wwPDB X-ray Structure Validation Summary Report (i)

Aug 5, 2026 – 09:02 PM JST

PDB ID	:	7DKZ / pdb_00007dkz
Title	:	Structure of plant photosystem I-light harvesting complex I supercomplex
Authors	:	Wang, J.; Yu, L.J.; Wang, W.
Deposited on	:	2020-11-25
Resolution	:	2.39 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:

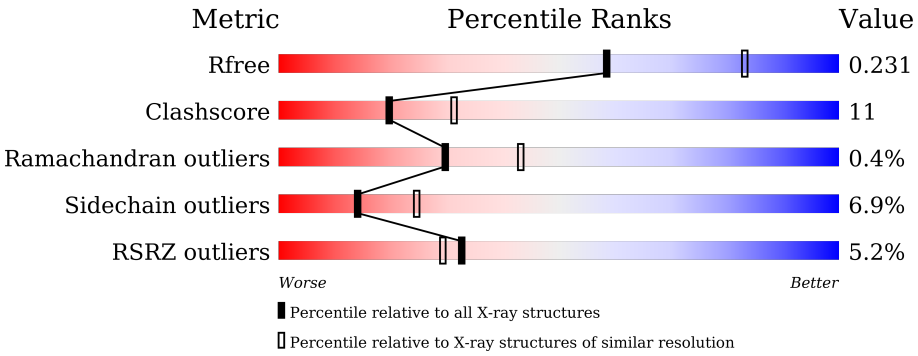
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.015 (Gargrove)
Density-Fitness	:	1.0.12
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 2.39 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	4912 (2.40-2.40)
Clashscore	190562	5391 (2.40-2.40)
Ramachandran outliers	187476	5320 (2.40-2.40)
Sidechain outliers	187428	5321 (2.40-2.40)
RSRZ outliers	180081	4916 (2.40-2.40)

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	195	8% 74% 22% ·
2	2	269	6% 54% 19% · 24%
3	3	275	8% 63% 14% · 21%
4	4	198	2% 76% 19% · ·
5	A	758	3% 77% 19% · ·
6	B	734	2% 80% 17% ·

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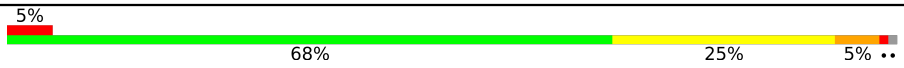
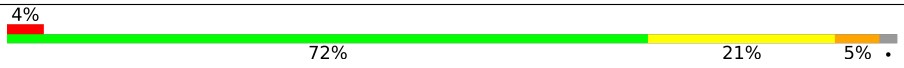
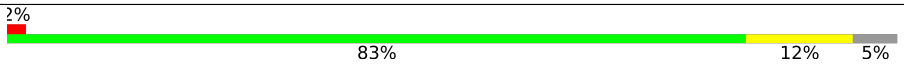
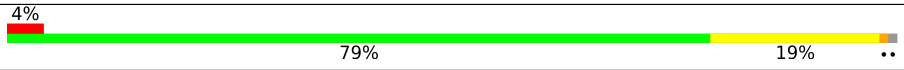
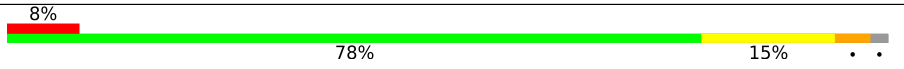
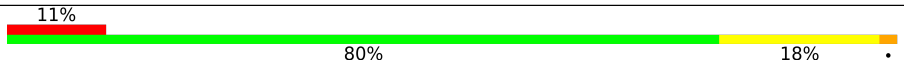
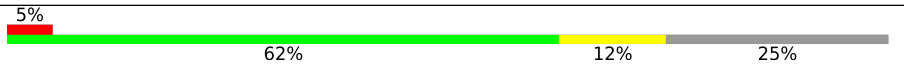
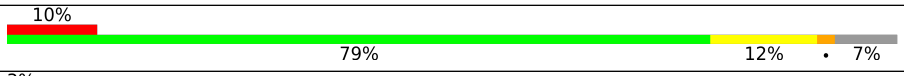
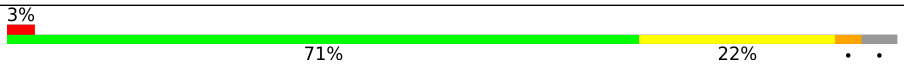
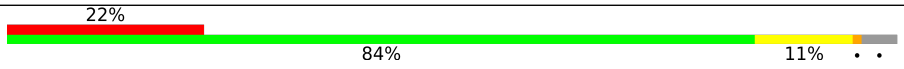
Mol	Chain	Length	Quality of chain
7	C	81	
8	D	143	
9	E	66	
10	F	154	
11	G	97	
12	H	88	
13	I	40	
14	J	42	
15	L	157	
16	K	80	

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	CLA	A	801	X	-	-	-
18	CHL	4	301	X	-	-	-
18	CHL	4	305	X	-	-	-
19	LUT	4	316	-	X	-	-
20	XAT	4	317	X	-	-	-
26	DGD	4	323	-	-	X	-

2 Entry composition (i)

There are 29 unique types of molecules in this entry. The entry contains 36093 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	195	Total	C	N	O	S	0	0	0
			1507	979	252	271	5			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	2	204	Total	C	N	O	S	0	0	0
			1592	1042	261	285	4			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	3	216	Total	C	N	O	S	0	0	0
			1661	1088	268	300	5			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	4	195	Total	C	N	O	S	0	0	0
			1535	1006	249	277	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	742	Total	C	N	O	S	0	0	0
			5852	3835	997	1002	18			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	223	ILE	VAL	conflict	UNP A0A0F6NFW5

- 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
			5856	3848	998	996	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
			611	379	107	114	11			

- Molecule 8 is a protein called PsaD.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	D	140	Total	C	N	O	S	0	0	0
			1110	716	191	200	3			

- Molecule 9 is a protein called PsaE.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
9	E	63	Total	C	N	O	0	0	0
			505	320	89	96			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	-1	PRO	-	expression tag	UNP E1C9K6
E	0	PRO	-	expression tag	UNP E1C9K6
E	14	GLN	LYS	conflict	UNP E1C9K6
E	60	VAL	-	expression tag	UNP E1C9K6
E	61	GLU	-	expression tag	UNP E1C9K6
E	62	GLU	-	expression tag	UNP E1C9K6
E	63	VAL	-	expression tag	UNP E1C9K6

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Chain	Residue	Modelled	Actual	Comment	Reference
E	64	LYS	-	expression tag	UNP E1C9K6

- Molecule 10 is a protein called PSI-F.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	F	152	Total	C	N	O	S	0	0	0
			1198	777	208	211	2			

There are 7 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
F	79	ALA	SER	conflict	UNP A0A0M3KL12
F	86	ASP	GLU	conflict	UNP A0A0M3KL12
F	107	LEU	ILE	conflict	UNP A0A0M3KL12
F	110	PRO	ALA	conflict	UNP A0A0M3KL12
F	133	GLY	ALA	conflict	UNP A0A0M3KL12
F	187	ASP	GLU	conflict	UNP A0A0M3KL12
F	203	THR	SER	conflict	UNP A0A0M3KL12

- Molecule 11 is a protein called PsaG.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
11	G	95	Total	C	N	O	0	0	0
			737	477	122	138			

- Molecule 12 is a protein called PsaH.

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

- 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
			226	156	34	35	1			

- Molecule 14 is a protein called Photosystem I reaction center subunit IX.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	J	39	Total	C	N	O	S	0	0	0
			309	208	48	52	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 PsaL.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
15	L	151	Total	C	N	O	S	0	0	0
			1122	737	182	202	1			

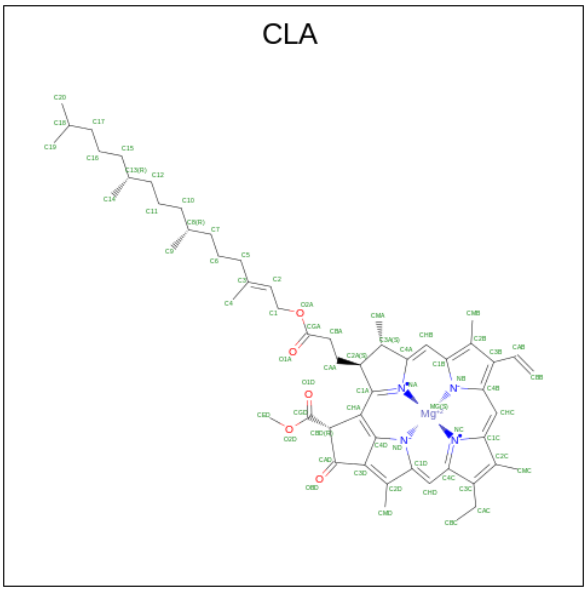
- Molecule 16 is a protein called PSI-K.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
16	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 17 is CHLOROPHYLL A (CCD ID: CLA) (formula: $C_{55}H_{72}MgN_4O_5$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
17	1	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
17	1	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
17	1	1	Total	C	Mg	N	O	0	0
			51	41	1	4	5		
17	1	1	Total	C	Mg	N	O	0	0
			42	34	1	4	3		
17	1	1	Total	C	Mg	N	O	0	0
			46	36	1	4	5		
17	1	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
17	1	1	Total	C	Mg	N	O	0	0
			60	50	1	4	5		
17	1	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
17	1	1	Total	C	Mg	N	O	0	0
			52	42	1	4	5		
17	1	1	Total	C	Mg	N	O	0	0
			60	50	1	4	5		
17	1	1	Total	C	Mg	N	O	0	0
			55	45	1	4	5		
17	1	1	Total	C	Mg	N	O	0	0
			46	36	1	4	5		
17	2	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
17	2	1	Total	C	Mg	N	O	0	0
			51	41	1	4	5		
17	2	1	Total	C	Mg	N	O	0	0
			60	50	1	4	5		
17	2	1	Total	C	Mg	N	O	0	0
			50	40	1	4	5		
17	2	1	Total	C	Mg	N	O	0	0
			60	50	1	4	5		
17	2	1	Total	C	Mg	N	O	0	0
			41	33	1	4	3		
17	2	1	Total	C	Mg	N	O	0	0
			52	42	1	4	5		
17	2	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
17	2	1	Total	C	Mg	N	O	0	0
			43	35	1	4	3		
17	2	1	Total	C	Mg	N	O	0	0
			46	36	1	4	5		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
17	3	1	Total	C	Mg	N	O	0	0
			60	50	1	4	5		
17	3	1	Total	C	Mg	N	O	0	0
			50	40	1	4	5		
17	3	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
17	3	1	Total	C	Mg	N	O	0	0
			42	34	1	4	3		
17	3	1	Total	C	Mg	N	O	0	0
			47	37	1	4	5		
17	3	1	Total	C	Mg	N	O	0	0
			50	40	1	4	5		
17	3	1	Total	C	Mg	N	O	0	0
			50	40	1	4	5		
17	3	1	Total	C	Mg	N	O	0	0
			52	42	1	4	5		
17	3	1	Total	C	Mg	N	O	0	0
			55	45	1	4	5		
17	3	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
17	3	1	Total	C	Mg	N	O	0	0
			46	36	1	4	5		
17	4	1	Total	C	Mg	N	O	0	0
			60	50	1	4	5		
17	4	1	Total	C	Mg	N	O	0	0
			60	50	1	4	5		
17	4	1	Total	C	Mg	N	O	0	0
			50	40	1	4	5		
17	4	1	Total	C	Mg	N	O	0	0
			50	40	1	4	5		
17	4	1	Total	C	Mg	N	O	0	0
			60	50	1	4	5		
17	4	1	Total	C	Mg	N	O	0	0
			60	50	1	4	5		
17	4	1	Total	C	Mg	N	O	0	0
			52	42	1	4	5		
17	4	1	Total	C	Mg	N	O	0	0
			56	46	1	4	5		
17	4	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
17	4	1	Total	C	Mg	N	O	0	0
			47	37	1	4	5		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
17	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
17	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
17	A	1	Total	C	Mg	N	O	0	0
			55	45	1	4	5		
17	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
17	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
17	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
17	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
17	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
17	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
17	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
17	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
17	A	1	Total	C	Mg	N	O	0	0
			54	44	1	4	5		
17	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
17	A	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
17	A	1	Total	C	Mg	N	O	0	0
			50	40	1	4	5		
17	A	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
17	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
17	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
17	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
17	A	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
17	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
17	A	1	Total	C	Mg	N	O	0	0
			49	39	1	4	5		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
17	A	1	Total	C	Mg	N	O	0	0
			51	41	1	4	5		
17	A	1	Total	C	Mg	N	O	0	0
			55	45	1	4	5		
17	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
17	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
17	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
17	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
17	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
17	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
17	A	1	Total	C	Mg	N	O	0	0
			50	40	1	4	5		
17	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
17	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
17	A	1	Total	C	Mg	N	O	0	0
			50	40	1	4	5		
17	A	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
17	A	1	Total	C	Mg	N	O	0	0
			51	41	1	4	5		
17	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
17	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
17	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
17	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
17	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
17	A	1	Total	C	Mg	N	O	0	0
			52	42	1	4	5		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
17	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
17	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
17	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
17	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
17	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
17	B	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
17	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
17	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
17	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
17	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
17	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
17	B	1	Total	C	Mg	N	O	0	0
			54	44	1	4	5		
17	B	1	Total	C	Mg	N	O	0	0
			55	45	1	4	5		
17	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
17	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
17	B	1	Total	C	Mg	N	O	0	0
			55	45	1	4	5		
17	B	1	Total	C	Mg	N	O	0	0
			55	45	1	4	5		
17	B	1	Total	C	Mg	N	O	0	0
			59	49	1	4	5		
17	B	1	Total	C	Mg	N	O	0	0
			60	50	1	4	5		
17	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
17	B	1	Total	C	Mg	N	O	0	0
			50	40	1	4	5		
17	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
17	B	1	Total	C	Mg	N	O	0	0
			55	45	1	4	5		
17	B	1	Total	C	Mg	N	O	0	0
			60	50	1	4	5		
17	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
17	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
17	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
17	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
17	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
17	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
17	B	1	Total	C	Mg	N	O	0	0
			50	40	1	4	5		
17	B	1	Total	C	Mg	N	O	0	0
			60	50	1	4	5		
17	B	1	Total	C	Mg	N	O	0	0
			58	48	1	4	5		
17	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
17	B	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
17	B	1	Total	C	Mg	N	O	0	0
			60	50	1	4	5		
17	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
17	B	1	Total	C	Mg	N	O	0	0
			47	37	1	4	5		
17	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
17	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
17	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		

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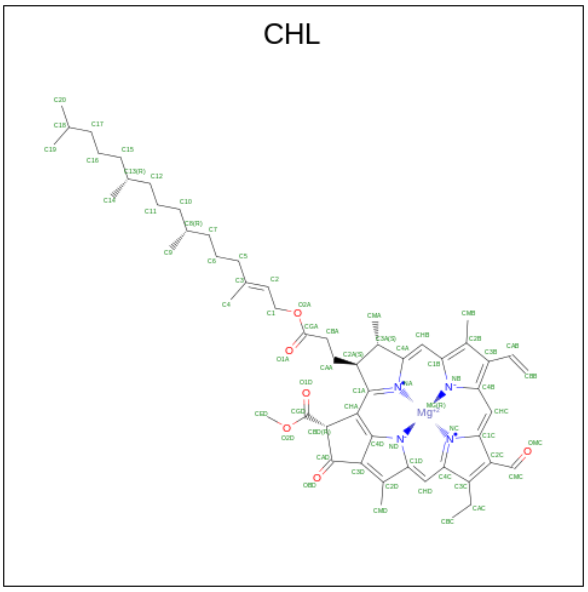
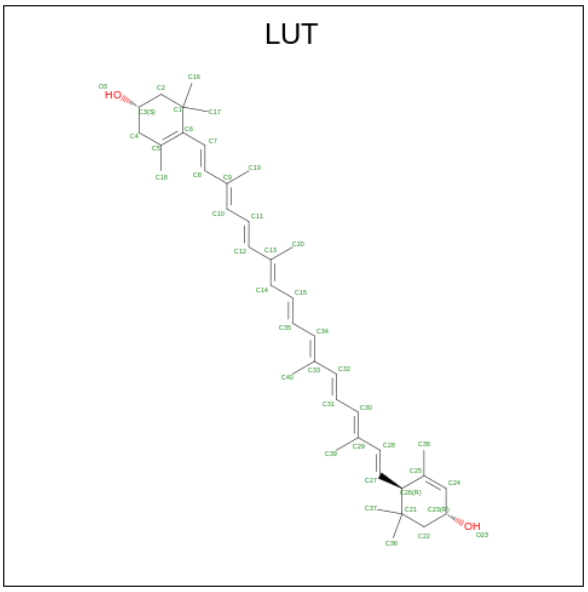
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
17	F	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
17	F	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
17	F	1	Total	C	Mg	N	O	0	0
			55	45	1	4	5		
17	G	1	Total	C	Mg	N	O	0	0
			41	33	1	4	3		
17	G	1	Total	C	Mg	N	O	0	0
			50	40	1	4	5		
17	G	1	Total	C	Mg	N	O	0	0
			46	36	1	4	5		
17	J	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
17	J	1	Total	C	Mg	N	O	0	0
			42	34	1	4	3		
17	L	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
17	L	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
17	L	1	Total	C	Mg	N	O	0	0
			50	40	1	4	5		
17	K	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
17	K	1	Total	C	Mg	N	O	0	0
			60	50	1	4	5		

- Molecule 18 is CHLOROPHYLL B (CCD ID: CHL) (formula: $C_{55}H_{70}MgN_4O_6$).



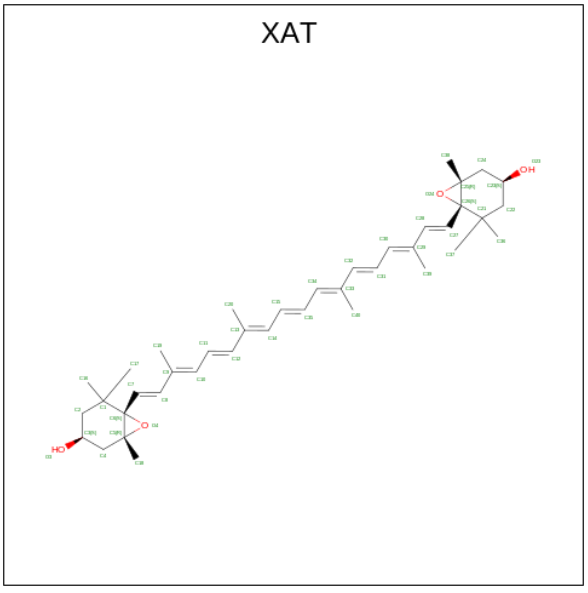
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
18	1	1	Total	C	Mg	N	O	0	0
			48	37	1	4	6		
18	2	1	Total	C	Mg	N	O	0	0
			43	34	1	4	4		
18	2	1	Total	C	Mg	N	O	0	0
			48	37	1	4	6		
18	2	1	Total	C	Mg	N	O	0	0
			51	40	1	4	6		
18	2	1	Total	C	Mg	N	O	0	0
			43	34	1	4	4		
18	3	1	Total	C	Mg	N	O	0	0
			56	45	1	4	6		
18	3	1	Total	C	Mg	N	O	0	0
			47	36	1	4	6		
18	4	1	Total	C	Mg	N	O	0	0
			61	50	1	4	6		
18	4	1	Total	C	Mg	N	O	0	0
			56	45	1	4	6		
18	4	1	Total	C	Mg	N	O	0	0
			51	40	1	4	6		
18	4	1	Total	C	Mg	N	O	0	0
			51	40	1	4	6		
18	4	1	Total	C	Mg	N	O	0	0
			43	34	1	4	4		

- Molecule 19 is (3R,3'R,6S)-4,5-DIDEHYDRO-5,6-DIHYDRO-BETA,BETA-CAROTENE-3 ,3'-DIOL (CCD ID: LUT) (formula: $C_{40}H_{56}O_2$).



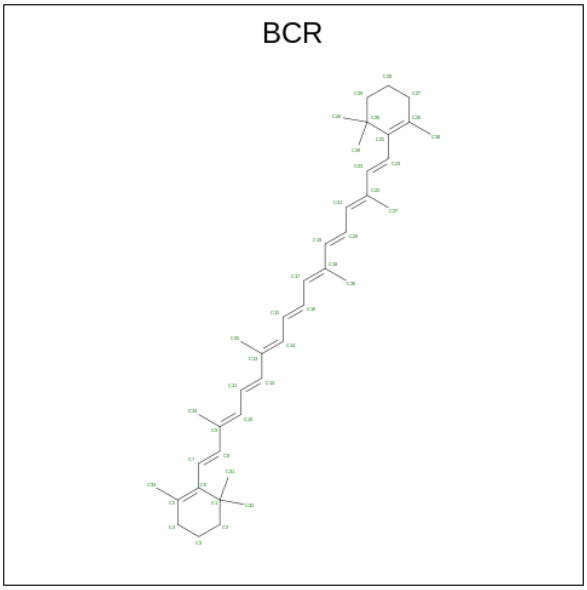
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
19	1	1	Total C O 42 40 2	0	0
19	2	1	Total C O 42 40 2	0	0
19	3	1	Total C O 42 40 2	0	0
19	4	1	Total C O 42 40 2	0	0

- Molecule 20 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
20	1	1	Total C O 44 40 4	0	0
20	2	1	Total C O 44 40 4	0	0
20	3	1	Total C O 44 40 4	0	0
20	4	1	Total C O 44 40 4	0	0

- Molecule 21 is BETA-CAROTENE (CCD ID: BCR) (formula: $C_{40}H_{56}$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
21	1	1	Total C 40 40	0	0
21	2	1	Total C 40 40	0	0
21	3	1	Total C 40 40	0	0
21	4	1	Total C 40 40	0	0
21	A	1	Total C 40 40	0	0
21	A	1	Total C 40 40	0	0
21	A	1	Total C 40 40	0	0
21	A	1	Total C 40 40	0	0

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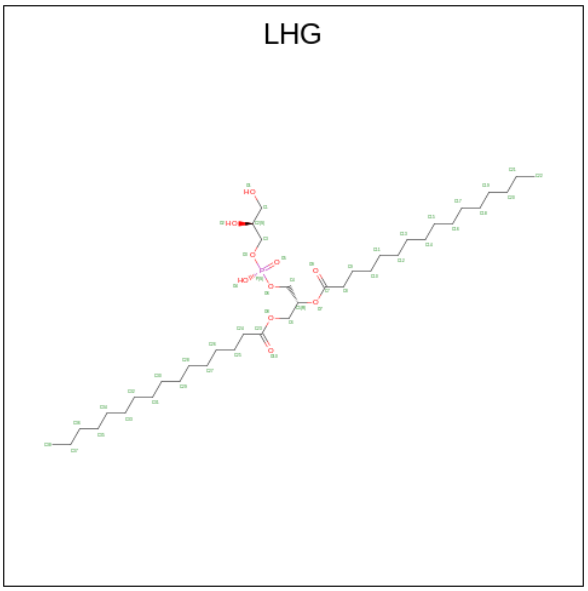
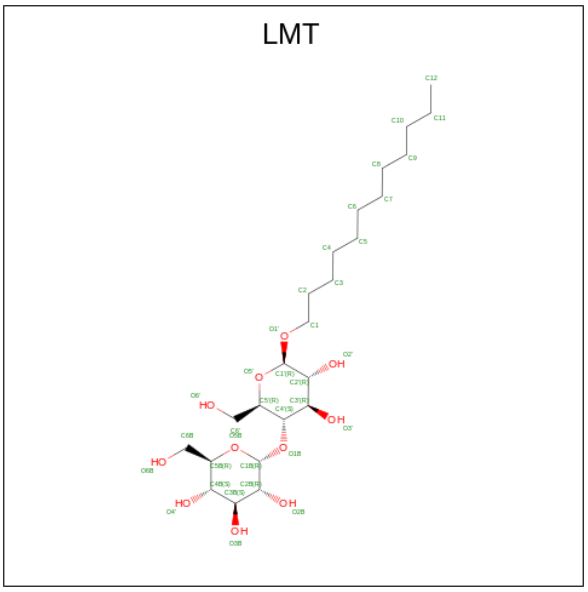
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
21	A	1	Total C 40 40	0	0
21	A	1	Total C 40 40	0	0
21	B	1	Total C 40 40	0	0
21	B	1	Total C 40 40	0	0
21	B	1	Total C 40 40	0	0
21	B	1	Total C 40 40	0	0
21	B	1	Total C 40 40	0	0
21	B	1	Total C 40 40	0	0
21	F	1	Total C 40 40	0	0
21	F	1	Total C 40 40	0	0
21	G	1	Total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

- Molecule 22 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (CCD ID: LHG) (formula: $C_{38}H_{75}O_{10}P$) (labeled as "Ligand of Interest" by depositor).



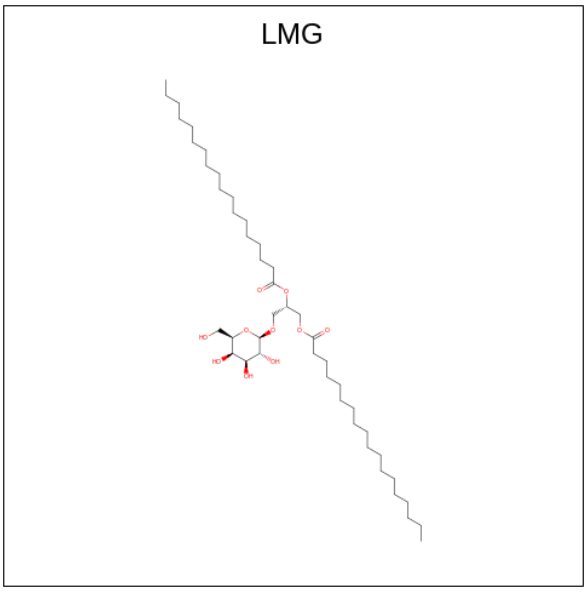
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
22	1	1	Total	C	O	P	0	0
			49	38	10	1		
22	2	1	Total	C	O	P	0	0
			37	26	10	1		
22	A	1	Total	C	O	P	0	0
			49	38	10	1		
22	A	1	Total	C	O	P	0	0
			27	16	10	1		
22	B	1	Total	C	O	P	0	0
			23	12	10	1		
22	F	1	Total	C	O	P	0	0
			40	29	10	1		
22	G	1	Total	C	O	P	0	0
			49	38	10	1		

- Molecule 23 is DODECYL-BETA-D-MALTOSIDE (CCD ID: LMT) (formula: $C_{24}H_{46}O_{11}$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
23	2	1	Total C O 35 24 11	0	0
23	A	1	Total C O 35 24 11	0	0

- Molecule 24 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (CCD ID: LMG) (formula: $C_{45}H_{86}O_{10}$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
24	4	1	Total C O 50 40 10	0	0

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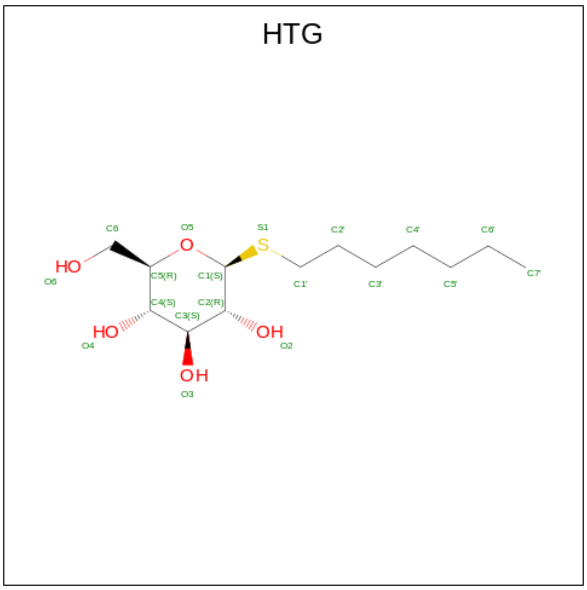
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
24	4	1	Total C O 49 39 10	0	0
24	B	1	Total C O 52 42 10	0	0
24	F	1	Total C O 55 45 10	0	0
24	G	1	Total C O 40 30 10	0	0

- Molecule 25 is heptyl 1-thio-beta-D-glucopyranoside (CCD ID: HTG) (formula: $C_{13}H_{26}O_5S$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
25	4	1	Total C O S 19 13 5 1	0	0
25	4	1	Total C O S 19 13 5 1	0	0
25	A	1	Total C O S 19 13 5 1	0	0
25	B	1	Total C O S 19 13 5 1	0	0
25	F	1	Total C O S 17 11 5 1	0	0
25	F	1	Total C O S 19 13 5 1	0	0
25	F	1	Total C O S 16 10 5 1	0	0

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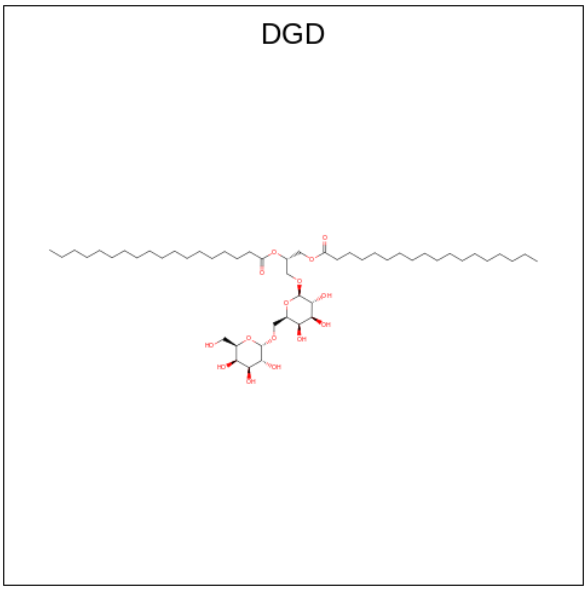
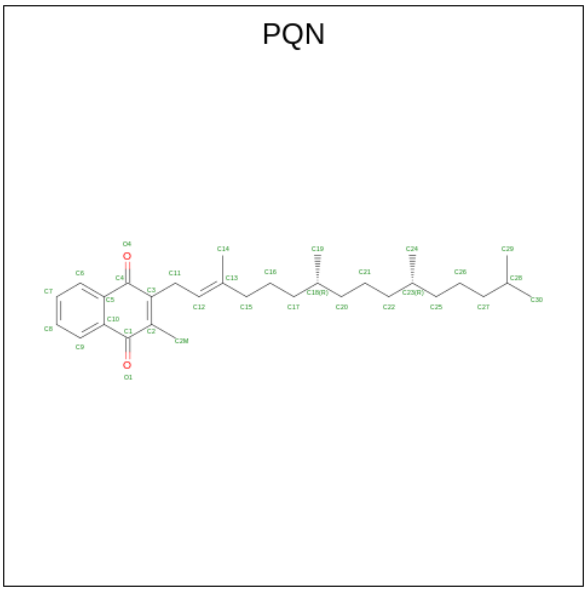
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
25	J	1	Total	C	O	S	0	0
			19	13	5	1		

- Molecule 26 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (CCD ID: DGD) (formula: $C_{51}H_{96}O_{15}$) (labeled as "Ligand of Interest" by depositor).



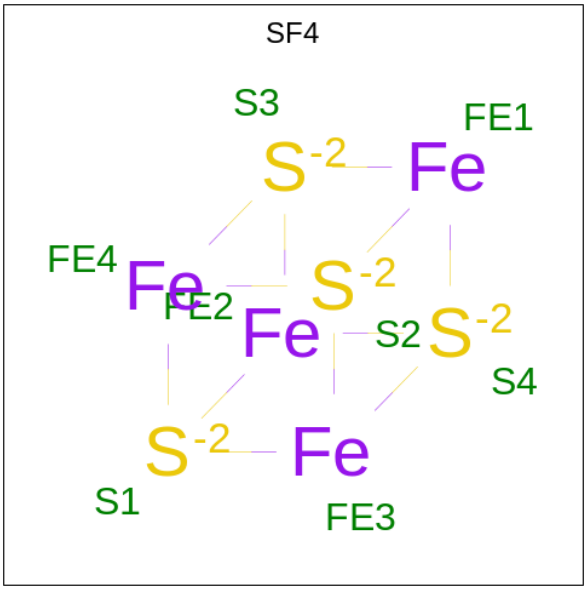
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
26	4	1	Total	C	O	0	0
			60	45	15		
26	B	1	Total	C	O	0	0
			66	51	15		

- Molecule 27 is PHYLLOQUINONE (CCD ID: PQN) (formula: $C_{31}H_{46}O_2$).



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

- 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 8 4 4	0	0
28	C	1	Total Fe S 8 4 4	0	0

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

- Molecule 29 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
29	1	3	Total O 3 3	0	0
29	2	5	Total O 5 5	0	0
29	3	3	Total O 3 3	0	0
29	4	7	Total O 7 7	0	0
29	A	25	Total O 25 25	0	0
29	B	39	Total O 39 39	0	0
29	C	3	Total O 3 3	0	0
29	F	5	Total O 5 5	0	0
29	G	1	Total O 1 1	0	0
29	J	1	Total O 1 1	0	0
29	L	1	Total O 1 1	0	0

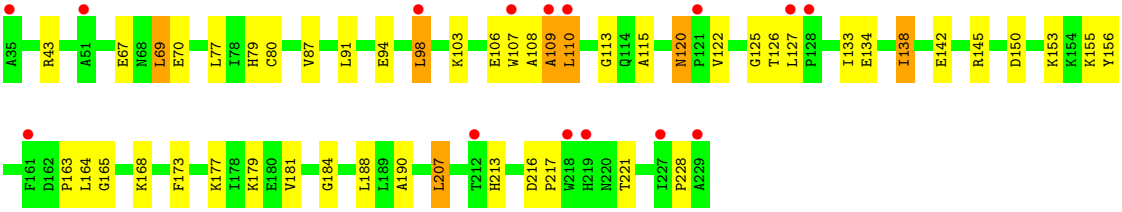
3 Residue-property plots (i)

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:

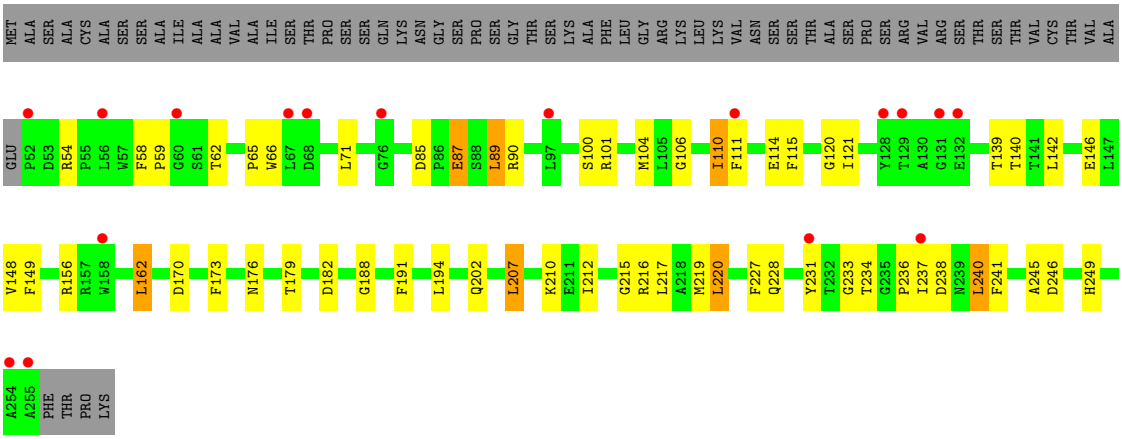




• Molecule 2: Chlorophyll a-b binding protein, chloroplastic

Chain 2:

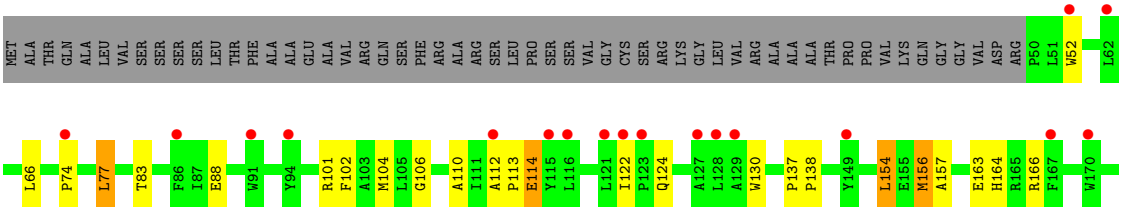


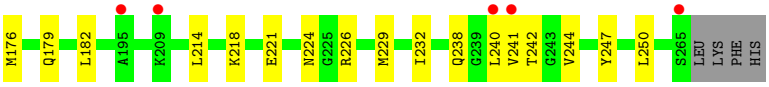


• Molecule 3: Chlorophyll a-b binding protein 3, chloroplastic

Chain 3:



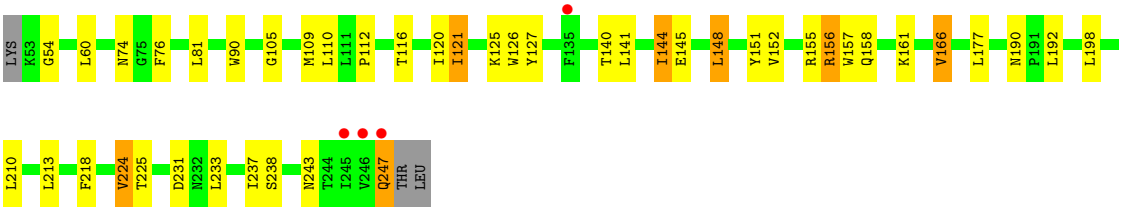




• Molecule 4: Chlorophyll a-b binding protein P4, chloroplastic

Chain 4:

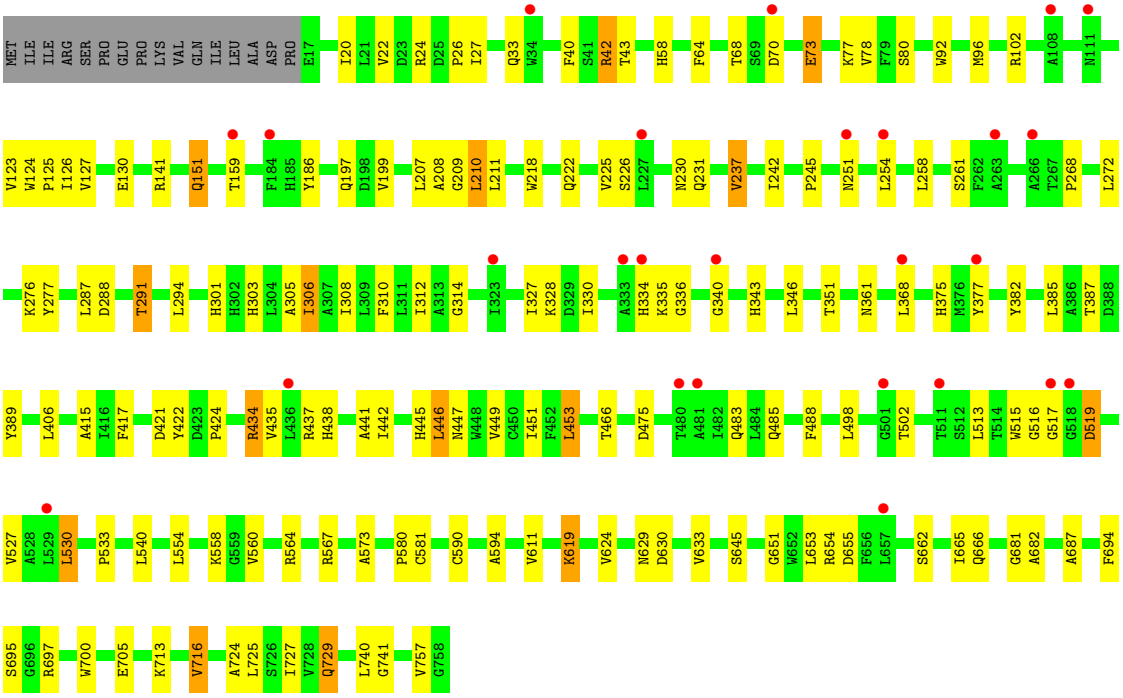




• Molecule 5: Photosystem I P700 chlorophyll a apoprotein A1

Chain A:

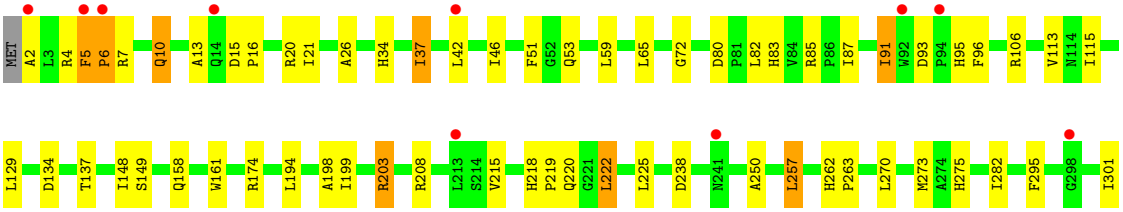


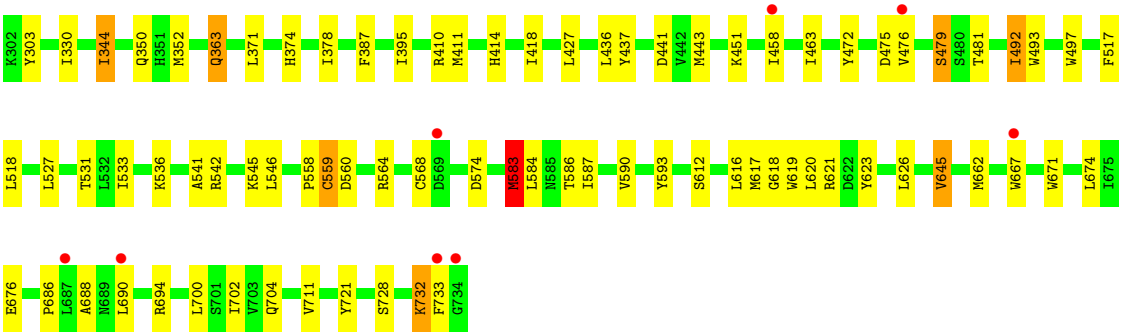


• Molecule 6: Photosystem I P700 chlorophyll a apoprotein A2

Chain B:

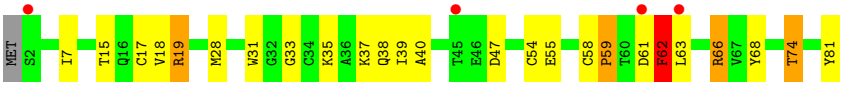






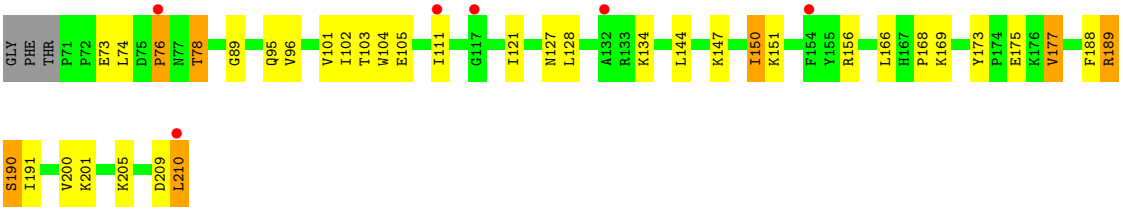
• Molecule 7: Photosystem I iron-sulfur center



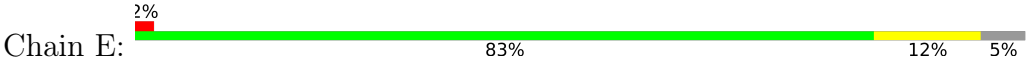


• Molecule 8: PsaD



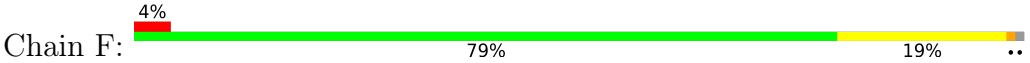


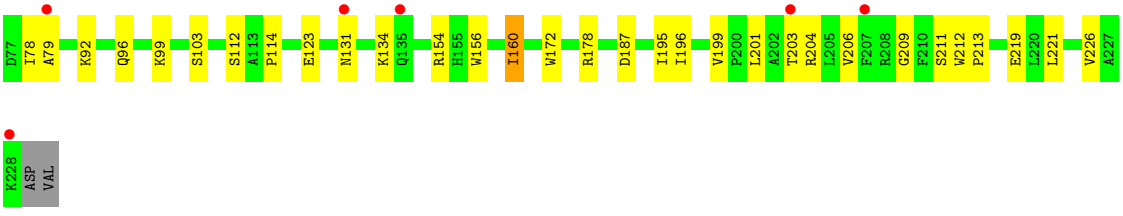
• Molecule 9: PsaE



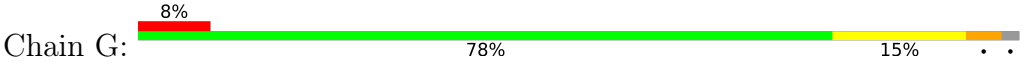


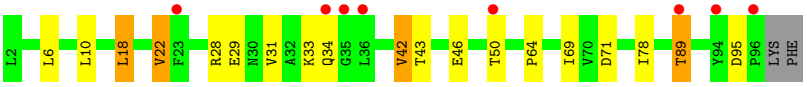
• Molecule 10: PSI-F



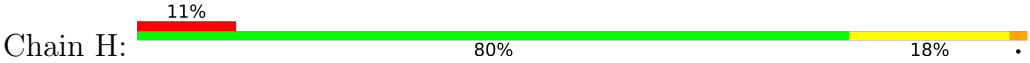


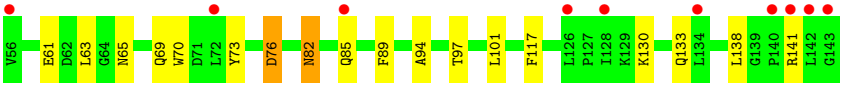
• Molecule 11: PsaG





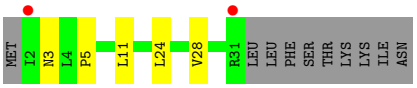
• Molecule 12: PsaH



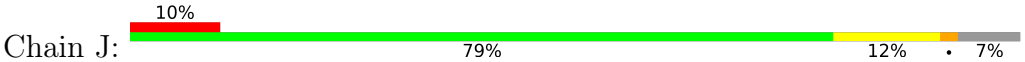


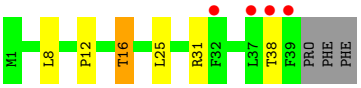
• Molecule 13: Photosystem I reaction center subunit VIII





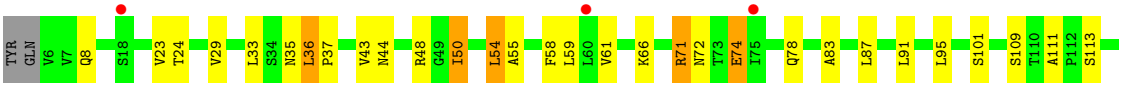
• Molecule 14: Photosystem I reaction center subunit IX





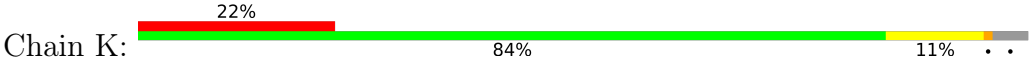
• Molecule 15: PsaL

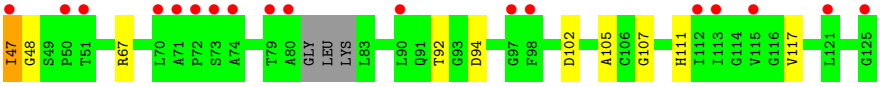






• Molecule 16: PSI-K





4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	225.65Å 168.95Å 185.22Å 90.00° 121.39° 90.00°	Depositor
Resolution (Å)	44.41 – 2.39 44.41 – 2.39	Depositor EDS
% Data completeness (in resolution range)	98.9 (44.41-2.39) 98.9 (44.41-2.39)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.75 (at 2.39Å)	Xtriage
Refinement program	PHENIX 1.11.1_2575	Depositor
R, R_{free}	0.189 , 0.227 0.195 , 0.231	Depositor DCC
R_{free} test set	11616 reflections (4.10%)	wwPDB-VP
Wilson B-factor (Å^2)	65.4	Xtriage
Anisotropy	0.534	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 70.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	36093	wwPDB-VP
Average B, all atoms (Å^2)	101.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.81% 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: LMT, LMG, DGD, XAT, CLA, HTG, SF4, LUT, PQN, CHL, BCR, LHG

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	0.28	0/1557	0.45	0/2127
2	2	0.21	0/1651	0.40	0/2262
3	3	0.14	0/1713	0.32	0/2326
4	4	0.45	0/1584	0.65	0/2159
5	A	0.30	0/6050	0.47	0/8254
6	B	0.46	1/6068 (0.0%)	0.65	1/8286 (0.0%)
7	C	0.99	2/624 (0.3%)	1.30	10/846 (1.2%)
8	D	0.31	0/1140	0.54	0/1540
9	E	0.39	0/515	0.56	0/700
10	F	0.46	0/1226	0.68	0/1658
11	G	0.54	0/755	0.70	0/1027
12	H	0.19	0/693	0.34	0/942
13	I	0.39	0/232	0.42	0/317
14	J	0.40	0/317	0.57	0/432
15	L	0.19	0/1153	0.36	0/1576
16	K	0.12	0/520	0.30	0/707
All	All	0.39	3/25798 (0.0%)	0.56	11/35159 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
7	C	1	0

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	C	59	PRO	N-CA	17.60	1.69	1.47
7	C	58	CYS	C-N	9.29	1.44	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	B	6	PRO	C-O	-5.05	1.17	1.24

The worst 5 of 11 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	C	58	CYS	CA-C-N	16.34	137.69	120.04
7	C	58	CYS	C-N-CA	16.34	137.69	120.04
7	C	62	PHE	CB-CA-C	11.20	132.72	110.42
7	C	62	PHE	CA-CB-CG	-6.52	107.28	113.80
7	C	59	PRO	CA-N-CD	-6.52	102.88	112.00

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
7	C	62	PHE	CA

There are no planarity outliers.

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	1	1507	0	1468	35	0
2	2	1592	0	1531	52	0
3	3	1661	0	1620	37	0
4	4	1535	0	1496	41	0
5	A	5852	0	5713	102	0
6	B	5856	0	5653	113	0
7	C	611	0	591	19	0
8	D	1110	0	1123	19	0
9	E	505	0	503	3	0
10	F	1198	0	1228	19	0
11	G	737	0	721	13	0
12	H	673	0	667	12	0
13	I	226	0	242	3	0
14	J	309	0	320	5	0
15	L	1122	0	1133	27	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
16	K	515	0	513	5	0
17	1	672	0	636	29	0
17	2	533	0	480	18	0
17	3	542	0	433	16	0
17	4	540	0	476	22	0
17	A	2582	0	2646	114	0
17	B	2493	0	2566	109	0
17	F	165	0	154	8	0
17	G	137	0	101	5	0
17	J	107	0	103	5	0
17	K	105	0	92	5	0
17	L	180	0	183	12	0
18	1	48	0	33	4	0
18	2	185	0	128	14	0
18	3	103	0	72	20	0
18	4	262	0	207	29	0
19	1	42	0	56	7	0
19	2	42	0	56	4	0
19	3	42	0	56	4	0
19	4	42	0	56	3	0
20	1	44	0	56	3	0
20	2	44	0	56	9	0
20	3	44	0	56	12	0
20	4	44	0	56	9	0
21	1	40	0	56	0	0
21	2	40	0	56	9	0
21	3	40	0	56	4	0
21	4	40	0	56	14	0
21	A	240	0	336	25	0
21	B	240	0	336	25	0
21	F	80	0	112	3	0
21	G	40	0	56	2	0
21	I	40	0	56	4	0
21	J	80	0	112	7	0
21	K	40	0	56	5	0
21	L	120	0	168	10	0
22	1	49	0	74	6	0
22	2	37	0	44	6	0
22	A	76	0	98	3	0
22	B	23	0	16	1	0
22	F	40	0	53	2	0
22	G	49	0	74	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
23	2	35	0	46	3	0
23	A	35	0	45	2	0
24	4	99	0	143	7	0
24	B	52	0	77	4	0
24	F	55	0	86	1	0
24	G	40	0	53	3	0
25	4	38	0	52	4	0
25	A	19	0	26	0	0
25	B	19	0	26	1	0
25	F	52	0	62	2	0
25	J	19	0	26	3	0
26	4	60	0	81	29	0
26	B	66	0	96	7	0
27	A	33	0	46	6	0
27	B	33	0	46	3	0
28	A	8	0	0	0	0
28	C	16	0	0	0	0
29	1	3	0	0	0	0
29	2	5	0	0	0	0
29	3	3	0	0	0	0
29	4	7	0	0	0	0
29	A	25	0	0	1	0
29	B	39	0	0	2	0
29	C	3	0	0	0	0
29	F	5	0	0	0	0
29	G	1	0	0	0	0
29	J	1	0	0	0	0
29	L	1	0	0	0	0
All	All	36093	0	36006	826	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 11.

The worst 5 of 826 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)
7:C:59:PRO:N	7:C:59:PRO:CA	1.69	1.32
6:B:303:TYR:CD2	11:G:34:GLN:HB3	1.94	1.03
3:3:74:PRO:HD2	20:3:615:XAT:O23	1.57	1.02
3:3:229:MET:HB3	20:3:615:XAT:H402	1.42	1.02
17:3:602:CLA:HAB	20:3:615:XAT:H32	1.44	0.99

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	193/195 (99%)	178 (92%)	12 (6%)	3 (2%)	7 11
2	2	202/269 (75%)	191 (95%)	9 (4%)	2 (1%)	12 20
3	3	214/275 (78%)	197 (92%)	17 (8%)	0	100 100
4	4	193/198 (98%)	179 (93%)	13 (7%)	1 (0%)	24 37
5	A	740/758 (98%)	707 (96%)	30 (4%)	3 (0%)	30 43
6	B	731/734 (100%)	709 (97%)	19 (3%)	3 (0%)	30 43
7	C	78/81 (96%)	74 (95%)	4 (5%)	0	100 100
8	D	138/143 (96%)	127 (92%)	9 (6%)	2 (1%)	9 13
9	E	61/66 (92%)	59 (97%)	2 (3%)	0	100 100
10	F	150/154 (97%)	148 (99%)	2 (1%)	0	100 100
11	G	93/97 (96%)	88 (95%)	5 (5%)	0	100 100
12	H	86/88 (98%)	80 (93%)	6 (7%)	0	100 100
13	I	28/40 (70%)	26 (93%)	2 (7%)	0	100 100
14	J	37/42 (88%)	37 (100%)	0	0	100 100
15	L	149/157 (95%)	145 (97%)	4 (3%)	0	100 100
16	K	73/80 (91%)	67 (92%)	6 (8%)	0	100 100
All	All	3166/3377 (94%)	3012 (95%)	140 (4%)	14 (0%)	30 43

5 of 14 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
5	A	516	GLY
6	B	5	PHE
8	D	76	PRO
1	1	109	ALA

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Mol	Chain	Res	Type
6	B	559	CYS

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	155/158 (98%)	145 (94%)	10 (6%)	15 27
2	2	164/216 (76%)	150 (92%)	14 (8%)	10 16
3	3	167/213 (78%)	158 (95%)	9 (5%)	20 35
4	4	161/164 (98%)	146 (91%)	15 (9%)	8 14
5	A	603/618 (98%)	569 (94%)	34 (6%)	19 33
6	B	598/599 (100%)	568 (95%)	30 (5%)	22 38
7	C	69/70 (99%)	65 (94%)	4 (6%)	18 32
8	D	120/122 (98%)	107 (89%)	13 (11%)	6 9
9	E	55/58 (95%)	51 (93%)	4 (7%)	13 22
10	F	124/127 (98%)	115 (93%)	9 (7%)	13 22
11	G	80/82 (98%)	69 (86%)	11 (14%)	3 4
12	H	71/71 (100%)	65 (92%)	6 (8%)	10 16
13	I	25/36 (69%)	23 (92%)	2 (8%)	11 19
14	J	32/35 (91%)	29 (91%)	3 (9%)	8 13
15	L	118/124 (95%)	106 (90%)	12 (10%)	7 11
16	K	51/58 (88%)	48 (94%)	3 (6%)	18 31
All	All	2593/2751 (94%)	2414 (93%)	179 (7%)	14 24

5 of 179 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
7	C	74	THR
11	G	10	LEU
8	D	96	VAL
9	E	44	LYS

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Mol	Chain	Res	Type
11	G	50	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 23 such sidechains are listed below:

Mol	Chain	Res	Type
6	B	236	ASN
6	B	608	GLN
6	B	504	ASN
9	E	49	ASN
5	A	185	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)

215 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
21	BCR	A	849	-	41,41,41	1.12	2 (4%)	56,56,56	1.26	7 (12%)
17	CLA	B	842	22	69,73,73	1.28	7 (10%)	83,113,113	1.49	13 (15%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
17	CLA	B	829	6	69,73,73	1.31	9 (13%)	83,113,113	1.23	8 (9%)
17	CLA	F	307	10	59,63,73	1.38	7 (11%)	71,101,113	1.39	9 (12%)
17	CLA	B	838	6	69,73,73	1.22	8 (11%)	83,113,113	1.45	8 (9%)
17	CLA	3	604	-	49,53,73	1.50	8 (16%)	59,89,113	1.41	7 (11%)
21	BCR	K	203	-	41,41,41	1.08	2 (4%)	56,56,56	1.21	6 (10%)
17	CLA	K	201	16	49,53,73	1.49	7 (14%)	59,89,113	1.45	6 (10%)
25	HTG	F	301	-	17,17,19	0.96	2 (11%)	21,22,24	0.69	0
17	CLA	B	836	29	49,53,73	1.51	7 (14%)	59,89,113	1.59	11 (18%)
17	CLA	A	808	5	69,73,73	1.22	6 (8%)	83,113,113	1.52	12 (14%)
25	HTG	4	322	-	19,19,19	1.07	2 (10%)	23,24,24	1.23	3 (13%)
17	CLA	B	818	6	59,63,73	1.36	7 (11%)	71,101,113	1.50	9 (12%)
17	CLA	A	840	5	69,73,73	1.26	9 (13%)	83,113,113	1.45	14 (16%)
17	CLA	A	807	5	69,73,73	1.25	10 (14%)	83,113,113	1.27	7 (8%)
17	CLA	1	304	-	46,50,73	1.54	7 (15%)	55,85,113	1.38	4 (7%)
17	CLA	B	840	29	69,73,73	1.21	6 (8%)	83,113,113	1.29	6 (7%)
17	CLA	A	810	5,17	69,73,73	1.27	7 (10%)	83,113,113	1.27	8 (9%)
17	CLA	B	823	-	69,73,73	1.20	6 (8%)	83,113,113	1.42	8 (9%)
17	CLA	B	833	6	64,68,73	1.27	8 (12%)	77,107,113	1.39	15 (19%)
25	HTG	4	321	-	19,19,19	1.14	2 (10%)	23,24,24	1.14	1 (4%)
17	CLA	B	811	6	69,73,73	1.27	7 (10%)	83,113,113	1.35	8 (9%)
22	LHG	A	844	-	48,48,48	0.67	1 (2%)	51,54,54	1.29	6 (11%)
17	CLA	L	202	15	69,73,73	1.27	7 (10%)	83,113,113	1.29	6 (7%)
17	CLA	1	306	29	50,54,73	1.49	7 (14%)	60,90,113	1.39	7 (11%)
17	CLA	2	312	2	47,51,73	1.53	8 (17%)	56,86,113	1.42	5 (8%)
17	CLA	B	803	5	69,73,73	1.29	8 (11%)	83,113,113	1.26	5 (6%)
20	XAT	3	615	-	39,47,47	4.99	17 (43%)	54,74,74	5.48	32 (59%)
17	CLA	A	805	5	69,73,73	1.27	7 (10%)	83,113,113	1.38	10 (12%)
18	CHL	2	304	29	47,51,74	2.22	15 (31%)	52,86,114	3.21	24 (46%)
20	XAT	1	315	-	39,47,47	5.00	17 (43%)	54,74,74	5.48	32 (59%)
21	BCR	F	308	-	41,41,41	1.05	2 (4%)	56,56,56	1.27	8 (14%)
17	CLA	2	309	-	45,49,73	1.54	6 (13%)	54,84,113	1.54	8 (14%)
17	CLA	B	812	6	69,73,73	1.28	7 (10%)	83,113,113	1.18	7 (8%)
17	CLA	A	806	-	69,73,73	1.34	9 (13%)	83,113,113	1.23	6 (7%)
17	CLA	A	834	5	49,53,73	1.51	8 (16%)	59,89,113	1.42	7 (11%)
17	CLA	4	309	4	64,68,73	1.43	7 (10%)	77,107,113	1.24	7 (9%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
18	CHL	4	315	4	47,51,74	2.26	17 (36%)	52,86,114	2.98	19 (36%)
21	BCR	B	846	-	41,41,41	1.02	2 (4%)	56,56,56	1.24	8 (14%)
17	CLA	A	833	5	54,58,73	1.43	8 (14%)	65,95,113	1.41	8 (12%)
22	LHG	A	845	17	26,26,48	0.87	1 (3%)	29,32,54	1.32	3 (10%)
21	BCR	3	616	-	41,41,41	1.09	2 (4%)	56,56,56	1.30	5 (8%)
17	CLA	A	804	5	69,73,73	1.33	6 (8%)	83,113,113	1.31	10 (12%)
17	CLA	1	312	1	59,63,73	1.41	7 (11%)	71,101,113	1.32	9 (12%)
17	CLA	3	610	-	56,60,73	1.42	7 (12%)	67,97,113	1.45	7 (10%)
17	CLA	B	816	6	69,73,73	1.31	8 (11%)	83,113,113	1.30	9 (10%)
17	CLA	A	822	5	55,59,73	1.41	7 (12%)	66,96,113	1.37	6 (9%)
17	CLA	1	313	1	50,54,73	1.45	8 (16%)	60,90,113	1.38	6 (10%)
24	LMG	4	319	-	50,50,55	0.88	3 (6%)	58,58,63	1.46	8 (13%)
17	CLA	1	307	1	69,73,73	1.31	9 (13%)	83,113,113	1.30	7 (8%)
17	CLA	A	809	5	69,73,73	1.24	8 (11%)	83,113,113	1.31	10 (12%)
17	CLA	A	823	5	59,63,73	1.39	7 (11%)	71,101,113	1.35	6 (8%)
17	CLA	A	811	5	58,62,73	1.40	7 (12%)	69,99,113	1.32	7 (10%)
17	CLA	3	608	3	54,58,73	1.45	7 (12%)	65,95,113	1.38	7 (10%)
17	CLA	3	609	3	54,58,73	1.44	6 (11%)	65,95,113	1.34	6 (9%)
17	CLA	4	312	4	60,64,73	1.36	8 (13%)	72,102,113	1.38	7 (9%)
17	CLA	B	805	-	69,73,73	1.29	9 (13%)	83,113,113	1.29	10 (12%)
17	CLA	B	824	6	59,63,73	1.40	9 (15%)	71,101,113	1.37	9 (12%)
24	LMG	F	309	-	55,55,55	0.85	2 (3%)	63,63,63	1.45	8 (12%)
17	CLA	2	308	2	64,68,73	1.31	7 (10%)	77,107,113	1.24	5 (6%)
17	CLA	3	605	-	46,50,73	1.60	7 (15%)	55,85,113	1.35	6 (10%)
18	CHL	3	601	2	57,61,74	2.09	16 (28%)	64,98,114	3.09	28 (43%)
17	CLA	G	103	29	45,49,73	1.57	9 (20%)	54,84,113	1.50	5 (9%)
22	LHG	G	102	-	48,48,48	0.67	1 (2%)	51,54,54	1.23	6 (11%)
17	CLA	G	105	11	50,54,73	1.46	7 (14%)	60,90,113	1.41	7 (11%)
21	BCR	L	206	-	41,41,41	1.09	2 (4%)	56,56,56	1.29	7 (12%)
17	CLA	B	806	6	49,53,73	1.39	6 (12%)	59,89,113	1.67	11 (18%)
20	XAT	4	317	-	39,47,47	5.05	17 (43%)	54,74,74	5.30	32 (59%)
17	CLA	B	817	-	59,63,73	1.38	8 (13%)	71,101,113	1.44	8 (11%)
17	CLA	A	835	5	55,59,73	1.42	9 (16%)	66,96,113	1.41	10 (15%)
17	CLA	2	319	4	50,54,73	1.48	7 (14%)	60,90,113	1.46	8 (13%)
17	CLA	B	822	6	54,58,73	1.39	6 (11%)	65,95,113	1.57	9 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
25	HTG	B	851	-	19,19,19	1.06	1 (5%)	23,24,24	1.87	7 (30%)
28	SF4	C	102	7	0,12,12	-	-	-		
24	LMG	B	852	-	52,52,55	1.09	4 (7%)	60,60,63	1.49	7 (11%)
17	CLA	B	831	6	69,73,73	1.26	8 (11%)	83,113,113	1.61	13 (15%)
17	CLA	3	603	3	54,58,73	1.41	7 (12%)	65,95,113	1.36	4 (6%)
21	BCR	A	848	-	41,41,41	1.05	2 (4%)	56,56,56	1.22	6 (10%)
17	CLA	2	311	2	69,73,73	1.30	7 (10%)	83,113,113	1.32	9 (10%)
17	CLA	G	104	11	54,58,73	1.48	8 (14%)	65,95,113	1.49	10 (15%)
21	BCR	B	848	-	41,41,41	1.06	2 (4%)	56,56,56	1.20	7 (12%)
18	CHL	4	301	1	65,69,74	2.11	20 (30%)	74,108,114	2.84	30 (40%)
23	LMT	2	318	-	36,36,36	1.09	5 (13%)	47,47,47	1.11	3 (6%)
17	CLA	A	836	5	69,73,73	1.22	7 (10%)	83,113,113	1.37	8 (9%)
17	CLA	3	611	3	59,63,73	1.38	6 (10%)	71,101,113	1.34	5 (7%)
21	BCR	4	318	-	41,41,41	0.97	1 (2%)	56,56,56	1.26	8 (14%)
17	CLA	A	818	5	69,73,73	1.27	9 (13%)	83,113,113	1.34	11 (13%)
17	CLA	2	302	2	55,59,73	1.44	9 (16%)	66,96,113	1.37	4 (6%)
17	CLA	4	308	4	54,58,73	1.42	9 (16%)	65,95,113	1.53	9 (13%)
22	LHG	F	302	-	39,39,48	0.65	0	42,45,54	1.25	6 (14%)
17	CLA	B	827	29	69,73,73	1.27	8 (11%)	83,113,113	1.46	9 (10%)
17	CLA	2	303	-	64,68,73	1.30	6 (9%)	77,107,113	1.26	6 (7%)
17	CLA	J	101	5	69,73,73	1.34	8 (11%)	83,113,113	1.41	10 (12%)
17	CLA	B	804	6	69,73,73	1.37	10 (14%)	83,113,113	1.21	7 (8%)
17	CLA	B	837	6	64,68,73	1.19	7 (10%)	77,107,113	1.55	11 (14%)
26	DGD	4	323	-	61,61,67	0.89	2 (3%)	75,75,81	1.76	21 (28%)
18	CHL	4	307	29	55,59,74	2.16	18 (32%)	62,96,114	2.86	24 (38%)
21	BCR	J	104	-	41,41,41	1.00	3 (7%)	56,56,56	1.23	4 (7%)
24	LMG	4	320	-	49,49,55	1.04	4 (8%)	57,57,63	1.46	5 (8%)
28	SF4	C	101	7	0,12,12	-	-	-		
17	CLA	A	838	5	69,73,73	1.27	8 (11%)	83,113,113	1.52	13 (15%)
19	LUT	3	614	-	42,43,43	5.66	20 (47%)	51,60,60	5.51	31 (60%)
17	CLA	3	613	3	50,54,73	1.48	9 (18%)	60,90,113	1.42	6 (10%)
17	CLA	A	837	5	69,73,73	1.31	6 (8%)	83,113,113	1.33	9 (10%)
21	BCR	L	201	-	41,41,41	1.02	2 (4%)	56,56,56	1.20	6 (10%)
17	CLA	B	820	6	64,68,73	1.31	7 (10%)	77,107,113	1.53	17 (22%)
17	CLA	B	821	29	69,73,73	1.26	6 (8%)	83,113,113	1.41	7 (8%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
24	LMG	G	101	-	40,40,55	0.87	2 (5%)	48,48,63	1.28	3 (6%)
27	PQN	B	843	-	34,34,34	4.45	14 (41%)	42,45,45	4.44	23 (54%)
17	CLA	A	802	29	69,73,73	1.21	7 (10%)	83,113,113	1.30	7 (8%)
17	CLA	A	853	29	69,73,73	1.31	9 (13%)	83,113,113	1.82	17 (20%)
22	LHG	2	317	-	36,36,48	0.71	1 (2%)	39,42,54	1.23	4 (10%)
17	CLA	A	824	29	69,73,73	1.29	8 (11%)	83,113,113	1.27	8 (9%)
17	CLA	A	821	-	53,57,73	1.42	7 (13%)	62,93,113	1.46	7 (11%)
17	CLA	B	826	29	69,73,73	1.36	10 (14%)	83,113,113	1.29	10 (12%)
17	CLA	1	303	29	55,59,73	1.39	6 (10%)	66,96,113	1.40	7 (10%)
27	PQN	A	842	-	34,34,34	4.59	16 (47%)	42,45,45	4.02	17 (40%)
17	CLA	B	813	6,17	58,62,73	1.38	6 (10%)	73,100,113	1.39	7 (9%)
28	SF4	A	852	6,5	0,12,12	-	-	-		
17	CLA	F	304	6	69,73,73	1.29	7 (10%)	83,113,113	1.47	10 (12%)
17	CLA	4	313	4	49,53,73	1.52	7 (14%)	59,89,113	1.48	5 (8%)
17	CLA	A	826	5	69,73,73	1.24	9 (13%)	83,113,113	1.29	5 (6%)
17	CLA	A	817	5	69,73,73	1.27	7 (10%)	83,113,113	1.32	8 (9%)
17	CLA	A	828	5	69,73,73	1.28	6 (8%)	83,113,113	1.29	8 (9%)
25	HTG	F	310	-	16,16,19	1.15	2 (12%)	20,21,24	1.41	4 (20%)
17	CLA	A	829	5	69,73,73	1.23	8 (11%)	83,113,113	1.39	7 (8%)
17	CLA	A	827	5	69,73,73	1.24	9 (13%)	83,113,113	1.43	11 (13%)
17	CLA	B	825	6	64,68,73	1.25	8 (12%)	77,107,113	1.55	12 (15%)
17	CLA	B	839	6	51,55,73	1.41	8 (15%)	61,91,113	1.86	16 (26%)
18	CHL	2	313	2	47,51,74	2.22	14 (29%)	52,86,114	3.20	23 (44%)
17	CLA	J	103	14	46,50,73	1.50	7 (15%)	55,85,113	1.51	5 (9%)
21	BCR	1	316	-	41,41,41	1.07	2 (4%)	56,56,56	1.24	6 (10%)
17	CLA	B	835	6	69,73,73	1.38	7 (10%)	83,113,113	1.21	8 (9%)
21	BCR	2	316	-	41,41,41	1.18	3 (7%)	56,56,56	1.25	8 (14%)
21	BCR	B	844	-	41,41,41	0.99	2 (4%)	56,56,56	1.28	7 (12%)
17	CLA	1	309	22	69,73,73	1.29	7 (10%)	83,113,113	1.23	9 (10%)
18	CHL	1	305	1	52,56,74	2.34	17 (32%)	58,92,114	2.82	24 (41%)
17	CLA	3	602	3	64,68,73	1.32	7 (10%)	77,107,113	1.27	5 (6%)
25	HTG	A	854	-	19,19,19	0.84	1 (5%)	23,24,24	0.92	0
21	BCR	A	847	-	41,41,41	1.08	3 (7%)	56,56,56	1.22	5 (8%)
17	CLA	4	314	-	51,55,73	1.34	7 (13%)	61,91,113	1.60	10 (16%)
17	CLA	A	843	22	56,60,73	1.43	7 (12%)	67,97,113	1.40	7 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
17	CLA	A	839	29	69,73,73	1.30	8 (11%)	83,113,113	1.31	7 (8%)
21	BCR	G	106	-	41,41,41	1.06	2 (4%)	56,56,56	1.13	5 (8%)
17	CLA	3	606	3	51,55,73	1.48	8 (15%)	61,91,113	1.38	7 (11%)
17	CLA	4	302	4	64,68,73	1.37	10 (15%)	77,107,113	1.40	10 (12%)
17	CLA	A	814	-	54,58,73	1.43	7 (12%)	65,95,113	1.36	6 (9%)
19	LUT	4	316	-	42,43,43	5.53	22 (52%)	51,60,60	5.74	35 (68%)
25	HTG	F	305	-	19,19,19	1.05	2 (10%)	23,24,24	1.73	4 (17%)
17	CLA	A	813	5	49,53,73	1.52	7 (14%)	59,89,113	1.33	5 (8%)
17	CLA	A	830	5	54,58,73	1.43	8 (14%)	65,95,113	1.39	8 (12%)
25	HTG	J	102	-	19,19,19	1.20	2 (10%)	23,24,24	1.30	3 (13%)
17	CLA	A	803	5,17	59,63,73	1.42	9 (15%)	71,101,113	1.31	6 (8%)
17	CLA	A	812	5	69,73,73	1.28	7 (10%)	83,113,113	1.28	7 (8%)
17	CLA	B	809	6	69,73,73	1.29	8 (11%)	83,113,113	1.23	8 (9%)
21	BCR	B	849	-	41,41,41	0.96	2 (4%)	56,56,56	1.19	3 (5%)
21	BCR	L	205	-	41,41,41	0.98	1 (2%)	56,56,56	1.10	4 (7%)
17	CLA	A	831	5	69,73,73	1.28	7 (10%)	83,113,113	1.37	9 (10%)
21	BCR	A	846	-	41,41,41	1.05	2 (4%)	56,56,56	1.33	8 (14%)
21	BCR	I	101	-	41,41,41	1.06	2 (4%)	56,56,56	1.21	4 (7%)
21	BCR	A	850	-	41,41,41	1.14	2 (4%)	56,56,56	1.33	8 (14%)
17	CLA	B	802	-	69,73,73	1.28	8 (11%)	83,113,113	1.35	12 (14%)
17	CLA	A	820	29	69,73,73	1.28	8 (11%)	83,113,113	1.21	7 (8%)
17	CLA	4	303	4	64,68,73	1.40	8 (12%)	77,107,113	1.35	8 (10%)
17	CLA	A	801	5	69,73,73	1.26	7 (10%)	83,113,113	1.60	14 (16%)
17	CLA	A	819	5	49,53,73	1.50	6 (12%)	59,89,113	1.47	7 (11%)
18	CHL	2	306	29	55,59,74	2.16	19 (34%)	62,96,114	2.94	24 (38%)
17	CLA	1	311	1	64,68,73	1.29	8 (12%)	77,107,113	1.29	7 (9%)
17	CLA	B	808	6	69,73,73	1.31	10 (14%)	83,113,113	1.36	8 (9%)
21	BCR	B	845	-	41,41,41	0.92	1 (2%)	56,56,56	1.36	9 (16%)
17	CLA	B	828	6	69,73,73	1.32	8 (11%)	83,113,113	1.47	14 (16%)
17	CLA	A	815	29	49,53,73	1.54	8 (16%)	59,89,113	1.43	7 (11%)
17	CLA	F	306	29	49,53,73	1.46	7 (14%)	59,89,113	1.39	6 (10%)
17	CLA	4	304	29	54,58,73	1.43	6 (11%)	65,95,113	1.57	12 (18%)
17	CLA	A	832	5	69,73,73	1.28	6 (8%)	83,113,113	1.36	9 (10%)
17	CLA	1	308	1	64,68,73	1.30	7 (10%)	77,107,113	1.22	5 (6%)
17	CLA	1	310	1	56,60,73	1.42	9 (16%)	67,97,113	1.31	6 (8%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
17	CLA	2	310	2	56,60,73	1.49	10 (17%)	67,97,113	1.27	5 (7%)
17	CLA	B	830	-	69,73,73	1.32	9 (13%)	83,113,113	1.39	11 (13%)
18	CHL	3	607	29	51,55,74	2.21	17 (33%)	57,91,114	2.97	22 (38%)
23	LMT	A	855	-	36,36,36	1.11	4 (11%)	47,47,47	0.92	1 (2%)
21	BCR	F	303	-	41,41,41	0.92	2 (4%)	56,56,56	1.43	11 (19%)
17	CLA	L	204	-	54,58,73	1.46	6 (11%)	65,95,113	1.36	7 (10%)
20	XAT	2	315	-	39,47,47	4.99	17 (43%)	54,74,74	5.48	32 (59%)
18	CHL	4	306	29	55,59,74	2.19	16 (29%)	62,96,114	3.00	24 (38%)
17	CLA	L	203	15	69,73,73	1.27	7 (10%)	83,113,113	1.34	6 (7%)
17	CLA	B	832	6	54,58,73	1.42	8 (14%)	65,95,113	1.50	9 (13%)
17	CLA	1	302	1	69,73,73	1.27	8 (11%)	83,113,113	1.29	9 (10%)
17	CLA	2	301	2	69,73,73	1.27	9 (13%)	83,113,113	1.26	8 (9%)
17	CLA	4	310	-	64,68,73	1.29	7 (10%)	77,107,113	1.54	13 (16%)
17	CLA	A	825	29	69,73,73	1.28	7 (10%)	83,113,113	1.37	11 (13%)
19	LUT	2	314	-	42,43,43	5.62	20 (47%)	51,60,60	5.61	32 (62%)
17	CLA	A	816	-	69,73,73	1.26	7 (10%)	83,113,113	1.22	7 (8%)
17	CLA	B	841	6	69,73,73	1.26	10 (14%)	83,113,113	1.36	11 (13%)
21	BCR	J	105	-	41,41,41	1.16	2 (4%)	56,56,56	1.43	9 (16%)
26	DGD	B	850	-	67,67,67	1.13	6 (8%)	81,81,81	1.50	10 (12%)
17	CLA	B	807	6	69,73,73	1.25	10 (14%)	83,113,113	1.34	10 (12%)
17	CLA	4	311	4	56,60,73	1.44	7 (12%)	67,97,113	1.37	6 (8%)
17	CLA	B	810	6	69,73,73	1.34	8 (11%)	83,113,113	1.21	9 (10%)
17	CLA	B	814	6,17	59,63,73	1.38	7 (11%)	71,101,113	1.45	9 (12%)
17	CLA	B	834	6	62,66,73	1.38	9 (14%)	74,104,113	1.44	11 (14%)
17	CLA	B	819	6	63,67,73	1.31	7 (11%)	75,105,113	1.39	11 (14%)
17	CLA	A	841	29	69,73,73	1.26	9 (13%)	83,113,113	1.33	9 (10%)
21	BCR	A	851	-	41,41,41	0.89	2 (4%)	56,56,56	1.21	6 (10%)
17	CLA	1	301	1	69,73,73	1.35	7 (10%)	83,113,113	1.26	9 (10%)
19	LUT	1	314	-	42,43,43	5.53	20 (47%)	51,60,60	5.67	33 (64%)
22	LHG	B	801	17	22,22,48	1.09	2 (9%)	25,28,54	1.10	2 (8%)
17	CLA	K	202	-	64,68,73	1.33	7 (10%)	77,107,113	1.32	6 (7%)
18	CHL	2	305	29	52,56,74	2.23	17 (32%)	58,92,114	3.03	23 (39%)
18	CHL	4	305	29	60,64,74	1.94	16 (26%)	68,102,114	3.00	24 (35%)
17	CLA	B	815	6	69,73,73	1.34	7 (10%)	83,113,113	1.30	8 (9%)
17	CLA	2	307	2	54,58,73	1.44	6 (11%)	65,95,113	1.36	8 (12%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
22	LHG	1	317	17	48,48,48	0.68	1 (2%)	51,54,54	1.23	6 (11%)
21	BCR	B	847	-	41,41,41	1.10	2 (4%)	56,56,56	1.45	10 (17%)
17	CLA	3	612	3	49,53,73	1.50	6 (12%)	59,89,113	1.42	5 (8%)

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
21	BCR	A	849	-	-	7/29/63/63	0/2/2/2
17	CLA	B	842	22	-	7/39/115/115	-
17	CLA	B	829	6	-	14/39/115/115	-
17	CLA	F	307	10	-	8/27/103/115	-
17	CLA	B	838	6	-	11/39/115/115	-
17	CLA	3	604	-	-	3/15/91/115	-
21	BCR	K	203	-	-	15/29/63/63	0/2/2/2
17	CLA	K	201	16	-	5/15/91/115	-
25	HTG	F	301	-	-	4/8/28/30	0/1/1/1
17	CLA	B	836	29	-	4/15/91/115	-
17	CLA	A	808	5	-	8/39/115/115	-
25	HTG	4	322	-	-	1/10/30/30	0/1/1/1
17	CLA	B	818	6	-	5/27/103/115	-
17	CLA	A	840	5	-	16/39/115/115	-
17	CLA	A	807	5	-	19/39/115/115	-
17	CLA	1	304	-	-	6/12/88/115	-
17	CLA	B	840	29	-	14/39/115/115	-
17	CLA	A	810	5,17	-	13/39/115/115	-
17	CLA	B	823	-	-	13/39/115/115	-
17	CLA	B	833	6	-	7/33/109/115	-
25	HTG	4	321	-	-	3/10/30/30	0/1/1/1
17	CLA	B	811	6	-	9/39/115/115	-
22	LHG	A	844	-	-	26/53/53/53	-
17	CLA	L	202	15	-	15/39/115/115	-
17	CLA	1	306	29	-	1/17/93/115	-
17	CLA	2	312	2	-	0/13/89/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
17	CLA	B	803	5	-	16/39/115/115	-
20	XAT	3	615	-	-	13/31/93/93	0/4/4/4
17	CLA	A	805	5	-	21/39/115/115	-
18	CHL	2	304	29	-	7/14/90/117	-
20	XAT	1	315	-	-	13/31/93/93	0/4/4/4
21	BCR	F	308	-	-	3/29/63/63	0/2/2/2
17	CLA	2	309	-	-	2/10/86/115	-
17	CLA	B	812	6	-	18/39/115/115	-
17	CLA	A	806	-	-	10/39/115/115	-
17	CLA	A	834	5	-	8/15/91/115	-
17	CLA	4	309	4	-	8/33/109/115	-
18	CHL	4	315	4	-	2/14/90/117	-
21	BCR	B	846	-	-	7/29/63/63	0/2/2/2
17	CLA	A	833	5	-	5/21/97/115	-
22	LHG	A	845	17	-	14/31/31/53	-
21	BCR	3	616	-	-	8/29/63/63	0/2/2/2
17	CLA	A	804	5	-	13/39/115/115	-
17	CLA	1	312	1	-	11/27/103/115	-
17	CLA	3	610	-	-	10/24/100/115	-
17	CLA	B	816	6	-	9/39/115/115	-
17	CLA	A	822	5	-	13/23/99/115	-
17	CLA	1	313	1	-	4/17/93/115	-
24	LMG	4	319	-	-	15/45/65/70	0/1/1/1
17	CLA	1	307	1	-	13/39/115/115	-
17	CLA	A	809	5	-	16/39/115/115	-
17	CLA	A	823	5	-	8/27/103/115	-
17	CLA	A	811	5	-	5/26/102/115	-
17	CLA	3	608	3	-	4/21/97/115	-
17	CLA	3	609	3	-	4/21/97/115	-
17	CLA	4	312	4	-	7/29/105/115	-
17	CLA	B	805	-	-	11/39/115/115	-
17	CLA	B	824	6	-	10/27/103/115	-
24	LMG	F	309	-	-	20/50/70/70	0/1/1/1
17	CLA	2	308	2	-	11/33/109/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
17	CLA	3	605	-	-	5/12/88/115	-
18	CHL	3	601	2	-	3/26/102/117	-
17	CLA	G	103	29	-	4/10/86/115	-
22	LHG	G	102	-	-	26/53/53/53	-
17	CLA	G	105	11	-	5/17/93/115	-
21	BCR	L	206	-	-	4/29/63/63	0/2/2/2
17	CLA	B	806	6	-	2/15/91/115	-
20	XAT	4	317	-	3/3/12/26	11/31/93/93	0/4/4/4
17	CLA	B	817	-	-	10/27/103/115	-
17	CLA	A	835	5	-	9/23/99/115	-
17	CLA	2	319	4	-	3/17/93/115	-
17	CLA	B	822	6	-	6/21/97/115	-
25	HTG	B	851	-	-	7/10/30/30	0/1/1/1
28	SF4	C	102	7	-	-	0/6/5/5
24	LMG	B	852	-	-	21/47/67/70	0/1/1/1
17	CLA	B	831	6	-	12/39/115/115	-
17	CLA	3	603	3	-	3/21/97/115	-
21	BCR	A	848	-	-	7/29/63/63	0/2/2/2
17	CLA	2	311	2	-	16/39/115/115	-
17	CLA	G	104	11	-	4/21/97/115	-
21	BCR	B	848	-	-	3/29/63/63	0/2/2/2
18	CHL	4	301	1	1/1/14/21	17/35/111/117	-
23	LMT	2	318	-	-	11/21/61/61	0/2/2/2
17	CLA	A	836	5	-	14/39/115/115	-
17	CLA	3	611	3	-	11/27/103/115	-
21	BCR	4	318	-	-	7/29/63/63	0/2/2/2
17	CLA	A	818	5	-	16/39/115/115	-
17	CLA	2	302	2	-	2/23/99/115	-
17	CLA	4	308	4	-	3/21/97/115	-
22	LHG	F	302	-	-	30/44/44/53	-
17	CLA	B	827	29	-	11/39/115/115	-
17	CLA	2	303	-	-	17/33/109/115	-
17	CLA	J	101	5	-	8/39/115/115	-
17	CLA	B	804	6	-	6/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
17	CLA	B	837	6	-	11/33/109/115	-
26	DGD	4	323	-	-	27/49/89/95	0/2/2/2
18	CHL	4	307	29	-	2/23/99/117	-
21	BCR	J	104	-	-	2/29/63/63	0/2/2/2
24	LMG	4	320	-	-	20/44/64/70	0/1/1/1
28	SF4	C	101	7	-	-	0/6/5/5
17	CLA	A	838	5	-	15/39/115/115	-
19	LUT	3	614	-	-	12/29/67/67	0/2/2/2
17	CLA	3	613	3	-	2/17/93/115	-
17	CLA	A	837	5	-	15/39/115/115	-
21	BCR	L	201	-	-	11/29/63/63	0/2/2/2
17	CLA	B	820	6	-	14/33/109/115	-
17	CLA	B	821	29	-	5/39/115/115	-
24	LMG	G	101	-	-	15/35/55/70	0/1/1/1
27	PQN	B	843	-	-	3/23/43/43	0/2/2/2
17	CLA	A	802	29	-	6/39/115/115	-
17	CLA	A	853	29	-	16/39/115/115	-
22	LHG	2	317	-	-	19/41/41/53	-
17	CLA	A	824	29	-	11/39/115/115	-
17	CLA	A	821	-	-	8/20/96/115	-
17	CLA	B	826	29	-	16/39/115/115	-
17	CLA	1	303	29	-	10/23/99/115	-
27	PQN	A	842	-	-	6/23/43/43	0/2/2/2
17	CLA	B	813	6,17	-	11/25/101/115	-
28	SF4	A	852	6,5	-	-	0/6/5/5
17	CLA	F	304	6	-	7/39/115/115	-
17	CLA	4	313	4	-	11/15/91/115	-
17	CLA	A	826	5	-	13/39/115/115	-
17	CLA	A	817	5	-	13/39/115/115	-
17	CLA	A	828	5	-	8/39/115/115	-
25	HTG	F	310	-	-	3/7/27/30	0/1/1/1
17	CLA	A	829	5	-	14/39/115/115	-
17	CLA	A	827	5	-	9/39/115/115	-
17	CLA	B	825	6	-	12/33/109/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
17	CLA	B	839	6	-	4/18/94/115	-
18	CHL	2	313	2	-	5/14/90/117	-
17	CLA	J	103	14	-	5/12/88/115	-
21	BCR	1	316	-	-	12/29/63/63	0/2/2/2
17	CLA	B	835	6	-	11/39/115/115	-
21	BCR	2	316	-	-	17/29/63/63	0/2/2/2
21	BCR	B	844	-	-	7/29/63/63	0/2/2/2
17	CLA	1	309	22	-	17/39/115/115	-
18	CHL	1	305	1	-	7/20/96/117	-
17	CLA	3	602	3	-	5/33/109/115	-
25	HTG	A	854	-	-	2/10/30/30	0/1/1/1
21	BCR	A	847	-	-	6/29/63/63	0/2/2/2
17	CLA	4	314	-	-	4/18/94/115	-
17	CLA	A	843	22	-	10/24/100/115	-
17	CLA	A	839	29	-	16/39/115/115	-
21	BCR	G	106	-	-	6/29/63/63	0/2/2/2
17	CLA	3	606	3	-	9/18/94/115	-
17	CLA	4	302	4	-	4/33/109/115	-
17	CLA	A	814	-	-	11/21/97/115	-
19	LUT	4	316	-	-	13/29/67/67	0/2/2/2
25	HTG	F	305	-	-	3/10/30/30	0/1/1/1
17	CLA	A	813	5	-	3/15/91/115	-
17	CLA	A	830	5	-	5/21/97/115	-
25	HTG	J	102	-	-	6/10/30/30	0/1/1/1
17	CLA	A	803	5,17	-	10/27/103/115	-
17	CLA	A	812	5	-	11/39/115/115	-
17	CLA	B	809	6	-	14/39/115/115	-
21	BCR	B	849	-	-	8/29/63/63	0/2/2/2
21	BCR	L	205	-	-	10/29/63/63	0/2/2/2
17	CLA	A	831	5	-	17/39/115/115	-
21	BCR	A	846	-	-	2/29/63/63	0/2/2/2
21	BCR	I	101	-	-	5/29/63/63	0/2/2/2
21	BCR	A	850	-	-	8/29/63/63	0/2/2/2
17	CLA	B	802	-	-	2/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
17	CLA	A	820	29	-	10/39/115/115	-
17	CLA	4	303	4	-	15/33/109/115	-
17	CLA	A	801	5	1/1/15/20	11/39/115/115	-
17	CLA	A	819	5	-	8/15/91/115	-
18	CHL	2	306	29	-	7/23/99/117	-
17	CLA	1	311	1	-	8/33/109/115	-
17	CLA	B	808	6	-	15/39/115/115	-
21	BCR	B	845	-	-	5/29/63/63	0/2/2/2
17	CLA	B	828	6	-	9/39/115/115	-
17	CLA	A	815	29	-	4/15/91/115	-
17	CLA	F	306	29	-	0/15/91/115	-
17	CLA	4	304	29	-	7/21/97/115	-
17	CLA	A	832	5	-	13/39/115/115	-
17	CLA	1	308	1	-	9/33/109/115	-
17	CLA	1	310	1	-	9/24/100/115	-
17	CLA	2	310	2	-	7/24/100/115	-
17	CLA	B	830	-	-	5/39/115/115	-
18	CHL	3	607	29	-	4/19/95/117	-
23	LMT	A	855	-	-	14/21/61/61	0/2/2/2
21	BCR	F	303	-	-	5/29/63/63	0/2/2/2
17	CLA	L	204	-	-	8/21/97/115	-
20	XAT	2	315	-	-	13/31/93/93	0/4/4/4
18	CHL	4	306	29	-	7/23/99/117	-
17	CLA	L	203	15	-	11/39/115/115	-
17	CLA	B	832	6	-	3/21/97/115	-
17	CLA	1	302	1	-	18/39/115/115	-
17	CLA	2	301	2	-	5/39/115/115	-
17	CLA	4	310	-	-	17/33/109/115	-
17	CLA	A	825	29	-	8/39/115/115	-
19	LUT	2	314	-	-	12/29/67/67	0/2/2/2
17	CLA	A	816	-	-	16/39/115/115	-
17	CLA	B	841	6	-	13/39/115/115	-
21	BCR	J	105	-	-	7/29/63/63	0/2/2/2
26	DGD	B	850	-	-	24/55/95/95	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
17	CLA	B	807	6	-	13/39/115/115	-
17	CLA	4	311	4	-	4/24/100/115	-
17	CLA	B	810	6	-	8/39/115/115	-
17	CLA	B	814	6,17	-	7/27/103/115	-
17	CLA	B	834	6	-	13/31/107/115	-
17	CLA	B	819	6	-	7/32/108/115	-
17	CLA	A	841	29	-	13/39/115/115	-
21	BCR	A	851	-	-	7/29/63/63	0/2/2/2
17	CLA	1	301	1	-	9/39/115/115	-
19	LUT	1	314	-	-	12/29/67/67	0/2/2/2
22	LHG	B	801	17	-	10/26/26/53	-
18	CHL	4	305	29	1/1/13/21	12/29/105/117	-
17	CLA	K	202	-	-	16/33/109/115	-
18	CHL	2	305	29	-	2/20/96/117	-
17	CLA	B	815	6	-	17/39/115/115	-
17	CLA	2	307	2	-	1/21/97/115	-
22	LHG	1	317	17	-	23/53/53/53	-
21	BCR	B	847	-	-	3/29/63/63	0/2/2/2
17	CLA	3	612	3	-	5/15/91/115	-

The worst 5 of 1546 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	1	314	LUT	C24-C25	15.75	1.52	1.33
19	2	314	LUT	C24-C25	15.50	1.52	1.33
19	3	614	LUT	C24-C25	15.40	1.52	1.33
19	4	316	LUT	C24-C25	15.00	1.51	1.33
19	3	614	LUT	C14-C13	12.92	1.52	1.35

The worst 5 of 2048 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
27	A	842	PQN	C6-C5-C10	-13.60	104.14	119.26
27	A	842	PQN	C9-C10-C5	-12.36	105.51	119.26
19	4	316	LUT	C31-C30-C29	-11.83	110.43	127.31
19	4	316	LUT	C11-C10-C9	-11.79	110.48	127.31
19	2	314	LUT	C35-C34-C33	-11.70	110.62	127.31

5 of 6 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
17	A	801	CLA	CBD
18	4	301	CHL	C8
18	4	305	CHL	C8
20	4	317	XAT	C26
20	4	317	XAT	C6

5 of 2018 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
17	1	304	CLA	CHA-CBD-CGD-O1D
17	1	307	CLA	CBA-CGA-O2A-C1
17	1	307	CLA	O1A-CGA-O2A-C1
17	1	309	CLA	C1A-C2A-CAA-CBA
17	1	311	CLA	C4B-C3B-CAB-CBB

There are no ring outliers.

190 monomers are involved in 543 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
21	A	849	BCR	3	0
17	B	842	CLA	3	0
17	B	829	CLA	6	0
17	F	307	CLA	2	0
17	B	838	CLA	4	0
21	K	203	BCR	5	0
17	K	201	CLA	3	0
17	B	836	CLA	2	0
17	A	808	CLA	5	0
25	4	322	HTG	2	0
17	B	818	CLA	2	0
17	A	840	CLA	4	0
17	A	807	CLA	2	0
17	1	304	CLA	4	0
17	A	810	CLA	7	0
17	B	823	CLA	4	0
17	B	833	CLA	1	0
25	4	321	HTG	2	0
17	B	811	CLA	5	0
22	A	844	LHG	2	0
17	L	202	CLA	5	0
17	2	312	CLA	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
17	B	803	CLA	6	0
20	3	615	XAT	12	0
17	A	805	CLA	3	0
18	2	304	CHL	2	0
20	1	315	XAT	3	0
21	F	308	BCR	3	0
17	2	309	CLA	1	0
17	B	812	CLA	3	0
17	A	806	CLA	1	0
17	A	834	CLA	2	0
17	4	309	CLA	1	0
18	4	315	CHL	4	0
21	B	846	BCR	3	0
22	A	845	LHG	1	0
21	3	616	BCR	4	0
17	A	804	CLA	6	0
17	1	312	CLA	2	0
17	3	610	CLA	1	0
17	B	816	CLA	3	0
17	A	822	CLA	1	0
17	1	307	CLA	3	0
17	A	809	CLA	3	0
17	A	823	CLA	4	0
17	A	811	CLA	3	0
17	3	608	CLA	3	0
17	3	609	CLA	2	0
17	B	805	CLA	3	0
17	B	824	CLA	2	0
24	F	309	LMG	1	0
17	2	308	CLA	5	0
17	3	605	CLA	1	0
18	3	601	CHL	18	0
17	G	103	CLA	1	0
22	G	102	LHG	2	0
17	G	105	CLA	1	0
21	L	206	BCR	4	0
17	B	806	CLA	2	0
20	4	317	XAT	9	0
17	B	817	CLA	1	0
17	A	835	CLA	3	0
17	B	822	CLA	2	0
25	B	851	HTG	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
24	B	852	LMG	4	0
17	B	831	CLA	2	0
17	3	603	CLA	2	0
21	A	848	BCR	3	0
17	2	311	CLA	4	0
17	G	104	CLA	3	0
21	B	848	BCR	4	0
18	4	301	CHL	11	0
23	2	318	LMT	3	0
17	A	836	CLA	3	0
21	4	318	BCR	14	0
17	A	818	CLA	3	0
17	4	308	CLA	1	0
22	F	302	LHG	2	0
17	B	827	CLA	9	0
17	2	303	CLA	1	0
17	J	101	CLA	5	0
17	B	804	CLA	2	0
17	B	837	CLA	7	0
26	4	323	DGD	29	0
18	4	307	CHL	4	0
21	J	104	BCR	2	0
24	4	320	LMG	7	0
17	A	838	CLA	4	0
19	3	614	LUT	4	0
17	3	613	CLA	2	0
17	A	837	CLA	6	0
21	L	201	BCR	2	0
17	B	820	CLA	2	0
17	B	821	CLA	2	0
24	G	101	LMG	3	0
27	B	843	PQN	3	0
17	A	853	CLA	7	0
22	2	317	LHG	6	0
17	A	824	CLA	1	0
17	A	821	CLA	1	0
17	B	826	CLA	7	0
17	1	303	CLA	2	0
27	A	842	PQN	6	0
17	F	304	CLA	2	0
17	A	826	CLA	1	0
17	A	817	CLA	5	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
17	A	828	CLA	3	0
25	F	310	HTG	1	0
17	A	829	CLA	2	0
17	A	827	CLA	1	0
17	B	825	CLA	3	0
17	B	839	CLA	2	0
18	2	313	CHL	5	0
17	B	835	CLA	3	0
21	2	316	BCR	9	0
21	B	844	BCR	4	0
17	1	309	CLA	5	0
18	1	305	CHL	4	0
17	3	602	CLA	6	0
21	A	847	BCR	1	0
17	4	314	CLA	2	0
17	A	843	CLA	6	0
17	A	839	CLA	3	0
21	G	106	BCR	2	0
17	4	302	CLA	6	0
17	A	814	CLA	4	0
19	4	316	LUT	3	0
25	F	305	HTG	1	0
17	A	813	CLA	1	0
25	J	102	HTG	3	0
17	A	803	CLA	7	0
17	A	812	CLA	2	0
17	B	809	CLA	6	0
21	B	849	BCR	3	0
21	L	205	BCR	4	0
17	A	831	CLA	2	0
21	A	846	BCR	10	0
21	I	101	BCR	4	0
21	A	850	BCR	3	0
17	B	802	CLA	3	0
17	A	820	CLA	6	0
17	4	303	CLA	4	0
17	A	801	CLA	1	0
17	A	819	CLA	4	0
18	2	306	CHL	6	0
17	1	311	CLA	6	0
17	B	808	CLA	1	0
21	B	845	BCR	4	0

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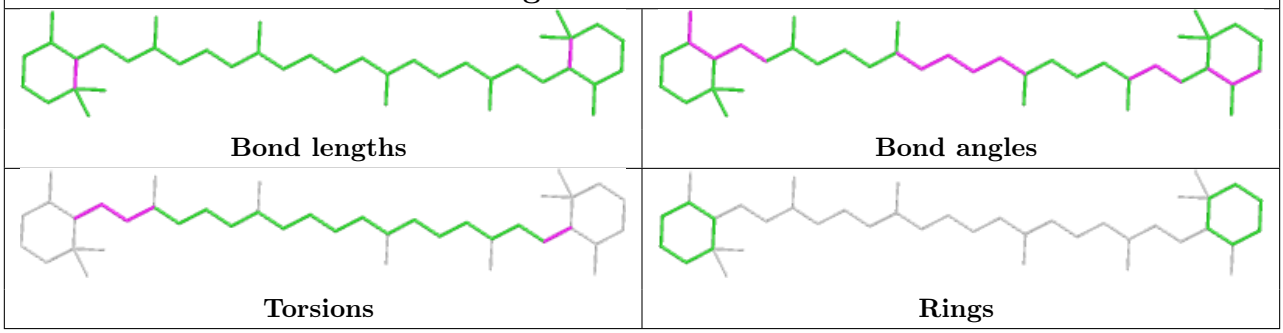
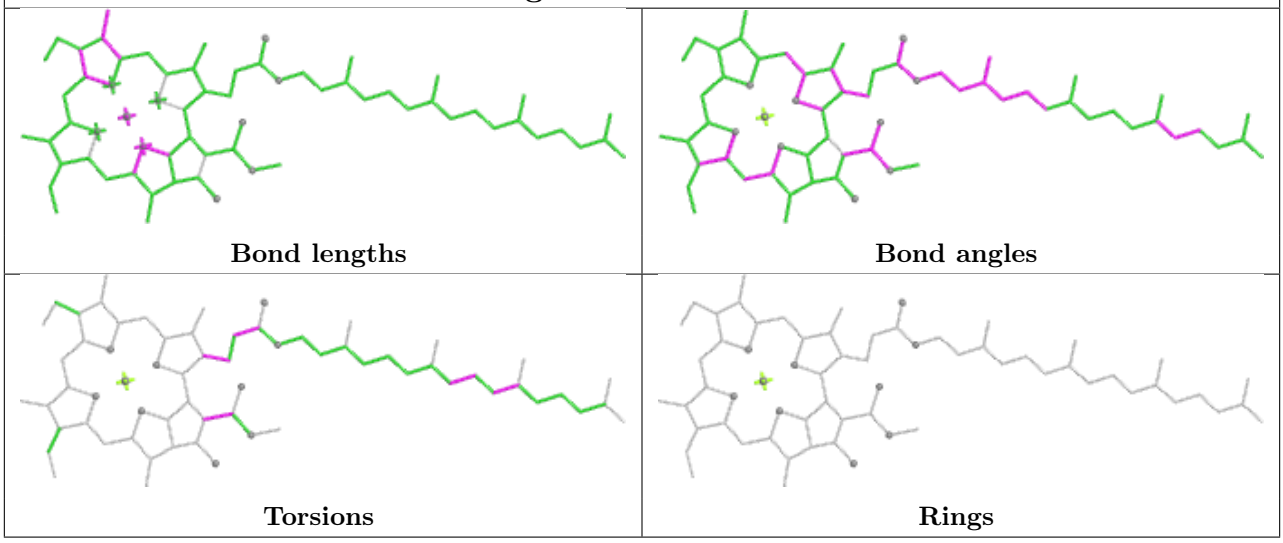
Mol	Chain	Res	Type	Clashes	Symm-Clashes
17	B	828	CLA	2	0
17	A	815	CLA	1	0
17	F	306	CLA	4	0
17	4	304	CLA	5	0
17	A	832	CLA	2	0
17	1	308	CLA	6	0
17	1	310	CLA	3	0
17	2	310	CLA	1	0
17	B	830	CLA	2	0
18	3	607	CHL	2	0
23	A	855	LMT	2	0
17	L	204	CLA	2	0
20	2	315	XAT	9	0
18	4	306	CHL	7	0
17	L	203	CLA	5	0
17	B	832	CLA	3	0
17	1	302	CLA	2	0
17	2	301	CLA	4	0
17	4	310	CLA	1	0
17	A	825	CLA	4	0
19	2	314	LUT	4	0
17	A	816	CLA	4	0
17	B	841	CLA	1	0
21	J	105	BCR	5	0
26	B	850	DGD	7	0
17	B	807	CLA	3	0
17	4	311	CLA	2	0
17	B	810	CLA	6	0
17	B	834	CLA	2	0
17	B	819	CLA	6	0
17	A	841	CLA	4	0
21	A	851	BCR	5	0
17	1	301	CLA	1	0
19	1	314	LUT	7	0
22	B	801	LHG	1	0
17	K	202	CLA	2	0
18	2	305	CHL	2	0
18	4	305	CHL	5	0
17	B	815	CLA	2	0
17	2	307	CLA	1	0
22	1	317	LHG	6	0
21	B	847	BCR	8	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.

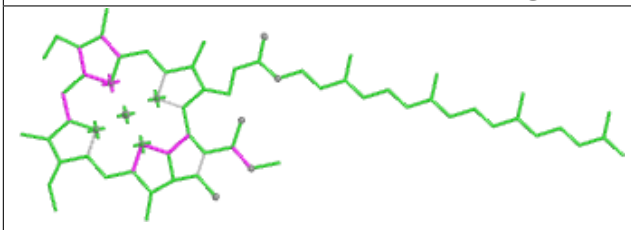
Ligand BCR A 849



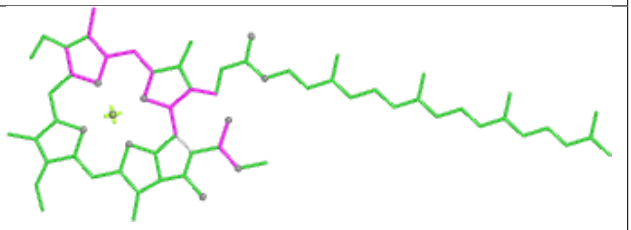
Ligand CLA B 842



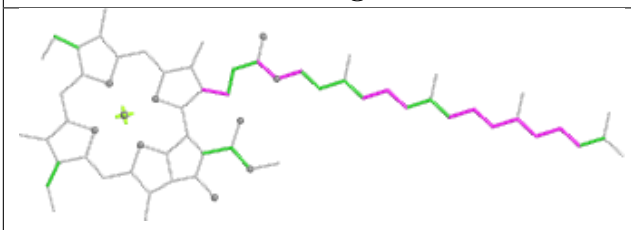
Ligand CLA B 829



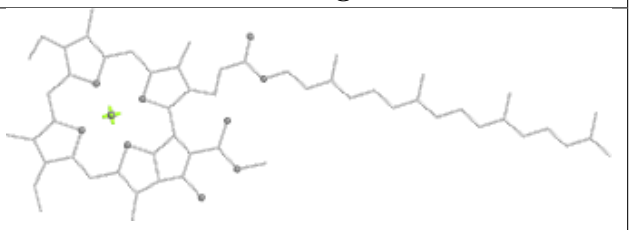
Bond lengths



Bond angles

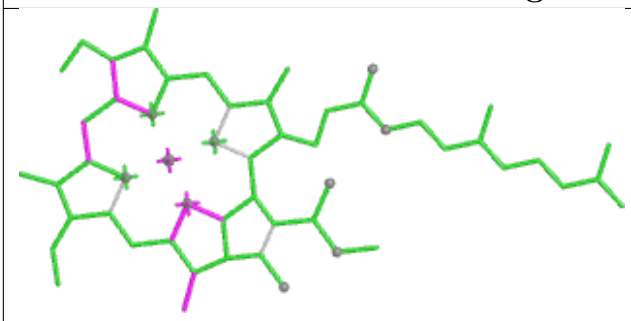


Torsions

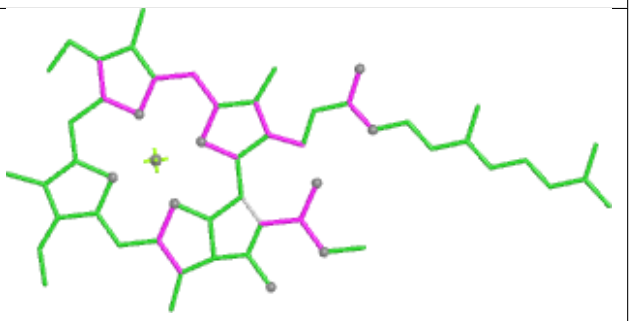


Rings

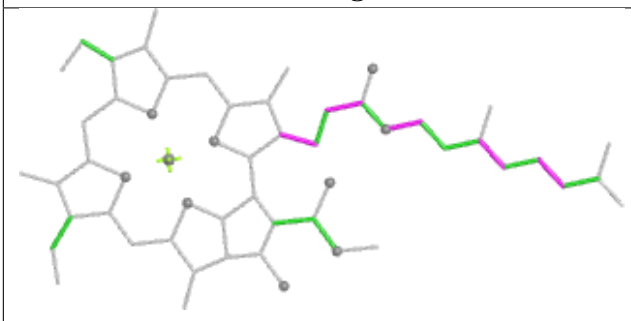
Ligand CLA F 307



Bond lengths



Bond angles



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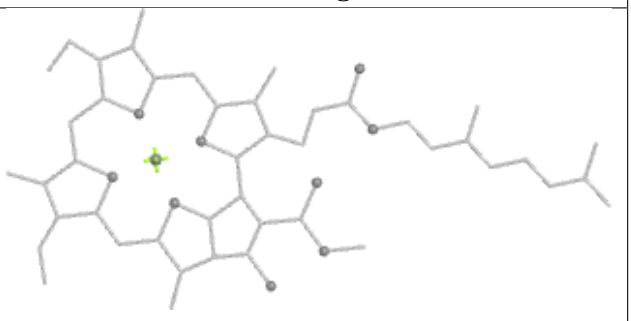
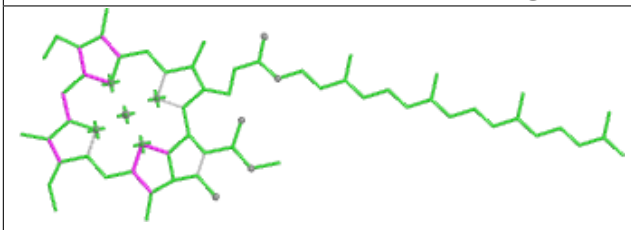


Rings

Ligand CLA B 838



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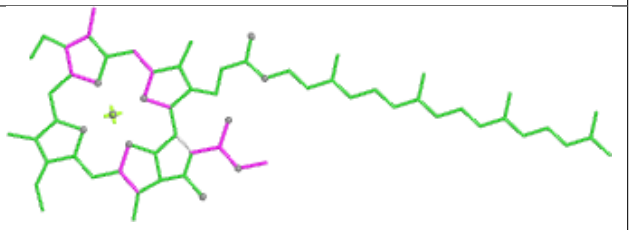
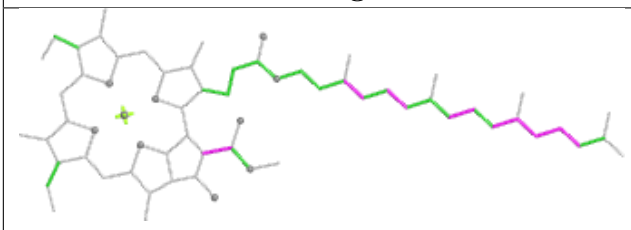
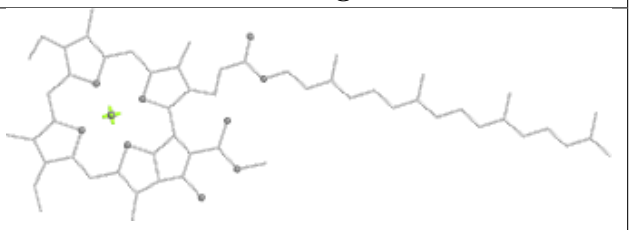


Bond angles

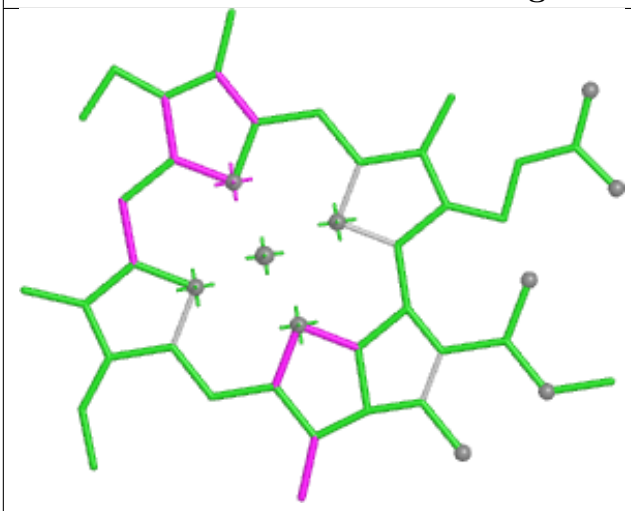


Torsions

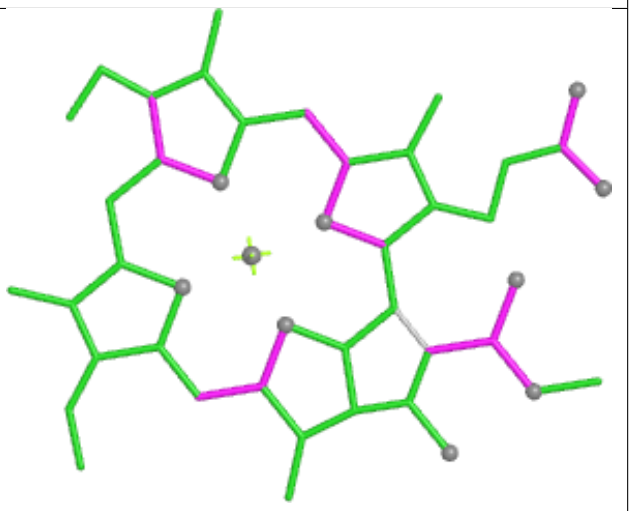


Rings

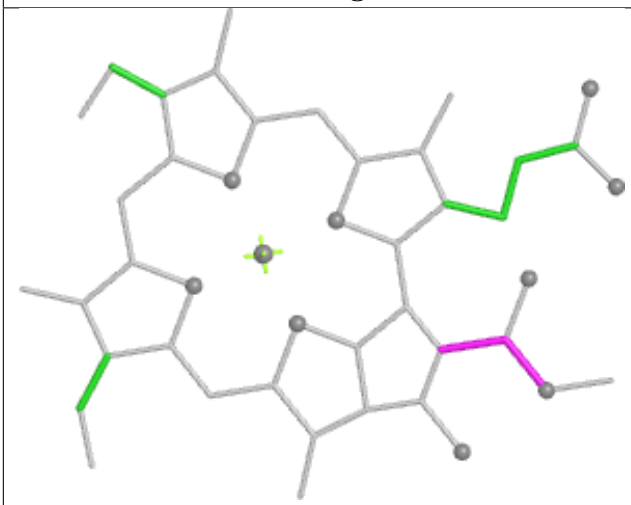
Ligand CLA 3 604



Bond lengths



Bond angles



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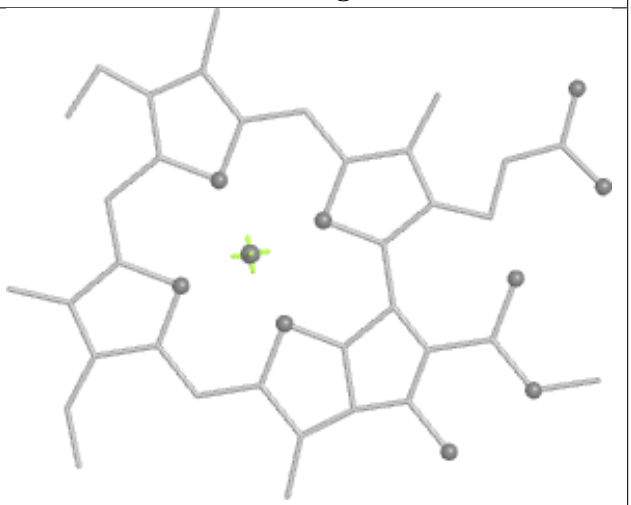
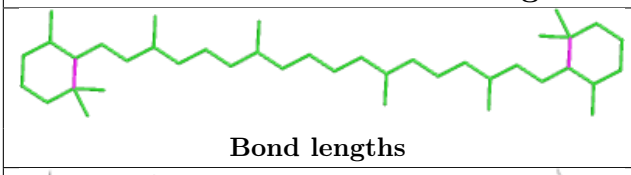


Rings

Ligand BCR K 203



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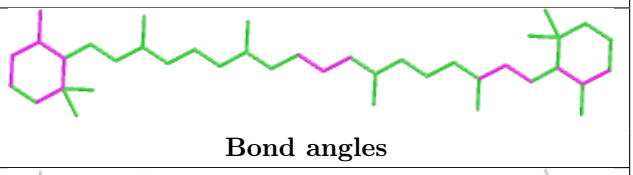

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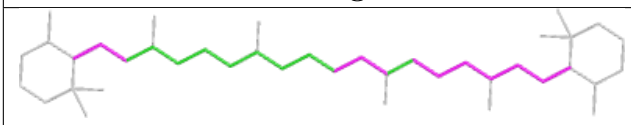

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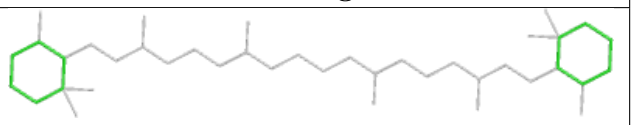
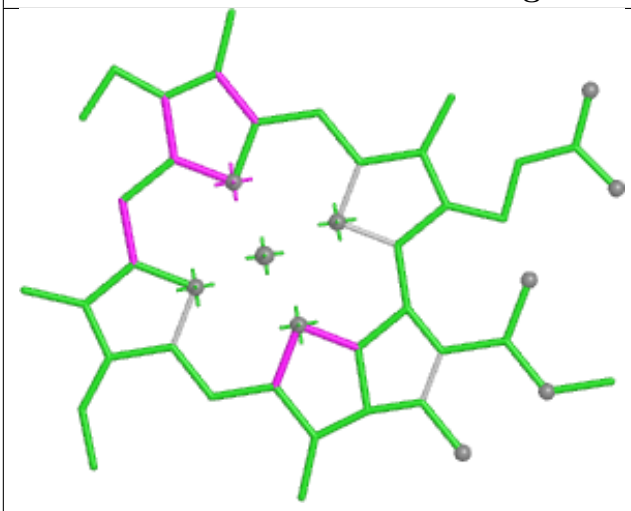


Rings

Ligand CLA K 201



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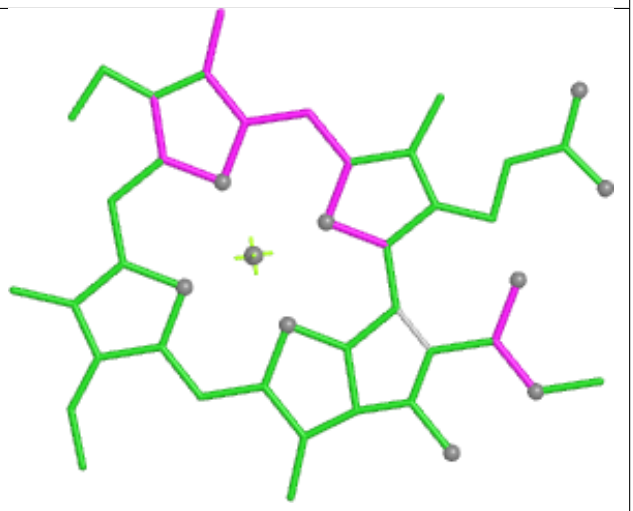

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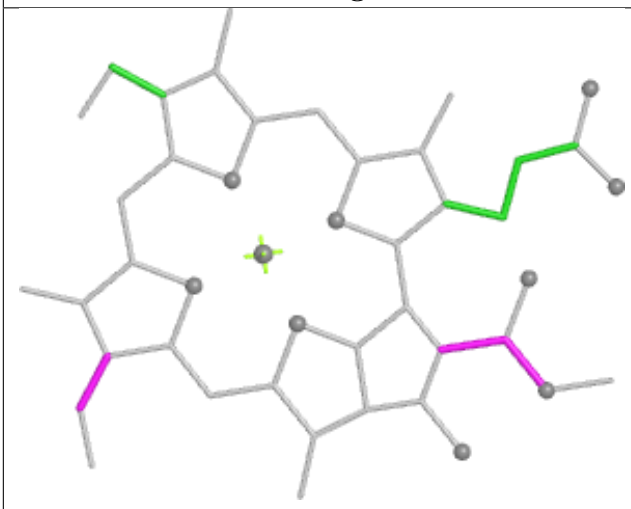

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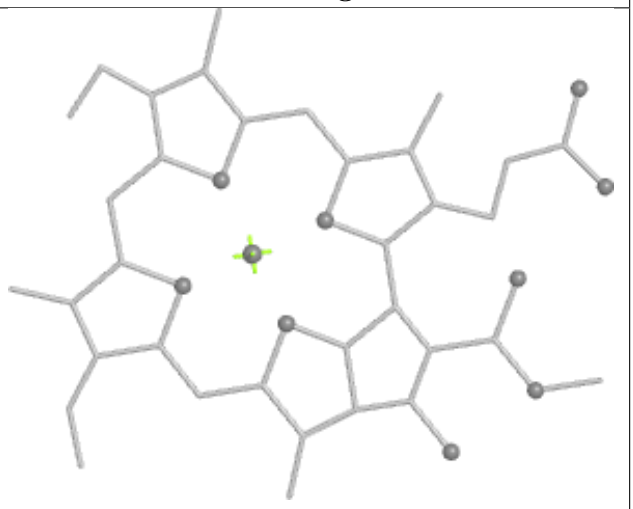
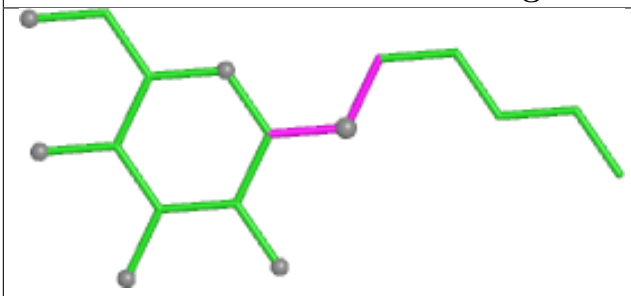


Rings

Ligand HTG F 301



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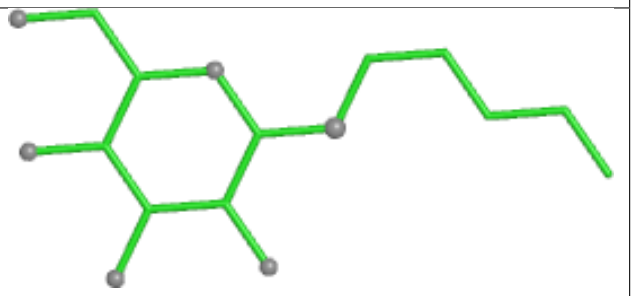

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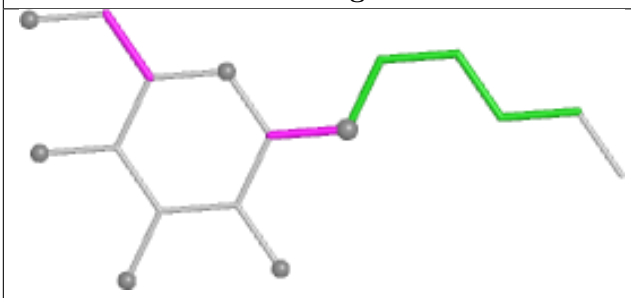

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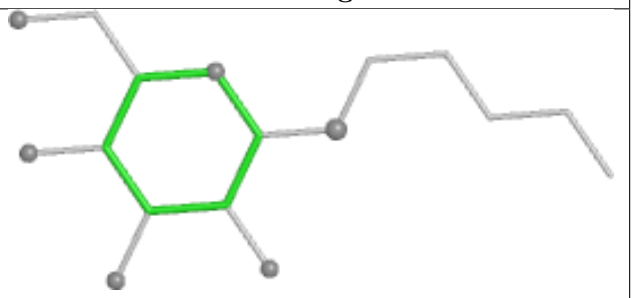
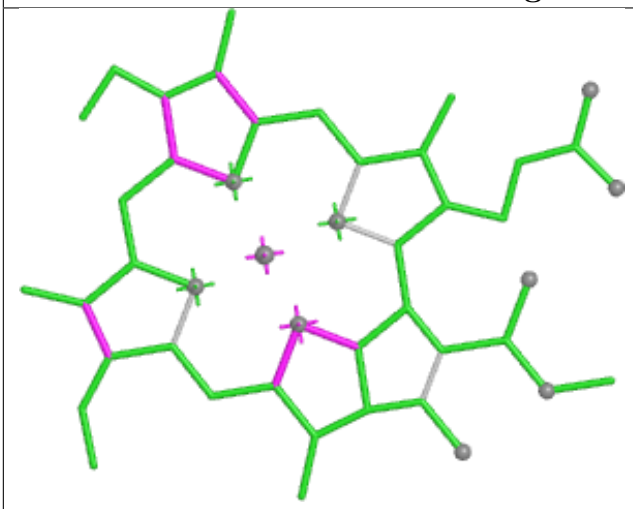


