wwPDB X-ray Structure Validation Summary Report (i)

Aug 8, 2020 – 08:26 AM BST

PDB ID	:	4XK8
Title	:	Crystal structure of plant photosystem I-LHCI super-complex at 2.8 angstrom resolution
Authors	:	Suga, M.; Qin, X.; Kuang, T.; Shen, J.R.
Deposited on	:	2015-01-10
Resolution	:	2.80 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 following versions of software and data (see references (1)) were used in the production of this report:

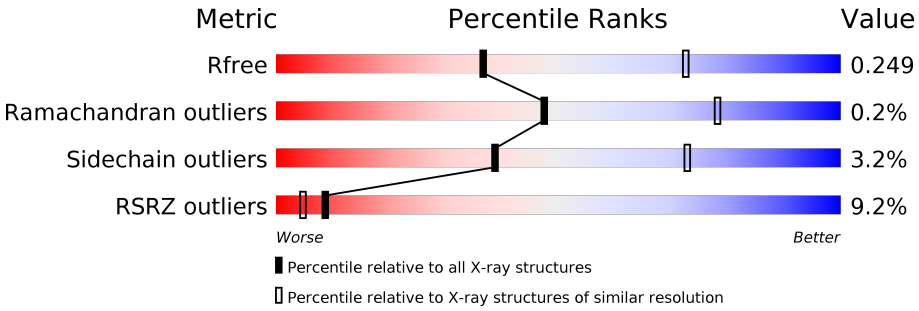
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.13.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.13.1

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 2.80 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}	130704	3140 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)
RSRZ outliers	127900	3078 (2.80-2.80)

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 on 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	A	742	4% 98% .
1	a	742	4% 98% .
2	B	733	9% 98% .
2	b	733	7% 98% .
3	C	80	6% 98% .
3	c	80	98% .
4	D	141	8% 96% .

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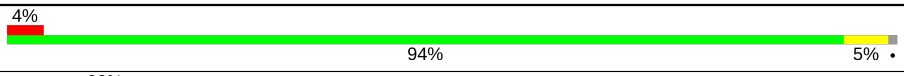
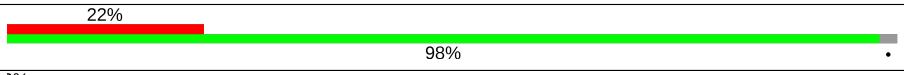
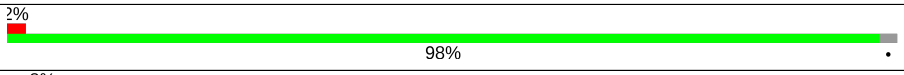
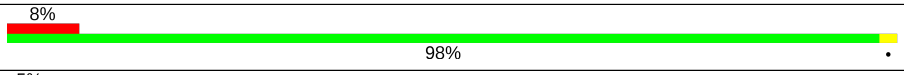
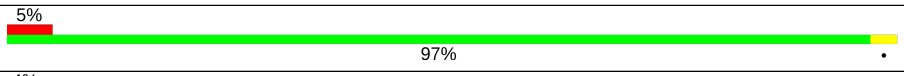
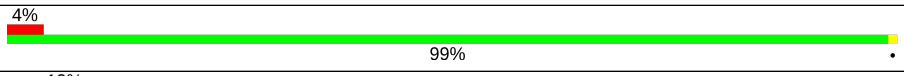
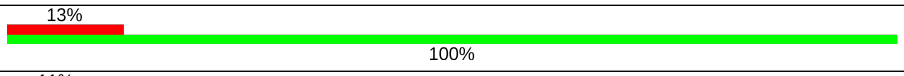
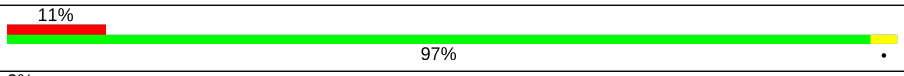
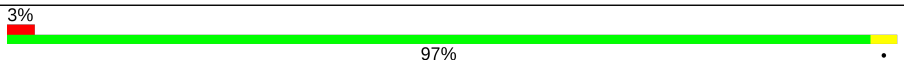
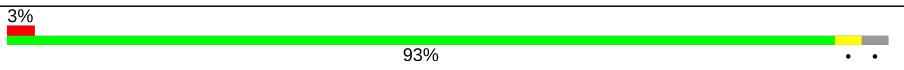
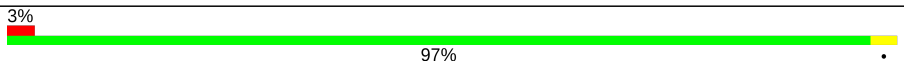
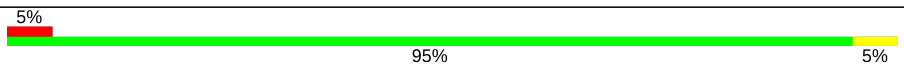
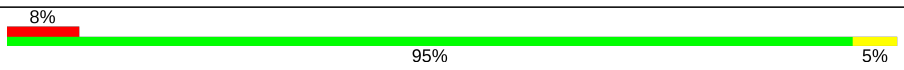
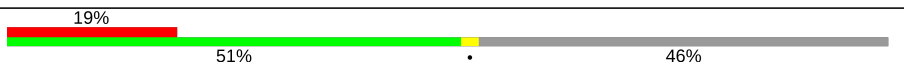
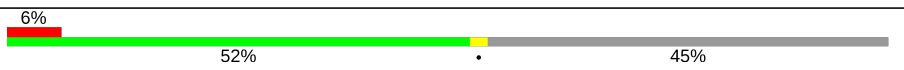
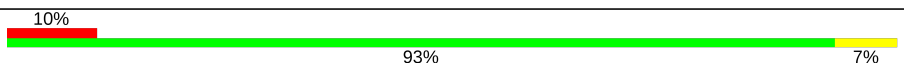
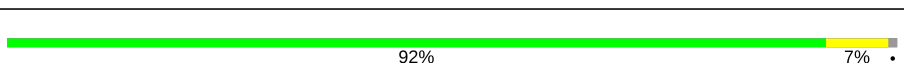
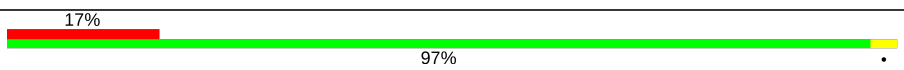
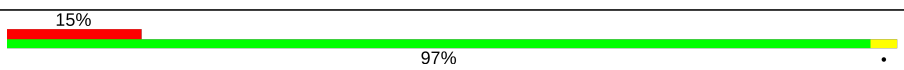
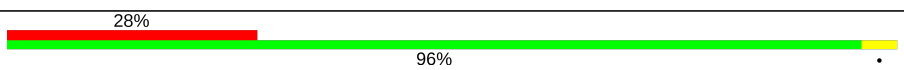
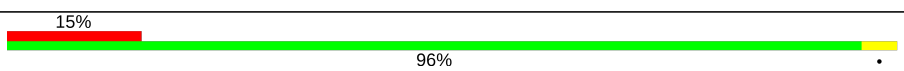
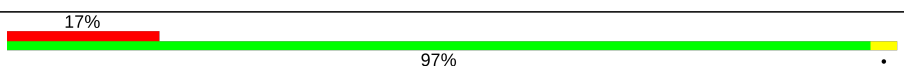
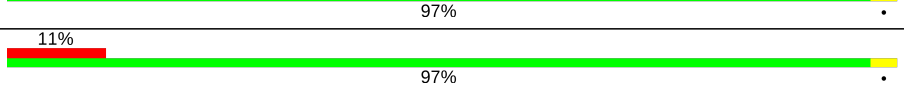
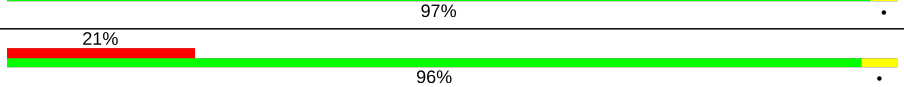
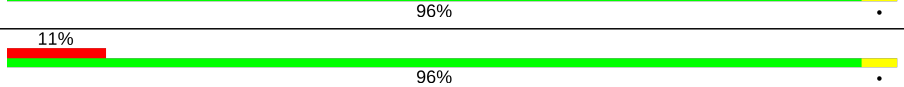
Mol	Chain	Length	Quality of chain
4	d	141	
5	E	64	
5	e	64	
6	F	151	
6	f	151	
7	G	95	
7	g	95	
8	H	90	
8	h	90	
9	I	30	
9	i	30	
10	J	39	
10	j	39	
11	K	84	
11	k	84	
12	L	153	
12	l	153	
13	1	195	
13	6	195	
14	2	206	
14	7	206	
15	3	218	
15	8	218	
16	4	196	
16	9	196	

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	1	303	X	-	-	-
17	CLA	1	304	X	-	-	-
17	CLA	1	305	X	-	-	-
17	CLA	1	306	X	-	-	-
17	CLA	1	308	X	-	-	-
17	CLA	1	309	X	-	-	-
17	CLA	1	310	X	-	-	-
17	CLA	1	311	X	-	-	-
17	CLA	1	312	X	-	-	-
17	CLA	1	313	X	-	-	-
17	CLA	1	314	X	-	-	-
17	CLA	1	315	X	-	-	-
17	CLA	2	602	X	-	-	-
17	CLA	2	603	X	-	-	-
17	CLA	2	604	X	-	-	-
17	CLA	2	608	X	-	-	-
17	CLA	2	609	X	-	-	-
17	CLA	2	610	X	-	-	-
17	CLA	2	611	X	-	-	-
17	CLA	2	612	X	-	-	-
17	CLA	2	613	X	-	-	-
17	CLA	3	301	X	-	-	X
17	CLA	3	302	X	-	-	-
17	CLA	3	303	X	-	-	-
17	CLA	3	304	X	-	-	-
17	CLA	3	305	X	-	-	-
17	CLA	3	306	X	-	-	-
17	CLA	3	308	X	-	-	-
17	CLA	3	309	X	-	-	-
17	CLA	3	310	X	-	-	-
17	CLA	3	311	X	-	-	-
17	CLA	3	312	X	-	-	-
17	CLA	3	313	X	-	-	-
17	CLA	3	314	X	-	-	-
17	CLA	3	315	X	-	-	-
17	CLA	4	601	X	-	-	-
17	CLA	4	602	X	-	-	-
17	CLA	4	603	X	-	-	-
17	CLA	4	604	X	-	-	-
17	CLA	4	608	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
17	CLA	4	609	X	-	-	-
17	CLA	4	610	X	-	-	-
17	CLA	4	611	X	-	-	-
17	CLA	4	612	X	-	-	-
17	CLA	4	613	X	-	-	-
17	CLA	4	614	X	-	-	-
17	CLA	6	304	X	-	-	-
17	CLA	6	305	X	-	-	-
17	CLA	6	306	X	-	-	-
17	CLA	6	307	X	-	-	-
17	CLA	6	309	X	-	-	-
17	CLA	6	310	X	-	-	-
17	CLA	6	311	X	-	-	-
17	CLA	6	312	X	-	-	-
17	CLA	6	313	X	-	-	-
17	CLA	6	314	X	-	-	-
17	CLA	6	315	X	-	-	-
17	CLA	6	316	X	-	-	-
17	CLA	7	602	X	-	-	-
17	CLA	7	603	X	-	-	-
17	CLA	7	604	X	-	-	-
17	CLA	7	608	X	-	-	-
17	CLA	7	609	X	-	-	-
17	CLA	7	610	X	-	-	-
17	CLA	7	611	X	-	-	-
17	CLA	7	612	X	-	-	-
17	CLA	7	613	X	-	-	-
17	CLA	8	301	X	-	-	-
17	CLA	8	302	X	-	-	-
17	CLA	8	303	X	-	-	-
17	CLA	8	304	X	-	-	-
17	CLA	8	305	X	-	-	-
17	CLA	8	307	X	-	-	-
17	CLA	8	308	X	-	-	-
17	CLA	8	309	X	-	-	X
17	CLA	8	310	X	-	-	-
17	CLA	8	311	X	-	-	-
17	CLA	8	312	X	-	-	-
17	CLA	8	313	X	-	-	-
17	CLA	9	601	X	-	-	-
17	CLA	9	602	X	-	-	-
17	CLA	9	603	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
17	CLA	9	604	X	-	-	-
17	CLA	9	608	X	-	-	-
17	CLA	9	609	X	-	-	-
17	CLA	9	610	X	-	-	-
17	CLA	9	611	X	-	-	-
17	CLA	9	612	X	-	-	-
17	CLA	9	613	X	-	-	-
17	CLA	9	614	X	-	-	-
17	CLA	A	801	X	-	-	-
17	CLA	A	802	X	-	-	-
17	CLA	A	803	X	-	-	-
17	CLA	A	804	X	-	-	-
17	CLA	A	805	X	-	-	-
17	CLA	A	806	X	-	-	-
17	CLA	A	807	X	-	-	-
17	CLA	A	808	X	-	-	-
17	CLA	A	809	X	-	-	-
17	CLA	A	810	X	-	-	-
17	CLA	A	811	X	-	-	-
17	CLA	A	812	X	-	-	-
17	CLA	A	813	X	-	-	-
17	CLA	A	814	X	-	-	-
17	CLA	A	815	X	-	-	-
17	CLA	A	816	X	-	-	-
17	CLA	A	817	X	-	-	-
17	CLA	A	818	X	-	-	-
17	CLA	A	819	X	-	-	-
17	CLA	A	820	X	-	-	-
17	CLA	A	821	X	-	-	-
17	CLA	A	822	X	-	-	-
17	CLA	A	823	X	-	-	-
17	CLA	A	824	X	-	-	-
17	CLA	A	825	X	-	-	-
17	CLA	A	826	X	-	-	-
17	CLA	A	827	X	-	-	-
17	CLA	A	828	X	-	-	-
17	CLA	A	829	X	-	-	-
17	CLA	A	830	X	-	-	-
17	CLA	A	831	X	-	-	-
17	CLA	A	832	X	-	-	-
17	CLA	A	833	X	-	-	-
17	CLA	A	834	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
17	CLA	A	835	X	-	-	-
17	CLA	A	836	X	-	-	-
17	CLA	A	837	X	-	-	-
17	CLA	A	838	X	-	-	-
17	CLA	A	839	X	-	-	-
17	CLA	A	840	X	-	-	-
17	CLA	A	841	X	-	-	-
17	CLA	A	842	X	-	-	-
17	CLA	A	843	X	-	-	-
17	CLA	A	845	X	-	-	-
17	CLA	A	854	X	-	-	-
17	CLA	B	802	X	-	-	-
17	CLA	B	803	X	-	-	-
17	CLA	B	804	X	-	-	-
17	CLA	B	805	X	-	-	-
17	CLA	B	806	X	-	-	-
17	CLA	B	807	X	-	-	-
17	CLA	B	808	X	-	-	-
17	CLA	B	809	X	-	-	-
17	CLA	B	810	X	-	-	-
17	CLA	B	811	X	-	-	-
17	CLA	B	812	X	-	-	-
17	CLA	B	813	X	-	-	-
17	CLA	B	814	X	-	-	-
17	CLA	B	815	X	-	-	-
17	CLA	B	816	X	-	-	-
17	CLA	B	817	X	-	-	-
17	CLA	B	818	X	-	-	-
17	CLA	B	819	X	-	-	-
17	CLA	B	820	X	-	-	-
17	CLA	B	821	X	-	-	-
17	CLA	B	822	X	-	-	-
17	CLA	B	823	X	-	-	-
17	CLA	B	824	X	-	-	-
17	CLA	B	825	X	-	-	-
17	CLA	B	826	X	-	-	-
17	CLA	B	827	X	-	-	-
17	CLA	B	828	X	-	-	-
17	CLA	B	829	X	-	-	-
17	CLA	B	830	X	-	-	-
17	CLA	B	831	X	-	-	-
17	CLA	B	832	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
17	CLA	B	833	X	-	-	-
17	CLA	B	834	X	-	-	-
17	CLA	B	835	X	-	-	-
17	CLA	B	836	X	-	-	-
17	CLA	B	837	X	-	-	-
17	CLA	B	838	X	-	-	-
17	CLA	B	839	X	-	-	-
17	CLA	B	840	X	-	-	-
17	CLA	B	841	X	-	-	-
17	CLA	F	301	X	-	-	-
17	CLA	F	303	X	-	-	-
17	CLA	F	304	X	-	-	-
17	CLA	G	101	X	-	-	-
17	CLA	G	103	X	-	-	-
17	CLA	G	104	X	-	-	-
17	CLA	J	3002	X	-	-	-
17	CLA	K	4002	X	-	-	X
17	CLA	K	4003	X	-	-	-
17	CLA	L	202	X	-	-	-
17	CLA	L	203	X	-	-	-
17	CLA	L	204	X	-	-	-
17	CLA	a	801	X	-	-	-
17	CLA	a	802	X	-	-	-
17	CLA	a	803	X	-	-	-
17	CLA	a	804	X	-	-	-
17	CLA	a	805	X	-	-	-
17	CLA	a	806	X	-	-	-
17	CLA	a	807	X	-	-	-
17	CLA	a	808	X	-	-	-
17	CLA	a	809	X	-	-	-
17	CLA	a	810	X	-	-	-
17	CLA	a	811	X	-	-	-
17	CLA	a	812	X	-	-	-
17	CLA	a	813	X	-	-	-
17	CLA	a	814	X	-	-	-
17	CLA	a	815	X	-	-	-
17	CLA	a	816	X	-	-	-
17	CLA	a	817	X	-	-	-
17	CLA	a	818	X	-	-	-
17	CLA	a	819	X	-	-	-
17	CLA	a	820	X	-	-	-
17	CLA	a	821	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
17	CLA	a	822	X	-	-	-
17	CLA	a	823	X	-	-	-
17	CLA	a	824	X	-	-	-
17	CLA	a	825	X	-	-	-
17	CLA	a	826	X	-	-	-
17	CLA	a	827	X	-	-	-
17	CLA	a	828	X	-	-	-
17	CLA	a	829	X	-	-	-
17	CLA	a	830	X	-	-	-
17	CLA	a	831	X	-	-	-
17	CLA	a	832	X	-	-	-
17	CLA	a	833	X	-	-	-
17	CLA	a	834	X	-	-	-
17	CLA	a	835	X	-	-	-
17	CLA	a	836	X	-	-	-
17	CLA	a	837	X	-	-	-
17	CLA	a	838	X	-	-	-
17	CLA	a	839	X	-	-	-
17	CLA	a	840	X	-	-	-
17	CLA	a	841	X	-	-	-
17	CLA	a	842	X	-	-	-
17	CLA	a	843	X	-	-	-
17	CLA	a	844	X	-	-	-
17	CLA	a	846	X	-	-	-
17	CLA	a	856	X	-	-	-
17	CLA	b	802	X	-	-	-
17	CLA	b	803	X	-	-	-
17	CLA	b	804	X	-	-	-
17	CLA	b	805	X	-	-	-
17	CLA	b	806	X	-	-	-
17	CLA	b	807	X	-	-	-
17	CLA	b	808	X	-	-	-
17	CLA	b	809	X	-	-	-
17	CLA	b	810	X	-	-	-
17	CLA	b	811	X	-	-	-
17	CLA	b	812	X	-	-	-
17	CLA	b	813	X	-	-	-
17	CLA	b	814	X	-	-	-
17	CLA	b	815	X	-	-	-
17	CLA	b	816	X	-	-	-
17	CLA	b	817	X	-	-	-
17	CLA	b	818	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
17	CLA	b	819	X	-	-	-
17	CLA	b	820	X	-	-	-
17	CLA	b	821	X	-	-	-
17	CLA	b	822	X	-	-	-
17	CLA	b	823	X	-	-	-
17	CLA	b	824	X	-	-	-
17	CLA	b	825	X	-	-	-
17	CLA	b	826	X	-	-	-
17	CLA	b	827	X	-	-	-
17	CLA	b	828	X	-	-	-
17	CLA	b	829	X	-	-	-
17	CLA	b	830	X	-	-	-
17	CLA	b	831	X	-	-	-
17	CLA	b	832	X	-	-	-
17	CLA	b	833	X	-	-	-
17	CLA	b	834	X	-	-	-
17	CLA	b	835	X	-	-	-
17	CLA	b	836	X	-	-	-
17	CLA	b	837	X	-	-	-
17	CLA	b	838	X	-	-	-
17	CLA	b	839	X	-	-	-
17	CLA	b	840	X	-	-	-
17	CLA	b	841	X	-	-	-
17	CLA	f	7002	X	-	-	-
17	CLA	f	7003	X	-	-	-
17	CLA	g	101	X	-	-	-
17	CLA	g	102	X	-	-	-
17	CLA	g	103	X	-	-	-
17	CLA	j	3002	X	-	-	-
17	CLA	k	1401	X	-	-	-
17	CLA	k	1402	X	-	-	-
17	CLA	k	1403	X	-	-	-
17	CLA	l	202	X	-	-	-
17	CLA	l	203	X	-	-	-
17	CLA	l	204	X	-	-	-
19	LHG	3	319	-	-	-	X
20	BCR	1	318	-	-	-	X
20	BCR	2	617	-	-	-	X
20	BCR	7	617	-	-	-	X
20	BCR	K	4001	-	-	-	X
20	BCR	K	4004	-	-	-	X
20	BCR	L	206	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
20	BCR	l	206	-	-	-	X
25	LMG	4	620	-	-	-	X
26	CHL	1	302	X	-	-	-
26	CHL	1	307	X	-	-	-
26	CHL	2	601	X	-	-	-
26	CHL	2	605	X	-	-	-
26	CHL	2	606	X	-	-	-
26	CHL	2	607	X	-	-	-
26	CHL	2	614	X	-	-	-
26	CHL	3	307	X	-	-	-
26	CHL	4	605	X	-	-	-
26	CHL	4	606	X	-	-	-
26	CHL	4	607	X	-	-	-
26	CHL	4	615	X	-	-	-
26	CHL	6	303	X	-	-	-
26	CHL	6	308	X	-	-	-
26	CHL	7	601	X	-	-	-
26	CHL	7	605	X	-	-	-
26	CHL	7	606	X	-	-	-
26	CHL	7	607	X	-	-	-
26	CHL	7	614	X	-	-	-
26	CHL	8	306	X	-	-	-
26	CHL	9	605	X	-	-	-
26	CHL	9	606	X	-	-	-
26	CHL	9	607	X	-	-	-
26	CHL	9	615	X	-	-	-
27	LUT	6	317	-	-	-	X
27	LUT	6	321	-	-	-	X

2 Entry composition

There are 29 unique types of molecules in this entry. The entry contains 71157 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 Photosystem I P700 chlorophyll a apoprotein A1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	742	Total	C	N	O	S	0	0	0
			5846	3831	994	1003	18			
1	a	742	Total	C	N	O	S	0	0	0
			5846	3831	994	1003	18			

- Molecule 2 is a protein called Photosystem I P700 chlorophyll a apoprotein A2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	733	Total	C	N	O	S	0	0	0
			5863	3853	1002	994	14			
2	b	733	Total	C	N	O	S	0	0	0
			5863	3853	1002	994	14			

- Molecule 3 is a protein called Photosystem I iron-sulfur center.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	80	Total	C	N	O	S	0	0	0
			611	379	107	114	11			
3	c	80	Total	C	N	O	S	0	0	0
			611	379	107	114	11			

- Molecule 4 is a protein called Uncharacterized protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	141	Total	C	N	O	S	0	0	0
			1114	716	193	202	3			
4	d	140	Total	C	N	O	S	0	0	0
			1107	712	192	200	3			

- Molecule 5 is a protein called Putative uncharacterized protein.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
5	E	63	Total 507	C 321	N 90	O 96	0	0	0
5	e	63	Total 506	C 322	N 90	O 94	0	0	0

- Molecule 6 is a protein called Photosystem I reaction center subunit III, chloroplastic.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	F	151	Total 1193	C 776	N 204	O 210	S 3	0	0	0
6	f	151	Total 1193	C 776	N 204	O 210	S 3	0	0	0

- Molecule 7 is a protein called Photosystem I reaction center subunit V, chloroplastic.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
7	G	95	Total 741	C 480	N 121	O 140	0	0	0
7	g	95	Total 737	C 478	N 121	O 138	0	0	0

- Molecule 8 is a protein called Putative uncharacterized protein.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
8	H	90	Total 678	C 439	N 110	O 129	0	0	0
8	h	90	Total 682	C 442	N 111	O 129	0	0	0

- Molecule 9 is a protein called Photosystem I reaction center subunit VIII.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	I	29	Total 221	C 153	N 33	O 34	S 1	0	0	0
9	i	30	Total 226	C 156	N 34	O 35	S 1	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	J	39	Total 311	C 211	N 48	O 51	S 1	0	0	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	j	39	Total	C	N	O	S	0	0	0
			311	211	48	51	1			

- Molecule 11 is a protein called Photosystem I reaction center subunit X psaK.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	K	45	Total	C	N	O	S	0	0	0
			311	204	48	56	3			
11	k	46	Total	C	N	O	S	0	0	0
			316	207	49	57	3			

- Molecule 12 is a protein called Putative uncharacterized protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	L	153	Total	C	N	O	S	0	0	0
			1136	746	183	206	1			
12	l	151	Total	C	N	O	S	0	0	0
			1122	738	180	203	1			

- Molecule 13 is a protein called Chlorophyll a-b binding protein 6, chloroplastic.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	1	195	Total	C	N	O	S	0	0	0
			1491	969	249	268	5			
13	6	195	Total	C	N	O	S	0	0	0
			1483	963	247	268	5			

- Molecule 14 is a protein called Type II chlorophyll a/b binding protein from photosystem I.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	2	206	Total	C	N	O	S	0	0	0
			1610	1055	263	288	4			
14	7	206	Total	C	N	O	S	0	0	0
			1610	1055	263	288	4			

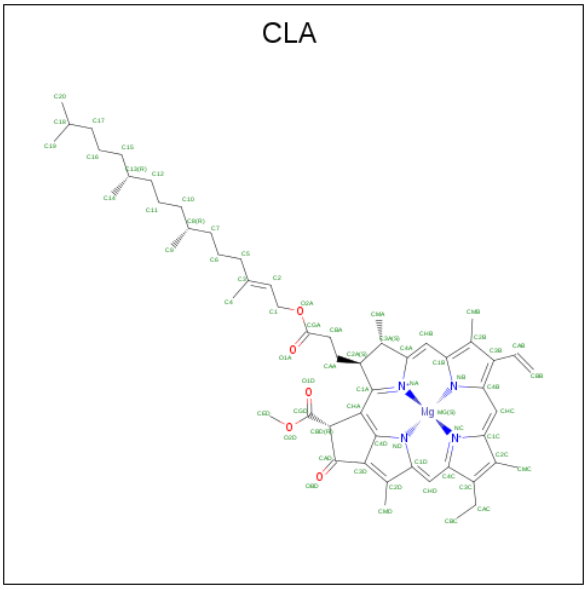
- Molecule 15 is a protein called Chlorophyll a-b binding protein 3, chloroplastic.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
15	3	218	Total	C	N	O	S	0	0	0
			1680	1100	273	302	5			
15	8	217	Total	C	N	O	S	0	0	0
			1672	1094	272	301	5			

- Molecule 16 is a protein called Chlorophyll a-b binding protein P4, chloroplastic.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
16	4	196	Total	C	N	O	S	0	0	0
			1540	1009	251	277	3			
16	9	196	Total	C	N	O	S	0	0	0
			1540	1009	251	277	3			

- Molecule 17 is CHLOROPHYLL A (three-letter code: CLA) (formula: $C_{55}H_{72}MgN_4O_5$).



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
			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		

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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
			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		
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		

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

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
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
			60	50	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		
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
			46	36	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		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
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
			49	39	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
			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		
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
			45	35	1	4	5		
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
			42	34	1	4	3		
17	K	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
17	K	1	Total	C	Mg	N	O	0	0
			46	36	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
			65	55	1	4	5		
17	L	1	Total	C	Mg	N	O	0	0
			50	40	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
			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
			52	42	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
			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
			41	33	1	4	3		
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
			65	55	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
			65	55	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		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
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	3	1	Total	C	Mg	N	O	0	0
			46	36	1	4	5		
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
			37	31	1	4	1		
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	3	1	Total	C	Mg	N		0	0
			25	20	1	4			
17	4	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
			46	36	1	4	5		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
17	4	1	Total C Mg N O 50 40 1 4 5	0	0
17	4	1	Total C Mg N O 50 40 1 4 5	0	0
17	4	1	Total C Mg N O 60 50 1 4 5	0	0
17	4	1	Total C Mg N O 55 45 1 4 5	0	0
17	4	1	Total C Mg N O 52 42 1 4 5	0	0
17	4	1	Total C Mg N O 56 46 1 4 5	0	0
17	4	1	Total C Mg N O 45 35 1 4 5	0	0
17	4	1	Total C Mg N O 50 40 1 4 5	0	0
17	a	1	Total C Mg N O 65 55 1 4 5	0	0
17	a	1	Total C Mg N O 65 55 1 4 5	0	0
17	a	1	Total C Mg N O 65 55 1 4 5	0	0
17	a	1	Total C Mg N O 65 55 1 4 5	0	0
17	a	1	Total C Mg N O 55 45 1 4 5	0	0
17	a	1	Total C Mg N O 65 55 1 4 5	0	0
17	a	1	Total C Mg N O 65 55 1 4 5	0	0
17	a	1	Total C Mg N O 65 55 1 4 5	0	0
17	a	1	Total C Mg N O 65 55 1 4 5	0	0
17	a	1	Total C Mg N O 65 55 1 4 5	0	0
17	a	1	Total C Mg N O 65 55 1 4 5	0	0
17	a	1	Total C Mg N O 65 55 1 4 5	0	0
17	a	1	Total C Mg N O 54 44 1 4 5	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
17	a	1	Total C Mg N O 65 55 1 4 5	0	0
17	a	1	Total C Mg N O 45 35 1 4 5	0	0
17	a	1	Total C Mg N O 50 40 1 4 5	0	0
17	a	1	Total C Mg N O 45 35 1 4 5	0	0
17	a	1	Total C Mg N O 65 55 1 4 5	0	0
17	a	1	Total C Mg N O 65 55 1 4 5	0	0
17	a	1	Total C Mg N O 65 55 1 4 5	0	0
17	a	1	Total C Mg N O 45 35 1 4 5	0	0
17	a	1	Total C Mg N O 65 55 1 4 5	0	0
17	a	1	Total C Mg N O 49 39 1 4 5	0	0
17	a	1	Total C Mg N O 51 41 1 4 5	0	0
17	a	1	Total C Mg N O 55 45 1 4 5	0	0
17	a	1	Total C Mg N O 65 55 1 4 5	0	0
17	a	1	Total C Mg N O 65 55 1 4 5	0	0
17	a	1	Total C Mg N O 65 55 1 4 5	0	0
17	a	1	Total C Mg N O 65 55 1 4 5	0	0
17	a	1	Total C Mg N O 65 55 1 4 5	0	0
17	a	1	Total C Mg N O 65 55 1 4 5	0	0
17	a	1	Total C Mg N O 50 40 1 4 5	0	0
17	a	1	Total C Mg N O 65 55 1 4 5	0	0
17	a	1	Total C Mg N O 65 55 1 4 5	0	0

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

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
17	b	1	Total C Mg N O 54 44 1 4 5	0	0
17	b	1	Total C Mg N O 55 45 1 4 5	0	0
17	b	1	Total C Mg N O 65 55 1 4 5	0	0
17	b	1	Total C Mg N O 65 55 1 4 5	0	0
17	b	1	Total C Mg N O 55 45 1 4 5	0	0
17	b	1	Total C Mg N O 55 45 1 4 5	0	0
17	b	1	Total C Mg N O 59 49 1 4 5	0	0
17	b	1	Total C Mg N O 60 50 1 4 5	0	0
17	b	1	Total C Mg N O 65 55 1 4 5	0	0
17	b	1	Total C Mg N O 50 40 1 4 5	0	0
17	b	1	Total C Mg N O 46 36 1 4 5	0	0
17	b	1	Total C Mg N O 55 45 1 4 5	0	0
17	b	1	Total C Mg N O 60 50 1 4 5	0	0
17	b	1	Total C Mg N O 65 55 1 4 5	0	0
17	b	1	Total C Mg N O 65 55 1 4 5	0	0
17	b	1	Total C Mg N O 65 55 1 4 5	0	0
17	b	1	Total C Mg N O 65 55 1 4 5	0	0
17	b	1	Total C Mg N O 65 55 1 4 5	0	0
17	b	1	Total C Mg N O 65 55 1 4 5	0	0
17	b	1	Total C Mg N O 50 40 1 4 5	0	0
17	b	1	Total C Mg N O 49 39 1 4 5	0	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
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
			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		
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
			42	34	1	4	3		
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
			46	36	1	4	5		
17	k	1	Total	C	Mg	N	O	0	0
			46	36	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
			65	55	1	4	5		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
17	l	1	Total	C	Mg	N	O	0	0
			50	40	1	4	5		
17	6	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
17	6	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
17	6	1	Total	C	Mg	N	O	0	0
			51	41	1	4	5		
17	6	1	Total	C	Mg	N	O	0	0
			42	34	1	4	3		
17	6	1	Total	C	Mg	N	O	0	0
			46	36	1	4	5		
17	6	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
17	6	1	Total	C	Mg	N	O	0	0
			60	50	1	4	5		
17	6	1	Total	C	Mg	N	O	0	0
			41	33	1	4	3		
17	6	1	Total	C	Mg	N	O	0	0
			52	42	1	4	5		
17	6	1	Total	C	Mg	N	O	0	0
			60	50	1	4	5		
17	6	1	Total	C	Mg	N	O	0	0
			55	45	1	4	5		
17	6	1	Total	C	Mg	N	O	0	0
			46	36	1	4	5		
17	7	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
17	7	1	Total	C	Mg	N	O	0	0
			51	41	1	4	5		
17	7	1	Total	C	Mg	N	O	0	0
			60	50	1	4	5		
17	7	1	Total	C	Mg	N	O	0	0
			50	40	1	4	5		
17	7	1	Total	C	Mg	N	O	0	0
			60	50	1	4	5		
17	7	1	Total	C	Mg	N	O	0	0
			41	33	1	4	3		
17	7	1	Total	C	Mg	N	O	0	0
			52	42	1	4	5		
17	7	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
17	7	1	Total	C	Mg	N	O	0	0
			43	35	1	4	3		
17	8	1	Total	C	Mg	N	O	0	0
			60	50	1	4	5		
17	8	1	Total	C	Mg	N	O	0	0
			50	40	1	4	5		
17	8	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
17	8	1	Total	C	Mg	N	O	0	0
			42	34	1	4	3		
17	8	1	Total	C	Mg	N	O	0	0
			47	37	1	4	5		
17	8	1	Total	C	Mg	N	O	0	0
			50	40	1	4	5		
17	8	1	Total	C	Mg	N	O	0	0
			50	40	1	4	5		
17	8	1	Total	C	Mg	N	O	0	0
			52	42	1	4	5		
17	8	1	Total	C	Mg	N	O	0	0
			55	45	1	4	5		
17	8	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
17	8	1	Total	C	Mg	N	O	0	0
			46	36	1	4	5		
17	8	1	Total	C	Mg	N		0	0
			25	20	1	4			
17	9	1	Total	C	Mg	N	O	0	0
			46	36	1	4	5		
17	9	1	Total	C	Mg	N	O	0	0
			60	50	1	4	5		
17	9	1	Total	C	Mg	N	O	0	0
			46	36	1	4	5		
17	9	1	Total	C	Mg	N	O	0	0
			50	40	1	4	5		
17	9	1	Total	C	Mg	N	O	0	0
			50	40	1	4	5		
17	9	1	Total	C	Mg	N	O	0	0
			60	50	1	4	5		
17	9	1	Total	C	Mg	N	O	0	0
			41	33	1	4	3		
17	9	1	Total	C	Mg	N	O	0	0
			52	42	1	4	5		

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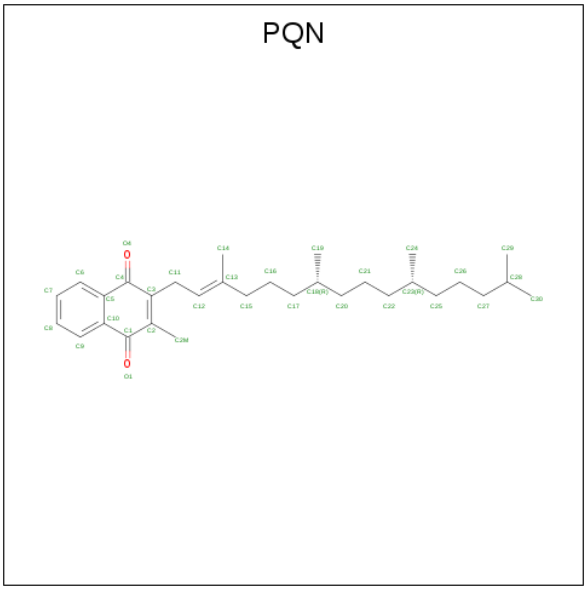
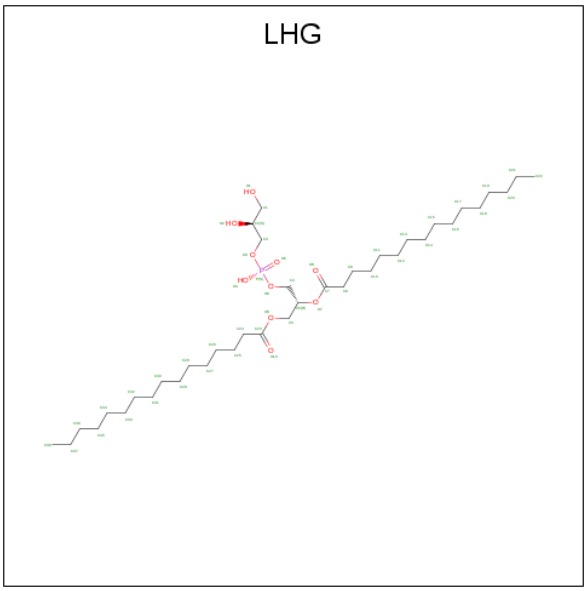
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
17	9	1	Total	C	Mg	N	O	0	0
			56	46	1	4	5		
17	9	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
17	9	1	Total	C	Mg	N	O	0	0
			47	37	1	4	5		

- Molecule 18 is PHYLLOQUINONE (three-letter code: PQN) (formula: $C_{31}H_{46}O_2$).



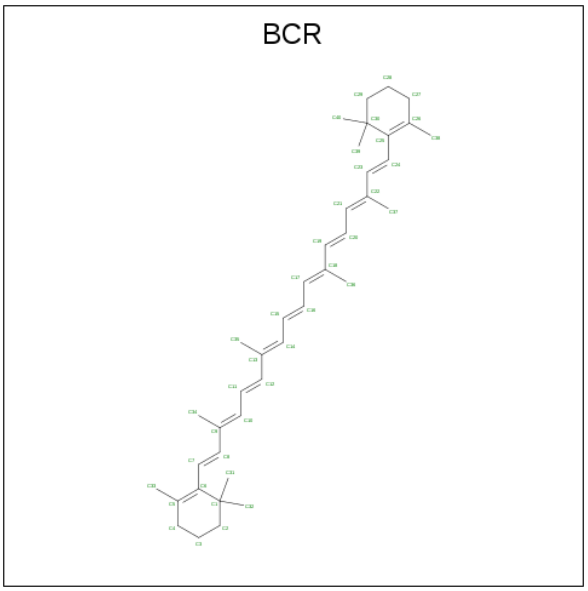
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
18	A	1	Total	C	O	0	0
			33	31	2		
18	B	1	Total	C	O	0	0
			33	31	2		
18	a	1	Total	C	O	0	0
			33	31	2		
18	b	1	Total	C	O	0	0
			33	31	2		

- Molecule 19 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (three-letter code: LHG) (formula: $C_{38}H_{75}O_{10}P$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
19	A	1	Total	C	O	P	0	0
			49	38	10	1		
19	A	1	Total	C	O	P	0	0
			27	16	10	1		
19	1	1	Total	C	O	P	0	0
			23	12	10	1		
19	1	1	Total	C	O	P	0	0
			49	38	10	1		
19	2	1	Total	C	O	P	0	0
			37	26	10	1		
19	3	1	Total	C	O	P	0	0
			20	10	9	1		
19	a	1	Total	C	O	P	0	0
			49	38	10	1		
19	a	1	Total	C	O	P	0	0
			27	16	10	1		
19	6	1	Total	C	O	P	0	0
			23	12	10	1		
19	6	1	Total	C	O	P	0	0
			49	38	10	1		
19	7	1	Total	C	O	P	0	0
			37	26	10	1		

- Molecule 20 is BETA-CAROTENE (three-letter code: BCR) (formula: $C_{40}H_{56}$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
20	A	1	Total C 40 40	0	0
20	A	1	Total C 40 40	0	0
20	A	1	Total C 40 40	0	0
20	A	1	Total C 40 40	0	0
20	A	1	Total C 40 40	0	0
20	A	1	Total C 40 40	0	0
20	B	1	Total C 40 40	0	0
20	B	1	Total C 40 40	0	0
20	B	1	Total C 40 40	0	0
20	B	1	Total C 40 40	0	0
20	B	1	Total C 40 40	0	0
20	B	1	Total C 40 40	0	0
20	B	1	Total C 40 40	0	0
20	F	1	Total C 40 40	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
20	G	1	Total C 40 40	0	0
20	I	1	Total C 40 40	0	0
20	J	1	Total C 40 40	0	0
20	K	1	Total C 40 40	0	0
20	K	1	Total C 40 40	0	0
20	L	1	Total C 40 40	0	0
20	L	1	Total C 40 40	0	0
20	L	1	Total C 40 40	0	0
20	1	1	Total C 40 40	0	0
20	2	1	Total C 40 40	0	0
20	3	1	Total C 40 40	0	0
20	4	1	Total C 40 40	0	0
20	a	1	Total C 40 40	0	0
20	a	1	Total C 40 40	0	0
20	a	1	Total C 40 40	0	0
20	a	1	Total C 40 40	0	0
20	a	1	Total C 40 40	0	0
20	a	1	Total C 40 40	0	0
20	b	1	Total C 40 40	0	0
20	b	1	Total C 40 40	0	0
20	b	1	Total C 40 40	0	0

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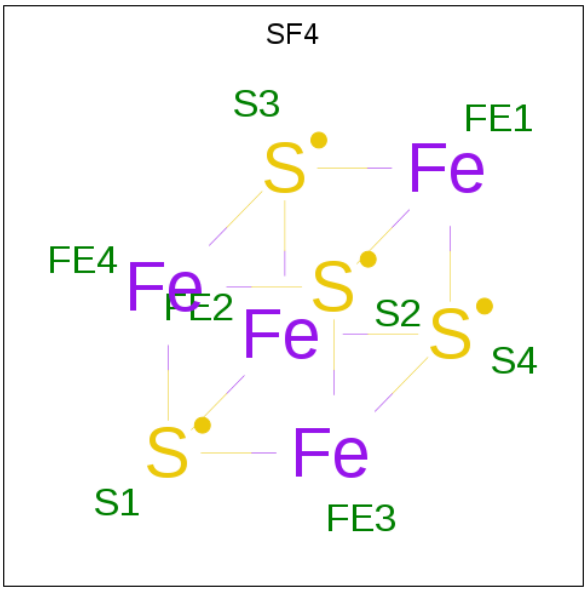
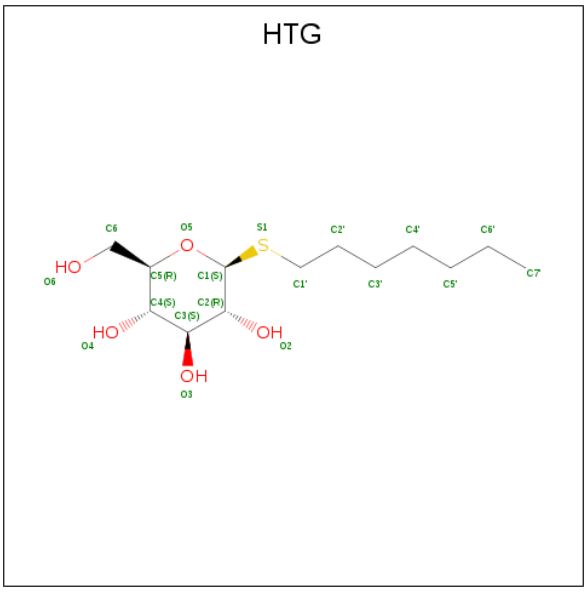
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
20	b	1	Total C 40 40	0	0
20	b	1	Total C 40 40	0	0
20	b	1	Total C 40 40	0	0
20	b	1	Total C 40 40	0	0
20	f	1	Total C 40 40	0	0
20	g	1	Total C 40 40	0	0
20	i	1	Total C 40 40	0	0
20	j	1	Total C 40 40	0	0
20	j	1	Total C 40 40	0	0
20	k	1	Total C 40 40	0	0
20	l	1	Total C 40 40	0	0
20	l	1	Total C 40 40	0	0
20	l	1	Total C 40 40	0	0
20	6	1	Total C 40 40	0	0
20	7	1	Total C 40 40	0	0
20	8	1	Total C 40 40	0	0
20	9	1	Total C 40 40	0	0

- Molecule 21 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe_4S_4).



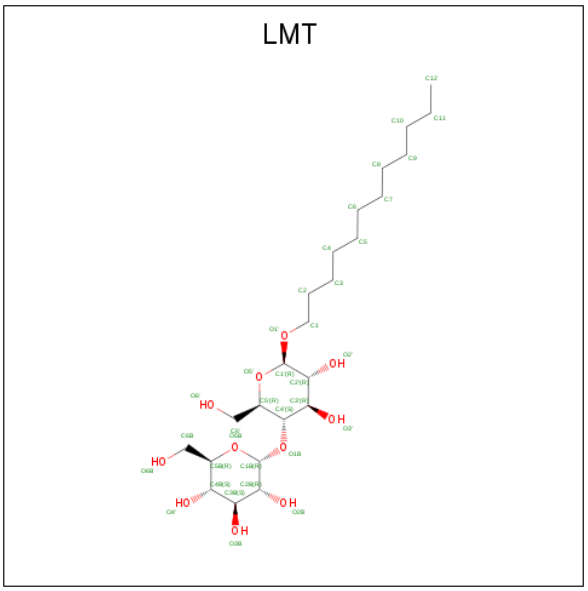
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
21	A	1	Total Fe S 8 4 4	0	0
21	C	1	Total Fe S 8 4 4	0	0
21	C	1	Total Fe S 8 4 4	0	0
21	a	1	Total Fe S 8 4 4	0	0
21	c	1	Total Fe S 8 4 4	0	0
21	c	1	Total Fe S 8 4 4	0	0

- Molecule 22 is heptyl 1-thio-beta-D-glucopyranoside (three-letter code: HTG) (formula: $C_{13}H_{26}O_5S$).



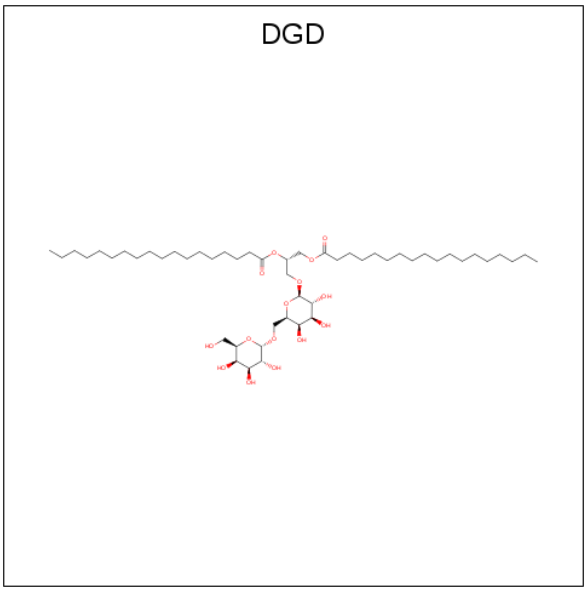
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
22	A	1	Total	C	O	S	0	0
			19	13	5	1		
22	F	1	Total	C	O	S	0	0
			19	13	5	1		
22	J	1	Total	C	O	S	0	0
			19	13	5	1		
22	a	1	Total	C	O	S	0	0
			19	13	5	1		
22	f	1	Total	C	O	S	0	0
			19	13	5	1		
22	j	1	Total	C	O	S	0	0
			19	13	5	1		

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



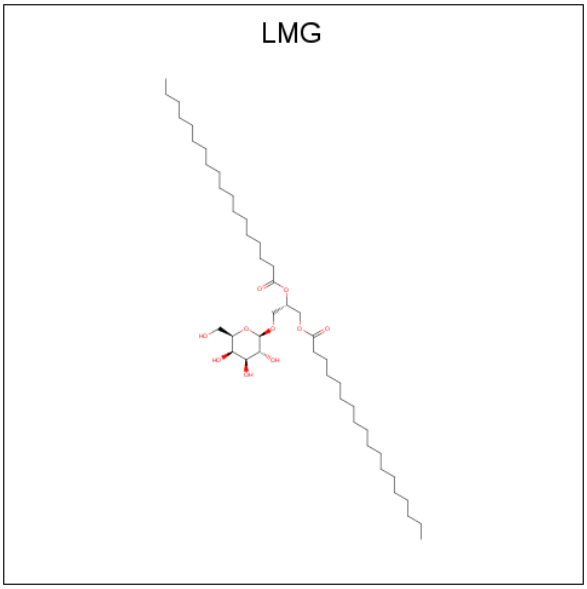
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
23	B	1	Total C O 35 24 11	0	0

- Molecule 24 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (three-letter code: DGD) (formula: $C_{51}H_{96}O_{15}$).



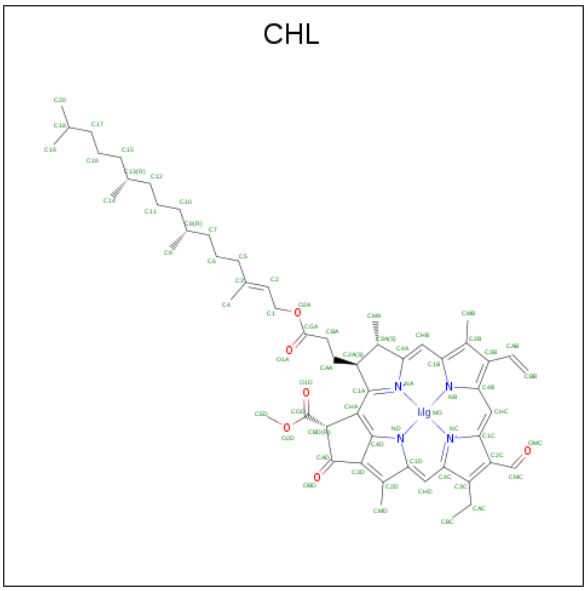
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
24	B	1	Total C O 66 51 15	0	0
24	b	1	Total C O 66 51 15	0	0

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



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
25	G	1	Total	C	O	0	0
			44	34	10		
25	4	1	Total	C	O	0	0
			44	34	10		
25	4	1	Total	C	O	0	0
			44	34	10		
25	6	1	Total	C	O	0	0
			40	30	10		
25	9	1	Total	C	O	0	0
			50	40	10		

- Molecule 26 is CHLOROPHYLL B (three-letter code: CHL) (formula: $C_{55}H_{70}MgN_4O_6$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
26	1	1	Total	C	Mg	N	O	0	0
			61	50	1	4	6		
26	1	1	Total	C	Mg	N	O	0	0
			48	37	1	4	6		
26	2	1	Total	C	Mg	N	O	0	0
			61	50	1	4	6		
26	2	1	Total	C	Mg	N	O	0	0
			43	34	1	4	4		
26	2	1	Total	C	Mg	N	O	0	0
			48	37	1	4	6		
26	2	1	Total	C	Mg	N	O	0	0
			51	40	1	4	6		
26	2	1	Total	C	Mg	N	O	0	0
			43	34	1	4	4		
26	3	1	Total	C	Mg	N	O	0	0
			47	36	1	4	6		
26	4	1	Total	C	Mg	N	O	0	0
			56	45	1	4	6		
26	4	1	Total	C	Mg	N	O	0	0
			51	40	1	4	6		
26	4	1	Total	C	Mg	N	O	0	0
			51	40	1	4	6		
26	4	1	Total	C	Mg	N	O	0	0
			43	34	1	4	4		
26	6	1	Total	C	Mg	N	O	0	0
			61	50	1	4	6		
26	6	1	Total	C	Mg	N	O	0	0
			47	36	1	4	6		

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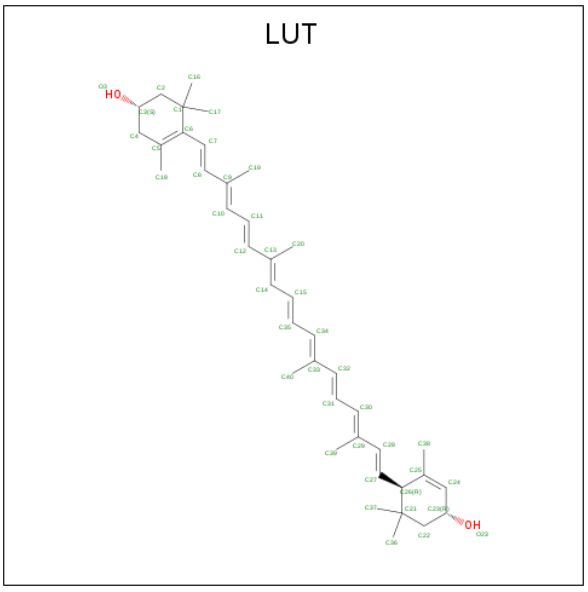
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
26	7	1	Total	C	Mg	N	O	0	0
			61	50	1	4	6		
26	7	1	Total	C	Mg	N	O	0	0
			43	34	1	4	4		
26	7	1	Total	C	Mg	N	O	0	0
			48	37	1	4	6		
26	7	1	Total	C	Mg	N	O	0	0
			51	40	1	4	6		
26	7	1	Total	C	Mg	N	O	0	0
			43	34	1	4	4		
26	8	1	Total	C	Mg	N	O	0	0
			47	36	1	4	6		
26	9	1	Total	C	Mg	N	O	0	0
			56	45	1	4	6		
26	9	1	Total	C	Mg	N	O	0	0
			51	40	1	4	6		
26	9	1	Total	C	Mg	N	O	0	0
			51	40	1	4	6		
26	9	1	Total	C	Mg	N	O	0	0
			43	34	1	4	4		

- Molecule 27 is (3R,3'R,6S)-4,5-DIDEHYDRO-5,6-DIHYDRO-BETA,BETA-CAROTENE-3 ,3'-DIOL (three-letter code: LUT) (formula: $C_{40}H_{56}O_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
27	1	1	Total	C	O	0	0
			42	40	2		

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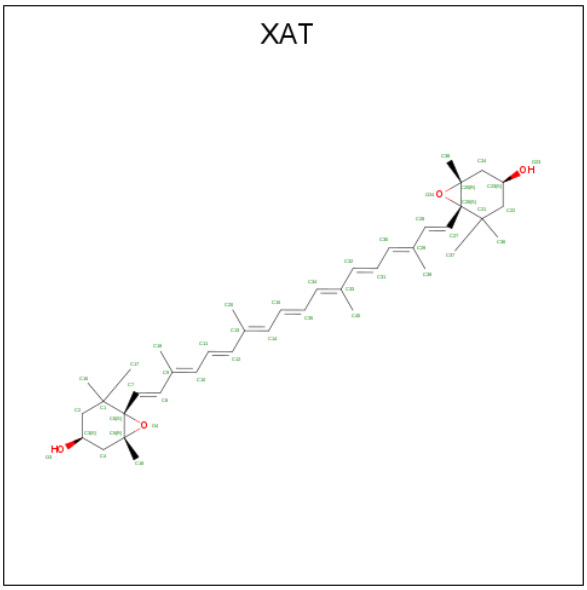
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
27	1	1	Total C O 42 40 2	0	0
27	2	1	Total C O 42 40 2	0	0
27	3	1	Total C O 42 40 2	0	0
27	4	1	Total C O 42 40 2	0	0
27	6	1	Total C O 42 40 2	0	0
27	6	1	Total C O 42 40 2	0	0
27	7	1	Total C O 42 40 2	0	0
27	8	1	Total C O 42 40 2	0	0
27	9	1	Total C O 42 40 2	0	0

- Molecule 28 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 (three-letter code: XAT) (formula: $C_{40}H_{56}O_4$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
28	1	1	Total C O 44 40 4	0	0
28	2	1	Total C O 44 40 4	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
28	3	1	Total C O 44 40 4	0	0
28	4	1	Total C O 44 40 4	0	0
28	6	1	Total C O 44 40 4	0	0
28	7	1	Total C O 44 40 4	0	0
28	8	1	Total C O 44 40 4	0	0
28	9	1	Total C O 44 40 4	0	0

- Molecule 29 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
29	A	29	Total O 29 29	0	0
29	B	42	Total O 42 42	0	0
29	C	1	Total O 1 1	0	0
29	D	2	Total O 2 2	0	0
29	F	5	Total O 5 5	0	0
29	I	1	Total O 1 1	0	0
29	L	1	Total O 1 1	0	0
29	1	3	Total O 3 3	0	0
29	2	4	Total O 4 4	0	0
29	3	3	Total O 3 3	0	0
29	4	6	Total O 6 6	0	0
29	a	30	Total O 30 30	0	0
29	b	32	Total O 32 32	0	0

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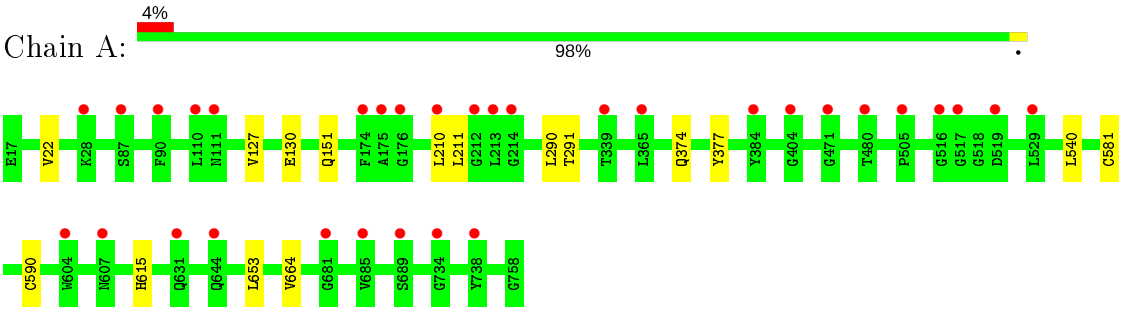
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
29	d	1	Total O 1 1	0	0
29	f	4	Total O 4 4	0	0
29	h	1	Total O 1 1	0	0
29	l	3	Total O 3 3	0	0
29	6	3	Total O 3 3	0	0
29	7	6	Total O 6 6	0	0
29	8	3	Total O 3 3	0	0
29	9	5	Total O 5 5	0	0

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.

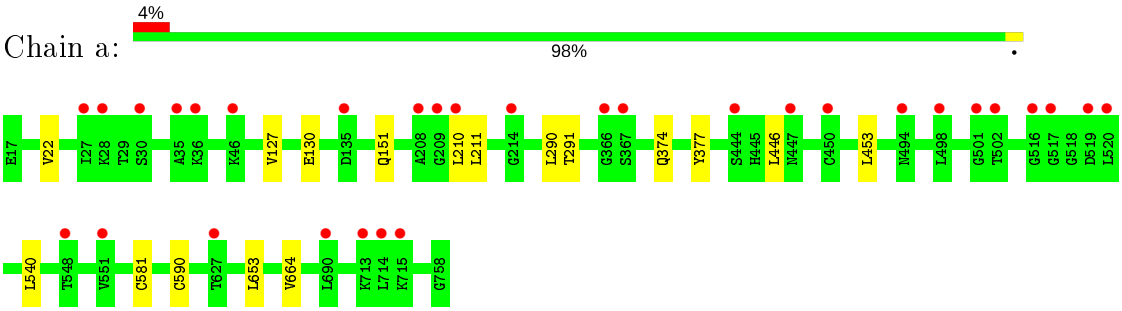
- Molecule 1: Photosystem I P700 chlorophyll a apoprotein A1

Chain A:



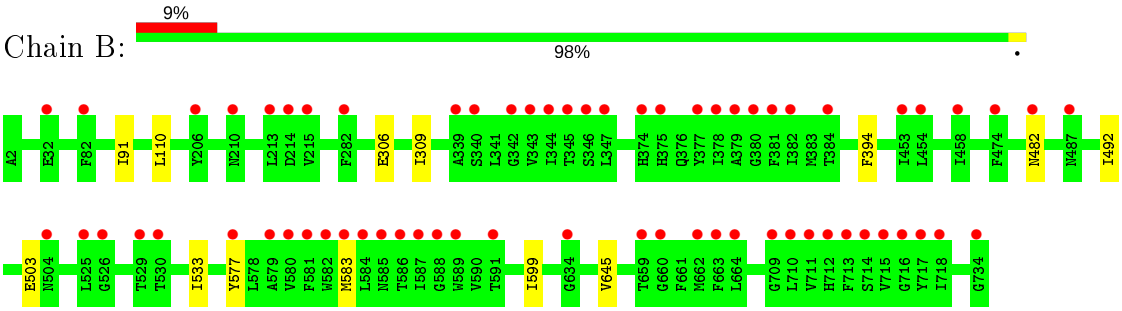
- Molecule 1: Photosystem I P700 chlorophyll a apoprotein A1

Chain a:



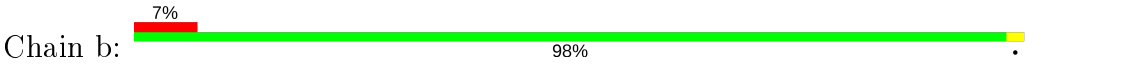
- Molecule 2: Photosystem I P700 chlorophyll a apoprotein A2

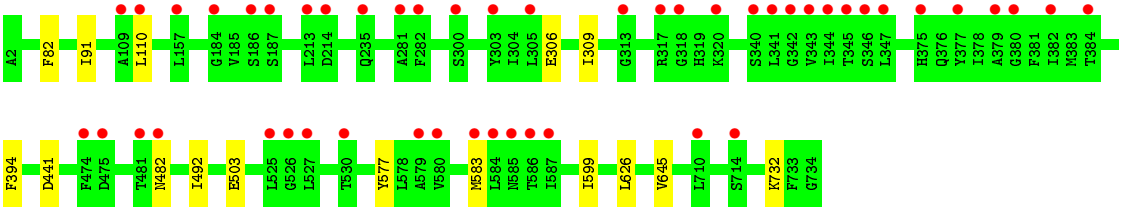
Chain B:



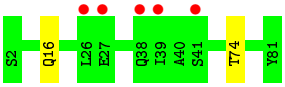
- Molecule 2: Photosystem I P700 chlorophyll a apoprotein A2

Chain b:



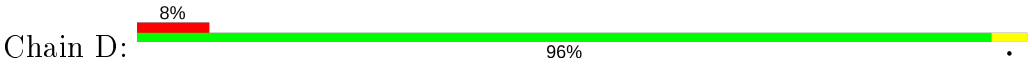


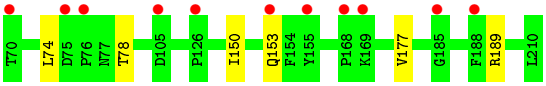
• Molecule 3: Photosystem I iron-sulfur center



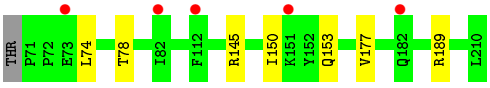
• Molecule 3: Photosystem I iron-sulfur center

• Molecule 4: Uncharacterized protein

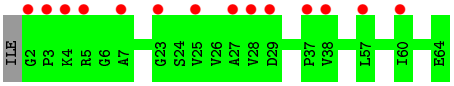




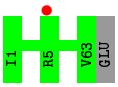
• Molecule 4: Uncharacterized protein



• Molecule 5: Putative uncharacterized protein

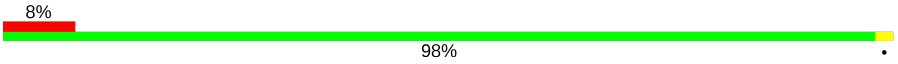


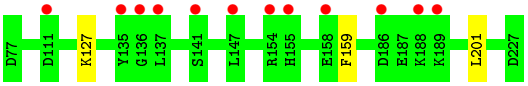
• Molecule 5: Putative uncharacterized protein



• Molecule 6: Photosystem I reaction center subunit III, chloroplastic

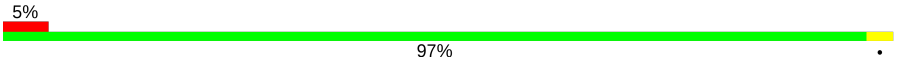
Chain F:

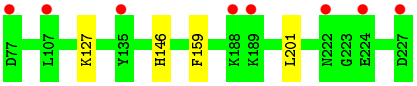




• Molecule 6: Photosystem I reaction center subunit III, chloroplastic

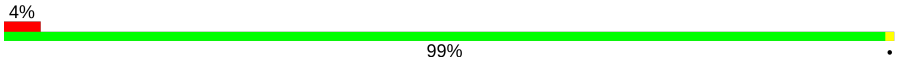
Chain f:

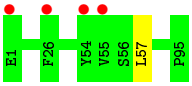




• Molecule 7: Photosystem I reaction center subunit V, chloroplastic

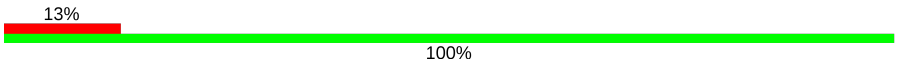
Chain G:

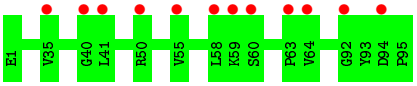




• Molecule 7: Photosystem I reaction center subunit V, chloroplastic

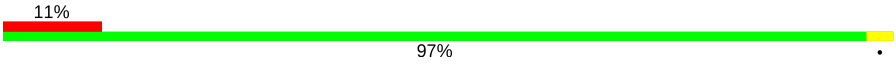
Chain g:

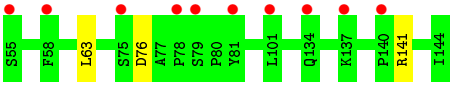




• Molecule 8: Putative uncharacterized protein

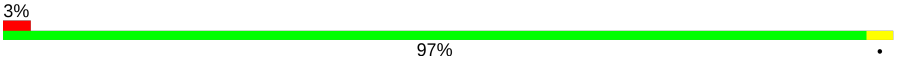
Chain H:





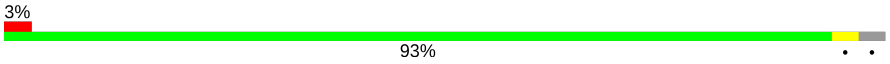
• Molecule 8: Putative uncharacterized protein

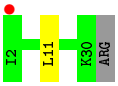
Chain h:



• Molecule 9: Photosystem I reaction center subunit VIII

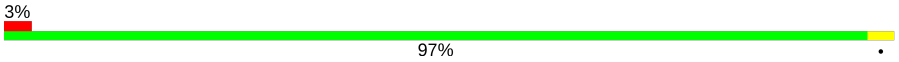
Chain I:





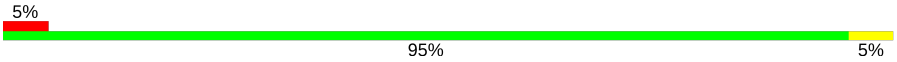
• Molecule 9: Photosystem I reaction center subunit VIII

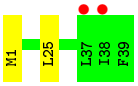
Chain i:



• Molecule 10: Photosystem I reaction center subunit IX

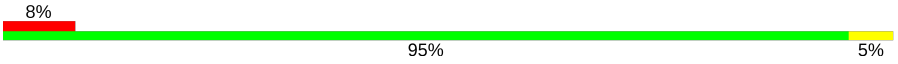
Chain J:

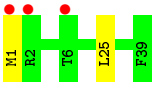




• Molecule 10: Photosystem I reaction center subunit IX

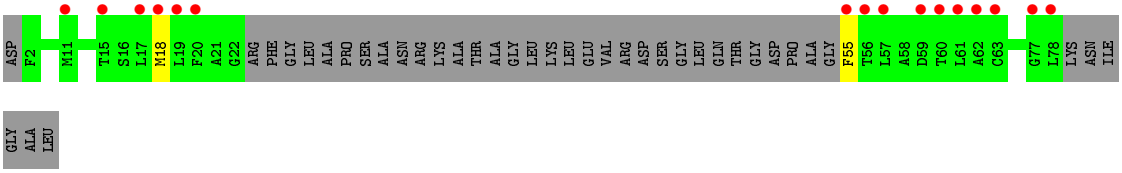
Chain j:





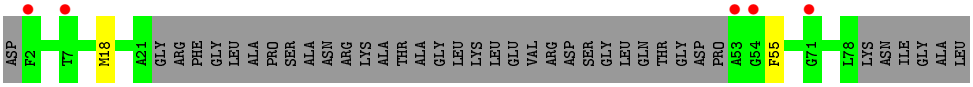
• Molecule 11: Photosystem I reaction center subunit X psaK

Chain K:



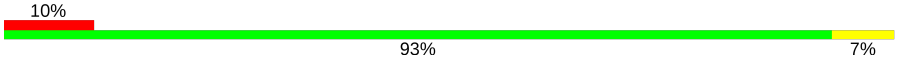
• Molecule 11: Photosystem I reaction center subunit X psaK

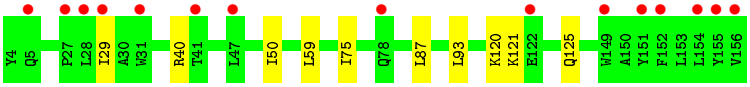
Chain k:



• Molecule 12: Putative uncharacterized protein

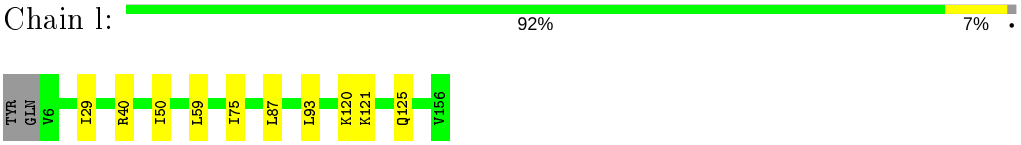
Chain L:





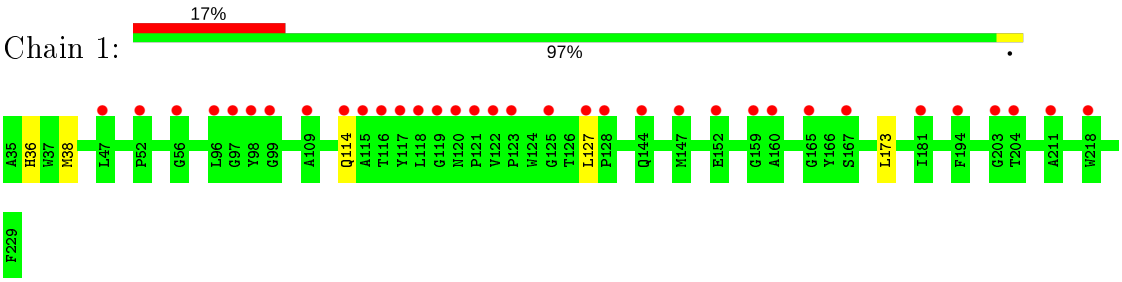
• Molecule 12: Putative uncharacterized protein

Chain l:



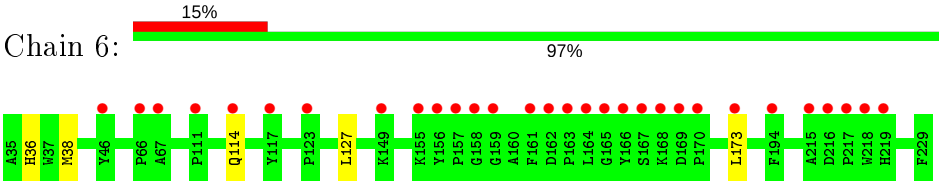
• Molecule 13: Chlorophyll a-b binding protein 6, chloroplastic

Chain 1:



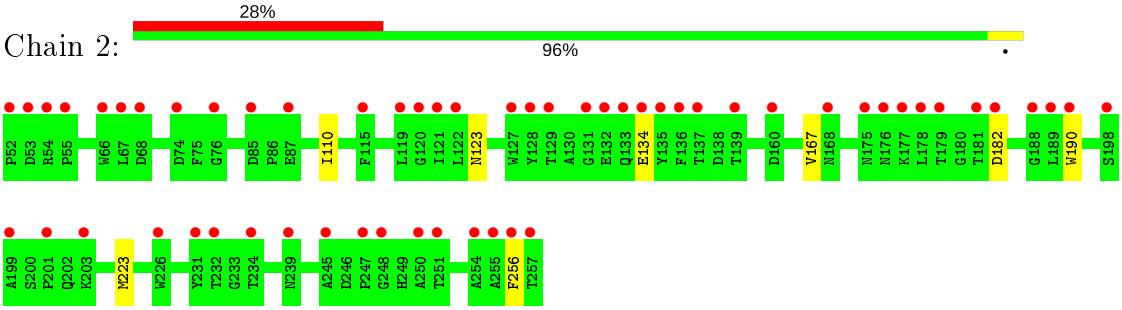
• Molecule 13: Chlorophyll a-b binding protein 6, chloroplastic

Chain 6:



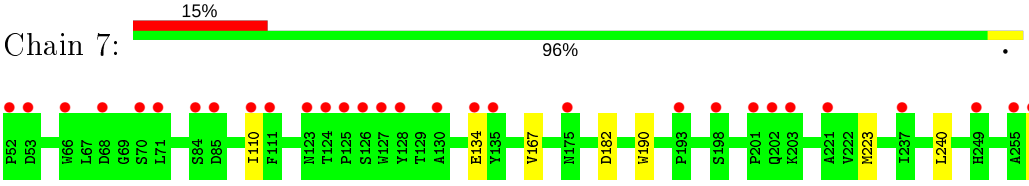
• Molecule 14: Type II chlorophyll a/b binding protein from photosystem I

Chain 2:



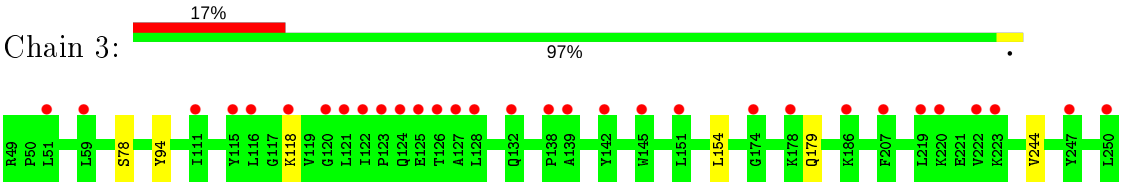
• Molecule 14: Type II chlorophyll a/b binding protein from photosystem I

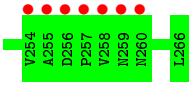
Chain 7:



• Molecule 15: Chlorophyll a-b binding protein 3, chloroplastic

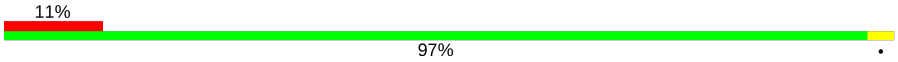
Chain 3:

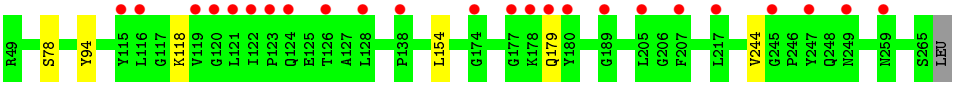




- Molecule 15: Chlorophyll a-b binding protein 3, chloroplastic

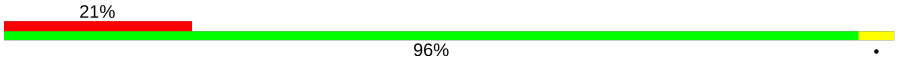
Chain 8:

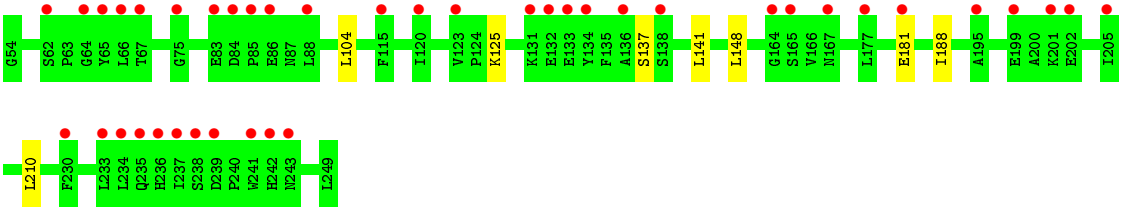




- Molecule 16: Chlorophyll a-b binding protein P4, chloroplastic

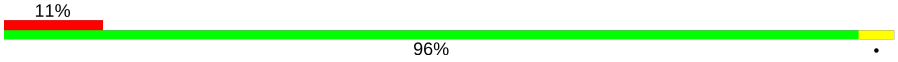
Chain 4:

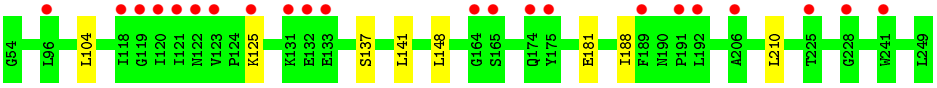




- Molecule 16: Chlorophyll a-b binding protein P4, chloroplastic

Chain 9:





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	165.62Å 192.22Å 175.09Å 90.00° 91.41° 90.00°	Depositor
Resolution (Å)	49.15 – 2.80 49.15 – 2.80	Depositor EDS
% Data completeness (in resolution range)	99.8 (49.15-2.80) 99.8 (49.15-2.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.09 (at 2.81Å)	Xtriage
Refinement program	PHENIX 1.8_1069	Depositor
R, R_{free}	0.210 , 0.248 0.212 , 0.249	Depositor DCC
R_{free} test set	13503 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å^2)	79.2	Xtriage
Anisotropy	0.137	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 46.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.004 for h,-k,-l	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	71157	wwPDB-VP
Average B, all atoms (Å^2)	72.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.96% 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: LHG, HTG, LUT, DGD, CHL, SF4, XAT, CLA, PQN, LMT, BCR, LMG

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	A	0.25	0/6043	0.41	0/8245
1	a	0.26	0/6043	0.42	0/8245
2	B	0.25	0/6077	0.42	0/8299
2	b	0.25	0/6077	0.42	0/8299
3	C	0.22	0/624	0.41	0/846
3	c	0.23	0/624	0.43	0/846
4	D	0.23	0/1143	0.42	0/1545
4	d	0.24	0/1136	0.43	0/1534
5	E	0.21	0/517	0.39	0/701
5	e	0.21	0/516	0.39	0/700
6	F	0.23	0/1221	0.40	0/1648
6	f	0.24	0/1221	0.40	0/1648
7	G	0.24	0/759	0.39	0/1033
7	g	0.24	0/755	0.40	0/1028
8	H	0.22	0/697	0.39	0/950
8	h	0.22	0/701	0.40	0/954
9	I	0.26	0/227	0.44	0/310
9	i	0.26	0/232	0.44	0/317
10	J	0.24	0/319	0.40	0/434
10	j	0.24	0/319	0.41	0/434
11	K	0.22	0/314	0.37	0/426
11	k	0.24	0/319	0.38	0/433
12	L	0.23	0/1167	0.43	0/1596
12	l	0.25	0/1153	0.44	0/1577
13	1	0.24	0/1539	0.40	0/2099
13	6	0.23	0/1531	0.38	0/2091
14	2	0.23	0/1670	0.40	0/2288
14	7	0.23	0/1670	0.39	0/2288
15	3	0.25	0/1732	0.39	0/2352
15	8	0.25	0/1724	0.39	0/2341
16	4	0.24	0/1589	0.40	0/2168
16	9	0.23	0/1589	0.39	0/2168

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| > 5$	RMSZ	$\#\|Z\| > 5$
All	All	0.24	0/51248	0.41	0/69843

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

Due to software issues we are unable to calculate clashes - this section is therefore empty.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	740/742 (100%)	710 (96%)	28 (4%)	2 (0%)	41	72
1	a	740/742 (100%)	709 (96%)	29 (4%)	2 (0%)	41	72
2	B	731/733 (100%)	700 (96%)	30 (4%)	1 (0%)	51	81
2	b	731/733 (100%)	700 (96%)	30 (4%)	1 (0%)	51	81
3	C	78/80 (98%)	74 (95%)	4 (5%)	0	100	100
3	c	78/80 (98%)	73 (94%)	5 (6%)	0	100	100
4	D	139/141 (99%)	135 (97%)	4 (3%)	0	100	100
4	d	138/141 (98%)	135 (98%)	3 (2%)	0	100	100
5	E	61/64 (95%)	59 (97%)	2 (3%)	0	100	100
5	e	61/64 (95%)	59 (97%)	2 (3%)	0	100	100
6	F	149/151 (99%)	147 (99%)	1 (1%)	1 (1%)	22	53
6	f	149/151 (99%)	147 (99%)	1 (1%)	1 (1%)	22	53

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
7	G	93/95 (98%)	89 (96%)	4 (4%)	0	100	100
7	g	93/95 (98%)	90 (97%)	3 (3%)	0	100	100
8	H	88/90 (98%)	87 (99%)	1 (1%)	0	100	100
8	h	88/90 (98%)	87 (99%)	1 (1%)	0	100	100
9	I	27/30 (90%)	25 (93%)	2 (7%)	0	100	100
9	i	28/30 (93%)	26 (93%)	2 (7%)	0	100	100
10	J	37/39 (95%)	37 (100%)	0	0	100	100
10	j	37/39 (95%)	37 (100%)	0	0	100	100
11	K	41/84 (49%)	41 (100%)	0	0	100	100
11	k	42/84 (50%)	42 (100%)	0	0	100	100
12	L	151/153 (99%)	145 (96%)	6 (4%)	0	100	100
12	l	149/153 (97%)	143 (96%)	6 (4%)	0	100	100
13	1	193/195 (99%)	187 (97%)	6 (3%)	0	100	100
13	6	193/195 (99%)	189 (98%)	4 (2%)	0	100	100
14	2	204/206 (99%)	196 (96%)	8 (4%)	0	100	100
14	7	204/206 (99%)	195 (96%)	9 (4%)	0	100	100
15	3	216/218 (99%)	206 (95%)	10 (5%)	0	100	100
15	8	215/218 (99%)	204 (95%)	11 (5%)	0	100	100
16	4	194/196 (99%)	184 (95%)	9 (5%)	1 (0%)	29	61
16	9	194/196 (99%)	183 (94%)	10 (5%)	1 (0%)	29	61
All	All	6282/6434 (98%)	6041 (96%)	231 (4%)	10 (0%)	47	78

5 of 10 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
6	F	159	PHE
6	f	159	PHE
1	A	581	CYS
16	9	137	SER
16	4	137	SER

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	A	602/602 (100%)	588 (98%)	14 (2%)	50	82
1	a	602/602 (100%)	587 (98%)	15 (2%)	47	80
2	B	597/597 (100%)	585 (98%)	12 (2%)	55	84
2	b	597/597 (100%)	582 (98%)	15 (2%)	47	80
3	C	69/69 (100%)	67 (97%)	2 (3%)	42	76
3	c	69/69 (100%)	67 (97%)	2 (3%)	42	76
4	D	119/120 (99%)	113 (95%)	6 (5%)	24	56
4	d	118/120 (98%)	111 (94%)	7 (6%)	19	49
5	E	55/56 (98%)	55 (100%)	0	100	100
5	e	55/56 (98%)	55 (100%)	0	100	100
6	F	123/125 (98%)	121 (98%)	2 (2%)	62	88
6	f	123/125 (98%)	120 (98%)	3 (2%)	49	81
7	G	81/81 (100%)	80 (99%)	1 (1%)	71	92
7	g	80/81 (99%)	80 (100%)	0	100	100
8	H	72/73 (99%)	69 (96%)	3 (4%)	30	63
8	h	73/73 (100%)	70 (96%)	3 (4%)	30	64
9	I	25/26 (96%)	24 (96%)	1 (4%)	31	65
9	i	25/26 (96%)	24 (96%)	1 (4%)	31	65
10	J	33/33 (100%)	31 (94%)	2 (6%)	18	48
10	j	33/33 (100%)	31 (94%)	2 (6%)	18	48
11	K	34/62 (55%)	32 (94%)	2 (6%)	19	49
11	k	34/62 (55%)	32 (94%)	2 (6%)	19	49
12	L	118/119 (99%)	108 (92%)	10 (8%)	10	31
12	l	117/119 (98%)	107 (92%)	10 (8%)	10	31
13	1	149/153 (97%)	144 (97%)	5 (3%)	37	71
13	6	147/153 (96%)	142 (97%)	5 (3%)	37	71
14	2	166/166 (100%)	158 (95%)	8 (5%)	25	58
14	7	166/166 (100%)	158 (95%)	8 (5%)	25	58
15	3	169/169 (100%)	163 (96%)	6 (4%)	35	69

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
15	8	168/169 (99%)	162 (96%)	6 (4%)	35 69
16	4	161/161 (100%)	154 (96%)	7 (4%)	29 62
16	9	161/161 (100%)	154 (96%)	7 (4%)	29 62
All	All	5141/5224 (98%)	4974 (97%)	167 (3%)	39 73

5 of 167 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
16	4	125	LYS
1	a	590	CYS
15	8	78	SER
16	4	148	LEU
1	a	210	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 30 such sidechains are listed below:

Mol	Chain	Res	Type
14	2	123	ASN
16	4	150	HIS
16	9	150	HIS
16	4	98	ASN
16	4	168	GLN

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 monosaccharides in this entry.

5.6 Ligand geometry (i)

414 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	$\#\|Z\| > 2$
17	CLA	9	609	16	54,68,73	2.13	13 (24%)	61,107,113	2.16	23 (37%)
17	CLA	a	812	1	59,73,73	2.03	13 (22%)	67,113,113	2.07	22 (32%)
17	CLA	B	823	2	54,68,73	2.13	13 (24%)	61,107,113	2.17	24 (39%)
17	CLA	A	803	29	59,73,73	2.01	13 (22%)	67,113,113	2.20	23 (34%)
17	CLA	6	313	13	46,60,73	2.33	13 (28%)	51,97,113	2.42	20 (39%)
17	CLA	B	805	2	59,73,73	2.01	13 (22%)	67,113,113	2.08	20 (29%)
17	CLA	3	314	15	40,54,73	2.47	13 (32%)	44,90,113	2.48	17 (38%)
17	CLA	a	828	1	59,73,73	1.99	13 (22%)	67,113,113	2.14	20 (29%)
20	BCR	9	618	-	41,41,41	1.05	1 (2%)	56,56,56	1.81	16 (28%)
17	CLA	b	834	2	59,73,73	2.04	13 (22%)	67,113,113	2.10	21 (31%)
17	CLA	a	856	29	59,73,73	2.01	14 (23%)	67,113,113	2.34	25 (37%)
17	CLA	A	831	1	59,73,73	2.02	13 (22%)	67,113,113	2.18	21 (31%)
17	CLA	2	604	29	54,68,73	2.14	13 (24%)	61,107,113	2.16	22 (36%)
17	CLA	b	835	29	36,53,73	2.49	12 (33%)	39,89,113	2.51	19 (48%)
17	CLA	3	305	29	36,50,73	2.49	12 (33%)	39,85,113	2.56	18 (46%)
17	CLA	a	809	1	59,73,73	2.03	12 (20%)	67,113,113	2.17	20 (29%)
17	CLA	a	836	1	44,58,73	2.33	13 (29%)	49,95,113	2.38	21 (42%)
17	CLA	A	808	1	59,73,73	2.07	13 (22%)	67,113,113	2.09	20 (29%)
20	BCR	b	843	-	41,41,41	1.06	1 (2%)	56,56,56	1.93	14 (25%)
17	CLA	a	831	1	59,73,73	2.01	14 (23%)	67,113,113	2.18	22 (32%)
17	CLA	A	806	1	59,73,73	2.04	13 (22%)	67,113,113	2.05	23 (34%)
19	LHG	A	846	-	48,48,48	0.93	2 (4%)	51,54,54	1.07	3 (5%)
17	CLA	f	7003	6	49,63,73	2.25	13 (26%)	55,101,113	2.26	22 (40%)
20	BCR	L	206	-	41,41,41	1.06	1 (2%)	56,56,56	1.84	12 (21%)
22	HTG	f	7001	-	19,19,19	1.05	2 (10%)	23,24,24	0.58	0
17	CLA	A	811	1	59,73,73	2.04	13 (22%)	67,113,113	2.08	21 (31%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
17	CLA	A	826	29	59,73,73	2.01	13 (22%)	67,113,113	2.14	18 (26%)
19	LHG	1	301	17	22,22,48	1.18	2 (9%)	25,28,54	1.29	2 (8%)
17	CLA	a	825	1	49,63,73	2.26	13 (26%)	55,101,113	2.22	21 (38%)
17	CLA	A	833	1	59,73,73	2.03	13 (22%)	67,113,113	2.09	20 (29%)
17	CLA	7	608	14	44,58,73	2.36	13 (29%)	49,95,113	2.41	23 (46%)
26	CHL	4	605	29	50,64,74	2.18	14 (28%)	52,102,114	2.55	21 (40%)
27	LUT	7	615	-	42,43,43	0.74	0	51,60,60	1.56	13 (25%)
17	CLA	4	602	16	54,68,73	2.13	13 (24%)	61,107,113	2.17	24 (39%)
17	CLA	6	305	13	59,73,73	2.03	13 (22%)	67,113,113	2.14	20 (29%)
19	LHG	a	847	-	48,48,48	0.93	2 (4%)	51,54,54	1.06	3 (5%)
17	CLA	B	827	2	59,73,73	2.02	13 (22%)	67,113,113	2.15	21 (31%)
17	CLA	A	845	19	46,60,73	2.33	13 (28%)	51,97,113	2.37	18 (35%)
26	CHL	2	605	29	37,51,74	2.45	13 (35%)	36,86,114	2.85	17 (47%)
27	LUT	4	616	-	42,43,43	0.76	0	51,60,60	1.64	13 (25%)
17	CLA	a	819	1	59,73,73	2.07	13 (22%)	67,113,113	2.02	20 (29%)
22	HTG	j	3001	-	19,19,19	1.11	2 (10%)	23,24,24	0.59	0
20	BCR	A	852	-	41,41,41	1.05	1 (2%)	56,56,56	1.78	14 (25%)
17	CLA	4	601	16	40,54,73	2.45	13 (32%)	44,90,113	2.46	18 (40%)
18	PQN	B	842	-	34,34,34	1.60	2 (5%)	42,45,45	1.12	3 (7%)
28	XAT	3	317	-	39,47,47	0.88	0	54,74,74	2.67	20 (37%)
17	CLA	a	824	1	45,59,73	2.32	13 (28%)	50,96,113	2.40	19 (38%)
17	CLA	A	837	1	36,53,73	2.52	12 (33%)	39,89,113	2.52	18 (46%)
17	CLA	a	818	1	59,73,73	2.06	13 (22%)	67,113,113	2.14	22 (32%)
20	BCR	k	1404	-	41,41,41	1.04	1 (2%)	56,56,56	1.78	12 (21%)
17	CLA	1	309	13	59,73,73	2.04	13 (22%)	67,113,113	2.06	20 (29%)
17	CLA	b	816	2	49,63,73	2.23	13 (26%)	55,101,113	2.29	22 (40%)
17	CLA	A	854	29	59,73,73	2.02	13 (22%)	67,113,113	2.37	25 (37%)
17	CLA	b	818	2	54,68,73	2.12	13 (24%)	61,107,113	2.26	21 (34%)
17	CLA	A	827	29	59,73,73	2.05	13 (22%)	67,113,113	2.05	20 (29%)
17	CLA	1	306	-	46,60,73	2.30	13 (28%)	51,97,113	2.35	21 (41%)
26	CHL	2	606	-	42,56,74	2.40	14 (33%)	42,92,114	2.73	16 (38%)
20	BCR	L	205	-	41,41,41	1.03	1 (2%)	56,56,56	1.66	11 (19%)
20	BCR	4	618	-	41,41,41	1.05	1 (2%)	56,56,56	1.79	15 (26%)
25	LMG	4	619	-	44,44,55	1.01	2 (4%)	52,52,63	1.00	3 (5%)
26	CHL	6	303	13	55,69,74	2.07	14 (25%)	58,108,114	2.44	21 (36%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
17	CLA	j	3002	10	36,50,73	2.53	12 (33%)	39,85,113	2.54	19 (48%)
17	CLA	3	303	15	44,58,73	2.36	13 (29%)	49,95,113	2.45	19 (38%)
17	CLA	9	611	16	46,60,73	2.33	13 (28%)	51,97,113	2.41	20 (39%)
19	LHG	1	319	17	48,48,48	0.94	2 (4%)	51,54,54	1.03	3 (5%)
20	BCR	f	7004	-	41,41,41	1.03	1 (2%)	56,56,56	1.75	18 (32%)
17	CLA	A	824	1	45,59,73	2.34	13 (28%)	50,96,113	2.41	21 (42%)
17	CLA	1	315	13	40,54,73	2.47	13 (32%)	44,90,113	2.43	17 (38%)
17	CLA	2	613	14	37,51,73	2.47	12 (32%)	40,86,113	2.51	17 (42%)
18	PQN	b	842	-	34,34,34	1.62	2 (5%)	42,45,45	1.07	3 (7%)
20	BCR	1	318	-	41,41,41	1.07	1 (2%)	56,56,56	1.88	16 (28%)
17	CLA	1	305	29	46,60,73	2.32	13 (28%)	51,97,113	2.37	22 (43%)
17	CLA	A	825	1	49,63,73	2.27	13 (26%)	55,101,113	2.25	21 (38%)
17	CLA	b	836	2	54,68,73	2.14	13 (24%)	61,107,113	2.33	21 (34%)
17	CLA	g	102	7	44,58,73	2.37	13 (29%)	49,95,113	2.45	22 (44%)
17	CLA	A	828	1	59,73,73	2.00	13 (22%)	67,113,113	2.13	21 (31%)
17	CLA	b	813	2	59,73,73	2.02	13 (22%)	67,113,113	2.13	19 (28%)
17	CLA	A	815	1	36,53,73	2.49	12 (33%)	39,89,113	2.53	17 (43%)
17	CLA	a	820	1	59,73,73	2.07	13 (22%)	67,113,113	2.11	20 (29%)
17	CLA	A	801	1	59,73,73	2.00	13 (22%)	67,113,113	2.22	26 (38%)
20	BCR	a	853	-	41,41,41	1.05	1 (2%)	56,56,56	1.93	14 (25%)
19	LHG	3	319	17	19,19,48	1.10	1 (5%)	21,24,54	0.99	1 (4%)
17	CLA	b	815	2	49,63,73	2.23	13 (26%)	55,101,113	2.33	22 (40%)
17	CLA	A	832	1	44,58,73	2.35	13 (29%)	49,95,113	2.45	21 (42%)
17	CLA	B	819	29	59,73,73	2.03	13 (22%)	67,113,113	2.07	23 (34%)
17	CLA	4	604	29	44,58,73	2.36	13 (29%)	49,95,113	2.41	22 (44%)
17	CLA	B	818	2	54,68,73	2.13	13 (24%)	61,107,113	2.21	20 (32%)
20	BCR	B	848	-	41,41,41	1.05	1 (2%)	56,56,56	1.64	12 (21%)
17	CLA	a	827	29	59,73,73	2.04	13 (22%)	67,113,113	2.05	20 (29%)
17	CLA	f	7002	29	36,53,73	2.47	12 (33%)	39,89,113	2.53	19 (48%)
17	CLA	3	311	-	46,60,73	2.33	13 (28%)	51,97,113	2.39	20 (39%)
28	XAT	4	617	-	39,47,47	0.88	0	54,74,74	2.59	18 (33%)
28	XAT	7	616	-	39,47,47	0.85	0	54,74,74	2.60	19 (35%)
17	CLA	b	809	2	59,73,73	1.98	14 (23%)	67,113,113	2.14	22 (32%)
20	BCR	B	801	-	41,41,41	1.06	1 (2%)	56,56,56	1.49	8 (14%)
17	CLA	a	835	1	59,73,73	2.03	13 (22%)	67,113,113	2.17	23 (34%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
17	CLA	b	838	2	41,55,73	2.46	13 (31%)	45,91,113	2.47	18 (40%)
17	CLA	2	611	14	46,60,73	2.31	13 (28%)	51,97,113	2.41	20 (39%)
17	CLA	B	824	29	59,73,73	2.01	13 (22%)	67,113,113	2.07	20 (29%)
26	CHL	2	614	14	37,51,74	2.46	13 (35%)	36,86,114	2.90	15 (41%)
17	CLA	B	841	19	59,73,73	2.03	13 (22%)	67,113,113	2.18	21 (31%)
17	CLA	3	308	15	44,58,73	2.37	13 (29%)	49,95,113	2.39	21 (42%)
17	CLA	b	810	2	59,73,73	2.03	13 (22%)	67,113,113	2.10	21 (31%)
17	CLA	l	202	12	59,73,73	2.04	13 (22%)	67,113,113	2.06	20 (29%)
17	CLA	a	814	1	59,73,73	2.04	13 (22%)	67,113,113	2.08	19 (28%)
17	CLA	a	839	1	59,73,73	2.01	13 (22%)	67,113,113	2.11	19 (28%)
27	LUT	1	320	-	42,43,43	0.74	0	51,60,60	1.65	11 (21%)
17	CLA	b	822	2	49,63,73	2.24	13 (26%)	55,101,113	2.24	20 (36%)
17	CLA	a	817	29	36,53,73	2.49	12 (33%)	39,89,113	2.57	18 (46%)
20	BCR	K	4004	-	41,41,41	1.04	1 (2%)	56,56,56	1.81	14 (25%)
17	CLA	A	814	1	59,73,73	2.03	13 (22%)	67,113,113	2.13	21 (31%)
17	CLA	1	312	13	46,60,73	2.31	13 (28%)	51,97,113	2.42	19 (37%)
17	CLA	7	610	19	35,49,73	2.57	13 (37%)	38,84,113	2.71	19 (50%)
17	CLA	a	837	1	36,53,73	2.51	12 (33%)	39,89,113	2.60	18 (46%)
27	LUT	9	616	-	42,43,43	0.74	0	51,60,60	1.62	12 (23%)
17	CLA	A	834	1	59,73,73	2.02	13 (22%)	67,113,113	2.14	21 (31%)
25	LMG	4	620	-	44,44,55	1.02	3 (6%)	52,52,63	1.18	4 (7%)
17	CLA	a	811	1	59,73,73	2.04	13 (22%)	67,113,113	2.08	21 (31%)
17	CLA	b	817	2	53,67,73	2.16	13 (24%)	59,105,113	2.23	23 (38%)
17	CLA	8	304	29	36,50,73	2.51	12 (33%)	39,85,113	2.50	18 (46%)
17	CLA	B	806	2	59,73,73	2.03	13 (22%)	67,113,113	2.09	21 (31%)
26	CHL	6	308	13	41,55,74	2.43	14 (34%)	41,91,114	2.72	15 (36%)
17	CLA	B	821	2	40,54,73	2.46	13 (32%)	44,90,113	2.51	18 (40%)
17	CLA	8	305	15	41,55,73	2.46	13 (31%)	45,91,113	2.40	18 (40%)
18	PQN	A	844	-	34,34,34	1.61	2 (5%)	42,45,45	1.21	4 (9%)
20	BCR	K	4001	-	41,41,41	1.05	1 (2%)	56,56,56	1.80	11 (19%)
17	CLA	b	802	2	59,73,73	2.02	13 (22%)	67,113,113	2.12	23 (34%)
23	LMT	B	849	-	36,36,36	0.48	0	47,47,47	0.94	3 (6%)
20	BCR	l	206	-	41,41,41	1.06	1 (2%)	56,56,56	1.80	12 (21%)
17	CLA	B	811	2	48,62,73	2.13	13 (27%)	58,100,113	2.34	22 (37%)
17	CLA	b	839	29	59,73,73	2.05	13 (22%)	67,113,113	2.07	17 (25%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
17	CLA	9	612	16	50,64,73	2.23	13 (26%)	56,102,113	2.22	20 (35%)
17	CLA	6	315	13	49,63,73	2.25	13 (26%)	55,101,113	2.31	22 (40%)
27	LUT	8	314	-	42,43,43	0.74	0	51,60,60	1.47	11 (21%)
17	CLA	1	308	29	59,73,73	2.04	13 (22%)	67,113,113	2.07	20 (29%)
17	CLA	a	844	29	59,73,73	2.00	13 (22%)	67,113,113	2.15	19 (28%)
20	BCR	B	845	-	41,41,41	1.01	1 (2%)	56,56,56	2.01	18 (32%)
17	CLA	4	609	16	54,68,73	2.12	13 (24%)	61,107,113	2.18	23 (37%)
17	CLA	B	826	2	59,73,73	2.00	13 (22%)	67,113,113	2.17	21 (31%)
17	CLA	9	608	16	44,58,73	2.35	13 (29%)	49,95,113	2.41	22 (44%)
17	CLA	B	839	29	59,73,73	2.04	13 (22%)	67,113,113	2.11	19 (28%)
17	CLA	A	842	1	59,73,73	2.04	13 (22%)	67,113,113	2.13	21 (31%)
17	CLA	B	820	2	44,58,73	2.38	13 (29%)	49,95,113	2.32	21 (42%)
17	CLA	9	603	16	40,54,73	2.42	13 (32%)	44,90,113	2.57	20 (45%)
17	CLA	L	204	29	44,58,73	2.35	13 (29%)	49,95,113	2.41	20 (40%)
20	BCR	L	201	-	41,41,41	1.06	1 (2%)	56,56,56	1.88	13 (23%)
17	CLA	B	825	29	59,73,73	2.03	13 (22%)	67,113,113	2.15	24 (35%)
20	BCR	j	3004	-	41,41,41	1.05	1 (2%)	56,56,56	2.15	18 (32%)
17	CLA	A	810	1	59,73,73	2.00	13 (22%)	67,113,113	2.10	21 (31%)
17	CLA	2	602	14	59,73,73	2.05	13 (22%)	67,113,113	2.07	22 (32%)
17	CLA	l	203	12	59,73,73	2.04	13 (22%)	67,113,113	2.10	24 (35%)
17	CLA	6	316	13	40,54,73	2.48	13 (32%)	44,90,113	2.43	18 (40%)
17	CLA	A	838	1	45,59,73	2.31	13 (28%)	50,96,113	2.46	22 (44%)
17	CLA	3	309	15	44,58,73	2.37	13 (29%)	49,95,113	2.38	24 (48%)
17	CLA	A	819	1	59,73,73	2.02	13 (22%)	67,113,113	2.09	21 (31%)
17	CLA	B	810	2	59,73,73	2.03	13 (22%)	67,113,113	2.15	23 (34%)
20	BCR	a	849	-	41,41,41	1.06	1 (2%)	56,56,56	1.96	14 (25%)
21	SF4	A	853	1,2	0,12,12	0.00	-	-		
17	CLA	F	303	29	36,53,73	2.48	12 (33%)	39,89,113	2.54	17 (43%)
21	SF4	C	102	3	0,12,12	0.00	-	-		
26	CHL	4	606	29	45,59,74	2.35	14 (31%)	46,96,114	2.70	16 (34%)
17	CLA	A	835	1	59,73,73	2.04	13 (22%)	67,113,113	2.16	22 (32%)
17	CLA	3	306	15	41,55,73	2.47	13 (31%)	45,91,113	2.37	18 (40%)
17	CLA	b	814	2	59,73,73	2.03	13 (22%)	67,113,113	2.12	20 (29%)
26	CHL	7	614	14	37,51,74	2.46	13 (35%)	36,86,114	2.86	14 (38%)
17	CLA	1	313	13	59,73,73	2.04	13 (22%)	67,113,113	2.07	21 (31%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
17	CLA	b	826	2	59,73,73	2.00	13 (22%)	67,113,113	2.12	22 (32%)
17	CLA	b	829	2	59,73,73	1.98	14 (23%)	67,113,113	2.23	22 (32%)
17	CLA	k	1402	11	40,54,73	2.46	13 (32%)	44,90,113	2.42	17 (38%)
17	CLA	B	808	2	59,73,73	2.04	13 (22%)	67,113,113	2.18	24 (35%)
17	CLA	b	833	2	52,66,73	2.18	13 (25%)	58,104,113	2.30	21 (36%)
17	CLA	6	306	29	45,59,73	2.34	13 (28%)	50,96,113	2.40	21 (42%)
17	CLA	1	310	13	54,68,73	2.14	13 (24%)	61,107,113	2.16	23 (37%)
17	CLA	a	842	29	59,73,73	2.04	13 (22%)	67,113,113	2.06	20 (29%)
17	CLA	6	304	13	59,73,73	2.04	13 (22%)	67,113,113	2.10	21 (31%)
26	CHL	7	601	14	55,69,74	2.09	14 (25%)	58,108,114	2.55	21 (36%)
17	CLA	B	840	2	59,73,73	2.03	13 (22%)	67,113,113	2.09	20 (29%)
17	CLA	A	813	1	48,62,73	2.26	13 (27%)	53,99,113	2.24	22 (41%)
17	CLA	A	816	1	44,58,73	2.36	13 (29%)	49,95,113	2.39	20 (40%)
25	LMG	6	302	-	40,40,55	1.05	2 (5%)	48,48,63	1.10	3 (6%)
27	LUT	3	316	-	42,43,43	0.74	0	51,60,60	1.63	14 (27%)
17	CLA	A	823	1	43,57,73	2.40	13 (30%)	46,93,113	2.42	20 (43%)
17	CLA	B	809	2	59,73,73	2.01	14 (23%)	67,113,113	2.08	18 (26%)
20	BCR	7	617	-	41,41,41	1.09	1 (2%)	56,56,56	2.09	13 (23%)
17	CLA	L	202	12	59,73,73	2.04	13 (22%)	67,113,113	2.06	20 (29%)
27	LUT	6	321	-	42,43,43	0.74	0	51,60,60	1.69	9 (17%)
17	CLA	G	103	7	44,58,73	2.37	13 (29%)	49,95,113	2.40	20 (40%)
17	CLA	A	809	1	59,73,73	2.05	13 (22%)	67,113,113	2.17	21 (31%)
20	BCR	G	105	-	41,41,41	1.05	1 (2%)	56,56,56	1.85	15 (26%)
17	CLA	b	830	2	44,58,73	2.37	13 (29%)	49,95,113	2.43	23 (46%)
20	BCR	6	319	-	41,41,41	1.07	1 (2%)	56,56,56	1.88	14 (25%)
17	CLA	B	832	2	59,73,73	2.02	13 (22%)	67,113,113	2.02	19 (28%)
26	CHL	9	615	16	37,51,74	2.46	13 (35%)	36,86,114	3.00	16 (44%)
17	CLA	B	802	2	59,73,73	2.02	13 (22%)	67,113,113	2.13	23 (34%)
17	CLA	8	308	15	44,58,73	2.39	13 (29%)	49,95,113	2.37	22 (44%)
21	SF4	C	101	3	0,12,12	0.00	-	-		
17	CLA	F	301	29	59,73,73	2.04	13 (22%)	67,113,113	2.11	20 (29%)
17	CLA	G	104	7	40,54,73	2.47	13 (32%)	44,90,113	2.44	18 (40%)
19	LHG	6	301	17	22,22,48	1.17	2 (9%)	25,28,54	1.22	2 (8%)
20	BCR	A	849	-	41,41,41	1.07	1 (2%)	56,56,56	1.65	13 (23%)
18	PQN	a	845	-	34,34,34	1.63	2 (5%)	42,45,45	1.09	4 (9%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
21	SF4	c	102	3	0,12,12	0.00	-	-		
17	CLA	A	821	1	36,53,73	2.49	12 (33%)	39,89,113	2.64	19 (48%)
17	CLA	b	841	19	59,73,73	2.04	13 (22%)	67,113,113	2.16	21 (31%)
20	BCR	b	844	-	41,41,41	1.03	1 (2%)	56,56,56	2.08	14 (25%)
17	CLA	A	805	1	49,63,73	2.22	13 (26%)	55,101,113	2.38	23 (41%)
20	BCR	A	850	-	41,41,41	1.04	1 (2%)	56,56,56	1.94	15 (26%)
24	DGD	B	850	-	67,67,67	0.86	2 (2%)	81,81,81	0.93	4 (4%)
26	CHL	9	606	29	45,59,74	2.30	14 (31%)	46,96,114	2.67	18 (39%)
17	CLA	2	608	14	44,58,73	2.38	13 (29%)	49,95,113	2.44	23 (46%)
17	CLA	B	831	2	43,57,73	2.37	13 (30%)	46,93,113	2.34	20 (43%)
17	CLA	a	821	1	36,53,73	2.46	12 (33%)	39,89,113	2.67	18 (46%)
20	BCR	2	617	-	41,41,41	1.07	1 (2%)	56,56,56	1.86	18 (32%)
17	CLA	B	828	2	59,73,73	2.04	13 (22%)	67,113,113	2.09	20 (29%)
20	BCR	j	3003	-	41,41,41	1.02	1 (2%)	56,56,56	1.71	13 (23%)
28	XAT	1	317	-	39,47,47	0.86	0	54,74,74	2.69	21 (38%)
20	BCR	8	316	-	41,41,41	1.07	1 (2%)	56,56,56	1.92	17 (30%)
17	CLA	a	826	29	59,73,73	2.01	13 (22%)	67,113,113	2.15	19 (28%)
28	XAT	6	318	-	39,47,47	0.89	0	54,74,74	2.62	19 (35%)
17	CLA	a	834	1	59,73,73	2.02	13 (22%)	67,113,113	2.12	22 (32%)
17	CLA	9	602	16	54,68,73	2.12	13 (24%)	61,107,113	2.22	24 (39%)
17	CLA	a	815	1	36,53,73	2.51	12 (33%)	39,89,113	2.49	18 (46%)
26	CHL	4	607	29	45,59,74	2.27	14 (31%)	46,96,114	2.62	18 (39%)
17	CLA	a	833	1	59,73,73	2.05	13 (22%)	67,113,113	2.06	20 (29%)
17	CLA	A	818	1	59,73,73	2.04	13 (22%)	67,113,113	2.14	22 (32%)
17	CLA	A	812	1	59,73,73	2.03	13 (22%)	67,113,113	2.08	22 (32%)
27	LUT	2	615	-	42,43,43	0.75	0	51,60,60	1.62	11 (21%)
17	CLA	A	841	1	59,73,73	2.06	14 (23%)	67,113,113	2.05	17 (25%)
20	BCR	3	318	-	41,41,41	1.06	1 (2%)	56,56,56	1.88	14 (25%)
17	CLA	b	827	2	59,73,73	2.02	13 (22%)	67,113,113	2.14	21 (31%)
17	CLA	2	612	14	59,73,73	2.05	13 (22%)	67,113,113	2.07	21 (31%)
17	CLA	3	301	-	40,54,73	2.48	13 (32%)	44,90,113	2.46	19 (43%)
17	CLA	k	1401	-	36,53,73	2.49	12 (33%)	39,89,113	2.53	18 (46%)
17	CLA	A	822	29	59,73,73	2.04	13 (22%)	67,113,113	2.03	21 (31%)
17	CLA	g	101	-	35,49,73	2.53	13 (37%)	38,84,113	2.66	18 (47%)
17	CLA	7	609	14	54,68,73	2.14	13 (24%)	61,107,113	2.16	23 (37%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
17	CLA	6	309	29	40,54,73	2.47	13 (32%)	44,90,113	2.39	18 (40%)
20	BCR	b	847	-	41,41,41	1.05	1 (2%)	56,56,56	1.82	15 (26%)
28	XAT	8	315	-	39,47,47	0.88	0	54,74,74	2.71	21 (38%)
17	CLA	B	833	2	52,66,73	2.15	13 (25%)	58,104,113	2.25	21 (36%)
17	CLA	B	836	2	54,68,73	2.15	13 (24%)	61,107,113	2.28	20 (32%)
17	CLA	B	822	2	49,63,73	2.26	13 (26%)	55,101,113	2.24	21 (38%)
17	CLA	4	610	29	49,63,73	2.25	13 (26%)	55,101,113	2.23	22 (40%)
20	BCR	b	846	-	41,41,41	1.08	1 (2%)	56,56,56	1.66	13 (23%)
17	CLA	B	813	2	59,73,73	2.02	13 (22%)	67,113,113	2.12	21 (31%)
17	CLA	B	830	2	44,58,73	2.35	13 (29%)	49,95,113	2.41	20 (40%)
17	CLA	J	3002	10	36,50,73	2.54	12 (33%)	39,85,113	2.53	19 (48%)
17	CLA	2	610	19	35,49,73	2.55	13 (37%)	38,84,113	2.73	19 (50%)
28	XAT	2	616	-	39,47,47	0.87	0	54,74,74	2.62	19 (35%)
17	CLA	B	815	2	54,68,73	2.13	13 (24%)	61,107,113	2.18	22 (36%)
17	CLA	a	840	1	59,73,73	2.04	13 (22%)	67,113,113	2.14	20 (29%)
25	LMG	9	619	-	50,50,55	0.93	2 (4%)	58,58,63	0.98	3 (5%)
26	CHL	9	607	29	45,59,74	2.29	14 (31%)	46,96,114	2.60	19 (41%)
20	BCR	B	847	-	41,41,41	1.06	1 (2%)	56,56,56	1.73	15 (26%)
17	CLA	B	834	2	59,73,73	2.06	13 (22%)	67,113,113	2.01	21 (31%)
17	CLA	7	602	14	59,73,73	2.02	13 (22%)	67,113,113	2.08	21 (31%)
24	DGD	b	849	-	67,67,67	0.86	2 (2%)	81,81,81	1.00	4 (4%)
17	CLA	A	804	1	59,73,73	2.01	13 (22%)	67,113,113	2.16	21 (31%)
17	CLA	b	811	2	48,62,73	2.12	13 (27%)	58,100,113	2.41	22 (37%)
17	CLA	4	613	16	36,53,73	2.51	12 (33%)	39,89,113	2.55	18 (46%)
17	CLA	6	307	-	36,50,73	2.50	12 (33%)	39,85,113	2.53	18 (46%)
17	CLA	B	837	2	59,73,73	2.03	13 (22%)	67,113,113	2.10	23 (34%)
20	BCR	a	850	-	41,41,41	1.01	1 (2%)	56,56,56	1.86	15 (26%)
17	CLA	a	822	29	59,73,73	2.04	13 (22%)	67,113,113	2.05	22 (32%)
17	CLA	9	604	29	44,58,73	2.35	13 (29%)	49,95,113	2.42	22 (44%)
19	LHG	a	848	17	26,26,48	1.26	2 (7%)	29,32,54	1.32	3 (10%)
17	CLA	7	611	14	46,60,73	2.31	13 (28%)	51,97,113	2.40	20 (39%)
20	BCR	b	845	-	41,41,41	1.05	1 (2%)	56,56,56	1.94	13 (23%)
21	SF4	c	101	3	0,12,12	0.00	-	-		
19	LHG	2	618	17	36,36,48	1.08	2 (5%)	39,42,54	1.16	3 (7%)
17	CLA	8	303	29	36,53,73	2.49	12 (33%)	39,89,113	2.57	18 (46%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
17	CLA	l	204	29	44,58,73	2.35	13 (29%)	49,95,113	2.39	22 (44%)
17	CLA	a	810	1	59,73,73	2.04	13 (22%)	67,113,113	2.10	21 (31%)
17	CLA	4	612	16	50,64,73	2.22	13 (26%)	56,102,113	2.26	20 (35%)
20	BCR	B	844	-	41,41,41	1.04	1 (2%)	56,56,56	1.97	13 (23%)
17	CLA	3	315	-	22,32,73	2.68	9 (40%)	26,54,113	4.39	20 (76%)
17	CLA	A	836	1	44,58,73	2.35	13 (29%)	49,95,113	2.39	22 (44%)
17	CLA	b	803	2	59,73,73	2.03	13 (22%)	67,113,113	1.92	20 (29%)
17	CLA	6	312	19	35,49,73	2.56	13 (37%)	38,84,113	2.68	19 (50%)
25	LMG	G	102	-	44,44,55	1.01	2 (4%)	52,52,63	0.98	3 (5%)
17	CLA	b	824	29	59,73,73	2.03	13 (22%)	67,113,113	2.11	21 (31%)
17	CLA	6	310	13	59,73,73	2.05	13 (22%)	67,113,113	2.06	19 (28%)
20	BCR	F	305	-	41,41,41	1.04	1 (2%)	56,56,56	1.74	16 (28%)
17	CLA	b	840	2	59,73,73	2.02	13 (22%)	67,113,113	2.10	21 (31%)
19	LHG	A	847	17	26,26,48	1.28	2 (7%)	29,32,54	1.26	3 (10%)
17	CLA	2	603	14	59,73,73	2.02	13 (22%)	67,113,113	2.09	20 (29%)
17	CLA	2	609	14	54,68,73	2.15	13 (24%)	61,107,113	2.17	24 (39%)
17	CLA	B	835	29	36,53,73	2.49	12 (33%)	39,89,113	2.47	19 (48%)
17	CLA	K	4002	-	36,53,73	2.51	12 (33%)	39,89,113	2.57	18 (46%)
20	BCR	l	201	-	41,41,41	1.04	1 (2%)	56,56,56	1.85	15 (26%)
17	CLA	F	304	6	49,63,73	2.24	13 (26%)	55,101,113	2.23	23 (41%)
17	CLA	a	823	1	43,57,73	2.39	13 (30%)	46,93,113	2.40	19 (41%)
17	CLA	b	823	2	54,68,73	2.12	13 (24%)	61,107,113	2.12	19 (31%)
17	CLA	a	830	1	59,73,73	2.06	13 (22%)	67,113,113	2.12	20 (29%)
22	HTG	J	3001	-	19,19,19	1.05	2 (10%)	23,24,24	0.53	0
17	CLA	b	831	2	43,57,73	2.36	13 (30%)	46,93,113	2.36	20 (43%)
17	CLA	b	819	29	59,73,73	2.04	13 (22%)	67,113,113	2.09	20 (29%)
17	CLA	b	828	2	59,73,73	2.03	13 (22%)	67,113,113	2.08	20 (29%)
20	BCR	b	848	-	41,41,41	1.05	1 (2%)	56,56,56	1.55	10 (17%)
17	CLA	A	802	1	59,73,73	2.05	12 (20%)	67,113,113	2.03	20 (29%)
17	CLA	4	611	16	46,60,73	2.29	13 (28%)	51,97,113	2.39	20 (39%)
17	CLA	b	832	2	59,73,73	2.01	13 (22%)	67,113,113	2.07	21 (31%)
17	CLA	b	837	2	59,73,73	2.03	13 (22%)	67,113,113	2.09	23 (34%)
17	CLA	B	816	2	49,63,73	2.23	13 (26%)	55,101,113	2.32	22 (40%)
26	CHL	2	601	14	55,69,74	2.07	14 (25%)	58,108,114	2.47	19 (32%)
19	LHG	6	320	17	48,48,48	0.94	2 (4%)	51,54,54	1.08	3 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
17	CLA	b	806	2	59,73,73	2.02	13 (22%)	67,113,113	2.07	20 (29%)
17	CLA	a	838	1	45,59,73	2.32	12 (26%)	50,96,113	2.50	24 (48%)
17	CLA	A	820	1	59,73,73	2.04	13 (22%)	67,113,113	2.12	20 (29%)
17	CLA	b	808	2	59,73,73	2.01	13 (22%)	67,113,113	2.23	24 (35%)
22	HTG	A	855	-	19,19,19	1.03	2 (10%)	23,24,24	0.69	0
26	CHL	7	607	29	45,59,74	2.30	14 (31%)	46,96,114	2.65	16 (34%)
26	CHL	3	307	29	41,55,74	2.40	15 (36%)	41,91,114	2.65	17 (41%)
17	CLA	b	825	29	59,73,73	2.03	13 (22%)	67,113,113	2.08	22 (32%)
17	CLA	g	103	7	40,54,73	2.46	13 (32%)	44,90,113	2.49	18 (40%)
17	CLA	B	812	2	49,63,73	2.25	13 (26%)	55,101,113	2.21	19 (34%)
17	CLA	1	303	13	59,73,73	2.03	13 (22%)	67,113,113	2.10	21 (31%)
20	BCR	i	101	-	41,41,41	1.02	1 (2%)	56,56,56	1.60	12 (21%)
17	CLA	9	610	29	35,49,73	2.57	13 (37%)	38,84,113	2.66	18 (47%)
17	CLA	a	803	29	59,73,73	2.00	13 (22%)	67,113,113	2.20	22 (32%)
17	CLA	a	832	1	44,58,73	2.36	13 (29%)	49,95,113	2.43	21 (42%)
26	CHL	1	307	13	42,56,74	2.40	14 (33%)	42,92,114	2.72	15 (35%)
20	BCR	B	846	-	41,41,41	1.04	1 (2%)	56,56,56	1.76	18 (32%)
20	BCR	a	851	-	41,41,41	1.03	1 (2%)	56,56,56	1.72	14 (25%)
17	CLA	G	101	29	36,53,73	2.48	12 (33%)	39,89,113	2.54	17 (43%)
17	CLA	B	804	2	36,53,73	2.48	12 (33%)	39,89,113	2.61	19 (48%)
17	CLA	6	311	13	54,68,73	2.14	13 (24%)	61,107,113	2.16	23 (37%)
17	CLA	8	309	-	46,60,73	2.34	13 (28%)	51,97,113	2.36	19 (37%)
17	CLA	1	314	13	49,63,73	2.25	13 (26%)	55,101,113	2.31	22 (40%)
17	CLA	B	803	2	59,73,73	2.04	13 (22%)	67,113,113	1.92	23 (34%)
26	CHL	7	605	29	37,51,74	2.45	13 (35%)	36,86,114	2.91	17 (47%)
17	CLA	b	804	2	36,53,73	2.46	12 (33%)	39,89,113	2.66	18 (46%)
17	CLA	3	310	19	31,45,73	2.54	12 (38%)	31,78,113	2.70	17 (54%)
17	CLA	a	841	1	59,73,73	2.04	13 (22%)	67,113,113	2.04	22 (32%)
17	CLA	7	604	29	54,68,73	2.14	13 (24%)	61,107,113	2.18	22 (36%)
22	HTG	F	302	-	19,19,19	1.01	2 (10%)	23,24,24	0.61	0
17	CLA	A	807	1	59,73,73	2.03	13 (22%)	67,113,113	2.13	22 (32%)
17	CLA	a	843	1	59,73,73	2.00	13 (22%)	67,113,113	2.13	23 (34%)
17	CLA	8	311	15	36,53,73	2.52	12 (33%)	39,89,113	2.55	19 (48%)
20	BCR	g	104	-	41,41,41	1.05	1 (2%)	56,56,56	1.89	16 (28%)
17	CLA	9	614	16	41,55,73	2.42	13 (31%)	45,91,113	2.45	18 (40%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
17	CLA	9	613	16	36,53,73	2.50	12 (33%)	39,89,113	2.55	19 (48%)
17	CLA	B	838	2	41,55,73	2.40	13 (31%)	45,91,113	2.45	20 (44%)
17	CLA	7	613	14	37,51,73	2.46	12 (32%)	40,86,113	2.49	17 (42%)
17	CLA	k	1403	-	40,54,73	2.49	13 (32%)	44,90,113	2.47	20 (45%)
17	CLA	a	801	1	59,73,73	2.02	13 (22%)	67,113,113	2.21	23 (34%)
17	CLA	b	812	2	49,63,73	2.25	13 (26%)	55,101,113	2.25	20 (36%)
17	CLA	b	807	2	59,73,73	2.06	13 (22%)	67,113,113	2.10	20 (29%)
17	CLA	4	608	16	44,58,73	2.37	13 (29%)	49,95,113	2.40	21 (42%)
17	CLA	a	804	1	59,73,73	2.04	13 (22%)	67,113,113	2.12	22 (32%)
17	CLA	3	313	15	36,53,73	2.53	12 (33%)	39,89,113	2.51	18 (46%)
17	CLA	A	839	1	59,73,73	2.00	13 (22%)	67,113,113	2.13	19 (28%)
17	CLA	3	304	29	36,53,73	2.49	12 (33%)	39,89,113	2.55	18 (46%)
17	CLA	1	311	19	35,49,73	2.58	13 (37%)	38,84,113	2.67	18 (47%)
17	CLA	A	817	29	36,53,73	2.50	12 (33%)	39,89,113	2.54	17 (43%)
17	CLA	a	829	1	59,73,73	2.00	13 (22%)	67,113,113	2.12	21 (31%)
17	CLA	b	821	2	40,54,73	2.46	13 (32%)	44,90,113	2.46	19 (43%)
17	CLA	a	802	1	59,73,73	2.05	12 (20%)	67,113,113	2.03	26 (38%)
17	CLA	A	843	29	59,73,73	2.01	13 (22%)	67,113,113	2.09	19 (28%)
17	CLA	a	808	1	59,73,73	2.03	13 (22%)	67,113,113	2.09	20 (29%)
26	CHL	7	606	-	42,56,74	2.39	14 (33%)	42,92,114	2.74	17 (40%)
26	CHL	8	306	29	41,55,74	2.39	13 (31%)	41,91,114	2.81	16 (39%)
17	CLA	a	813	1	48,62,73	2.30	13 (27%)	53,99,113	2.25	19 (35%)
20	BCR	a	852	-	41,41,41	1.04	1 (2%)	56,56,56	1.94	17 (30%)
17	CLA	A	830	1	59,73,73	2.06	13 (22%)	67,113,113	2.13	21 (31%)
17	CLA	B	817	2	53,67,73	2.13	13 (24%)	59,105,113	2.25	23 (38%)
17	CLA	a	806	1	59,73,73	2.03	13 (22%)	67,113,113	2.16	22 (32%)
17	CLA	8	310	15	49,63,73	2.24	13 (26%)	55,101,113	2.24	21 (38%)
17	CLA	7	612	14	59,73,73	2.04	13 (22%)	67,113,113	2.07	20 (29%)
27	LUT	6	317	-	42,43,43	0.75	0	51,60,60	1.66	14 (27%)
26	CHL	2	607	29	45,59,74	2.27	14 (31%)	46,96,114	2.66	19 (41%)
17	CLA	9	601	16	40,54,73	2.45	13 (32%)	44,90,113	2.46	20 (45%)
17	CLA	L	203	12	59,73,73	2.04	13 (22%)	67,113,113	2.07	22 (32%)
17	CLA	a	805	1	49,63,73	2.22	13 (26%)	55,101,113	2.28	21 (38%)
17	CLA	b	805	2	59,73,73	2.02	13 (22%)	67,113,113	2.12	22 (32%)
19	LHG	7	618	17	36,36,48	1.08	2 (5%)	39,42,54	1.16	4 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
17	CLA	A	829	1	59,73,73	1.99	13 (22%)	67,113,113	2.09	22 (32%)
20	BCR	A	856	-	41,41,41	1.03	1 (2%)	56,56,56	2.03	16 (28%)
17	CLA	8	313	-	22,32,73	2.70	9 (40%)	26,54,113	4.39	20 (76%)
20	BCR	J	3003	-	41,41,41	1.03	1 (2%)	56,56,56	1.76	14 (25%)
26	CHL	9	605	29	50,64,74	2.19	14 (28%)	52,102,114	2.55	21 (40%)
26	CHL	1	302	13	55,69,74	2.07	14 (25%)	58,108,114	2.44	20 (34%)
20	BCR	b	801	-	41,41,41	1.03	1 (2%)	56,56,56	1.43	6 (10%)
20	BCR	A	848	-	41,41,41	1.02	1 (2%)	56,56,56	1.82	13 (23%)
17	CLA	6	314	13	54,68,73	2.13	13 (24%)	61,107,113	2.19	21 (34%)
17	CLA	3	302	15	54,68,73	2.13	13 (24%)	61,107,113	2.20	22 (36%)
20	BCR	a	854	-	41,41,41	1.04	1 (2%)	56,56,56	1.74	12 (21%)
17	CLA	a	816	1	44,58,73	2.36	13 (29%)	49,95,113	2.37	21 (42%)
21	SF4	a	855	1,2	0,12,12	0.00	-	-		
22	HTG	a	857	-	19,19,19	1.05	2 (10%)	23,24,24	0.55	0
17	CLA	8	312	15	40,54,73	2.46	13 (32%)	44,90,113	2.46	19 (43%)
17	CLA	B	814	2	59,73,73	2.01	13 (22%)	67,113,113	2.08	23 (34%)
17	CLA	1	304	13	59,73,73	2.05	13 (22%)	67,113,113	2.14	20 (29%)
20	BCR	l	205	-	41,41,41	1.02	1 (2%)	56,56,56	1.59	10 (17%)
20	BCR	A	851	-	41,41,41	1.06	1 (2%)	56,56,56	2.02	14 (25%)
28	XAT	9	617	-	39,47,47	0.86	1 (2%)	54,74,74	2.61	17 (31%)
17	CLA	a	846	19	46,60,73	2.33	13 (28%)	51,97,113	2.35	18 (35%)
17	CLA	A	840	1	59,73,73	2.04	13 (22%)	67,113,113	2.13	21 (31%)
20	BCR	B	843	-	41,41,41	1.06	1 (2%)	56,56,56	1.88	14 (25%)
27	LUT	1	316	-	42,43,43	0.74	0	51,60,60	1.55	12 (23%)
26	CHL	4	615	16	37,51,74	2.45	13 (35%)	36,86,114	2.89	13 (36%)
17	CLA	a	807	1	59,73,73	2.03	13 (22%)	67,113,113	2.18	23 (34%)
17	CLA	B	829	2	59,73,73	2.02	13 (22%)	67,113,113	2.21	22 (32%)
17	CLA	b	820	2	44,58,73	2.36	13 (29%)	49,95,113	2.43	21 (42%)
17	CLA	4	614	16	44,58,73	2.36	13 (29%)	49,95,113	2.46	21 (42%)
20	BCR	I	101	-	41,41,41	1.04	1 (2%)	56,56,56	1.93	15 (26%)
17	CLA	4	603	16	40,54,73	2.40	13 (32%)	44,90,113	2.60	19 (43%)
17	CLA	8	301	15	54,68,73	2.14	13 (24%)	61,107,113	2.18	22 (36%)
17	CLA	B	807	2	59,73,73	2.06	13 (22%)	67,113,113	2.13	24 (35%)
17	CLA	3	312	15	49,63,73	2.25	13 (26%)	55,101,113	2.24	21 (38%)
17	CLA	K	4003	11	40,54,73	2.48	13 (32%)	44,90,113	2.47	19 (43%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
17	CLA	8	302	15	44,58,73	2.35	13 (29%)	49,95,113	2.50	21 (42%)
17	CLA	8	307	15	44,58,73	2.36	13 (29%)	49,95,113	2.34	21 (42%)
17	CLA	7	603	14	45,59,73	2.32	13 (28%)	50,96,113	2.41	21 (42%)

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
17	CLA	9	609	16	3/3/19/25	4/31/129/135	-
17	CLA	a	812	1	3/3/20/25	13/37/135/135	-
17	CLA	B	823	2	3/3/19/25	12/31/129/135	-
17	CLA	A	803	29	1/1/20/25	2/37/135/135	-
17	CLA	6	313	13	3/3/17/25	10/22/120/135	-
17	CLA	B	805	2	3/3/20/25	16/37/135/135	-
17	CLA	3	314	15	2/2/16/25	1/15/113/135	-
17	CLA	a	828	1	3/3/20/25	10/37/135/135	-
20	BCR	9	618	-	-	6/29/63/63	0/2/2/2
17	CLA	b	834	2	3/3/20/25	13/37/135/135	-
17	CLA	a	856	29	1/1/20/25	11/37/135/135	-
17	CLA	b	810	2	3/3/20/25	14/37/135/135	-
17	CLA	2	604	29	3/3/19/25	9/31/129/135	-
21	SF4	C	102	3	-	-	0/6/5/5
17	CLA	b	835	29	3/3/16/25	2/11/111/135	-
17	CLA	3	305	29	3/3/15/25	2/10/108/135	-
17	CLA	a	809	1	3/3/20/25	13/37/135/135	-
17	CLA	a	836	1	3/3/17/25	2/19/117/135	-
17	CLA	A	808	1	3/3/20/25	8/37/135/135	-
20	BCR	b	843	-	-	0/29/63/63	0/2/2/2
28	XAT	4	617	-	-	0/31/93/93	0/4/4/4
17	CLA	a	831	1	3/3/20/25	16/37/135/135	-
17	CLA	A	806	1	3/3/20/25	19/37/135/135	-
19	LHG	A	846	-	-	10/53/53/53	-
17	CLA	f	7003	6	1/1/18/25	9/25/123/135	-
20	BCR	L	206	-	-	3/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
17	CLA	A	821	1	3/3/16/25	0/11/111/135	-
17	CLA	A	811	1	3/3/20/25	9/37/135/135	-
17	CLA	A	826	29	3/3/20/25	14/37/135/135	-
20	BCR	B	845	-	-	6/29/63/63	0/2/2/2
19	LHG	1	301	17	-	9/26/26/53	-
17	CLA	a	825	1	3/3/18/25	6/25/123/135	-
17	CLA	b	812	2	3/3/18/25	11/25/123/135	-
17	CLA	7	608	14	3/3/17/25	6/19/117/135	-
26	CHL	4	605	29	2/2/18/26	8/27/125/137	-
27	LUT	7	615	-	-	1/29/67/67	0/2/2/2
17	CLA	4	602	16	3/3/19/25	6/31/129/135	-
17	CLA	6	305	13	3/3/20/25	10/37/135/135	-
19	LHG	a	847	-	-	10/53/53/53	-
20	BCR	I	101	-	-	3/29/63/63	0/2/2/2
17	CLA	B	827	2	1/1/20/25	8/37/135/135	-
17	CLA	A	845	19	3/3/17/25	10/22/120/135	-
26	CHL	2	605	29	2/2/15/26	0/12/110/137	-
27	LUT	4	616	-	-	2/29/67/67	0/2/2/2
17	CLA	a	819	1	3/3/20/25	14/37/135/135	-
22	HTG	j	3001	-	-	1/10/30/30	0/1/1/1
20	BCR	A	852	-	-	6/29/63/63	0/2/2/2
17	CLA	4	601	16	3/3/16/25	3/15/113/135	-
18	PQN	B	842	-	-	3/23/43/43	0/2/2/2
28	XAT	3	317	-	-	2/31/93/93	0/4/4/4
20	BCR	B	844	-	-	6/29/63/63	0/2/2/2
17	CLA	b	816	2	3/3/18/25	11/25/123/135	-
17	CLA	a	818	1	3/3/20/25	12/37/135/135	-
20	BCR	k	1404	-	-	6/29/63/63	0/2/2/2
17	CLA	1	309	13	3/3/20/25	10/37/135/135	-
17	CLA	A	854	29	1/1/20/25	10/37/135/135	-
17	CLA	b	818	2	3/3/19/25	13/31/129/135	-
17	CLA	A	827	29	3/3/20/25	7/37/135/135	-
17	CLA	1	306	-	3/3/17/25	2/22/120/135	-
26	CHL	2	606	-	3/3/16/26	2/18/116/137	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
20	BCR	L	205	-	-	6/29/63/63	0/2/2/2
20	BCR	B	843	-	-	0/29/63/63	0/2/2/2
25	LMG	4	619	-	-	9/39/59/70	0/1/1/1
26	CHL	6	303	13	3/3/19/26	15/33/131/137	-
17	CLA	j	3002	10	3/3/15/25	1/10/108/135	-
17	CLA	3	303	15	3/3/17/25	2/19/117/135	-
17	CLA	9	611	16	3/3/17/25	6/22/120/135	-
19	LHG	1	319	17	-	10/53/53/53	-
20	BCR	f	7004	-	-	4/29/63/63	0/2/2/2
17	CLA	A	824	1	3/3/17/25	9/21/119/135	-
17	CLA	1	315	13	3/3/16/25	1/15/113/135	-
17	CLA	2	613	14	3/3/15/25	6/11/109/135	-
20	BCR	1	318	-	-	6/29/63/63	0/2/2/2
17	CLA	1	305	29	3/3/17/25	6/22/120/135	-
17	CLA	A	825	1	3/3/18/25	7/25/123/135	-
17	CLA	A	817	29	2/2/16/25	1/11/111/135	-
17	CLA	g	102	7	3/3/17/25	1/19/117/135	-
17	CLA	A	828	1	3/3/20/25	13/37/135/135	-
20	BCR	B	801	-	-	1/29/63/63	0/2/2/2
17	CLA	A	815	1	3/3/16/25	1/11/111/135	-
17	CLA	a	820	1	3/3/20/25	11/37/135/135	-
17	CLA	A	801	1	4/4/20/25	7/37/135/135	-
20	BCR	a	853	-	-	7/29/63/63	0/2/2/2
27	LUT	9	616	-	-	2/29/67/67	0/2/2/2
17	CLA	A	834	1	2/2/20/25	10/37/135/135	-
17	CLA	A	832	1	2/2/17/25	2/19/117/135	-
17	CLA	B	819	29	2/2/20/25	9/37/135/135	-
17	CLA	4	604	29	3/3/17/25	5/19/117/135	-
17	CLA	B	818	2	2/2/19/25	10/31/129/135	-
20	BCR	B	848	-	-	2/29/63/63	0/2/2/2
17	CLA	f	7002	29	3/3/16/25	1/11/111/135	-
17	CLA	3	311	-	3/3/17/25	6/22/120/135	-
17	CLA	A	840	1	3/3/20/25	7/37/135/135	-
28	XAT	7	616	-	-	1/31/93/93	0/4/4/4
17	CLA	b	809	2	3/3/20/25	8/37/135/135	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
17	CLA	a	835	1	3/3/20/25	10/37/135/135	-
17	CLA	b	838	2	3/3/16/25	2/16/114/135	-
17	CLA	2	611	14	3/3/17/25	5/22/120/135	-
17	CLA	B	824	29	2/2/20/25	7/37/135/135	-
26	CHL	2	614	14	3/3/15/26	0/12/110/137	-
17	CLA	B	841	19	3/3/20/25	8/37/135/135	-
17	CLA	3	308	15	3/3/17/25	5/19/117/135	-
17	CLA	A	831	1	3/3/20/25	13/37/135/135	-
17	CLA	l	202	12	3/3/20/25	10/37/135/135	-
17	CLA	a	814	1	3/3/20/25	11/37/135/135	-
17	CLA	a	839	1	3/3/20/25	10/37/135/135	-
27	LUT	1	320	-	-	2/29/67/67	0/2/2/2
17	CLA	b	822	2	3/3/18/25	10/25/123/135	-
17	CLA	a	817	29	2/2/16/25	0/11/111/135	-
20	BCR	K	4004	-	-	4/29/63/63	0/2/2/2
17	CLA	A	814	1	3/3/20/25	16/37/135/135	-
17	CLA	1	312	13	3/3/17/25	8/22/120/135	-
28	XAT	6	318	-	-	1/31/93/93	0/4/4/4
17	CLA	7	610	19	3/3/15/25	0/8/106/135	-
17	CLA	a	837	1	2/2/16/25	3/11/111/135	-
17	CLA	b	815	2	3/3/18/25	7/25/123/135	-
17	CLA	2	602	14	3/3/20/25	13/37/135/135	-
17	CLA	a	811	1	3/3/20/25	9/37/135/135	-
17	CLA	A	836	1	3/3/17/25	0/19/117/135	-
17	CLA	8	304	29	3/3/15/25	0/10/108/135	-
17	CLA	B	806	2	3/3/20/25	16/37/135/135	-
26	CHL	6	308	13	3/3/16/26	1/17/115/137	-
17	CLA	B	821	2	3/3/16/25	1/15/113/135	-
17	CLA	8	305	15	3/3/16/25	3/16/114/135	-
18	PQN	A	844	-	-	8/23/43/43	0/2/2/2
20	BCR	K	4001	-	-	1/29/63/63	0/2/2/2
17	CLA	b	802	2	2/2/20/25	5/37/135/135	-
23	LMT	B	849	-	-	3/21/61/61	0/2/2/2
20	BCR	l	206	-	-	0/29/63/63	0/2/2/2
17	CLA	B	811	2	3/3/18/25	4/25/121/135	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
17	CLA	A	818	1	3/3/20/25	12/37/135/135	-
17	CLA	9	612	16	3/3/18/25	10/27/125/135	-
17	CLA	6	315	13	3/3/18/25	6/25/123/135	-
27	LUT	8	314	-	-	2/29/67/67	0/2/2/2
17	CLA	1	308	29	3/3/20/25	5/37/135/135	-
17	CLA	a	844	29	3/3/20/25	12/37/135/135	-
26	CHL	2	601	14	2/2/19/26	11/33/131/137	-
17	CLA	4	609	16	3/3/19/25	5/31/129/135	-
17	CLA	B	826	2	3/3/20/25	10/37/135/135	-
17	CLA	9	608	16	3/3/17/25	4/19/117/135	-
17	CLA	B	839	29	3/3/20/25	7/37/135/135	-
17	CLA	b	823	2	3/3/19/25	6/31/129/135	-
17	CLA	B	820	2	3/3/17/25	3/19/117/135	-
17	CLA	9	603	16	3/3/16/25	4/15/113/135	-
17	CLA	L	204	29	3/3/17/25	3/19/117/135	-
20	BCR	L	201	-	-	8/29/63/63	0/2/2/2
17	CLA	B	825	29	3/3/20/25	7/37/135/135	-
20	BCR	j	3004	-	-	9/29/63/63	0/2/2/2
17	CLA	A	810	1	3/3/20/25	4/37/135/135	-
25	LMG	4	620	-	-	11/39/59/70	0/1/1/1
17	CLA	l	203	12	3/3/20/25	6/37/135/135	-
17	CLA	6	316	13	3/3/16/25	3/15/113/135	-
17	CLA	b	819	29	3/3/20/25	5/37/135/135	-
17	CLA	3	309	15	3/3/17/25	1/19/117/135	-
17	CLA	A	819	1	3/3/20/25	13/37/135/135	-
20	BCR	a	849	-	-	2/29/63/63	0/2/2/2
21	SF4	A	853	1,2	-	-	0/6/5/5
17	CLA	F	303	29	3/3/16/25	0/11/111/135	-
17	CLA	B	810	2	3/3/20/25	9/37/135/135	-
26	CHL	4	606	29	3/3/17/26	6/21/119/137	-
26	CHL	4	615	16	3/3/15/26	0/12/110/137	-
17	CLA	3	306	15	3/3/16/25	3/16/114/135	-
17	CLA	A	835	1	3/3/20/25	10/37/135/135	-
26	CHL	7	614	14	3/3/15/26	3/12/110/137	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
17	CLA	1	313	13	3/3/20/25	5/37/135/135	-
17	CLA	b	826	2	3/3/20/25	8/37/135/135	-
17	CLA	b	829	2	3/3/20/25	6/37/135/135	-
18	PQN	b	842	-	-	3/23/43/43	0/2/2/2
17	CLA	B	808	2	3/3/20/25	7/37/135/135	-
17	CLA	A	812	1	3/3/20/25	13/37/135/135	-
17	CLA	6	306	29	3/3/17/25	3/21/119/135	-
17	CLA	1	310	13	3/3/19/25	3/31/129/135	-
17	CLA	a	842	29	3/3/20/25	5/37/135/135	-
17	CLA	6	304	13	3/3/20/25	9/37/135/135	-
26	CHL	7	601	14	3/3/19/26	8/33/131/137	-
17	CLA	B	840	2	2/2/20/25	9/37/135/135	-
17	CLA	b	832	2	3/3/20/25	12/37/135/135	-
17	CLA	b	837	2	3/3/20/25	9/37/135/135	-
25	LMG	6	302	-	-	6/35/55/70	0/1/1/1
27	LUT	3	316	-	-	2/29/67/67	0/2/2/2
17	CLA	A	823	1	3/3/16/25	5/18/116/135	-
17	CLA	B	809	2	3/3/20/25	7/37/135/135	-
22	HTG	f	7001	-	-	1/10/30/30	0/1/1/1
20	BCR	7	617	-	-	4/29/63/63	0/2/2/2
17	CLA	b	806	2	3/3/20/25	9/37/135/135	-
27	LUT	6	321	-	-	2/29/67/67	0/2/2/2
17	CLA	G	103	7	3/3/17/25	1/19/117/135	-
17	CLA	A	809	1	3/3/20/25	18/37/135/135	-
20	BCR	G	105	-	-	3/29/63/63	0/2/2/2
17	CLA	b	830	2	3/3/17/25	3/19/117/135	-
20	BCR	6	319	-	-	4/29/63/63	0/2/2/2
17	CLA	B	832	2	3/3/20/25	14/37/135/135	-
26	CHL	9	615	16	3/3/15/26	0/12/110/137	-
17	CLA	B	802	2	2/2/20/25	13/37/135/135	-
17	CLA	8	308	15	3/3/17/25	1/19/117/135	-
21	SF4	C	101	3	-	-	0/6/5/5
17	CLA	F	301	29	3/3/20/25	8/37/135/135	-
17	CLA	G	104	7	3/3/16/25	2/15/113/135	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
19	LHG	6	301	17	-	7/26/26/53	-
20	BCR	A	849	-	-	2/29/63/63	0/2/2/2
18	PQN	a	845	-	-	5/23/43/43	0/2/2/2
21	SF4	c	102	3	-	-	0/6/5/5
17	CLA	b	840	2	3/3/20/25	5/37/135/135	-
17	CLA	A	820	1	3/3/20/25	12/37/135/135	-
20	BCR	b	844	-	-	6/29/63/63	0/2/2/2
17	CLA	A	805	1	3/3/18/25	8/25/123/135	-
20	BCR	A	850	-	-	3/29/63/63	0/2/2/2
24	DGD	B	850	-	-	12/55/95/95	0/2/2/2
26	CHL	9	606	29	3/3/17/26	4/21/119/137	-
17	CLA	2	608	14	3/3/17/25	3/19/117/135	-
17	CLA	B	831	2	3/3/16/25	8/18/116/135	-
17	CLA	a	821	1	3/3/16/25	2/11/111/135	-
20	BCR	2	617	-	-	3/29/63/63	0/2/2/2
17	CLA	B	828	2	3/3/20/25	5/37/135/135	-
20	BCR	j	3003	-	-	6/29/63/63	0/2/2/2
28	XAT	1	317	-	-	0/31/93/93	0/4/4/4
20	BCR	8	316	-	-	4/29/63/63	0/2/2/2
17	CLA	a	826	29	3/3/20/25	6/37/135/135	-
17	CLA	k	1402	11	3/3/16/25	0/15/113/135	-
17	CLA	a	834	1	3/3/20/25	10/37/135/135	-
17	CLA	9	602	16	3/3/19/25	10/31/129/135	-
17	CLA	a	815	1	3/3/16/25	3/11/111/135	-
26	CHL	4	607	29	3/3/17/26	3/21/119/137	-
17	CLA	a	833	1	3/3/20/25	5/37/135/135	-
17	CLA	b	839	29	3/3/20/25	9/37/135/135	-
17	CLA	b	833	2	3/3/18/25	8/29/127/135	-
27	LUT	2	615	-	-	2/29/67/67	0/2/2/2
17	CLA	A	841	1	3/3/20/25	10/37/135/135	-
20	BCR	3	318	-	-	6/29/63/63	0/2/2/2
17	CLA	b	827	2	2/2/20/25	14/37/135/135	-
17	CLA	2	612	14	3/3/20/25	9/37/135/135	-
17	CLA	3	301	-	3/3/16/25	2/15/113/135	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
17	CLA	k	1401	-	3/3/16/25	3/11/111/135	-
17	CLA	A	822	29	3/3/20/25	5/37/135/135	-
17	CLA	g	101	-	2/2/15/25	3/8/106/135	-
17	CLA	7	609	14	3/3/19/25	7/31/129/135	-
17	CLA	6	309	29	3/3/16/25	3/15/113/135	-
20	BCR	b	847	-	-	3/29/63/63	0/2/2/2
28	XAT	8	315	-	-	0/31/93/93	0/4/4/4
17	CLA	B	833	2	3/3/18/25	9/29/127/135	-
17	CLA	B	836	2	3/3/19/25	5/31/129/135	-
17	CLA	B	822	2	3/3/18/25	11/25/123/135	-
17	CLA	4	610	29	3/3/18/25	5/25/123/135	-
20	BCR	b	846	-	-	5/29/63/63	0/2/2/2
17	CLA	B	813	2	3/3/20/25	16/37/135/135	-
17	CLA	B	830	2	3/3/17/25	5/19/117/135	-
17	CLA	J	3002	10	3/3/15/25	4/10/108/135	-
17	CLA	2	610	19	2/2/15/25	0/8/106/135	-
28	XAT	2	616	-	-	0/31/93/93	0/4/4/4
17	CLA	B	815	2	3/3/19/25	10/31/129/135	-
17	CLA	a	840	1	2/2/20/25	9/37/135/135	-
25	LMG	9	619	-	-	10/45/65/70	0/1/1/1
26	CHL	9	607	29	3/3/17/26	3/21/119/137	-
20	BCR	B	847	-	-	5/29/63/63	0/2/2/2
17	CLA	B	834	2	3/3/20/25	16/37/135/135	-
17	CLA	7	602	14	3/3/20/25	8/37/135/135	-
24	DGD	b	849	-	-	10/55/95/95	0/2/2/2
17	CLA	A	804	1	3/3/20/25	7/37/135/135	-
17	CLA	b	811	2	3/3/18/25	10/25/121/135	-
17	CLA	4	613	16	3/3/16/25	0/11/111/135	-
17	CLA	6	307	-	3/3/15/25	4/10/108/135	-
17	CLA	B	837	2	3/3/20/25	9/37/135/135	-
20	BCR	a	850	-	-	6/29/63/63	0/2/2/2
17	CLA	a	822	29	3/3/20/25	3/37/135/135	-
17	CLA	9	604	29	3/3/17/25	5/19/117/135	-
19	LHG	a	848	17	-	12/31/31/53	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
17	CLA	7	611	14	3/3/17/25	5/22/120/135	-
20	BCR	b	845	-	-	6/29/63/63	0/2/2/2
19	LHG	3	319	17	-	11/23/23/53	-
21	SF4	c	101	3	-	-	0/6/5/5
19	LHG	2	618	17	-	9/41/41/53	-
17	CLA	8	303	29	3/3/16/25	1/11/111/135	-
17	CLA	a	832	1	2/2/17/25	4/19/117/135	-
17	CLA	a	810	1	3/3/20/25	2/37/135/135	-
17	CLA	4	612	16	3/3/18/25	9/27/125/135	-
17	CLA	a	824	1	3/3/17/25	8/21/119/135	-
17	CLA	3	315	-	3/3/7/25	-	-
17	CLA	b	817	2	3/3/18/25	11/30/128/135	-
17	CLA	b	803	2	3/3/20/25	6/37/135/135	-
17	CLA	6	312	19	3/3/15/25	0/8/106/135	-
25	LMG	G	102	-	-	10/39/59/70	0/1/1/1
17	CLA	b	824	29	3/3/20/25	10/37/135/135	-
17	CLA	6	310	13	3/3/20/25	7/37/135/135	-
20	BCR	F	305	-	-	4/29/63/63	0/2/2/2
19	LHG	A	847	17	-	9/31/31/53	-
17	CLA	2	603	14	3/3/20/25	11/37/135/135	-
17	CLA	2	609	14	3/3/19/25	8/31/129/135	-
17	CLA	B	835	29	3/3/16/25	1/11/111/135	-
17	CLA	K	4002	-	3/3/16/25	2/11/111/135	-
20	BCR	l	201	-	-	8/29/63/63	0/2/2/2
17	CLA	F	304	6	3/3/18/25	8/25/123/135	-
17	CLA	a	823	1	3/3/16/25	5/18/116/135	-
17	CLA	A	842	1	3/3/20/25	13/37/135/135	-
17	CLA	a	830	1	3/3/20/25	11/37/135/135	-
22	HTG	J	3001	-	-	4/10/30/30	0/1/1/1
17	CLA	b	831	2	2/2/16/25	7/18/116/135	-
17	CLA	A	838	1	3/3/17/25	3/21/119/135	-
20	BCR	B	846	-	-	4/29/63/63	0/2/2/2
17	CLA	b	828	2	3/3/20/25	9/37/135/135	-
20	BCR	b	848	-	-	2/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
17	CLA	A	802	1	3/3/20/25	5/37/135/135	-
17	CLA	4	611	16	3/3/17/25	7/22/120/135	-
17	CLA	A	813	1	3/3/17/25	7/24/122/135	-
17	CLA	A	816	1	3/3/17/25	3/19/117/135	-
17	CLA	B	816	2	3/3/18/25	9/25/123/135	-
19	LHG	6	320	17	-	14/53/53/53	-
17	CLA	L	202	12	3/3/20/25	8/37/135/135	-
17	CLA	a	838	1	3/3/17/25	9/21/119/135	-
20	BCR	4	618	-	-	6/29/63/63	0/2/2/2
17	CLA	b	841	19	3/3/20/25	4/37/135/135	-
17	CLA	b	808	2	3/3/20/25	8/37/135/135	-
22	HTG	A	855	-	-	1/10/30/30	0/1/1/1
26	CHL	7	607	29	3/3/17/26	4/21/119/137	-
26	CHL	3	307	29	3/3/16/26	2/17/115/137	-
17	CLA	b	825	29	3/3/20/25	8/37/135/135	-
17	CLA	b	813	2	3/3/20/25	13/37/135/135	-
17	CLA	g	103	7	3/3/16/25	2/15/113/135	-
17	CLA	B	812	2	3/3/18/25	8/25/123/135	-
17	CLA	1	303	13	3/3/20/25	9/37/135/135	-
20	BCR	i	101	-	-	1/29/63/63	0/2/2/2
17	CLA	9	610	29	3/3/15/25	0/8/106/135	-
17	CLA	a	803	29	1/1/20/25	1/37/135/135	-
17	CLA	l	204	29	3/3/17/25	4/19/117/135	-
26	CHL	1	307	13	3/3/16/26	3/18/116/137	-
17	CLA	A	837	1	3/3/16/25	3/11/111/135	-
20	BCR	a	851	-	-	1/29/63/63	0/2/2/2
17	CLA	G	101	29	3/3/16/25	2/11/111/135	-
17	CLA	B	804	2	3/3/16/25	6/11/111/135	-
17	CLA	6	311	13	3/3/19/25	9/31/129/135	-
17	CLA	8	309	-	3/3/17/25	5/22/120/135	-
17	CLA	1	314	13	2/2/18/25	4/25/123/135	-
17	CLA	B	803	2	3/3/20/25	5/37/135/135	-
26	CHL	7	605	29	3/3/15/26	4/12/110/137	-
17	CLA	b	804	2	3/3/16/25	4/11/111/135	-
17	CLA	b	807	2	3/3/20/25	6/37/135/135	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
17	CLA	3	310	19	3/3/13/25	0/2/96/135	-
17	CLA	a	841	1	3/3/20/25	12/37/135/135	-
17	CLA	7	604	29	3/3/19/25	11/31/129/135	-
22	HTG	F	302	-	-	2/10/30/30	0/1/1/1
17	CLA	A	807	1	3/3/20/25	12/37/135/135	-
17	CLA	a	843	1	3/3/20/25	14/37/135/135	-
17	CLA	8	311	15	2/2/16/25	1/11/111/135	-
20	BCR	g	104	-	-	2/29/63/63	0/2/2/2
17	CLA	9	614	16	3/3/16/25	4/16/114/135	-
17	CLA	B	838	2	2/2/16/25	0/16/114/135	-
17	CLA	7	613	14	2/2/15/25	0/11/109/135	-
17	CLA	k	1403	-	3/3/16/25	4/15/113/135	-
17	CLA	a	801	1	4/4/20/25	8/37/135/135	-
17	CLA	A	833	1	3/3/20/25	7/37/135/135	-
17	CLA	L	203	12	3/3/20/25	5/37/135/135	-
17	CLA	4	608	16	3/3/17/25	3/19/117/135	-
17	CLA	a	804	1	3/3/20/25	16/37/135/135	-
17	CLA	3	313	15	3/3/16/25	2/11/111/135	-
17	CLA	A	839	1	3/3/20/25	5/37/135/135	-
17	CLA	3	304	29	3/3/16/25	1/11/111/135	-
17	CLA	1	311	19	3/3/15/25	0/8/106/135	-
17	CLA	b	836	2	3/3/19/25	5/31/129/135	-
17	CLA	a	829	1	1/1/20/25	12/37/135/135	-
17	CLA	b	821	2	3/3/16/25	3/15/113/135	-
17	CLA	a	802	1	3/3/20/25	16/37/135/135	-
17	CLA	A	843	29	3/3/20/25	16/37/135/135	-
17	CLA	a	808	1	3/3/20/25	8/37/135/135	-
26	CHL	7	606	-	3/3/16/26	0/18/116/137	-
26	CHL	8	306	29	3/3/16/26	3/17/115/137	-
17	CLA	a	813	1	3/3/17/25	6/24/122/135	-
20	BCR	a	852	-	-	6/29/63/63	0/2/2/2
17	CLA	A	830	1	3/3/20/25	13/37/135/135	-
17	CLA	B	817	2	3/3/18/25	10/30/128/135	-
17	CLA	a	806	1	3/3/20/25	16/37/135/135	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
17	CLA	8	310	15	3/3/18/25	8/25/123/135	-
17	CLA	7	612	14	3/3/20/25	8/37/135/135	-
27	LUT	6	317	-	-	2/29/67/67	0/2/2/2
26	CHL	2	607	29	3/3/17/26	5/21/119/137	-
17	CLA	9	601	16	3/3/16/25	5/15/113/135	-
17	CLA	a	805	1	3/3/18/25	9/25/123/135	-
17	CLA	b	805	2	3/3/20/25	19/37/135/135	-
19	LHG	7	618	17	-	10/41/41/53	-
17	CLA	A	829	1	2/2/20/25	11/37/135/135	-
20	BCR	A	856	-	-	4/29/63/63	0/2/2/2
17	CLA	8	313	-	3/3/7/25	-	-
20	BCR	J	3003	-	-	2/29/63/63	0/2/2/2
26	CHL	9	605	29	2/2/18/26	8/27/125/137	-
26	CHL	1	302	13	3/3/19/26	7/33/131/137	-
20	BCR	b	801	-	-	0/29/63/63	0/2/2/2
20	BCR	A	848	-	-	6/29/63/63	0/2/2/2
17	CLA	6	314	13	3/3/19/25	6/31/129/135	-
17	CLA	3	302	15	3/3/19/25	8/31/129/135	-
20	BCR	a	854	-	-	4/29/63/63	0/2/2/2
17	CLA	a	816	1	3/3/17/25	9/19/117/135	-
17	CLA	b	814	2	3/3/20/25	10/37/135/135	-
21	SF4	a	855	1,2	-	-	0/6/5/5
22	HTG	a	857	-	-	0/10/30/30	0/1/1/1
17	CLA	8	312	15	2/2/16/25	1/15/113/135	-
17	CLA	B	814	2	3/3/20/25	12/37/135/135	-
17	CLA	1	304	13	3/3/20/25	12/37/135/135	-
20	BCR	l	205	-	-	6/29/63/63	0/2/2/2
20	BCR	A	851	-	-	5/29/63/63	0/2/2/2
28	XAT	9	617	-	-	0/31/93/93	0/4/4/4
17	CLA	a	846	19	3/3/17/25	13/22/120/135	-
17	CLA	a	827	29	3/3/20/25	8/37/135/135	-
27	LUT	1	316	-	-	2/29/67/67	0/2/2/2
17	CLA	a	807	1	3/3/20/25	14/37/135/135	-
17	CLA	B	829	2	3/3/20/25	9/37/135/135	-
17	CLA	b	820	2	3/3/17/25	2/19/117/135	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
17	CLA	4	614	16	3/3/17/25	2/19/117/135	-
17	CLA	9	613	16	3/3/16/25	0/11/111/135	-
17	CLA	4	603	16	3/3/16/25	2/15/113/135	-
17	CLA	8	301	15	3/3/19/25	11/31/129/135	-
17	CLA	B	807	2	2/2/20/25	14/37/135/135	-
17	CLA	3	312	15	3/3/18/25	9/25/123/135	-
17	CLA	K	4003	11	3/3/16/25	2/15/113/135	-
17	CLA	8	302	15	3/3/17/25	1/19/117/135	-
17	CLA	8	307	15	3/3/17/25	5/19/117/135	-
17	CLA	7	603	14	3/3/17/25	3/21/119/135	-

The worst 5 of 4107 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	a	845	PQN	C3-C2	7.78	1.49	1.35
18	b	842	PQN	C3-C2	7.70	1.49	1.35
18	A	844	PQN	C3-C2	7.61	1.49	1.35
18	B	842	PQN	C3-C2	7.59	1.49	1.35
17	B	836	CLA	C3B-C2B	6.44	1.49	1.40

The worst 5 of 7347 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	8	306	CHL	C4A-NA-C1A	-9.69	102.35	106.71
26	9	615	CHL	C4A-NA-C1A	-9.19	102.57	106.71
26	7	605	CHL	C4A-NA-C1A	-8.75	102.77	106.71
26	7	601	CHL	C4A-NA-C1A	-8.69	102.80	106.71
26	4	606	CHL	C4A-NA-C1A	-8.62	102.83	106.71

5 of 886 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
17	9	609	CLA	NC
17	9	609	CLA	ND
17	9	609	CLA	NA
17	a	812	CLA	NC
17	a	812	CLA	ND

5 of 2517 torsion outliers are listed below:

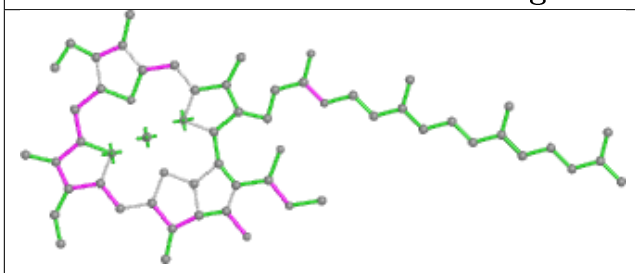
Mol	Chain	Res	Type	Atoms
17	B	805	CLA	C3A-C2A-CAA-CBA
20	9	618	BCR	C7-C8-C9-C10
20	9	618	BCR	C7-C8-C9-C34
17	A	831	CLA	CHA-CBD-CGD-O1D
17	A	831	CLA	CHA-CBD-CGD-O2D

There are no ring outliers.

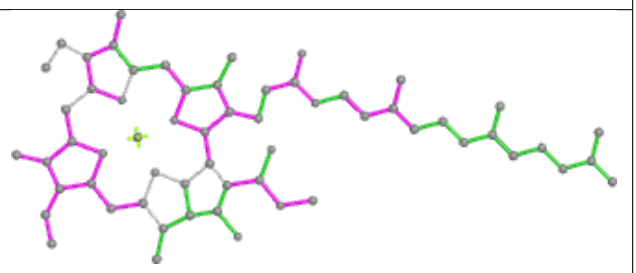
No monomer is involved in short contacts.

