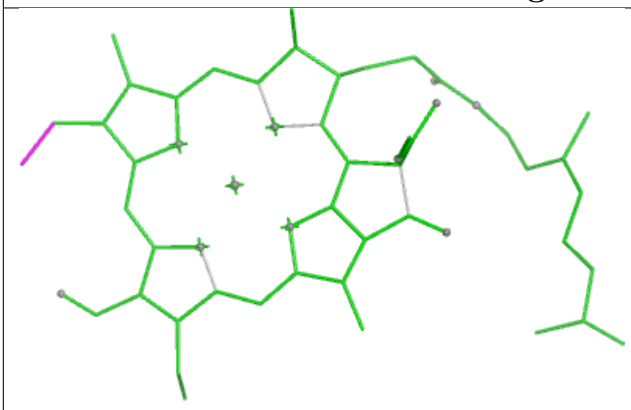


Torsions



Rings

Ligand CHL 2 516



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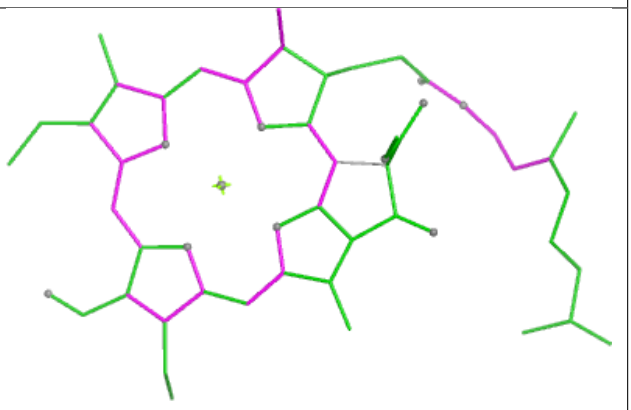
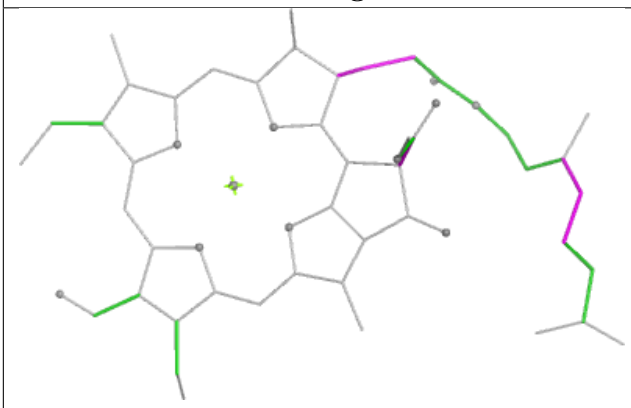


Bond angles



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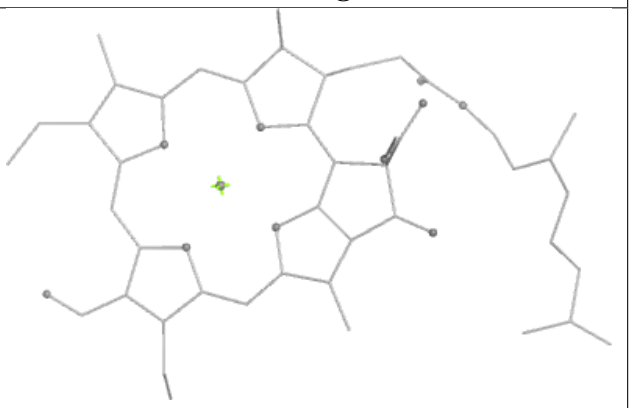
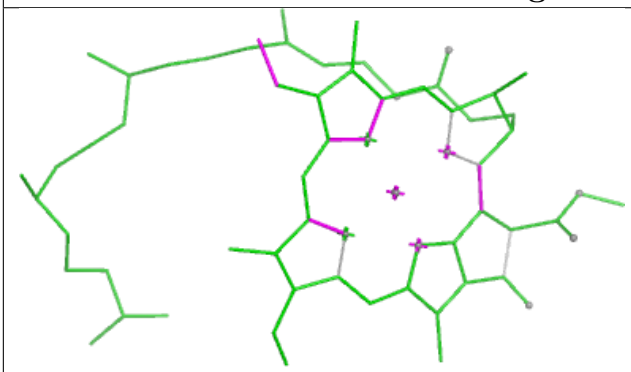
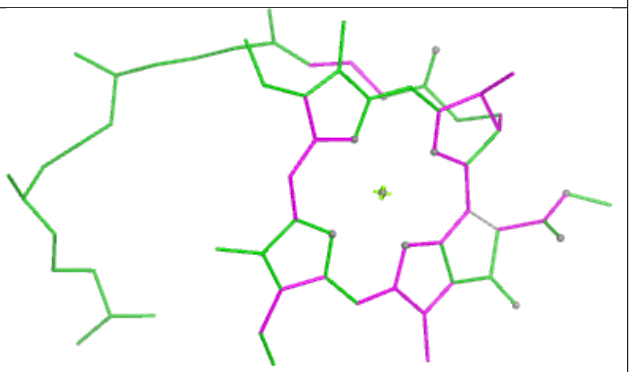


Rings

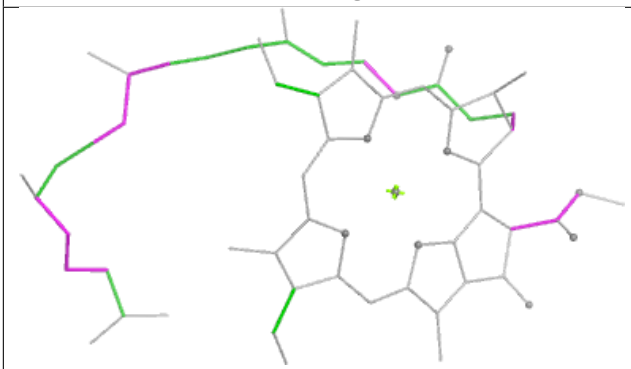
Ligand CLA 1 504



Bond lengths



Bond angles



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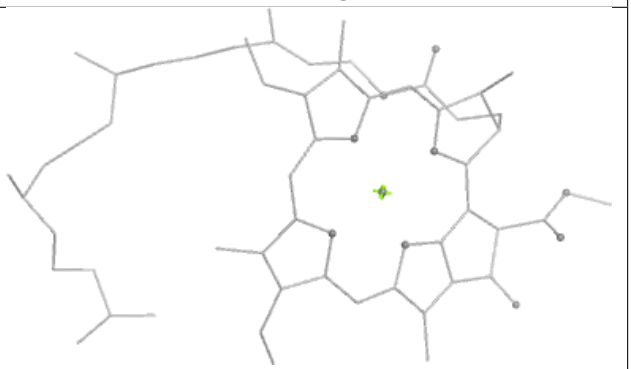
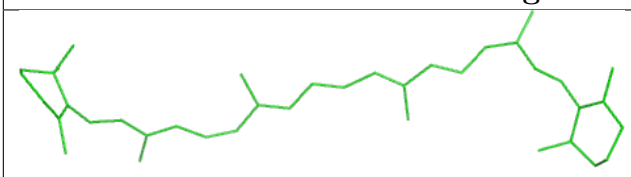


Rings

Ligand BCR B 851



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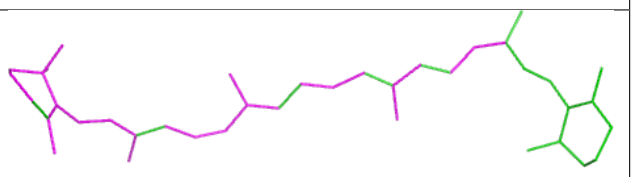
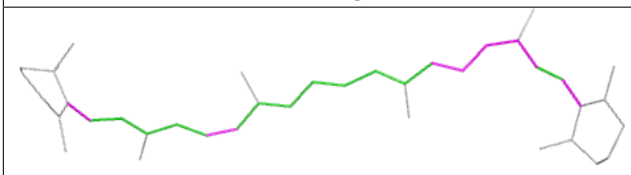


Bond angles



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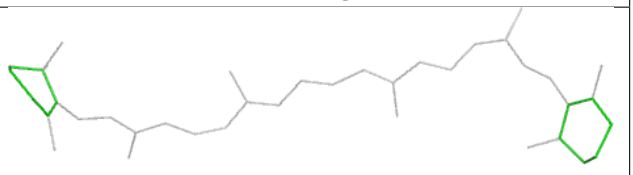
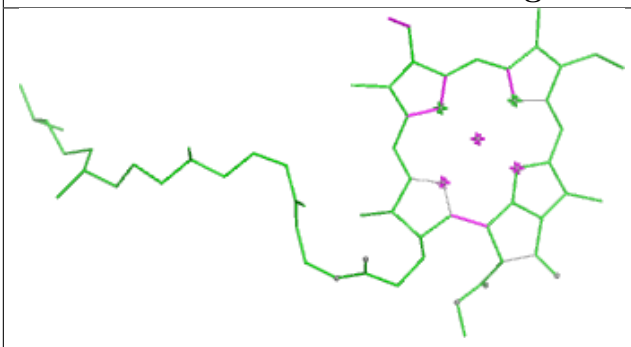
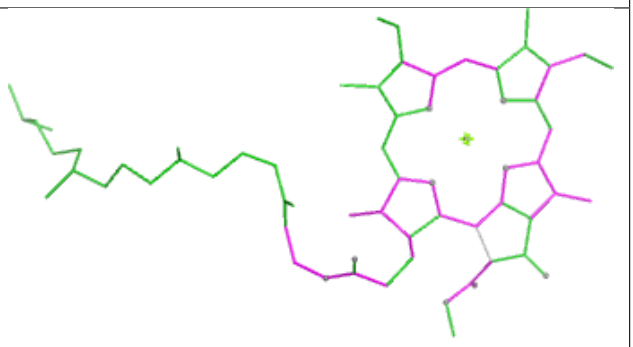


Rings

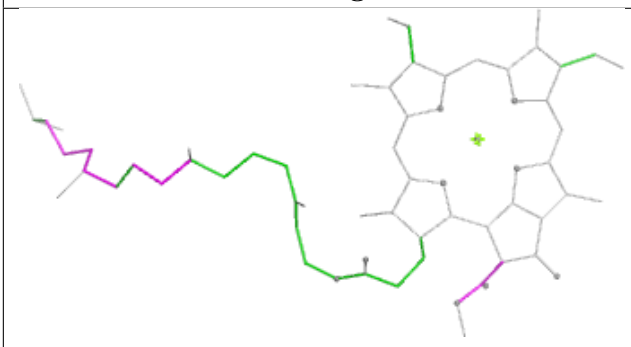
Ligand CLA B 804



Bond lengths



Bond angles

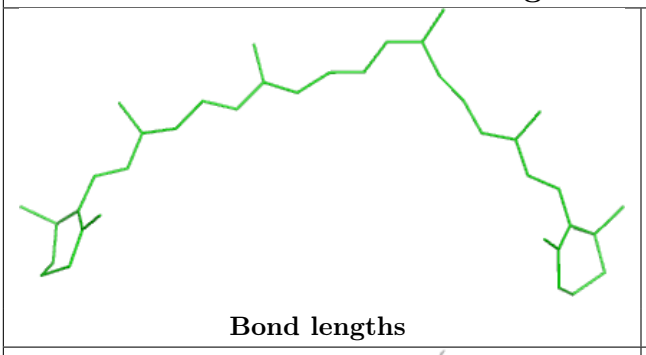


Torsions



Rings

Ligand BCR F 306



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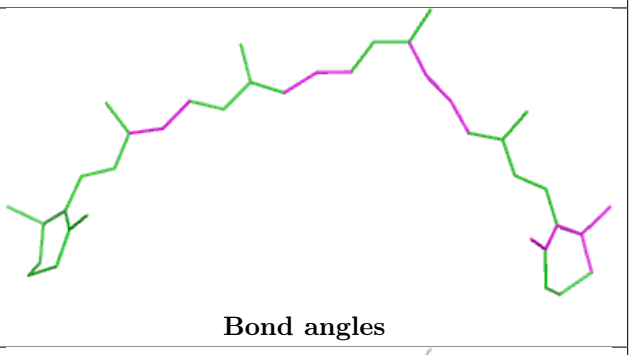
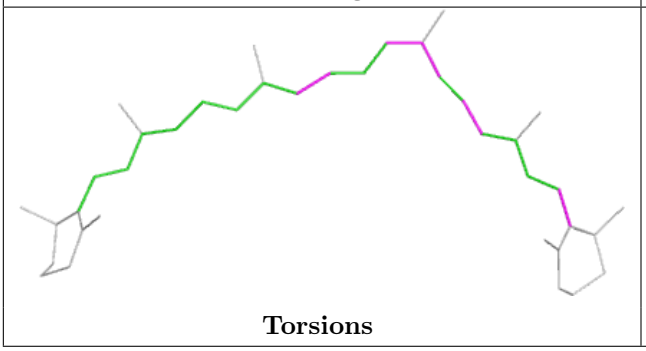


Bond angles



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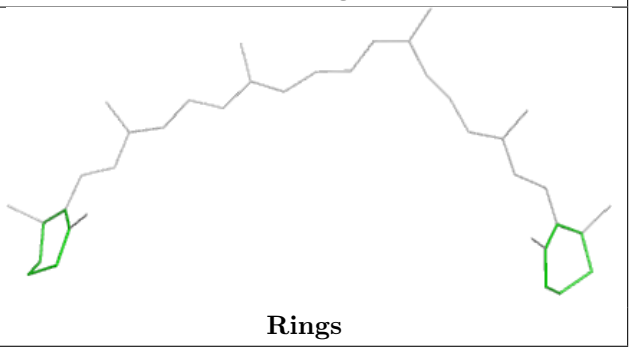
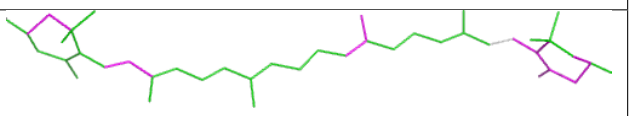


Rings

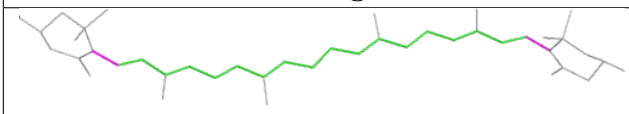
Ligand LUT 3 301



Bond lengths



Bond angles



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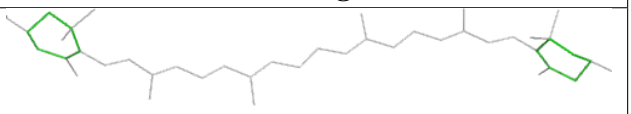
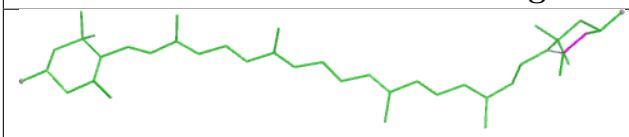
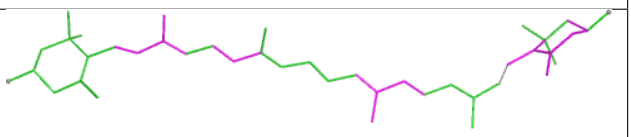


Rings

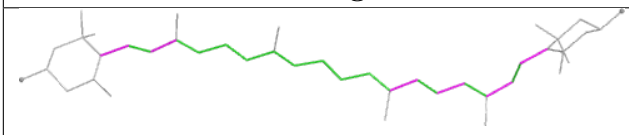
Ligand LUT 1 502



Bond lengths



Bond angles



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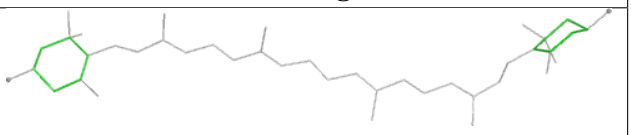
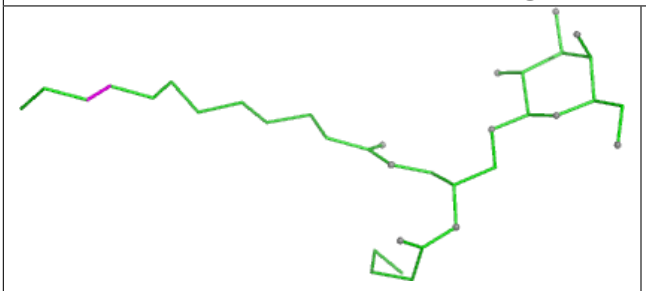


Rings

Ligand LMG F 305



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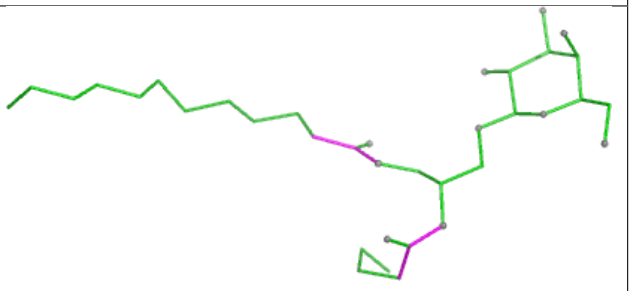
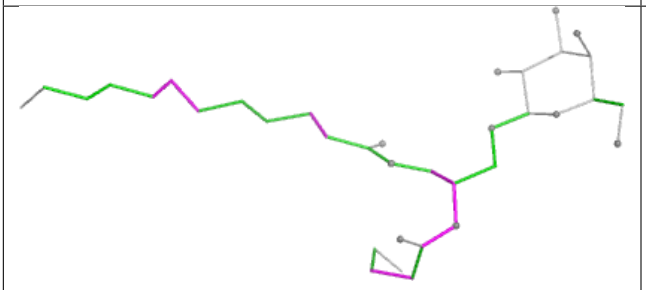


Bond angles



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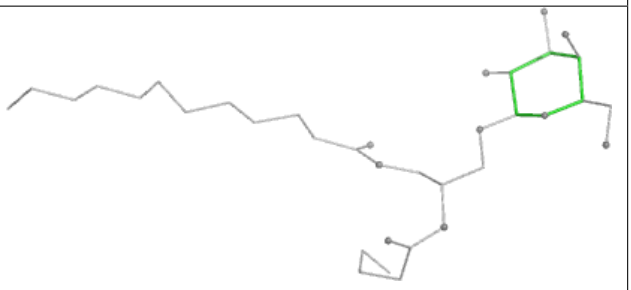
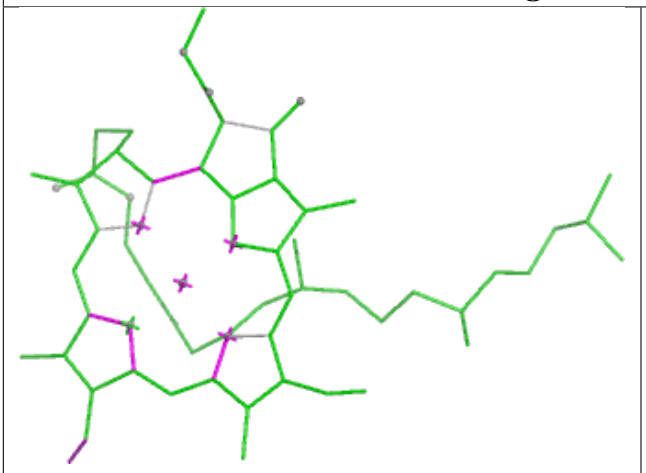


Rings

Ligand CLA B 827



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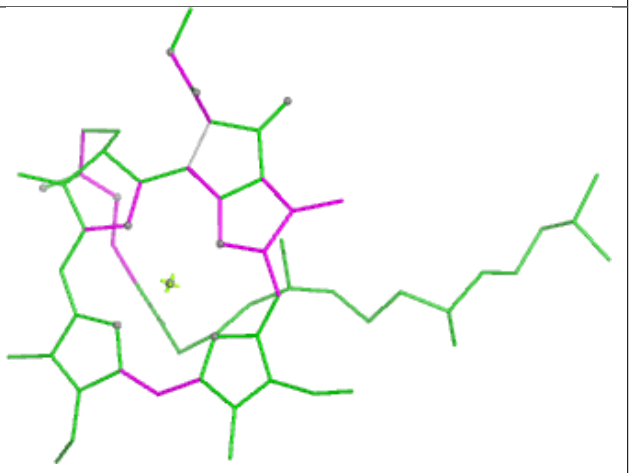
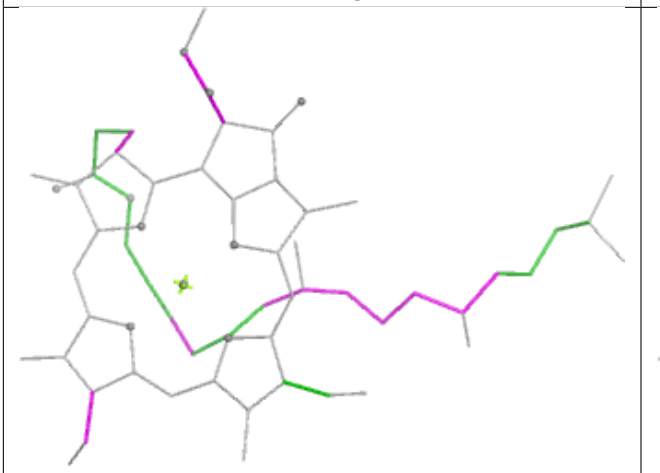


Bond angles



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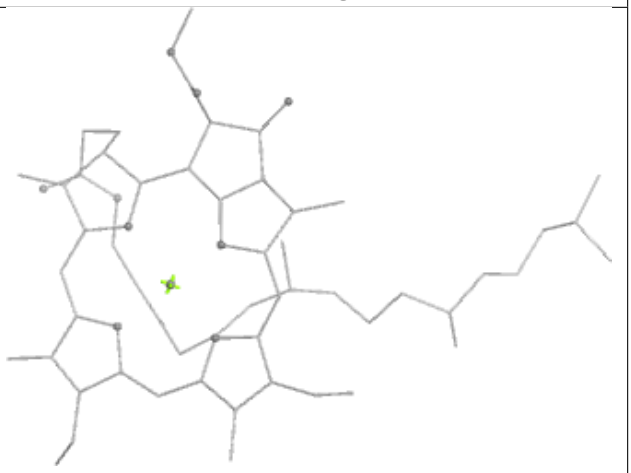
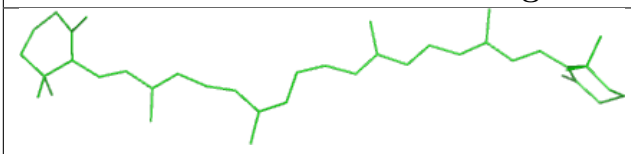


Rings

Ligand BCR A 850



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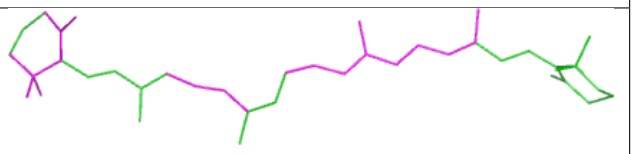
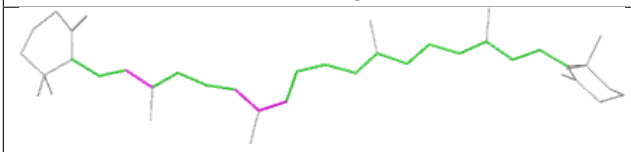


Bond angles



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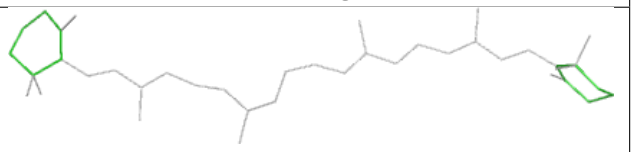
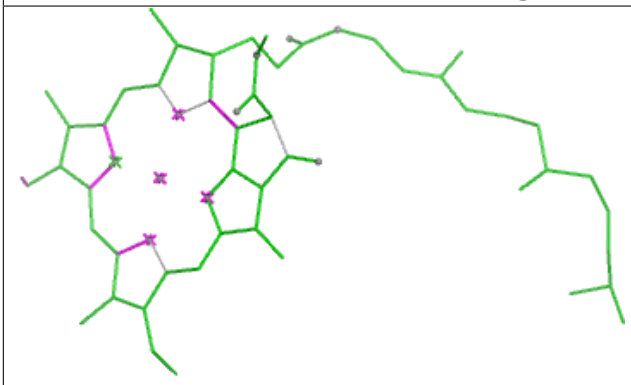


Rings

Ligand CLA K 1002



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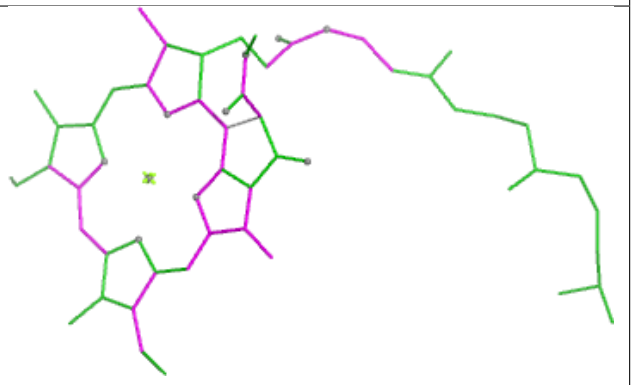
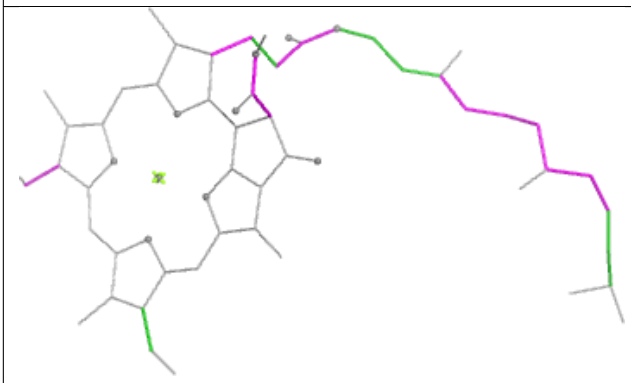


Bond angles



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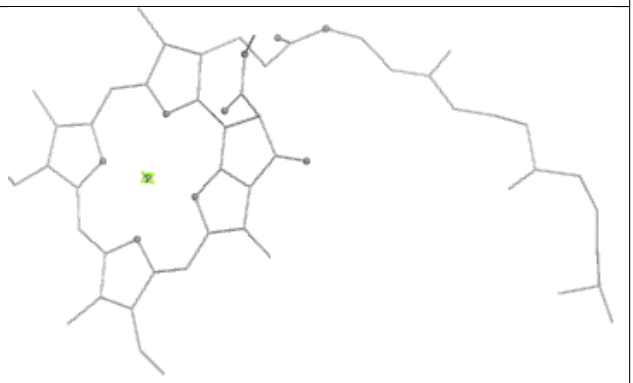
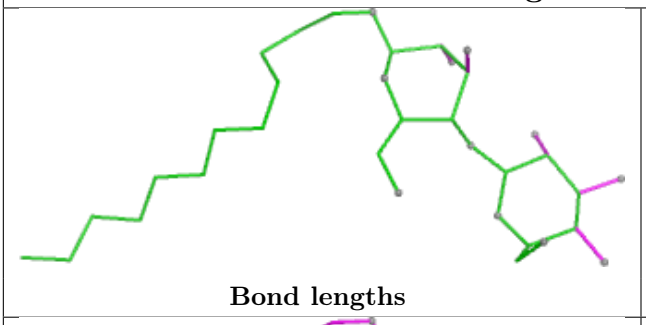


Rings

Ligand LMT 2 523



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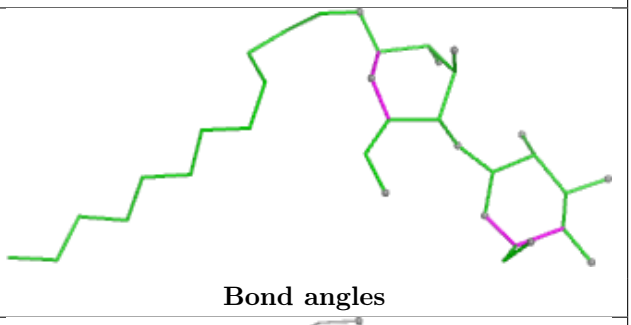
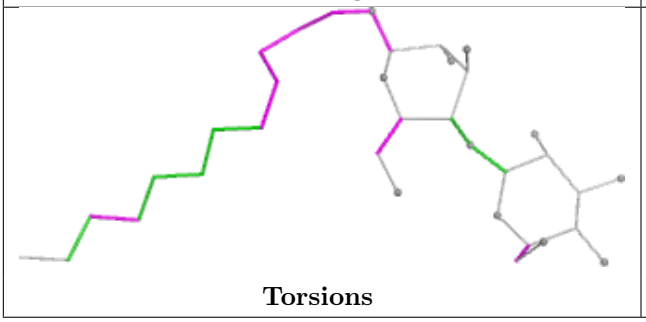


Bond angles



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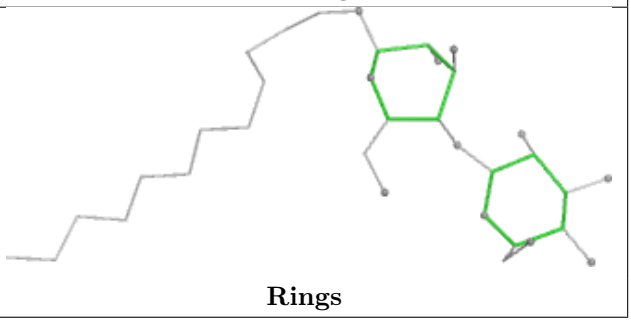
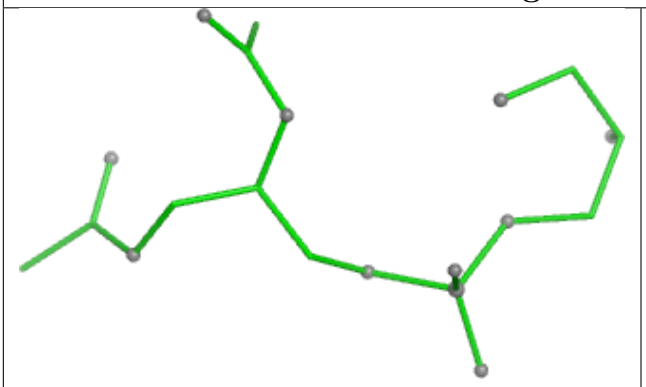


Rings

Ligand LHG B 842



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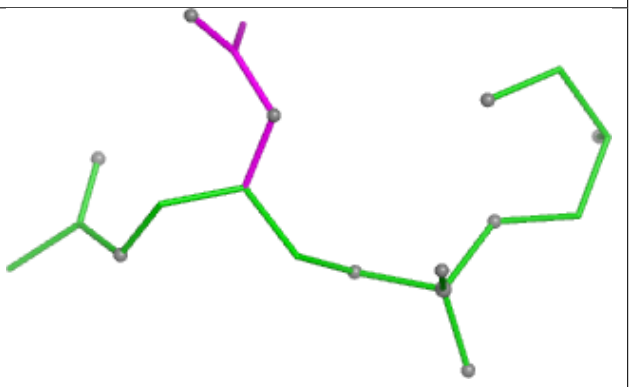
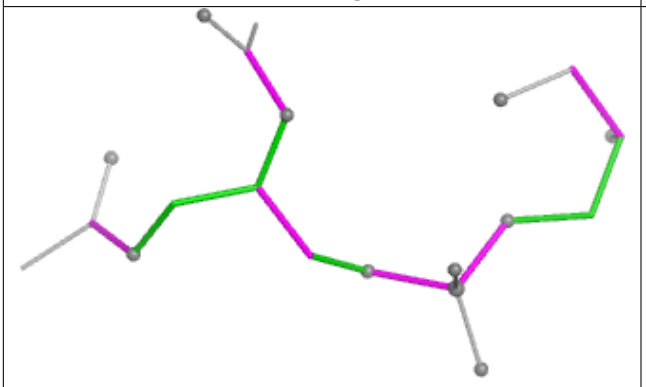


Bond angles



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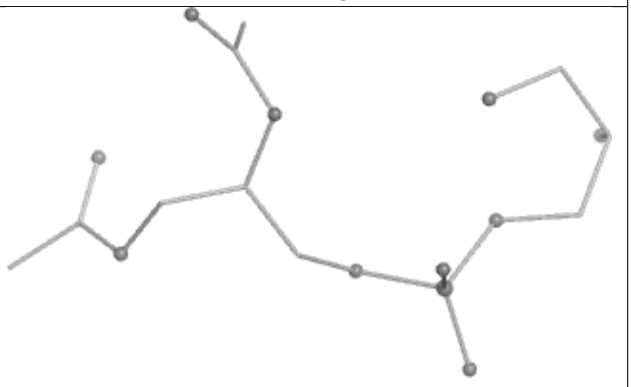
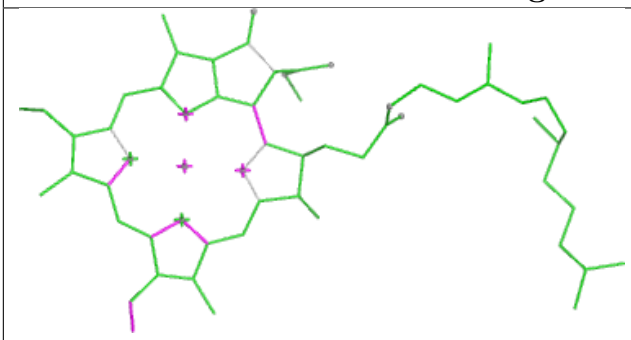
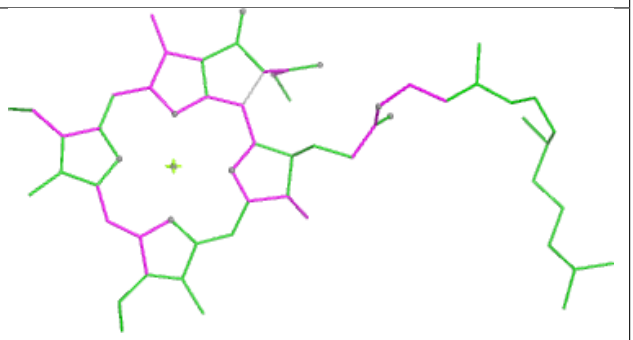


Rings

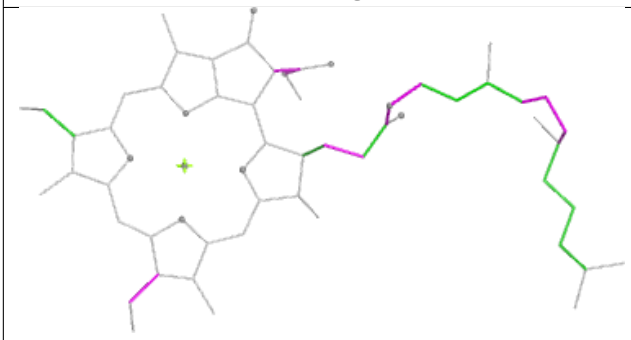
Ligand CLA 1 516



Bond lengths



Bond angles



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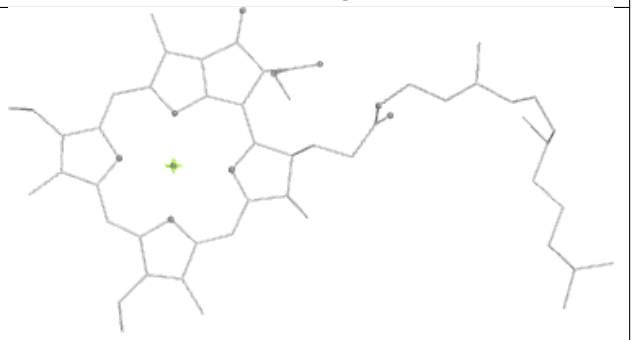
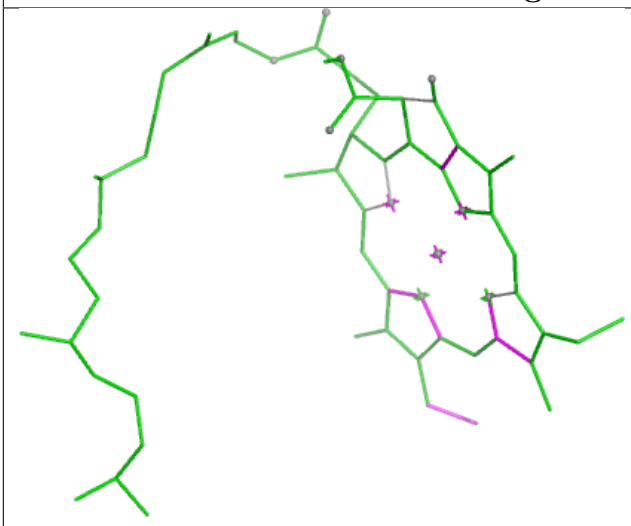
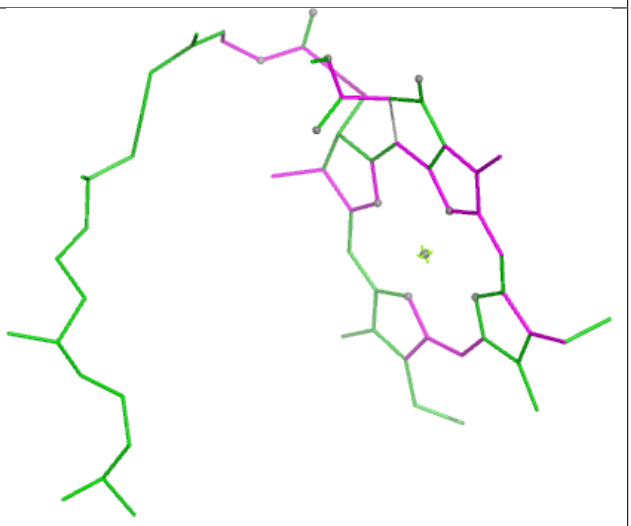


Rings

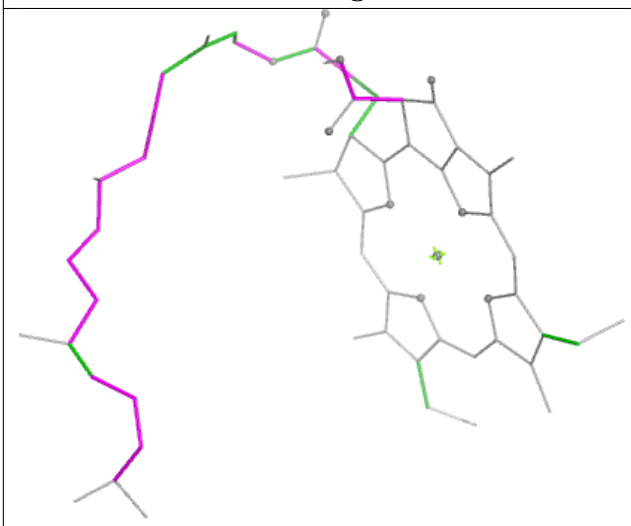
Ligand CLA B 811



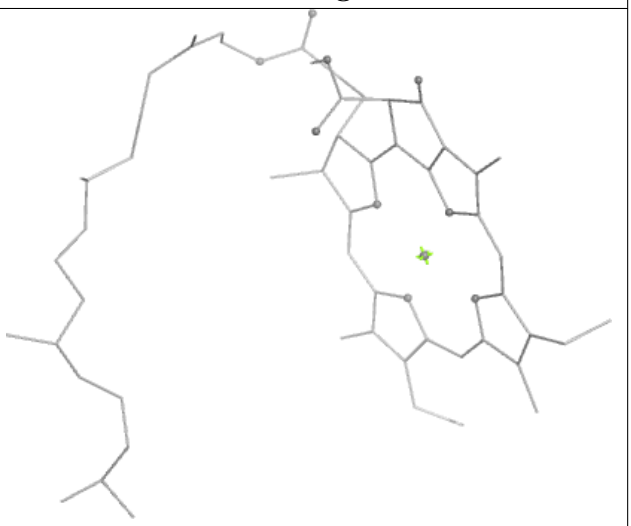
Bond lengths



Bond angles

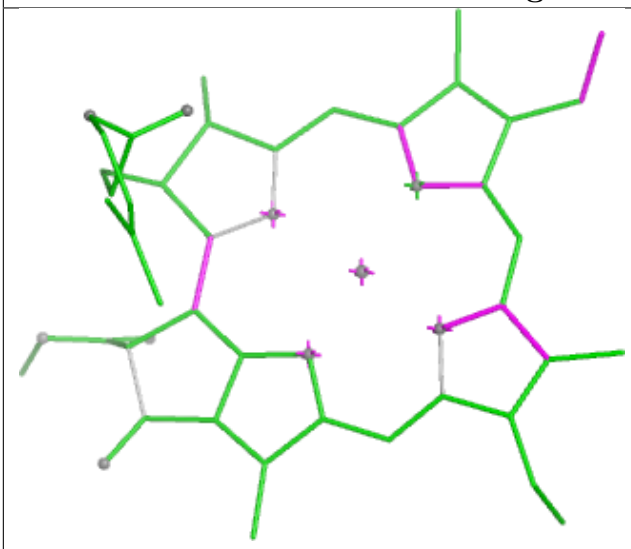


Torsions



Rings

Ligand CLA L 305



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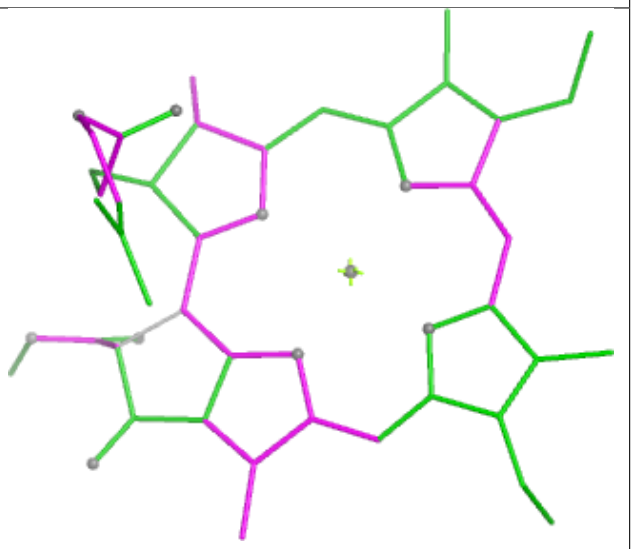
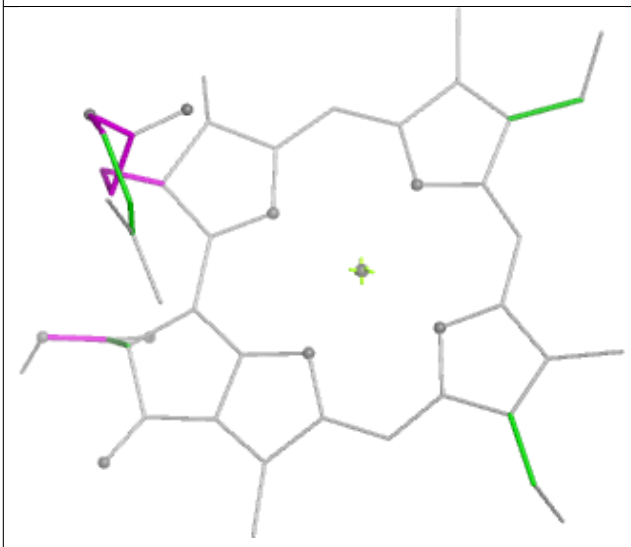


Bond angles



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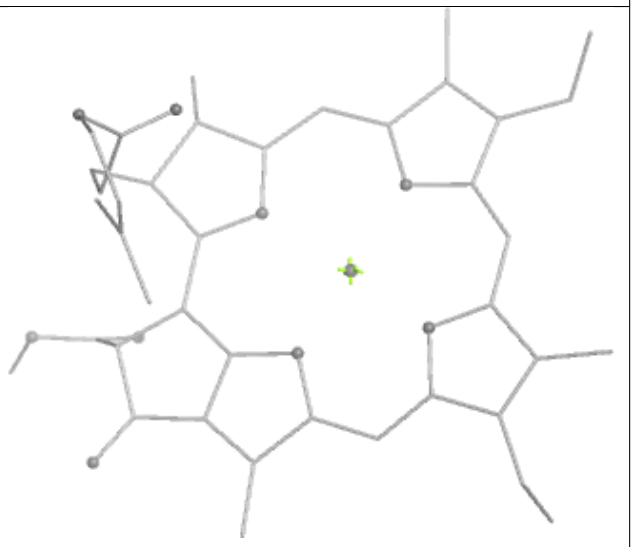
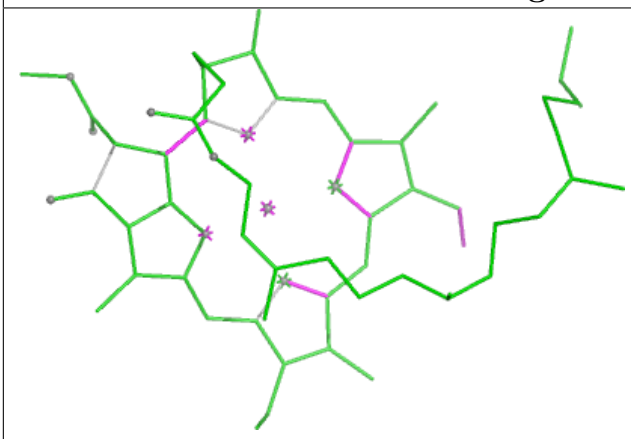


Rings

Ligand CLA 4 306



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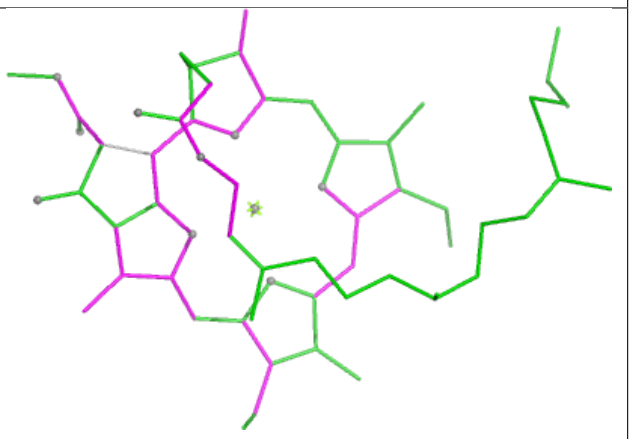
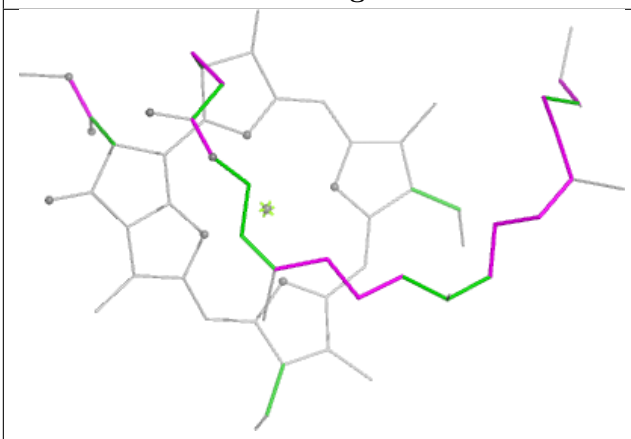


Bond angles

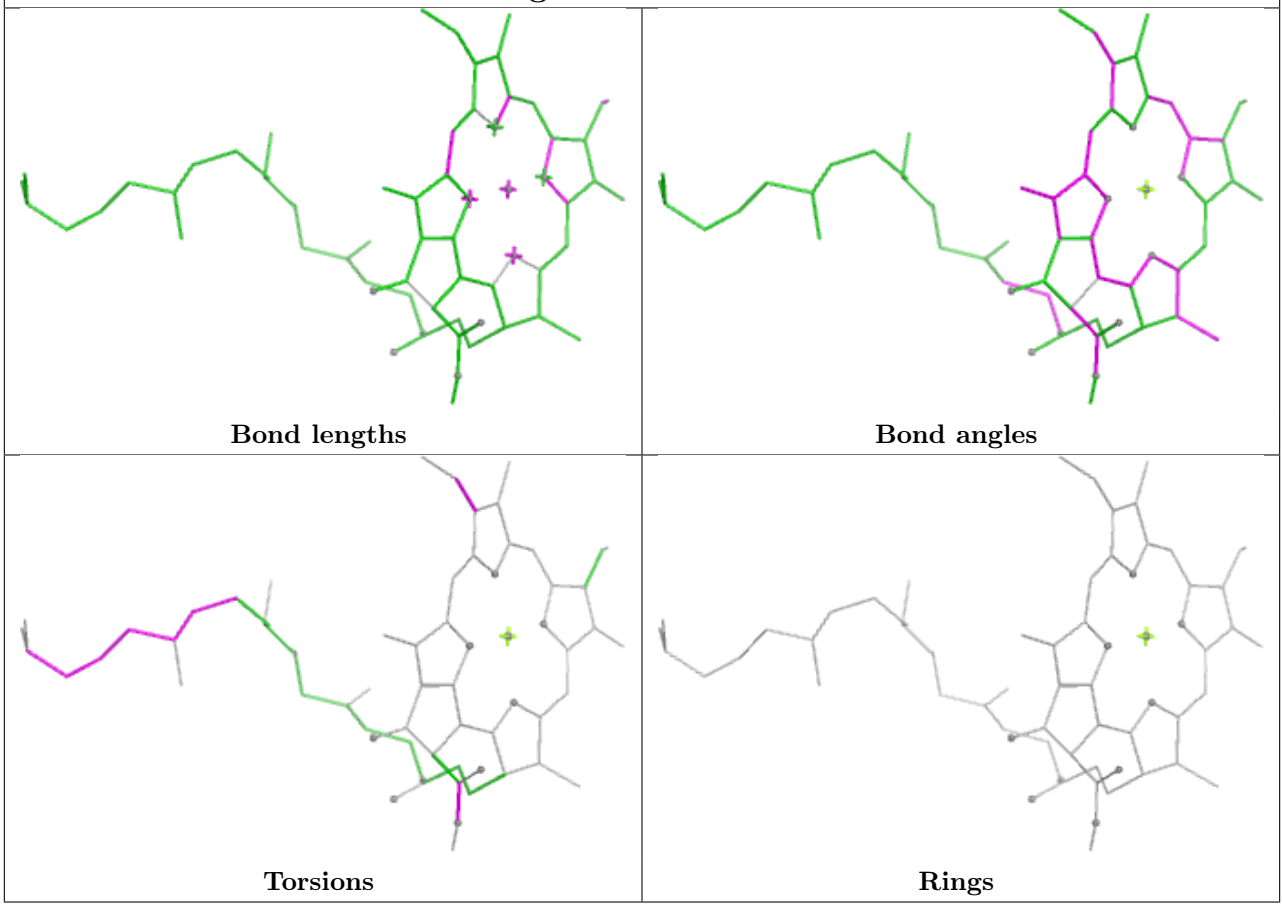


Torsions

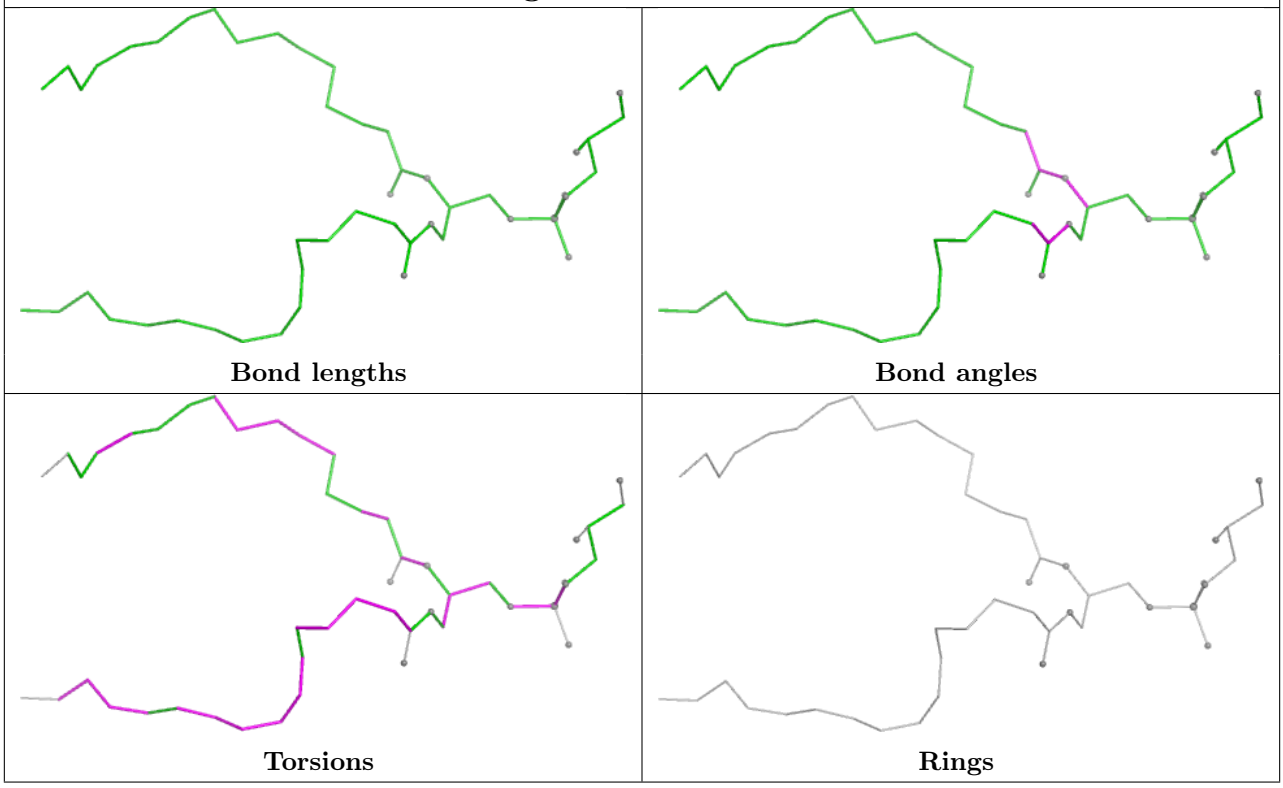


Rings

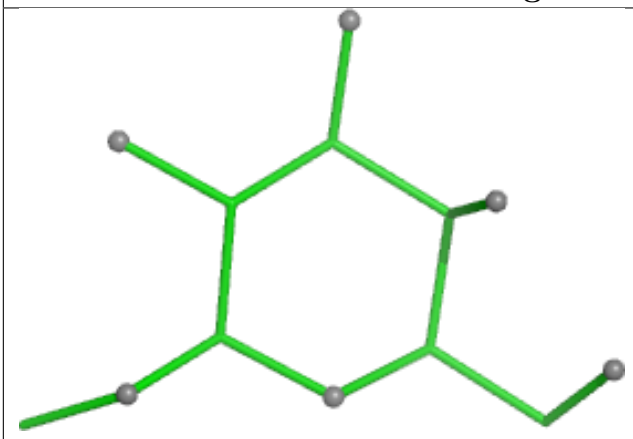
Ligand CLA 4 315



Ligand LHG A 853



Ligand LMG 2 522



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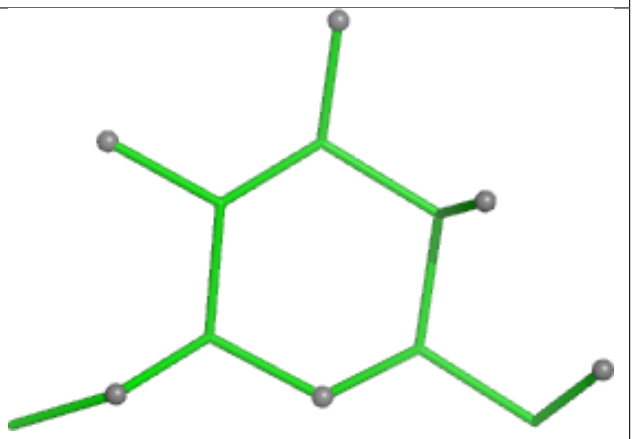
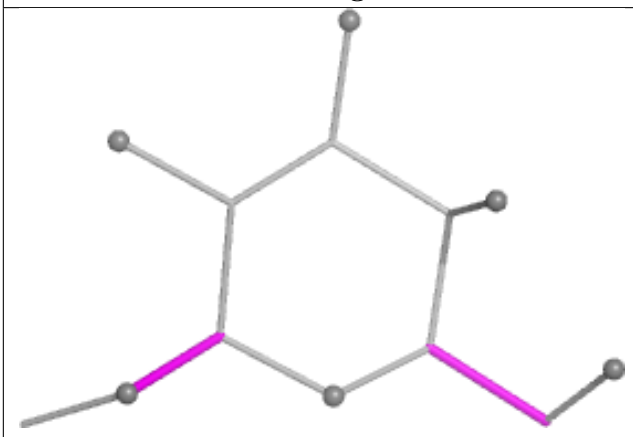
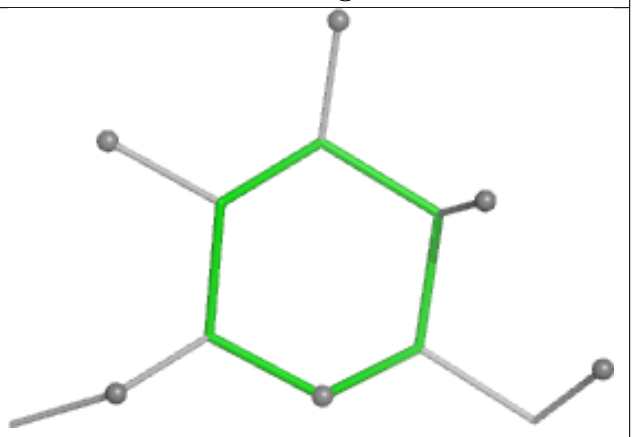


Bond angles

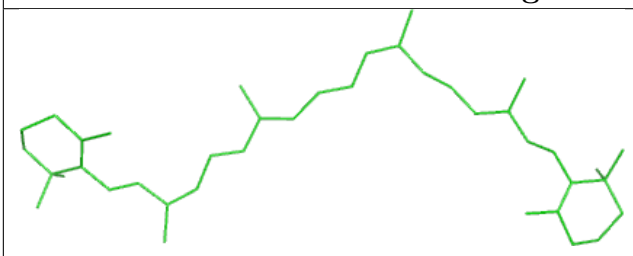


Torsions



Rings

Ligand BCR A 852



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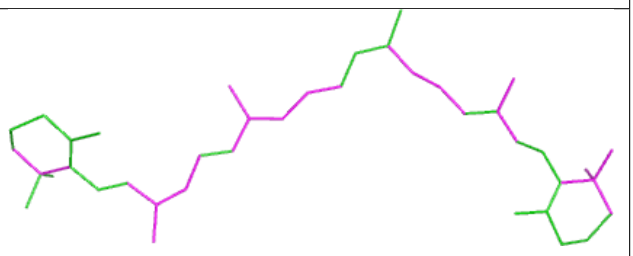
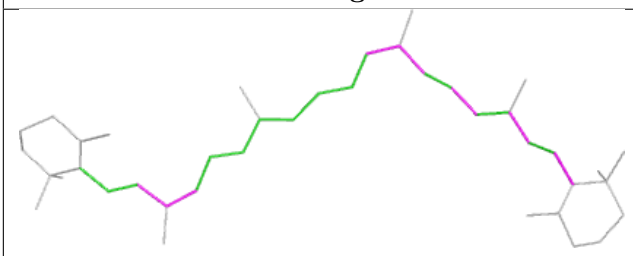


Bond angles



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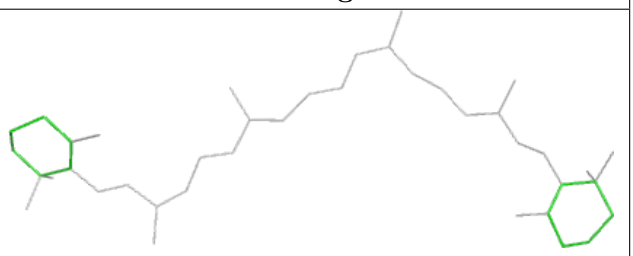
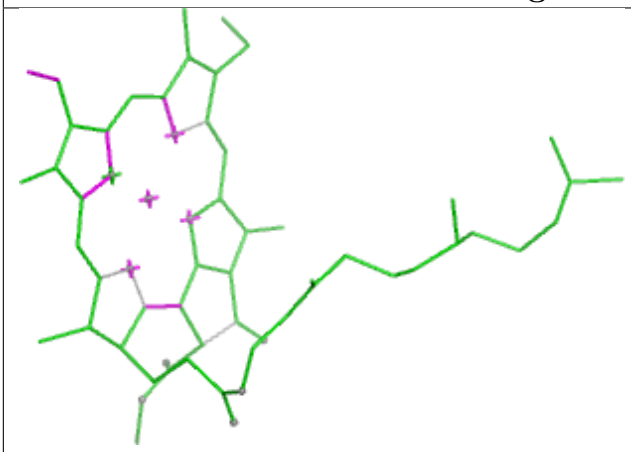


Rings

Ligand CLA 2 510



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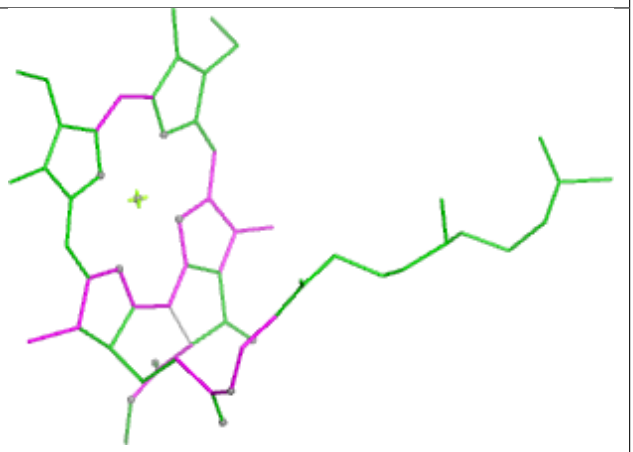
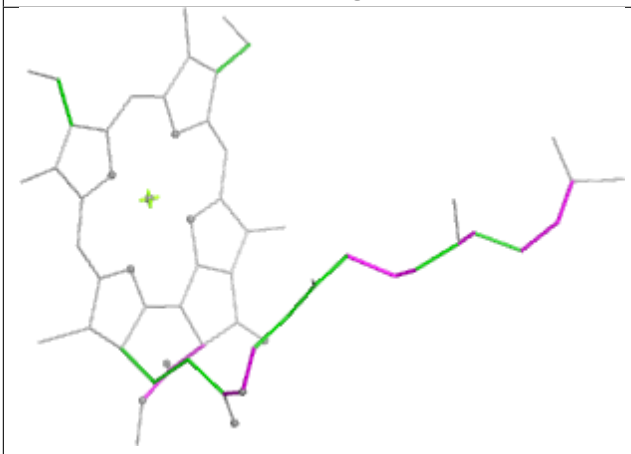


Bond angles



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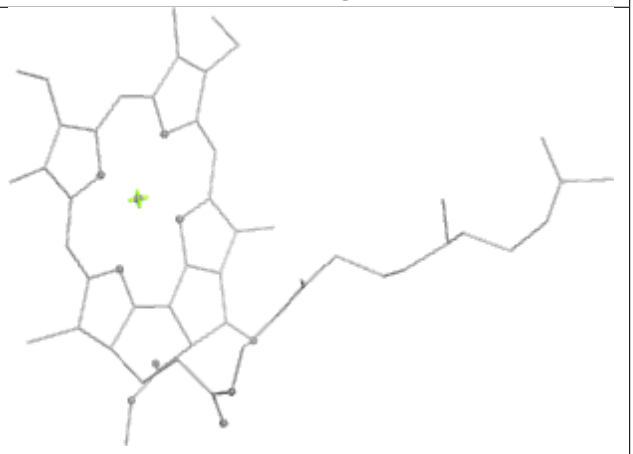
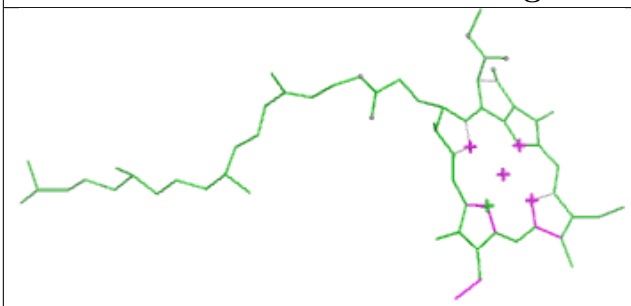


Rings

Ligand CLA A 803



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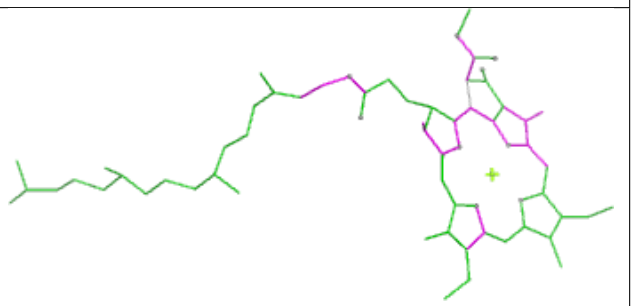
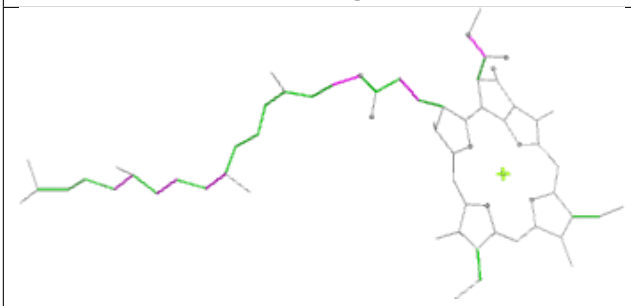
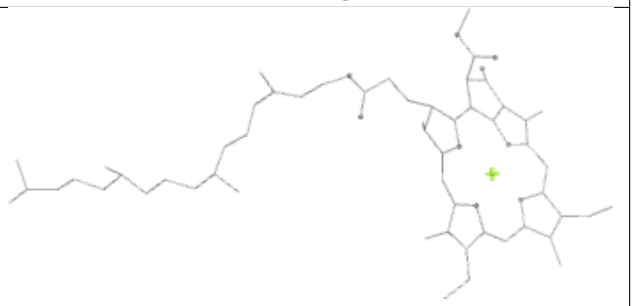


Bond angles

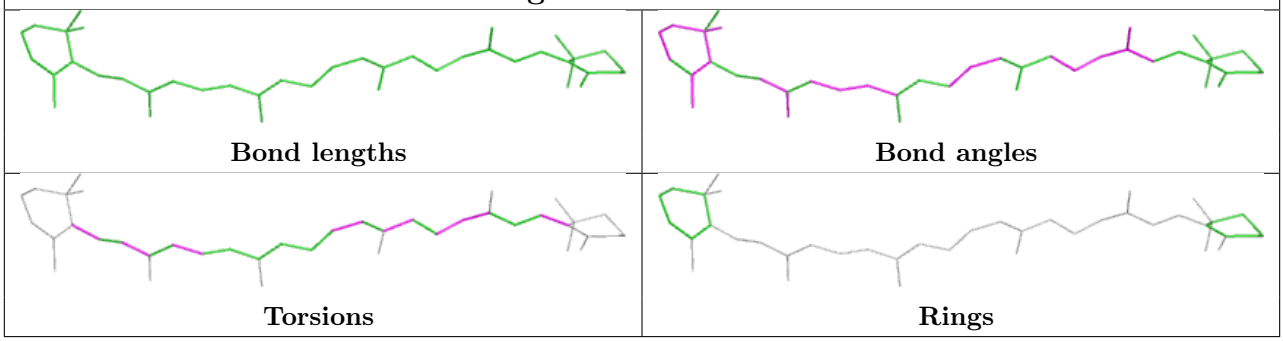


Torsions



Rings

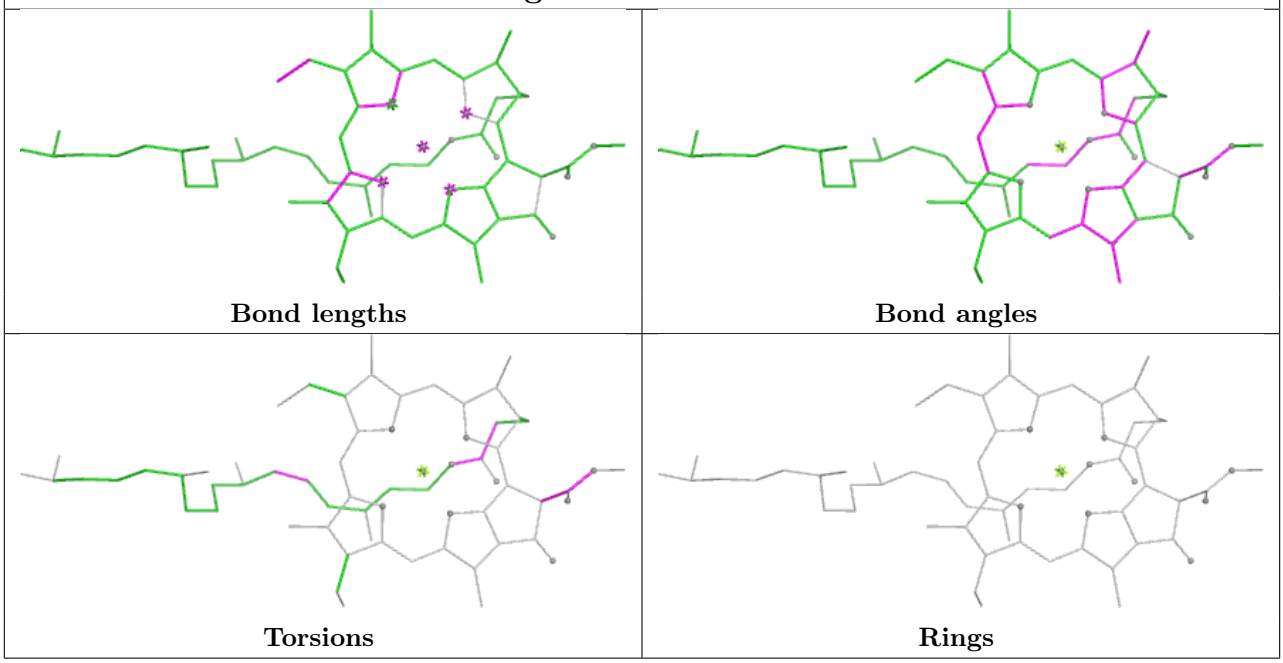
Ligand BCR 3 303



Bond lengths | Bond angles

Torsions | Rings

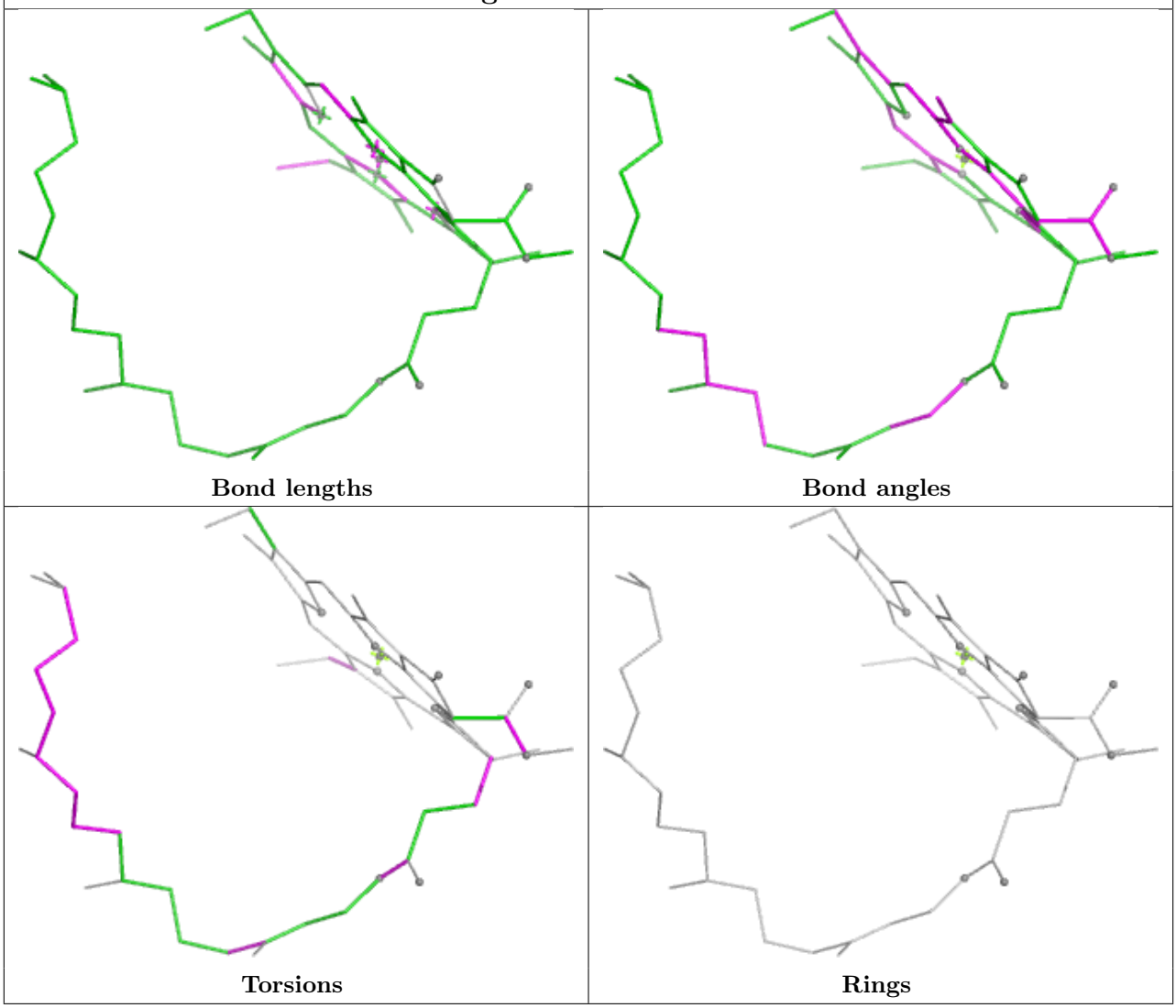
Ligand CLA A 837



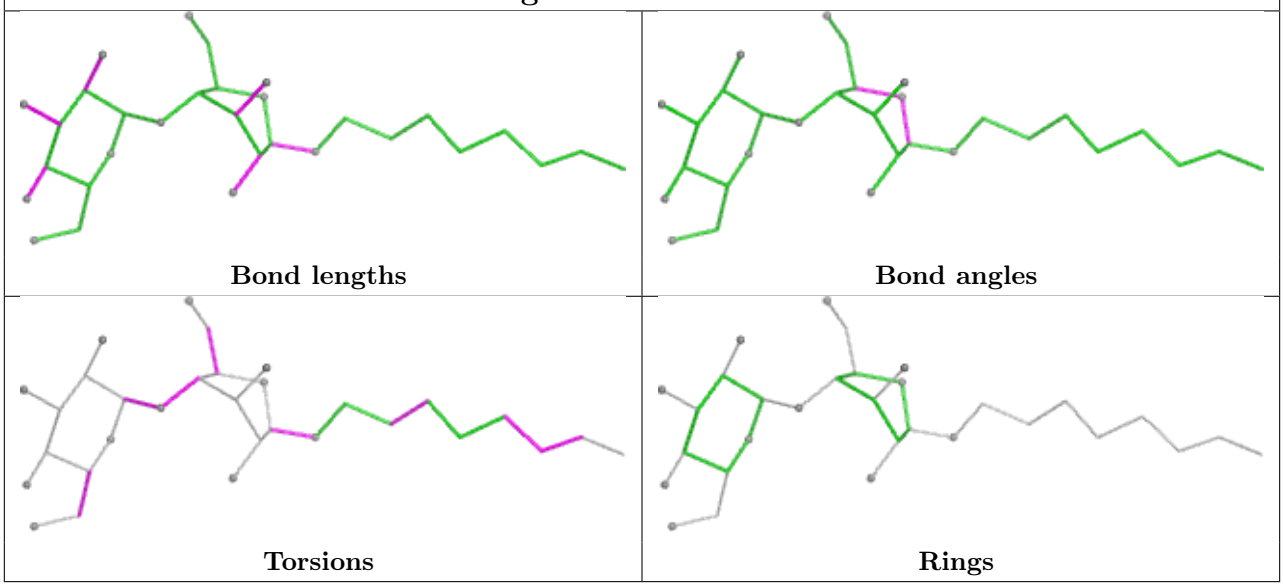
Bond lengths | Bond angles

Torsions | Rings

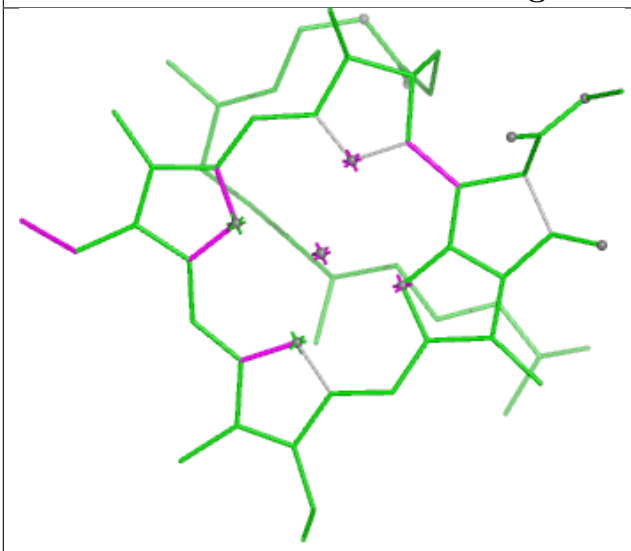
Ligand CLA B 820



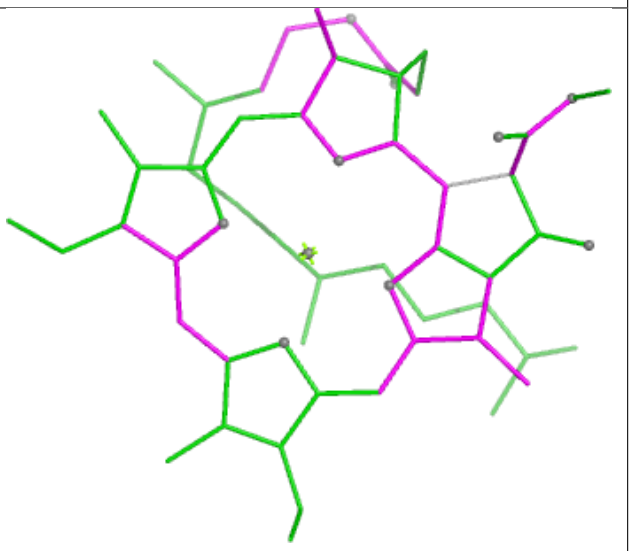
Ligand LMT G 209



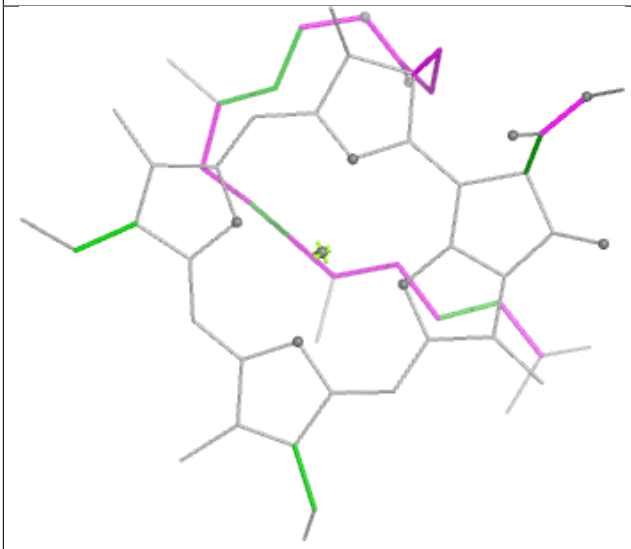
Ligand CLA 3 313



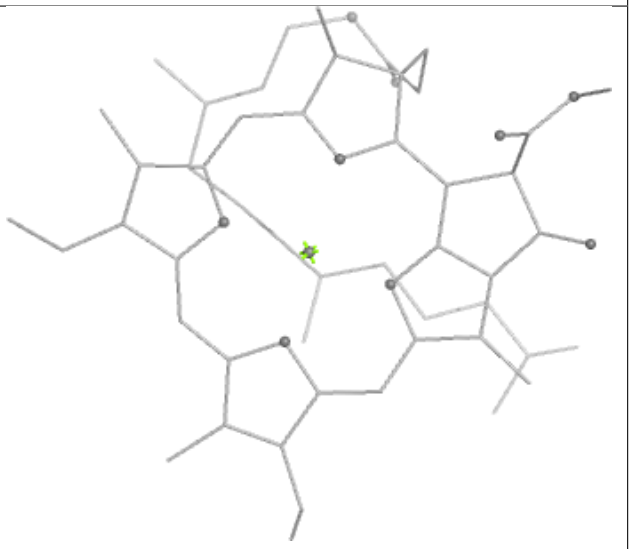
Bond lengths



Bond angles

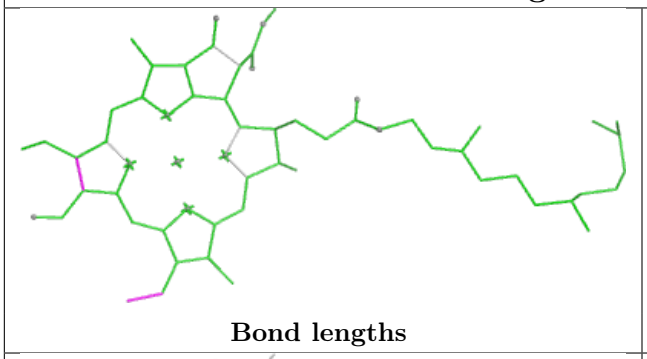


Torsions



Rings

Ligand CHL 4 316



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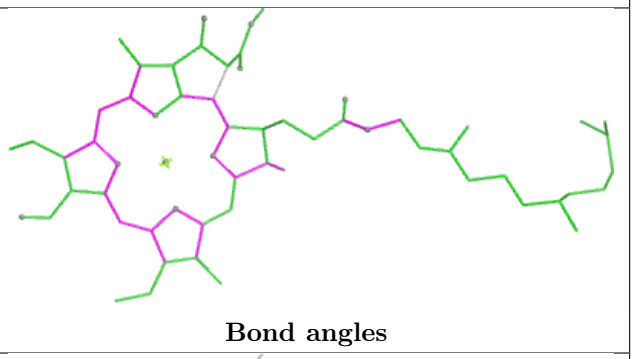
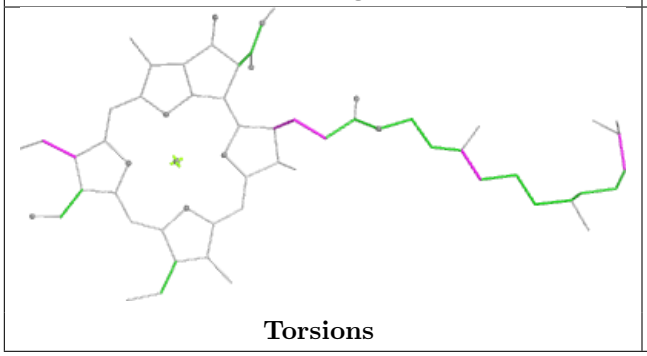
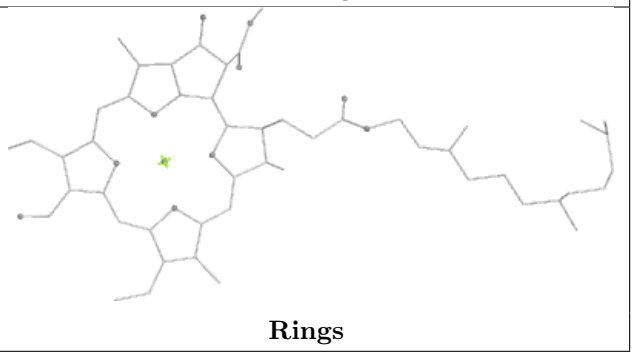


Bond angles

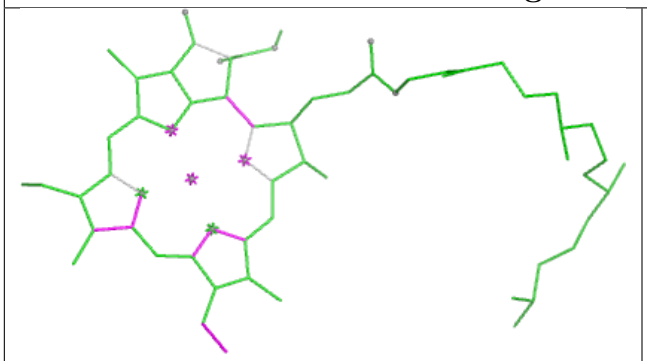


Torsions



Rings

Ligand CLA A 827



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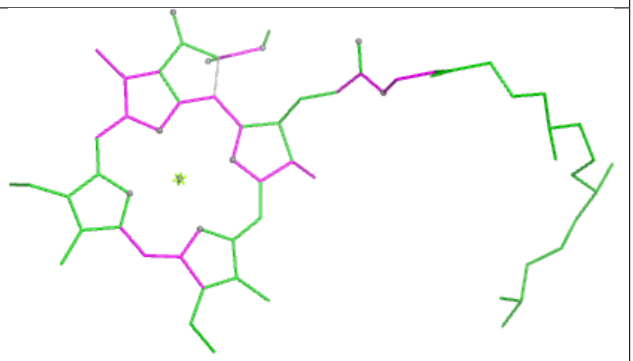
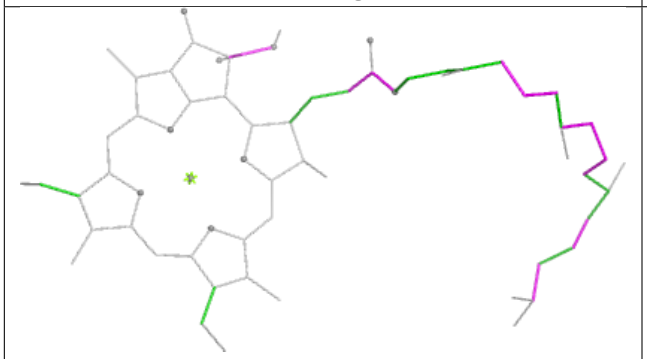


Bond angles



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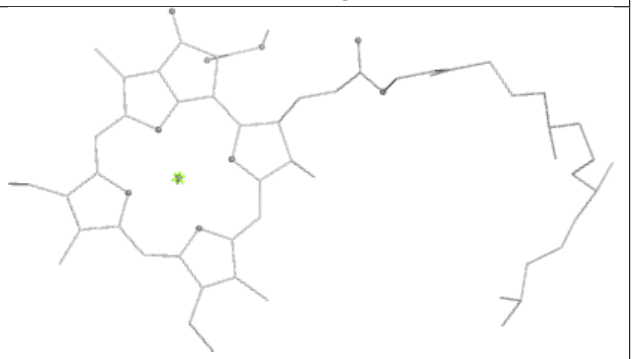
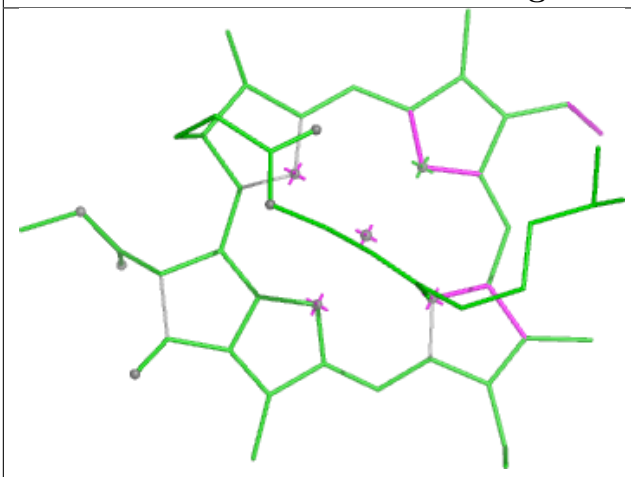


Rings

Ligand CLA 1 506



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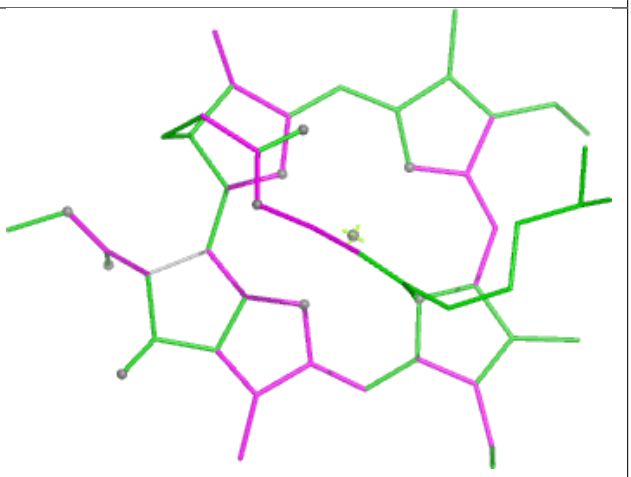
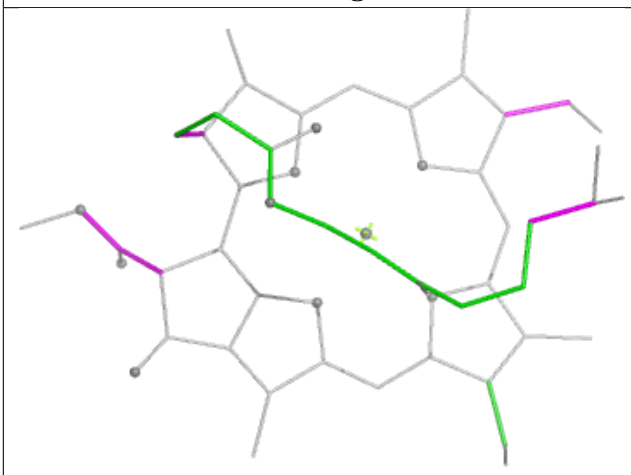


Bond angles



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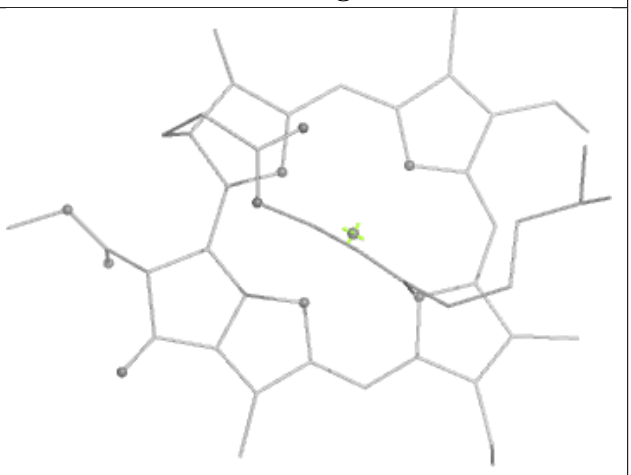
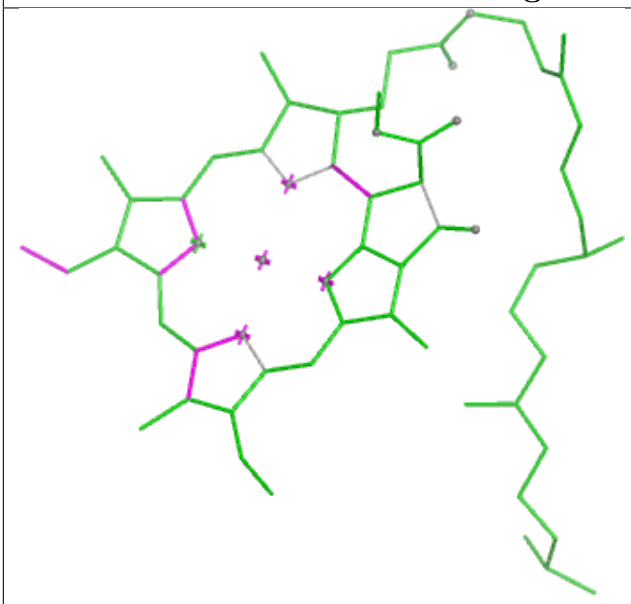


Rings

Ligand CLA A 825



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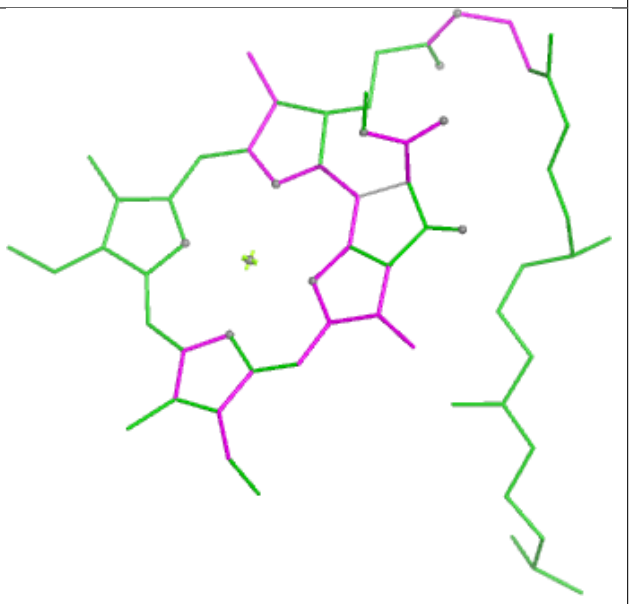
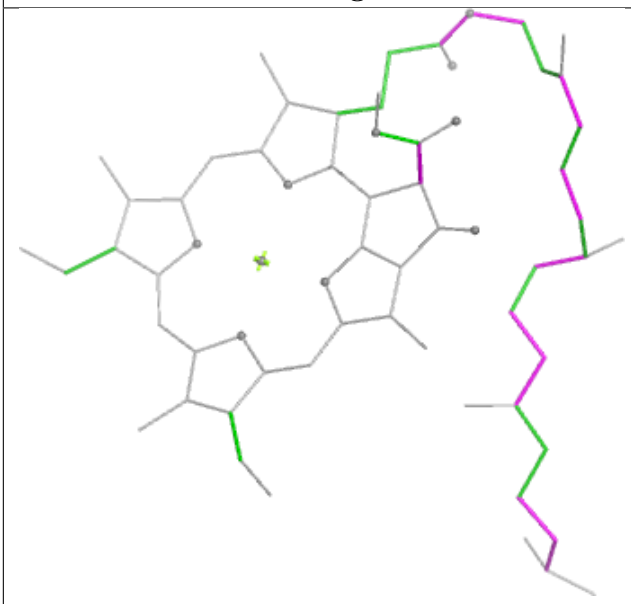


Bond angles



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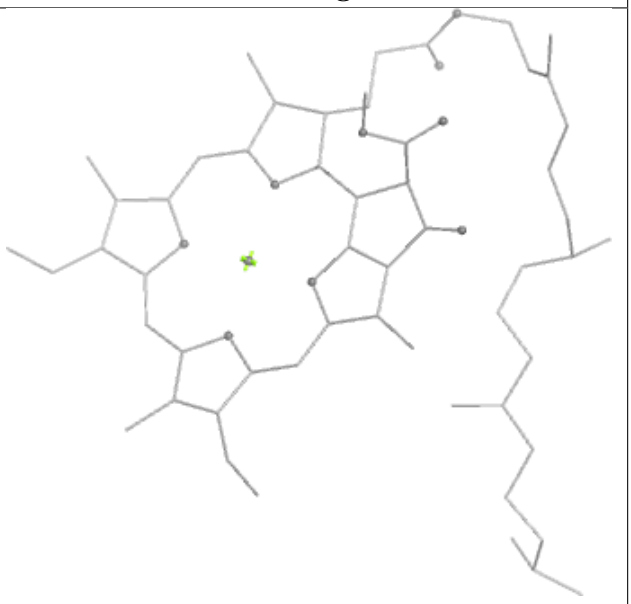
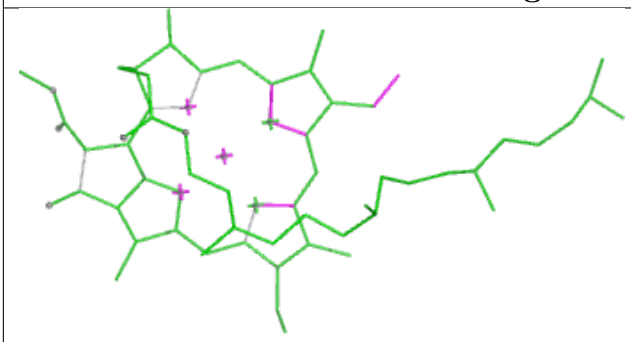


Rings

Ligand CLA A 839



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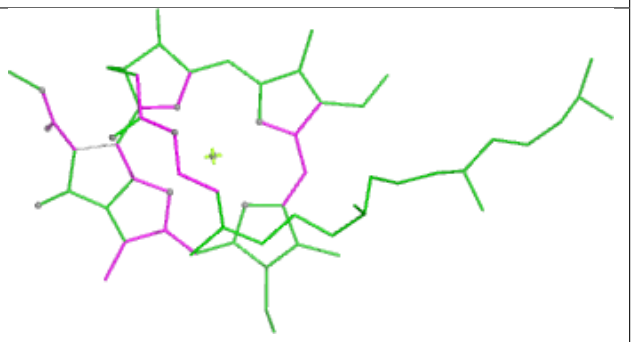
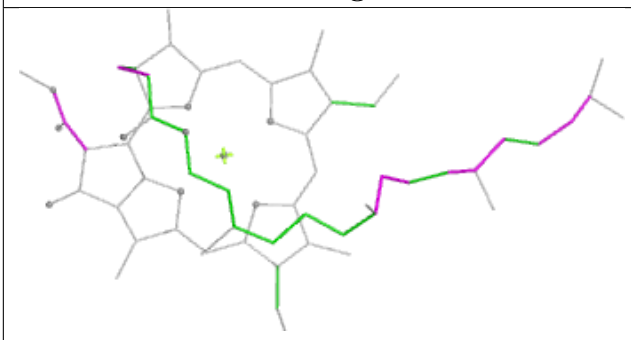


Bond angles



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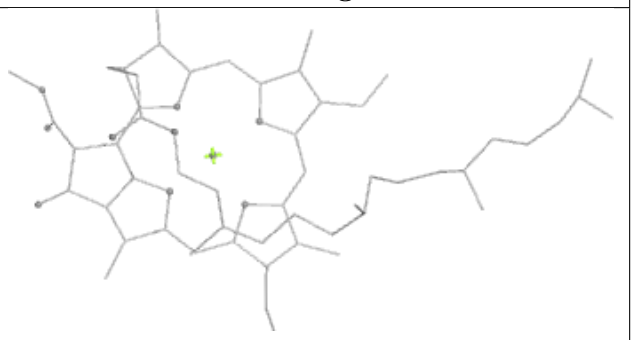
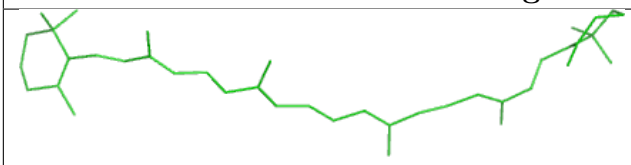
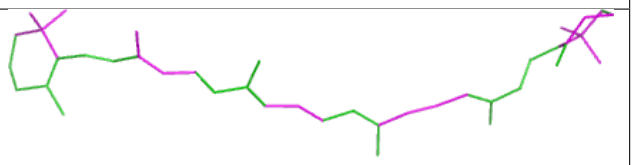


Rings

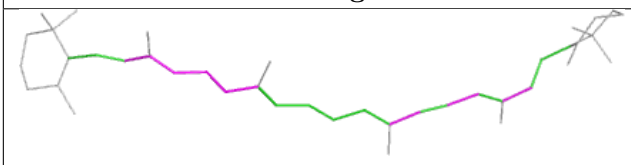
Ligand BCR B 856



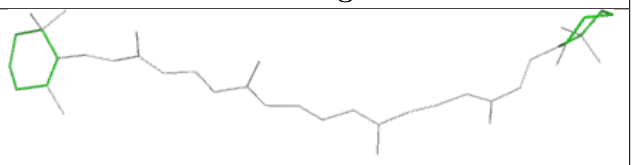
Bond lengths



Bond angles

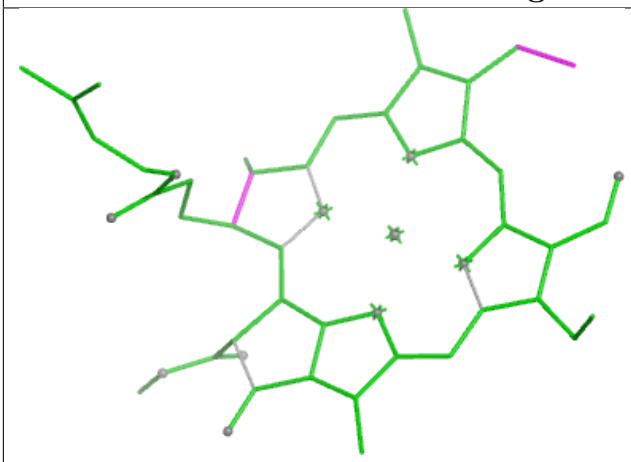


Torsions

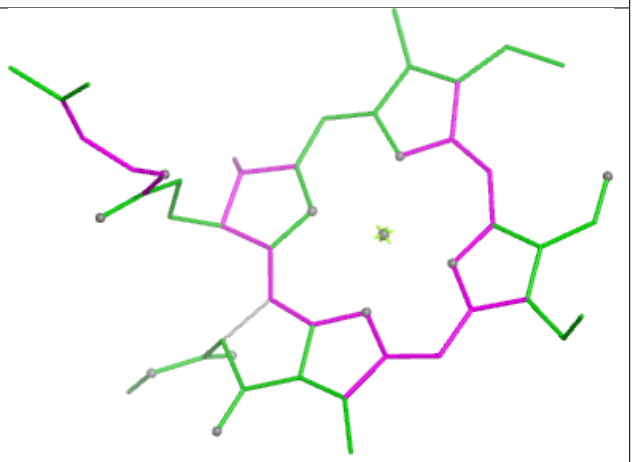


Rings

Ligand CHL 4 314



Bond lengths



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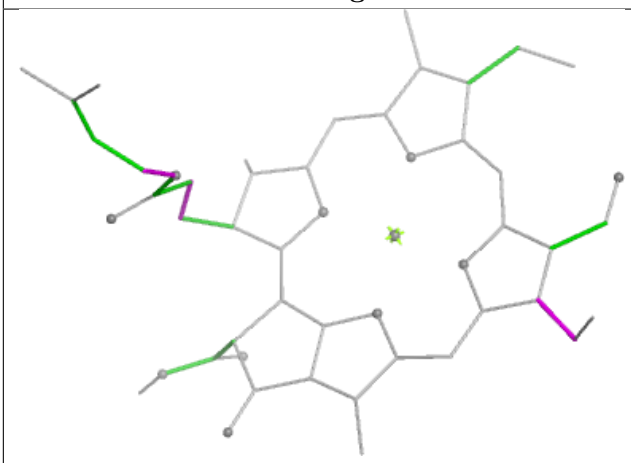

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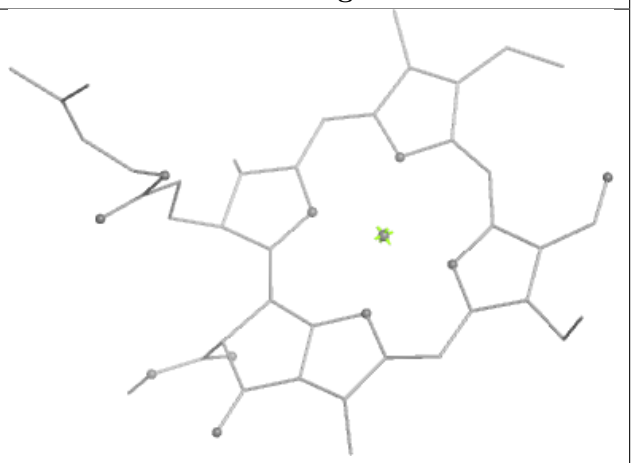
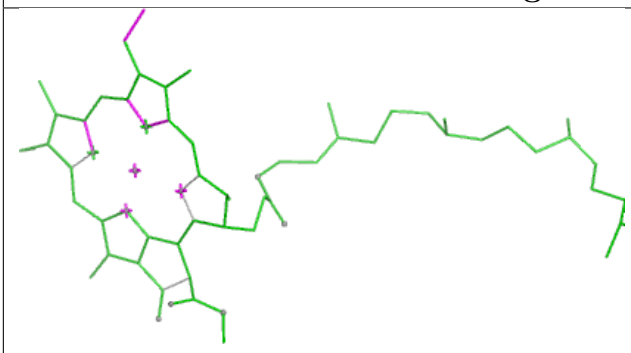
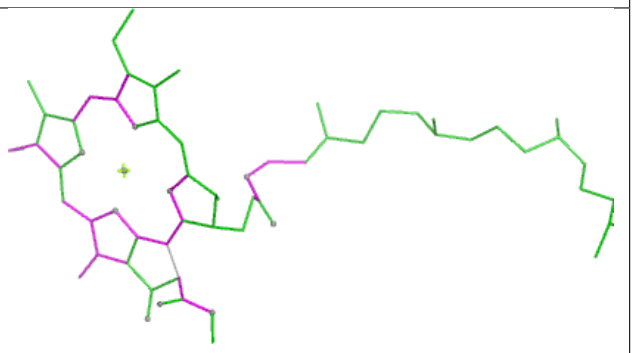


Rings

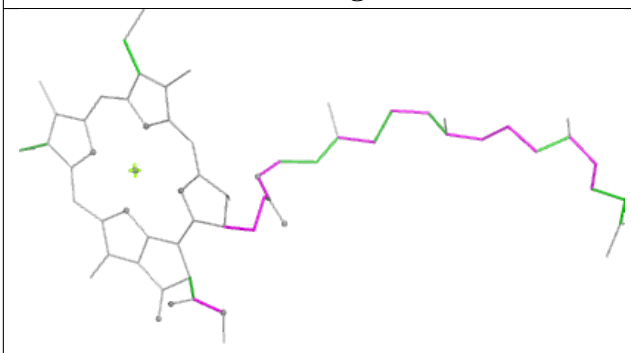
Ligand CLA A 821



Bond lengths



Bond angles



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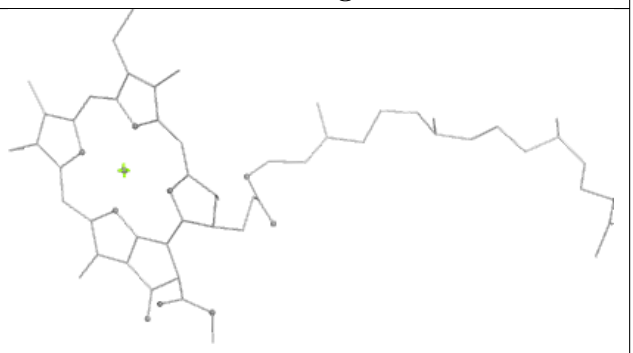
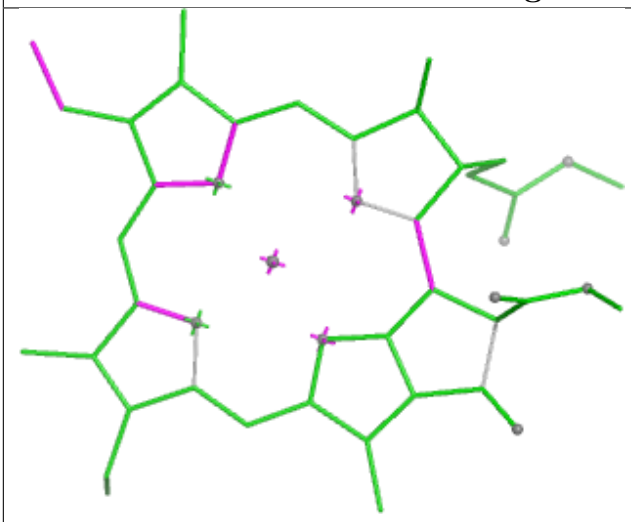


Rings

Ligand CLA B 813



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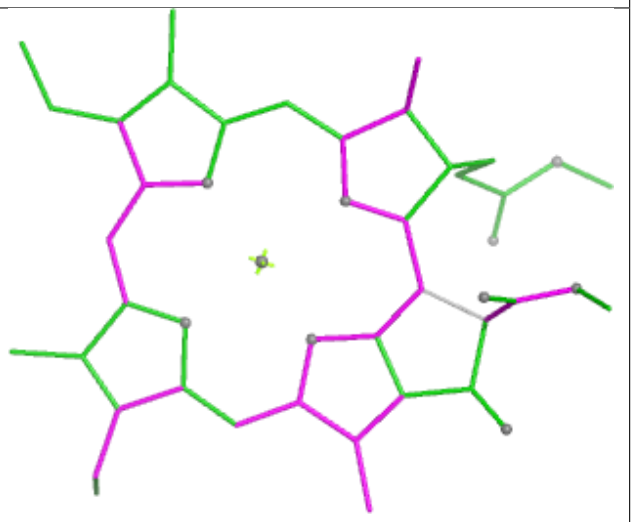
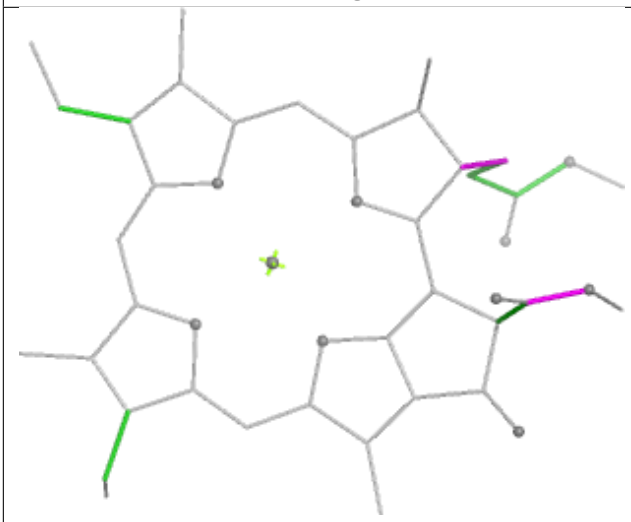
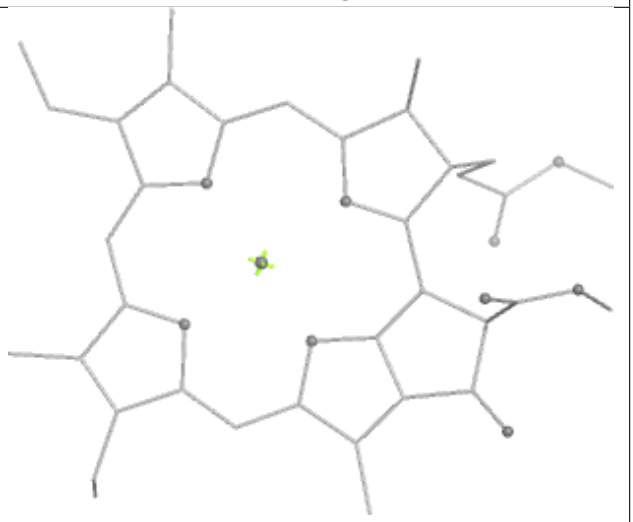


Bond angles

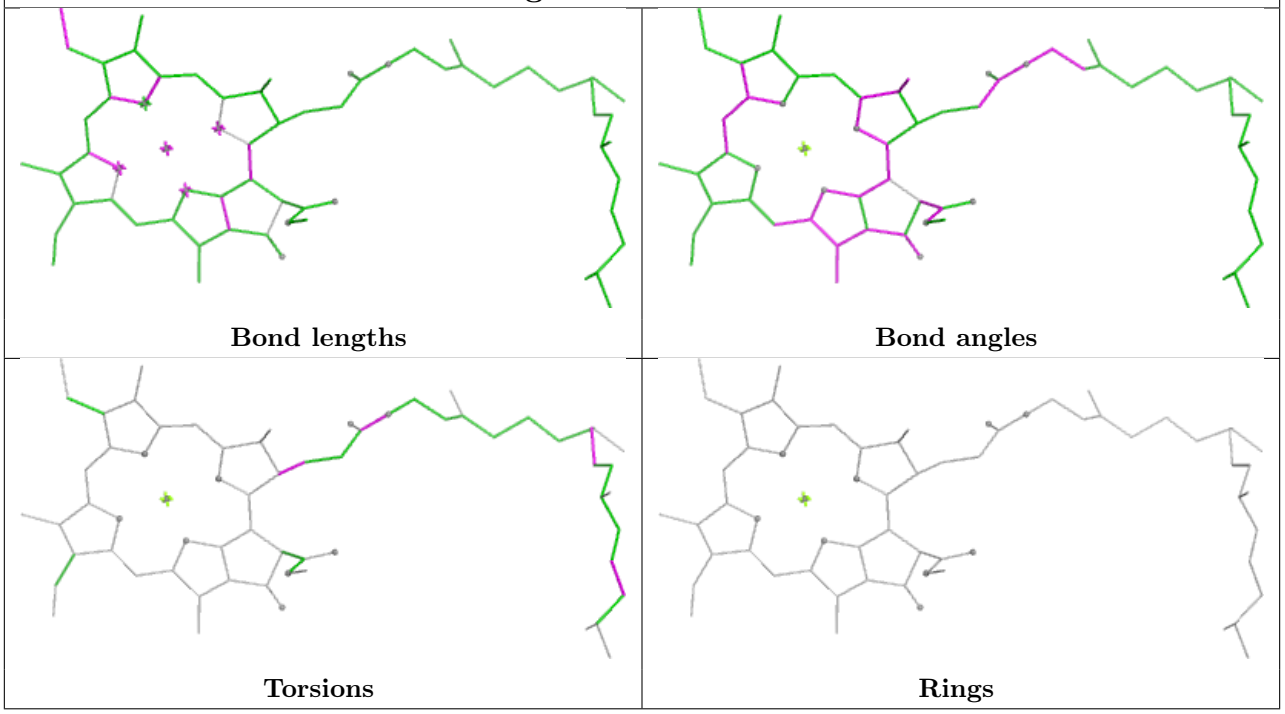


Torsions

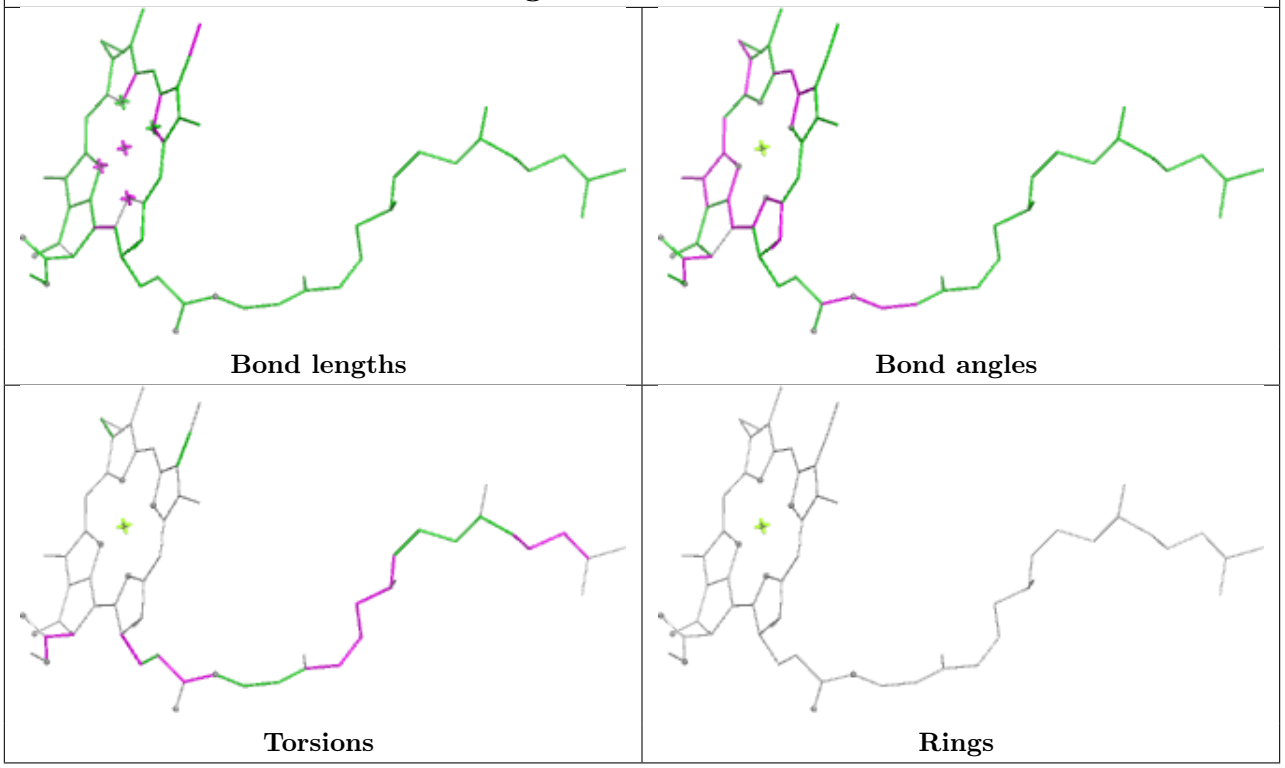


Rings

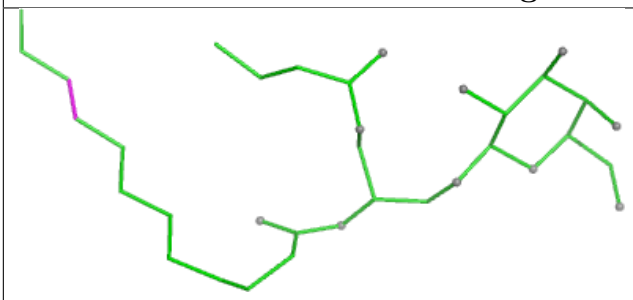
Ligand CLA B 826



Ligand CLA G 201



Ligand LMG B 844



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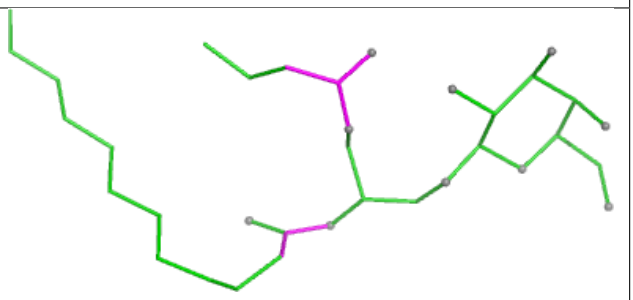
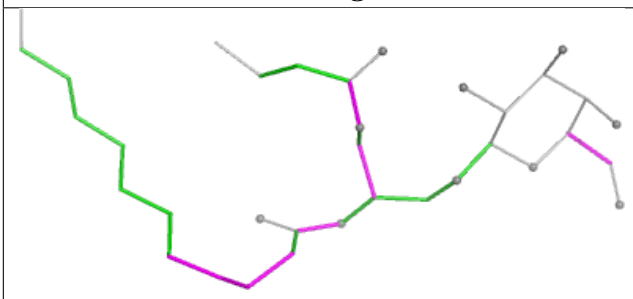


Bond angles



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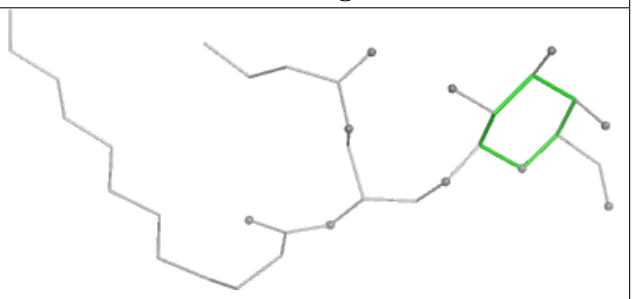
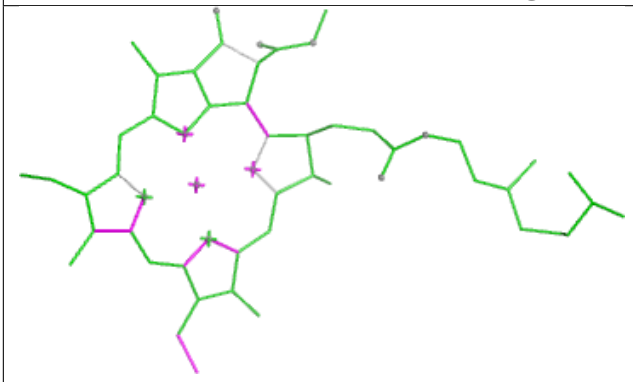


Rings

Ligand CLA G 202



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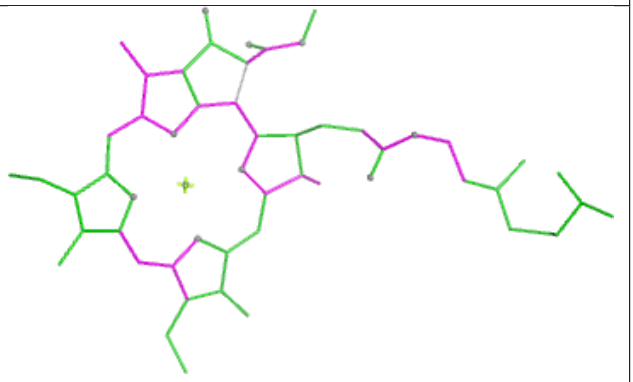
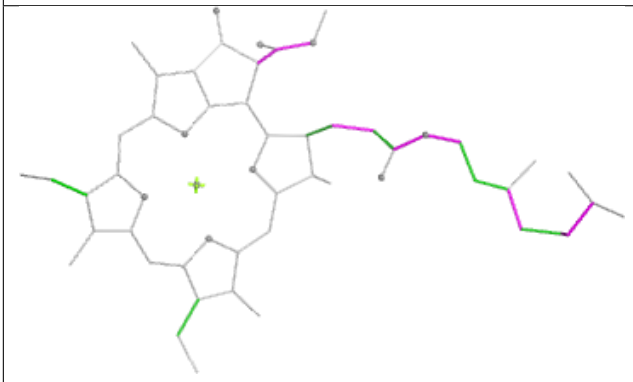


Bond angles

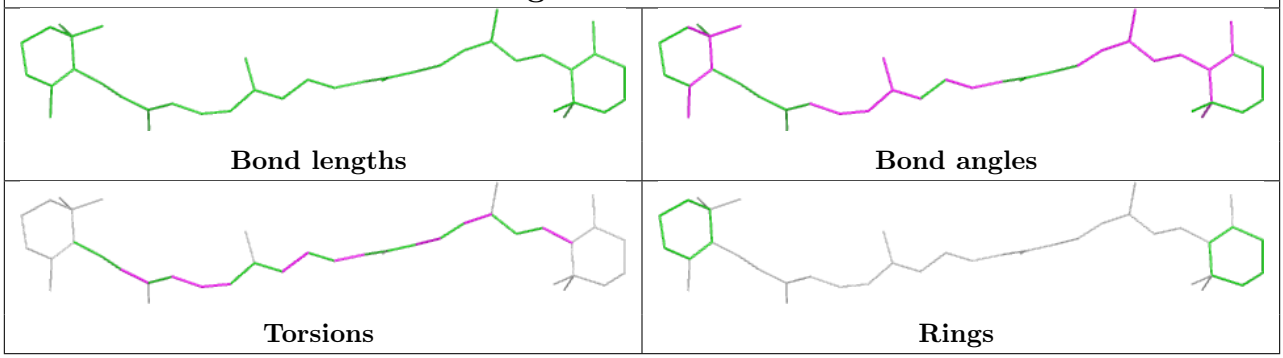


Torsions

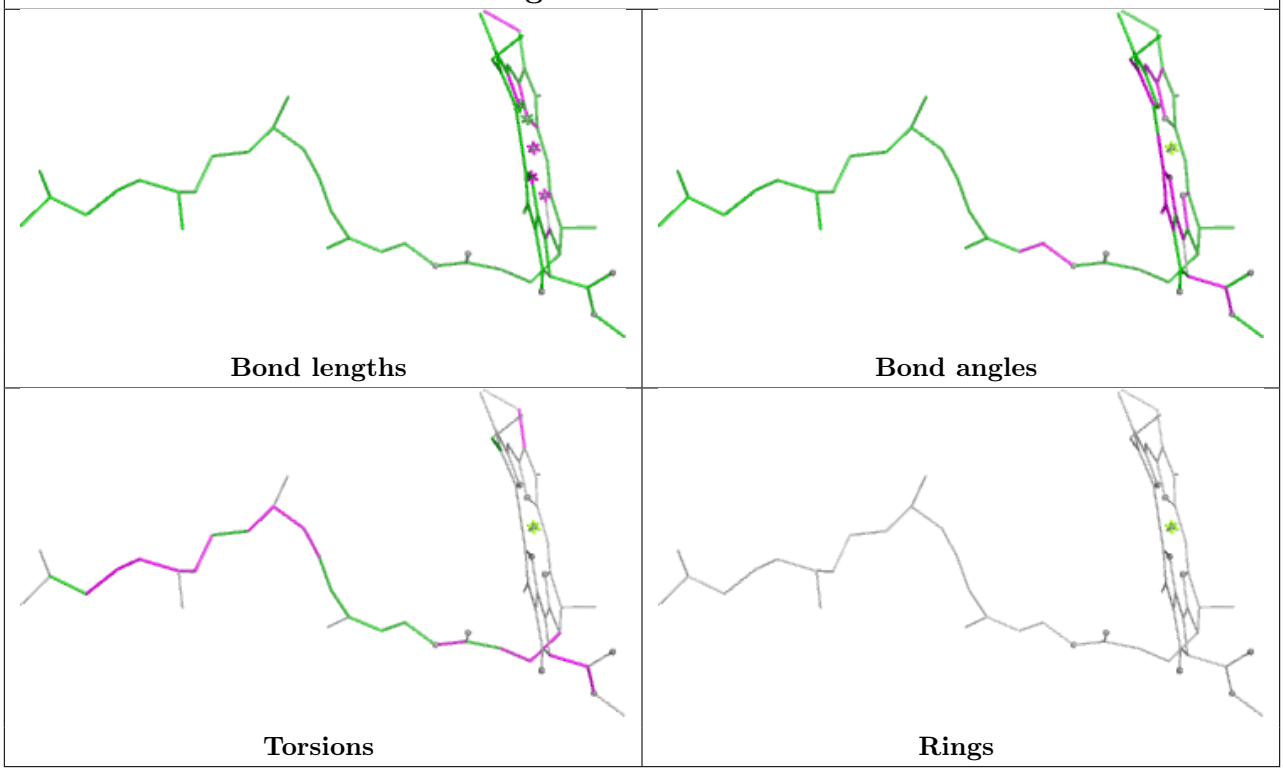


Rings

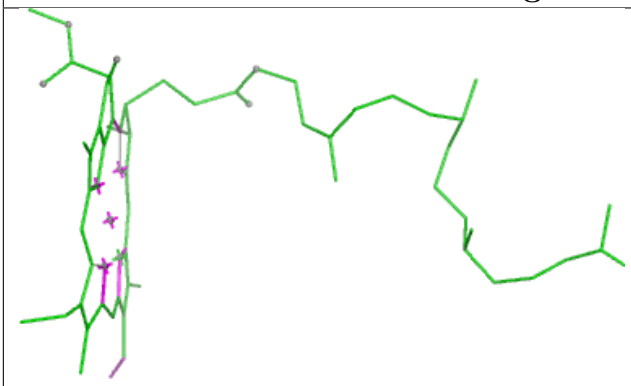
Ligand BCR 2 503



Ligand CLA B 805



Ligand CLA A 814



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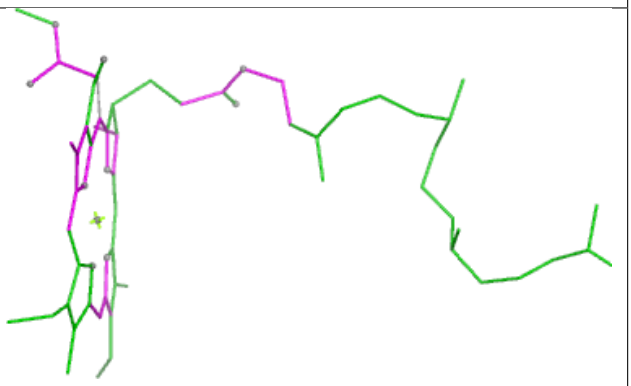
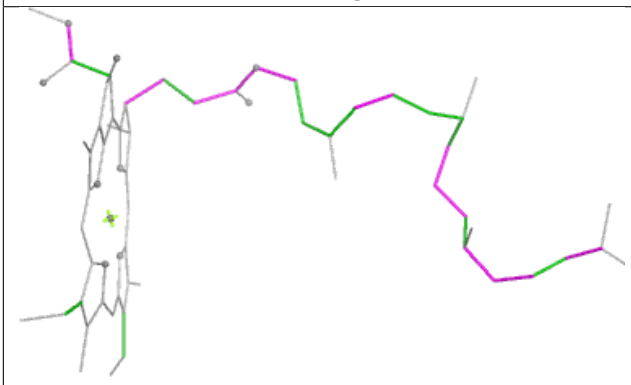


Bond angles



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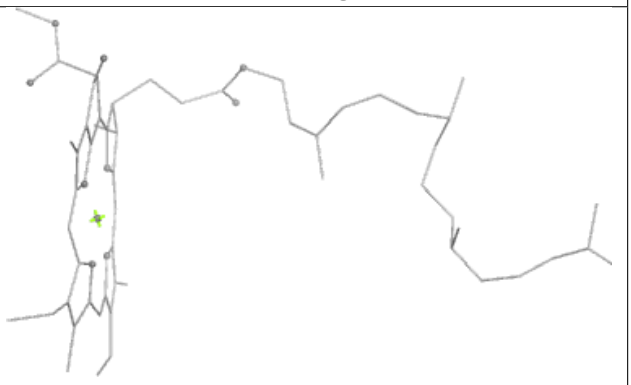
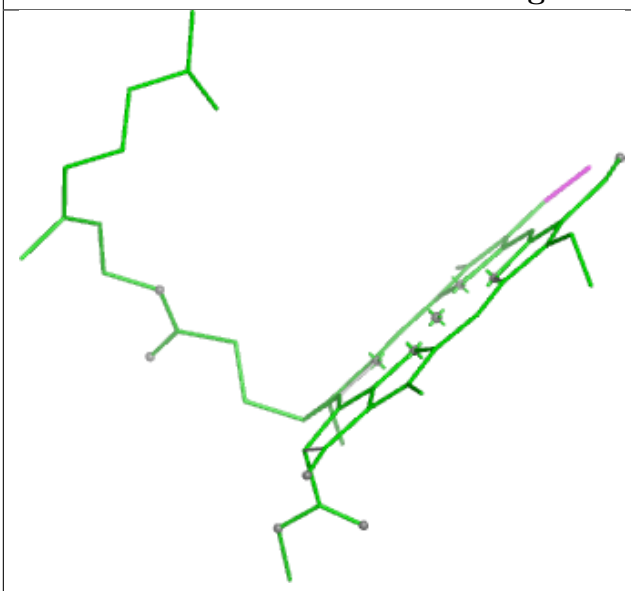


Rings

Ligand CHL 1 521



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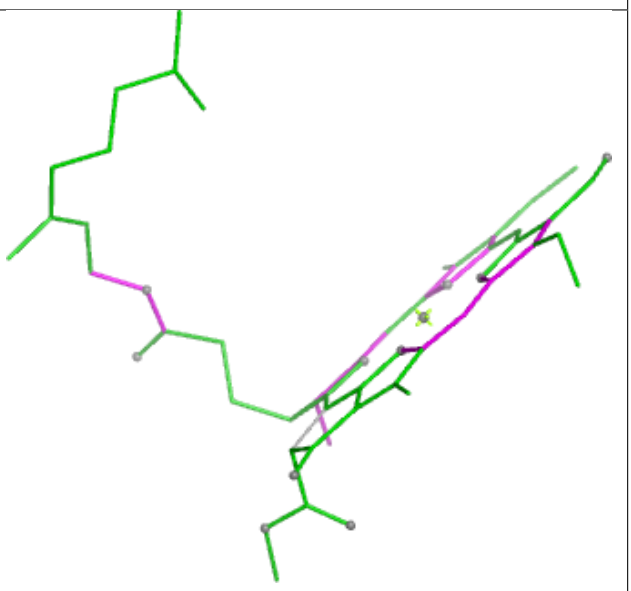
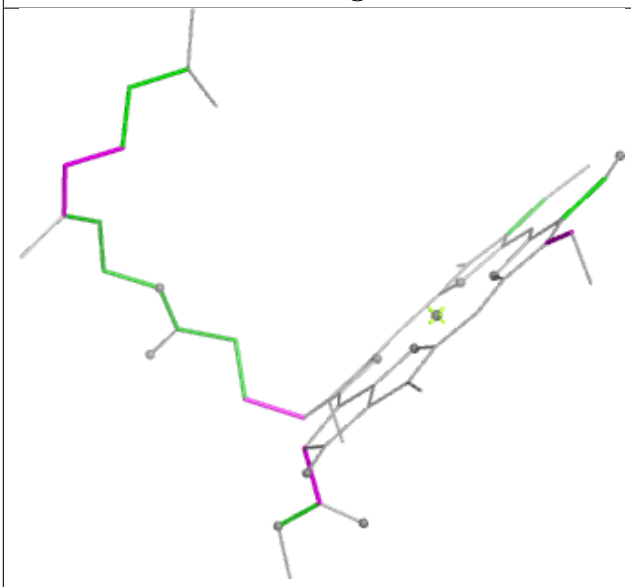


Bond angles



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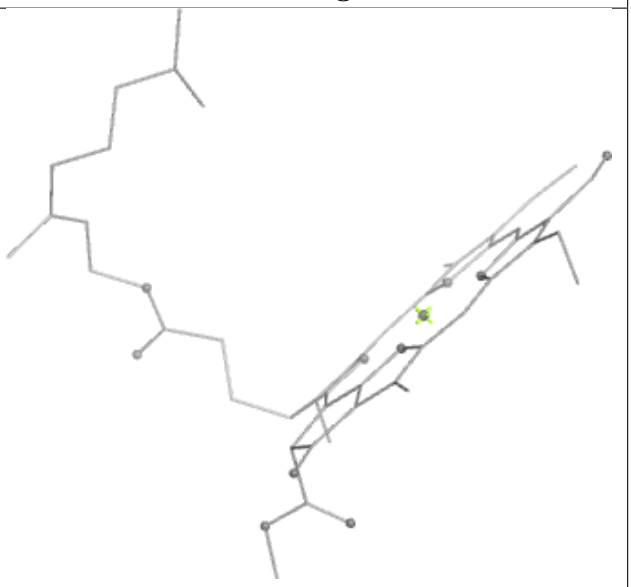
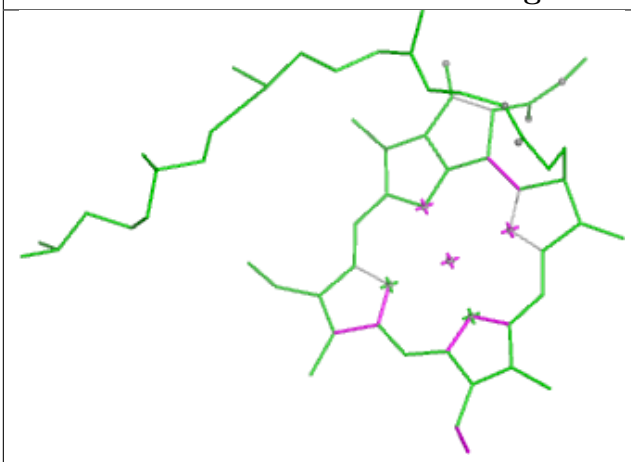


Rings

Ligand CLA A 829



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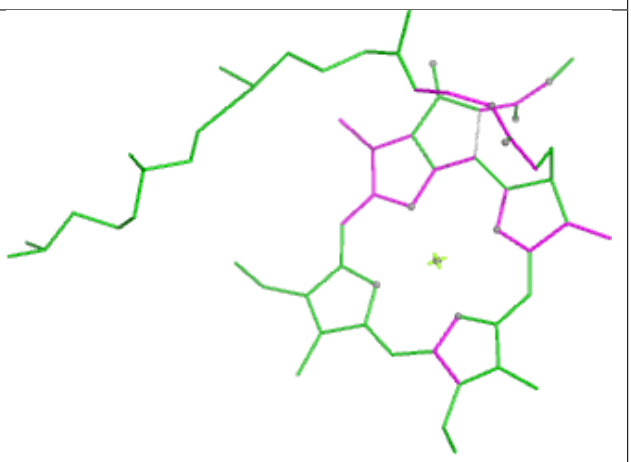
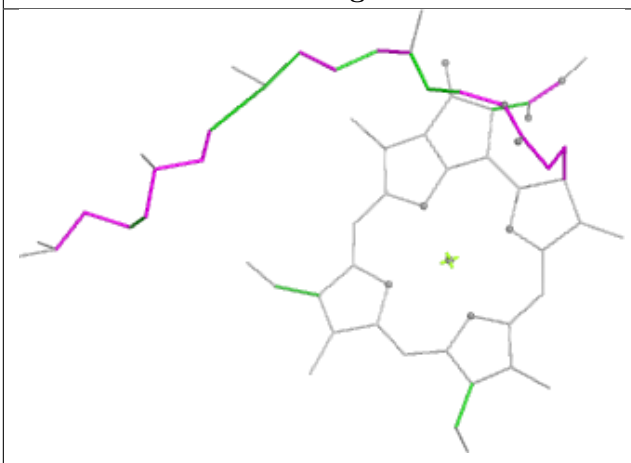