Rings

Ligand CLA B 836



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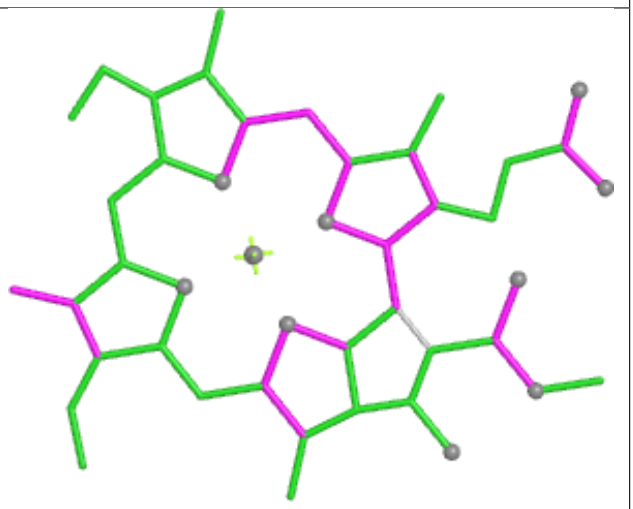

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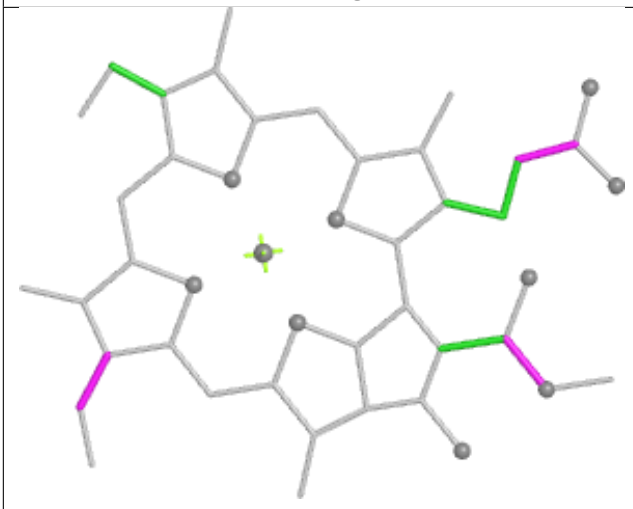
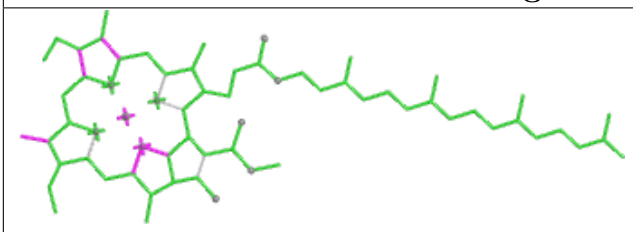


Torsions



Rings

Ligand CLA A 808



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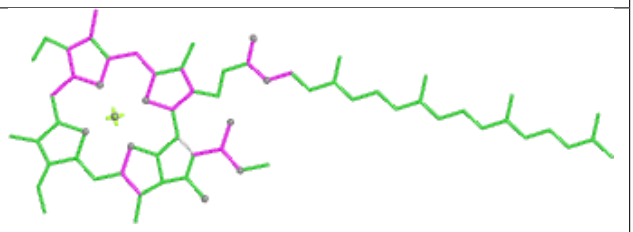

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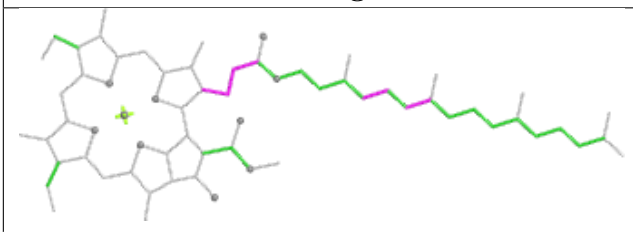

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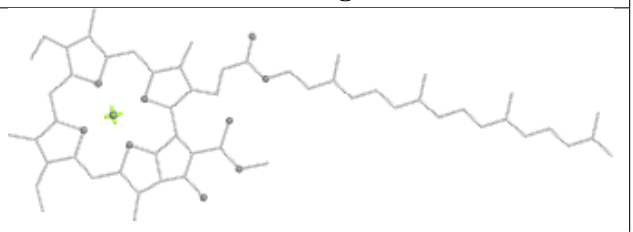
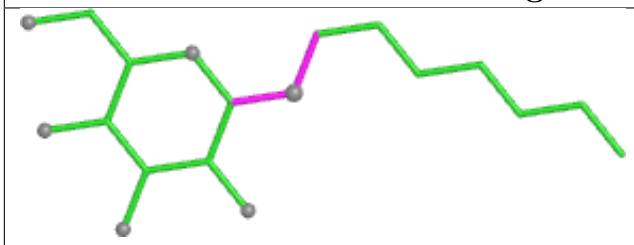


Rings

Ligand HTG 4 322



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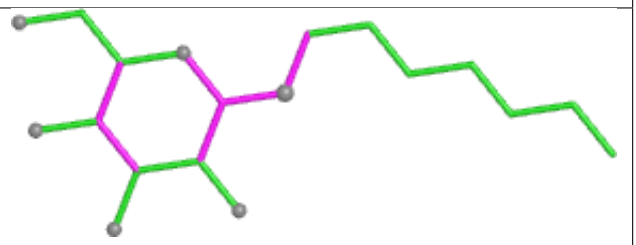

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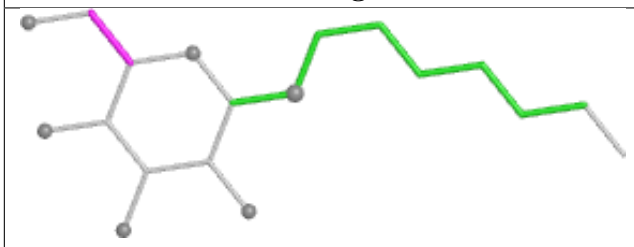

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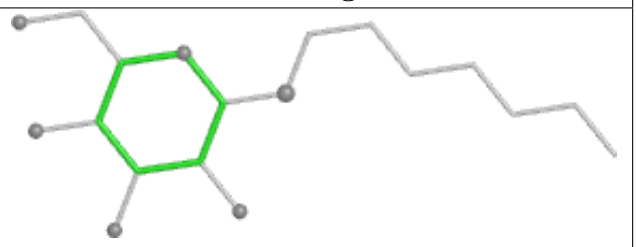
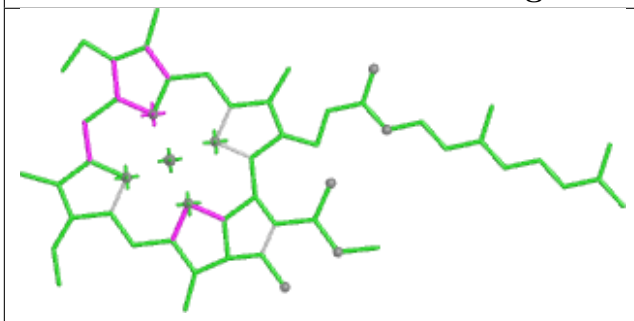


Rings

Ligand CLA B 818



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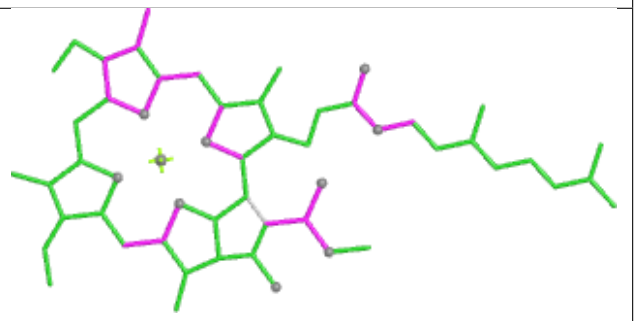

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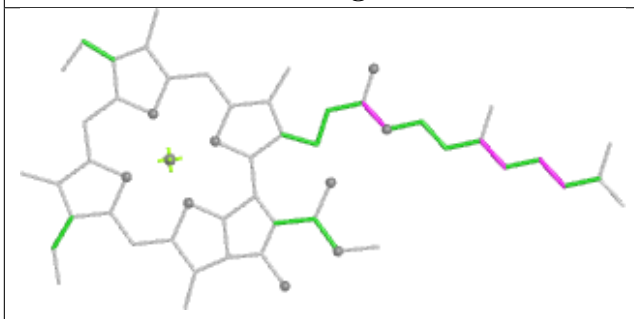

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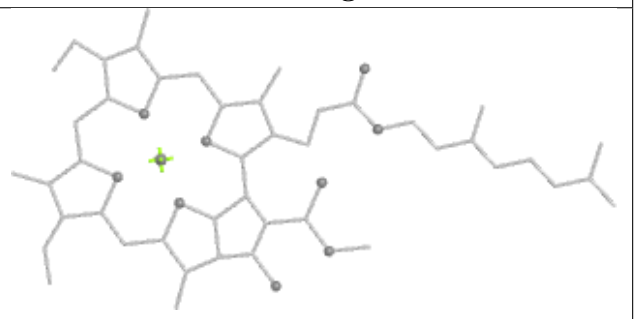
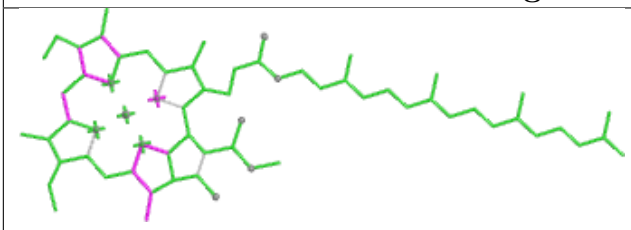
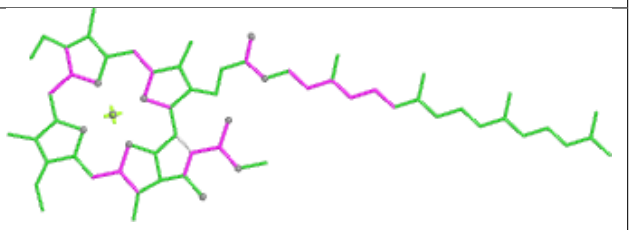
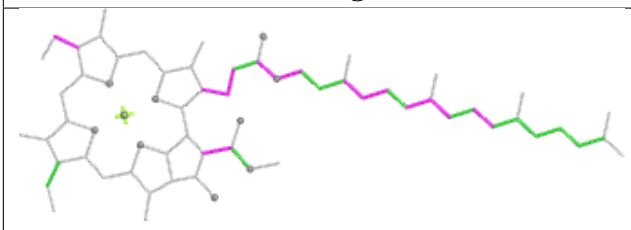
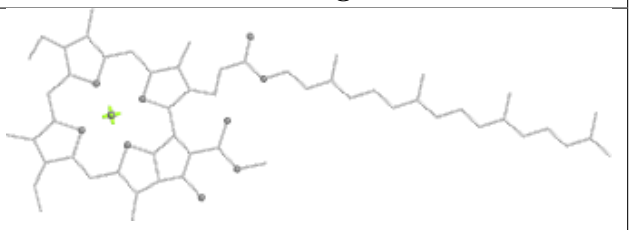


Rings

Ligand CLA A 840	
	
Bond lengths	Bond angles
	
Torsions	Rings

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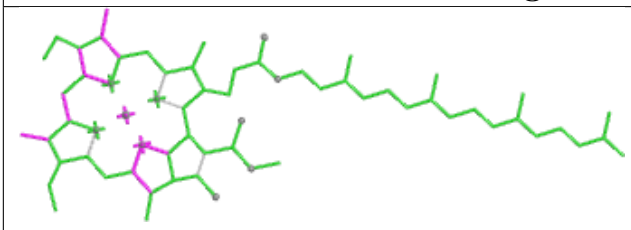
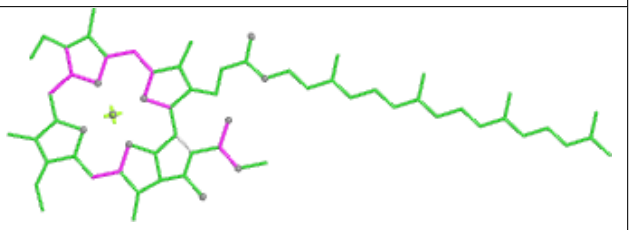
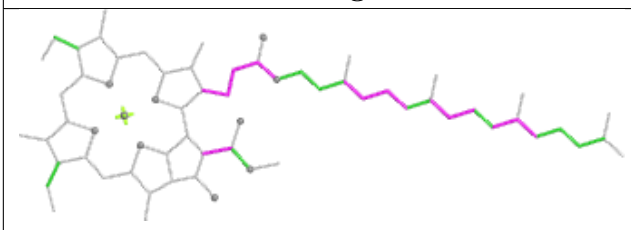
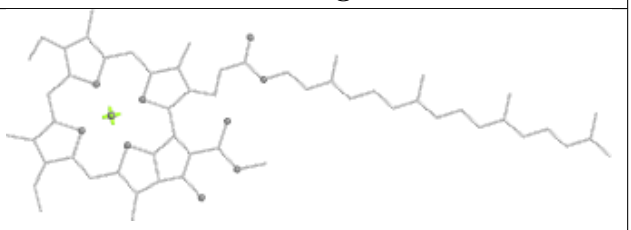
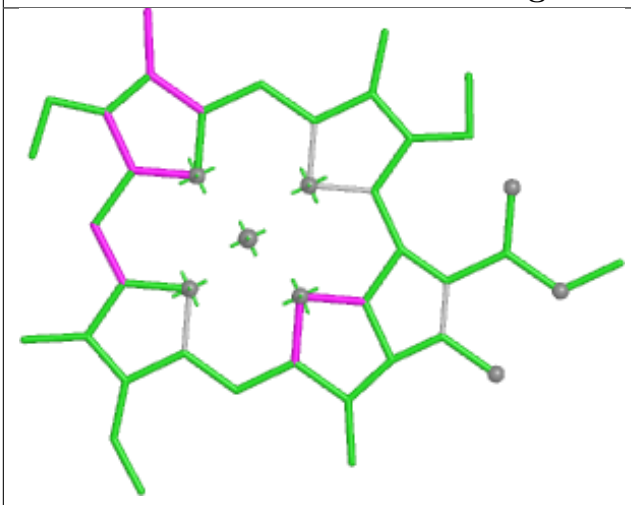
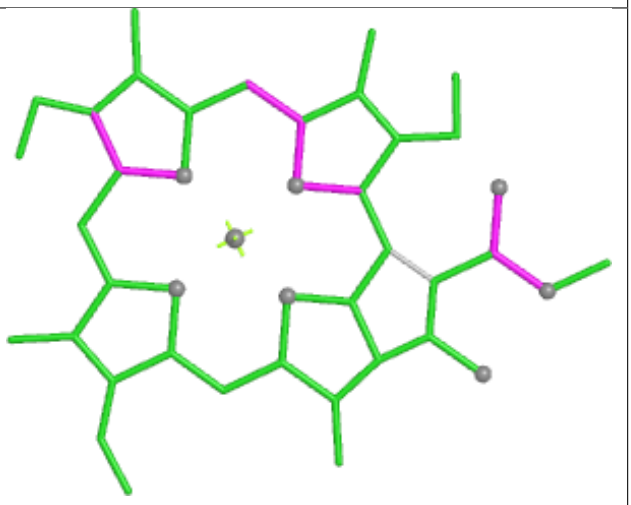
	
Bond lengths	Bond angles
	
Torsions	Rings

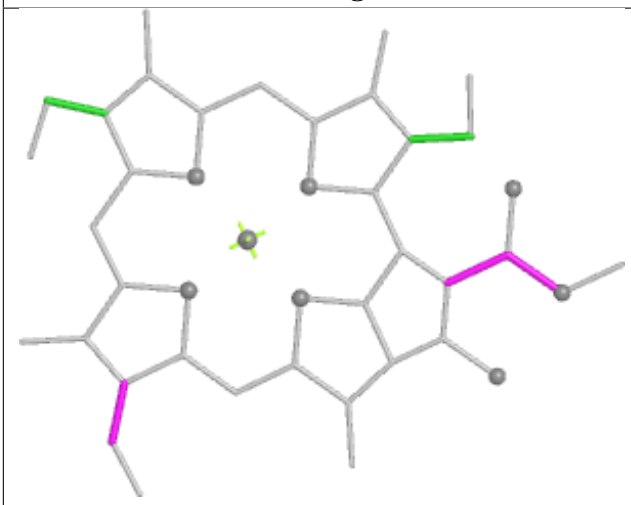
Ligand CLA 1 304



Bond lengths



Bond angles

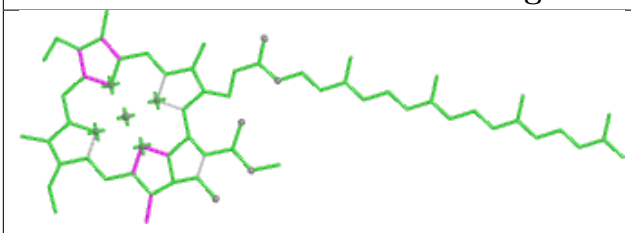


Torsions

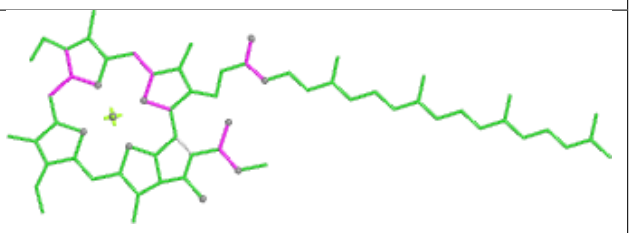


Rings

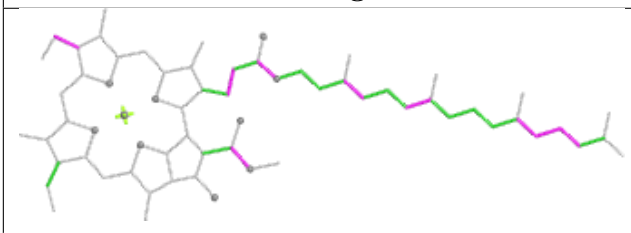
Ligand CLA B 840



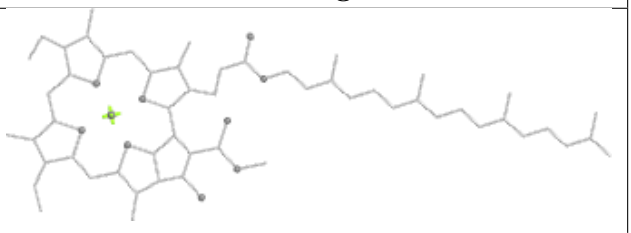
Bond lengths



Bond angles

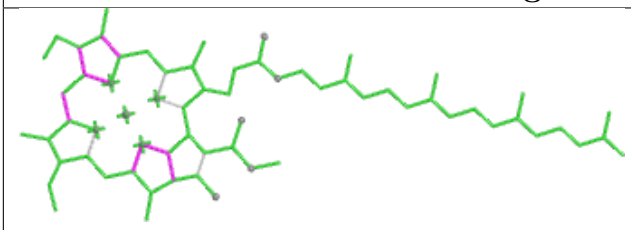


Torsions

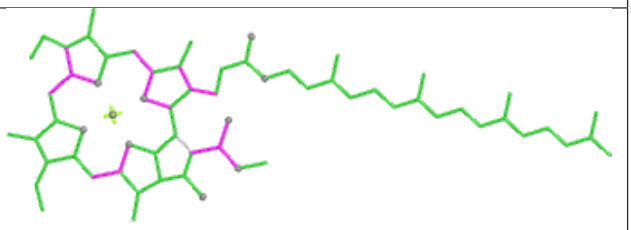


Rings

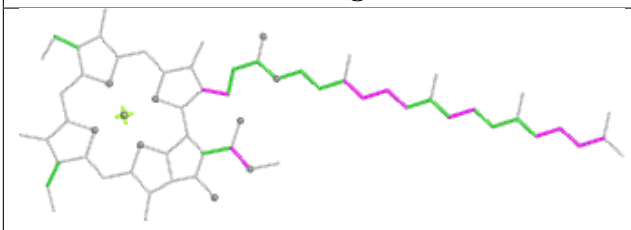
Ligand CLA A 810



Bond lengths



Bond angles



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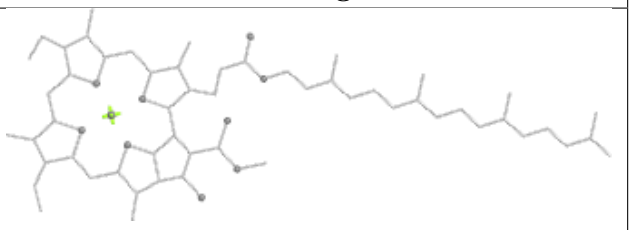
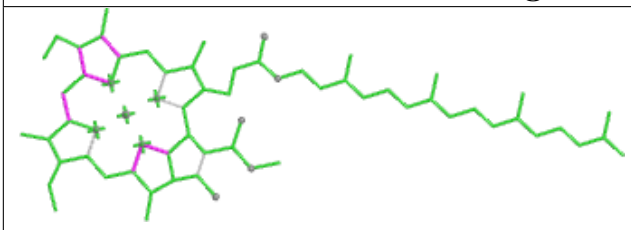
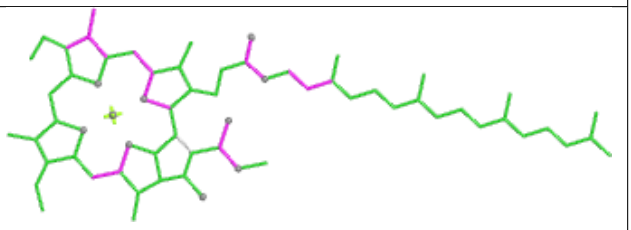


Rings

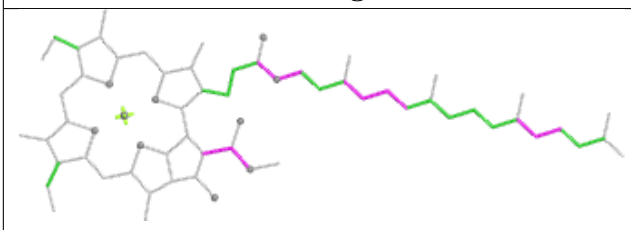
Ligand CLA B 823



Bond lengths



Bond angles



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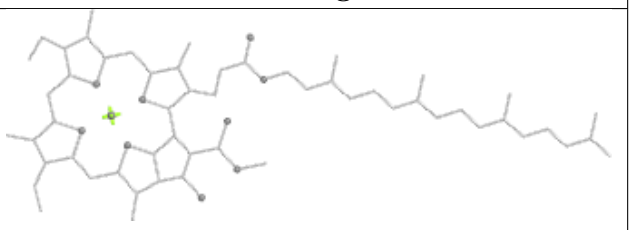
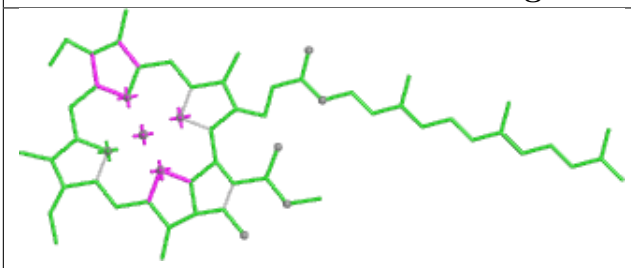
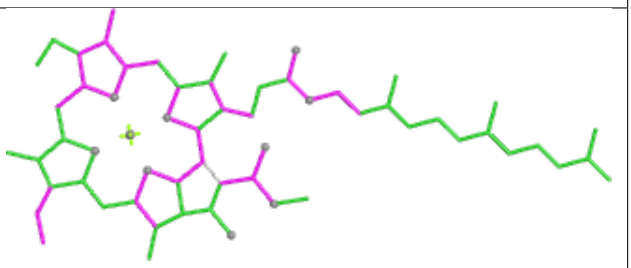
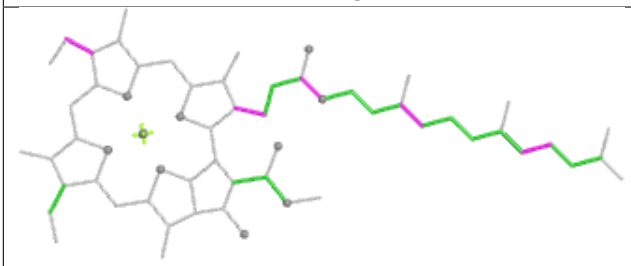
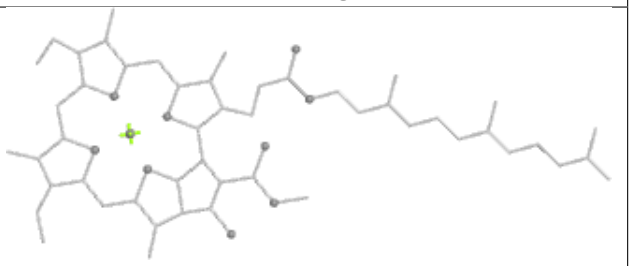
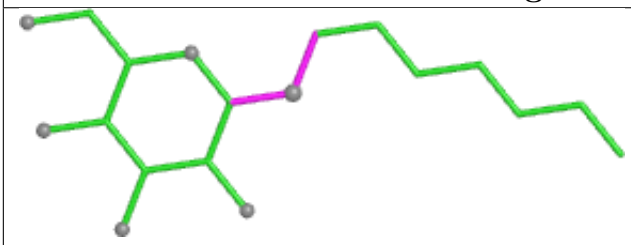
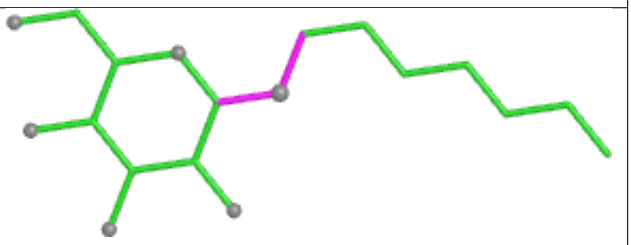
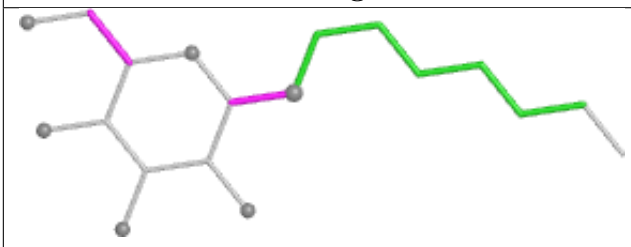
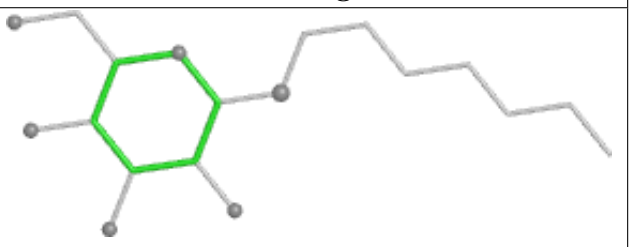
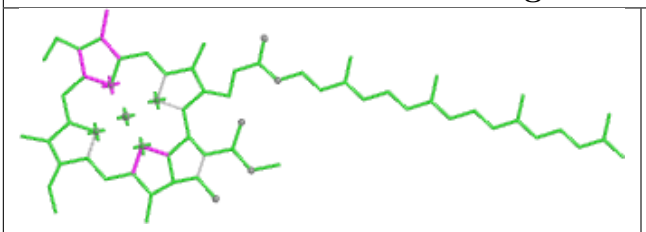


Rings

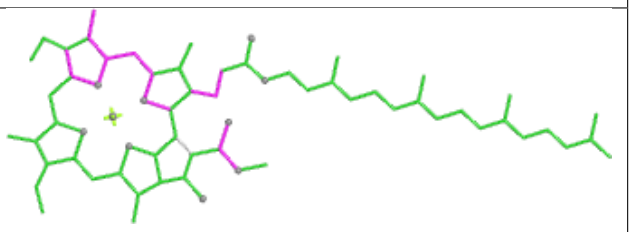
Ligand CLA B 833	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand HTG 4 321	
	
Bond lengths	Bond angles
	
Torsions	Rings

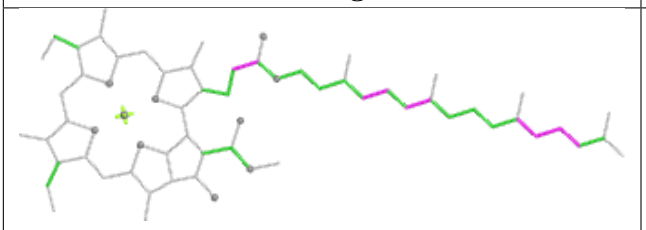
Ligand CLA B 811



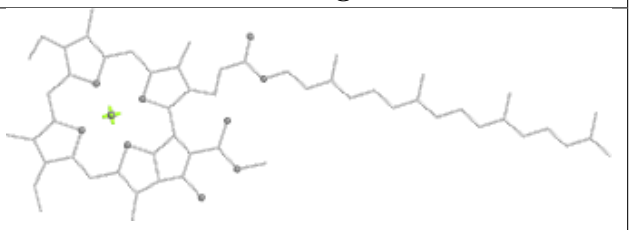
Bond lengths



Bond angles

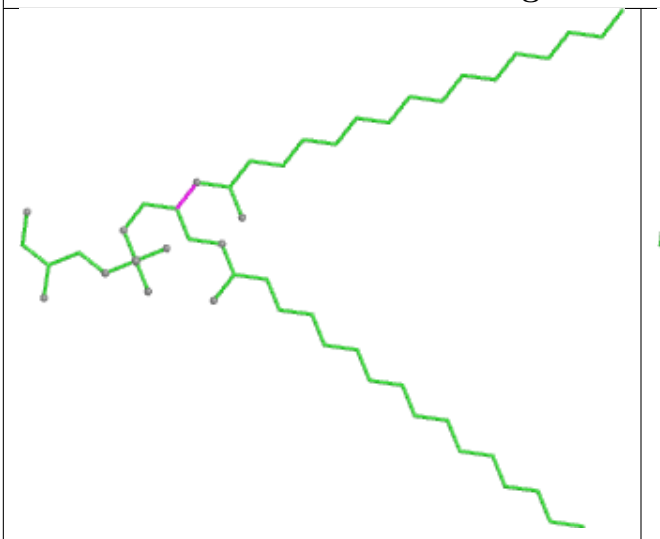


Torsions



Rings

Ligand LHG A 844



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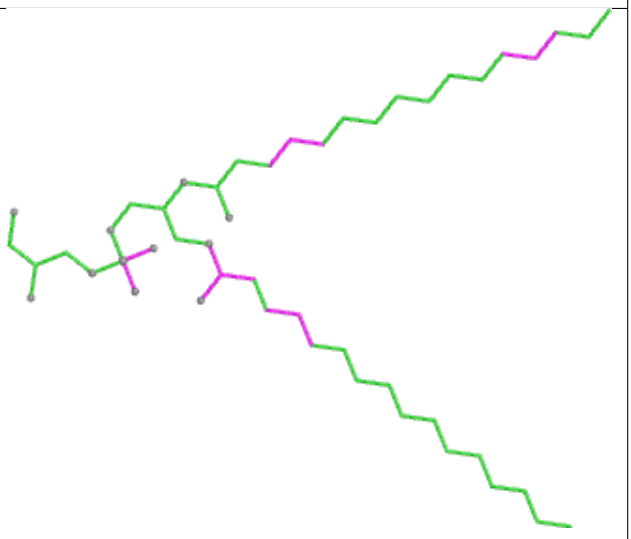
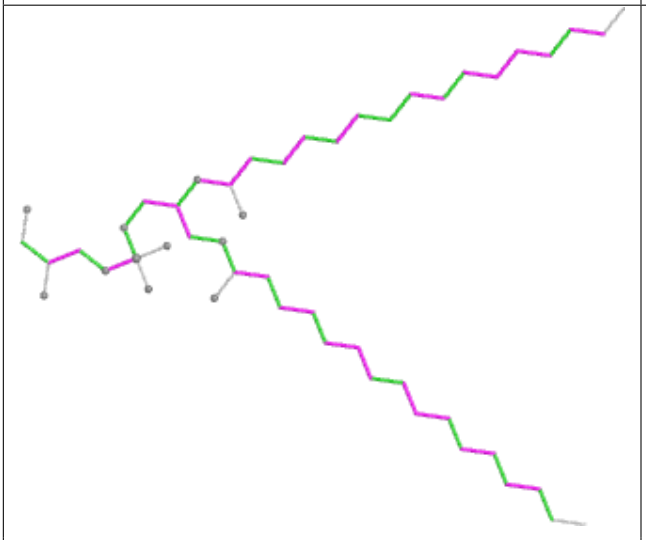


Bond angles



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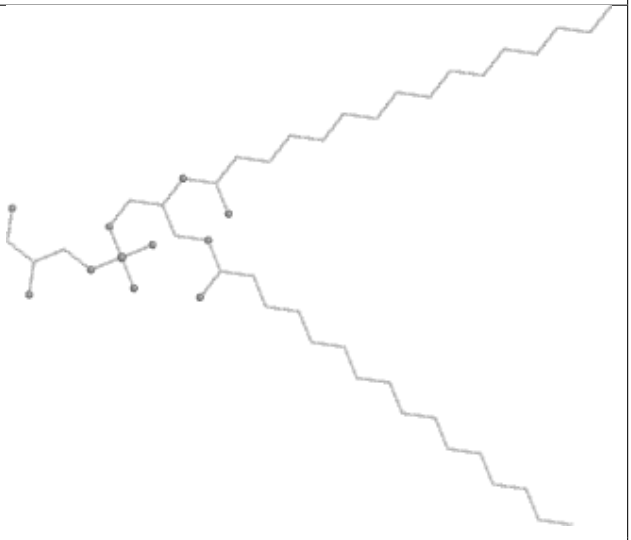
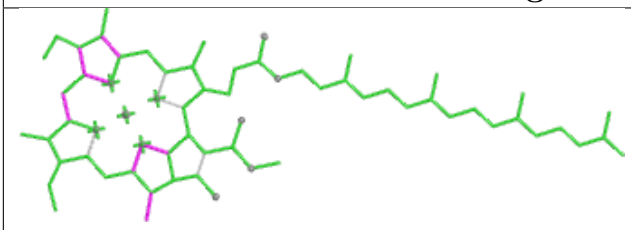


Rings

Ligand CLA L 202



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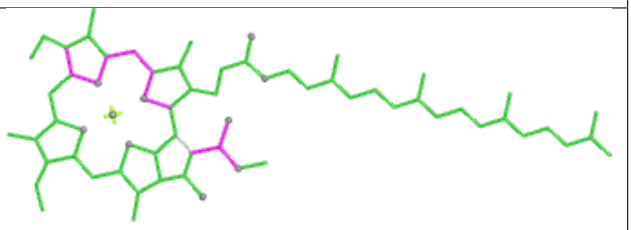
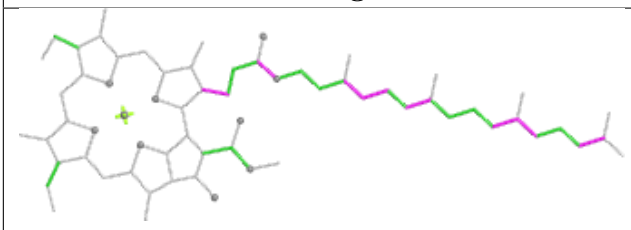


Bond angles



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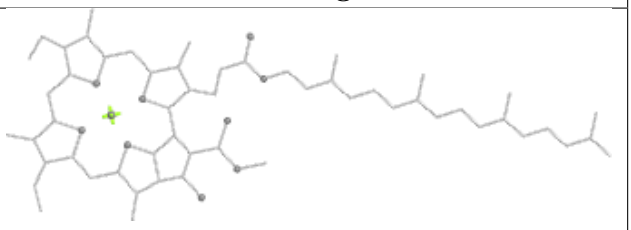
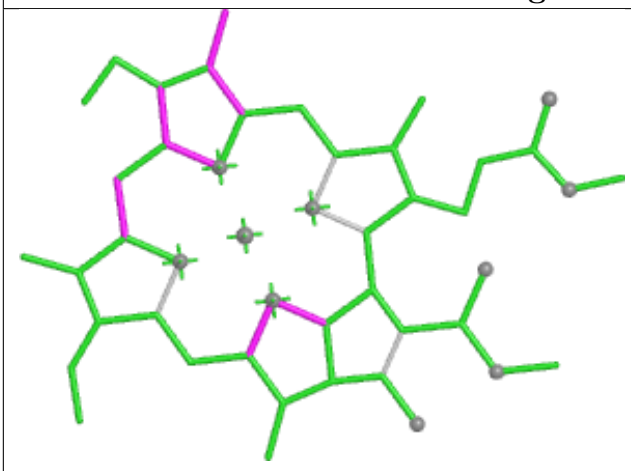


Rings

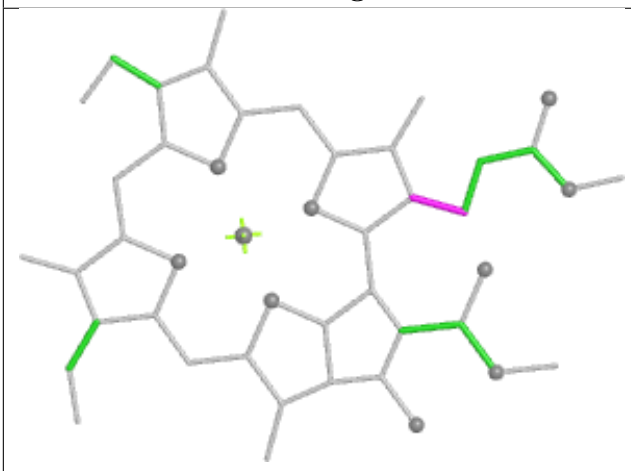
Ligand CLA 1 306



Bond lengths



Bond angles

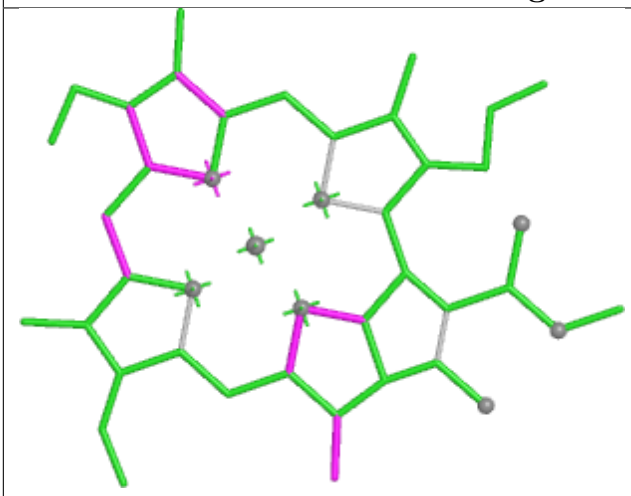


Torsions



Rings

Ligand CLA 2 312



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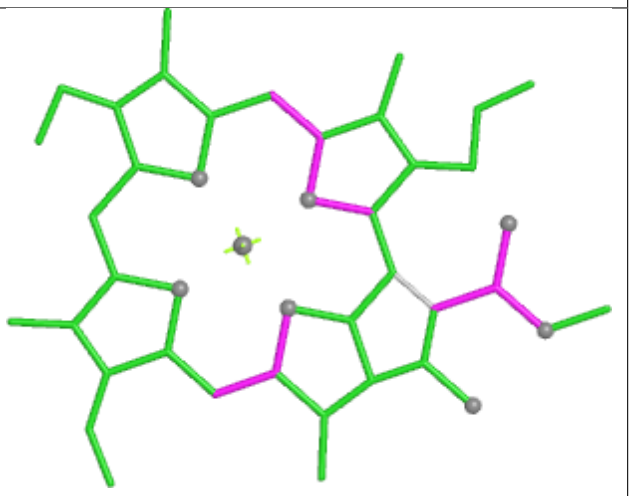
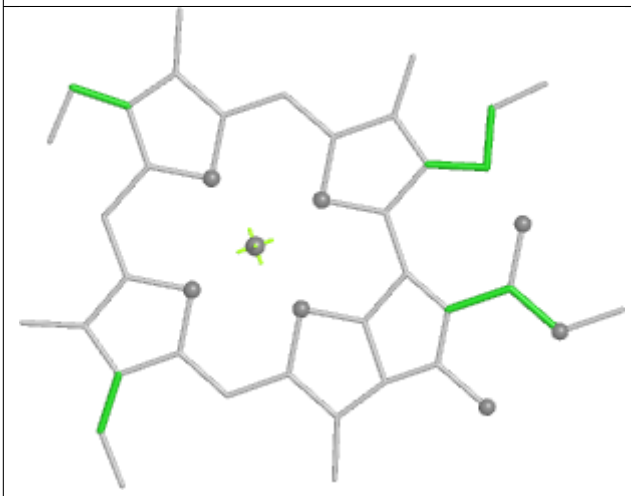


Bond angles



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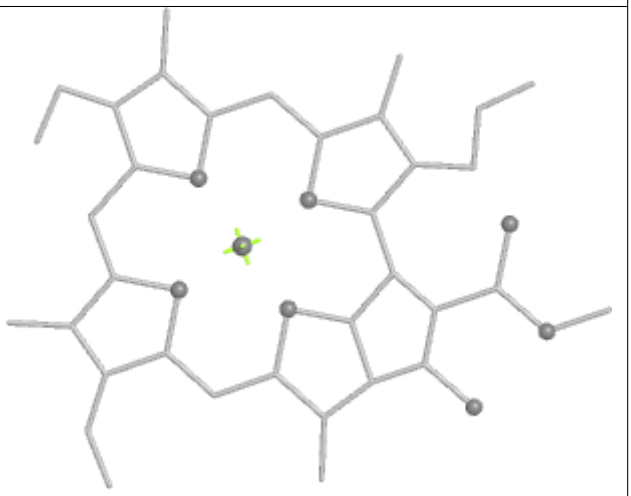
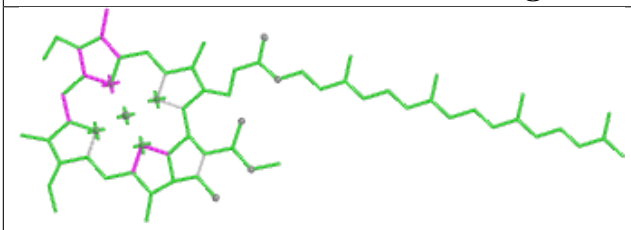


Rings

Ligand CLA B 803



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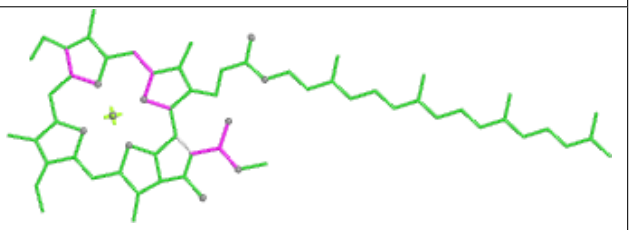
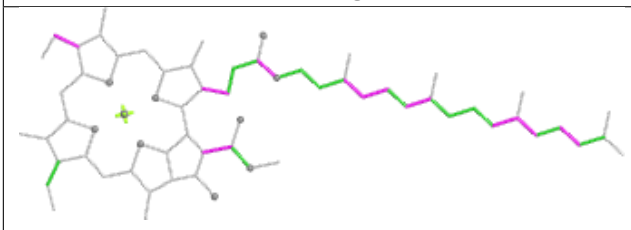


Bond angles



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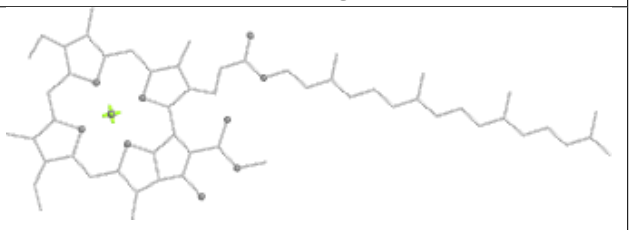
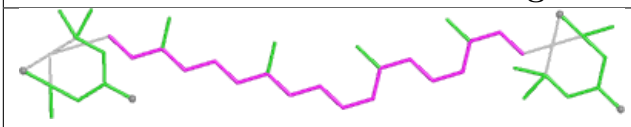
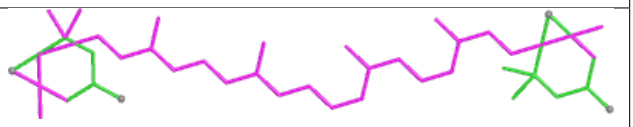
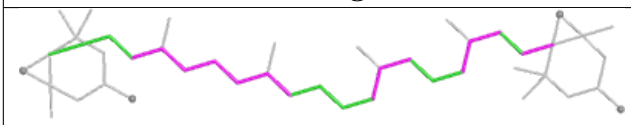
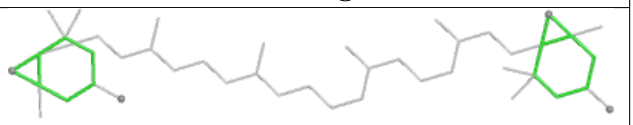
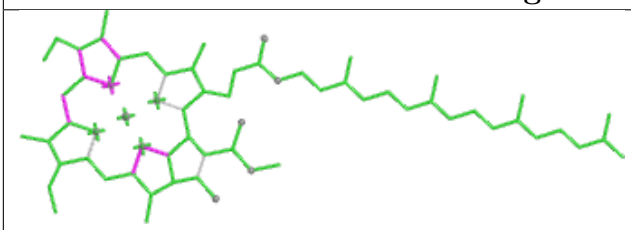
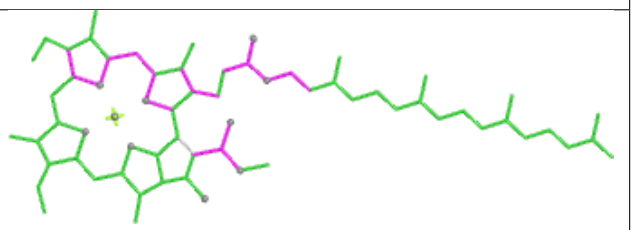
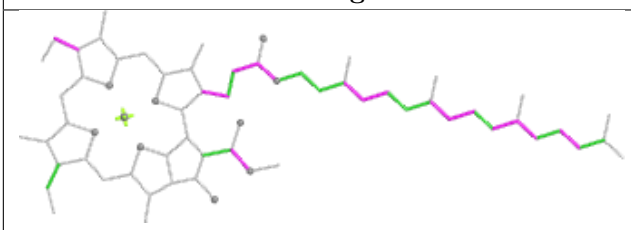
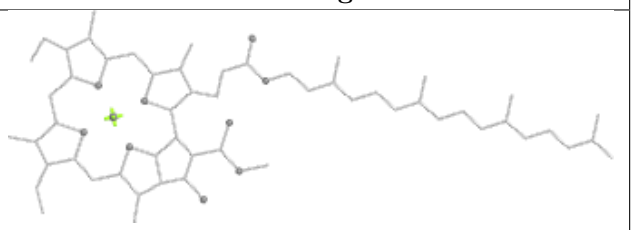
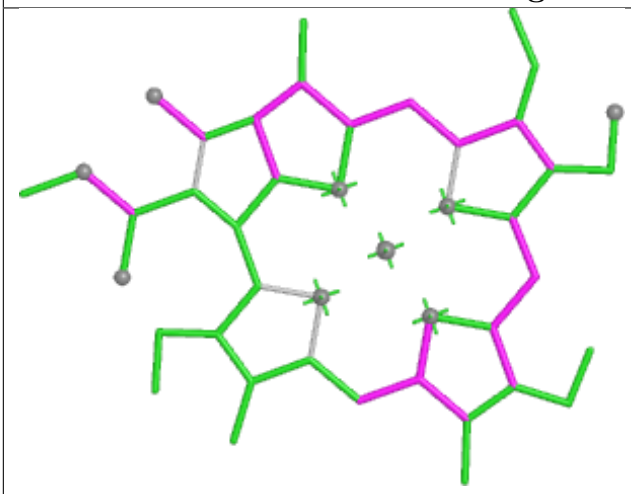


Rings

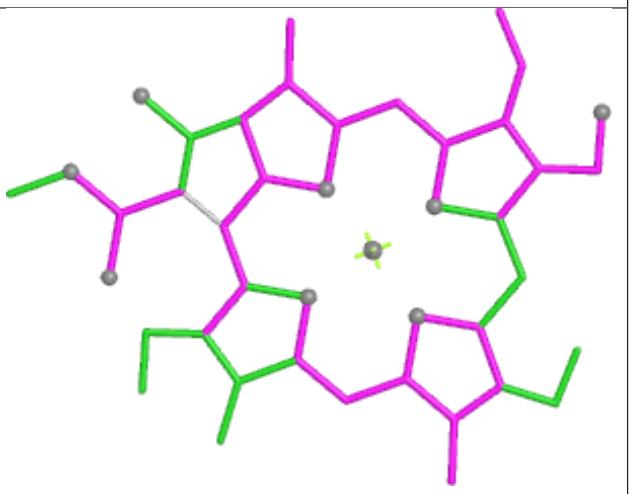
Ligand XAT 3 615	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA A 805	
 Bond lengths	 Bond angles
 Torsions	 Rings

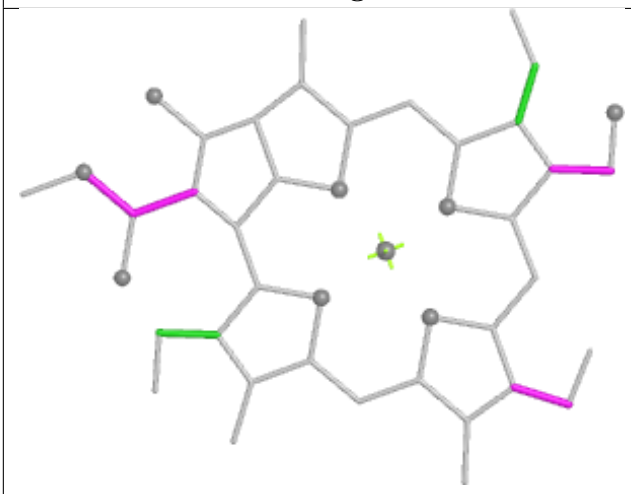
Ligand CHL 2 304



Bond lengths



Bond angles

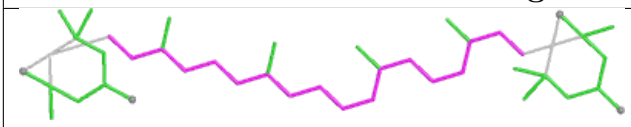


Torsions



Rings

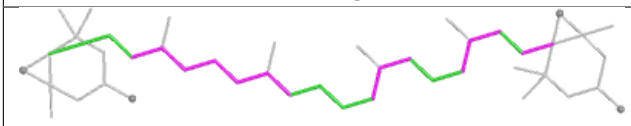
Ligand XAT 1 315



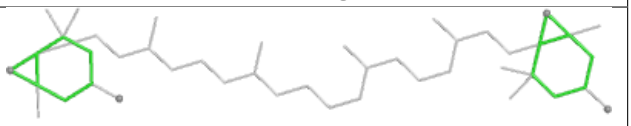
Bond lengths



Bond angles

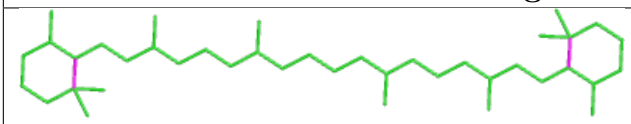


Torsions

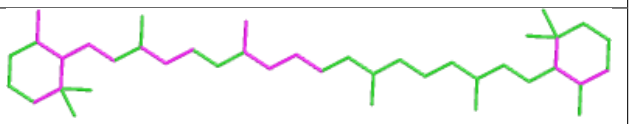


Rings

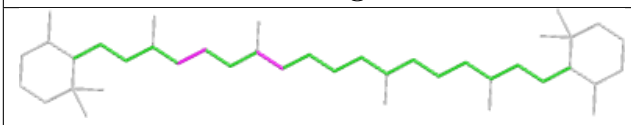
Ligand BCR F 308



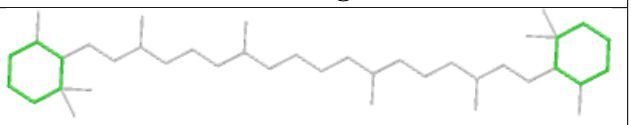
Bond lengths



Bond angles

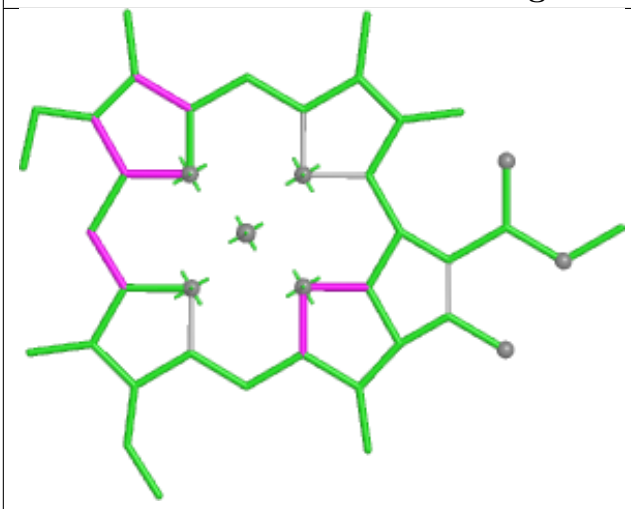


Torsions



Rings

Ligand CLA 2 309



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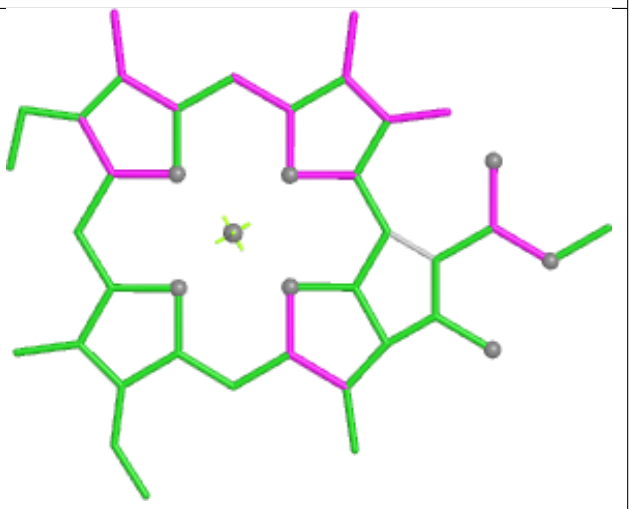

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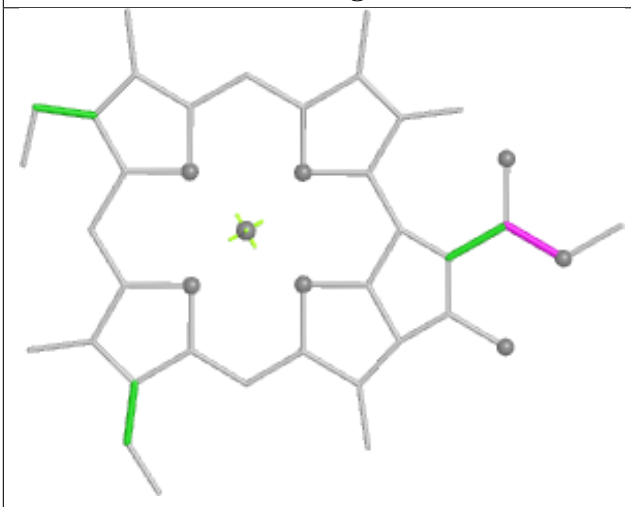

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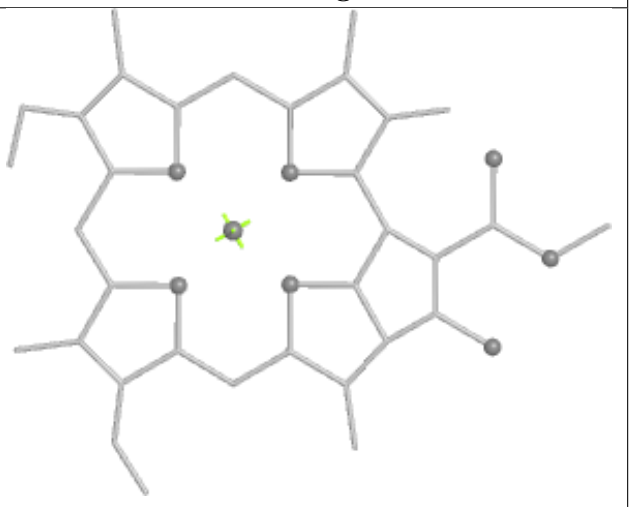
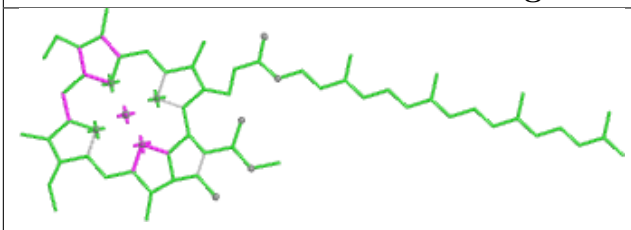
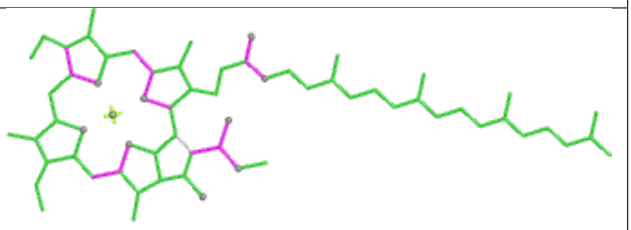
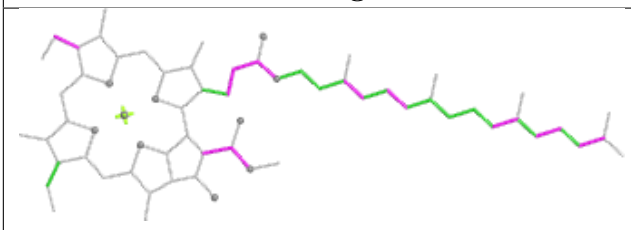
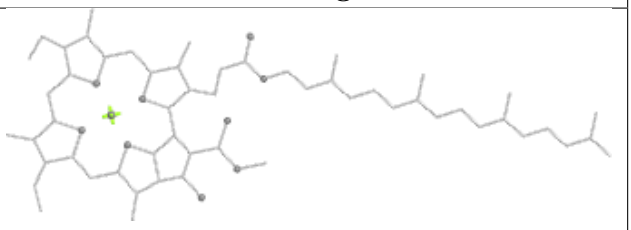
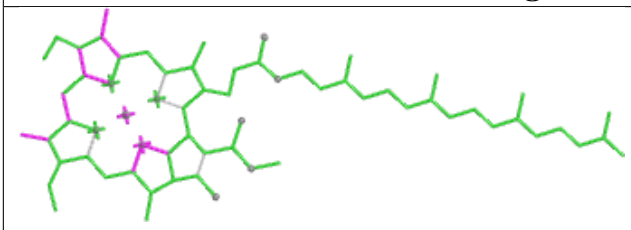
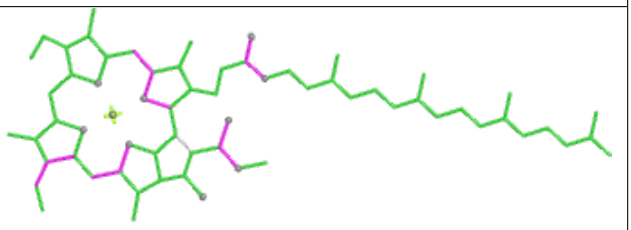
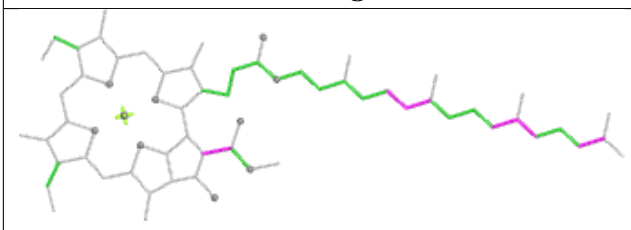
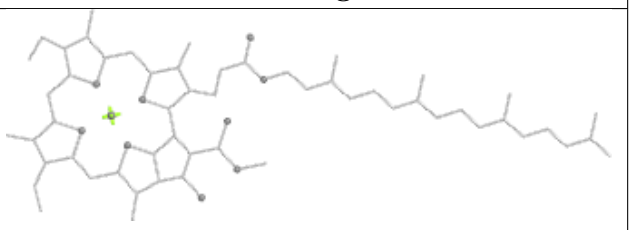
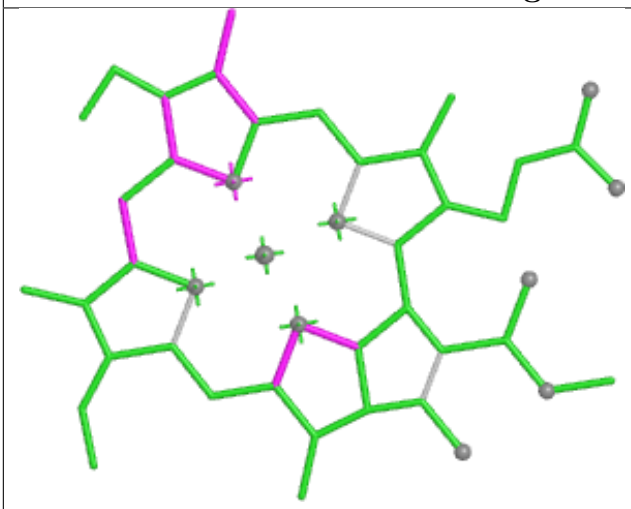


Rings

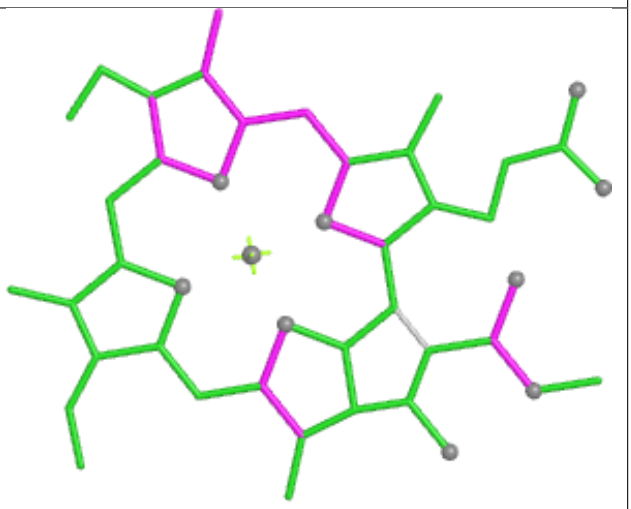
Ligand CLA B 812	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA A 806	
	
Bond lengths	Bond angles
	
Torsions	Rings

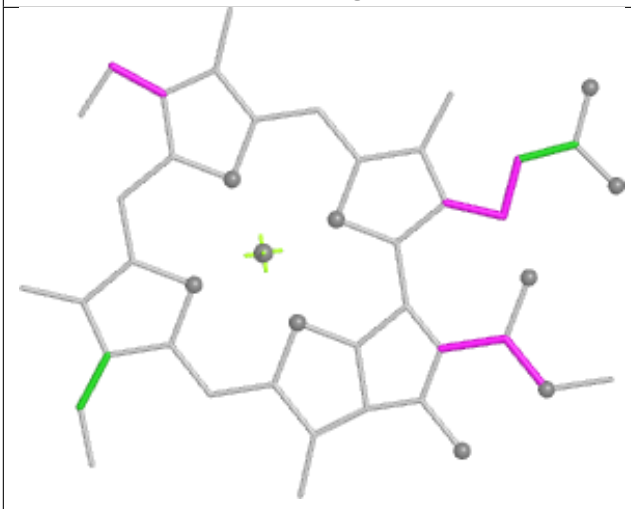
Ligand CLA A 834



Bond lengths



Bond angles

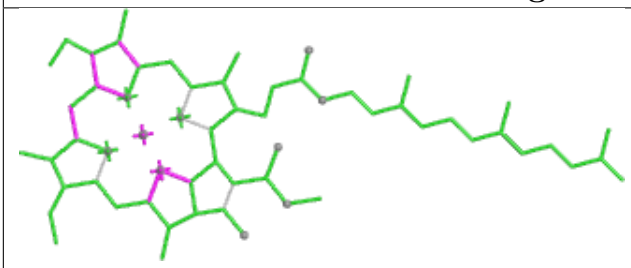


Torsions



Rings

Ligand CLA 4 309



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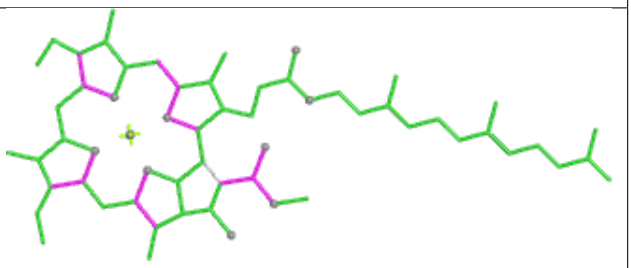
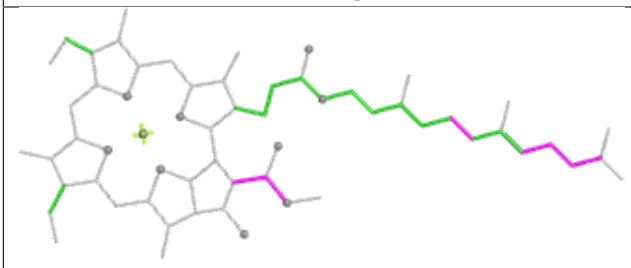


Bond angles



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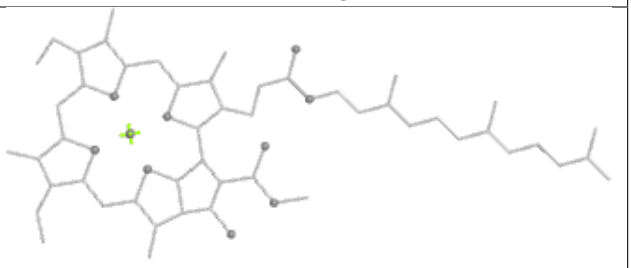
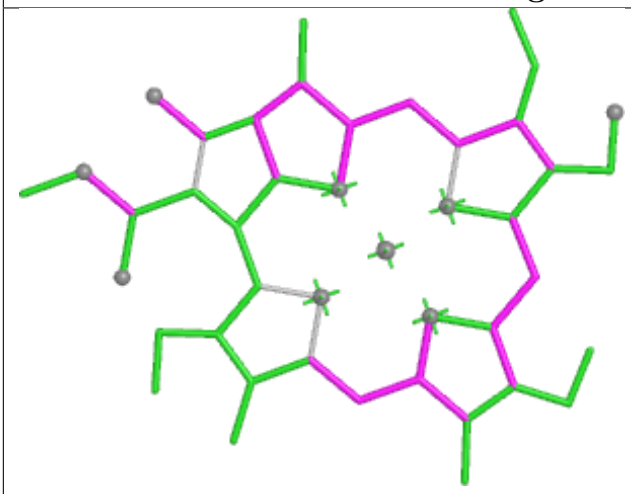


Rings

Ligand CHL 4 315



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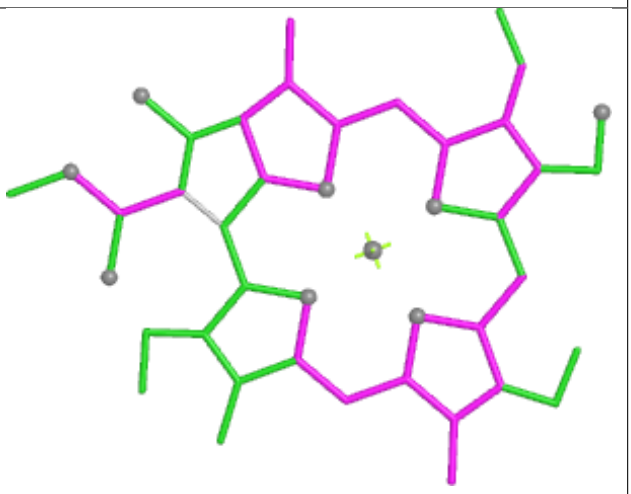
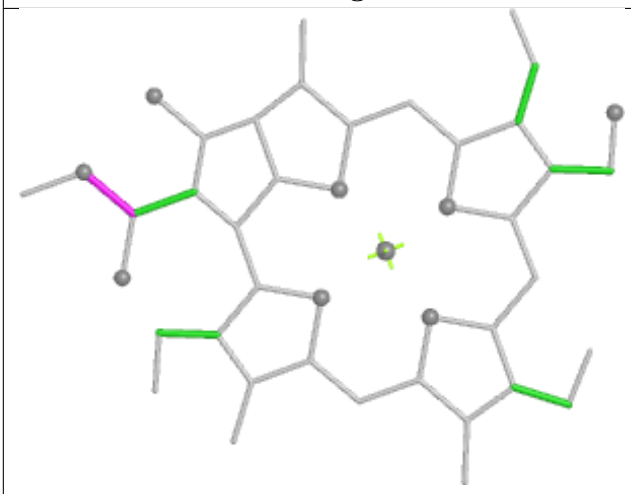


Bond angles



Torsions

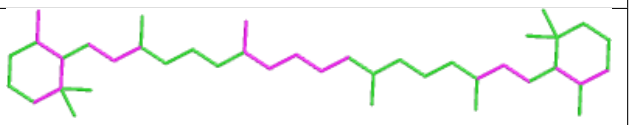


Rings

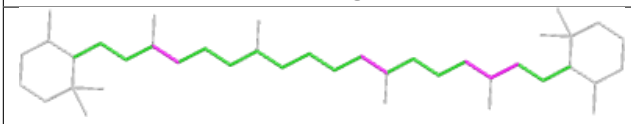
Ligand BCR B 846



Bond lengths



Bond angles



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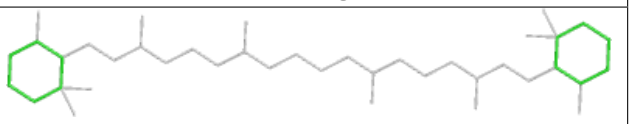
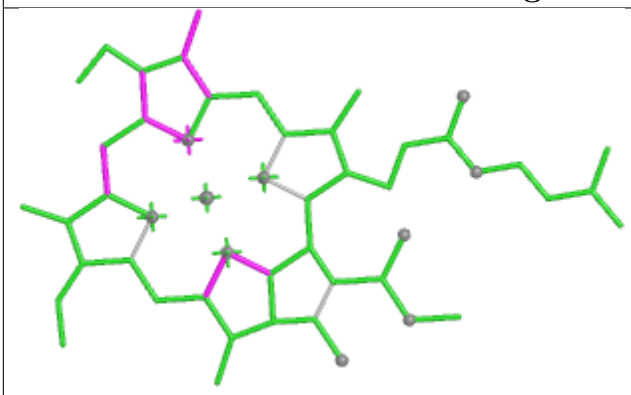


Rings

Ligand CLA A 833



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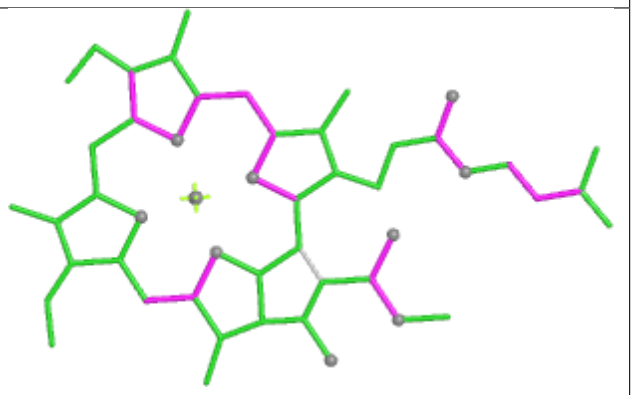
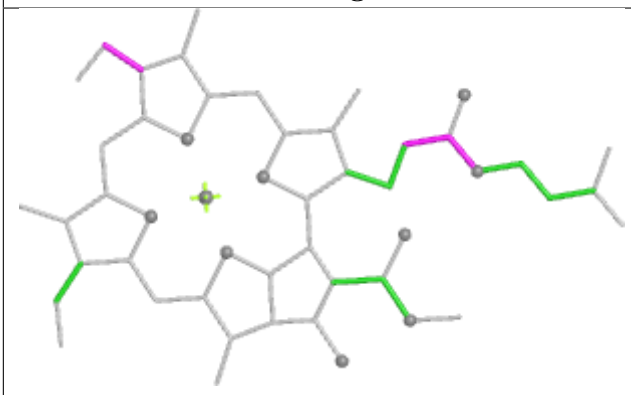


Bond angles



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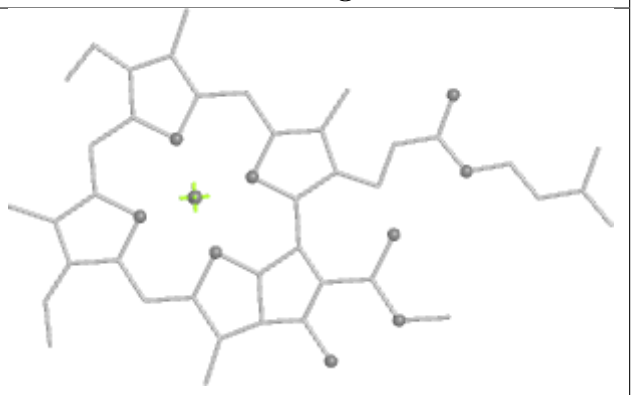
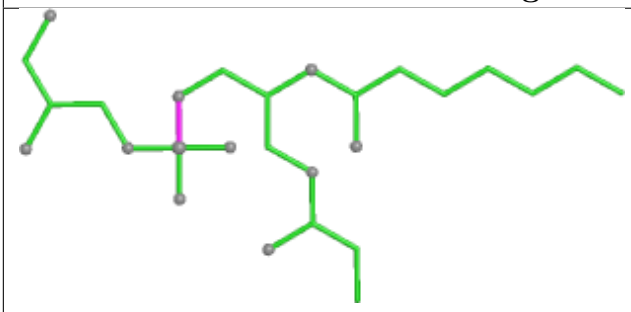


Rings

Ligand LHG A 845



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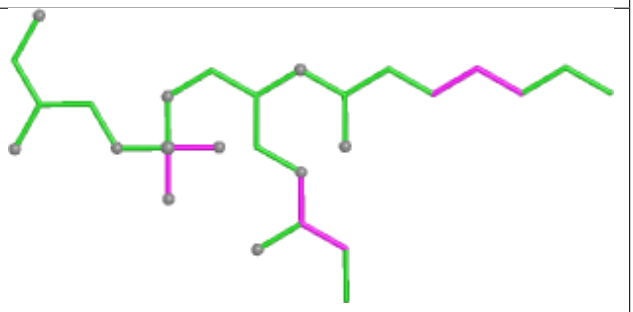
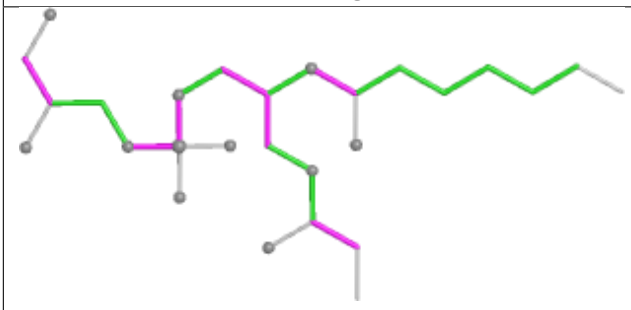
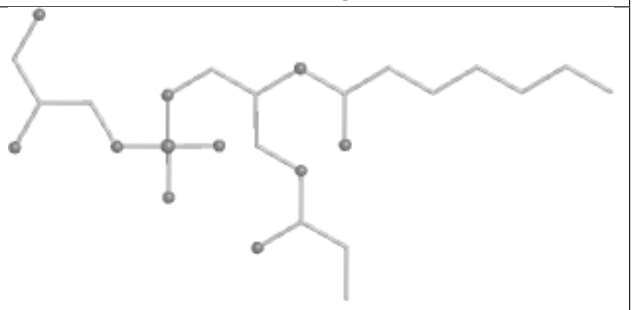


Bond angles

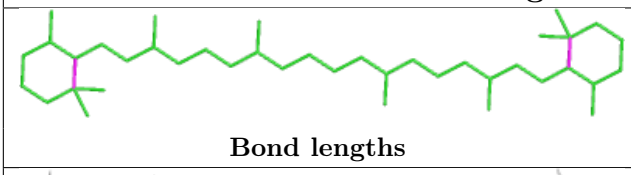


Torsions



Rings

Ligand BCR 3 616



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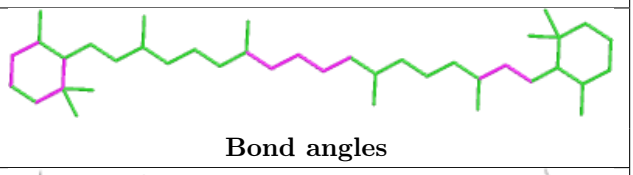
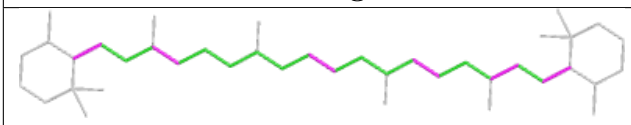


Bond angles



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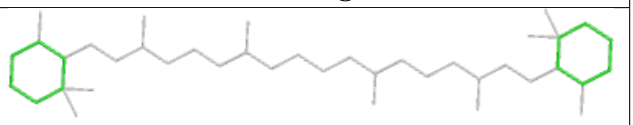
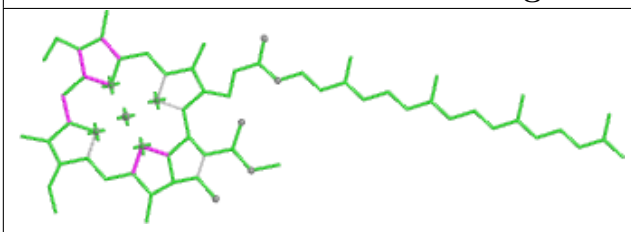
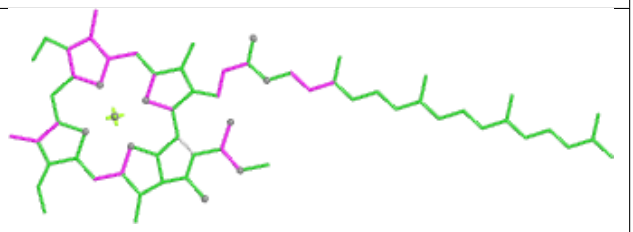


Rings

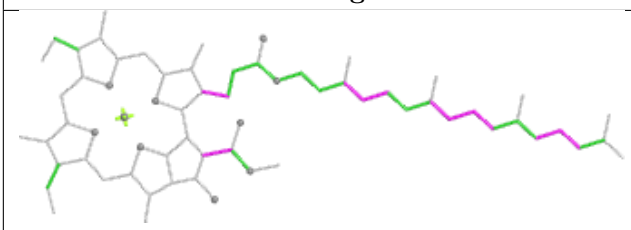
Ligand CLA A 804



Bond lengths



Bond angles



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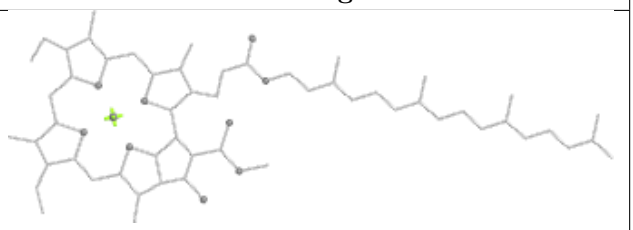
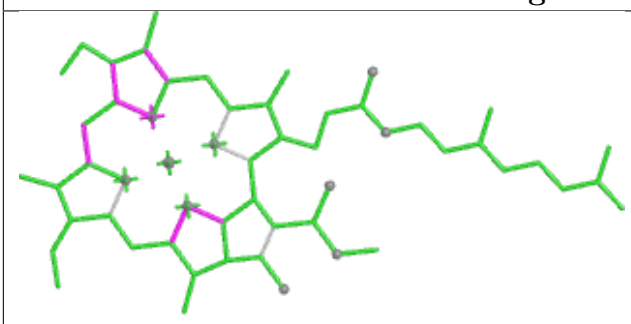


Rings

Ligand CLA 1 312



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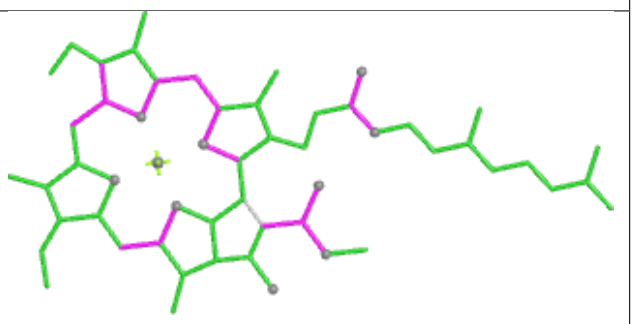
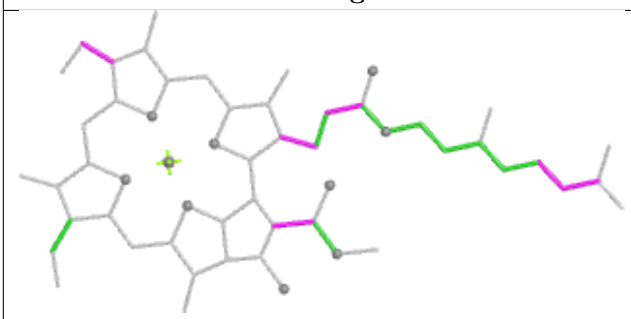


Bond angles



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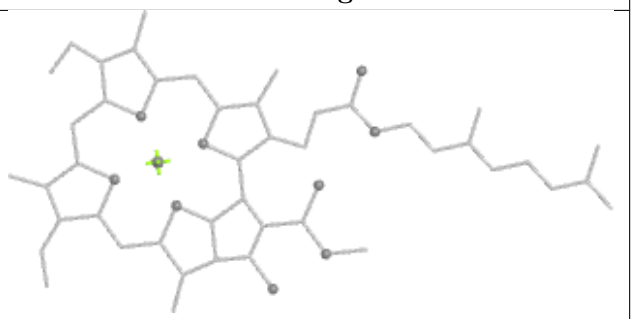
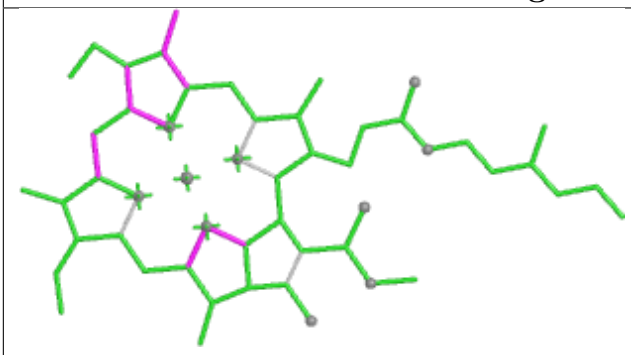


Rings

Ligand CLA 3 610



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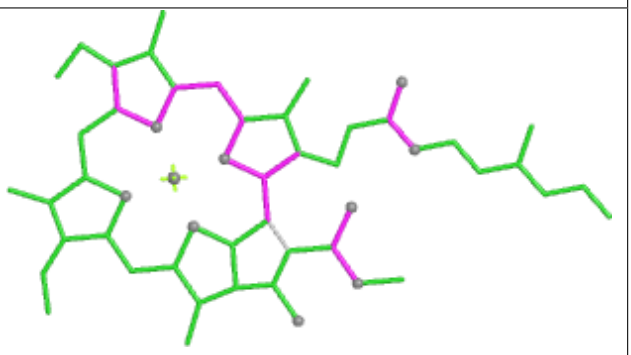
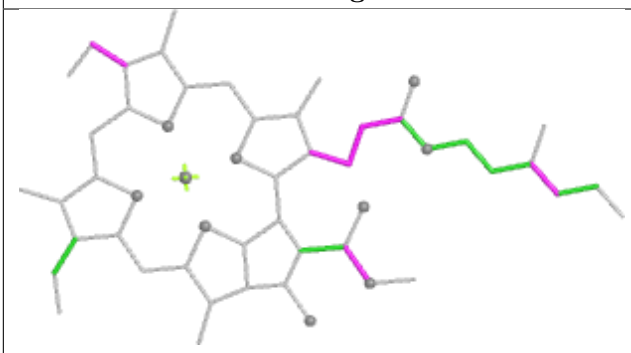


Bond angles



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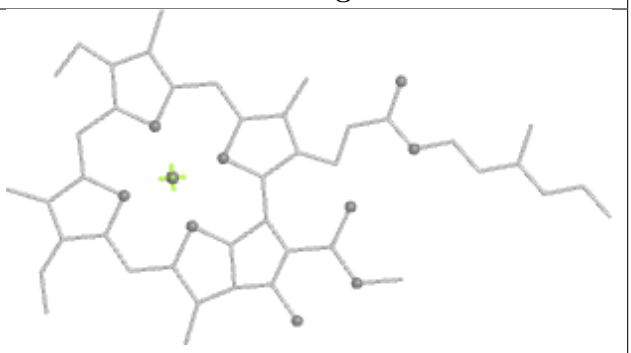
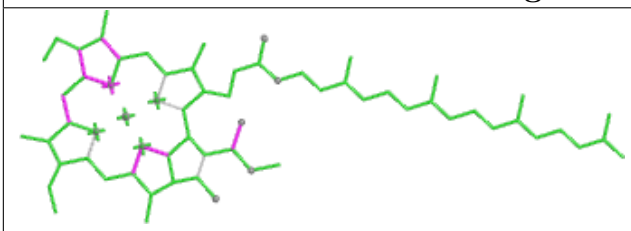
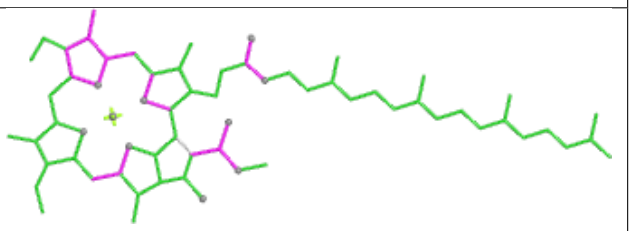


Rings

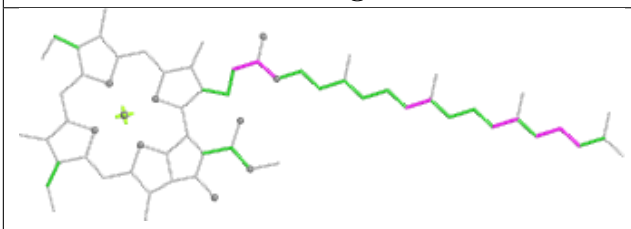
Ligand CLA B 816



Bond lengths



Bond angles



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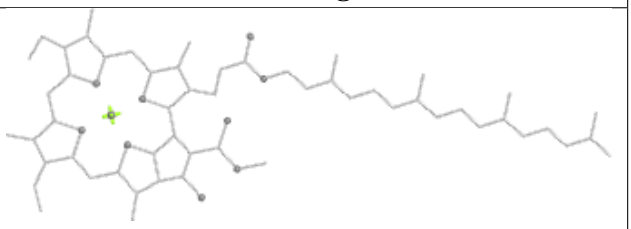
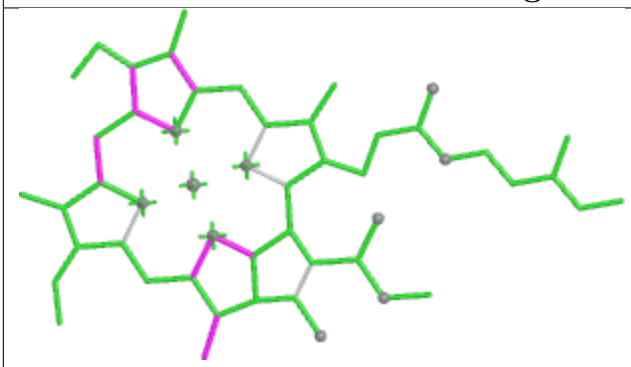
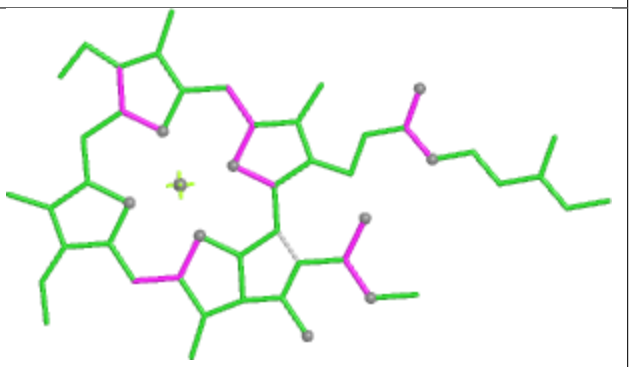


Rings

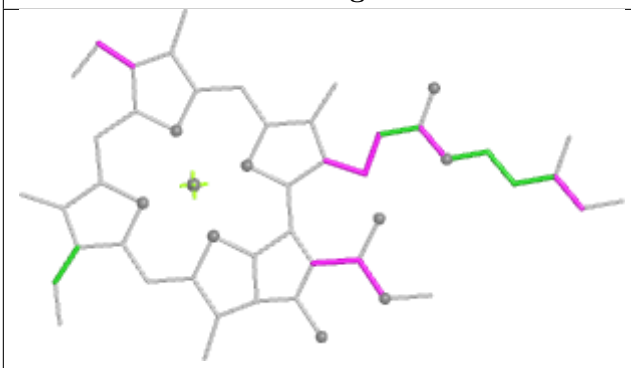
Ligand CLA A 822



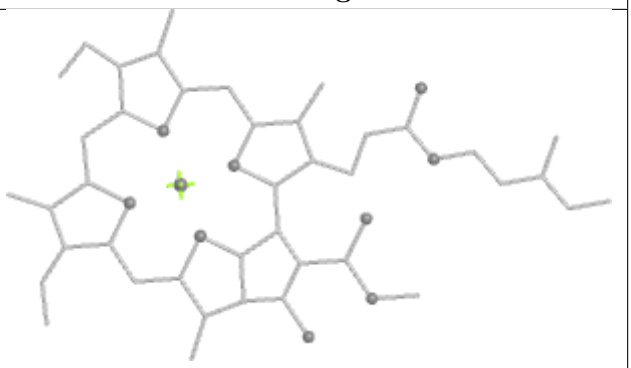
Bond lengths



Bond angles

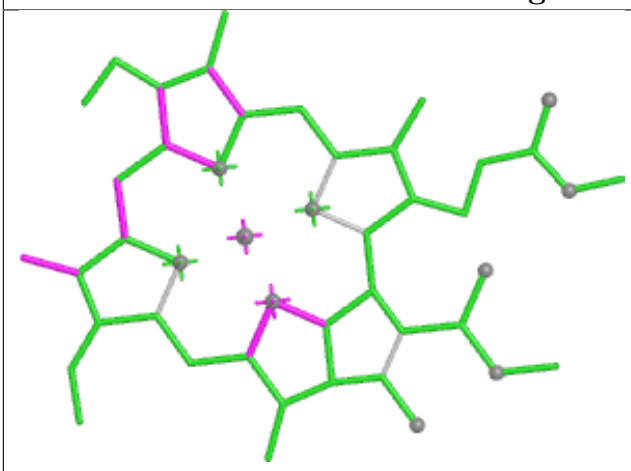


Torsions



Rings

Ligand CLA 1 313



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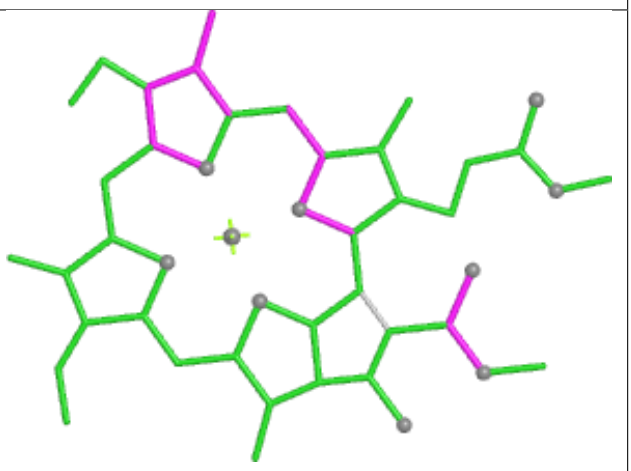
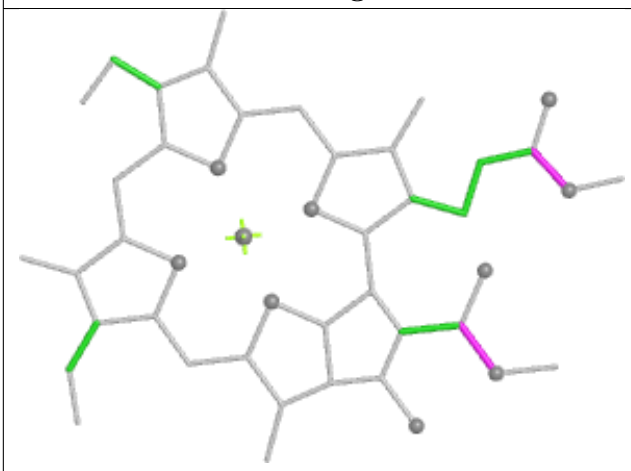


Bond angles



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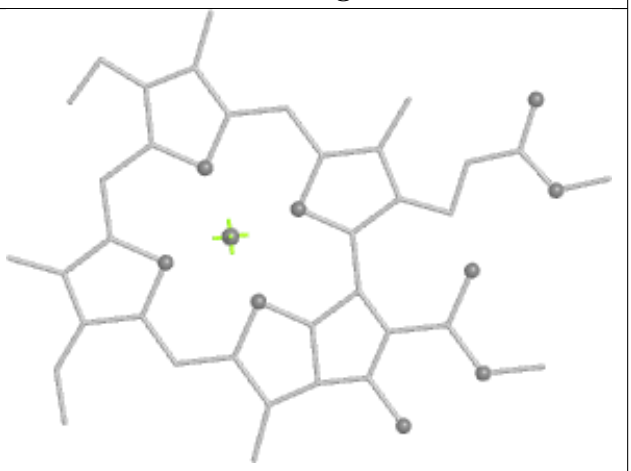
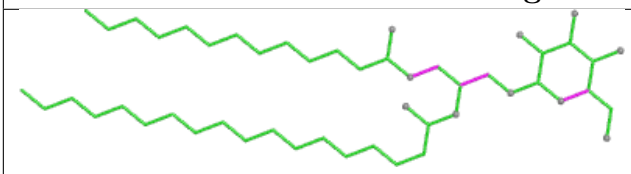


Rings

Ligand LMG 4 319



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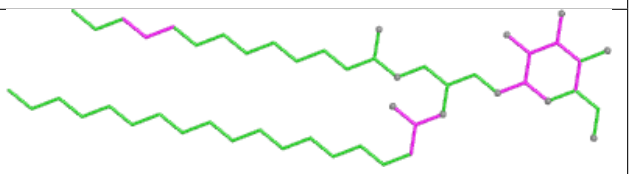

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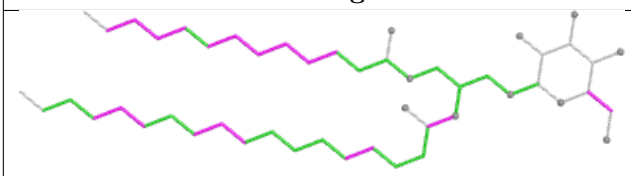

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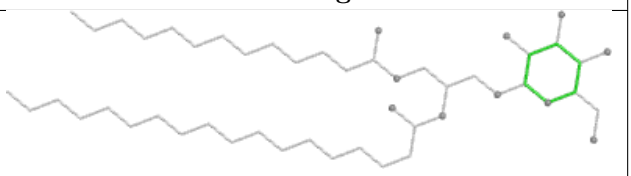
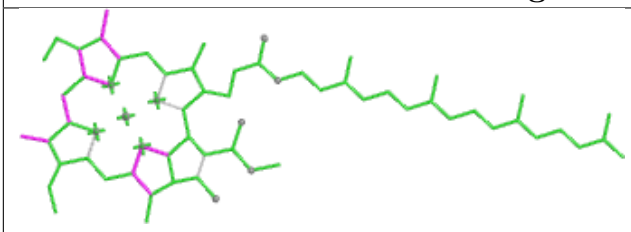


Rings

Ligand CLA 1 307



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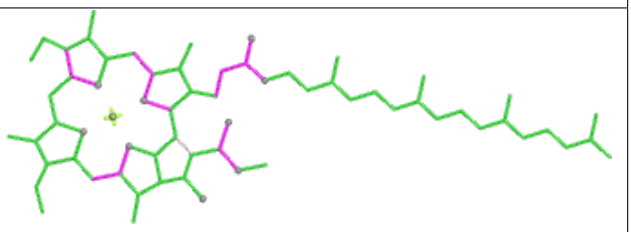

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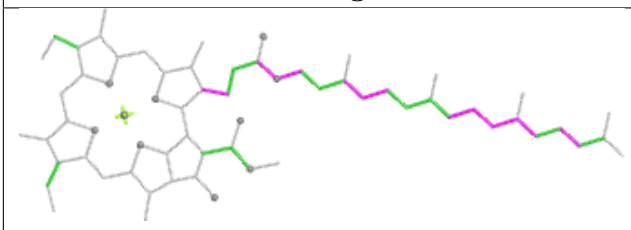

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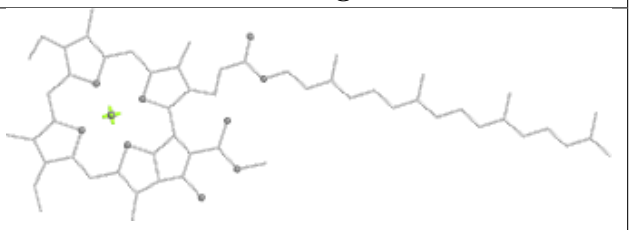
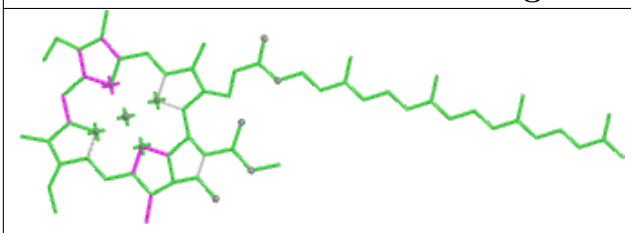


Rings

Ligand CLA A 809



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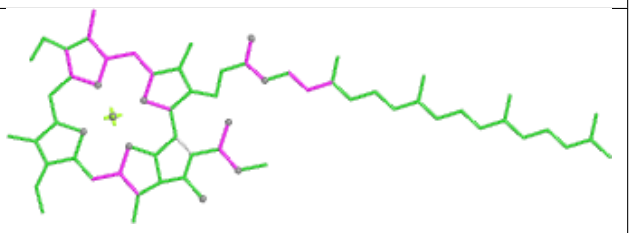

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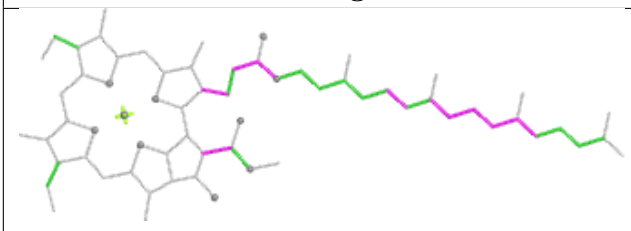

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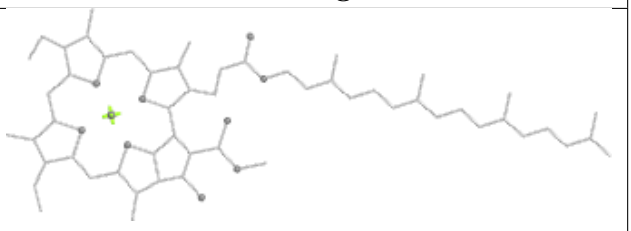
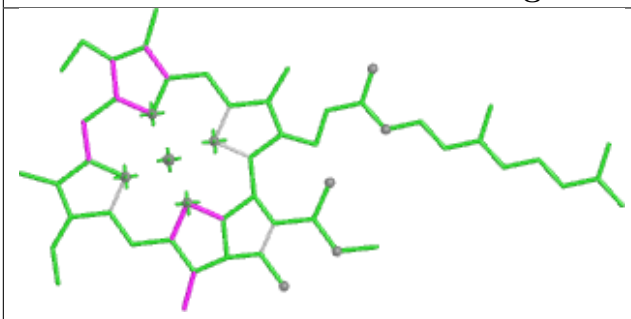


Rings

Ligand CLA A 823



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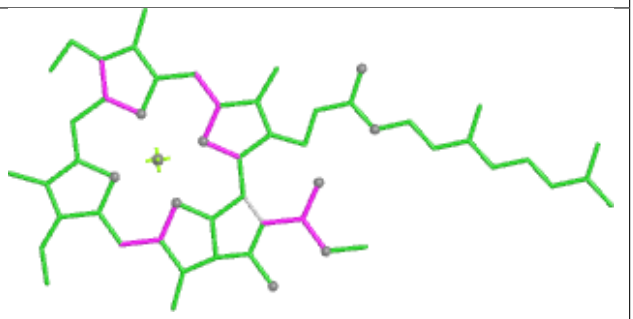

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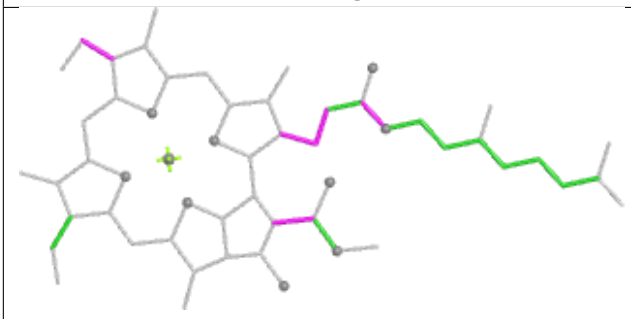

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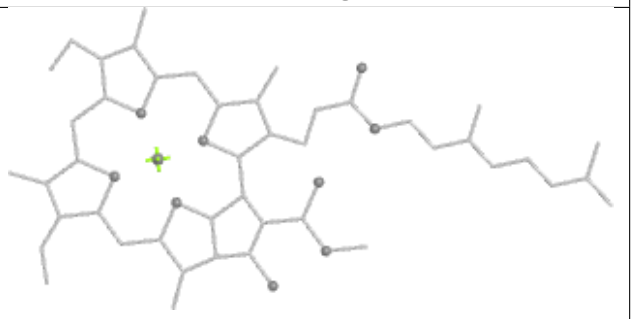
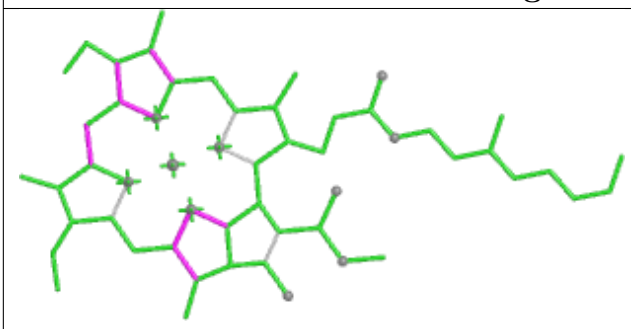


Rings

Ligand CLA A 811



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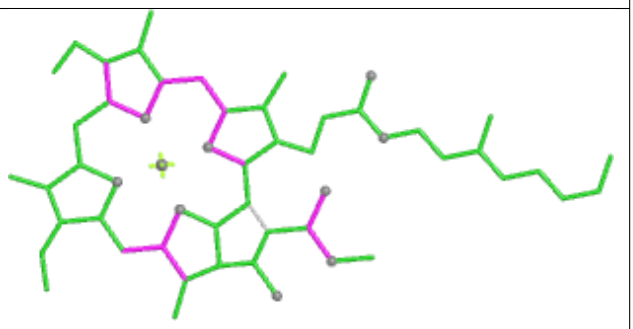
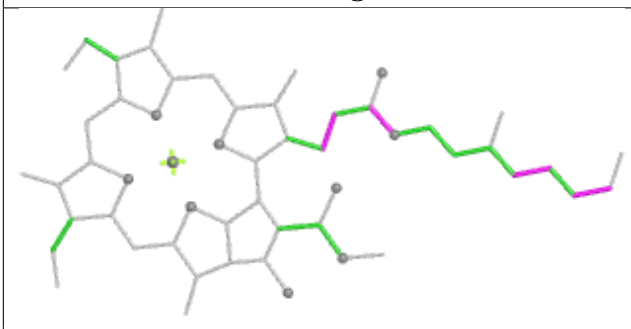


Bond angles



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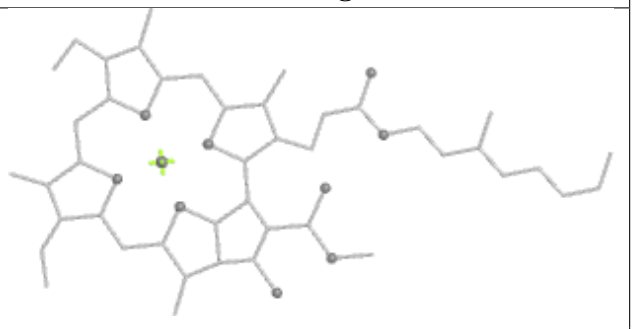
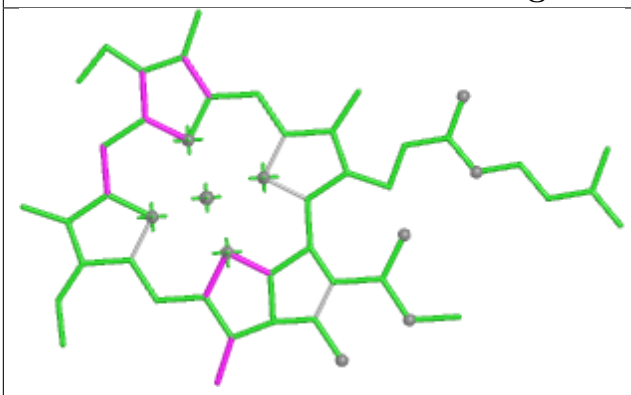


Rings

Ligand CLA 3 608



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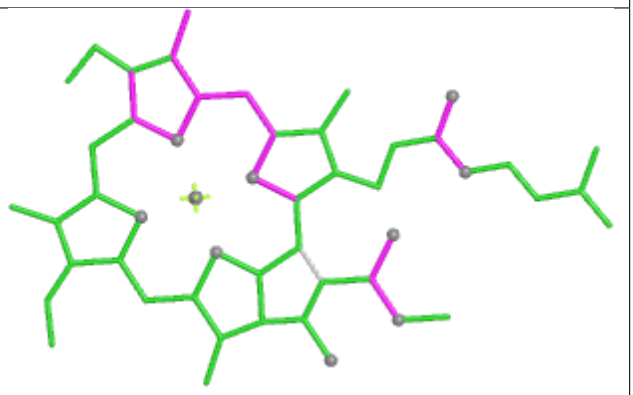

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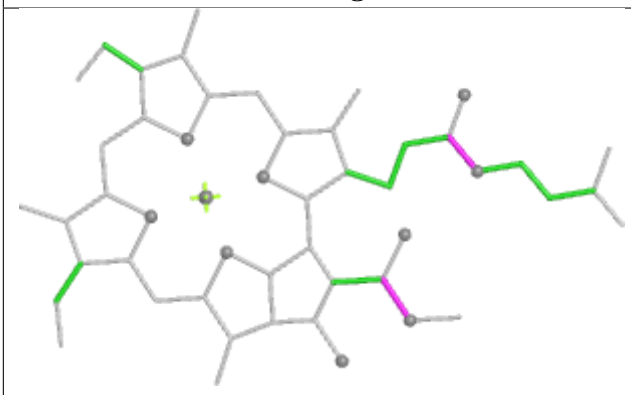

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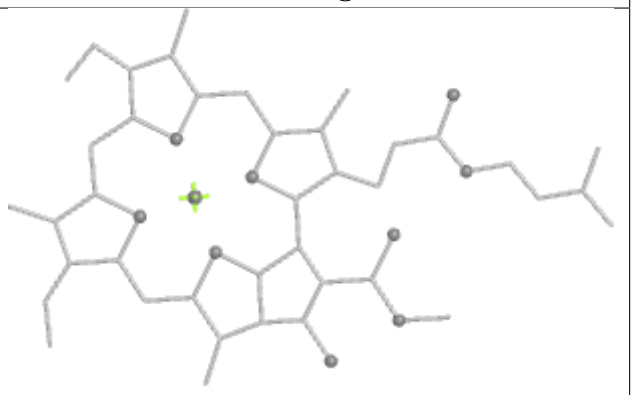

Rings

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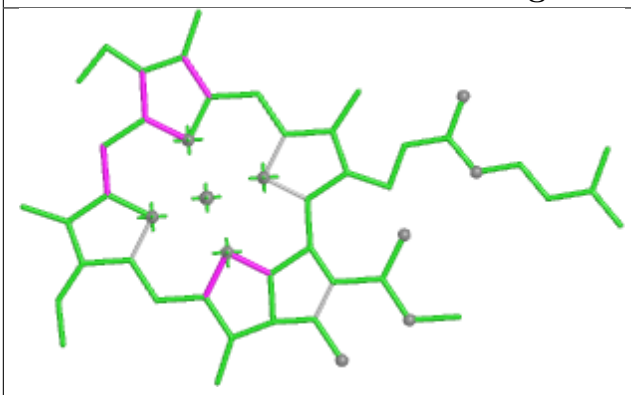

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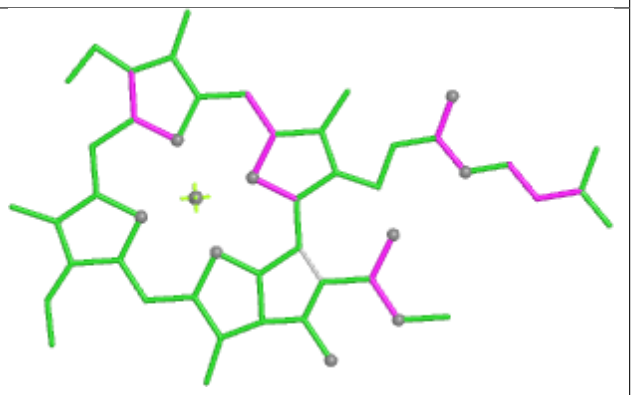
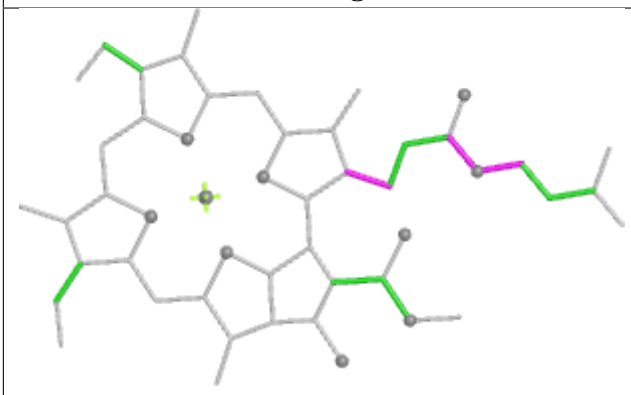


Bond angles



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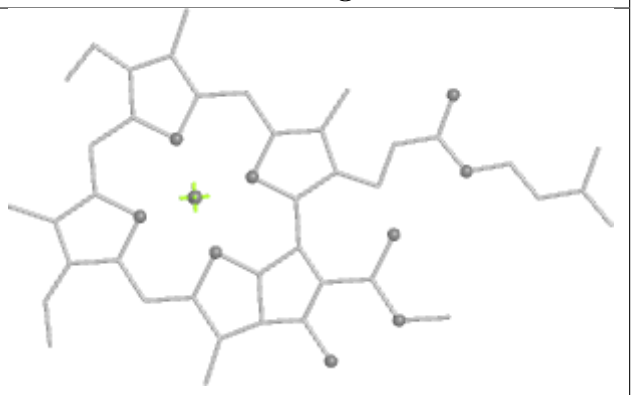
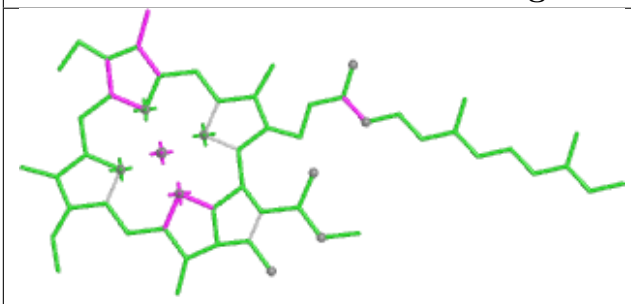


Rings

Ligand CLA 4 312



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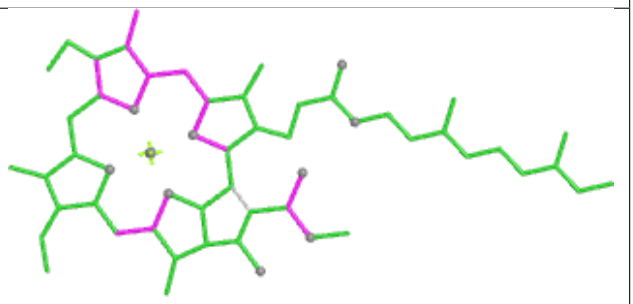

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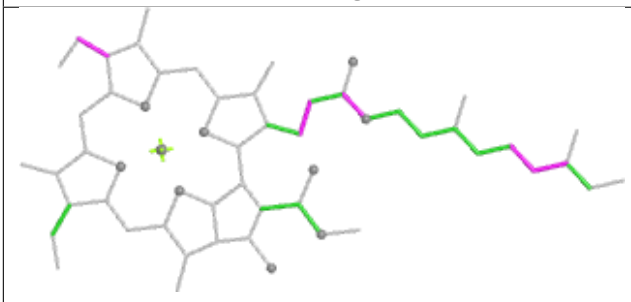

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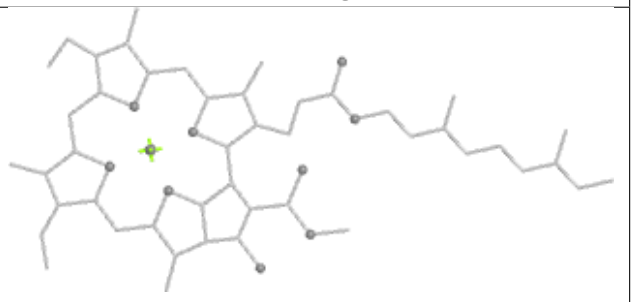
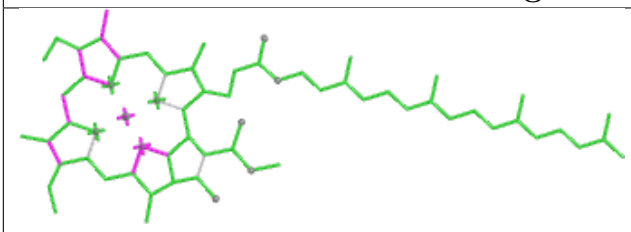


Rings

Ligand CLA B 805



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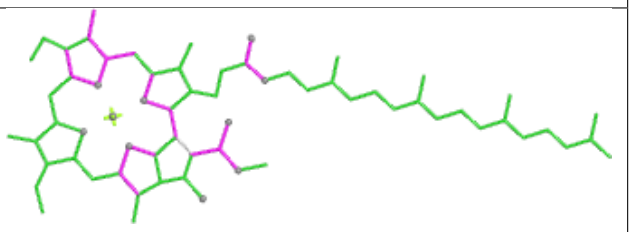
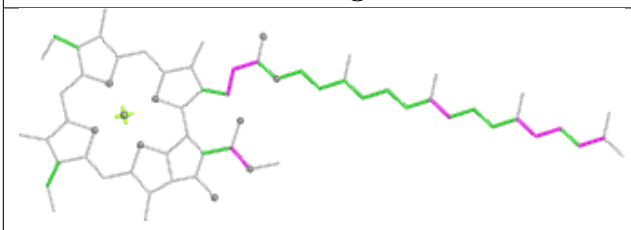


Bond angles



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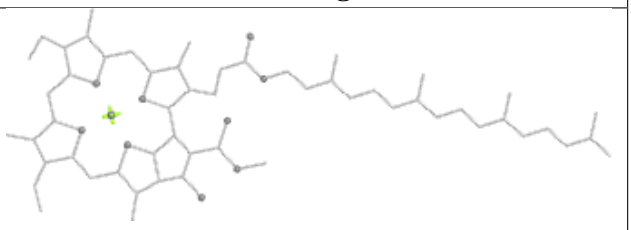
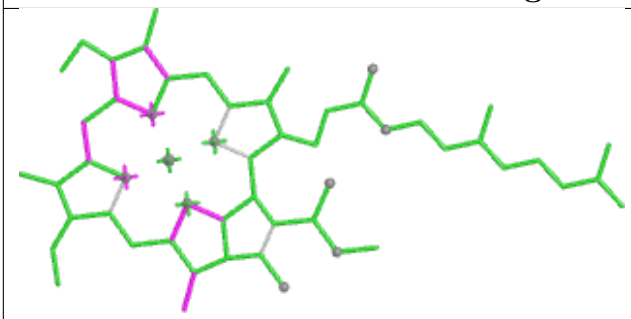


Rings

Ligand CLA B 824



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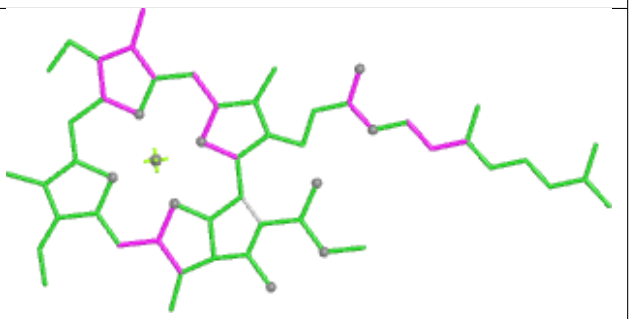

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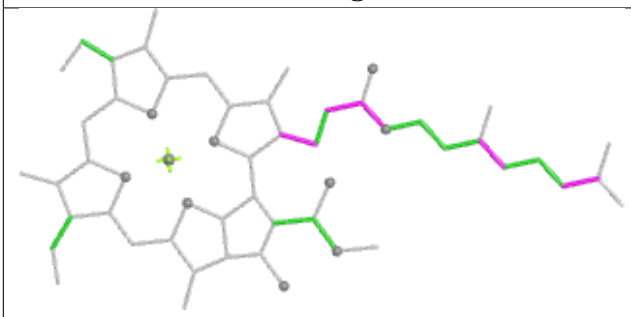

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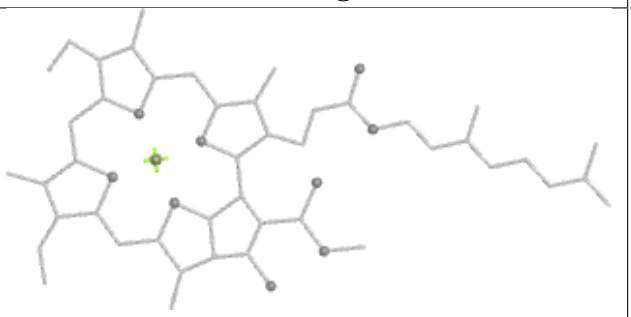
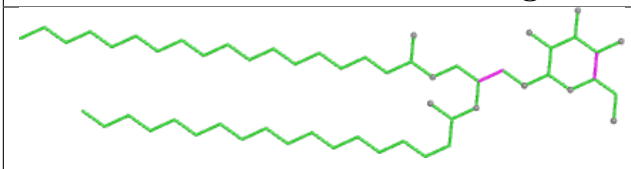


Rings

Ligand LMG F 309



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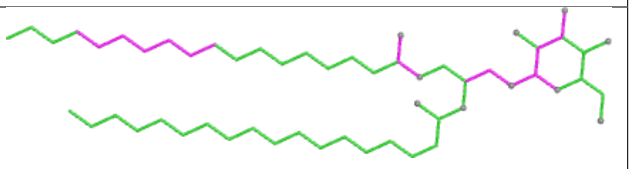

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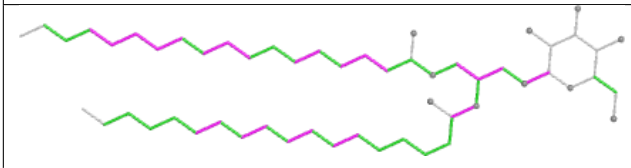

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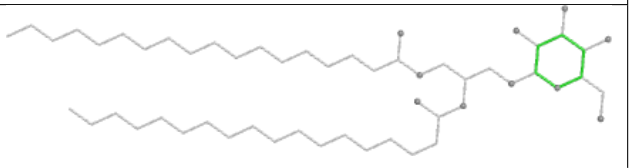
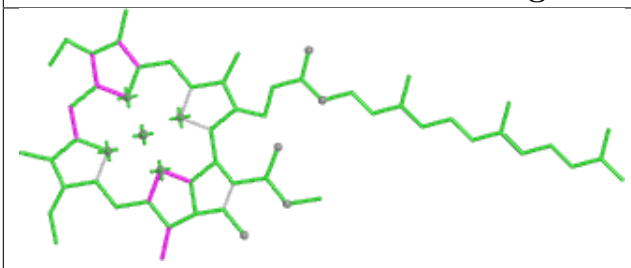


Rings

Ligand CLA 2 308



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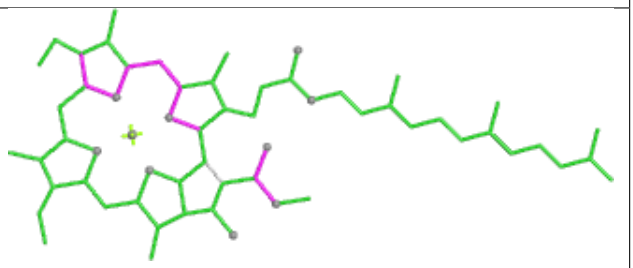
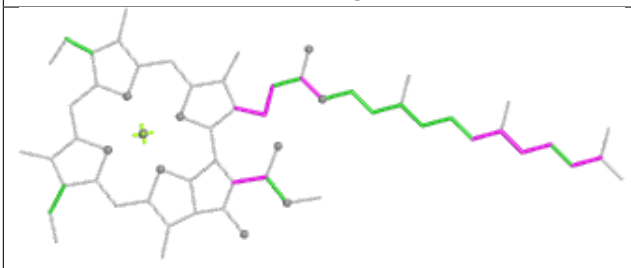


Bond angles



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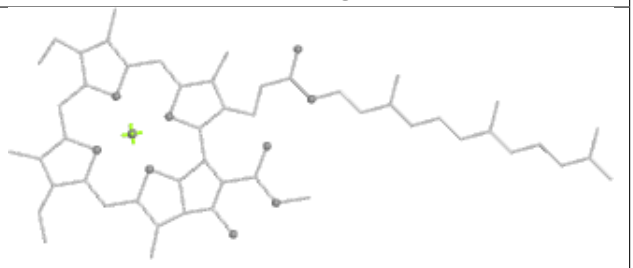
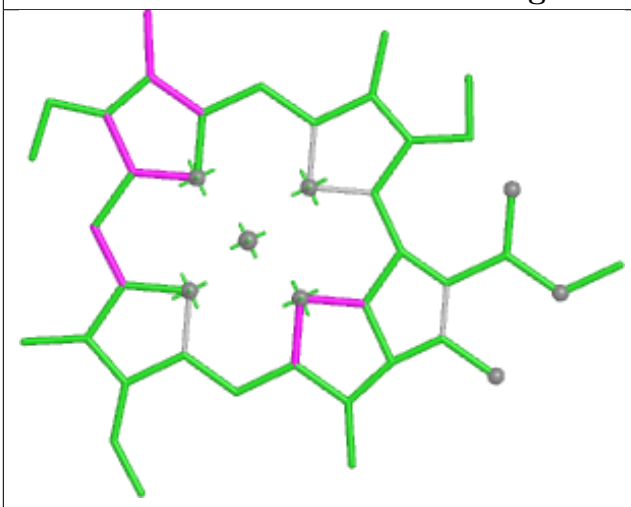