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

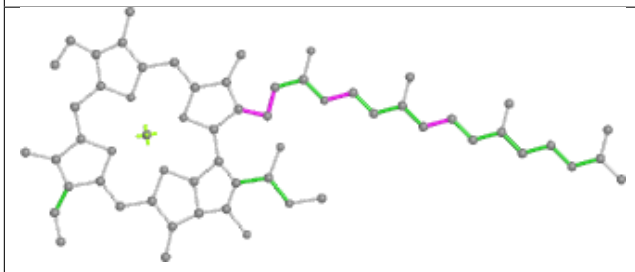
Ligand CLA 9 609



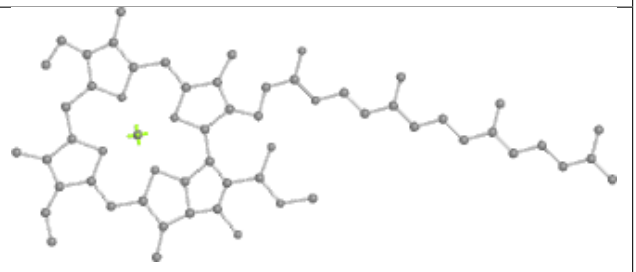
Bond lengths



Bond angles

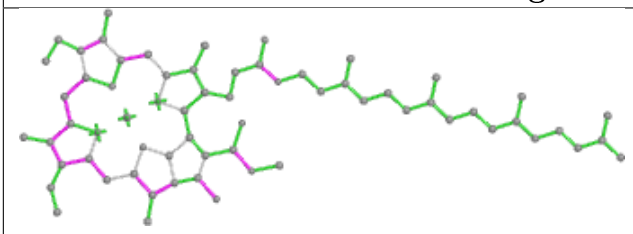


Torsions

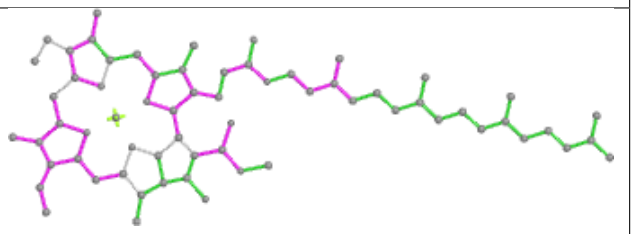


Rings

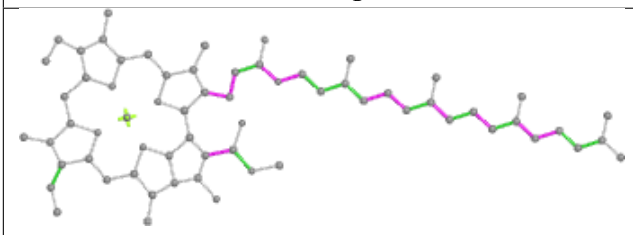
Ligand CLA a 812



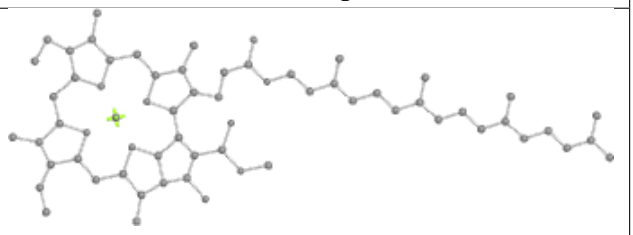
Bond lengths



Bond angles

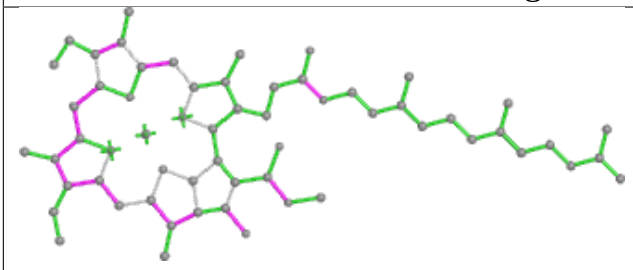


Torsions

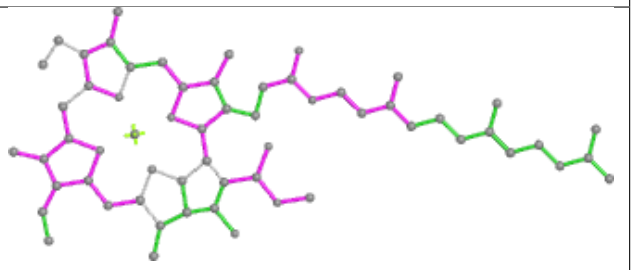


Rings

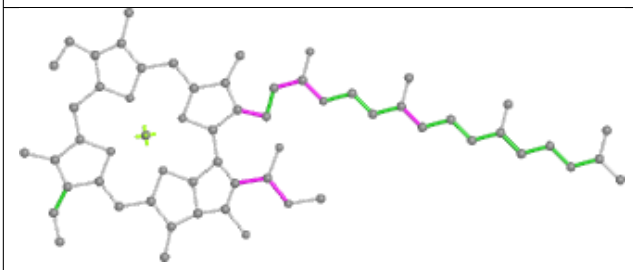
Ligand CLA B 823



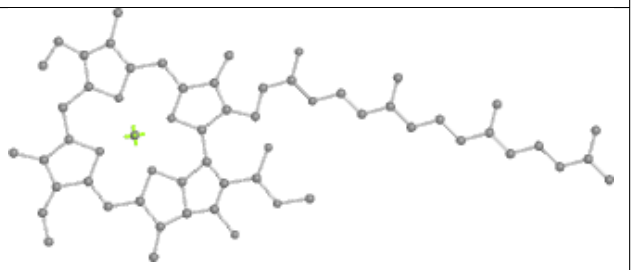
Bond lengths



Bond angles

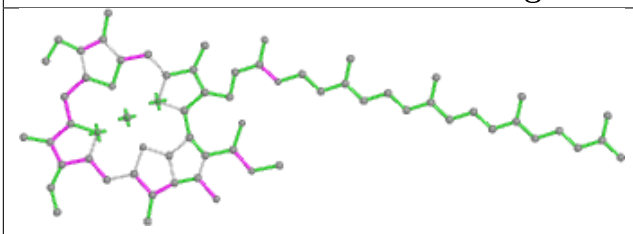


Torsions

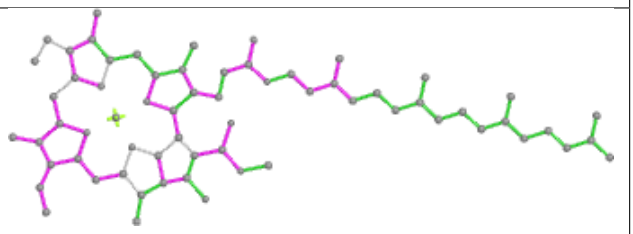


Rings

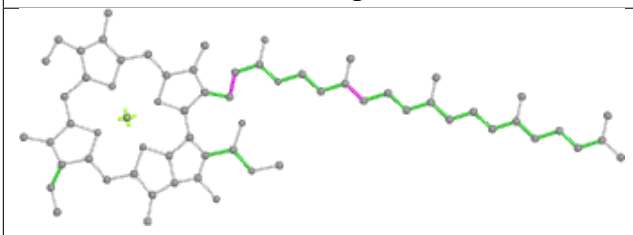
Ligand CLA A 803



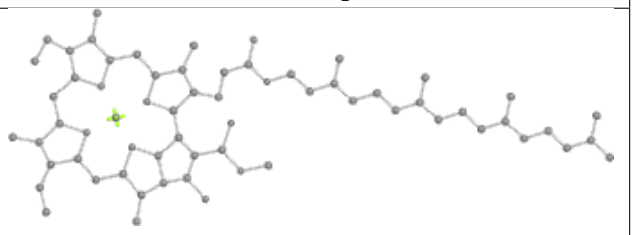
Bond lengths



Bond angles

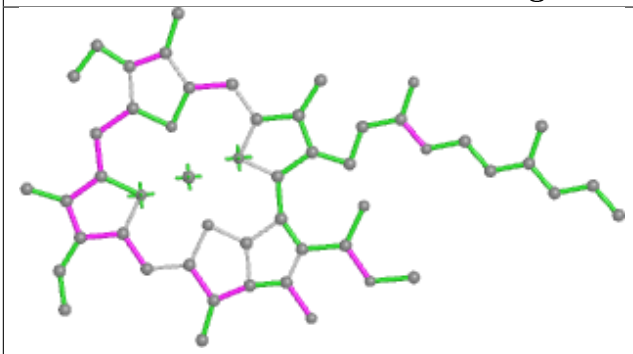


Torsions

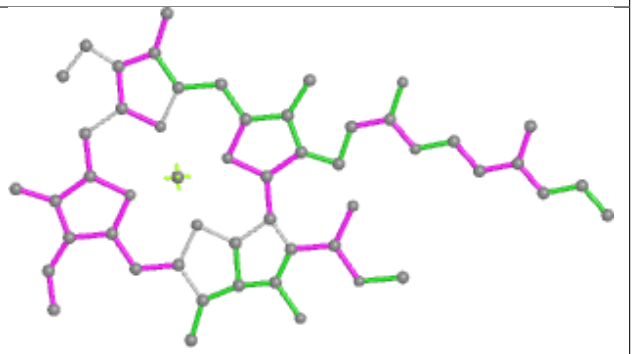


Rings

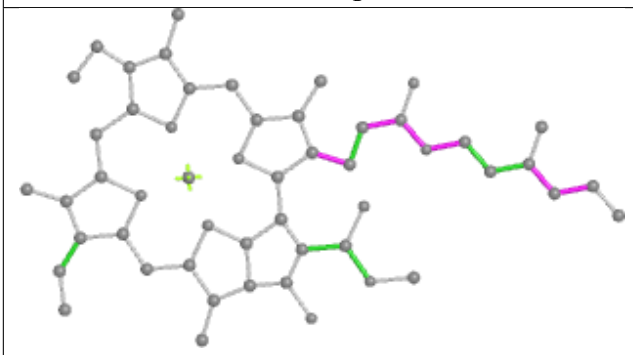
Ligand CLA 6 313



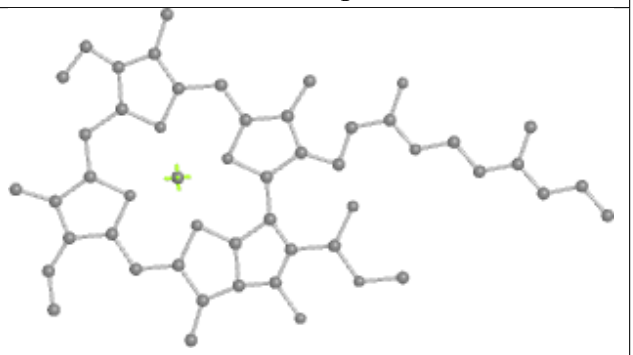
Bond lengths



Bond angles

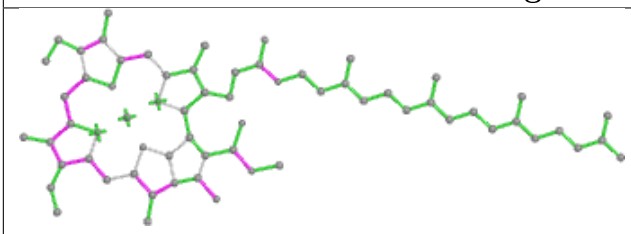


Torsions

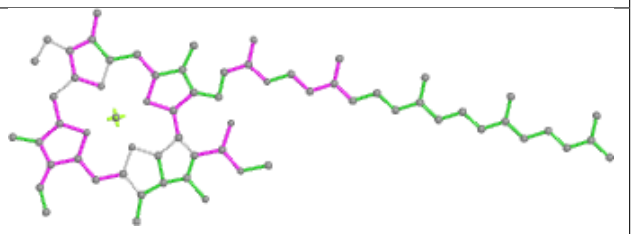


Rings

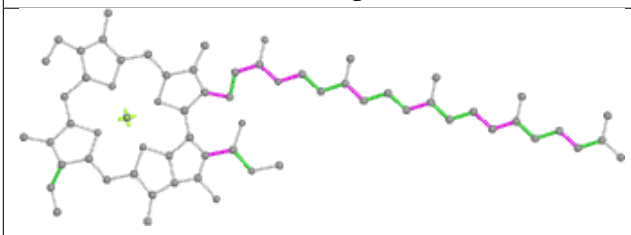
Ligand CLA B 805



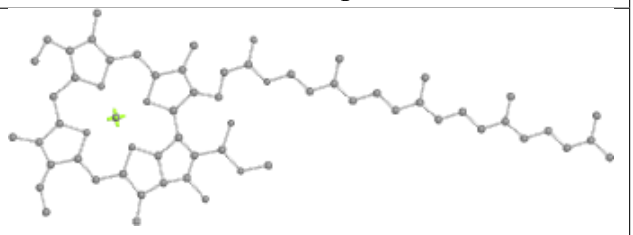
Bond lengths



Bond angles

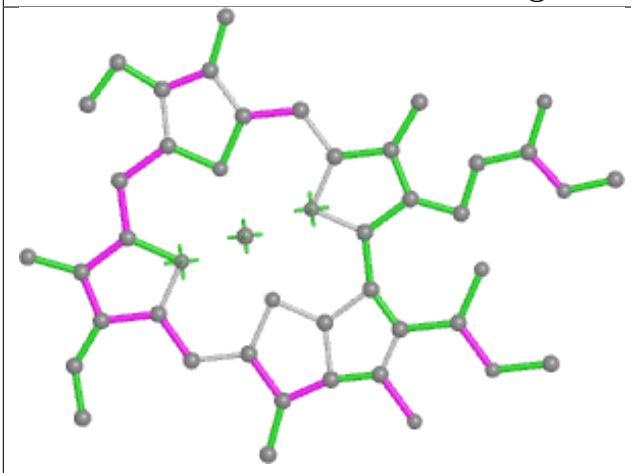


Torsions

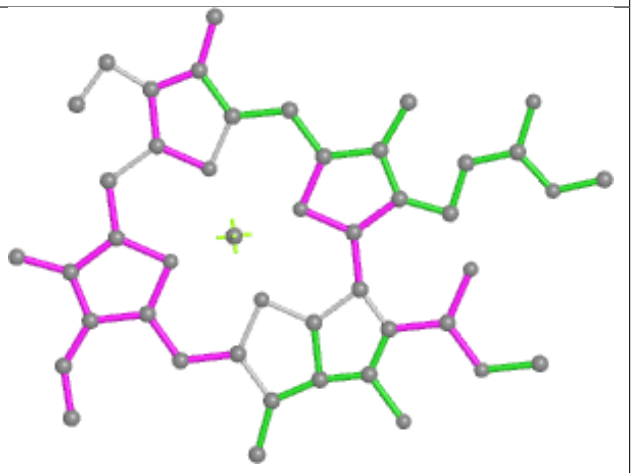


Rings

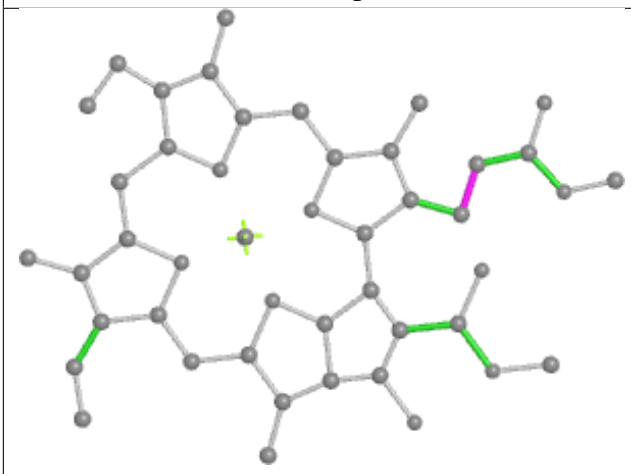
Ligand CLA 3 314



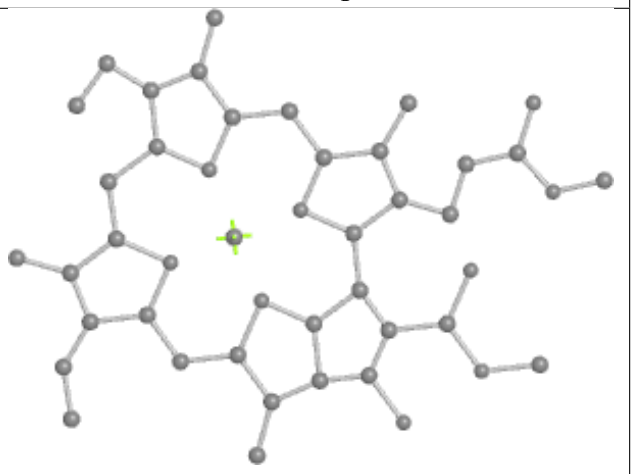
Bond lengths



Bond angles

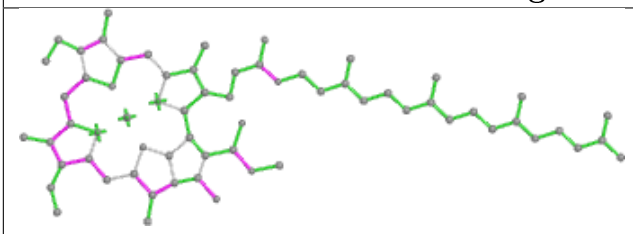


Torsions



Rings

Ligand CLA a 828



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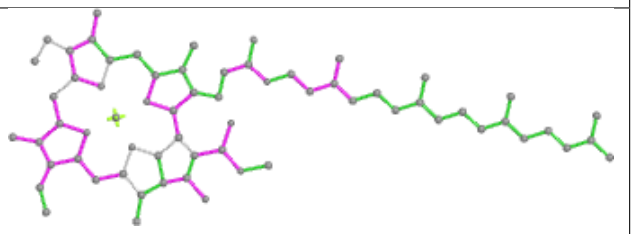
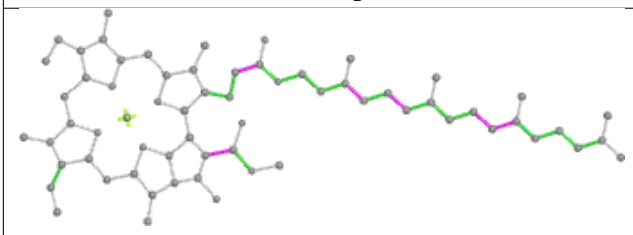


Bond angles



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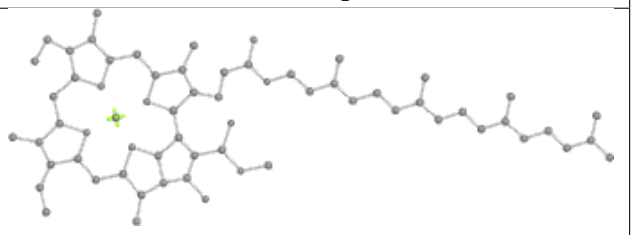
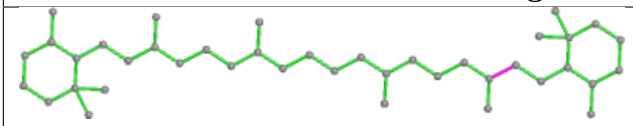


Rings

Ligand BCR 9 618



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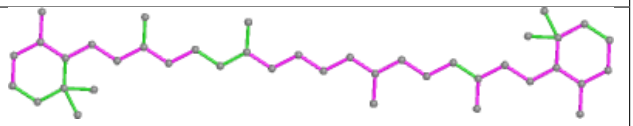

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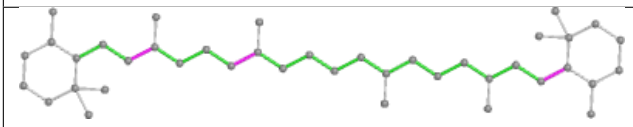
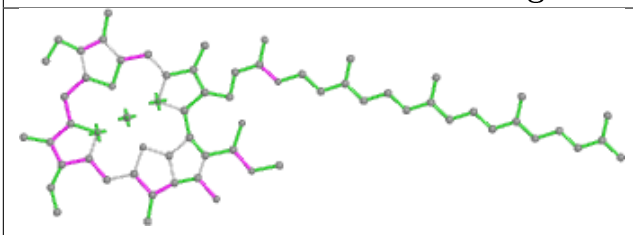


Torsions

Rings

Ligand CLA b 834



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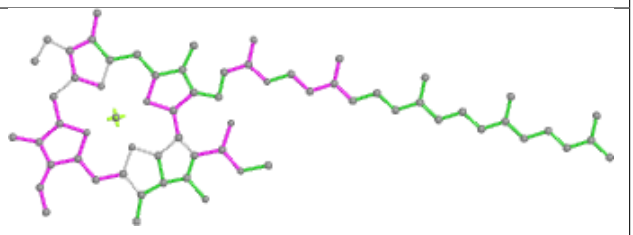
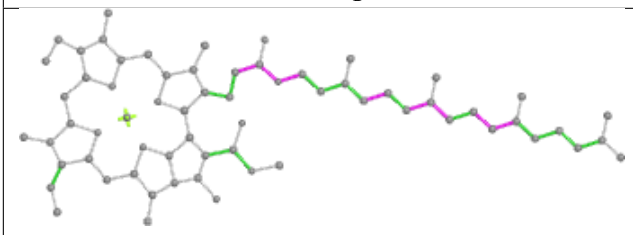
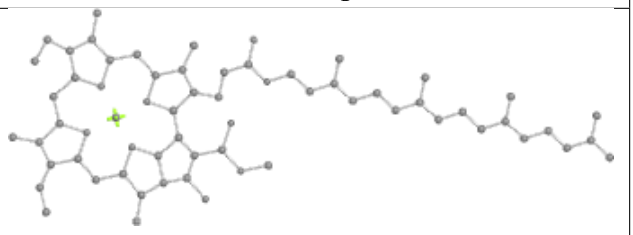


Bond angles

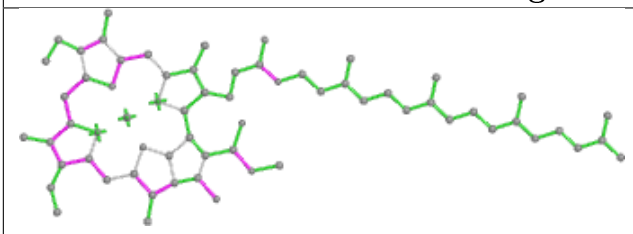


Torsions



Rings

Ligand CLA a 856



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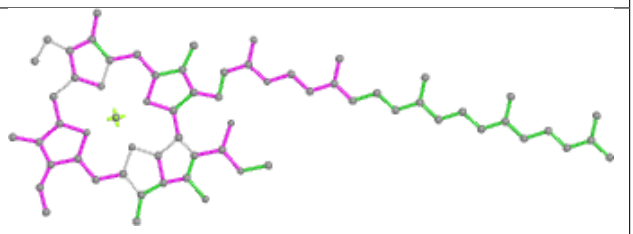
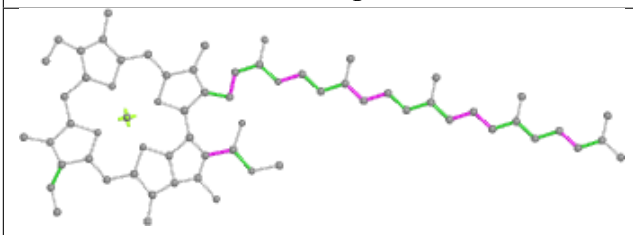


Bond angles



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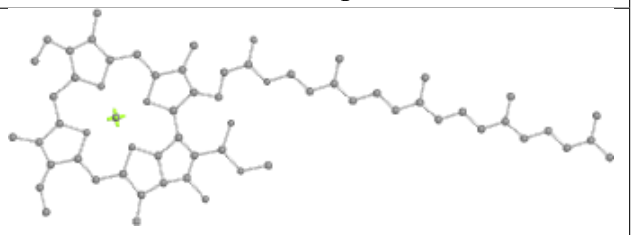
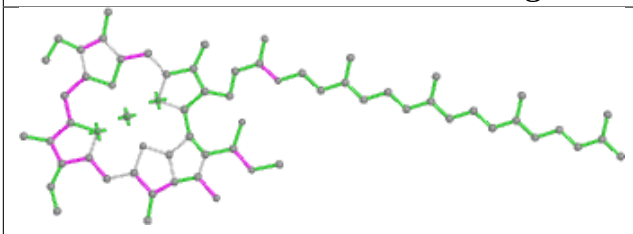


Rings

Ligand CLA A 831



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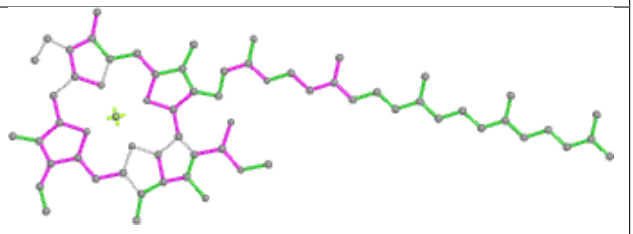
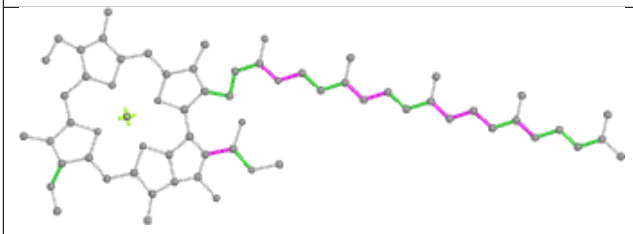


Bond angles



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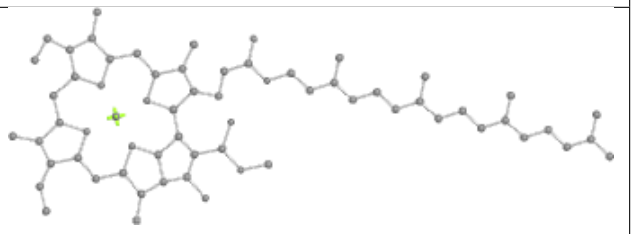
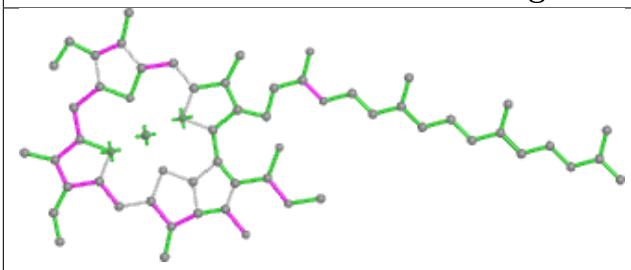


Rings

Ligand CLA 2 604



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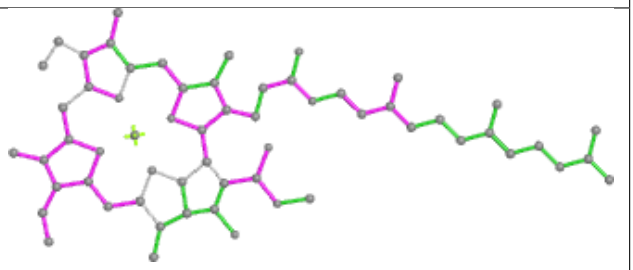
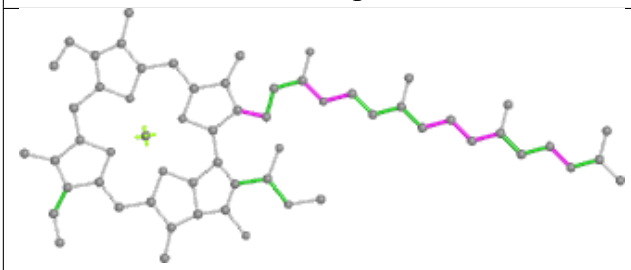


Bond angles



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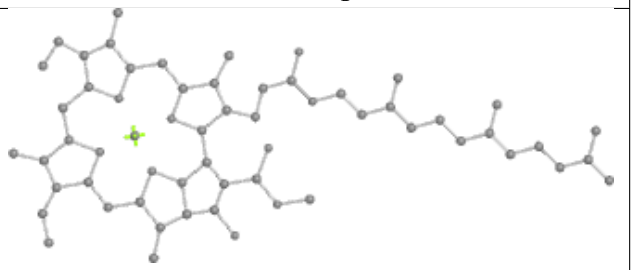
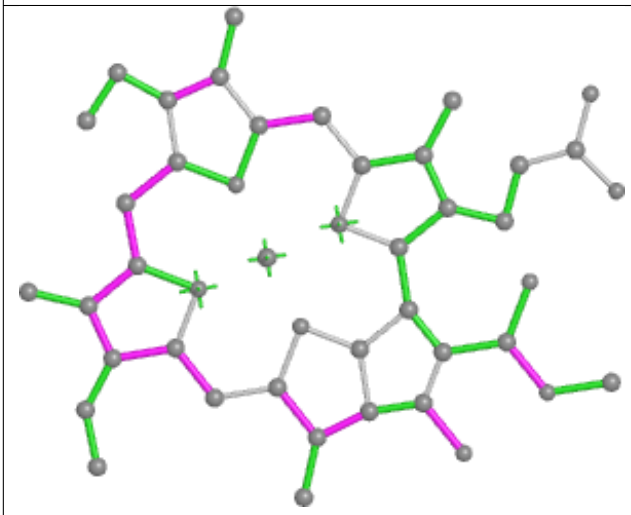


Rings

Ligand CLA b 835



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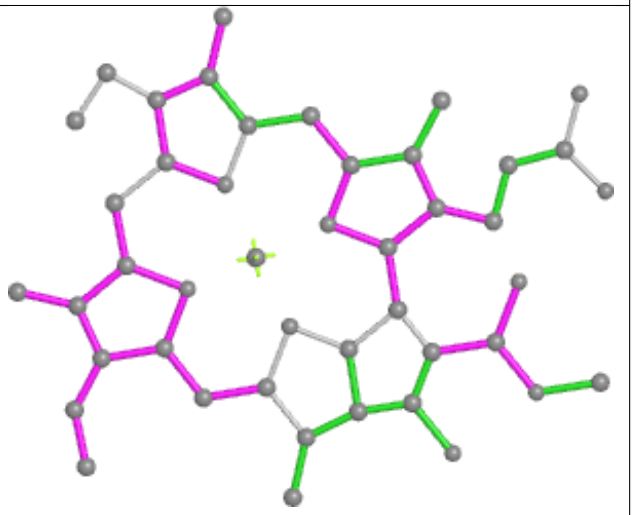
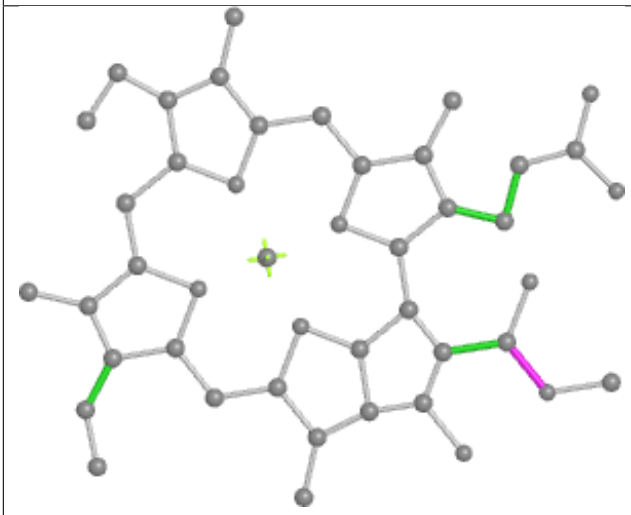


Bond angles



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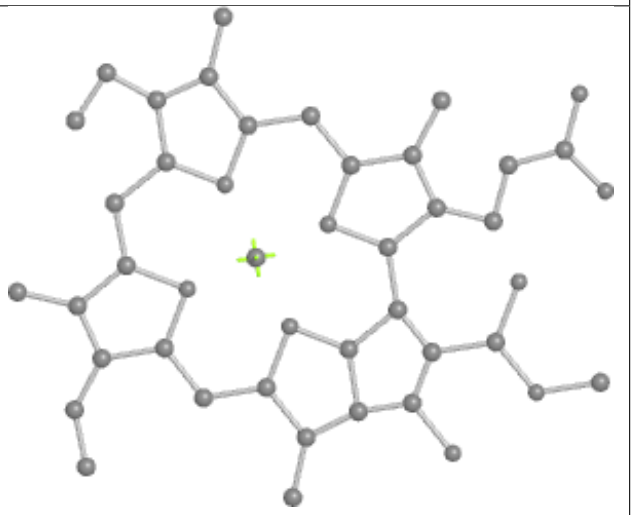
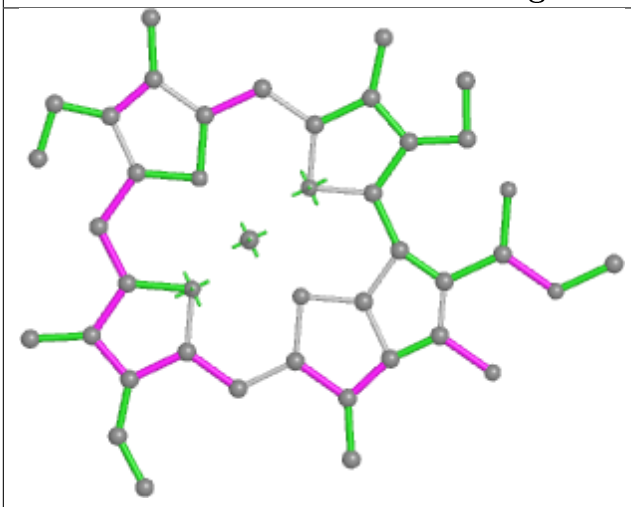


Rings

Ligand CLA 3 305



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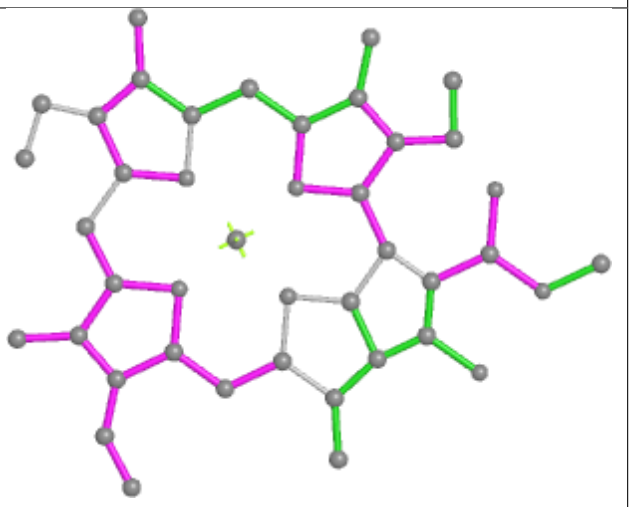
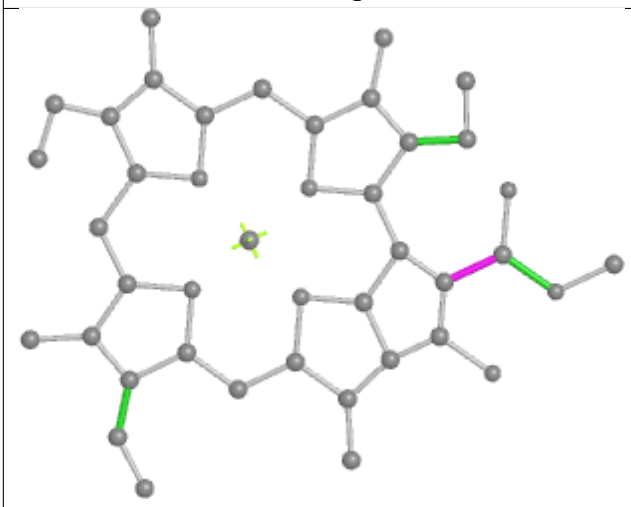


Bond angles



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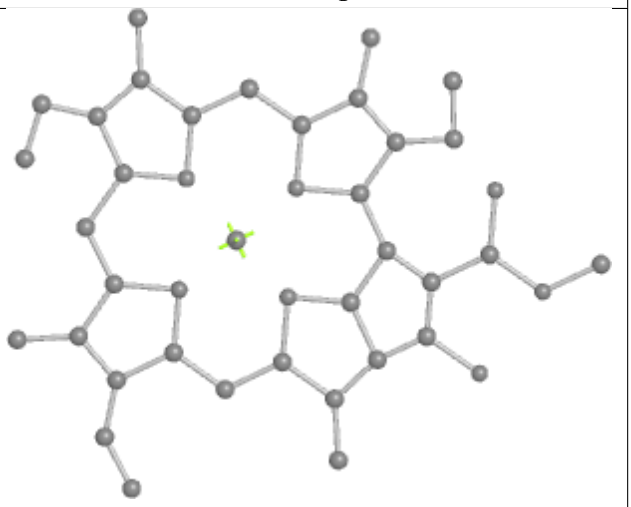
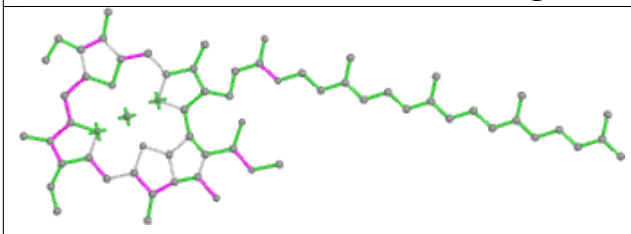


Rings

Ligand CLA a 809



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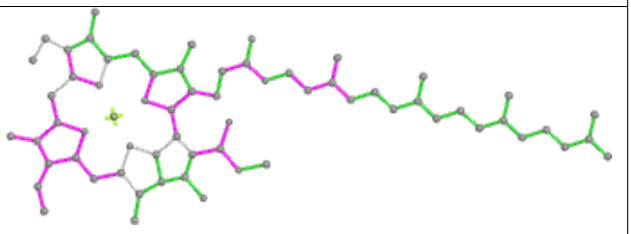
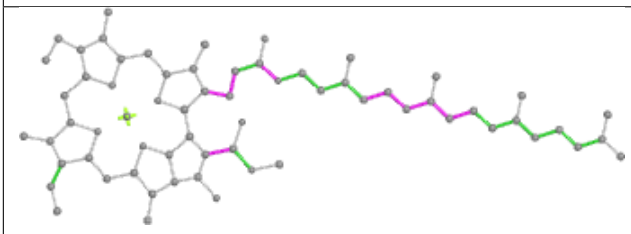


Bond angles



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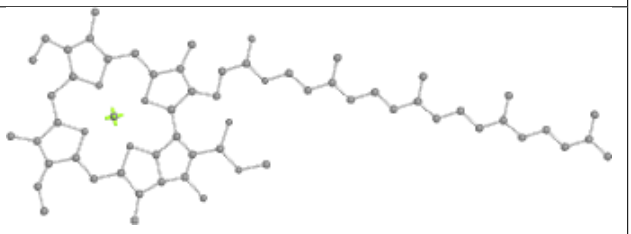
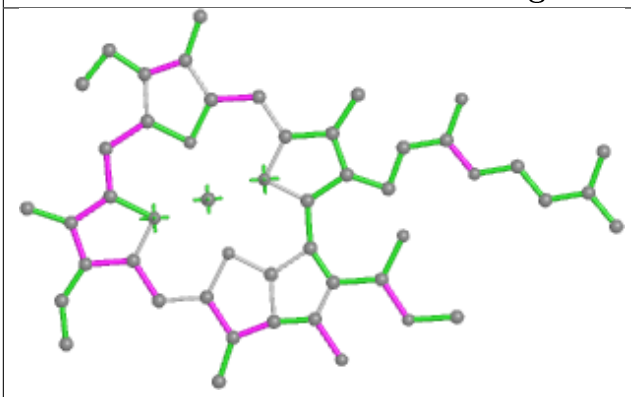


Rings

Ligand CLA a 836



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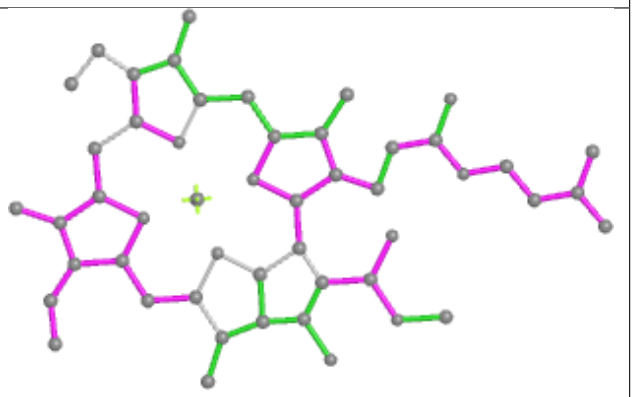
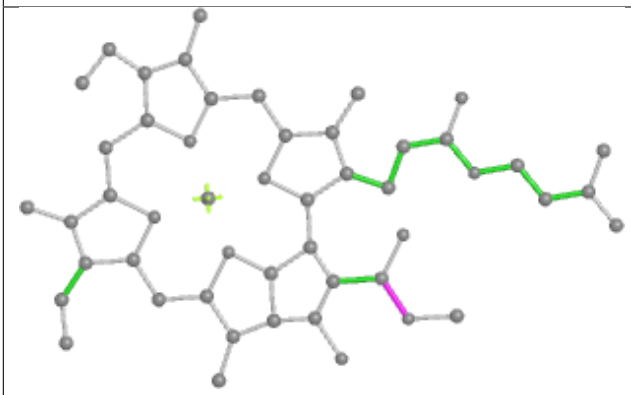


Bond angles



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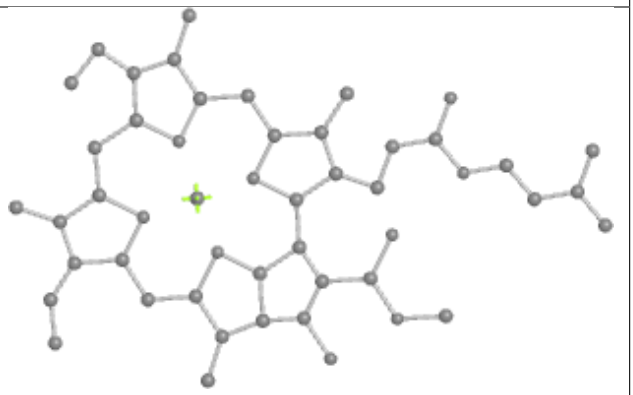
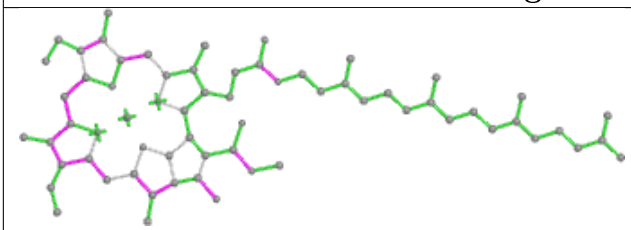


Rings

Ligand CLA A 808



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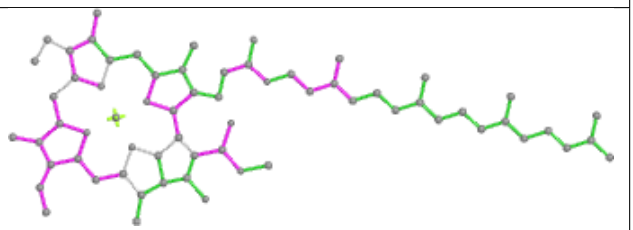
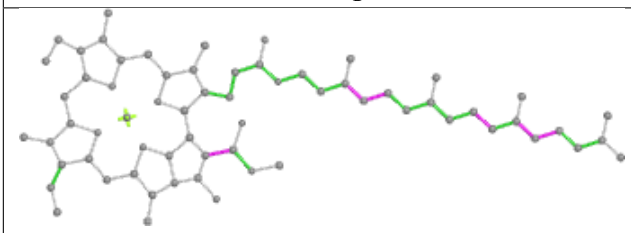
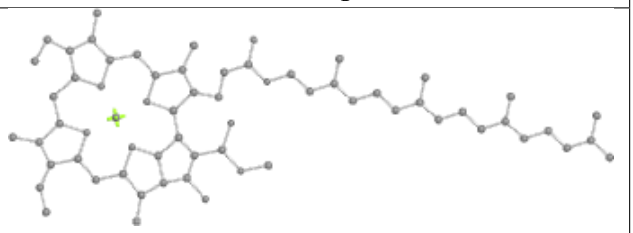


Bond angles

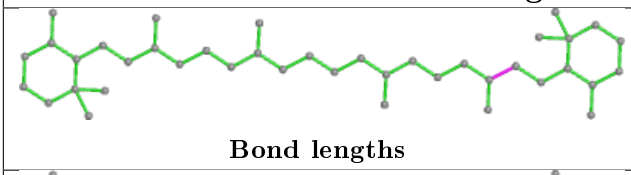


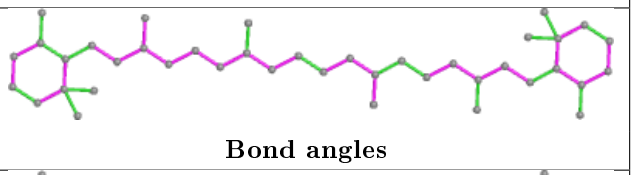
Torsions

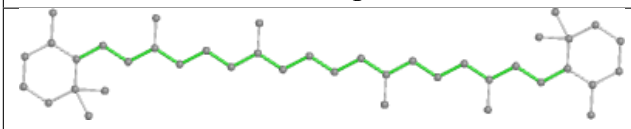


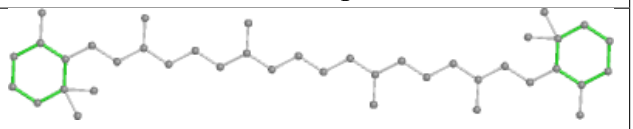
Rings

Ligand BCR b 843

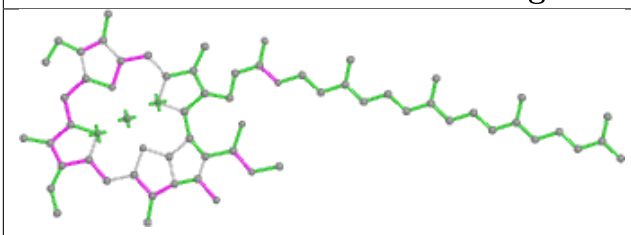

Bond lengths


Bond angles


Torsions


Rings

Ligand CLA a 831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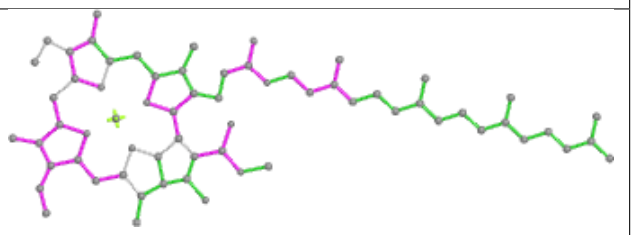
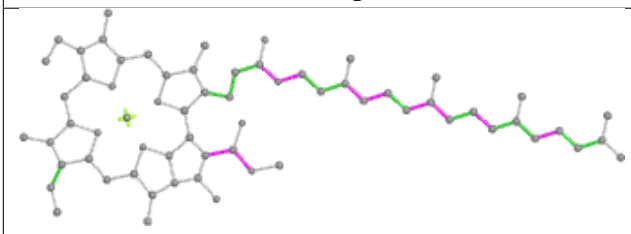
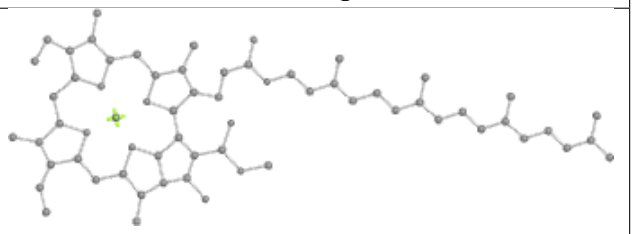
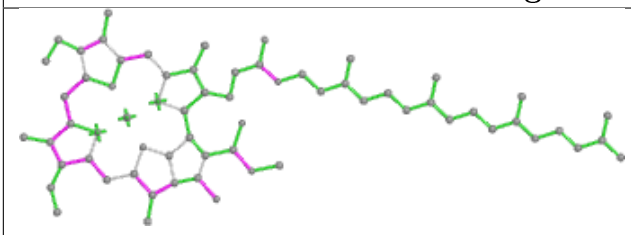
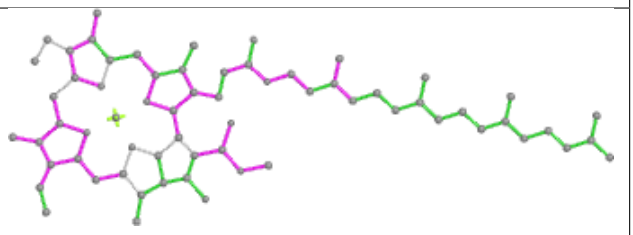

Bond angles

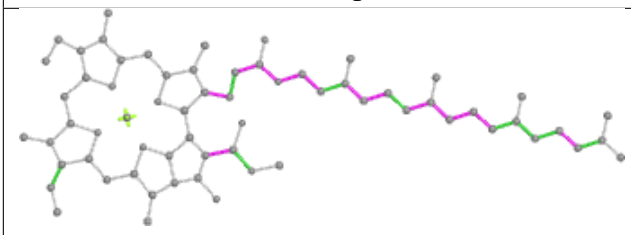

Torsions

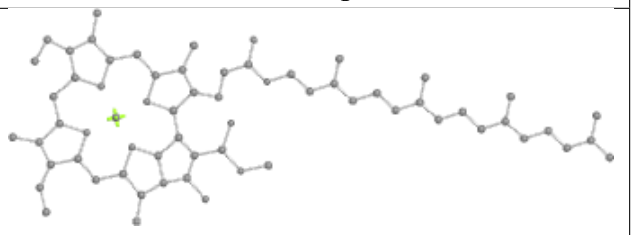

Rings

Ligand CLA A 806

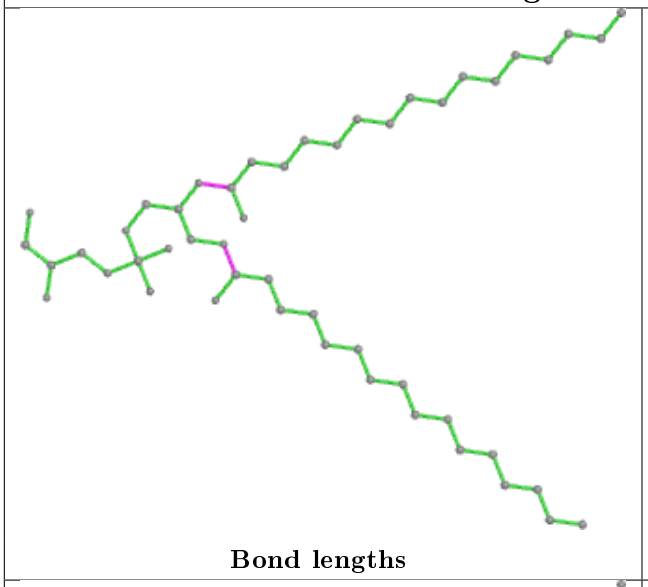

Bond lengths


Bond angles

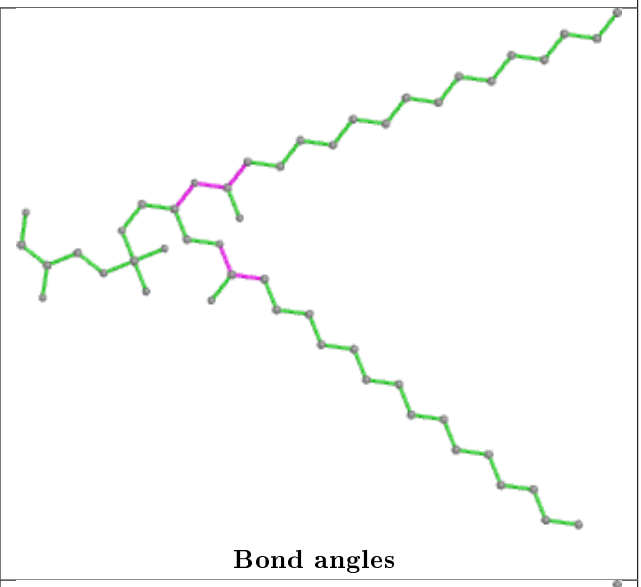

Torsions


Rings

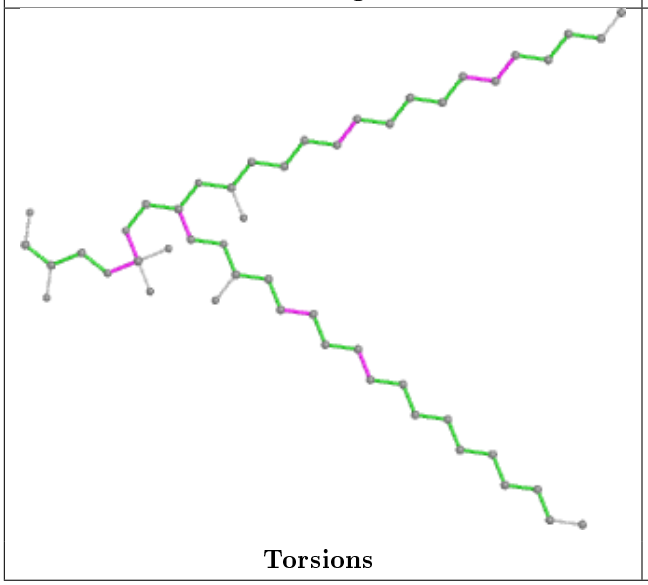
Ligand LHG A 846



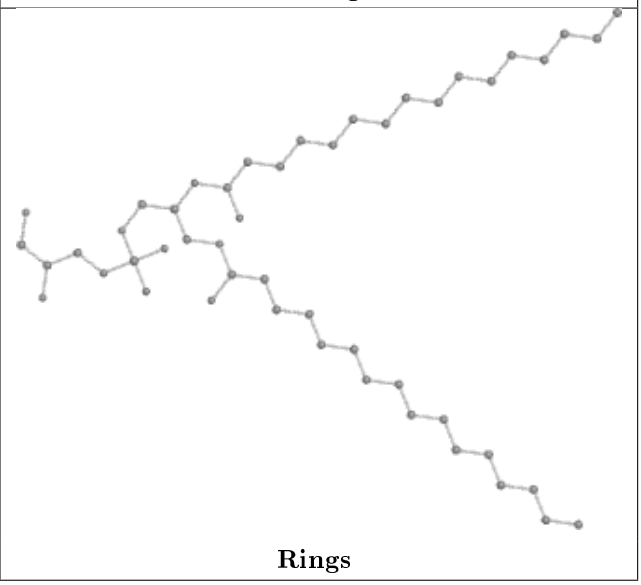
Bond lengths



Bond angles

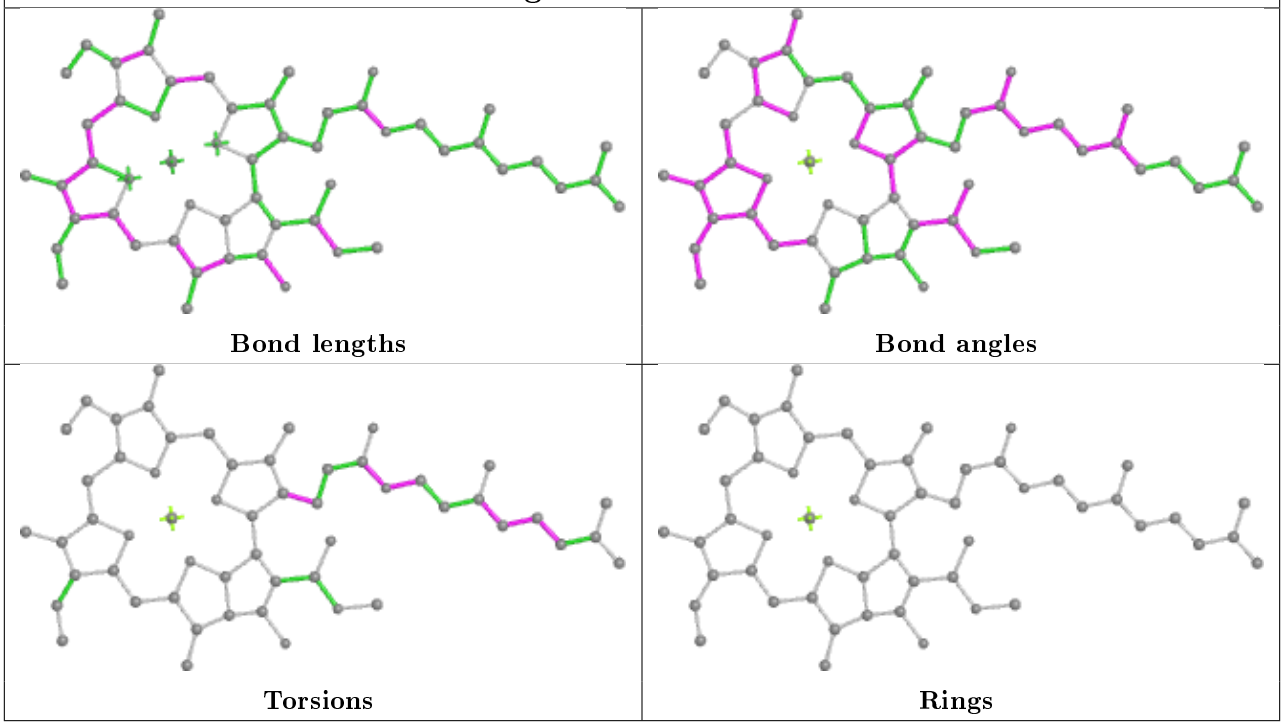


Torsions

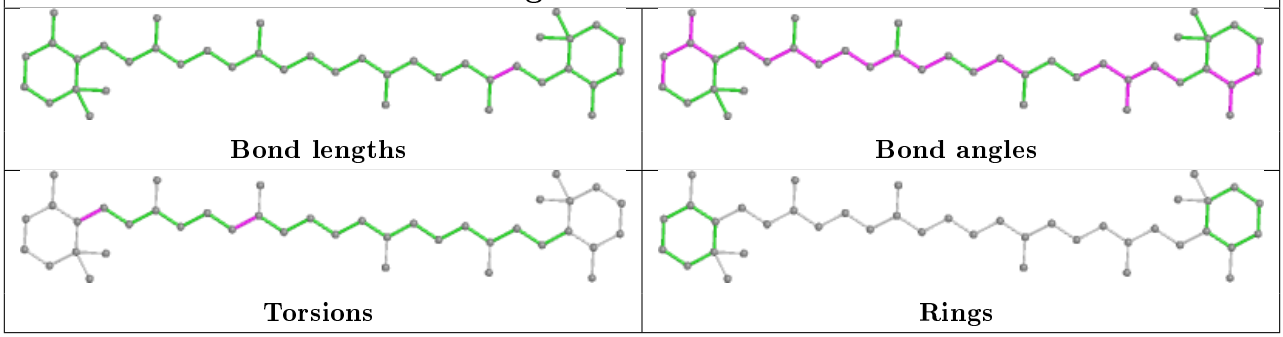


Rings

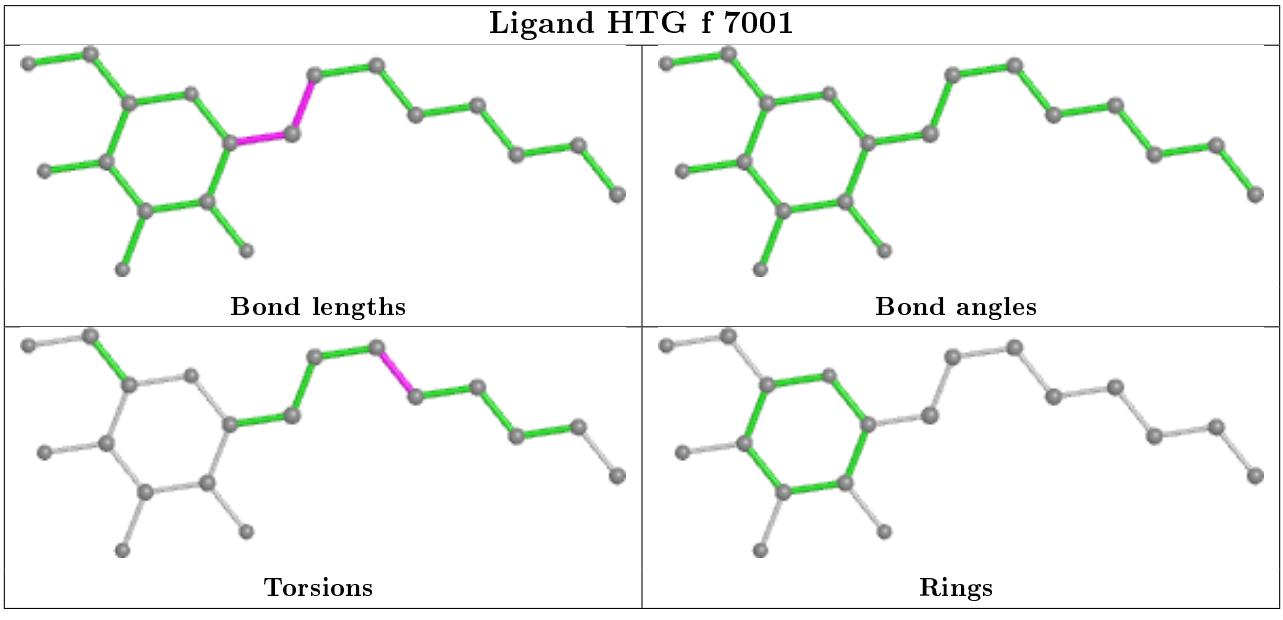
Ligand CLA f 7003



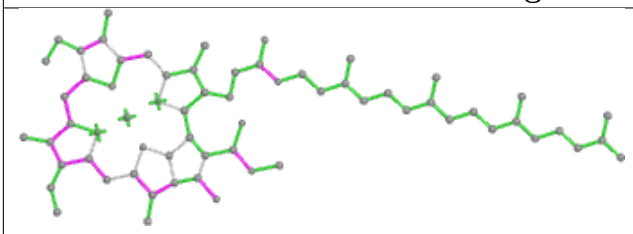
Ligand BCR L 206



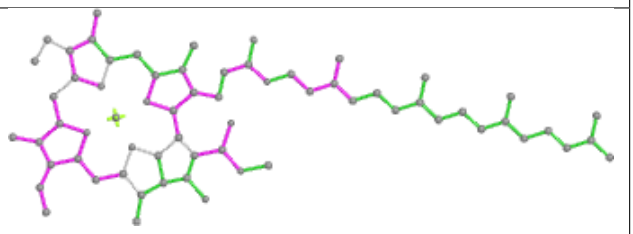
Ligand HTG f 7001



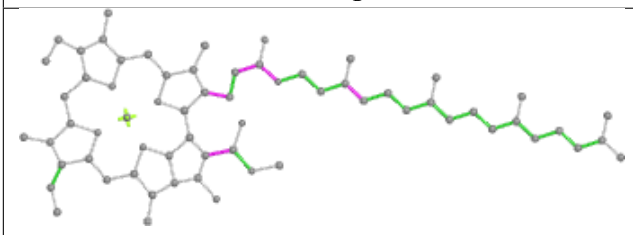
Ligand CLA A 811



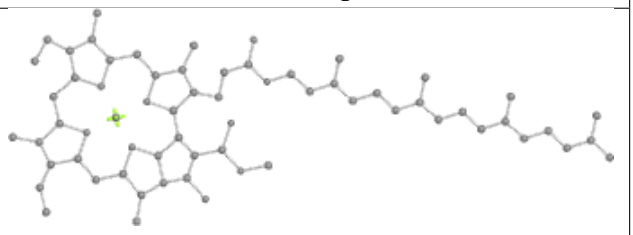
Bond lengths



Bond angles

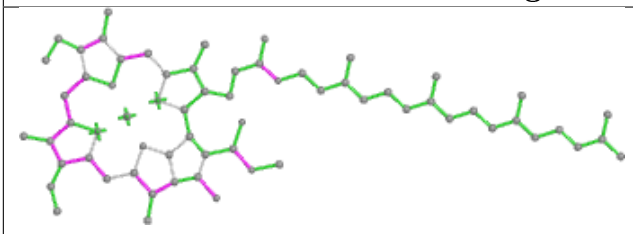


Torsions

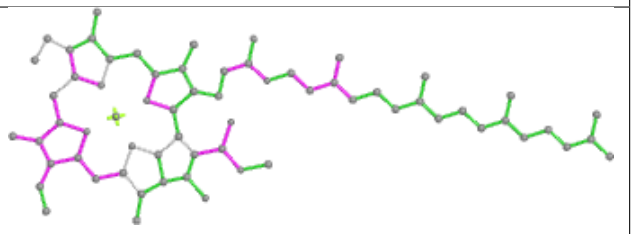


Rings

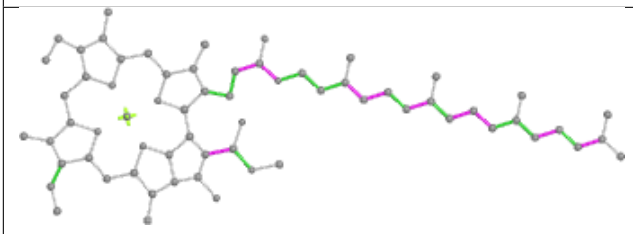
Ligand CLA A 826



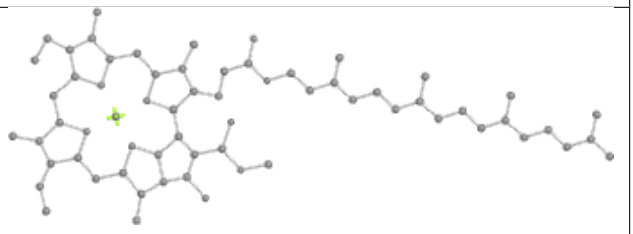
Bond lengths



Bond angles

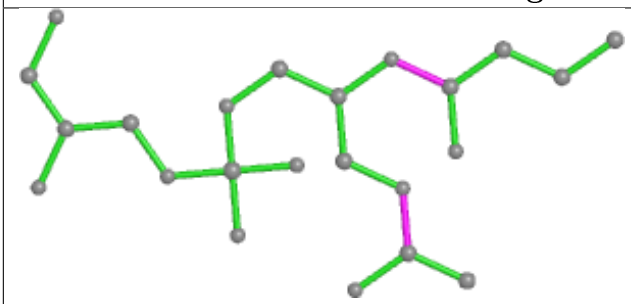


Torsions



Rings

Ligand LHG 1 301



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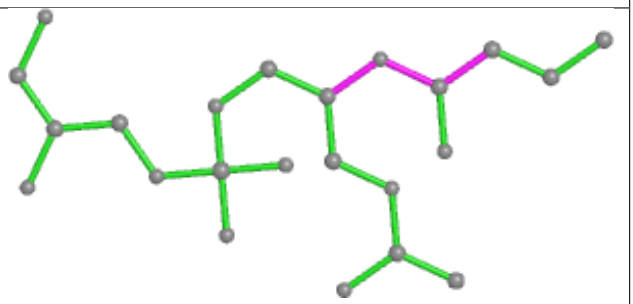
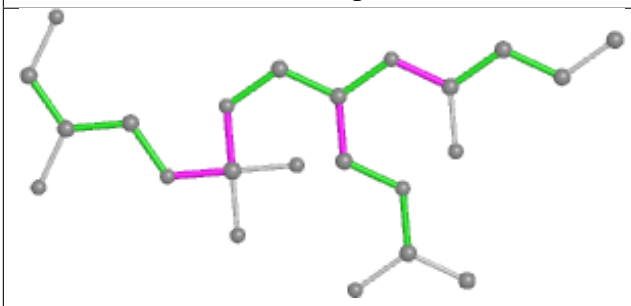


Bond angles



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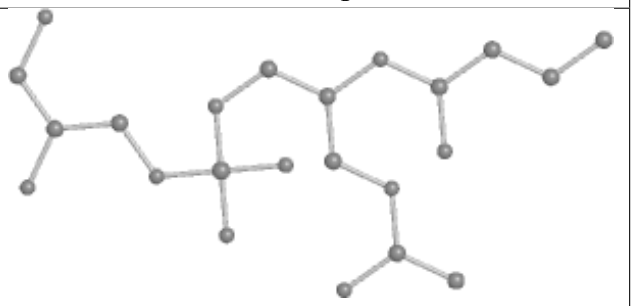
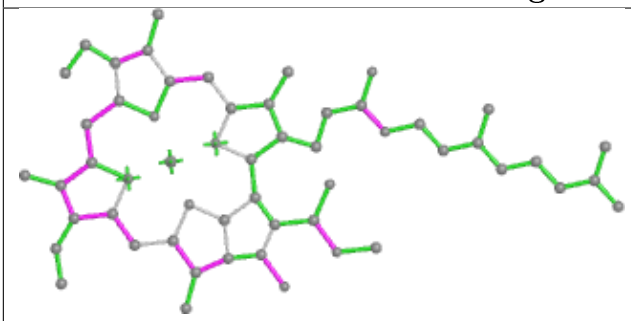


Rings

Ligand CLA a 825



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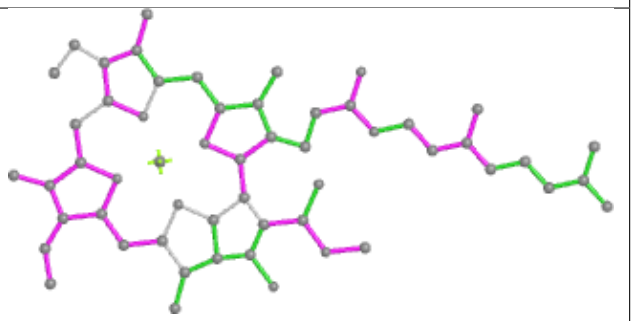
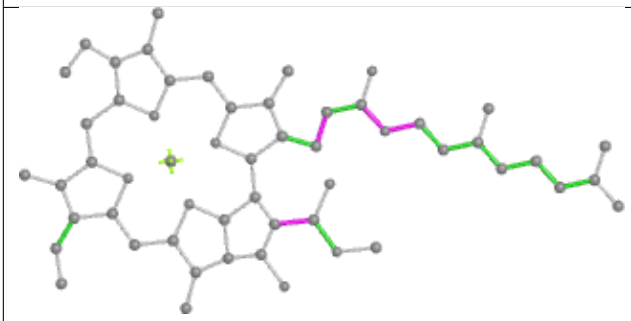


Bond angles



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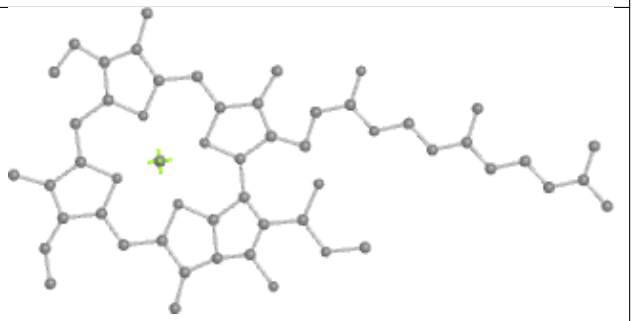
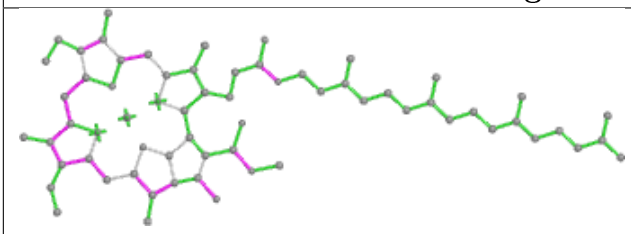
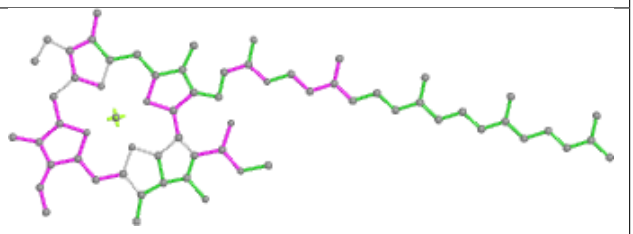


Rings

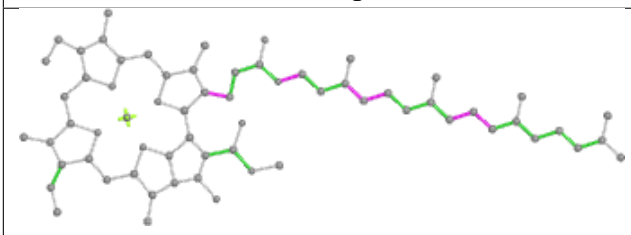
Ligand CLA A 833



Bond lengths



Bond angles



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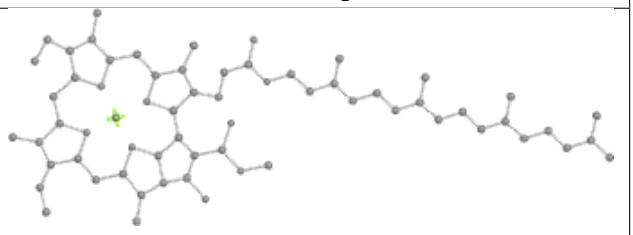
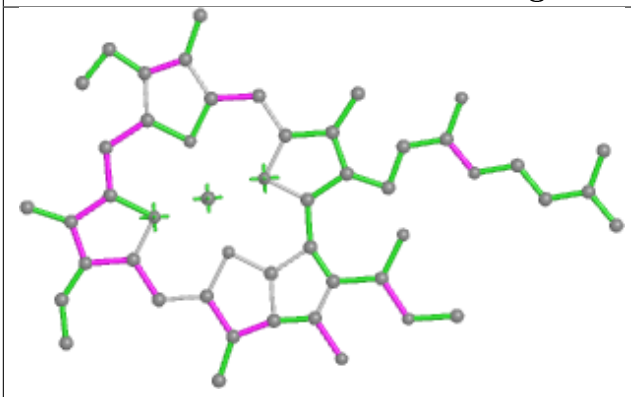
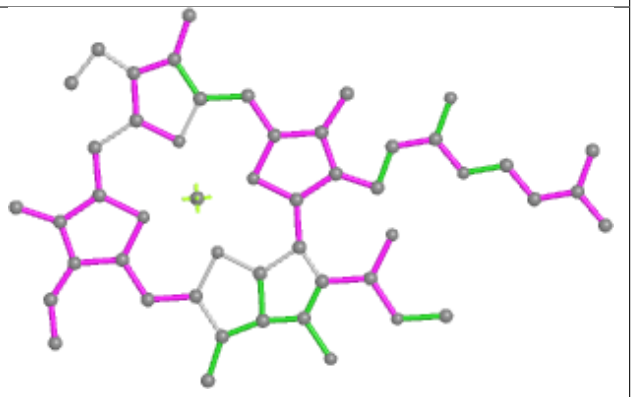


Rings

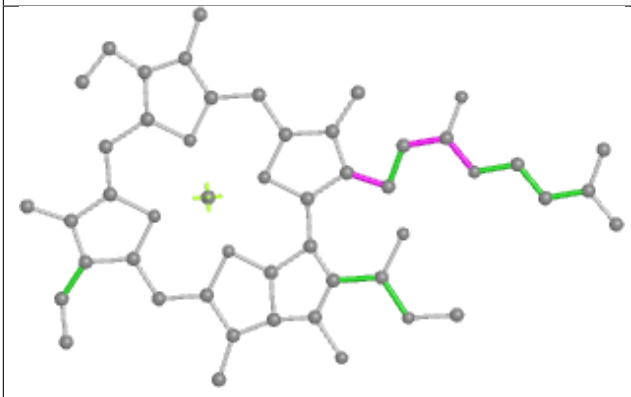
Ligand CLA 7 608



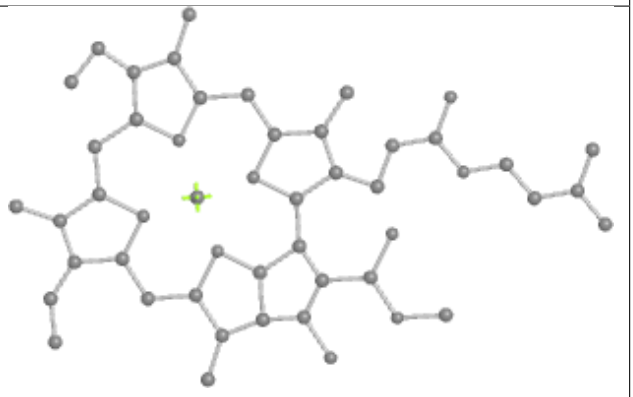
Bond lengths



Bond angles

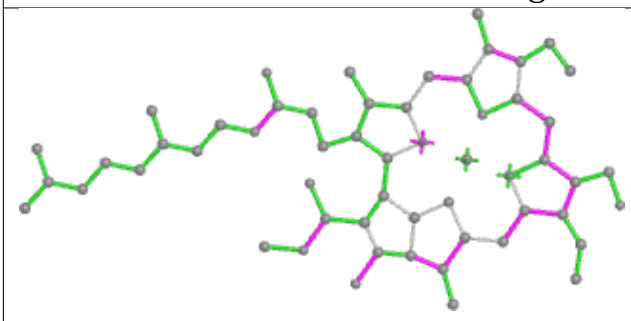


Torsions

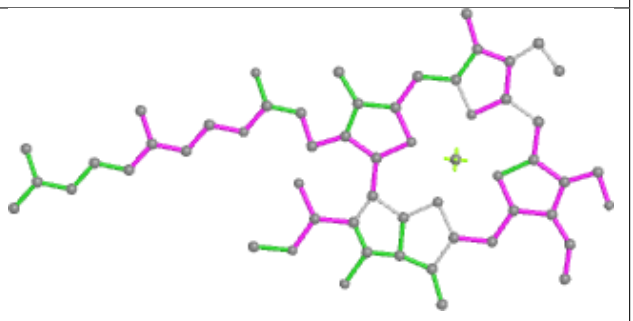


Rings

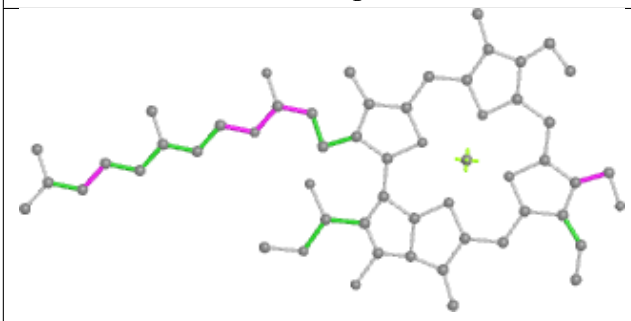
Ligand CHL 4 605



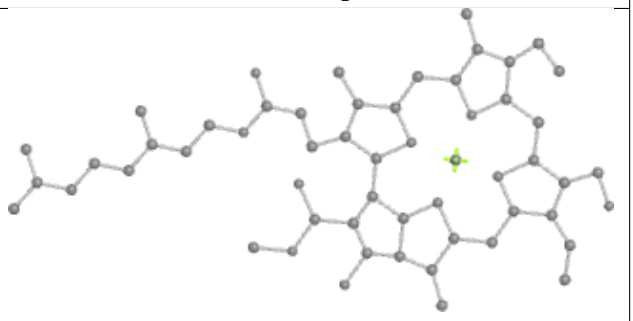
Bond lengths



Bond angles

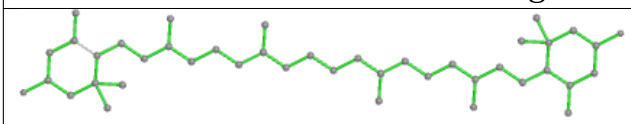


Torsions



Rings

Ligand LUT 7 615



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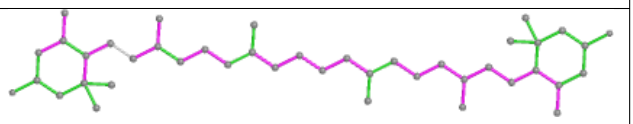
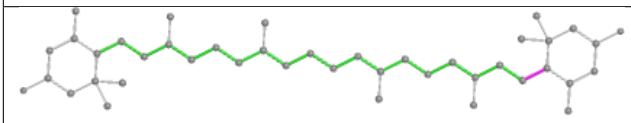
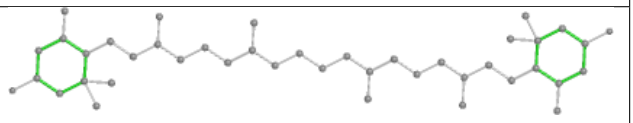


Bond angles

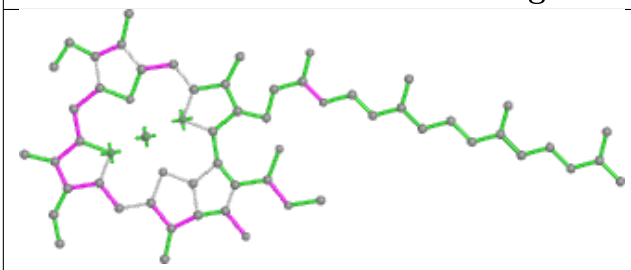


Torsions



Rings

Ligand CLA 4 602



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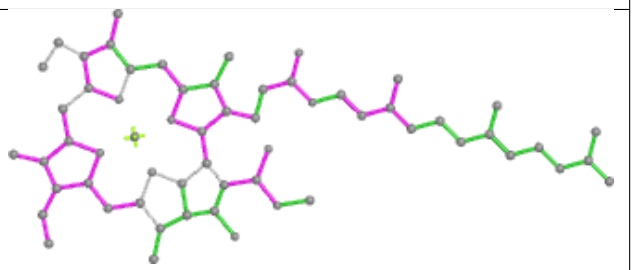
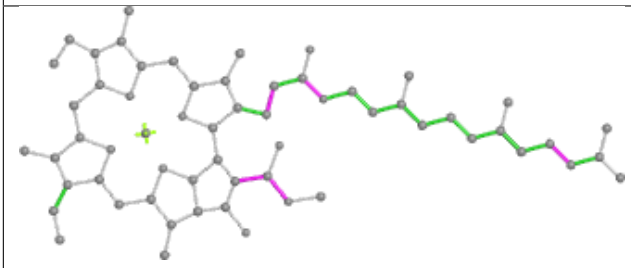
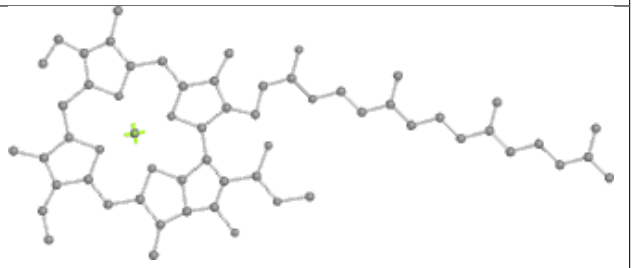


Bond angles

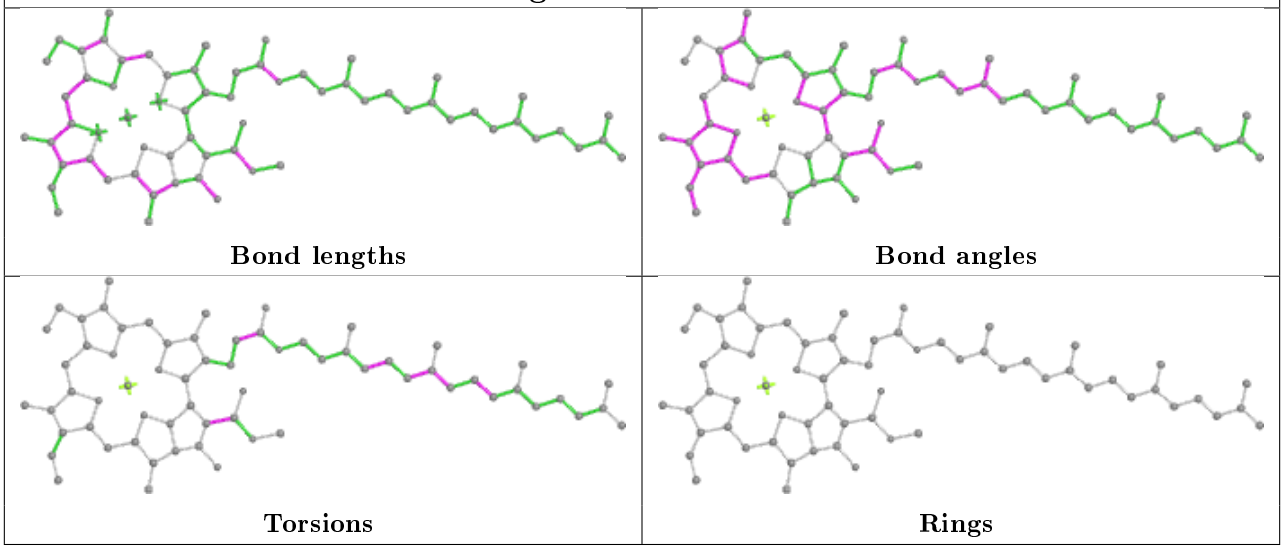


Torsions

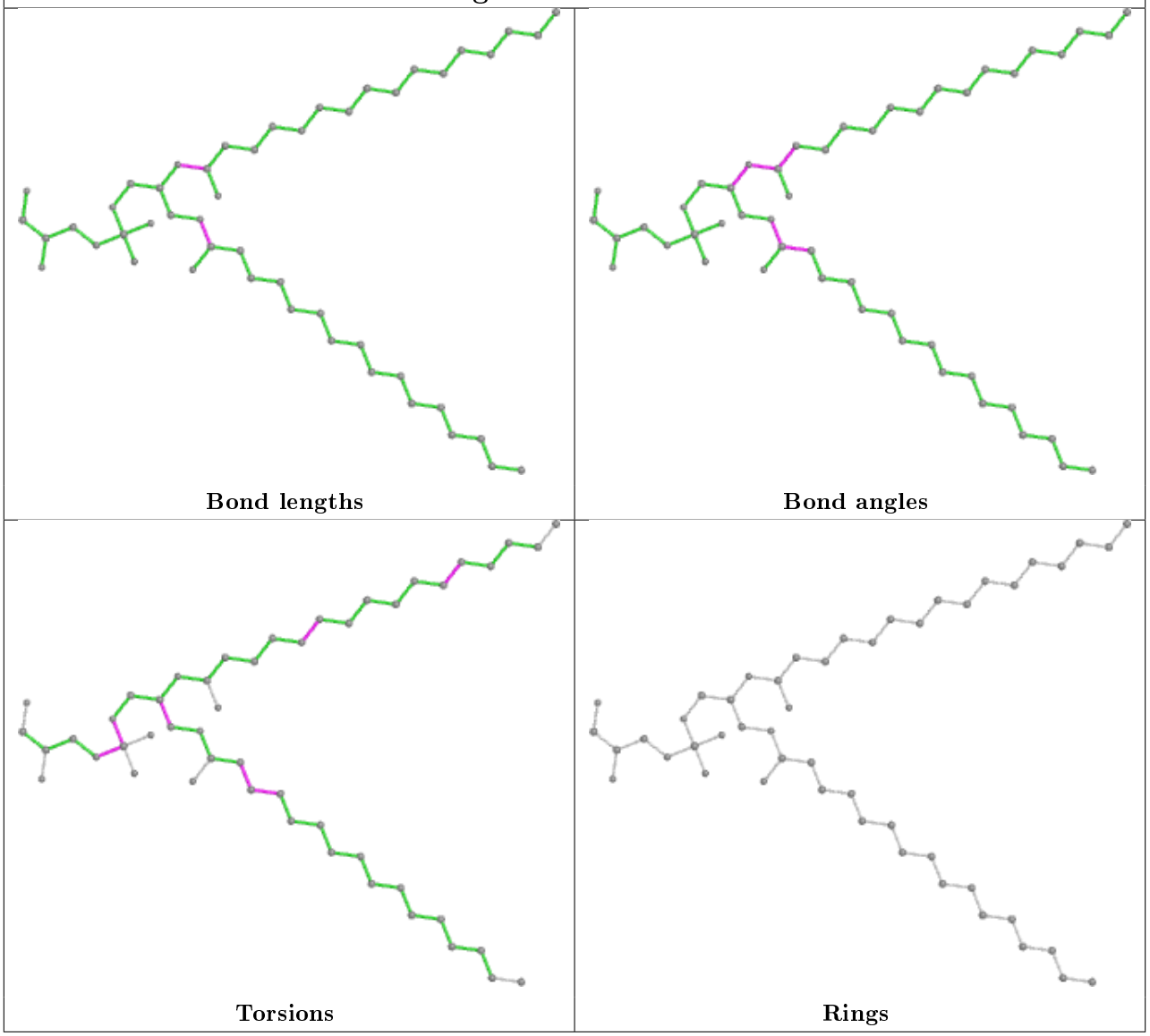


Rings

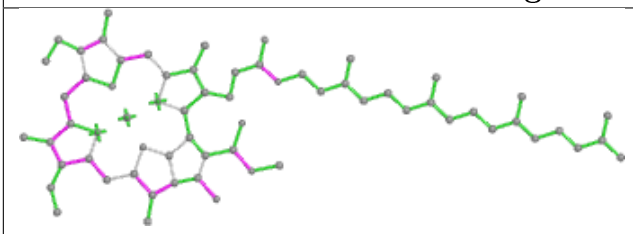
Ligand CLA 6 305



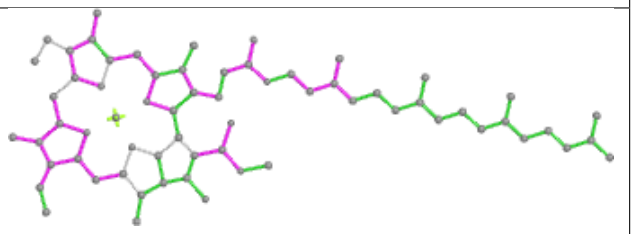
Ligand LHG a 847



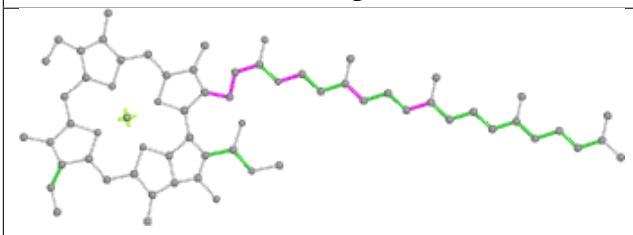
Ligand CLA B 827



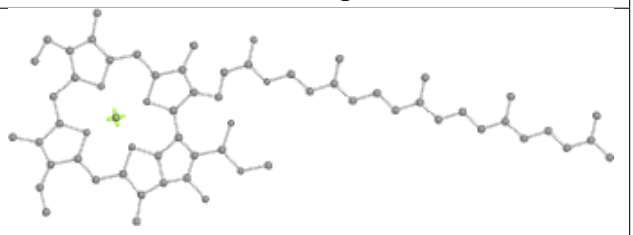
Bond lengths



Bond angles

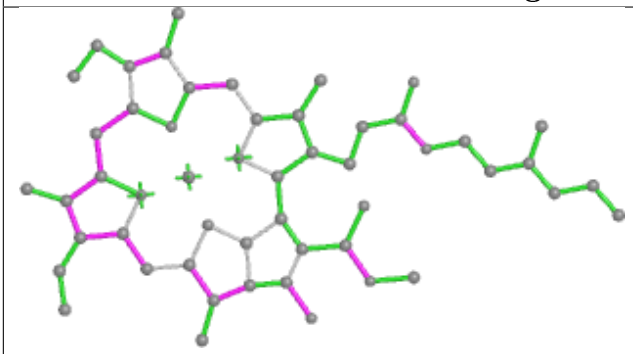


Torsions

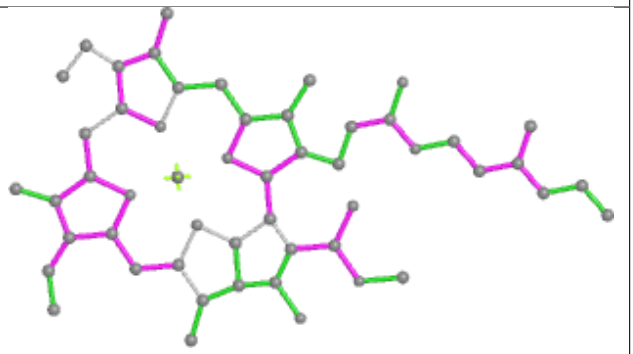


Rings

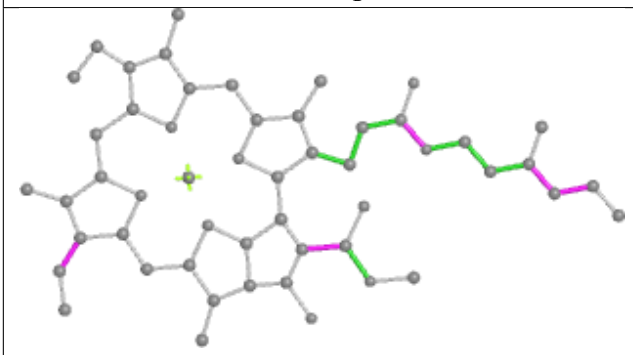
Ligand CLA A 845



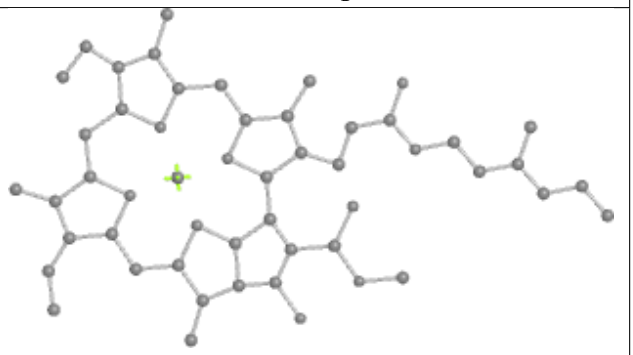
Bond lengths



Bond angles

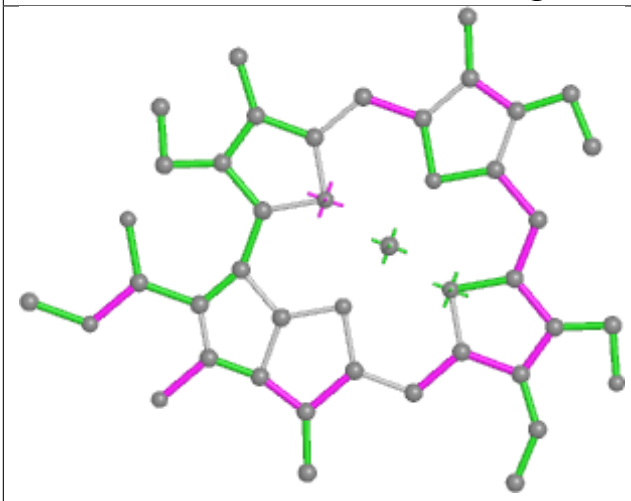


Torsions

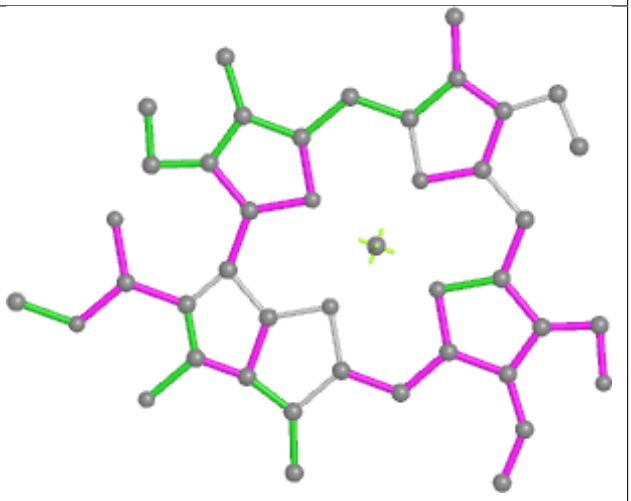


Rings

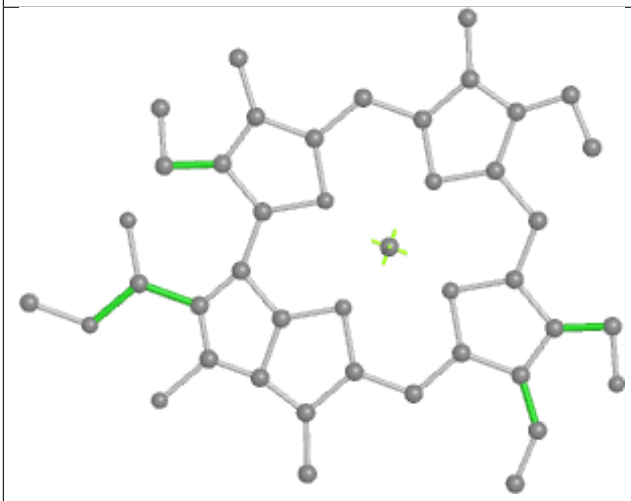
Ligand CHL 2 605



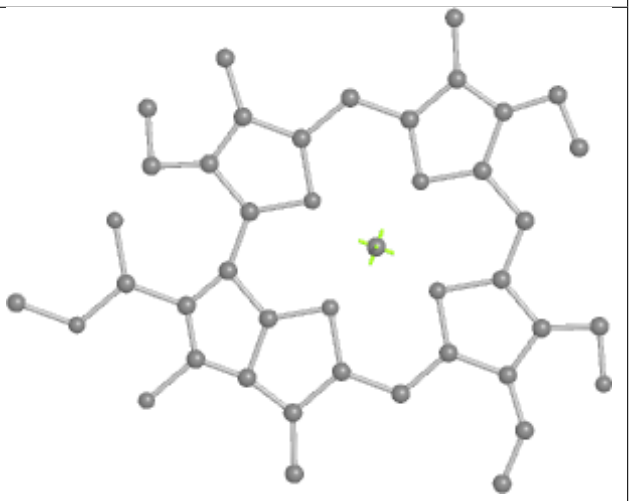
Bond lengths



Bond angles

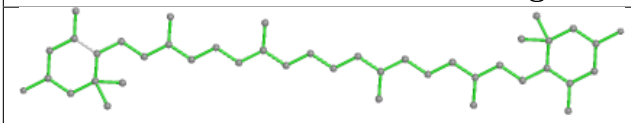


Torsions

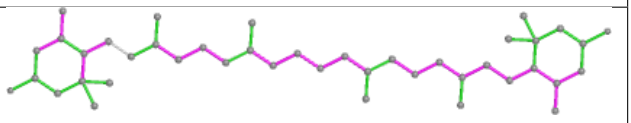


Rings

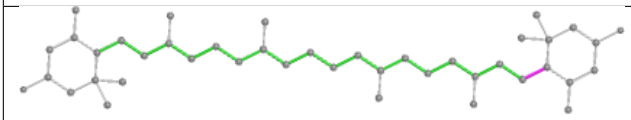
Ligand LUT 4 616



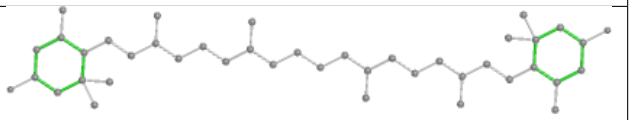
Bond lengths



Bond angles

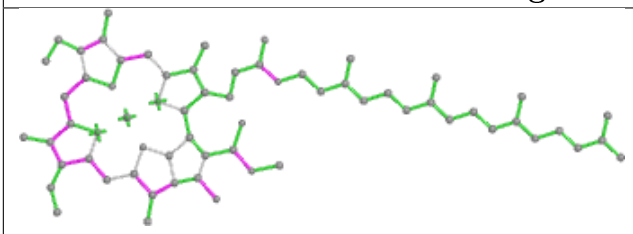


Torsions

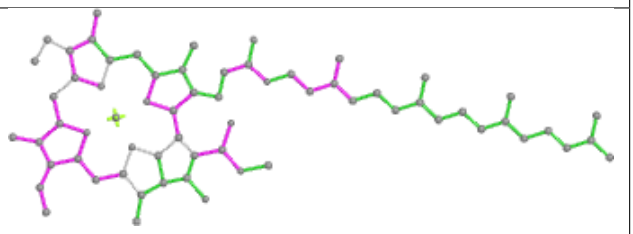


Rings

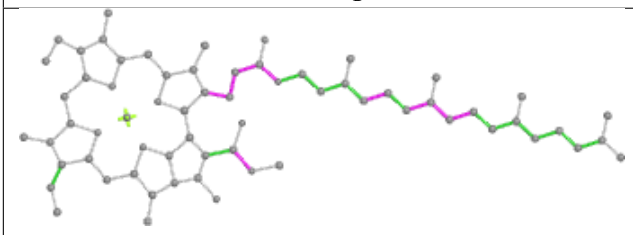
Ligand CLA a 819



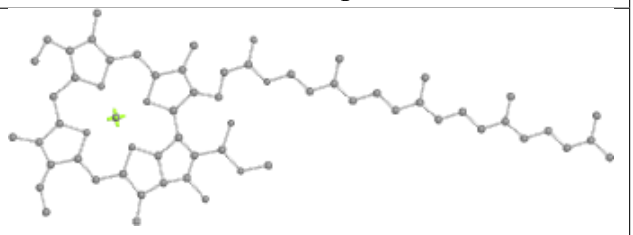
Bond lengths



Bond angles

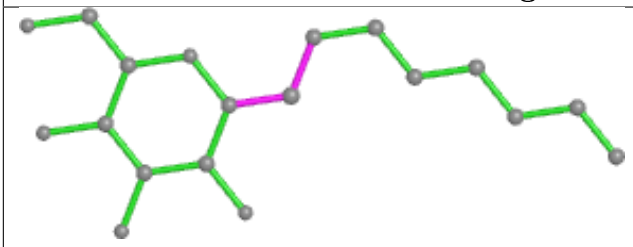


Torsions



Rings

Ligand HTG j 3001



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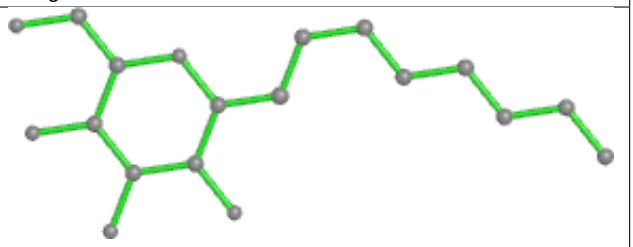
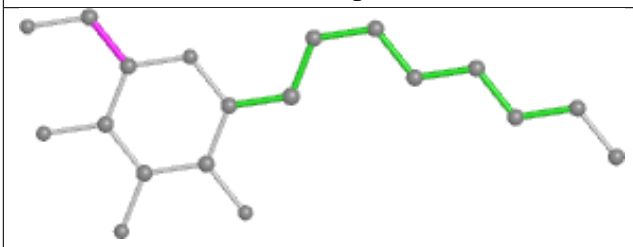
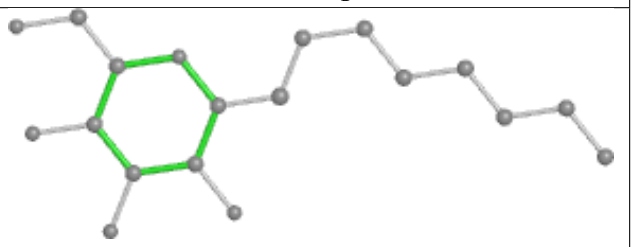


Bond angles

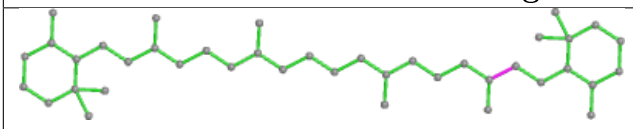


Torsions



Rings

Ligand BCR A 852



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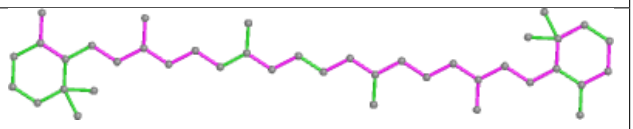
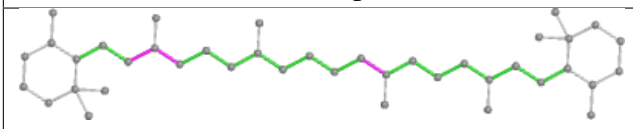


Bond angles



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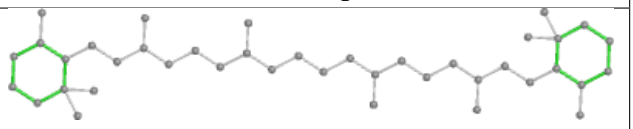
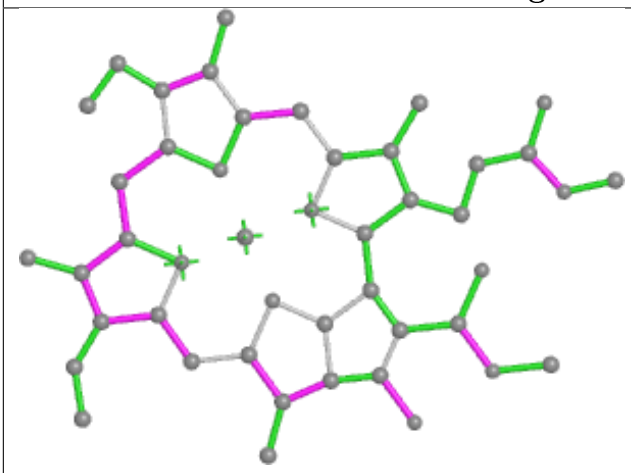


Rings

Ligand CLA 4 601



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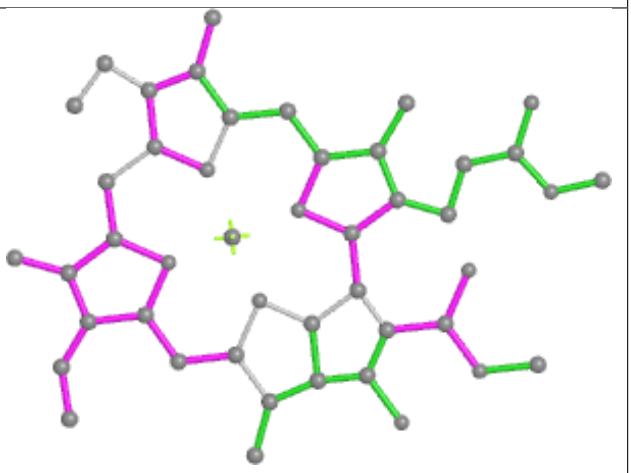
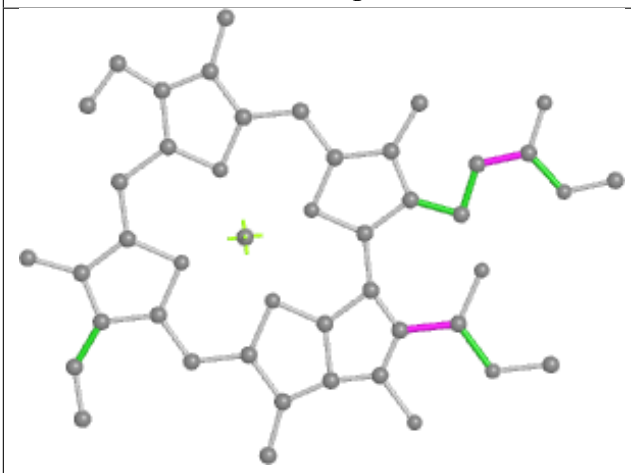


Bond angles



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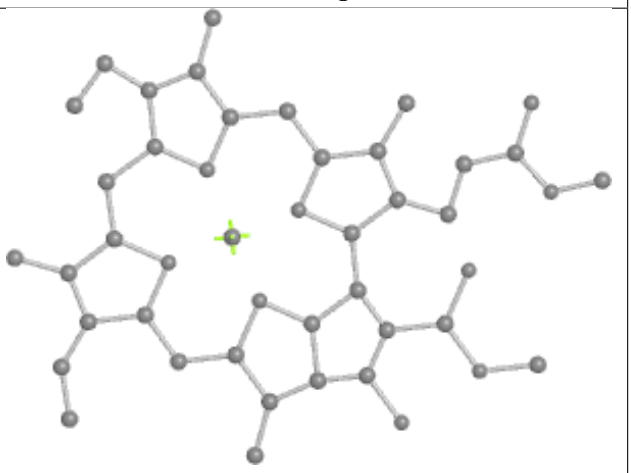
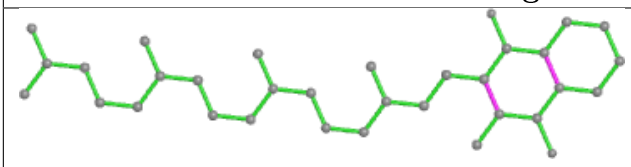


Rings

Ligand PQN B 842



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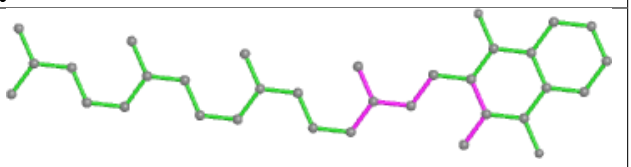
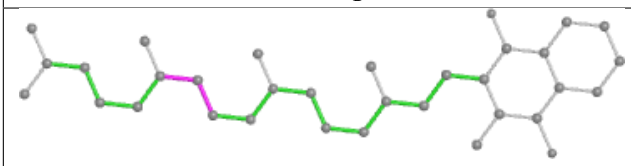


Bond angles



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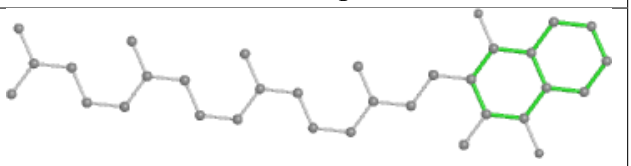
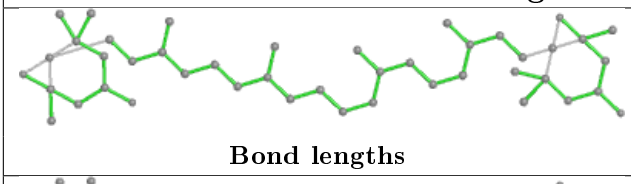


Rings

Ligand XAT 3 317



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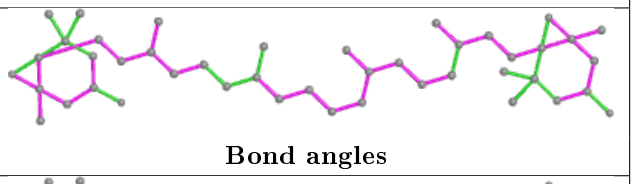
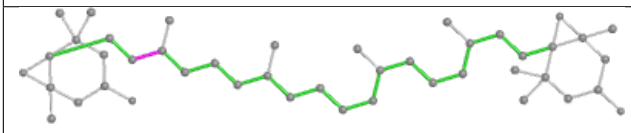


Bond angles



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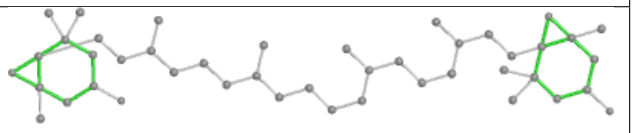
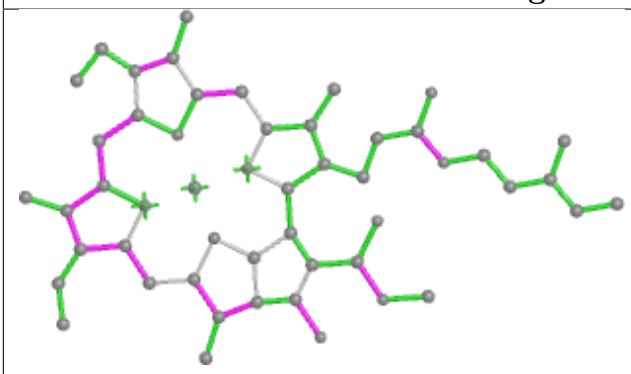


Rings

Ligand CLA a 824



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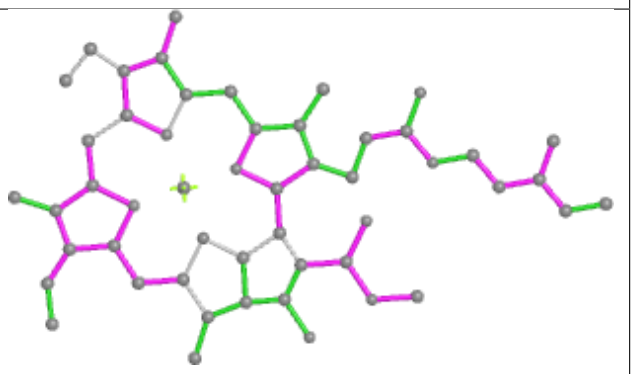
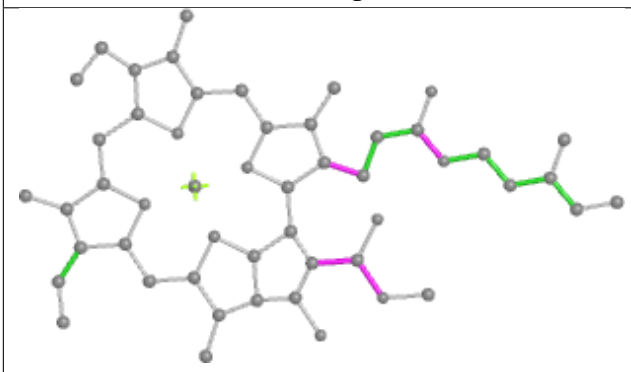


Bond angles



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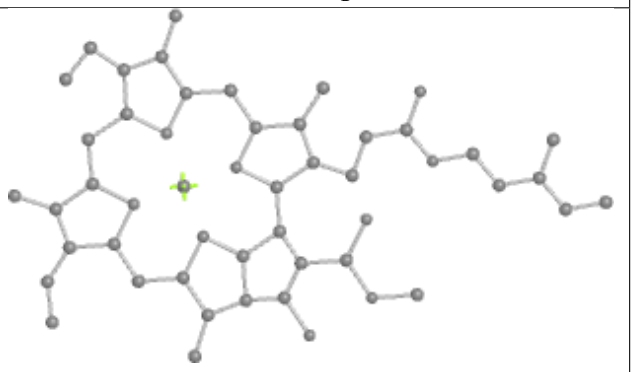
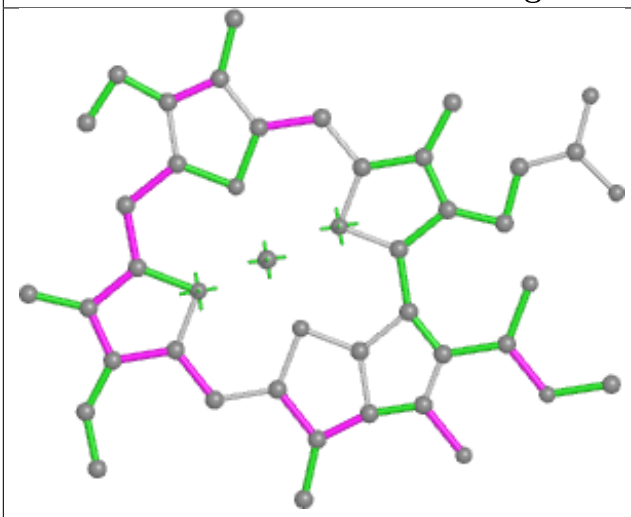
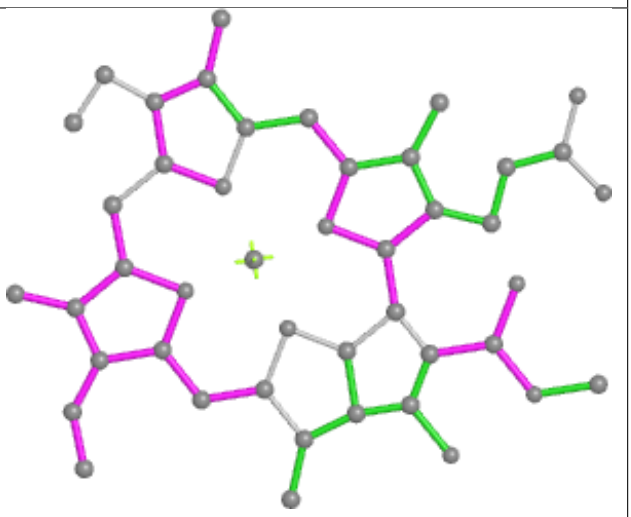


Rings

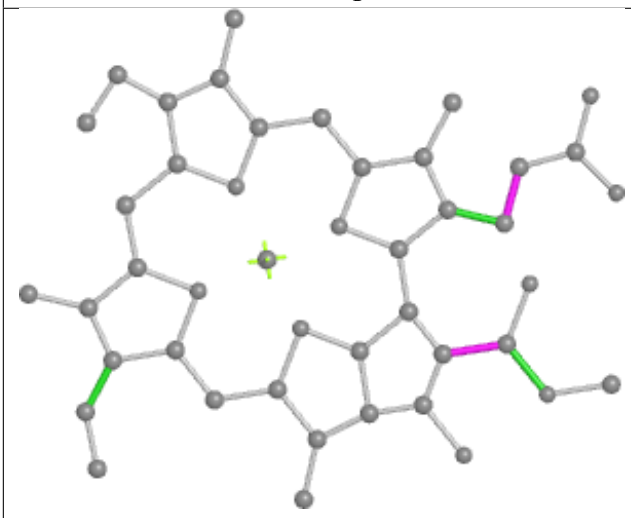
Ligand CLA A 837



Bond lengths



Bond angles



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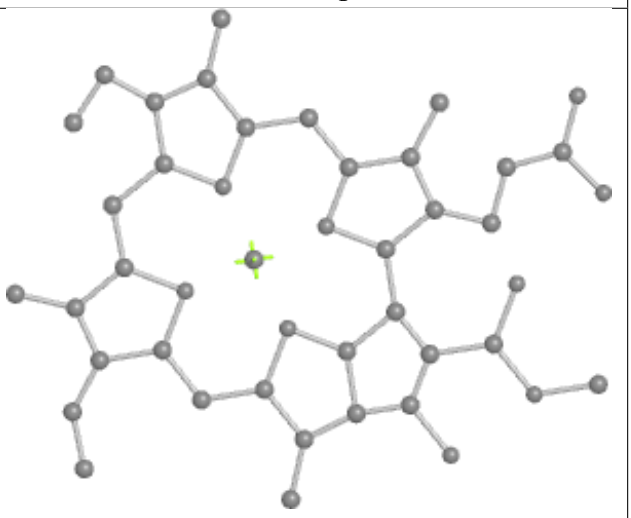
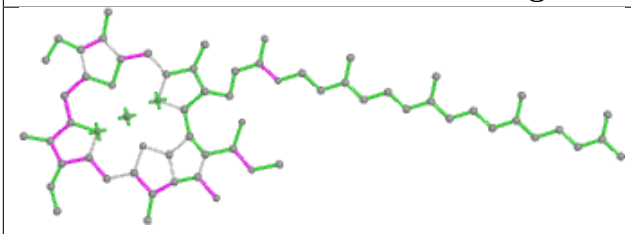
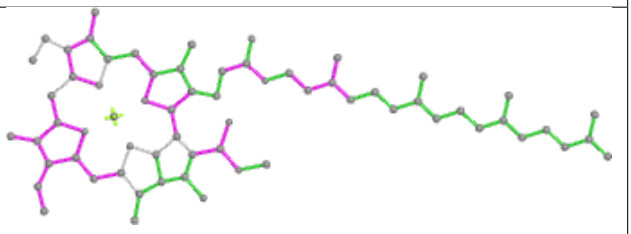


Rings

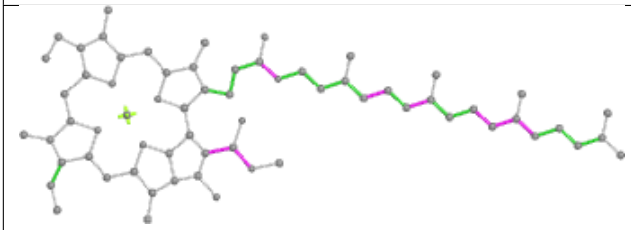
Ligand CLA a 818



Bond lengths



Bond angles



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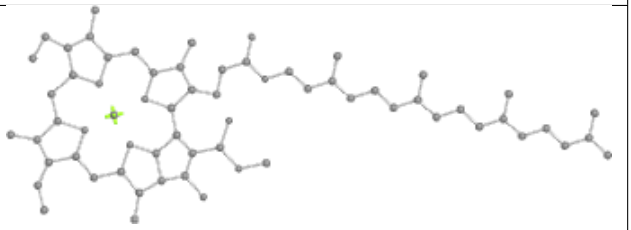
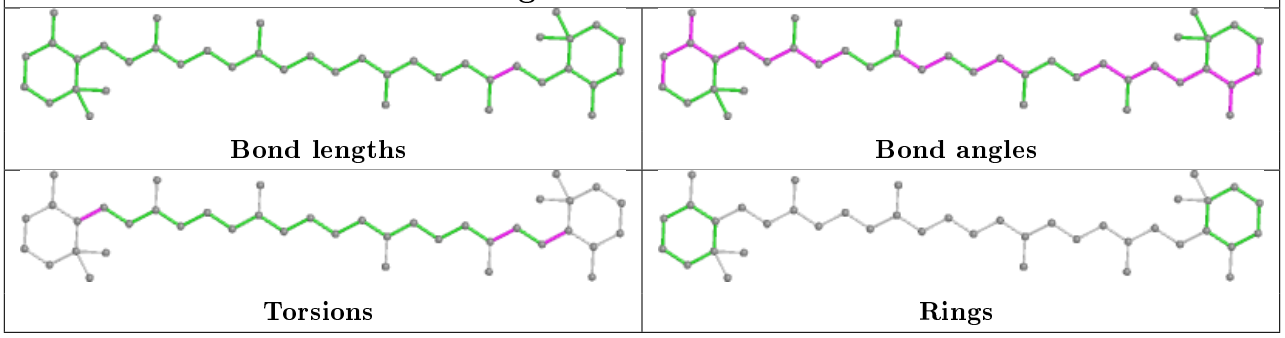
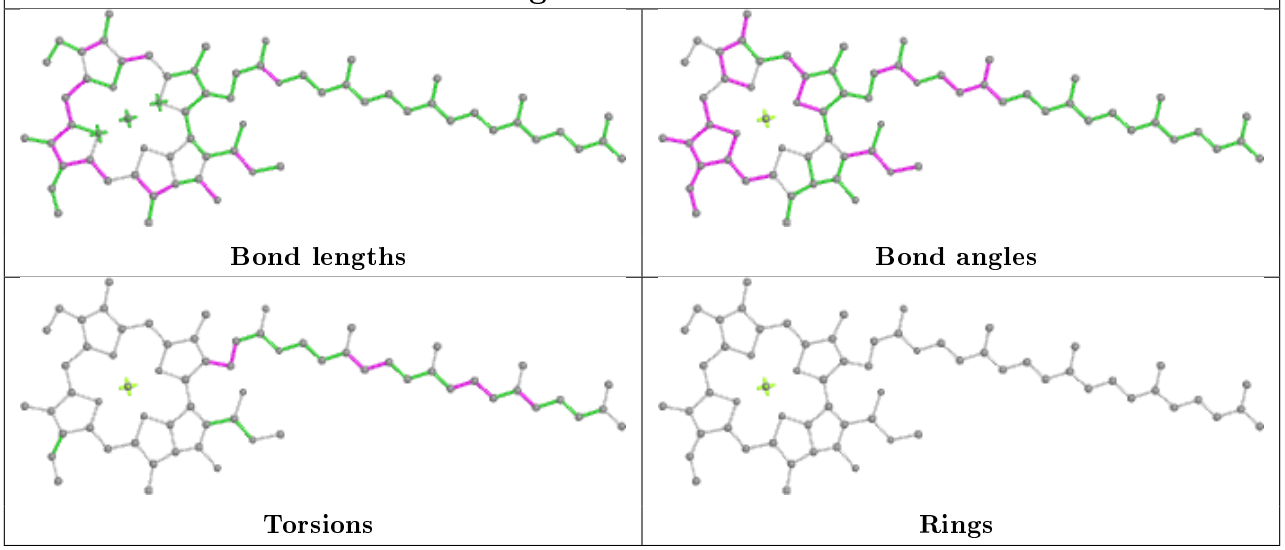


Rings

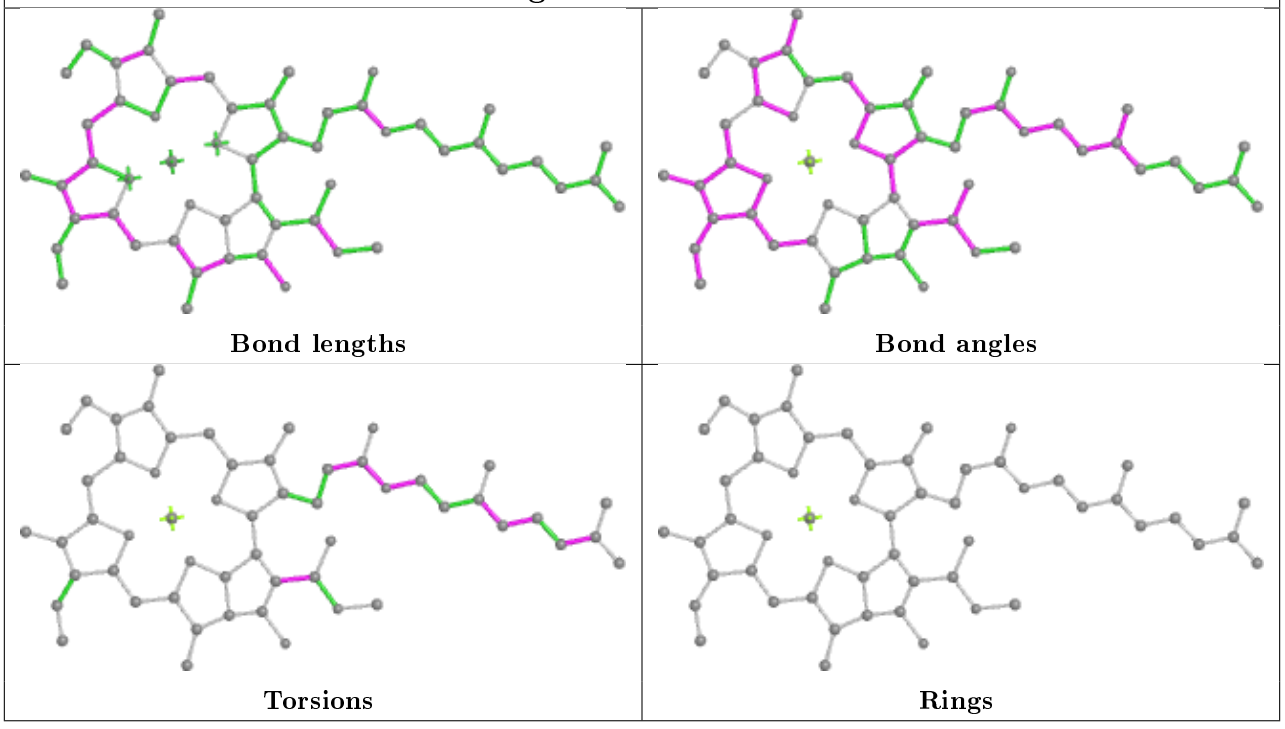
Ligand BCR k 1404



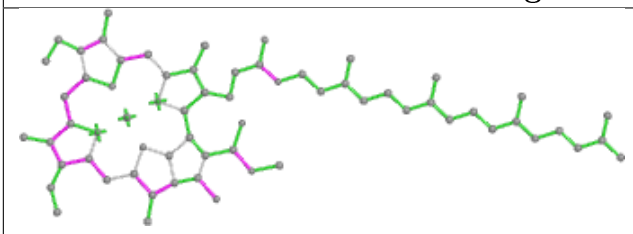
Ligand CLA 1 309



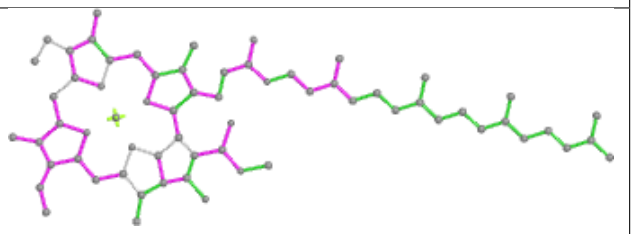
Ligand CLA b 816



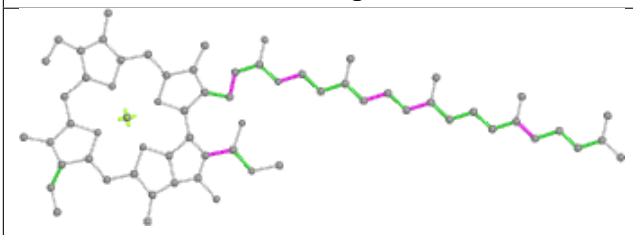
Ligand CLA A 854



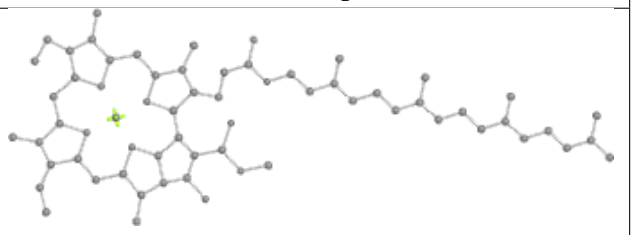
Bond lengths



Bond angles

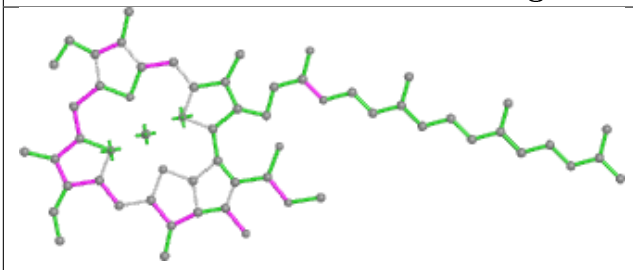


Torsions



Rings

Ligand CLA b 818



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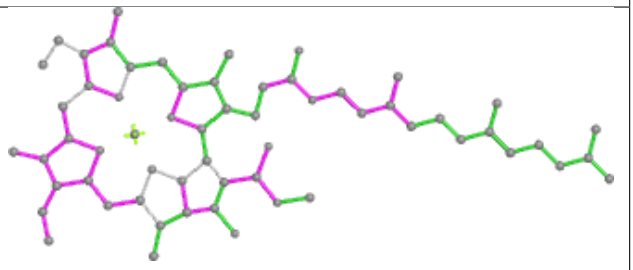
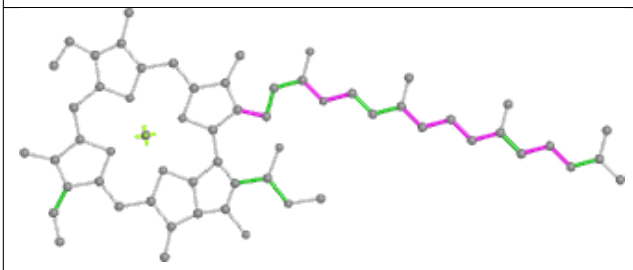


Bond angles



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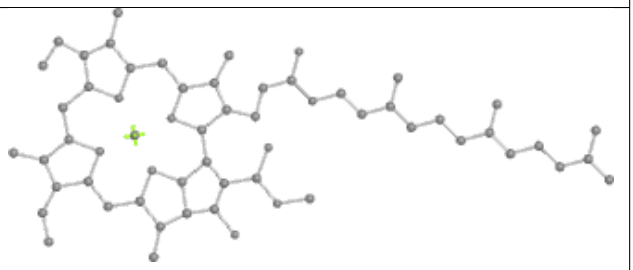
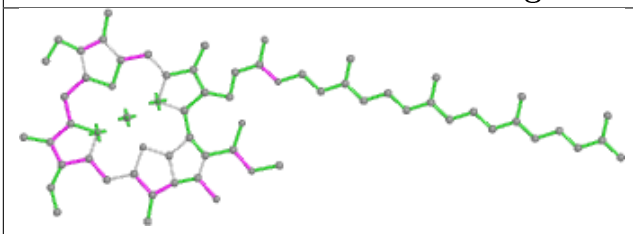
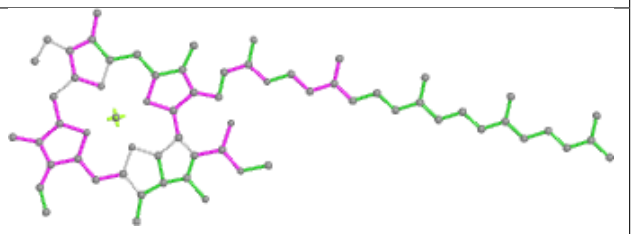


Rings

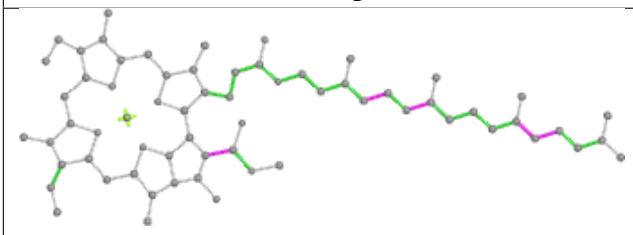
Ligand CLA A 827



Bond lengths



Bond angles



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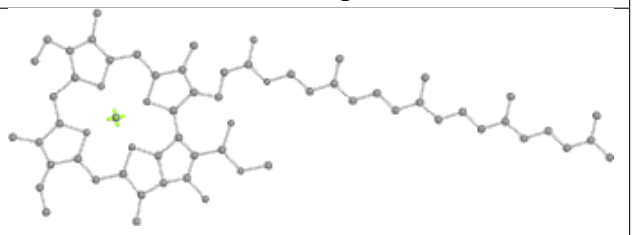
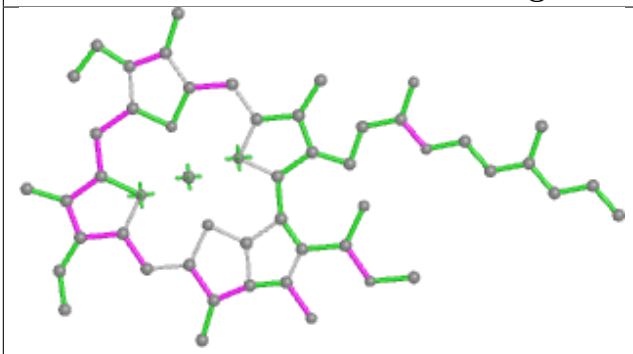
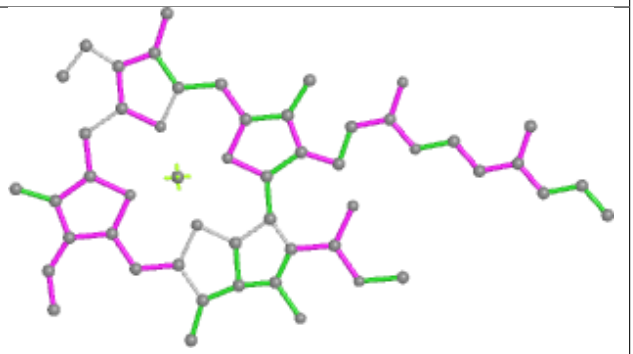


Rings

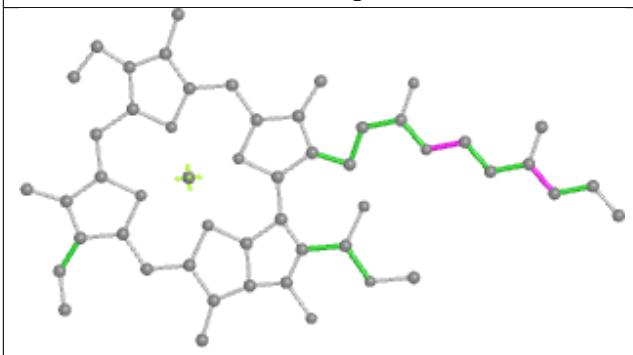
Ligand CLA 1 306



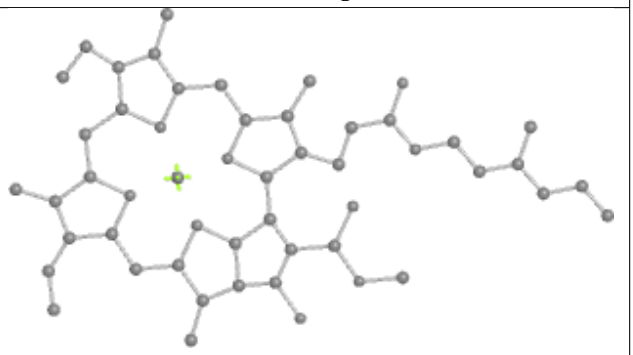
Bond lengths



Bond angles

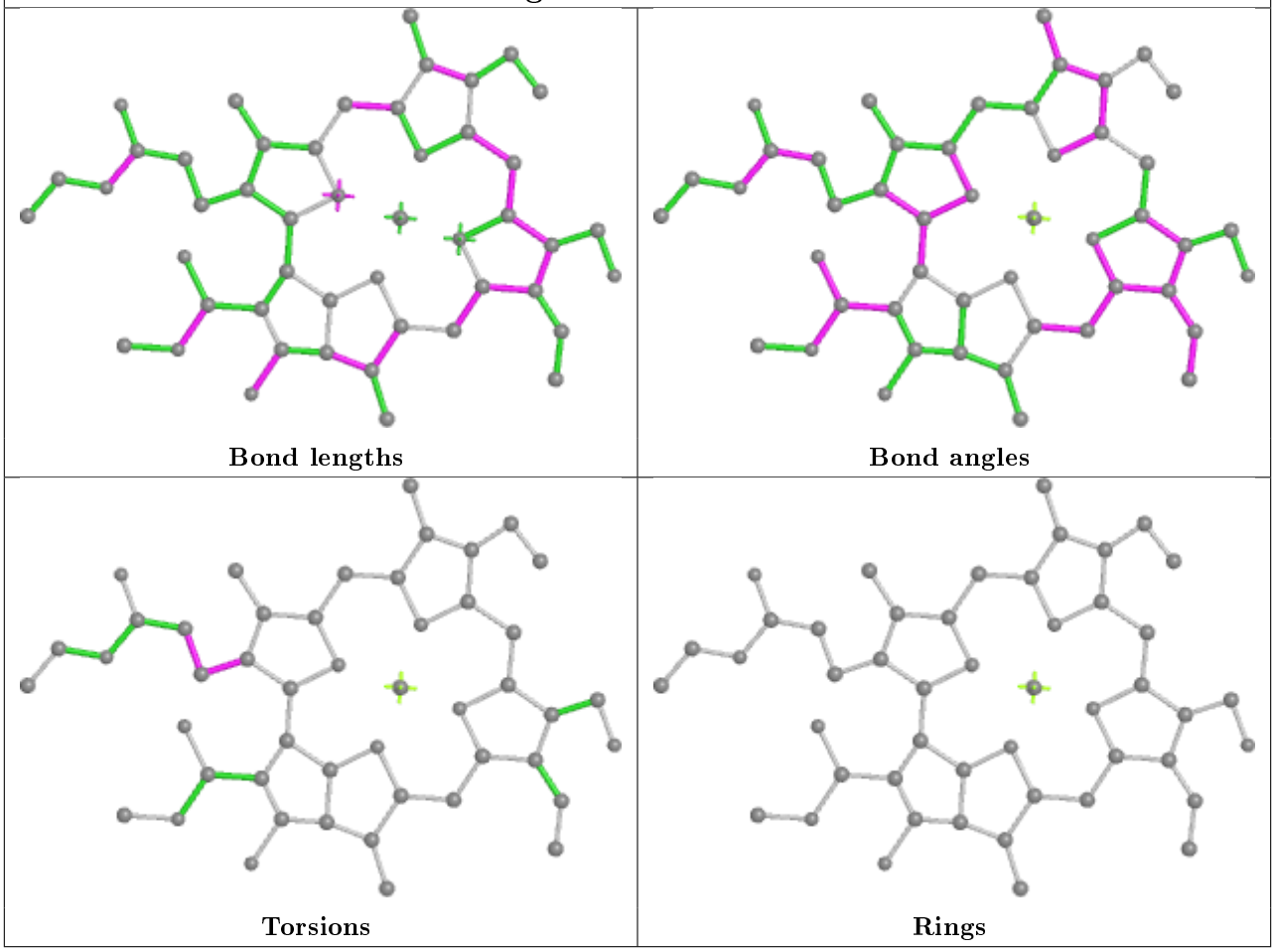


Torsions

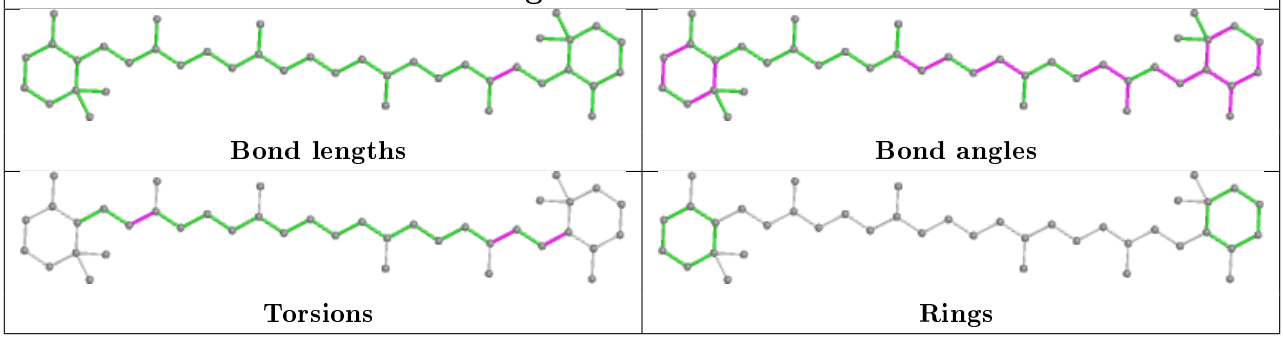


Rings

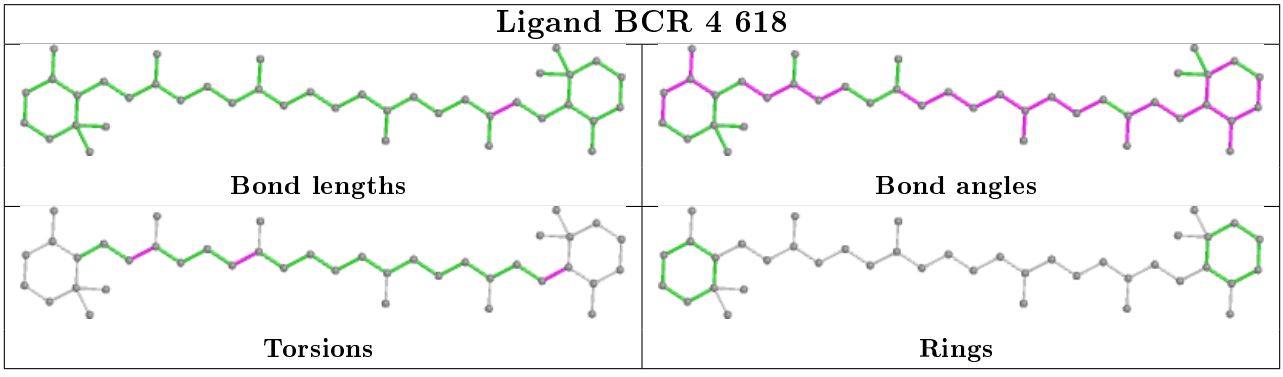
Ligand CHL 2 606



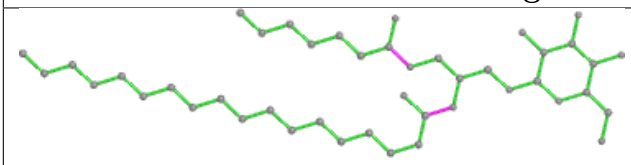
Ligand BCR L 205



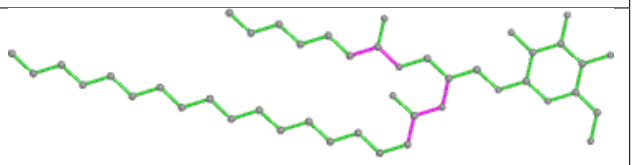
Ligand BCR 4 618



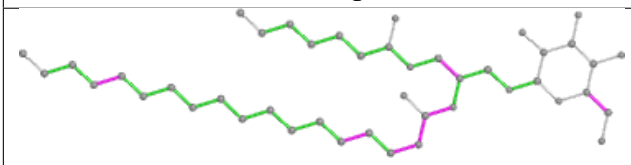
Ligand LMG 4 619



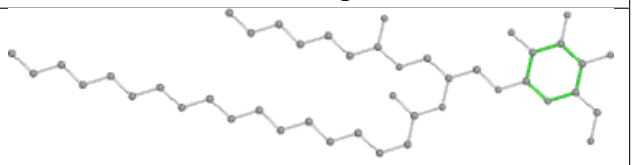
Bond lengths



Bond angles

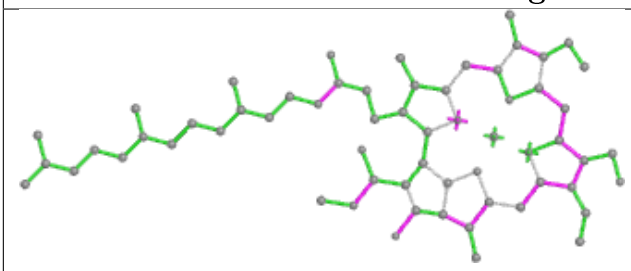


Torsions



Rings

Ligand CHL 6 303



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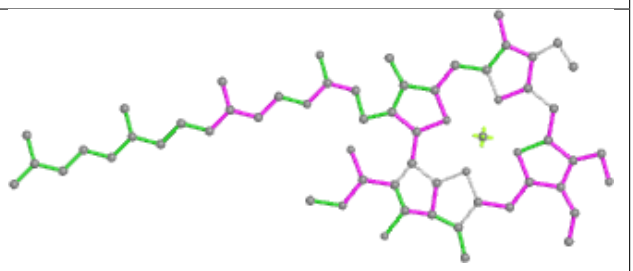
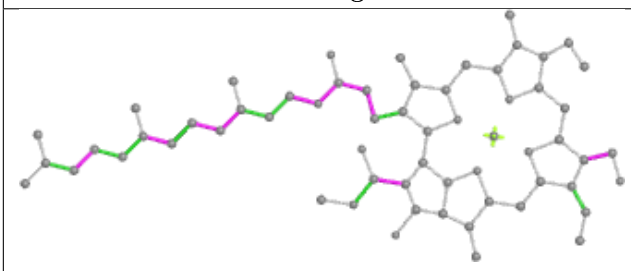


Bond angles



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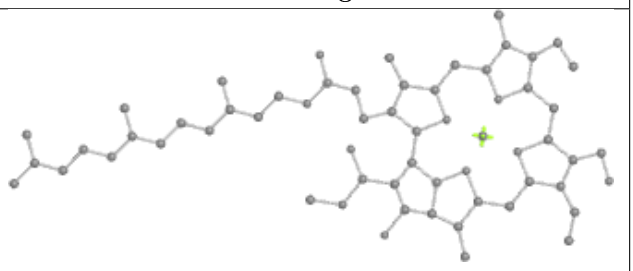
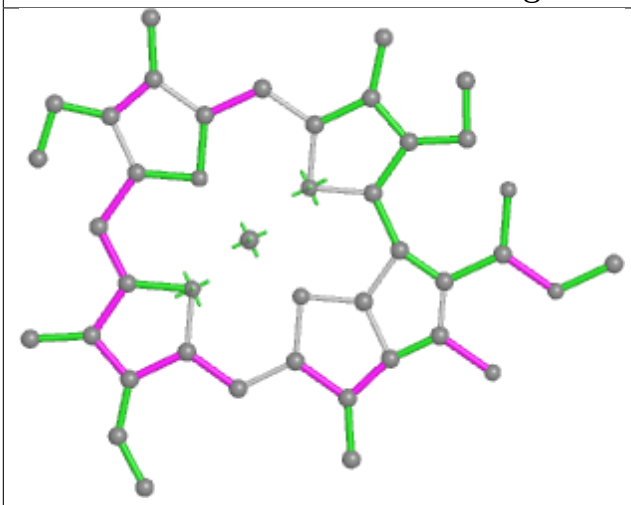


Rings

Ligand CLA j 3002



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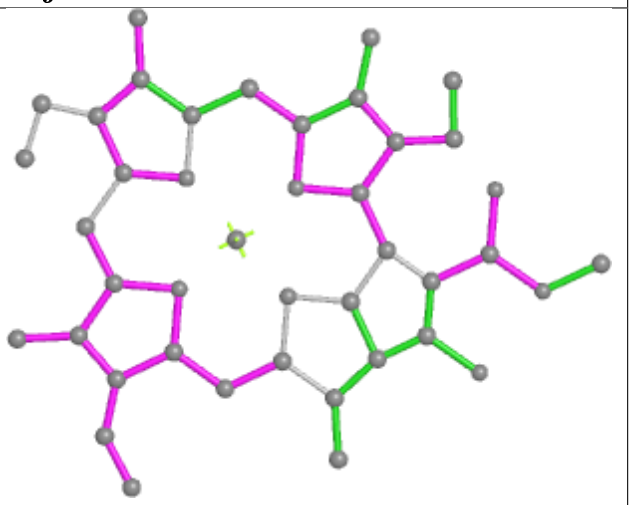
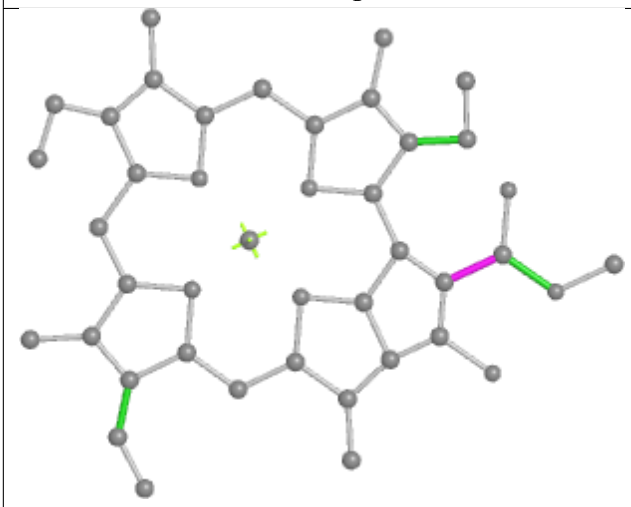


Bond angles



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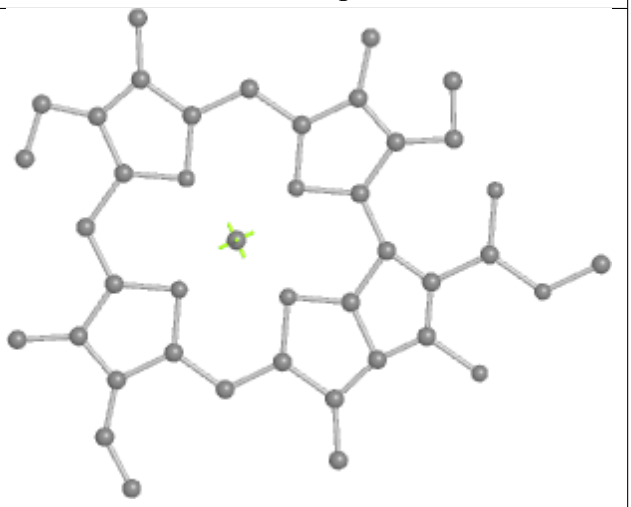
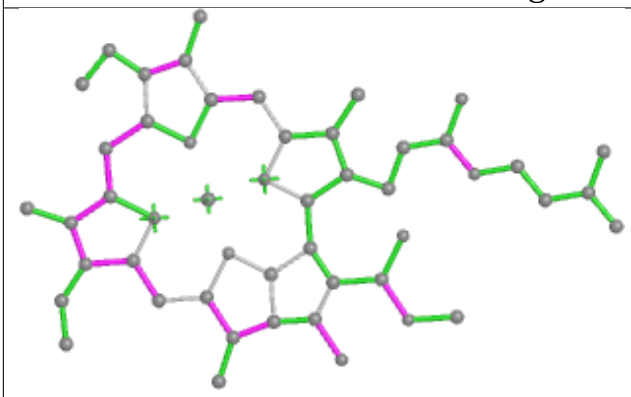


Rings

Ligand CLA 3 303



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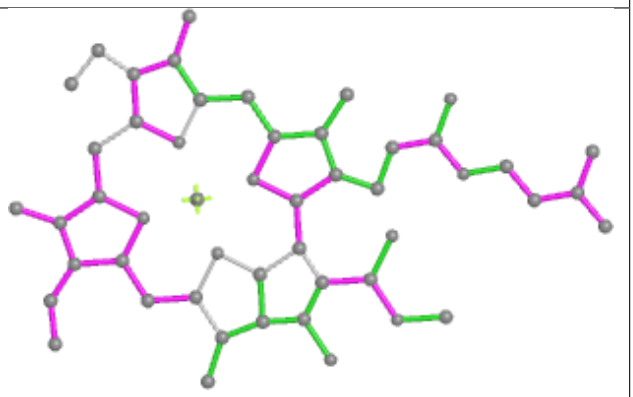
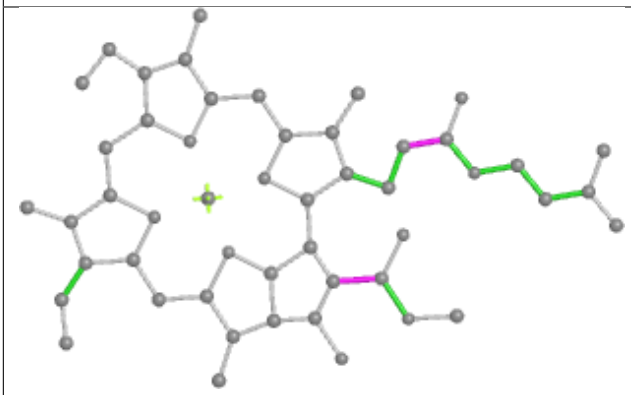


Bond angles



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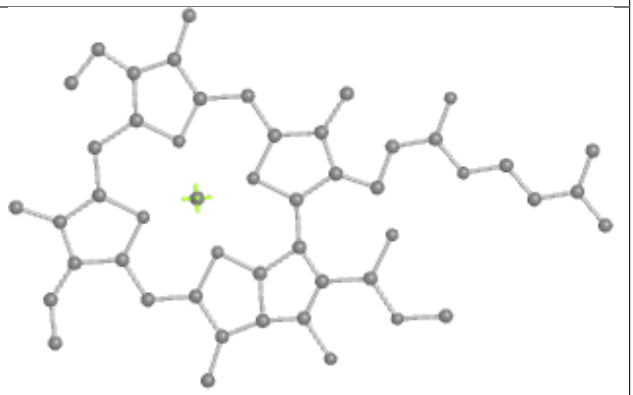
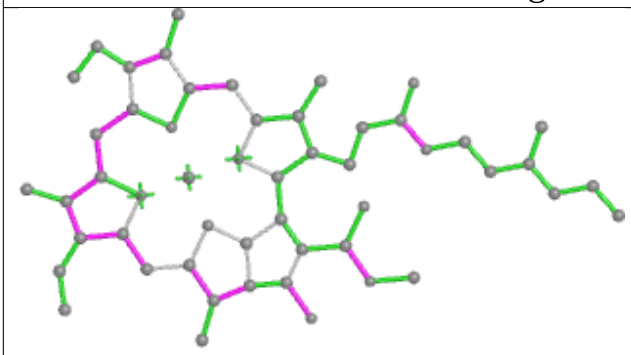


Rings

Ligand CLA 9 611



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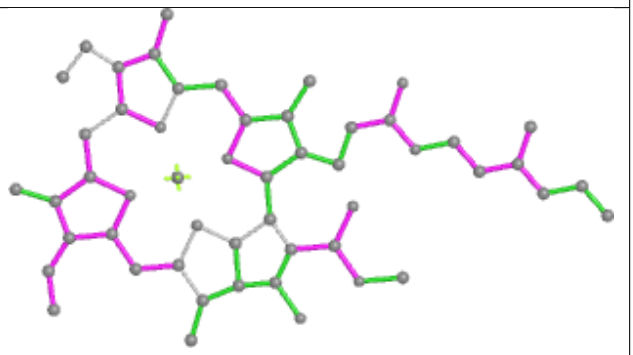
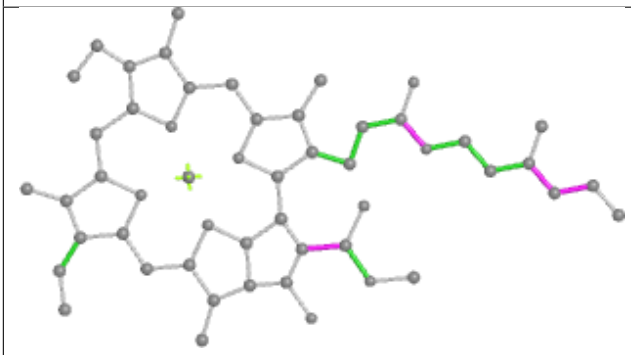


Bond angles



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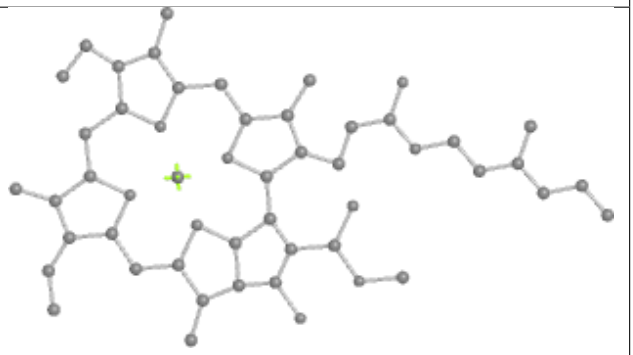
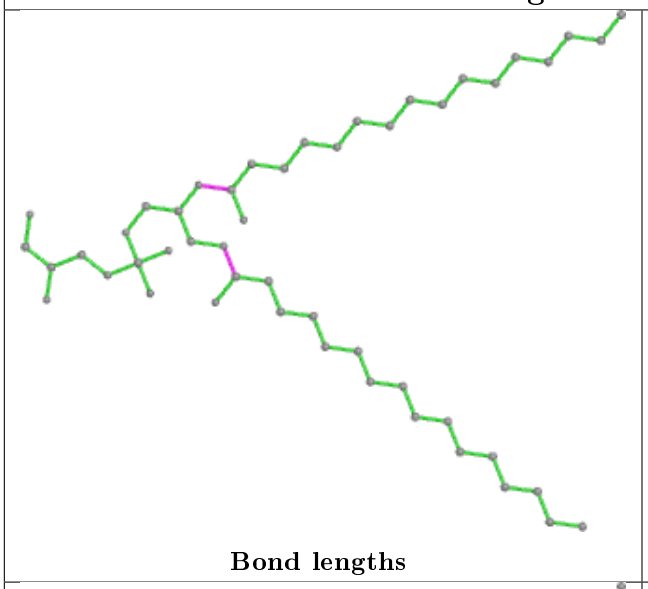


Rings

Ligand LHG 1 319



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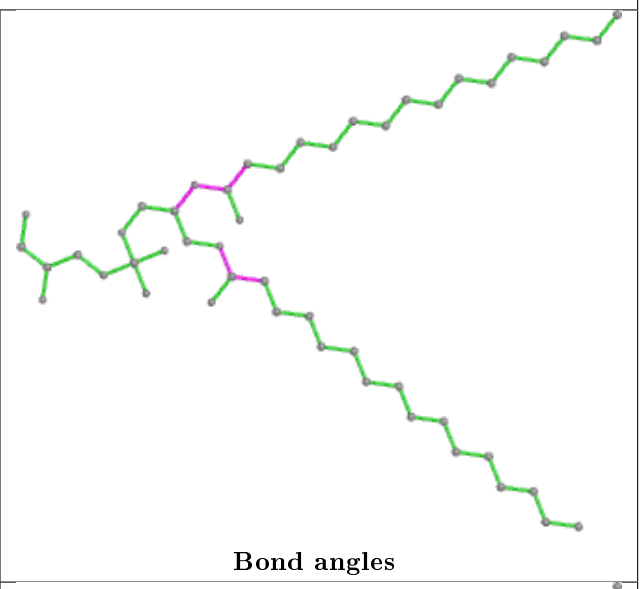

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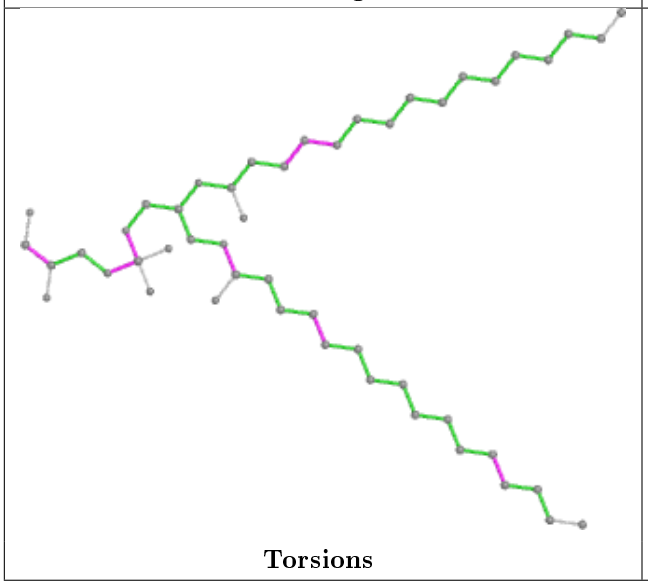

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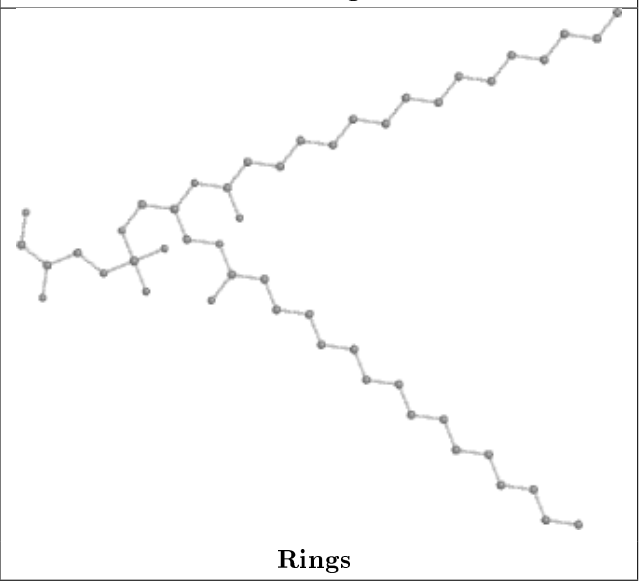
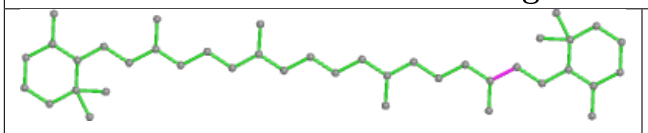


Rings

Ligand BCR f 7004



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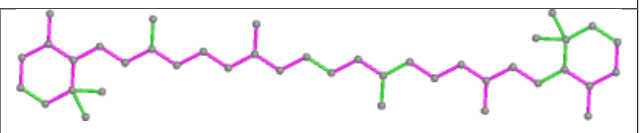
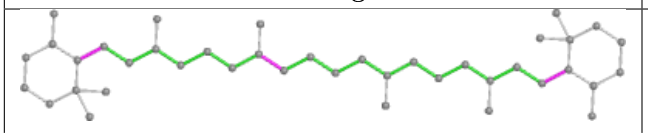


Bond angles



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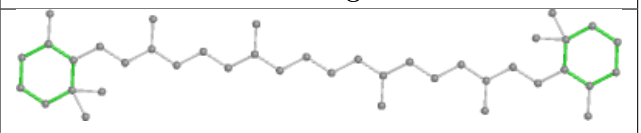
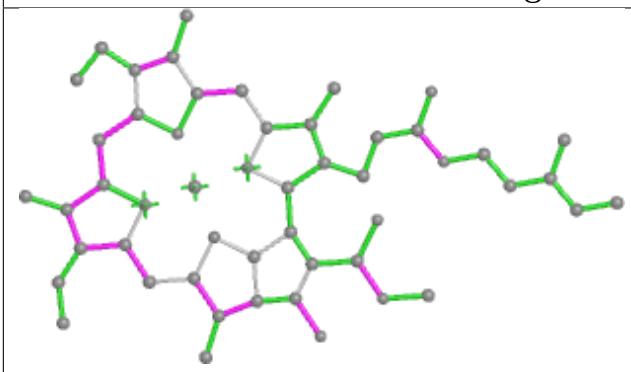


Rings

Ligand CLA A 824



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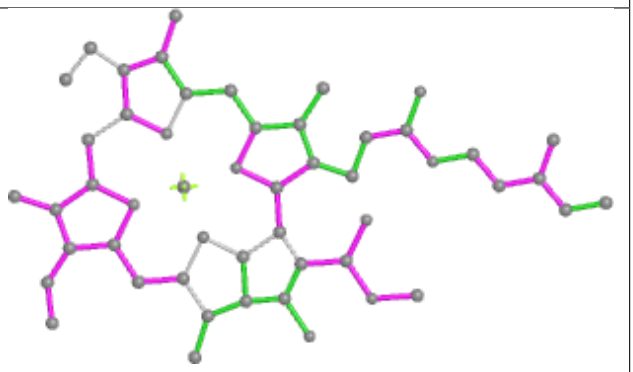
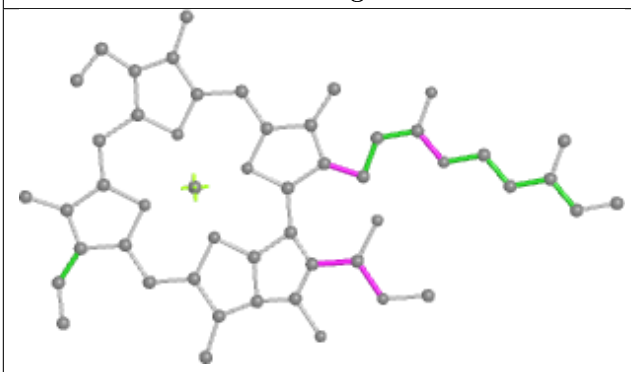


Bond angles



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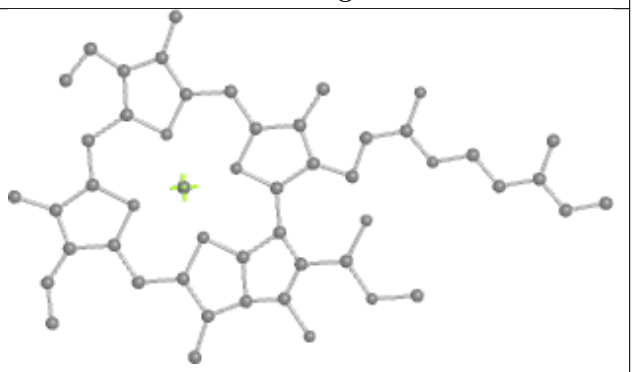
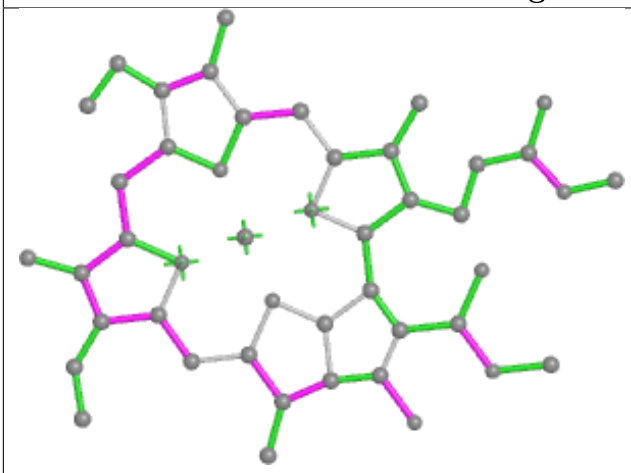


Rings

Ligand CLA 1 315



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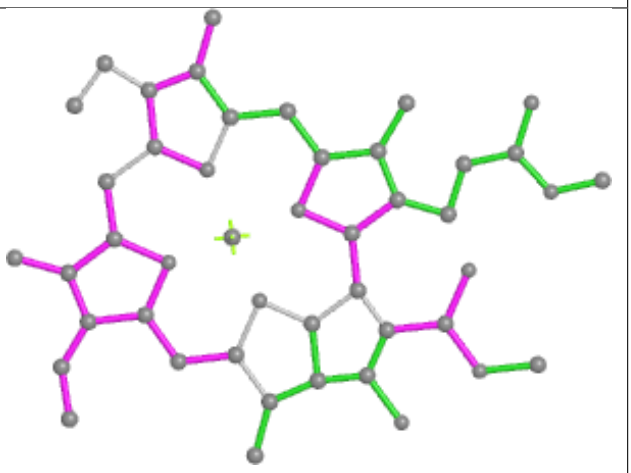
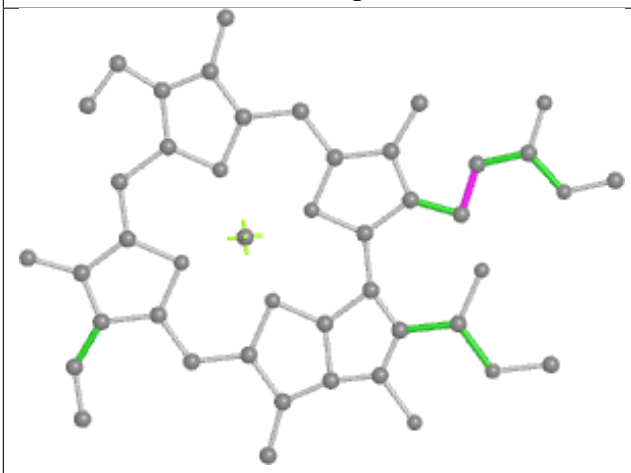


Bond angles



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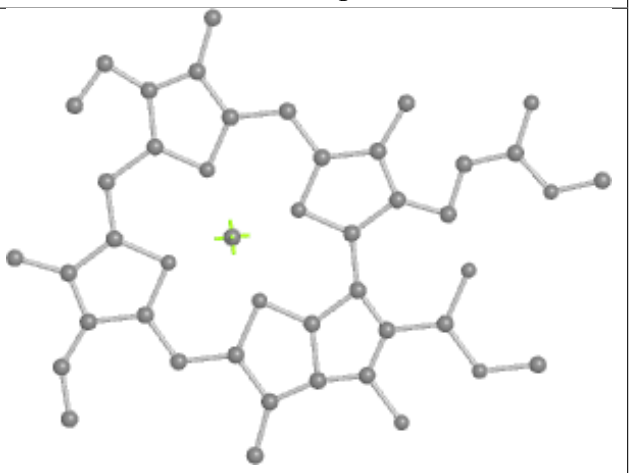
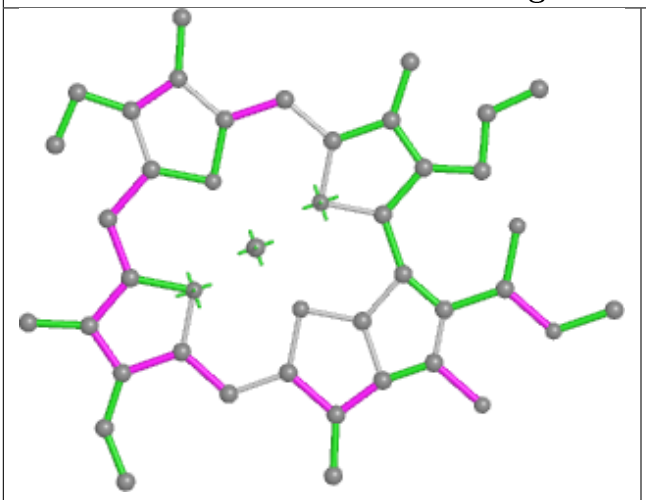


Rings

Ligand CLA 2 613



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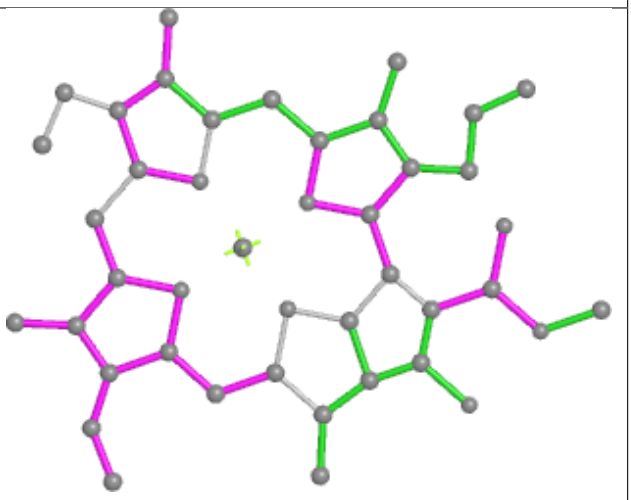
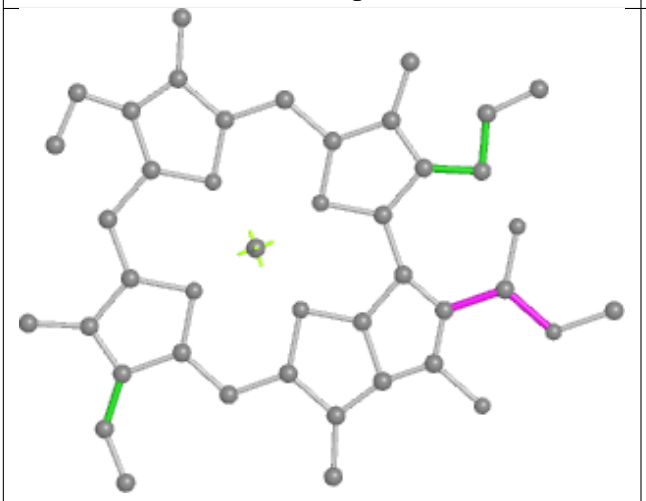


Bond angles



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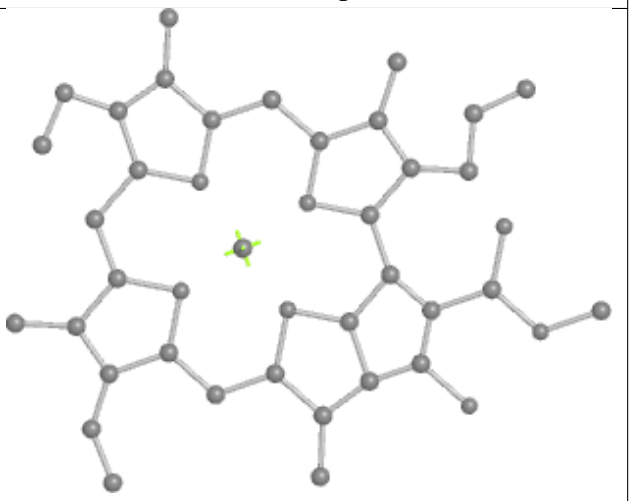
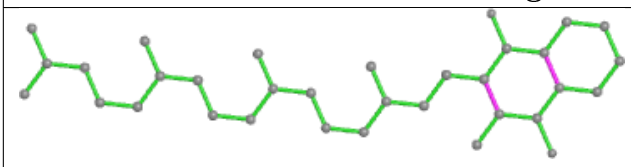


Rings

Ligand PQN b 842



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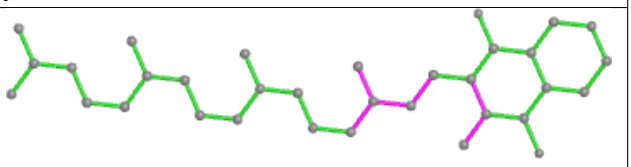
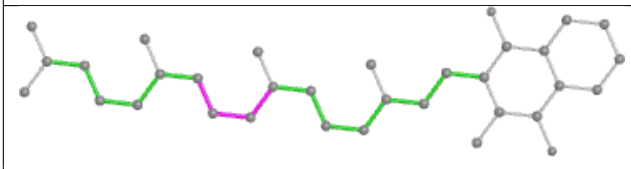
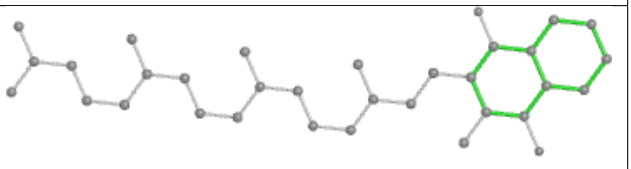


Bond angles

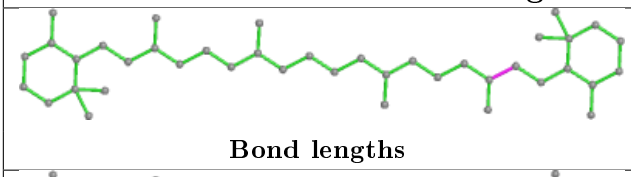


Torsions



Rings

Ligand BCR 1 318



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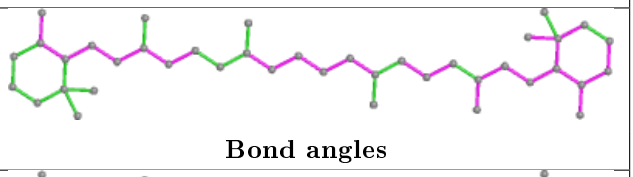
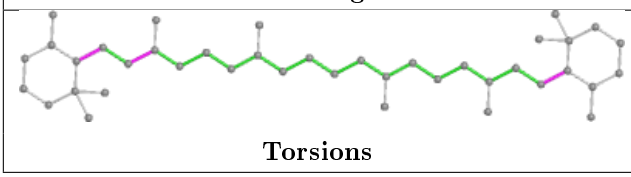


Bond angles



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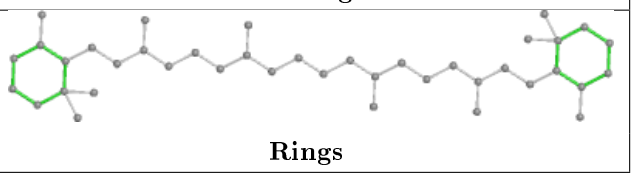
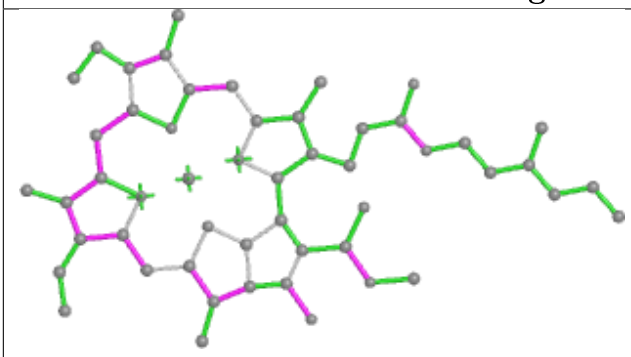
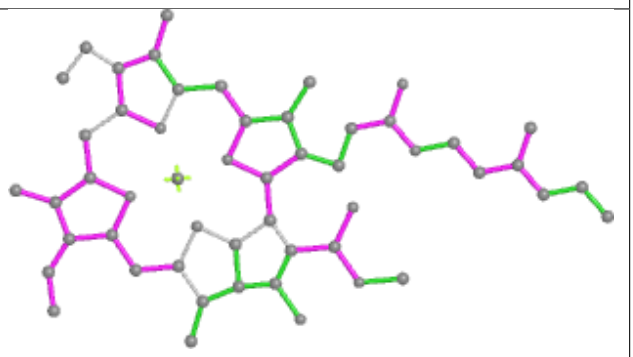


Rings

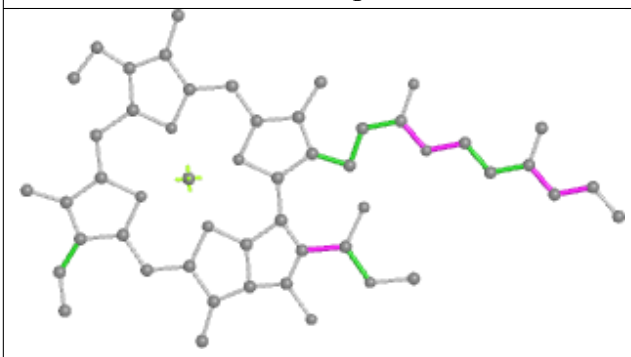
Ligand CLA 1 305



Bond lengths



Bond angles



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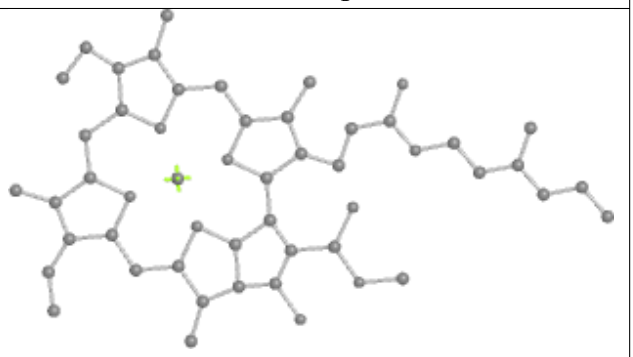
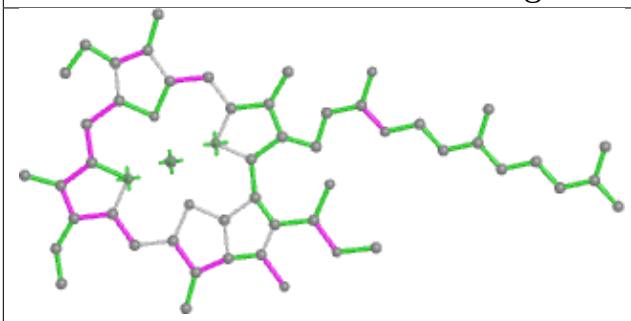
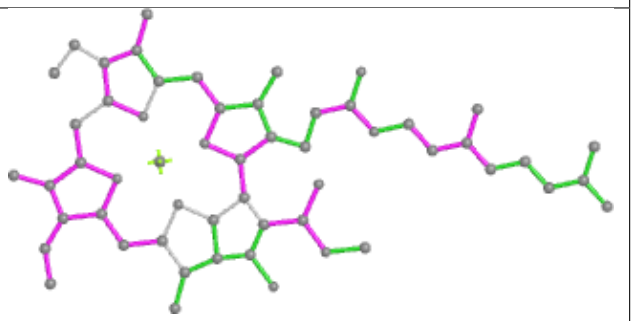


Rings

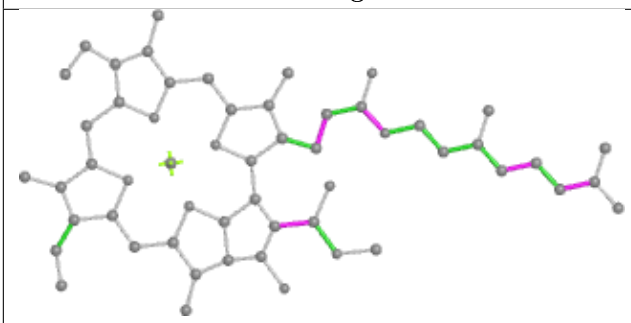
Ligand CLA A 825



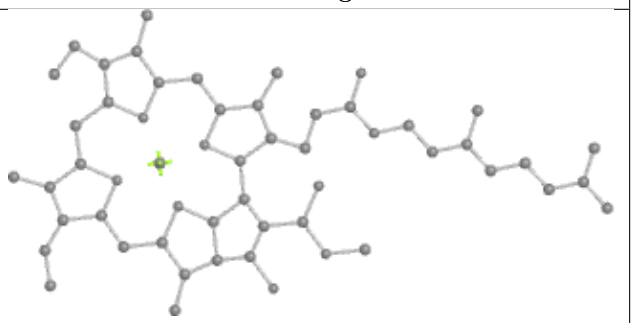
Bond lengths



Bond angles

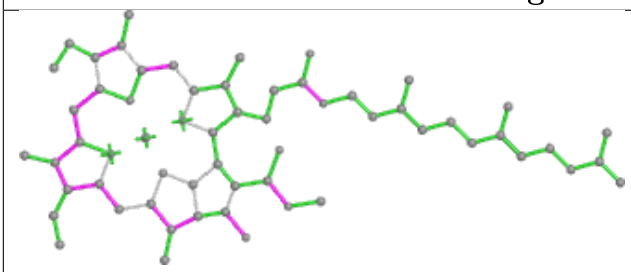


Torsions

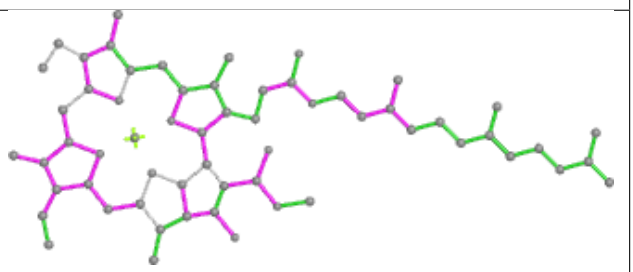


Rings

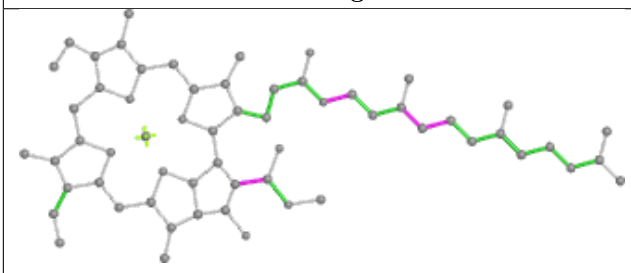
Ligand CLA b 836



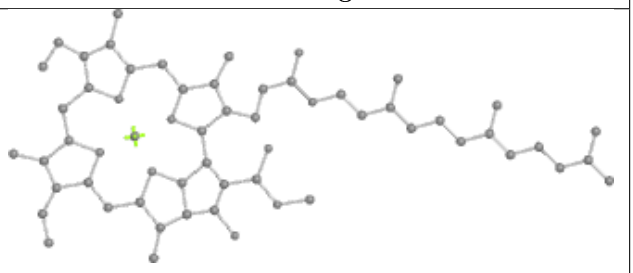
Bond lengths



Bond angles

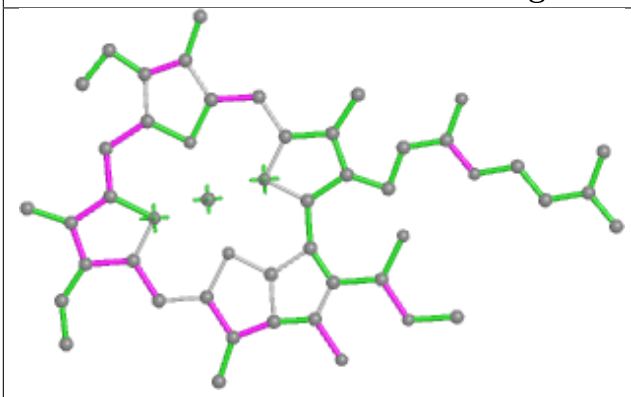


Torsions

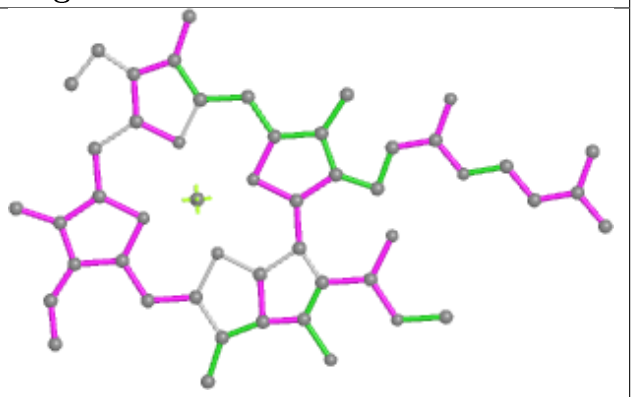


Rings

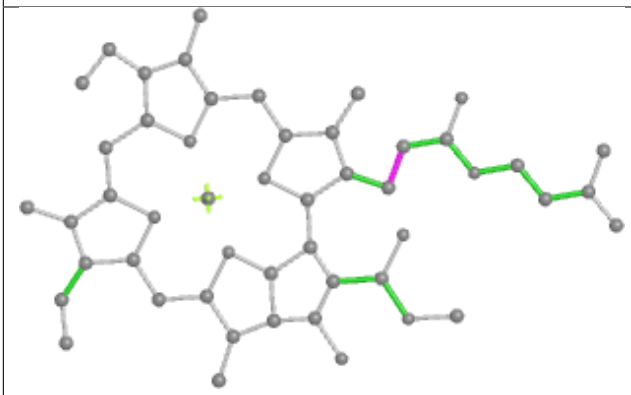
Ligand CLA g 102



Bond lengths



Bond angles



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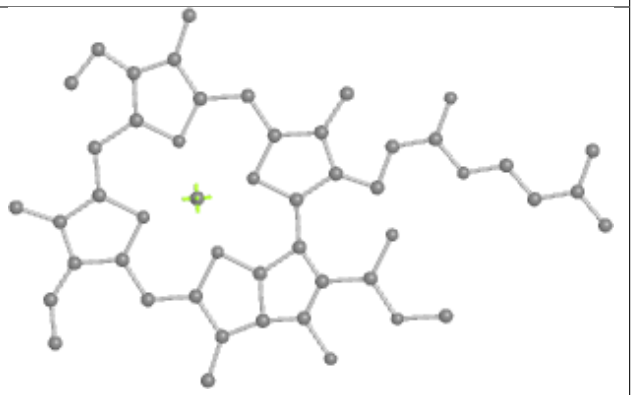
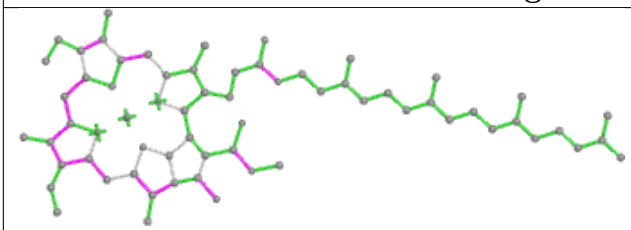


Rings

Ligand CLA A 828



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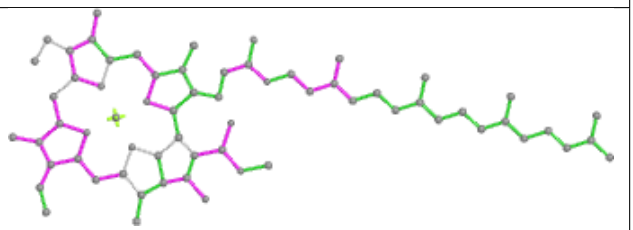
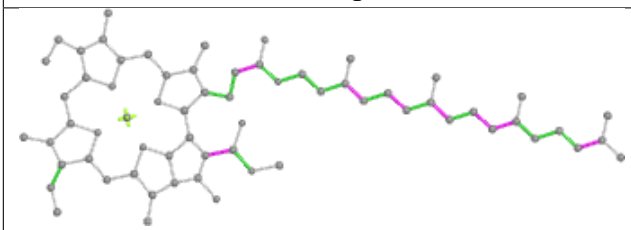
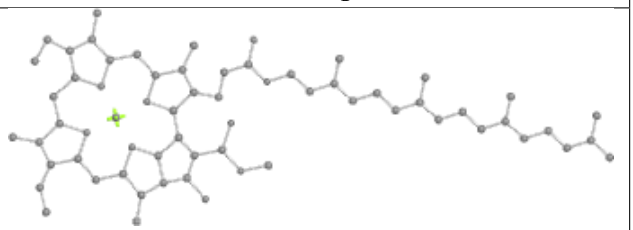


Bond angles

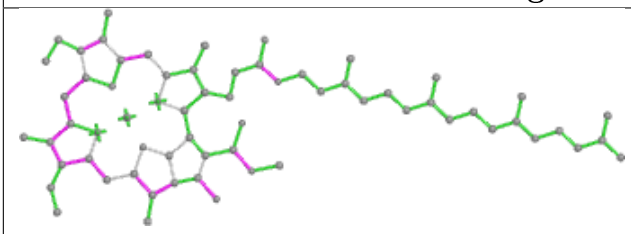


Torsions



Rings

Ligand CLA b 813



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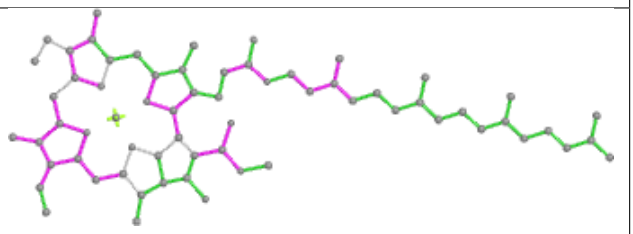
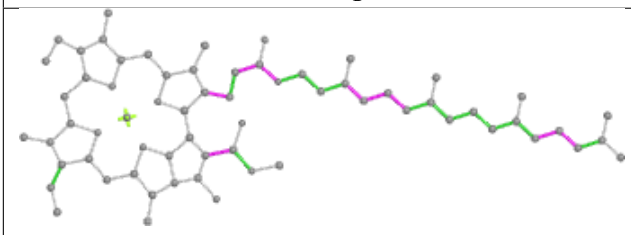


Bond angles



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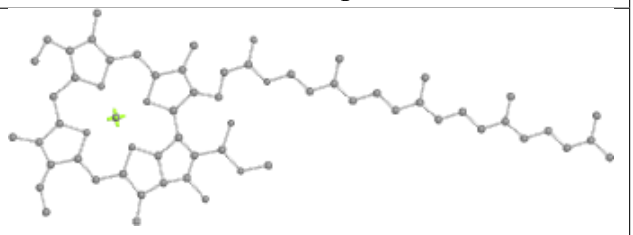
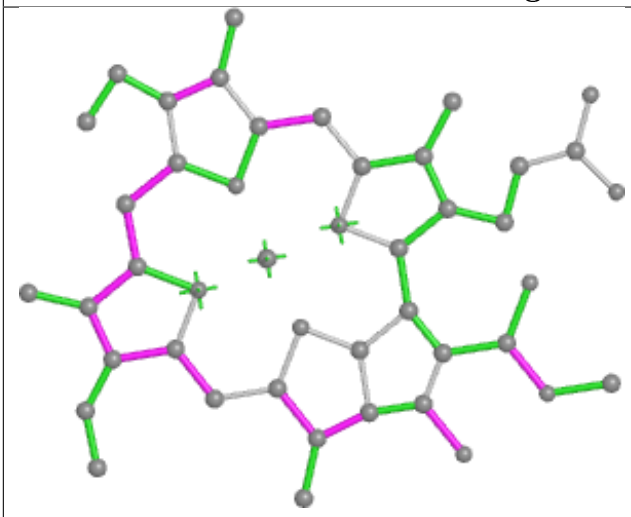


Rings

Ligand CLA A 815



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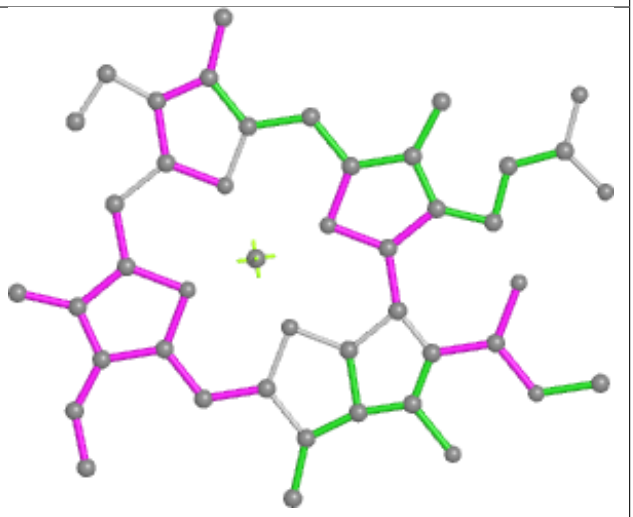

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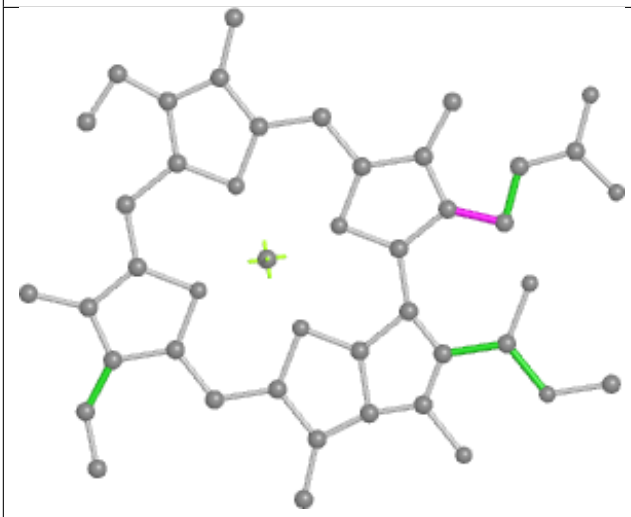

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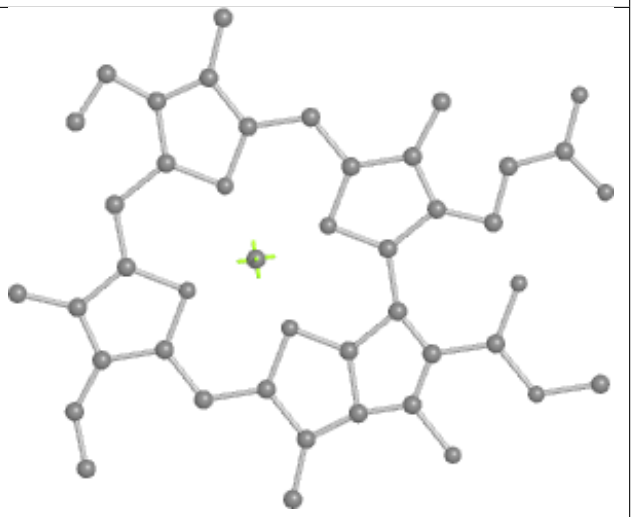
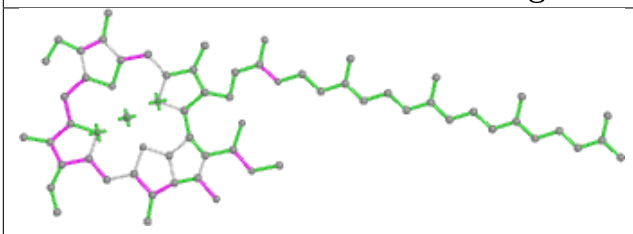


Rings

Ligand CLA a 820



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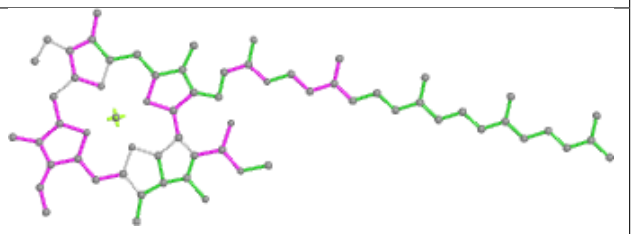
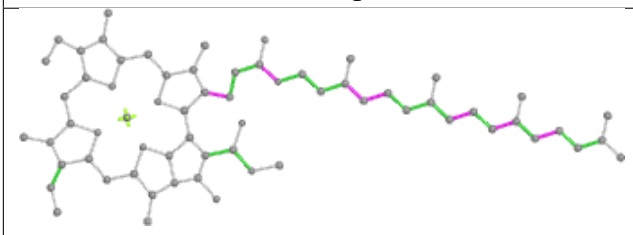


Bond angles



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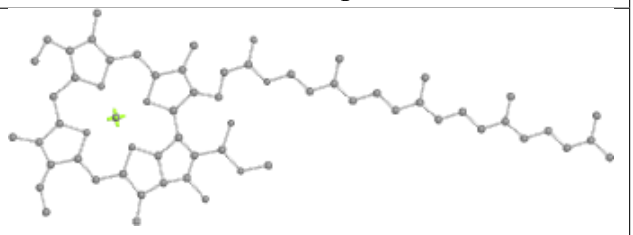
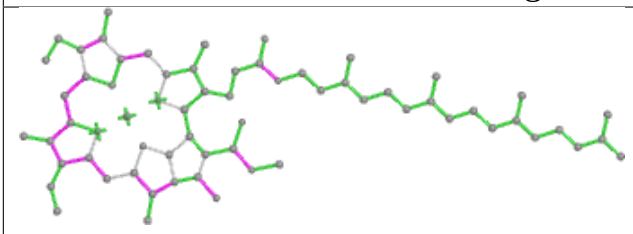


Rings

Ligand CLA A 801



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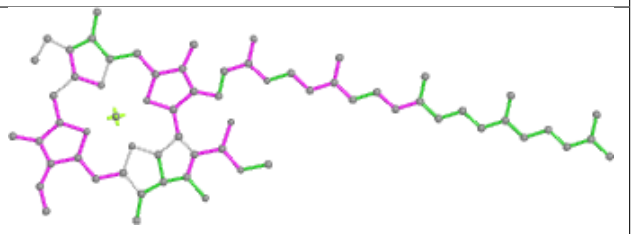
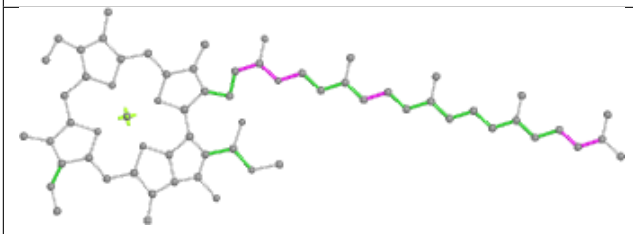


Bond angles



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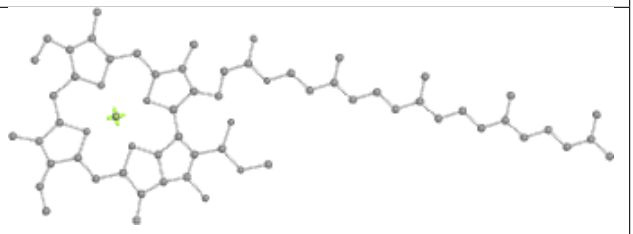
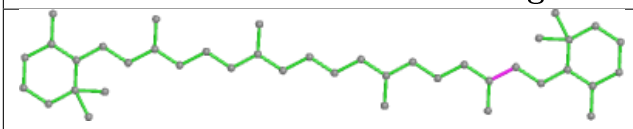


Rings

Ligand BCR a 853



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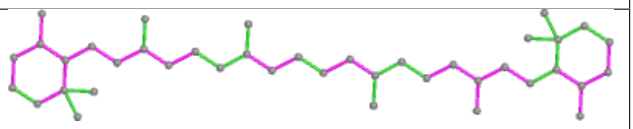
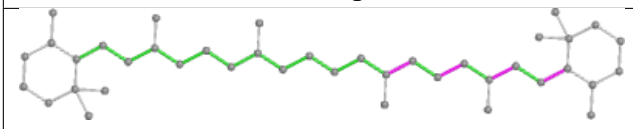


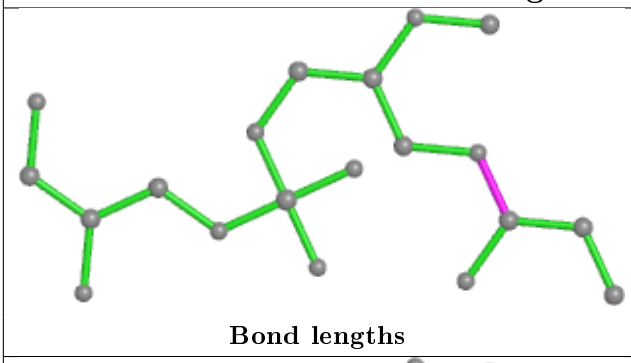
Bond angles



Torsions

Rings

Ligand LHG 3 319



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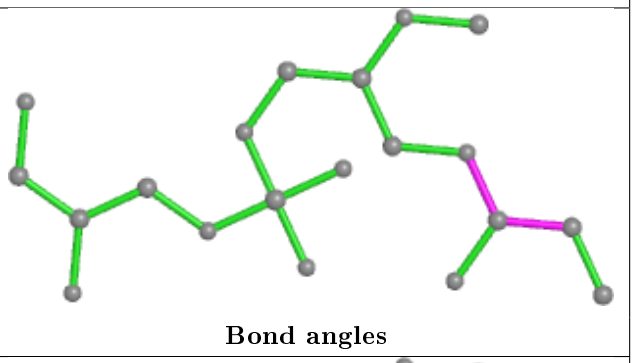
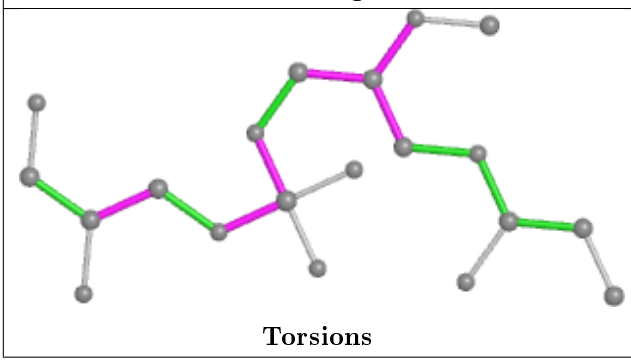
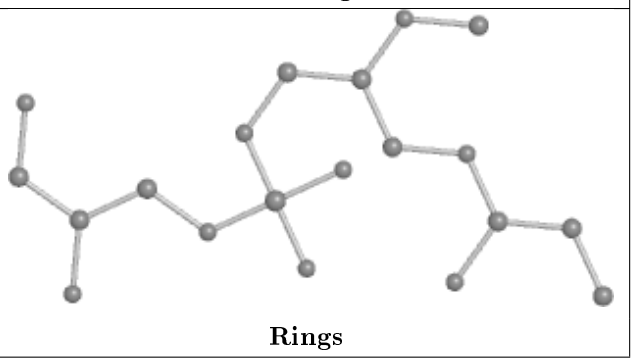