Bond angles

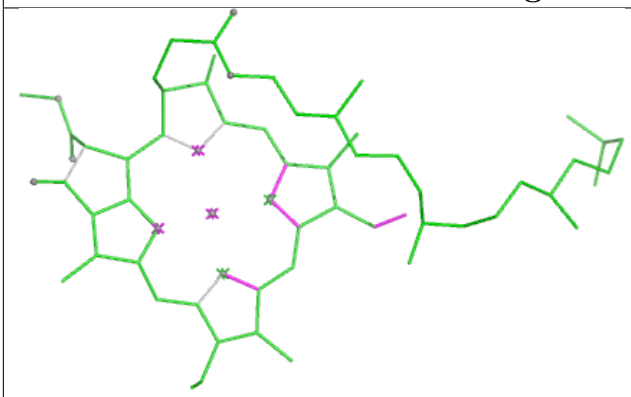


Torsions



Rings

Ligand CLA B 819



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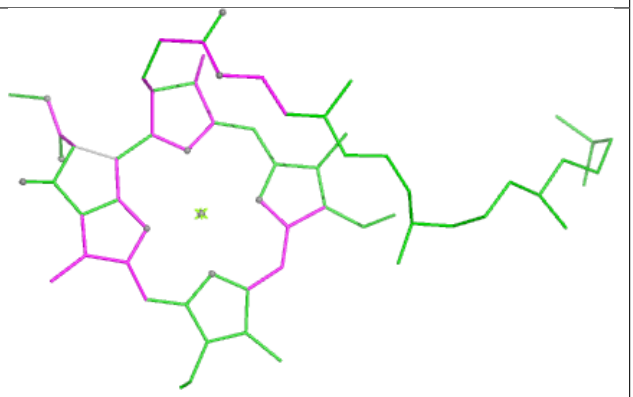
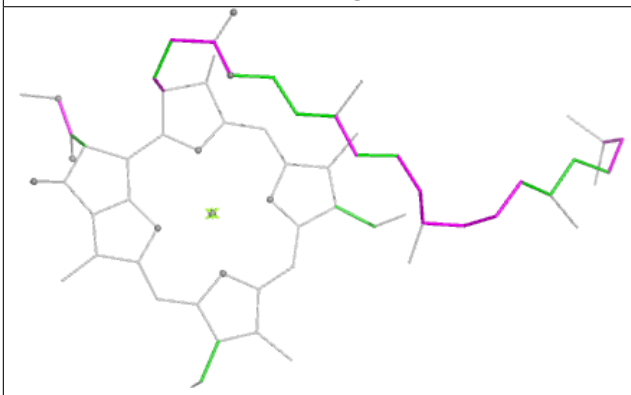


Bond angles



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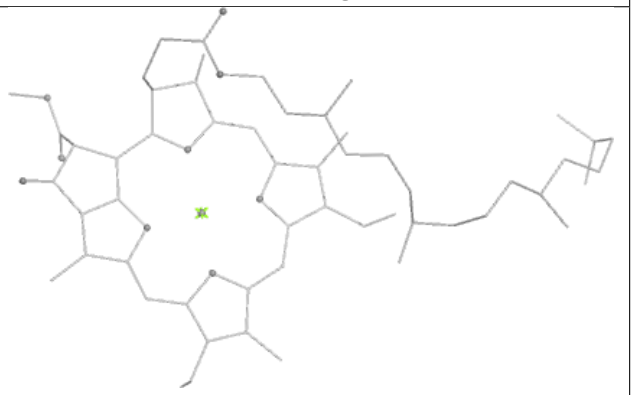
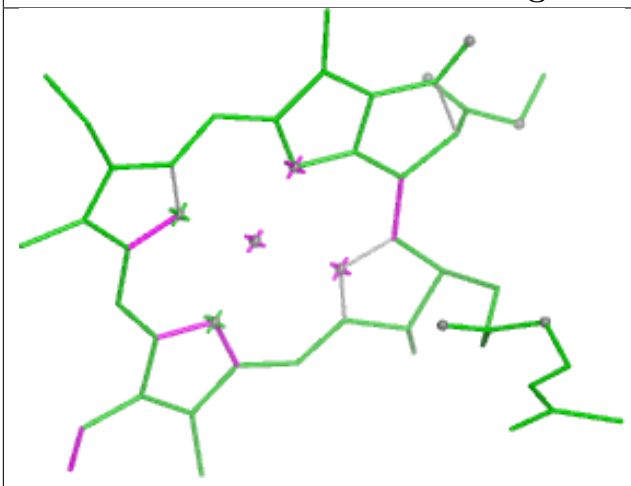


Rings

Ligand CLA 2 511



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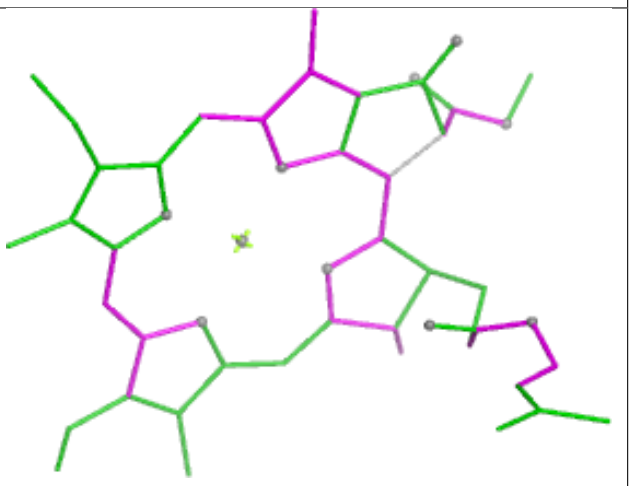
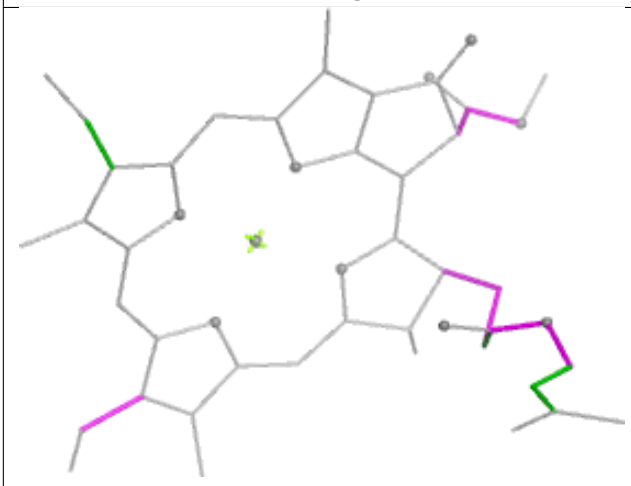


Bond angles



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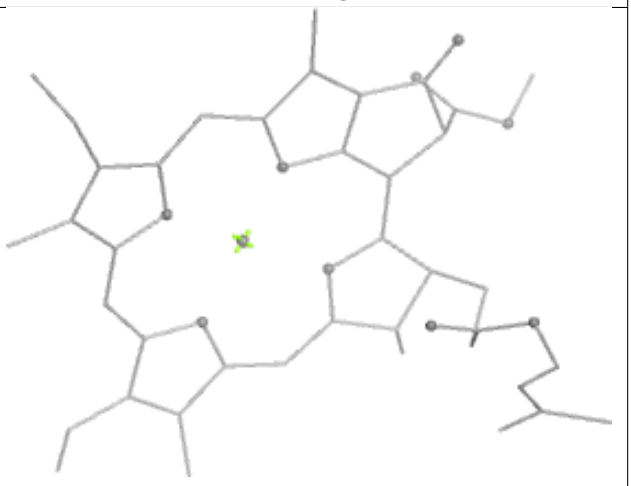
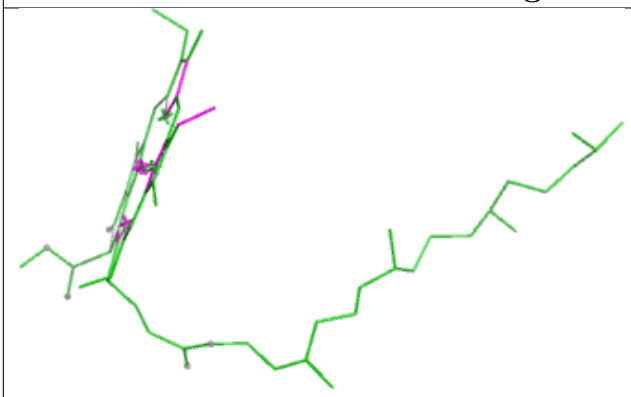


Rings

Ligand CLA A 804



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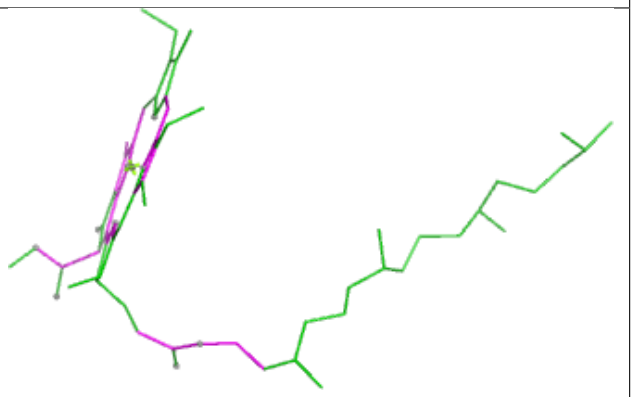
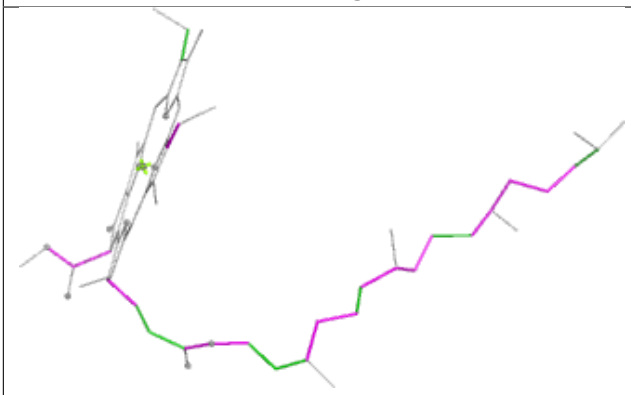


Bond angles



Torsions

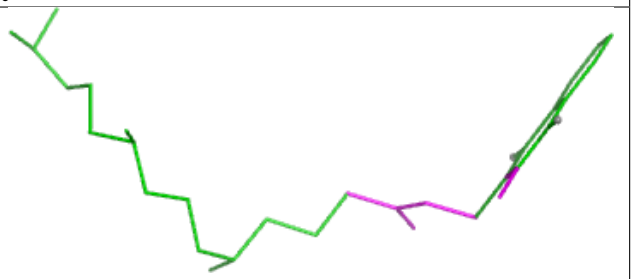


Rings

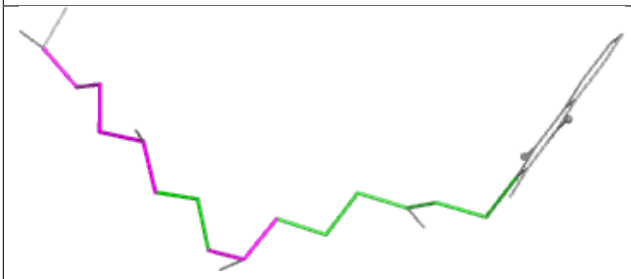
Ligand PQN B 841



Bond lengths



Bond angles



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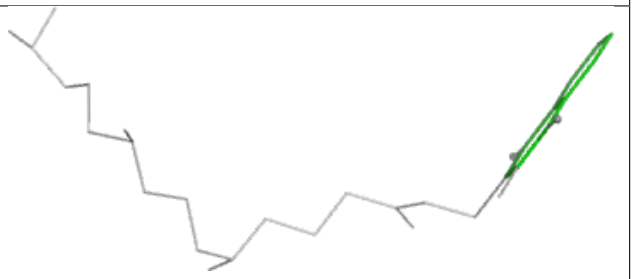
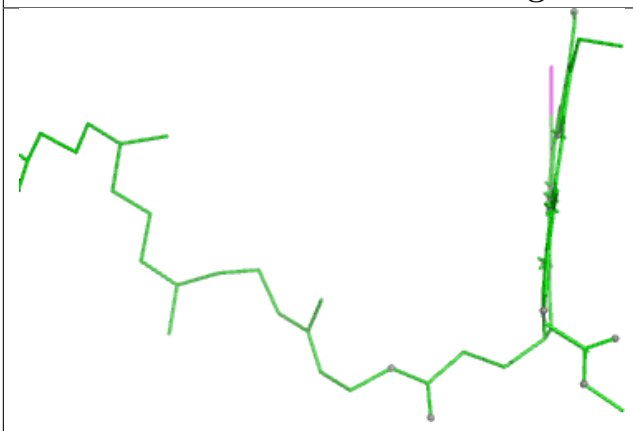
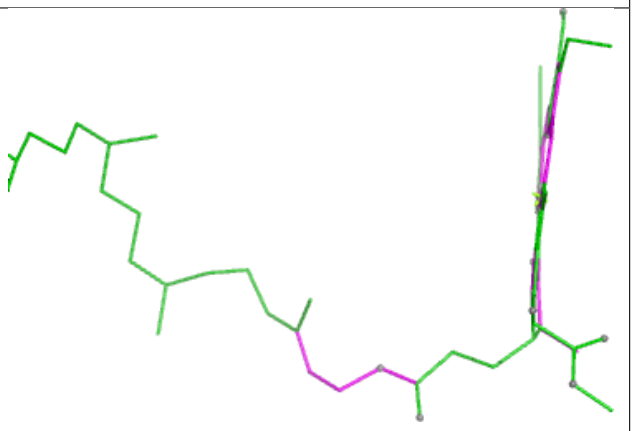


Rings

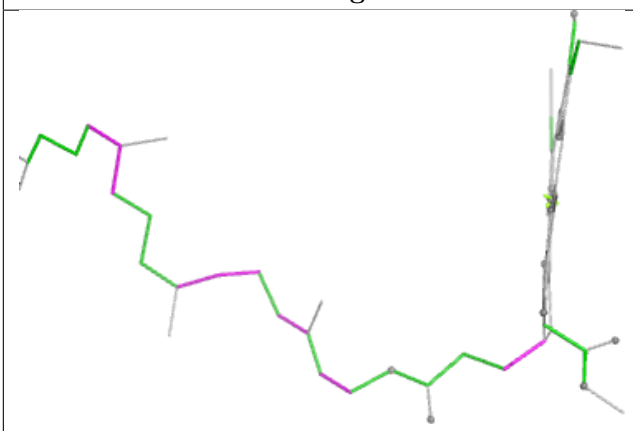
Ligand CHL 2 526



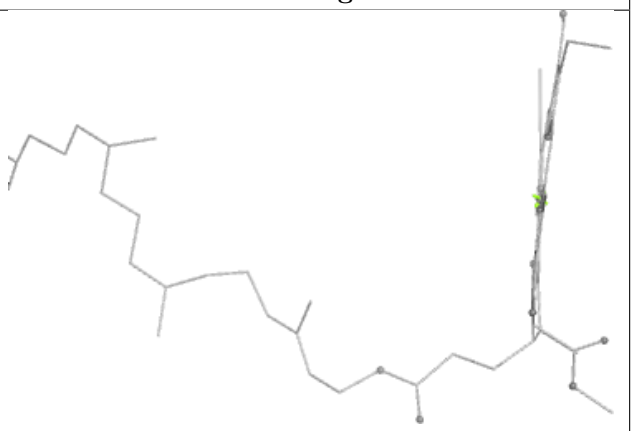
Bond lengths



Bond angles

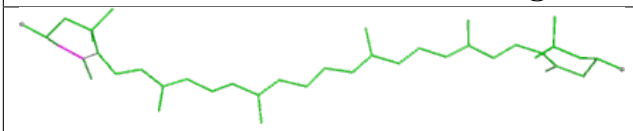


Torsions

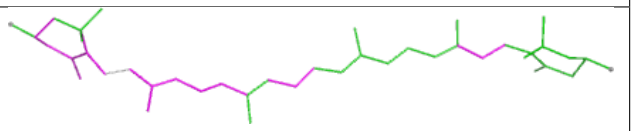


Rings

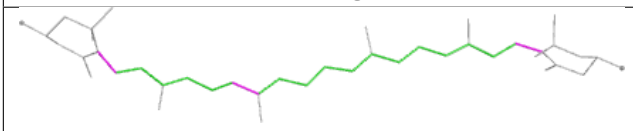
Ligand LUT 2 501



Bond lengths



Bond angles



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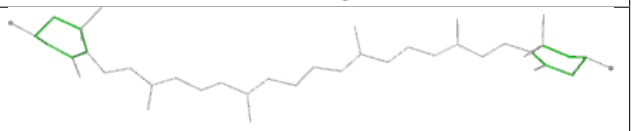
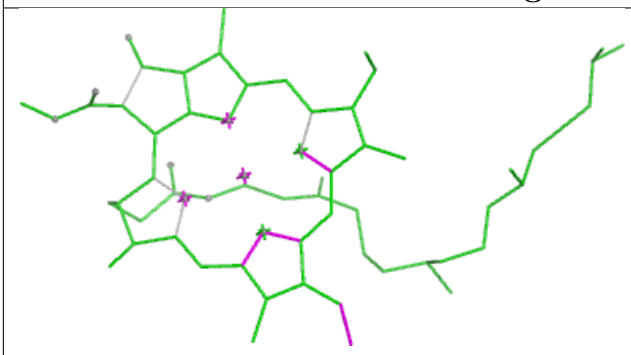
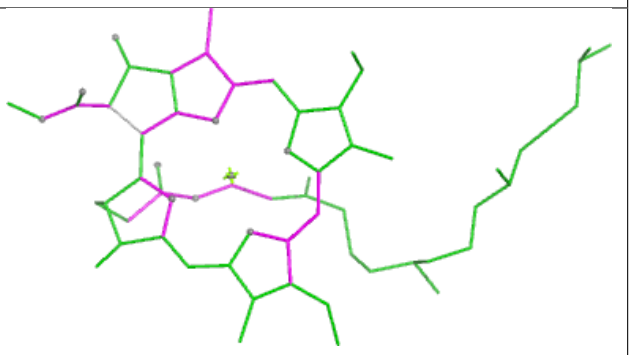


Rings

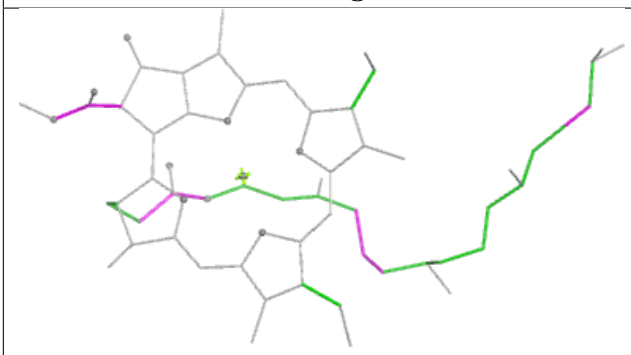
Ligand CLA B 836



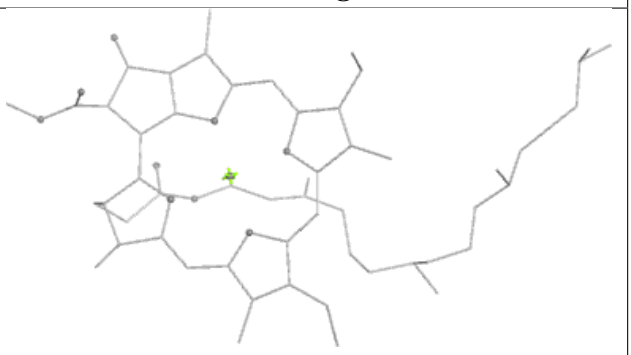
Bond lengths



Bond angles

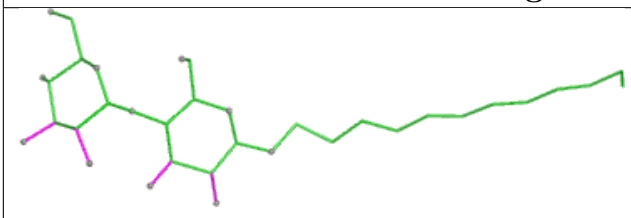


Torsions



Rings

Ligand LMT 4 320



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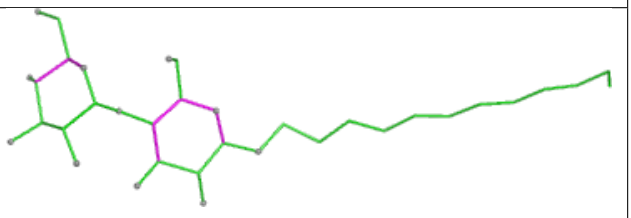

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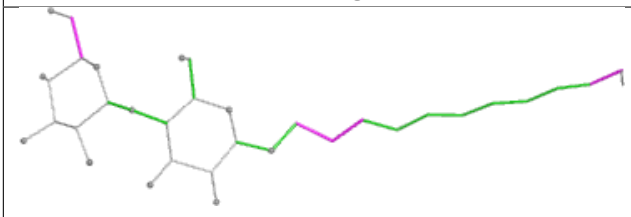

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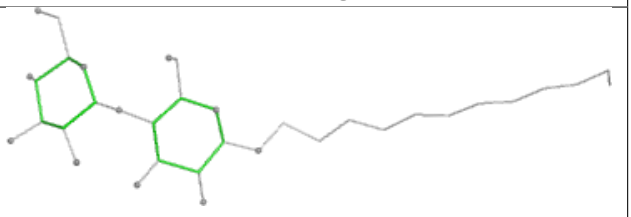
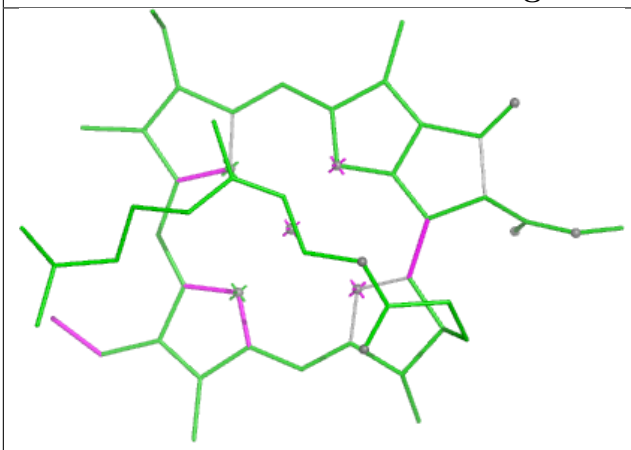


Rings

Ligand CLA A 812



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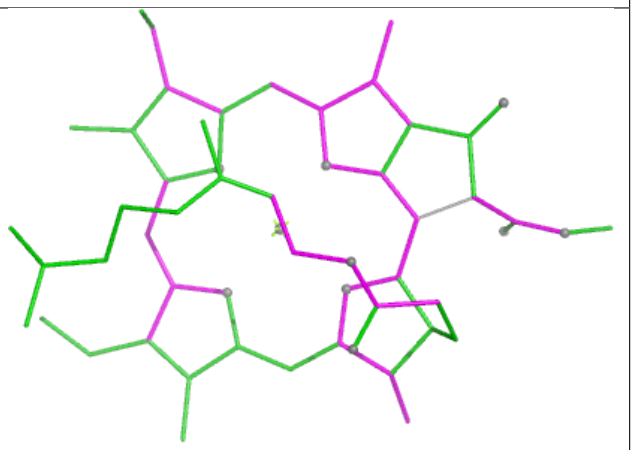

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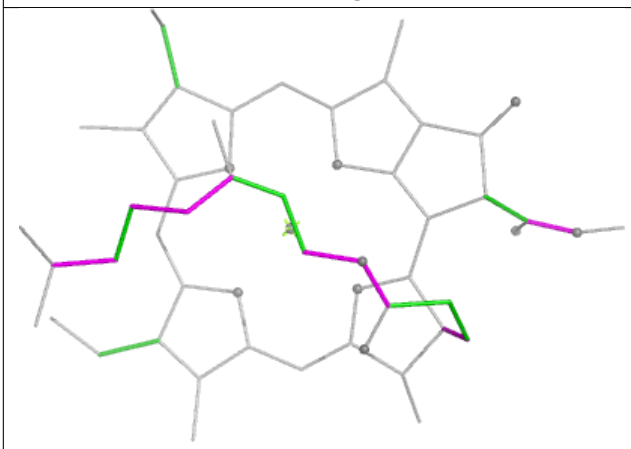

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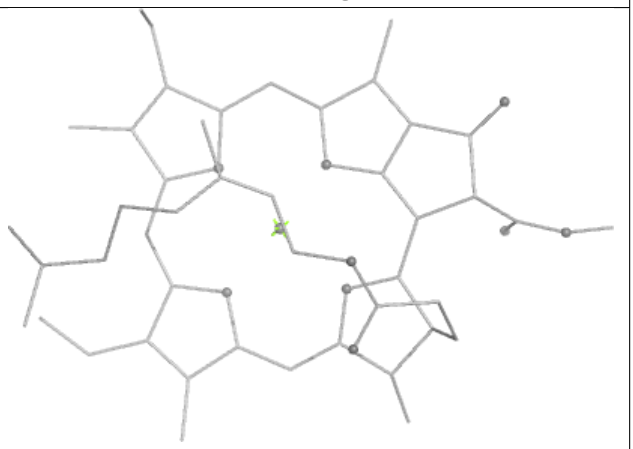
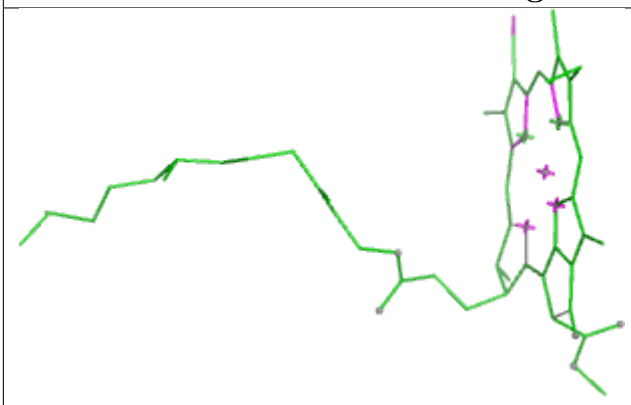


Rings

Ligand CLA L 304



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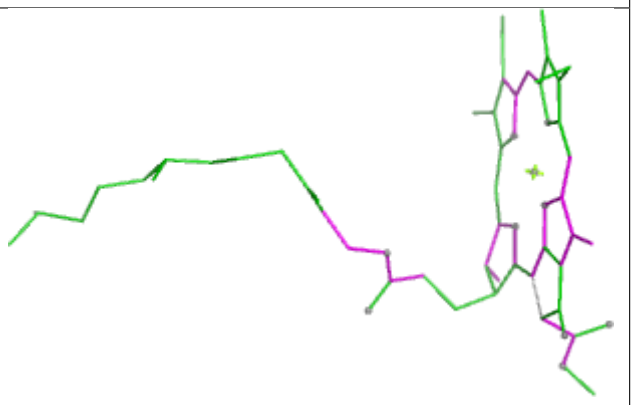
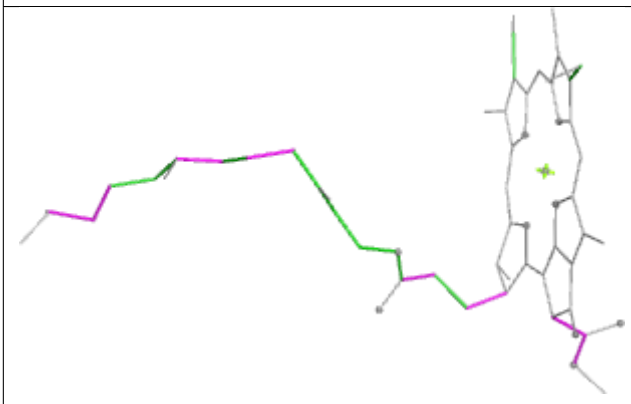


Bond angles

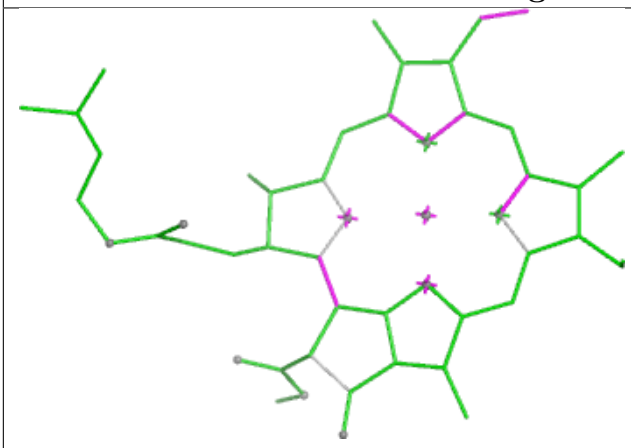


Torsions



Rings

Ligand CLA 4 312



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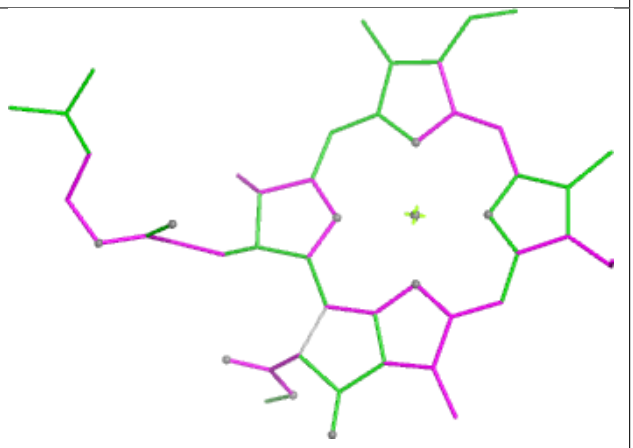
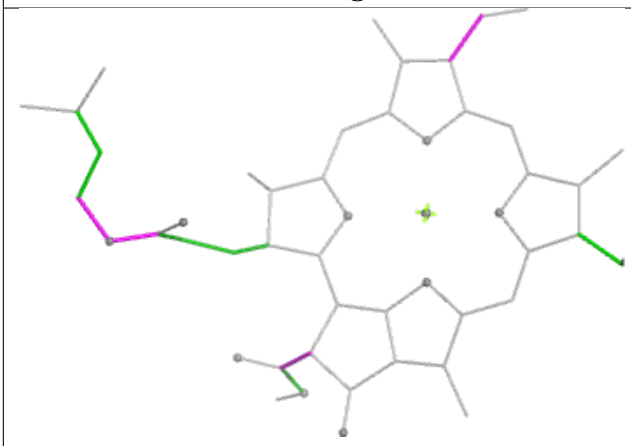


Bond angles



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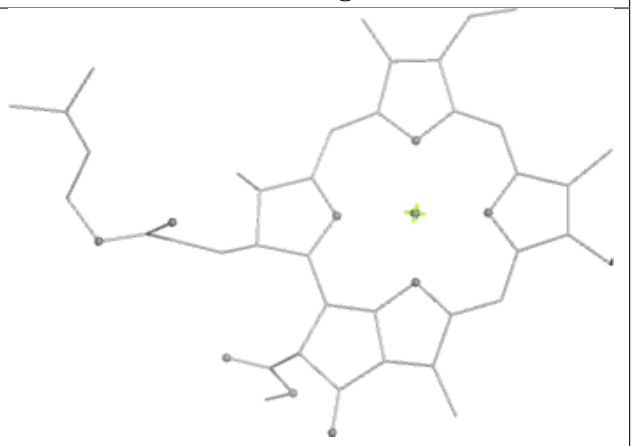
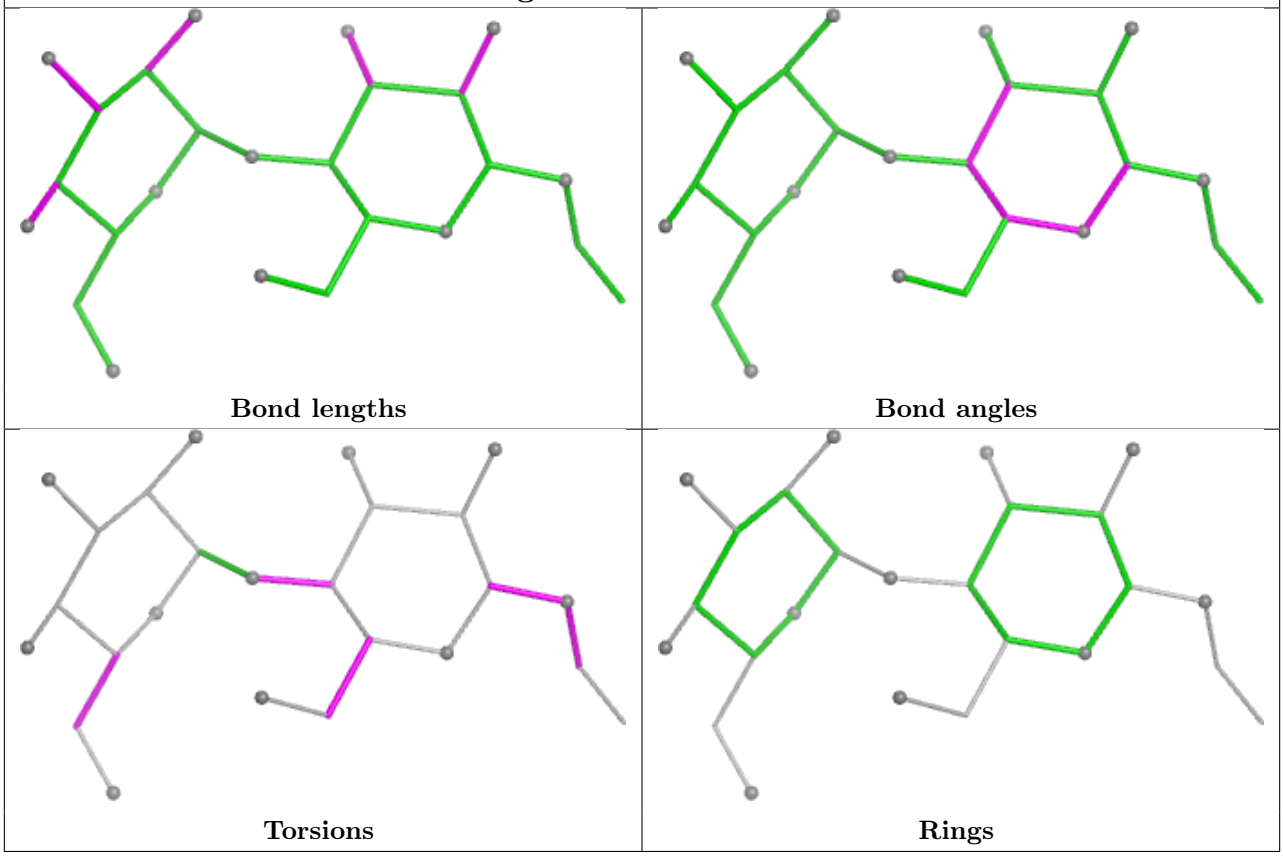
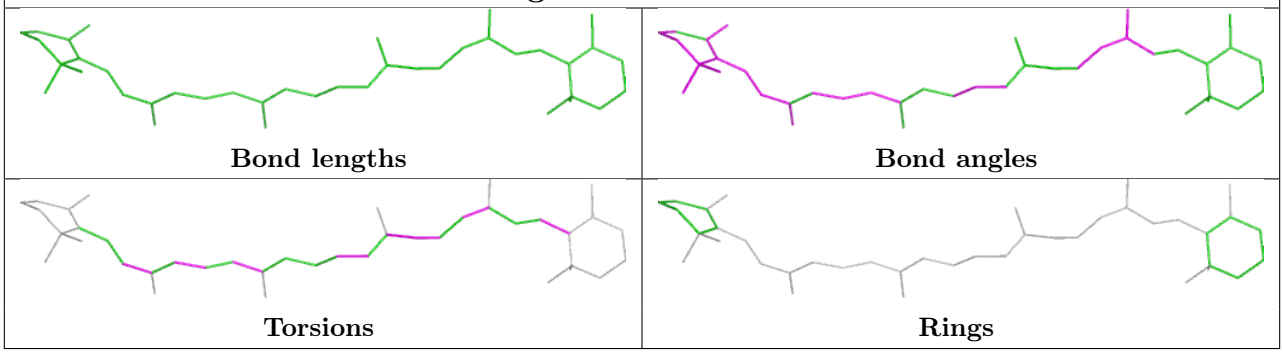


Rings

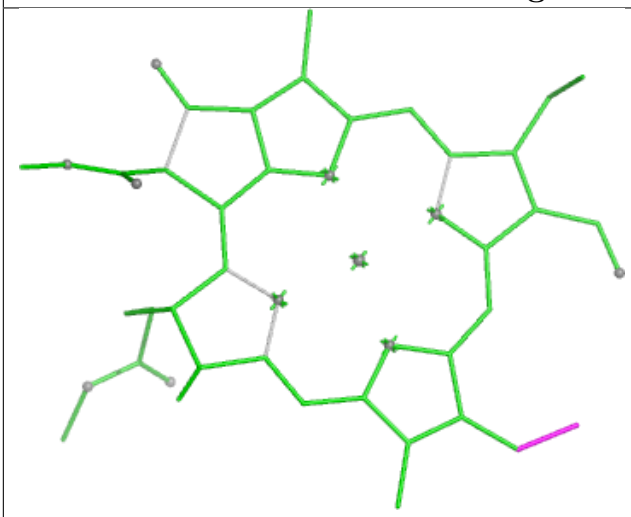
Ligand LMT J 1107



Ligand BCR 4 301



Ligand CHL 1 512



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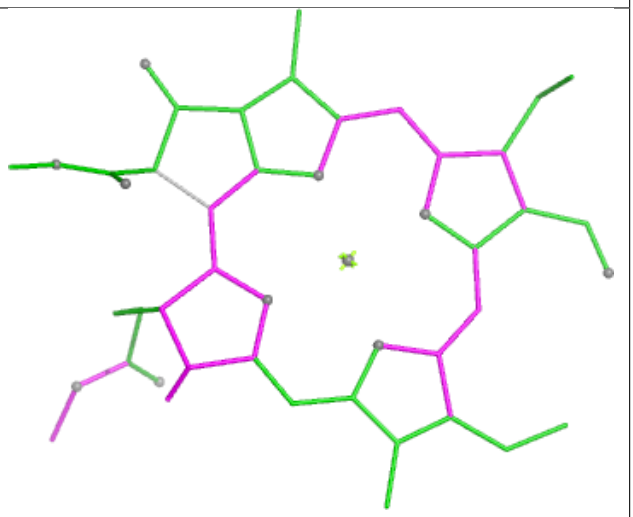
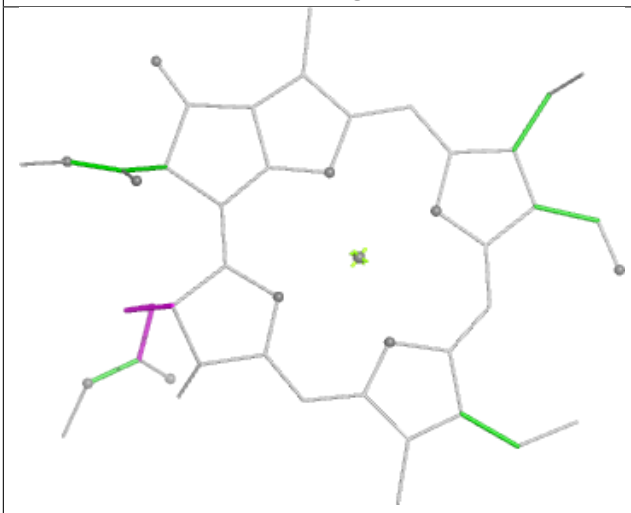


Bond angles



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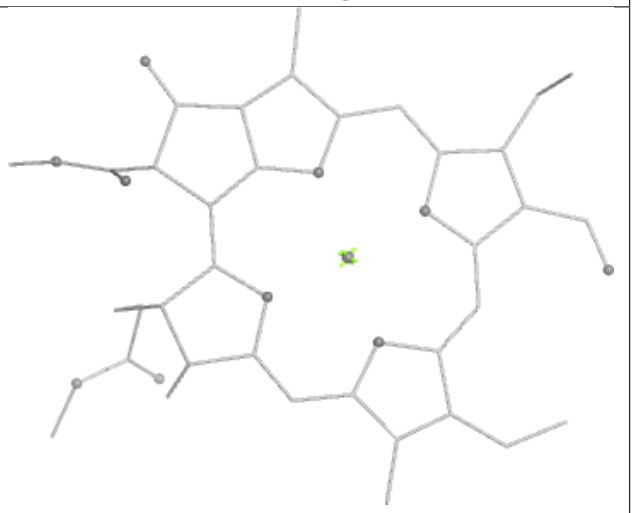
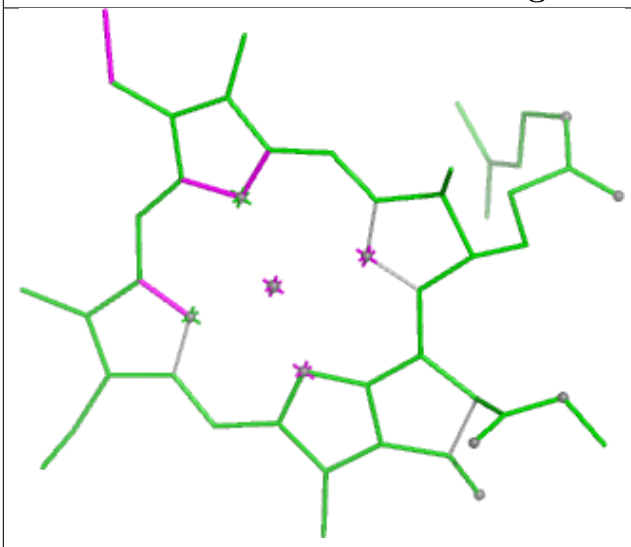


Rings

Ligand CLA 3 315



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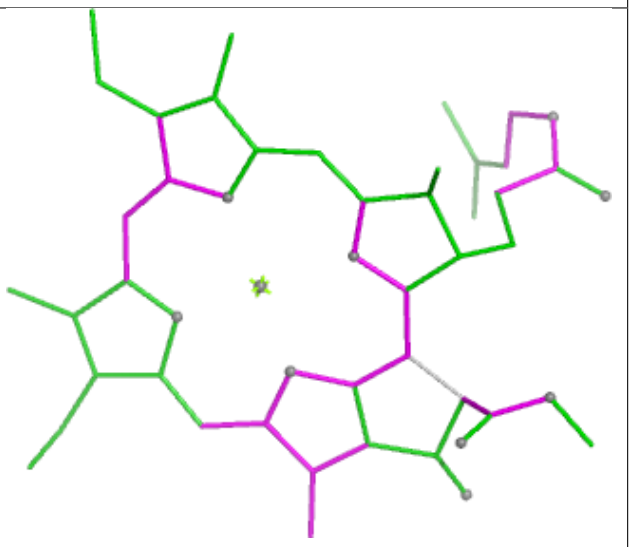
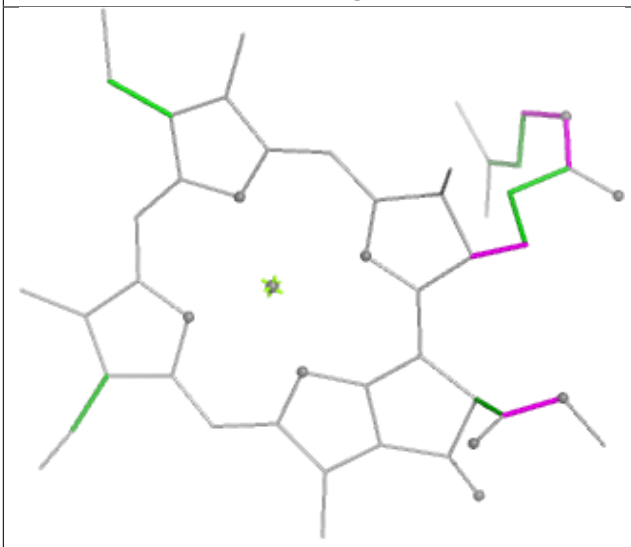


Bond angles



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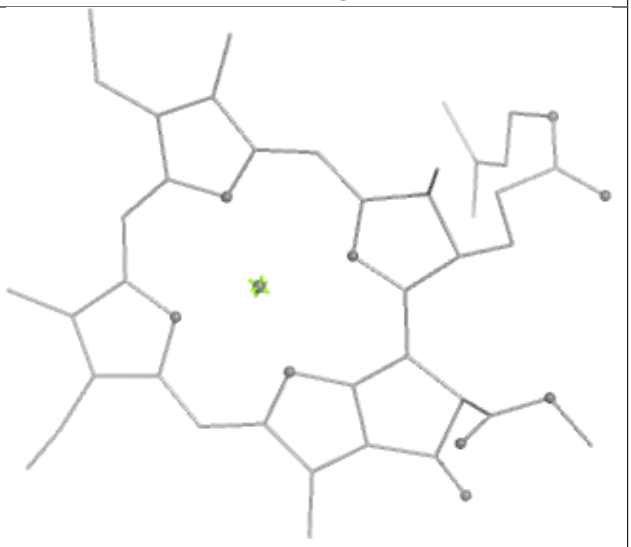
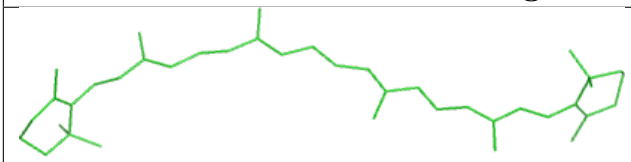


Rings

Ligand BCR B 853



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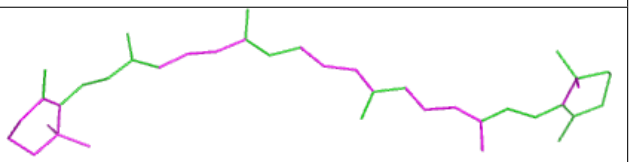
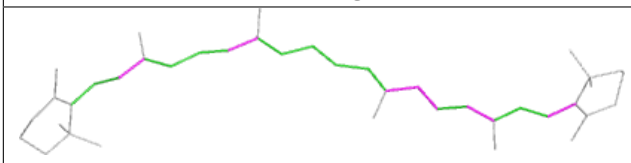


Bond angles



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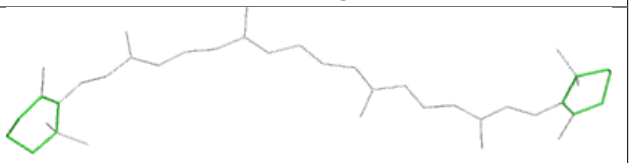
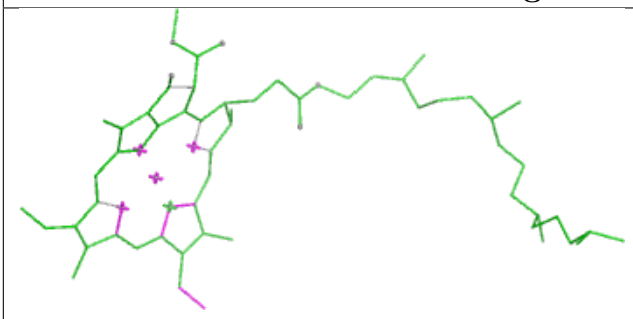


Rings

Ligand CLA A 854



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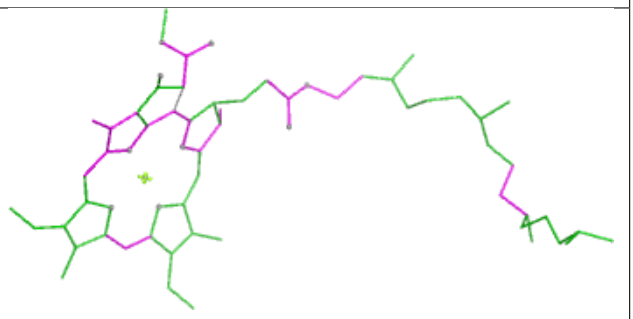
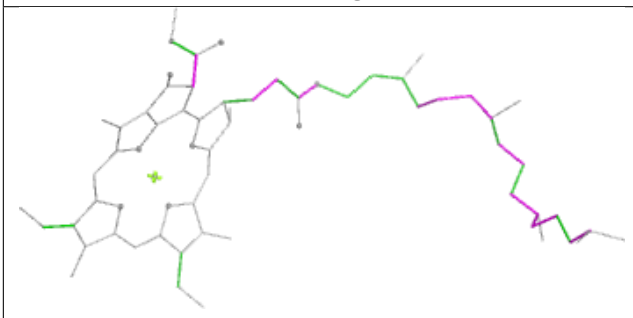


Bond angles



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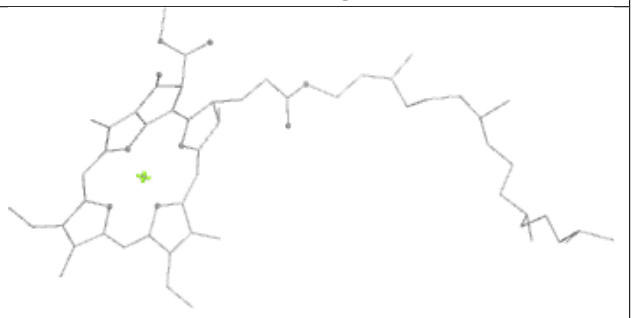
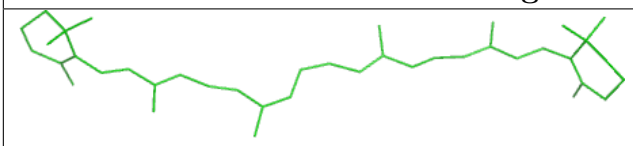


Rings

Ligand BCR G 205



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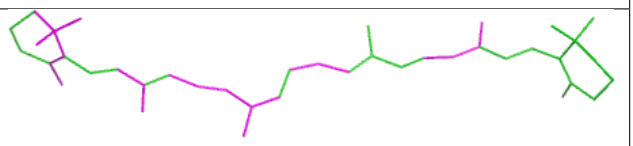

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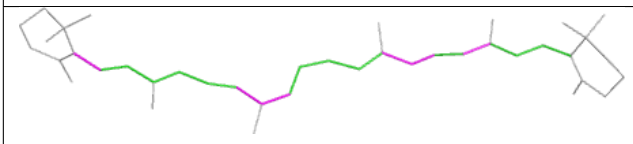

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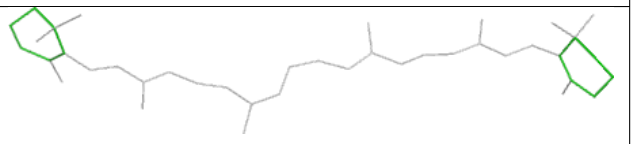


Rings

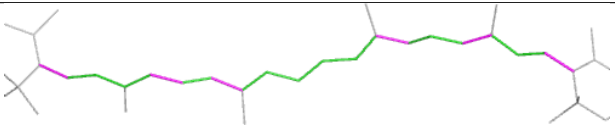
Ligand BCR J 1108



Bond lengths



Bond angles



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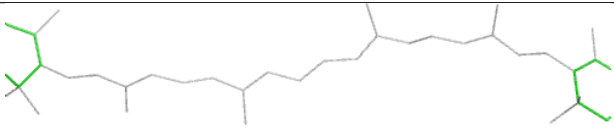
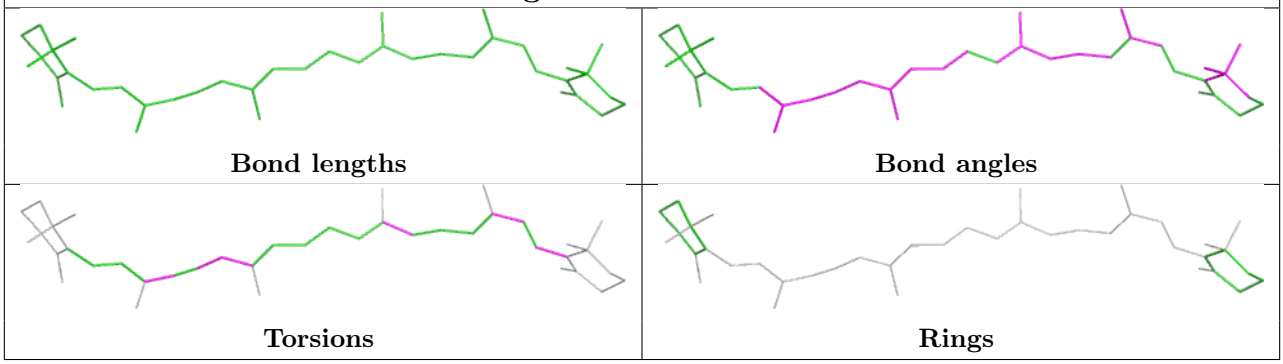
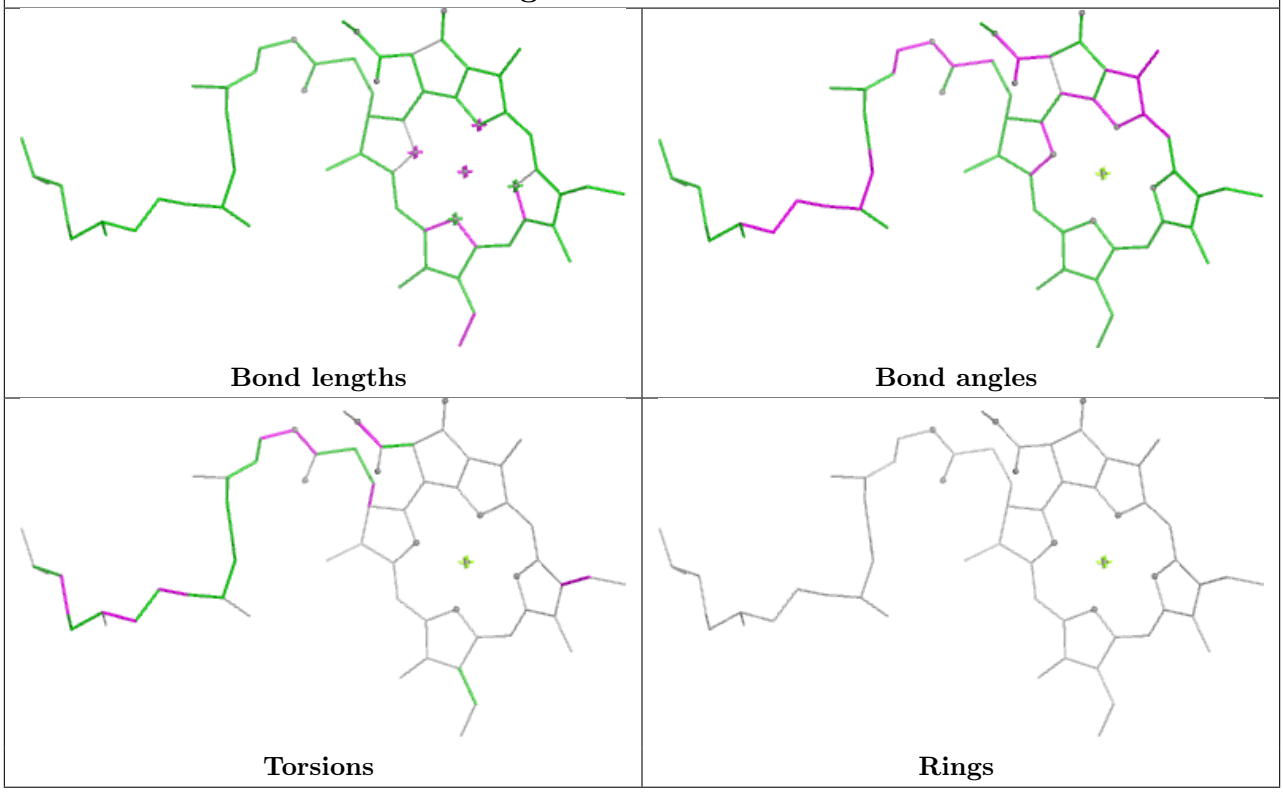


Rings

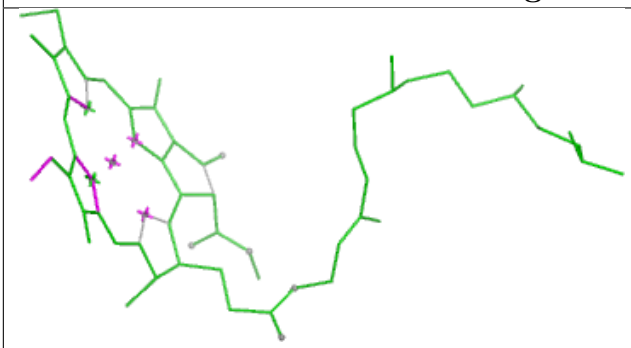
Ligand BCR A 849



Ligand CLA J 1101



Ligand CLA B 803



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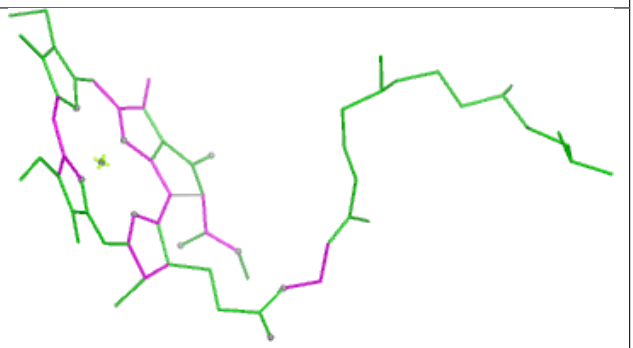
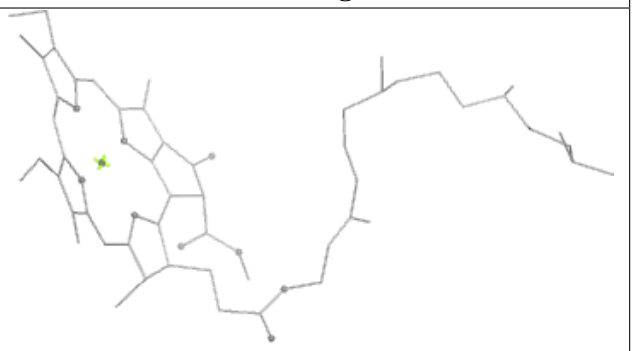


Bond angles

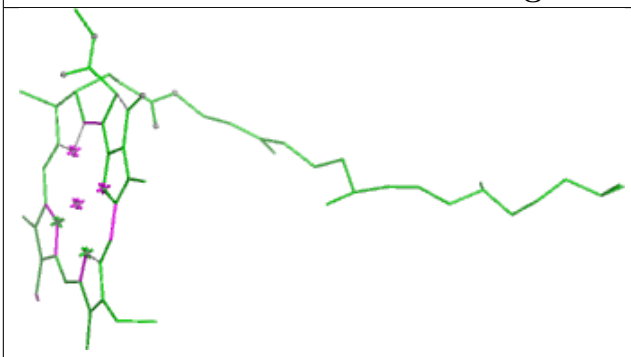


Torsions



Rings

Ligand CLA B 828



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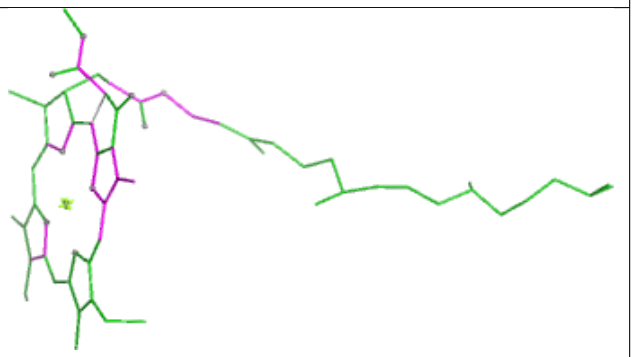
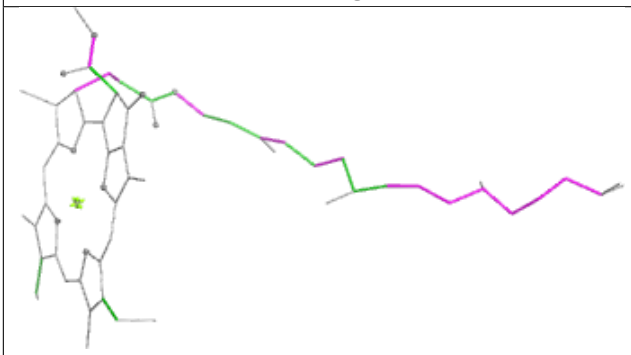


Bond angles



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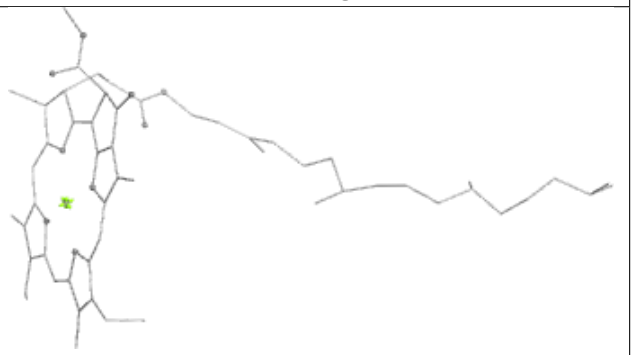
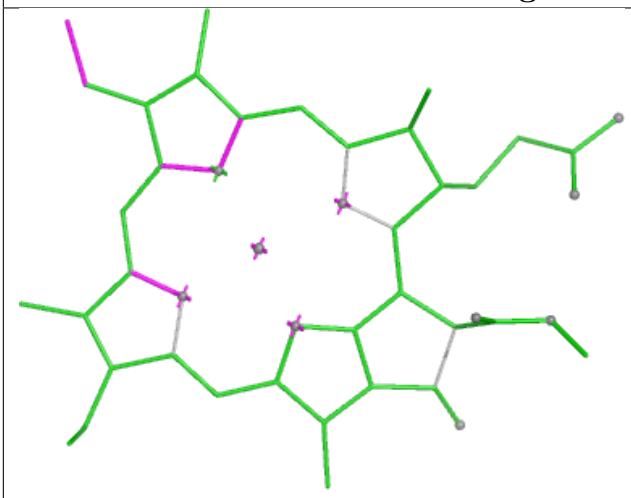
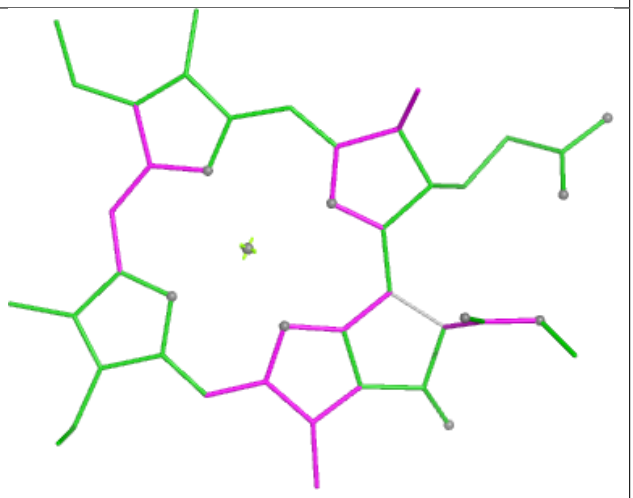


Rings

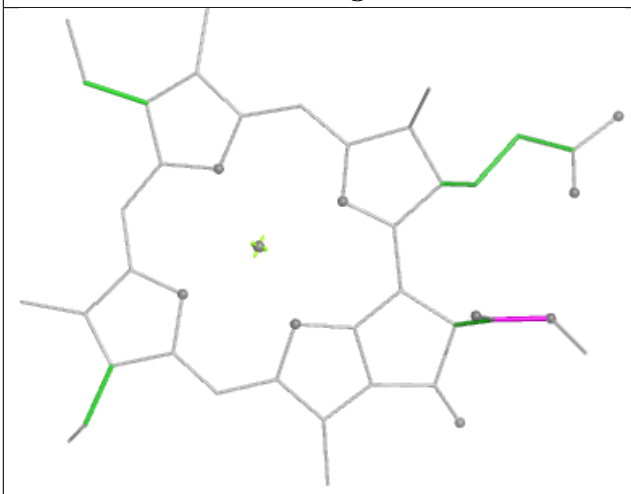
Ligand CLA J 1102



Bond lengths



Bond angles



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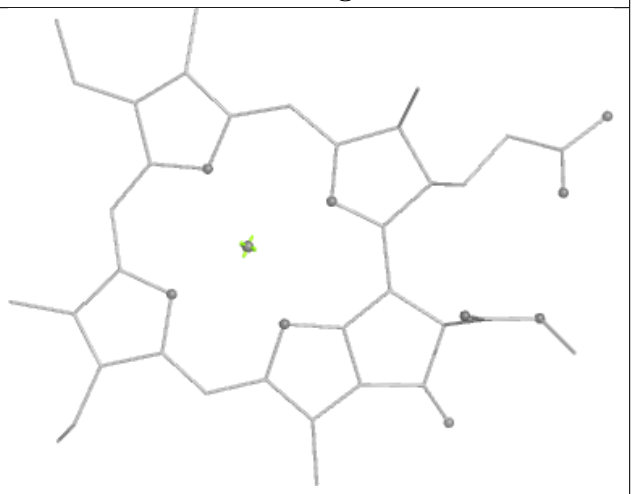
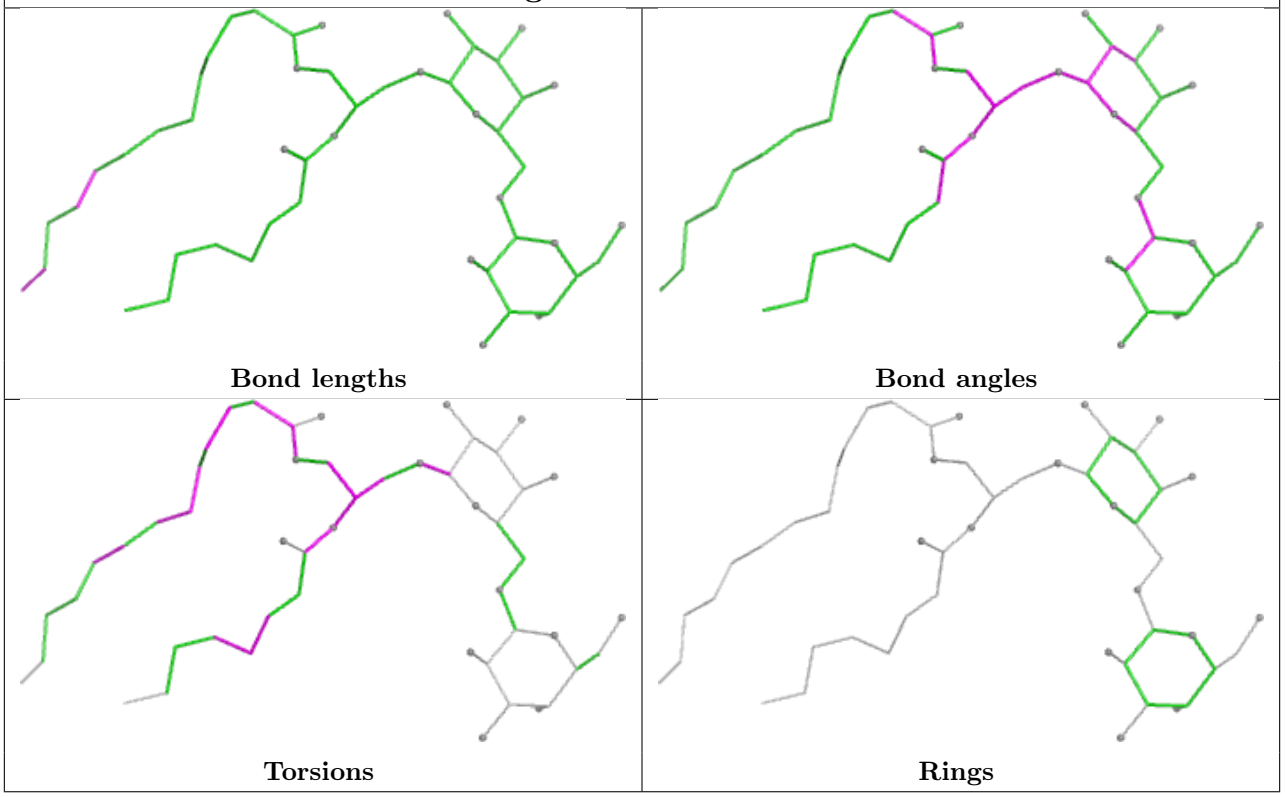
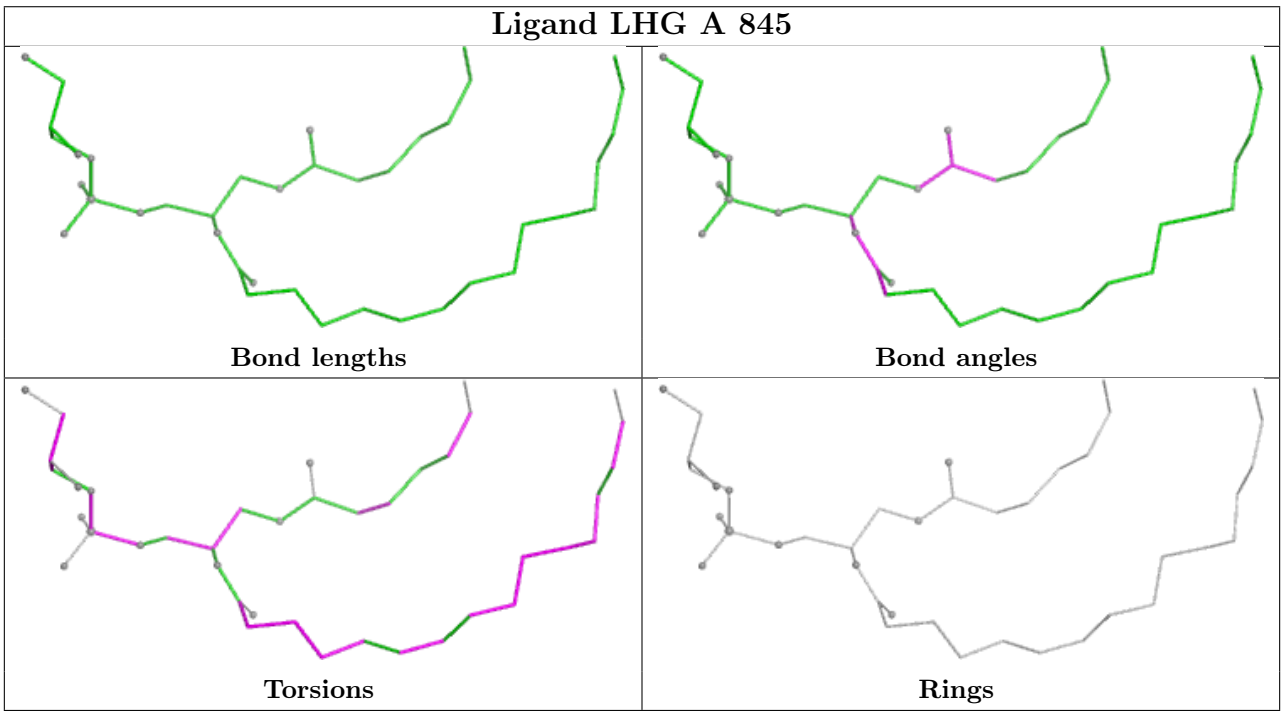


Rings

Ligand DGD 4 319



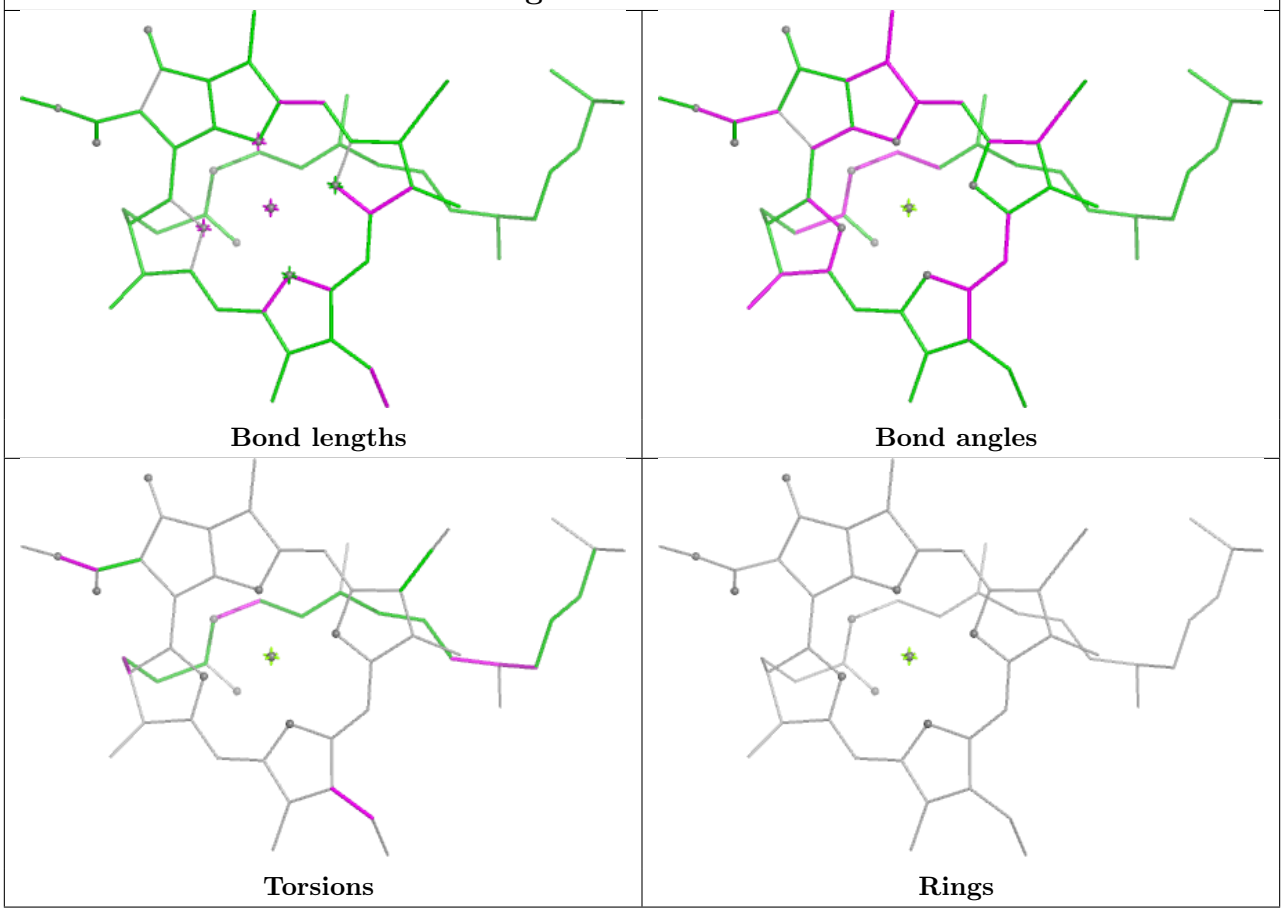
Ligand LHG A 845



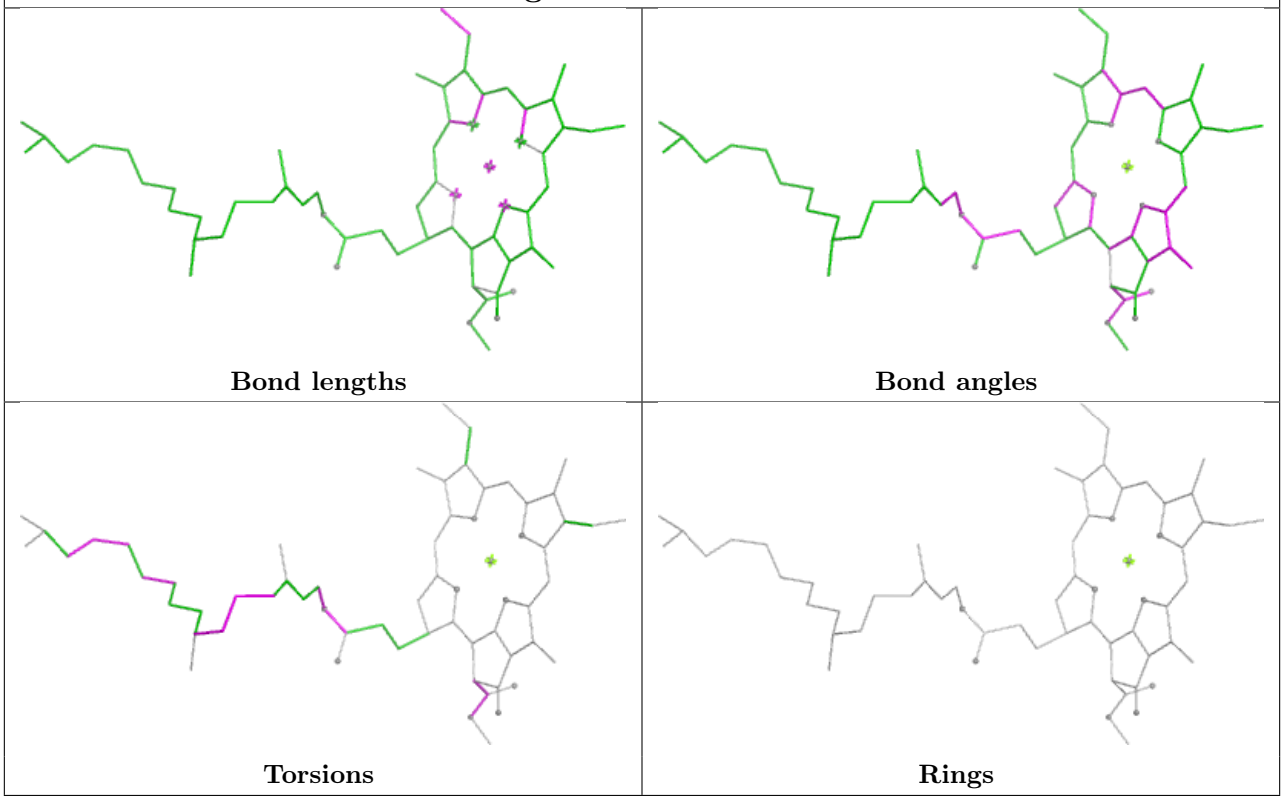
Ligand LUT 3 302



Ligand CLA B 817



Ligand CLA A 831



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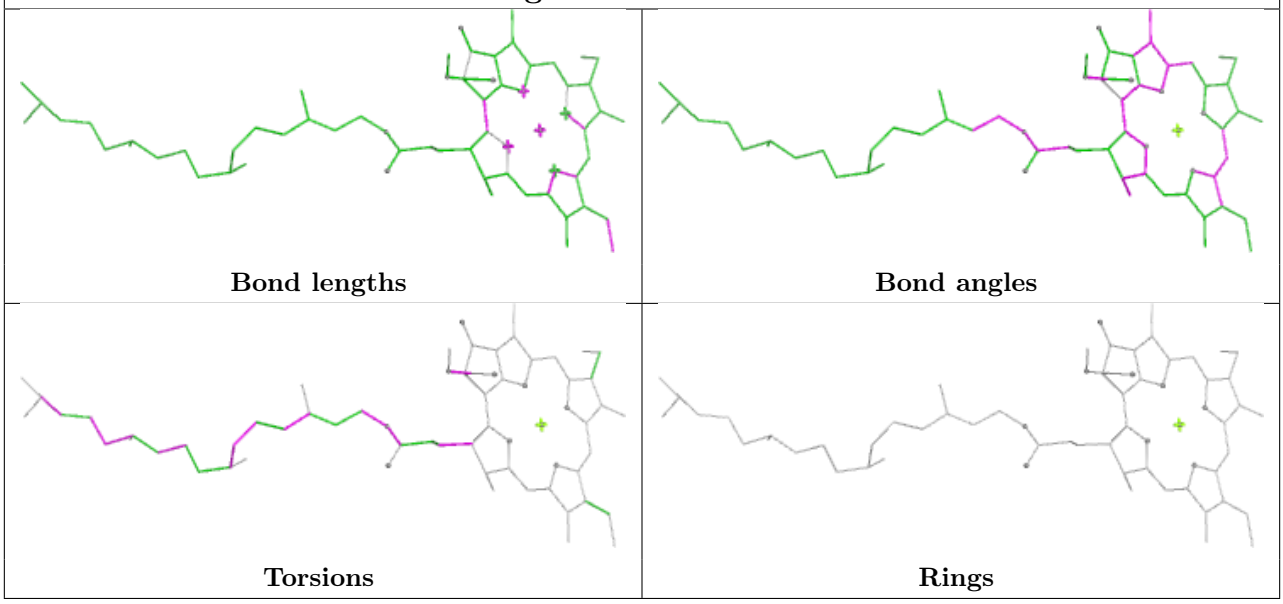

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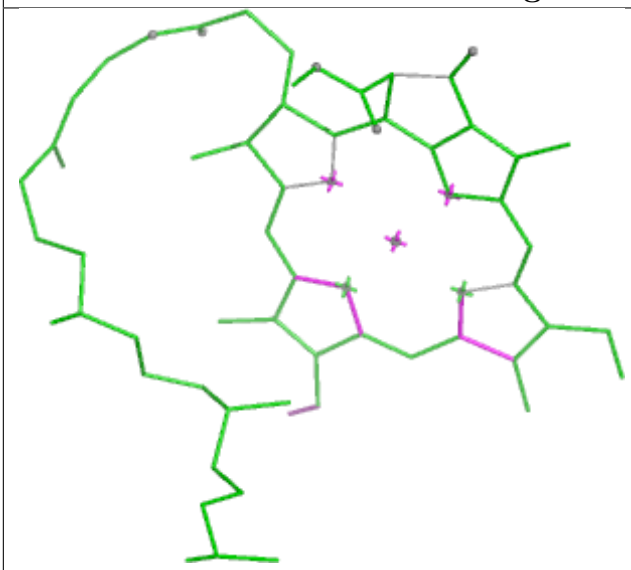
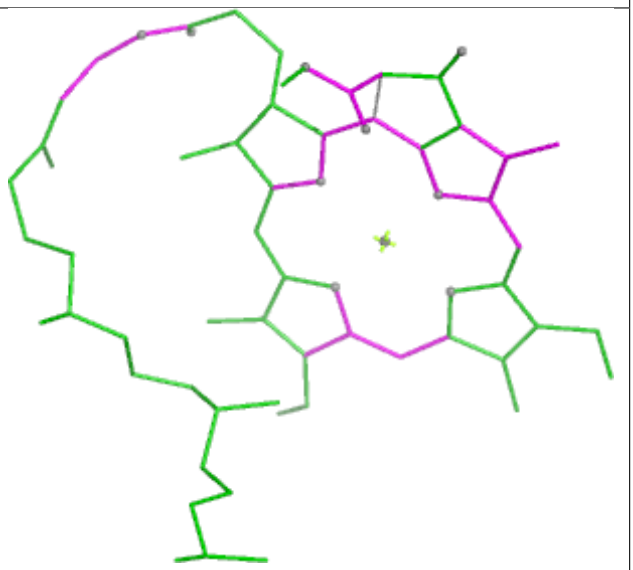
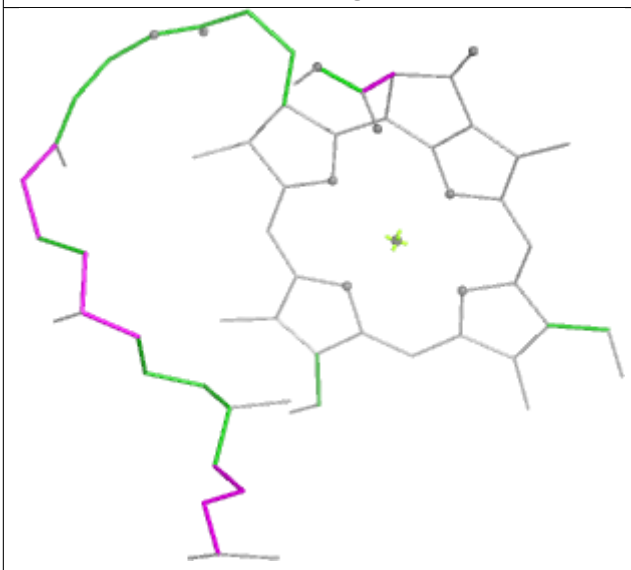


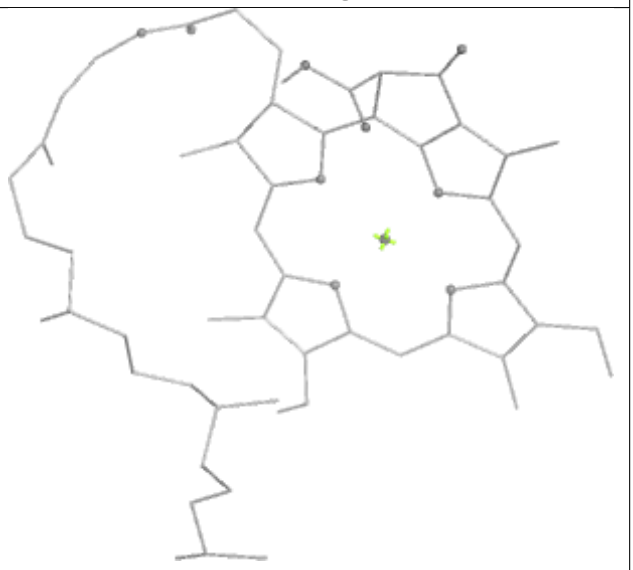
Bond lengths



Bond angles

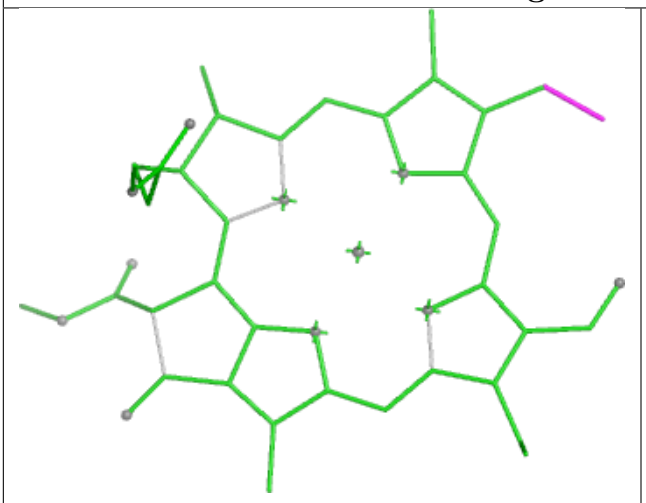


Torsions



Rings

Ligand CHL 3 314



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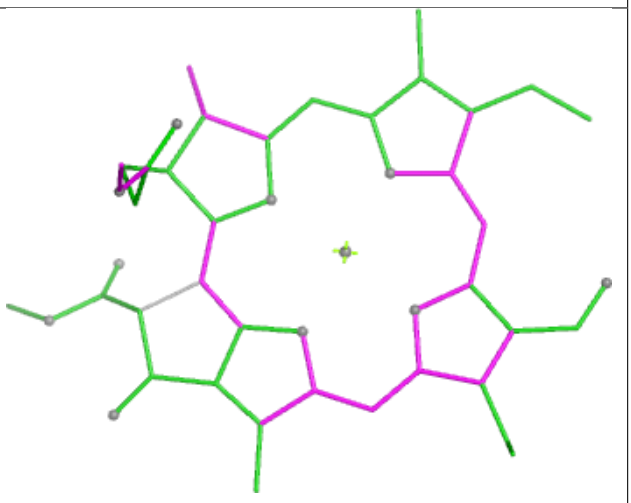
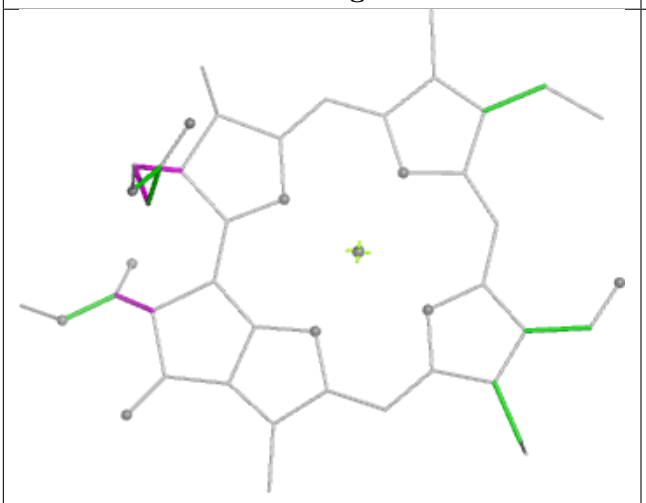


Bond angles



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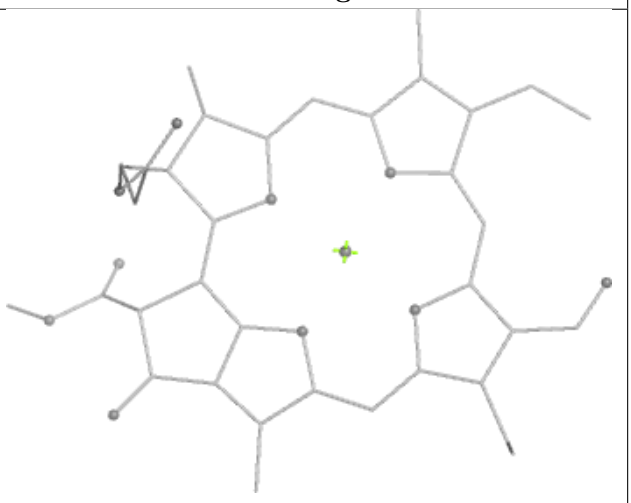
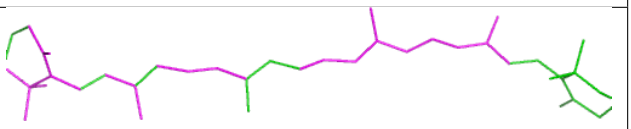


Rings

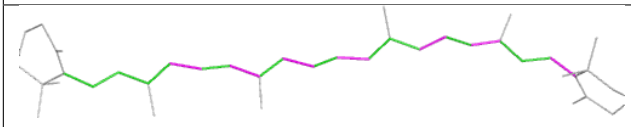
Ligand BCR A 848



Bond lengths



Bond angles



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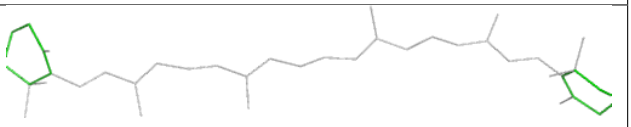
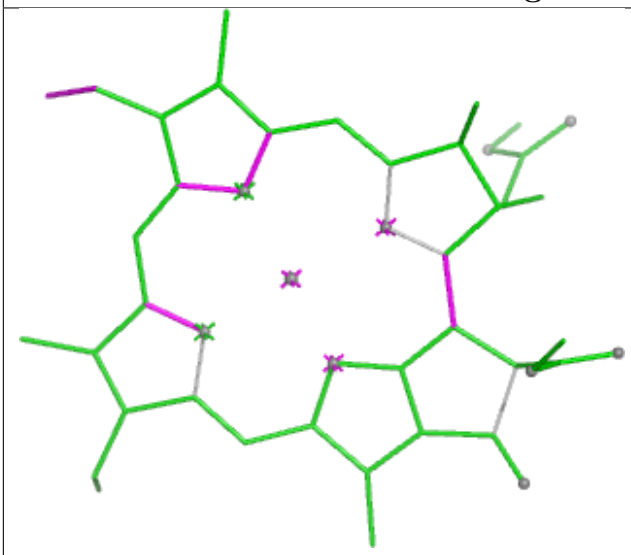


Rings

Ligand CLA B 821



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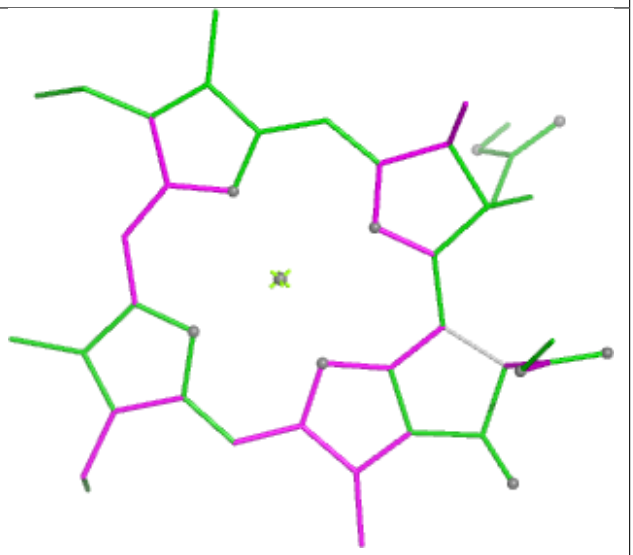
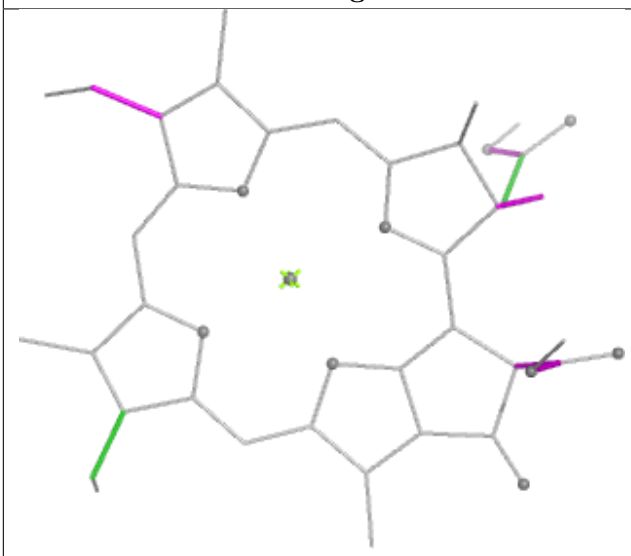


Bond angles



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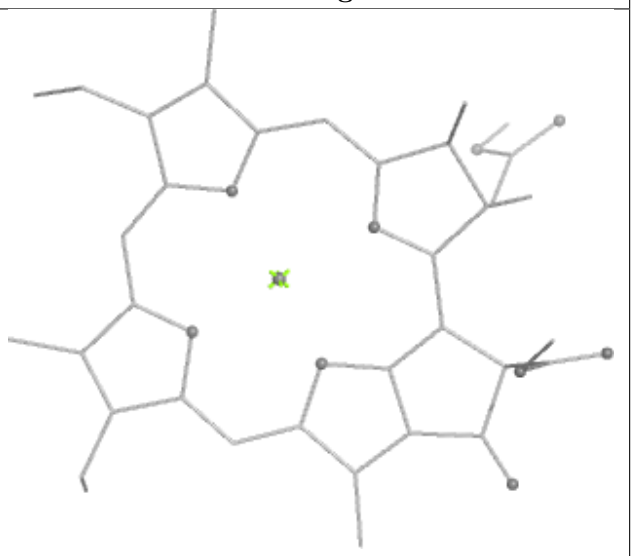
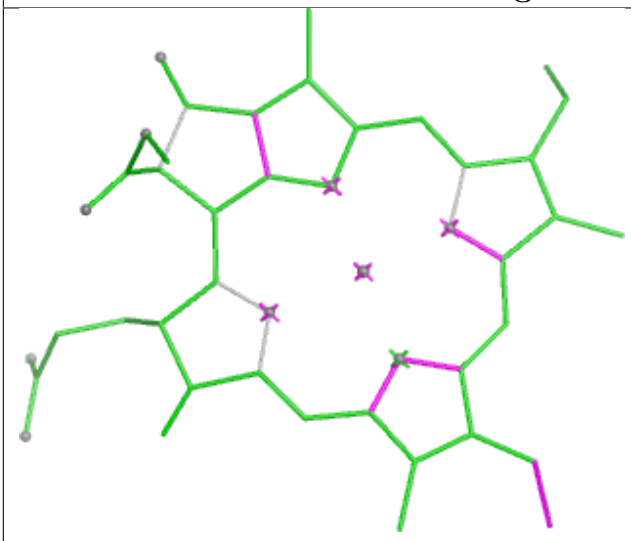


Rings

Ligand CLA K 1001



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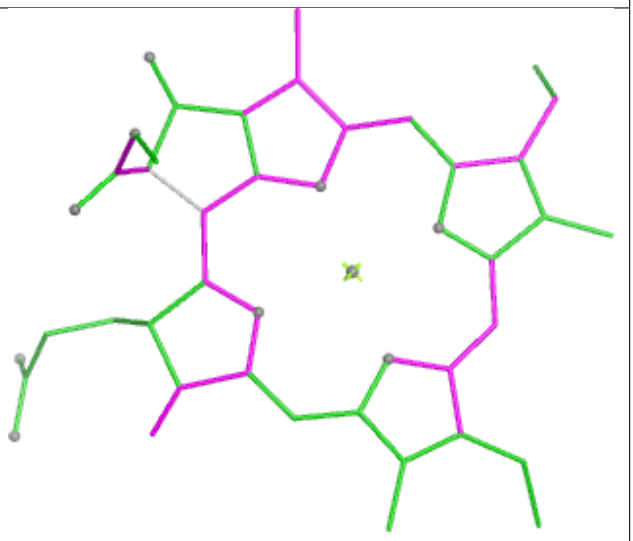
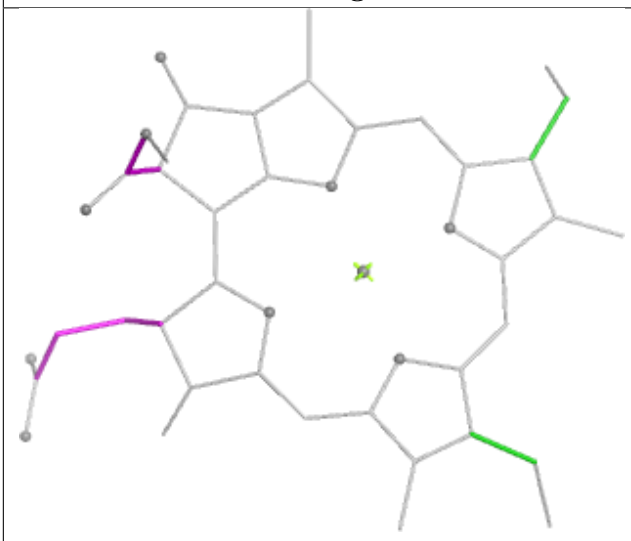


Bond angles



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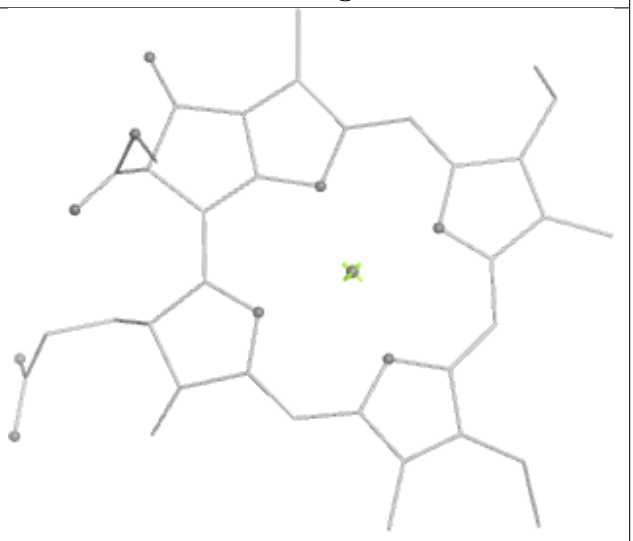
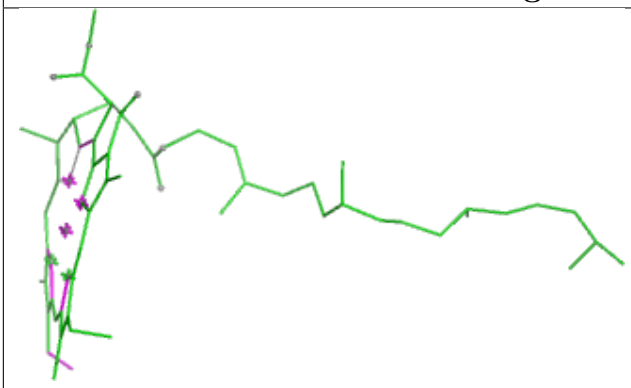


Rings

Ligand CLA A 828



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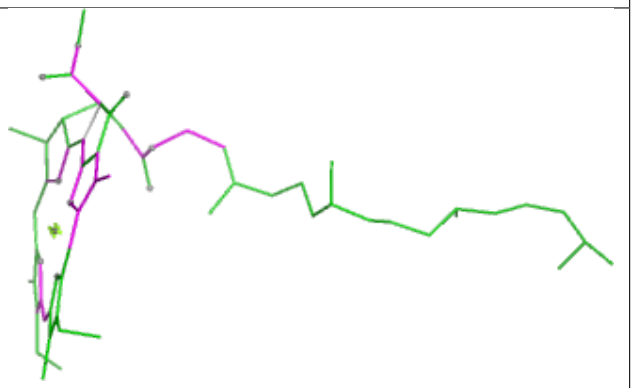
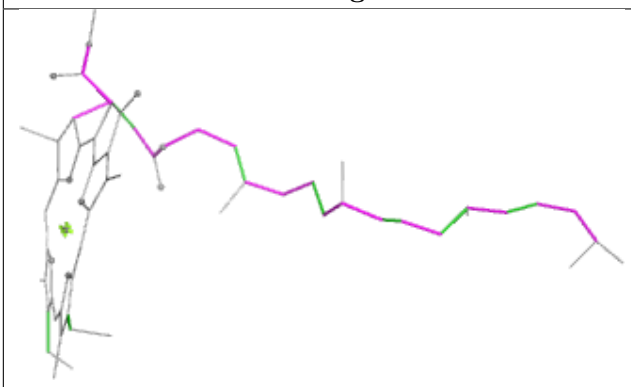


Bond angles



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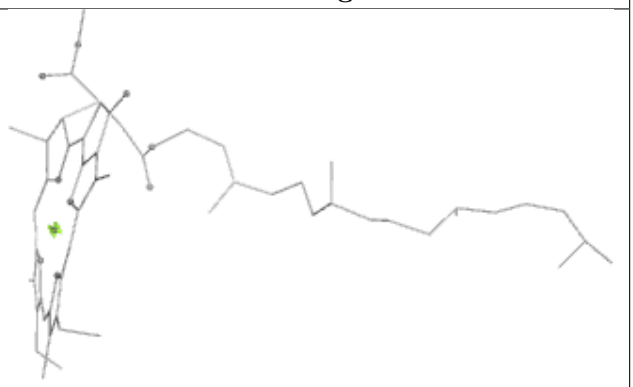
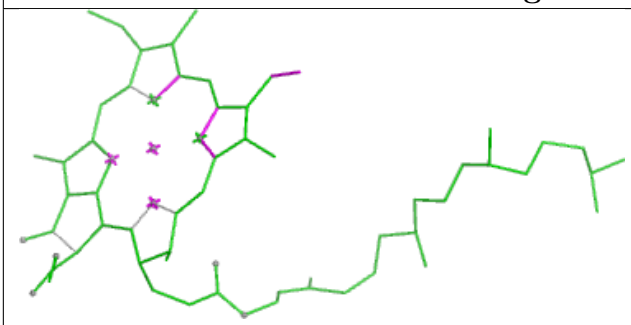


Rings

Ligand CLA A 808



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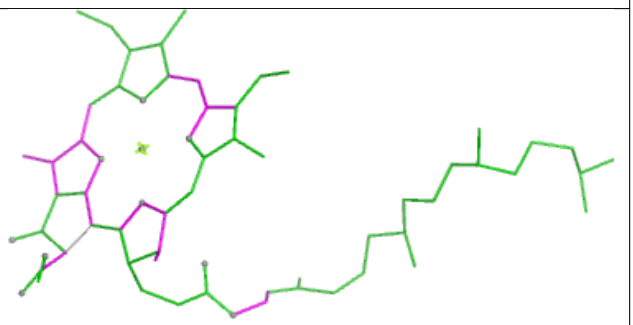
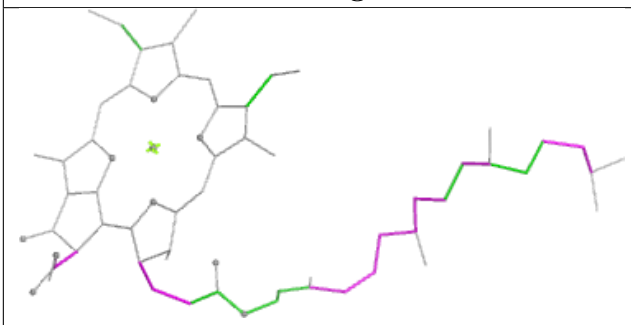


Bond angles

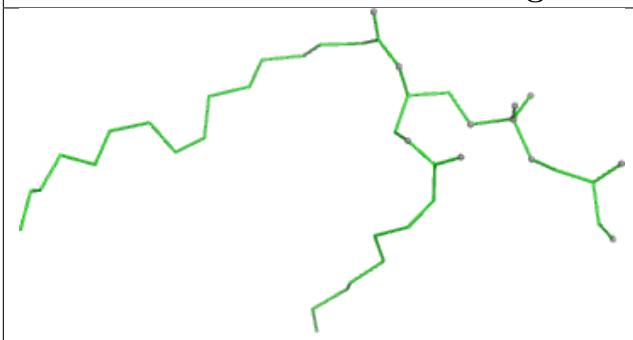


Torsions



Rings

Ligand LHG 1 520



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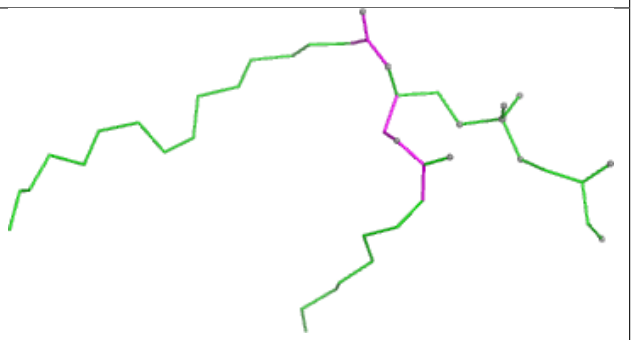
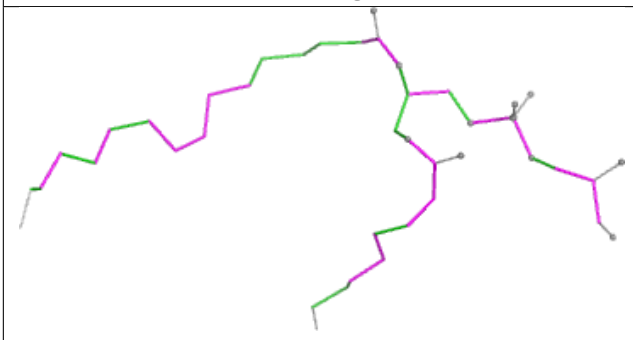


Bond angles



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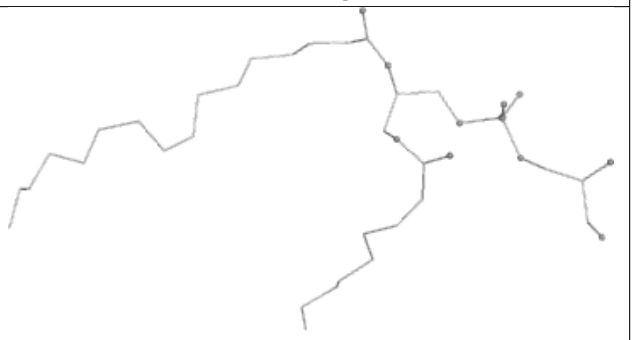
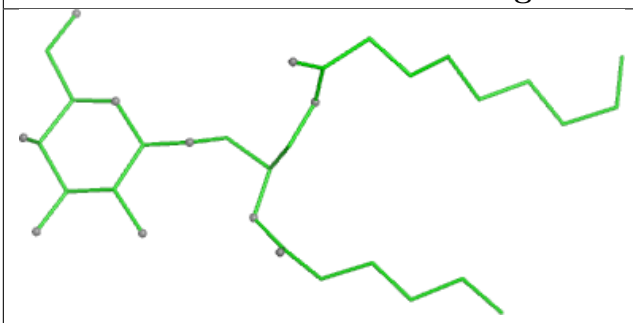


Rings

Ligand LMG J 1104



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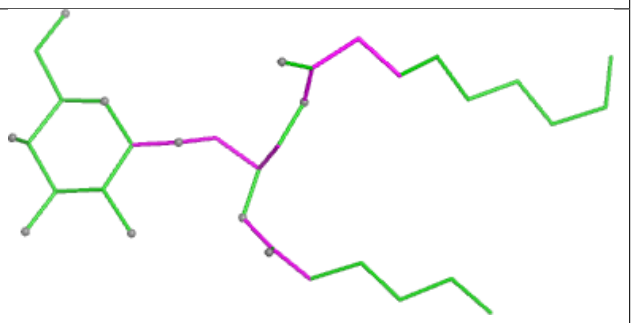
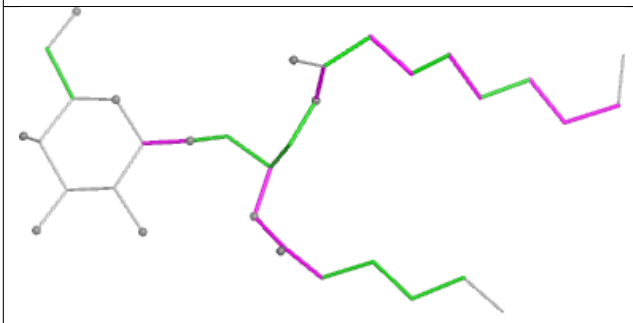


Bond angles



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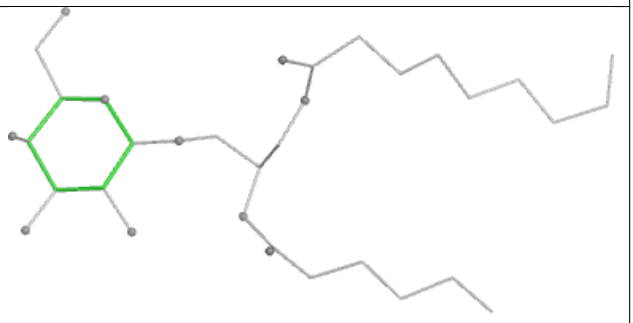
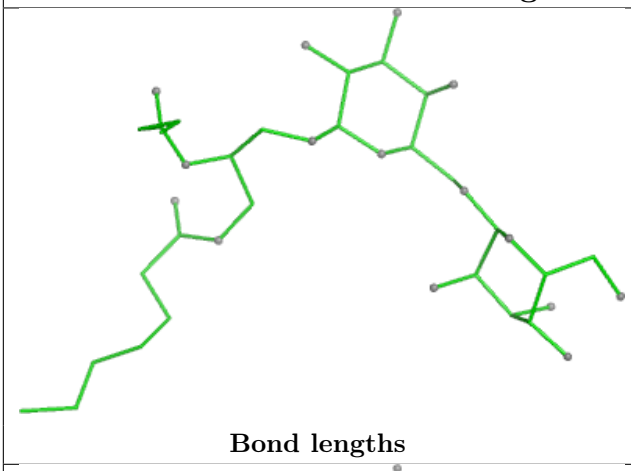


Rings

Ligand DGD B 801



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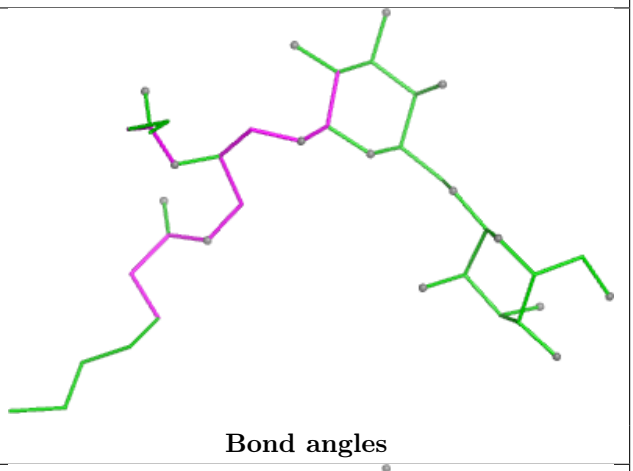
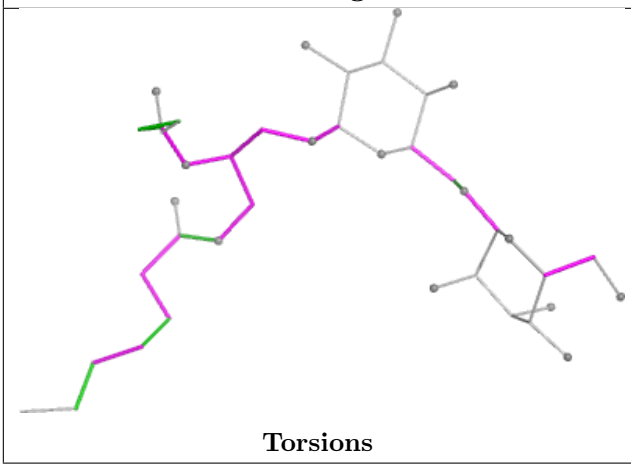


Bond angles



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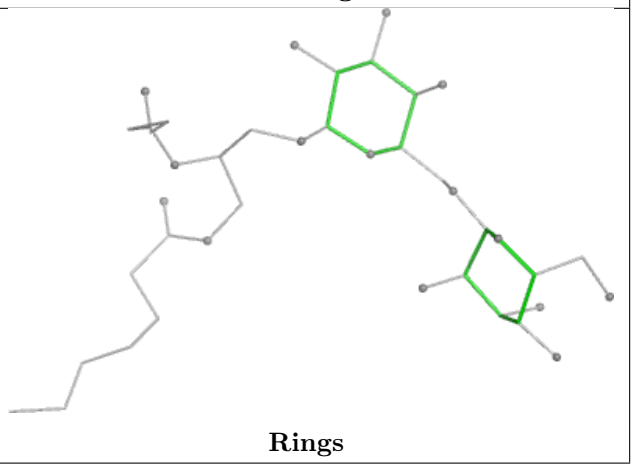
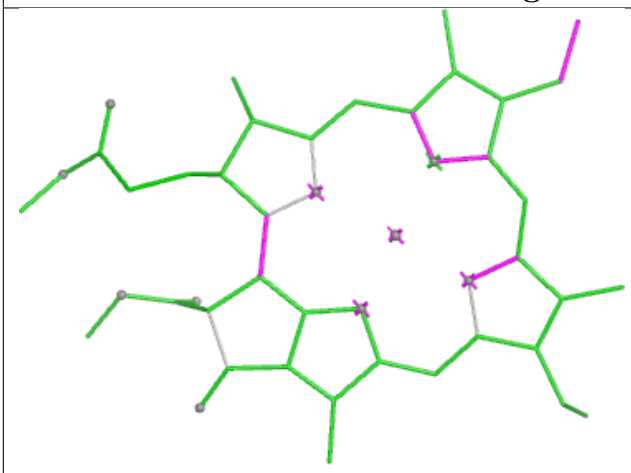


Rings

Ligand CLA G 203



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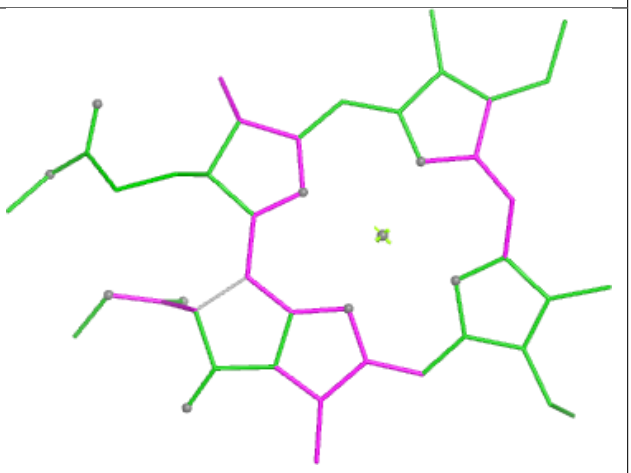
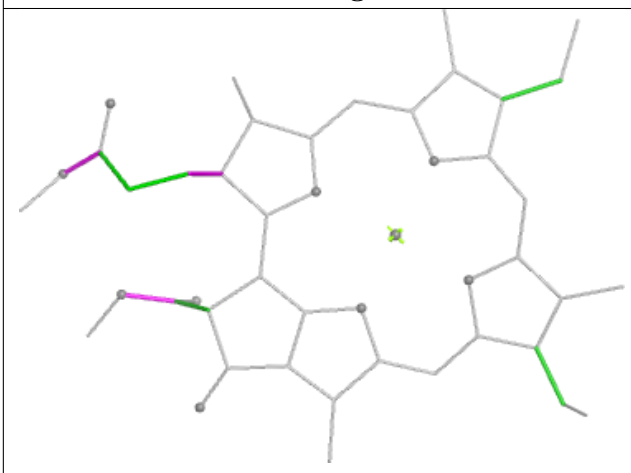


Bond angles



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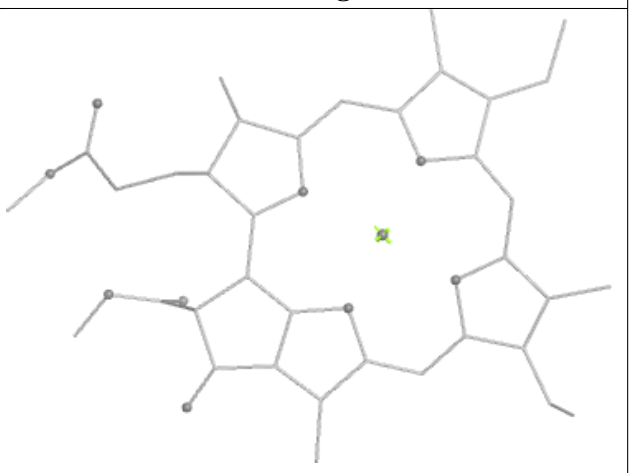
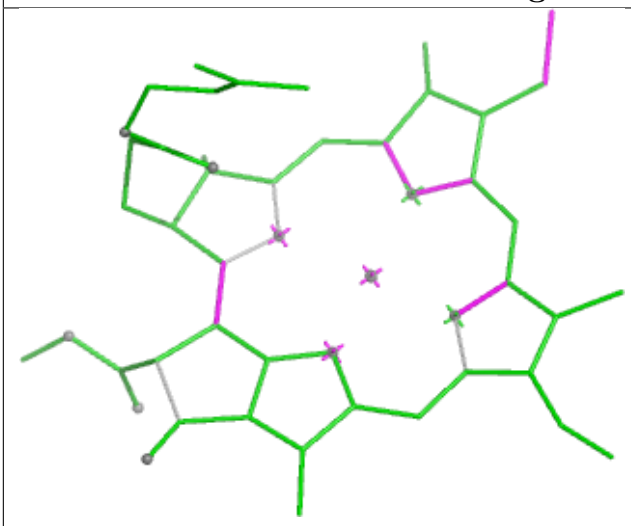


Rings

Ligand CLA 4 309



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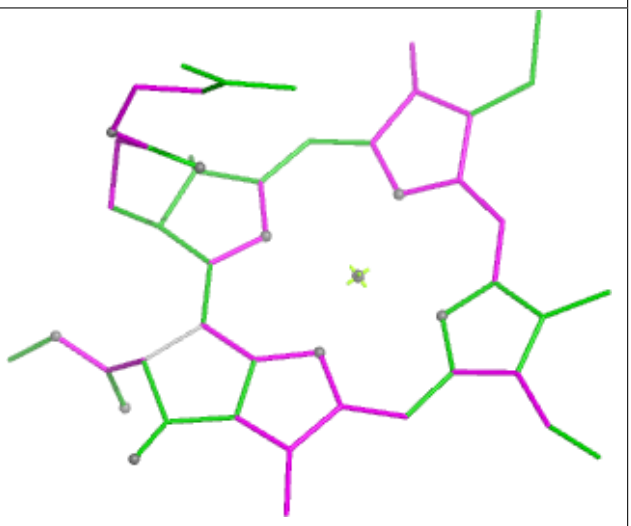
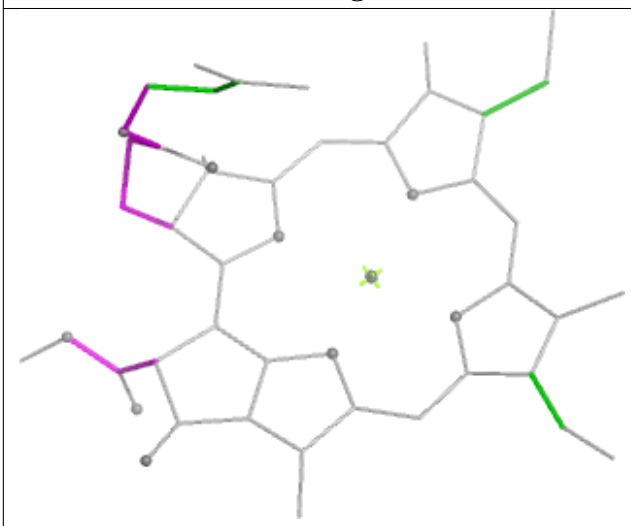


Bond angles



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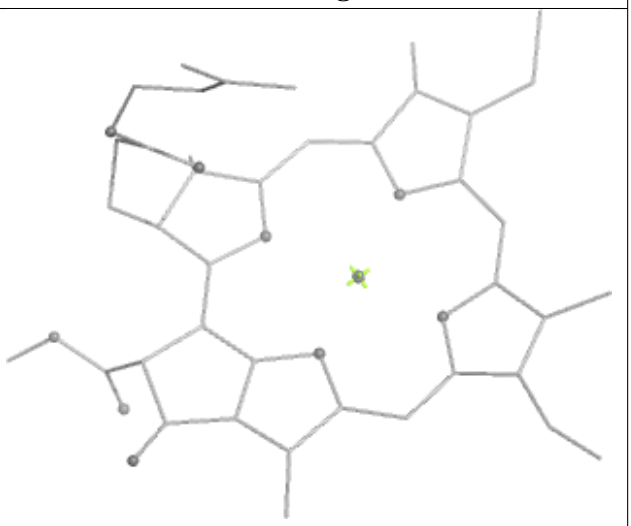
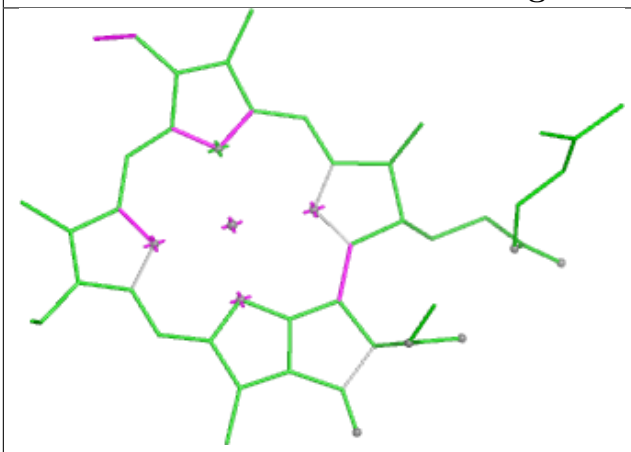


Rings

Ligand CLA 4 305



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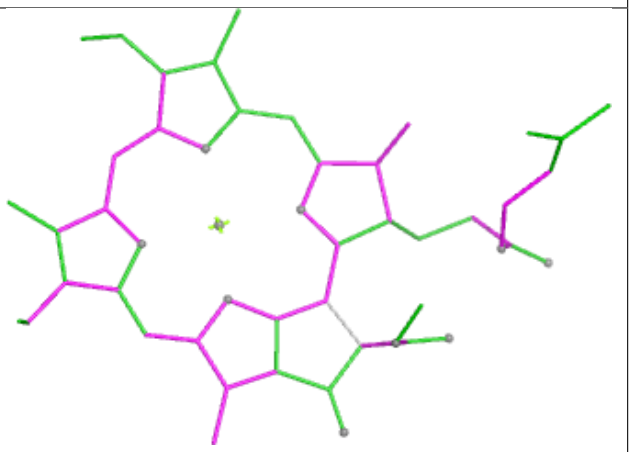
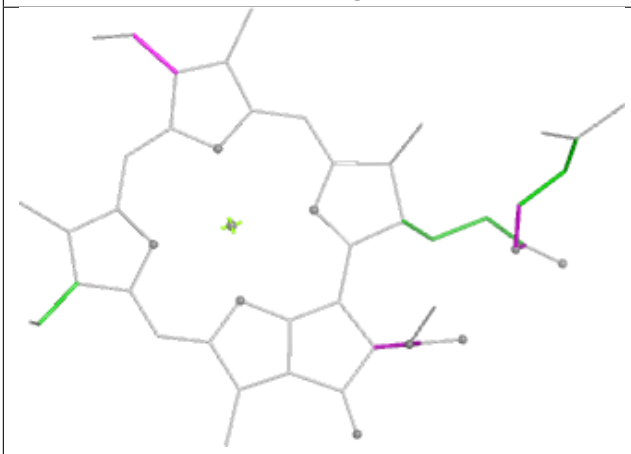


Bond angles

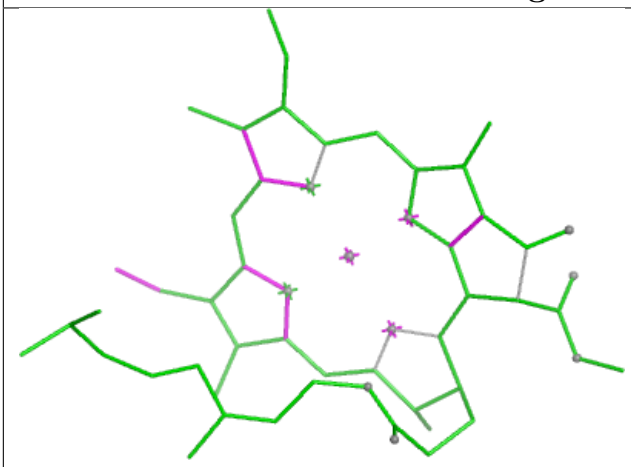


Torsions



Rings

Ligand CLA 3 305



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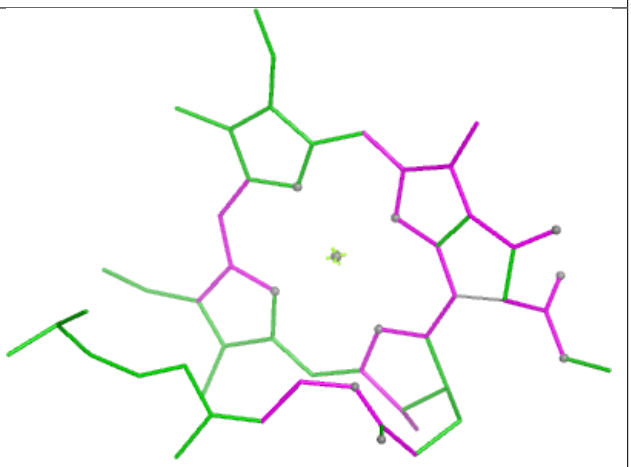
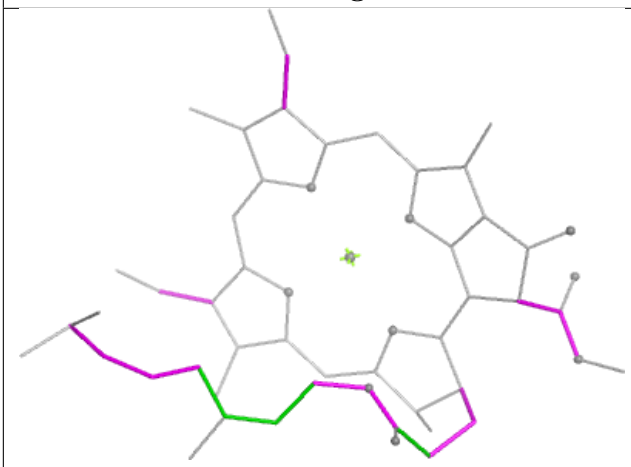


Bond angles



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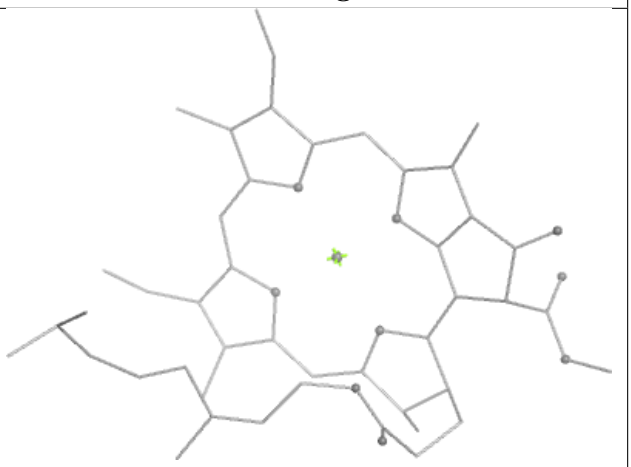
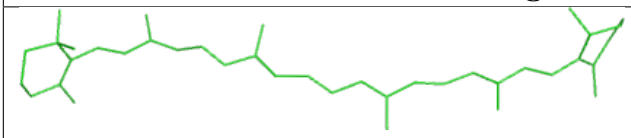


Rings

Ligand BCR L 306



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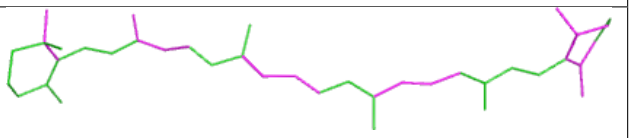
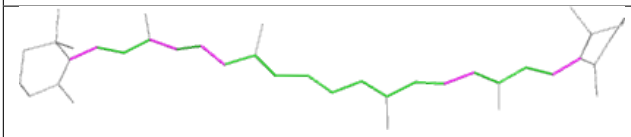
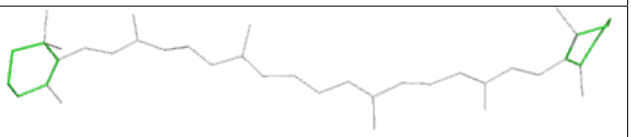


Bond angles

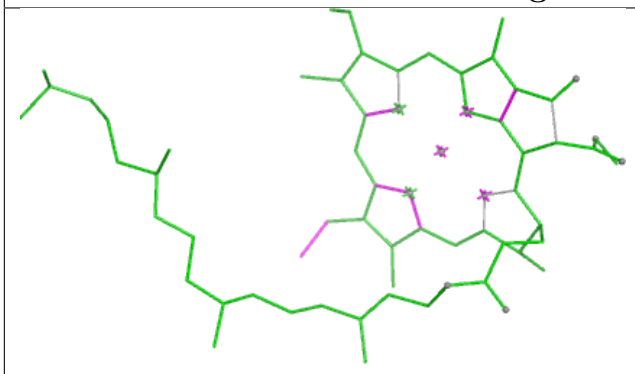


Torsions

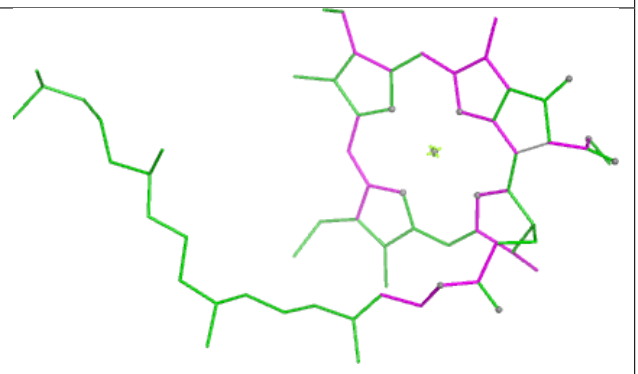


Rings

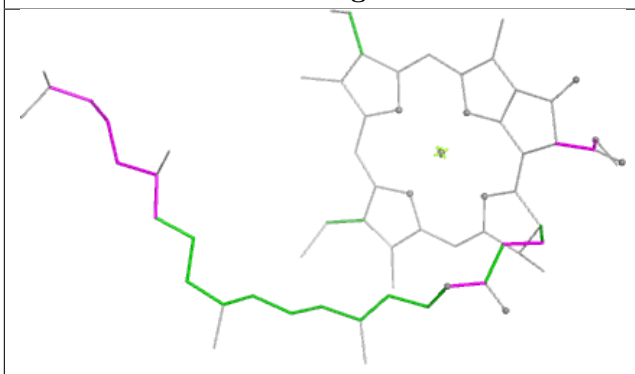
Ligand CLA 1 507



Bond lengths



Bond angles



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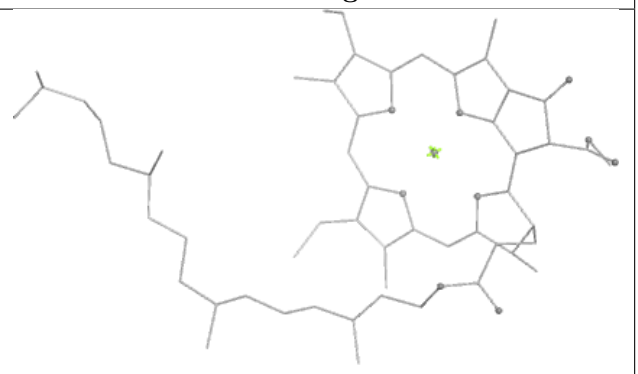
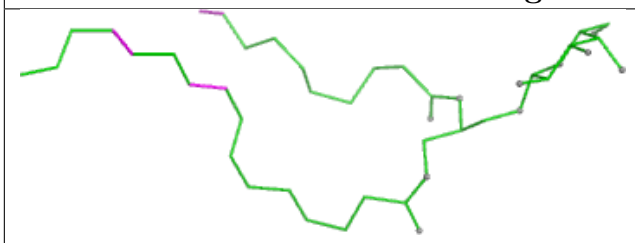


Rings

Ligand LMG 4 322



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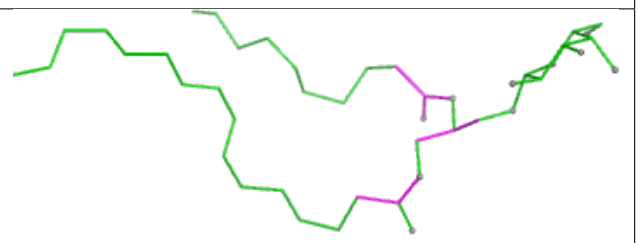
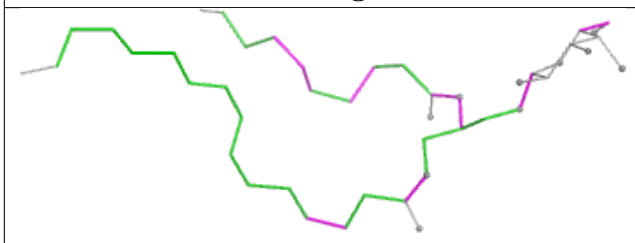


Bond angles



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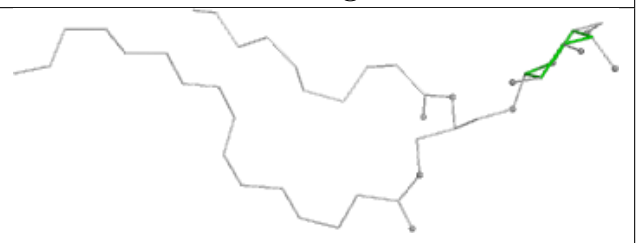
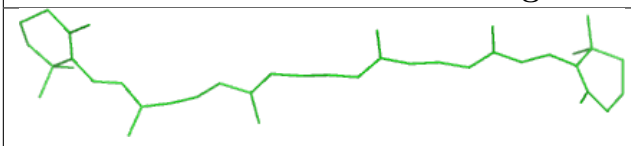


Rings

Ligand BCR A 851



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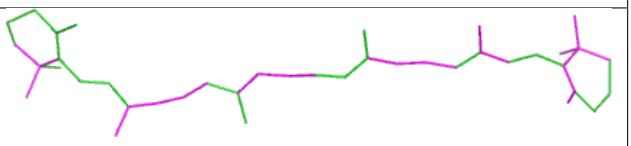
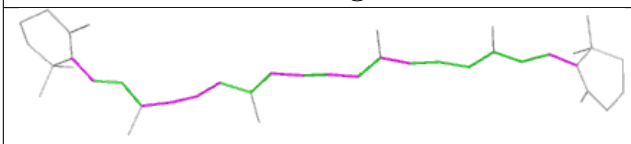


Bond angles



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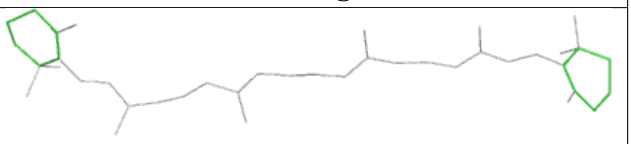
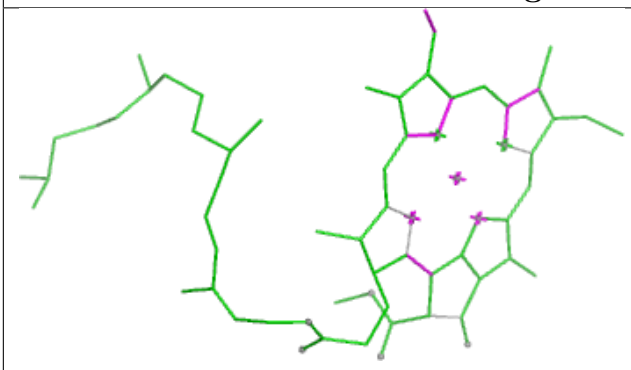