Rings

Ligand CLA 3 605



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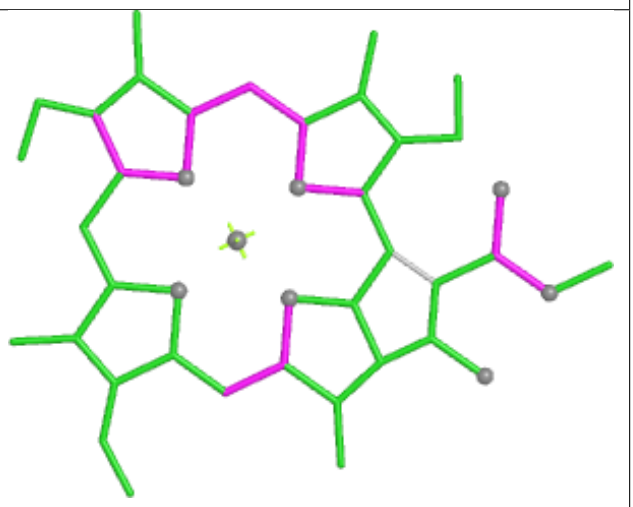
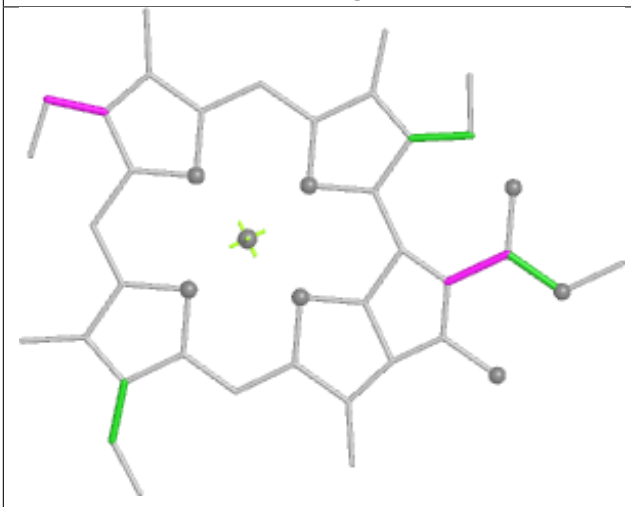


Bond angles



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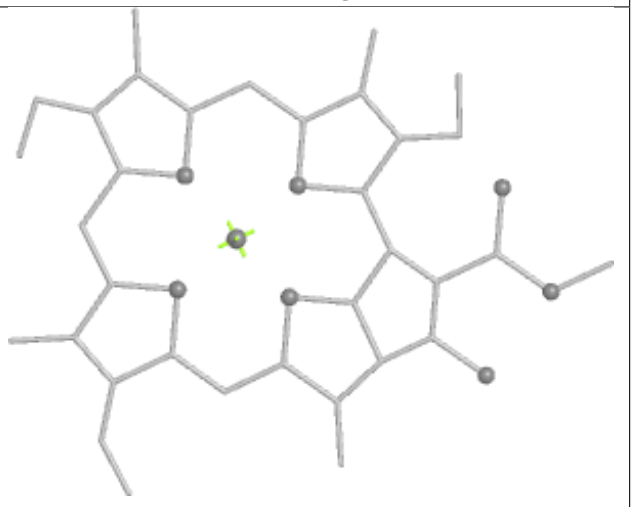
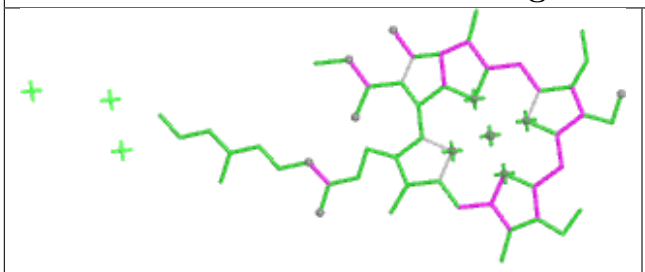
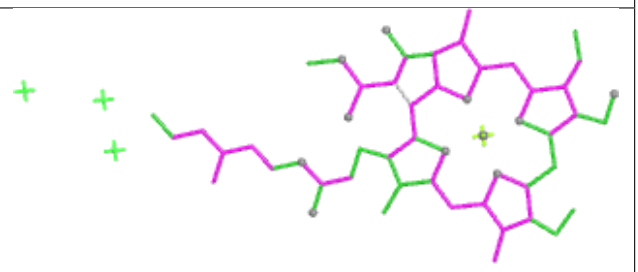


Rings

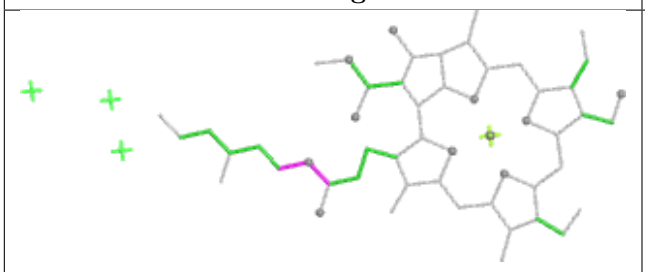
Ligand CHL 3 601



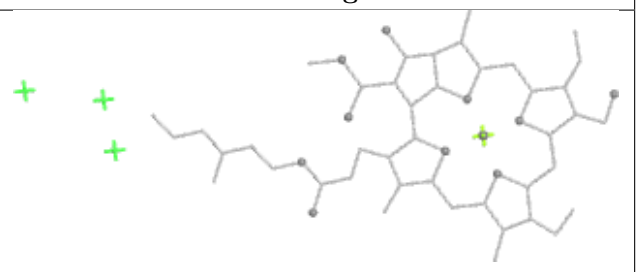
Bond lengths



Bond angles

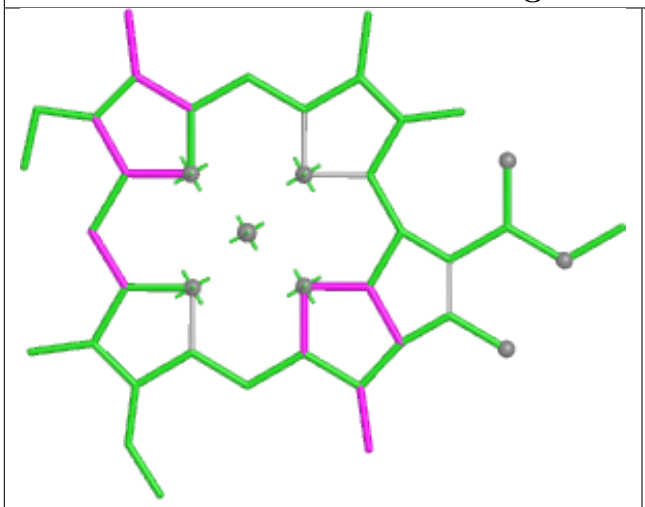


Torsions



Rings

Ligand CLA G 103



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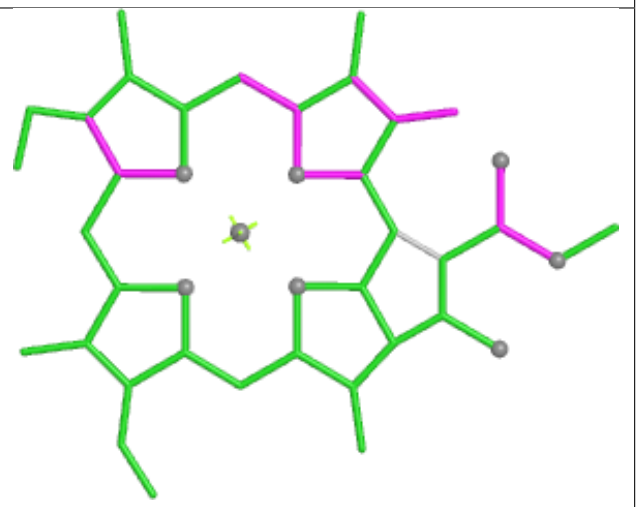

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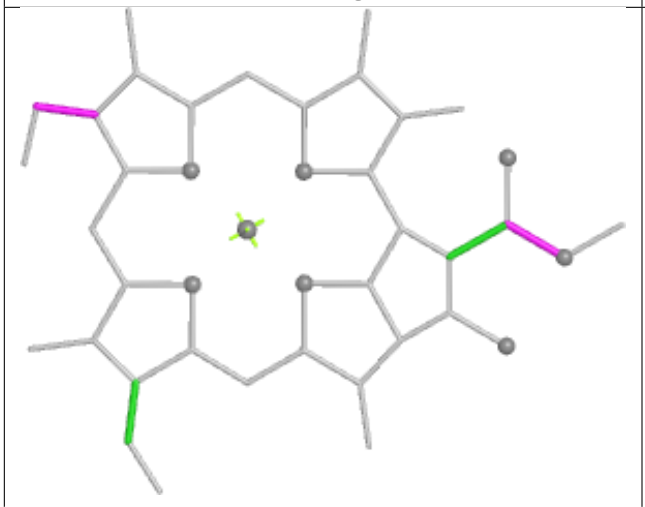

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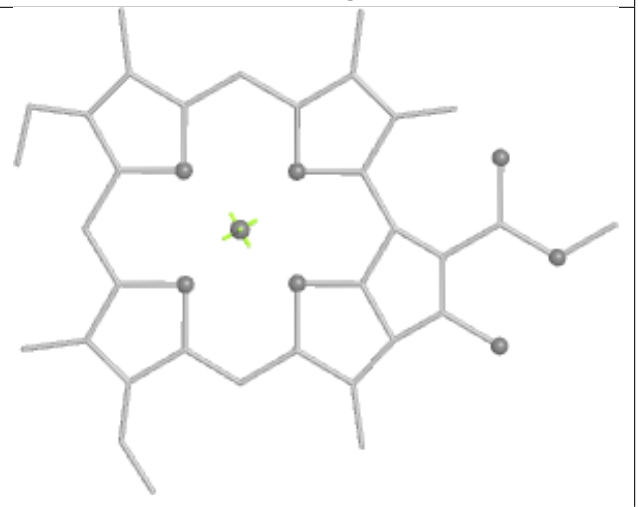
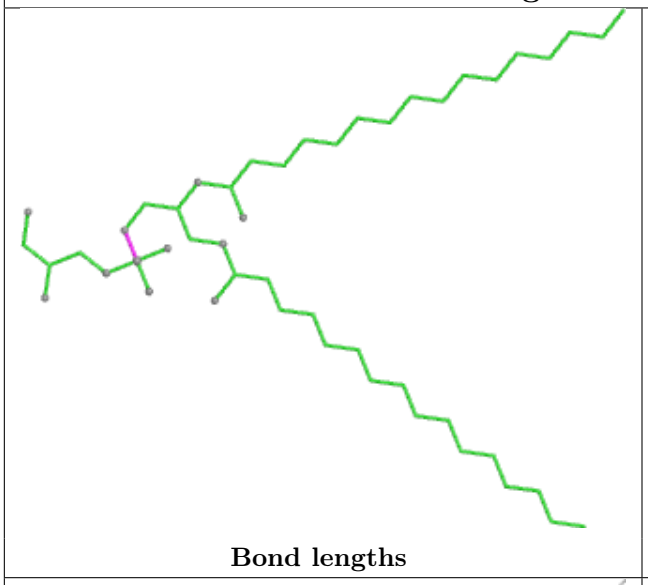


Rings

Ligand LHG G 102



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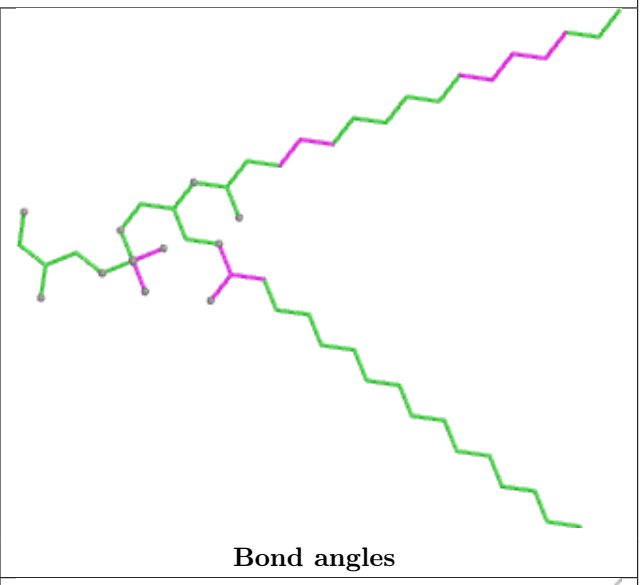
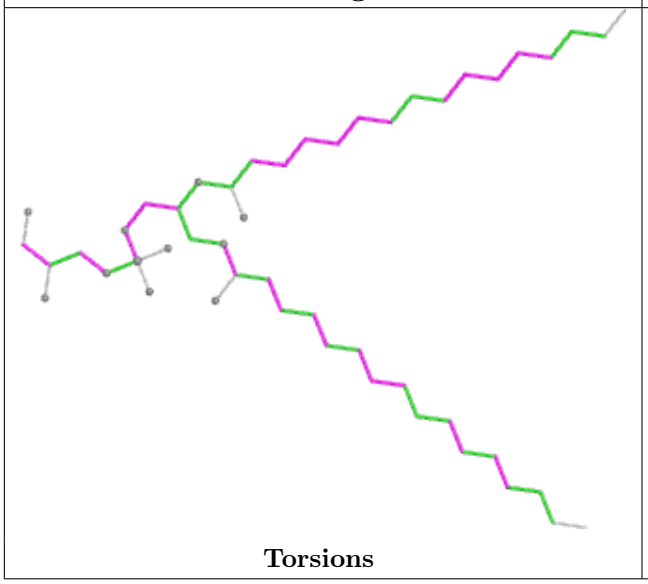


Bond angles



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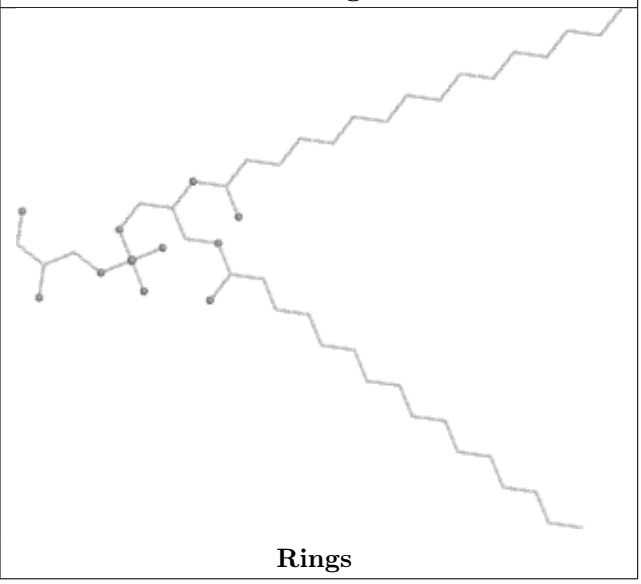
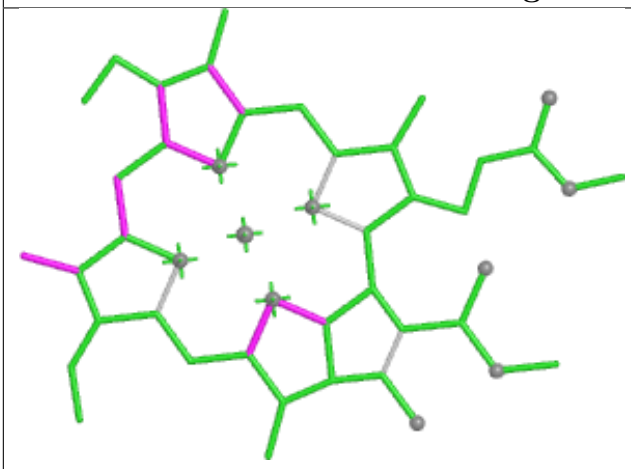


Rings

Ligand CLA G 105



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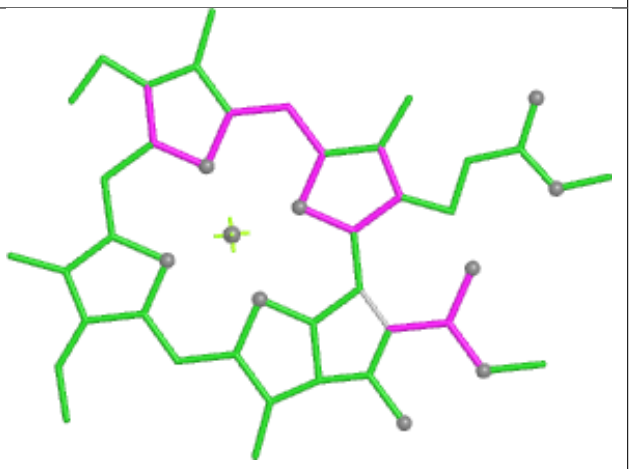

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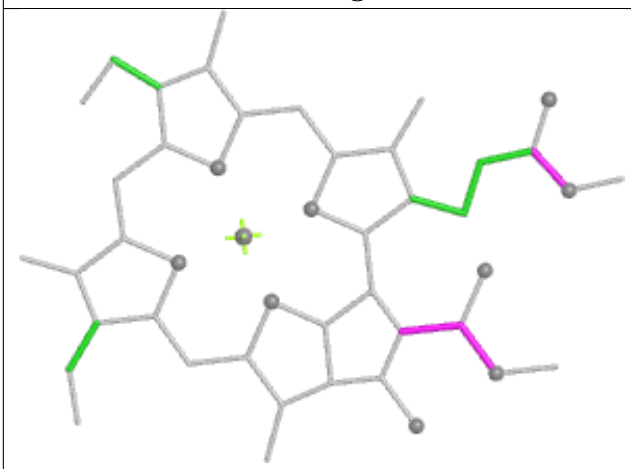

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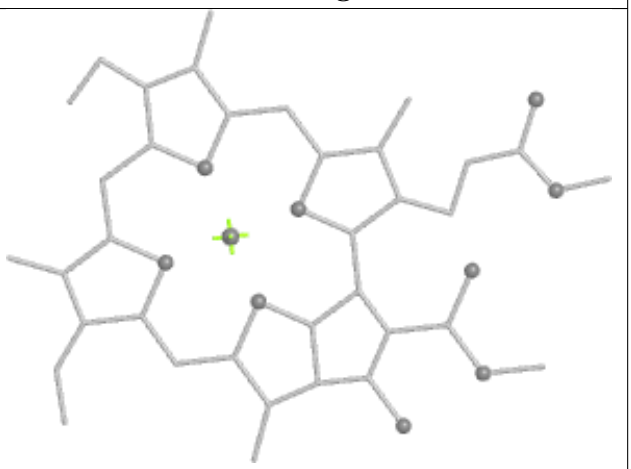
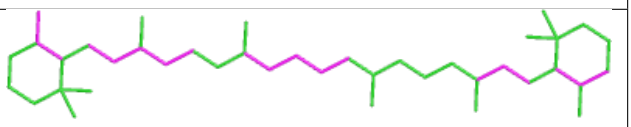


Rings

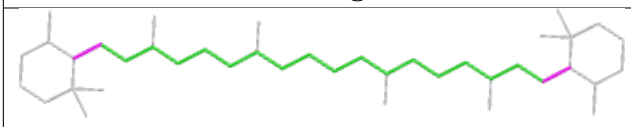
Ligand BCR L 206



Bond lengths



Bond angles



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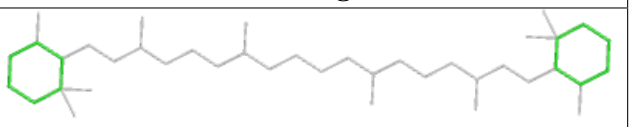
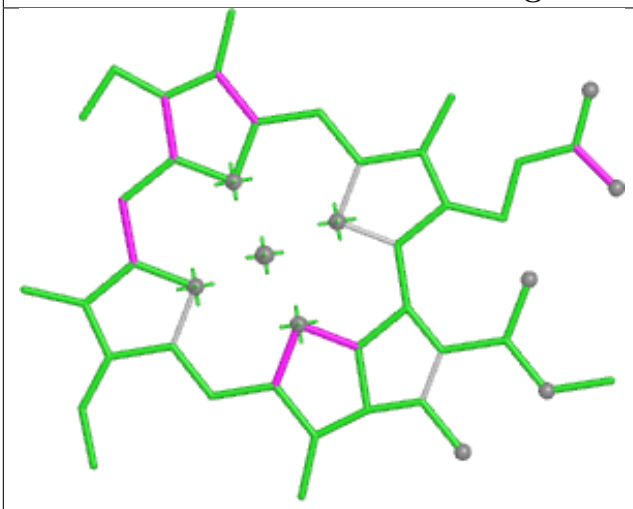


Rings

Ligand CLA B 806



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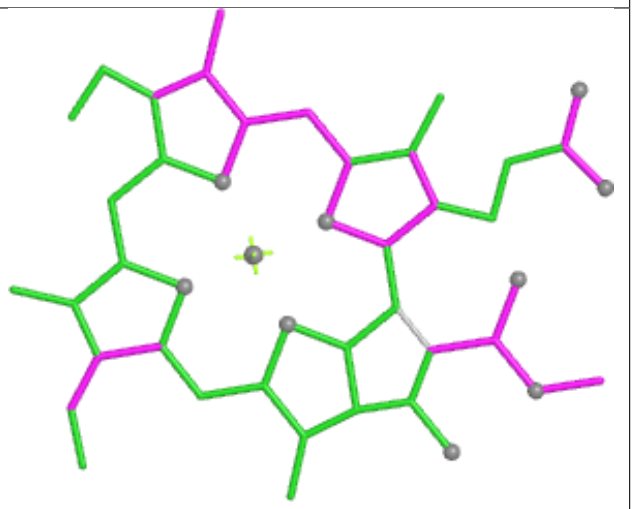
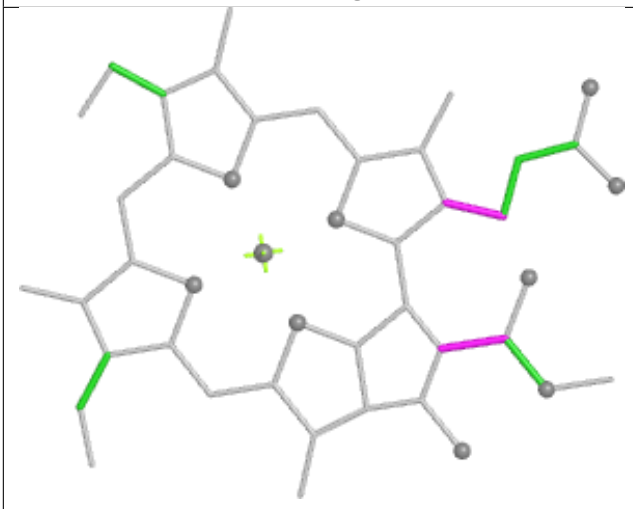


Bond angles

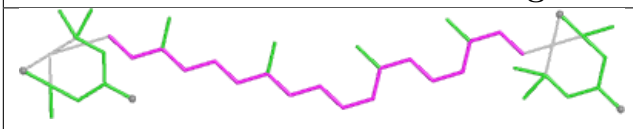


Torsions



Rings

Ligand XAT 4 317



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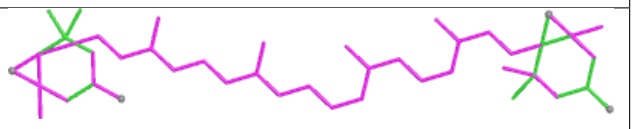
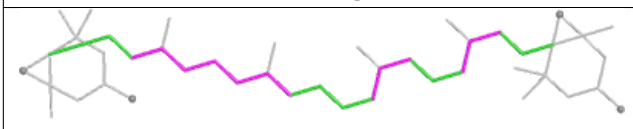


Bond angles



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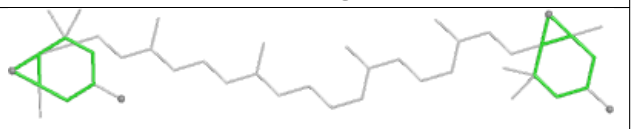
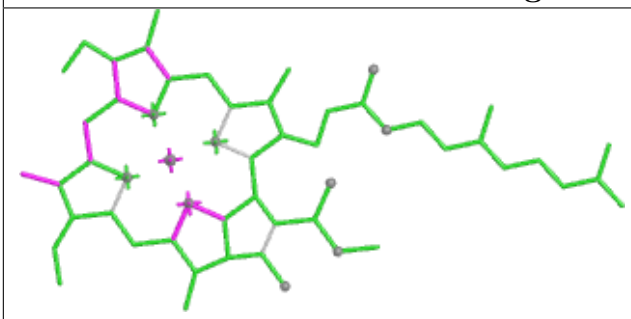


Rings

Ligand CLA B 817



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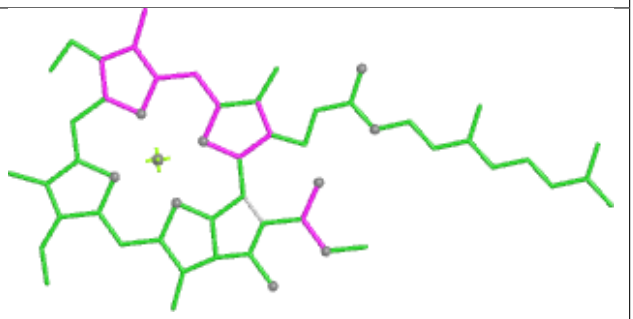

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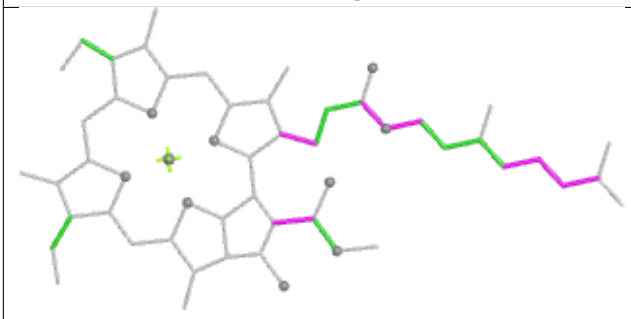

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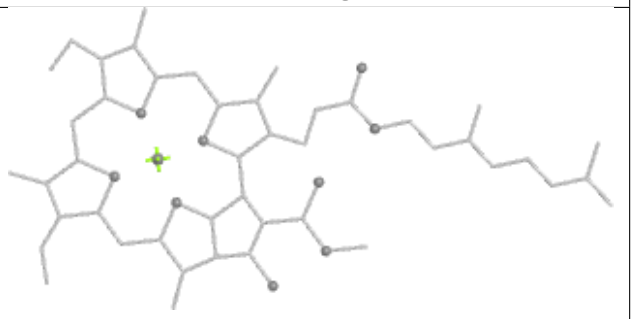
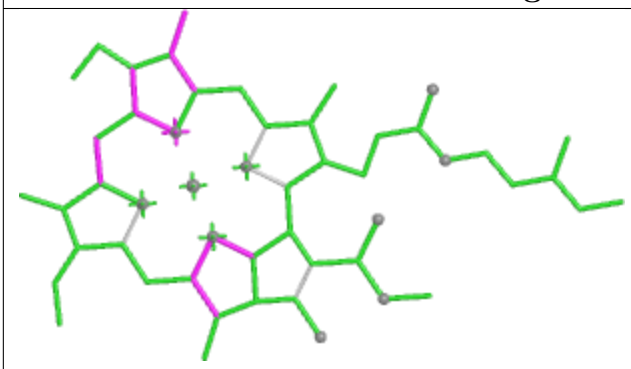


Rings

Ligand CLA A 835



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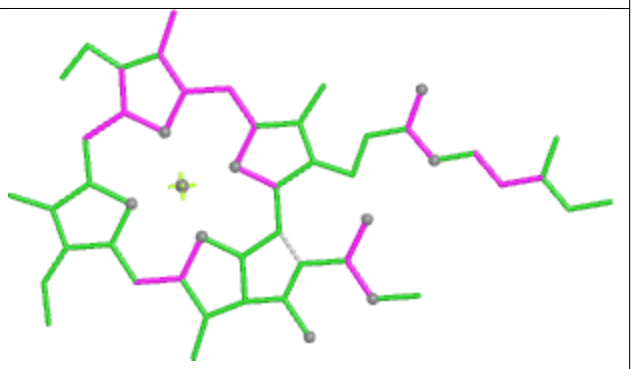
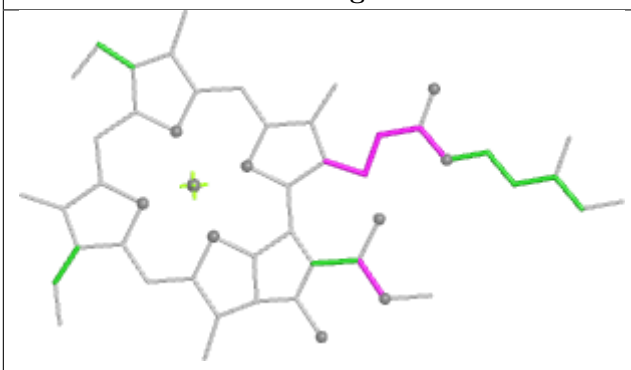


Bond angles



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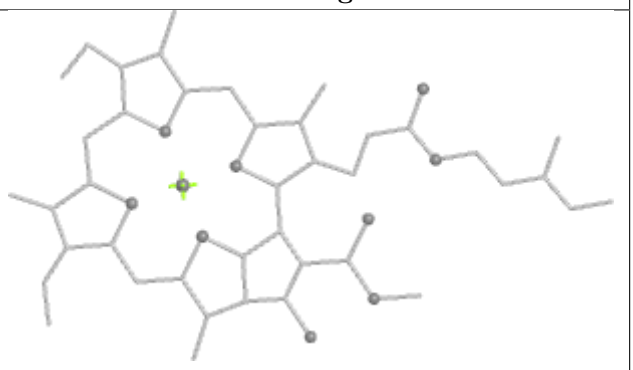
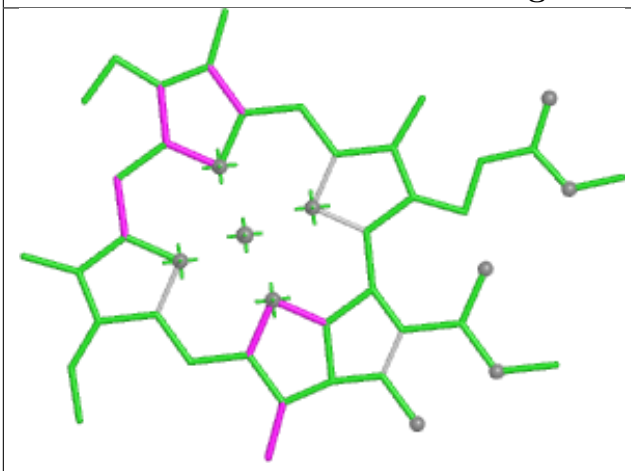


Rings

Ligand CLA 2 319



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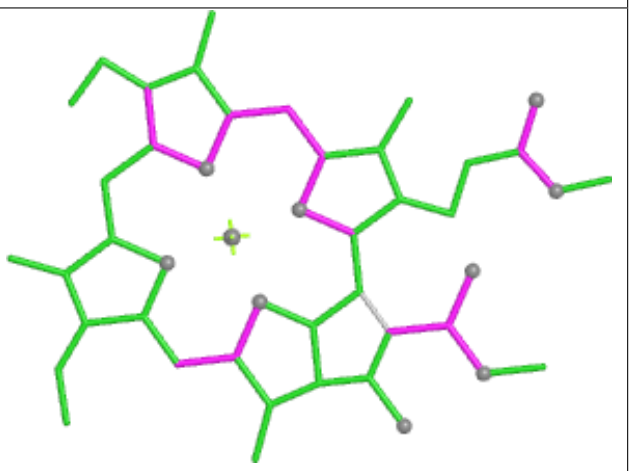
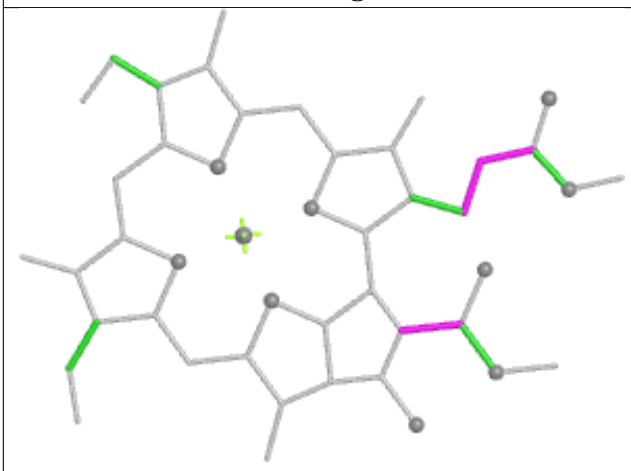


Bond angles



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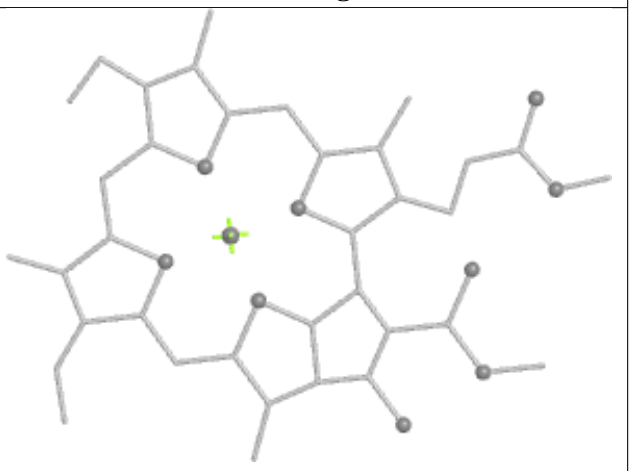
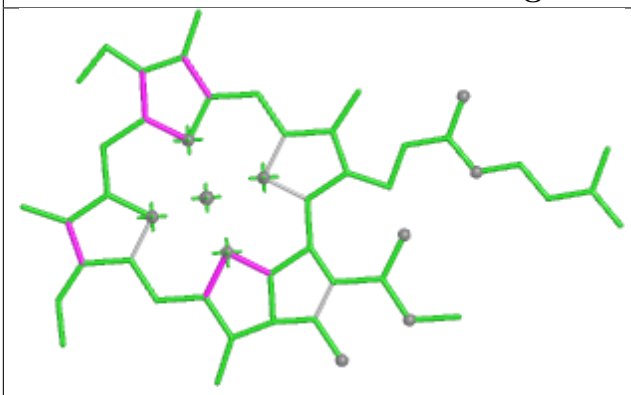


Rings

Ligand CLA B 822



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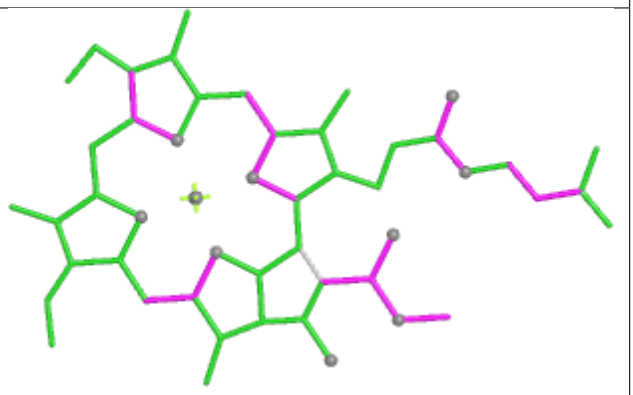
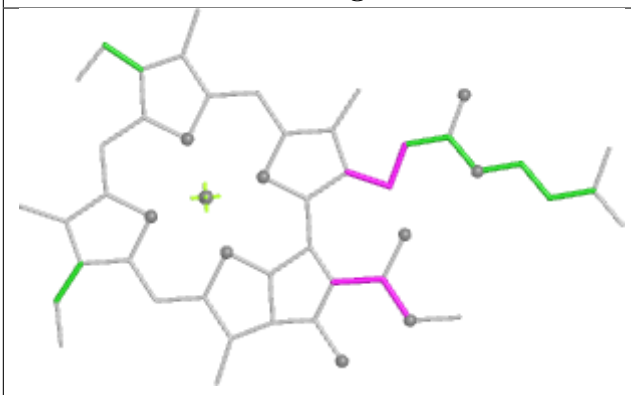


Bond angles



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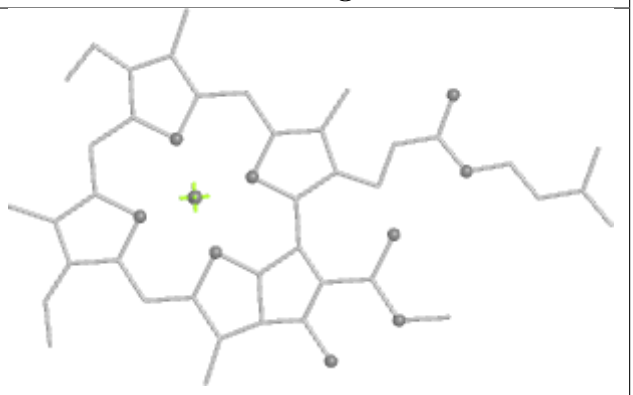
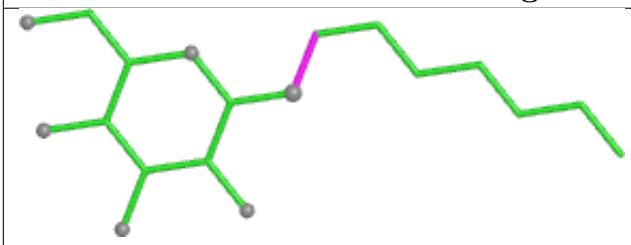


Rings

Ligand HTG B 851



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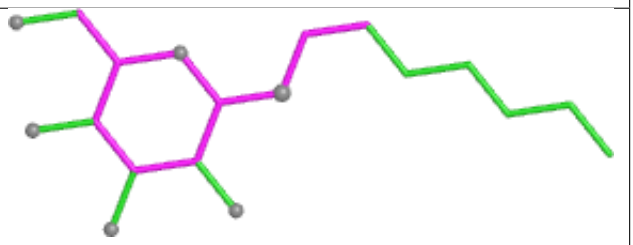
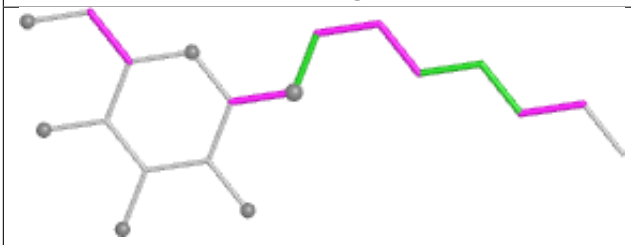


Bond angles



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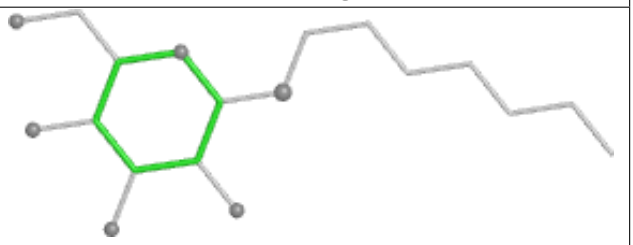
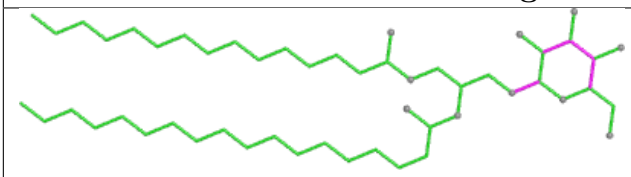
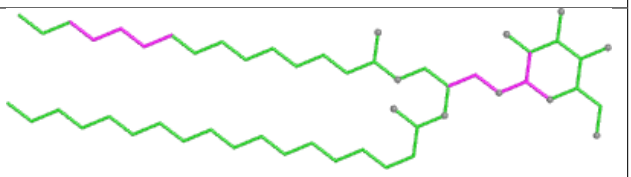


Rings

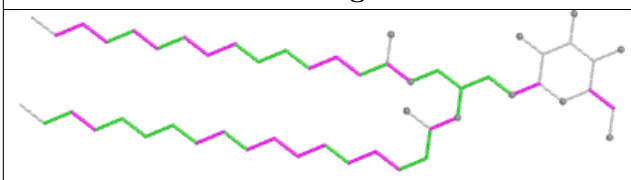
Ligand LMG B 852



Bond lengths



Bond angles



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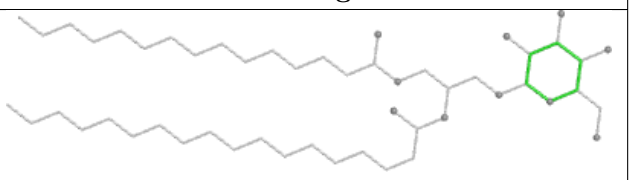
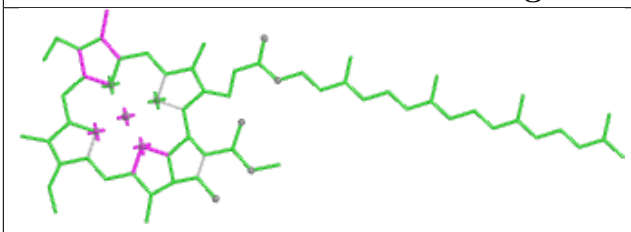


Rings

Ligand CLA B 831



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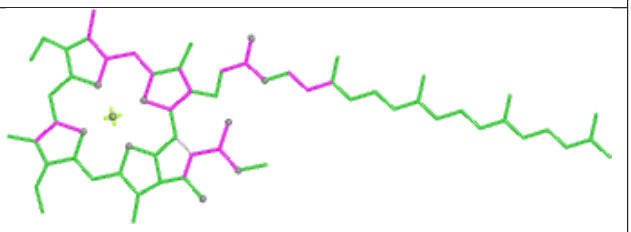
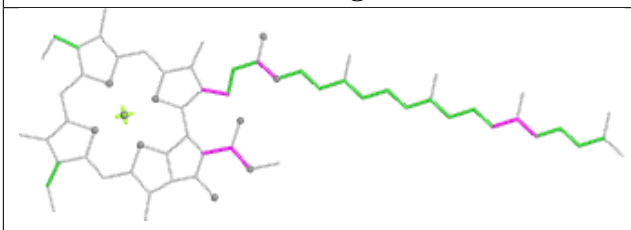
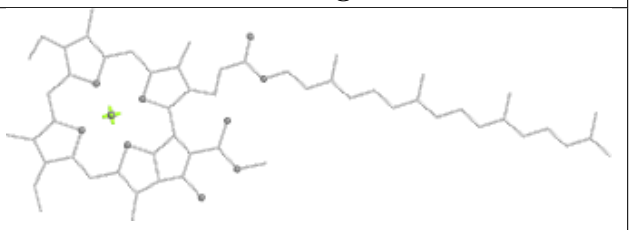


Bond angles

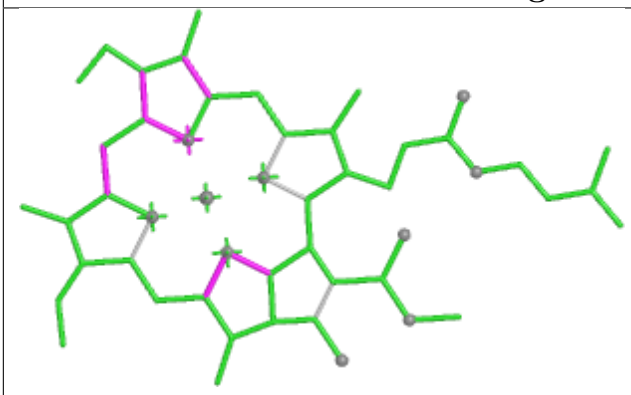


Torsions



Rings

Ligand CLA 3 603



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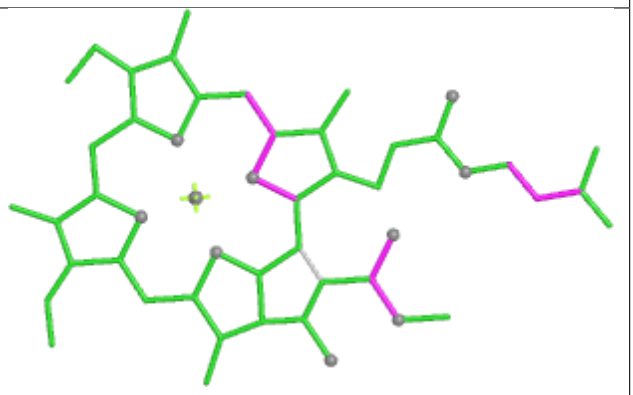
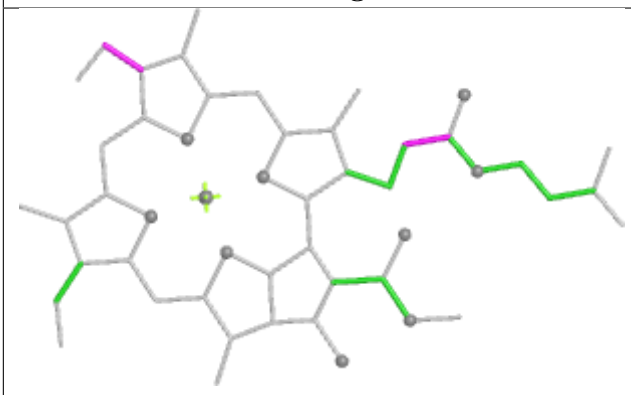


Bond angles



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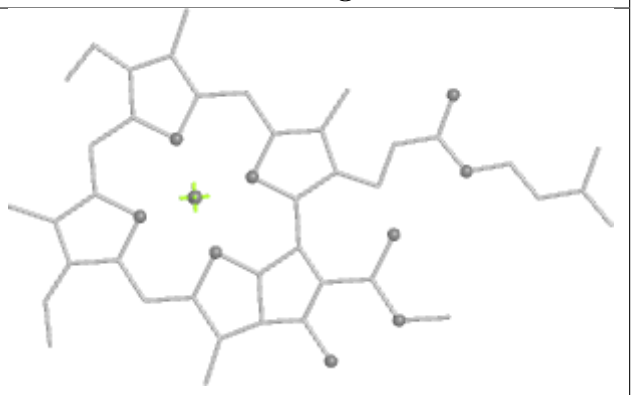
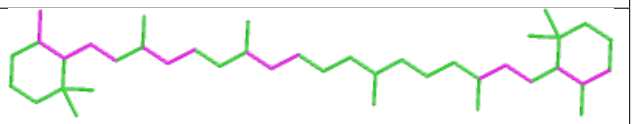


Rings

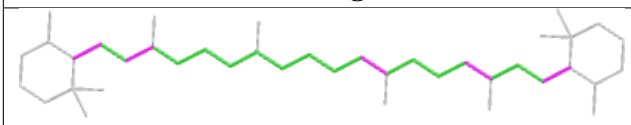
Ligand BCR A 848



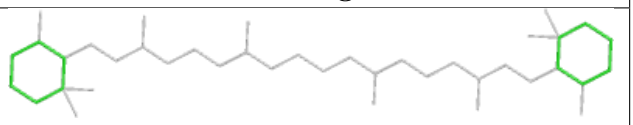
Bond lengths



Bond angles

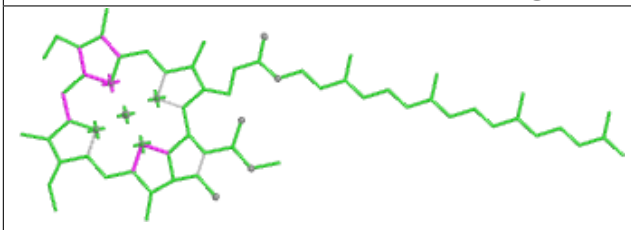


Torsions

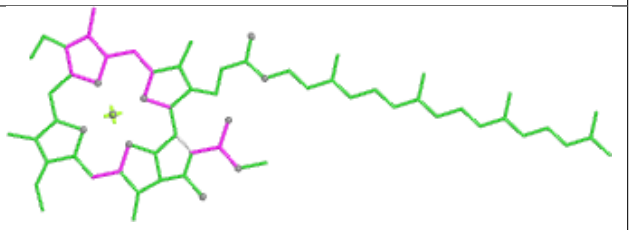


Rings

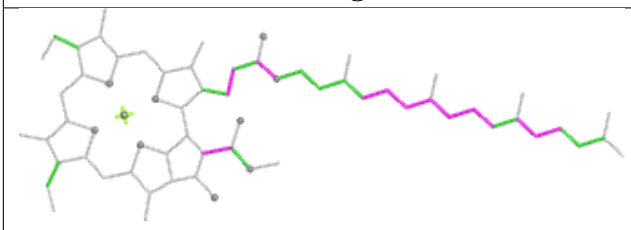
Ligand CLA 2 311



Bond lengths



Bond angles



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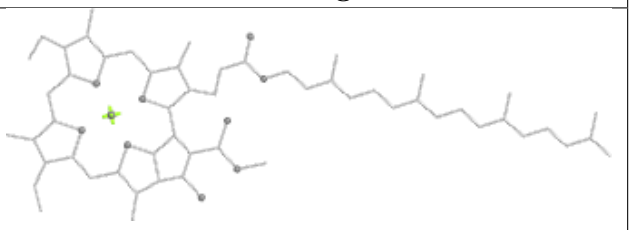
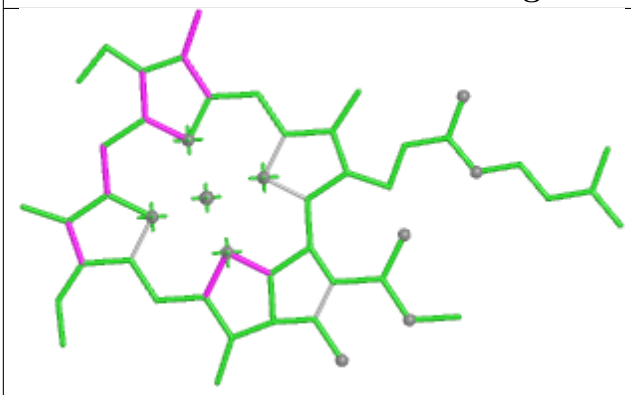


Rings

Ligand CLA G 104



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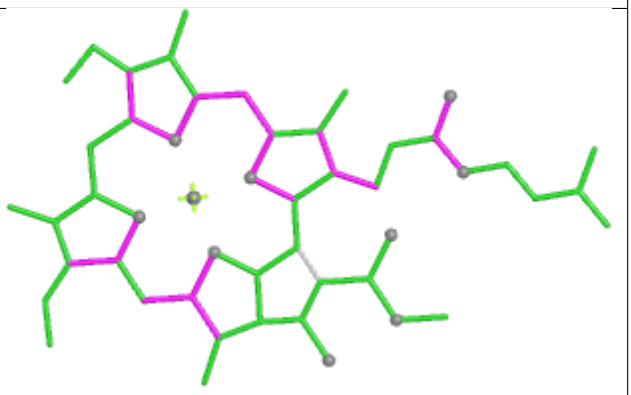

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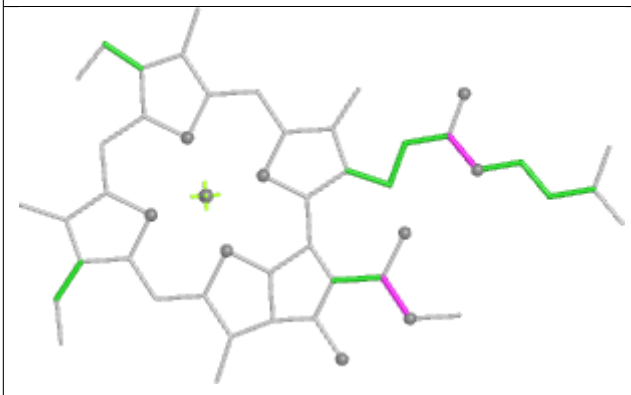

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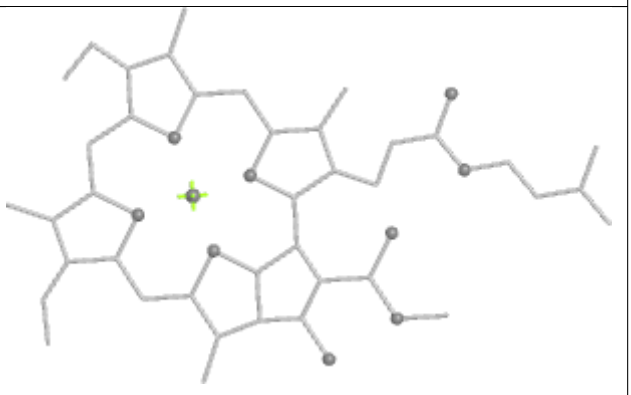
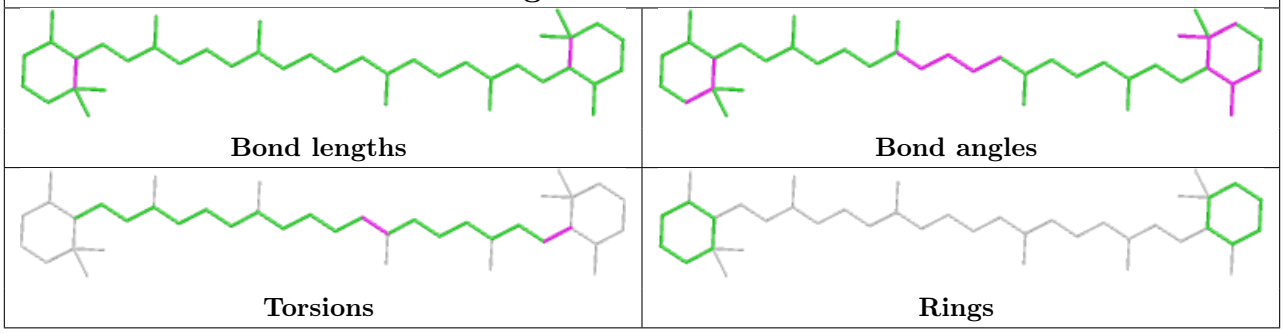
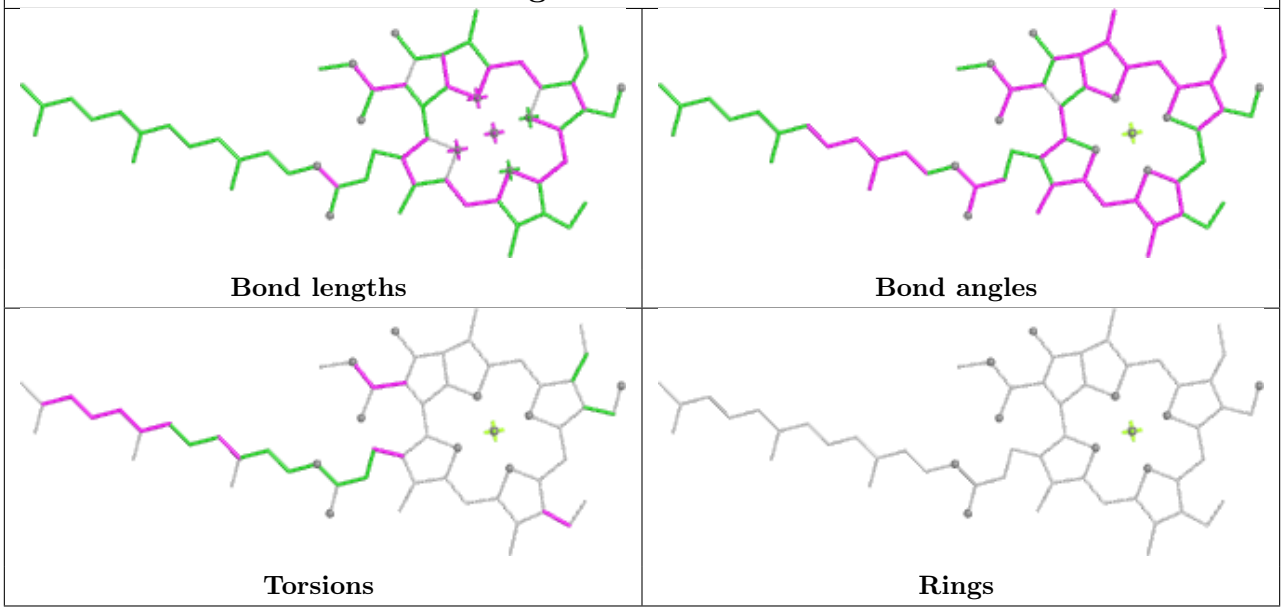


Rings

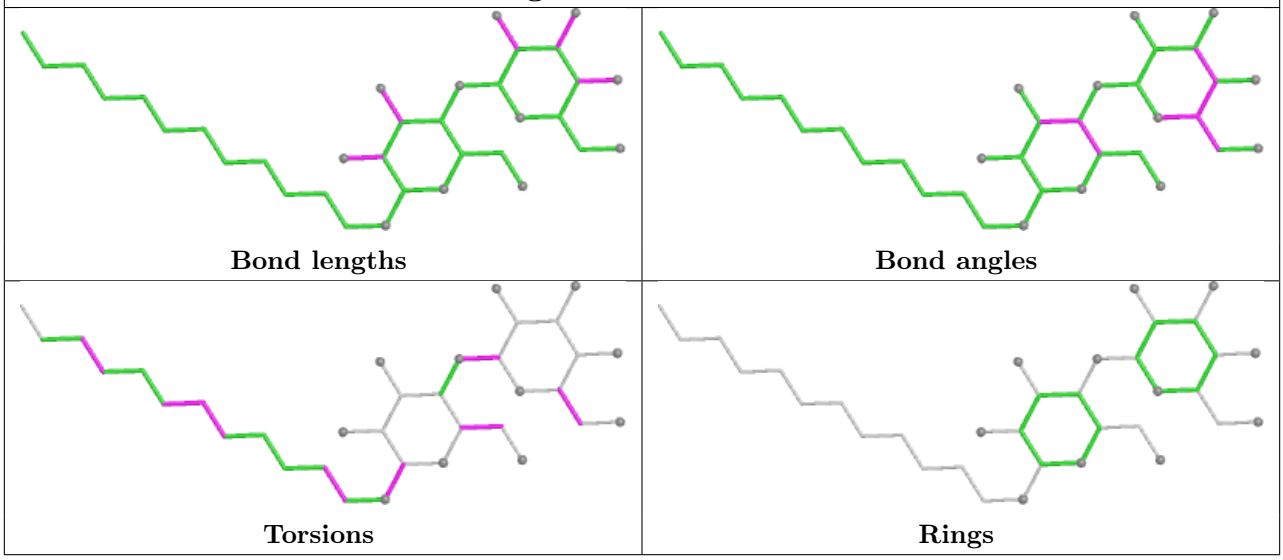
Ligand BCR B 848



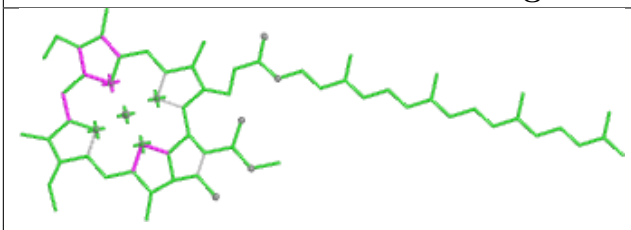
Ligand CHL 4 301



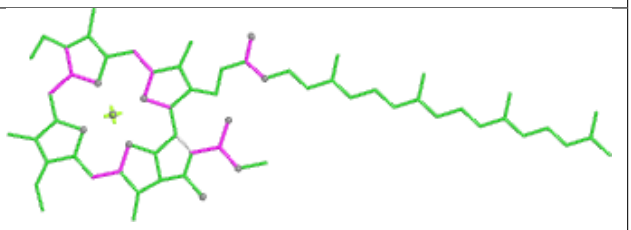
Ligand LMT 2 318



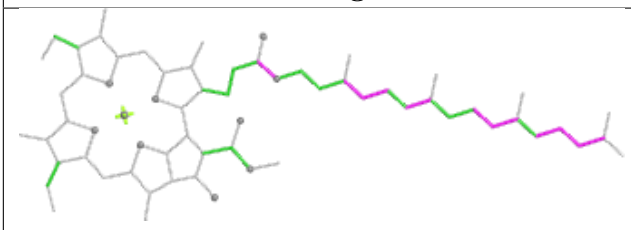
Ligand CLA A 836



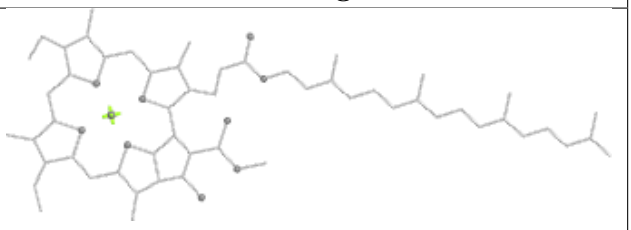
Bond lengths



Bond angles

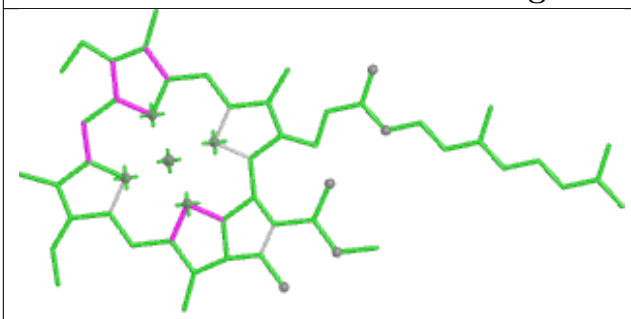


Torsions



Rings

Ligand CLA 3 611



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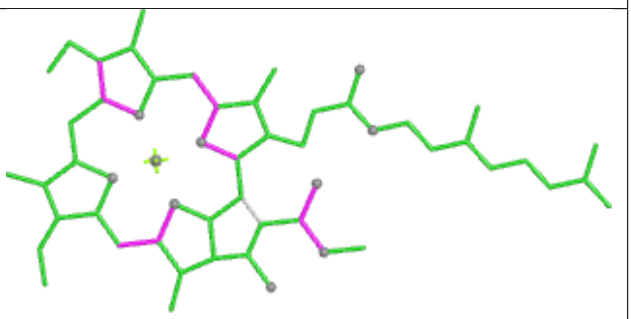
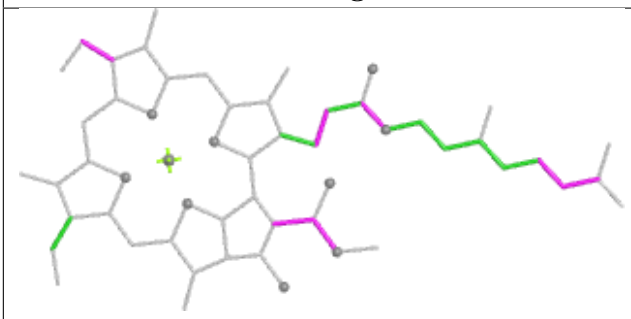


Bond angles



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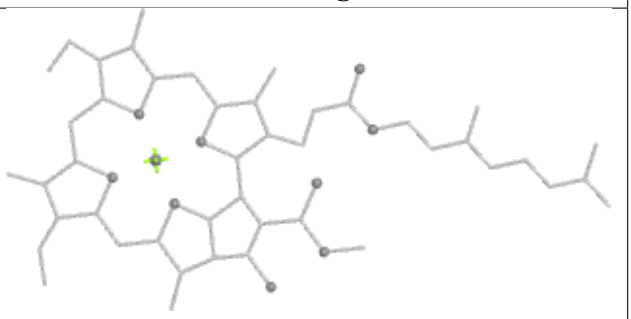
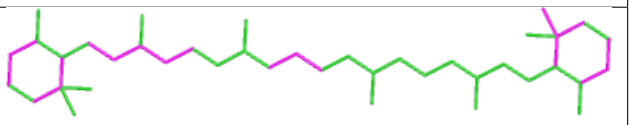


Rings

Ligand BCR 4 318



Bond lengths



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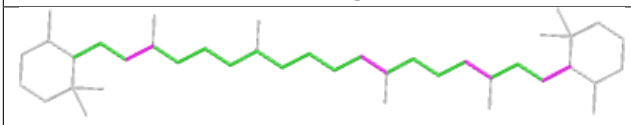

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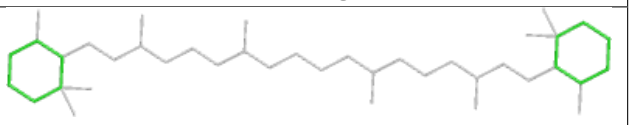
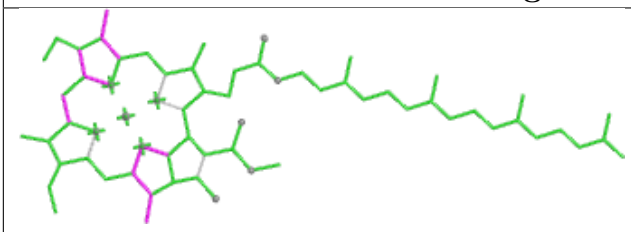


Rings

Ligand CLA A 818



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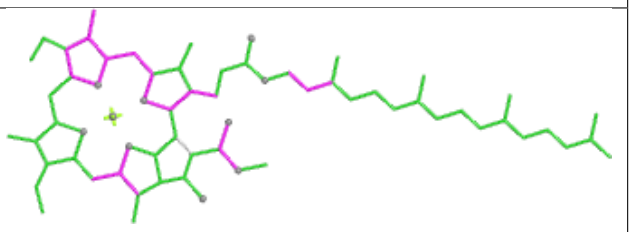
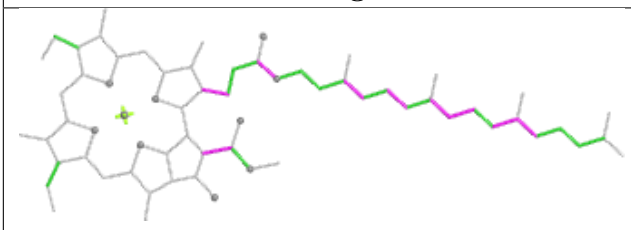


Bond angles



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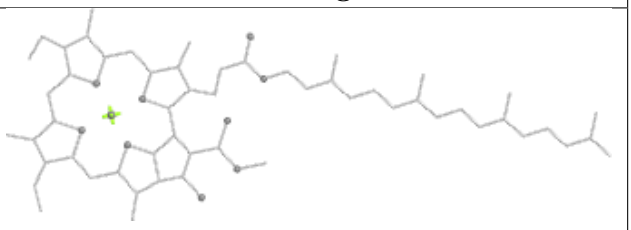
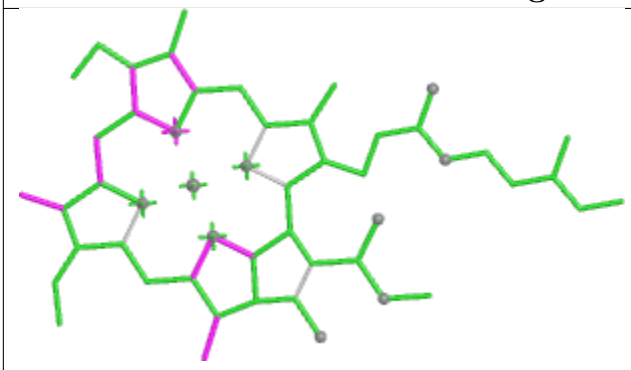


Rings

Ligand CLA 2 302



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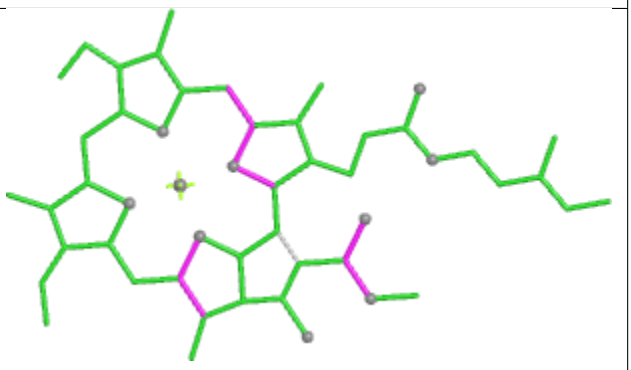
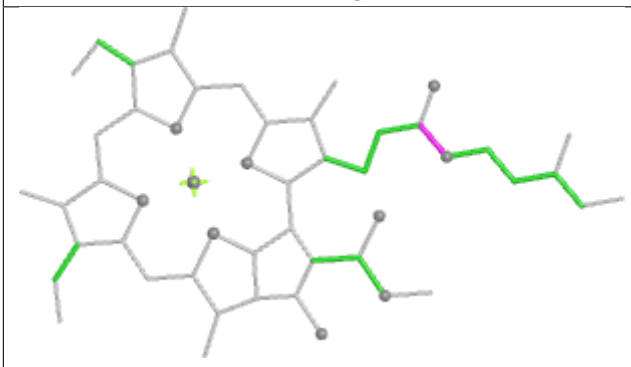


Bond angles



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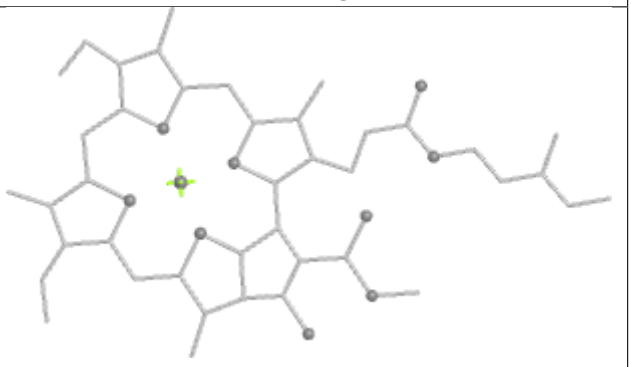
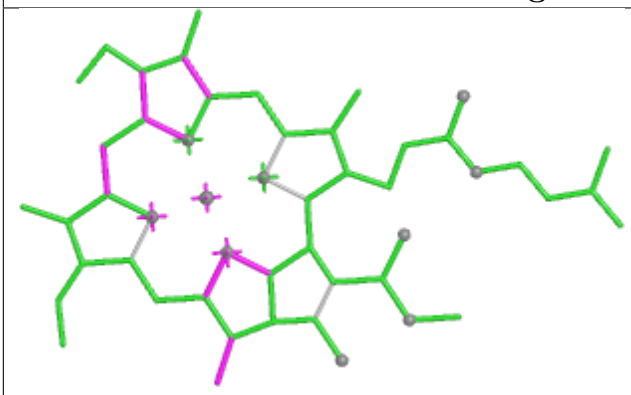


Rings

Ligand CLA 4 308



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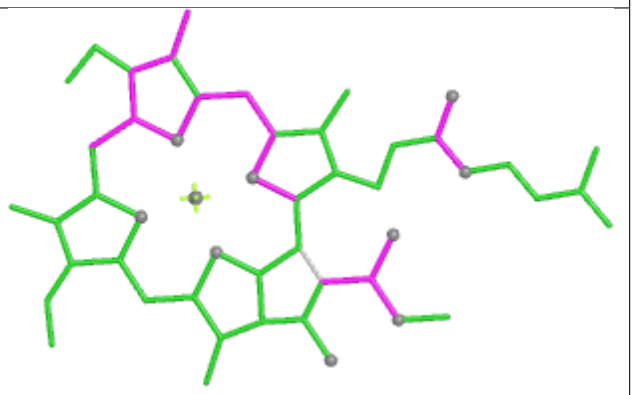
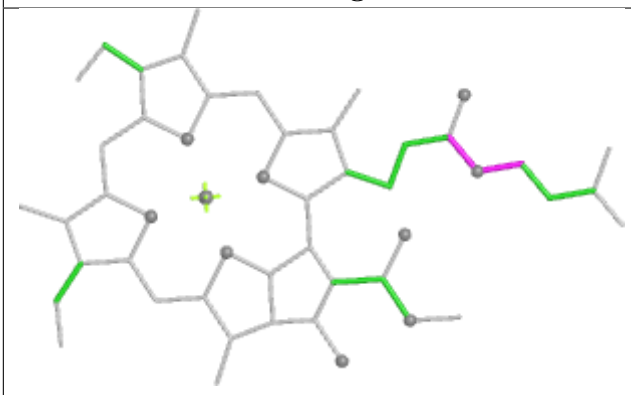


Bond angles



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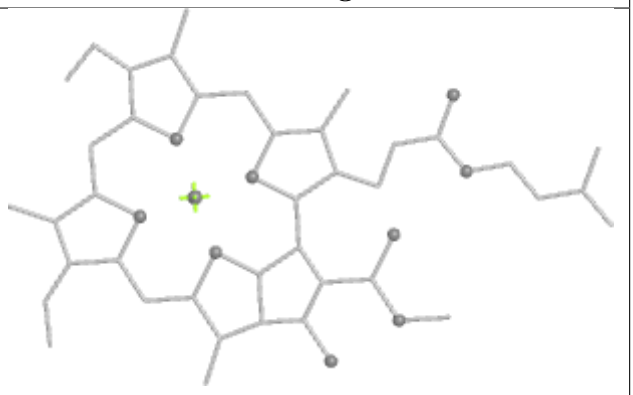
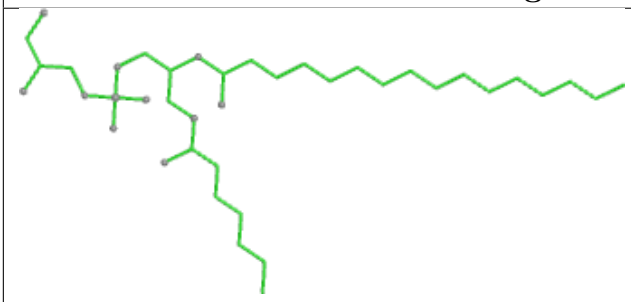


Rings

Ligand LHG F 302



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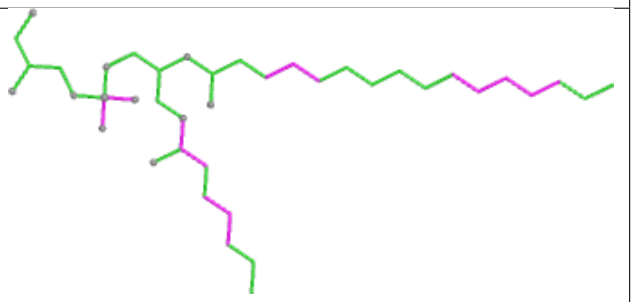

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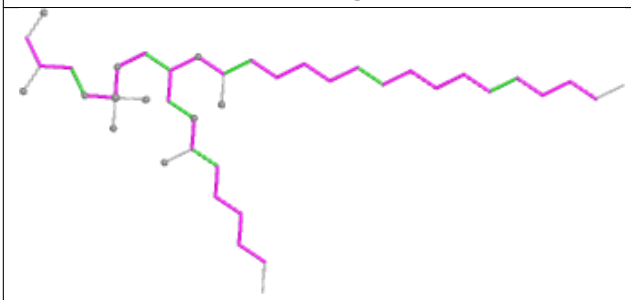

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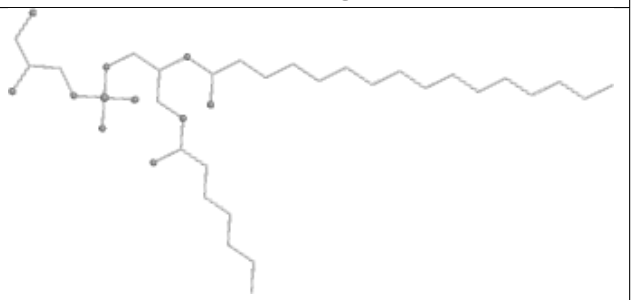
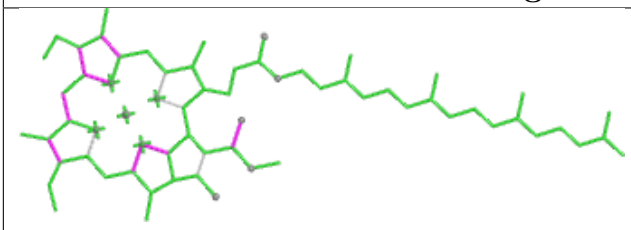


Rings

Ligand CLA B 827



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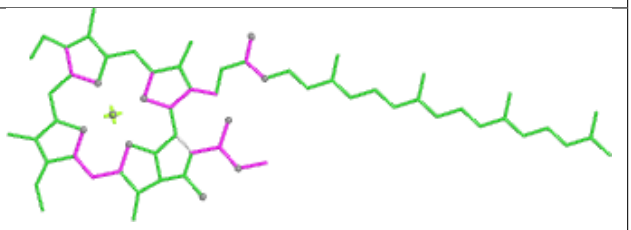
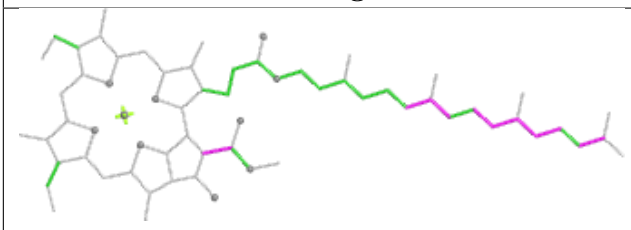


Bond angles



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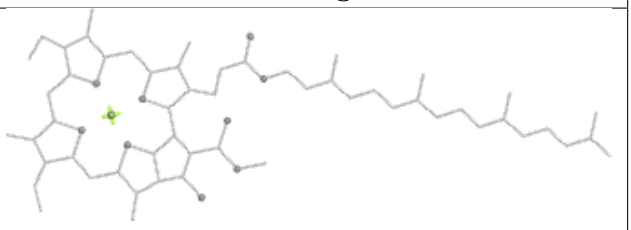
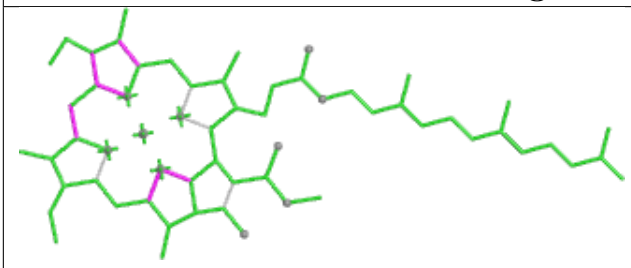


Rings

Ligand CLA 2 303



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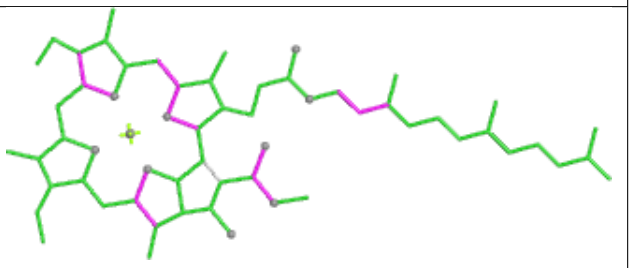
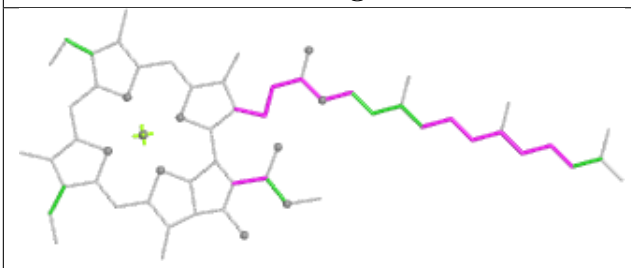


Bond angles



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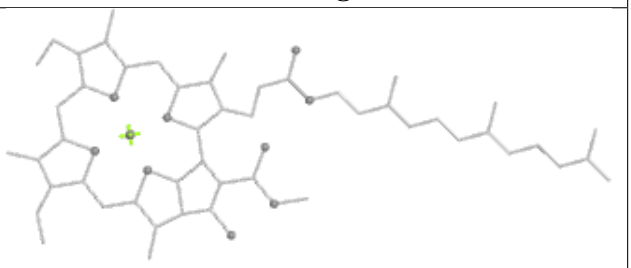
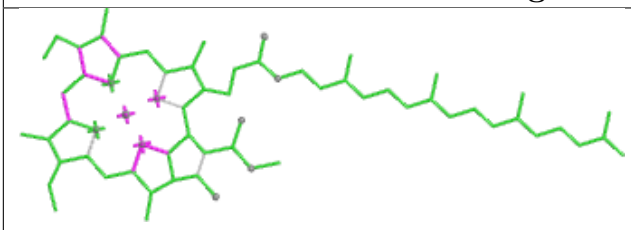
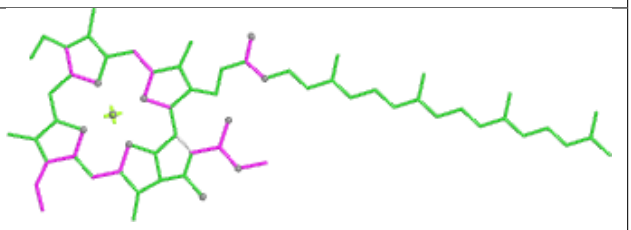
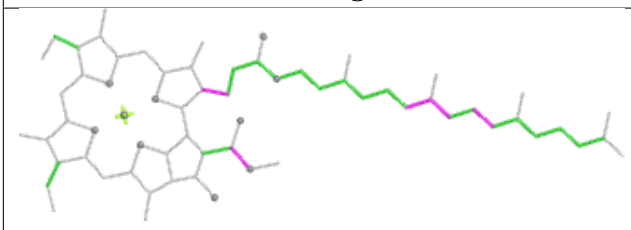
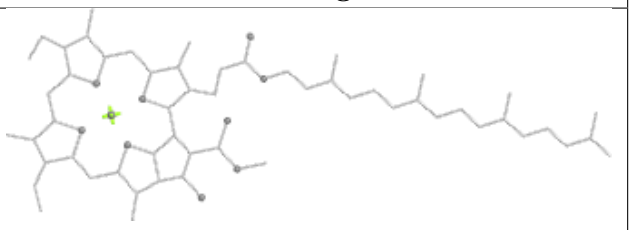
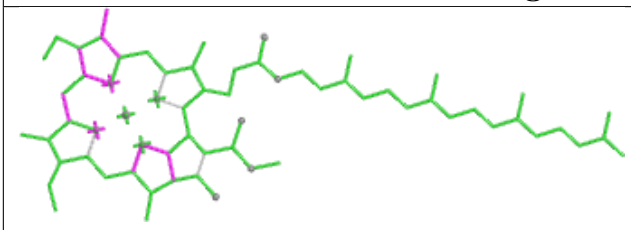
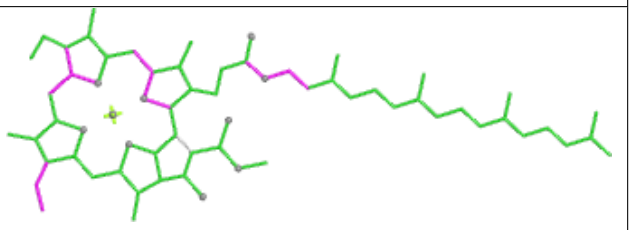
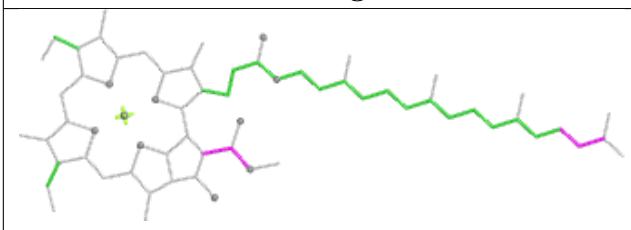
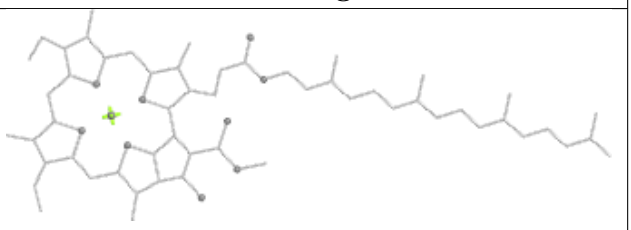
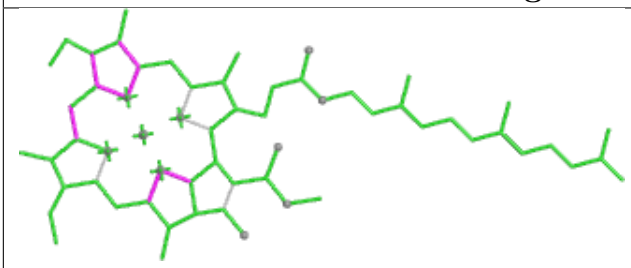


Rings

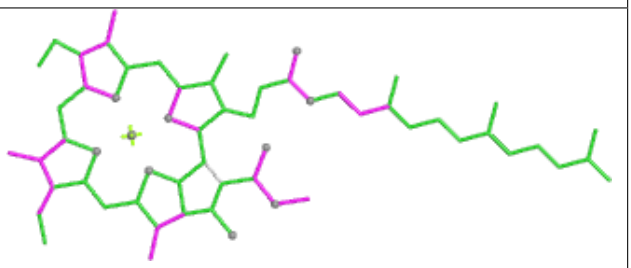
Ligand CLA J 101	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA B 804	
	
Bond lengths	Bond angles
	
Torsions	Rings

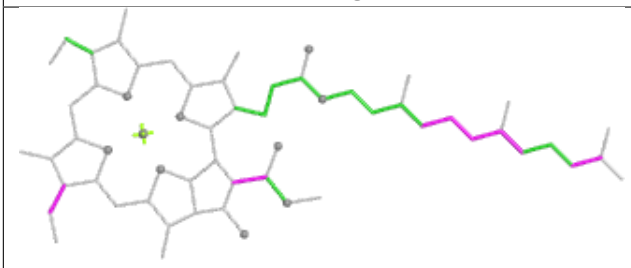
Ligand CLA B 837



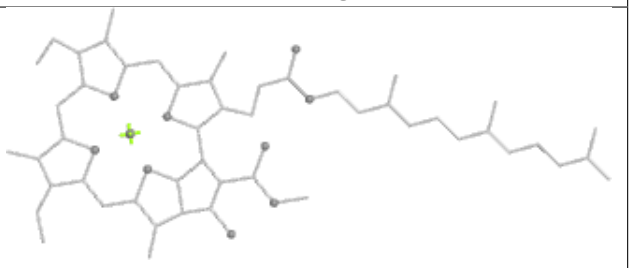
Bond lengths



Bond angles

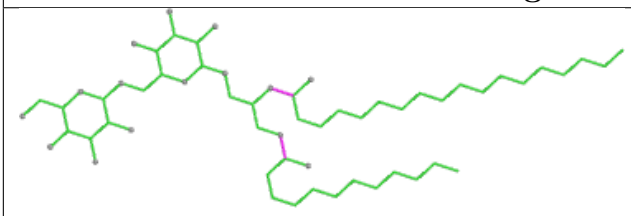


Torsions

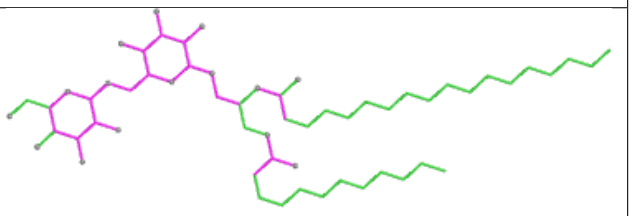


Rings

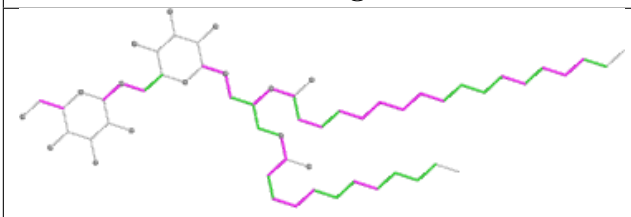
Ligand DGD 4 323



Bond lengths



Bond angles



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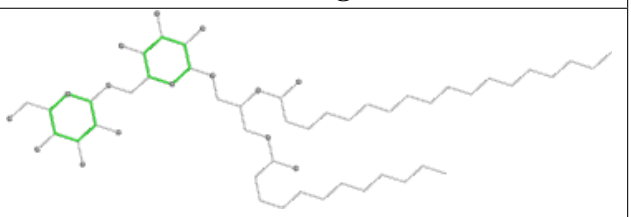
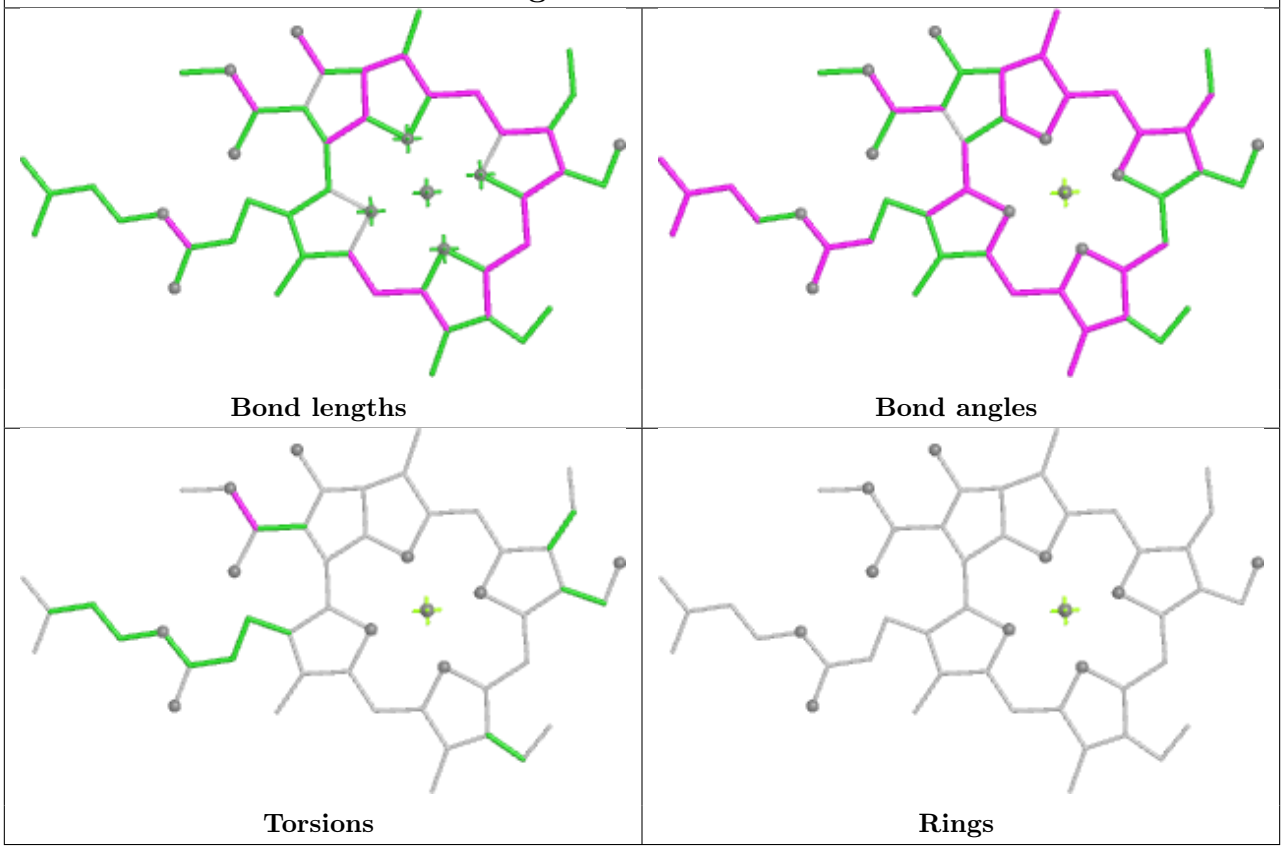
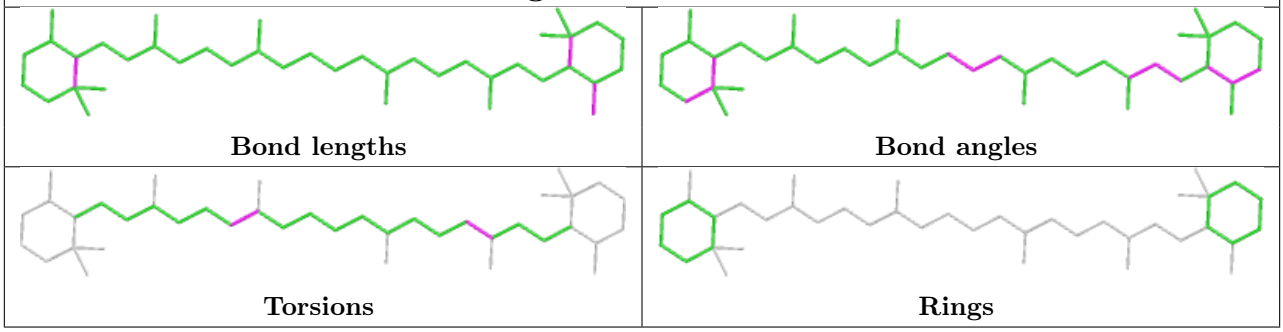


Rings

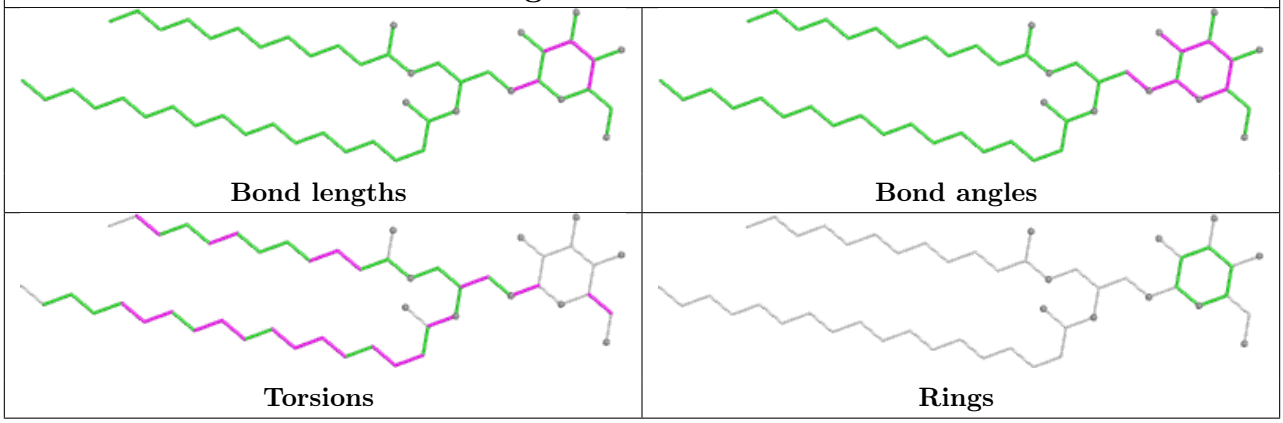
Ligand CHL 4 307



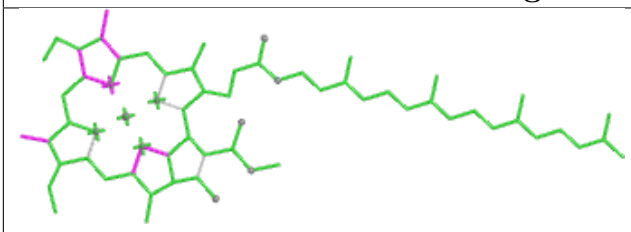
Ligand BCR J 104



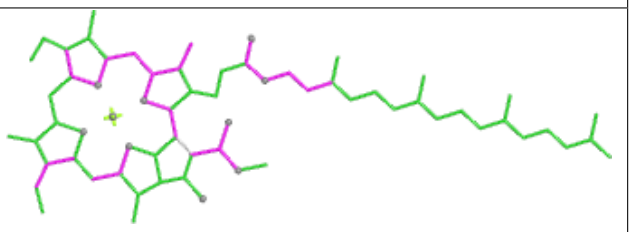
Ligand LMG 4 320



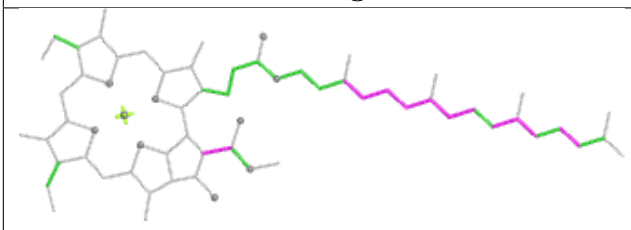
Ligand CLA A 838



Bond lengths



Bond angles



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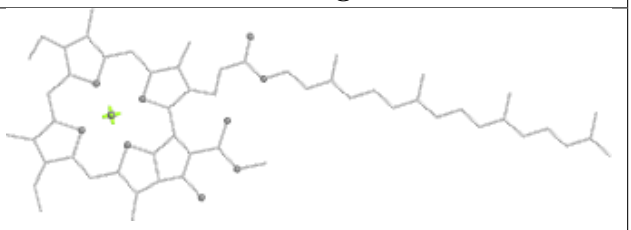
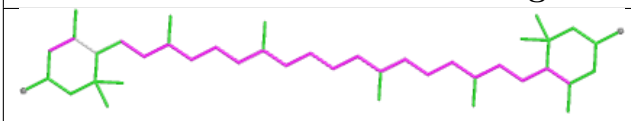


Rings

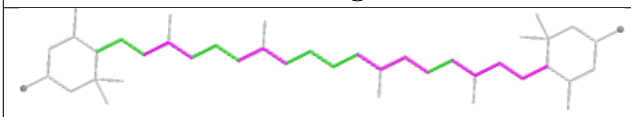
Ligand LUT 3 614



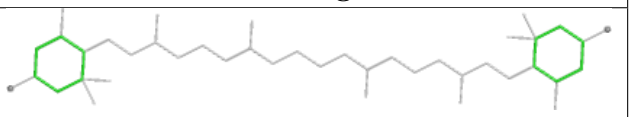
Bond lengths



Bond angles

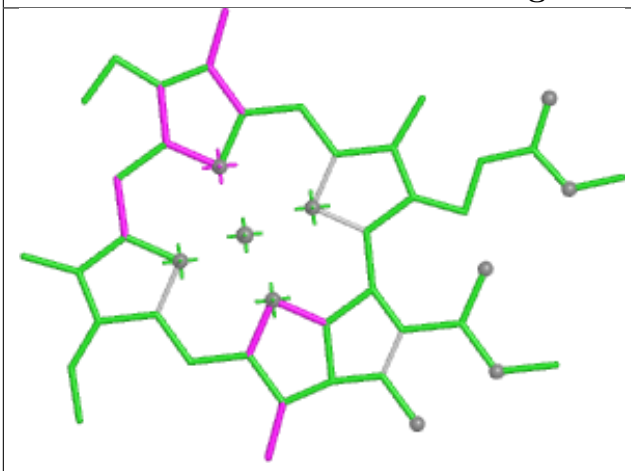


Torsions

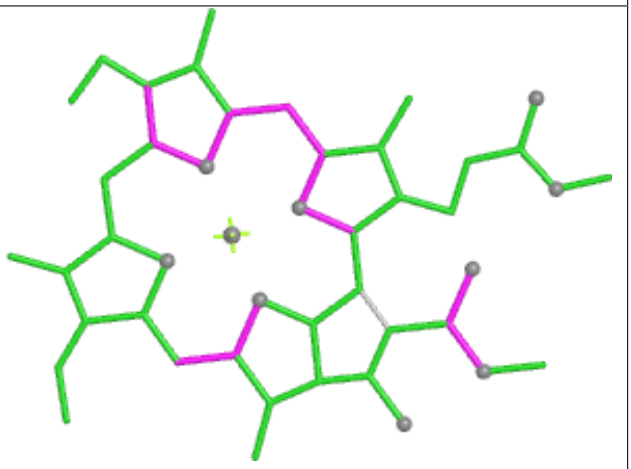


Rings

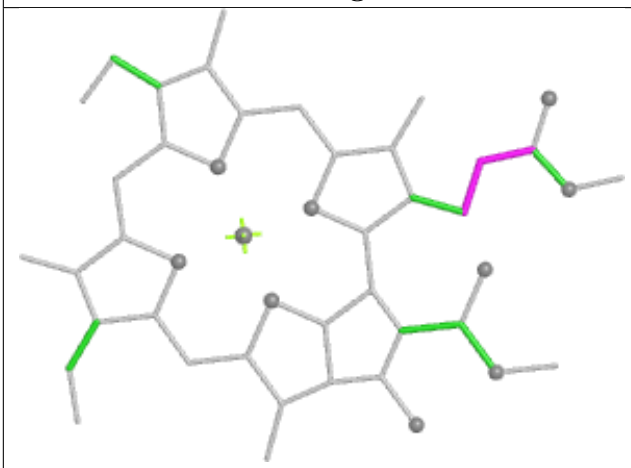
Ligand CLA 3 613



Bond lengths



Bond angles



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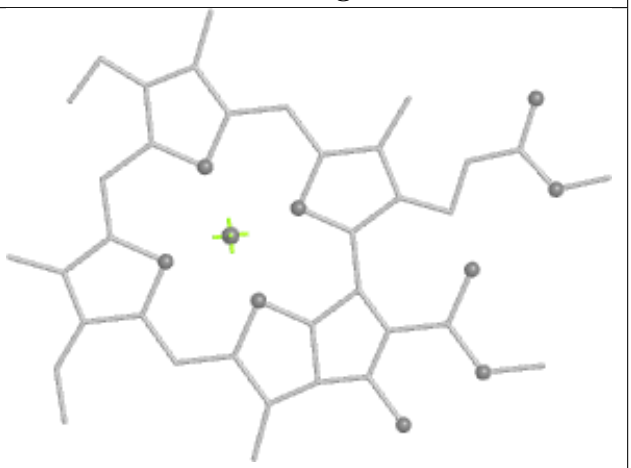
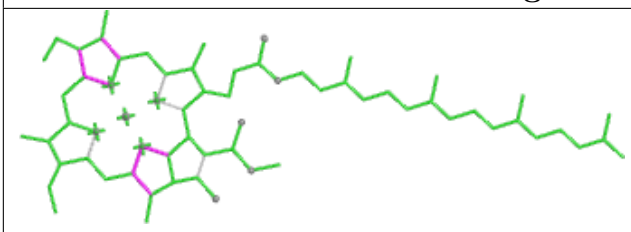


Rings

Ligand CLA A 837



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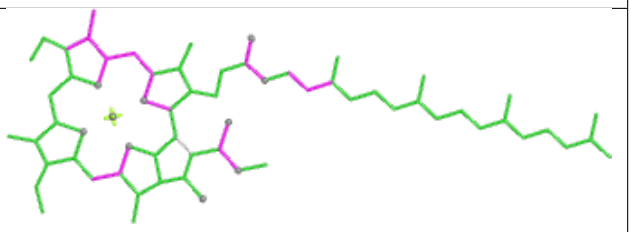
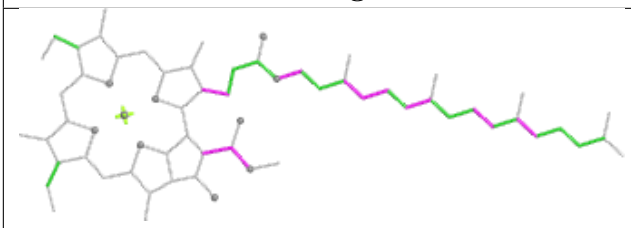
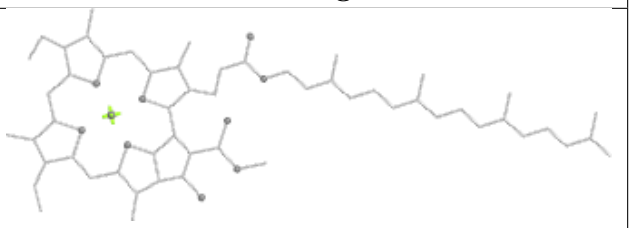


Bond angles

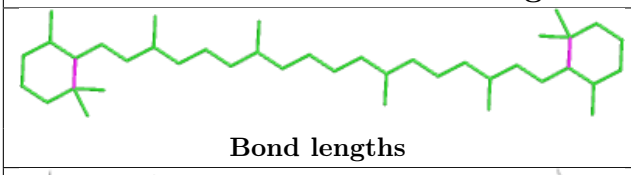


Torsions



Rings

Ligand BCR L 201



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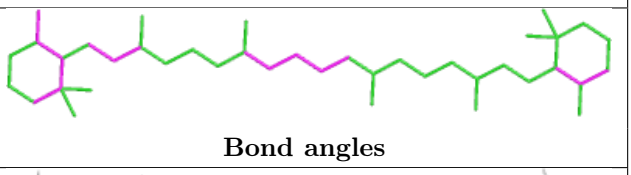
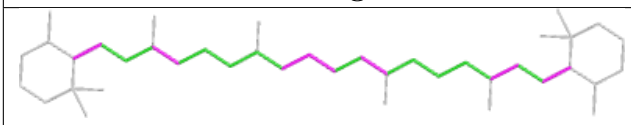


Bond angles



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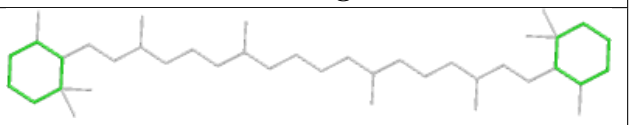
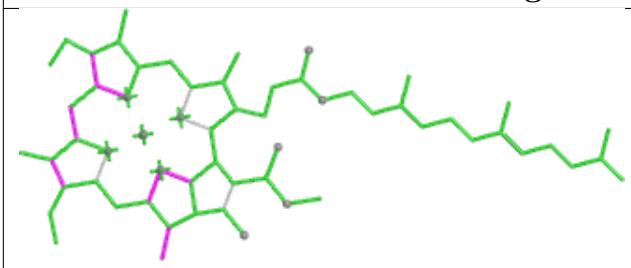


Rings

Ligand CLA B 820



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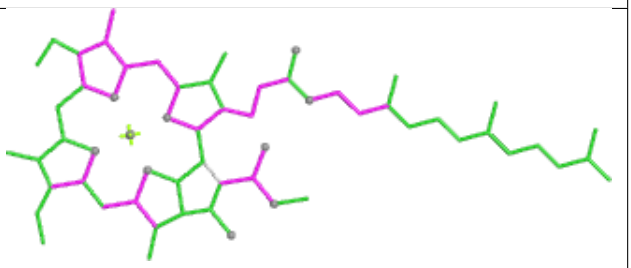
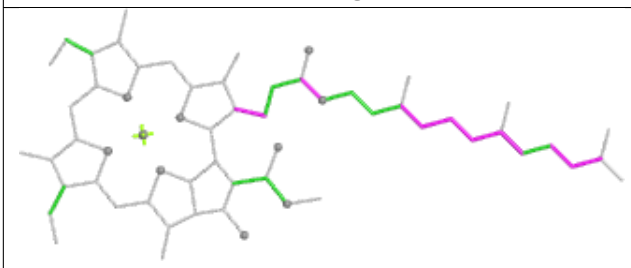


Bond angles



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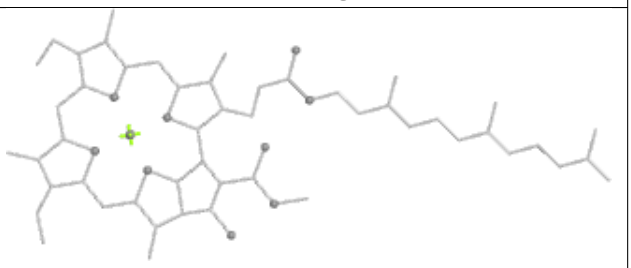
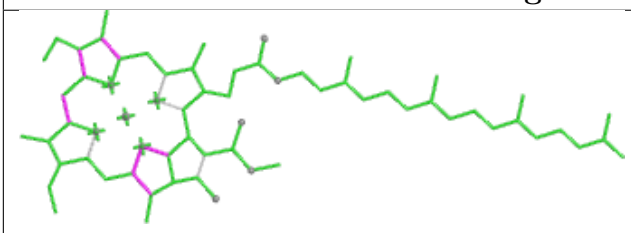


Rings

Ligand CLA B 821



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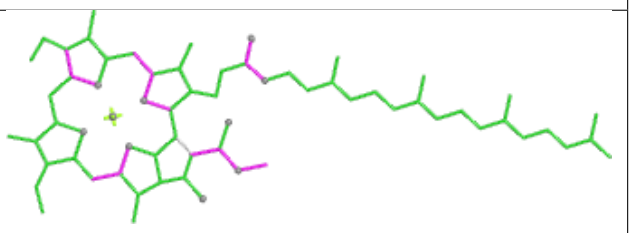
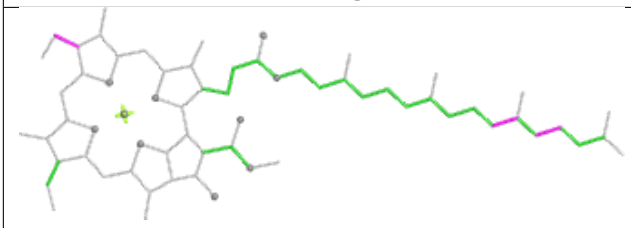


Bond angles



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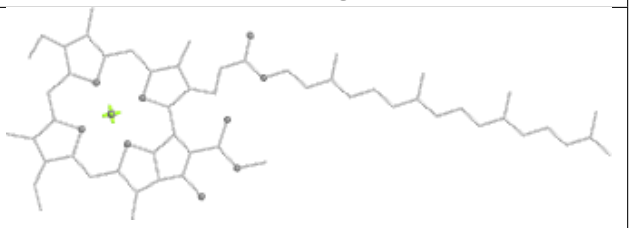
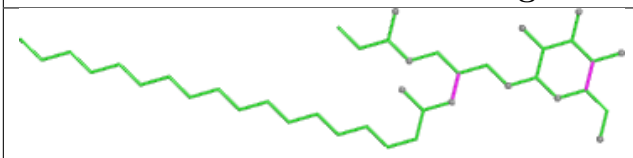


Rings

Ligand LMG G 101



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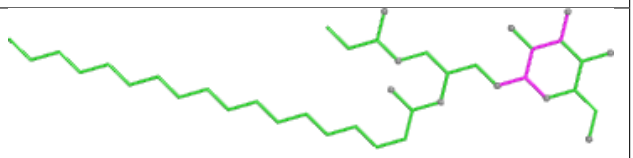
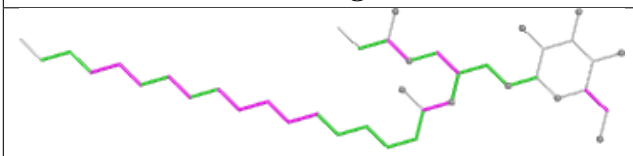


Bond angles



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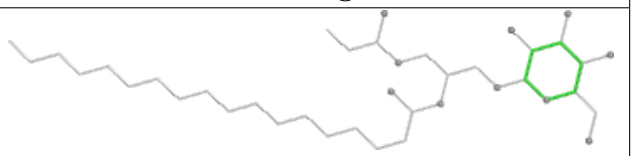
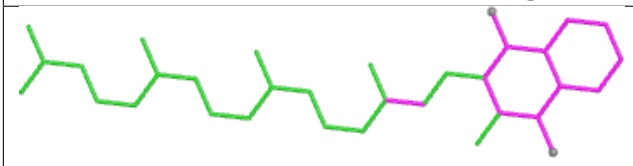


Rings

Ligand PQN B 843



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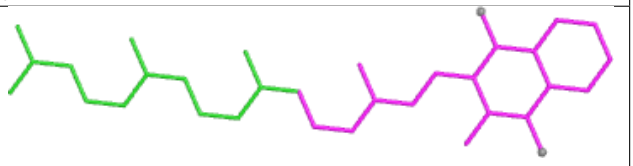
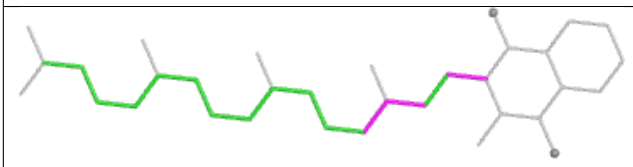


Bond angles



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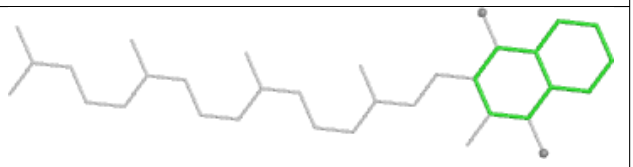
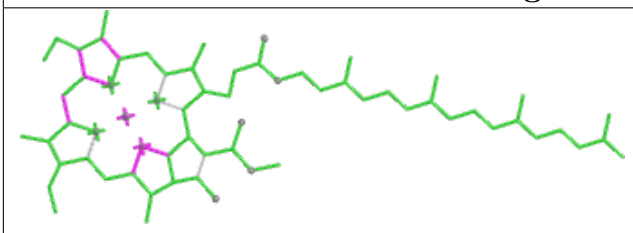


Rings

Ligand CLA A 802



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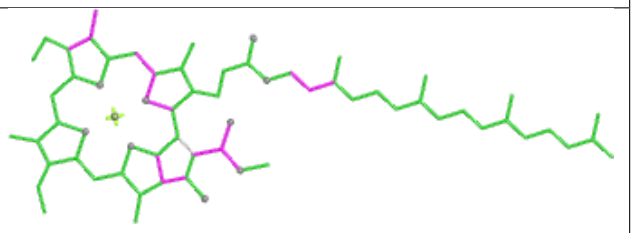
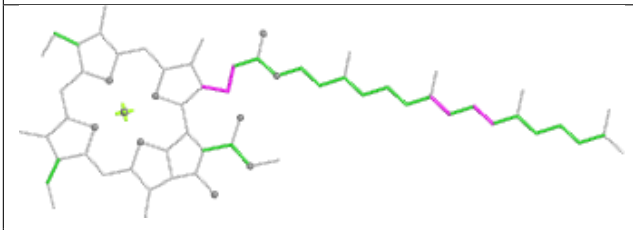


Bond angles



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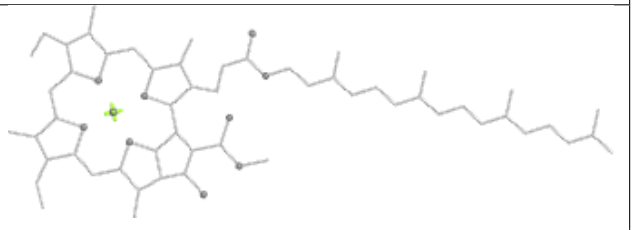
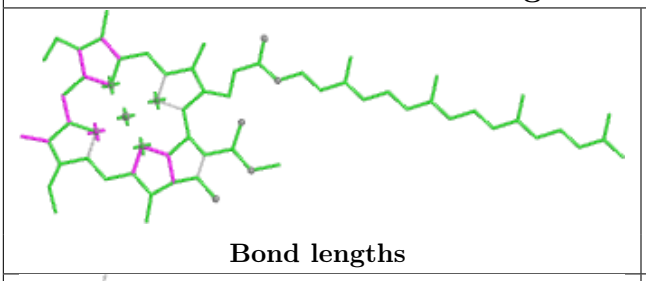
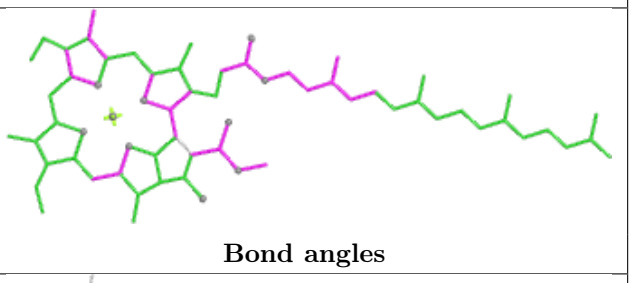


Rings

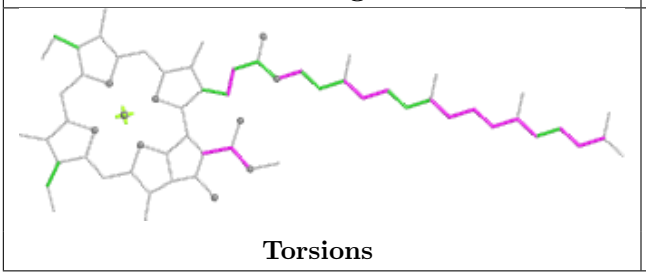
Ligand CLA A 853



Bond lengths



Bond angles



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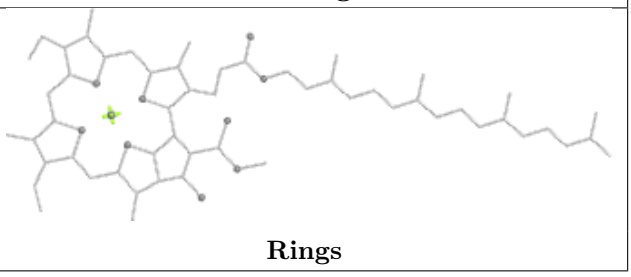
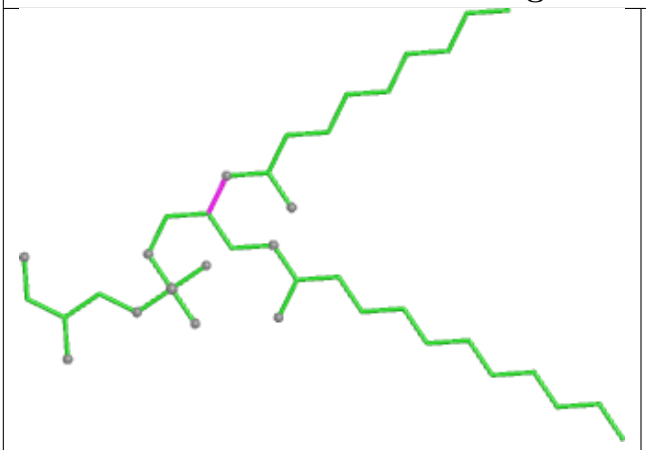


Rings

Ligand LHG 2 317



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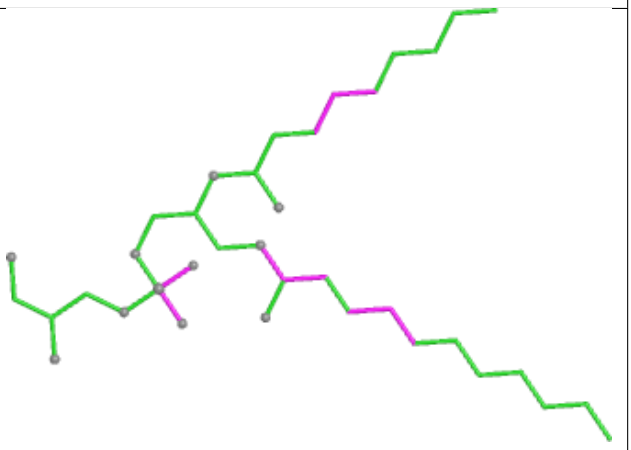
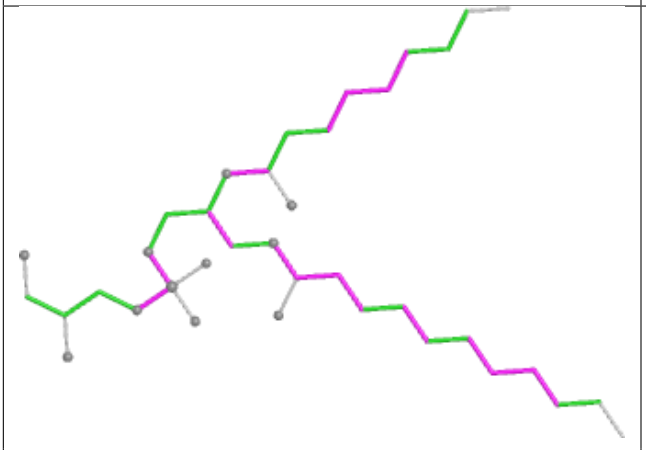


Bond angles



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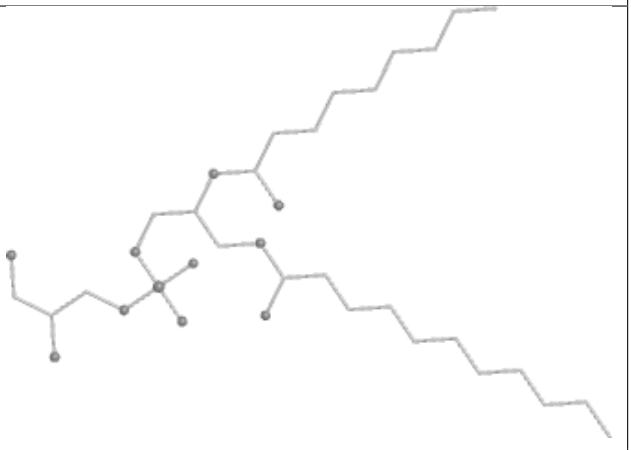
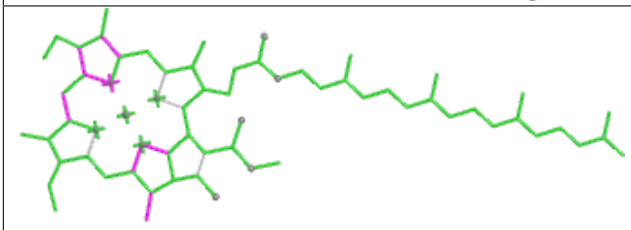
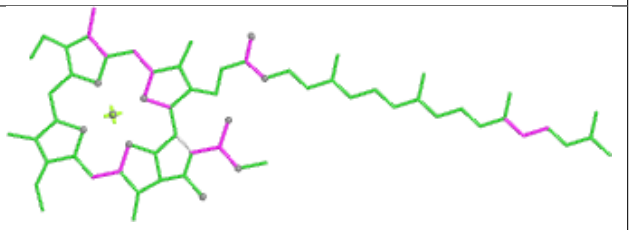


Rings

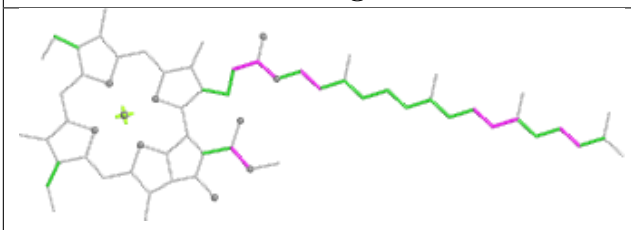
Ligand CLA A 824



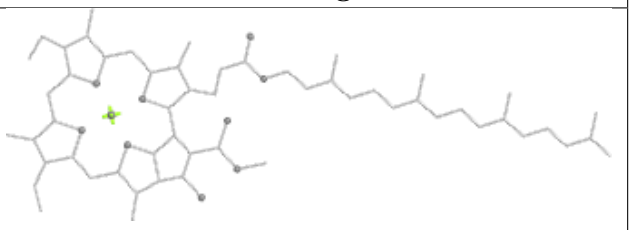
Bond lengths



Bond angles

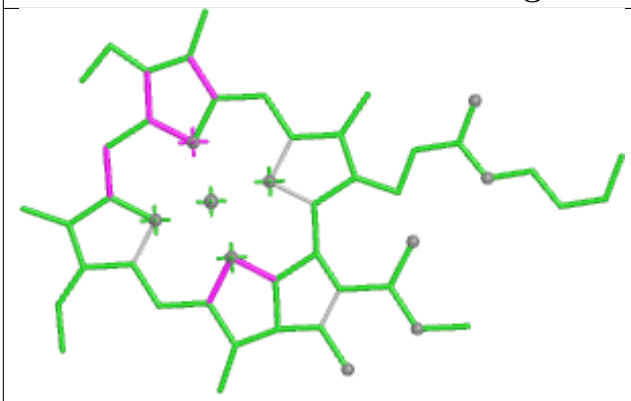


Torsions

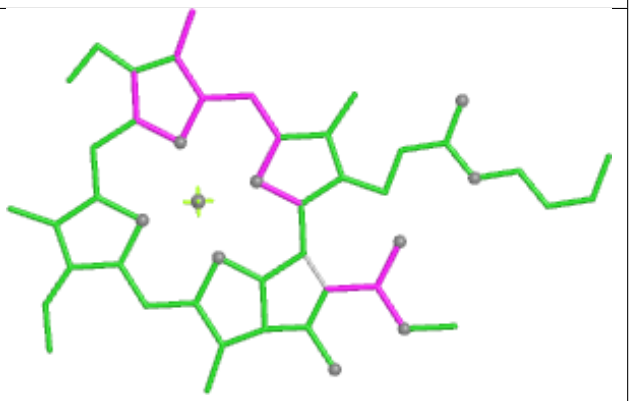


Rings

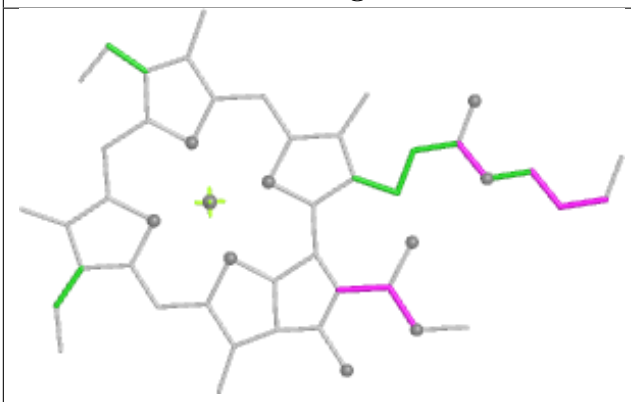
Ligand CLA A 821



Bond lengths



Bond angles



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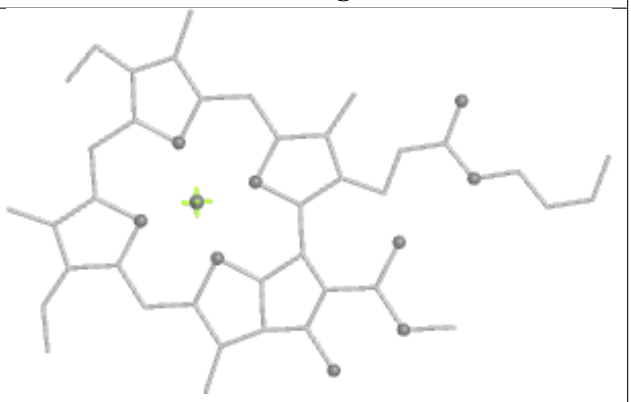
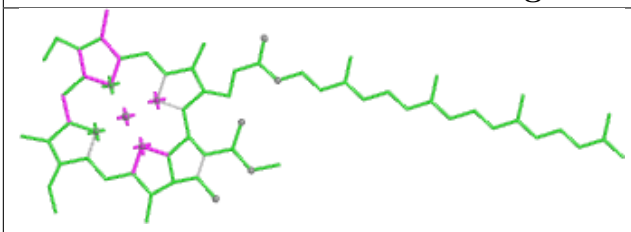