Bond angles

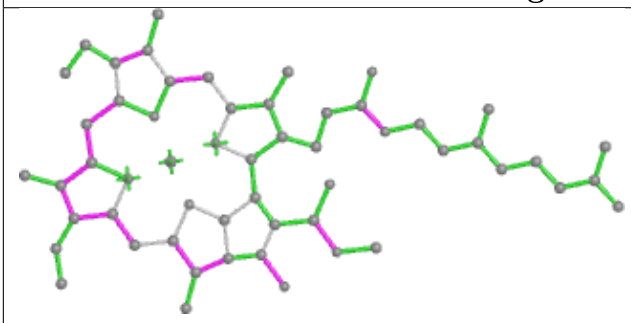


Torsions



Rings

Ligand CLA b 815



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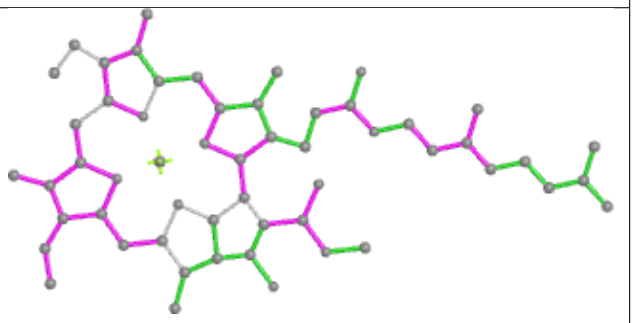
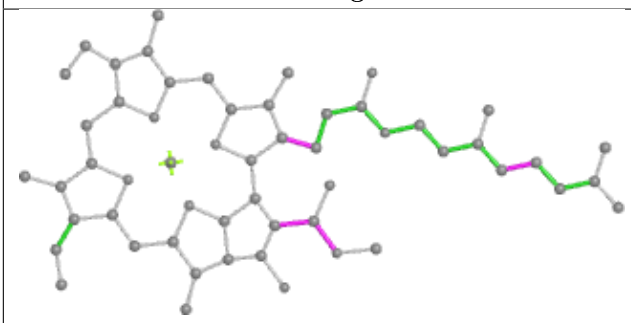


Bond angles



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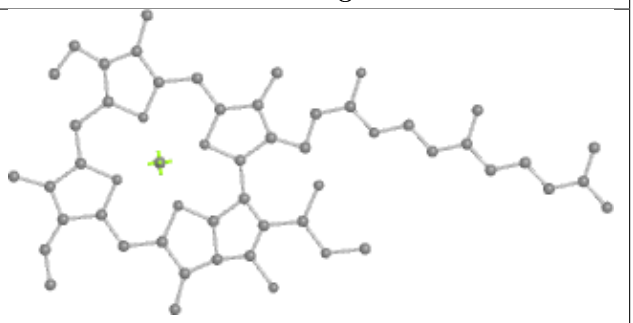
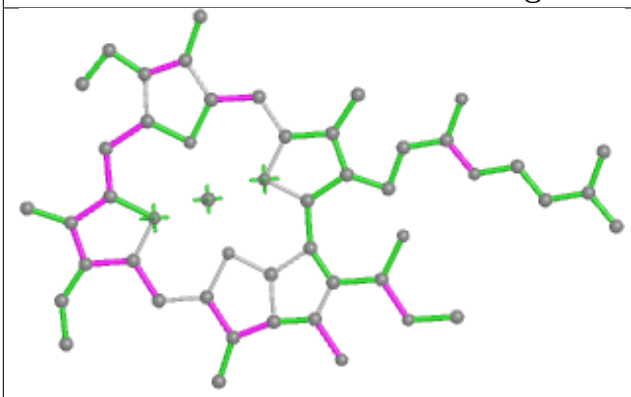


Rings

Ligand CLA A 832



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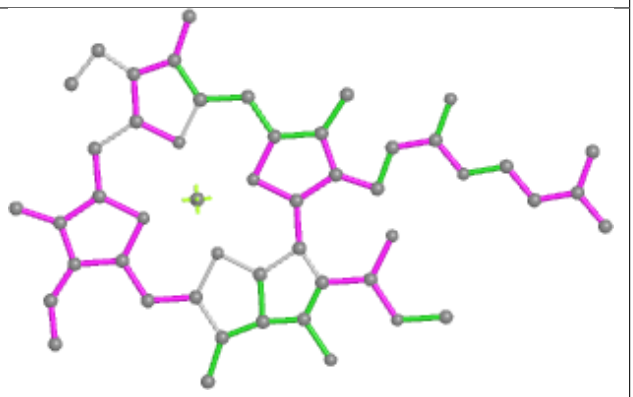
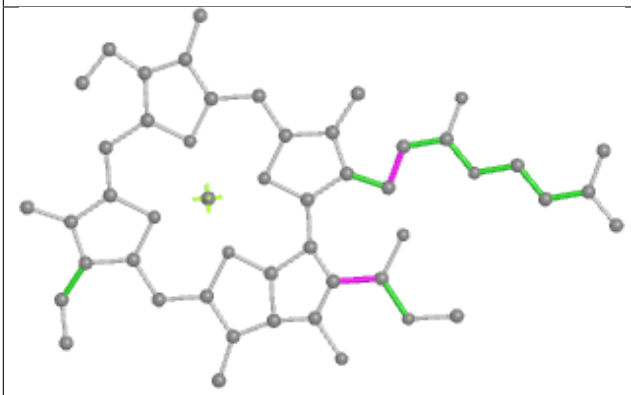


Bond angles



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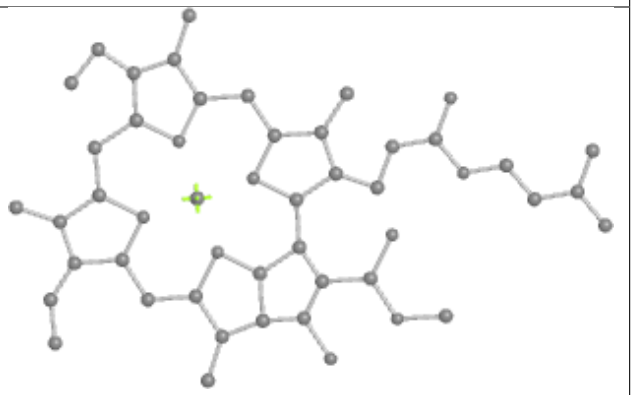
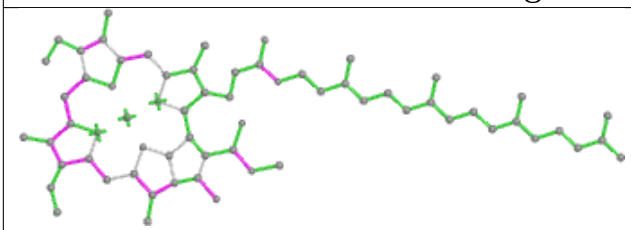
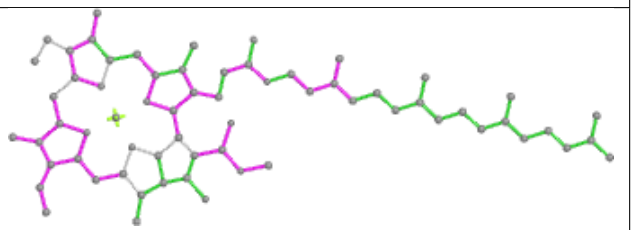


Rings

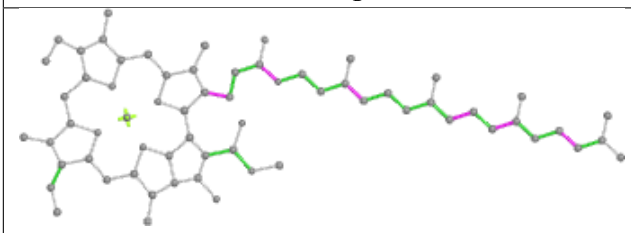
Ligand CLA B 819



Bond lengths



Bond angles



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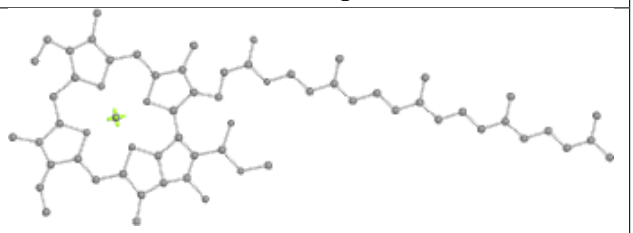
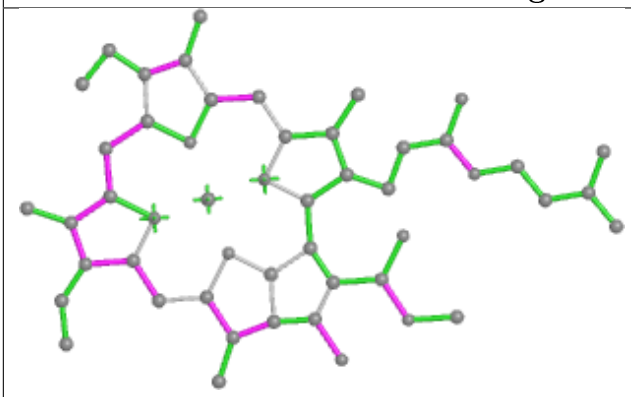
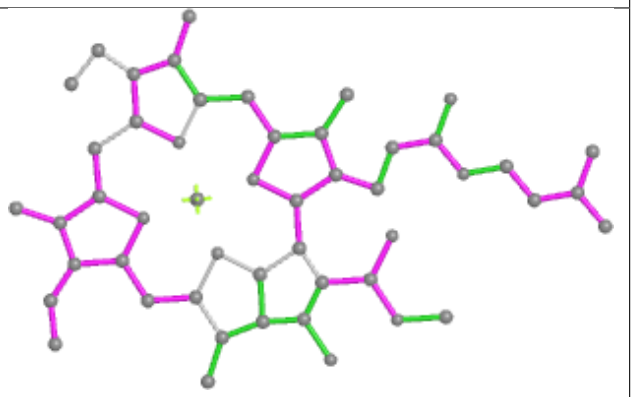


Rings

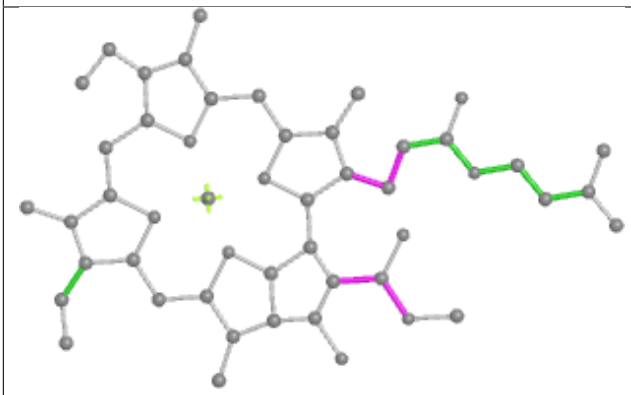
Ligand CLA 4 604



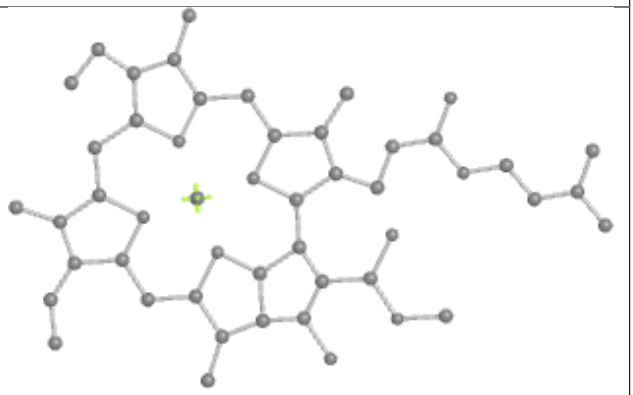
Bond lengths



Bond angles

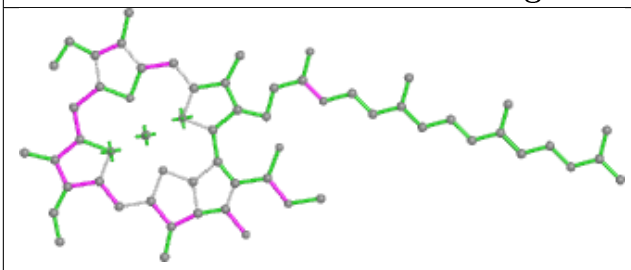


Torsions

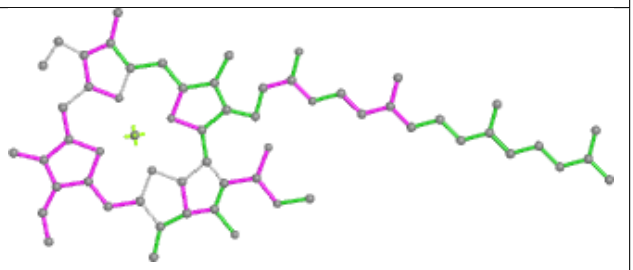


Rings

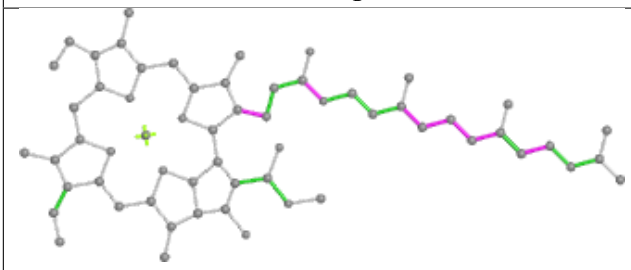
Ligand CLA B 818



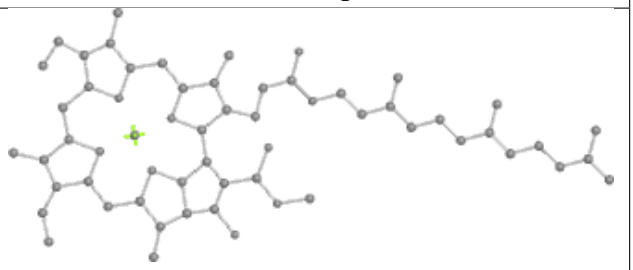
Bond lengths



Bond angles

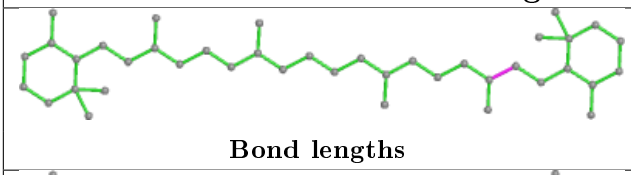


Torsions



Rings

Ligand BCR B 848



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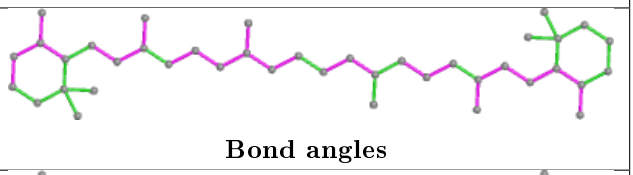
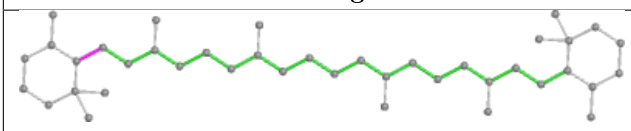
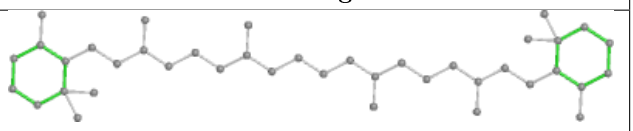


Bond angles

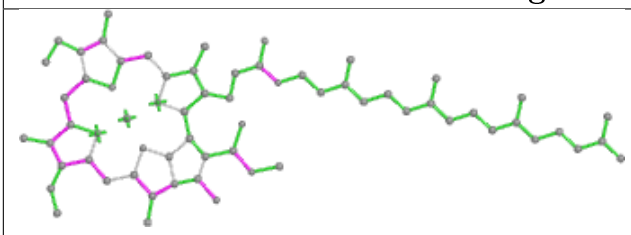


Torsions

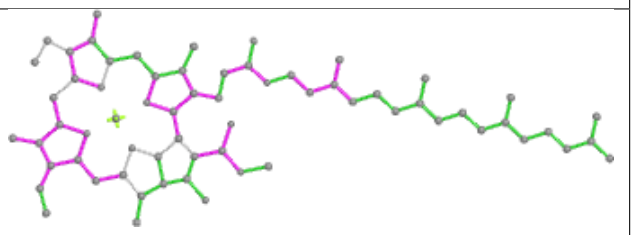


Rings

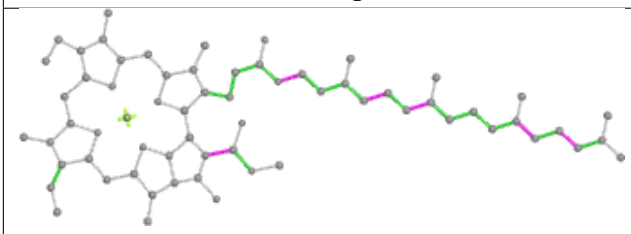
Ligand CLA a 827



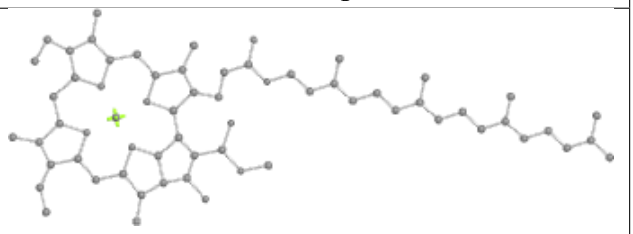
Bond lengths



Bond angles

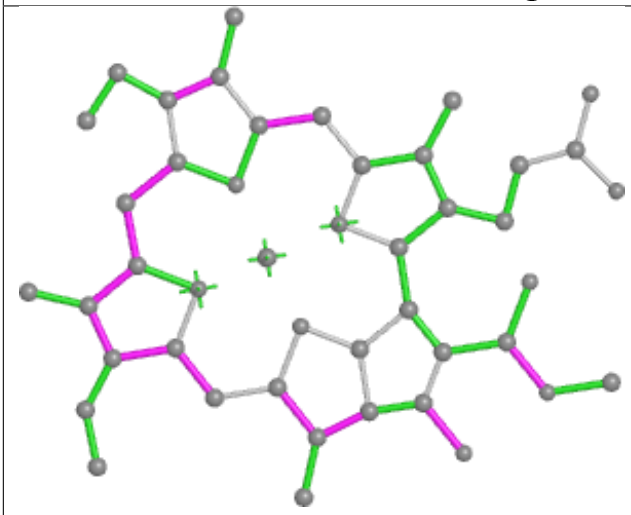


Torsions



Rings

Ligand CLA f 7002



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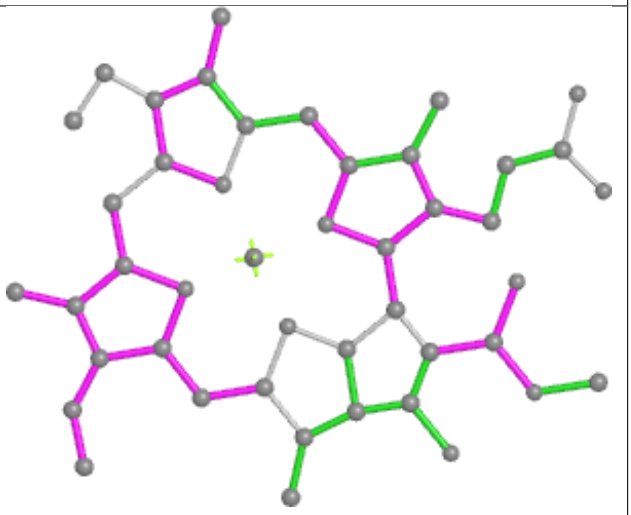
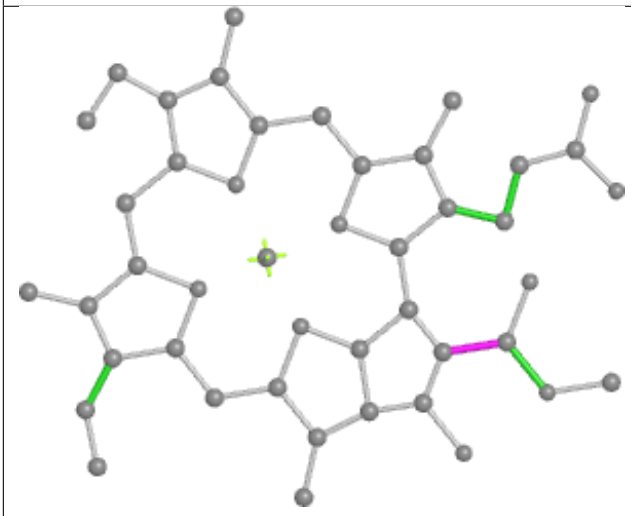


Bond angles



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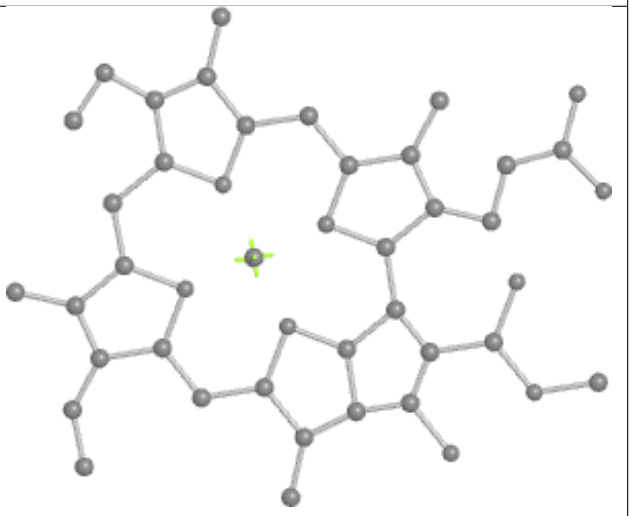
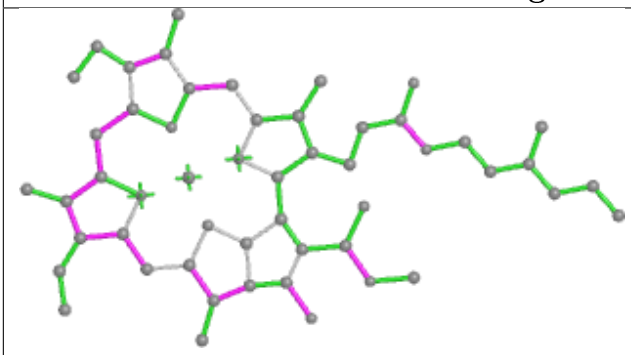
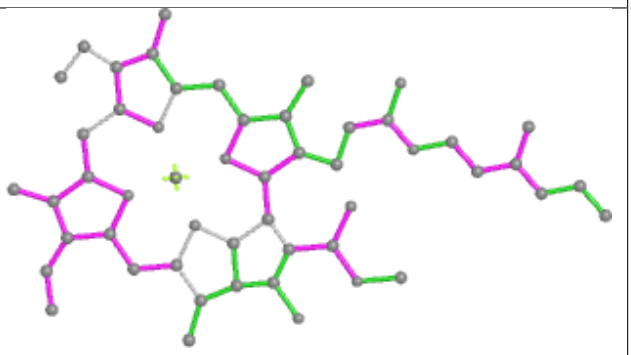


Rings

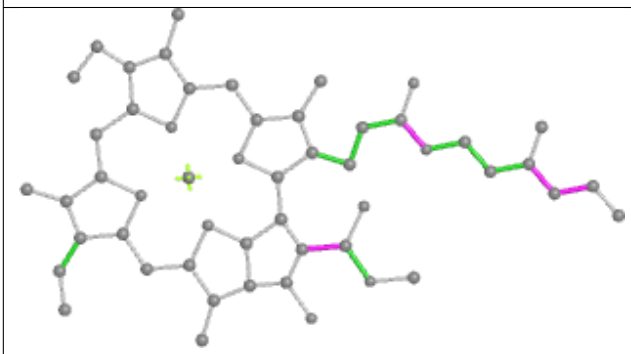
Ligand CLA 3 311



Bond lengths



Bond angles



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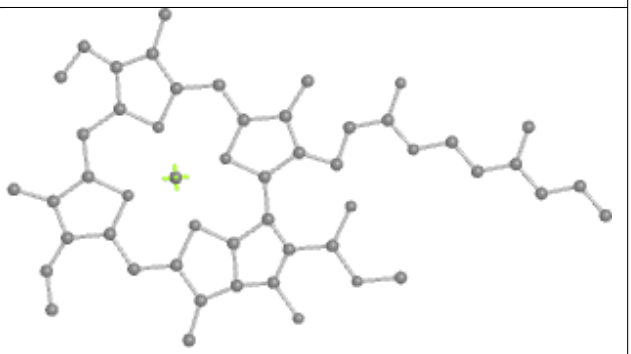
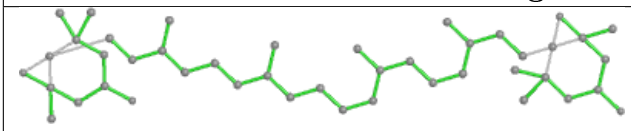


Rings

Ligand XAT 4 617



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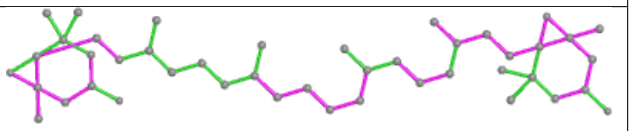
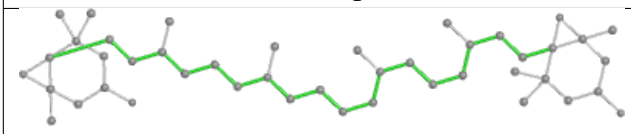


Bond angles



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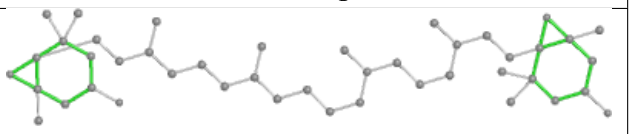
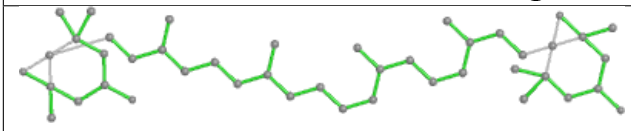


Rings

Ligand XAT 7 616



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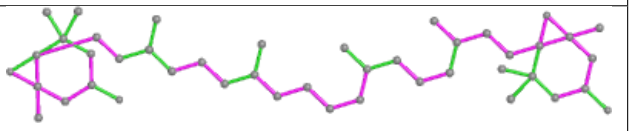

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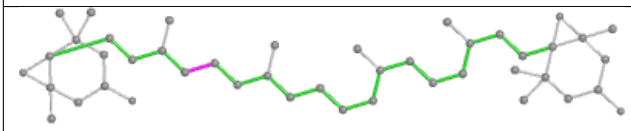

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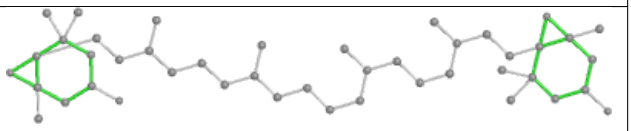
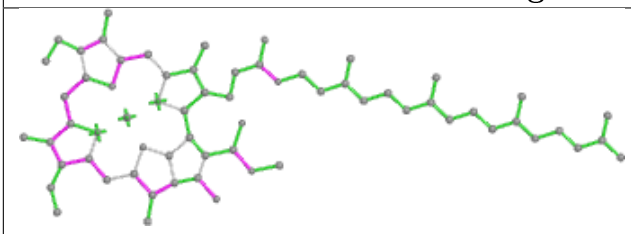


Rings

Ligand CLA b 809



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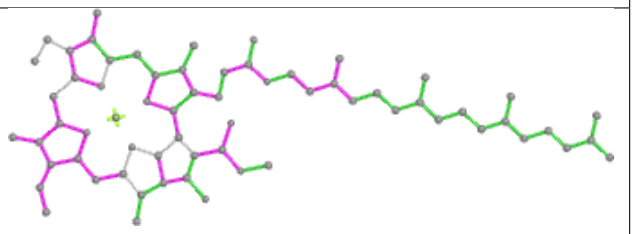

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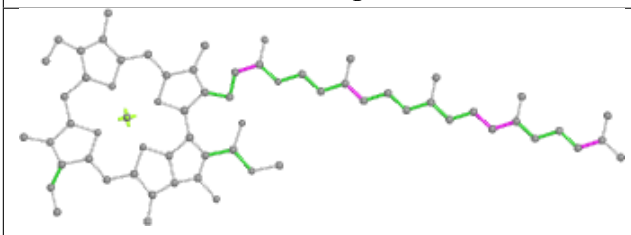

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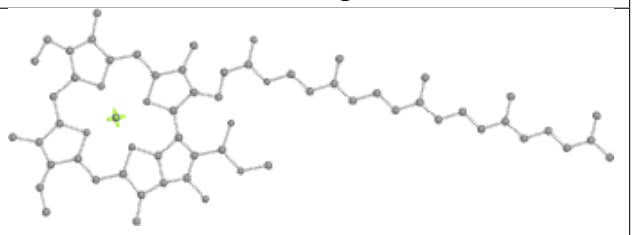
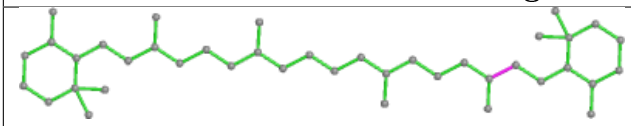


Rings

Ligand BCR B 801



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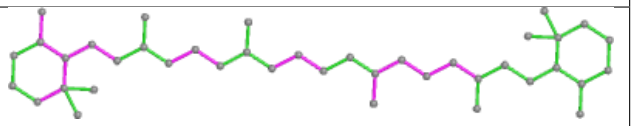
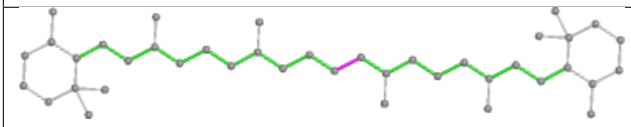


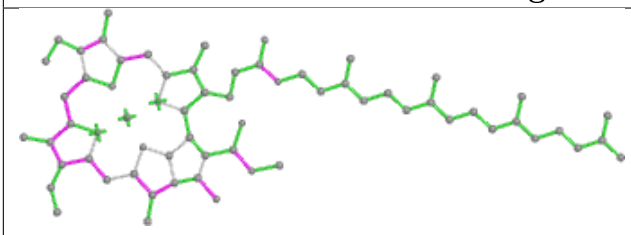
Bond angles



Torsions

Rings

Ligand CLA a 835



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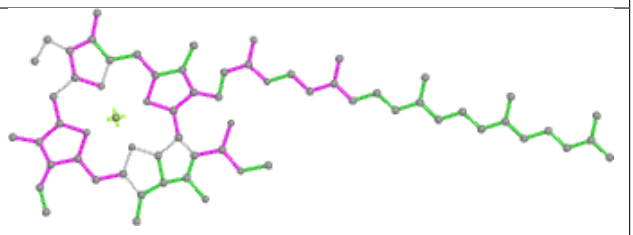
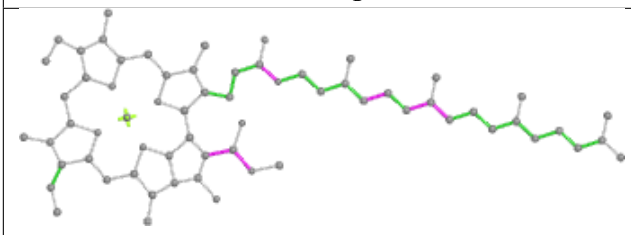


Bond angles



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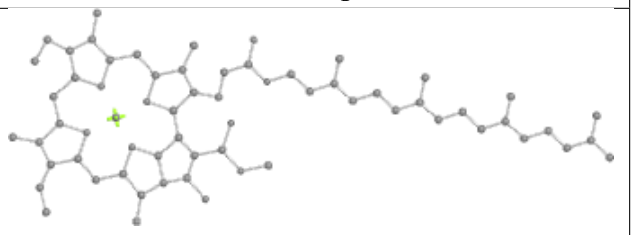
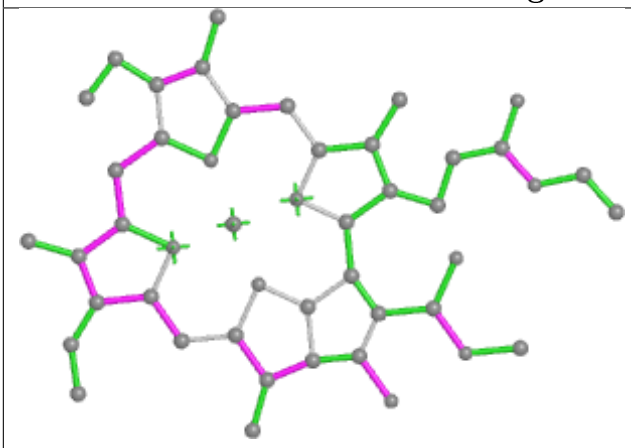


Rings

Ligand CLA b 838



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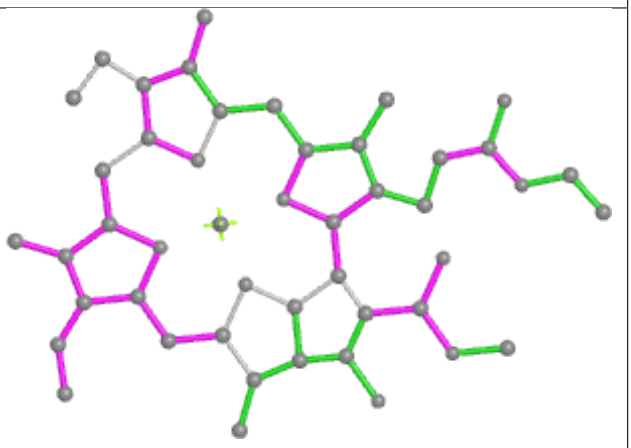
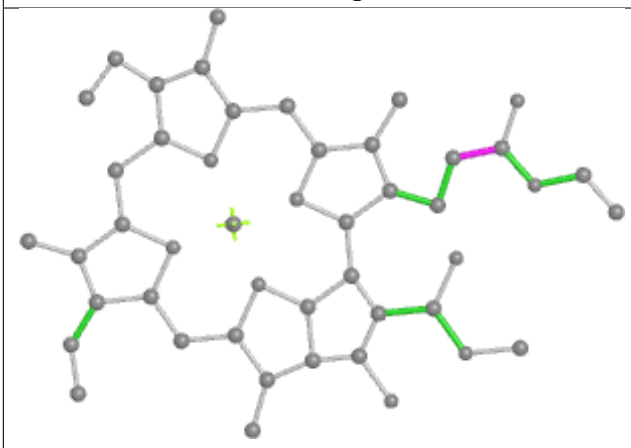


Bond angles



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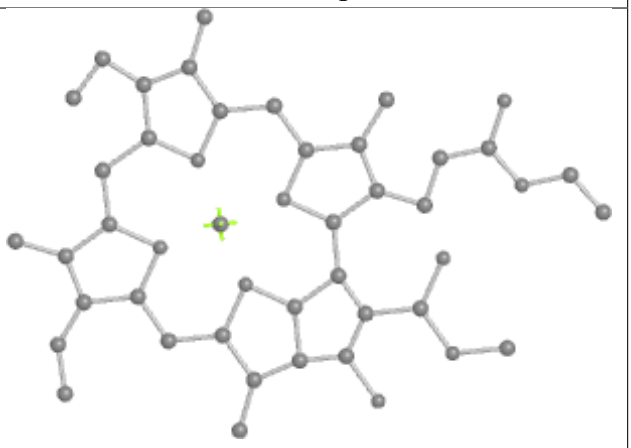
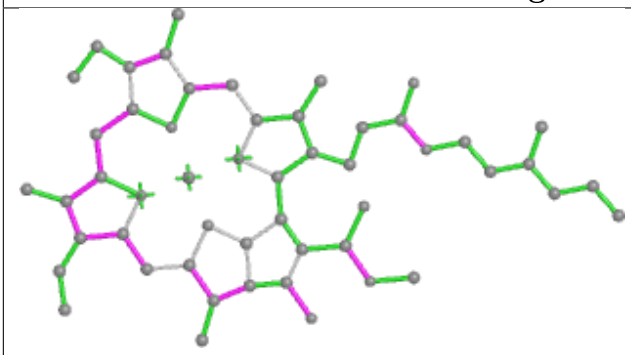
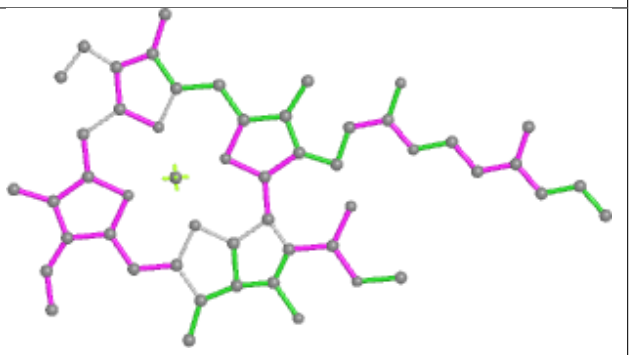
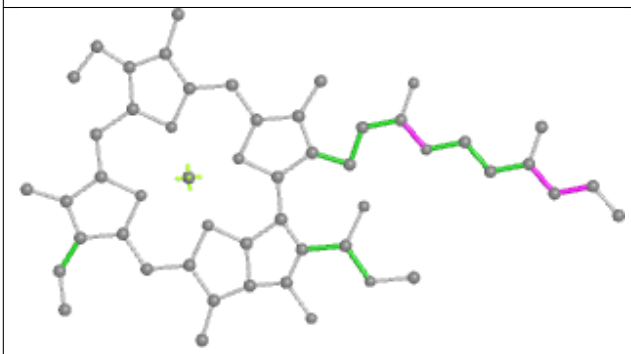
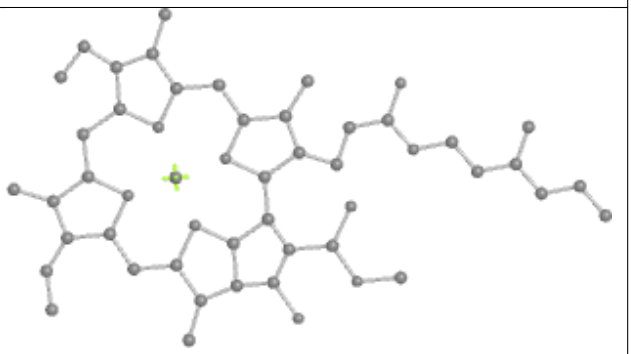
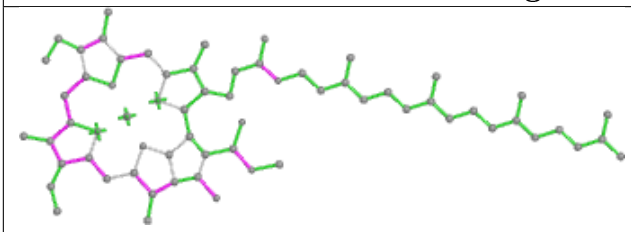
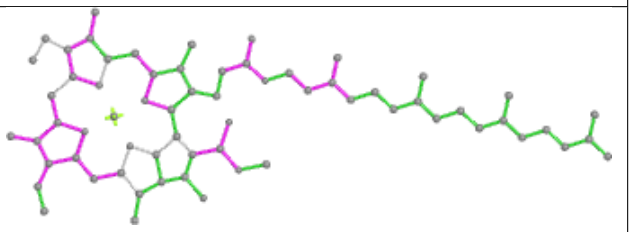
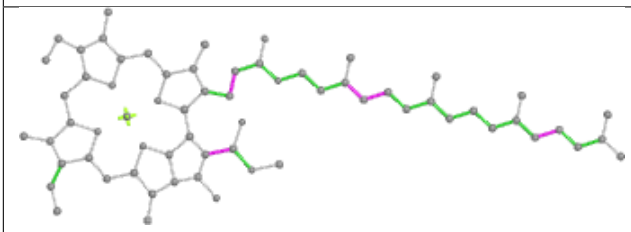
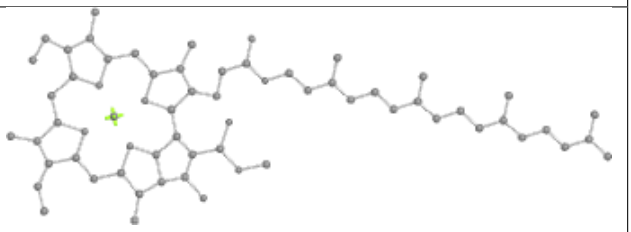
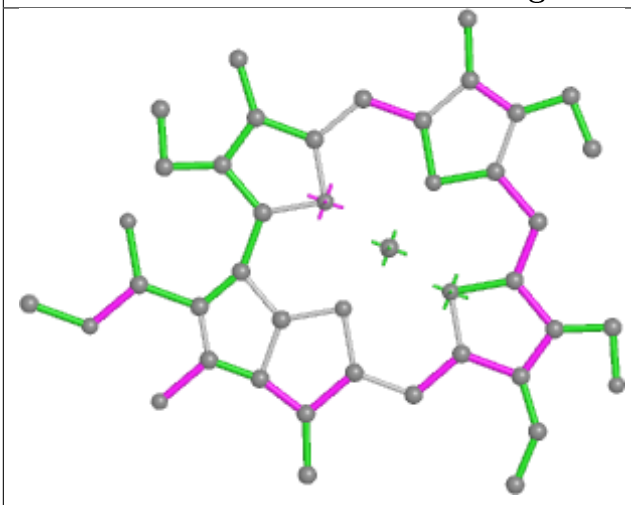


Rings

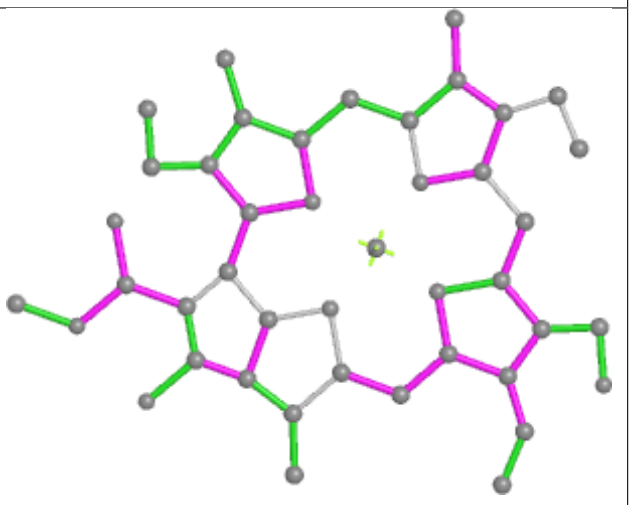
Ligand CLA 2 611	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA B 824	
 Bond lengths	 Bond angles
 Torsions	 Rings

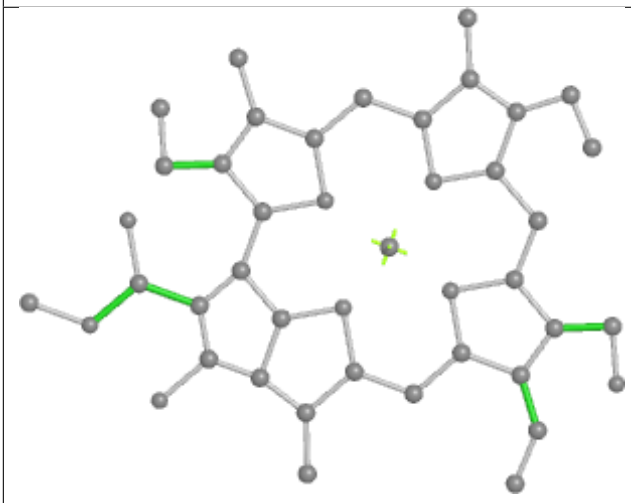
Ligand CHL 2 614



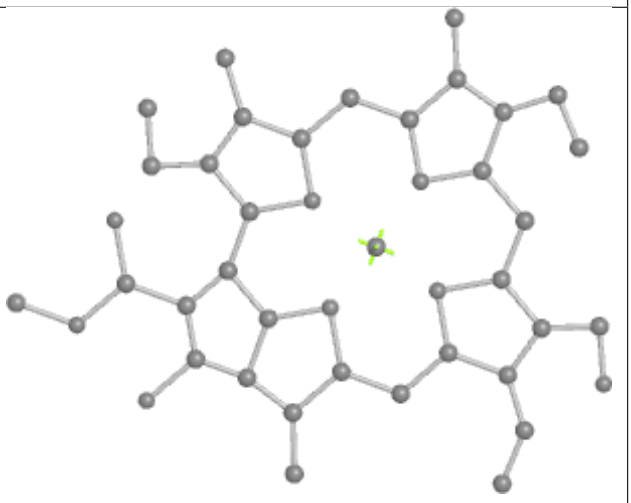
Bond lengths



Bond angles

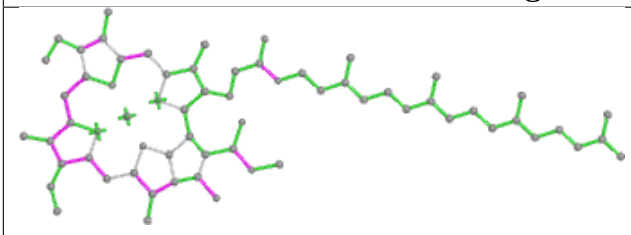


Torsions

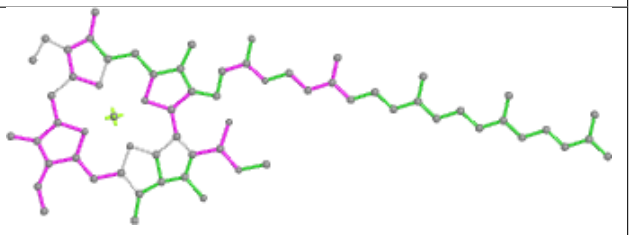


Rings

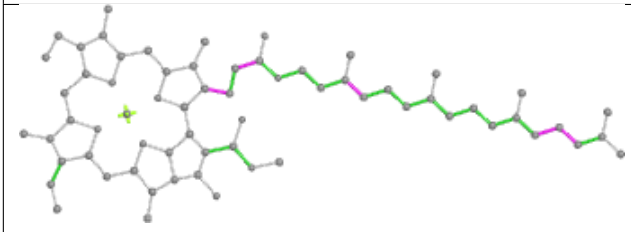
Ligand CLA B 841



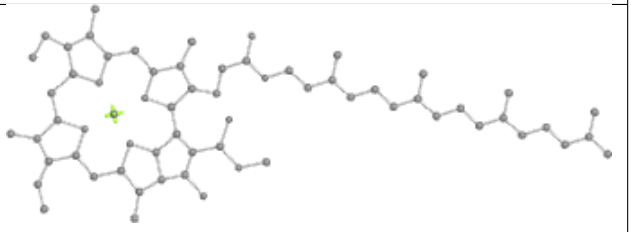
Bond lengths



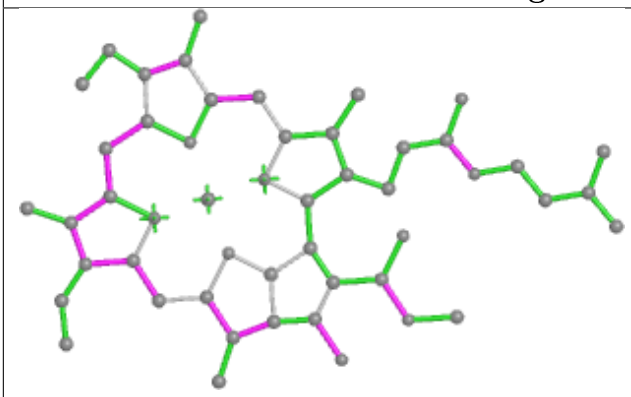
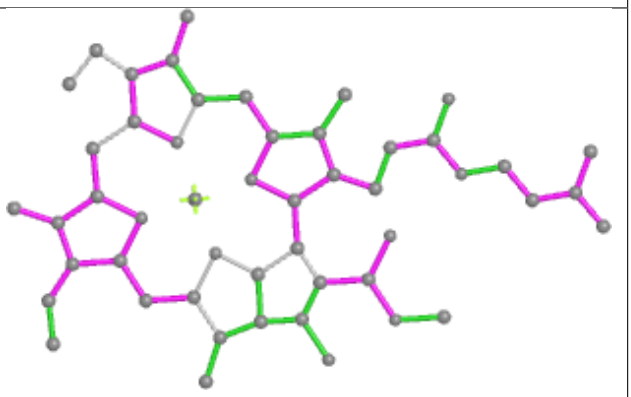
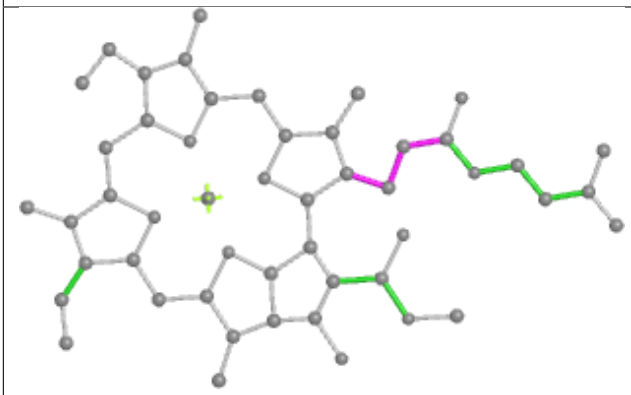
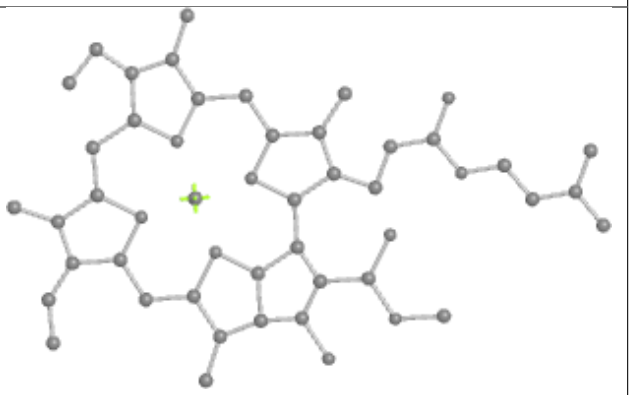
Bond angles

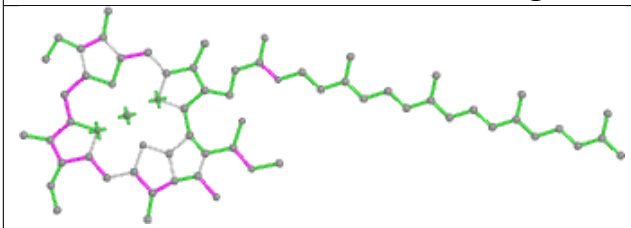
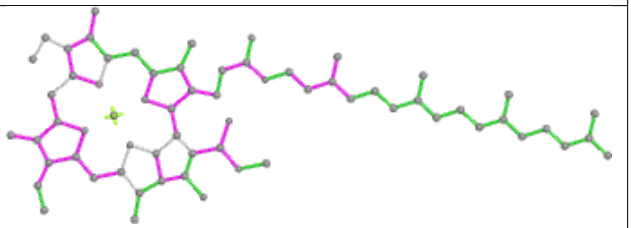
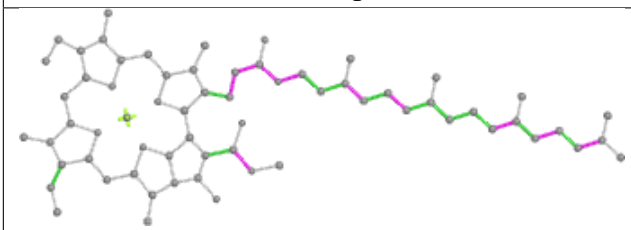
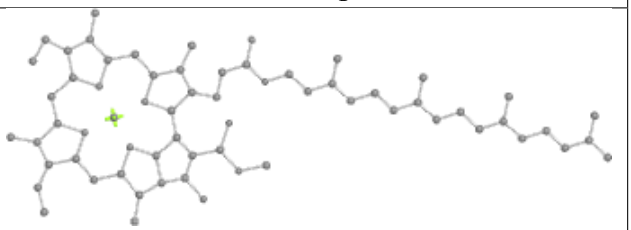


Torsions

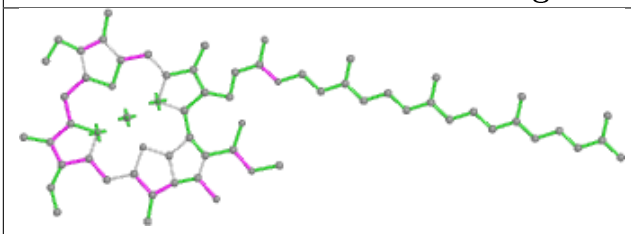


Rings

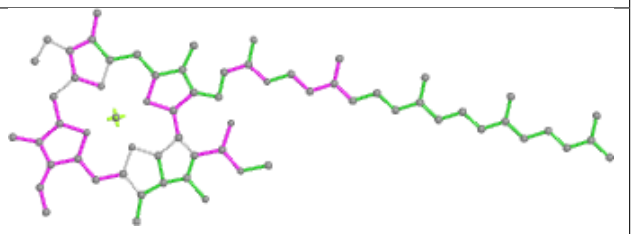
Ligand CLA 3 308	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA b 810	
 Bond lengths	 Bond angles
 Torsions	 Rings

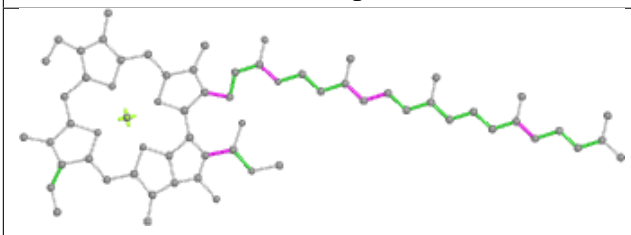
Ligand CLA l 202



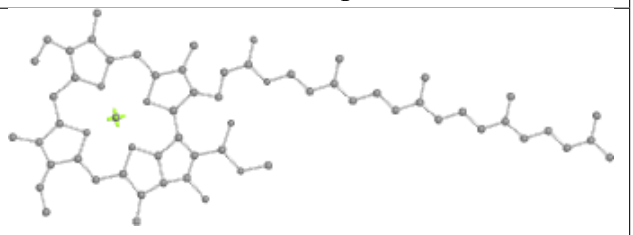
Bond lengths



Bond angles



Torsions



Rings

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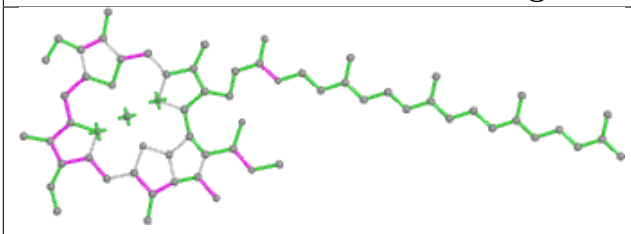

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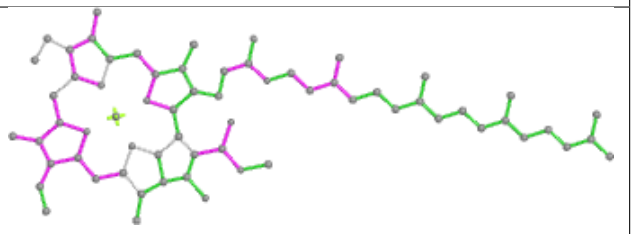

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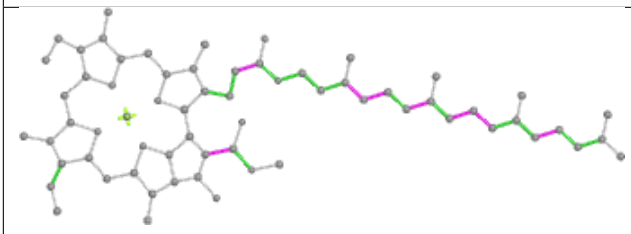

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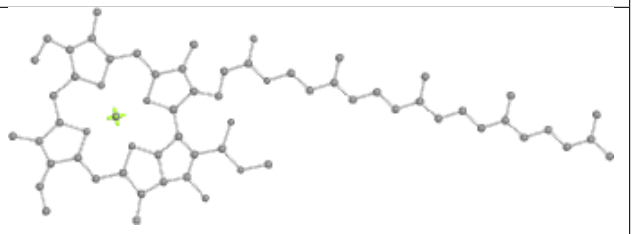

Rings

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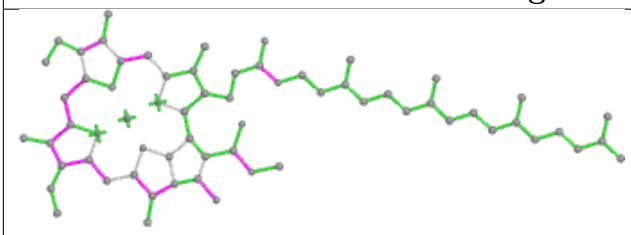

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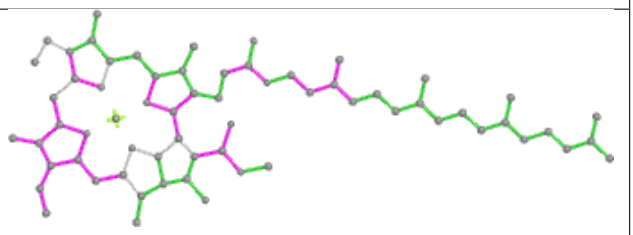

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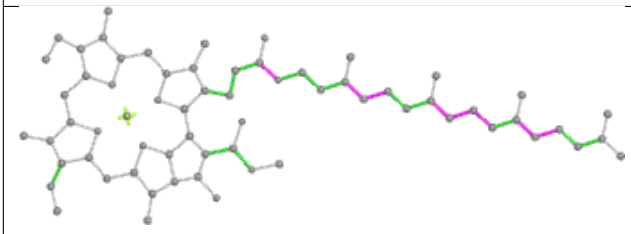

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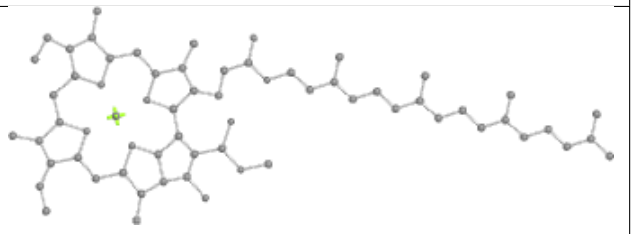
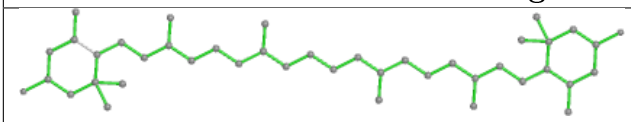


Rings

Ligand LUT 1 320



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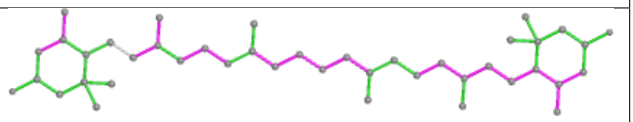

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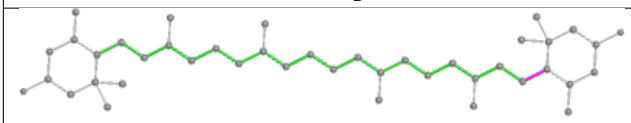

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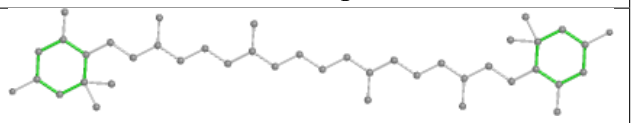
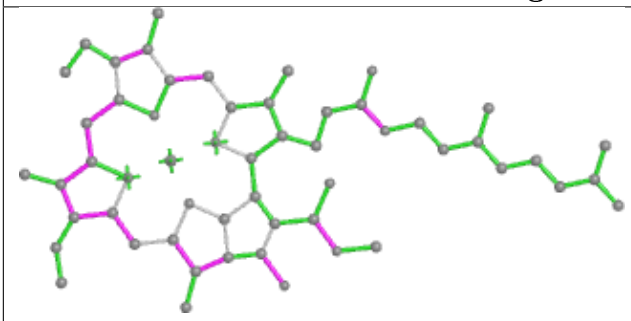


Rings

Ligand CLA b 822



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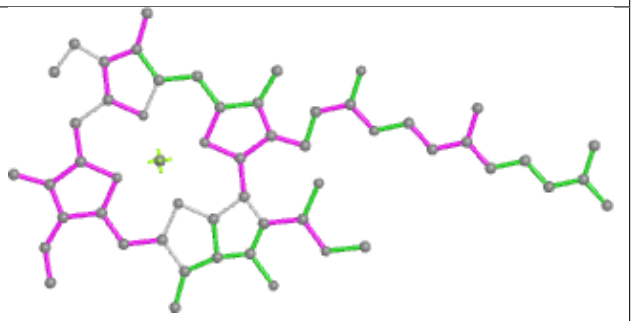

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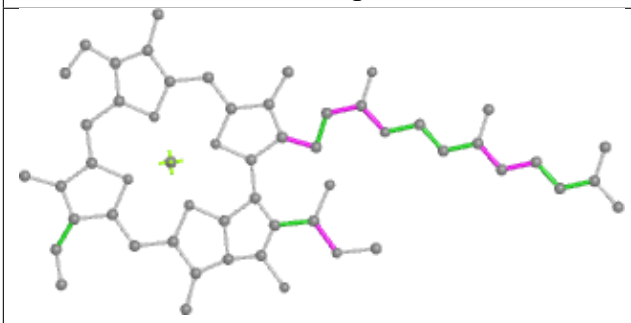

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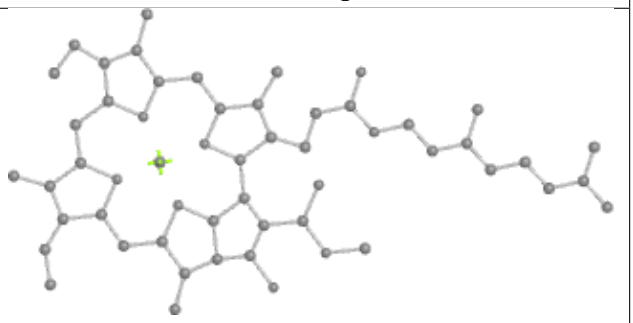

Rings

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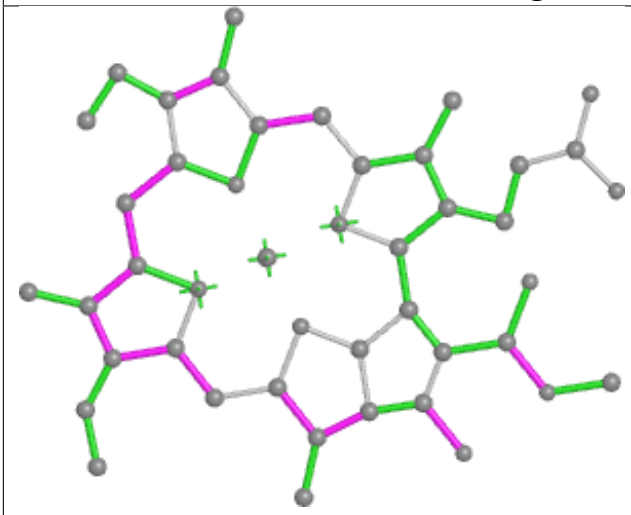

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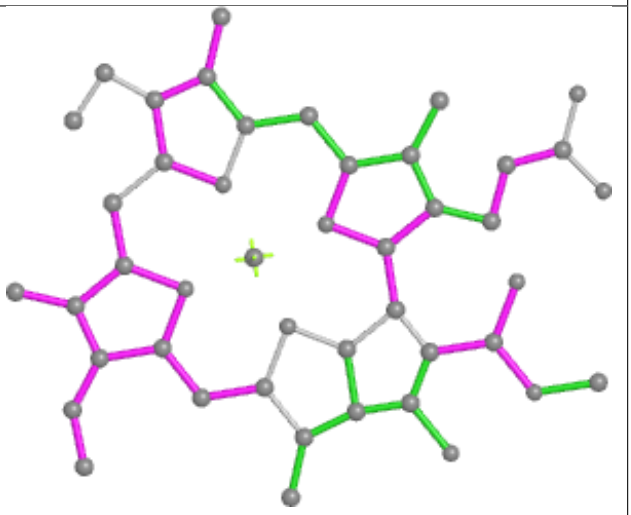

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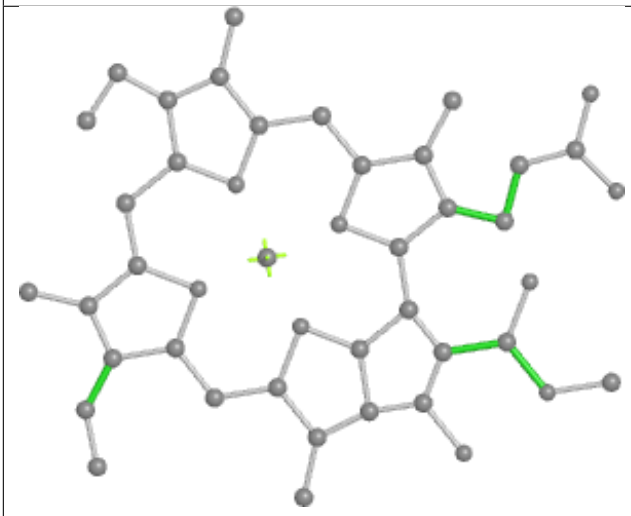

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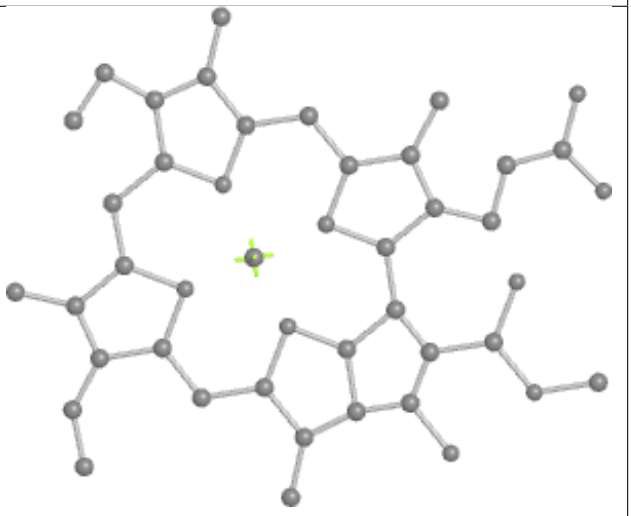
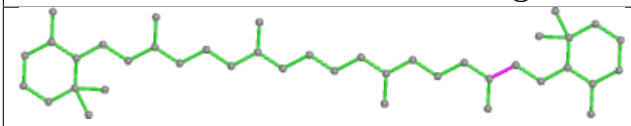


Rings

Ligand BCR K 4004



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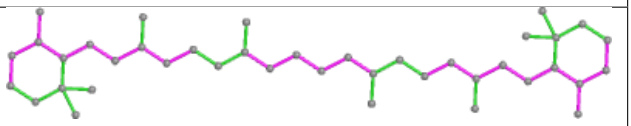

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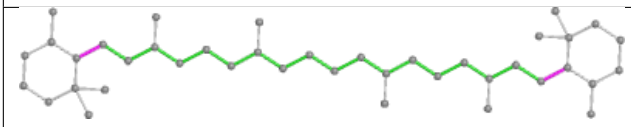
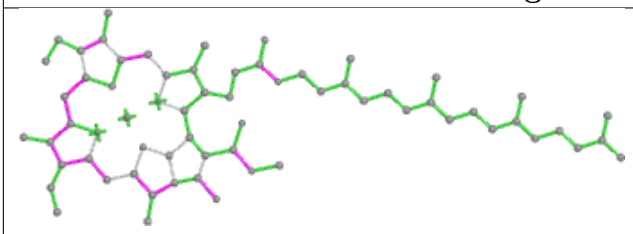


Torsions

Rings

Ligand CLA A 814



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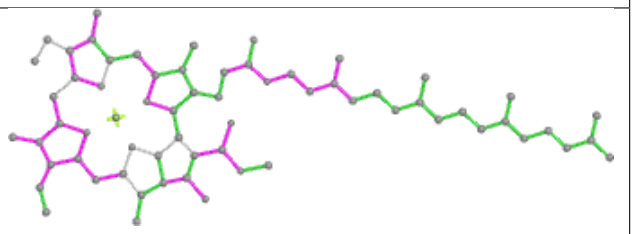

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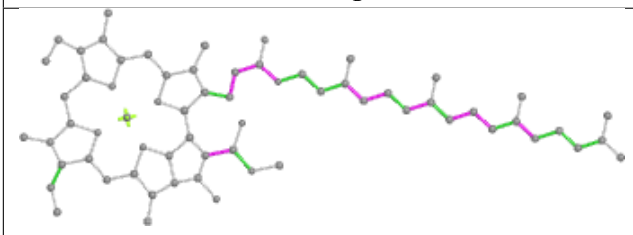

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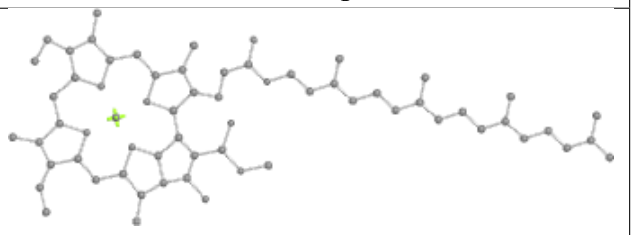
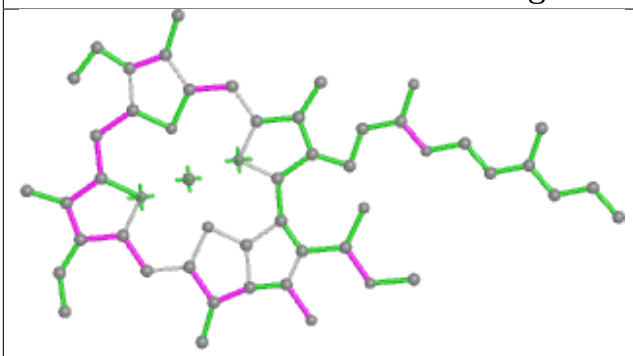


Rings

Ligand CLA 1 312



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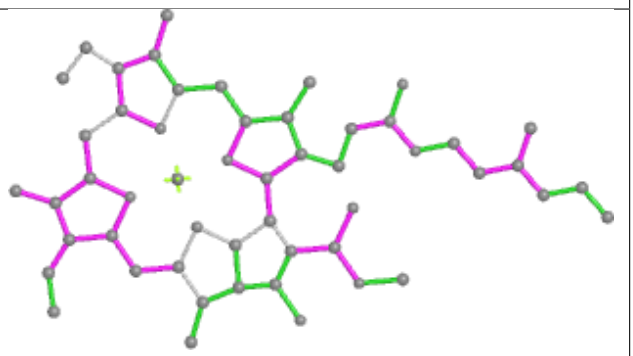

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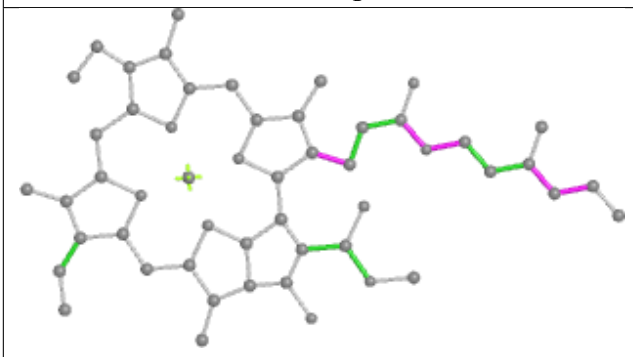

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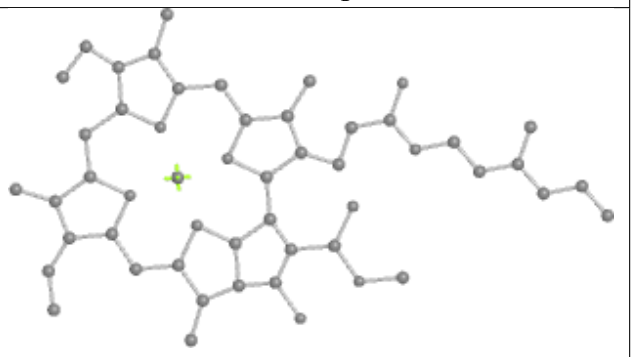
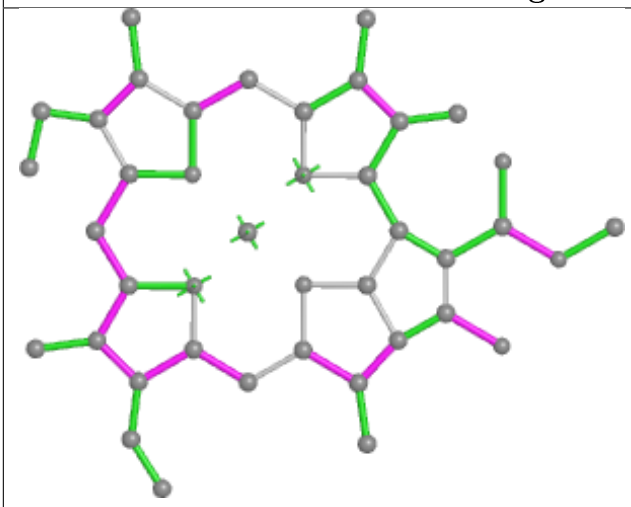


Rings

Ligand CLA 7 610



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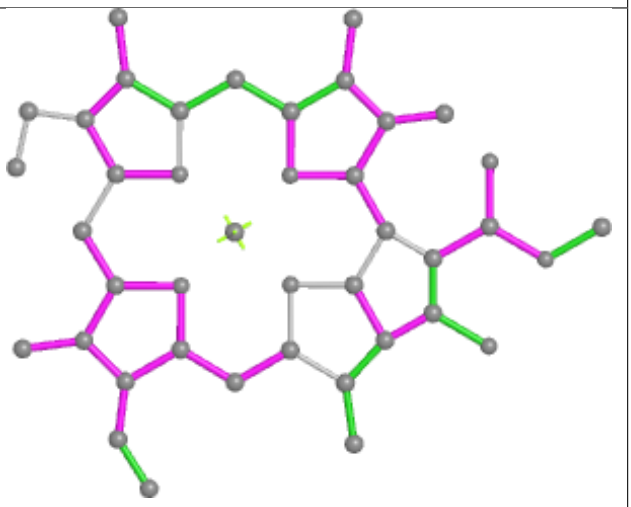

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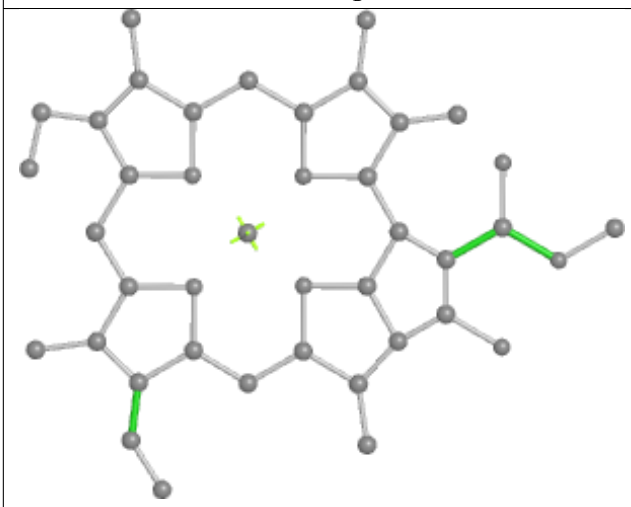

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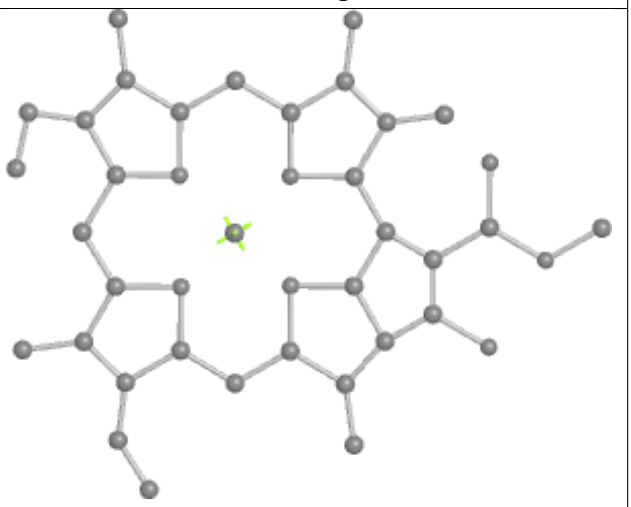
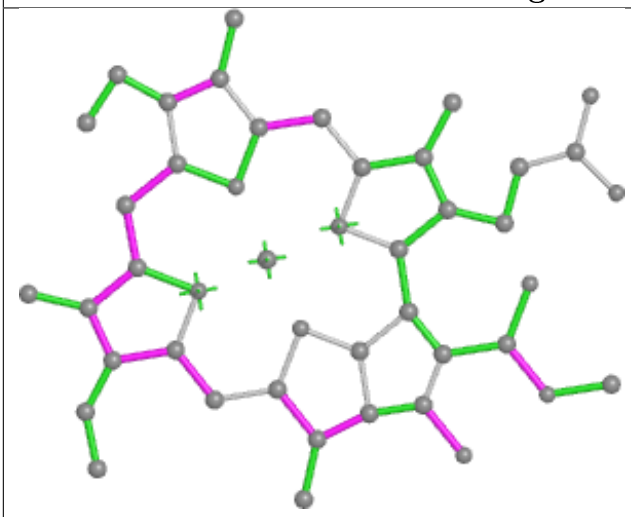


Rings

Ligand CLA a 837



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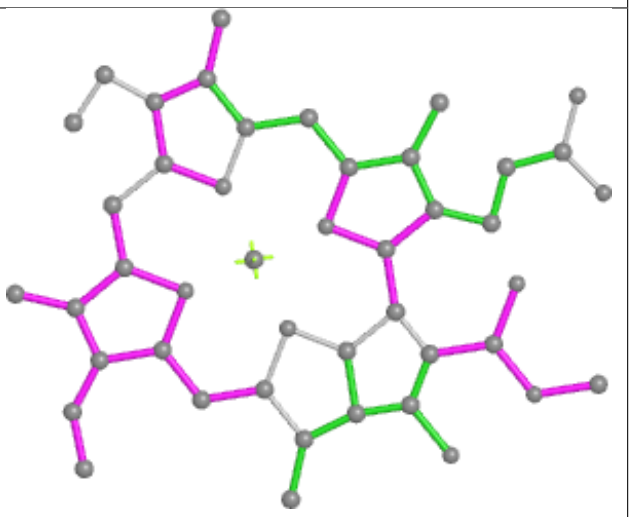

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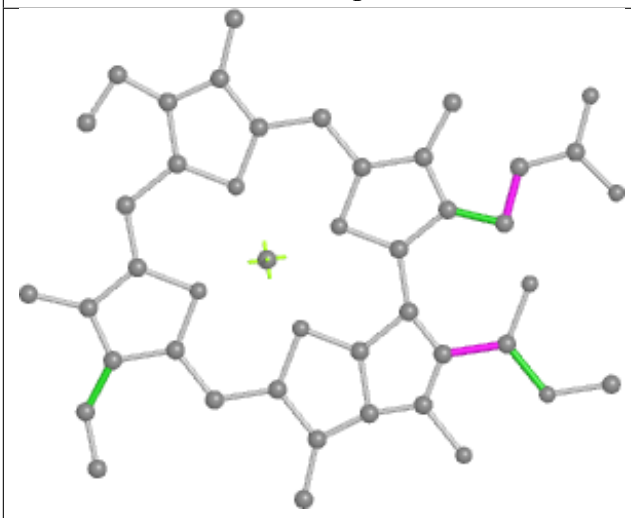

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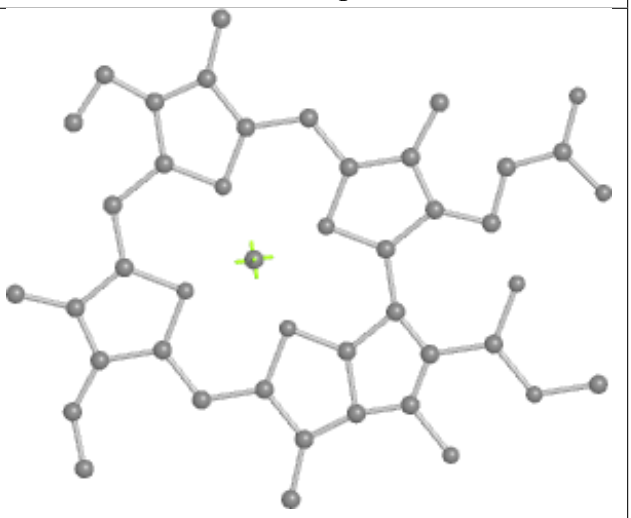
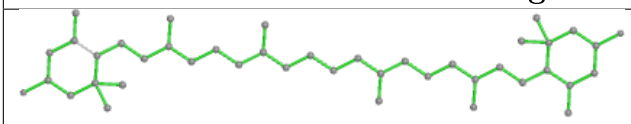


Rings

Ligand LUT 9 616



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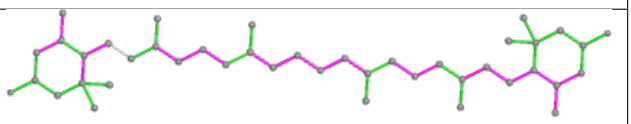

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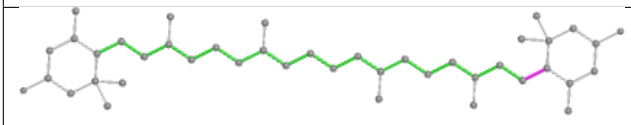
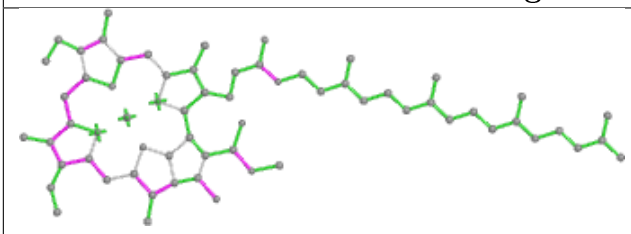


Torsions

Rings

Ligand CLA A 834



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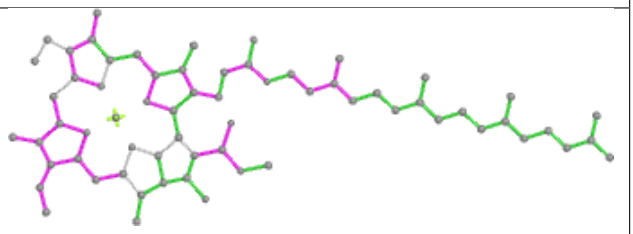

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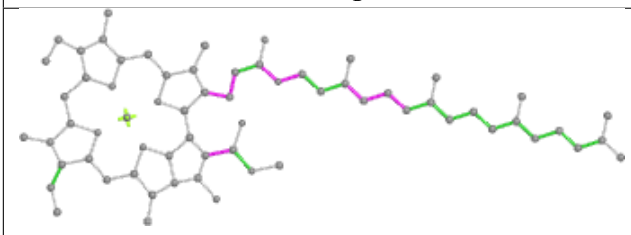

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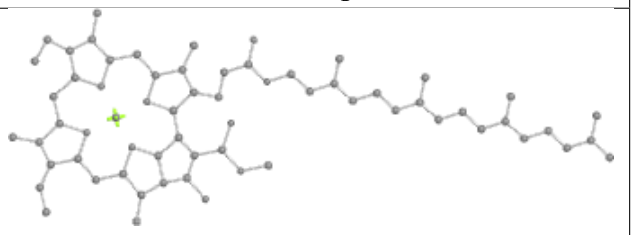
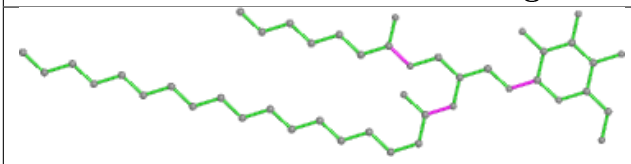


Rings

Ligand LMG 4 620



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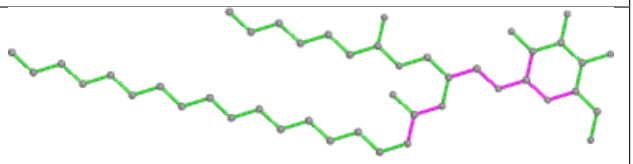
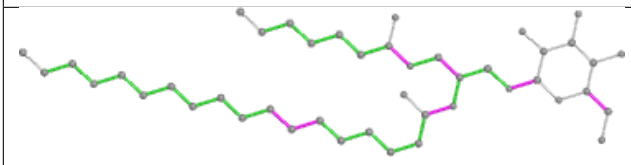


Bond angles



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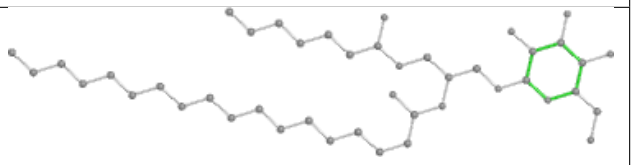
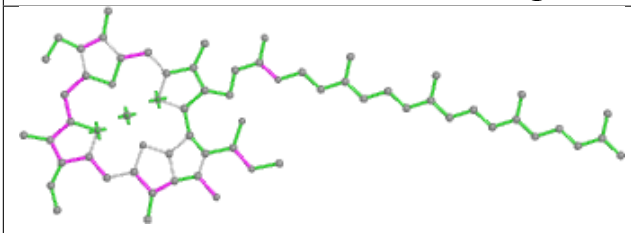


Rings

Ligand CLA a 811



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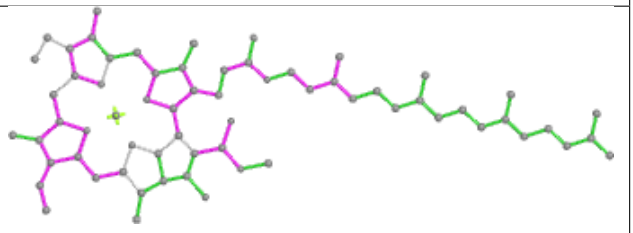

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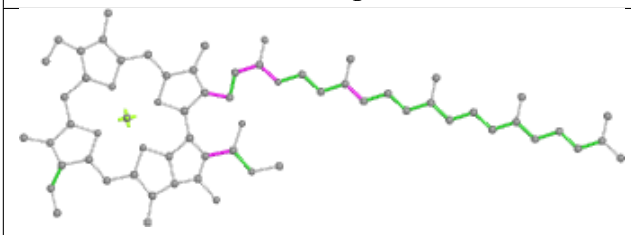
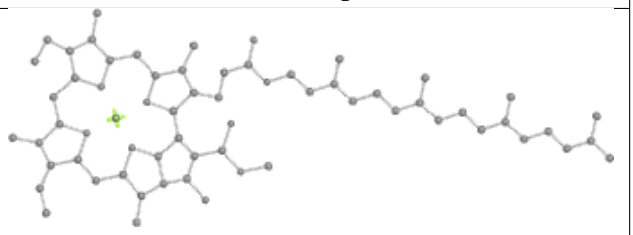
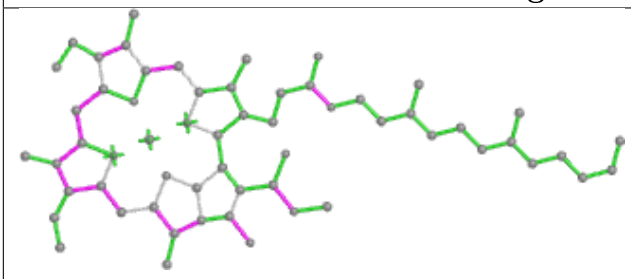


Torsions

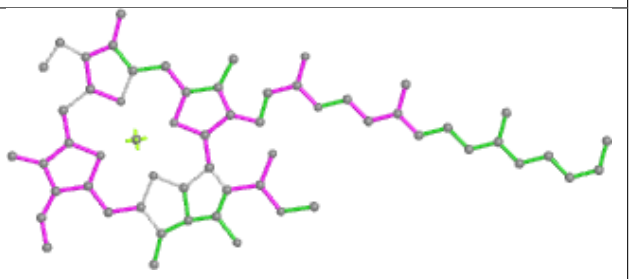


Rings

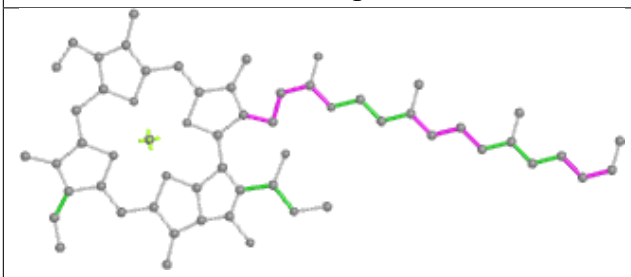
Ligand CLA b 817



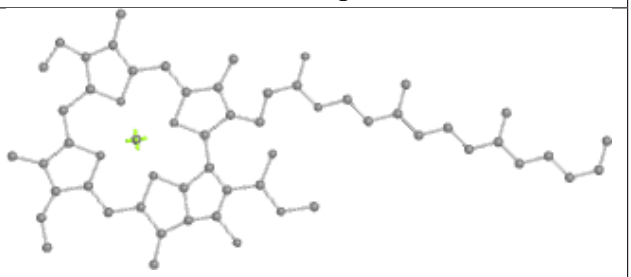
Bond lengths



Bond angles

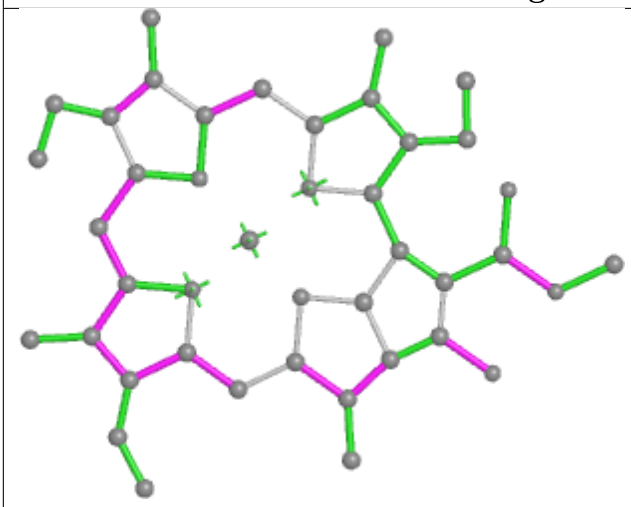


Torsions

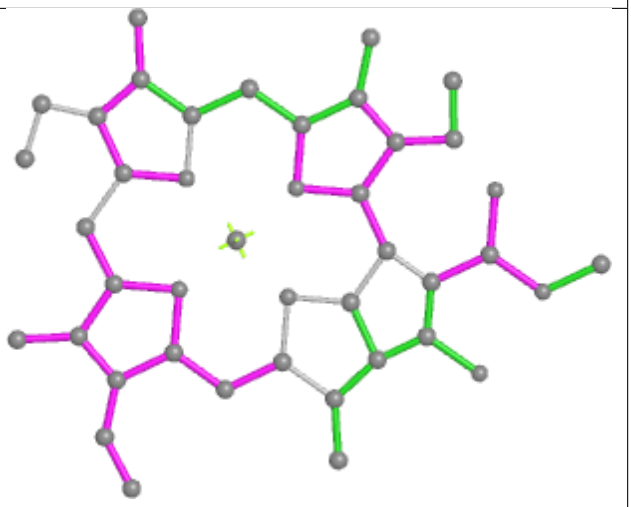


Rings

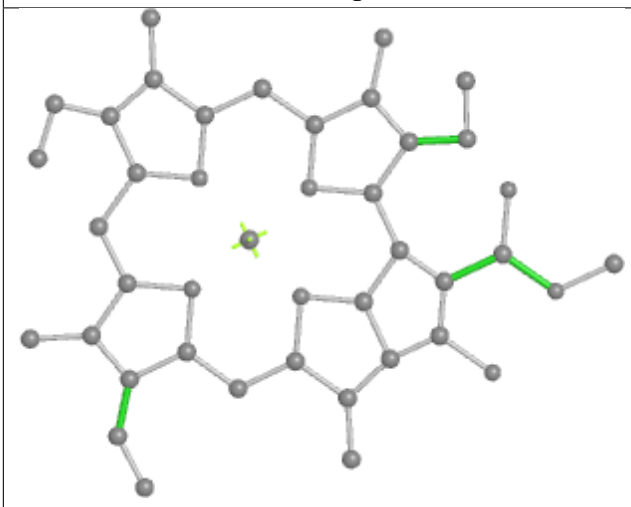
Ligand CLA 8 304



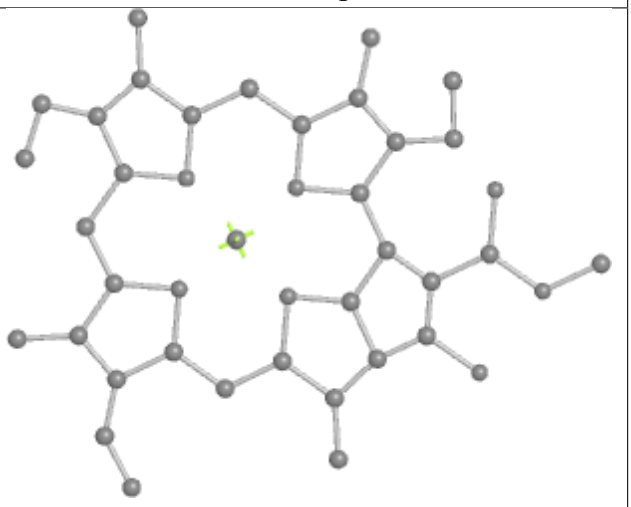
Bond lengths



Bond angles

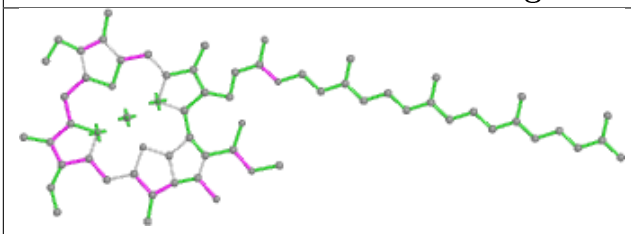


Torsions

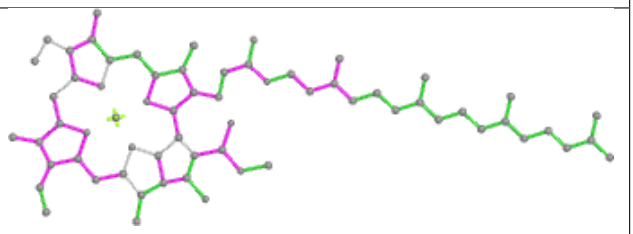


Rings

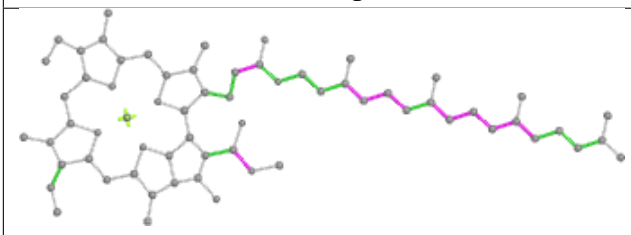
Ligand CLA B 806



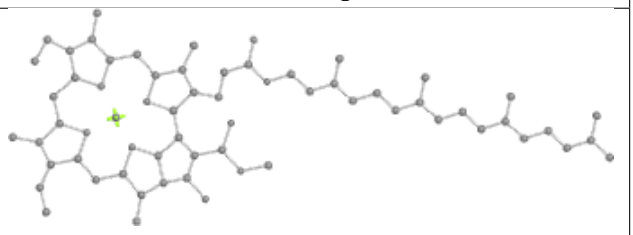
Bond lengths



Bond angles

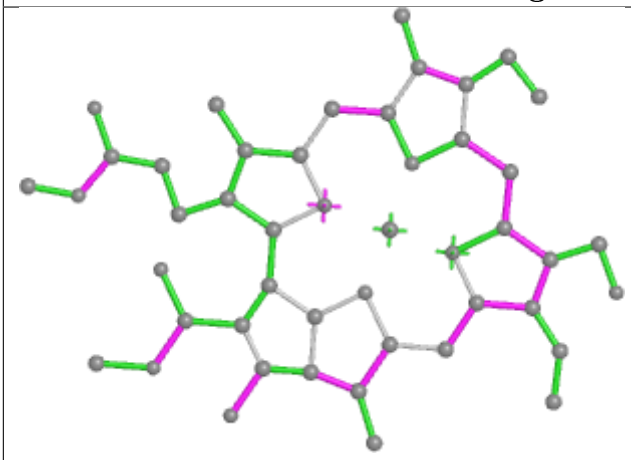


Torsions



Rings

Ligand CHL 6 308



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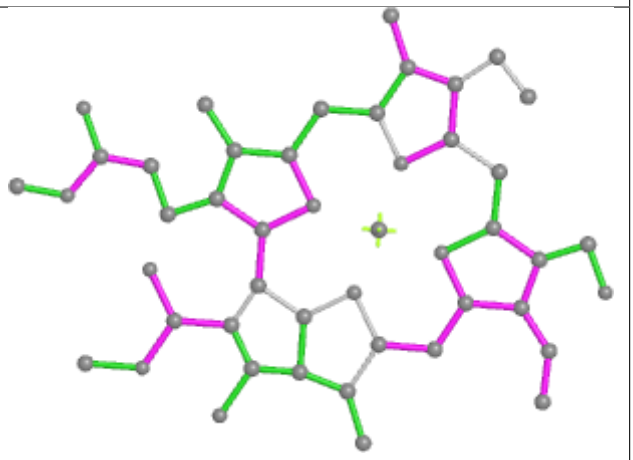
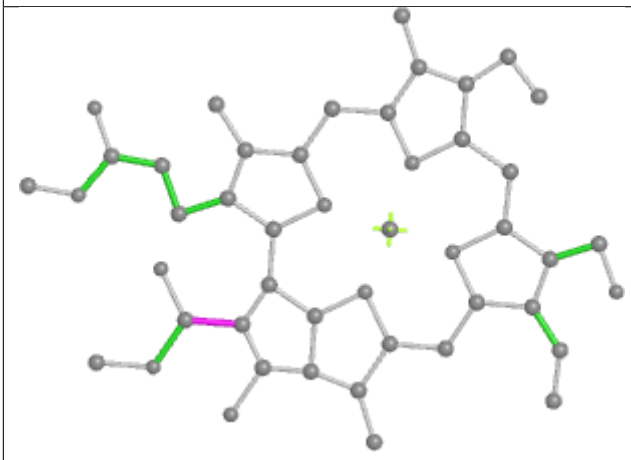
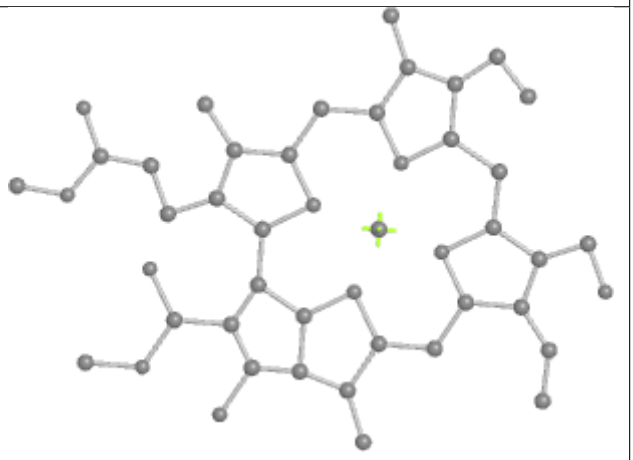


Bond angles

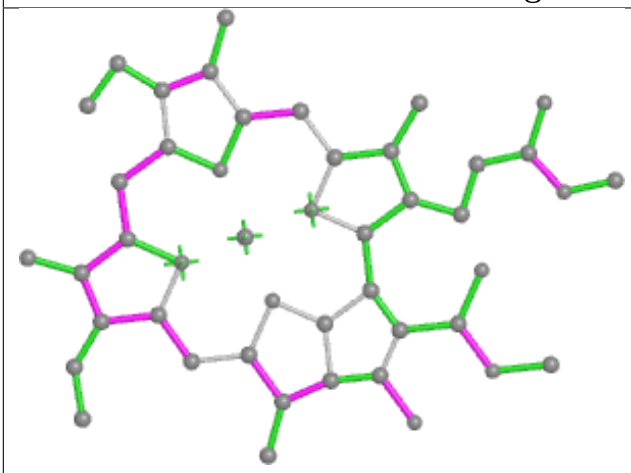


Torsions

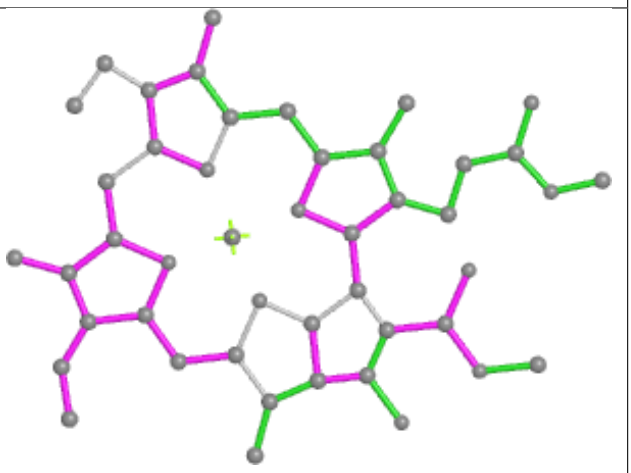


Rings

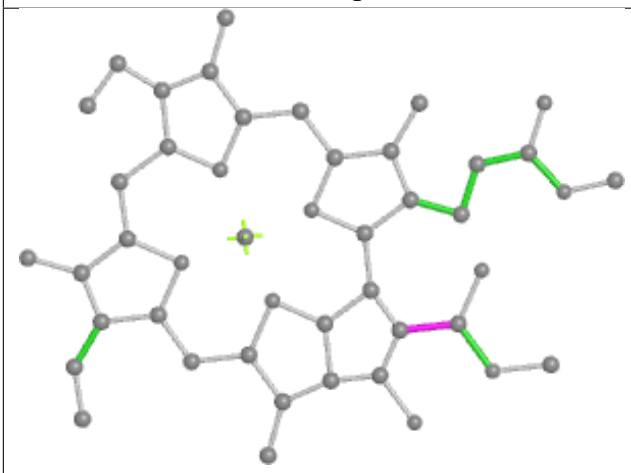
Ligand CLA B 821



Bond lengths



Bond angles



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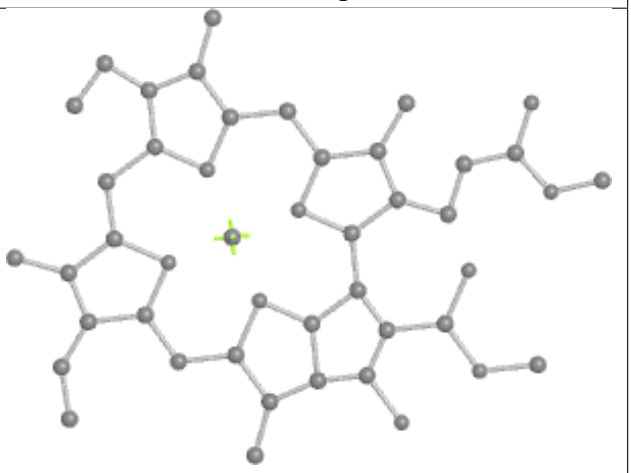
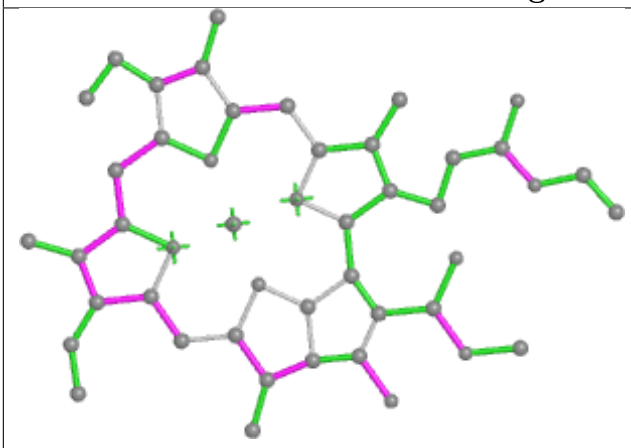


Rings

Ligand CLA 8 305



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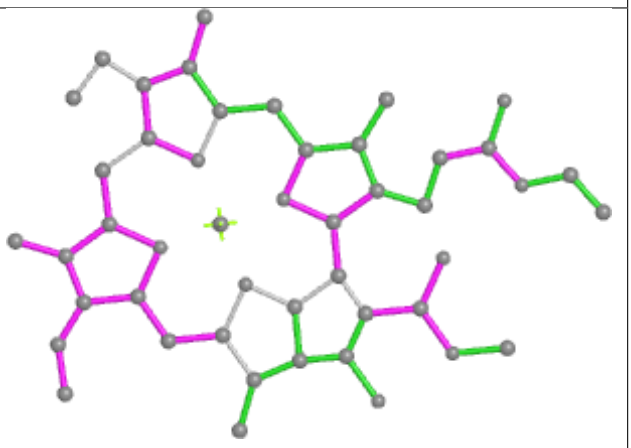
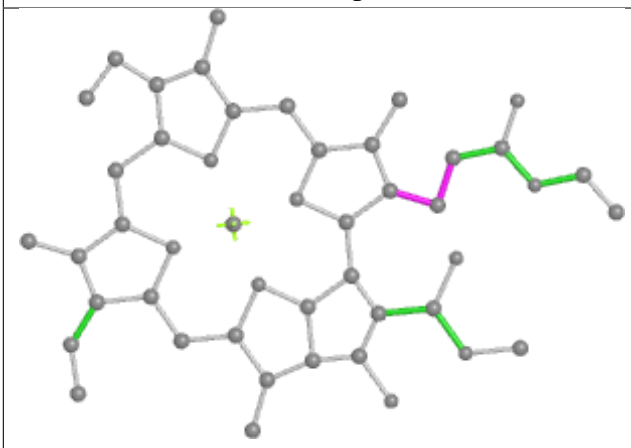


Bond angles



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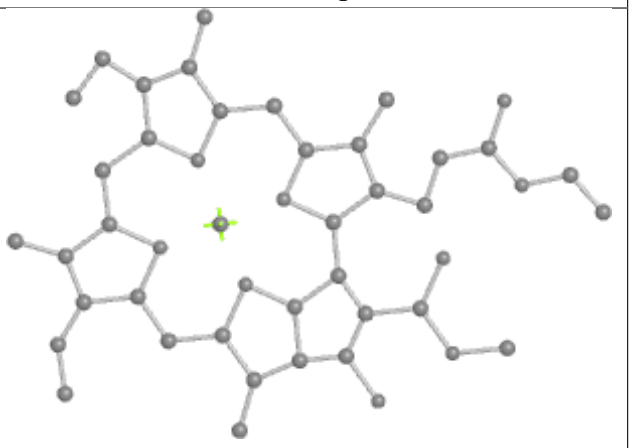
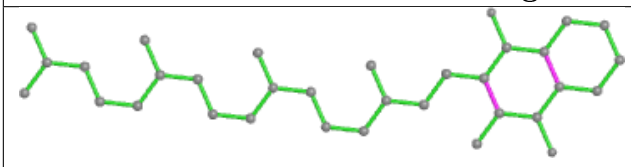


Rings

Ligand PQN A 844



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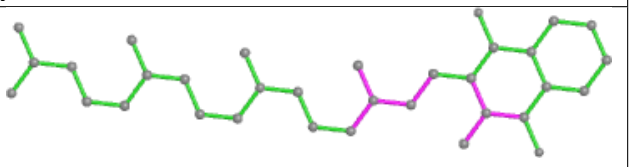
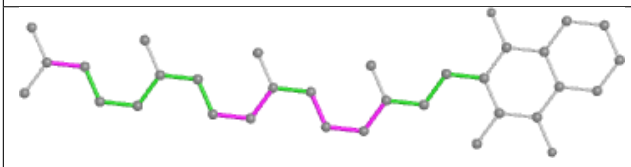


Bond angles



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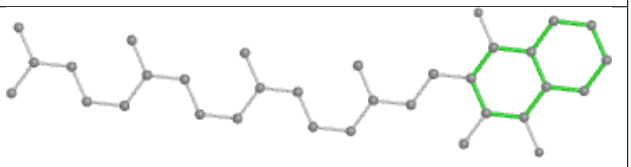
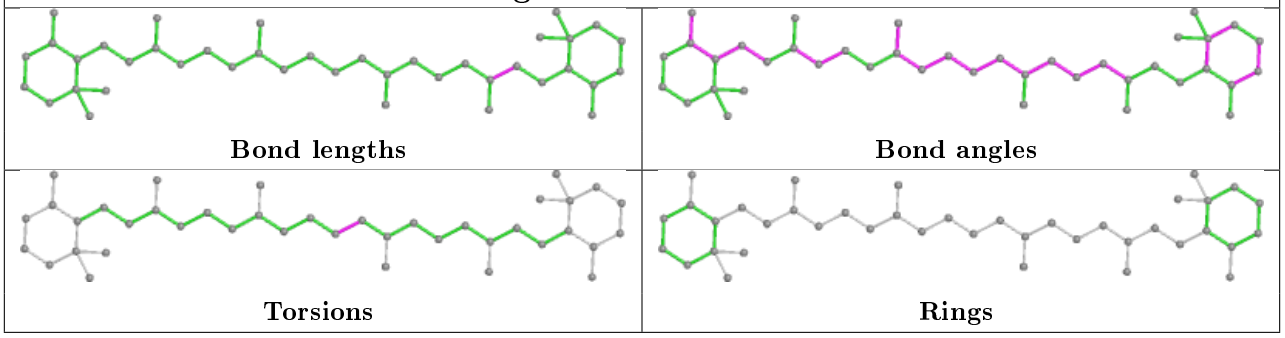
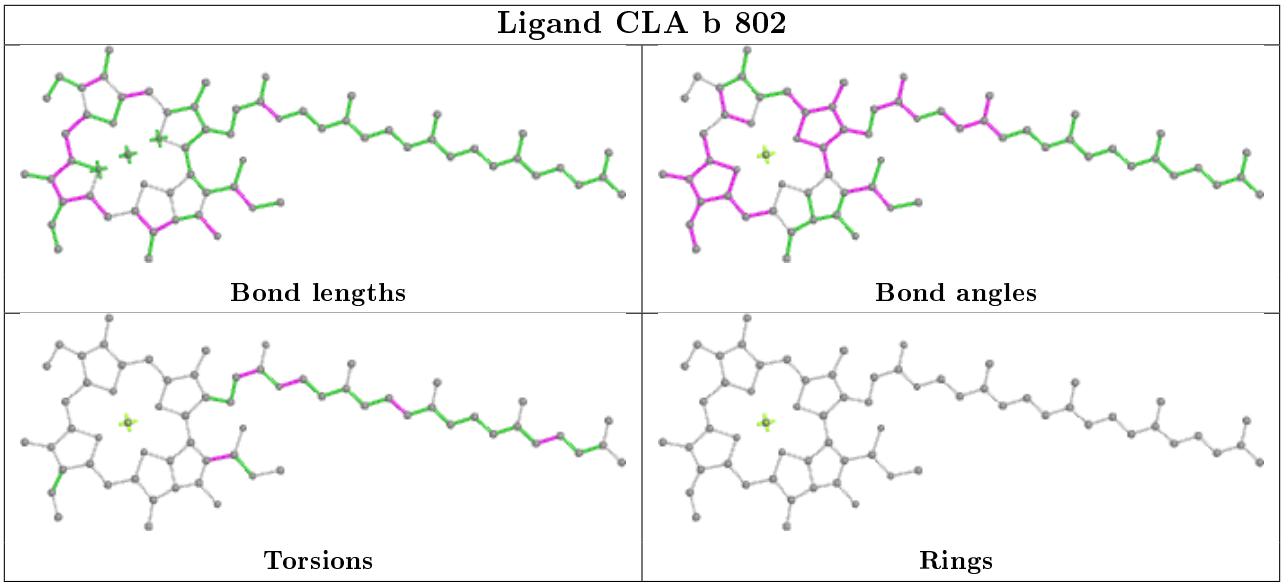


Rings

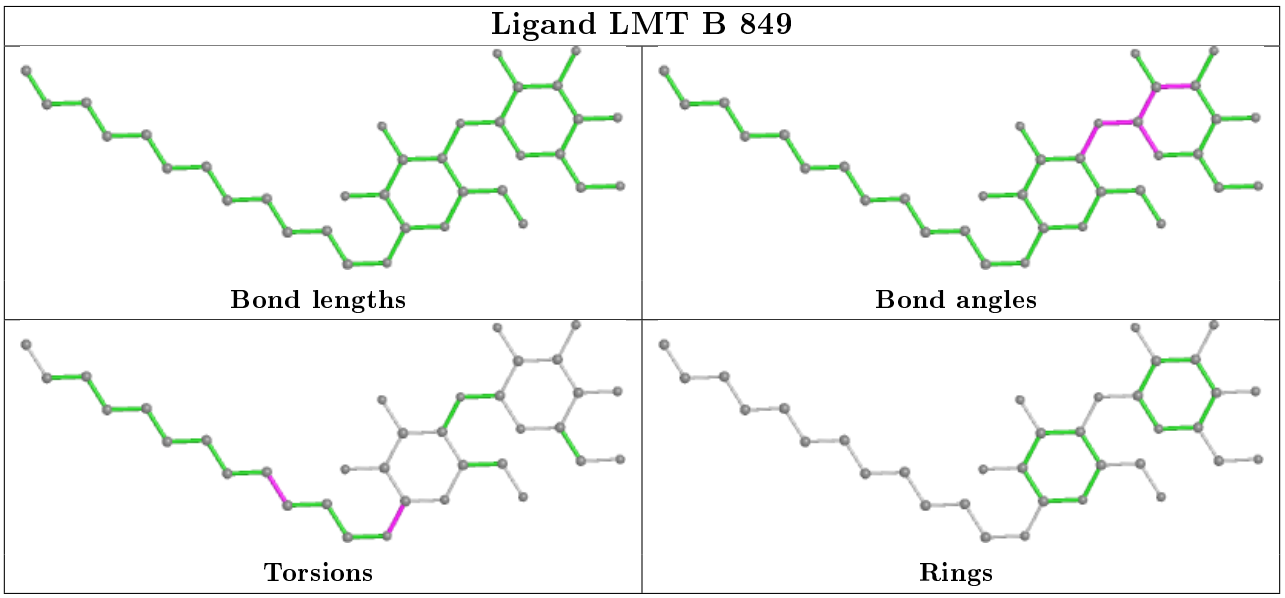
Ligand BCR K 4001



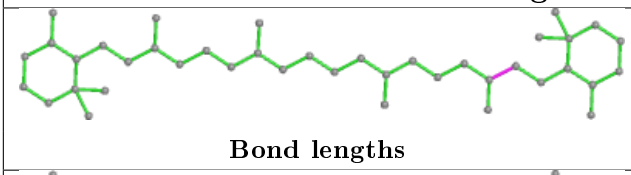
Ligand CLA b 802

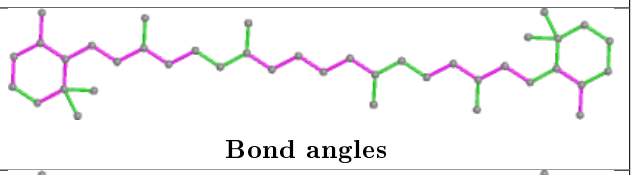


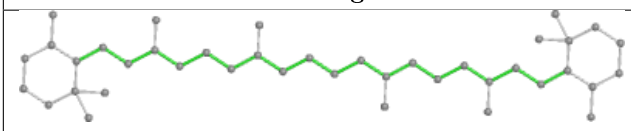
Ligand LMT B 849

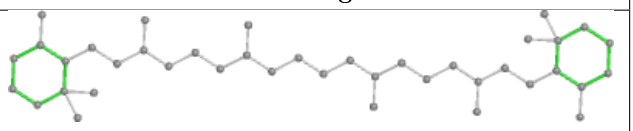


Ligand BCR l 206

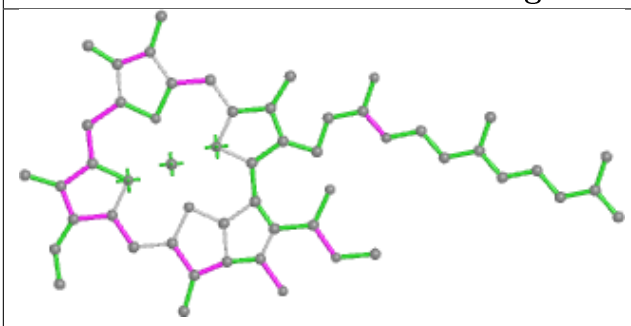

Bond lengths

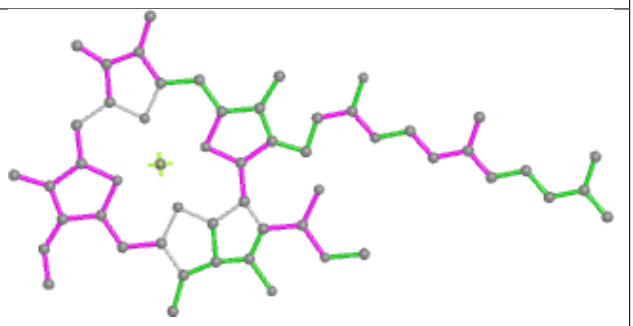

Bond angles

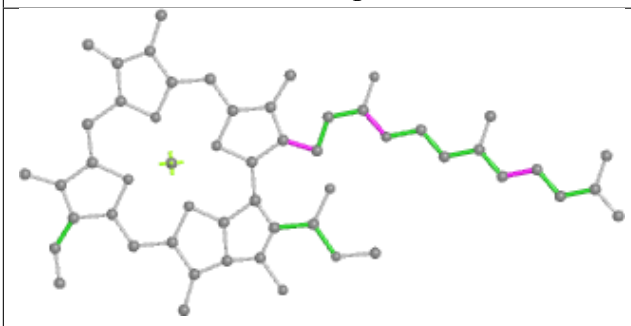

Torsions


Rings

Ligand CLA B 811


Bond lengths


Bond angles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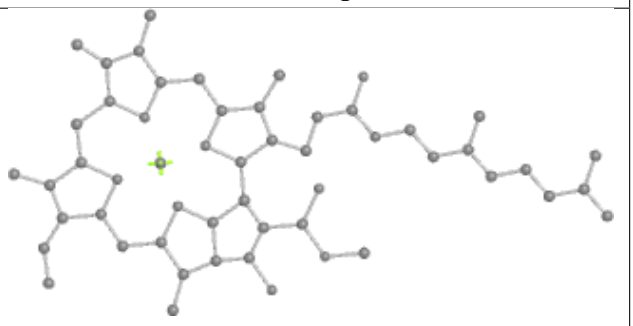
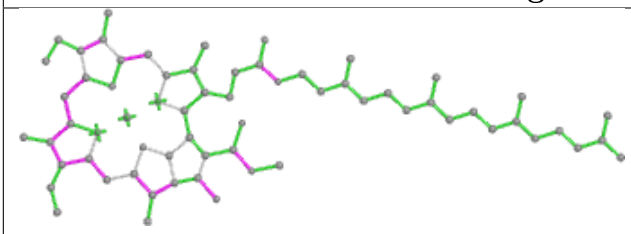
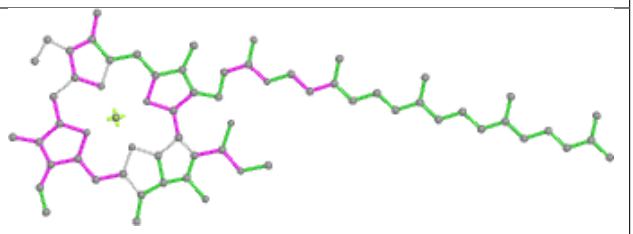
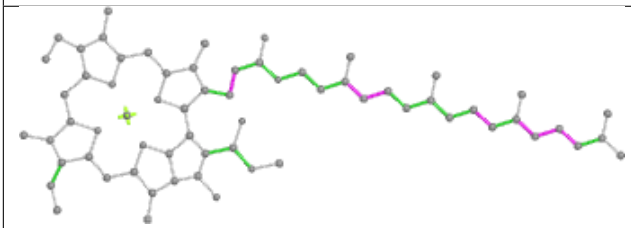

Rings

Ligand CLA b 839


Bond lengths


Bond angles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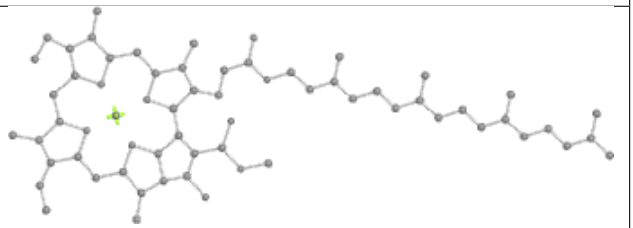
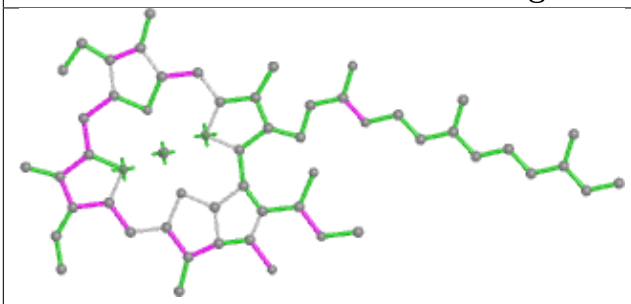
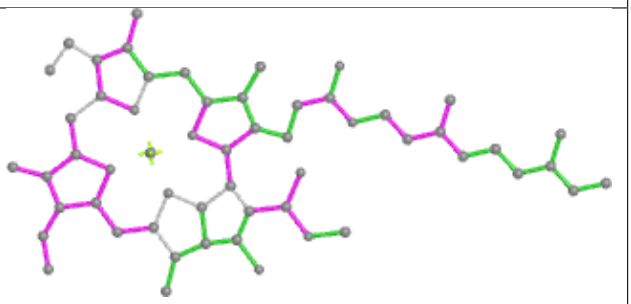

Rings

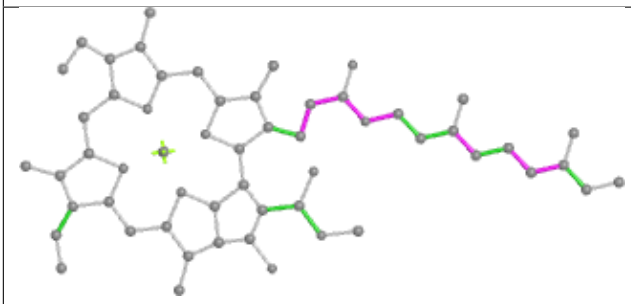
Ligand CLA 9 612



Bond lengths



Bond angles



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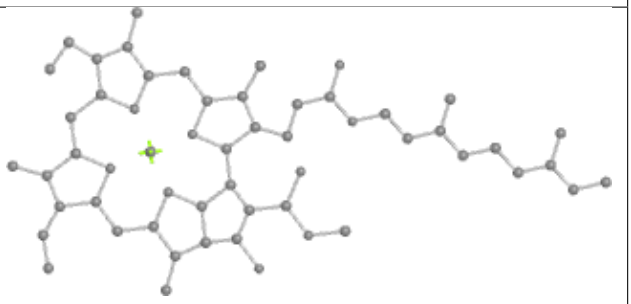
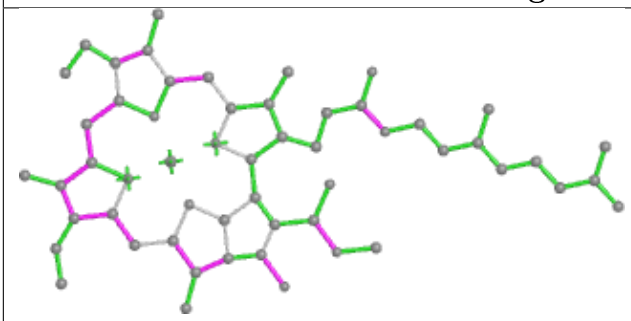
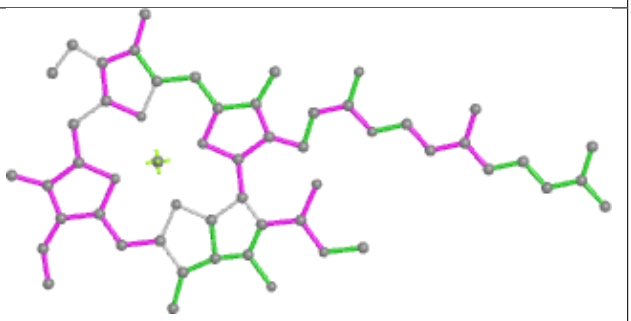


Rings

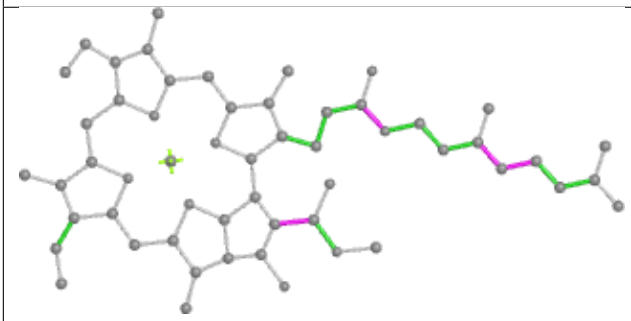
Ligand CLA 6 315



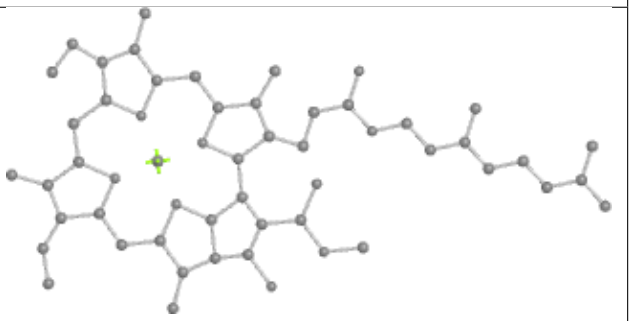
Bond lengths



Bond angles

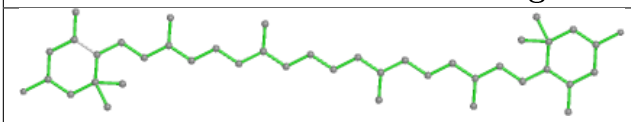


Torsions

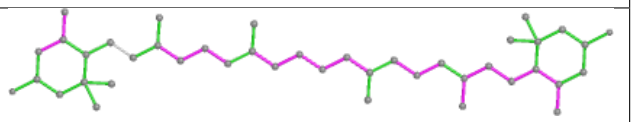


Rings

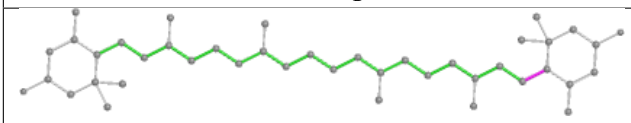
Ligand LUT 8 314



Bond lengths



Bond angles



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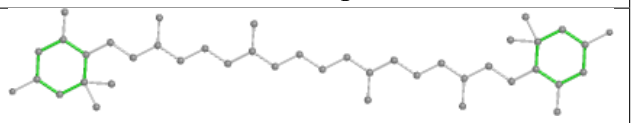
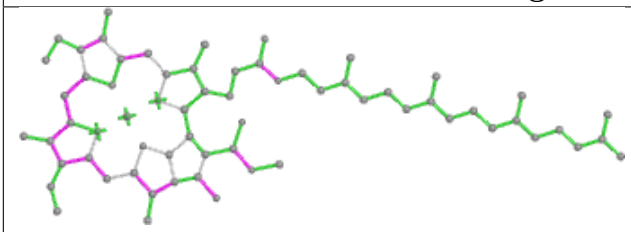
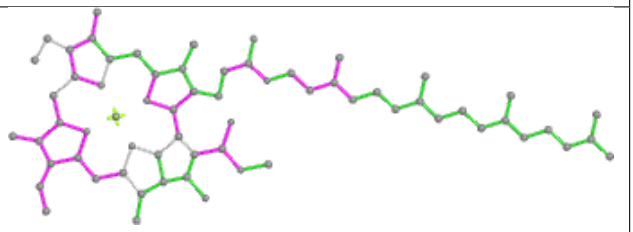


Rings

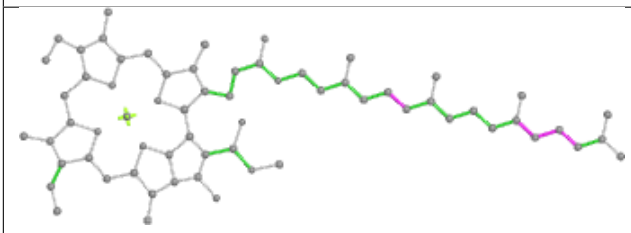
Ligand CLA 1 308



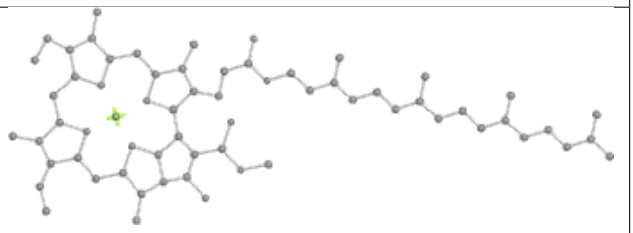
Bond lengths



Bond angles

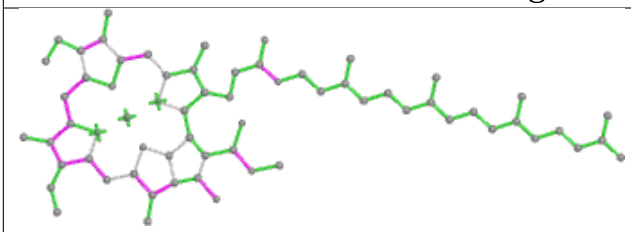


Torsions

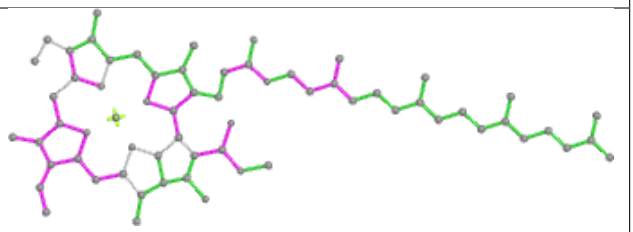


Rings

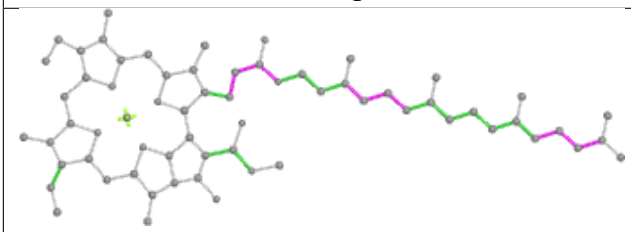
Ligand CLA a 844



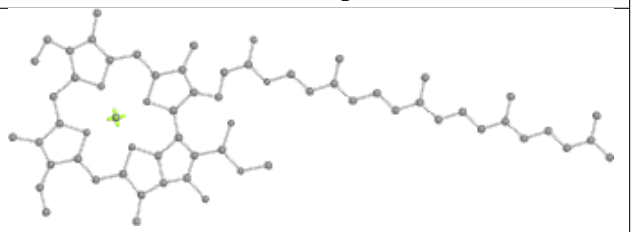
Bond lengths



Bond angles

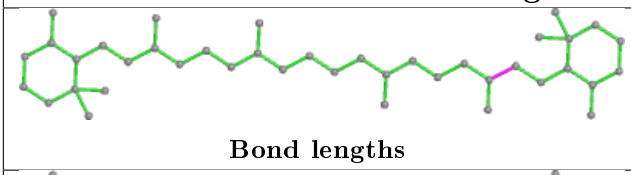


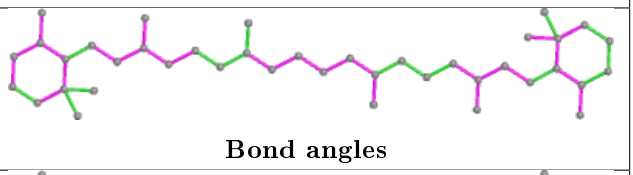
Torsions

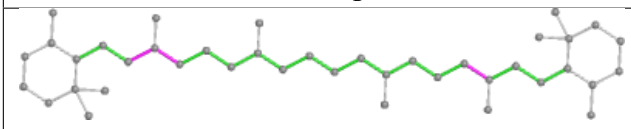


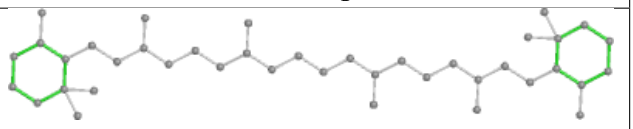
Rings

Ligand BCR B 845

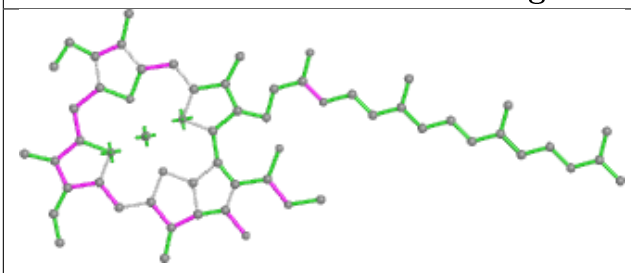

Bond lengths

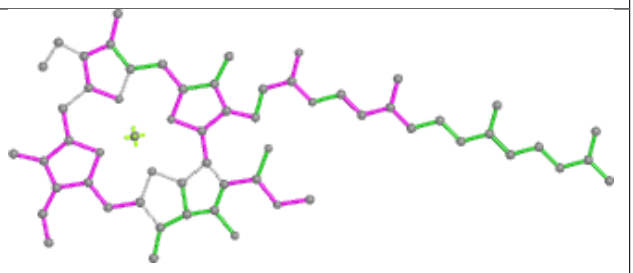

Bond angles

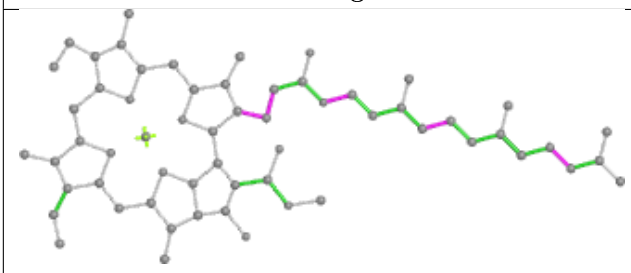

Torsions

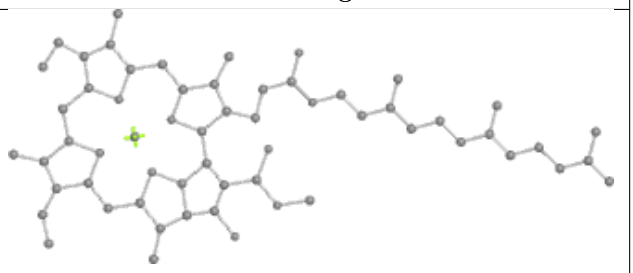

Rings

Ligand CLA 4 609

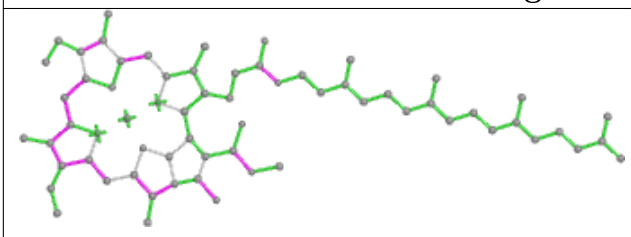

Bond lengths

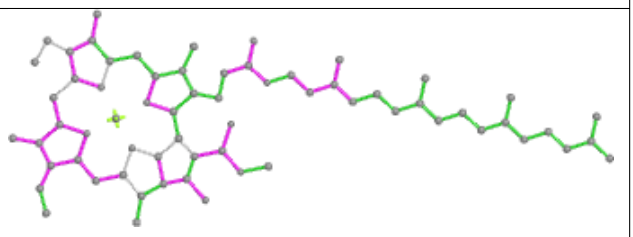

Bond angles

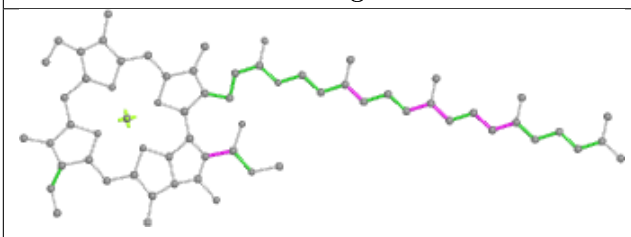

Torsions


Rings

Ligand CLA B 826


Bond lengths


Bond angles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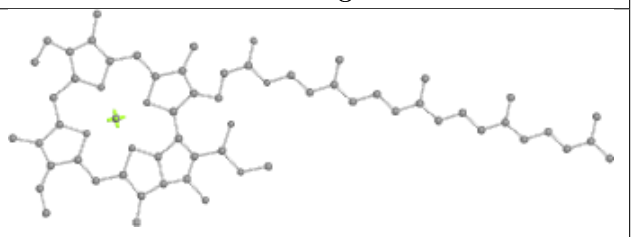
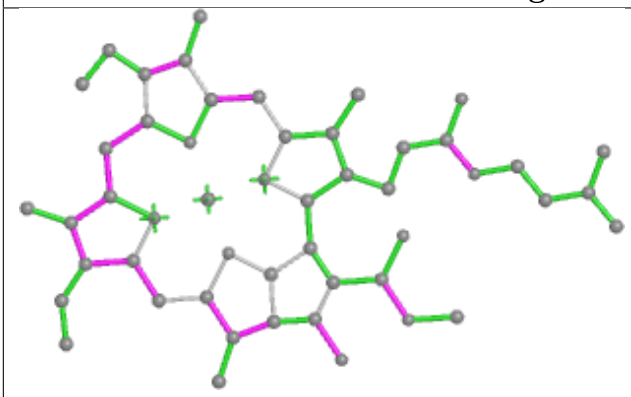
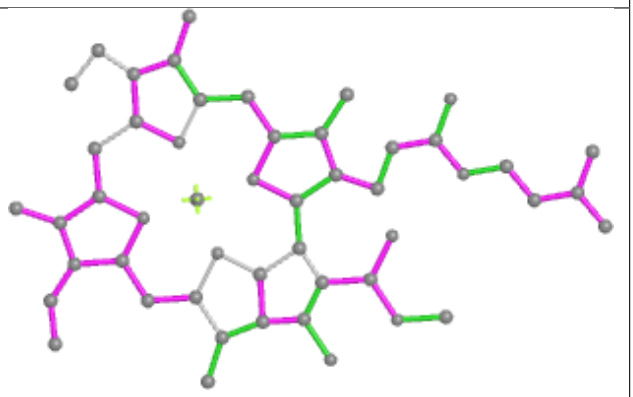

Rings

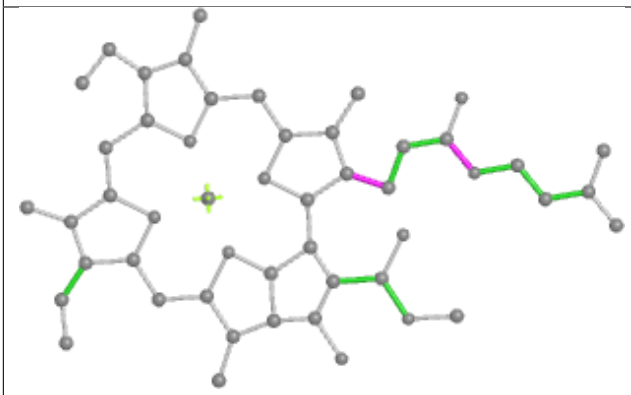
Ligand CLA 9 608



Bond lengths



Bond angles



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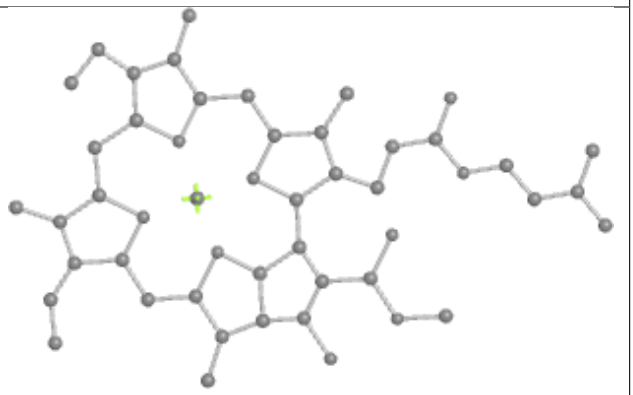
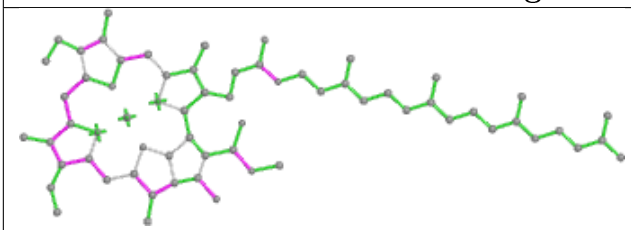
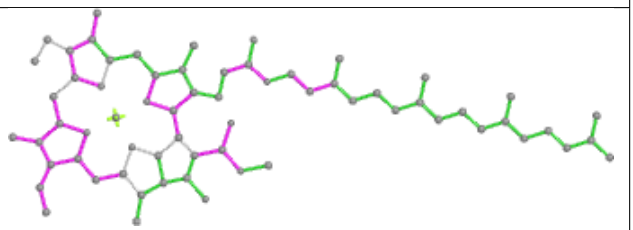


Rings

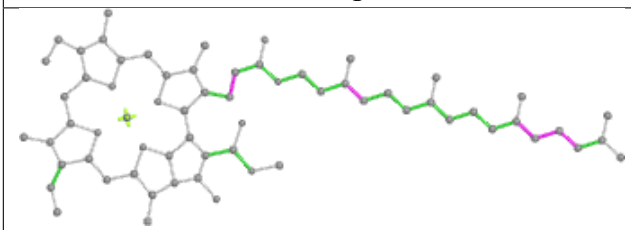
Ligand CLA B 839



Bond lengths



Bond angles



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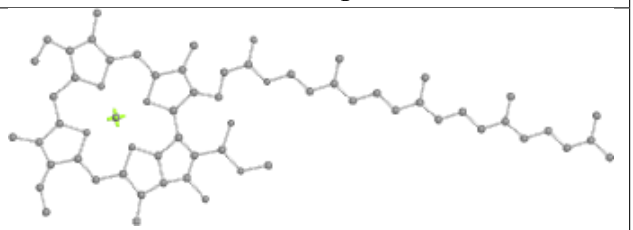
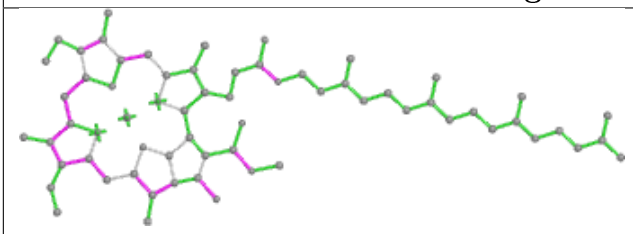
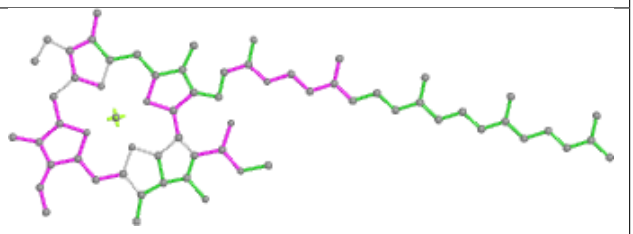


Rings

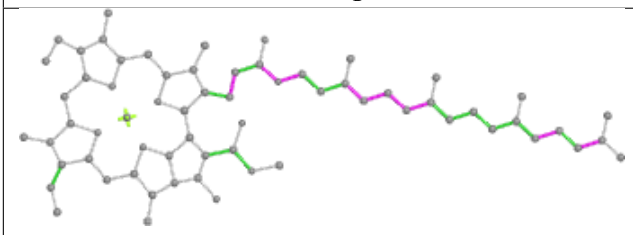
Ligand CLA A 842



Bond lengths



Bond angles



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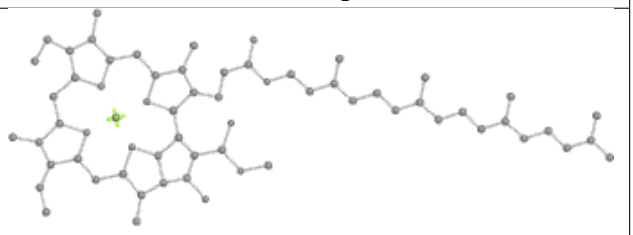
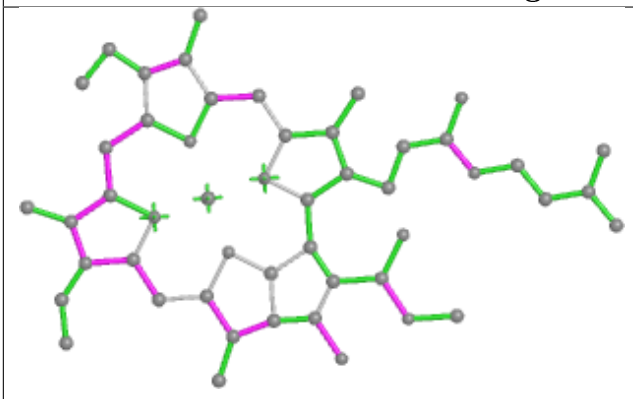


Rings

Ligand CLA B 820



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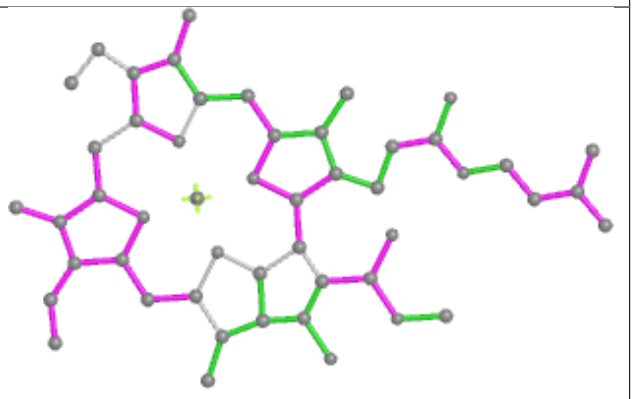
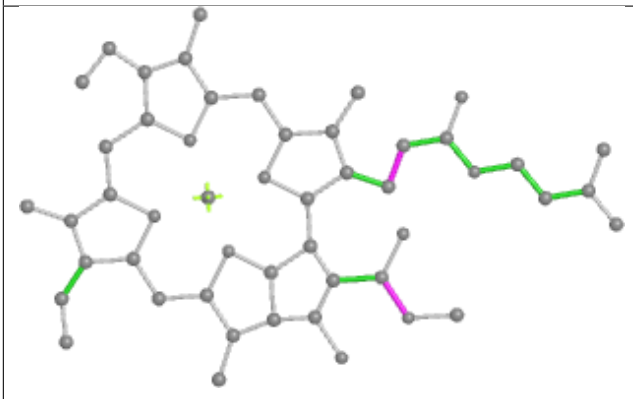


Bond angles



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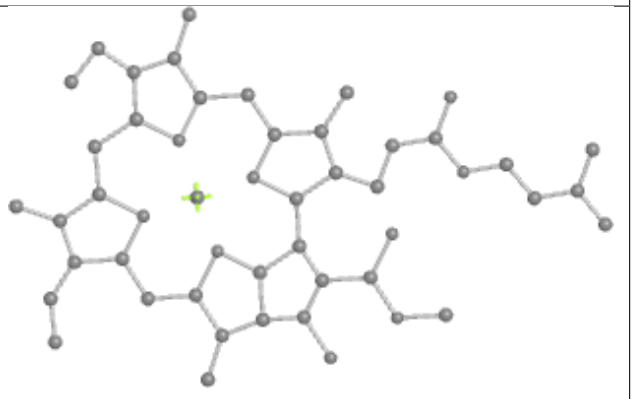
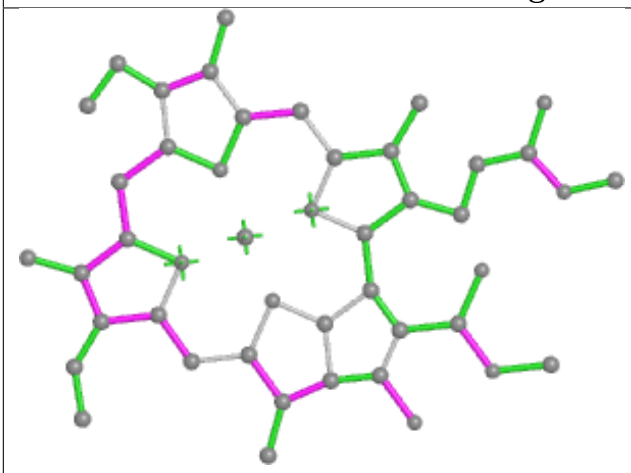
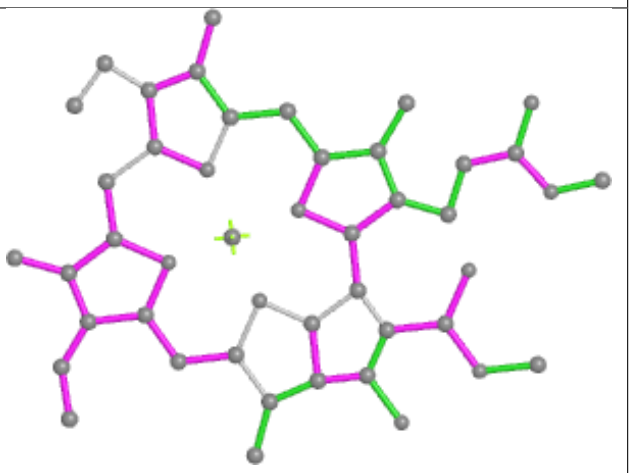


Rings

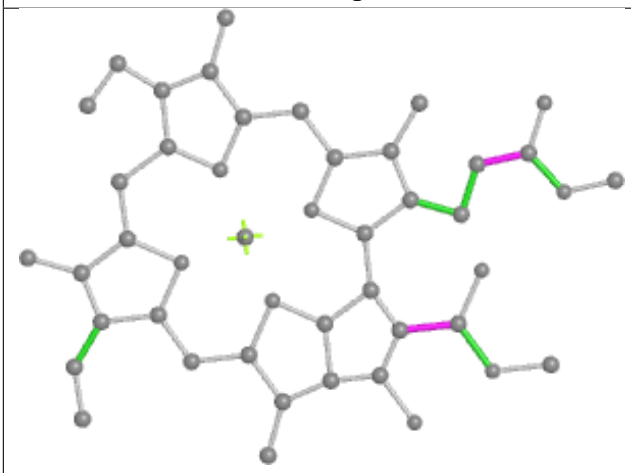
Ligand CLA 9 603



Bond lengths



Bond angles



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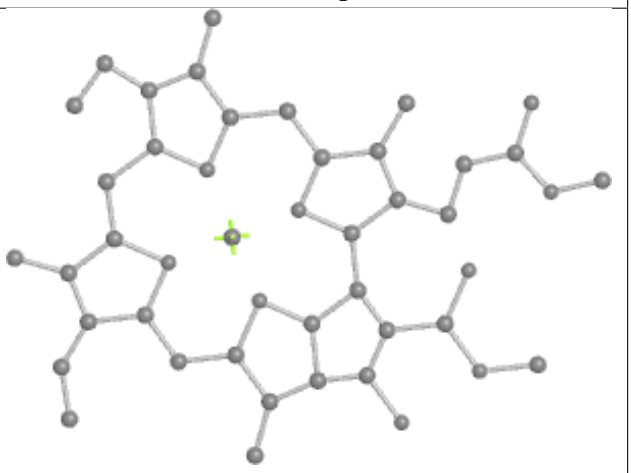
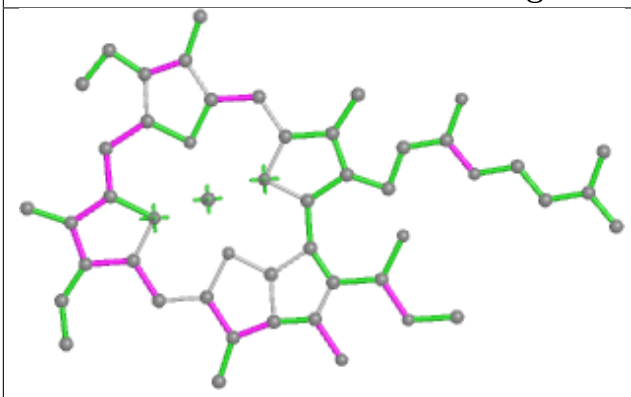


Rings

Ligand CLA L 204



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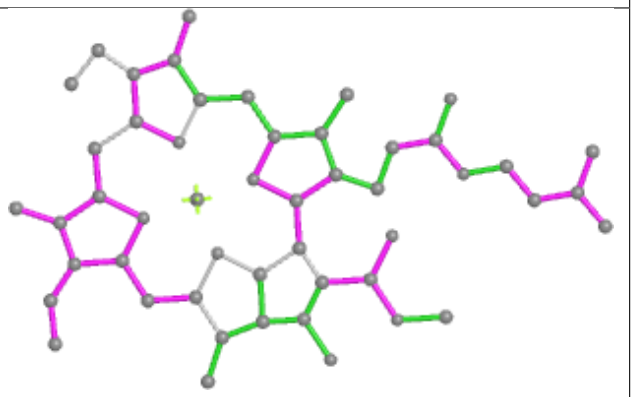
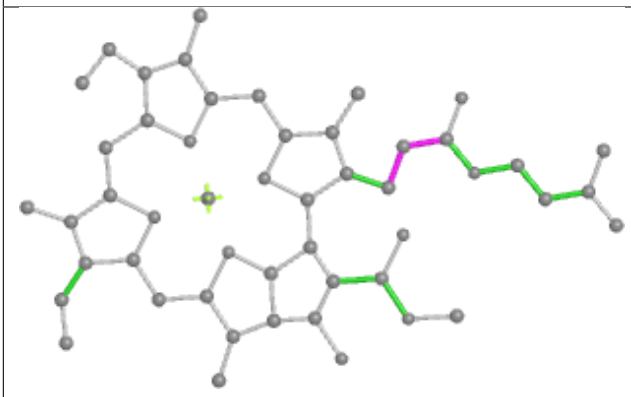
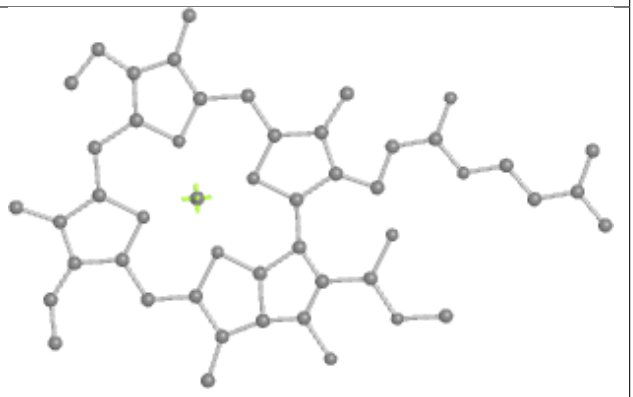


Bond angles

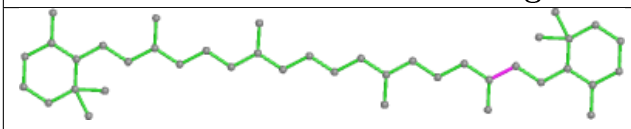


Torsions

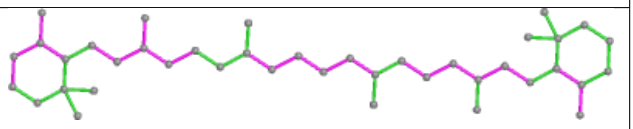


Rings

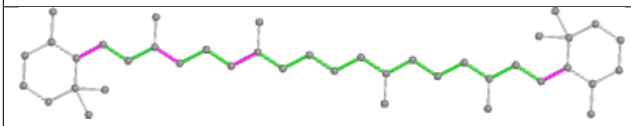
Ligand BCR L 201



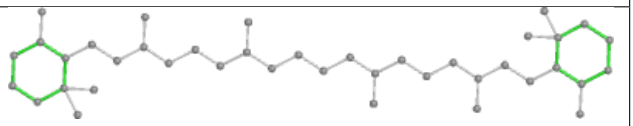
Bond lengths



Bond angles

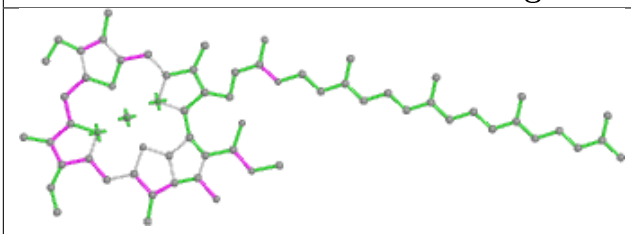


Torsions



Rings

Ligand CLA B 825



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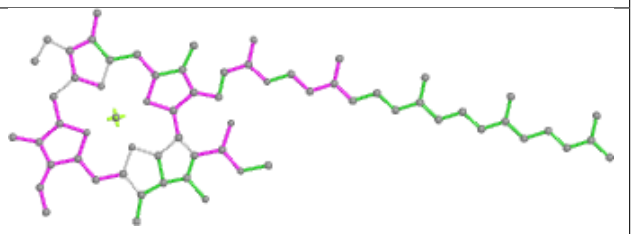
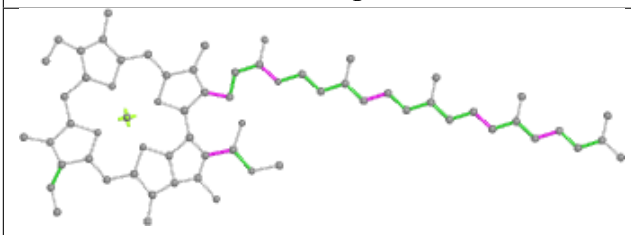
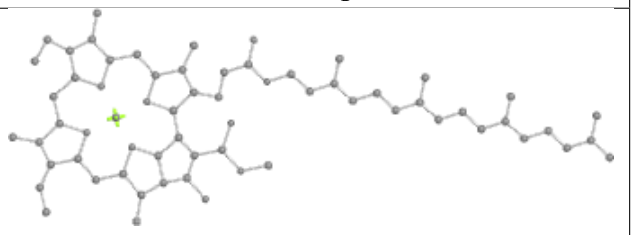


Bond angles

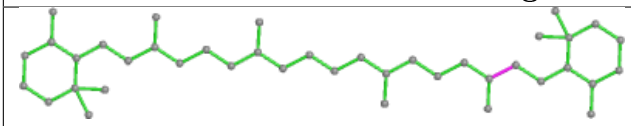


Torsions

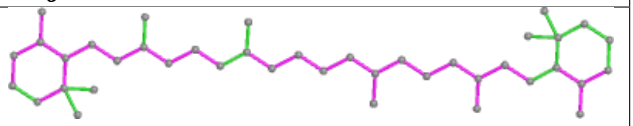


Rings

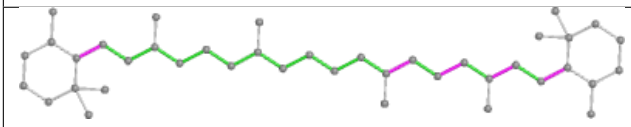
Ligand BCR j 3004



Bond lengths



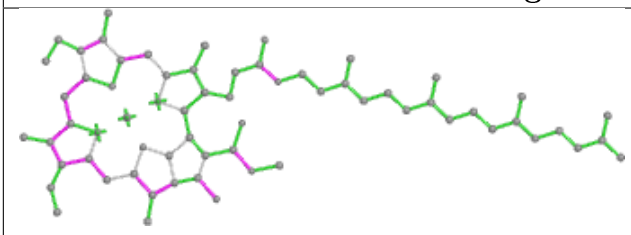
Bond angles



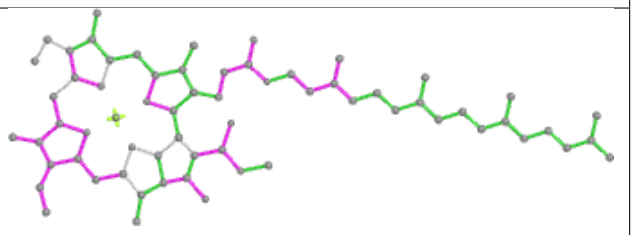
Torsions

Rings

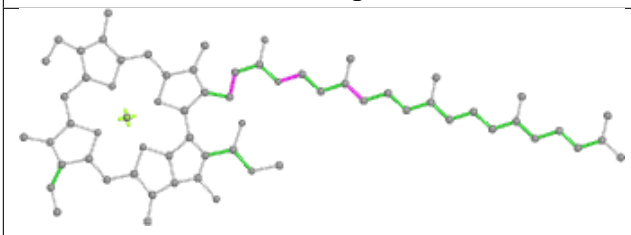
Ligand CLA A 810



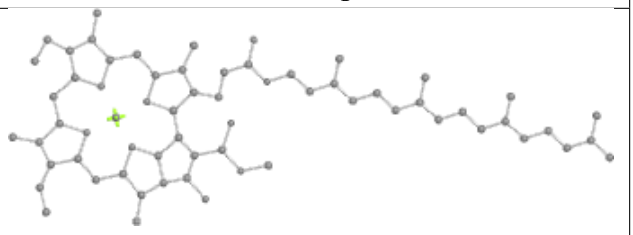
Bond lengths



Bond angles

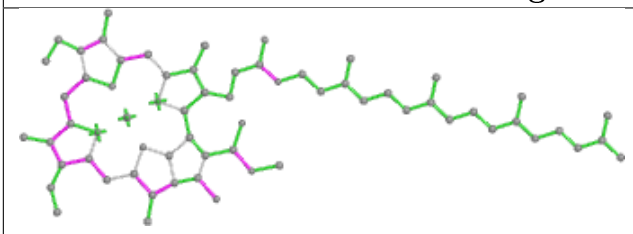


Torsions

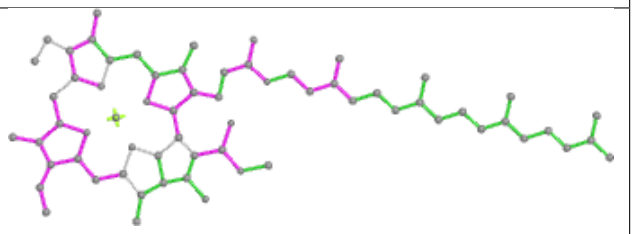


Rings

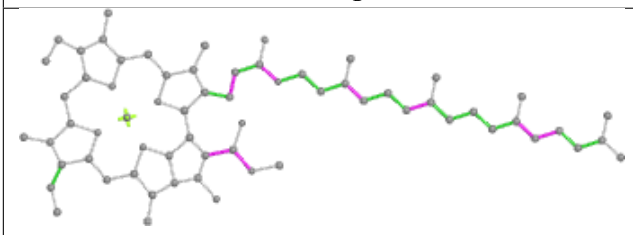
Ligand CLA 2 602



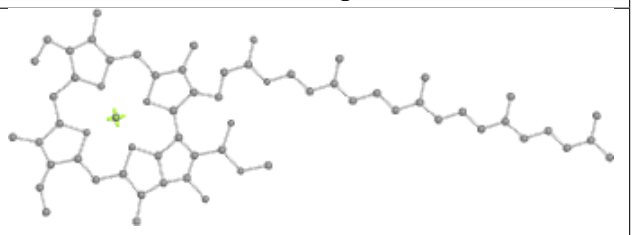
Bond lengths



Bond angles

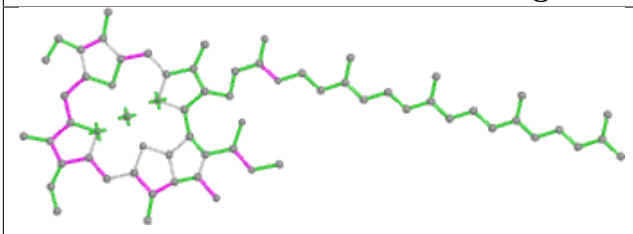


Torsions



Rings

Ligand CLA l 203



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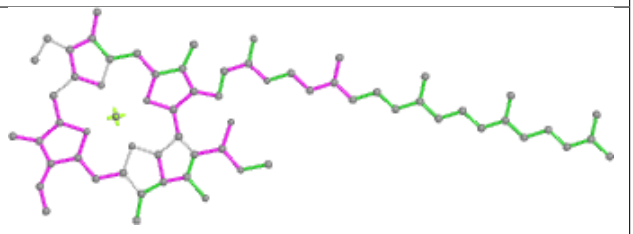
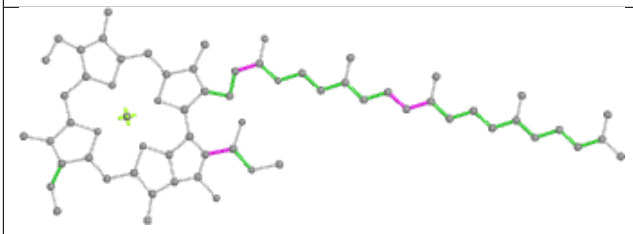


Bond angles



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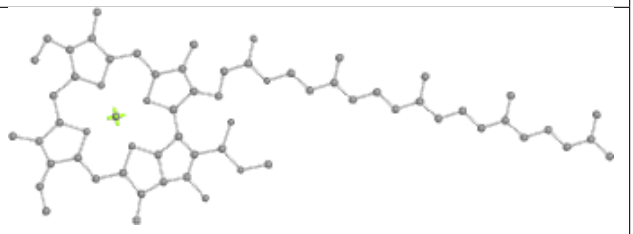
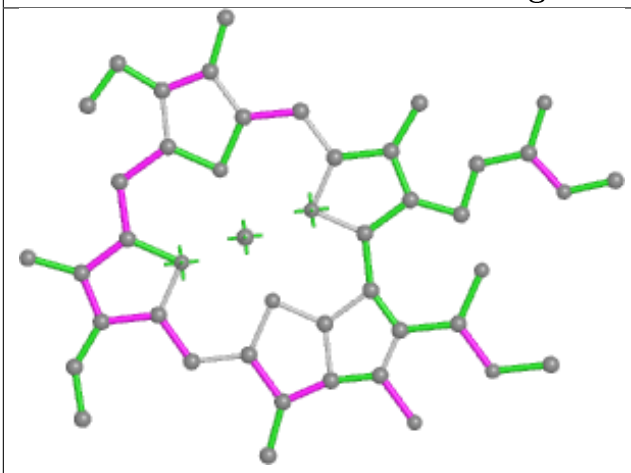


Rings

Ligand CLA 6 316



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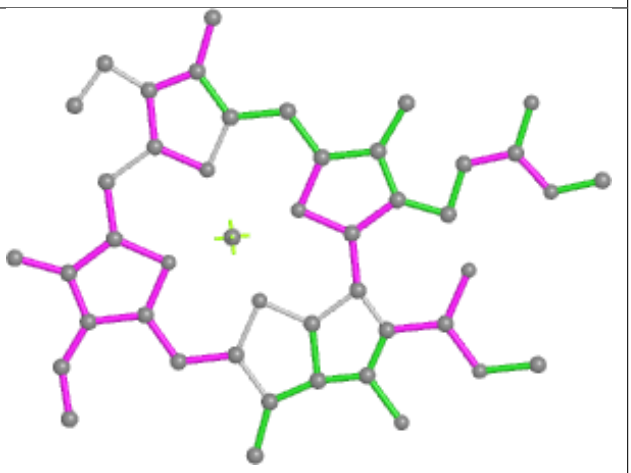
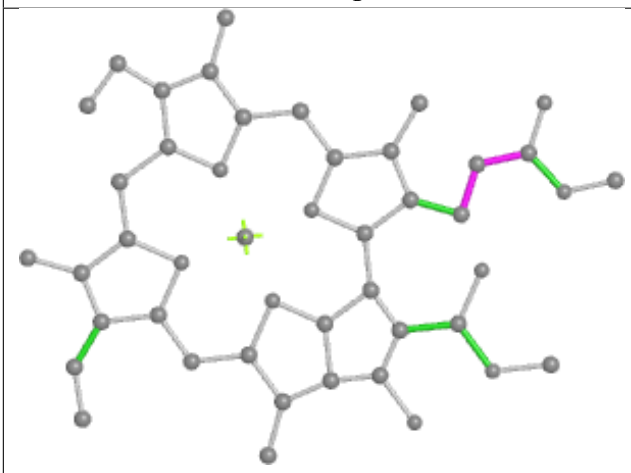


Bond angles



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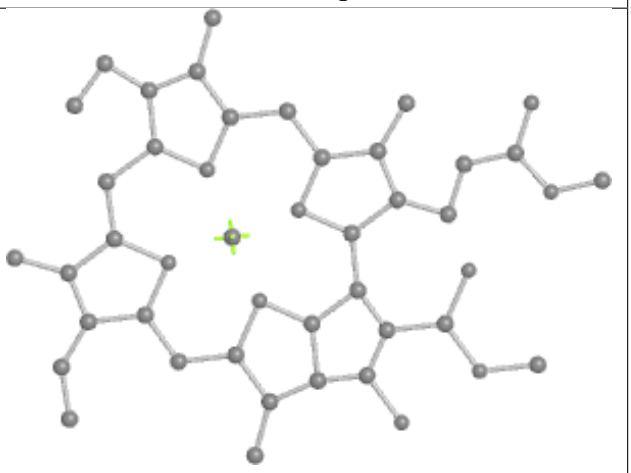
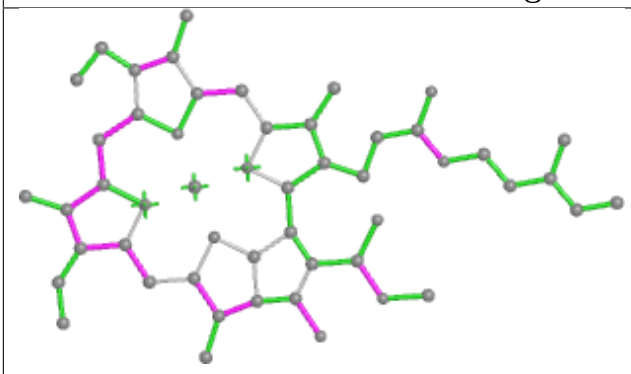


Rings

Ligand CLA A 838



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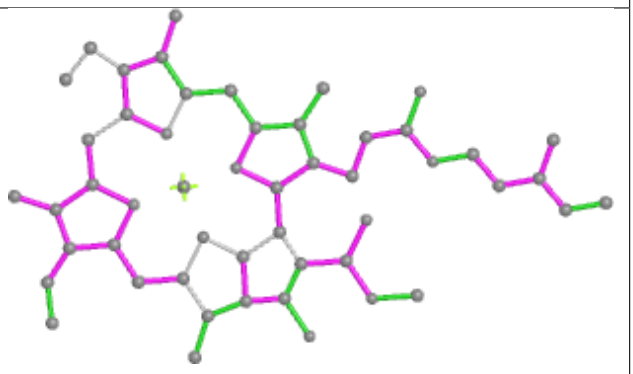
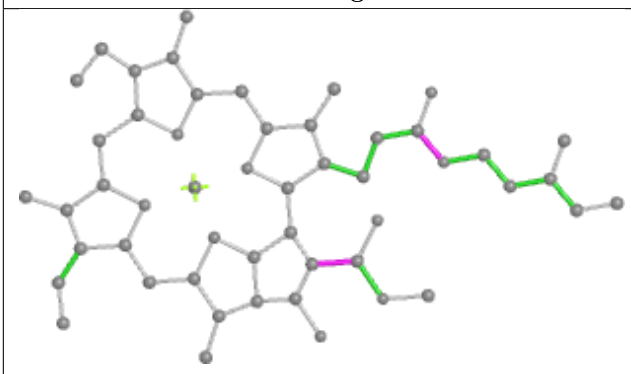


Bond angles



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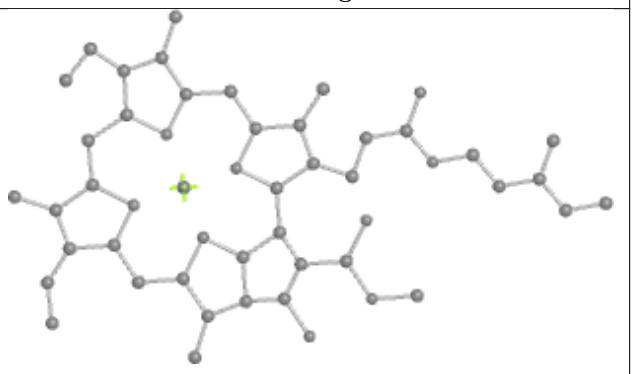
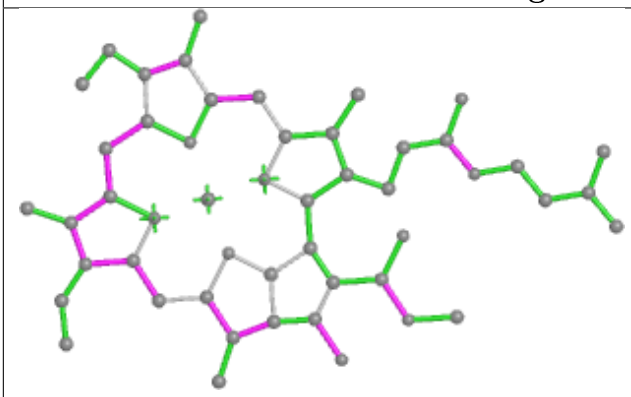


Rings

Ligand CLA 3 309



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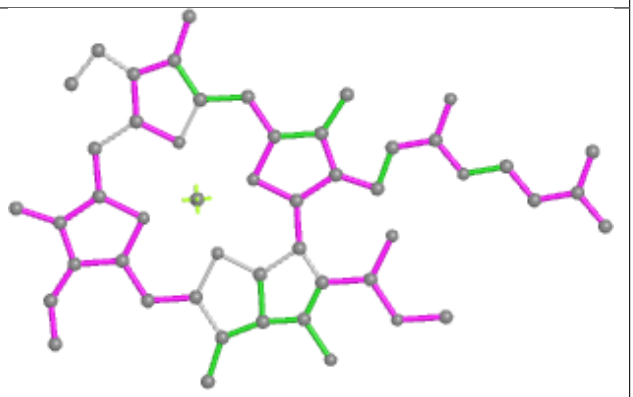

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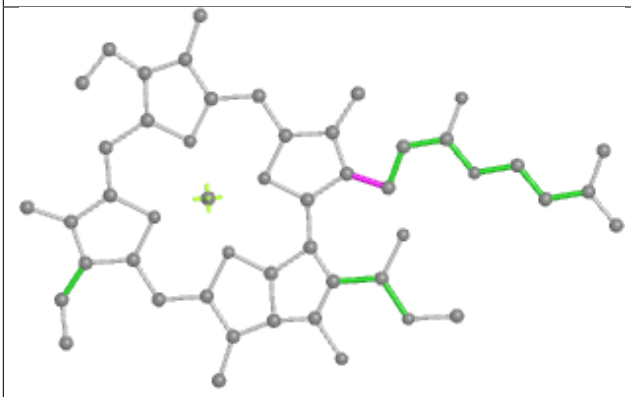

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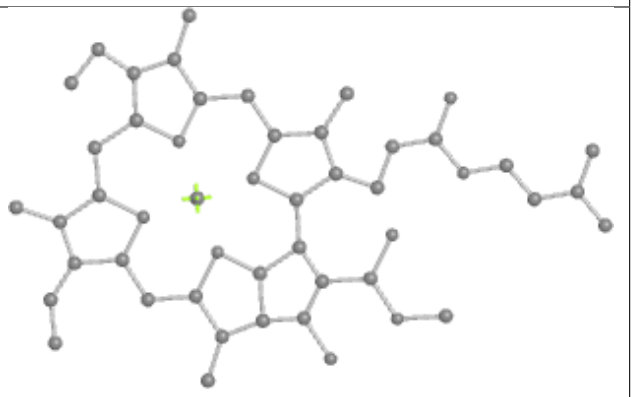
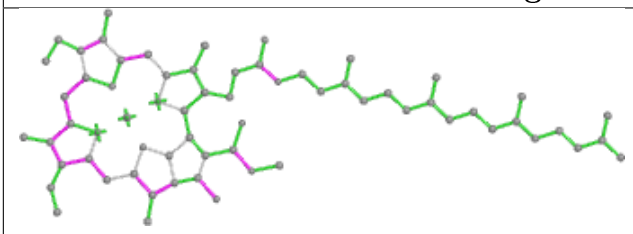


Rings

Ligand CLA A 819



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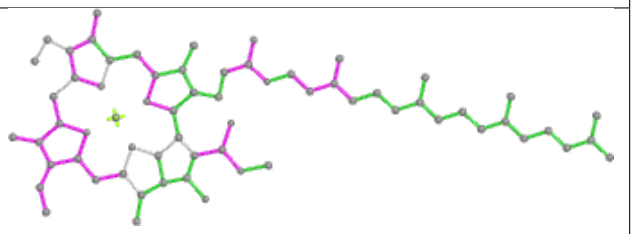

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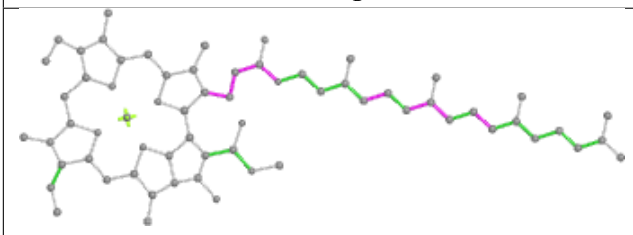

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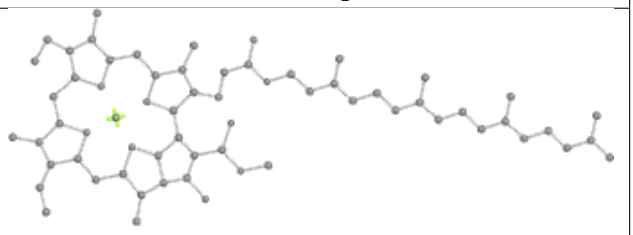
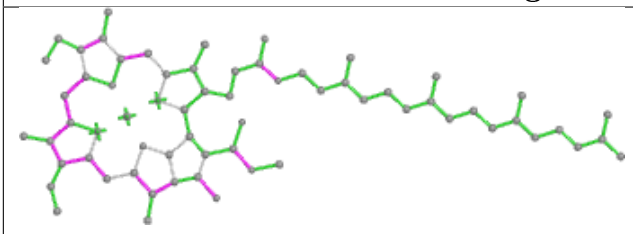


Rings

Ligand CLA B 810



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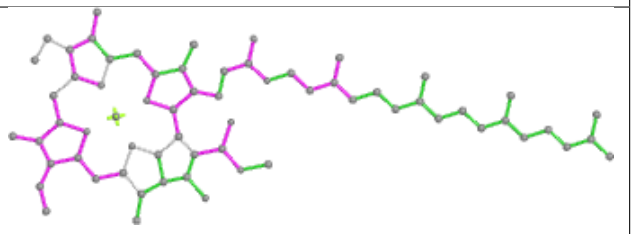
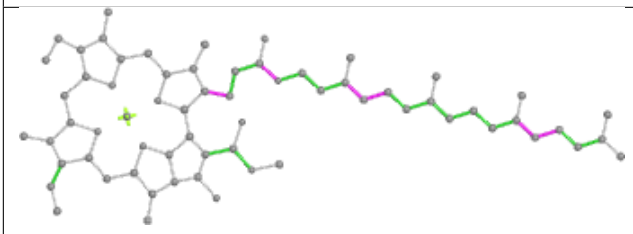


Bond angles



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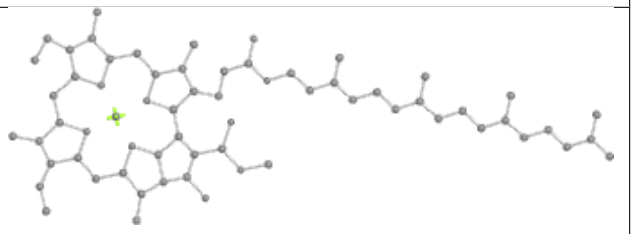
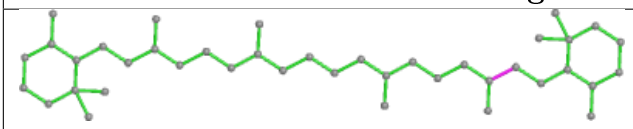


Rings

Ligand BCR a 849



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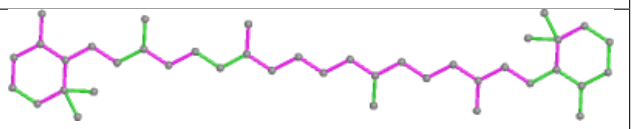

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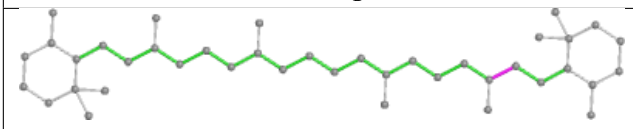
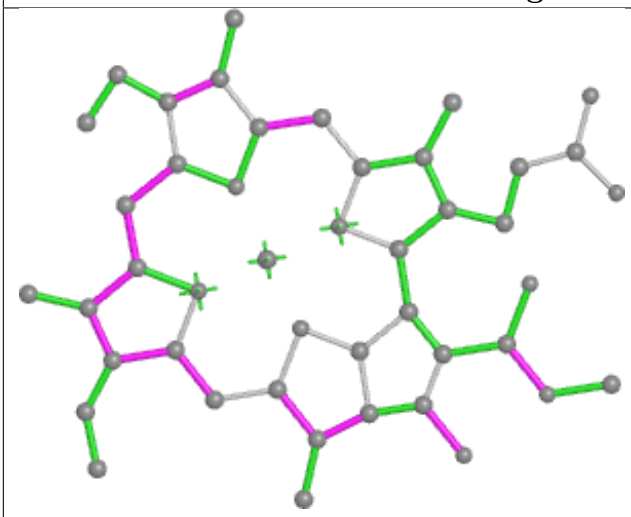


Torsions

Rings

Ligand CLA F 303



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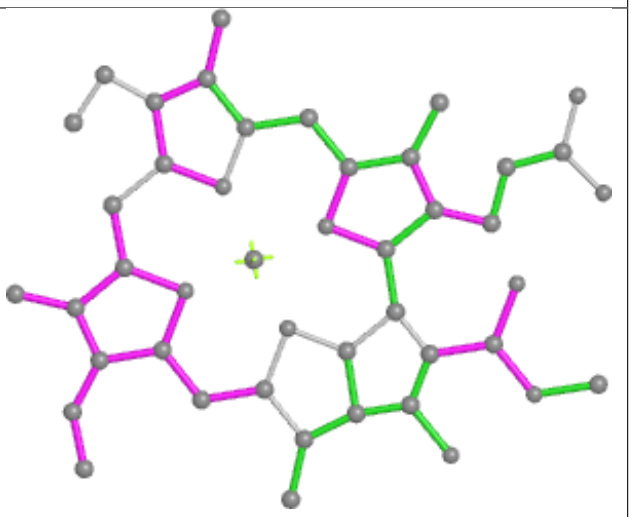
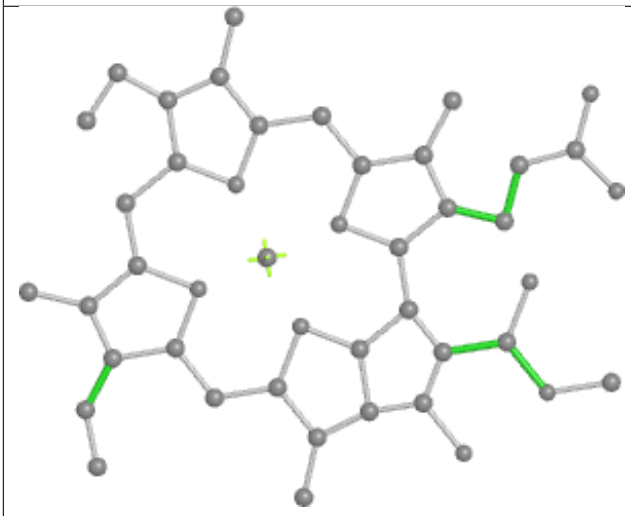