Rings

Ligand CLA B 824



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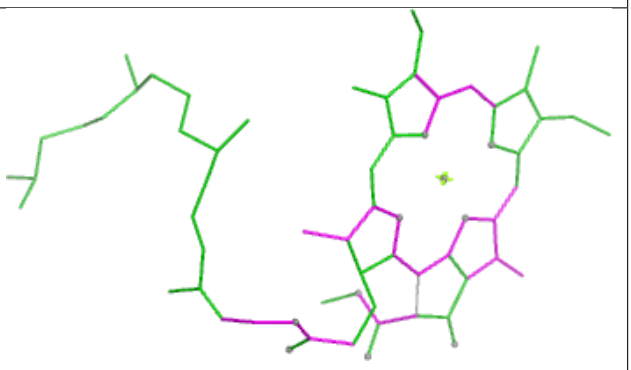

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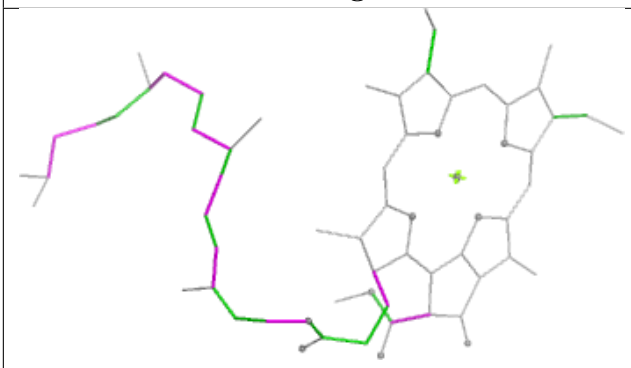

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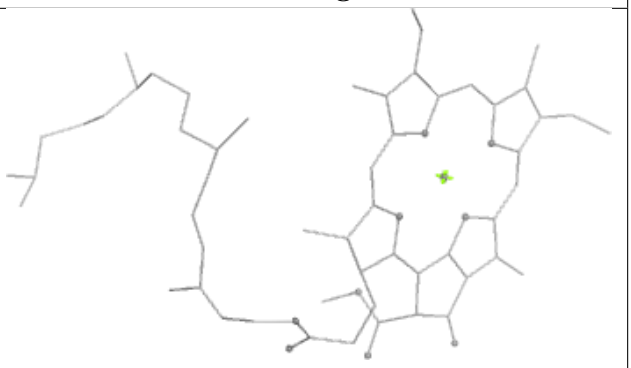
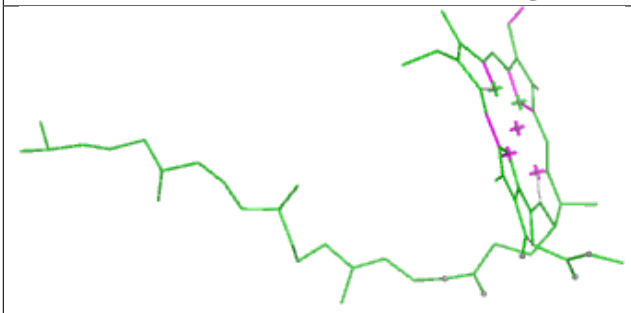


Rings

Ligand CLA B 829



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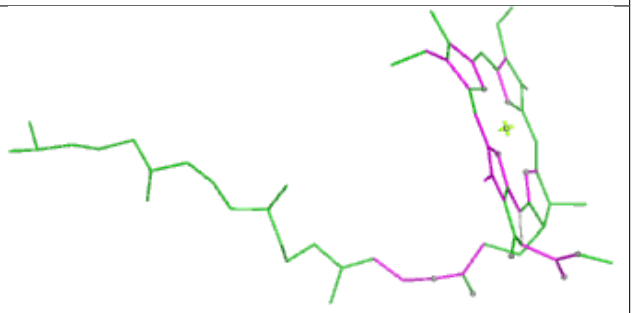
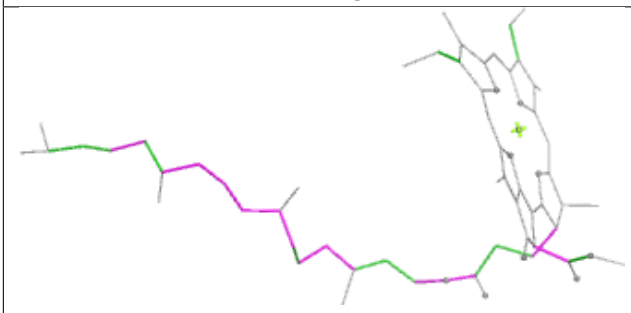


Bond angles



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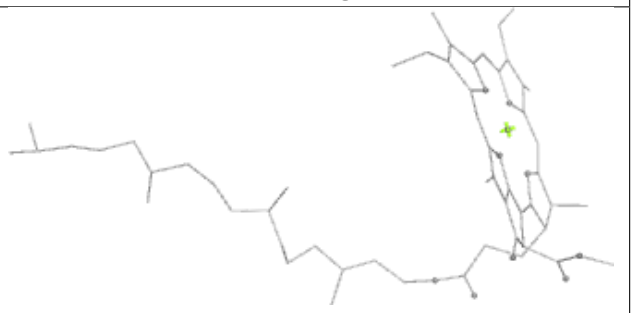
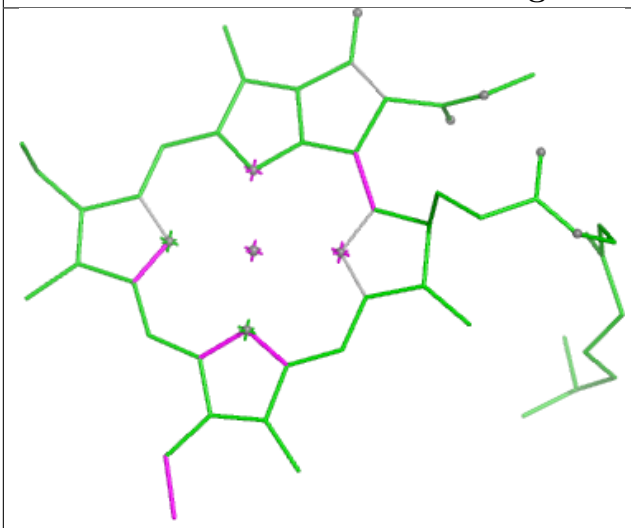


Rings

Ligand CLA 2 508



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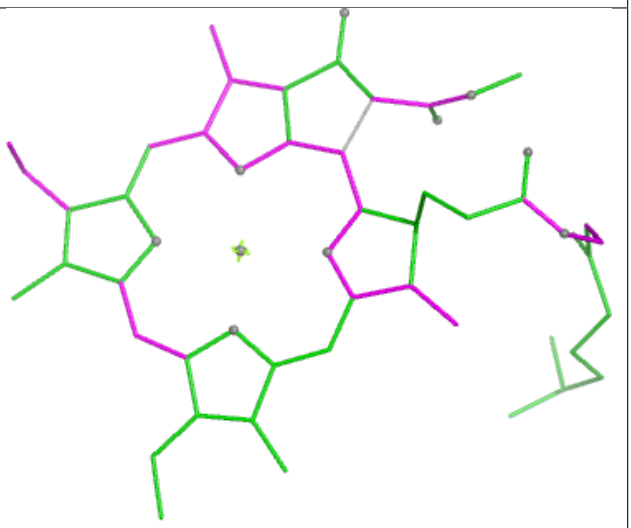
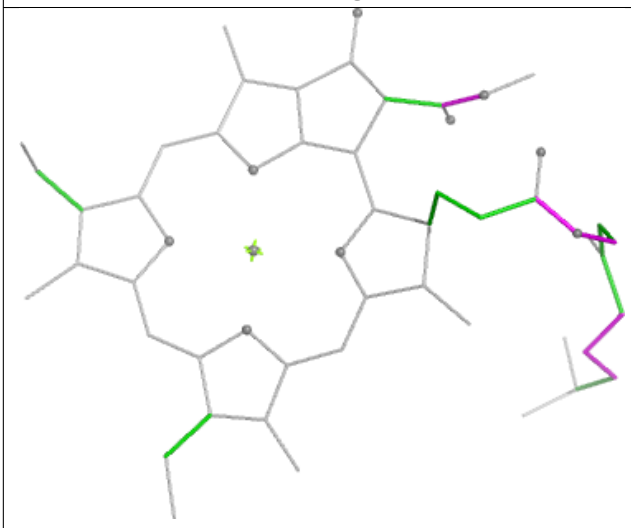


Bond angles



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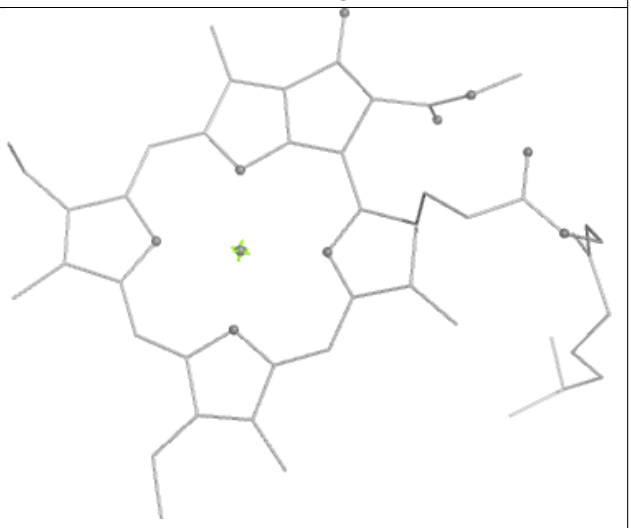
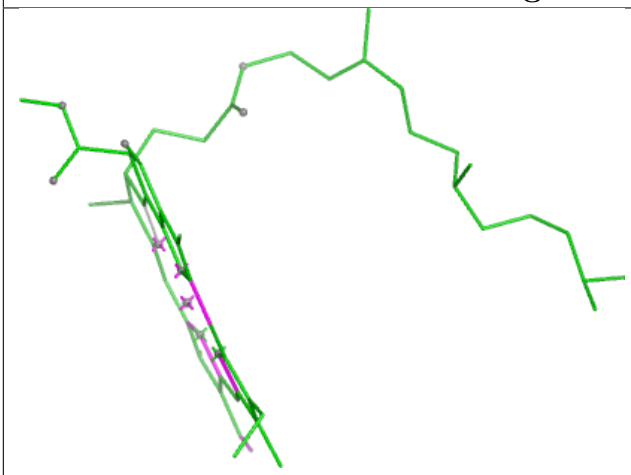


Rings

Ligand CLA A 807



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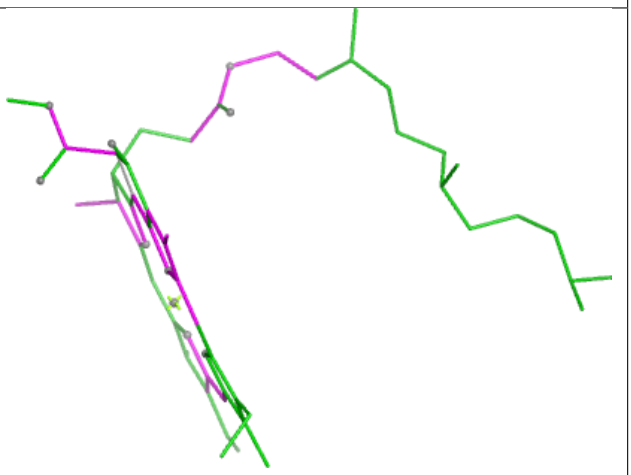

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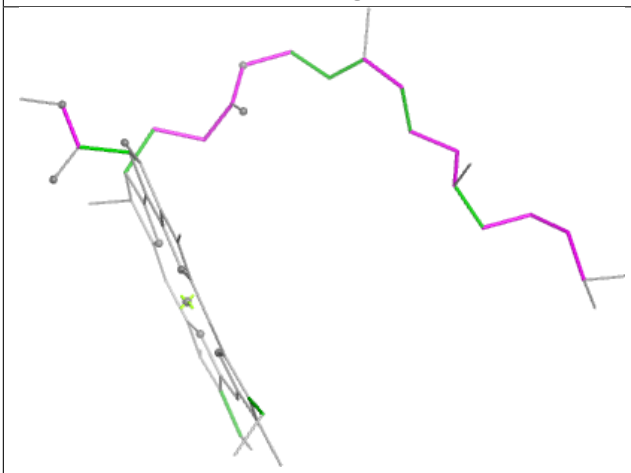

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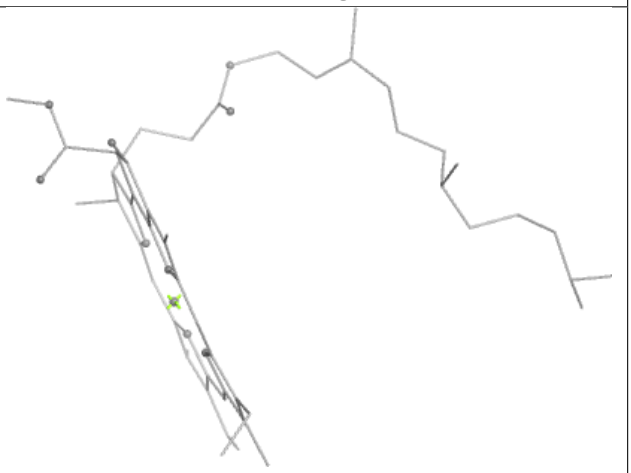
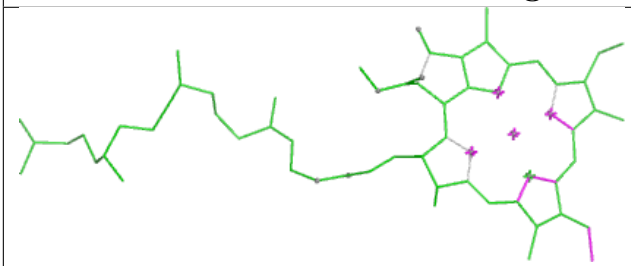


Rings

Ligand CLA A 840



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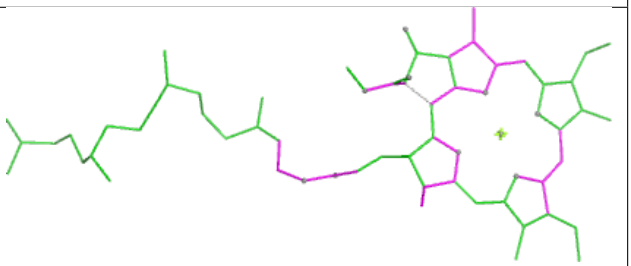
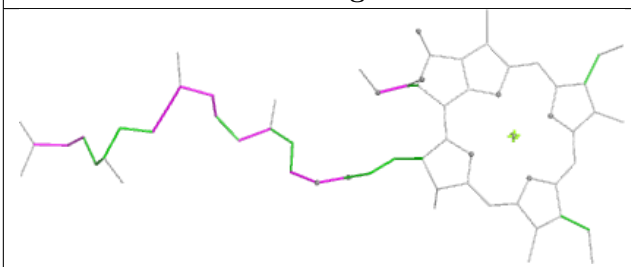


Bond angles



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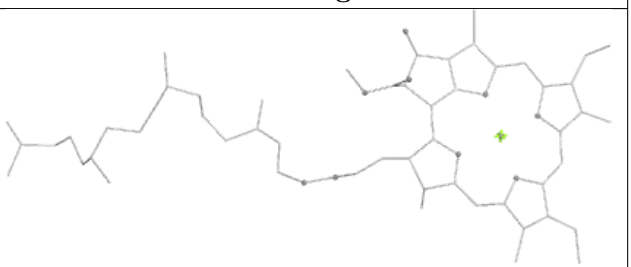
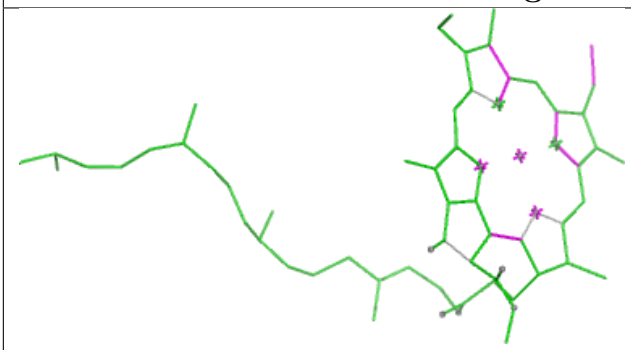


Rings

Ligand CLA B 822



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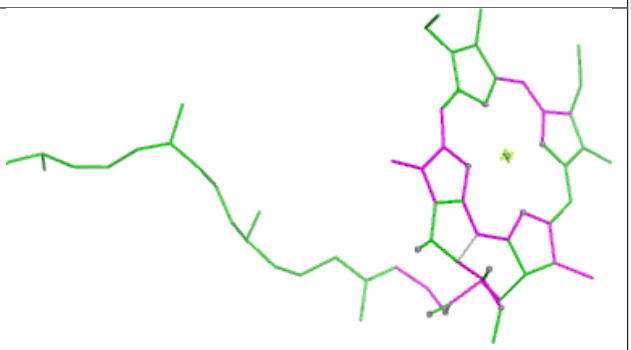
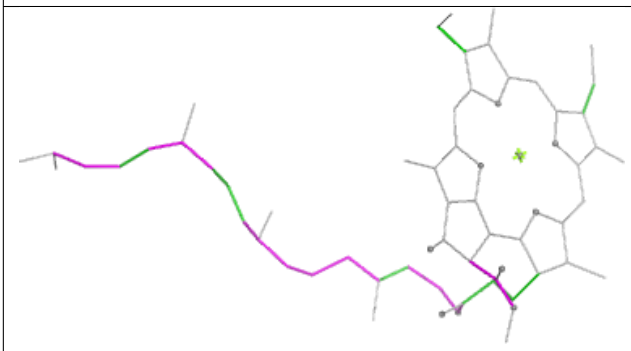


Bond angles



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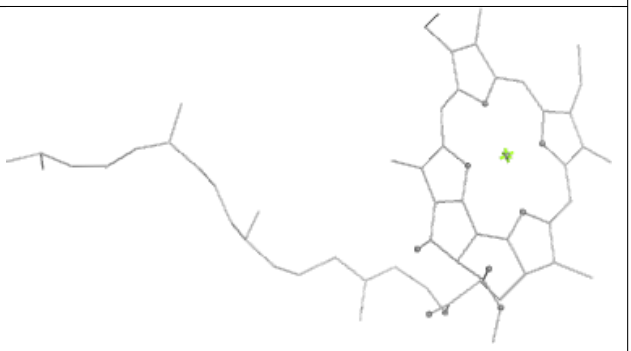
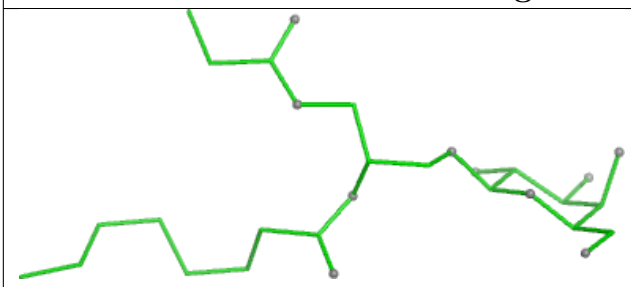


Rings

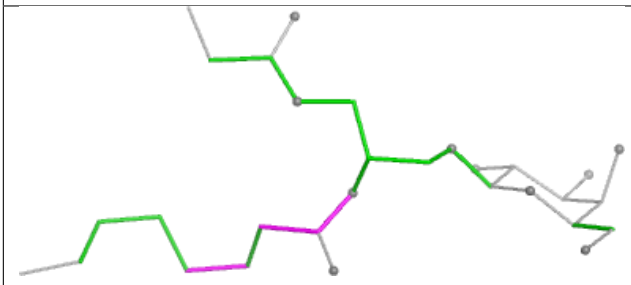
Ligand LMG J 1103



Bond lengths



Bond angles



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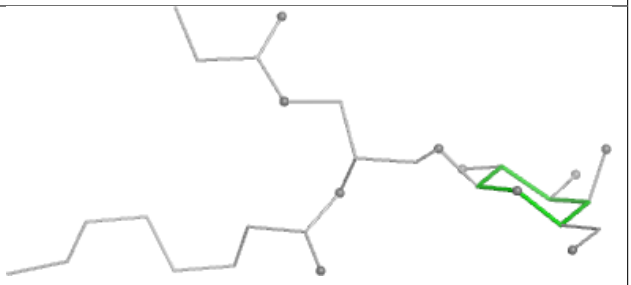
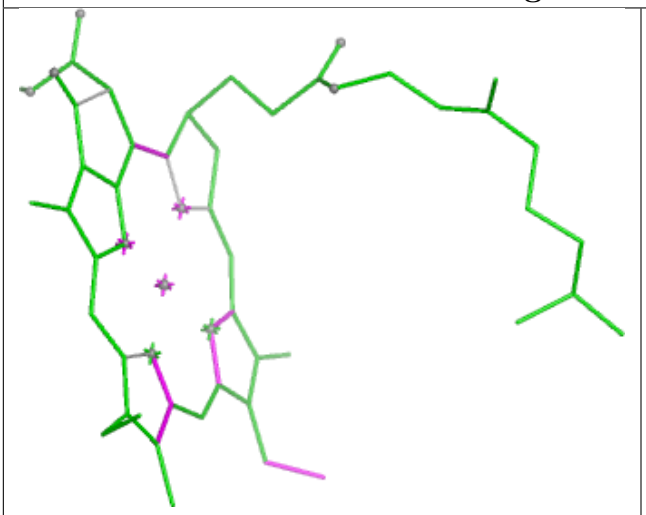


Rings

Ligand CLA B 816



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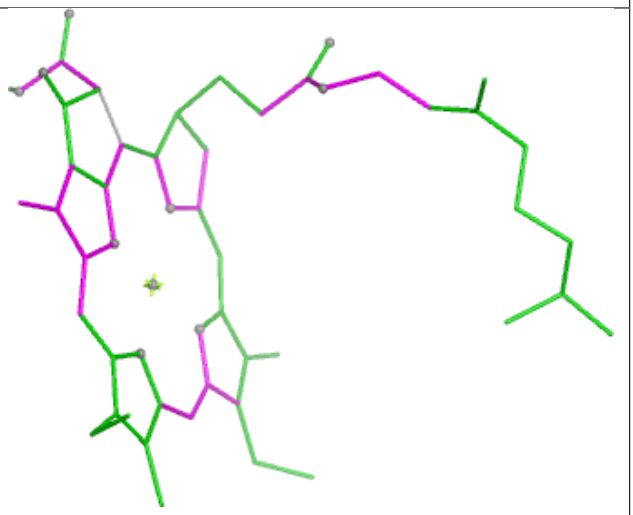
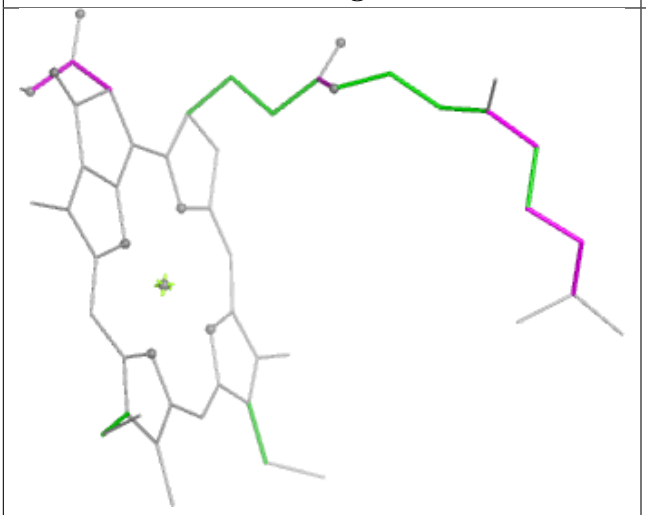


Bond angles



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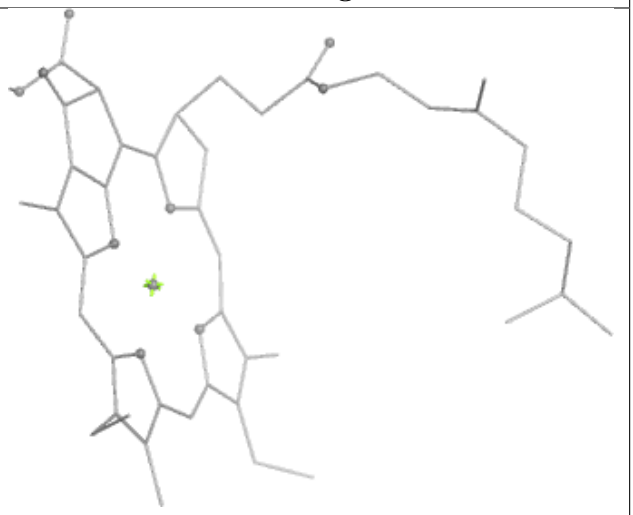
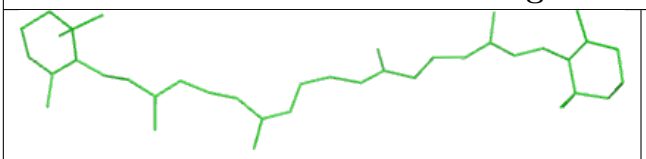


Rings

Ligand BCR 3 304



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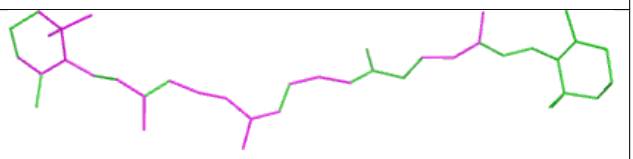
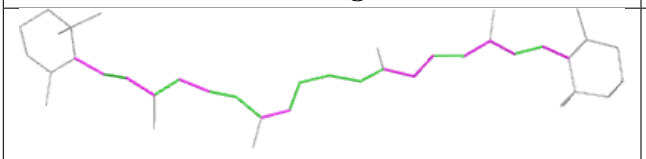


Bond angles



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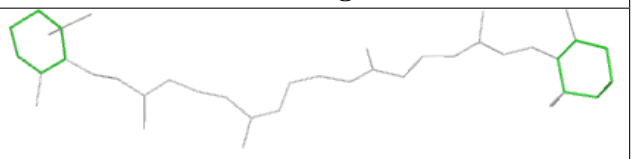
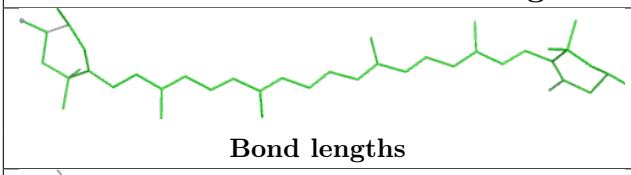


Rings

Ligand ZEX F 301



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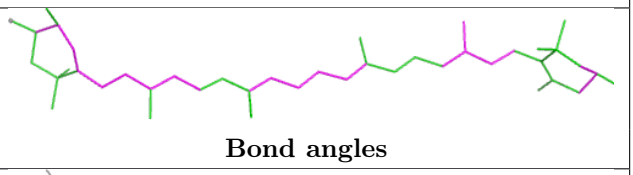
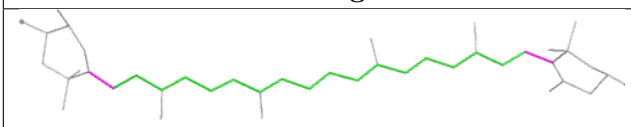


Bond angles



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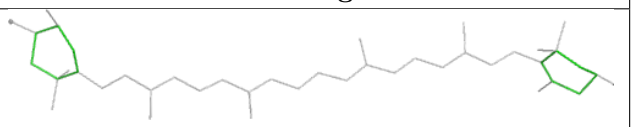
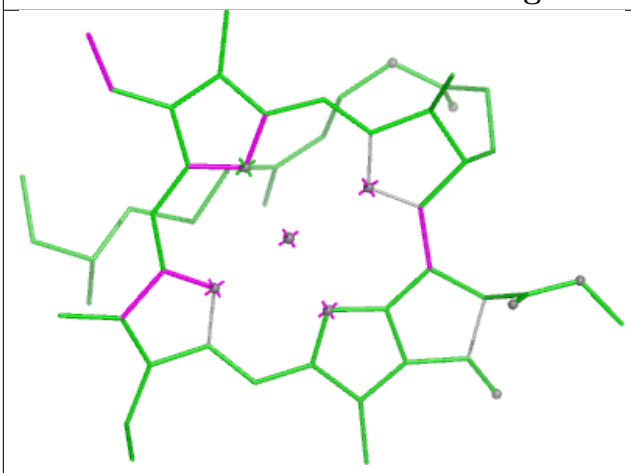


Rings

Ligand CLA A 818



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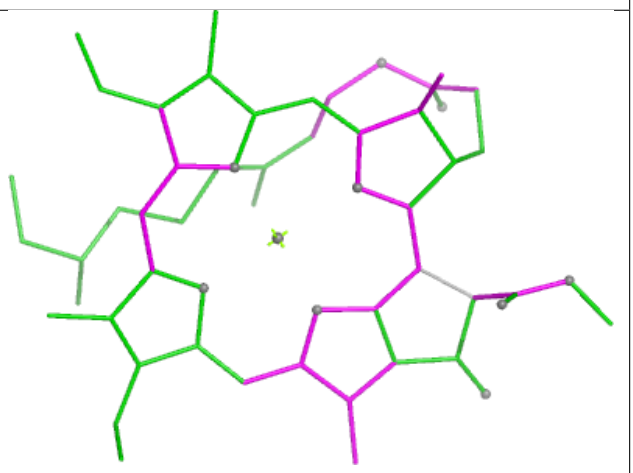
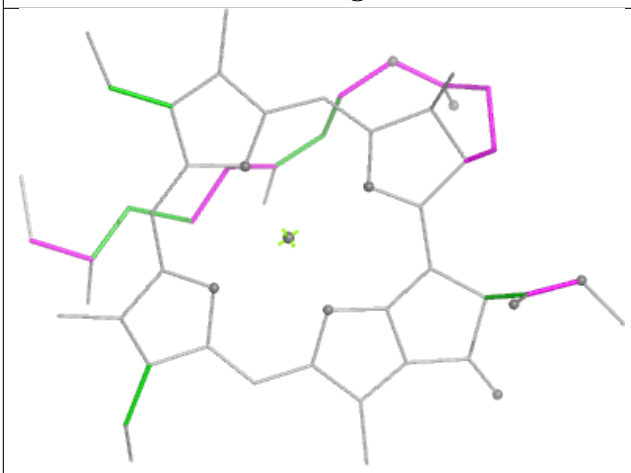


Bond angles



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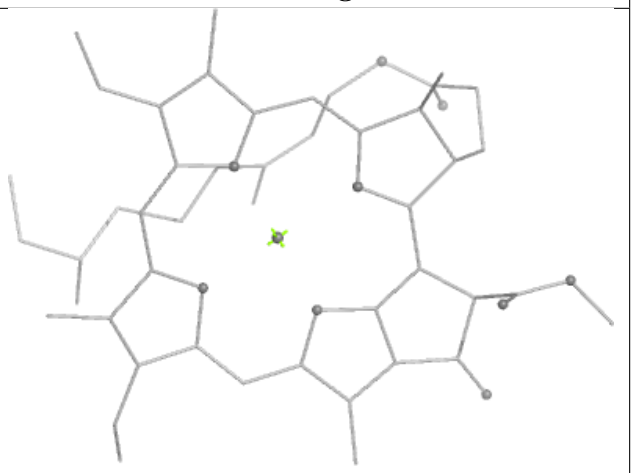
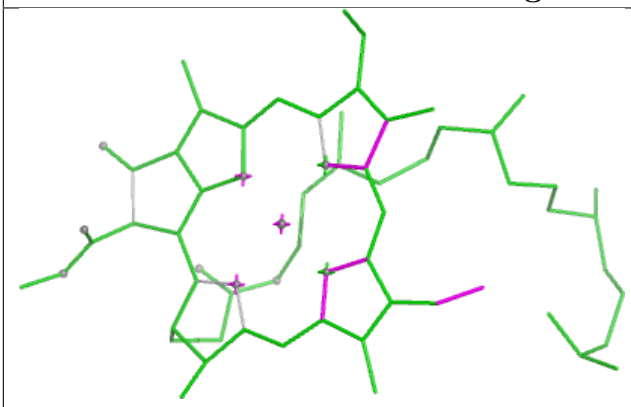
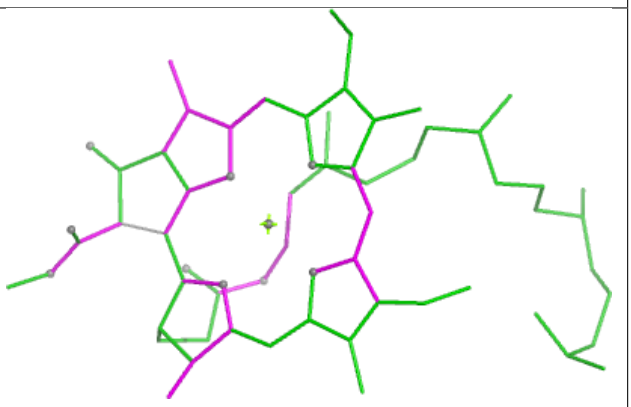


Rings

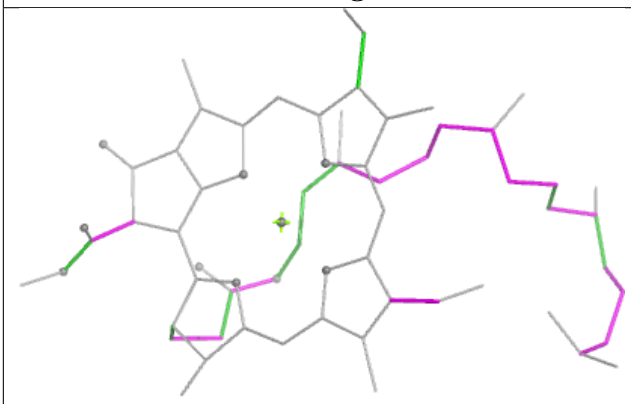
Ligand CLA B 808



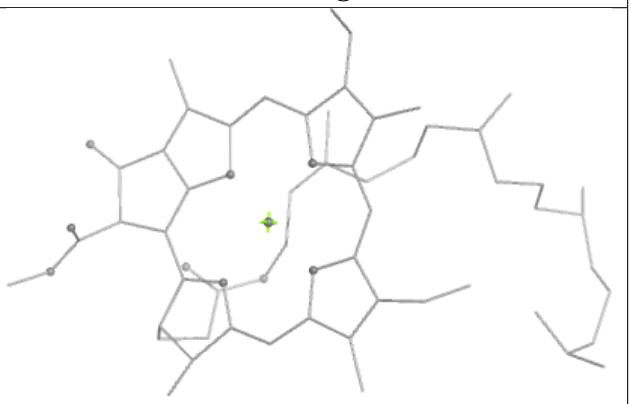
Bond lengths



Bond angles

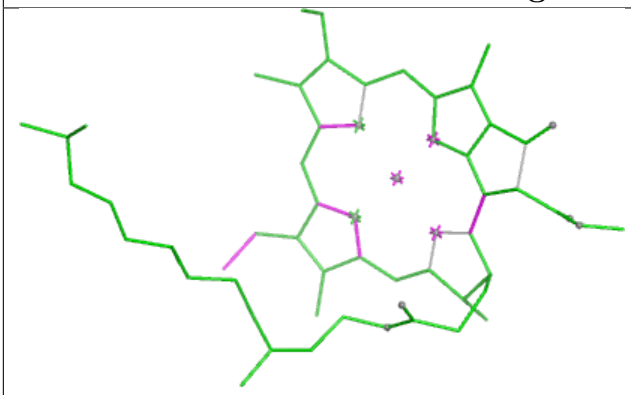


Torsions

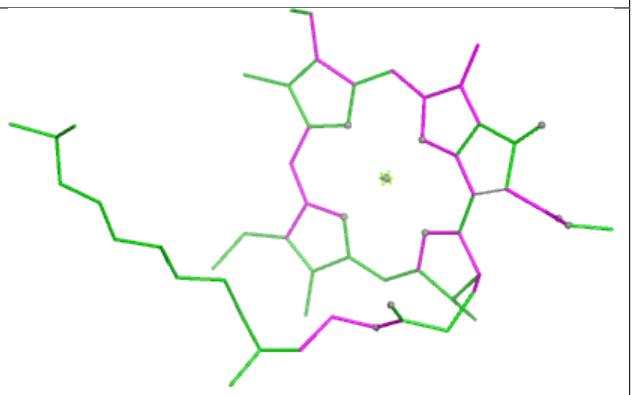


Rings

Ligand CLA 2 504



Bond lengths



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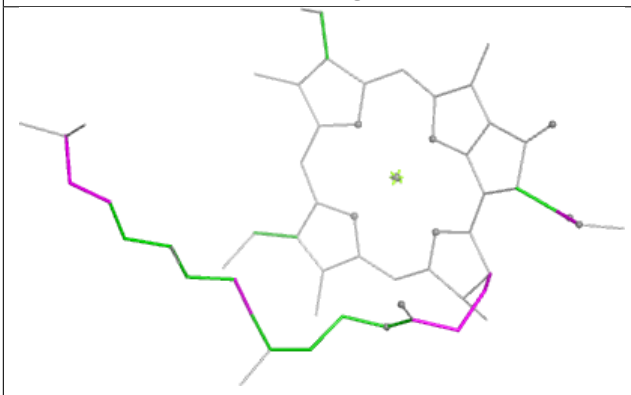

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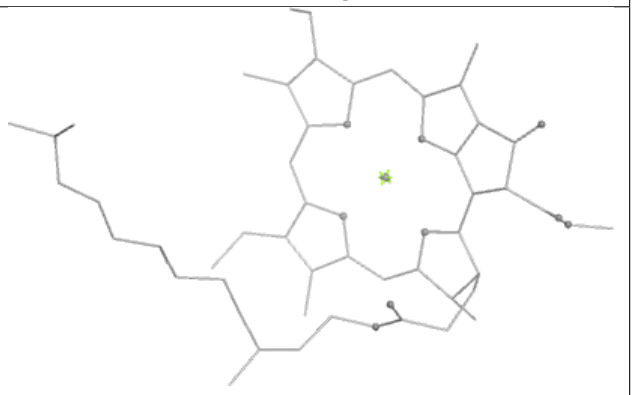
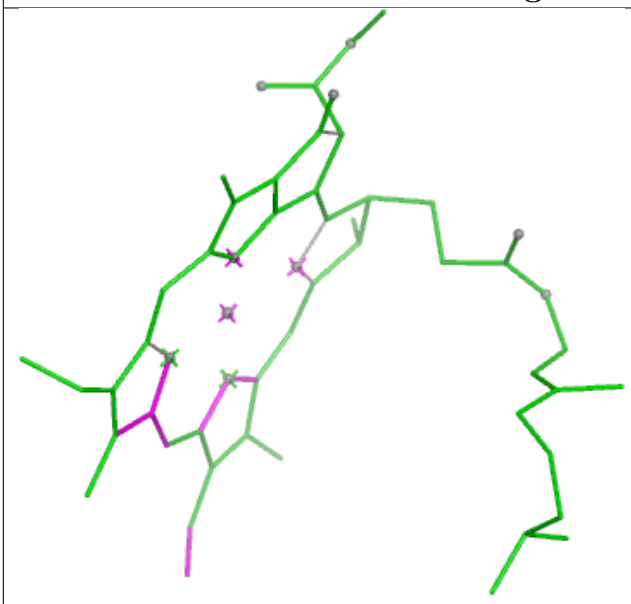
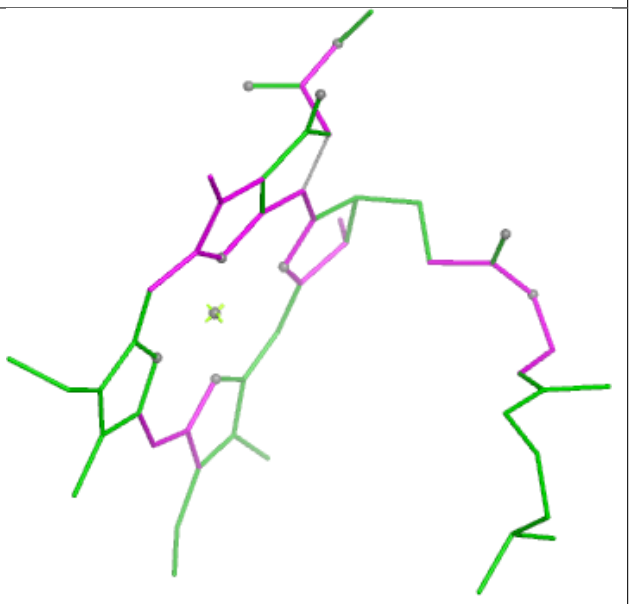


Rings

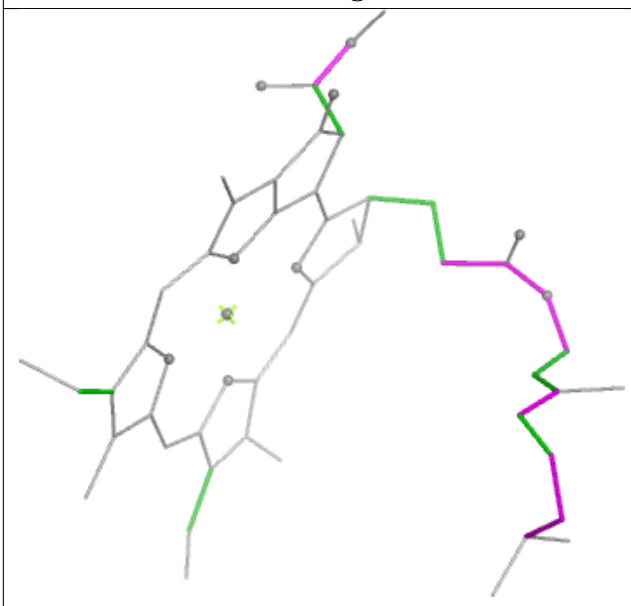
Ligand CLA B 834



Bond lengths



Bond angles



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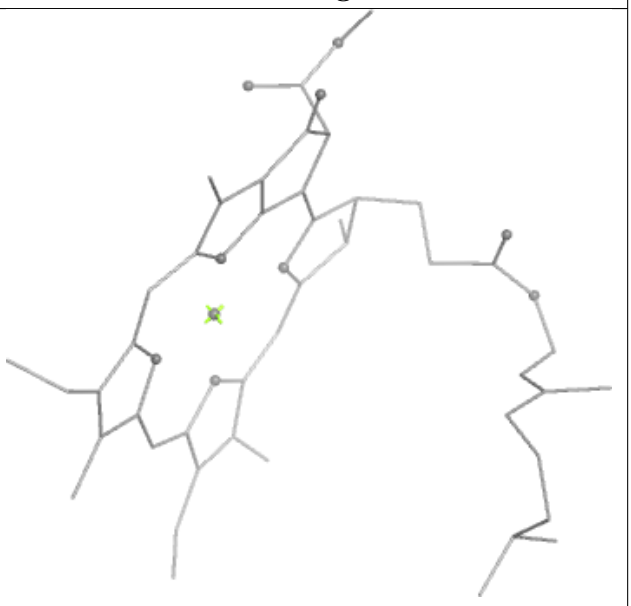
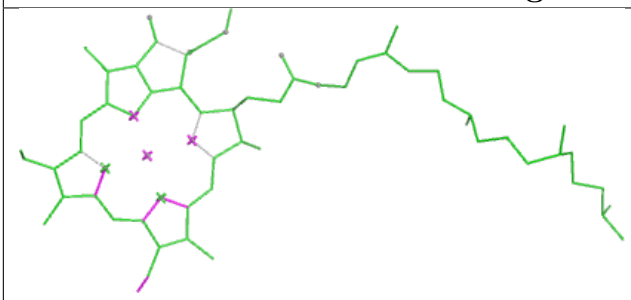


Rings

Ligand CLA F 303



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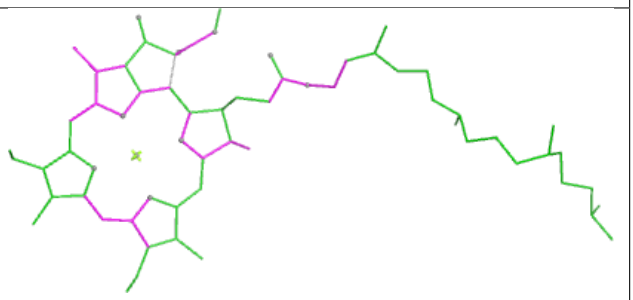
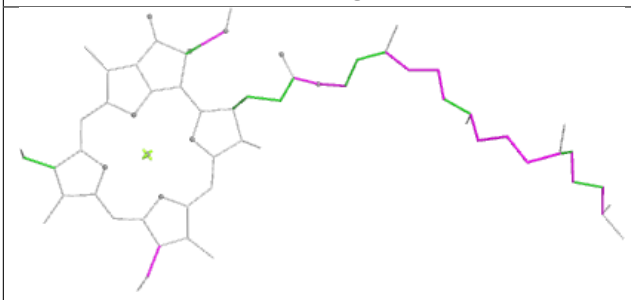
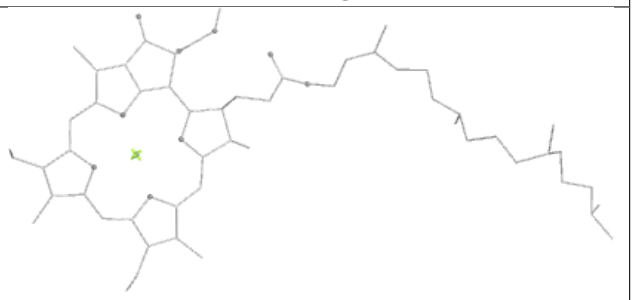


Bond angles

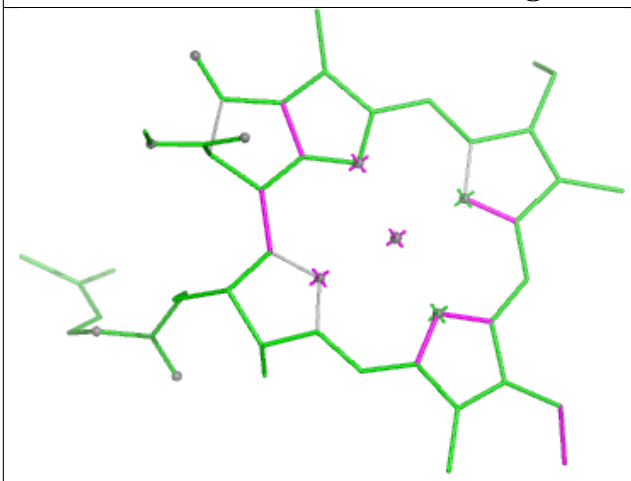


Torsions



Rings

Ligand CLA B 837



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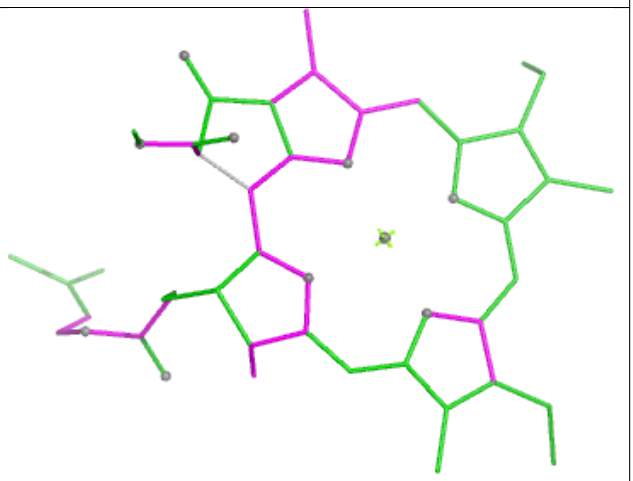
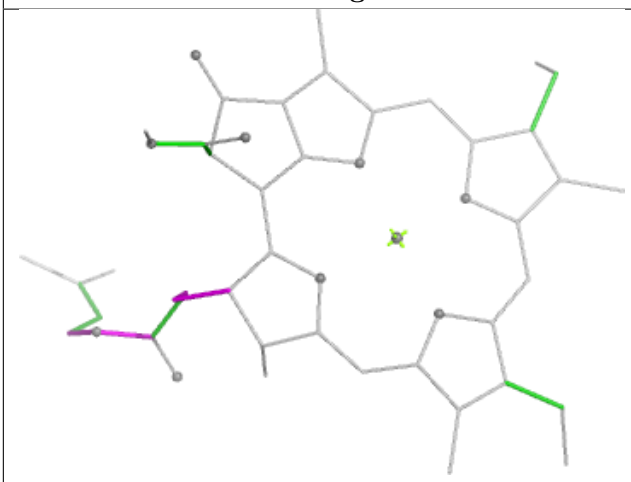


Bond angles

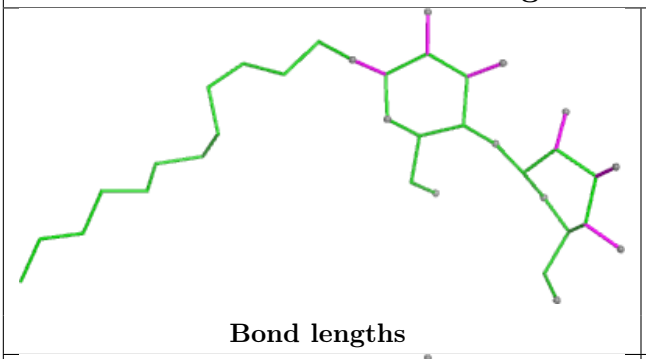


Torsions



Rings

Ligand LMT B 846



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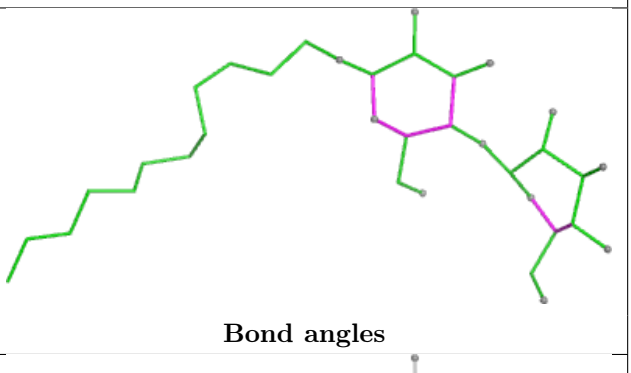
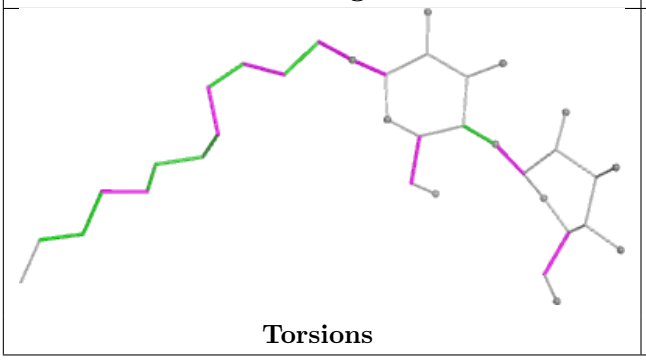


Bond angles



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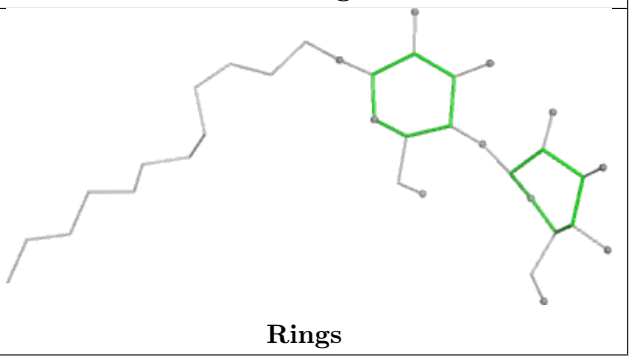
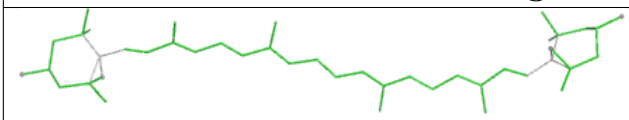


Rings

Ligand XAT 4 303



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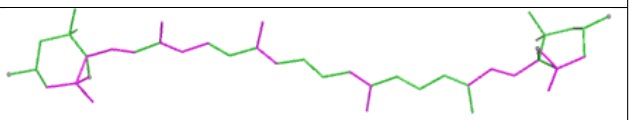
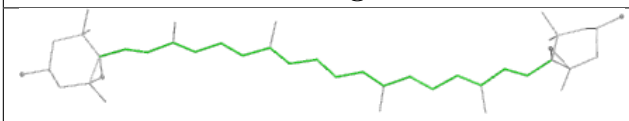


Bond angles



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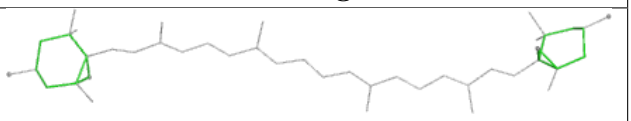
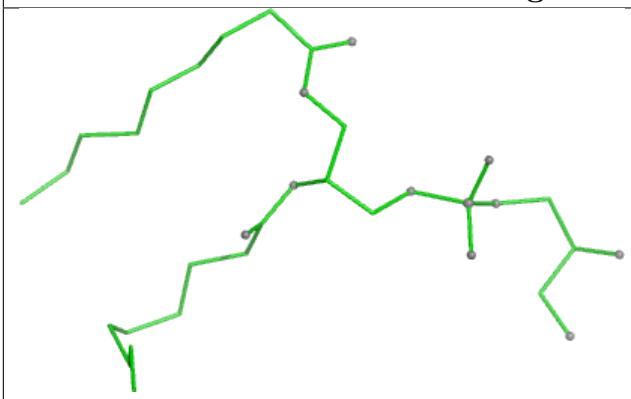


Rings

Ligand LHG 2 517



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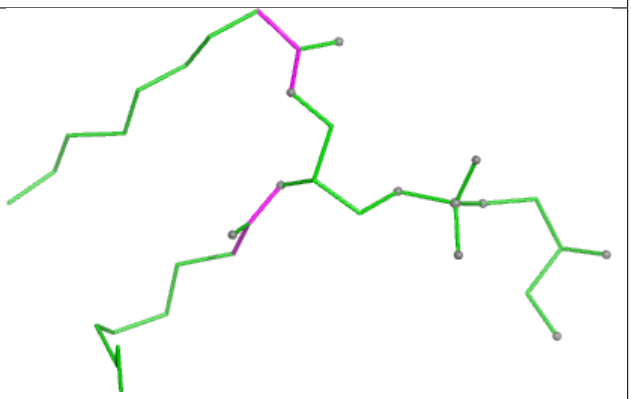
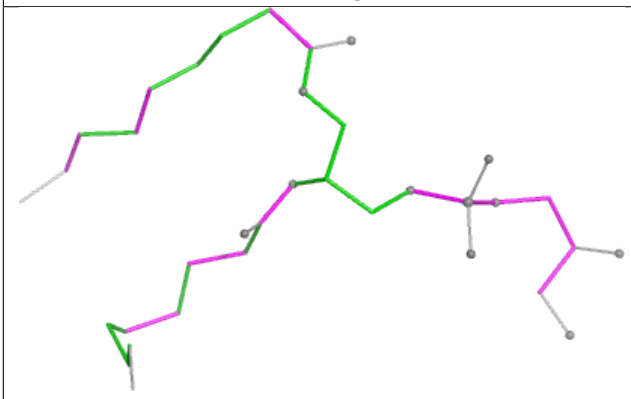


Bond angles



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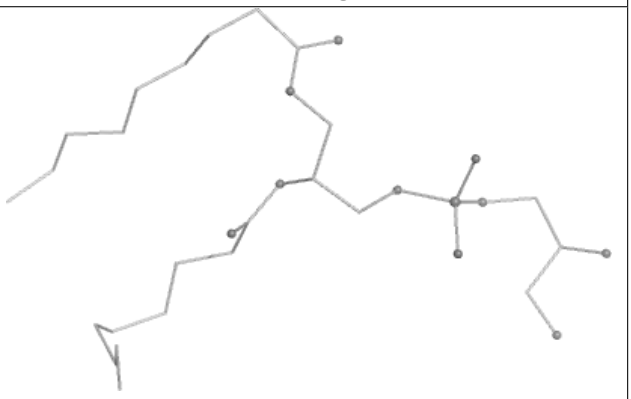
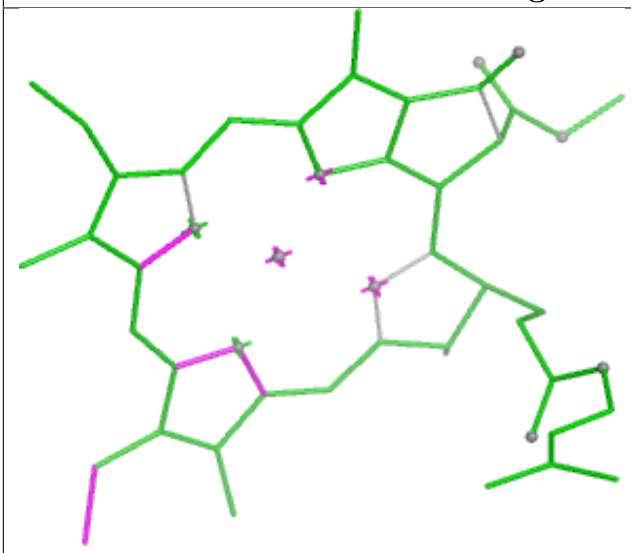


Rings

Ligand CLA 2 509



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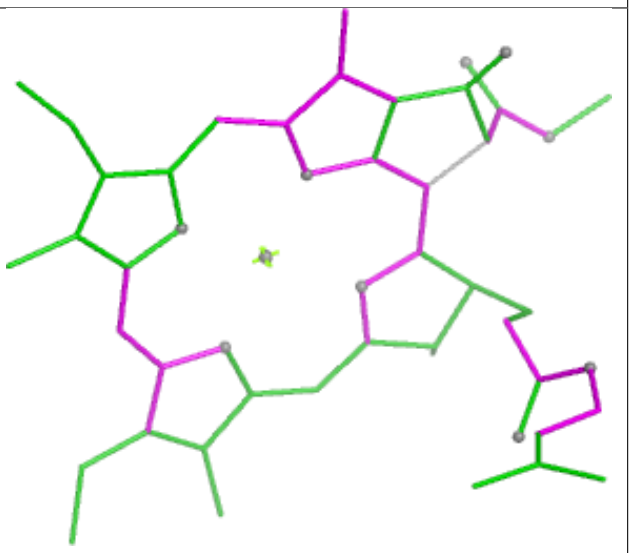
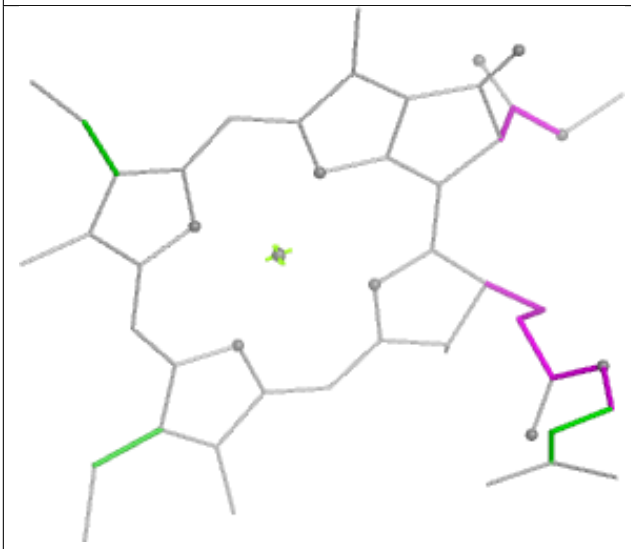


Bond angles



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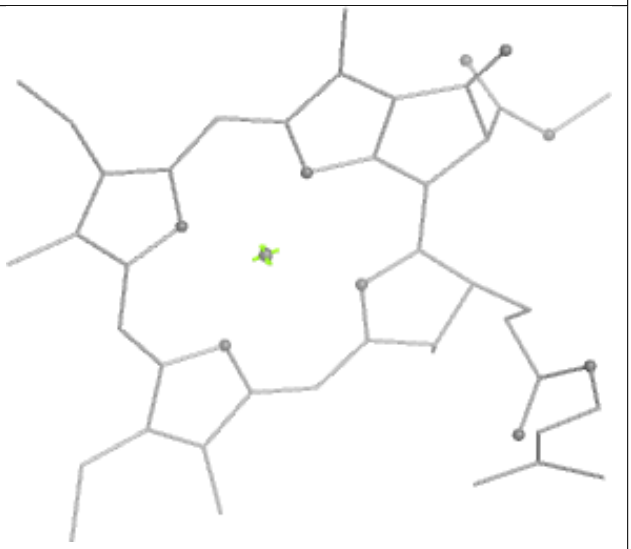
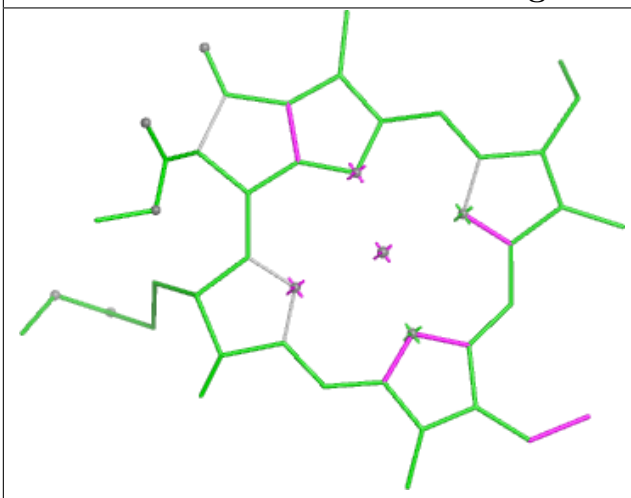


Rings

Ligand CLA 1 510



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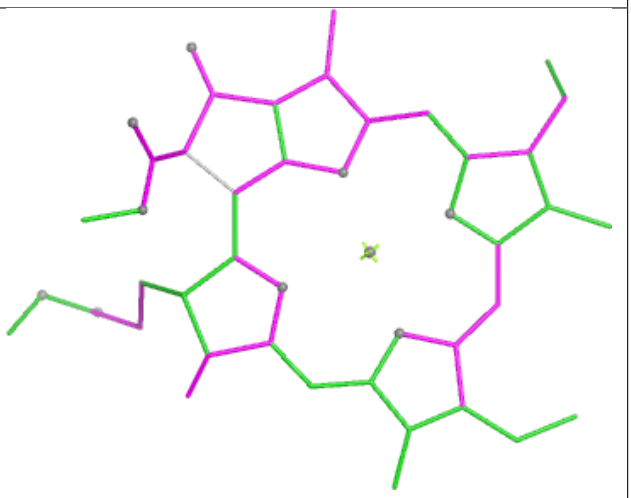
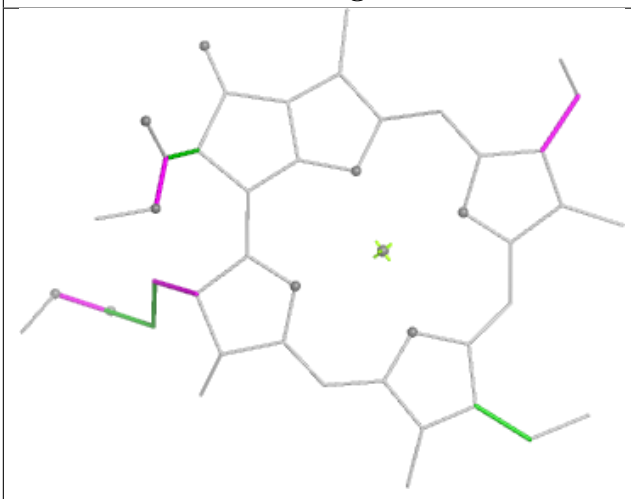


Bond angles



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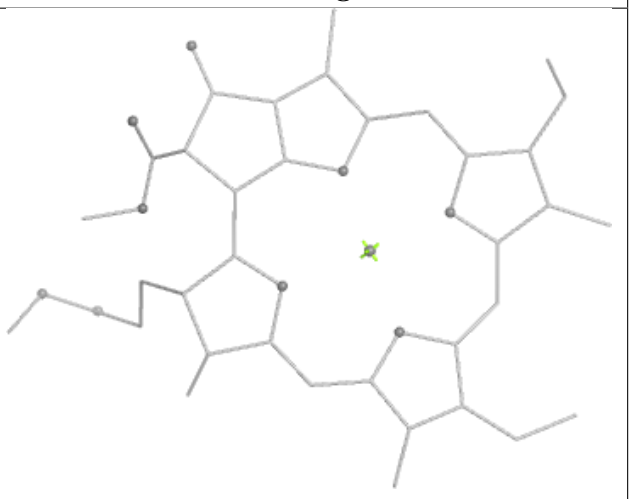
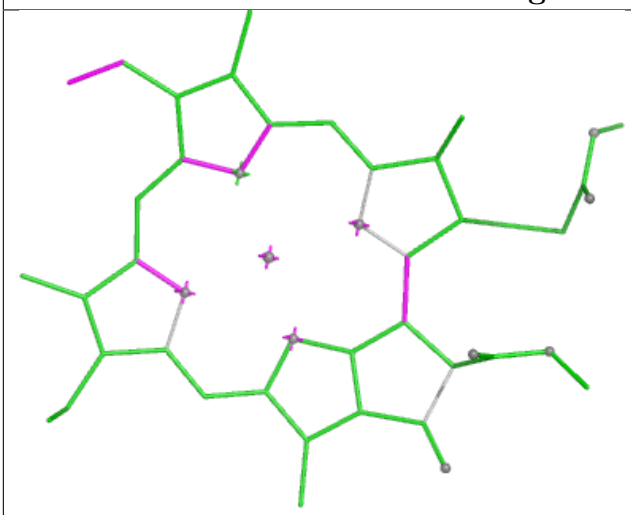
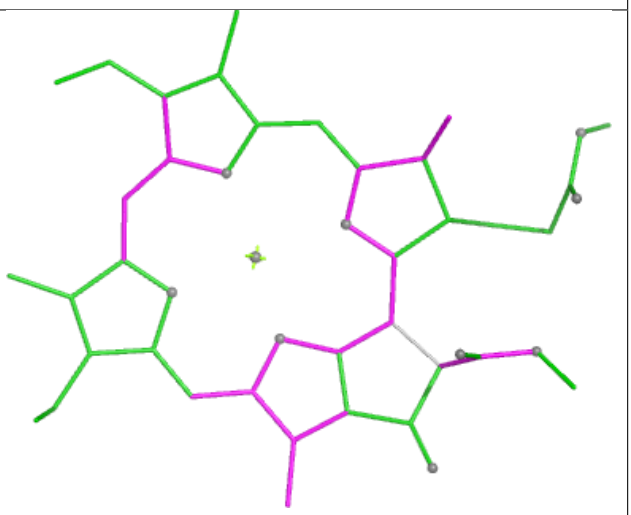


Rings

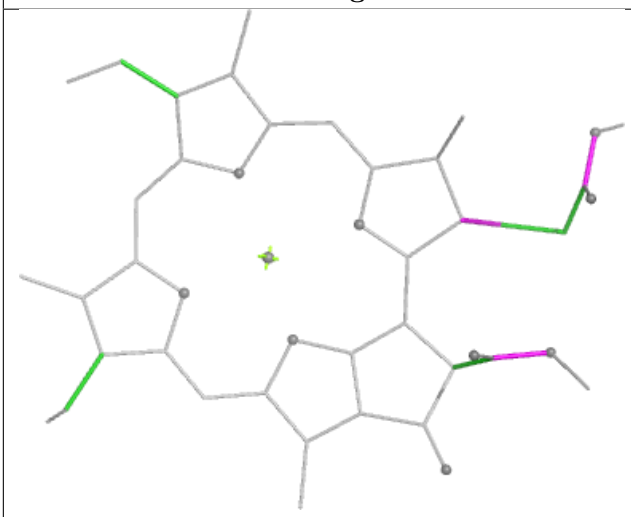
Ligand CLA 1 505



Bond lengths



Bond angles



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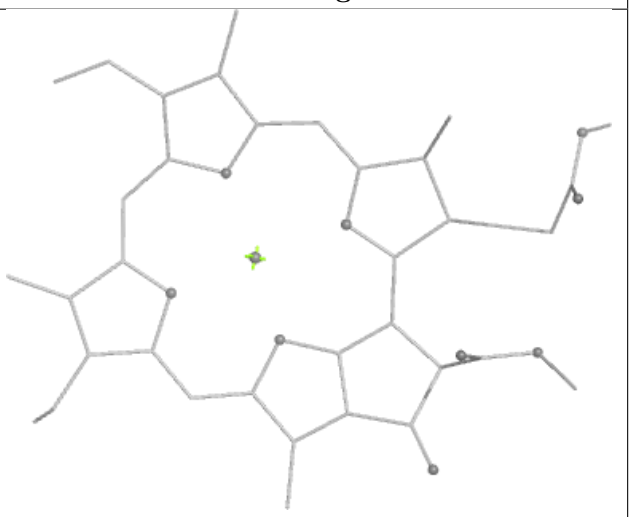
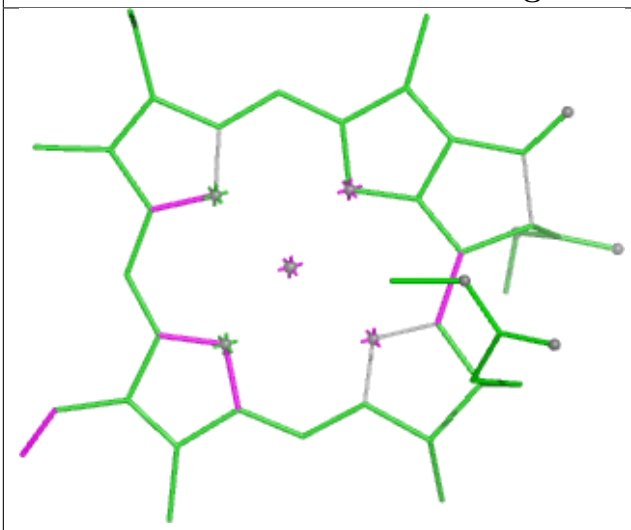


Rings

Ligand CLA A 816



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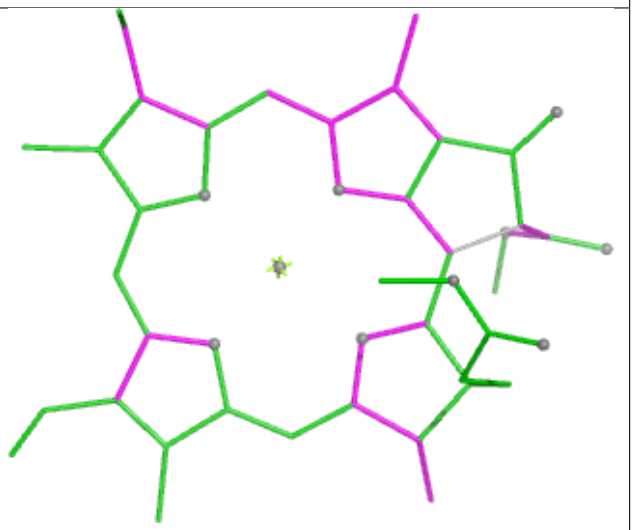
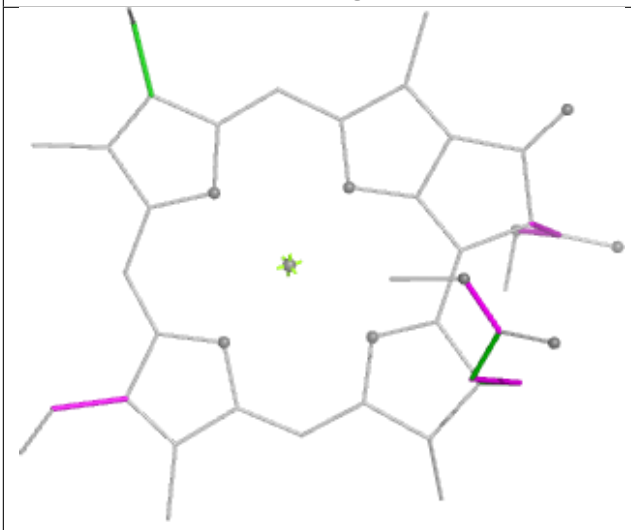


Bond angles



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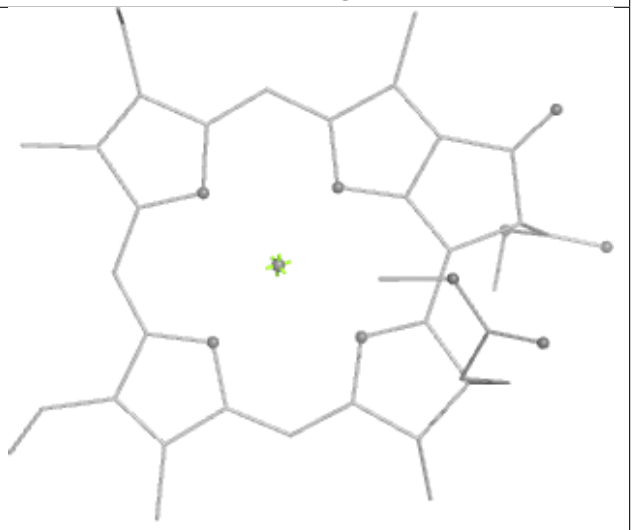
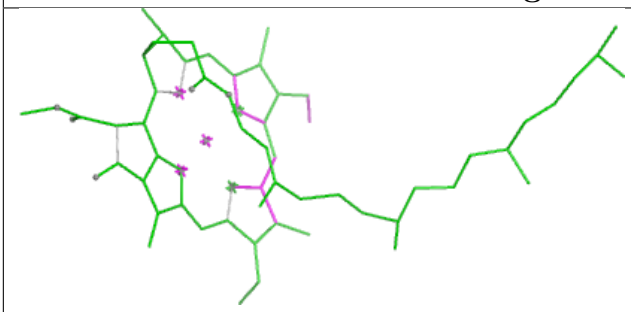


Rings

Ligand CLA A 841



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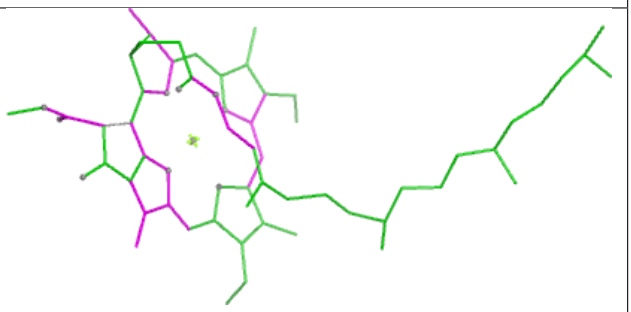
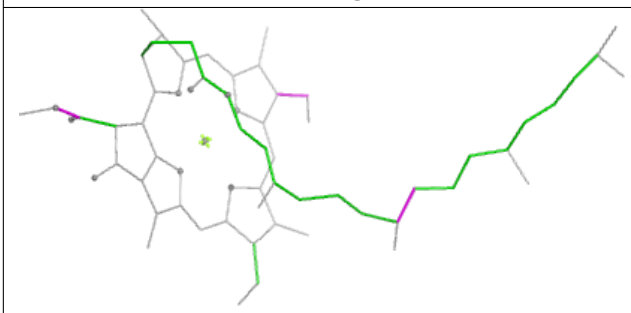


Bond angles



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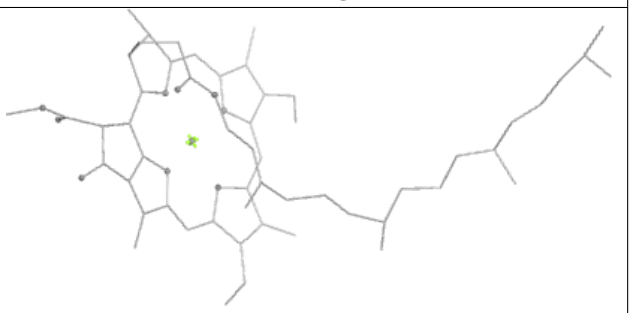
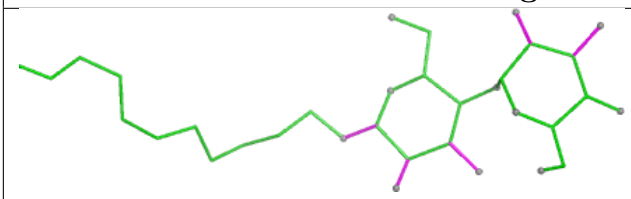
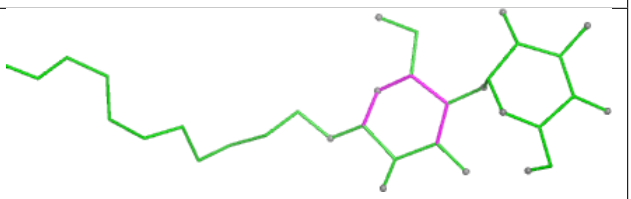


Rings

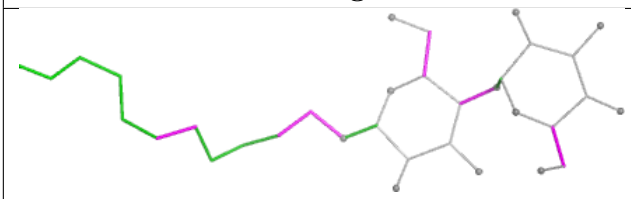
Ligand LMT G 208



Bond lengths



Bond angles



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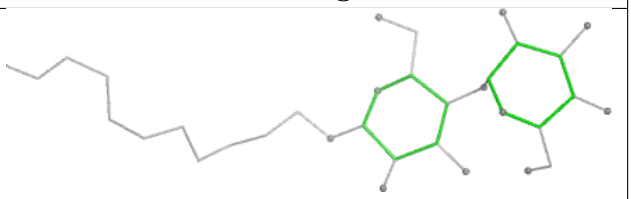
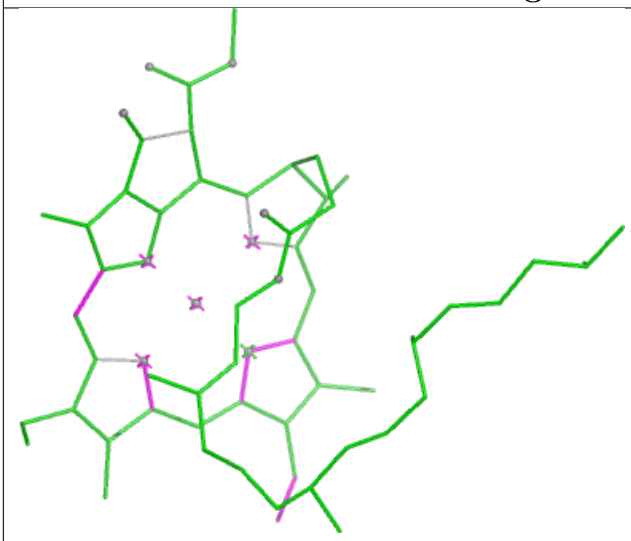
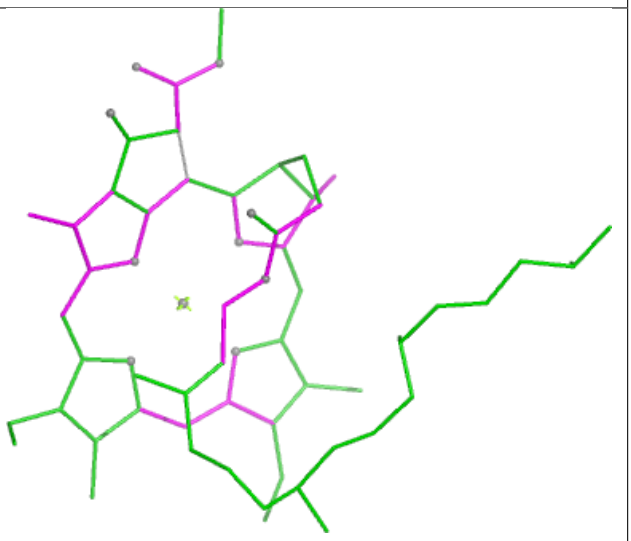


Rings

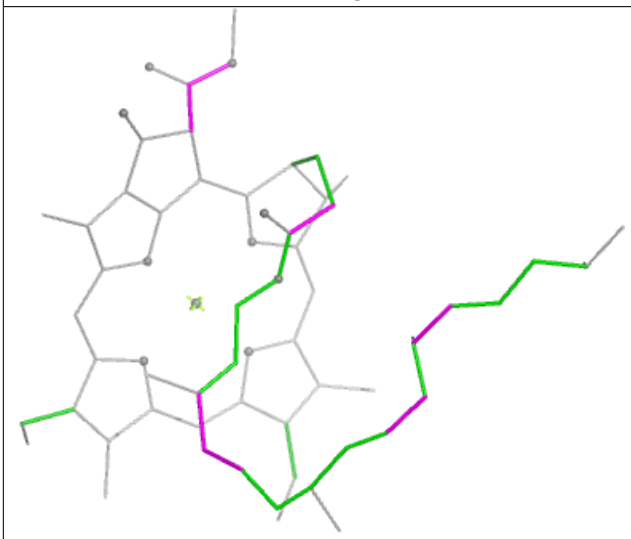
Ligand CLA B 809



Bond lengths



Bond angles



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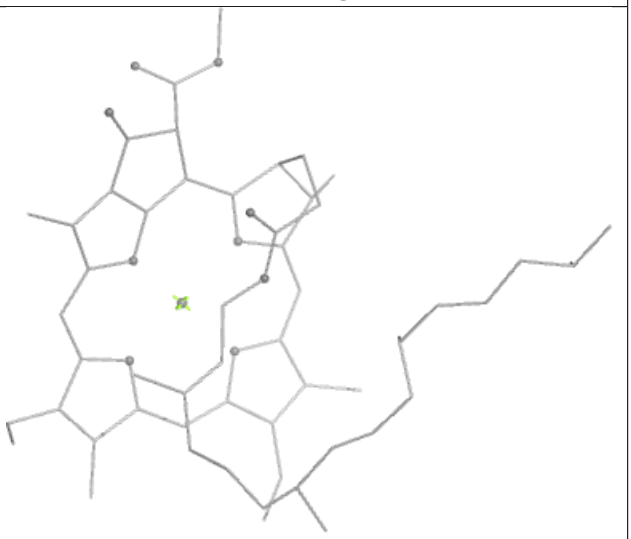
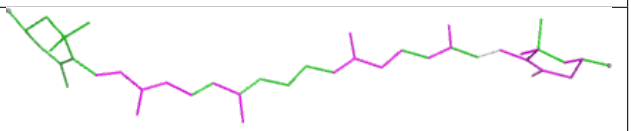


Rings

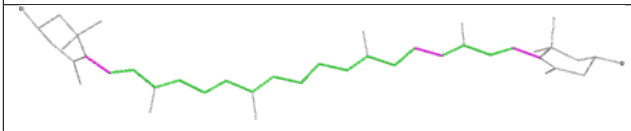
Ligand LUT 4 302



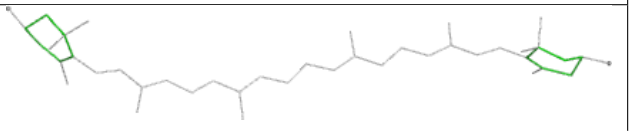
Bond lengths



Bond angles

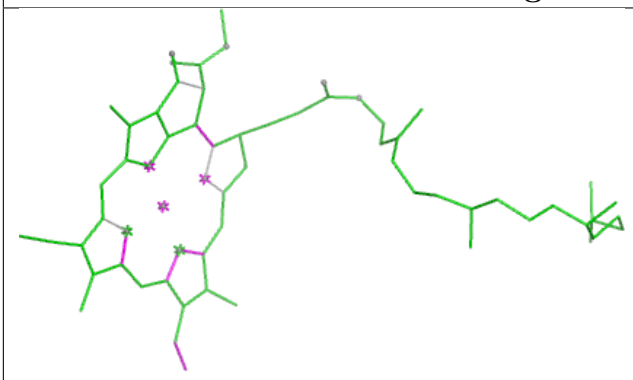


Torsions

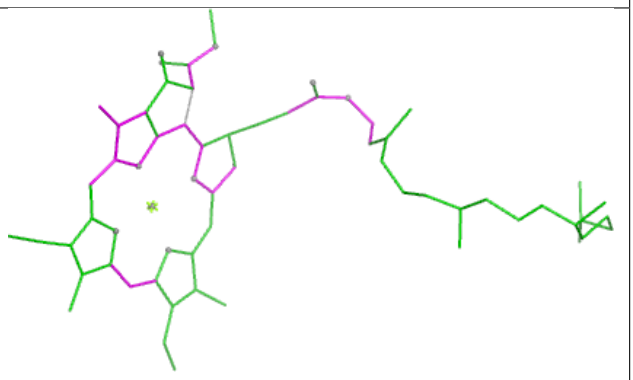


Rings

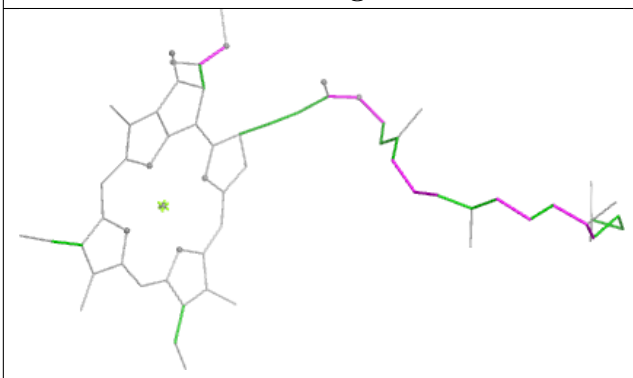
Ligand CLA B 810



Bond lengths



Bond angles



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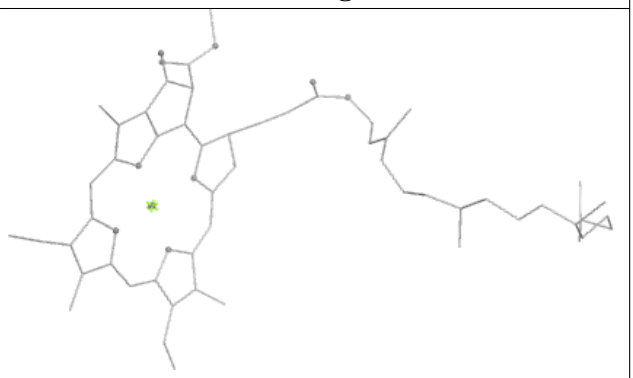
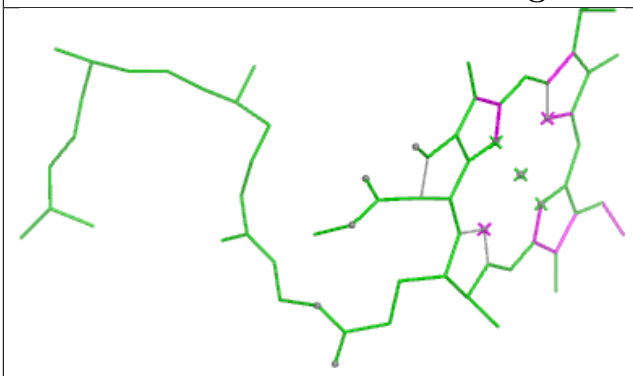


Rings

Ligand CL0 A 801



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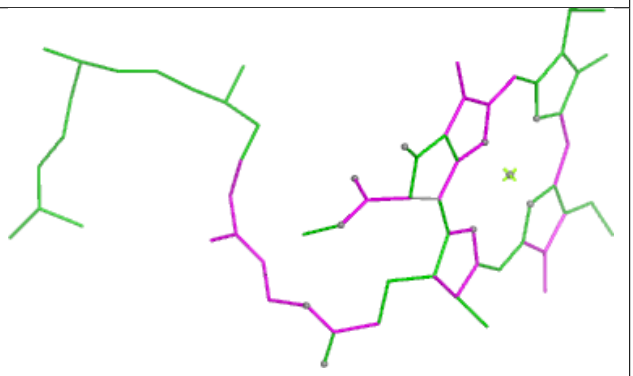

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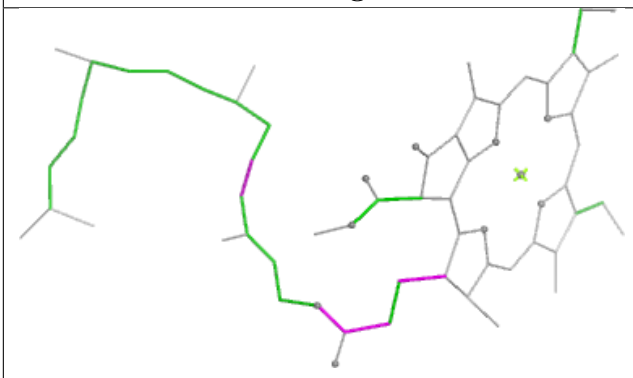

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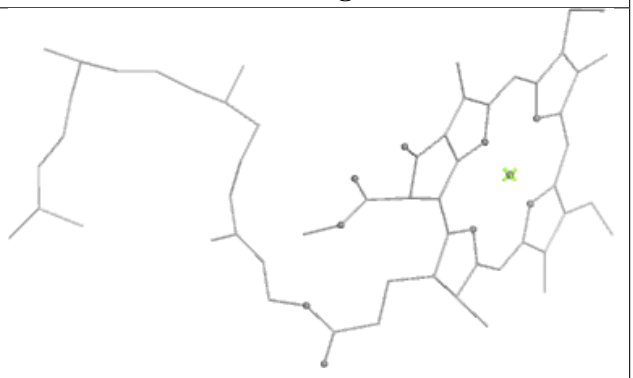
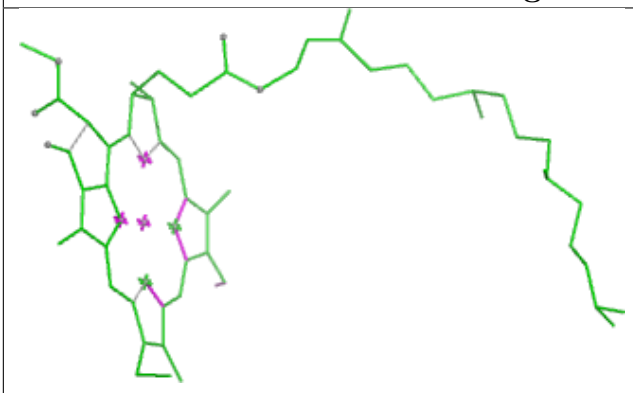


Rings

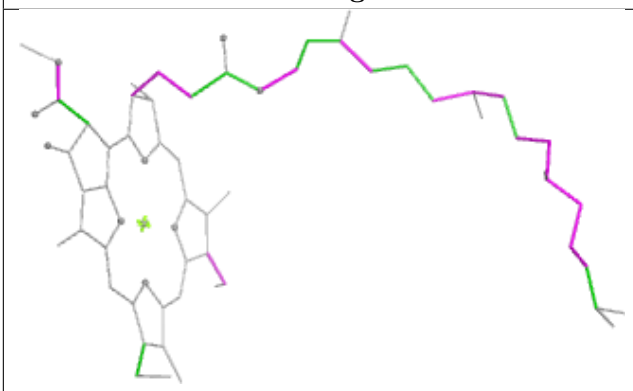
Ligand CLA A 834



Bond lengths



Bond angles

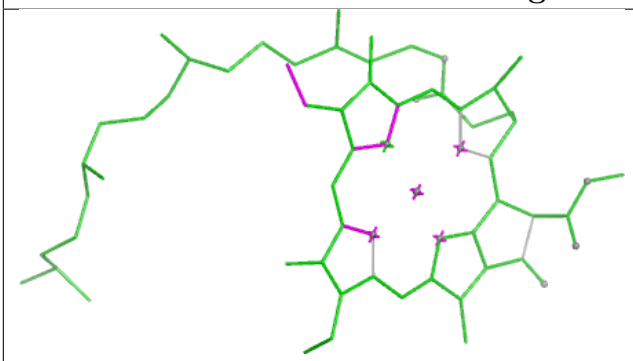


Torsions



Rings

Ligand CLA 3 308



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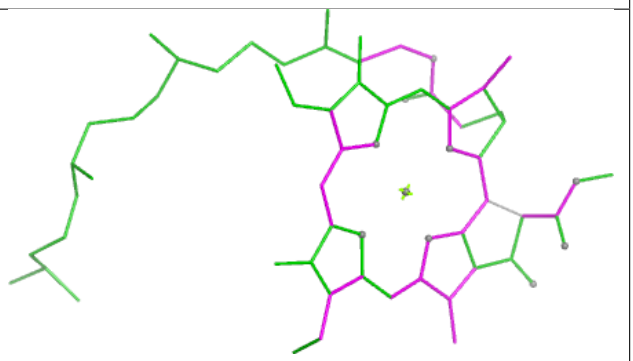

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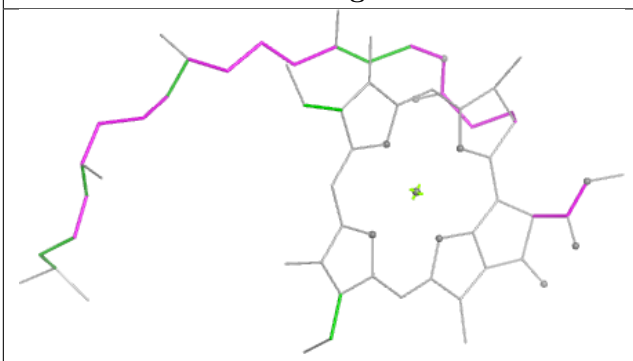

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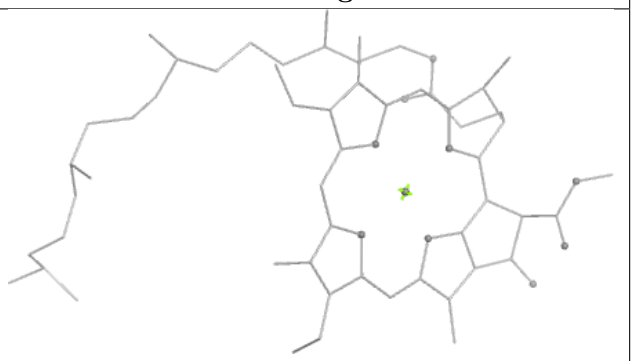
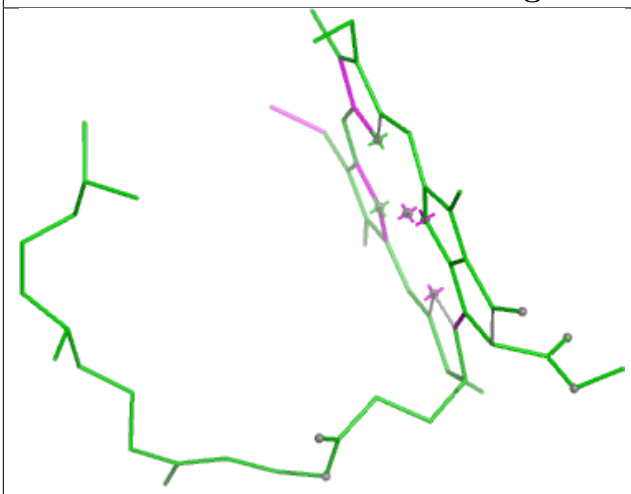


Rings

Ligand CLA A 823



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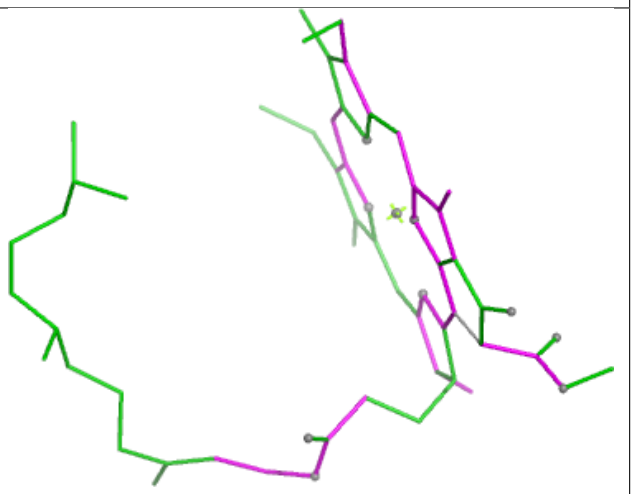
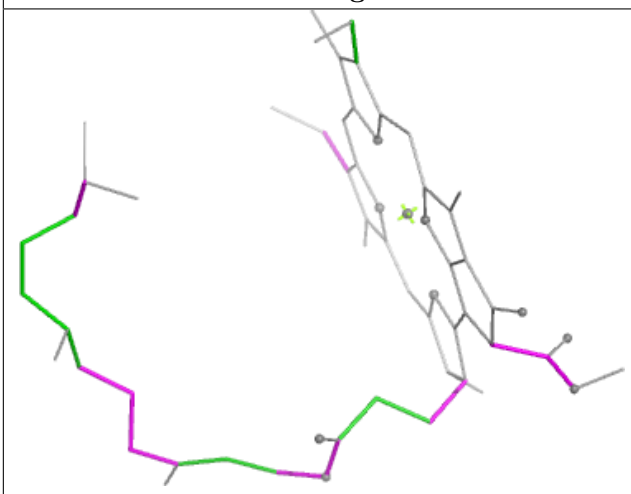


Bond angles

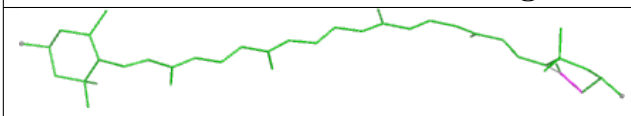


Torsions



Rings

Ligand LUT J 1109



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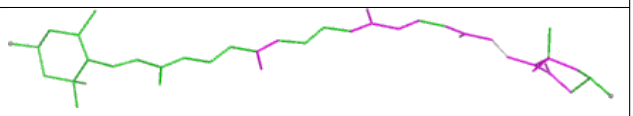

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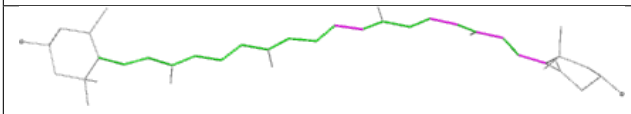

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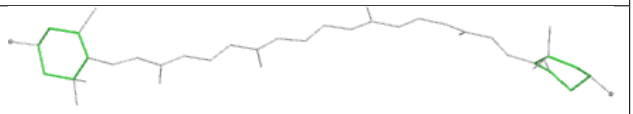
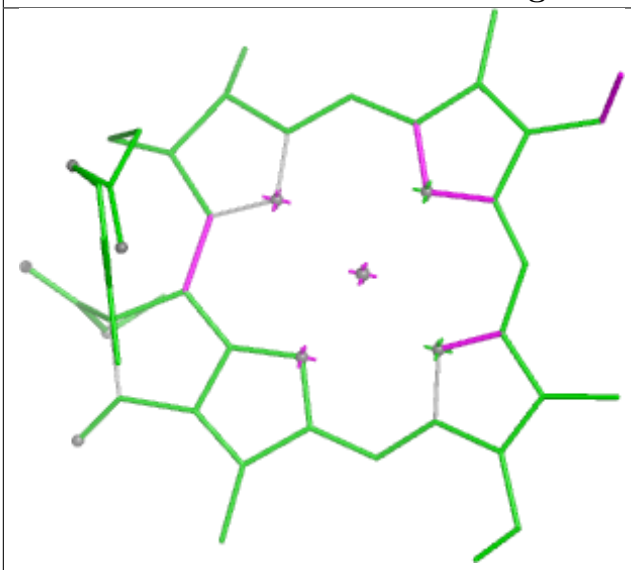


Rings

Ligand CLA 3 310



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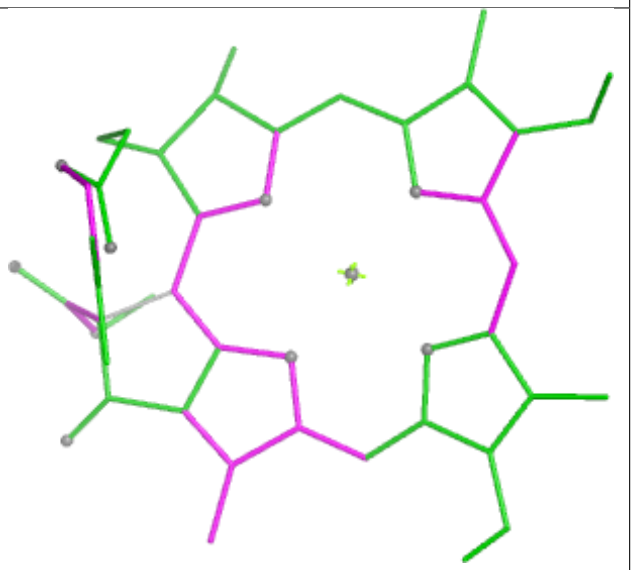
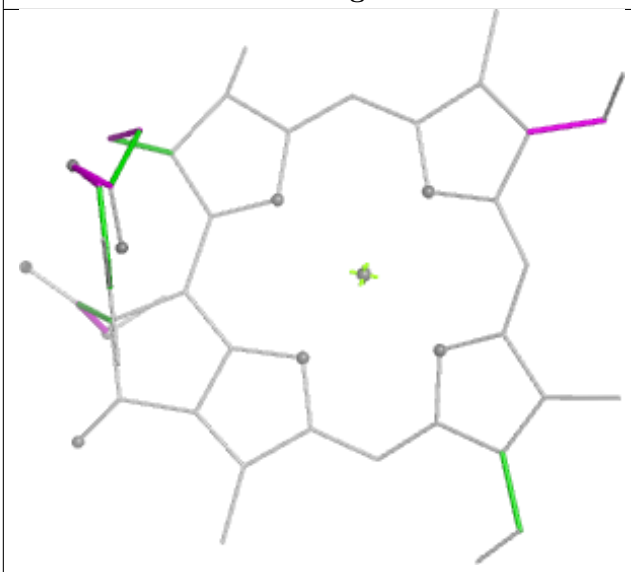


Bond angles

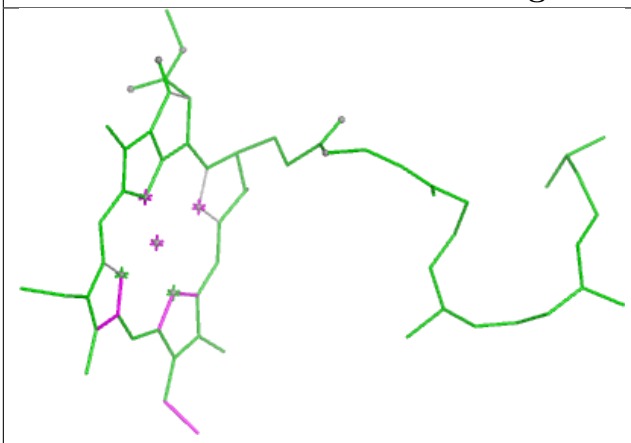


Torsions



Rings

Ligand CLA 1 513



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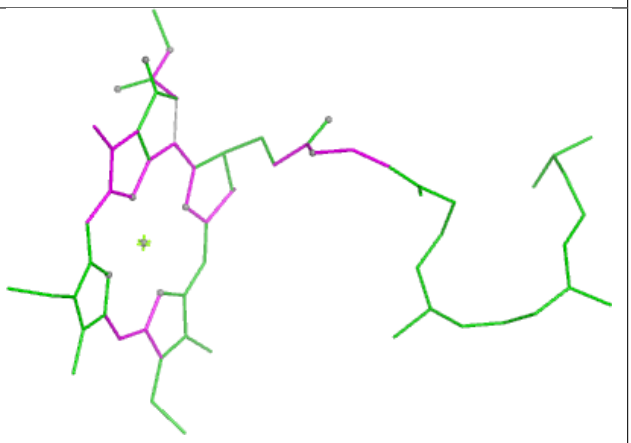

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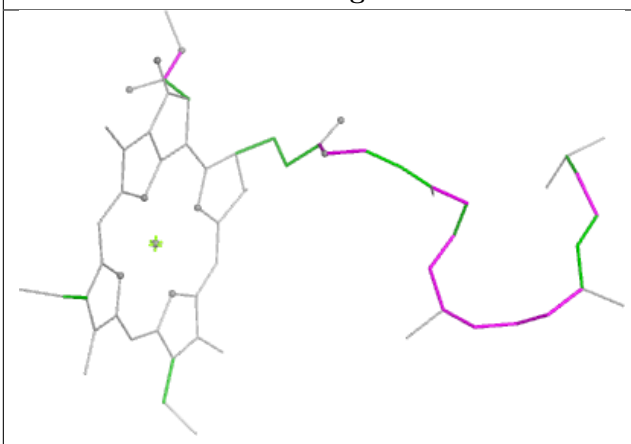

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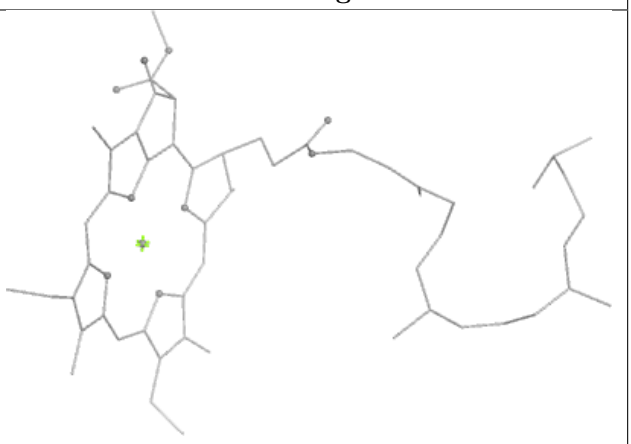
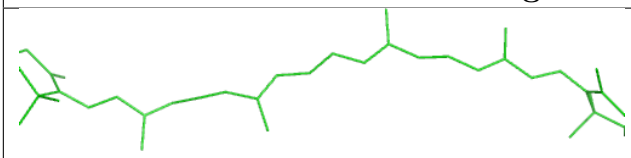


Rings

Ligand BCR B 852



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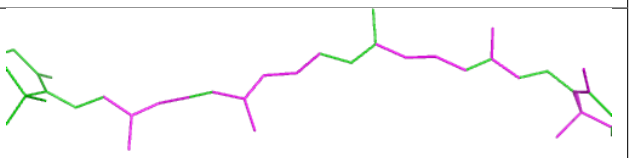
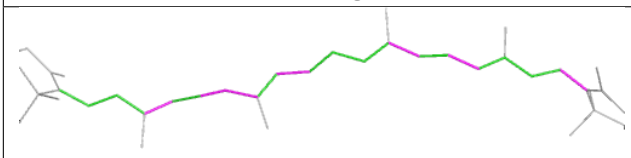


Bond angles



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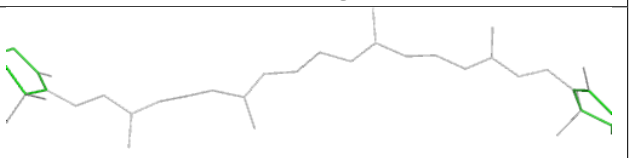
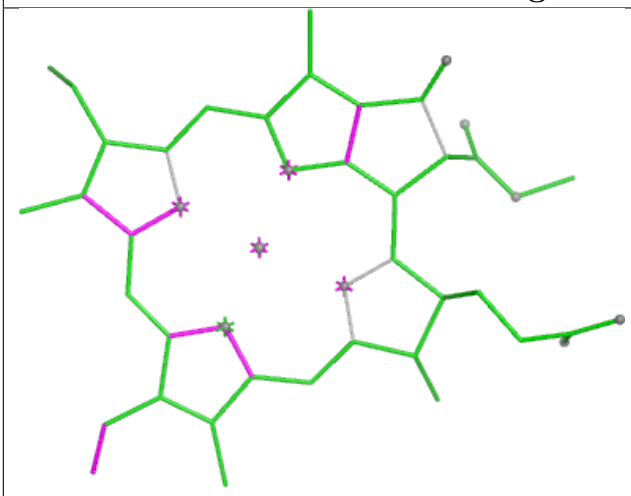


Rings

Ligand CLA 1 515



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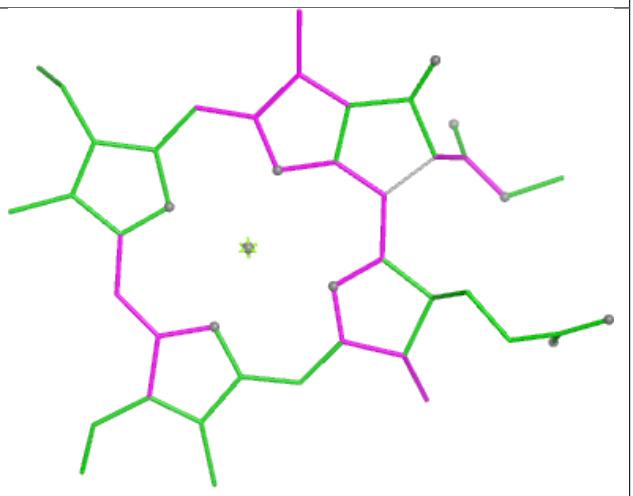

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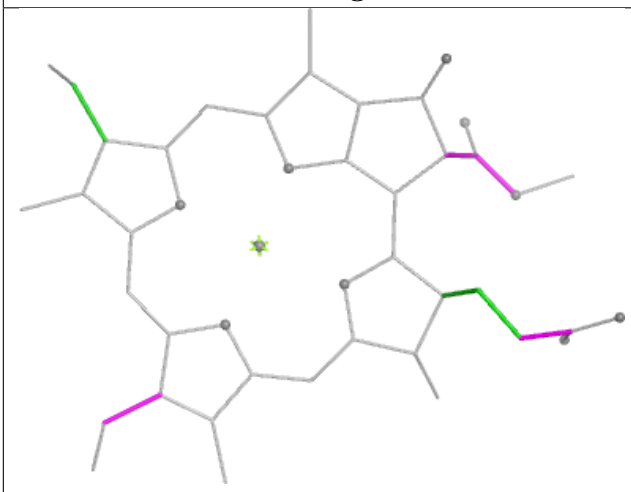

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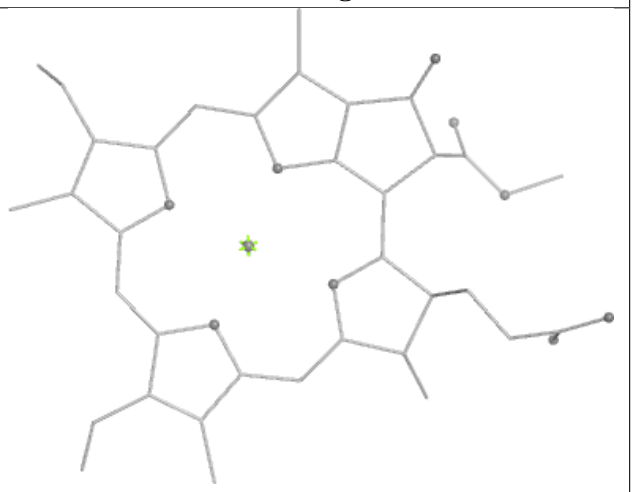
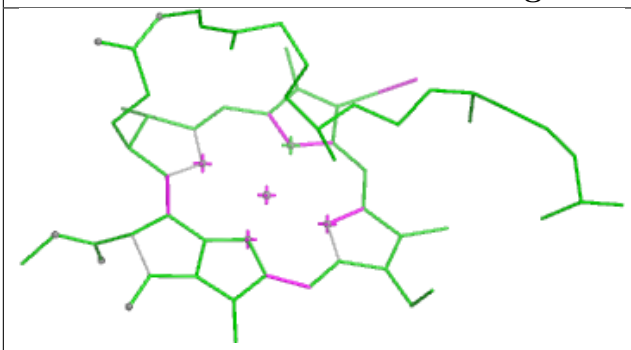


Rings

Ligand CLA B 818



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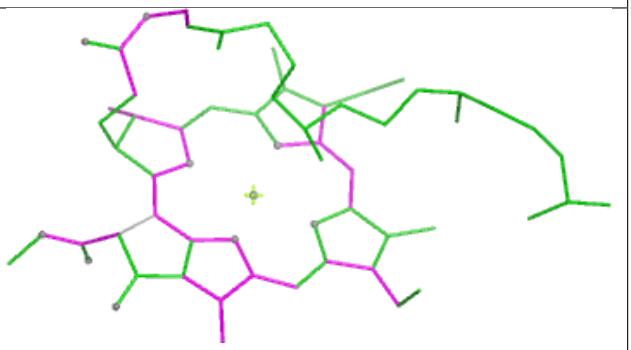

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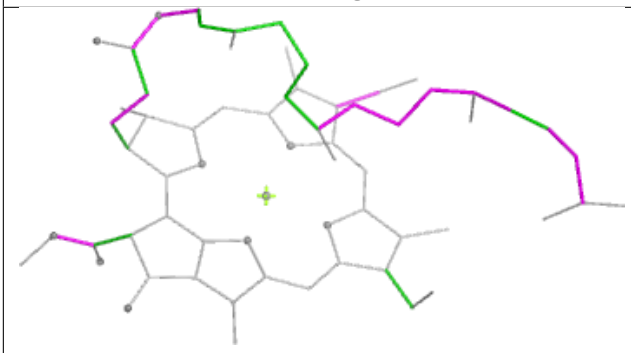

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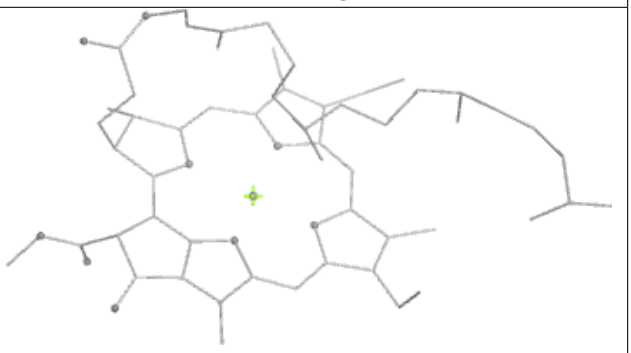
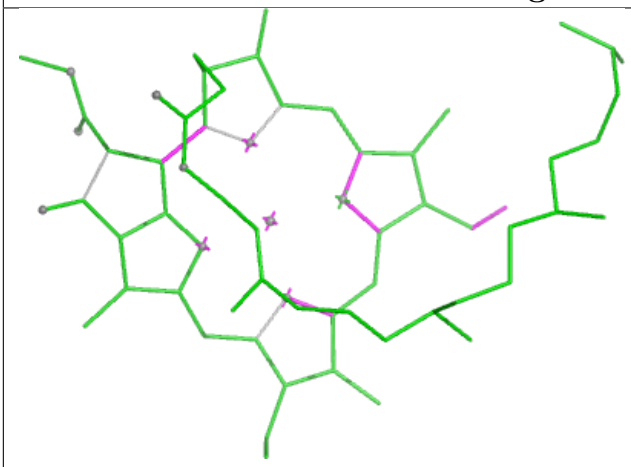


Rings

Ligand CLA 2 506



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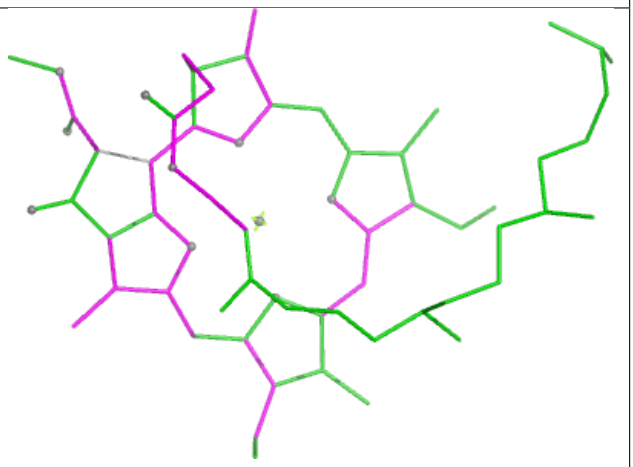
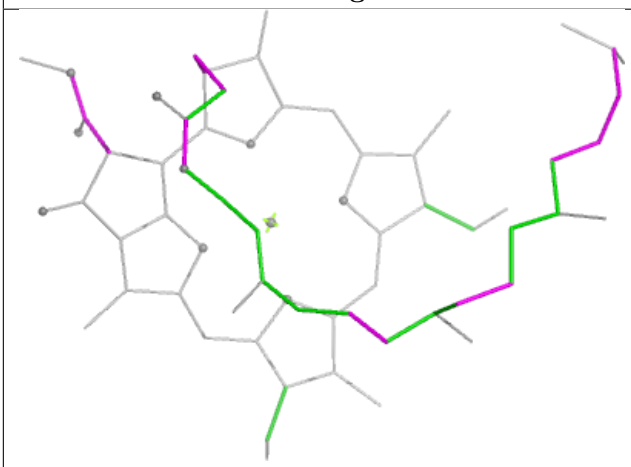


Bond angles

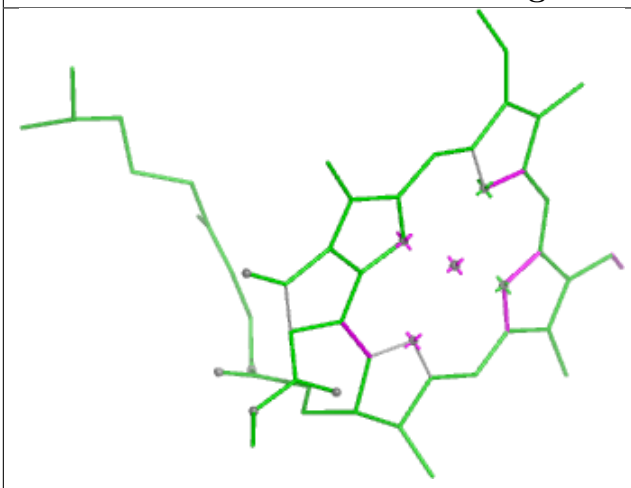


Torsions



Rings

Ligand CLA 2 514



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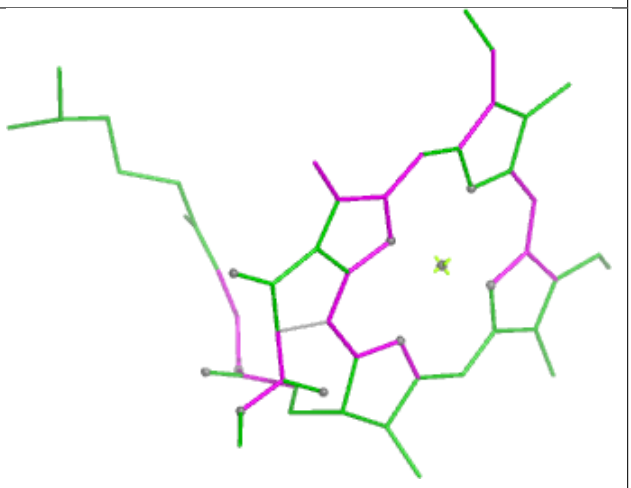
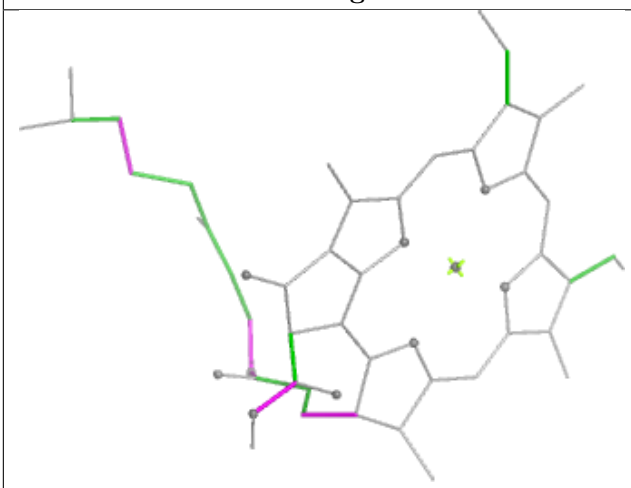


Bond angles



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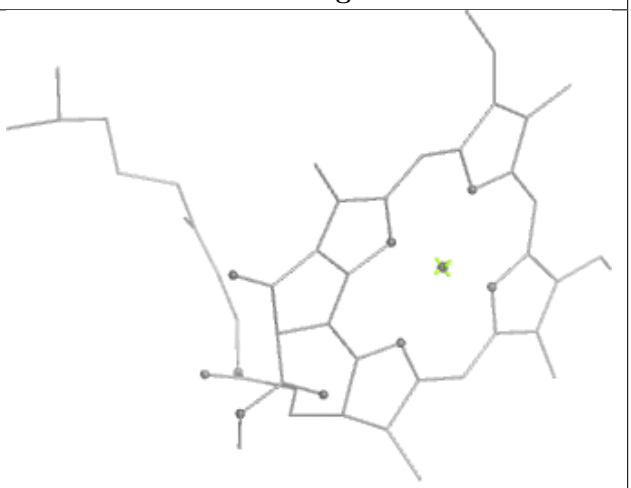
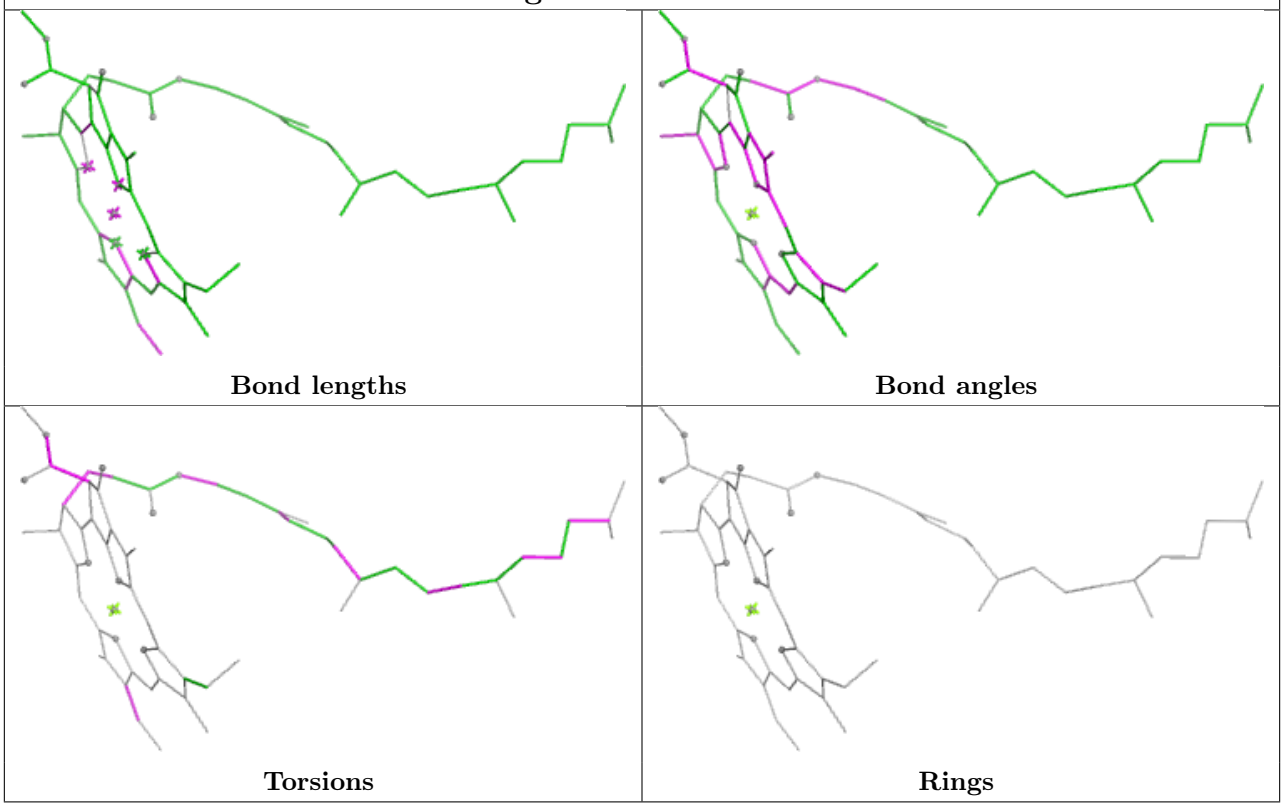
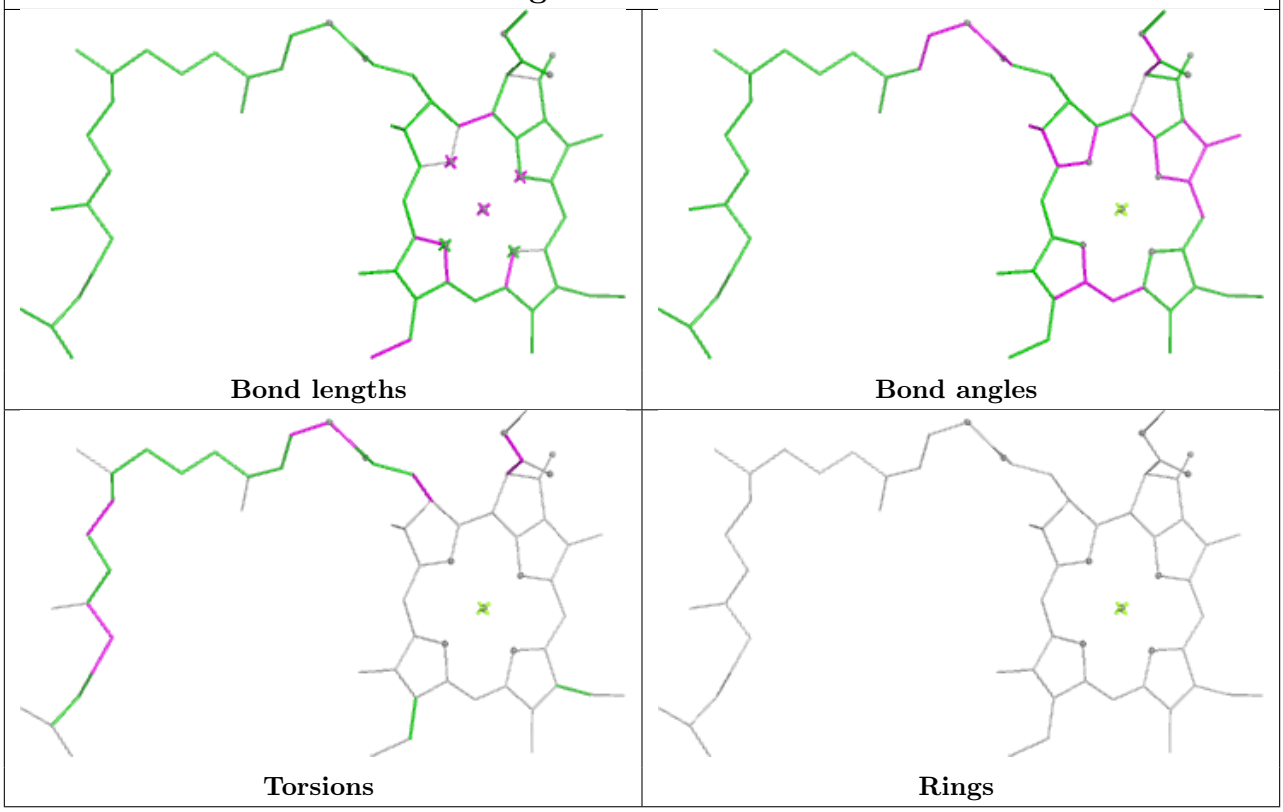


Rings

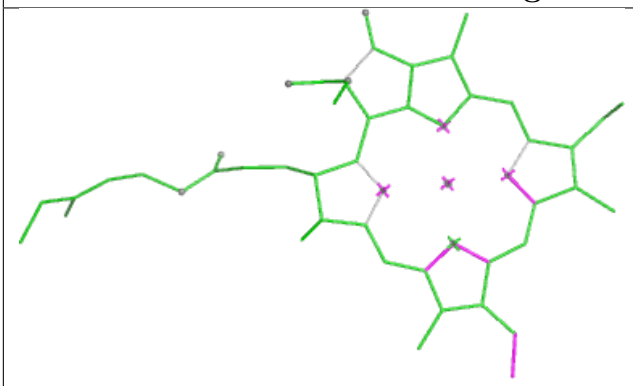
Ligand CLA A 811



Ligand CLA 4 318



Ligand CLA A 836



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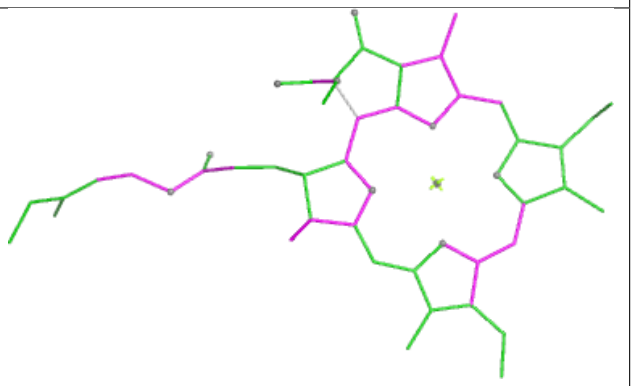
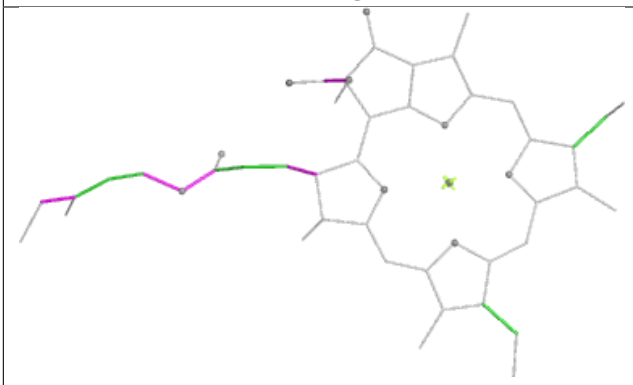


Bond angles



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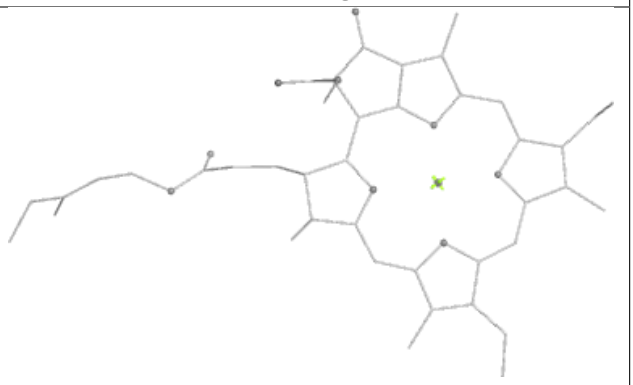
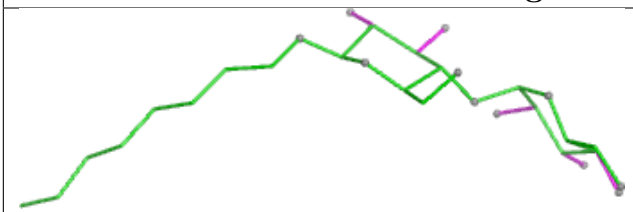


Rings

Ligand LMT 3 318



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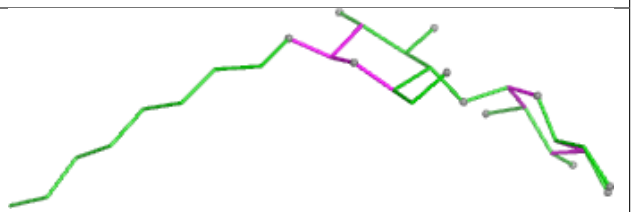
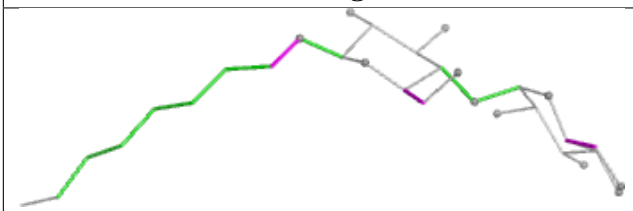


Bond angles



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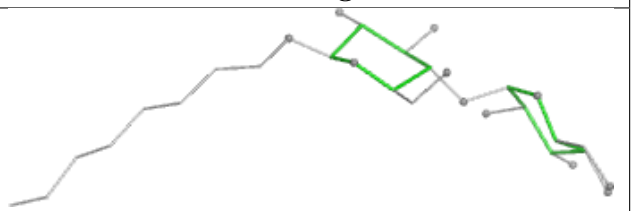
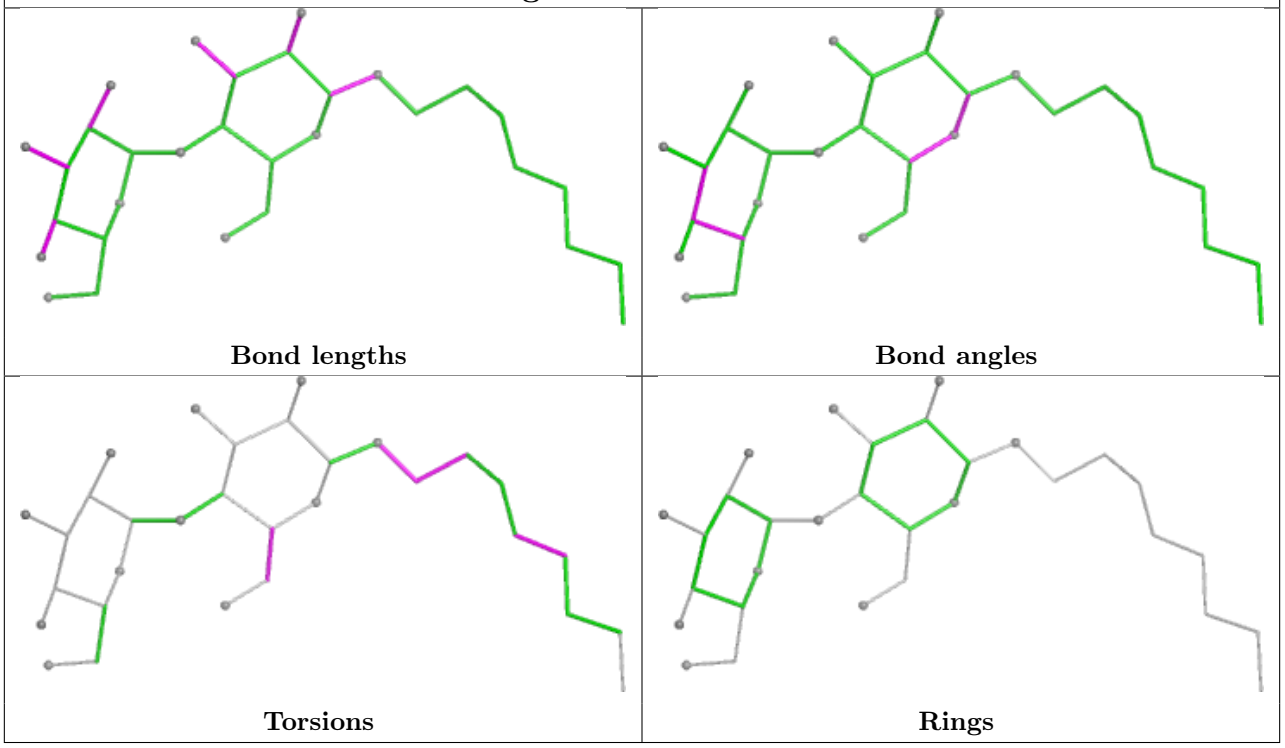
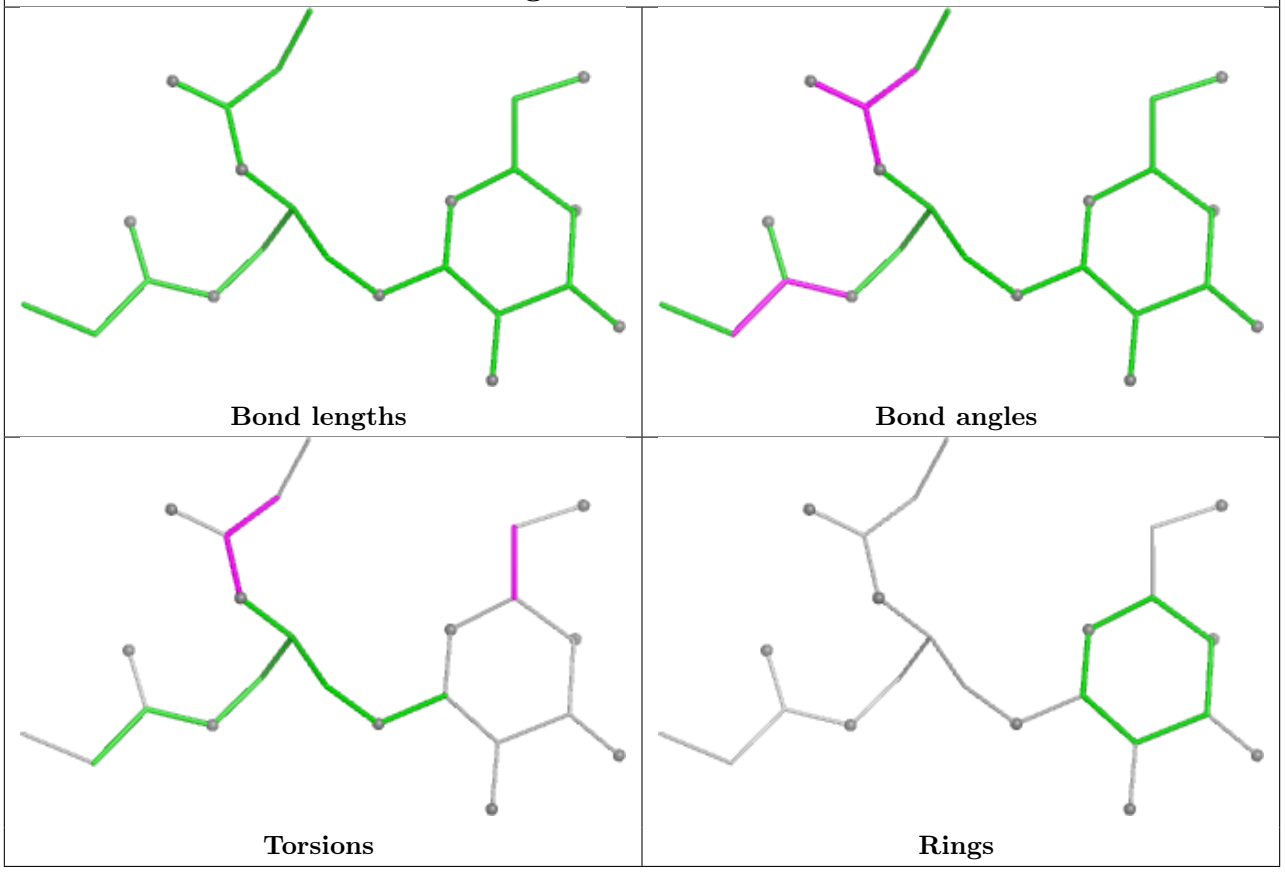