Rings

Ligand CLA B 826



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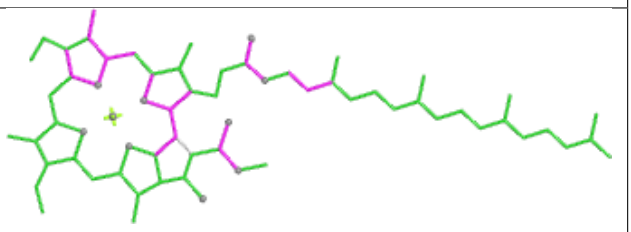

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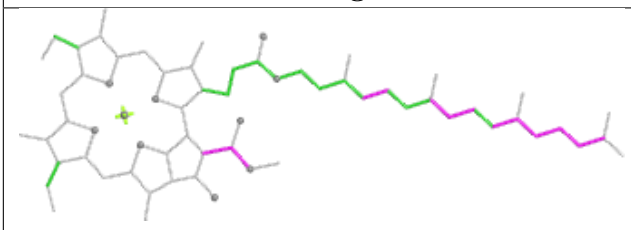

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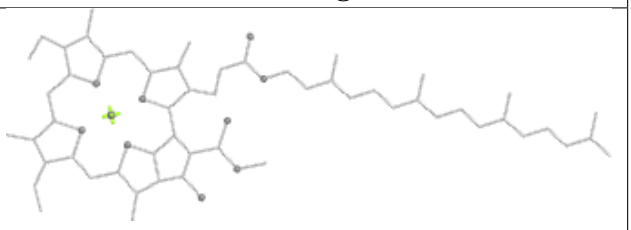
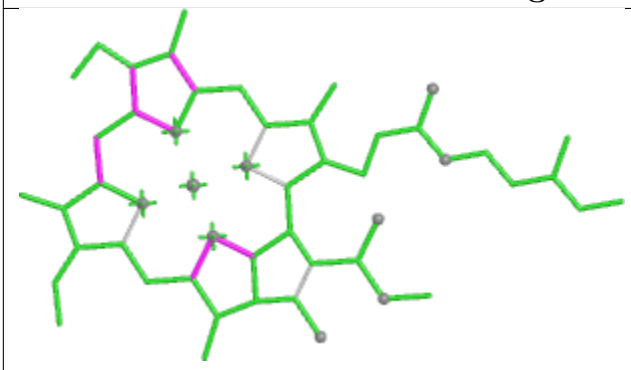


Rings

Ligand CLA 1 303



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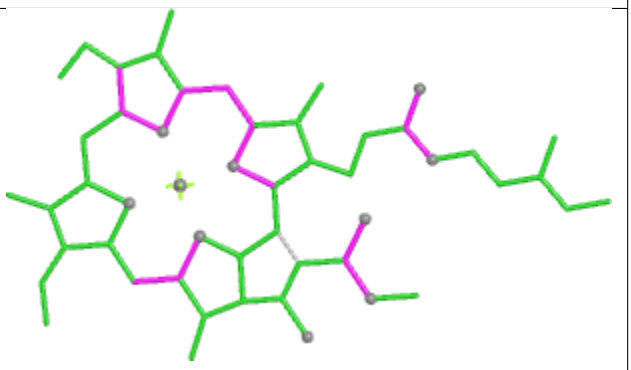
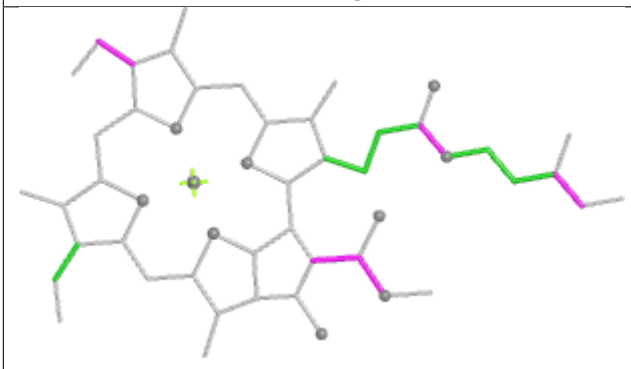


Bond angles



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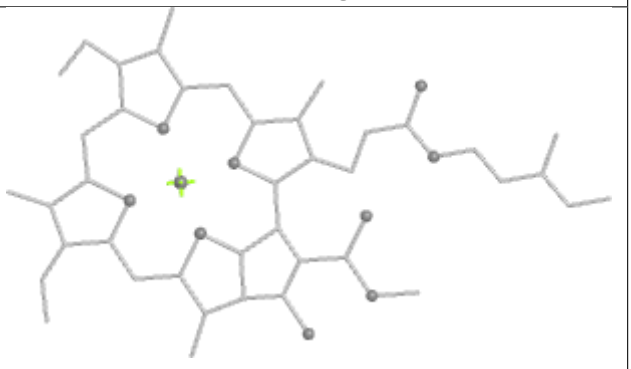
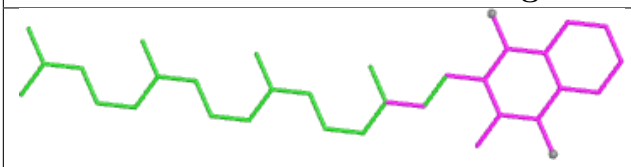


Rings

Ligand PQN A 842



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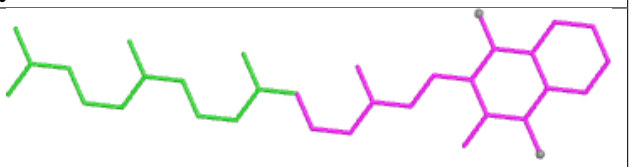
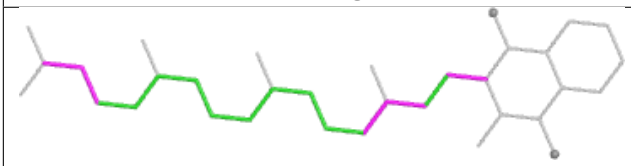


Bond angles



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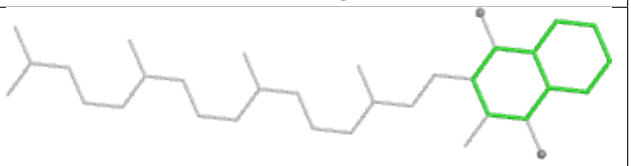
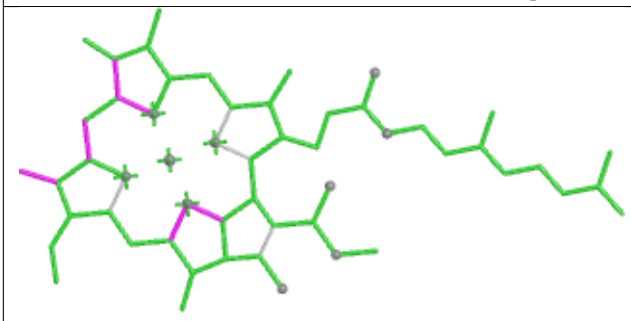


Rings

Ligand CLA B 813



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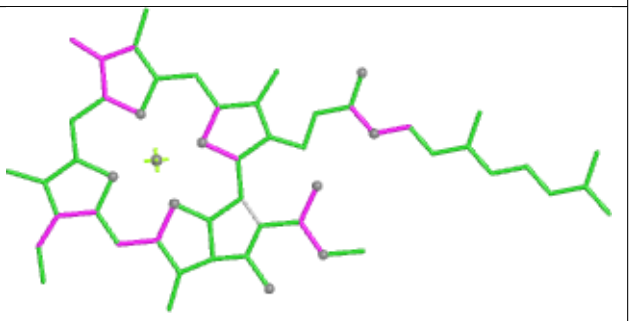
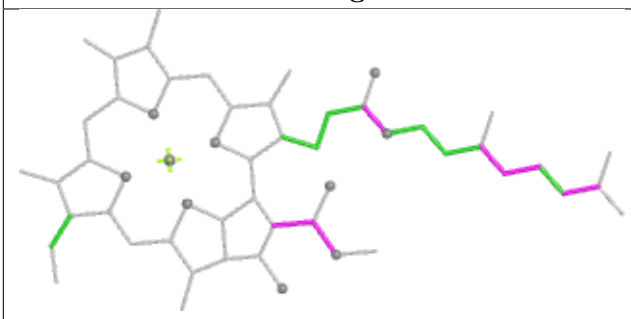


Bond angles



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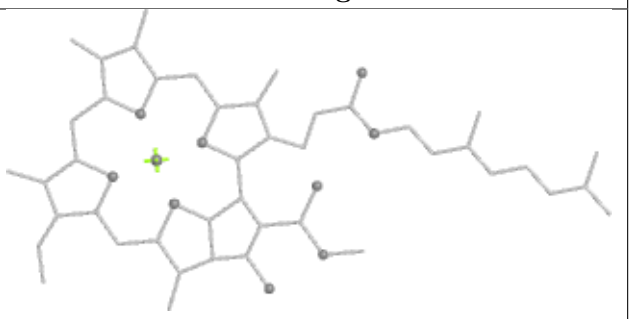
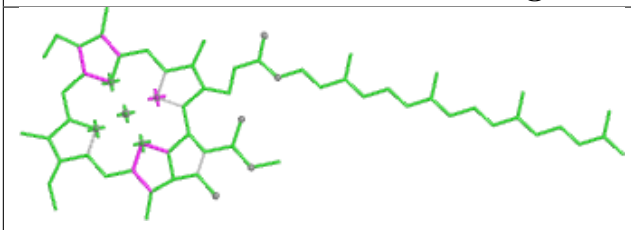


Rings

Ligand CLA F 304



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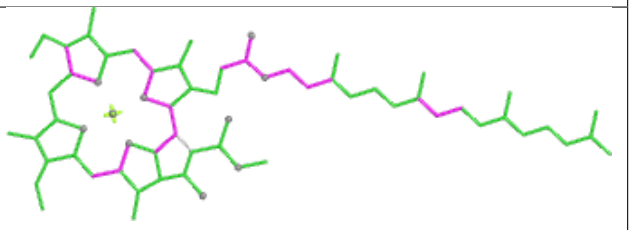
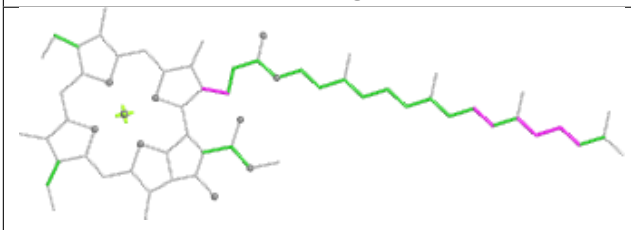


Bond angles



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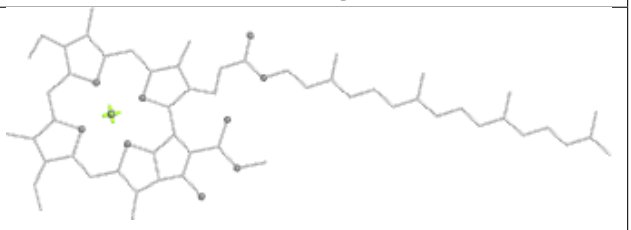
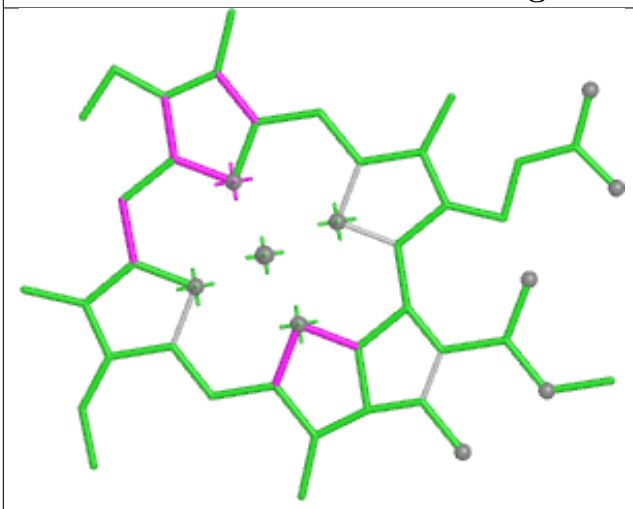


Rings

Ligand CLA 4 313



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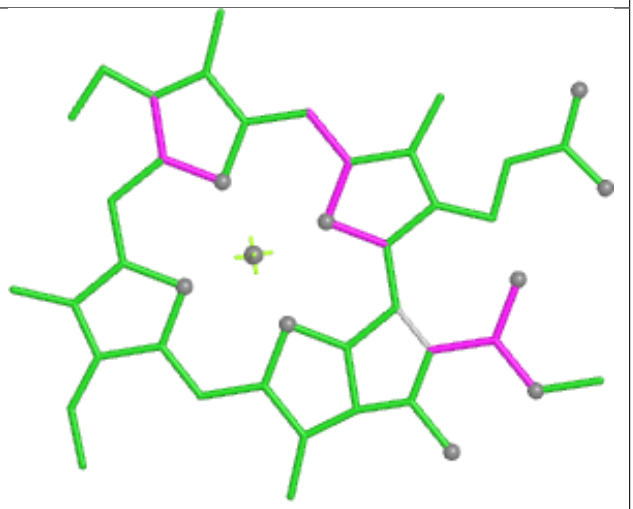
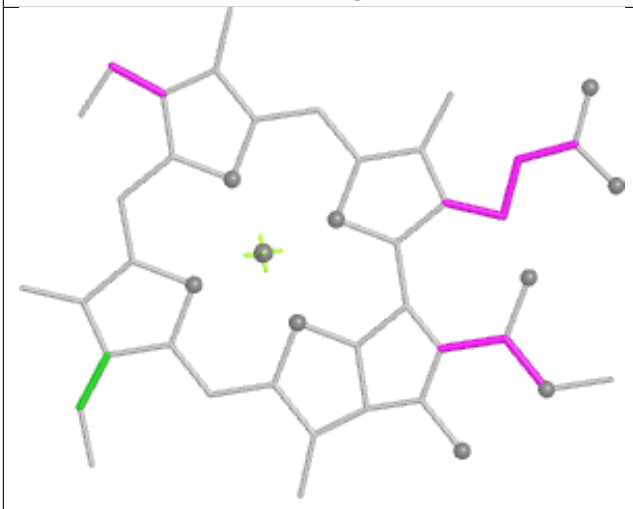


Bond angles

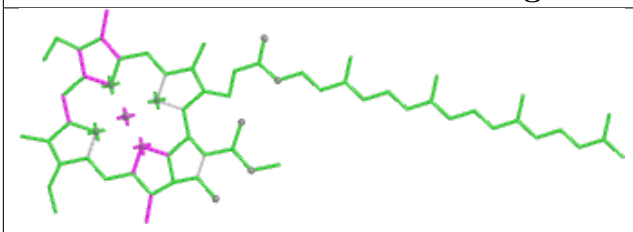


Torsions



Rings

Ligand CLA A 826



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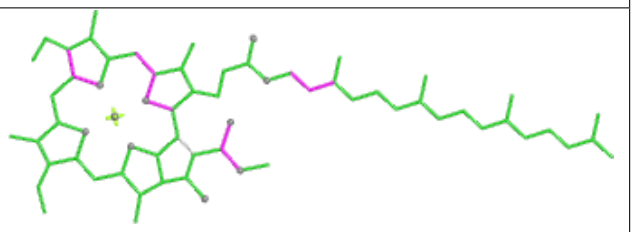

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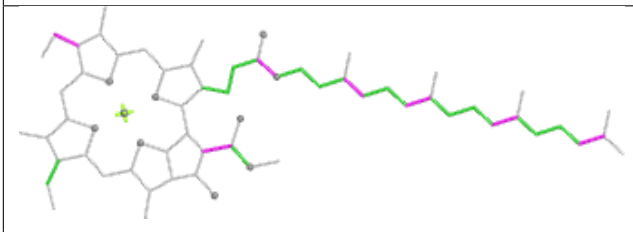

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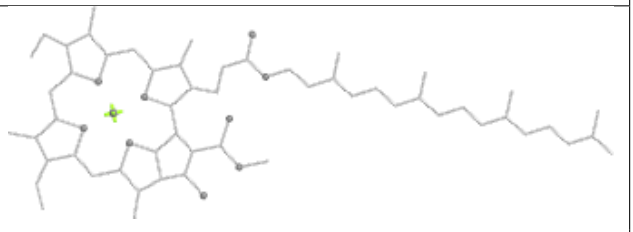
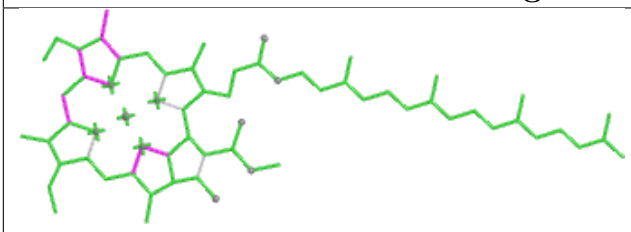
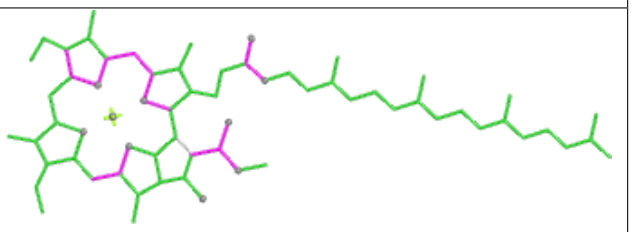


Rings

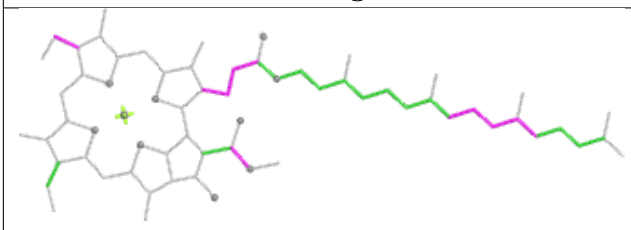
Ligand CLA A 817



Bond lengths



Bond angles



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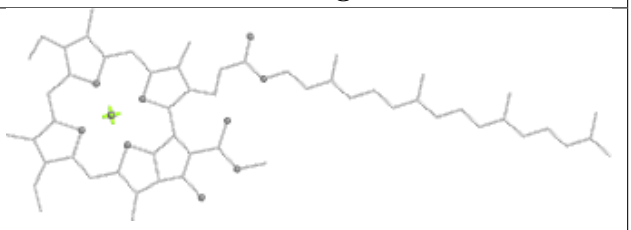
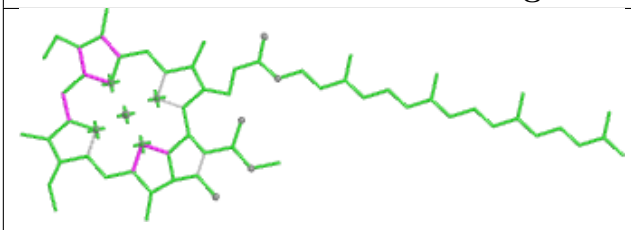


Rings

Ligand CLA A 828



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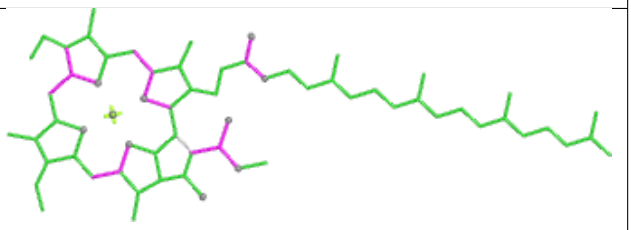
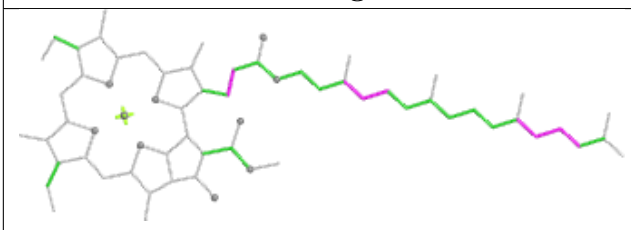


Bond angles



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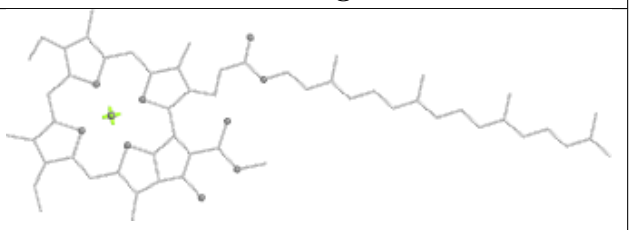
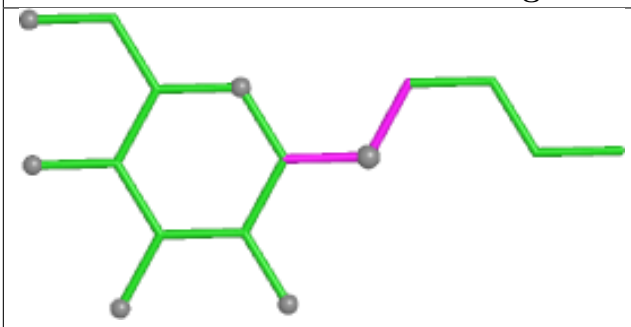


Rings

Ligand HTG F 310



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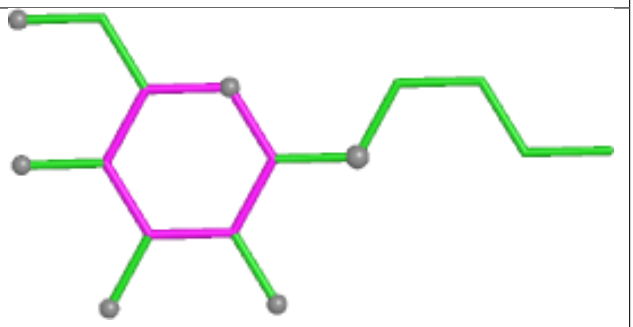
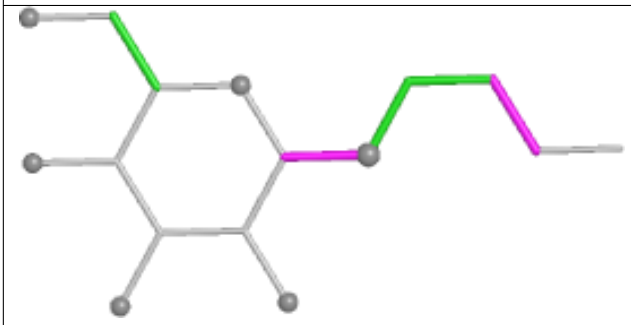


Bond angles



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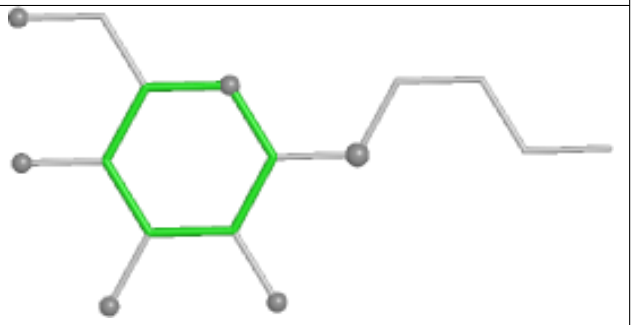
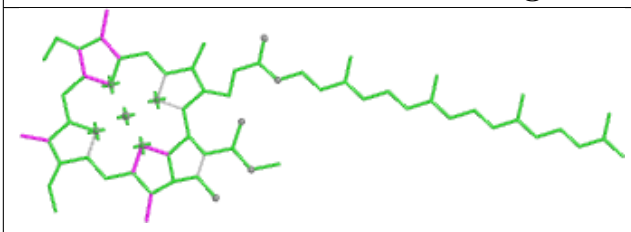


Rings

Ligand CLA A 829



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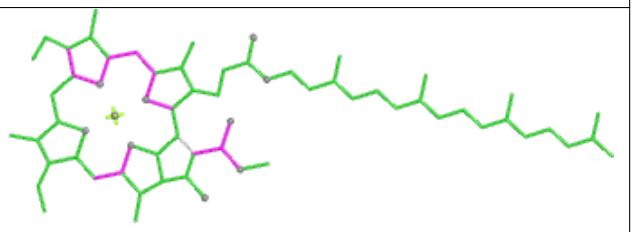
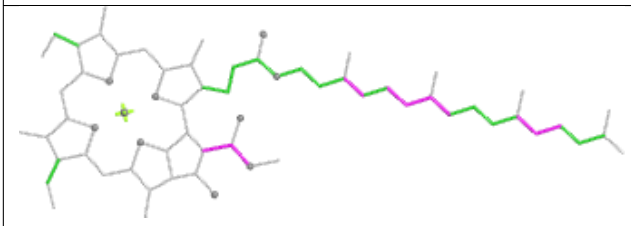


Bond angles



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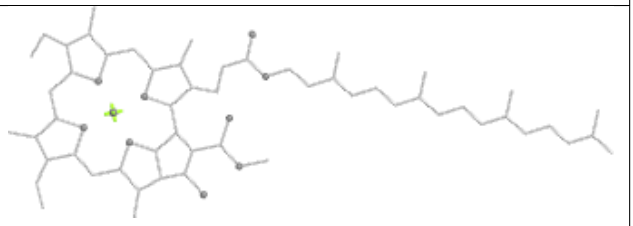
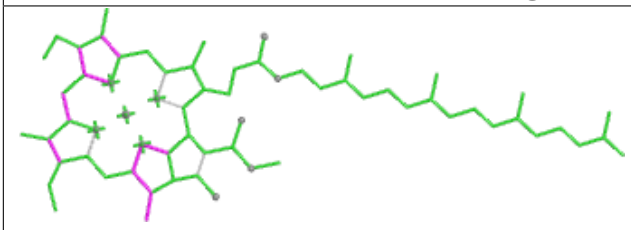
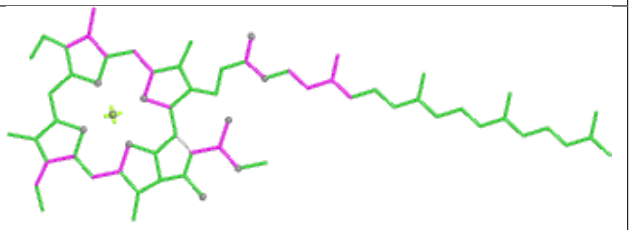
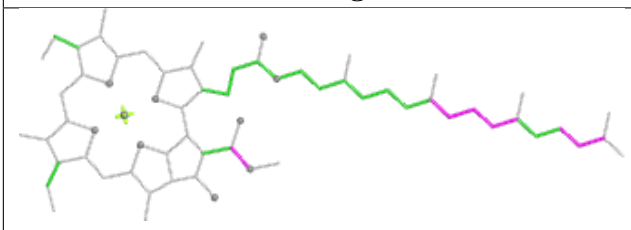
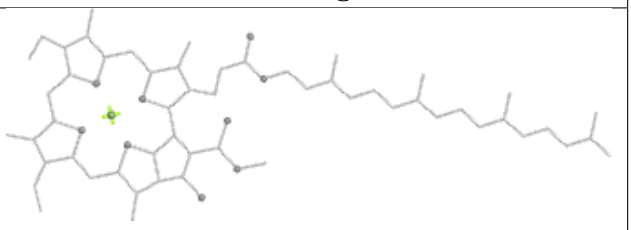
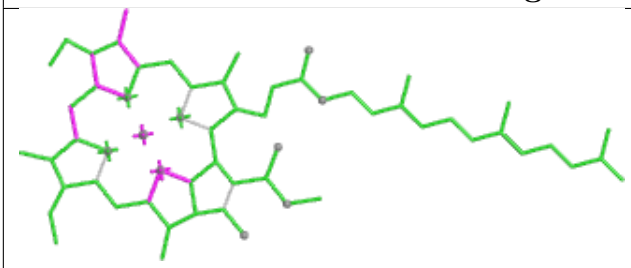
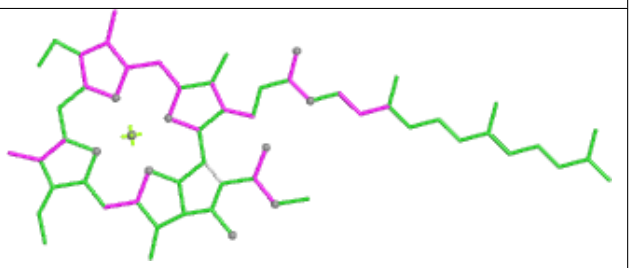
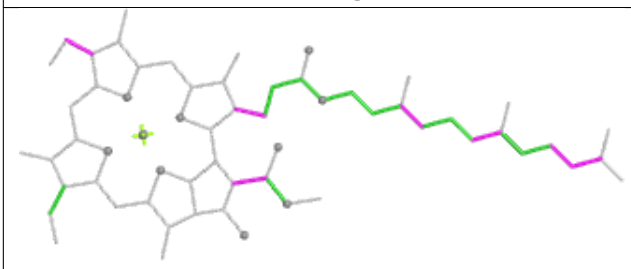
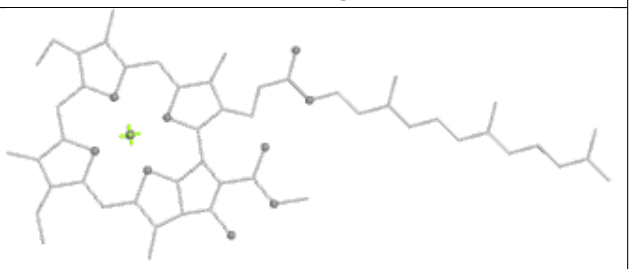
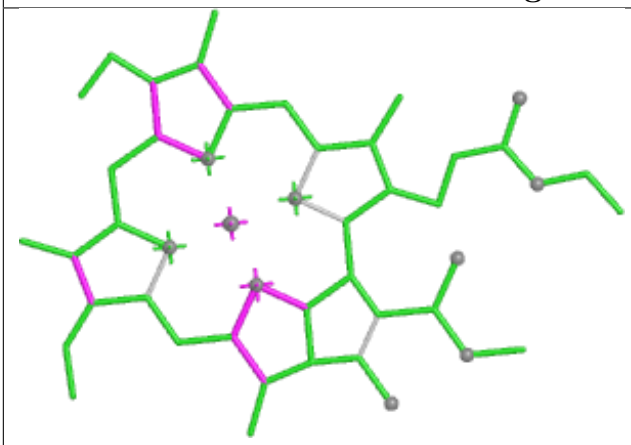


Rings

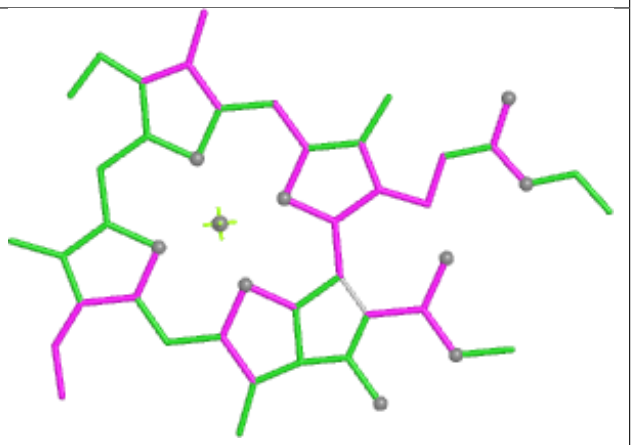
Ligand CLA A 827	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA B 825	
 Bond lengths	 Bond angles
 Torsions	 Rings

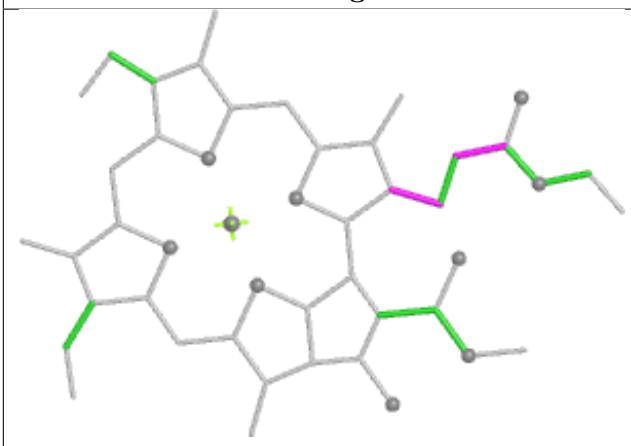
Ligand CLA B 839



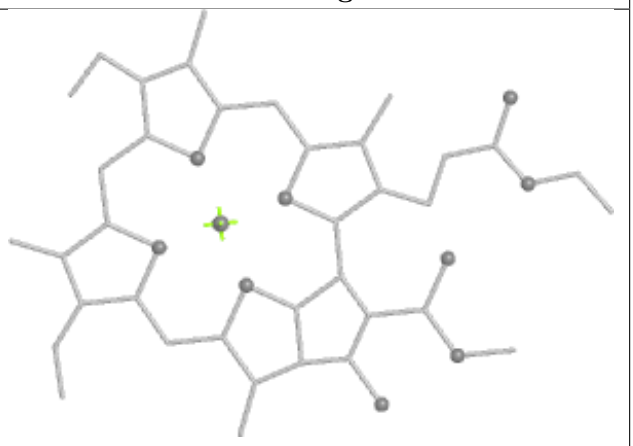
Bond lengths



Bond angles

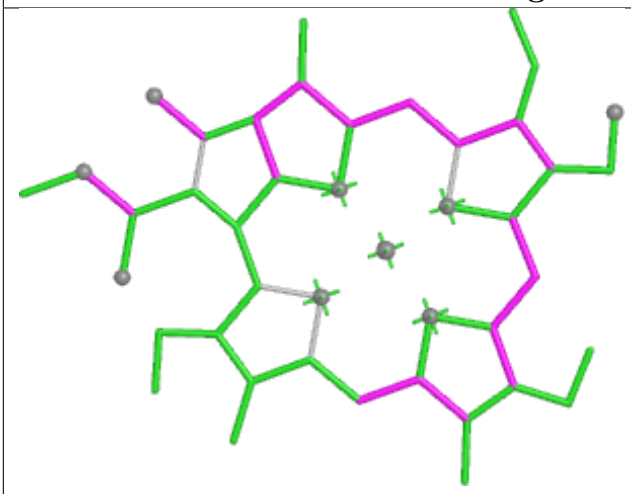


Torsions

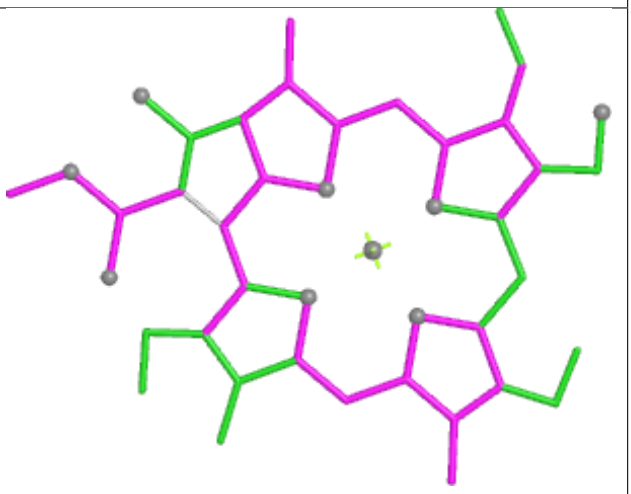


Rings

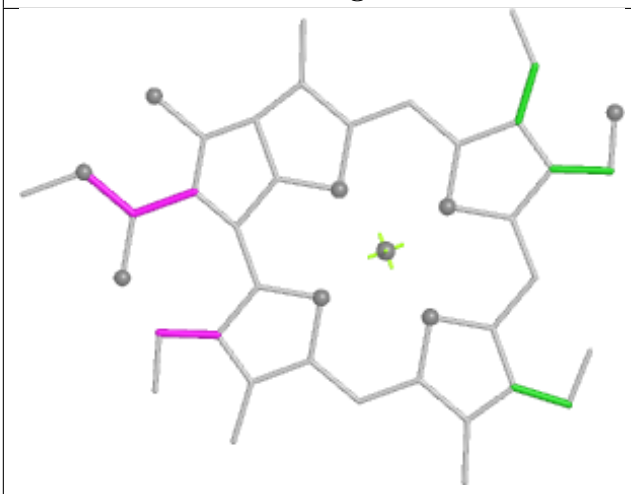
Ligand CHL 2 313



Bond lengths



Bond angles

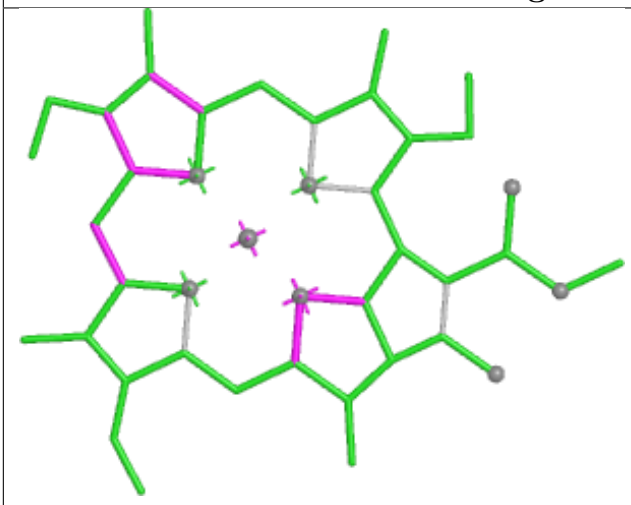


Torsions



Rings

Ligand CLA J 103



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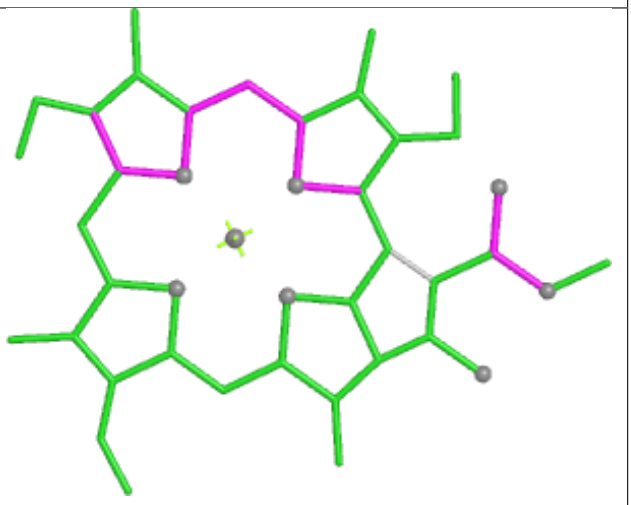

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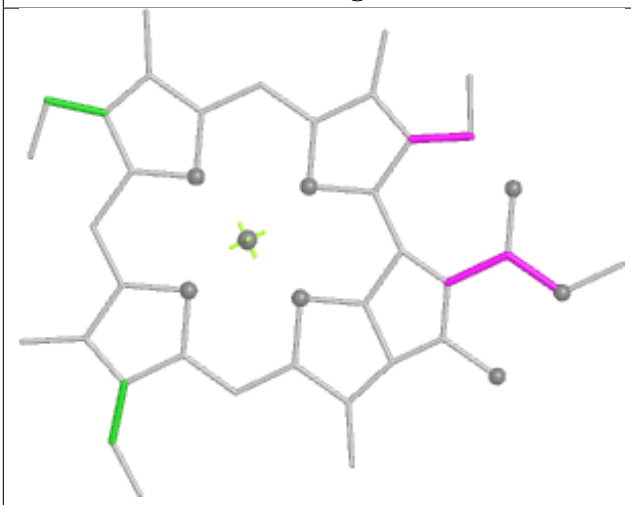


Torsions

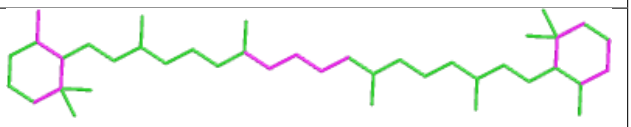


Rings

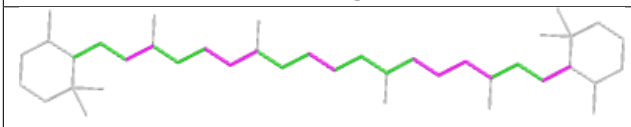
Ligand BCR 1 316



Bond lengths



Bond angles



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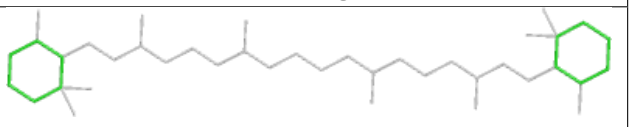
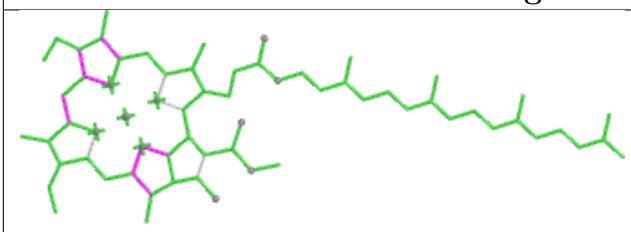


Rings

Ligand CLA B 835



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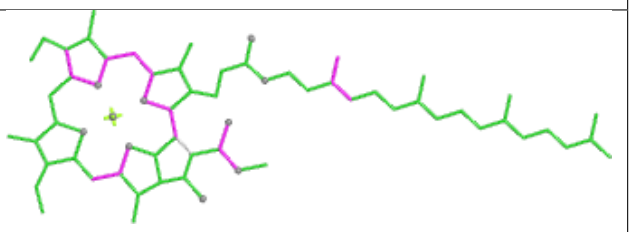
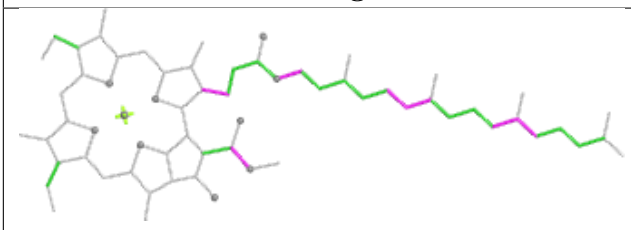


Bond angles



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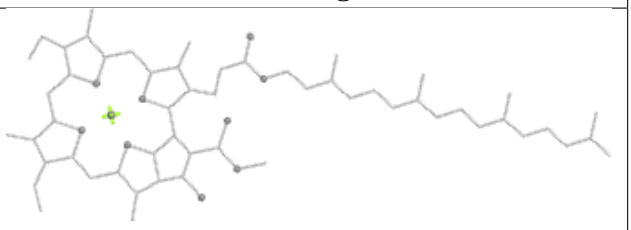
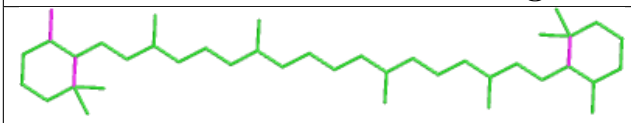


Rings

Ligand BCR 2 316



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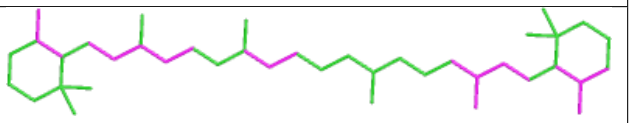
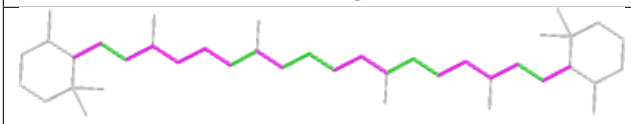


Bond angles



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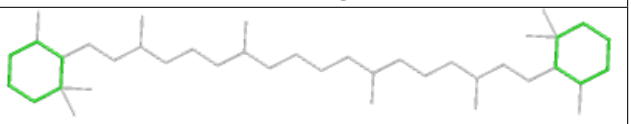
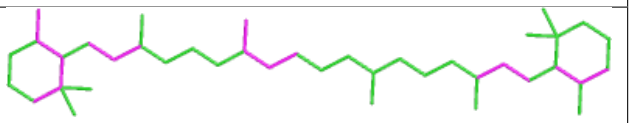


Rings

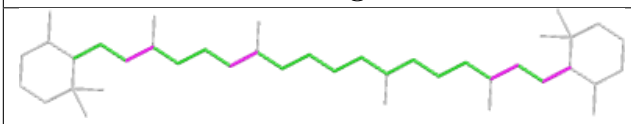
Ligand BCR B 844



Bond lengths



Bond angles



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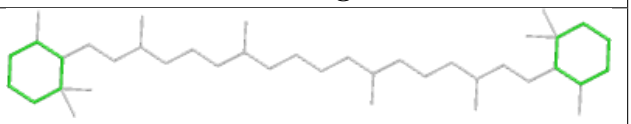
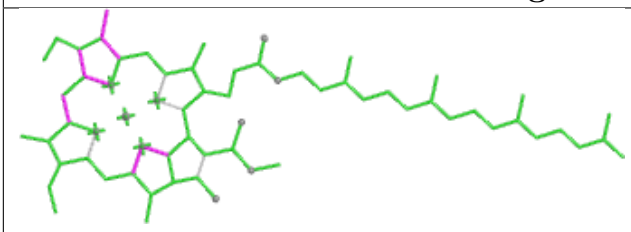


Rings

Ligand CLA 1 309



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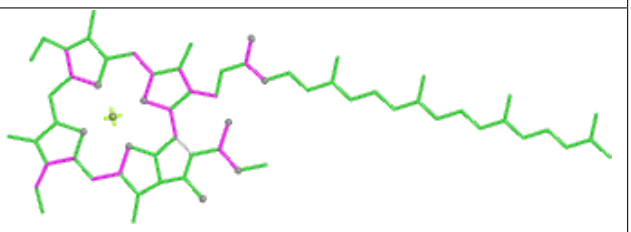
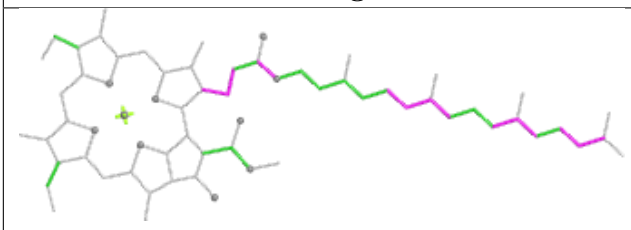


Bond angles



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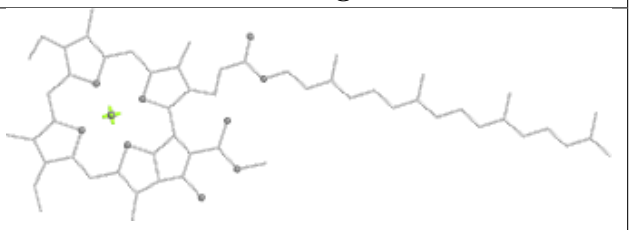
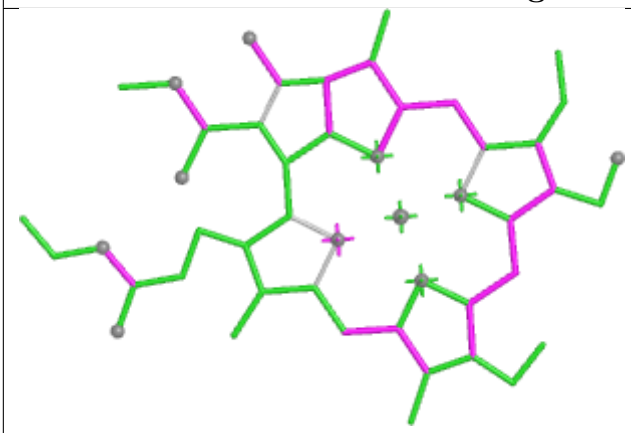


Rings

Ligand CHL 1 305



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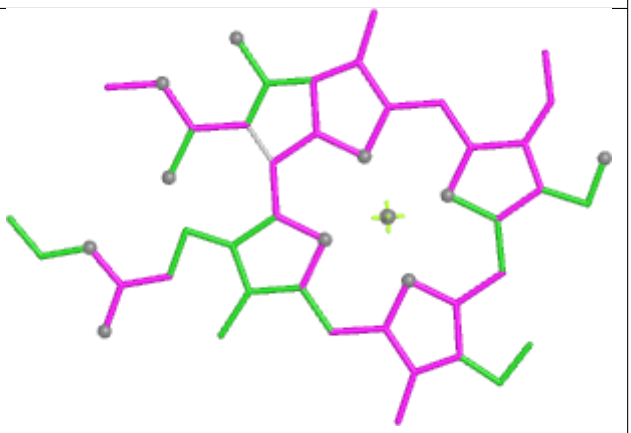
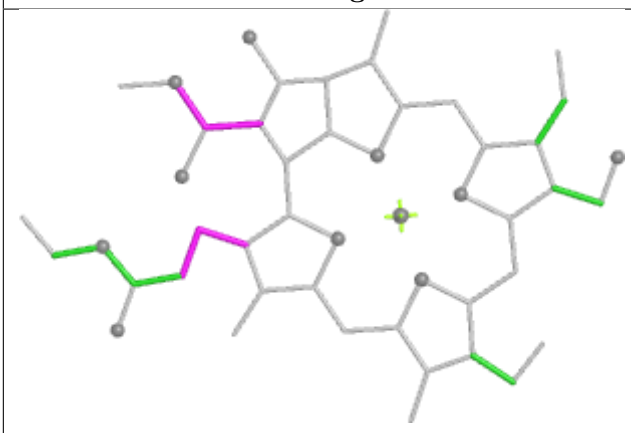


Bond angles



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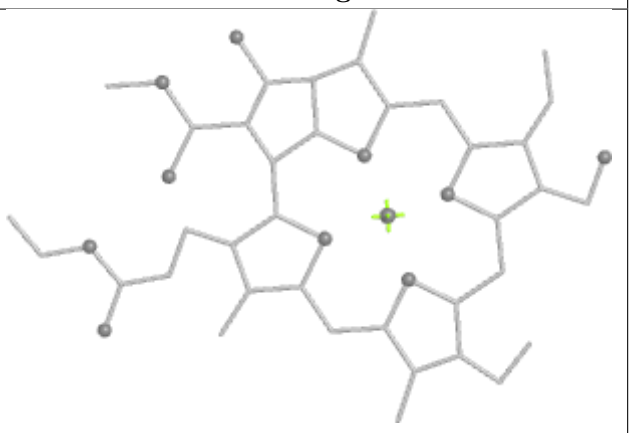
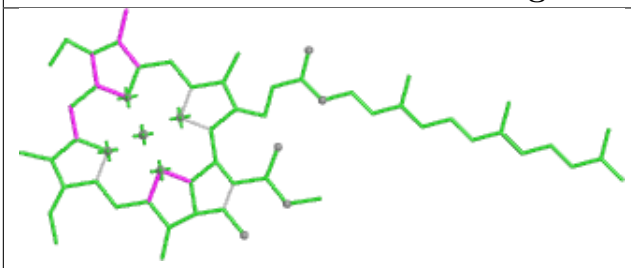


Rings

Ligand CLA 3 602



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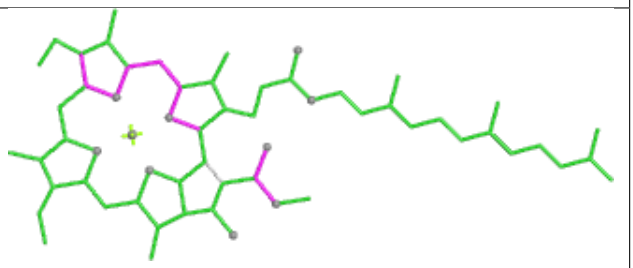
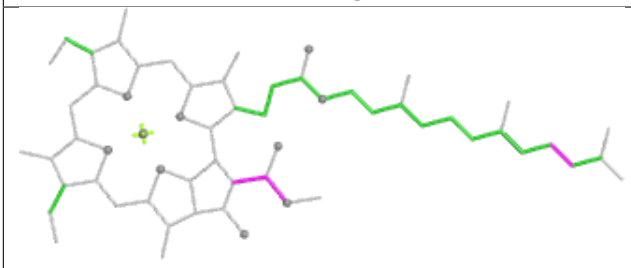


Bond angles



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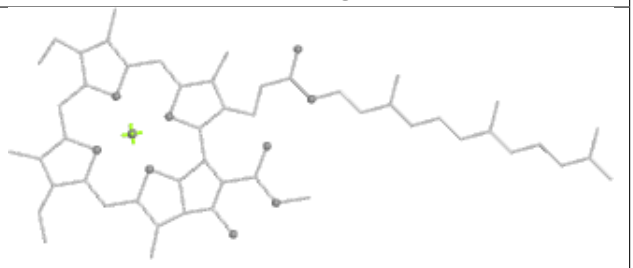
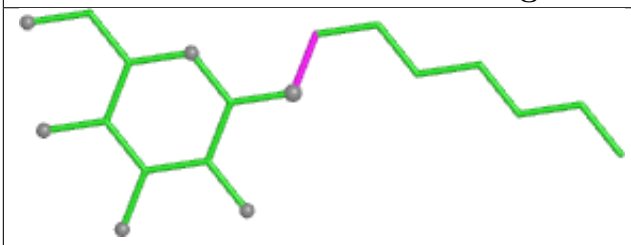


Rings

Ligand HTG A 854



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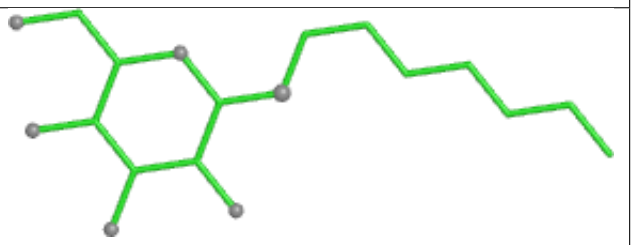
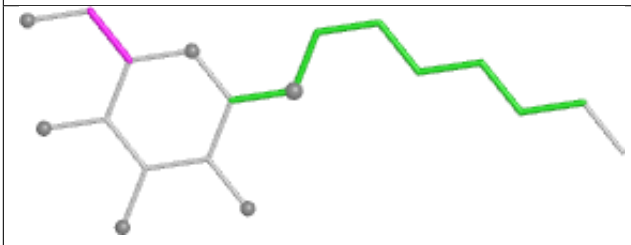


Bond angles



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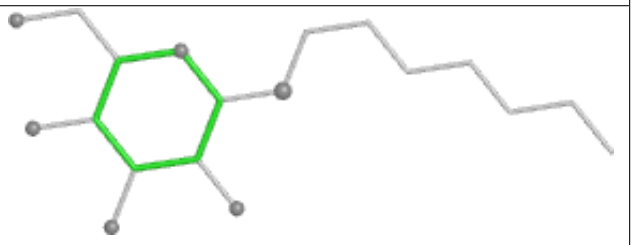
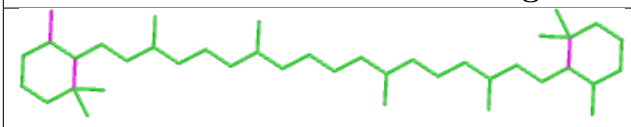


Rings

Ligand BCR A 847



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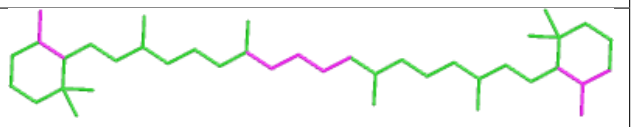
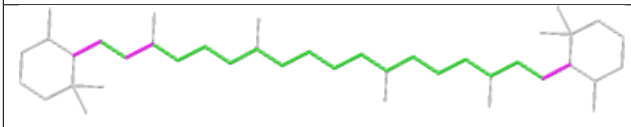


Bond angles



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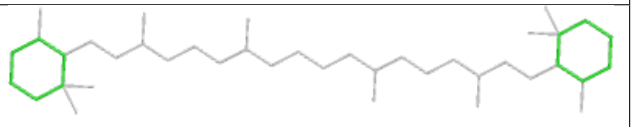
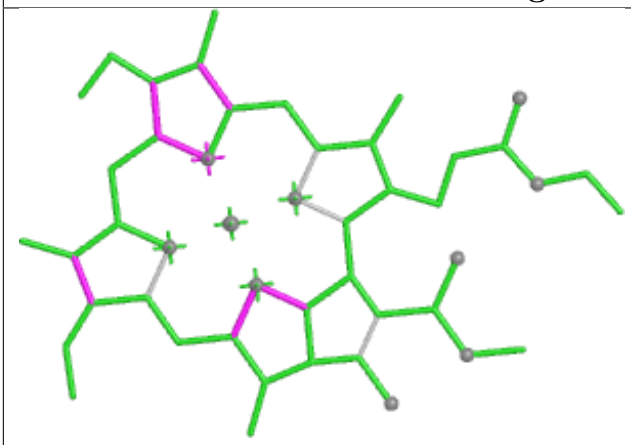


Rings

Ligand CLA 4 314



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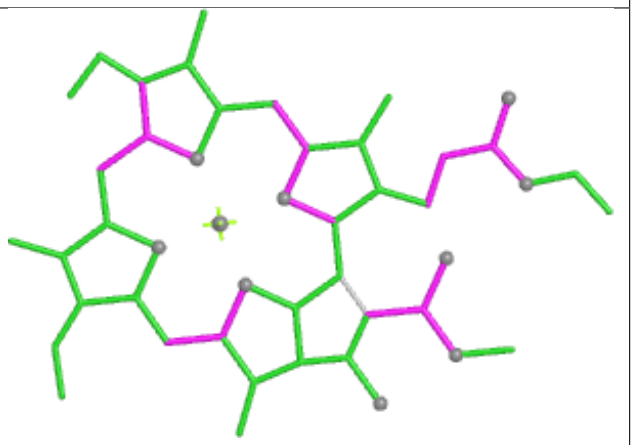
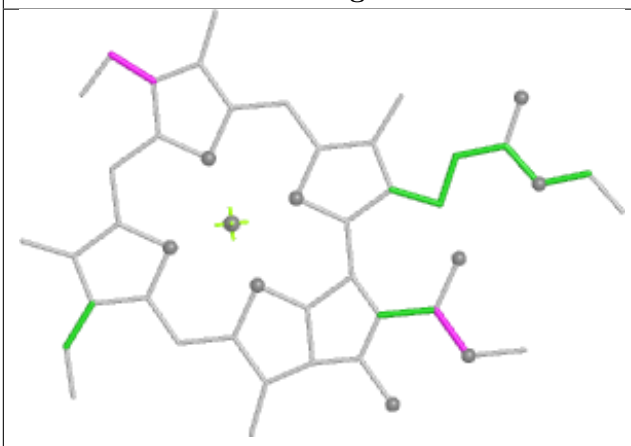


Bond angles



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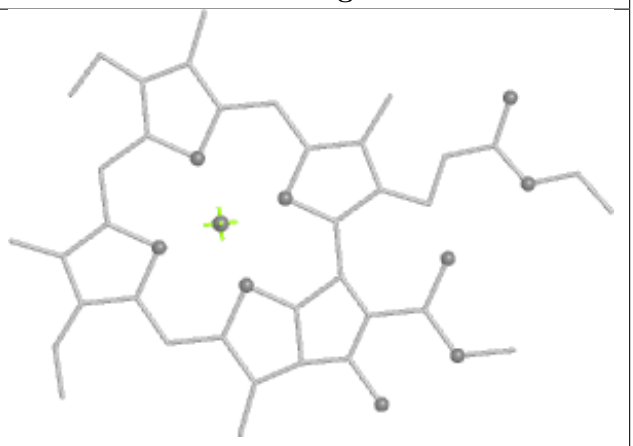
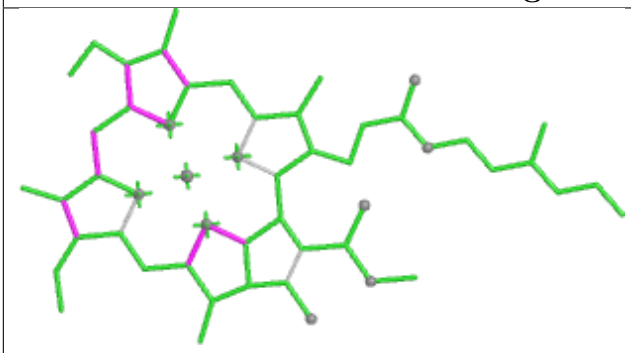


Rings

Ligand CLA A 843



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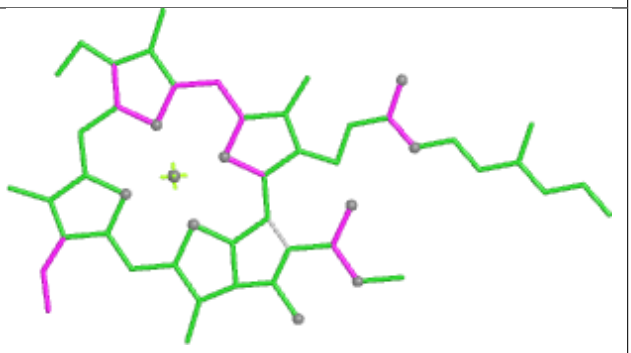
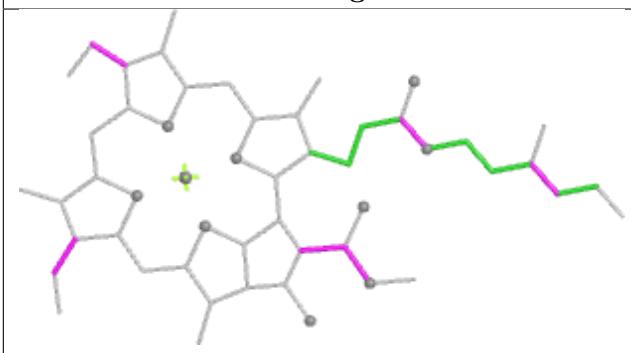


Bond angles



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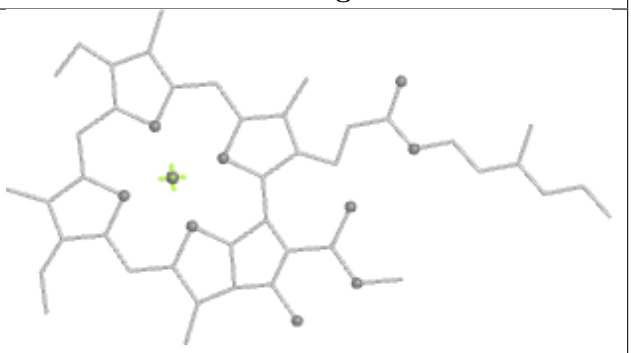
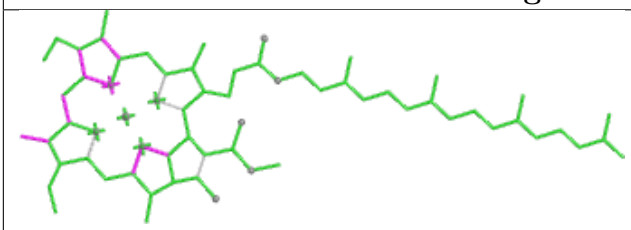


Rings

Ligand CLA A 839



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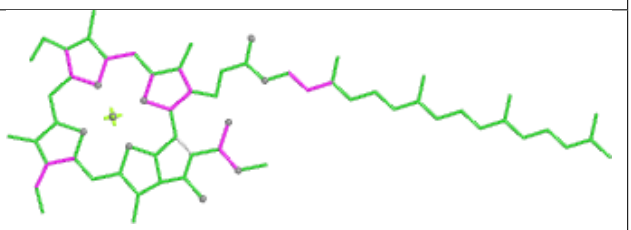
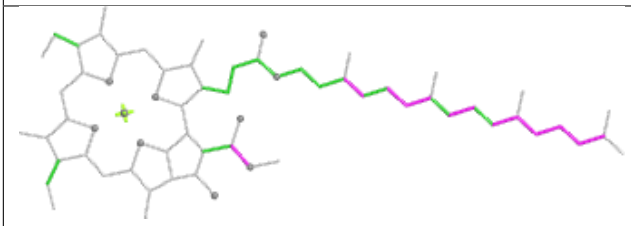


Bond angles



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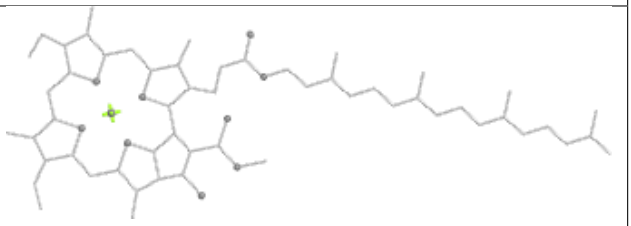
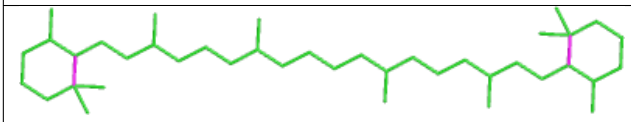


Rings

Ligand BCR G 106



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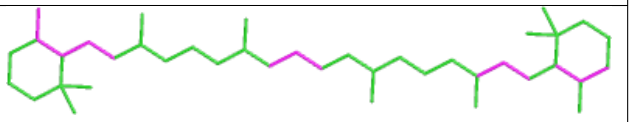
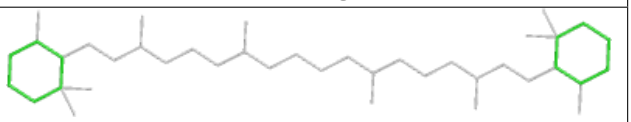


Bond angles

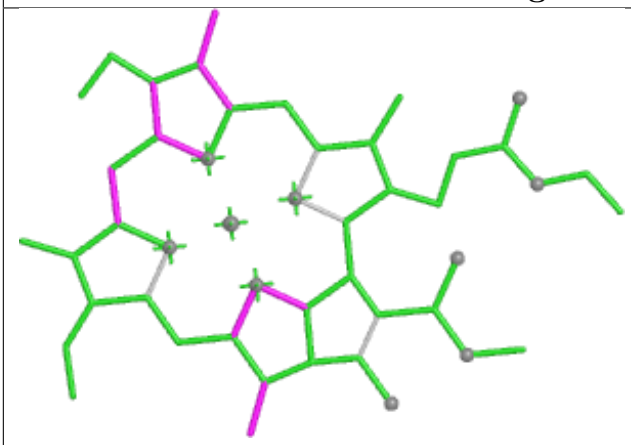


Torsions

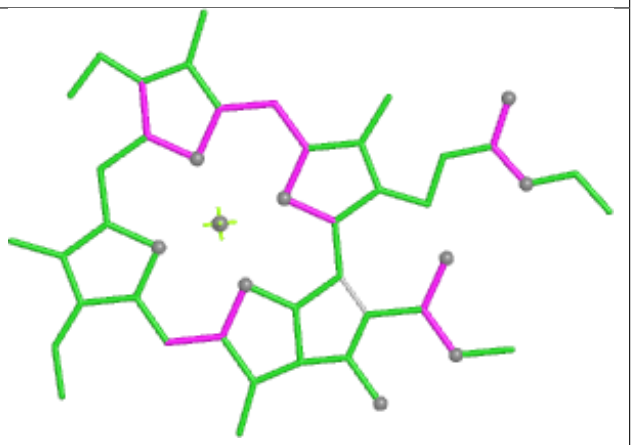


Rings

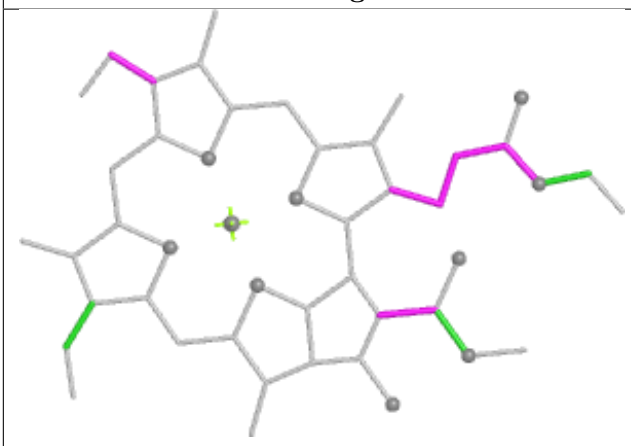
Ligand CLA 3 606



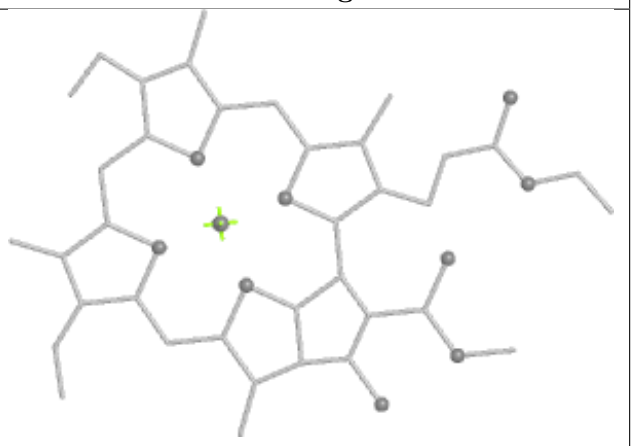
Bond lengths



Bond angles

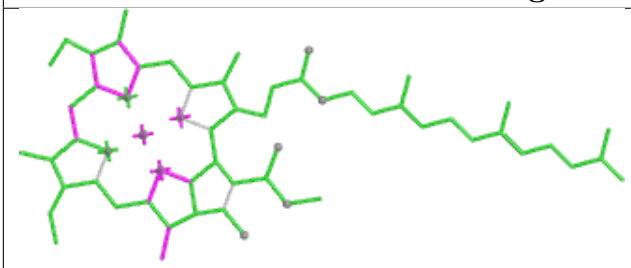


Torsions



Rings

Ligand CLA 4 302



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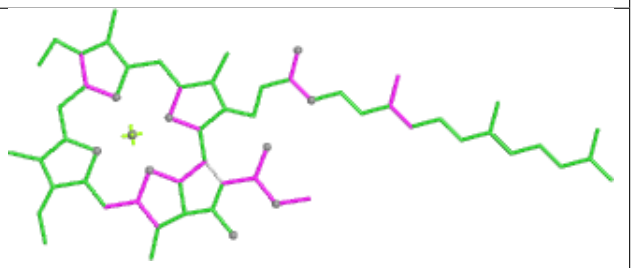
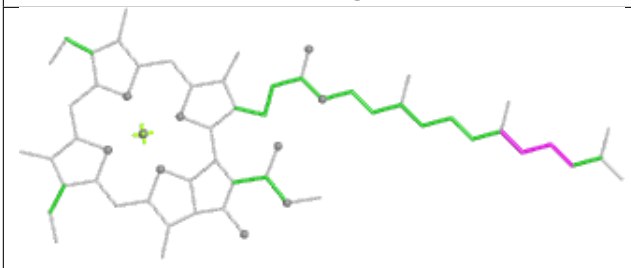


Bond angles



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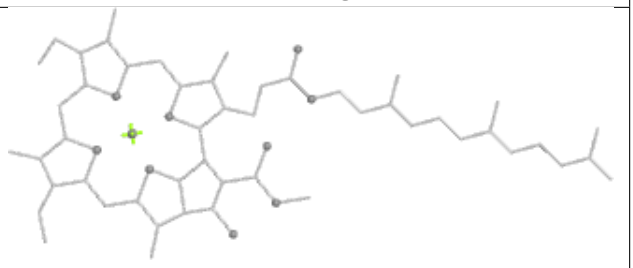
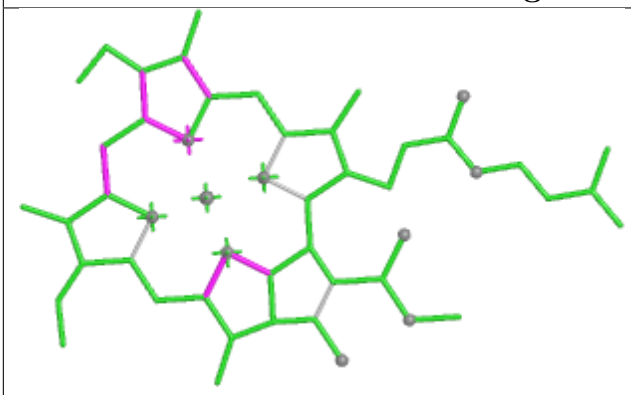


Rings

Ligand CLA A 814



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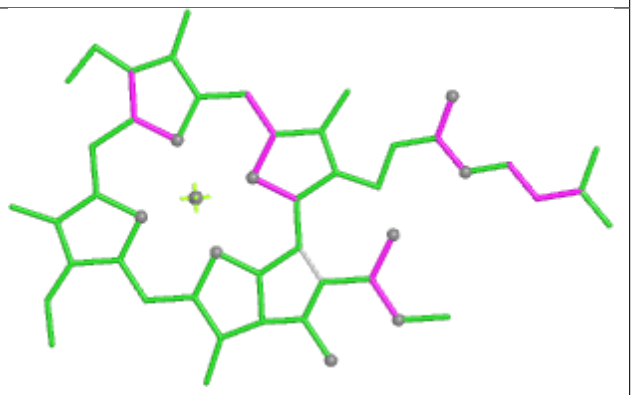
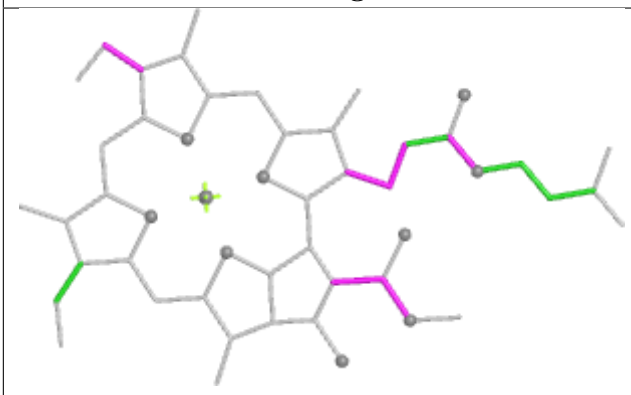


Bond angles



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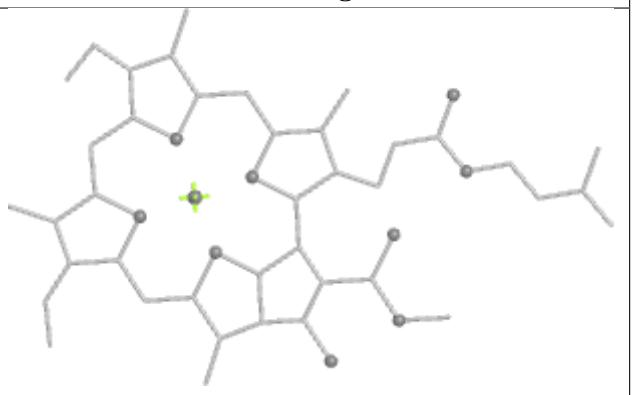
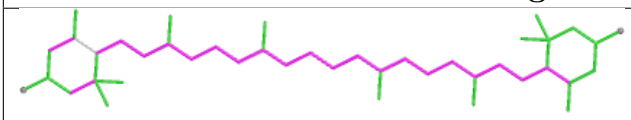


Rings

Ligand LUT 4 316



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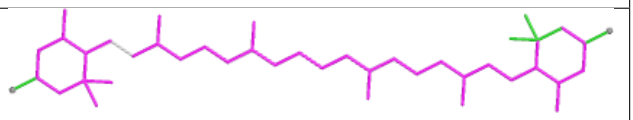
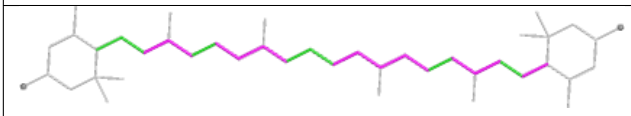


Bond angles



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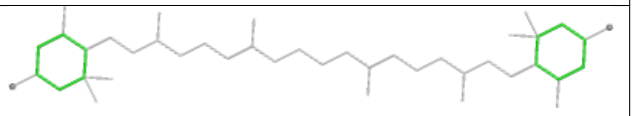
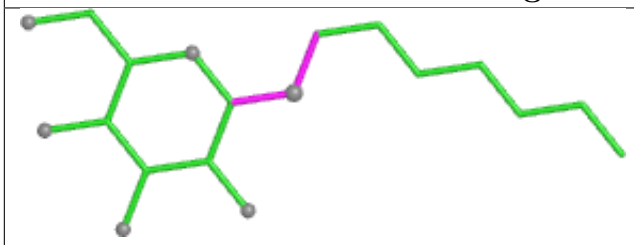


Rings

Ligand HTG F 305



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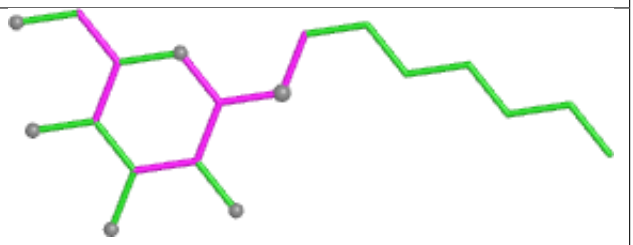
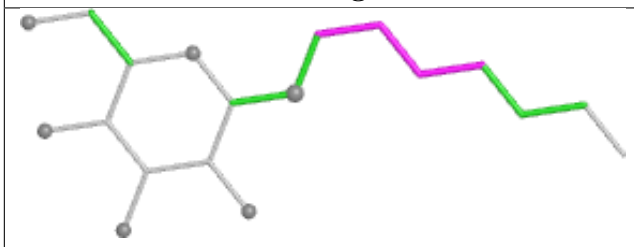


Bond angles



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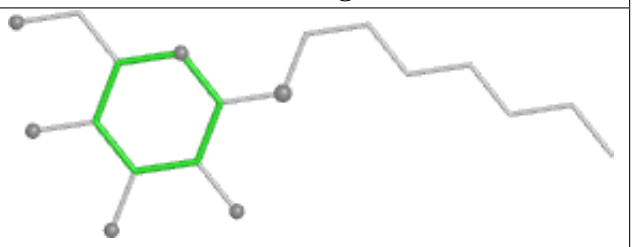
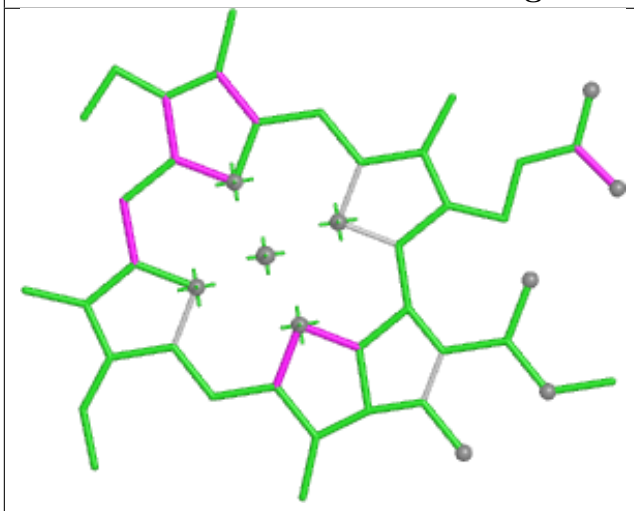


Rings

Ligand CLA A 813



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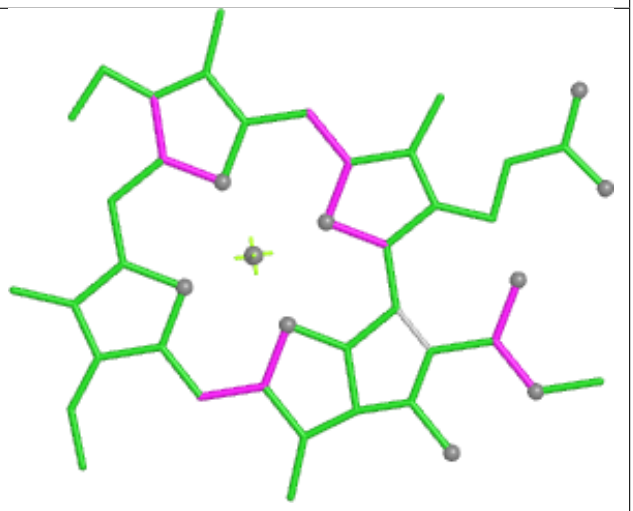
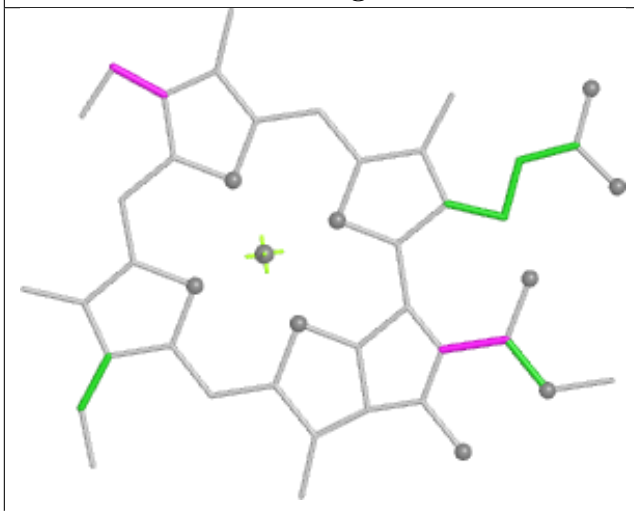


Bond angles

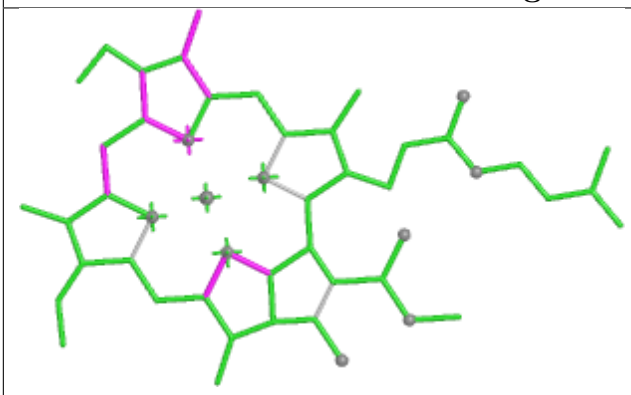


Torsions



Rings

Ligand CLA A 830



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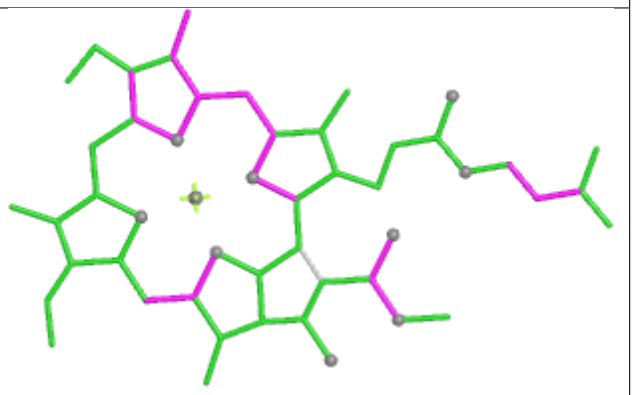
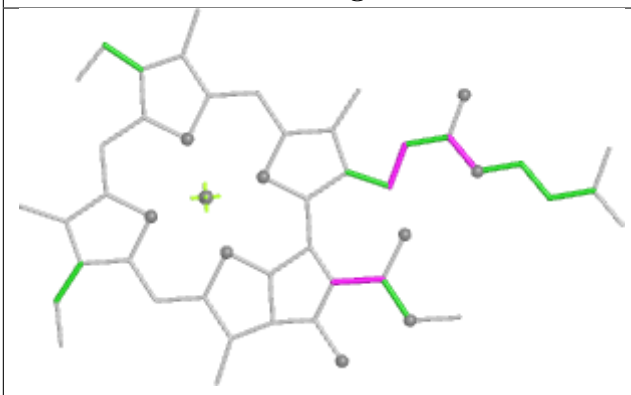
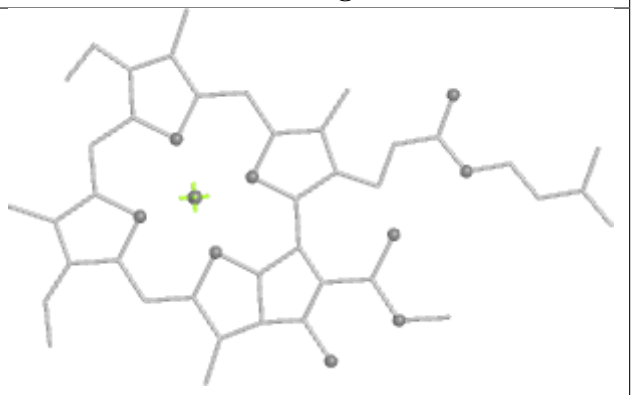


Bond angles

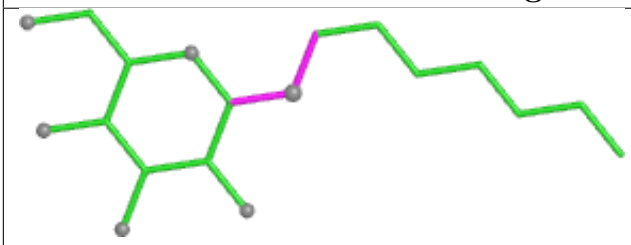


Torsions



Rings

Ligand HTG J 102



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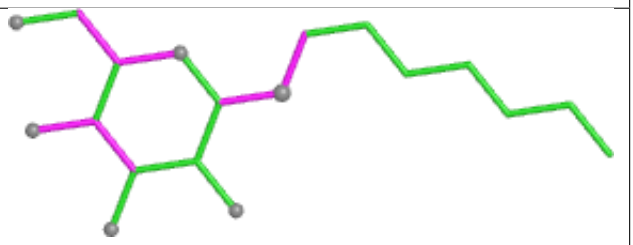
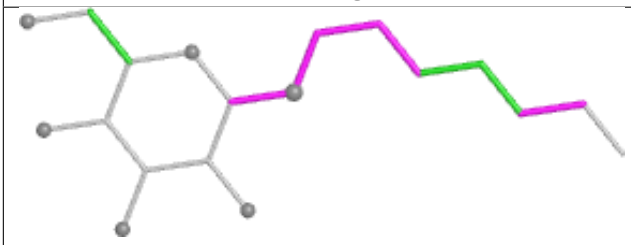


Bond angles



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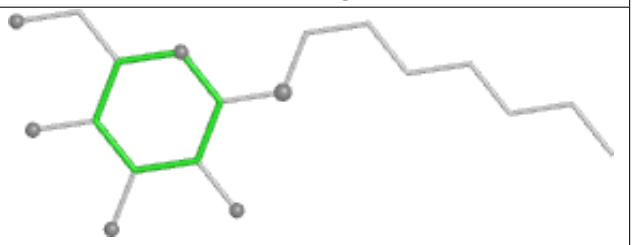
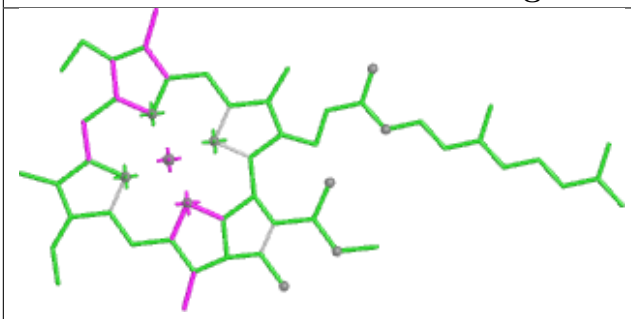


Rings

Ligand CLA A 803



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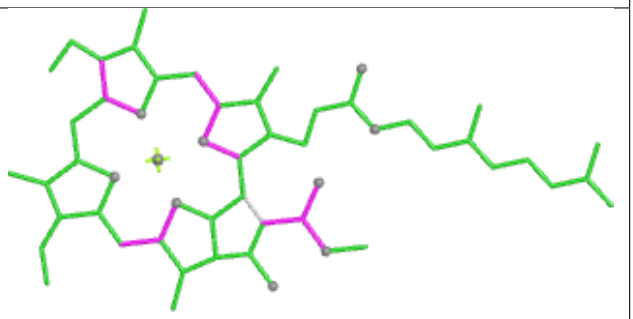
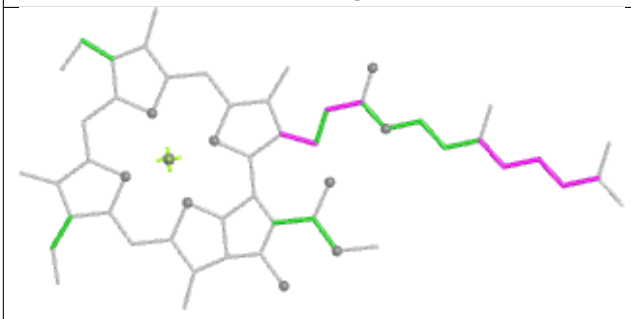


Bond angles



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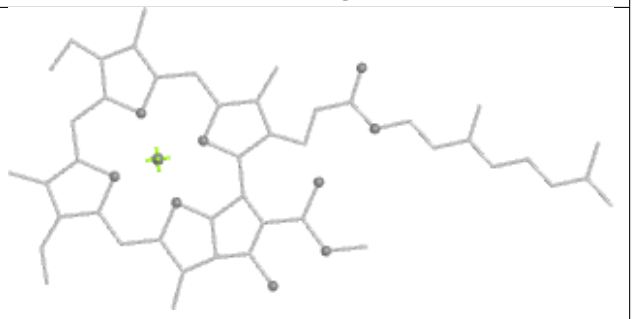
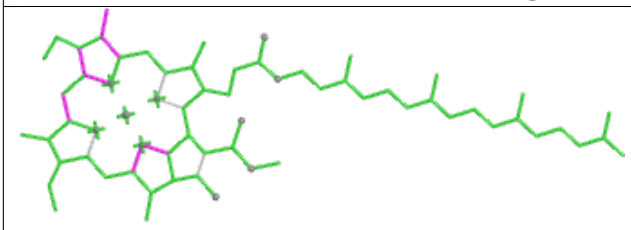


Rings

Ligand CLA A 812



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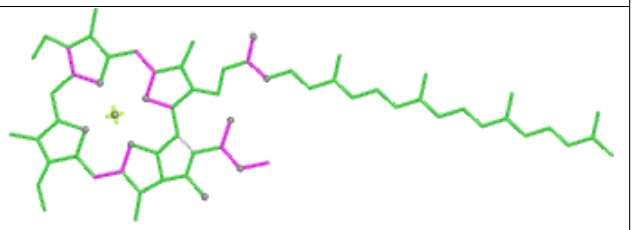
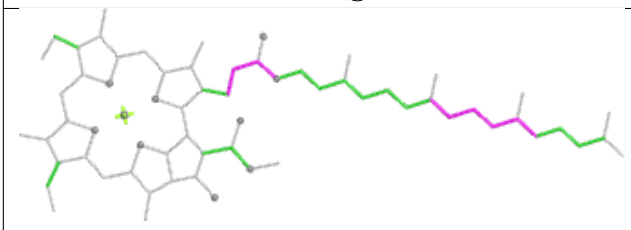


Bond angles



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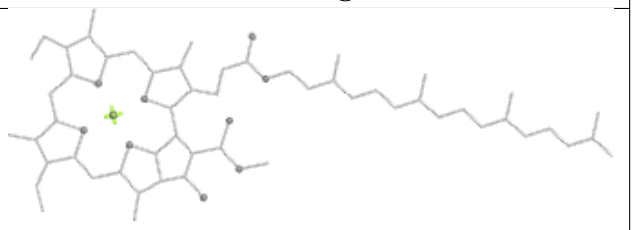
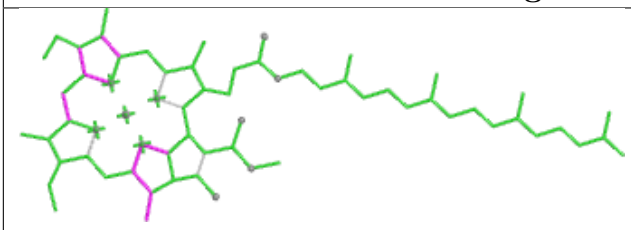


Rings

Ligand CLA B 809



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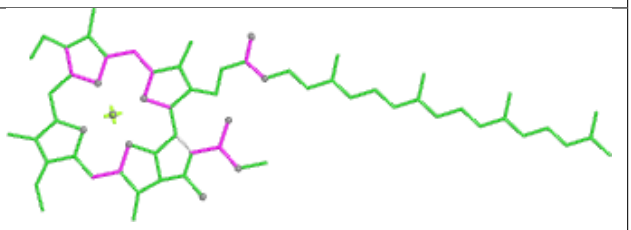
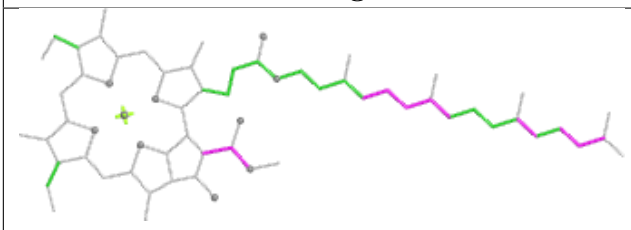


Bond angles



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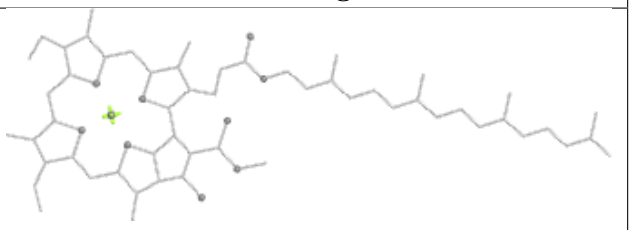
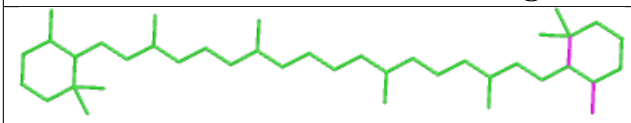


Rings

Ligand BCR B 849



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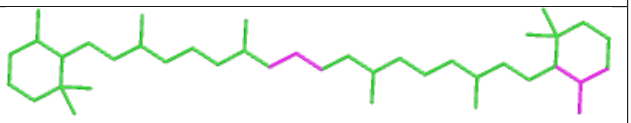
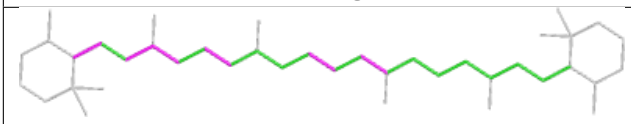


Bond angles



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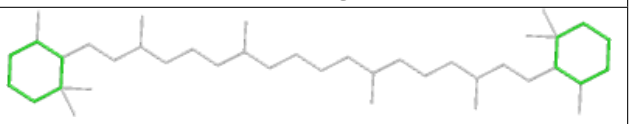


Rings

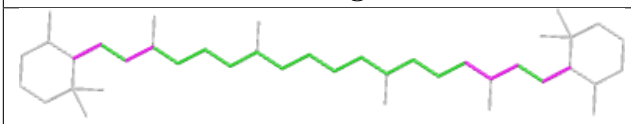
Ligand BCR L 205



Bond lengths



Bond angles



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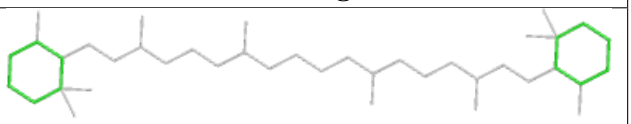
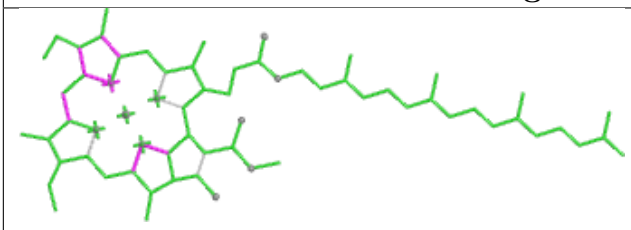
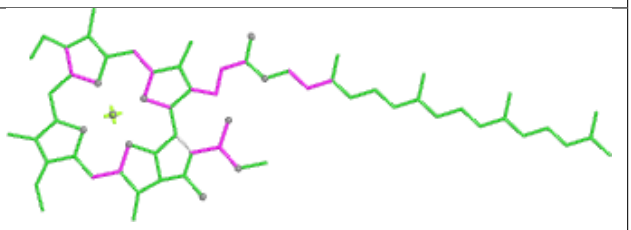
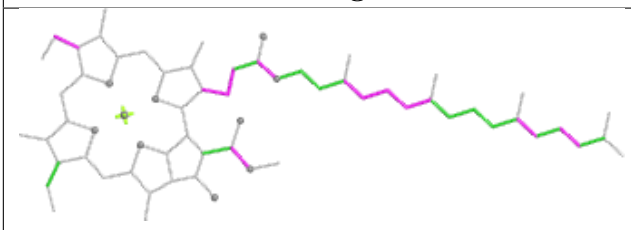


Rings

Ligand CLA A 831


Bond lengths


Bond angles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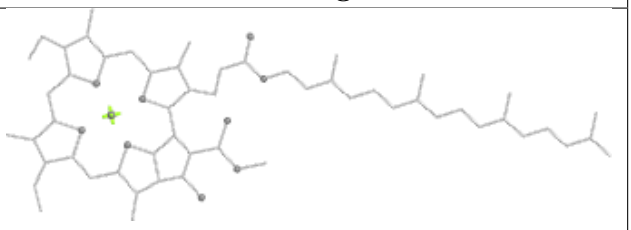
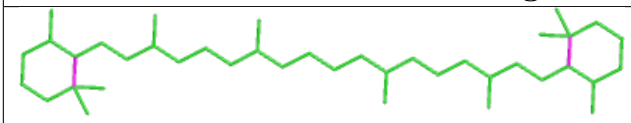

Rings

Ligand BCR A 846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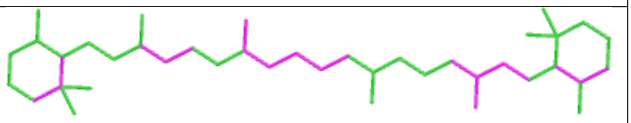
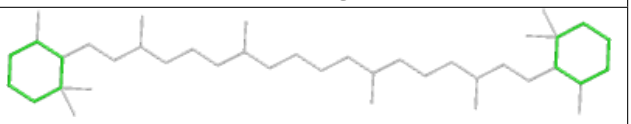
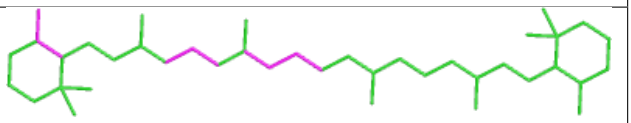

Bond angles

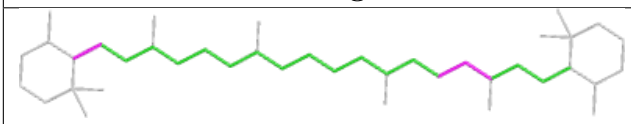

Torsions


Rings

Ligand BCR I 101


Bond lengths


Bond angles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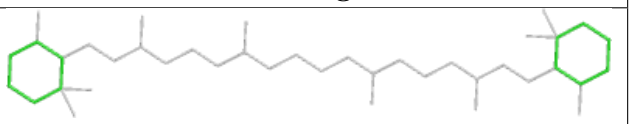
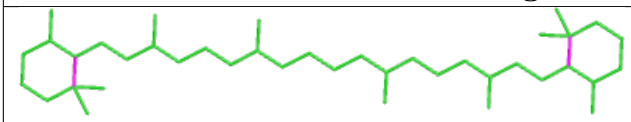

Rings

Ligand BCR A 850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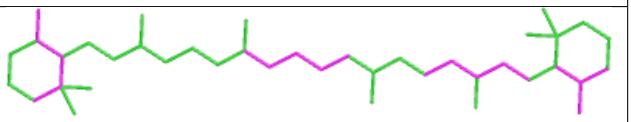
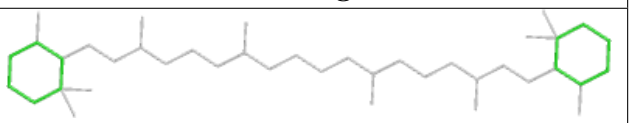
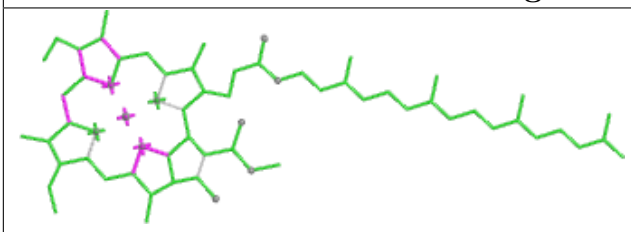

Bond angles


Torsions


Rings

Ligand CLA B 802



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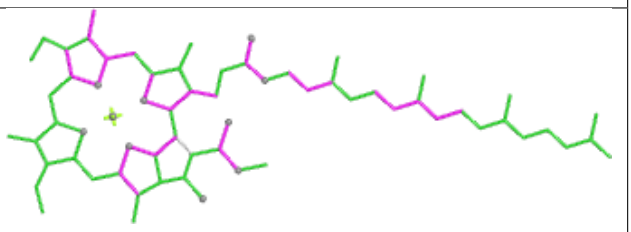
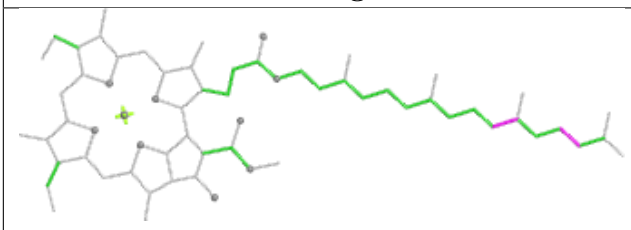


Bond angles



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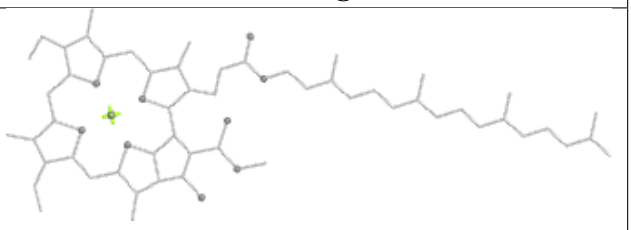
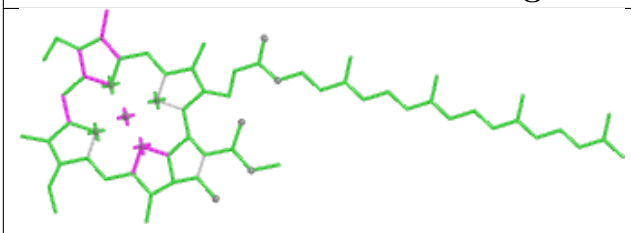


Rings

Ligand CLA A 820



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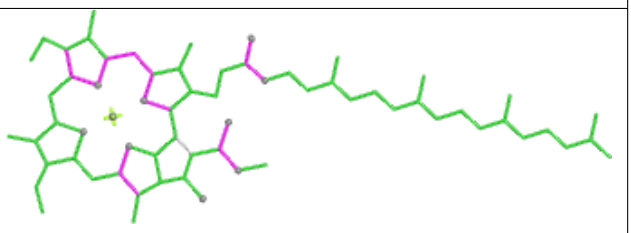

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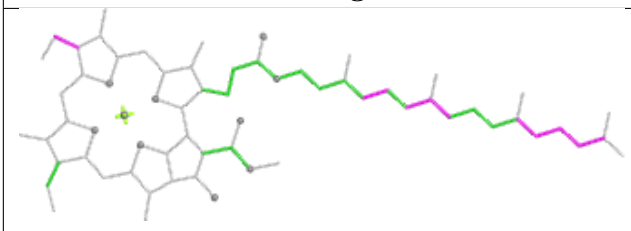

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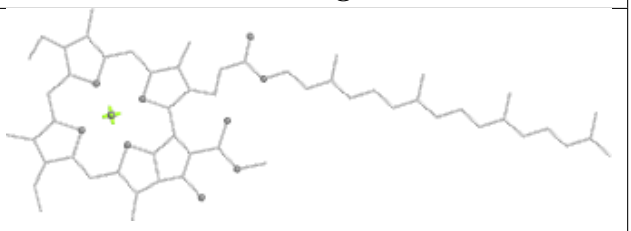
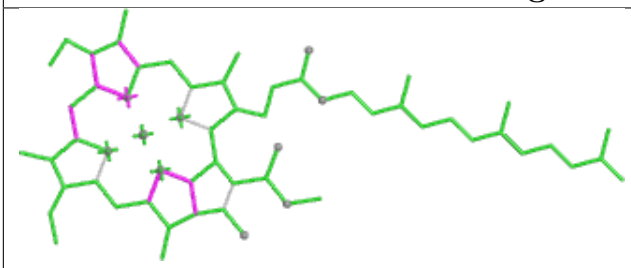
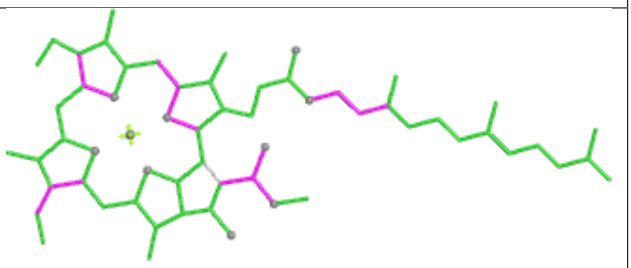
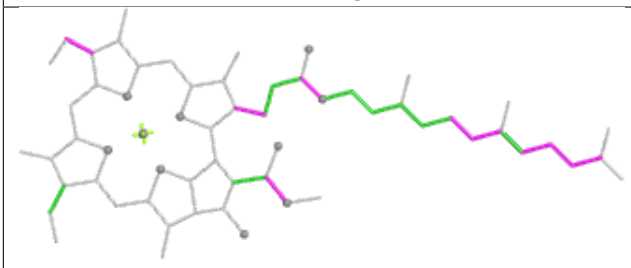
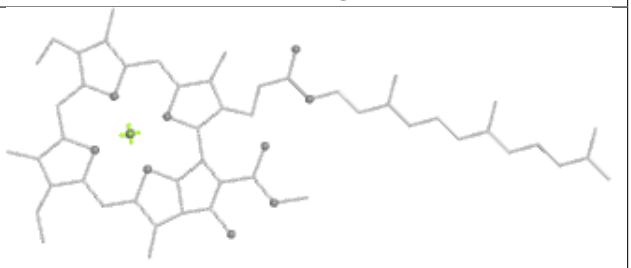


Rings

Ligand CLA 4 303	
	
Bond lengths	Bond angles
	
Torsions	Rings

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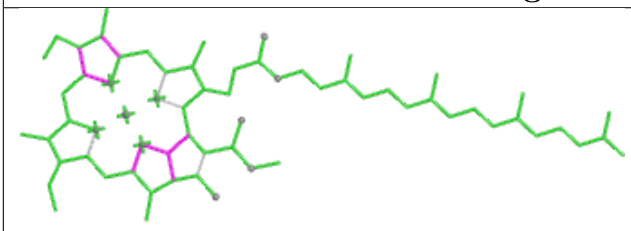	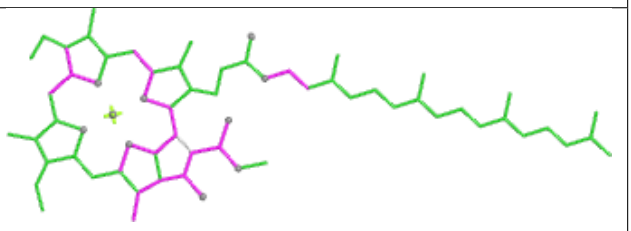
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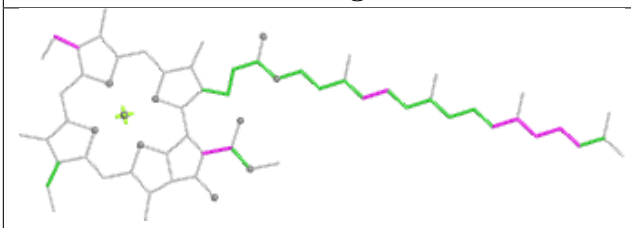
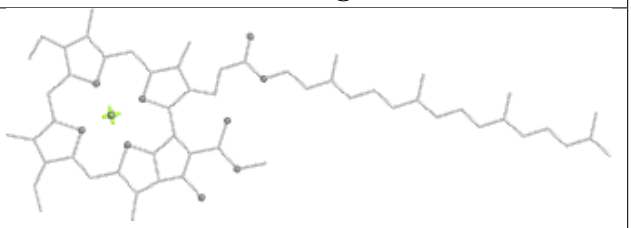
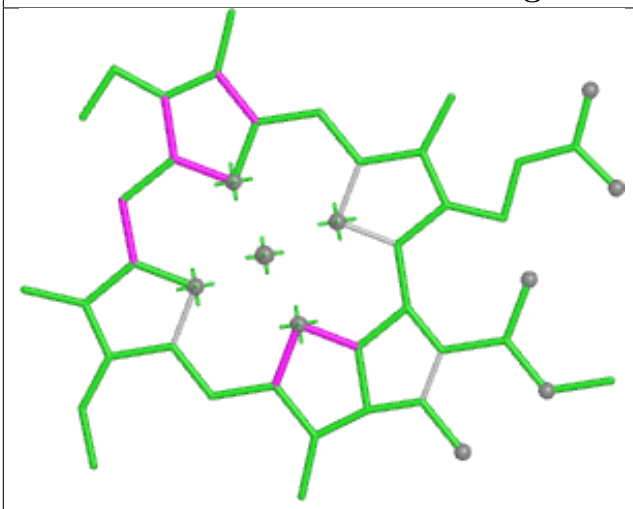
	
Torsions	Rings

Ligand CLA A 819



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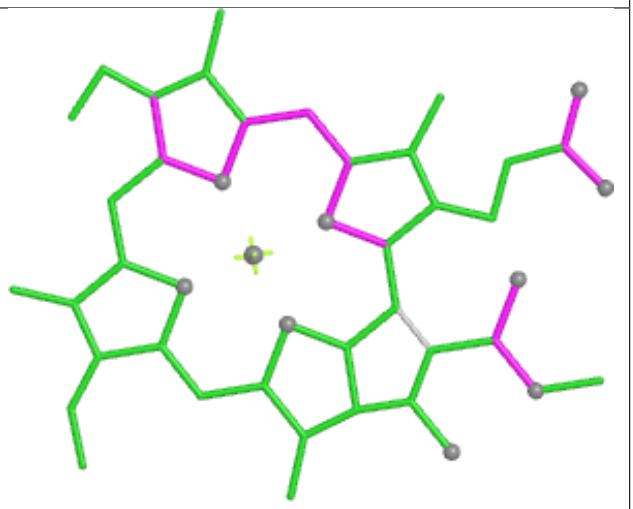

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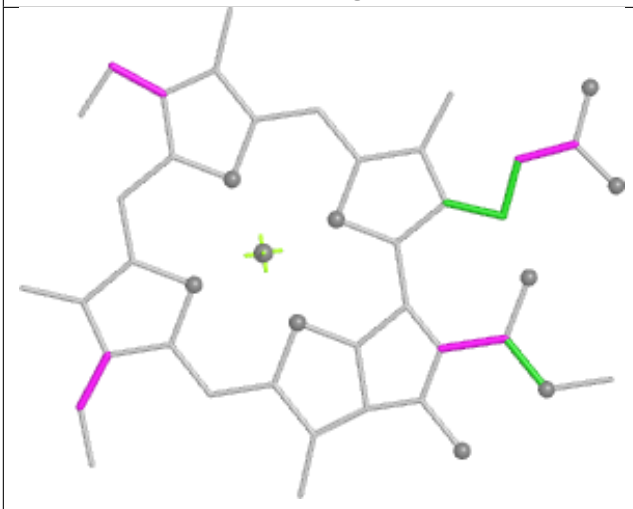
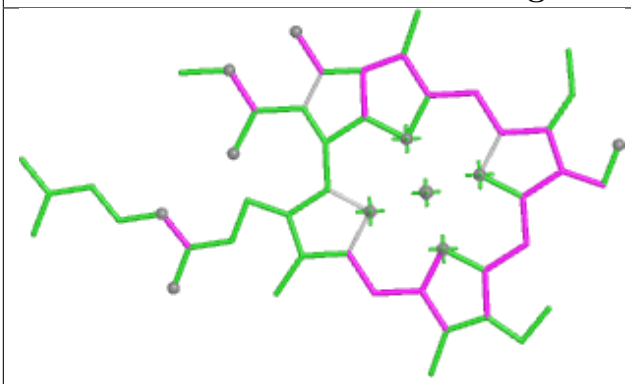


Torsions



Rings

Ligand CHL 2 306



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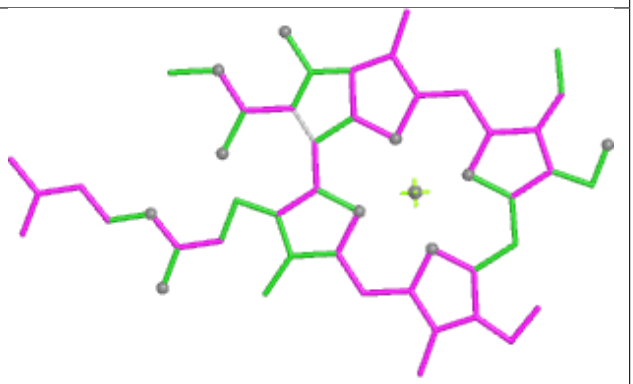

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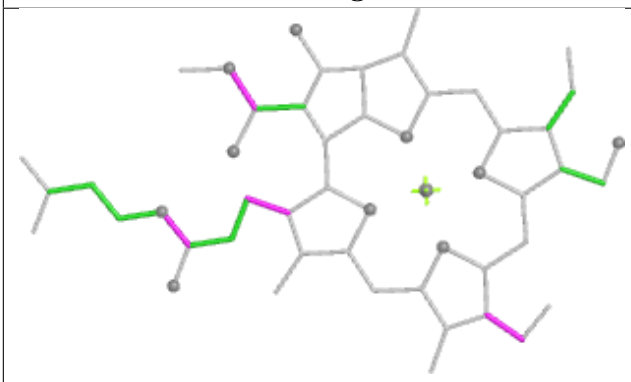

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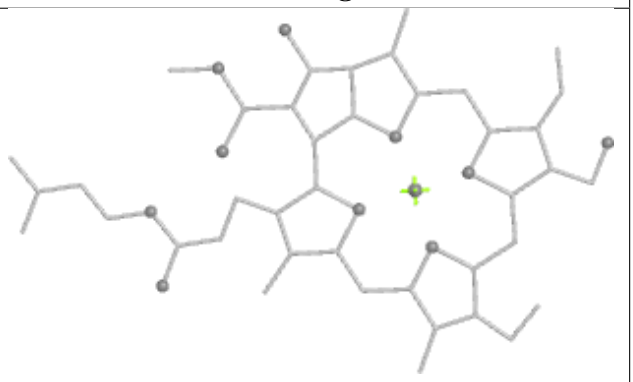
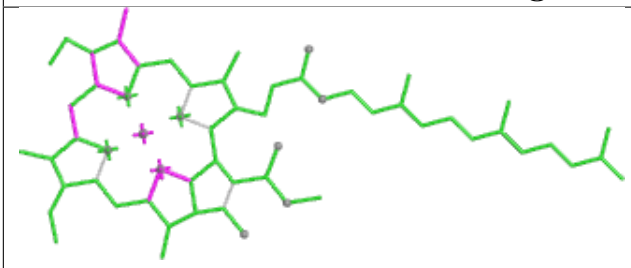


Rings

Ligand CLA 1 311



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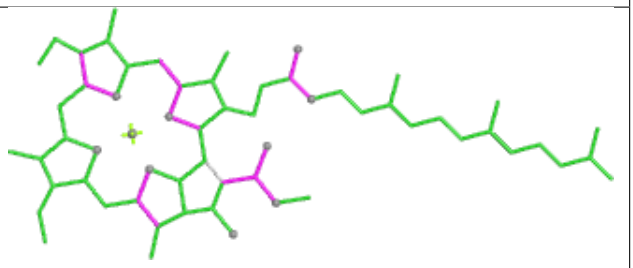
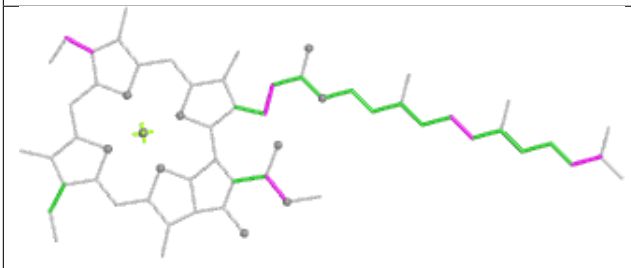


Bond angles



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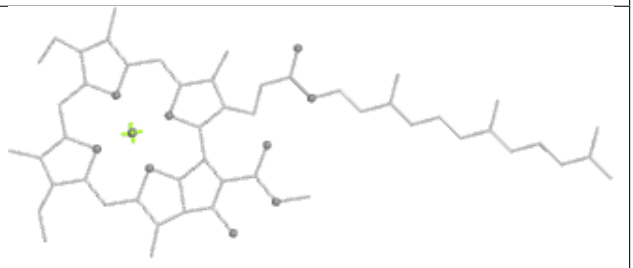
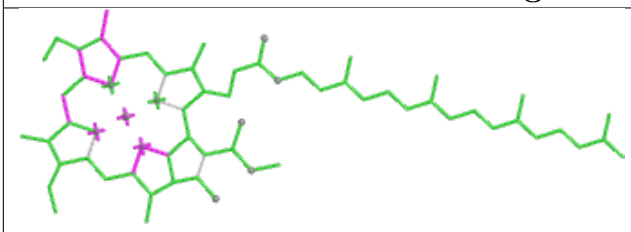


Rings

Ligand CLA B 808



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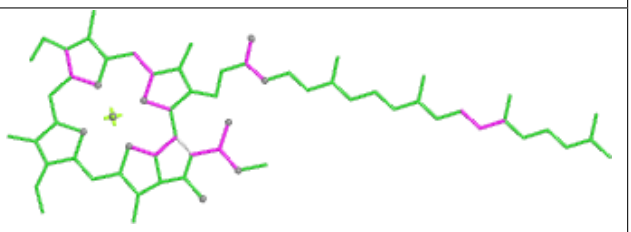

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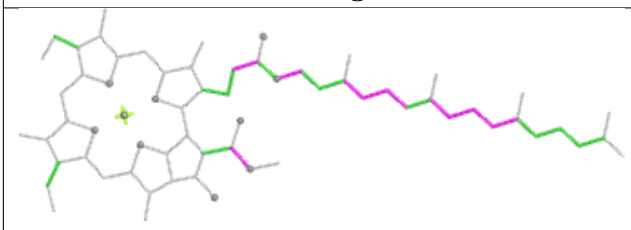

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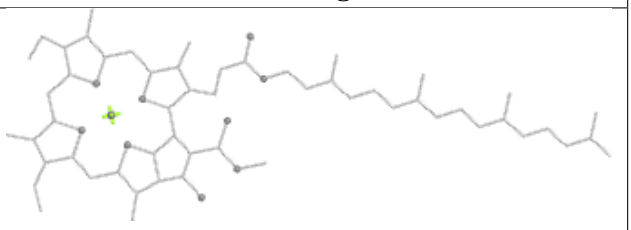
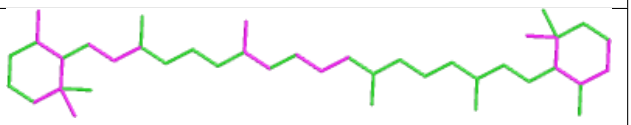


Rings

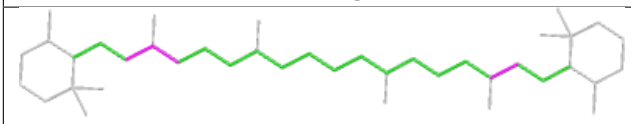
Ligand BCR B 845



Bond lengths



Bond angles



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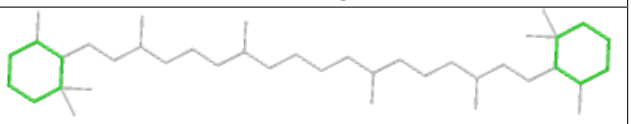
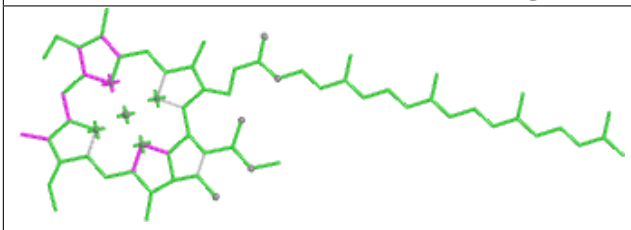


Rings

Ligand CLA B 828



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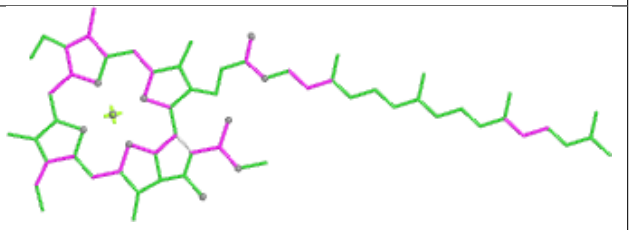

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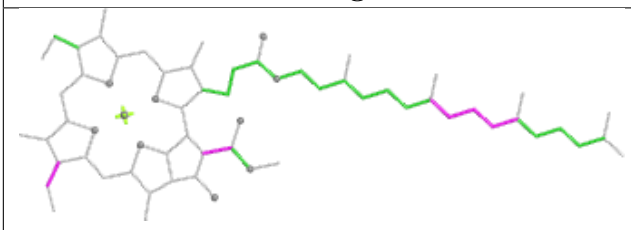

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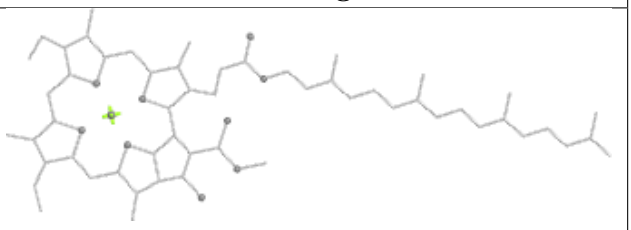
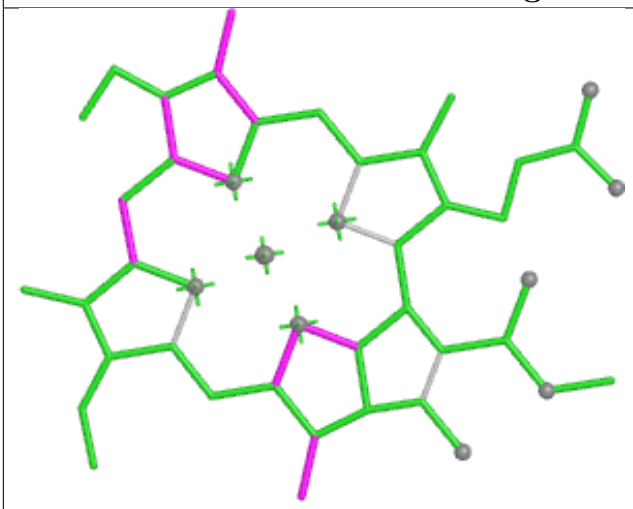


Rings

Ligand CLA A 815



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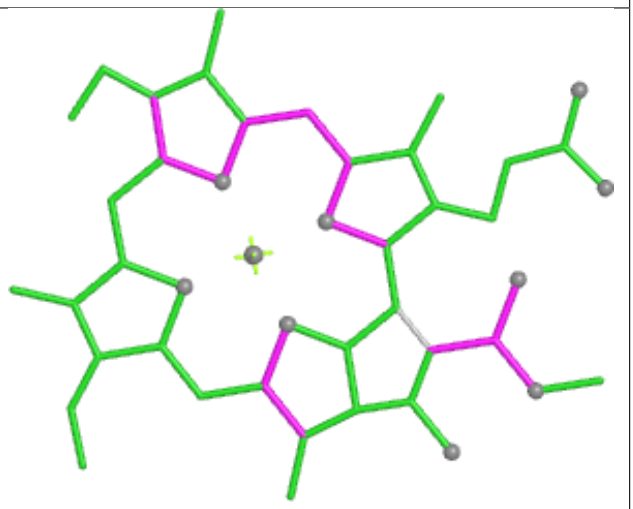