Bond angles



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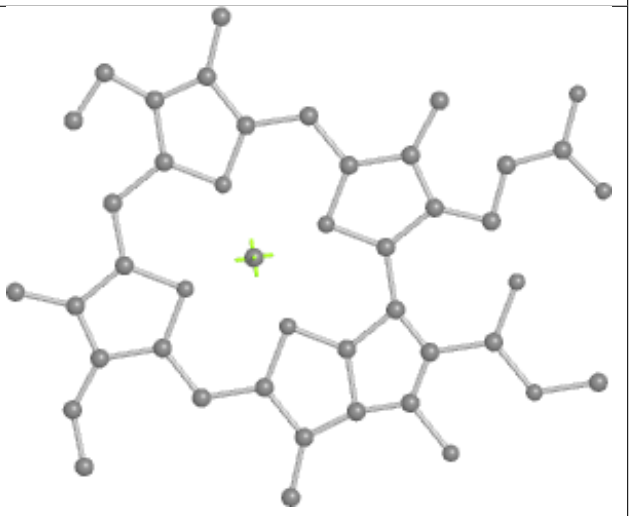
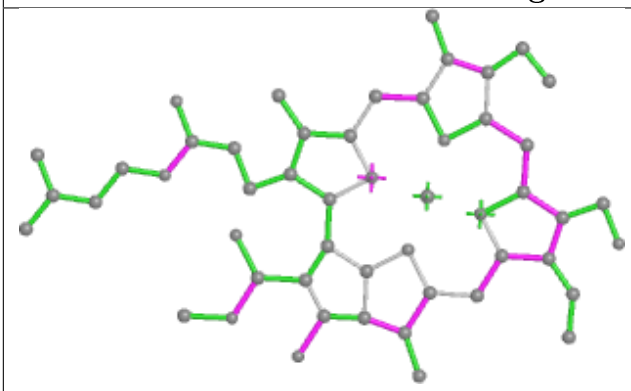


Rings

Ligand CHL 4 606



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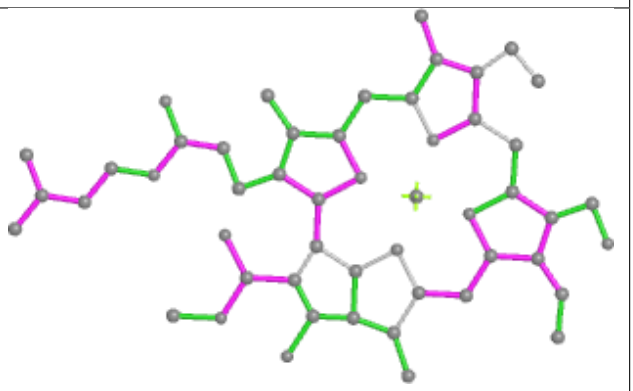
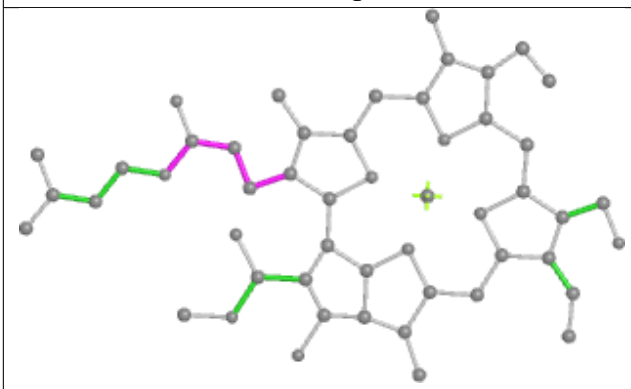


Bond angles



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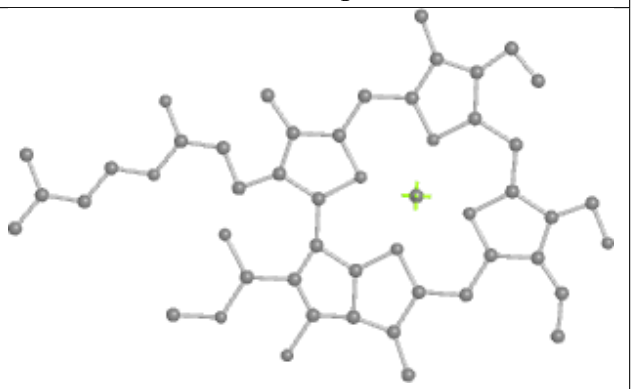
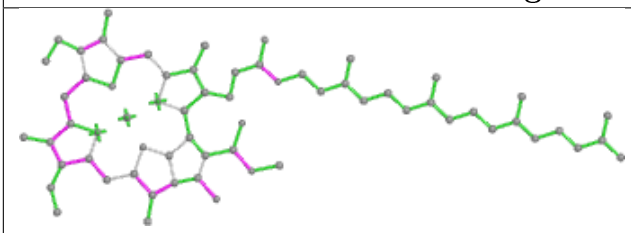


Rings

Ligand CLA A 835



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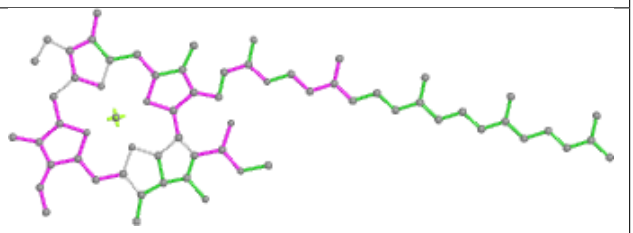
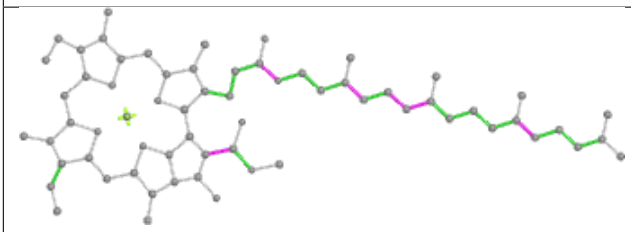


Bond angles



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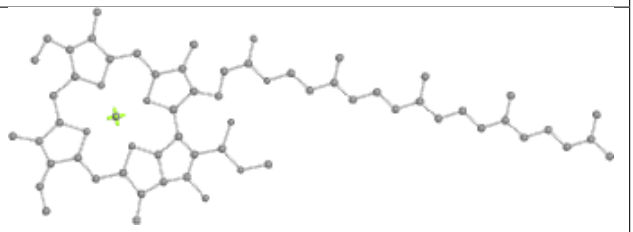
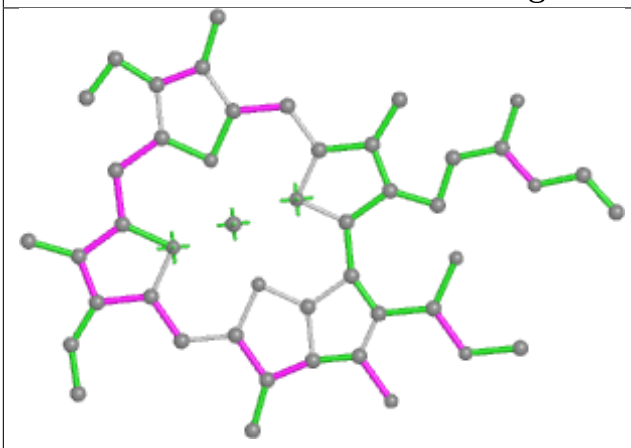


Rings

Ligand CLA 3 306



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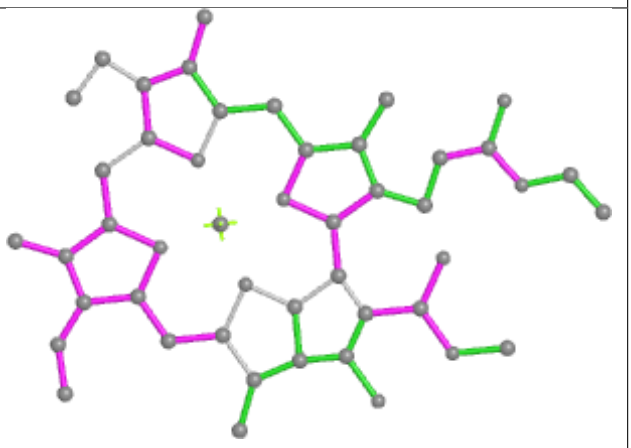
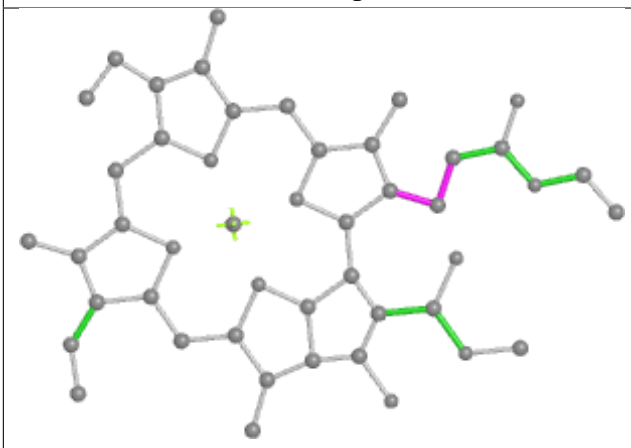


Bond angles



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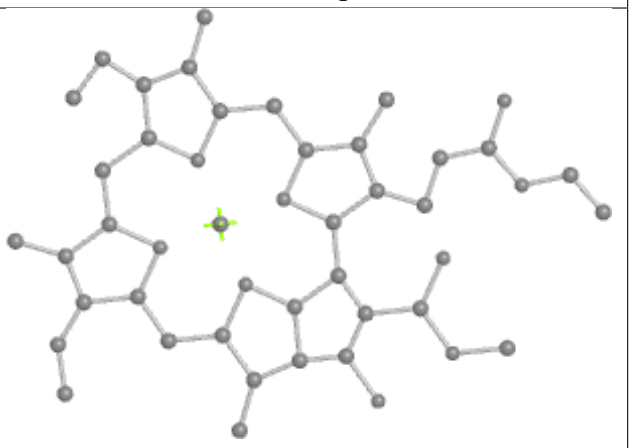
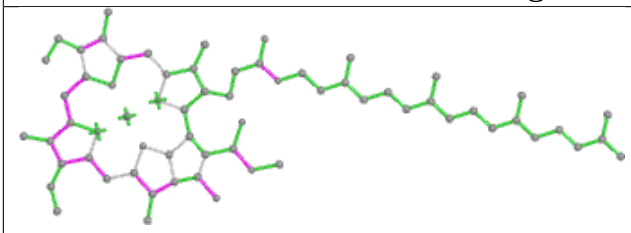
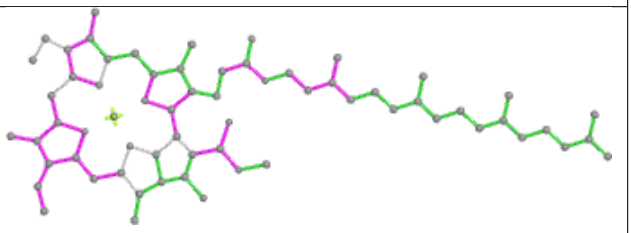


Rings

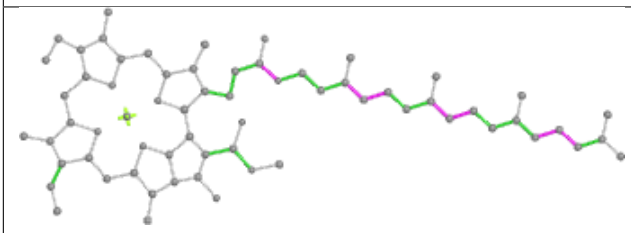
Ligand CLA b 814



Bond lengths



Bond angles



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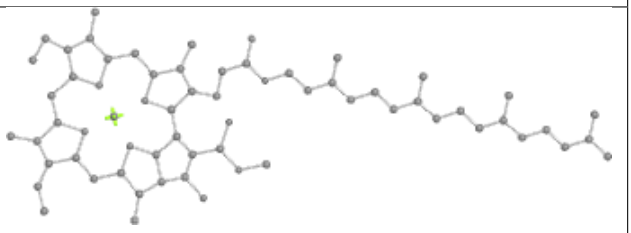
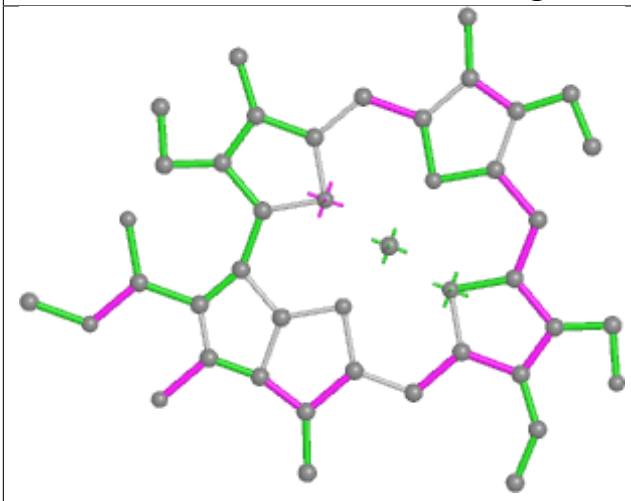


Rings

Ligand CHL 7 614



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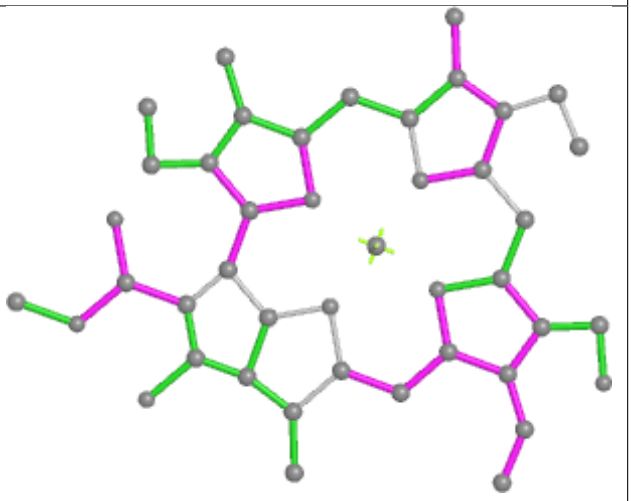
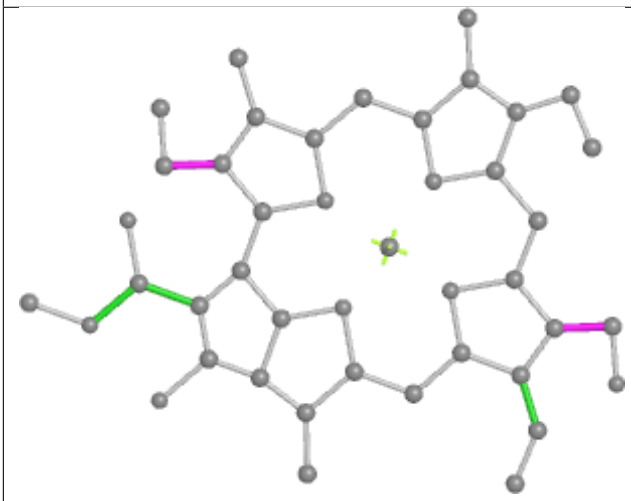


Bond angles



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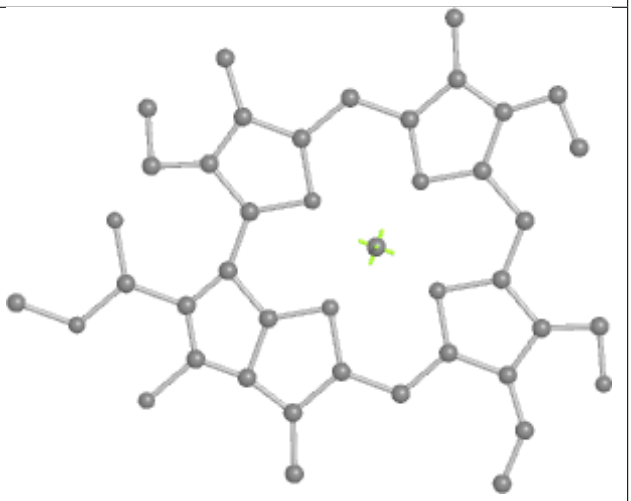
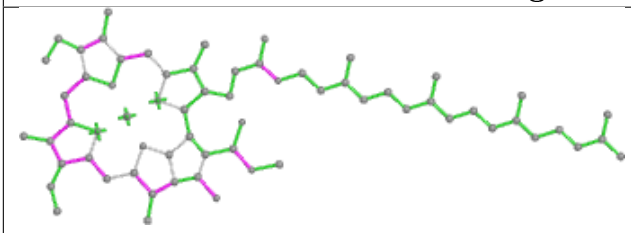


Rings

Ligand CLA 1 313



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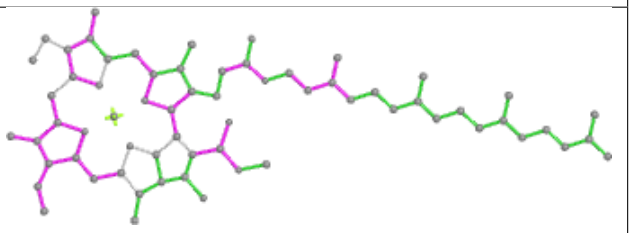
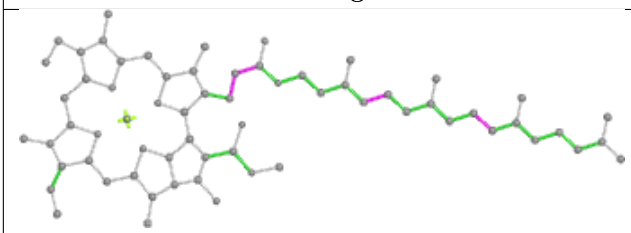


Bond angles



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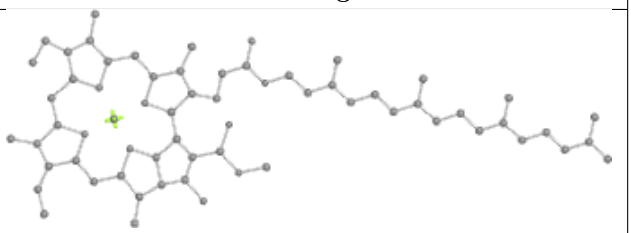
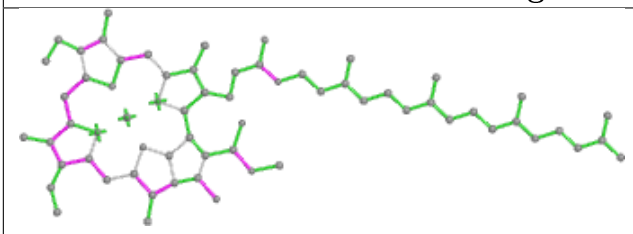
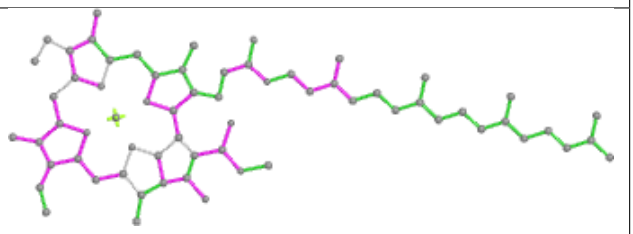


Rings

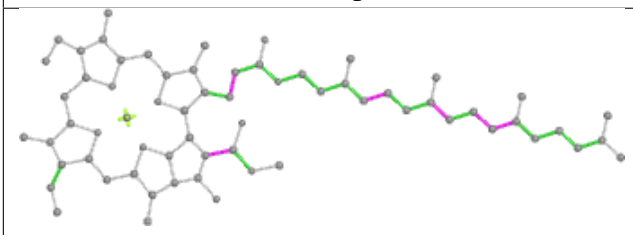
Ligand CLA b 826



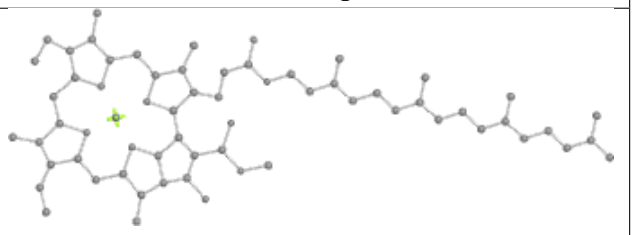
Bond lengths



Bond angles

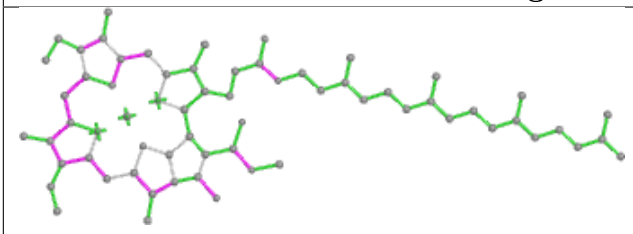


Torsions



Rings

Ligand CLA b 829



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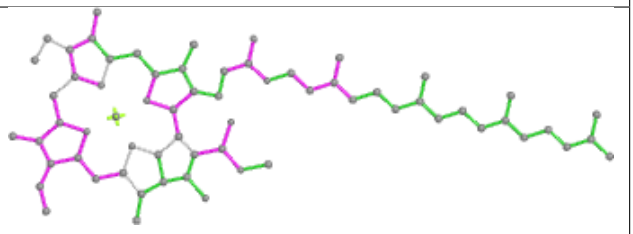
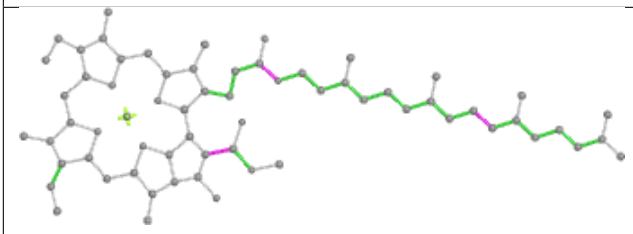
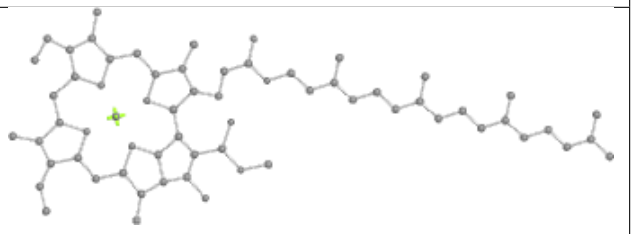


Bond angles

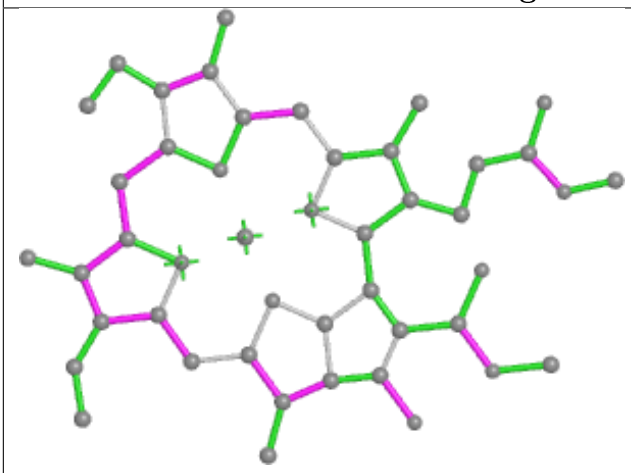


Torsions

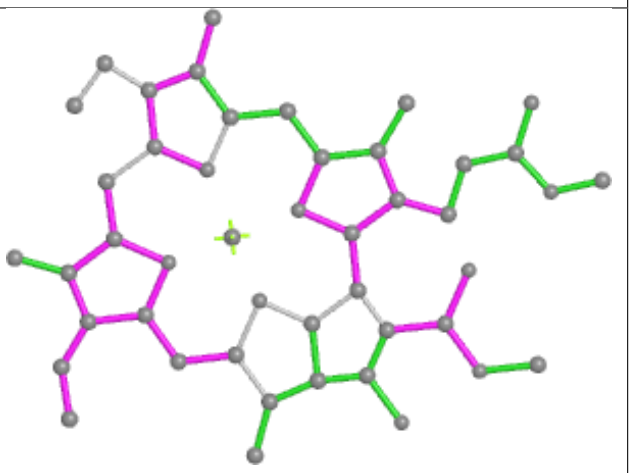


Rings

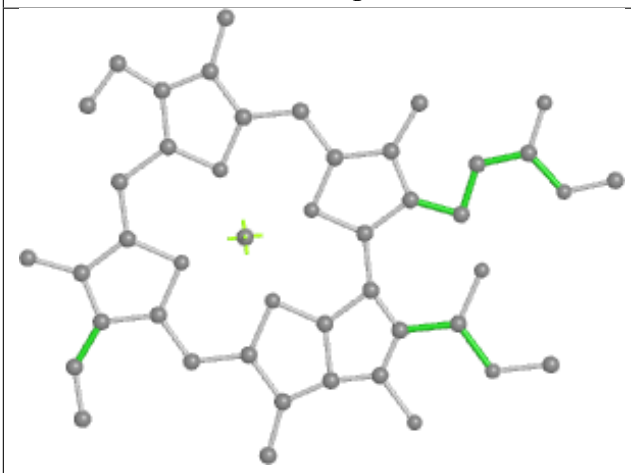
Ligand CLA k 1402



Bond lengths



Bond angles



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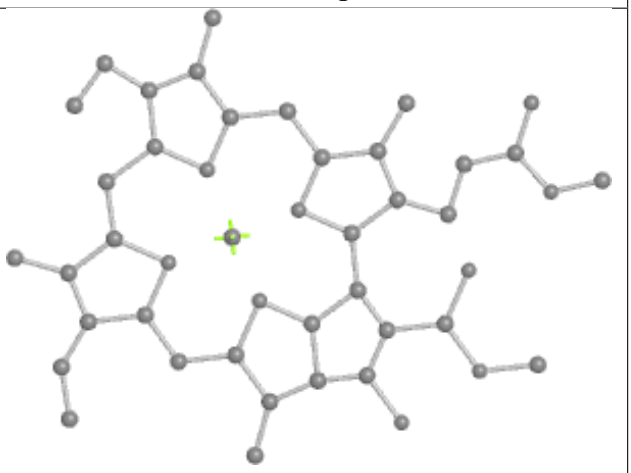
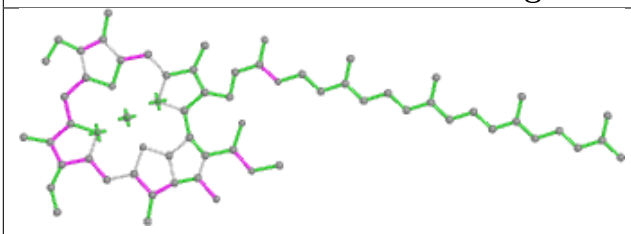


Rings

Ligand CLA B 808



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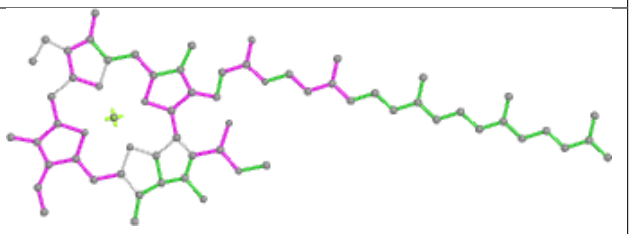
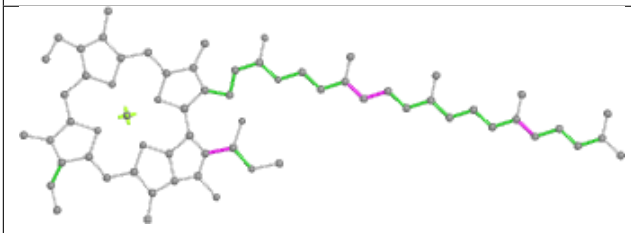


Bond angles



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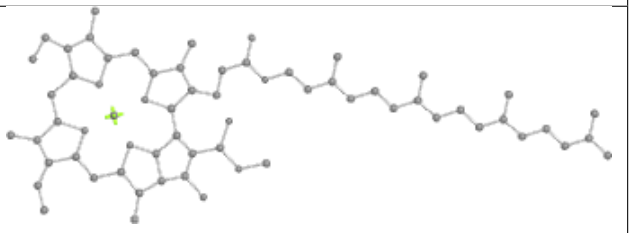
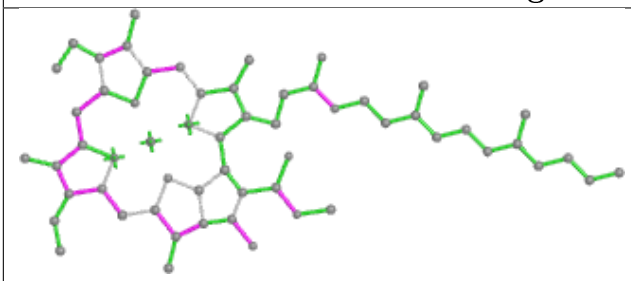


Rings

Ligand CLA b 833



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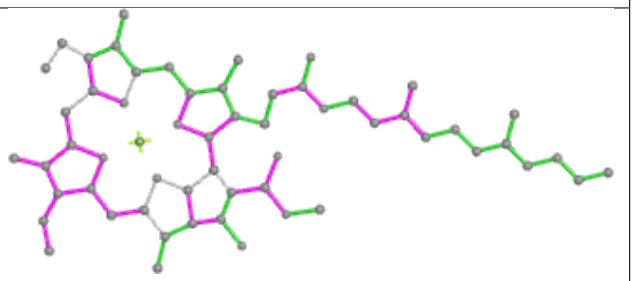
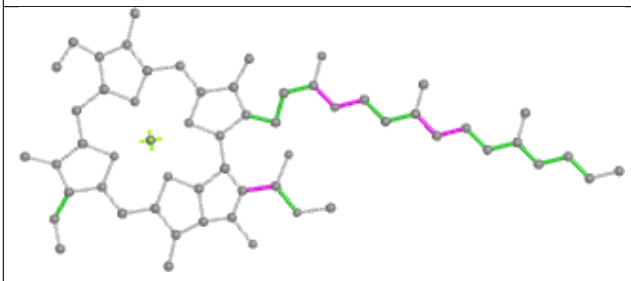


Bond angles



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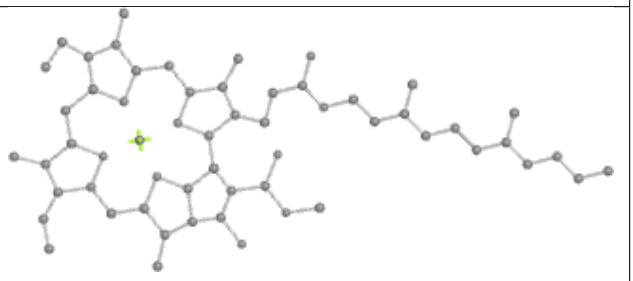
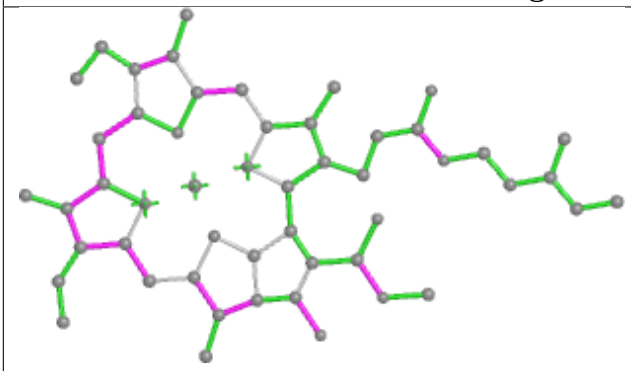


Rings

Ligand CLA 6 306



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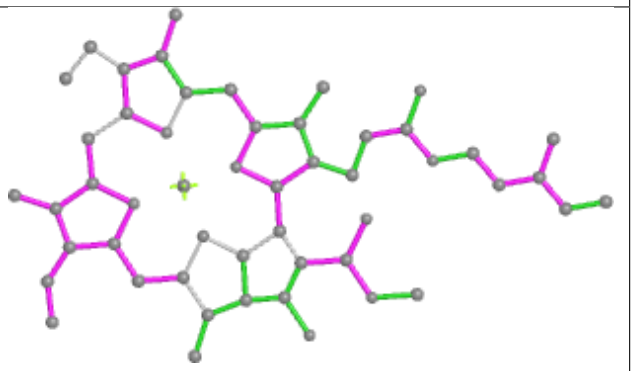
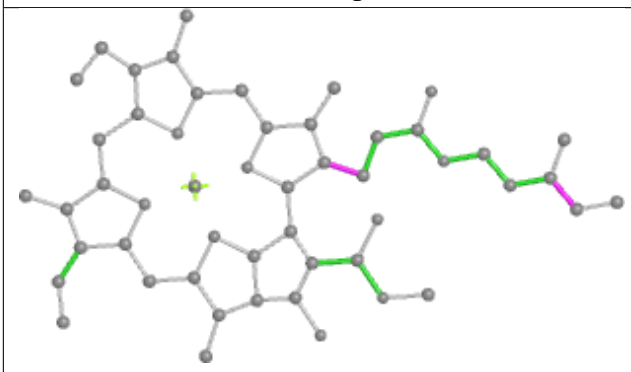


Bond angles



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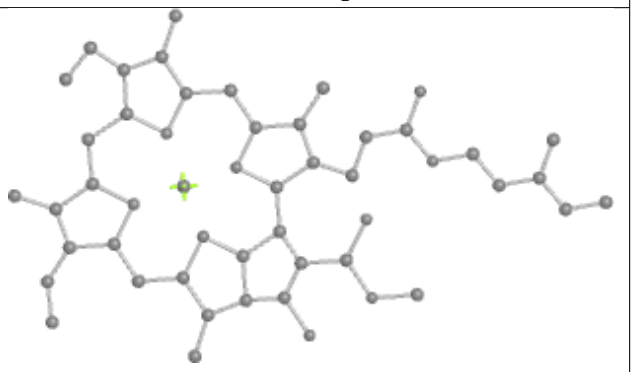
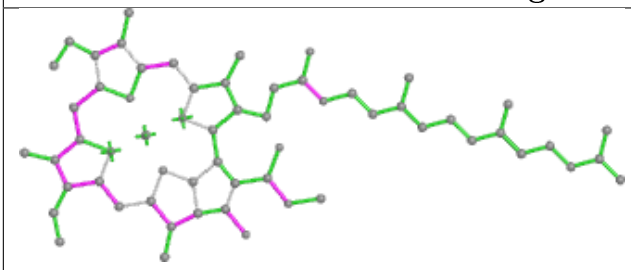


Rings

Ligand CLA 1 310



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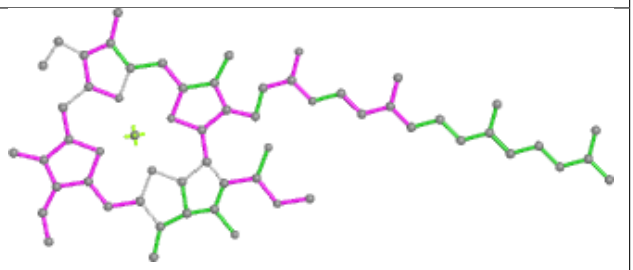
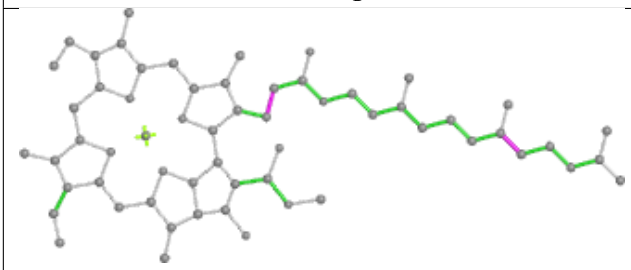


Bond angles



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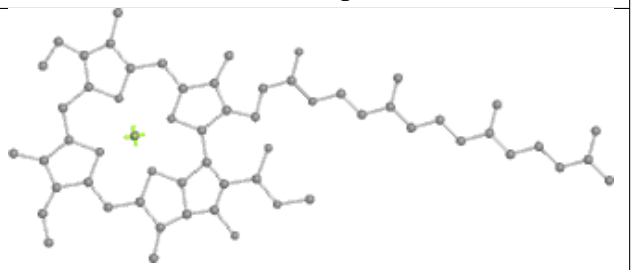
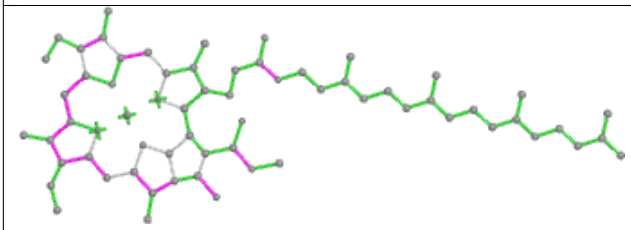


Rings

Ligand CLA a 842



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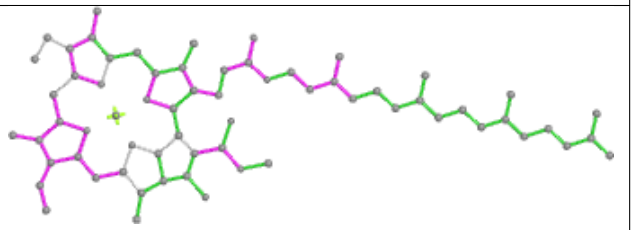
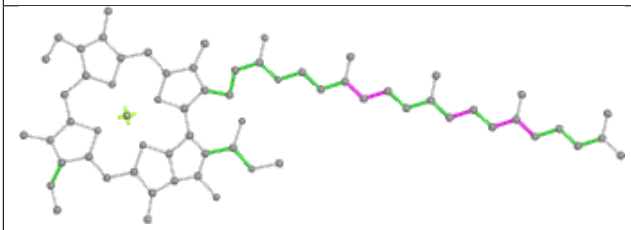


Bond angles



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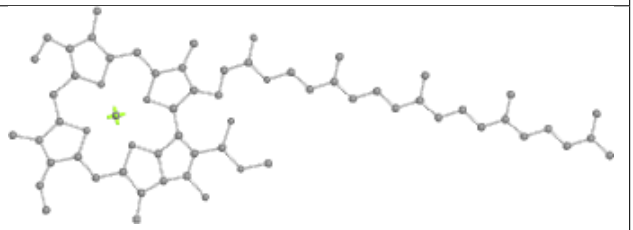
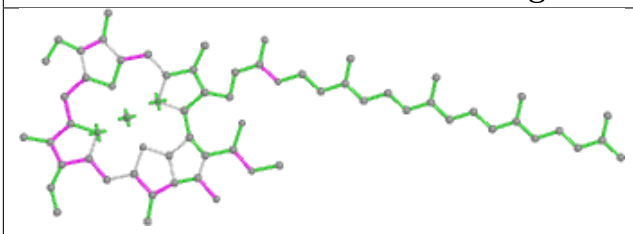
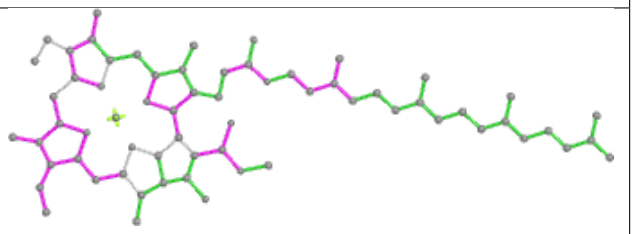


Rings

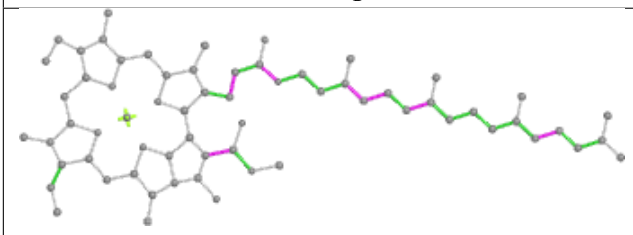
Ligand CLA 6 304



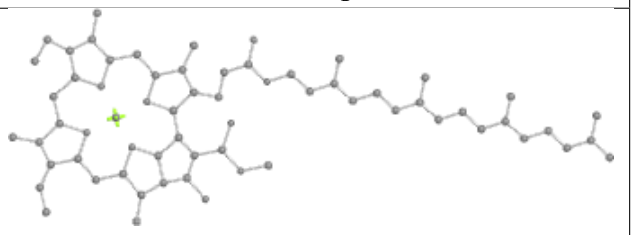
Bond lengths



Bond angles

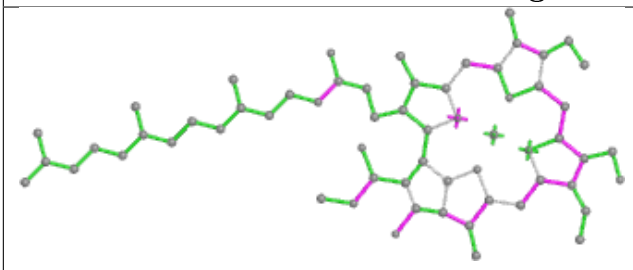


Torsions



Rings

Ligand CHL 7 601



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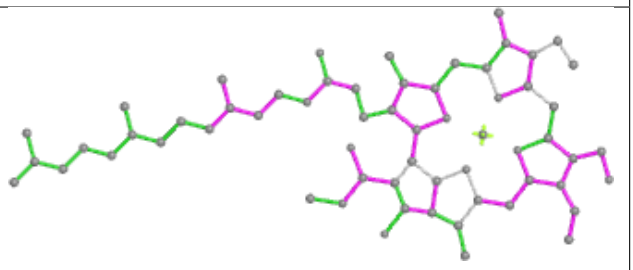
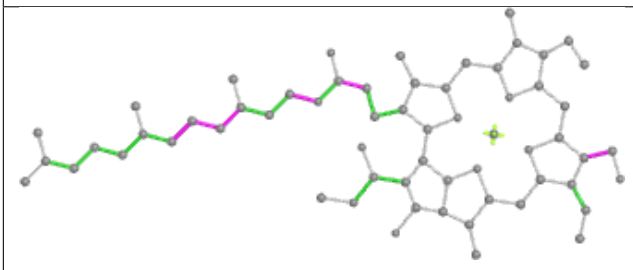


Bond angles



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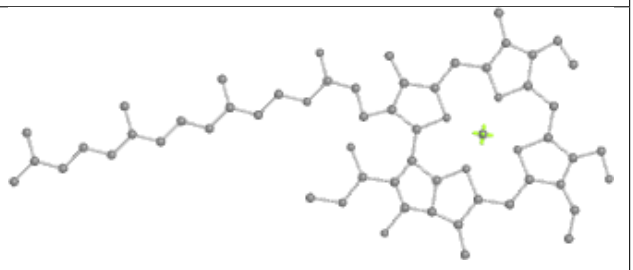
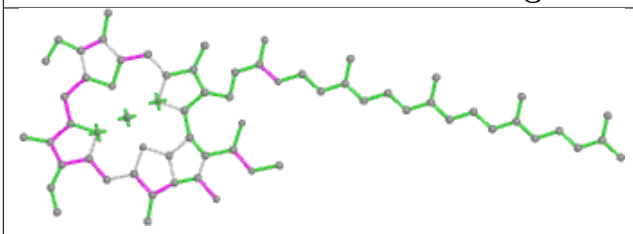


Rings

Ligand CLA B 840



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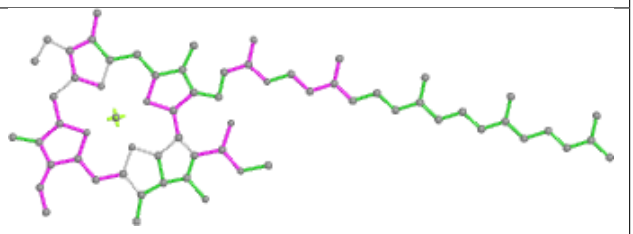
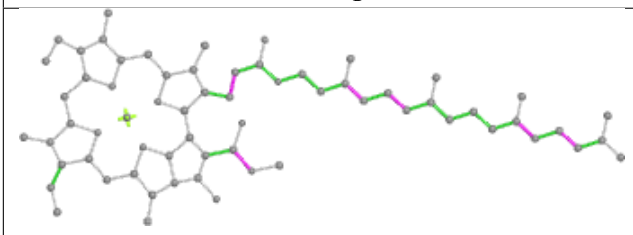
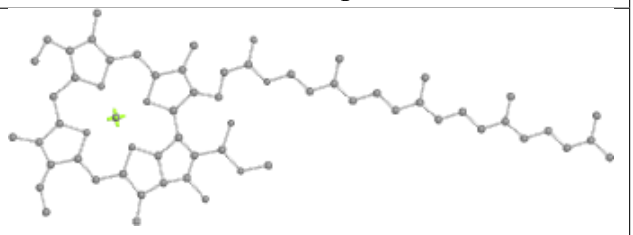


Bond angles

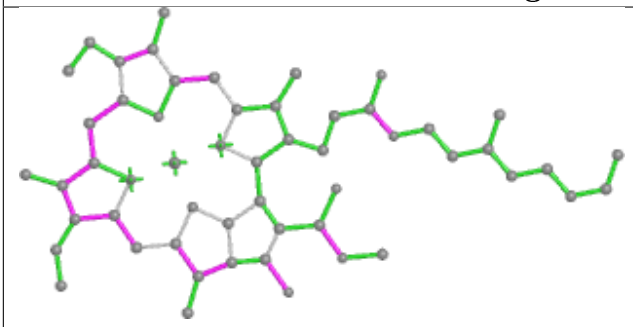


Torsions



Rings

Ligand CLA A 813



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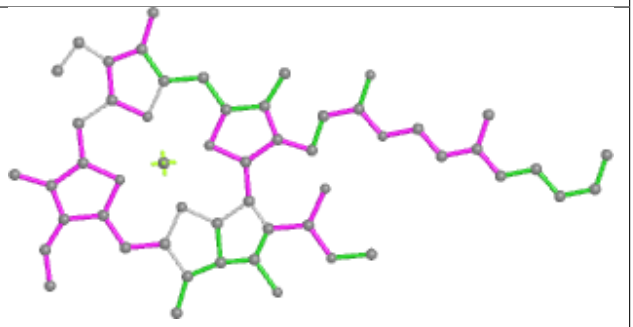
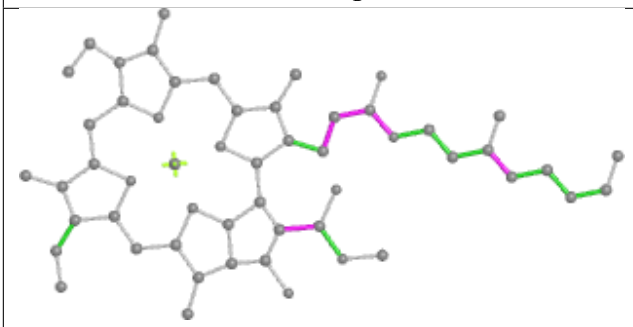
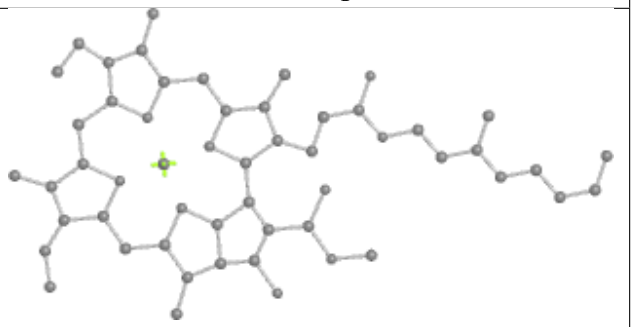


Bond angles

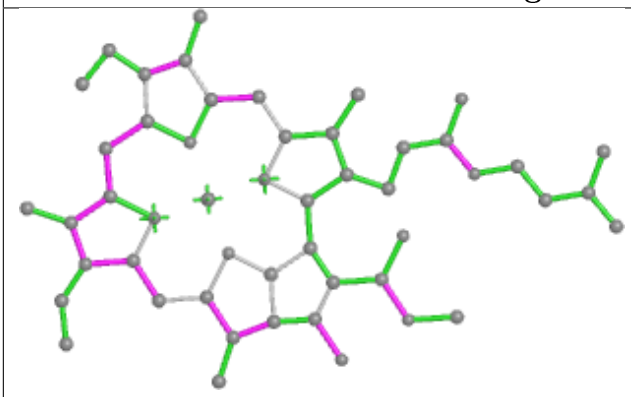


Torsions

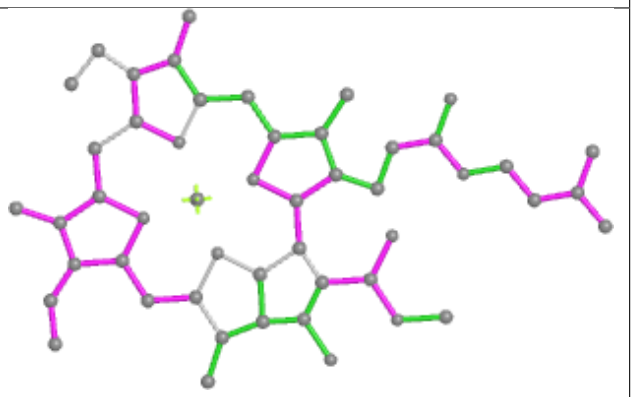


Rings

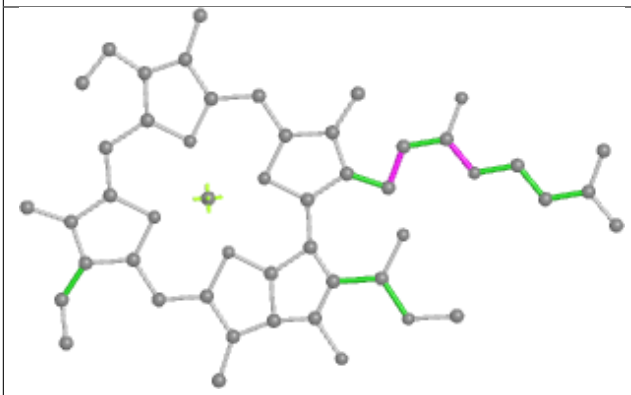
Ligand CLA A 816



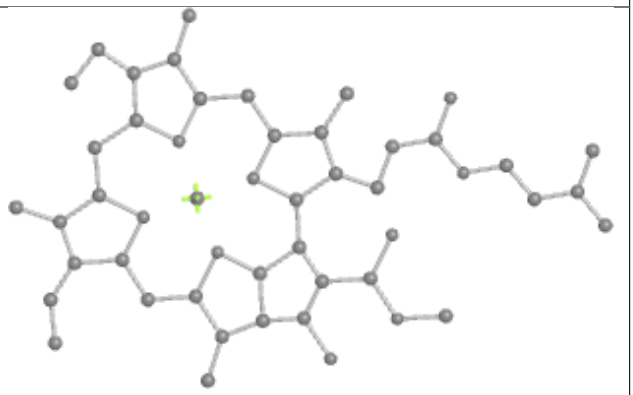
Bond lengths



Bond angles

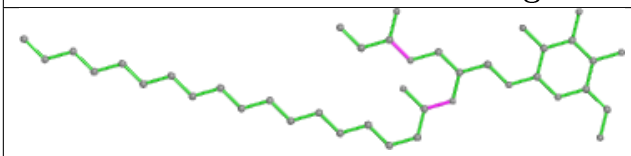


Torsions

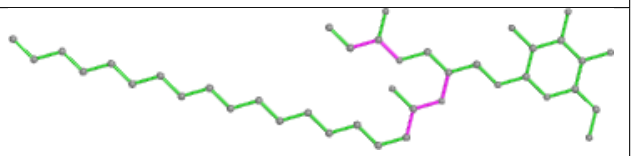


Rings

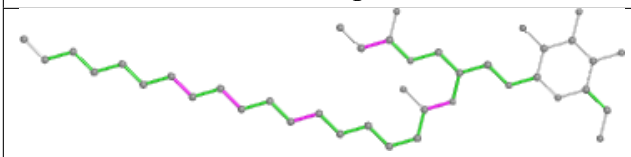
Ligand LMG 6 302



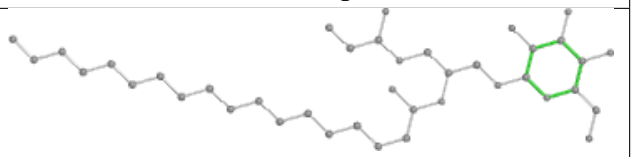
Bond lengths



Bond angles

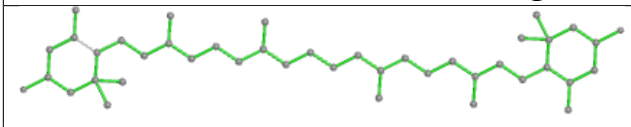


Torsions

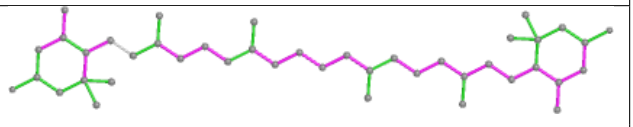


Rings

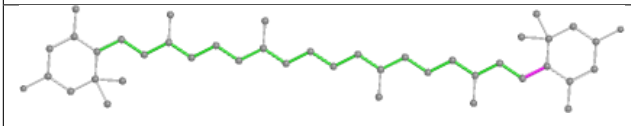
Ligand LUT 3 316



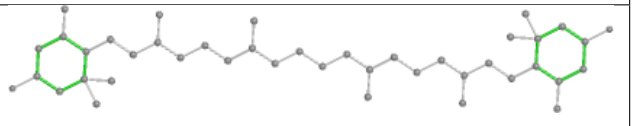
Bond lengths



Bond angles

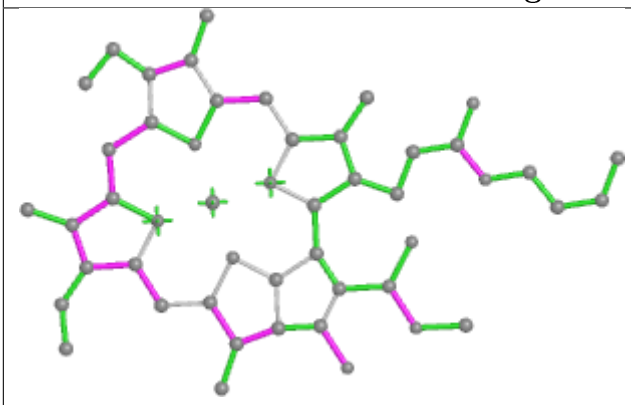


Torsions

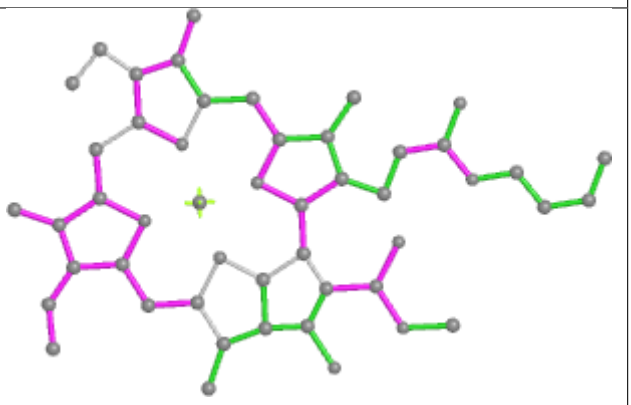


Rings

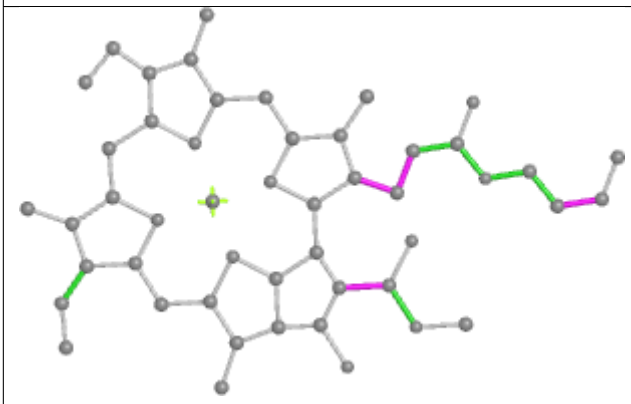
Ligand CLA A 823



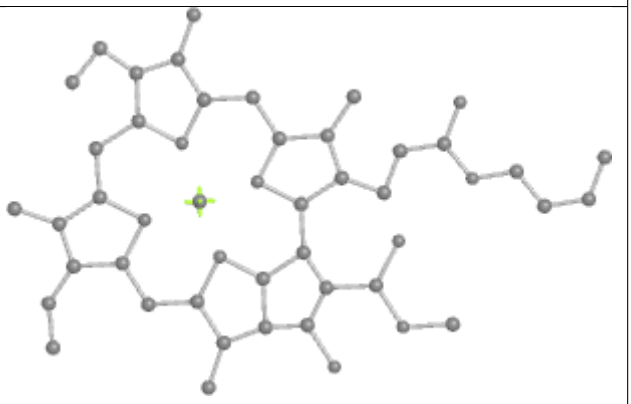
Bond lengths



Bond angles

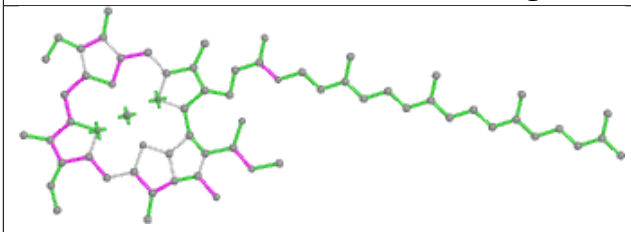


Torsions



Rings

Ligand CLA B 809



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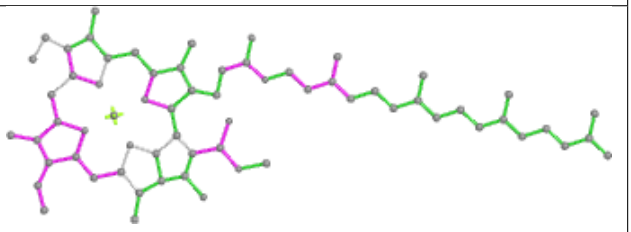
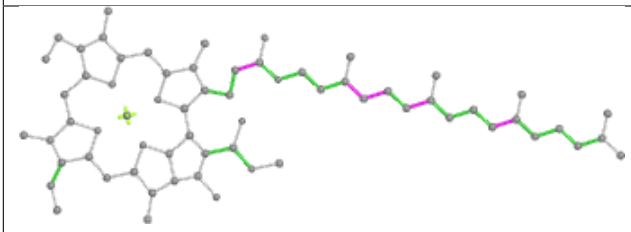
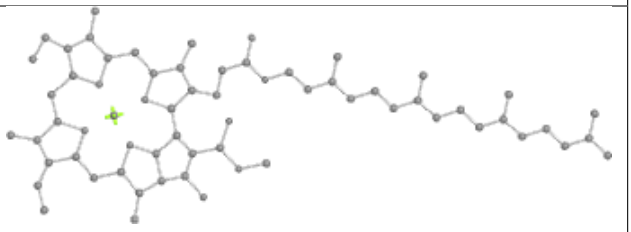


Bond angles

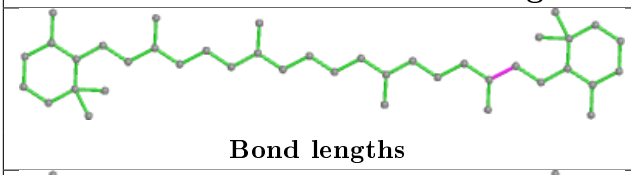


Torsions

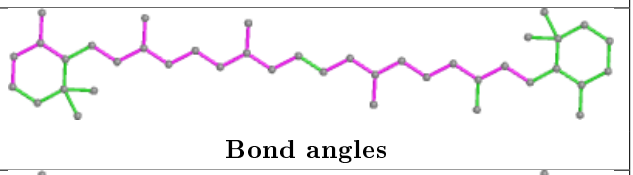


Rings

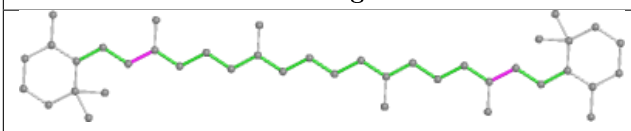
Ligand BCR 7 617



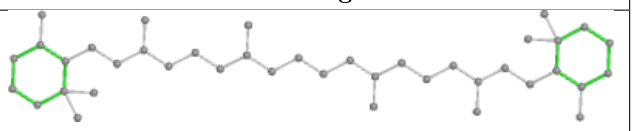
Bond lengths



Bond angles

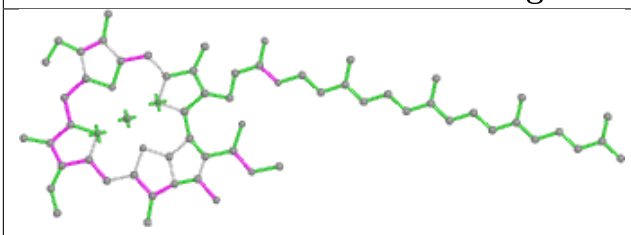


Torsions

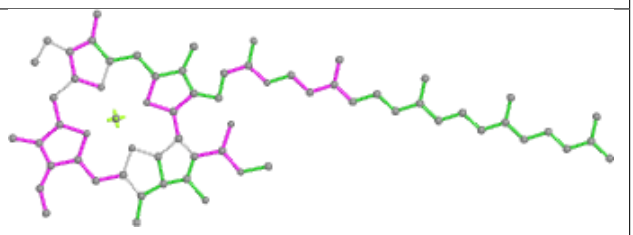


Rings

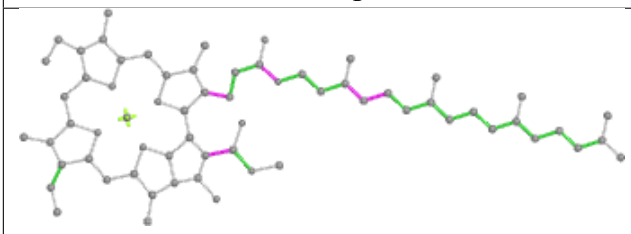
Ligand CLA L 202



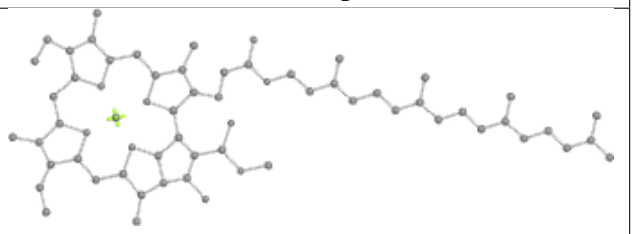
Bond lengths



Bond angles

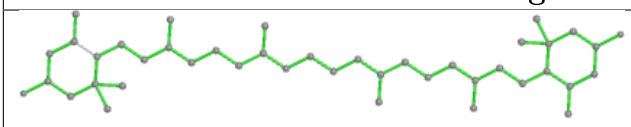


Torsions



Rings

Ligand LUT 6 321



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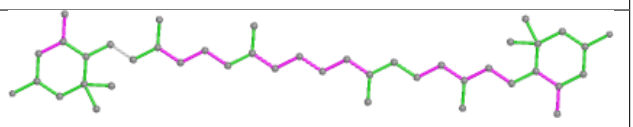
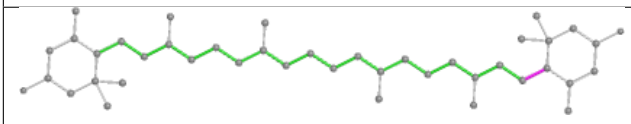


Bond angles



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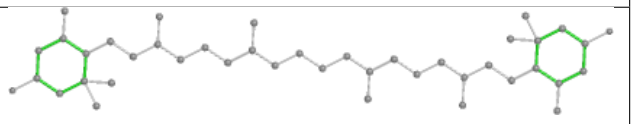
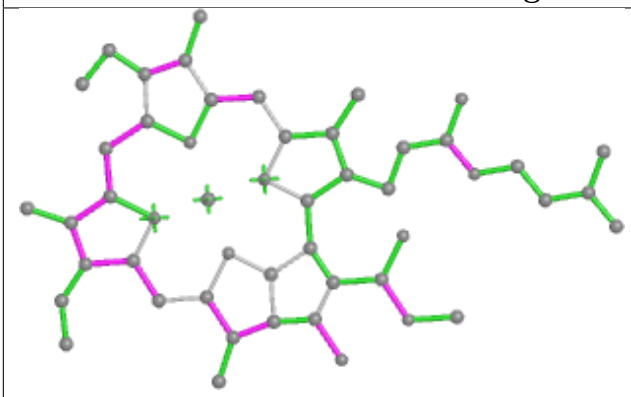


Rings

Ligand CLA G 103



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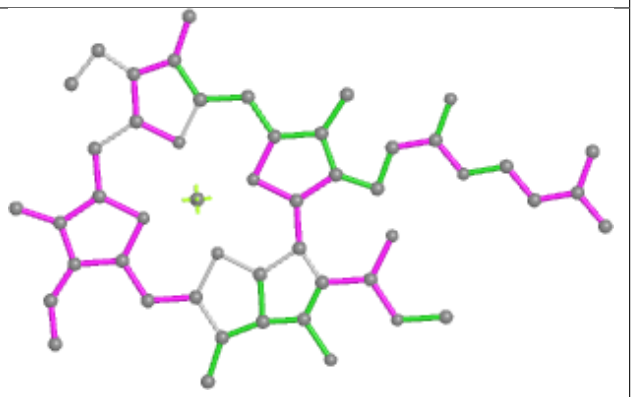
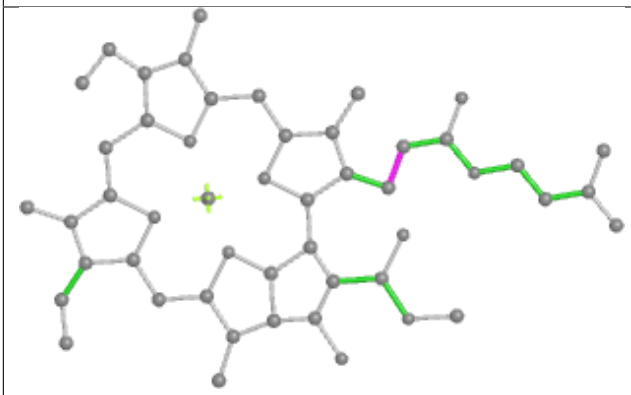


Bond angles



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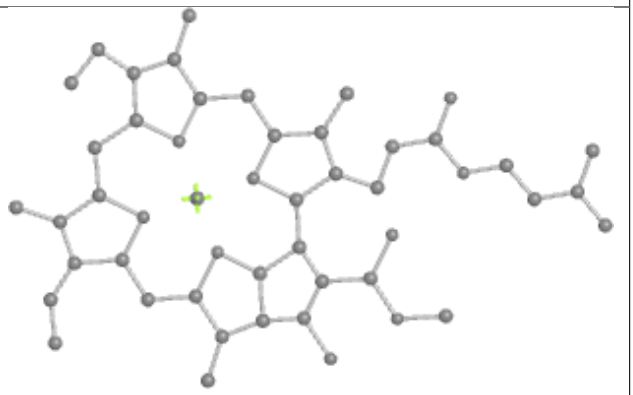
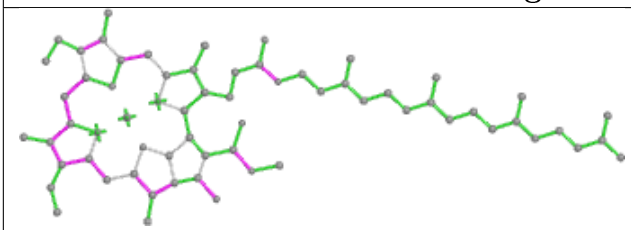


Rings

Ligand CLA A 809



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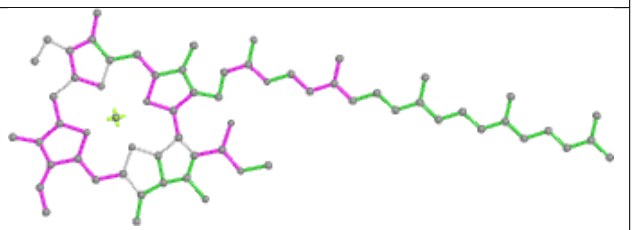
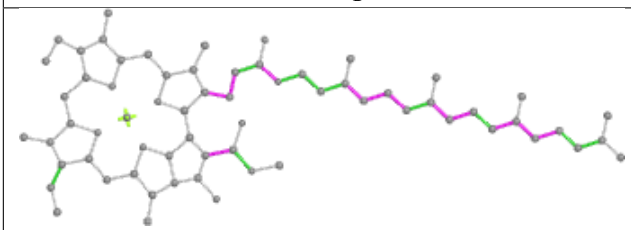


Bond angles



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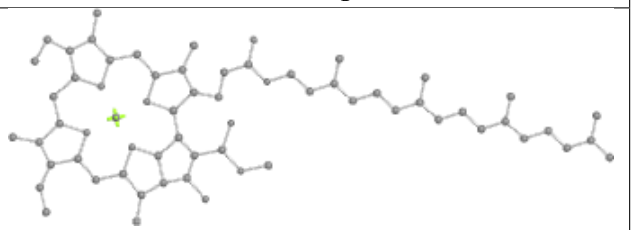
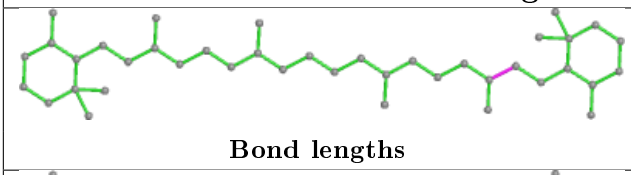
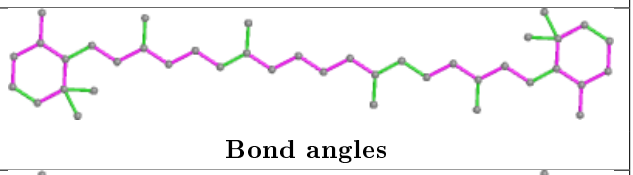


Rings

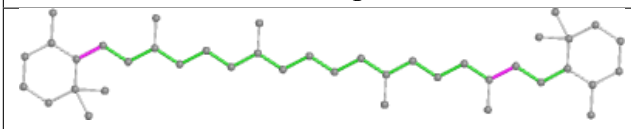
Ligand BCR G 105



Bond lengths



Bond angles



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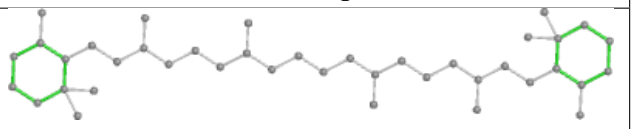
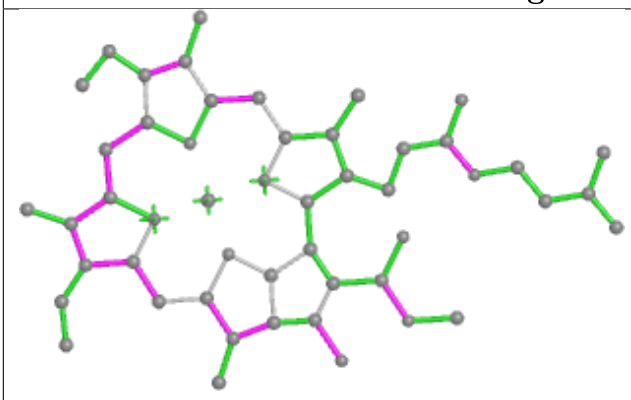
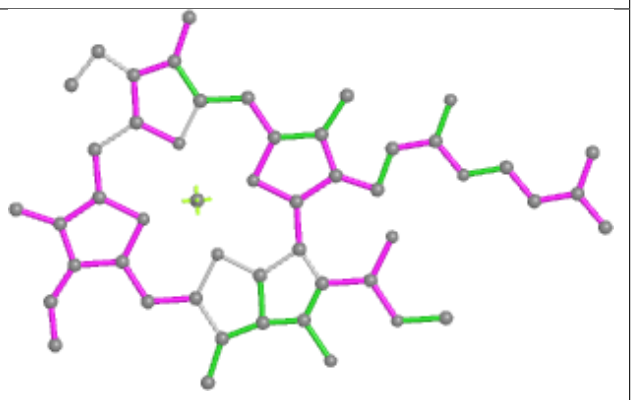


Rings

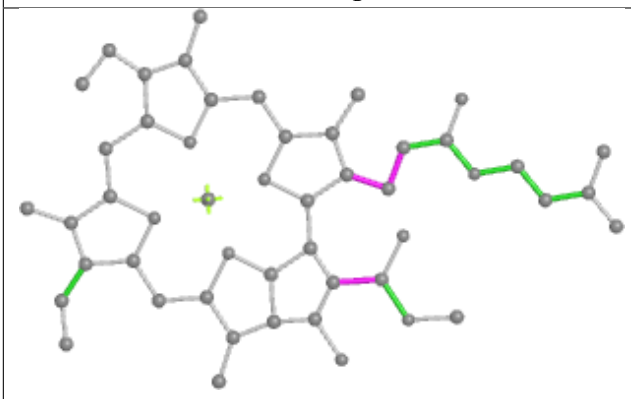
Ligand CLA b 830



Bond lengths



Bond angles



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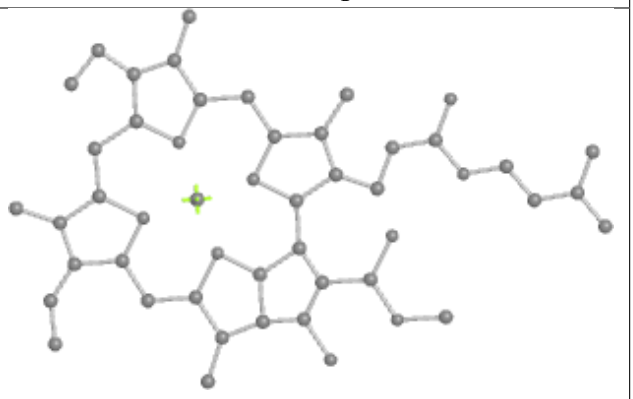
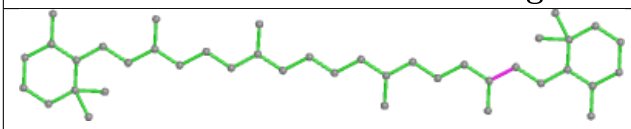


Rings

Ligand BCR 6 319



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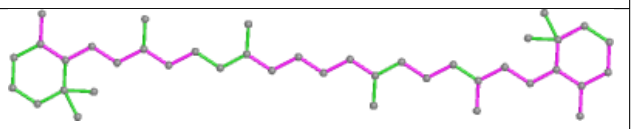
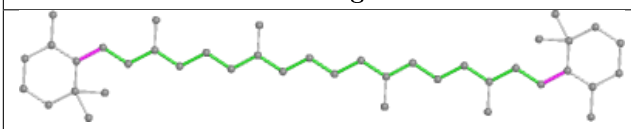


Bond angles



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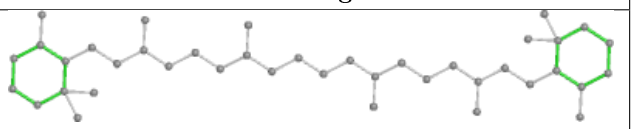
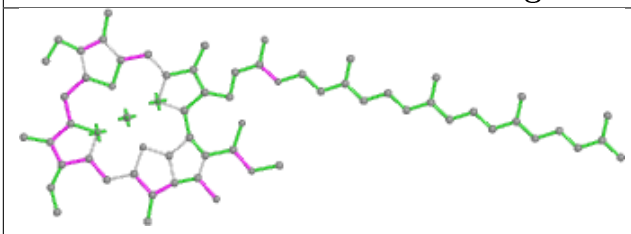
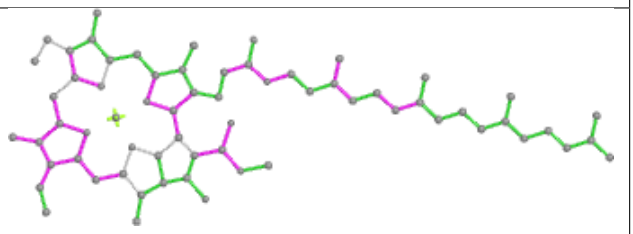


Rings

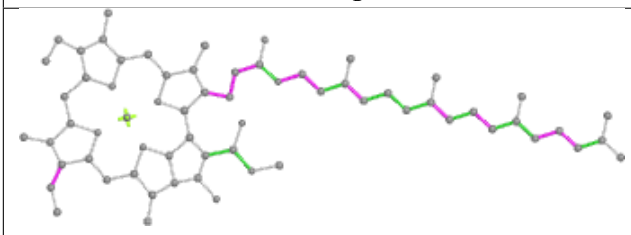
Ligand CLA B 832



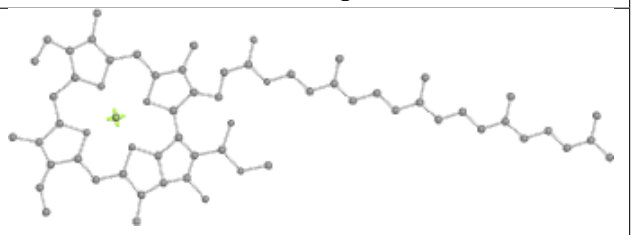
Bond lengths



Bond angles

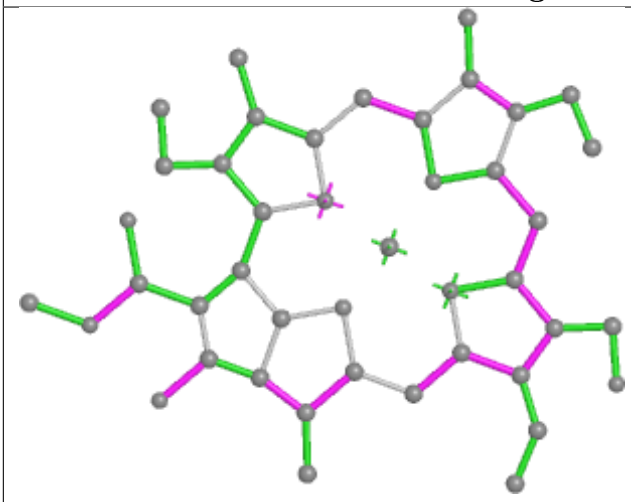


Torsions



Rings

Ligand CHL 9 615



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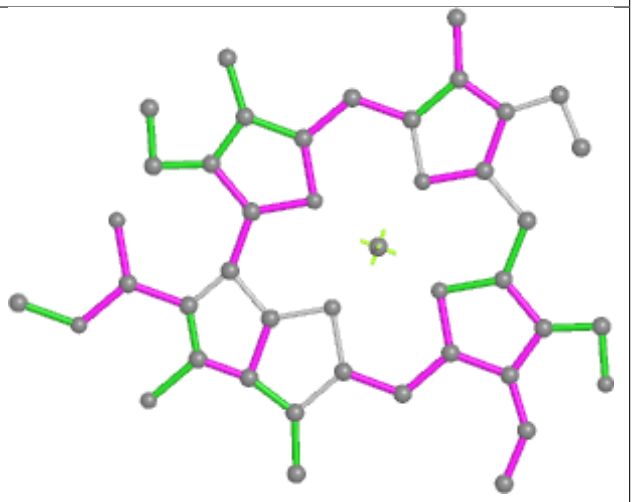
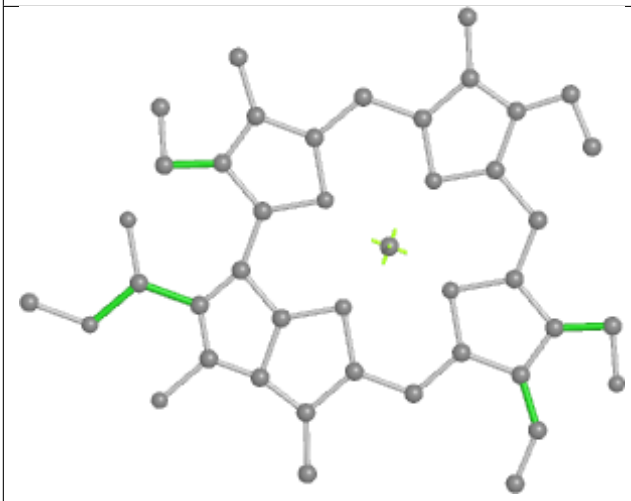


Bond angles



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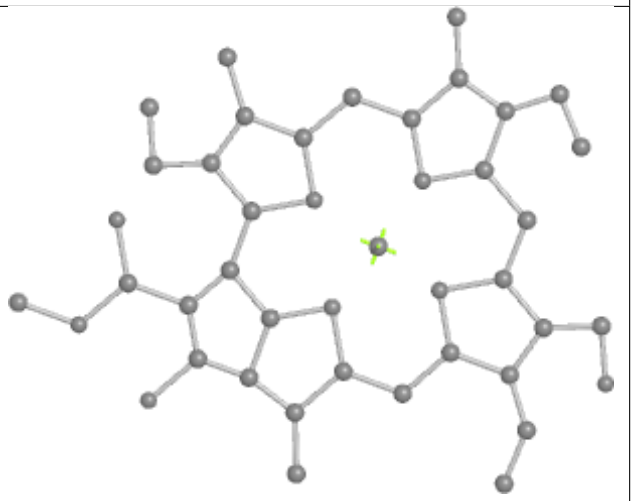
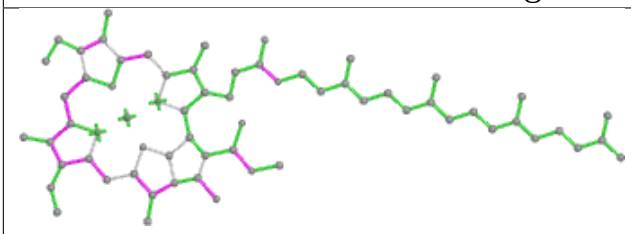
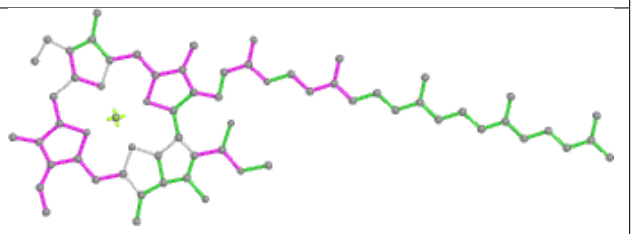


Rings

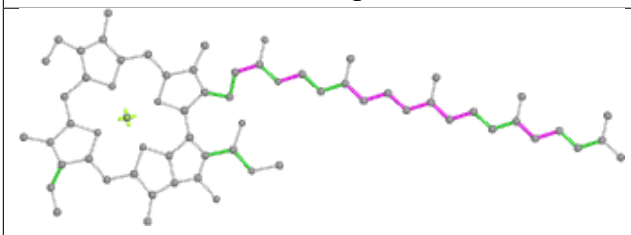
Ligand CLA B 802



Bond lengths



Bond angles



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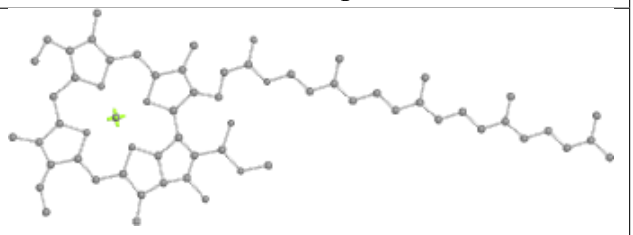
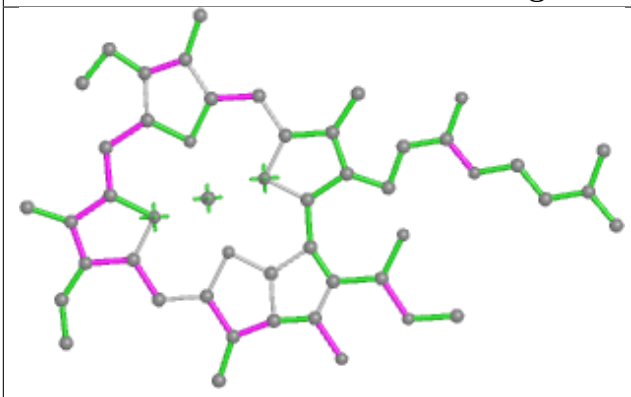
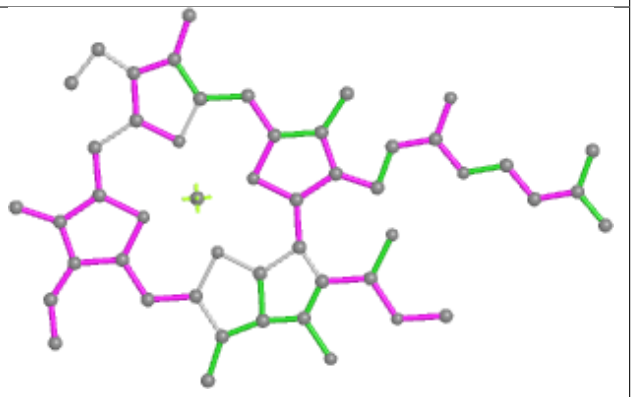


Rings

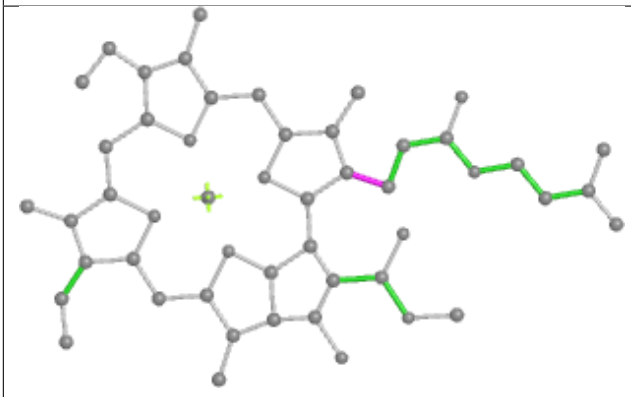
Ligand CLA 8 308



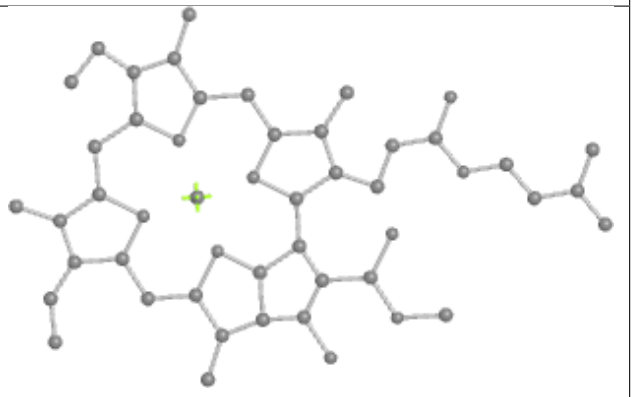
Bond lengths



Bond angles

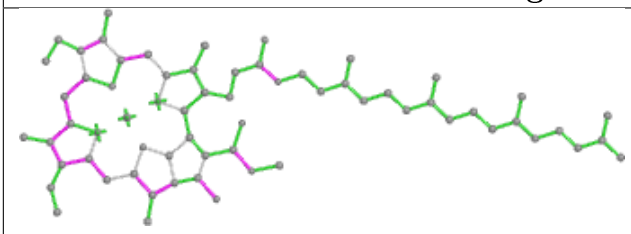


Torsions

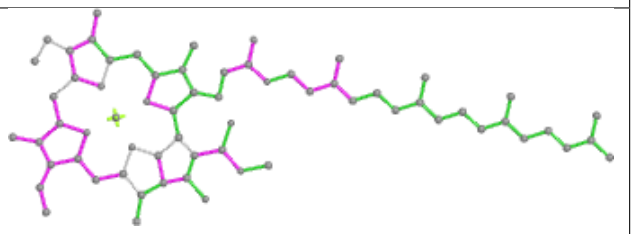


Rings

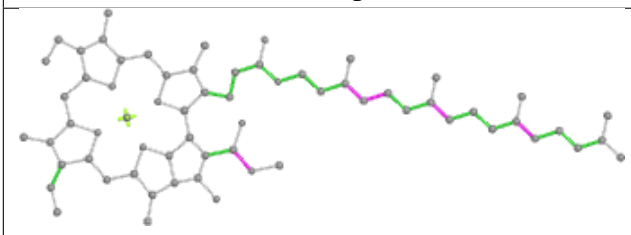
Ligand CLA F 301



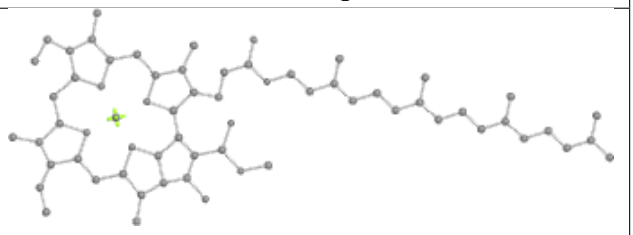
Bond lengths



Bond angles

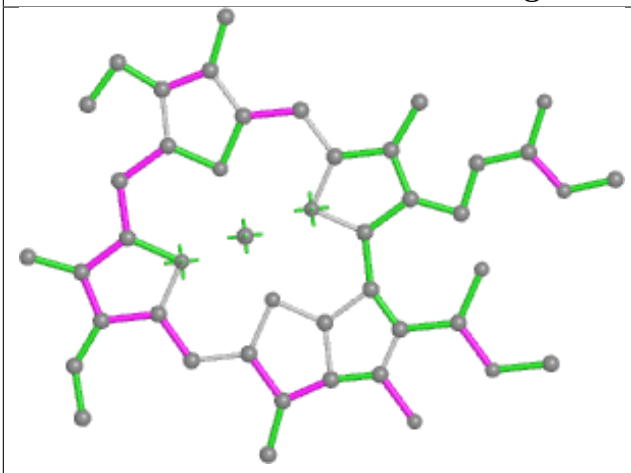


Torsions

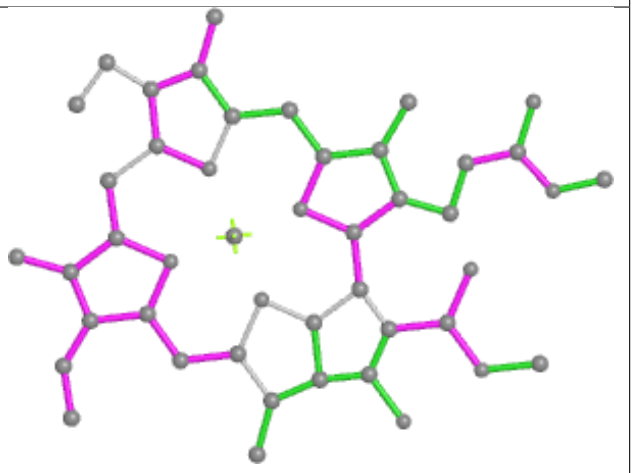


Rings

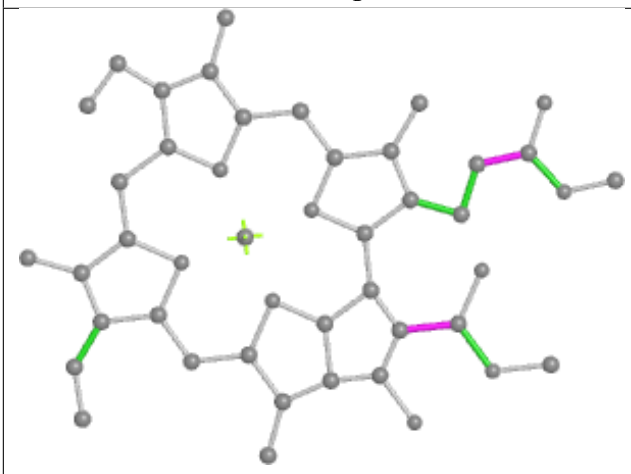
Ligand CLA G 104



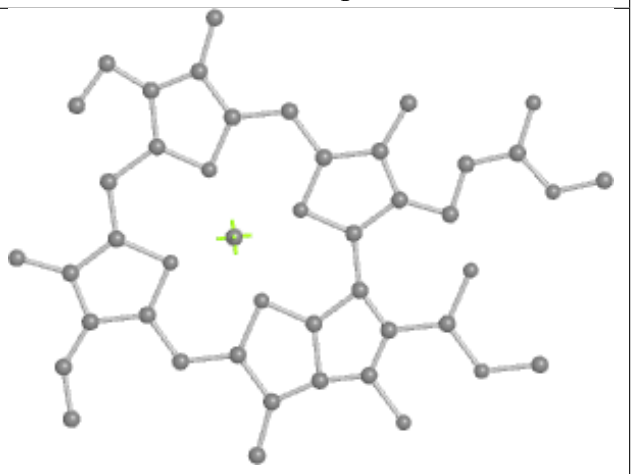
Bond lengths



Bond angles

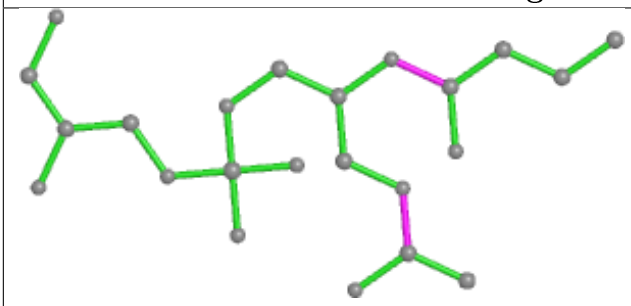


Torsions

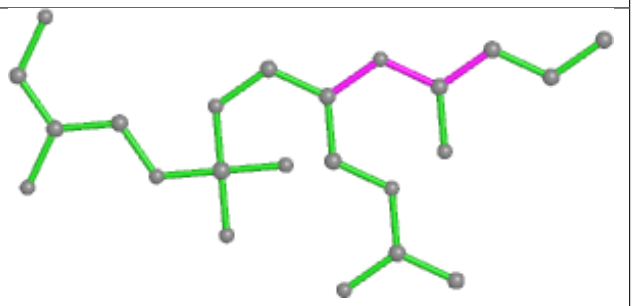


Rings

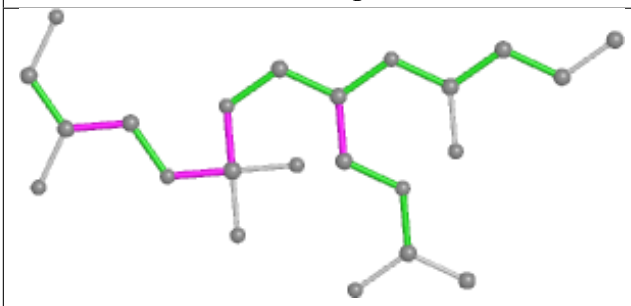
Ligand LHG 6 301



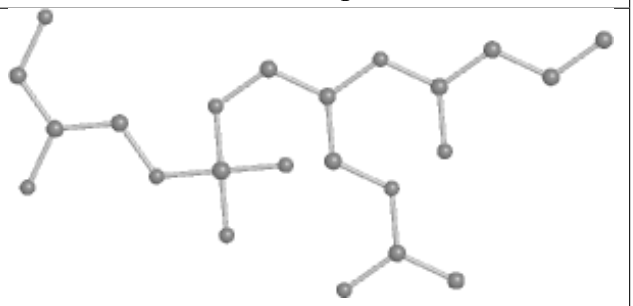
Bond lengths



Bond angles

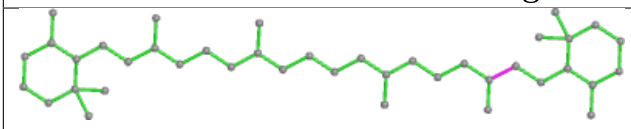


Torsions

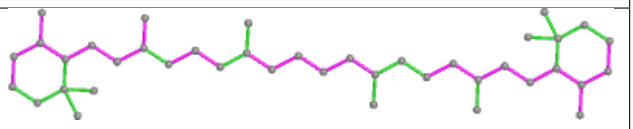


Rings

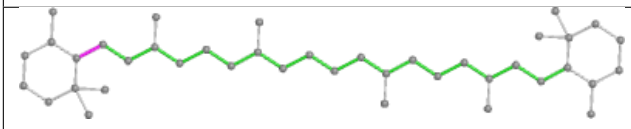
Ligand BCR A 849



Bond lengths



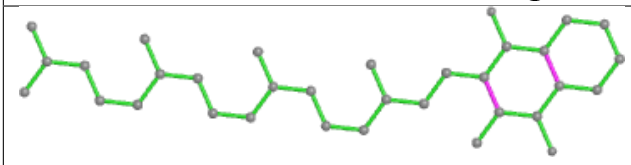
Bond angles



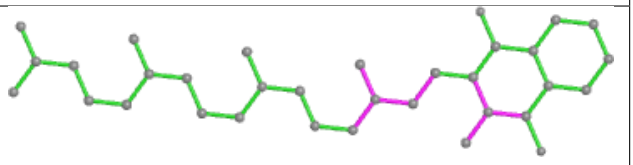
Torsions

Rings

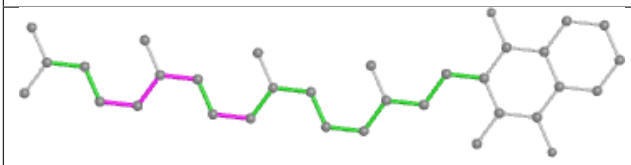
Ligand PQN a 845



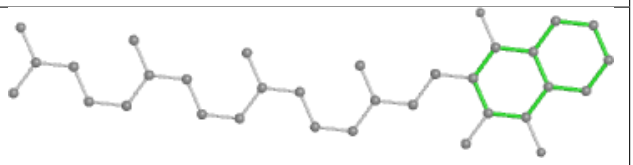
Bond lengths



Bond angles

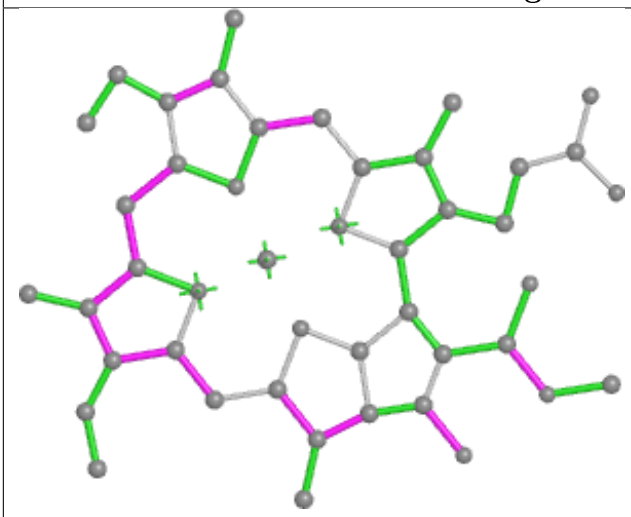


Torsions

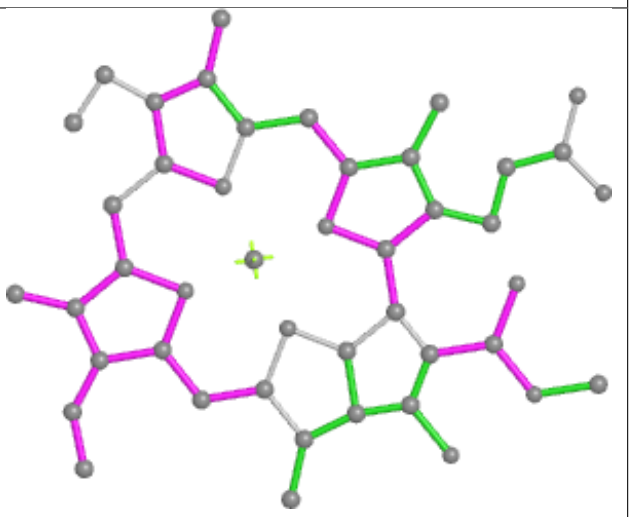


Rings

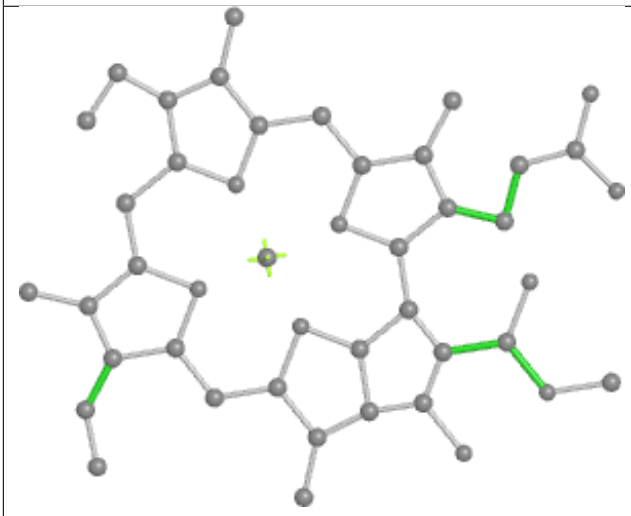
Ligand CLA A 821



Bond lengths



Bond angles



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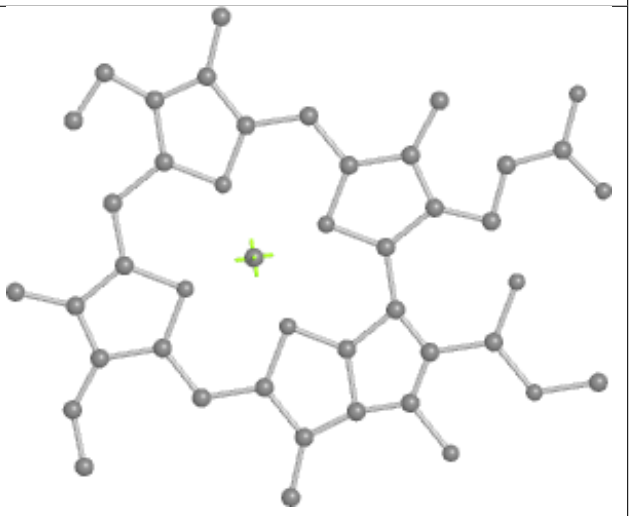
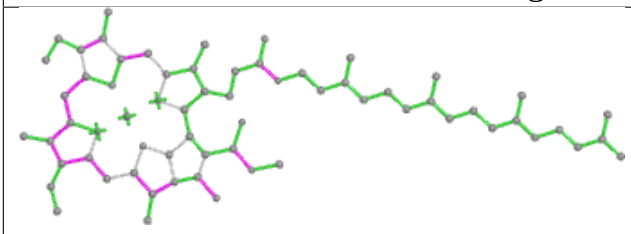


Rings

Ligand CLA b 841



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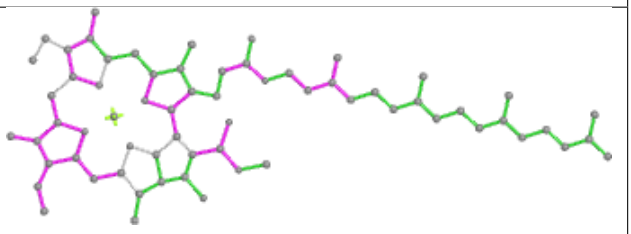
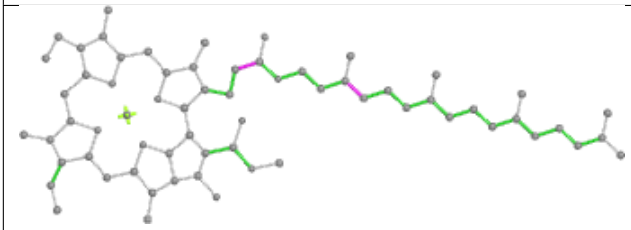
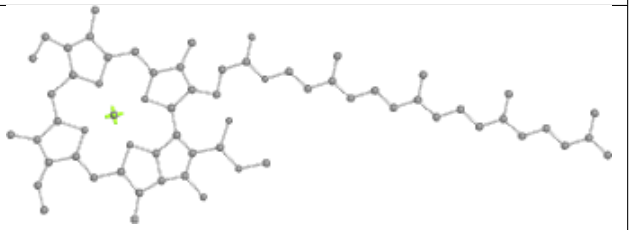


Bond angles

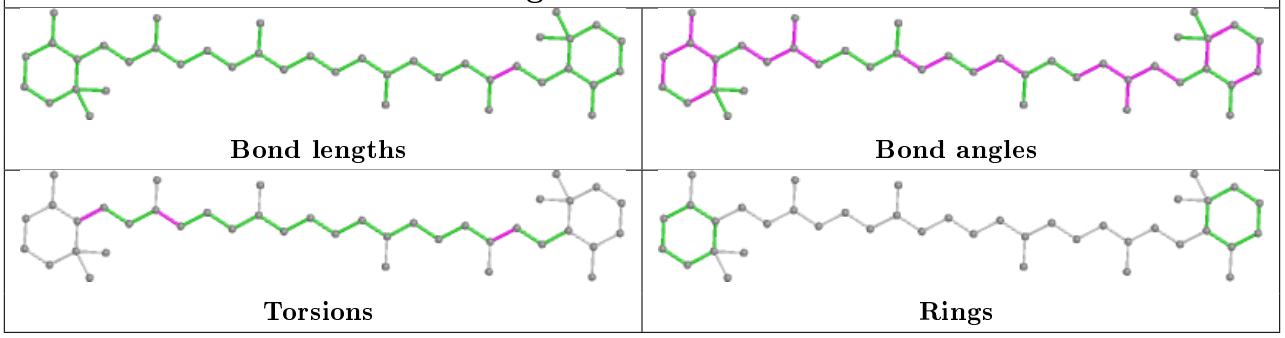


Torsions

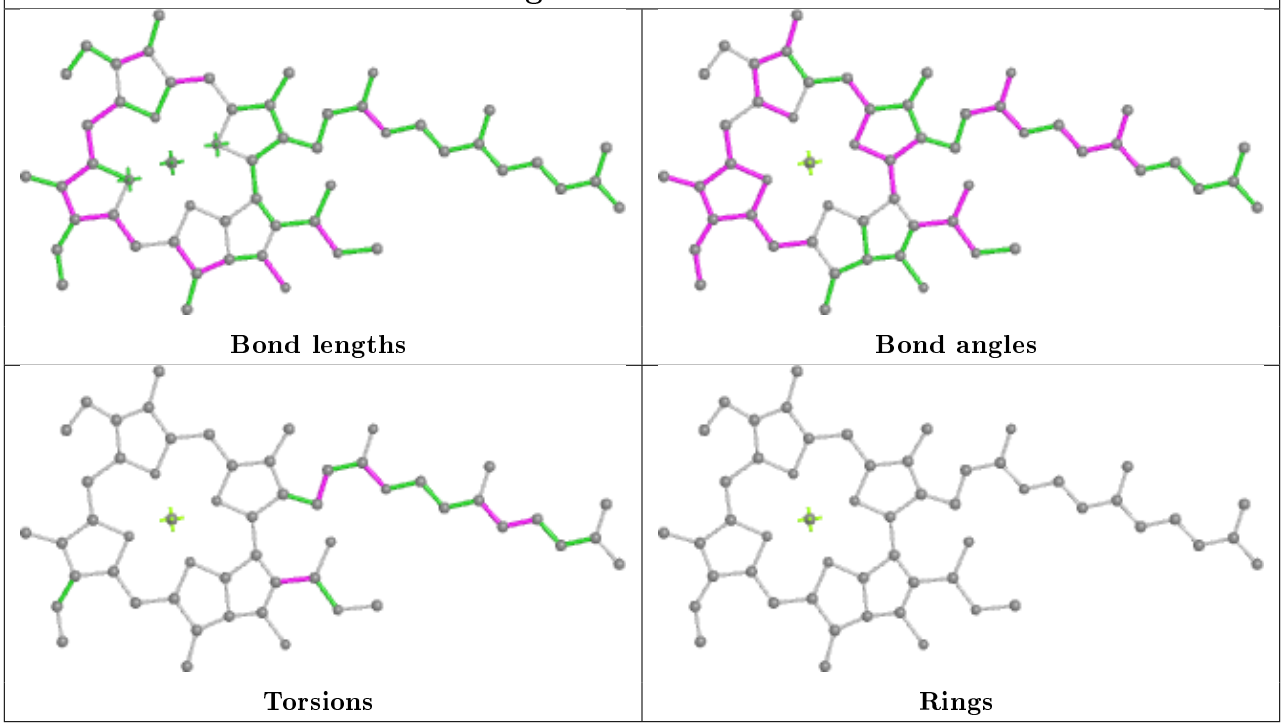


Rings

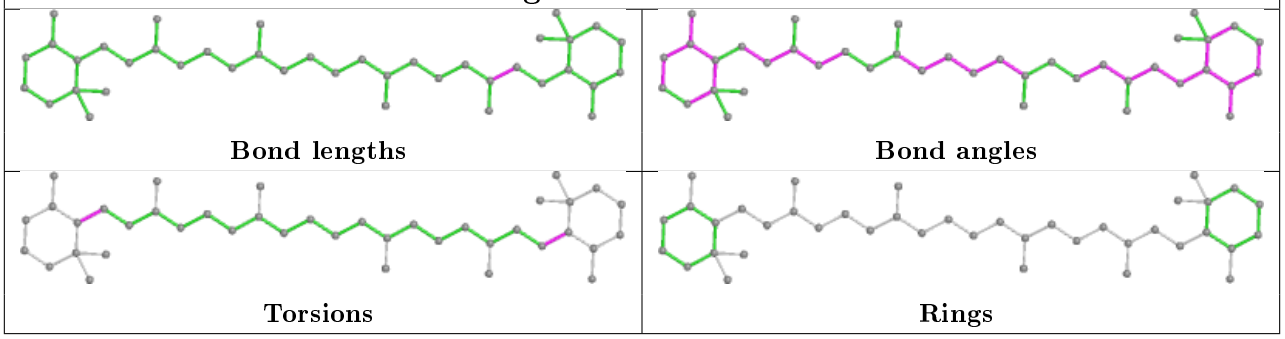
Ligand BCR b 844



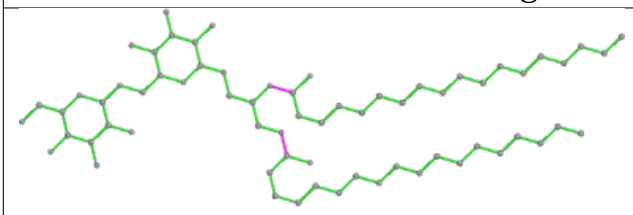
Ligand CLA A 805



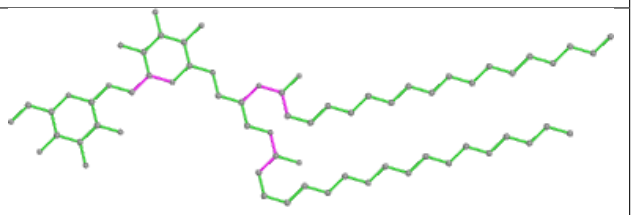
Ligand BCR A 850



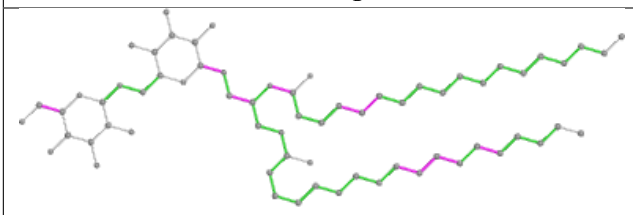
Ligand DGD B 850



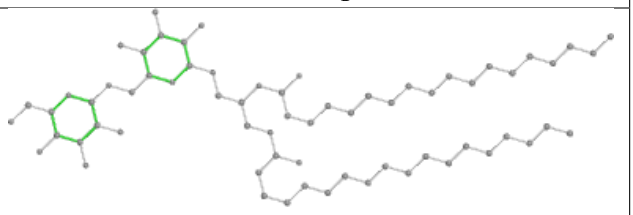
Bond lengths



Bond angles

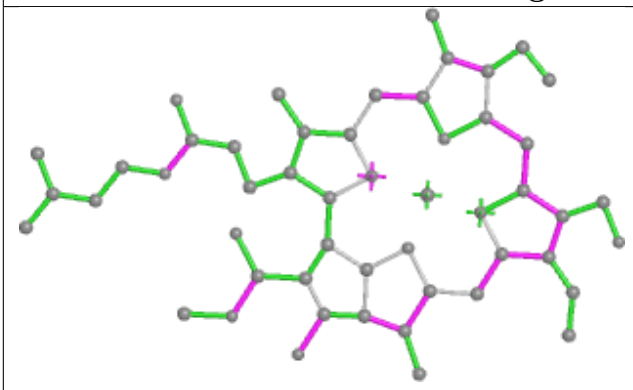


Torsions



Rings

Ligand CHL 9 606



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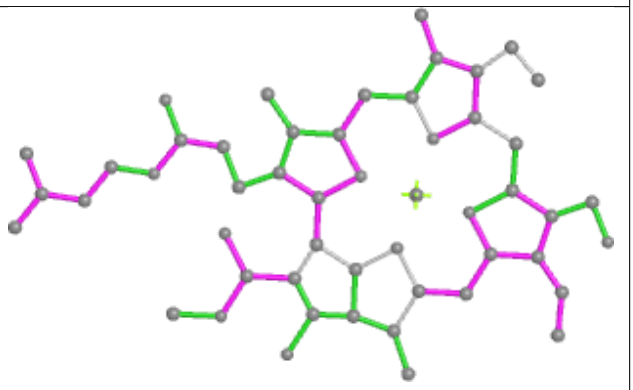
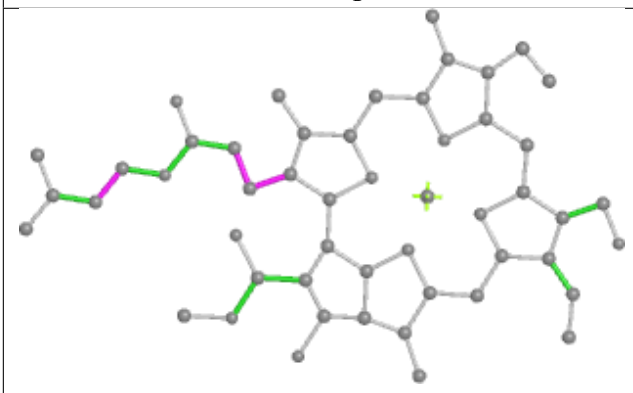
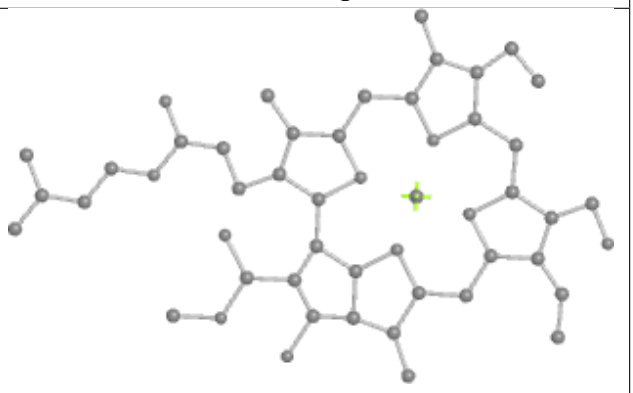


Bond angles

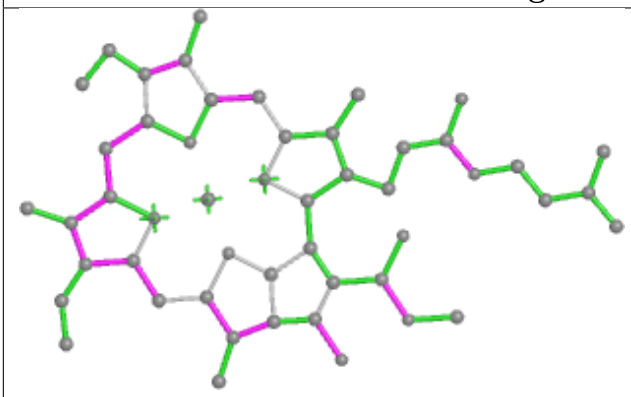


Torsions

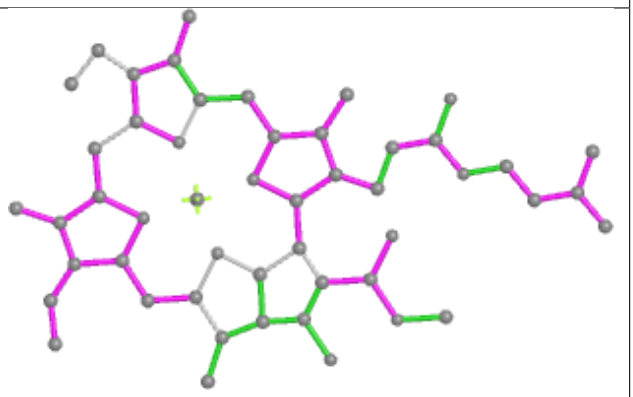


Rings

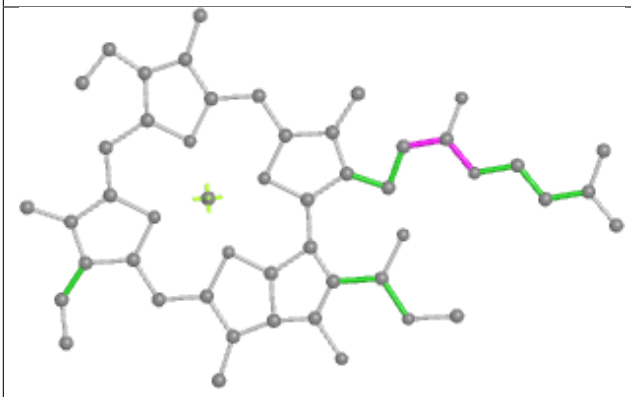
Ligand CLA 2 608



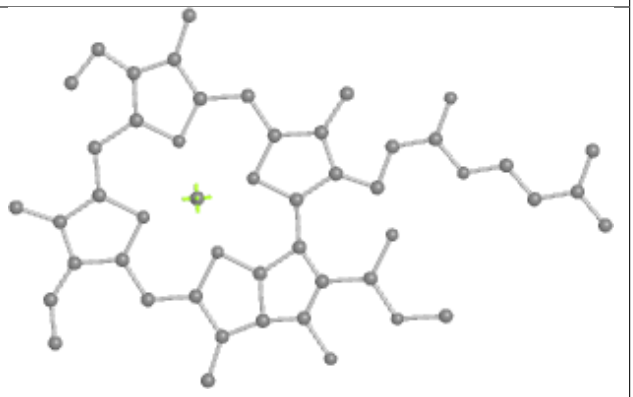
Bond lengths



Bond angles

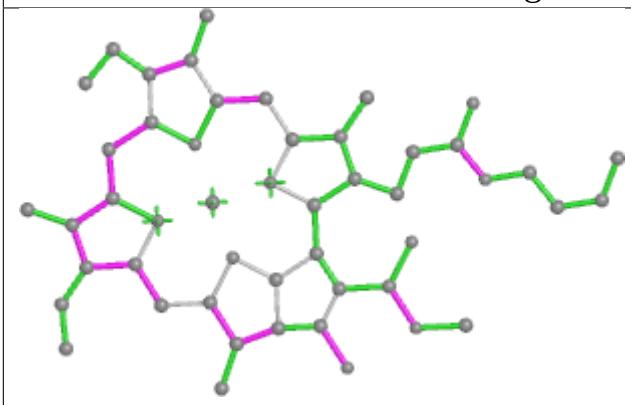


Torsions

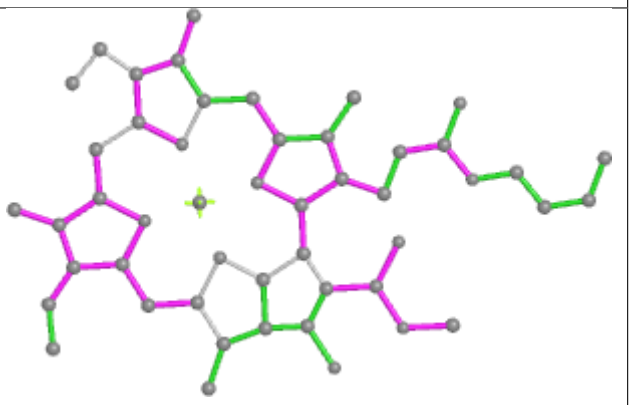


Rings

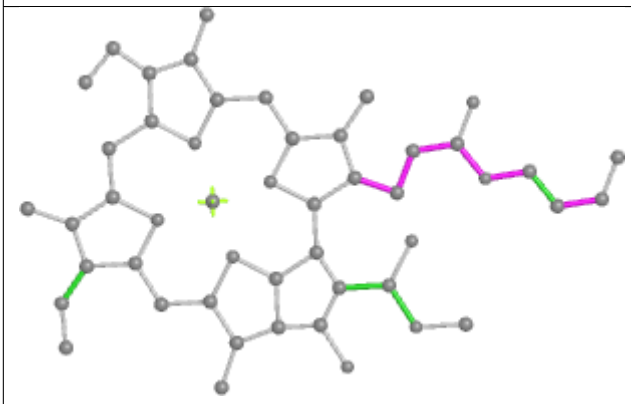
Ligand CLA B 831



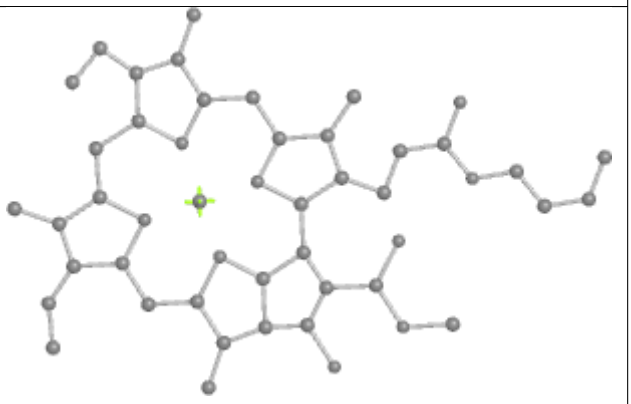
Bond lengths



Bond angles

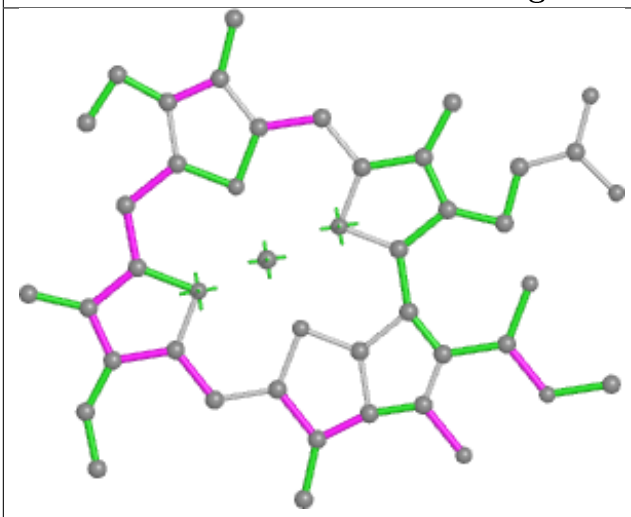


Torsions

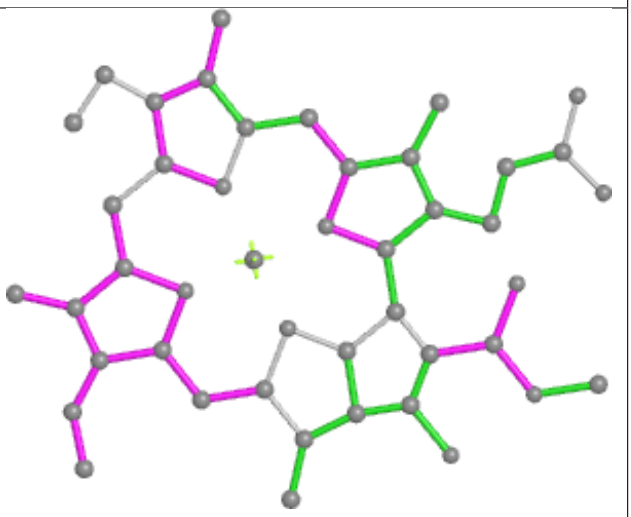


Rings

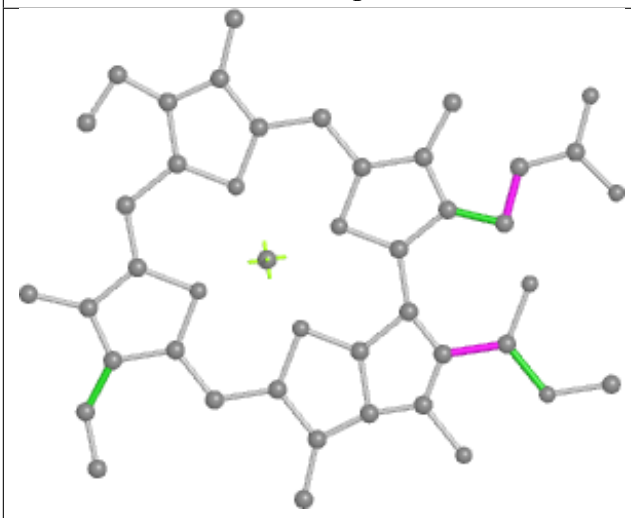
Ligand CLA a 821



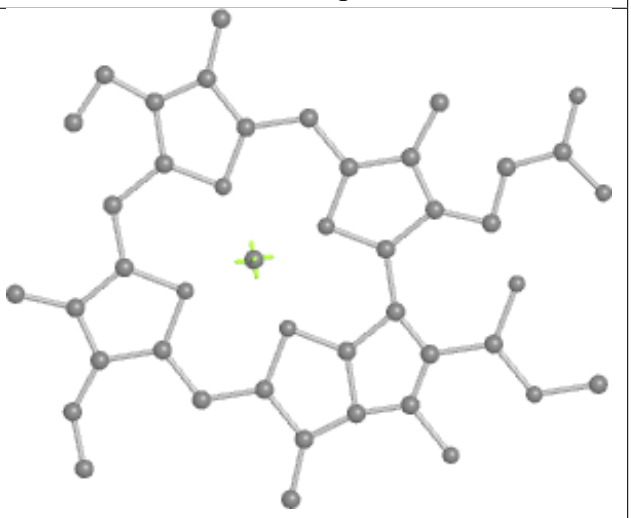
Bond lengths



Bond angles

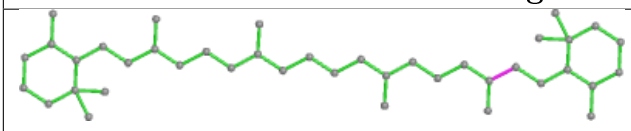


Torsions

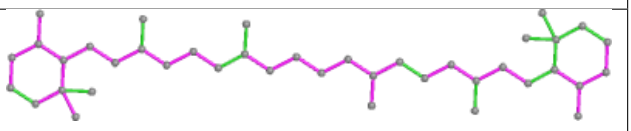


Rings

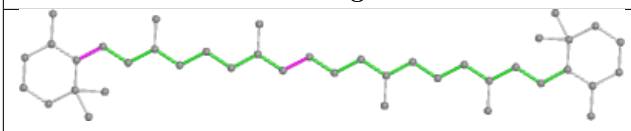
Ligand BCR 2 617



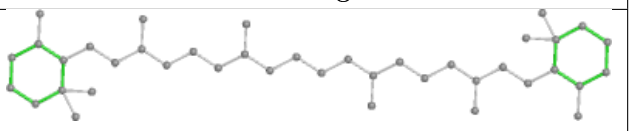
Bond lengths



Bond angles

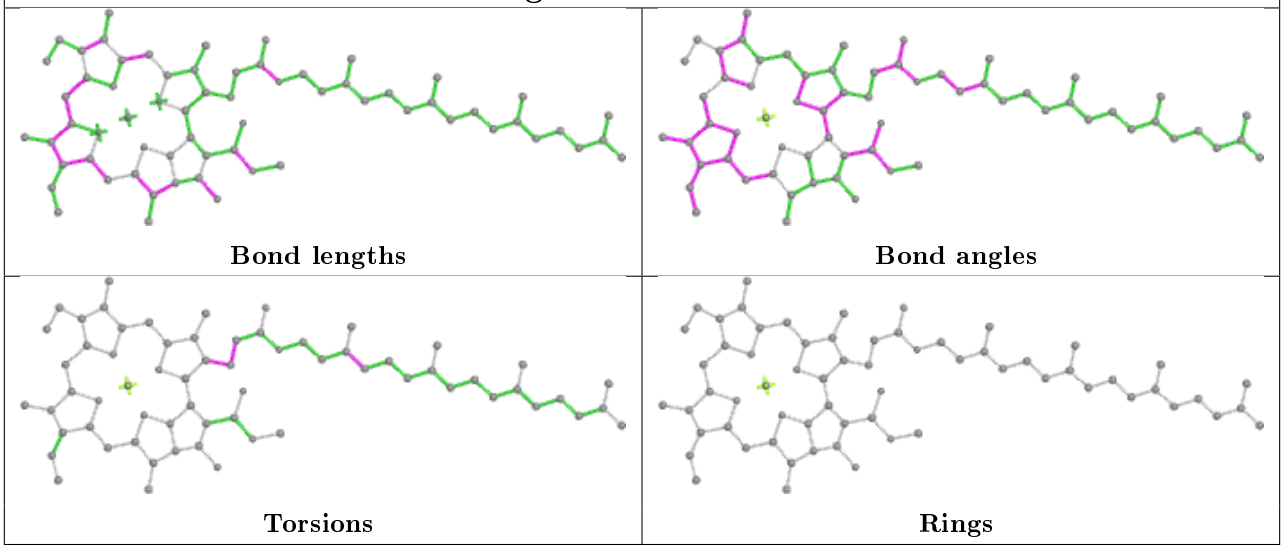


Torsions

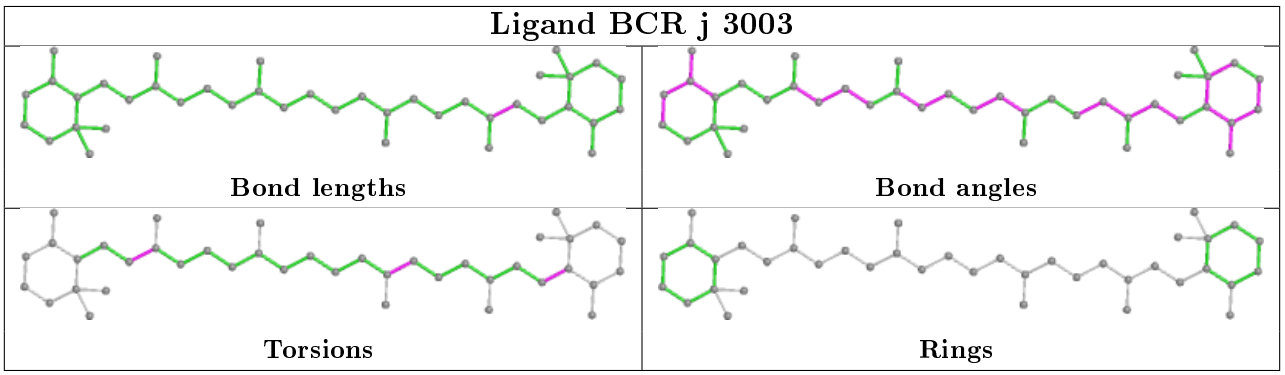


Rings

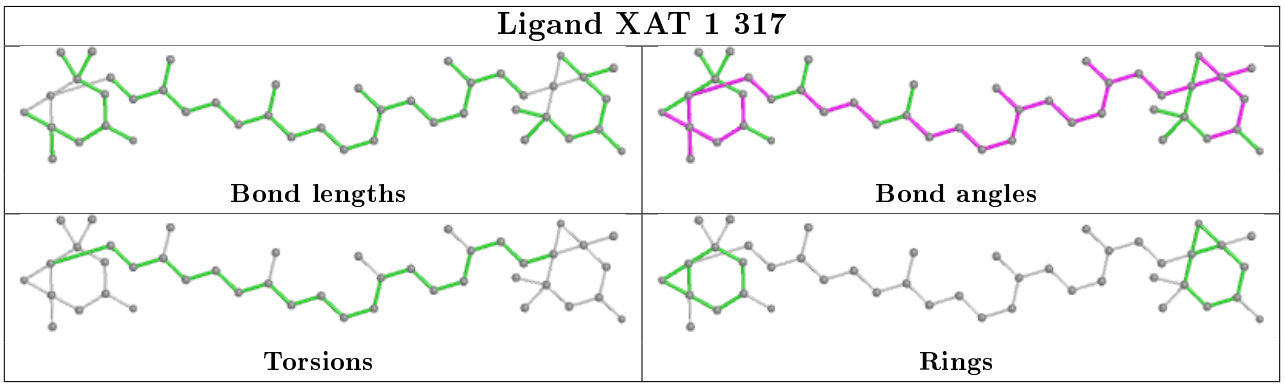
Ligand CLA B 828



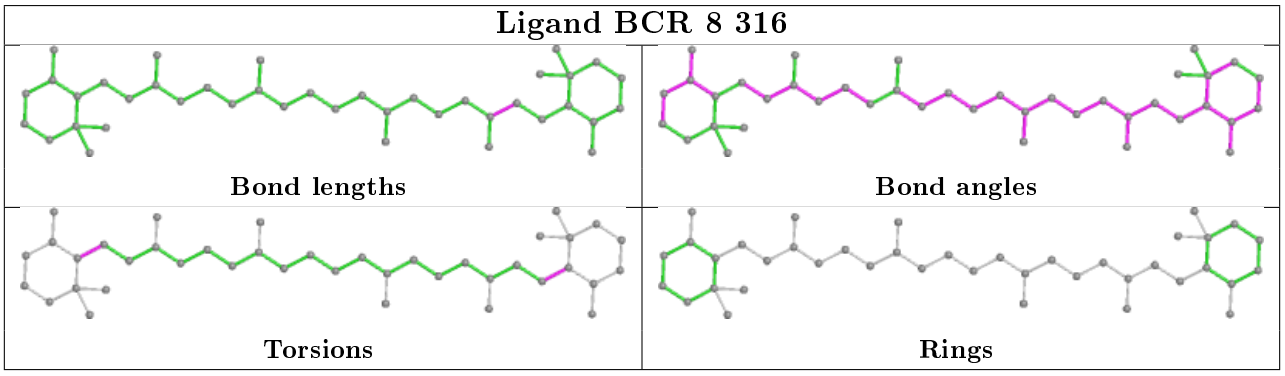
Ligand BCR j 3003



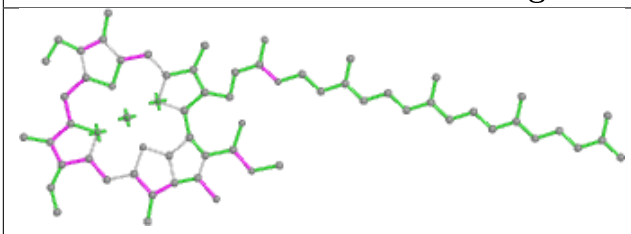
Ligand XAT 1 317



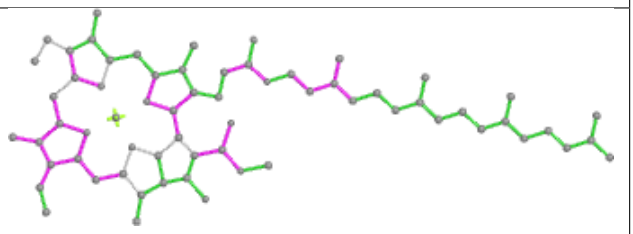
Ligand BCR 8 316



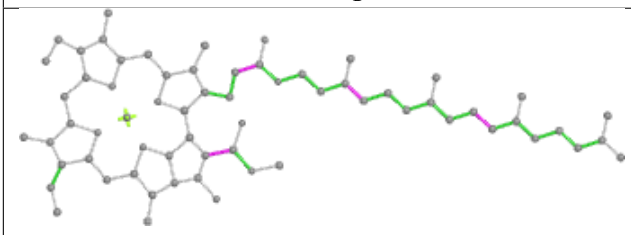
Ligand CLA a 826



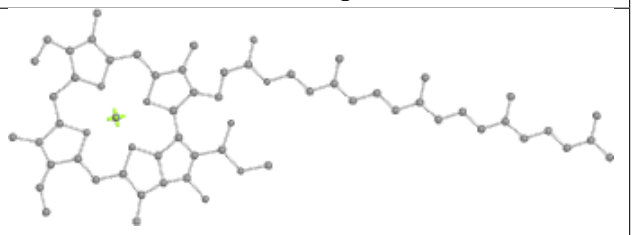
Bond lengths



Bond angles

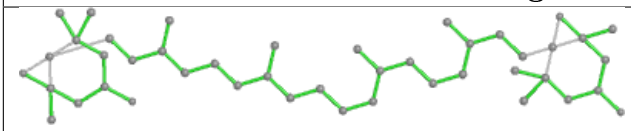


Torsions



Rings

Ligand XAT 6 318



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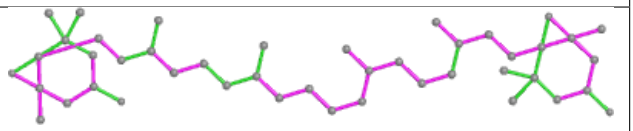

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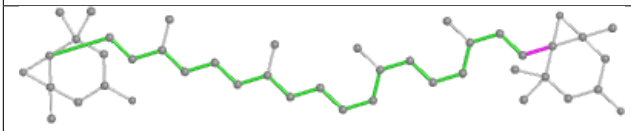

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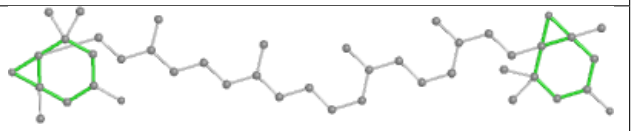
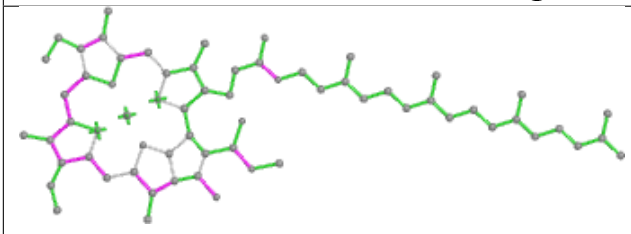


Rings

Ligand CLA a 834



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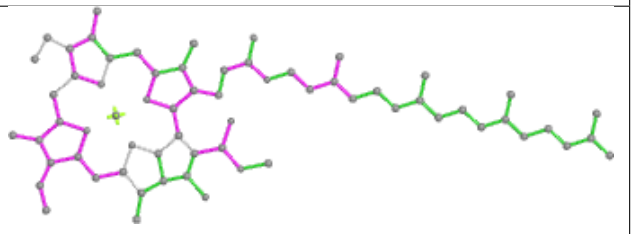
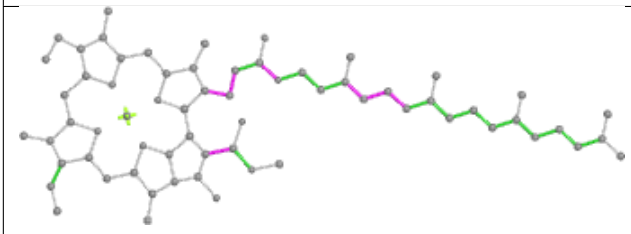


Bond angles



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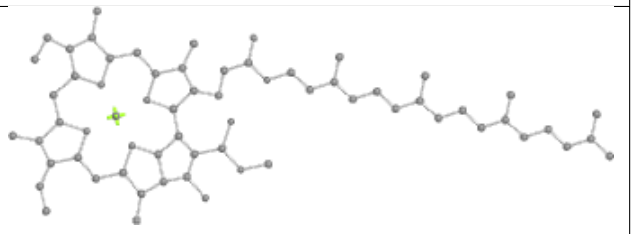
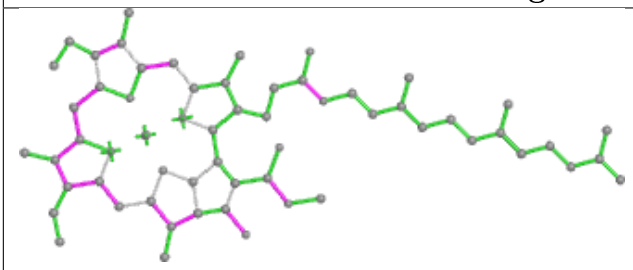


Rings

Ligand CLA 9 602



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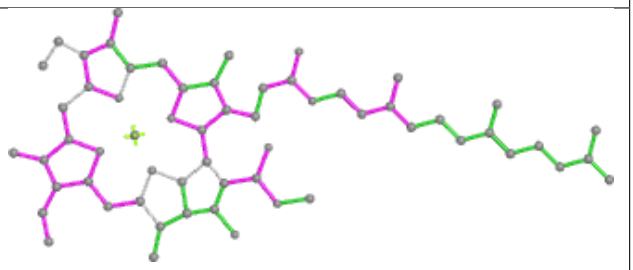

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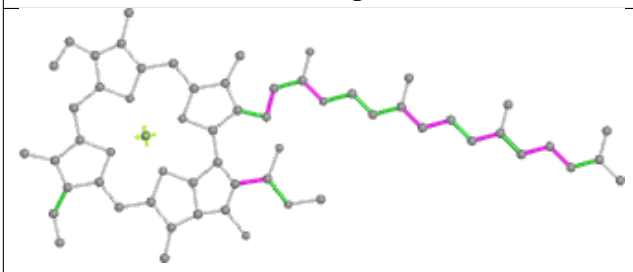

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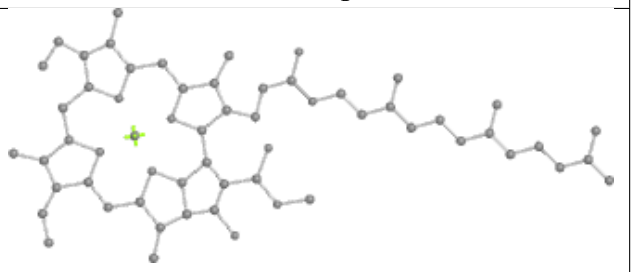

Rings

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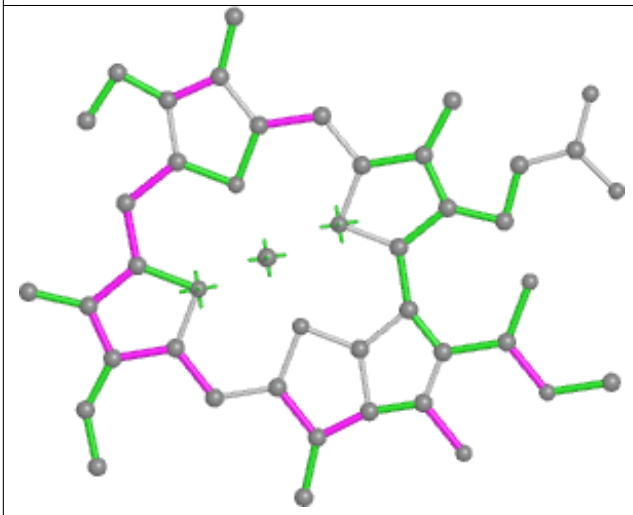

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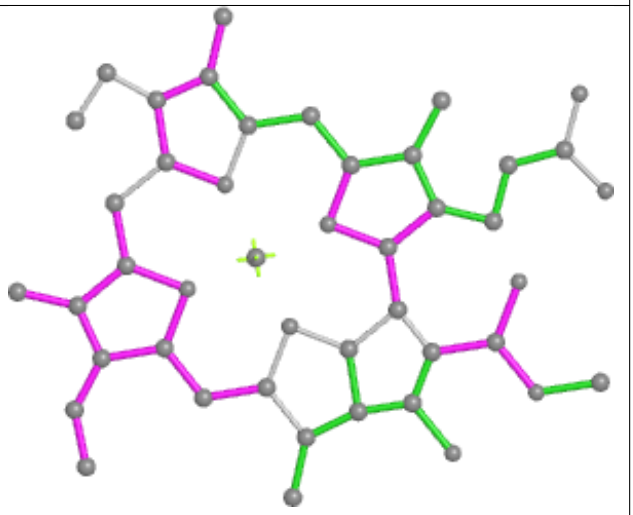

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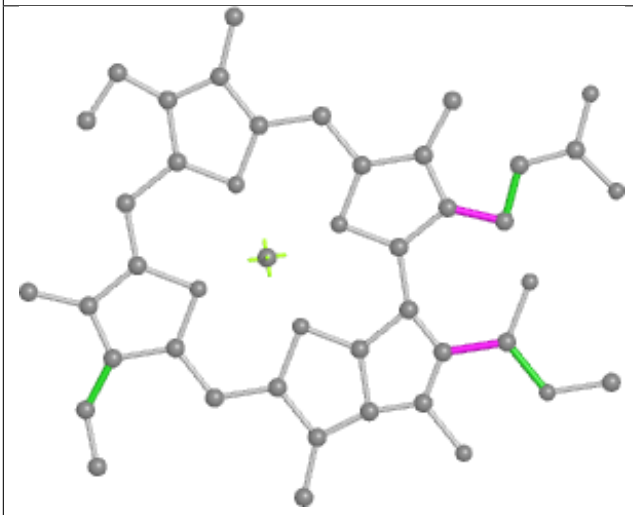

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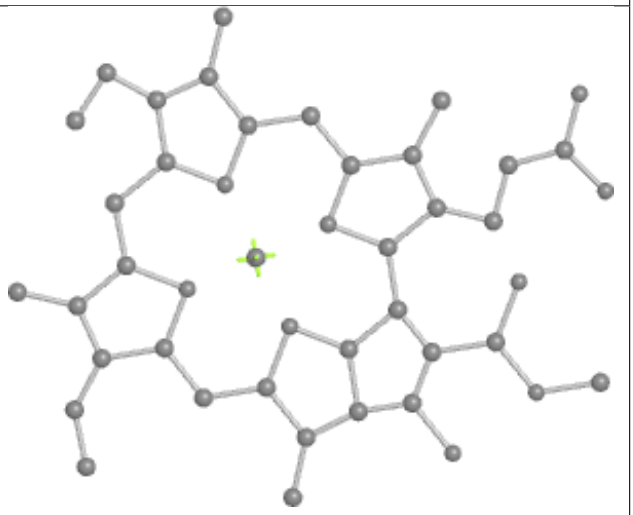
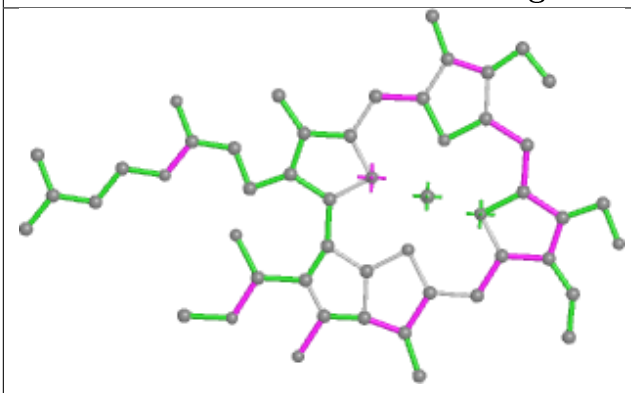


Rings

Ligand CHL 4 607



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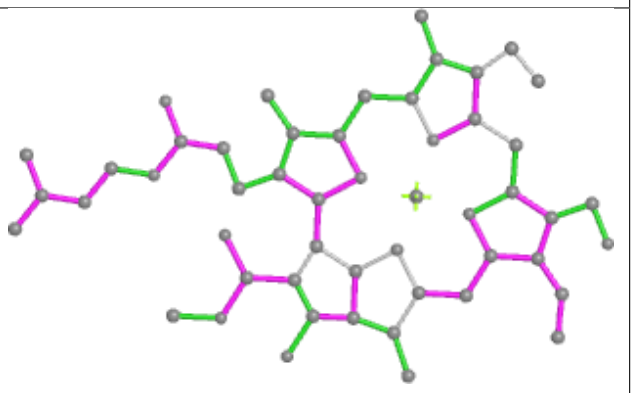

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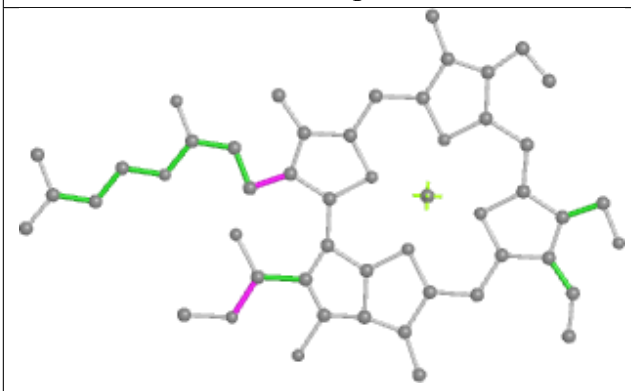

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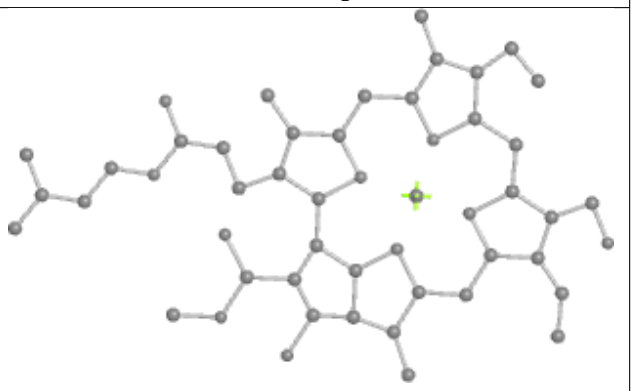

Rings

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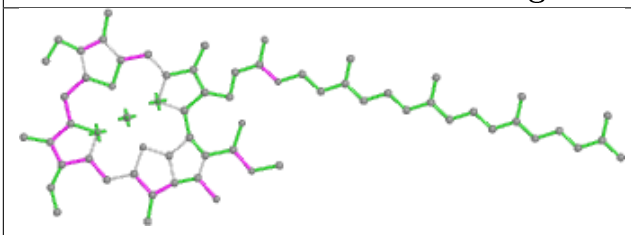

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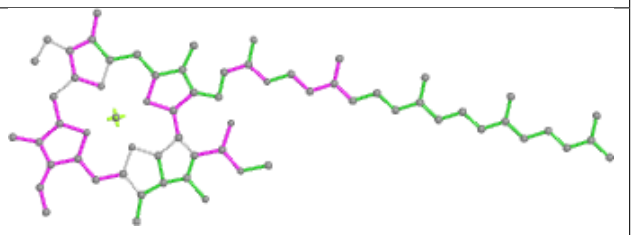
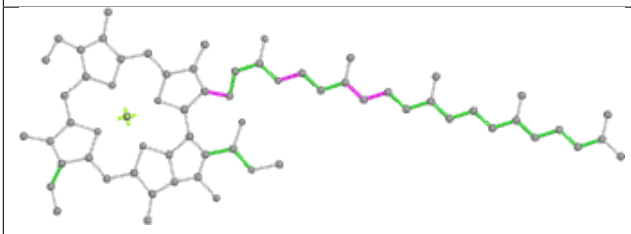


Bond angles



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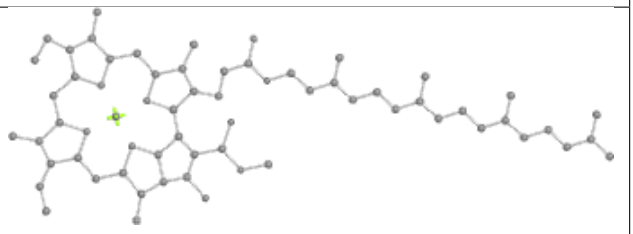
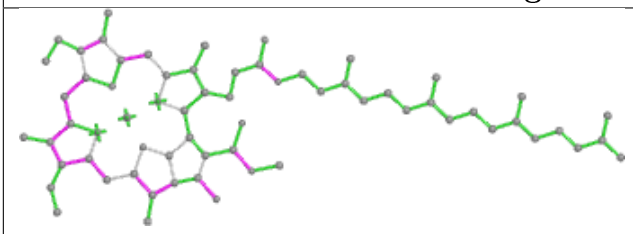


Rings

Ligand CLA A 818



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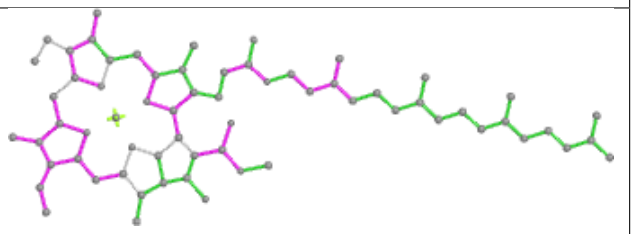
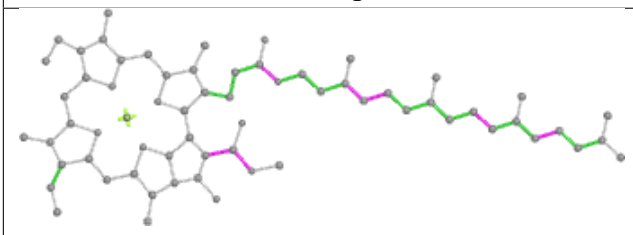


Bond angles



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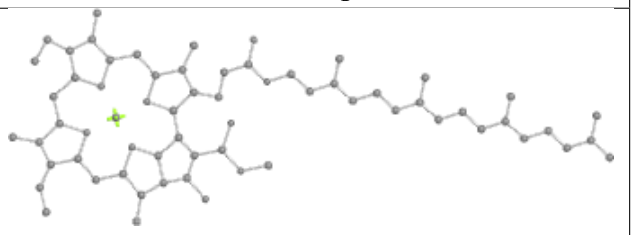
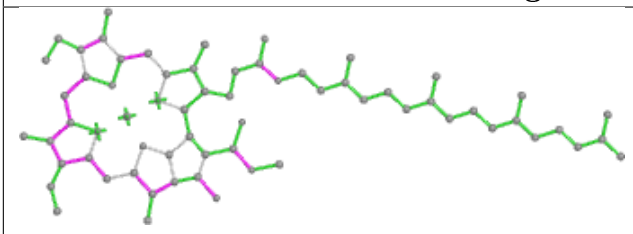


Rings

Ligand CLA A 812



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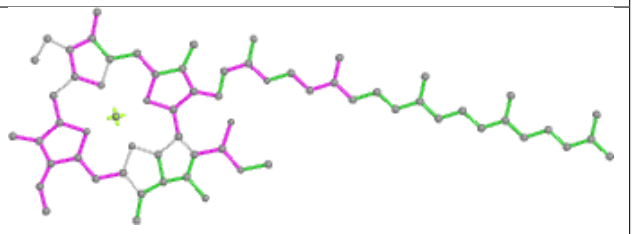

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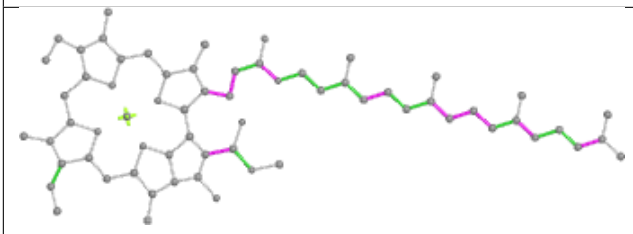

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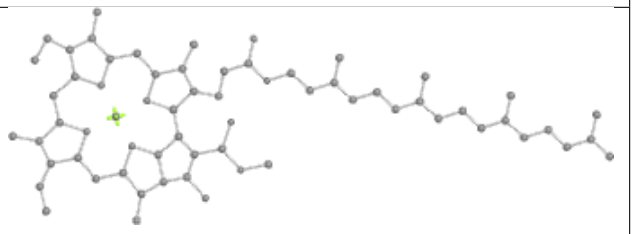
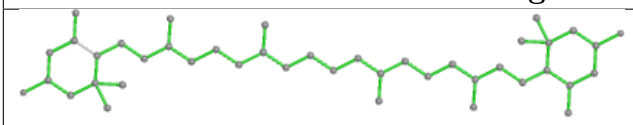


Rings

Ligand LUT 2 615



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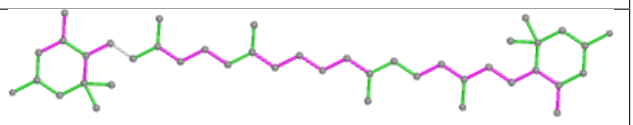

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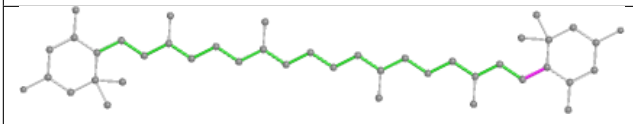

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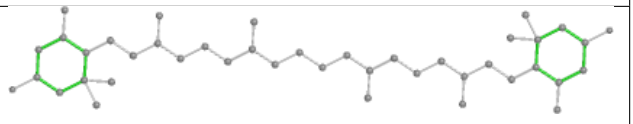
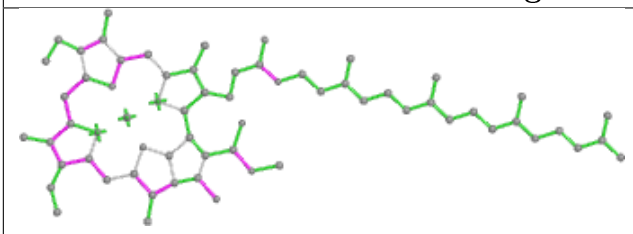


Rings

Ligand CLA A 841



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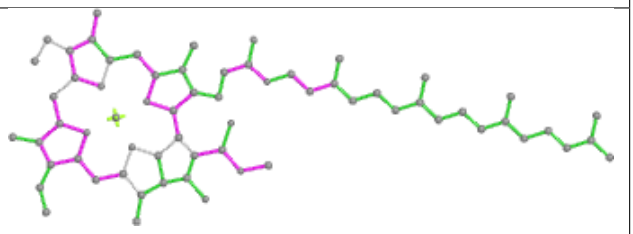
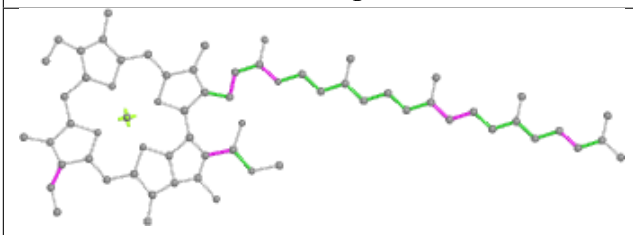


Bond angles



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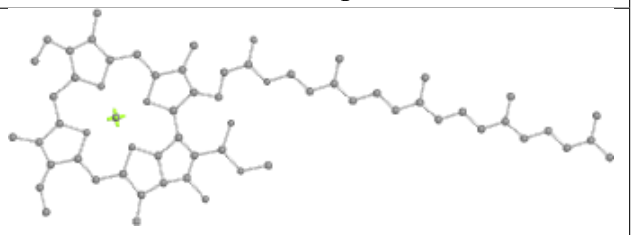
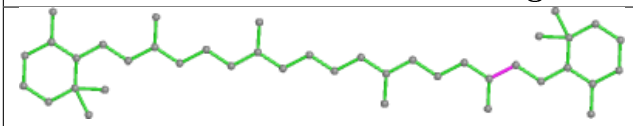


Rings

Ligand BCR 3 318



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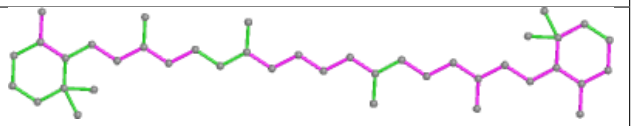

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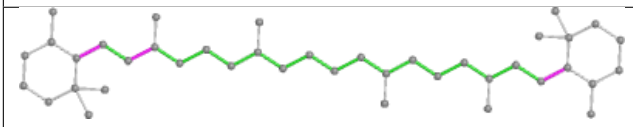
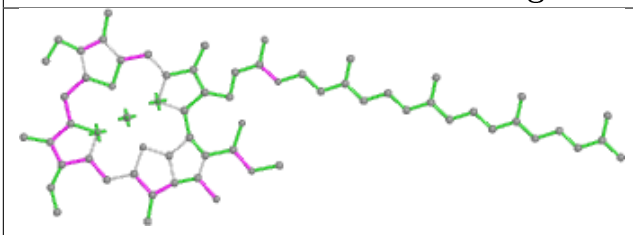


Torsions

Rings

Ligand CLA b 827



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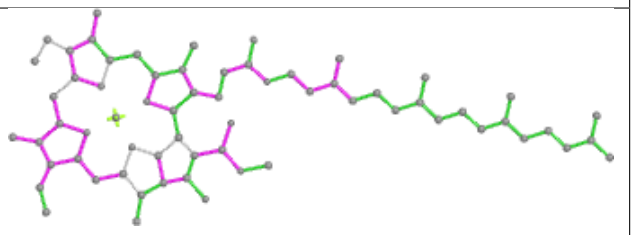
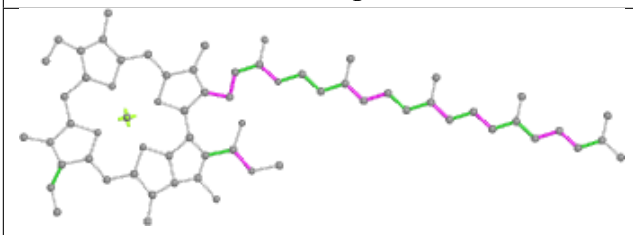


Bond angles



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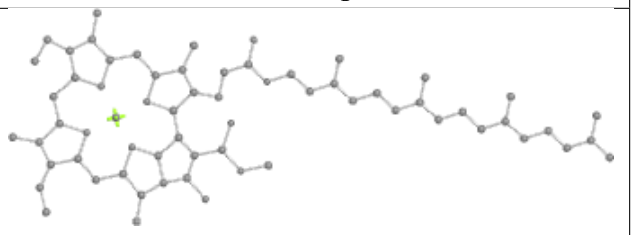
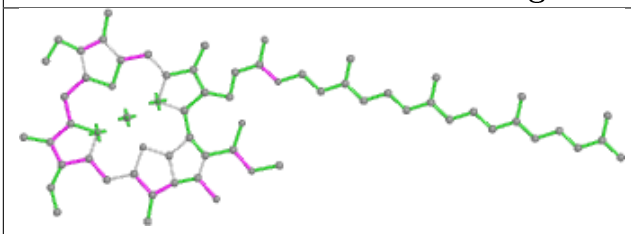
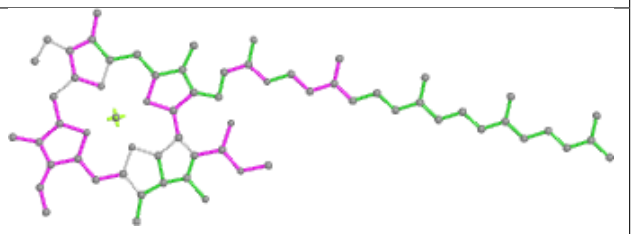


Rings

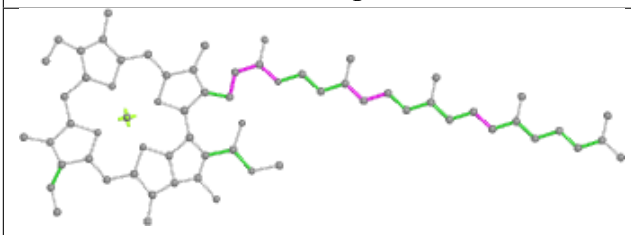
Ligand CLA 2 612



Bond lengths



Bond angles



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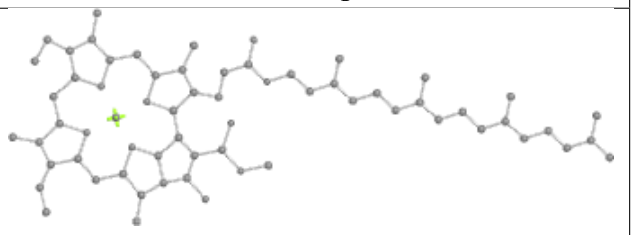
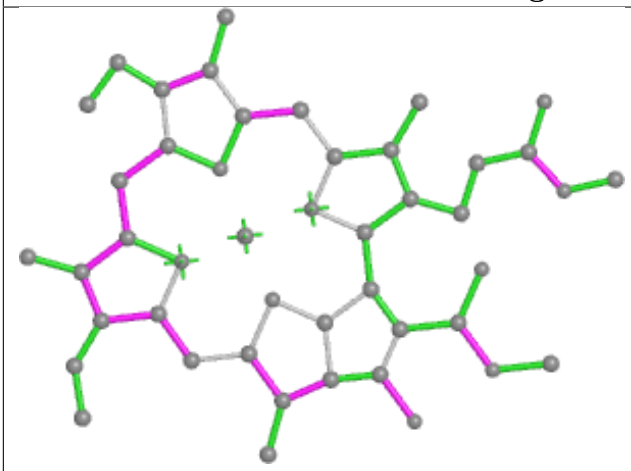


Rings

Ligand CLA 3 301



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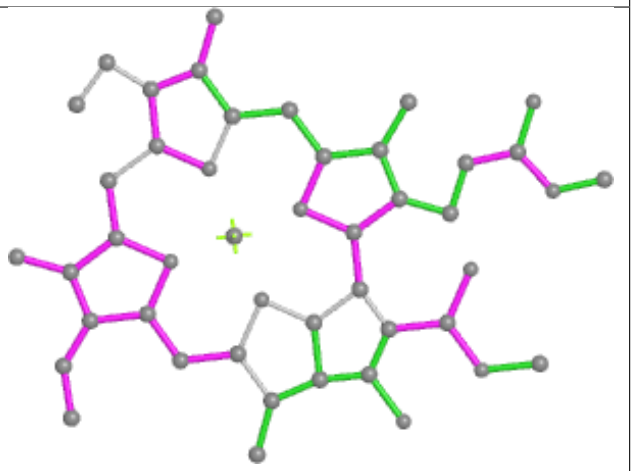
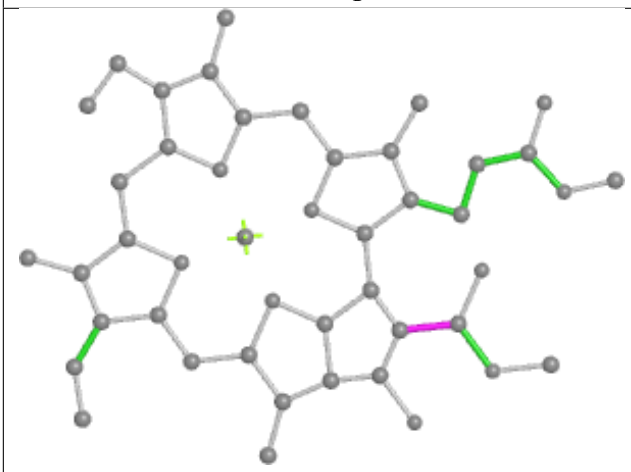


Bond angles



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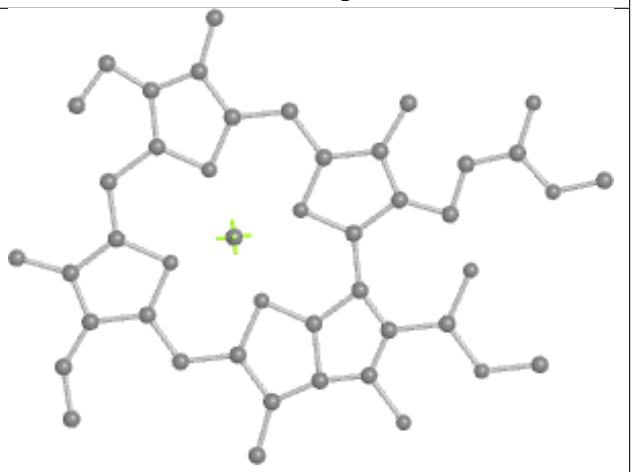
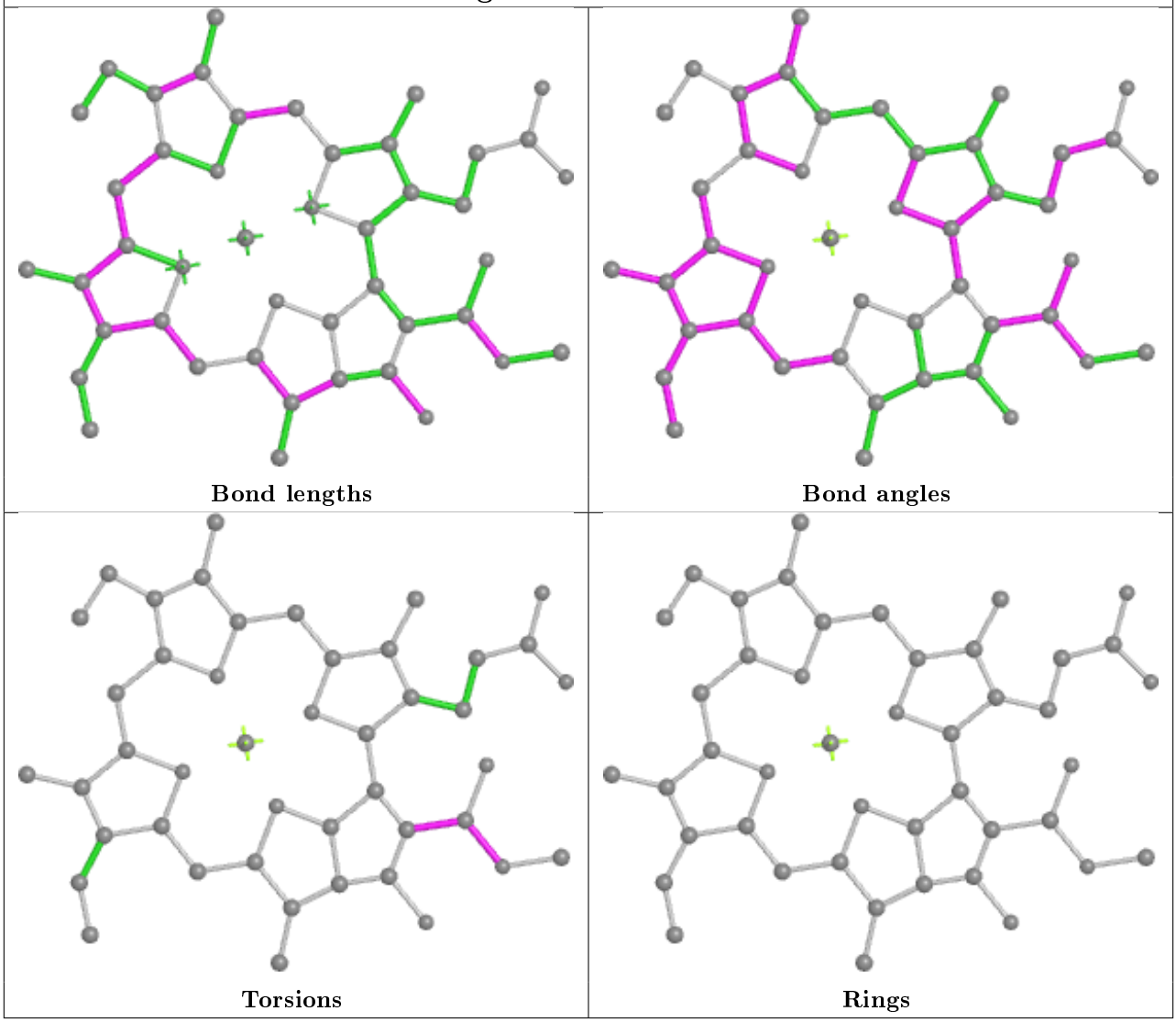
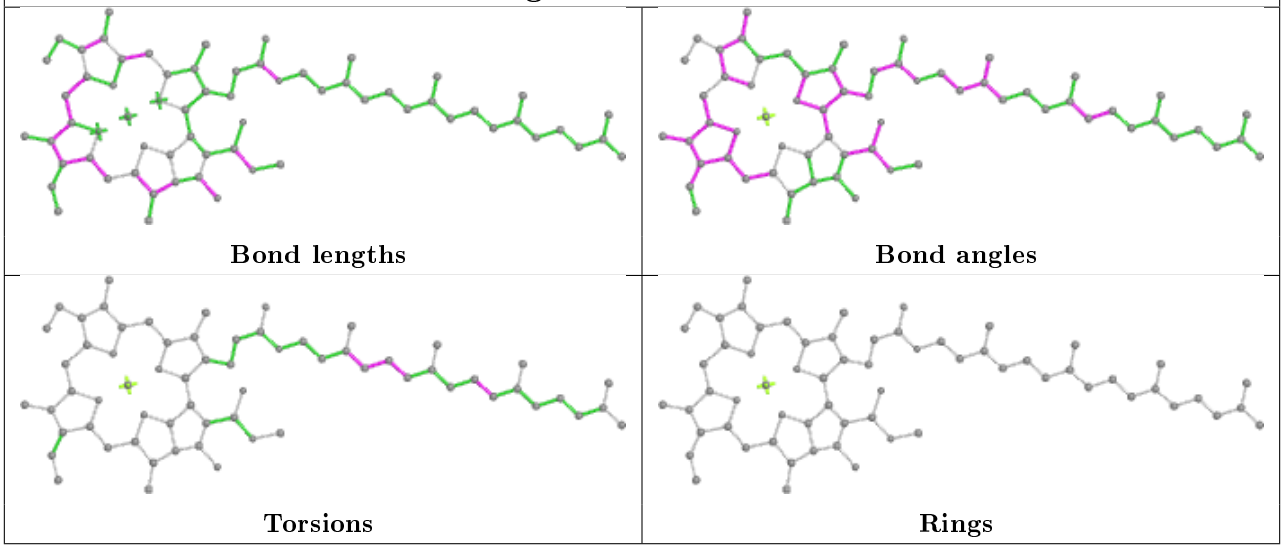


Rings

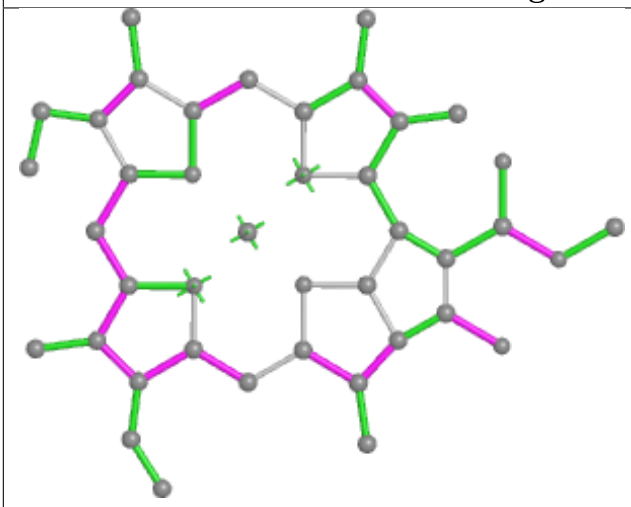
Ligand CLA k 1401



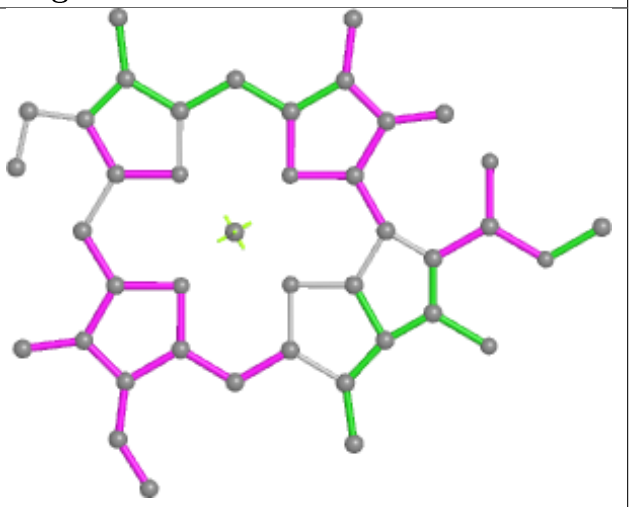
Ligand CLA A 822



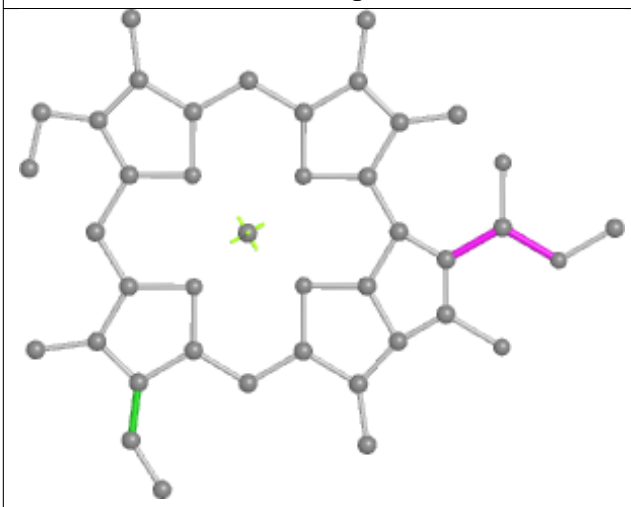
Ligand CLA g 101



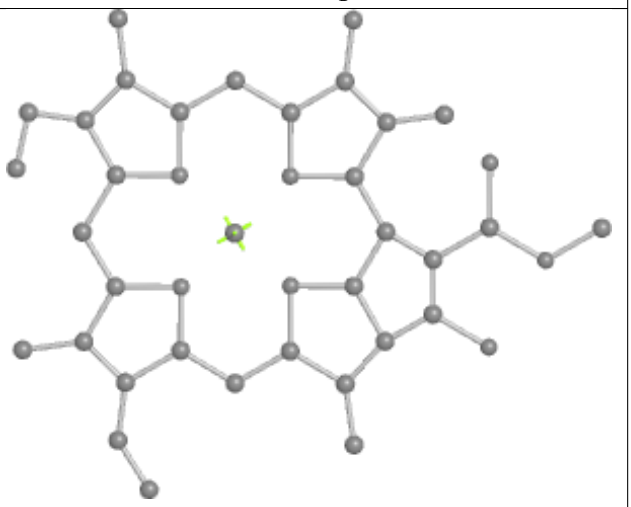
Bond lengths



Bond angles

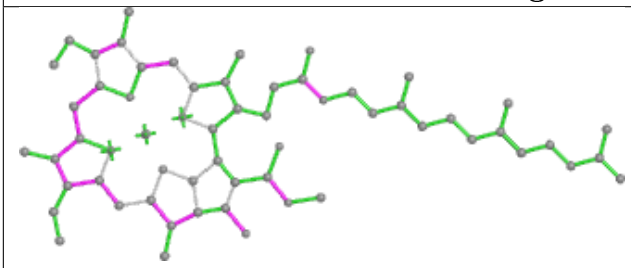


Torsions

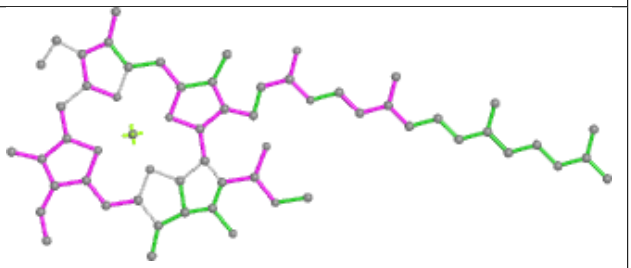


Rings

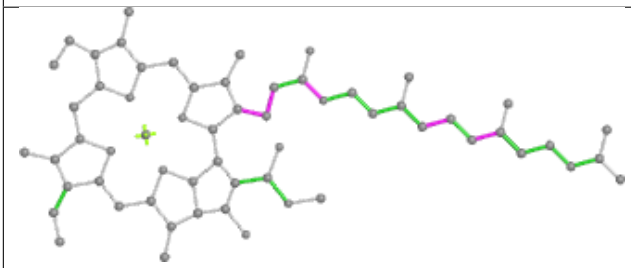
Ligand CLA 7 609



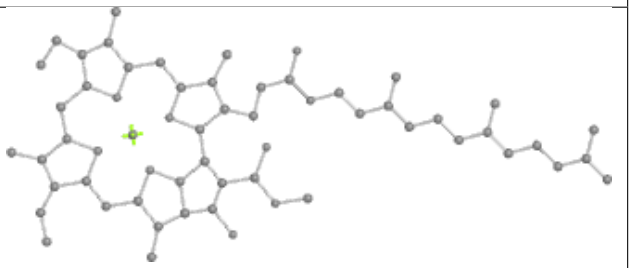
Bond lengths



Bond angles

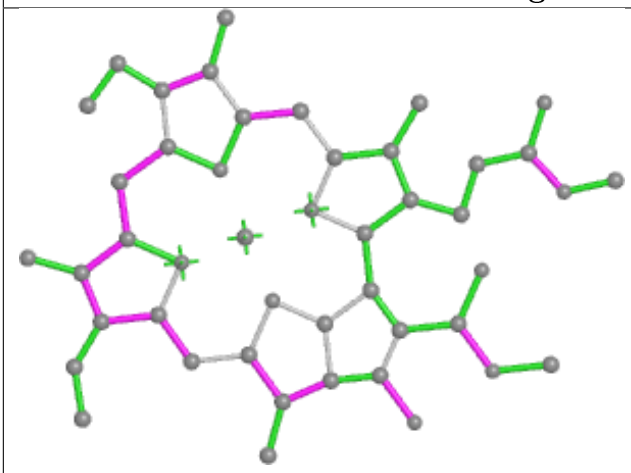


Torsions



Rings

Ligand CLA 6 309



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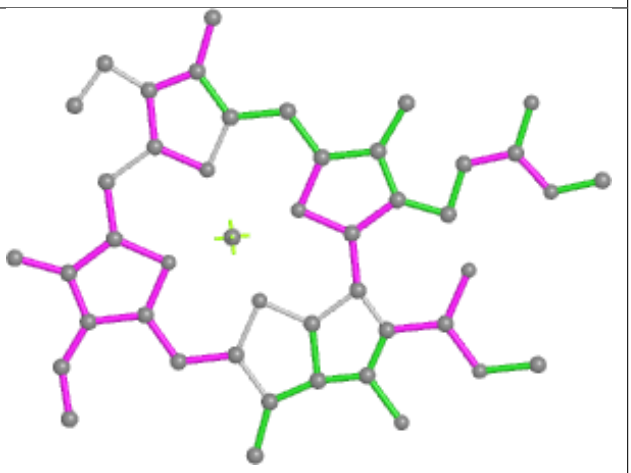
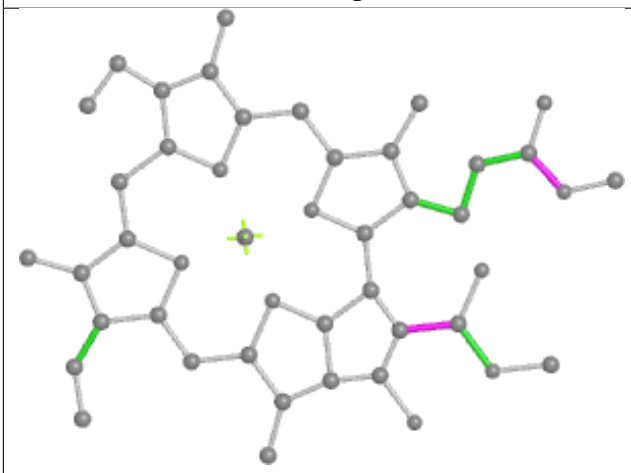


Bond angles



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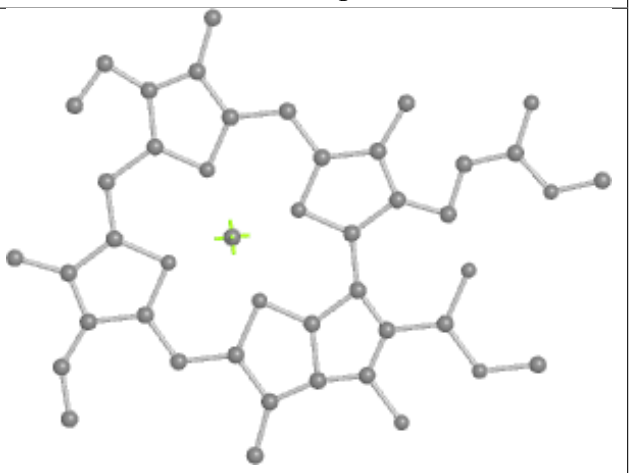
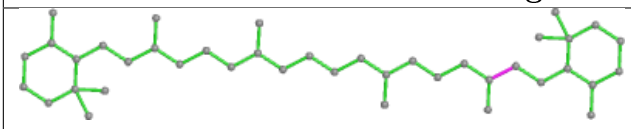


Rings

Ligand BCR b 847



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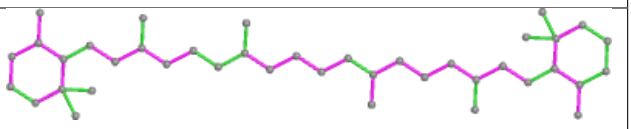
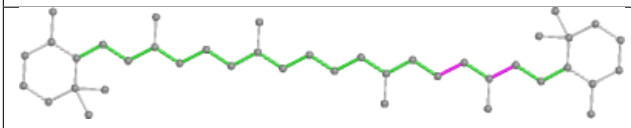


Bond angles



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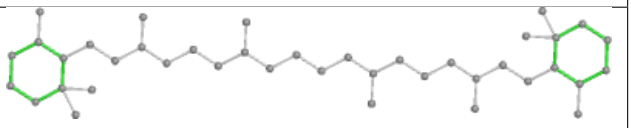
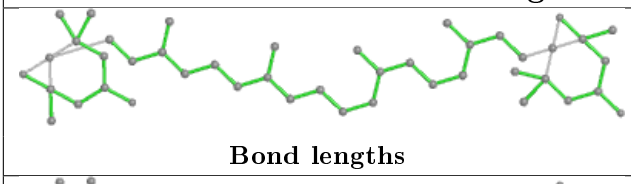