Rings

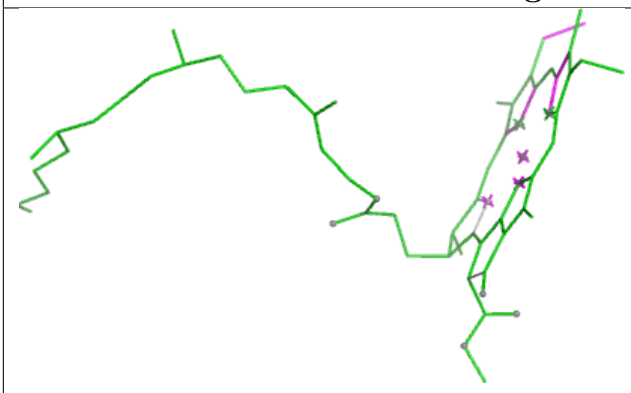
Ligand LMT B 855



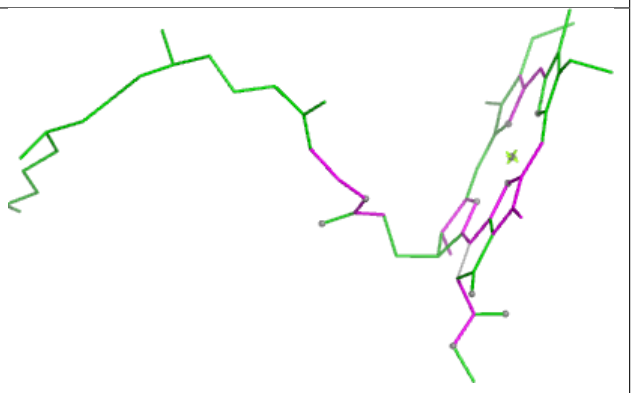
Ligand LMG 2 518



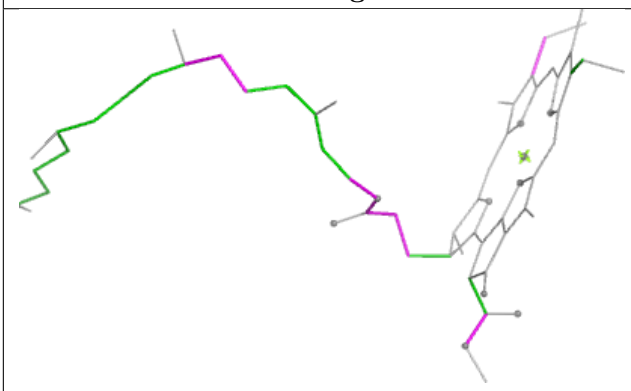
Ligand CLA B 838



Bond lengths



Bond angles

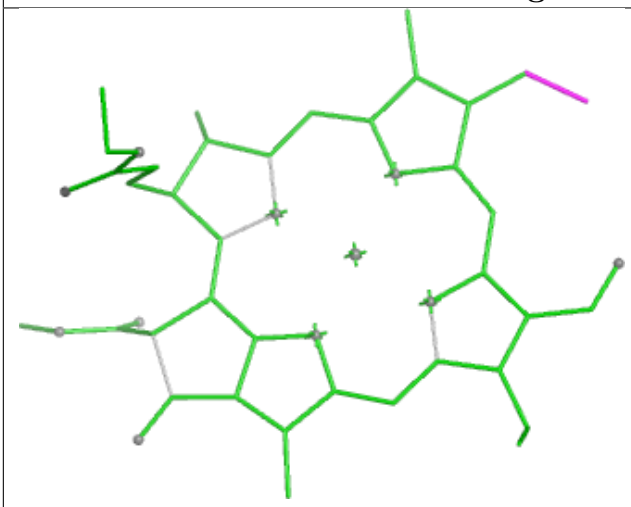


Torsions



Rings

Ligand CHL 2 513



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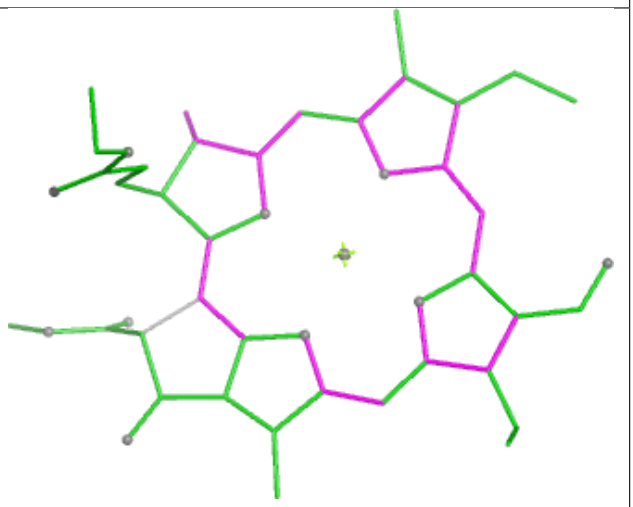
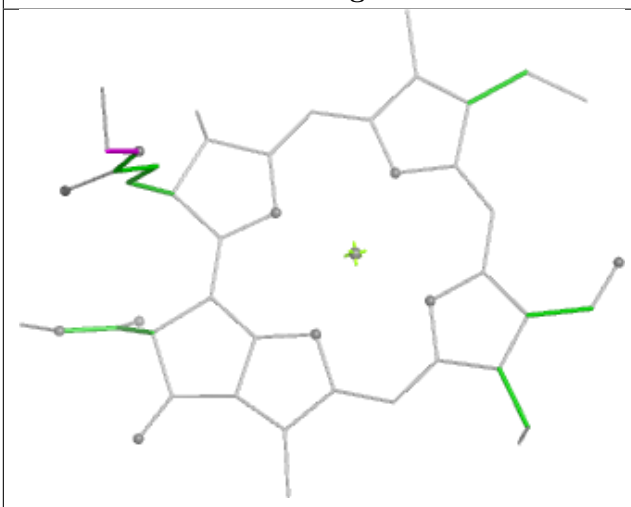


Bond angles



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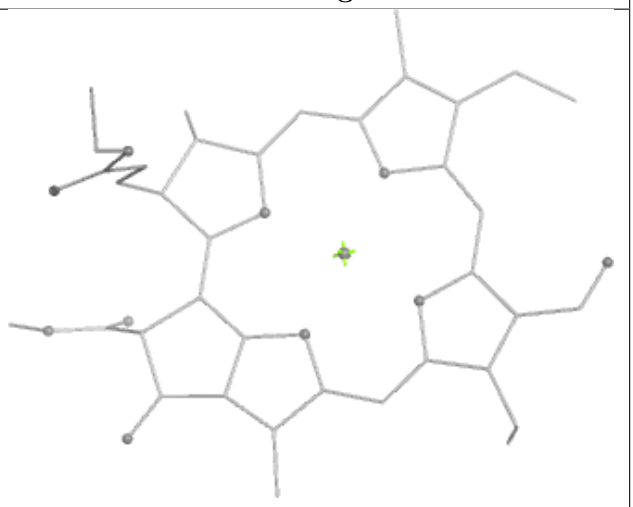
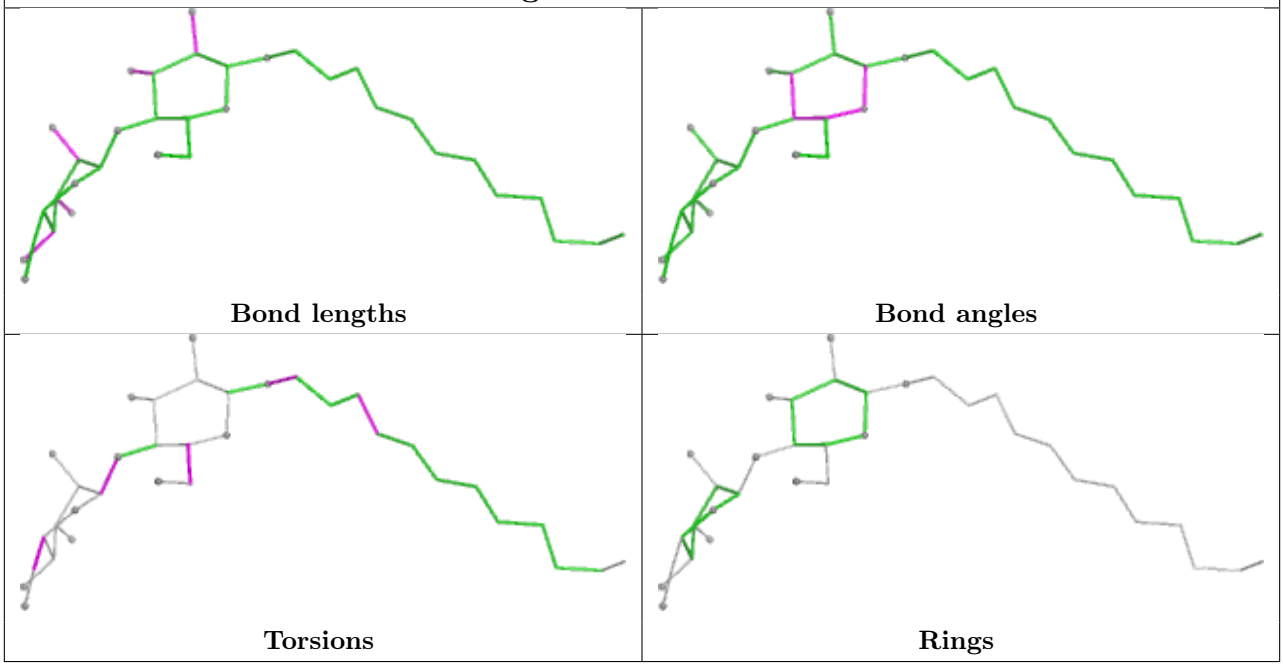
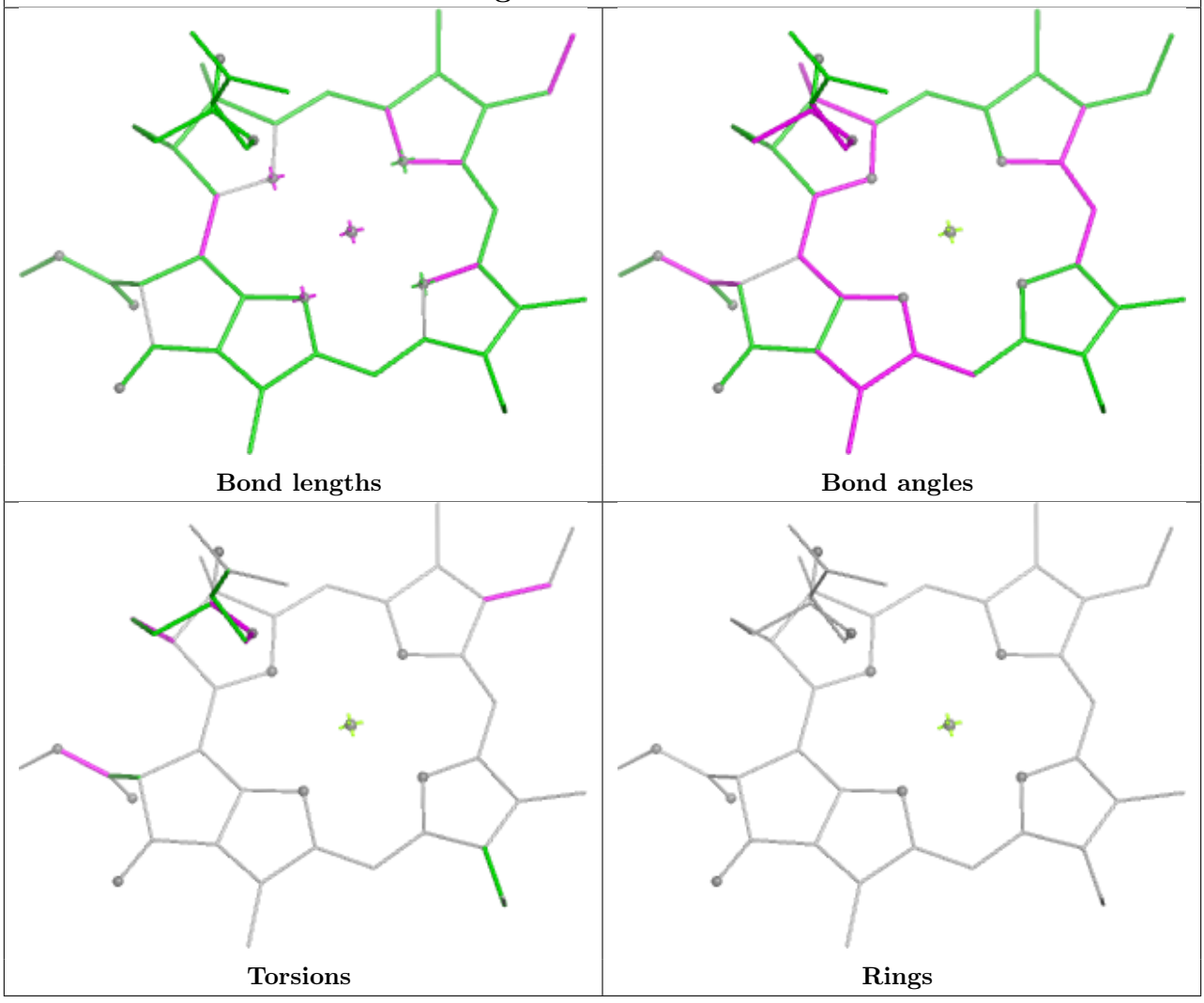


Rings

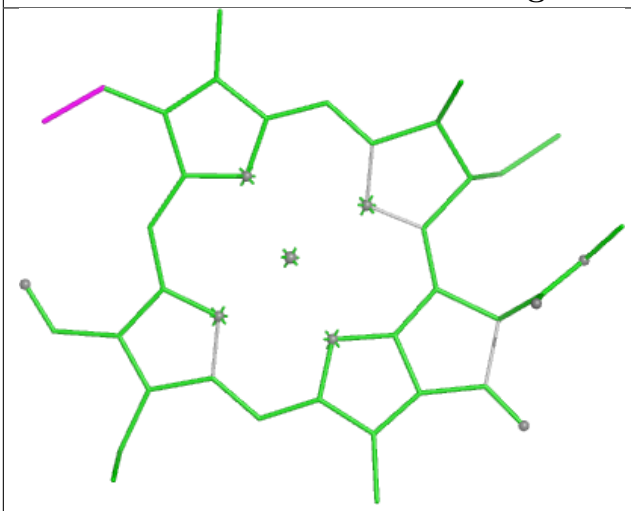
Ligand LMT A 846



Ligand CLA L 303



Ligand CHL 4 317



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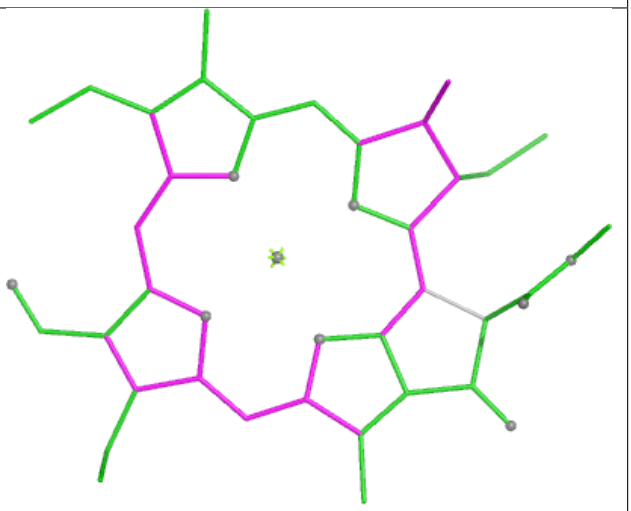
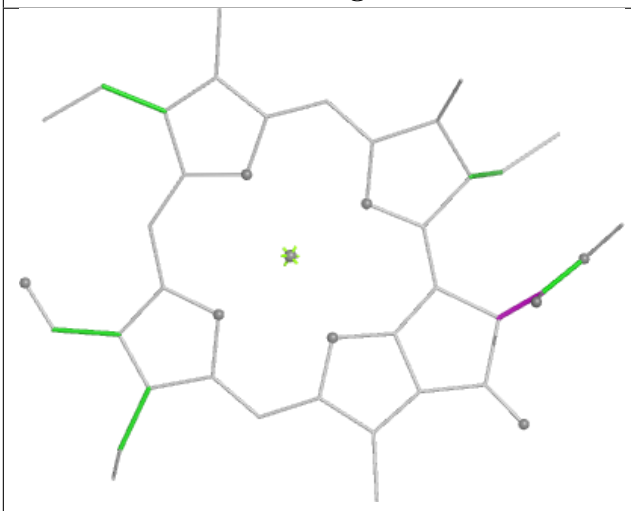


Bond angles



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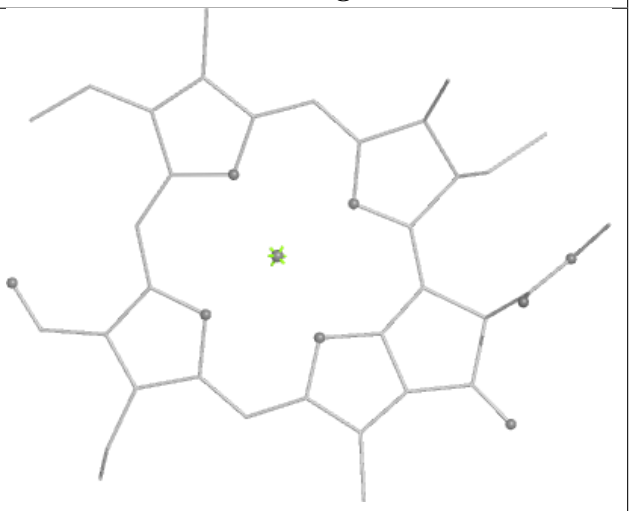
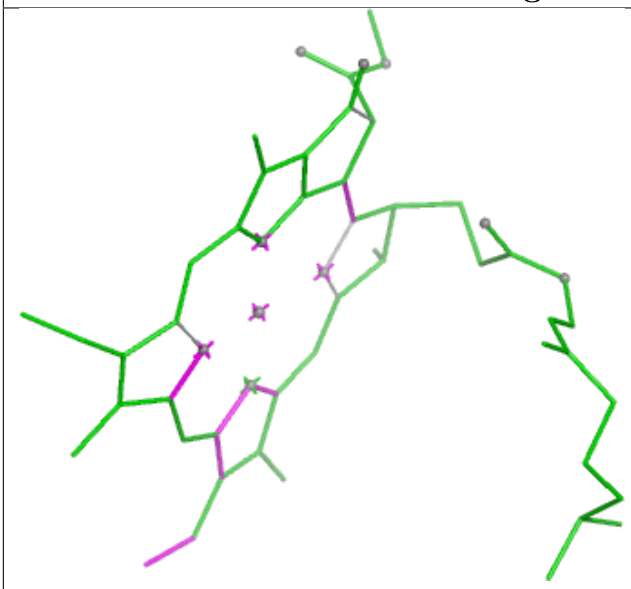


Rings

Ligand CLA A 835



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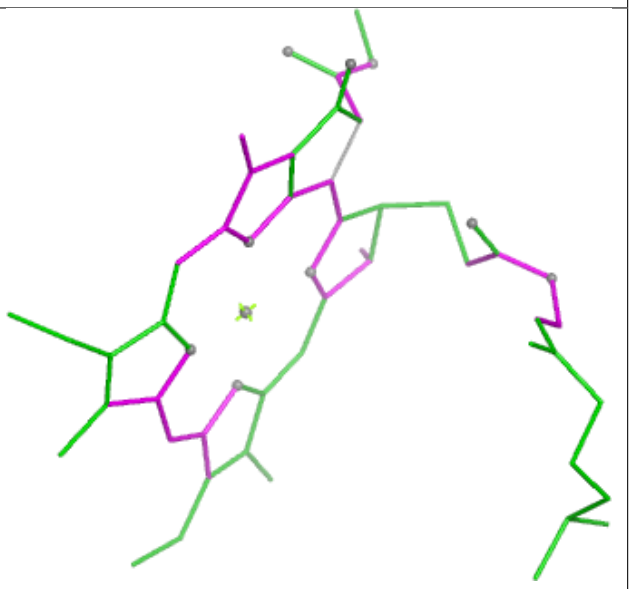
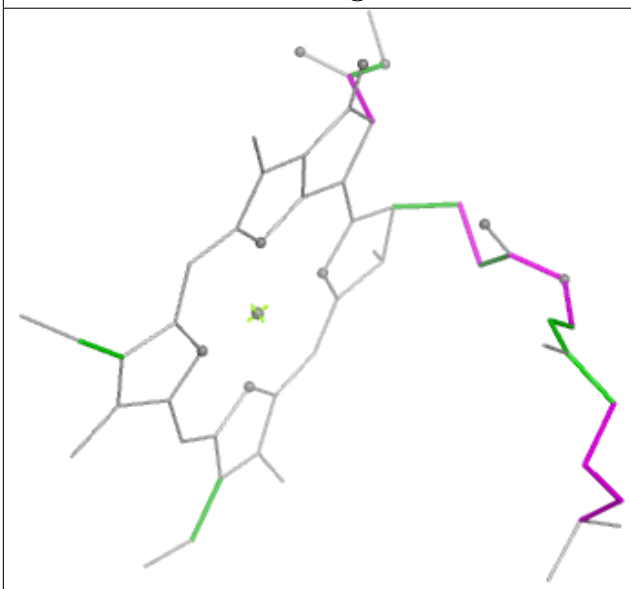


Bond angles



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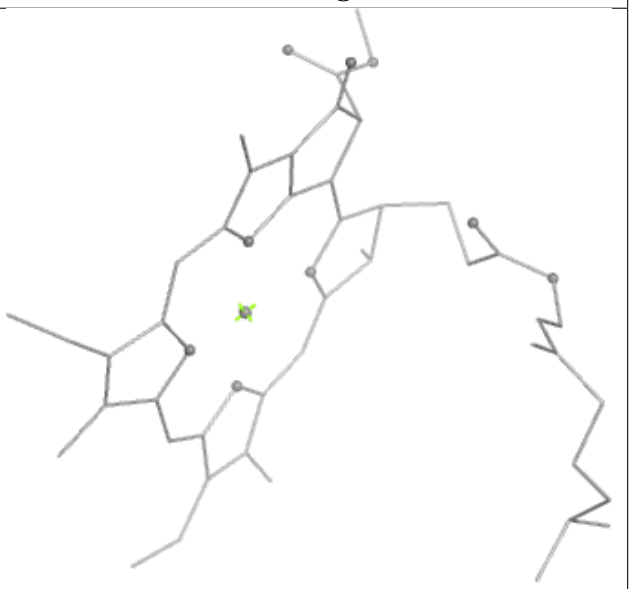
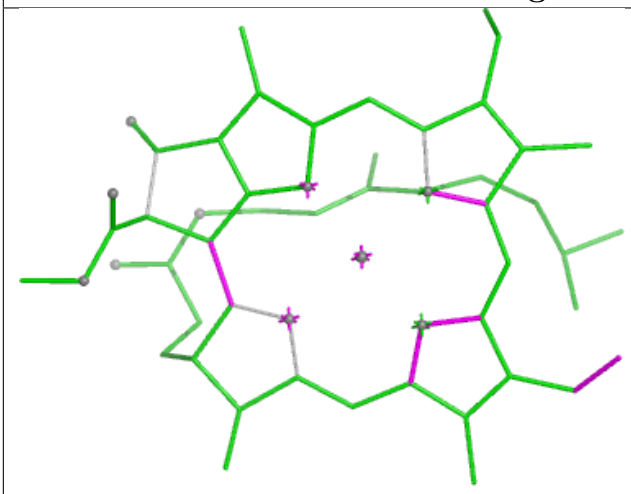


Rings

Ligand CLA 3 307



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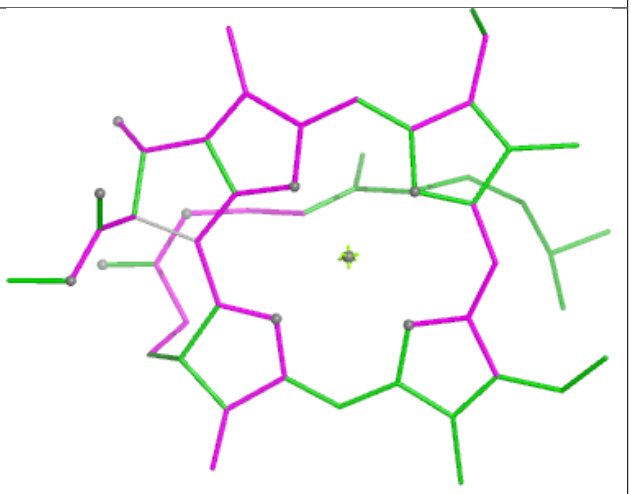
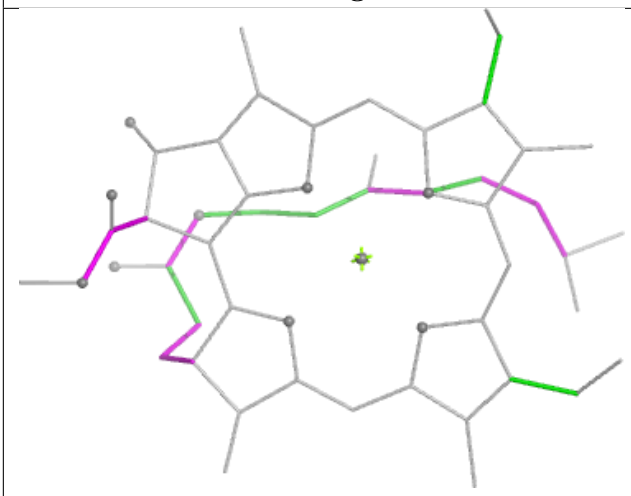


Bond angles



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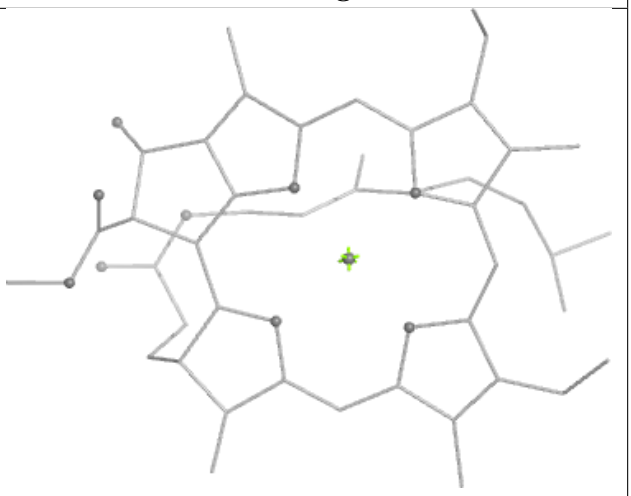
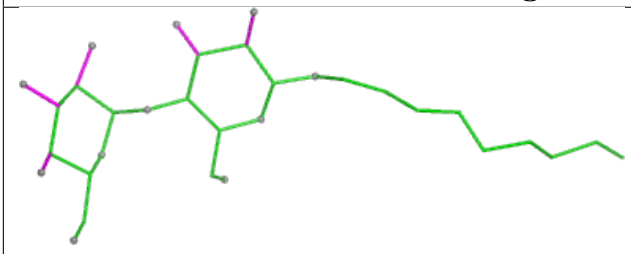


Rings

Ligand LMT B 847



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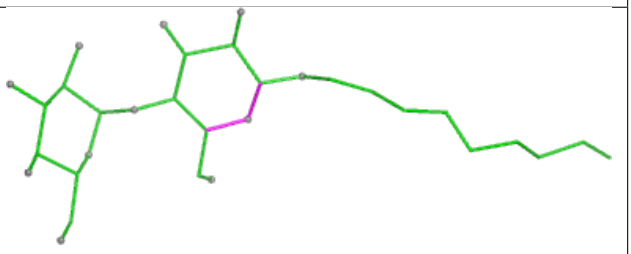
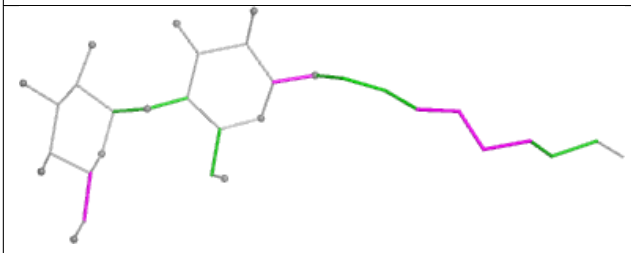


Bond angles



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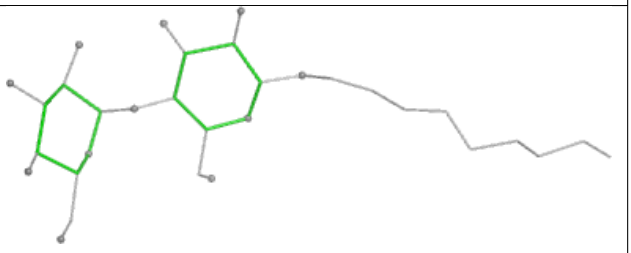
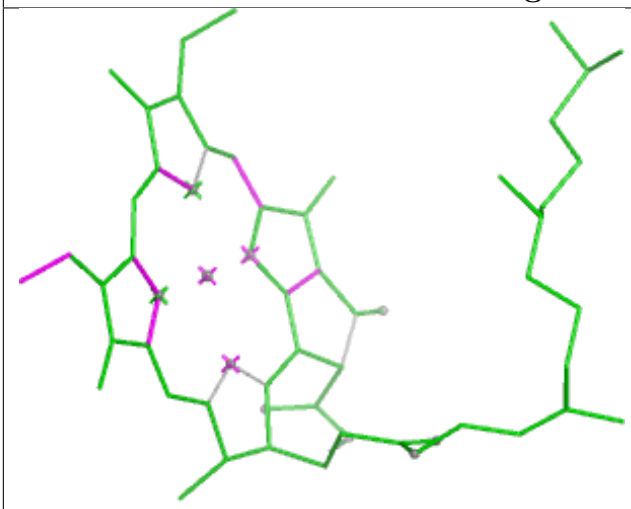


Rings

Ligand CLA B 833



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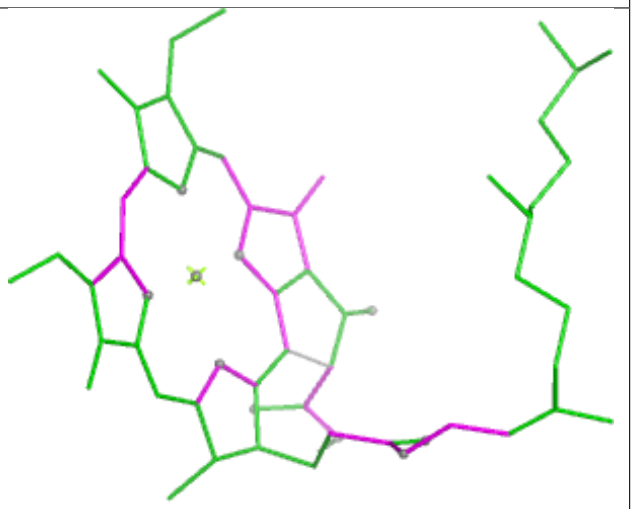

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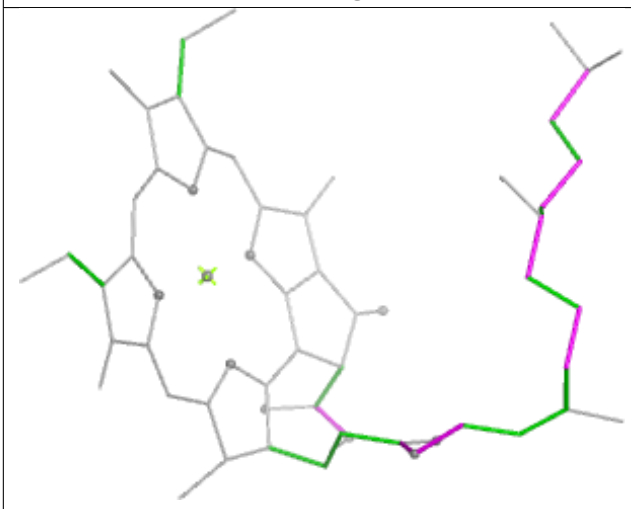
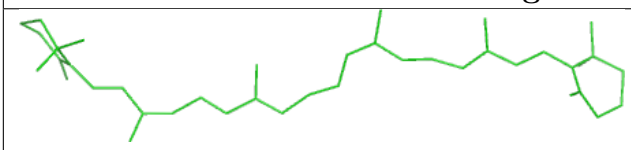


Torsions



Rings

Ligand BCR B 802



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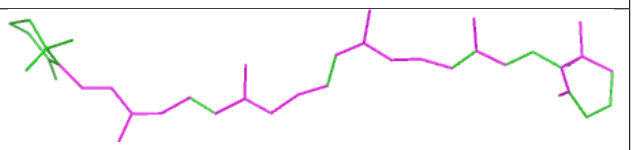
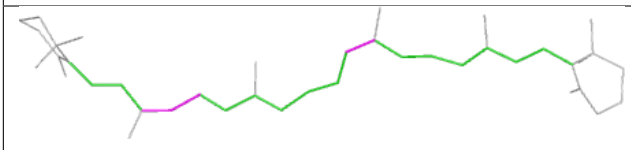


Bond angles



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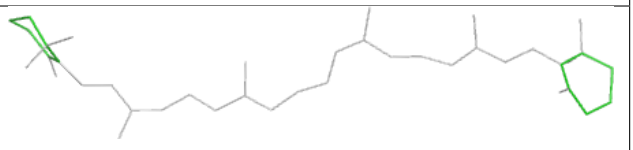
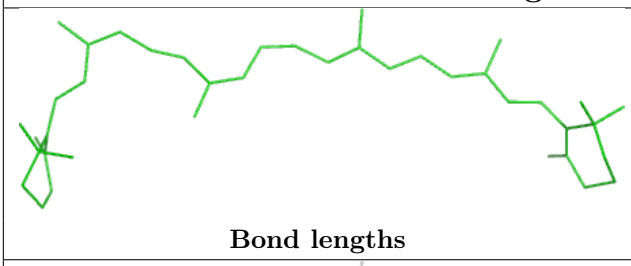


Rings

Ligand BCR L 302



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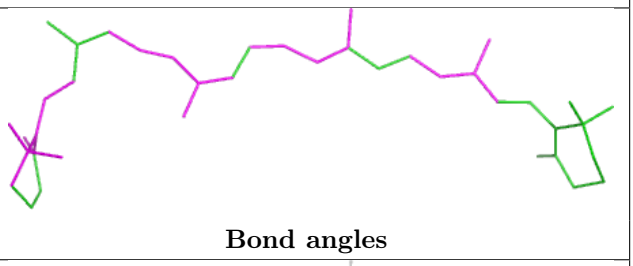
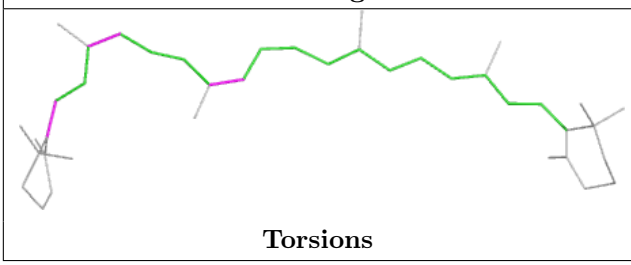


Bond angles



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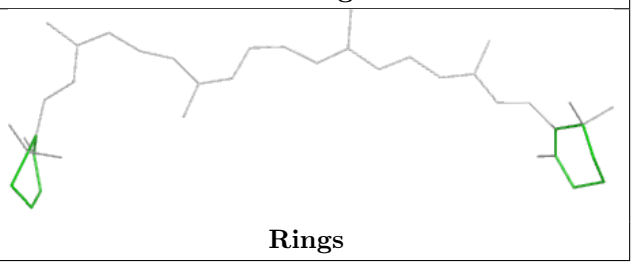
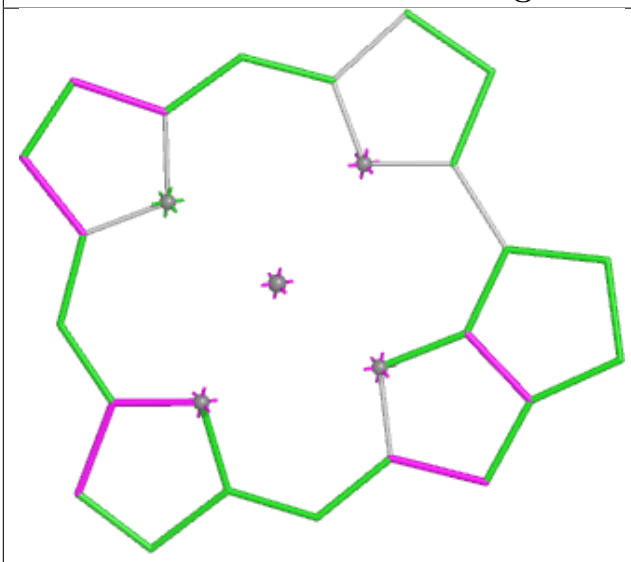


Rings

Ligand CLA K 1004



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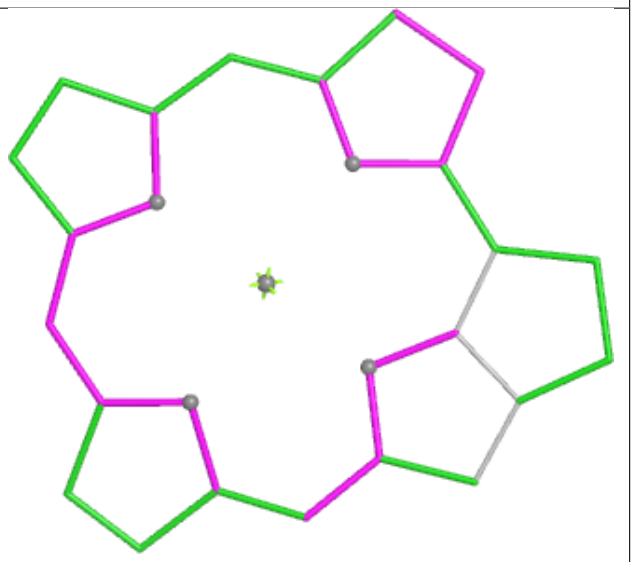
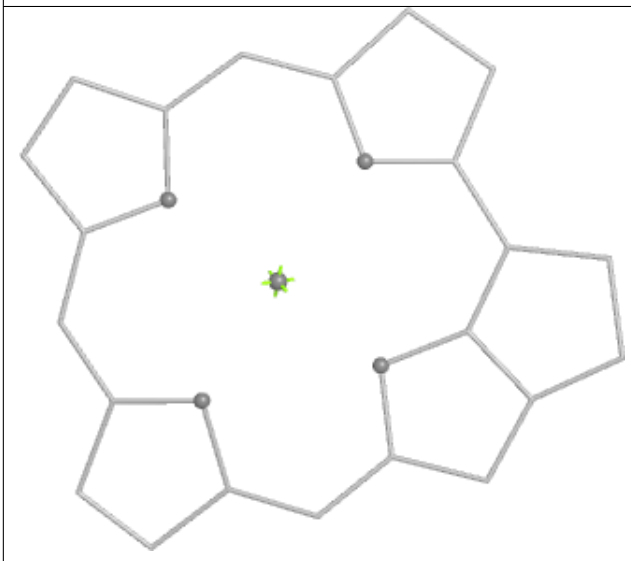


Bond angles



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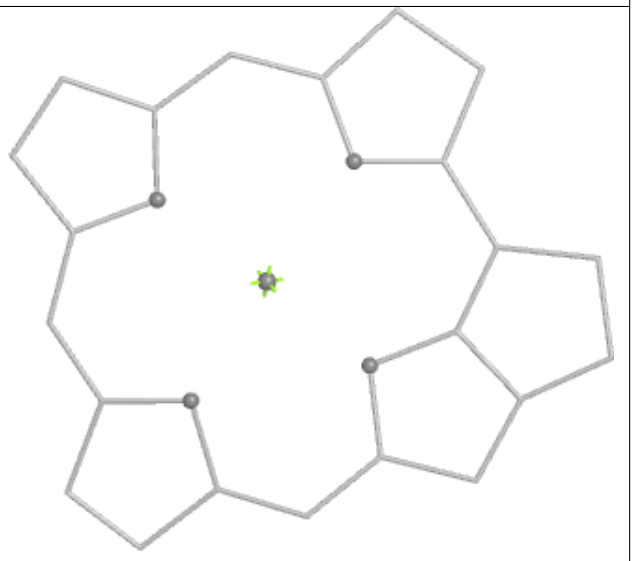
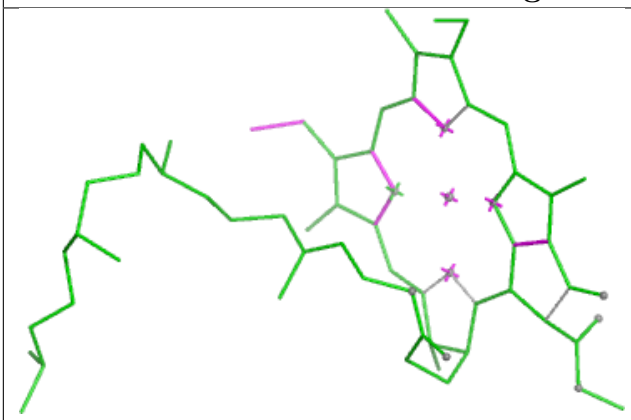


Rings

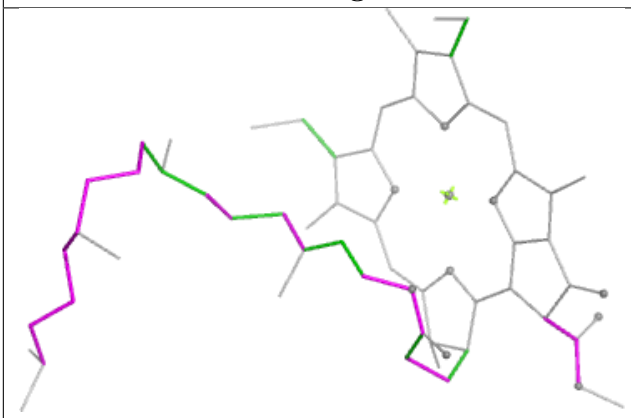
Ligand CLA A 855



Bond lengths



Bond angles

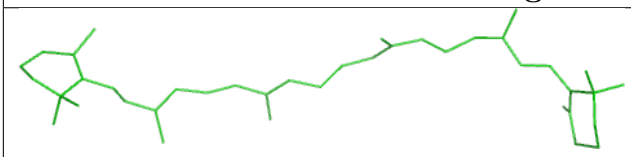


Torsions



Rings

Ligand BCR L 307



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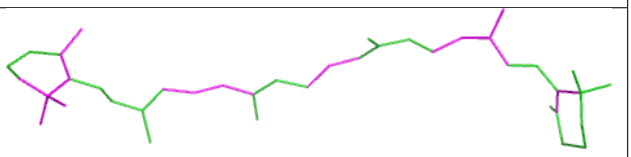
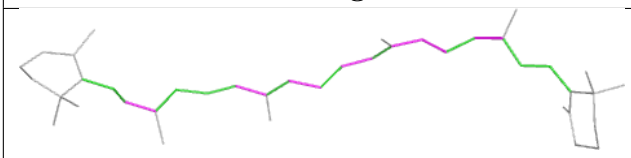


Bond angles

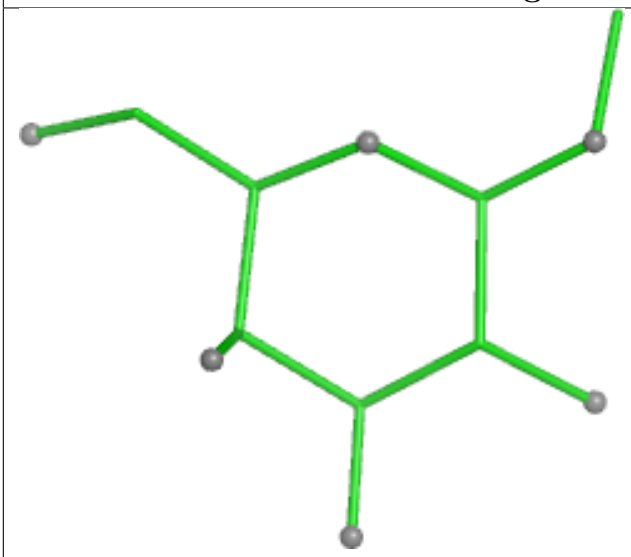


Torsions



Rings

Ligand LMG 2 524



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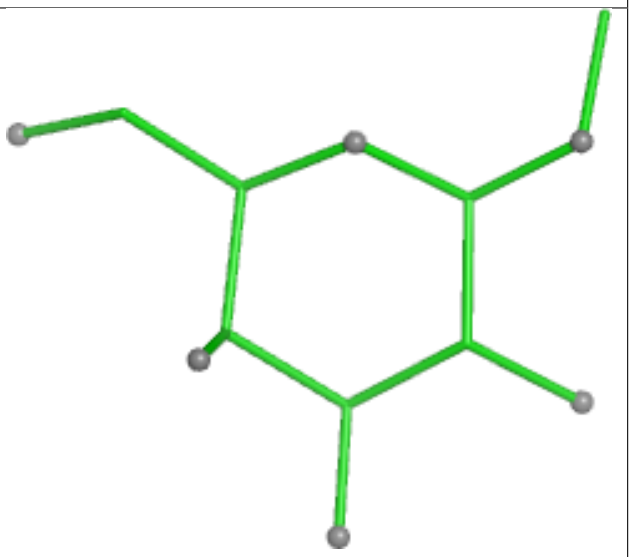
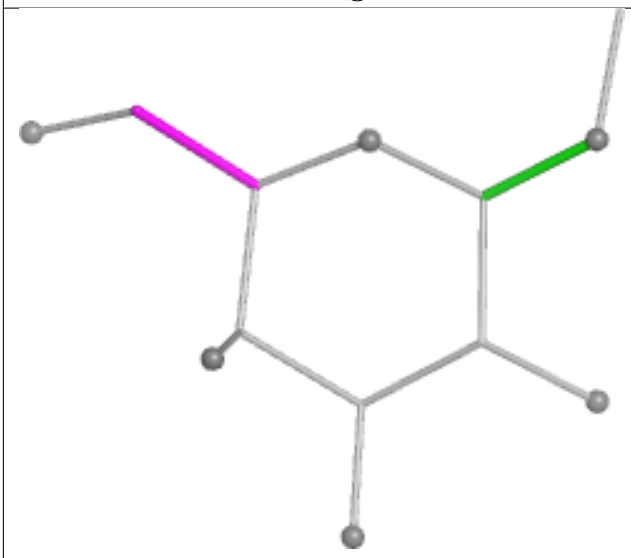
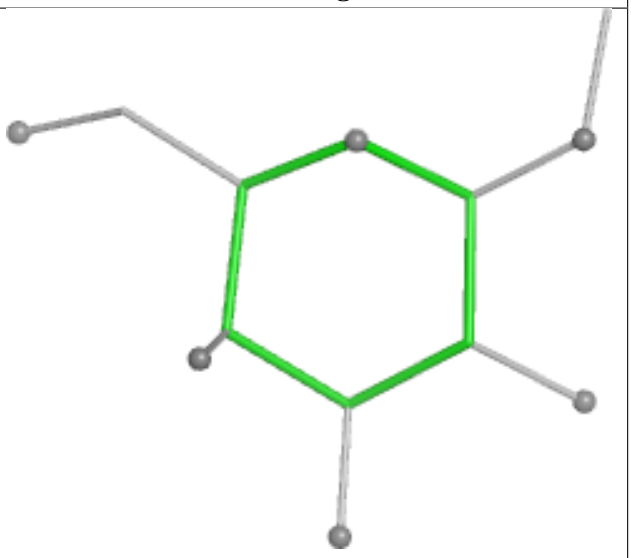


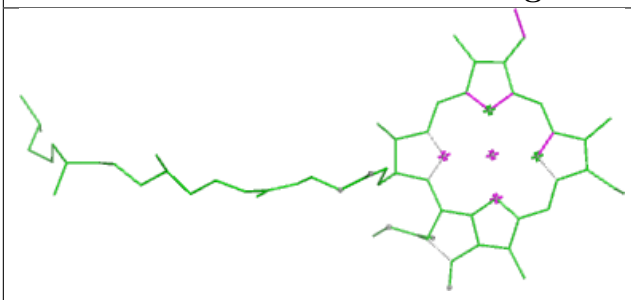
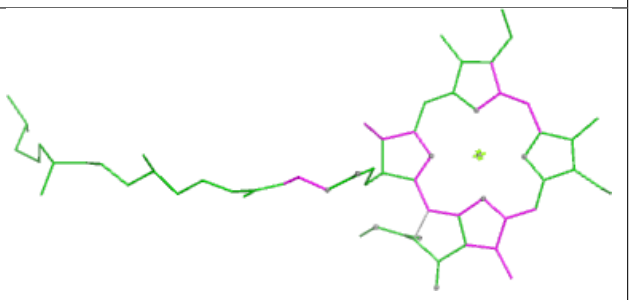
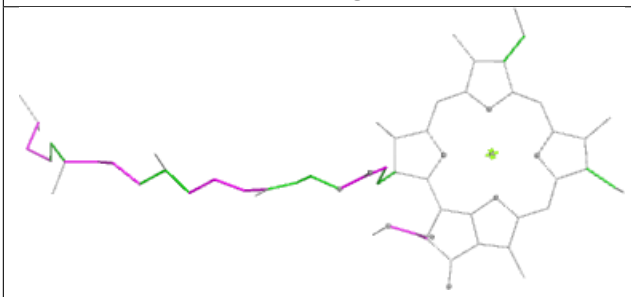
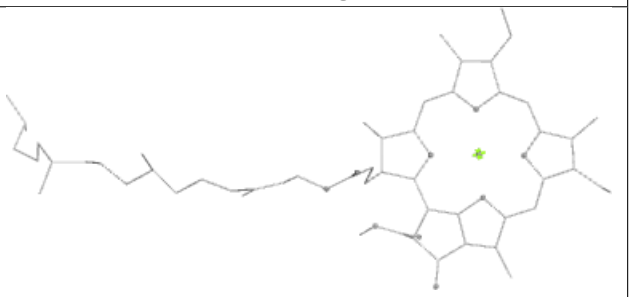
Bond angles

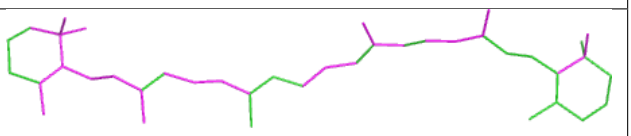
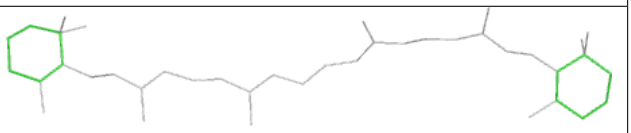


Torsions

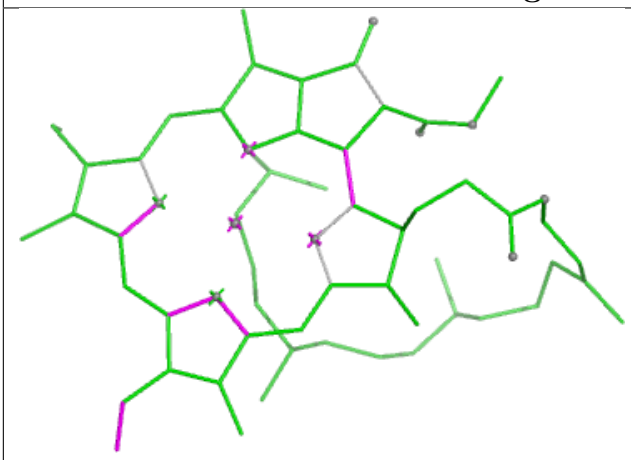


Rings

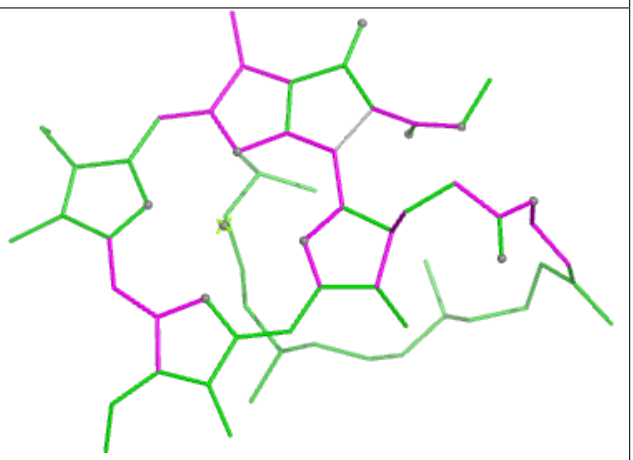
Ligand CLA B 840	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand BCR I 102	
 Bond lengths	 Bond angles
 Torsions	 Rings

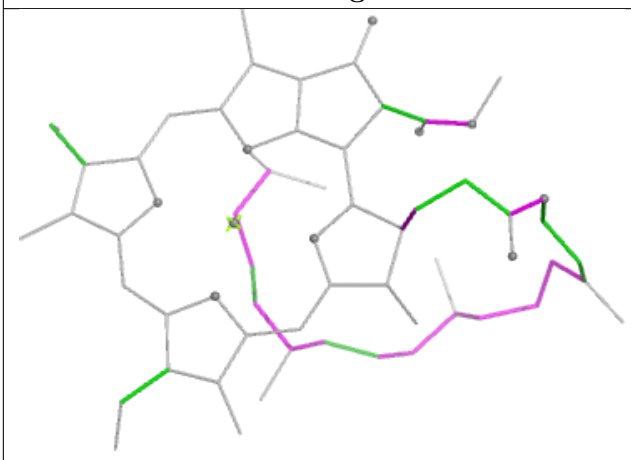
Ligand CLA A 806



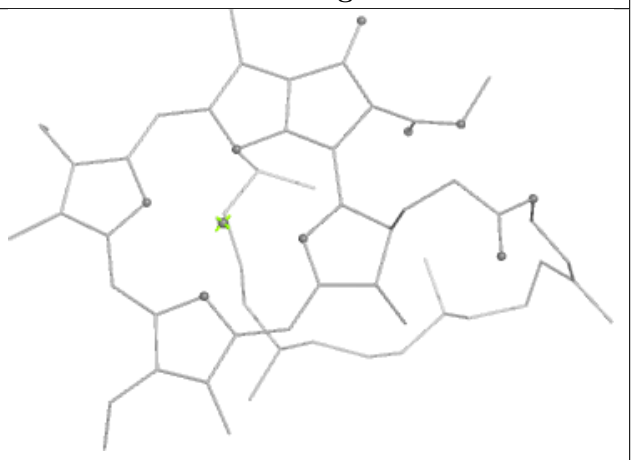
Bond lengths



Bond angles

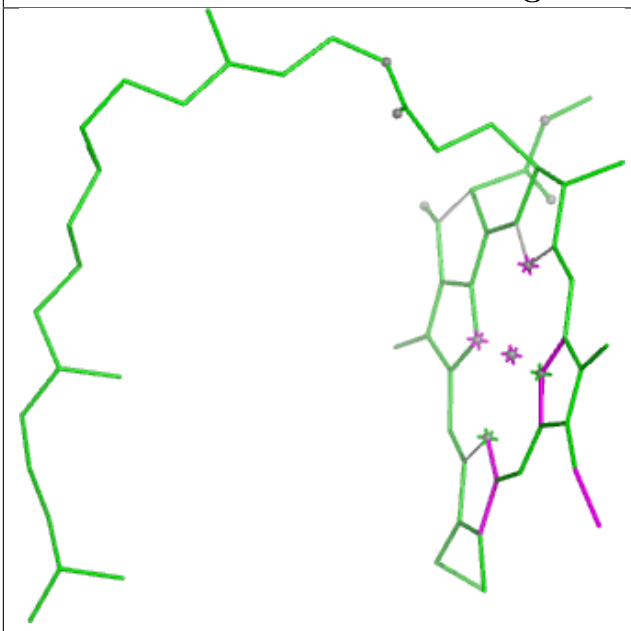


Torsions

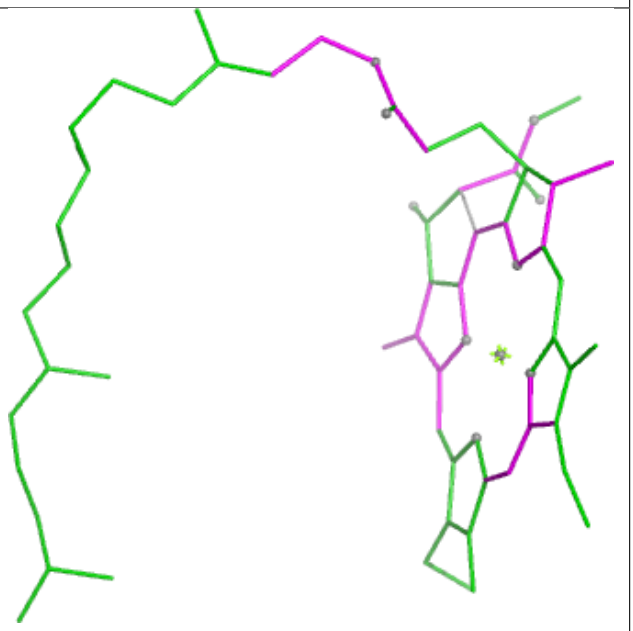


Rings

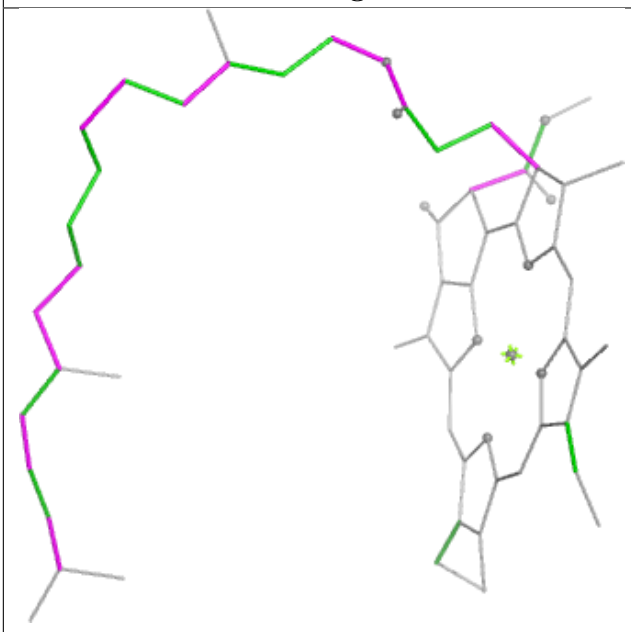
Ligand CLA A 838



Bond lengths



Bond angles



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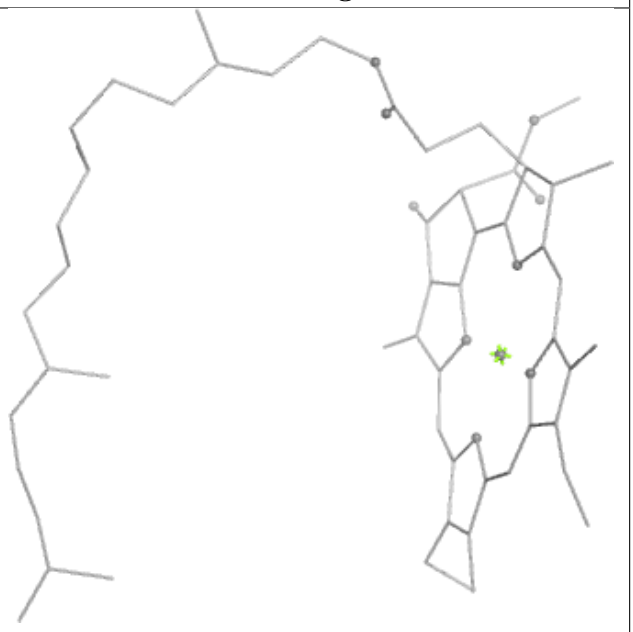
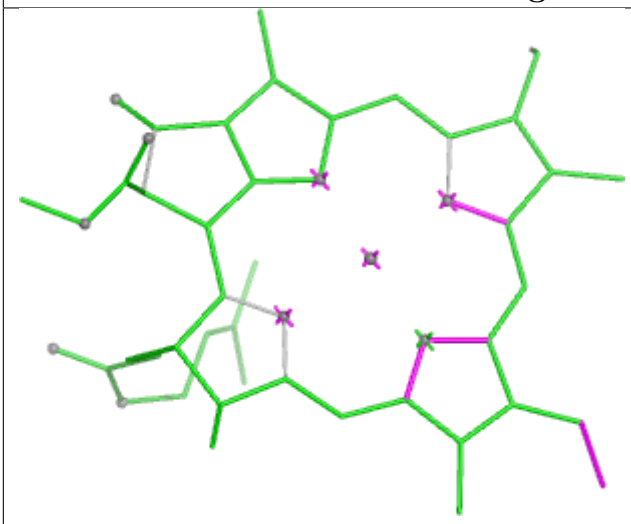


Rings

Ligand CLA 1 509



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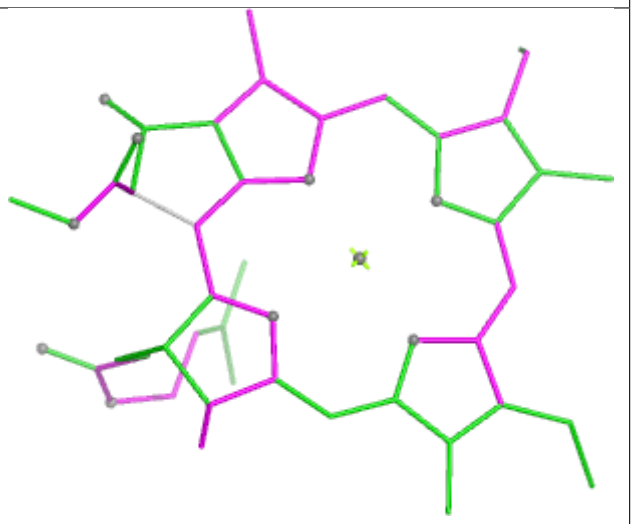

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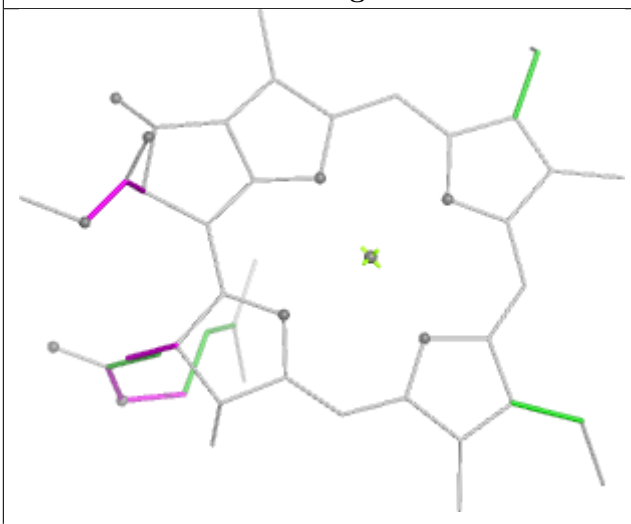

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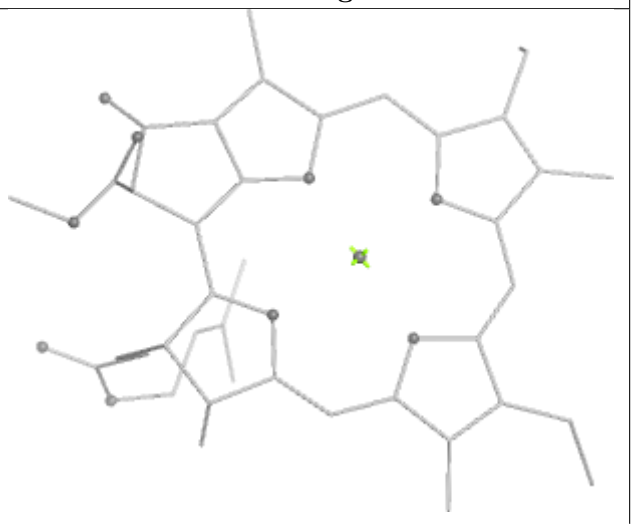
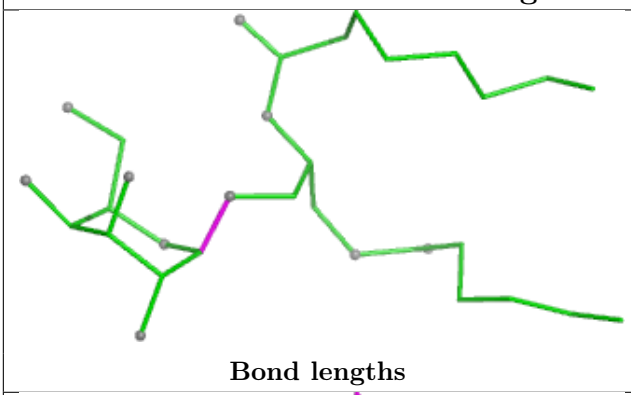


Rings

Ligand LMG B 845



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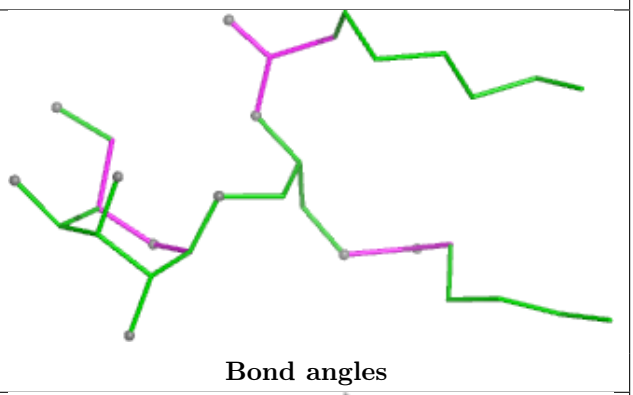
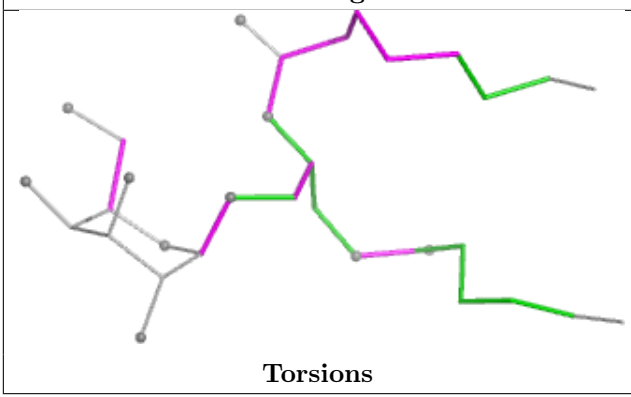


Bond angles



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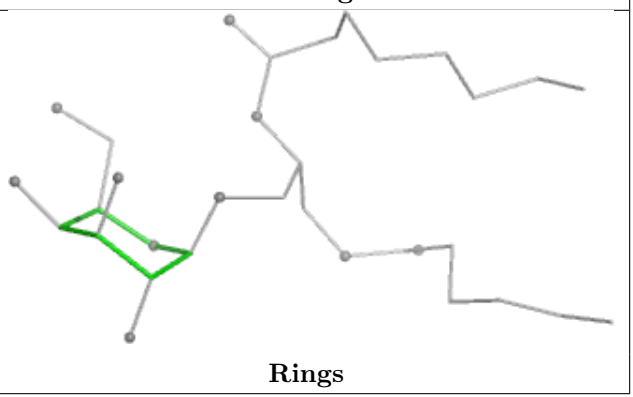
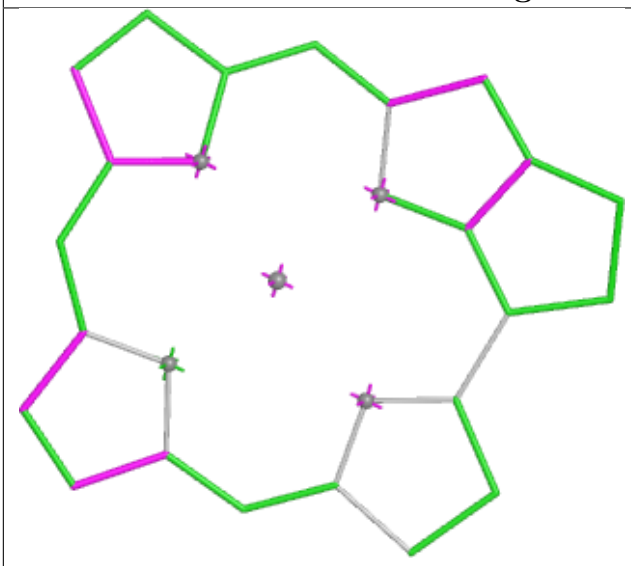


Rings

Ligand CLA K 1003



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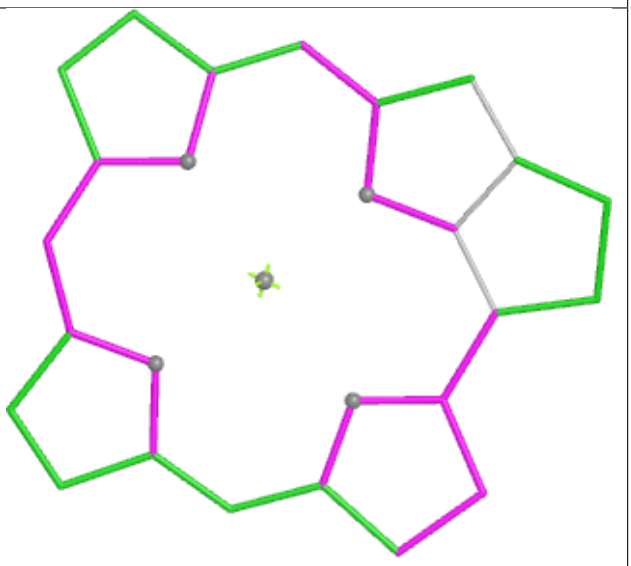
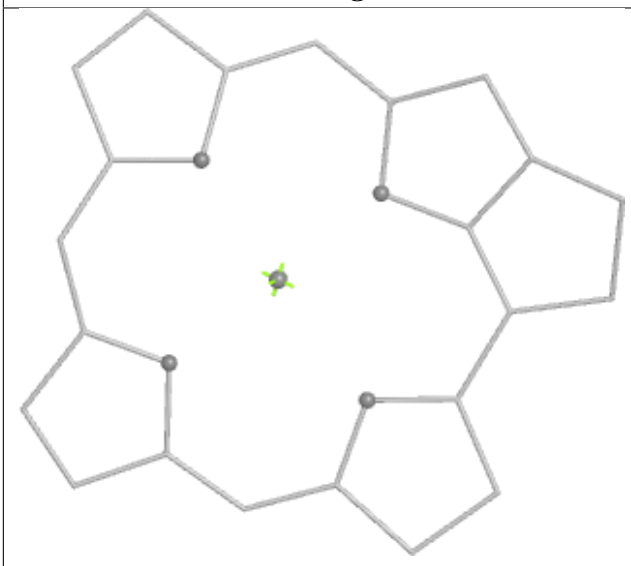


Bond angles



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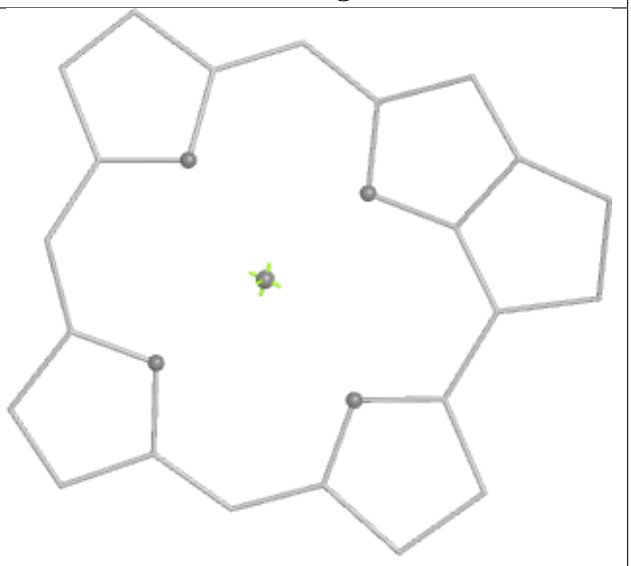
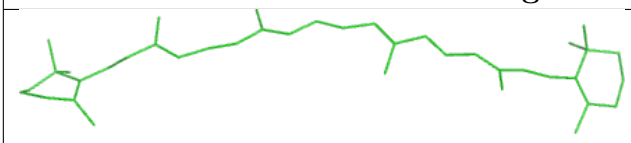


Rings

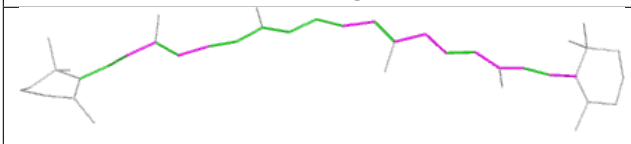
Ligand BCR A 856



Bond lengths



Bond angles

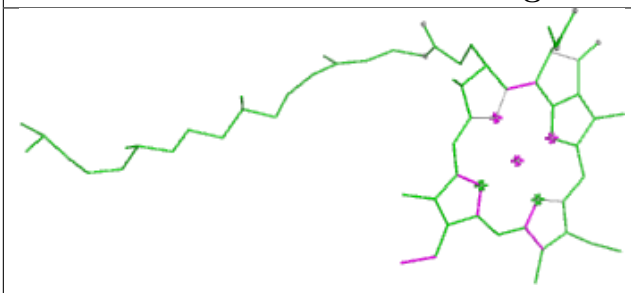


Torsions



Rings

Ligand CLA A 833



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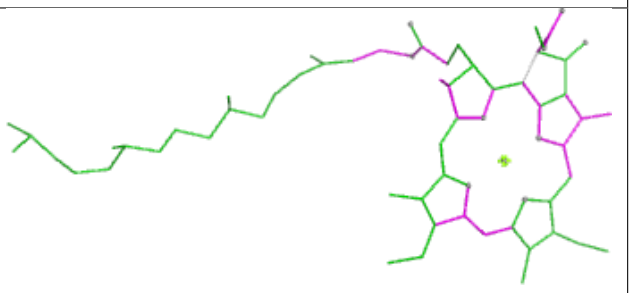
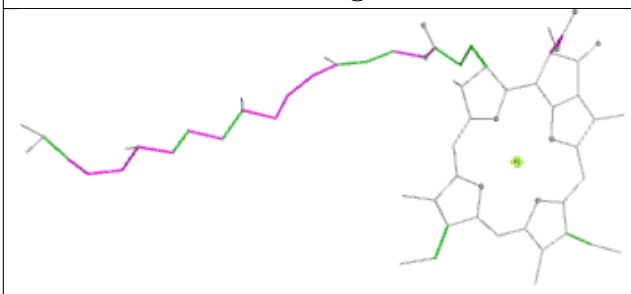


Bond angles



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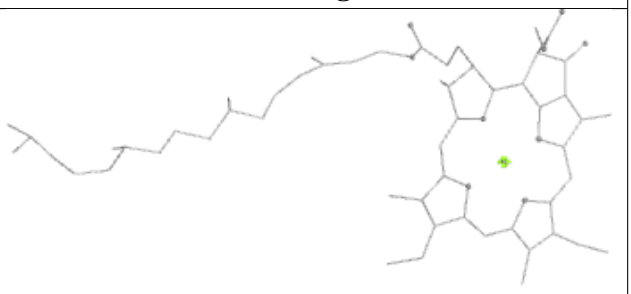
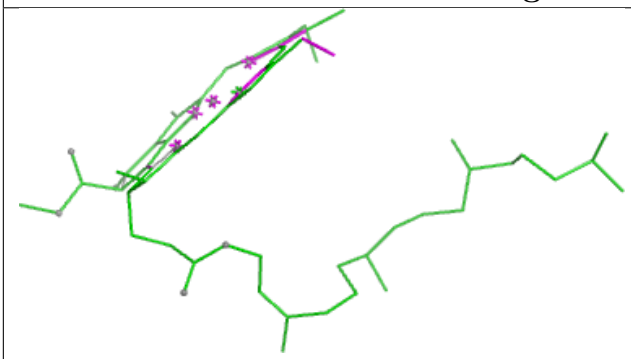


Rings

Ligand CLA G 204



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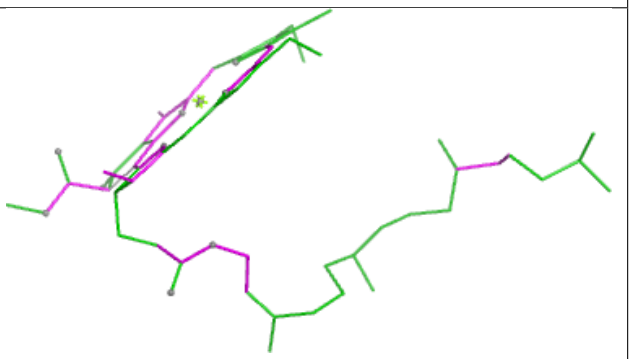
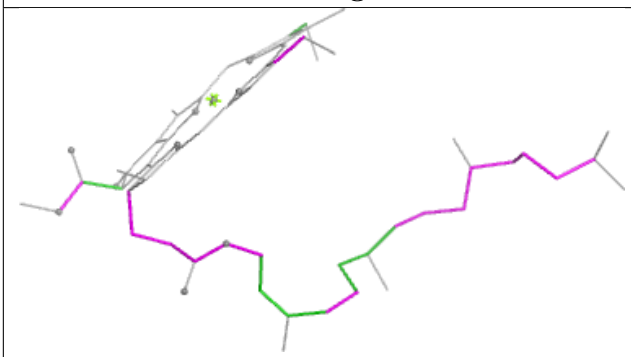


Bond angles



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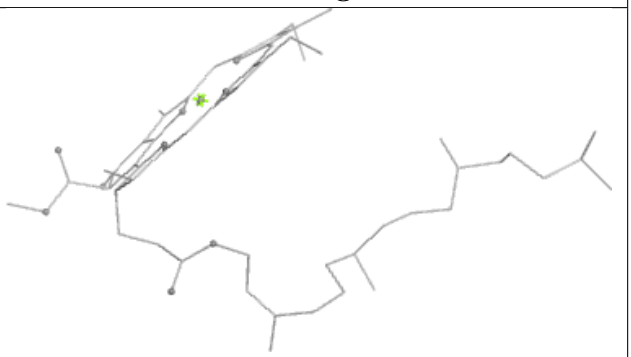
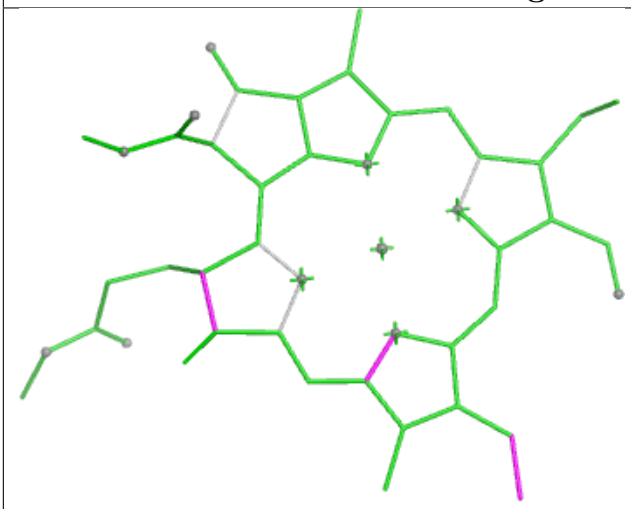


Rings

Ligand CHL 2 512



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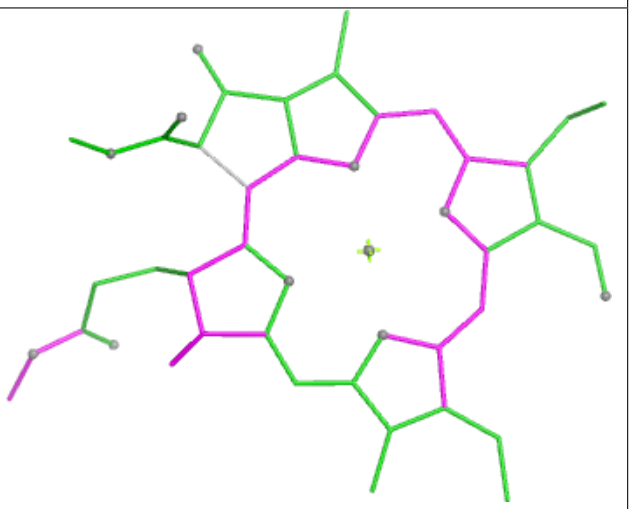
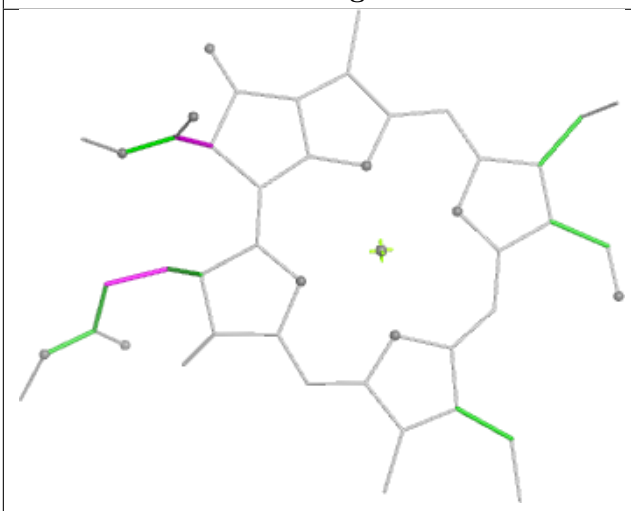


Bond angles



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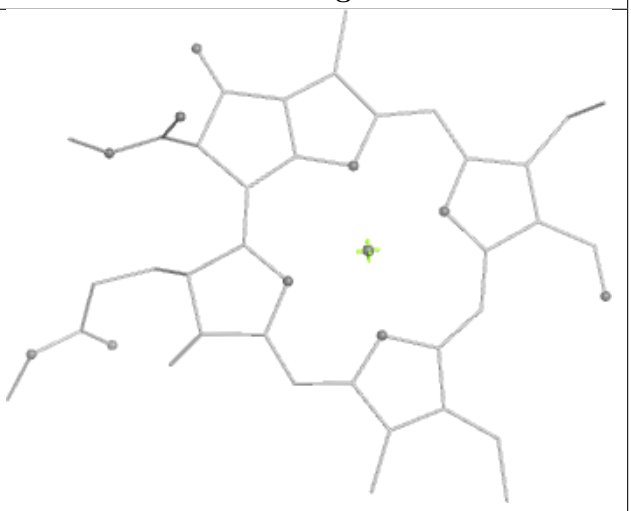
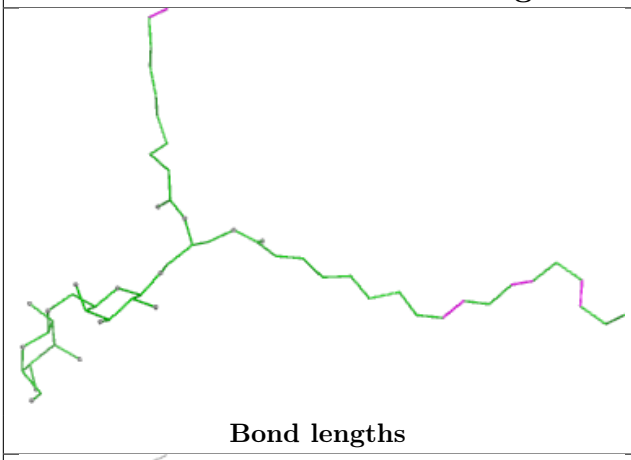


Rings

Ligand DGD J 1106



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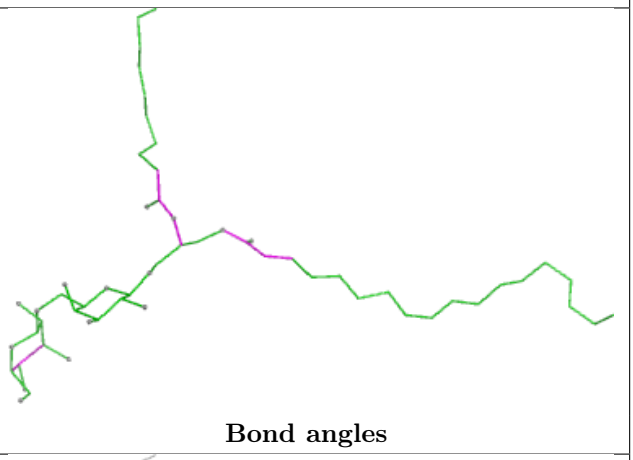
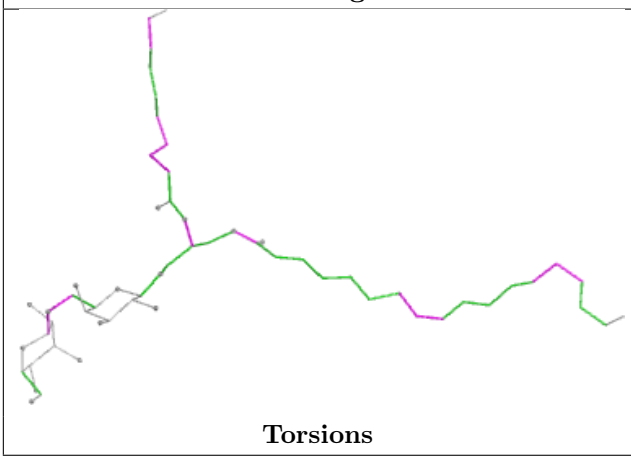


Bond angles



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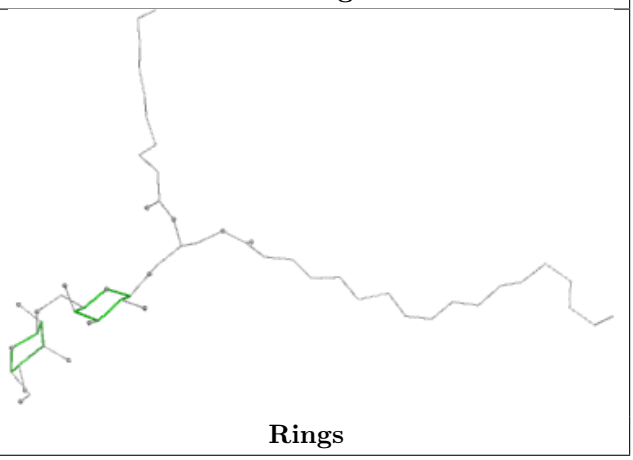
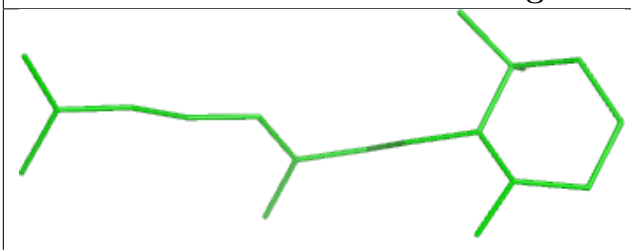


Rings

Ligand BCR 1 503



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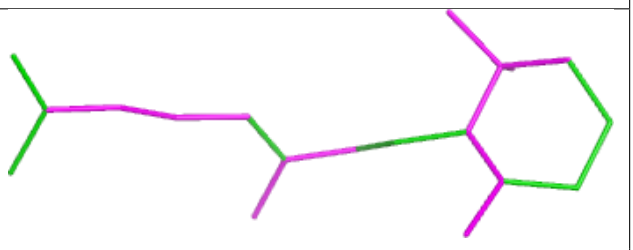
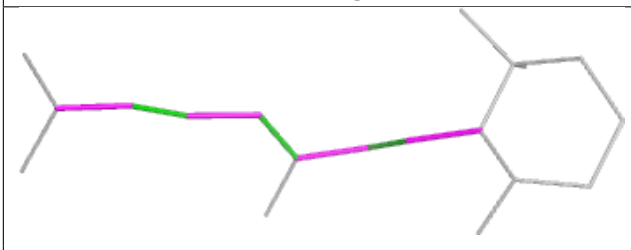


Bond angles



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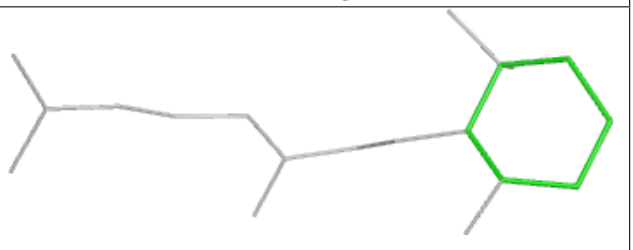
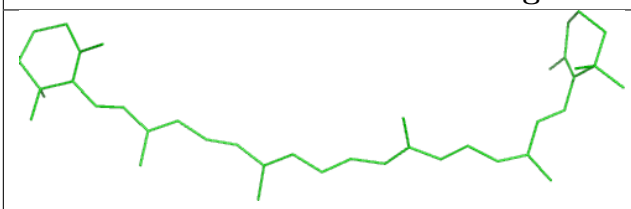


Rings

Ligand BCR B 850



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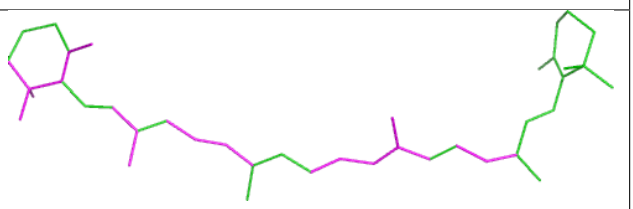
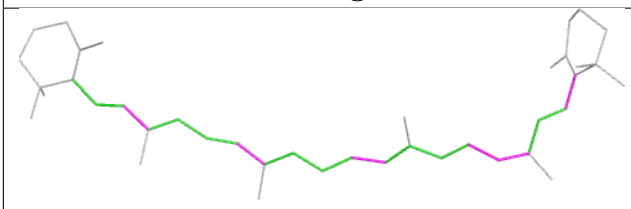


Bond angles



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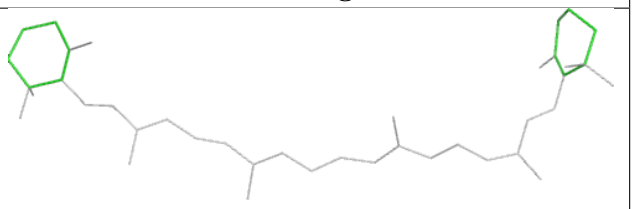
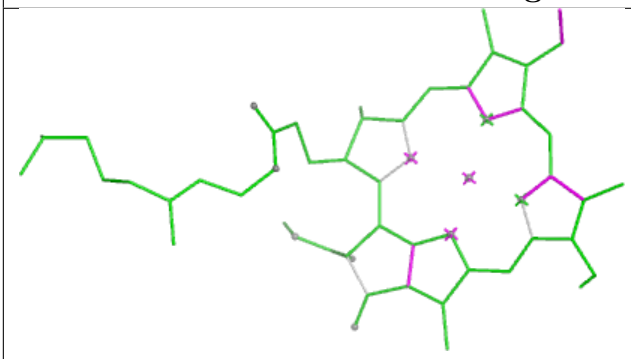


Rings

Ligand CLA B 823



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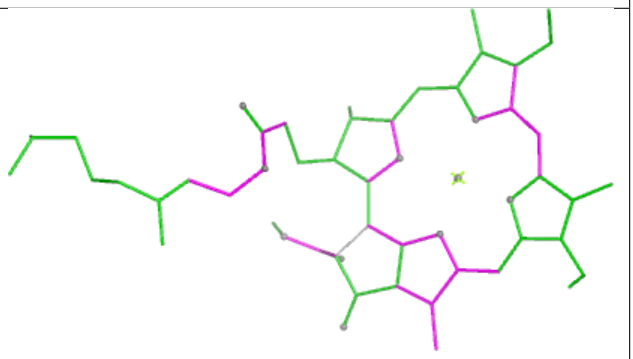
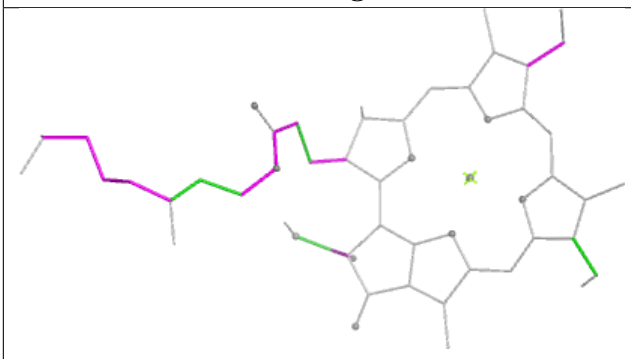


Bond angles



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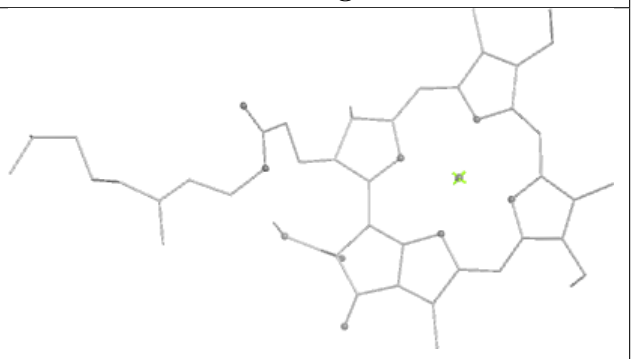
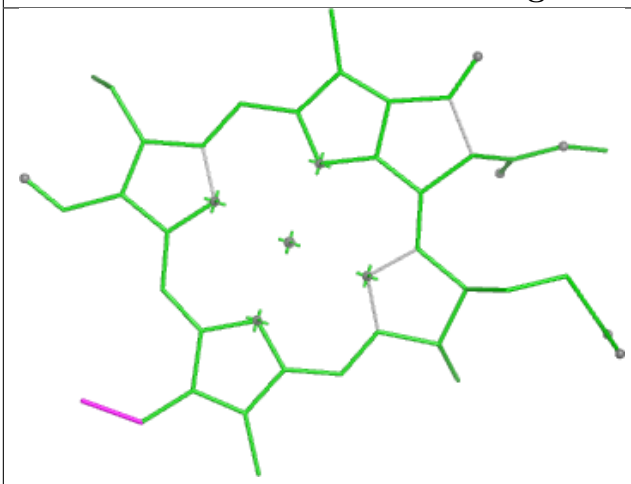


Rings

Ligand CHL 2 515



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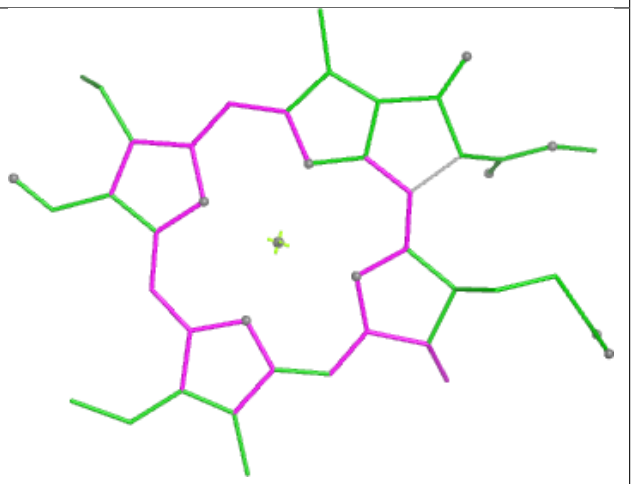
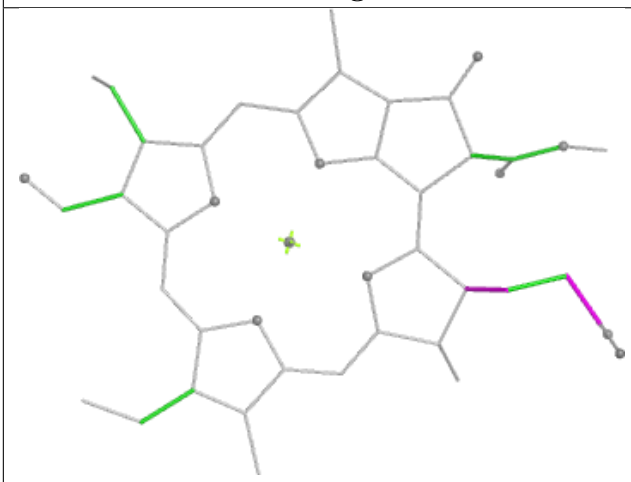


Bond angles



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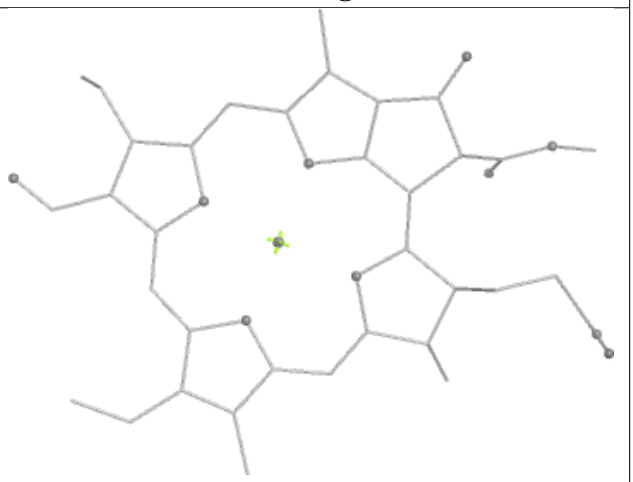
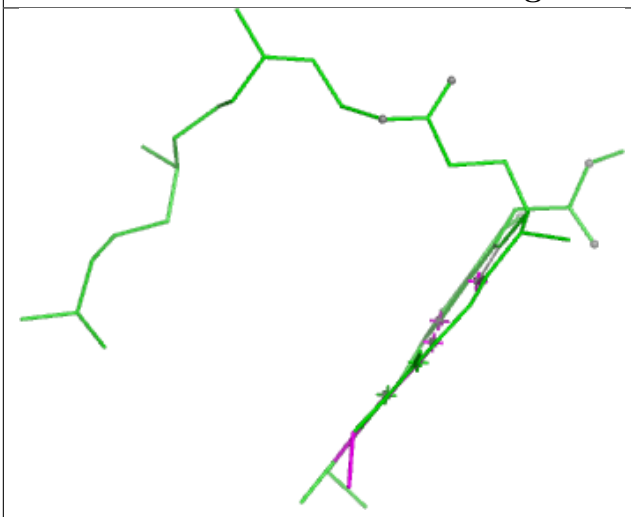
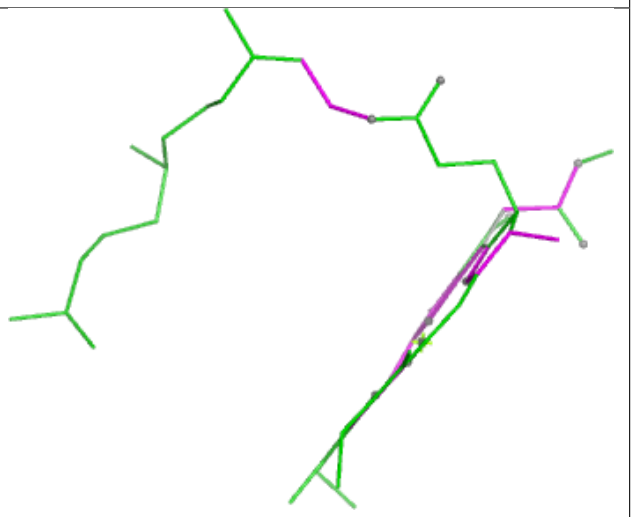


Rings

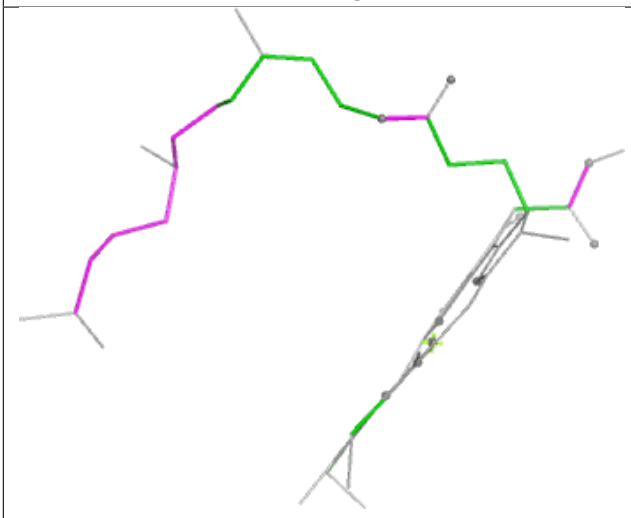
Ligand CLA B 812



Bond lengths



Bond angles



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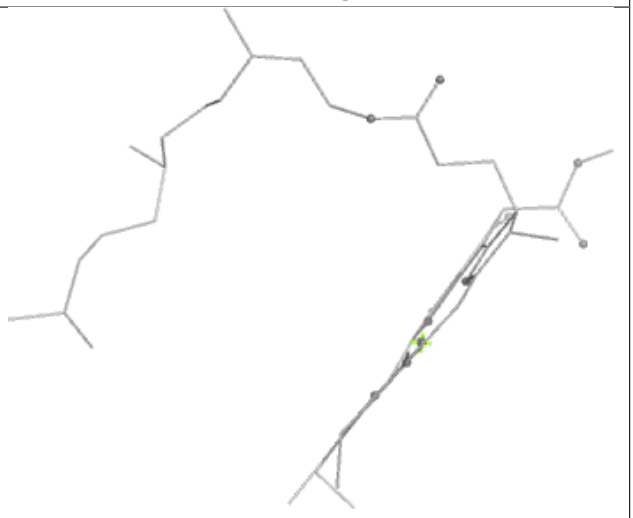
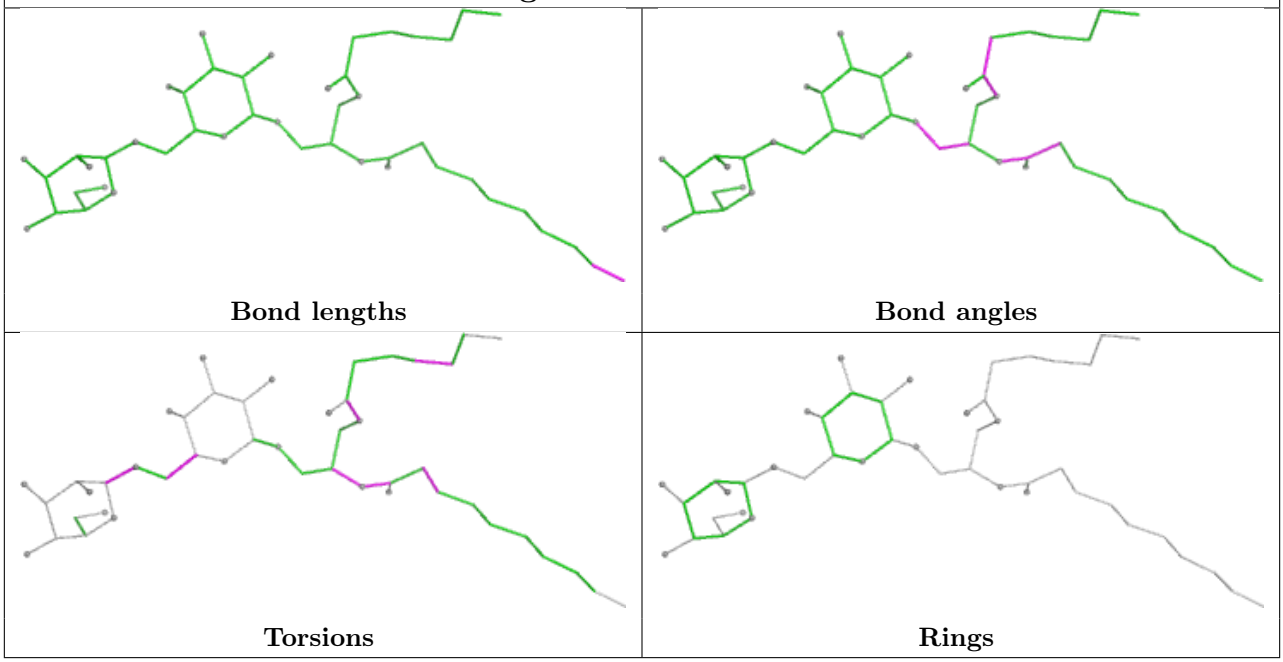
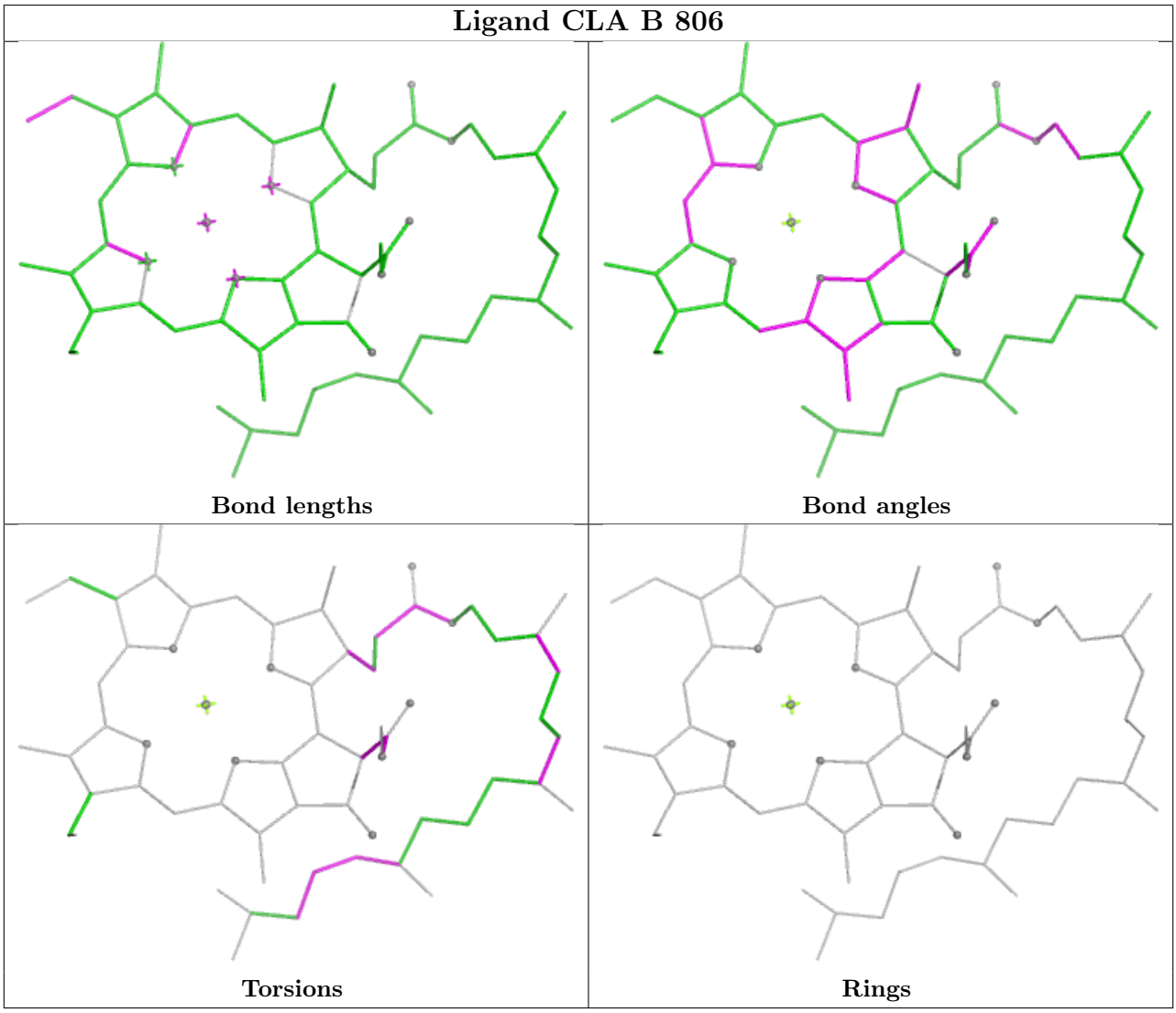


Rings

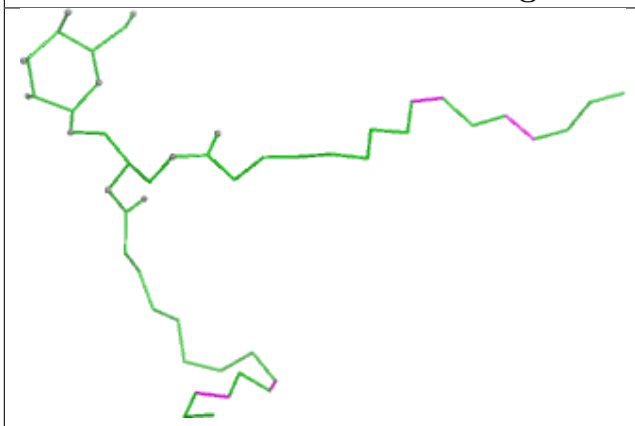
Ligand DGD G 207



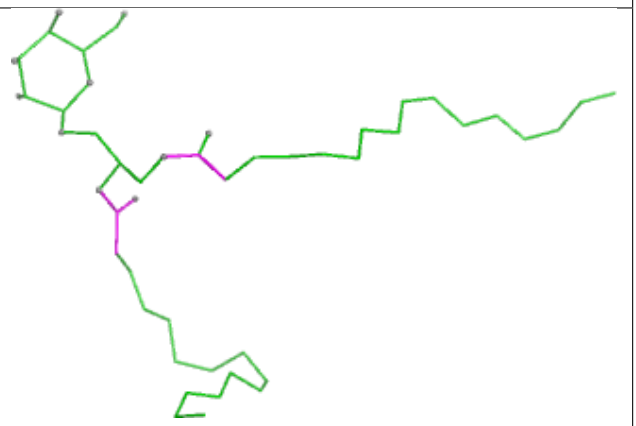
Ligand CLA B 806



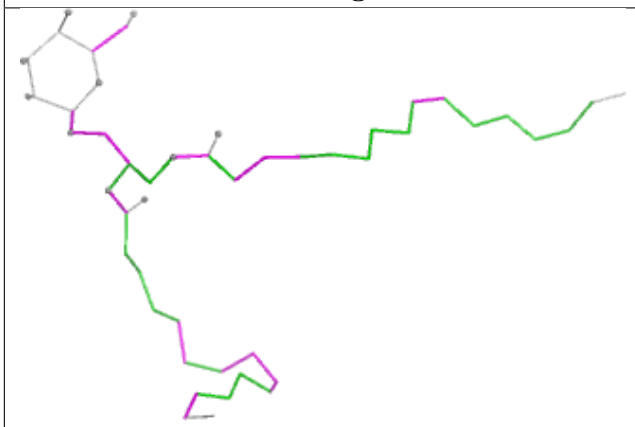
Ligand LMG G 206



Bond lengths



Bond angles

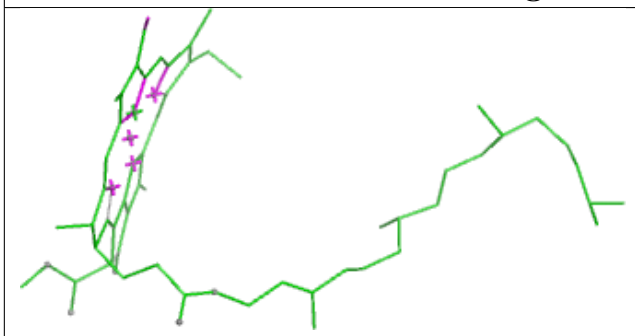


Torsions

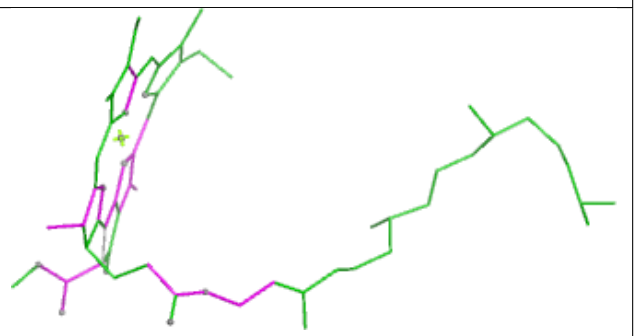


Rings

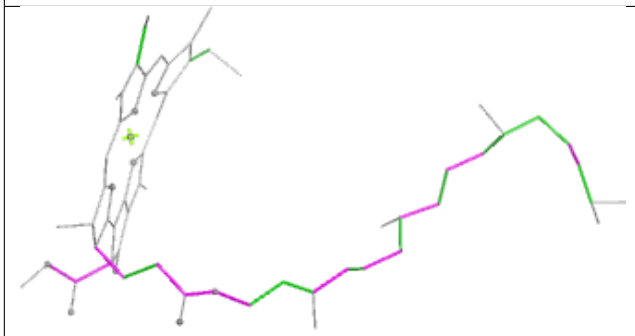
Ligand CLA A 830



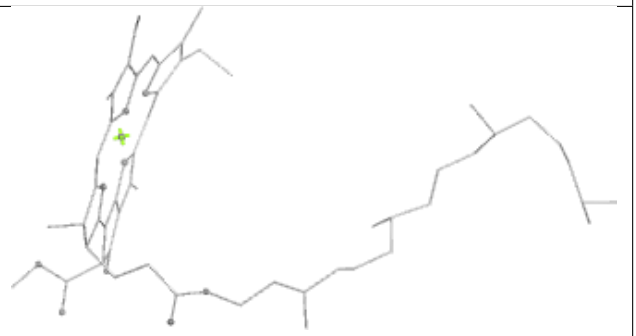
Bond lengths



Bond angles

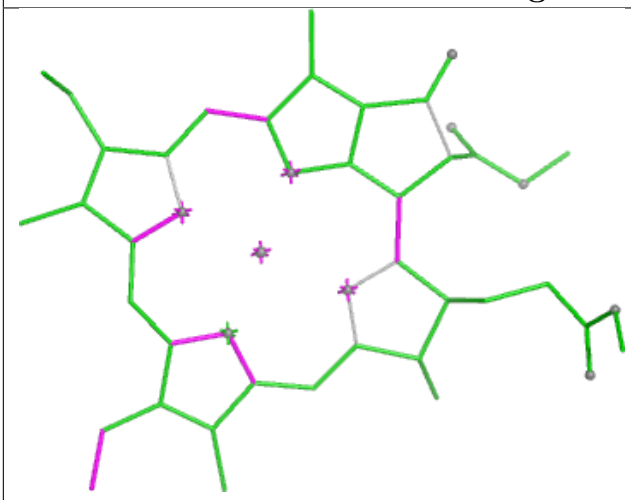


Torsions



Rings

Ligand CLA 3 316



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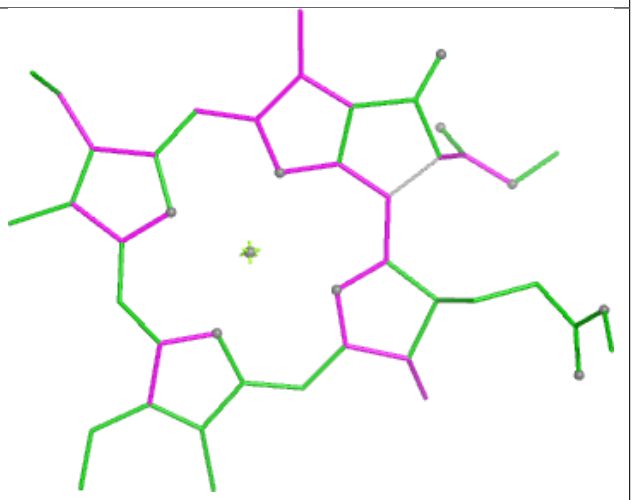
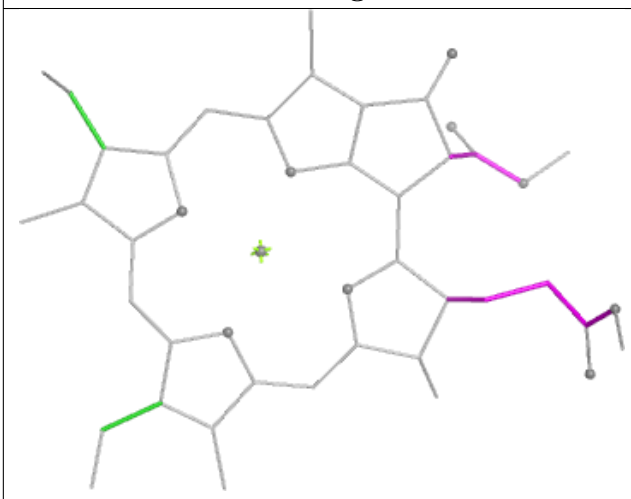


Bond angles



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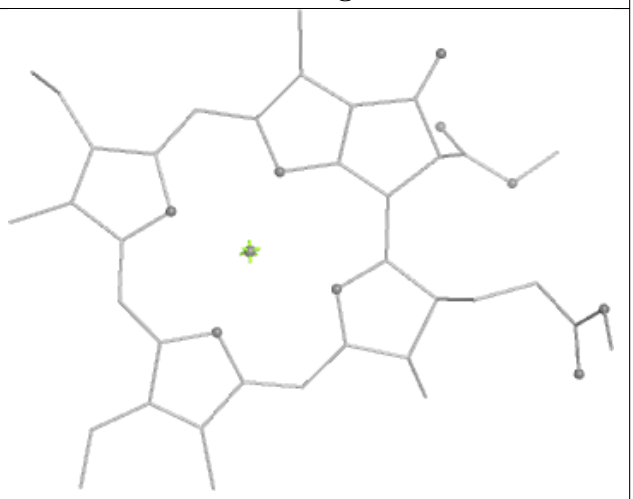
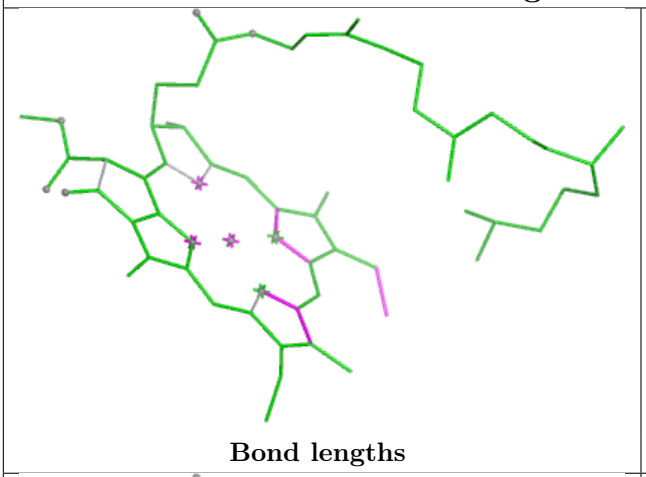


Rings

Ligand CLA A 824



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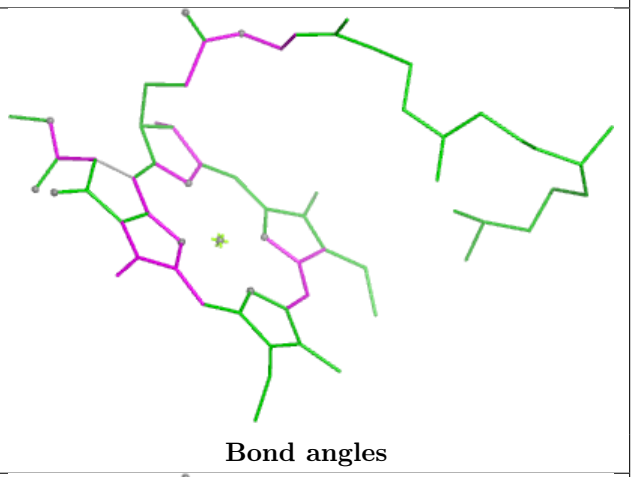

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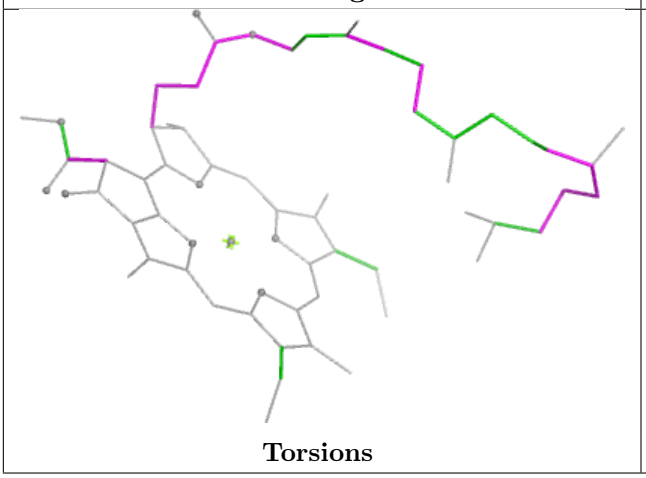

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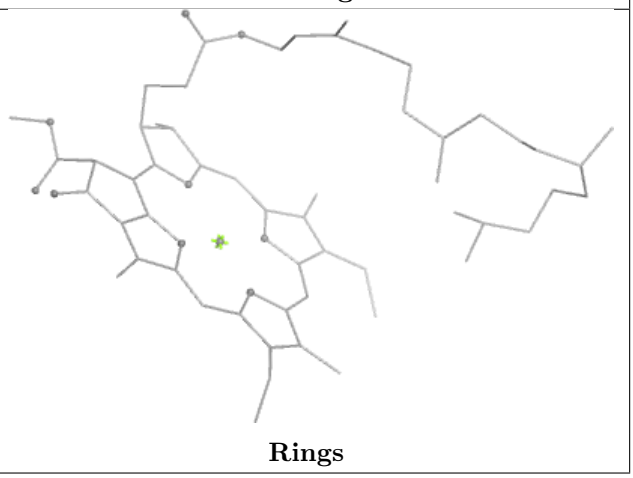
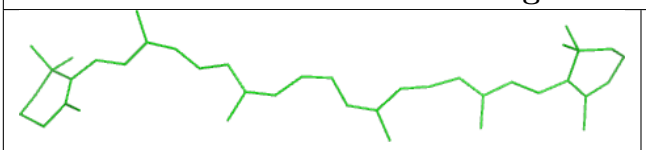


Rings

Ligand BCR B 849



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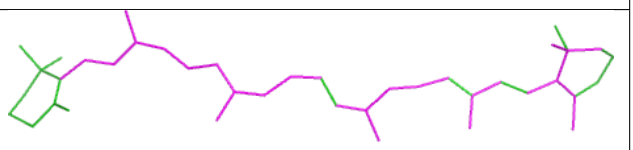
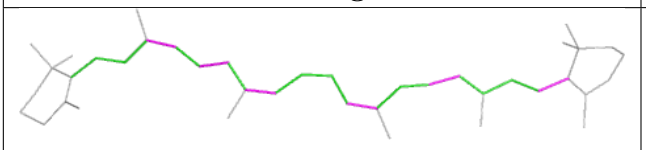


Bond angles



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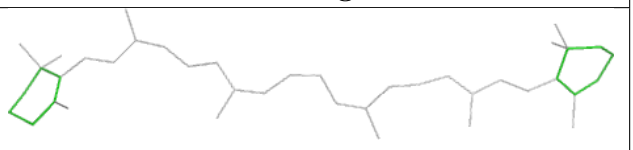
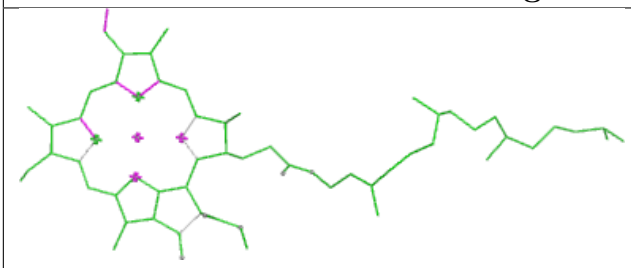


Rings

Ligand CLA A 832



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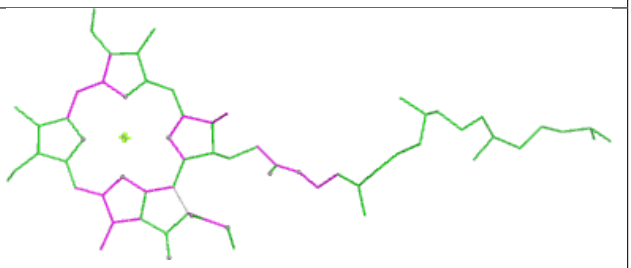
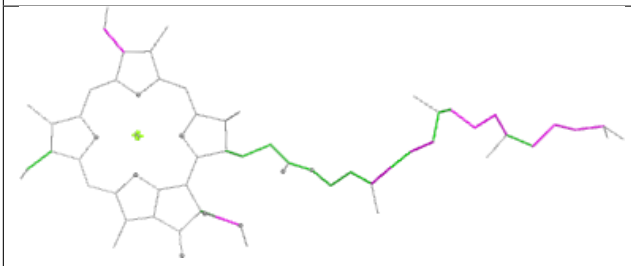


Bond angles



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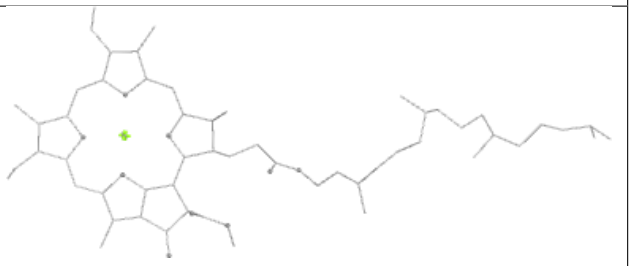
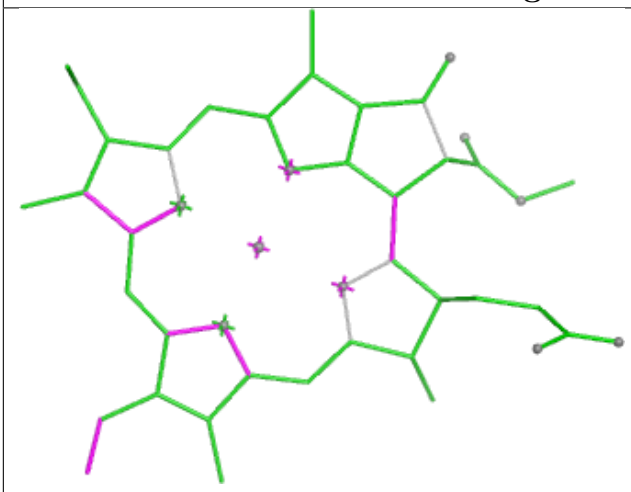


Rings

Ligand CLA A 815



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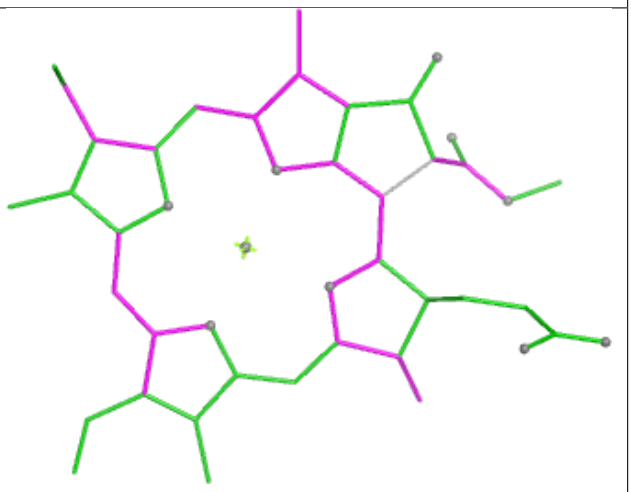
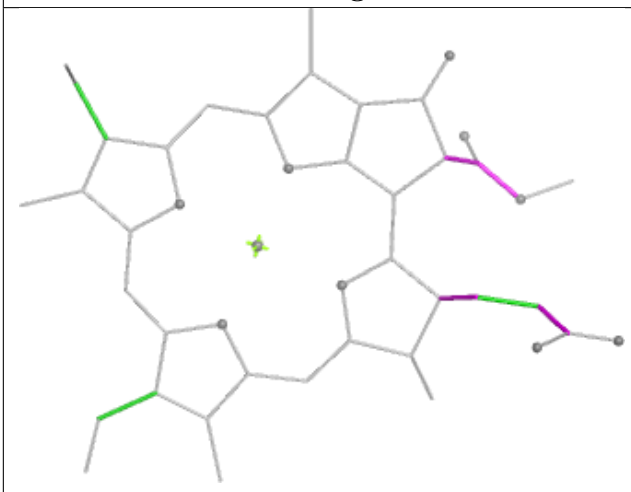


Bond angles



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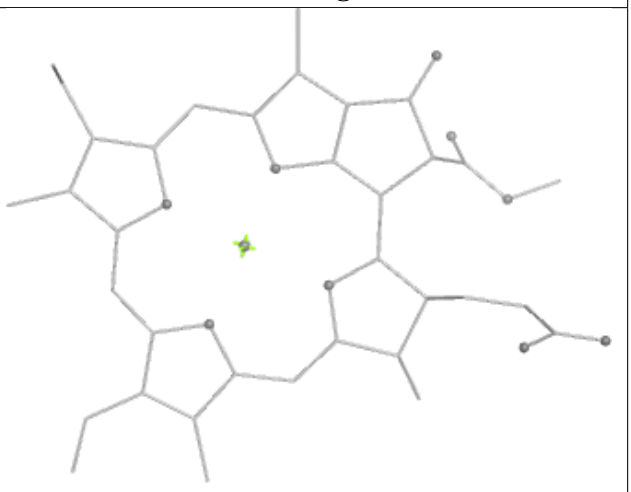
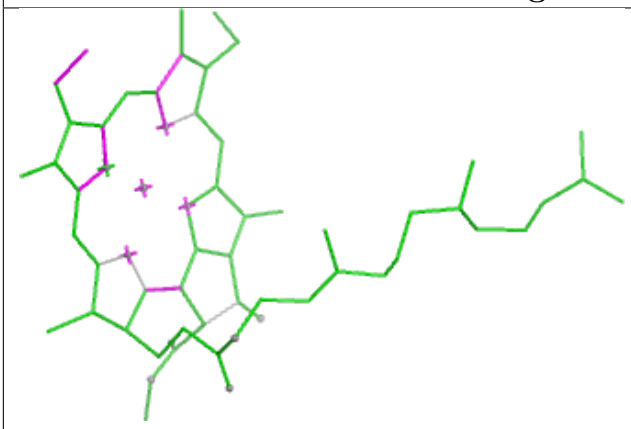


Rings

Ligand CLA 4 310



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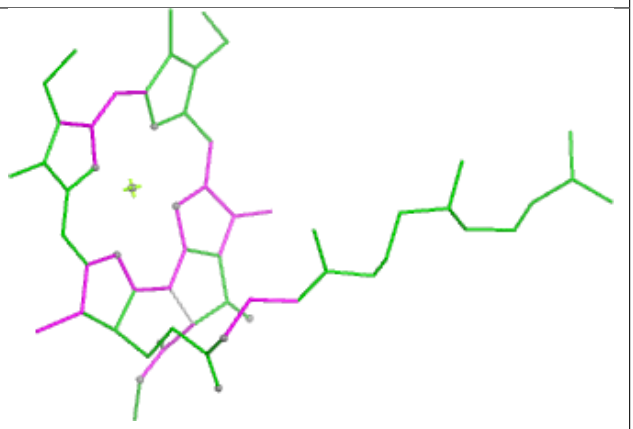
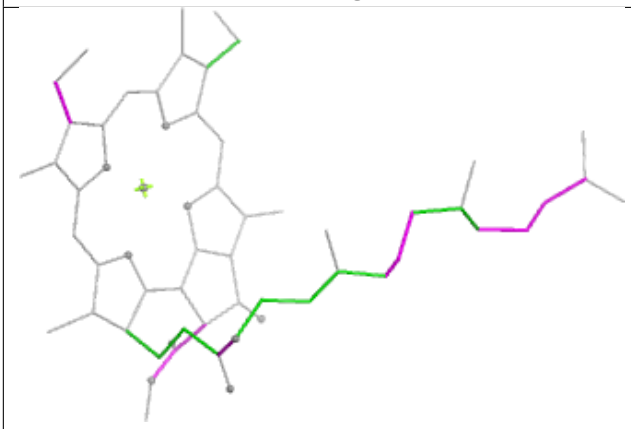


Bond angles



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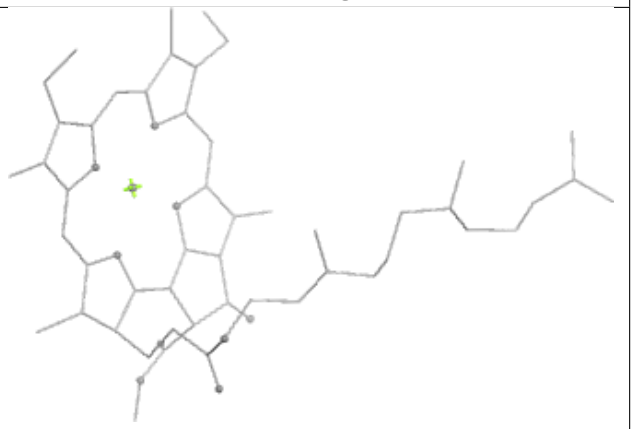
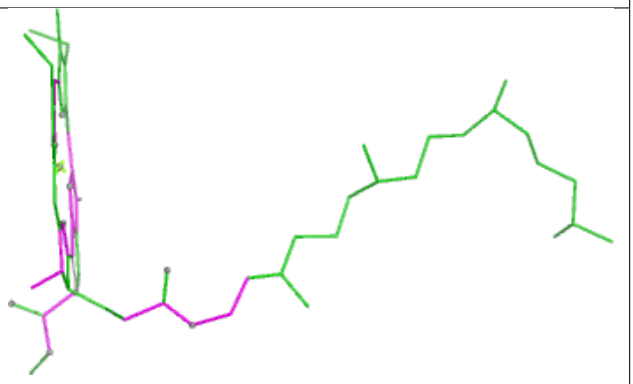


Rings

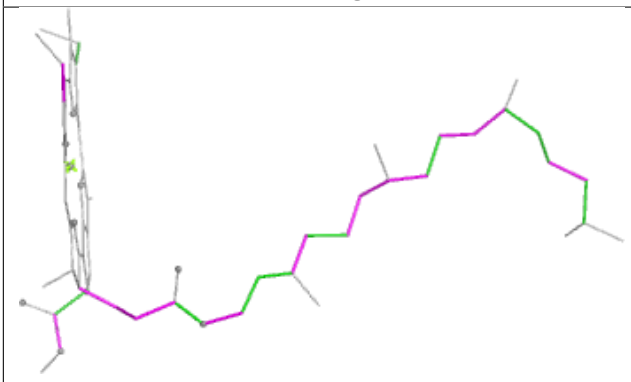
Ligand CLA B 839



Bond lengths



Bond angles



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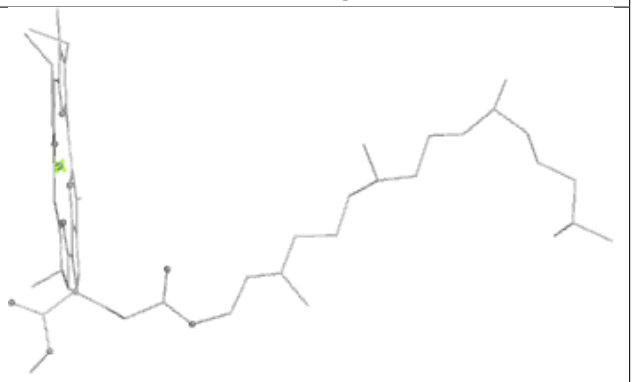
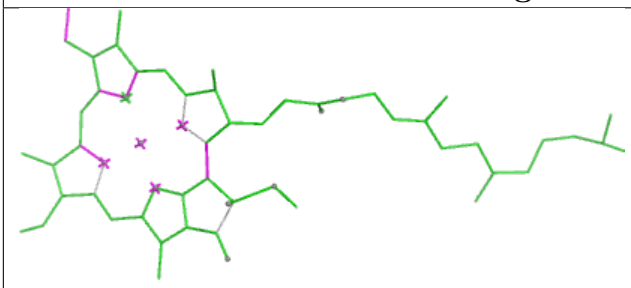