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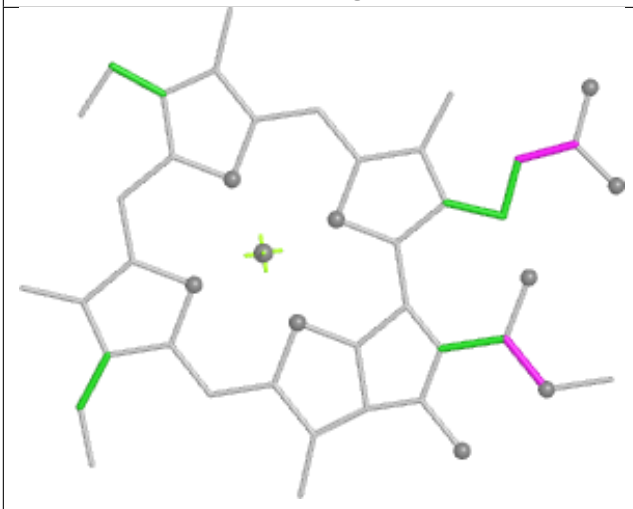
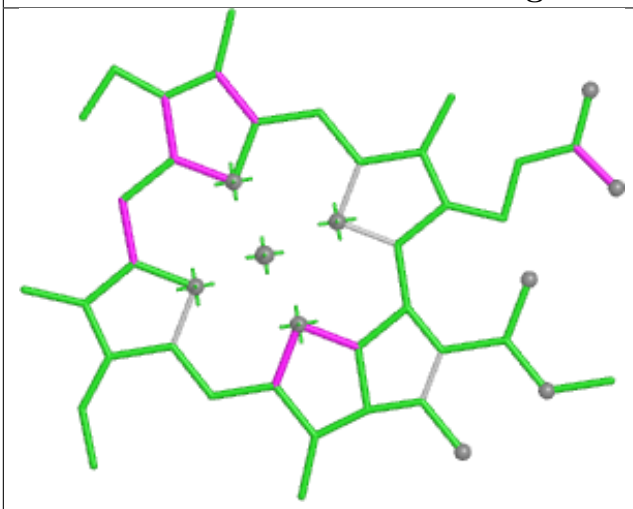


Torsions



Rings

Ligand CLA F 306



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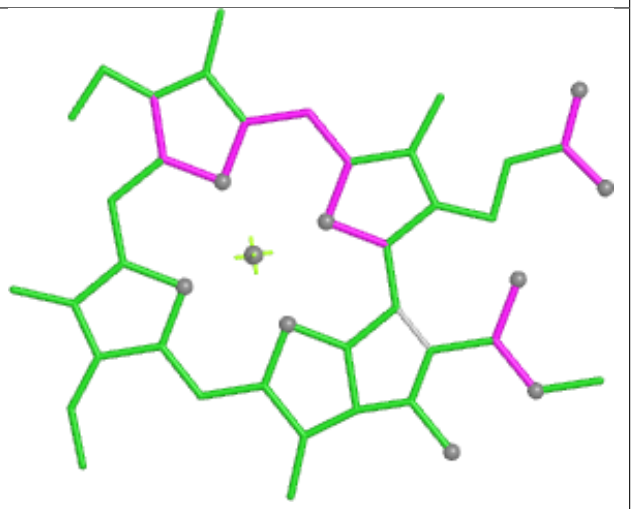
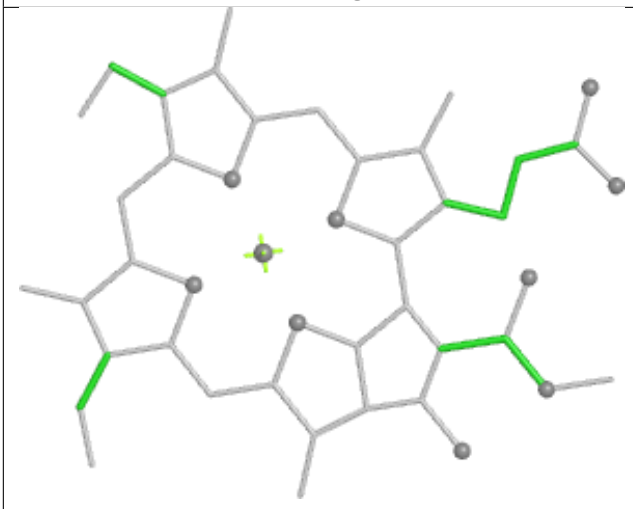


Bond angles

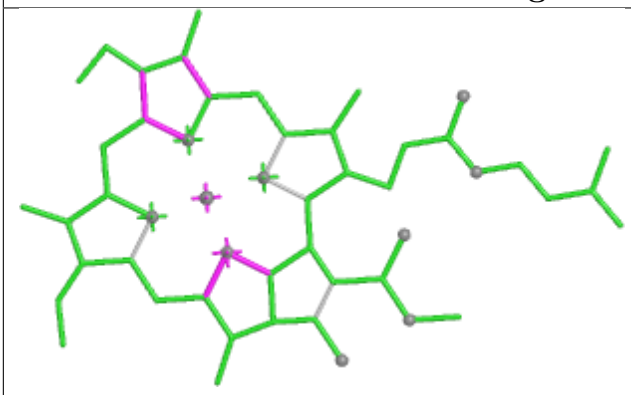


Torsions



Rings

Ligand CLA 4 304



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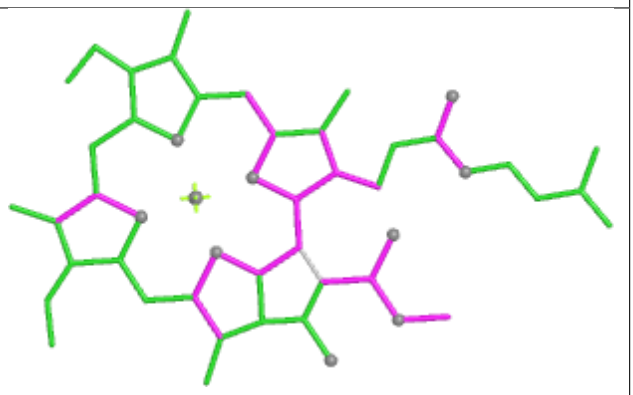
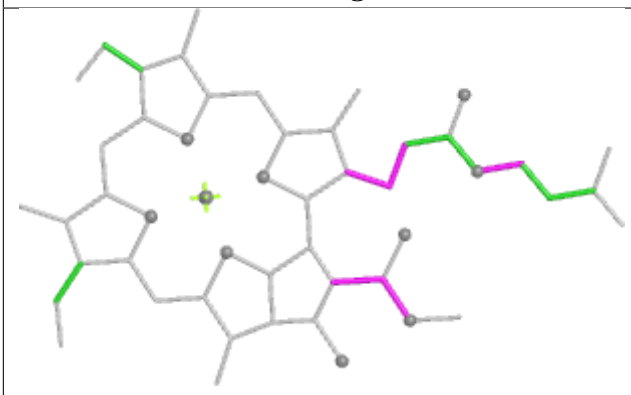


Bond angles



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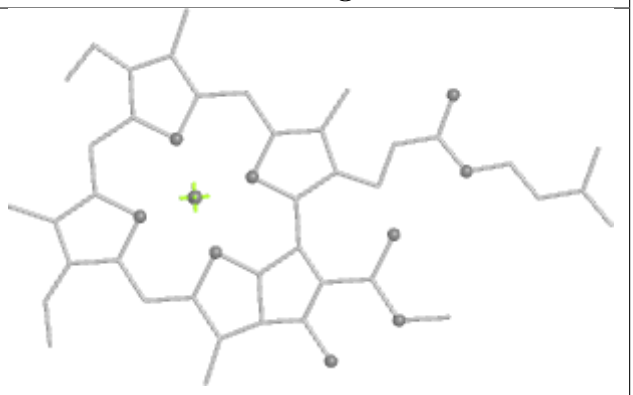
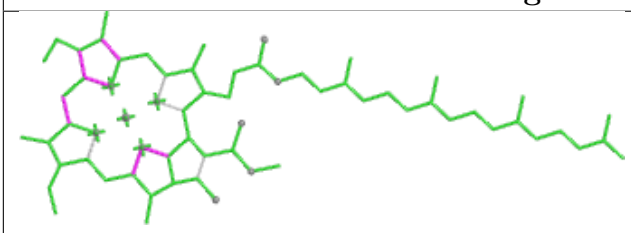


Rings

Ligand CLA A 832



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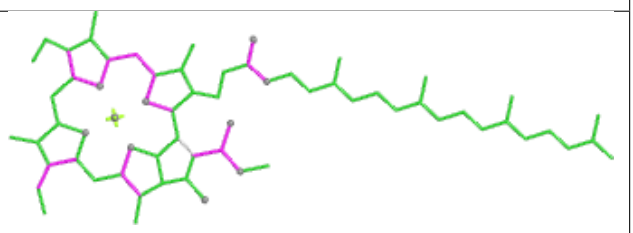
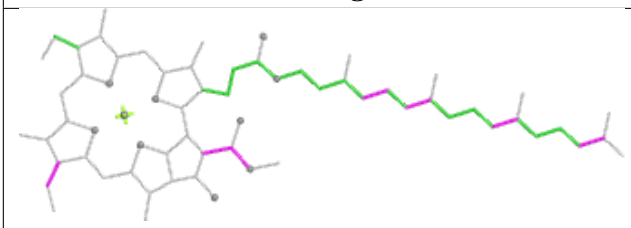


Bond angles



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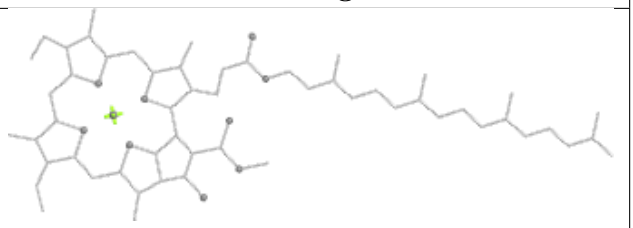
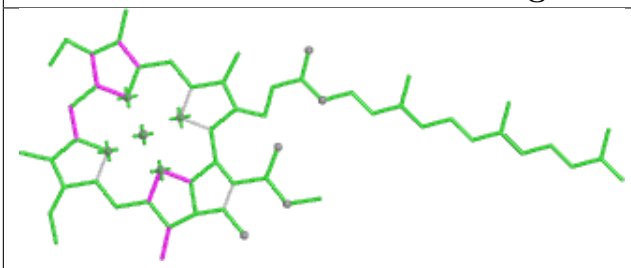


Rings

Ligand CLA 1 308



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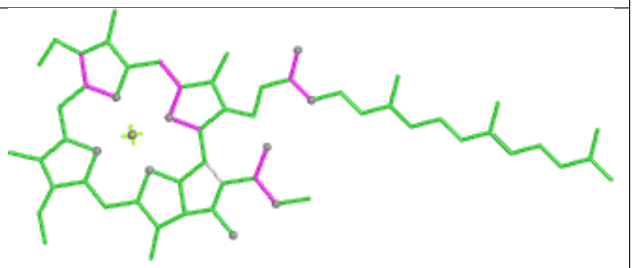
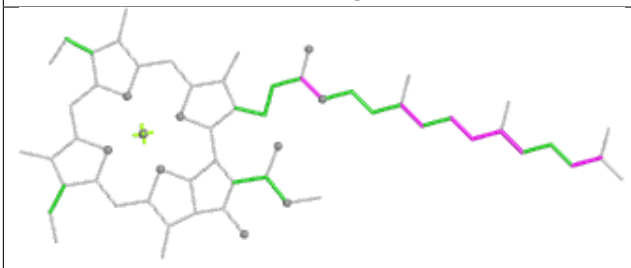


Bond angles



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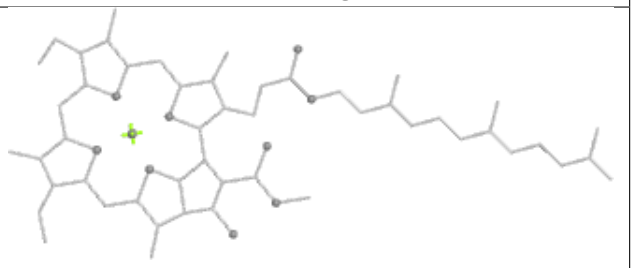
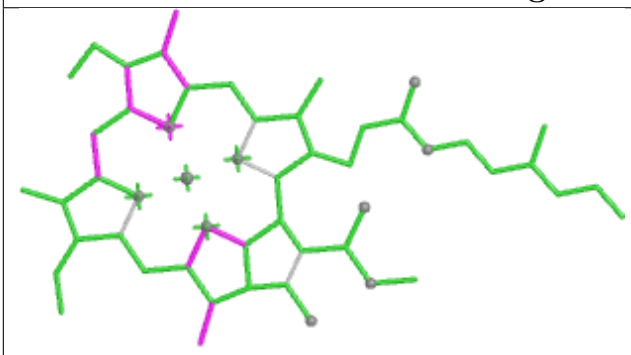
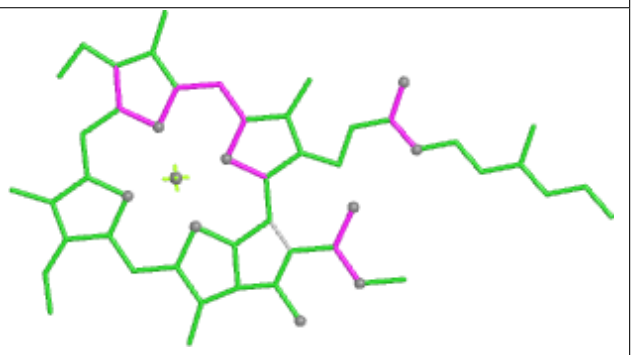


Rings

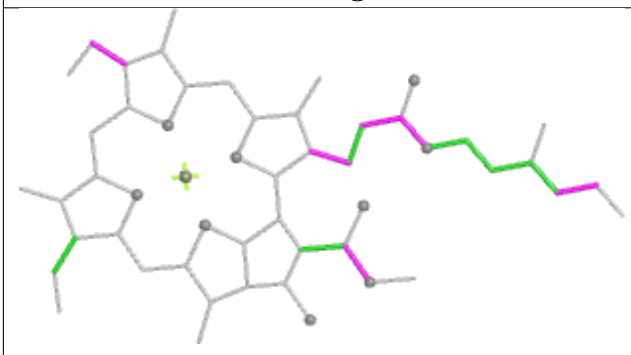
Ligand CLA 1 310



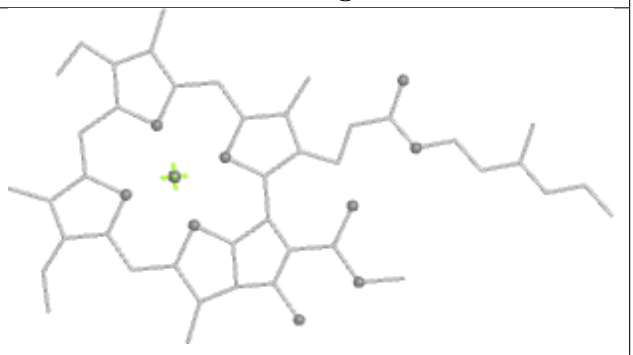
Bond lengths



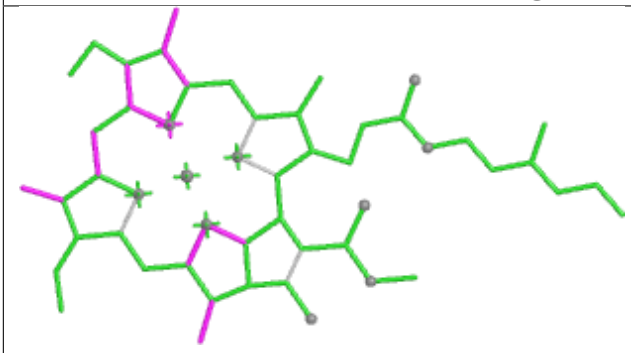
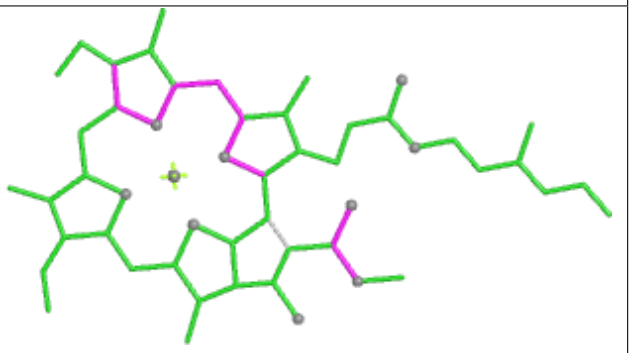
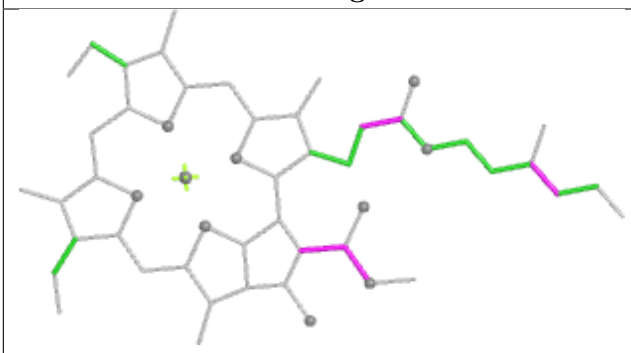
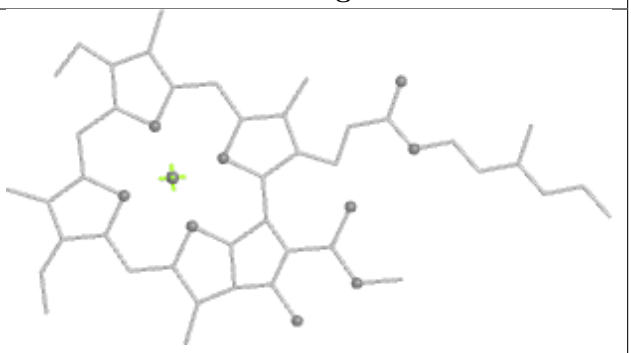
Bond angles

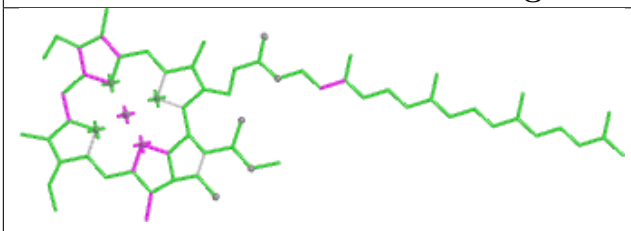
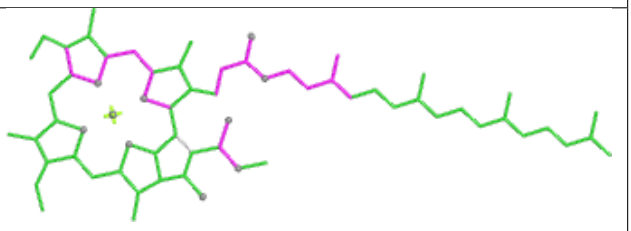
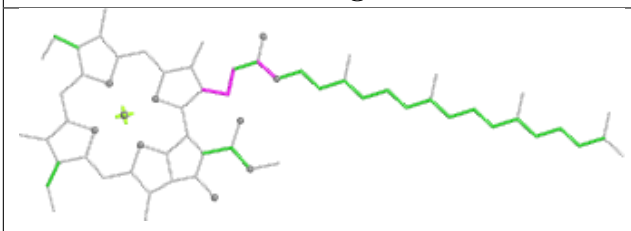
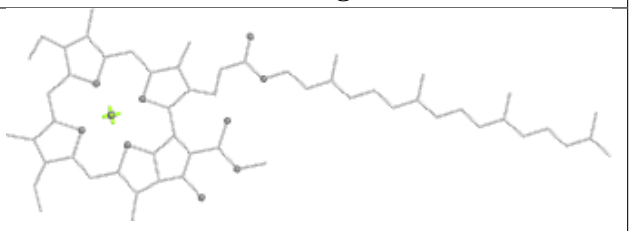


Torsions

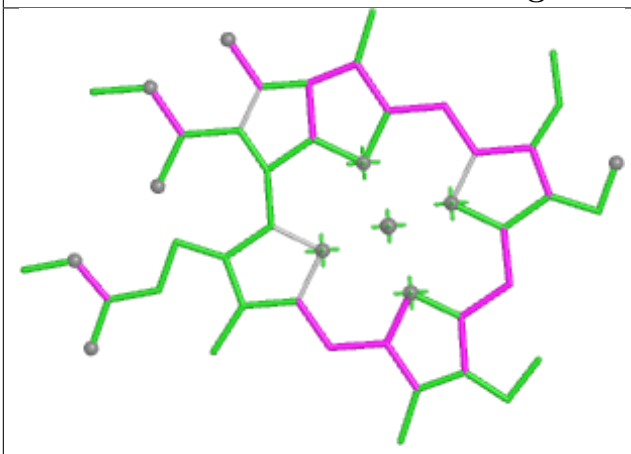


Rings

Ligand CLA 2 310	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA B 830	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CHL 3 607



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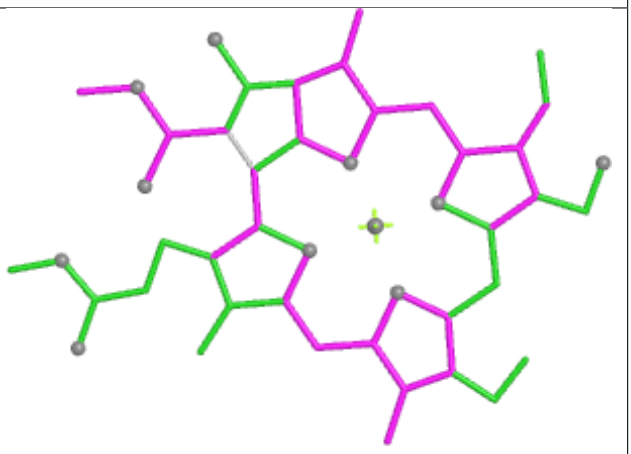
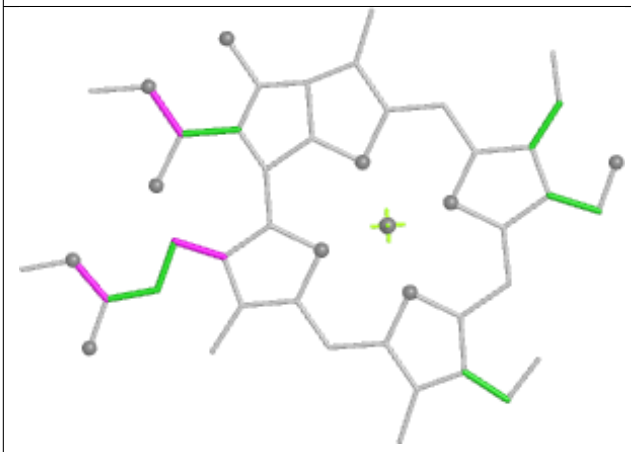


Bond angles



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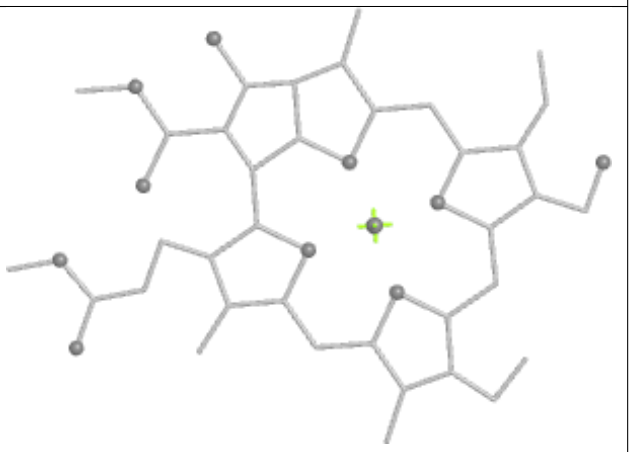
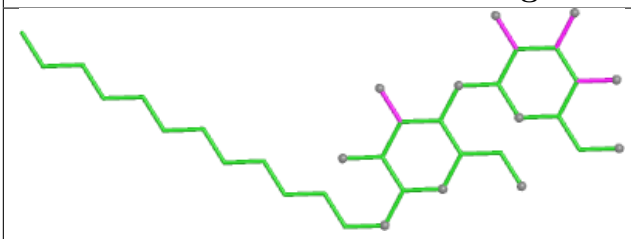


Rings

Ligand LMT A 855



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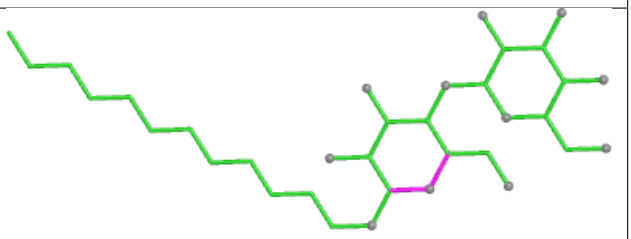
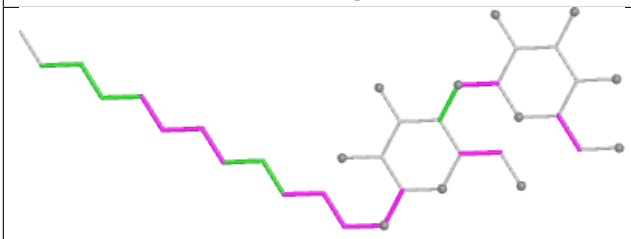


Bond angles



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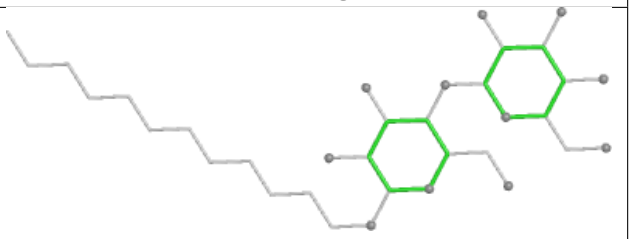
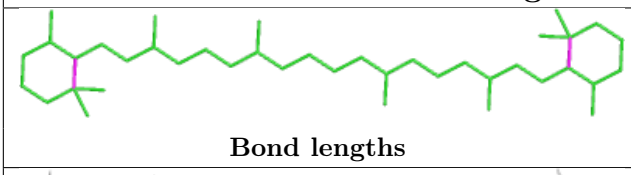


Rings

Ligand BCR F 303



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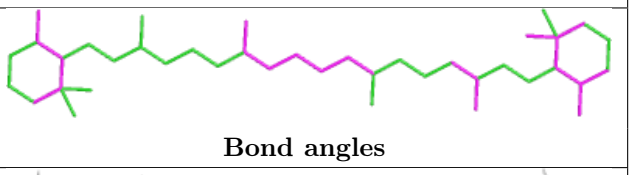
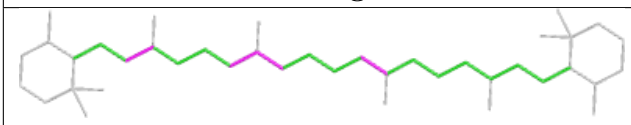


Bond angles



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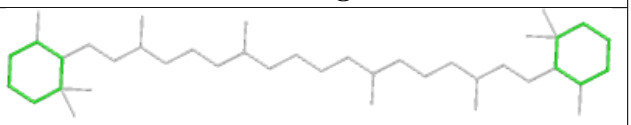
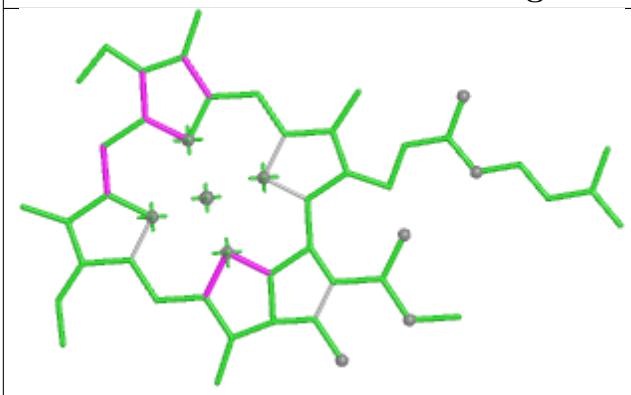


Rings

Ligand CLA L 204



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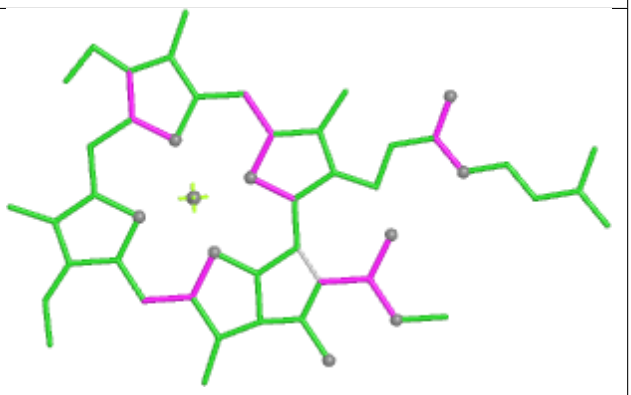
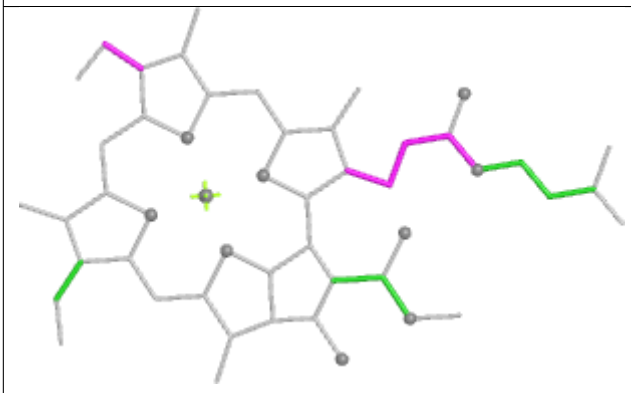


Bond angles



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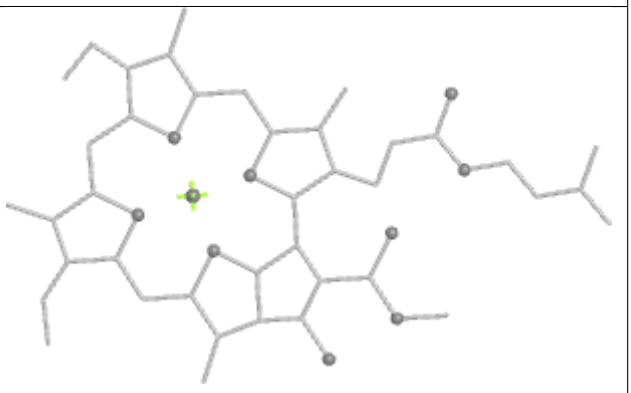
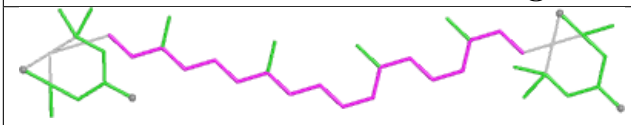


Rings

Ligand XAT 2 315



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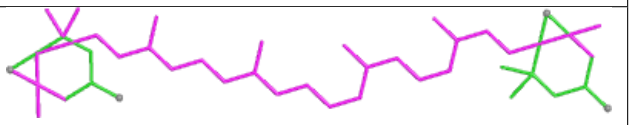

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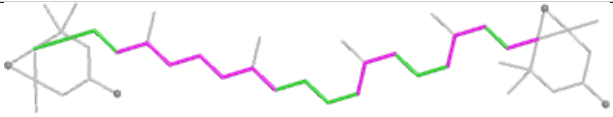

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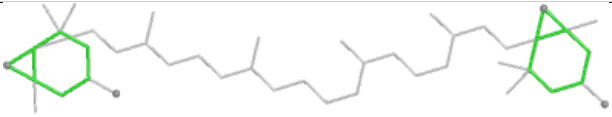
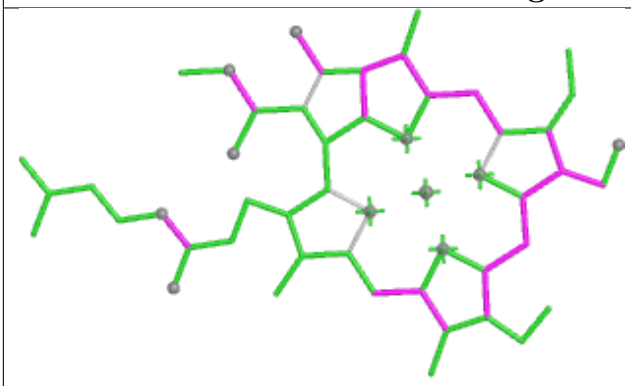


Rings

Ligand CHL 4 306



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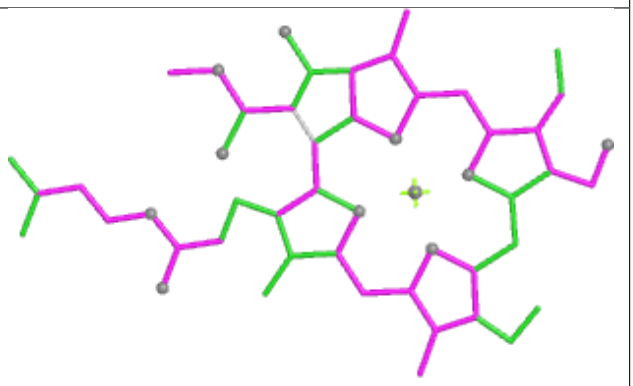
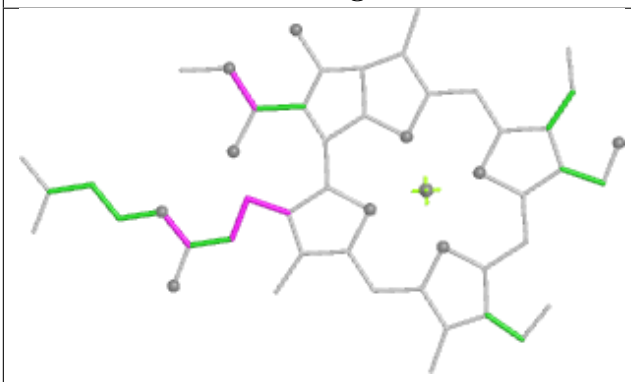


Bond angles



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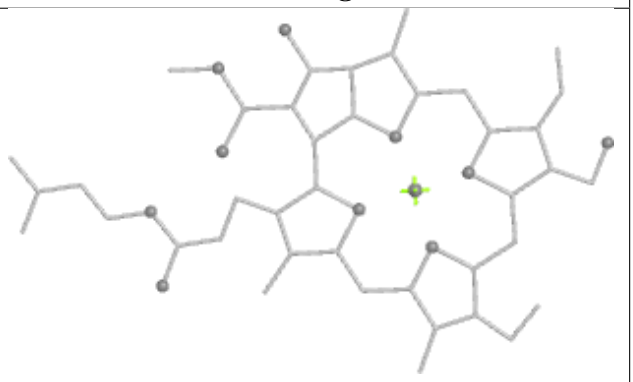
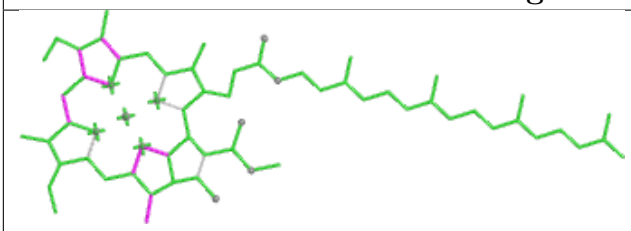


Rings

Ligand CLA L 203



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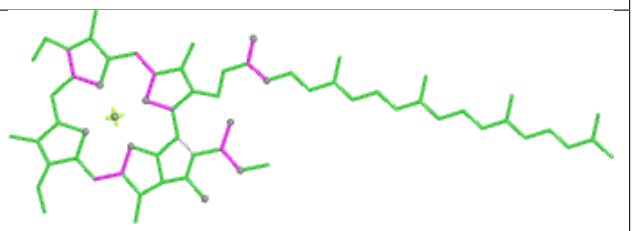

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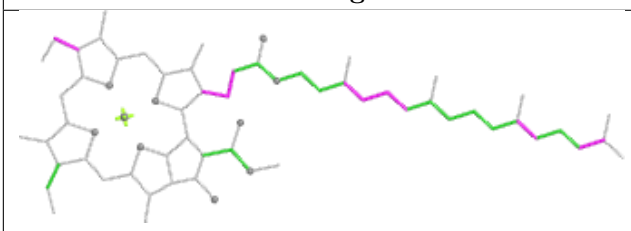

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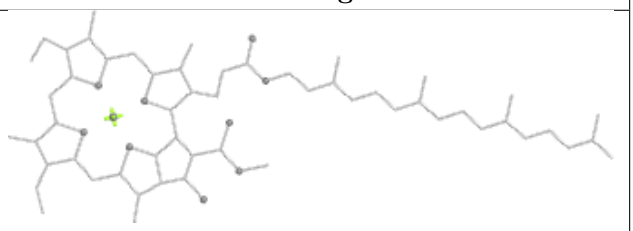
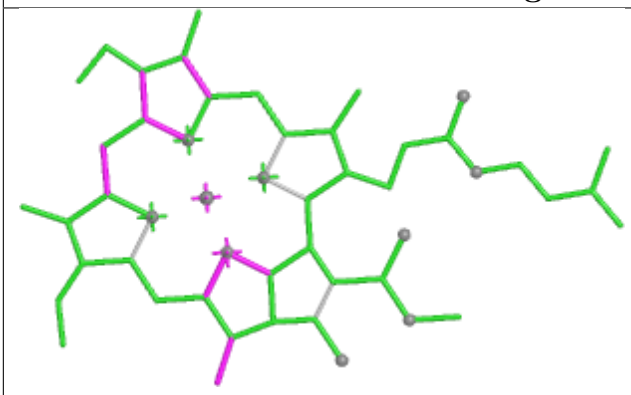


Rings

Ligand CLA B 832



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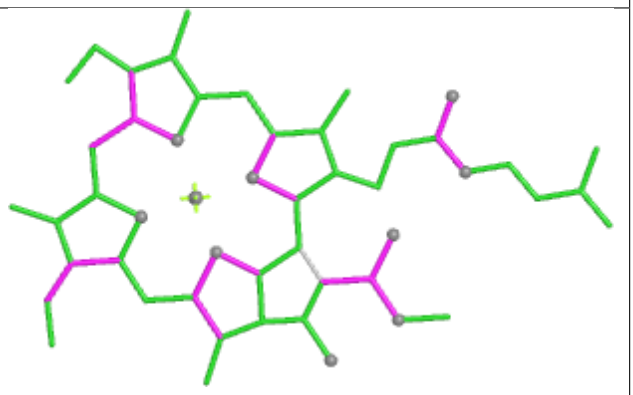

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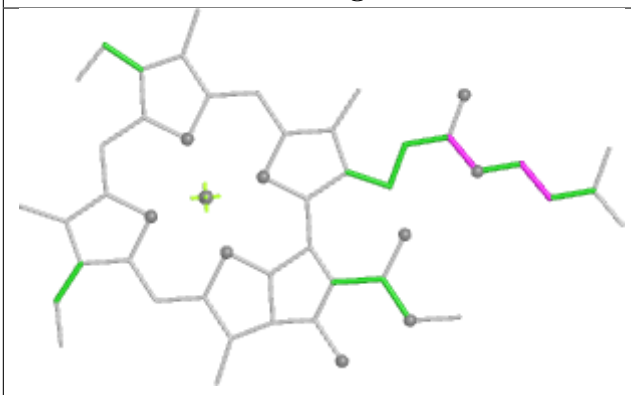

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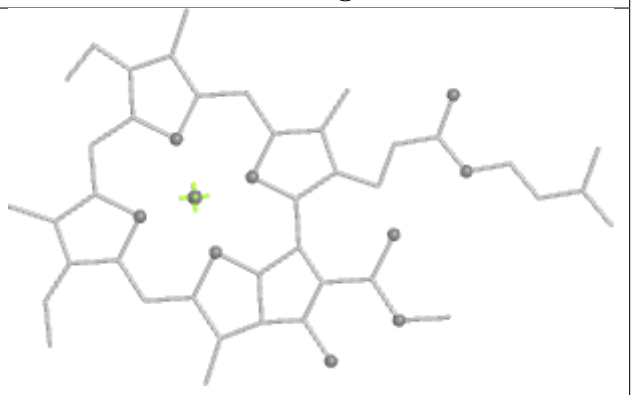
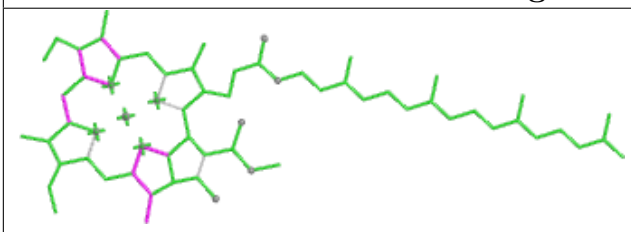


Rings

Ligand CLA 1 302



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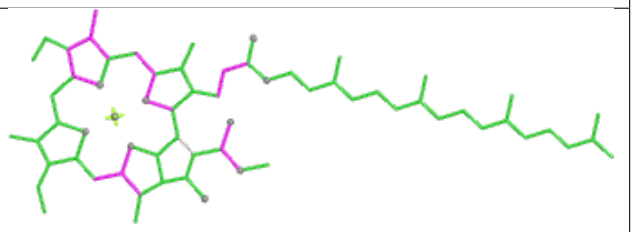

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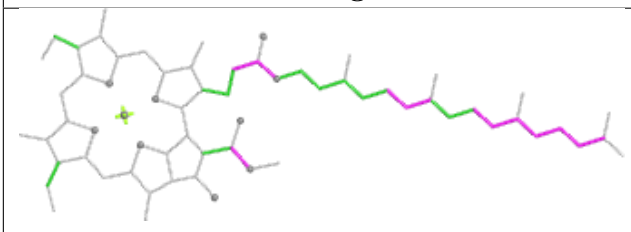

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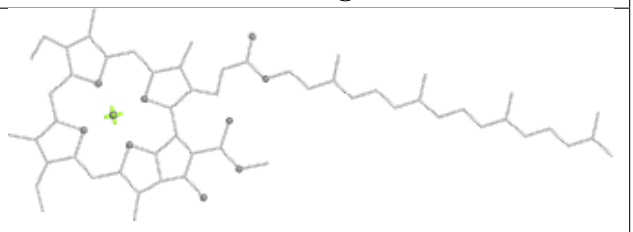
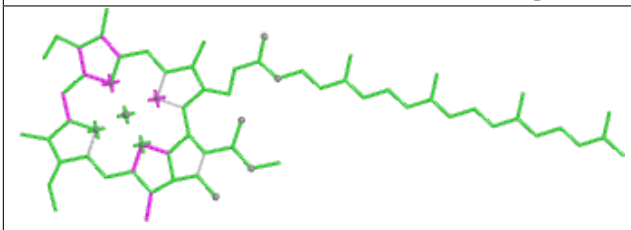


Rings

Ligand CLA 2 301



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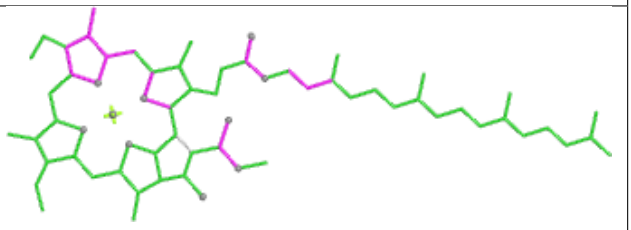

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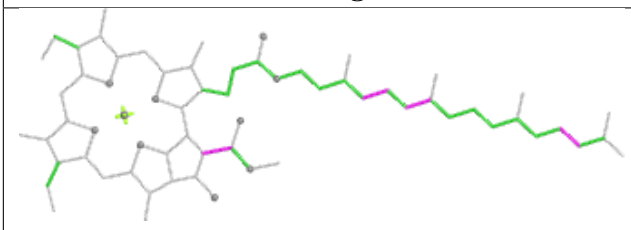

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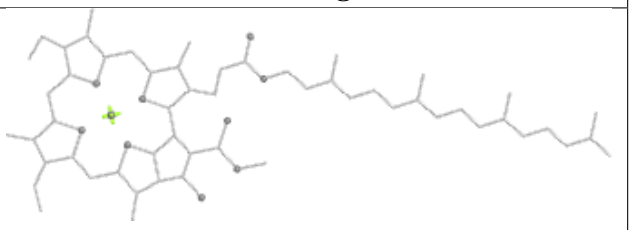
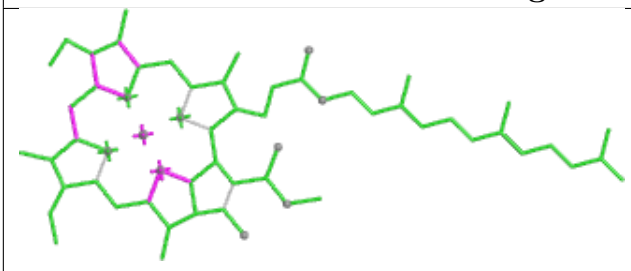


Rings

Ligand CLA 4 310



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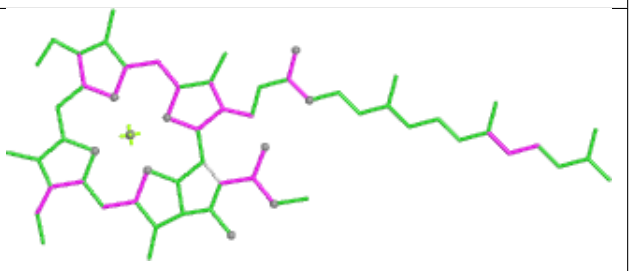
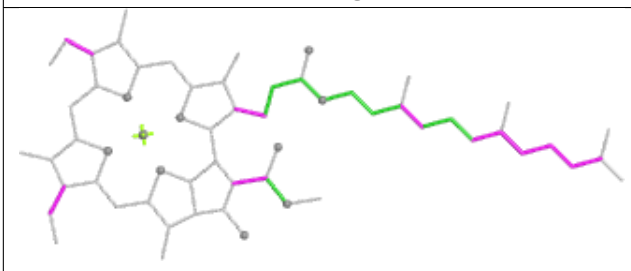


Bond angles



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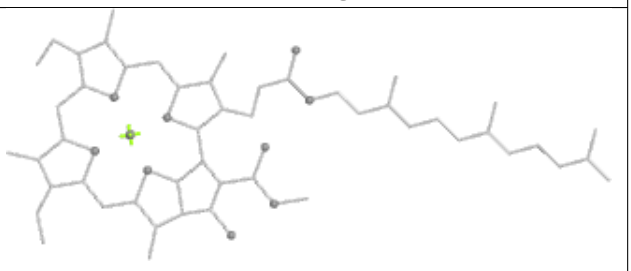
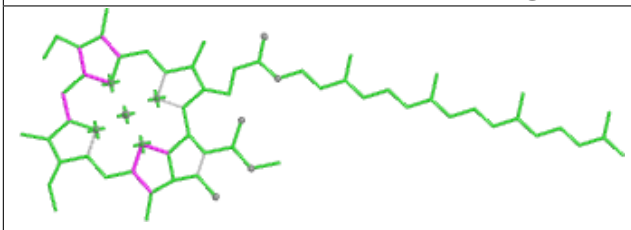
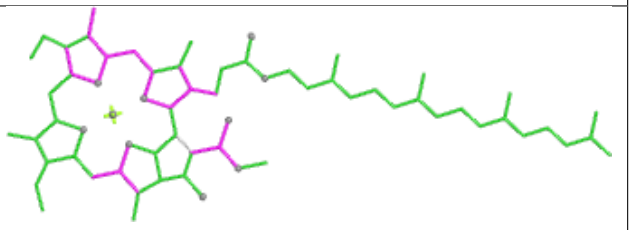


Rings

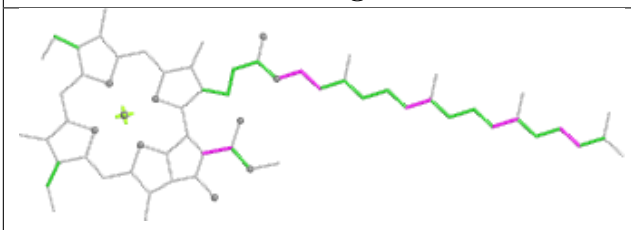
Ligand CLA A 825



Bond lengths



Bond angles



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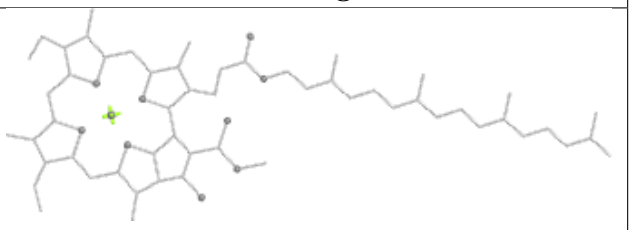
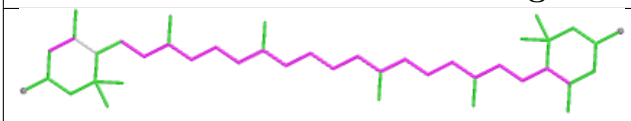


Rings

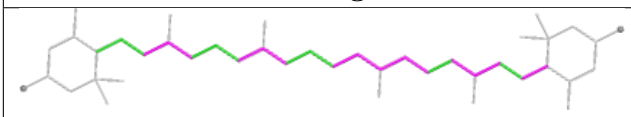
Ligand LUT 2 314



Bond lengths



Bond angles



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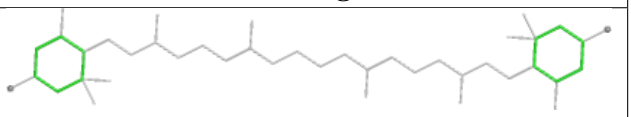
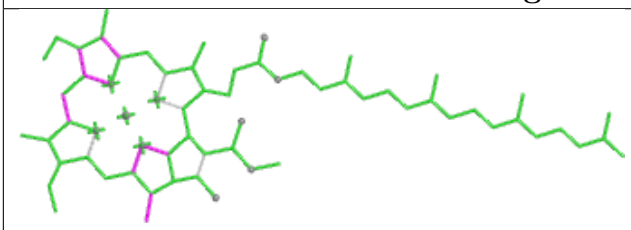
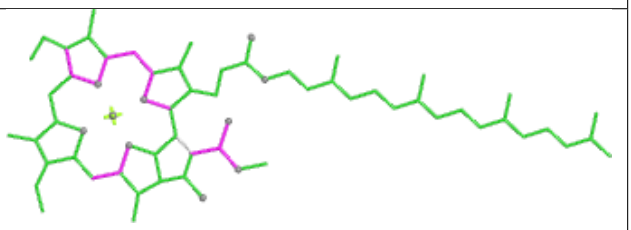


Rings

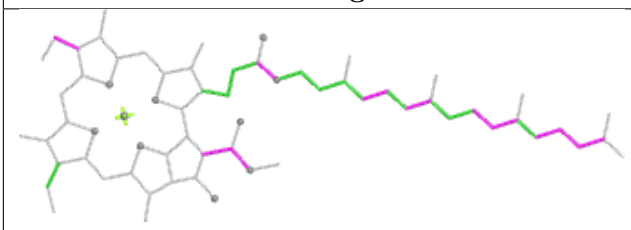
Ligand CLA A 816



Bond lengths



Bond angles



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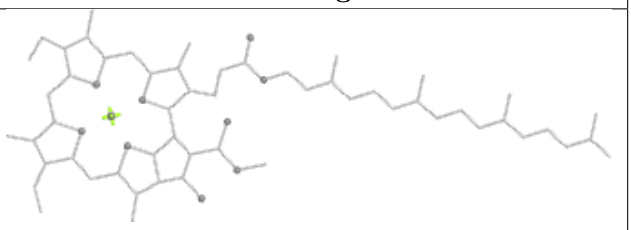
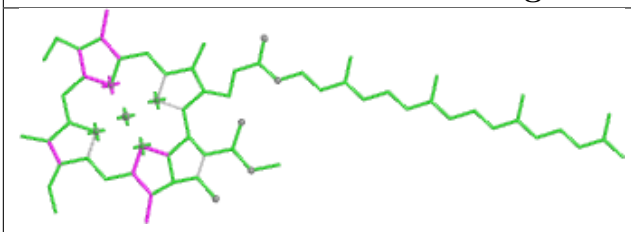


Rings

Ligand CLA B 841



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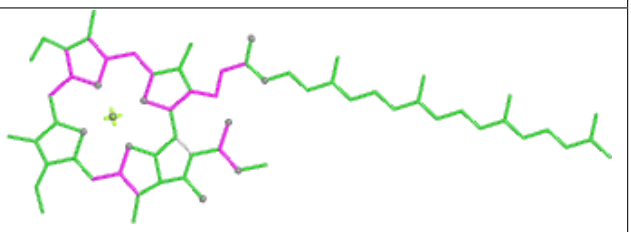
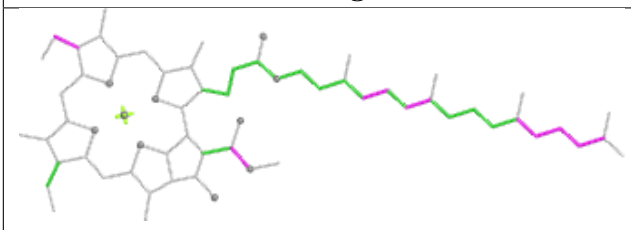


Bond angles



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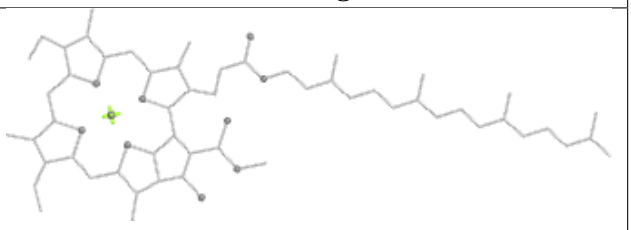
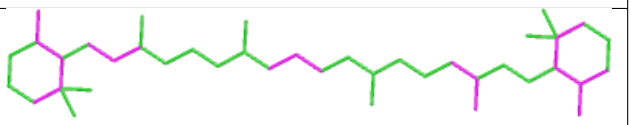


Rings

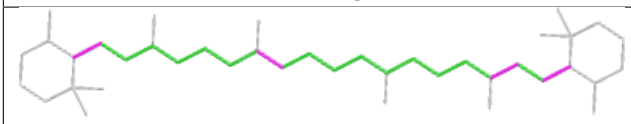
Ligand BCR J 105



Bond lengths



Bond angles



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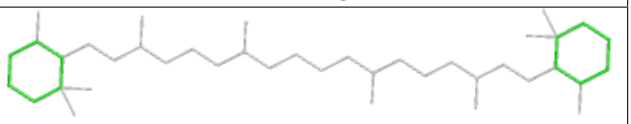
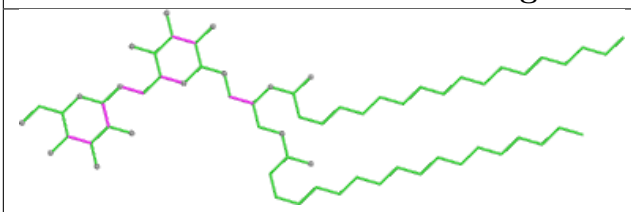
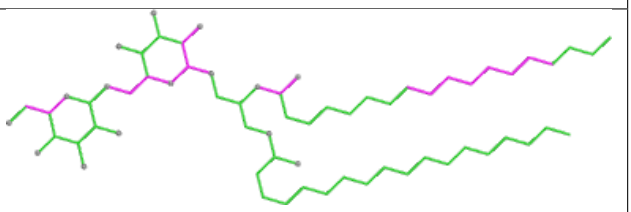


Rings

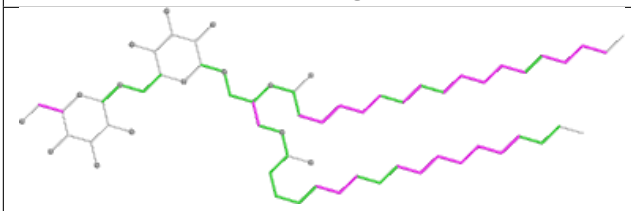
Ligand DGD B 850



Bond lengths



Bond angles



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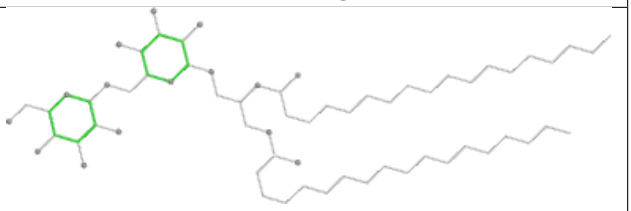
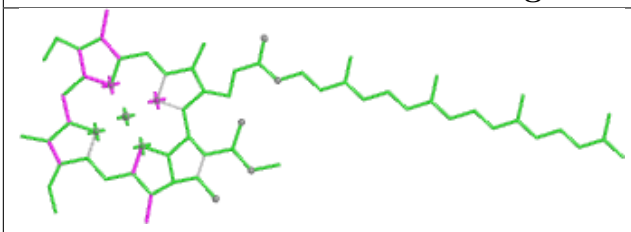


Rings

Ligand CLA B 807



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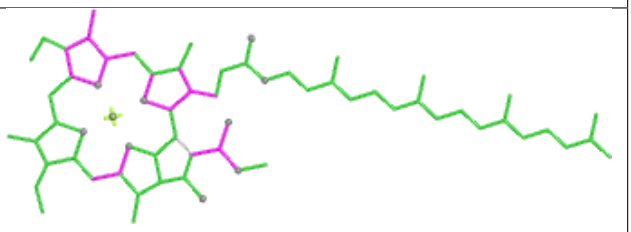
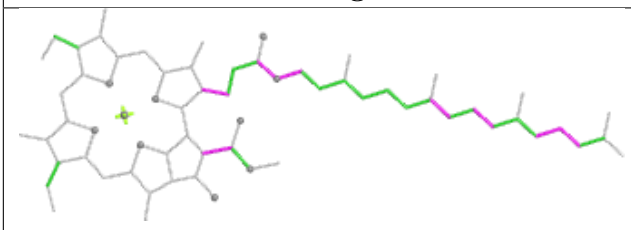


Bond angles



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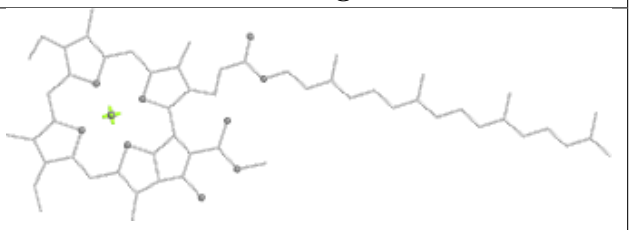
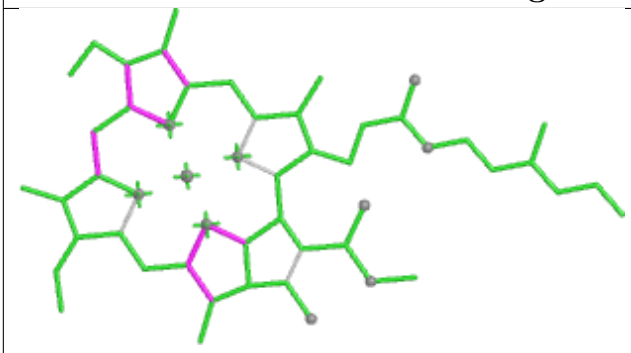


Rings

Ligand CLA 4 311



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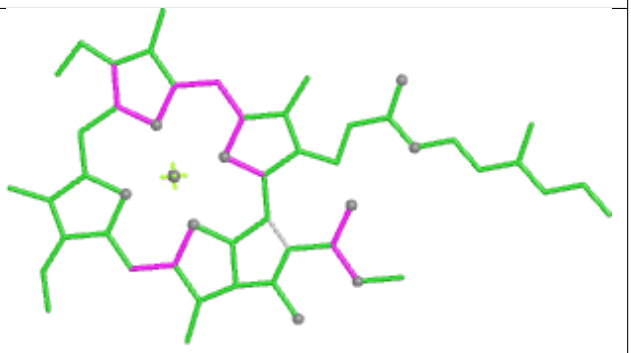
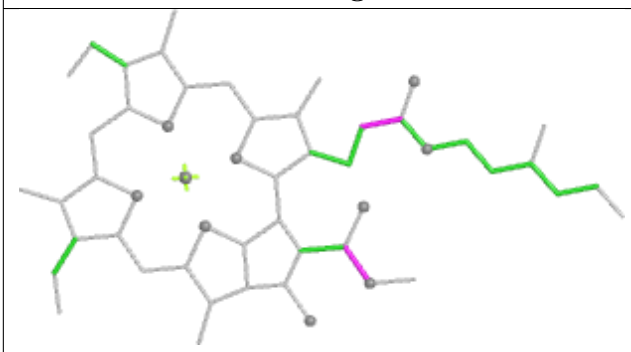


Bond angles



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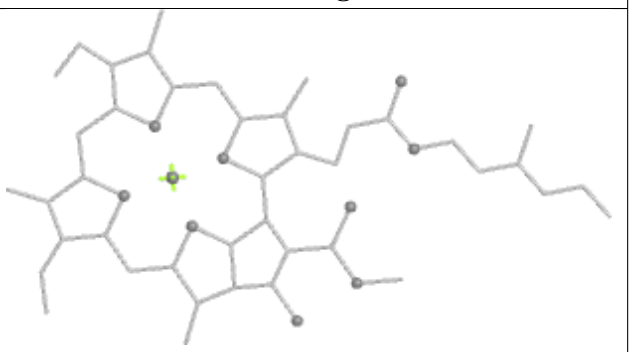
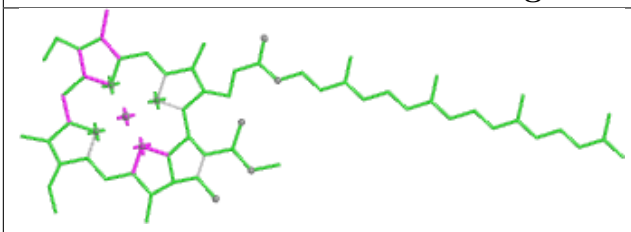


Rings

Ligand CLA B 810



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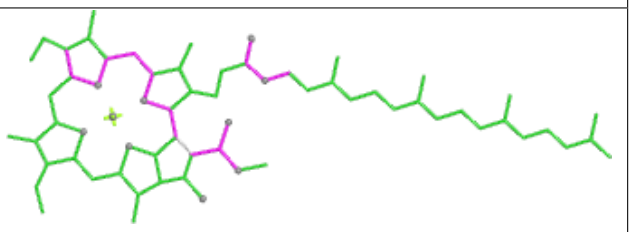
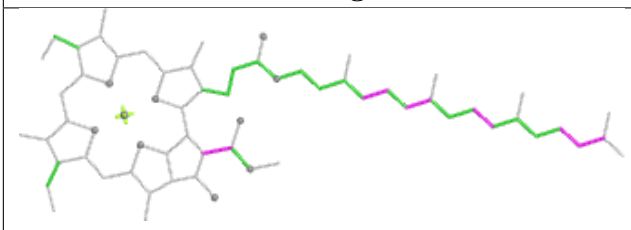


Bond angles



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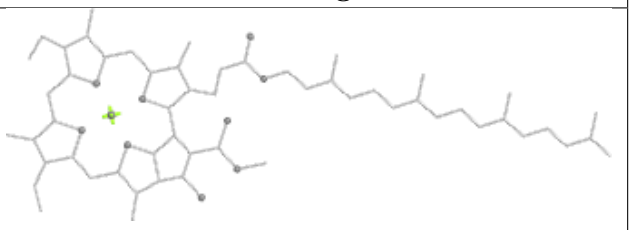
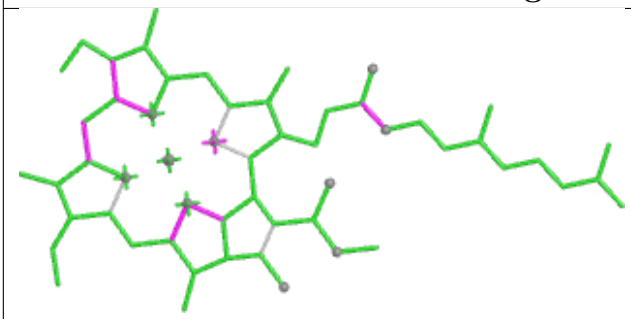


Rings

Ligand CLA B 814



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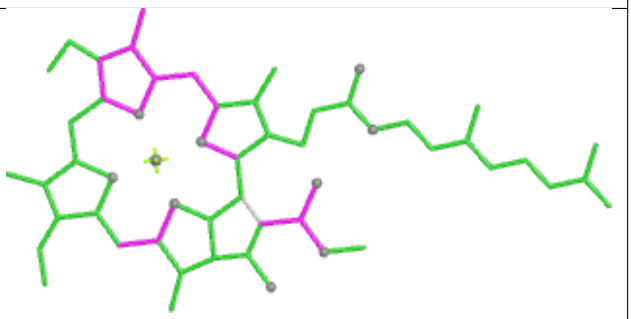
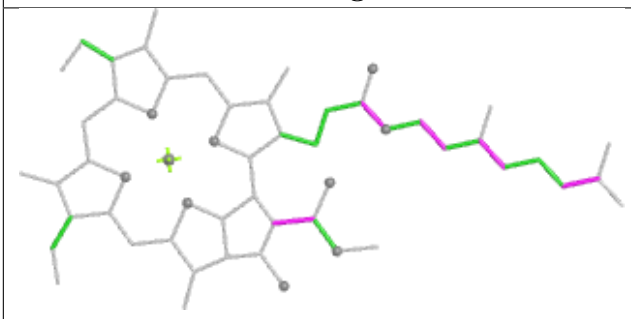


Bond angles



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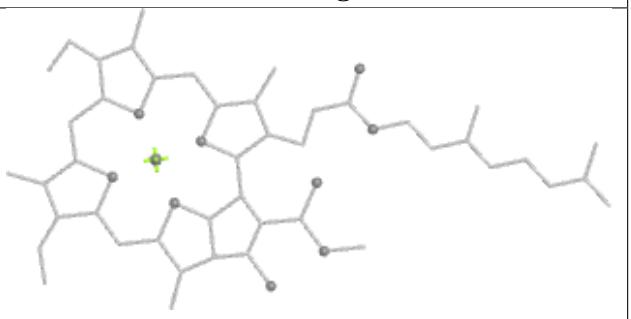
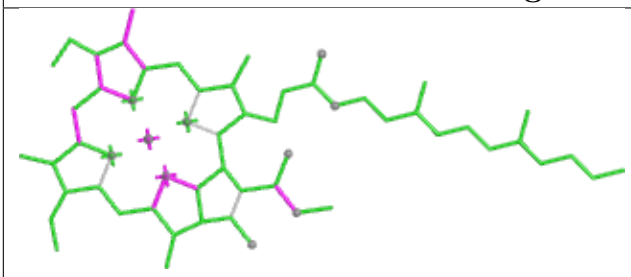


Rings

Ligand CLA B 834



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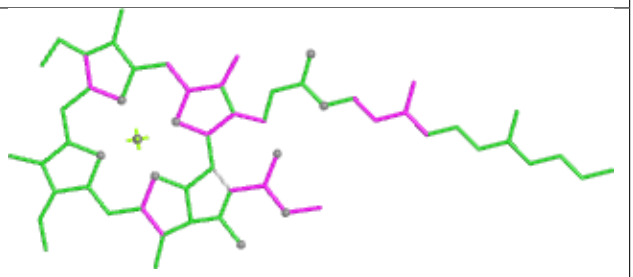
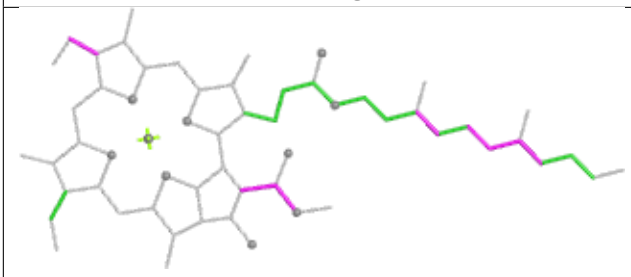


Bond angles



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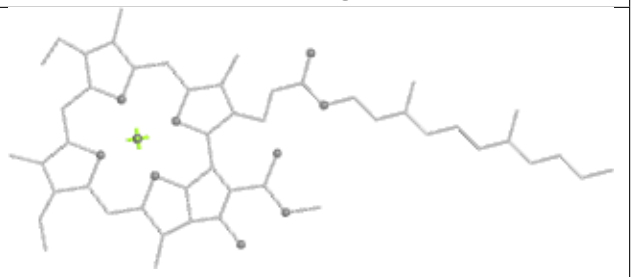
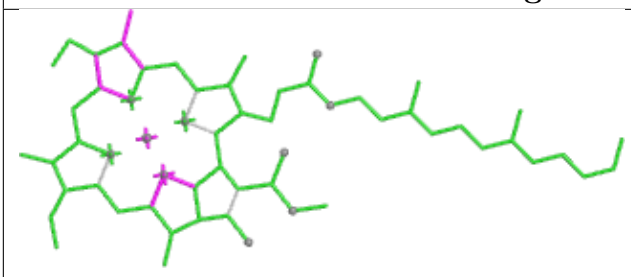


Rings

Ligand CLA B 819



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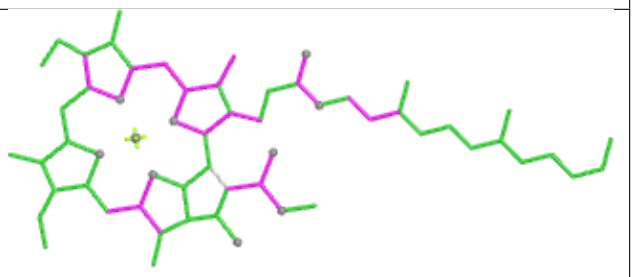
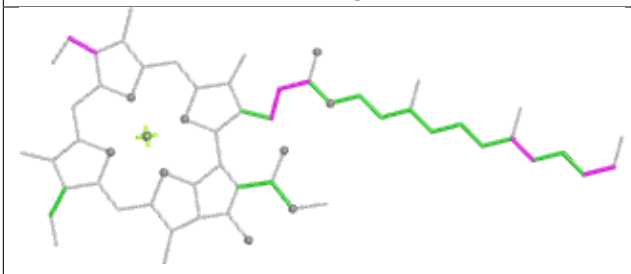


Bond angles



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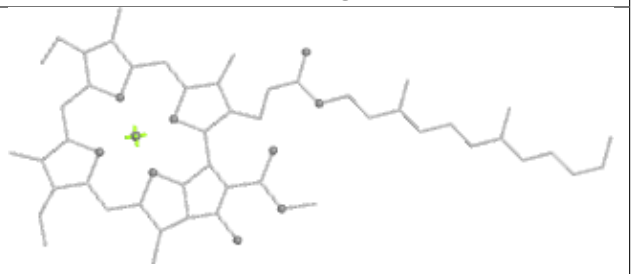
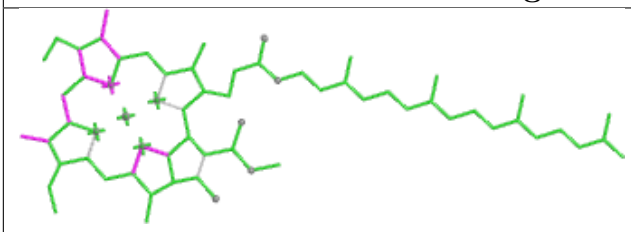


Rings

Ligand CLA A 841



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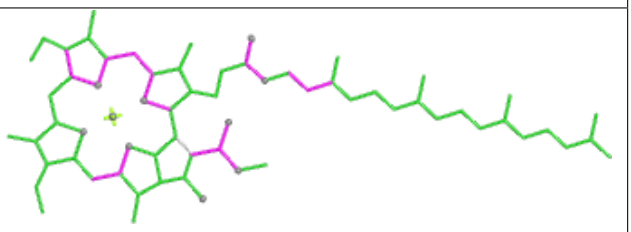
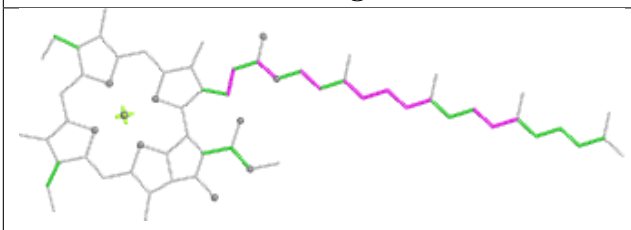


Bond angles



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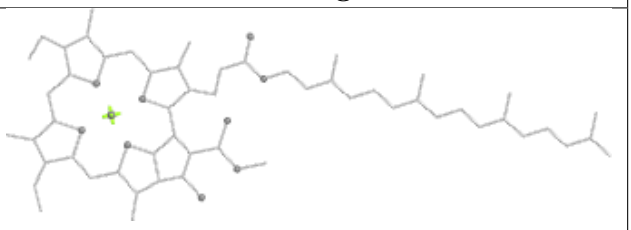
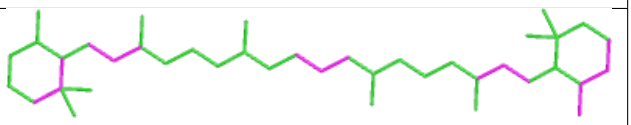


Rings

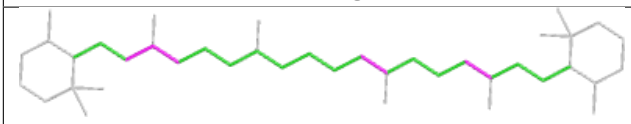
Ligand BCR A 851



Bond lengths



Bond angles



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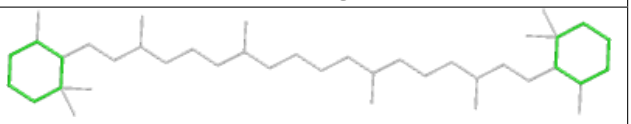
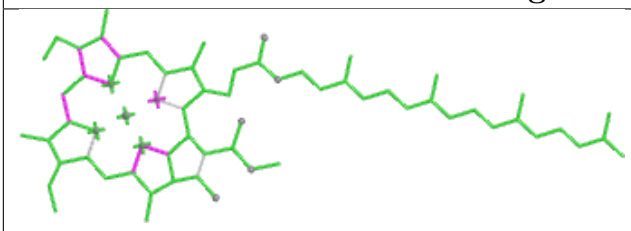
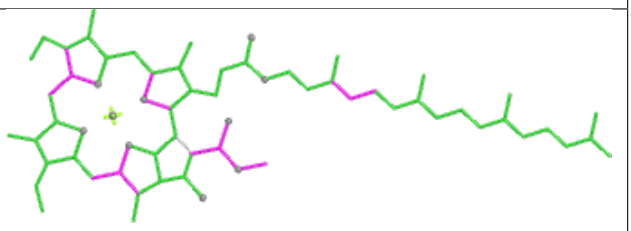


Rings

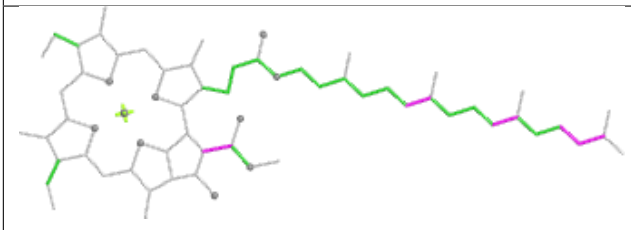
Ligand CLA 1 301



Bond lengths



Bond angles



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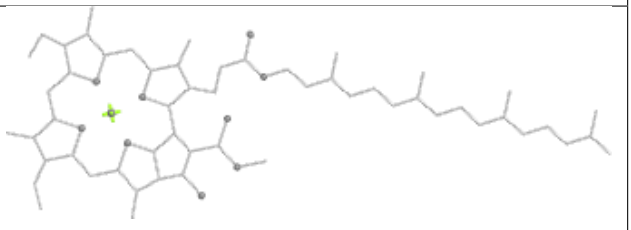
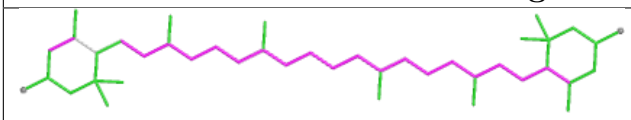
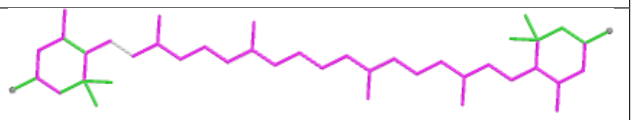


Rings

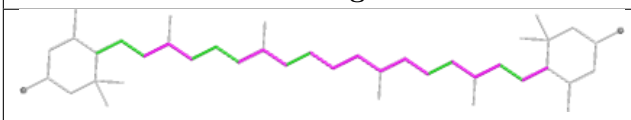
Ligand LUT 1 314



Bond lengths



Bond angles



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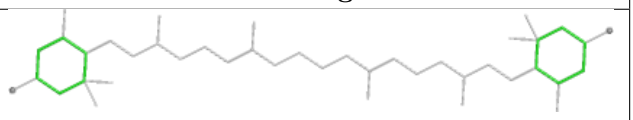
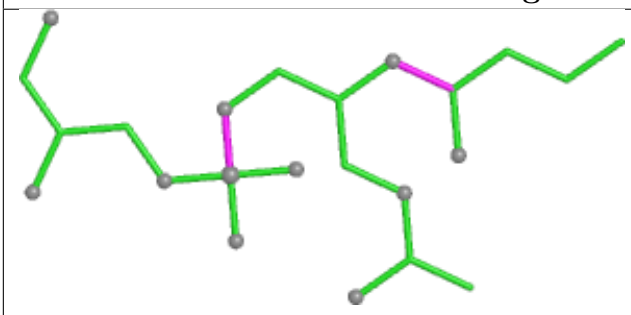
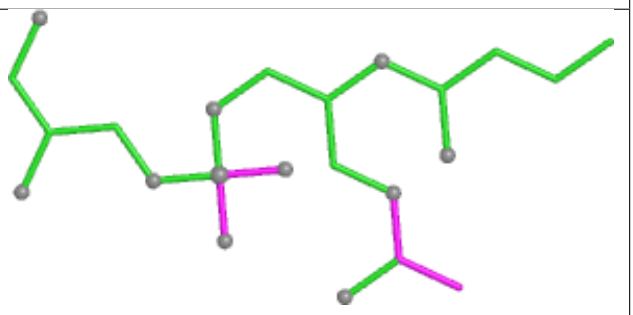


Rings

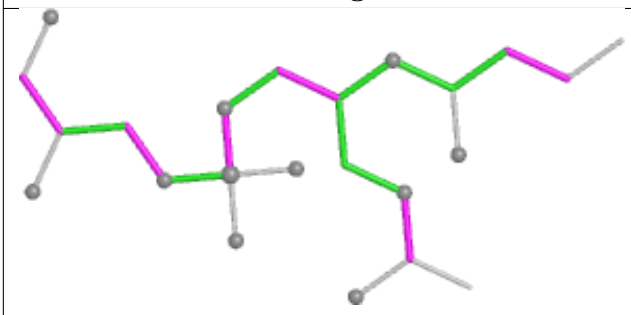
Ligand LHG B 801



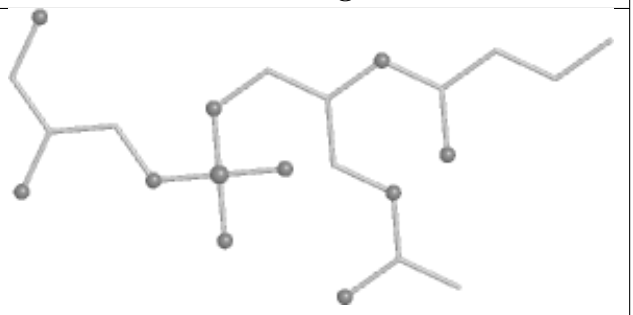
Bond lengths



Bond angles

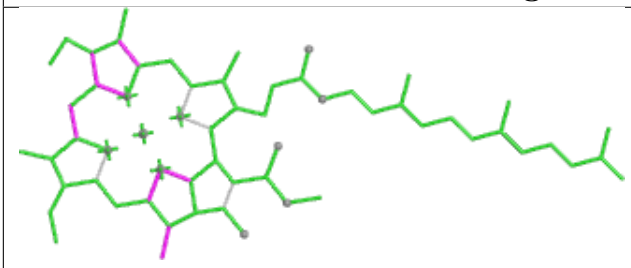


Torsions

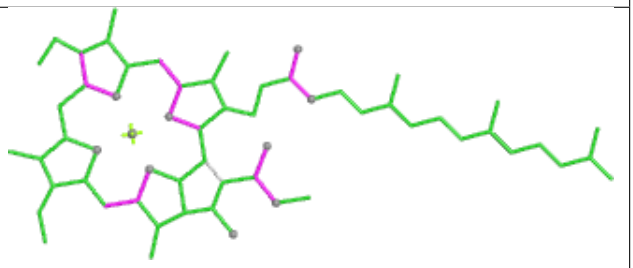


Rings

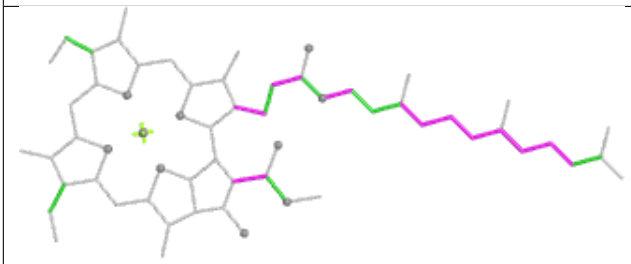
Ligand CLA K 202



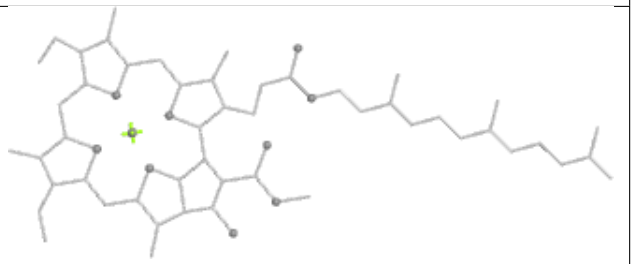
Bond lengths



Bond angles

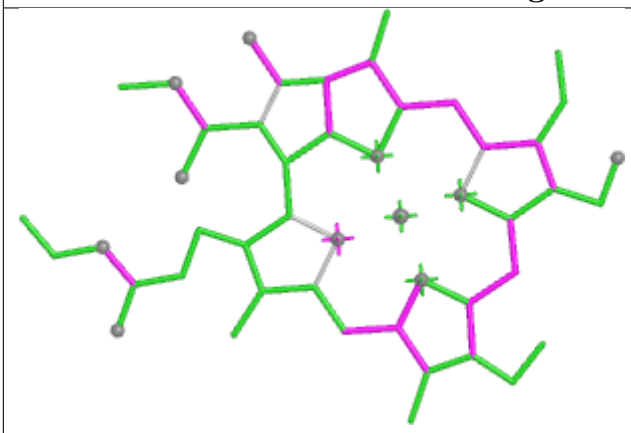


Torsions

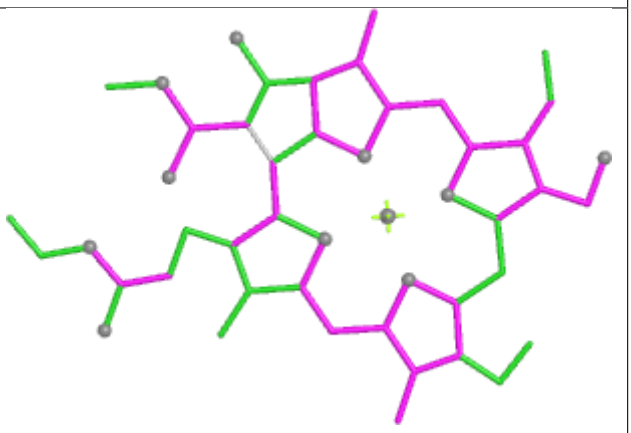


Rings

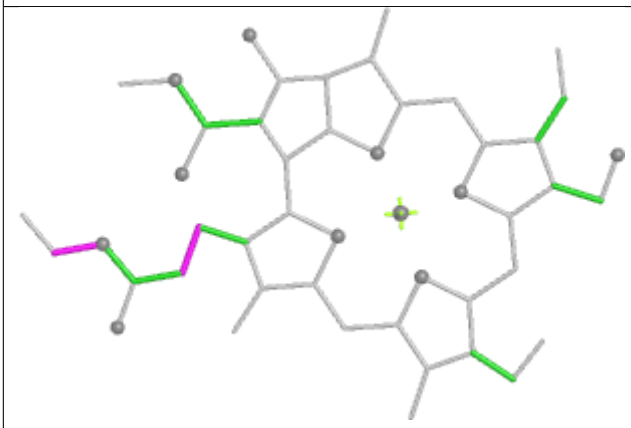
Ligand CHL 2 305



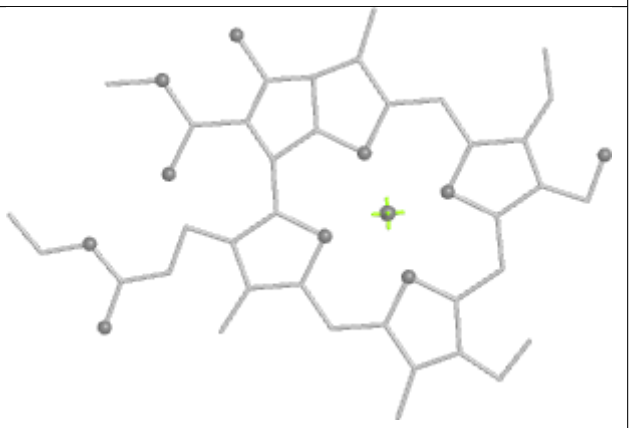
Bond lengths



Bond angles

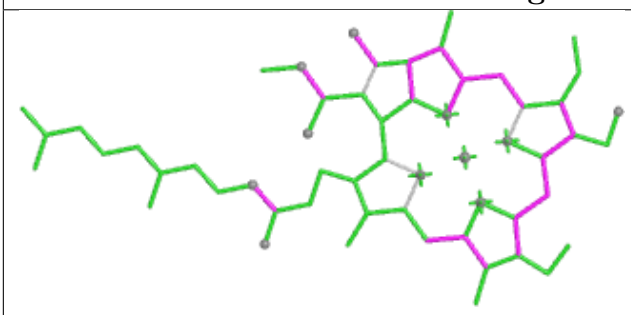


Torsions

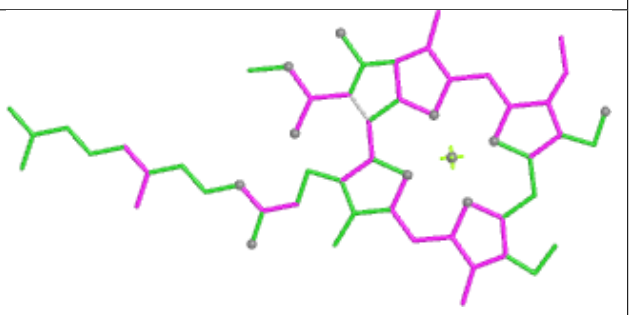


Rings

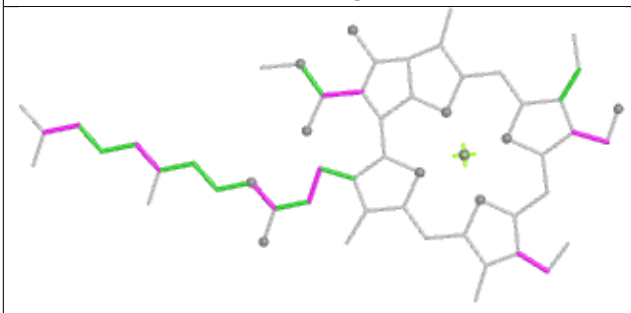
Ligand CHL 4 305



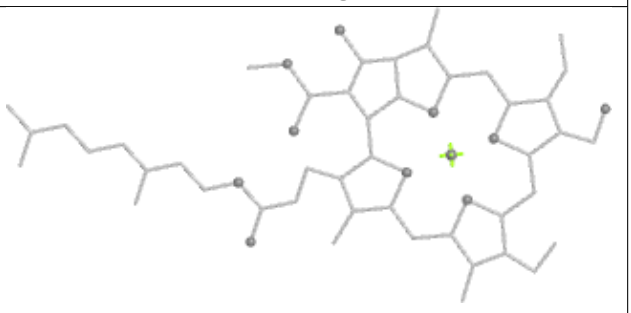
Bond lengths



Bond angles

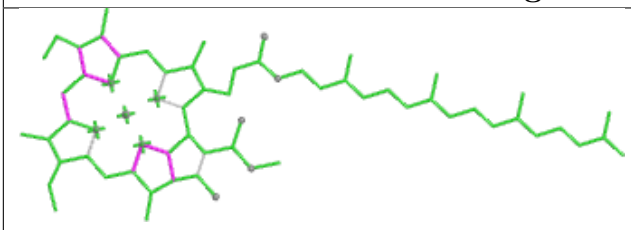


Torsions

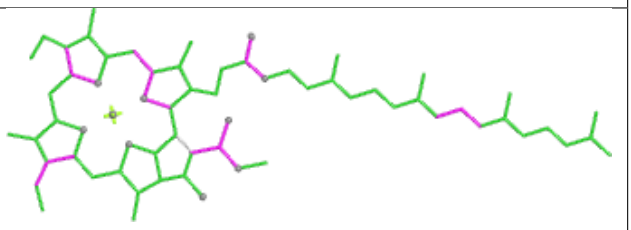


Rings

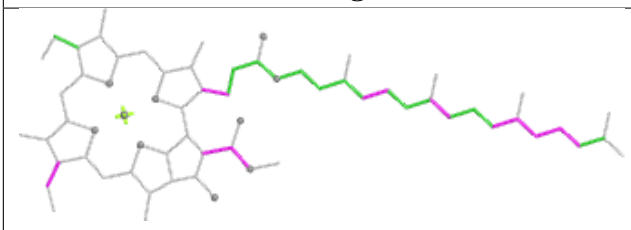
Ligand CLA B 815



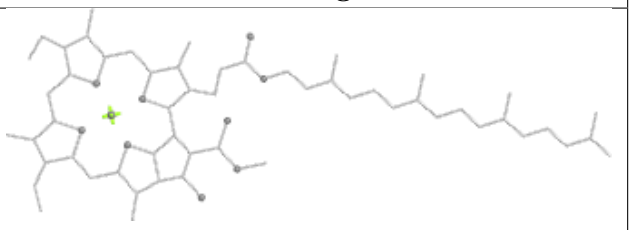
Bond lengths



Bond angles

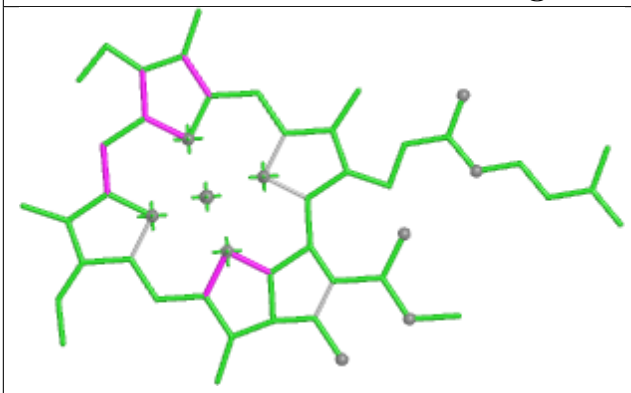


Torsions

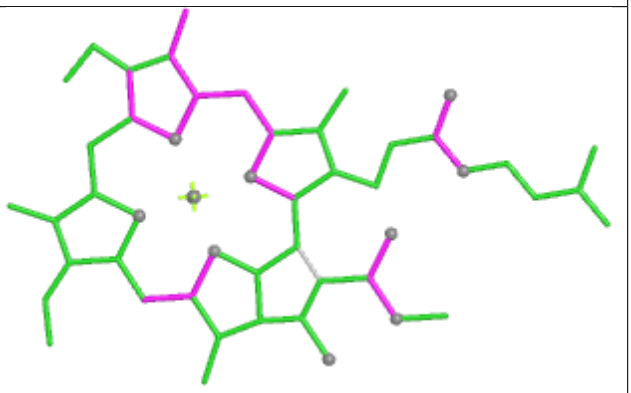


Rings

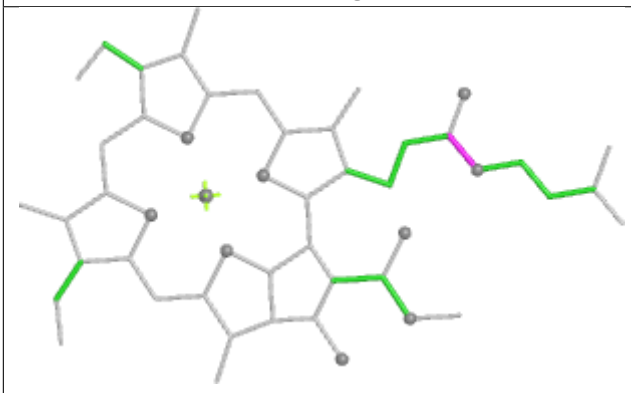
Ligand CLA 2 307



Bond lengths



Bond angles



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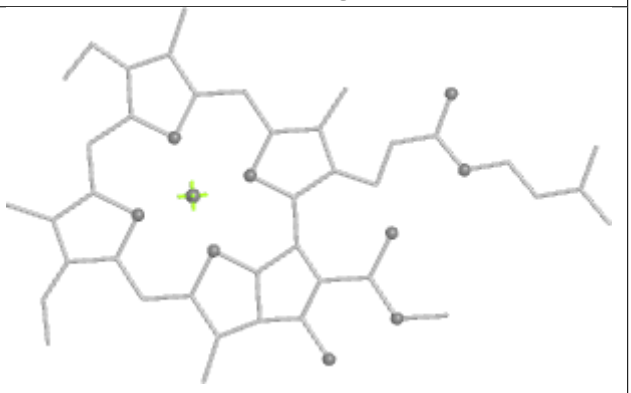
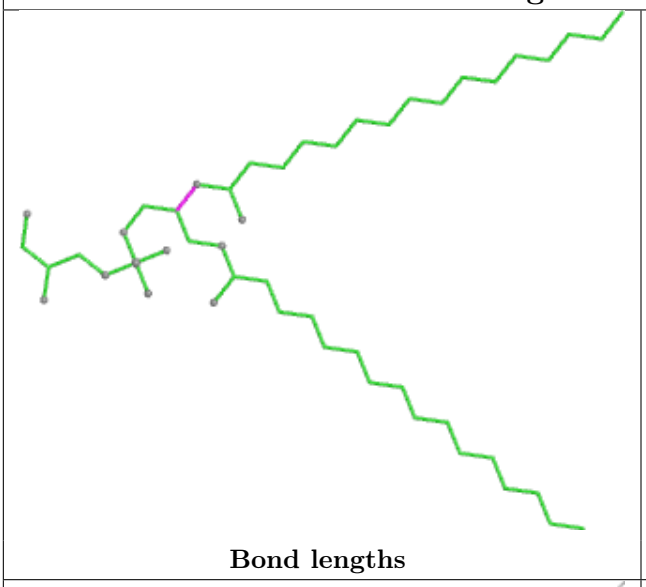
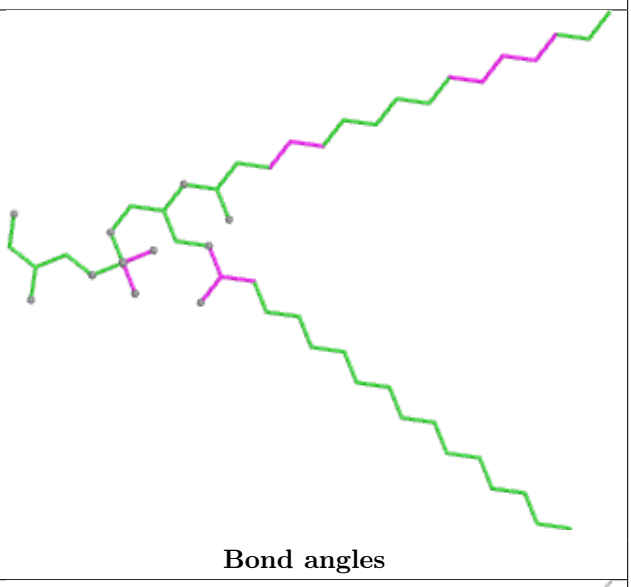


Rings

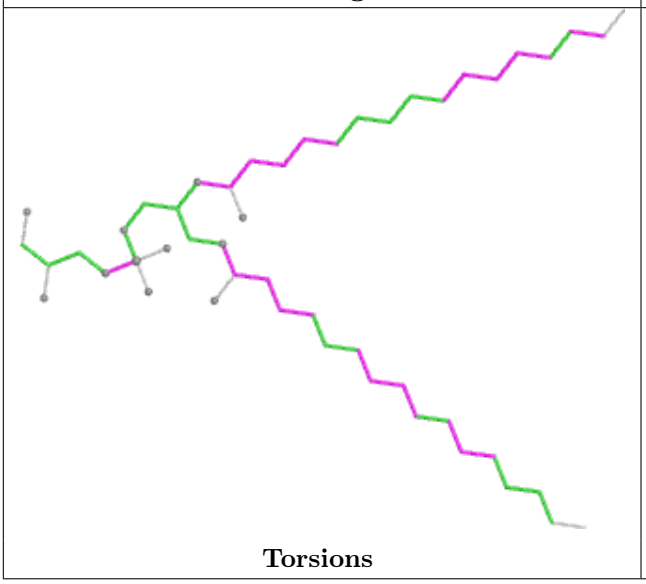
Ligand LHG 1 317



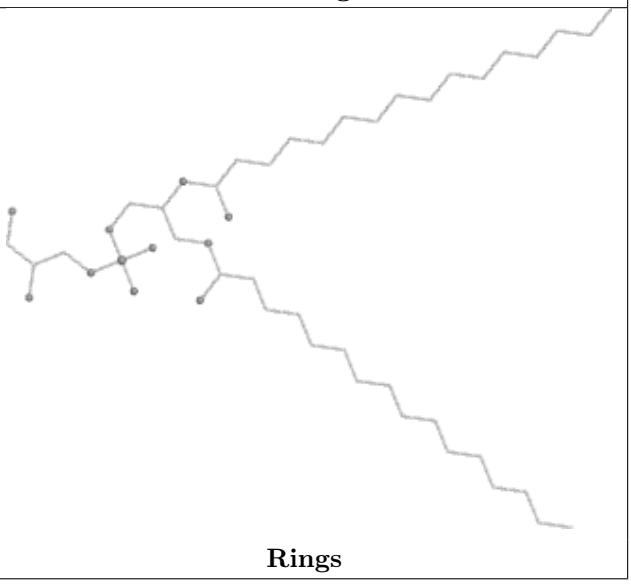
Bond lengths



Bond angles



Torsions

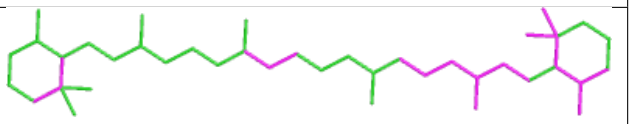


Rings

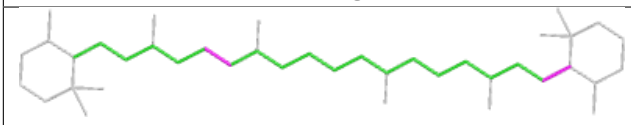
Ligand BCR B 847



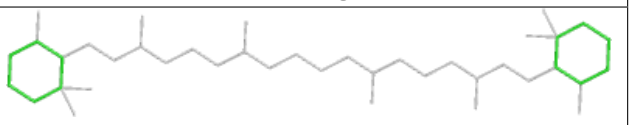
Bond lengths



Bond angles

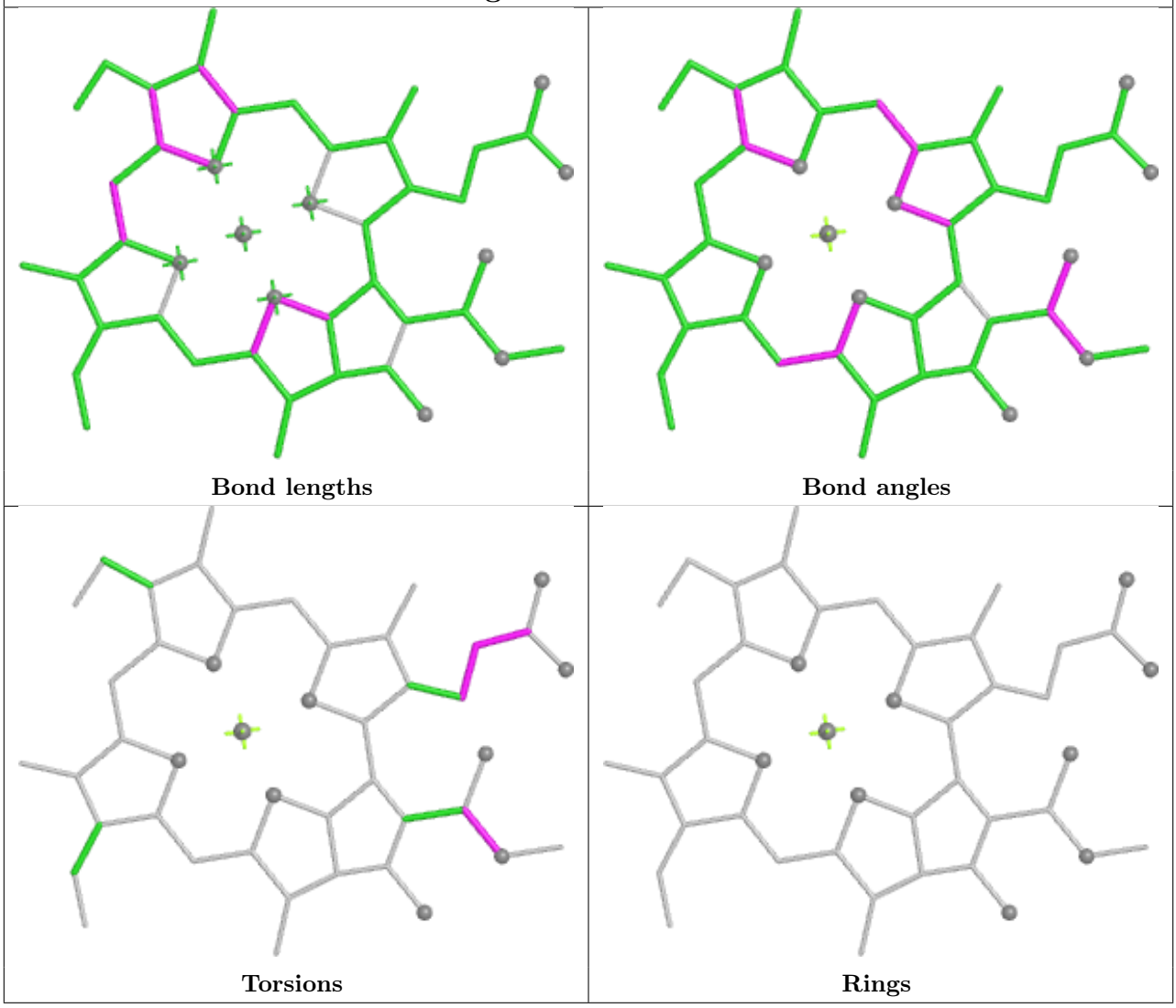


Torsions



Rings

Ligand CLA 3 612



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	195/195 (100%)	0.58	15 (7%) 19 16	66, 95, 152, 193	0
2	2	204/269 (75%)	0.68	17 (8%) 17 14	87, 121, 159, 212	0
3	3	216/275 (78%)	0.76	23 (10%) 11 8	114, 161, 229, 257	0
4	4	195/198 (98%)	0.12	4 (2%) 63 59	60, 74, 111, 143	0
5	A	742/758 (97%)	0.30	26 (3%) 47 43	52, 94, 150, 233	0
6	B	733/734 (99%)	0.03	18 (2%) 58 54	30, 69, 98, 132	0
7	C	80/81 (98%)	0.33	4 (5%) 34 30	30, 78, 94, 120	0
8	D	140/143 (97%)	0.32	6 (4%) 40 36	66, 101, 137, 158	0
9	E	63/66 (95%)	-0.03	1 (1%) 70 66	65, 84, 111, 129	0
10	F	152/154 (98%)	0.11	6 (3%) 43 39	30, 70, 96, 138	0
11	G	95/97 (97%)	0.41	8 (8%) 17 14	30, 91, 125, 156	0
12	H	88/88 (100%)	0.76	10 (11%) 10 7	96, 132, 182, 259	0
13	I	30/40 (75%)	0.60	2 (6%) 24 20	92, 108, 146, 208	0
14	J	39/42 (92%)	0.23	4 (10%) 12 9	60, 73, 101, 112	0
15	L	151/157 (96%)	0.41	4 (2%) 57 53	102, 137, 165, 192	0
16	K	77/80 (96%)	1.33	18 (23%) 2 1	137, 198, 248, 302	0
All	All	3200/3377 (94%)	0.33	166 (5%) 33 29	30, 91, 178, 302	0

The worst 5 of 166 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
16	K	90	LEU	6.2
3	3	128	LEU	5.9
12	H	142	LEU	5.7
1	1	109	ALA	5.5
16	K	72	PRO	5.5

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
17	CLA	A	843	52/65	0.66	0.14	173,188,196,199	0
25	HTG	4	322	19/19	0.71	0.16	107,129,140,145	0
25	HTG	F	310	16/19	0.71	0.14	114,141,144,146	0
26	DGD	4	323	60/66	0.72	0.17	90,115,130,138	0
22	LHG	G	102	49/49	0.74	0.20	92,119,171,174	0
25	HTG	F	301	17/19	0.75	0.16	124,149,155,159	0
25	HTG	B	851	19/19	0.77	0.16	107,134,142,143	0
22	LHG	F	302	40/49	0.77	0.21	111,140,164,167	0
17	CLA	3	610	52/65	0.77	0.14	177,188,210,215	0
21	BCR	K	203	40/40	0.77	0.18	142,185,227,229	0
24	LMG	B	852	52/55	0.78	0.17	100,127,143,148	0
21	BCR	2	316	40/40	0.78	0.19	148,157,172,173	0
20	XAT	3	615	44/44	0.79	0.15	62,89,98,100	0
24	LMG	4	320	49/55	0.80	0.16	96,119,174,176	0
24	LMG	F	309	55/55	0.81	0.14	91,108,120,124	0
17	CLA	L	204	50/65	0.82	0.12	122,147,157,163	0
17	CLA	J	103	42/65	0.82	0.12	83,101,120,125	0
24	LMG	G	101	40/55	0.83	0.15	110,157,180,181	0
23	LMT	2	318	35/35	0.83	0.15	120,133,143,146	0
22	LHG	A	845	27/49	0.83	0.12	128,174,191,196	0
17	CLA	A	821	49/65	0.84	0.12	130,142,169,175	0
21	BCR	3	616	40/40	0.85	0.14	156,164,187,189	0
17	CLA	L	202	65/65	0.85	0.12	142,154,170,175	0
17	CLA	3	612	45/65	0.85	0.11	197,212,229,235	0
22	LHG	B	801	23/49	0.85	0.15	67,88,119,120	0
23	LMT	A	855	35/35	0.86	0.13	97,154,171,172	0
17	CLA	A	822	51/65	0.86	0.11	137,148,164,169	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
18	CHL	3	601	56/66	0.86	0.13	108,134,146,147	0
20	XAT	2	315	44/44	0.86	0.14	62,89,98,100	0
17	CLA	2	303	60/65	0.86	0.11	120,132,139,142	0
17	CLA	L	203	65/65	0.87	0.13	119,143,157,167	0
17	CLA	K	201	45/65	0.87	0.11	172,184,191,193	0
18	CHL	2	305	48/66	0.87	0.13	105,129,162,162	0
24	LMG	4	319	50/55	0.87	0.15	68,89,131,132	0
25	HTG	4	321	19/19	0.87	0.16	125,139,147,147	0
17	CLA	4	304	50/65	0.88	0.11	55,78,112,117	0
21	BCR	L	206	40/40	0.88	0.12	156,168,177,178	0
17	CLA	3	609	50/65	0.88	0.10	147,163,173,175	0
22	LHG	2	317	37/49	0.88	0.19	155,163,179,187	0
17	CLA	1	304	42/65	0.88	0.12	80,107,125,133	0
17	CLA	A	837	65/65	0.88	0.13	92,103,174,177	0
17	CLA	3	604	45/65	0.88	0.11	137,162,170,173	0
17	CLA	3	605	42/65	0.89	0.11	125,135,143,147	0
17	CLA	G	103	41/65	0.89	0.14	105,122,131,136	0
17	CLA	1	307	65/65	0.89	0.12	74,93,123,129	0
18	CHL	4	301	61/66	0.89	0.12	66,78,116,118	0
26	DGD	B	850	66/66	0.89	0.14	80,94,119,120	0
17	CLA	3	602	60/65	0.90	0.12	132,157,174,178	0
17	CLA	A	817	65/65	0.90	0.13	103,129,169,173	0
17	CLA	2	310	52/65	0.90	0.09	106,113,156,164	0
19	LUT	3	614	42/42	0.90	0.11	127,146,163,166	0
22	LHG	1	317	49/49	0.90	0.16	85,100,127,130	0
17	CLA	2	312	43/65	0.90	0.10	122,142,146,147	0
17	CLA	K	202	60/65	0.90	0.09	146,176,193,196	0
21	BCR	1	316	40/40	0.90	0.12	98,125,149,151	0
17	CLA	2	309	41/65	0.91	0.10	126,134,143,146	0
17	CLA	A	819	45/65	0.91	0.11	126,138,151,155	0
17	CLA	1	303	51/65	0.91	0.12	112,124,138,143	0
17	CLA	1	312	55/65	0.91	0.11	74,88,119,123	0
17	CLA	A	825	65/65	0.91	0.11	76,98,163,165	0
18	CHL	1	305	48/66	0.91	0.13	102,114,132,134	0
17	CLA	A	833	50/65	0.91	0.11	120,135,146,157	0
17	CLA	A	834	45/65	0.91	0.09	156,170,177,185	0
17	CLA	A	835	51/65	0.91	0.11	78,102,129,135	0
17	CLA	2	302	51/65	0.91	0.10	89,102,120,127	0
17	CLA	1	306	46/65	0.91	0.11	91,101,117,120	0
17	CLA	B	803	65/65	0.91	0.11	106,119,153,161	0
17	CLA	B	814	55/65	0.91	0.11	61,75,121,123	0
17	CLA	B	817	55/65	0.91	0.11	72,86,123,134	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
17	CLA	4	310	60/65	0.91	0.10	68,89,116,121	0
21	BCR	4	318	40/40	0.91	0.12	61,90,99,104	0
21	BCR	A	846	40/40	0.91	0.12	116,137,151,153	0
21	BCR	J	105	40/40	0.91	0.14	73,85,100,101	0
17	CLA	G	105	46/65	0.91	0.10	92,122,136,144	0
17	CLA	A	814	50/65	0.91	0.14	119,141,161,164	0
17	CLA	4	311	52/65	0.92	0.10	72,83,118,119	0
17	CLA	B	824	55/65	0.92	0.12	63,74,104,112	0
21	BCR	A	849	40/40	0.92	0.14	100,137,196,199	0
21	BCR	B	845	40/40	0.92	0.11	62,73,118,122	0
21	BCR	B	847	40/40	0.92	0.12	49,65,85,92	0
18	CHL	2	313	43/66	0.92	0.08	99,119,137,139	0
17	CLA	A	830	50/65	0.92	0.12	102,117,152,156	0
17	CLA	A	809	65/65	0.92	0.13	100,120,149,151	0
17	CLA	3	613	46/65	0.92	0.09	106,121,156,159	0
17	CLA	A	816	65/65	0.92	0.12	116,134,152,155	0
17	CLA	4	303	60/65	0.92	0.10	52,67,108,113	0
17	CLA	2	301	65/65	0.92	0.12	86,105,122,135	0
25	HTG	J	102	19/19	0.92	0.10	75,82,115,120	0
17	CLA	4	309	60/65	0.92	0.11	61,72,98,100	0
17	CLA	1	309	65/65	0.92	0.10	84,105,142,147	0
21	BCR	J	104	40/40	0.93	0.11	63,73,87,91	0
17	CLA	B	812	65/65	0.93	0.13	76,107,137,144	0
21	BCR	L	201	40/40	0.93	0.10	95,107,120,123	0
18	CHL	2	304	43/66	0.93	0.11	101,117,129,137	0
17	CLA	B	813	54/65	0.93	0.09	61,90,114,117	0
17	CLA	3	606	47/65	0.93	0.09	113,124,135,138	0
17	CLA	1	302	65/65	0.93	0.10	70,87,125,128	0
17	CLA	B	818	55/65	0.93	0.11	63,73,95,102	0
18	CHL	4	305	56/66	0.93	0.10	68,77,116,118	0
18	CHL	4	306	51/66	0.93	0.09	66,79,130,133	0
18	CHL	4	315	43/66	0.93	0.09	67,88,102,117	0
19	LUT	1	314	42/42	0.93	0.10	67,95,116,120	0
19	LUT	2	314	42/42	0.93	0.10	97,114,124,130	0
17	CLA	B	820	60/65	0.93	0.10	46,66,85,87	0
19	LUT	4	316	42/42	0.93	0.10	63,72,86,91	0
17	CLA	1	313	46/65	0.93	0.08	73,84,105,117	0
17	CLA	3	611	55/65	0.93	0.10	143,177,193,195	0
17	CLA	G	104	50/65	0.93	0.09	76,95,125,133	0
17	CLA	A	811	54/65	0.93	0.11	107,127,140,140	0
17	CLA	2	307	50/65	0.93	0.10	90,95,110,113	0
25	HTG	A	854	19/19	0.93	0.07	63,78,85,96	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
17	CLA	A	815	45/65	0.93	0.09	114,125,135,140	0
17	CLA	A	836	65/65	0.93	0.11	86,106,146,154	0
25	HTG	F	305	19/19	0.93	0.14	62,83,100,104	0
17	CLA	3	603	50/65	0.93	0.10	116,128,132,135	0
17	CLA	2	308	60/65	0.93	0.12	111,122,145,151	0
17	CLA	1	310	52/65	0.93	0.10	88,103,145,147	0
21	BCR	F	303	40/40	0.93	0.12	48,60,65,66	0
17	CLA	2	311	65/65	0.94	0.09	109,127,142,147	0
17	CLA	A	826	65/65	0.94	0.10	90,119,149,154	0
17	CLA	B	816	65/65	0.94	0.12	65,78,97,99	0
17	CLA	4	308	50/65	0.94	0.09	52,64,103,109	0
17	CLA	1	301	65/65	0.94	0.10	60,72,107,115	0
17	CLA	1	308	60/65	0.94	0.11	89,100,129,133	0
18	CHL	2	306	51/66	0.94	0.12	84,101,141,144	0
17	CLA	B	822	50/65	0.94	0.10	70,80,109,113	0
21	BCR	A	847	40/40	0.94	0.12	87,120,171,173	0
21	BCR	A	848	40/40	0.94	0.12	92,116,163,164	0
17	CLA	3	608	50/65	0.94	0.09	120,130,136,139	0
18	CHL	3	607	47/66	0.94	0.10	124,135,160,166	0
21	BCR	B	846	40/40	0.94	0.10	62,77,125,126	0
17	CLA	B	834	58/65	0.94	0.10	46,59,102,105	0
17	CLA	4	312	56/65	0.94	0.09	70,84,109,112	0
21	BCR	G	106	40/40	0.94	0.10	71,90,129,130	0
21	BCR	I	101	40/40	0.94	0.10	92,99,112,114	0
17	CLA	A	820	65/65	0.94	0.11	103,126,143,144	0
17	CLA	4	314	47/65	0.94	0.08	57,70,104,106	0
17	CLA	1	311	60/65	0.94	0.10	64,75,111,113	0
21	BCR	L	205	40/40	0.94	0.13	101,116,137,137	0
17	CLA	B	809	65/65	0.94	0.11	71,88,138,144	0
17	CLA	A	824	65/65	0.94	0.11	90,102,108,111	0
17	CLA	B	833	60/65	0.95	0.08	44,58,104,110	0
17	CLA	A	803	55/65	0.95	0.10	64,82,119,124	0
17	CLA	B	835	65/65	0.95	0.09	53,67,106,116	0
17	CLA	B	836	45/65	0.95	0.07	62,71,94,97	0
17	CLA	B	839	47/65	0.95	0.08	52,58,84,93	0
17	CLA	F	304	65/65	0.95	0.10	44,58,76,84	0
21	BCR	A	850	40/40	0.95	0.11	72,108,147,148	0
21	BCR	A	851	40/40	0.95	0.09	45,63,77,79	0
17	CLA	F	307	55/65	0.95	0.07	49,67,123,125	0
17	CLA	A	804	65/65	0.95	0.10	77,91,115,117	0
17	CLA	A	827	65/65	0.95	0.10	64,76,89,94	0
17	CLA	A	829	65/65	0.95	0.09	68,82,94,98	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
21	BCR	F	308	40/40	0.95	0.09	53,62,72,78	0
17	CLA	J	101	65/65	0.95	0.11	62,76,93,101	0
17	CLA	A	853	65/65	0.95	0.11	48,61,88,96	0
17	CLA	A	806	65/65	0.95	0.10	72,81,131,134	0
17	CLA	2	319	46/65	0.95	0.09	68,80,109,111	0
17	CLA	B	823	65/65	0.95	0.10	62,75,131,140	0
17	CLA	A	810	65/65	0.95	0.10	80,88,102,113	0
20	XAT	4	317	44/44	0.95	0.09	58,67,81,88	0
17	CLA	B	825	60/65	0.95	0.09	51,60,107,115	0
17	CLA	B	826	65/65	0.95	0.09	50,67,87,92	0
17	CLA	A	812	65/65	0.96	0.09	88,112,121,122	0
21	BCR	B	848	40/40	0.96	0.07	48,58,74,79	0
21	BCR	B	849	40/40	0.96	0.07	60,75,82,83	0
17	CLA	A	823	55/65	0.96	0.09	105,121,137,143	0
17	CLA	A	805	65/65	0.96	0.10	69,82,91,93	0
17	CLA	B	821	65/65	0.96	0.07	56,67,98,103	0
17	CLA	A	801	65/65	0.96	0.10	52,67,83,87	0
17	CLA	A	838	65/65	0.96	0.09	45,55,71,78	0
17	CLA	A	839	65/65	0.96	0.09	47,59,97,101	0
17	CLA	A	840	65/65	0.96	0.08	52,63,76,90	0
17	CLA	A	841	65/65	0.96	0.10	82,100,138,149	0
17	CLA	B	827	65/65	0.96	0.08	43,58,106,109	0
17	CLA	B	829	65/65	0.96	0.10	54,65,124,133	0
17	CLA	B	830	65/65	0.96	0.09	48,68,83,97	0
17	CLA	B	831	65/65	0.96	0.10	48,63,105,107	0
17	CLA	B	832	50/65	0.96	0.08	53,62,96,105	0
17	CLA	A	807	65/65	0.96	0.09	59,73,104,120	0
17	CLA	A	808	65/65	0.96	0.08	54,69,114,118	0
17	CLA	A	828	65/65	0.96	0.09	73,89,106,107	0
17	CLA	B	804	65/65	0.96	0.10	50,60,68,74	0
17	CLA	B	837	60/65	0.96	0.09	46,57,105,106	0
17	CLA	B	838	65/65	0.96	0.08	43,58,72,81	0
17	CLA	B	805	65/65	0.96	0.09	62,78,101,112	0
17	CLA	B	840	65/65	0.96	0.08	70,91,118,124	0
17	CLA	B	841	65/65	0.96	0.09	57,72,127,136	0
17	CLA	B	842	65/65	0.96	0.09	57,69,84,94	0
17	CLA	B	806	45/65	0.96	0.07	62,71,90,114	0
17	CLA	B	808	65/65	0.96	0.08	49,70,88,92	0
17	CLA	A	802	65/65	0.96	0.09	59,73,82,90	0
17	CLA	B	811	65/65	0.96	0.09	70,83,118,125	0
17	CLA	4	313	45/65	0.96	0.07	73,98,120,127	0
17	CLA	A	831	65/65	0.96	0.08	84,103,108,110	0

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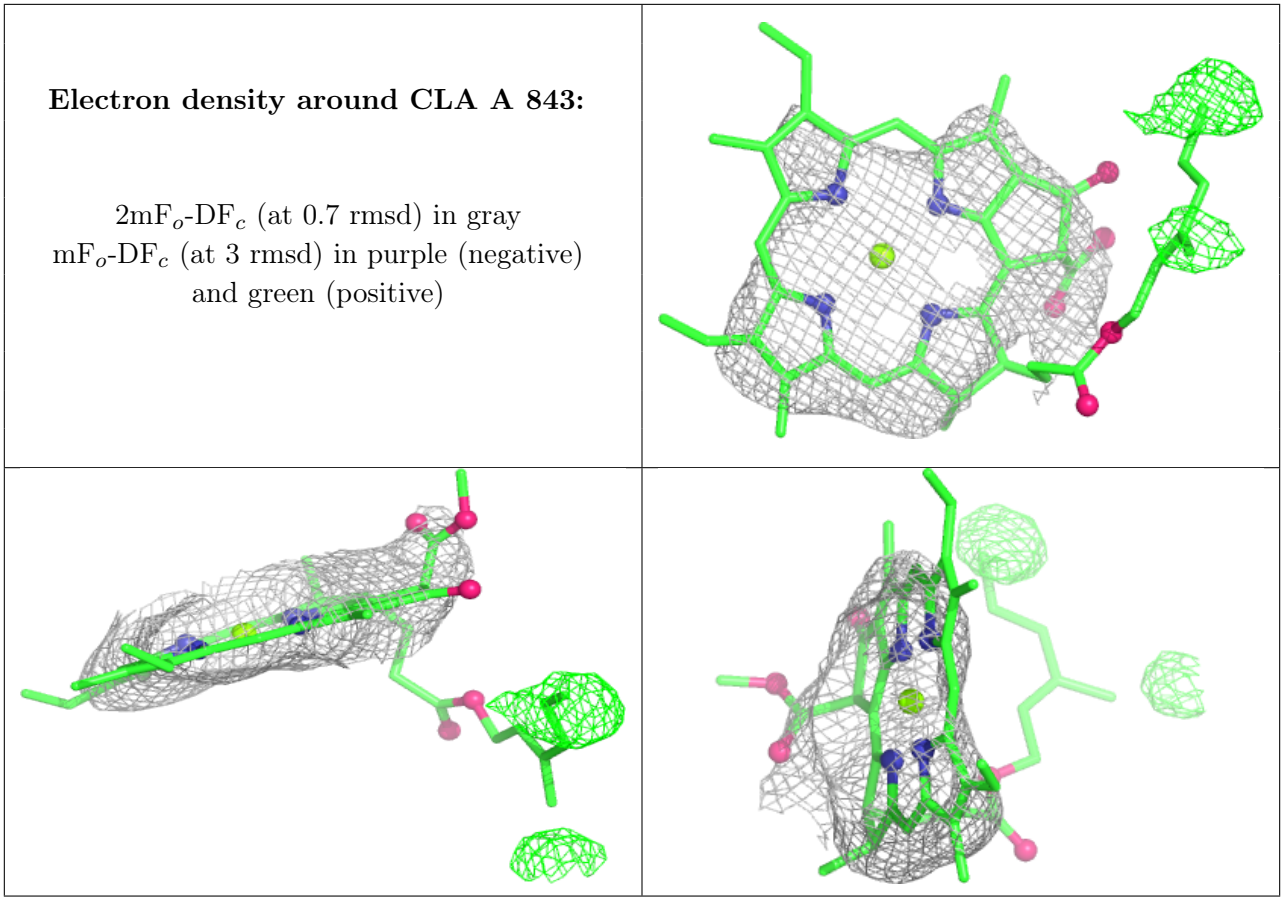
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
17	CLA	A	832	65/65	0.96	0.10	89,101,142,149	0
21	BCR	B	844	40/40	0.96	0.11	69,83,97,102	0
17	CLA	B	815	65/65	0.96	0.08	57,67,75,77	0
17	CLA	4	302	60/65	0.96	0.08	50,62,94,97	0
27	PQN	A	842	33/33	0.96	0.10	49,61,85,91	0
27	PQN	B	843	33/33	0.96	0.10	65,84,91,97	0
17	CLA	B	810	65/65	0.97	0.09	63,73,95,101	0
18	CHL	4	307	51/66	0.97	0.07	60,73,90,101	0
17	CLA	B	828	65/65	0.97	0.07	45,58,72,78	0
17	CLA	A	818	65/65	0.97	0.10	91,103,125,130	0
17	CLA	F	306	45/65	0.97	0.06	55,66,75,85	0
17	CLA	B	807	65/65	0.97	0.10	57,69,79,82	0
17	CLA	A	813	45/65	0.97	0.08	89,111,120,126	0
20	XAT	1	315	44/44	0.97	0.09	62,89,98,100	0
17	CLA	B	819	59/65	0.97	0.09	55,66,81,85	0
22	LHG	A	844	49/49	0.97	0.09	69,83,92,96	0
17	CLA	B	802	65/65	0.97	0.07	48,60,81,93	0
28	SF4	A	852	8/8	0.99	0.04	55,67,73,74	0
28	SF4	C	101	8/8	0.99	0.03	69,76,84,85	0
28	SF4	C	102	8/8	0.99	0.03	75,76,85,89	0