Rings

Ligand XAT 8 315



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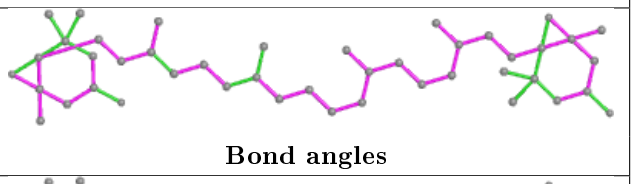
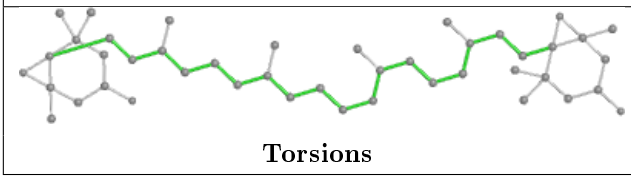


Bond angles



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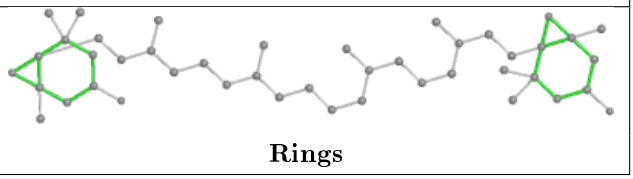
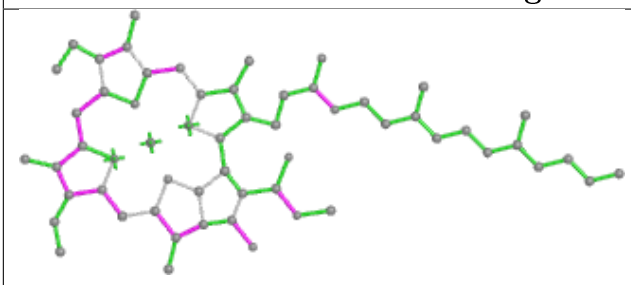


Rings

Ligand CLA B 833



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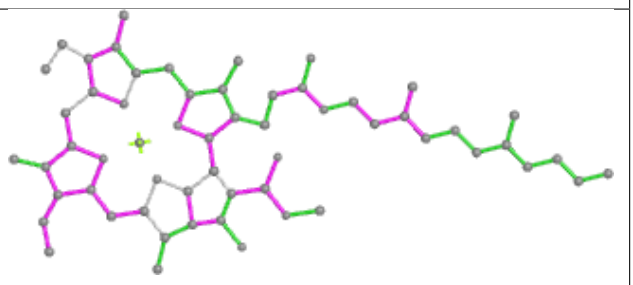

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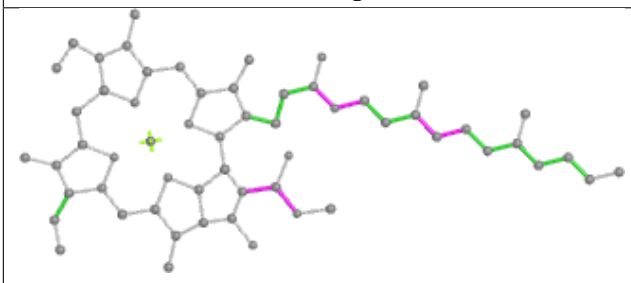

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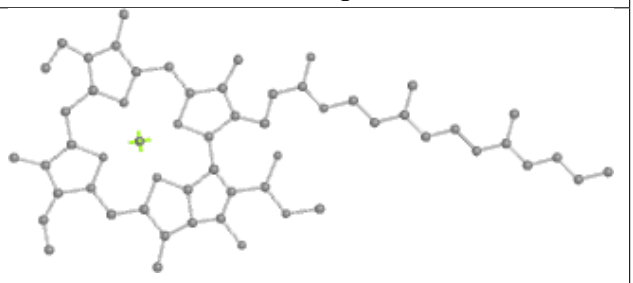
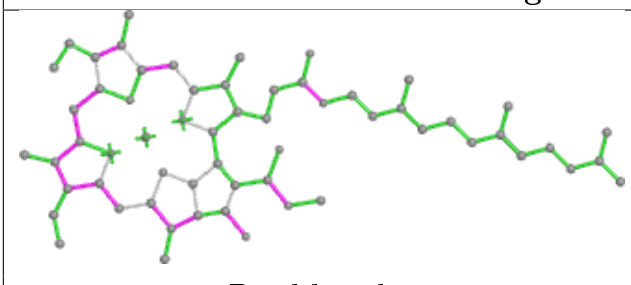


Rings

Ligand CLA B 836



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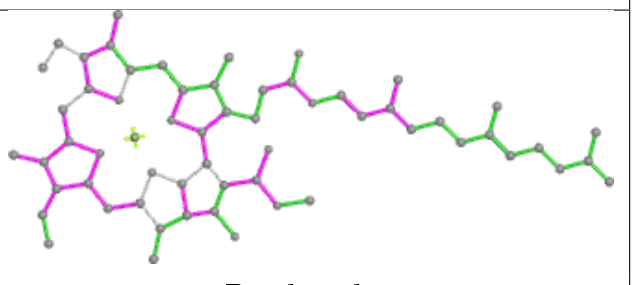
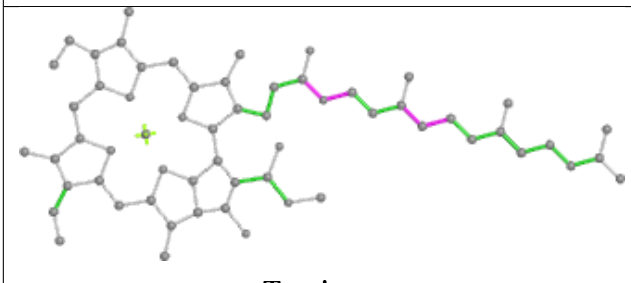


Bond angles



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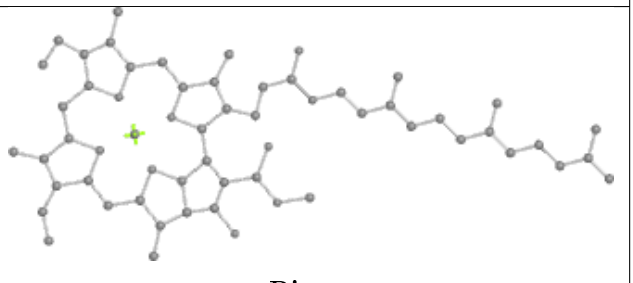
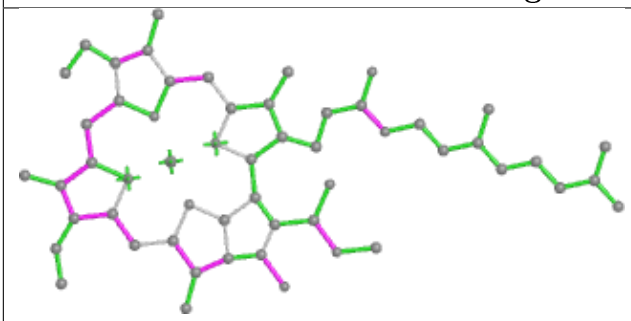


Rings

Ligand CLA B 822



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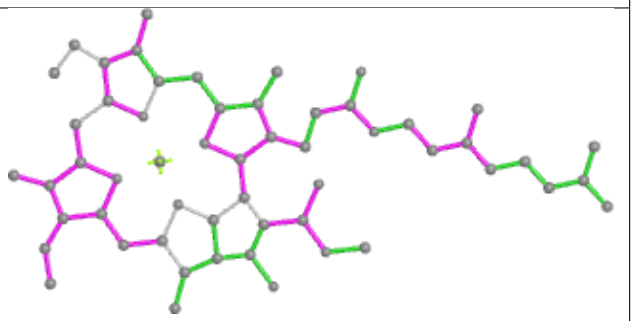
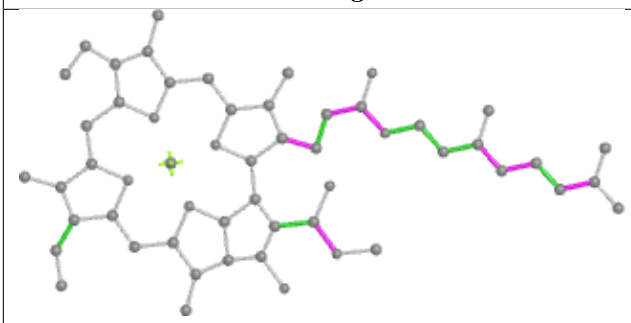


Bond angles



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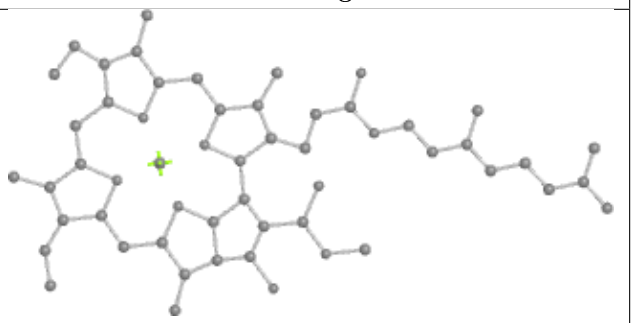
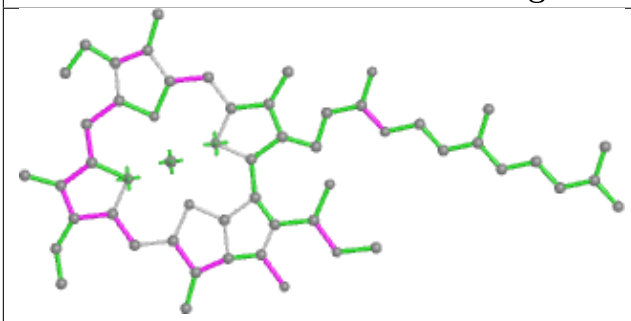
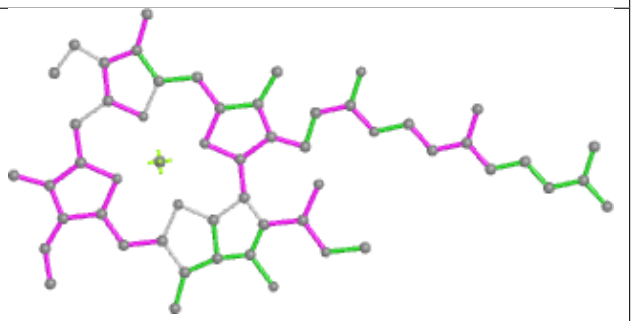


Rings

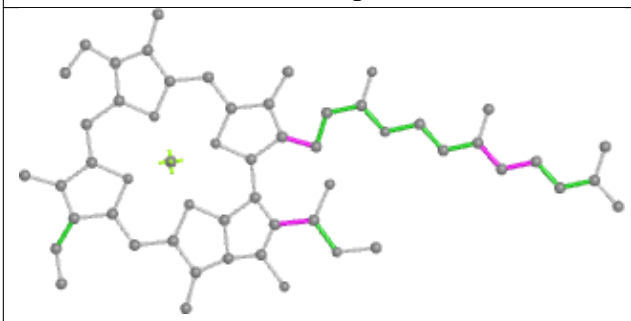
Ligand CLA 4 610



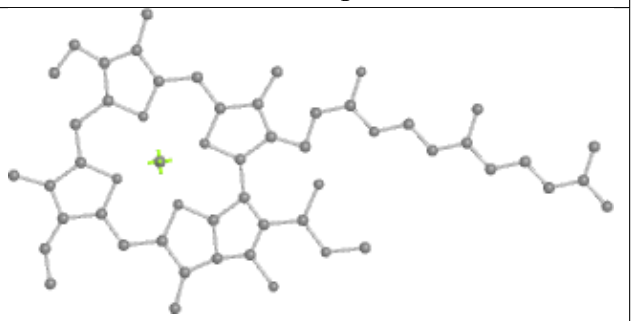
Bond lengths



Bond angles

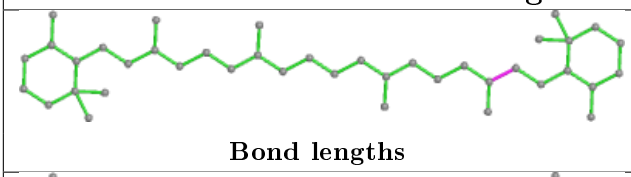


Torsions



Rings

Ligand BCR b 846



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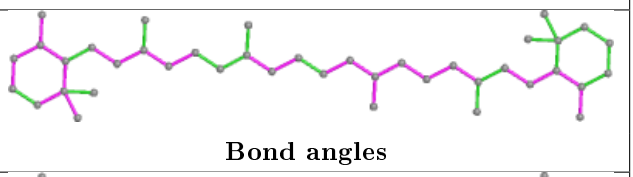
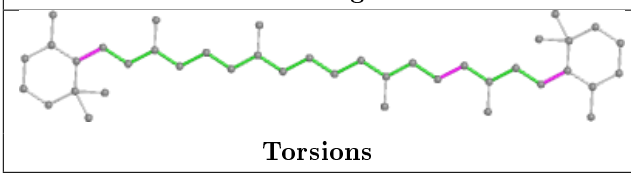


Bond angles



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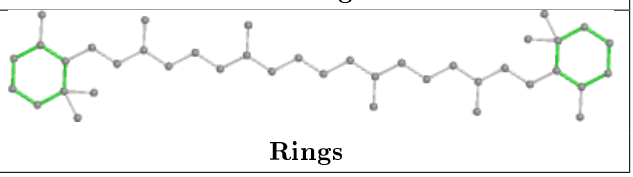
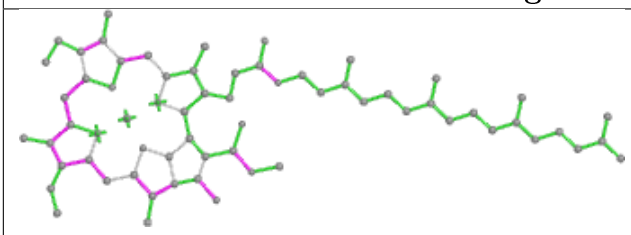


Rings

Ligand CLA B 813



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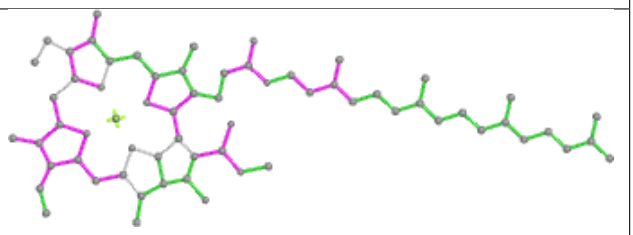
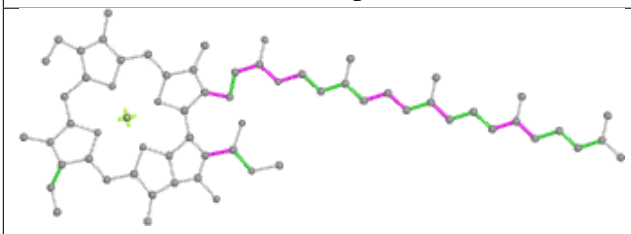


Bond angles



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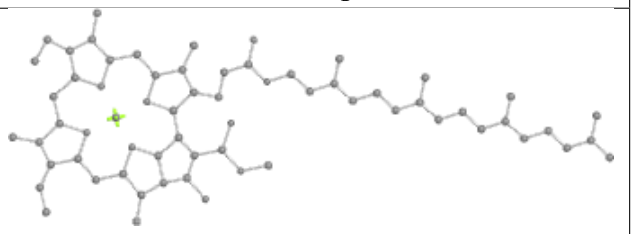
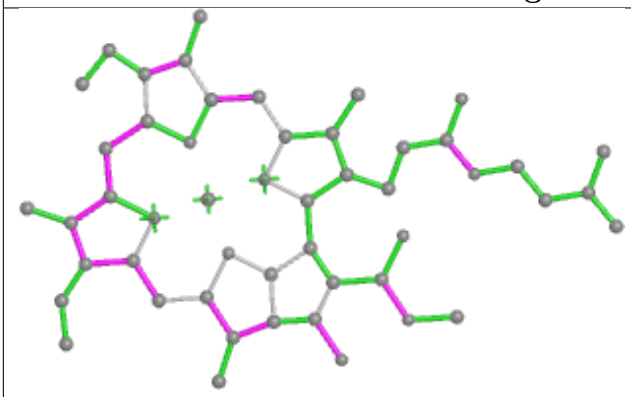
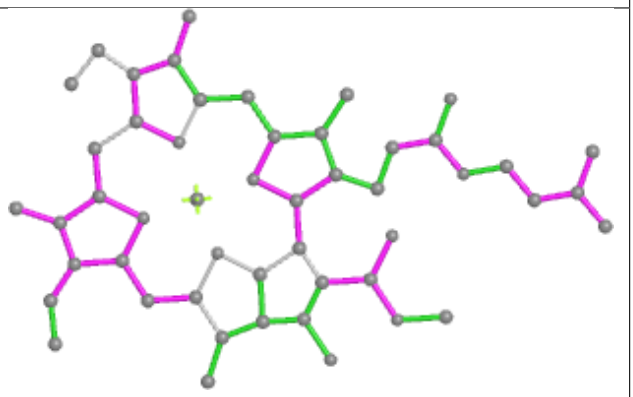


Rings

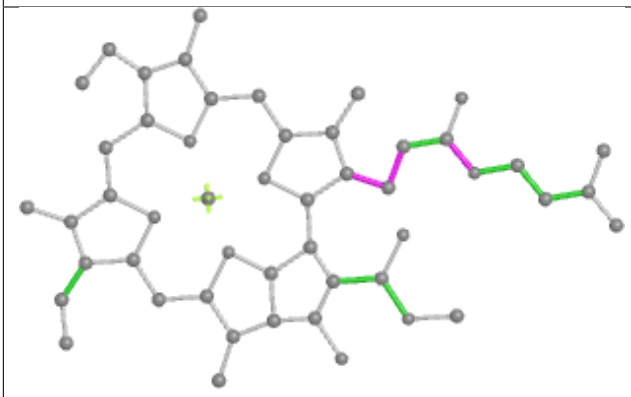
Ligand CLA B 830



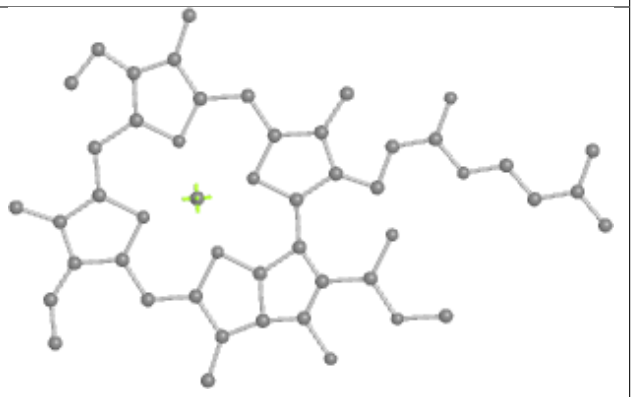
Bond lengths



Bond angles

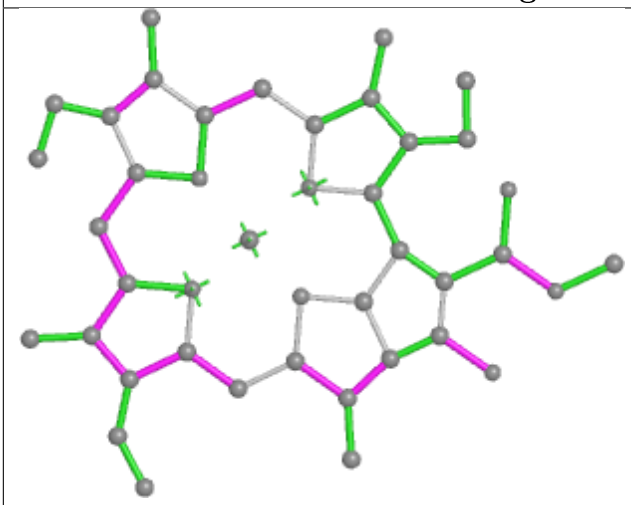


Torsions

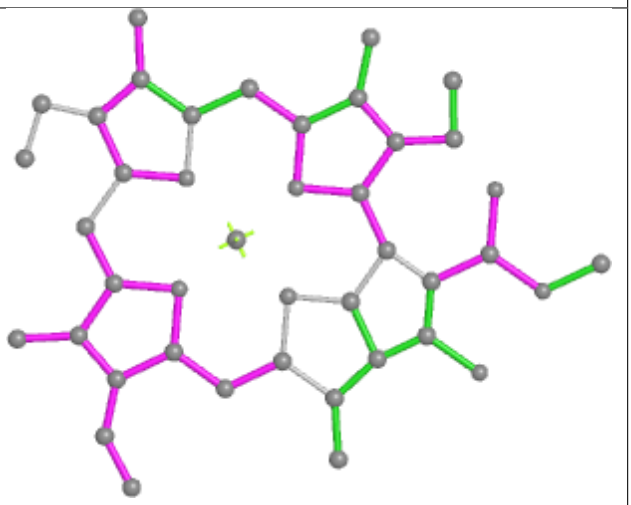


Rings

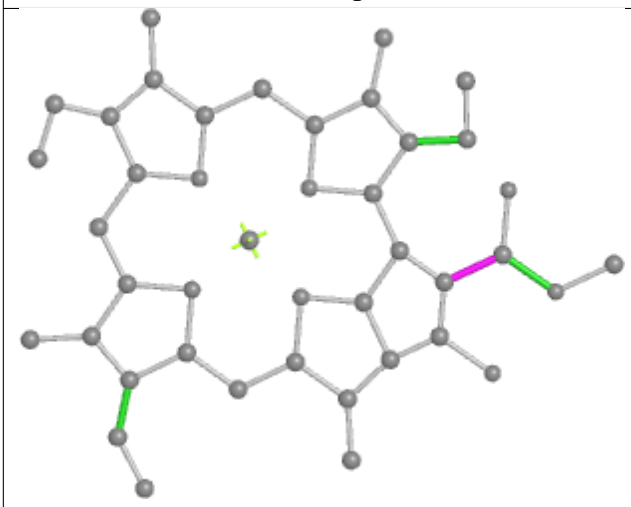
Ligand CLA J 3002



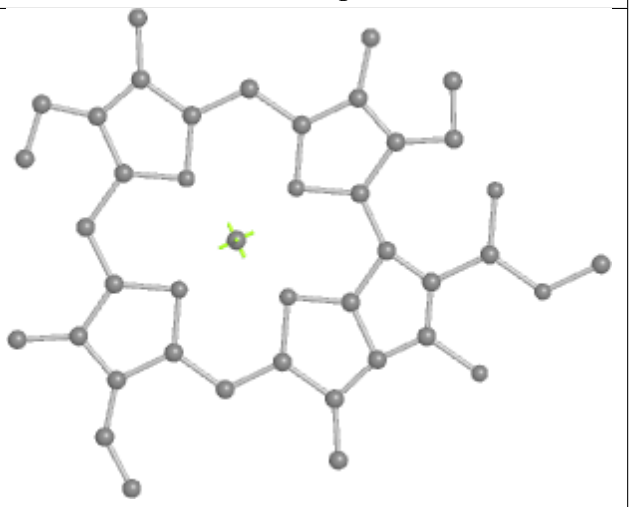
Bond lengths



Bond angles

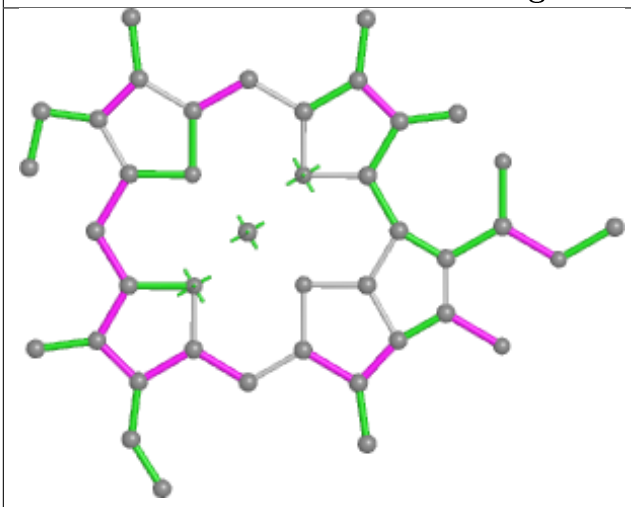


Torsions

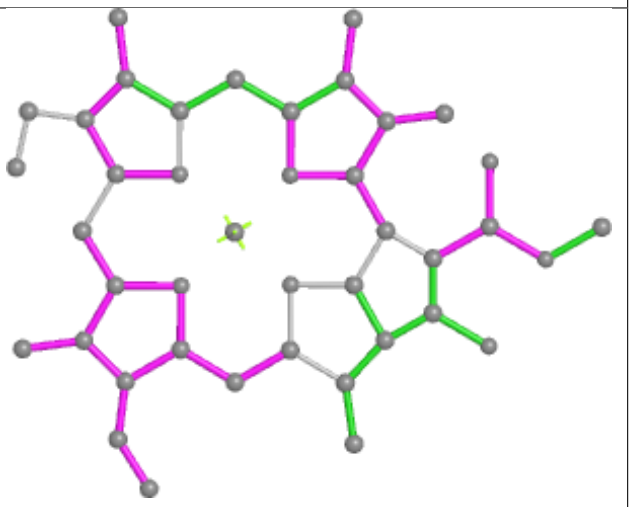


Rings

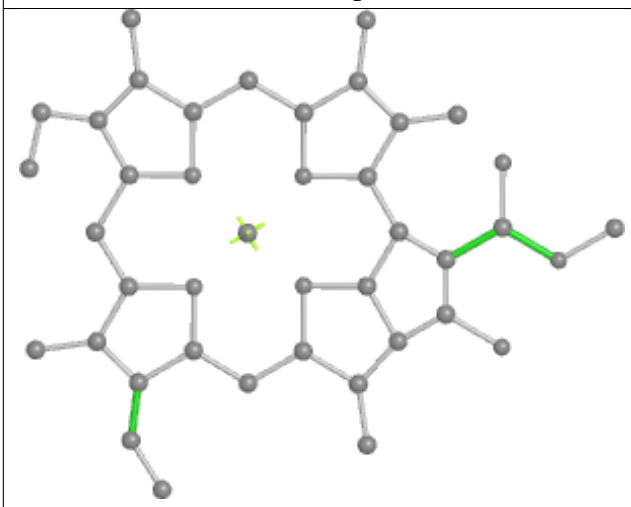
Ligand CLA 2 610



Bond lengths



Bond angles



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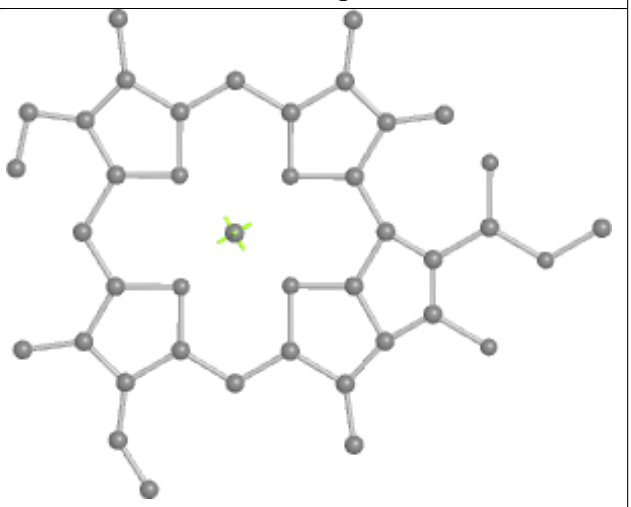
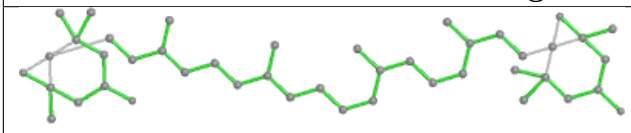
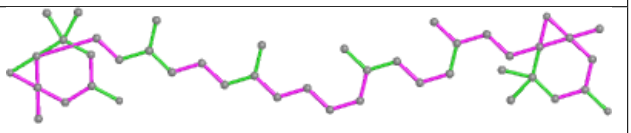


Rings

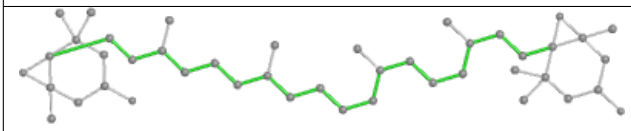
Ligand XAT 2 616



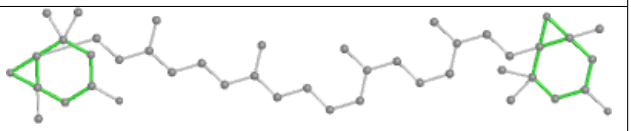
Bond lengths



Bond angles

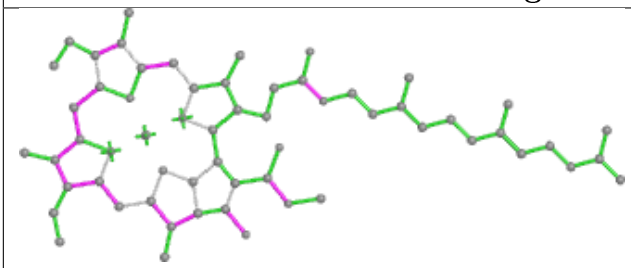


Torsions

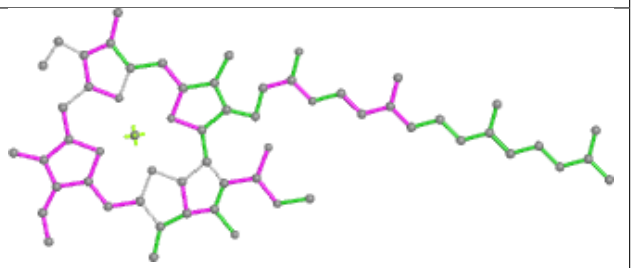


Rings

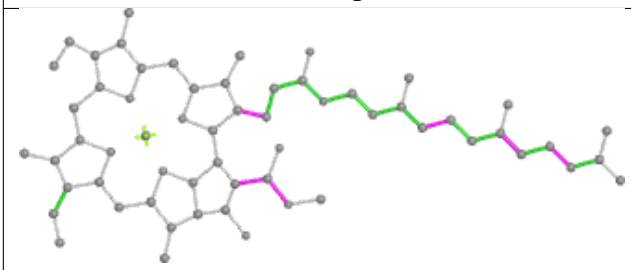
Ligand CLA B 815



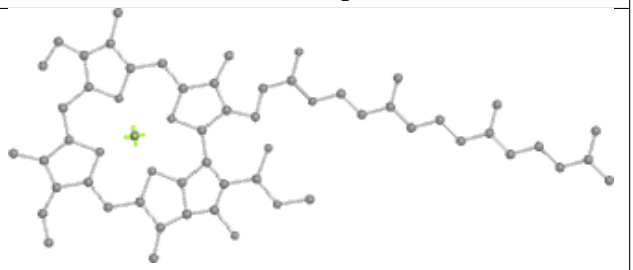
Bond lengths



Bond angles

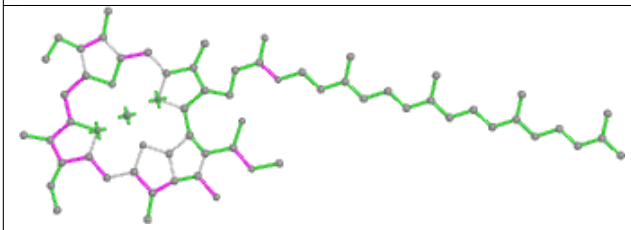


Torsions

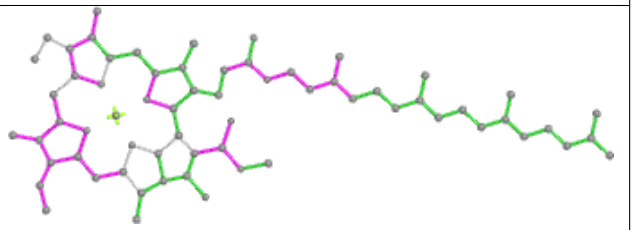


Rings

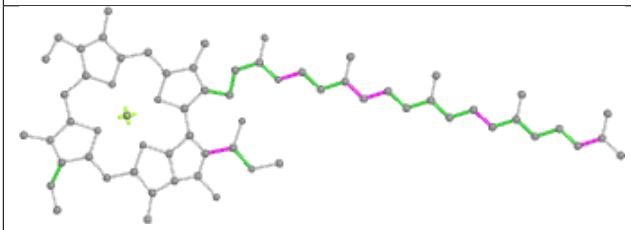
Ligand CLA a 840



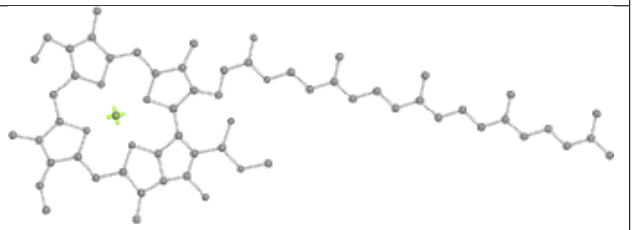
Bond lengths



Bond angles

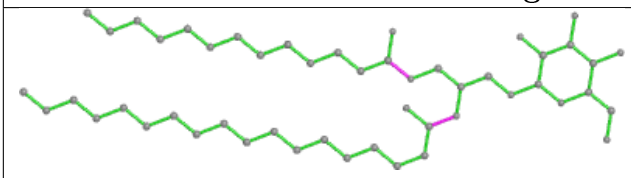


Torsions



Rings

Ligand LMG 9 619



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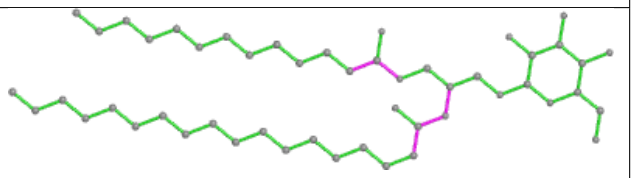
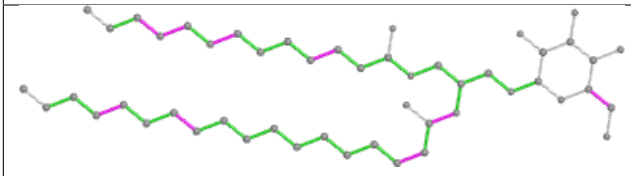
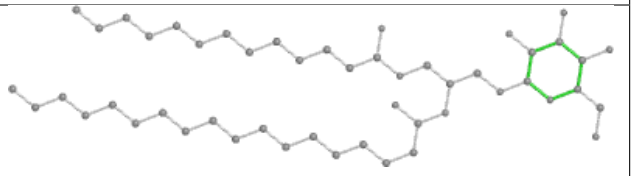


Bond angles

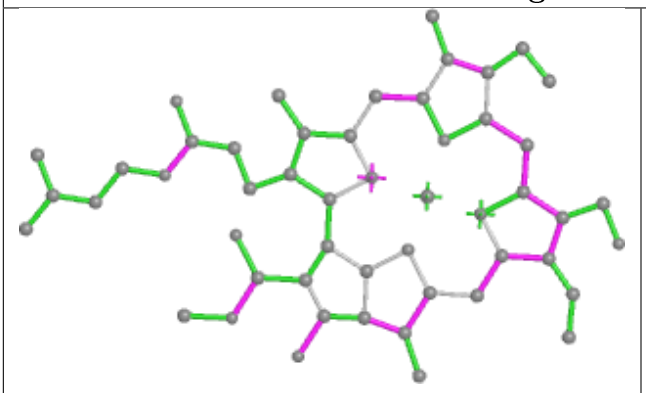


Torsions



Rings

Ligand CHL 9 607



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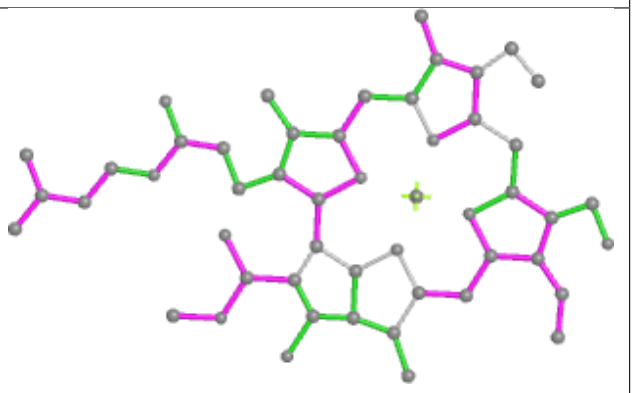
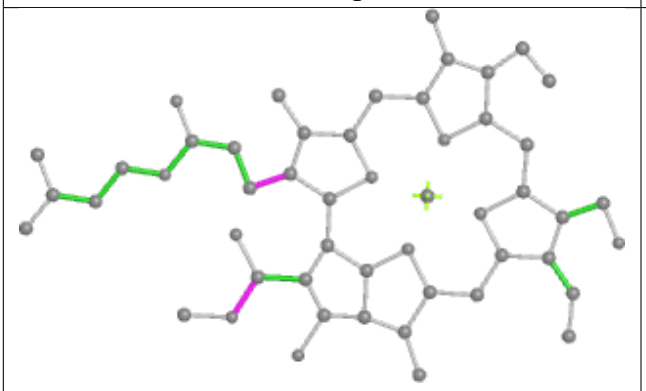


Bond angles



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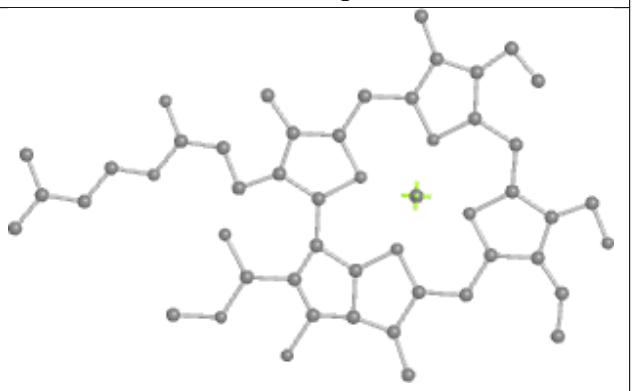
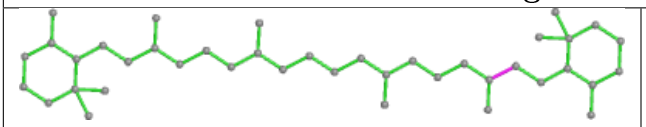


Rings

Ligand BCR B 847



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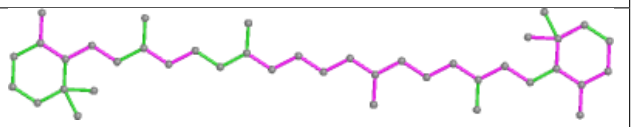
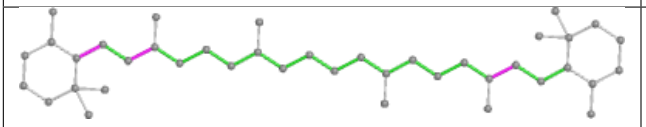


Bond angles



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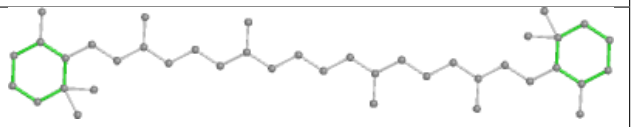
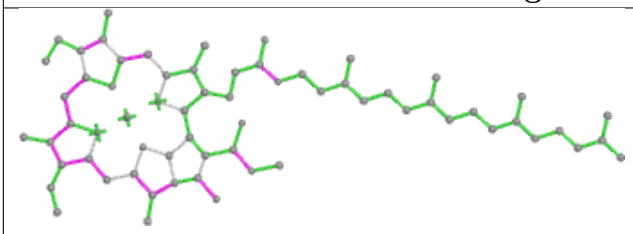


Rings

Ligand CLA B 834



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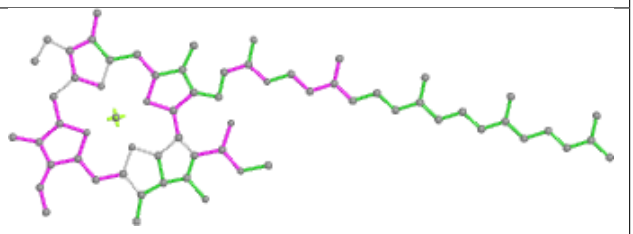
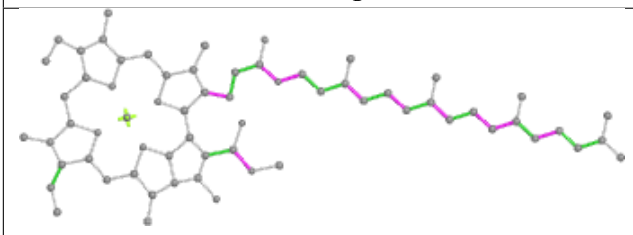


Bond angles



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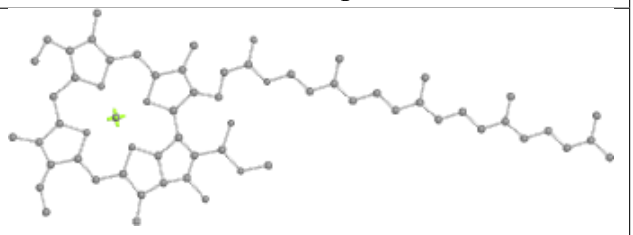
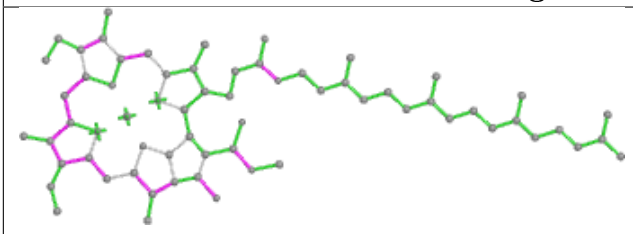


Rings

Ligand CLA 7 602



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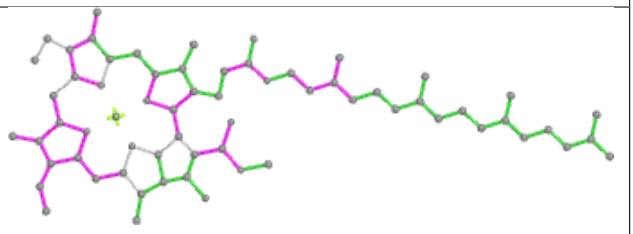
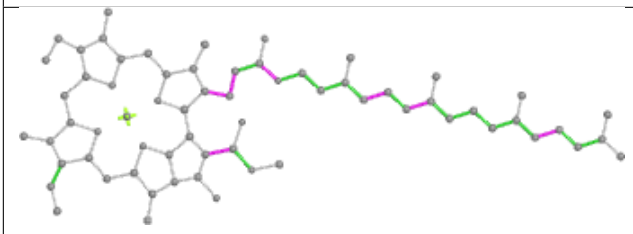
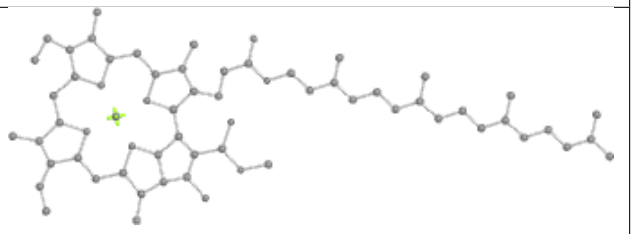


Bond angles

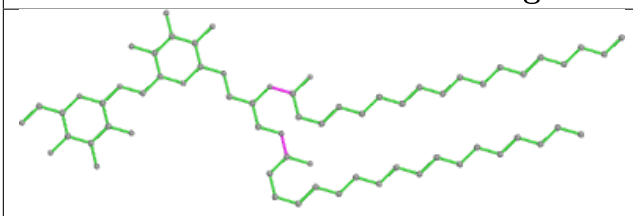


Torsions



Rings

Ligand DGD b 849



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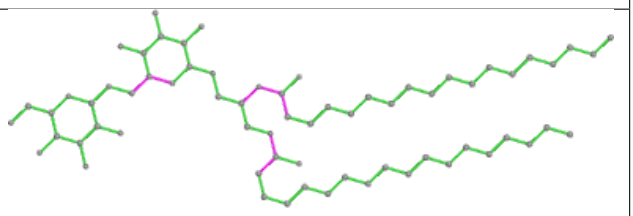
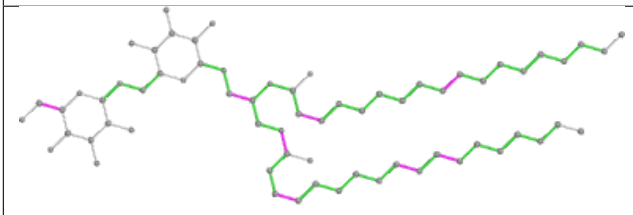
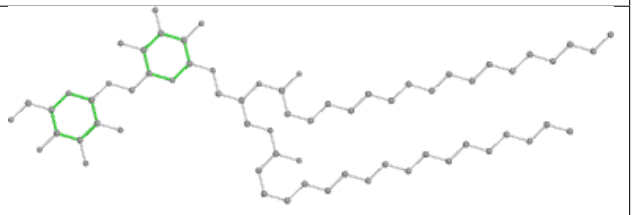


Bond angles

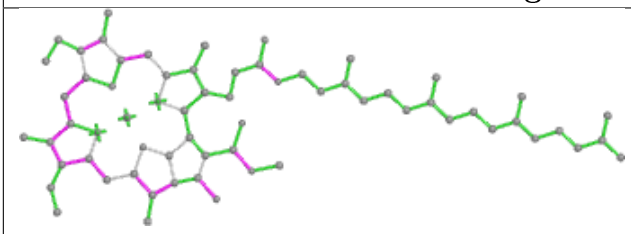


Torsions



Rings

Ligand CLA A 804



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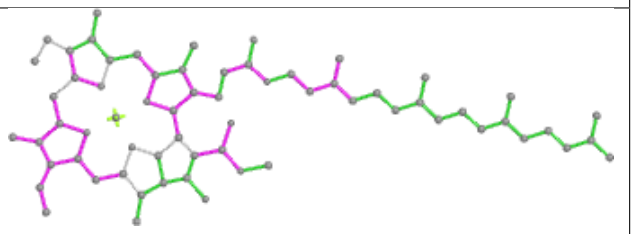
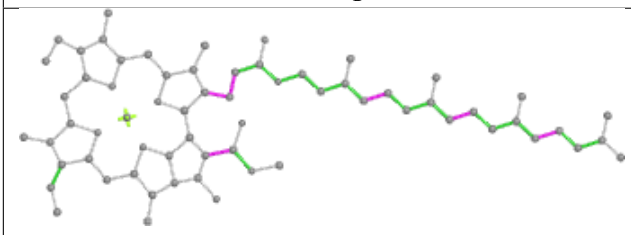
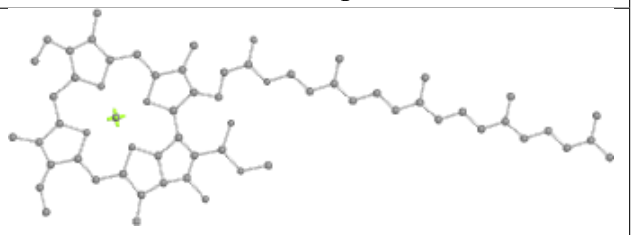


Bond angles

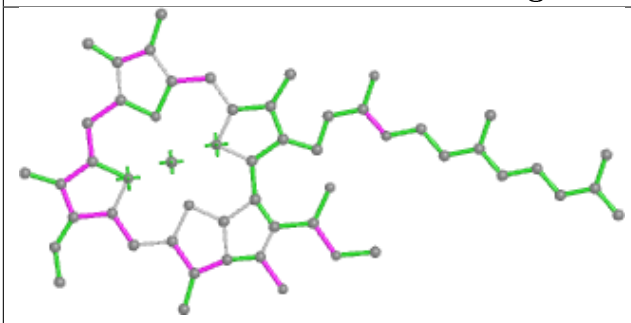


Torsions



Rings

Ligand CLA b 811



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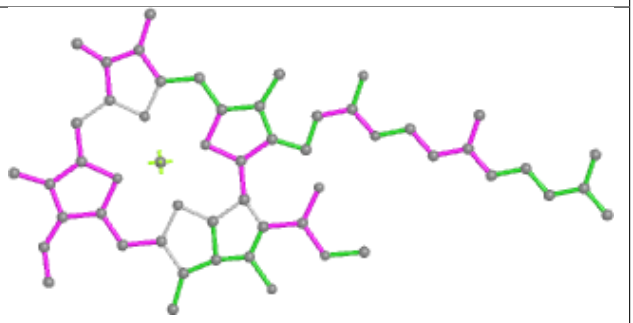
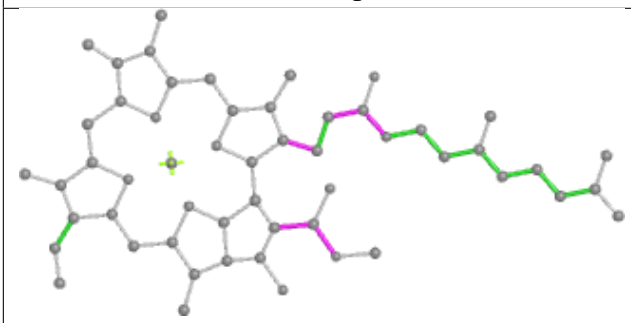


Bond angles



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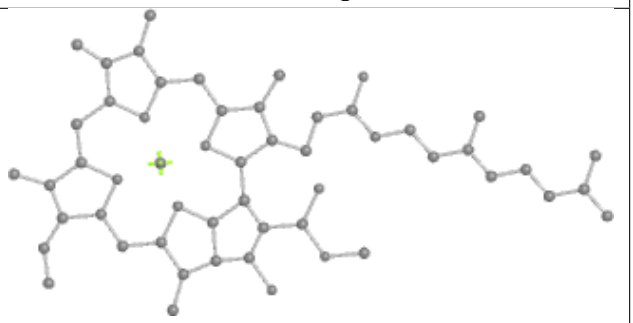
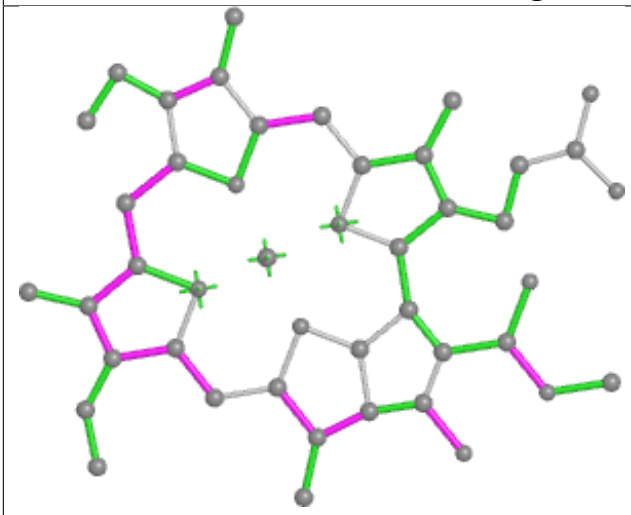


Rings

Ligand CLA 4 613



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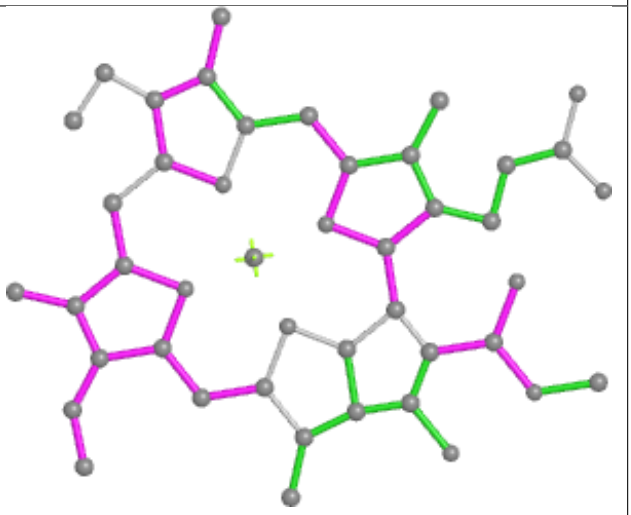
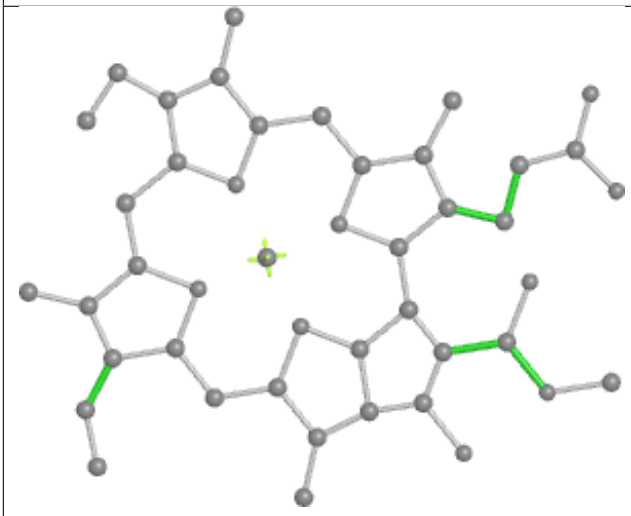
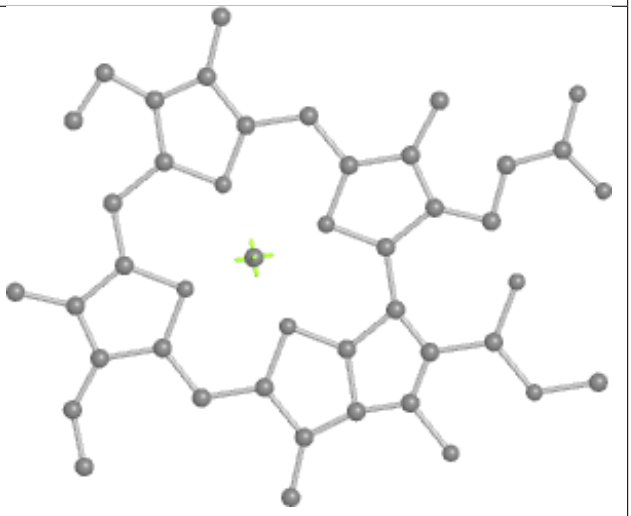


Bond angles

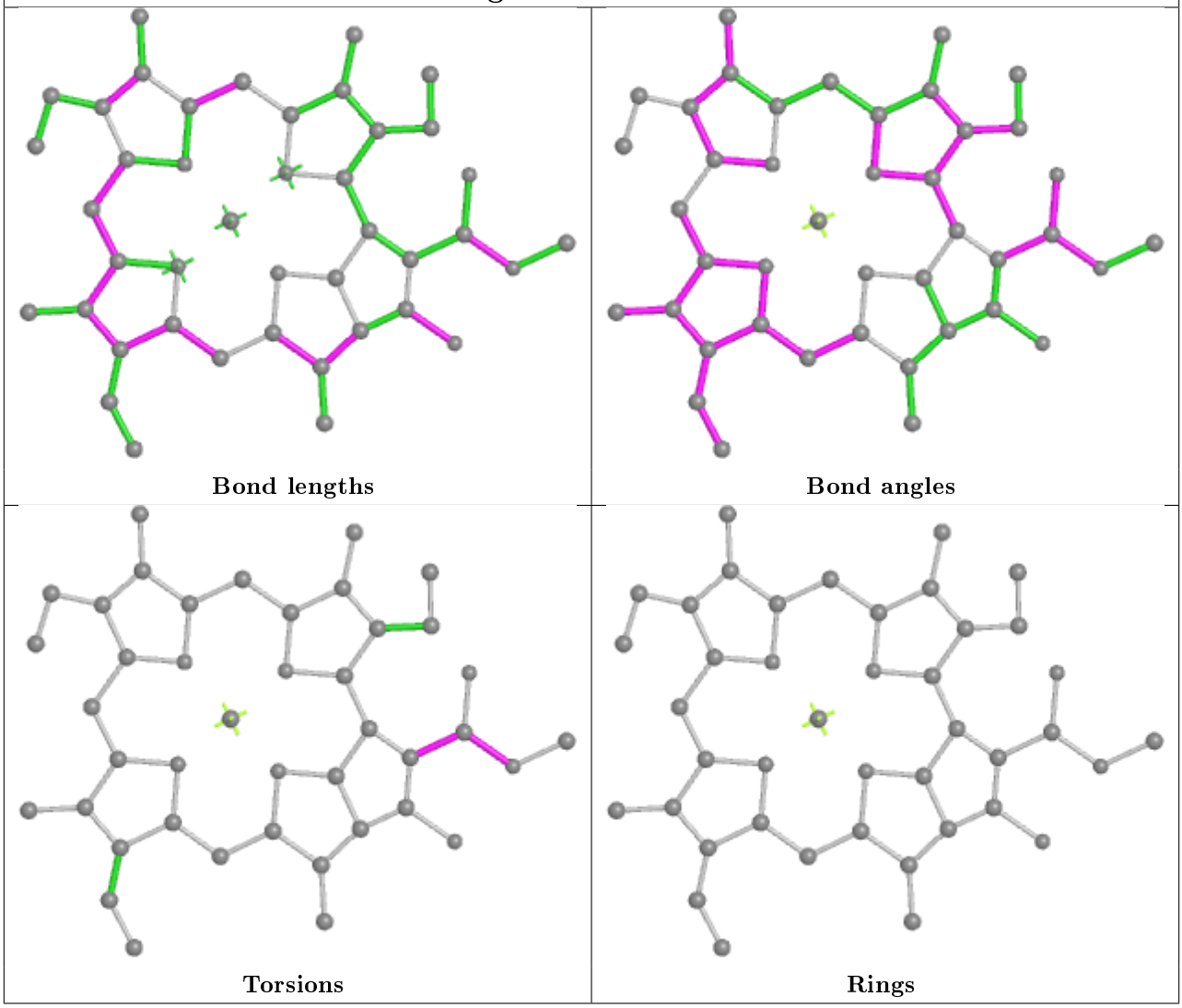


Torsions

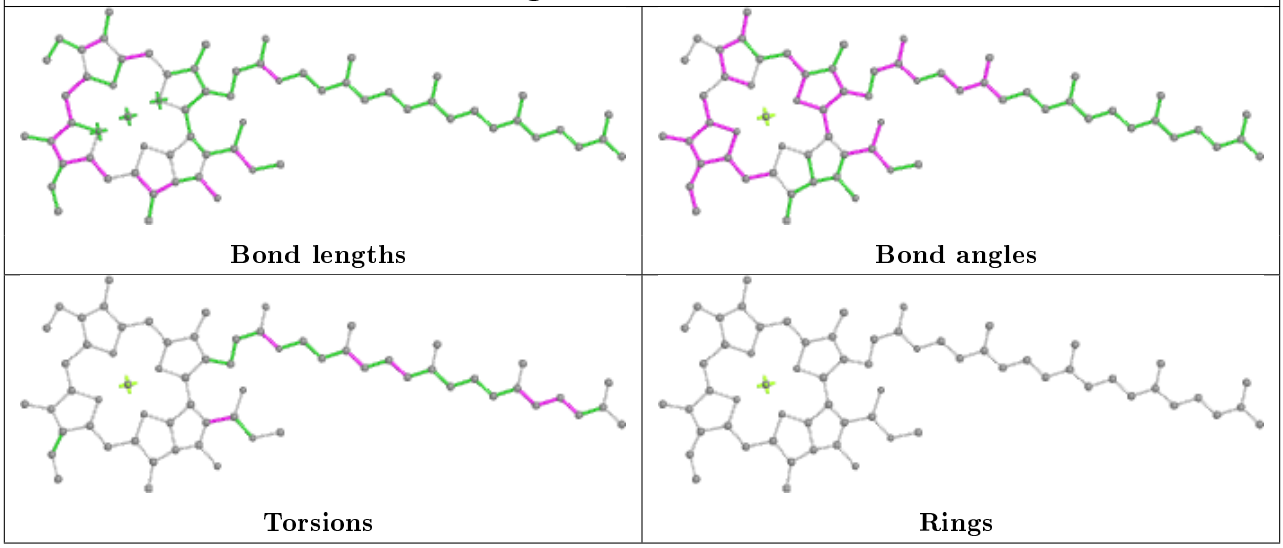


Rings

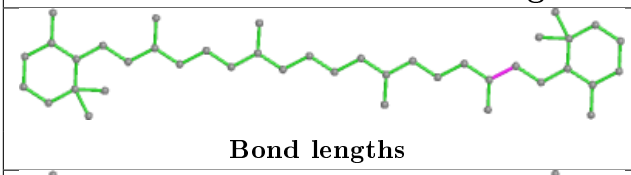
Ligand CLA 6 307



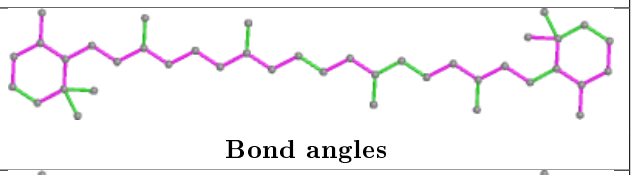
Ligand CLA B 837



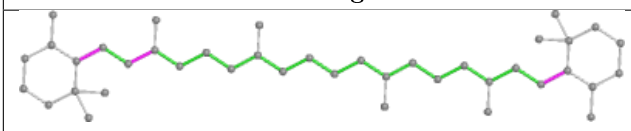
Ligand BCR a 850



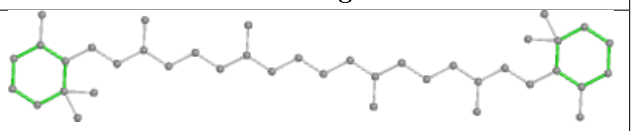
Bond lengths



Bond angles

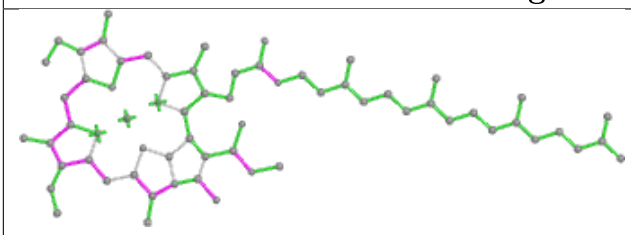


Torsions

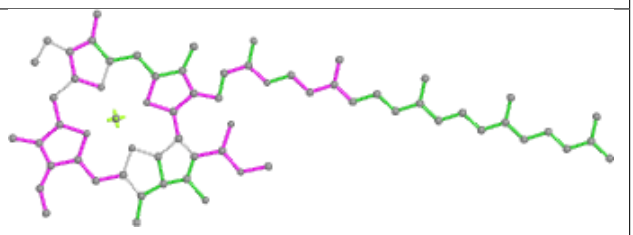


Rings

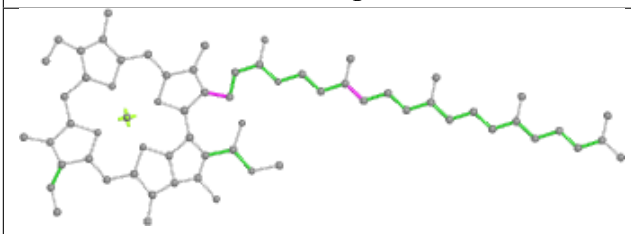
Ligand CLA a 822



Bond lengths



Bond angles



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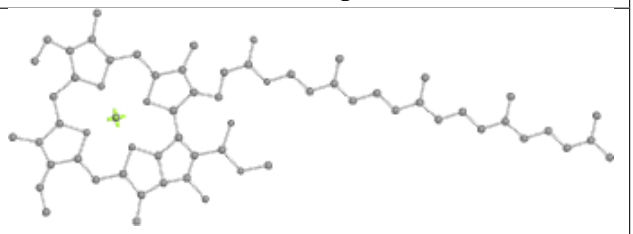
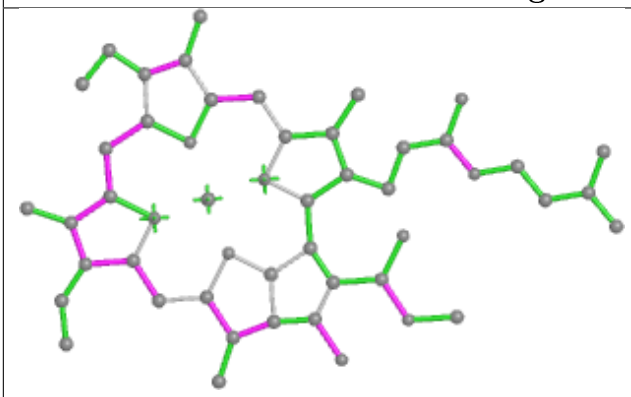
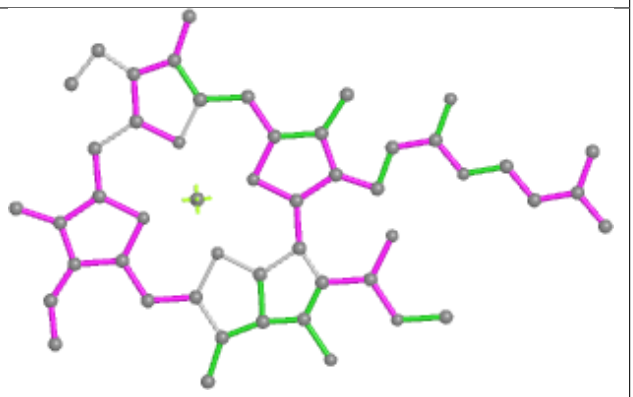


Rings

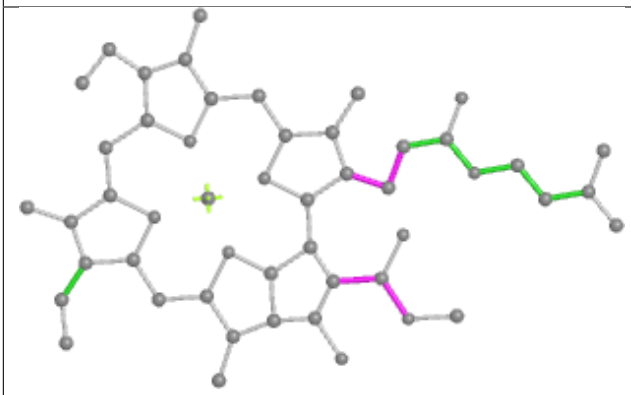
Ligand CLA 9 604



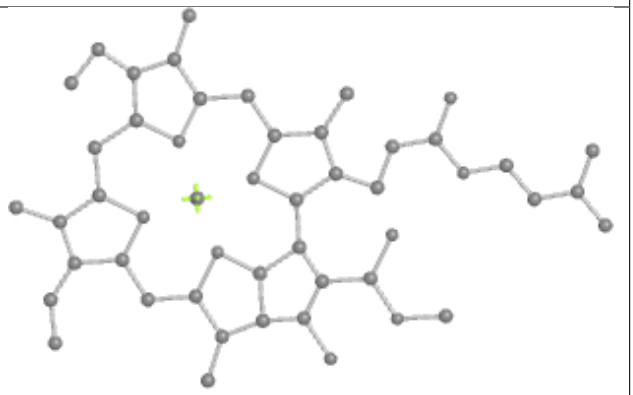
Bond lengths



Bond angles

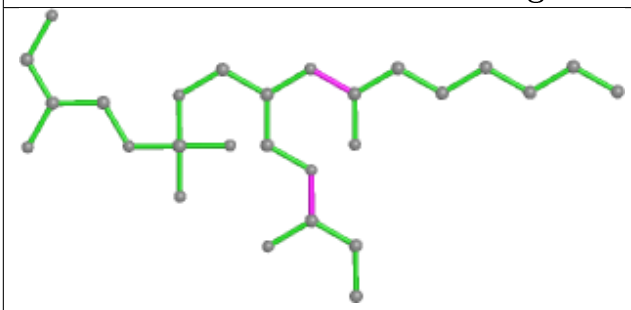


Torsions



Rings

Ligand LHG a 848



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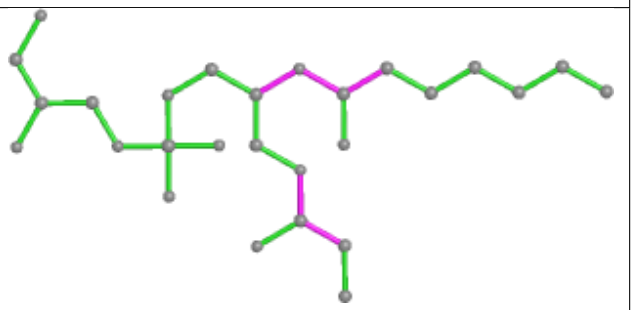
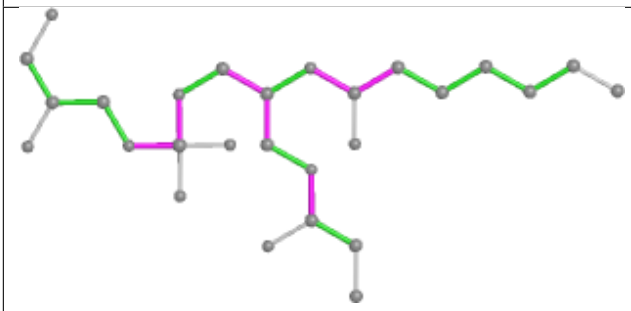


Bond angles



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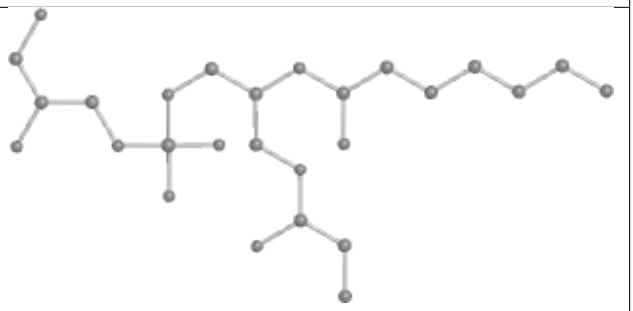
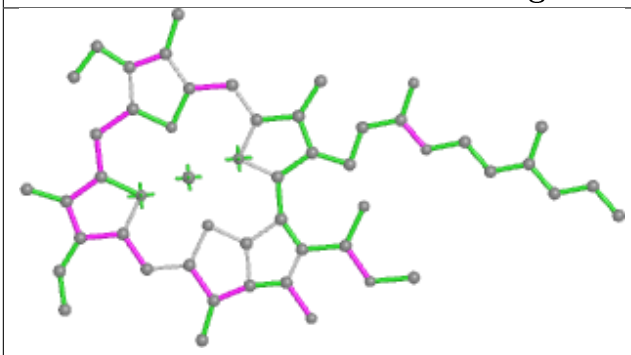
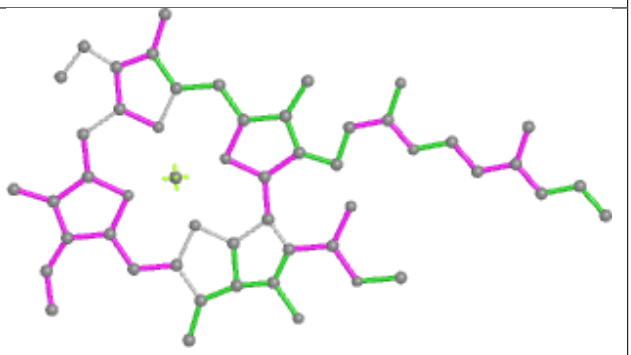


Rings

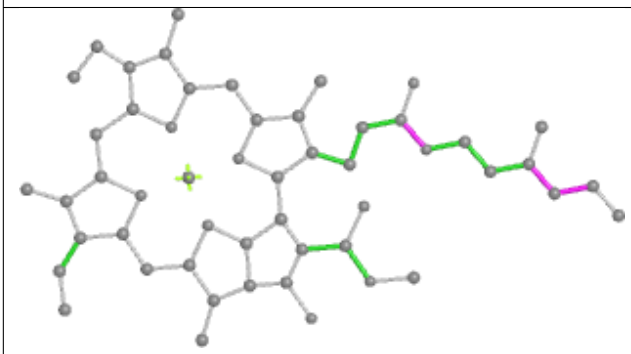
Ligand CLA 7 611



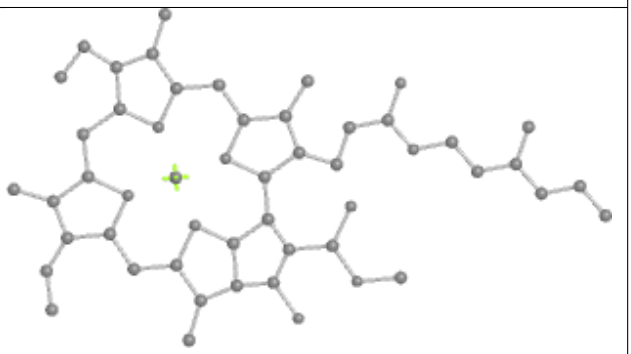
Bond lengths



Bond angles

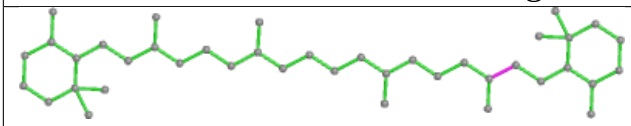


Torsions



Rings

Ligand BCR b 845



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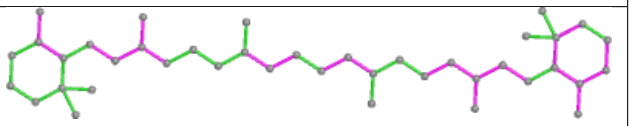
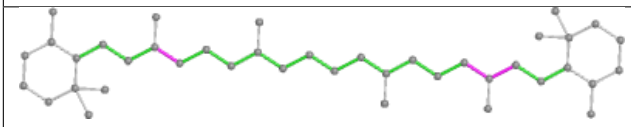
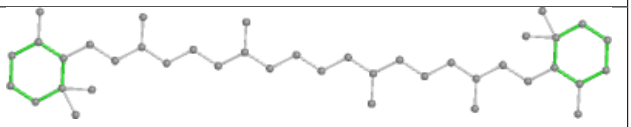


Bond angles

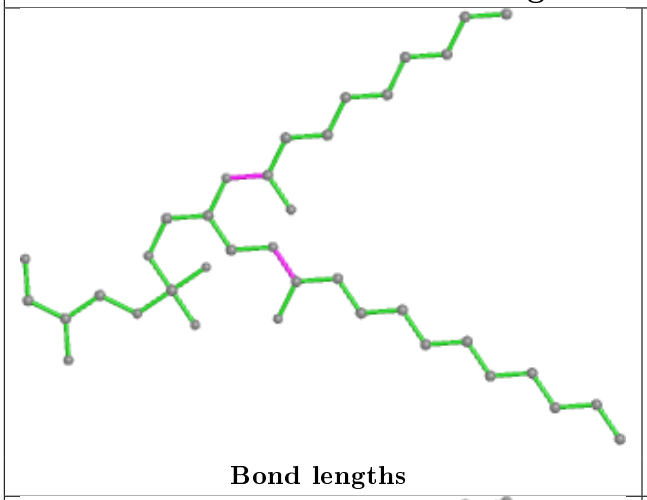


Torsions

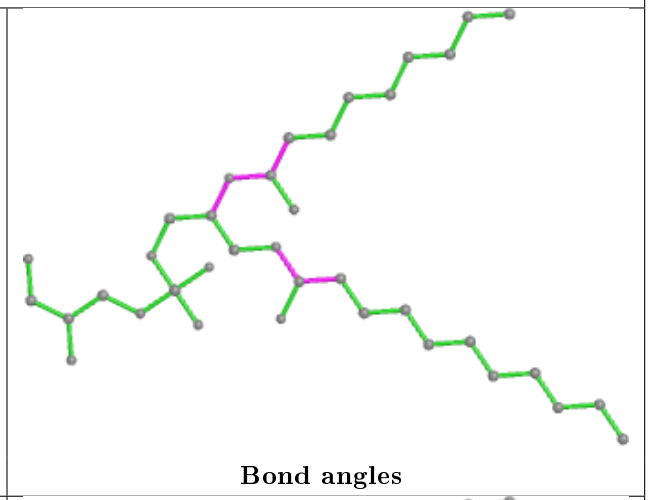


Rings

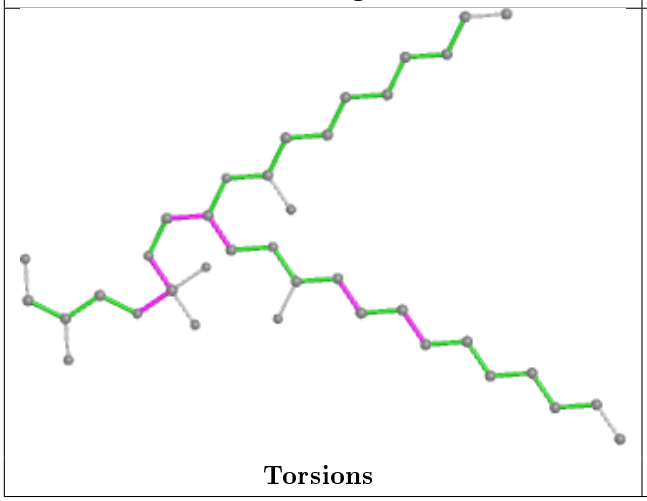
Ligand LHG 2 618



Bond lengths



Bond angles



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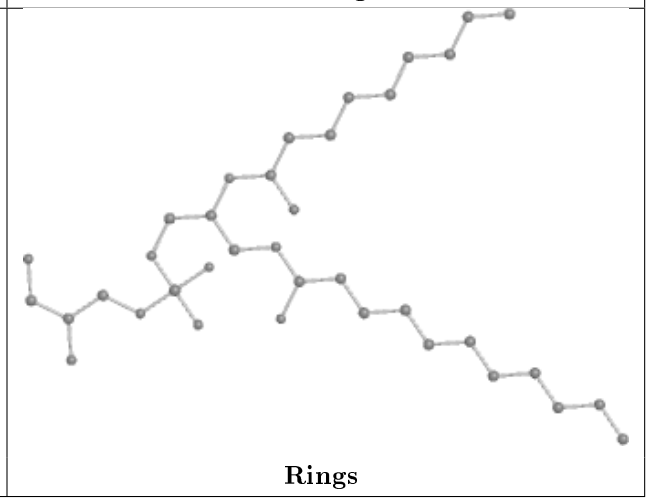
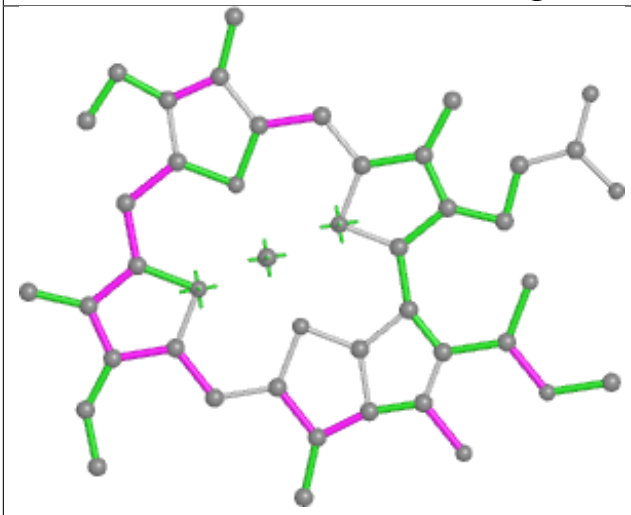


Rings

Ligand CLA 8 303



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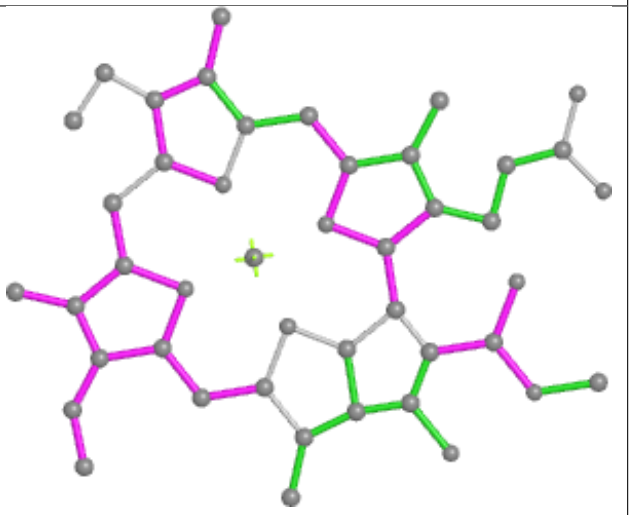
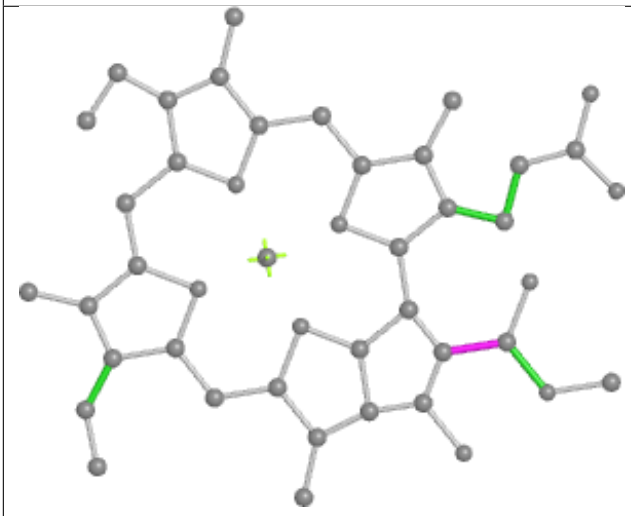


Bond angles



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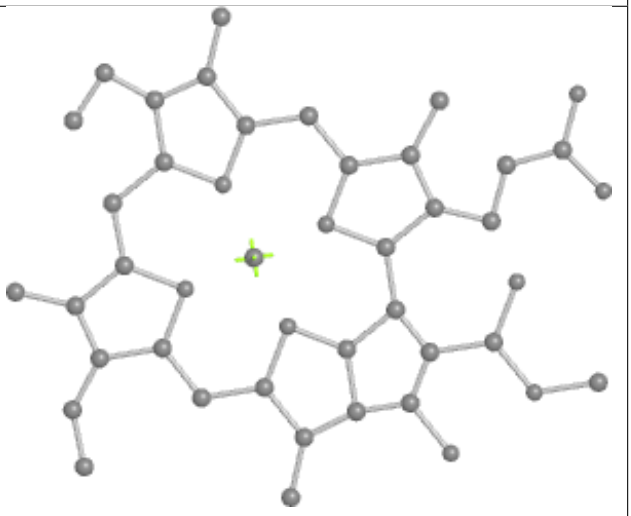
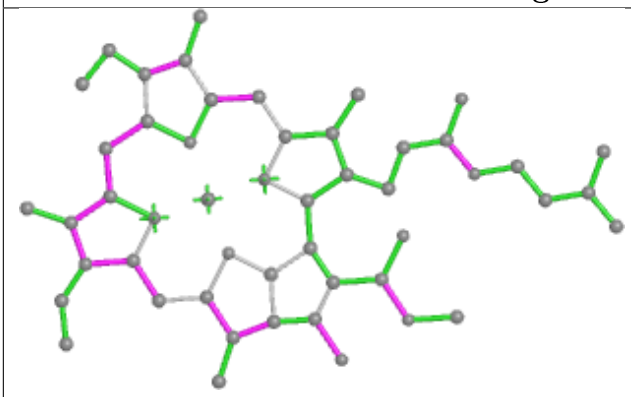
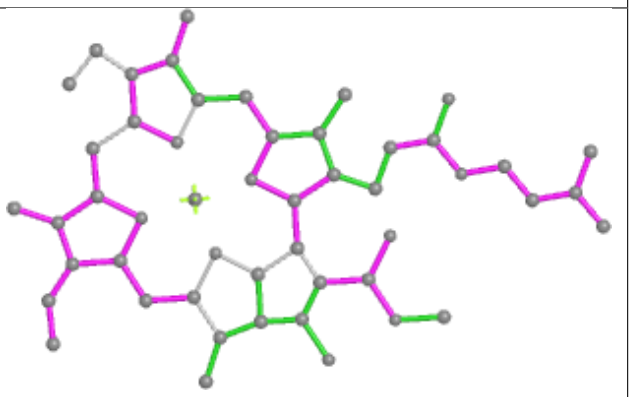
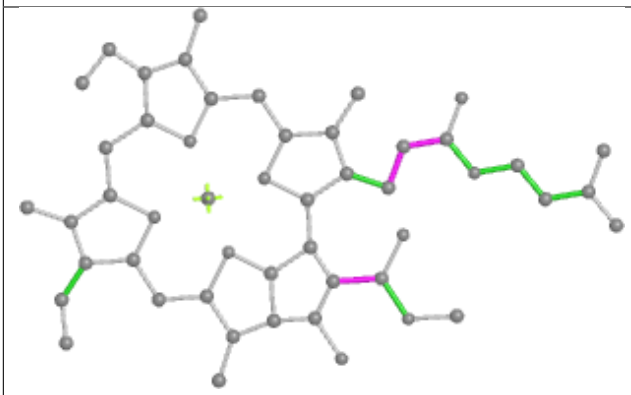
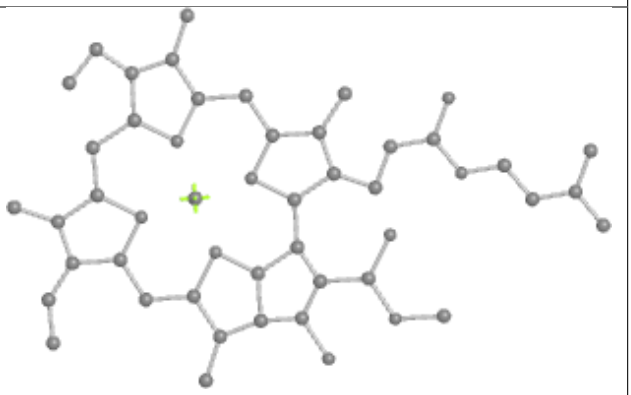
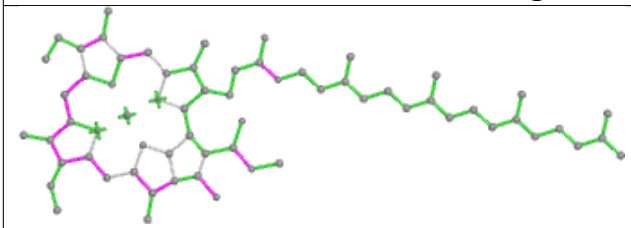
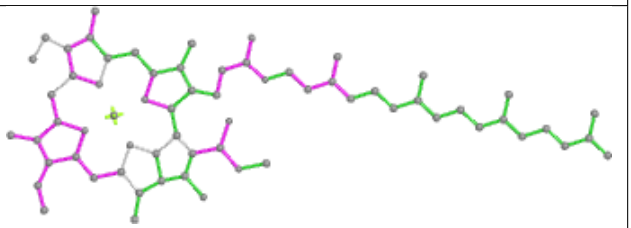
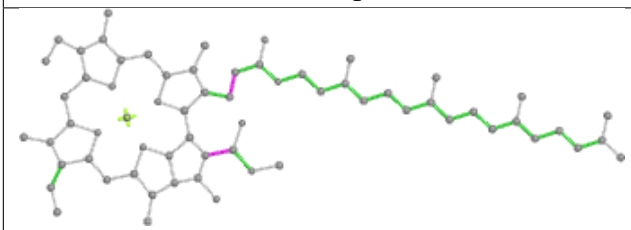
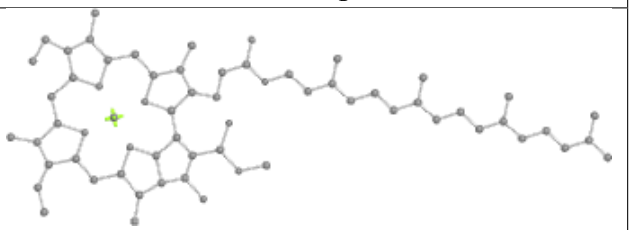
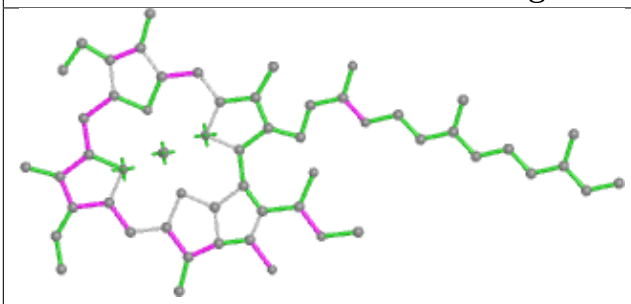


Rings

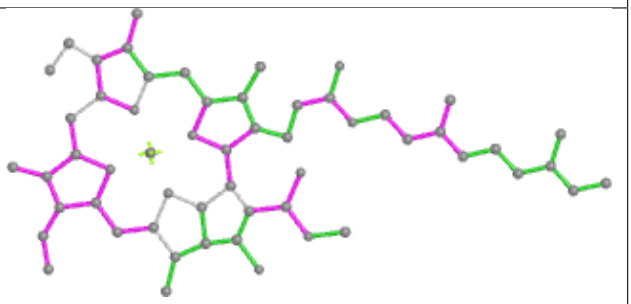
Ligand CLA l 204	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA a 810	
 Bond lengths	 Bond angles
 Torsions	 Rings

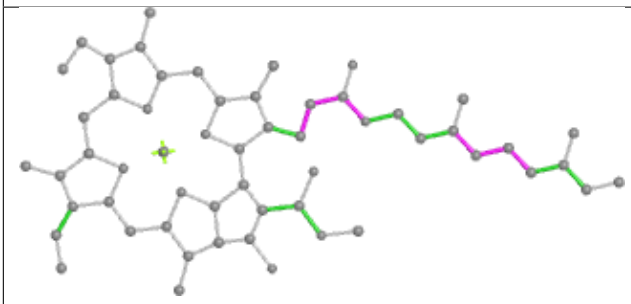
Ligand CLA 4 612



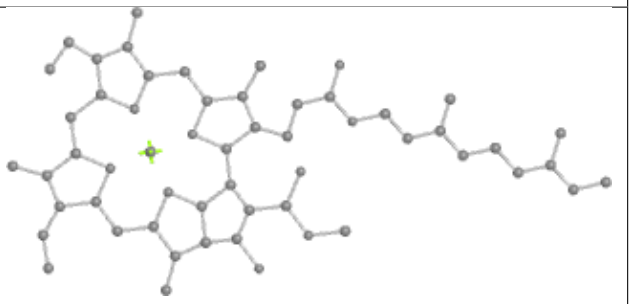
Bond lengths



Bond angles

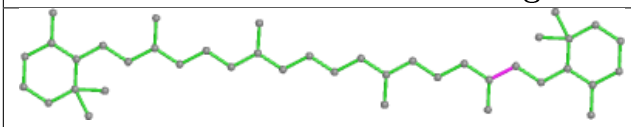


Torsions

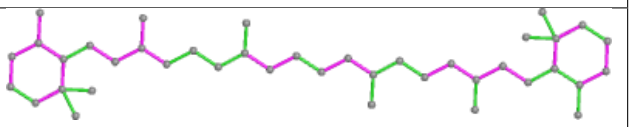


Rings

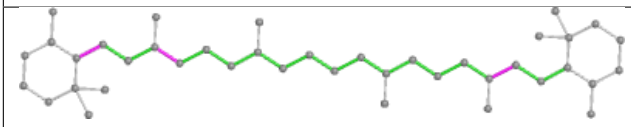
Ligand BCR B 844



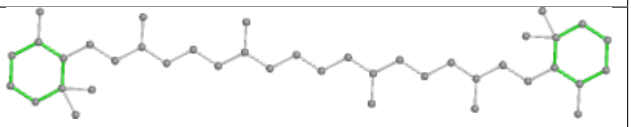
Bond lengths



Bond angles

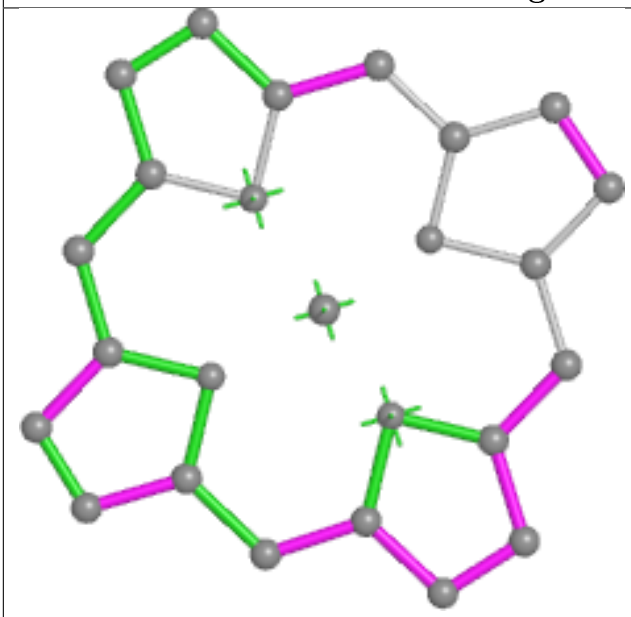


Torsions

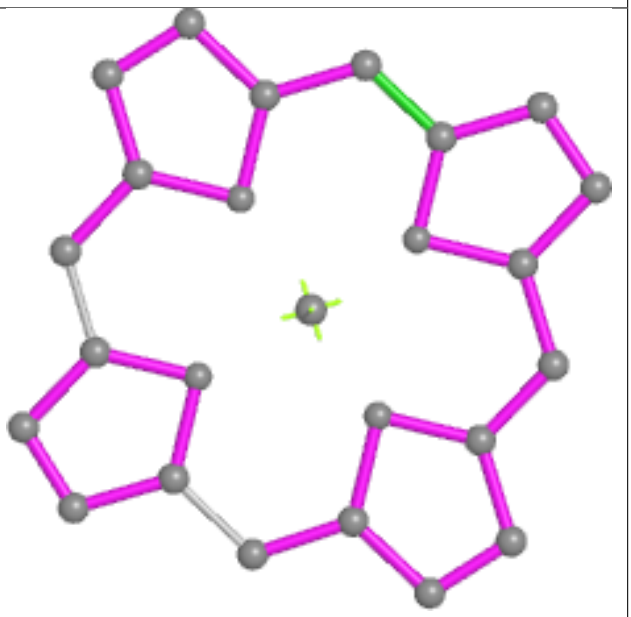


Rings

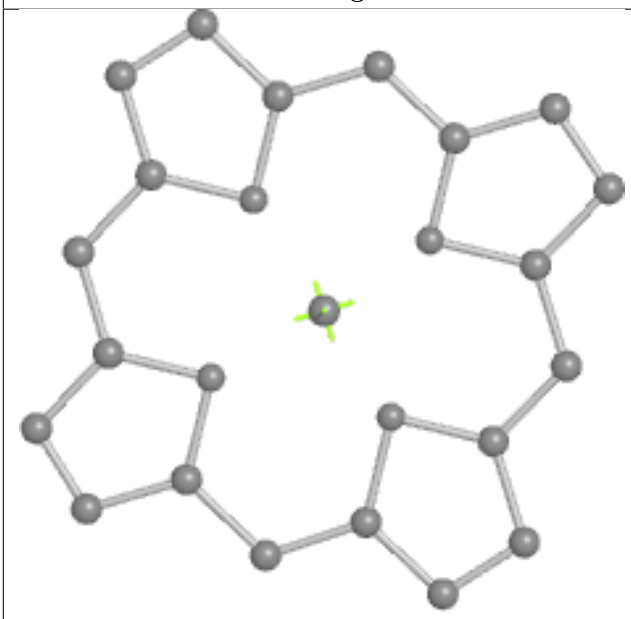
Ligand CLA 3 315



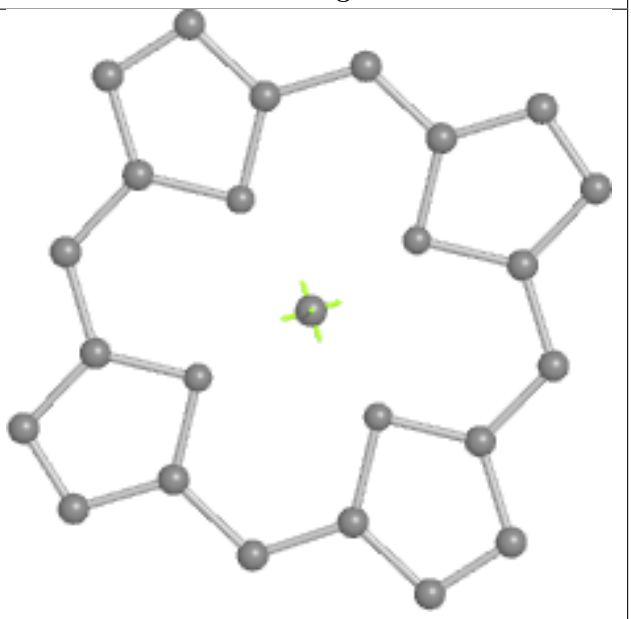
Bond lengths



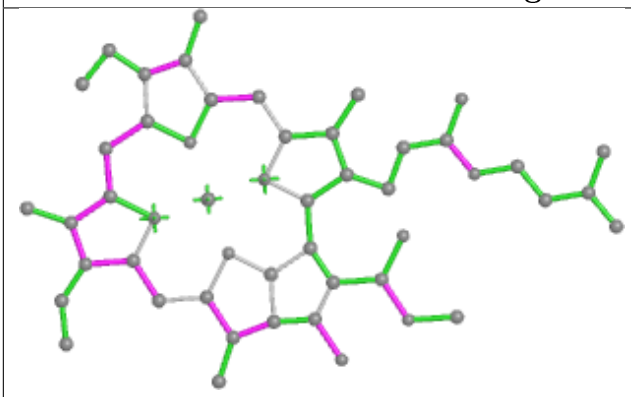
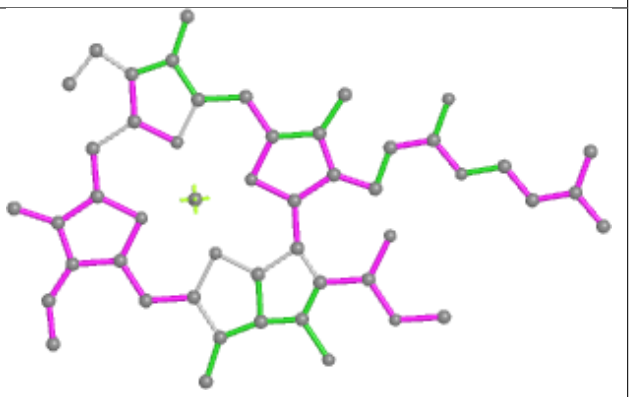
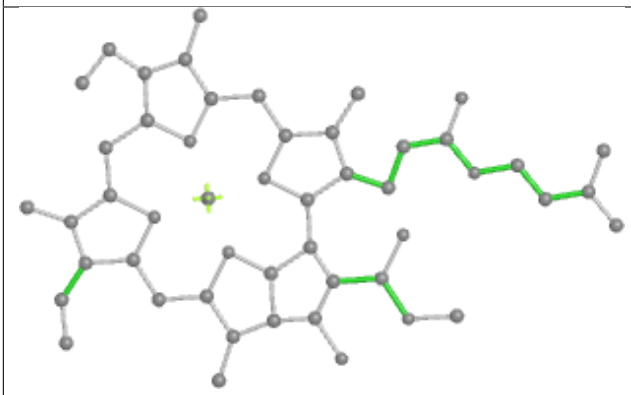
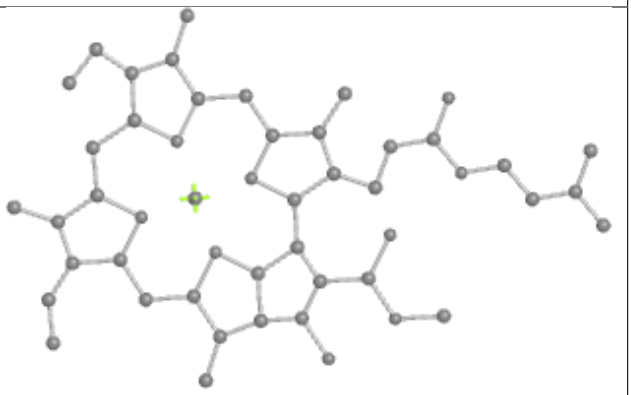
Bond angles

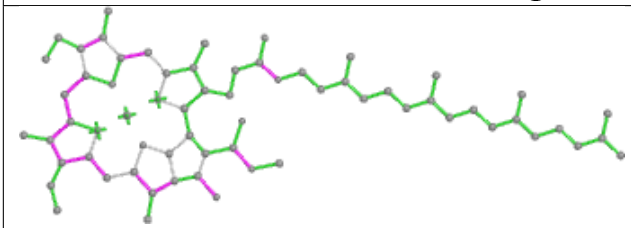
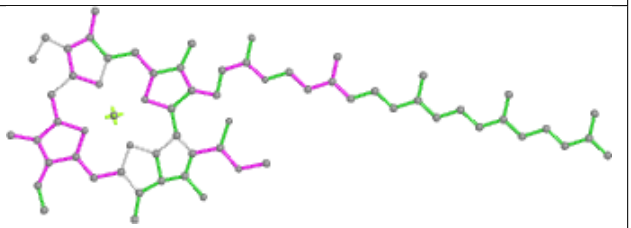
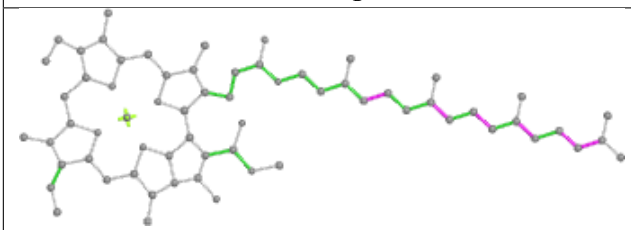
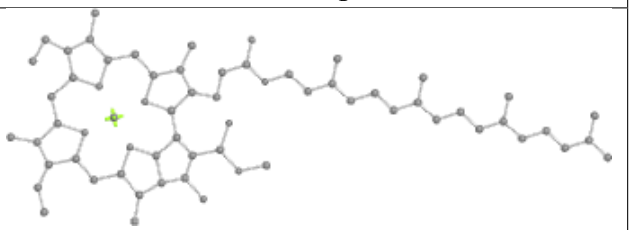


Torsions

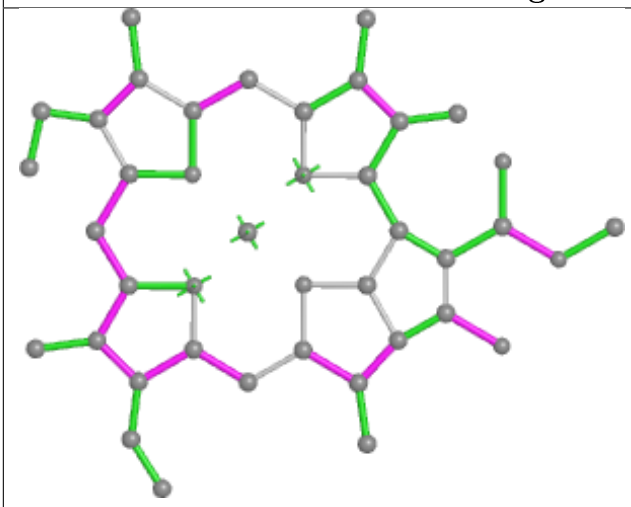


Rings

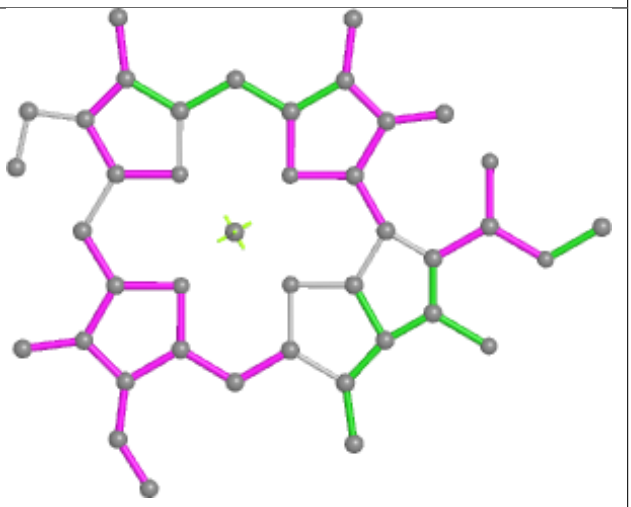
Ligand CLA A 836	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA b 803	
 Bond lengths	 Bond angles
 Torsions	 Rings

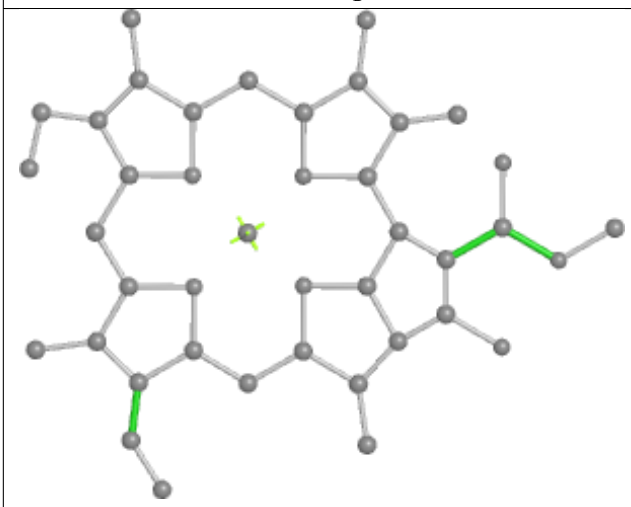
Ligand CLA 6 312



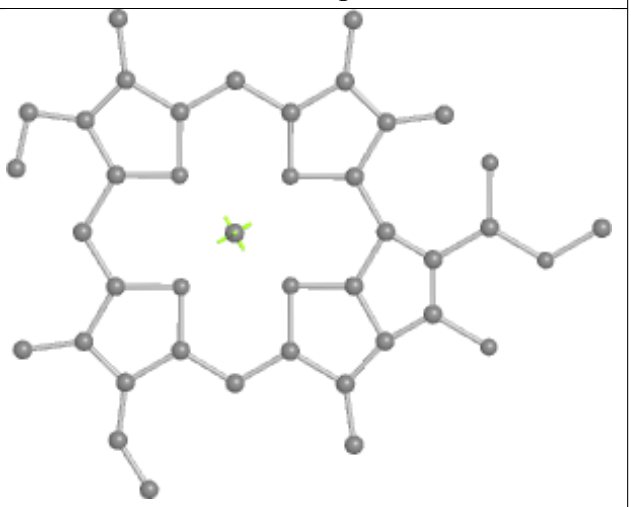
Bond lengths



Bond angles

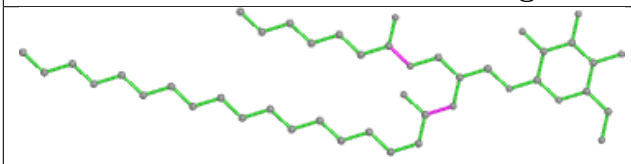


Torsions

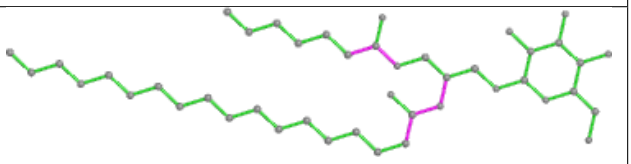


Rings

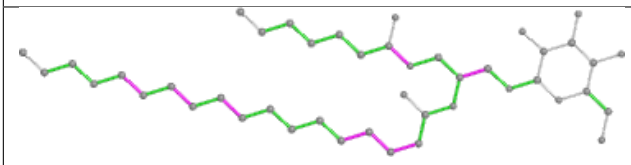
Ligand LMG G 102



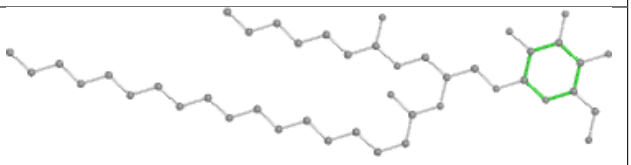
Bond lengths



Bond angles

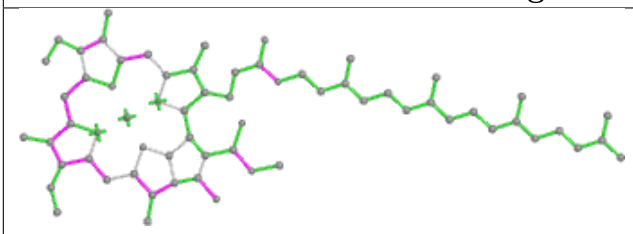


Torsions

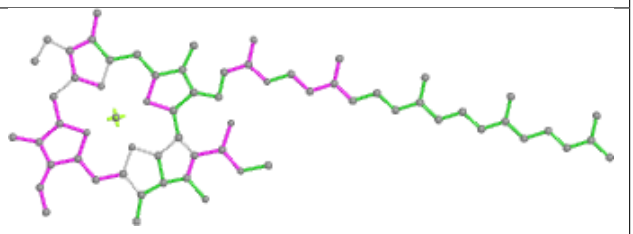


Rings

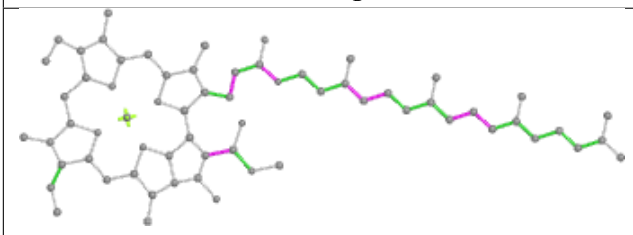
Ligand CLA b 824



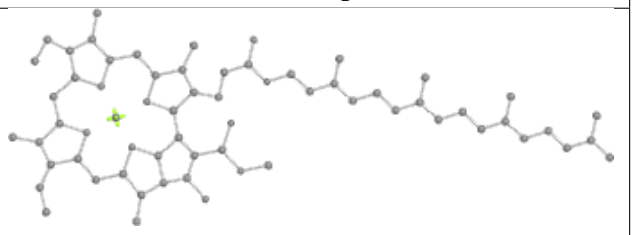
Bond lengths



Bond angles

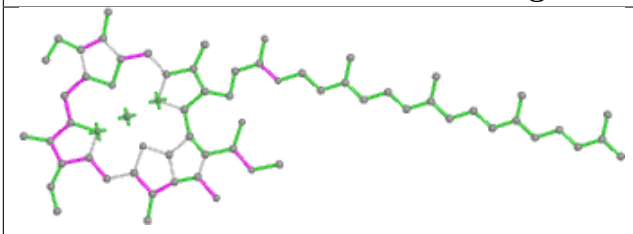


Torsions

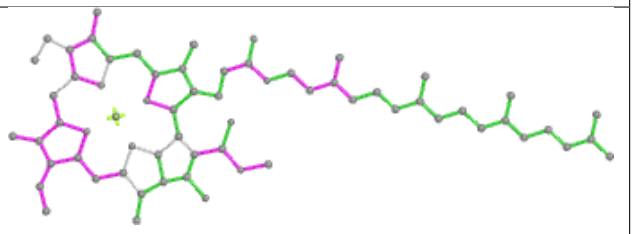


Rings

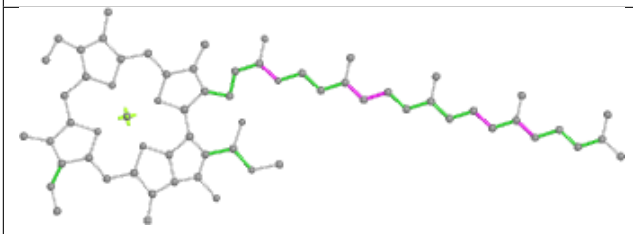
Ligand CLA 6 310



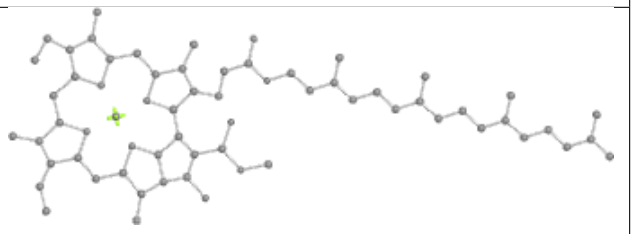
Bond lengths



Bond angles

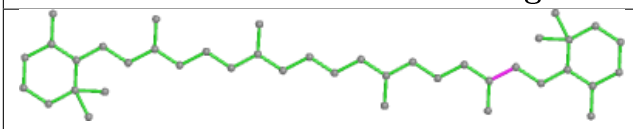


Torsions

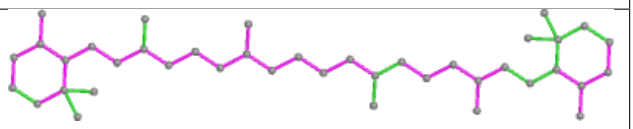


Rings

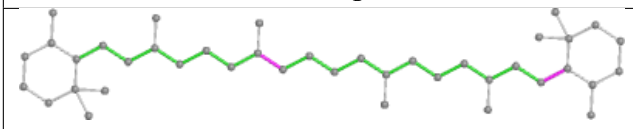
Ligand BCR F 305



Bond lengths



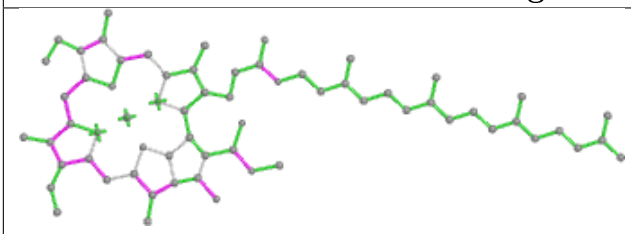
Bond angles



Torsions

Rings

Ligand CLA b 840



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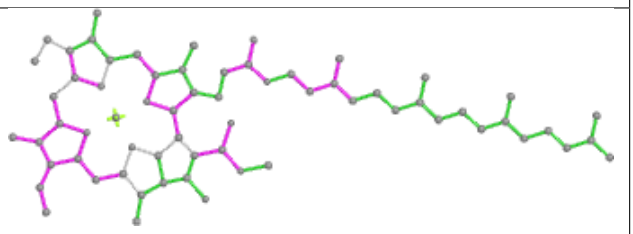
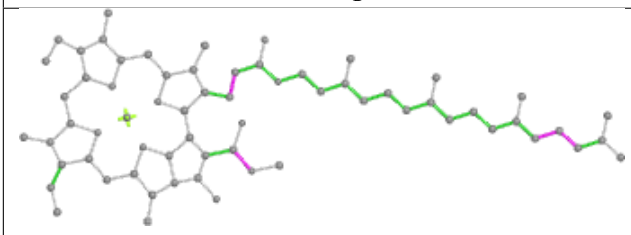


Bond angles



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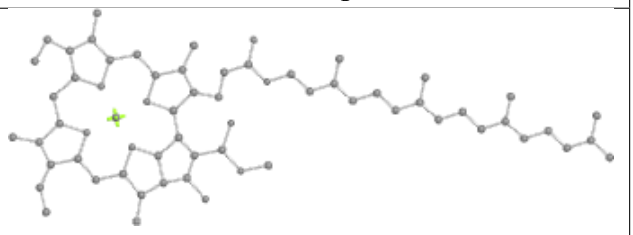
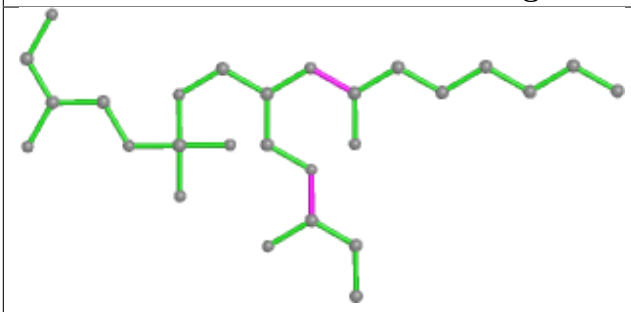


Rings

Ligand LHG A 847



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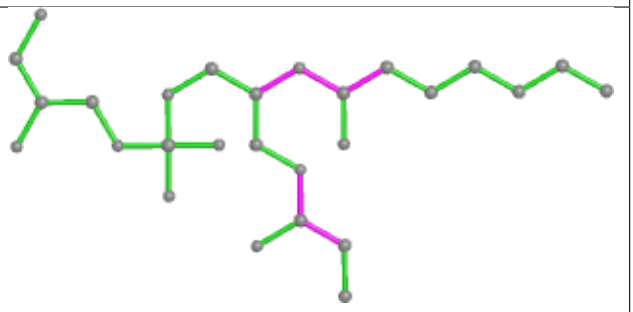
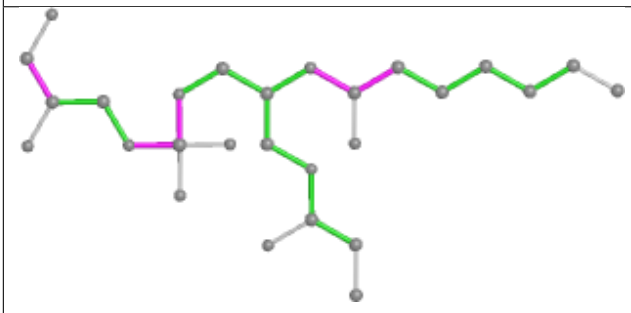


Bond angles



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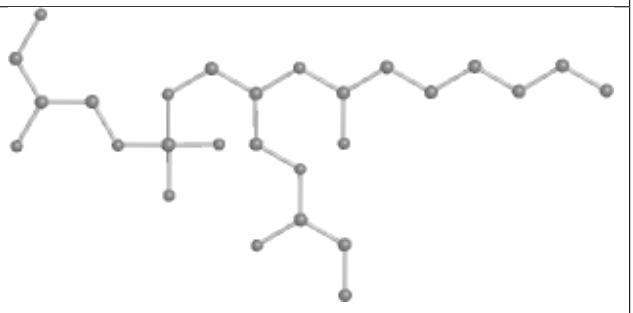
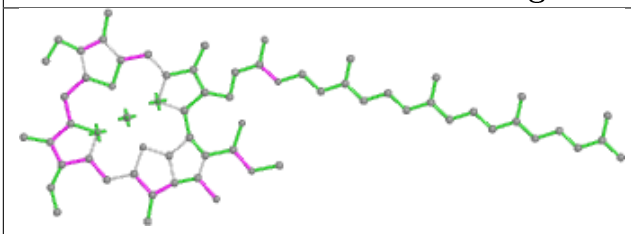


Rings

Ligand CLA 2 603



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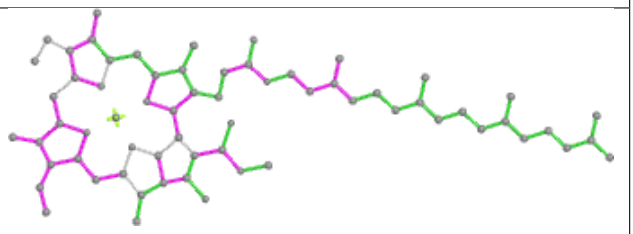
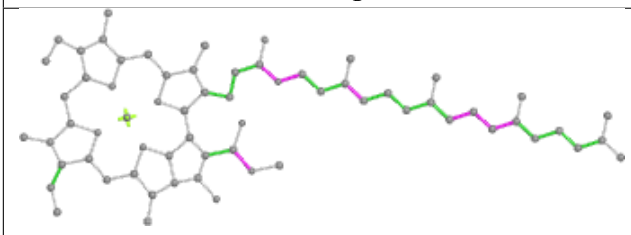


Bond angles



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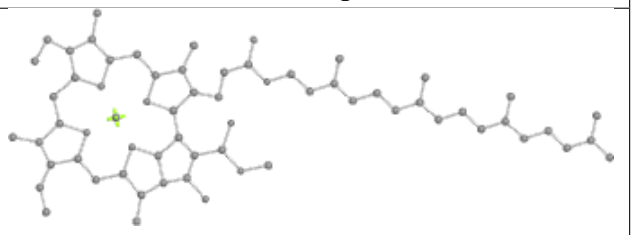
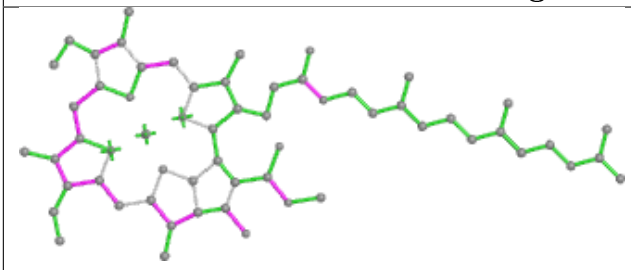


Rings

Ligand CLA 2 609



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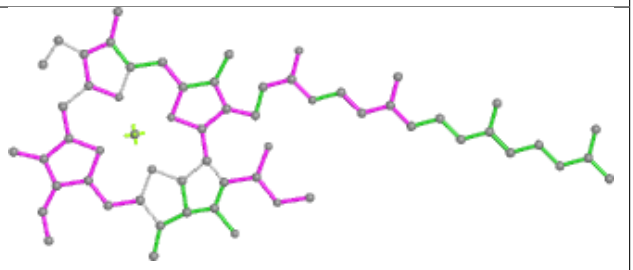
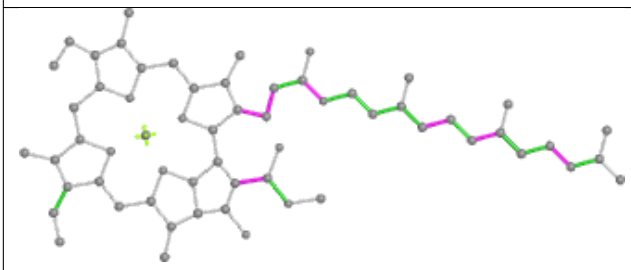


Bond angles



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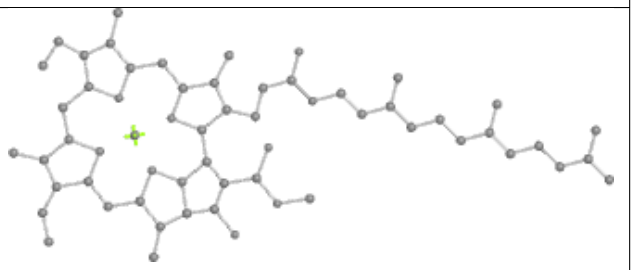
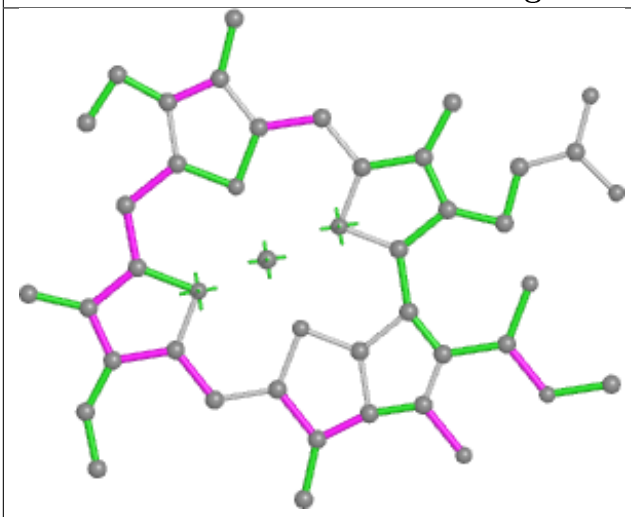


Rings

Ligand CLA B 835



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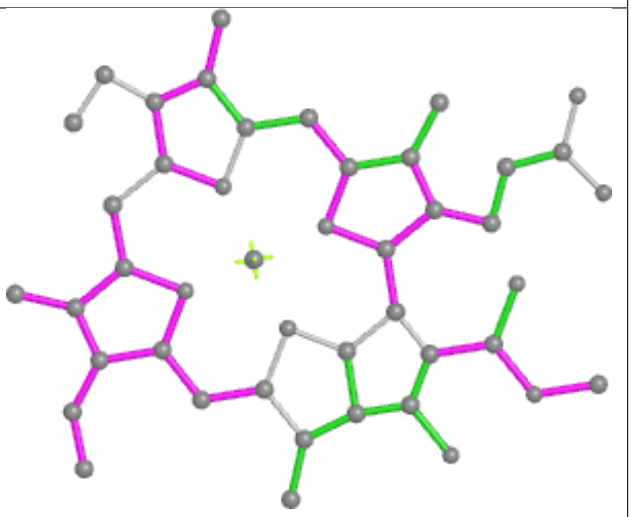
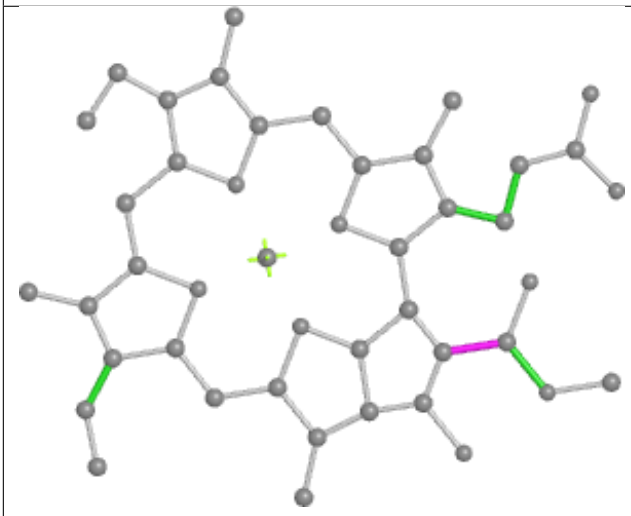


Bond angles



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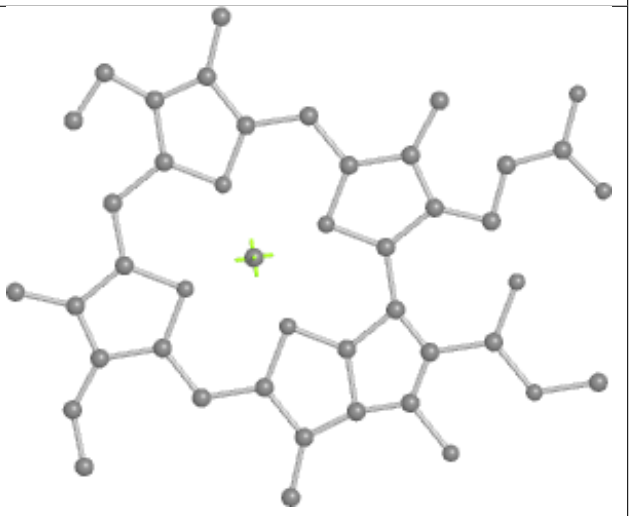
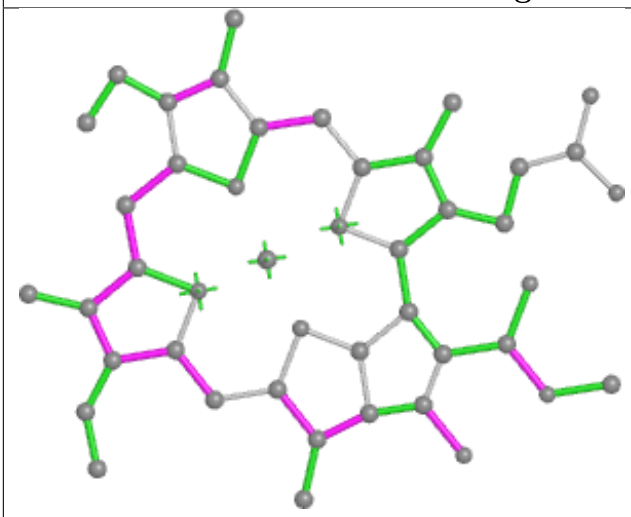
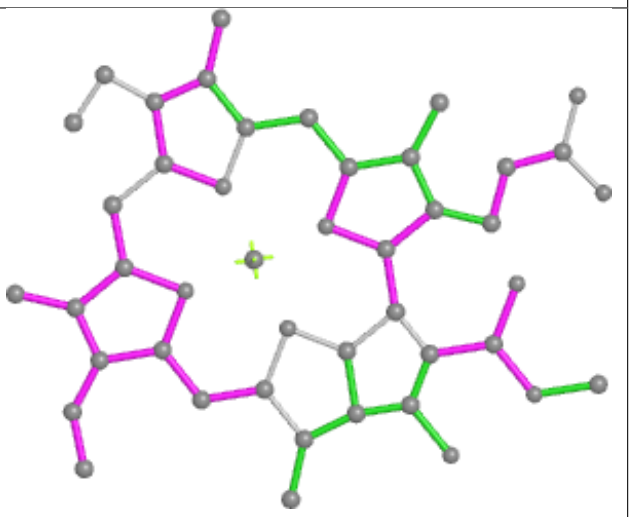


Rings

Ligand CLA K 4002



Bond lengths



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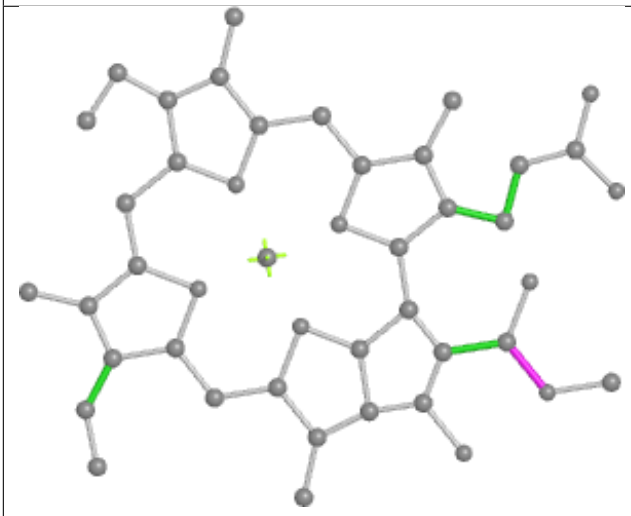
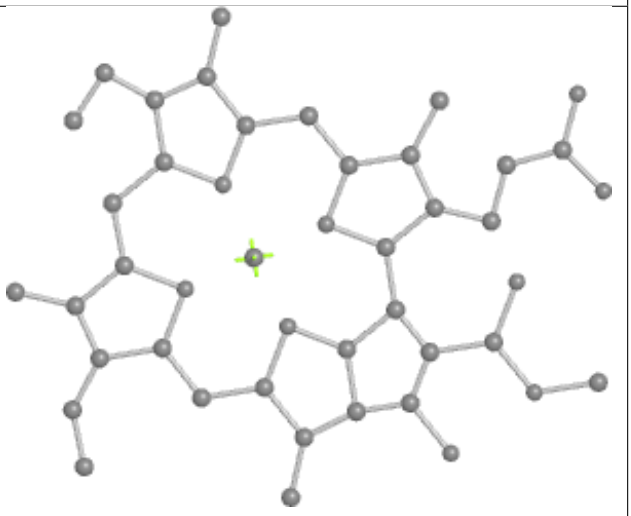
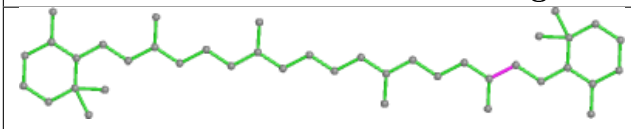


Torsions



Rings

Ligand BCR l 201



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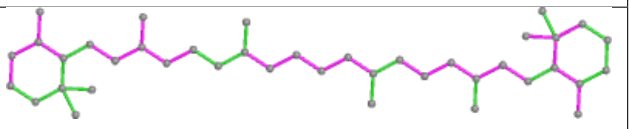
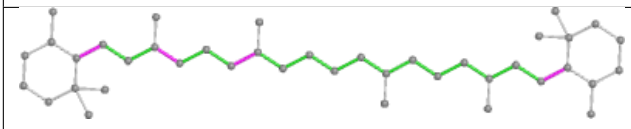


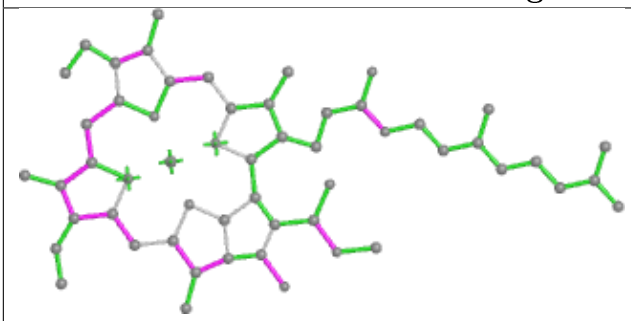
Bond angles



Torsions

Rings

Ligand CLA F 304



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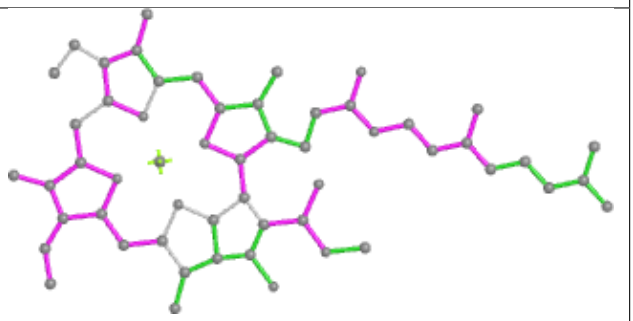

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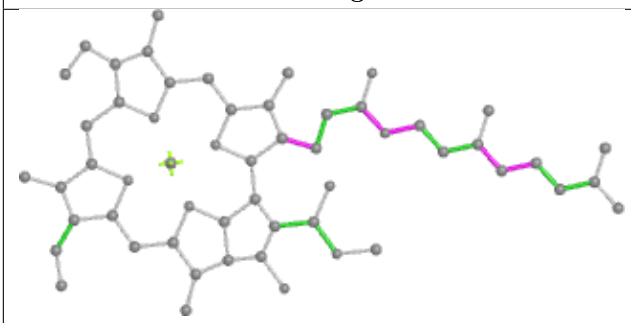

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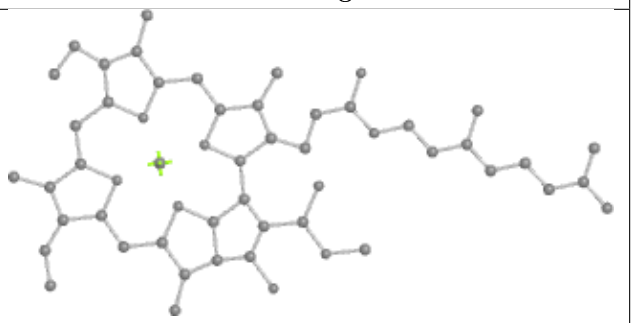
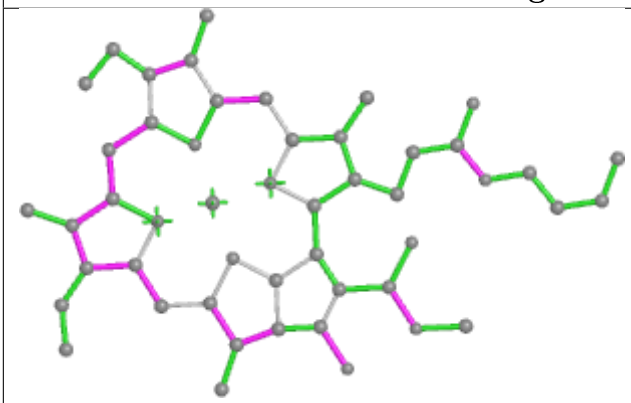


Rings

Ligand CLA a 823



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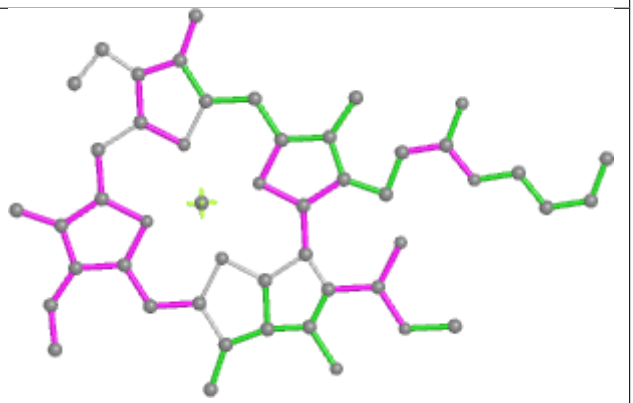
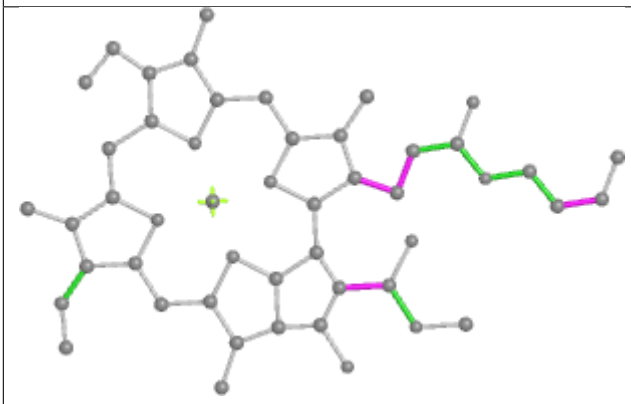


Bond angles



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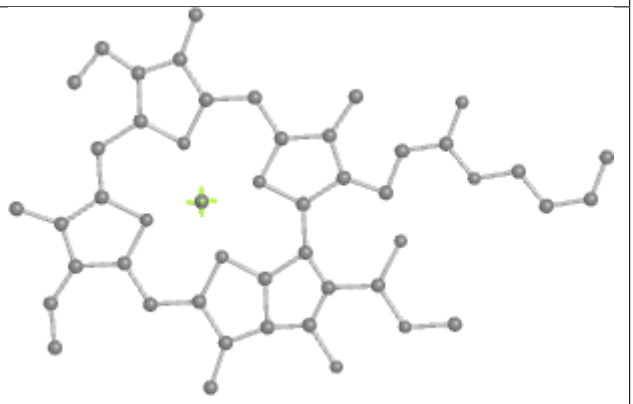
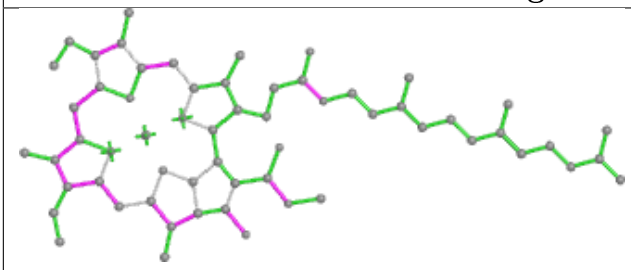
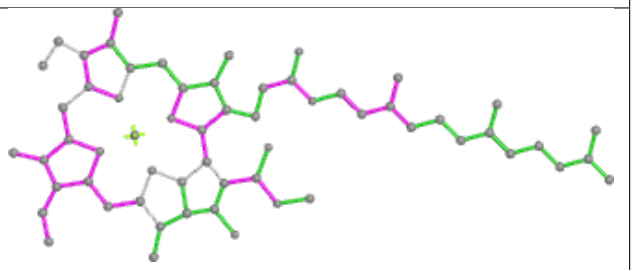


Rings

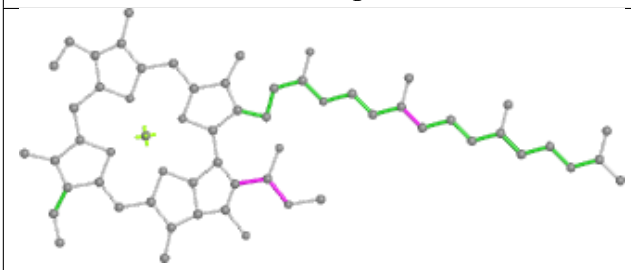
Ligand CLA b 823



Bond lengths



Bond angles



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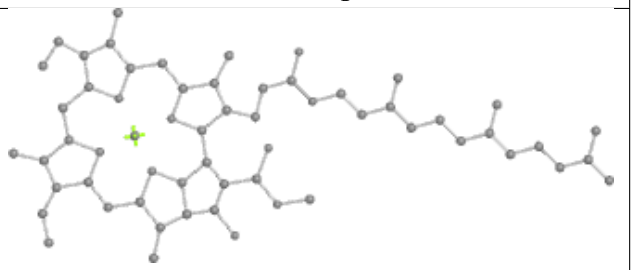
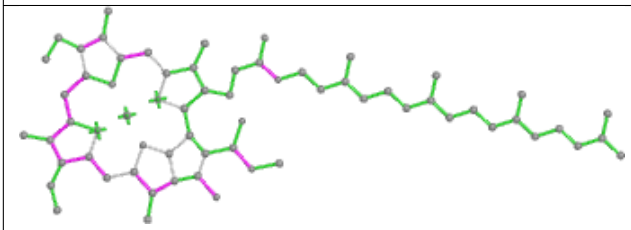
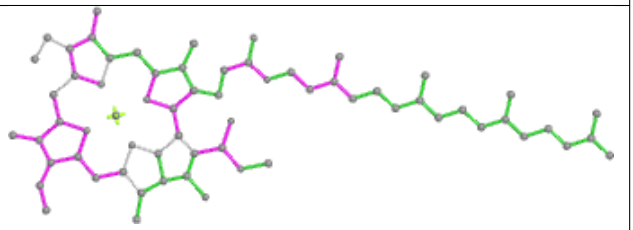


Rings

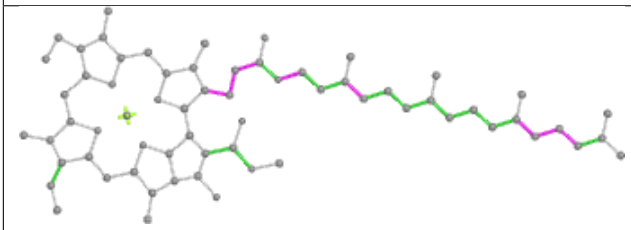
Ligand CLA a 830



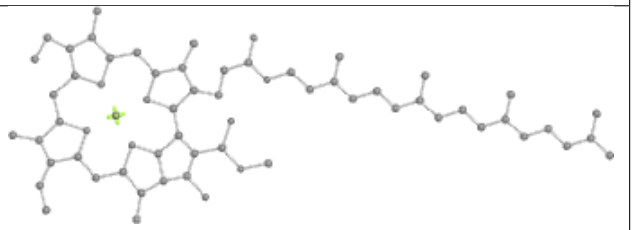
Bond lengths



Bond angles

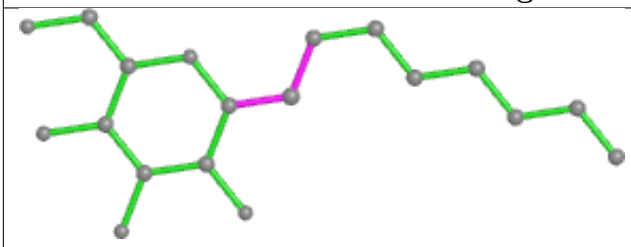


Torsions



Rings

Ligand HTG J 3001



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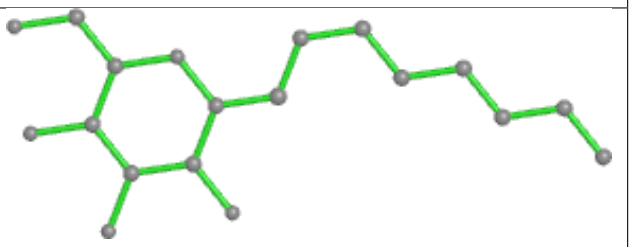
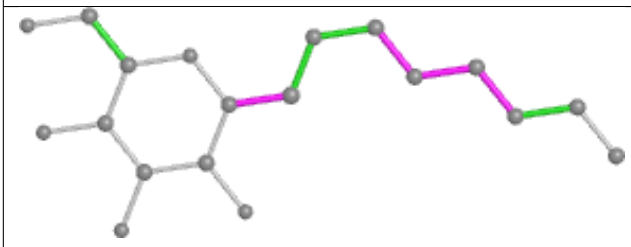
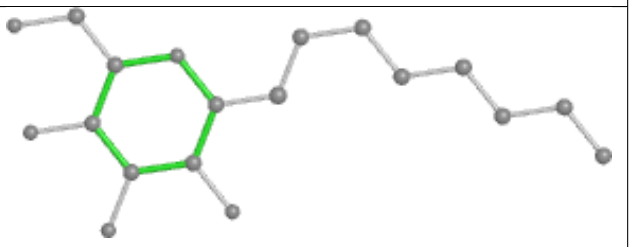


Bond angles

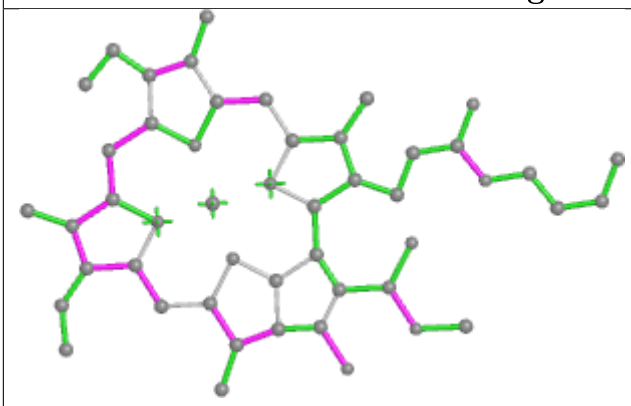


Torsions

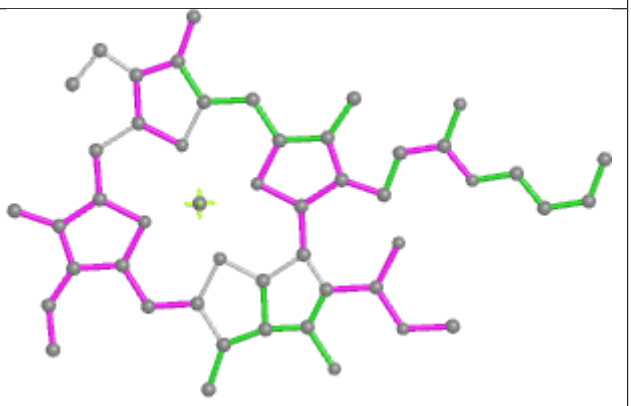


Rings

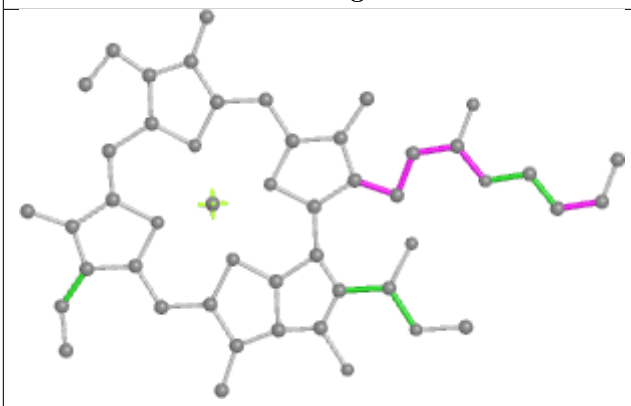
Ligand CLA b 831



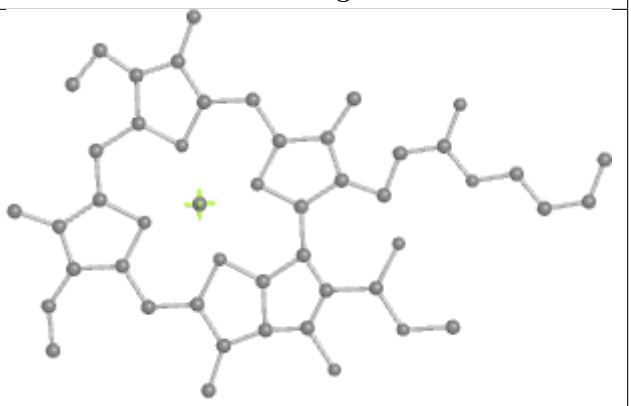
Bond lengths



Bond angles

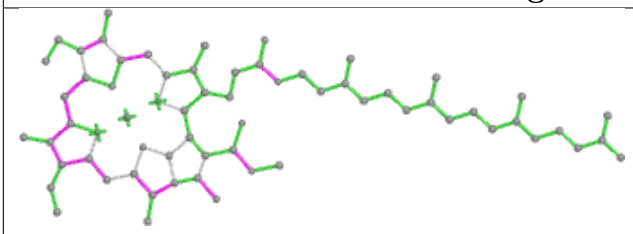


Torsions

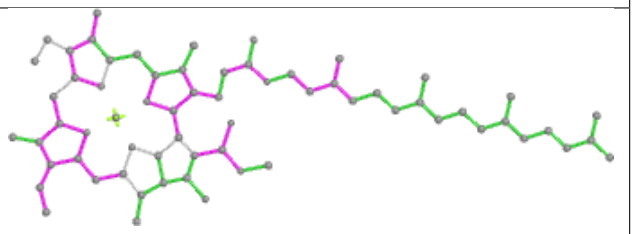


Rings

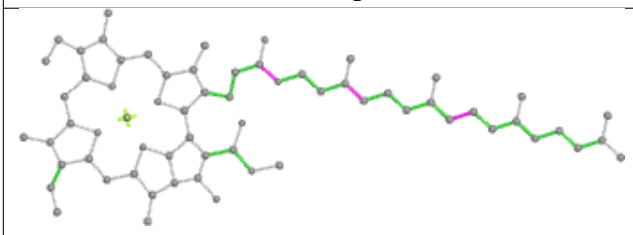
Ligand CLA b 819



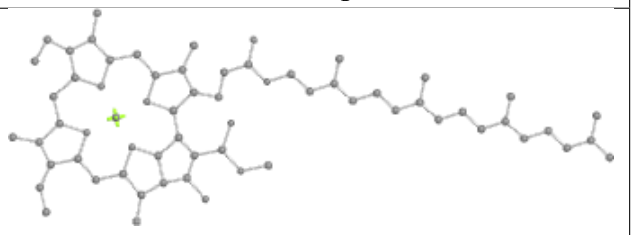
Bond lengths



Bond angles

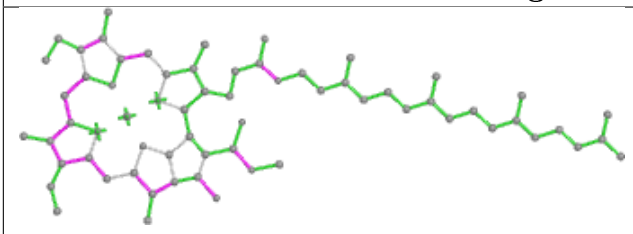


Torsions



Rings

Ligand CLA b 828



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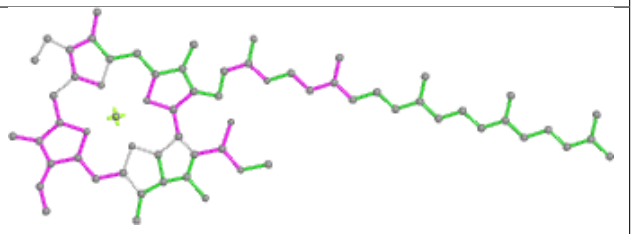
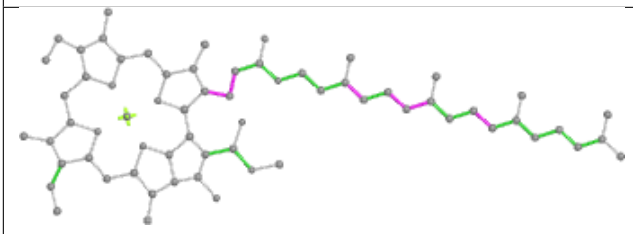
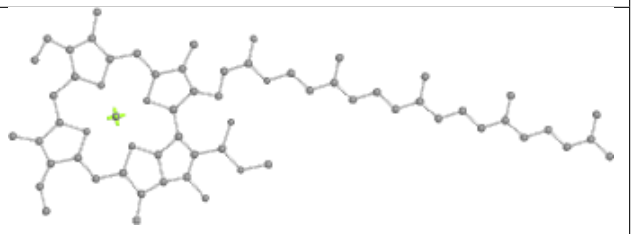


Bond angles

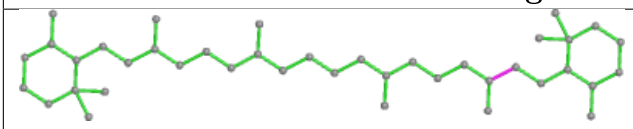


Torsions

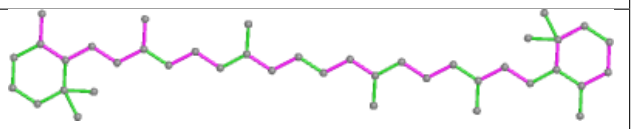


Rings

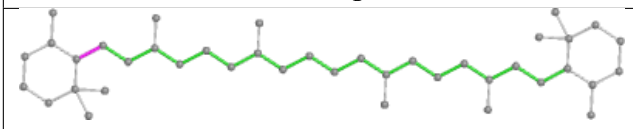
Ligand BCR b 848



Bond lengths



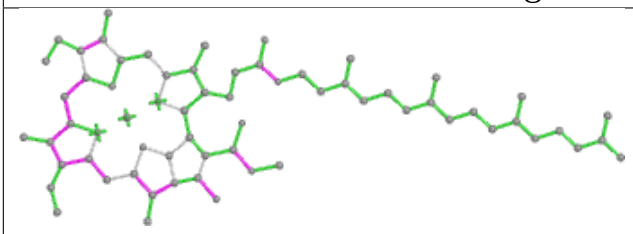
Bond angles



Torsions

Rings

Ligand CLA A 802



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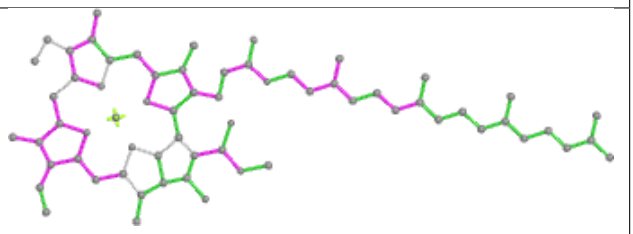
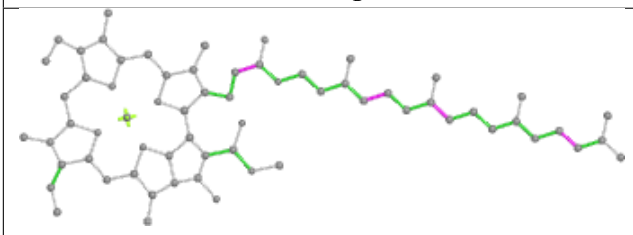


Bond angles



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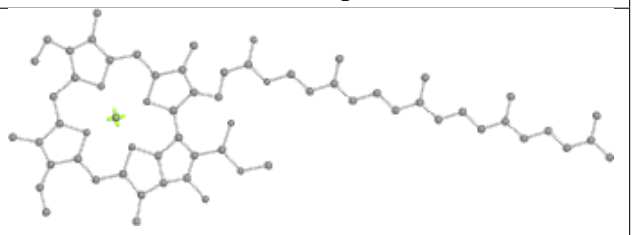
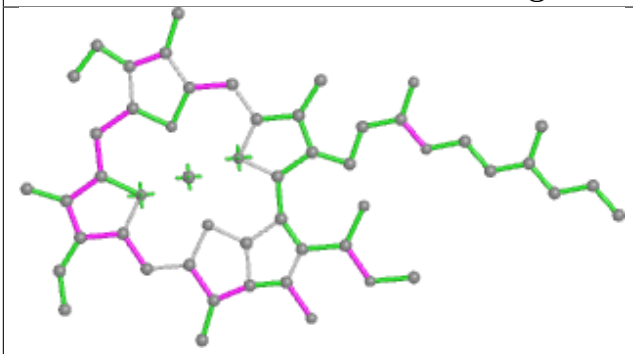


Rings

Ligand CLA 4 611



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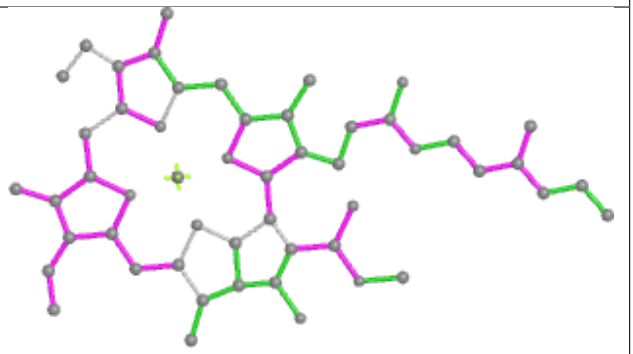
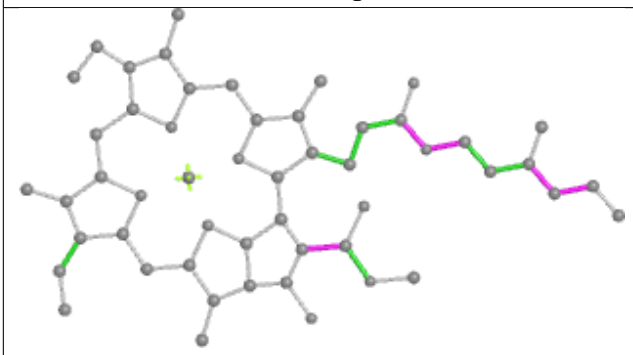


Bond angles



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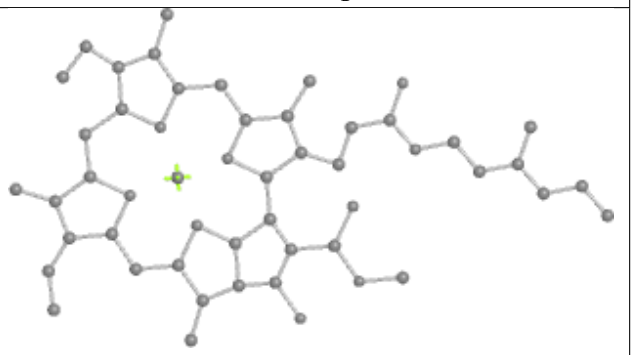
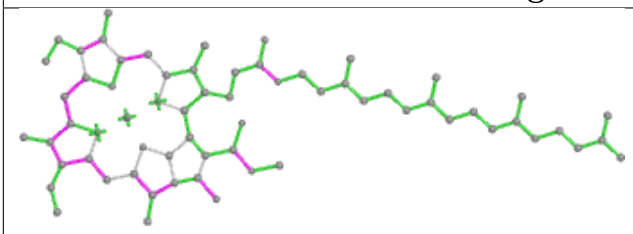


Rings

Ligand CLA b 832



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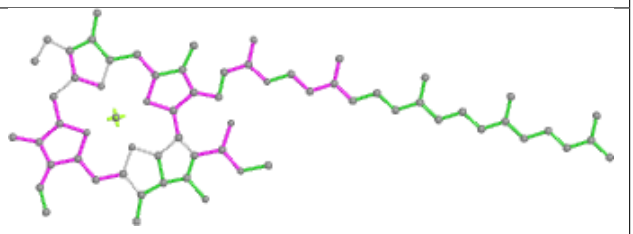
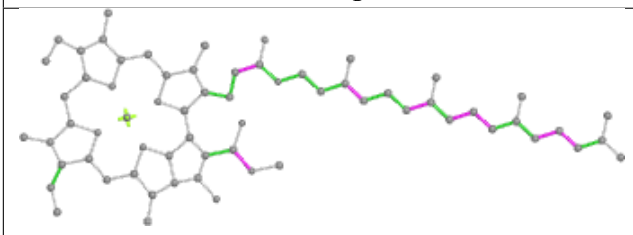


Bond angles



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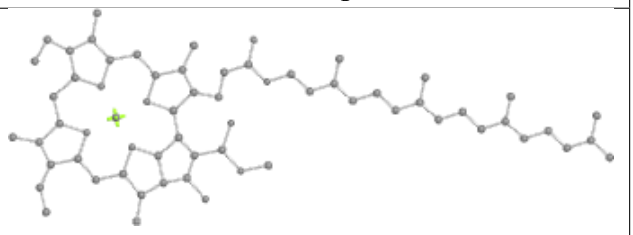
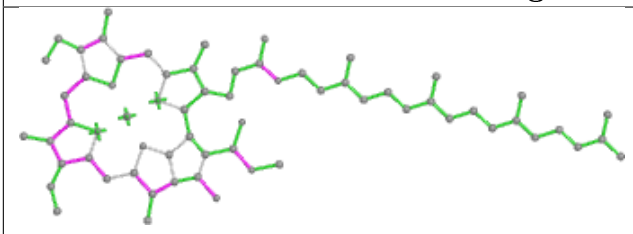


Rings

Ligand CLA b 837



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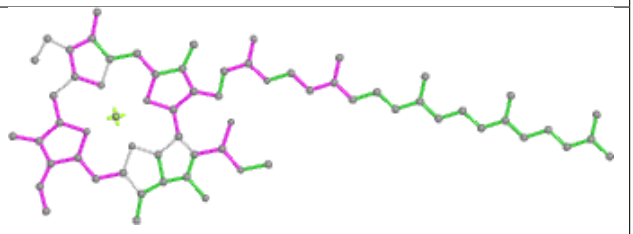
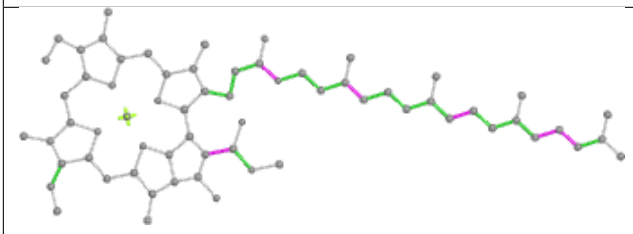


Bond angles



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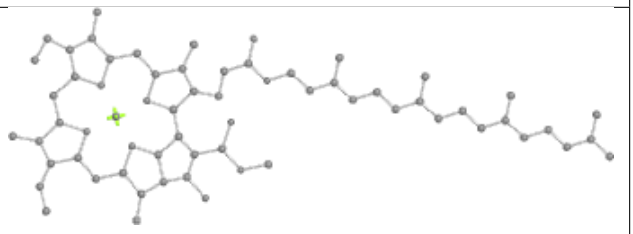
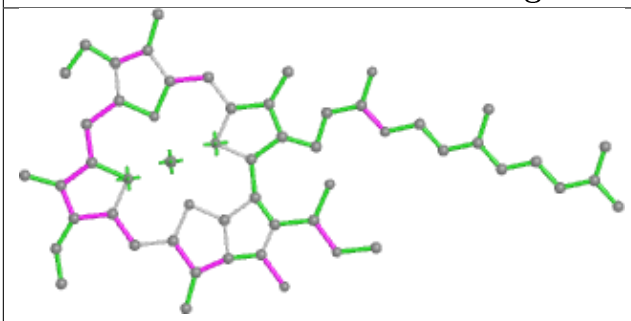
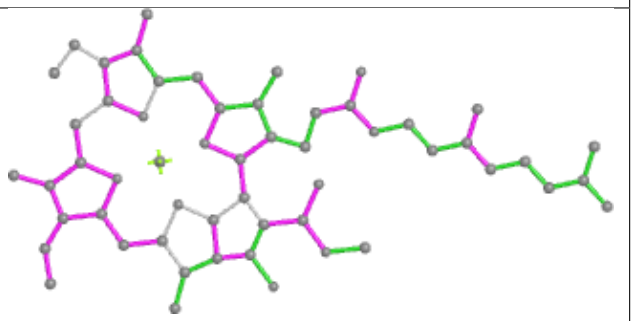


Rings

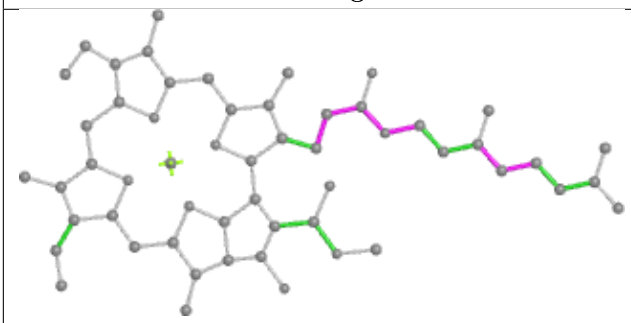
Ligand CLA B 816



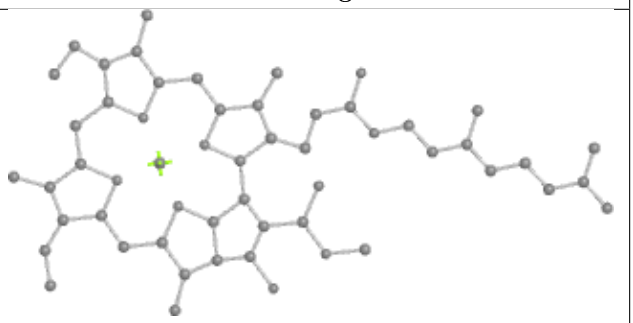
Bond lengths



Bond angles

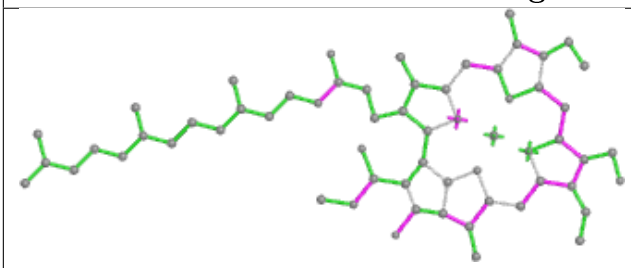


Torsions



Rings

Ligand CHL 2 601



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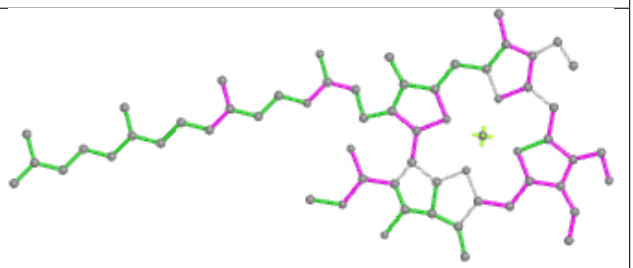
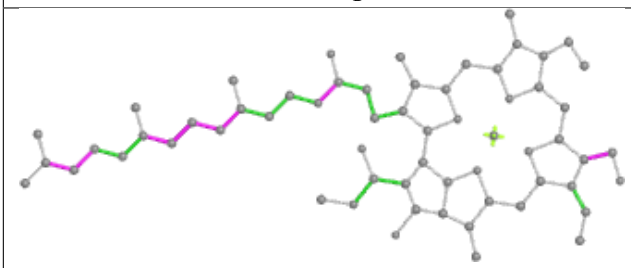


Bond angles



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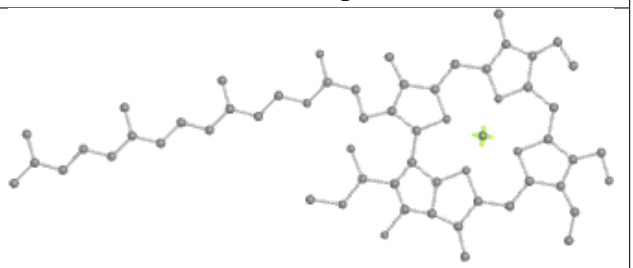
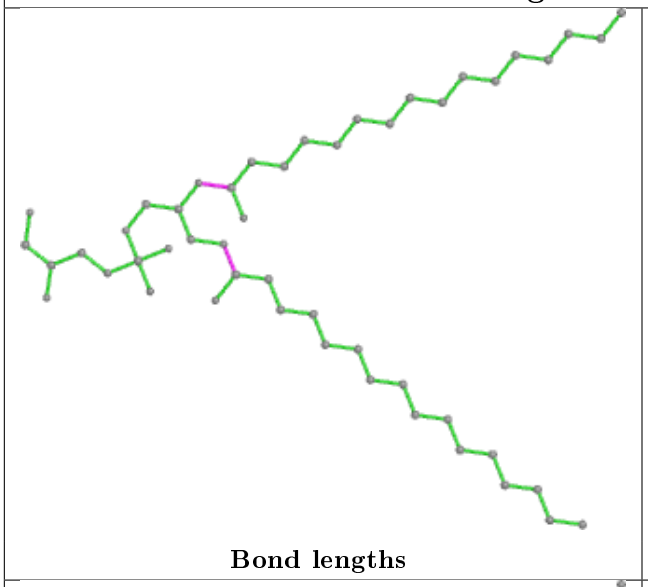


Rings

Ligand LHG 6 320



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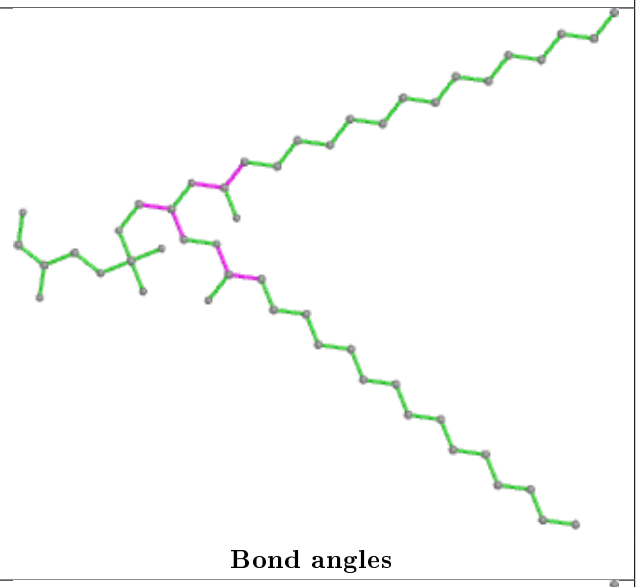
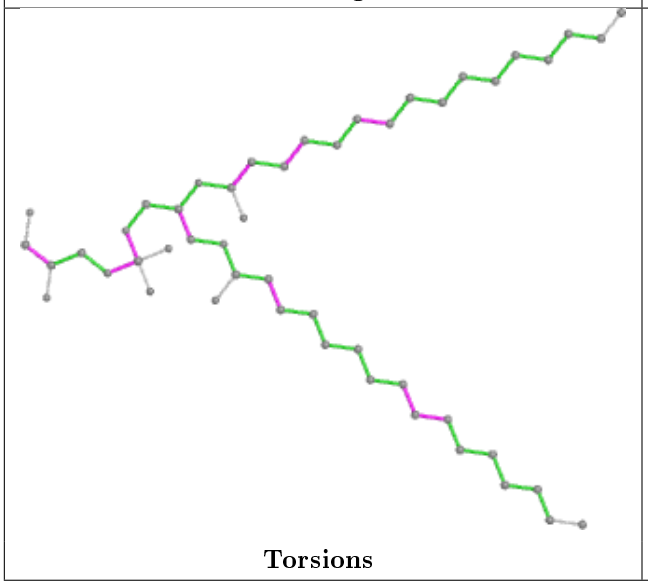


Bond angles



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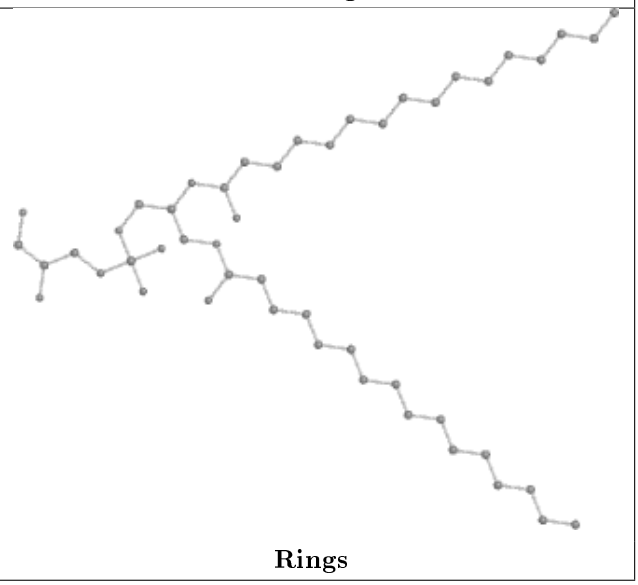
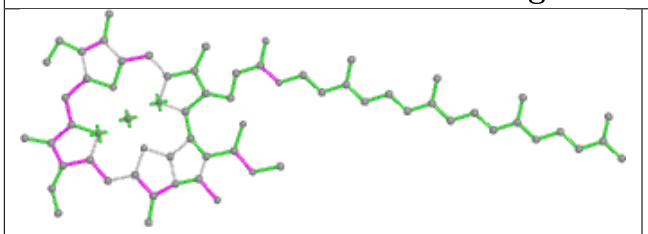


Rings

Ligand CLA b 806



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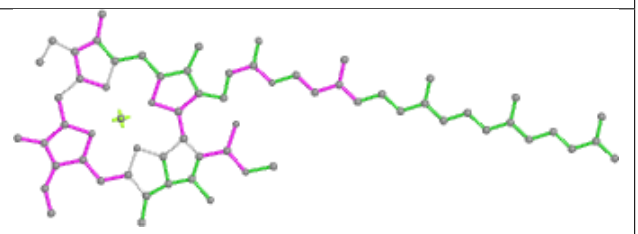
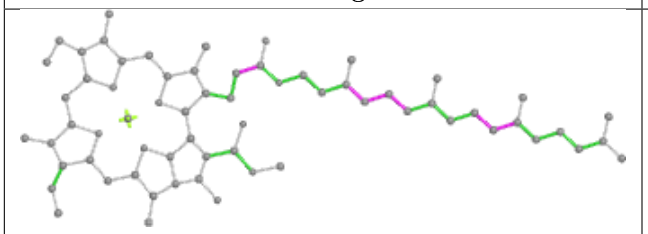


Bond angles



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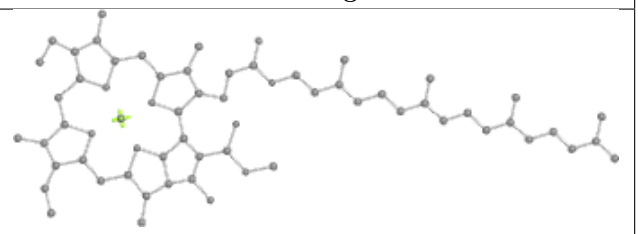
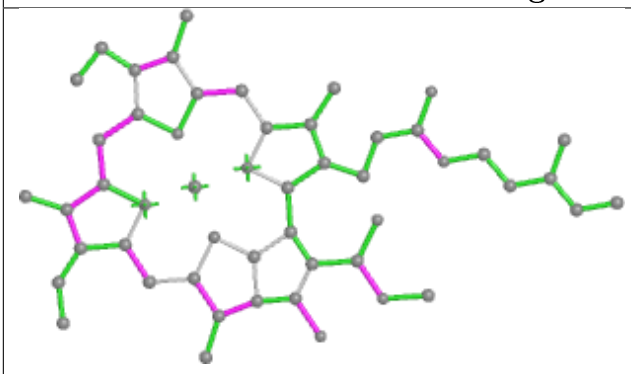
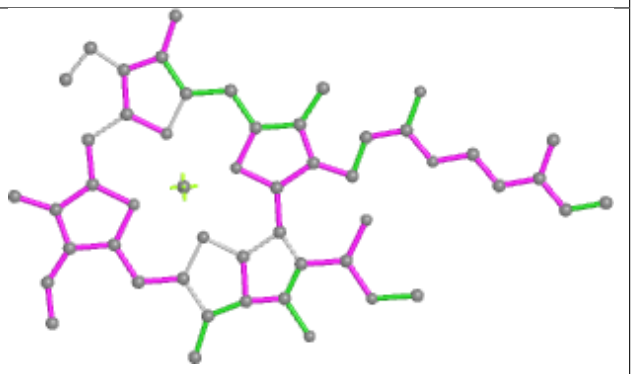


Rings

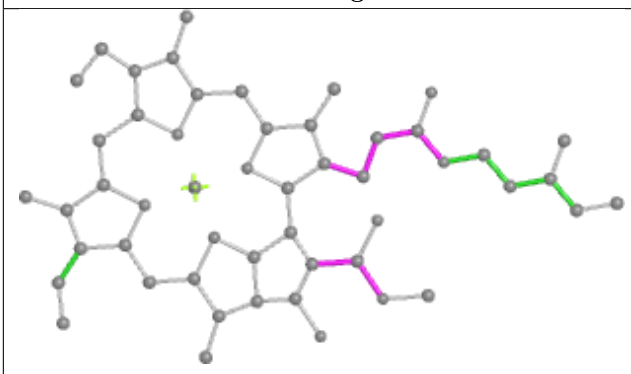
Ligand CLA a 838



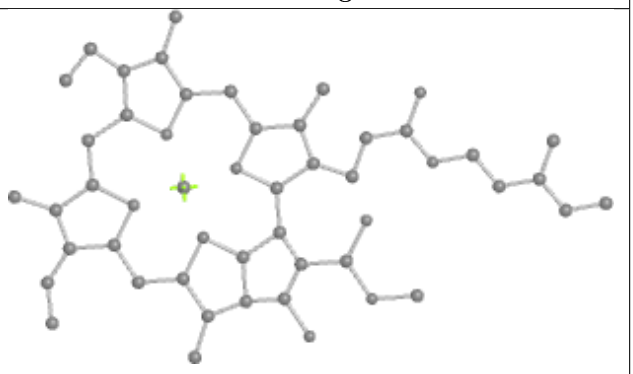
Bond lengths



Bond angles

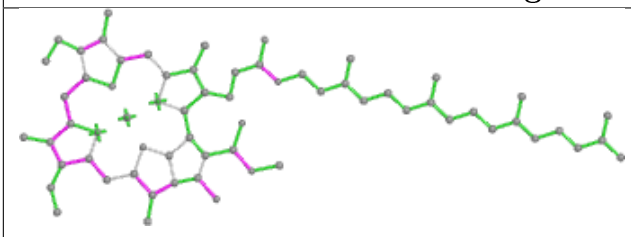


Torsions

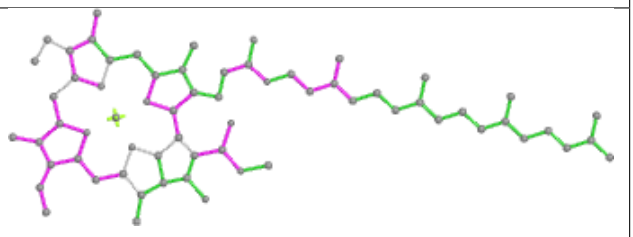


Rings

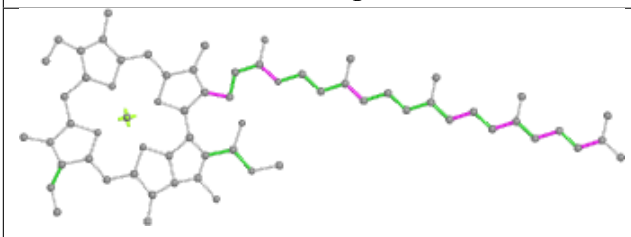
Ligand CLA A 820



Bond lengths



Bond angles



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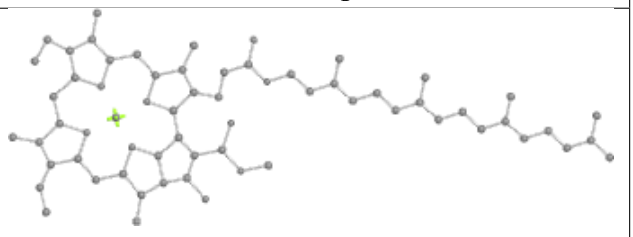
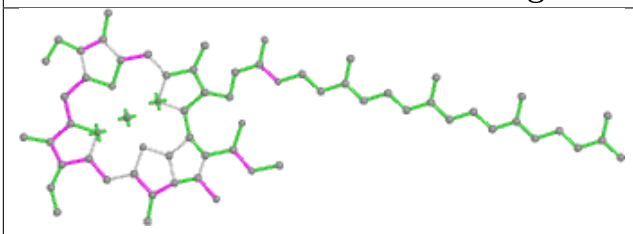
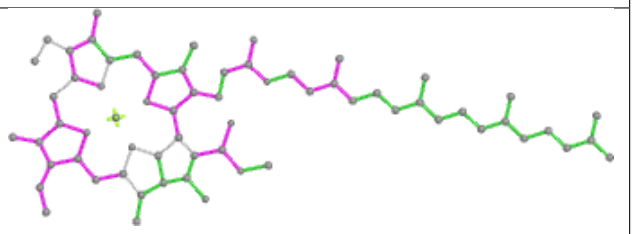


Rings

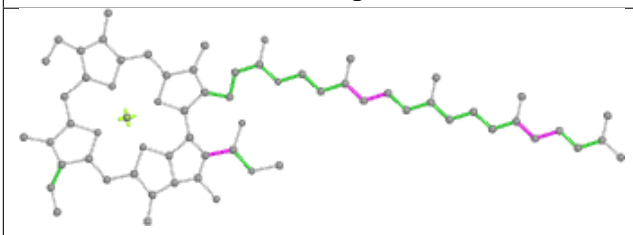
Ligand CLA b 808



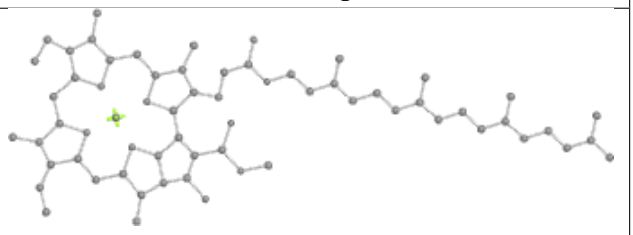
Bond lengths



Bond angles

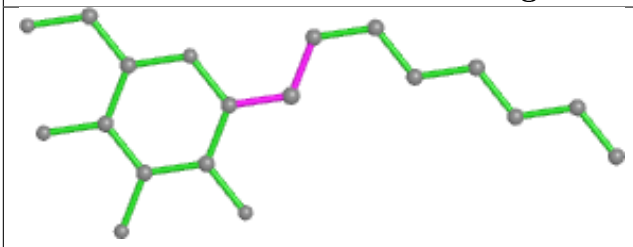


Torsions

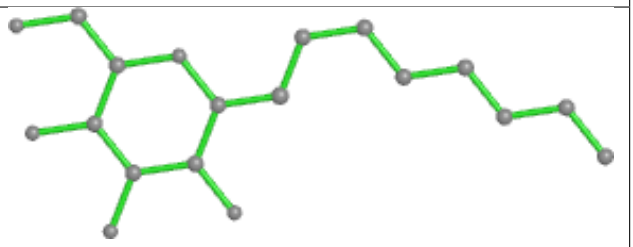


Rings

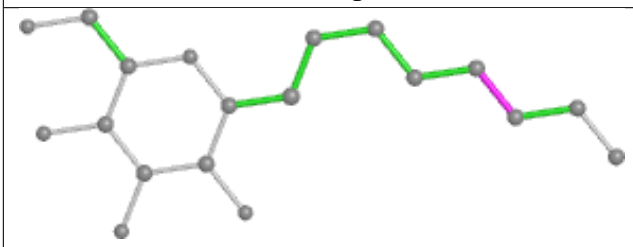
Ligand HTG A 855



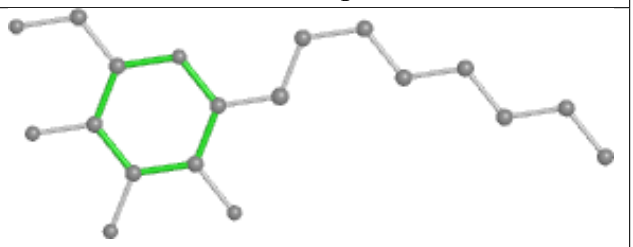
Bond lengths



Bond angles

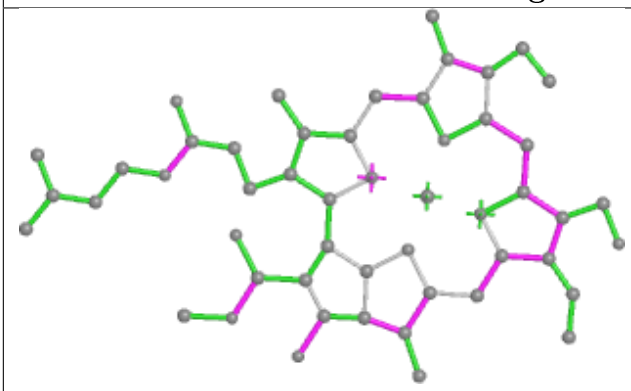


Torsions



Rings

Ligand CHL 7 607



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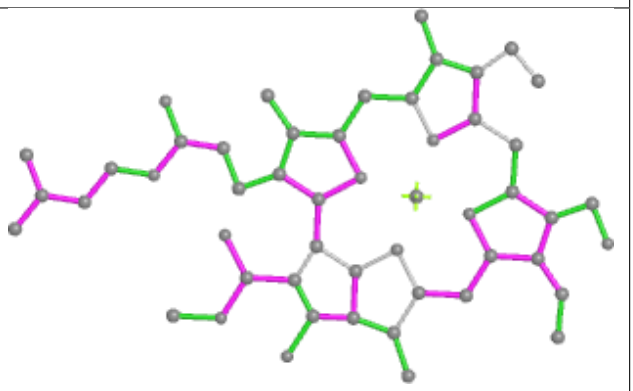