Rings

Ligand CLA H 1000



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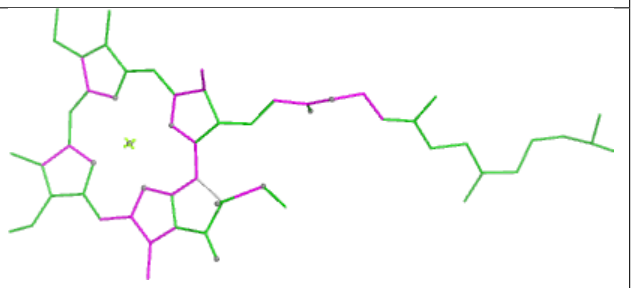
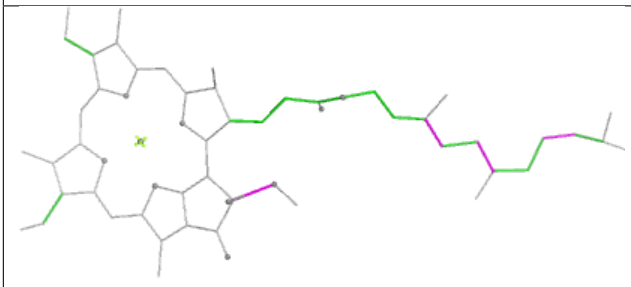


Bond angles



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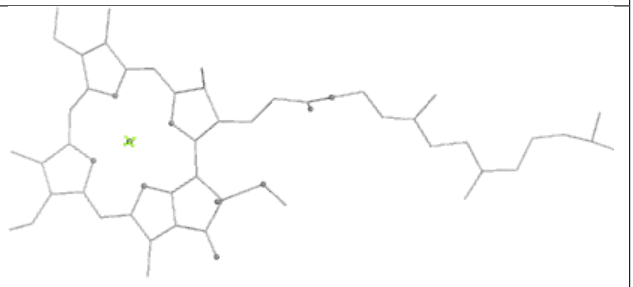
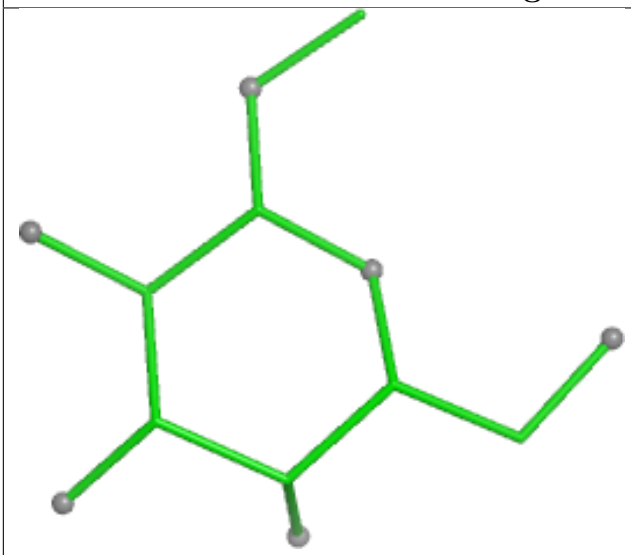


Rings

Ligand LMG 1 519



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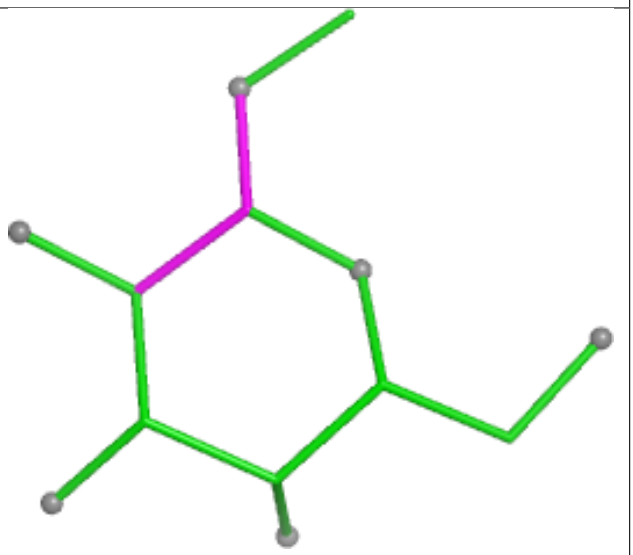
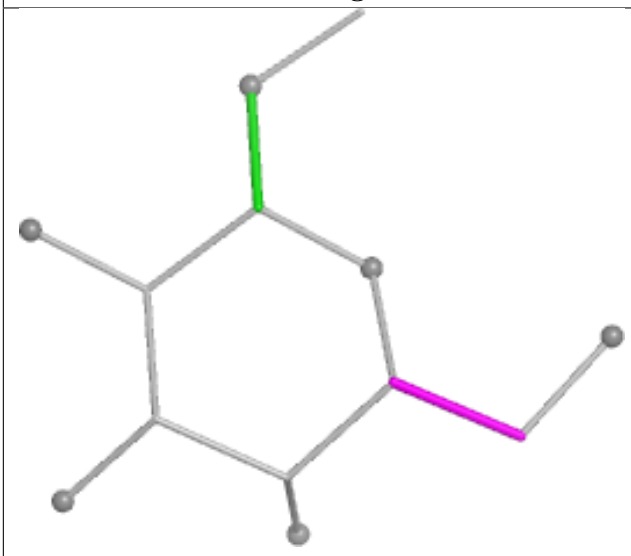


Bond angles



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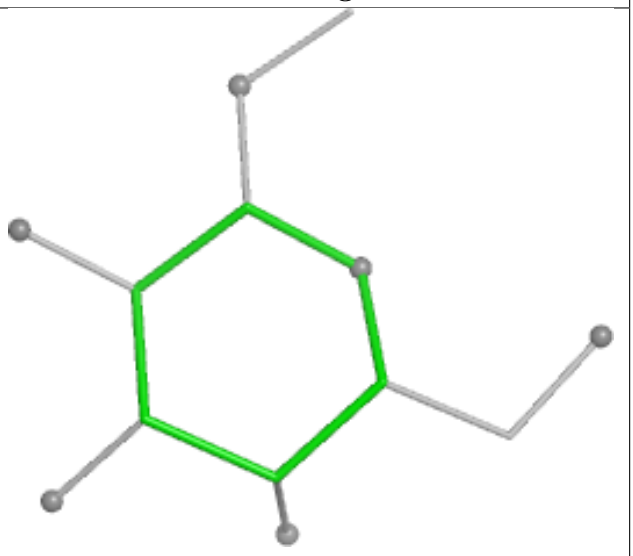
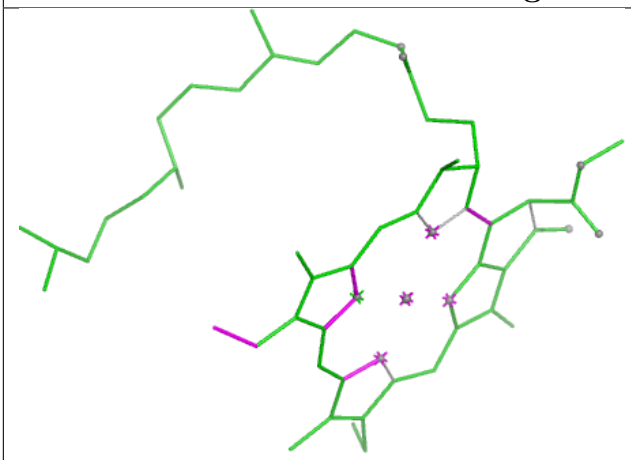


Rings

Ligand CLA A 842



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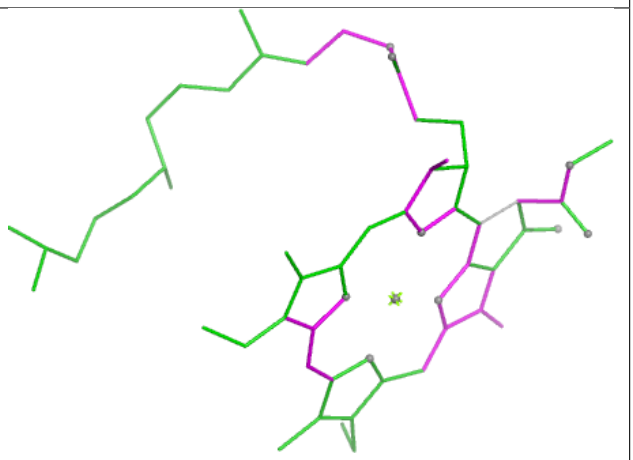
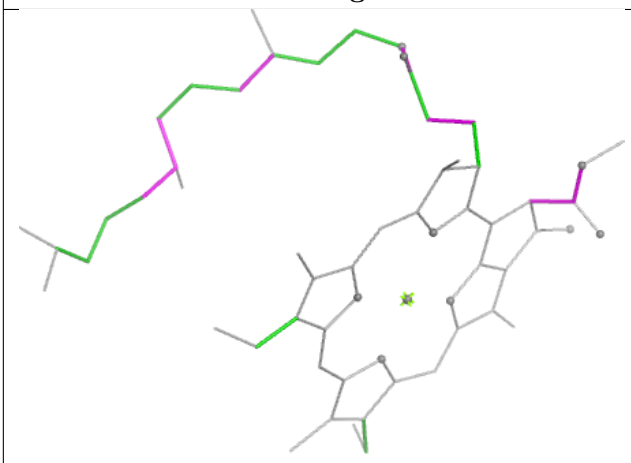


Bond angles

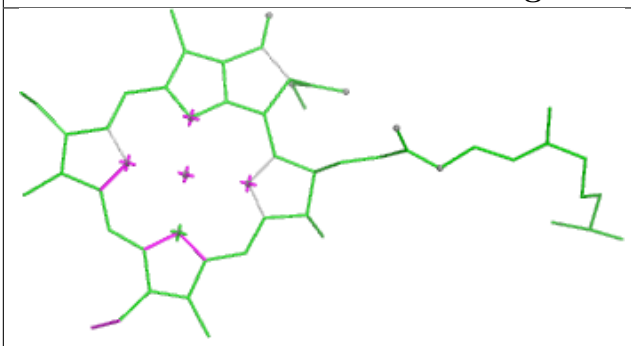


Torsions



Rings

Ligand CLA B 835



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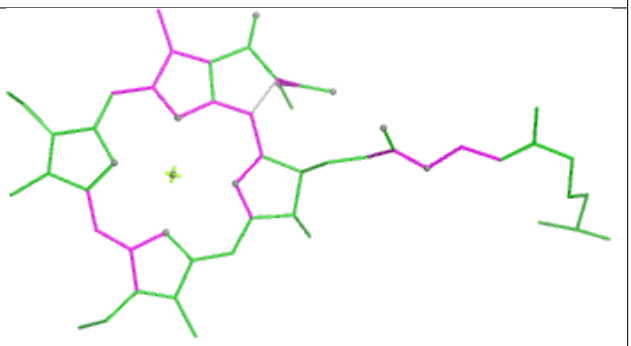
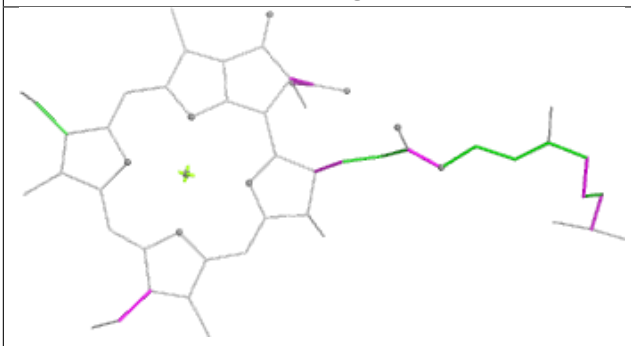


Bond angles



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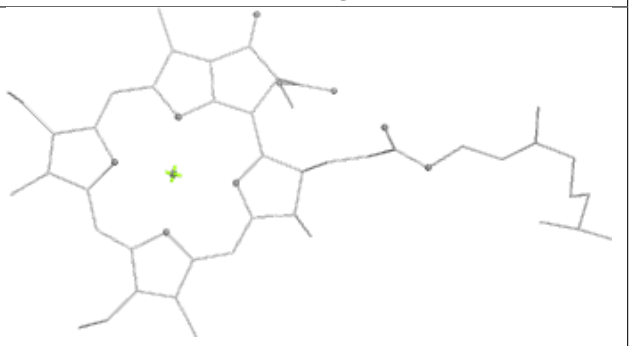
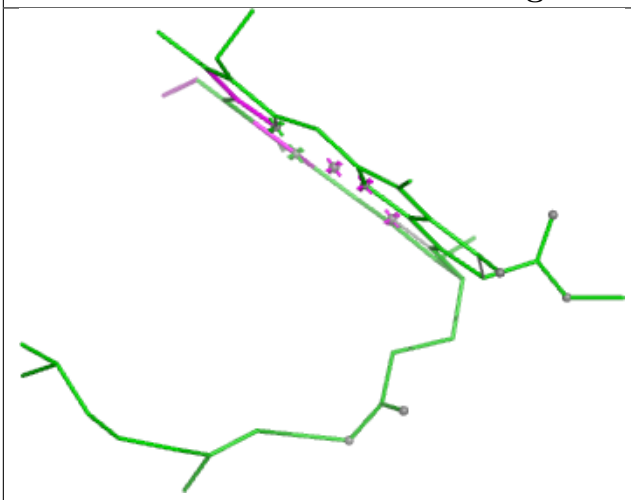


Rings

Ligand CLA L 301



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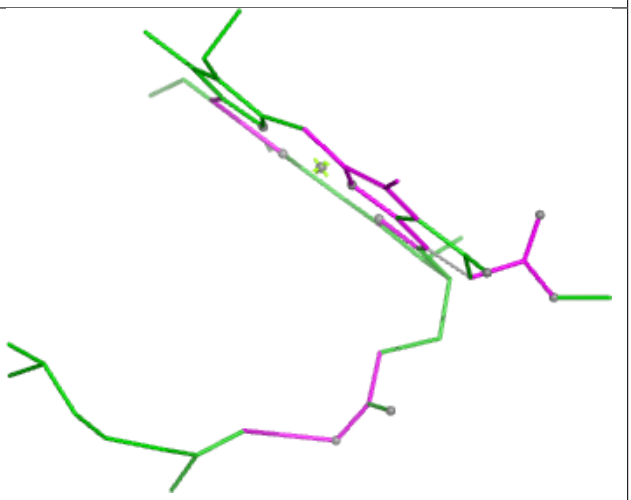
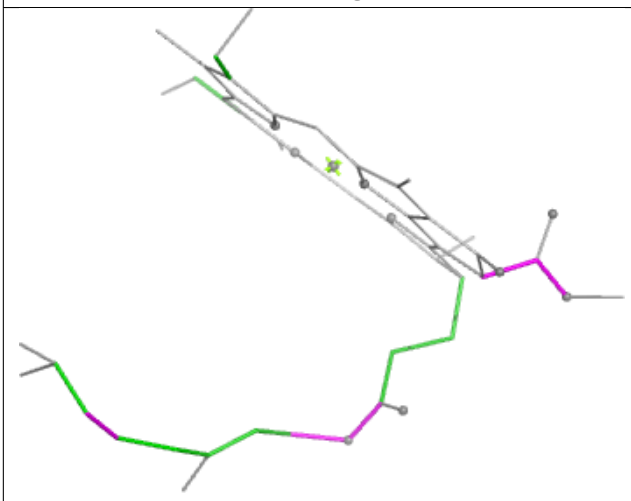


Bond angles

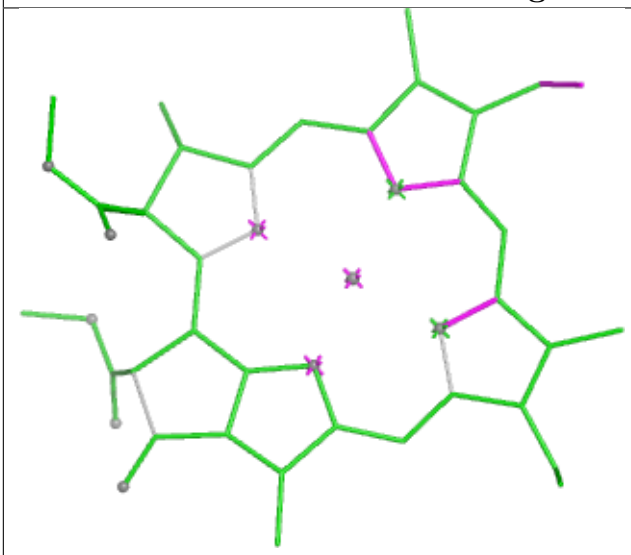


Torsions



Rings

Ligand CLA 1 511



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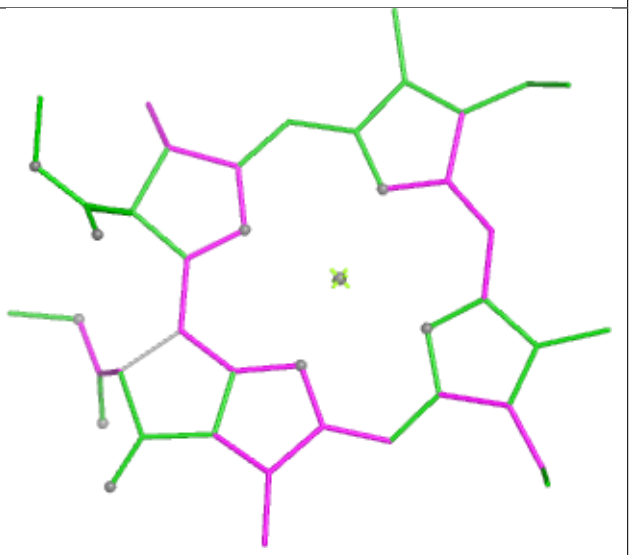
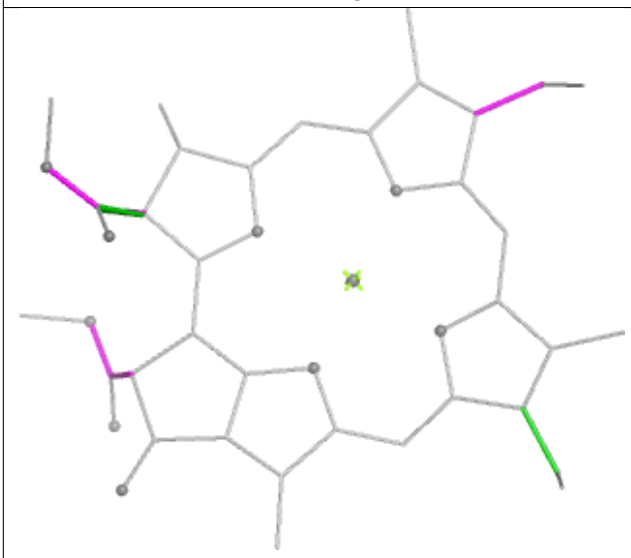
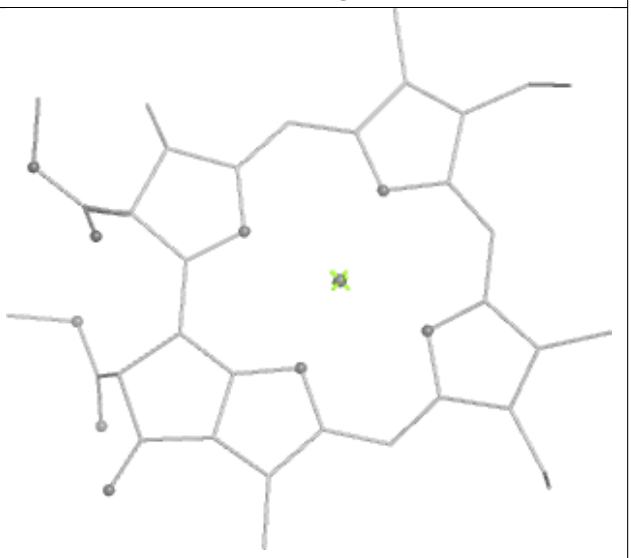


Bond angles

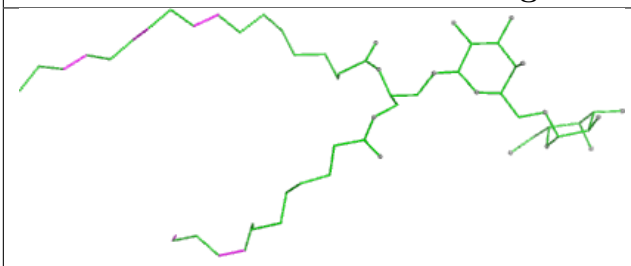


Torsions

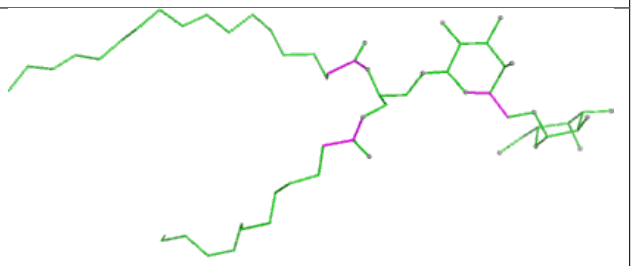


Rings

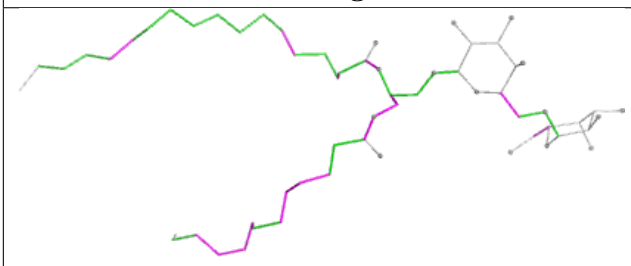
Ligand DGD B 854



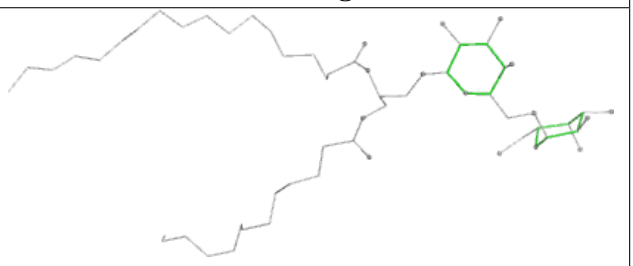
Bond lengths



Bond angles

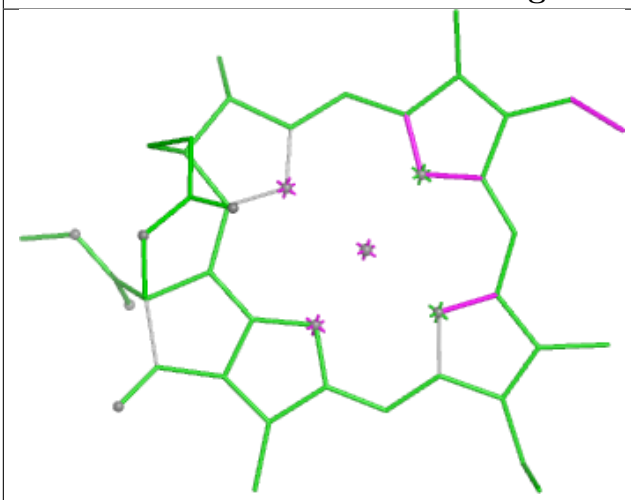


Torsions



Rings

Ligand CLA 4 311



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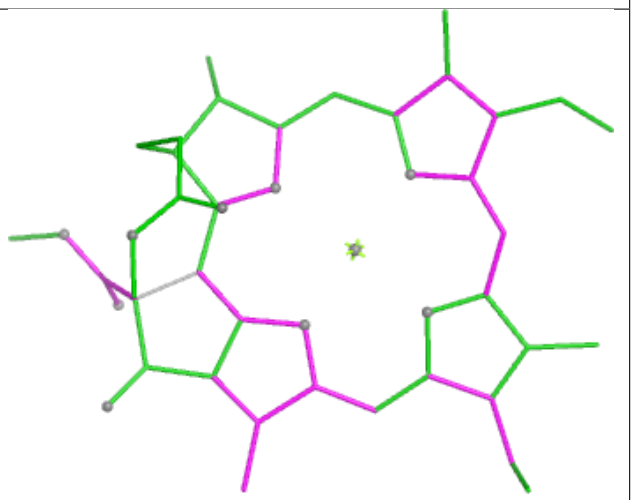
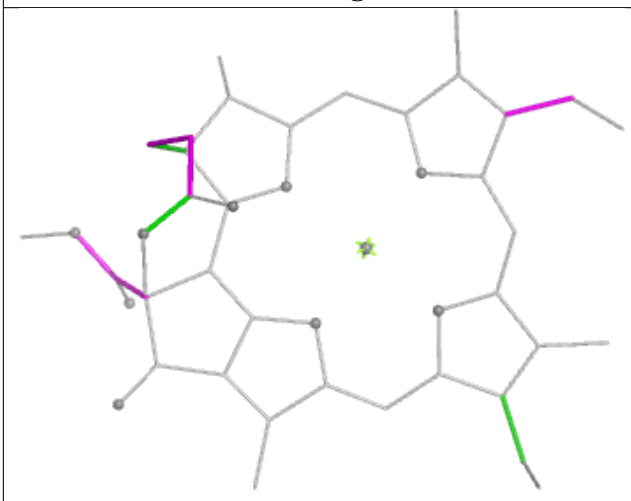


Bond angles



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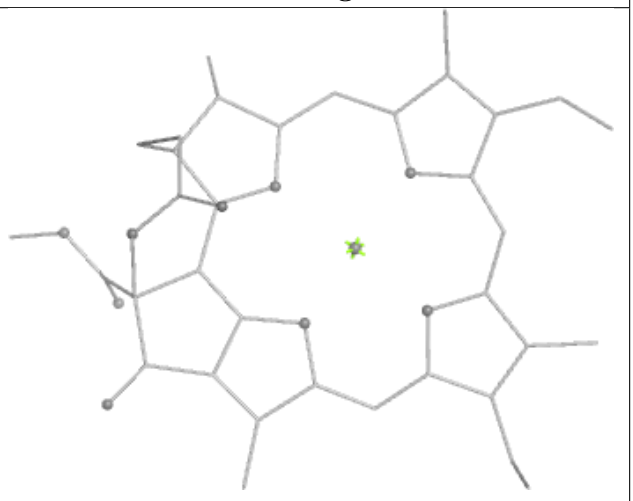
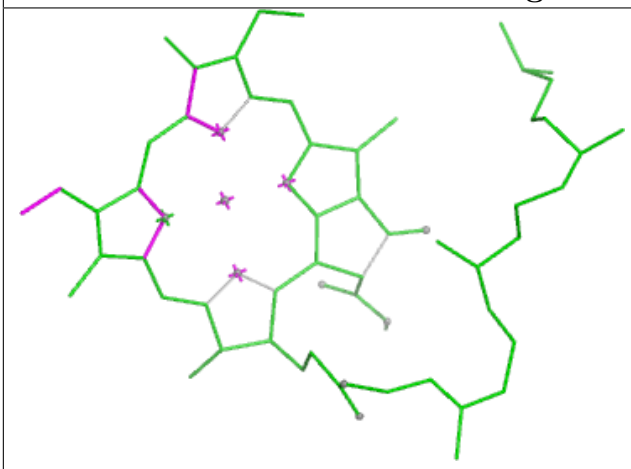


Rings

Ligand CLA F 302



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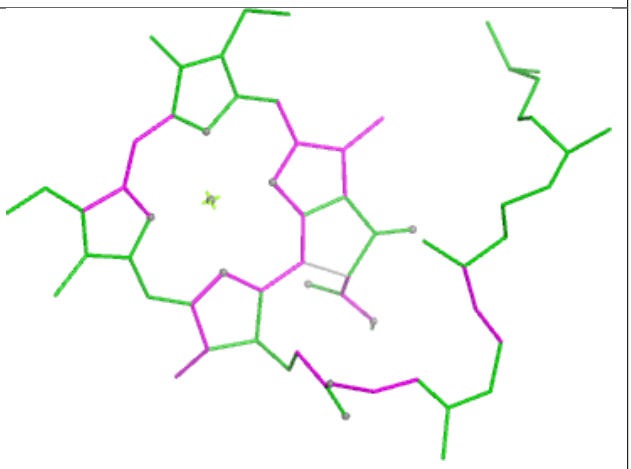
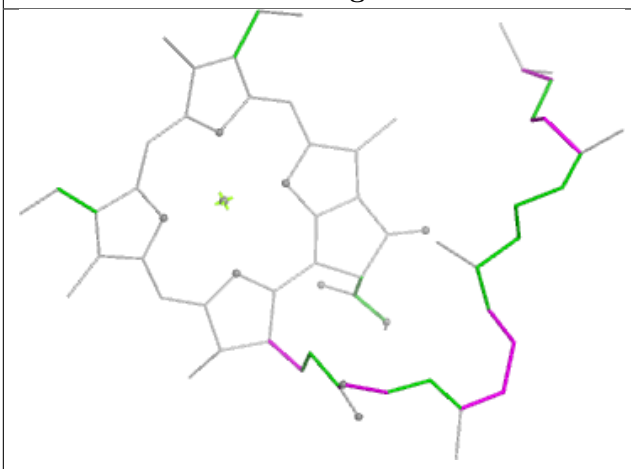


Bond angles



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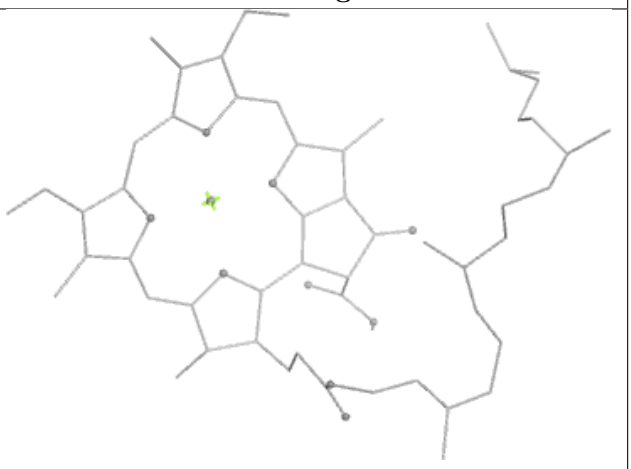
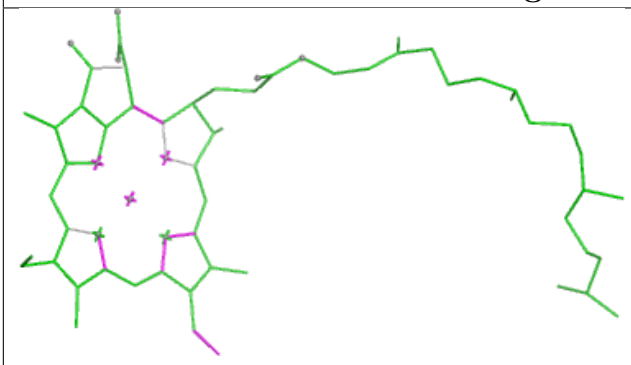
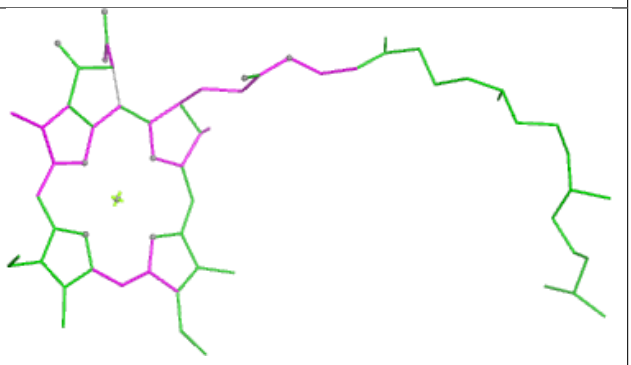


Rings

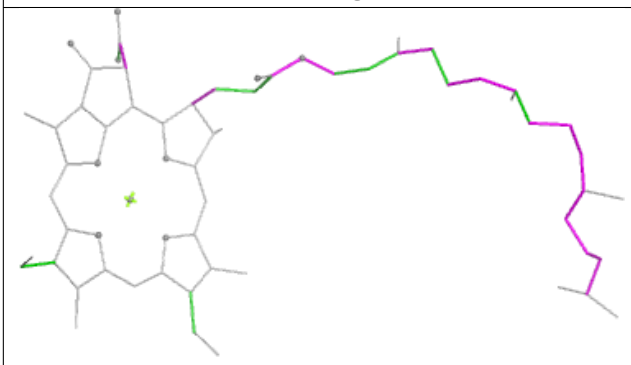
Ligand CLA B 825



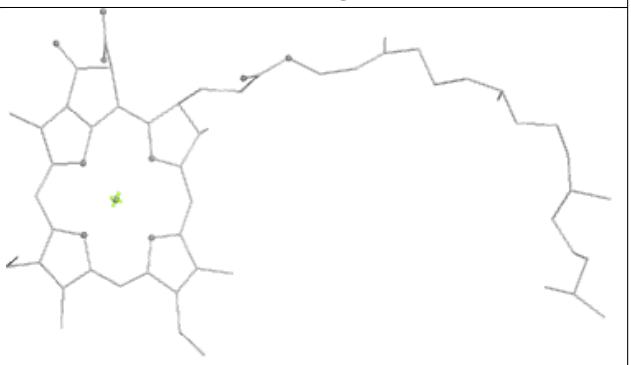
Bond lengths



Bond angles

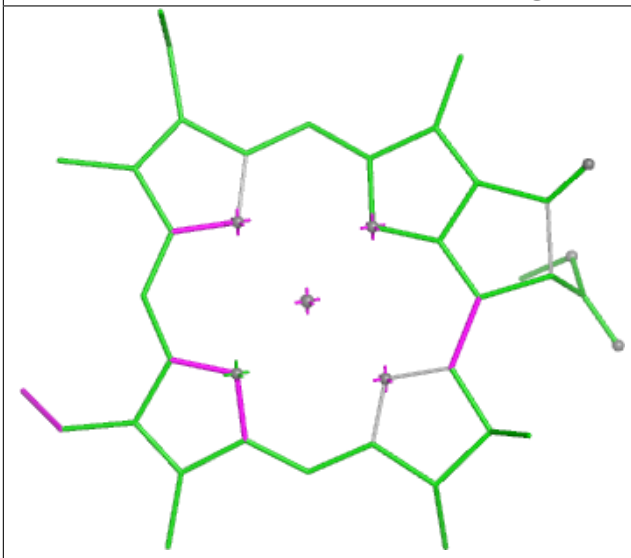


Torsions



Rings

Ligand CLA 3 311



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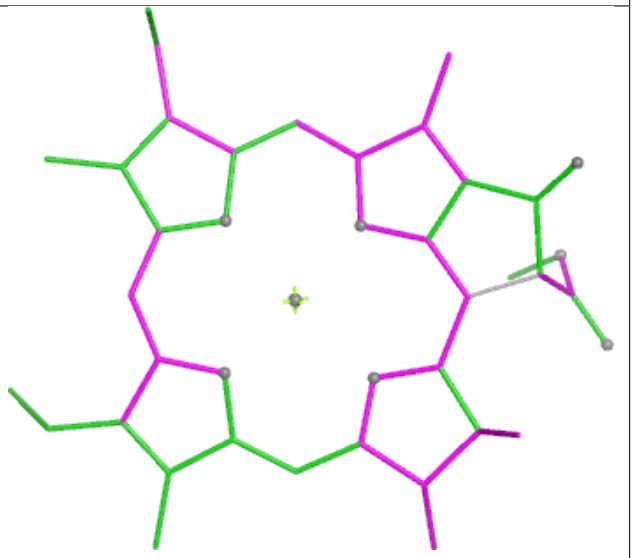
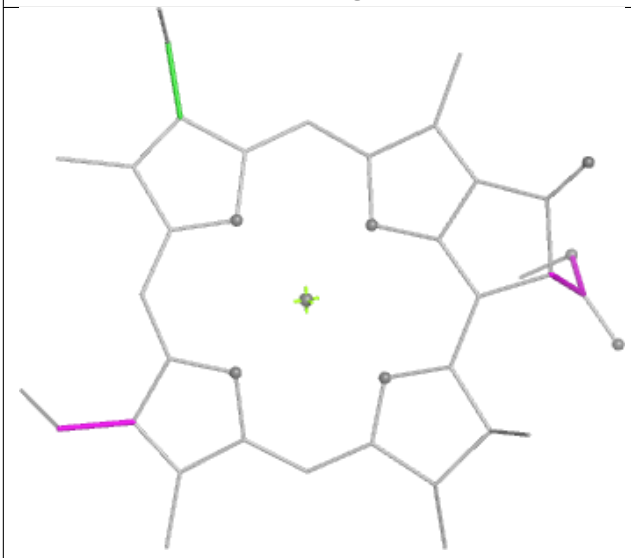


Bond angles



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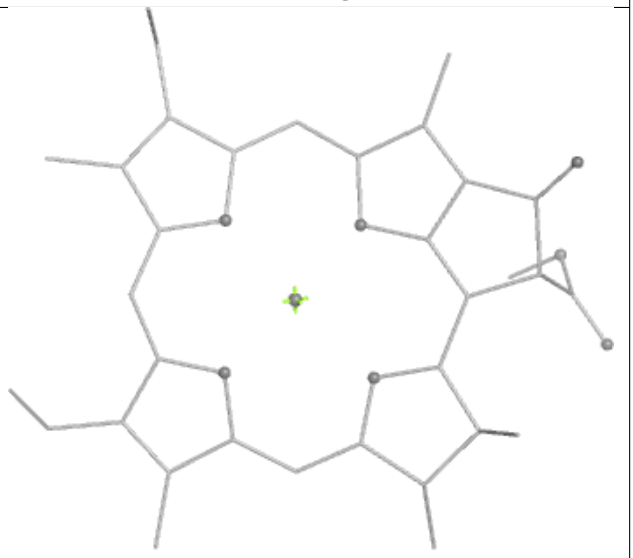
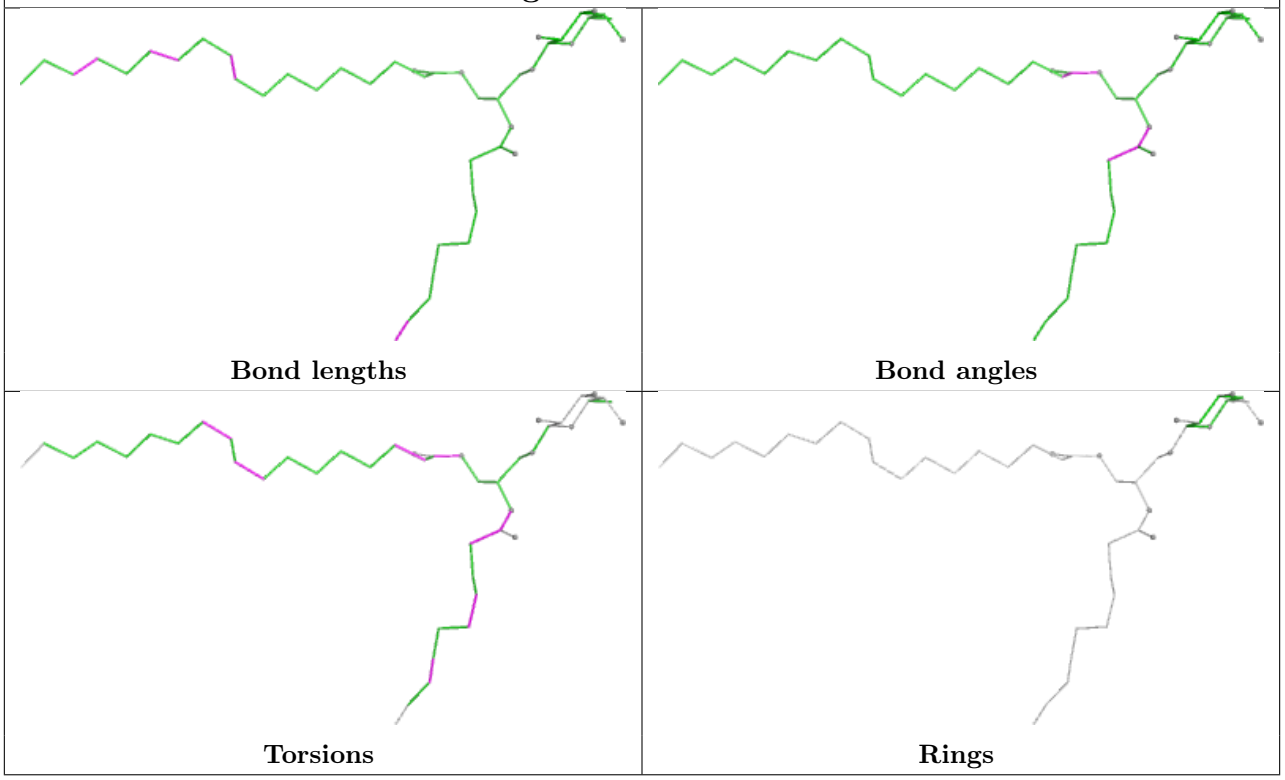
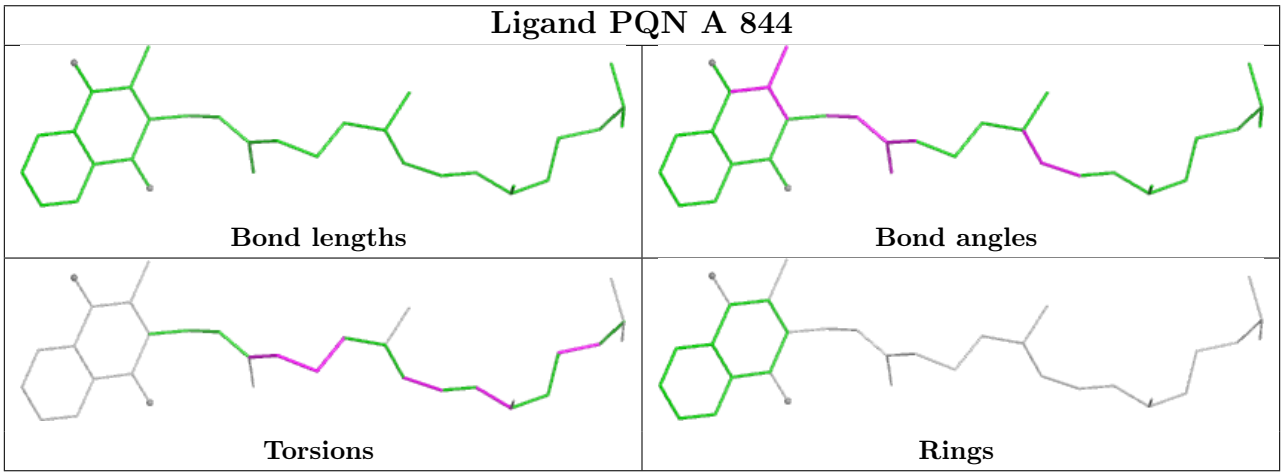


Rings

Ligand LMG F 304



Ligand PQN A 844



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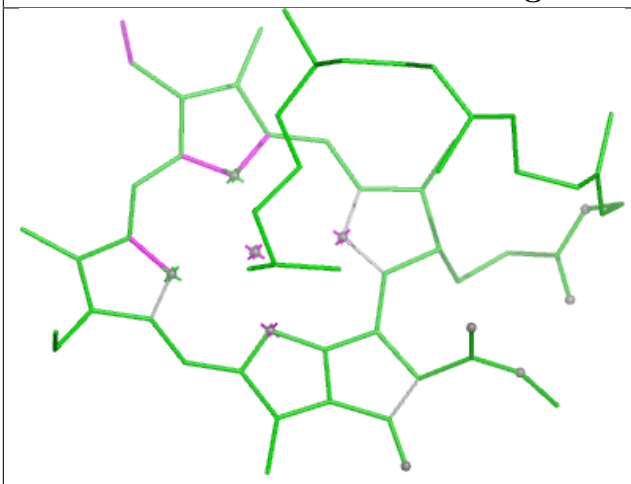

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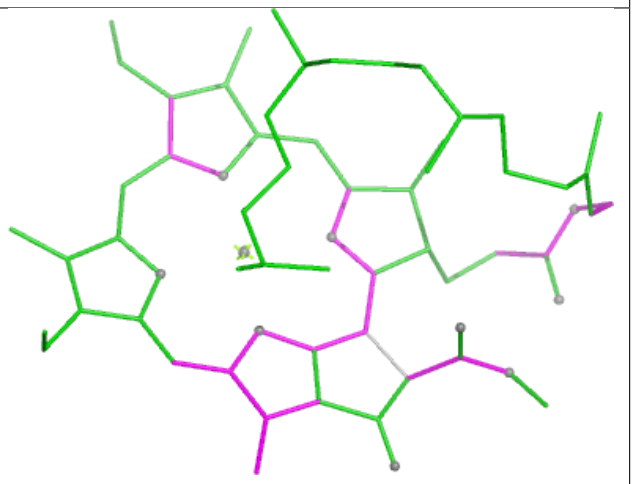
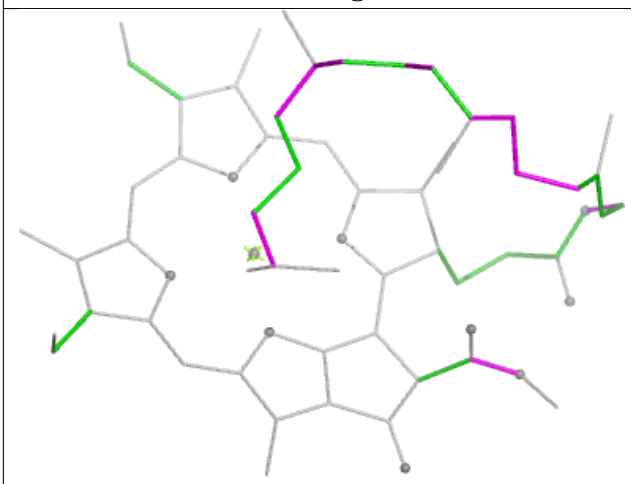


Bond angles



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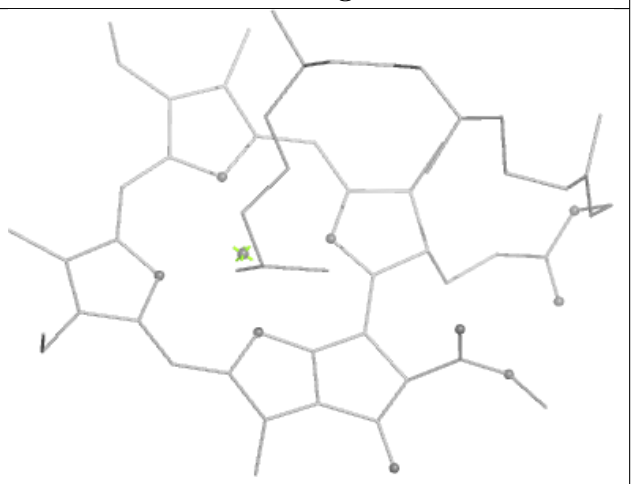
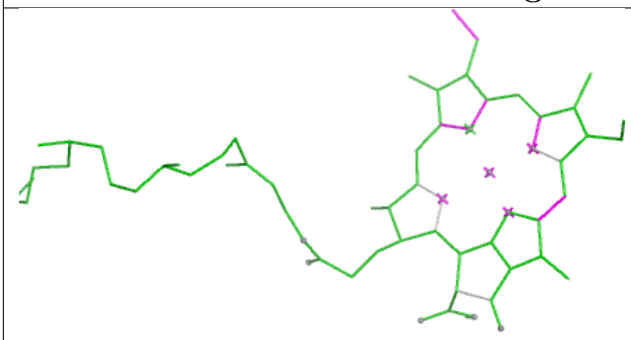


Rings

Ligand CLA B 814



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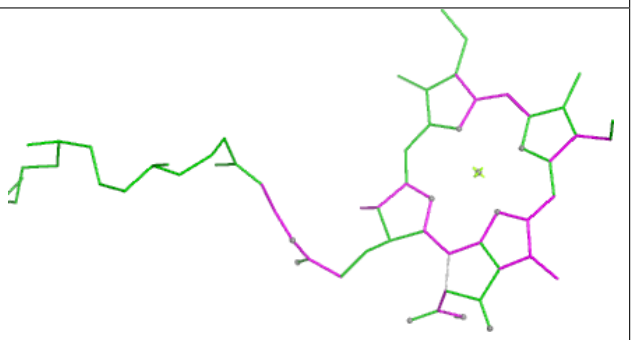
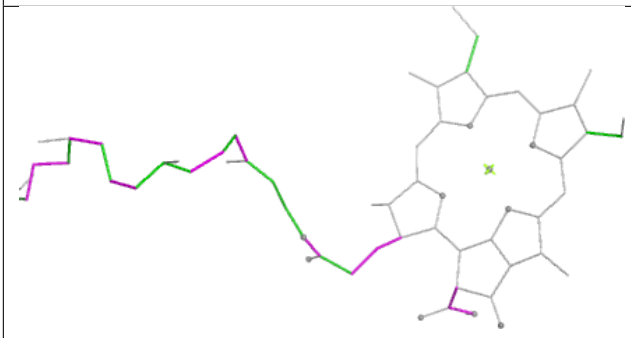


Bond angles



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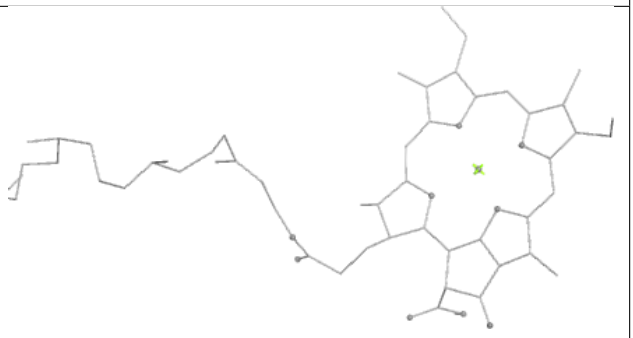
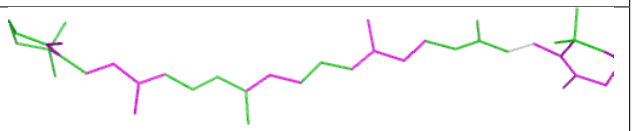


Rings

Ligand LUT 1 501



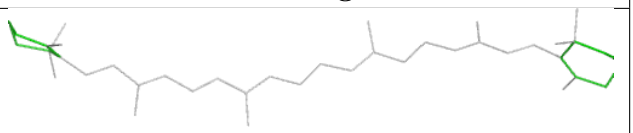
Bond lengths



Bond angles

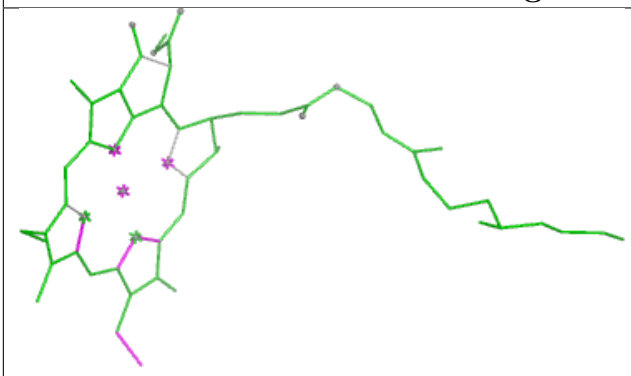


Torsions



Rings

Ligand CLA B 832



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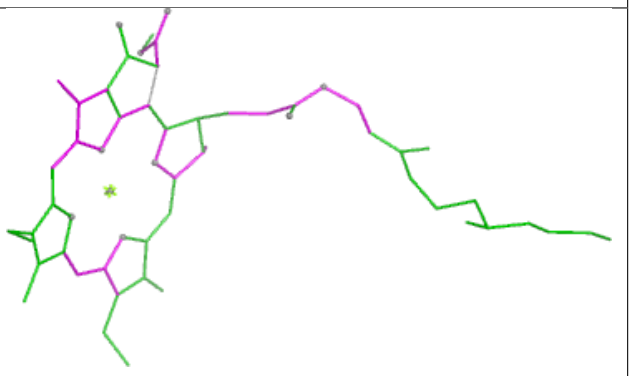
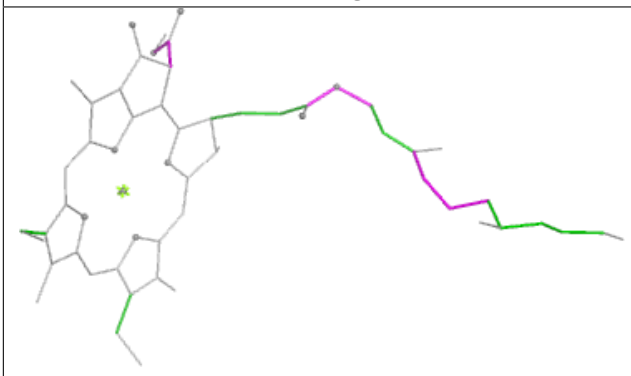


Bond angles



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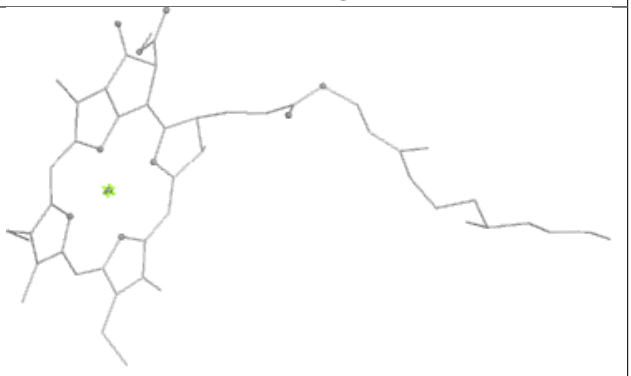
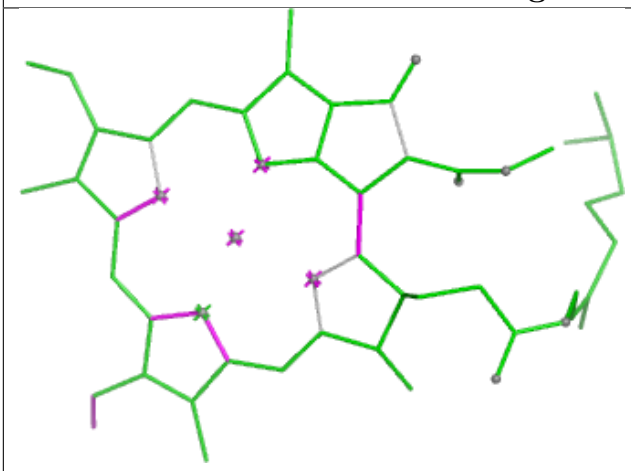


Rings

Ligand CLA 3 309



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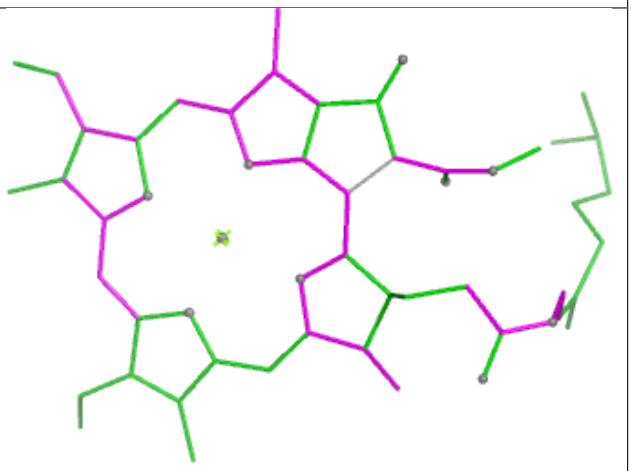
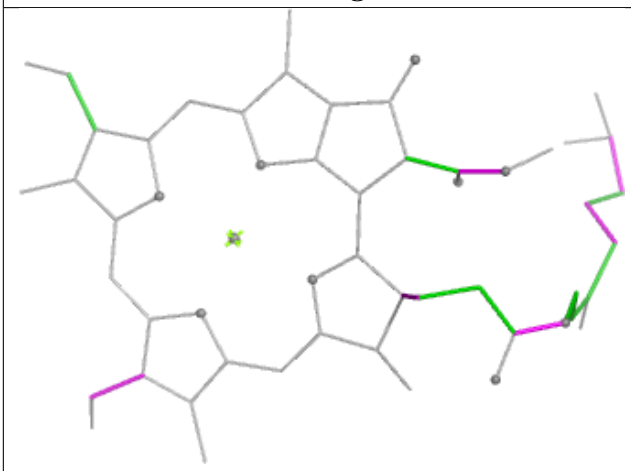


Bond angles



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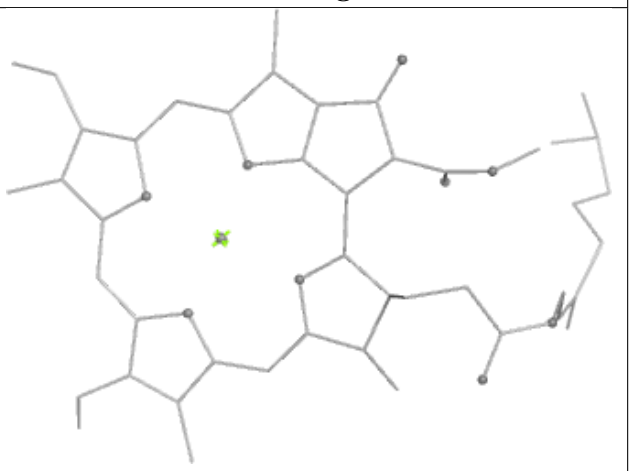
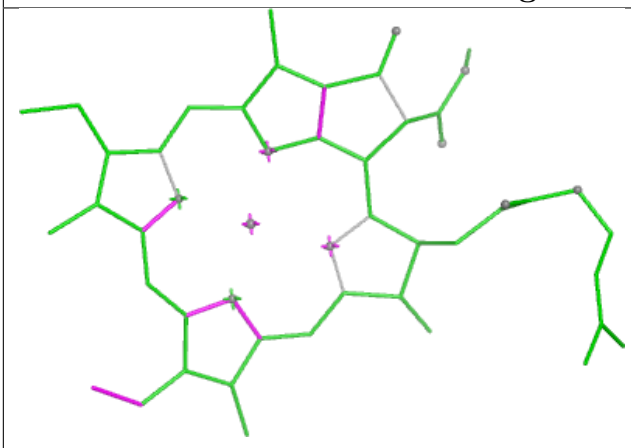


Rings

Ligand CLA J 1105



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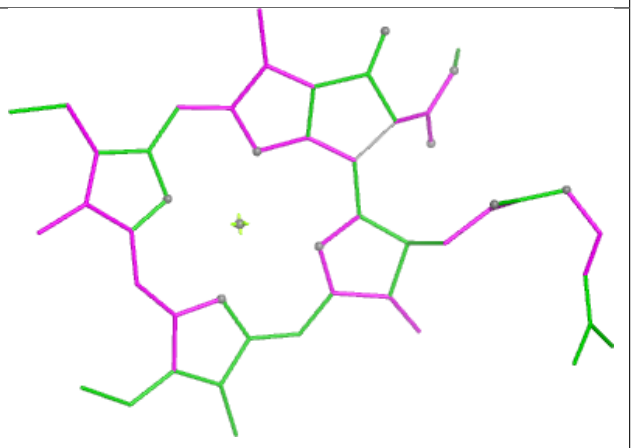
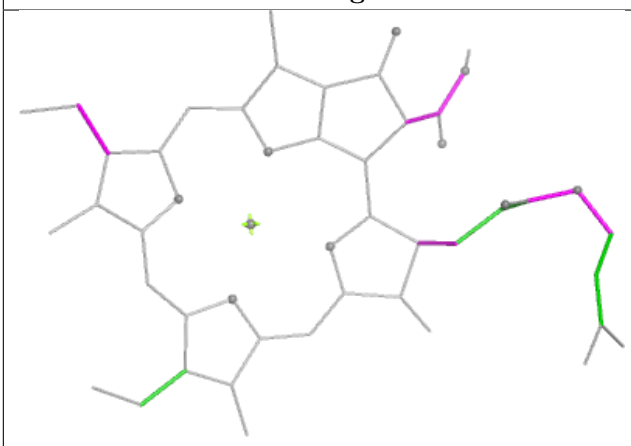


Bond angles



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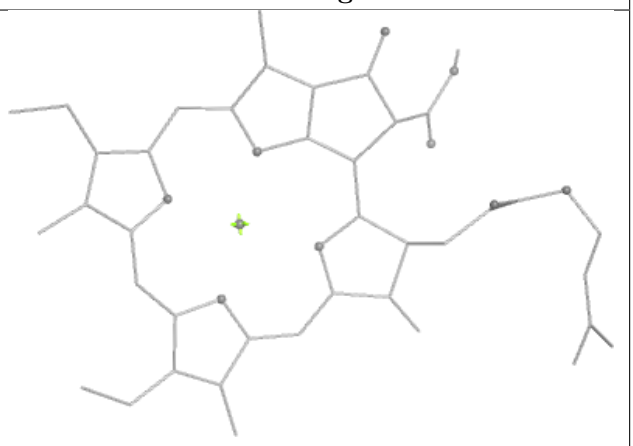
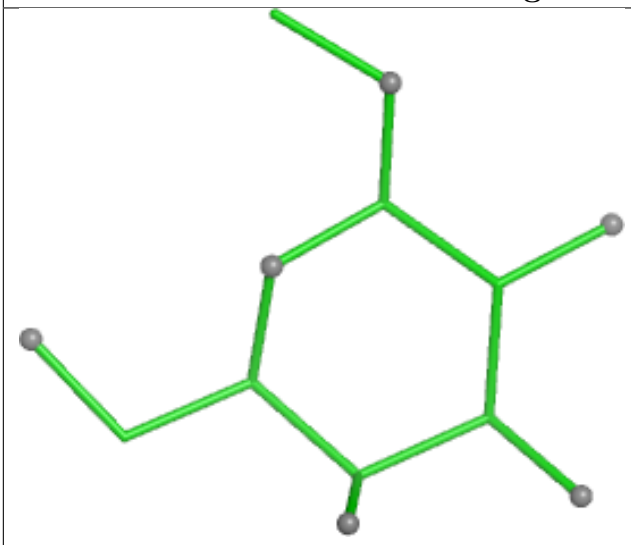


Rings

Ligand LMG 2 520



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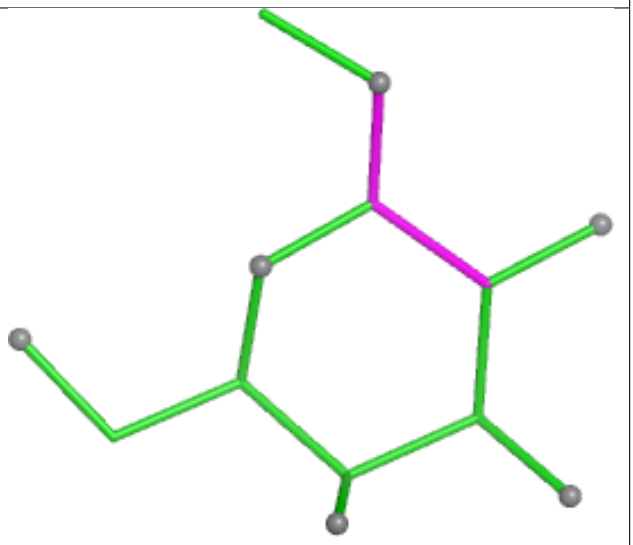
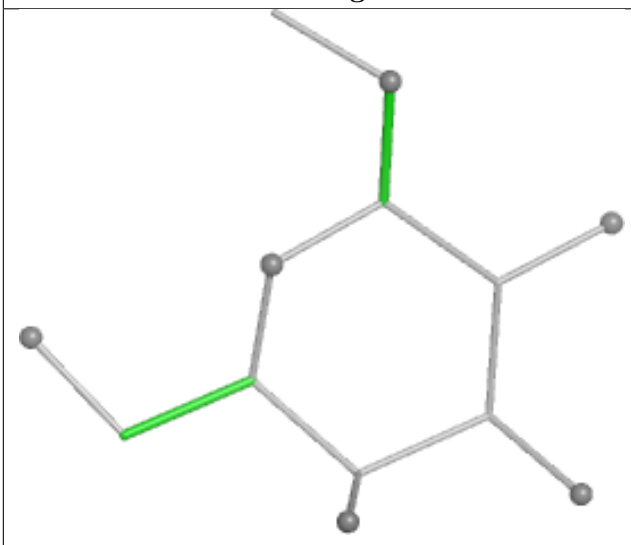


Bond angles



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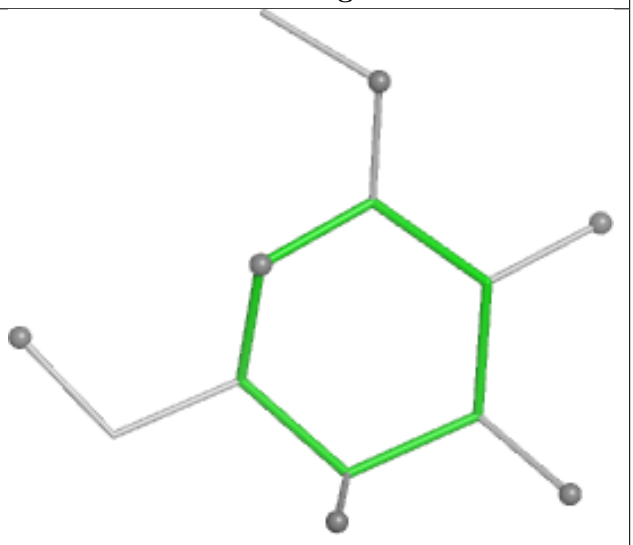
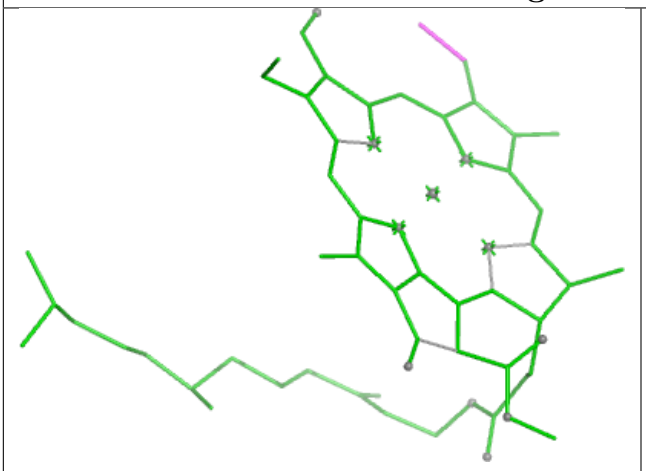


Rings

Ligand CHL 1 514



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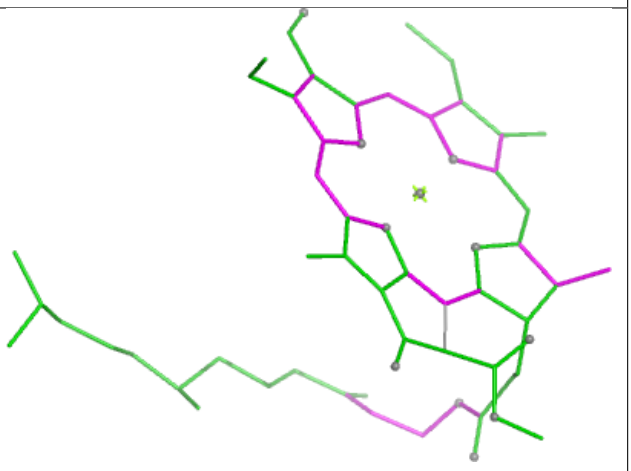
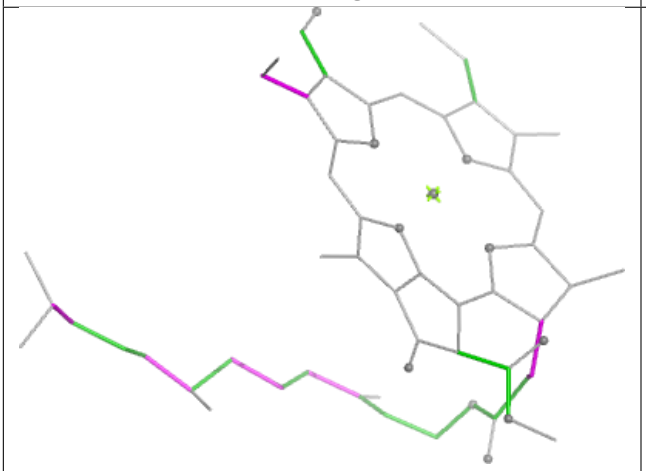


Bond angles



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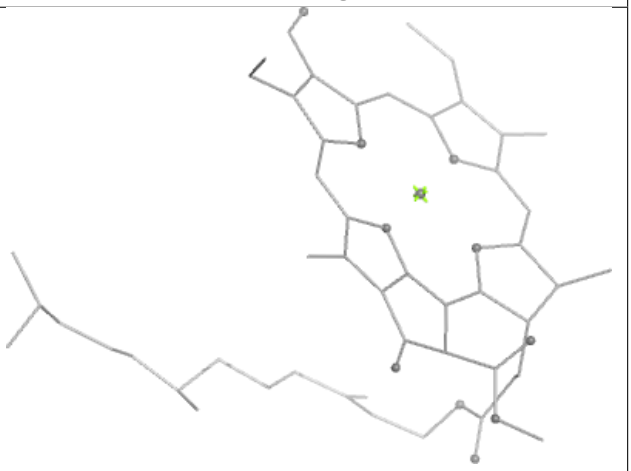
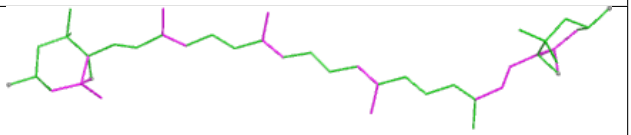


Rings

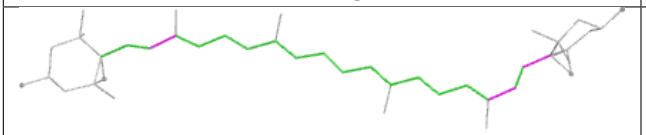
Ligand XAT 2 502



Bond lengths



Bond angles



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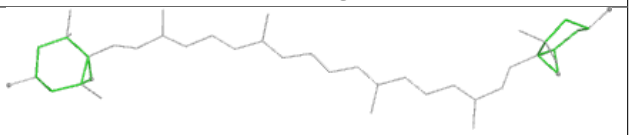
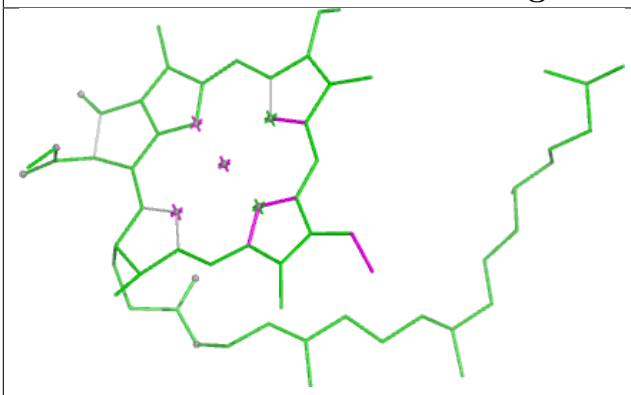
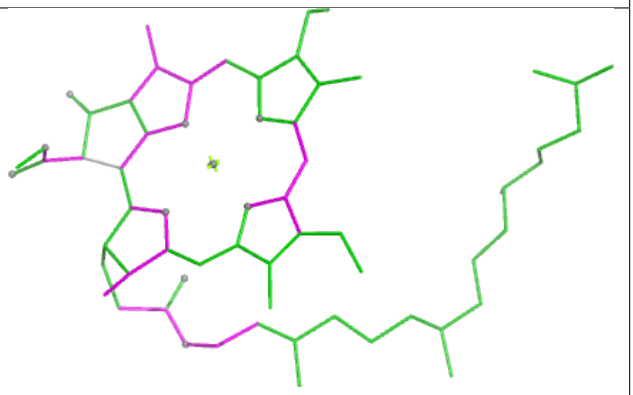


Rings

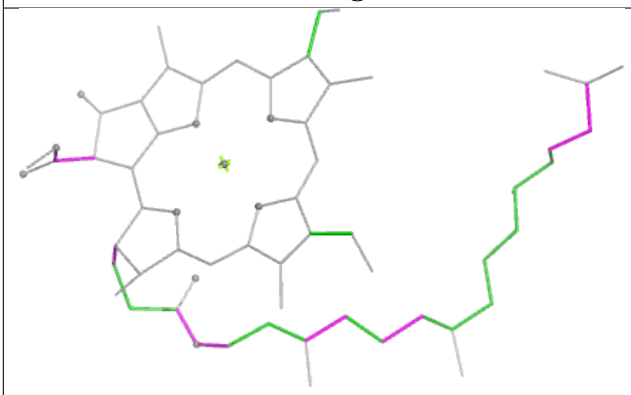
Ligand CLA 2 507



Bond lengths



Bond angles



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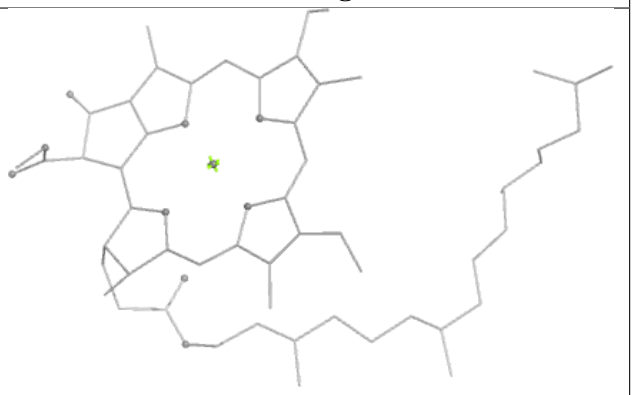


Rings

Ligand CLA B 830



Bond lengths



Bond angles

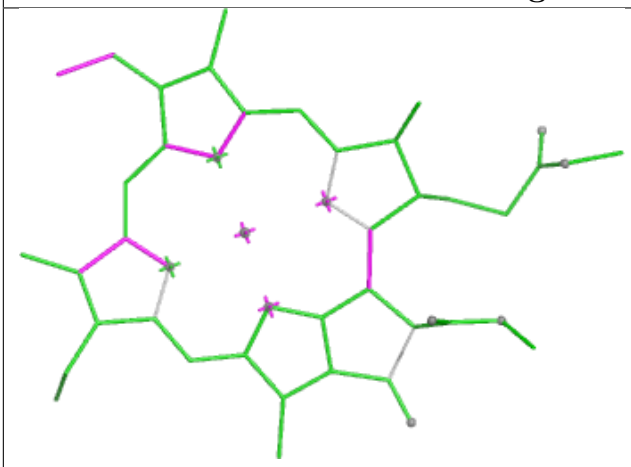


Torsions

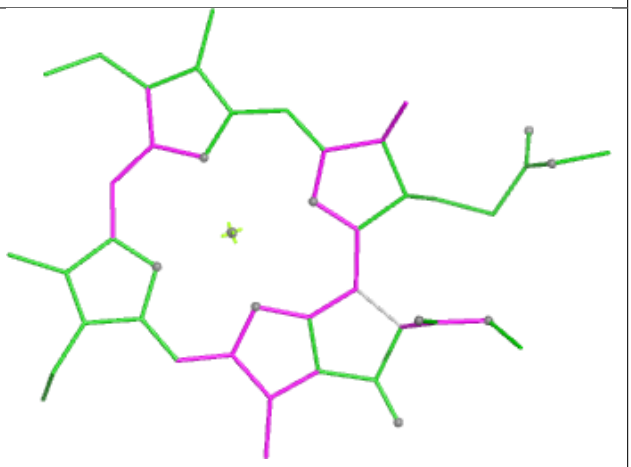


Rings

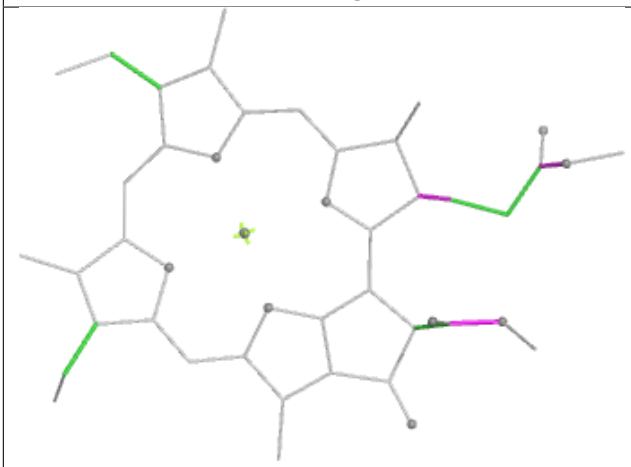
Ligand CLA 3 317



Bond lengths



Bond angles



Torsions

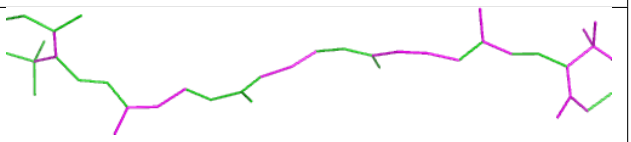


Rings

Ligand BCR K 1005



Bond lengths



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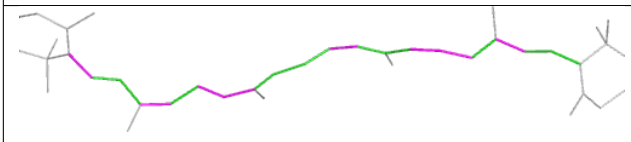

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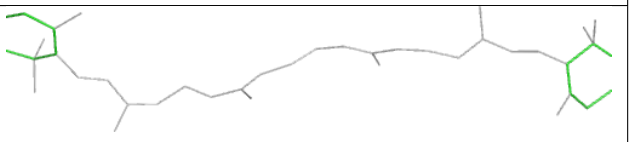
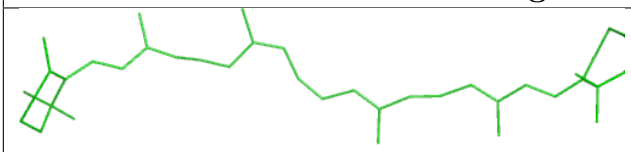


Rings

Ligand BCR I 101



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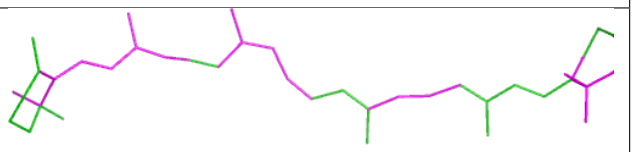

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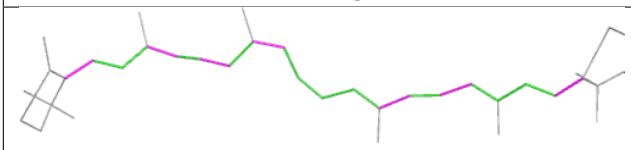

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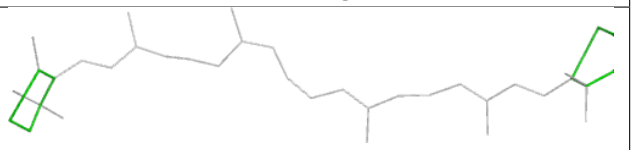
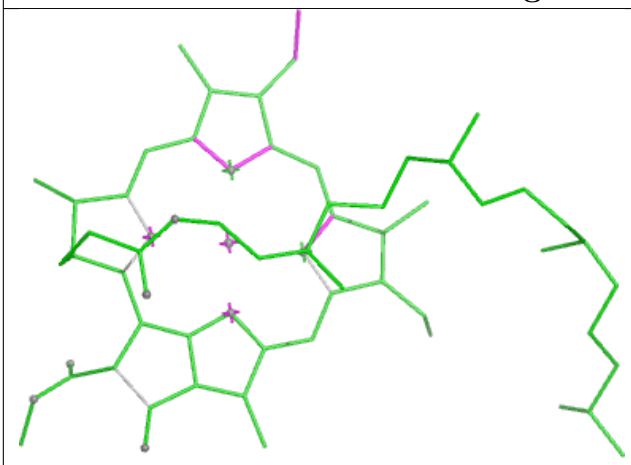


Rings

Ligand CLA A 817



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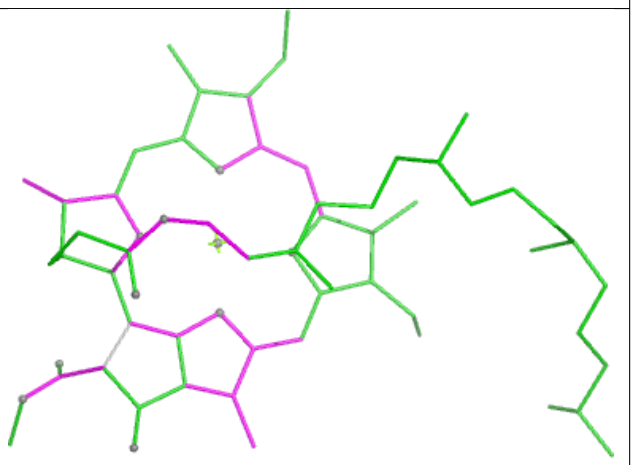

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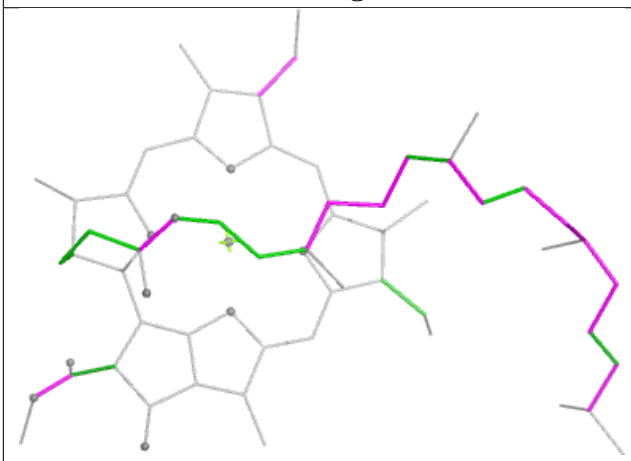

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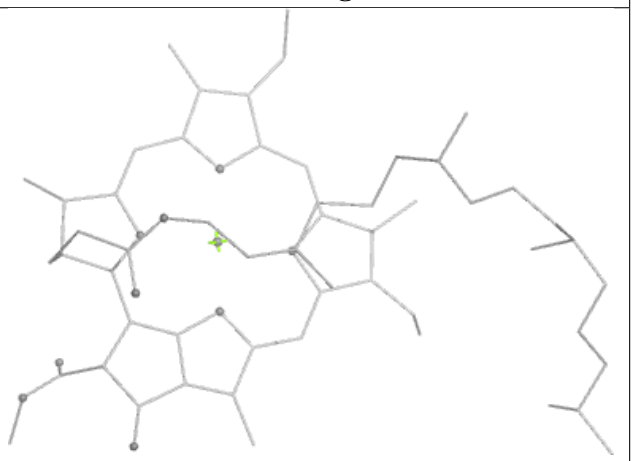
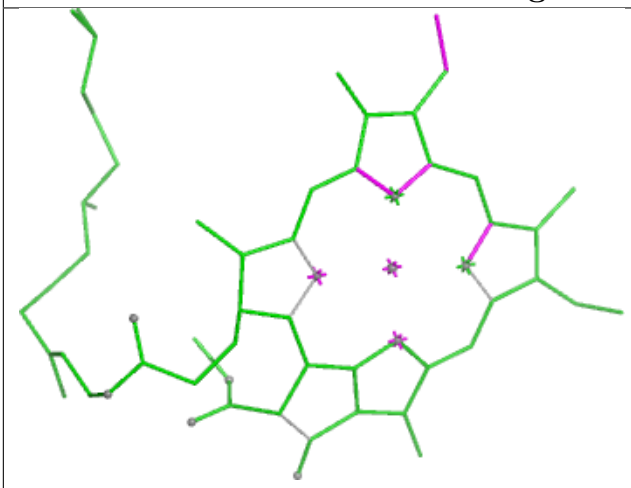


Rings

Ligand CLA 4 308



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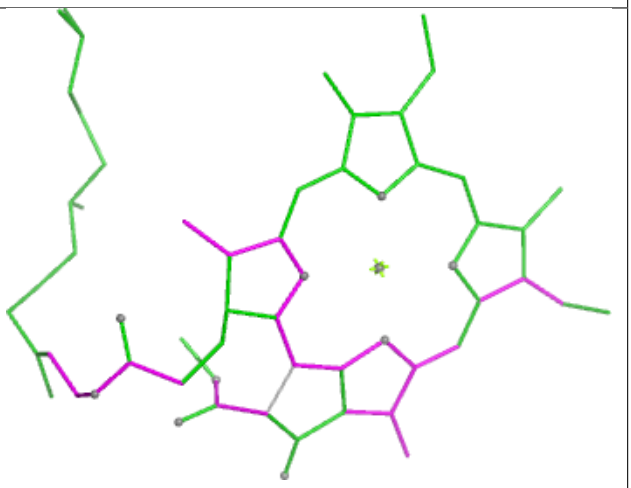
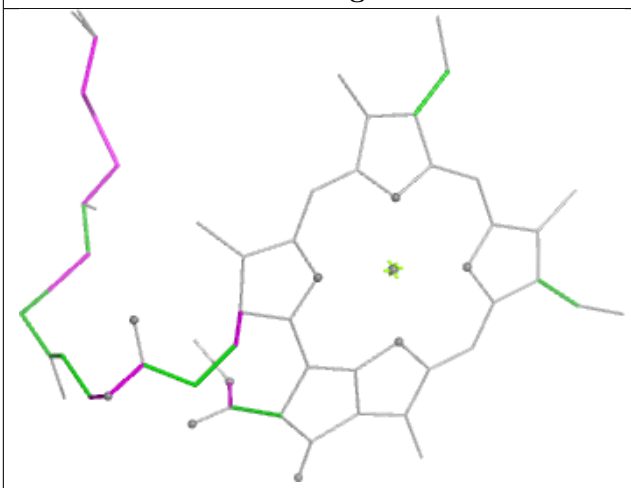


Bond angles



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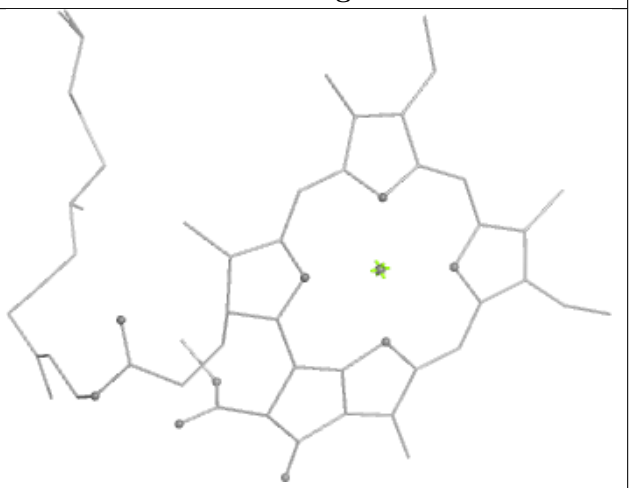
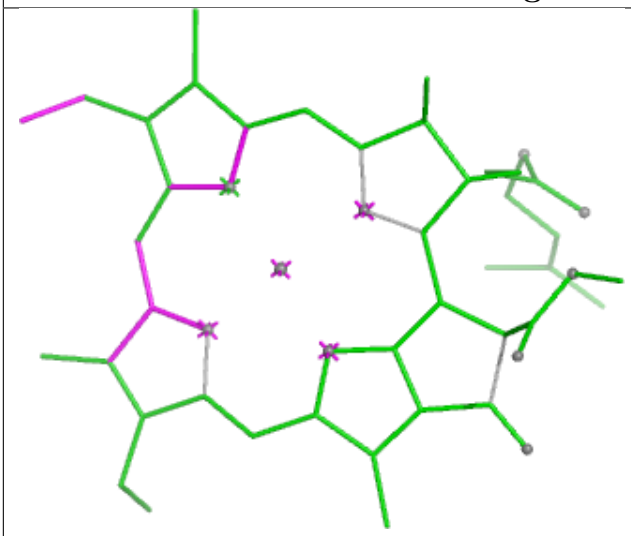


Rings

Ligand CLA A 810



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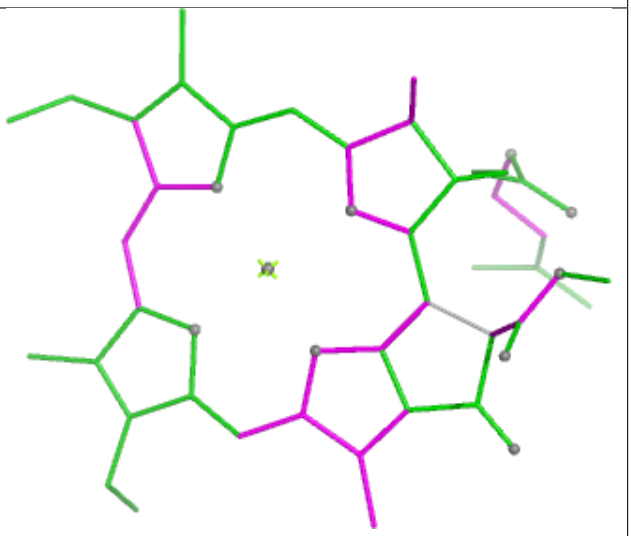

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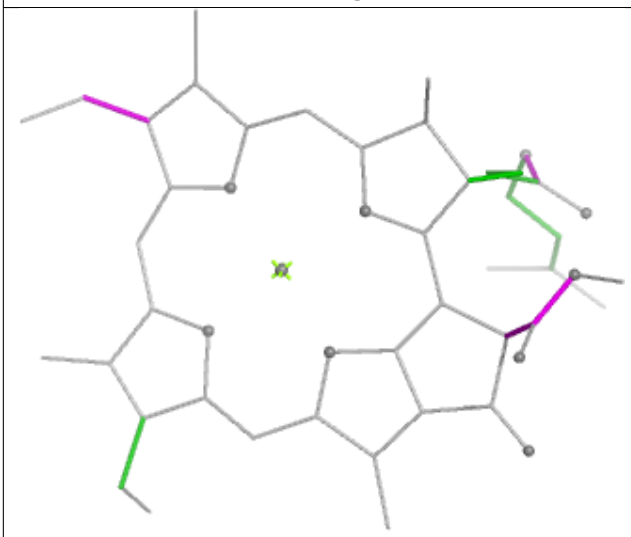

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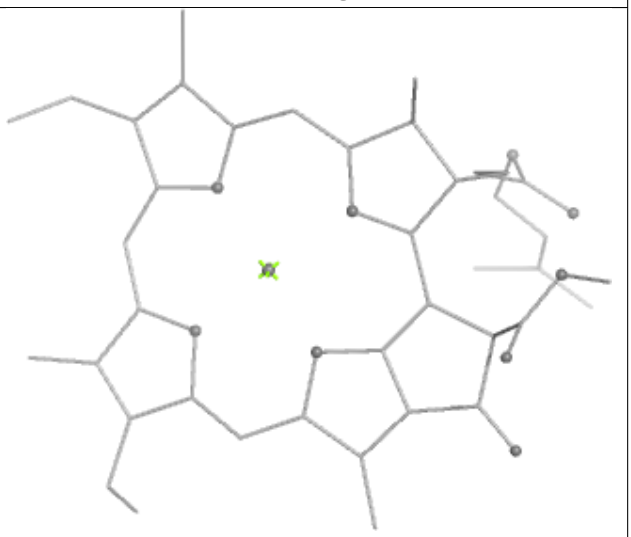
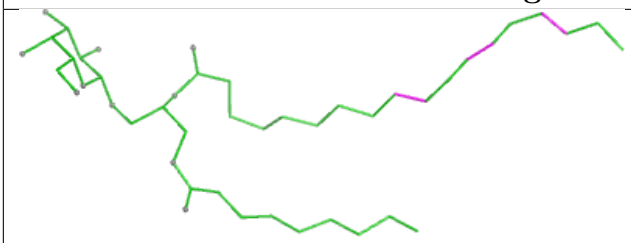


Rings

Ligand LMG 1 518



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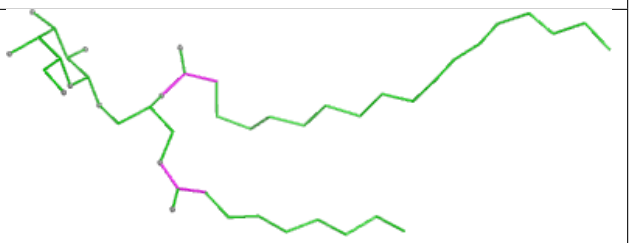
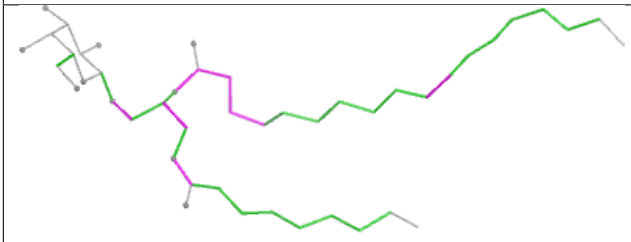


Bond angles



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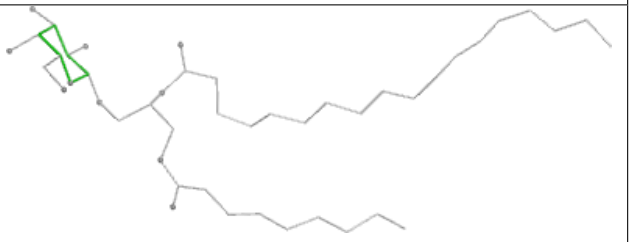
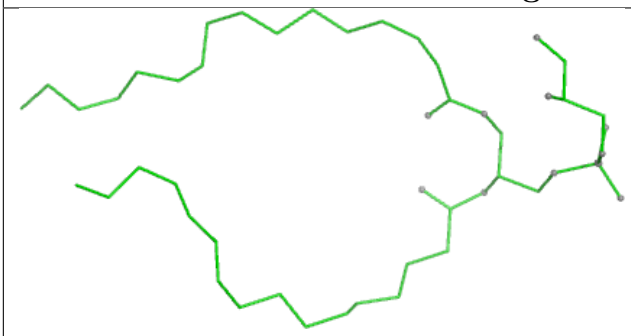


Rings

Ligand LHG B 843



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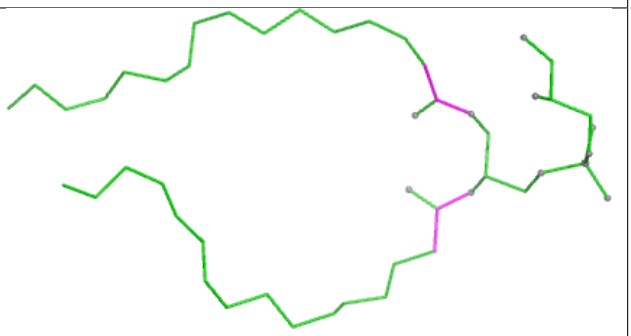
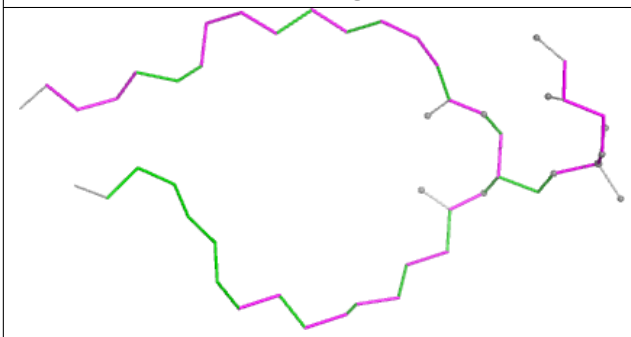


Bond angles



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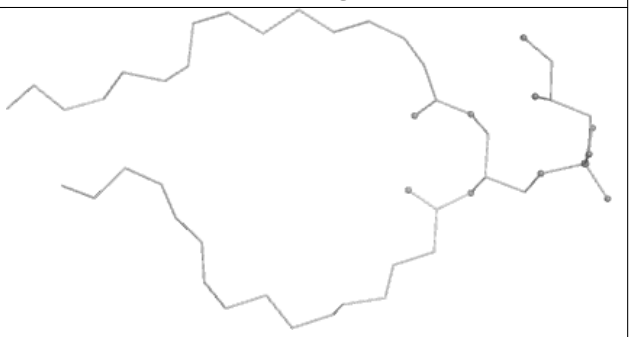
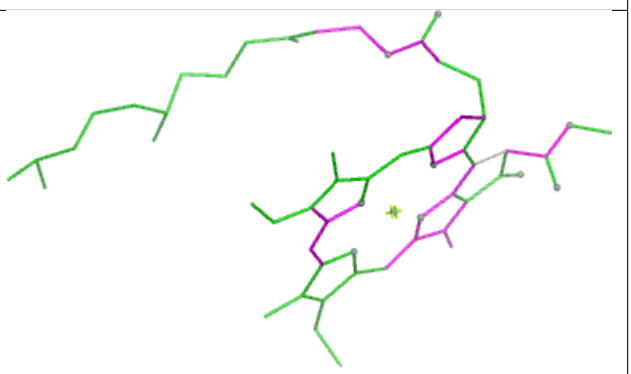


Rings

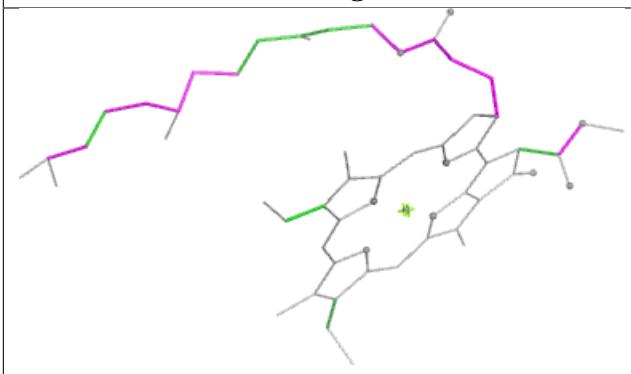
Ligand CLA B 831



Bond lengths



Bond angles



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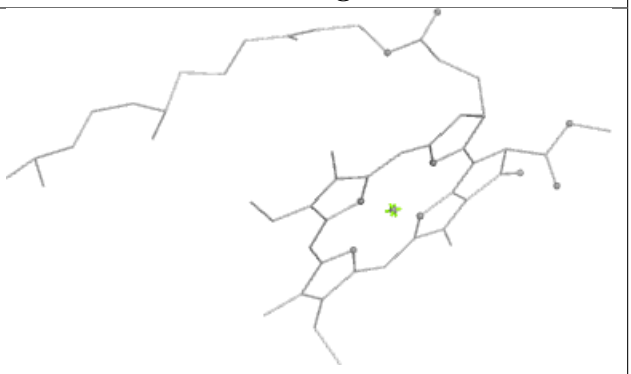
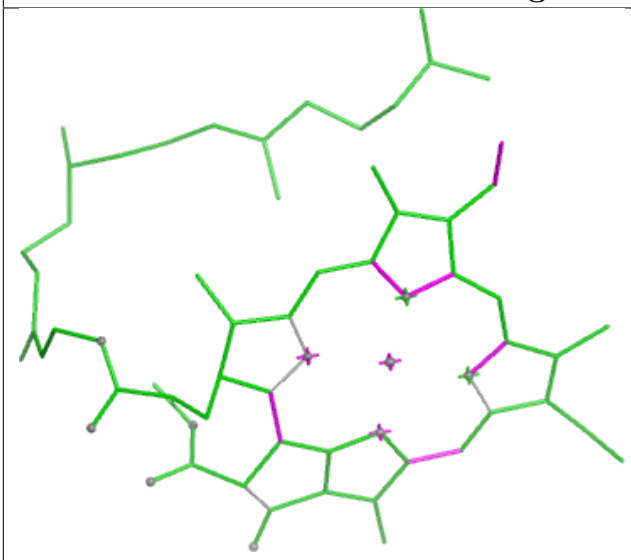


Rings

Ligand CLA 1 508



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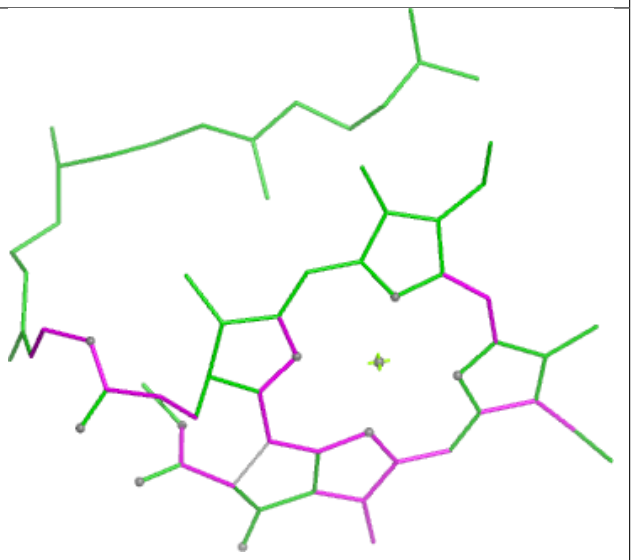
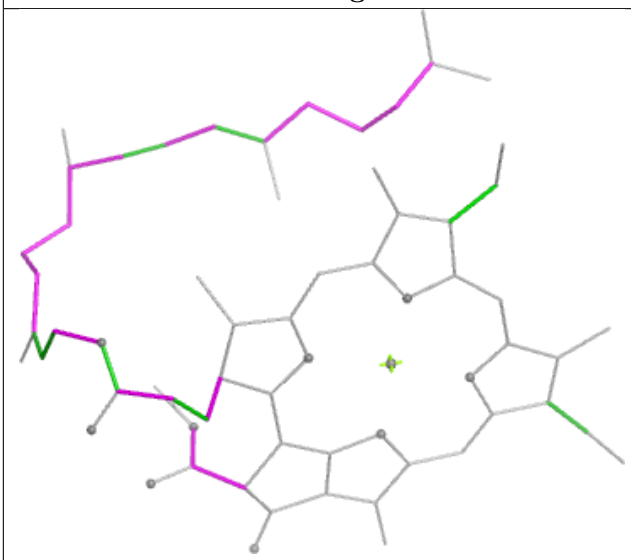


Bond angles



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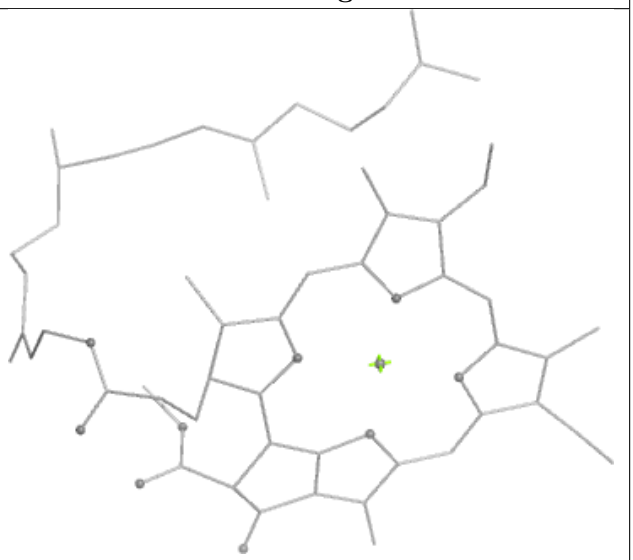
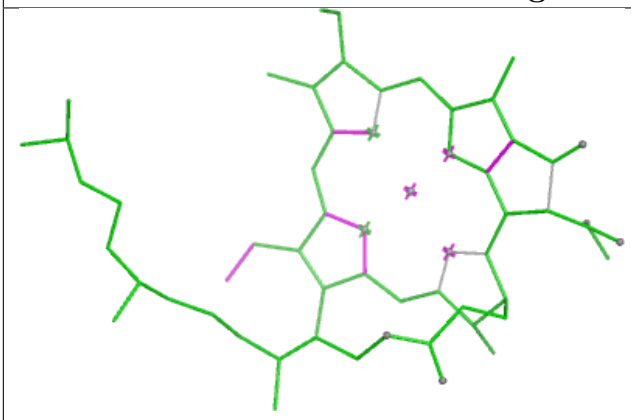


Rings

Ligand CLA 4 307



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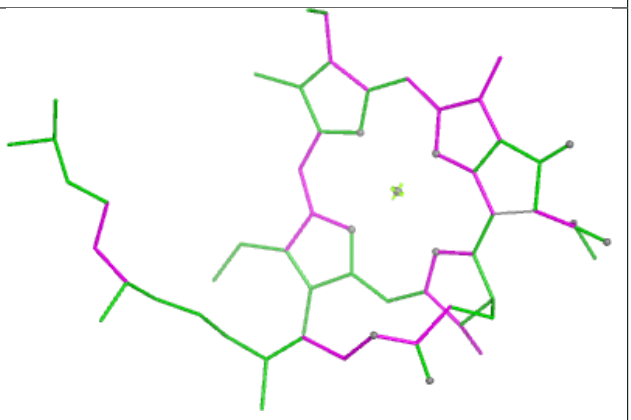
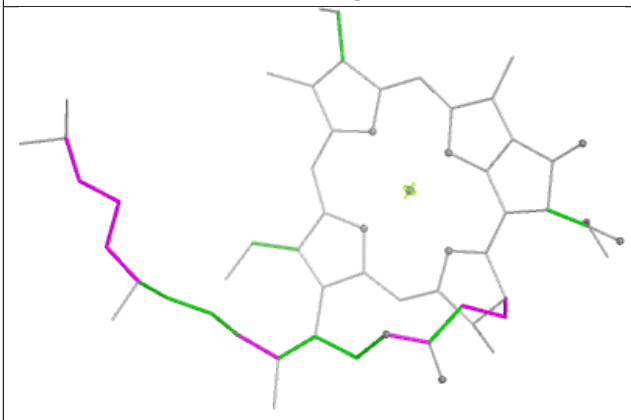


Bond angles



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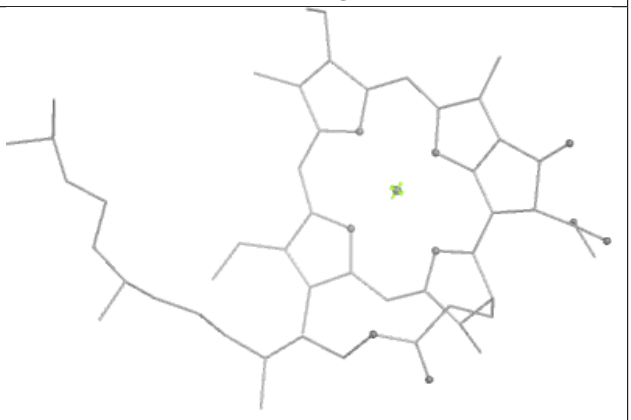
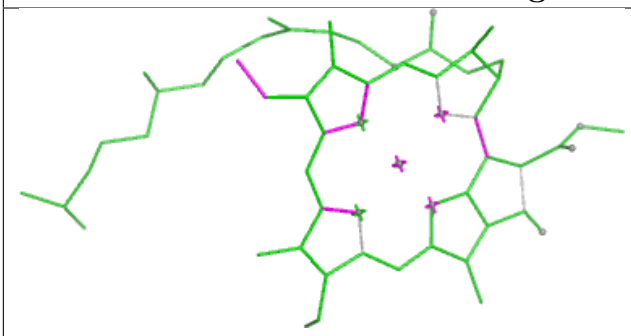


Rings

Ligand CLA 4 304



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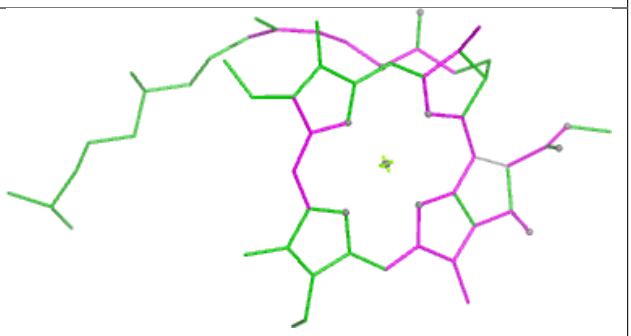
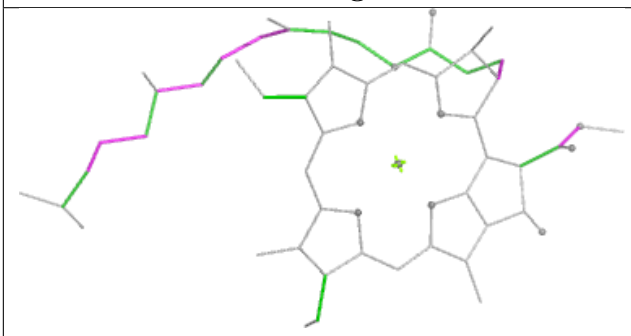


Bond angles



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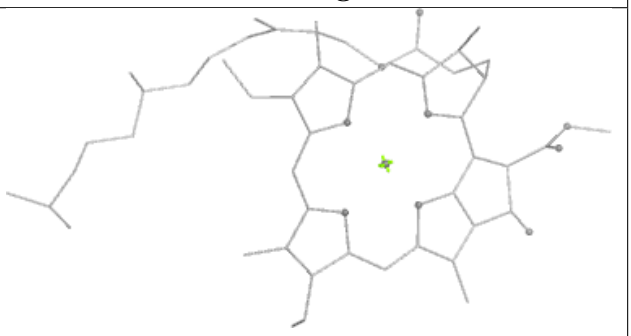
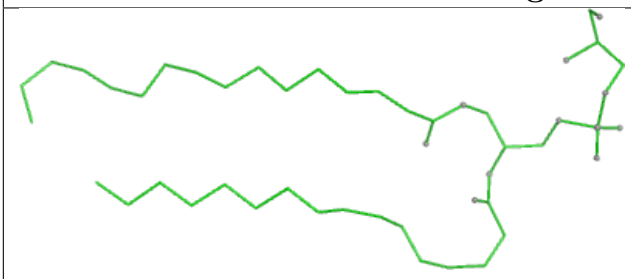


Rings

Ligand LHG 1 517



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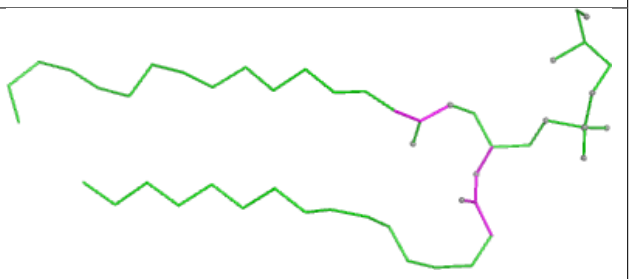
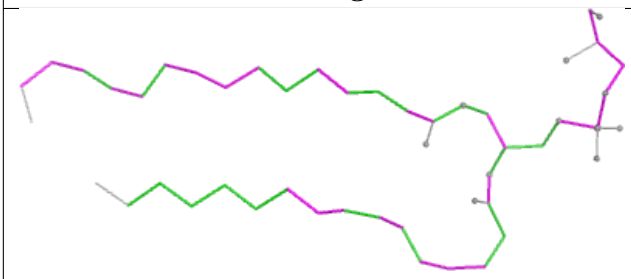


Bond angles



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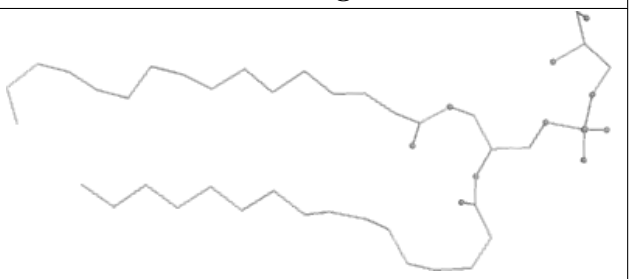
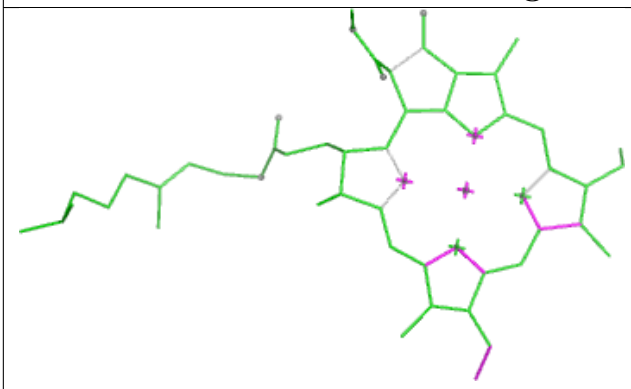


Rings

Ligand CLA A 826



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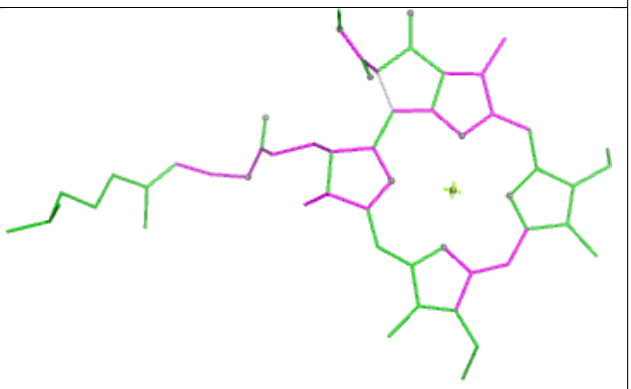
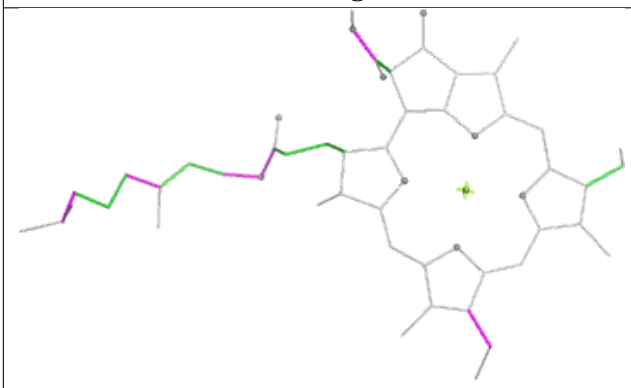


Bond angles



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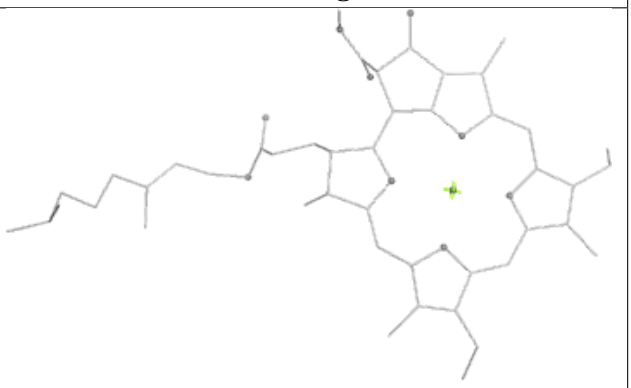
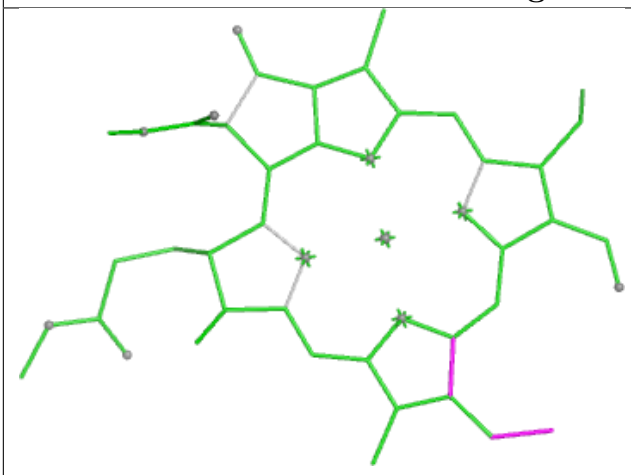


Rings

Ligand CHL 4 313



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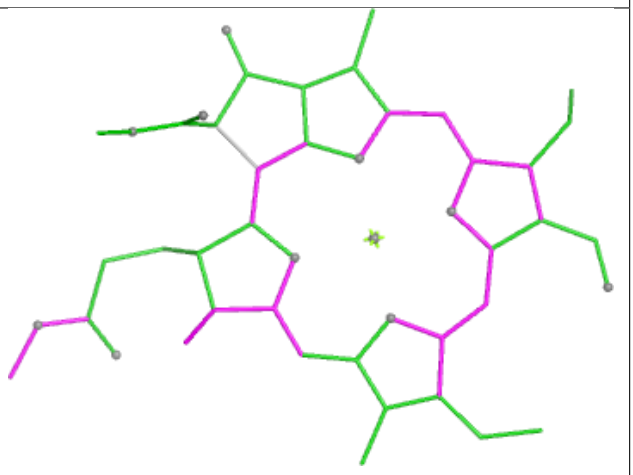
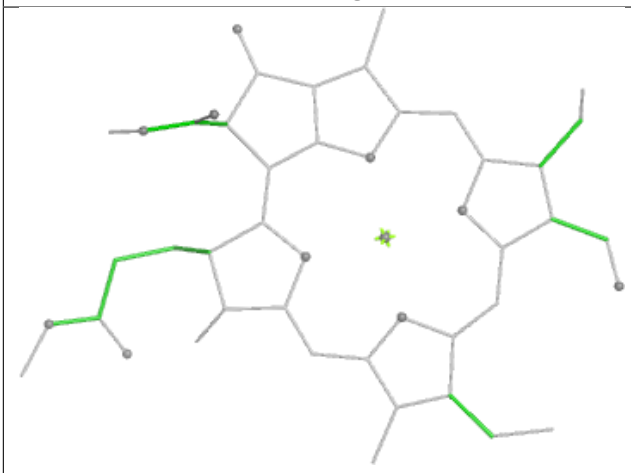


Bond angles



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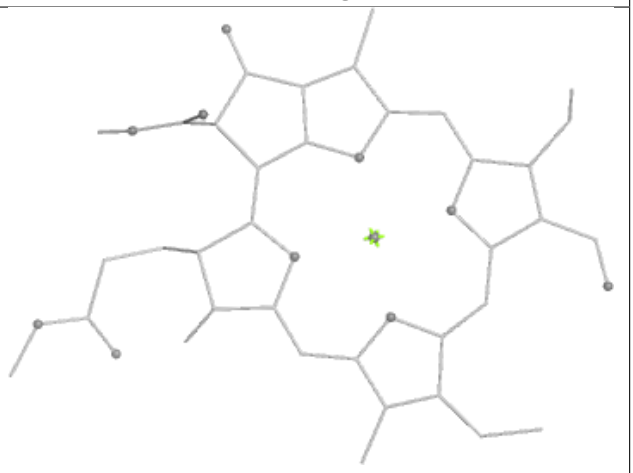
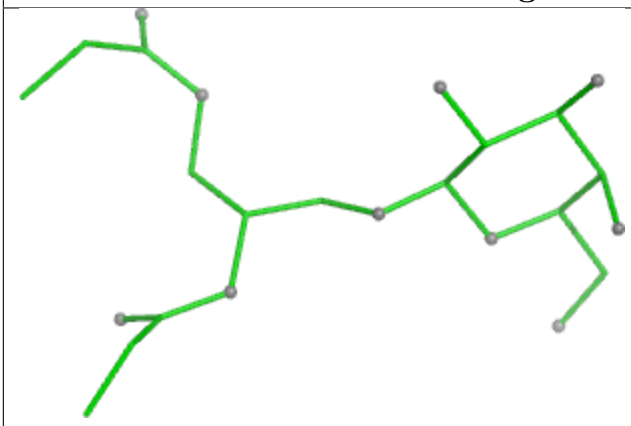


Rings

Ligand LMG G 210



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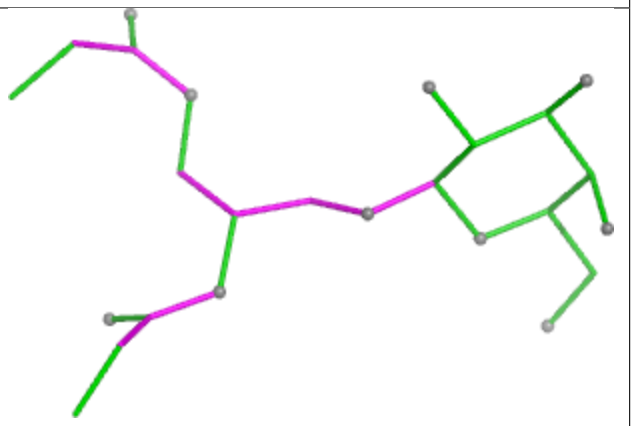
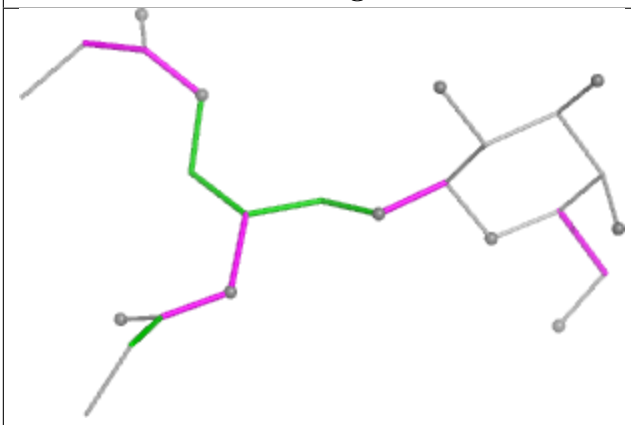
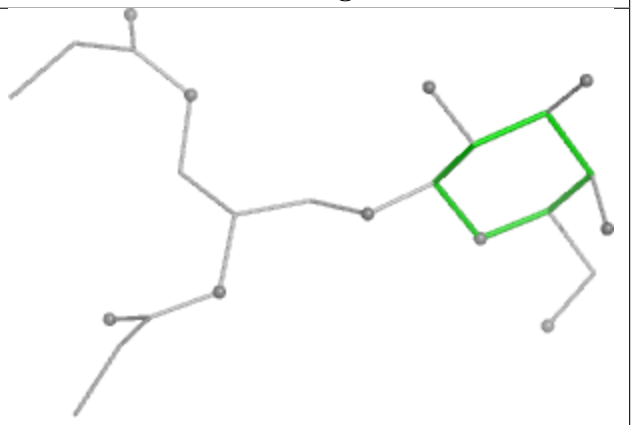


Bond angles

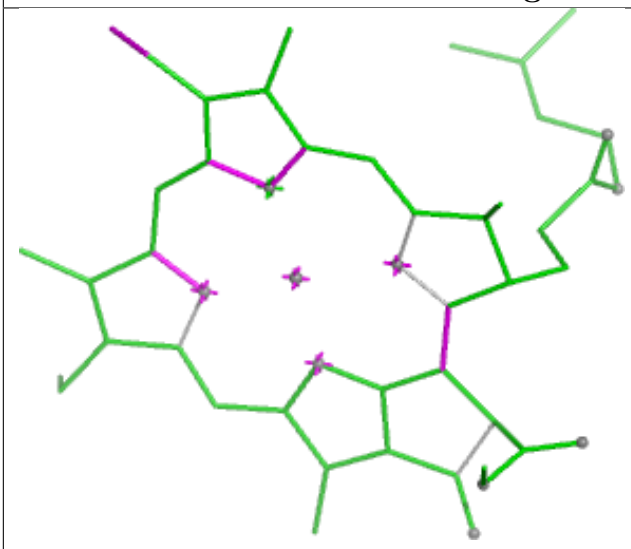


Torsions

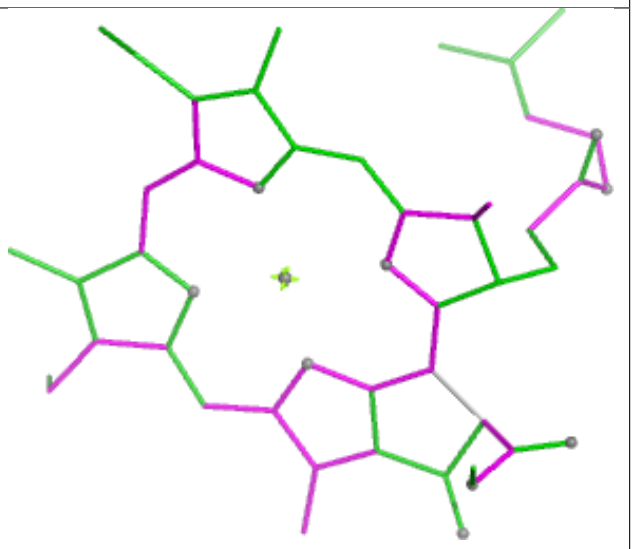


Rings

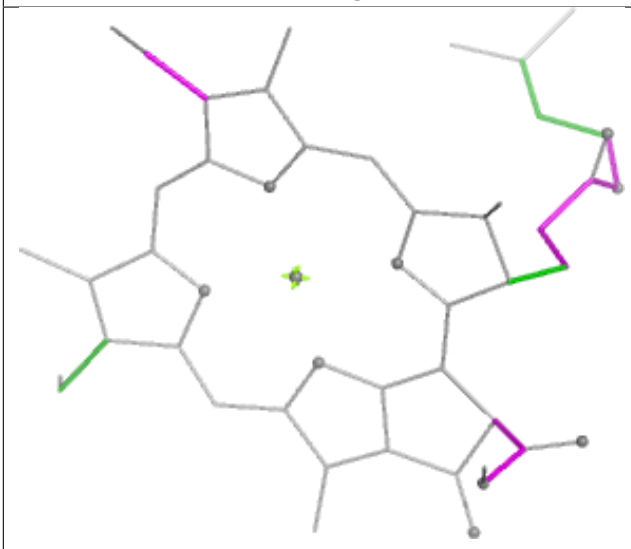
Ligand CLA A 820



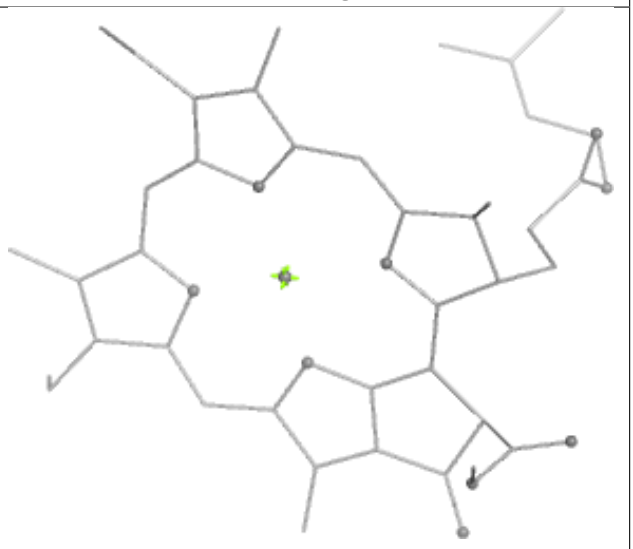
Bond lengths



Bond angles

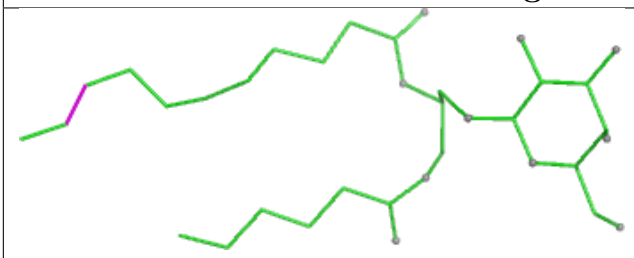


Torsions

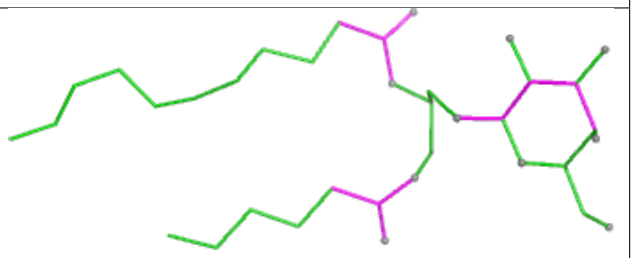


Rings

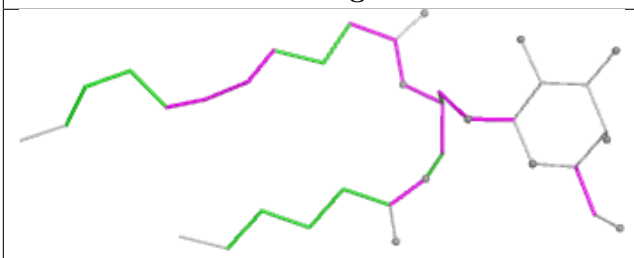
Ligand LMG 2 519



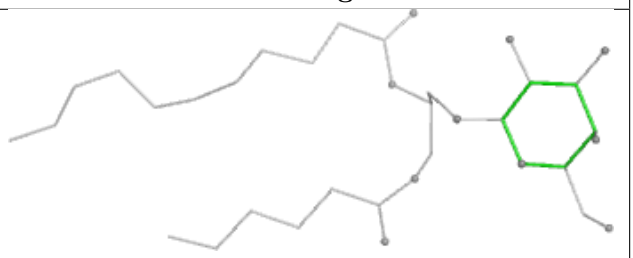
Bond lengths



Bond angles

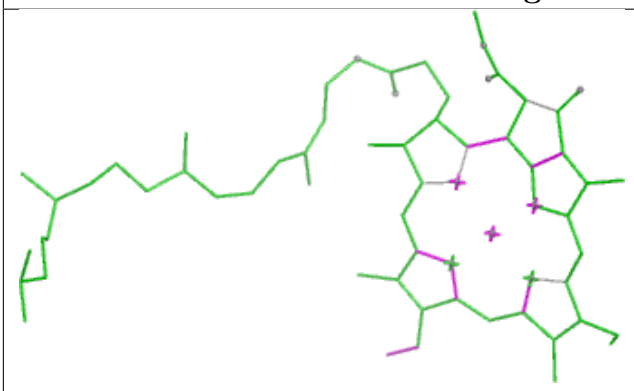


Torsions

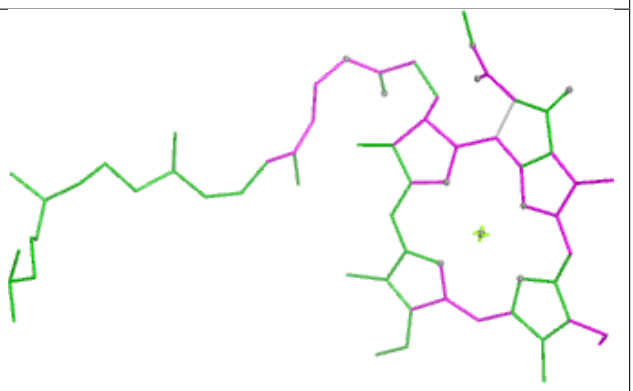


Rings

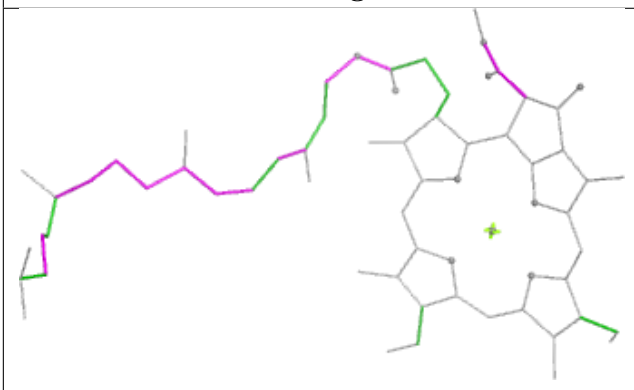
Ligand CLA A 802



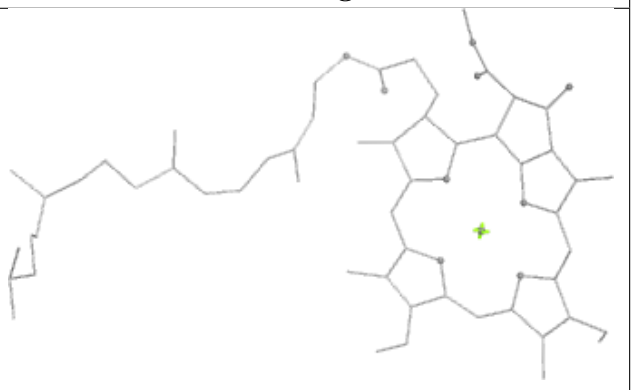
Bond lengths



Bond angles

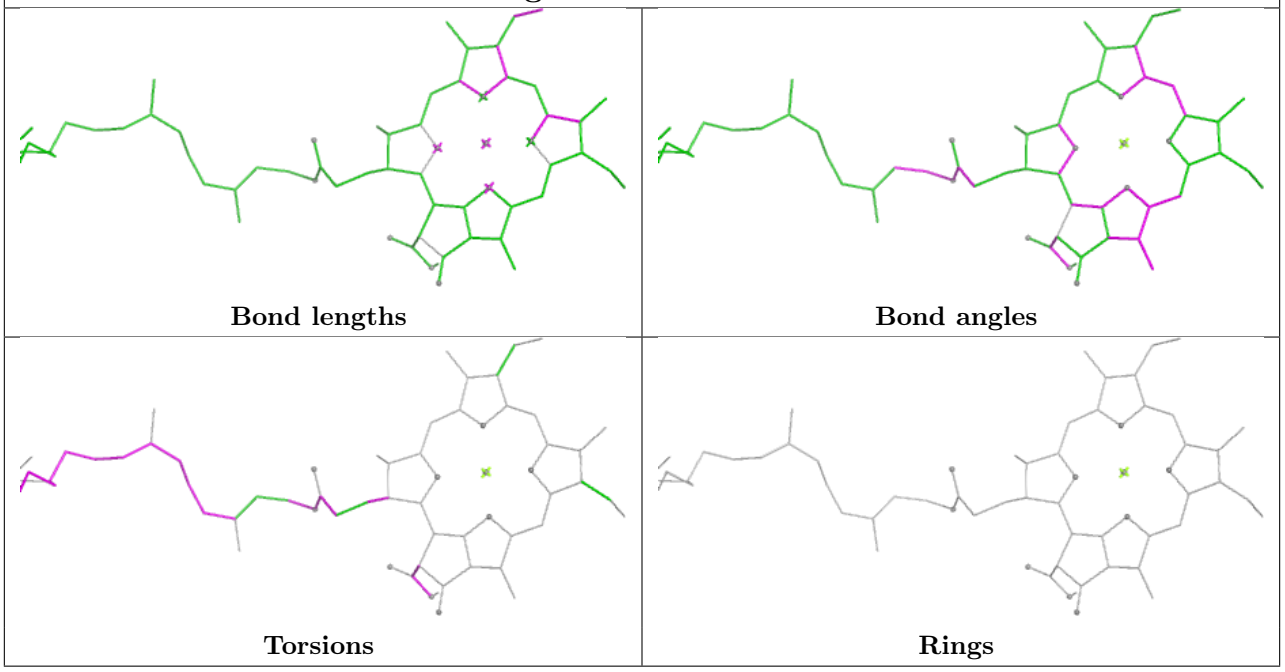


Torsions



Rings

Ligand CLA A 805



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	1	193/193 (100%)	1.08	37 (19%) 3 2	86, 127, 178, 218	0
2	2	208/269 (77%)	0.35	11 (5%) 32 26	82, 113, 154, 201	0
3	3	221/275 (80%)	0.86	35 (15%) 5 4	101, 148, 202, 253	0
4	4	198/198 (100%)	0.35	14 (7%) 22 17	73, 107, 149, 196	0
5	A	743/758 (98%)	0.34	45 (6%) 27 22	47, 79, 137, 192	0
6	B	733/734 (99%)	0.29	49 (6%) 24 19	49, 76, 116, 160	0
7	C	80/81 (98%)	0.42	6 (7%) 20 16	55, 66, 89, 121	0
8	D	143/143 (100%)	0.78	18 (12%) 8 6	60, 77, 107, 153	0
9	E	66/66 (100%)	0.36	4 (6%) 27 22	51, 81, 122, 147	0
10	F	154/154 (100%)	0.03	4 (2%) 57 51	54, 76, 116, 168	0
11	G	97/97 (100%)	0.67	11 (11%) 10 8	76, 113, 151, 161	0
12	H	88/88 (100%)	0.66	8 (9%) 15 11	80, 112, 146, 178	0
13	I	30/40 (75%)	0.32	2 (6%) 24 19	76, 99, 136, 138	0
14	J	42/42 (100%)	0.06	2 (4%) 35 30	57, 69, 96, 145	0
15	K	77/80 (96%)	1.21	16 (20%) 2 2	131, 168, 192, 218	0
16	L	157/157 (100%)	0.78	21 (13%) 7 5	77, 105, 151, 209	0
All	All	3230/3375 (95%)	0.47	283 (8%) 15 12	47, 94, 164, 253	0

The worst 5 of 283 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	1	103	GLY	11.1
1	1	101	GLY	11.0
8	D	196	VAL	9.8
8	D	200	GLU	8.4
3	3	177	ALA	8.3

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

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

6.3 Carbohydrates (i)

There are no oligosaccharides in this entry.