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

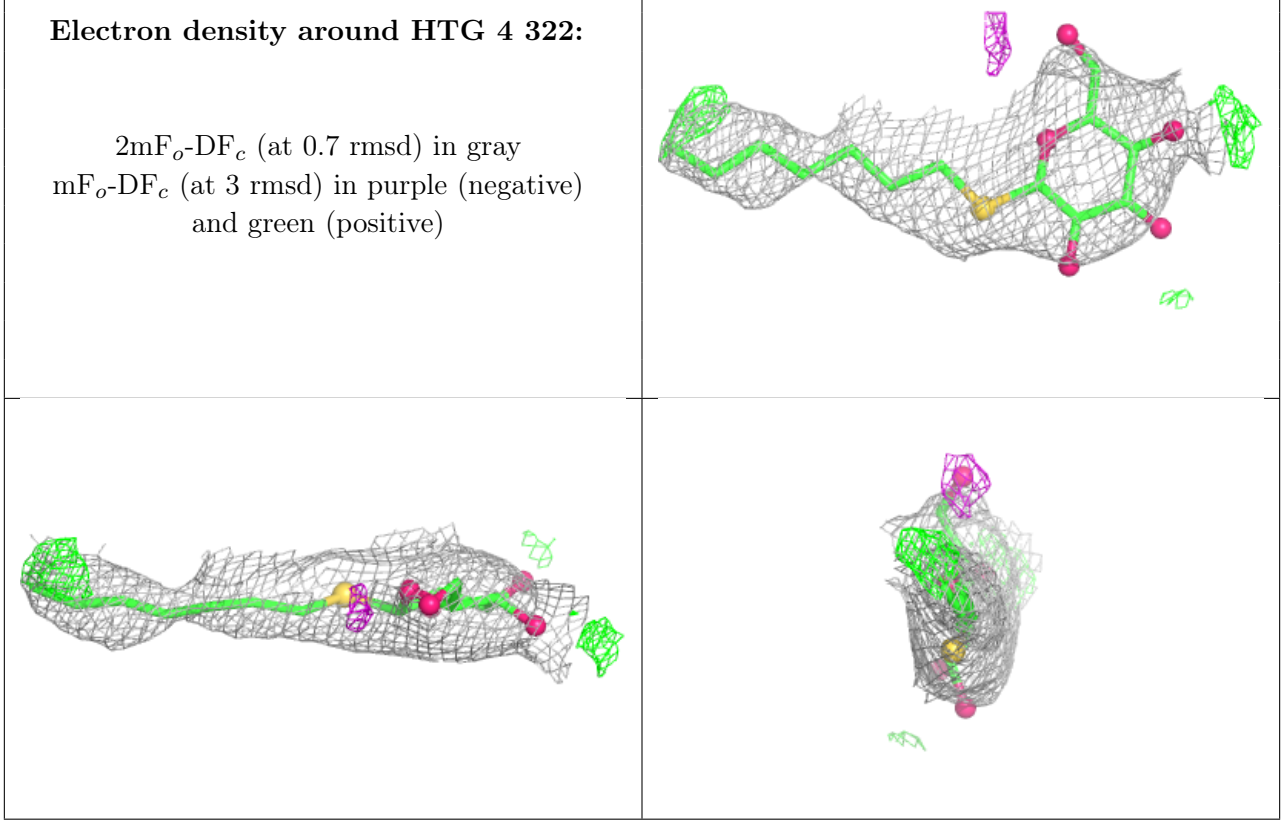
Electron density around CLA A 843:

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



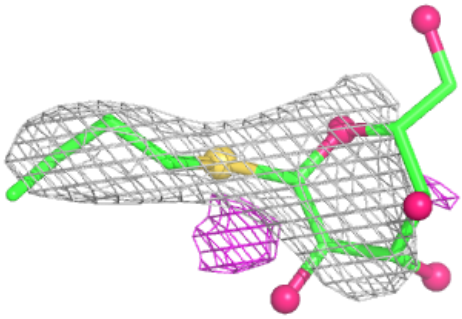
Electron density around HTG 4 322:

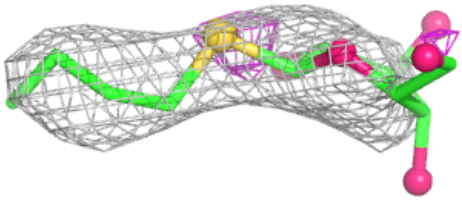
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

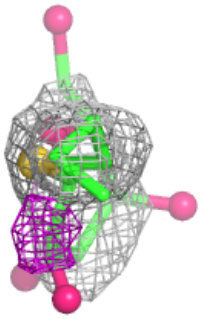


Electron density around HTG F 310:

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

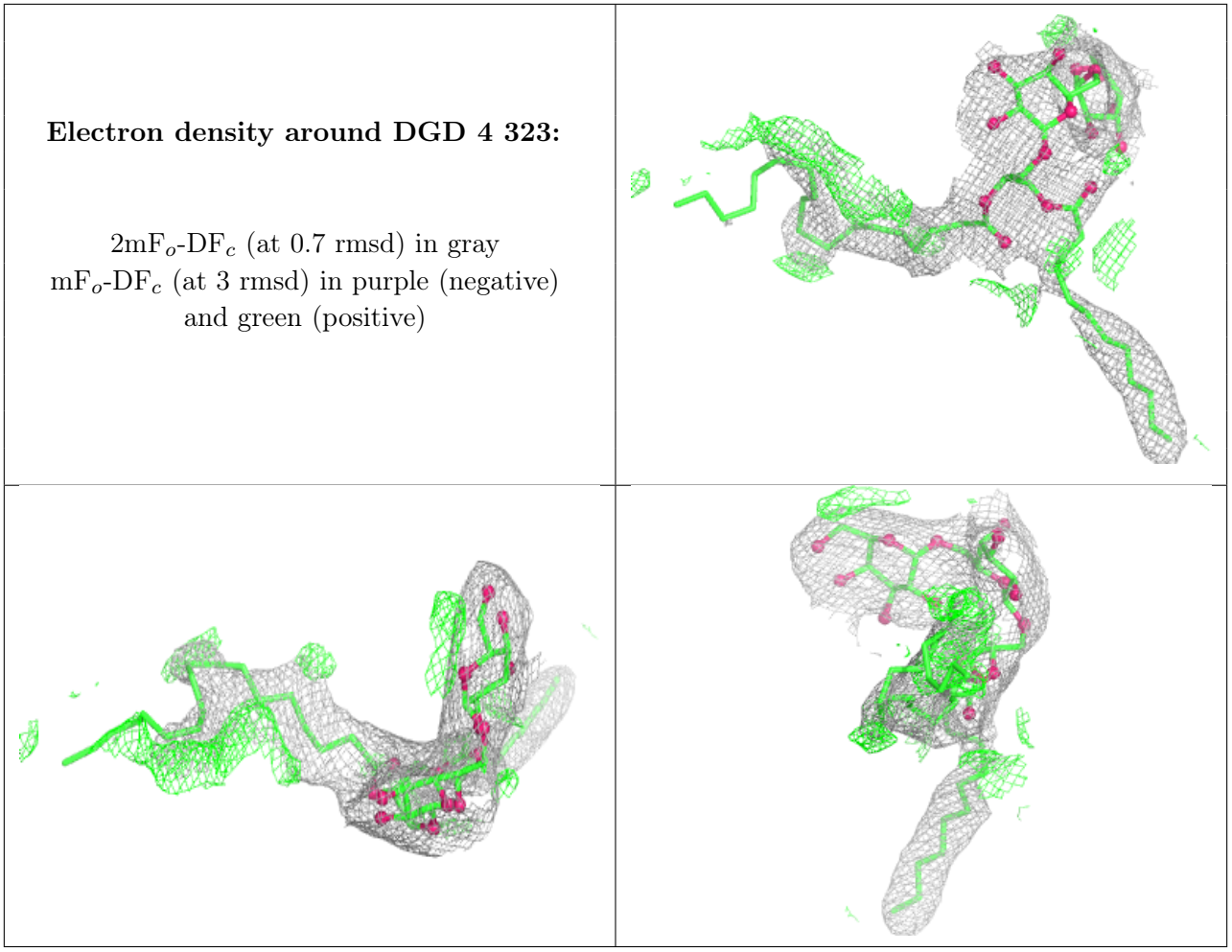






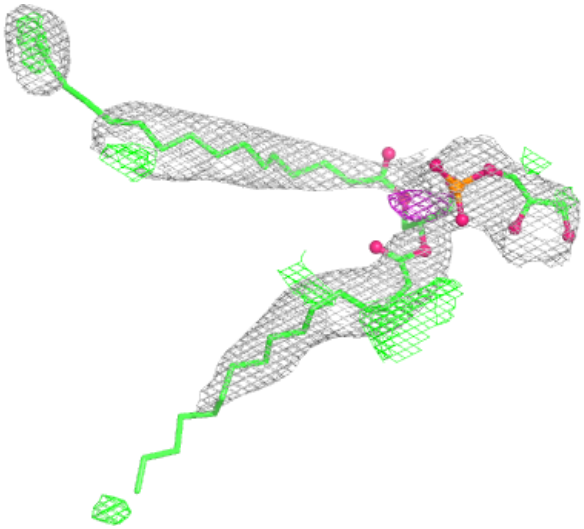
Electron density around DGD 4 323:

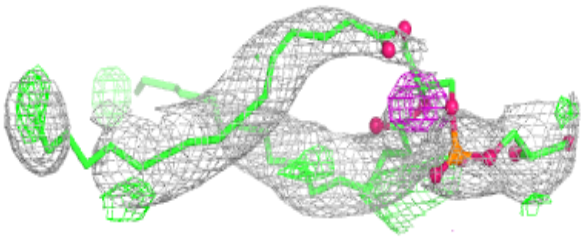
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

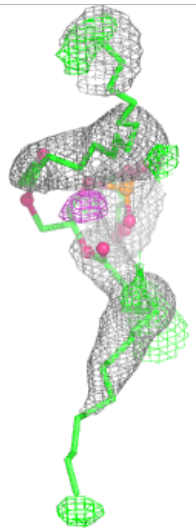


Electron density around LHG G 102:

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

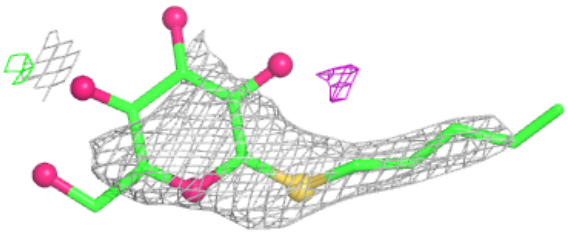


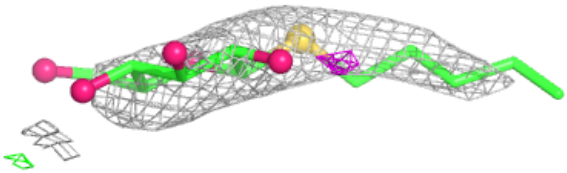


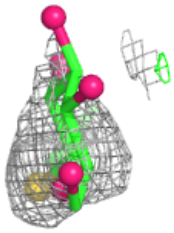


Electron density around HTG F 301:

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

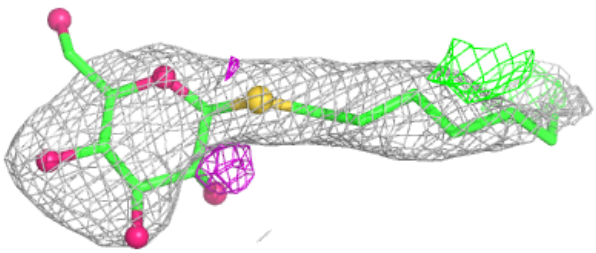


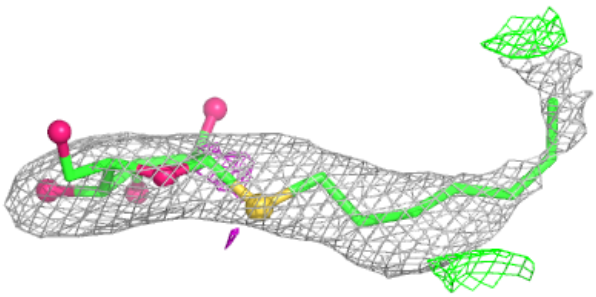


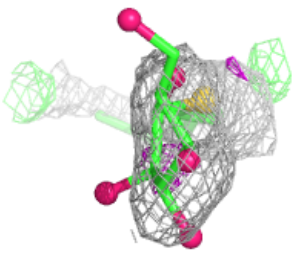


Electron density around HTG B 851:

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

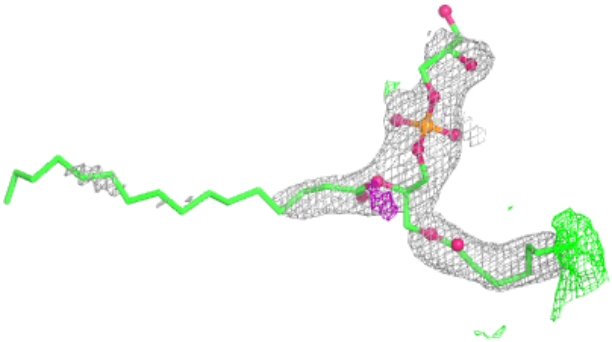


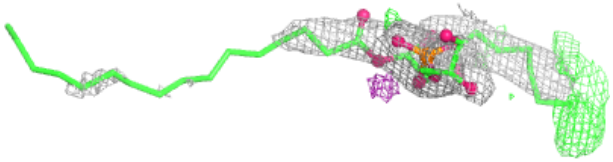


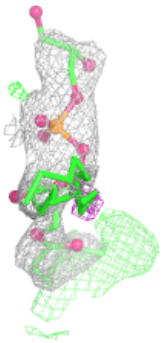


Electron density around LHG F 302:

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

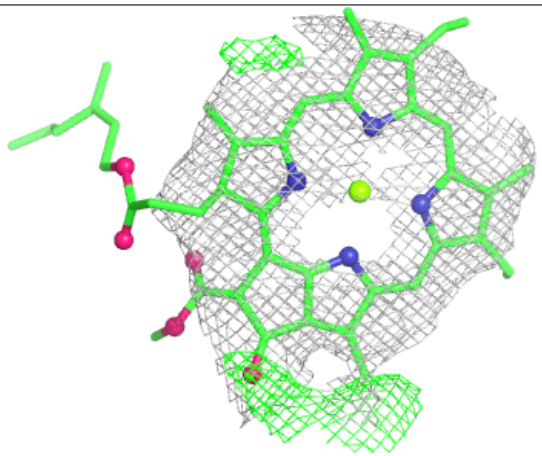


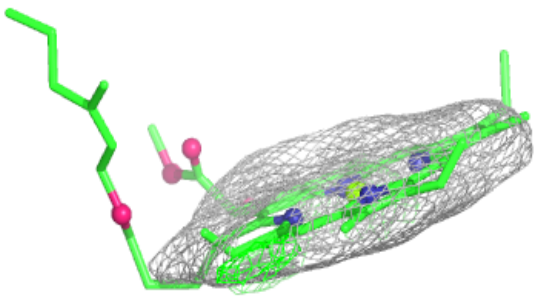


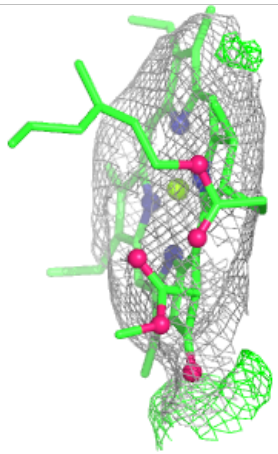


Electron density around CLA 3 610:

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

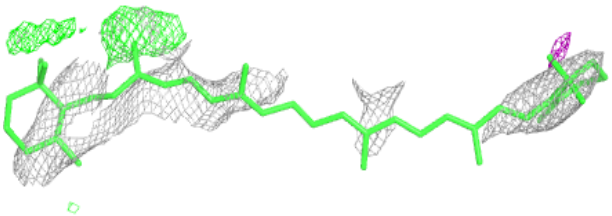


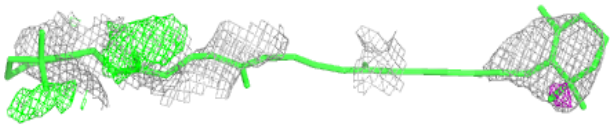


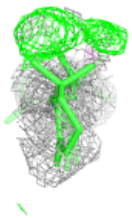


Electron density around BCR K 203:

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

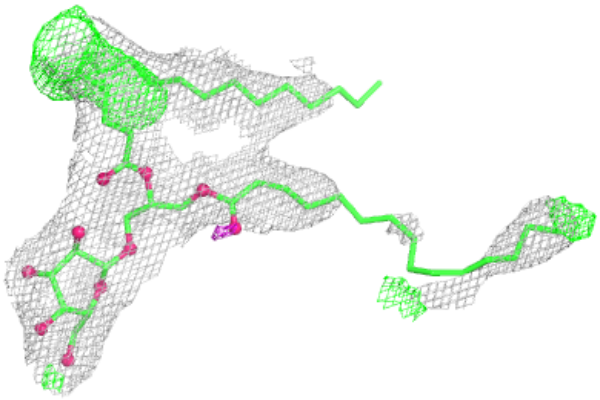


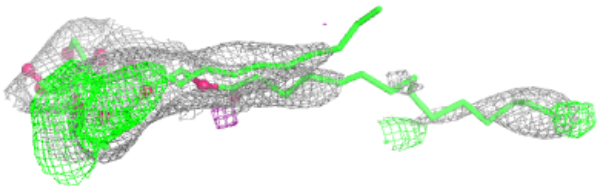




Electron density around LMG B 852:

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

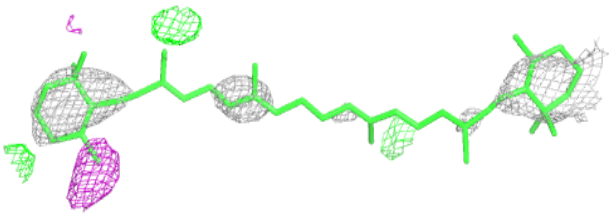


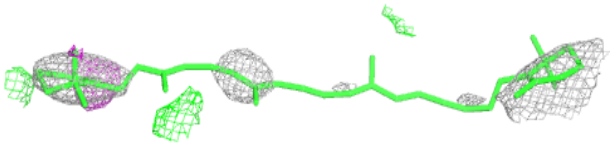


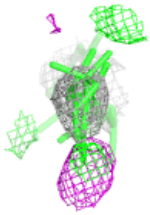


Electron density around BCR 2 316:

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

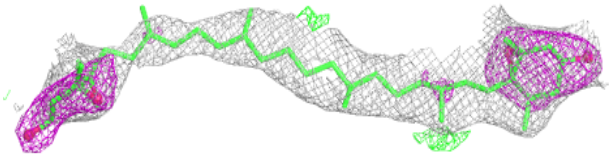


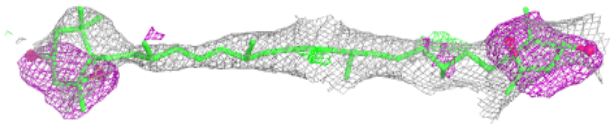


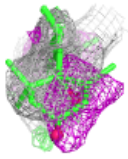


Electron density around XAT 3 615:

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

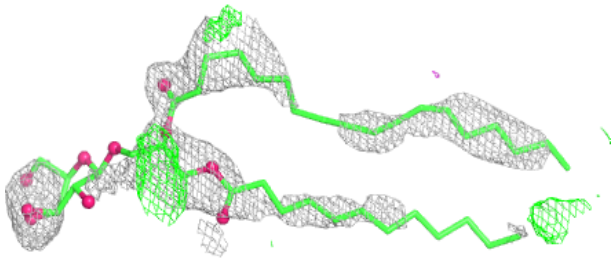


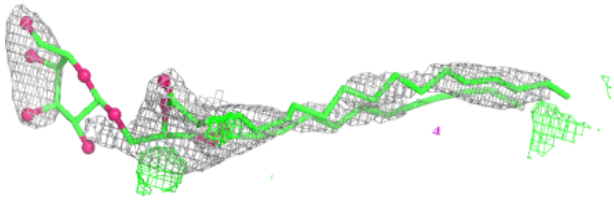


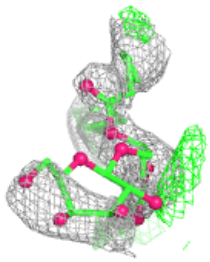


Electron density around LMG 4 320:

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

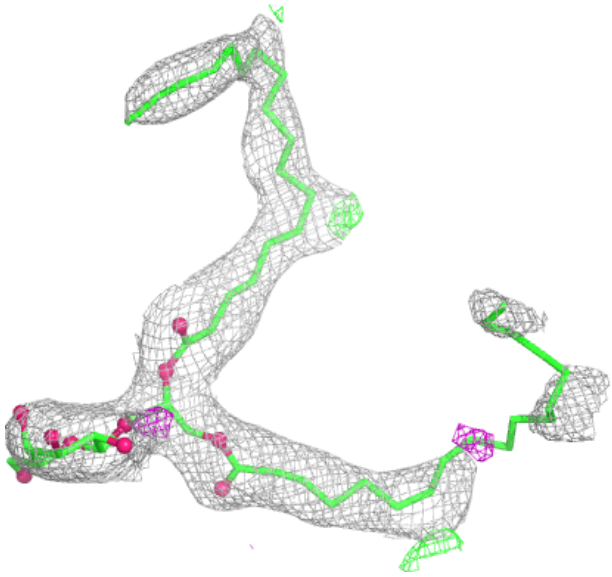


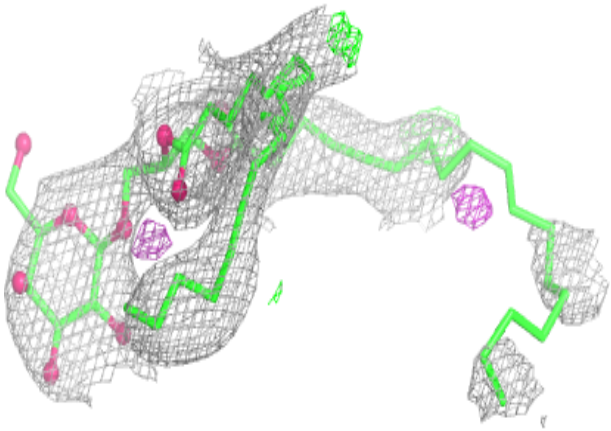


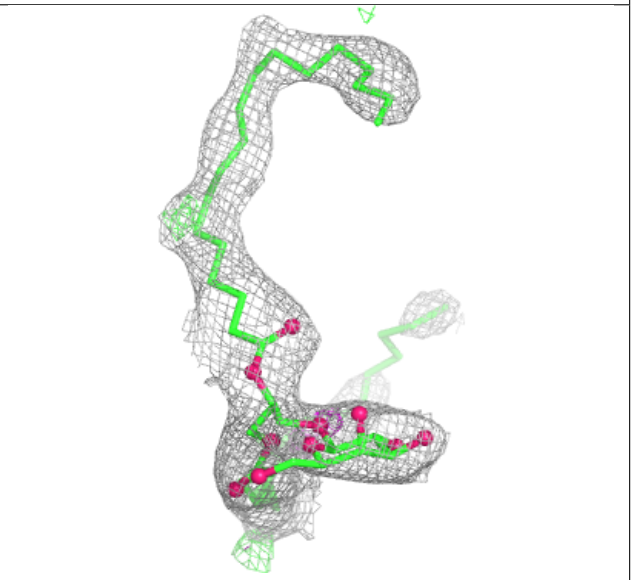


Electron density around LMG F 309:

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

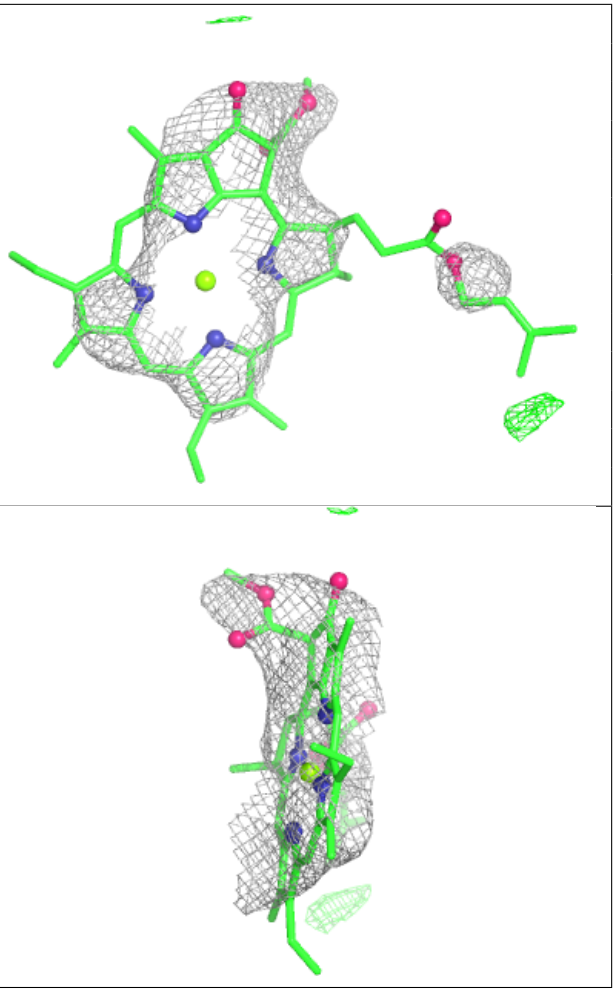






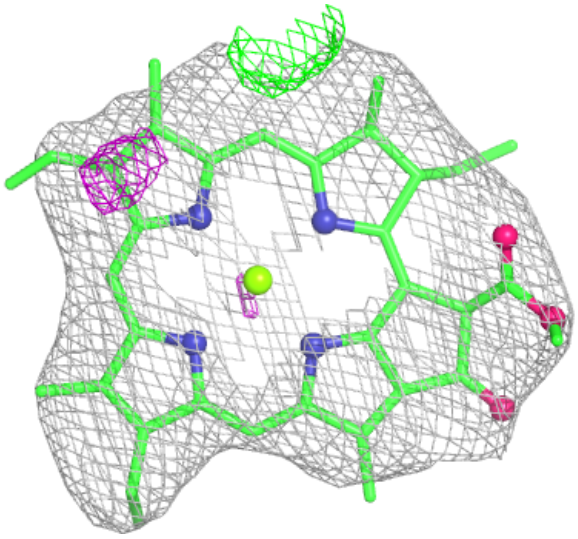
Electron density around CLA L 204:

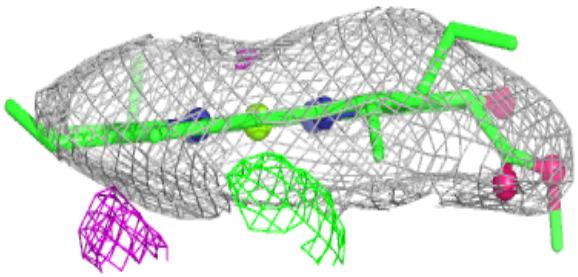
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

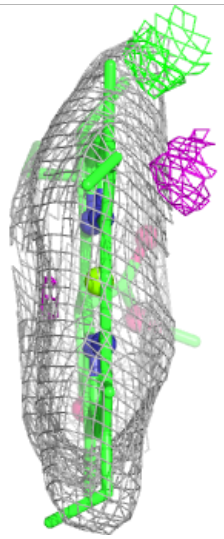


Electron density around CLA J 103:

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

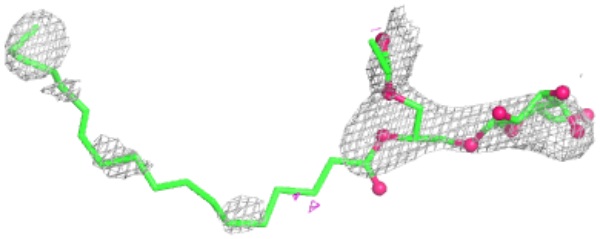


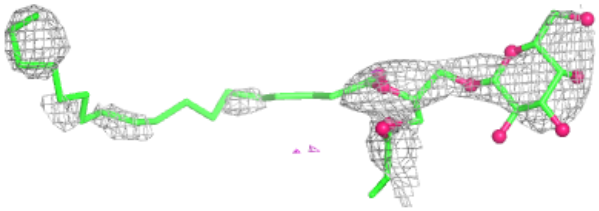


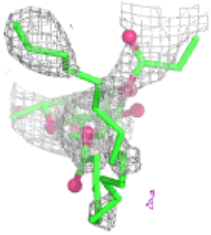


Electron density around LMG G 101:

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

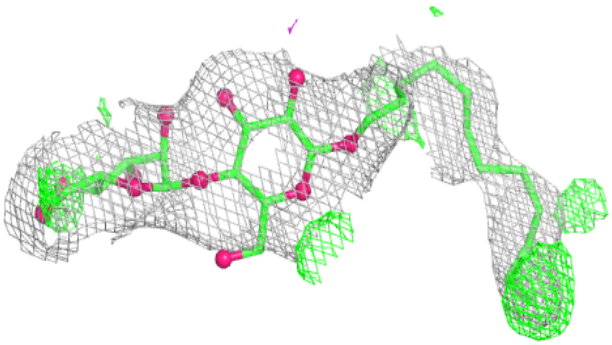


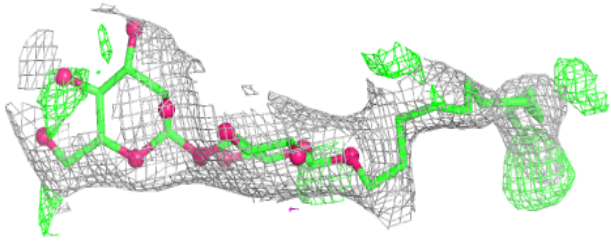


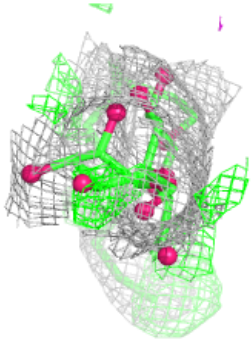


Electron density around LMT 2 318:

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

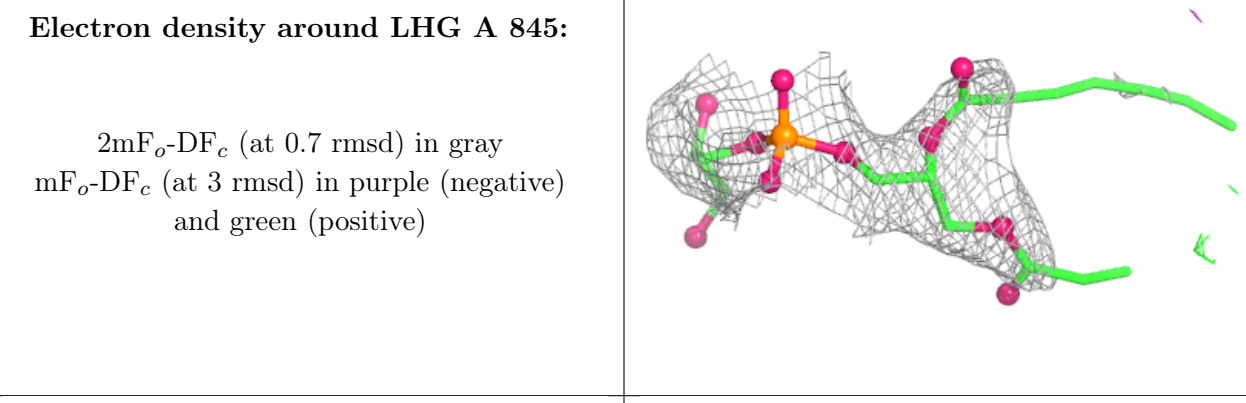






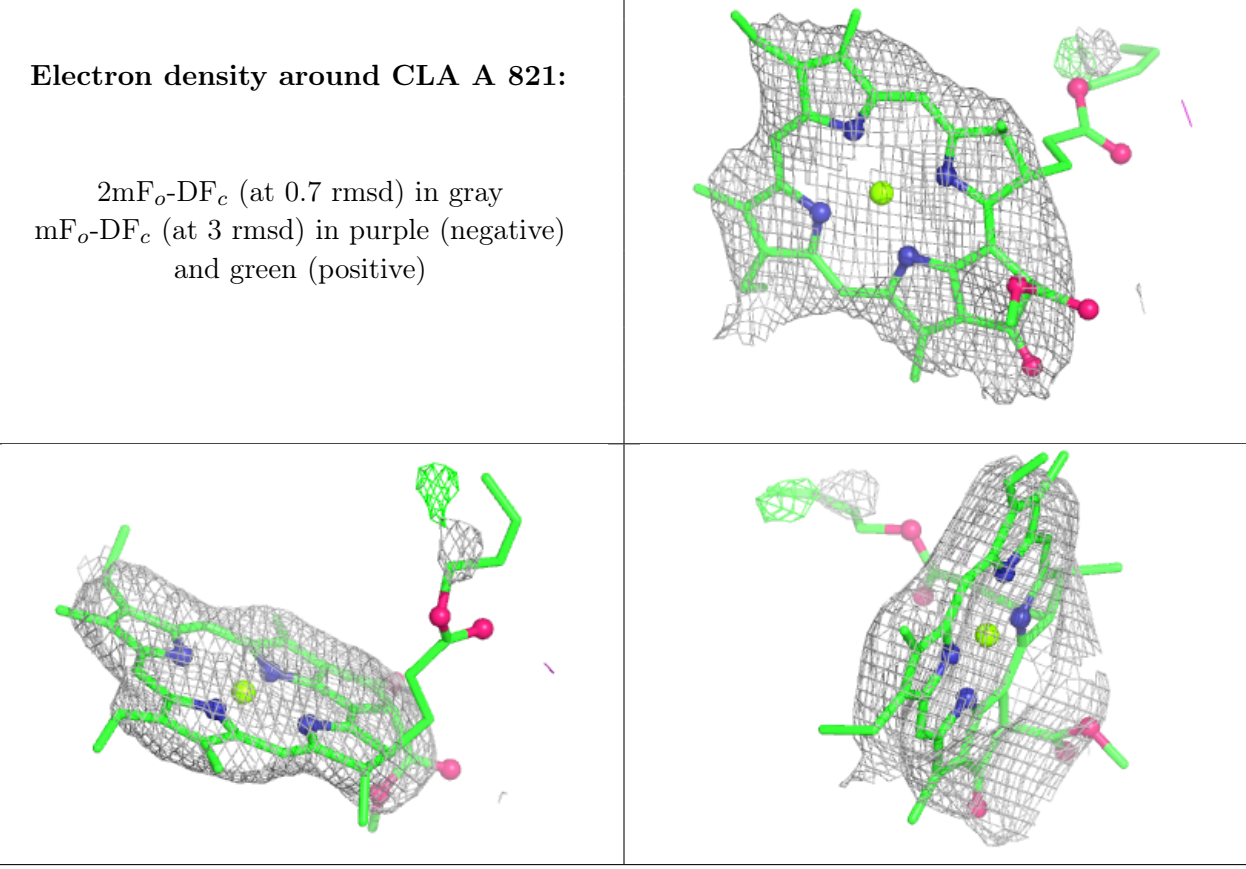
Electron density around LHG A 845:

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



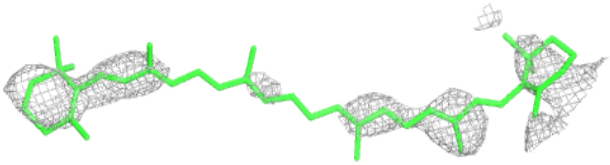
Electron density around CLA A 821:

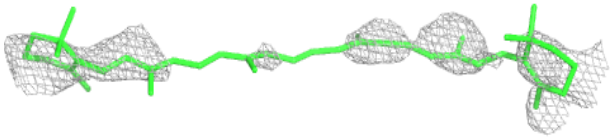
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

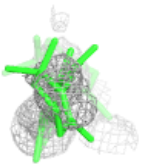


Electron density around BCR 3 616:

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

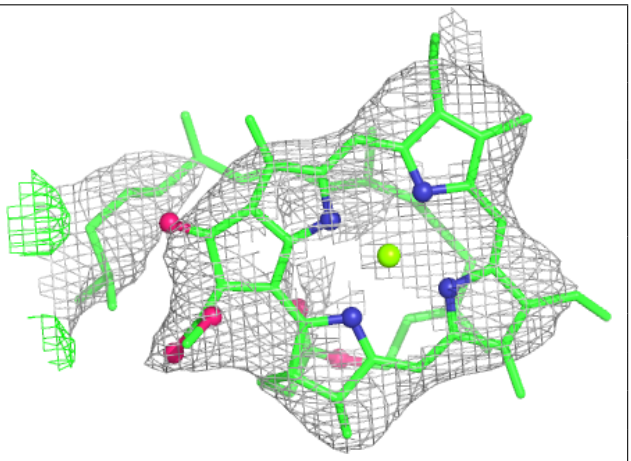


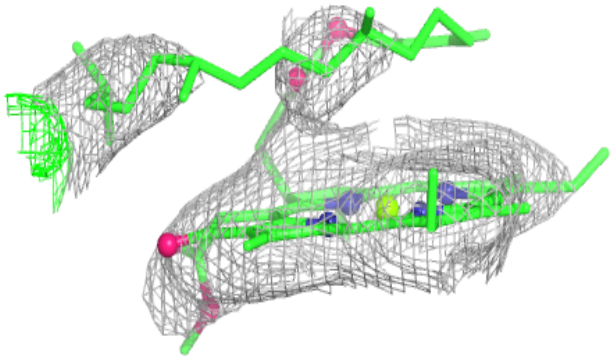


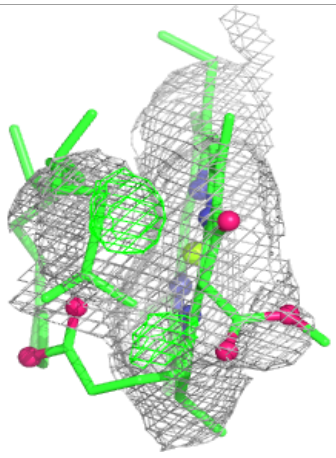


Electron density around CLA L 202:

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

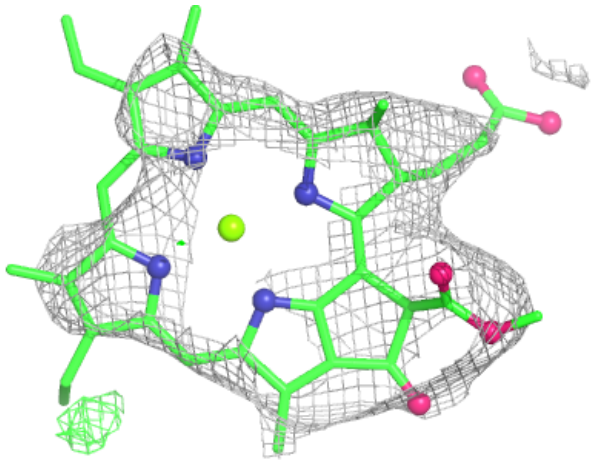


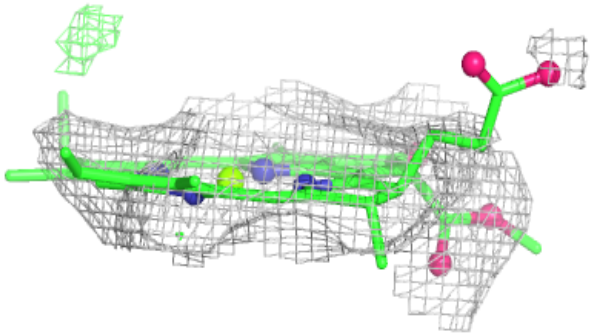


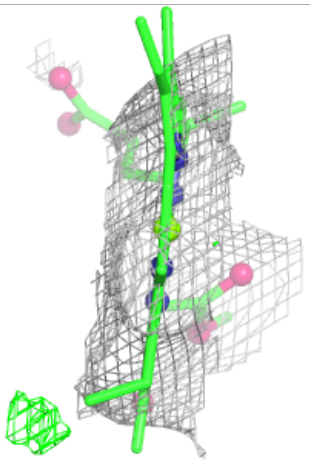


Electron density around CLA 3 612:

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

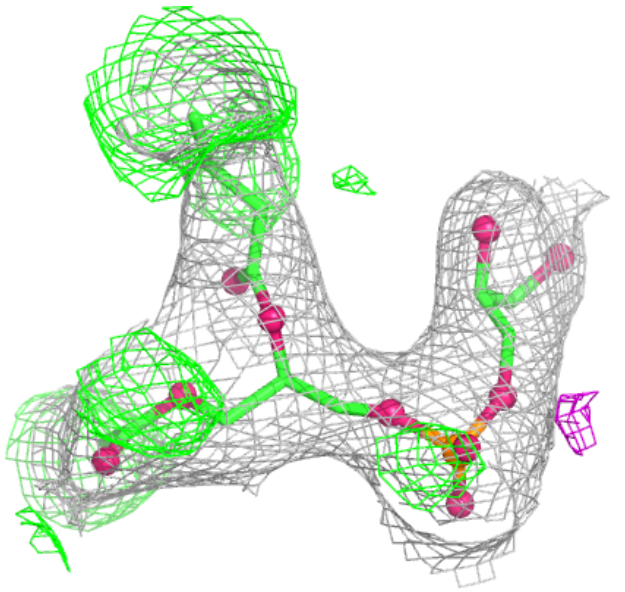


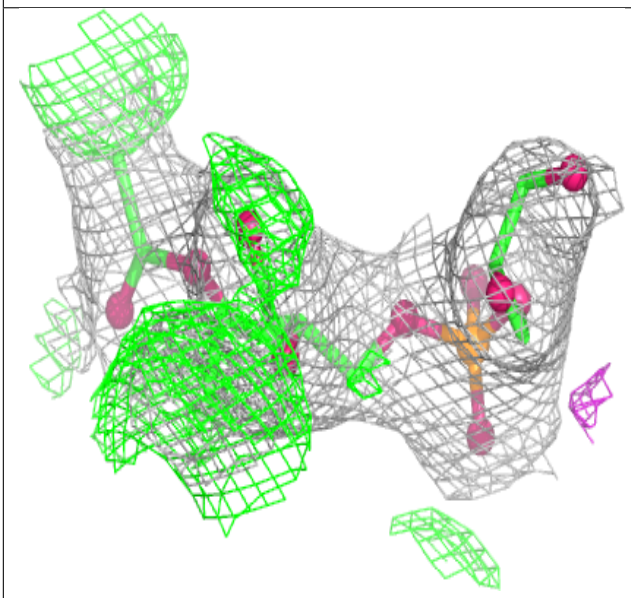


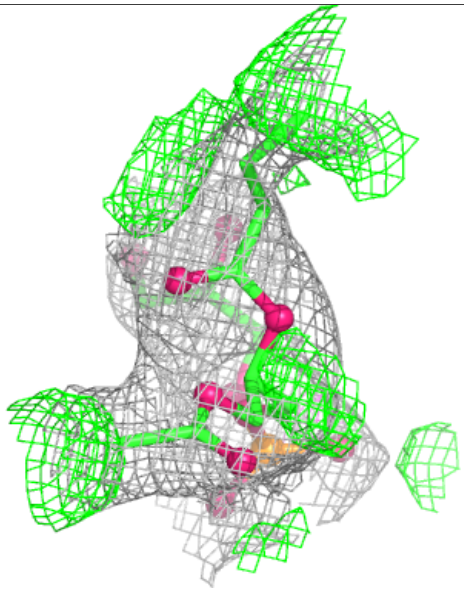


Electron density around LHG B 801:

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



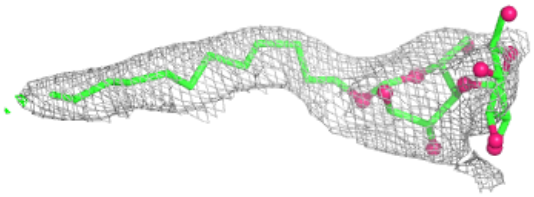


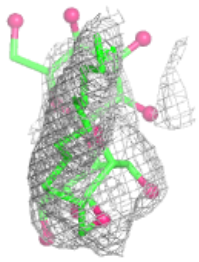


Electron density around LMT A 855:

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

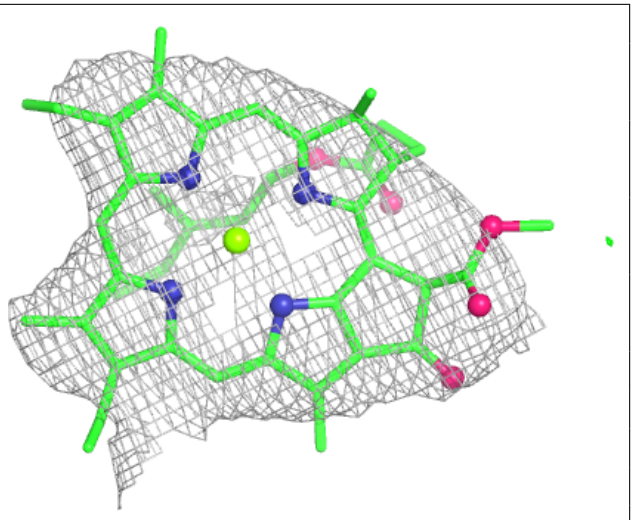


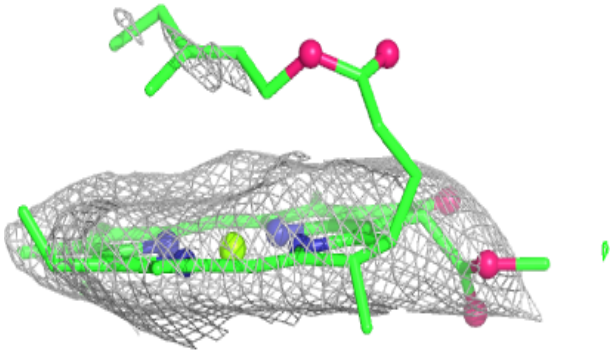


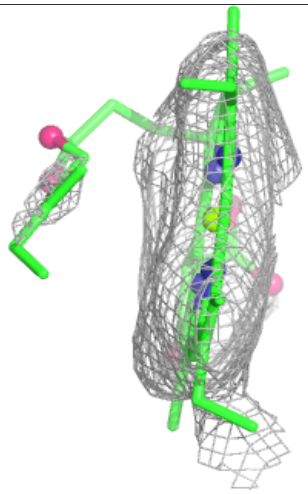


Electron density around CLA A 822:

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

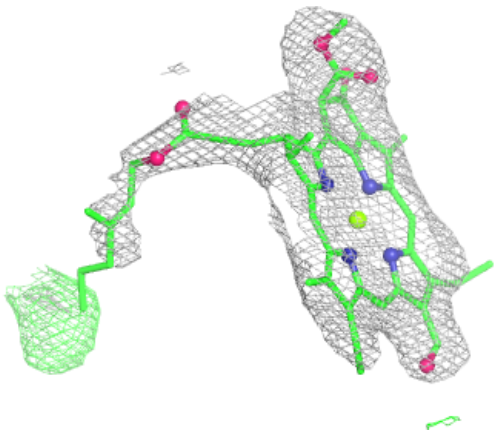


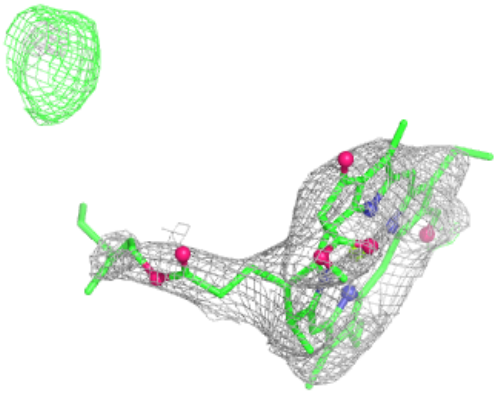


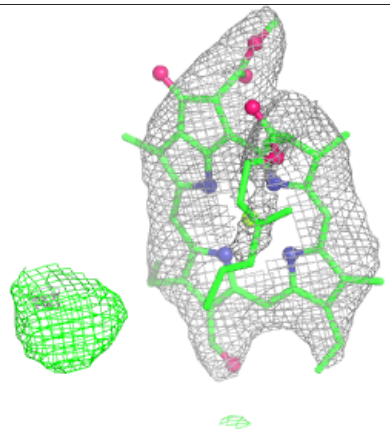


Electron density around CHL 3 601:

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

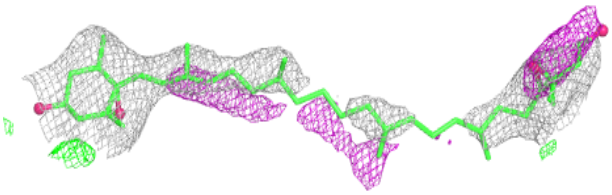


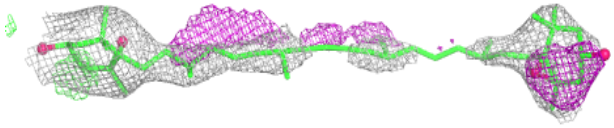


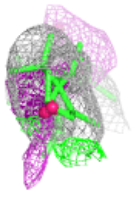


Electron density around XAT 2 315:

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

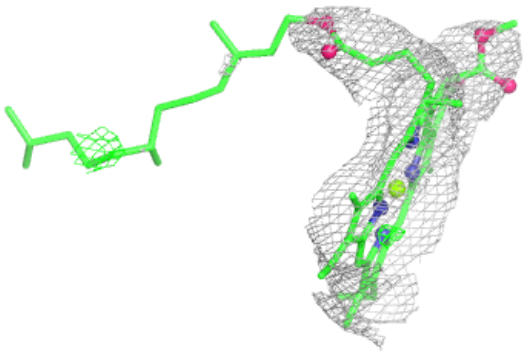


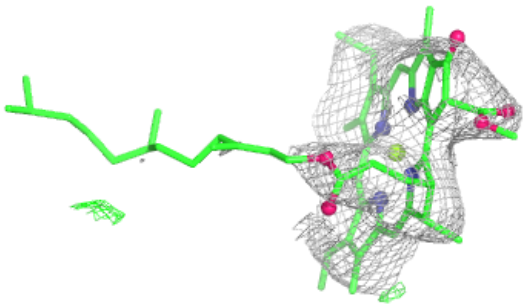


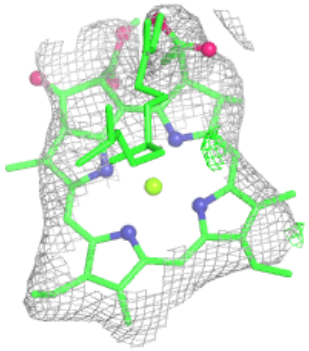


Electron density around CLA 2 303:

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

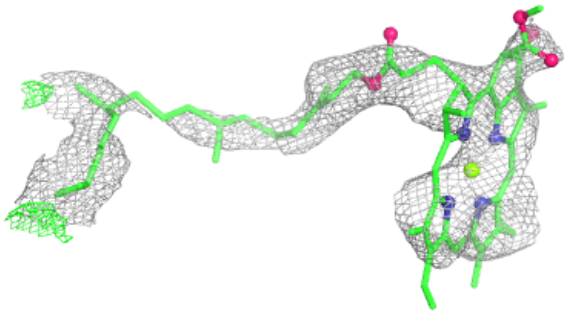


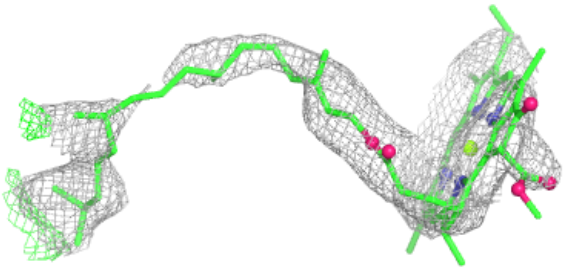


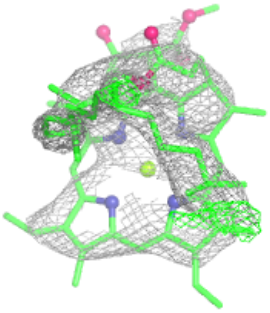


Electron density around CLA L 203:

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

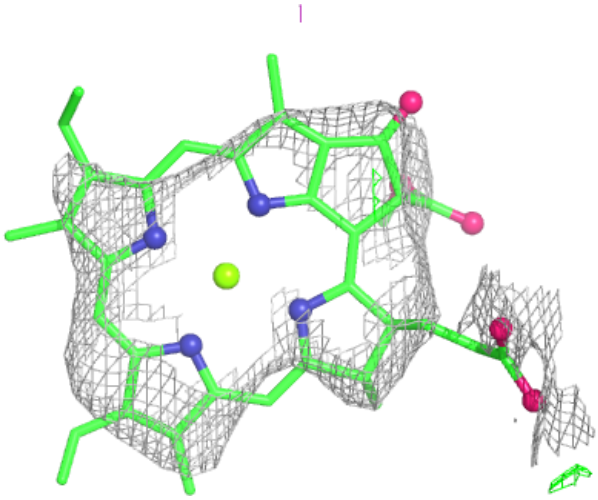


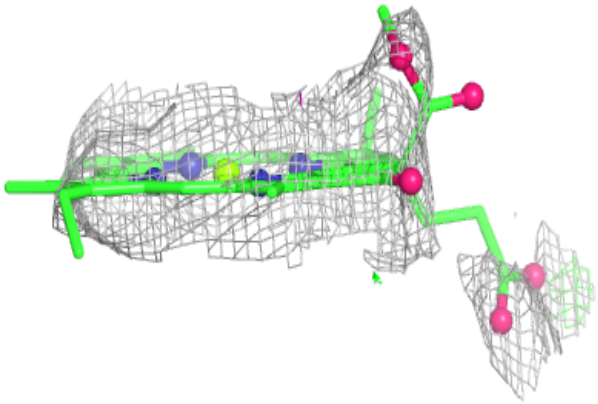


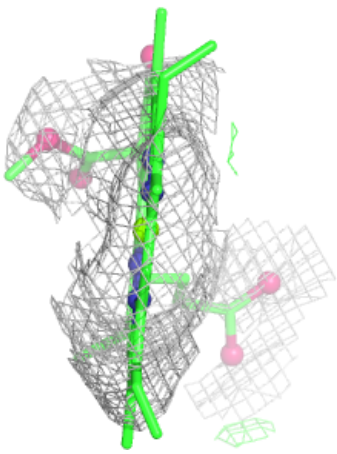


Electron density around CLA K 201:

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

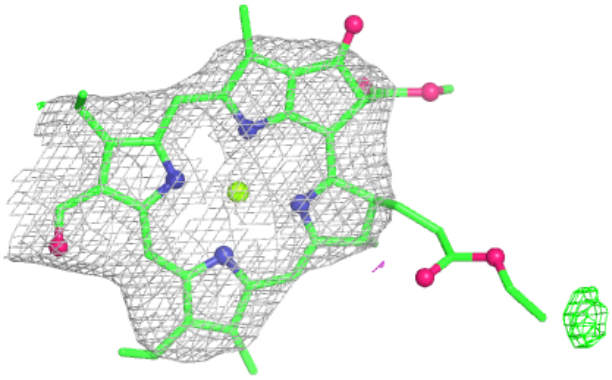


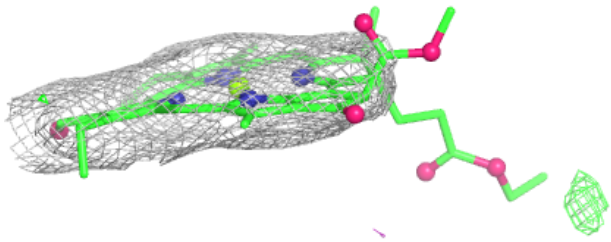


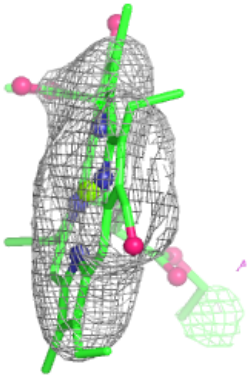


Electron density around CHL 2 305:

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

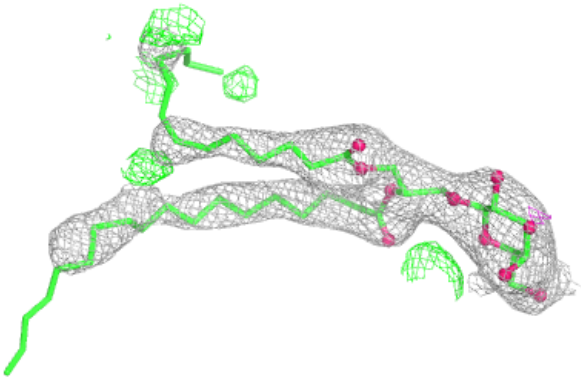


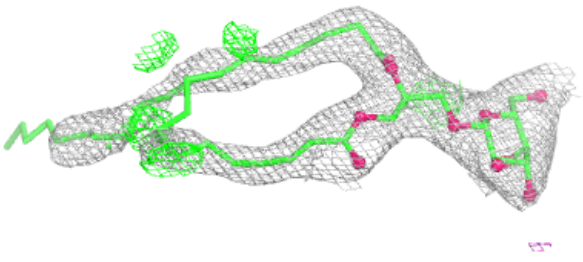


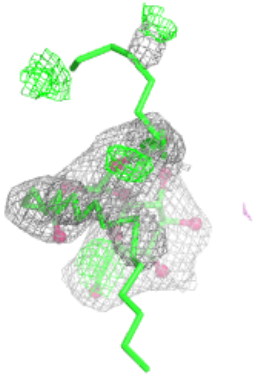


Electron density around LMG 4 319:

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

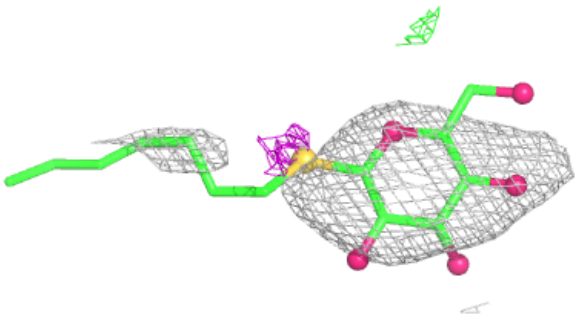


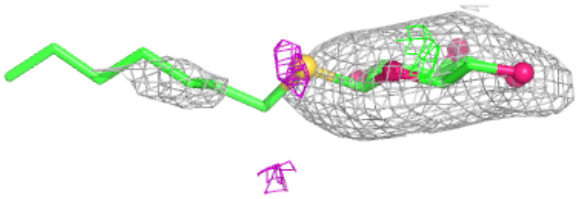


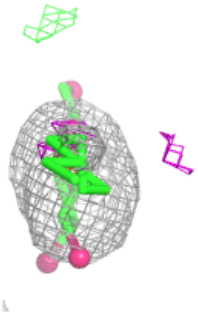


Electron density around HTG 4 321:

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

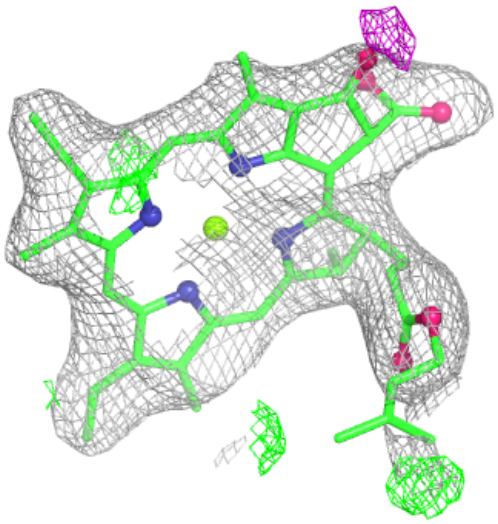


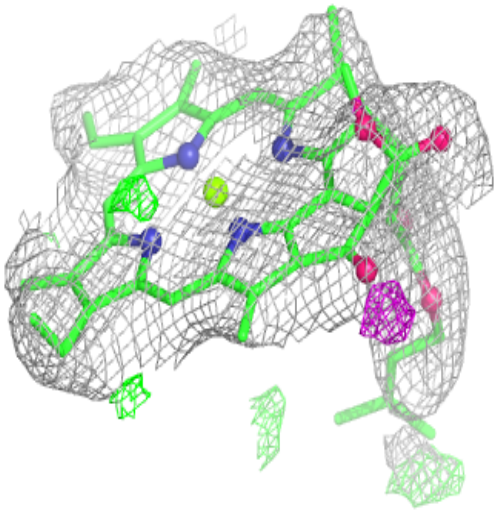


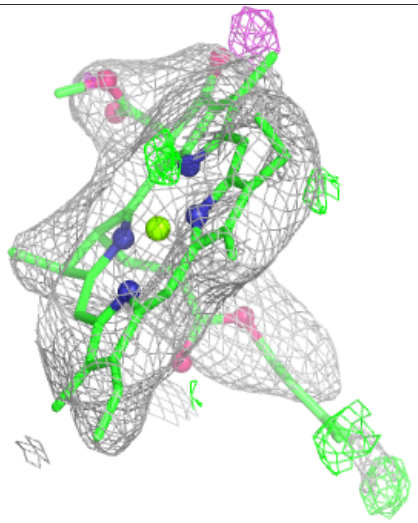


Electron density around CLA 4 304:

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

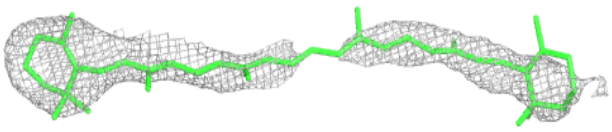


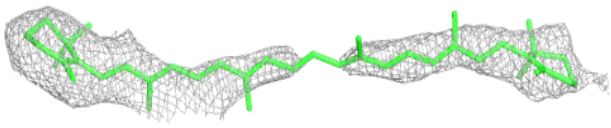


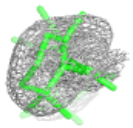


Electron density around BCR L 206:

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

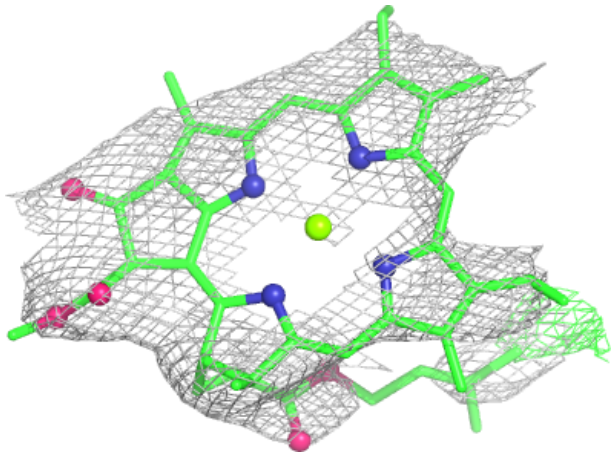


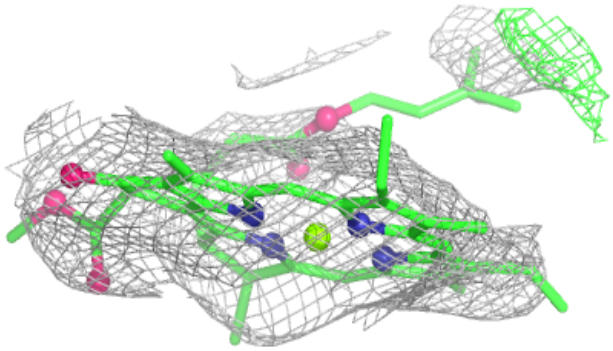


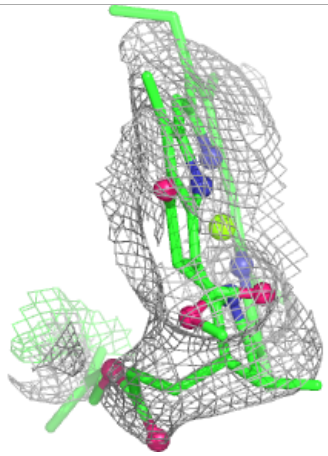


Electron density around CLA 3 609:

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

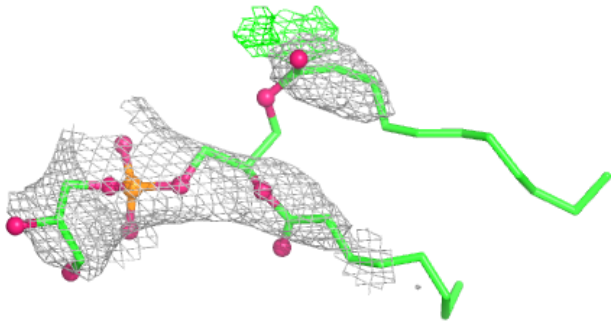


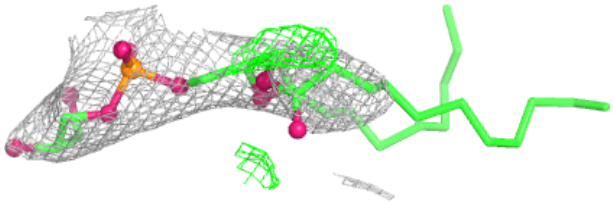


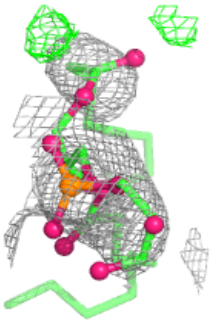


Electron density around LHG 2 317:

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

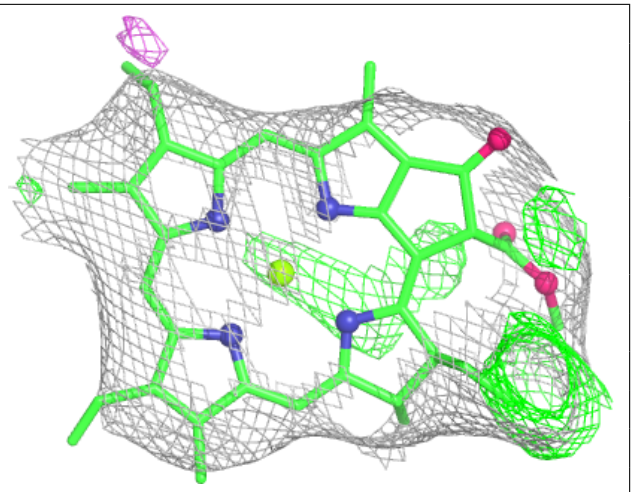


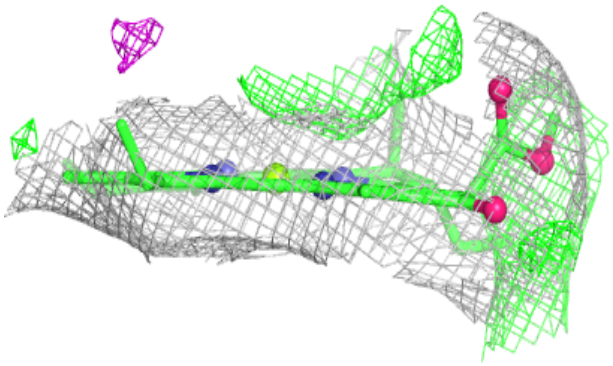


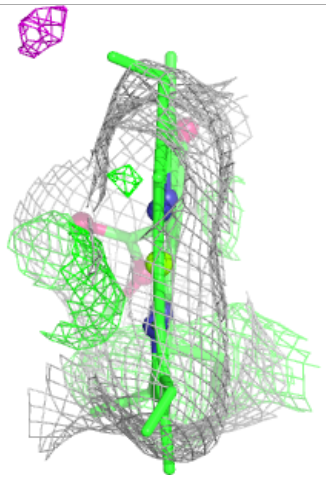


Electron density around CLA 1 304:

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

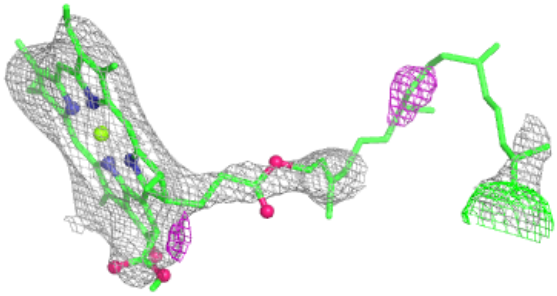


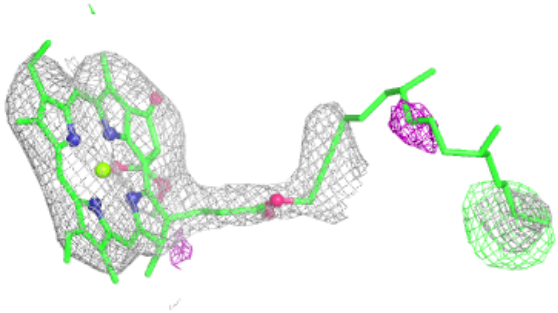


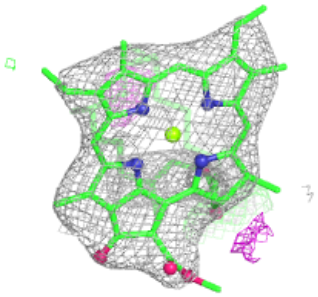


Electron density around CLA A 837:

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

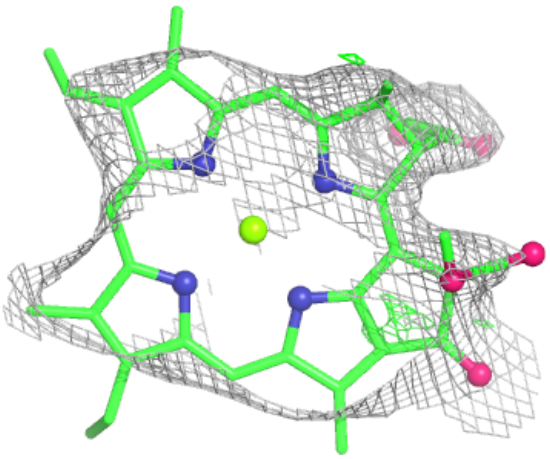


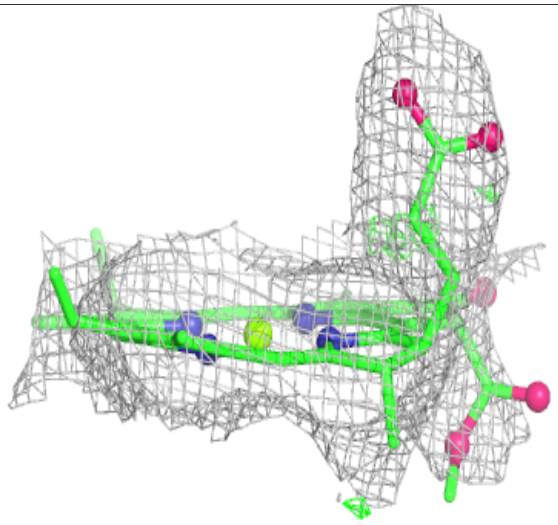


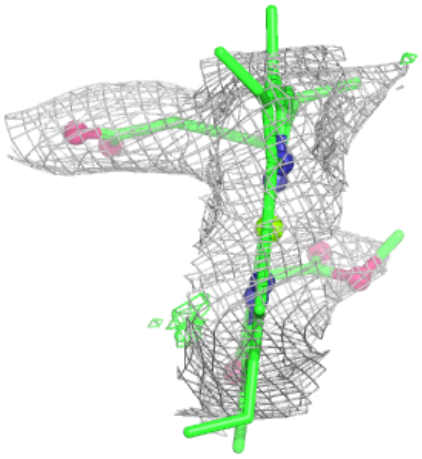


Electron density around CLA 3 604:

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

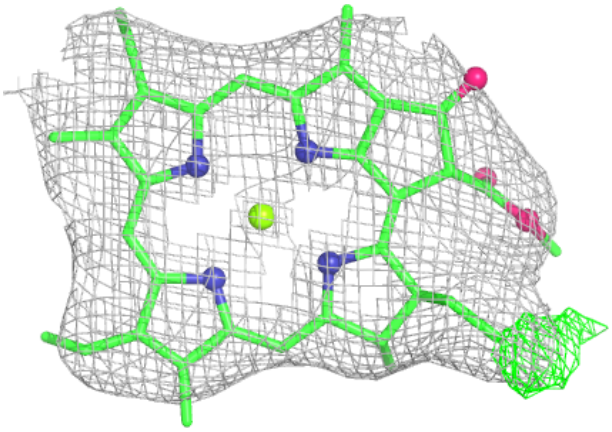


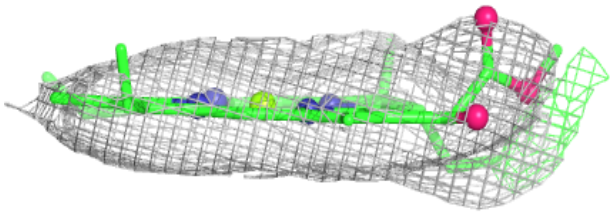


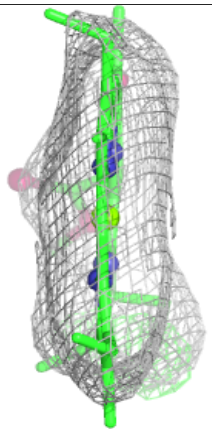


Electron density around CLA 3 605:

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

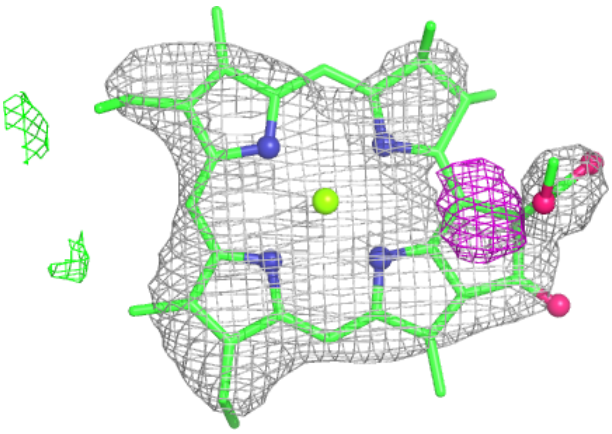


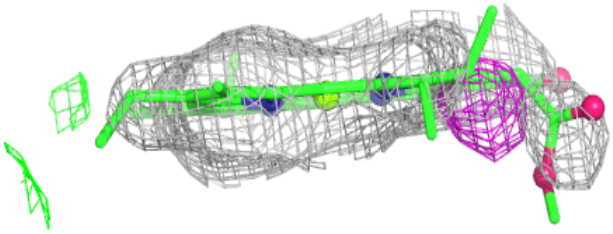


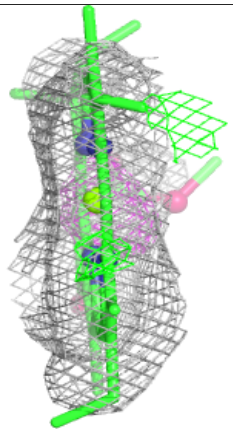


Electron density around CLA G 103:

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

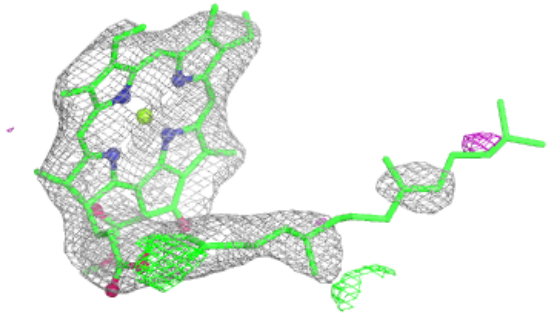


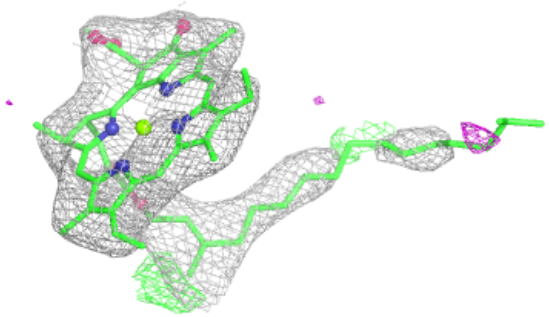


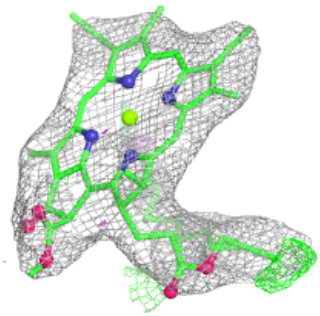


Electron density around CLA 1 307:

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

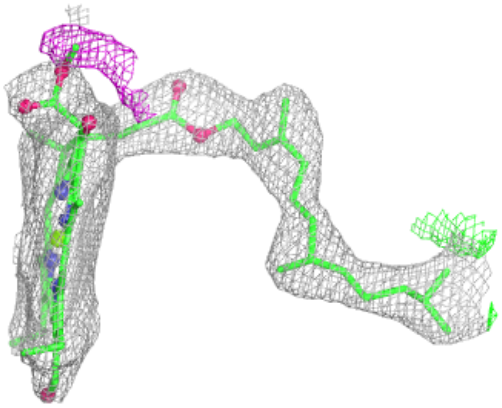


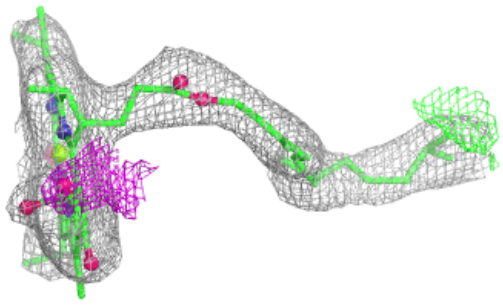


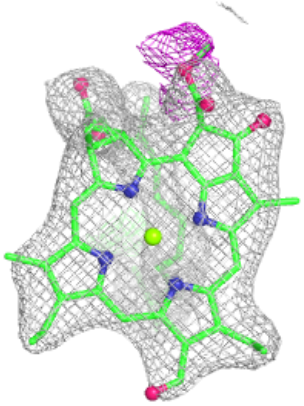


Electron density around CHL 4 301:

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

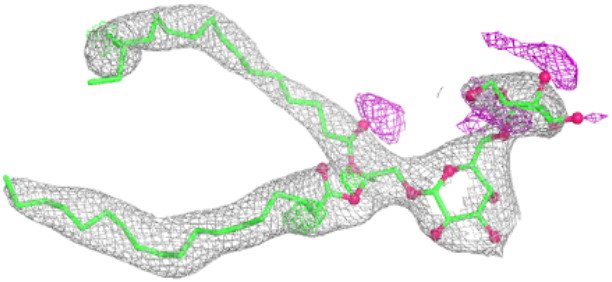


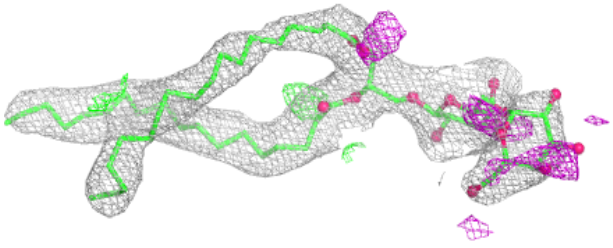


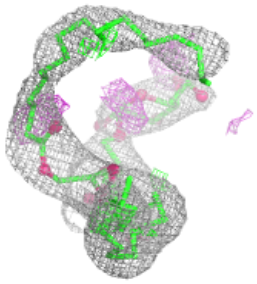


Electron density around DGD B 850:

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

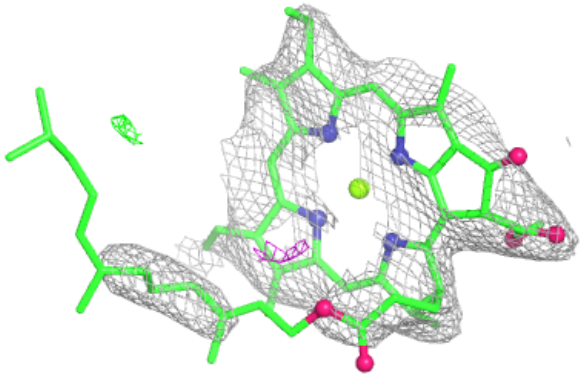


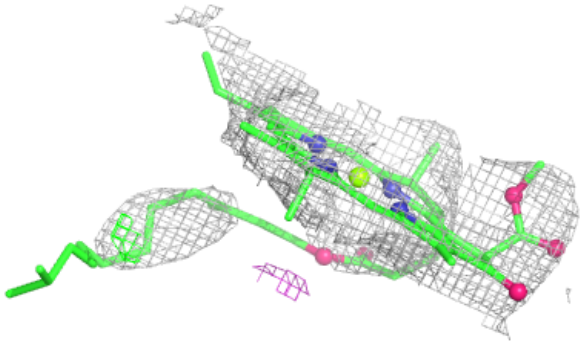


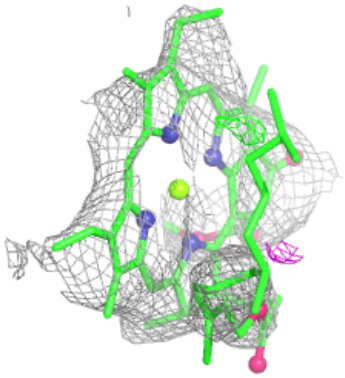


Electron density around CLA 3 602:

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

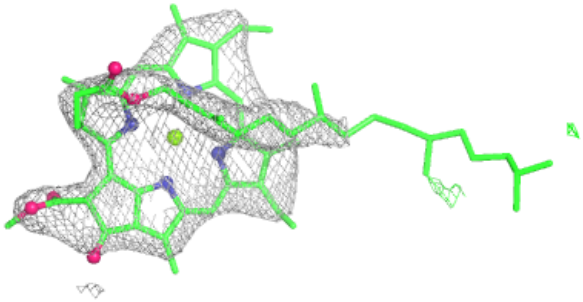


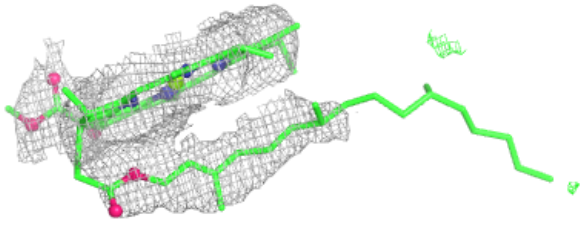


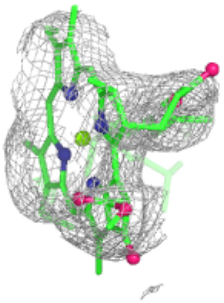


Electron density around CLA A 817:

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

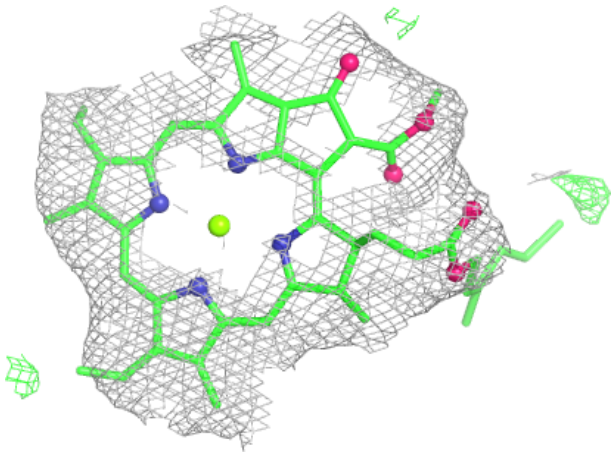


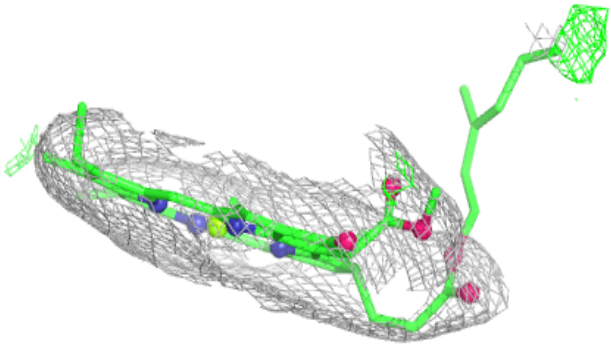




Electron density around CLA 2 310:

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

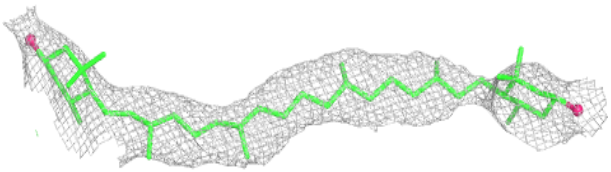


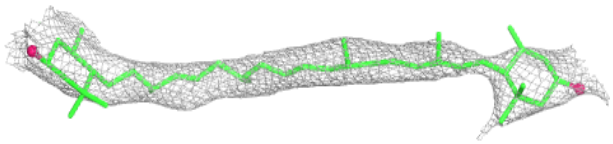


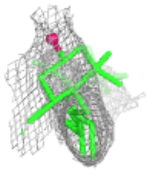


Electron density around LUT 3 614:

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

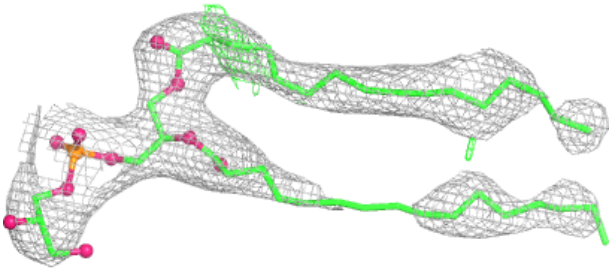


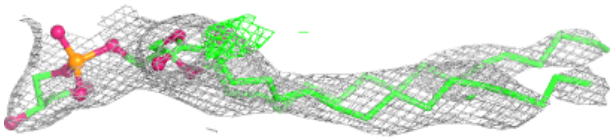


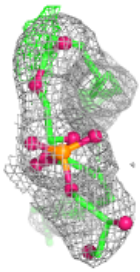


Electron density around LHG 1 317:

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

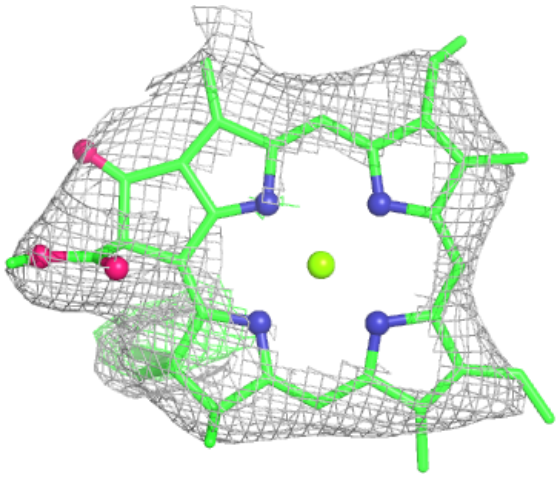


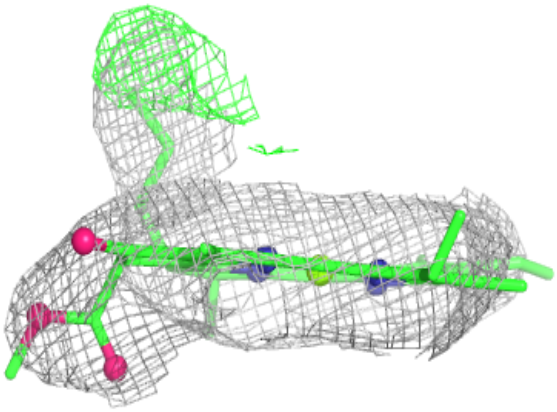


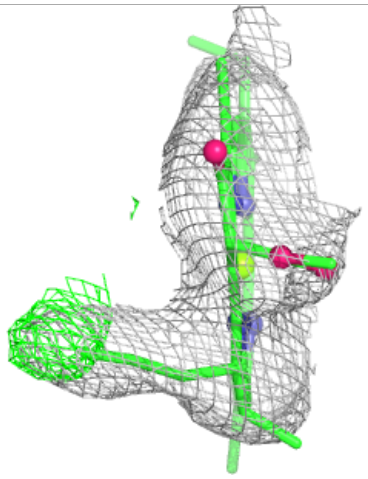


Electron density around CLA 2 312:

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

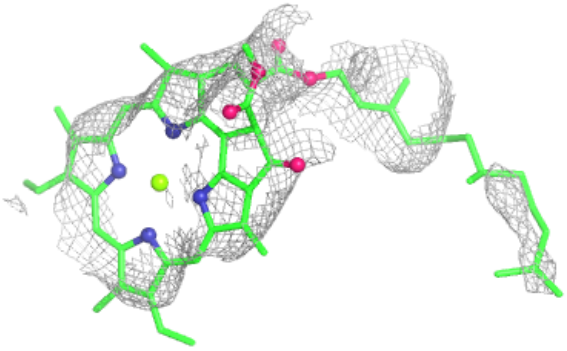


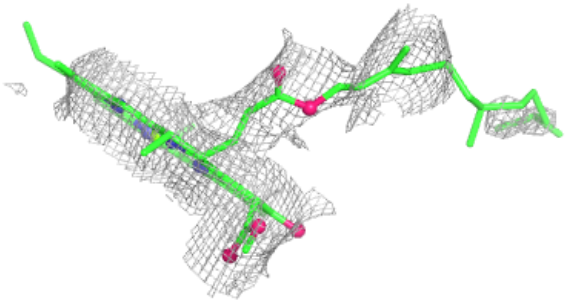


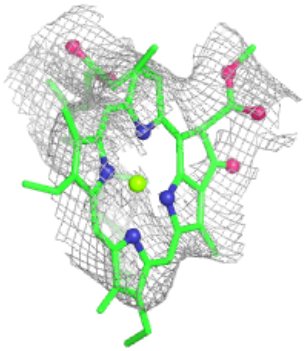


Electron density around CLA K 202:

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

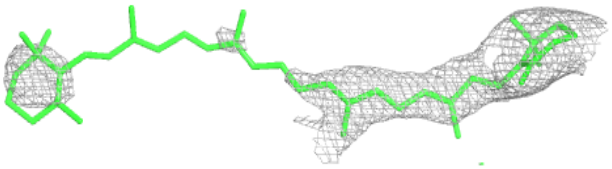


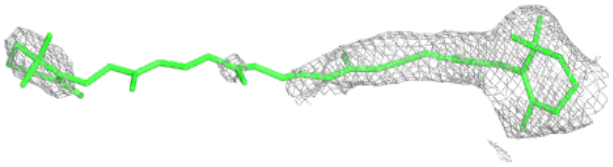


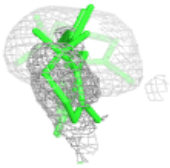


Electron density around BCR 1 316:

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

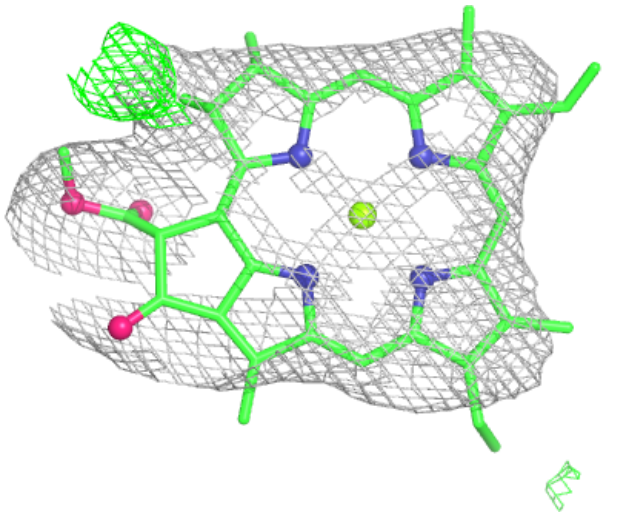


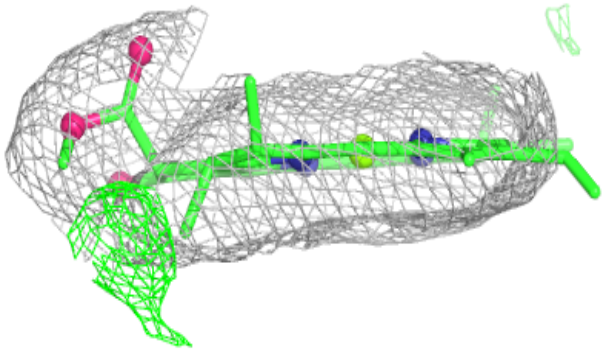


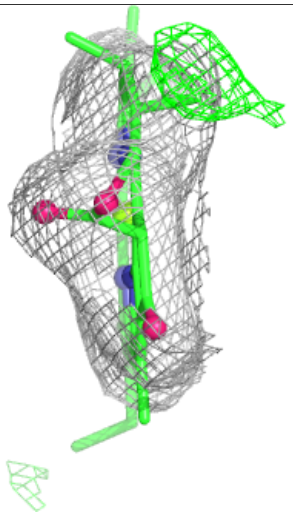


Electron density around CLA 2 309:

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

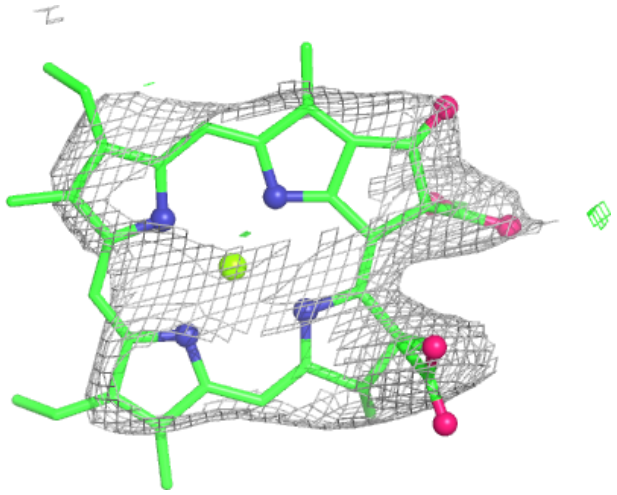


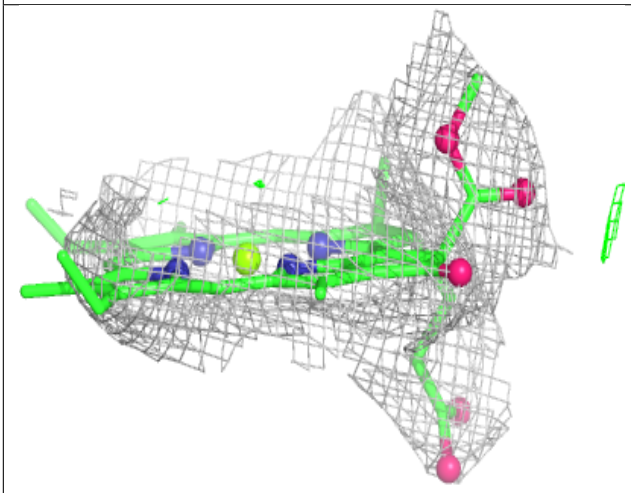


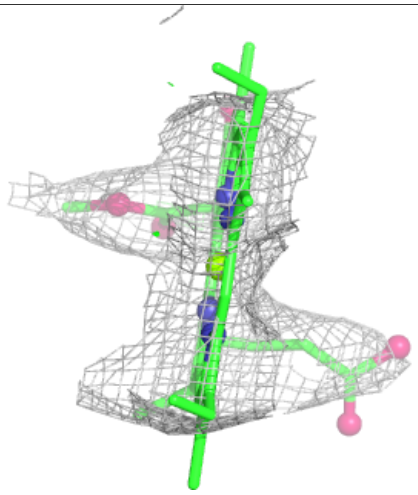


Electron density around CLA A 819:

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

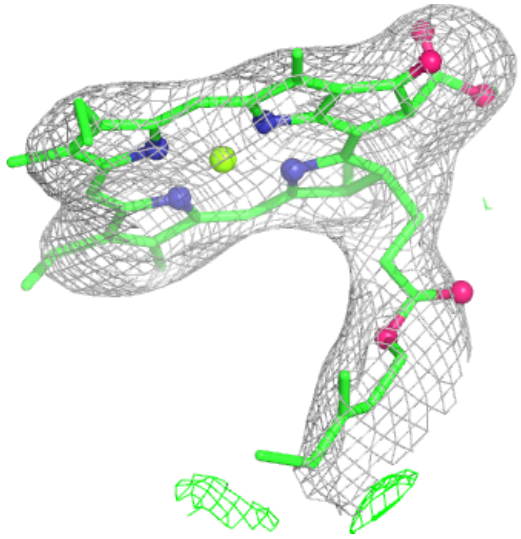


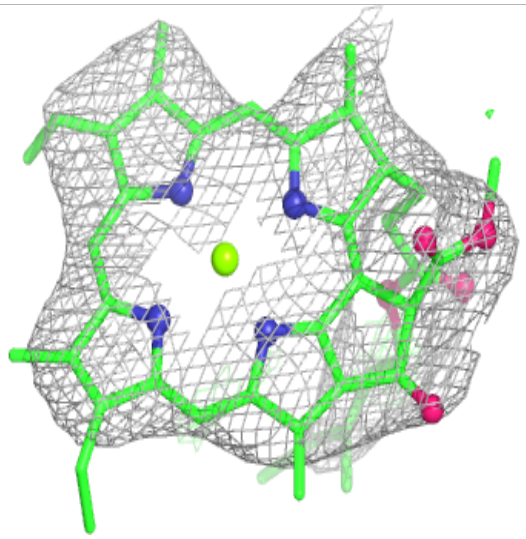


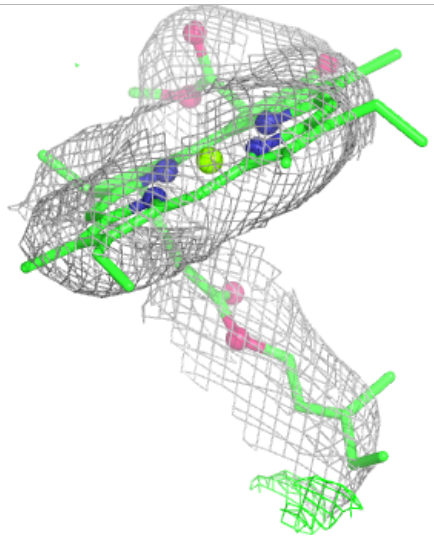


Electron density around CLA 1 303:

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

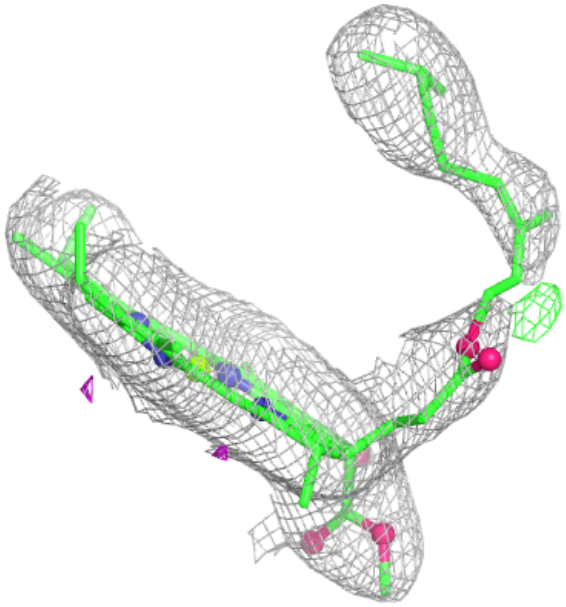


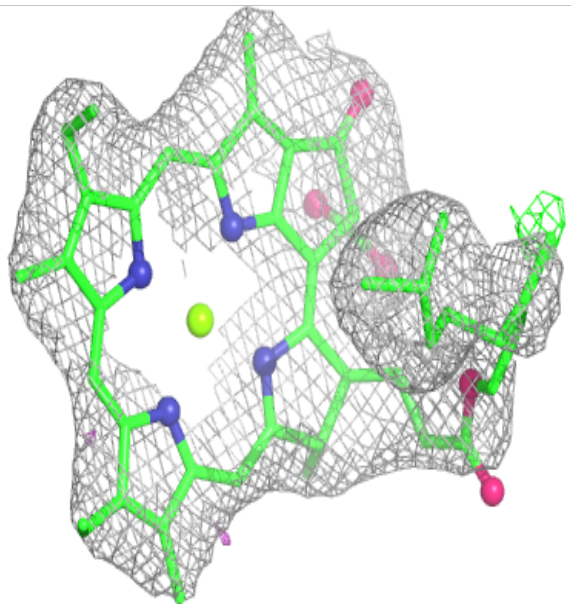


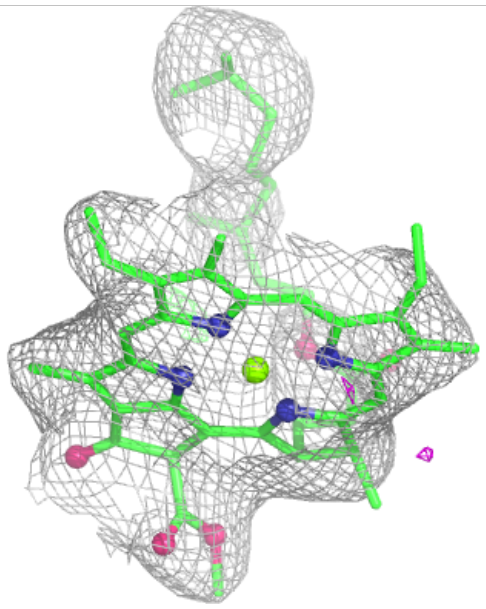


Electron density around CLA 1 312:

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

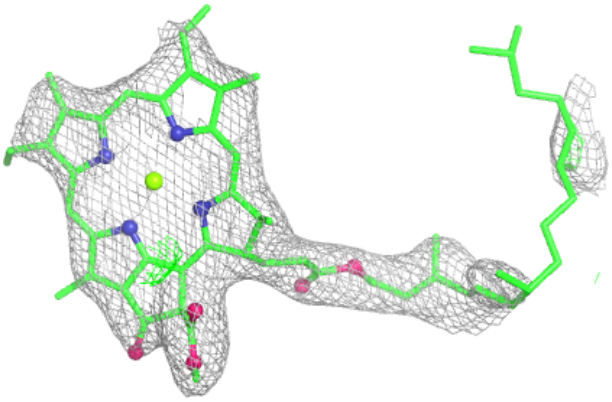


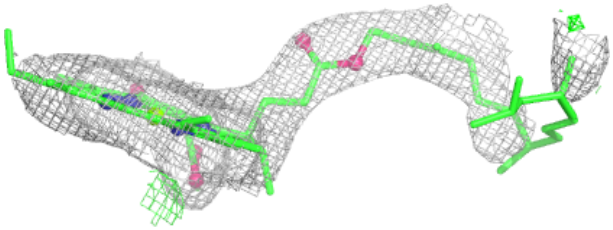


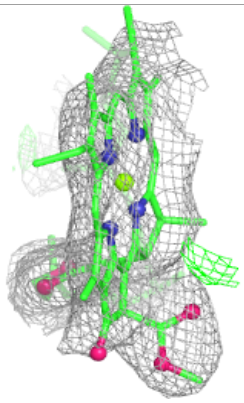


Electron density around CLA A 825:

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

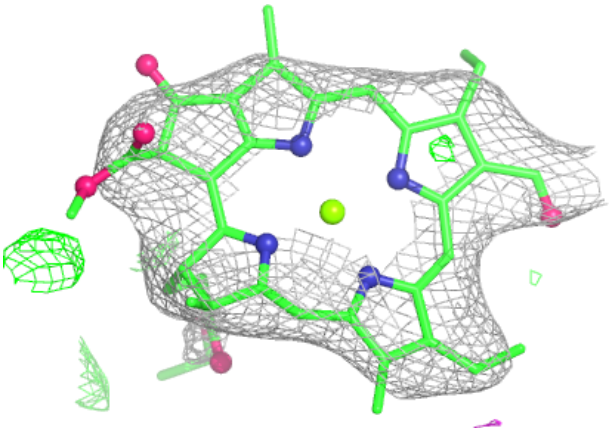


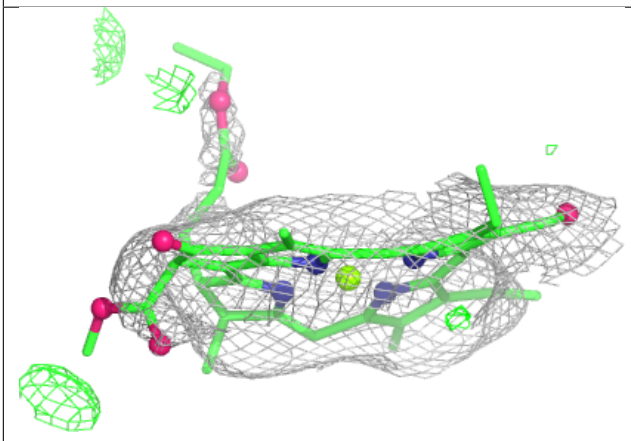


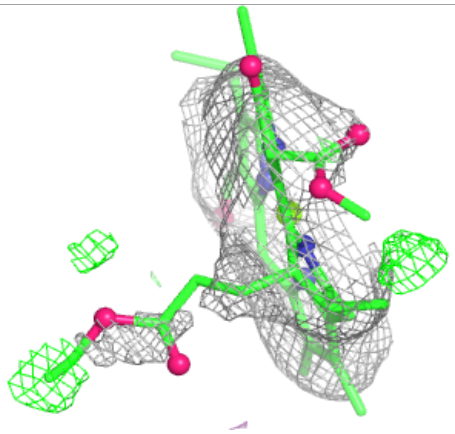


Electron density around CHL 1 305:

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

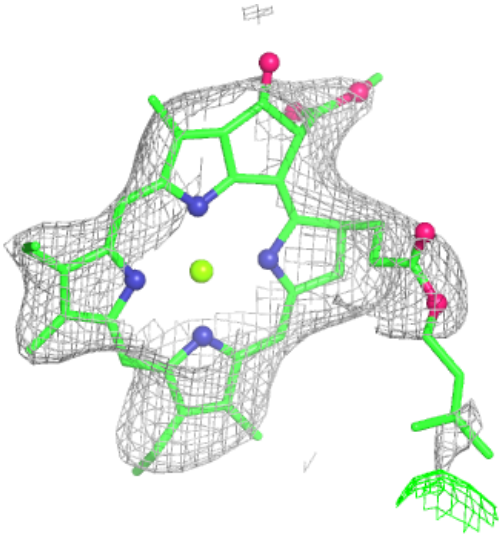


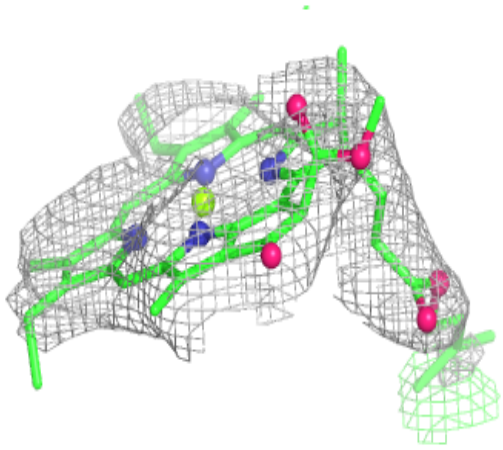


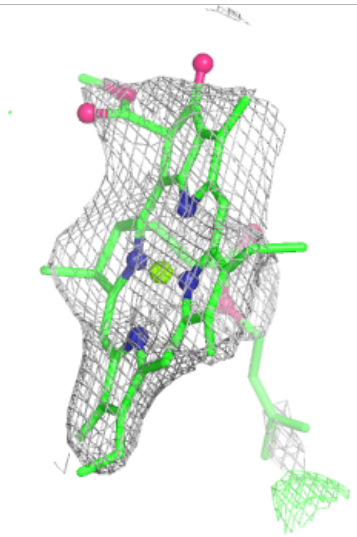


Electron density around CLA A 833:

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

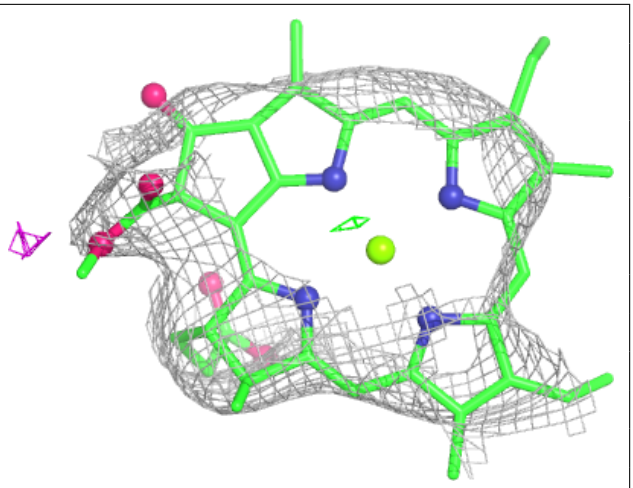


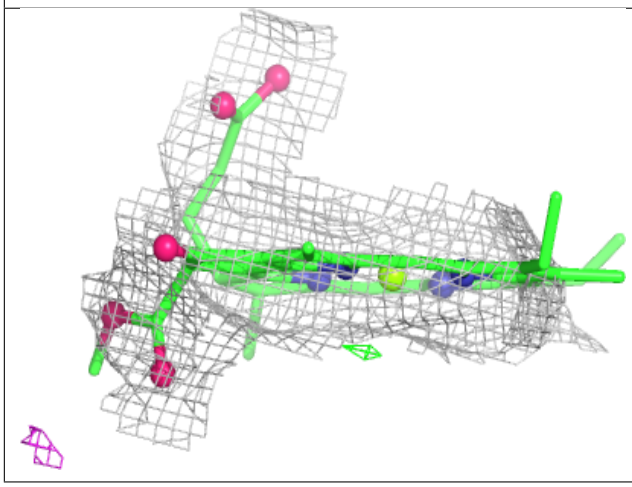


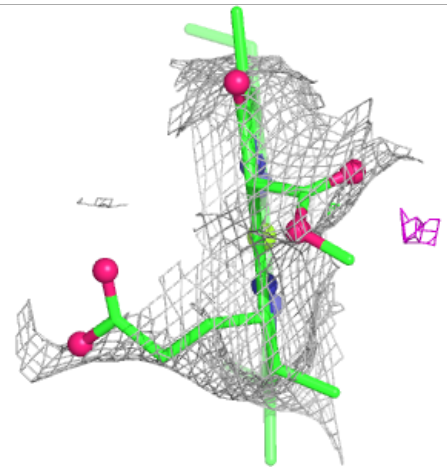


Electron density around CLA A 834:

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

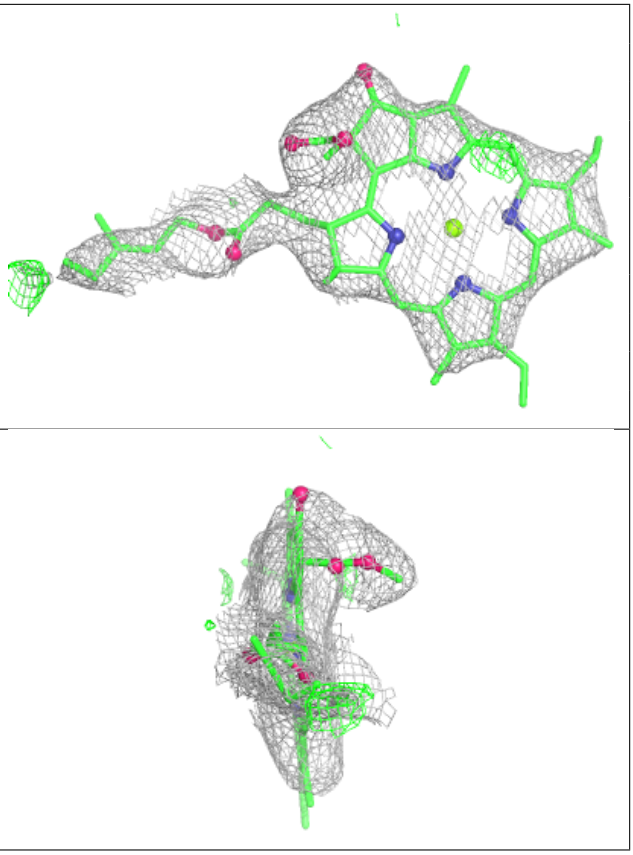


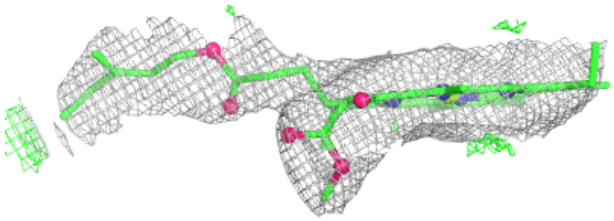




Electron density around CLA A 835:

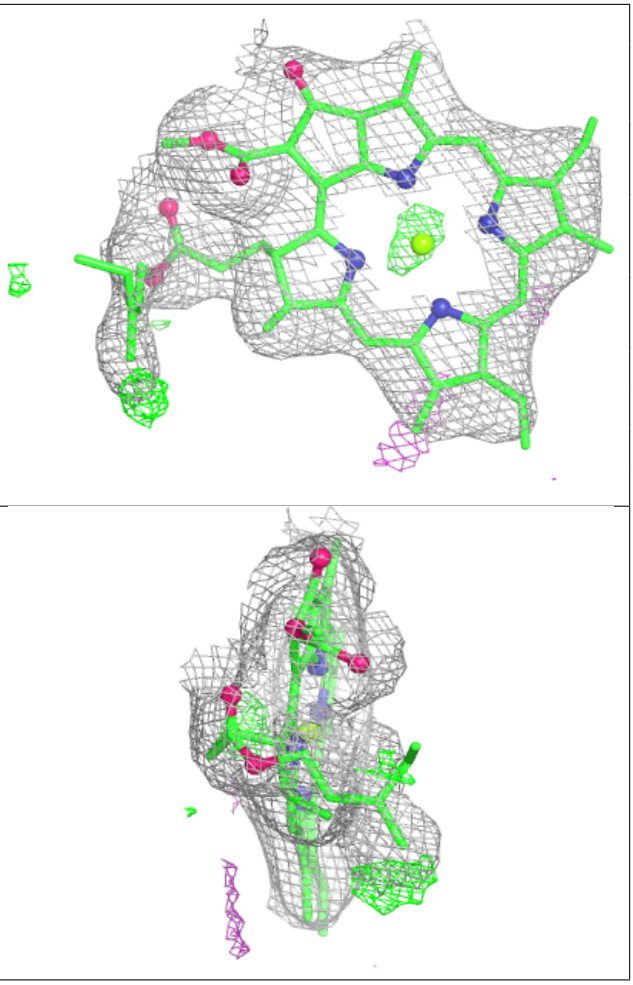
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)





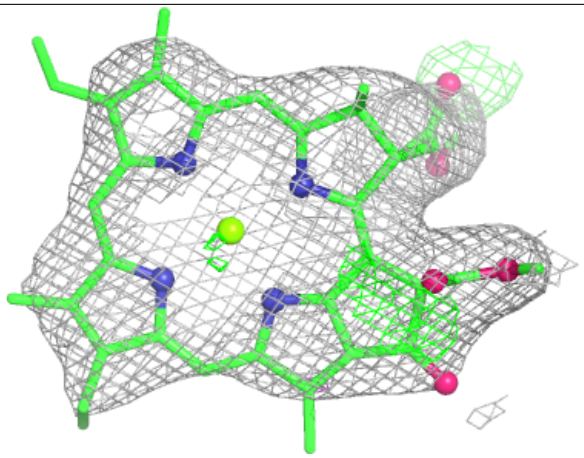
Electron density around CLA 2 302:

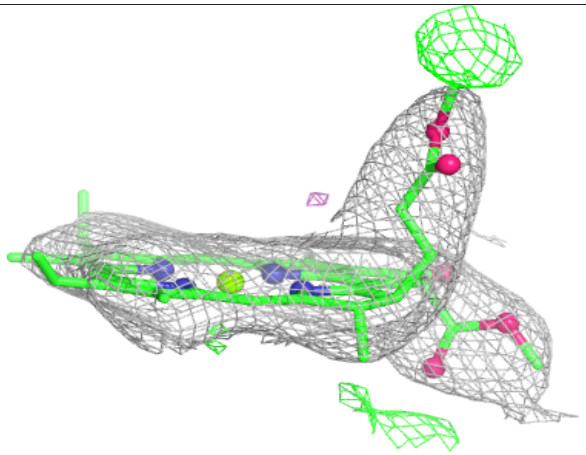
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

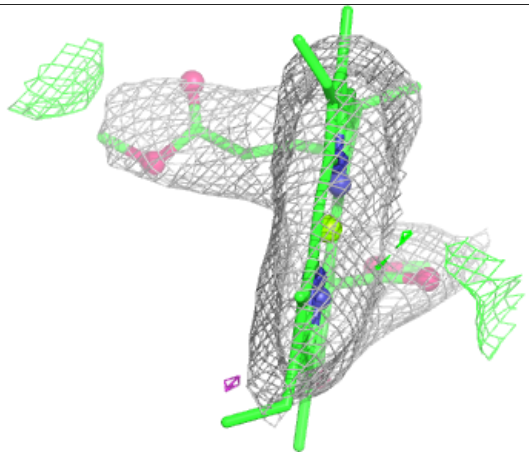


Electron density around CLA 1 306:

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

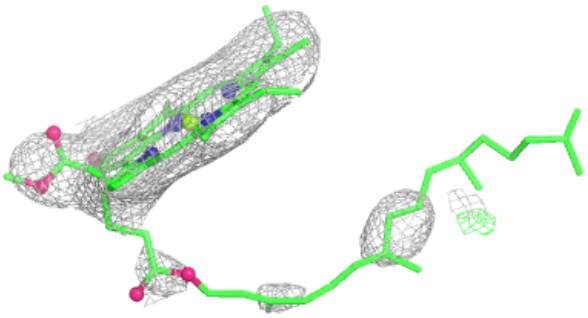


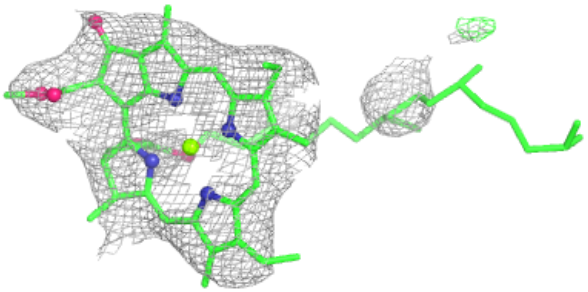


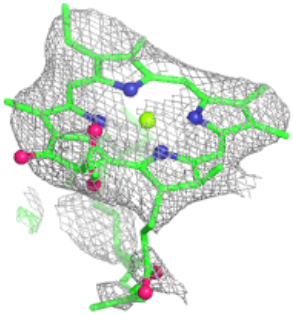


Electron density around CLA B 803:

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

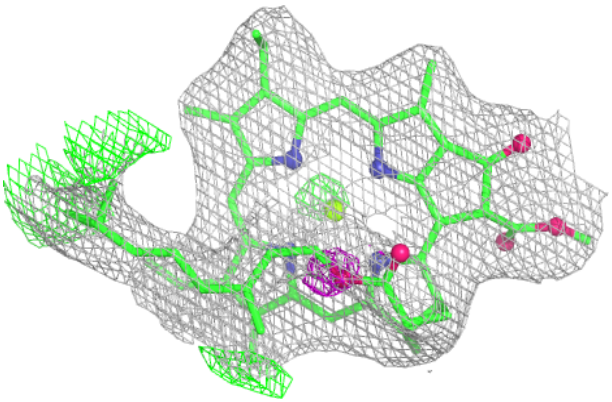


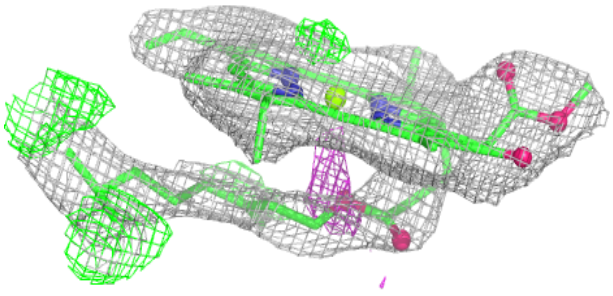


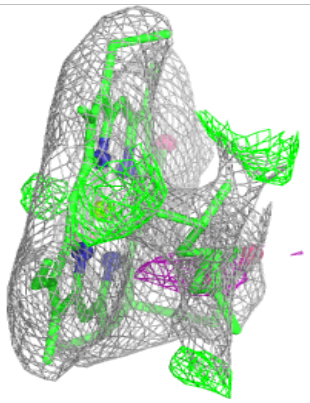


Electron density around CLA B 814:

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

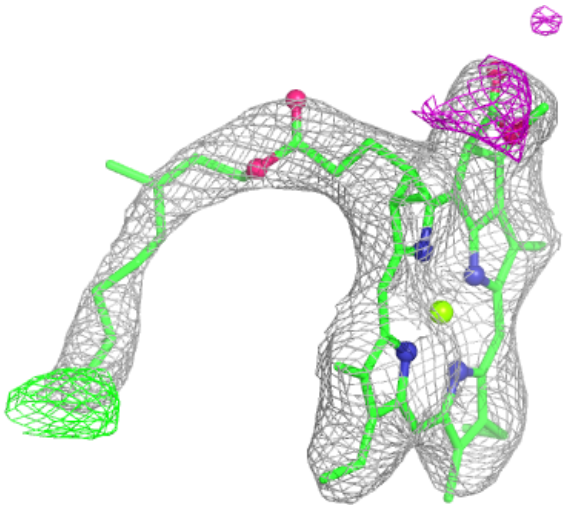


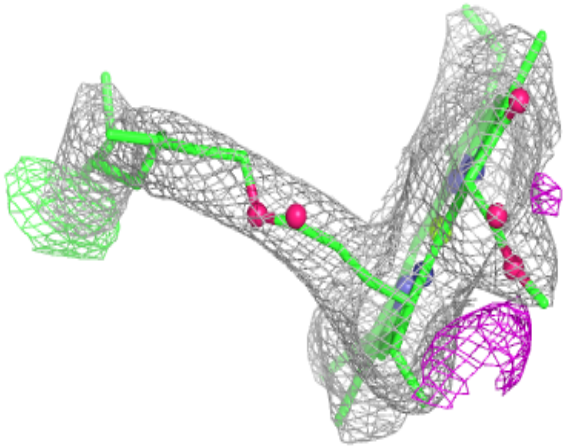


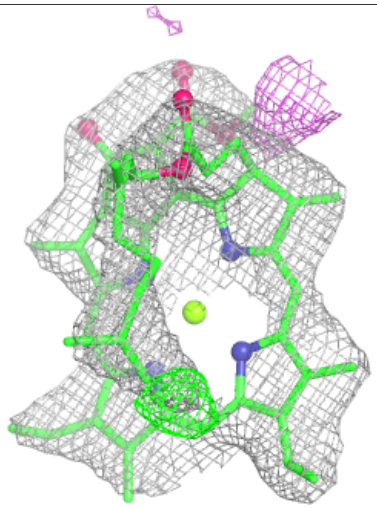


Electron density around CLA B 817:

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

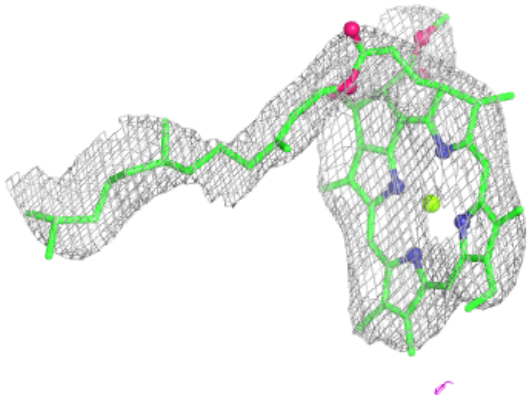


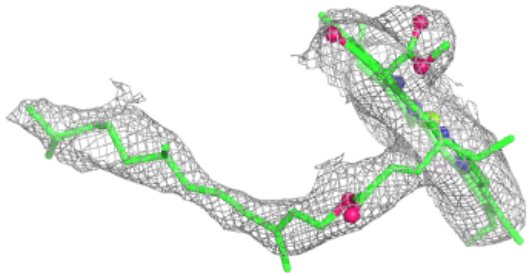


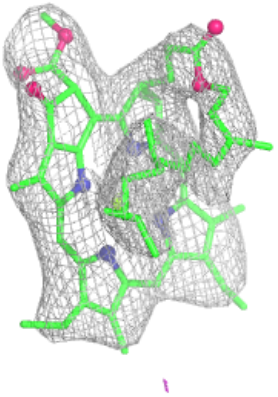


Electron density around CLA 4 310:

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

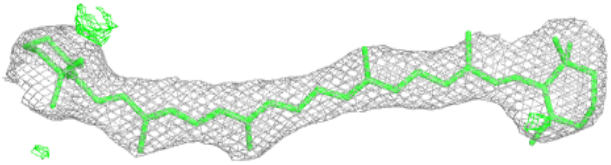


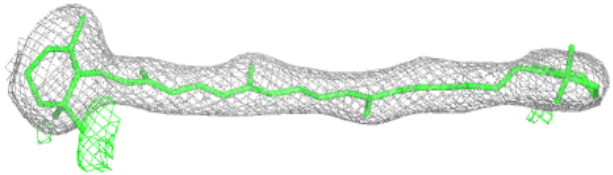


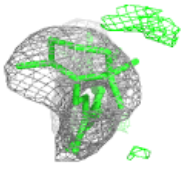


Electron density around BCR 4 318:

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

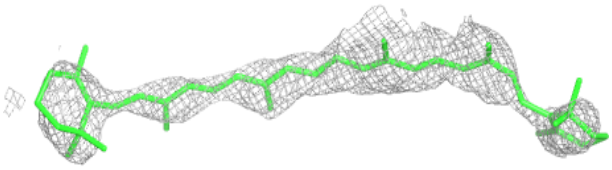


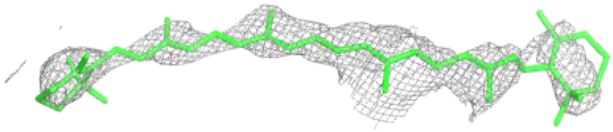


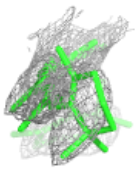


Electron density around BCR A 846:

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

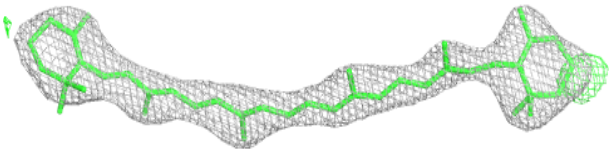


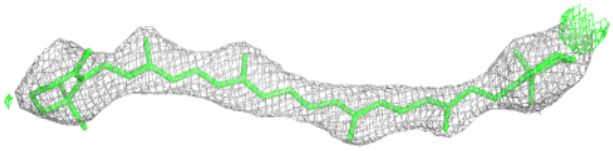


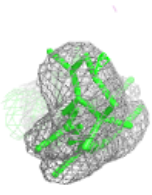


Electron density around BCR J 105:

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

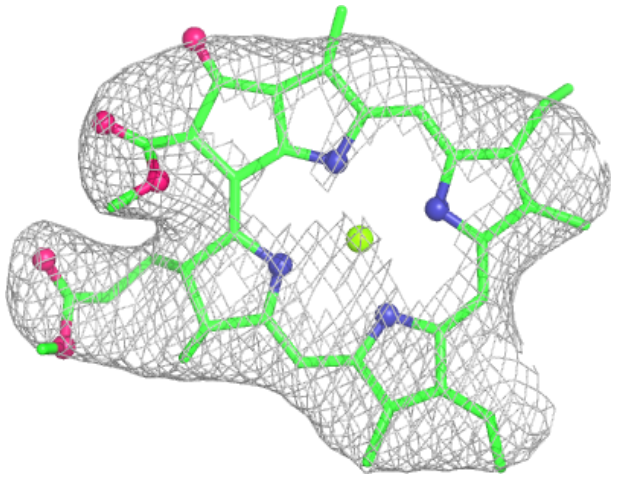


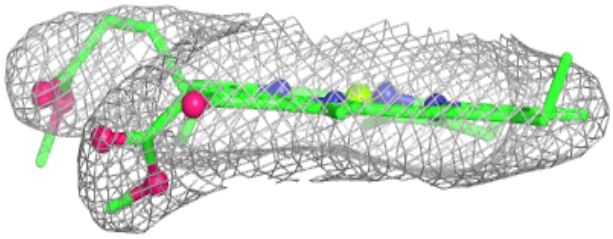


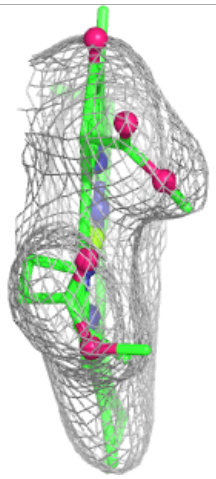


Electron density around CLA G 105:

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

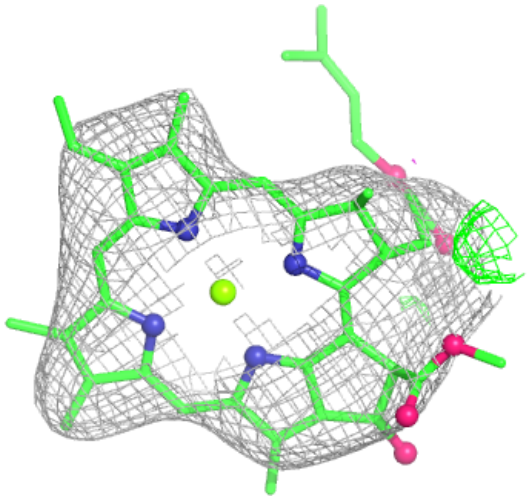


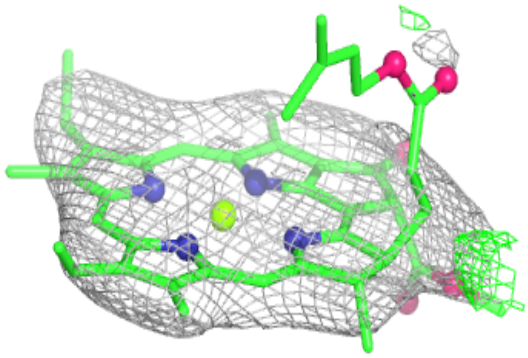


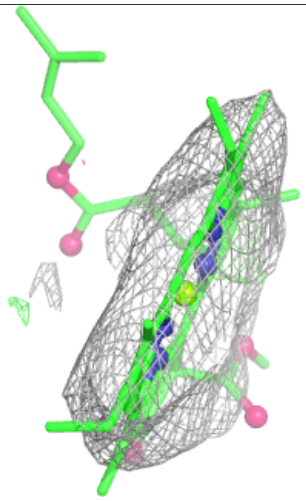


Electron density around CLA A 814:

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

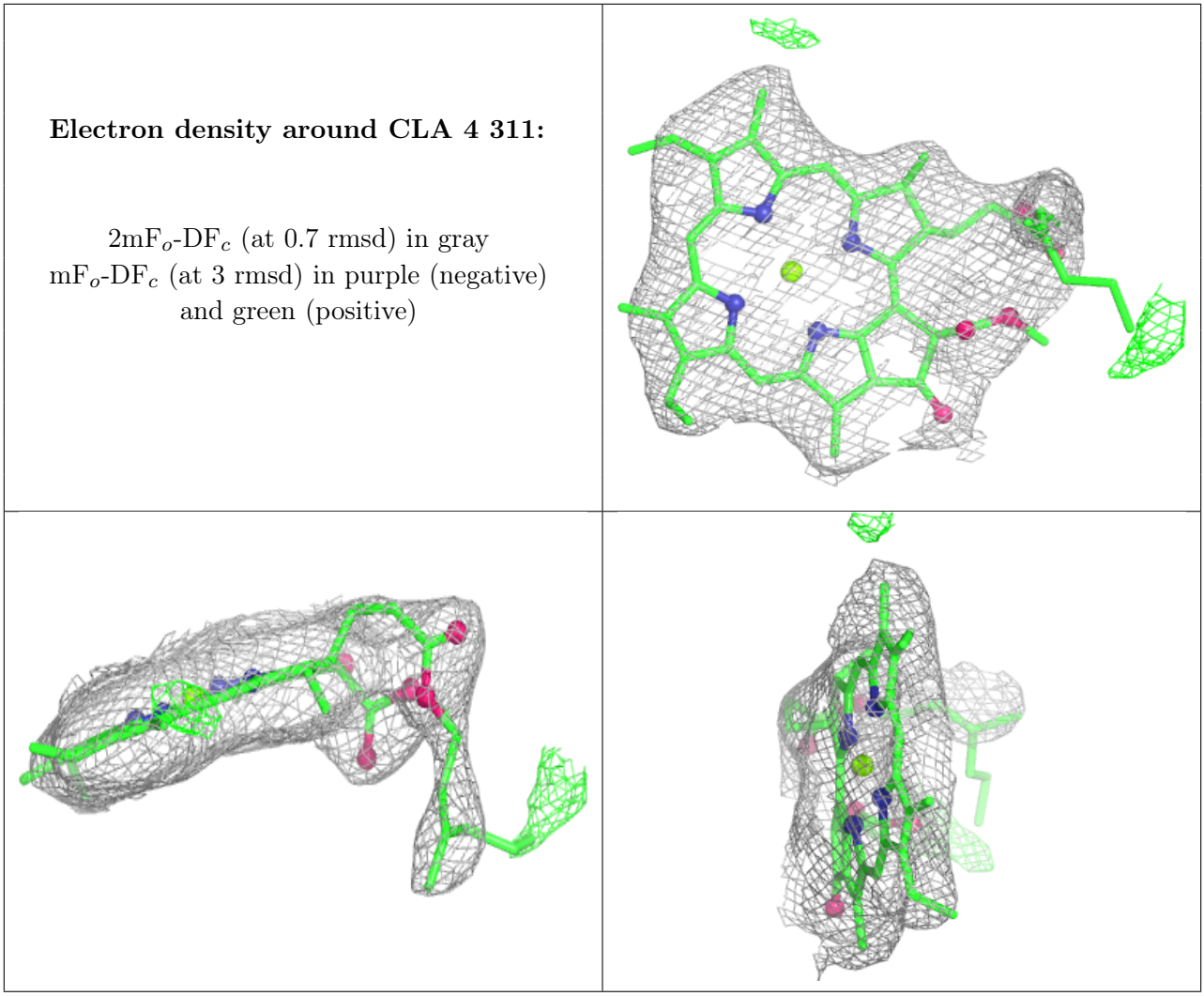






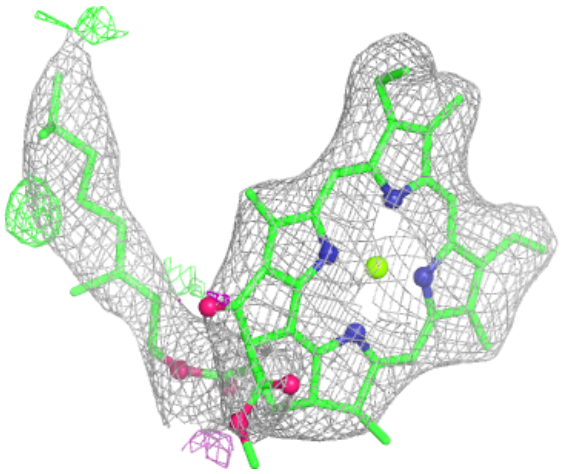
Electron density around CLA 4 311:

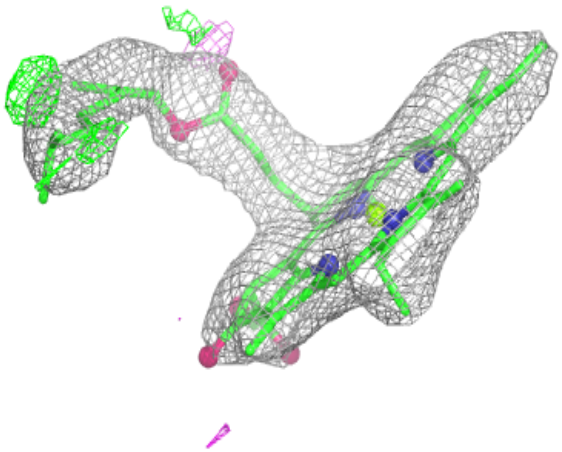
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

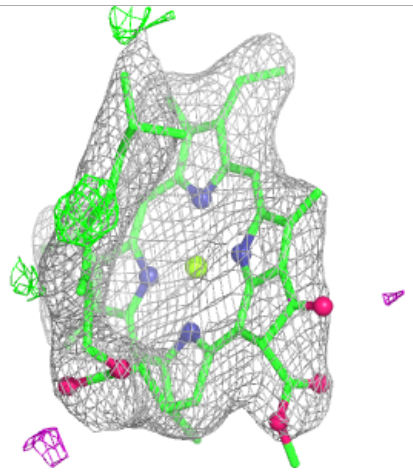


Electron density around CLA B 824:

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

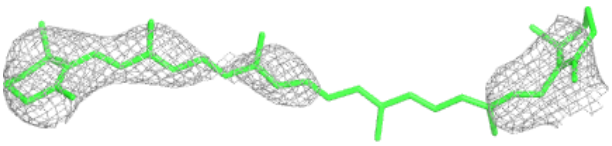


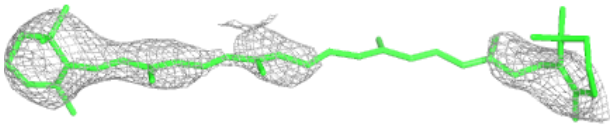


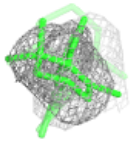


Electron density around BCR A 849:

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

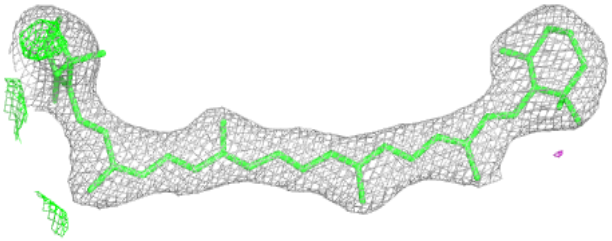


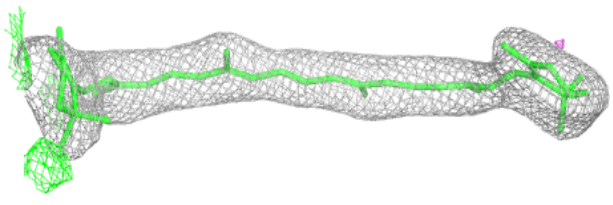


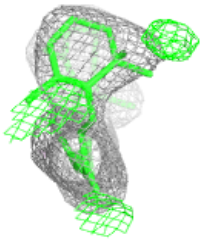


Electron density around BCR B 845:

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

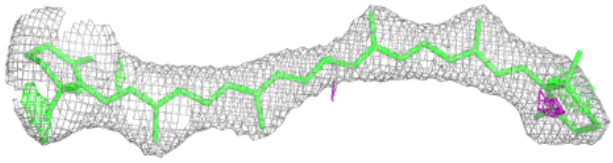


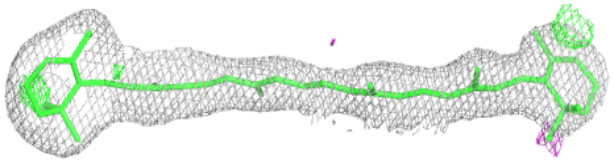


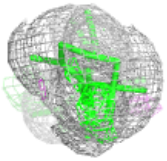


Electron density around BCR B 847:

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

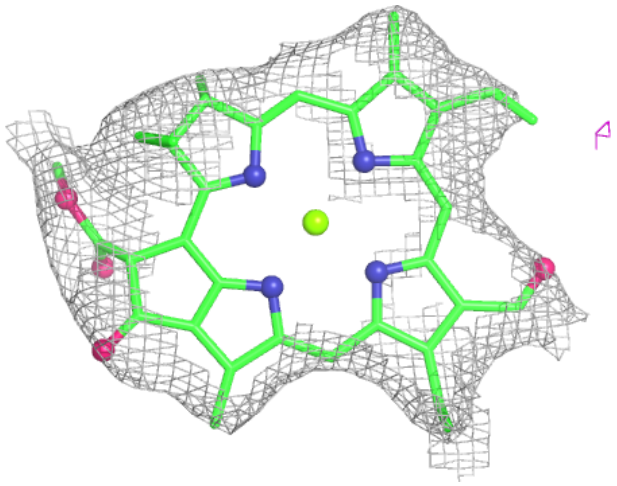


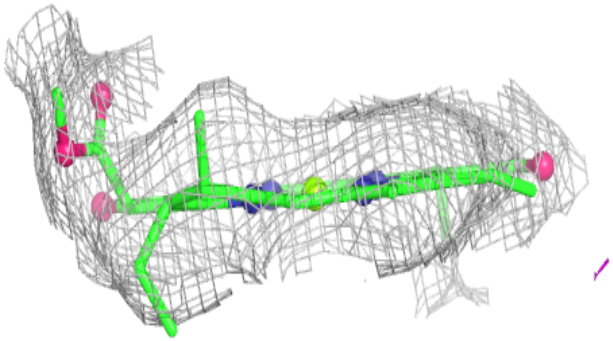


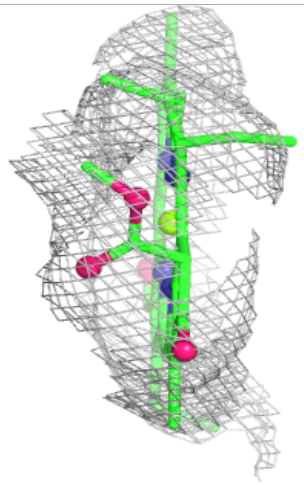


Electron density around CHL 2 313:

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

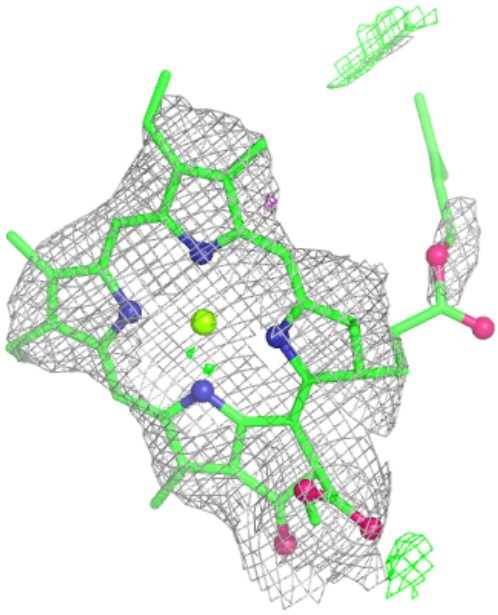


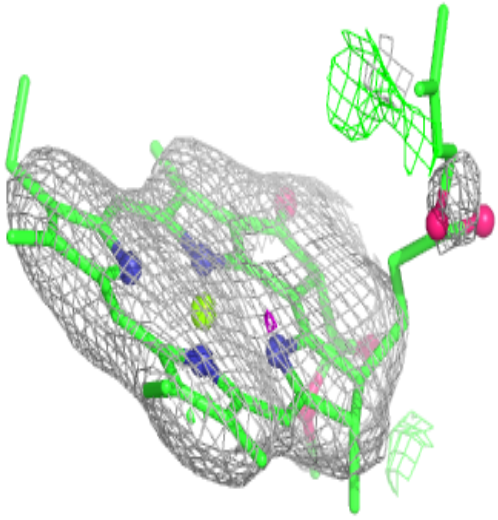


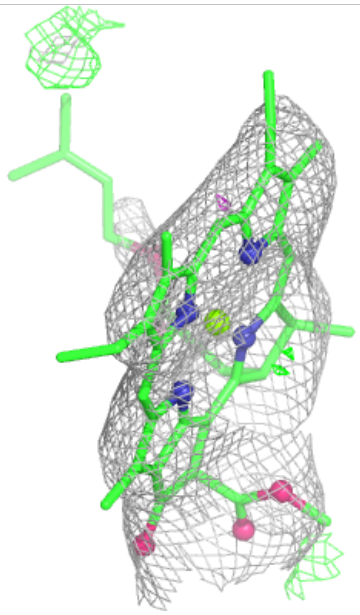


Electron density around CLA A 830:

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

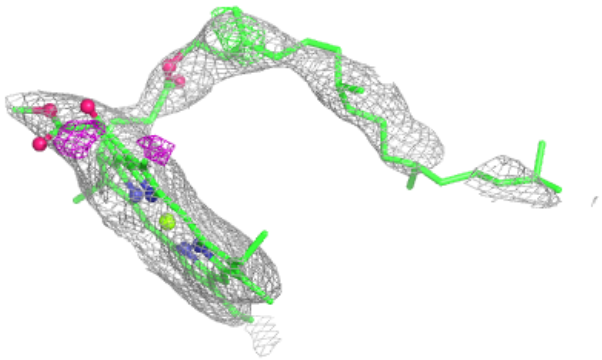


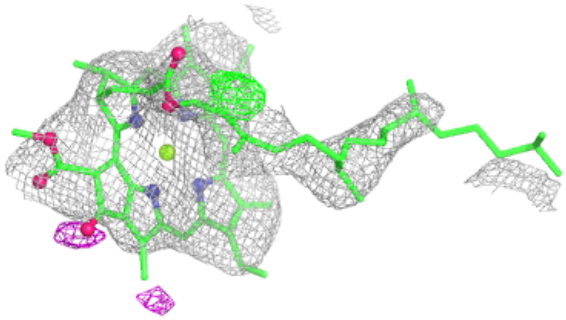


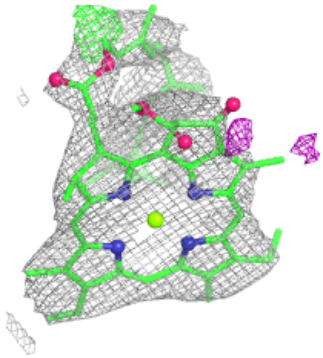


Electron density around CLA A 809:

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

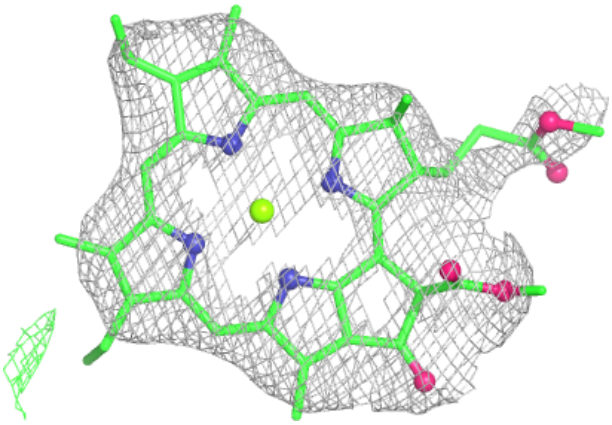


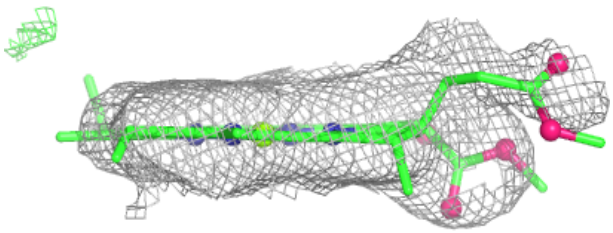


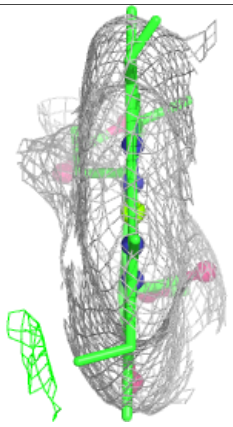


Electron density around CLA 3 613:

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

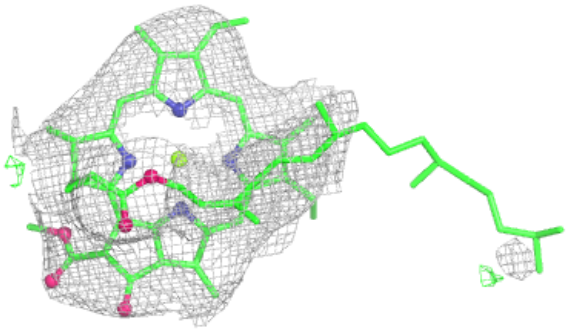


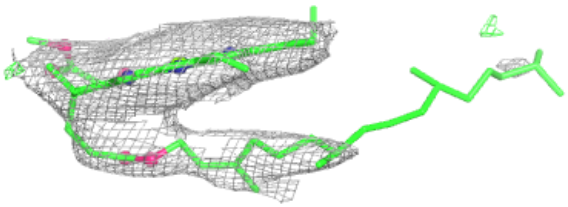


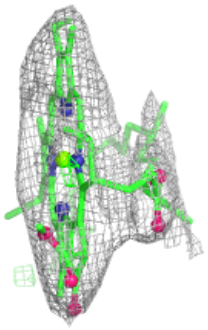


Electron density around CLA A 816:

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

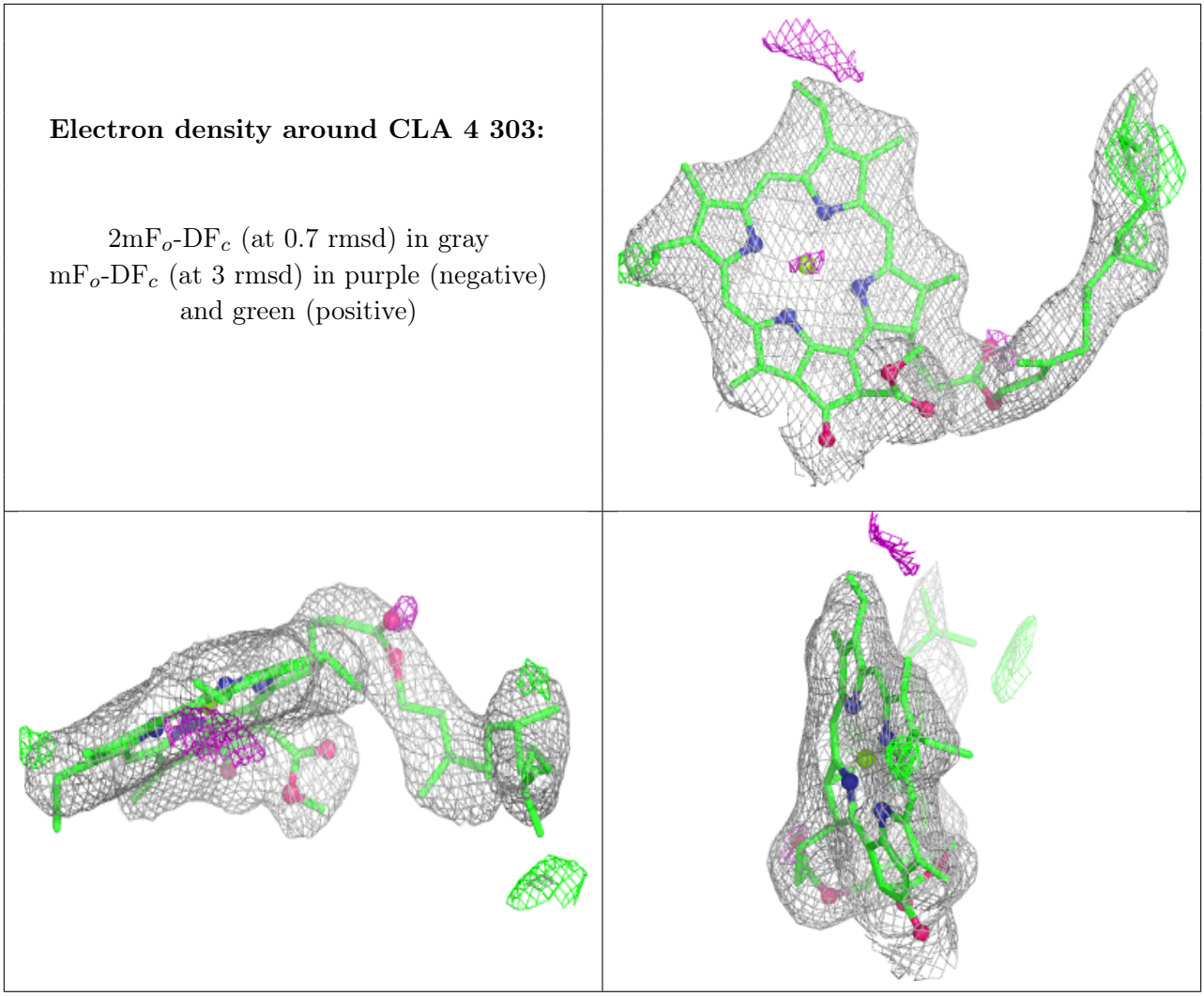






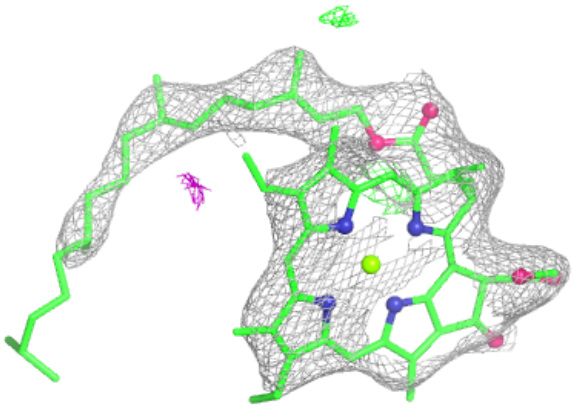
Electron density around CLA 4 303:

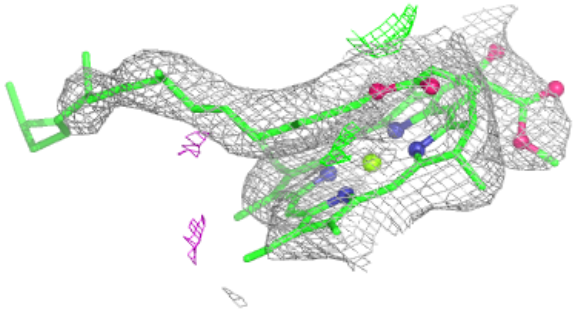
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



Electron density around CLA 2 301:

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

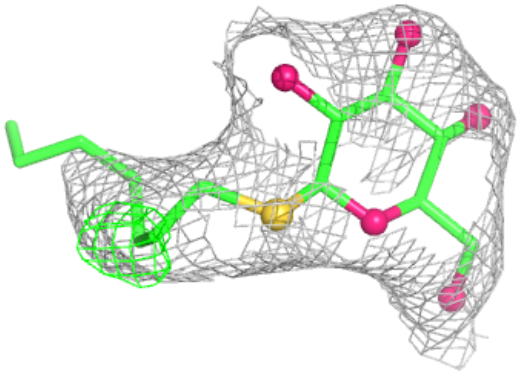


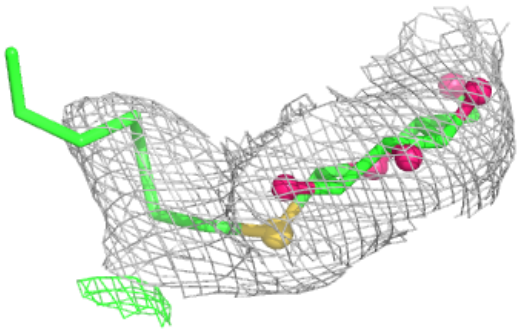


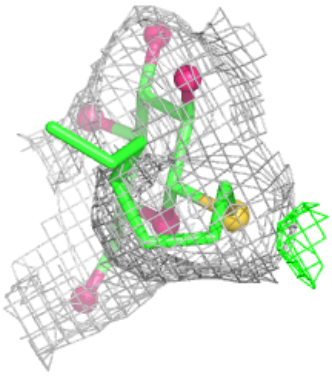


Electron density around HTG J 102:

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

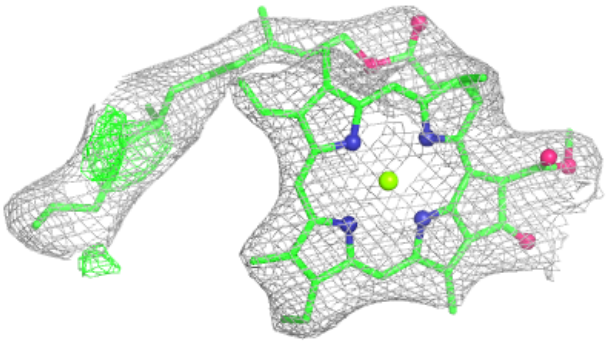


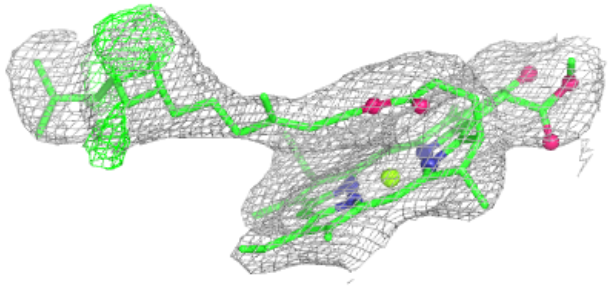


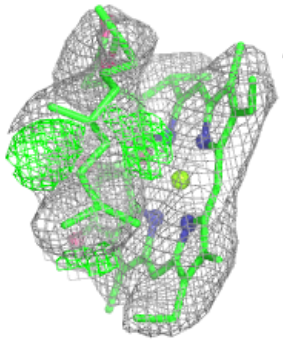


Electron density around CLA 4 309:

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

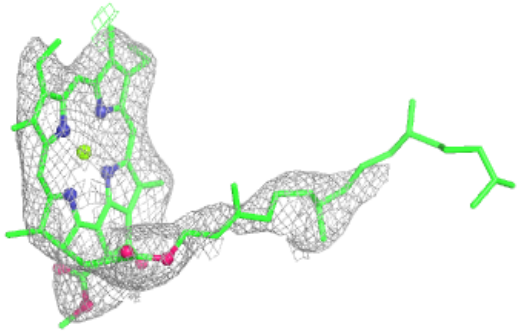


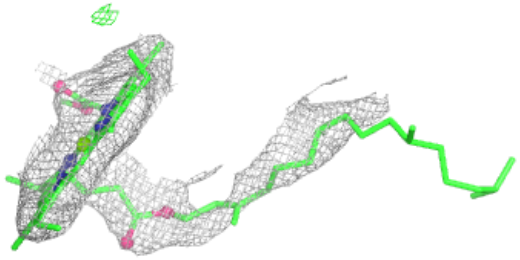


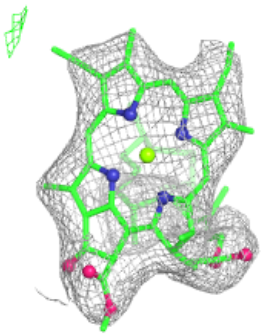


Electron density around CLA 1 309:

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

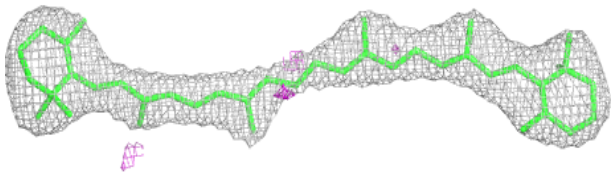


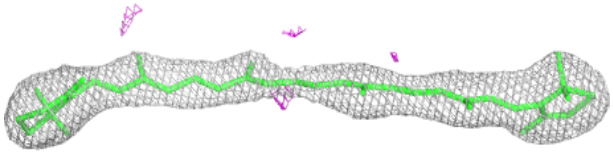


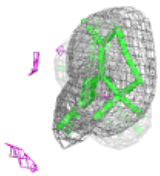


Electron density around BCR J 104:

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

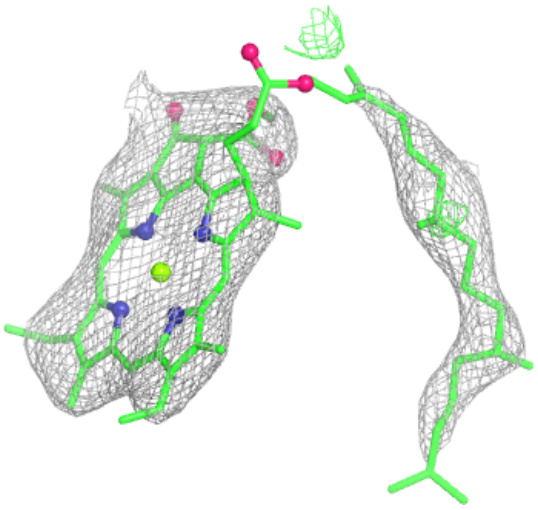


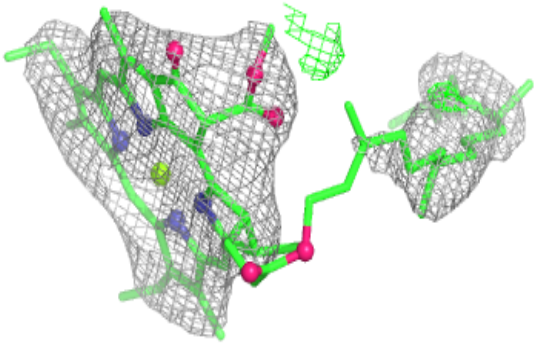


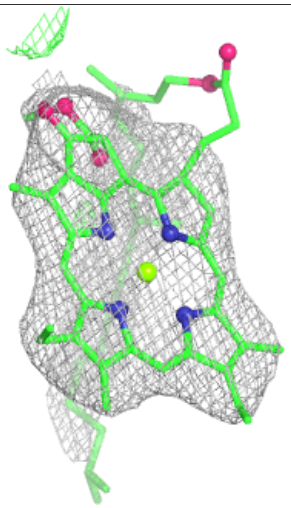


Electron density around CLA B 812:

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

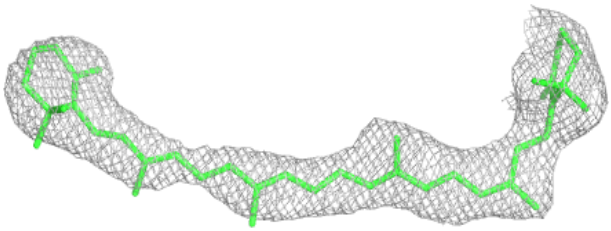


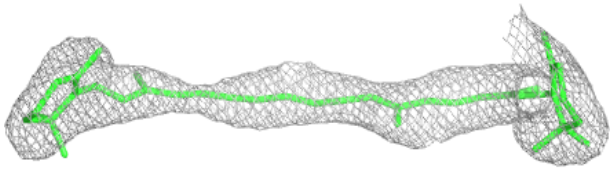


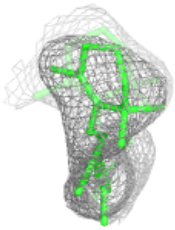


Electron density around BCR L 201:

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

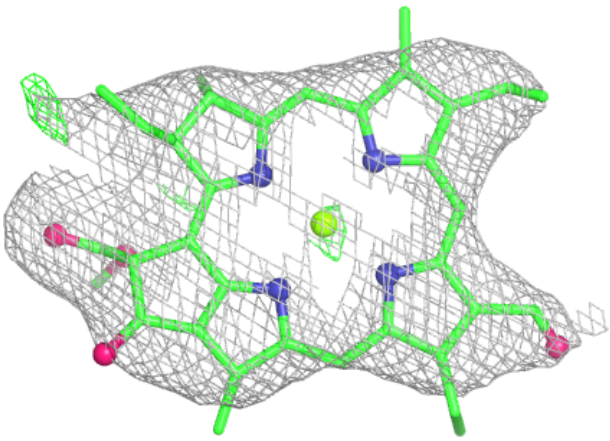


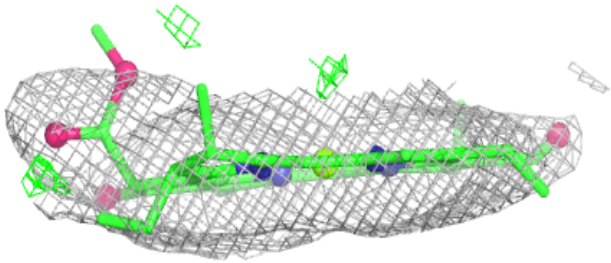


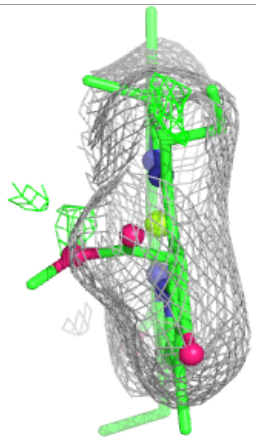


Electron density around CHL 2 304:

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

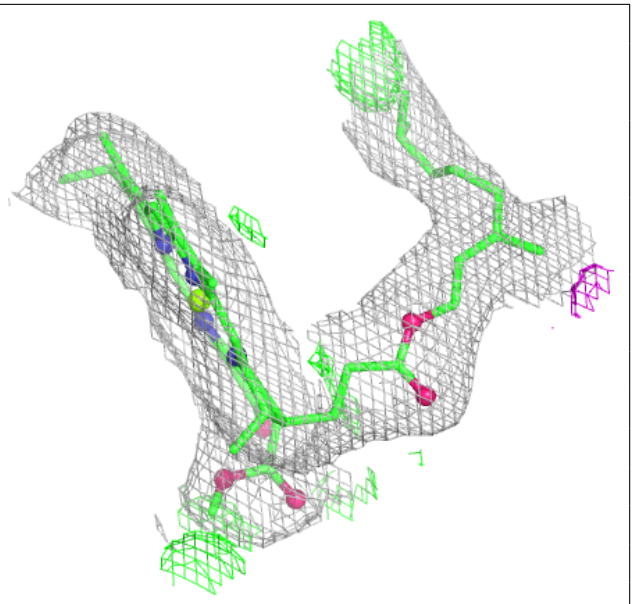


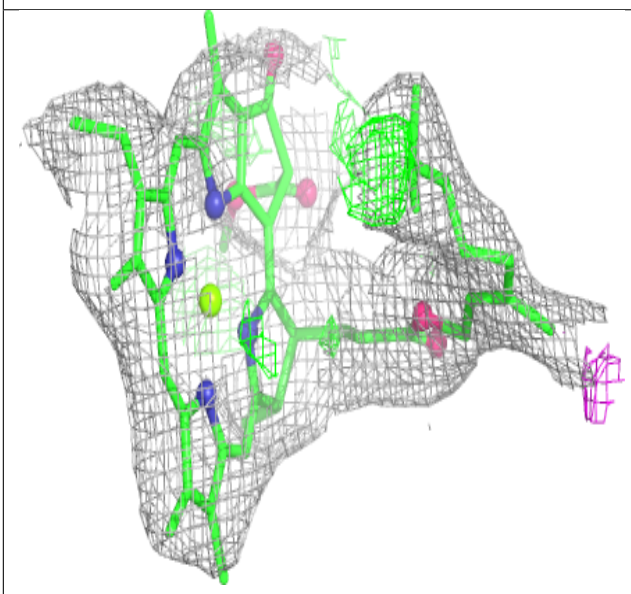


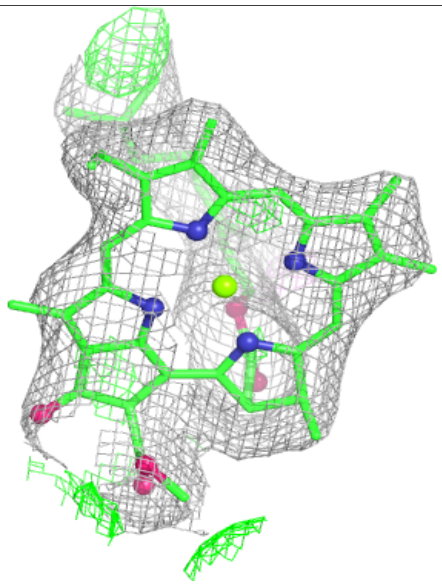


Electron density around CLA B 813:

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

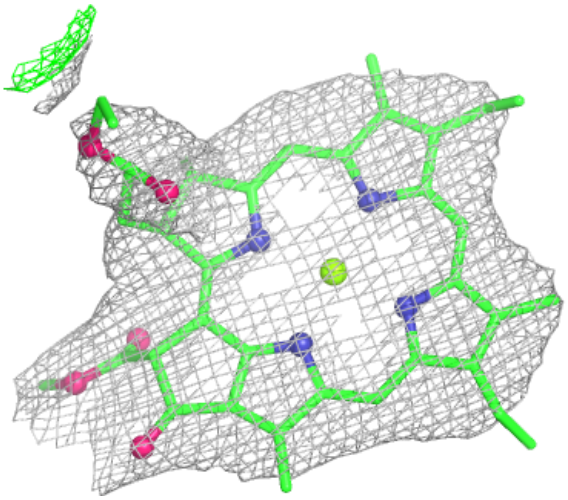


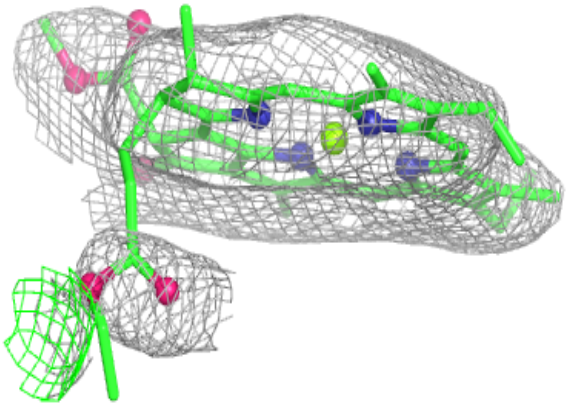


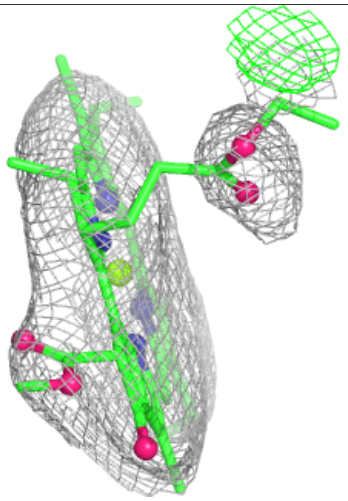


Electron density around CLA 3 606:

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

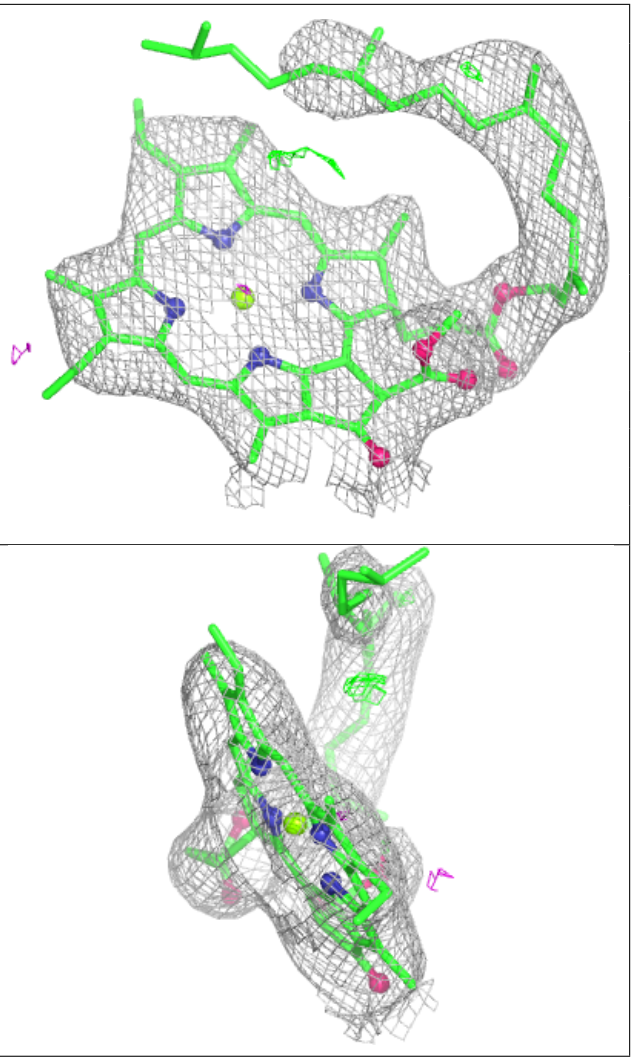






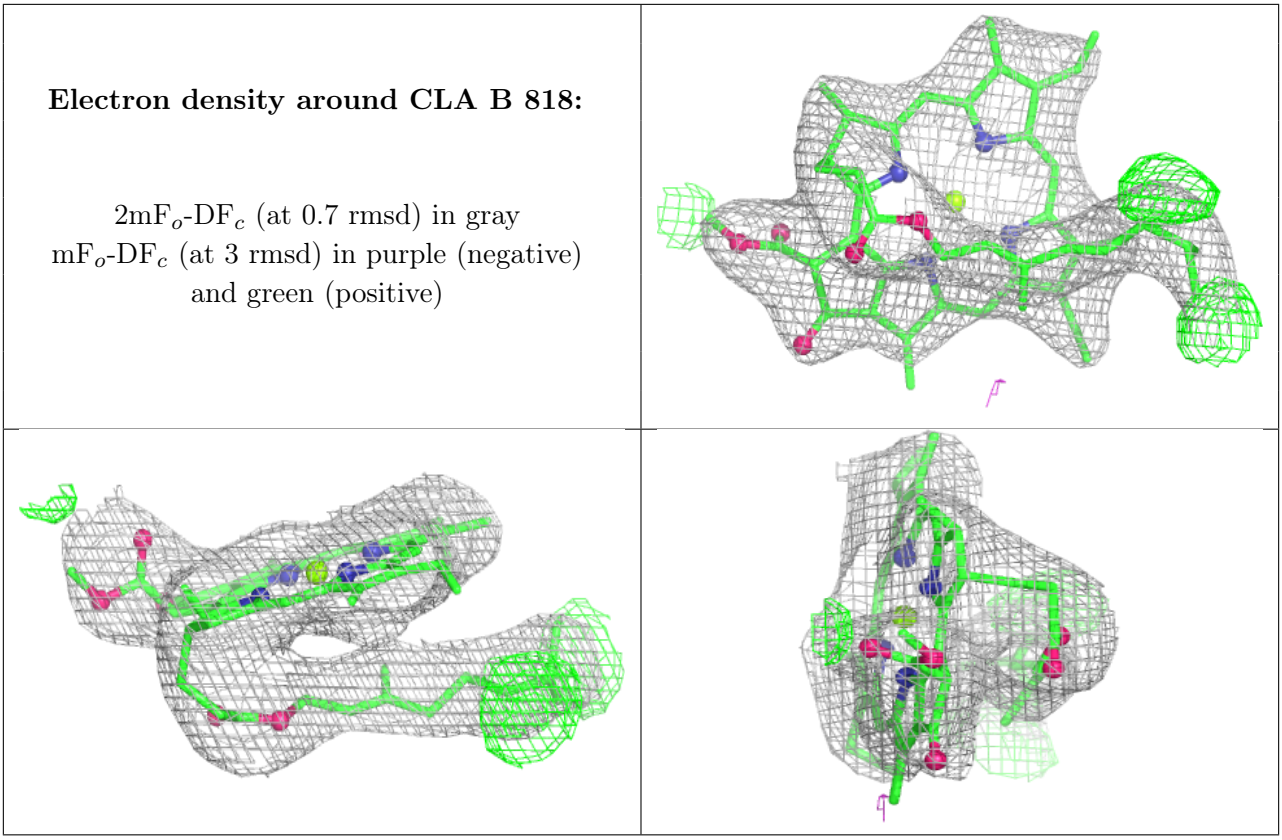
Electron density around CLA 1 302:

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



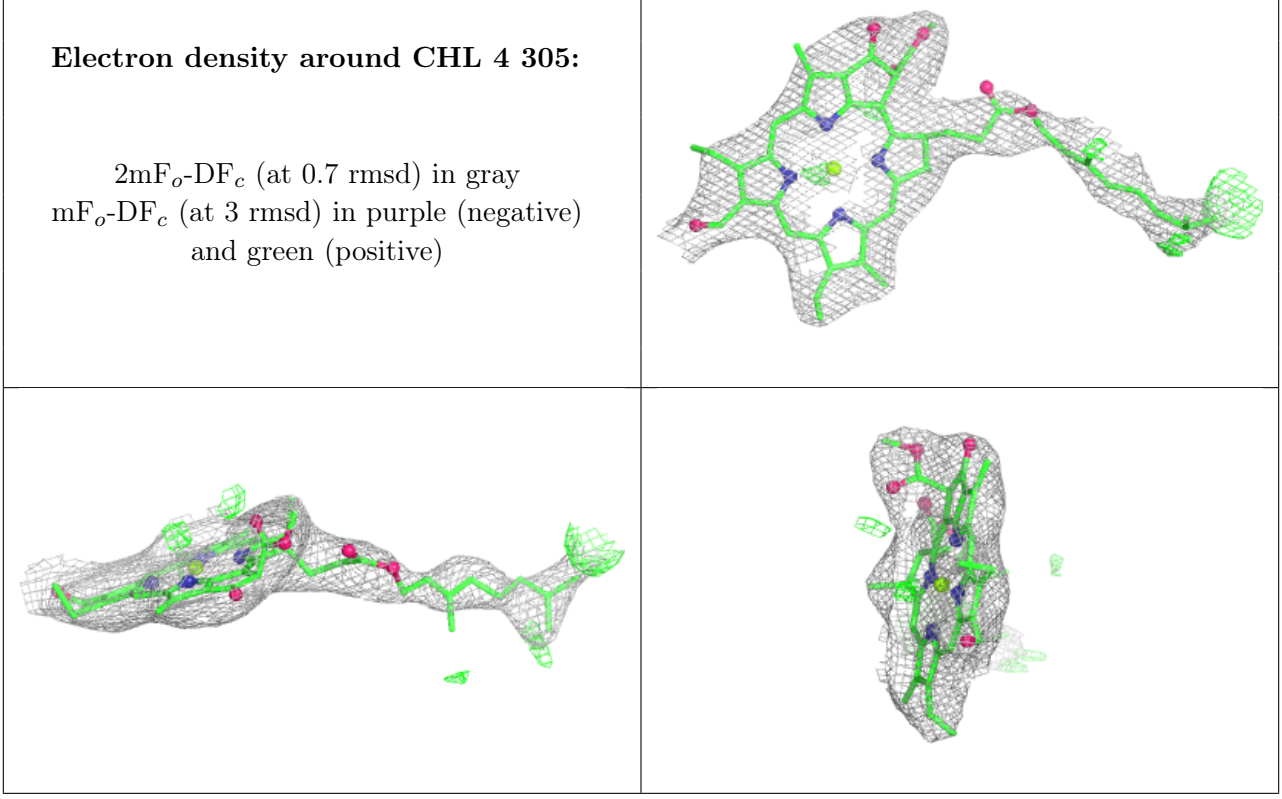
Electron density around CLA B 818:

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



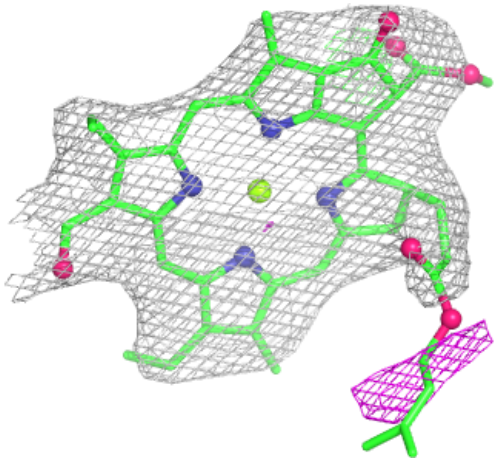
Electron density around CHL 4 305:

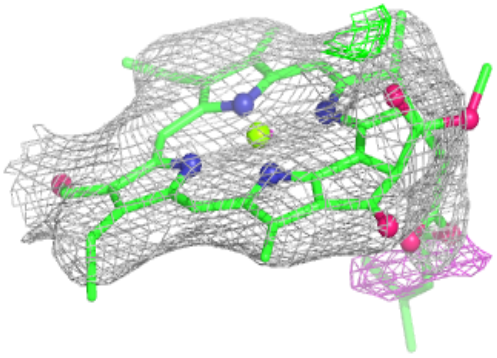
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

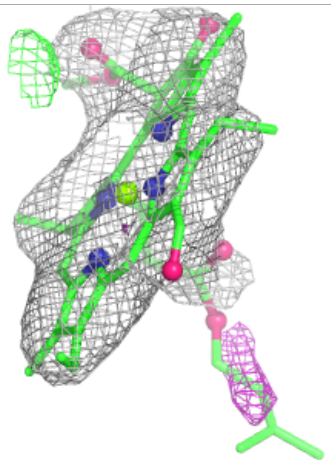


Electron density around CHL 4 306:

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

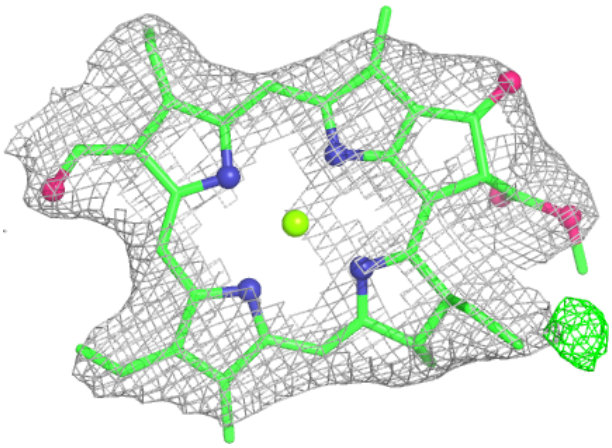


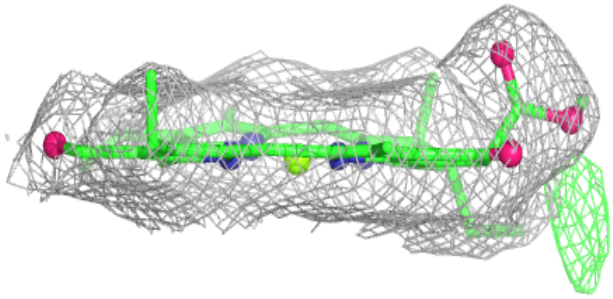


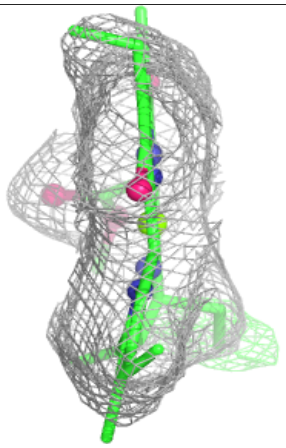


Electron density around CHL 4 315:

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

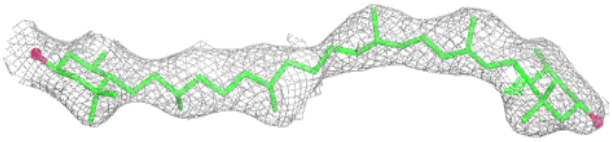


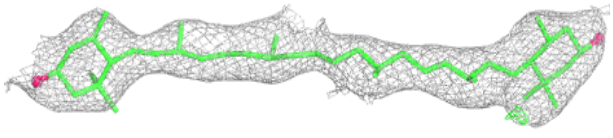


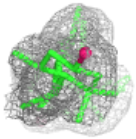


Electron density around LUT 1 314:

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

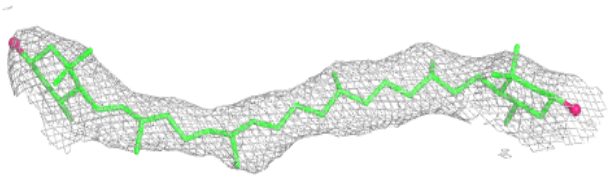


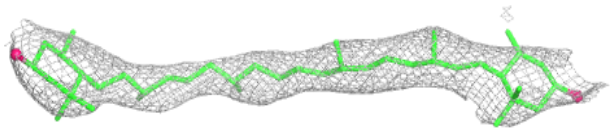


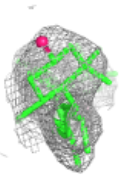


Electron density around LUT 2 314:

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

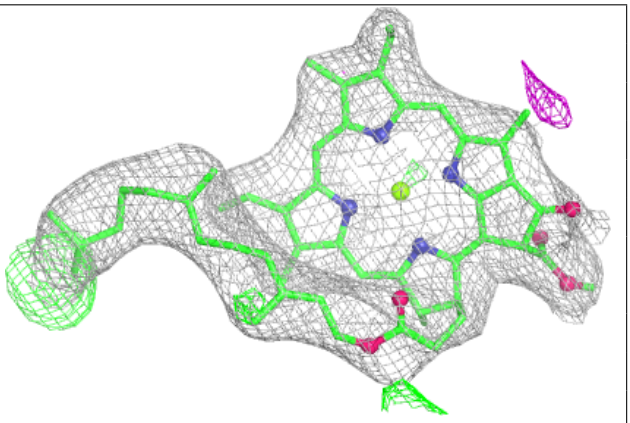


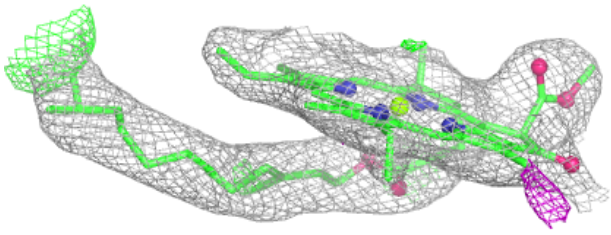


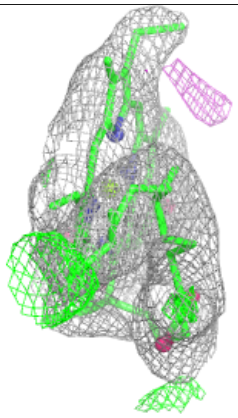


Electron density around CLA B 820:

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

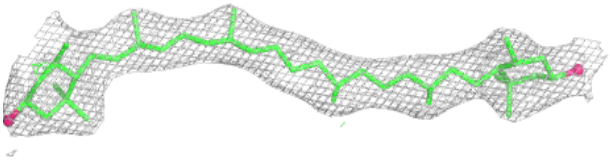


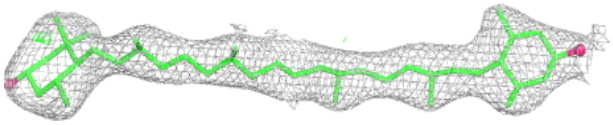


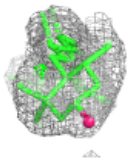


Electron density around LUT 4 316:

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

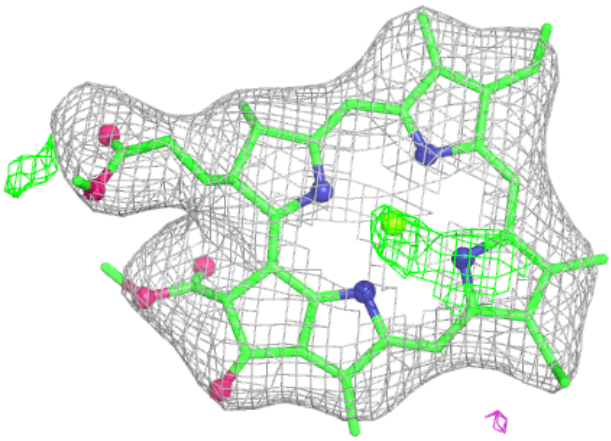


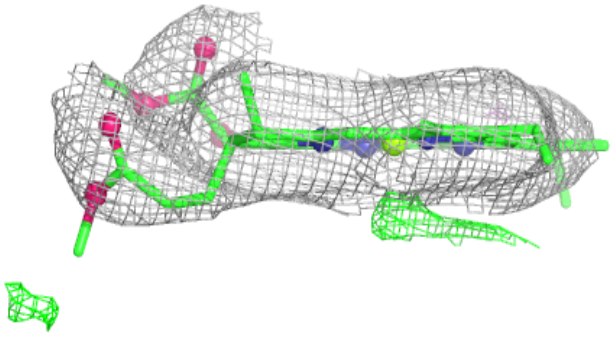


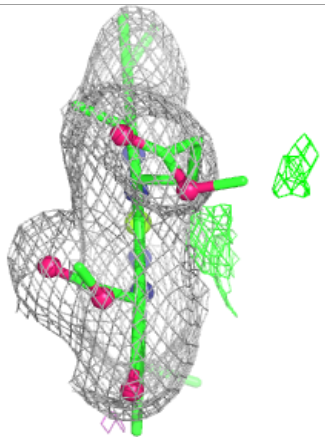


Electron density around CLA 1 313:

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

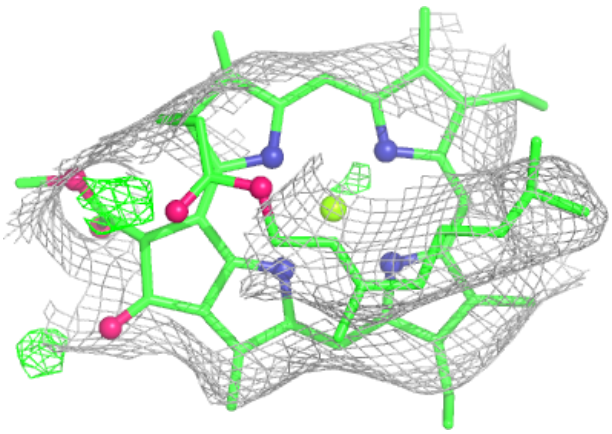


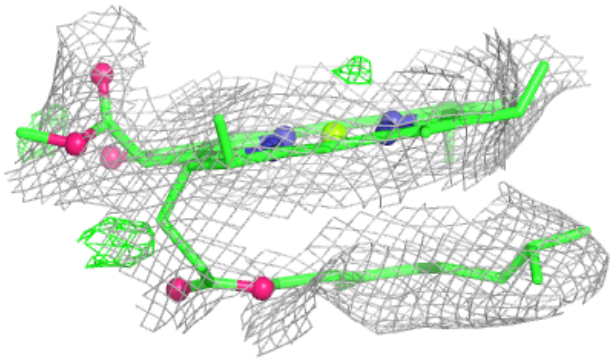


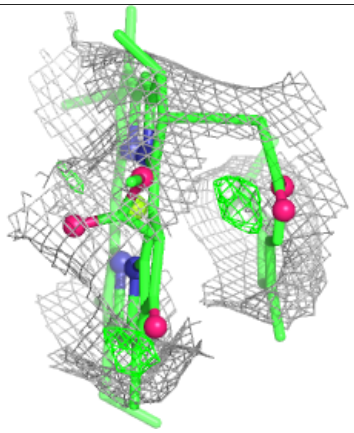


Electron density around CLA 3 611:

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

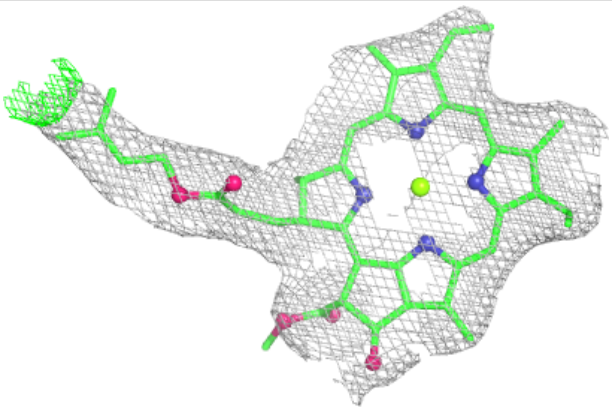


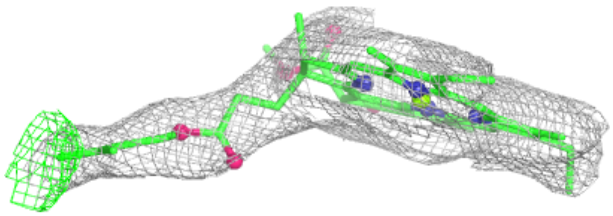


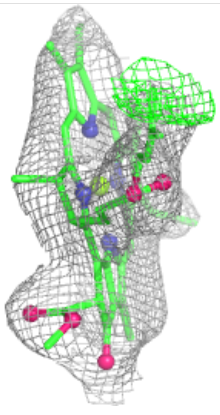


Electron density around CLA G 104:

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

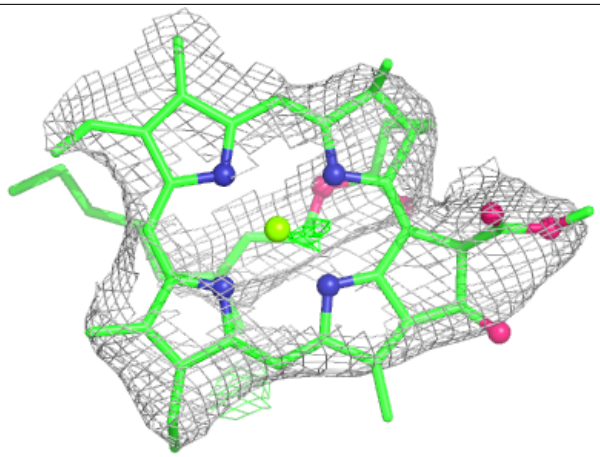


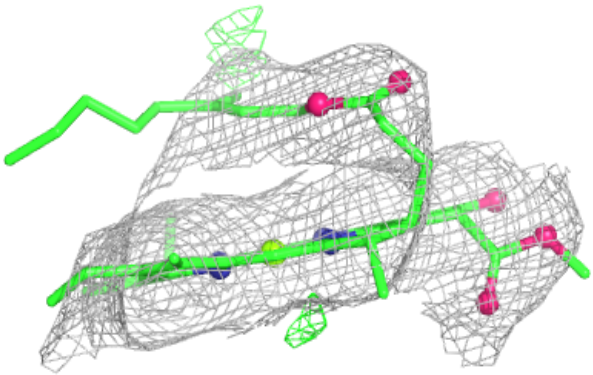


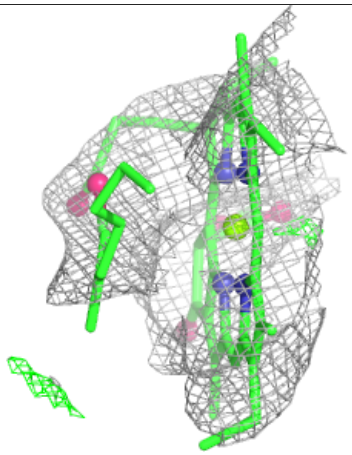


Electron density around CLA A 811:

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

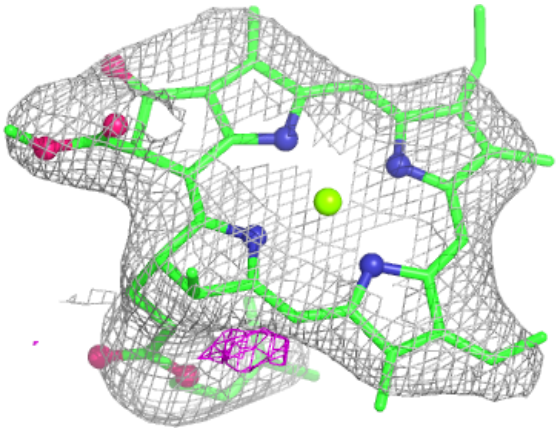


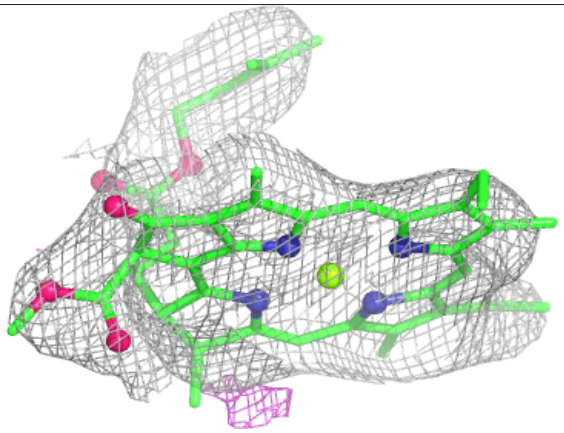


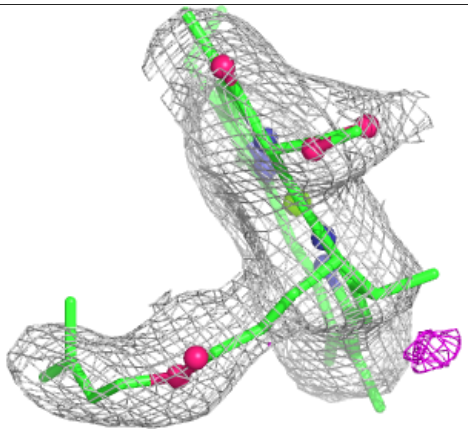


Electron density around CLA 2 307:

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

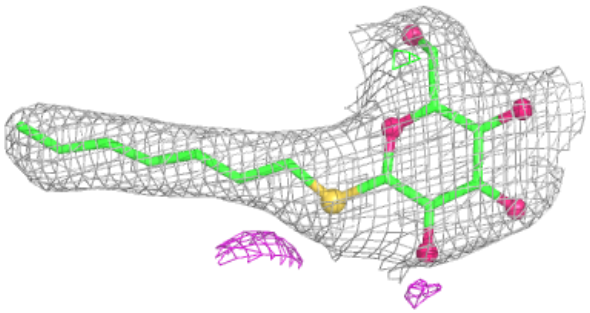


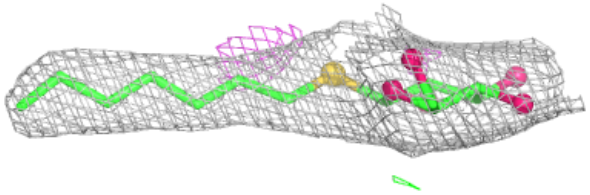


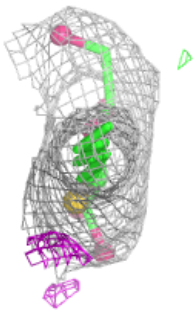


Electron density around HTG A 854:

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

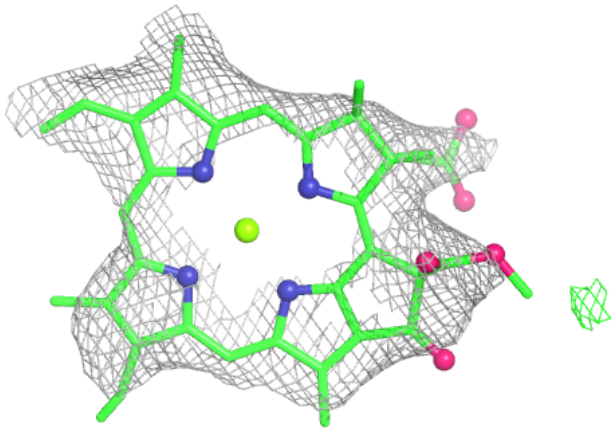


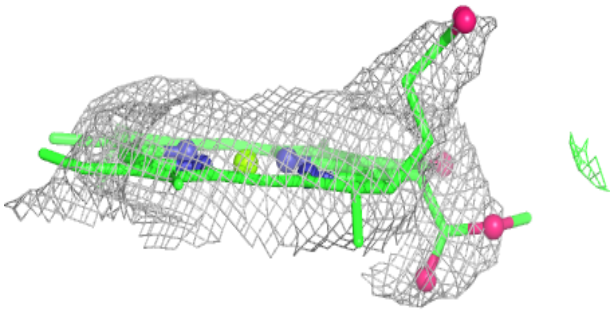


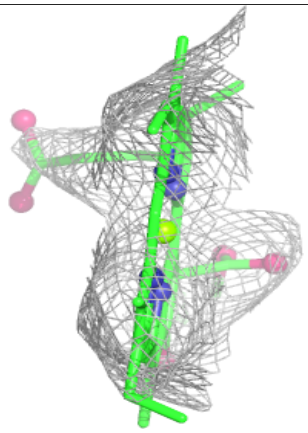


Electron density around CLA A 815:

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

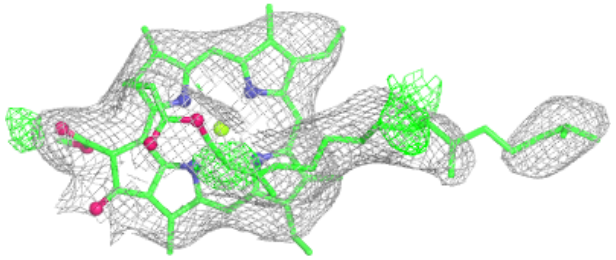


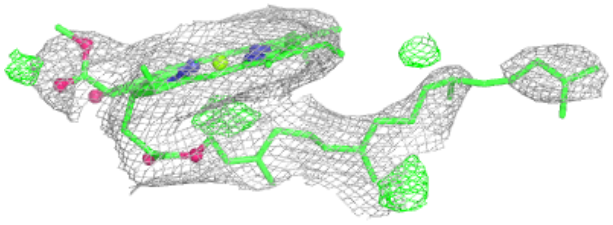


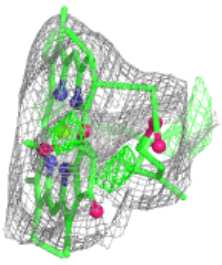


Electron density around CLA A 836:

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

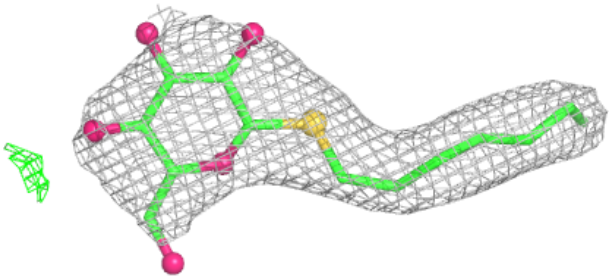


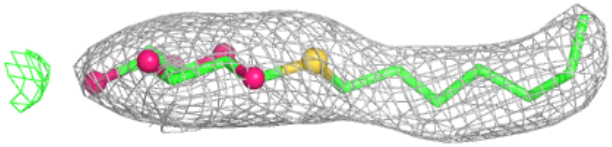


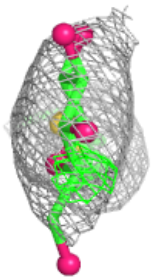


Electron density around HTG F 305:

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

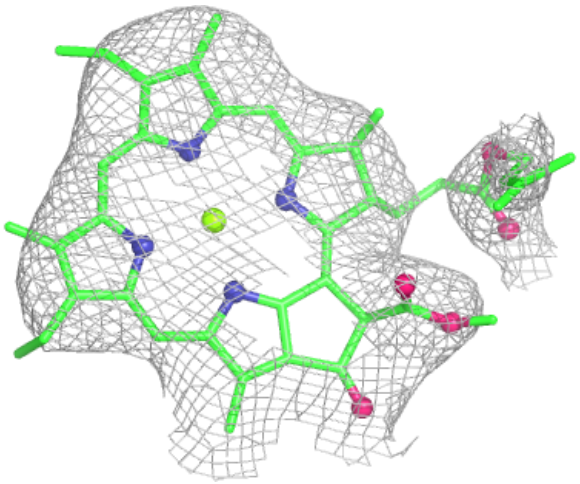


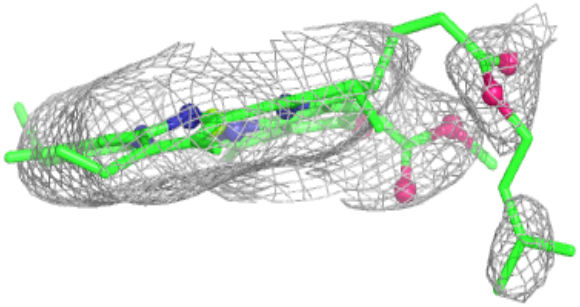


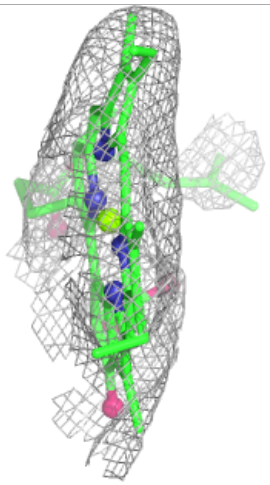


Electron density around CLA 3 603:

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

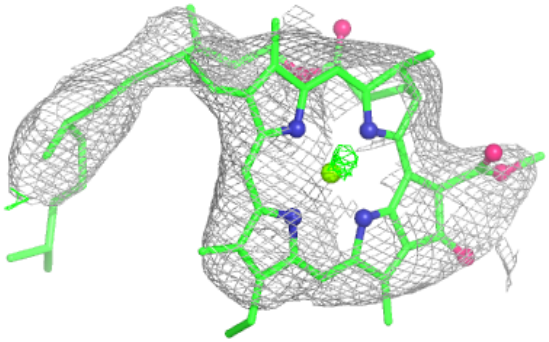


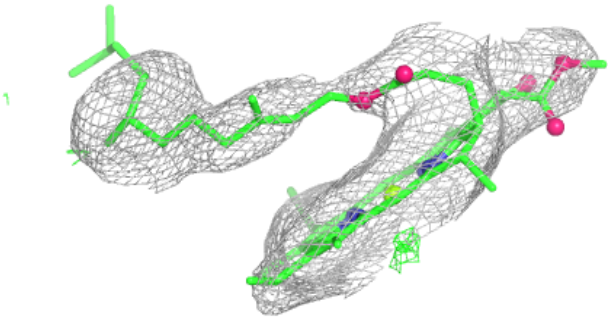


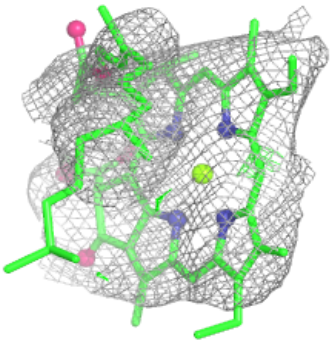


Electron density around CLA 2 308:

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

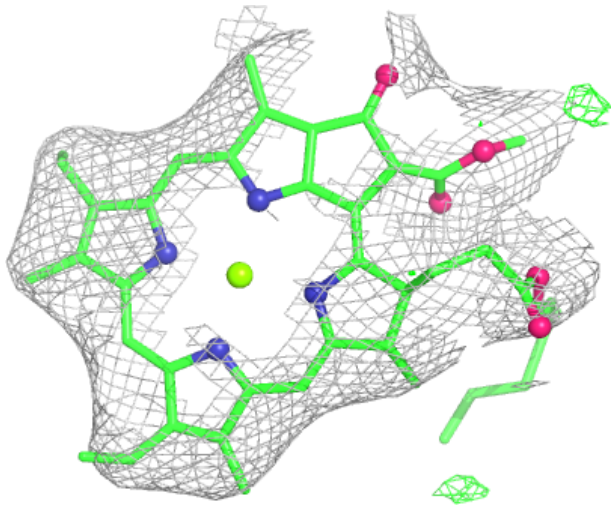


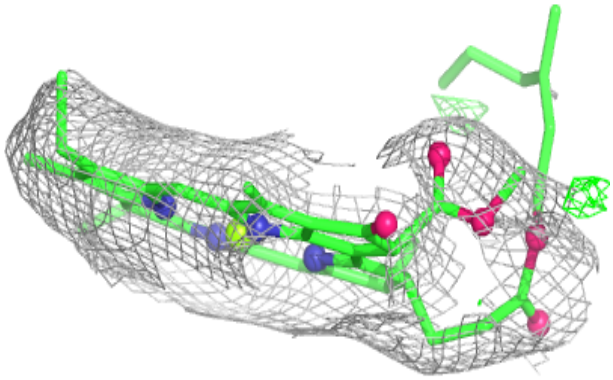


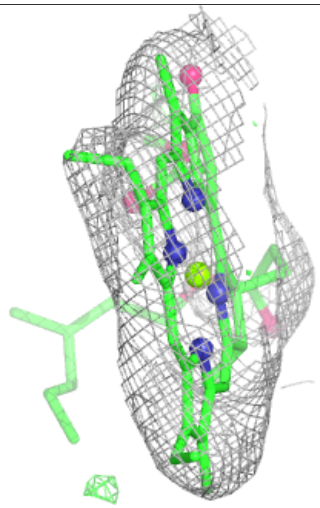


Electron density around CLA 1 310:

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

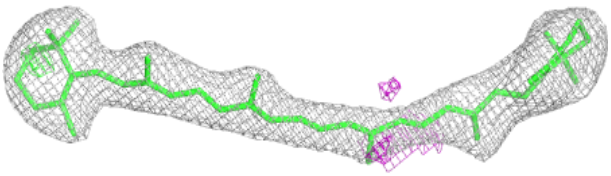


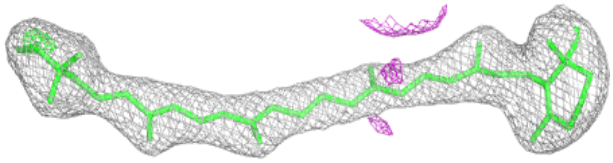


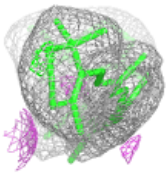


Electron density around BCR F 303:

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

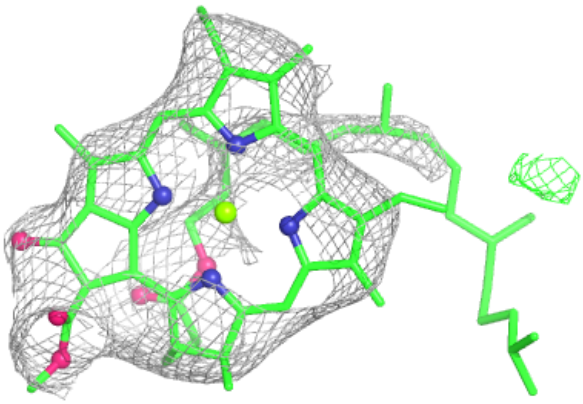


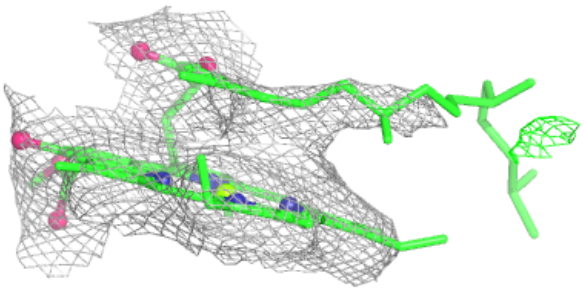


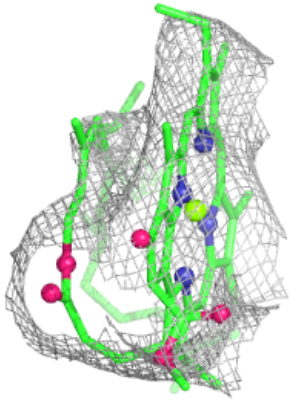


Electron density around CLA 2 311:

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

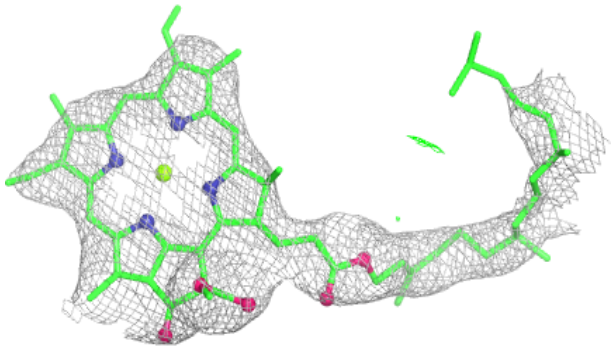


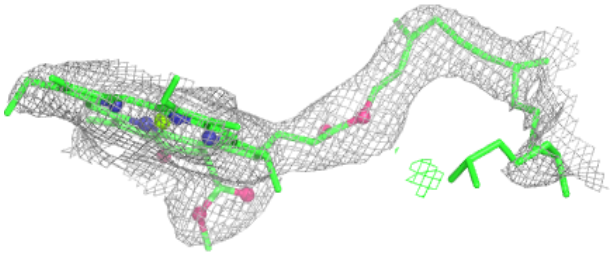


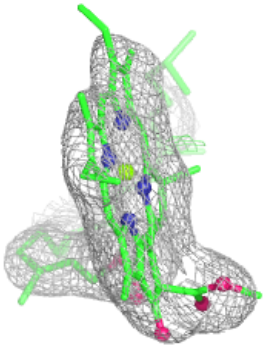


Electron density around CLA A 826:

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

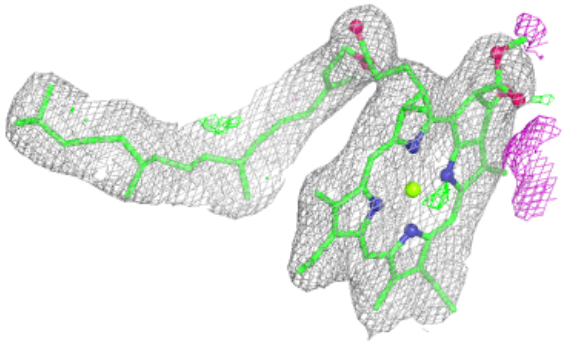


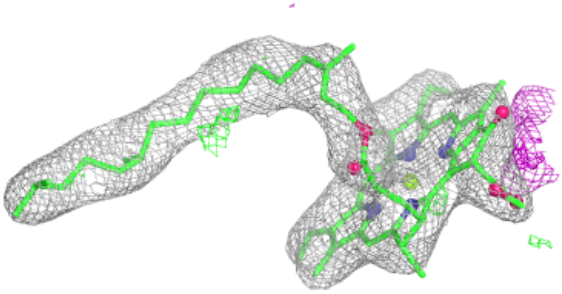


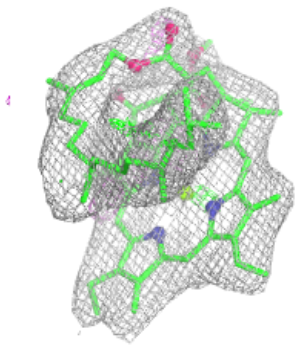


Electron density around CLA B 816:

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

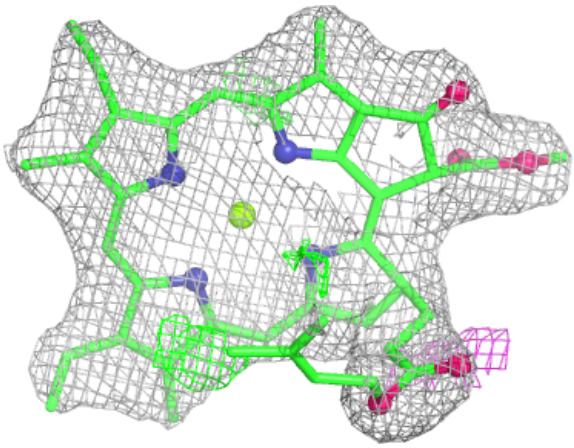


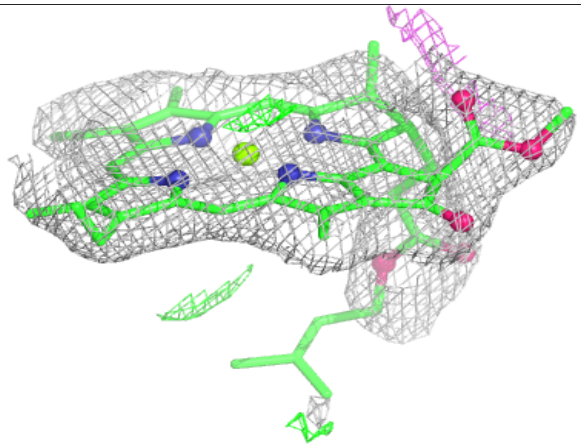


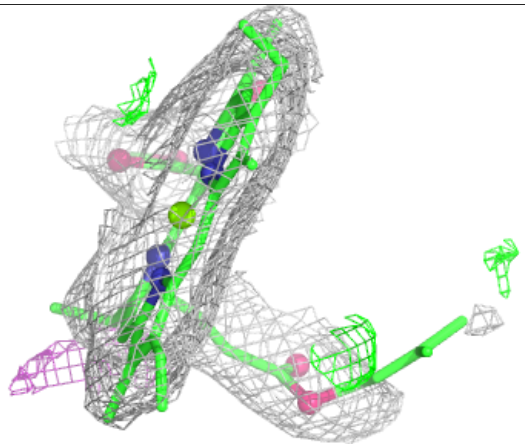


Electron density around CLA 4 308:

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

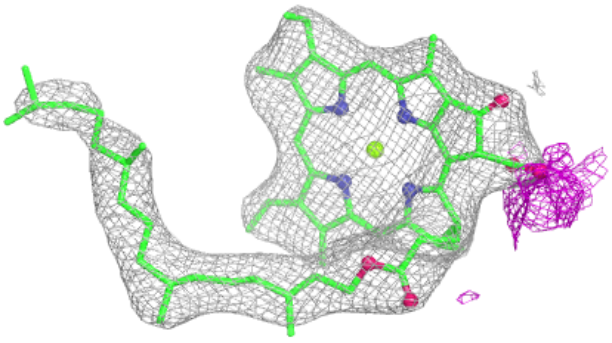


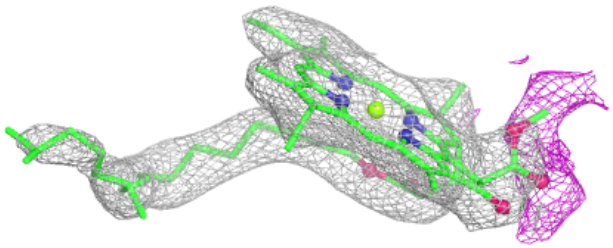


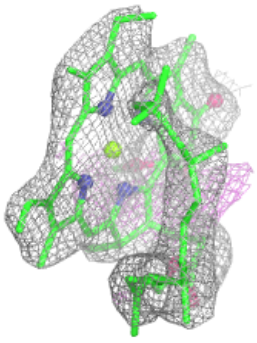


Electron density around CLA 1 301:

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

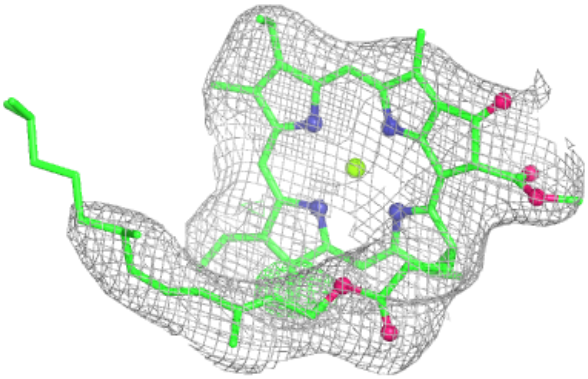


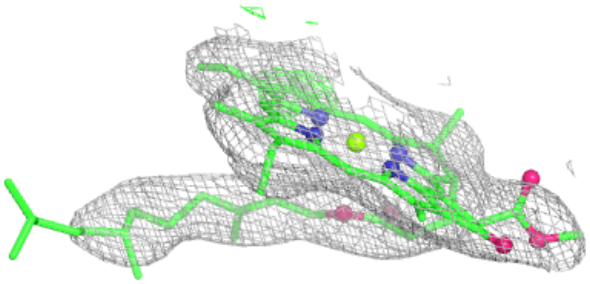




Electron density around CLA 1 308:

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

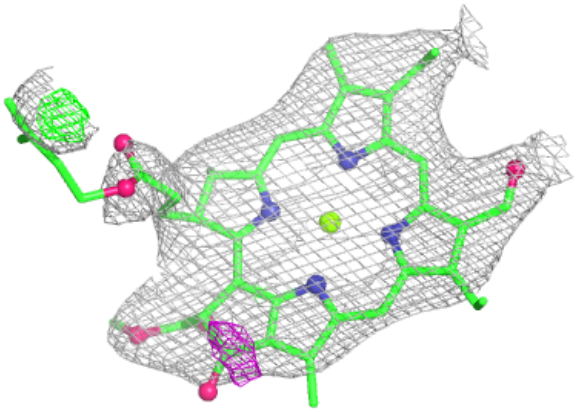


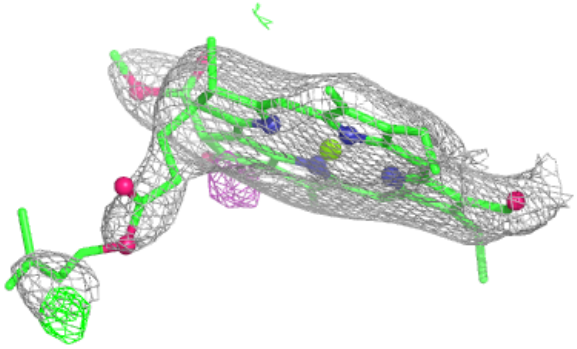


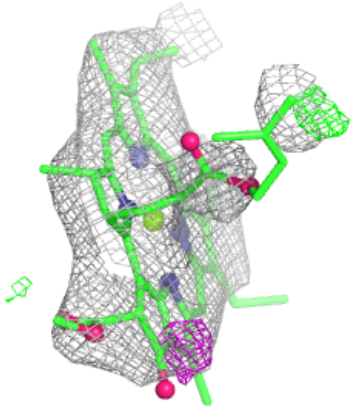


Electron density around CHL 2 306:

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

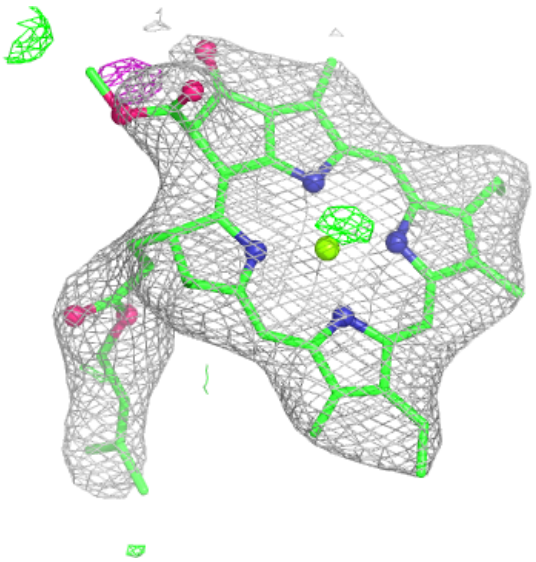


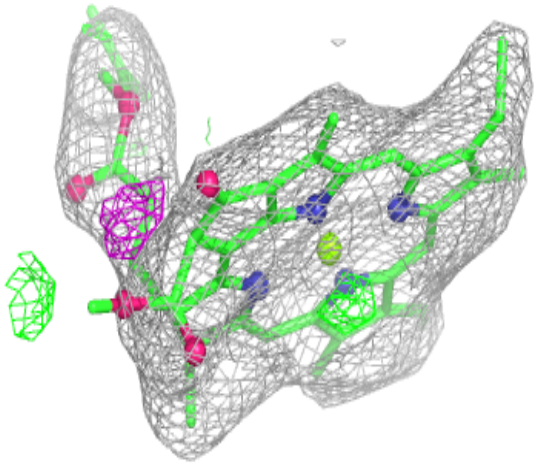


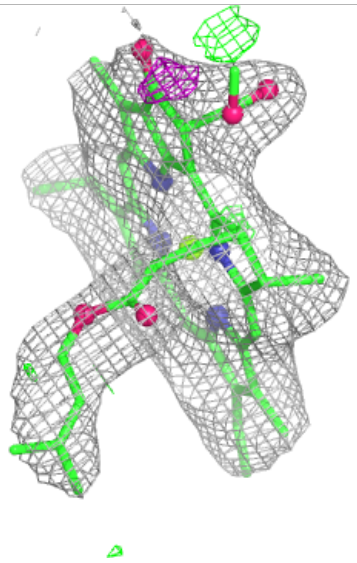


Electron density around CLA B 822:

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

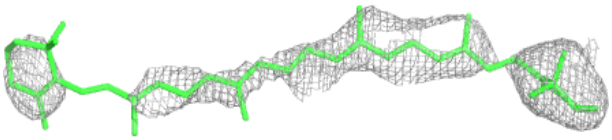


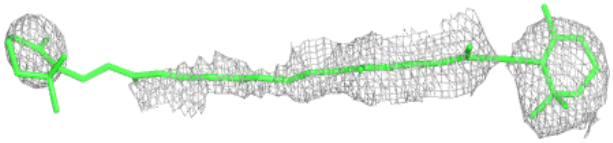


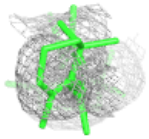


Electron density around BCR A 847:

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

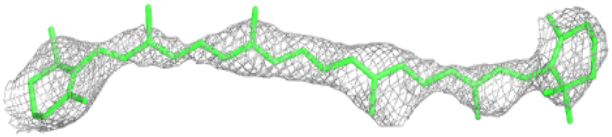


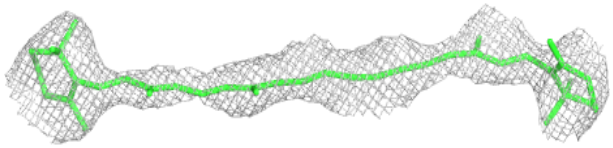


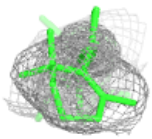


Electron density around BCR A 848:

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

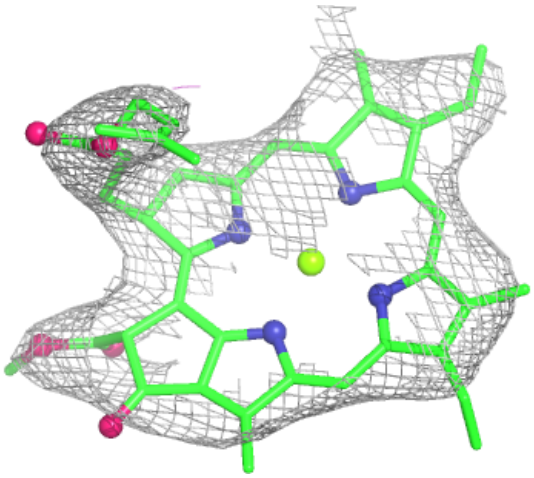


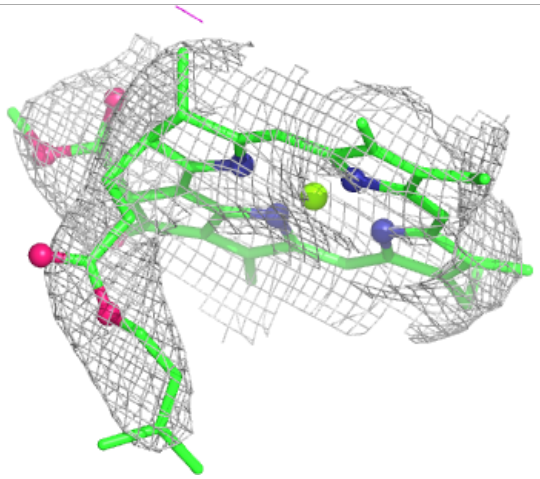


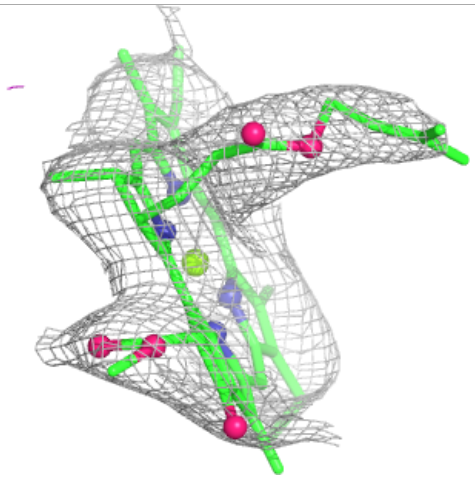


Electron density around CLA 3 608:

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

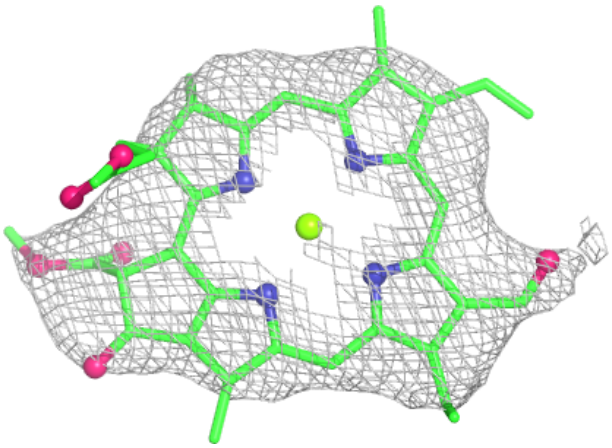


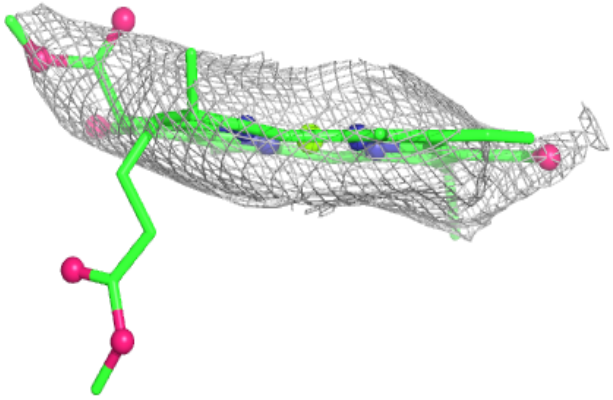


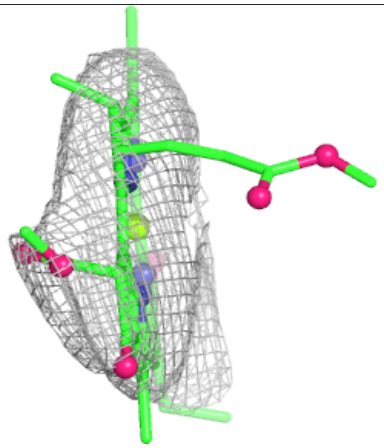


Electron density around CHL 3 607:

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

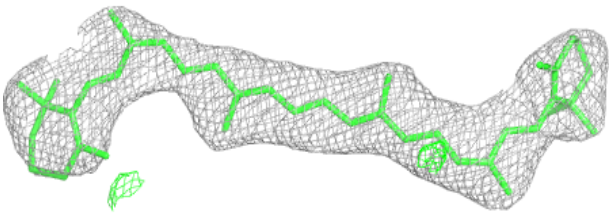


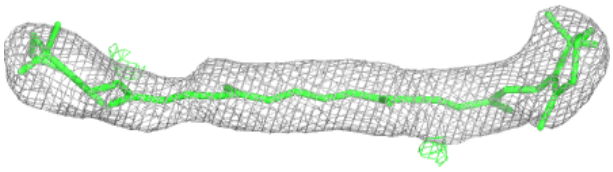


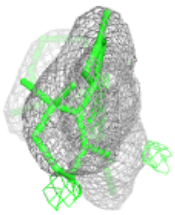


Electron density around BCR B 846:

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

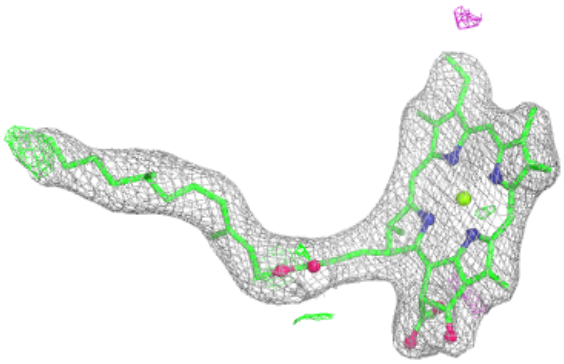


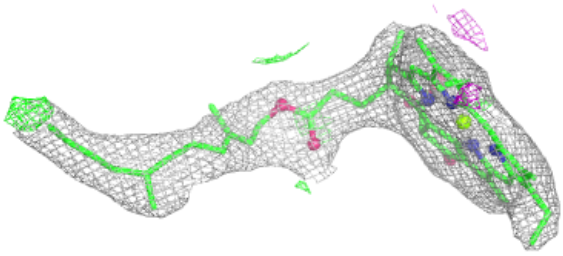


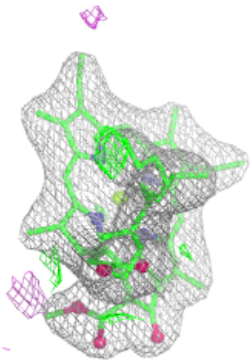


Electron density around CLA B 834:

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

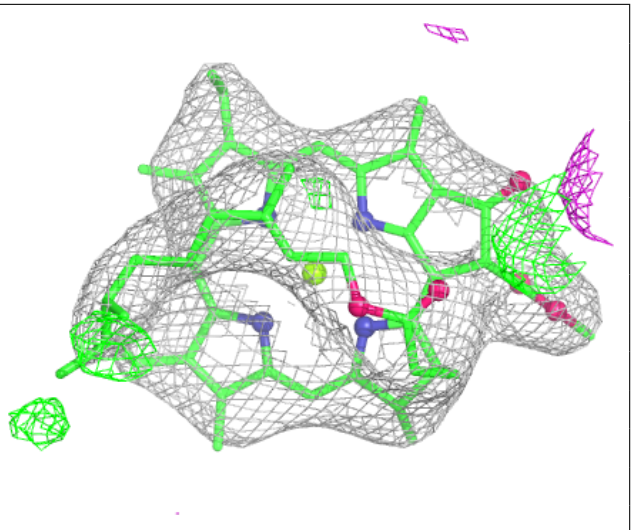


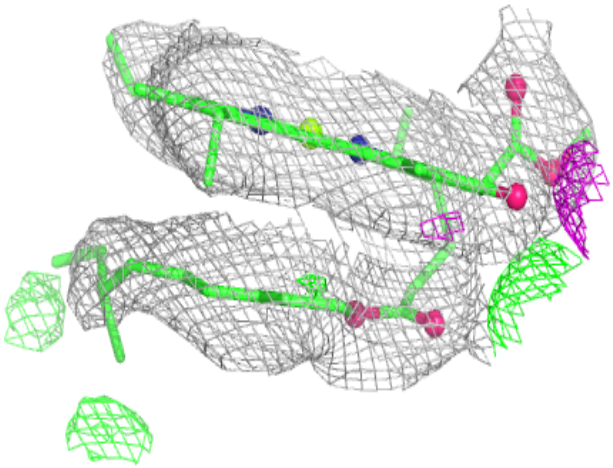


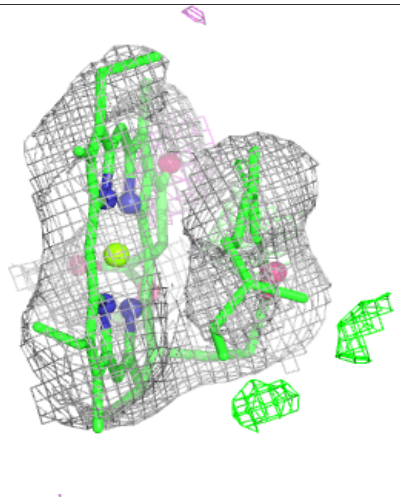


Electron density around CLA 4 312:

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

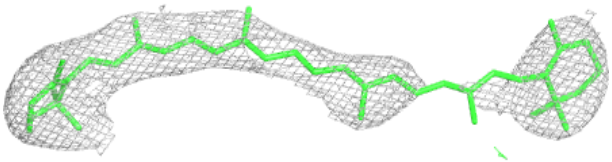


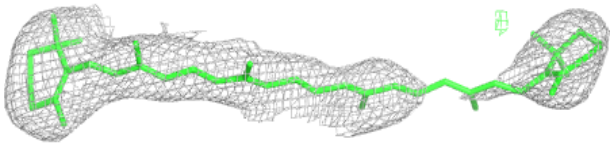


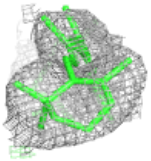


Electron density around BCR G 106:

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

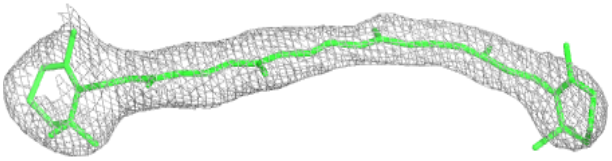


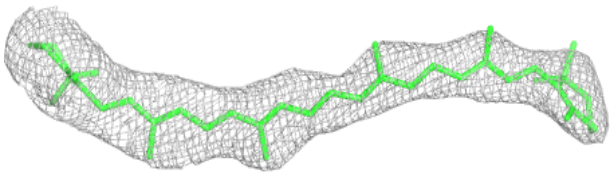


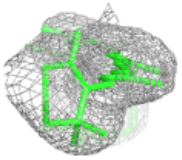


Electron density around BCR I 101:

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

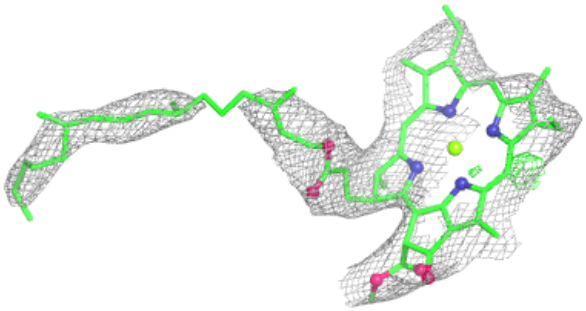


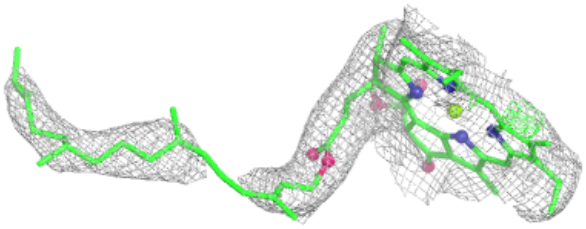


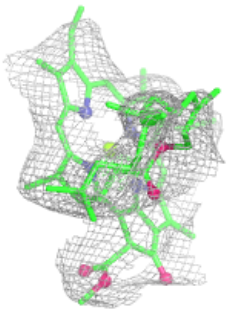


Electron density around CLA A 820:

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

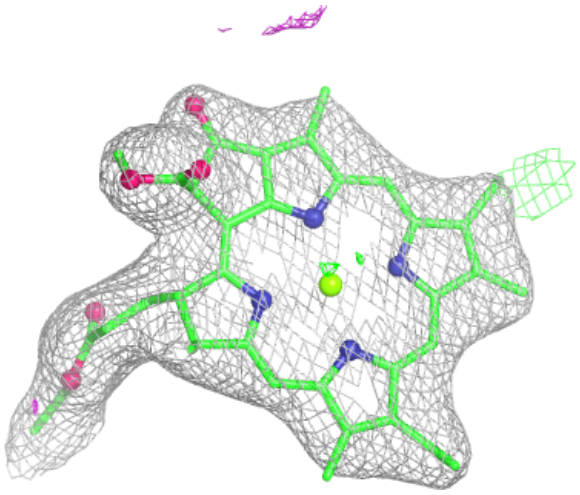


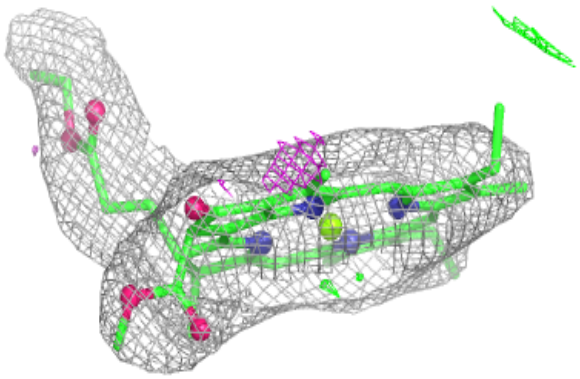


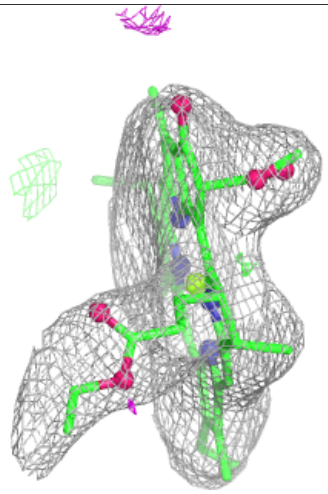


Electron density around CLA 4 314:

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

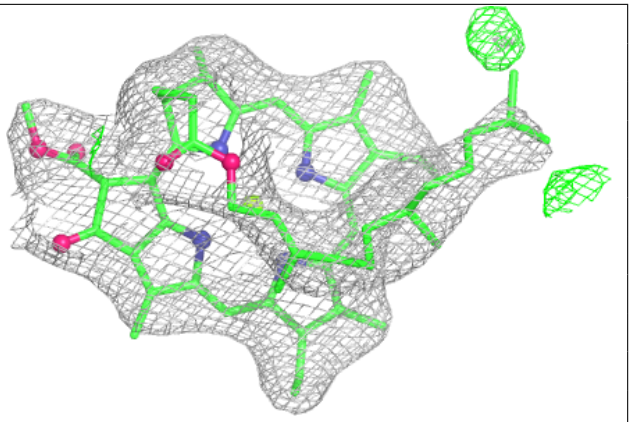


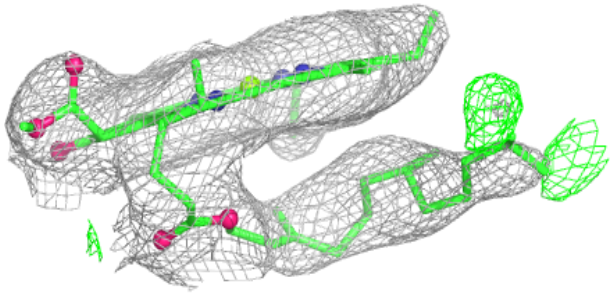


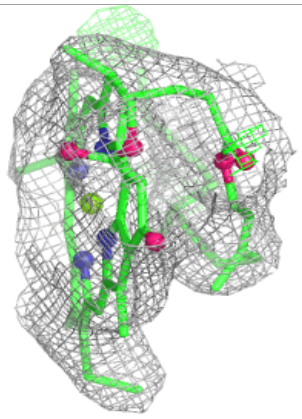


Electron density around CLA 1 311:

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

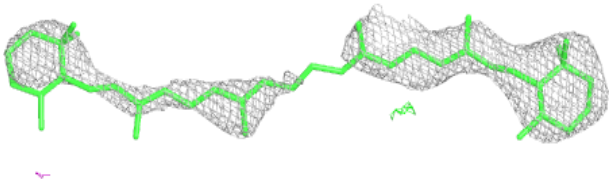


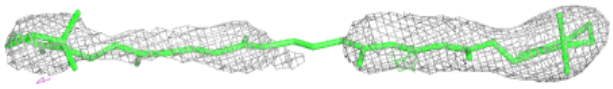


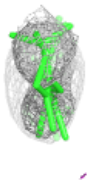


Electron density around BCR L 205:

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

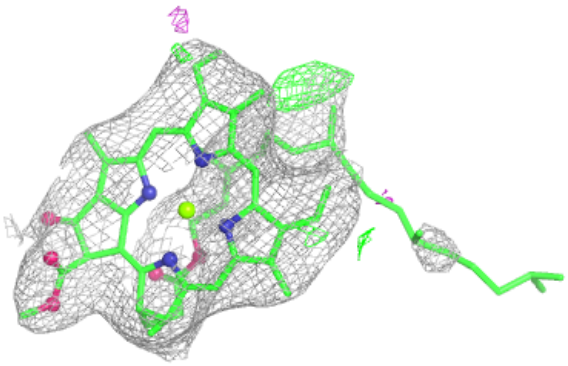


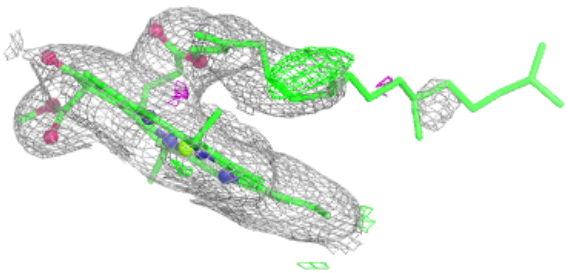


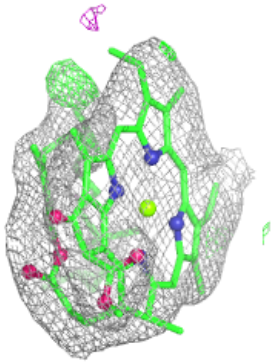


Electron density around CLA B 809:

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

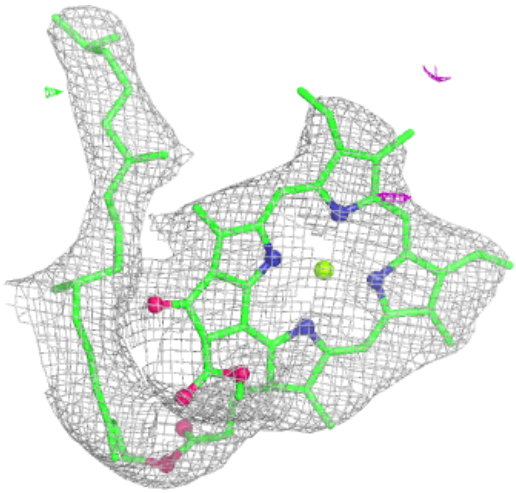


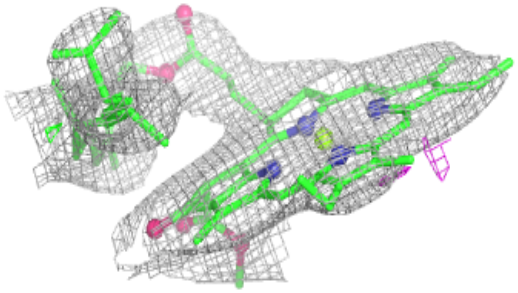


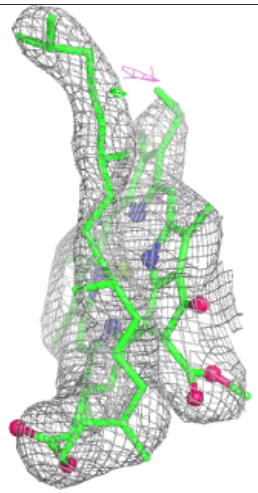


Electron density around CLA A 824:

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

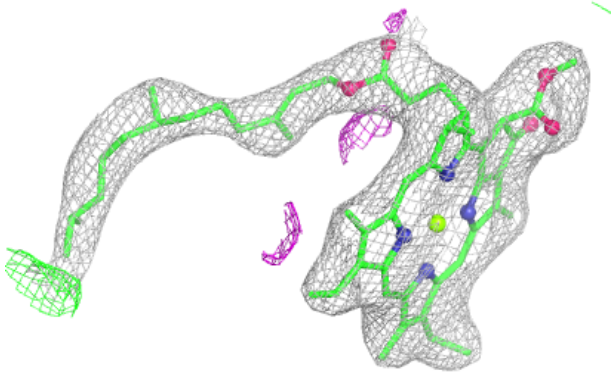


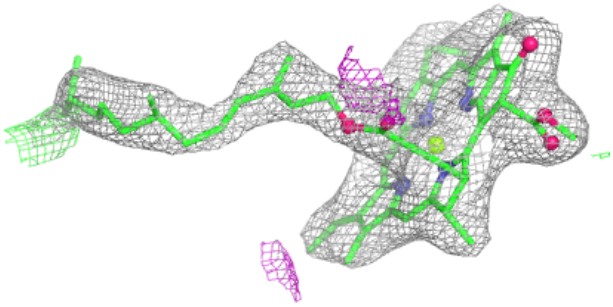


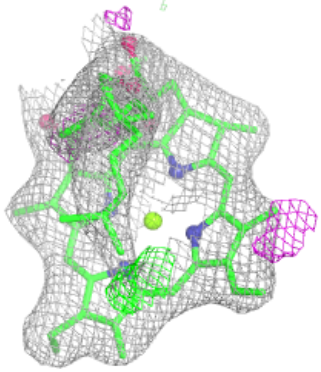


Electron density around CLA B 833:

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

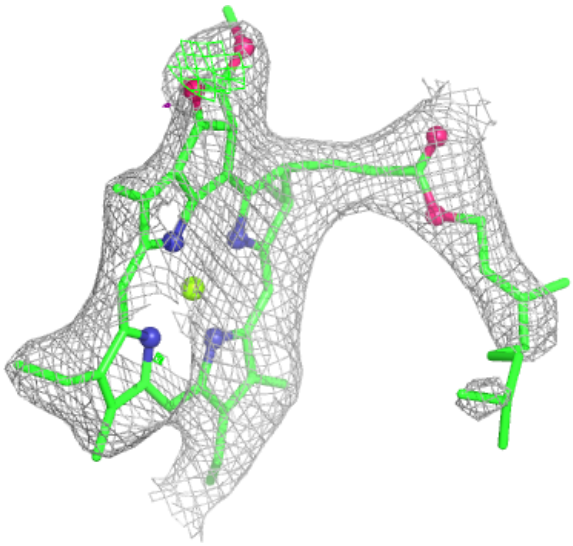


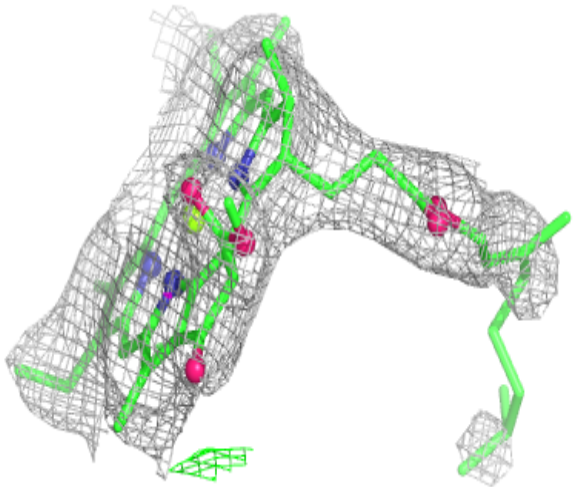


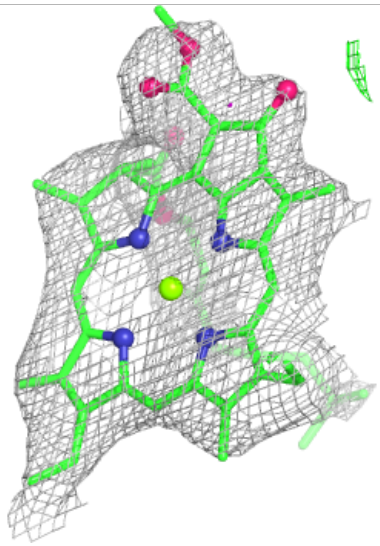


Electron density around CLA A 803:

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

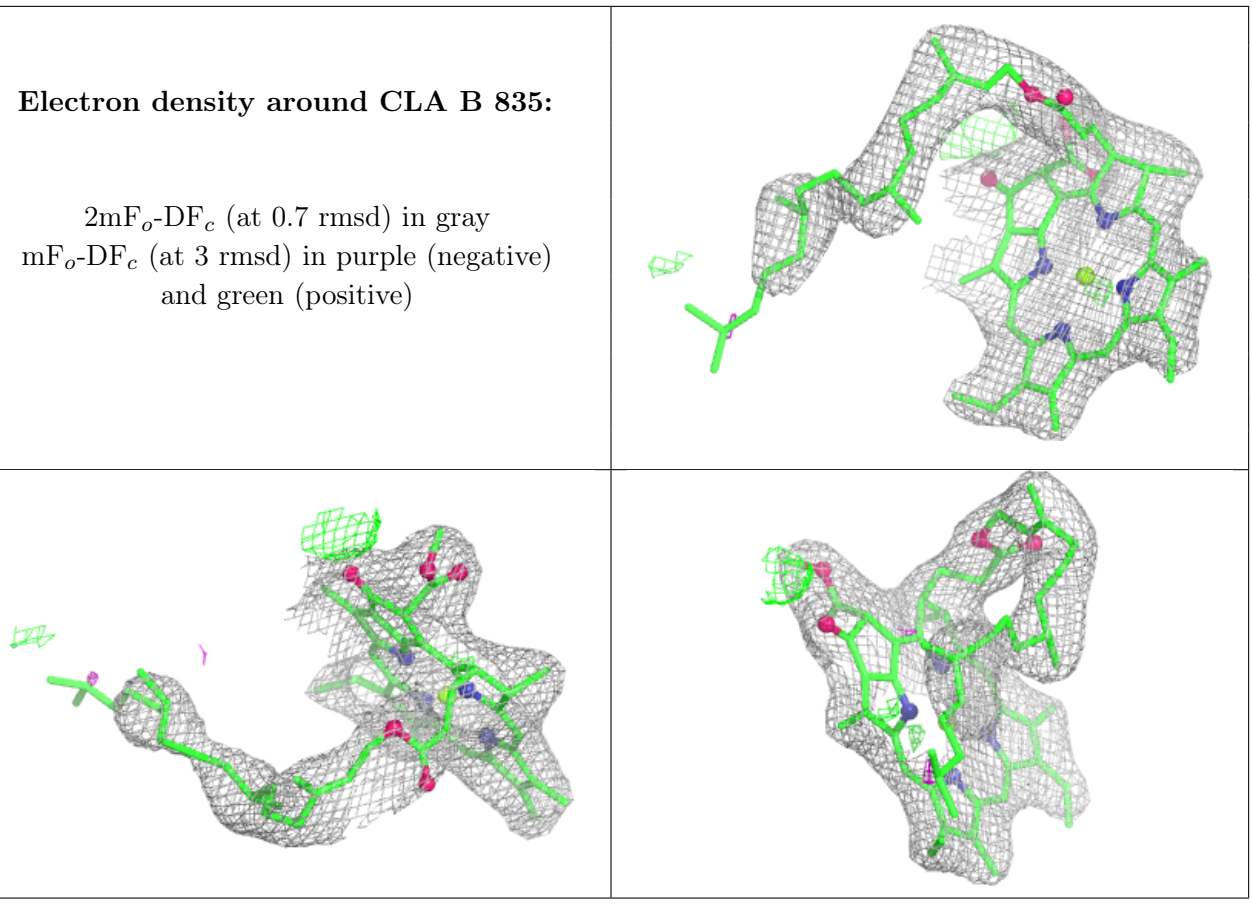






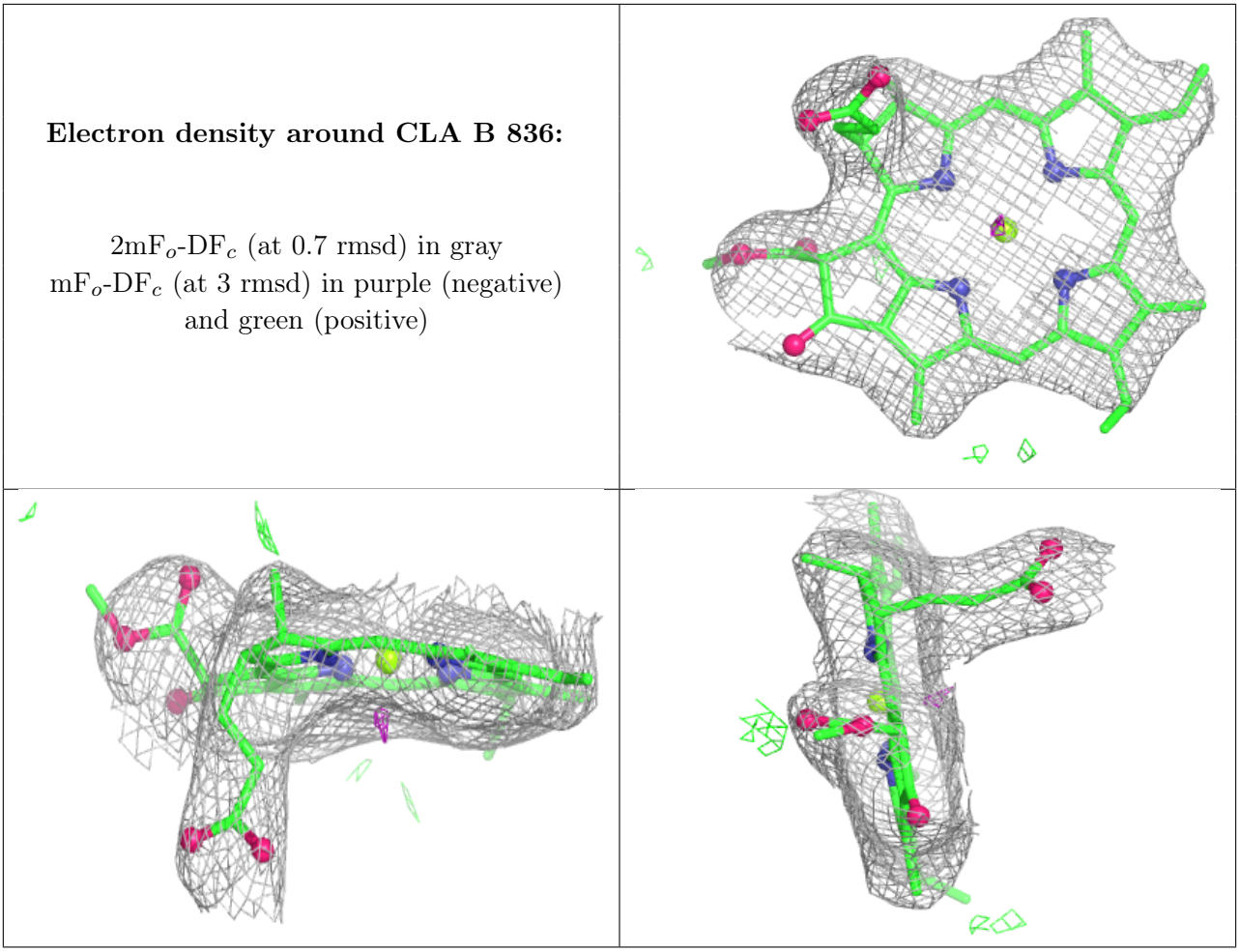
Electron density around CLA B 835:

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



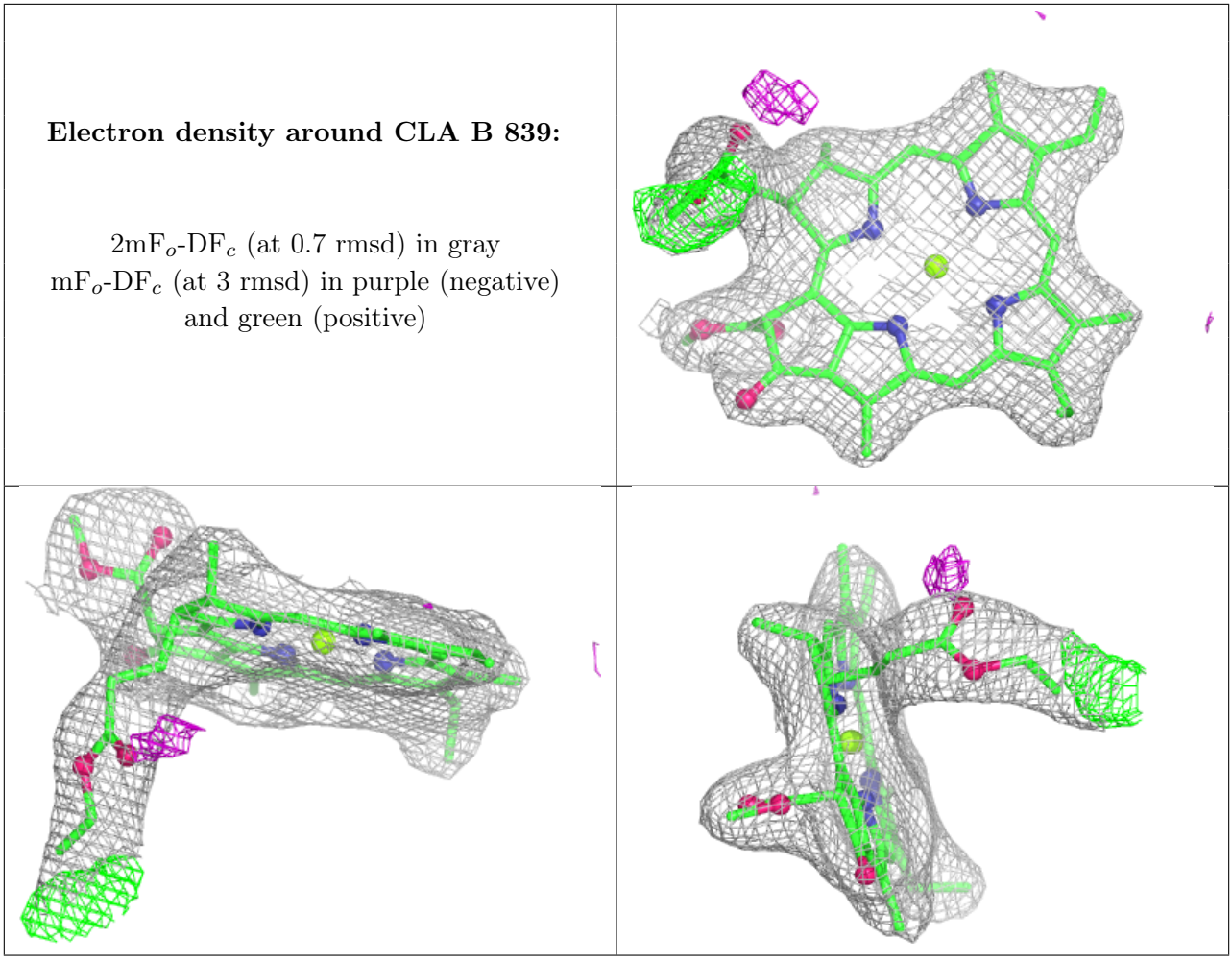
Electron density around CLA B 836:

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



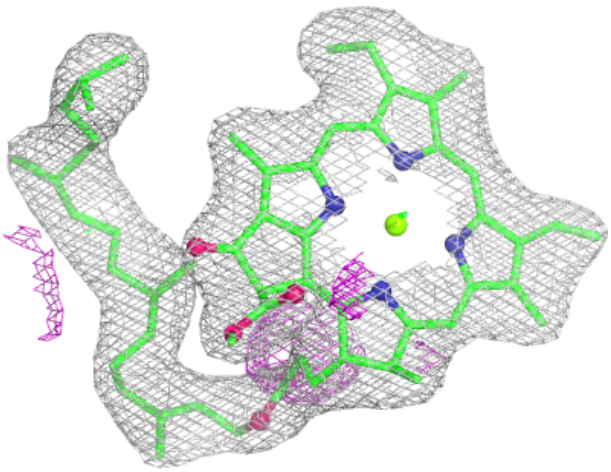
Electron density around CLA B 839:

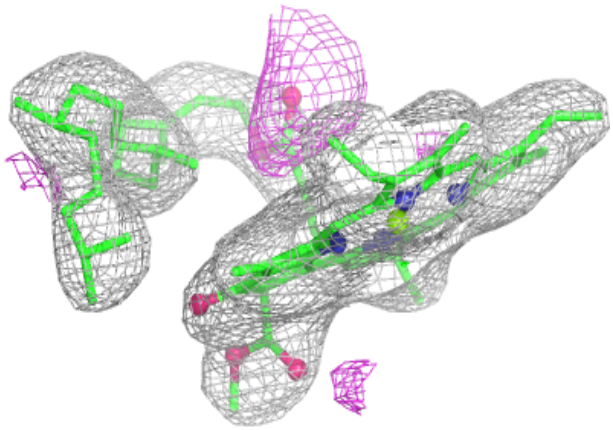
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

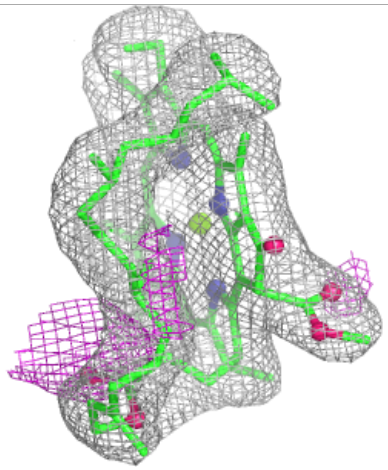


Electron density around CLA F 304:

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

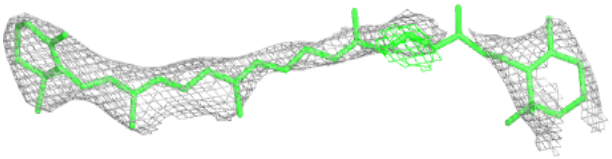


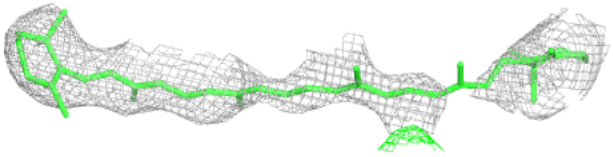


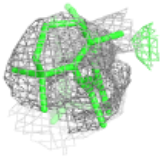


Electron density around BCR A 850:

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

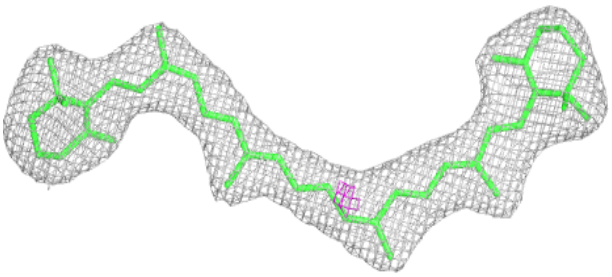


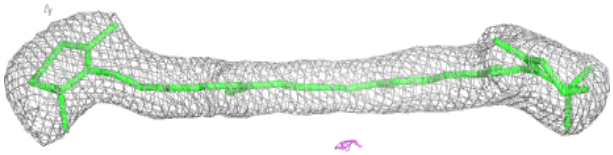


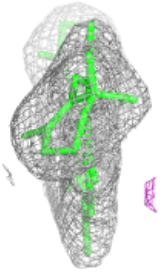


Electron density around BCR A 851:

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

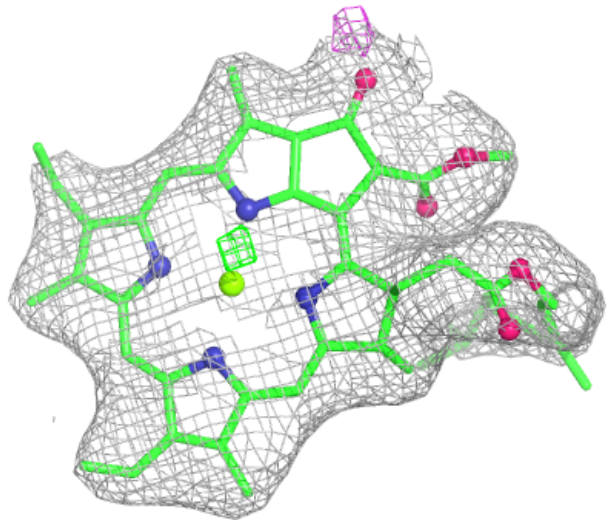


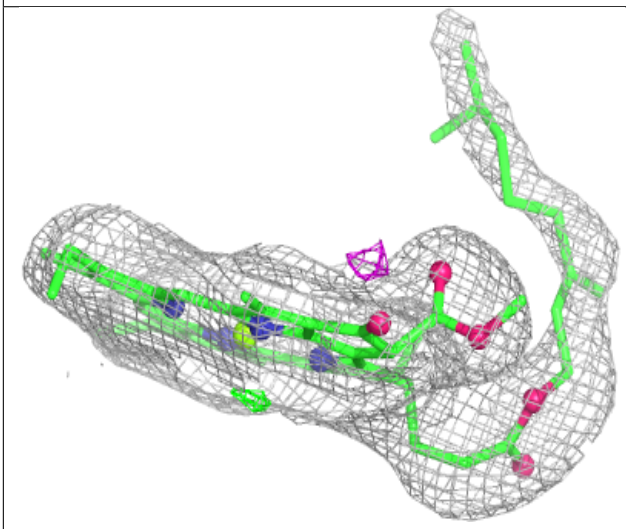


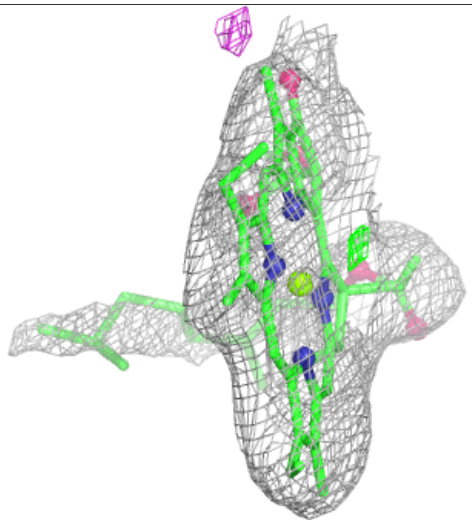


Electron density around CLA F 307:

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

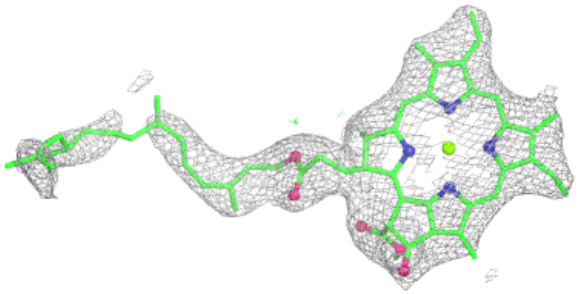


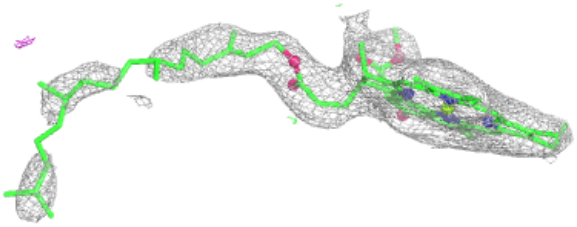


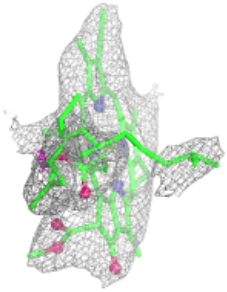


Electron density around CLA A 804:

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

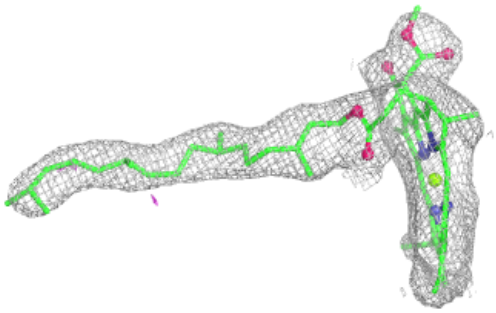


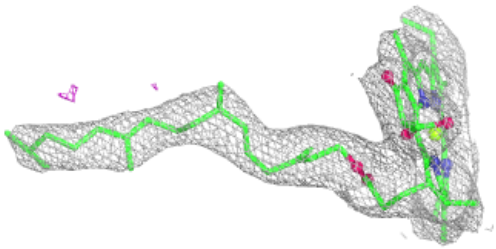


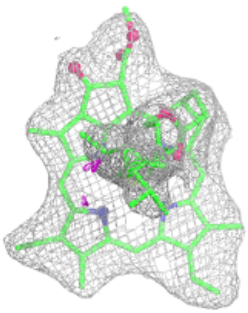


Electron density around CLA A 827:

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

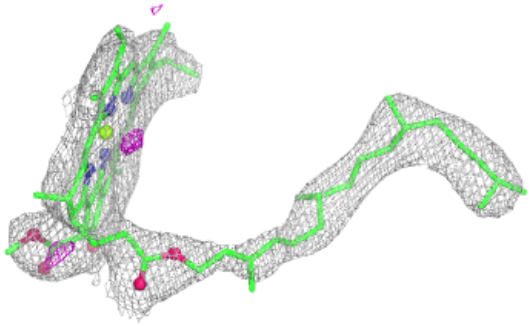


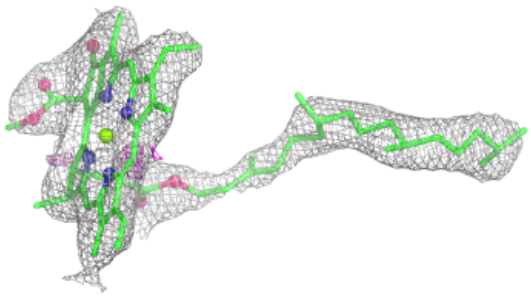


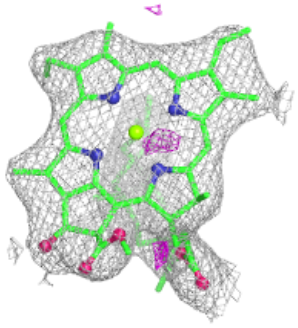


Electron density around CLA A 829:

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

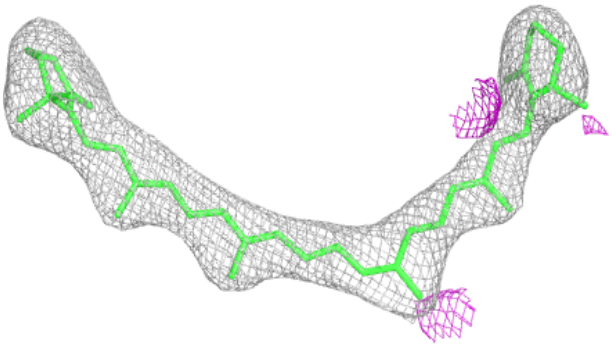


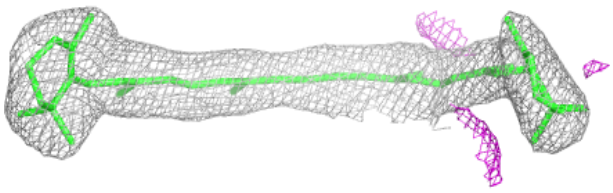


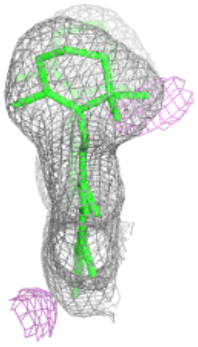


Electron density around BCR F 308:

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

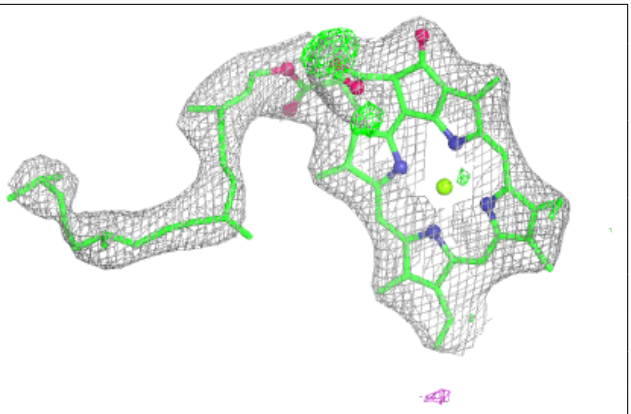


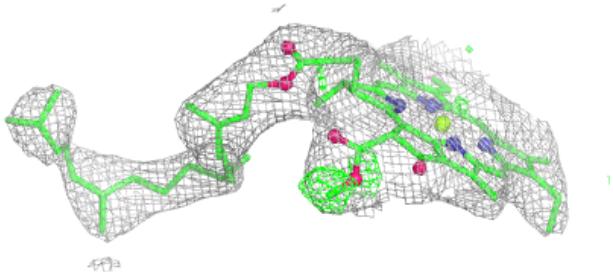


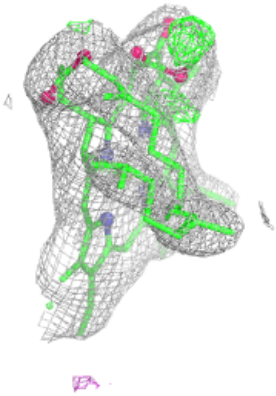


Electron density around CLA J 101:

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

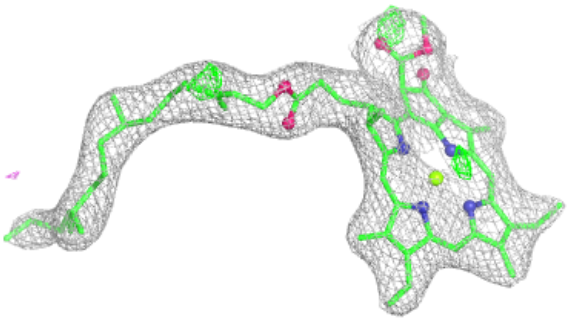


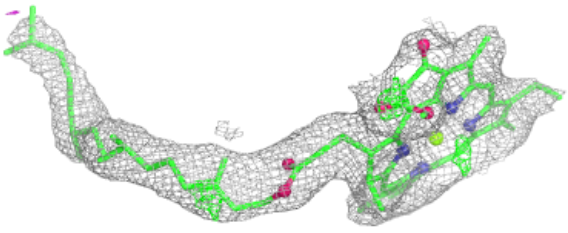


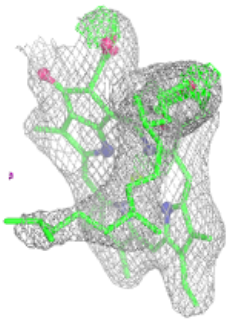


Electron density around CLA A 853:

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

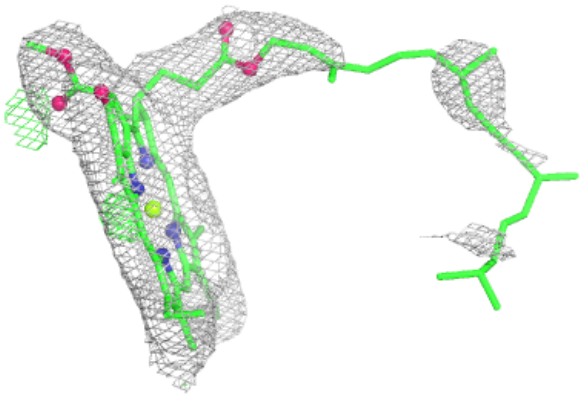


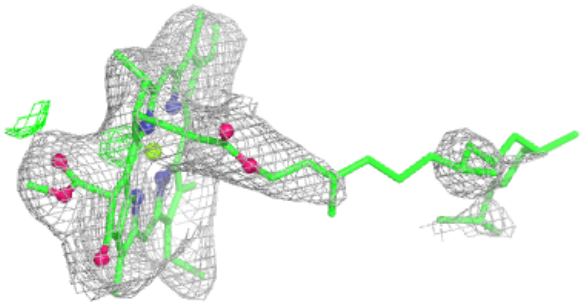


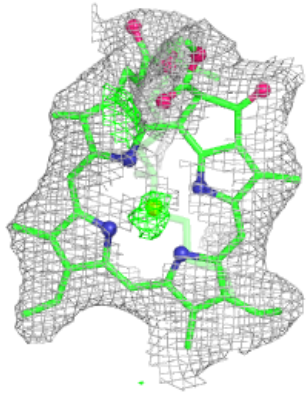


Electron density around CLA A 806:

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

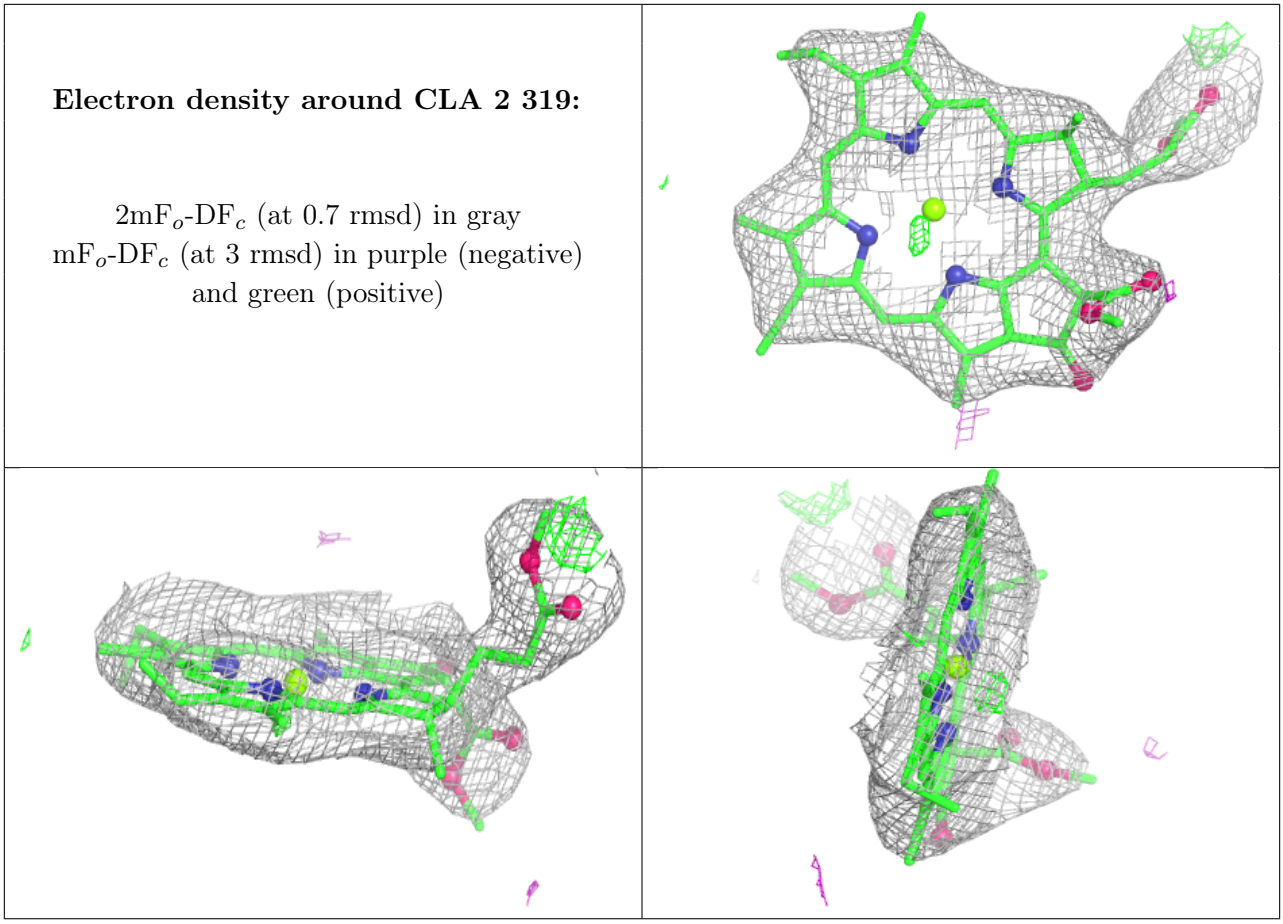






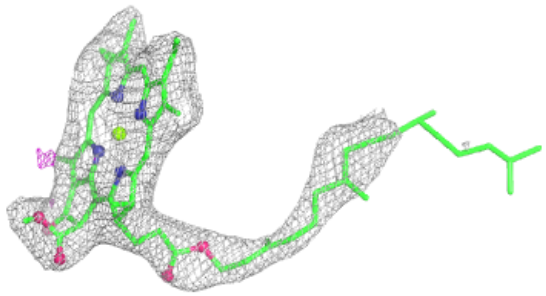
Electron density around CLA 2 319:

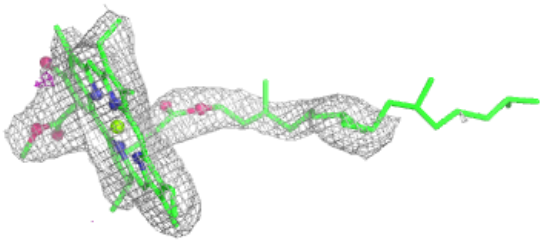
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

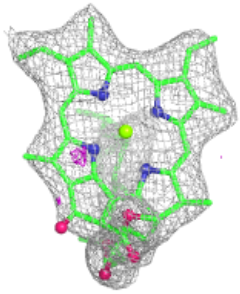


Electron density around CLA B 823:

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

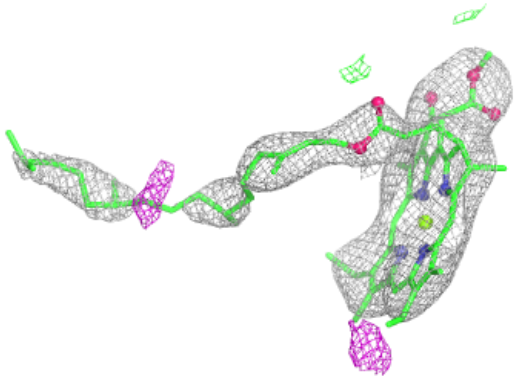


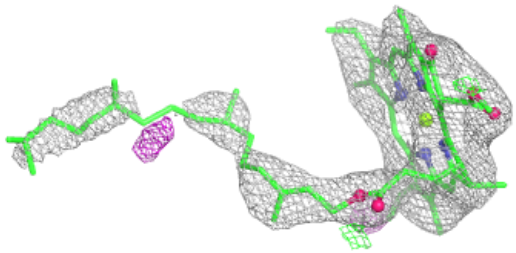


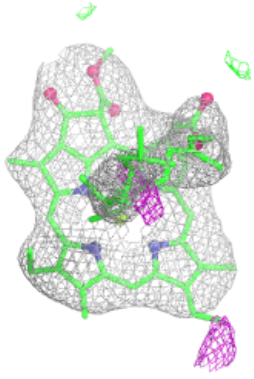


Electron density around CLA A 810:

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

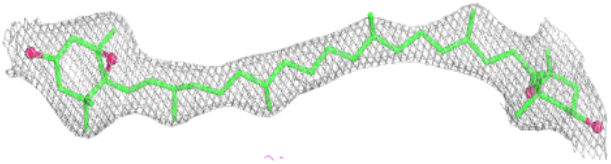


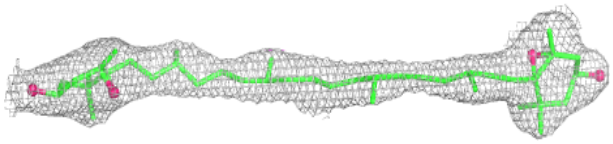


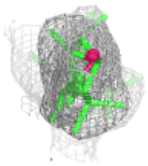


Electron density around XAT 4 317:

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

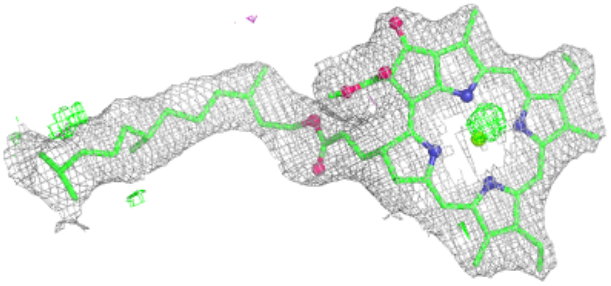


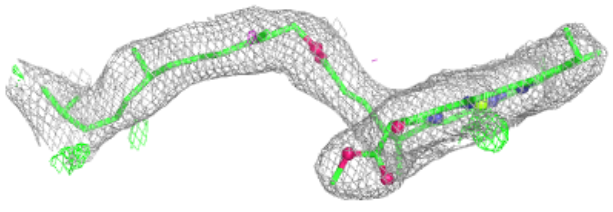




Electron density around CLA B 825:

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

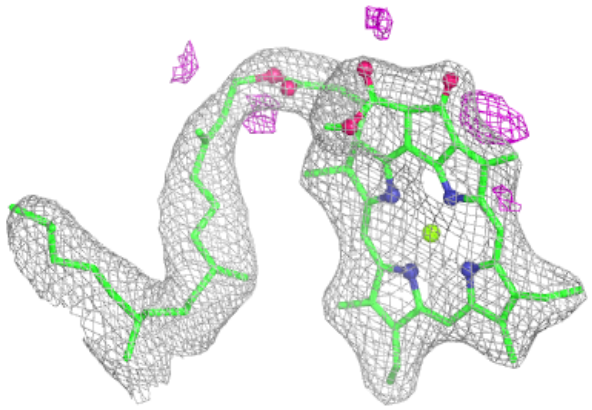


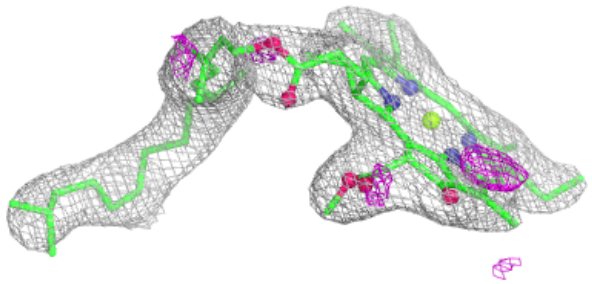


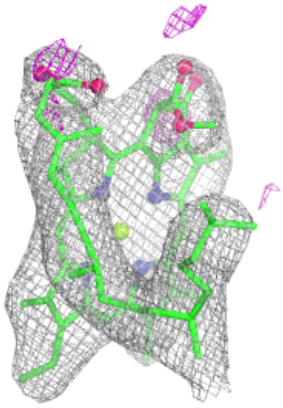


Electron density around CLA B 826:

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

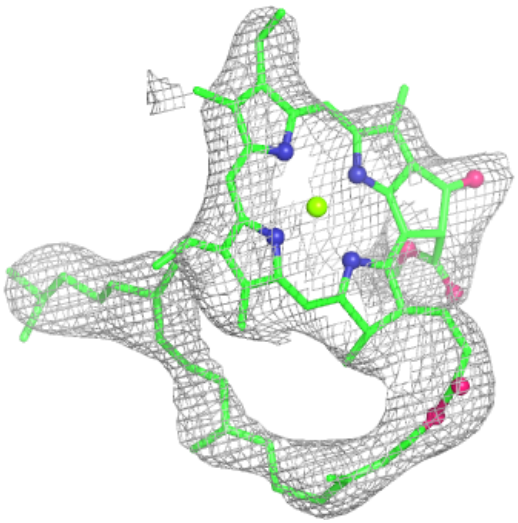


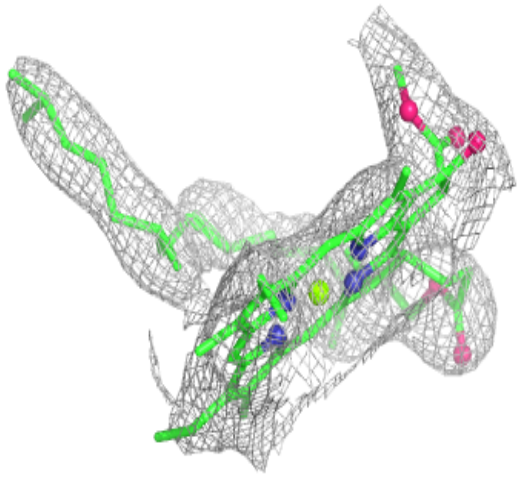


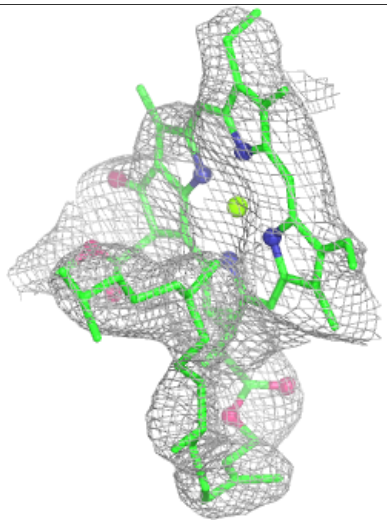


Electron density around CLA A 812:

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

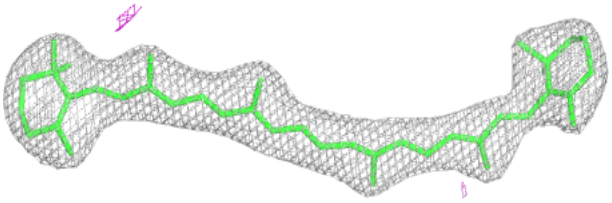


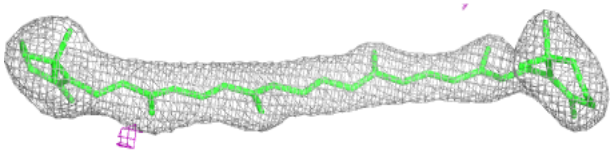


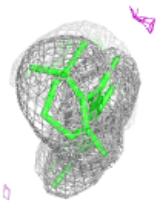


Electron density around BCR B 848:

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

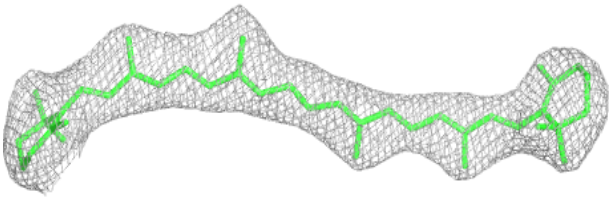


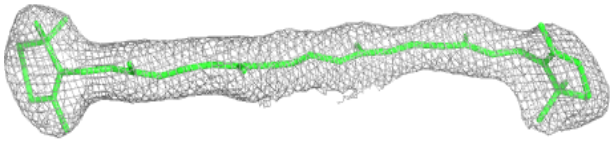


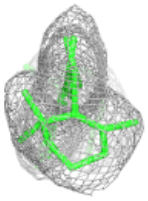


Electron density around BCR B 849:

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

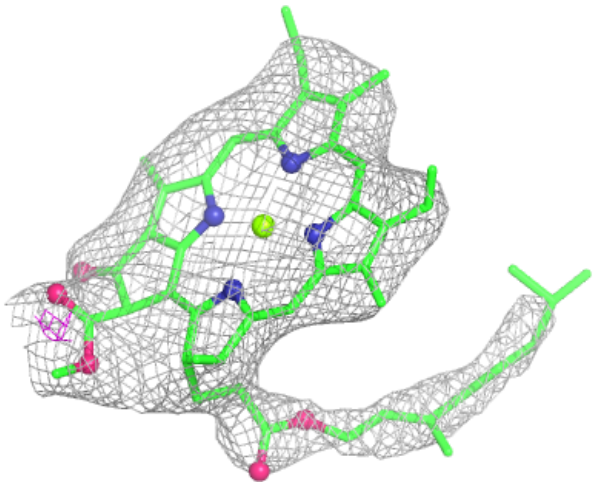


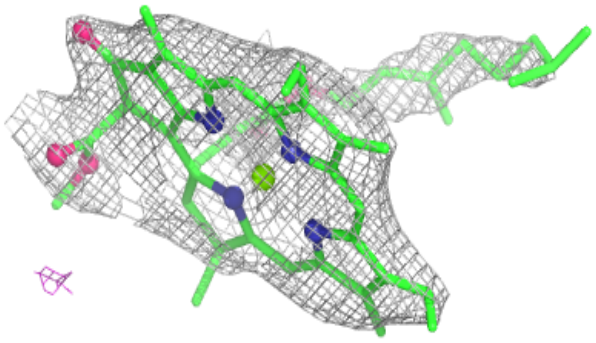


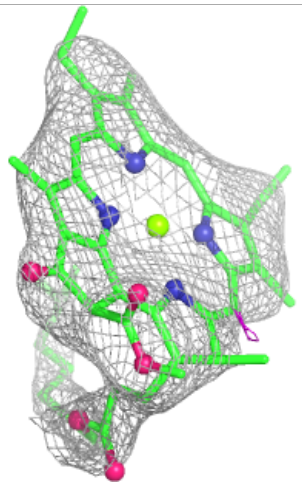


Electron density around CLA A 823:

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

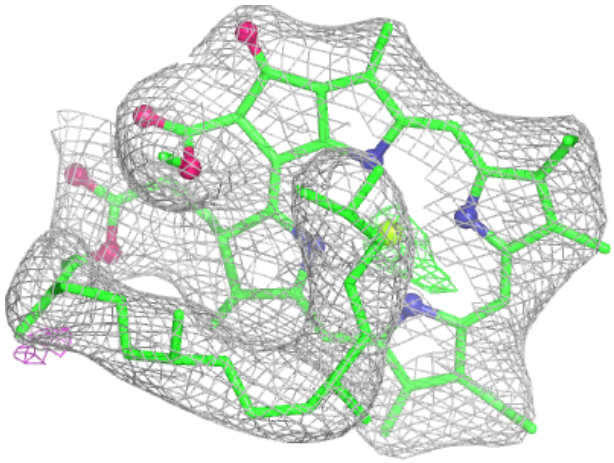


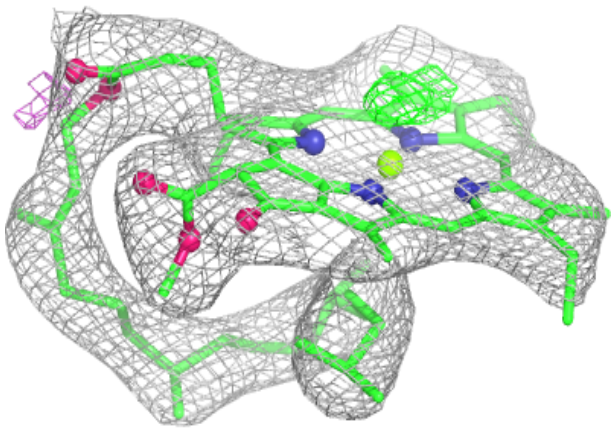


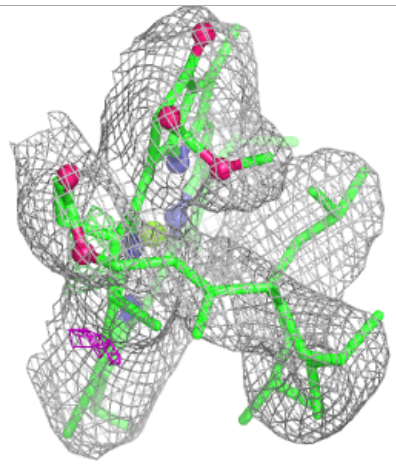


Electron density around CLA A 805:

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

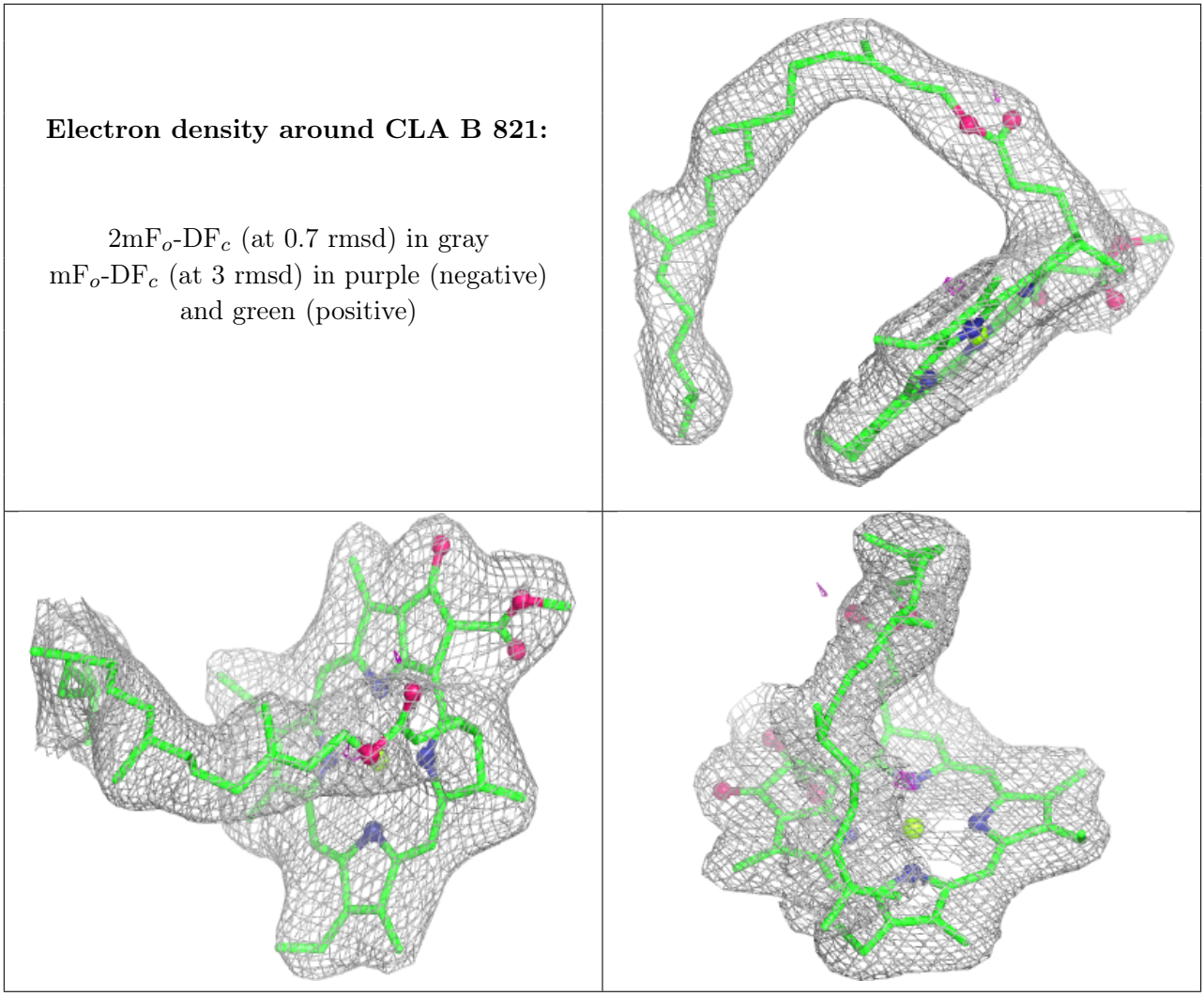






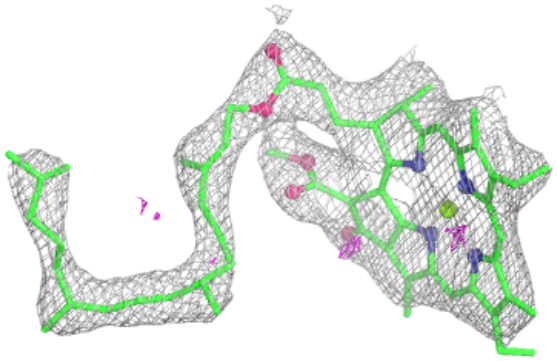
Electron density around CLA B 821:

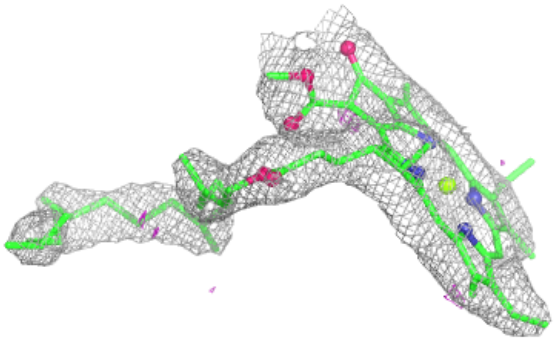
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

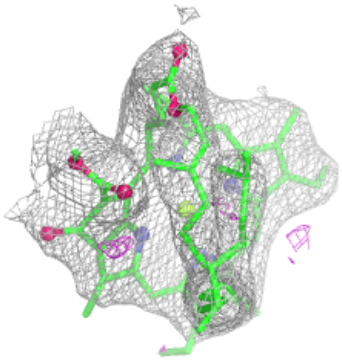


Electron density around CLA A 801:

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

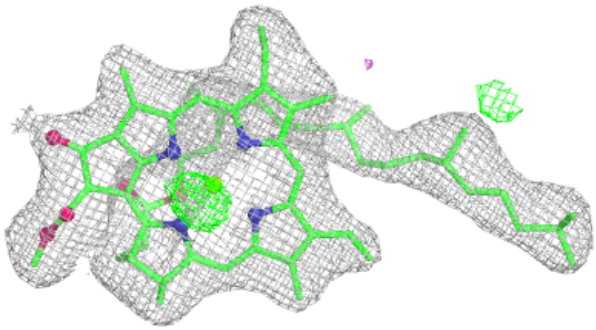


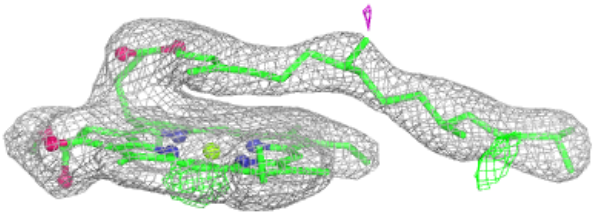


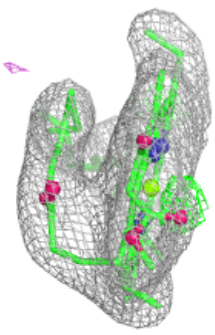


Electron density around CLA A 838:

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

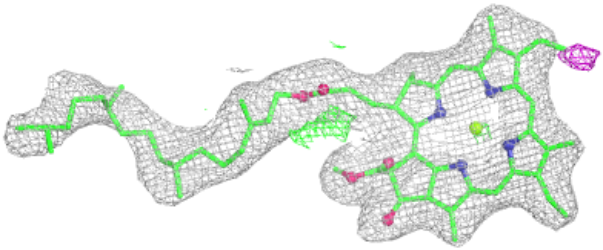


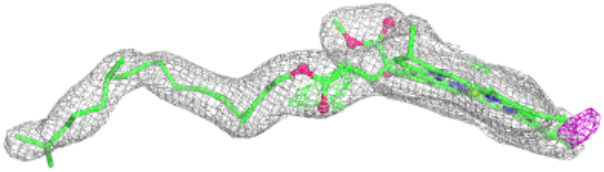


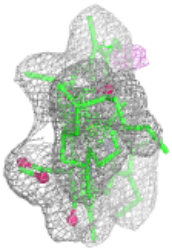


Electron density around CLA A 839:

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

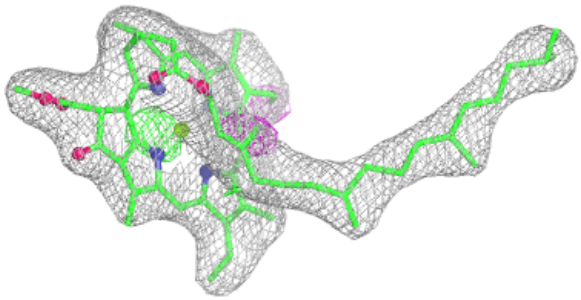


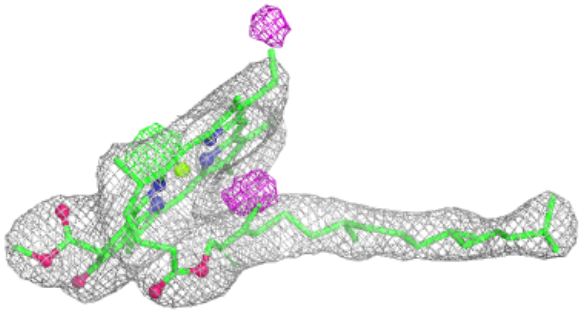


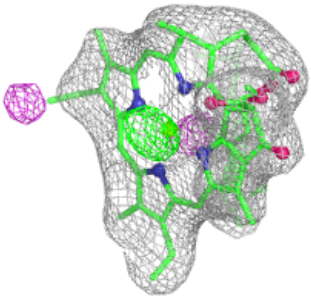


Electron density around CLA A 840:

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

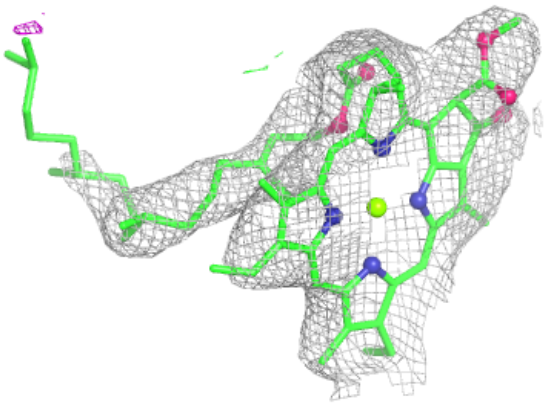


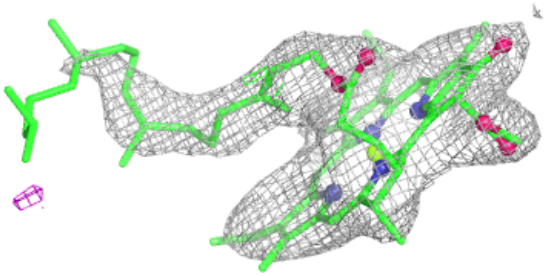


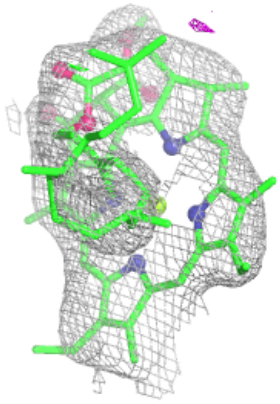


Electron density around CLA A 841:

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

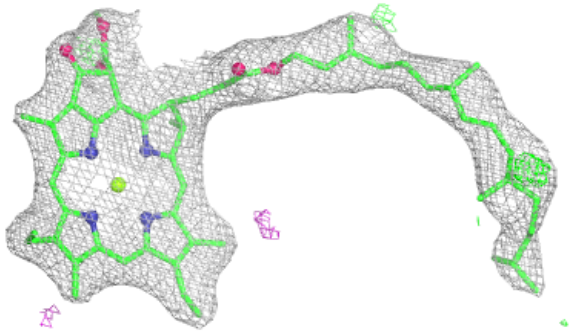


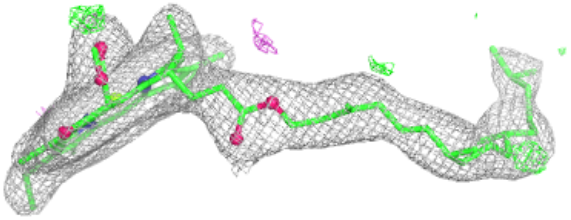


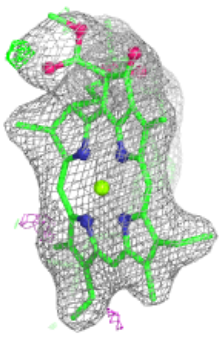


Electron density around CLA B 827:

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

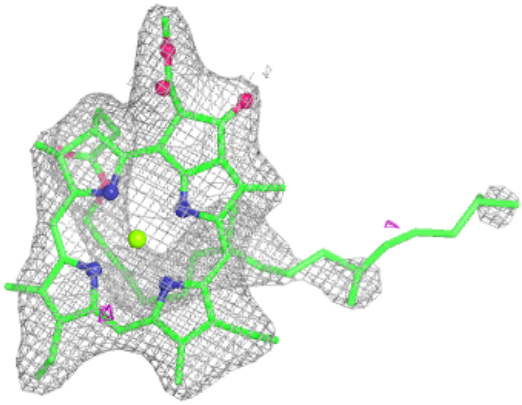


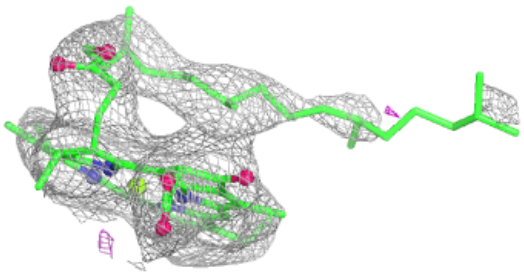


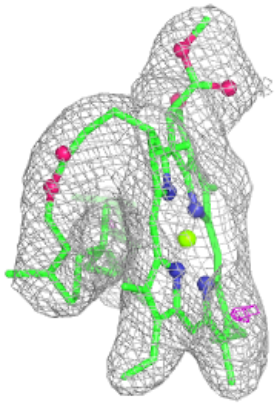


Electron density around CLA B 829:

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

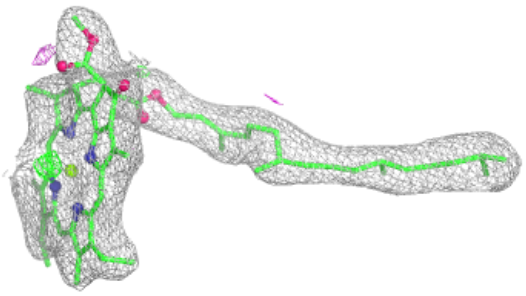


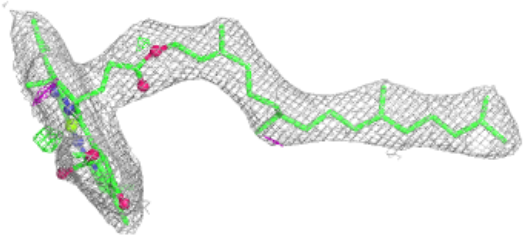


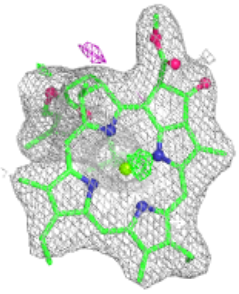


Electron density around CLA B 830:

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

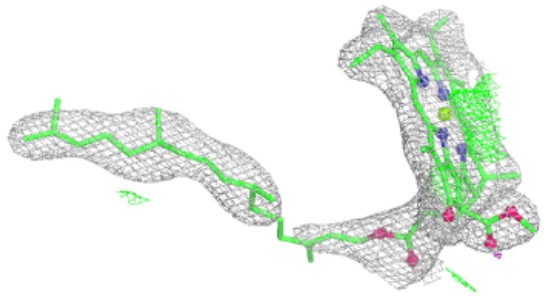


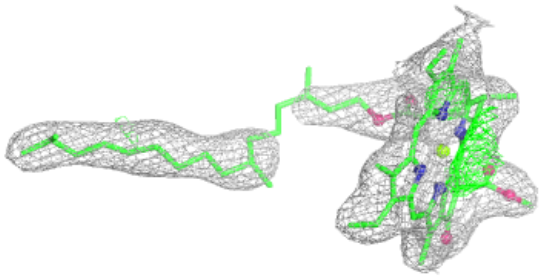


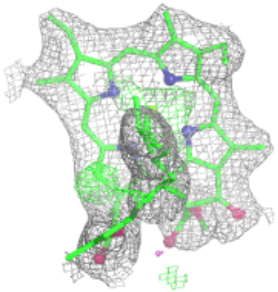


Electron density around CLA B 831:

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

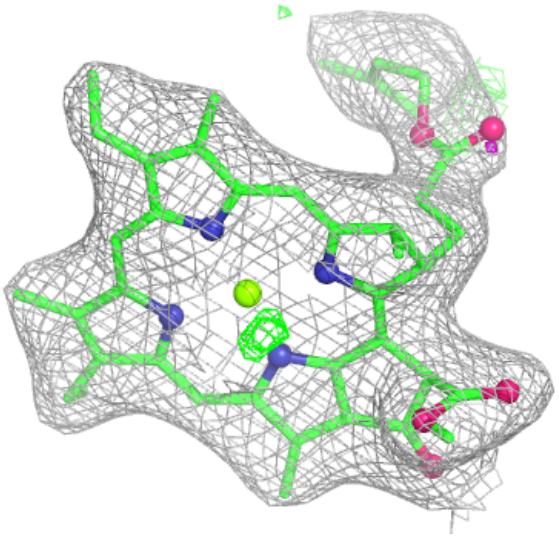


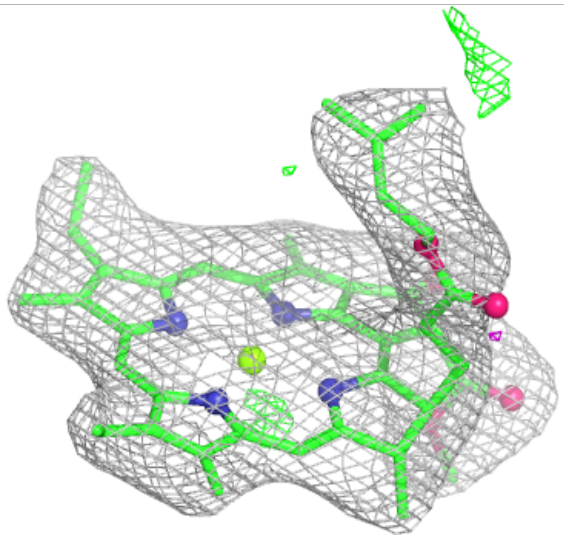


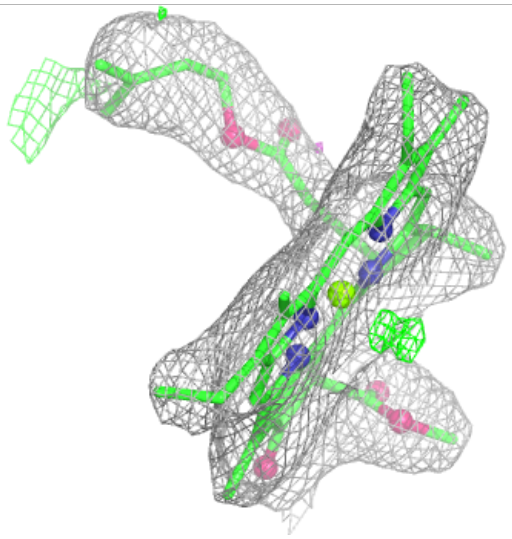


Electron density around CLA B 832:

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

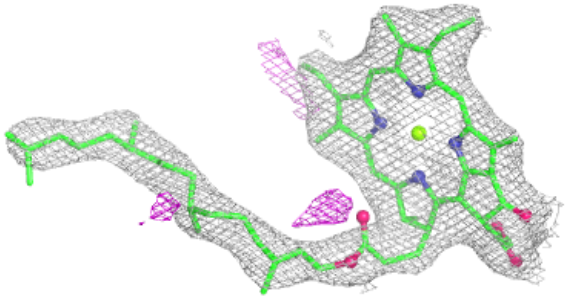


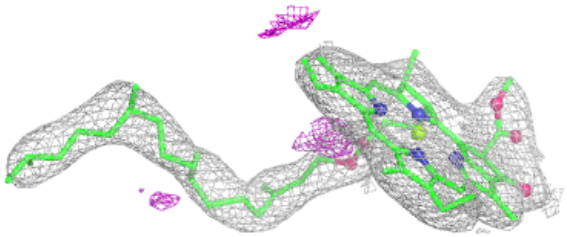


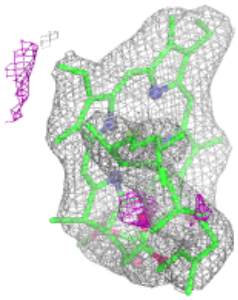


Electron density around CLA A 807:

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

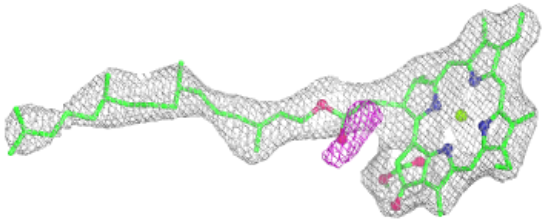


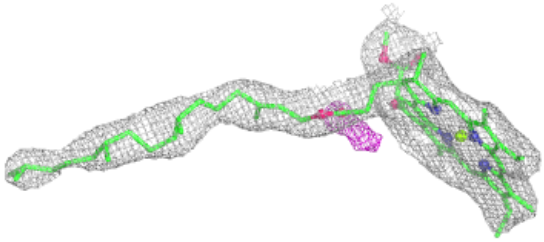


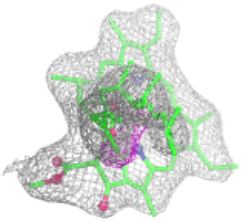


Electron density around CLA A 808:

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

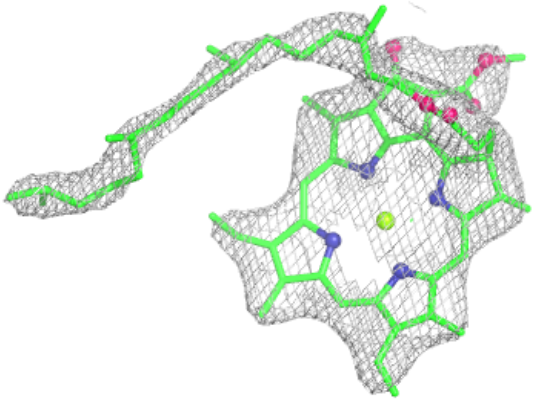


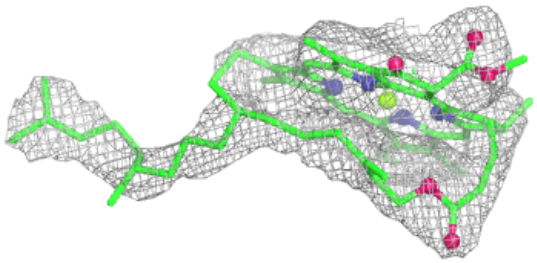


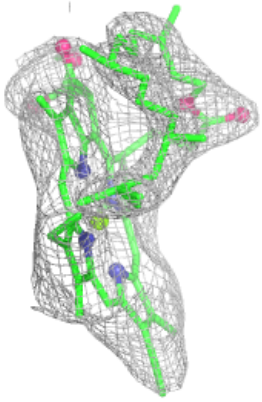


Electron density around CLA A 828:

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

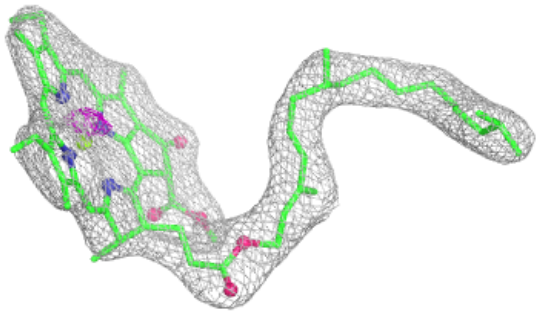


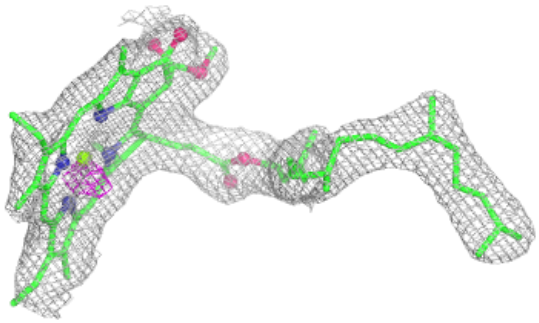


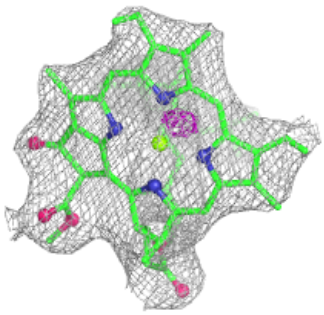


Electron density around CLA B 804:

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

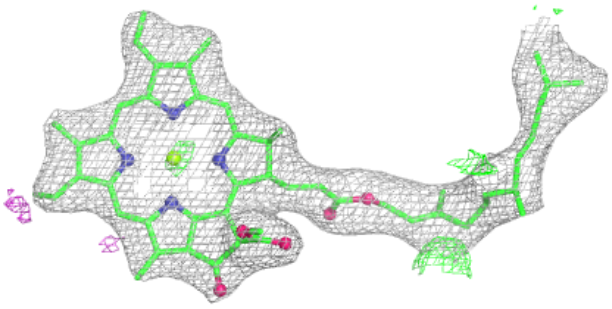


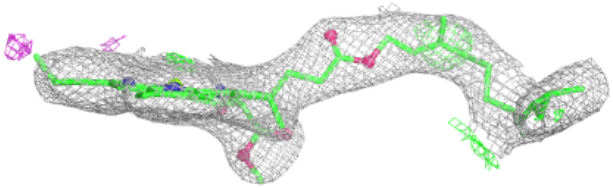


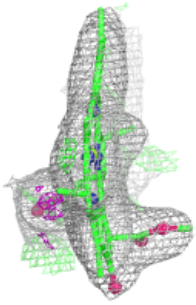


Electron density around CLA B 837:

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

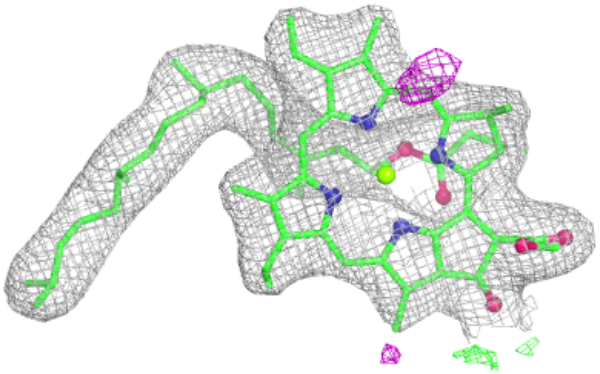


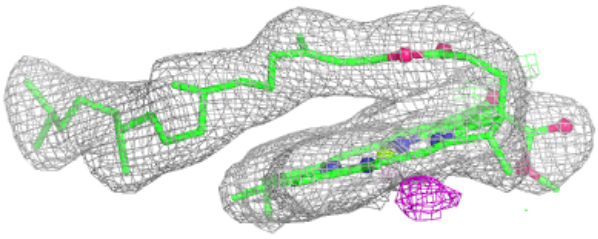


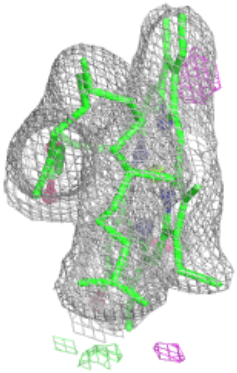


Electron density around CLA B 838:

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

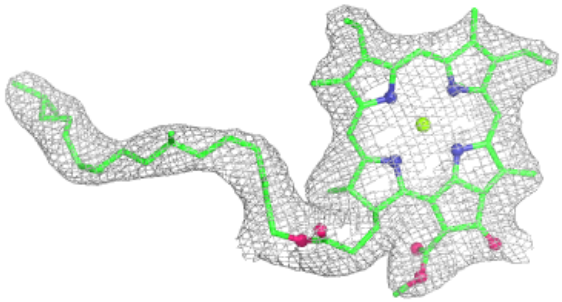


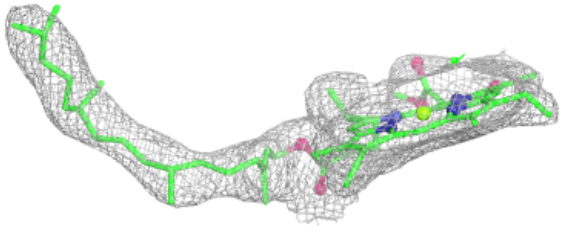


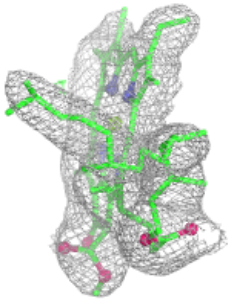


Electron density around CLA B 805:

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

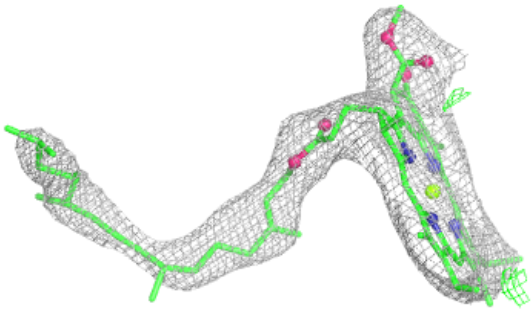


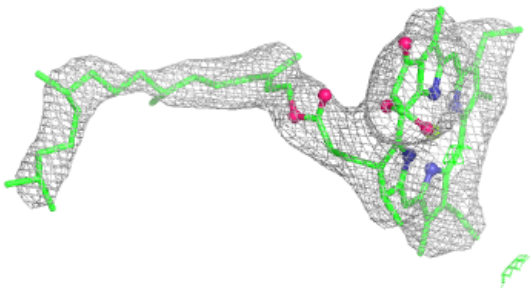


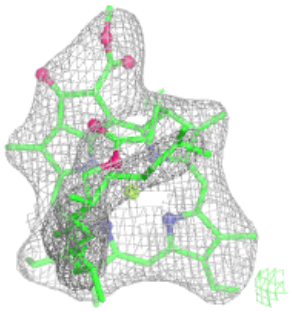


Electron density around CLA B 840:

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



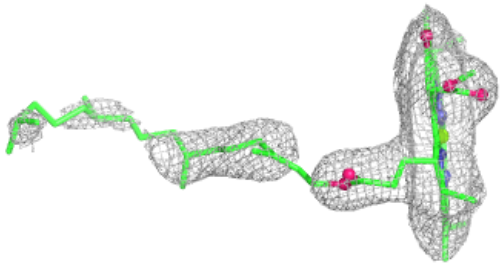


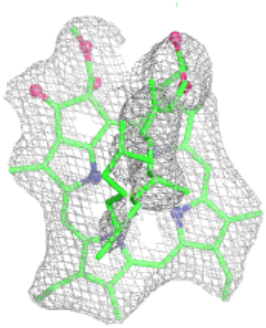


Electron density around CLA B 841:

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

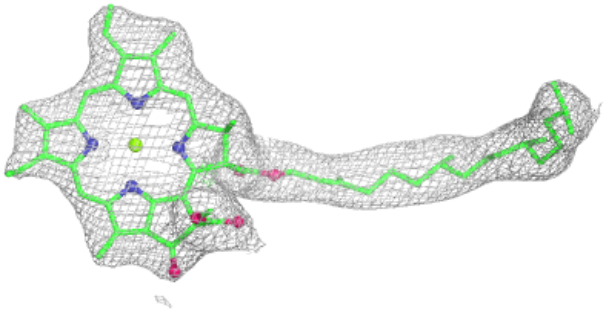


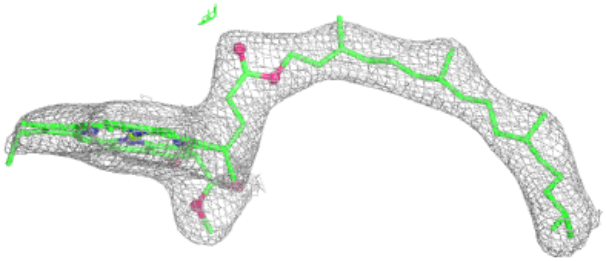


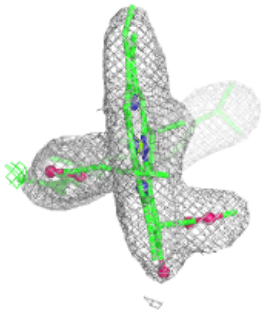


Electron density around CLA B 842:

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

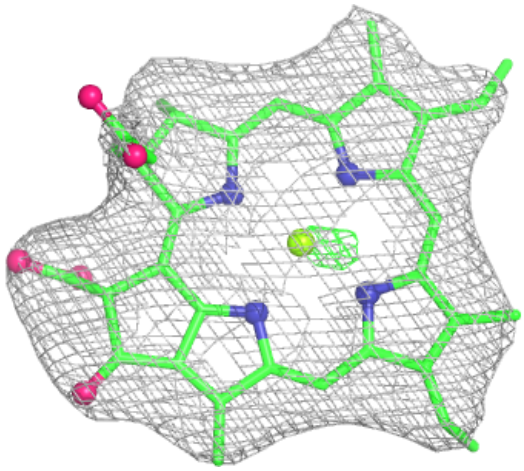


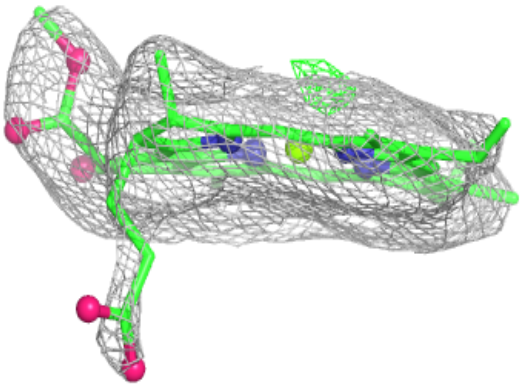


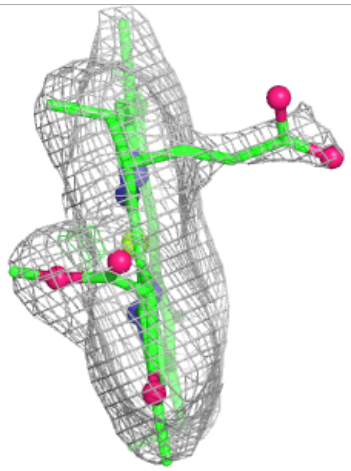


Electron density around CLA B 806:

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

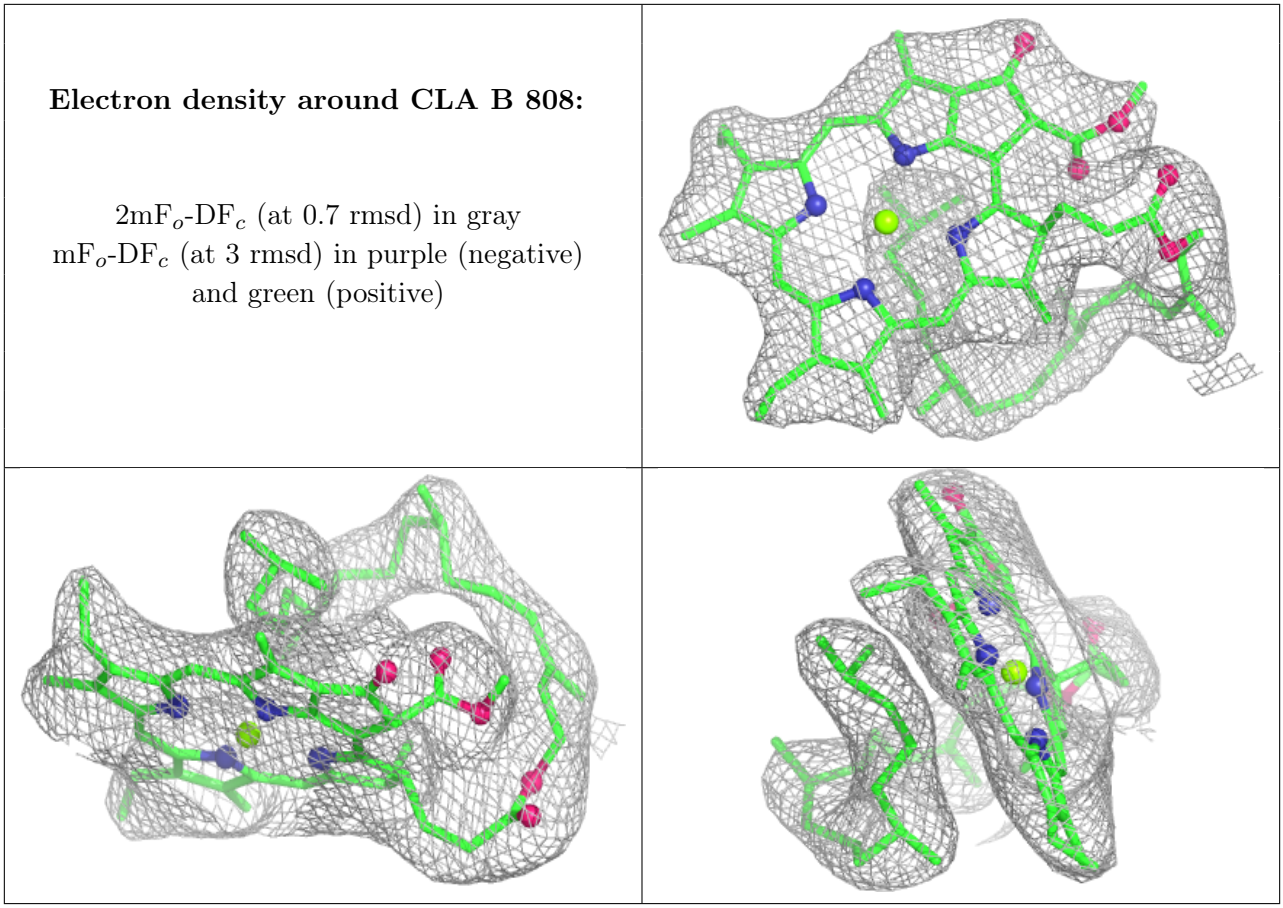






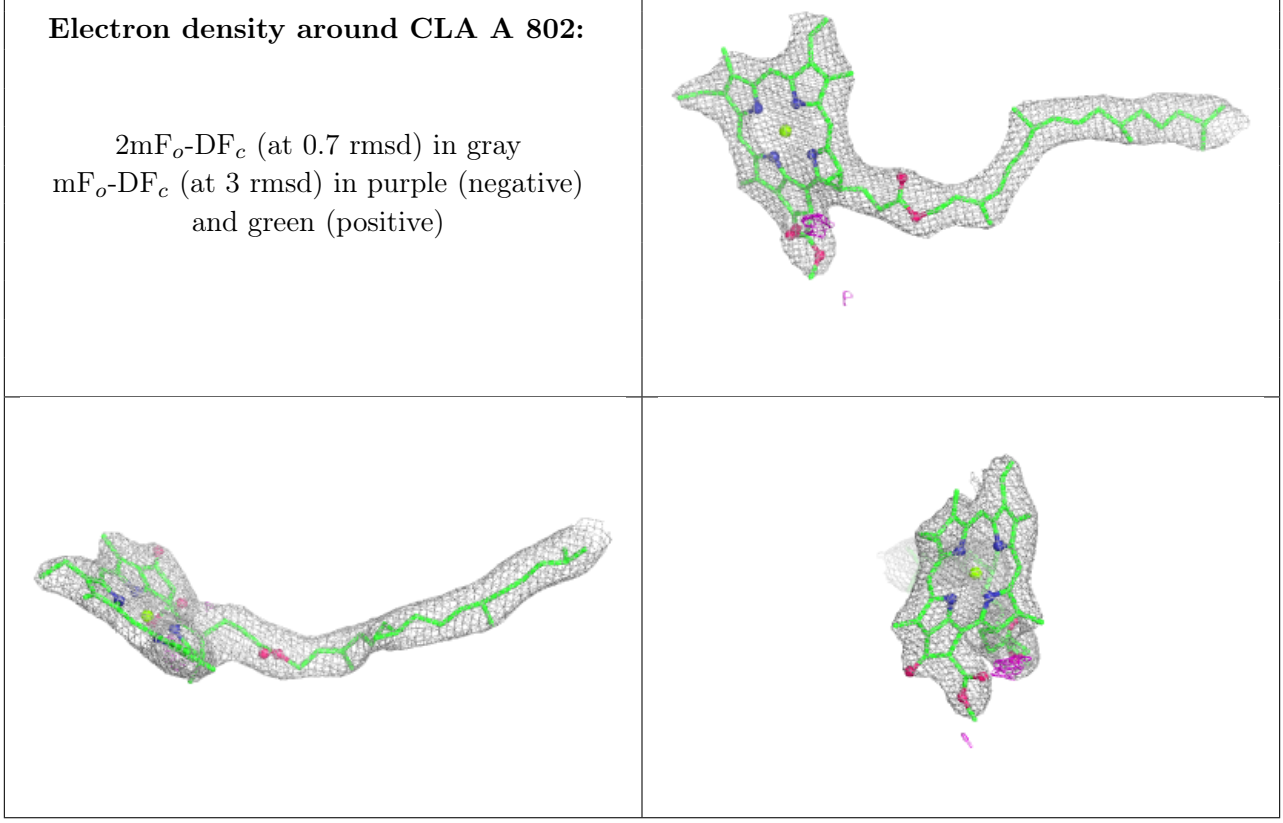
Electron density around CLA B 808:

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



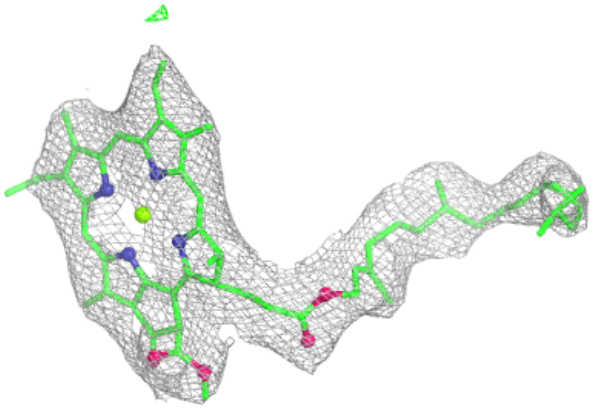
Electron density around CLA A 802:

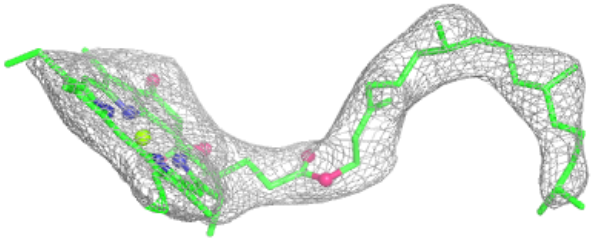
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

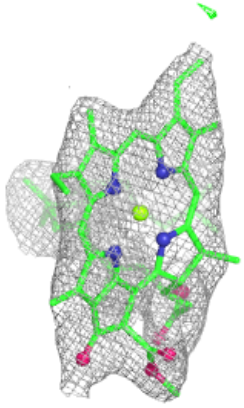


Electron density around CLA B 811:

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

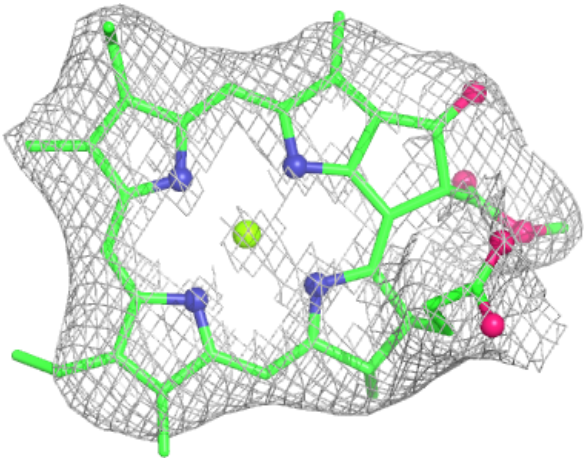


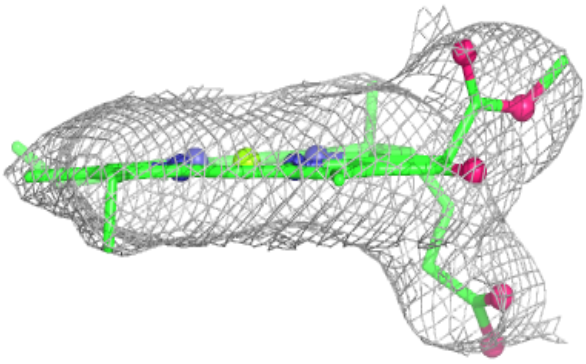


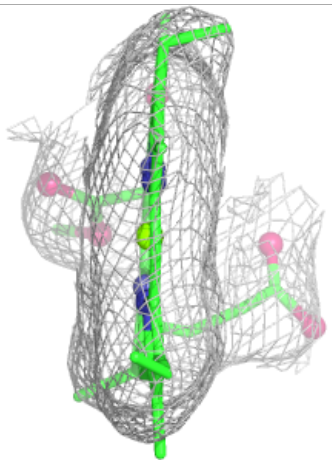


Electron density around CLA 4 313:

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

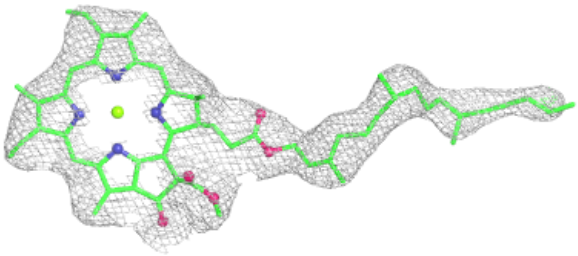


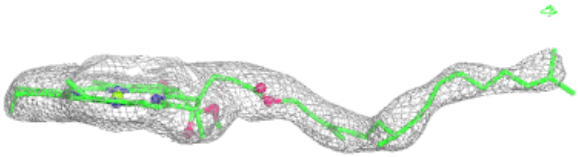


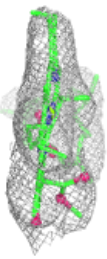


Electron density around CLA A 831:

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

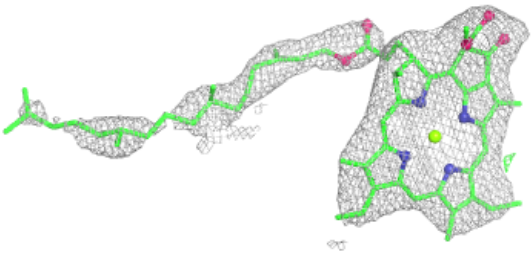


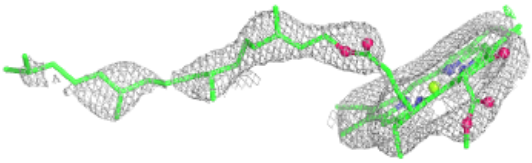


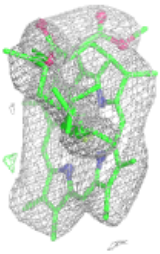


Electron density around CLA A 832:

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

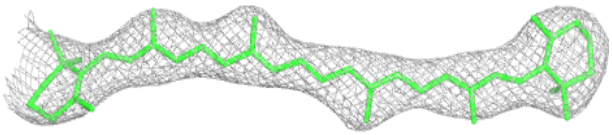


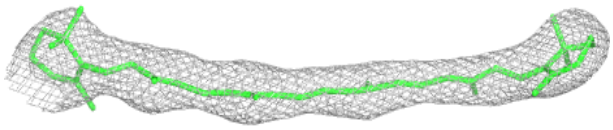


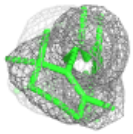


Electron density around BCR B 844:

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

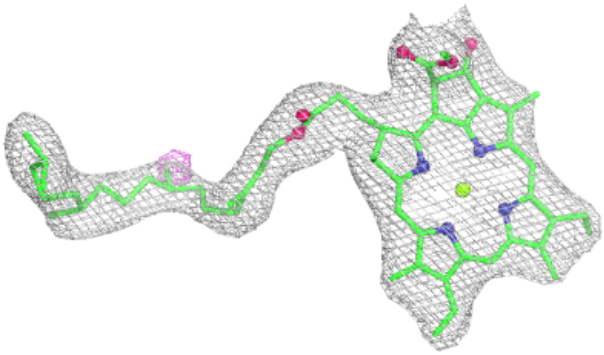


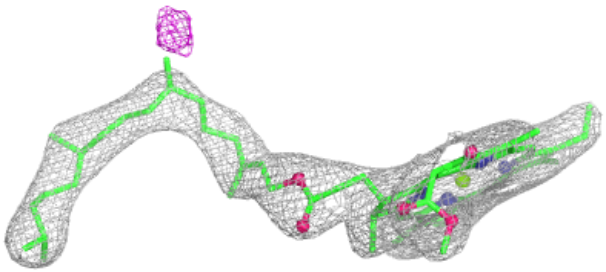


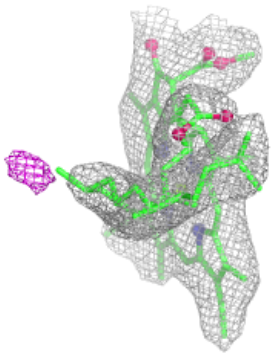


Electron density around CLA B 815:

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

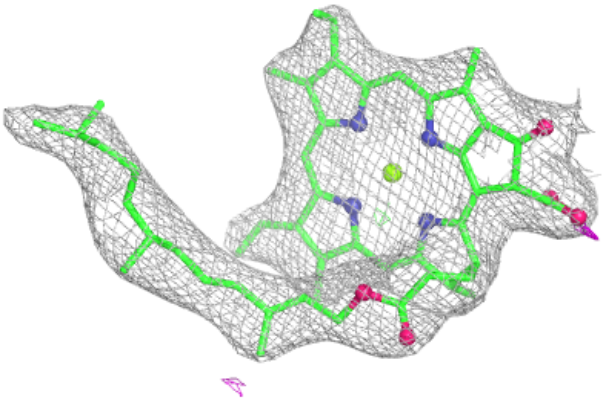


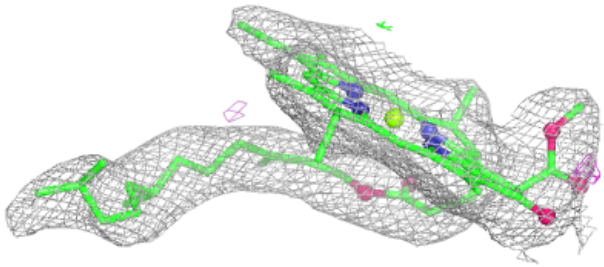


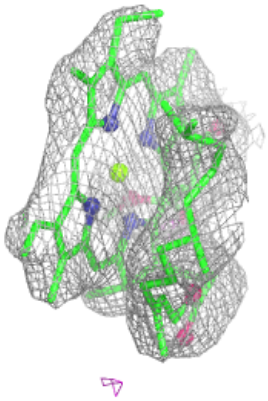


Electron density around CLA 4 302:

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

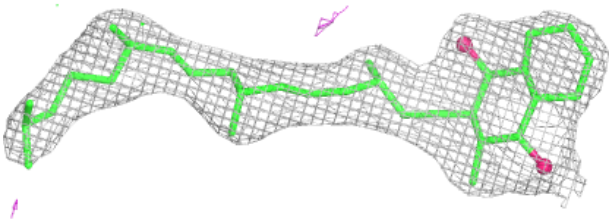


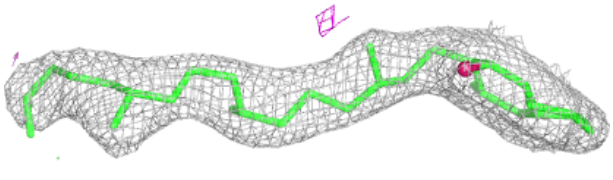


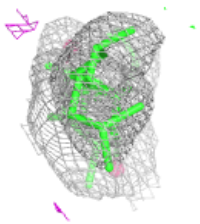


Electron density around PQN A 842:

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

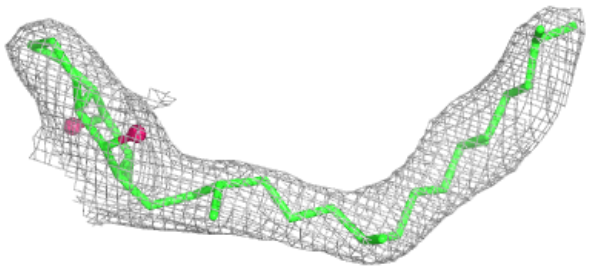


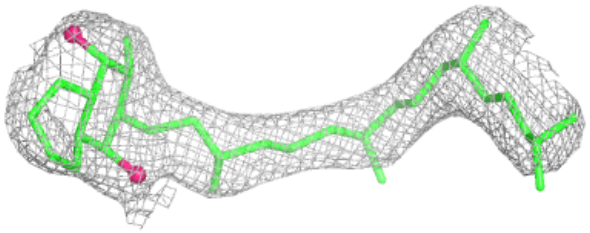


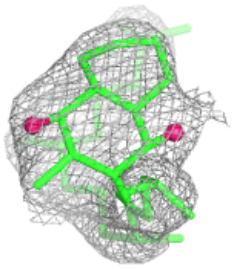


Electron density around PQN B 843:

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

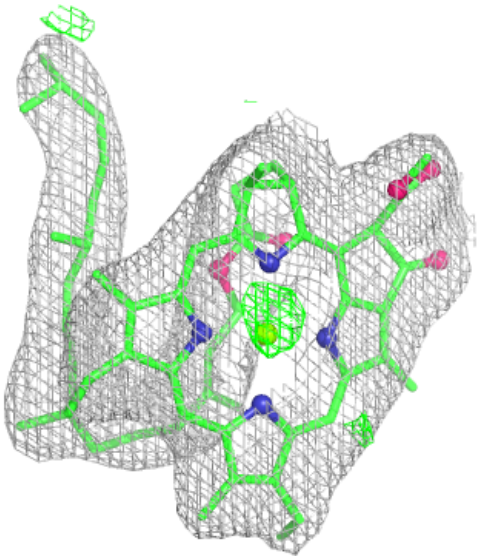


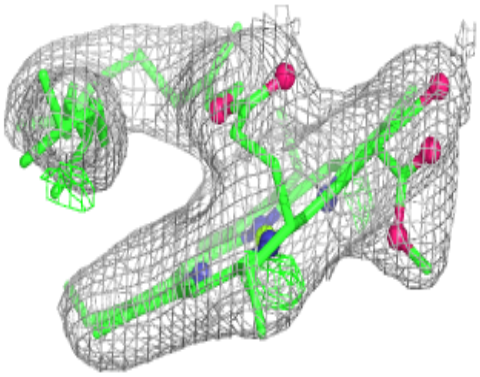


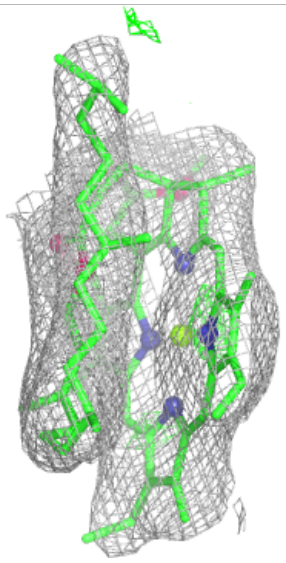


Electron density around CLA B 810:

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

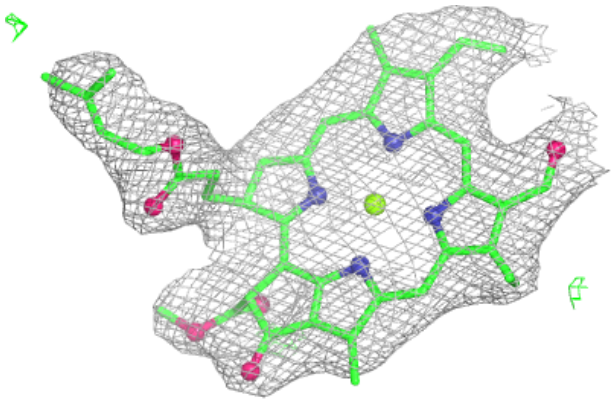


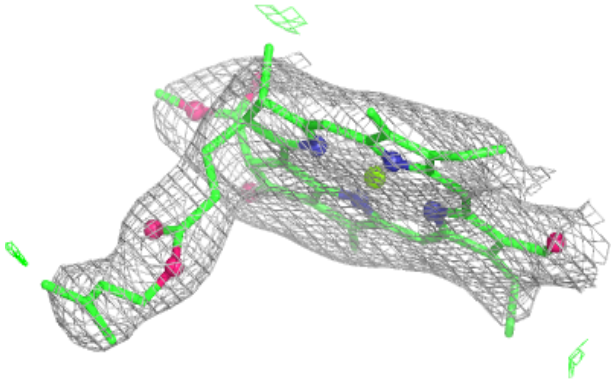


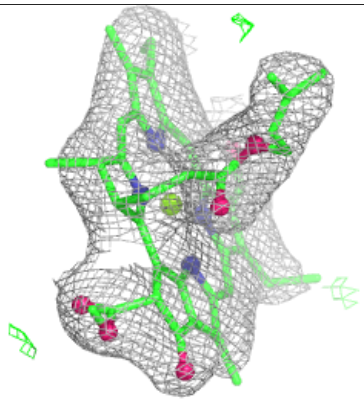


Electron density around CHL 4 307:

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

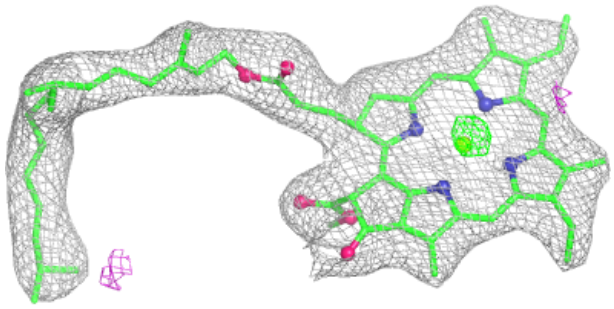


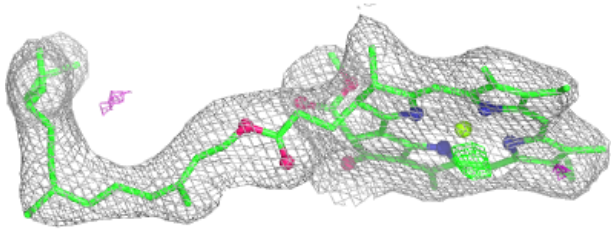




Electron density around CLA B 828:

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

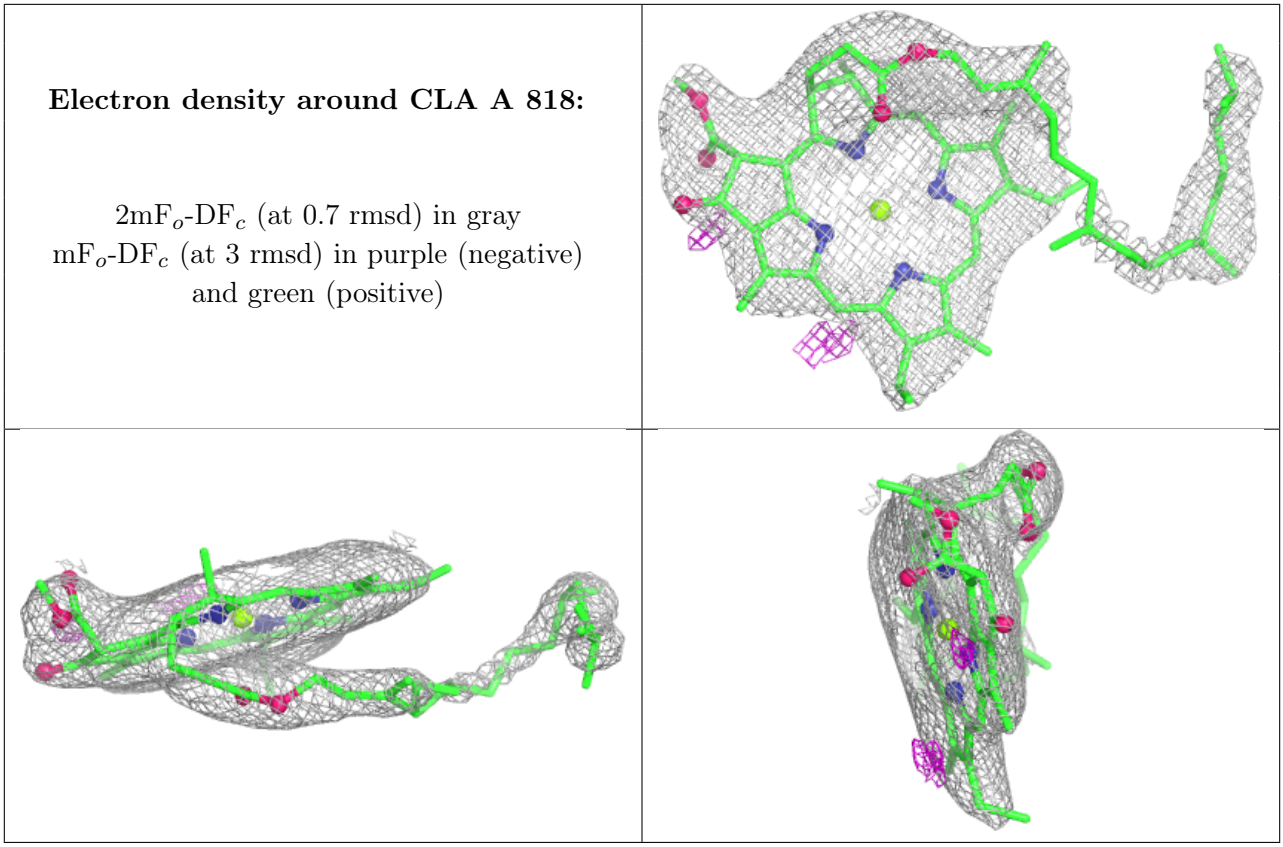






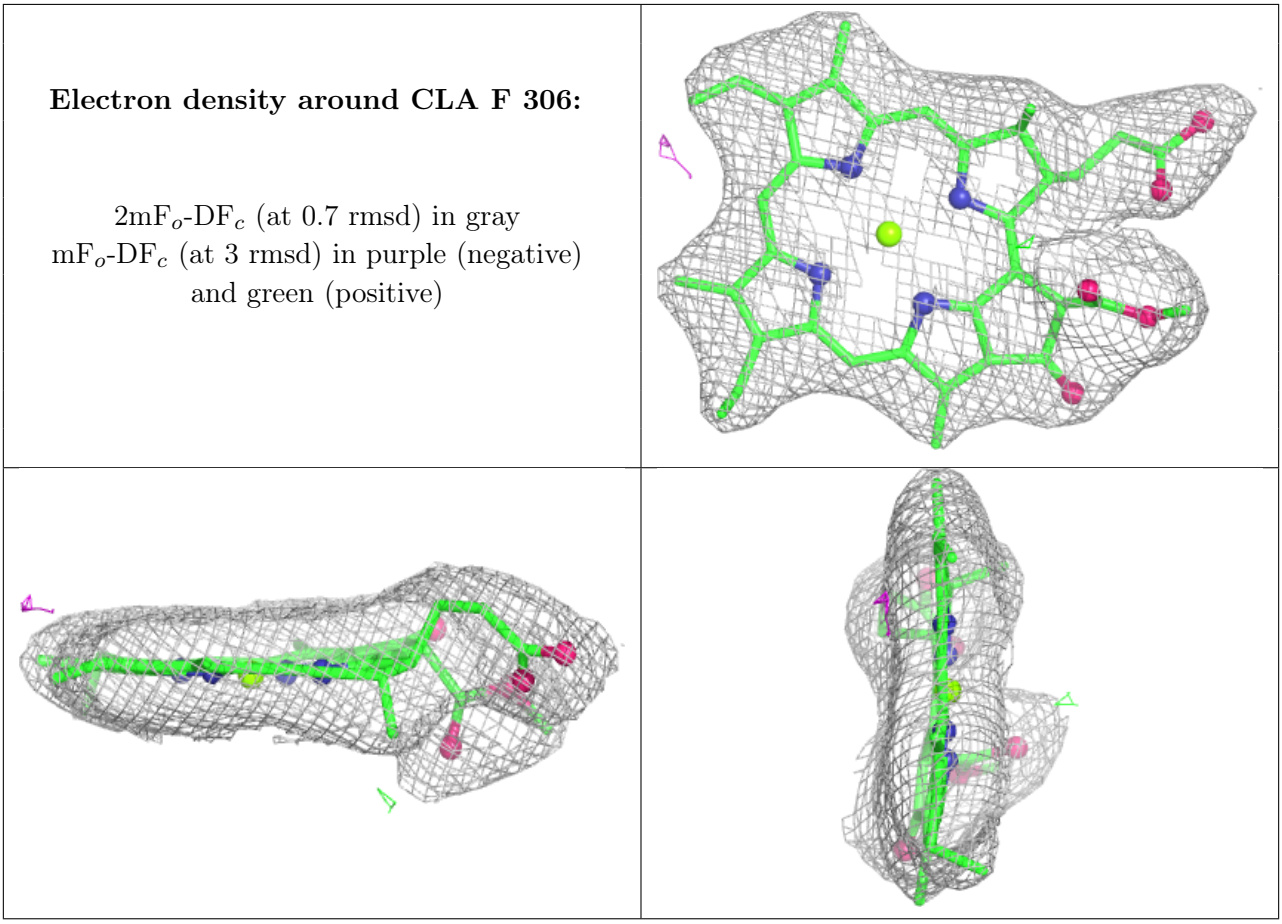
Electron density around CLA A 818:

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



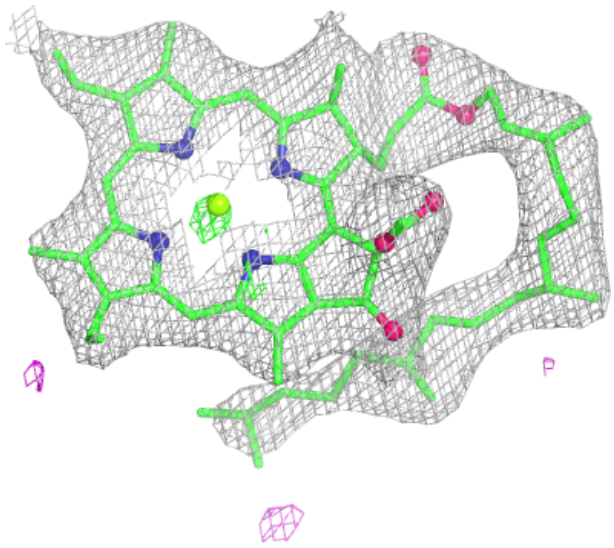
Electron density around CLA F 306:

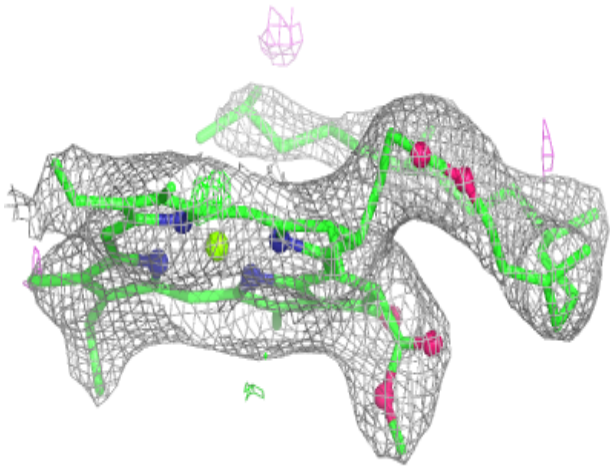
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

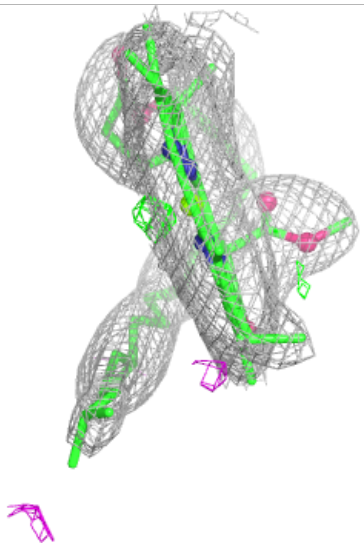


Electron density around CLA B 807:

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

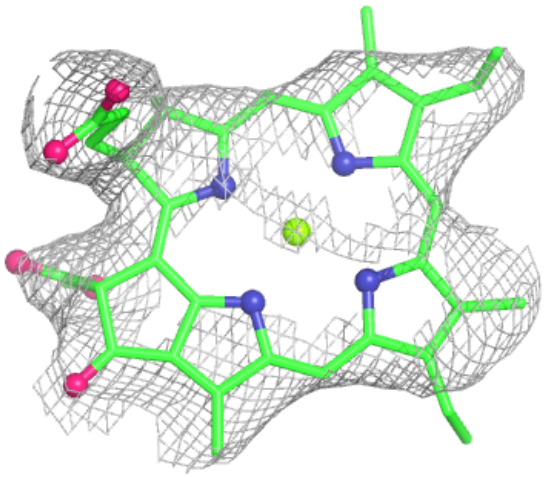


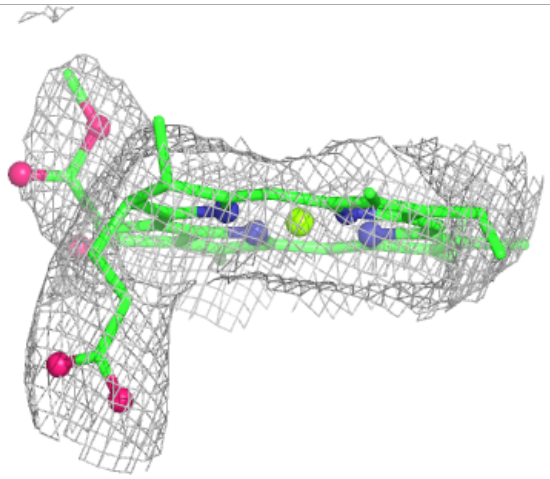


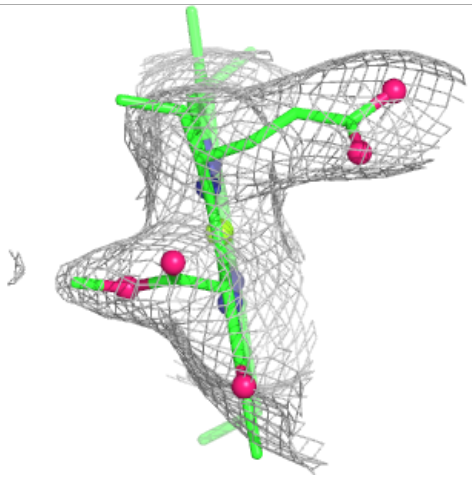


Electron density around CLA A 813:

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

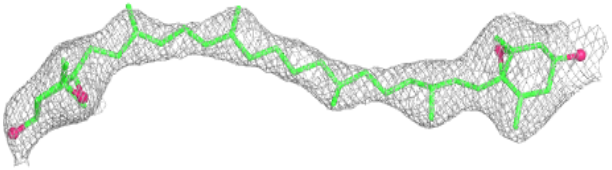


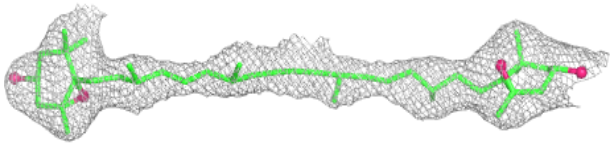


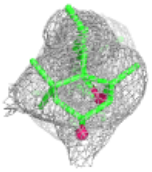


Electron density around XAT 1 315:

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

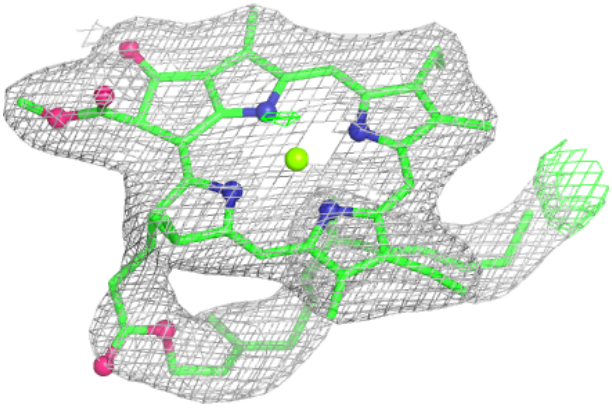


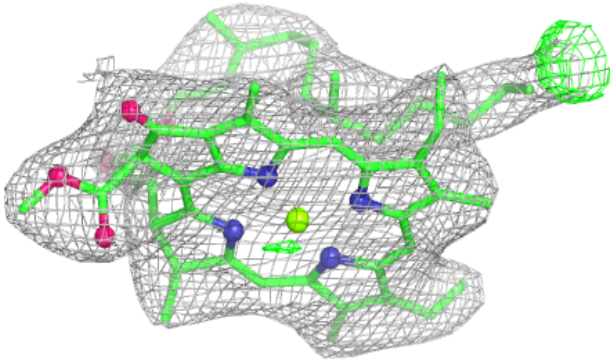


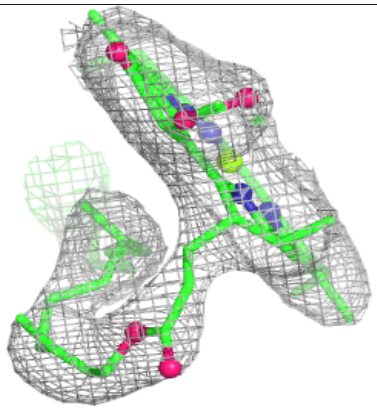


Electron density around CLA B 819:

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

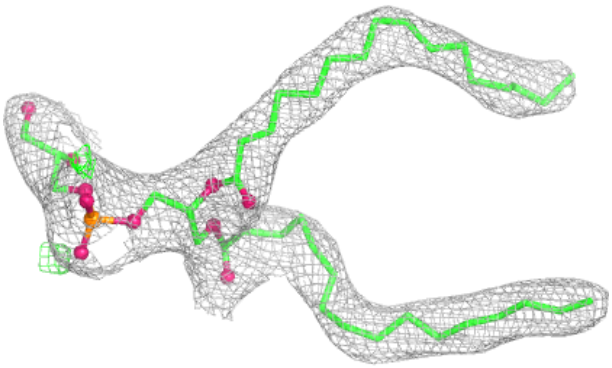


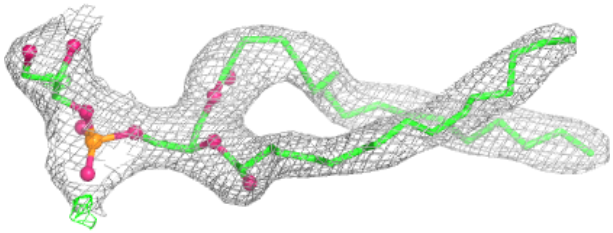


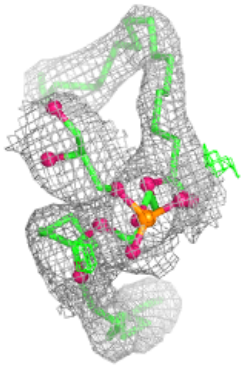


Electron density around LHG A 844:

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

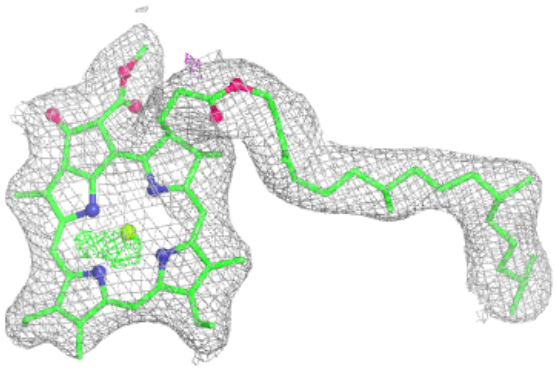


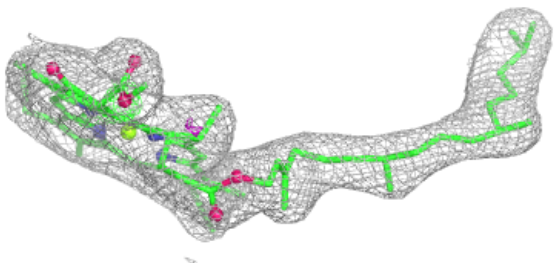




Electron density around CLA B 802:

$2mF_o$-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.