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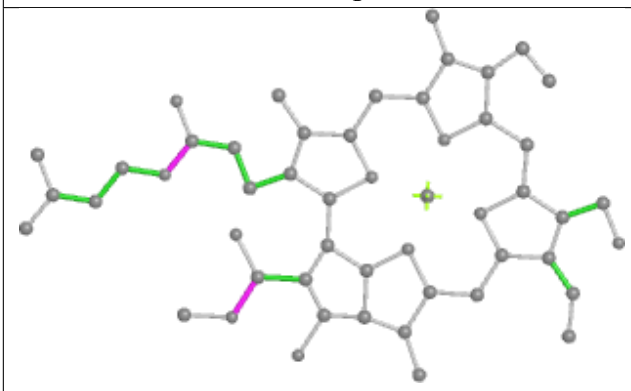

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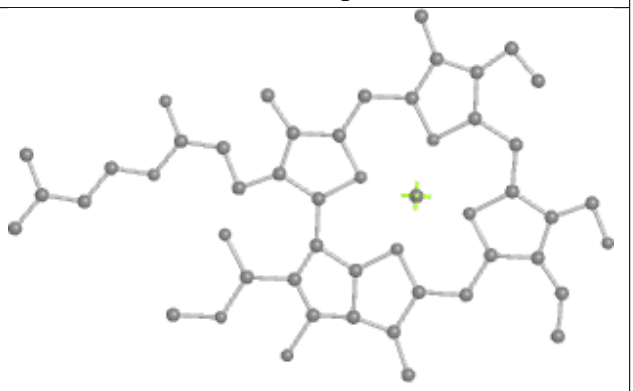
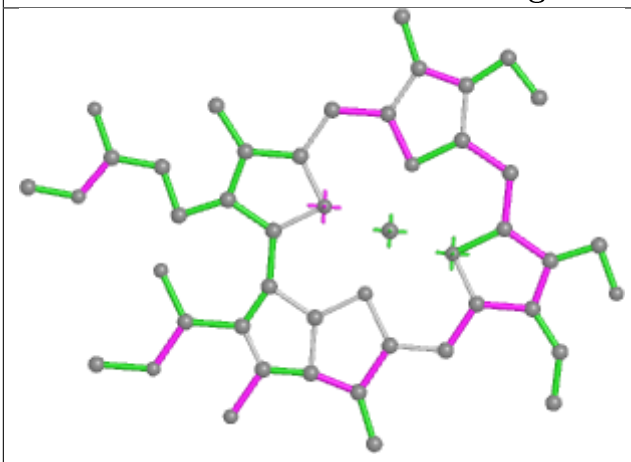


Rings

Ligand CHL 3 307



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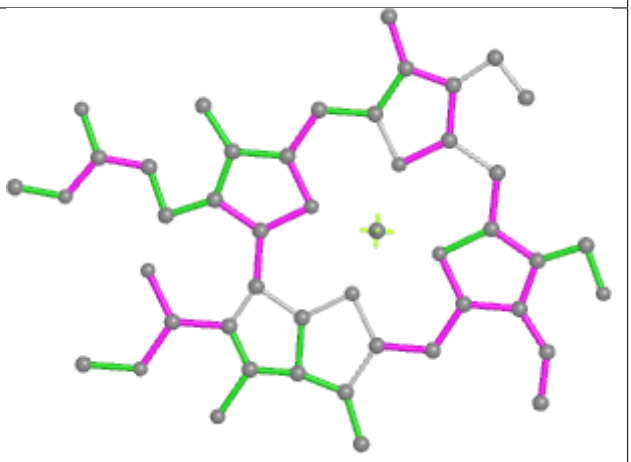
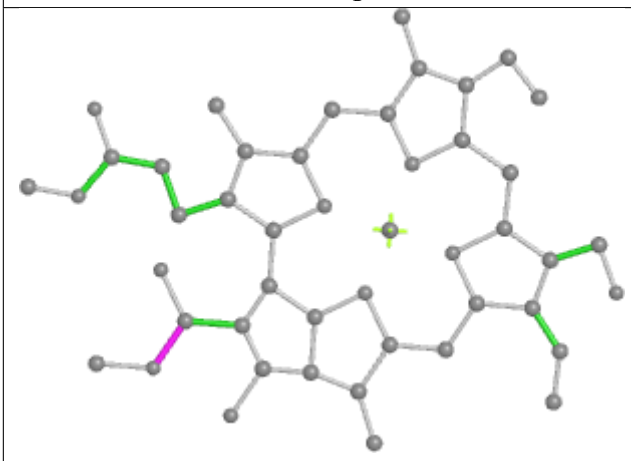


Bond angles



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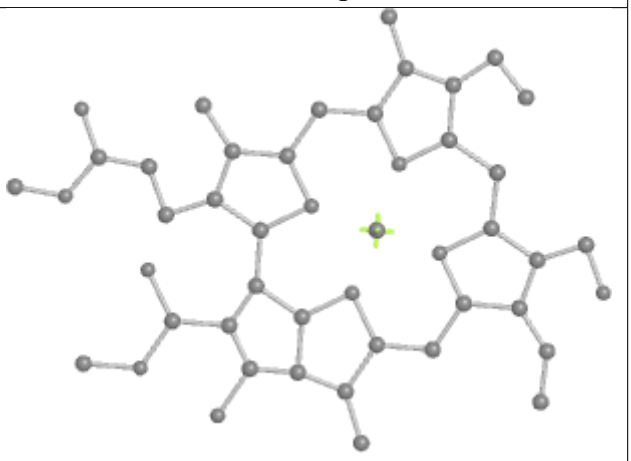
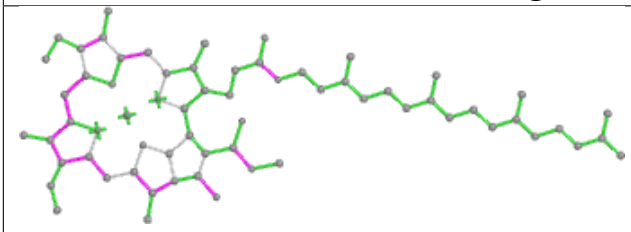


Rings

Ligand CLA b 825



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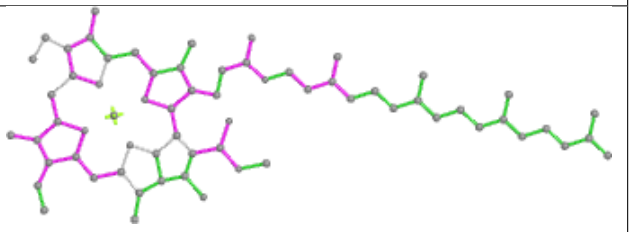
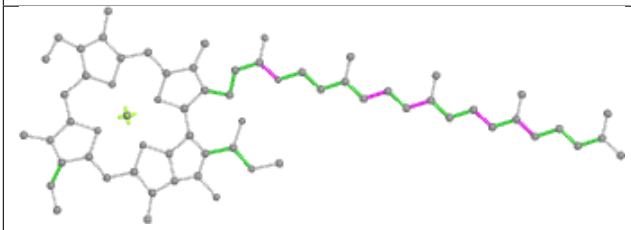


Bond angles



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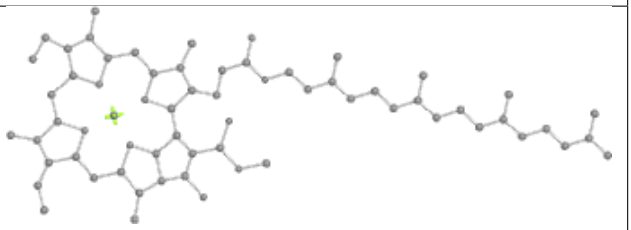
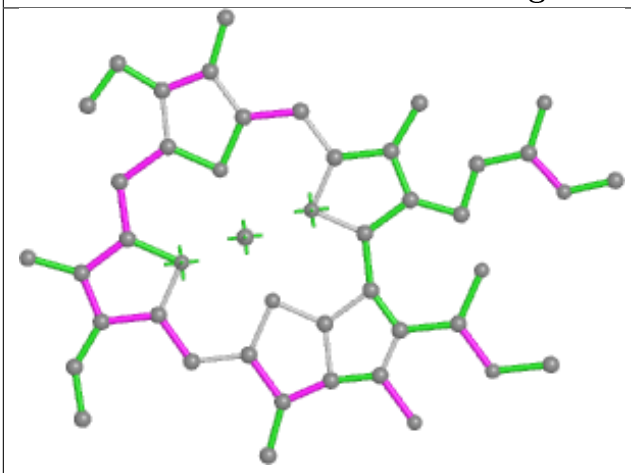


Rings

Ligand CLA g 103



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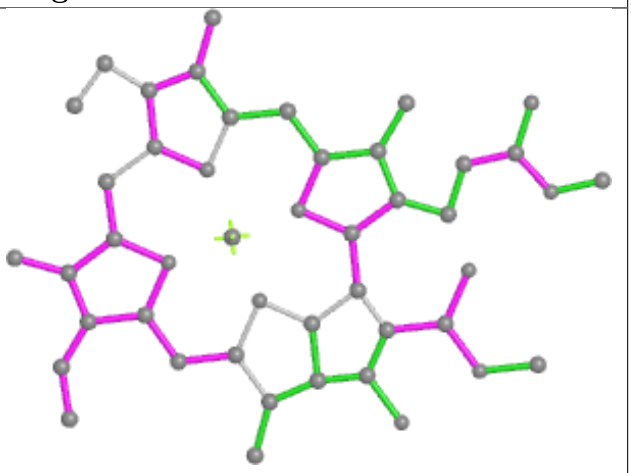
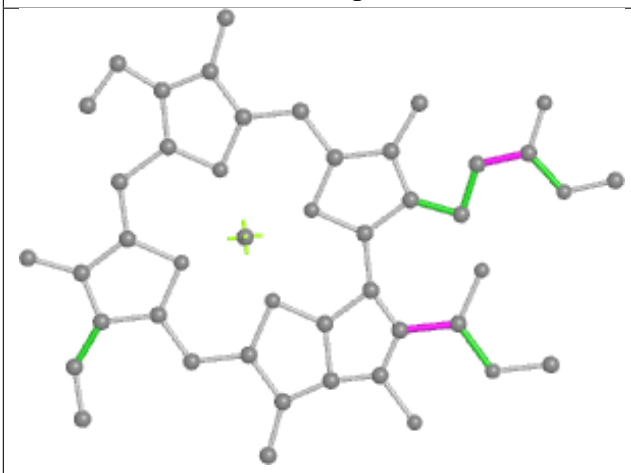


Bond angles



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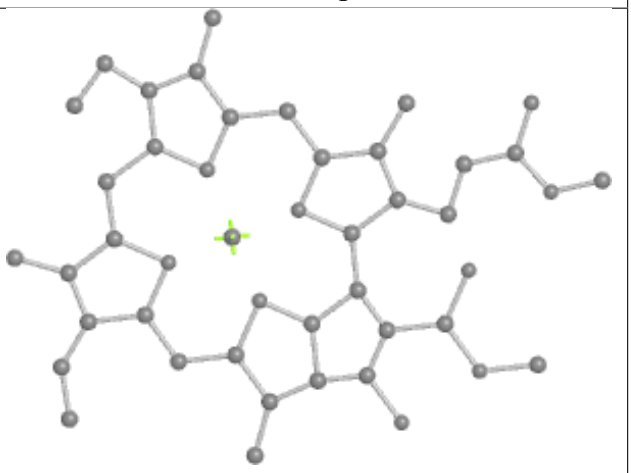
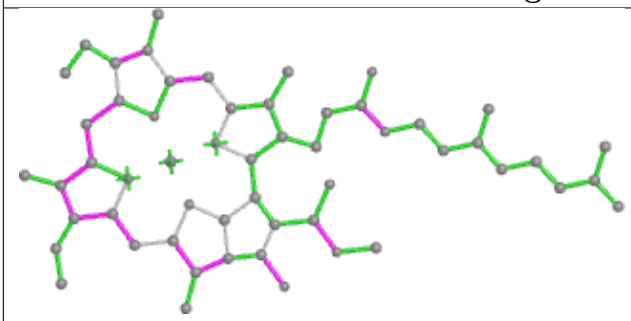


Rings

Ligand CLA B 812



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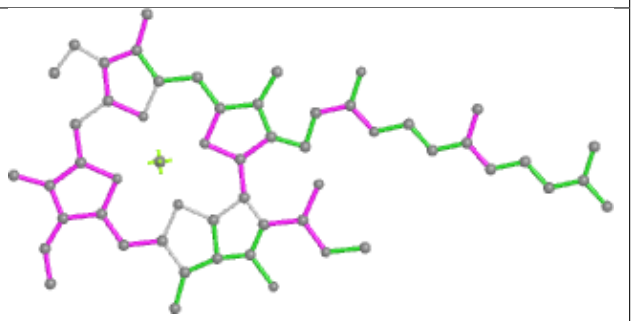
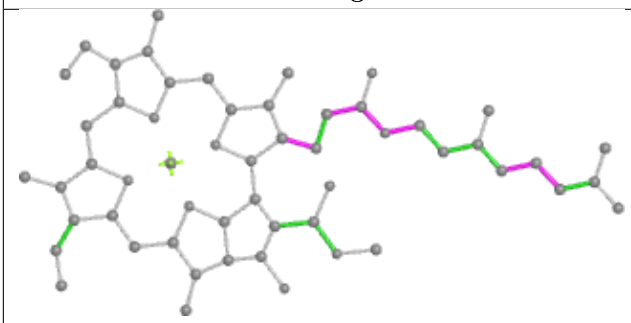


Bond angles



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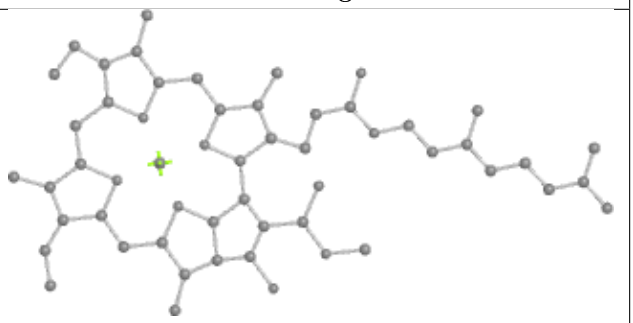
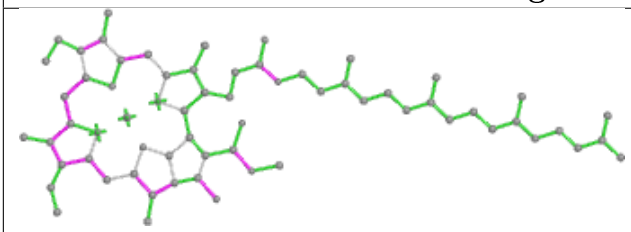


Rings

Ligand CLA 1 303



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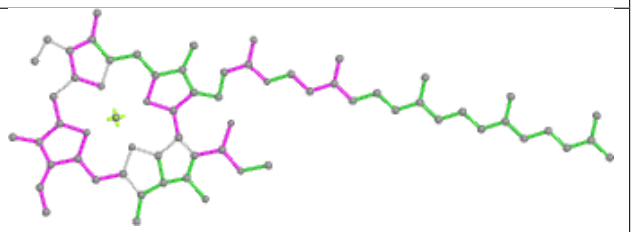
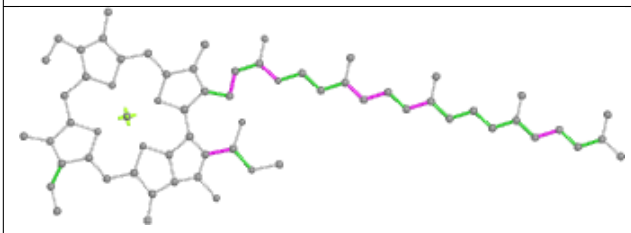


Bond angles



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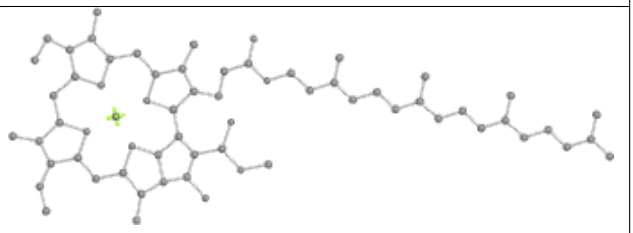
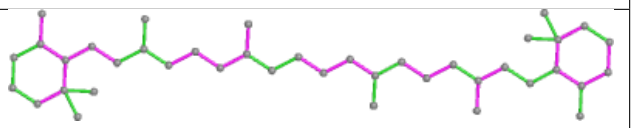


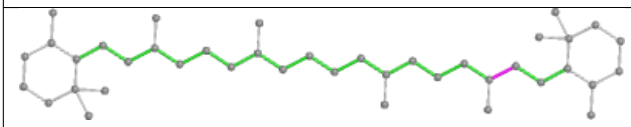
Rings

Ligand BCR i 101

Bond lengths



Bond angles



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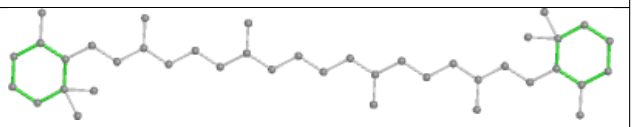
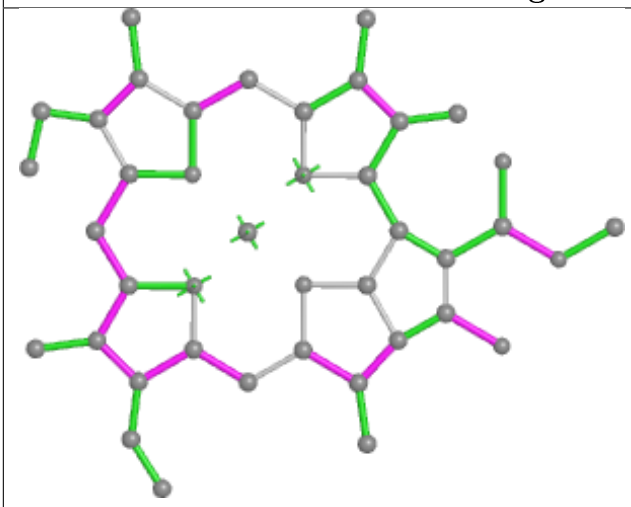


Rings

Ligand CLA 9 610



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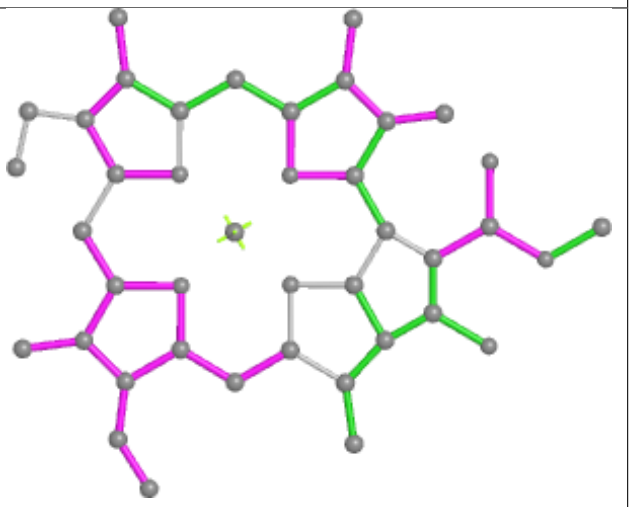
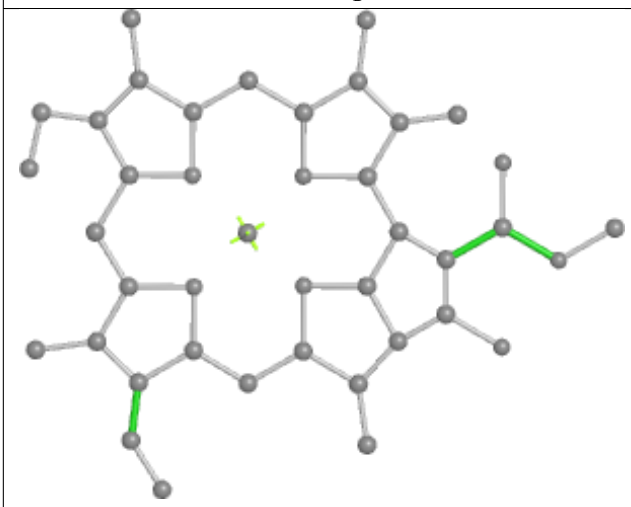
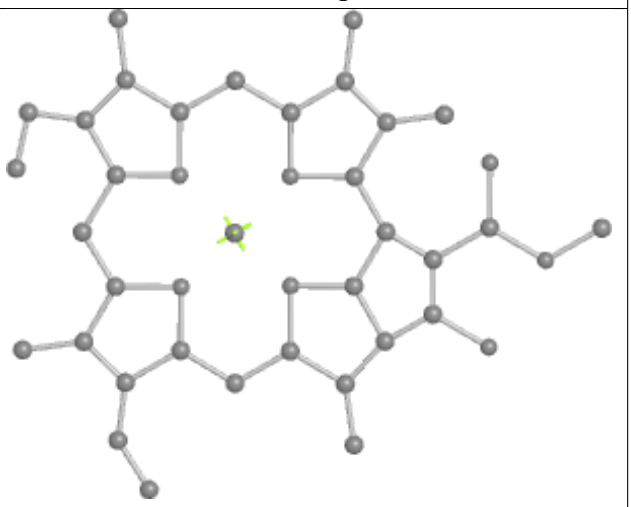


Bond angles

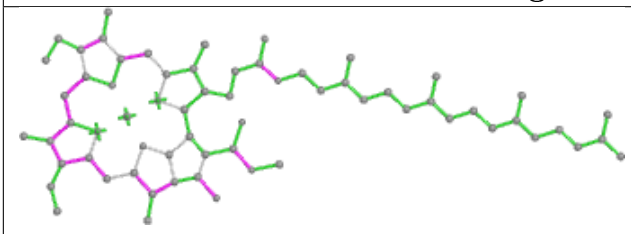


Torsions



Rings

Ligand CLA a 803



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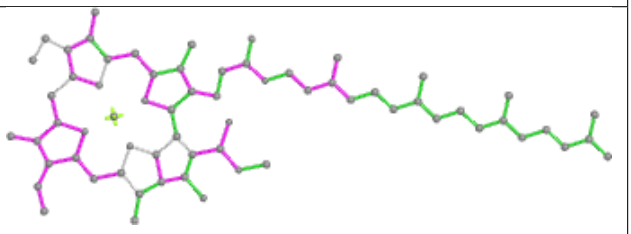
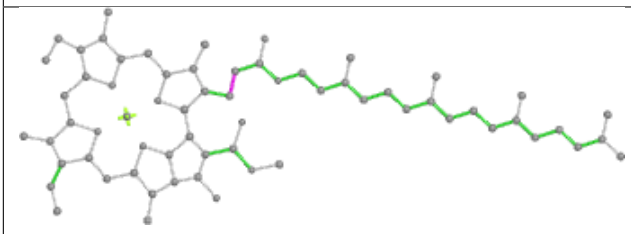
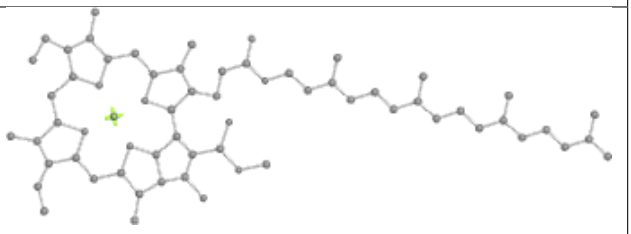


Bond angles

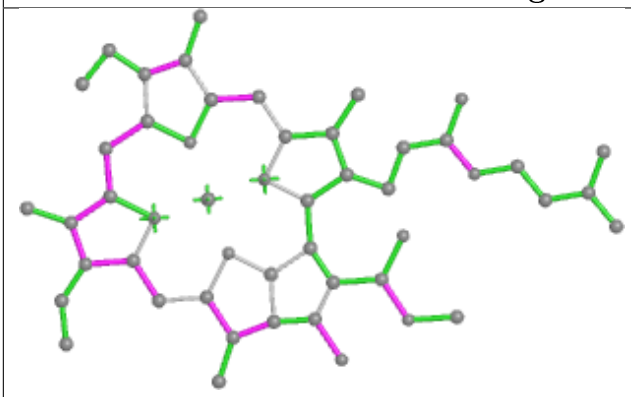


Torsions



Rings

Ligand CLA a 832



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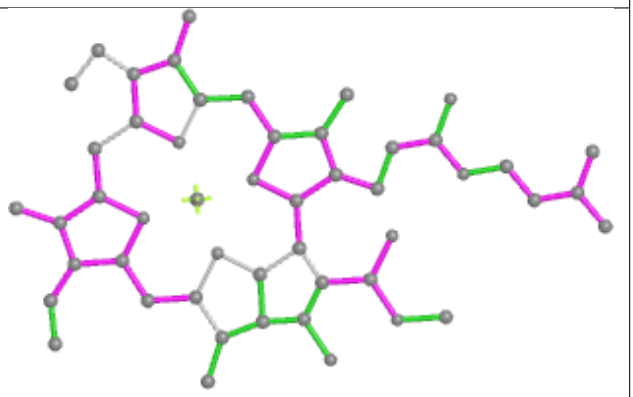
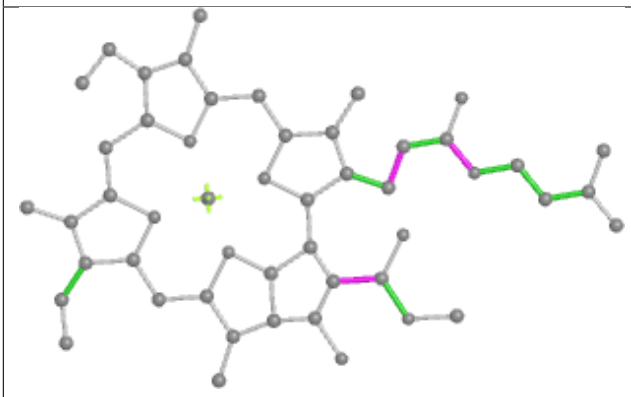


Bond angles



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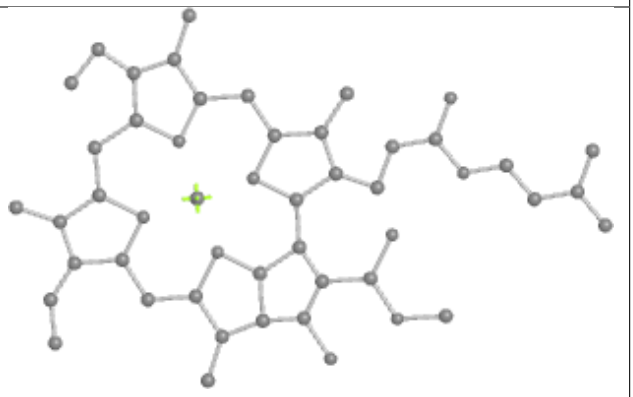
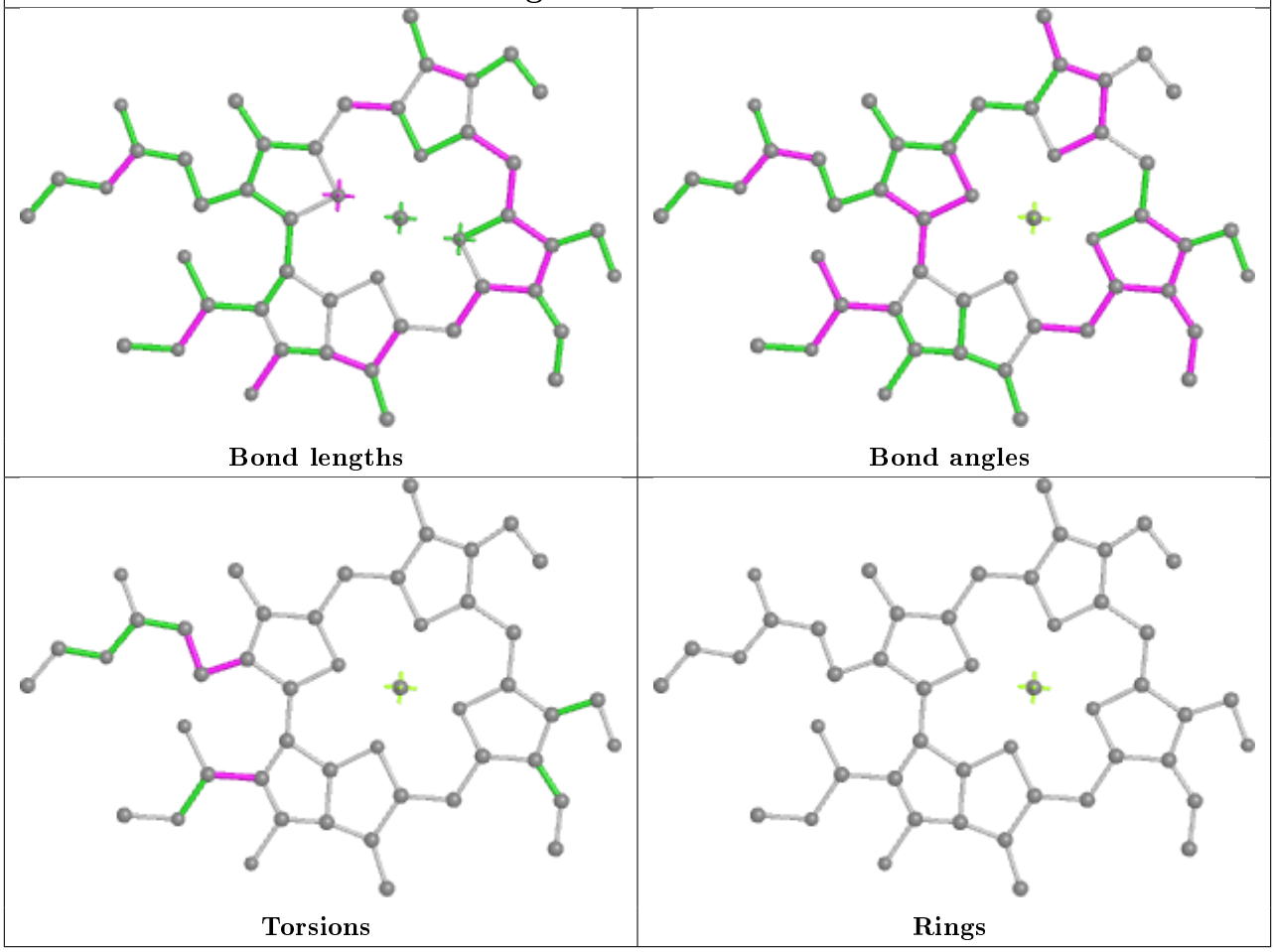
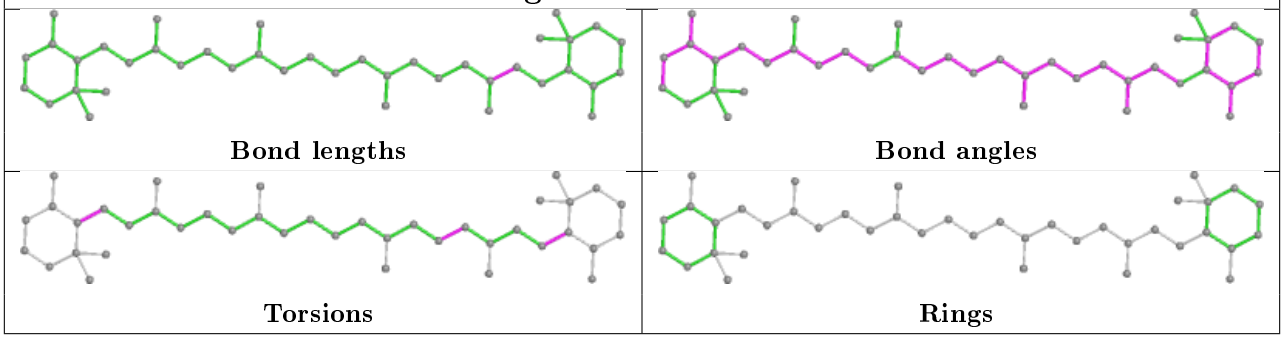


Rings

Ligand CHL 1 307



Ligand BCR B 846



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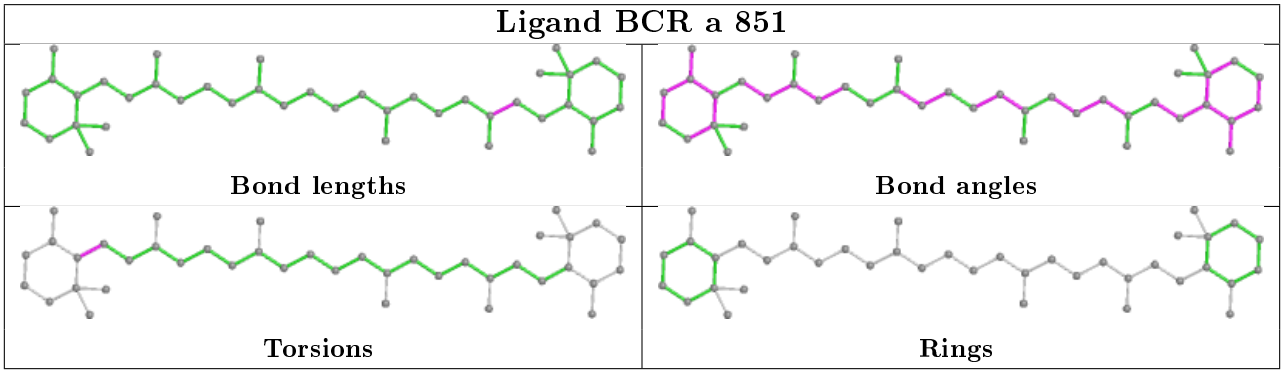
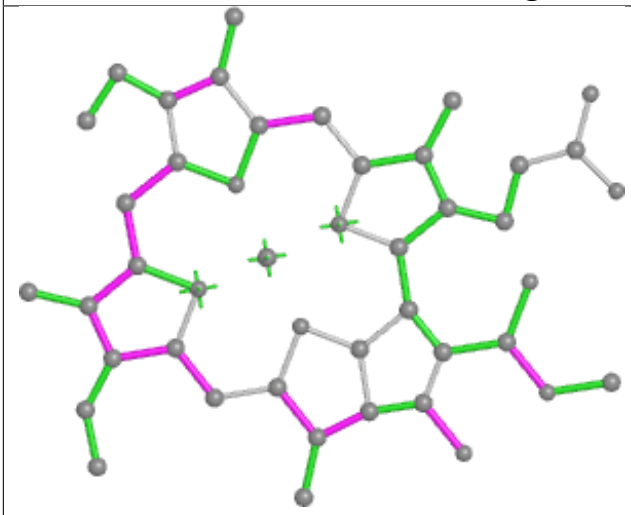
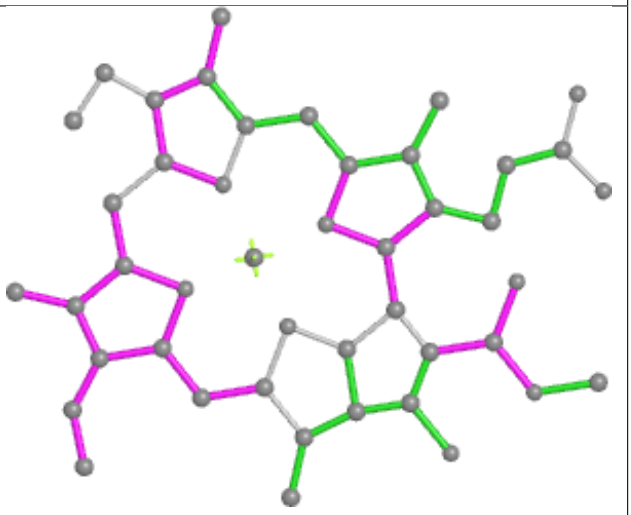


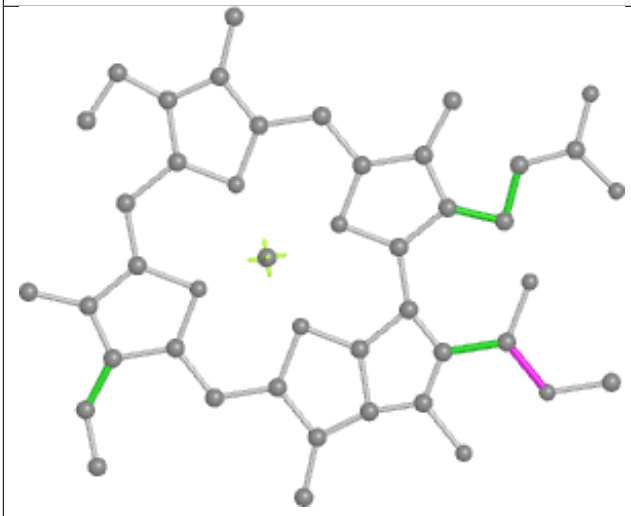
Ligand CLA G 101



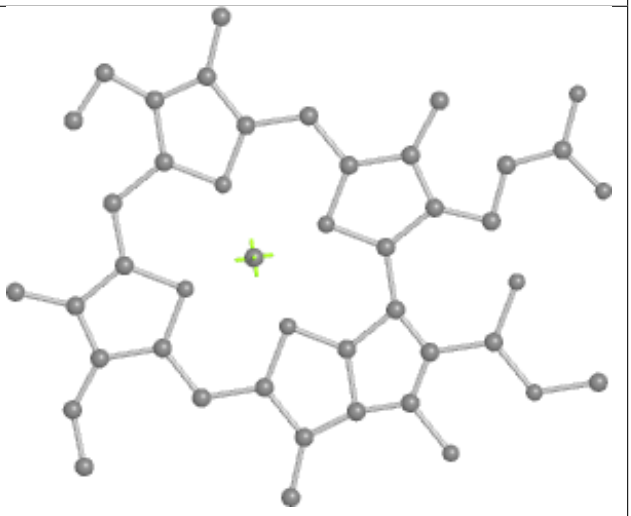
Bond lengths



Bond angles

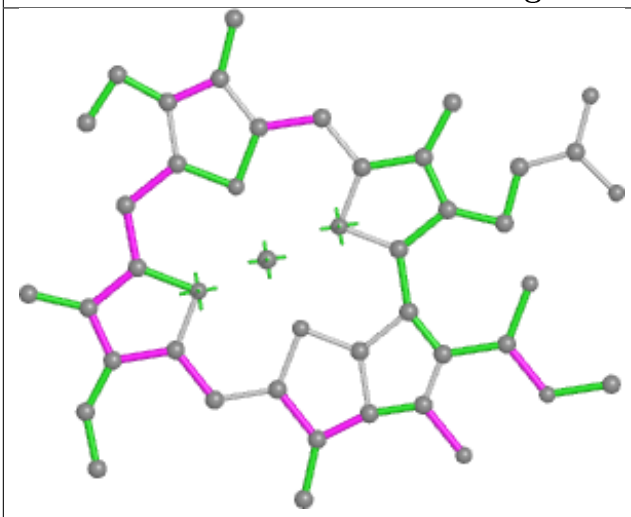


Torsions

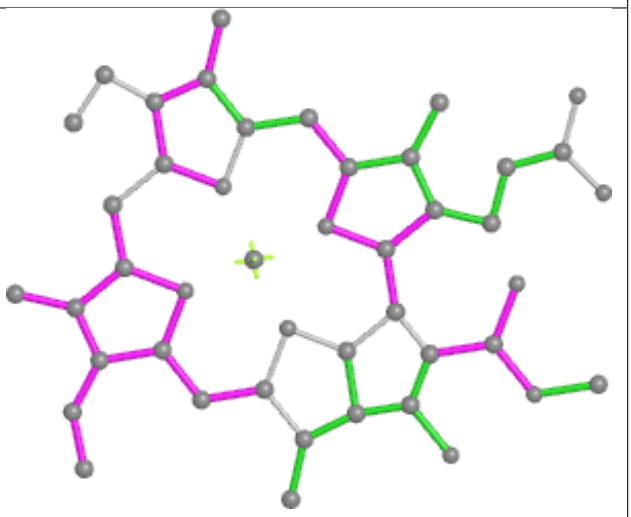


Rings

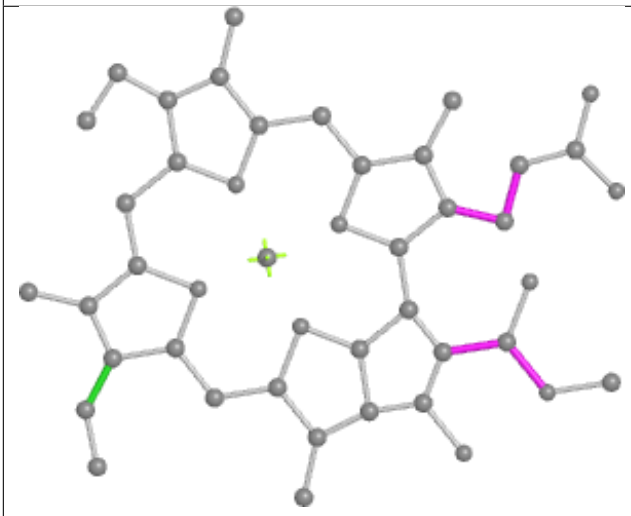
Ligand CLA B 804



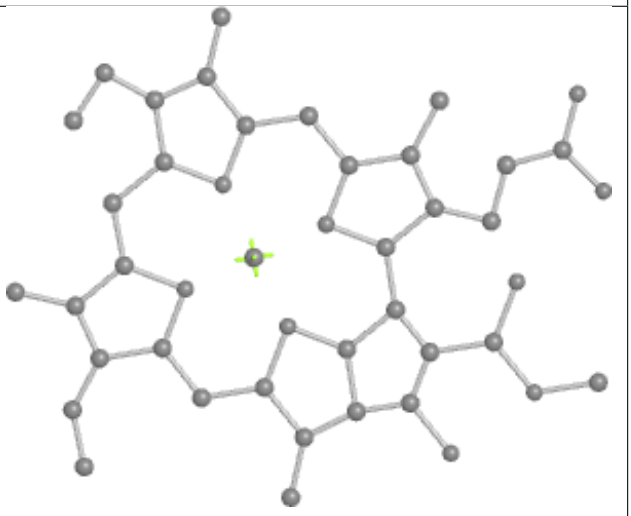
Bond lengths



Bond angles

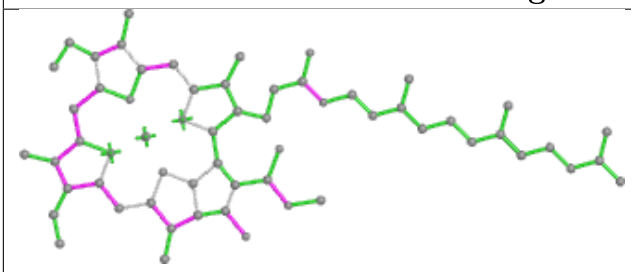


Torsions

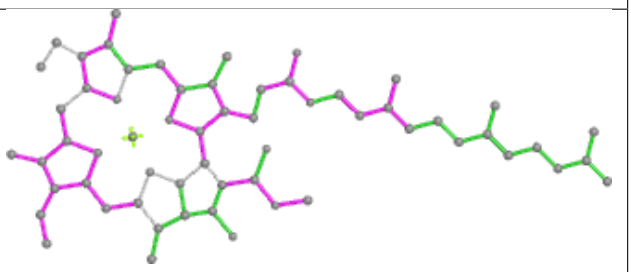


Rings

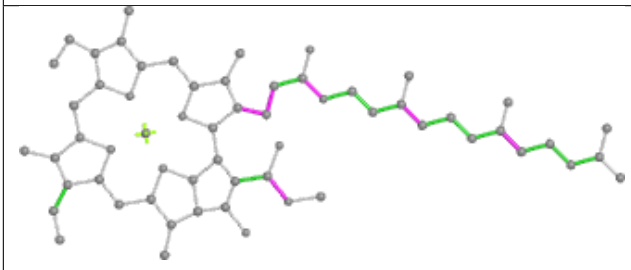
Ligand CLA 6 311



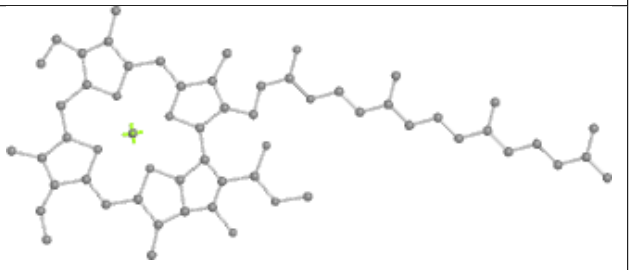
Bond lengths



Bond angles

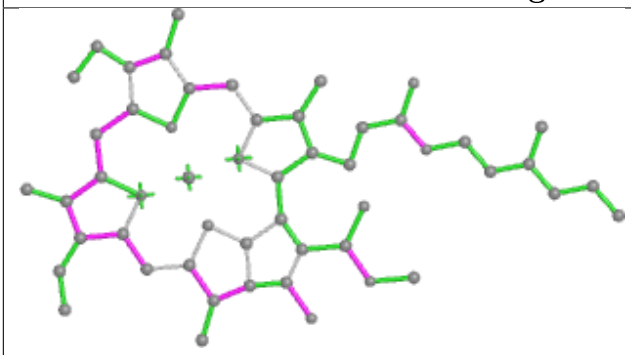


Torsions

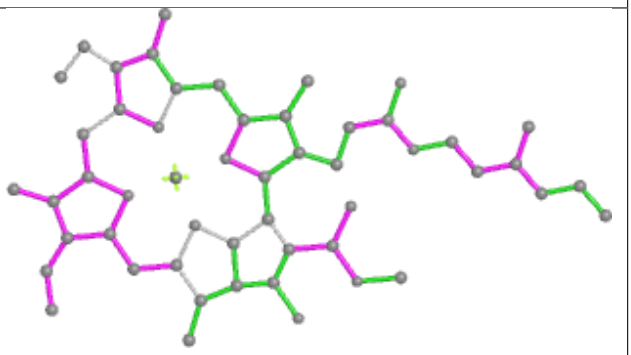


Rings

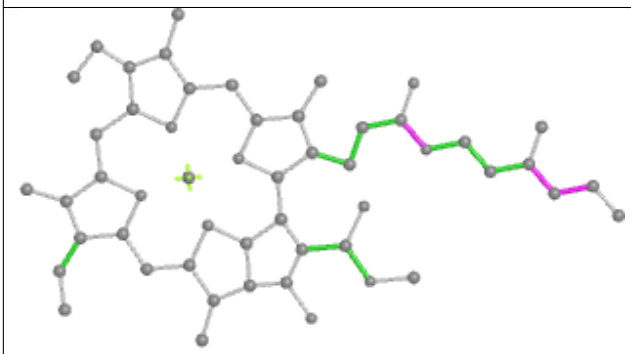
Ligand CLA 8 309



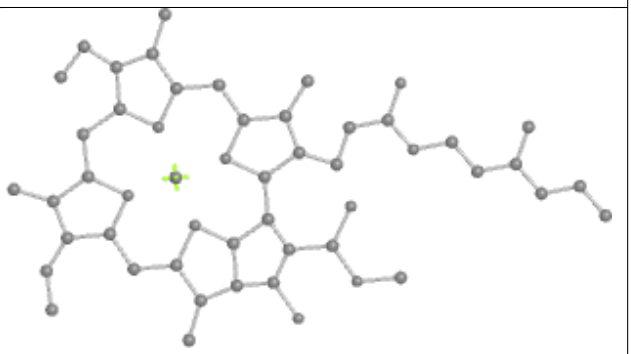
Bond lengths



Bond angles

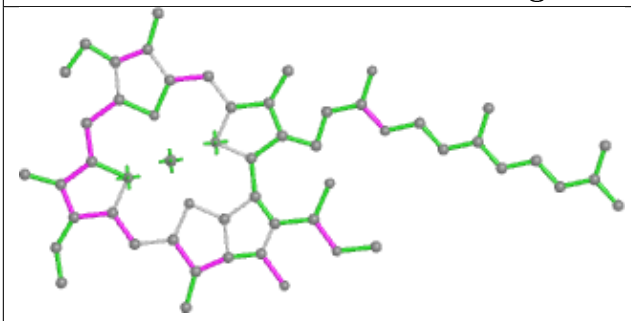


Torsions



Rings

Ligand CLA 1 314



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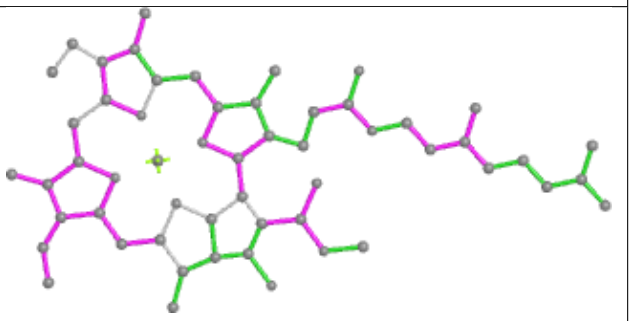
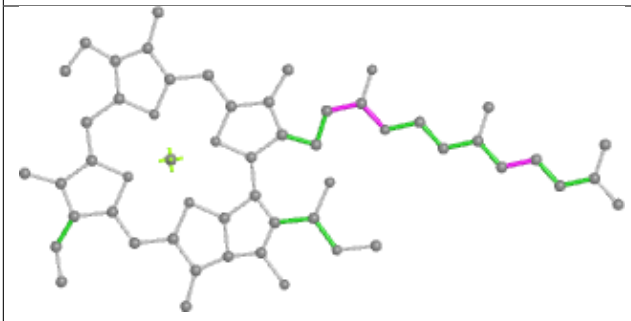
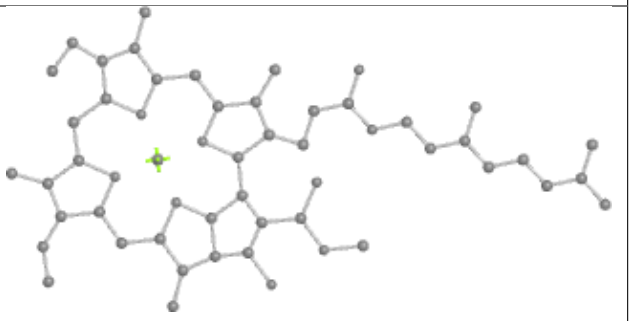


Bond angles

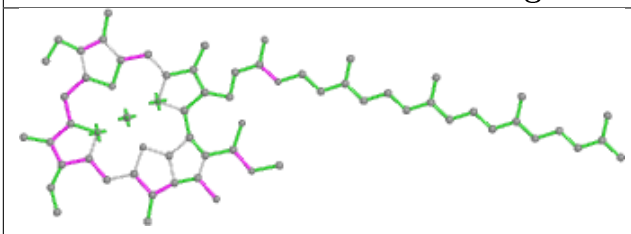


Torsions



Rings

Ligand CLA B 803



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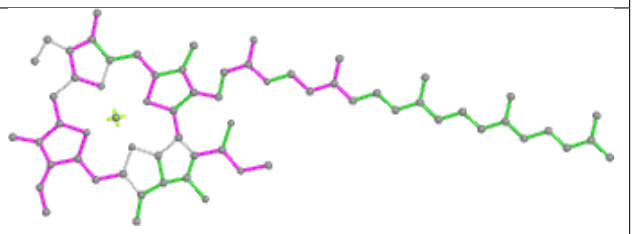
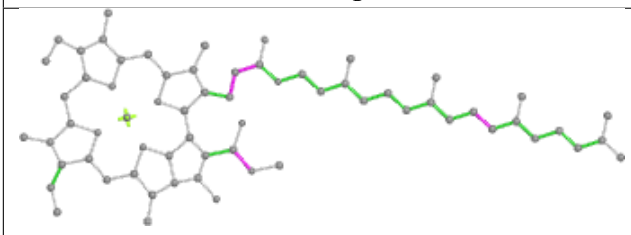
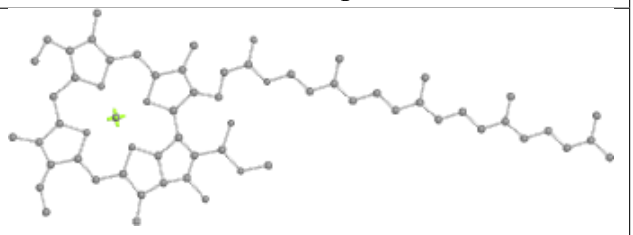


Bond angles

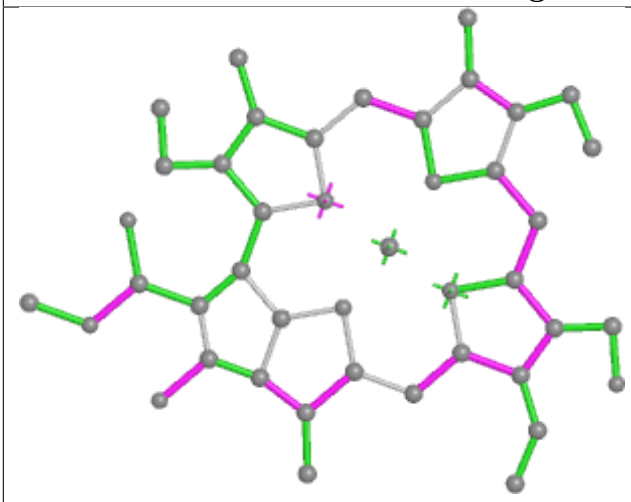


Torsions



Rings

Ligand CHL 7 605



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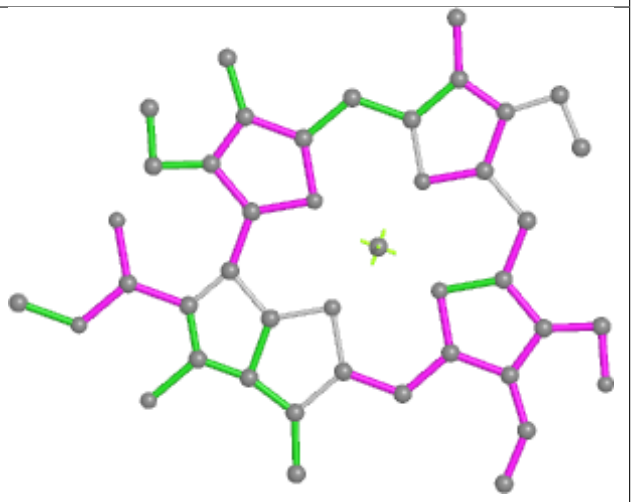
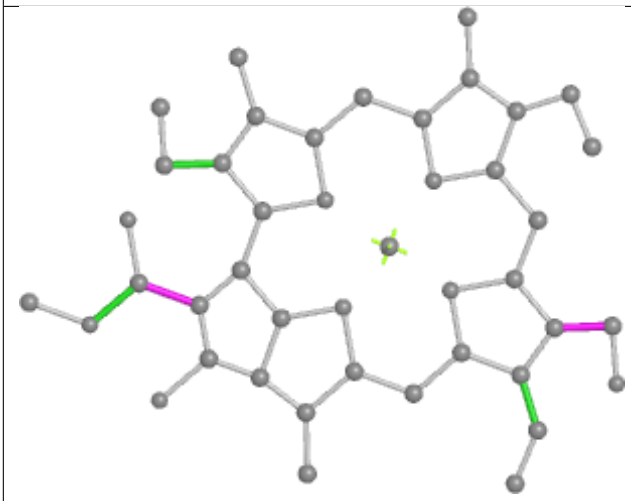


Bond angles



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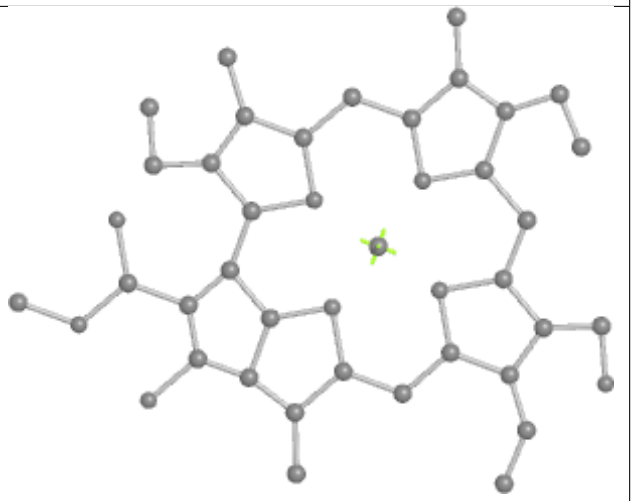
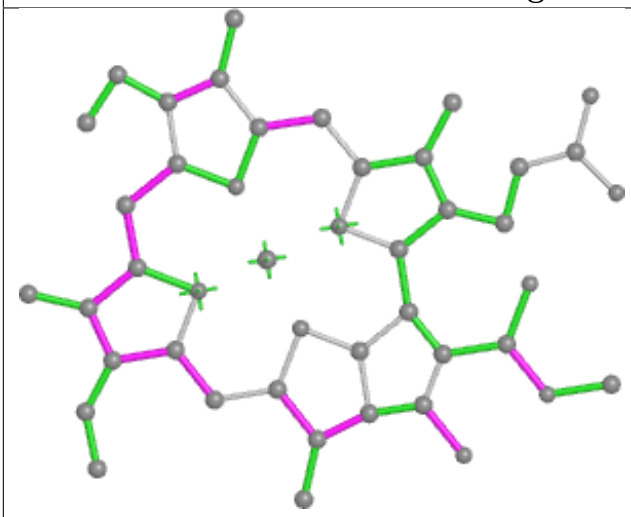


Rings

Ligand CLA b 804



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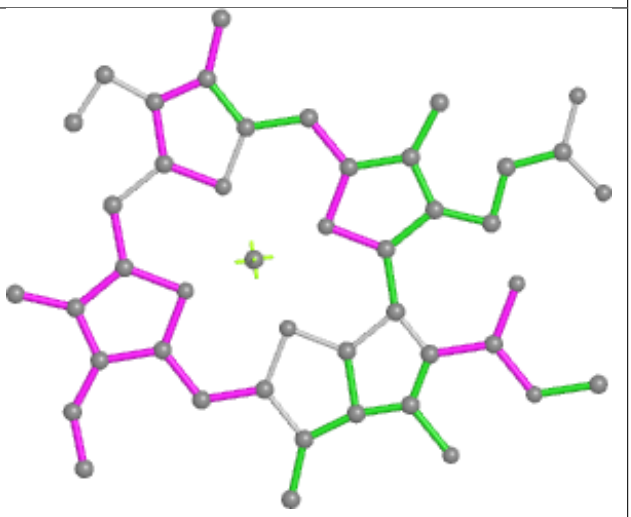
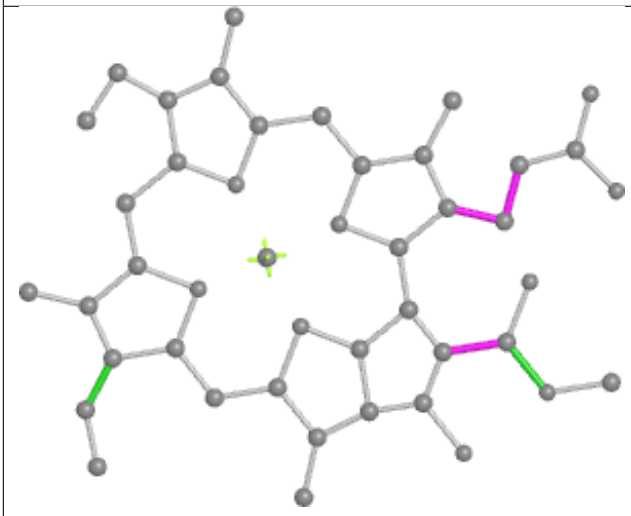


Bond angles



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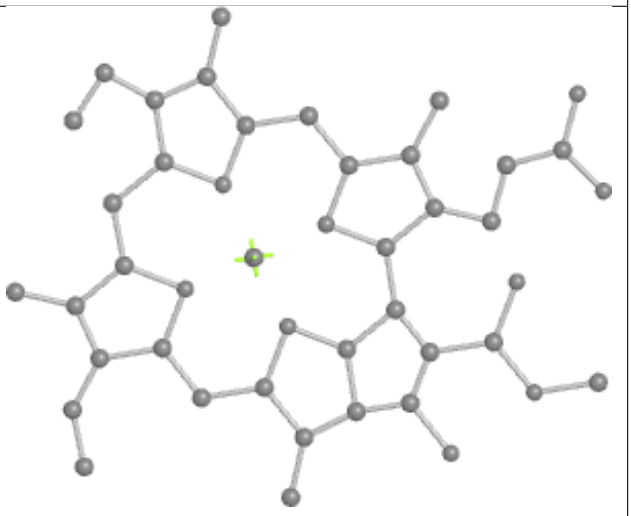
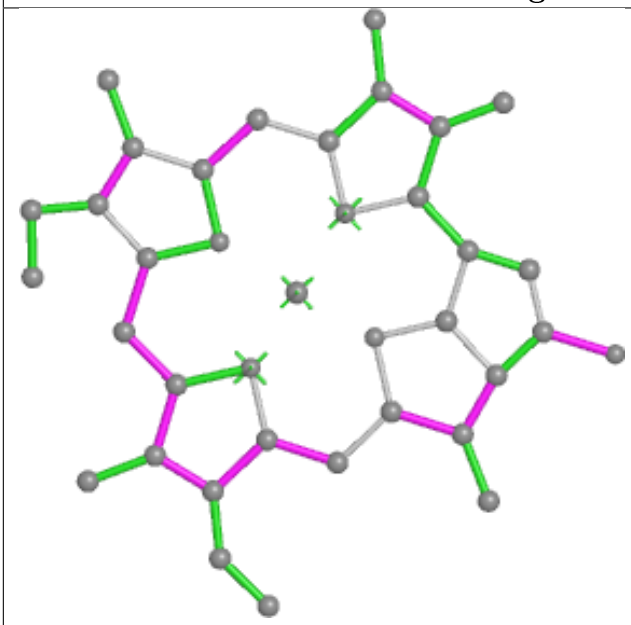
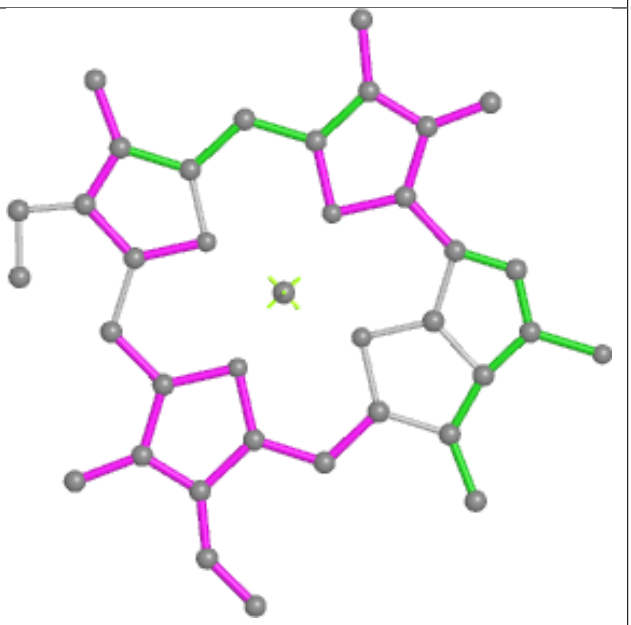


Rings

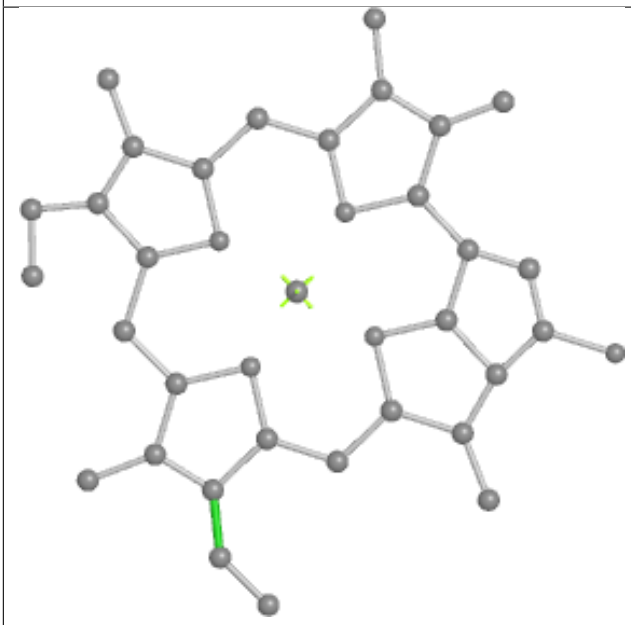
Ligand CLA 3 310



Bond lengths



Bond angles



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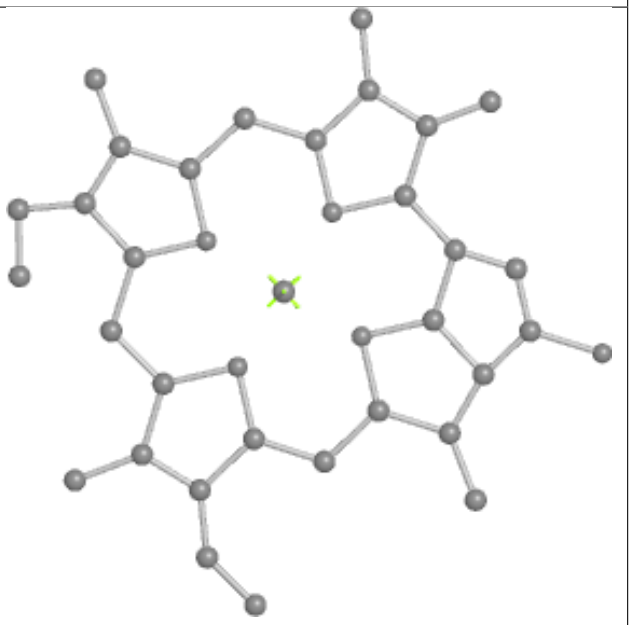
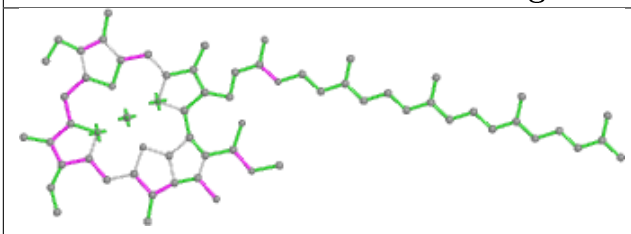


Rings

Ligand CLA a 841



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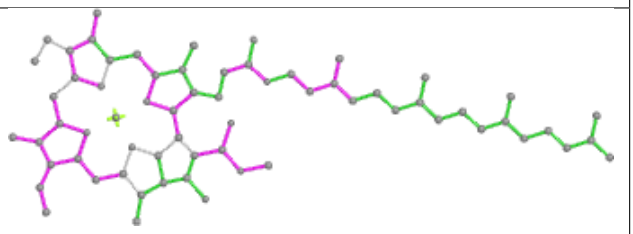
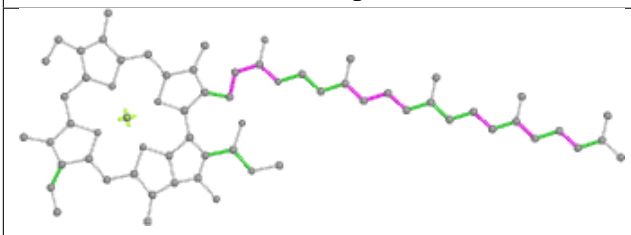


Bond angles



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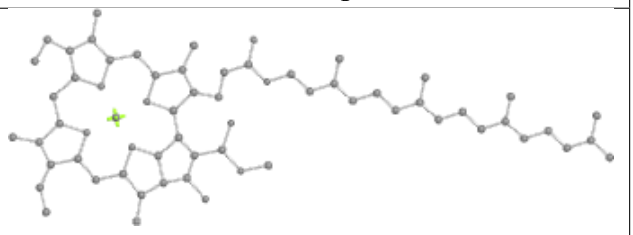
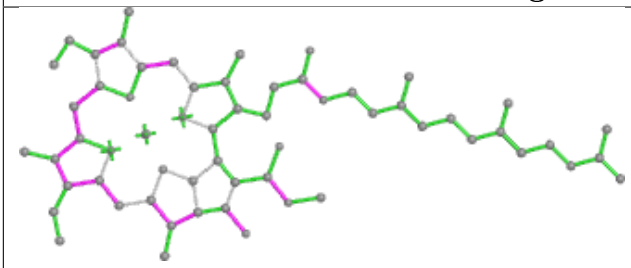


Rings

Ligand CLA 7 604



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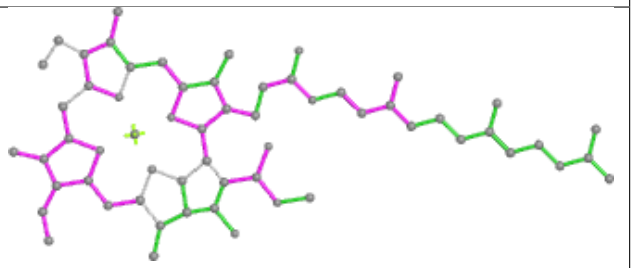
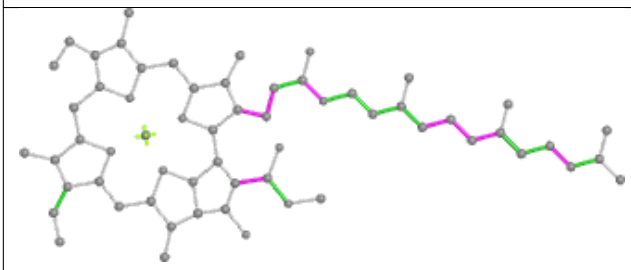


Bond angles



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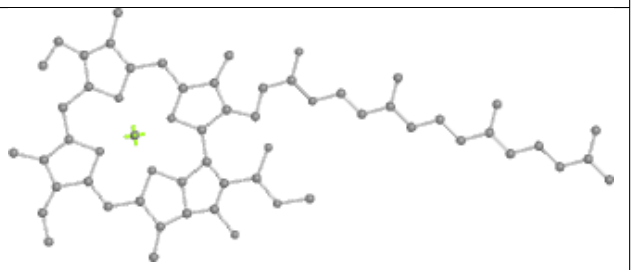
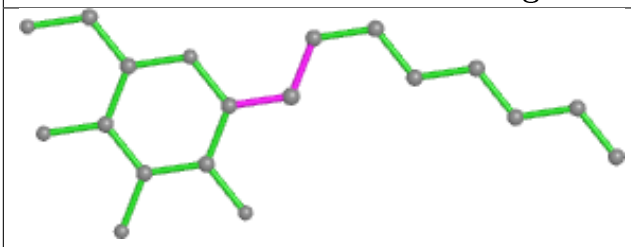


Rings

Ligand HTG F 302



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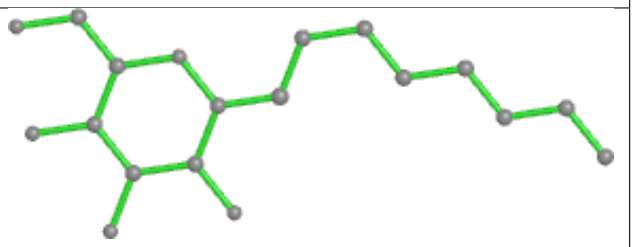
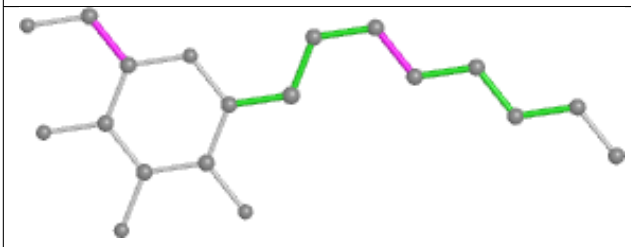


Bond angles



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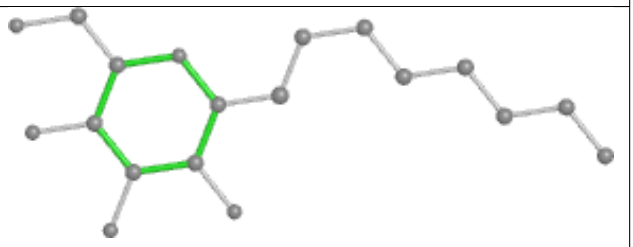
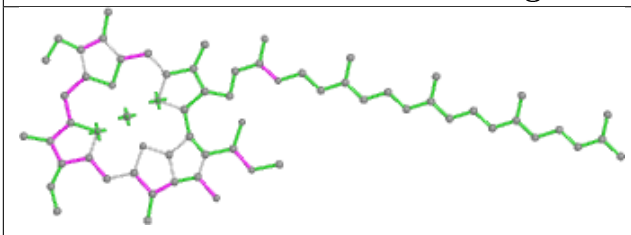


Rings

Ligand CLA A 807



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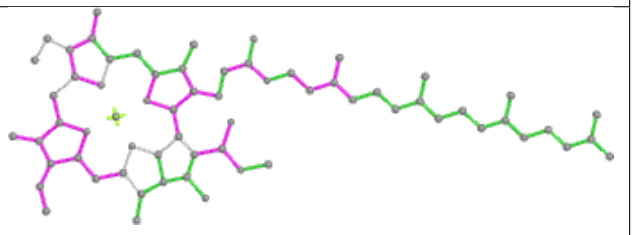

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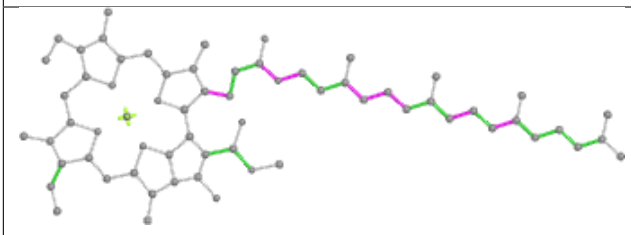

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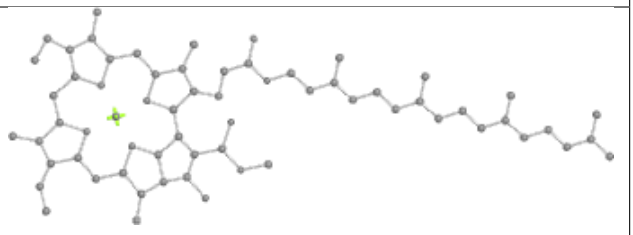
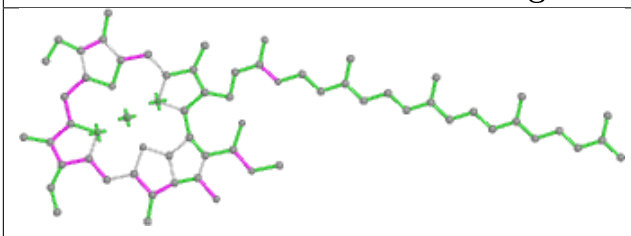


Rings

Ligand CLA a 843



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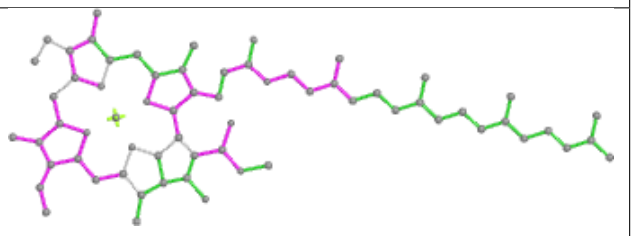
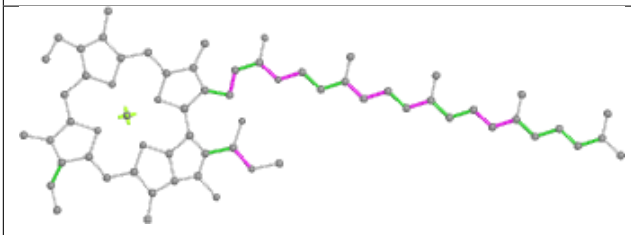


Bond angles



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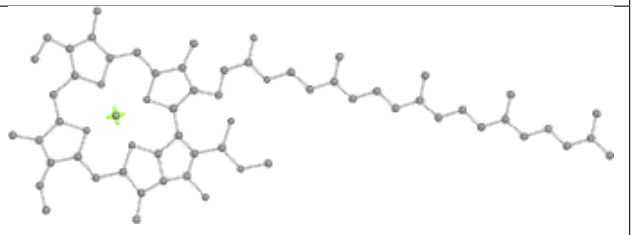
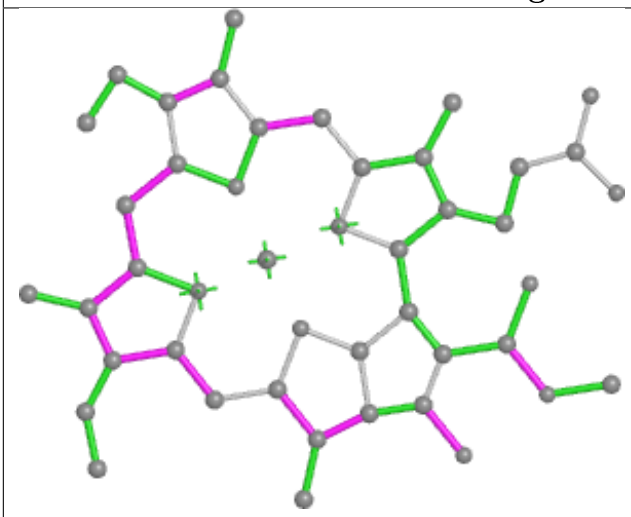


Rings

Ligand CLA 8 311



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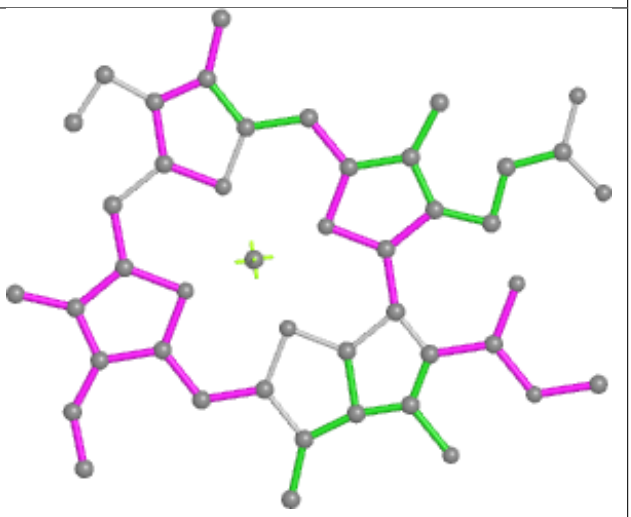
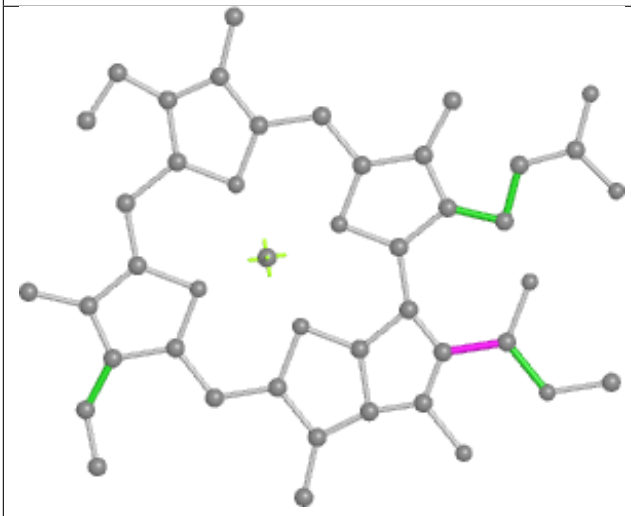
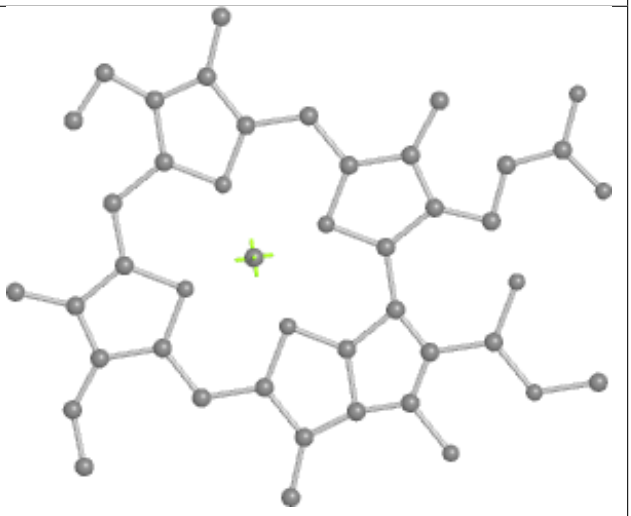


Bond angles

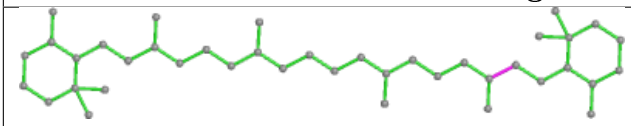


Torsions



Rings

Ligand BCR g 104



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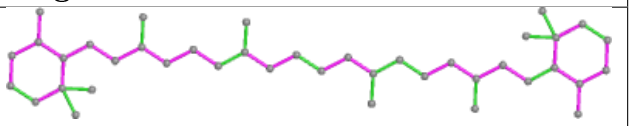
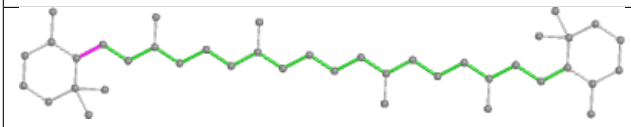


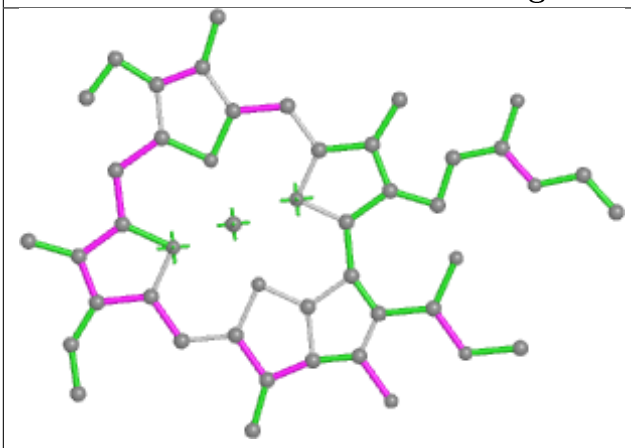
Bond angles



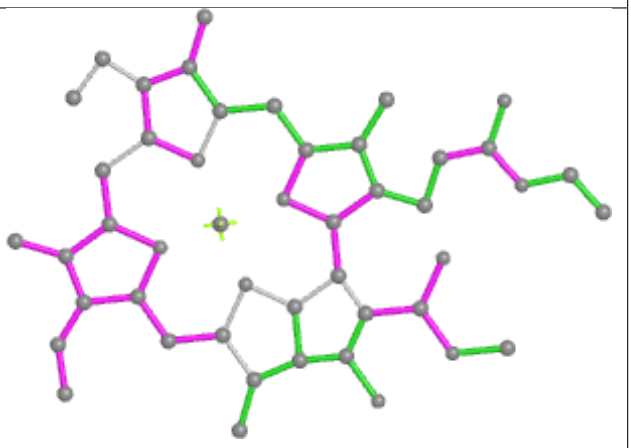
Torsions

Rings

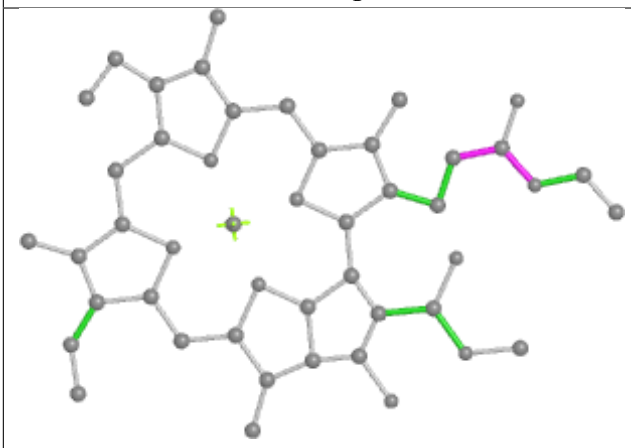
Ligand CLA 9 614



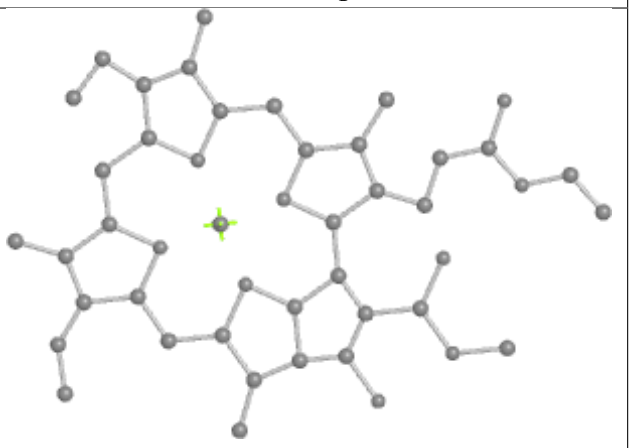
Bond lengths



Bond angles

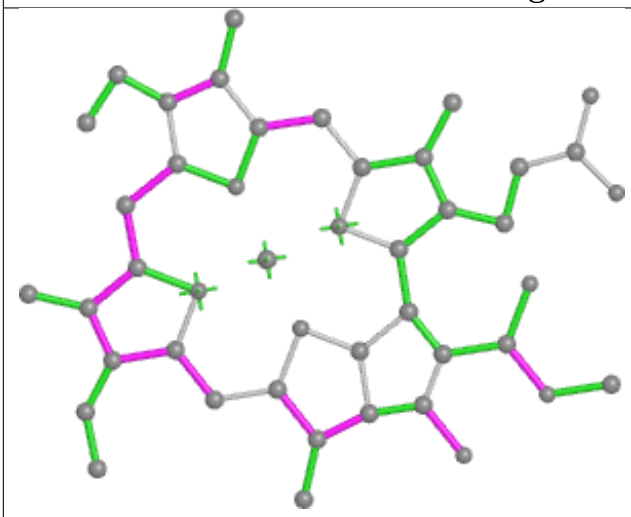


Torsions

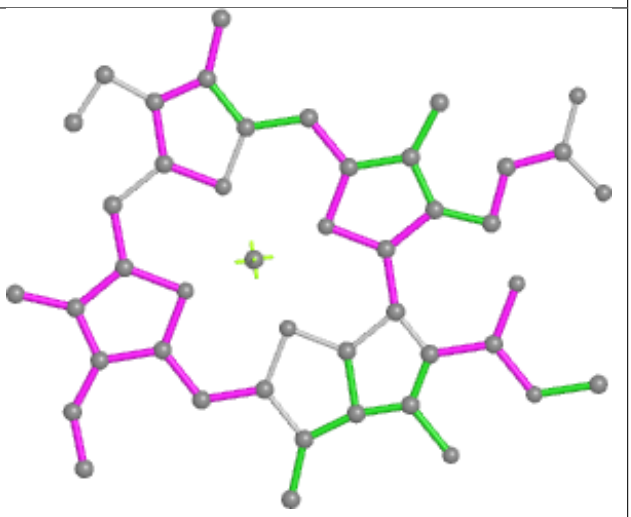


Rings

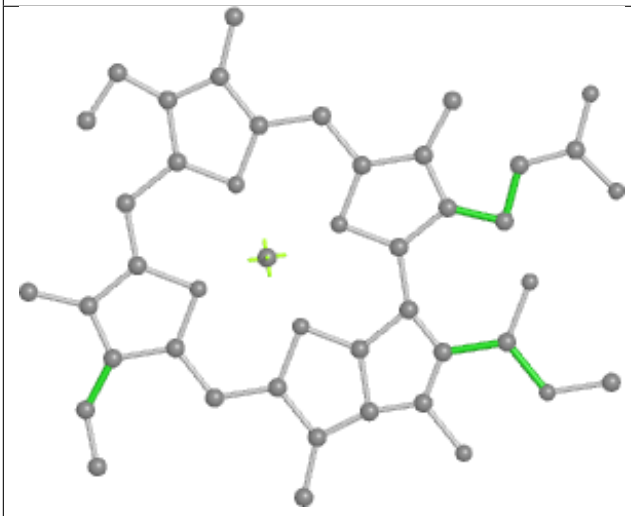
Ligand CLA 9 613



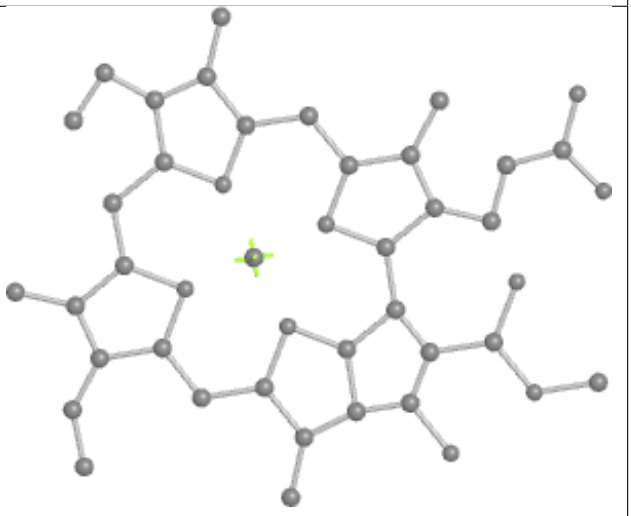
Bond lengths



Bond angles

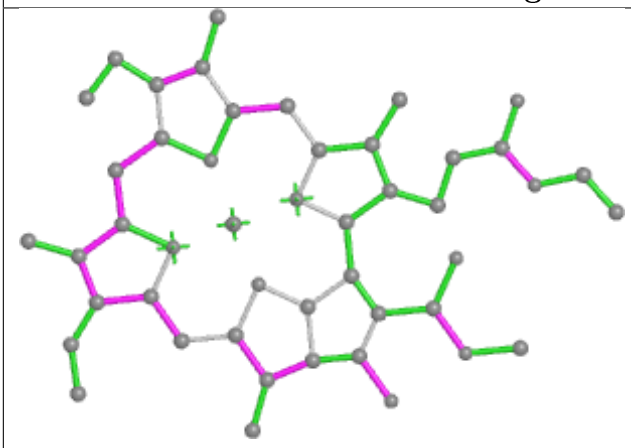


Torsions



Rings

Ligand CLA B 838



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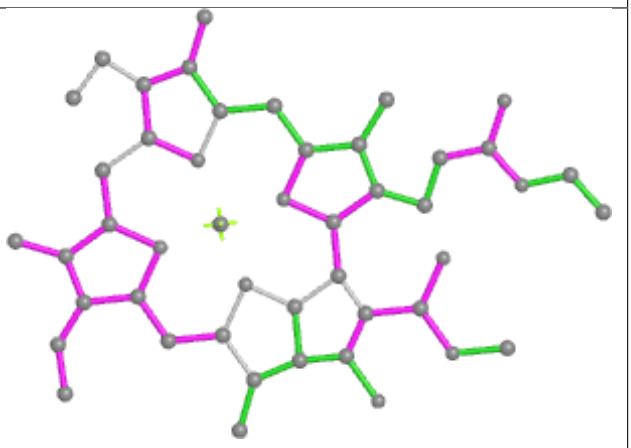
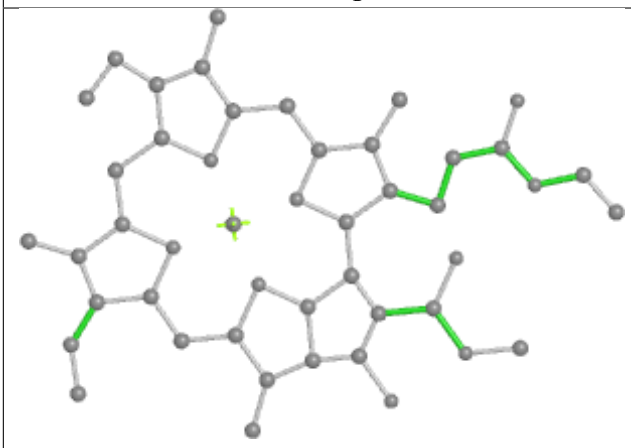
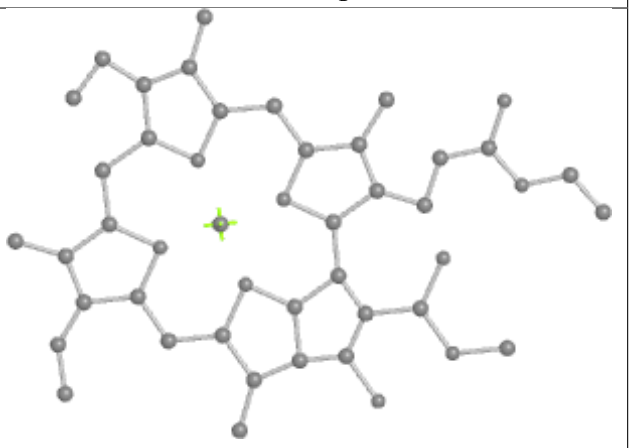


Bond angles

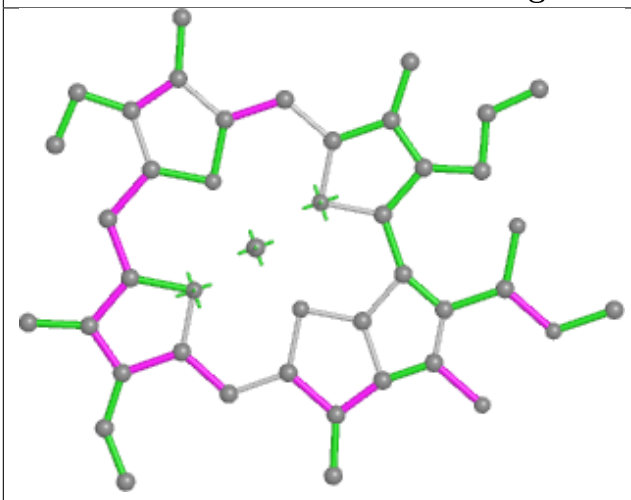


Torsions



Rings

Ligand CLA 7 613



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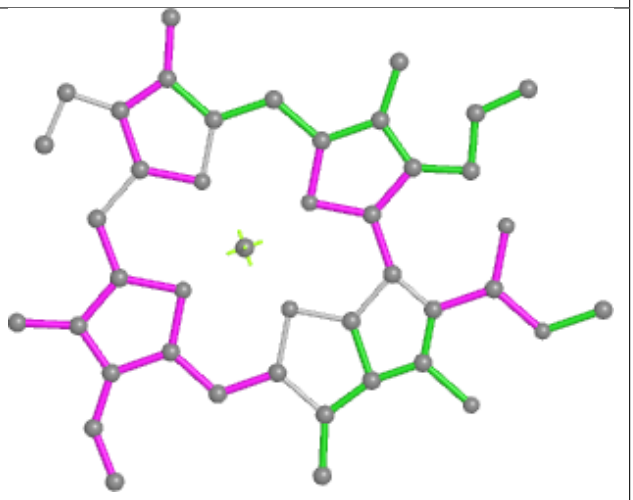
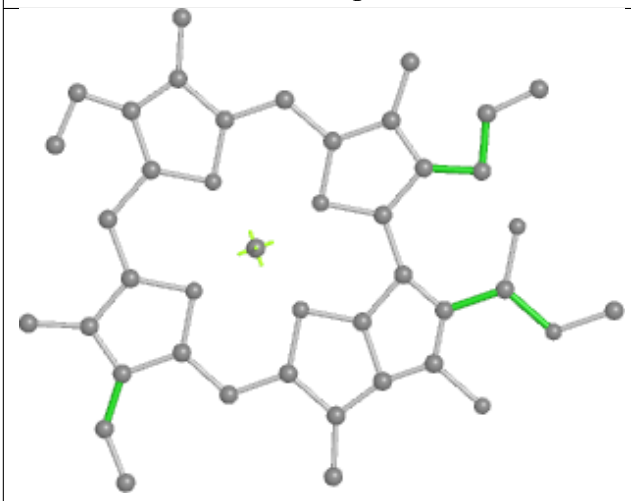


Bond angles



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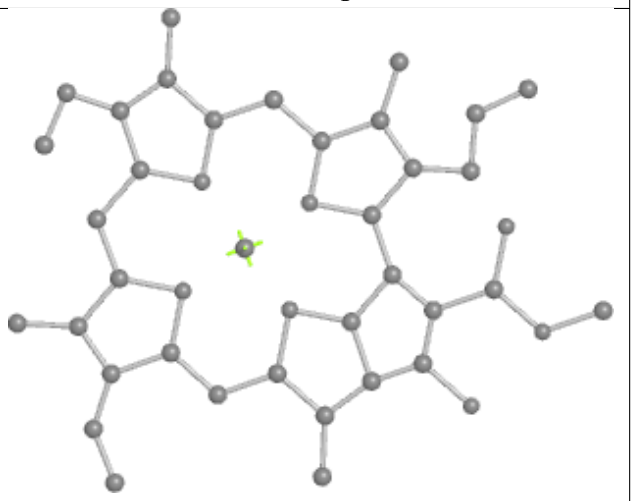
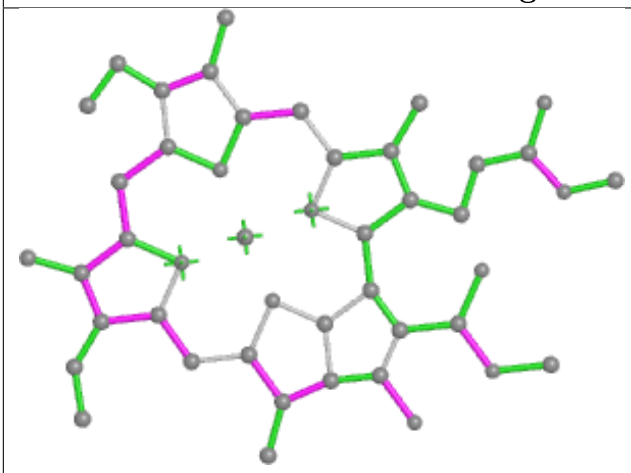


Rings

Ligand CLA k 1403



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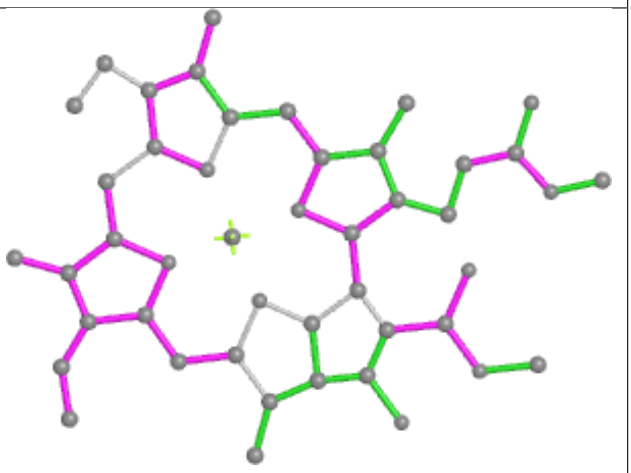
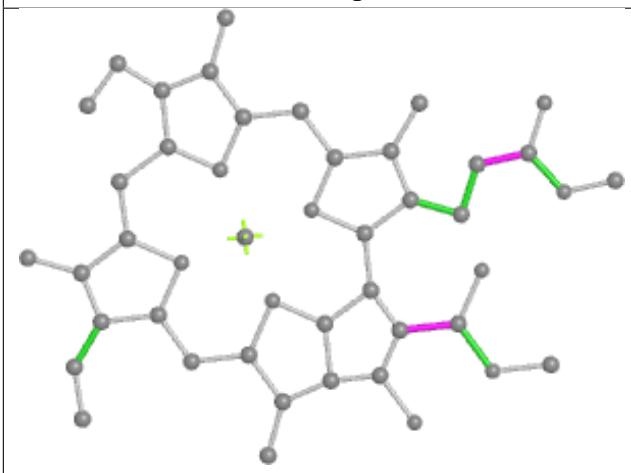


Bond angles



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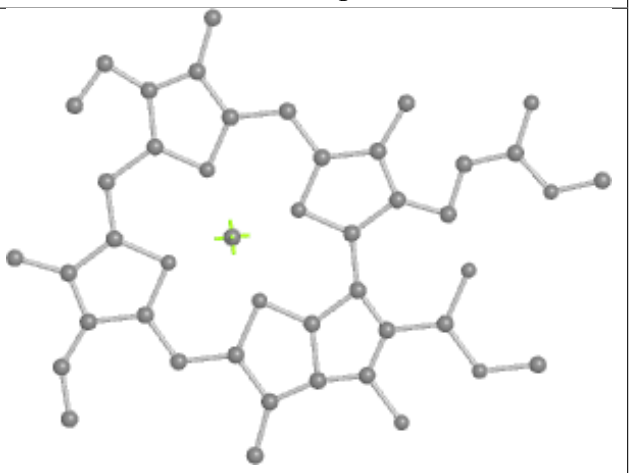
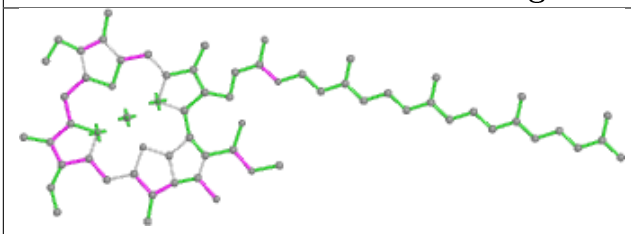


Rings

Ligand CLA a 801



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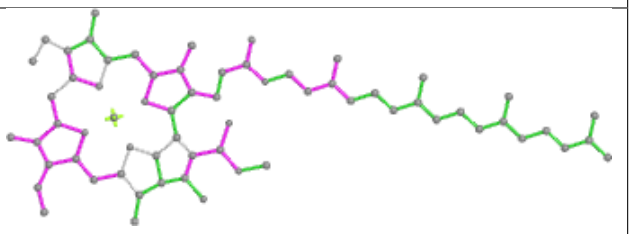
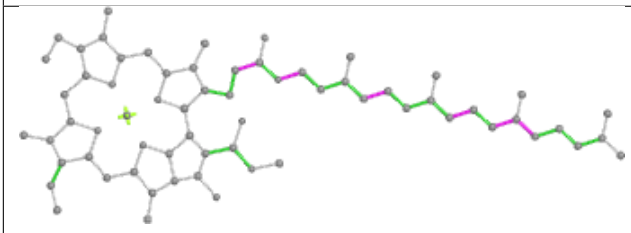


Bond angles



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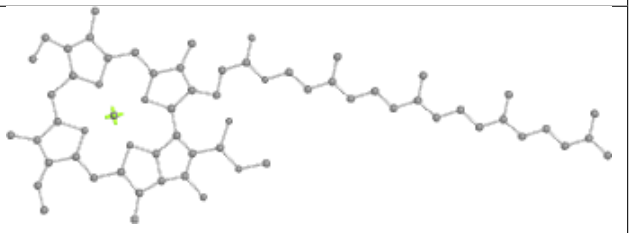
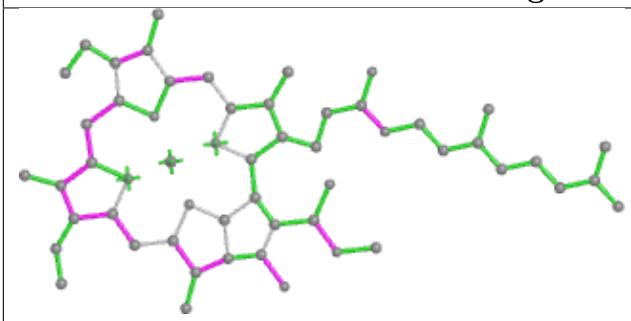
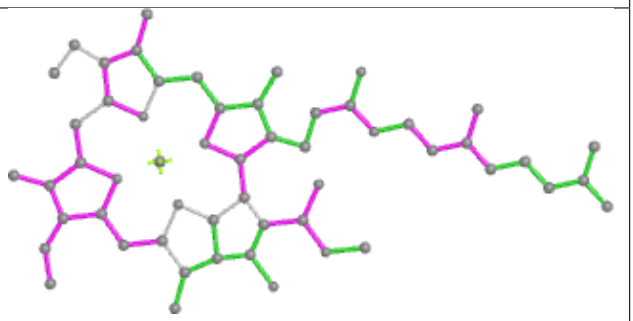


Rings

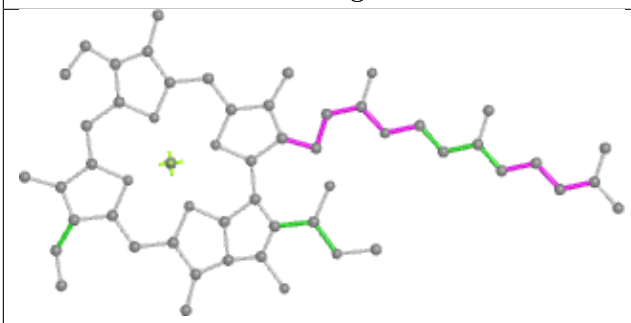
Ligand CLA b 812



Bond lengths



Bond angles



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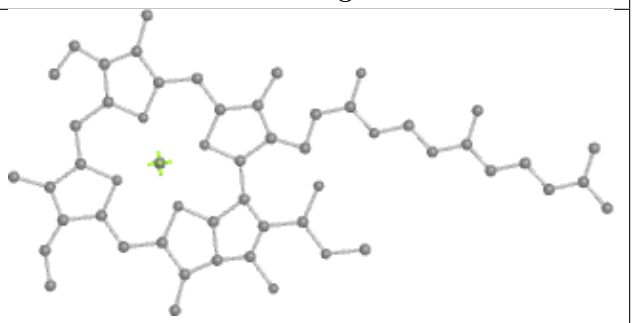
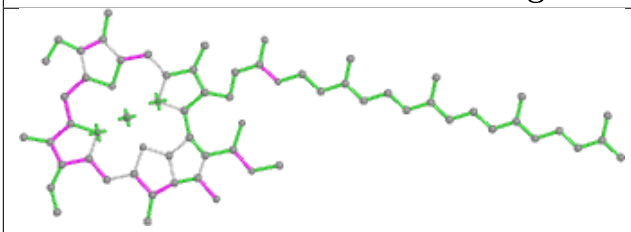
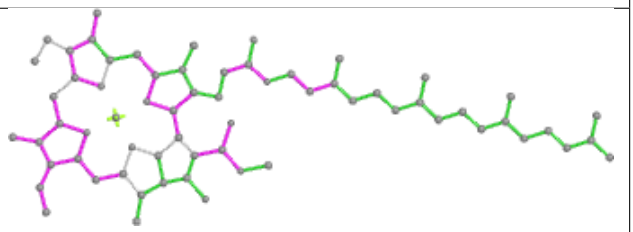


Rings

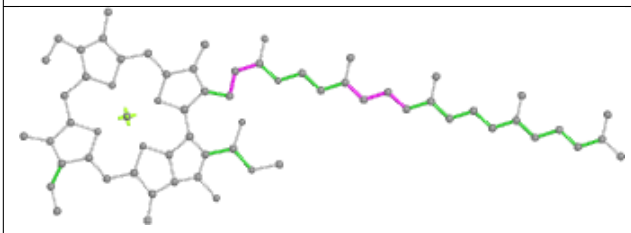
Ligand CLA b 807



Bond lengths



Bond angles



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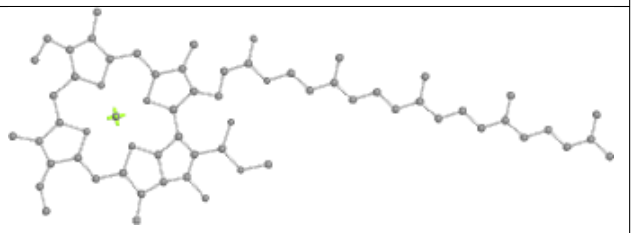
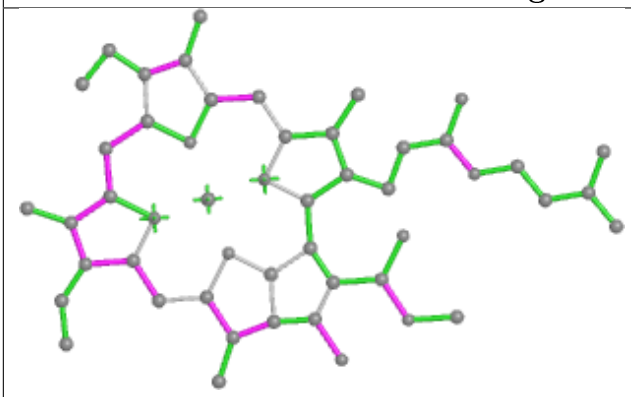
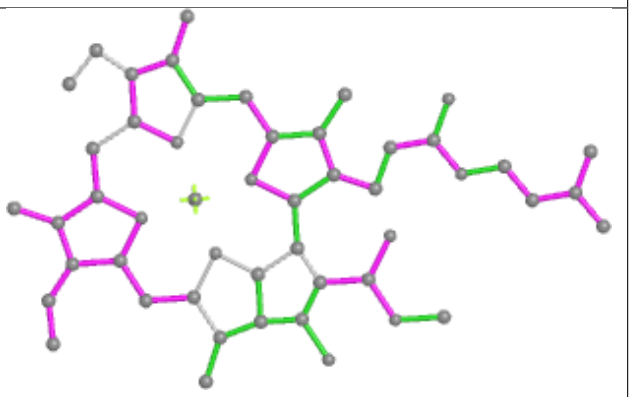
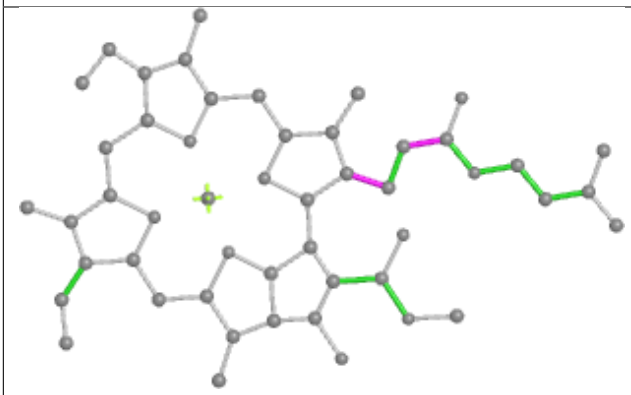
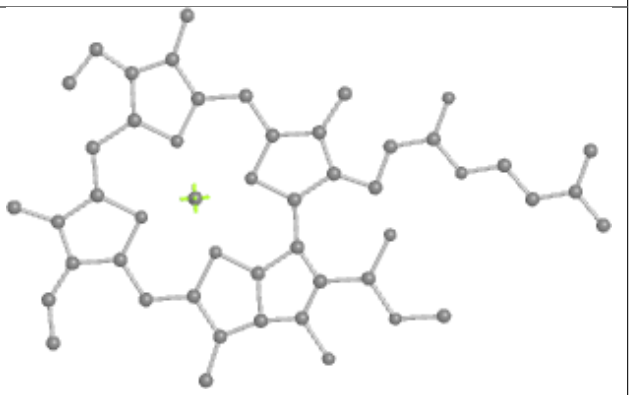
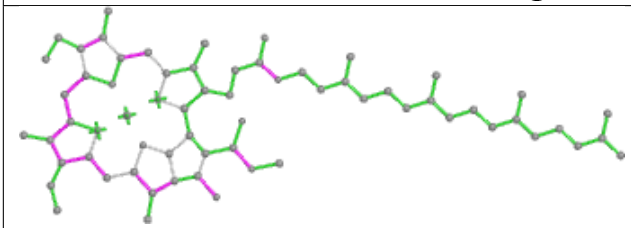
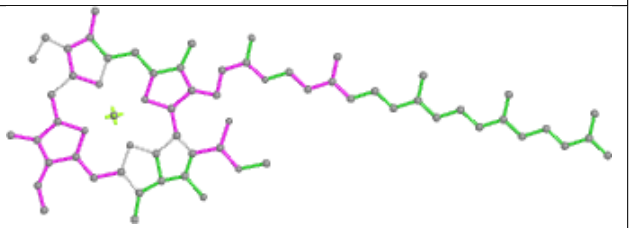
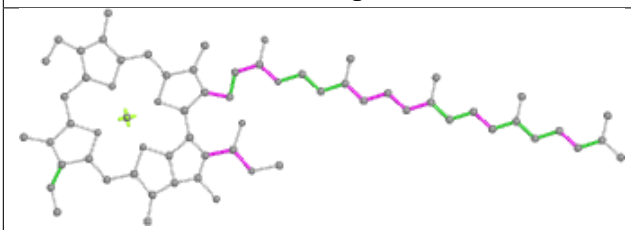
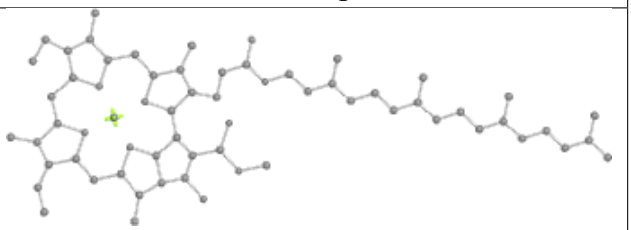
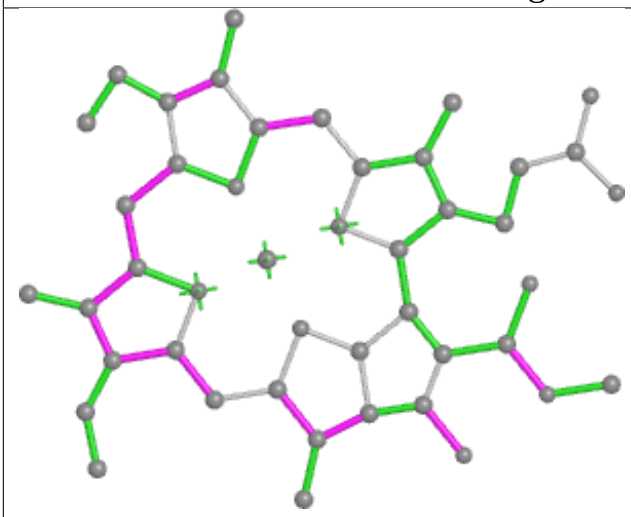


Rings

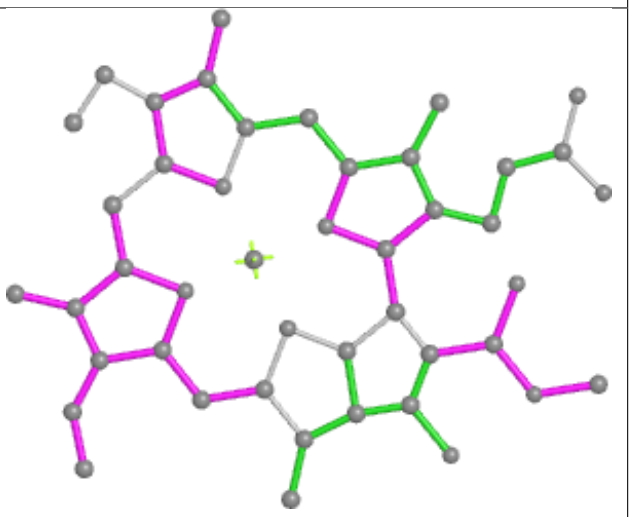
Ligand CLA 4 608	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA a 804	
 Bond lengths	 Bond angles
 Torsions	 Rings

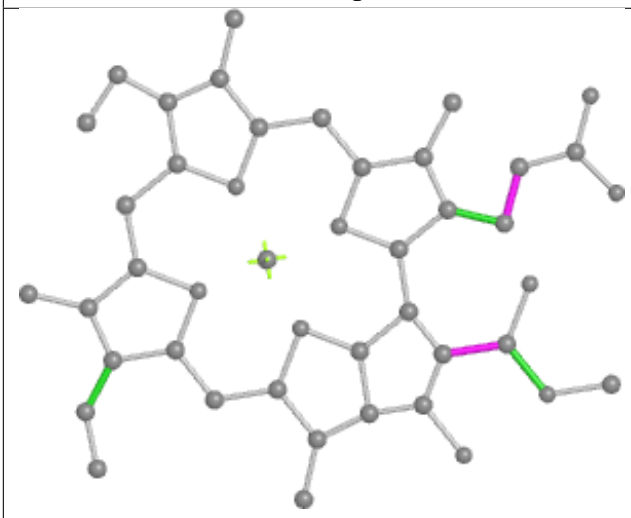
Ligand CLA 3 313



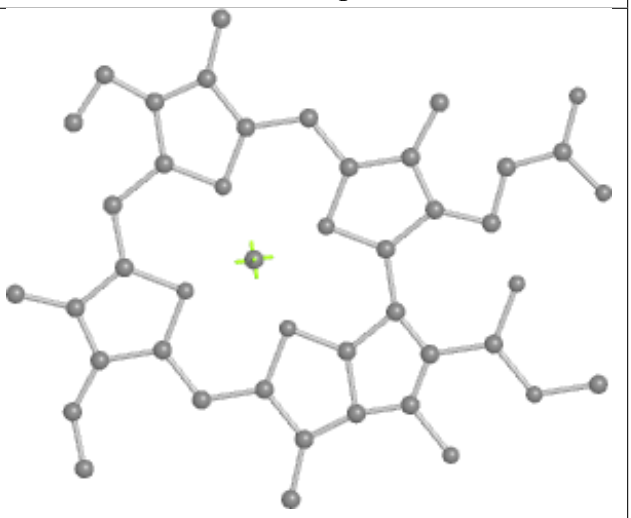
Bond lengths



Bond angles

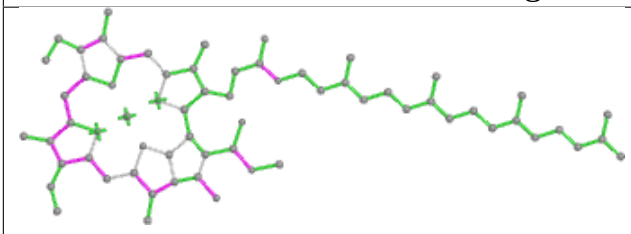


Torsions

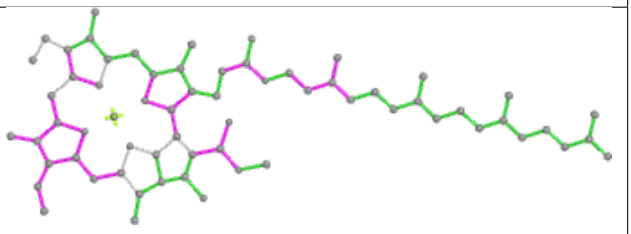


Rings

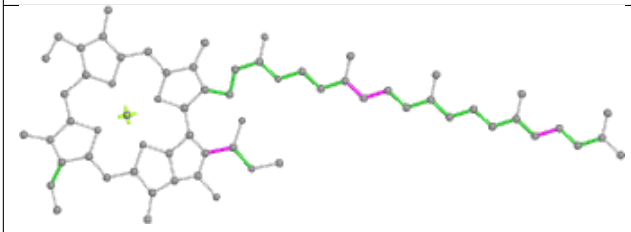
Ligand CLA A 839



Bond lengths



Bond angles



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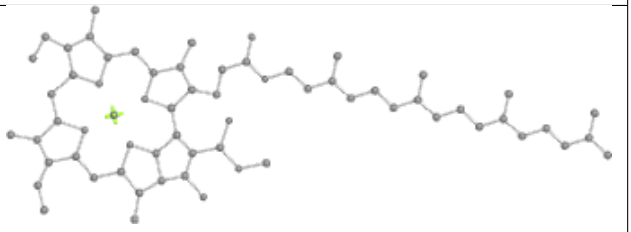
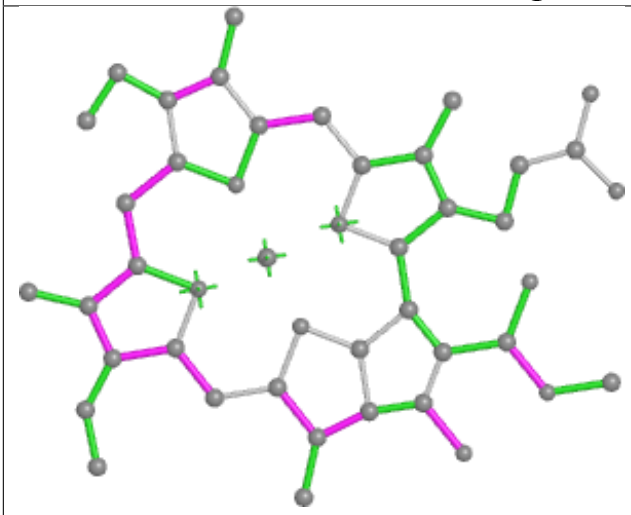


Rings

Ligand CLA 3 304



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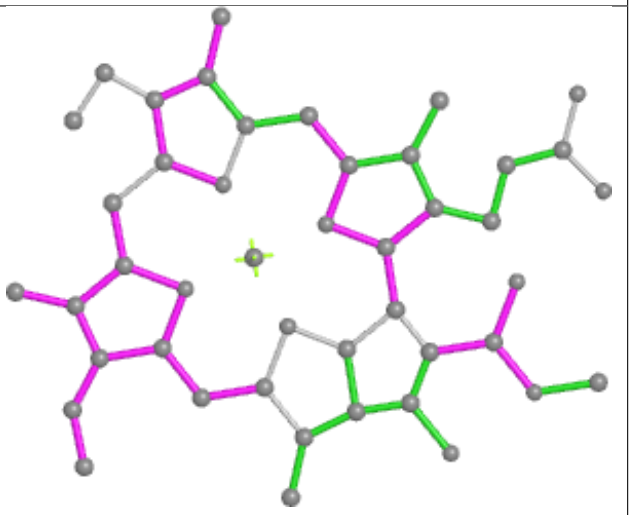
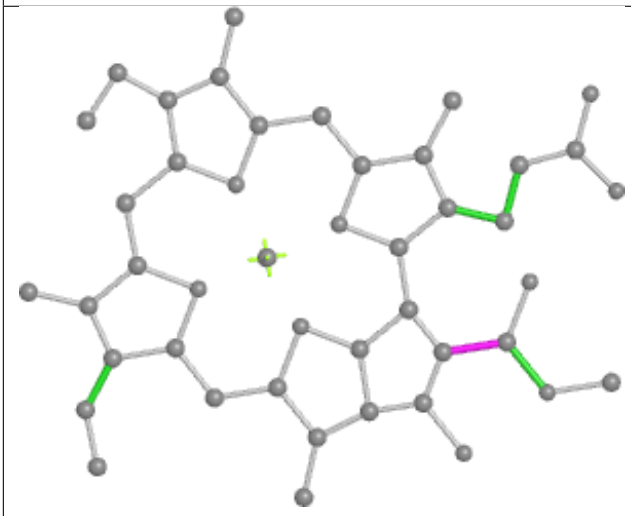
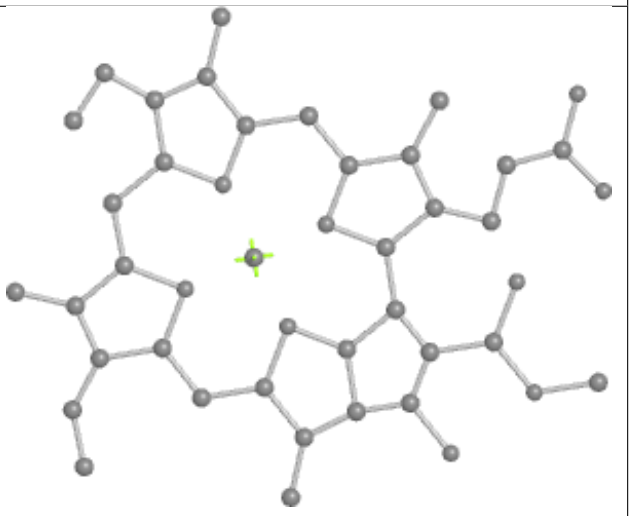


Bond angles

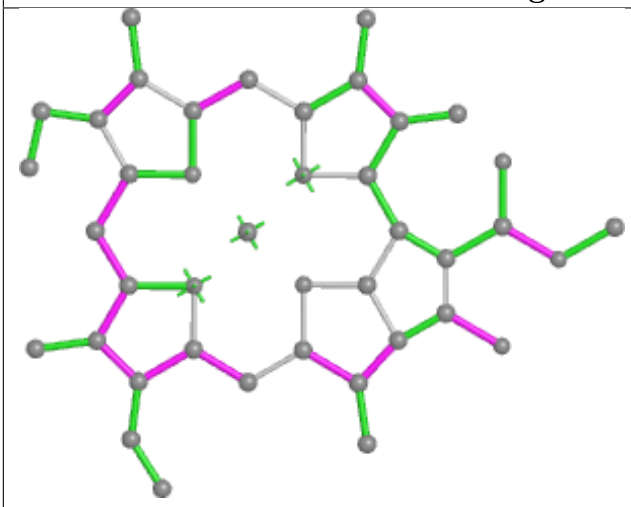


Torsions



Rings

Ligand CLA 1 311



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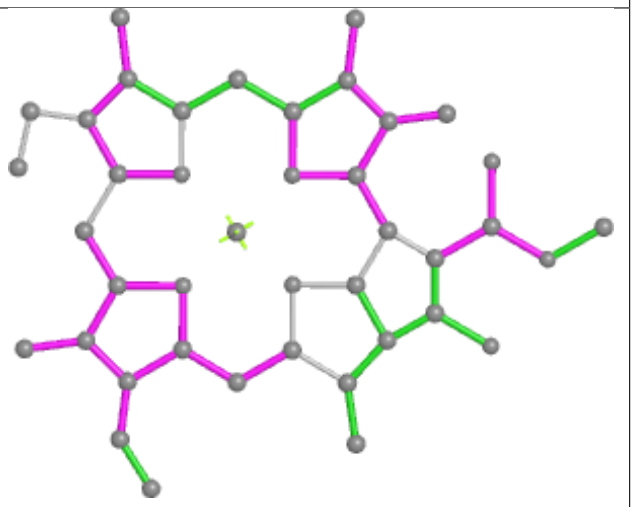
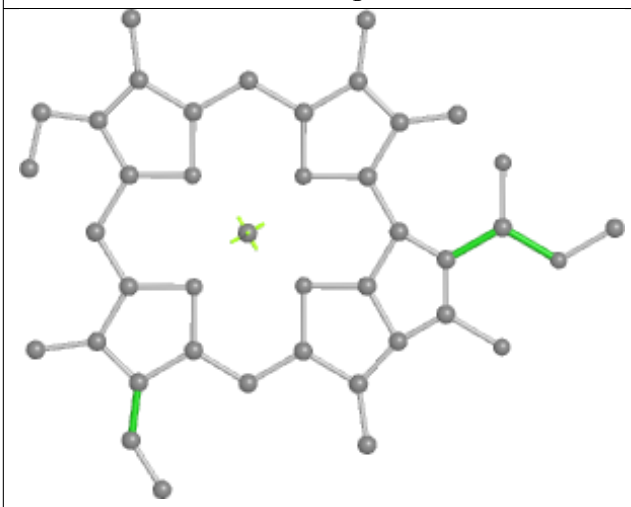
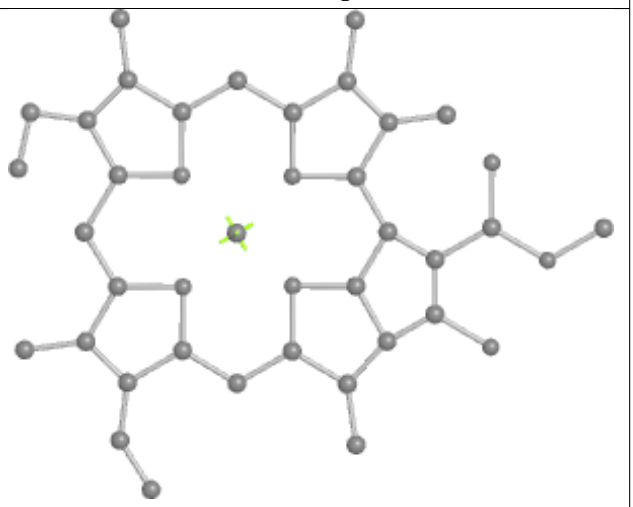


Bond angles

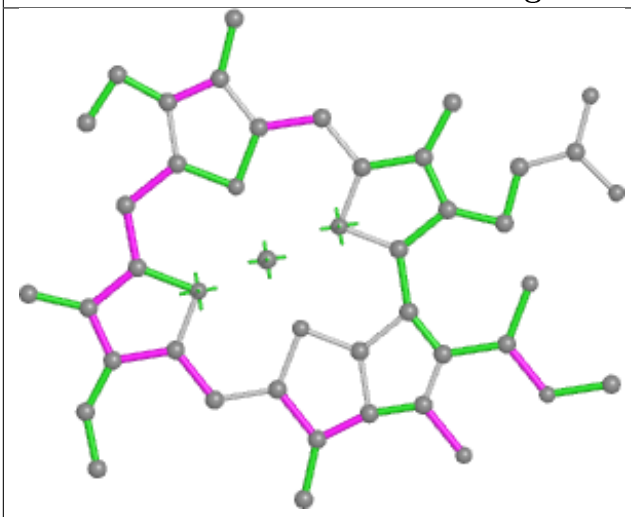


Torsions

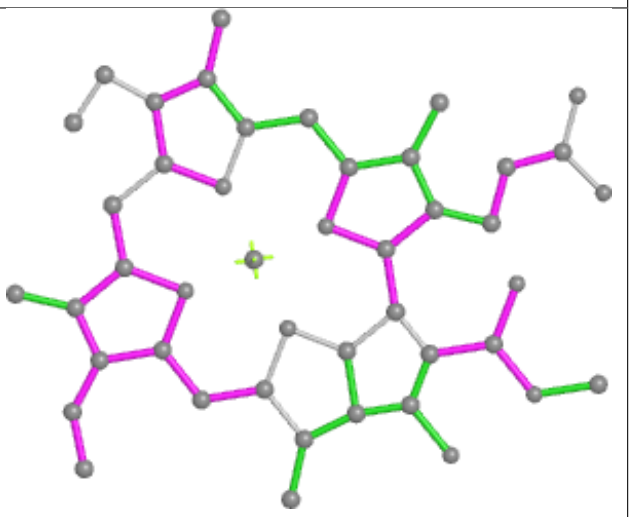


Rings

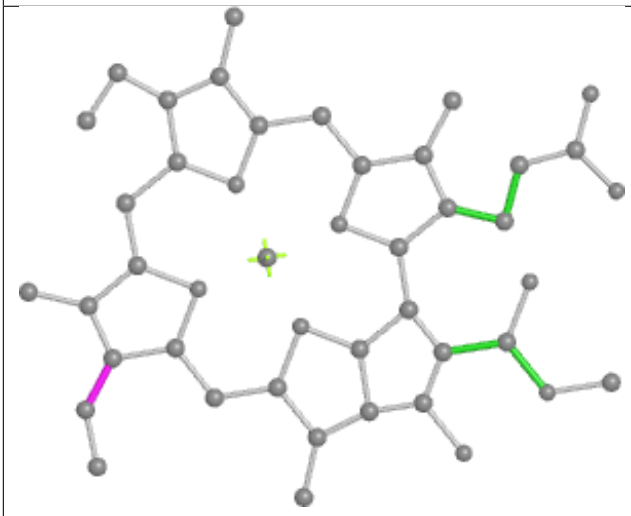
Ligand CLA A 817



Bond lengths



Bond angles



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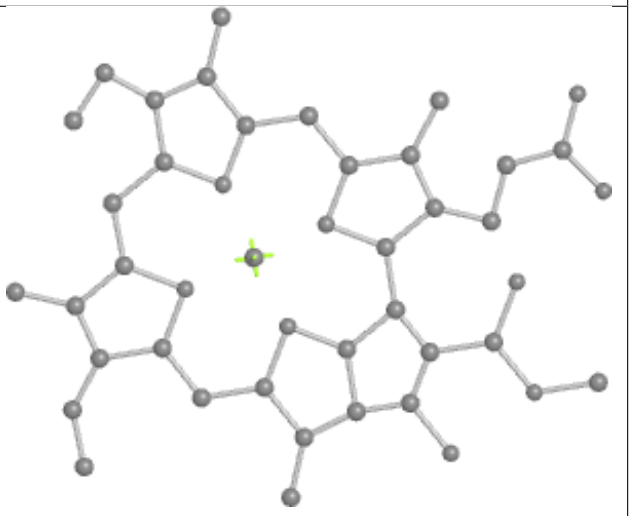
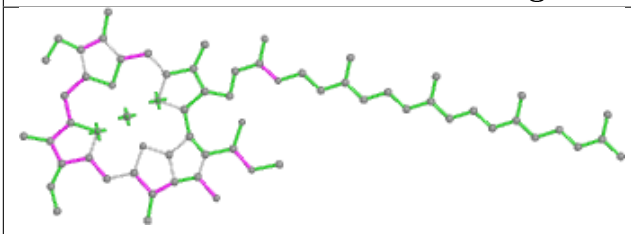
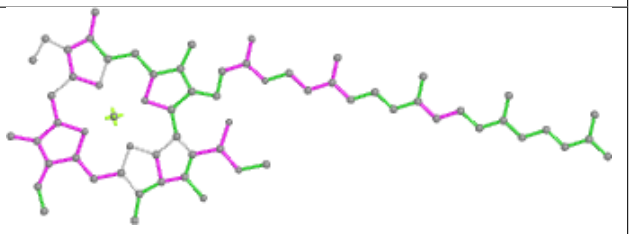


Rings

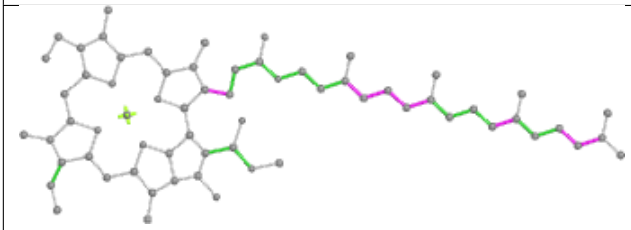
Ligand CLA a 829



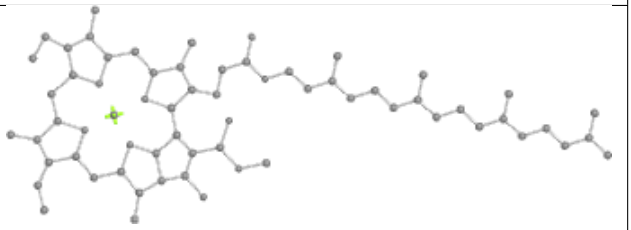
Bond lengths



Bond angles

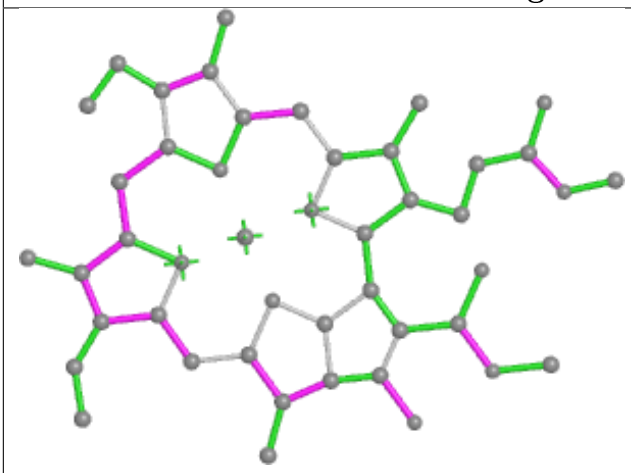


Torsions

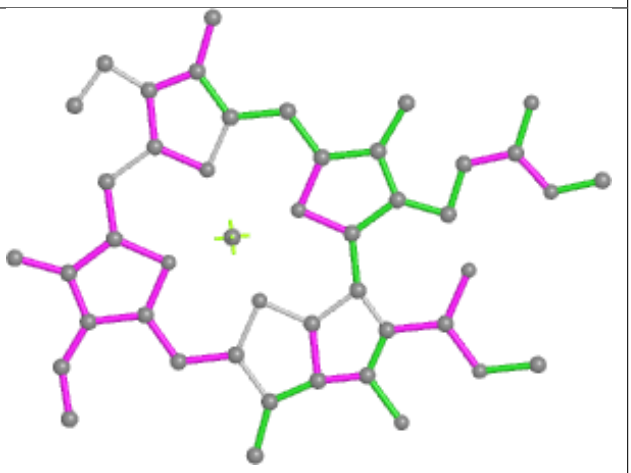


Rings

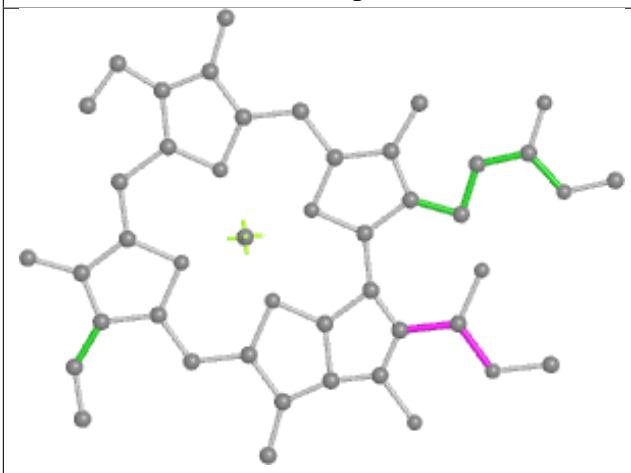
Ligand CLA b 821



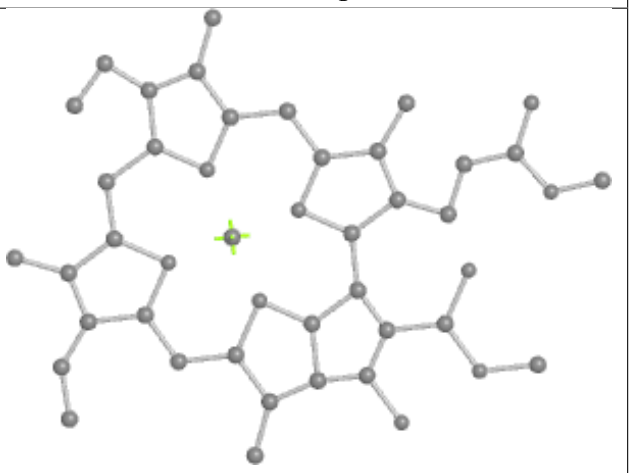
Bond lengths



Bond angles

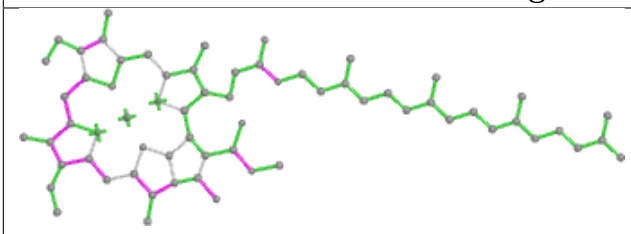


Torsions

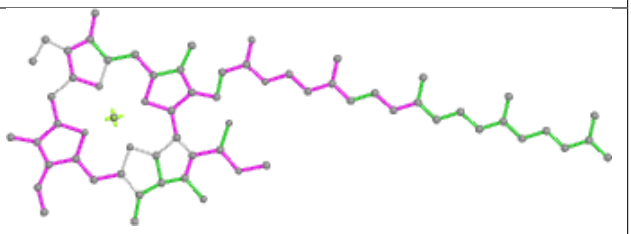


Rings

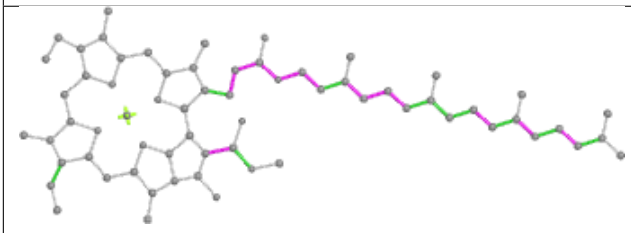
Ligand CLA a 802



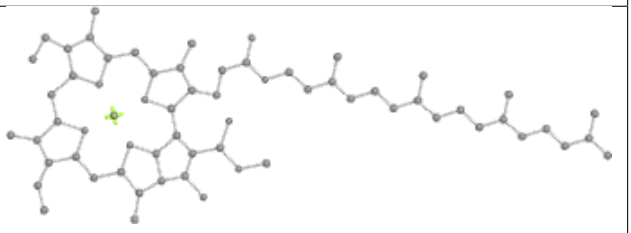
Bond lengths



Bond angles

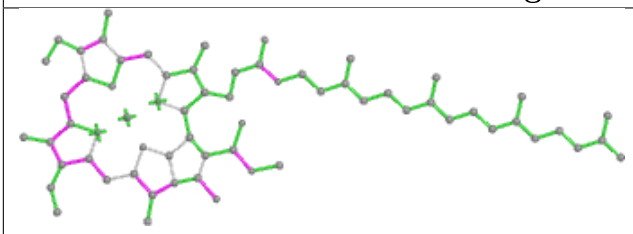


Torsions



Rings

Ligand CLA A 843



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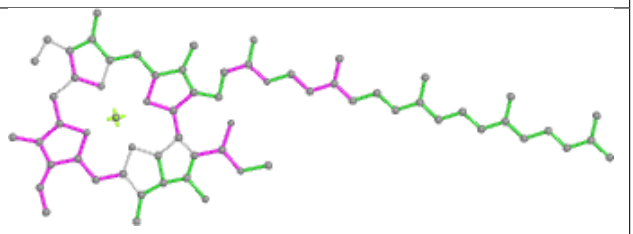
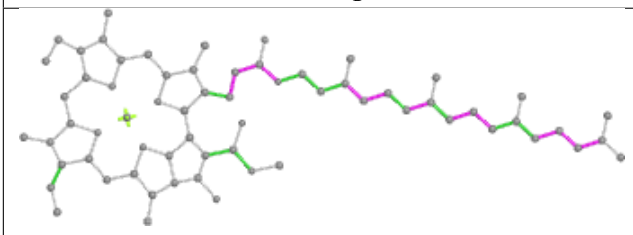
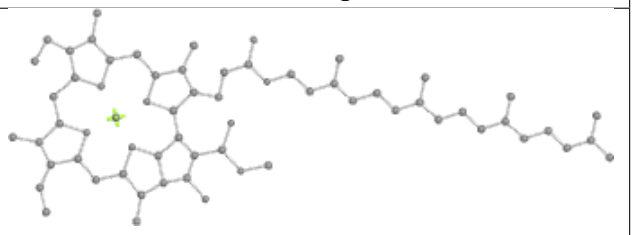


Bond angles

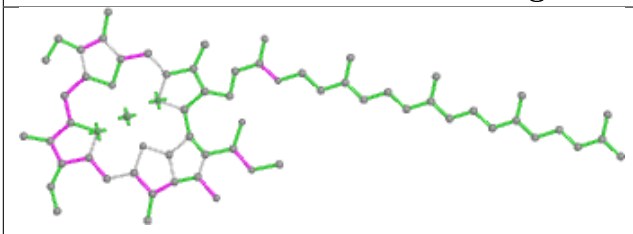


Torsions

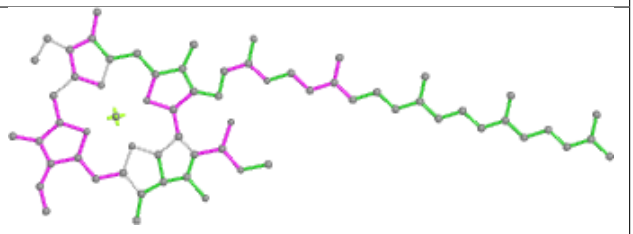


Rings

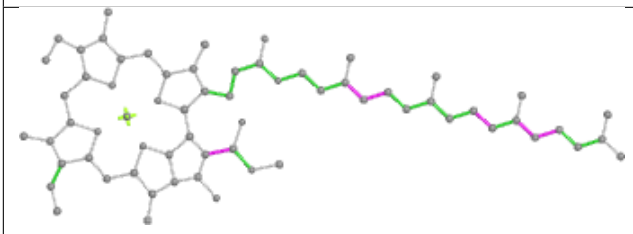
Ligand CLA a 808



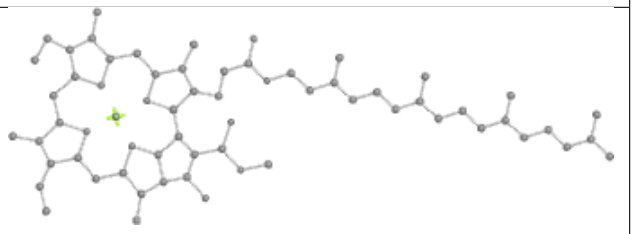
Bond lengths



Bond angles

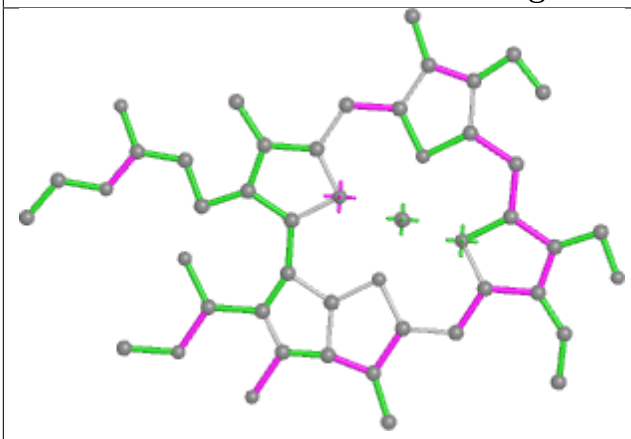


Torsions



Rings

Ligand CHL 7 606



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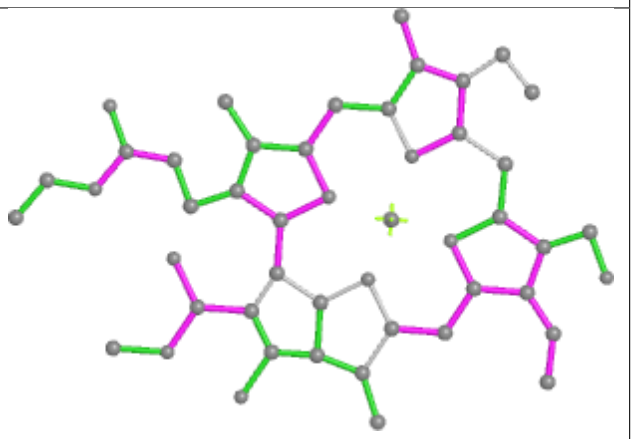
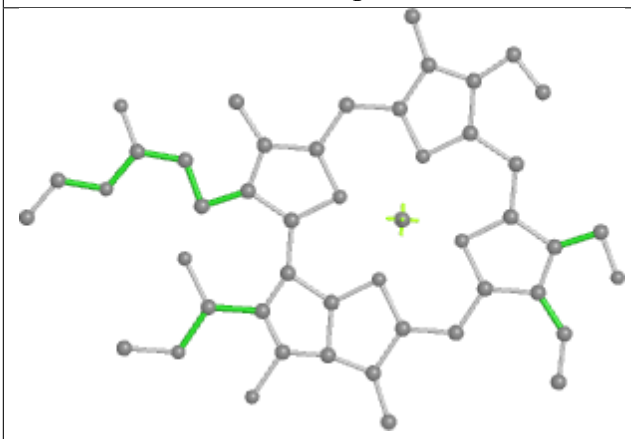
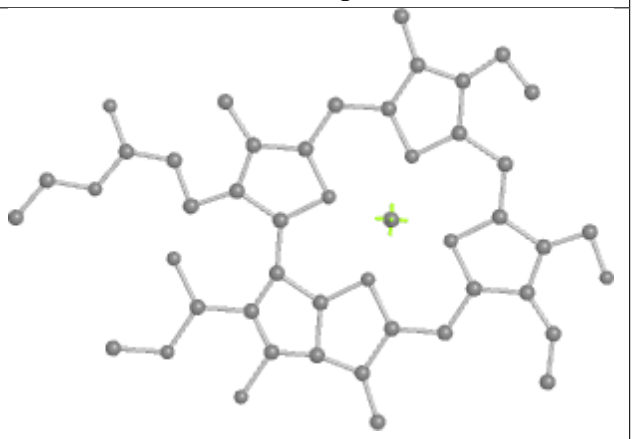


Bond angles

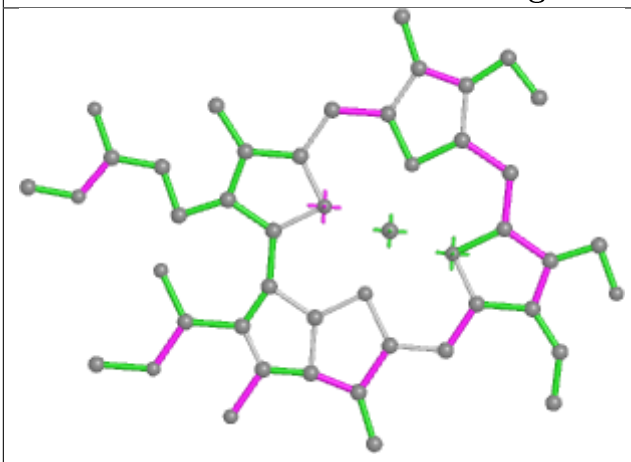


Torsions



Rings

Ligand CHL 8 306



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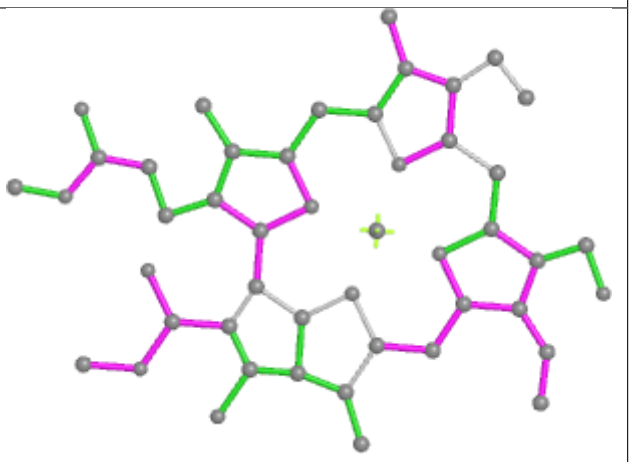
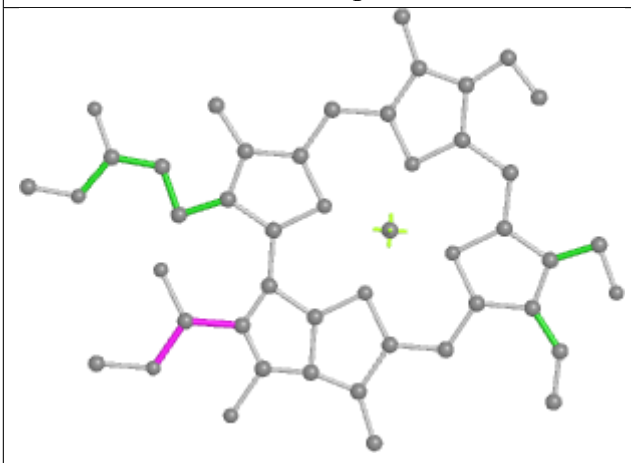
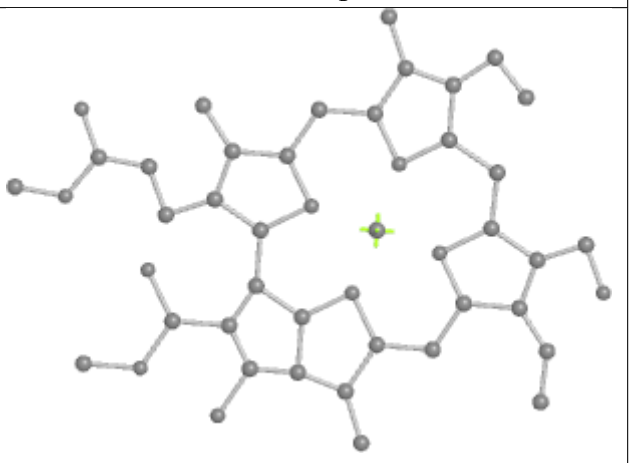


Bond angles

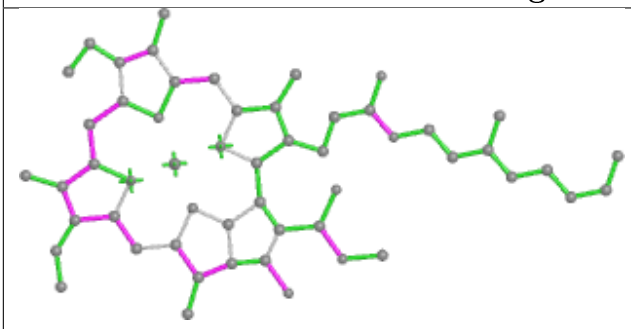


Torsions



Rings

Ligand CLA a 813



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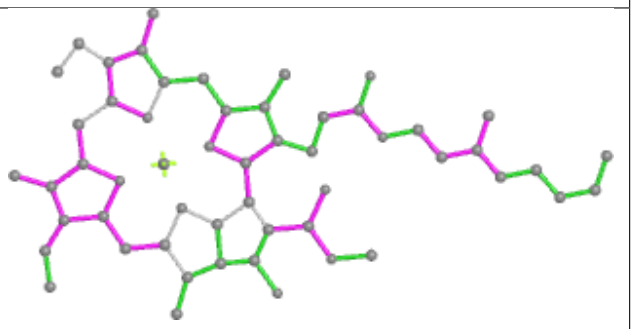
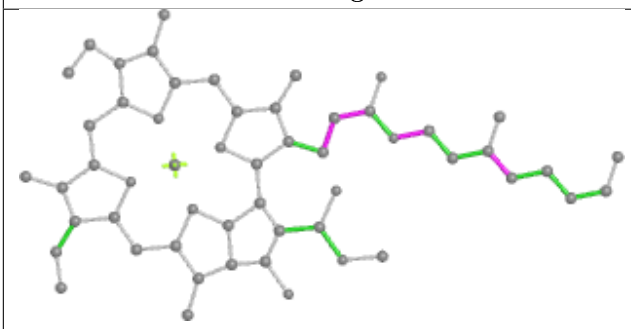
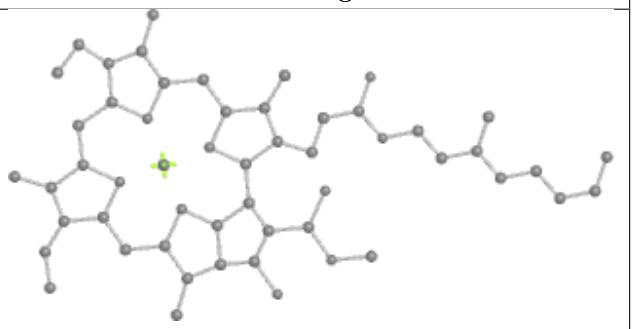


Bond angles

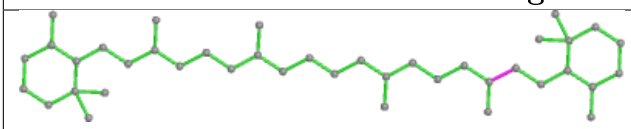


Torsions

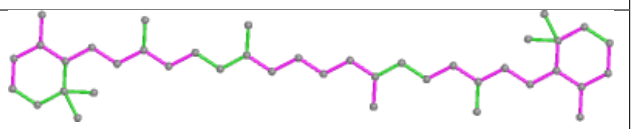


Rings

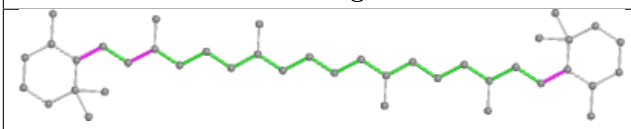
Ligand BCR a 852



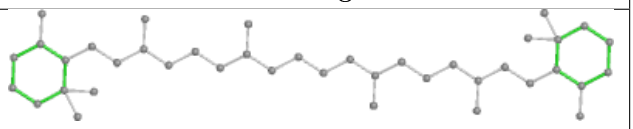
Bond lengths



Bond angles

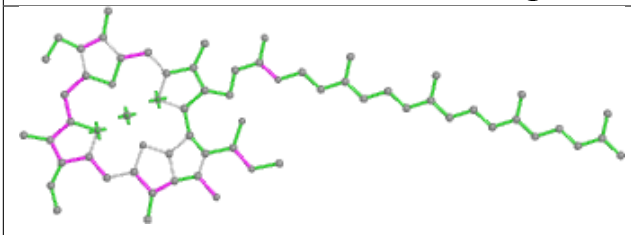


Torsions



Rings

Ligand CLA A 830



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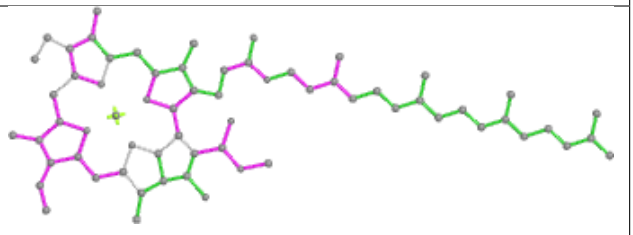
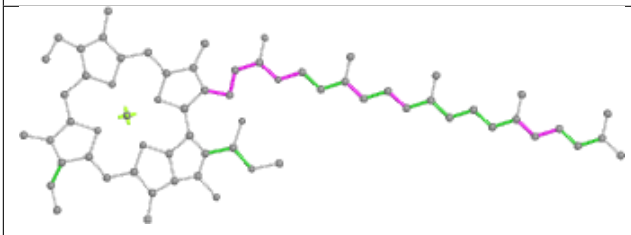
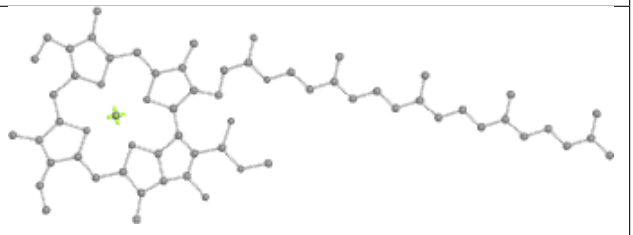


Bond angles

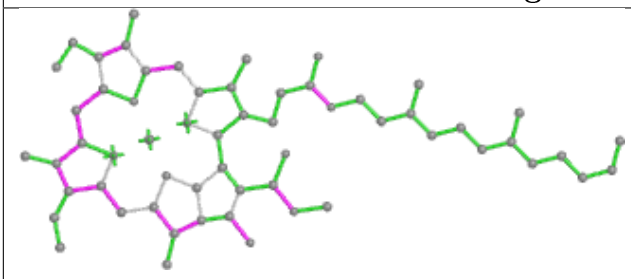


Torsions

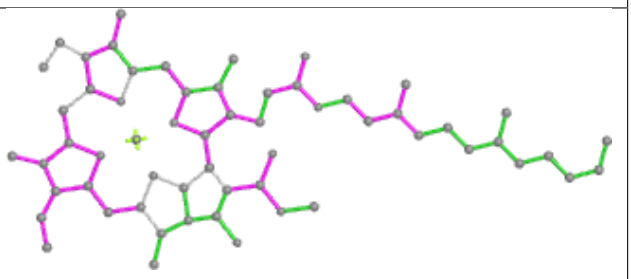


Rings

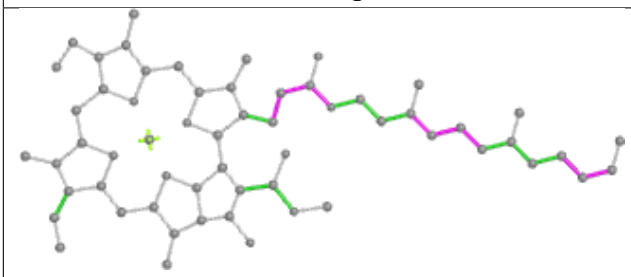
Ligand CLA B 817



Bond lengths



Bond angles



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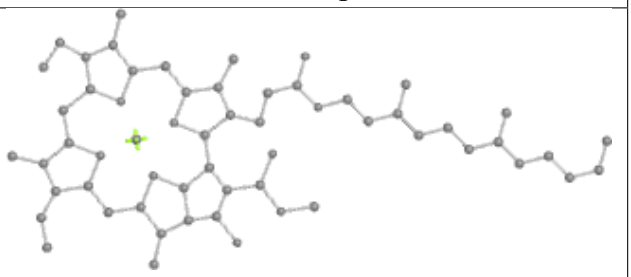
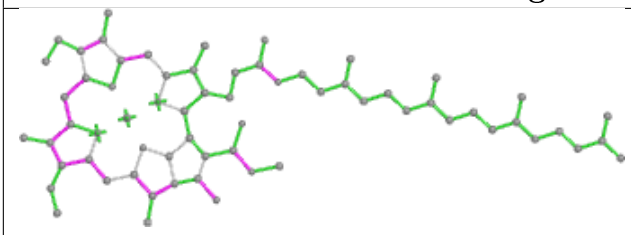


Rings

Ligand CLA a 806



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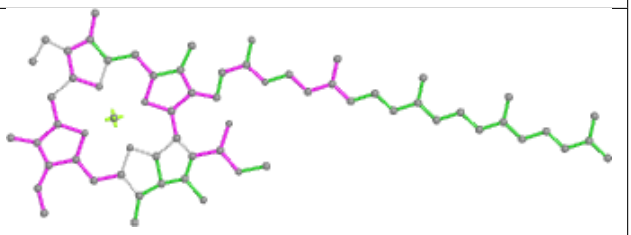
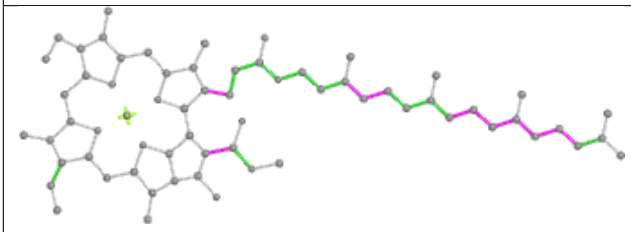
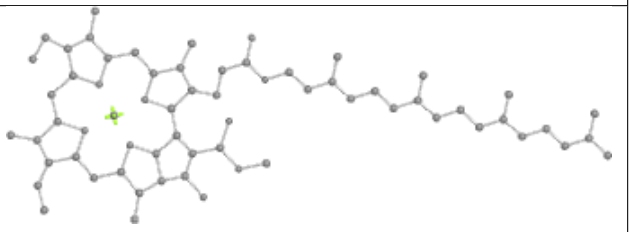


Bond angles

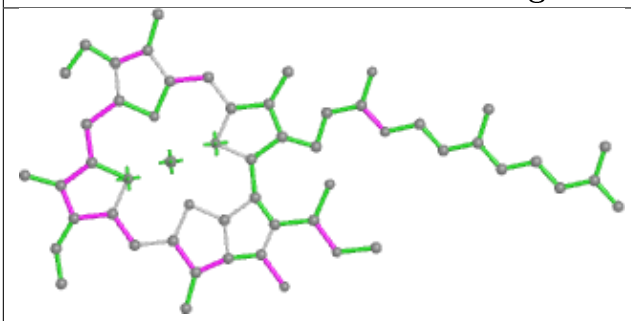


Torsions



Rings

Ligand CLA 8 310



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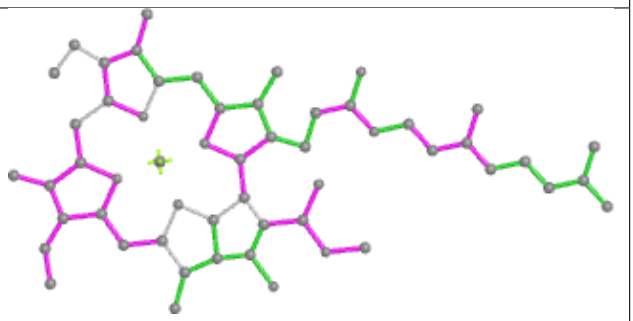
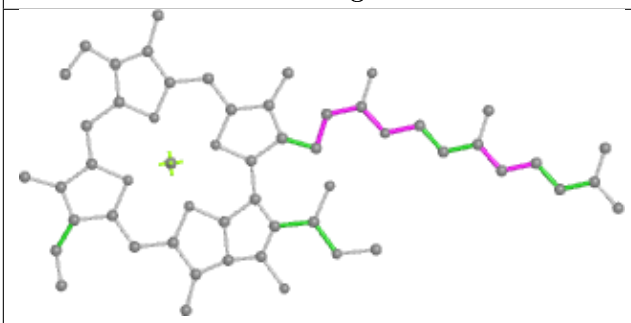
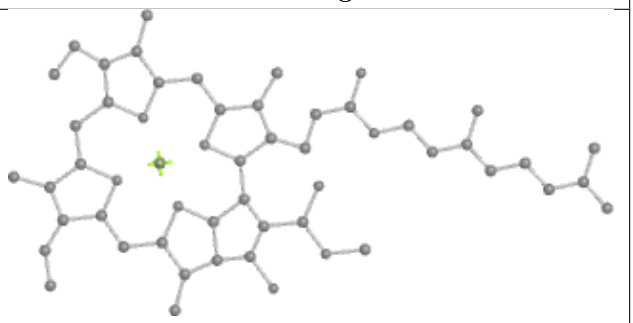


Bond angles

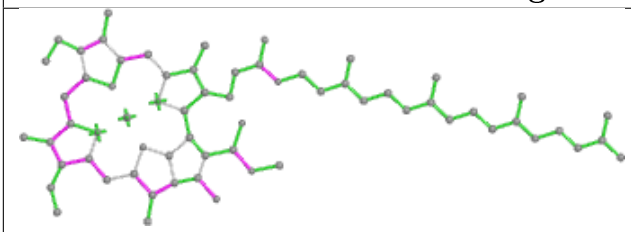


Torsions

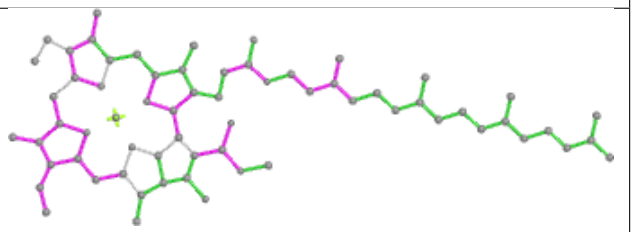


Rings

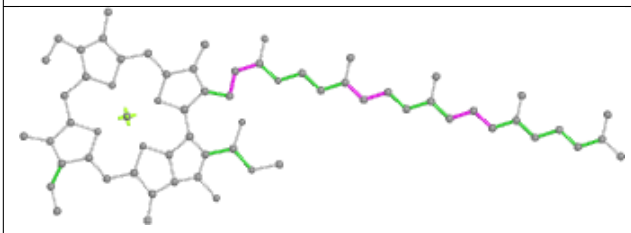
Ligand CLA 7 612



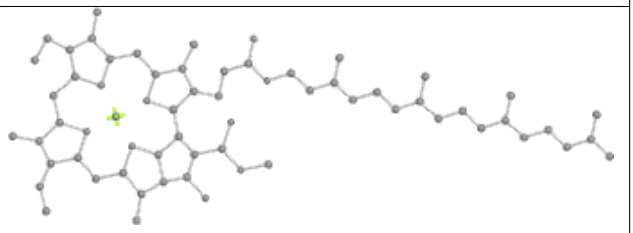
Bond lengths



Bond angles

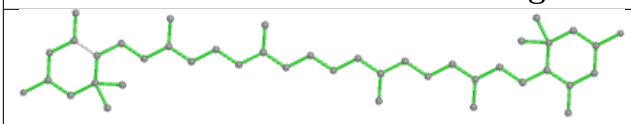


Torsions

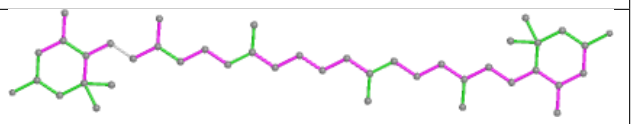


Rings

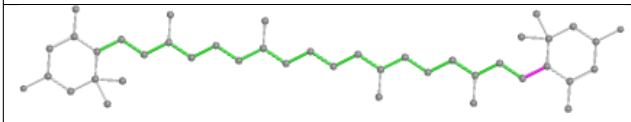
Ligand LUT 6 317



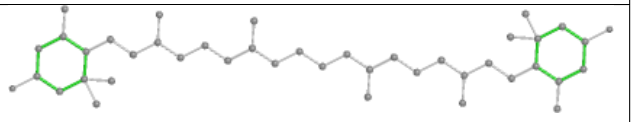
Bond lengths



Bond angles

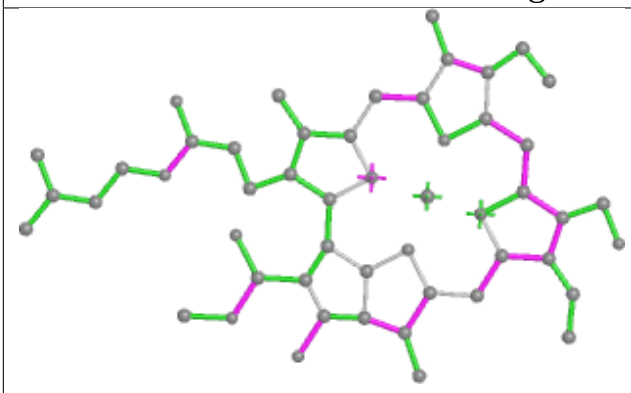


Torsions

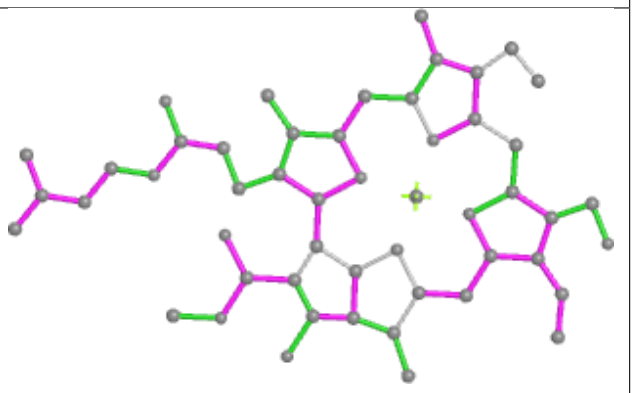


Rings

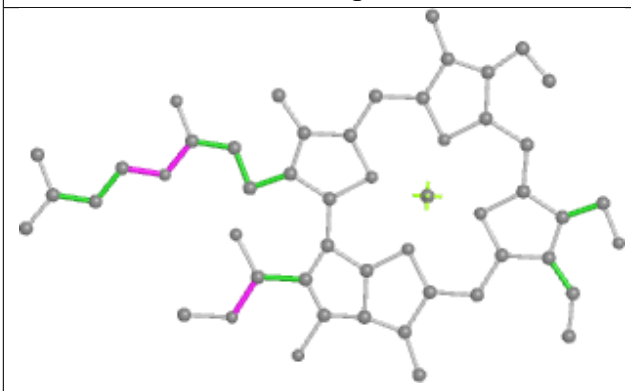
Ligand CHL 2 607



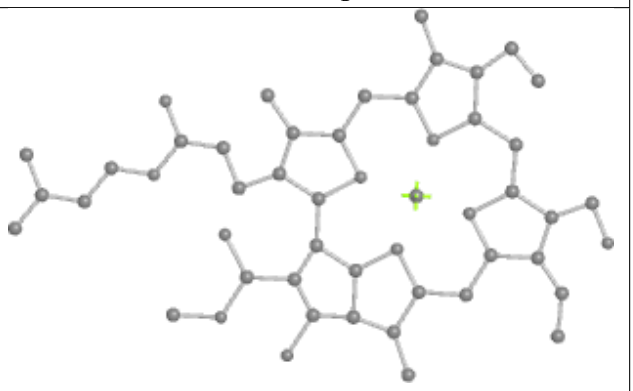
Bond lengths



Bond angles

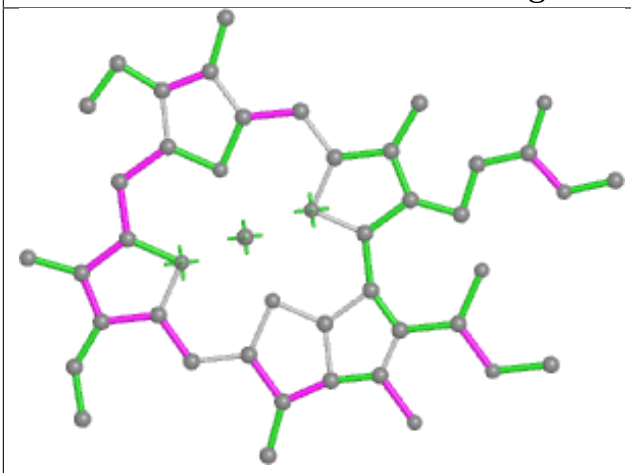


Torsions

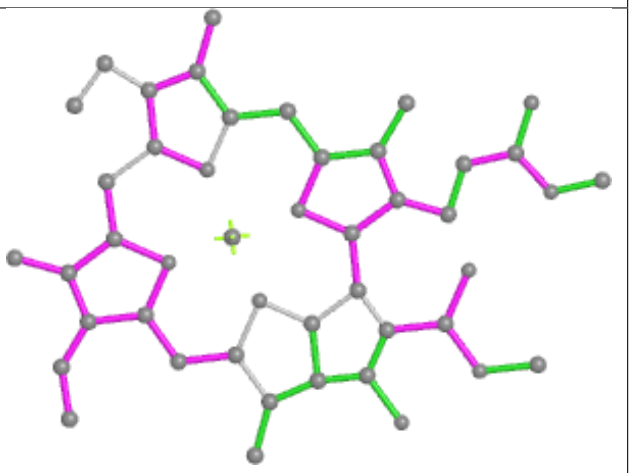


Rings

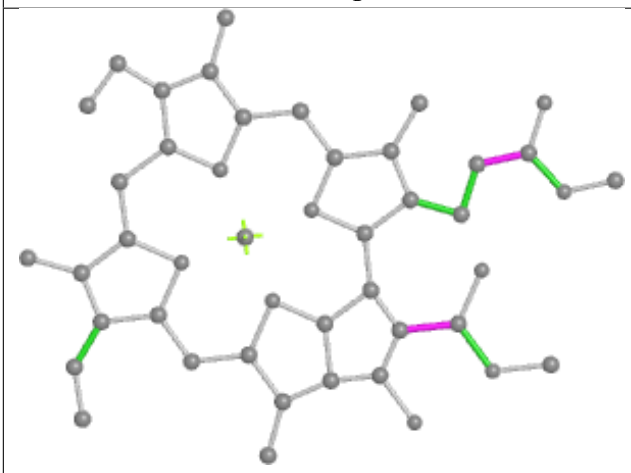
Ligand CLA 9 601



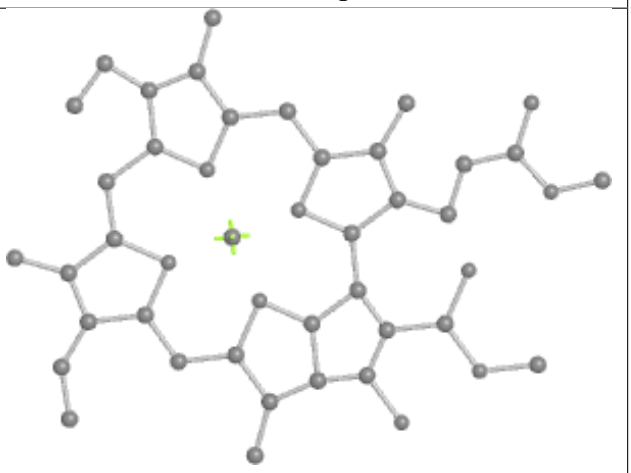
Bond lengths



Bond angles

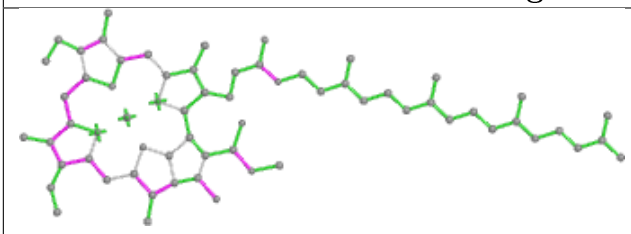


Torsions

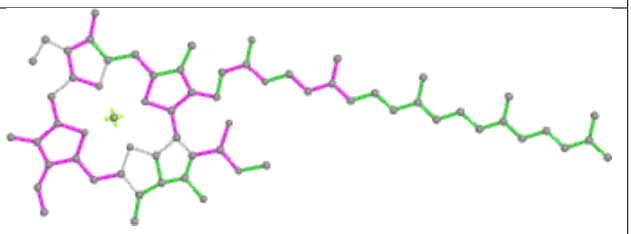


Rings

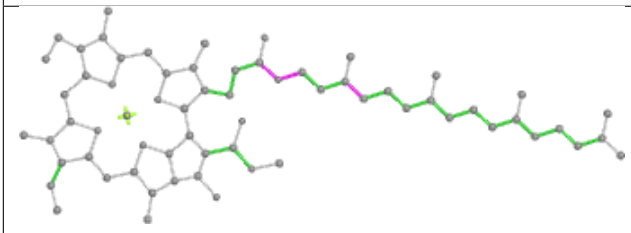
Ligand CLA L 203



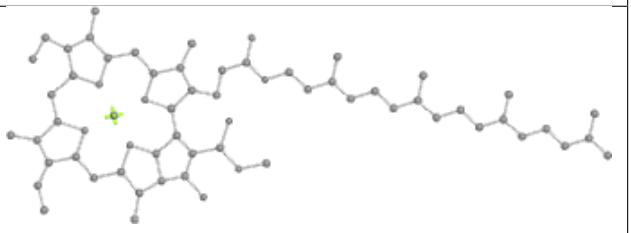
Bond lengths



Bond angles

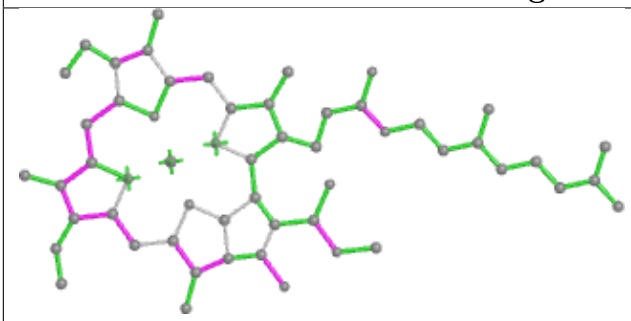


Torsions

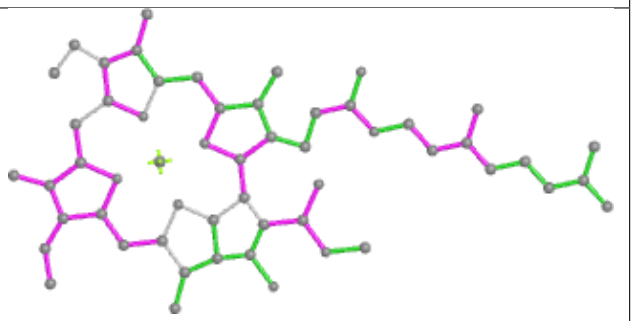


Rings

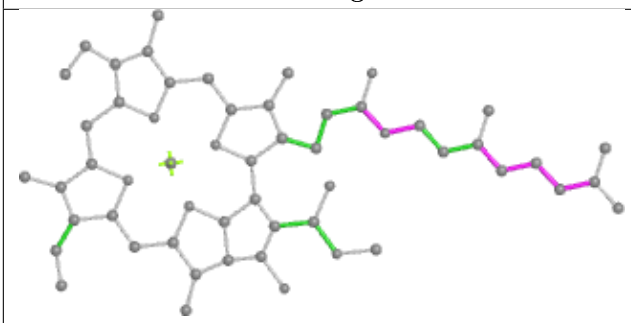
Ligand CLA a 805



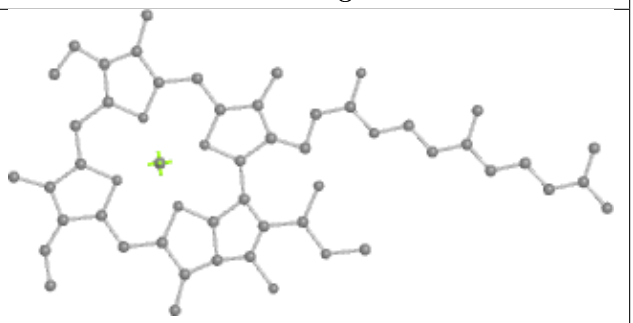
Bond lengths



Bond angles

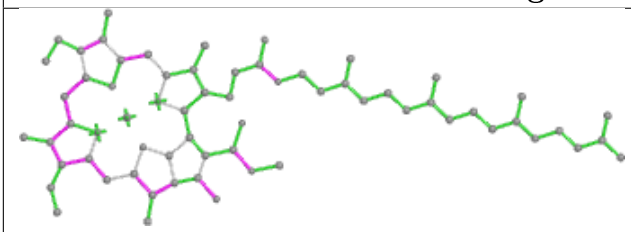


Torsions

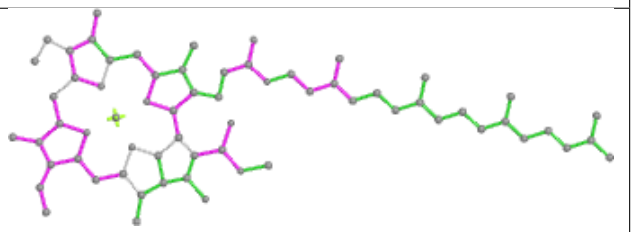


Rings

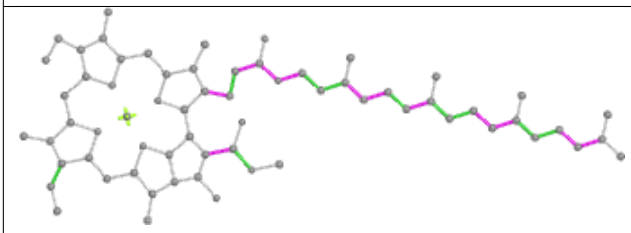
Ligand CLA b 805



Bond lengths



Bond angles



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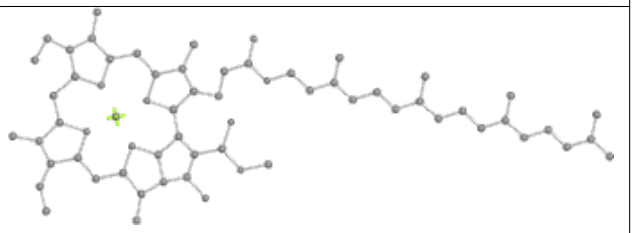
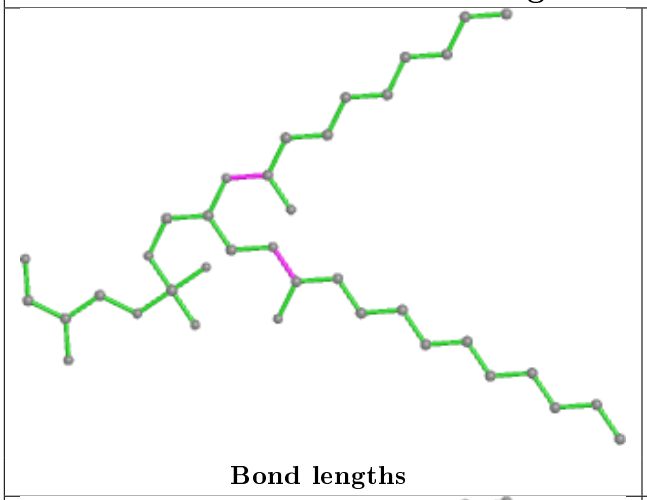
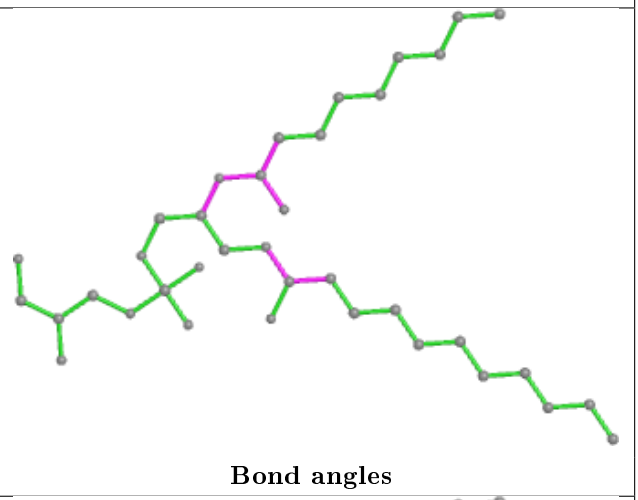