6.4 Ligands (i)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
22	LMG	2	520	13/55	0.39	0.19	101,133,145,149	0
24	LMT	J	1107	25/35	0.39	0.16	174,178,183,184	0
24	LMT	2	523	35/35	0.44	0.23	182,208,216,216	0
19	CLA	K	1004	27/65	0.46	0.18	166,177,185,190	0
26	DGD	B	801	41/66	0.56	0.24	170,200,207,208	0
24	LMT	G	209	31/35	0.58	0.17	136,187,203,205	0
22	LMG	2	521	13/55	0.62	0.24	120,140,149,150	0
22	LMG	2	522	13/55	0.64	0.16	166,181,188,190	0
22	LMG	G	210	25/55	0.64	0.23	145,173,190,195	0
19	CLA	K	1003	27/65	0.65	0.16	189,198,202,205	0
24	LMT	A	846	35/35	0.67	0.17	90,128,143,148	0
22	LMG	B	845	33/55	0.68	0.17	107,163,172,176	0
22	LMG	2	524	13/55	0.68	0.15	143,153,159,162	0
22	LMG	A	847	50/55	0.68	0.18	133,155,181,184	0
24	LMT	3	318	31/35	0.68	0.17	127,164,183,187	0
22	LMG	2	525	13/55	0.70	0.17	100,129,143,143	0
19	CLA	H	1000	60/65	0.70	0.18	124,150,167,178	0
22	LMG	2	519	36/55	0.71	0.16	108,148,158,160	0
22	LMG	4	321	13/55	0.73	0.15	159,168,171,172	0
19	CLA	J	1105	50/65	0.75	0.17	113,150,159,164	0
21	LHG	B	843	49/49	0.76	0.22	104,125,175,186	0
19	CLA	3	312	48/65	0.76	0.15	176,192,204,209	0
21	LHG	1	520	42/49	0.76	0.22	86,136,161,165	0
22	LMG	B	844	35/55	0.76	0.14	59,114,124,125	0
26	DGD	G	207	47/66	0.76	0.22	162,204,212,214	0
19	CLA	K	1002	60/65	0.77	0.16	119,151,162,167	0
19	CLA	3	311	41/65	0.78	0.19	184,202,209,211	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
24	LMT	B	855	31/35	0.78	0.14	117,141,151,154	0
24	LMT	B	846	35/35	0.79	0.14	153,194,203,209	0
22	LMG	J	1104	34/55	0.79	0.14	97,129,137,141	0
22	LMG	F	305	36/55	0.79	0.19	124,141,152,159	0
19	CLA	3	306	52/65	0.80	0.15	152,181,190,195	0
19	CLA	1	513	65/65	0.81	0.21	129,151,169,170	0
24	LMT	B	847	32/35	0.82	0.13	103,134,152,153	0
20	CHL	4	317	43/66	0.82	0.12	116,136,152,161	0
18	BCR	K	1005	40/40	0.82	0.19	145,157,181,184	0
22	LMG	1	519	13/55	0.83	0.13	131,138,144,147	0
22	LMG	G	206	50/55	0.83	0.20	123,149,163,164	0
22	LMG	2	518	25/55	0.83	0.16	110,121,138,142	0
24	LMT	4	320	35/35	0.83	0.15	98,133,152,158	0
19	CLA	3	310	50/65	0.84	0.14	135,159,166,168	0
18	BCR	L	307	40/40	0.84	0.18	126,138,165,167	0
19	CLA	K	1001	45/65	0.85	0.15	148,174,184,185	0
24	LMT	G	208	35/35	0.85	0.14	101,158,170,173	0
18	BCR	3	304	40/40	0.85	0.23	144,156,180,182	0
19	CLA	1	510	46/65	0.85	0.15	105,140,169,174	0
18	BCR	2	503	40/40	0.85	0.25	134,153,166,170	0
19	CLA	L	303	50/65	0.85	0.13	105,127,146,157	0
20	CHL	4	313	47/66	0.86	0.12	80,110,137,147	0
20	CHL	2	512	47/66	0.86	0.11	101,123,140,175	0
22	LMG	4	322	45/55	0.87	0.20	87,126,133,138	0
21	LHG	1	517	49/49	0.87	0.18	96,108,141,145	0
19	CLA	L	305	50/65	0.87	0.13	88,104,132,135	0
19	CLA	G	204	65/65	0.87	0.16	91,119,134,140	0
19	CLA	A	816	46/65	0.88	0.12	109,126,142,148	0
19	CLA	A	842	60/65	0.88	0.11	94,119,157,159	0
19	CLA	1	509	50/65	0.88	0.13	130,145,153,162	0
19	CLA	1	516	60/65	0.88	0.13	79,105,143,146	0
17	LUT	3	301	42/42	0.88	0.15	146,159,165,171	0
22	LMG	1	518	46/55	0.88	0.17	81,129,140,144	0
19	CLA	3	313	60/65	0.88	0.15	108,137,146,156	0
19	CLA	A	835	55/65	0.89	0.13	107,124,142,152	0
18	BCR	G	205	40/40	0.89	0.17	93,120,154,157	0
20	CHL	2	516	56/66	0.89	0.12	102,129,157,164	0
19	CLA	3	305	55/65	0.89	0.11	154,168,178,185	0
22	LMG	F	304	47/55	0.89	0.11	89,102,119,134	0
18	BCR	3	303	40/40	0.89	0.18	115,133,145,150	0
18	BCR	A	850	40/40	0.89	0.14	61,78,127,129	0
30	ZEX	F	301	42/42	0.89	0.17	84,105,116,122	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
19	CLA	A	823	60/65	0.90	0.12	106,123,152,160	0
19	CLA	1	504	65/65	0.90	0.14	118,136,149,153	0
19	CLA	4	309	50/65	0.90	0.13	109,120,137,143	0
20	CHL	4	316	61/66	0.90	0.14	104,118,136,142	0
19	CLA	B	831	60/65	0.90	0.14	48,59,97,100	0
19	CLA	F	303	65/65	0.90	0.13	63,81,109,121	0
19	CLA	G	201	65/65	0.90	0.14	75,90,116,123	0
22	LMG	J	1103	30/55	0.90	0.11	72,82,102,102	0
25	CA	3	319	1/1	0.90	0.10	118,118,118,118	0
21	LHG	A	845	40/49	0.90	0.14	78,102,116,124	0
19	CLA	G	203	46/65	0.90	0.09	125,139,150,154	0
18	BCR	B	851	40/40	0.90	0.20	84,110,134,137	0
19	CLA	1	515	45/65	0.91	0.13	149,166,184,188	0
19	CLA	B	808	65/65	0.91	0.13	73,91,117,121	0
17	LUT	J	1109	42/42	0.91	0.12	62,88,104,109	0
18	BCR	I	102	40/40	0.91	0.18	70,86,109,113	0
17	LUT	1	502	42/42	0.91	0.19	79,114,132,135	0
19	CLA	A	817	65/65	0.91	0.15	104,135,150,154	0
19	CLA	1	511	46/65	0.91	0.16	99,129,147,160	0
26	DGD	4	319	51/66	0.91	0.16	97,112,143,149	0
19	CLA	A	831	65/65	0.91	0.13	66,93,128,132	0
26	DGD	B	854	61/66	0.91	0.16	53,79,99,120	0
20	CHL	3	314	47/66	0.91	0.11	134,140,156,163	0
17	LUT	3	302	42/42	0.91	0.18	120,141,154,161	0
19	CLA	A	838	65/65	0.92	0.14	63,80,126,130	0
18	BCR	A	856	40/40	0.92	0.20	137,144,158,161	0
20	CHL	1	512	47/66	0.92	0.11	108,140,147,152	0
20	CHL	1	514	61/66	0.92	0.13	114,131,139,162	0
19	CLA	B	805	65/65	0.92	0.12	80,93,126,135	0
19	CLA	1	505	46/65	0.92	0.11	111,135,149,157	0
19	CLA	B	816	55/65	0.92	0.12	92,110,131,141	0
17	LUT	4	302	42/42	0.92	0.14	90,106,118,128	0
18	BCR	L	306	40/40	0.92	0.13	99,119,127,132	0
28	SF4	C	102	8/8	0.92	0.16	67,106,137,151	0
18	BCR	A	851	40/40	0.92	0.17	63,90,106,108	0
19	CLA	4	310	60/65	0.93	0.13	104,115,132,138	0
19	CLA	4	318	65/65	0.93	0.14	87,106,128,131	0
19	CLA	A	804	65/65	0.93	0.13	49,65,110,119	0
19	CLA	A	813	65/65	0.93	0.14	67,89,108,109	0
19	CLA	A	814	65/65	0.93	0.13	89,113,129,135	0
18	BCR	B	852	40/40	0.93	0.13	50,66,83,89	0
19	CLA	2	509	50/65	0.93	0.11	99,120,140,143	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
19	CLA	2	510	60/65	0.93	0.12	108,128,143,151	0
19	CLA	2	511	50/65	0.93	0.12	112,133,142,146	0
20	CHL	2	526	66/66	0.93	0.14	97,120,138,144	0
19	CLA	2	514	55/65	0.93	0.12	81,94,116,121	0
23	XAT	2	502	44/44	0.93	0.15	82,99,114,118	0
23	XAT	4	303	44/44	0.93	0.12	72,92,116,128	0
19	CLA	A	836	51/65	0.93	0.12	66,82,95,110	0
18	BCR	B	853	40/40	0.93	0.13	50,64,74,78	0
18	BCR	F	306	40/40	0.93	0.10	48,64,72,77	0
19	CLA	3	307	55/65	0.93	0.13	154,177,191,198	0
19	CLA	3	309	55/65	0.93	0.13	97,123,131,135	0
21	LHG	2	517	35/49	0.93	0.15	116,124,130,132	0
17	LUT	2	501	42/42	0.93	0.16	108,118,128,134	0
19	CLA	B	822	65/65	0.93	0.14	70,89,119,127	0
18	BCR	B	849	40/40	0.93	0.17	90,98,109,114	0
19	CLA	B	840	65/65	0.93	0.11	52,80,91,102	0
18	BCR	J	1108	40/40	0.93	0.13	52,64,79,82	0
18	BCR	B	850	40/40	0.93	0.18	69,89,130,131	0
19	CLA	3	315	50/65	0.93	0.12	109,125,133,147	0
19	CLA	3	316	46/65	0.93	0.10	142,149,159,163	0
19	CLA	3	317	46/65	0.93	0.12	91,105,132,138	0
26	DGD	J	1106	58/66	0.93	0.11	52,80,117,120	0
19	CLA	4	305	50/65	0.93	0.12	107,126,138,142	0
18	BCR	A	848	40/40	0.93	0.17	75,105,142,143	0
19	CLA	A	821	65/65	0.94	0.12	60,86,95,101	0
19	CLA	A	822	60/65	0.94	0.11	94,114,155,161	0
18	BCR	I	101	40/40	0.94	0.13	72,86,105,107	0
19	CLA	A	827	65/65	0.94	0.13	69,87,107,114	0
18	BCR	1	503	19/40	0.94	0.13	121,134,143,146	0
19	CLA	A	832	65/65	0.94	0.13	62,81,91,98	0
19	CLA	A	834	65/65	0.94	0.11	79,98,117,132	0
18	BCR	A	849	40/40	0.94	0.17	69,91,119,124	0
19	CLA	4	311	46/65	0.94	0.10	109,121,132,139	0
20	CHL	1	521	56/66	0.94	0.13	100,112,123,126	0
19	CLA	4	315	65/65	0.94	0.13	74,96,118,123	0
17	LUT	1	501	42/42	0.94	0.13	105,125,144,146	0
19	CLA	1	507	65/65	0.94	0.12	77,101,114,120	0
19	CLA	A	807	60/65	0.94	0.10	67,88,115,118	0
19	CLA	B	815	65/65	0.94	0.13	84,97,119,123	0
19	CLA	A	811	65/65	0.94	0.10	56,73,87,108	0
19	CLA	B	817	60/65	0.94	0.12	87,97,110,129	0
19	CLA	B	821	46/65	0.94	0.10	86,100,118,122	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
19	CLA	A	812	55/65	0.94	0.13	80,104,117,123	0
19	CLA	B	825	65/65	0.94	0.11	48,64,93,98	0
19	CLA	B	827	65/65	0.94	0.15	54,77,98,103	0
19	CLA	B	830	65/65	0.94	0.11	50,63,97,110	0
19	CLA	1	508	65/65	0.94	0.13	89,115,123,137	0
19	CLA	B	833	60/65	0.94	0.10	59,75,106,107	0
19	CLA	B	839	65/65	0.94	0.13	54,70,104,119	0
19	CLA	2	504	60/65	0.94	0.11	99,111,133,136	0
19	CLA	A	815	45/65	0.94	0.11	108,124,153,163	0
19	CLA	3	308	65/65	0.94	0.14	118,129,139,143	0
19	CLA	4	304	60/65	0.94	0.12	99,113,137,139	0
27	CL0	A	801	65/65	0.94	0.11	48,59,71,80	0
19	CLA	A	818	56/65	0.94	0.12	79,107,125,133	0
19	CLA	A	820	50/65	0.94	0.13	88,110,136,137	0
19	CLA	4	306	65/65	0.95	0.12	74,105,121,130	0
19	CLA	B	834	55/65	0.95	0.09	66,88,118,124	0
19	CLA	B	835	55/65	0.95	0.11	54,68,96,100	0
19	CLA	B	836	65/65	0.95	0.09	48,61,68,73	0
19	CLA	A	833	65/65	0.95	0.11	67,85,101,113	0
19	CLA	4	308	60/65	0.95	0.11	64,85,96,102	0
19	CLA	1	506	55/65	0.95	0.12	89,115,132,141	0
18	BCR	L	302	40/40	0.95	0.12	77,84,97,97	0
19	CLA	G	202	55/65	0.95	0.09	109,131,152,153	0
19	CLA	A	837	65/65	0.95	0.11	69,88,110,121	0
18	BCR	4	301	40/40	0.95	0.14	105,124,131,136	0
18	BCR	B	856	40/40	0.95	0.11	42,57,69,76	0
19	CLA	J	1102	45/65	0.95	0.09	52,65,80,89	0
19	CLA	A	854	65/65	0.95	0.12	44,57,76,89	0
19	CLA	A	855	65/65	0.95	0.11	63,77,98,107	0
19	CLA	B	803	65/65	0.95	0.11	46,59,68,71	0
19	CLA	B	804	65/65	0.95	0.10	48,62,82,85	0
19	CLA	2	505	52/65	0.95	0.11	116,134,141,144	0
19	CLA	L	301	55/65	0.95	0.11	74,85,116,125	0
19	CLA	B	807	65/65	0.95	0.10	54,72,82,95	0
19	CLA	L	304	60/65	0.95	0.10	79,93,113,122	0
19	CLA	2	508	55/65	0.95	0.10	74,87,111,116	0
19	CLA	B	810	65/65	0.95	0.11	70,84,102,108	0
19	CLA	B	811	65/65	0.95	0.11	71,95,111,114	0
19	CLA	B	812	60/65	0.95	0.10	79,100,117,126	0
19	CLA	A	805	65/65	0.95	0.11	54,71,89,93	0
20	CHL	2	513	48/66	0.95	0.11	91,105,114,141	0
20	CHL	2	515	46/66	0.95	0.09	113,121,131,142	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
18	BCR	B	802	40/40	0.95	0.13	57,71,85,94	0
19	CLA	A	809	65/65	0.95	0.11	51,65,99,102	0
19	CLA	B	818	65/65	0.95	0.12	66,82,104,109	0
19	CLA	A	824	65/65	0.95	0.12	67,85,106,124	0
20	CHL	4	314	51/66	0.95	0.13	89,114,129,133	0
19	CLA	A	826	55/65	0.95	0.11	59,71,96,109	0
19	CLA	A	810	50/65	0.95	0.11	78,96,106,121	0
19	CLA	A	828	65/65	0.95	0.12	53,67,78,88	0
19	CLA	B	828	65/65	0.95	0.12	60,71,91,103	0
19	CLA	B	829	65/65	0.95	0.12	50,67,92,100	0
19	CLA	A	829	65/65	0.95	0.12	60,75,86,95	0
28	SF4	A	843	8/8	0.95	0.14	45,78,104,173	0
21	LHG	B	842	21/49	0.95	0.09	69,92,102,116	0
18	BCR	A	852	40/40	0.95	0.12	45,55,71,75	0
19	CLA	A	825	65/65	0.96	0.11	64,79,85,89	0
19	CLA	A	803	65/65	0.96	0.10	49,64,79,83	0
19	CLA	B	809	65/65	0.96	0.11	66,82,95,126	0
21	LHG	A	853	49/49	0.96	0.10	49,60,72,79	0
19	CLA	2	506	65/65	0.96	0.11	88,121,139,150	0
19	CLA	A	819	65/65	0.96	0.13	77,88,99,104	0
19	CLA	B	832	58/65	0.96	0.08	48,60,76,78	0
19	CLA	A	840	65/65	0.96	0.10	43,58,88,96	0
19	CLA	B	813	46/65	0.96	0.08	84,95,120,135	0
19	CLA	4	312	50/65	0.96	0.10	79,91,116,121	0
19	CLA	A	830	65/65	0.96	0.10	46,58,72,78	0
19	CLA	B	837	50/65	0.96	0.10	48,58,81,100	0
19	CLA	B	838	65/65	0.96	0.10	58,75,94,115	0
19	CLA	A	806	65/65	0.96	0.10	52,61,79,86	0
19	CLA	2	507	65/65	0.96	0.10	78,91,100,102	0
19	CLA	F	302	65/65	0.96	0.10	45,60,75,80	0
19	CLA	B	820	65/65	0.96	0.12	61,78,98,105	0
19	CLA	A	808	65/65	0.96	0.10	54,65,82,91	0
19	CLA	4	307	60/65	0.96	0.10	73,86,97,99	0
19	CLA	B	823	55/65	0.96	0.09	54,74,98,105	0
19	CLA	B	824	65/65	0.96	0.10	59,69,90,93	0
19	CLA	B	806	65/65	0.96	0.12	58,72,82,99	0
19	CLA	J	1101	65/65	0.96	0.09	48,64,87,101	0
29	PQN	B	841	33/33	0.96	0.10	49,64,82,85	0
19	CLA	B	826	65/65	0.96	0.10	52,69,80,84	0
19	CLA	A	839	65/65	0.97	0.08	44,53,62,70	0
25	CA	B	848	1/1	0.97	0.09	83,83,83,83	0
19	CLA	A	802	65/65	0.97	0.09	42,50,63,75	0

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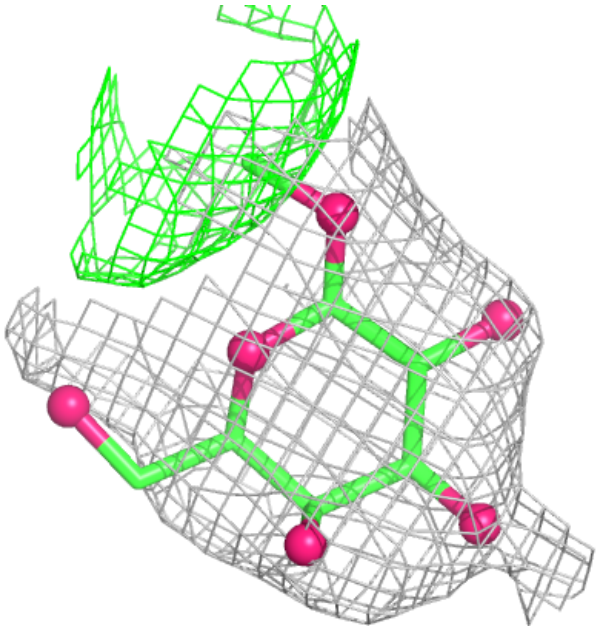
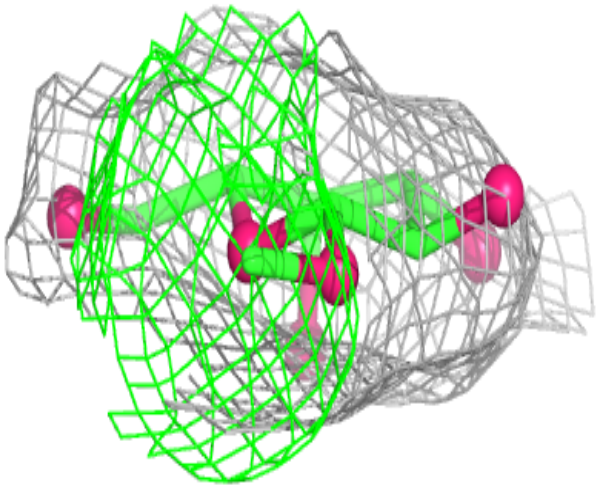
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
19	CLA	B	814	65/65	0.97	0.10	71,80,87,92	0
29	PQN	A	844	33/33	0.97	0.09	42,54,68,74	0
19	CLA	B	819	65/65	0.97	0.10	69,76,96,101	0
19	CLA	A	841	65/65	0.97	0.09	44,57,65,67	0
28	SF4	C	101	8/8	0.99	0.10	53,58,74,74	0

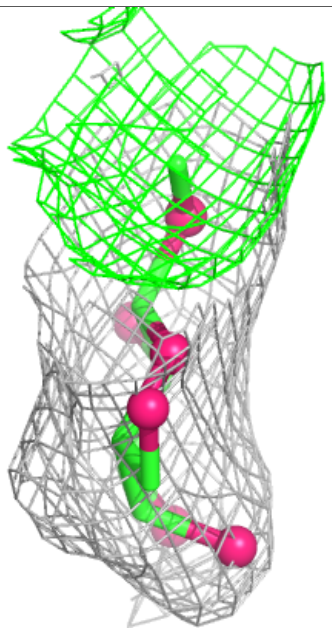
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around LMG 2 520:

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

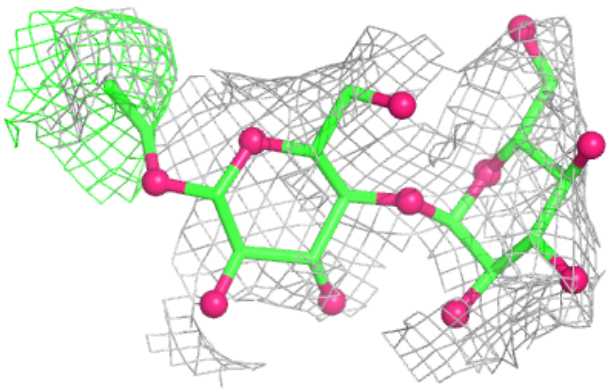


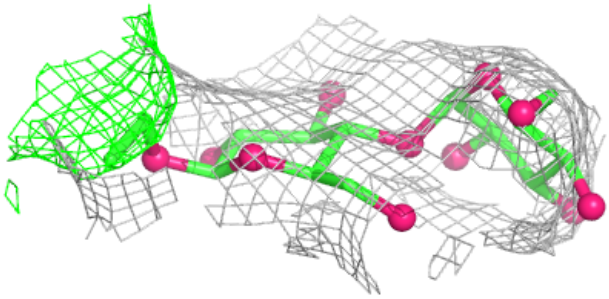


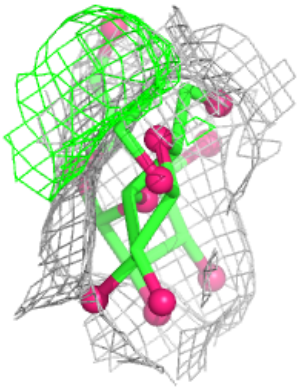


Electron density around LMT J 1107:

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



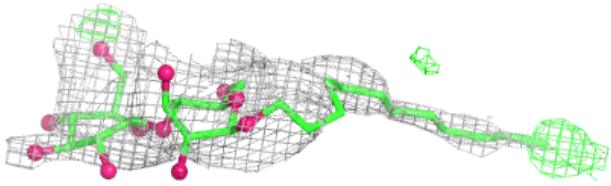


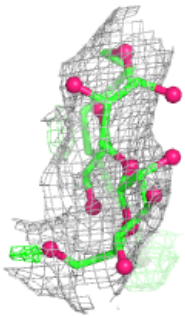


Electron density around LMT 2 523:

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

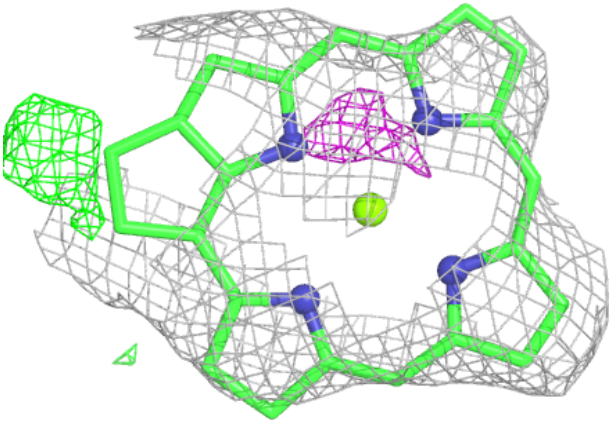


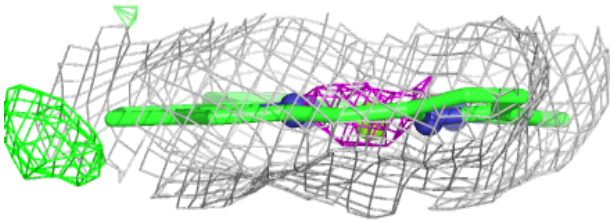


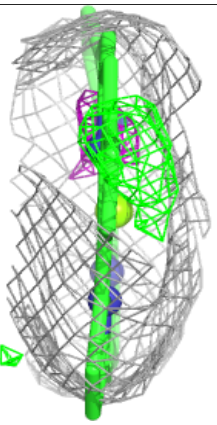


Electron density around CLA K 1004:

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

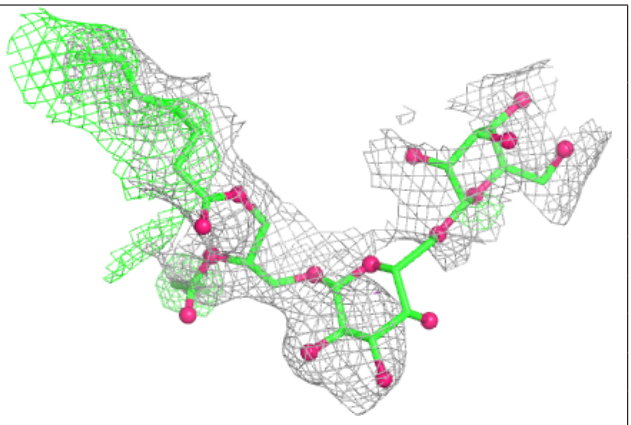


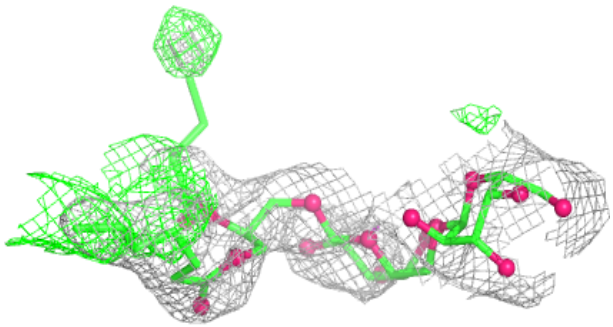


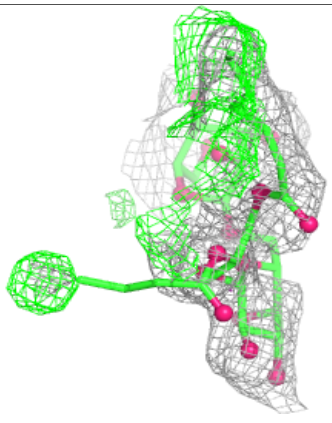


Electron density around DGD B 801:

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

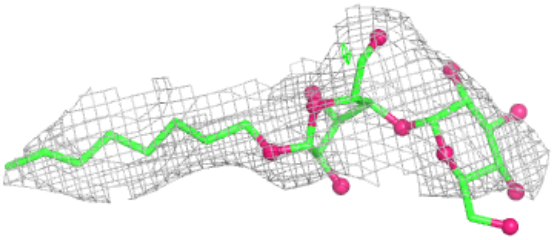


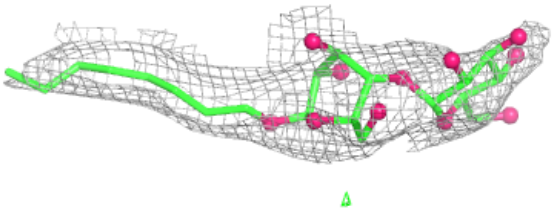


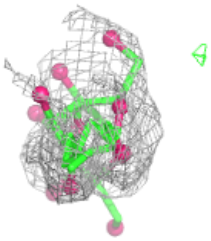


Electron density around LMT G 209:

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

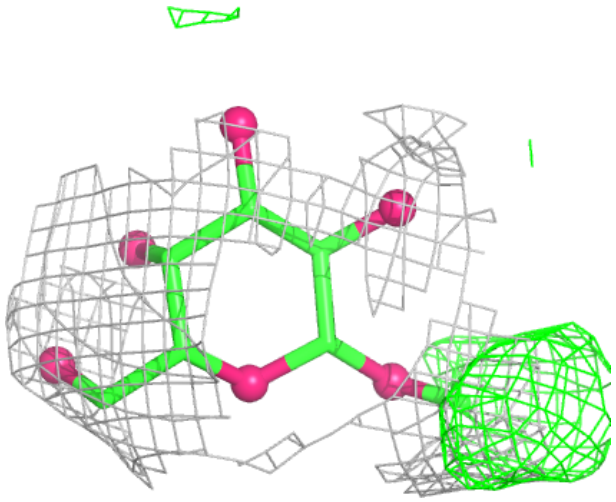


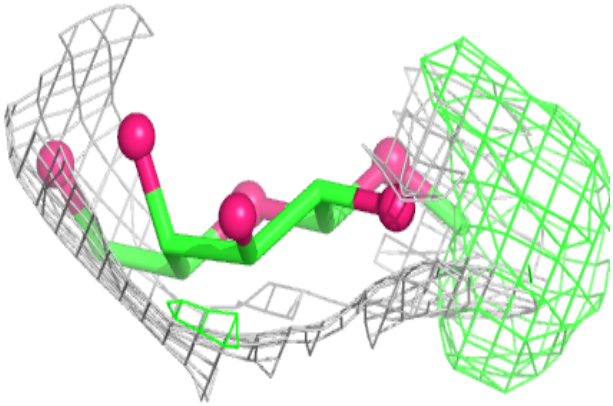


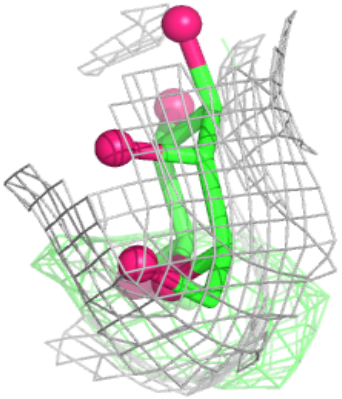


Electron density around LMG 2 522:

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

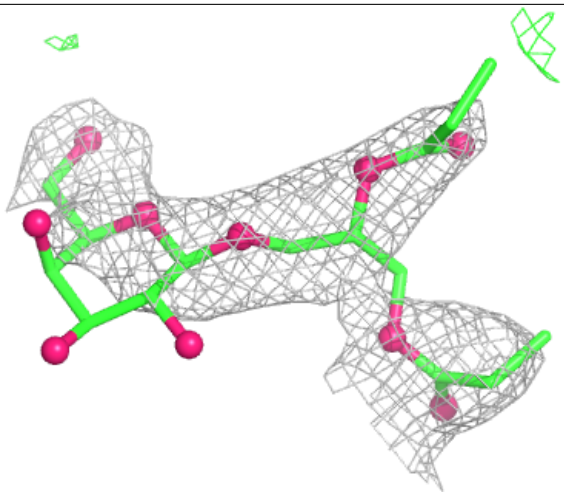


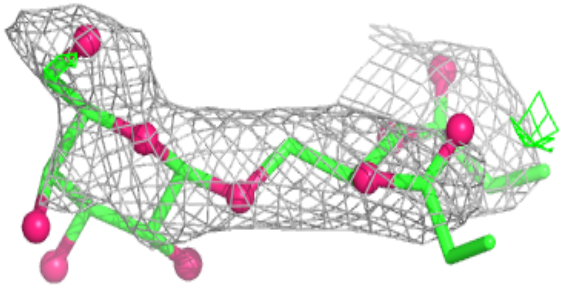


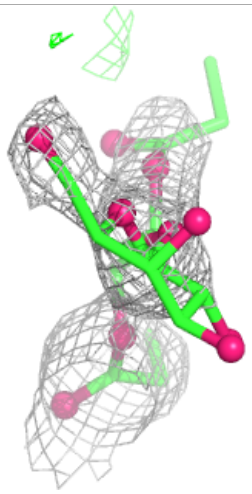


Electron density around LMG G 210:

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

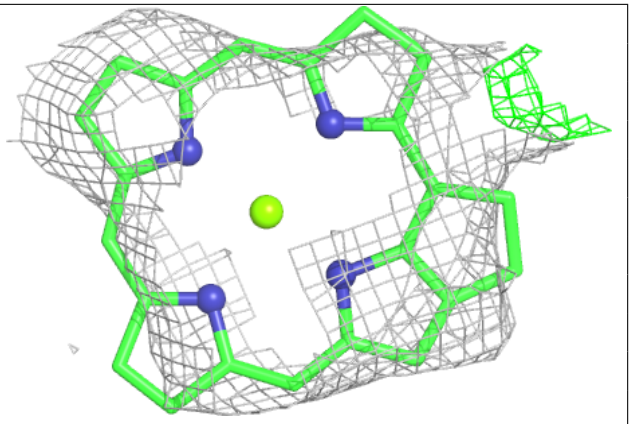


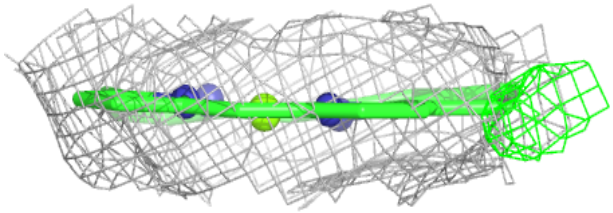


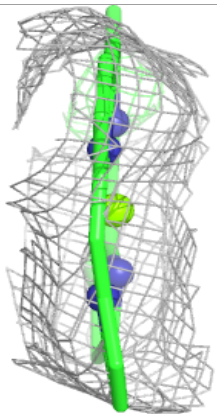


Electron density around CLA K 1003:

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

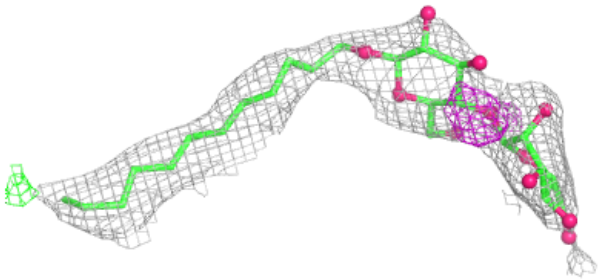


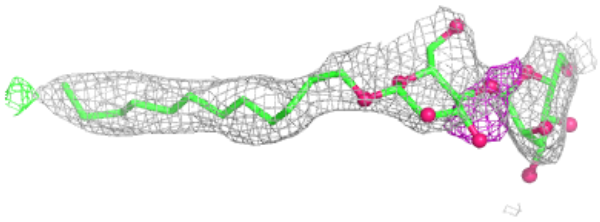


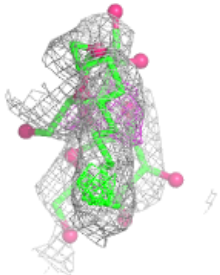


Electron density around LMT A 846:

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

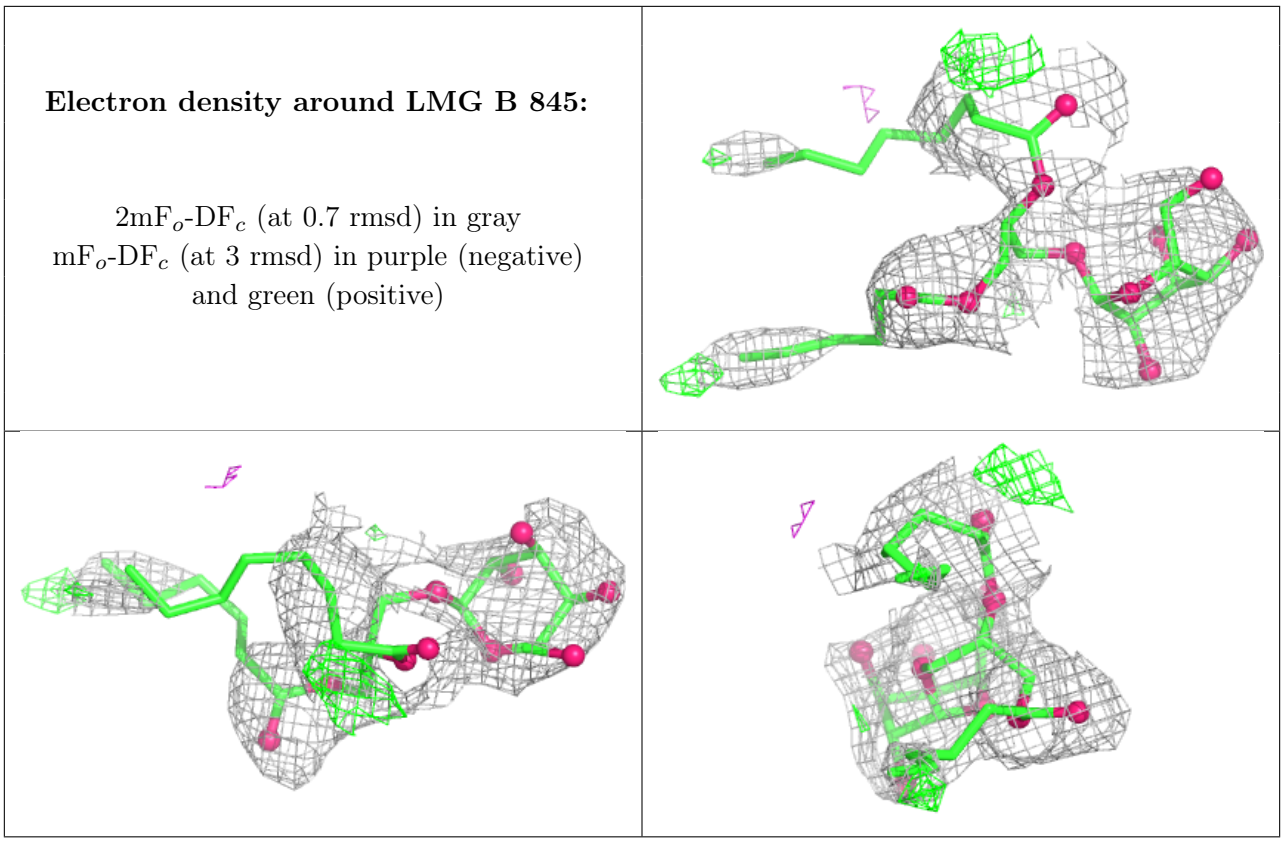






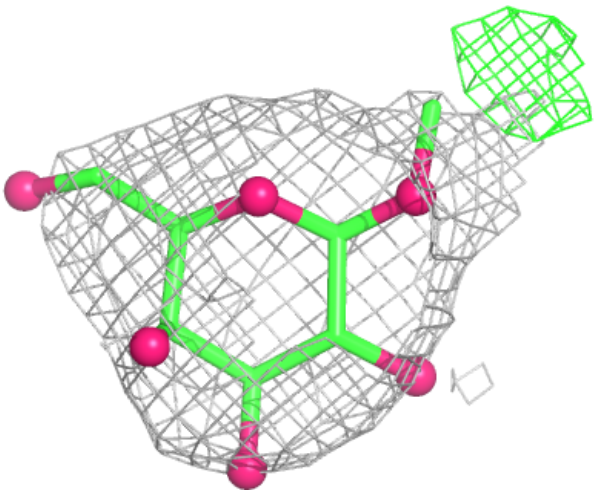
Electron density around LMG B 845:

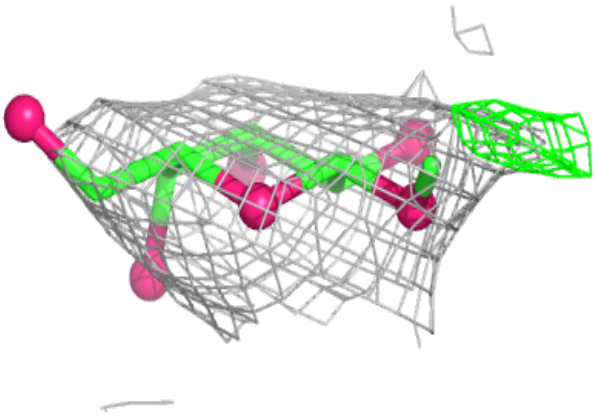
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

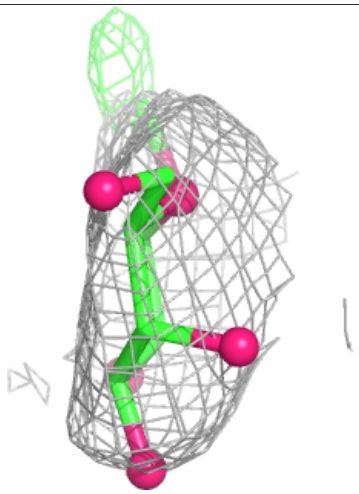


Electron density around LMG 2 524:

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

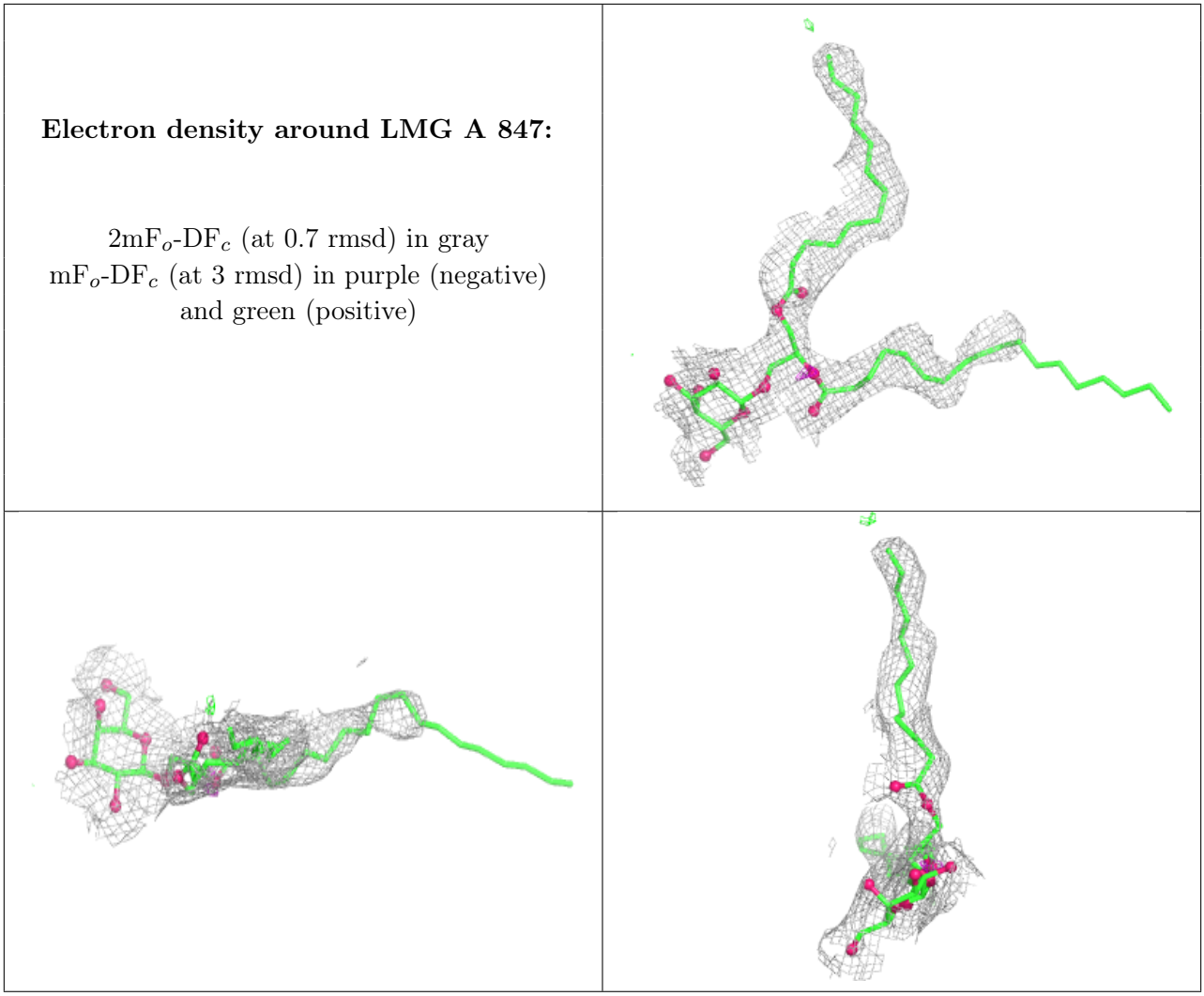






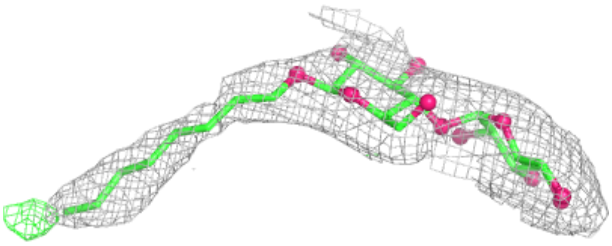
Electron density around LMG A 847:

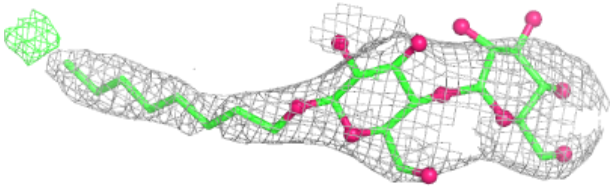
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

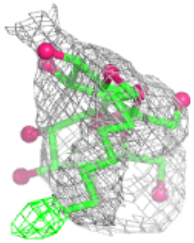


Electron density around LMT 3 318:

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

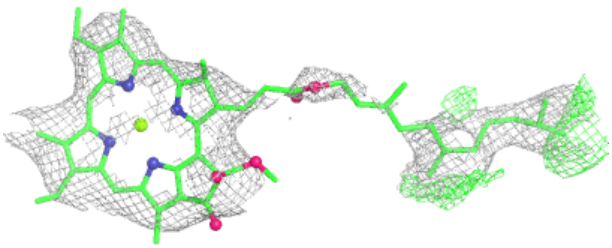


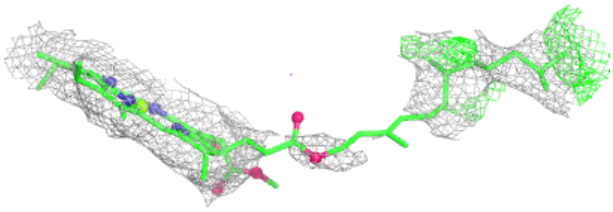


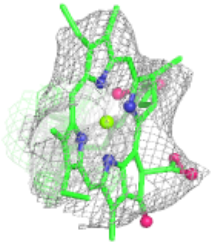


Electron density around CLA H 1000:

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

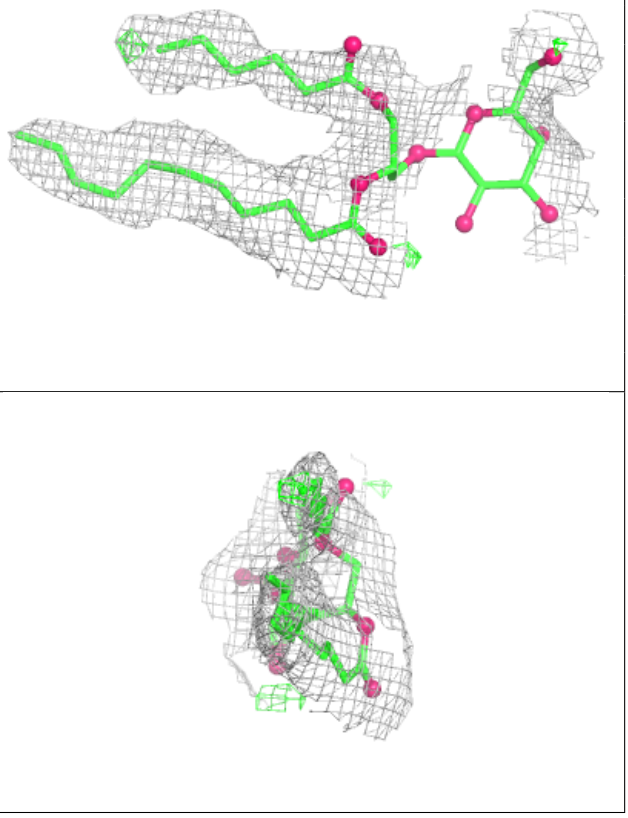


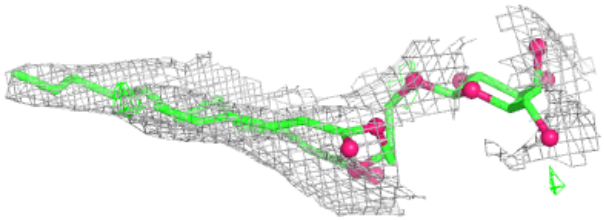




Electron density around LMG 2 519:

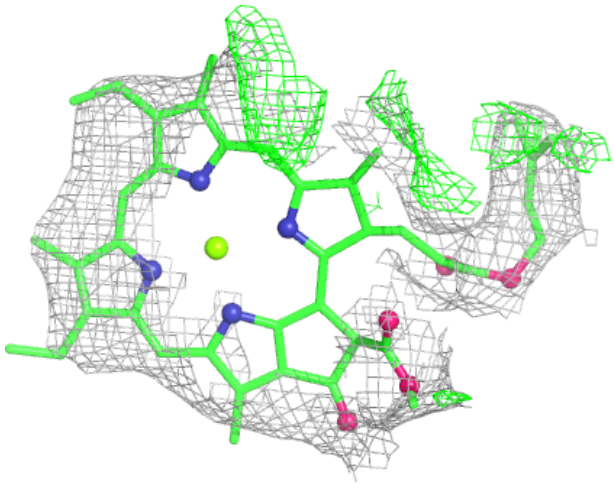
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

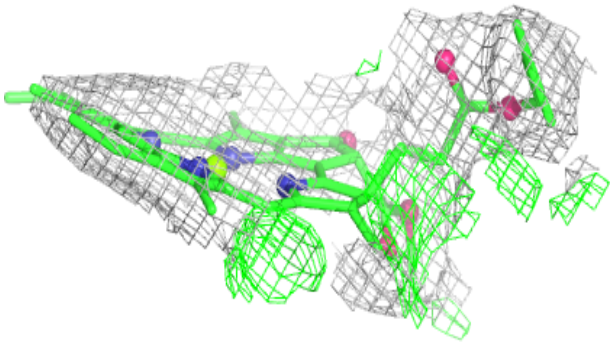




Electron density around CLA J 1105:

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

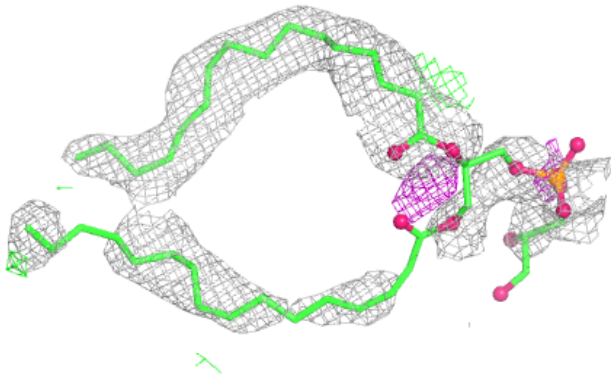


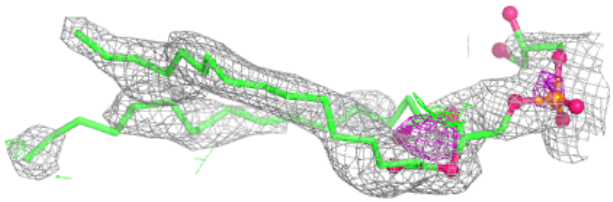


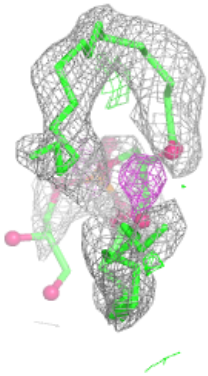


Electron density around LHG B 843:

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

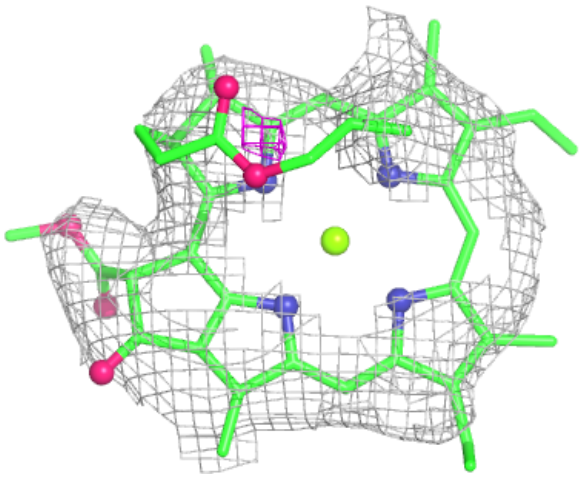


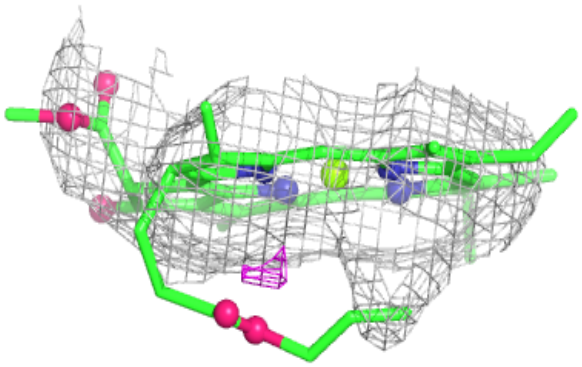




Electron density around CLA 3 312:

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

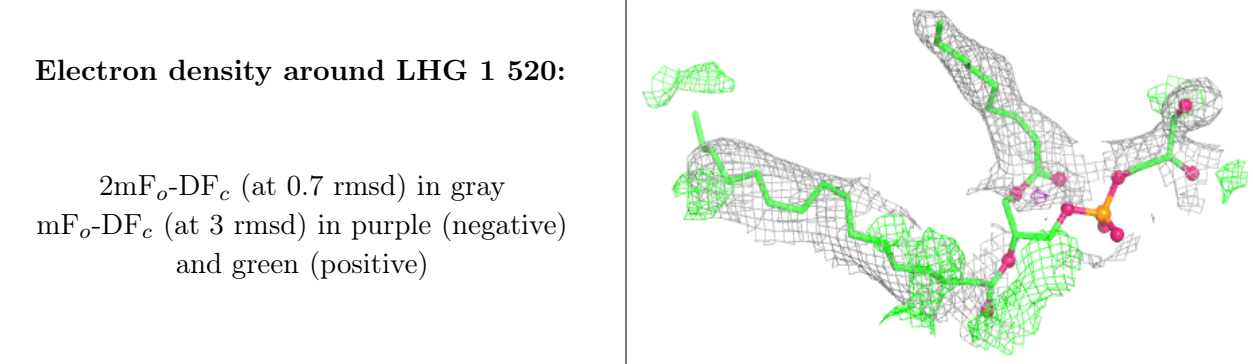


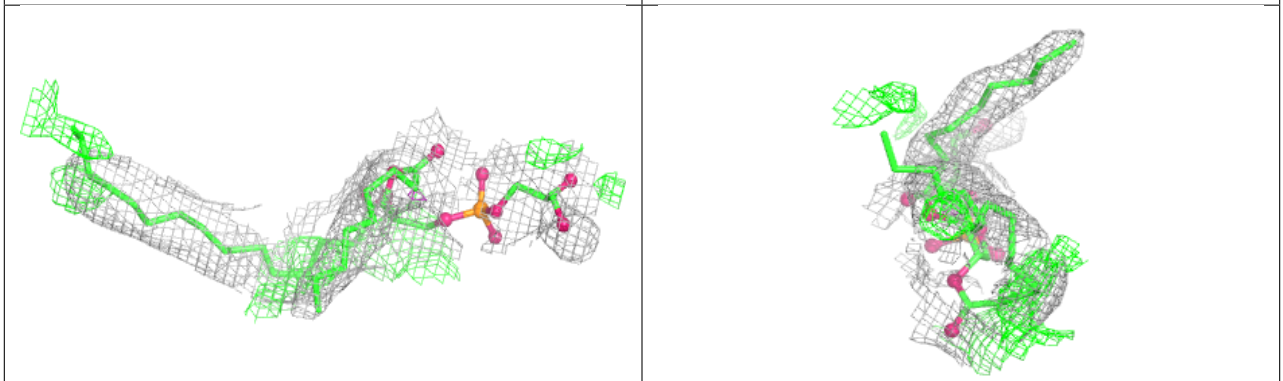




Electron density around LHG 1 520:

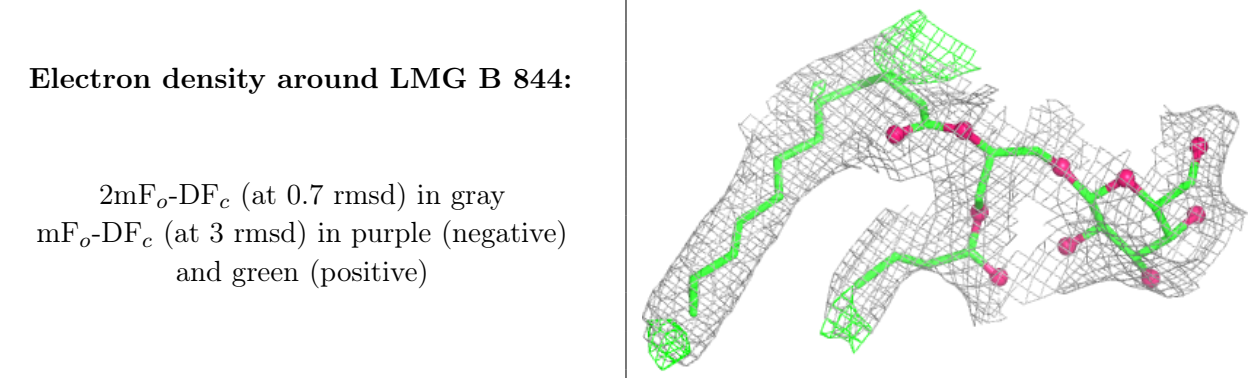
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

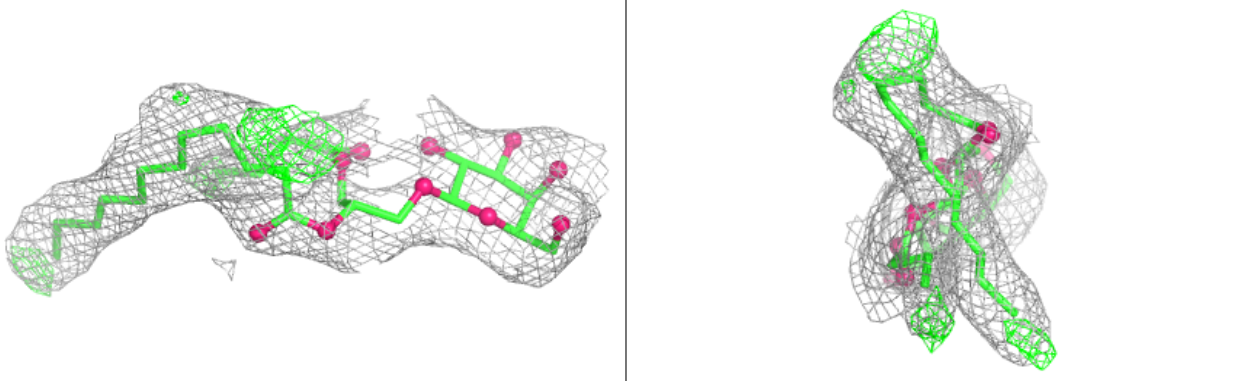




Electron density around LMG B 844:

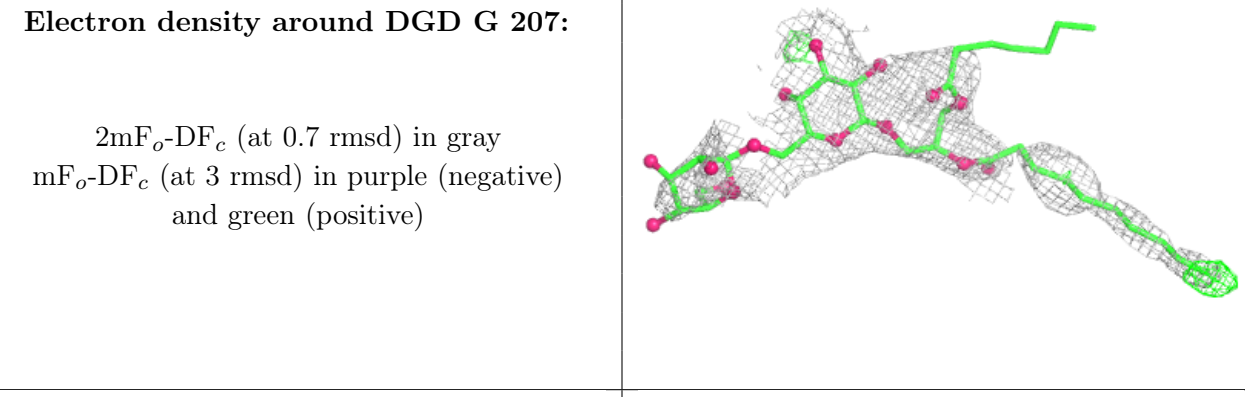
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)





Electron density around DGD G 207:

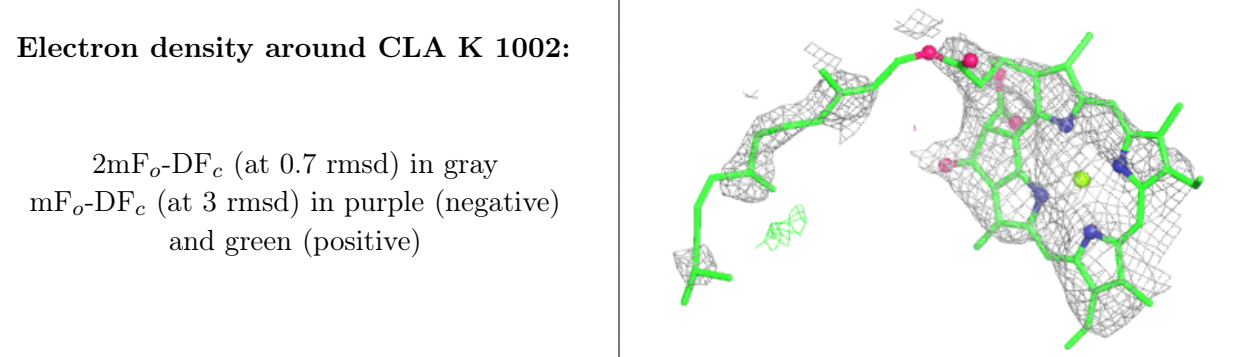
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

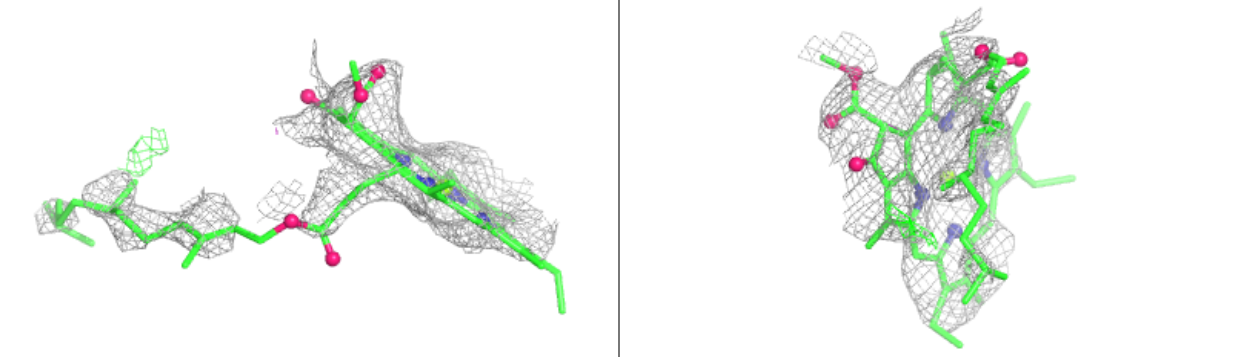




Electron density around CLA K 1002:

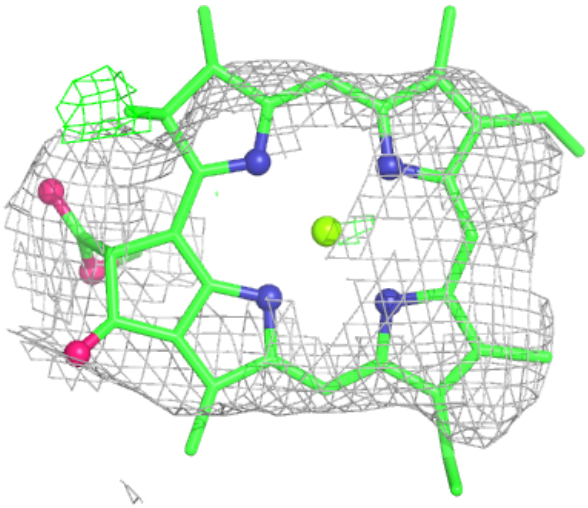
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

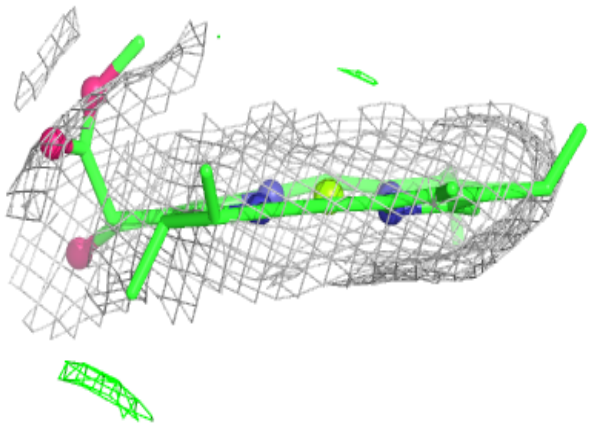


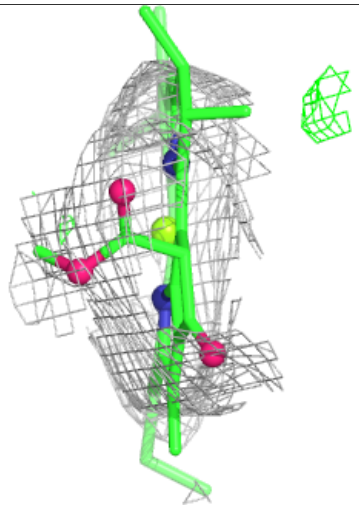


Electron density around CLA 3 311:

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

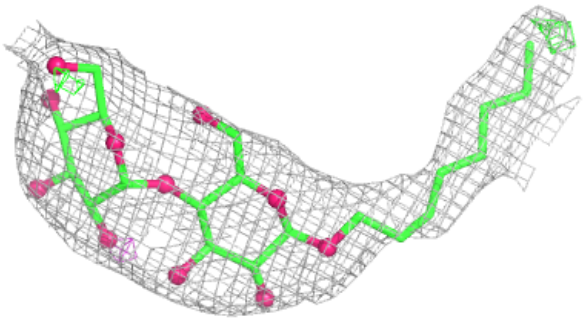


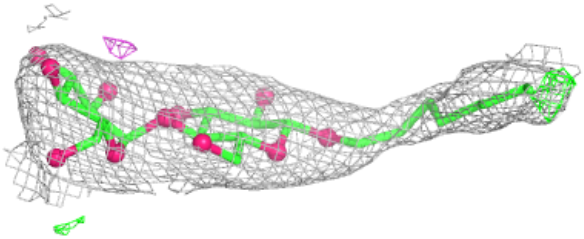


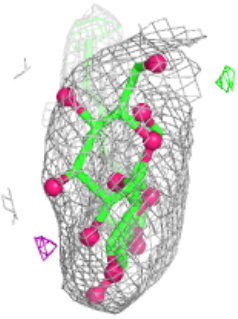


Electron density around LMT B 855:

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

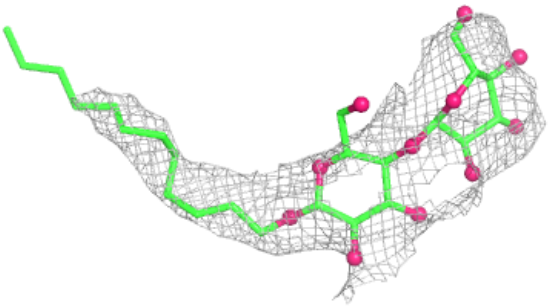


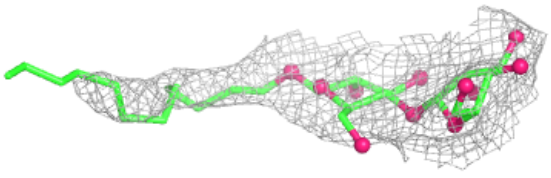




Electron density around LMT B 846:

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

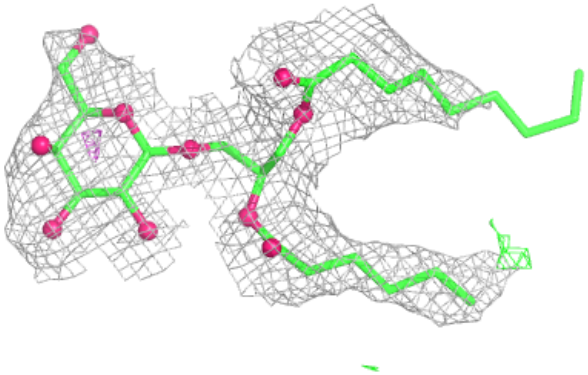


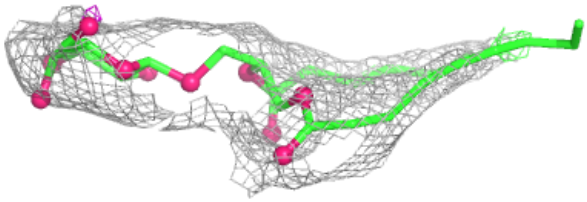


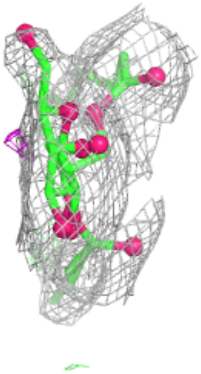


Electron density around LMG J 1104:

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



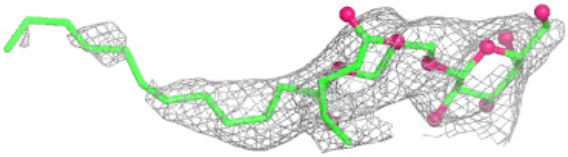


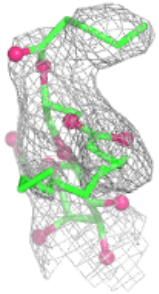


Electron density around LMG F 305:

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

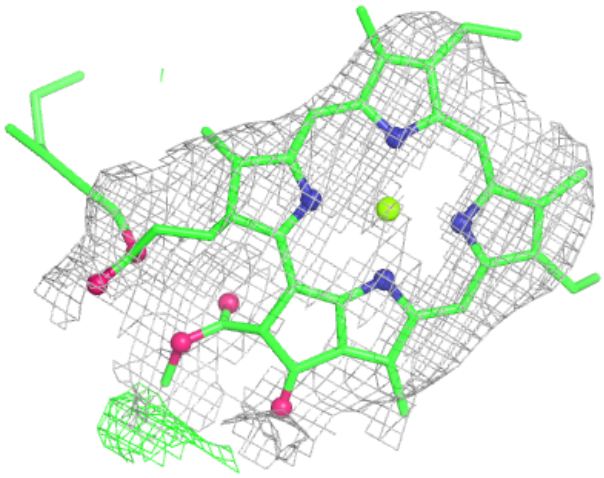


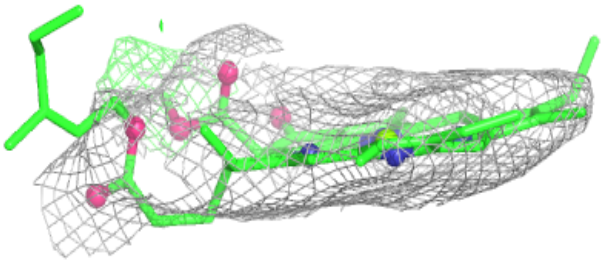


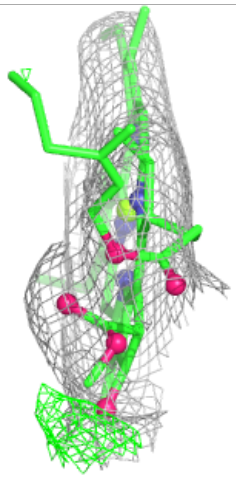


Electron density around CLA 3 306:

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

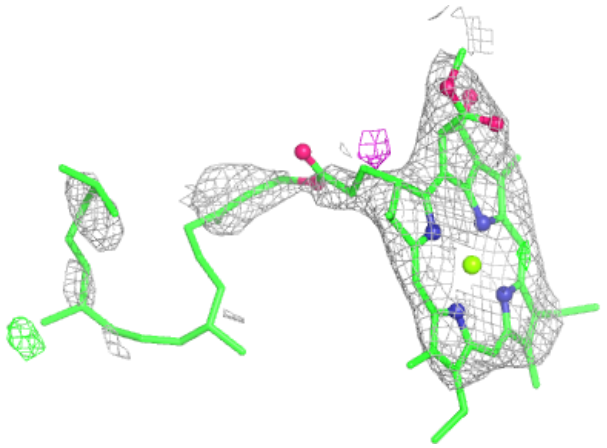


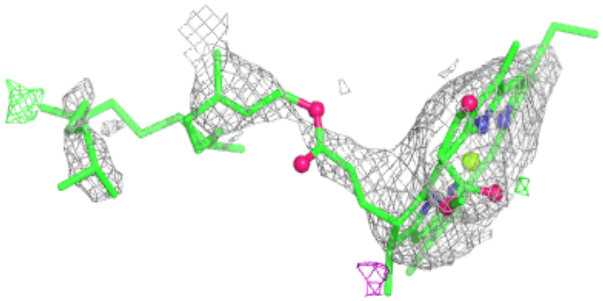


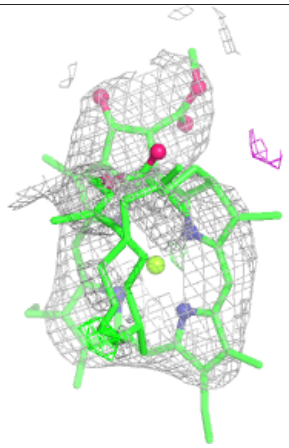


Electron density around CLA 1 513:

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

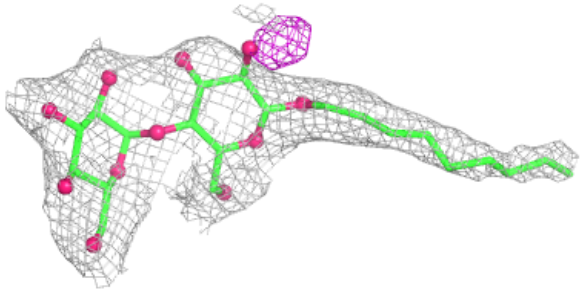


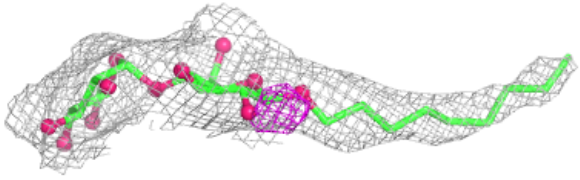


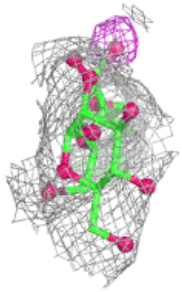


Electron density around LMT B 847:

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

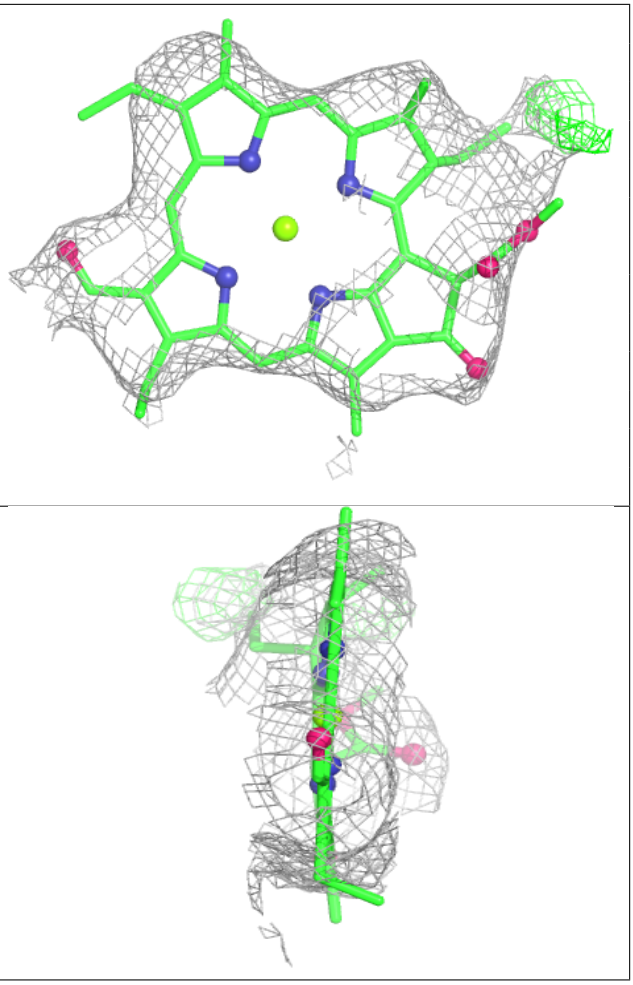






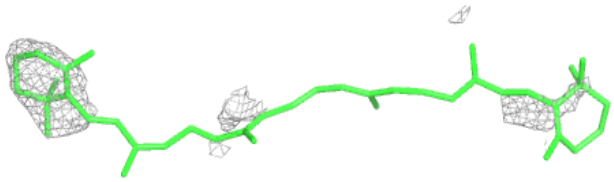
Electron density around CHL 4 317:

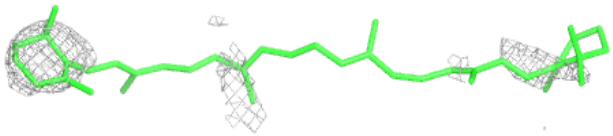
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

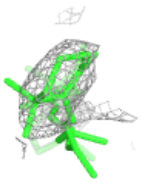


Electron density around BCR K 1005:

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

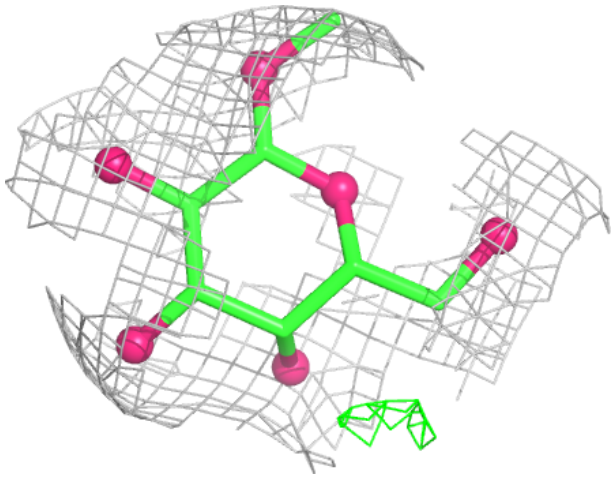


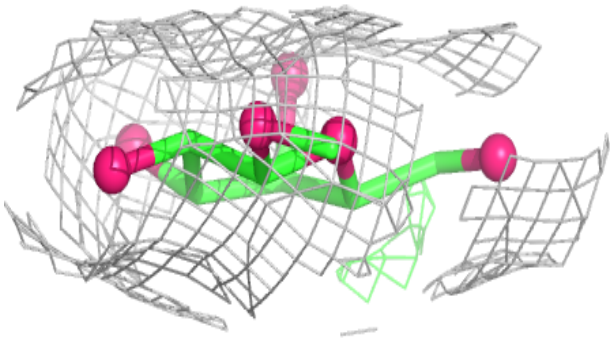


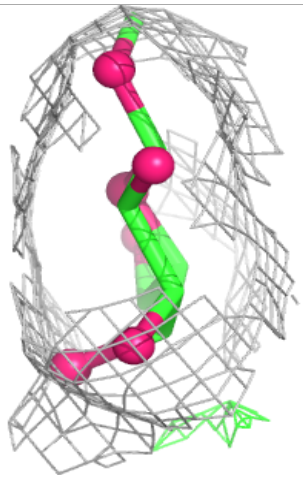


Electron density around LMG 1 519:

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

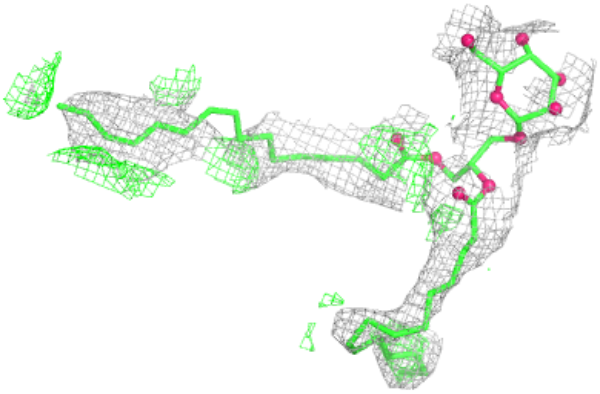


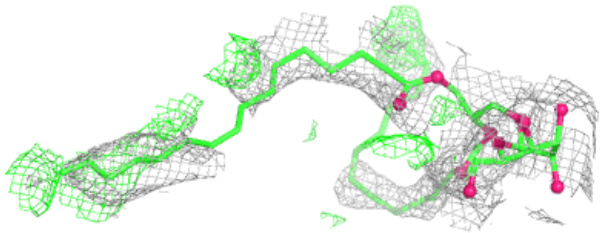


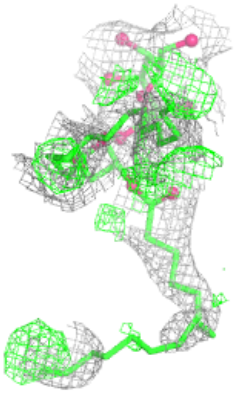


Electron density around LMG G 206:

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

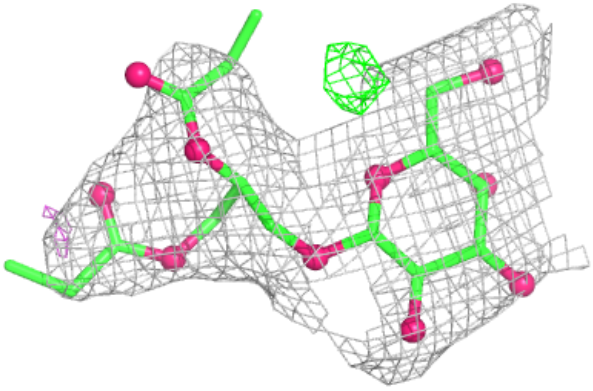


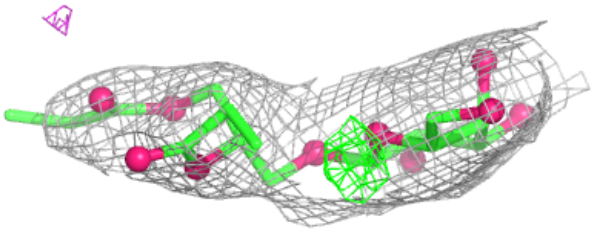


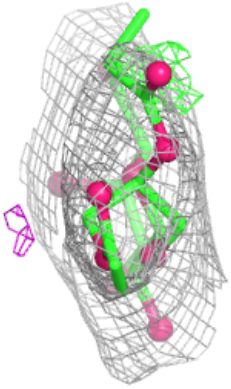


Electron density around LMG 2 518:

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

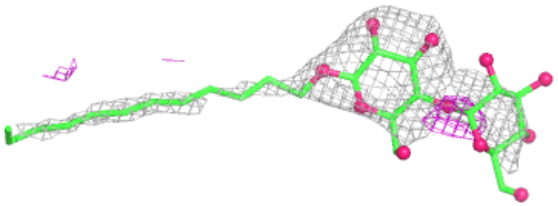


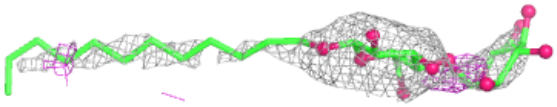


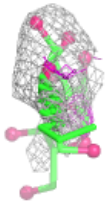


Electron density around LMT 4 320:

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

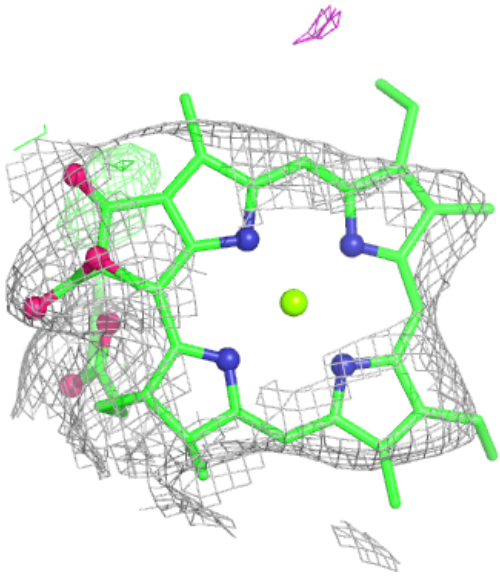


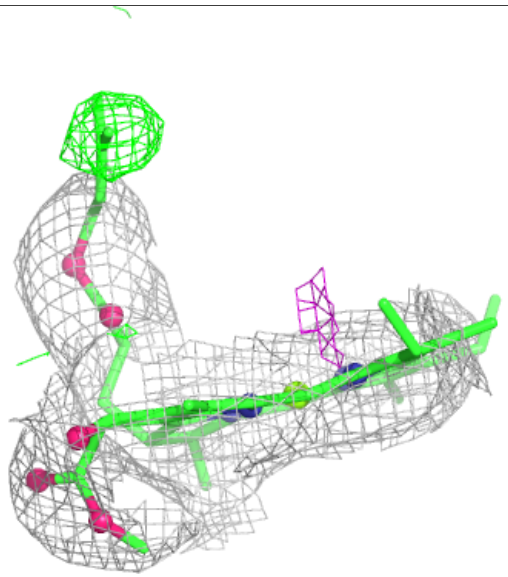


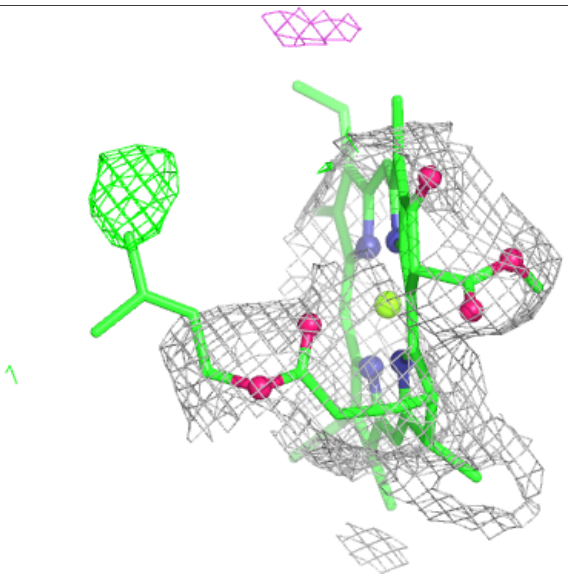


Electron density around CLA 3 310:

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

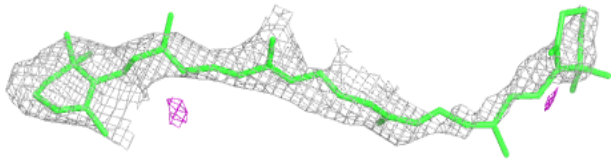


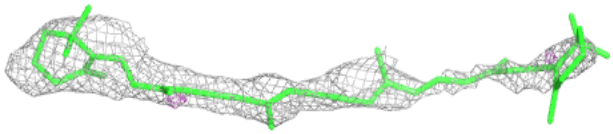


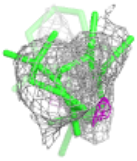


Electron density around BCR L 307:

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

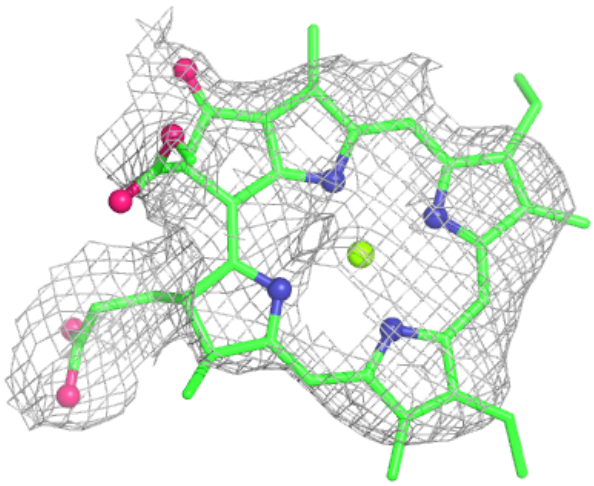


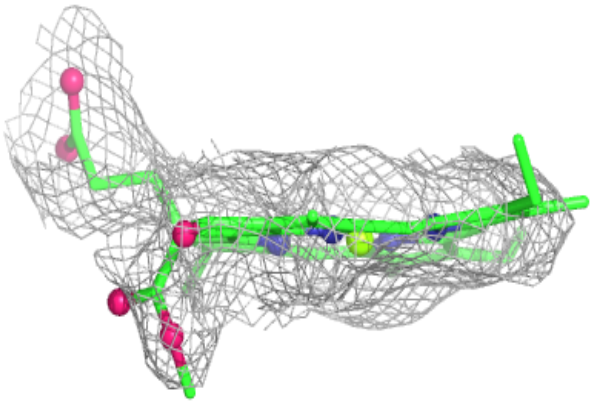


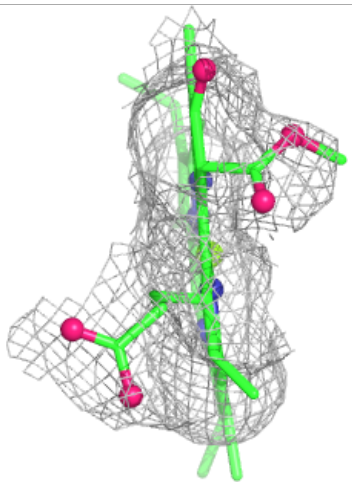


Electron density around CLA K 1001:

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

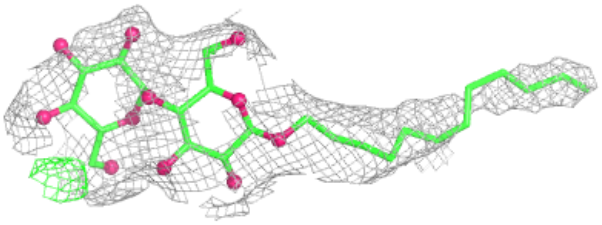


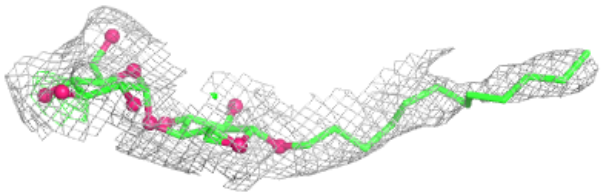


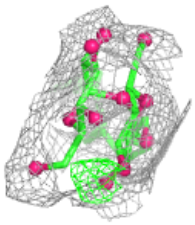


Electron density around LMT G 208:

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

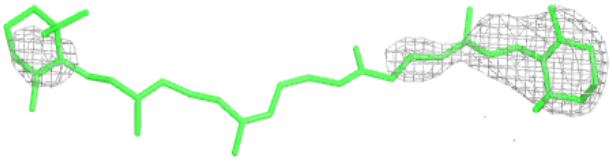


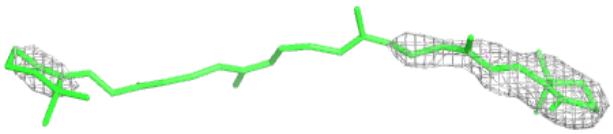


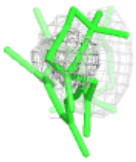


Electron density around BCR 3 304:

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

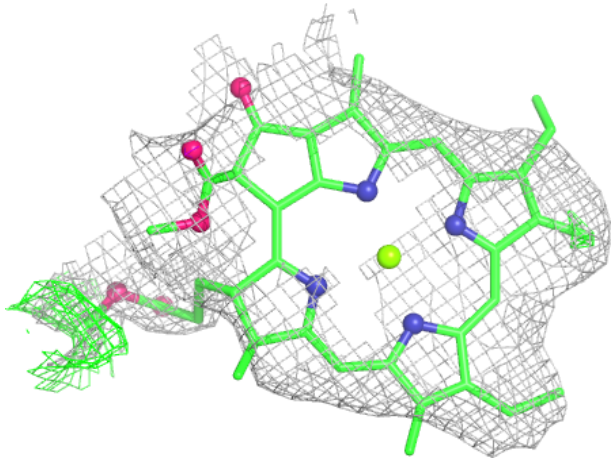


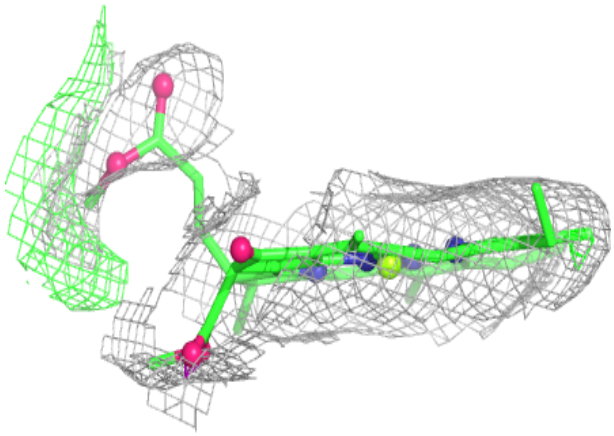




Electron density around CLA 1 510:

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

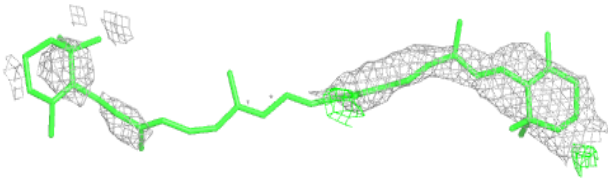


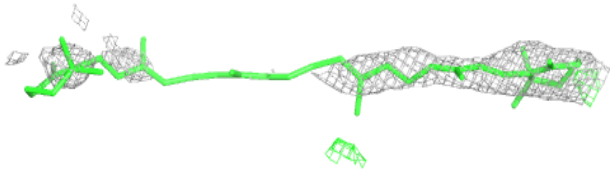


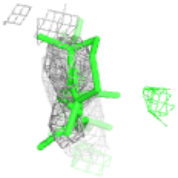


Electron density around BCR 2 503:

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

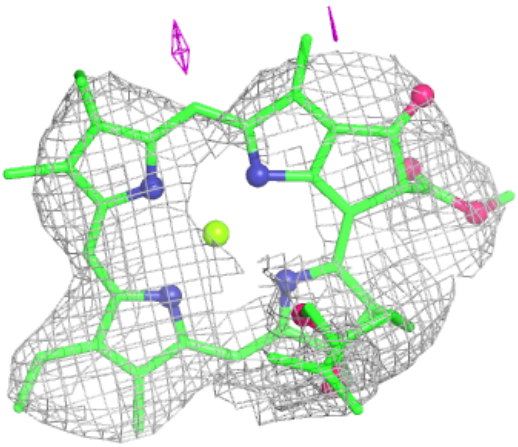


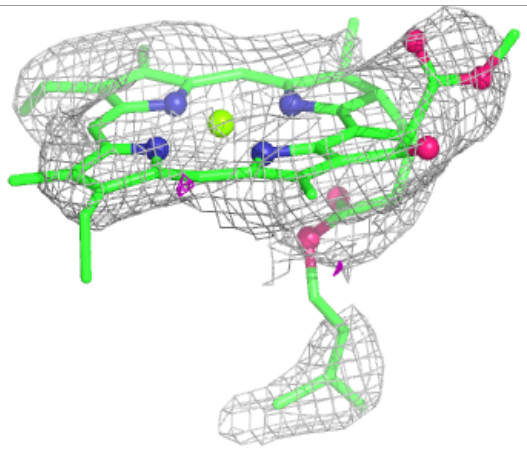


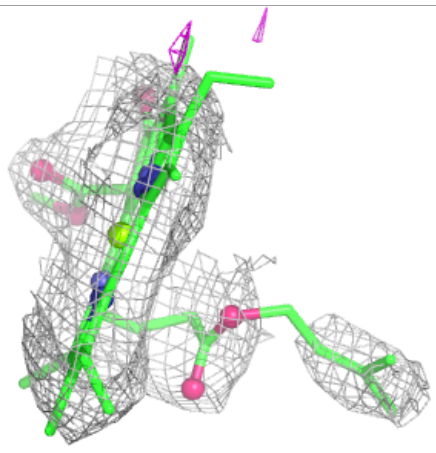


Electron density around CLA L 303:

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

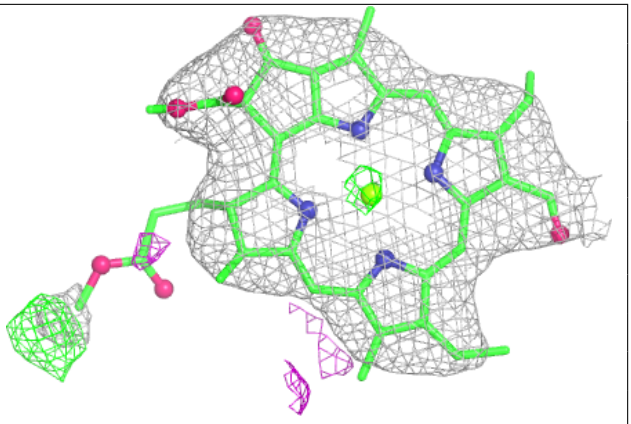


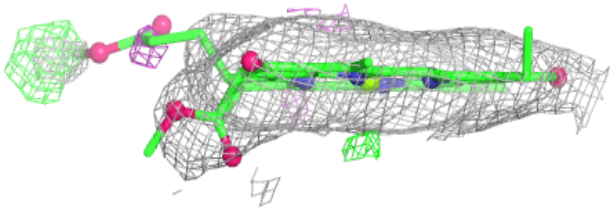


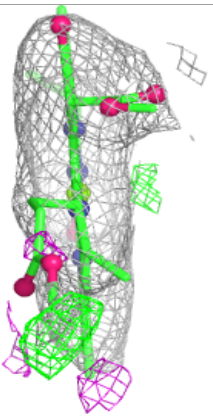


Electron density around CHL 4 313:

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

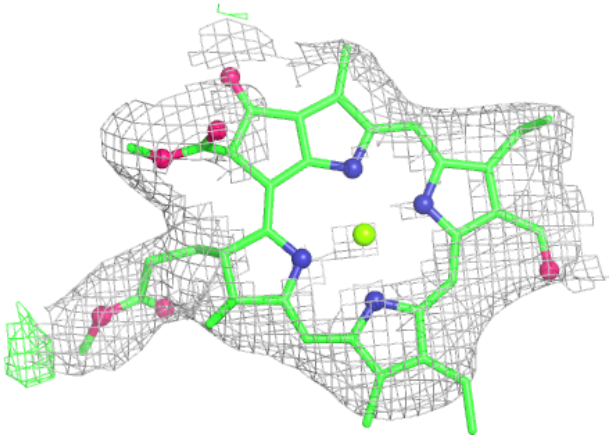


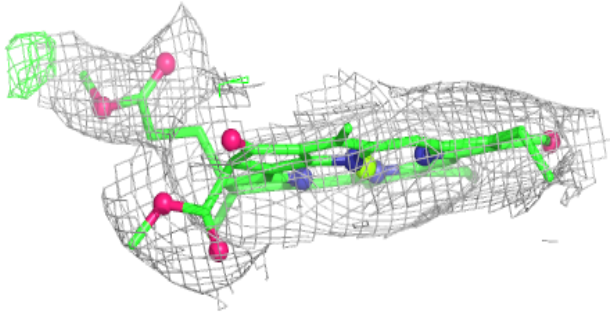


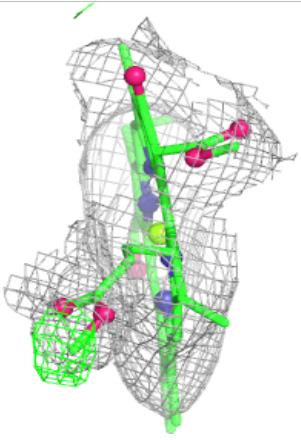


Electron density around CHL 2 512:

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



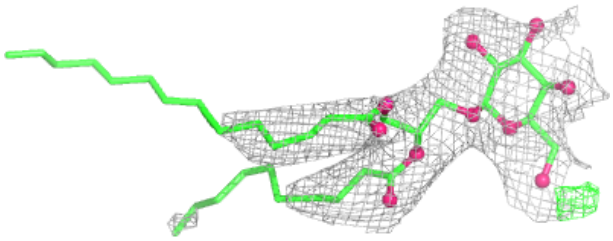


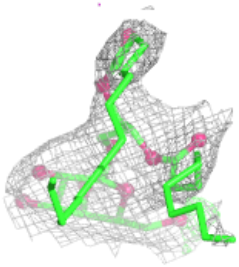


Electron density around LMG 4 322:

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

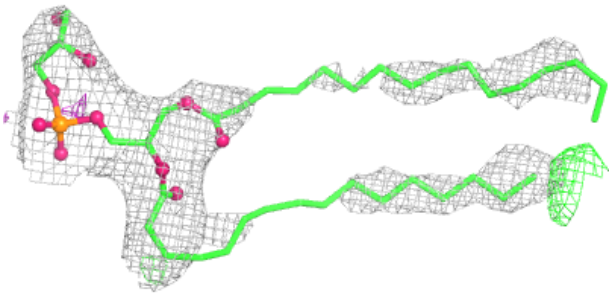


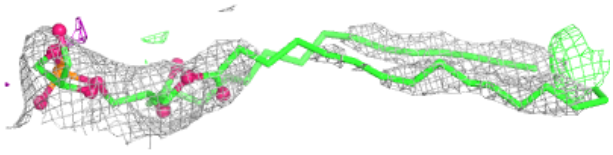




Electron density around LHG 1 517:

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

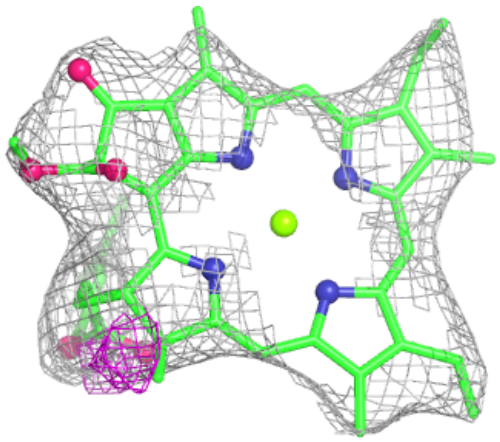


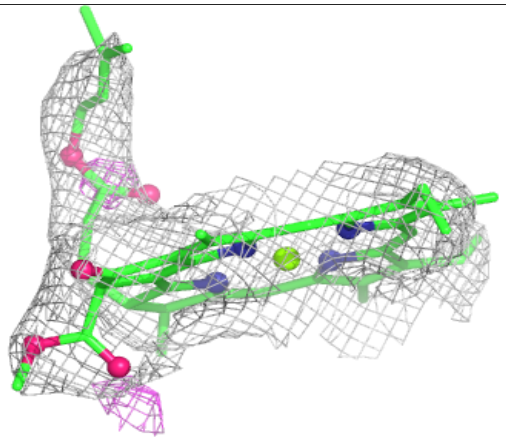


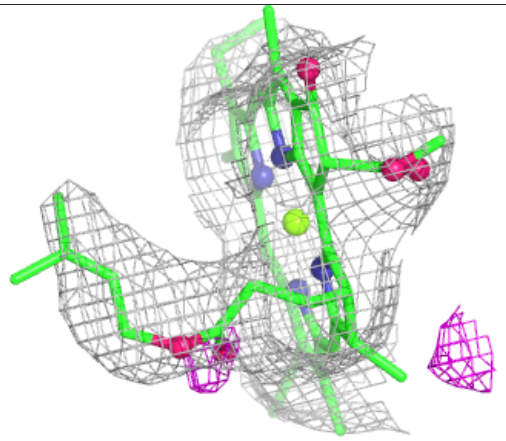


Electron density around CLA L 305:

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

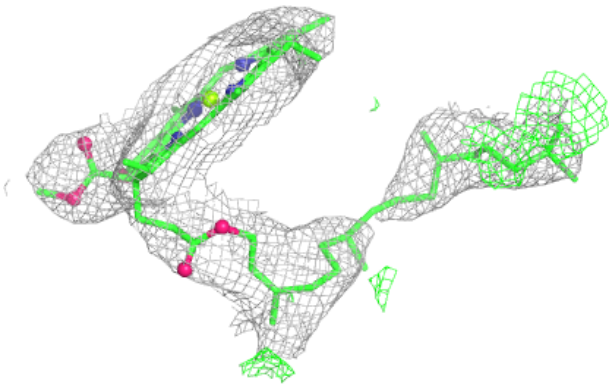


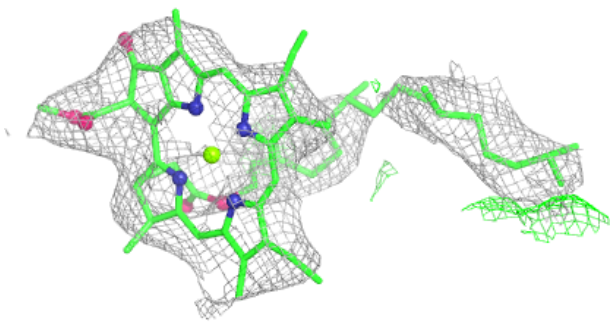


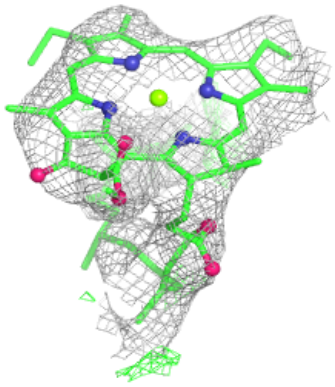


Electron density around CLA G 204:

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

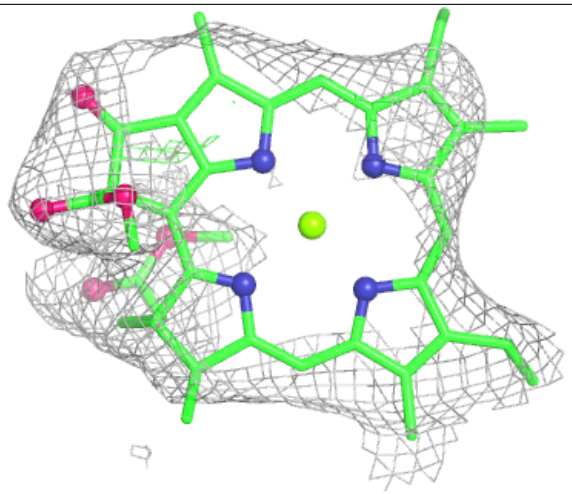


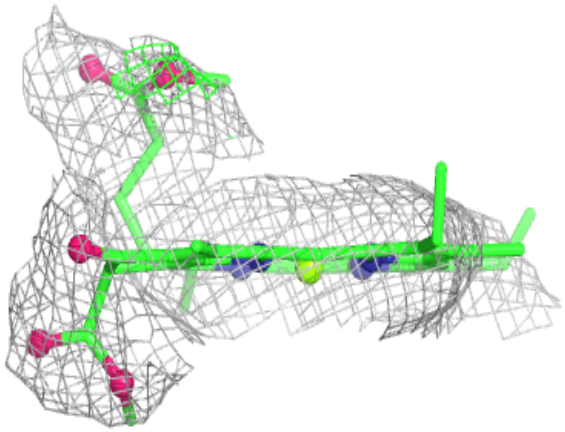


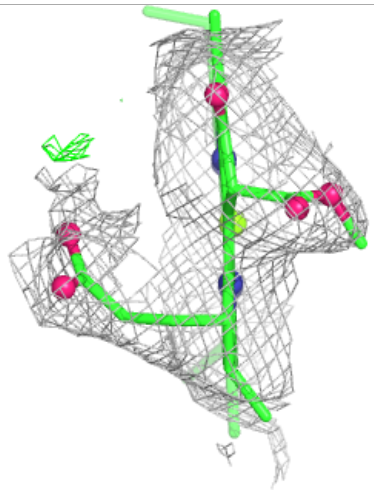


Electron density around CLA A 816:

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

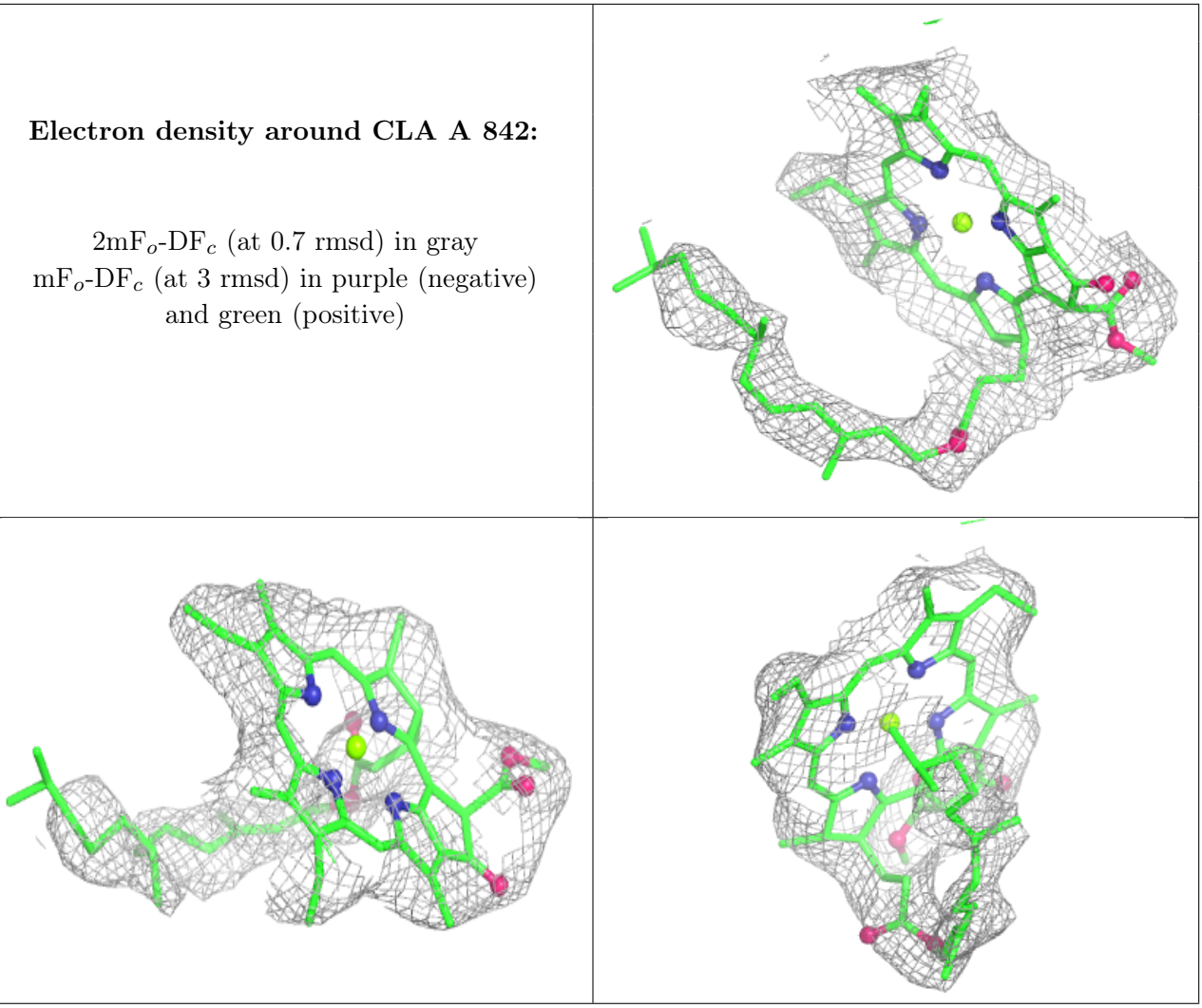






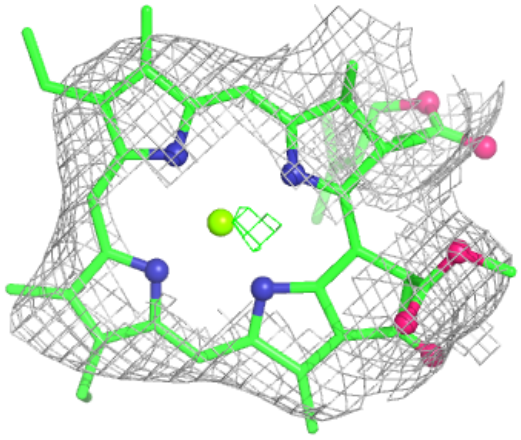
Electron density around CLA A 842:

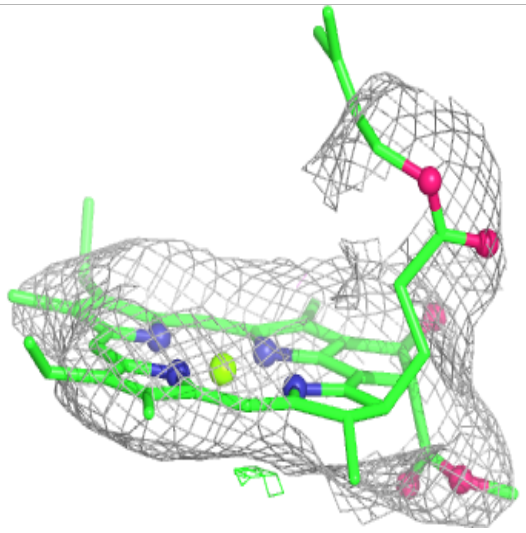
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

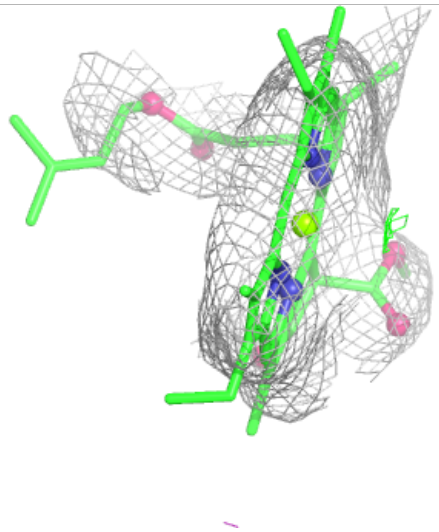


Electron density around CLA 1 509:

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

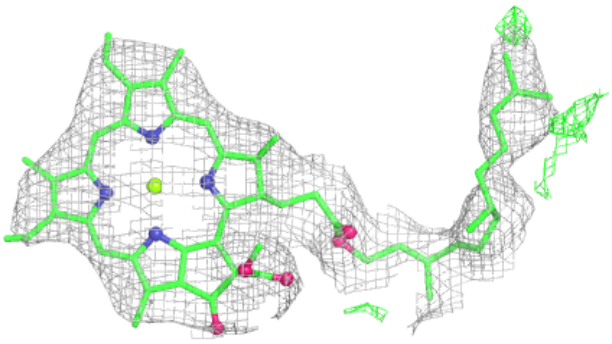


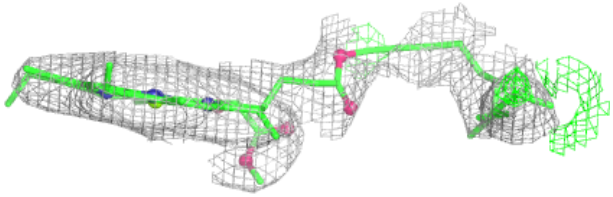


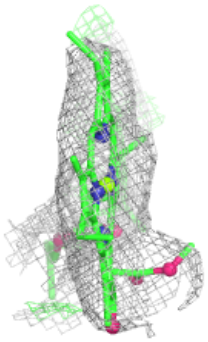


Electron density around CLA 1 516:

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

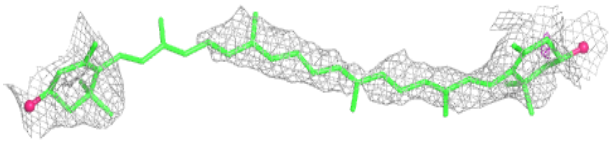


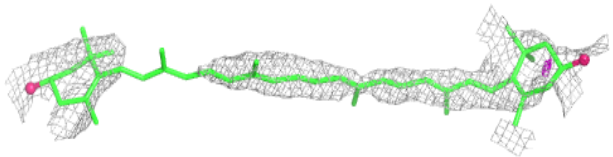


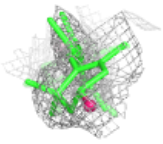


Electron density around LUT 3 301:

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

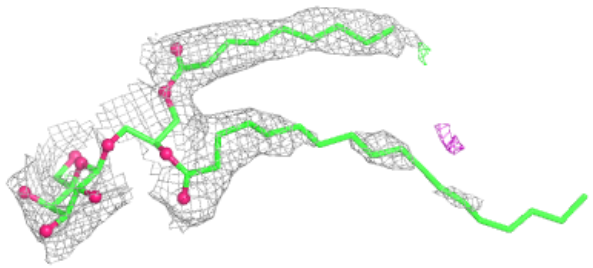


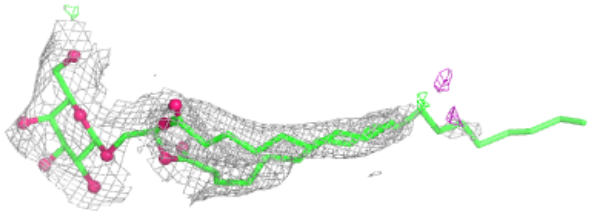




Electron density around LMG 1 518:

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

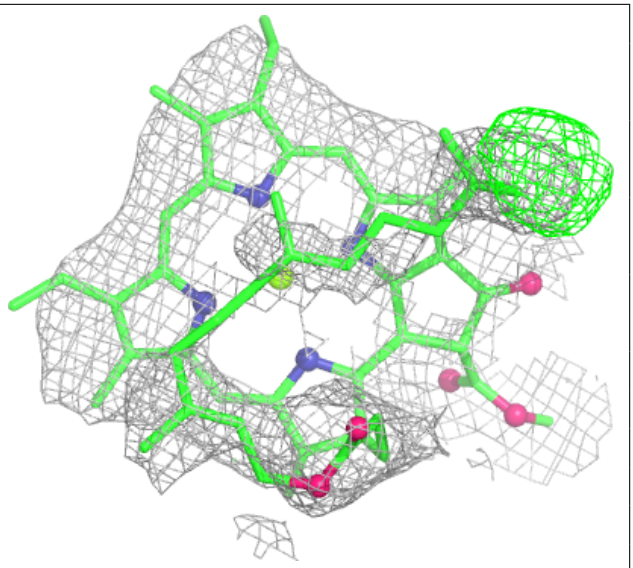


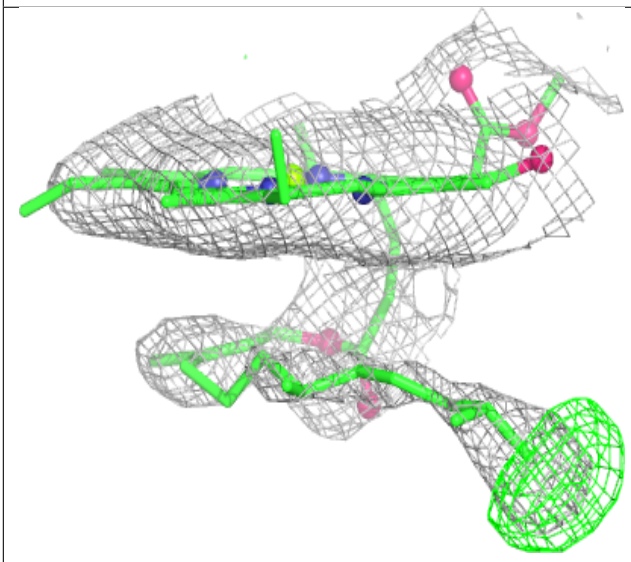


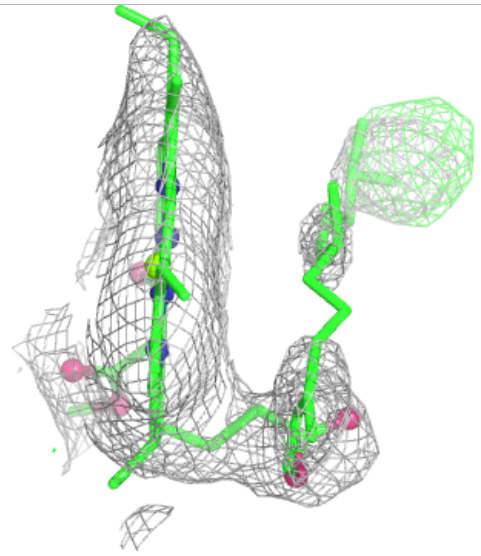


Electron density around CLA 3 313:

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

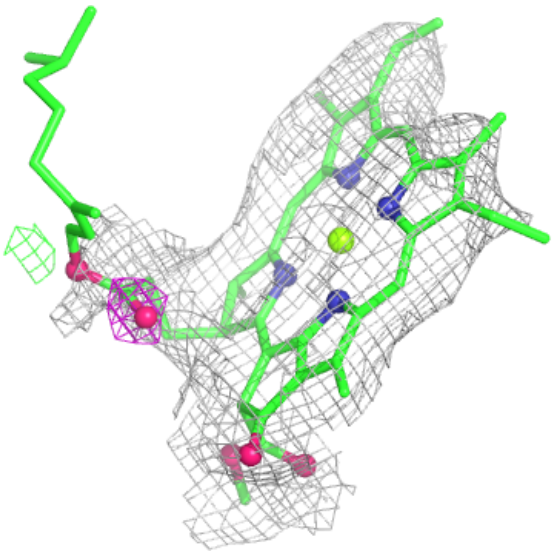


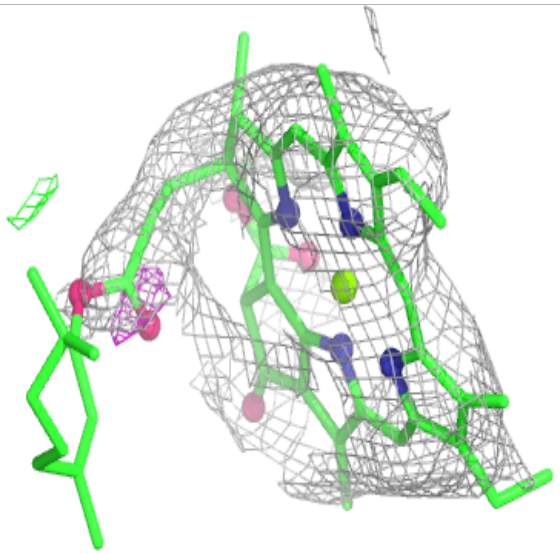


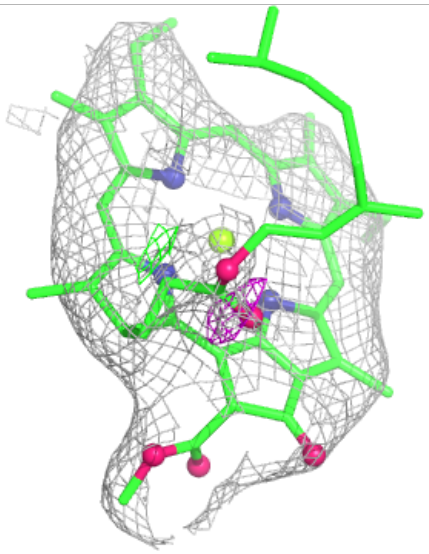


Electron density around CLA A 835:

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

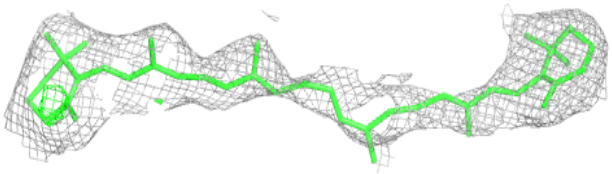


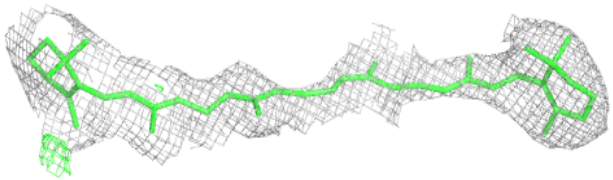


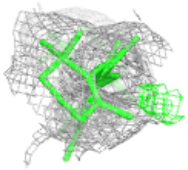


Electron density around BCR G 205:

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

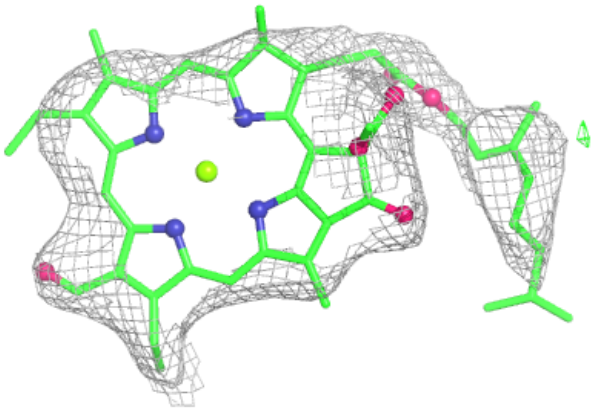


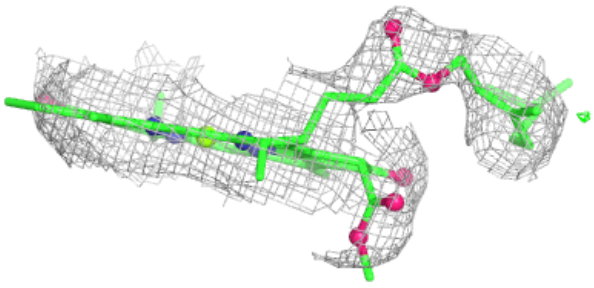


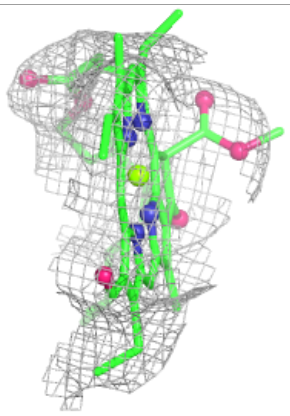


Electron density around CHL 2 516:

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

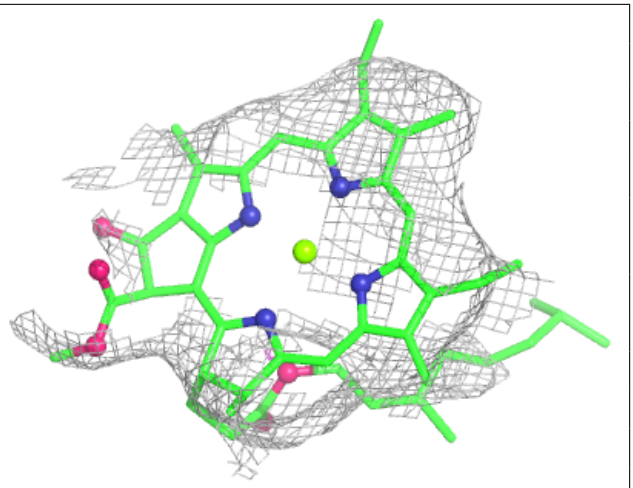


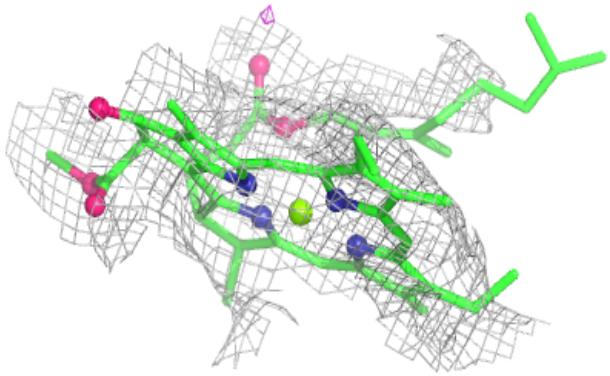


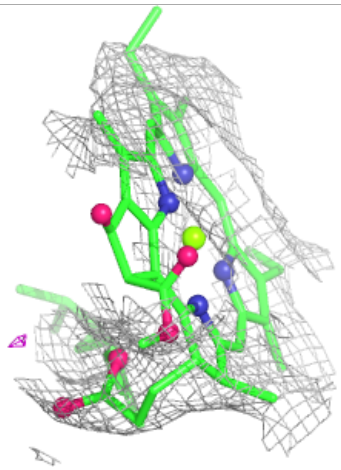


Electron density around CLA 3 305:

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

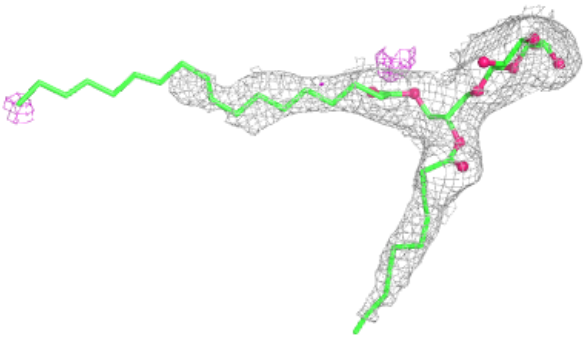


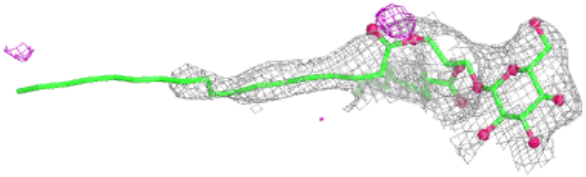


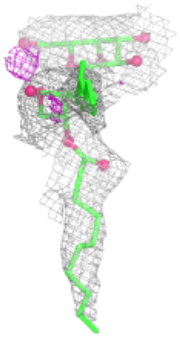


Electron density around LMG F 304:

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

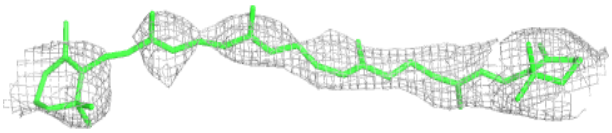


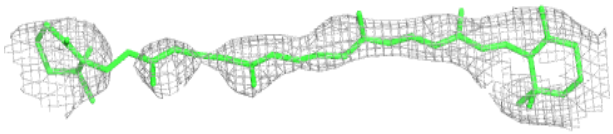


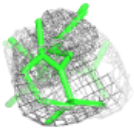


Electron density around BCR 3 303:

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

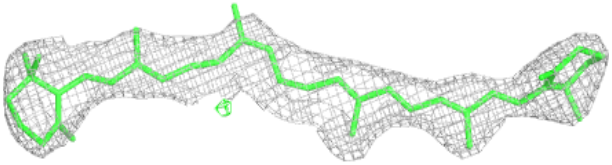


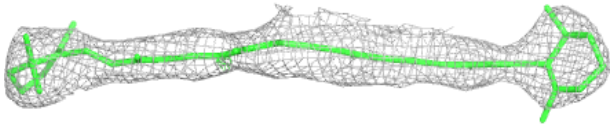


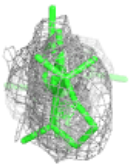


Electron density around BCR A 850:

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

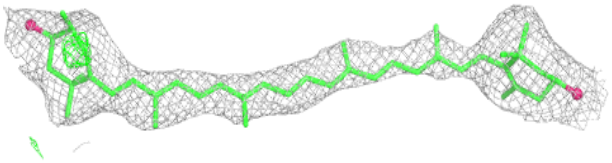


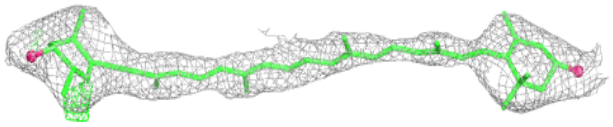


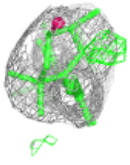


Electron density around ZEX F 301:

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

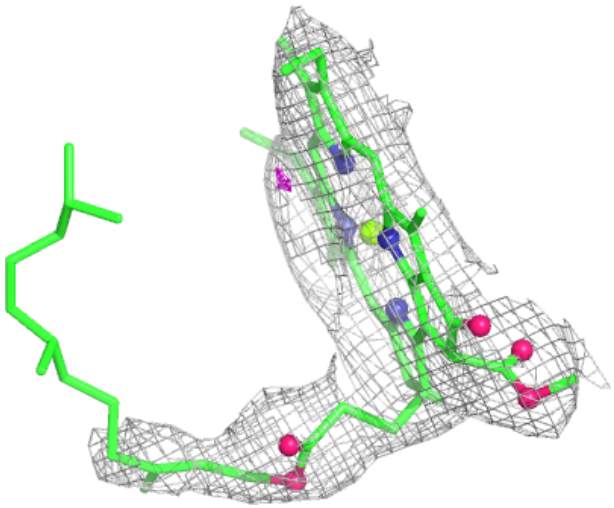


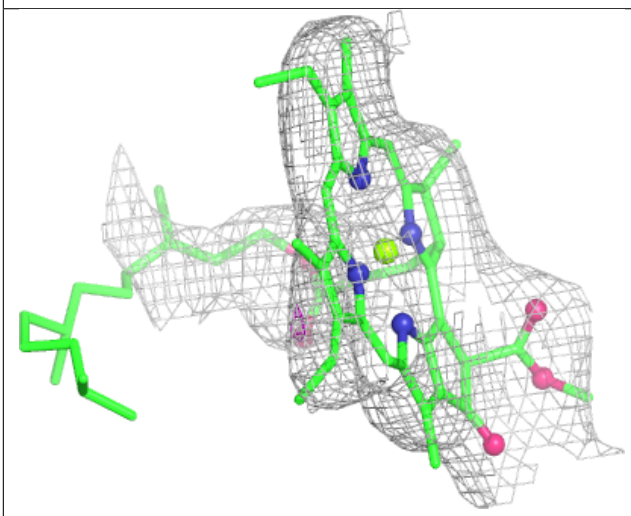


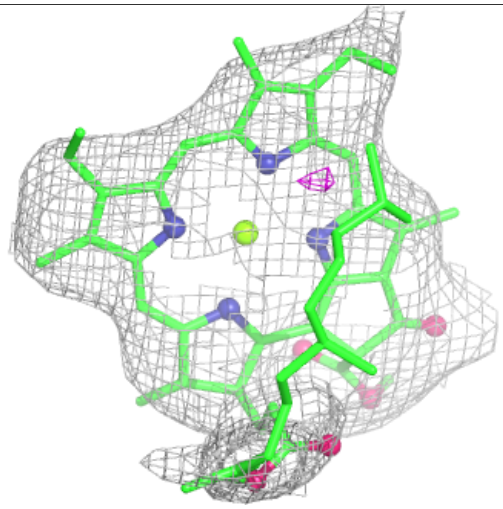


Electron density around CLA A 823:

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

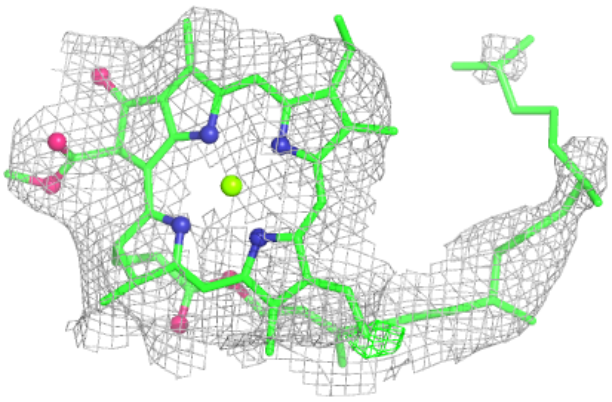


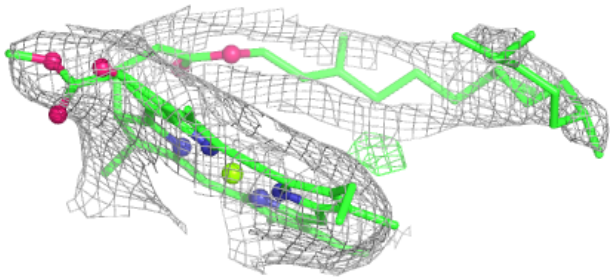


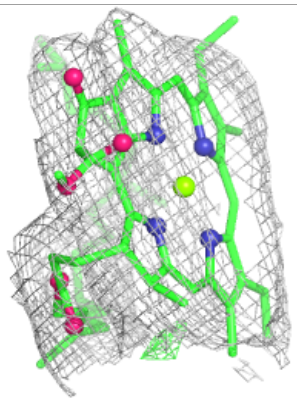


Electron density around CLA 1 504:

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

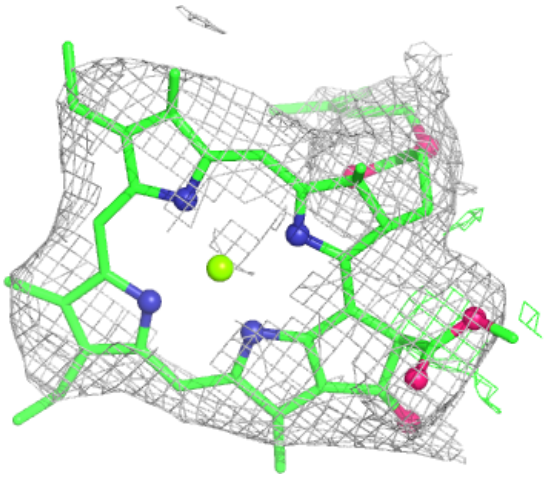


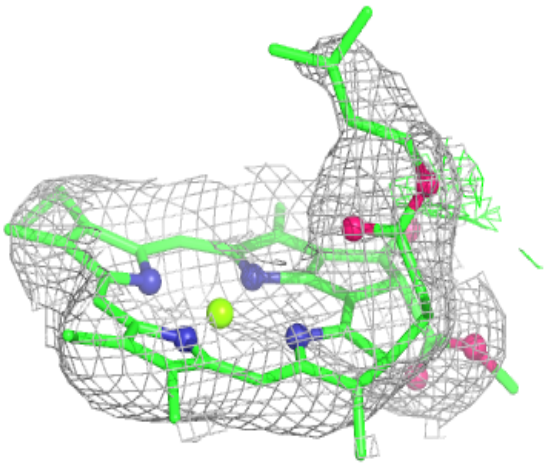




Electron density around CLA 4 309:

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

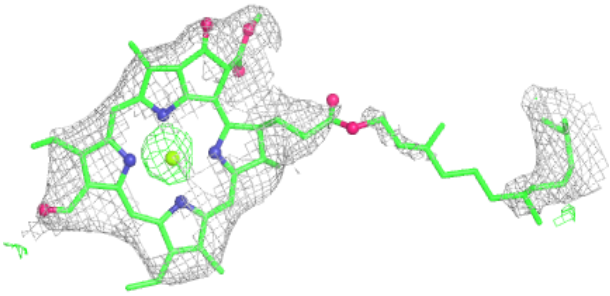


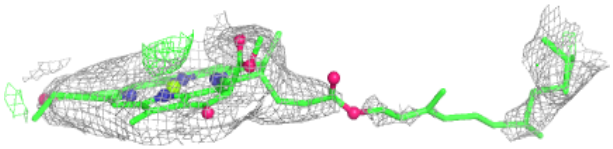


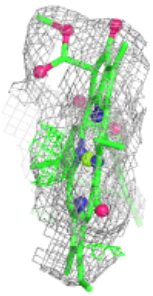


Electron density around CHL 4 316:

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

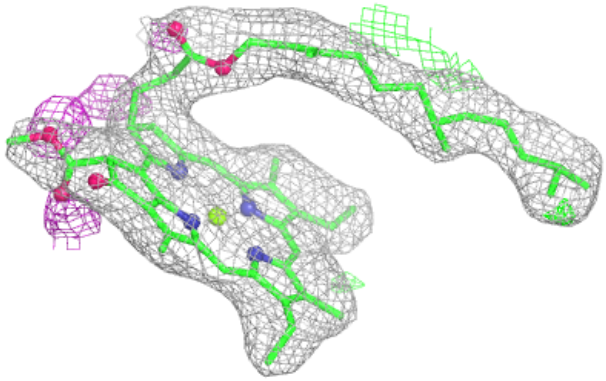


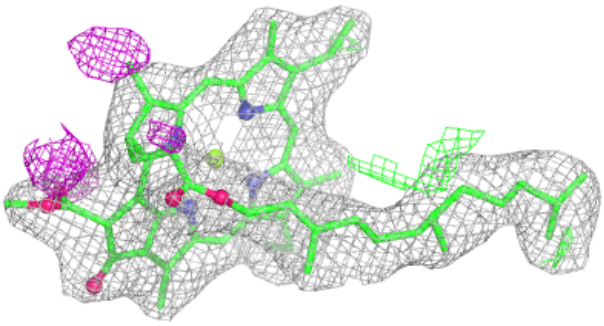


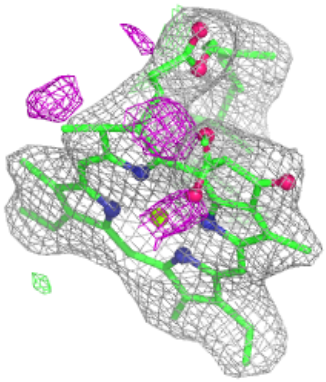


Electron density around CLA B 831:

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

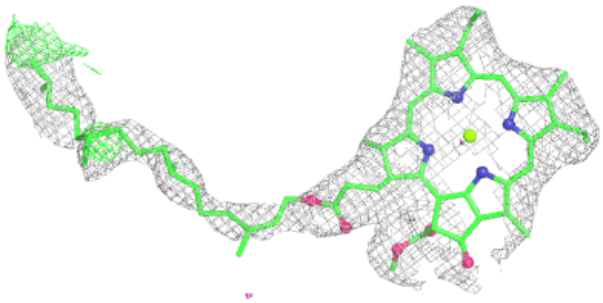


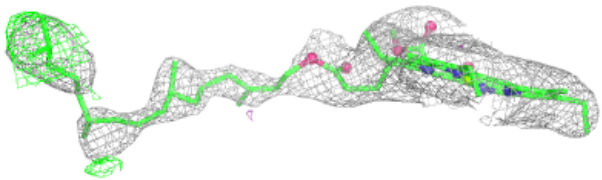


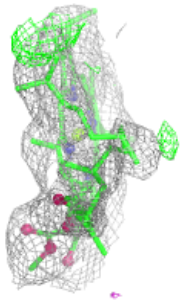


Electron density around CLA F 303:

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

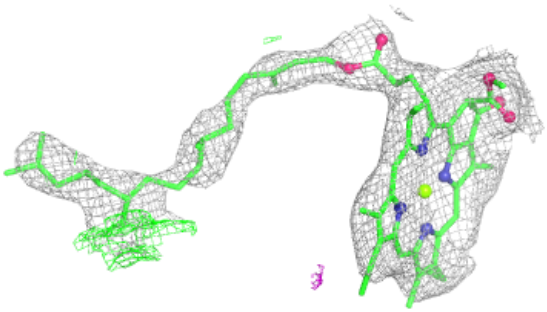


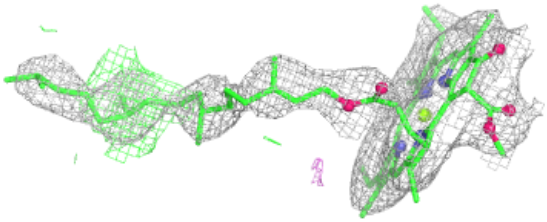


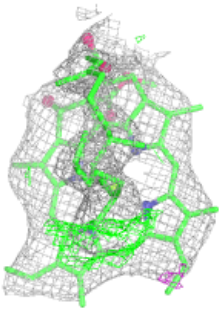


Electron density around CLA G 201:

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

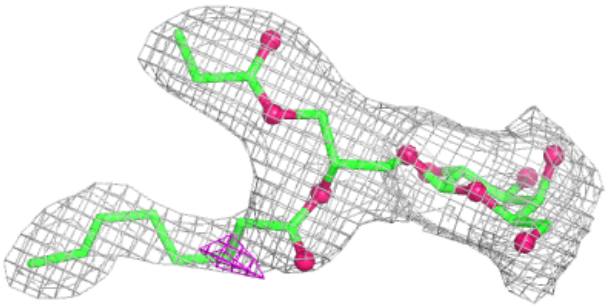


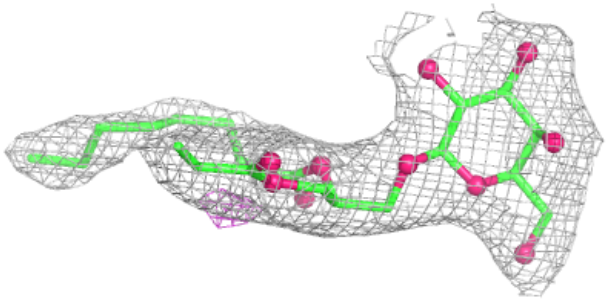


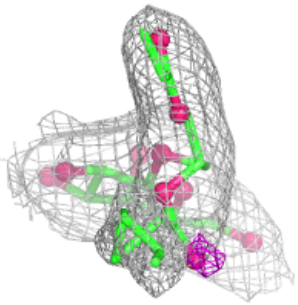


Electron density around LMG J 1103:

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

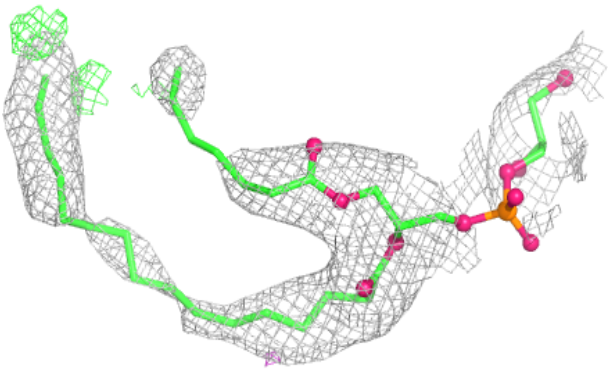


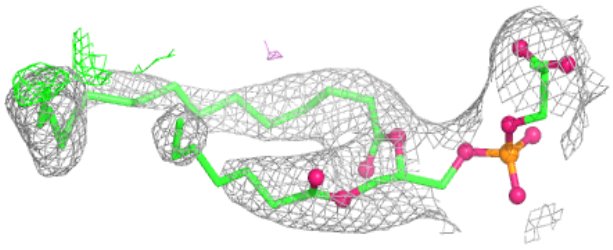


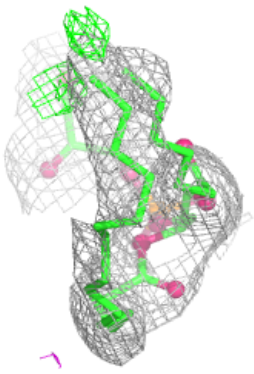


Electron density around LHG A 845:

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

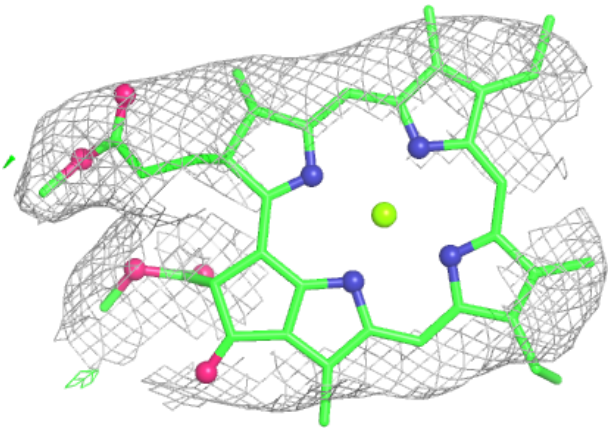


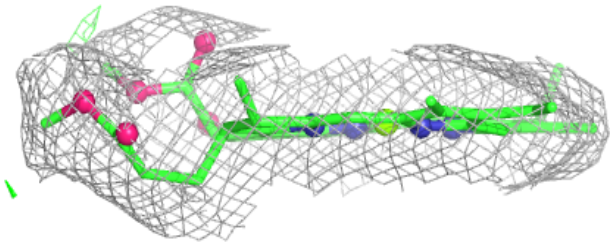


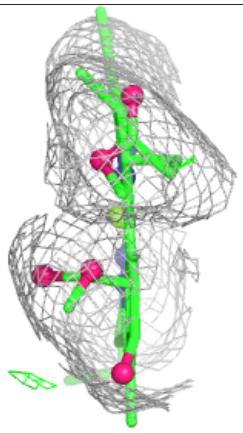


Electron density around CLA G 203:

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

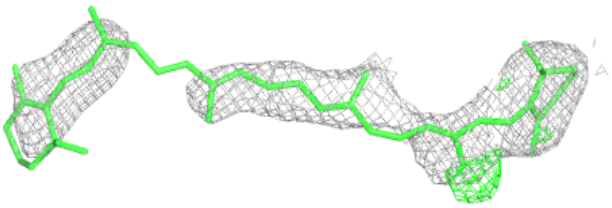


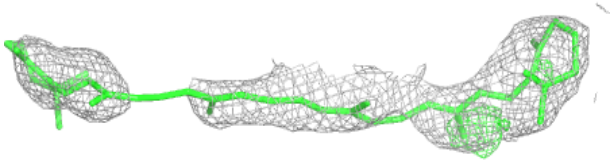


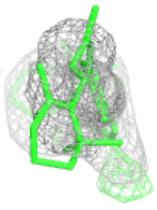


Electron density around BCR B 851:

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

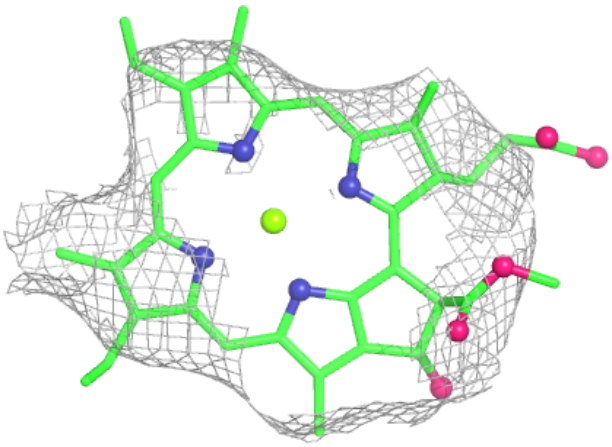


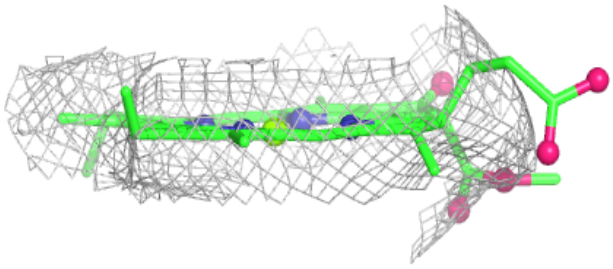


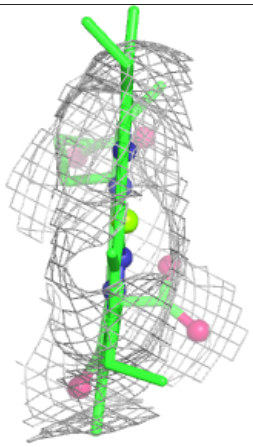


Electron density around CLA 1 515:

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

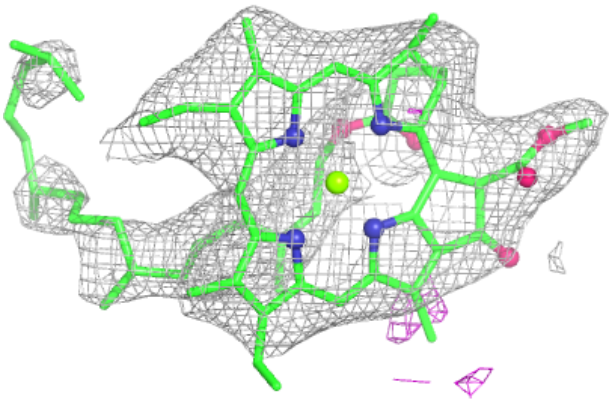




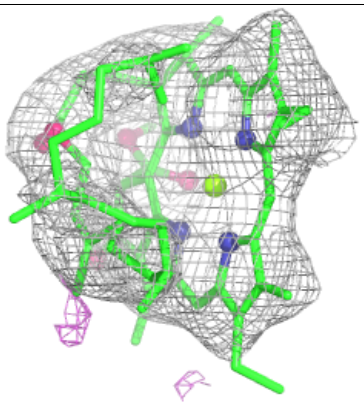


Electron density around CLA B 808:

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

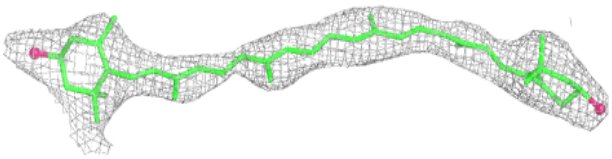


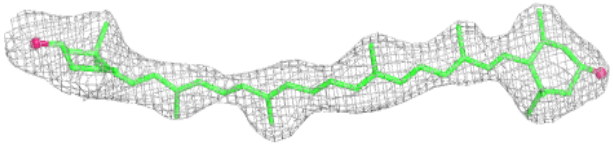


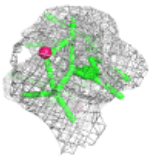


Electron density around LUT J 1109:

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



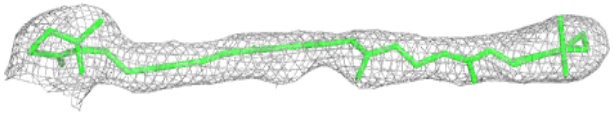


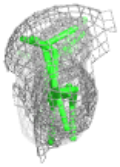


Electron density around BCR I 102:

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

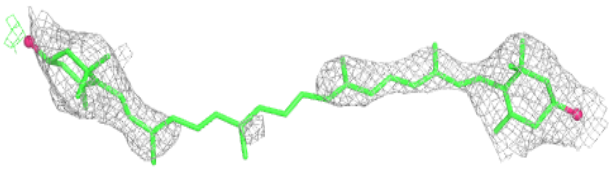


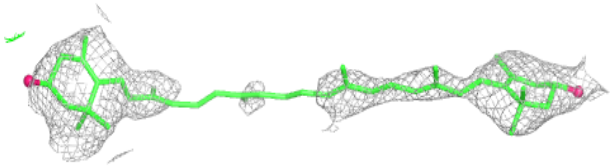


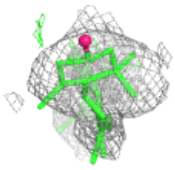


Electron density around LUT 1 502:

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

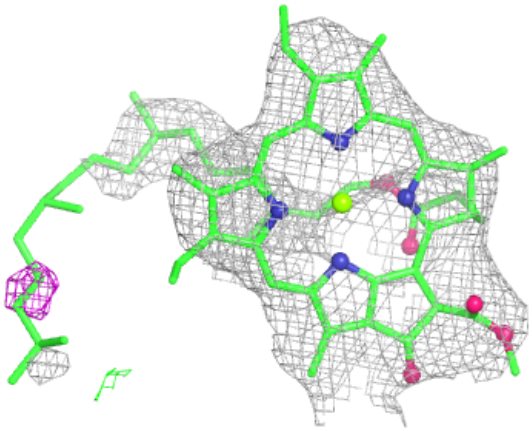


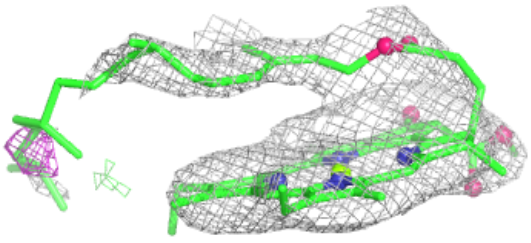


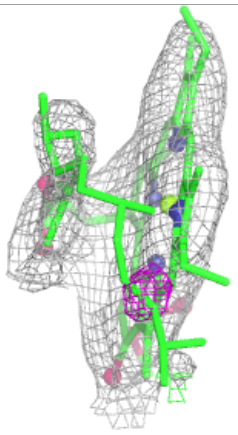


Electron density around CLA A 817:

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

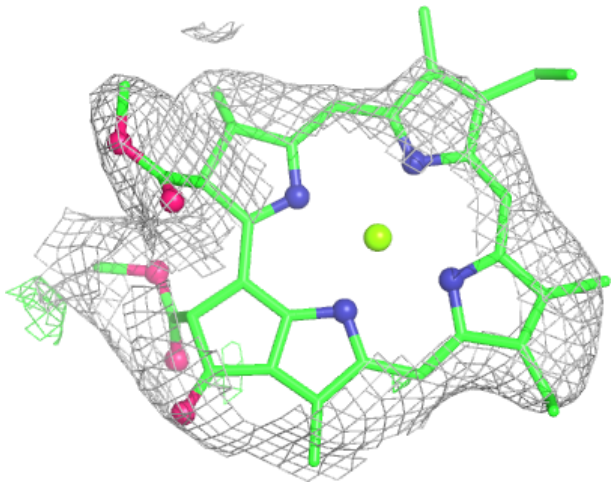


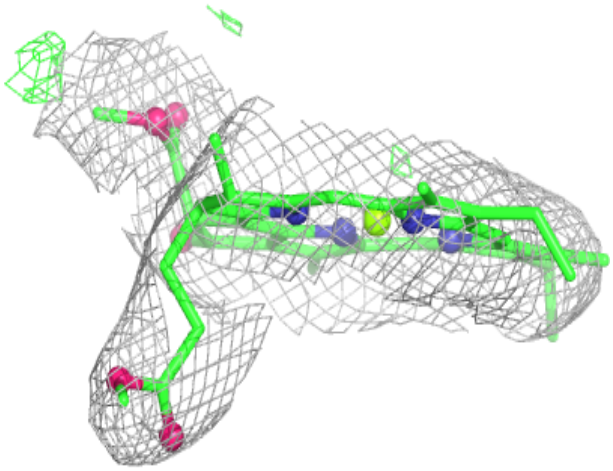


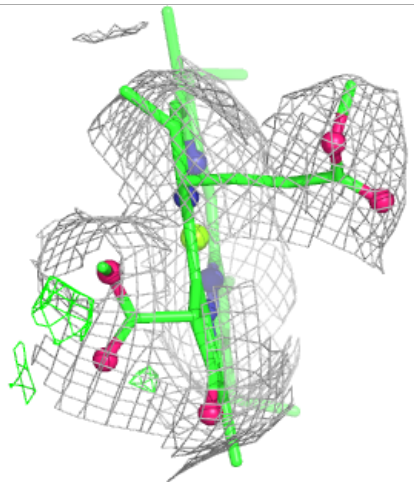


Electron density around CLA 1 511:

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

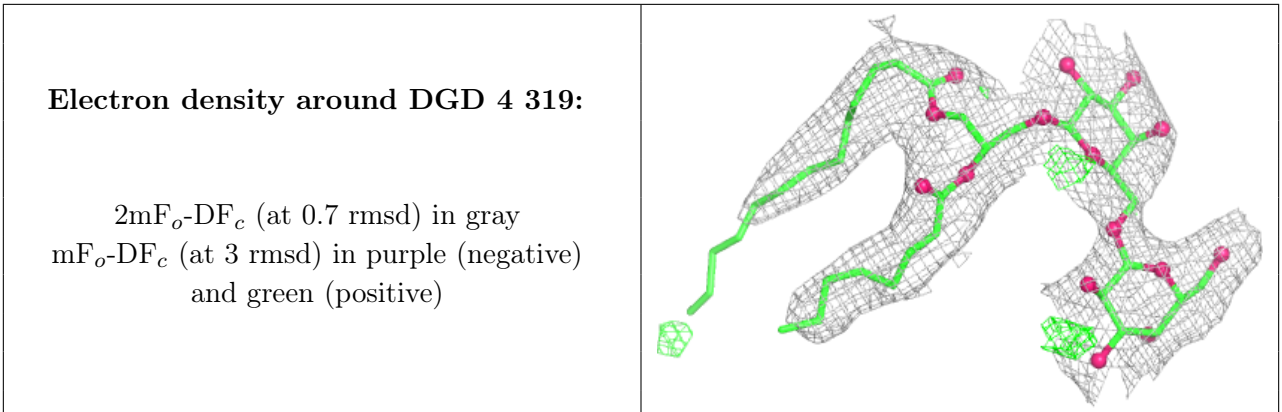


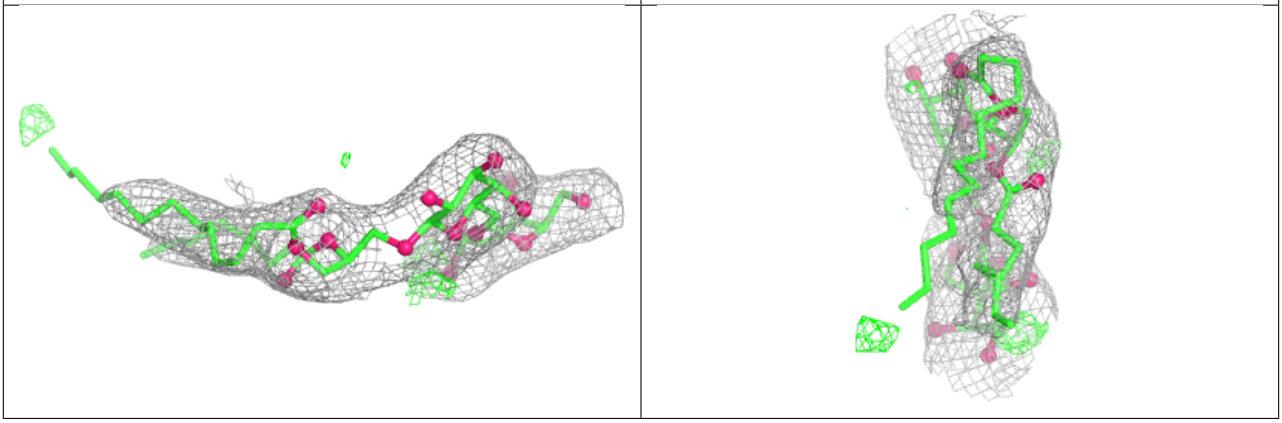




Electron density around DGD 4 319:

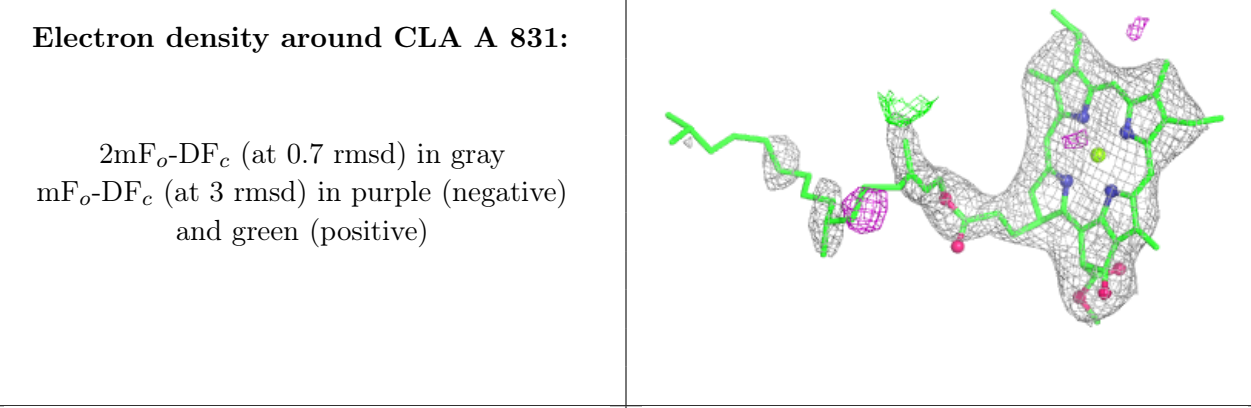
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

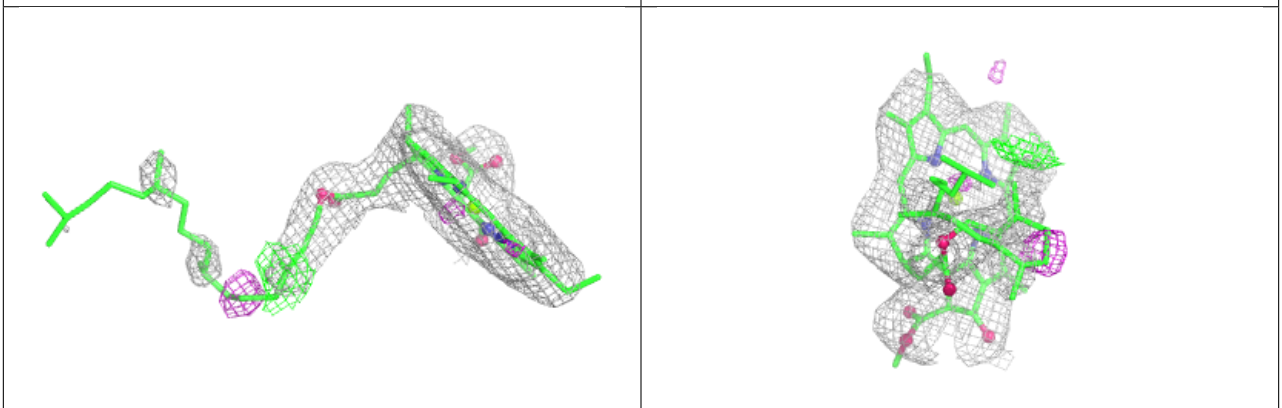




Electron density around CLA A 831:

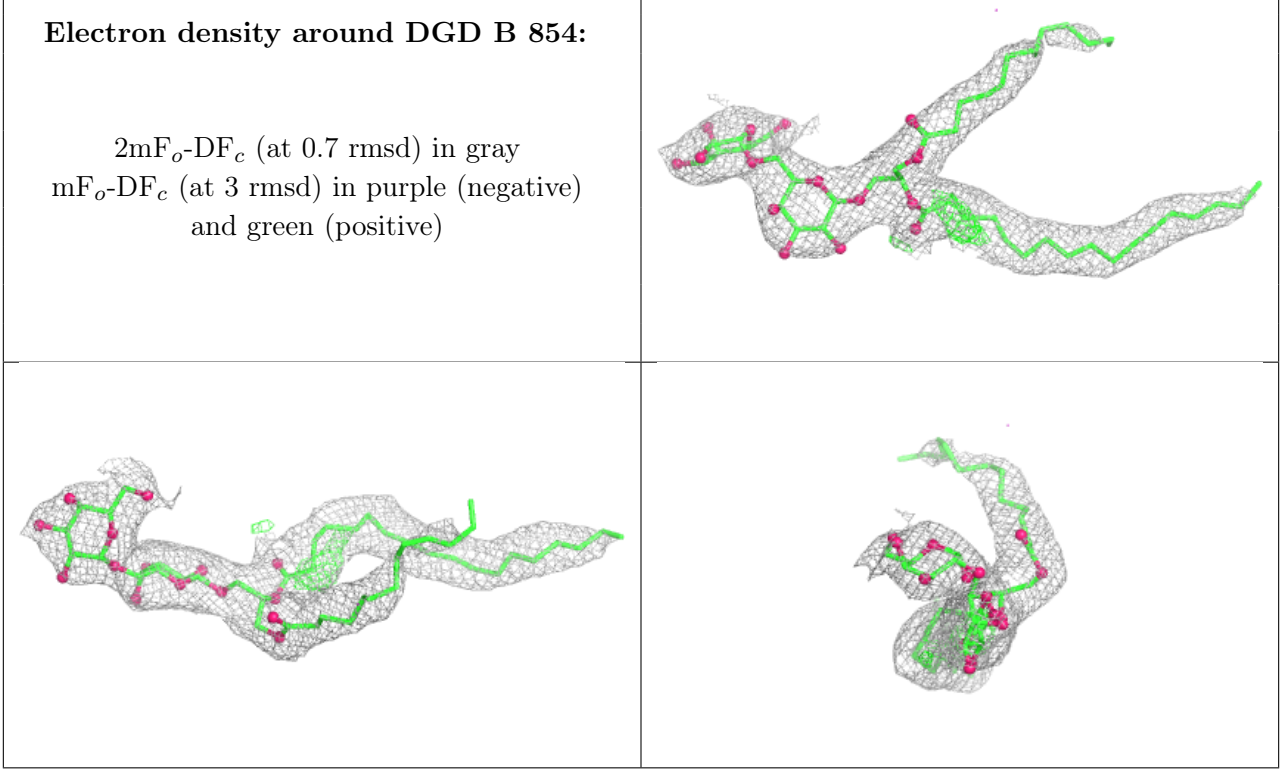
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)





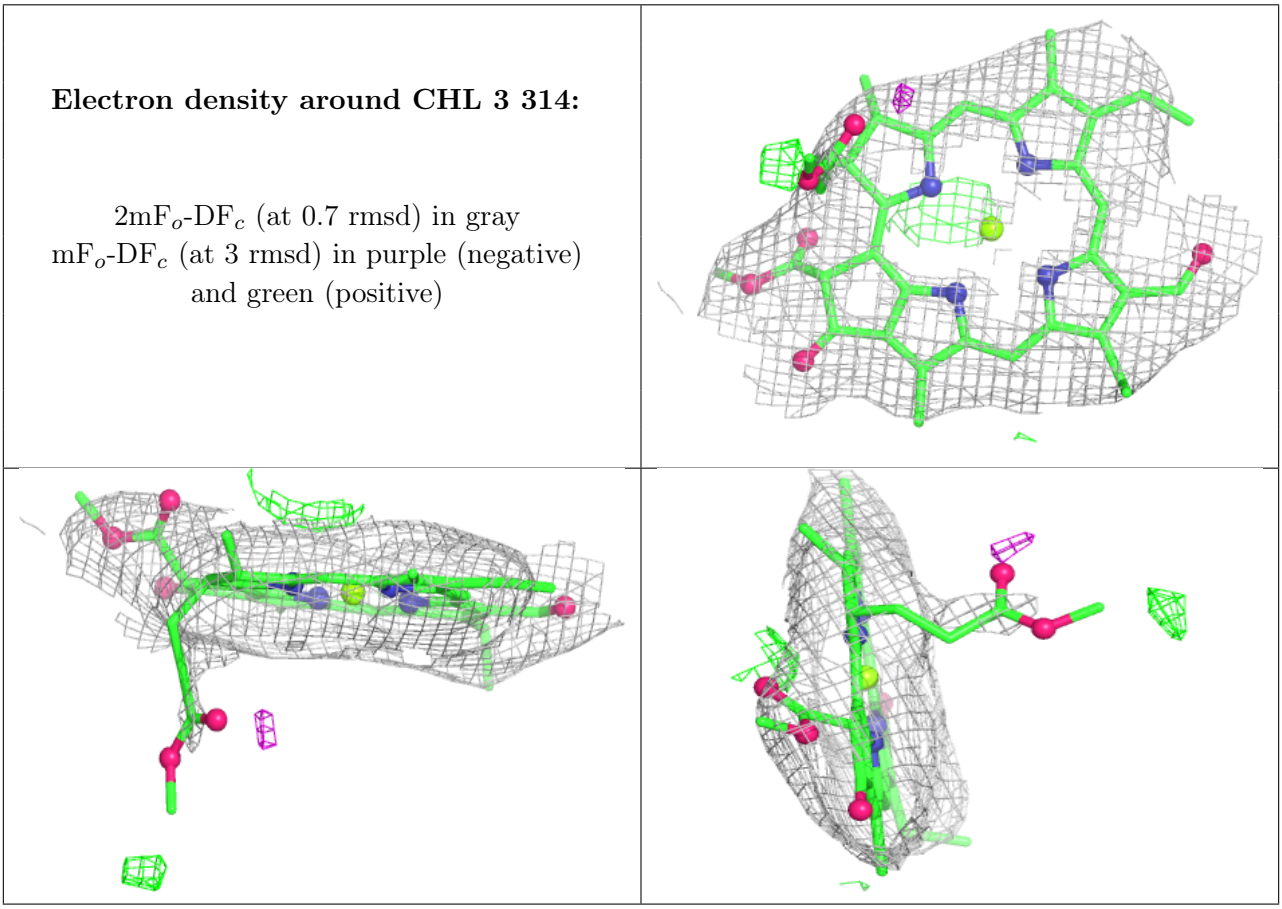
Electron density around DGD B 854:

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



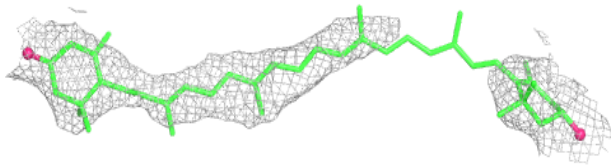
Electron density around CHL 3 314:

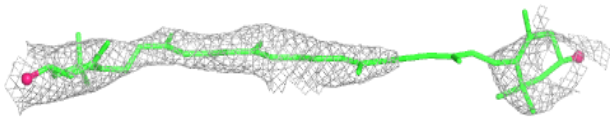
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

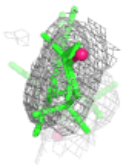


Electron density around LUT 3 302:

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

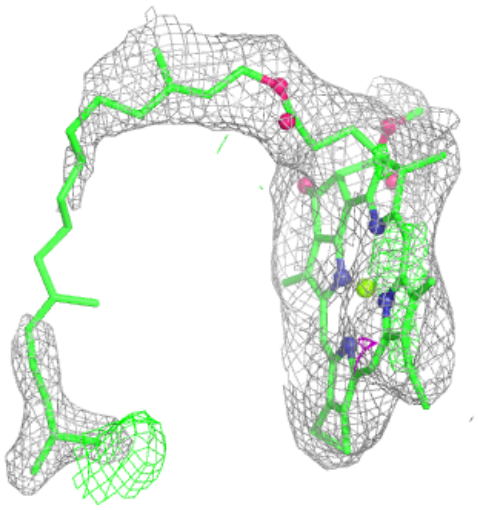


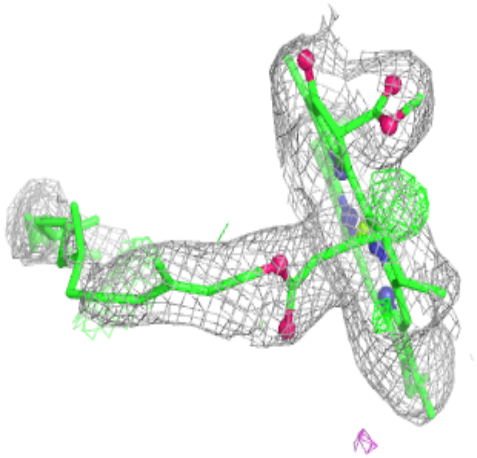


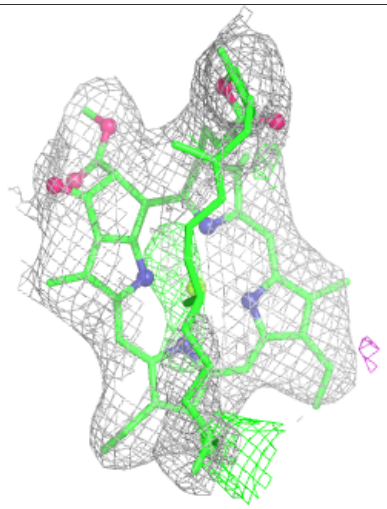


Electron density around CLA A 838:

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

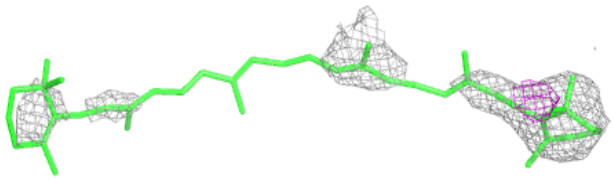


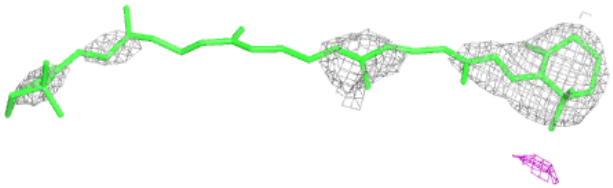


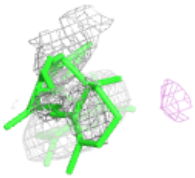


Electron density around BCR A 856:

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

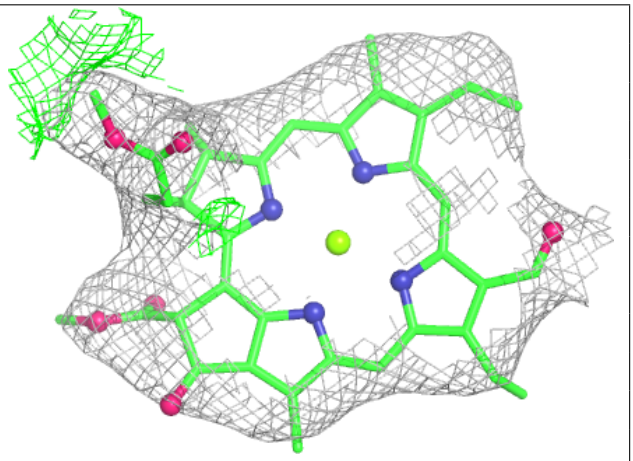


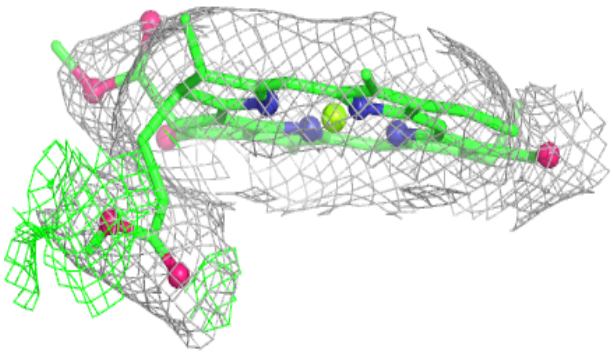


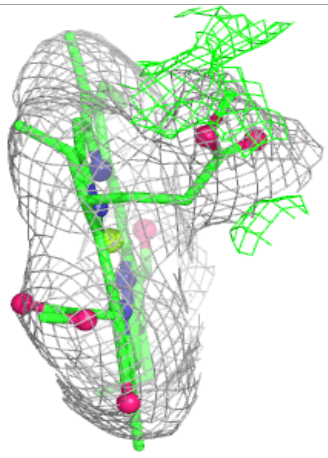


Electron density around CHL 1 512:

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

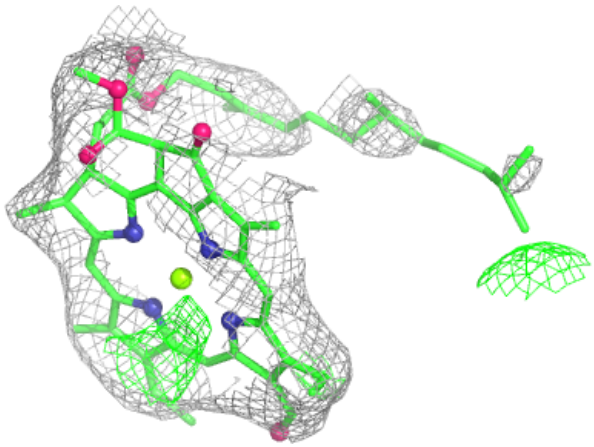


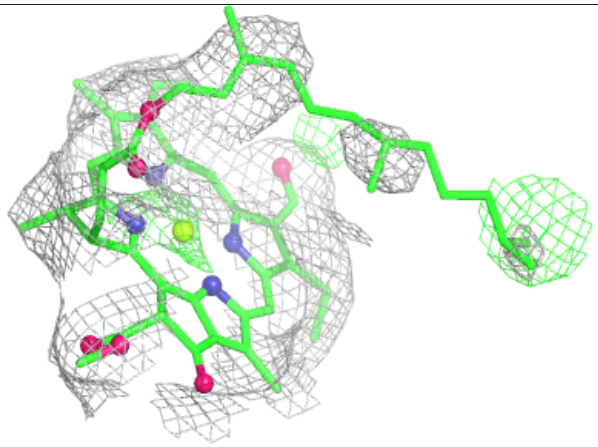


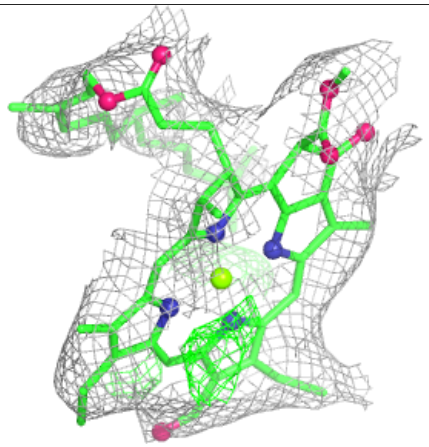


Electron density around CHL 1 514:

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

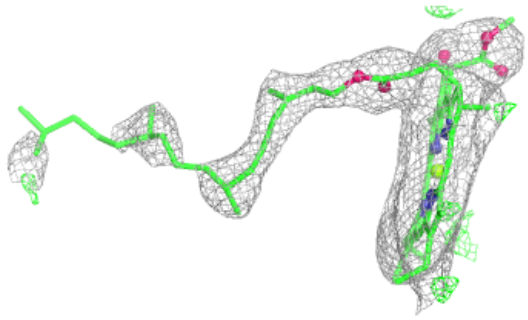


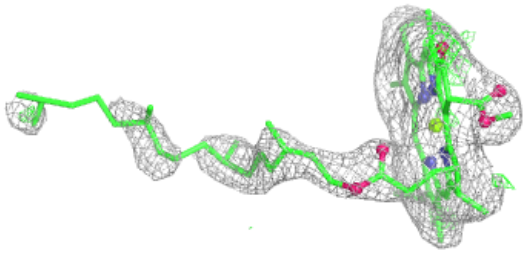


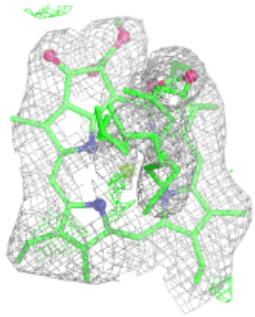


Electron density around CLA B 805:

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

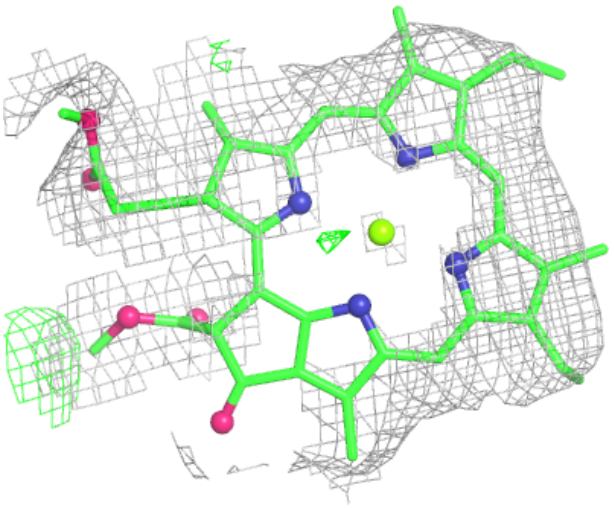


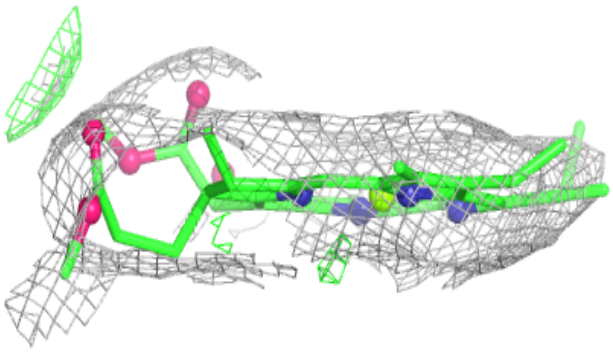


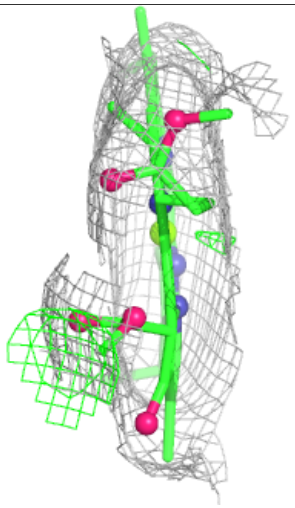


Electron density around CLA 1 505:

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

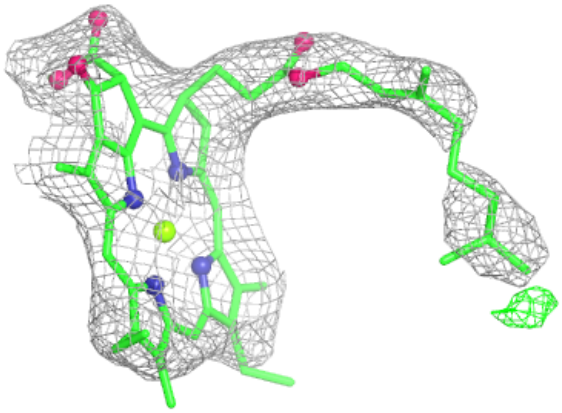


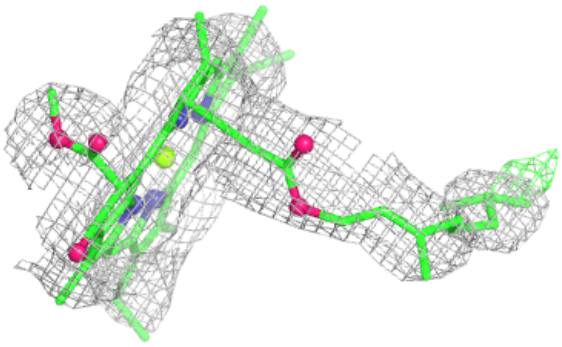


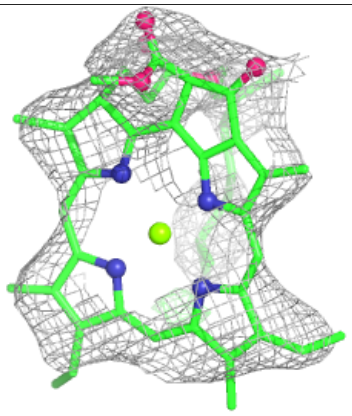


Electron density around CLA B 816:

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

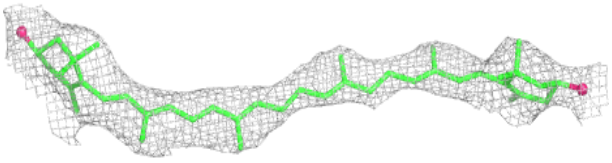


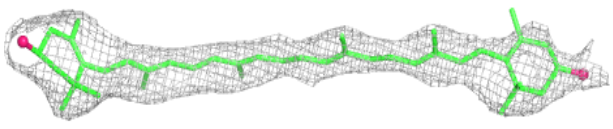




Electron density around LUT 4 302:

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

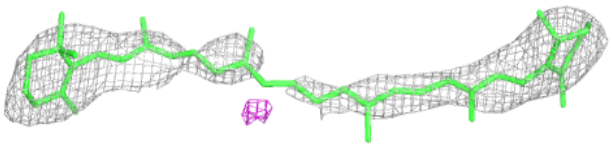


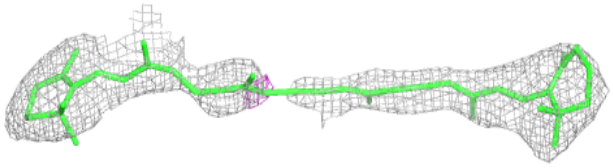


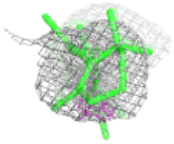


Electron density around BCR L 306:

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

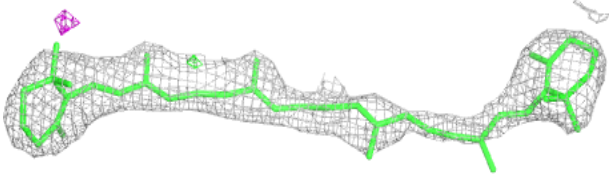


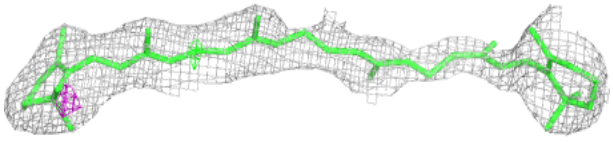


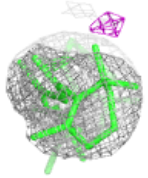


Electron density around BCR A 851:

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

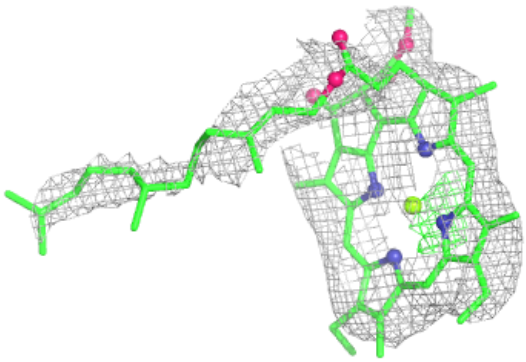


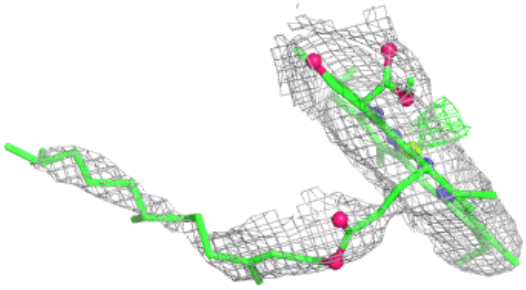


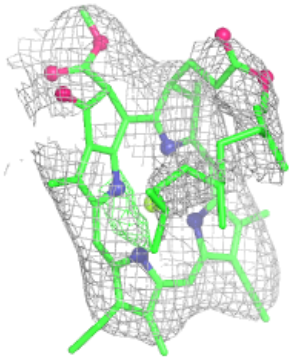


Electron density around CLA 4 310:

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

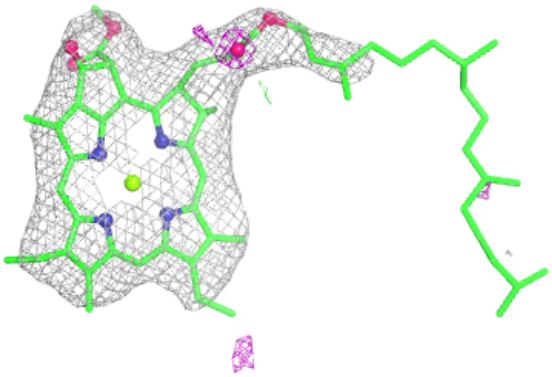


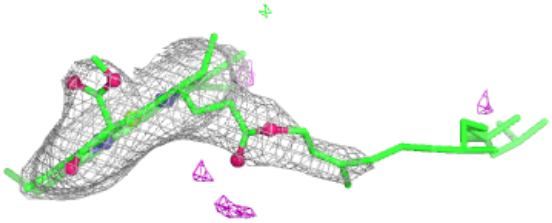


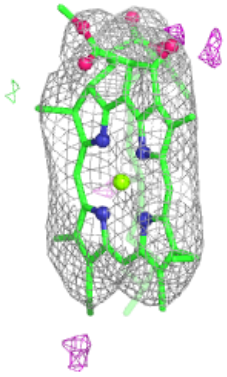


Electron density around CLA 4 318:

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

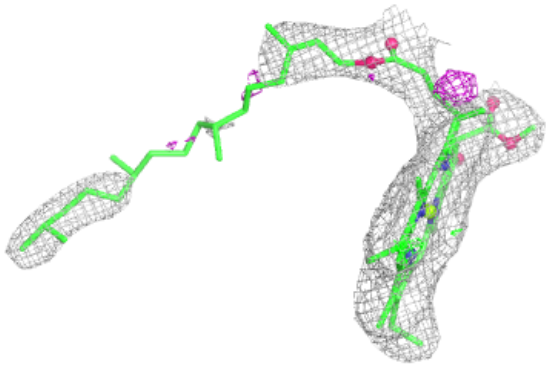


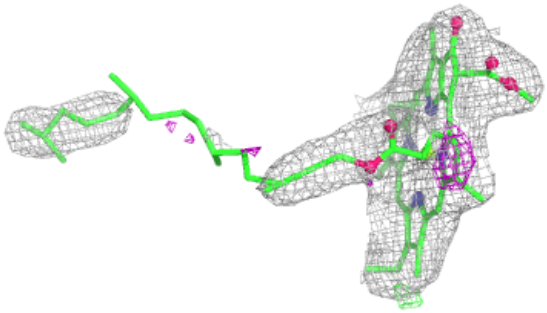


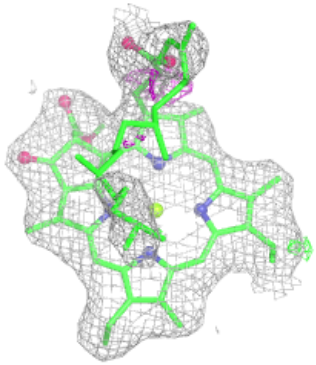


Electron density around CLA A 804:

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

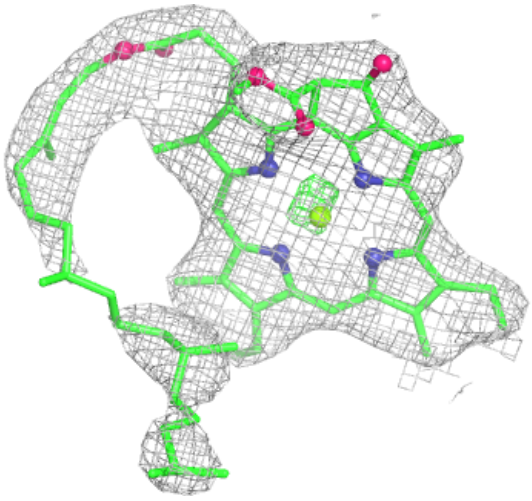


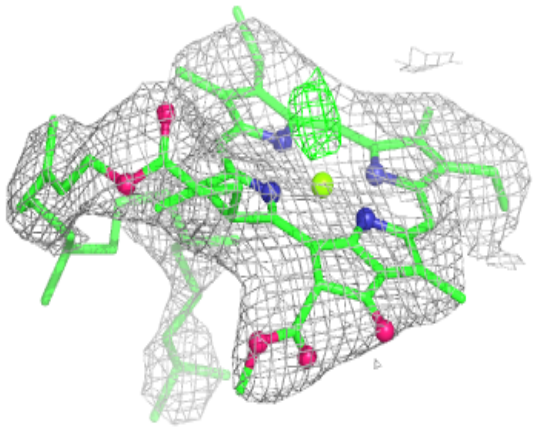


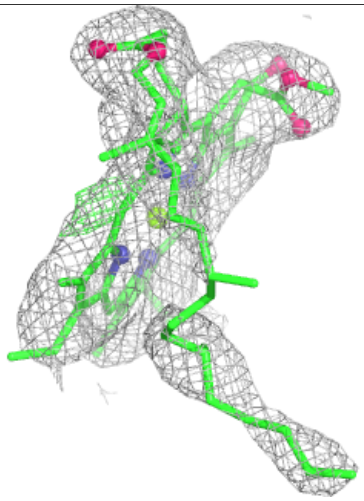


Electron density around CLA A 813:

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

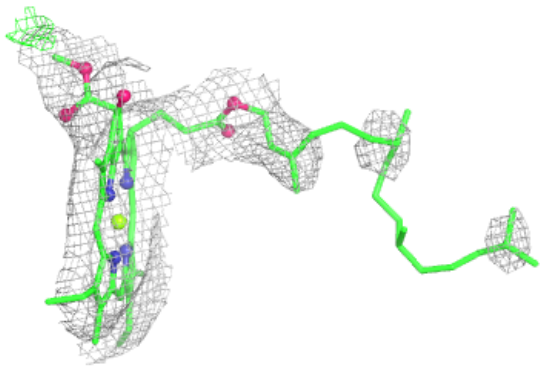


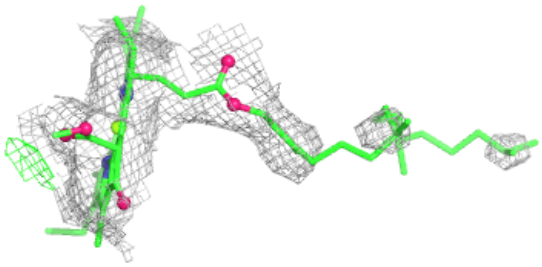


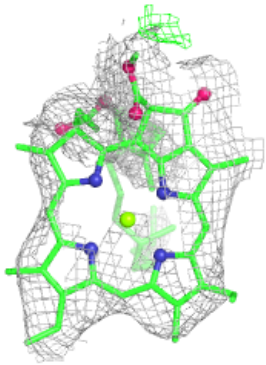


Electron density around CLA A 814:

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

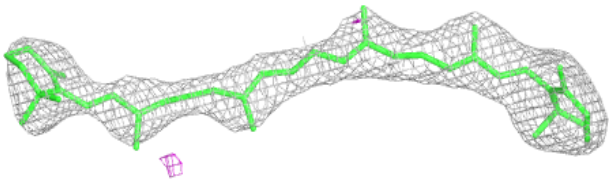


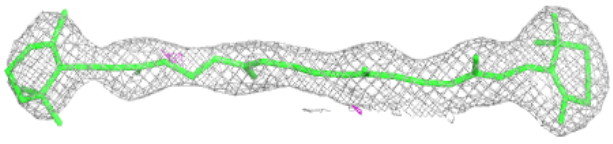


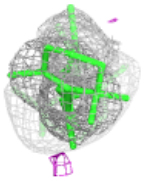


Electron density around BCR B 852:

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

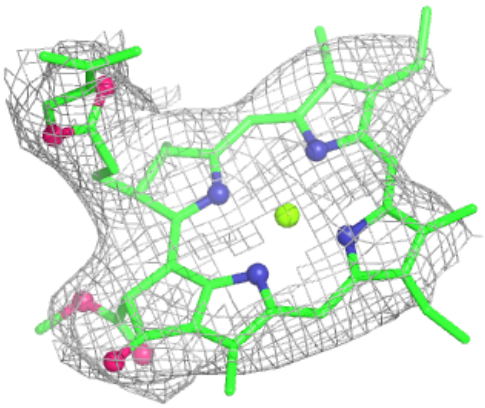


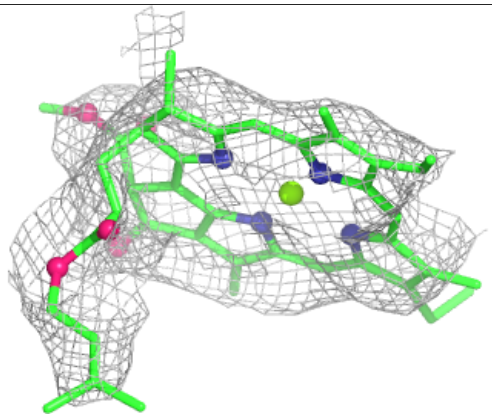


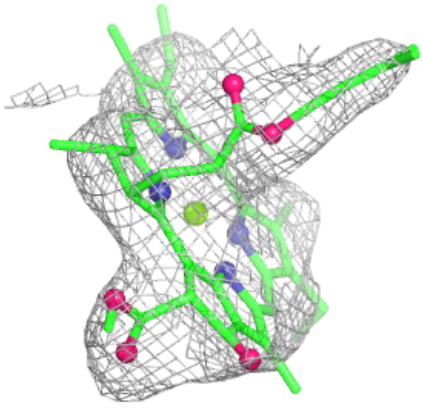


Electron density around CLA 2 509:

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

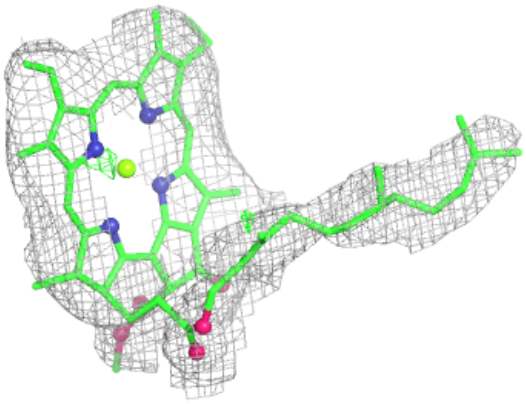


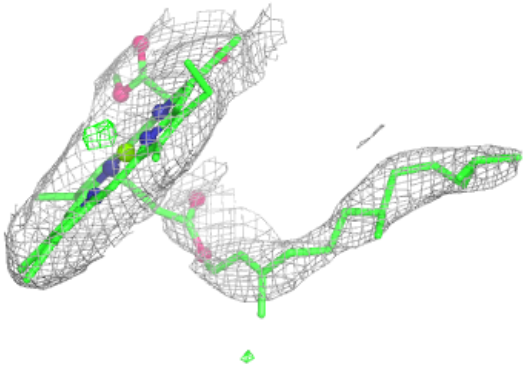


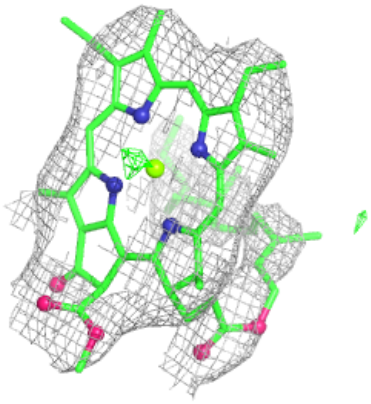


Electron density around CLA 2 510:

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

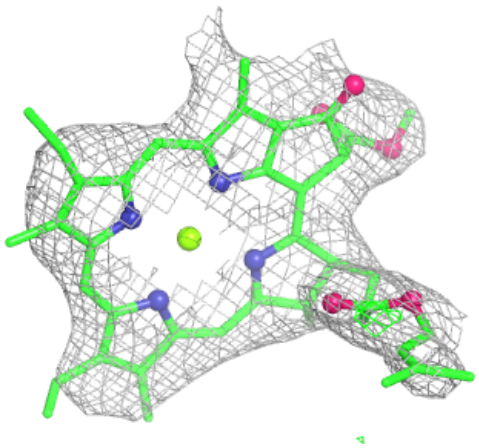


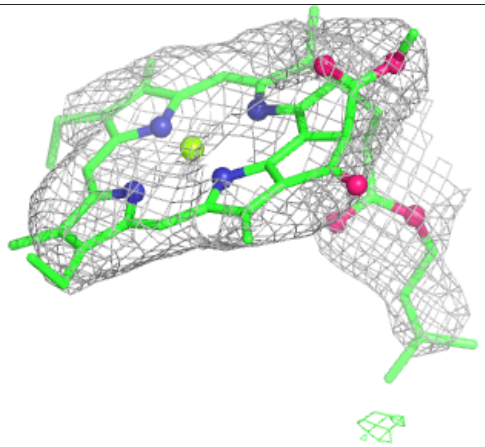


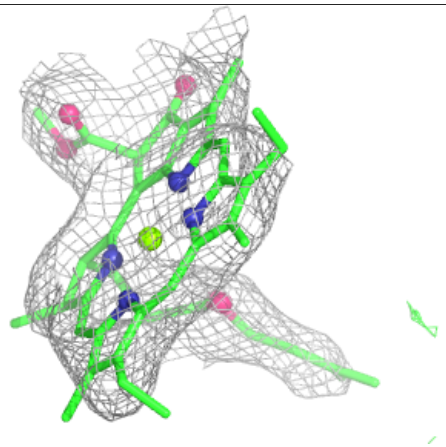


Electron density around CLA 2 511:

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

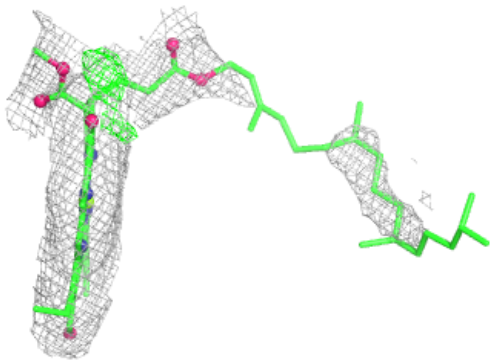


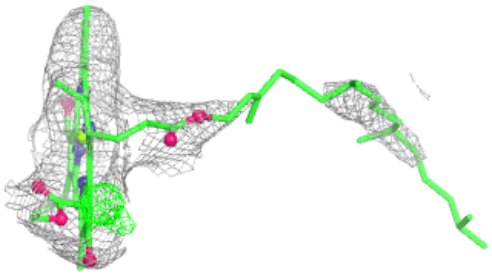


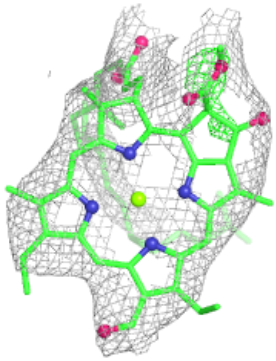


Electron density around CHL 2 526:

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

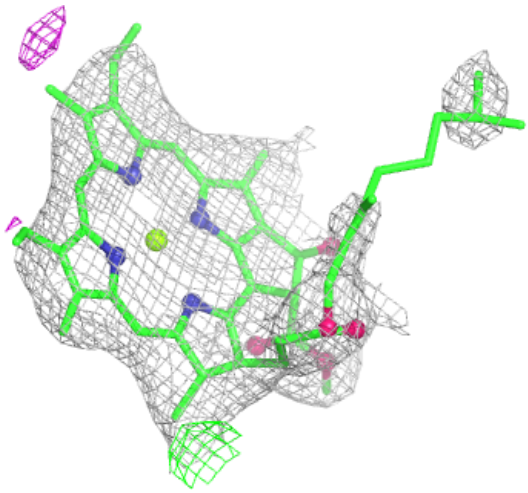


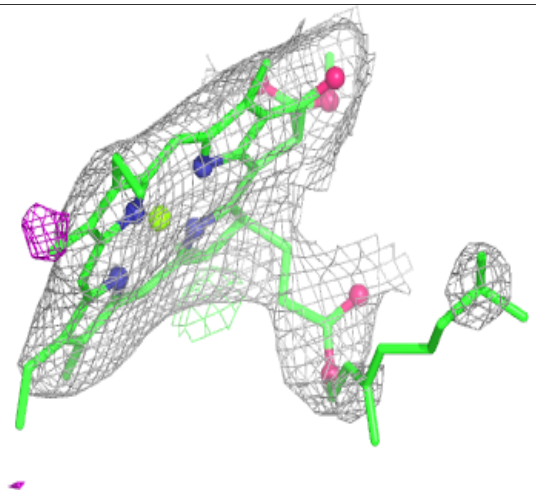


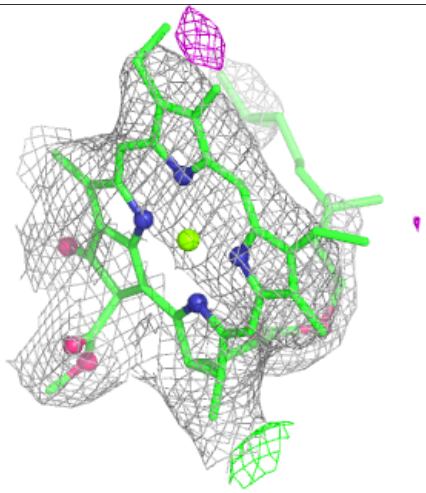


Electron density around CLA 2 514:

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

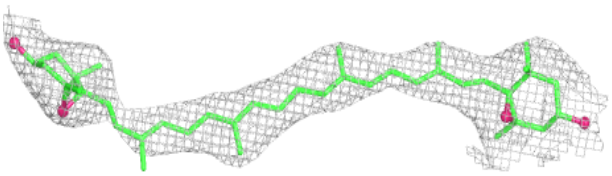


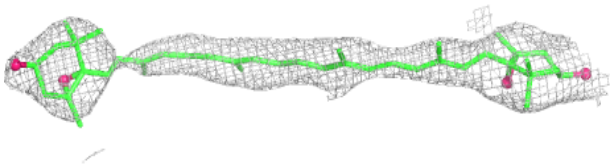


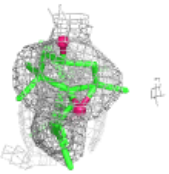


Electron density around XAT 2 502:

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

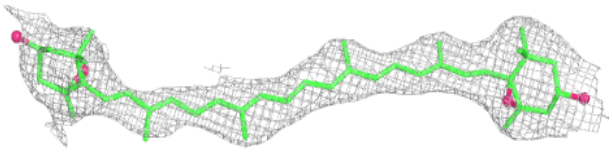


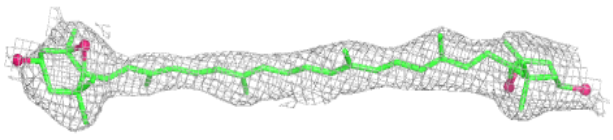


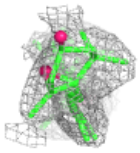


Electron density around XAT 4 303:

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

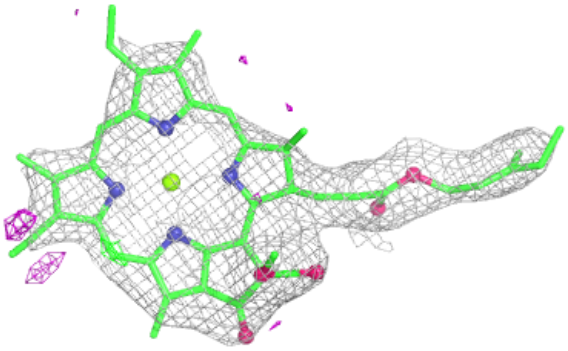


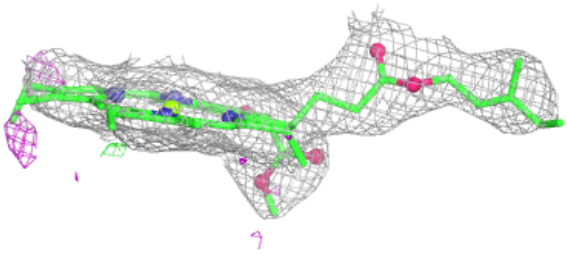


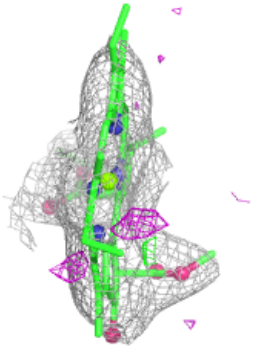


Electron density around CLA A 836:

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

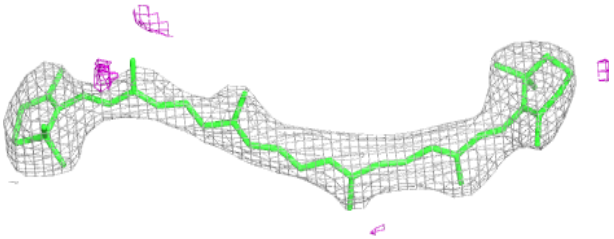


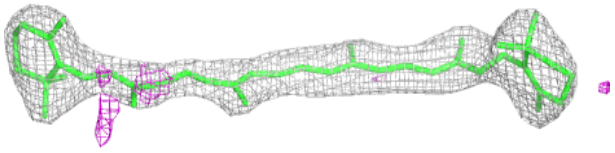


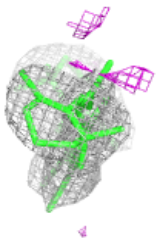


Electron density around BCR B 853:

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

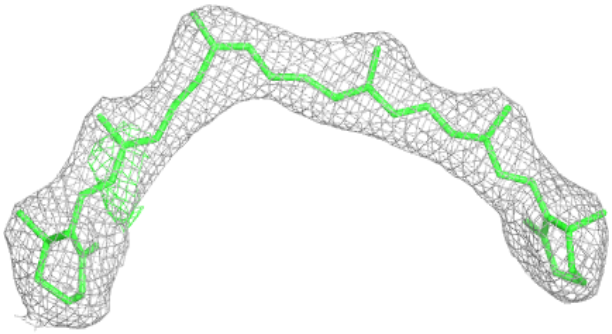


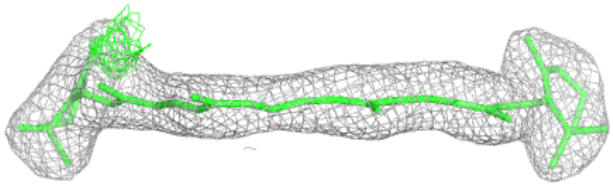


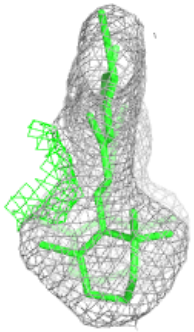


Electron density around BCR F 306:

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

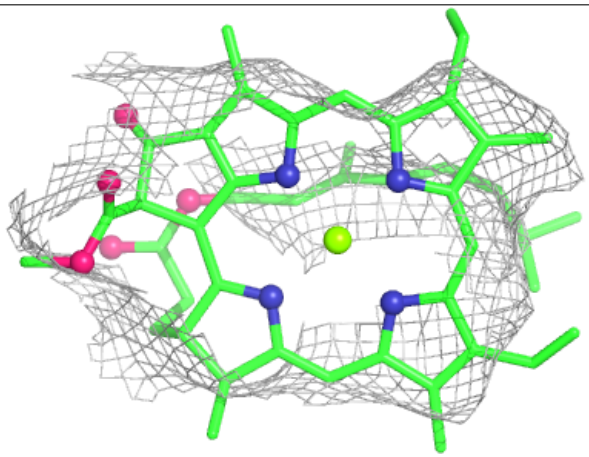


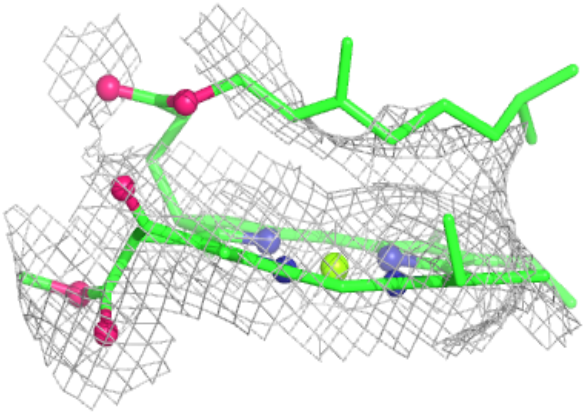


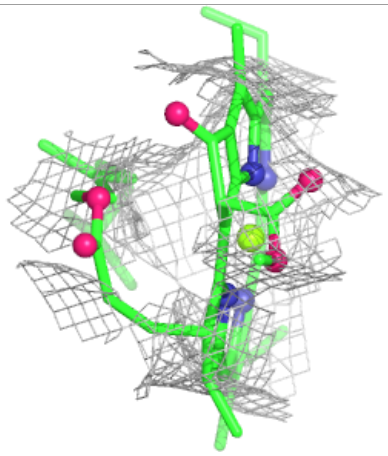


Electron density around CLA 3 307:

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

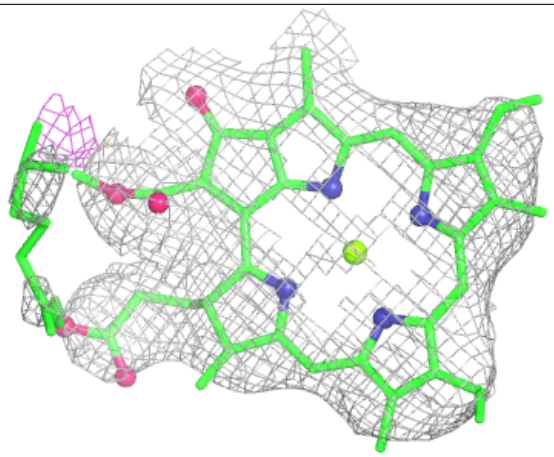


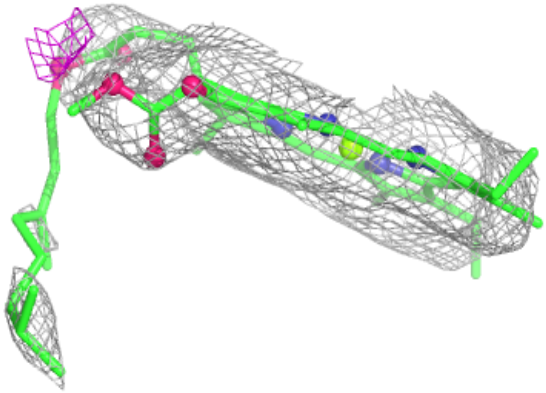


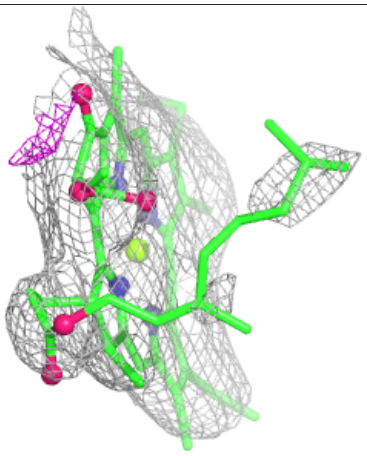


Electron density around CLA 3 309:

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

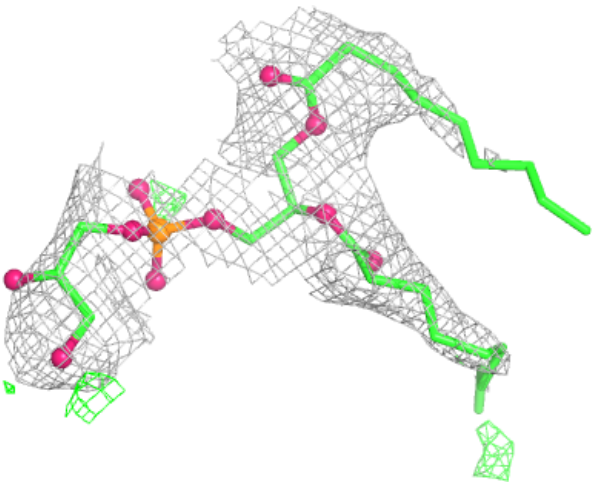


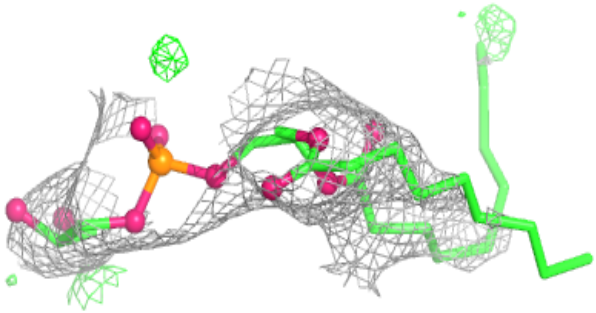




Electron density around LHG 2 517:

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

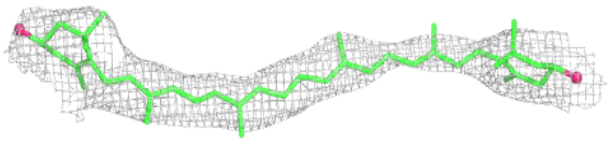


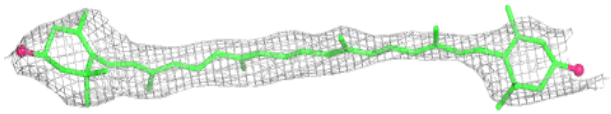




Electron density around LUT 2 501:

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

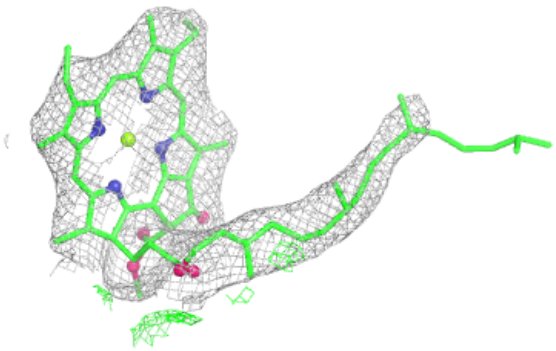


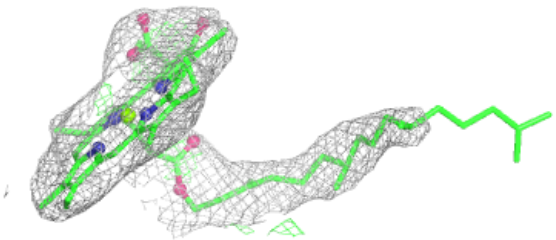


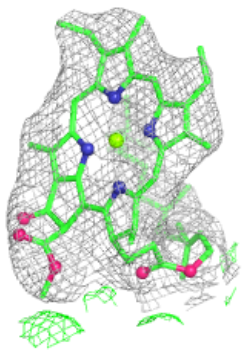


Electron density around CLA B 822:

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

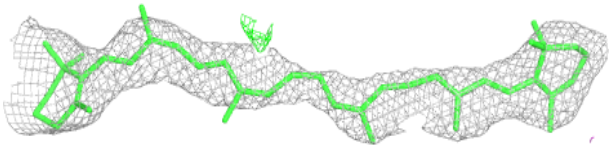


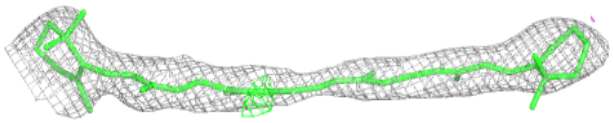


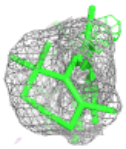


Electron density around BCR B 849:

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

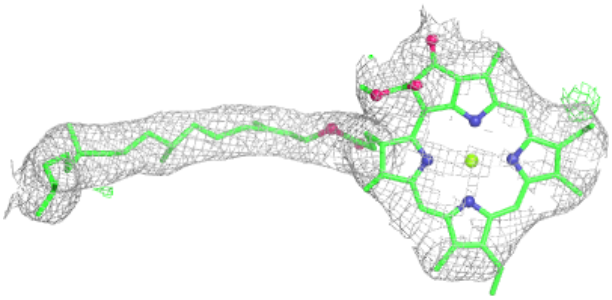


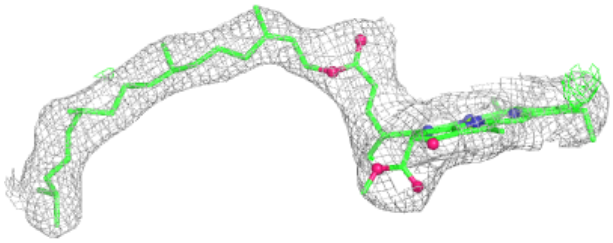


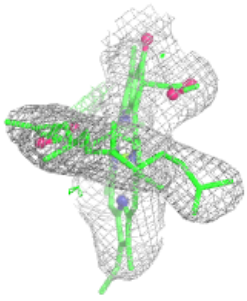


Electron density around CLA B 840:

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

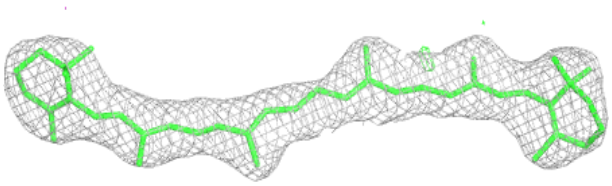


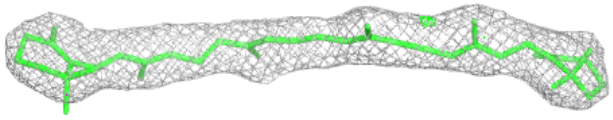


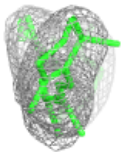


Electron density around BCR J 1108:

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

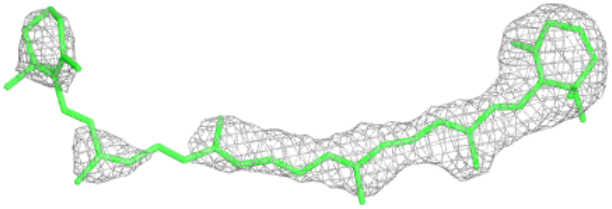


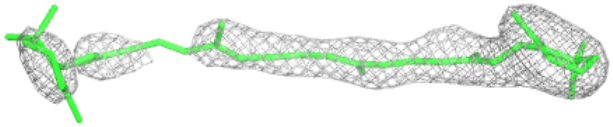


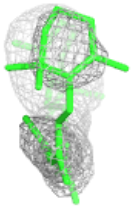


Electron density around BCR B 850:

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

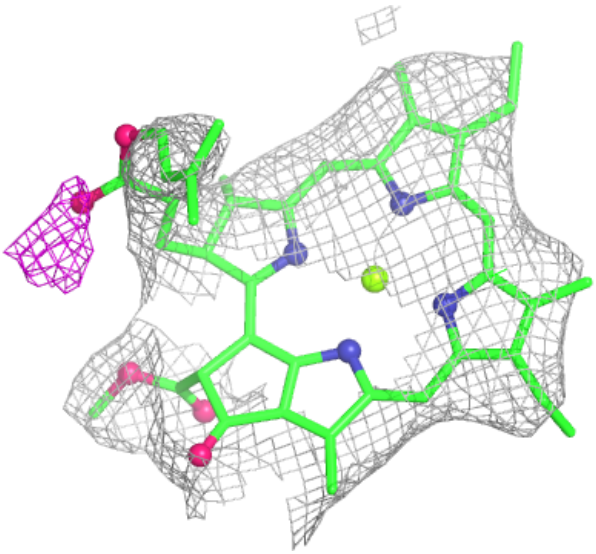


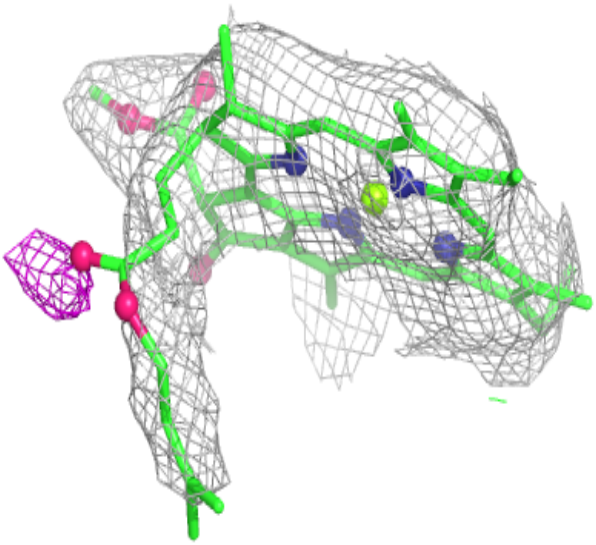


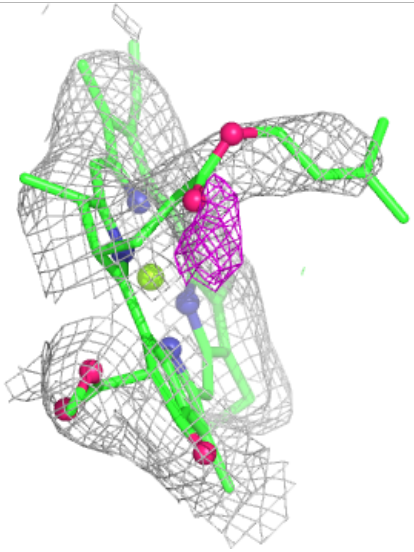


Electron density around CLA 3 315:

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

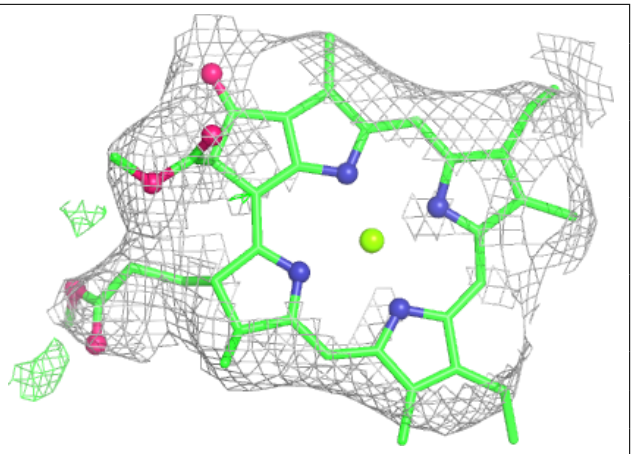


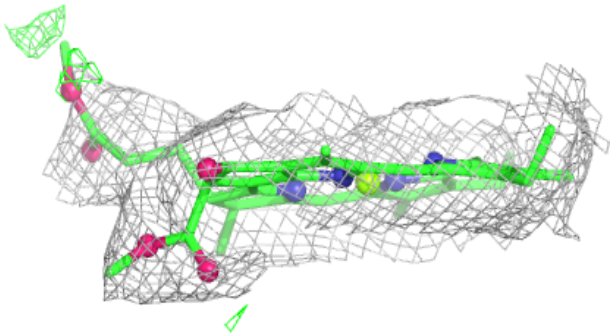


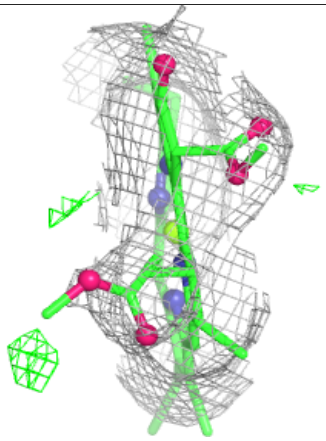


Electron density around CLA 3 316:

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

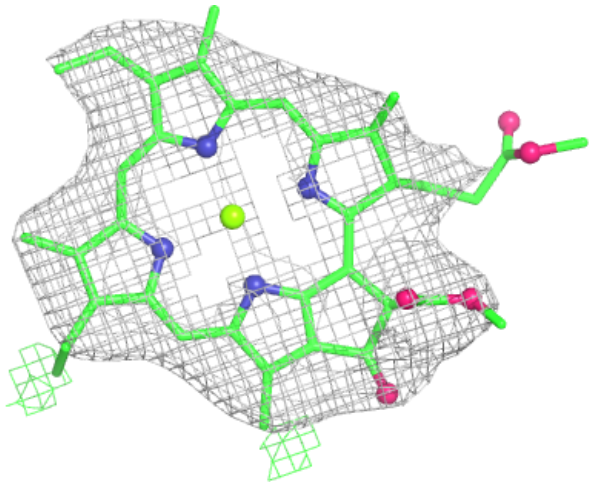


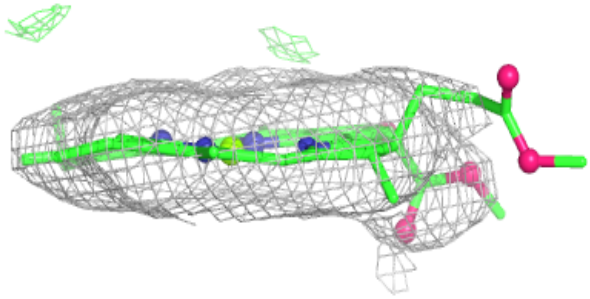


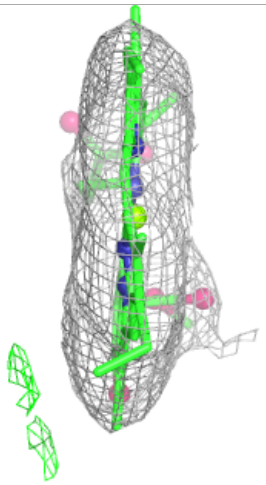


Electron density around CLA 3 317:

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

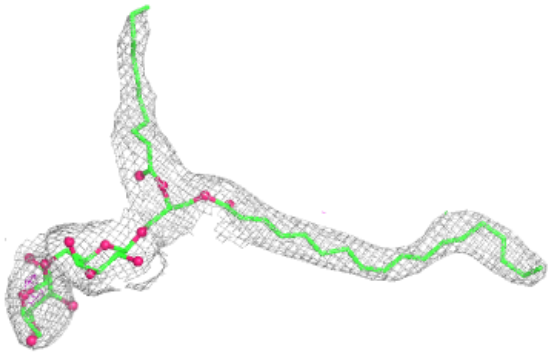


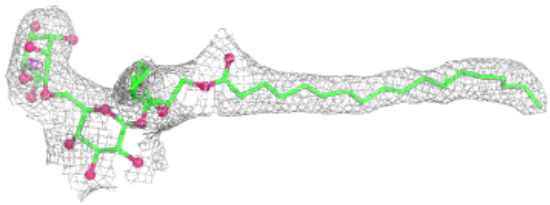




Electron density around DGD J 1106:

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

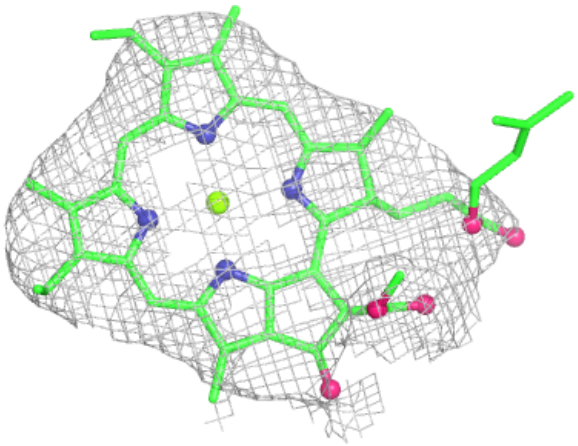


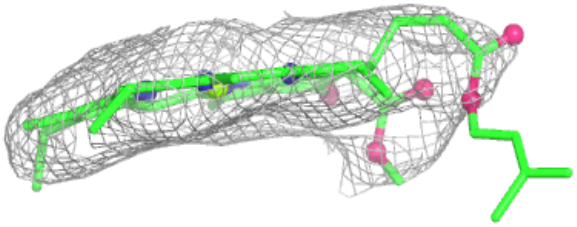


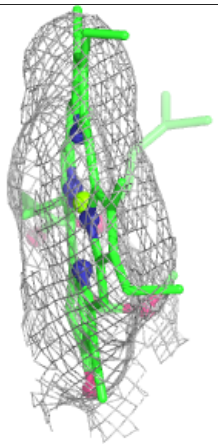


Electron density around CLA 4 305:

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

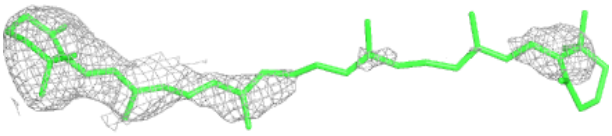


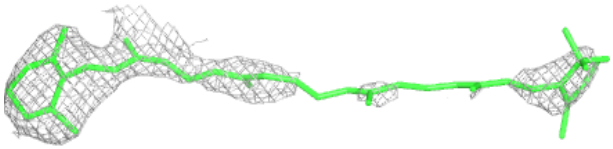


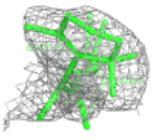


Electron density around BCR A 848:

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

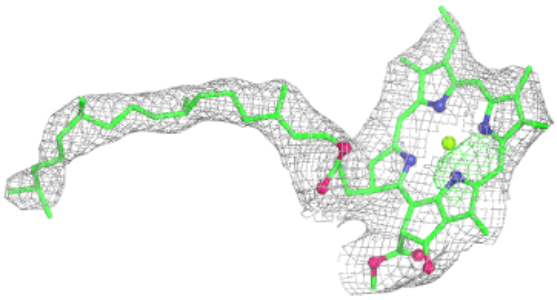


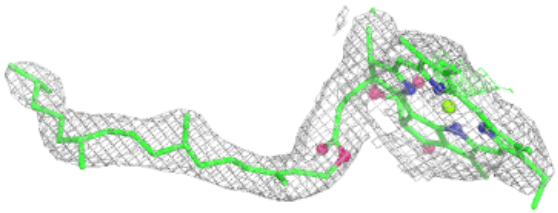


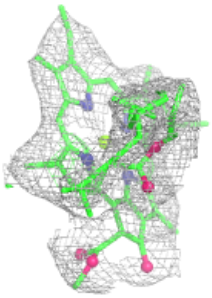


Electron density around CLA A 821:

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

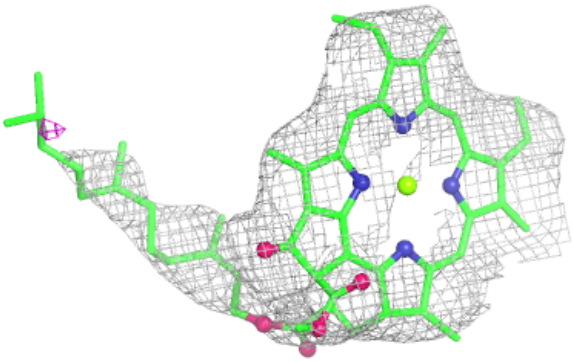


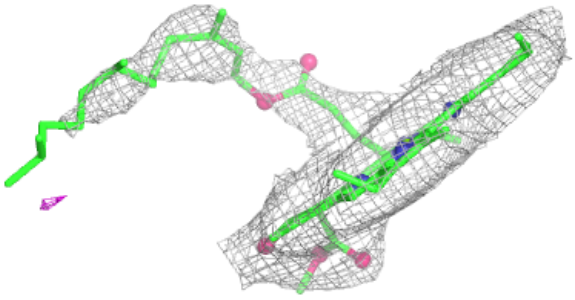


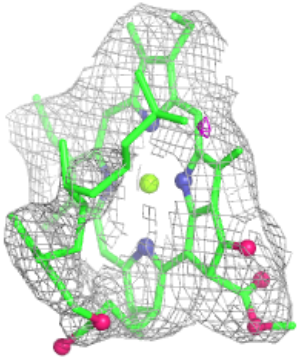


Electron density around CLA A 822:

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

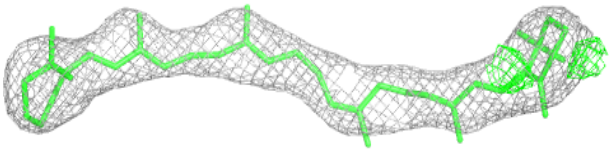


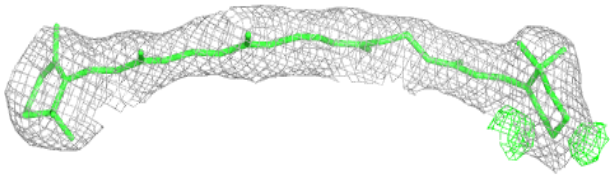


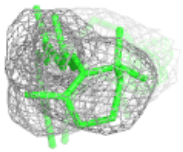


Electron density around BCR I 101:

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

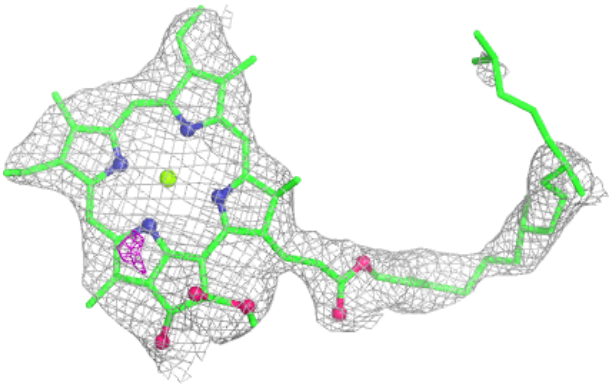


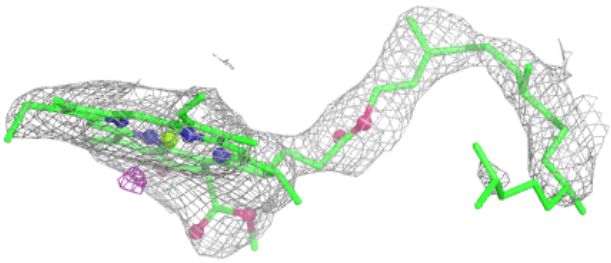


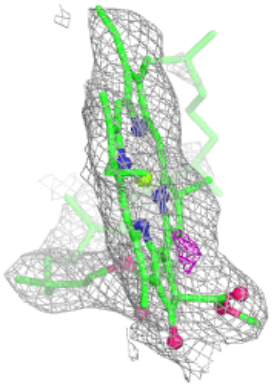


Electron density around CLA A 827:

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

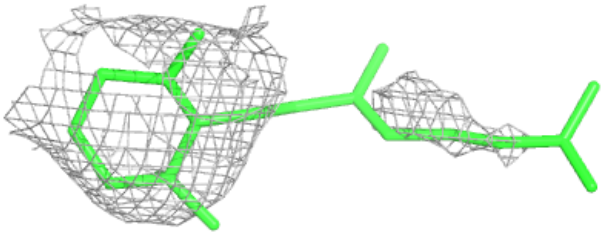


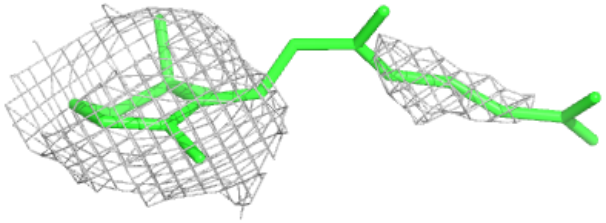


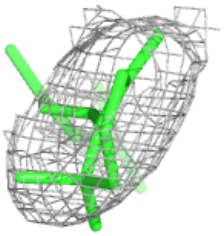


Electron density around BCR 1 503:

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

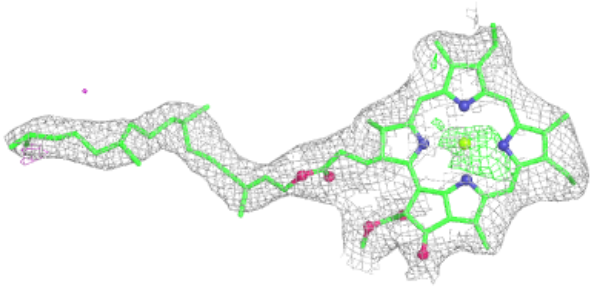


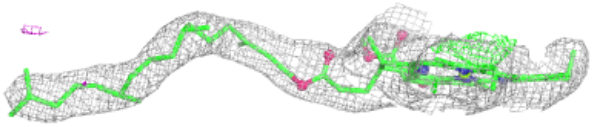




Electron density around CLA A 832:

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

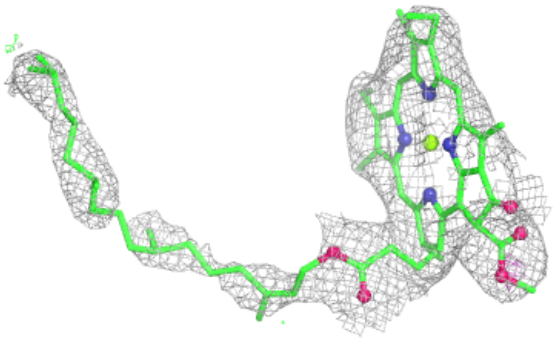


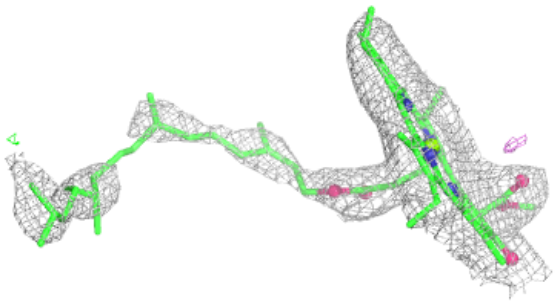


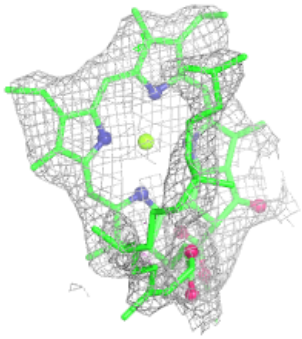


Electron density around CLA A 834:

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

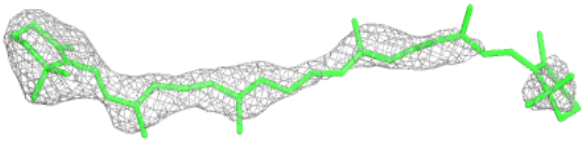


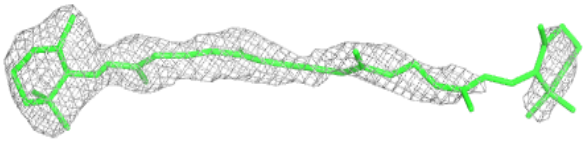


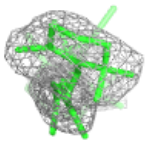


Electron density around BCR A 849:

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

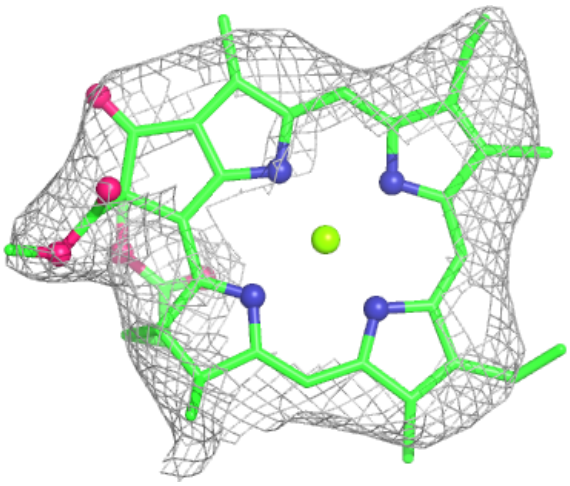


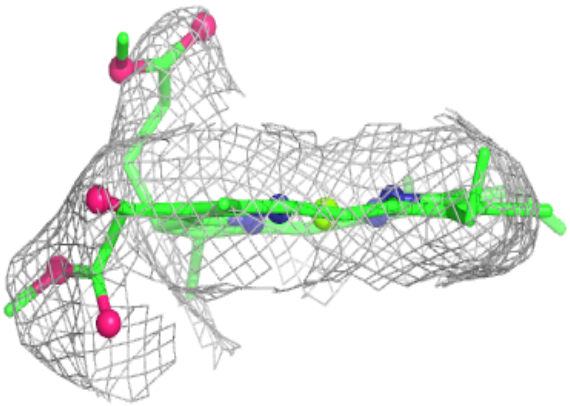


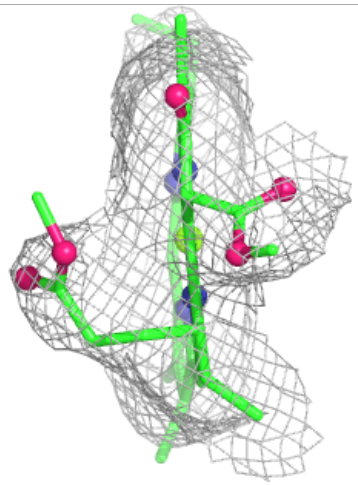


Electron density around CLA 4 311:

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

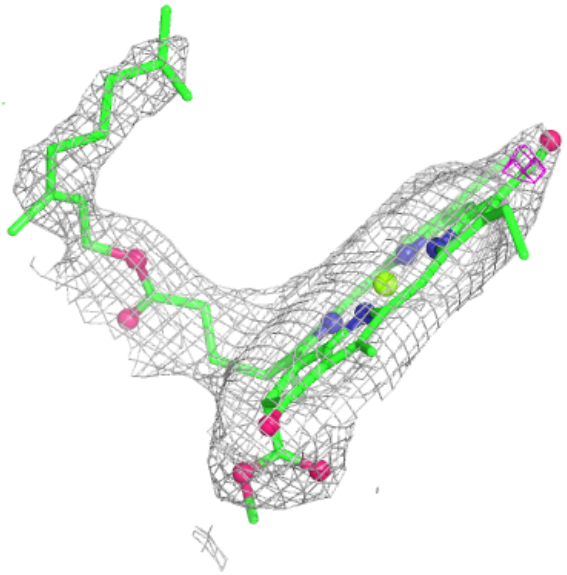


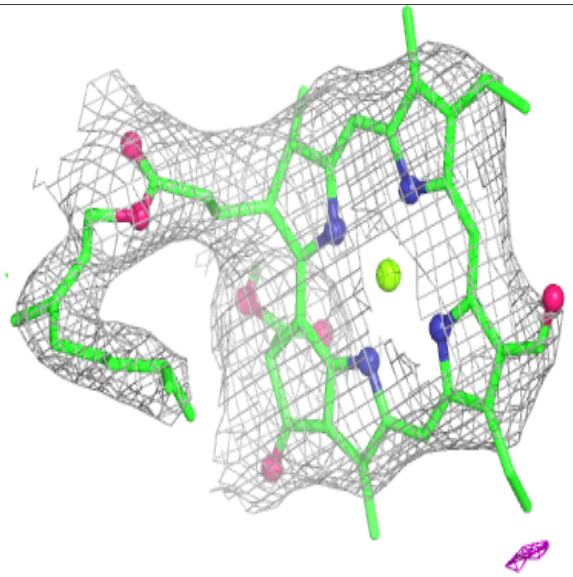


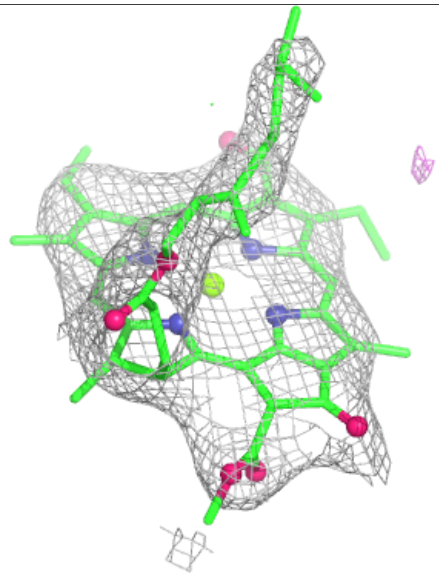


Electron density around CHL 1 521:

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

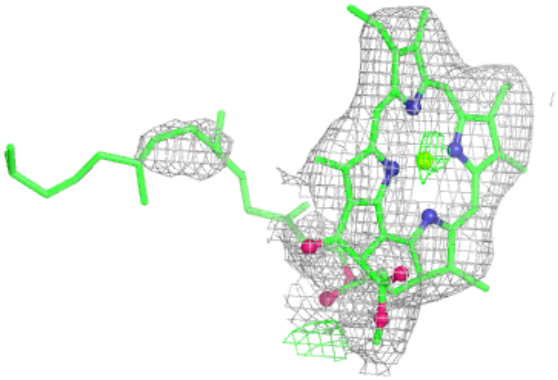


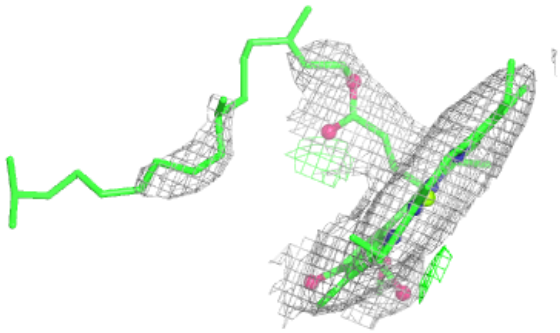


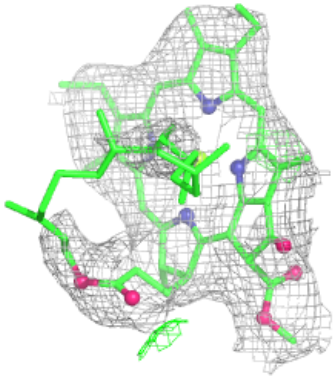


Electron density around CLA 4 315:

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

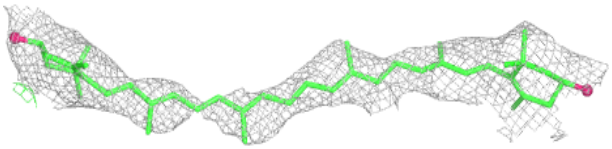


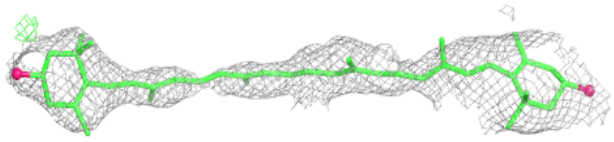


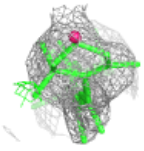


Electron density around LUT 1 501:

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

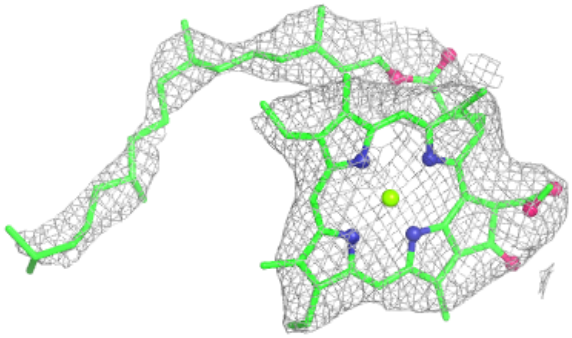


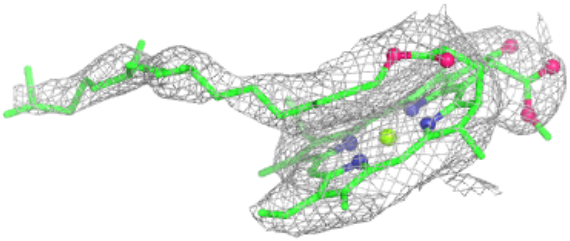


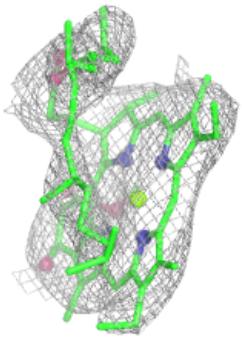


Electron density around CLA 1 507:

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

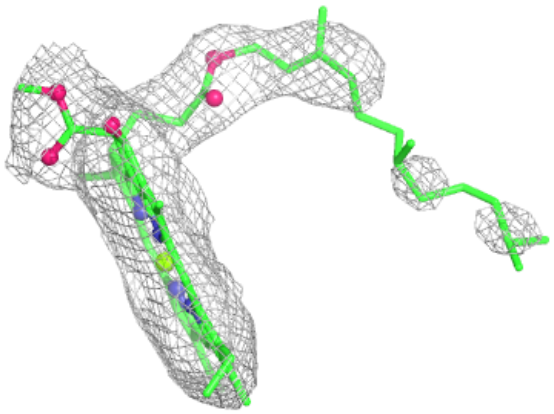


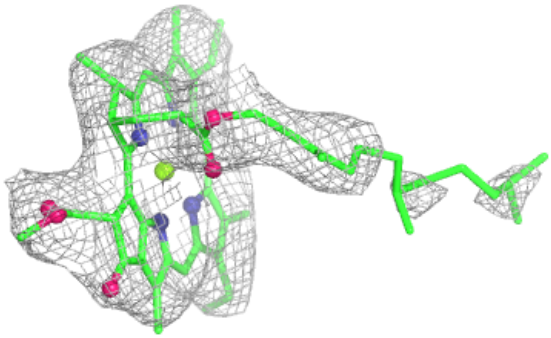


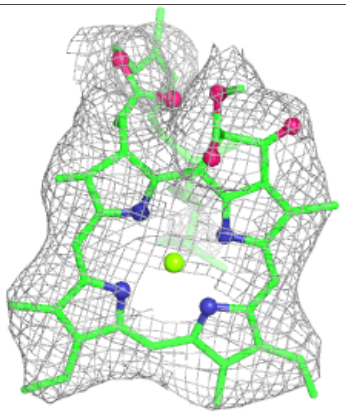


Electron density around CLA A 807:

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

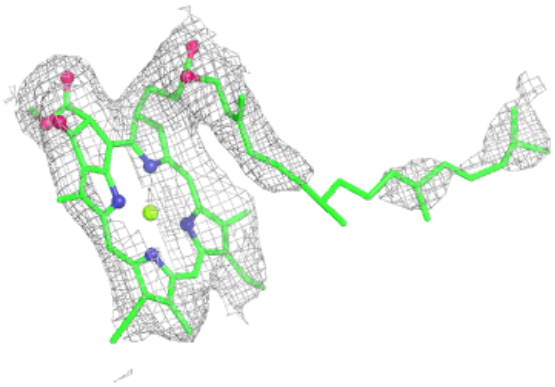


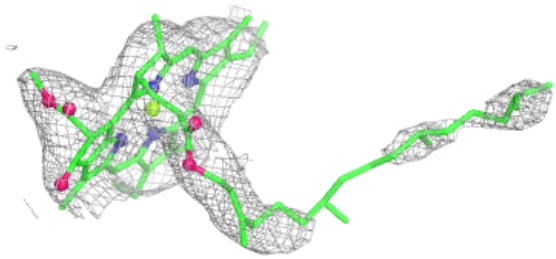


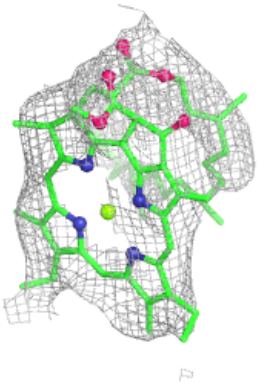


Electron density around CLA B 815:

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

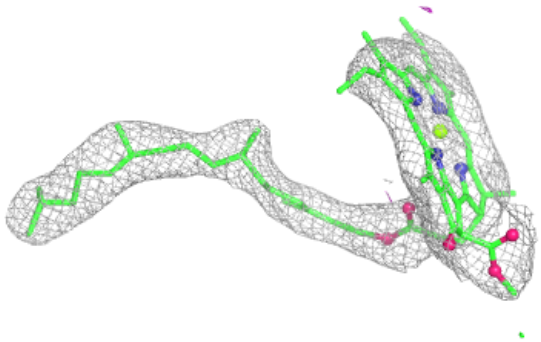


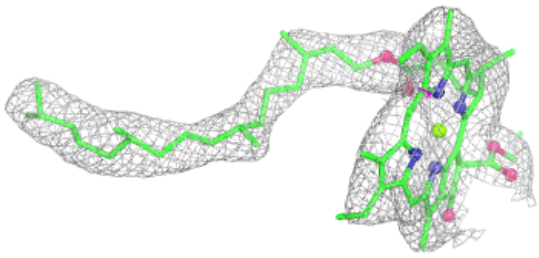


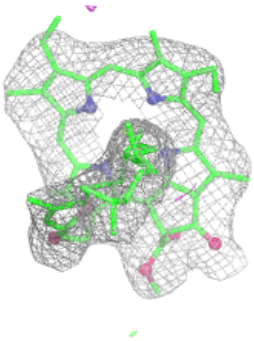


Electron density around CLA A 811:

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

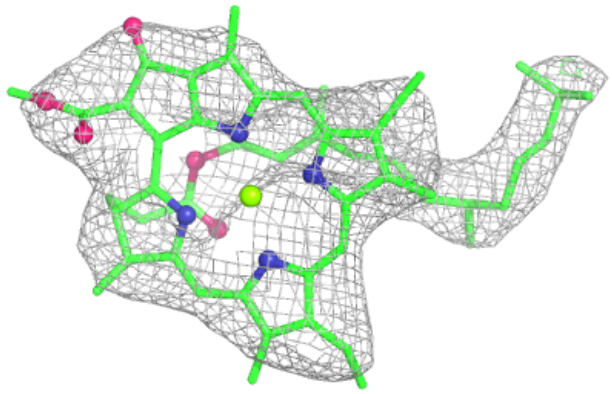


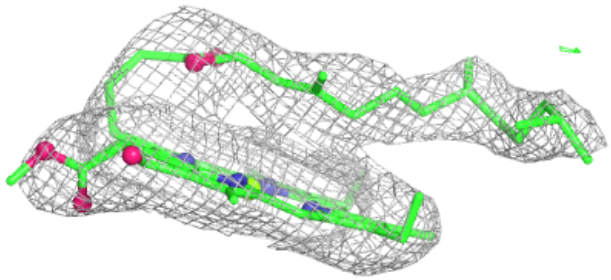


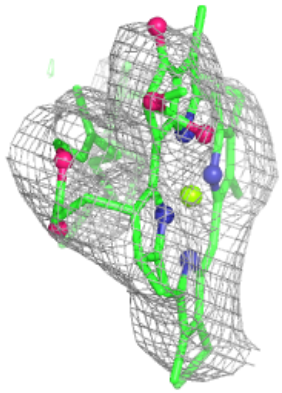


Electron density around CLA B 817:

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

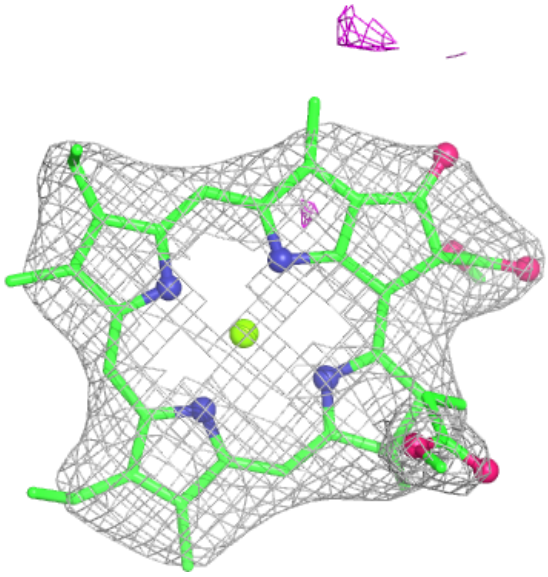


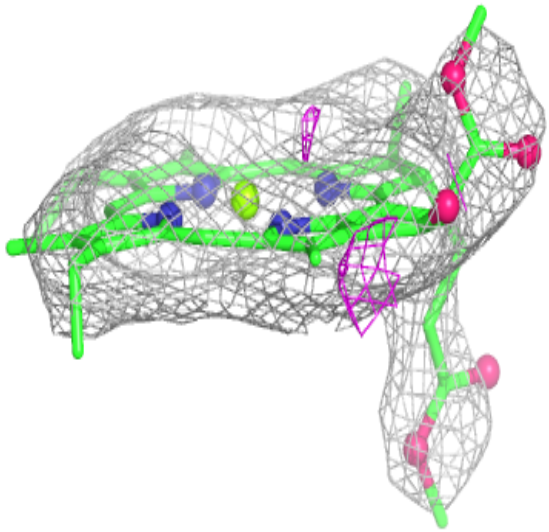


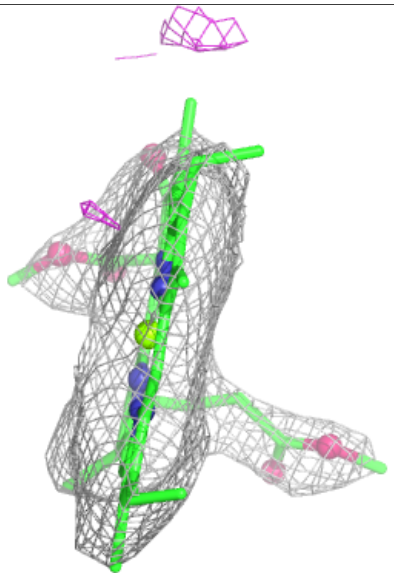


Electron density around CLA B 821:

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

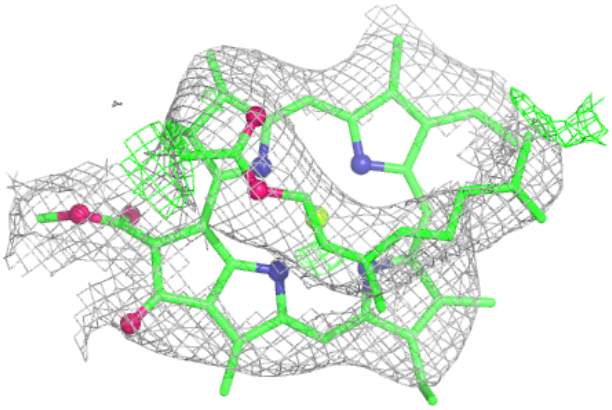


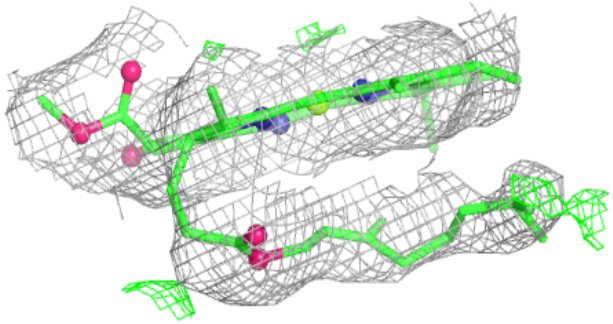


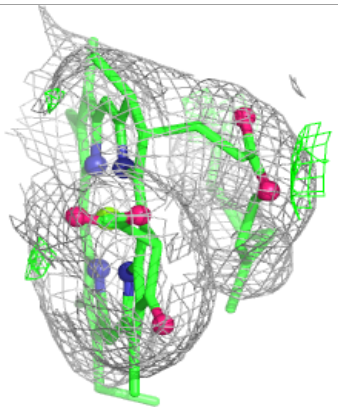


Electron density around CLA A 812:

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

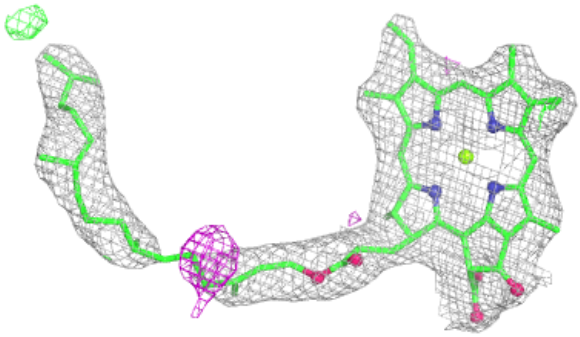


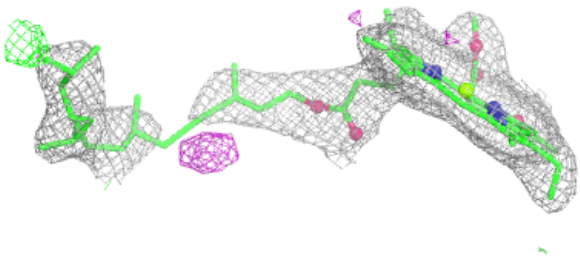


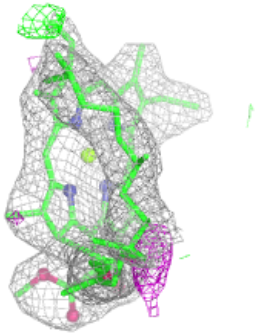


Electron density around CLA B 825:

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

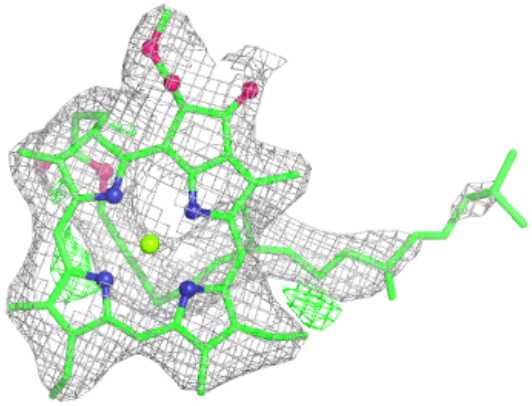


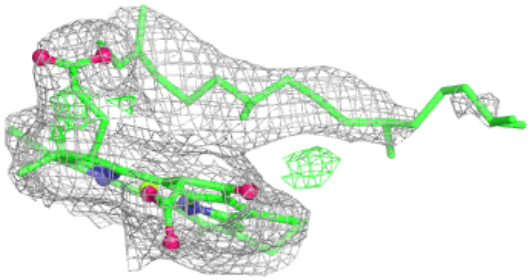


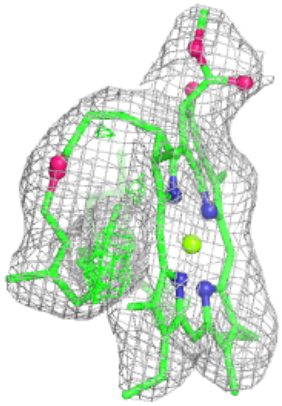


Electron density around CLA B 827:

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

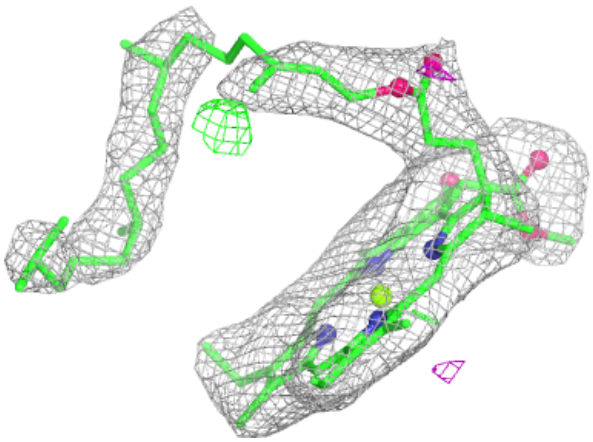


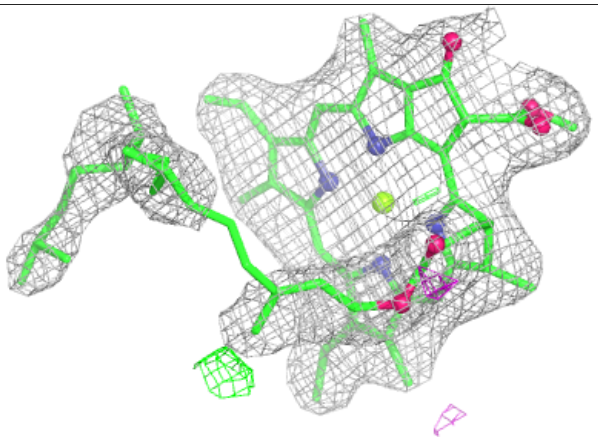


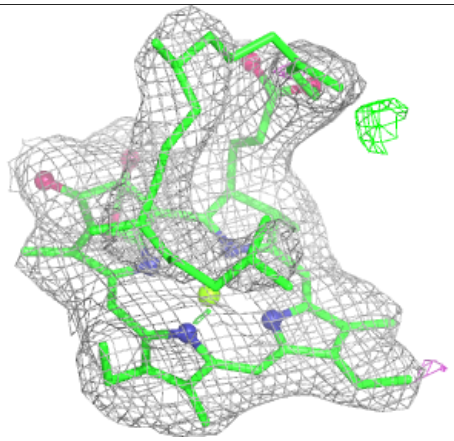


Electron density around CLA B 830:

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

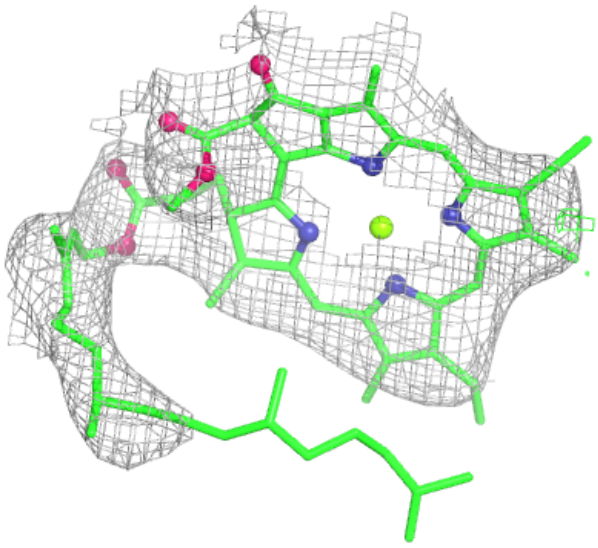


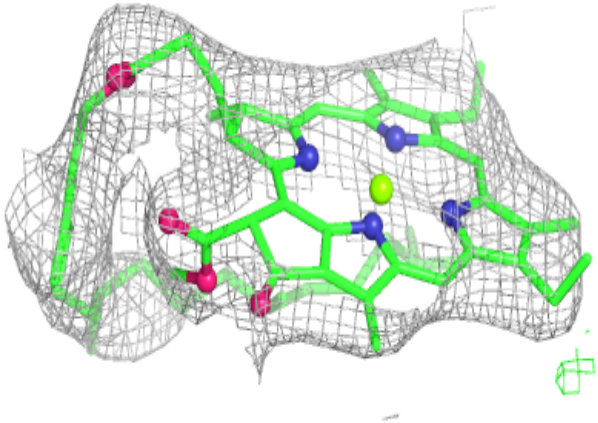


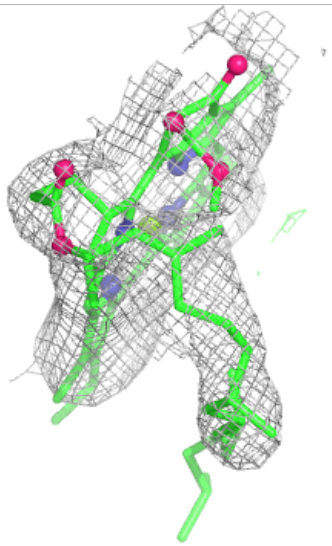


Electron density around CLA 1 508:

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

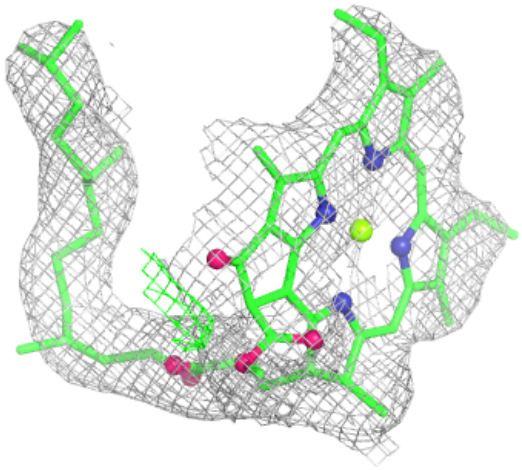


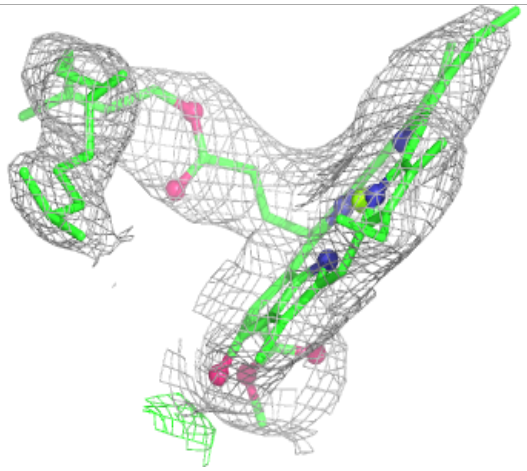


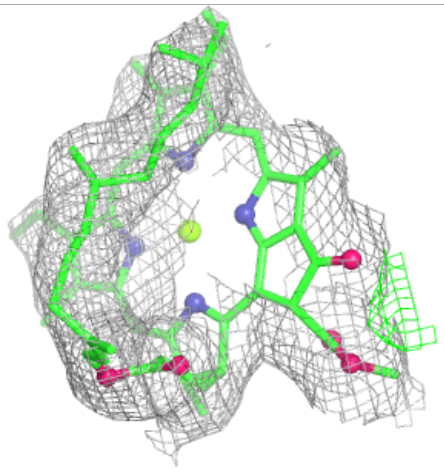


Electron density around CLA B 833:

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

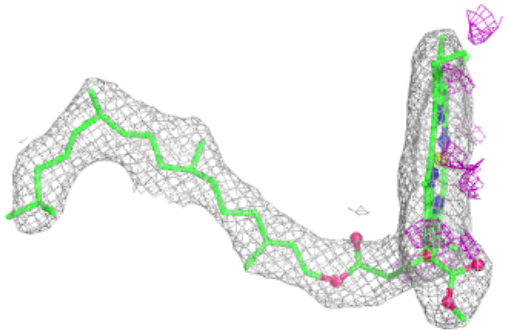


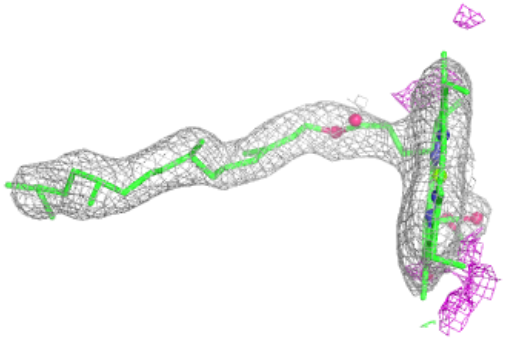


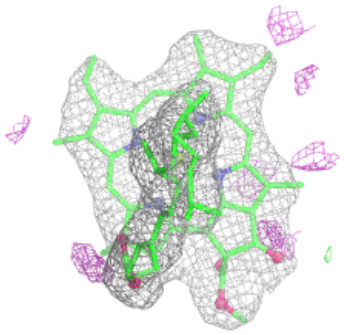


Electron density around CLA B 839:

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

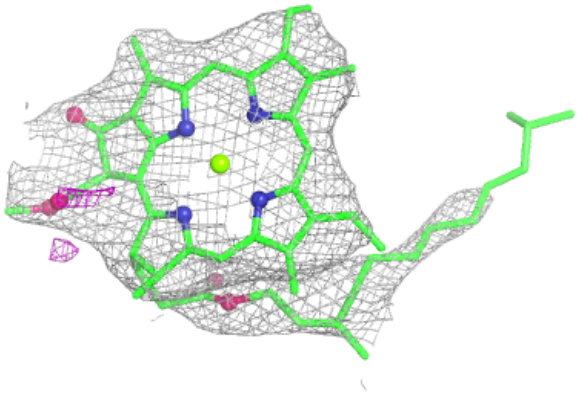


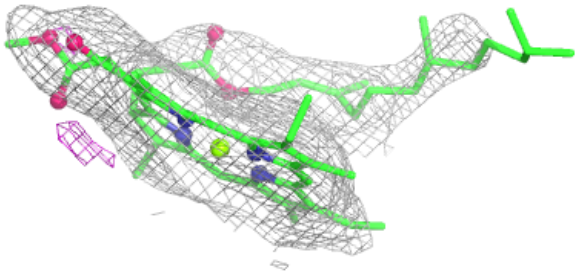


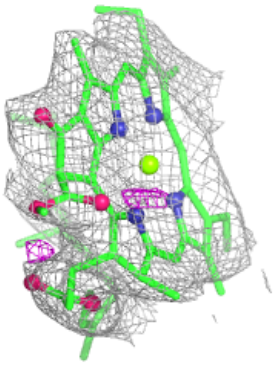


Electron density around CLA 2 504:

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

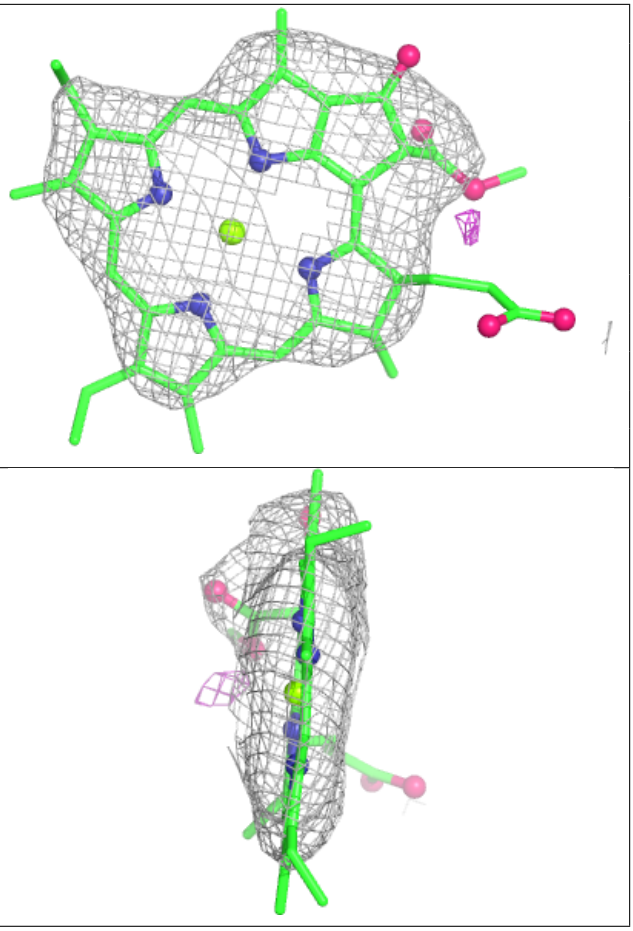


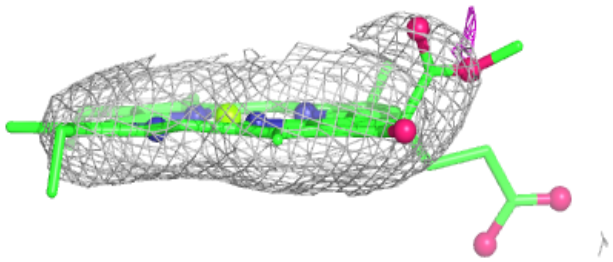




Electron density around CLA A 815:

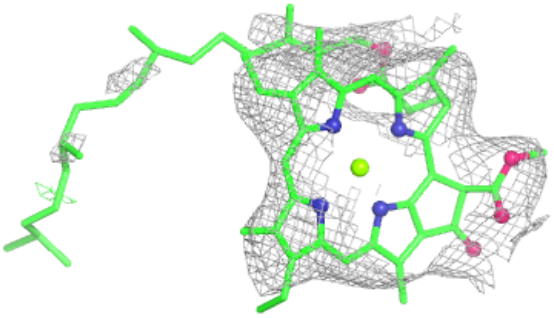
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

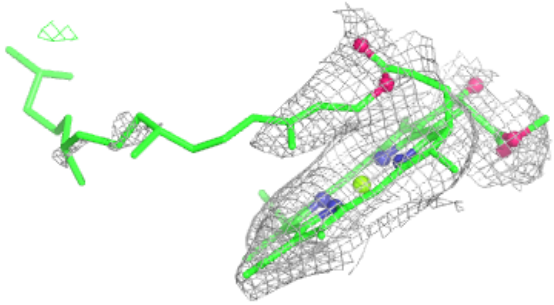


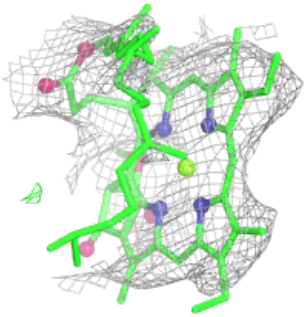


Electron density around CLA 3 308:

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

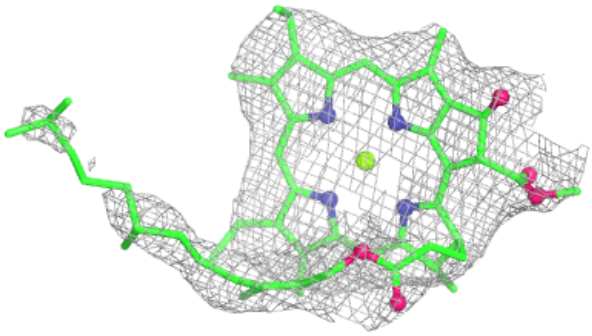


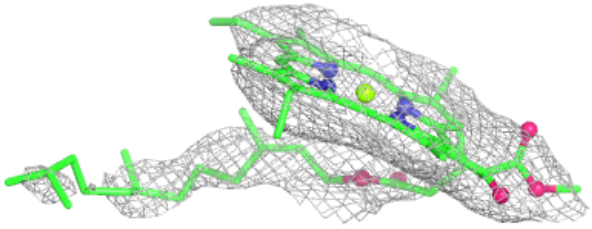


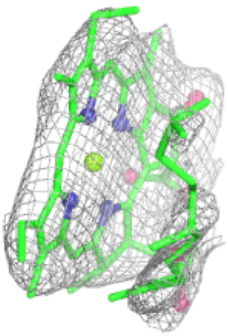


Electron density around CLA 4 304:

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

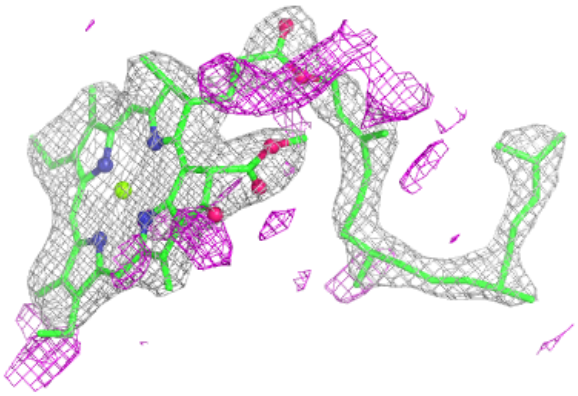


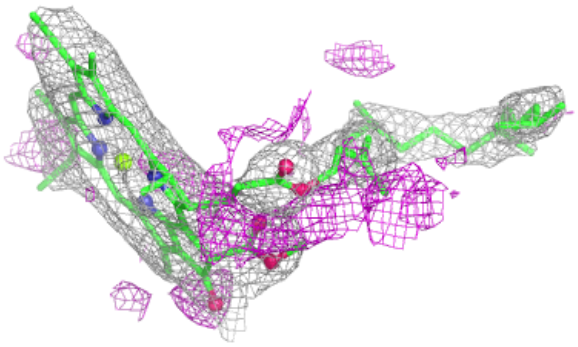


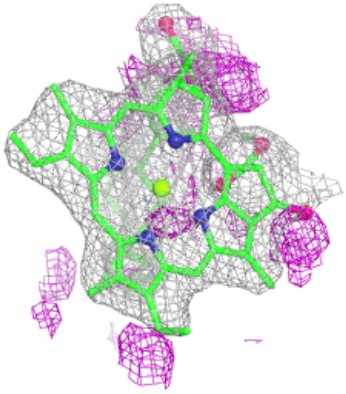


Electron density around CL0 A 801:

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

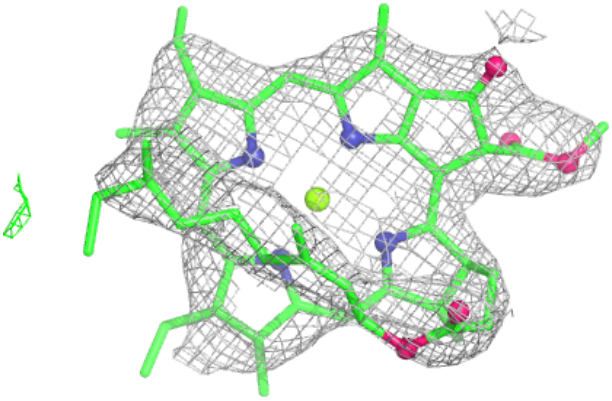


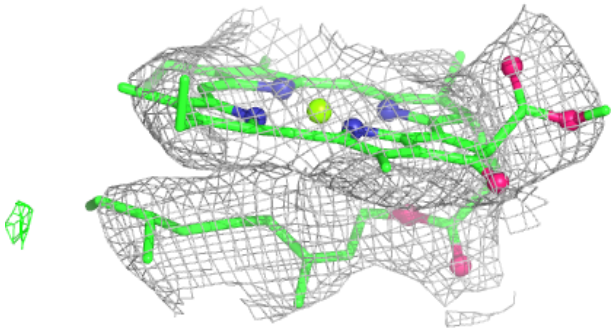


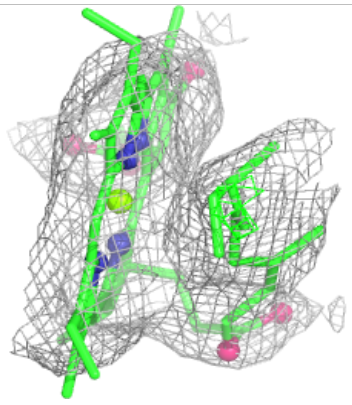


Electron density around CLA A 818:

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

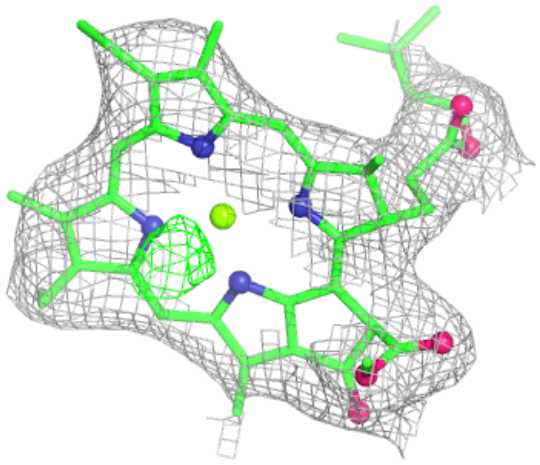


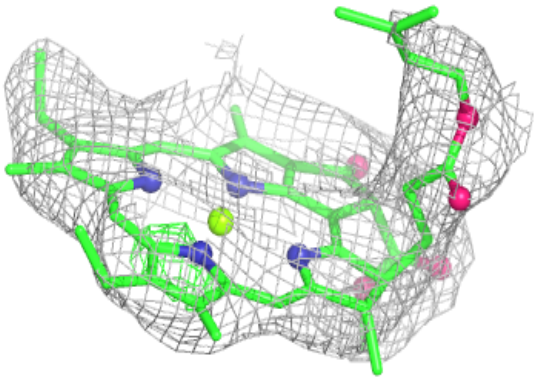


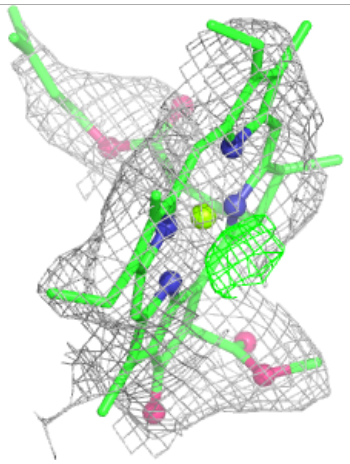


Electron density around CLA A 820:

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

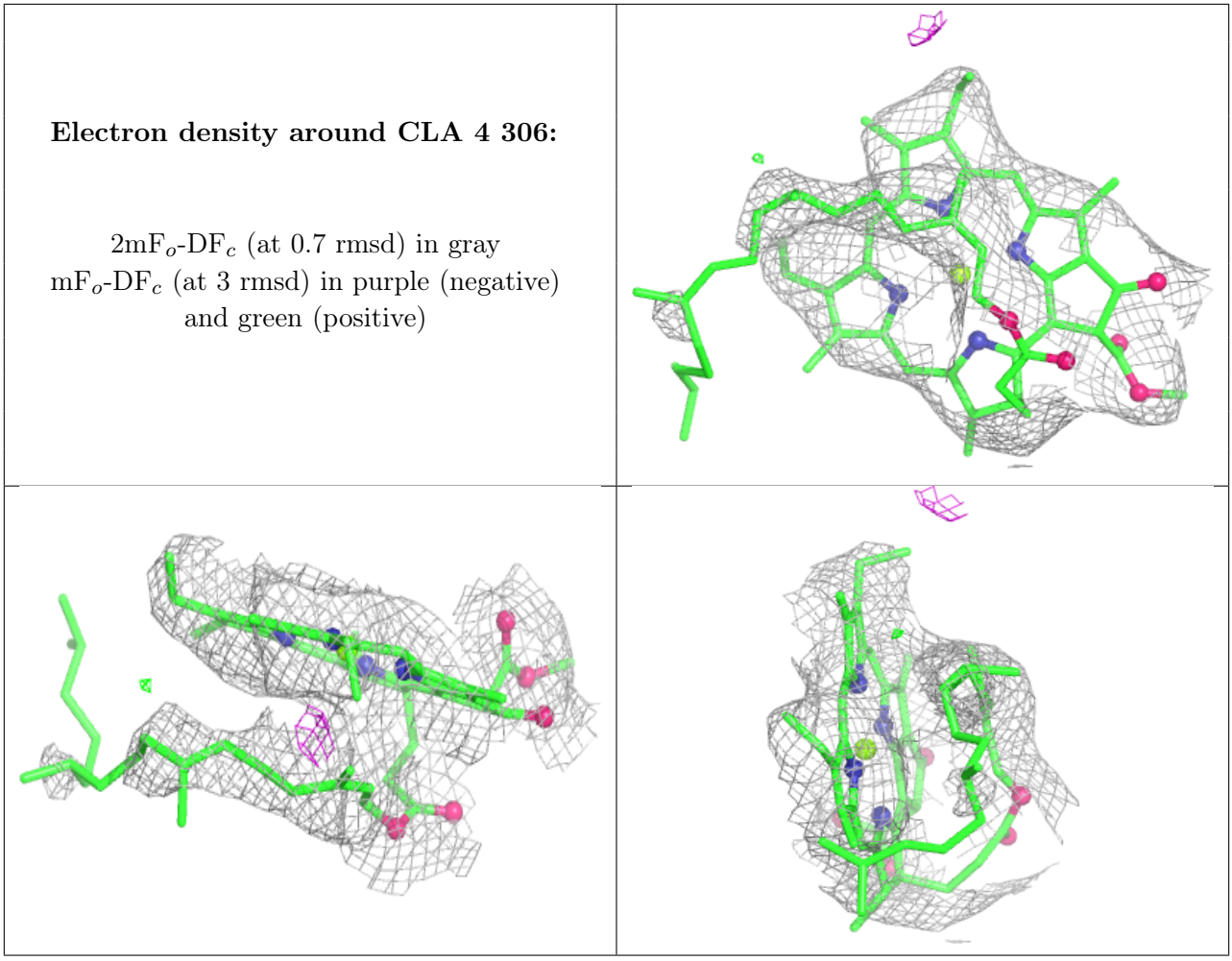






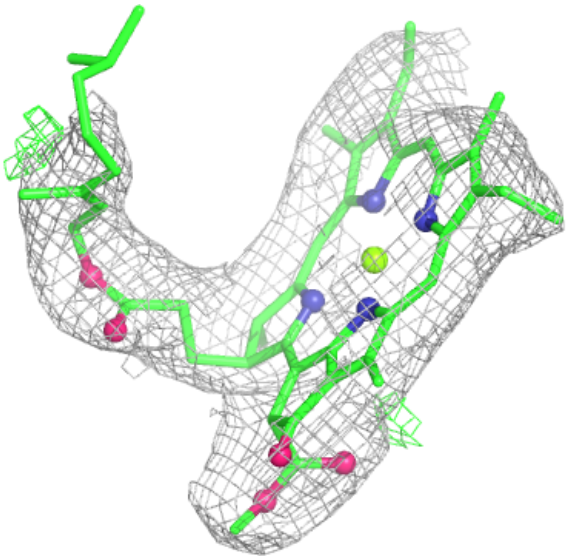
Electron density around CLA 4 306:

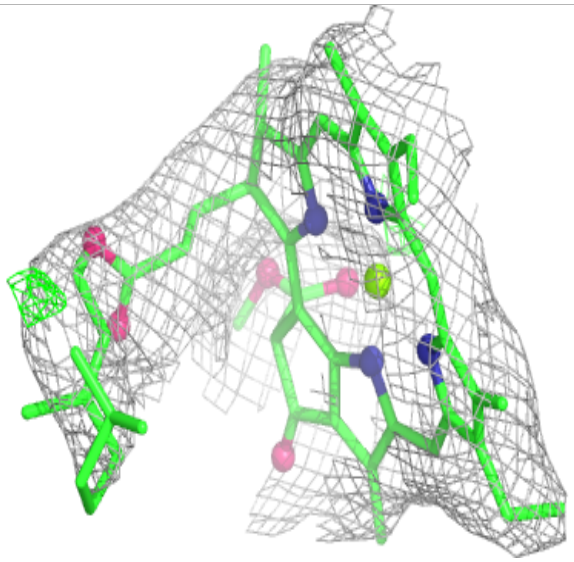
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

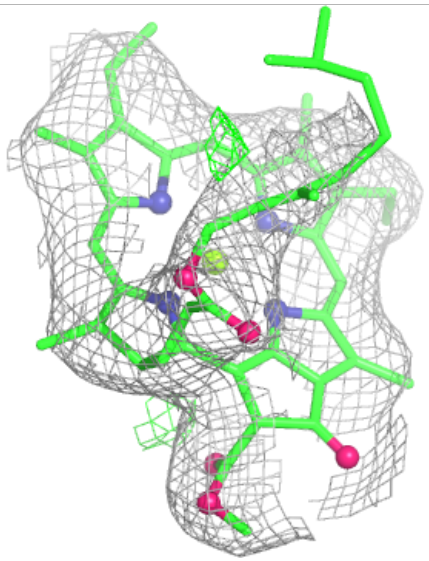


Electron density around CLA B 834:

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

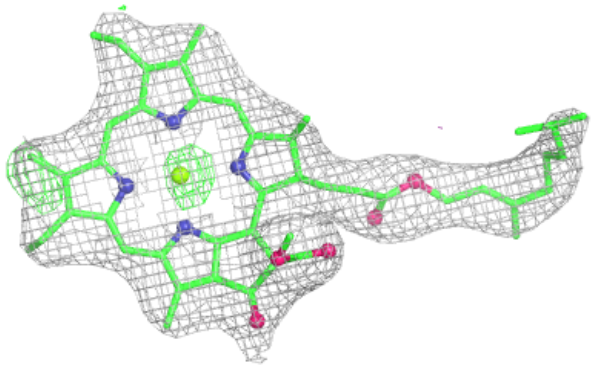


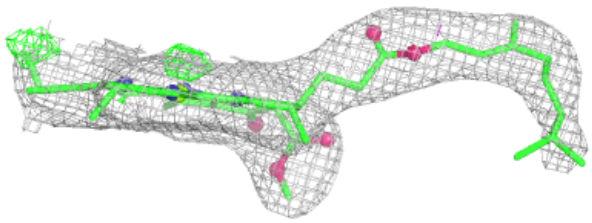


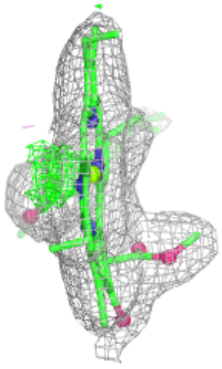


Electron density around CLA B 835:

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

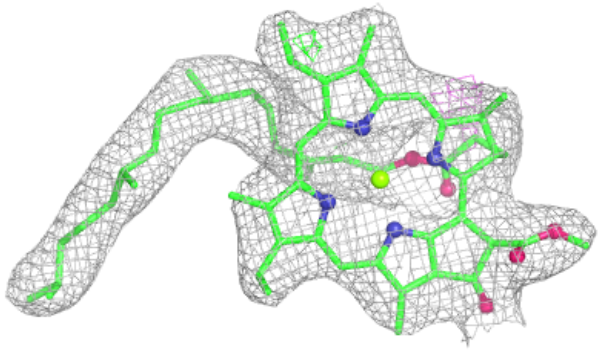


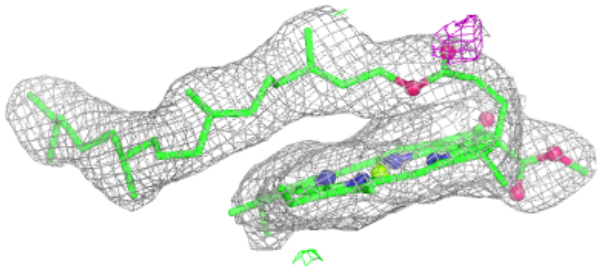


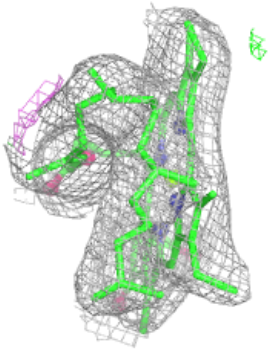


Electron density around CLA B 836:

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

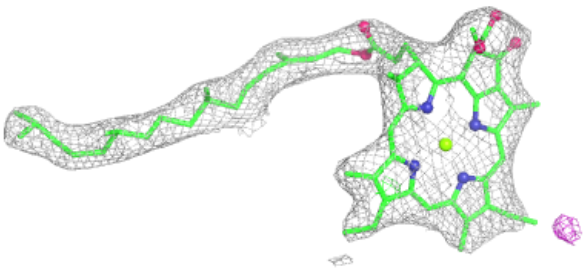


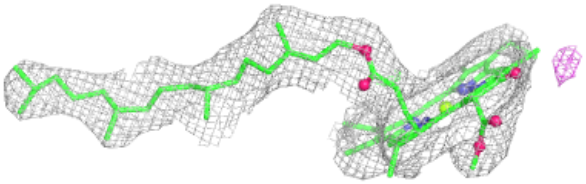


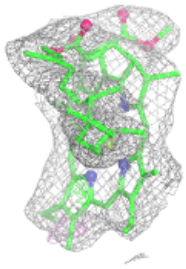


Electron density around CLA A 833:

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

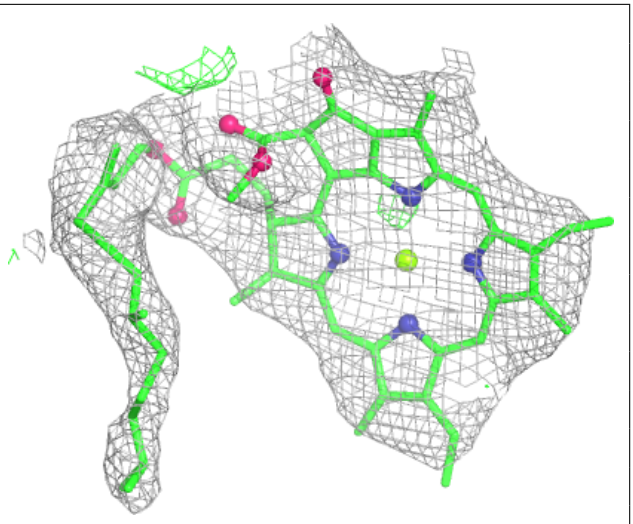


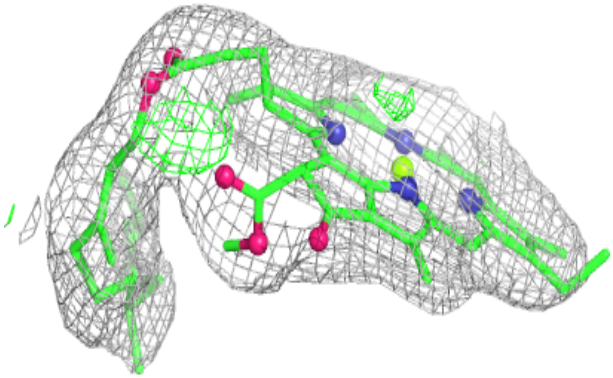


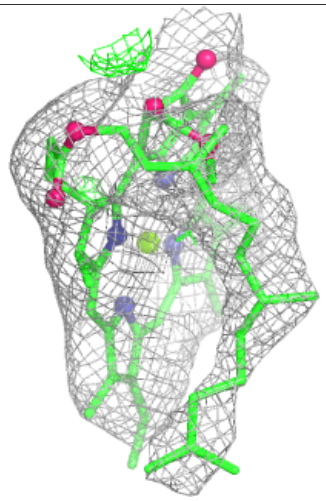


Electron density around CLA 4 308:

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

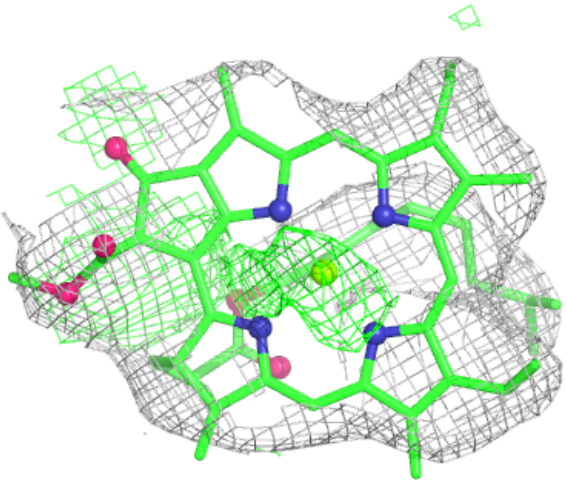


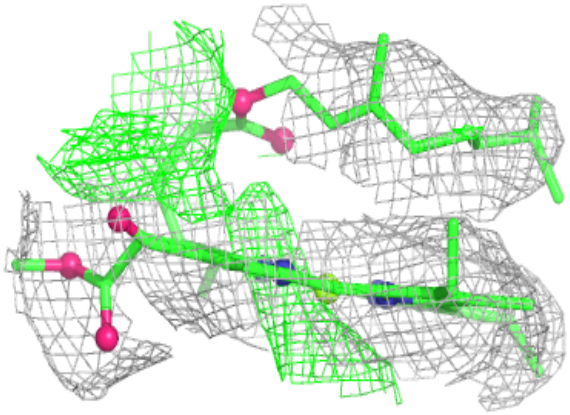


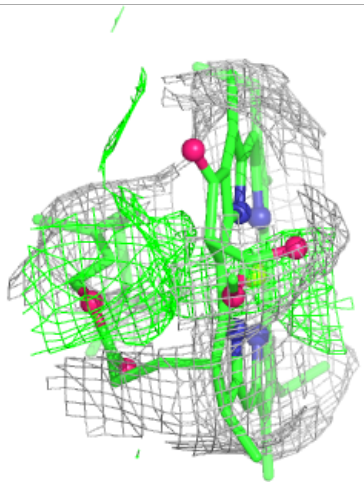


Electron density around CLA 1 506:

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

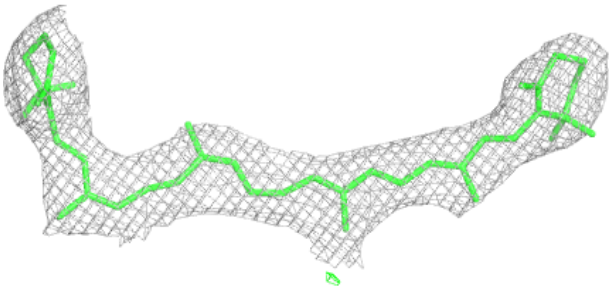


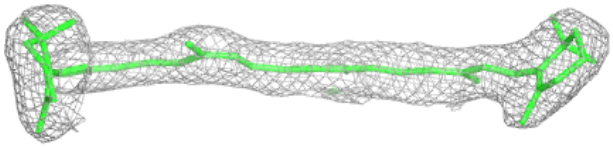


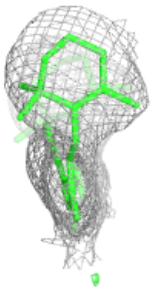


Electron density around BCR L 302:

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

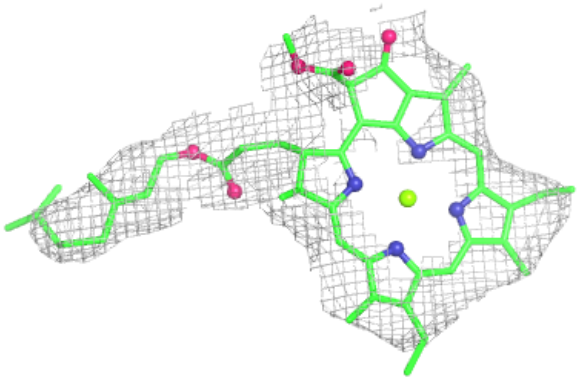


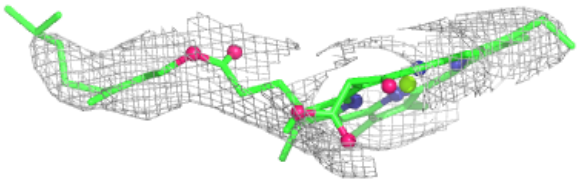




Electron density around CLA G 202:

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

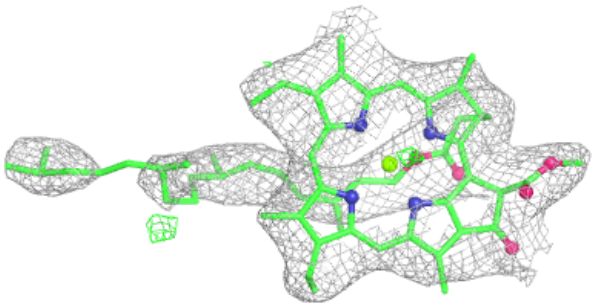


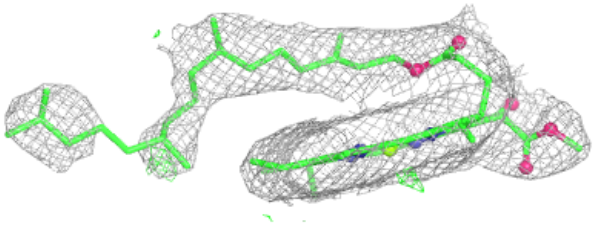


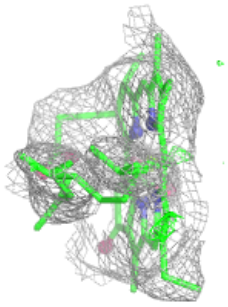


Electron density around CLA A 837:

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

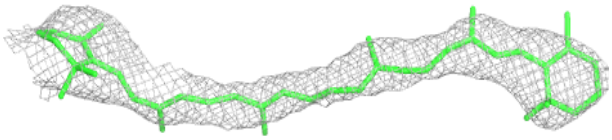


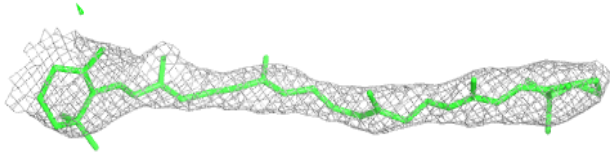


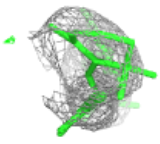


Electron density around BCR 4 301:

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

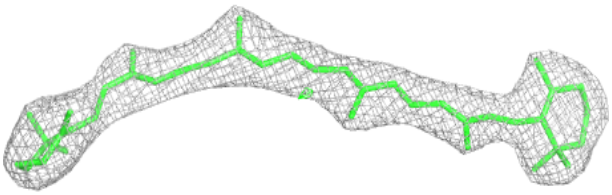


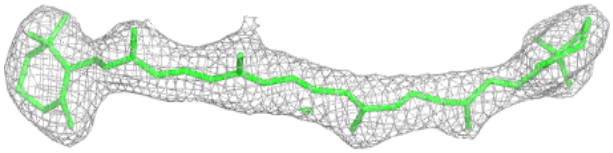


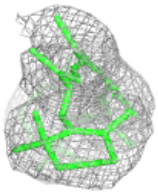


Electron density around BCR B 856:

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

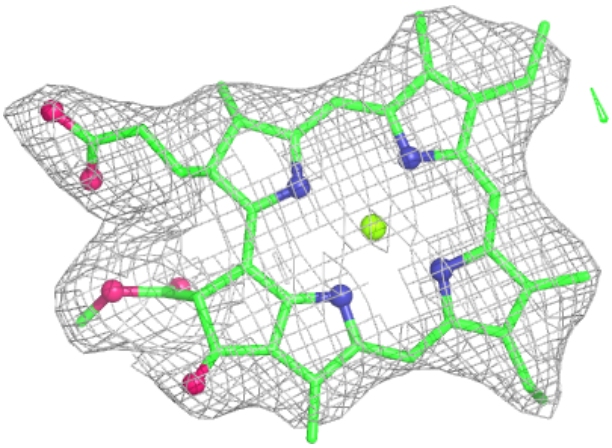


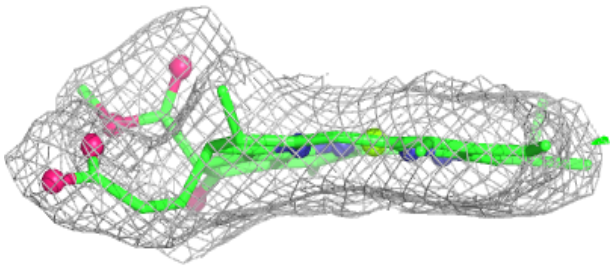


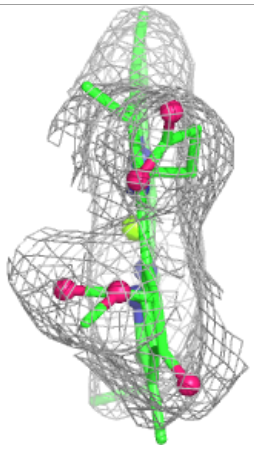


Electron density around CLA J 1102:

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

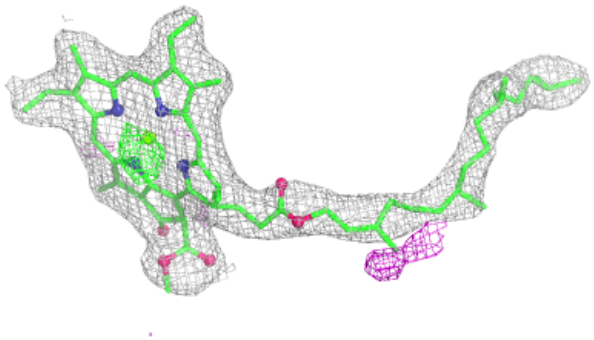


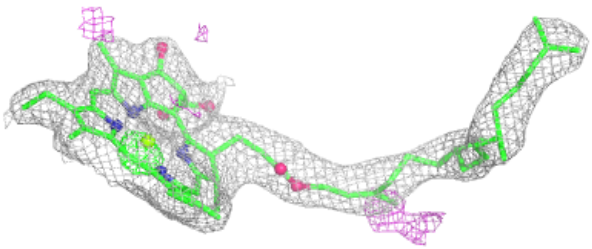


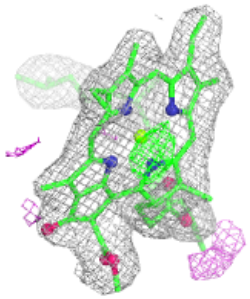


Electron density around CLA A 854:

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

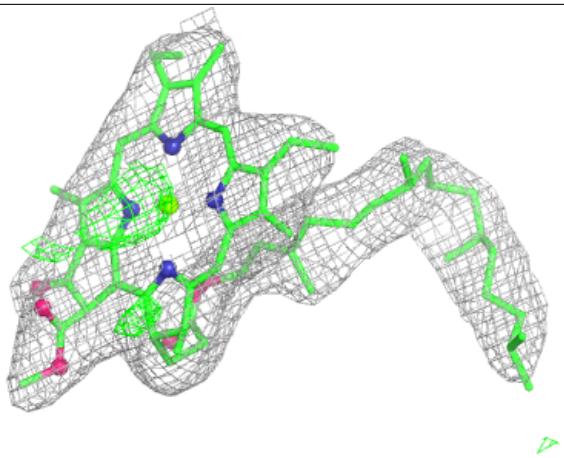


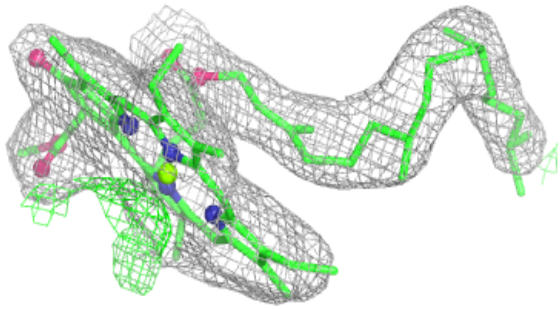


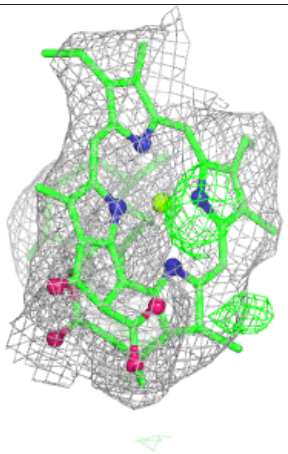


Electron density around CLA A 855:

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

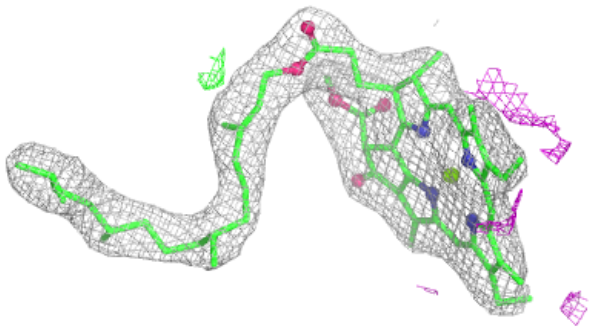


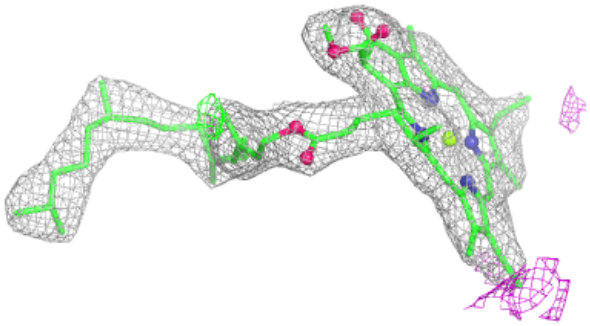


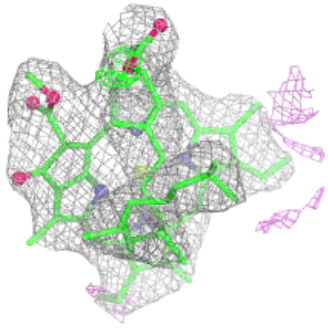


Electron density around CLA B 803:

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

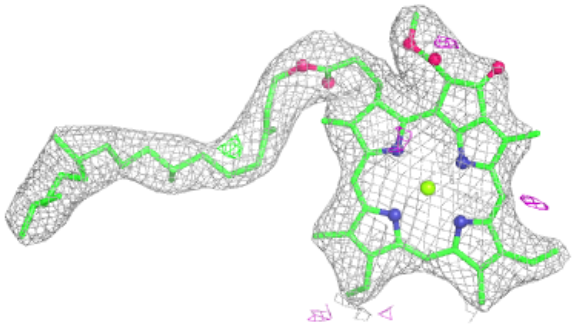


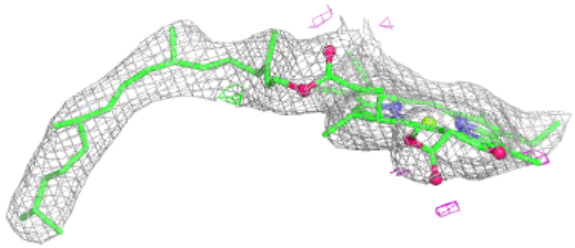




Electron density around CLA B 804:

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

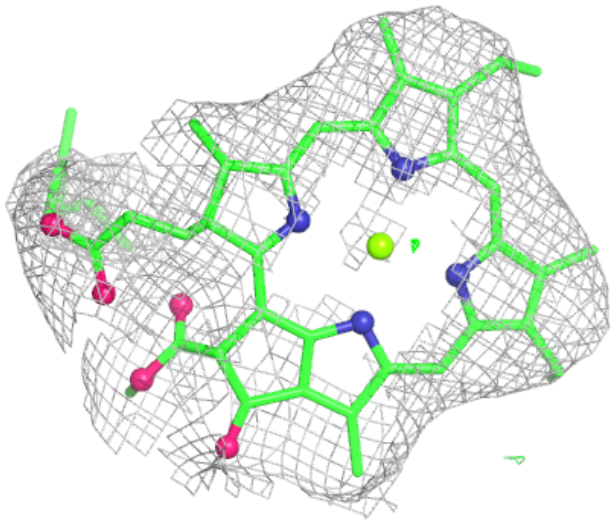


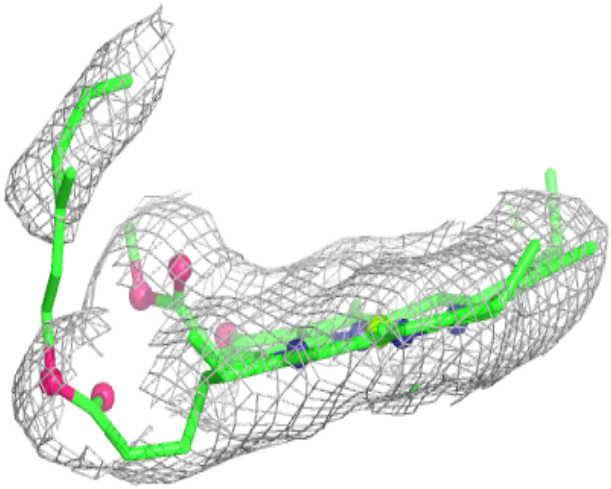


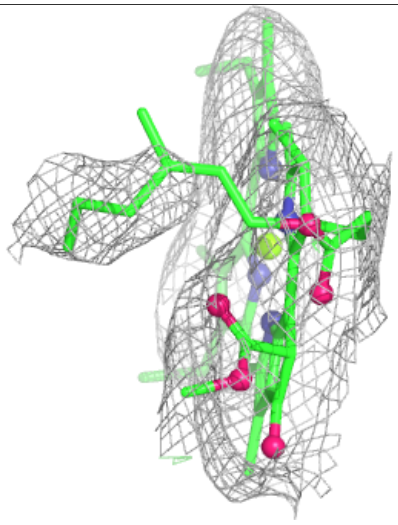


Electron density around CLA 2 505:

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

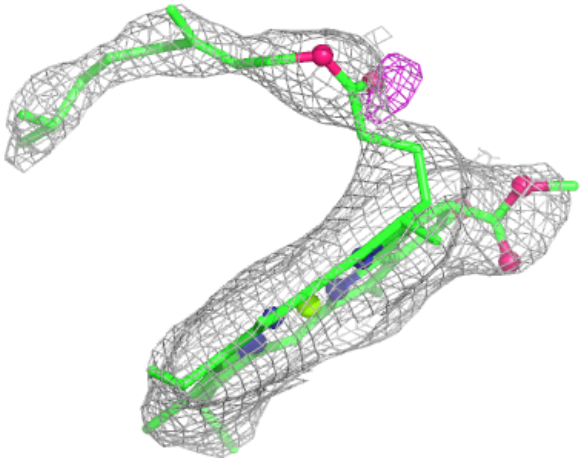


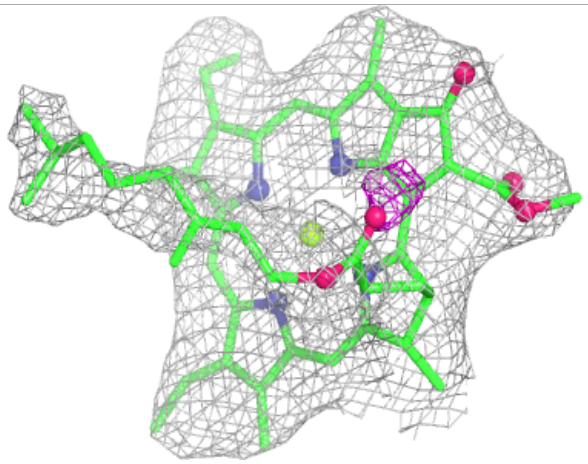


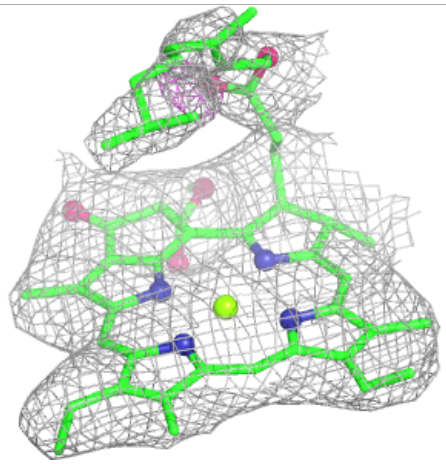


Electron density around CLA L 301:

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

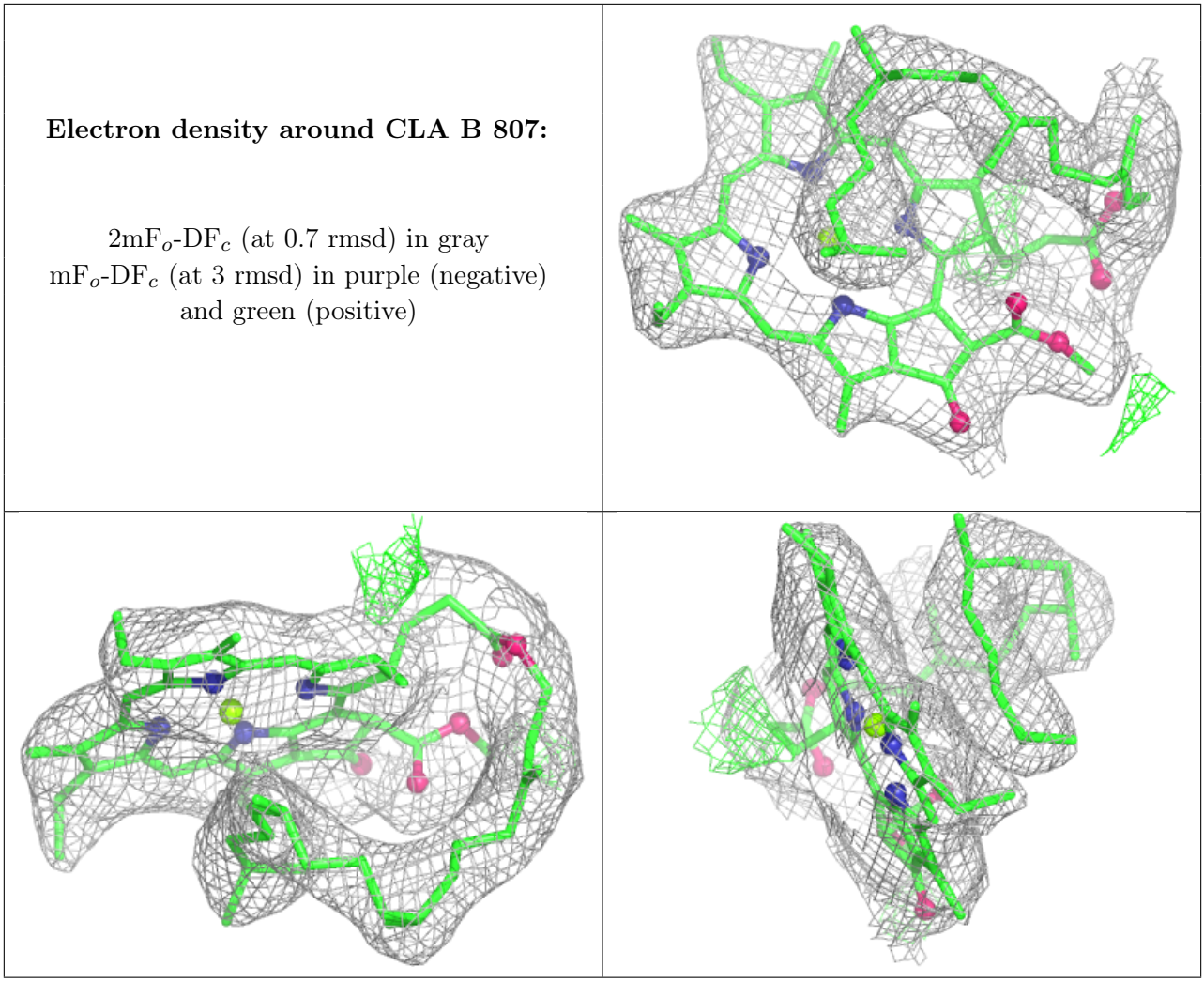






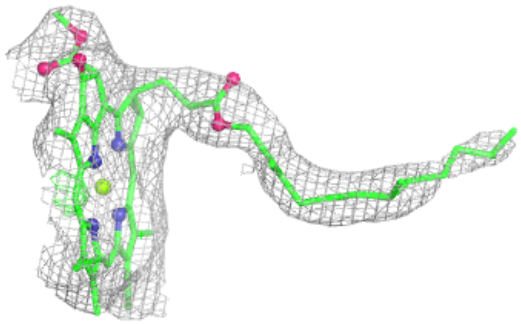
Electron density around CLA B 807:

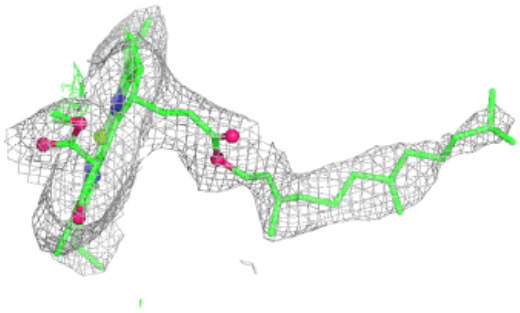
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

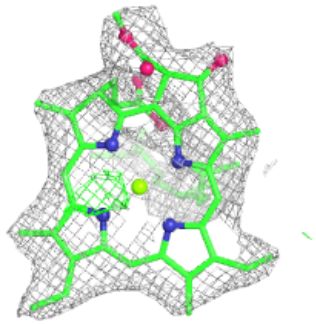


Electron density around CLA L 304:

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

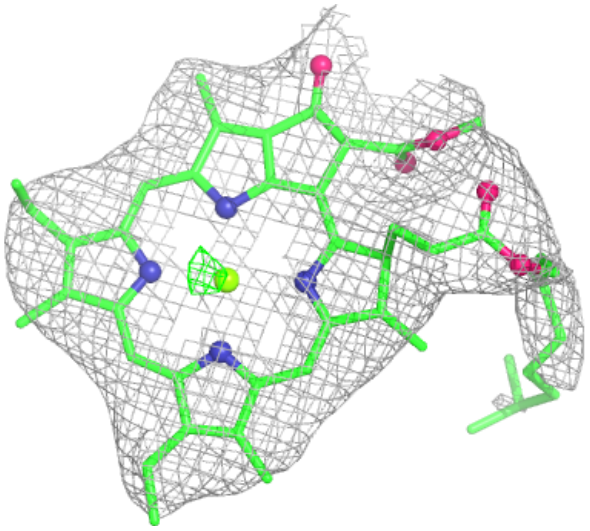


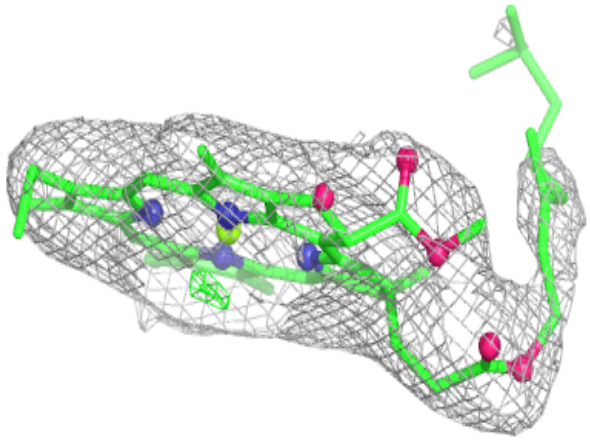


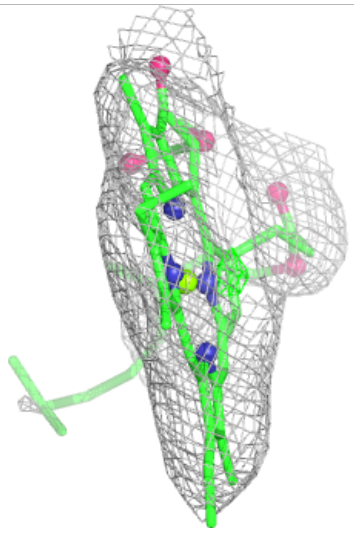


Electron density around CLA 2 508:

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

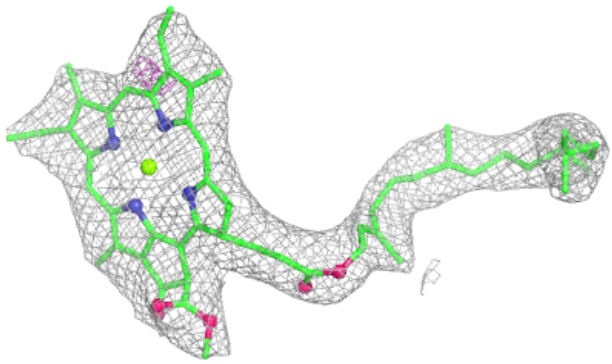


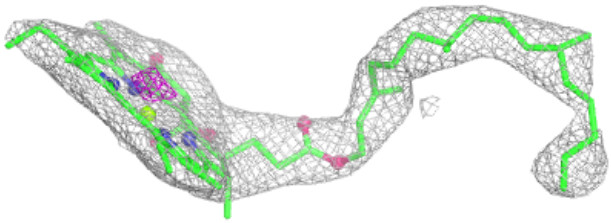


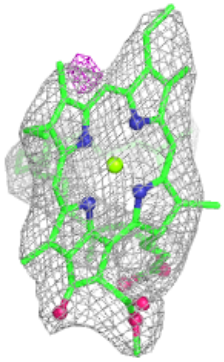


Electron density around CLA B 810:

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

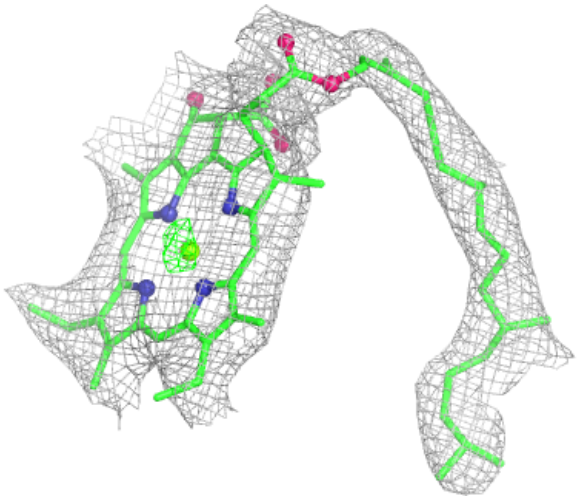


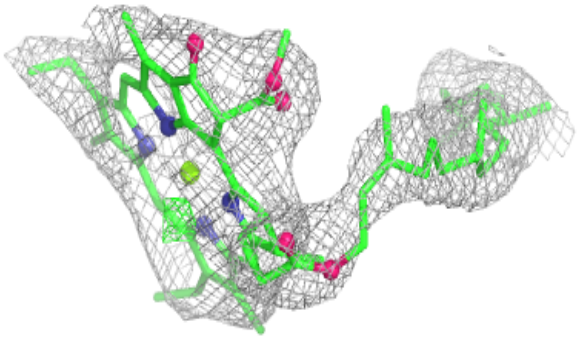


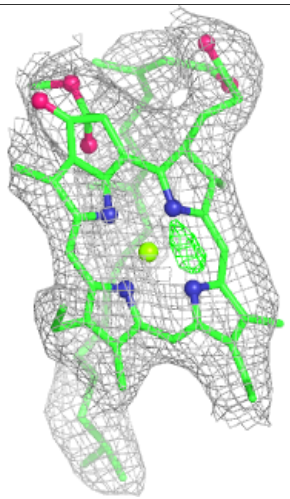


Electron density around CLA B 811:

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

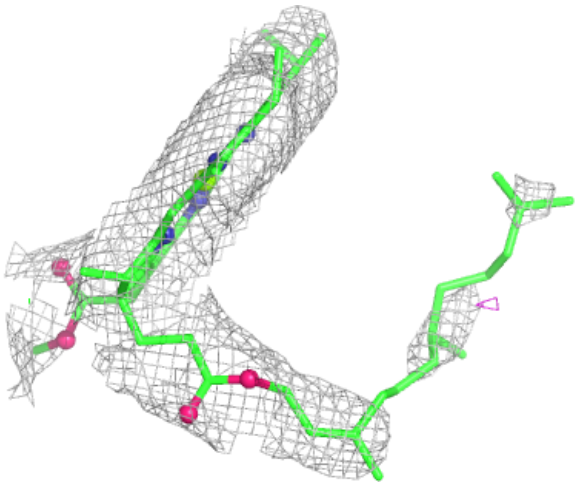


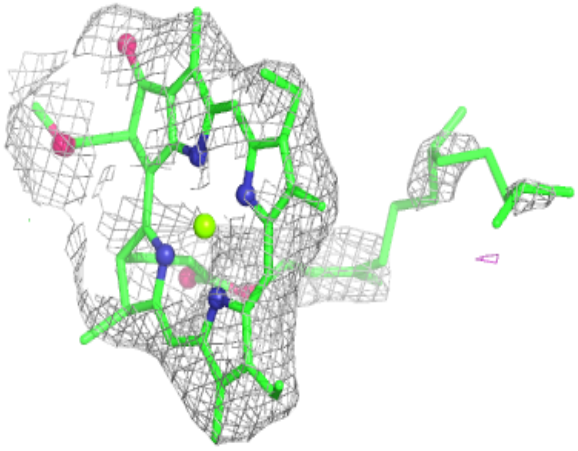


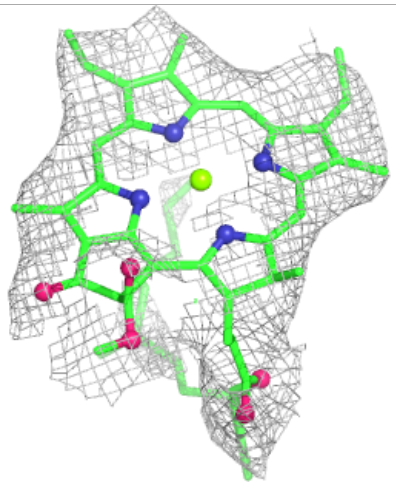


Electron density around CLA B 812:

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

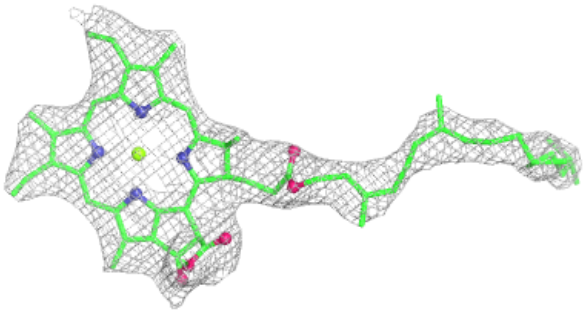


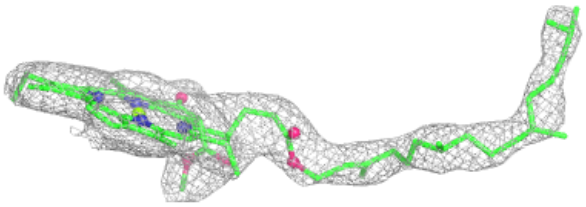


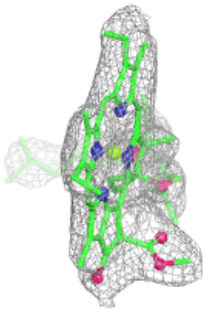


Electron density around CLA A 805:

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

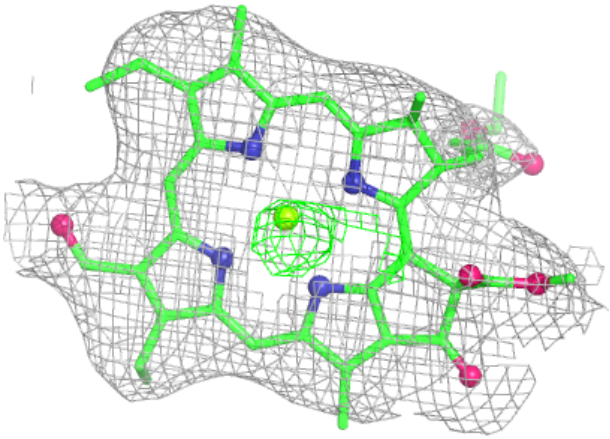


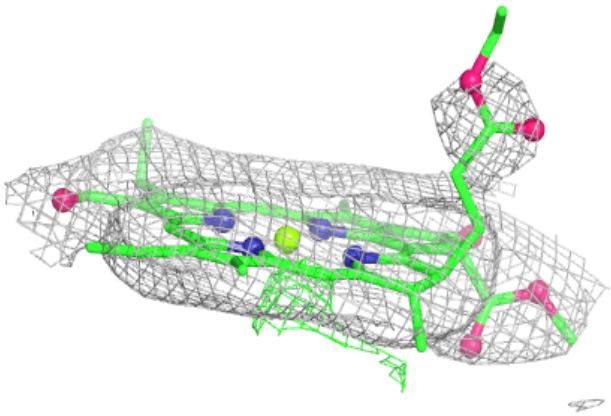




Electron density around CHL 2 513:

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

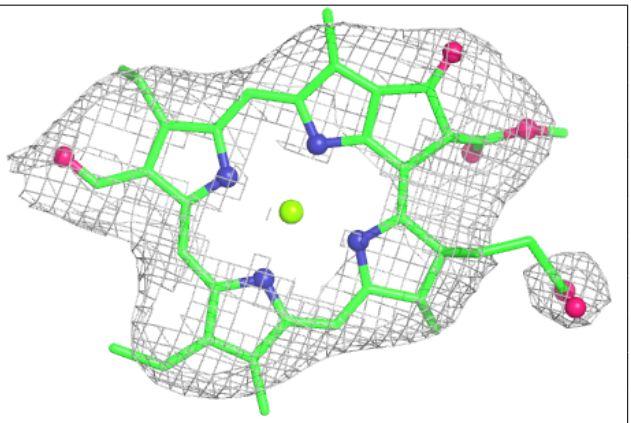


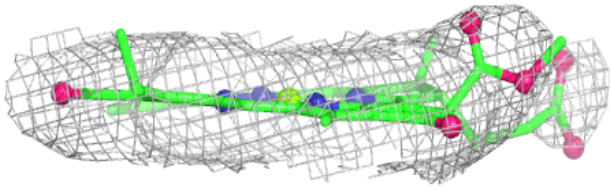


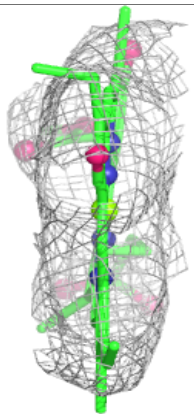


Electron density around CHL 2 515:

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

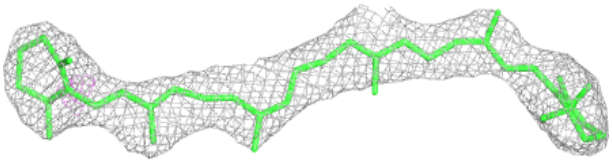


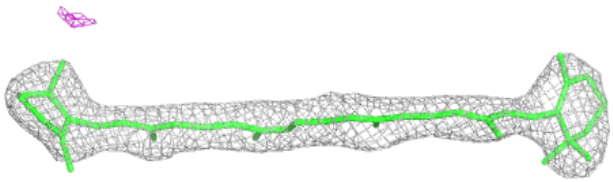


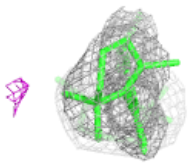


Electron density around BCR B 802:

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

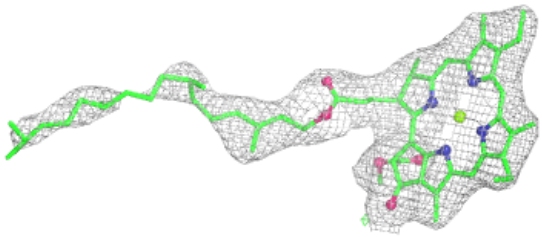


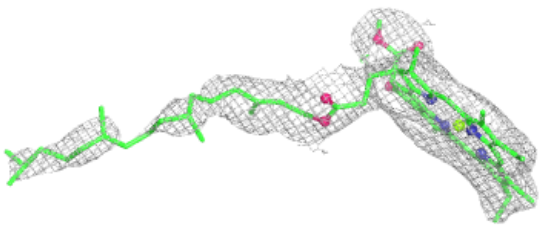


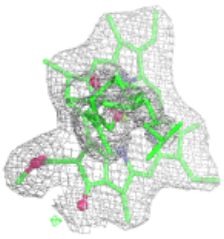


Electron density around CLA A 809:

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

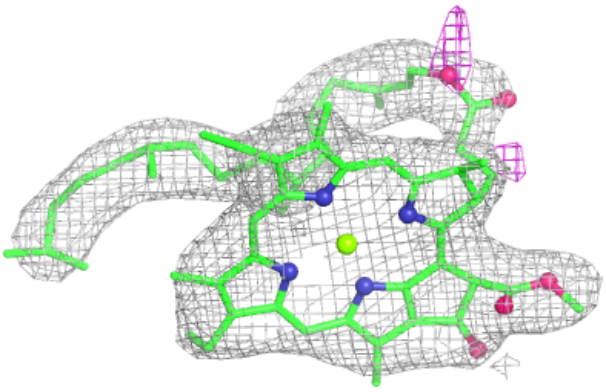


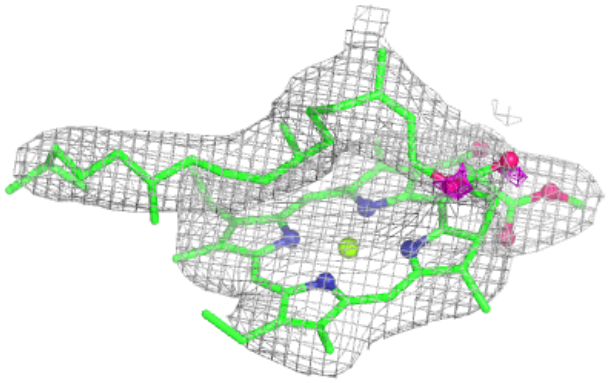


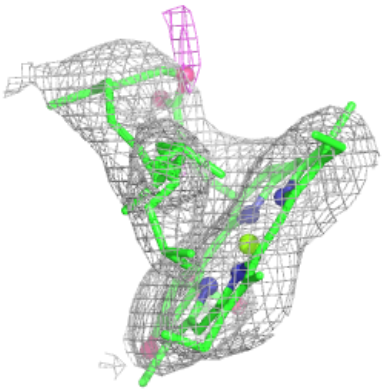


Electron density around CLA B 818:

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

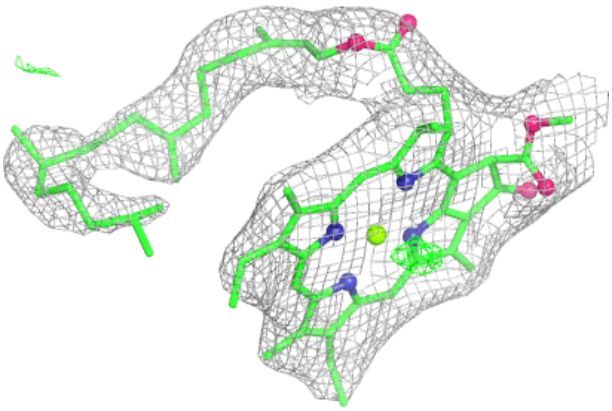


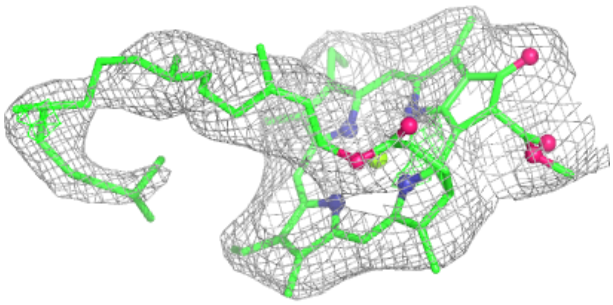


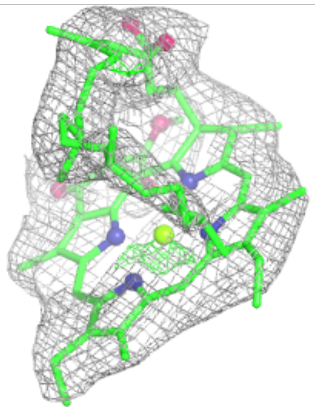


Electron density around CLA A 824:

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

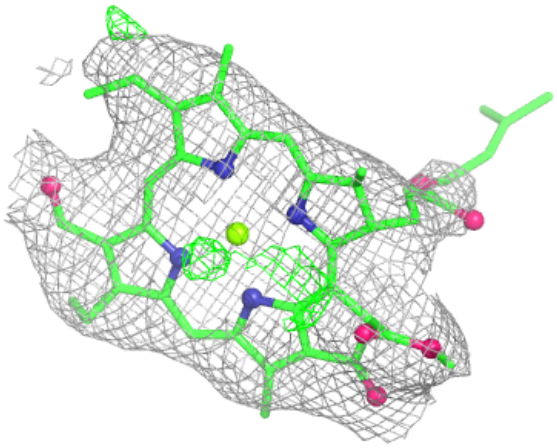


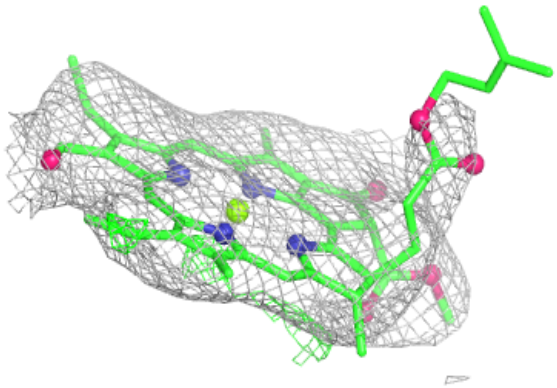


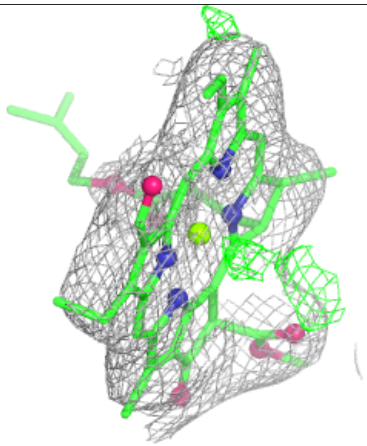


Electron density around CHL 4 314:

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

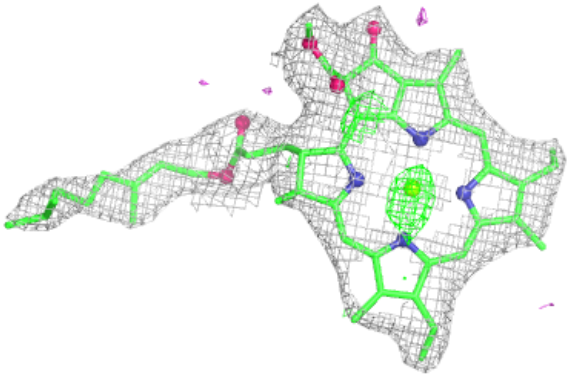


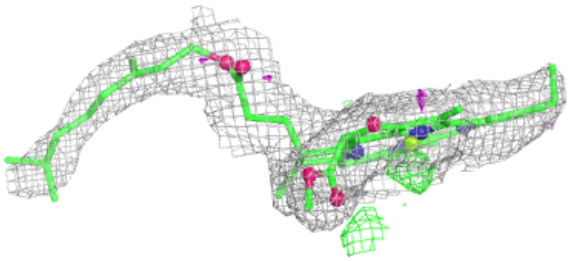


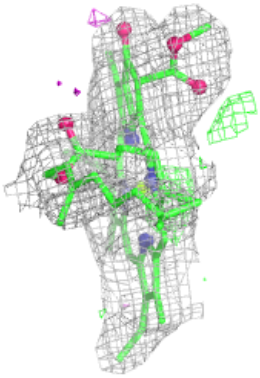


Electron density around CLA A 826:

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

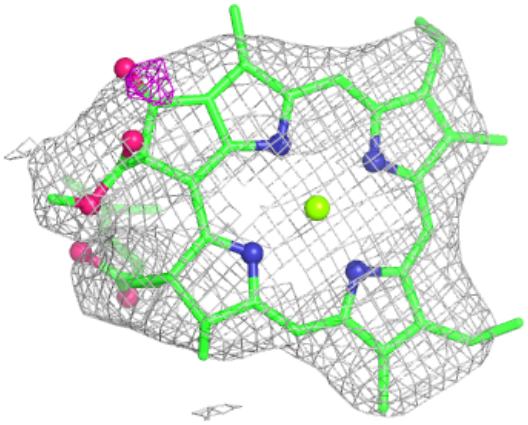


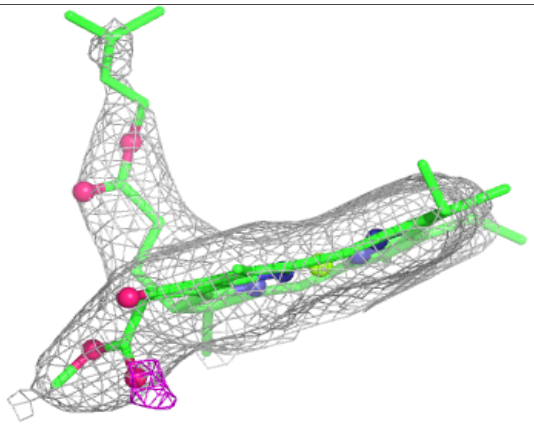


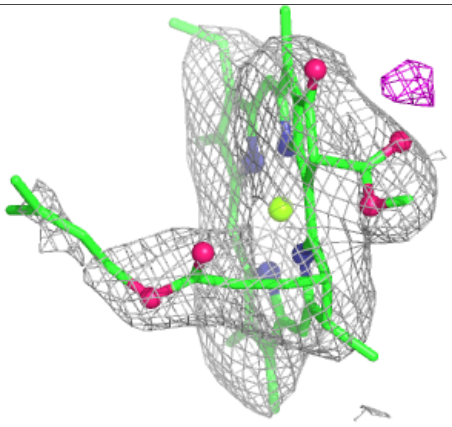


Electron density around CLA A 810:

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

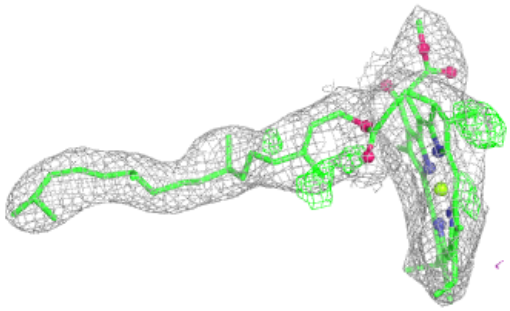


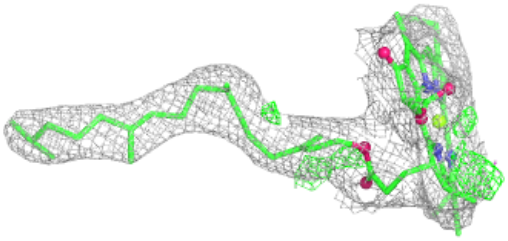


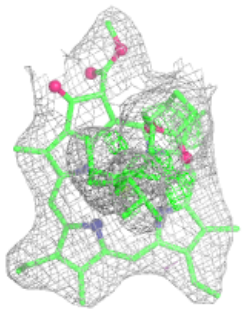


Electron density around CLA A 828:

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

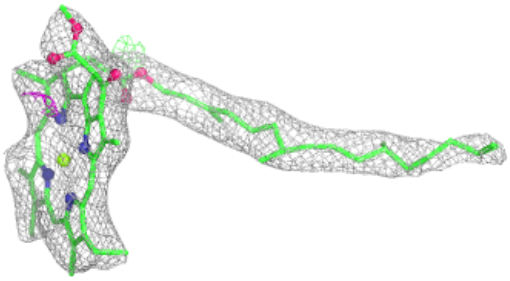


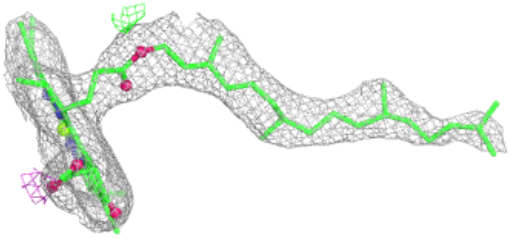


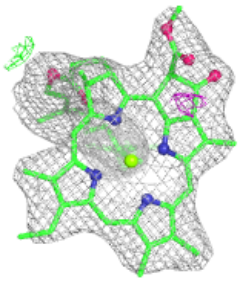


Electron density around CLA B 828:

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

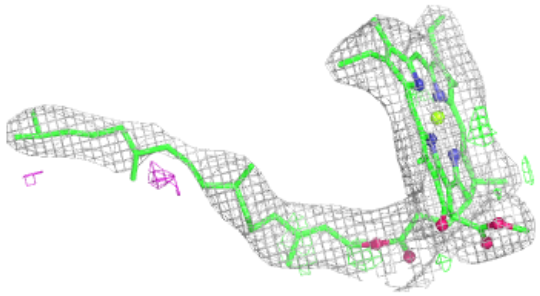


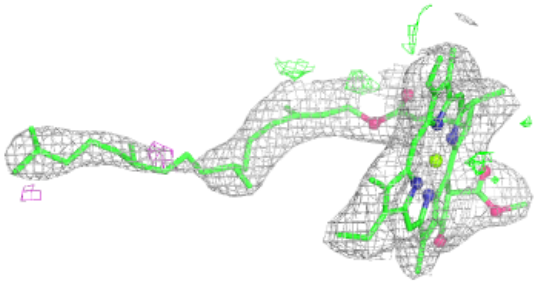


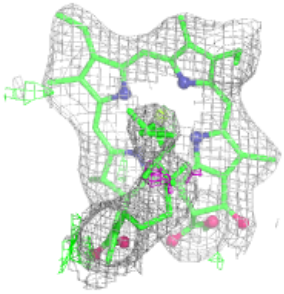


Electron density around CLA B 829:

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

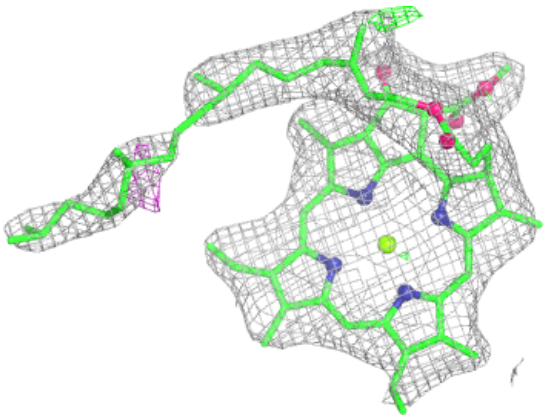


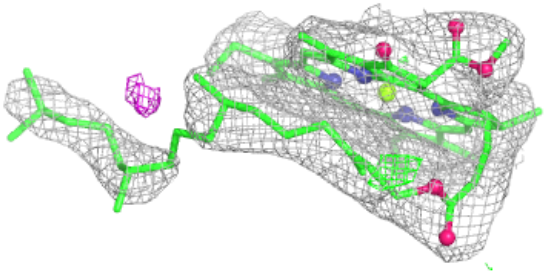


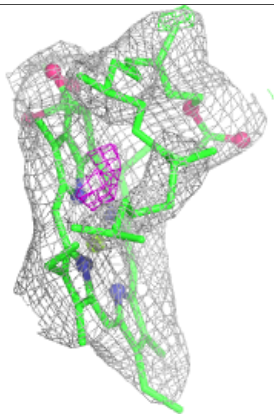


Electron density around CLA A 829:

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

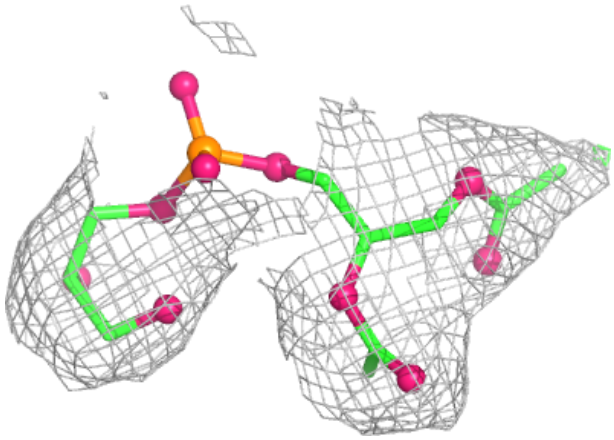


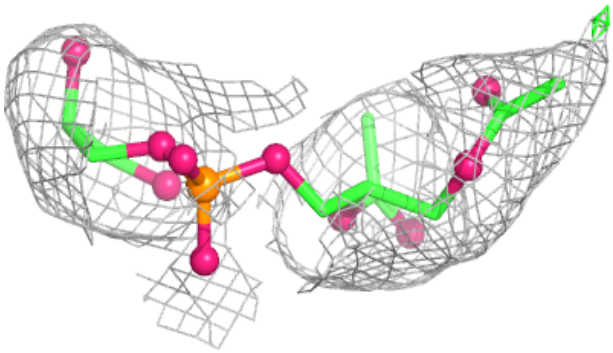


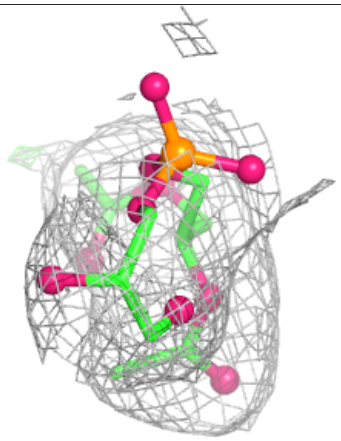


Electron density around LHG B 842:

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

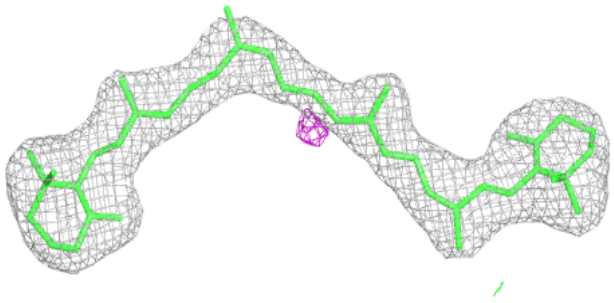


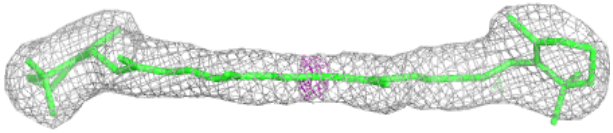


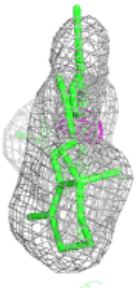


Electron density around BCR A 852:

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

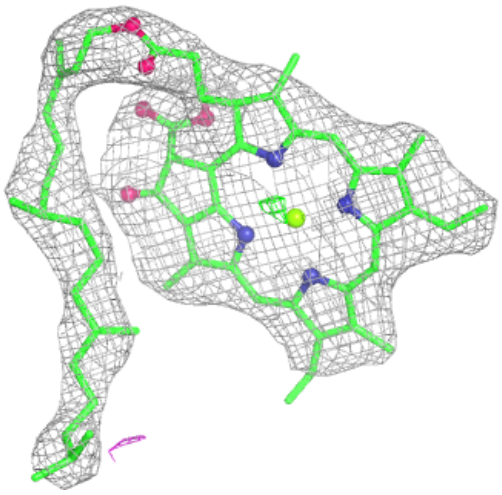


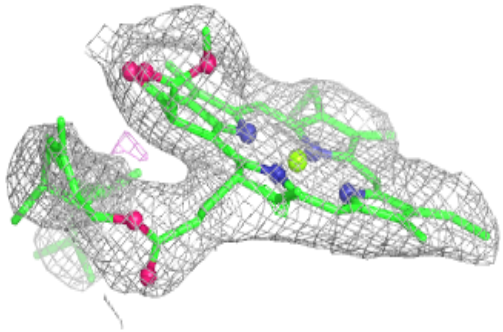


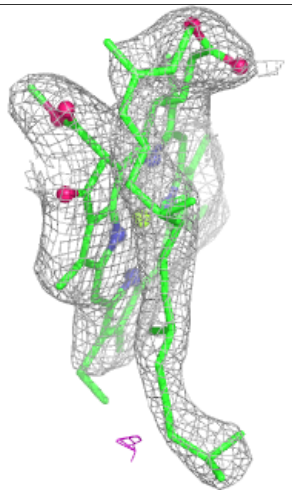


Electron density around CLA A 825:

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

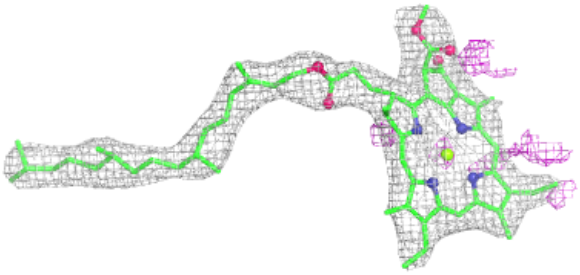


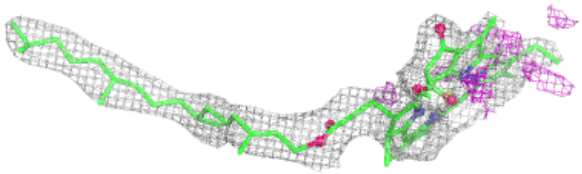




Electron density around CLA A 803:

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

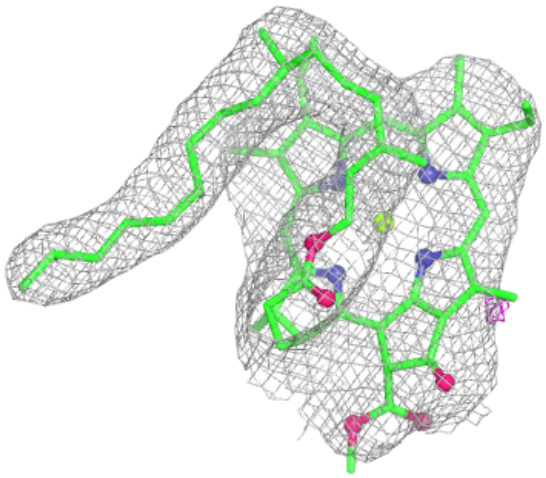


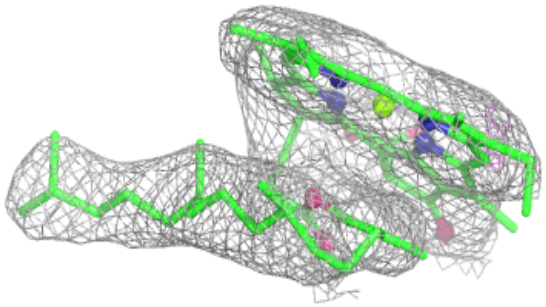


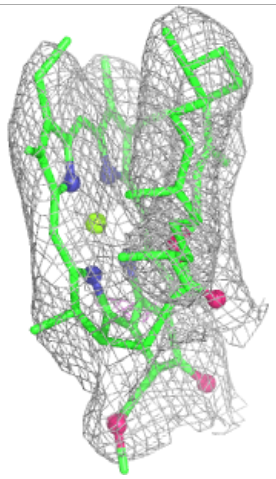


Electron density around CLA B 809:

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

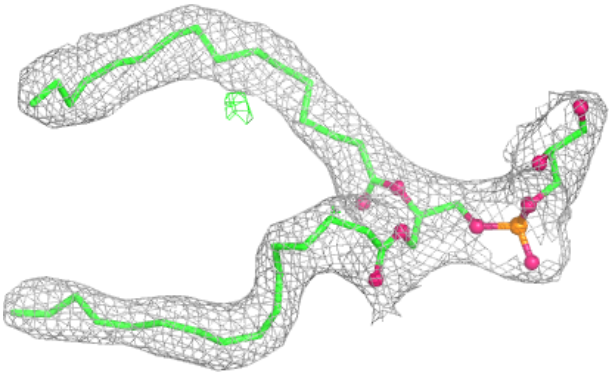


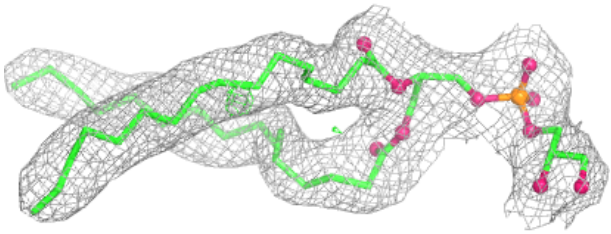


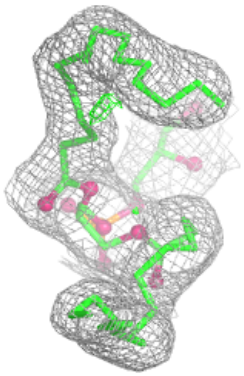


Electron density around LHG A 853:

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

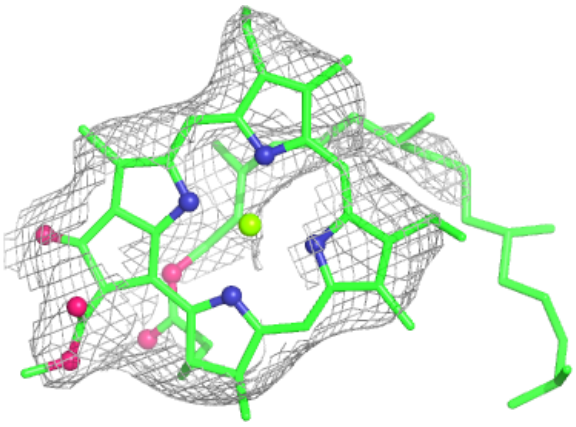


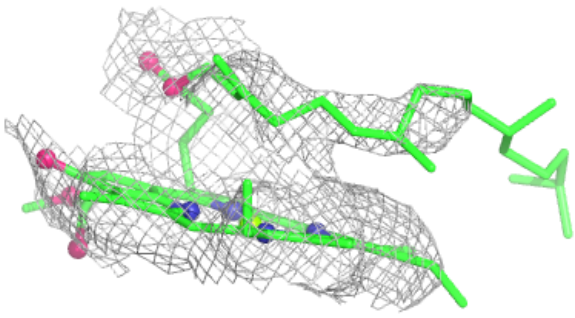


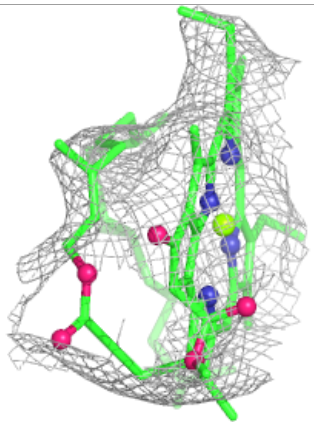


Electron density around CLA 2 506:

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

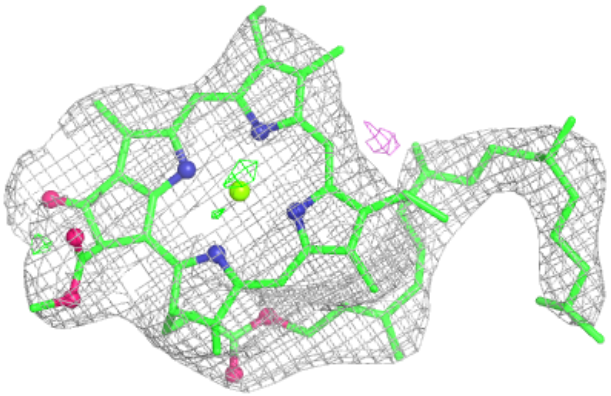


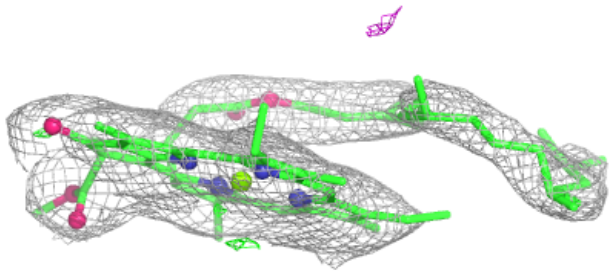


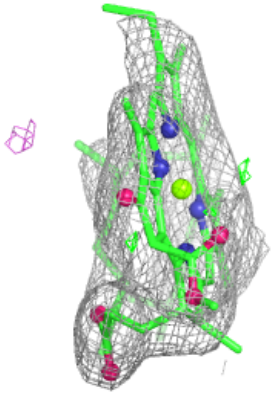


Electron density around CLA A 819:

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

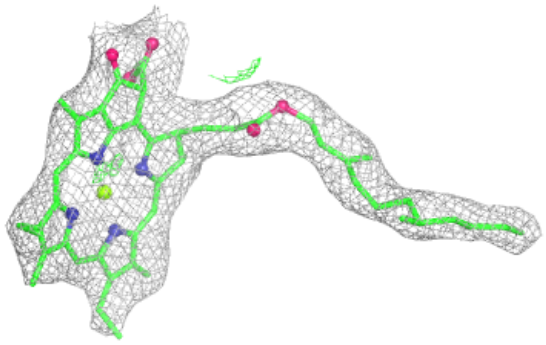


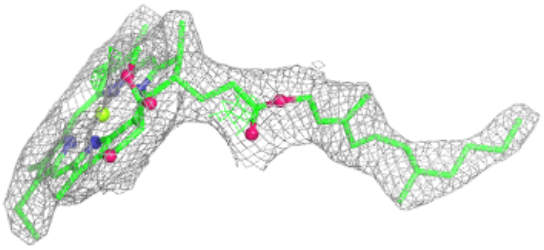


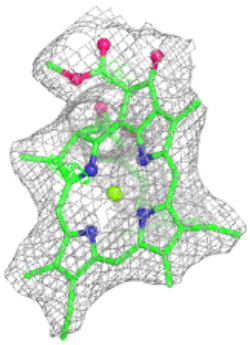


Electron density around CLA B 832:

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

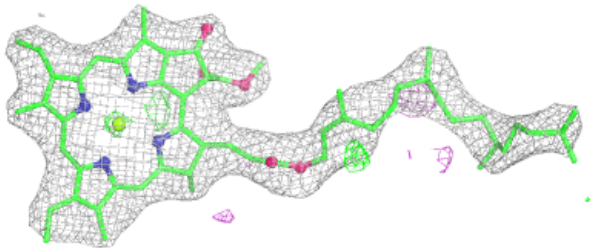


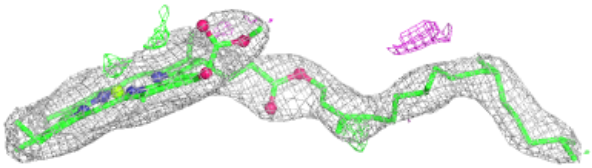


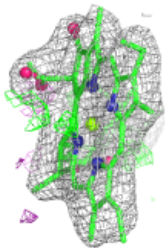


Electron density around CLA A 840:

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

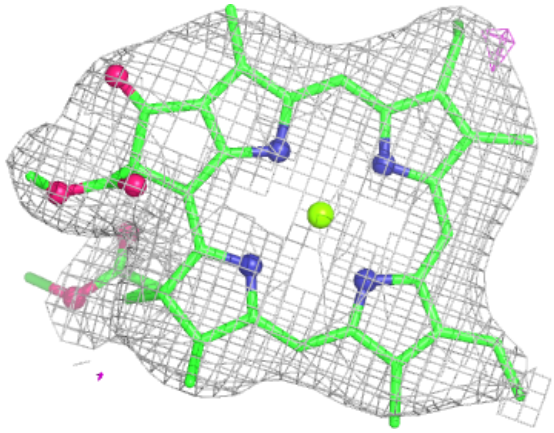


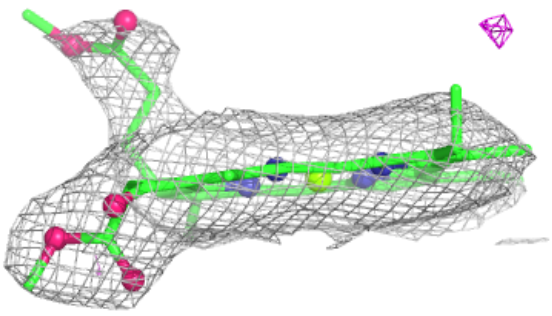


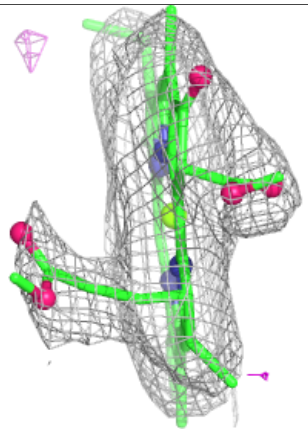


Electron density around CLA B 813:

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

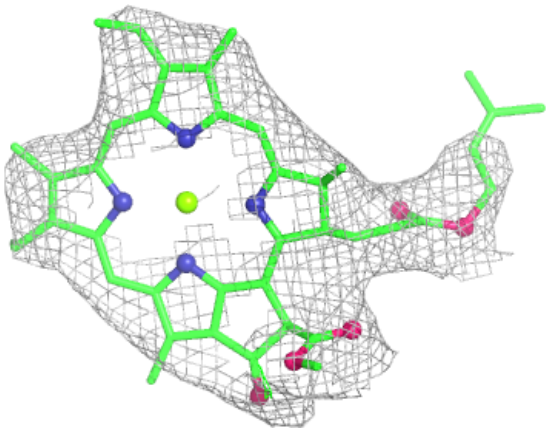


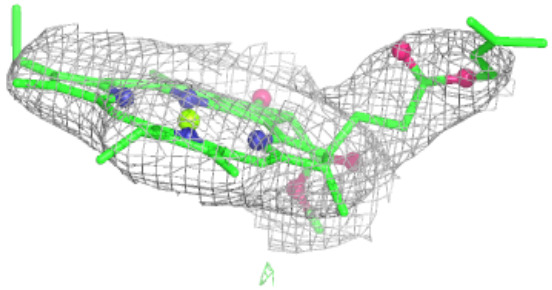


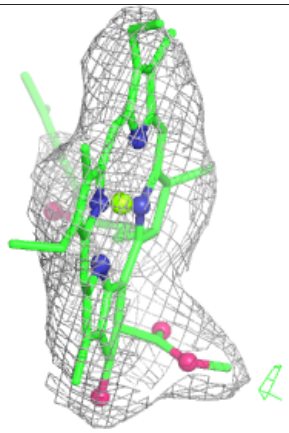


Electron density around CLA 4 312:

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

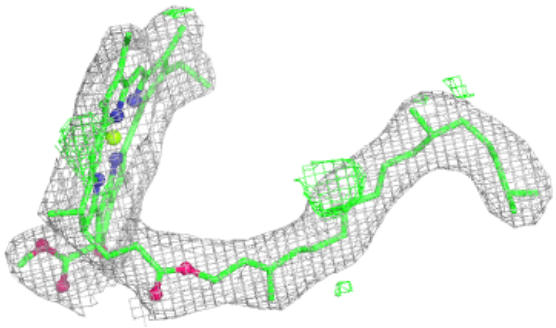


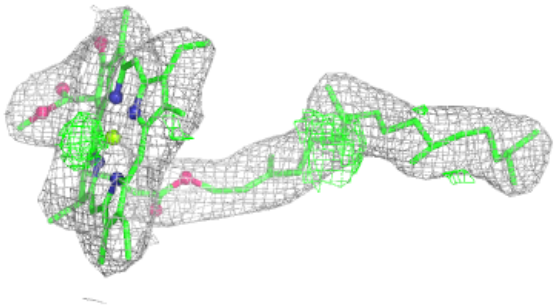


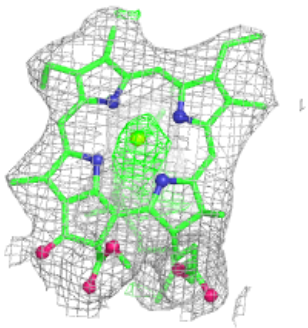


Electron density around CLA A 830:

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

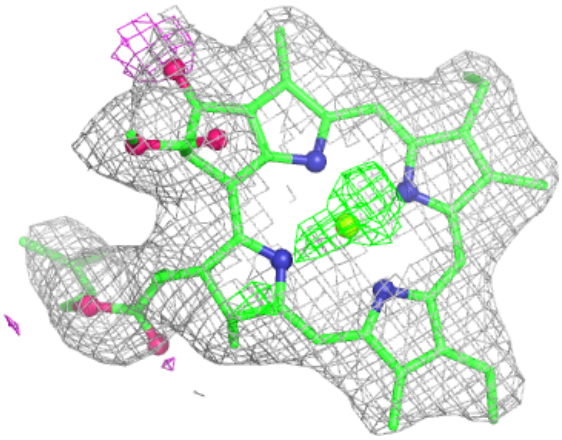


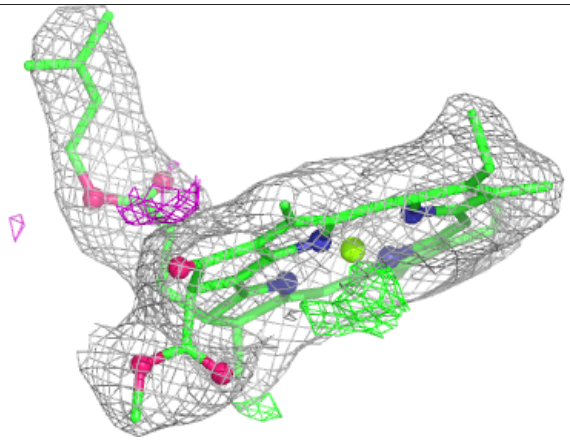


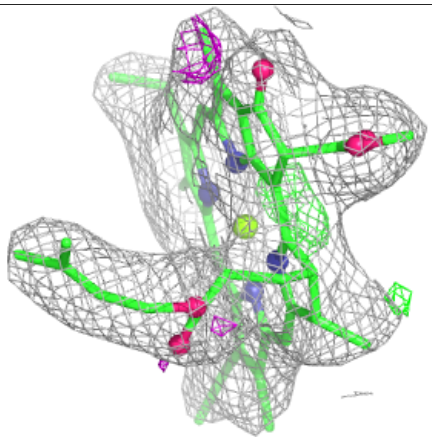


Electron density around CLA B 837:

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

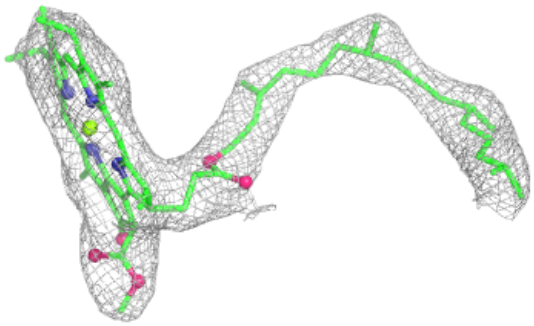


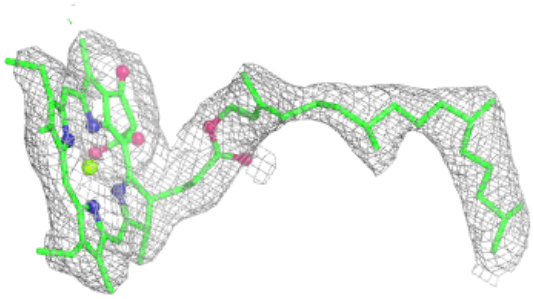


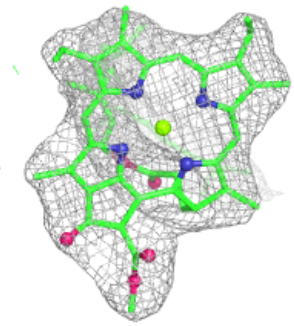


Electron density around CLA B 838:

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

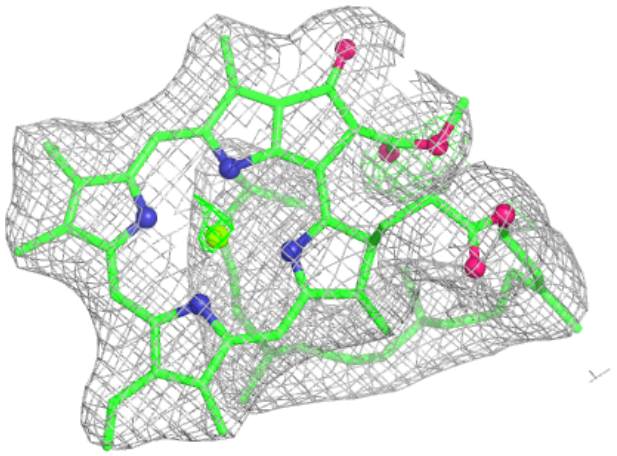


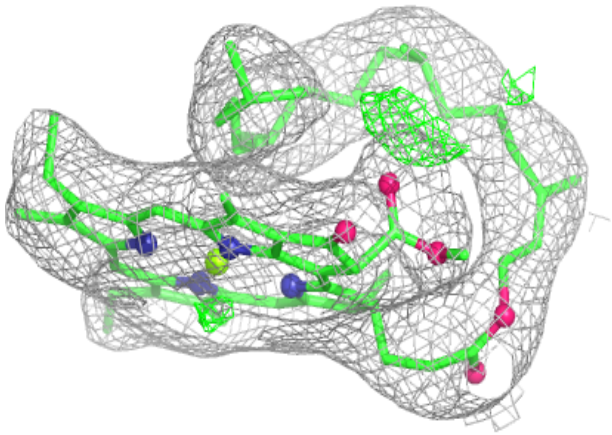


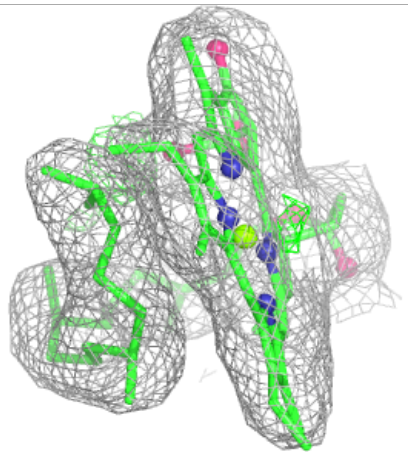


Electron density around CLA A 806:

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

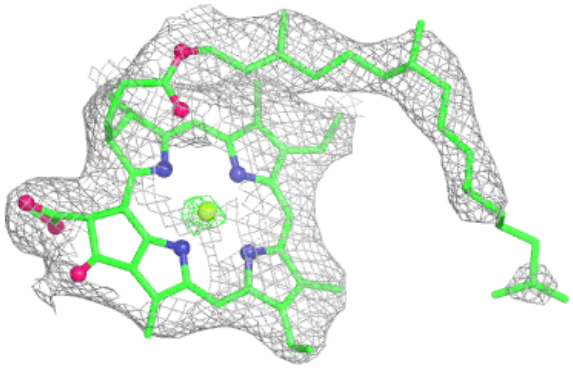


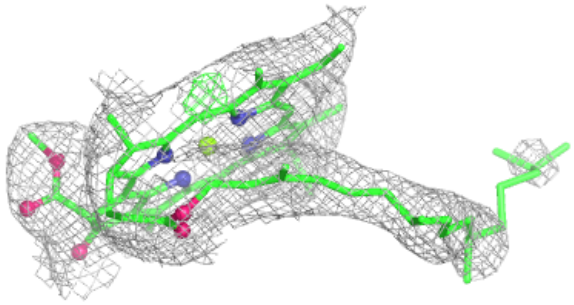


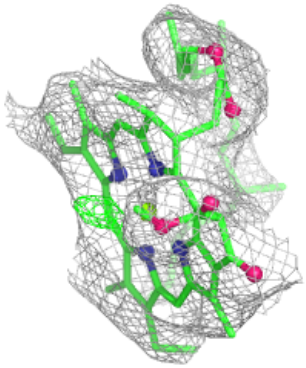


Electron density around CLA 2 507:

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

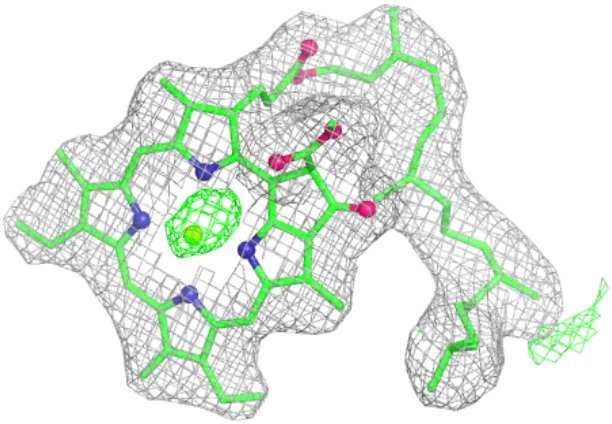


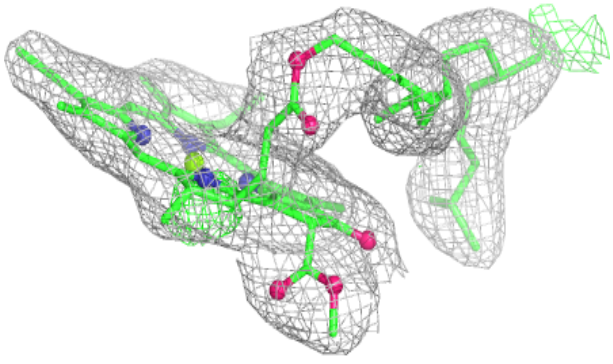


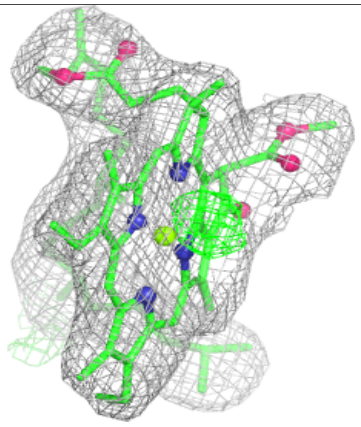


Electron density around CLA F 302:

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

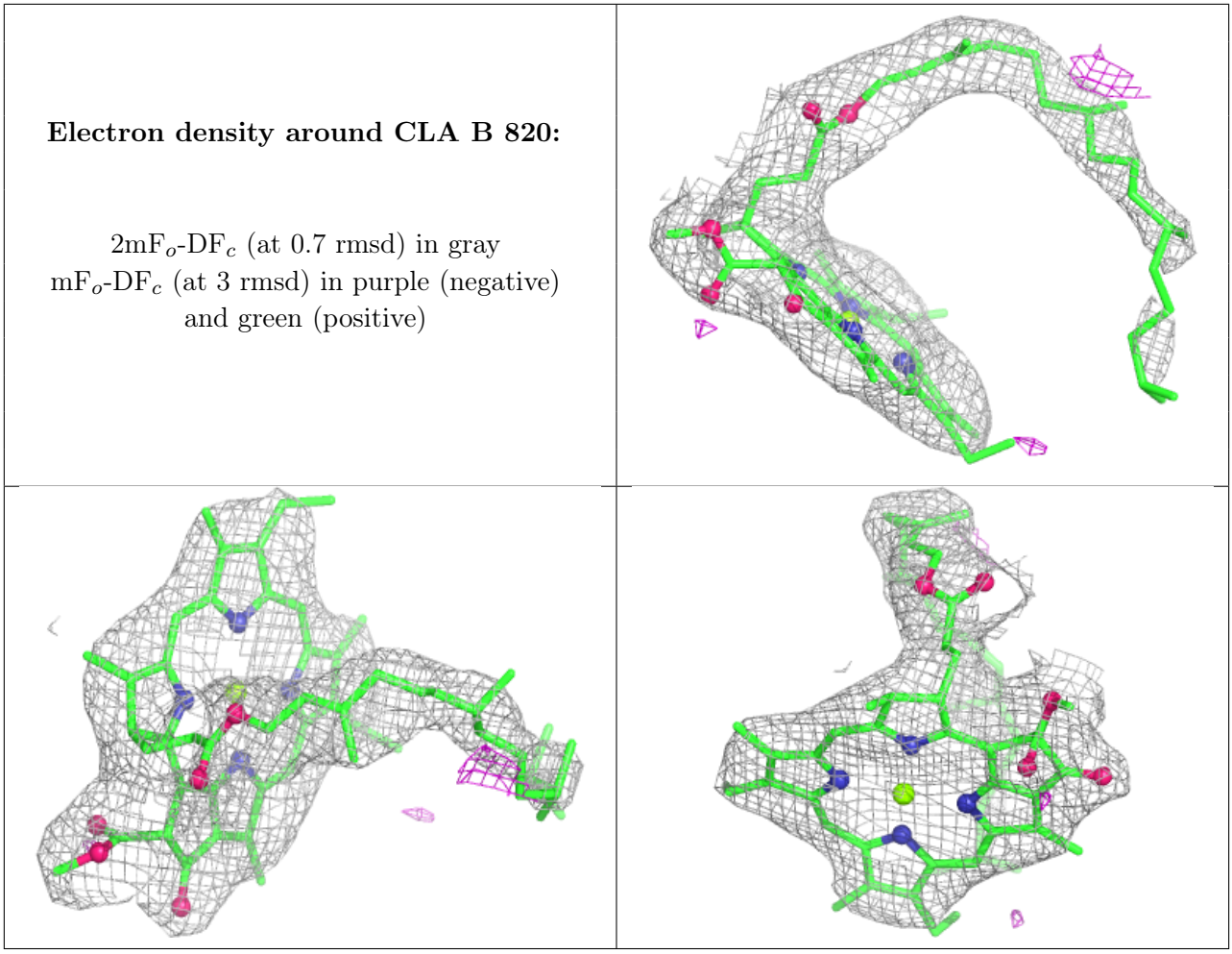






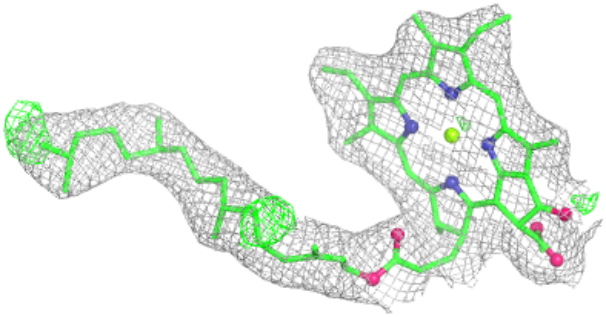
Electron density around CLA B 820:

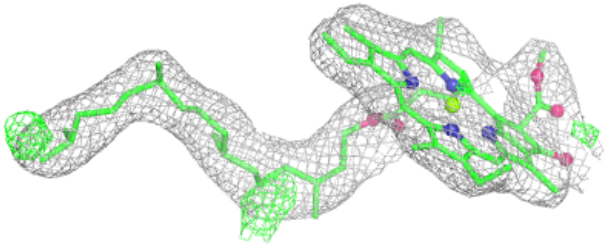
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

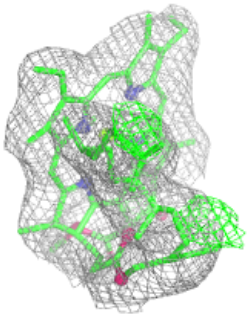


Electron density around CLA A 808:

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

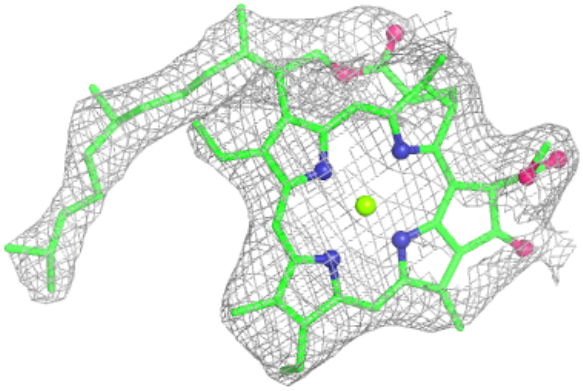


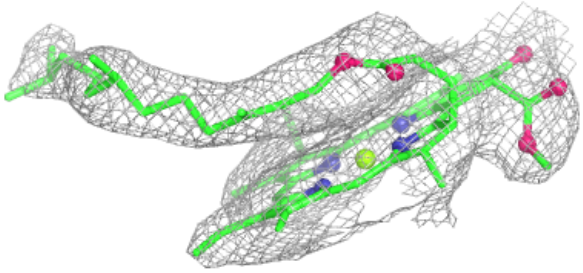




Electron density around CLA 4 307:

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

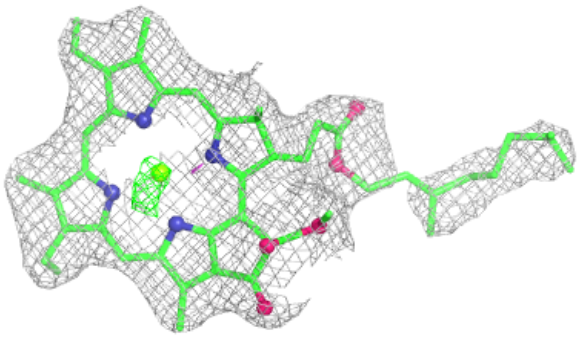


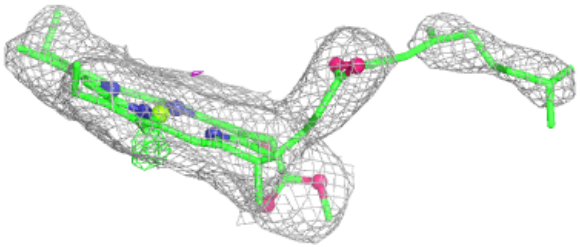


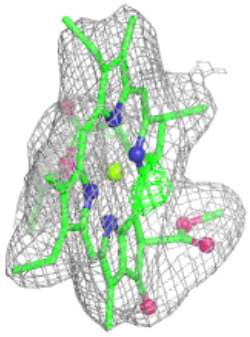


Electron density around CLA B 823:

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

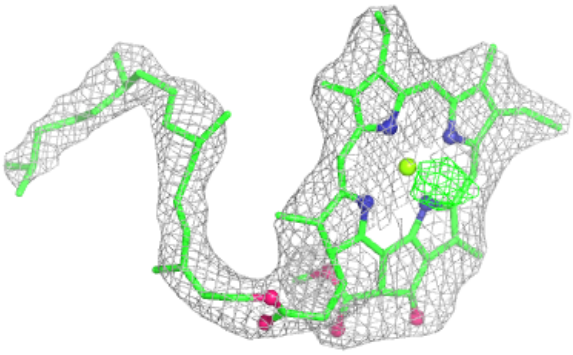


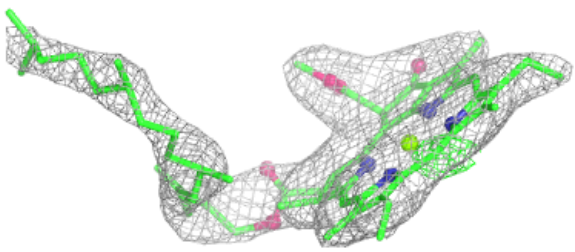


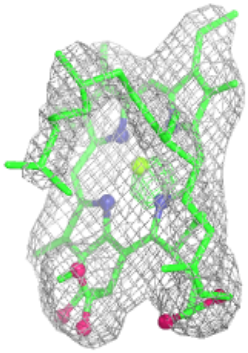


Electron density around CLA B 824:

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

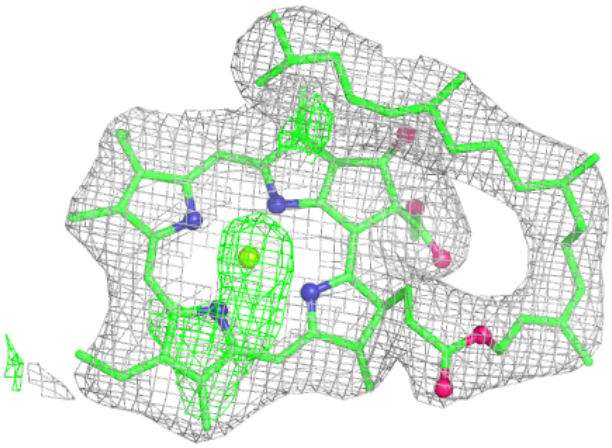


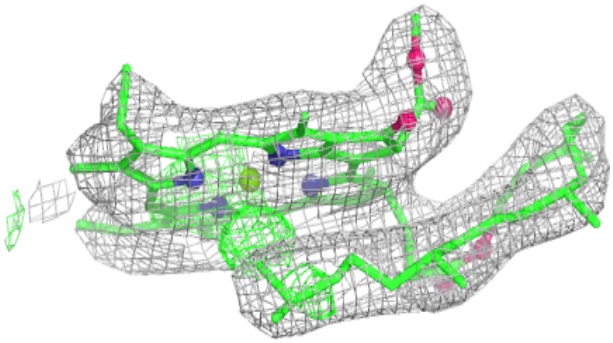


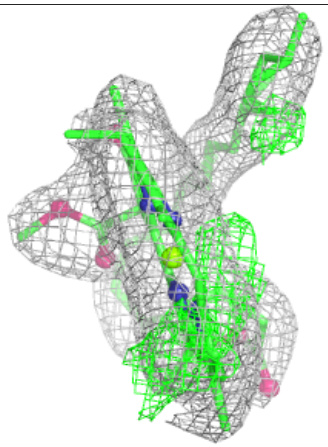


Electron density around CLA B 806:

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

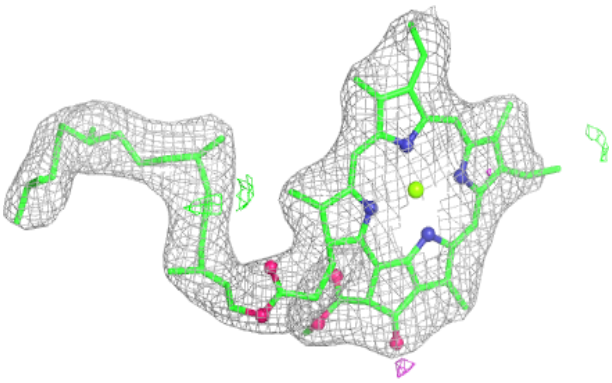


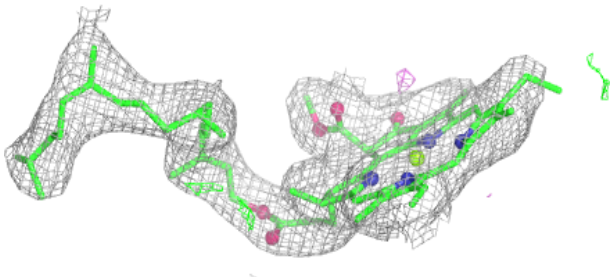




Electron density around CLA J 1101:

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

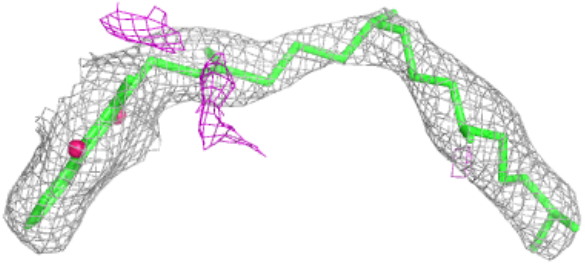


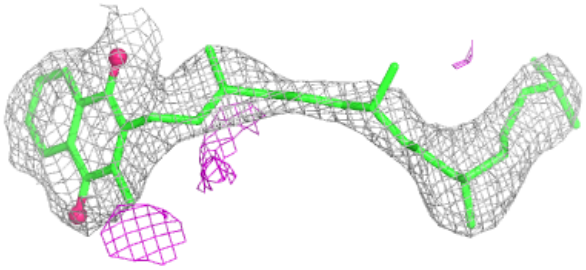


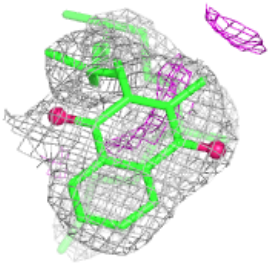


Electron density around PQN B 841:

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

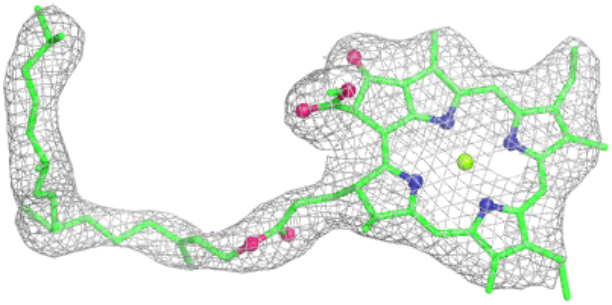


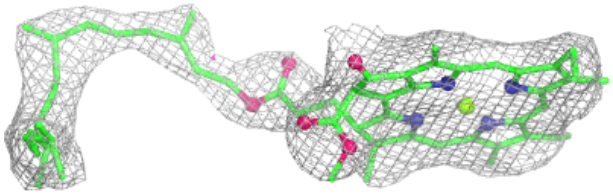


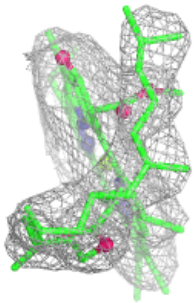


Electron density around CLA B 826:

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

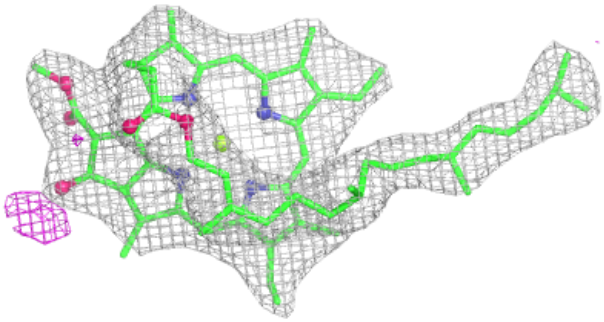


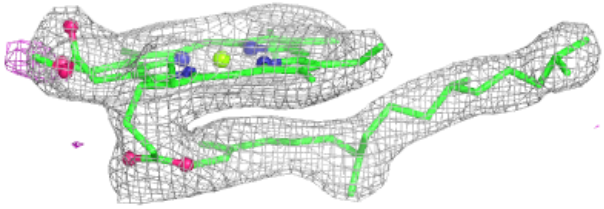


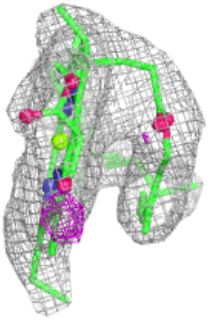


Electron density around CLA A 839:

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

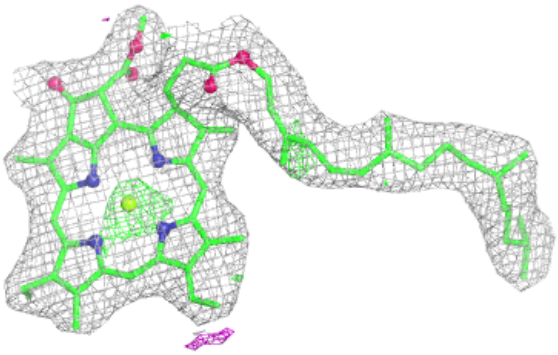


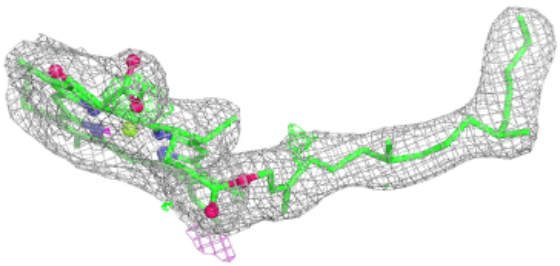


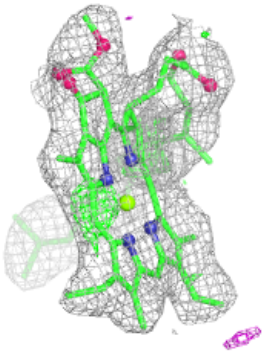


Electron density around CLA A 802:

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

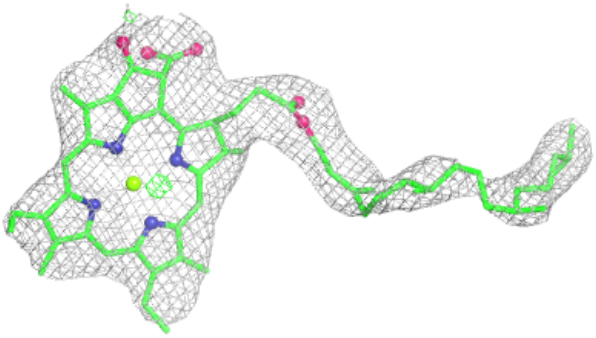


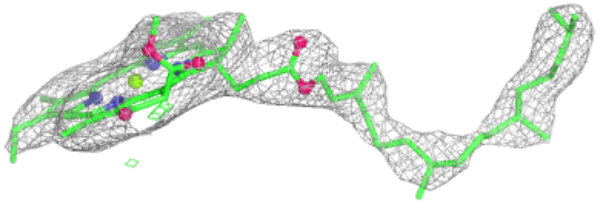


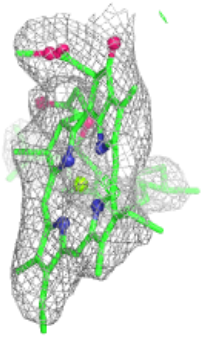


Electron density around CLA B 814:

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

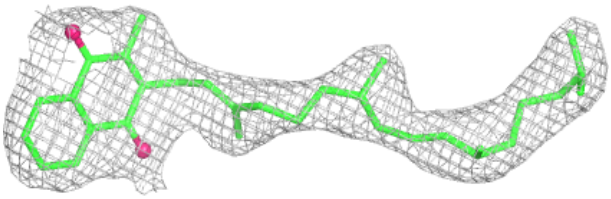


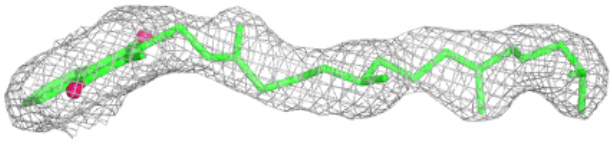


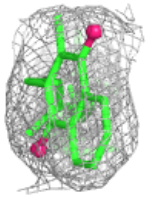


Electron density around PQN A 844:

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

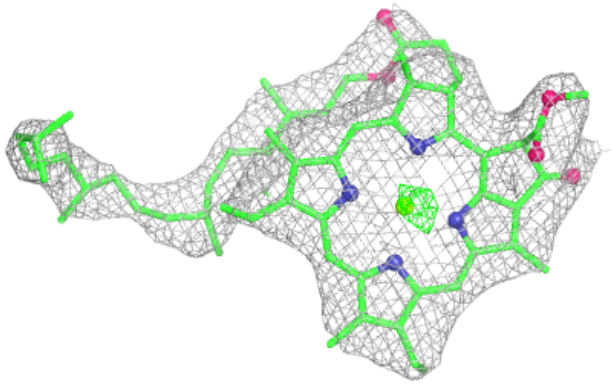


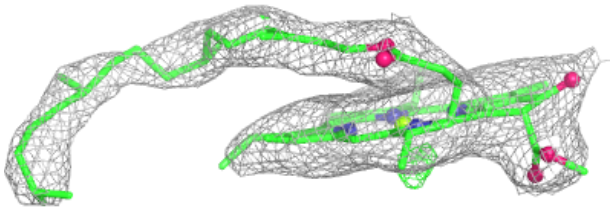


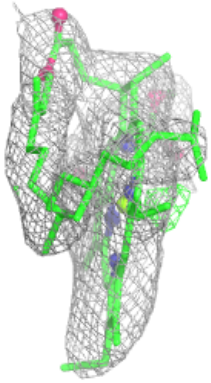


Electron density around CLA B 819:

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

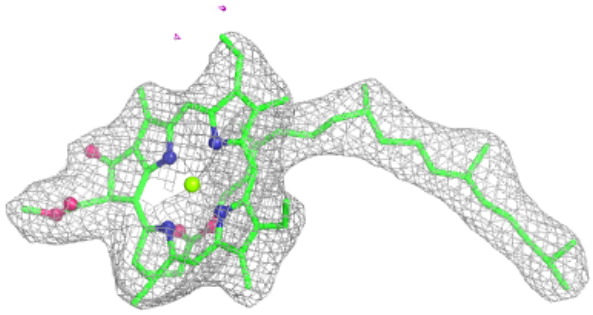


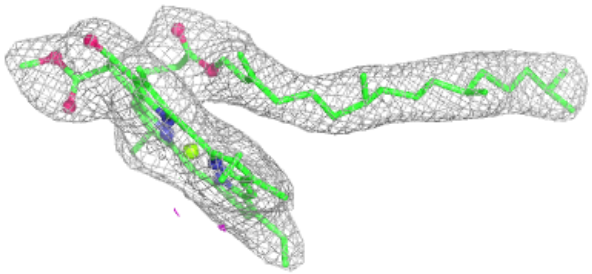


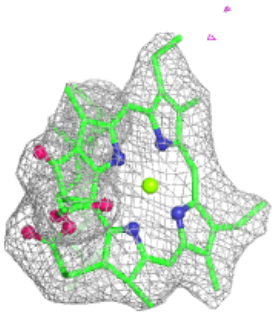


Electron density around CLA A 841:

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







6.5 Other polymers (i)

There are no such residues in this entry.