Rings

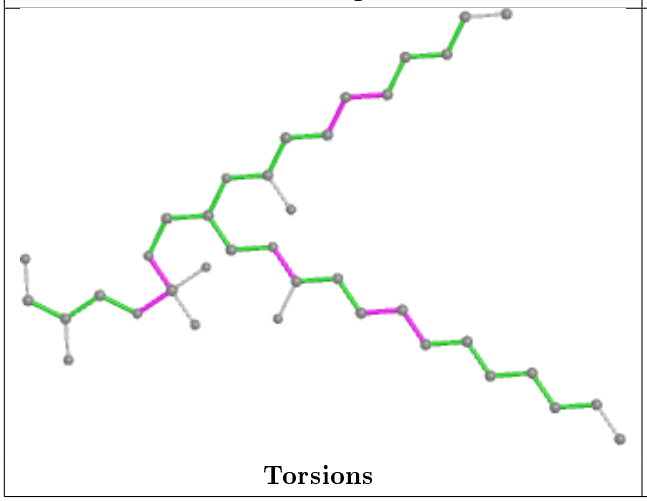
Ligand LHG 7 618



Bond lengths



Bond angles



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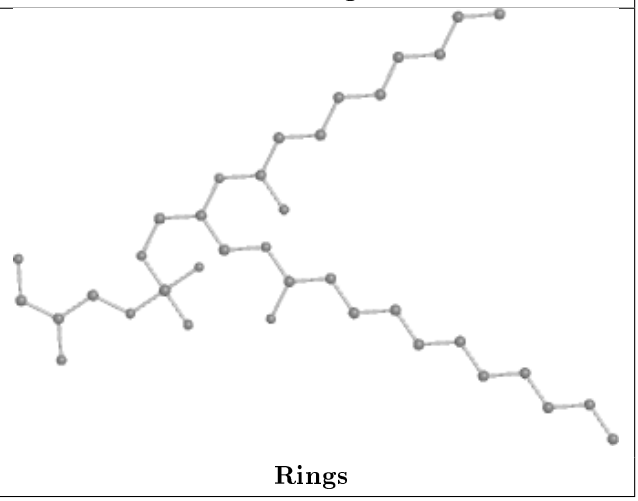
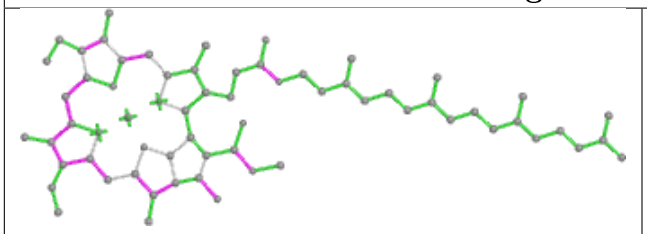
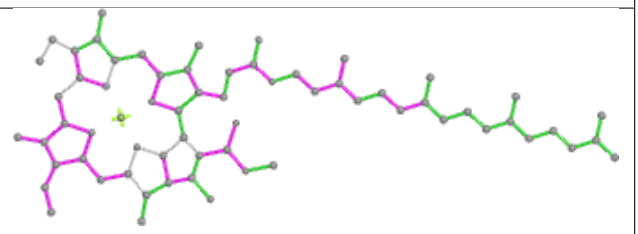


Rings

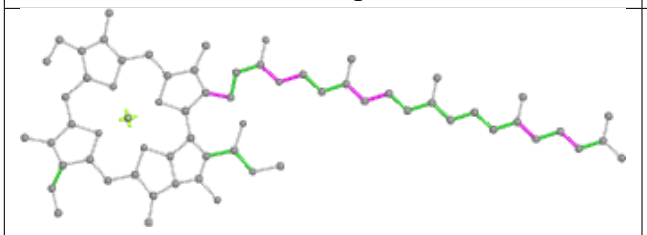
Ligand CLA A 829



Bond lengths



Bond angles



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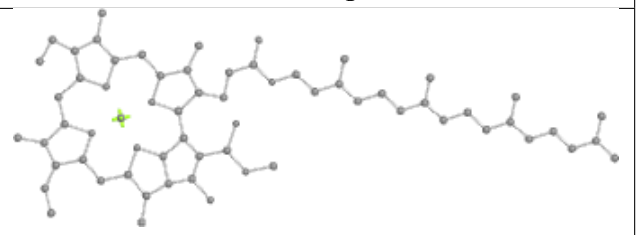
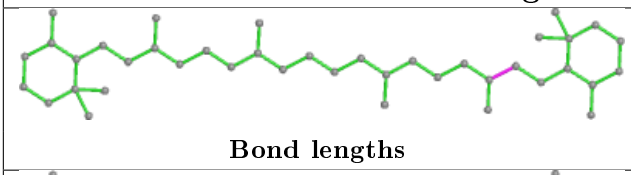
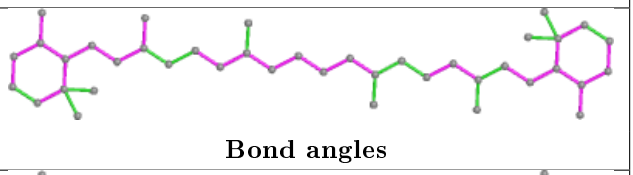


Rings

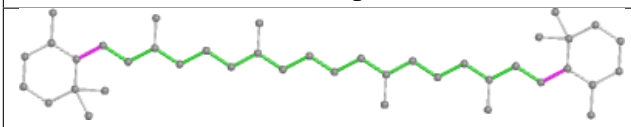
Ligand BCR A 856



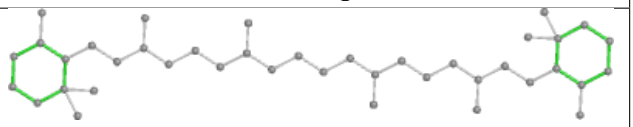
Bond lengths



Bond angles

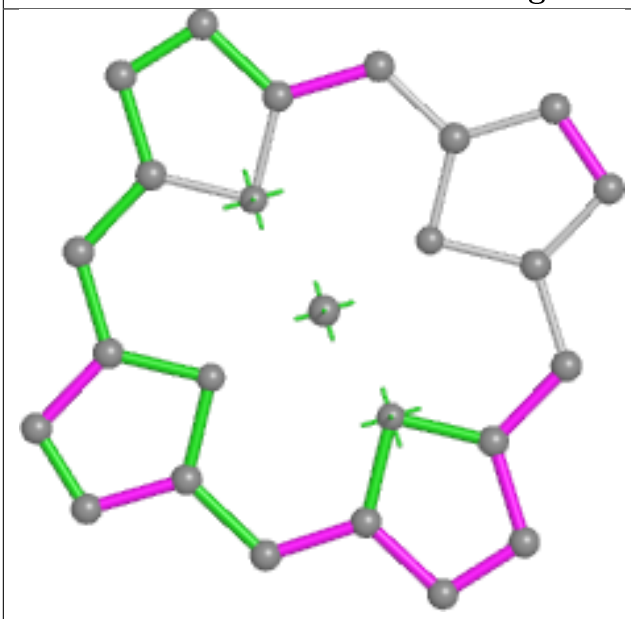


Torsions

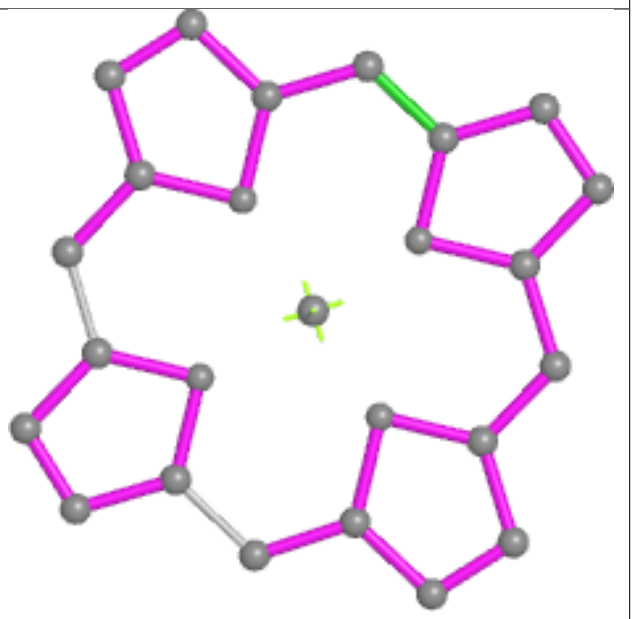


Rings

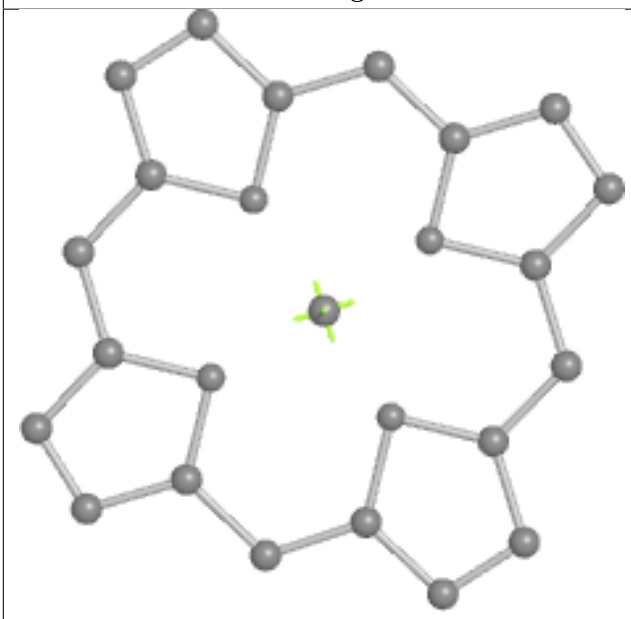
Ligand CLA 8 313



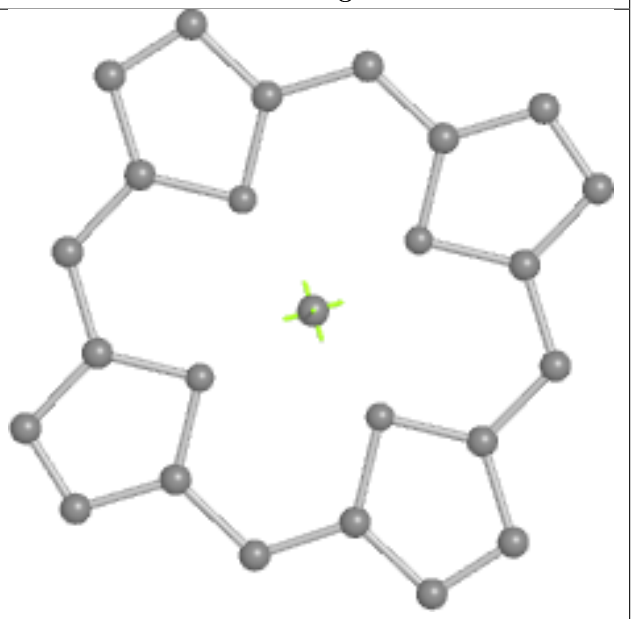
Bond lengths



Bond angles

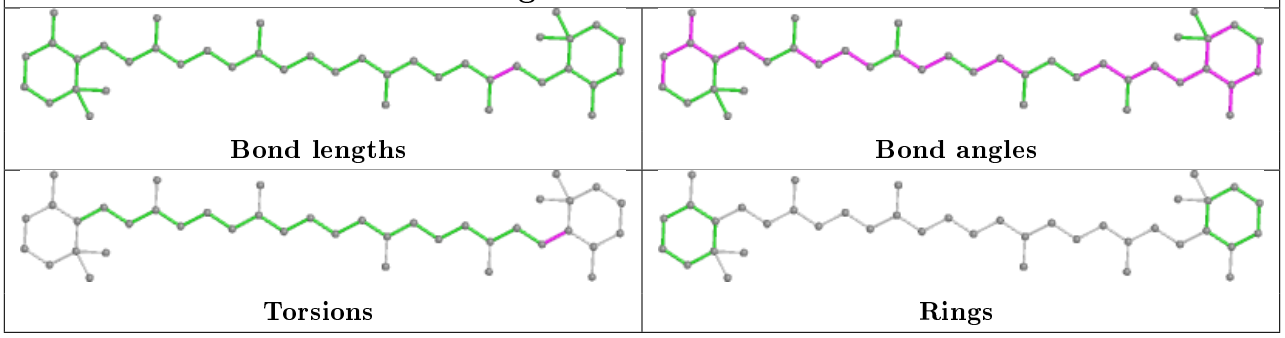


Torsions

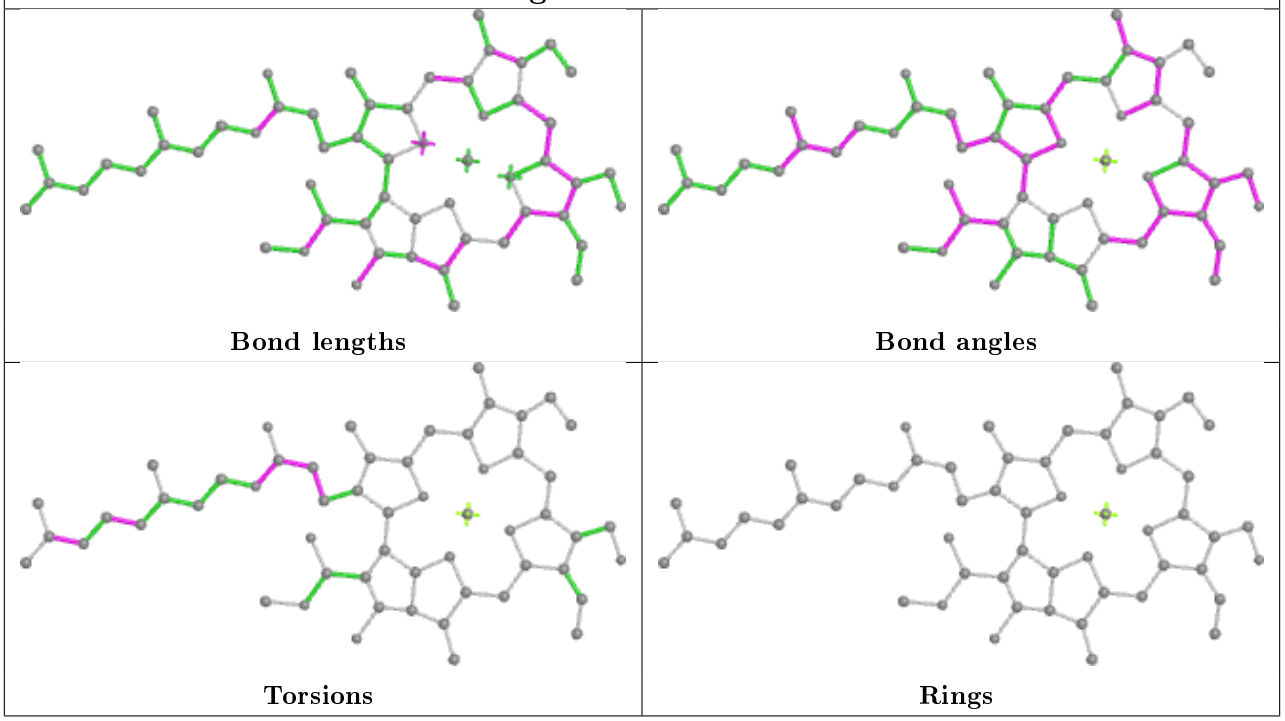


Rings

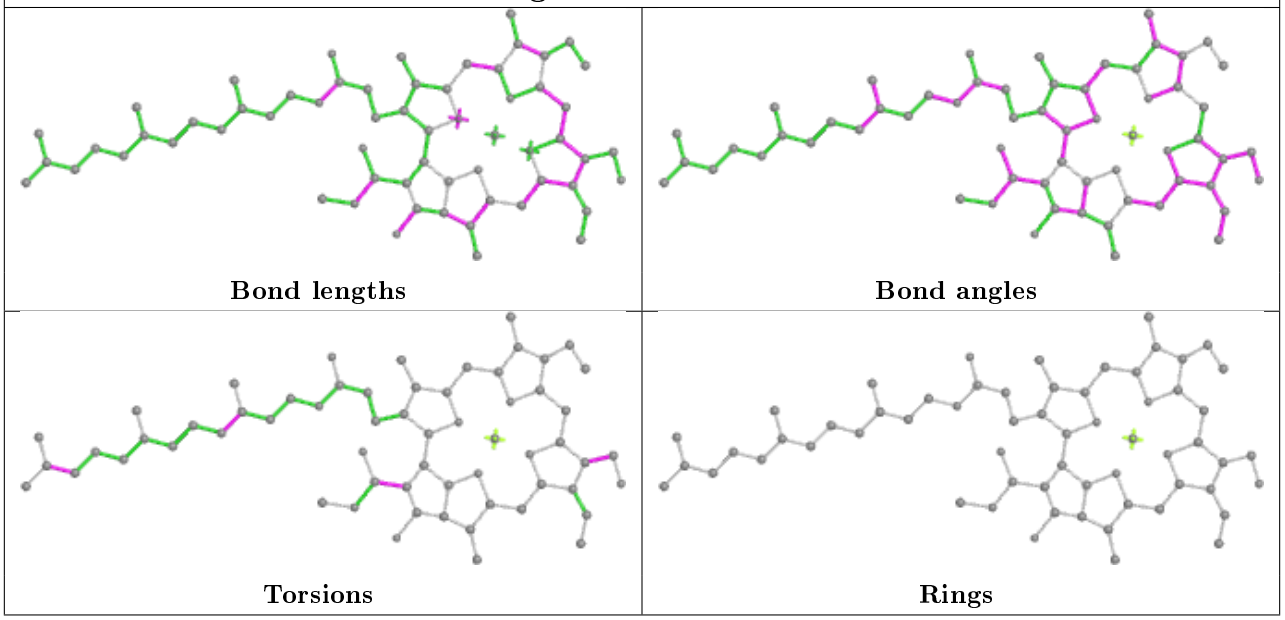
Ligand BCR J 3003



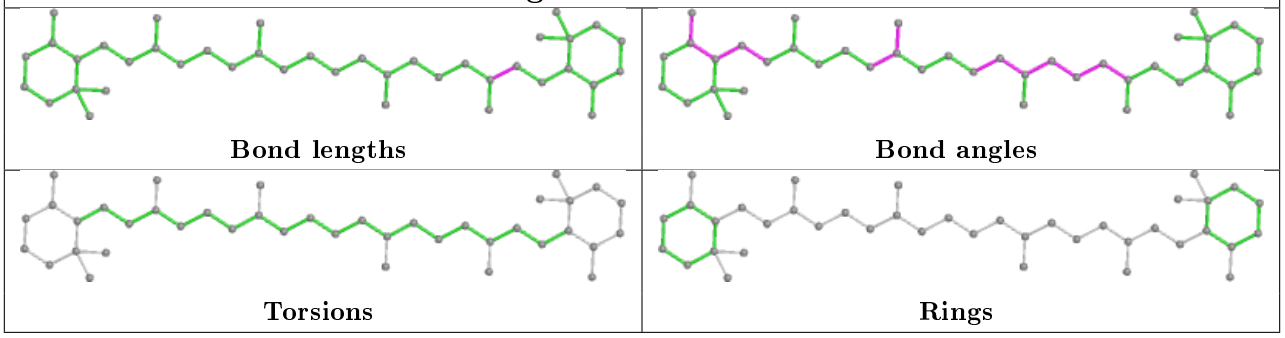
Ligand CHL 9 605



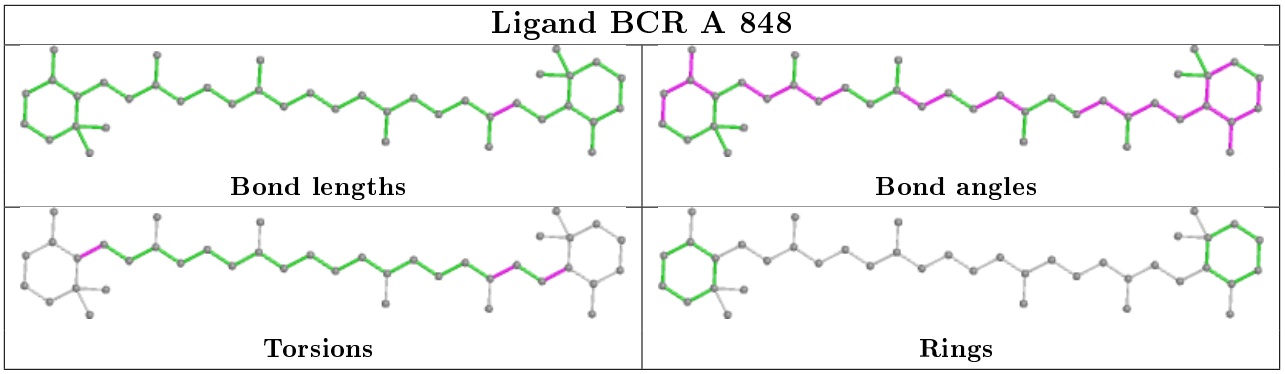
Ligand CHL 1 302



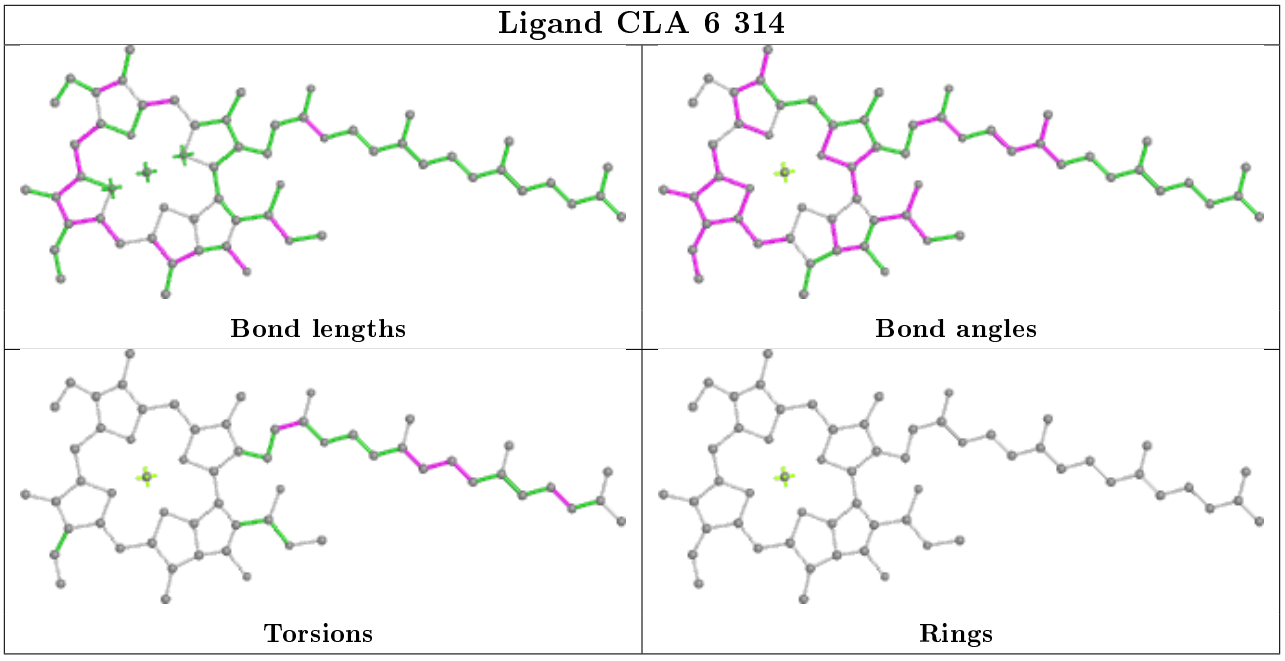
Ligand BCR b 801



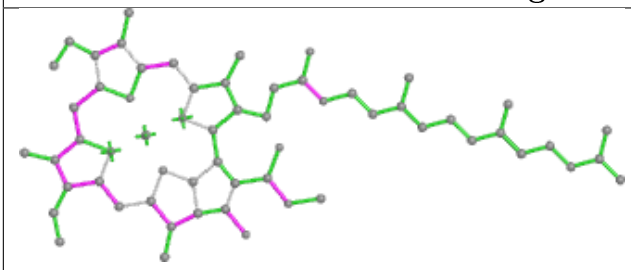
Ligand BCR A 848



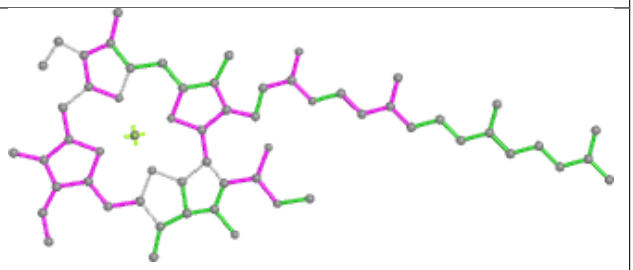
Ligand CLA 6 314



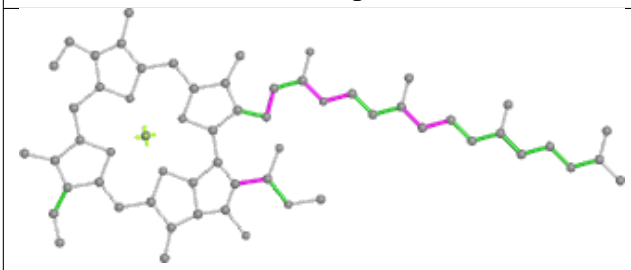
Ligand CLA 3 302



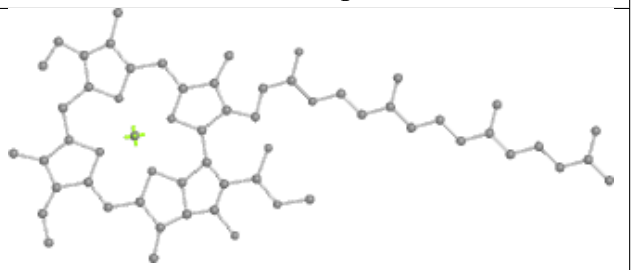
Bond lengths



Bond angles

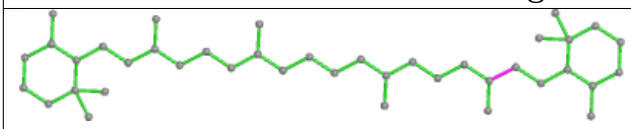


Torsions



Rings

Ligand BCR a 854



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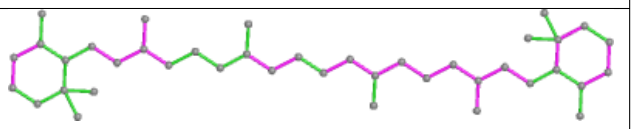
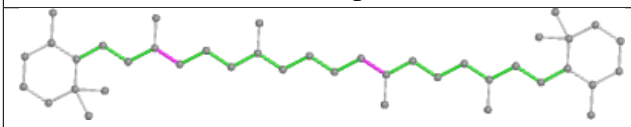
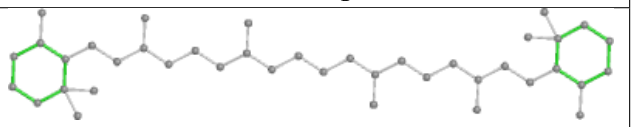


Bond angles

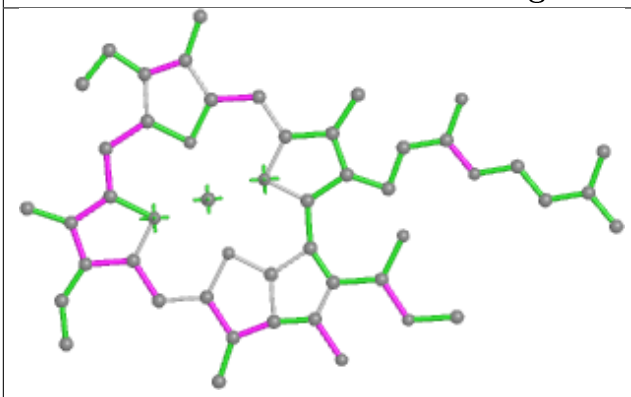


Torsions

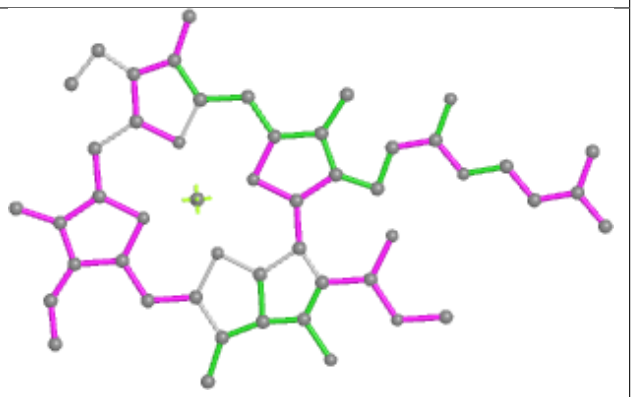


Rings

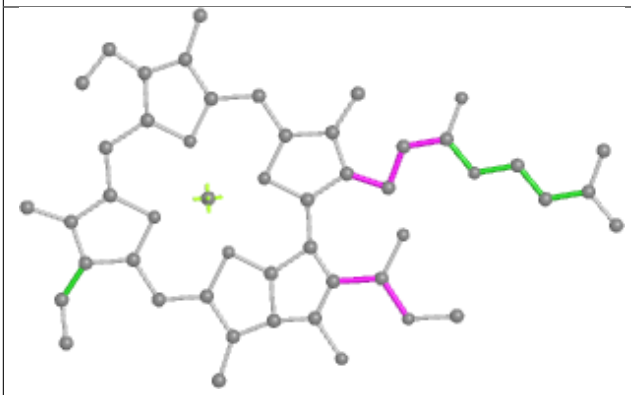
Ligand CLA a 816



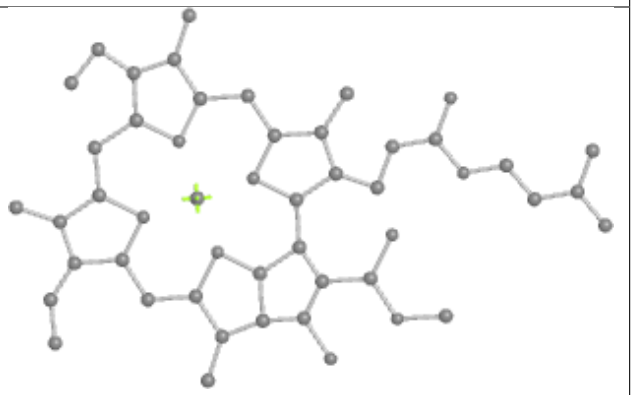
Bond lengths



Bond angles

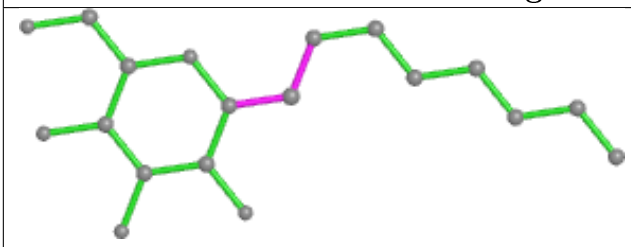


Torsions

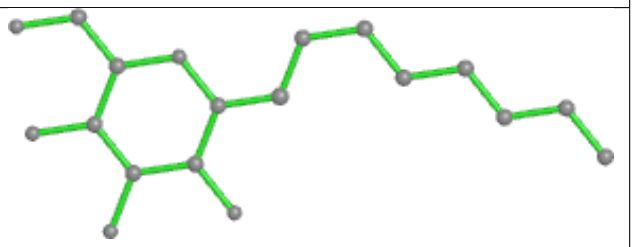


Rings

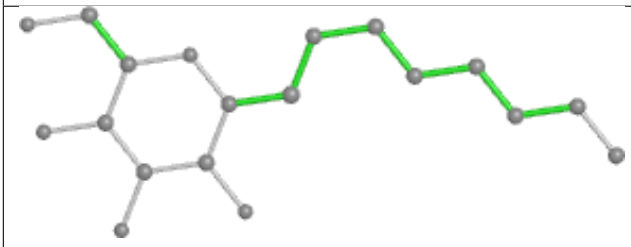
Ligand HTG a 857



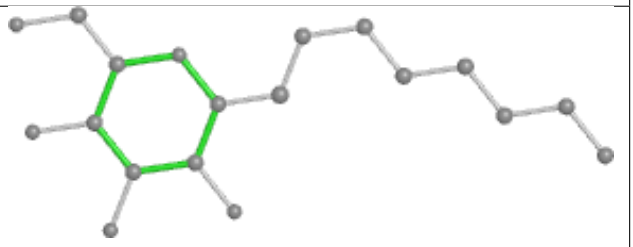
Bond lengths



Bond angles

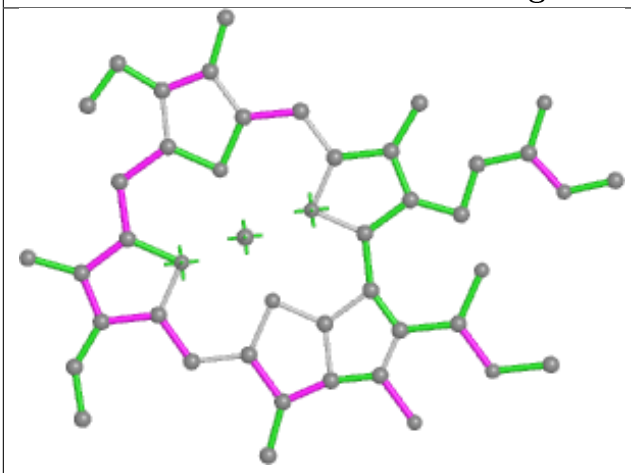


Torsions

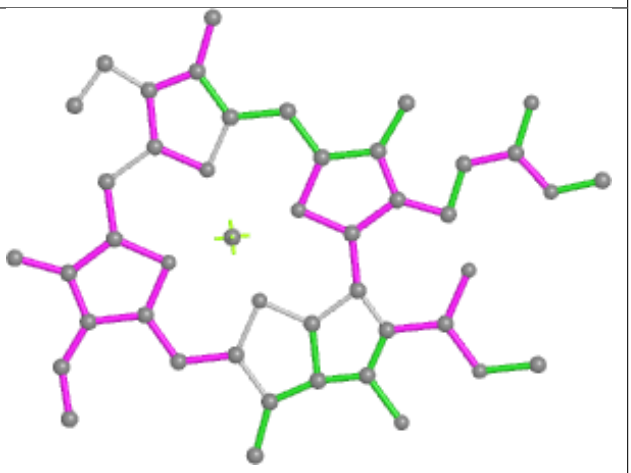


Rings

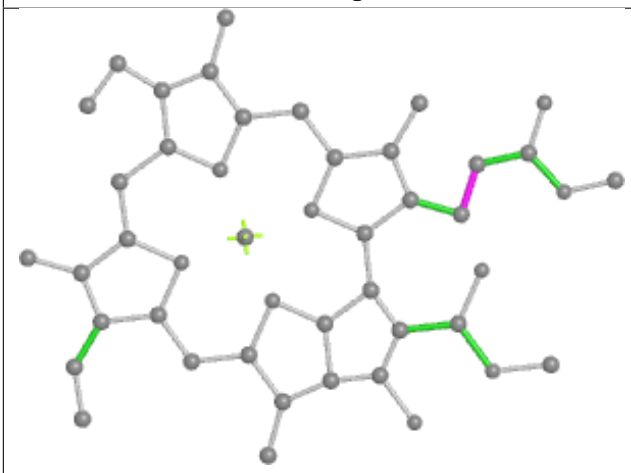
Ligand CLA 8 312



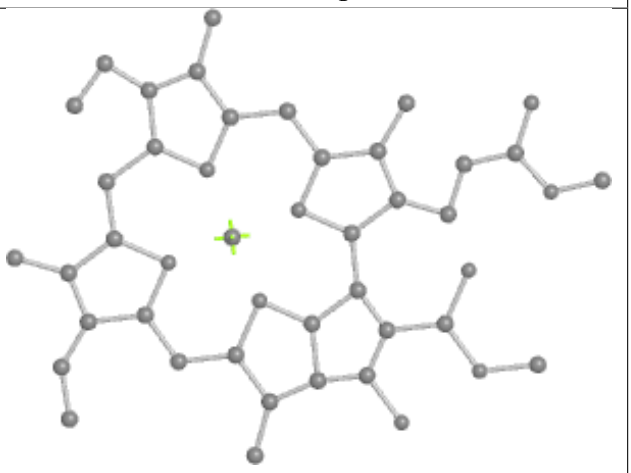
Bond lengths



Bond angles

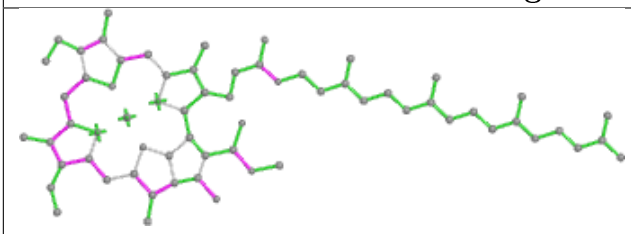


Torsions

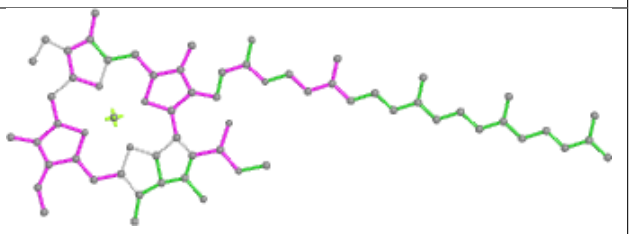


Rings

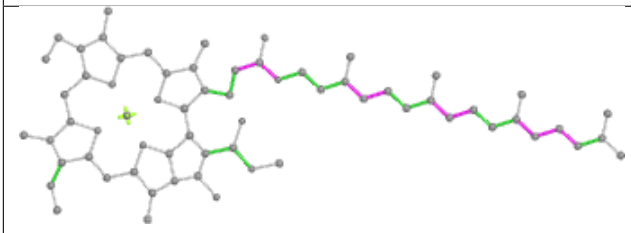
Ligand CLA B 814



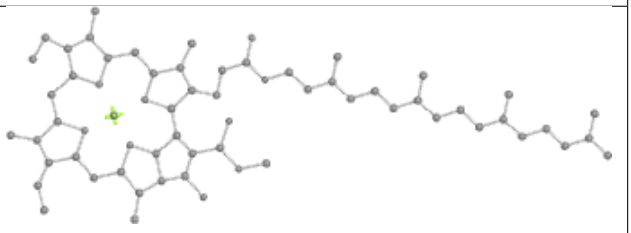
Bond lengths



Bond angles

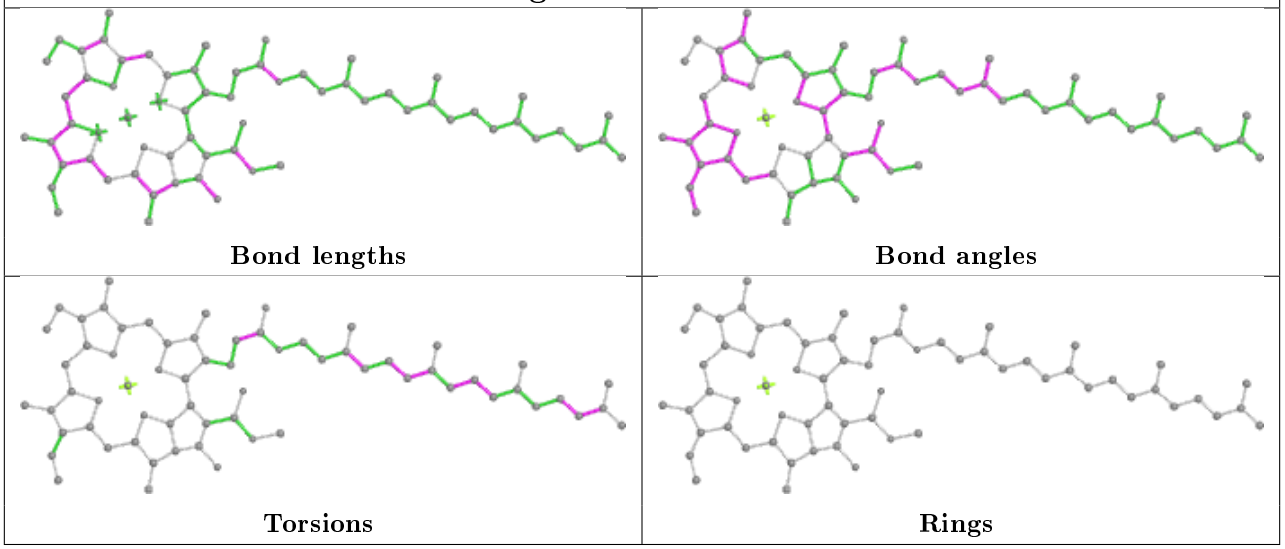


Torsions

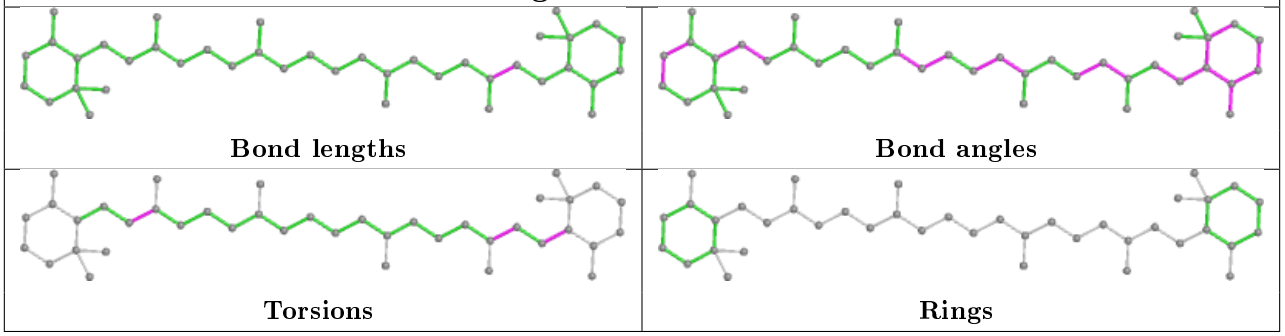


Rings

Ligand CLA 1 304



Ligand BCR l 205



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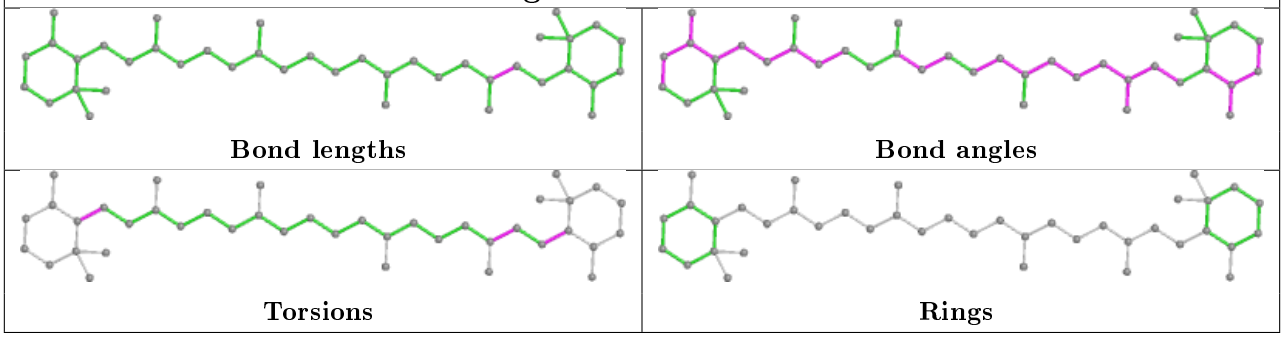
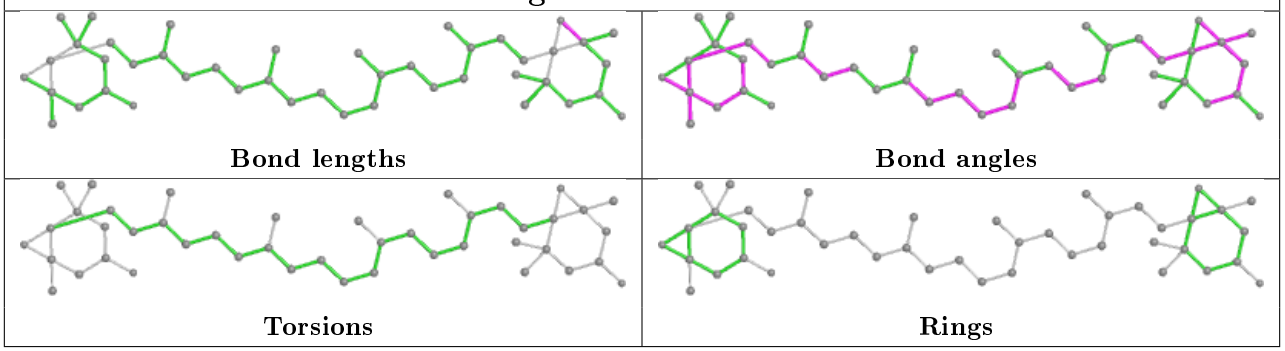
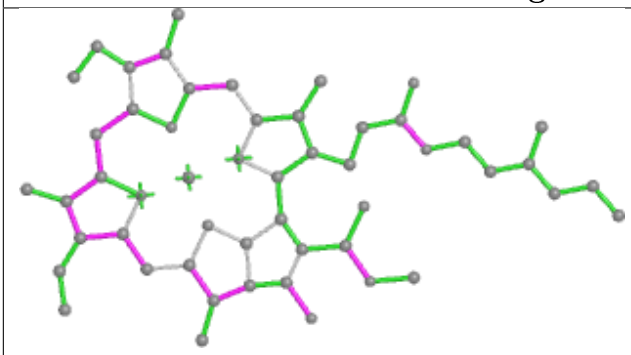


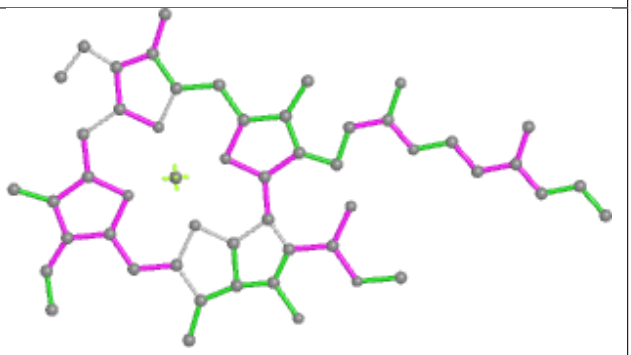
Ligand XAT 9 617



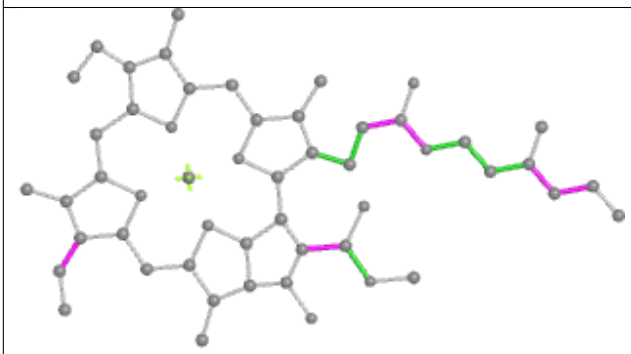
Ligand CLA a 846



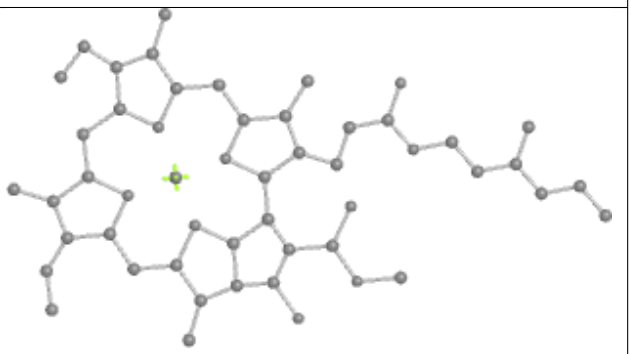
Bond lengths



Bond angles

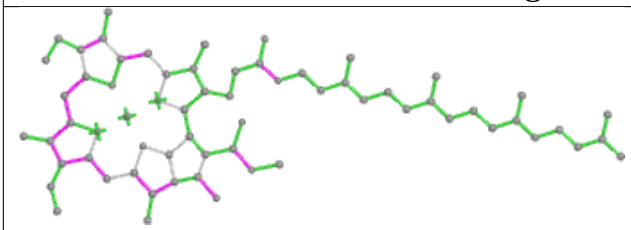


Torsions

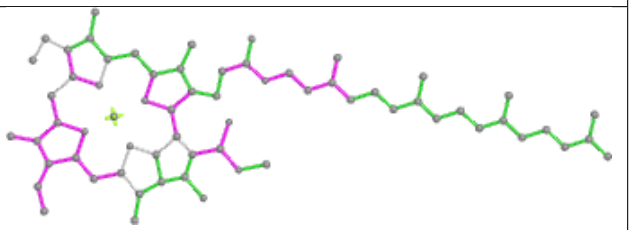


Rings

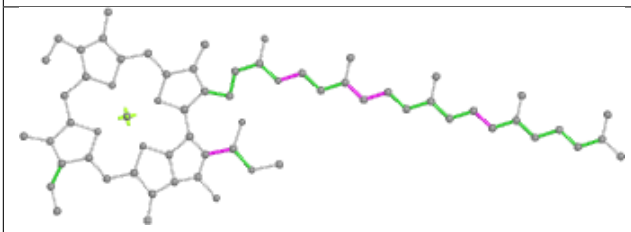
Ligand CLA A 840



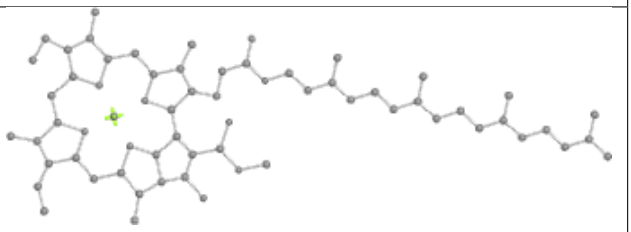
Bond lengths



Bond angles

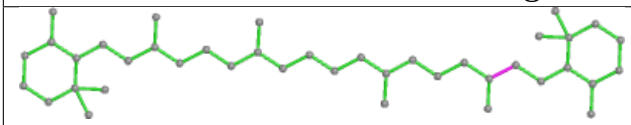


Torsions

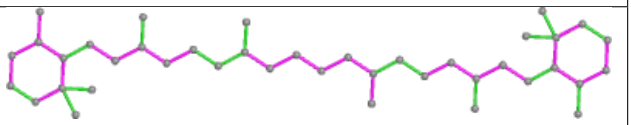


Rings

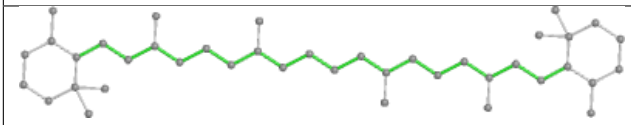
Ligand BCR B 843



Bond lengths



Bond angles



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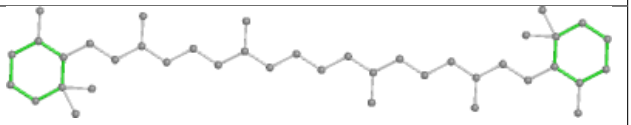
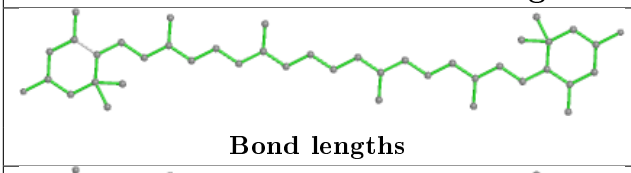


Rings

Ligand LUT 1 316



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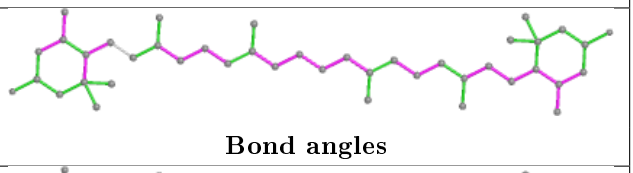
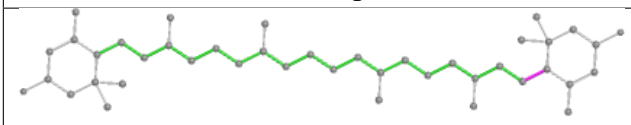
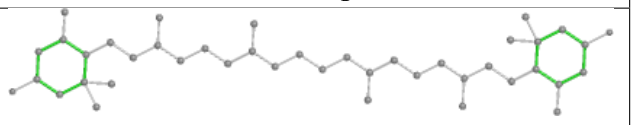


Bond angles

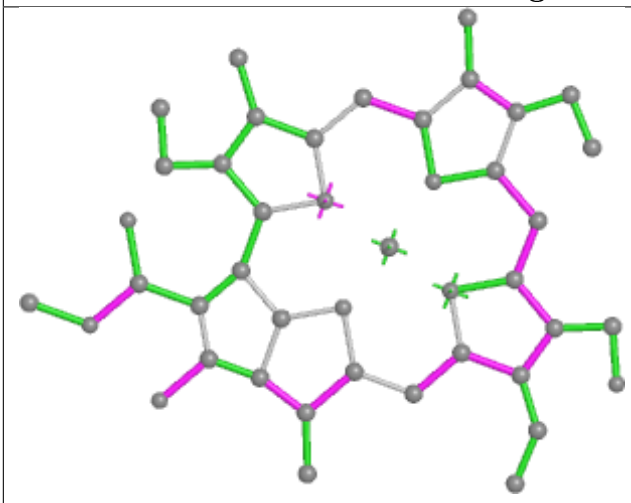


Torsions



Rings

Ligand CHL 4 615



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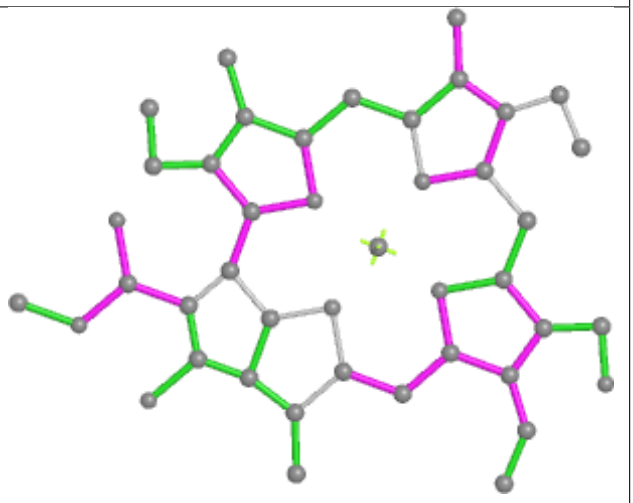
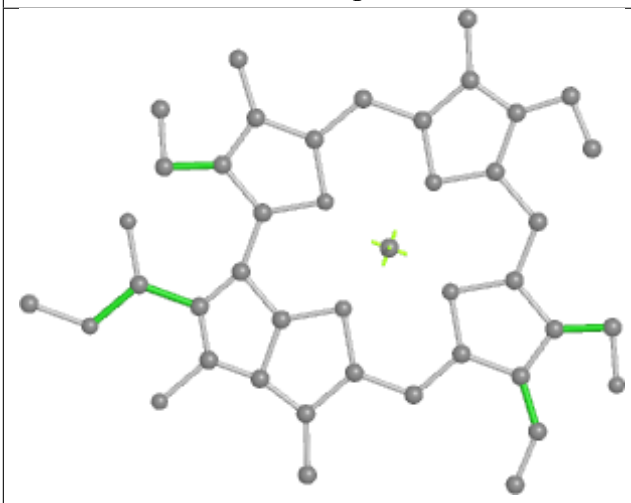
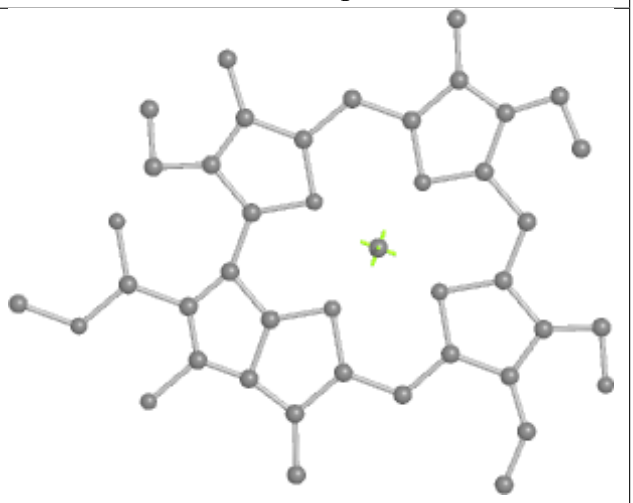


Bond angles

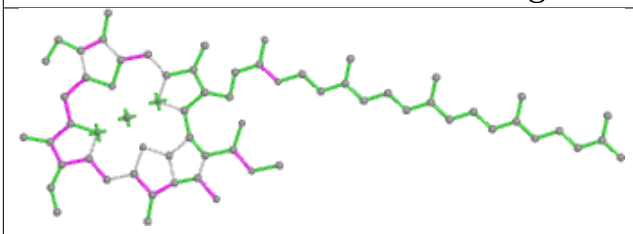


Torsions



Rings

Ligand CLA a 807



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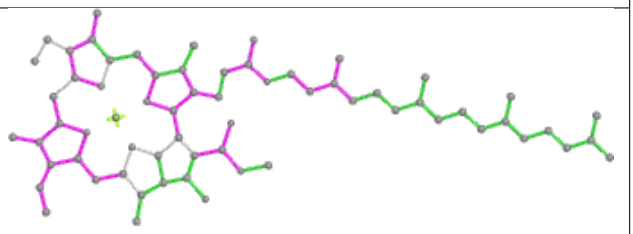
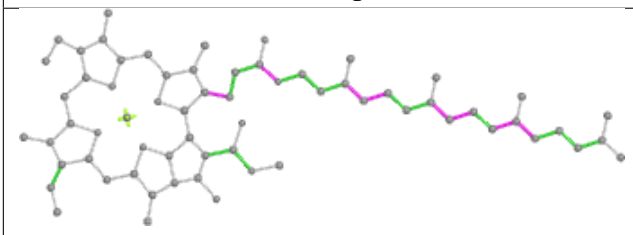
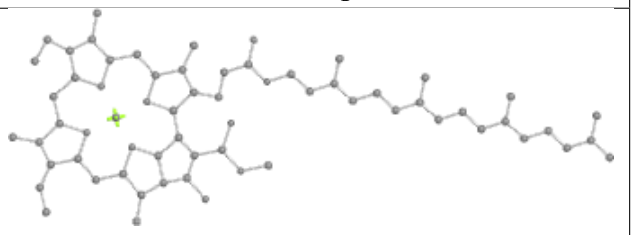


Bond angles

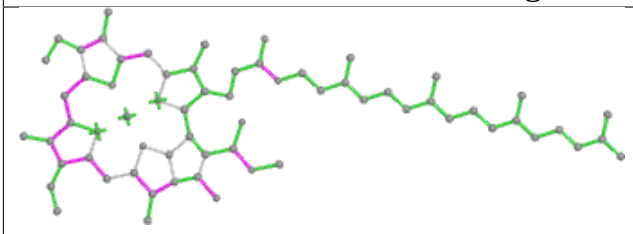


Torsions



Rings

Ligand CLA B 829



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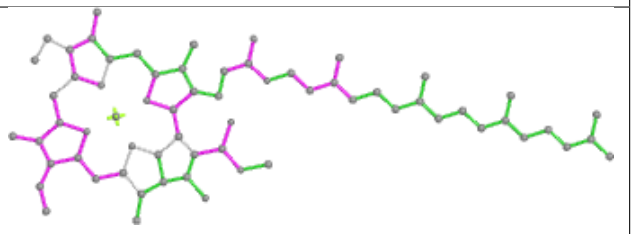
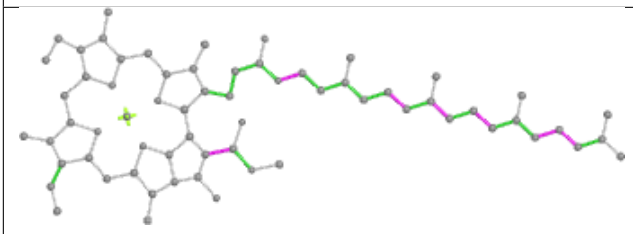
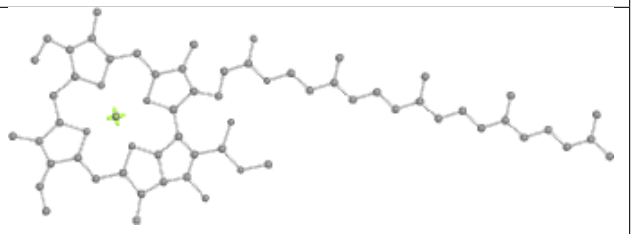


Bond angles

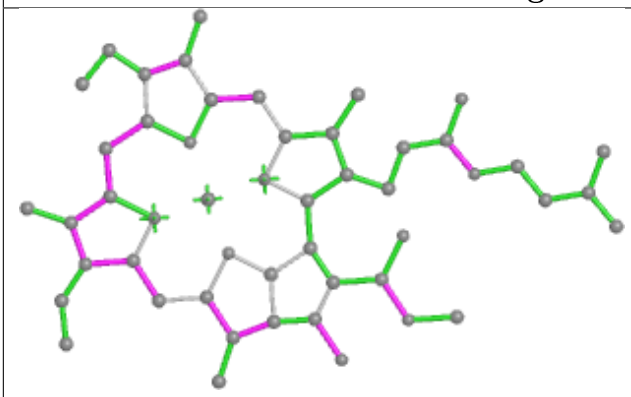


Torsions



Rings

Ligand CLA b 820



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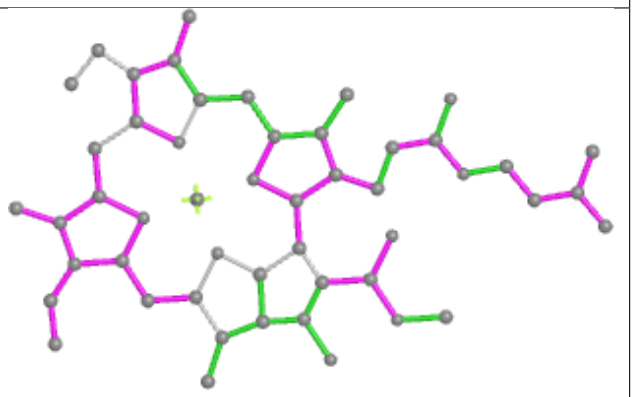
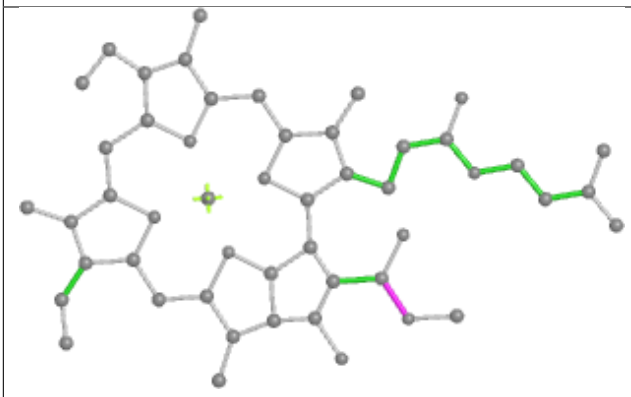


Bond angles



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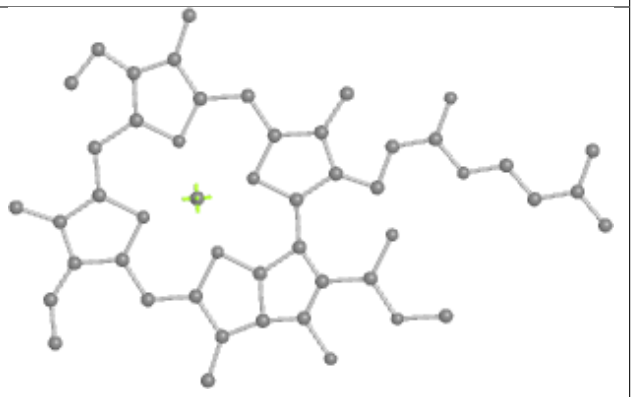
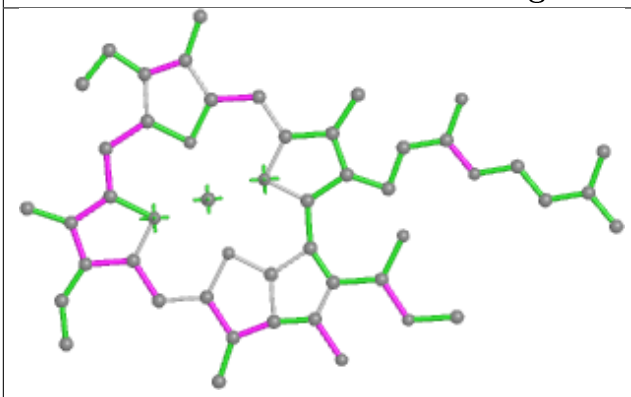


Rings

Ligand CLA 4 614



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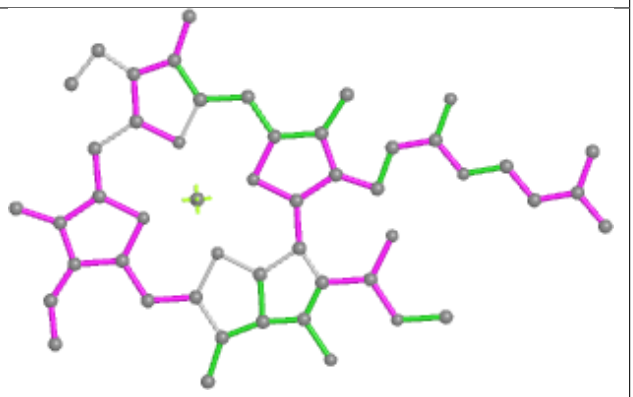
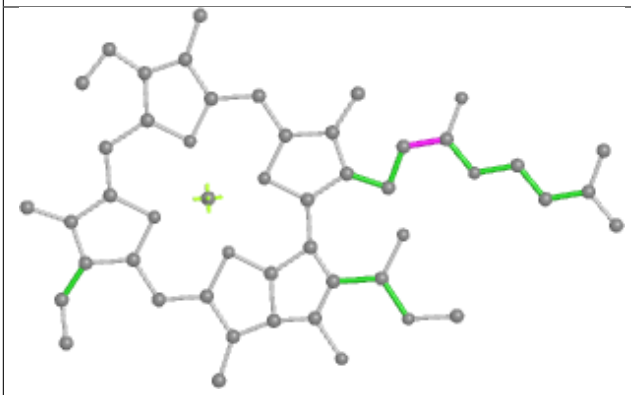
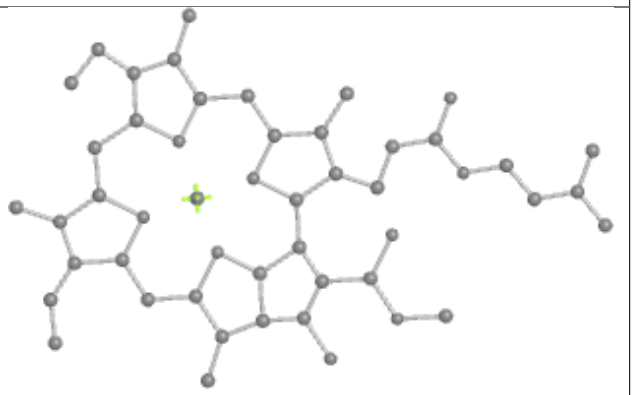


Bond angles

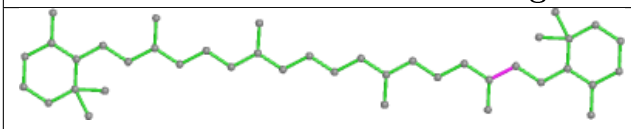


Torsions

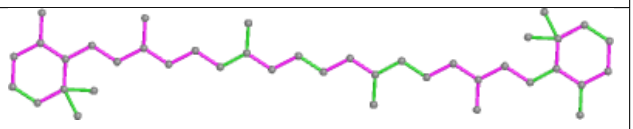


Rings

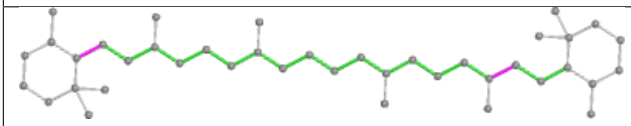
Ligand BCR I 101



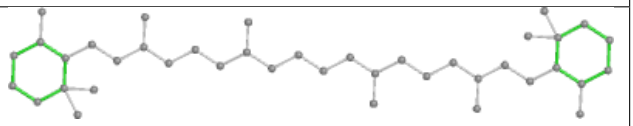
Bond lengths



Bond angles

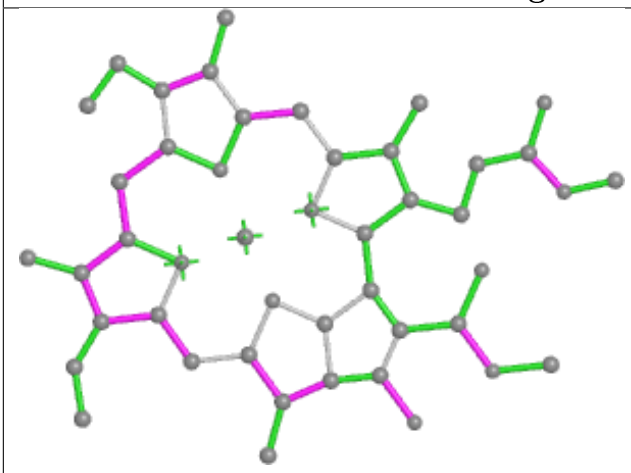


Torsions

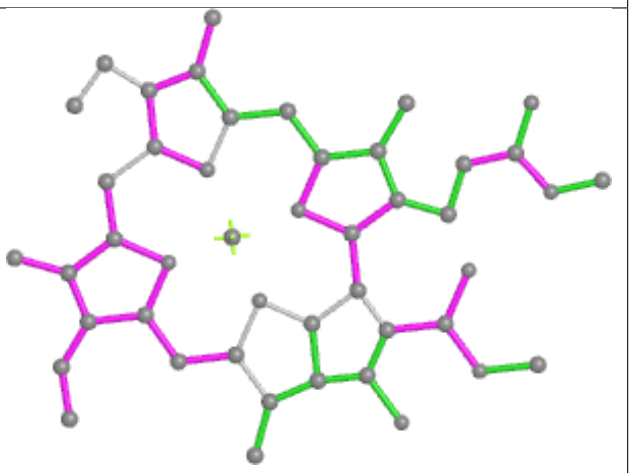


Rings

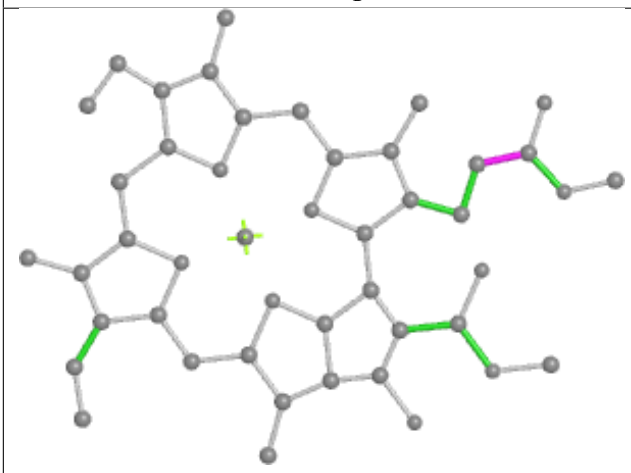
Ligand CLA 4 603



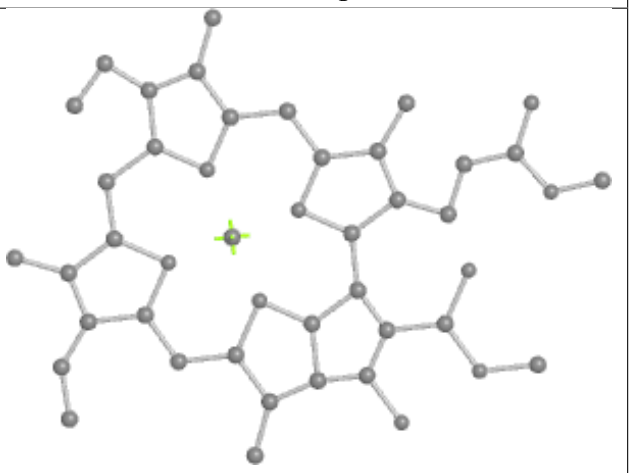
Bond lengths



Bond angles

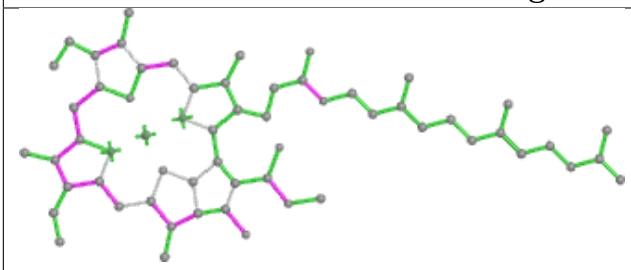


Torsions

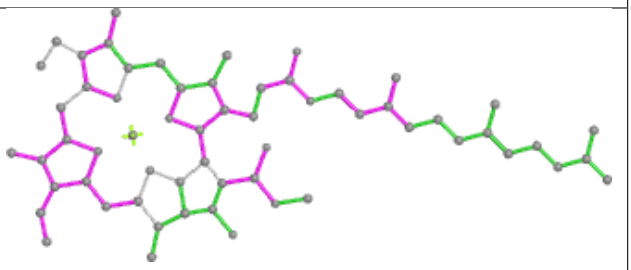


Rings

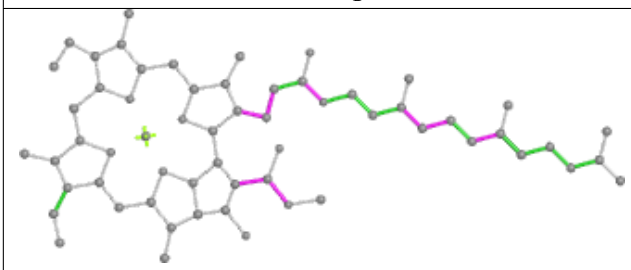
Ligand CLA 8 301



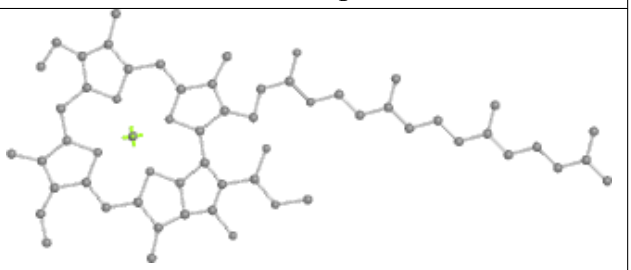
Bond lengths



Bond angles

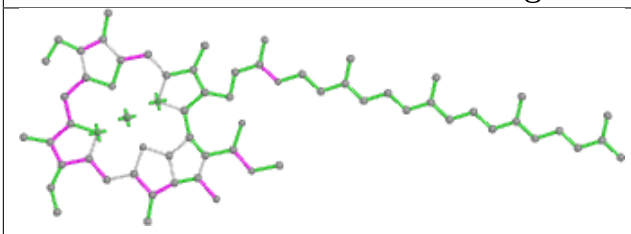


Torsions

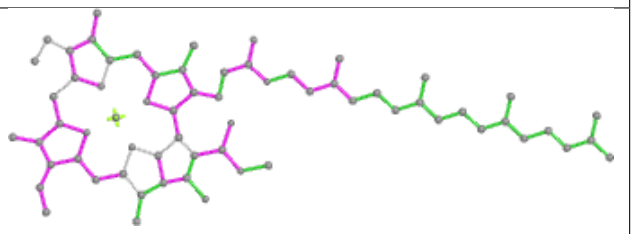


Rings

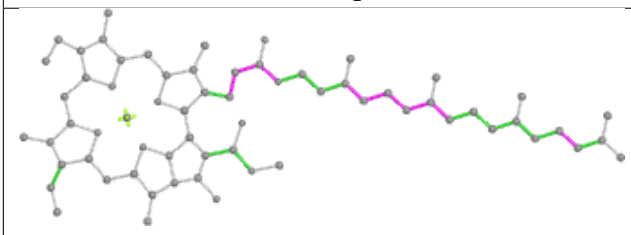
Ligand CLA B 807



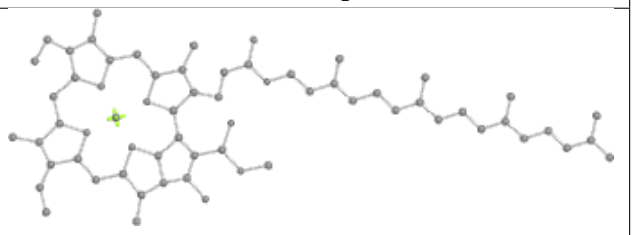
Bond lengths



Bond angles

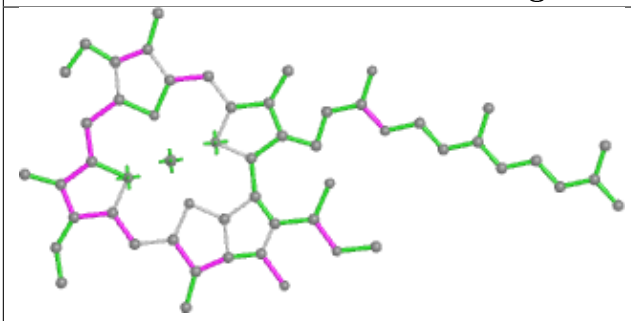


Torsions

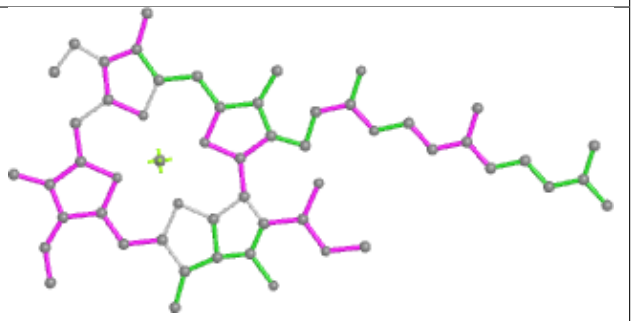


Rings

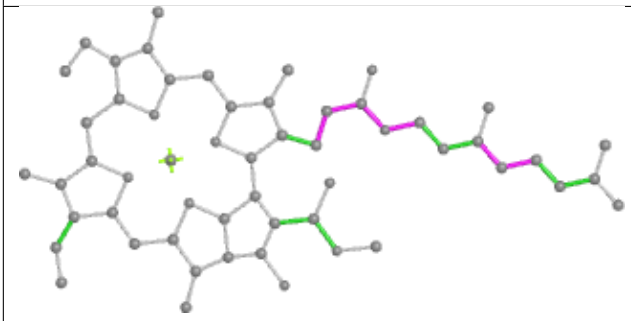
Ligand CLA 3 312



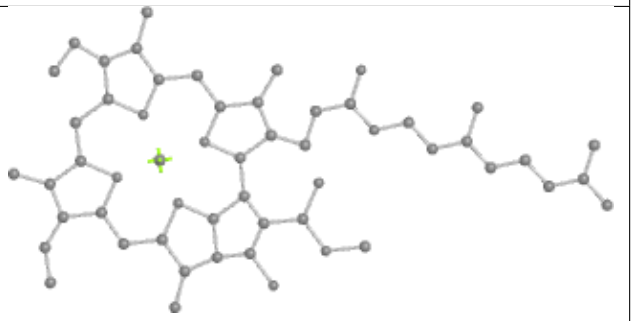
Bond lengths



Bond angles

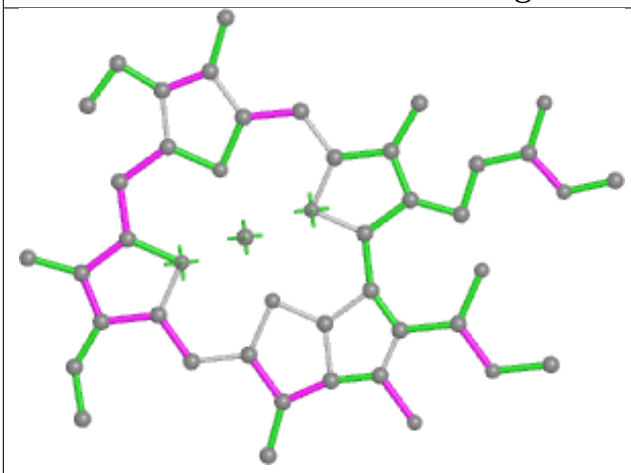


Torsions

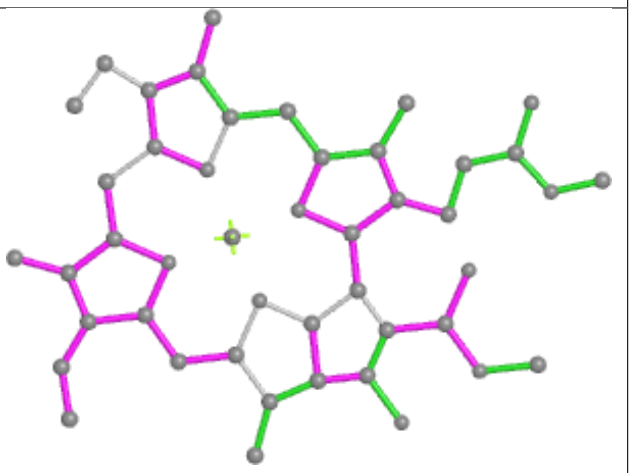


Rings

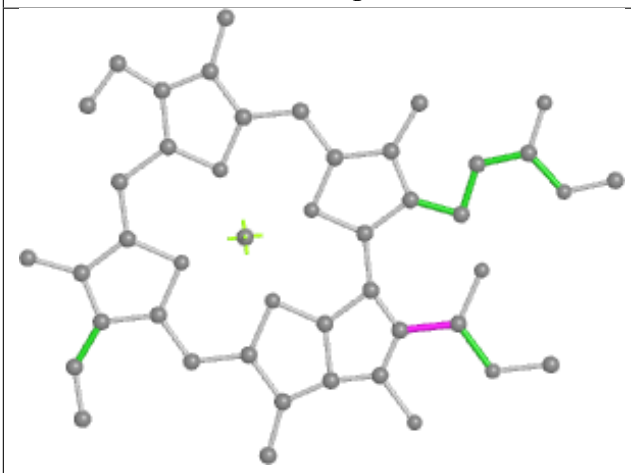
Ligand CLA K 4003



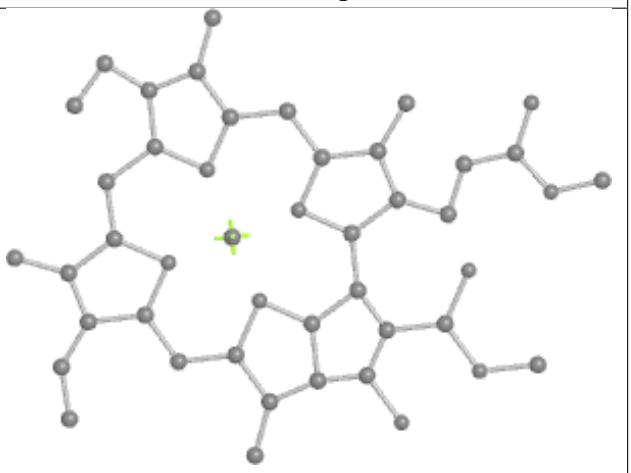
Bond lengths



Bond angles

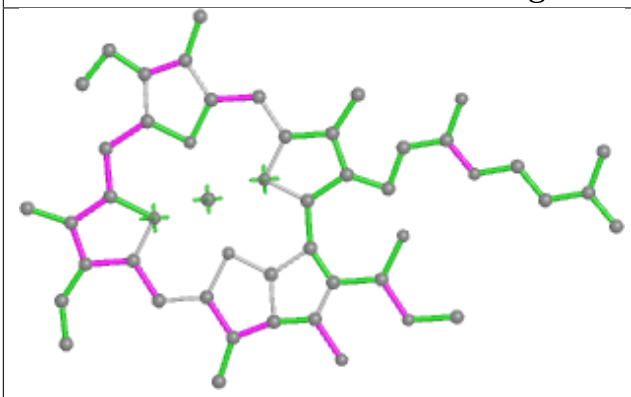


Torsions

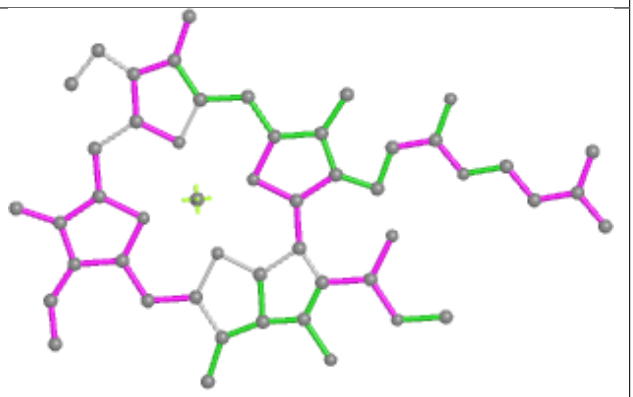


Rings

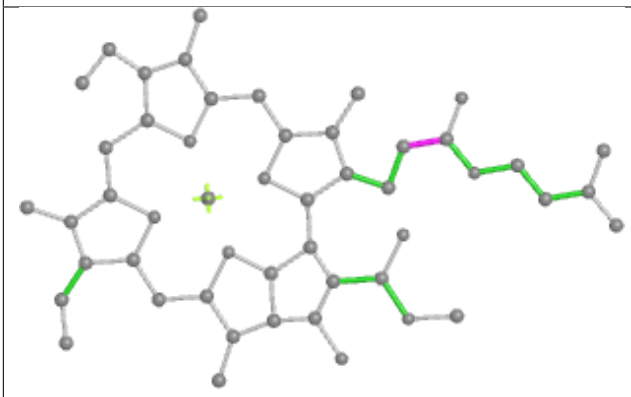
Ligand CLA 8 302



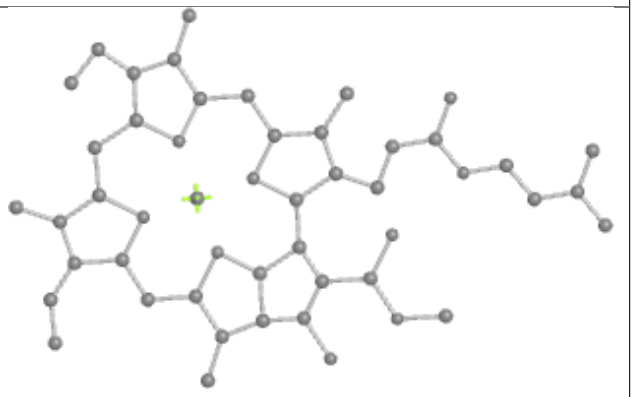
Bond lengths



Bond angles

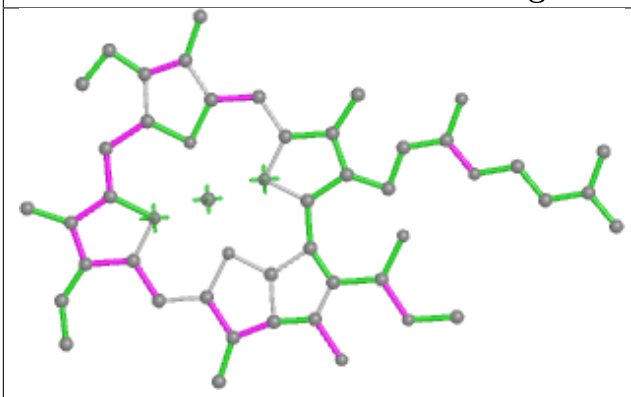


Torsions

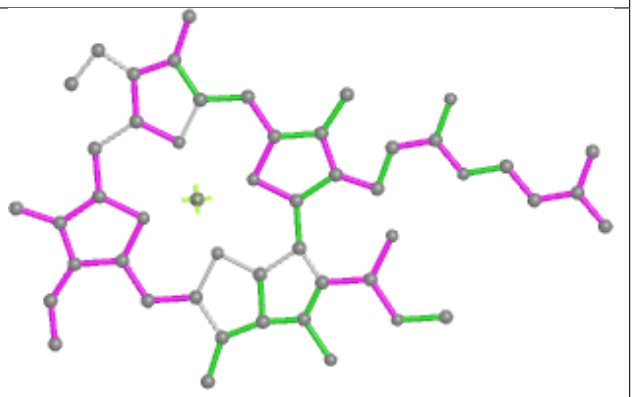


Rings

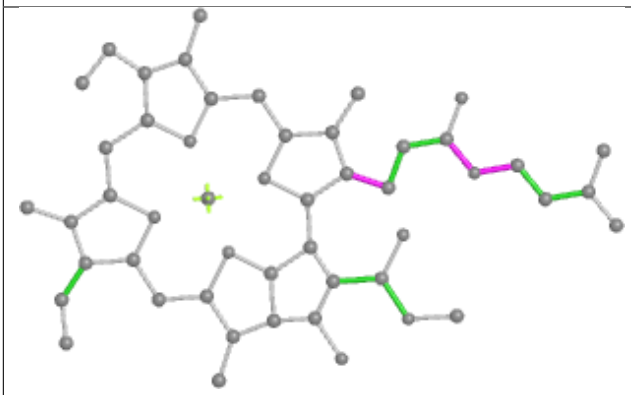
Ligand CLA 8 307



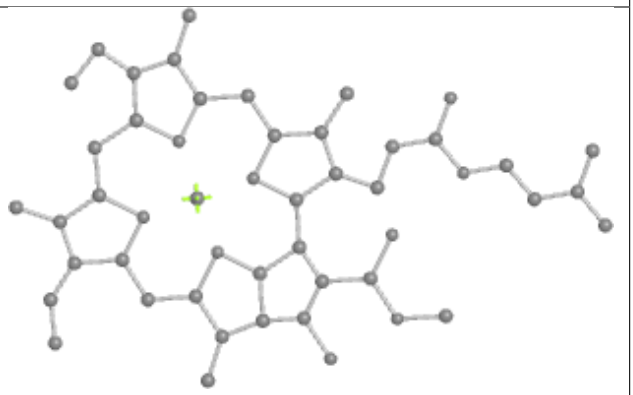
Bond lengths



Bond angles

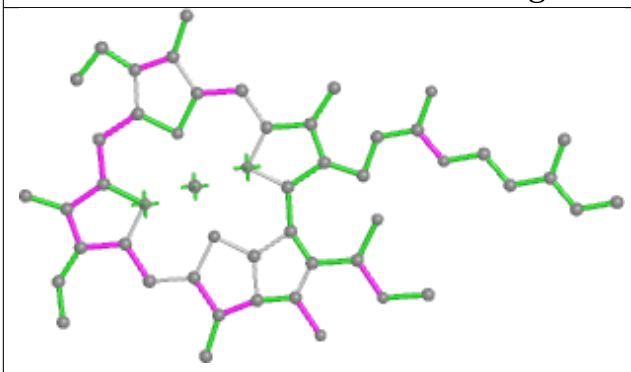


Torsions

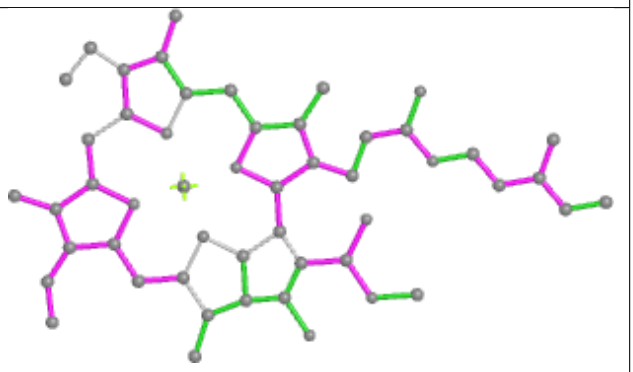


Rings

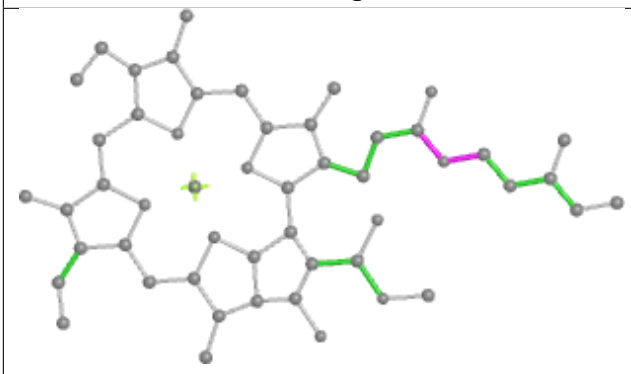
Ligand CLA 7 603



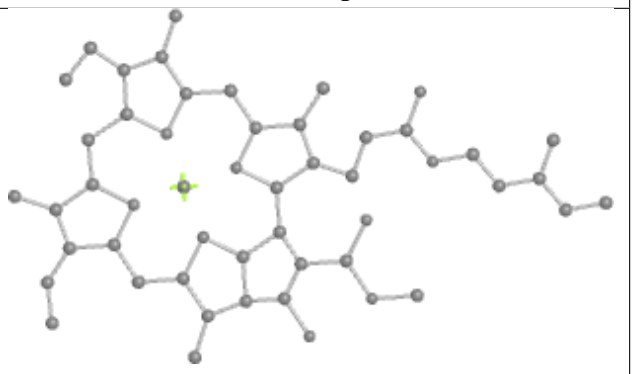
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

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, 95^{th} 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	A	742/742 (100%)	0.17	32 (4%) 35 25	42, 58, 91, 169	0
1	a	742/742 (100%)	0.10	31 (4%) 36 26	36, 48, 81, 140	0
2	B	733/733 (100%)	0.34	66 (9%) 9 5	42, 56, 80, 121	0
2	b	733/733 (100%)	0.24	49 (6%) 17 10	36, 55, 86, 139	0
3	C	80/80 (100%)	0.15	5 (6%) 20 12	50, 62, 77, 96	0
3	c	80/80 (100%)	-0.18	0 100 100	44, 55, 72, 88	0
4	D	141/141 (100%)	0.38	11 (7%) 13 7	53, 71, 103, 163	0
4	d	140/141 (99%)	0.29	5 (3%) 42 32	45, 61, 92, 132	0
5	E	63/64 (98%)	0.96	14 (22%) 0 0	51, 77, 115, 127	0
5	e	63/64 (98%)	-0.09	1 (1%) 72 66	51, 78, 96, 119	0
6	F	151/151 (100%)	0.25	12 (7%) 12 7	50, 69, 98, 126	0
6	f	151/151 (100%)	0.15	8 (5%) 26 17	49, 73, 101, 132	0
7	G	95/95 (100%)	0.26	4 (4%) 36 26	60, 79, 103, 127	0
7	g	95/95 (100%)	0.45	12 (12%) 3 2	62, 83, 123, 171	0
8	H	90/90 (100%)	0.41	10 (11%) 5 3	61, 83, 116, 127	0
8	h	90/90 (100%)	-0.07	3 (3%) 46 36	51, 70, 100, 111	0
9	I	29/30 (96%)	-0.22	1 (3%) 45 35	53, 65, 87, 117	0
9	i	30/30 (100%)	-0.20	1 (3%) 46 36	48, 56, 80, 129	0
10	J	39/39 (100%)	0.00	2 (5%) 28 19	51, 62, 97, 100	0
10	j	39/39 (100%)	0.27	3 (7%) 13 7	48, 65, 95, 100	0
11	K	45/84 (53%)	1.76	16 (35%) 0 0	92, 111, 131, 143	0
11	k	46/84 (54%)	0.87	5 (10%) 5 3	68, 86, 126, 134	0
12	L	153/153 (100%)	0.23	15 (9%) 7 4	56, 80, 120, 143	0
12	l	151/153 (98%)	-0.32	0 100 100	42, 60, 87, 119	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2		OWAB(Å^2)	Q<0.9
13	1	195/195 (100%)	0.57	34 (17%)	1	1	61, 87, 119, 136	0
13	6	195/195 (100%)	0.60	30 (15%)	2	1	74, 114, 164, 176	0
14	2	206/206 (100%)	1.23	57 (27%)	0	0	67, 97, 133, 188	0
14	7	206/206 (100%)	0.63	30 (14%)	2	1	61, 89, 122, 158	0
15	3	218/218 (100%)	0.81	38 (17%)	1	1	62, 96, 133, 155	0
15	8	217/218 (99%)	0.38	24 (11%)	5	3	56, 81, 112, 142	0
16	4	196/196 (100%)	0.83	41 (20%)	1	0	61, 85, 115, 160	0
16	9	196/196 (100%)	0.46	22 (11%)	5	3	65, 97, 134, 155	0
All	All	6350/6434 (98%)	0.34	582 (9%)	9	5	36, 68, 116, 188	0

The worst 5 of 582 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
15	3	259	ASN	8.7
9	i	2	ILE	8.2
5	E	2	GLY	7.1
15	8	121	LEU	7.1
14	2	121	ILE	6.7

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 monosaccharides 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
20	BCR	L	206	40/40	0.48	0.79	146,151,156,156	0
20	BCR	K	4004	40/40	0.49	0.62	94,115,138,138	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
20	BCR	K	4001	40/40	0.59	0.41	91,94,96,96	0
17	CLA	8	309	52/65	0.60	0.51	155,164,169,259	0
20	BCR	2	617	40/40	0.67	0.77	125,133,163,164	0
27	LUT	6	317	42/42	0.67	0.43	86,93,118,120	0
20	BCR	7	617	40/40	0.69	0.63	112,119,127,128	0
25	LMG	4	620	44/55	0.69	0.42	89,97,111,113	0
19	LHG	a	848	27/49	0.73	0.33	74,95,125,127	0
25	LMG	6	302	40/55	0.75	0.34	116,148,163,164	0
27	LUT	6	321	42/42	0.75	0.49	107,113,133,134	0
17	CLA	K	4002	45/65	0.76	0.46	115,123,125,154	0
20	BCR	l	206	40/40	0.77	0.52	77,82,93,93	0
20	BCR	1	318	40/40	0.77	0.50	94,105,126,127	0
19	LHG	3	319	20/49	0.79	0.50	152,157,193,194	0
25	LMG	4	619	44/55	0.80	0.35	82,92,103,104	0
24	DGD	B	850	66/66	0.80	0.33	52,71,93,102	0
23	LMT	B	849	35/35	0.80	0.33	80,97,102,103	0
17	CLA	3	301	46/65	0.80	0.78	142,149,154,175	0
20	BCR	A	856	40/40	0.81	0.25	65,71,85,85	0
17	CLA	3	310	37/65	0.82	0.63	179,186,191,221	0
17	CLA	6	316	46/65	0.82	0.30	152,162,171,203	0
20	BCR	6	319	40/40	0.82	0.47	104,124,138,140	0
19	LHG	A	847	27/49	0.83	0.26	68,88,113,113	0
20	BCR	b	844	40/40	0.83	0.32	52,67,91,93	0
25	LMG	G	102	44/55	0.83	0.21	72,95,110,113	0
17	CLA	8	313	25/65	0.83	0.28	102,110,116,146	0
17	CLA	K	4003	46/65	0.83	0.29	81,119,128,130	0
22	HTG	F	302	19/19	0.84	0.31	43,98,105,107	0
20	BCR	A	850	40/40	0.84	0.30	53,72,112,112	0
25	LMG	9	619	50/55	0.84	0.29	68,88,96,98	0
17	CLA	L	202	65/65	0.84	0.37	83,111,131,132	0
17	CLA	A	824	51/65	0.84	0.38	77,89,118,118	0
17	CLA	k	1403	46/65	0.85	0.21	89,95,103,110	0
22	HTG	J	3001	19/19	0.85	0.19	73,76,78,82	0
20	BCR	G	105	40/40	0.85	0.30	63,71,83,83	0
17	CLA	A	845	52/65	0.85	0.41	90,115,146,149	0
28	XAT	9	617	44/44	0.85	0.23	72,81,97,98	0
20	BCR	4	618	40/40	0.85	0.30	79,86,89,90	0
27	LUT	4	616	42/42	0.85	0.31	71,90,94,95	0
20	BCR	g	104	40/40	0.86	0.40	57,102,117,118	0
26	CHL	2	606	48/66	0.86	0.46	89,97,105,107	0
20	BCR	a	852	40/40	0.86	0.33	40,62,120,120	0
26	CHL	2	605	43/66	0.86	0.27	77,89,100,106	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
17	CLA	g	101	41/65	0.86	0.21	146,164,166,167	0
17	CLA	A	837	45/65	0.86	0.28	84,95,103,165	0
17	CLA	1	309	65/65	0.86	0.25	71,79,106,108	0
24	DGD	b	849	66/66	0.86	0.27	41,64,90,91	0
22	HTG	f	7001	19/19	0.86	0.33	49,104,107,108	0
28	XAT	3	317	44/44	0.87	0.26	61,74,100,101	0
17	CLA	7	604	60/65	0.87	0.34	92,101,106,109	0
20	BCR	a	849	40/40	0.87	0.25	56,63,75,76	0
20	BCR	k	1404	40/40	0.87	0.26	49,89,103,104	0
20	BCR	B	844	40/40	0.87	0.28	50,53,85,87	0
17	CLA	3	313	45/65	0.87	0.41	85,97,102,106	0
17	CLA	3	315	25/65	0.87	0.26	112,115,121,157	0
20	BCR	8	316	40/40	0.87	0.36	66,71,88,90	0
17	CLA	l	202	65/65	0.87	0.40	57,88,111,113	0
27	LUT	1	320	42/42	0.87	0.22	71,79,90,91	0
26	CHL	9	615	43/66	0.87	0.34	90,144,147,148	0
27	LUT	7	615	42/42	0.87	0.47	72,83,97,98	0
26	CHL	7	605	43/66	0.87	0.27	85,89,93,99	0
20	BCR	b	845	40/40	0.88	0.24	46,67,106,106	0
17	CLA	2	613	43/65	0.88	0.23	80,88,94,95	0
17	CLA	b	841	65/65	0.88	0.20	64,80,92,94	0
17	CLA	k	1401	45/65	0.88	0.34	75,83,94,96	0
17	CLA	b	824	65/65	0.88	0.28	45,51,69,72	0
17	CLA	2	604	60/65	0.88	0.35	100,111,118,119	0
17	CLA	2	609	60/65	0.88	0.23	73,87,98,101	0
20	BCR	j	3004	40/40	0.88	0.24	56,71,82,84	0
17	CLA	6	313	52/65	0.88	0.24	83,94,119,120	0
17	CLA	3	302	60/65	0.88	0.20	67,79,85,95	0
20	BCR	A	851	40/40	0.88	0.28	43,66,78,79	0
26	CHL	2	614	43/66	0.88	0.33	116,134,143,145	0
17	CLA	a	846	52/65	0.88	0.32	86,102,115,140	0
17	CLA	b	811	54/65	0.88	0.29	50,74,114,114	0
17	CLA	B	821	46/65	0.88	0.23	51,60,72,80	0
17	CLA	8	311	45/65	0.89	0.34	100,110,122,161	0
17	CLA	B	815	60/65	0.89	0.22	60,72,100,102	0
17	CLA	6	310	65/65	0.89	0.25	80,90,121,126	0
17	CLA	4	609	60/65	0.89	0.31	69,86,106,111	0
17	CLA	3	311	52/65	0.89	0.40	129,142,154,157	0
17	CLA	A	832	50/65	0.89	0.24	52,70,98,99	0
17	CLA	9	604	50/65	0.89	0.23	105,116,125,126	0
19	LHG	6	320	49/49	0.89	0.32	90,100,111,113	0
20	BCR	A	848	40/40	0.89	0.32	50,59,95,95	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
28	XAT	7	616	44/44	0.89	0.33	57,64,73,74	0
17	CLA	1	314	55/65	0.89	0.23	78,93,105,110	0
27	LUT	9	616	42/42	0.89	0.38	68,79,103,104	0
17	CLA	6	305	65/65	0.89	0.23	83,87,104,110	0
17	CLA	A	823	49/65	0.89	0.25	66,79,104,105	0
17	CLA	B	829	65/65	0.89	0.26	42,50,76,77	0
17	CLA	4	610	55/65	0.89	0.28	72,88,94,122	0
17	CLA	g	103	46/65	0.90	0.28	87,99,103,116	0
17	CLA	1	303	65/65	0.90	0.24	60,67,83,90	0
17	CLA	k	1402	46/65	0.90	0.26	62,78,100,106	0
17	CLA	2	610	41/65	0.90	0.21	80,94,108,110	0
17	CLA	1	310	60/65	0.90	0.25	63,80,90,92	0
17	CLA	A	805	55/65	0.90	0.23	45,54,89,89	0
20	BCR	B	847	40/40	0.90	0.31	44,49,52,53	0
17	CLA	B	834	65/65	0.90	0.21	46,58,90,90	0
17	CLA	A	834	65/65	0.90	0.24	49,60,71,75	0
17	CLA	B	811	54/65	0.90	0.21	58,74,103,104	0
20	BCR	B	845	40/40	0.90	0.18	47,63,102,102	0
20	BCR	9	618	40/40	0.90	0.30	86,92,100,101	0
17	CLA	3	304	45/65	0.90	0.21	109,122,133,162	0
26	CHL	7	606	48/66	0.90	0.29	71,87,104,105	0
17	CLA	4	604	50/65	0.90	0.30	75,84,111,114	0
17	CLA	A	812	65/65	0.90	0.21	49,63,74,82	0
19	LHG	7	618	37/49	0.90	0.25	83,95,102,104	0
27	LUT	2	615	42/42	0.90	0.27	77,84,89,89	0
17	CLA	2	612	65/65	0.90	0.32	70,93,113,118	0
17	CLA	9	611	52/65	0.90	0.37	76,89,102,103	0
19	LHG	1	319	49/49	0.90	0.27	77,84,109,109	0
17	CLA	b	830	50/65	0.90	0.21	46,59,70,74	0
26	CHL	4	606	51/66	0.90	0.22	71,81,109,110	0
17	CLA	6	309	46/65	0.90	0.30	92,99,106,137	0
17	CLA	F	304	55/65	0.90	0.21	52,69,95,95	0
28	XAT	8	315	44/44	0.90	0.23	64,69,80,83	0
17	CLA	b	814	65/65	0.90	0.19	47,55,69,71	0
17	CLA	j	3002	42/65	0.91	0.15	91,94,96,97	0
17	CLA	a	836	50/65	0.91	0.17	42,54,73,74	0
17	CLA	2	608	50/65	0.91	0.18	65,69,108,111	0
26	CHL	1	307	48/66	0.91	0.19	75,95,109,110	0
20	BCR	B	846	40/40	0.91	0.23	49,53,70,70	0
17	CLA	6	311	60/65	0.91	0.46	81,99,115,116	0
17	CLA	L	203	65/65	0.91	0.23	64,74,87,89	0
17	CLA	B	824	65/65	0.91	0.27	48,53,70,74	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
17	CLA	7	602	65/65	0.91	0.20	62,70,88,93	0
17	CLA	9	612	56/65	0.91	0.24	68,77,89,92	0
17	CLA	a	824	51/65	0.91	0.23	61,74,91,93	0
17	CLA	4	613	45/65	0.91	0.25	92,103,108,160	0
17	CLA	6	307	42/65	0.91	0.27	112,126,137,139	0
20	BCR	I	101	40/40	0.91	0.23	54,60,65,65	0
17	CLA	9	613	45/65	0.91	0.20	87,105,115,137	0
17	CLA	A	806	65/65	0.91	0.29	46,51,59,59	0
17	CLA	b	812	55/65	0.91	0.22	59,70,103,104	0
17	CLA	b	807	65/65	0.91	0.22	42,51,102,104	0
17	CLA	a	804	65/65	0.91	0.21	36,52,71,73	0
17	CLA	G	103	50/65	0.91	0.23	61,80,91,93	0
17	CLA	7	611	52/65	0.91	0.33	87,104,123,126	0
17	CLA	9	609	60/65	0.91	0.37	72,93,107,108	0
17	CLA	4	612	56/65	0.91	0.19	63,78,87,88	0
17	CLA	B	817	59/65	0.91	0.22	46,53,59,64	0
17	CLA	7	608	50/65	0.91	0.20	60,65,93,96	0
17	CLA	3	309	50/65	0.91	0.23	76,95,104,107	0
17	CLA	1	305	52/65	0.91	0.23	76,101,105,108	0
17	CLA	8	308	50/65	0.91	0.33	75,81,87,88	0
20	BCR	b	847	40/40	0.91	0.24	40,49,69,70	0
20	BCR	B	843	40/40	0.91	0.23	54,64,72,72	0
17	CLA	B	814	65/65	0.91	0.20	50,57,80,82	0
26	CHL	4	605	56/66	0.91	0.26	69,88,96,102	0
17	CLA	B	818	60/65	0.91	0.26	45,50,57,61	0
17	CLA	B	813	65/65	0.91	0.23	47,51,54,55	0
17	CLA	J	3002	42/65	0.91	0.18	92,105,119,148	0
17	CLA	b	831	49/65	0.91	0.23	51,55,71,71	0
17	CLA	b	820	50/65	0.91	0.21	65,72,77,82	0
17	CLA	4	611	52/65	0.91	0.28	71,88,123,125	0
17	CLA	A	836	50/65	0.92	0.17	60,73,80,86	0
17	CLA	a	823	49/65	0.92	0.17	60,67,102,104	0
17	CLA	b	823	60/65	0.92	0.23	50,60,92,94	0
17	CLA	3	314	46/65	0.92	0.18	73,78,101,103	0
27	LUT	3	316	42/42	0.92	0.25	74,78,97,99	0
26	CHL	6	308	47/66	0.92	0.23	103,135,146,149	0
26	CHL	2	601	61/66	0.92	0.32	68,99,113,115	0
17	CLA	b	815	55/65	0.92	0.28	62,78,93,94	0
17	CLA	b	825	65/65	0.92	0.32	38,55,82,83	0
17	CLA	b	817	59/65	0.92	0.24	56,59,67,68	0
17	CLA	B	836	60/65	0.92	0.22	43,46,97,97	0
20	BCR	L	205	40/40	0.92	0.21	51,61,70,71	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
17	CLA	f	7003	55/65	0.92	0.24	68,87,121,122	0
20	BCR	b	846	40/40	0.92	0.22	48,56,76,77	0
22	HTG	j	3001	19/19	0.92	0.37	61,71,80,84	0
17	CLA	4	601	46/65	0.92	0.20	84,92,95,111	0
17	CLA	4	602	60/65	0.92	0.19	54,67,73,74	0
28	XAT	2	616	44/44	0.92	0.25	69,79,86,87	0
17	CLA	B	823	60/65	0.92	0.20	46,57,84,84	0
17	CLA	a	840	65/65	0.92	0.32	36,41,87,89	0
17	CLA	1	308	65/65	0.92	0.37	57,92,120,121	0
26	CHL	9	607	51/66	0.92	0.27	67,77,98,99	0
27	LUT	8	314	42/42	0.92	0.39	57,73,82,84	0
17	CLA	B	802	65/65	0.92	0.30	40,44,50,52	0
17	CLA	B	827	65/65	0.92	0.40	49,61,78,80	0
17	CLA	L	204	50/65	0.92	0.19	76,84,109,109	0
17	CLA	A	804	65/65	0.92	0.23	46,58,70,71	0
17	CLA	B	825	65/65	0.92	0.35	42,50,83,88	0
17	CLA	a	817	45/65	0.92	0.19	64,73,78,79	0
17	CLA	A	839	65/65	0.92	0.19	54,60,80,83	0
17	CLA	A	808	65/65	0.92	0.18	52,61,113,115	0
17	CLA	A	817	45/65	0.92	0.22	66,75,86,92	0
17	CLA	A	814	65/65	0.92	0.31	50,59,67,68	0
26	CHL	9	606	51/66	0.92	0.19	86,106,118,119	0
28	XAT	6	318	44/44	0.92	0.24	71,81,94,95	0
17	CLA	8	310	55/65	0.92	0.33	74,88,99,104	0
17	CLA	B	810	65/65	0.92	0.22	59,77,84,86	0
20	BCR	j	3003	40/40	0.92	0.22	42,52,59,61	0
17	CLA	8	303	45/65	0.92	0.26	75,92,99,133	0
17	CLA	A	827	65/65	0.92	0.27	40,60,97,98	0
20	BCR	J	3003	40/40	0.92	0.21	45,54,67,68	0
26	CHL	9	605	56/66	0.92	0.18	80,94,97,126	0
20	BCR	b	801	40/40	0.92	0.20	36,43,52,55	0
17	CLA	A	835	65/65	0.92	0.23	58,67,75,81	0
17	CLA	A	818	65/65	0.92	0.22	58,71,95,97	0
17	CLA	6	312	41/65	0.92	0.20	90,102,109,129	0
17	CLA	1	306	52/65	0.92	0.17	90,99,109,111	0
26	CHL	7	614	43/66	0.92	0.29	105,120,127,139	0
20	BCR	3	318	40/40	0.92	0.23	77,83,105,108	0
17	CLA	1	313	65/65	0.92	0.21	81,88,108,112	0
27	LUT	1	316	42/42	0.92	0.19	69,74,100,101	0
26	CHL	4	615	43/66	0.92	0.19	61,74,87,89	0
17	CLA	g	102	50/65	0.92	0.33	92,107,123,124	0
17	CLA	B	835	45/65	0.92	0.17	57,66,70,72	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
17	CLA	6	306	51/65	0.92	0.24	118,123,130,131	0
28	XAT	4	617	44/44	0.93	0.19	63,72,87,88	0
17	CLA	B	822	55/65	0.93	0.22	48,58,82,83	0
17	CLA	b	816	55/65	0.93	0.19	57,65,72,75	0
17	CLA	6	315	55/65	0.93	0.28	105,114,131,131	0
20	BCR	f	7004	40/40	0.93	0.20	55,62,66,66	0
20	BCR	i	101	40/40	0.93	0.18	36,45,49,50	0
17	CLA	a	839	65/65	0.93	0.24	36,43,65,69	0
17	CLA	a	812	65/65	0.93	0.23	47,59,70,77	0
17	CLA	G	101	45/65	0.93	0.21	74,79,85,89	0
17	CLA	b	822	55/65	0.93	0.16	46,60,80,83	0
17	CLA	B	839	65/65	0.93	0.25	53,60,69,72	0
17	CLA	1	315	46/65	0.93	0.15	76,87,93,132	0
17	CLA	b	835	45/65	0.93	0.16	86,92,94,96	0
17	CLA	3	305	42/65	0.93	0.20	67,78,84,90	0
17	CLA	G	104	46/65	0.93	0.31	70,93,100,111	0
19	LHG	6	301	23/49	0.93	0.15	67,101,110,111	0
20	BCR	A	849	40/40	0.93	0.44	54,62,83,84	0
17	CLA	A	821	45/65	0.93	0.21	69,74,88,109	0
17	CLA	A	810	65/65	0.93	0.19	43,51,85,89	0
17	CLA	7	613	43/65	0.93	0.23	73,78,82,86	0
17	CLA	2	602	65/65	0.93	0.21	66,73,80,83	0
17	CLA	l	203	65/65	0.93	0.20	40,51,71,73	0
17	CLA	1	312	52/65	0.93	0.20	70,76,99,100	0
17	CLA	A	826	65/65	0.93	0.23	47,57,65,66	0
17	CLA	a	837	45/65	0.93	0.17	57,65,74,77	0
17	CLA	A	825	55/65	0.93	0.16	58,67,74,78	0
17	CLA	A	833	65/65	0.93	0.22	54,61,101,102	0
17	CLA	b	834	65/65	0.93	0.22	61,74,105,106	0
28	XAT	1	317	44/44	0.93	0.21	63,68,93,96	0
17	CLA	a	813	54/65	0.93	0.19	43,51,60,70	0
17	CLA	l	204	50/65	0.93	0.18	46,59,100,104	0
17	CLA	a	811	65/65	0.93	0.20	42,59,94,96	0
20	BCR	a	853	40/40	0.93	0.26	44,48,66,67	0
26	CHL	4	607	51/66	0.93	0.20	57,73,82,85	0
26	CHL	2	607	51/66	0.93	0.21	66,75,117,118	0
17	CLA	9	601	46/65	0.93	0.18	81,91,95,110	0
17	CLA	8	304	42/65	0.93	0.18	59,72,78,80	0
17	CLA	b	829	65/65	0.93	0.23	39,54,67,69	0
17	CLA	a	819	65/65	0.93	0.22	38,54,96,99	0
17	CLA	b	833	58/65	0.93	0.20	48,63,77,78	0
17	CLA	B	805	65/65	0.93	0.25	45,47,53,60	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
17	CLA	A	831	65/65	0.93	0.21	43,52,59,61	0
26	CHL	7	601	61/66	0.93	0.20	62,74,93,95	0
17	CLA	6	314	60/65	0.93	0.23	66,109,124,125	0
17	CLA	B	840	65/65	0.93	0.33	41,50,72,78	0
17	CLA	a	816	50/65	0.93	0.23	43,52,94,96	0
22	HTG	a	857	19/19	0.93	0.24	53,70,79,81	0
20	BCR	l	201	40/40	0.93	0.21	38,46,54,54	0
20	BCR	l	205	40/40	0.93	0.24	39,46,52,54	0
17	CLA	A	813	54/65	0.93	0.21	60,68,77,95	0
17	CLA	7	609	60/65	0.93	0.27	64,86,97,97	0
26	CHL	6	303	61/66	0.93	0.20	78,91,102,103	0
20	BCR	b	843	40/40	0.93	0.20	54,60,68,69	0
17	CLA	b	821	46/65	0.93	0.18	58,69,90,118	0
17	CLA	B	833	58/65	0.93	0.18	43,52,79,80	0
17	CLA	b	832	65/65	0.93	0.22	36,55,70,79	0
17	CLA	B	816	55/65	0.93	0.20	60,67,73,91	0
17	CLA	B	807	65/65	0.93	0.21	51,66,113,117	0
17	CLA	3	312	55/65	0.93	0.15	86,107,114,117	0
17	CLA	B	809	65/65	0.93	0.23	41,50,81,82	0
17	CLA	b	813	65/65	0.94	0.23	44,57,67,69	0
19	LHG	A	846	49/49	0.94	0.21	44,49,58,59	0
17	CLA	a	826	65/65	0.94	0.22	39,43,48,56	0
17	CLA	4	608	50/65	0.94	0.17	56,66,76,86	0
17	CLA	3	306	47/65	0.94	0.18	67,79,90,91	0
17	CLA	9	602	60/65	0.94	0.18	60,67,74,86	0
17	CLA	a	815	45/65	0.94	0.19	41,54,63,63	0
17	CLA	A	809	65/65	0.94	0.19	44,51,63,65	0
17	CLA	a	833	65/65	0.94	0.25	39,46,98,102	0
17	CLA	A	843	65/65	0.94	0.26	48,64,79,81	0
17	CLA	b	819	65/65	0.94	0.24	50,57,92,95	0
26	CHL	8	306	47/66	0.94	0.21	60,64,79,84	0
20	BCR	b	848	40/40	0.94	0.20	37,42,45,47	0
17	CLA	b	809	65/65	0.94	0.20	39,50,72,75	0
17	CLA	A	830	65/65	0.94	0.28	45,53,58,61	0
17	CLA	2	611	52/65	0.94	0.17	68,83,119,128	0
17	CLA	A	801	65/65	0.94	0.27	40,44,49,53	0
17	CLA	7	612	65/65	0.94	0.24	56,66,87,89	0
18	PQN	B	842	33/33	0.94	0.44	46,56,63,63	0
17	CLA	9	608	50/65	0.94	0.18	72,78,103,105	0
17	CLA	A	820	65/65	0.94	0.22	46,50,57,58	0
17	CLA	a	805	55/65	0.94	0.18	38,43,76,78	0
17	CLA	b	805	65/65	0.94	0.21	42,45,52,58	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
26	CHL	7	607	51/66	0.94	0.20	64,70,92,98	0
17	CLA	A	829	65/65	0.94	0.23	42,46,55,58	0
17	CLA	B	841	65/65	0.94	0.19	49,56,63,68	0
17	CLA	F	301	65/65	0.94	0.19	48,55,83,87	0
17	CLA	3	308	50/65	0.94	0.20	76,86,93,104	0
20	BCR	L	201	40/40	0.94	0.18	51,59,72,73	0
26	CHL	1	302	61/66	0.94	0.21	64,74,101,105	0
17	CLA	a	842	65/65	0.94	0.21	47,59,96,98	0
17	CLA	a	832	50/65	0.94	0.20	41,54,78,83	0
17	CLA	6	304	65/65	0.94	0.20	66,79,104,106	0
19	LHG	2	618	37/49	0.94	0.30	80,91,127,130	0
17	CLA	a	834	65/65	0.94	0.24	37,44,48,50	0
17	CLA	B	804	45/65	0.94	0.18	44,50,68,77	0
17	CLA	a	814	65/65	0.94	0.24	39,47,64,67	0
17	CLA	1	304	65/65	0.94	0.21	63,70,95,97	0
17	CLA	B	806	65/65	0.94	0.27	43,52,60,64	0
17	CLA	b	840	65/65	0.94	0.23	36,41,59,67	0
17	CLA	B	803	65/65	0.94	0.33	39,50,61,68	0
17	CLA	A	811	65/65	0.94	0.26	54,69,89,90	0
17	CLA	b	836	60/65	0.94	0.24	43,53,106,107	0
17	CLA	a	856	65/65	0.94	0.26	36,41,56,59	0
17	CLA	a	821	45/65	0.94	0.19	51,62,70,87	0
20	BCR	B	848	40/40	0.94	0.33	40,45,51,52	0
17	CLA	B	830	50/65	0.94	0.17	45,56,75,75	0
17	CLA	4	614	50/65	0.94	0.20	60,68,90,91	0
17	CLA	B	837	65/65	0.94	0.23	49,55,61,65	0
17	CLA	9	614	47/65	0.94	0.22	62,75,97,99	0
17	CLA	2	603	65/65	0.94	0.16	64,72,106,108	0
17	CLA	A	828	65/65	0.94	0.22	49,61,79,84	0
17	CLA	b	827	65/65	0.95	0.28	40,53,83,83	0
17	CLA	B	808	65/65	0.95	0.25	41,45,70,73	0
17	CLA	1	311	41/65	0.95	0.17	67,74,81,82	0
17	CLA	b	837	65/65	0.95	0.21	46,57,69,70	0
17	CLA	a	829	65/65	0.95	0.23	35,41,56,58	0
17	CLA	A	840	65/65	0.95	0.23	48,55,95,96	0
17	CLA	a	802	65/65	0.95	0.27	35,42,56,62	0
17	CLA	9	603	46/65	0.95	0.17	62,64,77,78	0
17	CLA	a	808	65/65	0.95	0.20	54,63,86,87	0
17	CLA	b	838	47/65	0.95	0.22	38,44,54,64	0
17	CLA	a	822	65/65	0.95	0.17	42,46,53,57	0
17	CLA	b	806	65/65	0.95	0.26	39,43,52,65	0
17	CLA	a	838	51/65	0.95	0.19	36,40,63,68	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
17	CLA	b	818	60/65	0.95	0.28	44,47,53,56	0
17	CLA	b	808	65/65	0.95	0.18	39,47,53,59	0
17	CLA	a	806	65/65	0.95	0.21	37,39,49,51	0
17	CLA	A	822	65/65	0.95	0.20	49,67,76,79	0
26	CHL	3	307	47/66	0.95	0.17	72,77,94,97	0
17	CLA	8	305	47/65	0.95	0.15	61,71,78,79	0
17	CLA	3	303	50/65	0.95	0.21	60,67,75,76	0
17	CLA	b	802	65/65	0.95	0.24	36,41,45,52	0
17	CLA	B	812	55/65	0.95	0.21	53,62,106,107	0
20	BCR	B	801	40/40	0.95	0.21	43,46,54,55	0
17	CLA	7	610	41/65	0.95	0.19	74,82,94,99	0
17	CLA	9	610	41/65	0.95	0.26	99,103,113,114	0
17	CLA	a	810	65/65	0.95	0.19	44,59,94,95	0
17	CLA	A	816	50/65	0.95	0.20	52,70,108,108	0
19	LHG	1	301	23/49	0.95	0.20	63,84,93,94	0
17	CLA	A	838	51/65	0.95	0.17	45,60,67,68	0
20	BCR	a	851	40/40	0.95	0.32	37,53,66,67	0
17	CLA	a	809	65/65	0.95	0.20	36,39,53,57	0
17	CLA	A	819	65/65	0.95	0.21	54,65,117,120	0
17	CLA	B	828	65/65	0.95	0.29	43,48,58,61	0
17	CLA	b	810	65/65	0.95	0.17	39,49,59,62	0
20	BCR	F	305	40/40	0.95	0.20	46,51,58,60	0
17	CLA	F	303	45/65	0.95	0.20	51,60,71,76	0
17	CLA	8	312	46/65	0.95	0.15	57,66,99,103	0
17	CLA	a	841	65/65	0.95	0.21	55,62,65,67	0
17	CLA	A	815	45/65	0.95	0.19	54,59,65,70	0
17	CLA	a	827	65/65	0.95	0.27	35,41,82,85	0
17	CLA	a	843	65/65	0.95	0.24	35,39,60,65	0
17	CLA	a	818	65/65	0.95	0.21	45,53,81,83	0
17	CLA	a	828	65/65	0.95	0.22	37,44,67,72	0
17	CLA	B	826	65/65	0.95	0.28	44,50,56,64	0
17	CLA	A	803	65/65	0.95	0.27	39,44,54,59	0
17	CLA	B	838	47/65	0.95	0.30	43,48,65,68	0
17	CLA	a	807	65/65	0.95	0.22	35,41,50,54	0
17	CLA	A	854	65/65	0.95	0.31	40,44,57,59	0
17	CLA	B	832	65/65	0.95	0.23	43,48,73,76	0
17	CLA	b	826	65/65	0.95	0.27	48,55,59,62	0
17	CLA	A	842	65/65	0.95	0.23	42,45,56,65	0
17	CLA	4	603	46/65	0.95	0.19	54,62,69,72	0
17	CLA	A	841	65/65	0.95	0.19	44,50,55,60	0
17	CLA	B	820	50/65	0.95	0.20	53,69,95,100	0
17	CLA	A	802	65/65	0.95	0.29	41,45,51,53	0

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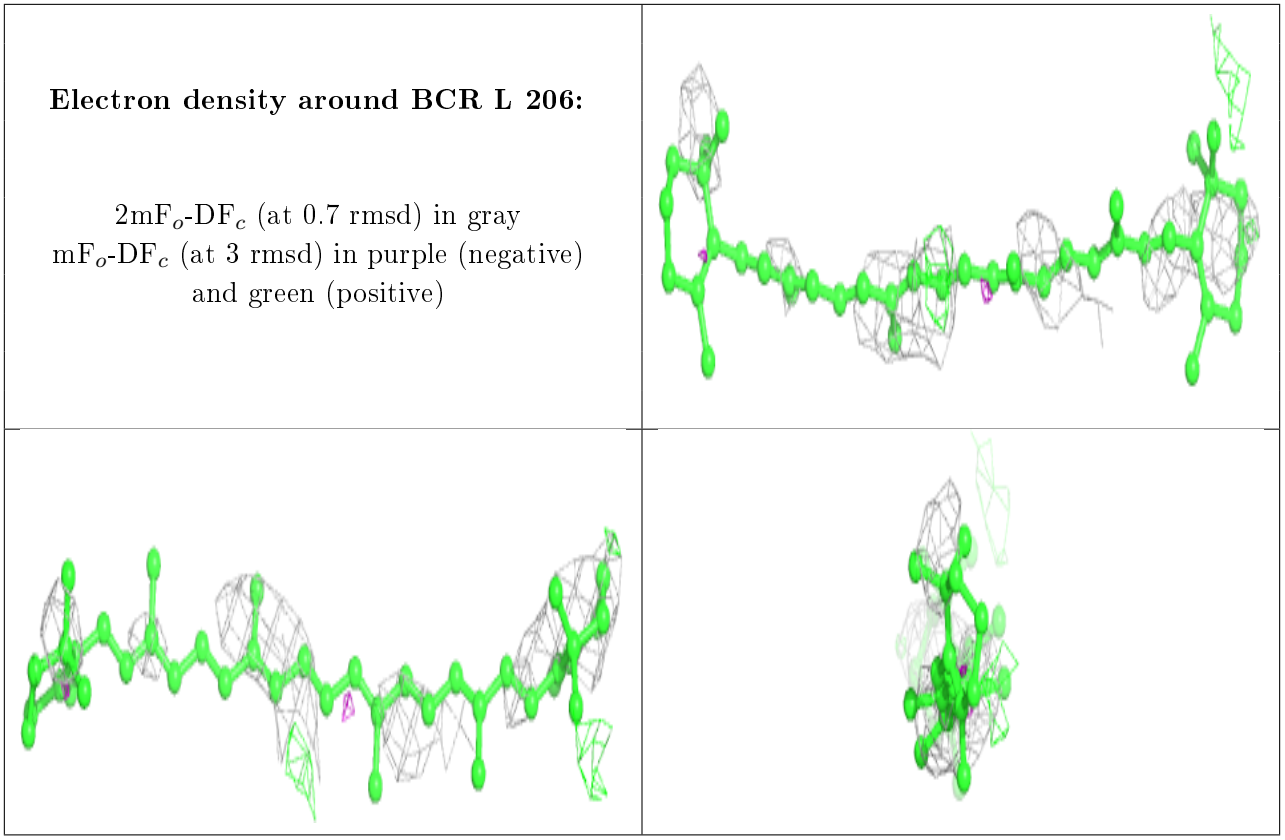
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
17	CLA	8	302	50/65	0.95	0.16	46,54,73,74	0
17	CLA	7	603	51/65	0.95	0.19	52,60,97,98	0
20	BCR	A	852	40/40	0.96	0.23	42,44,49,50	0
18	PQN	a	845	33/33	0.96	0.22	35,48,54,58	0
17	CLA	b	828	65/65	0.96	0.29	41,47,56,56	0
17	CLA	b	804	45/65	0.96	0.14	42,52,68,75	0
17	CLA	a	831	65/65	0.96	0.19	36,43,54,56	0
17	CLA	a	835	65/65	0.96	0.19	36,43,48,49	0
17	CLA	b	839	65/65	0.96	0.18	38,44,50,53	0
17	CLA	a	825	55/65	0.96	0.18	39,44,58,68	0
17	CLA	A	807	65/65	0.96	0.27	44,47,58,69	0
18	PQN	b	842	33/33	0.96	0.22	36,41,49,50	0
17	CLA	f	7002	45/65	0.96	0.16	54,59,76,77	0
17	CLA	a	803	65/65	0.96	0.23	35,38,50,53	0
18	PQN	A	844	33/33	0.96	0.24	42,45,57,58	0
17	CLA	B	819	65/65	0.96	0.23	46,53,80,83	0
17	CLA	a	844	65/65	0.96	0.23	38,49,59,64	0
17	CLA	8	301	60/65	0.96	0.17	56,64,68,72	0
17	CLA	B	831	49/65	0.96	0.18	45,53,62,65	0
19	LHG	a	847	49/49	0.96	0.21	35,41,47,48	0
17	CLA	a	801	65/65	0.96	0.21	35,39,44,46	0
20	BCR	a	850	40/40	0.96	0.23	39,48,79,81	0
17	CLA	8	307	50/65	0.96	0.18	52,65,91,93	0
22	HTG	A	855	19/19	0.96	0.16	68,72,74,75	0
17	CLA	b	803	65/65	0.97	0.27	35,40,47,49	0
20	BCR	a	854	40/40	0.97	0.19	35,40,47,47	0
17	CLA	a	830	65/65	0.97	0.21	36,40,47,49	0
17	CLA	a	820	65/65	0.98	0.20	38,43,48,50	0
21	SF4	a	855	8/8	0.98	0.20	37,37,43,43	0
21	SF4	A	853	8/8	0.99	0.18	43,44,48,51	0
21	SF4	c	102	8/8	0.99	0.12	41,50,62,77	0
21	SF4	c	101	8/8	0.99	0.16	41,46,54,56	0
21	SF4	C	101	8/8	0.99	0.14	47,49,53,57	0
21	SF4	C	102	8/8	0.99	0.09	51,62,72,84	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.

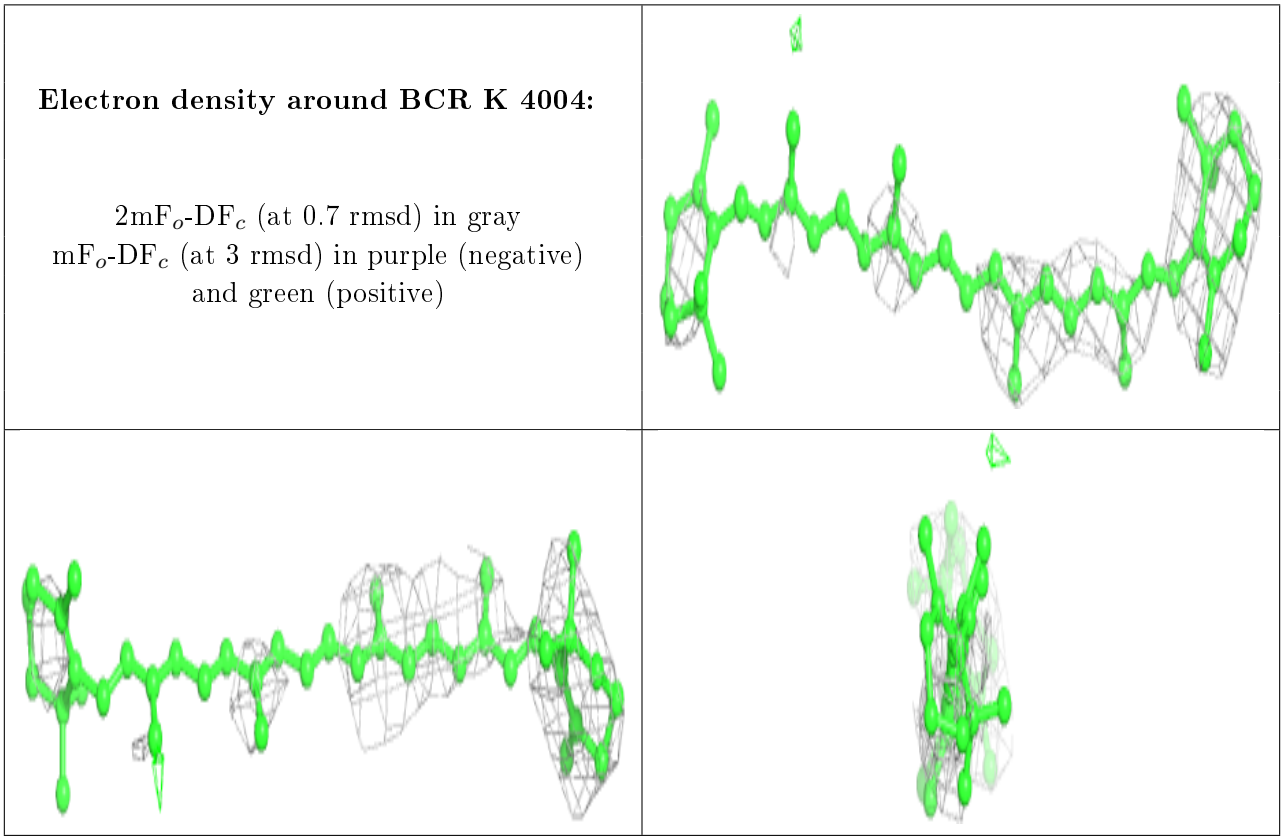
Electron density around BCR L 206:

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



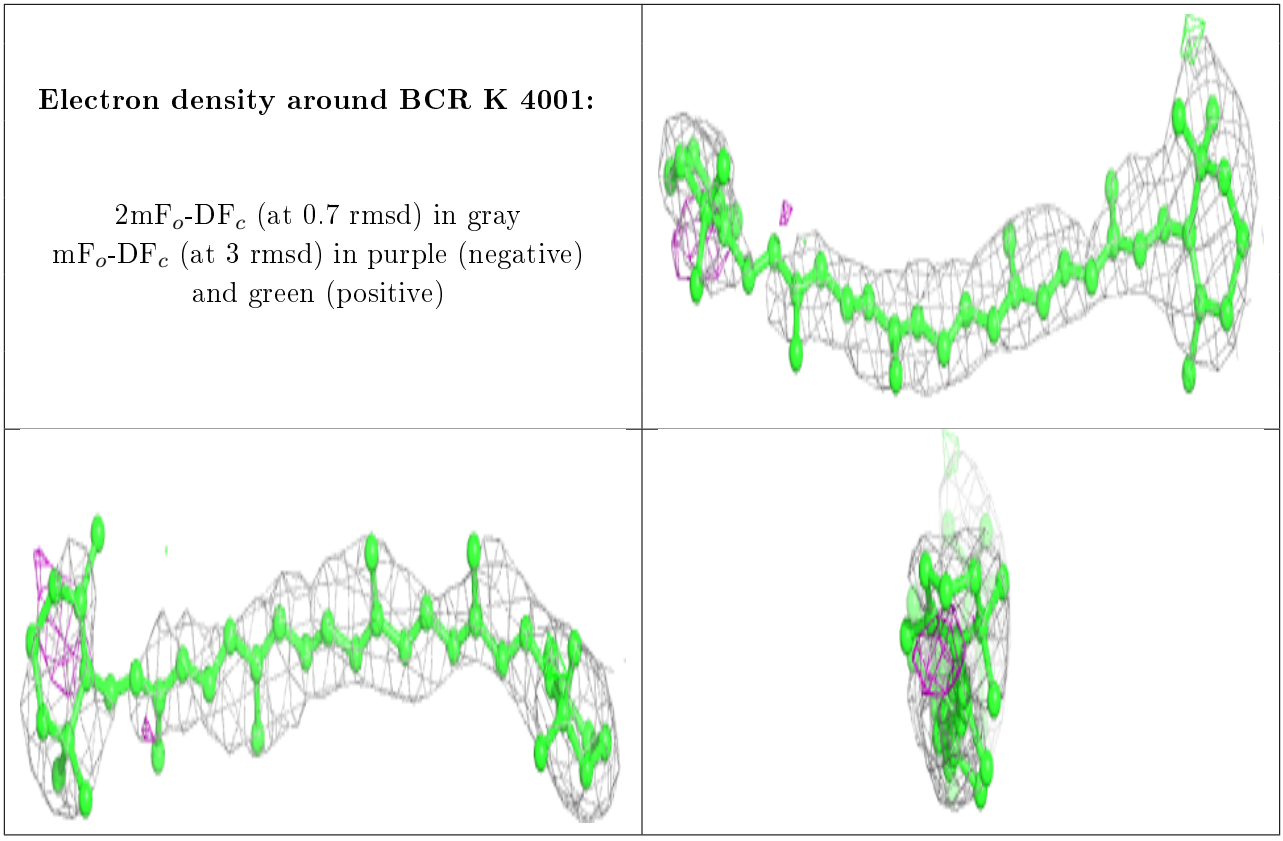
Electron density around BCR K 4004:

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



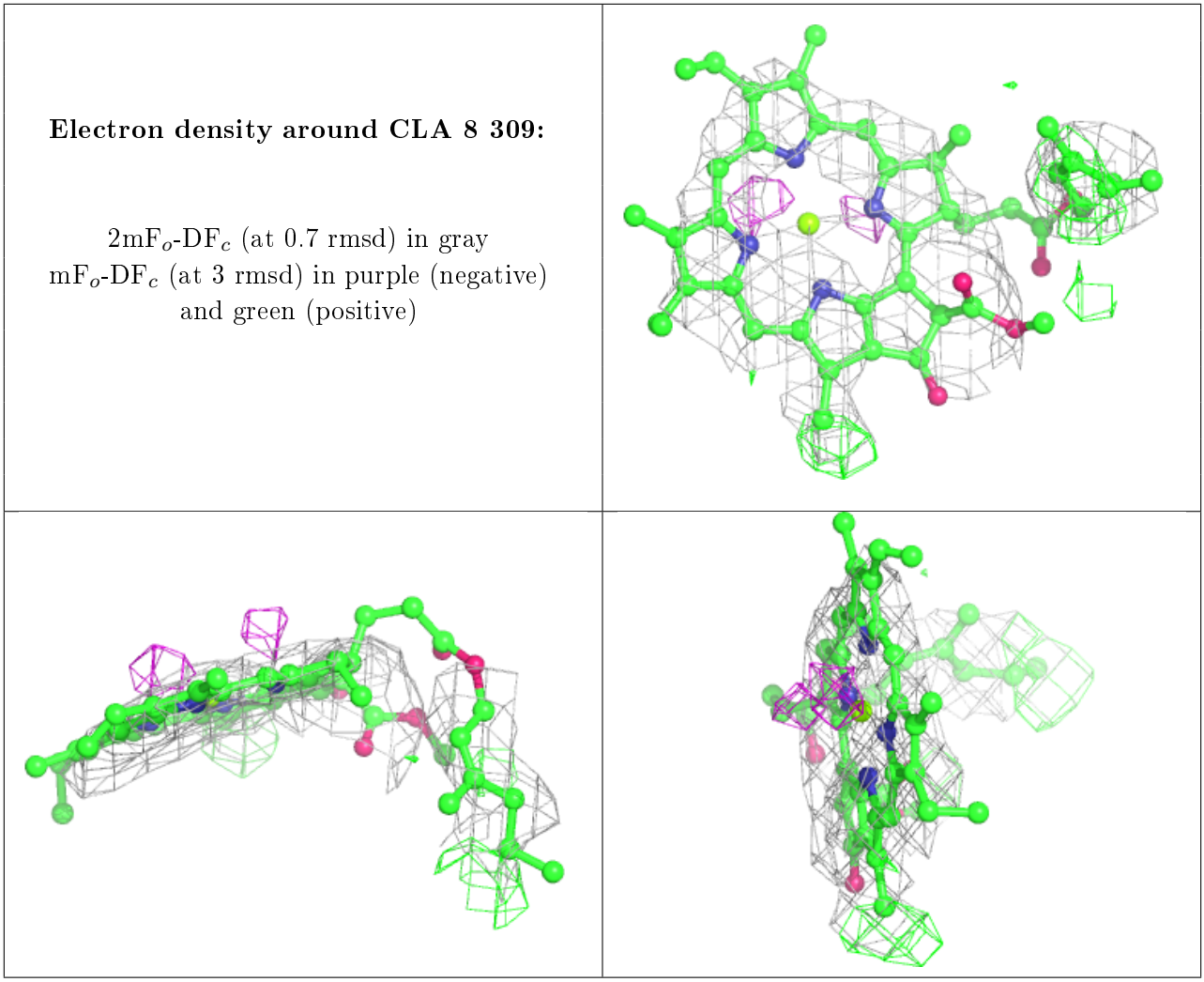
Electron density around BCR K 4001:

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



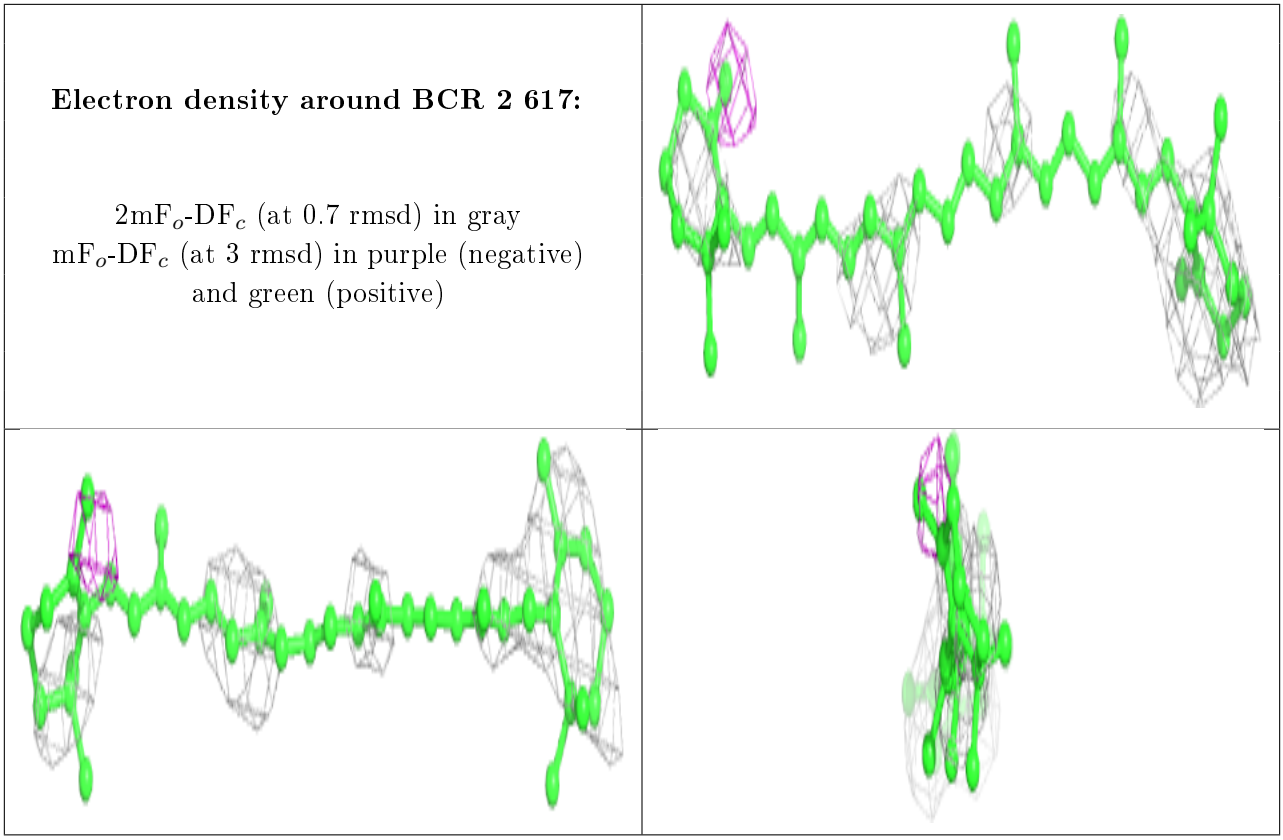
Electron density around CLA 8 309:

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



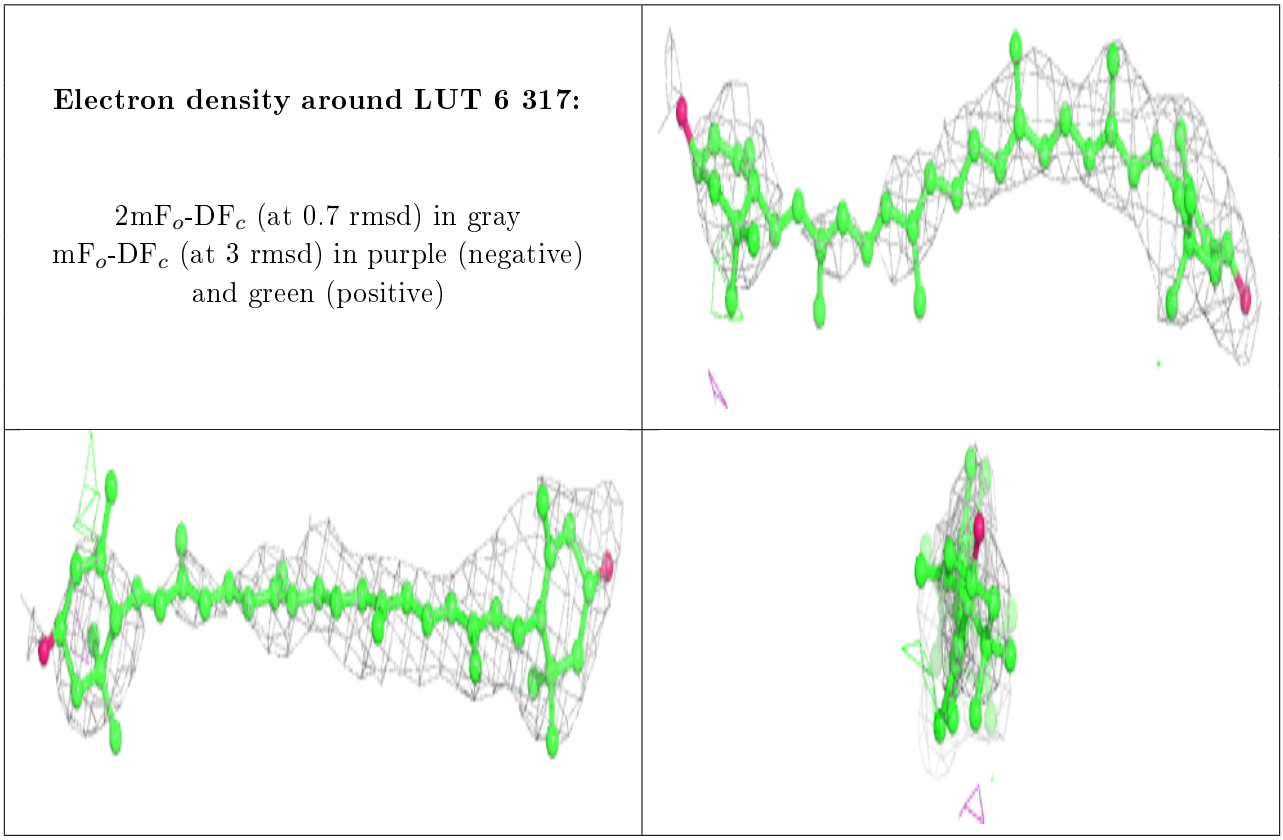
Electron density around BCR 2 617:

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



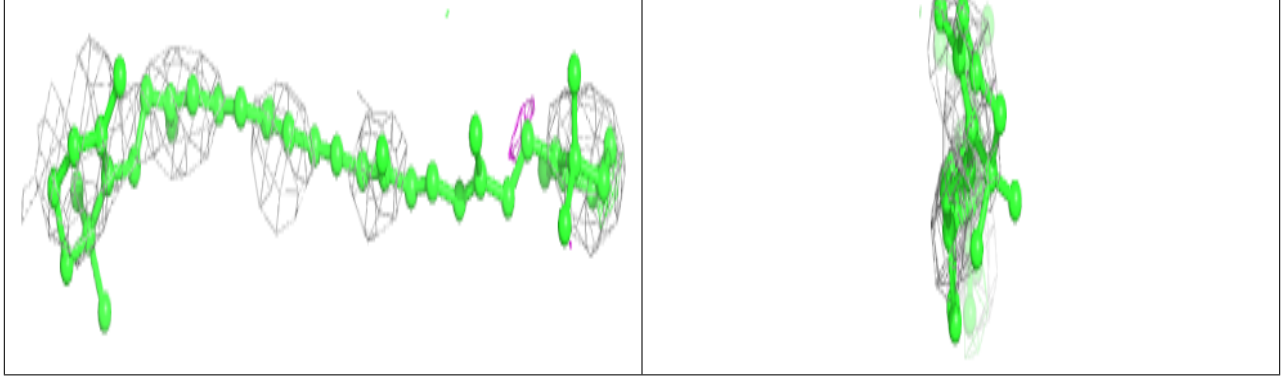
Electron density around LUT 6 317:

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



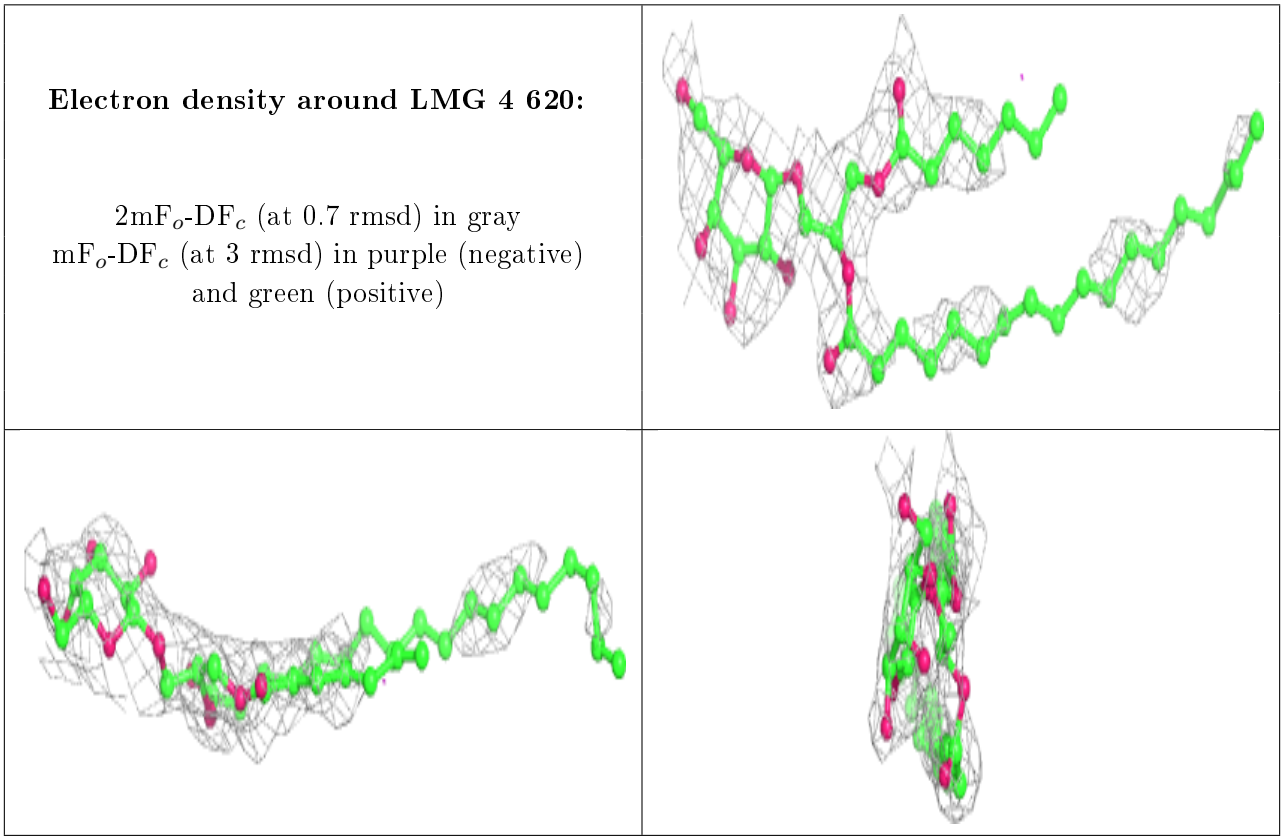
Electron density around BCR 7 617:

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



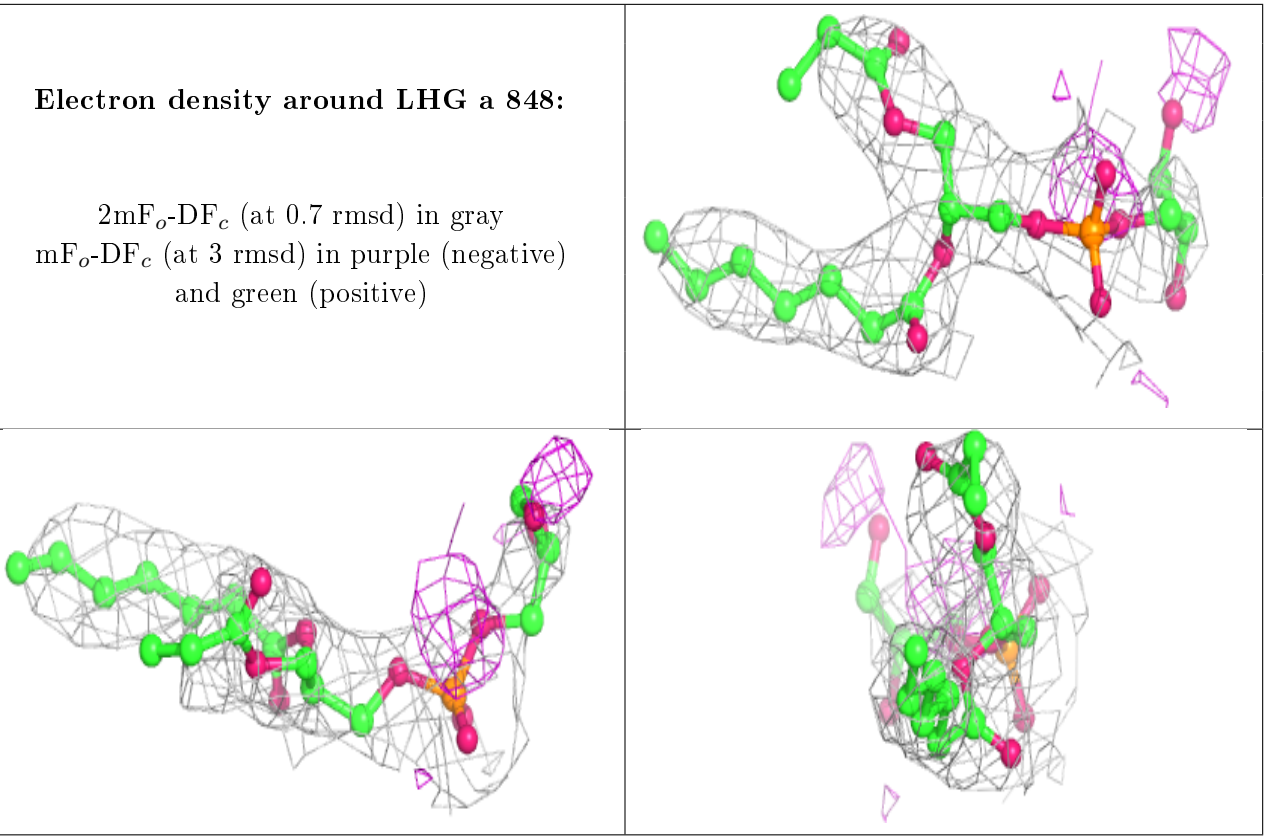
Electron density around LMG 4 620:

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



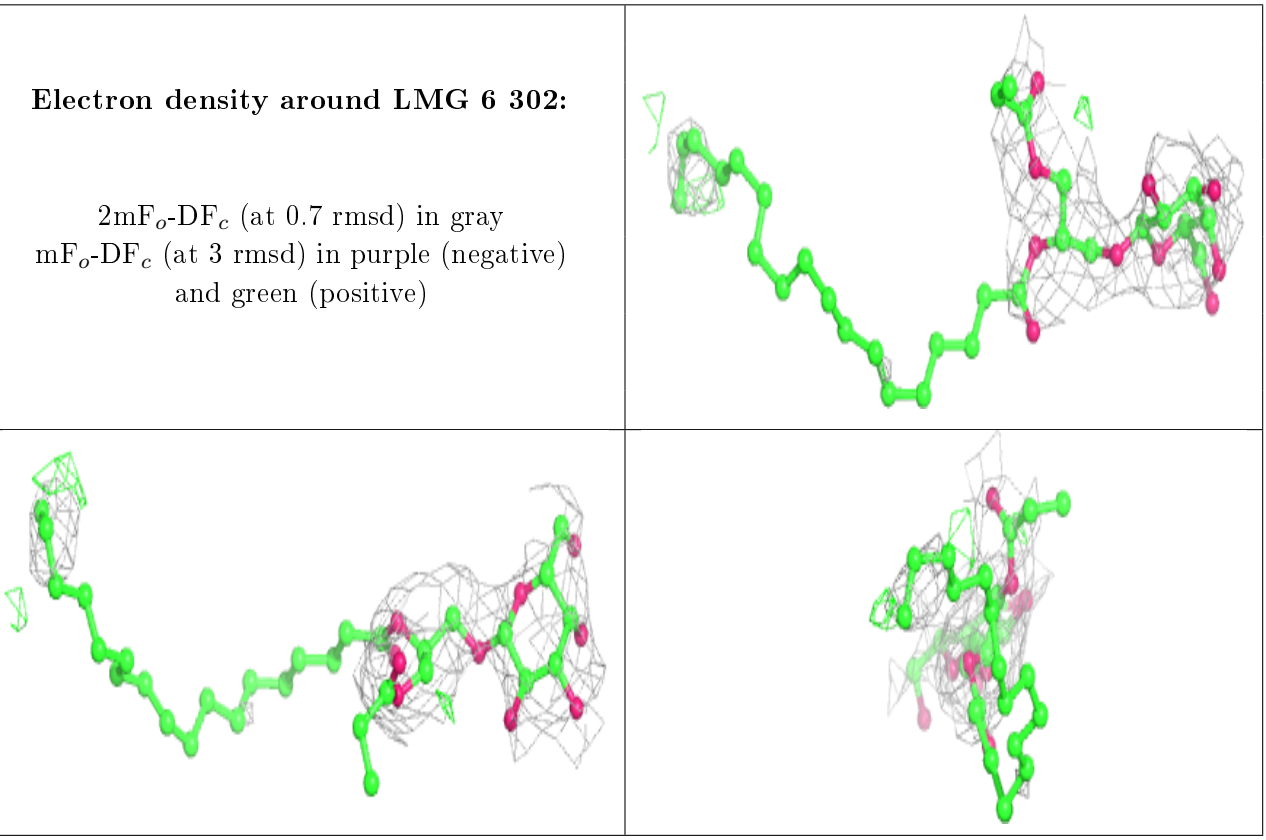
Electron density around LHG a 848:

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



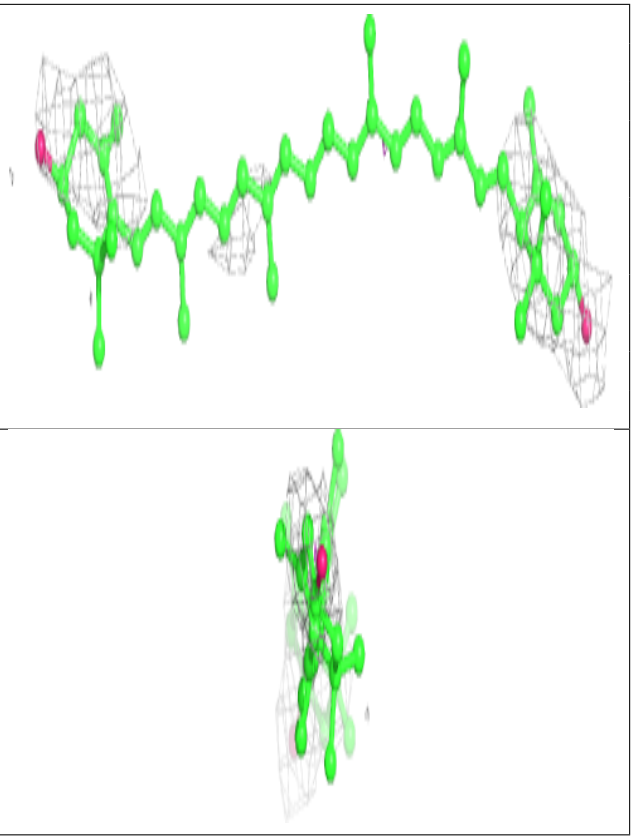
Electron density around LMG 6 302:

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



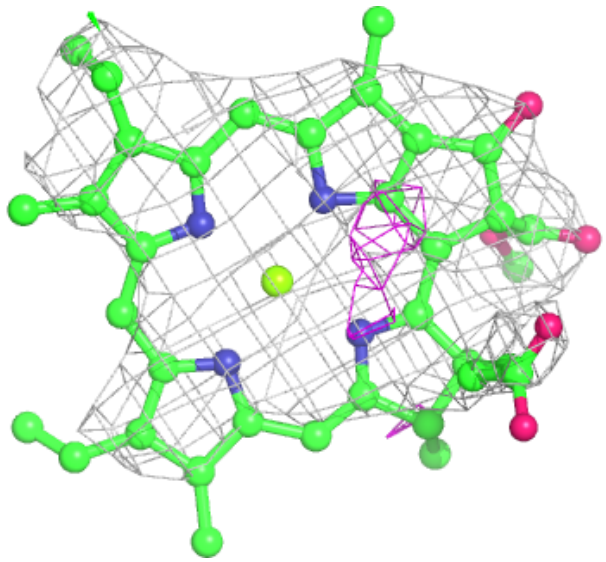
Electron density around LUT 6 321:

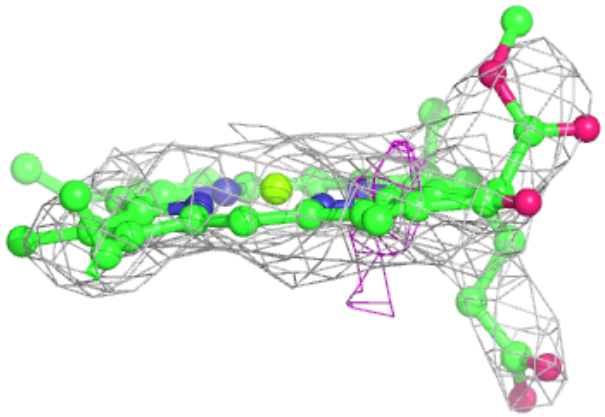
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

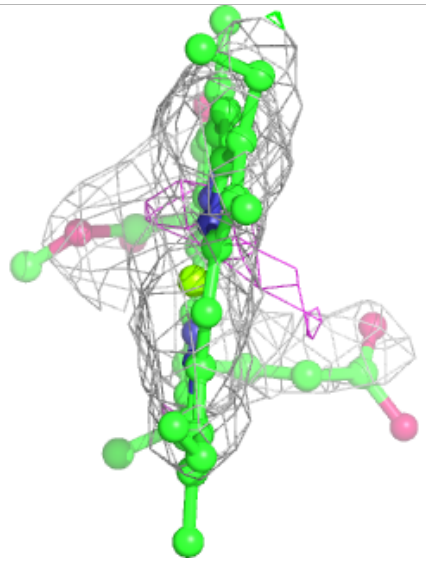


Electron density around CLA K 4002:

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

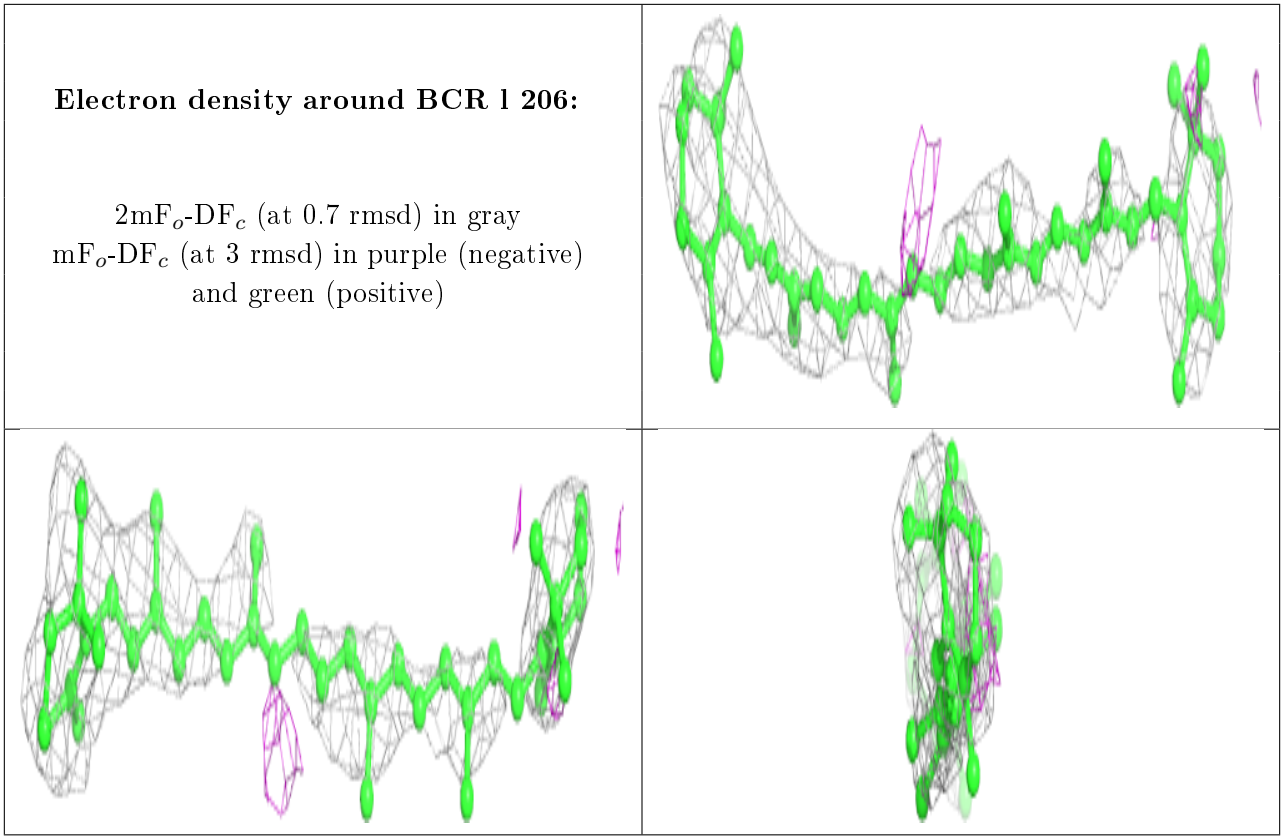






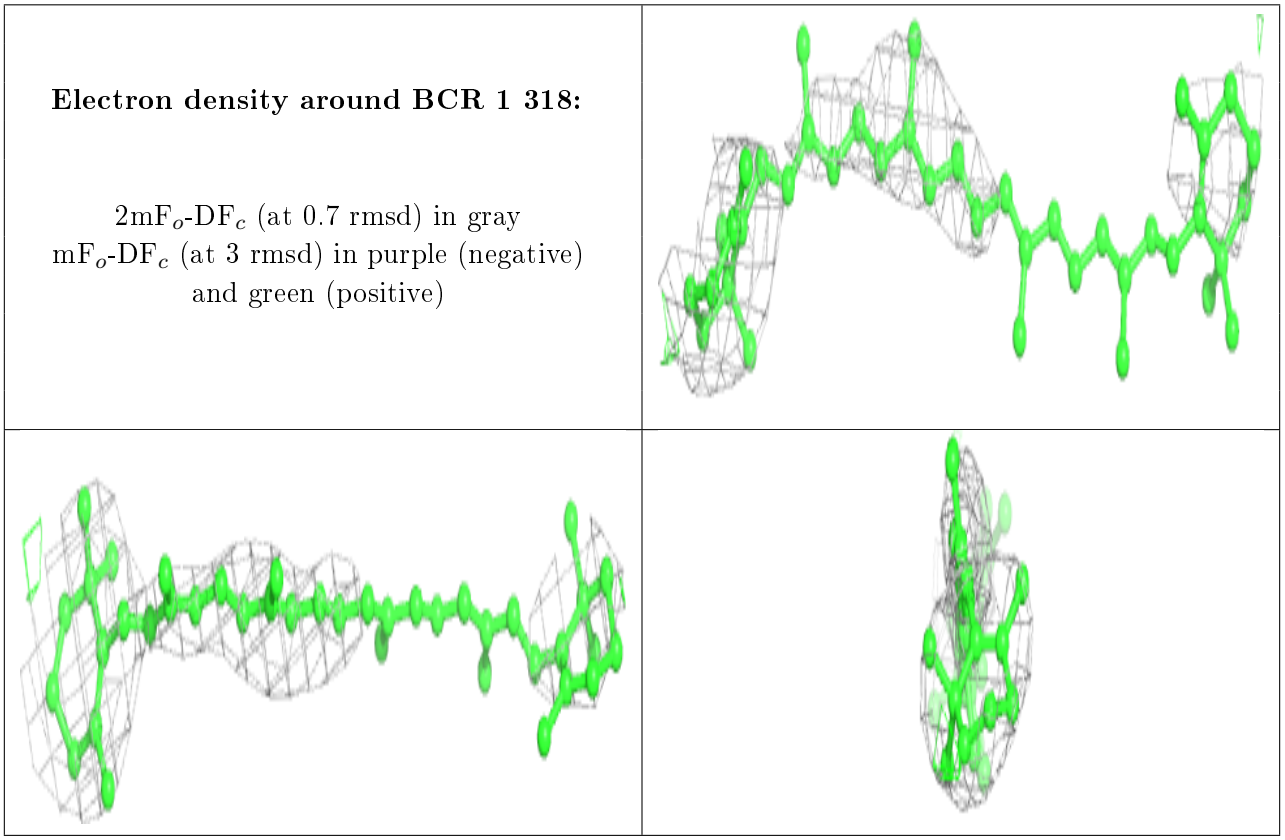
Electron density around BCR l 206:

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



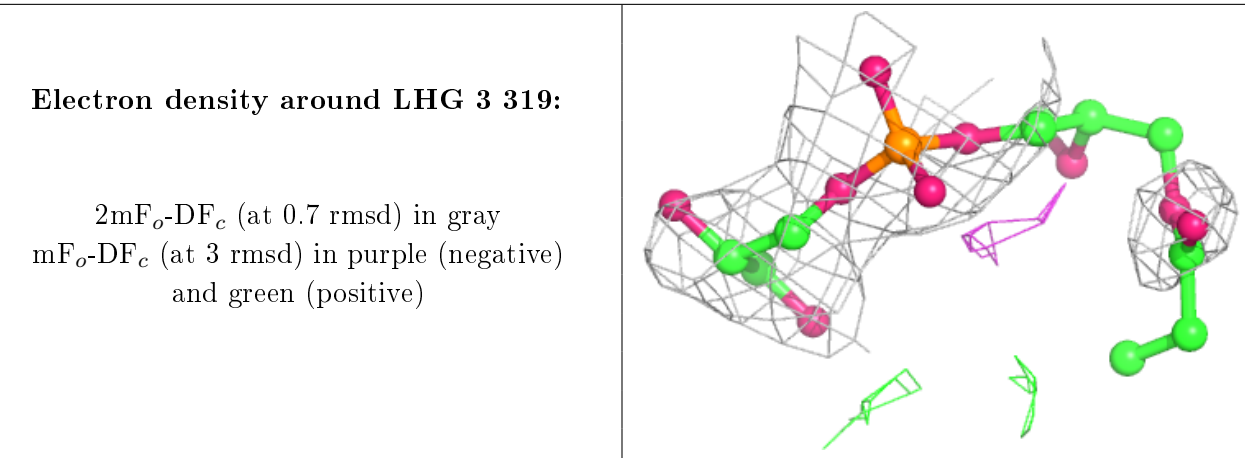
Electron density around BCR 1 318:

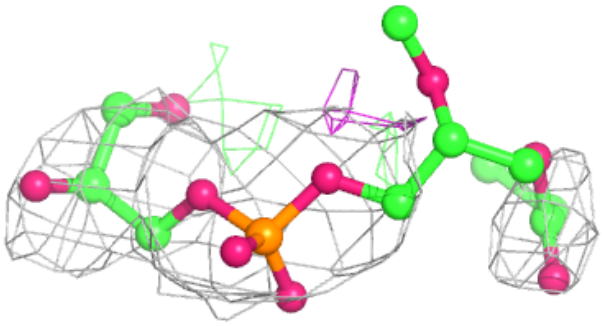
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

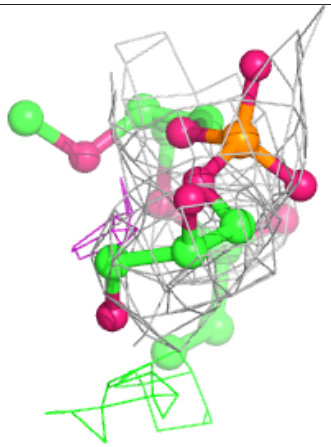


Electron density around LHG 3 319:

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

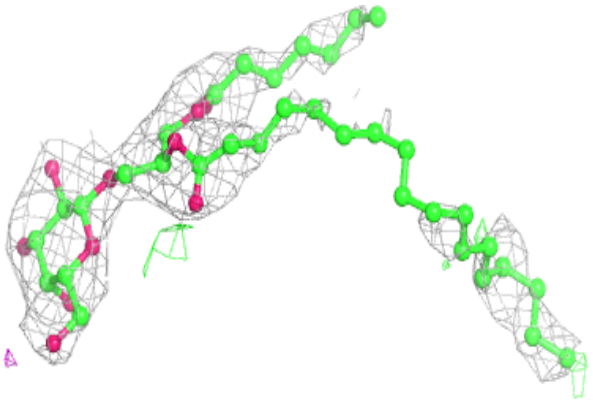


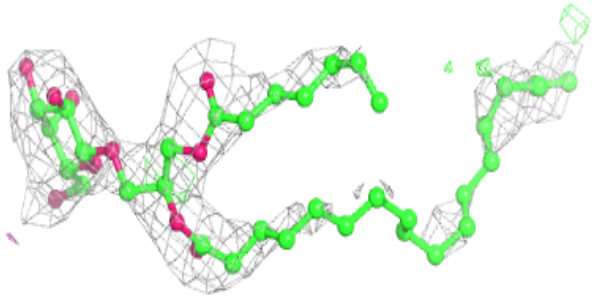


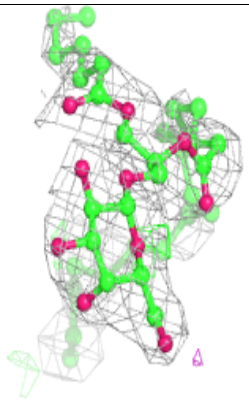


Electron density around LMG 4 619:

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

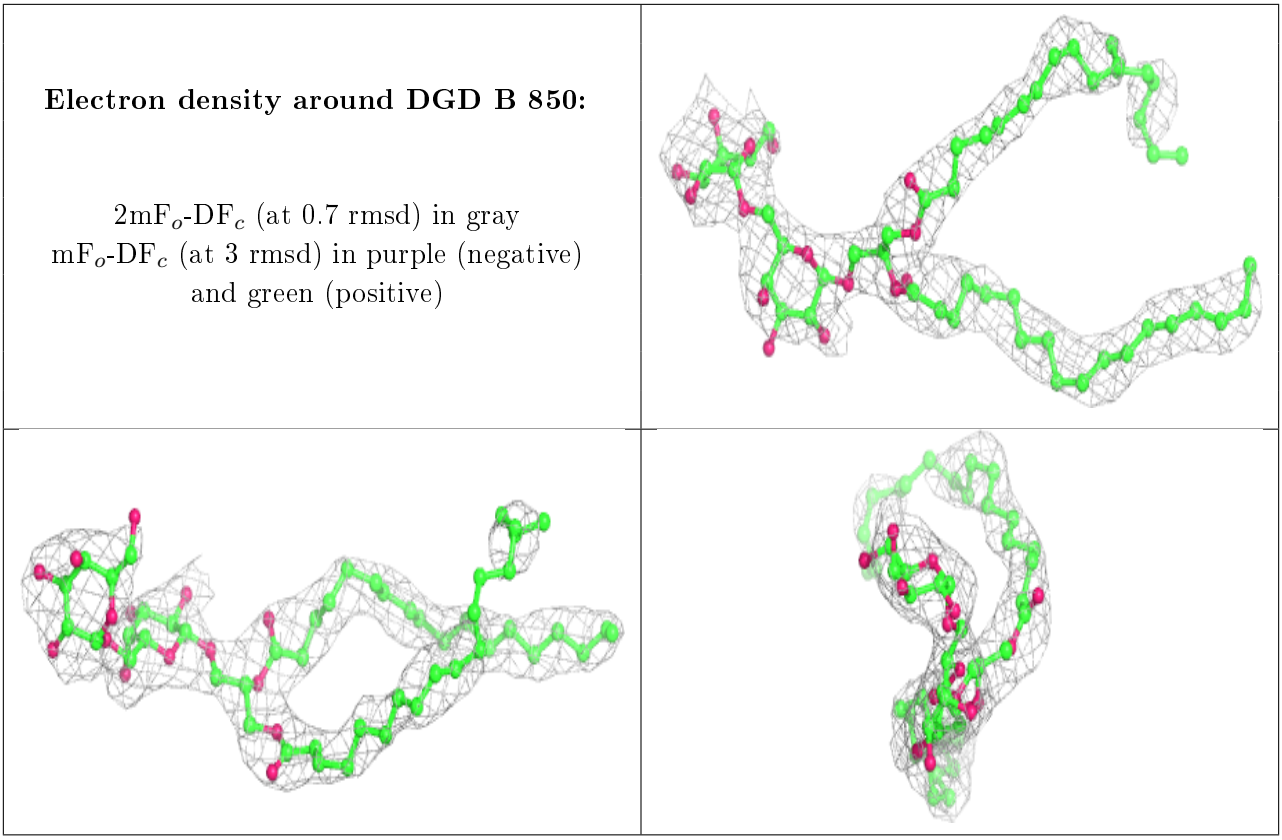






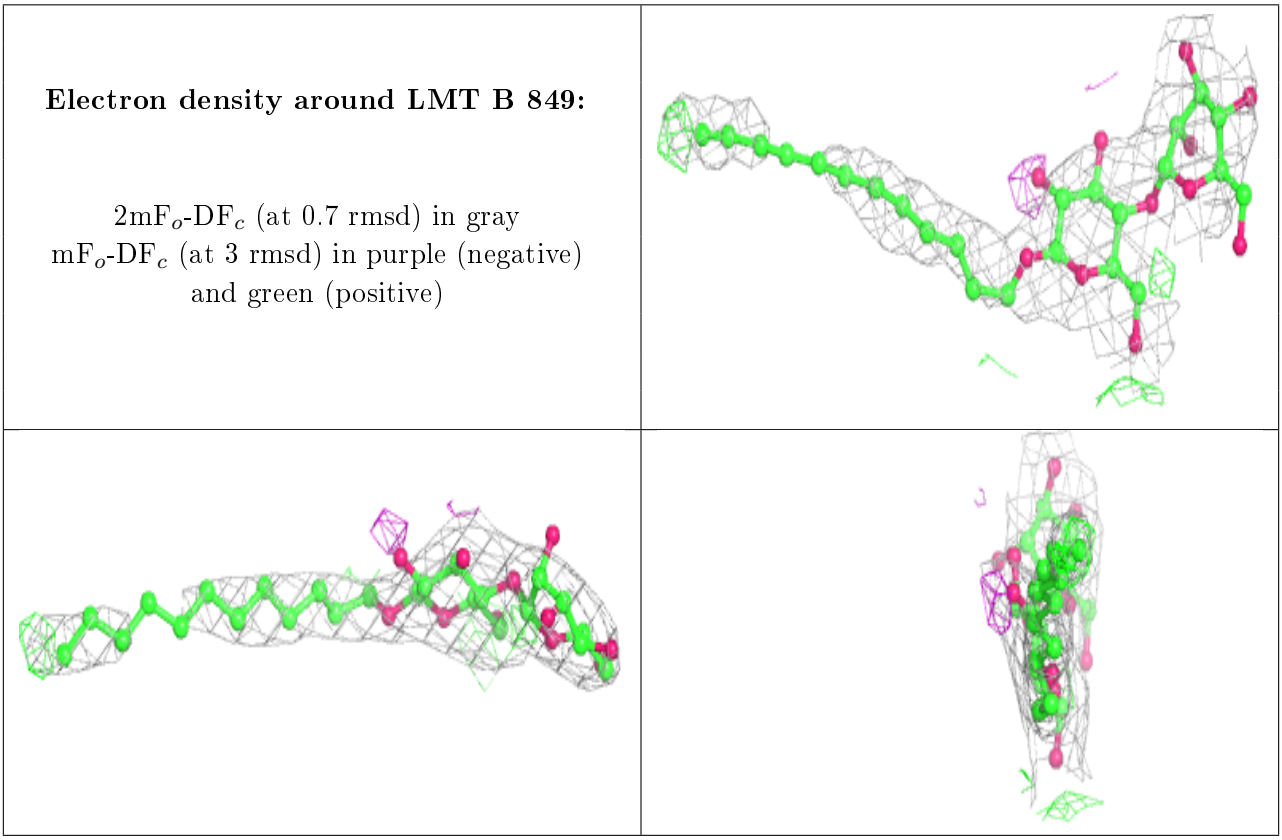
Electron density around DGD B 850:

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



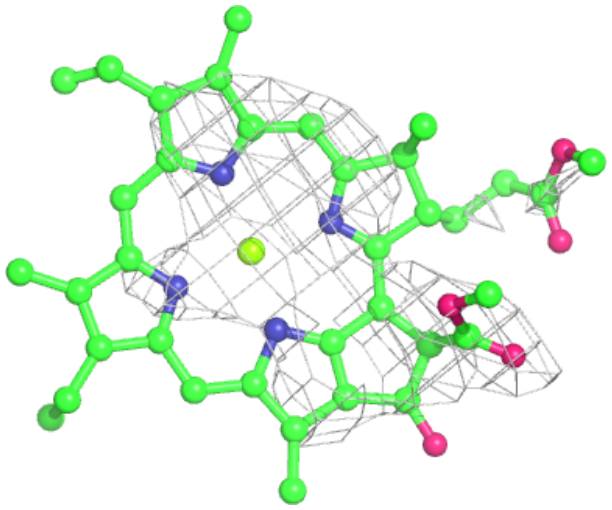
Electron density around LMT B 849:

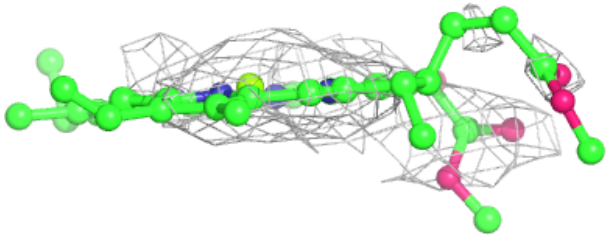
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

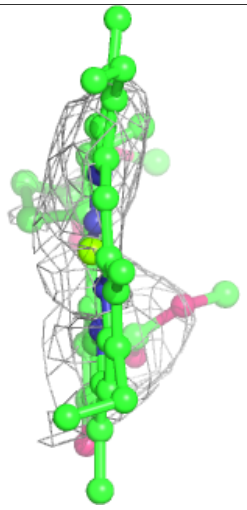


Electron density around CLA 3 301:

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

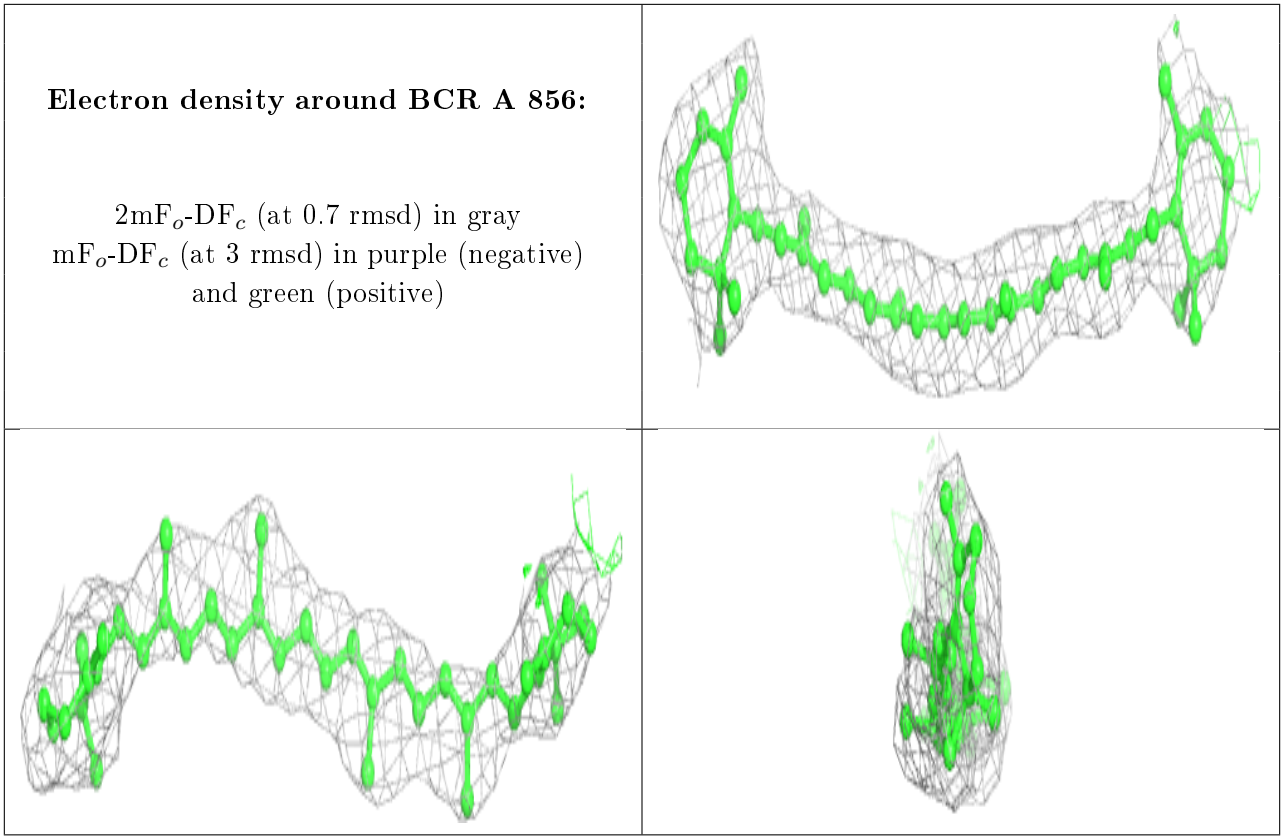






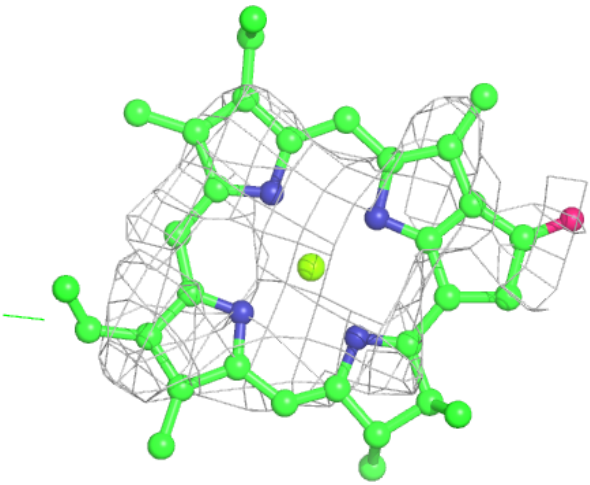
Electron density around BCR A 856:

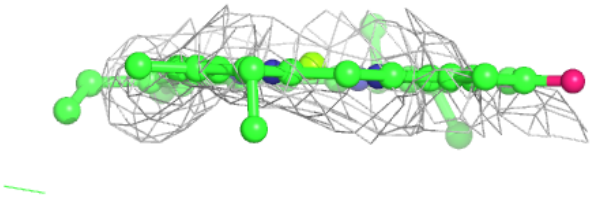
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

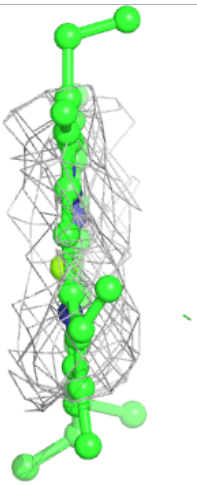


Electron density around CLA 3 310:

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

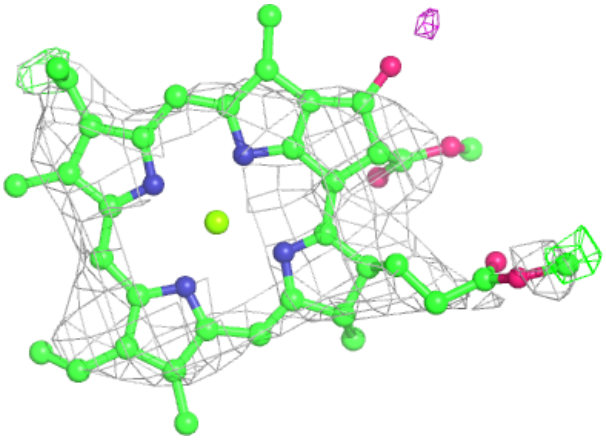


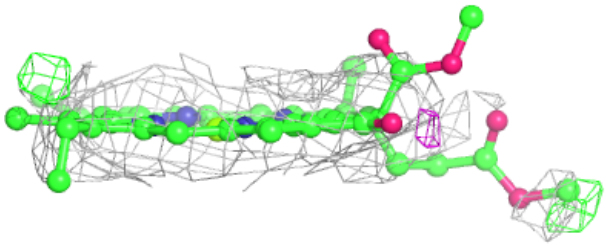


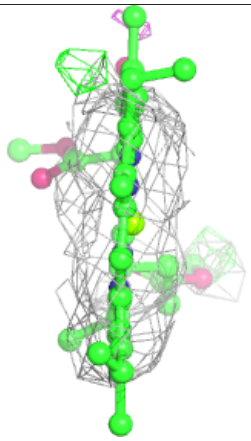


Electron density around CLA 6 316:

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

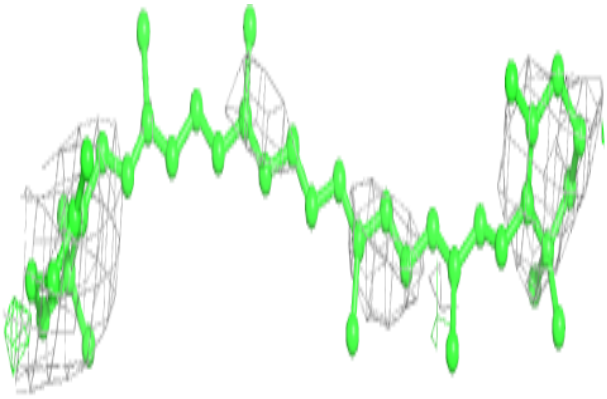


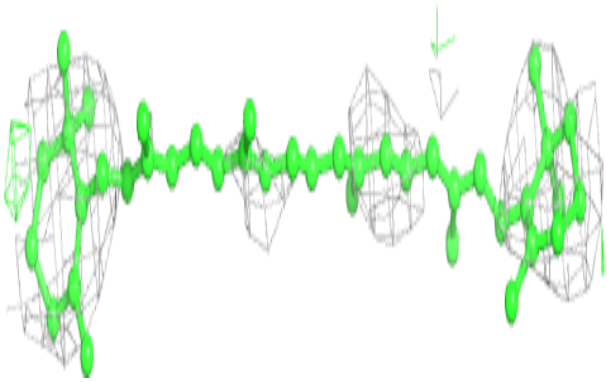


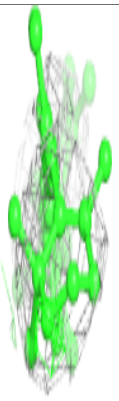


Electron density around BCR 6 319:

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

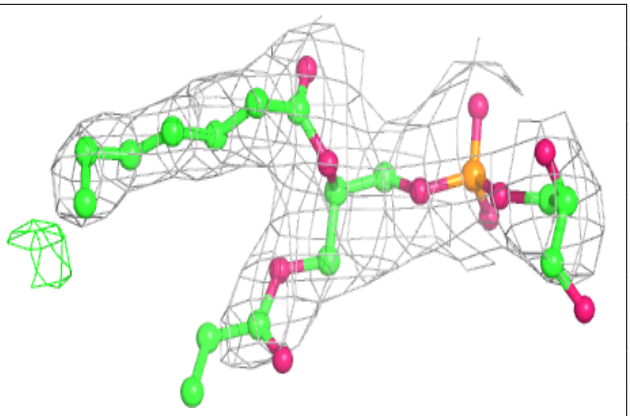


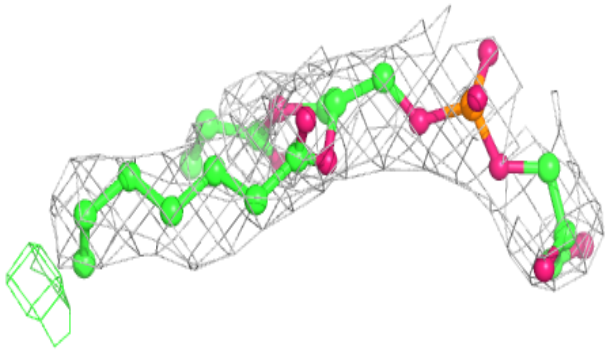


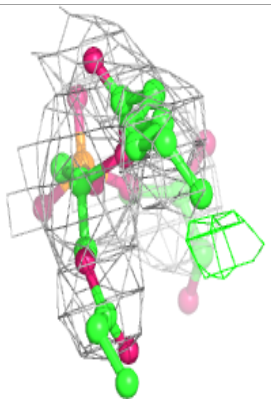


Electron density around LHG A 847:

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

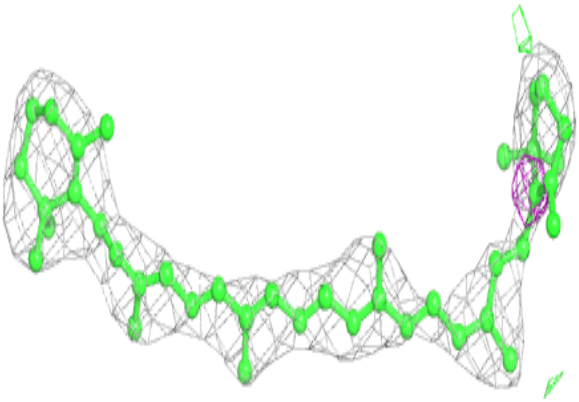


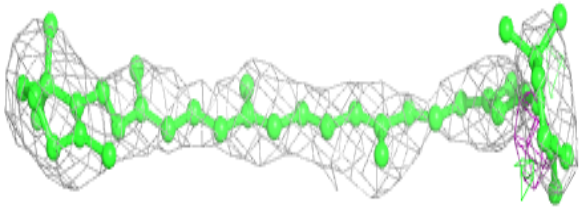


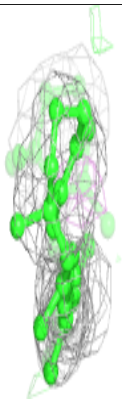


Electron density around BCR b 844:

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

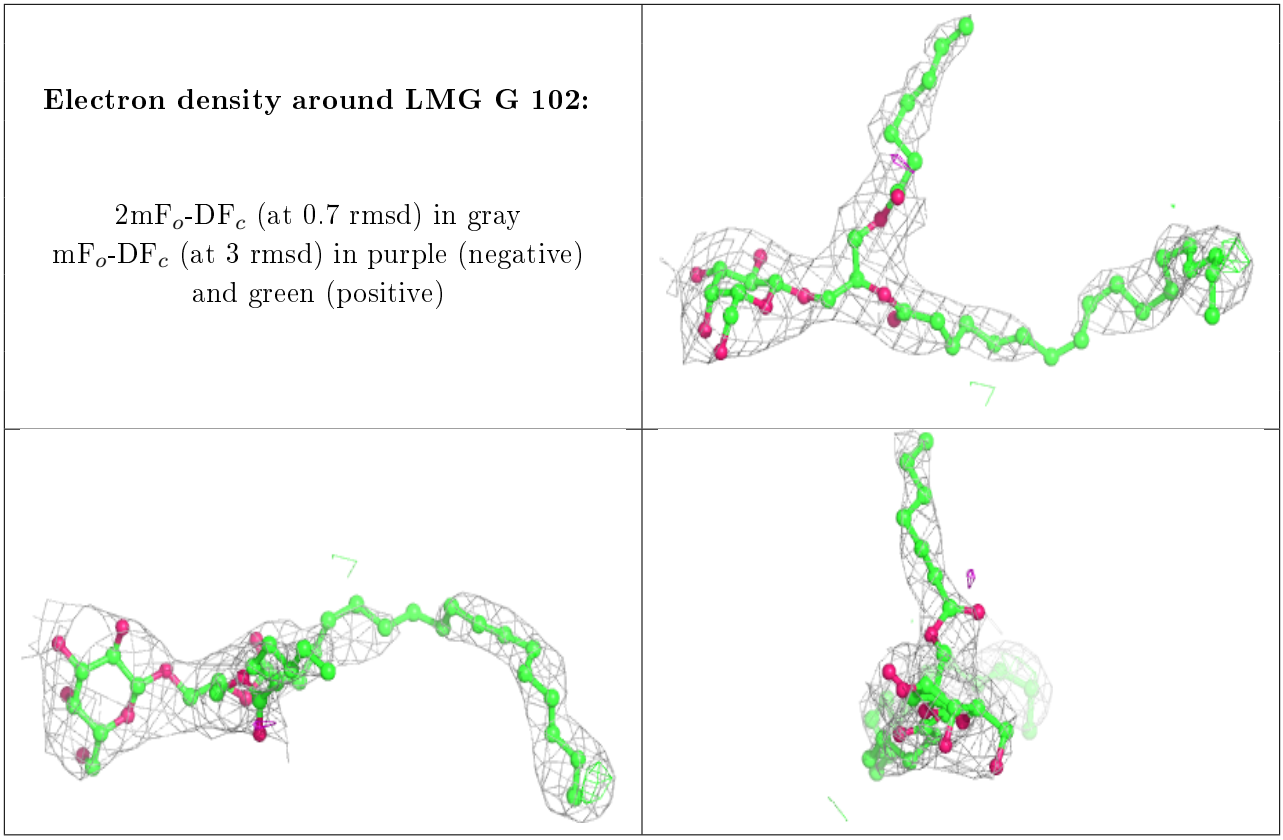






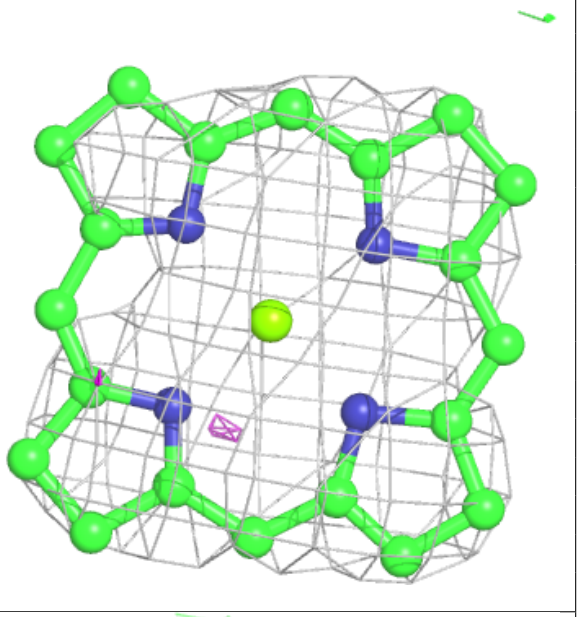
Electron density around LMG G 102:

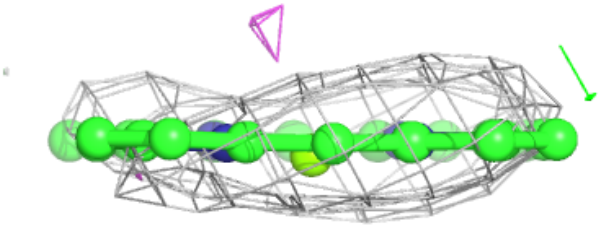
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

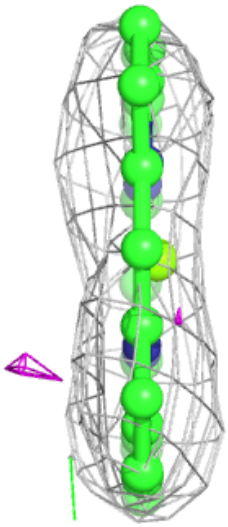


Electron density around CLA 8 313:

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

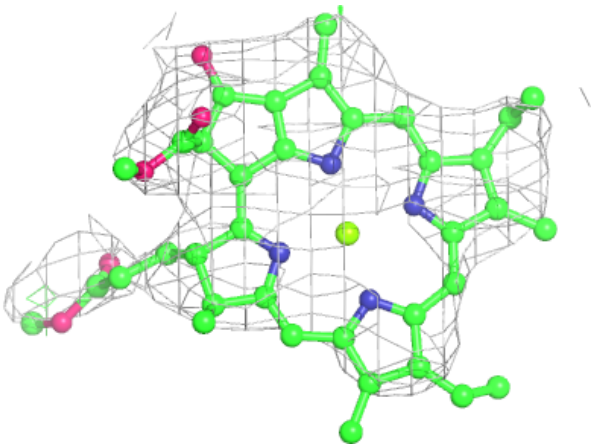


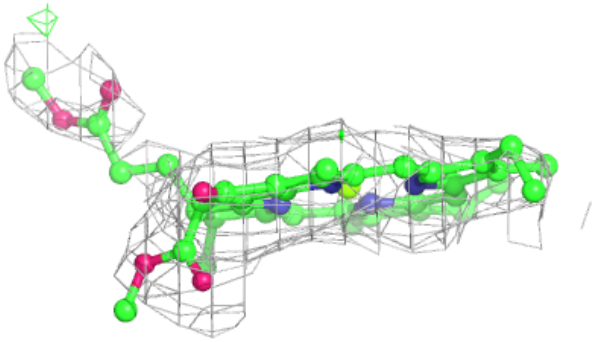


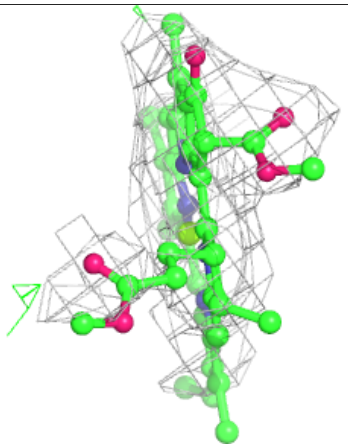


Electron density around CLA K 4003:

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

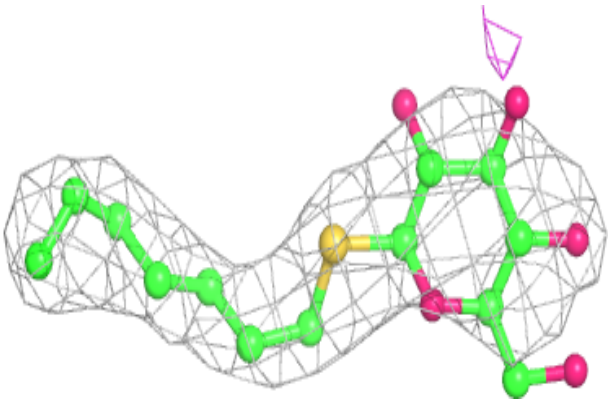


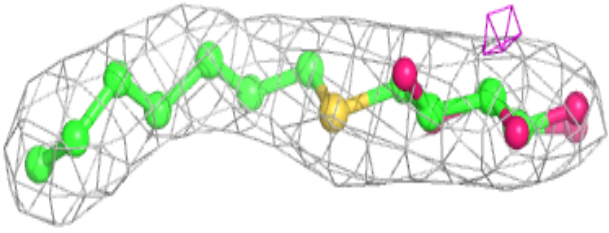




Electron density around HTG F 302:

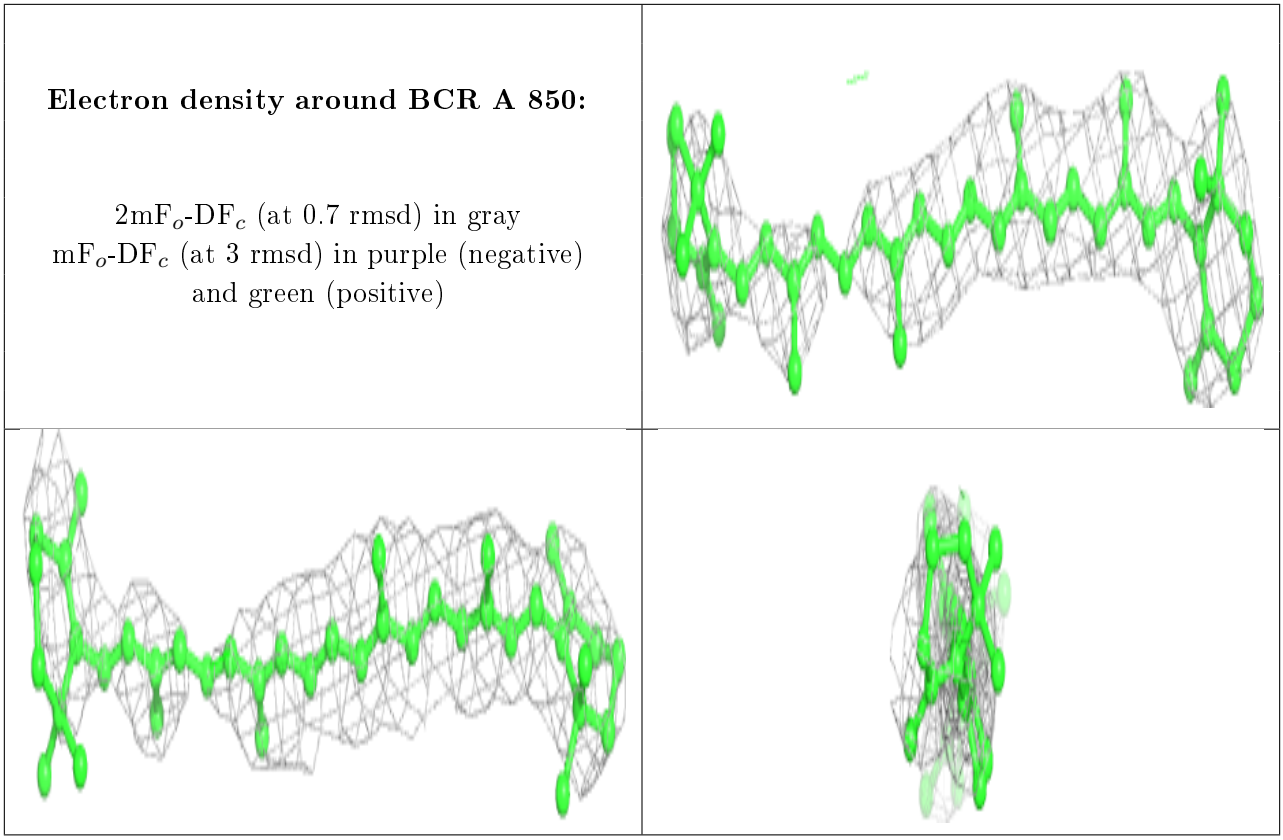
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)





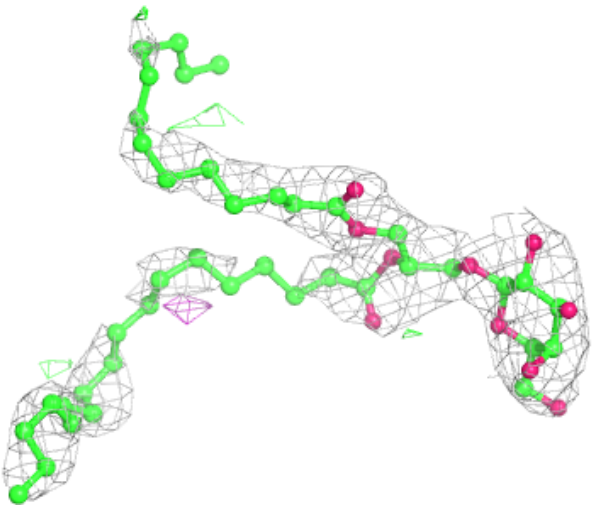
Electron density around BCR A 850:

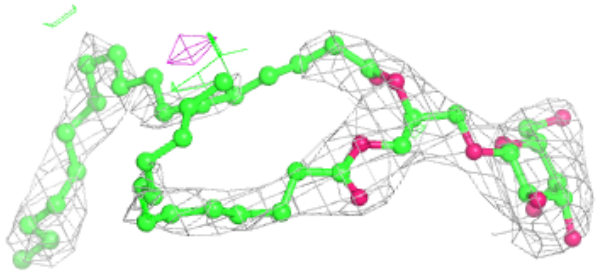
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

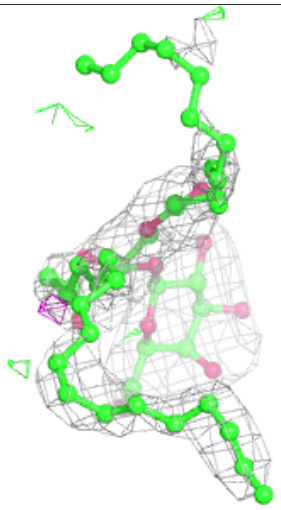


Electron density around LMG 9 619:

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

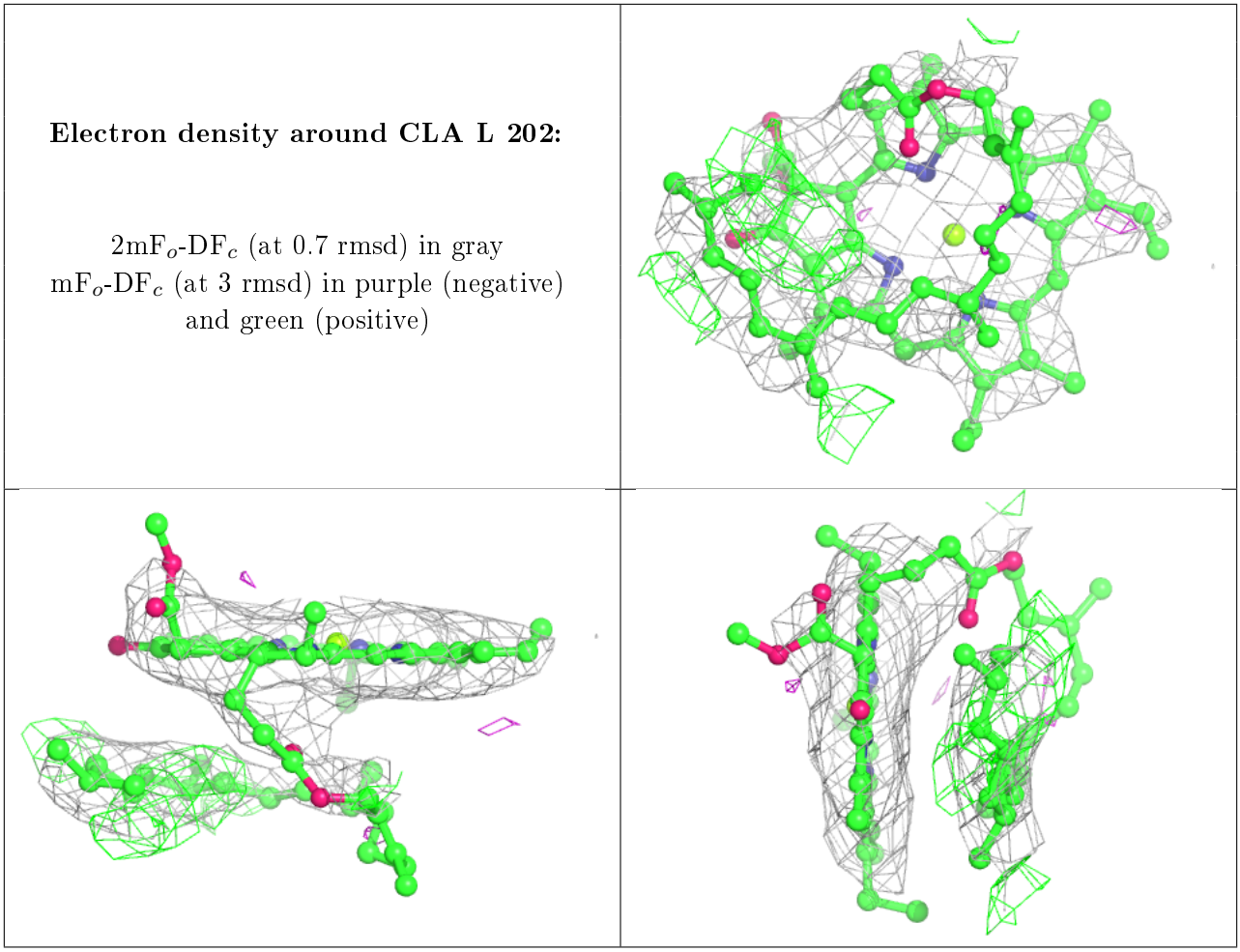






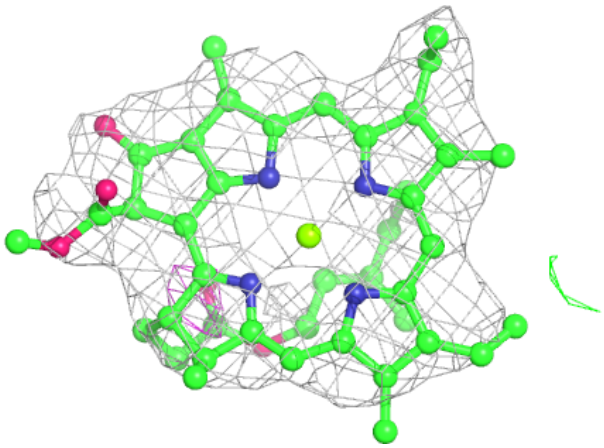
Electron density around CLA L 202:

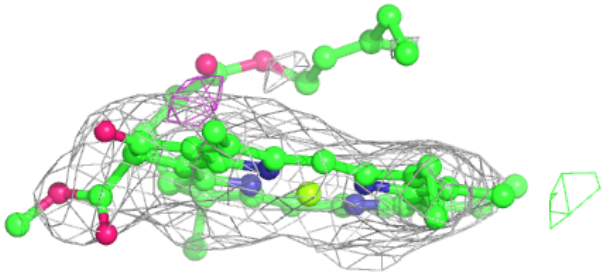
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

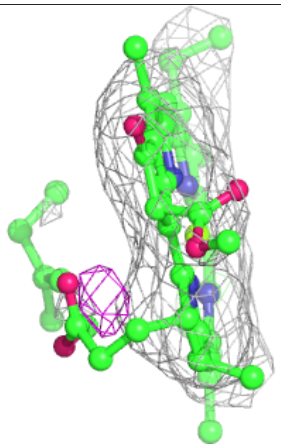


Electron density around CLA A 824:

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

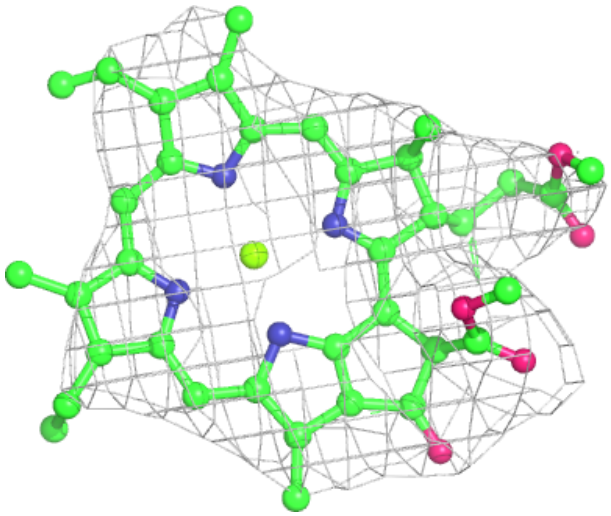


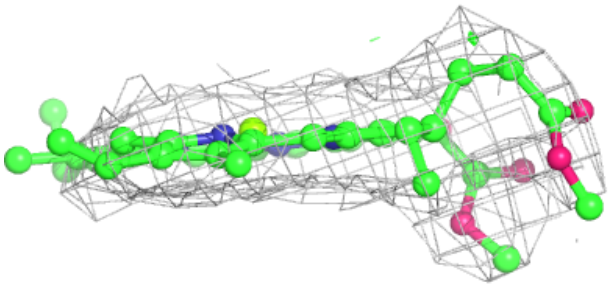


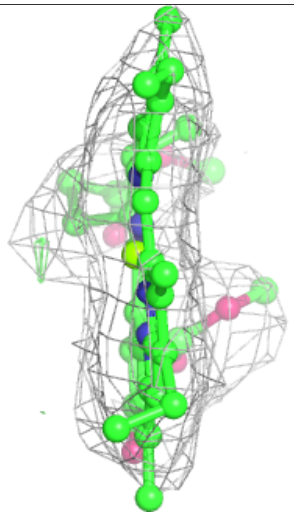


Electron density around CLA k 1403:

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

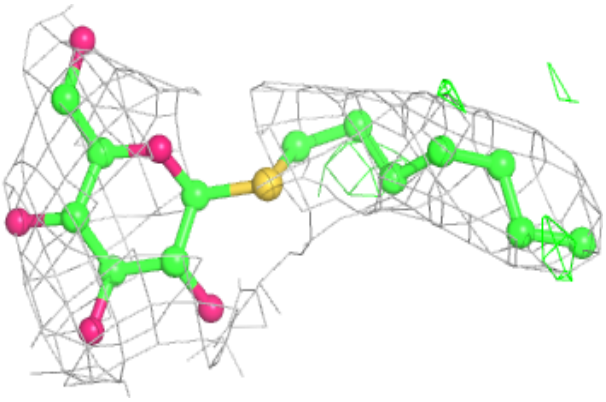


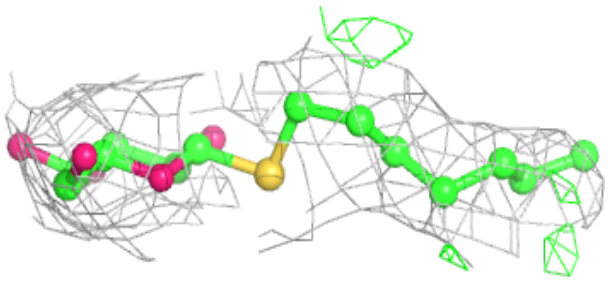


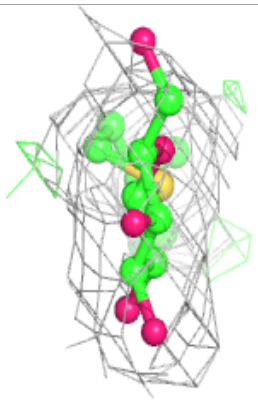


Electron density around HTG J 3001:

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

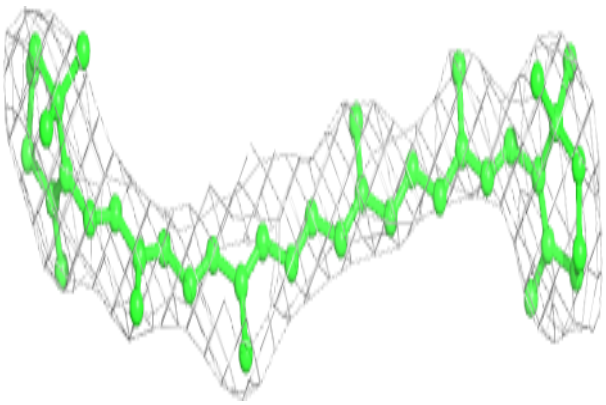


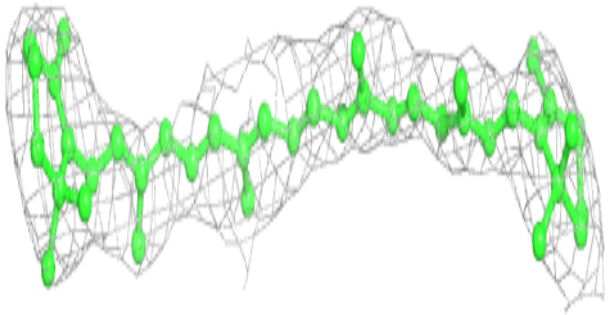


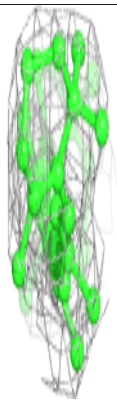


Electron density around BCR G 105:

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

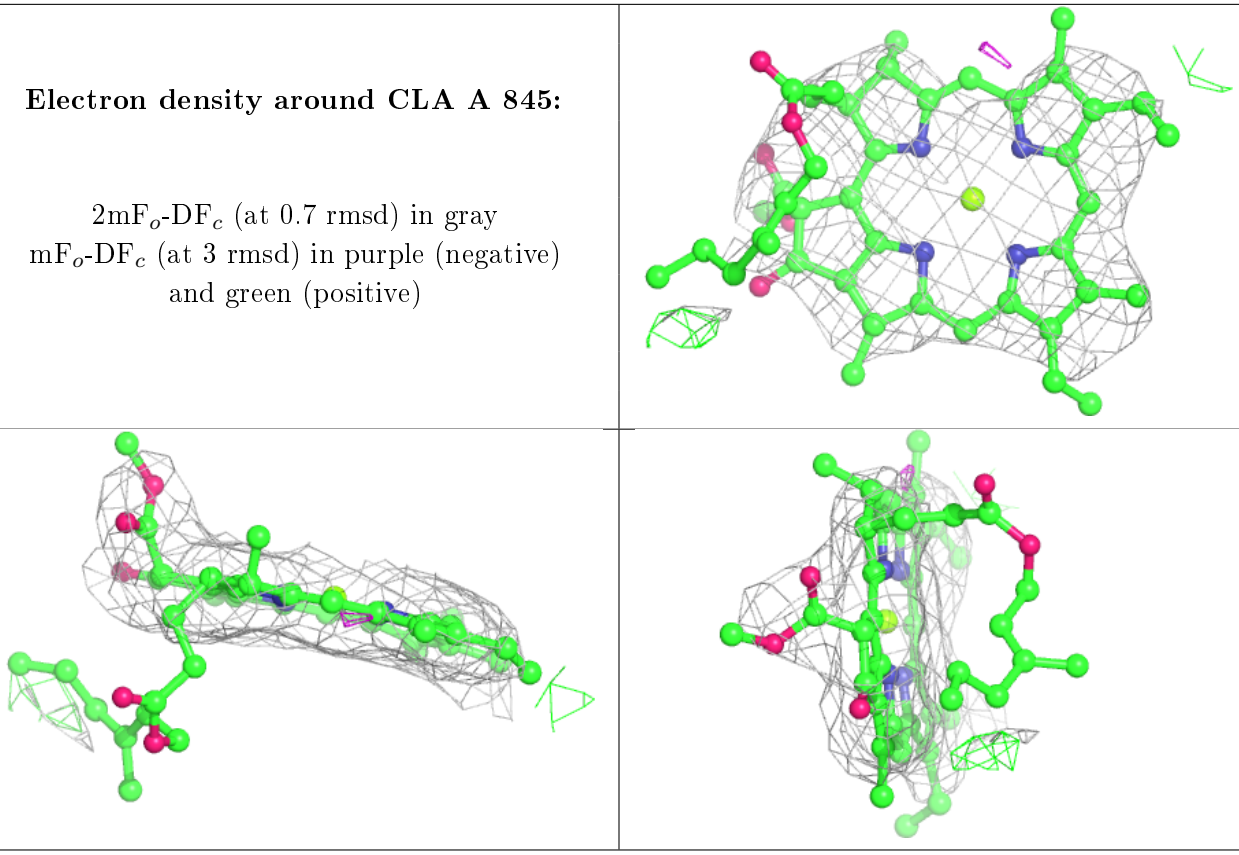






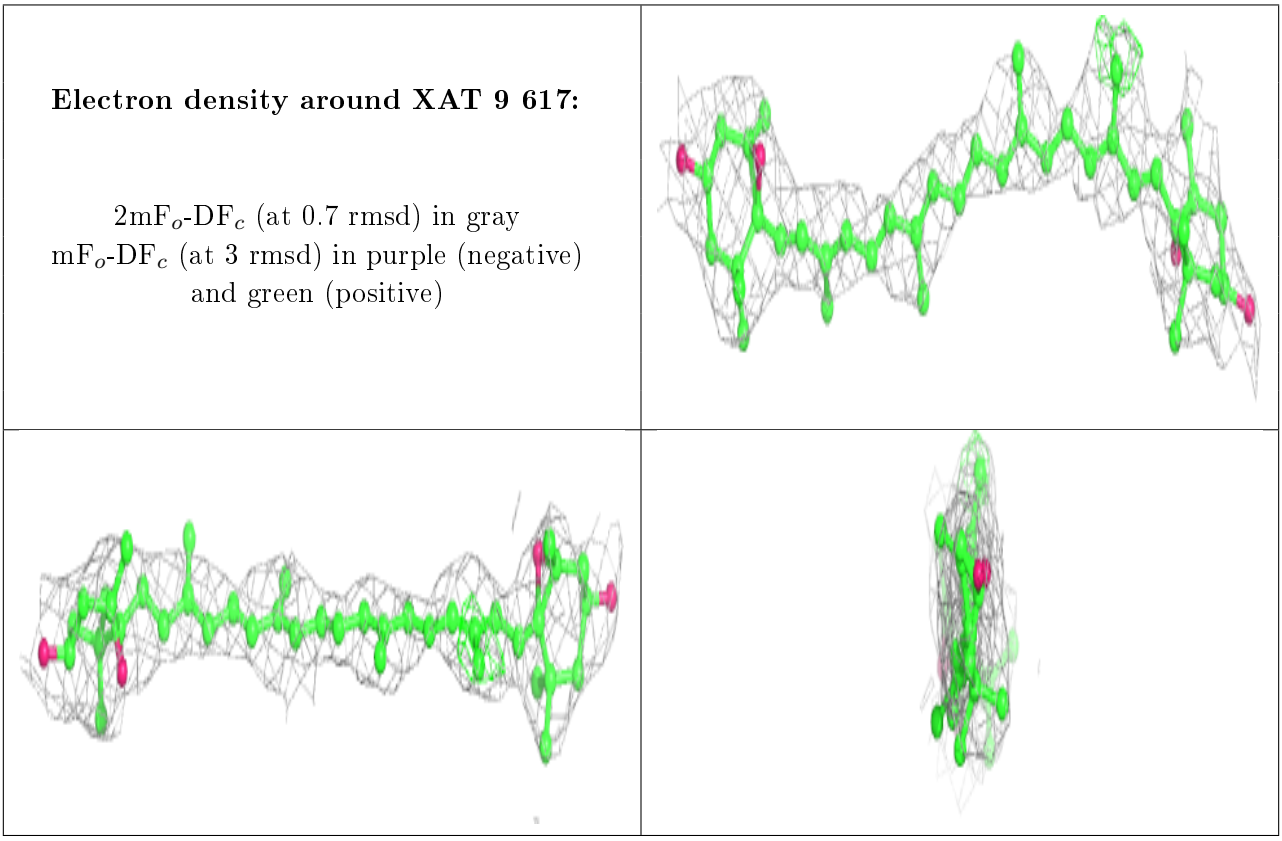
Electron density around CLA A 845:

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



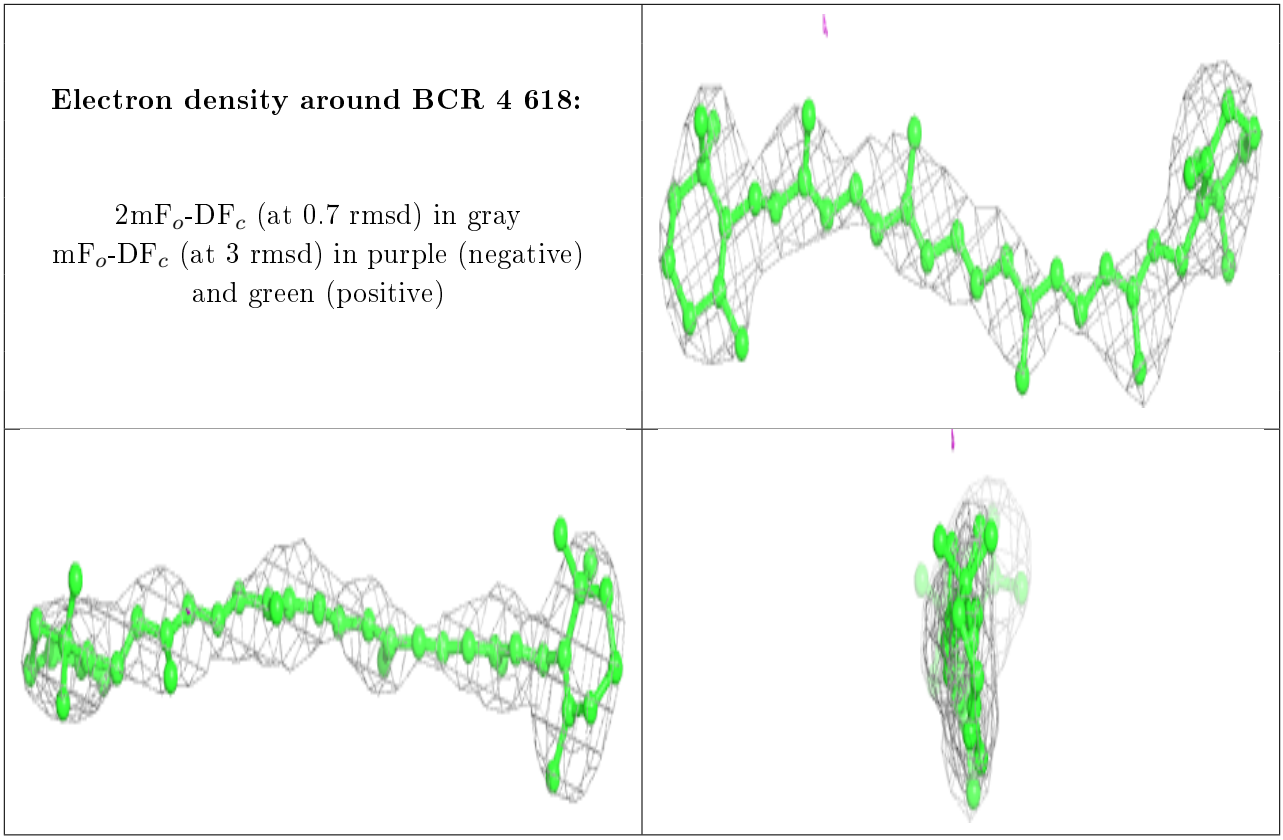
Electron density around XAT 9 617:

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



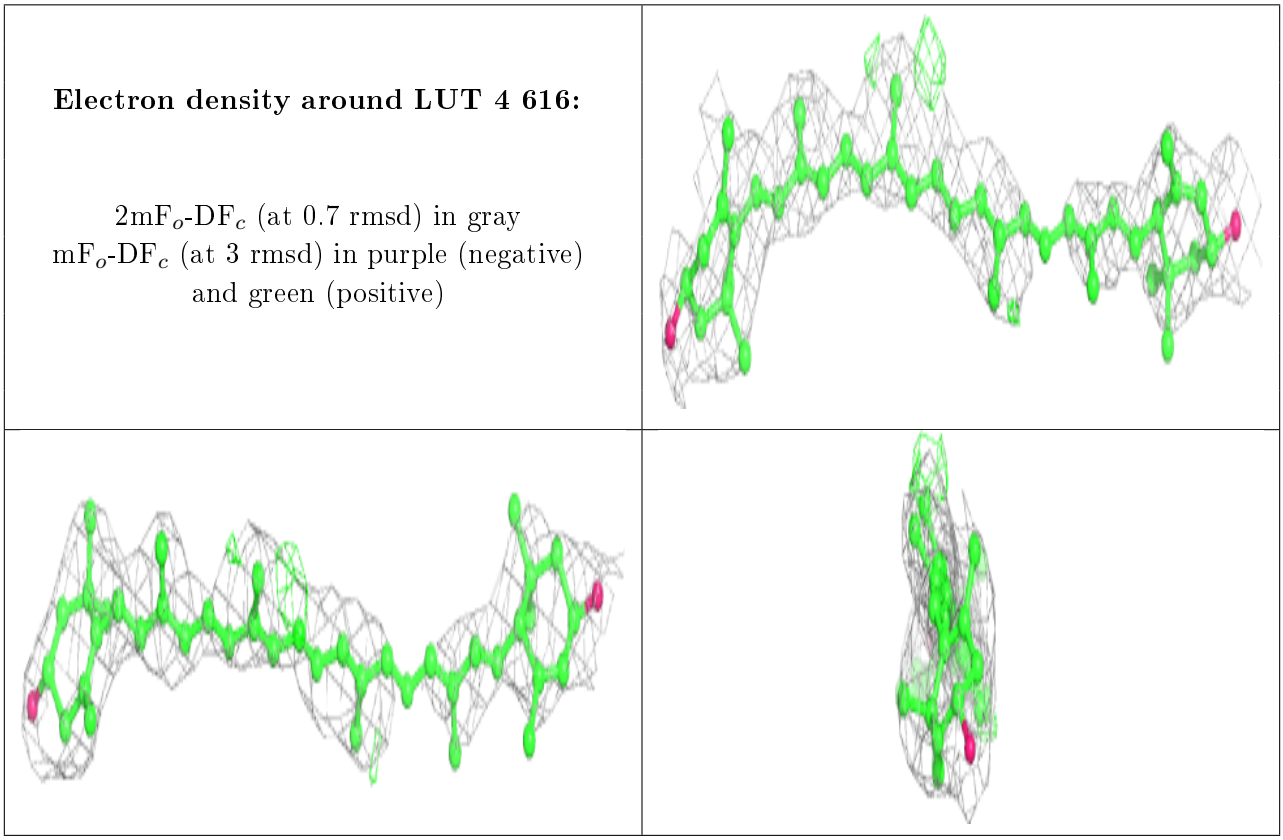
Electron density around BCR 4 618:

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



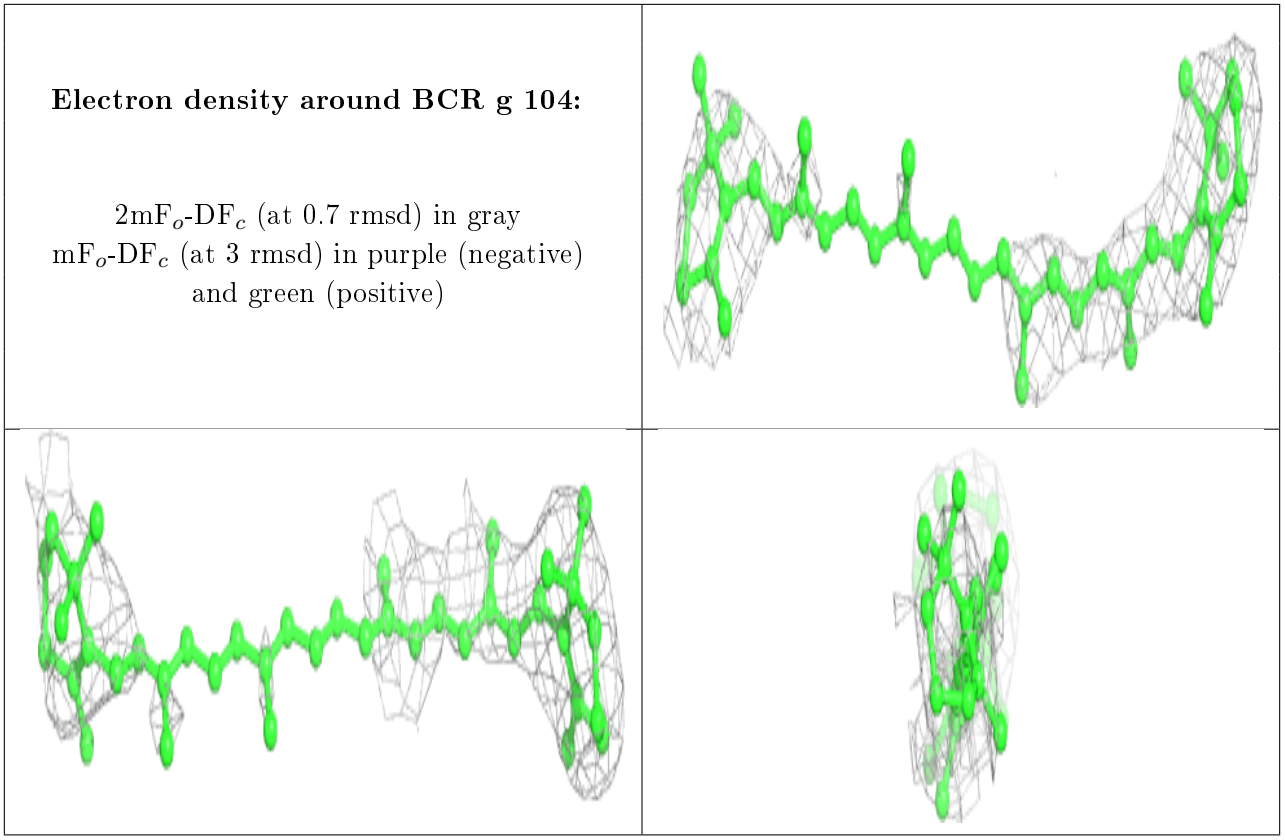
Electron density around LUT 4 616:

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



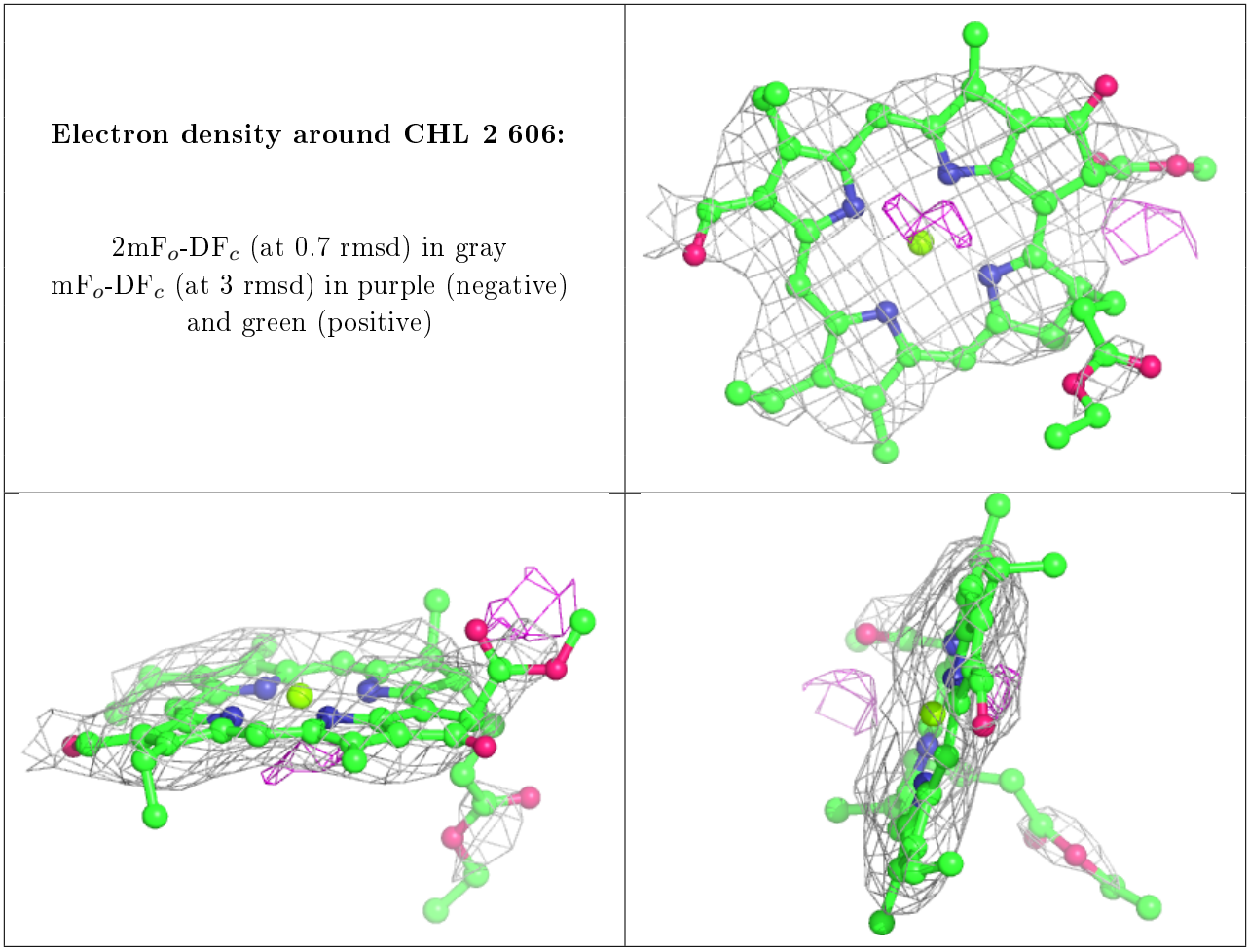
Electron density around BCR g 104:

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



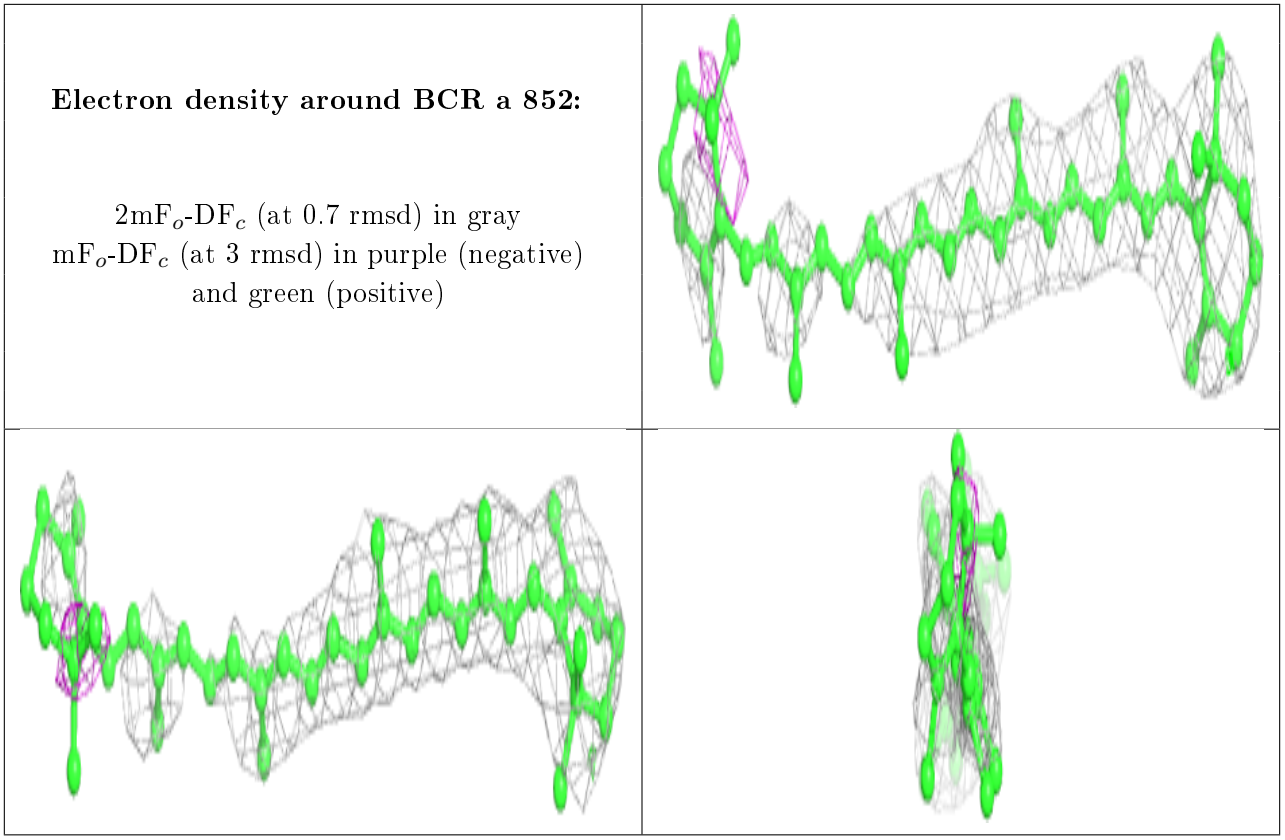
Electron density around CHL 2 606:

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



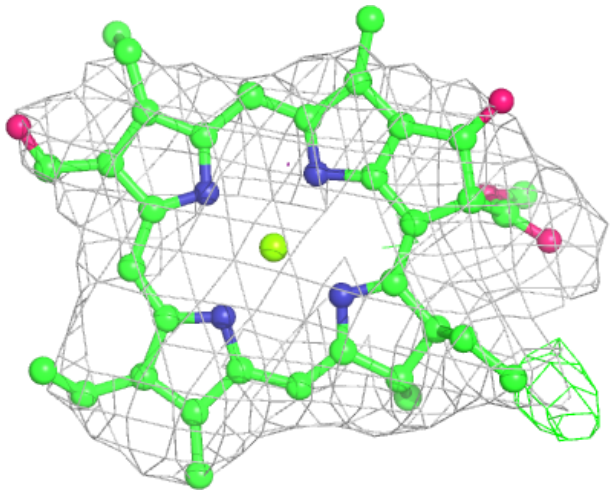
Electron density around BCR a 852:

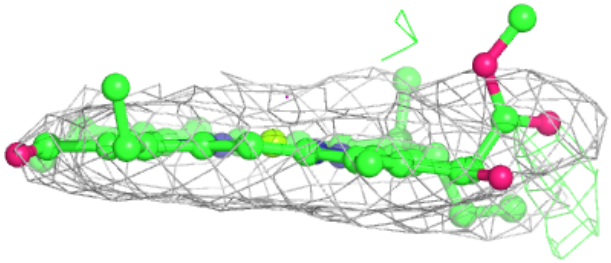
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

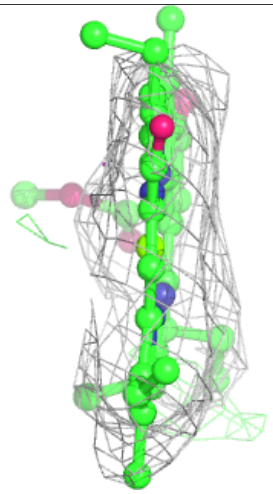


Electron density around CHL 2 605:

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

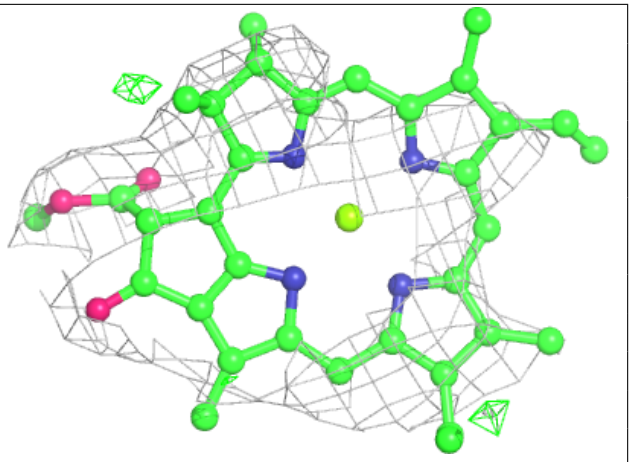


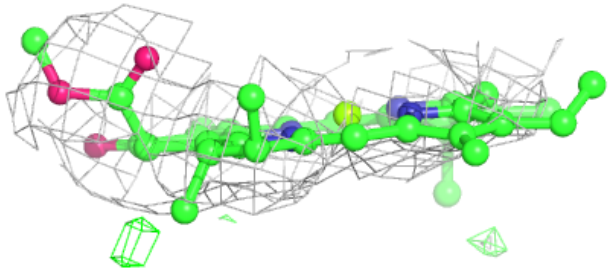


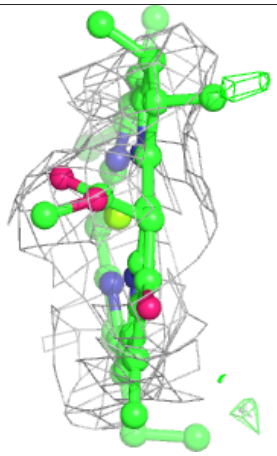


Electron density around CLA g 101:

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

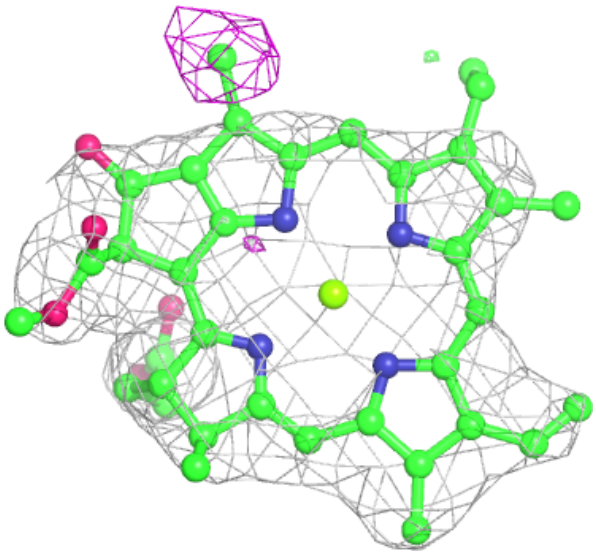


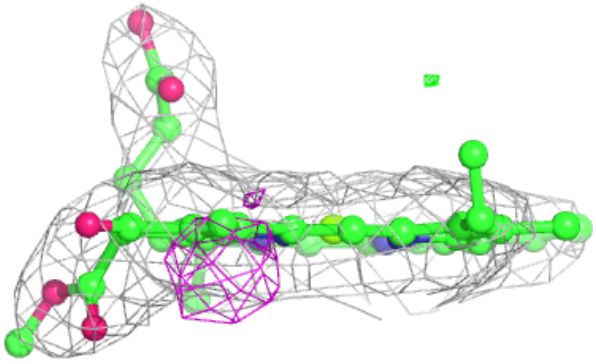


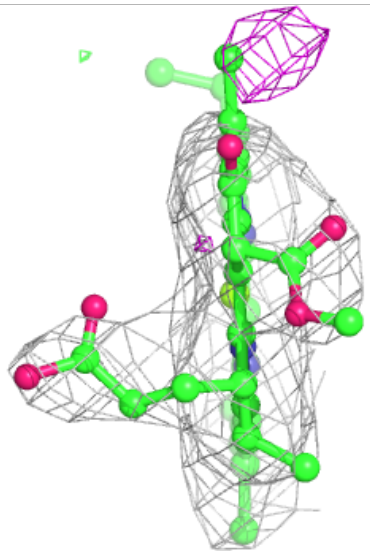


Electron density around CLA A 837:

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

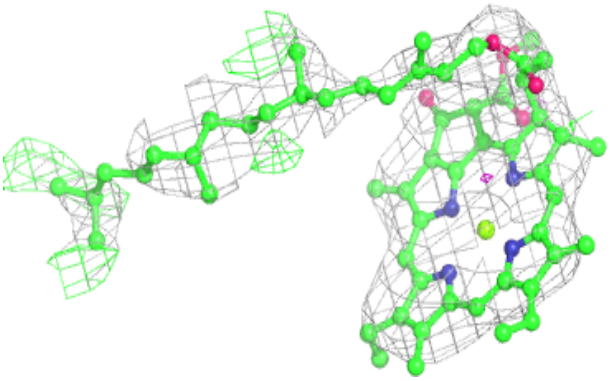


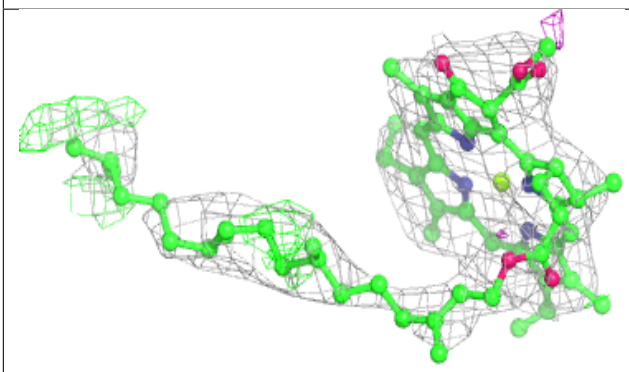


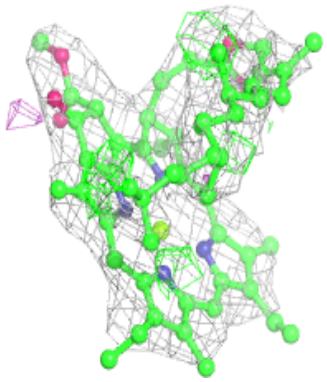


Electron density around CLA 1 309:

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

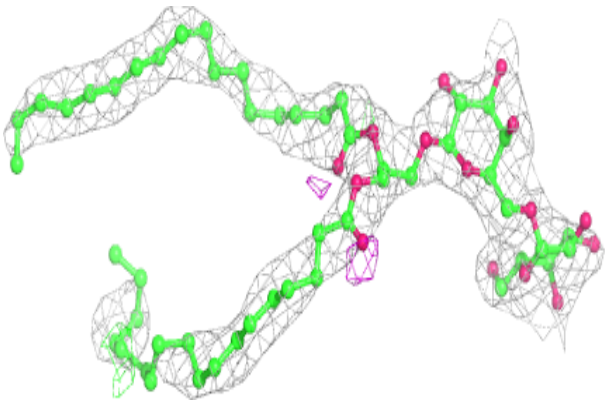


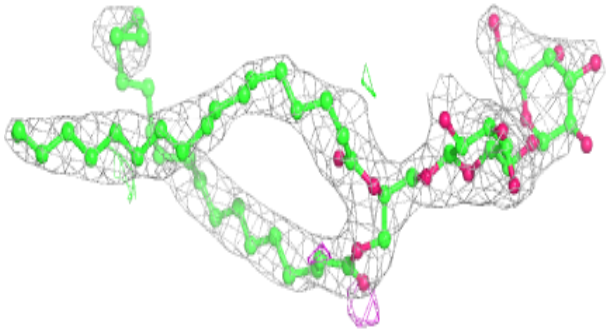


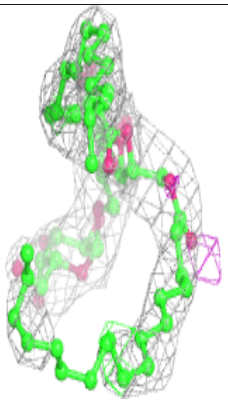


Electron density around DGD b 849:

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

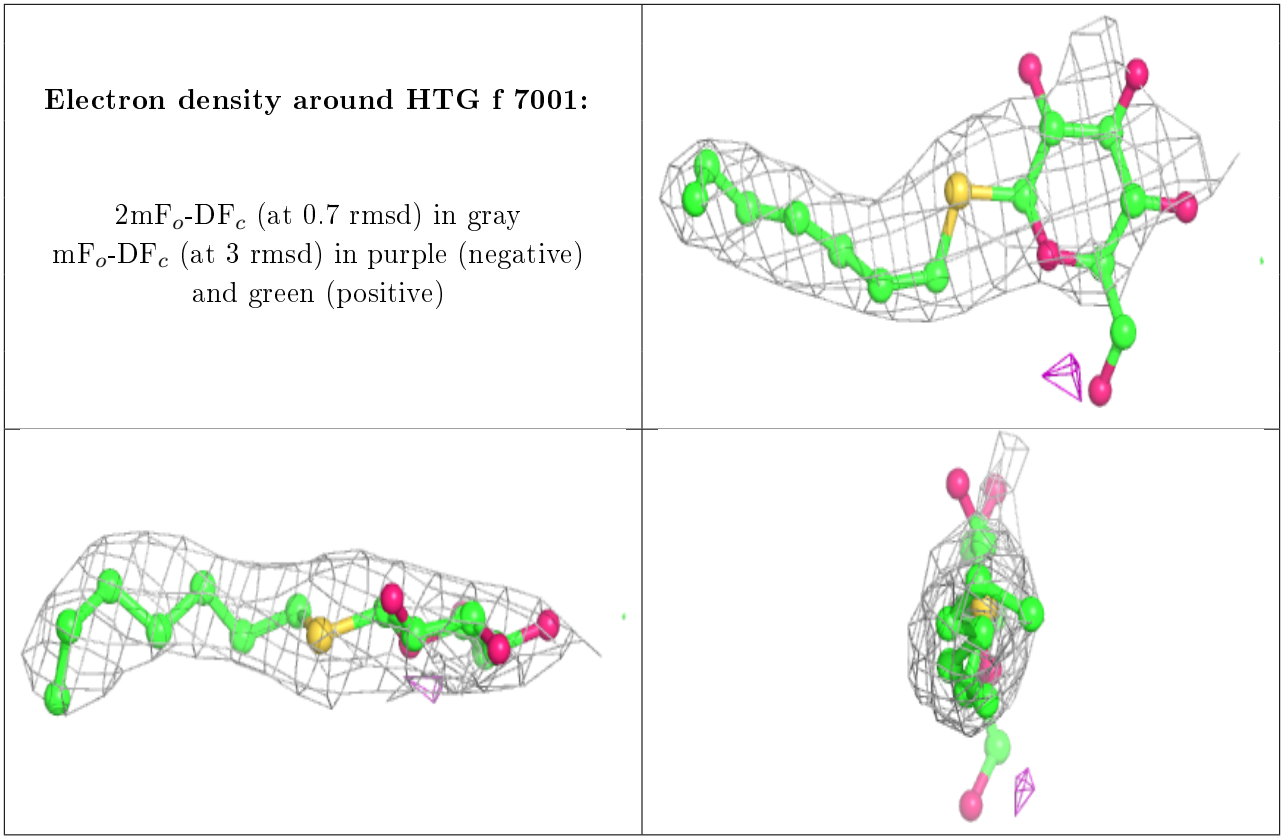






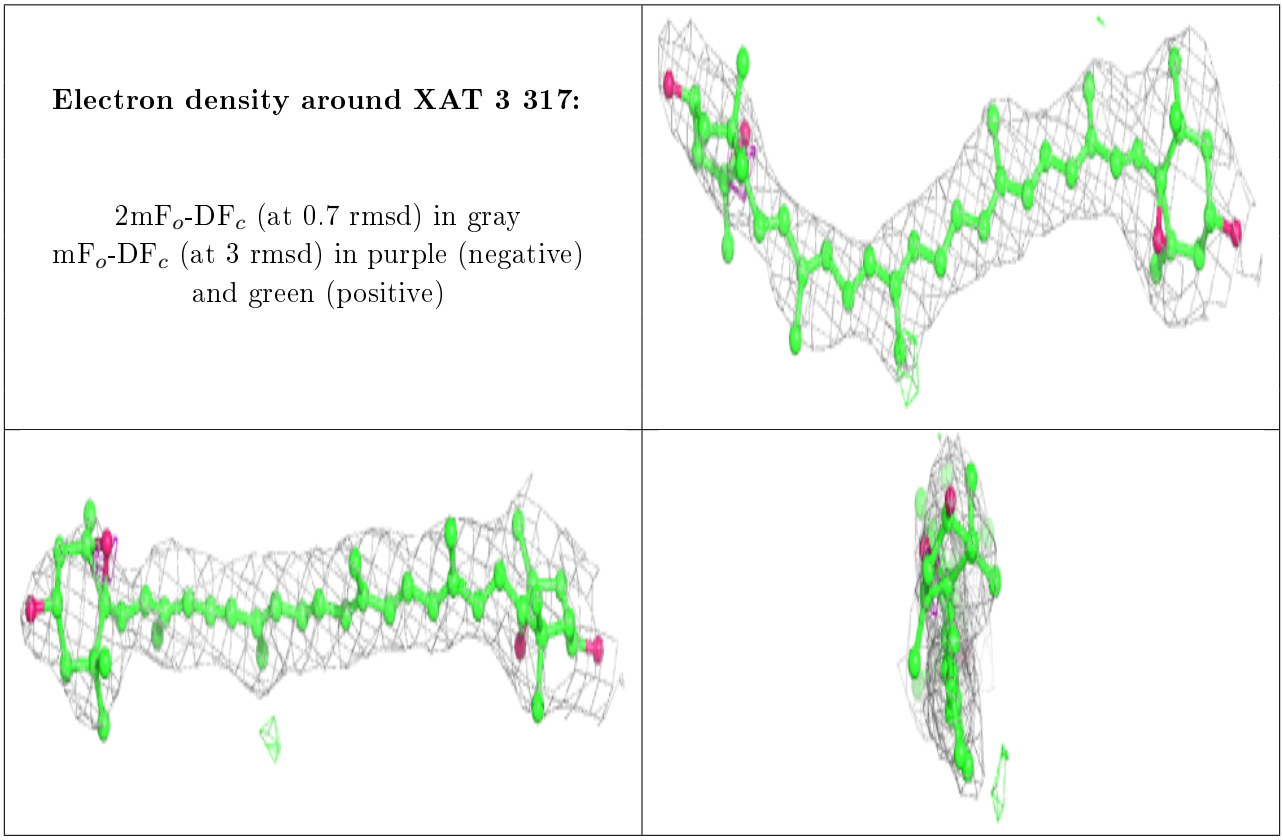
Electron density around HTG f 7001:

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



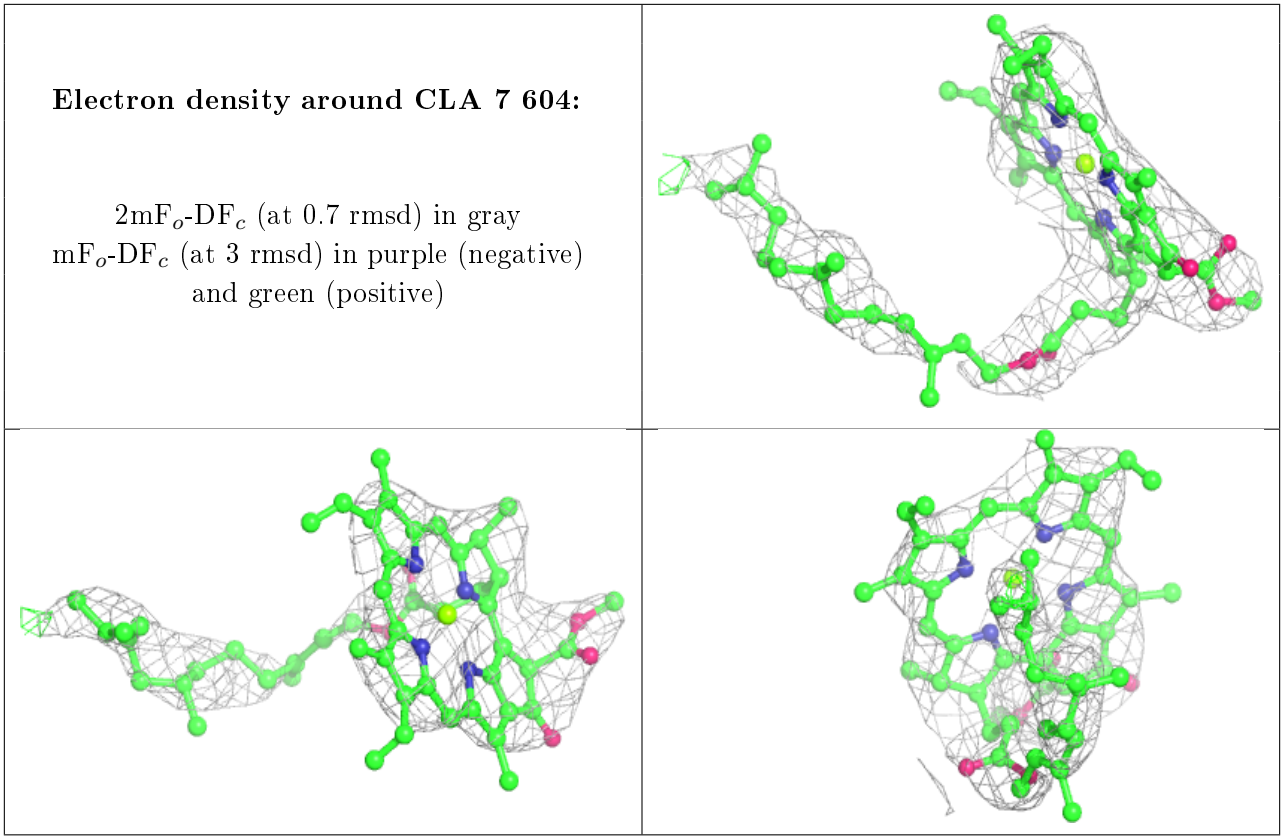
Electron density around XAT 3 317:

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



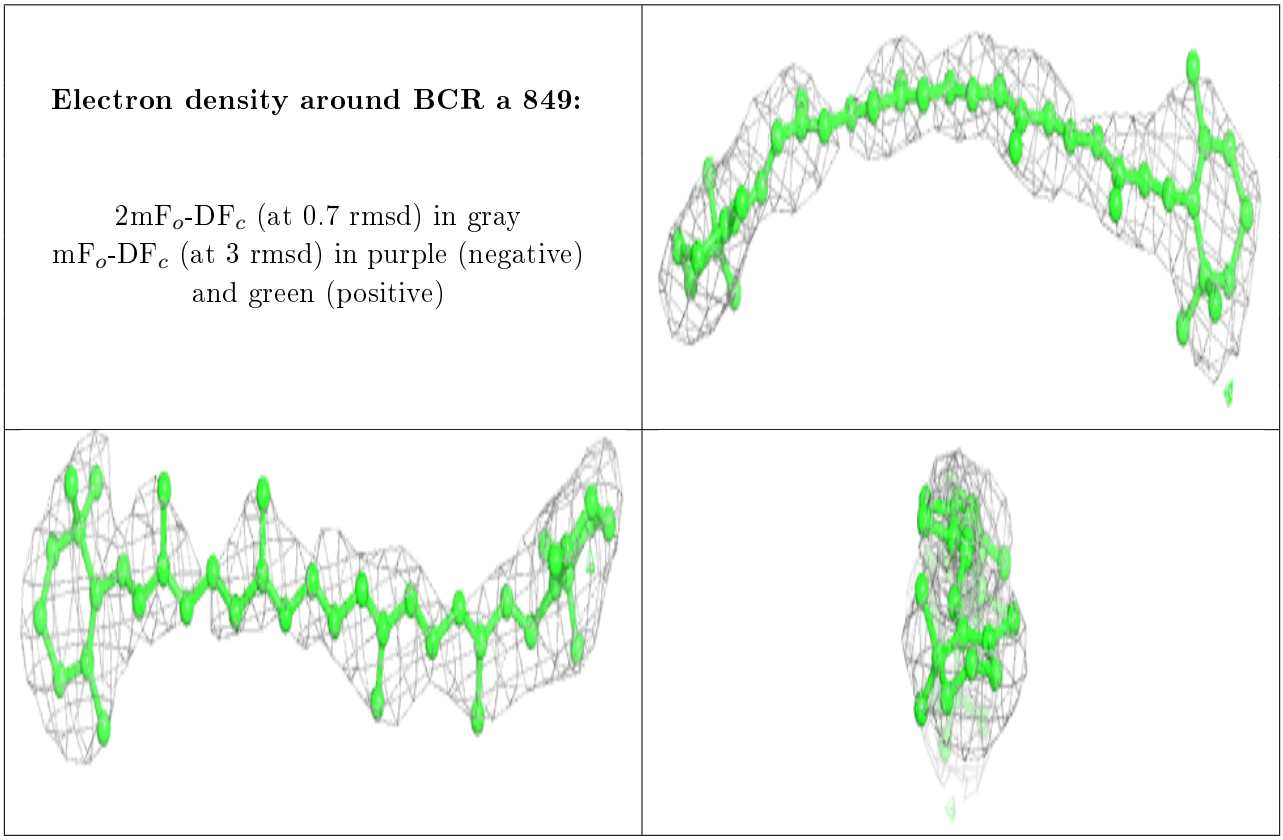
Electron density around CLA 7 604:

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



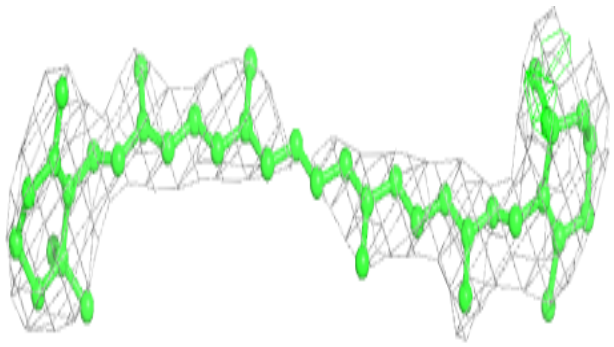
Electron density around BCR a 849:

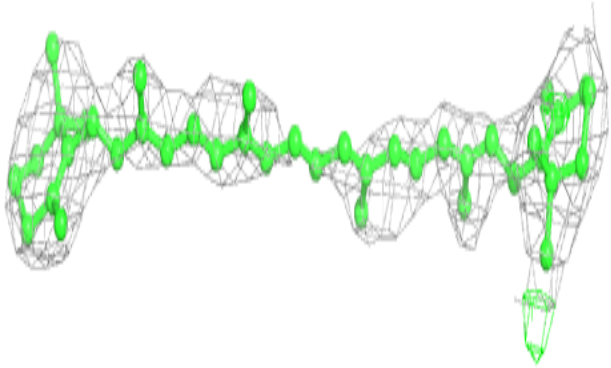
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

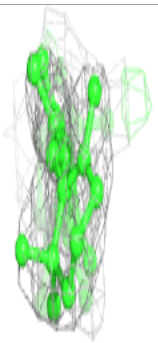


Electron density around BCR k 1404:

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

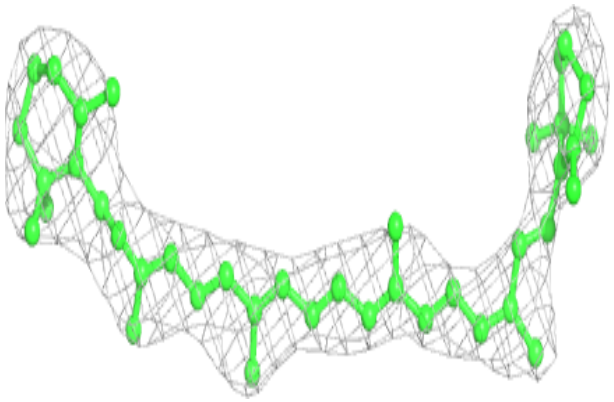


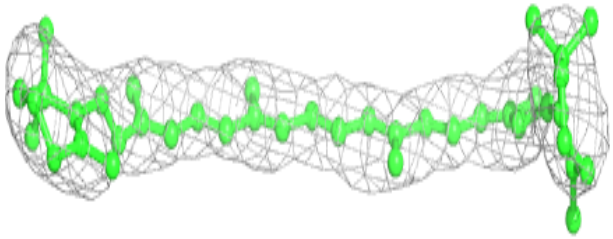


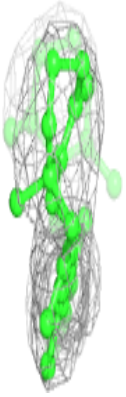


Electron density around BCR B 844:

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

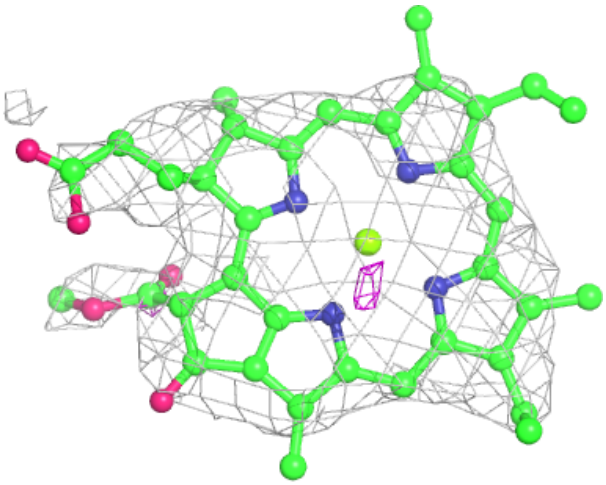


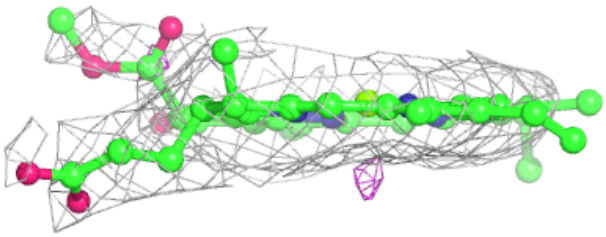


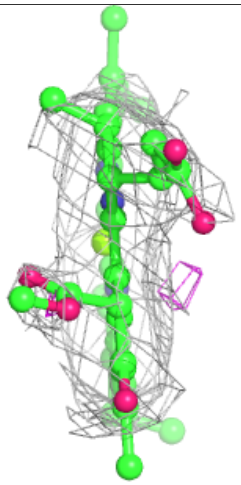


Electron density around CLA 3 313:

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

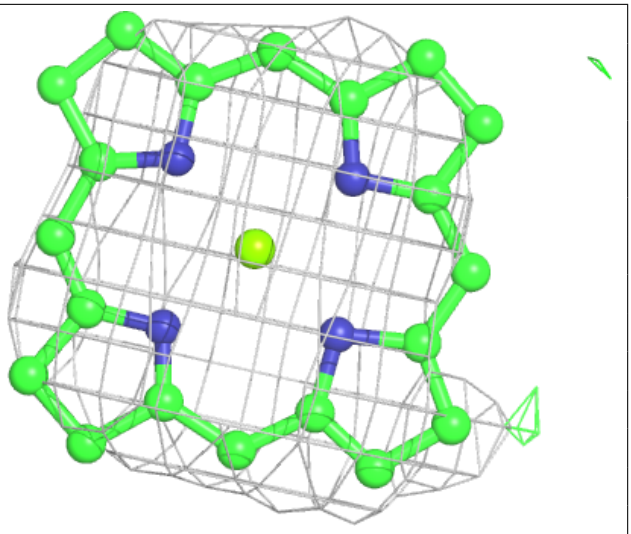


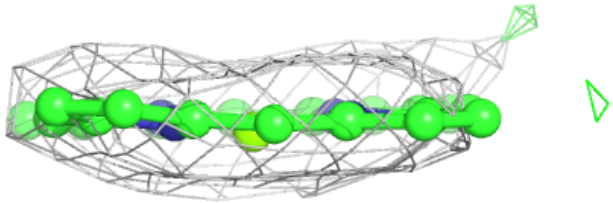


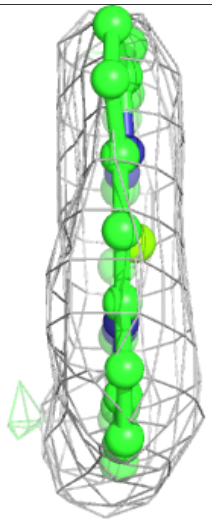


Electron density around CLA 3 315:

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

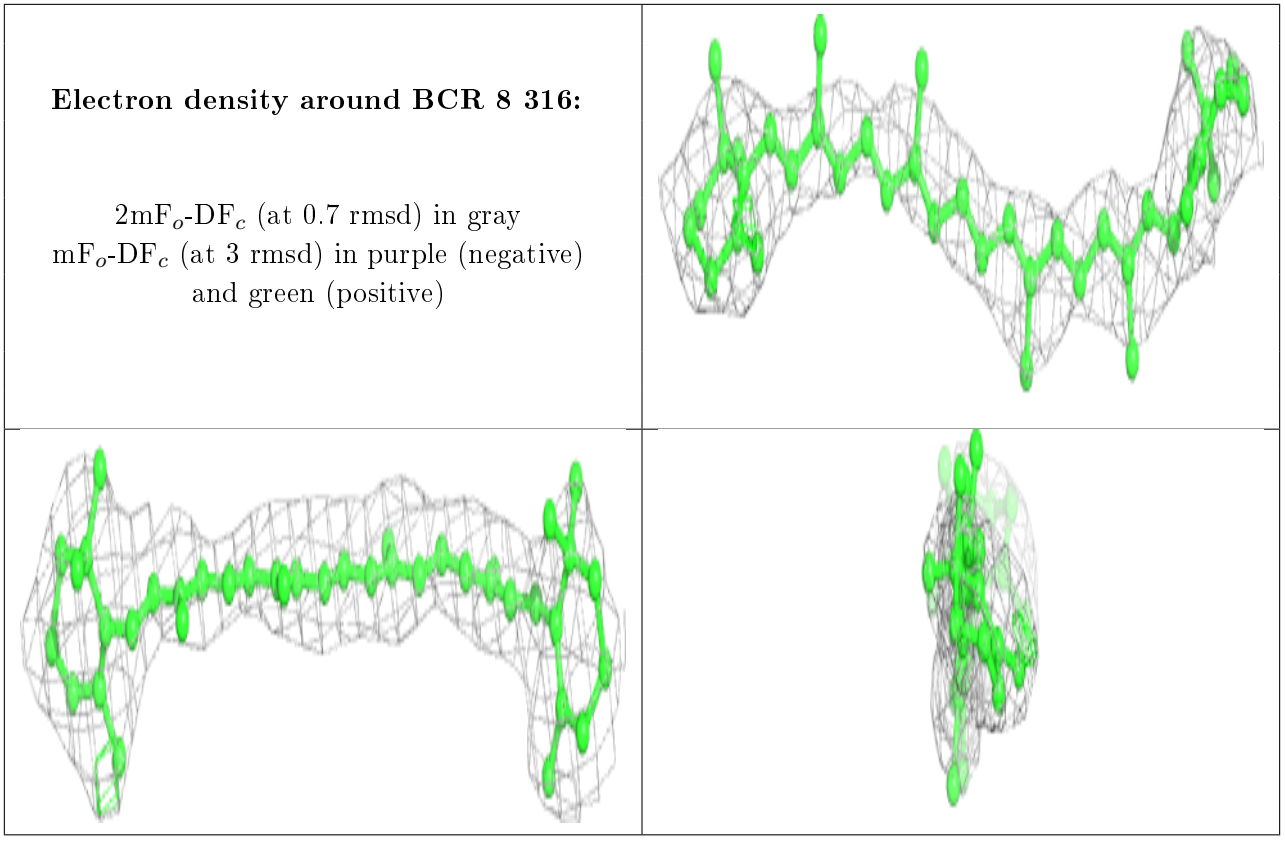






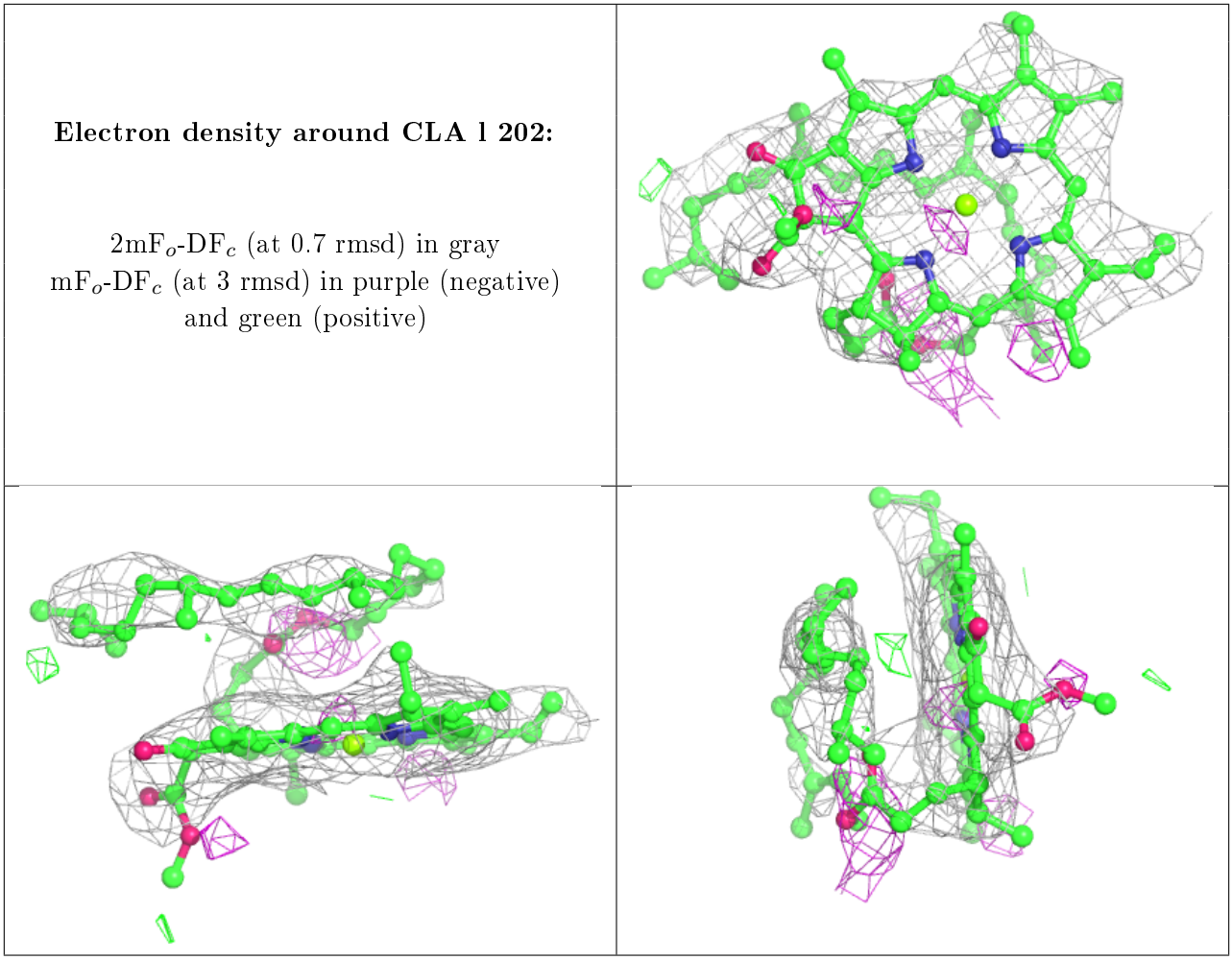
Electron density around BCR 8 316:

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



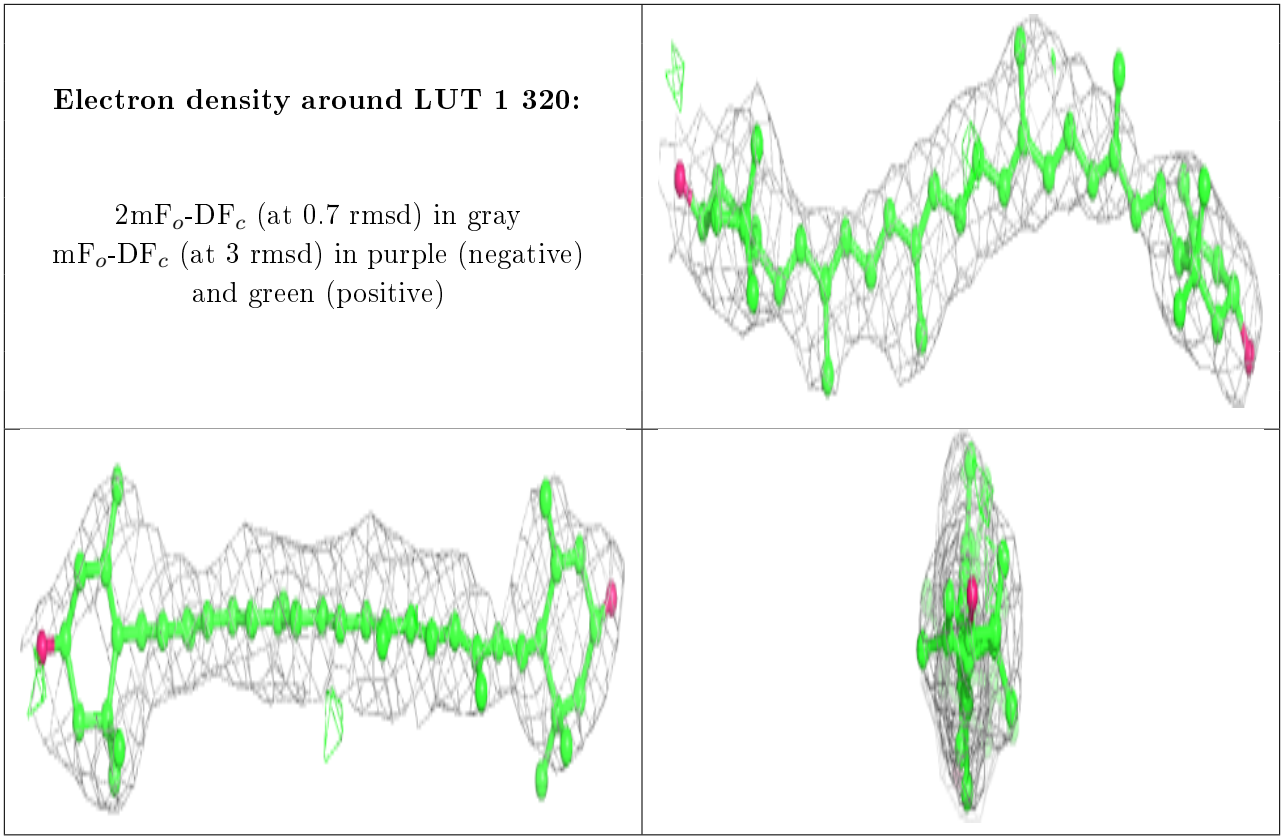
Electron density around CLA l 202:

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



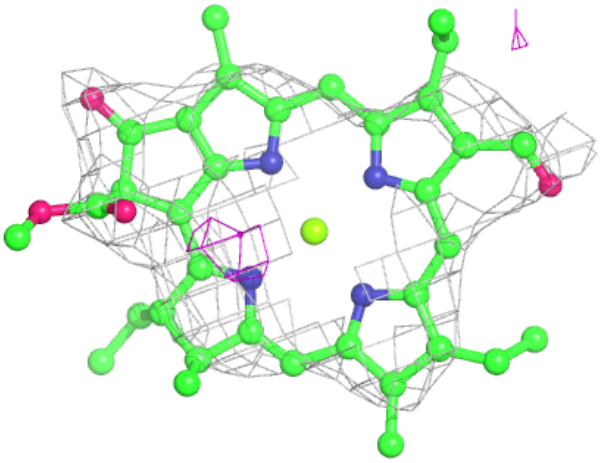
Electron density around LUT 1 320:

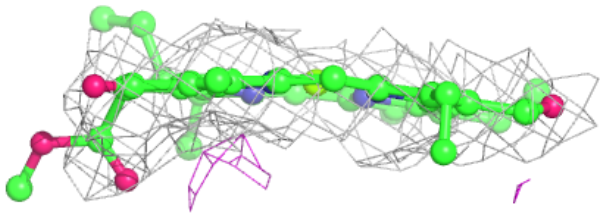
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

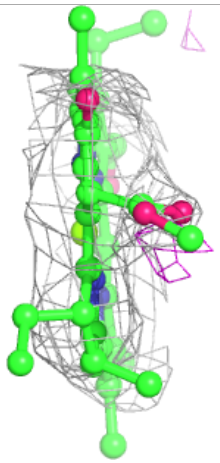


Electron density around CHL 9 615:

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

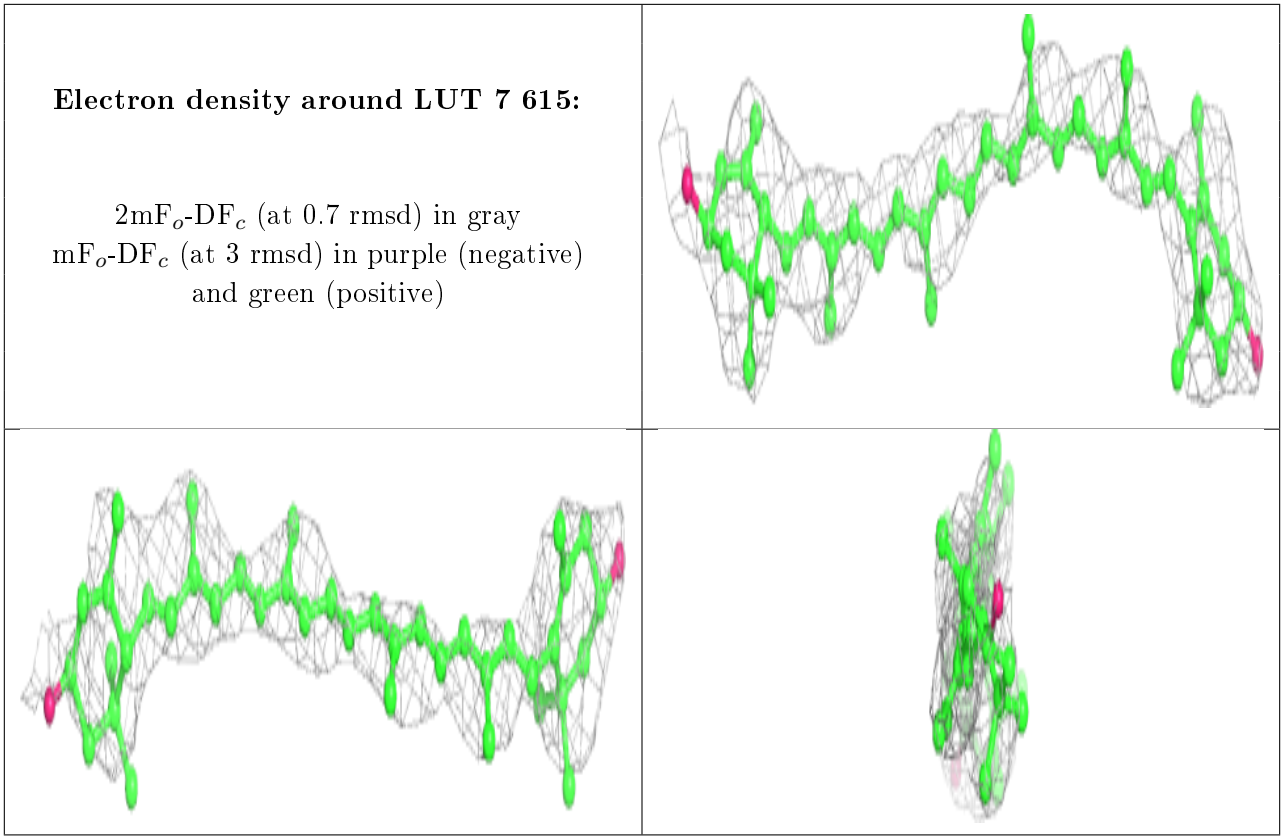






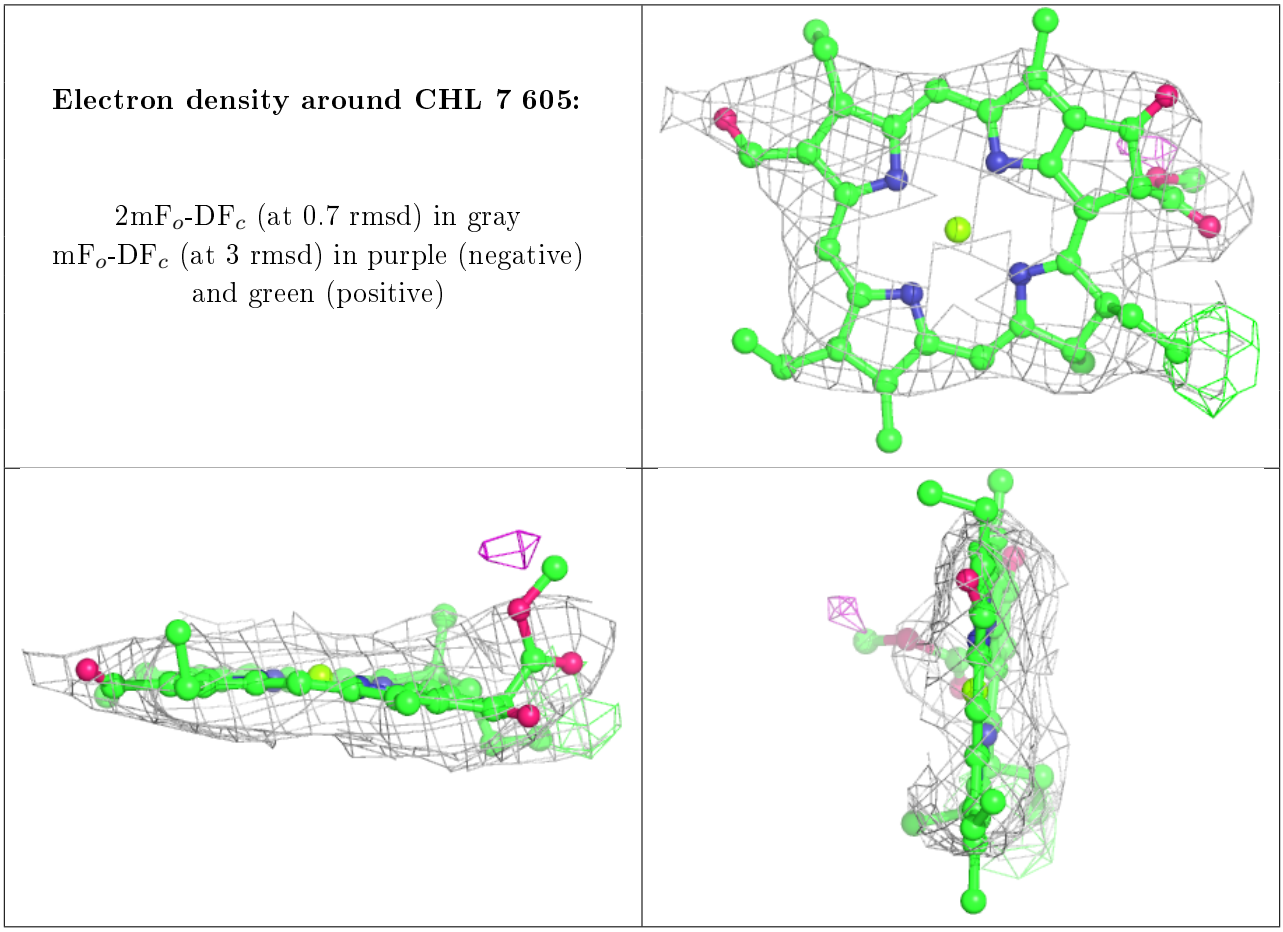
Electron density around LUT 7 615:

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



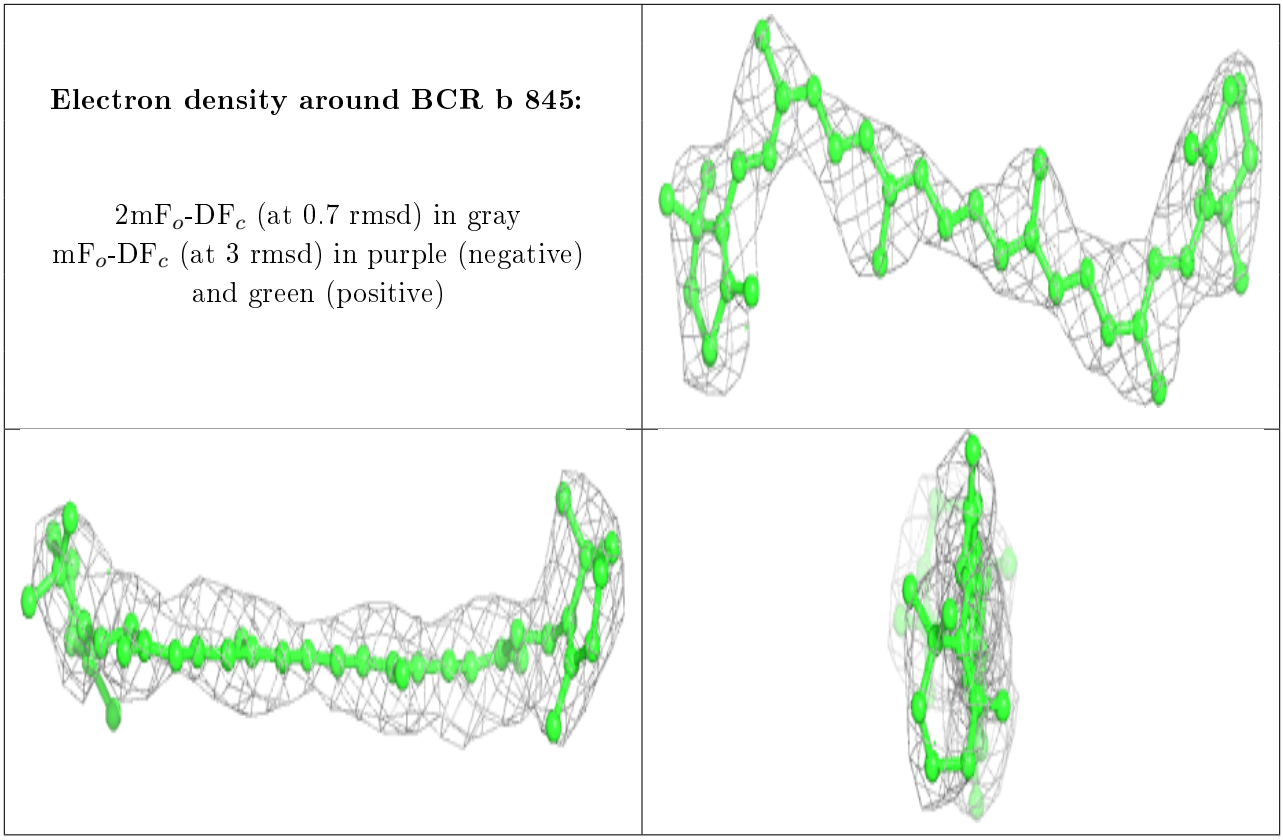
Electron density around CHL 7 605:

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



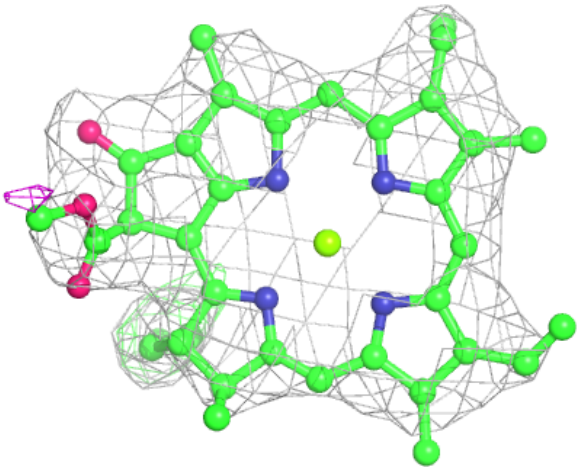
Electron density around BCR b 845:

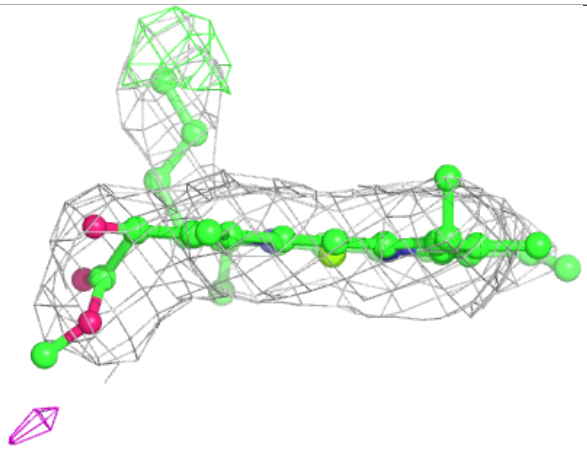
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

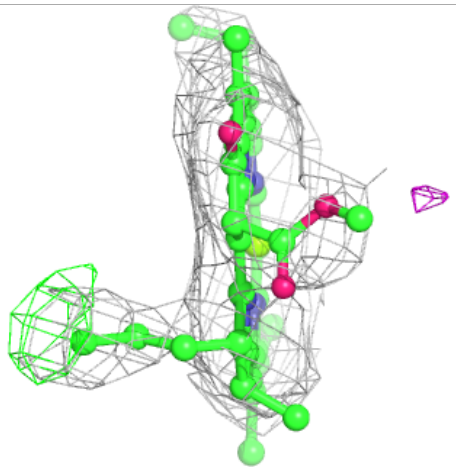


Electron density around CLA 2 613:

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

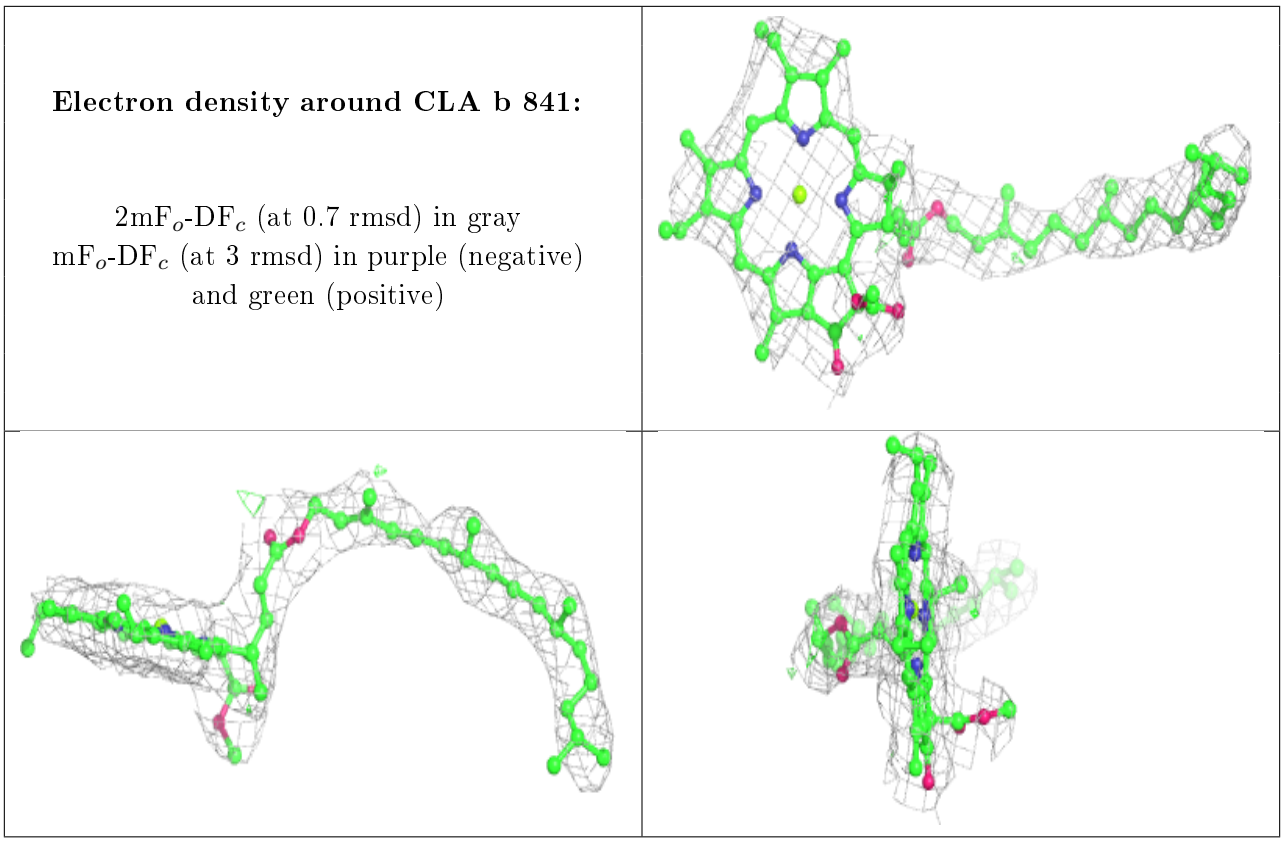






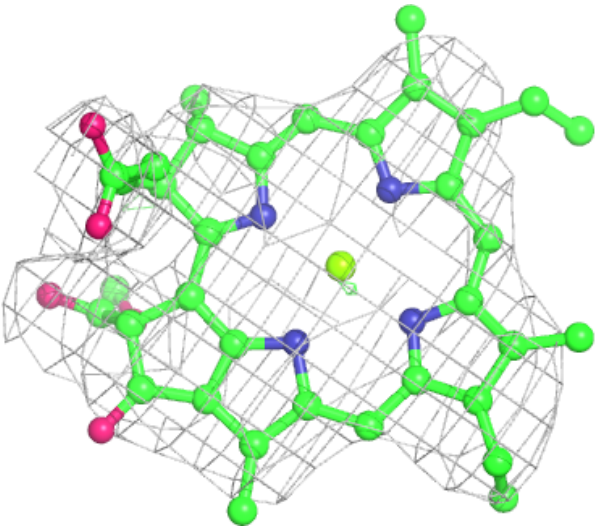
Electron density around CLA b 841:

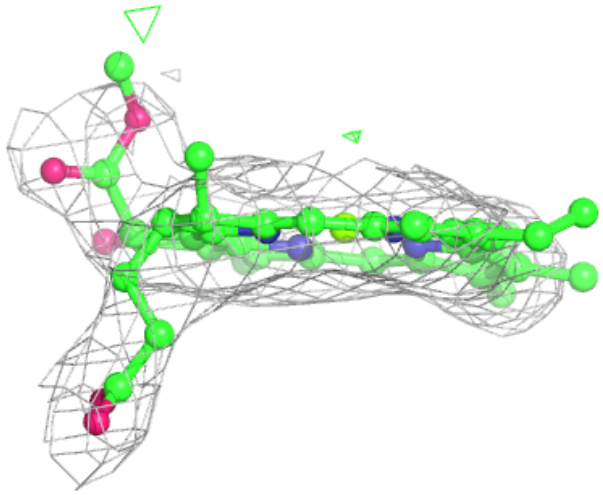
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

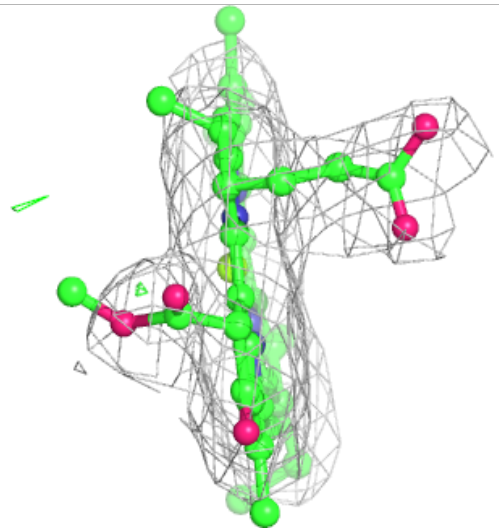


Electron density around CLA k 1401:

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

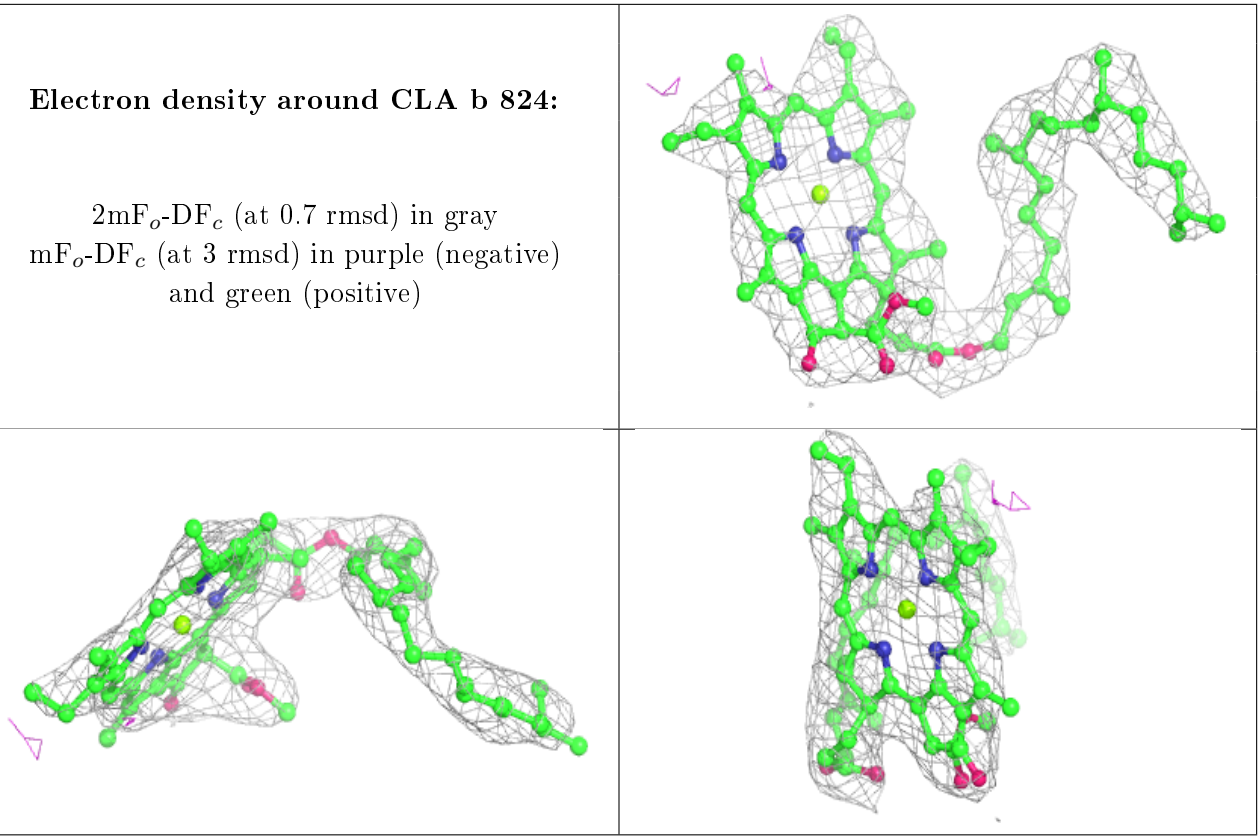






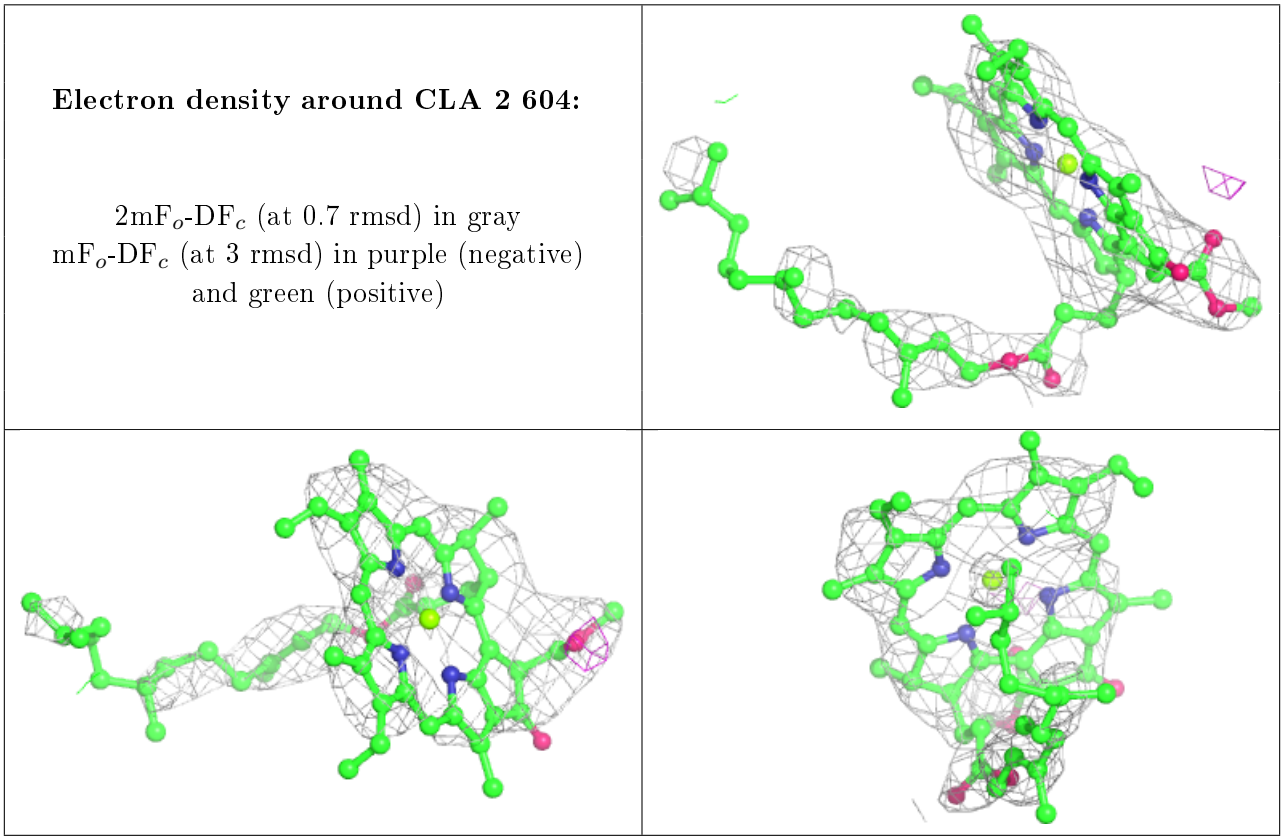
Electron density around CLA b 824:

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



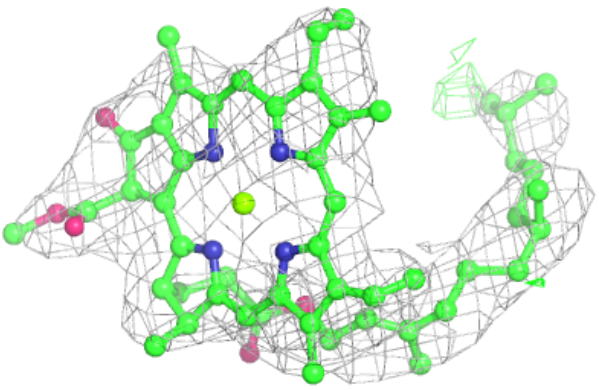
Electron density around CLA 2 604:

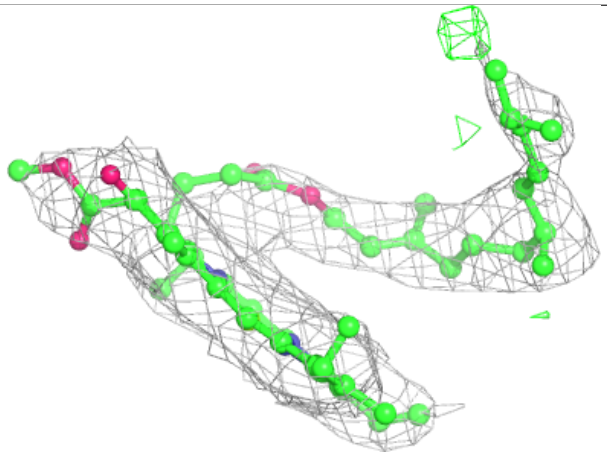
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

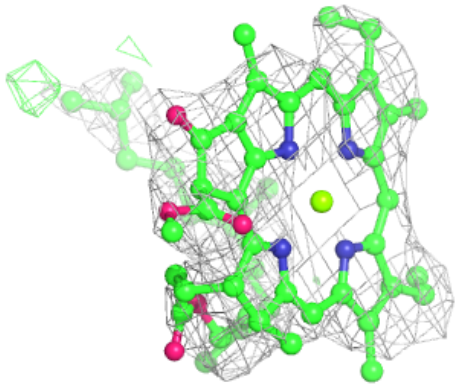


Electron density around CLA 2 609:

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

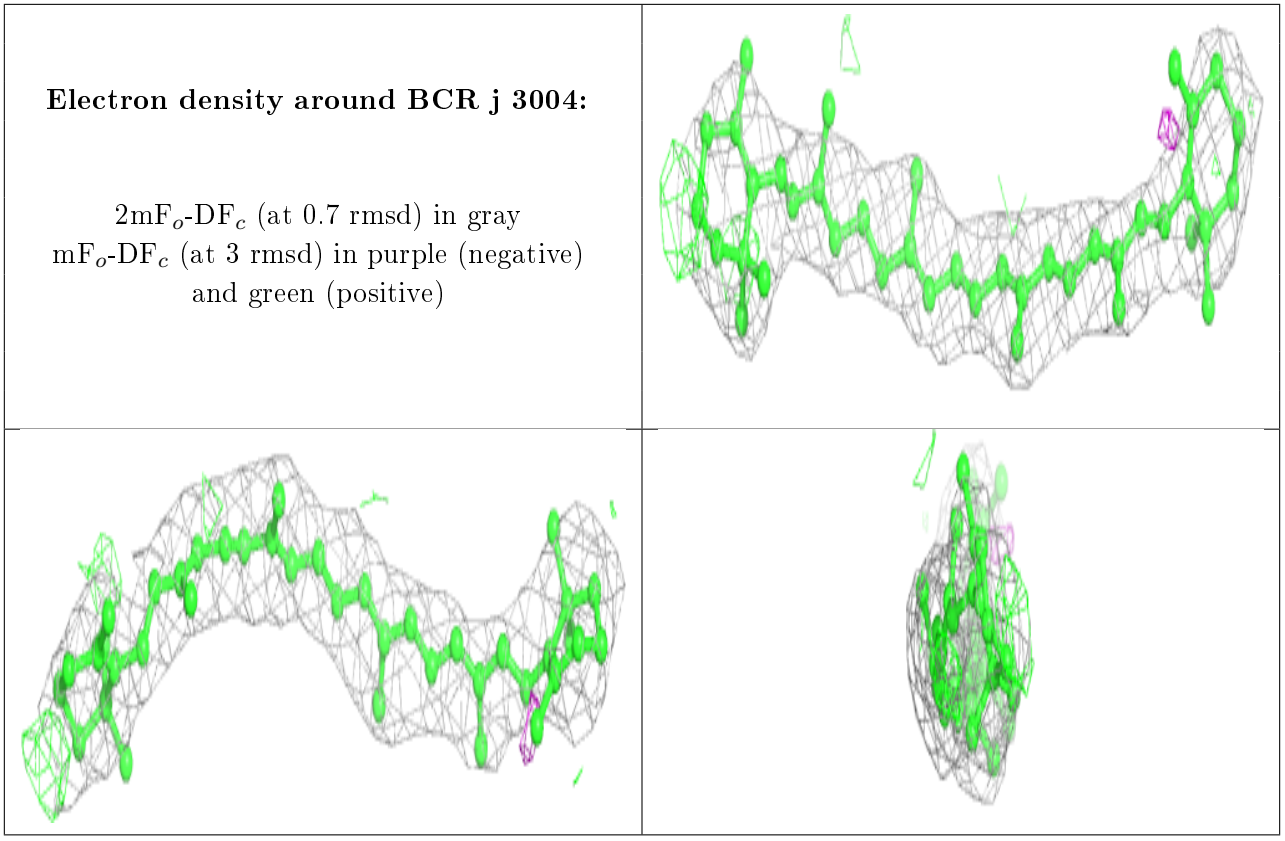






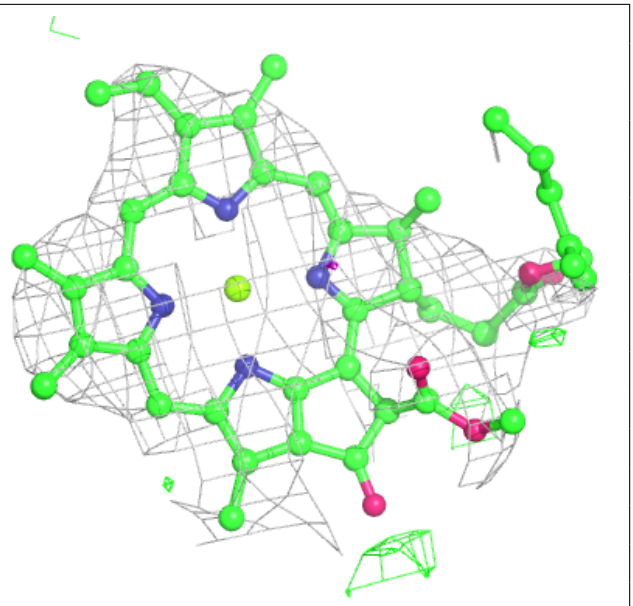
Electron density around BCR j 3004:

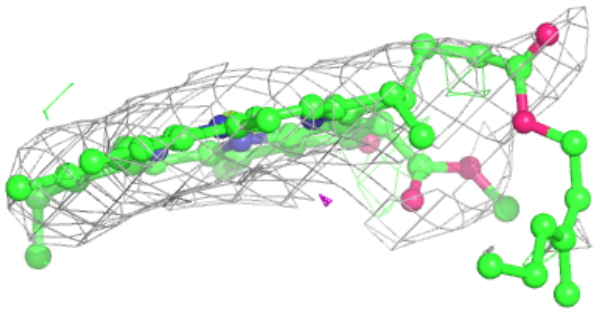
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

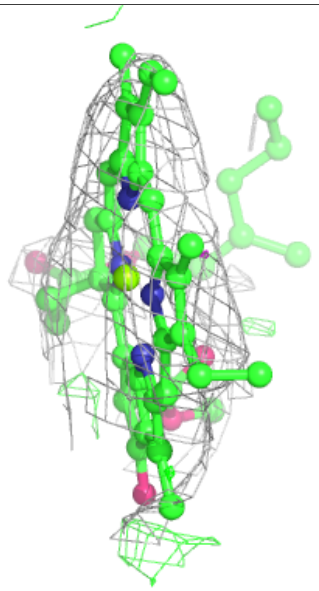


Electron density around CLA 6 313:

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

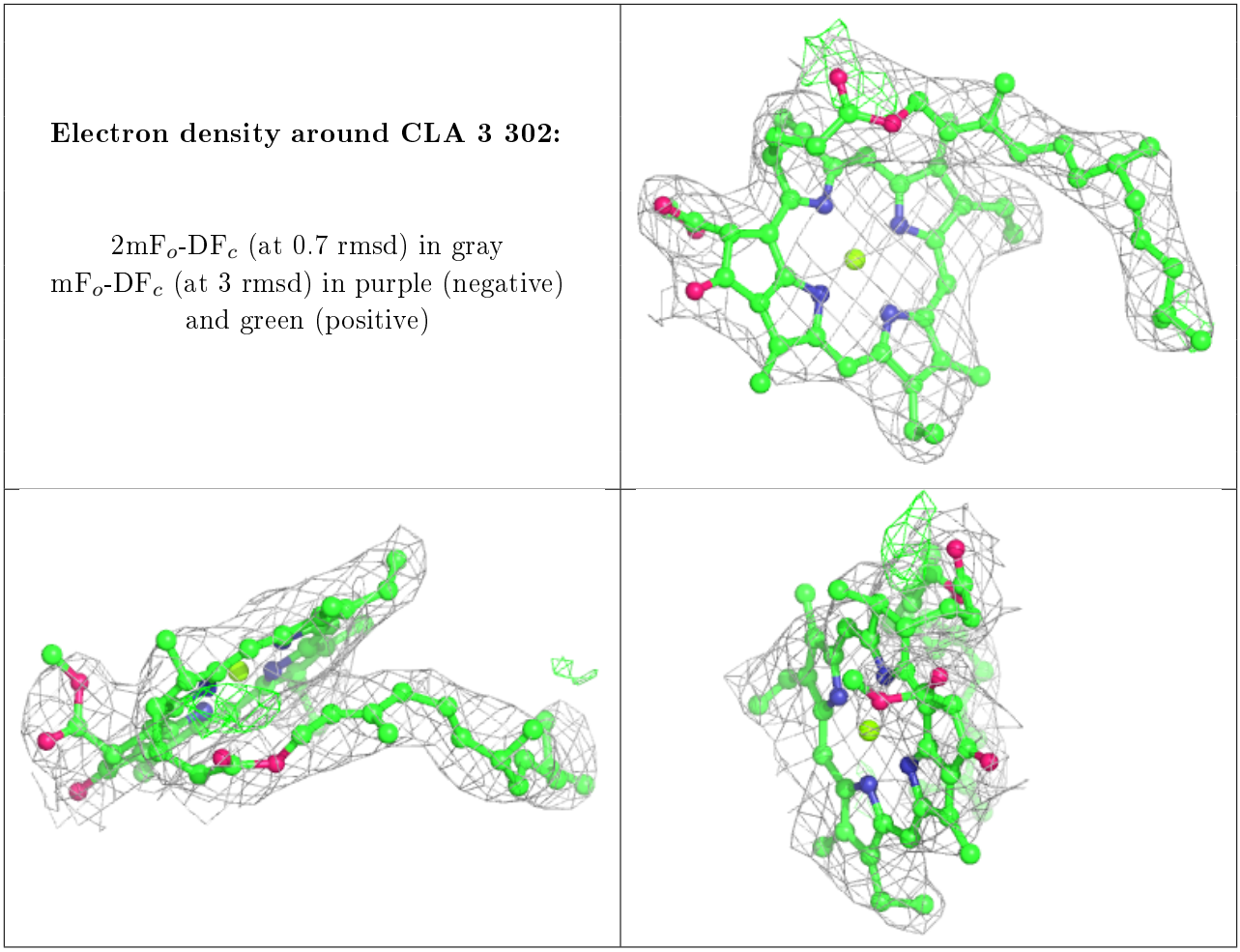






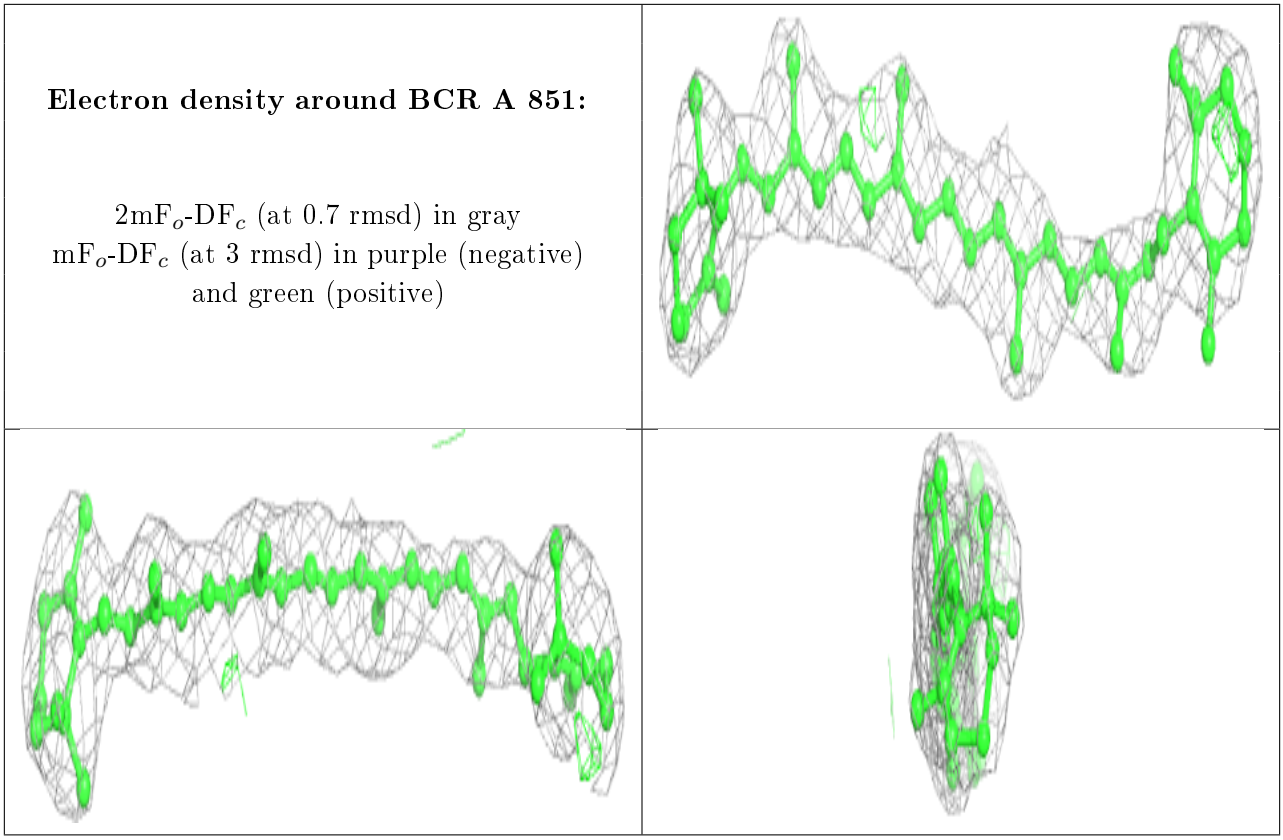
Electron density around CLA 3 302:

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



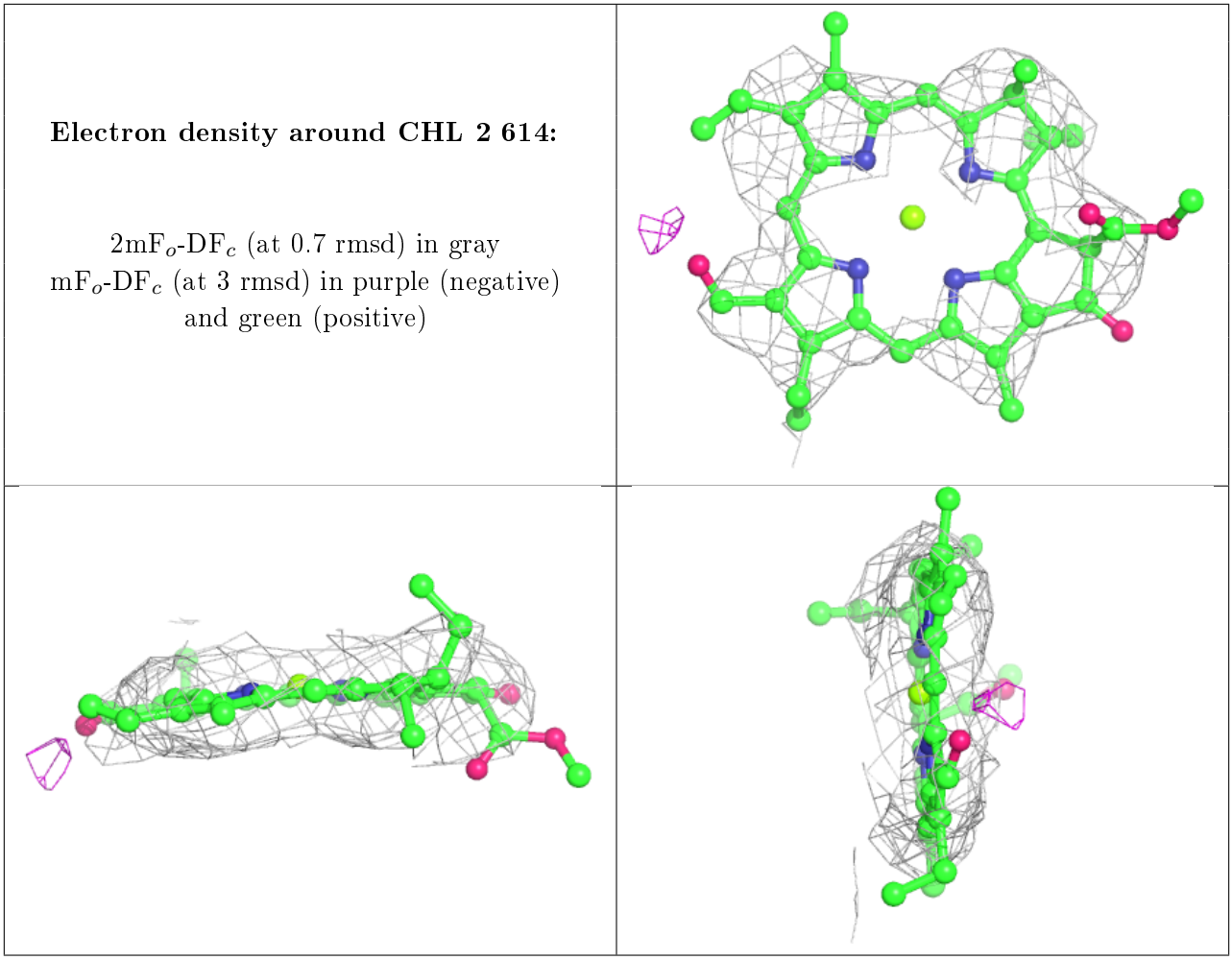
Electron density around BCR A 851:

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



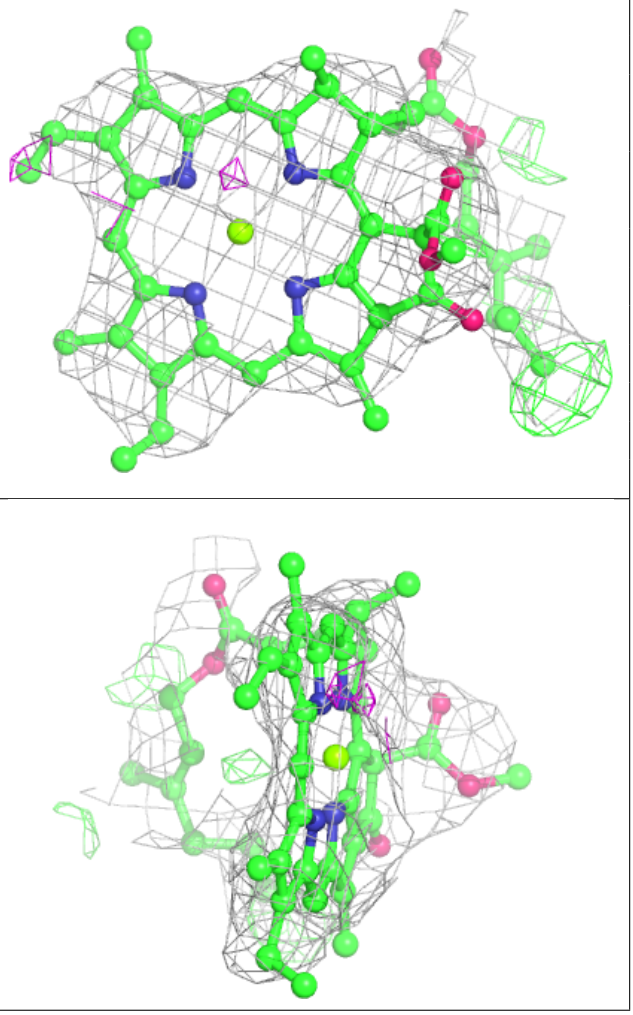
Electron density around CHL 2 614:

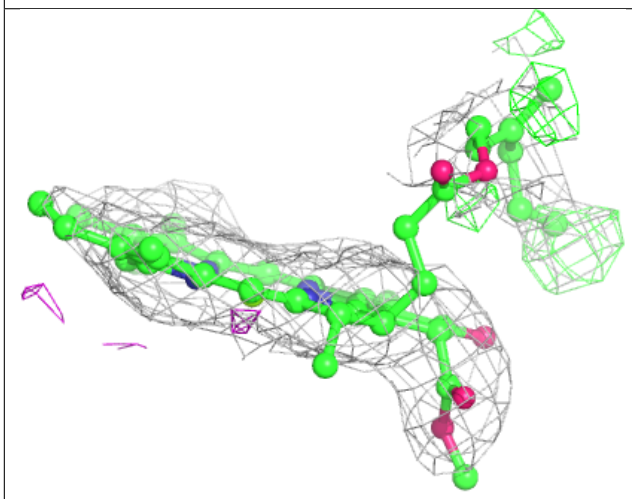
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



Electron density around CLA a 846:

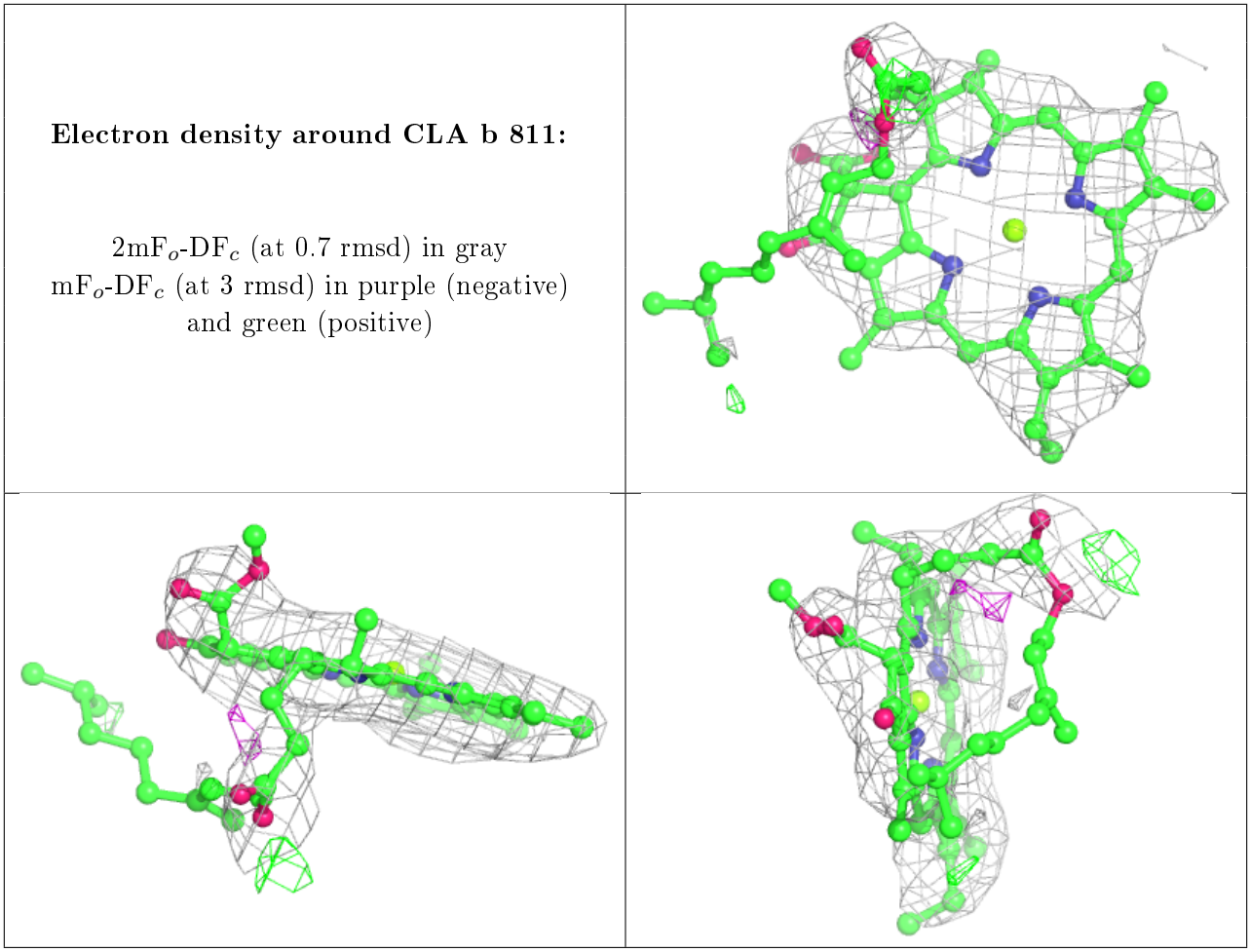
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)





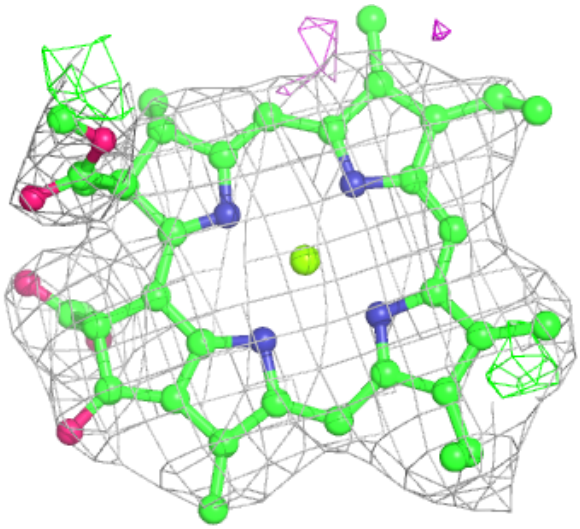
Electron density around CLA b 811:

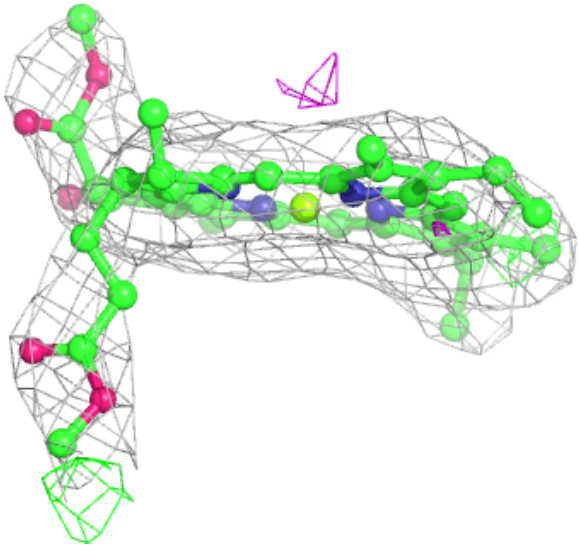
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

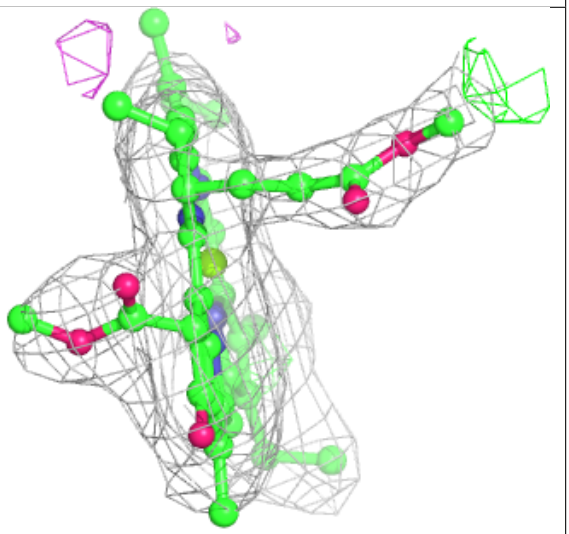


Electron density around CLA B 821:

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

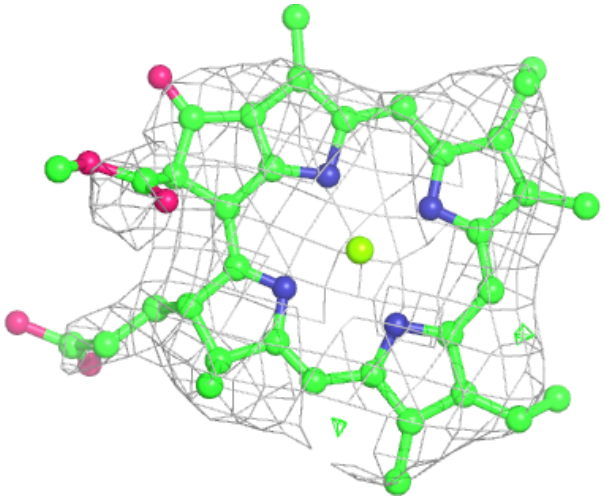


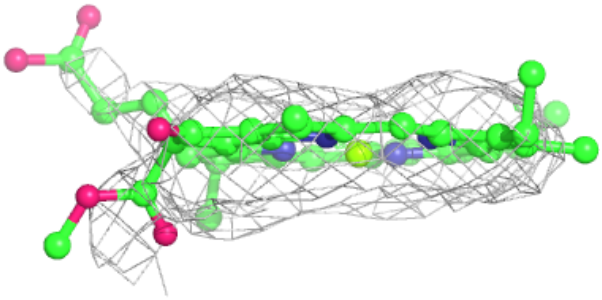


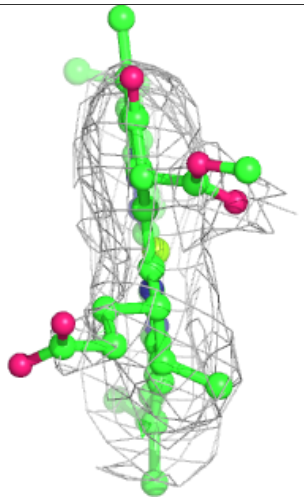


Electron density around CLA 8 311:

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

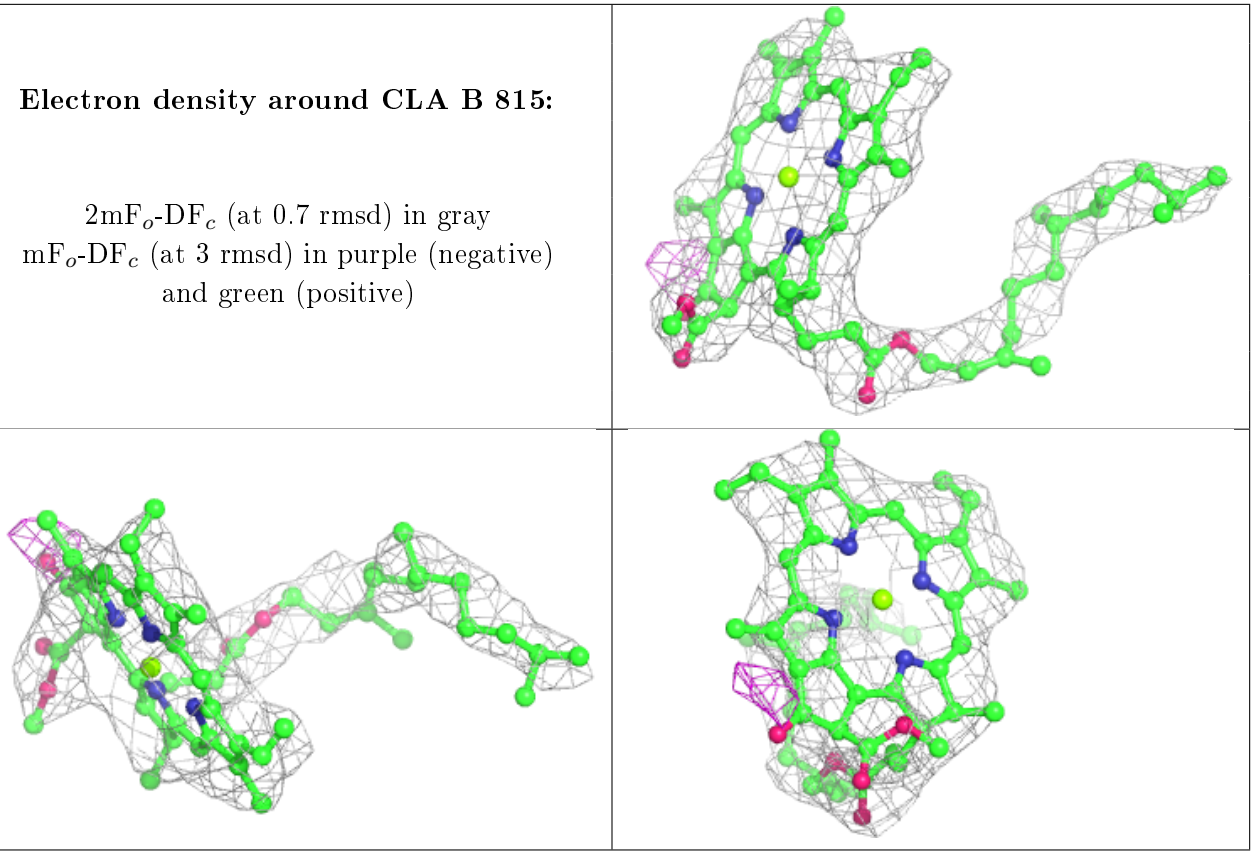






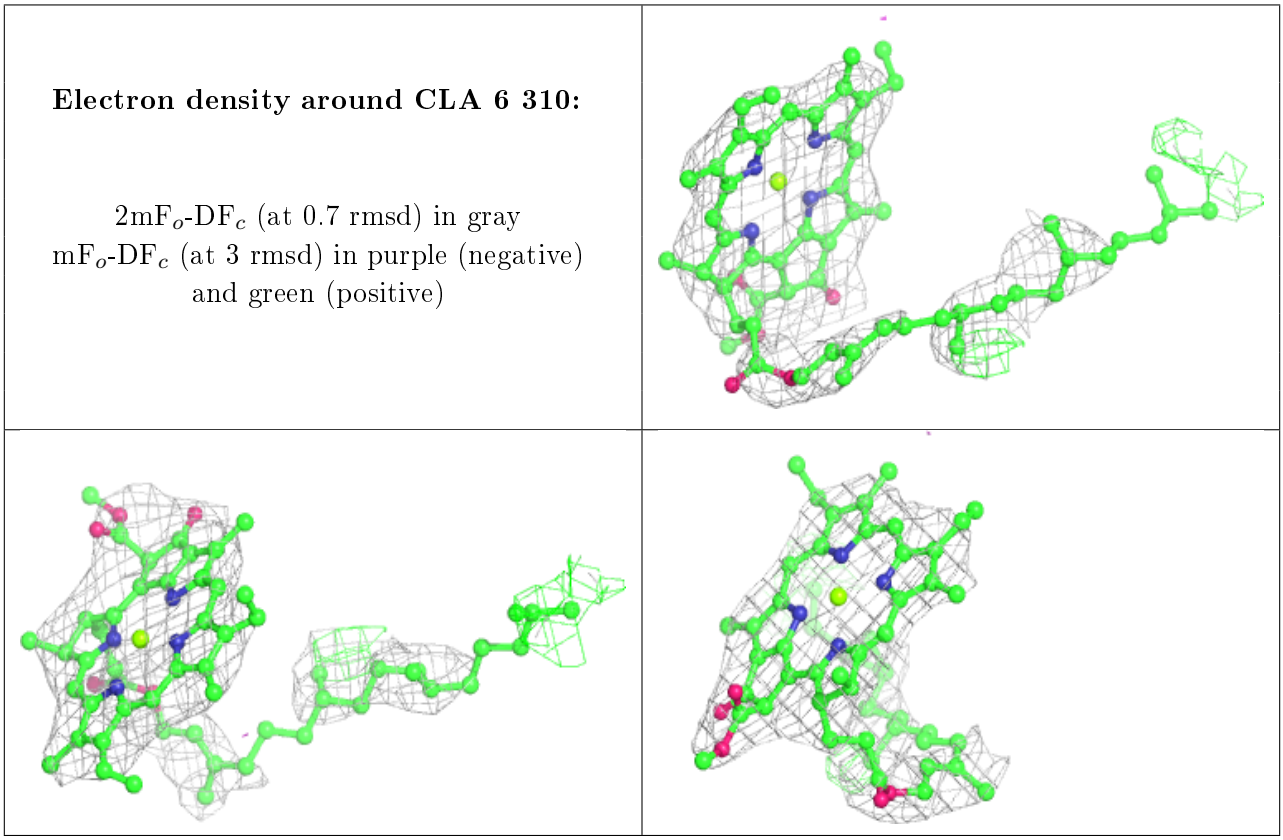
Electron density around CLA B 815:

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



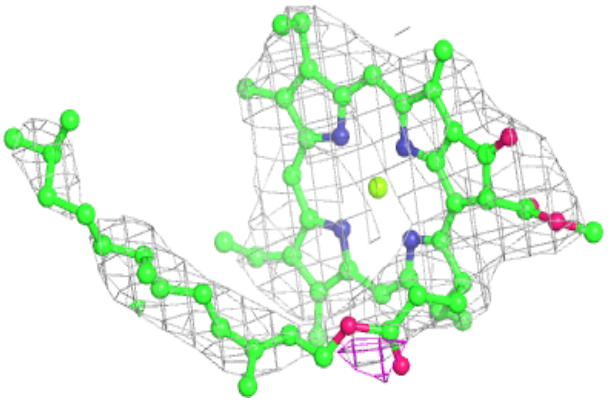
Electron density around CLA 6 310:

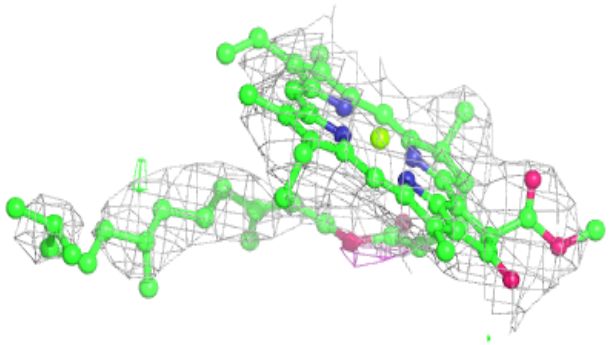
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

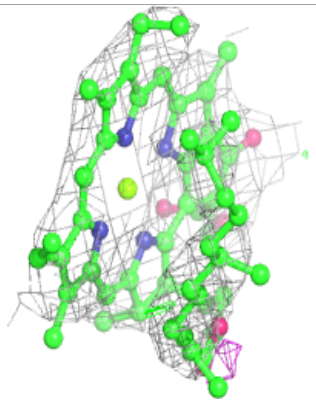


Electron density around CLA 4 609:

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

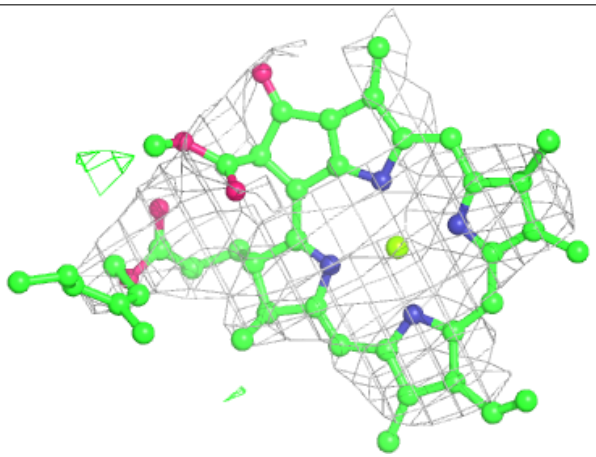


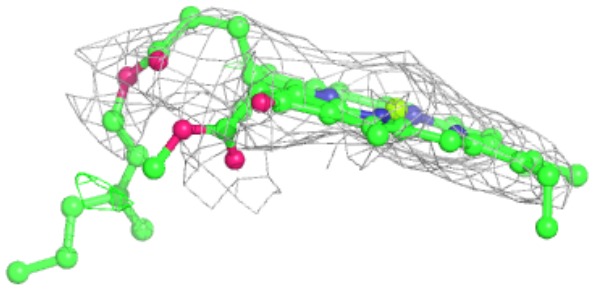


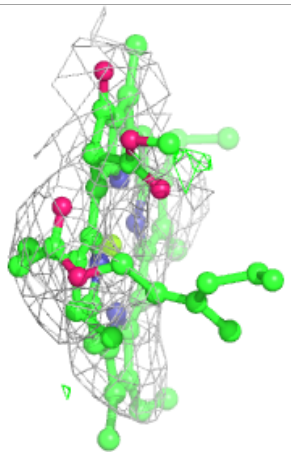


Electron density around CLA 3 311:

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

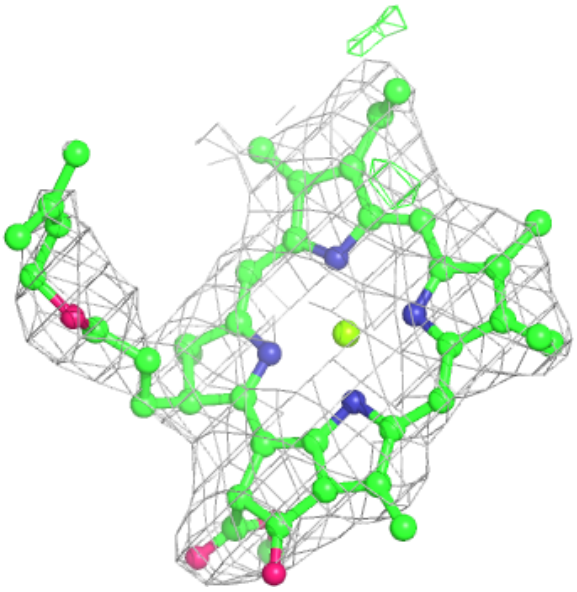


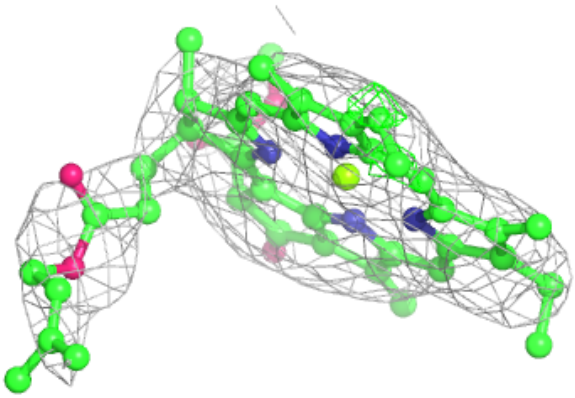


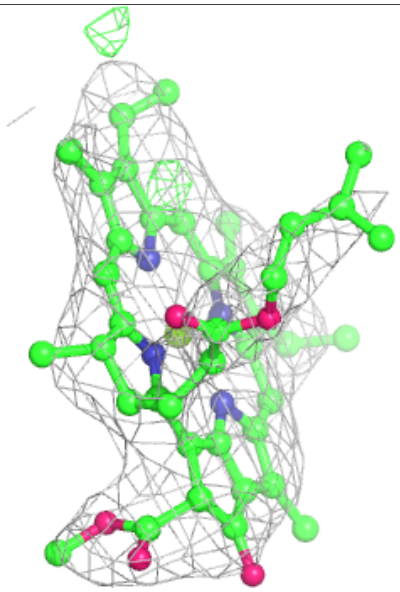


Electron density around CLA A 832:

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

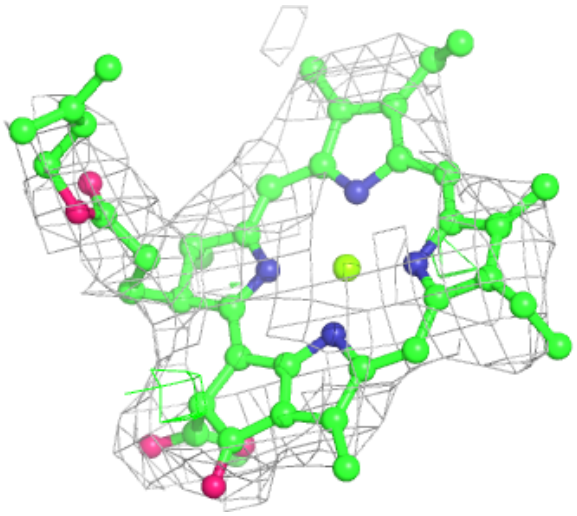


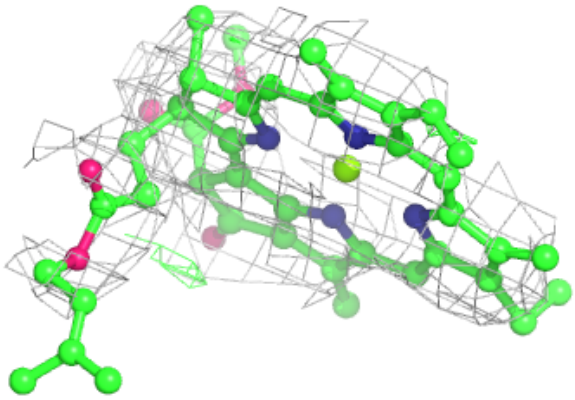


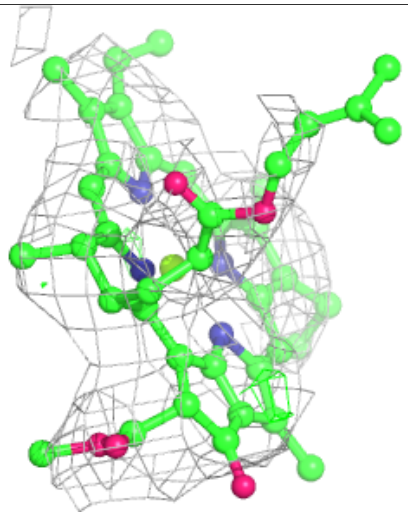


Electron density around CLA 9 604:

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

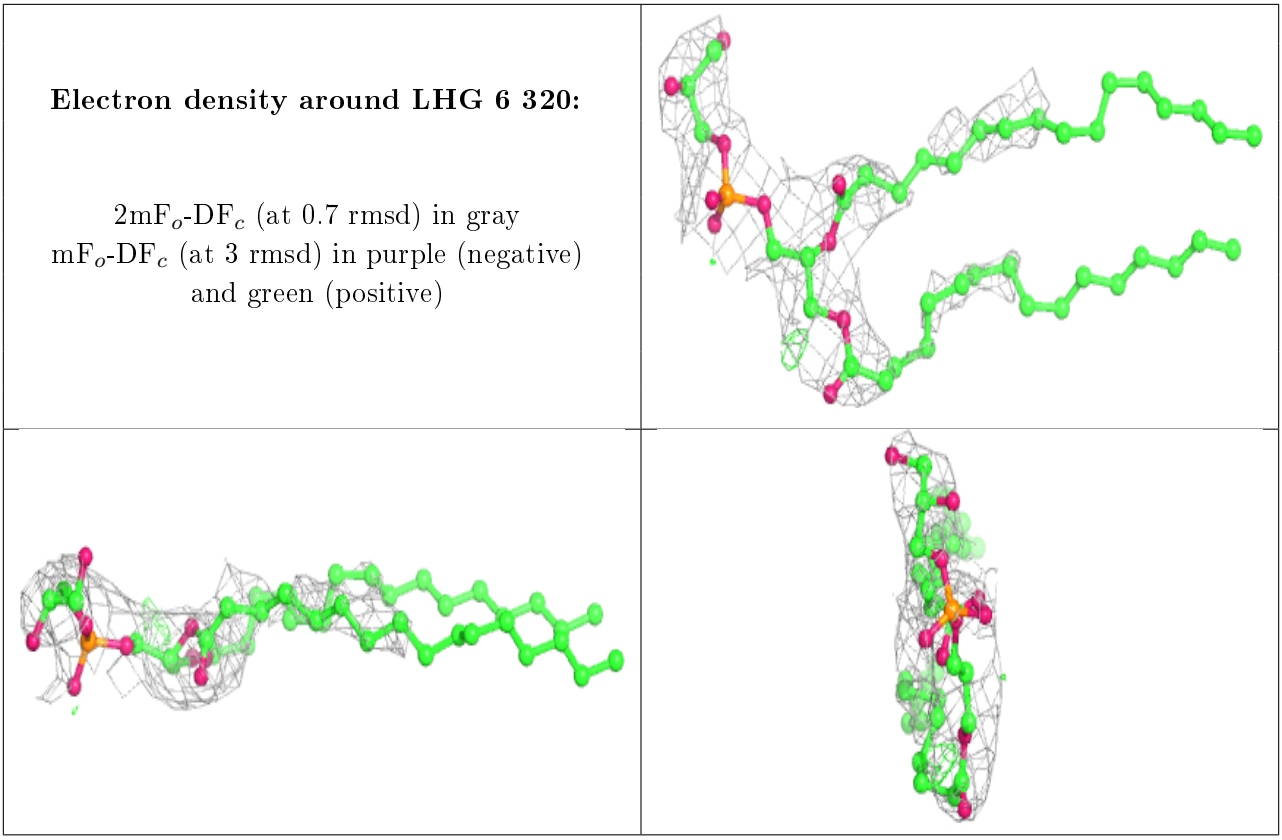






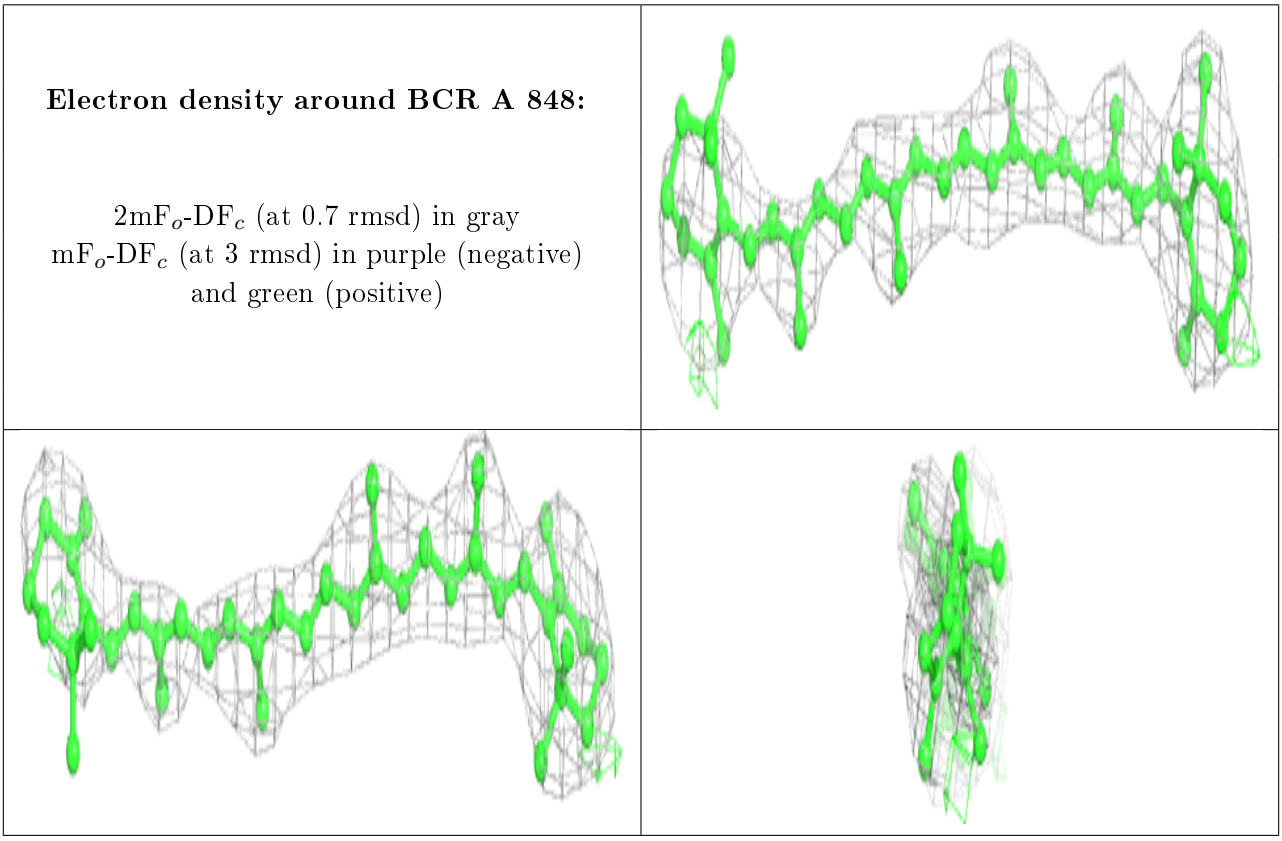
Electron density around LHG 6 320:

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



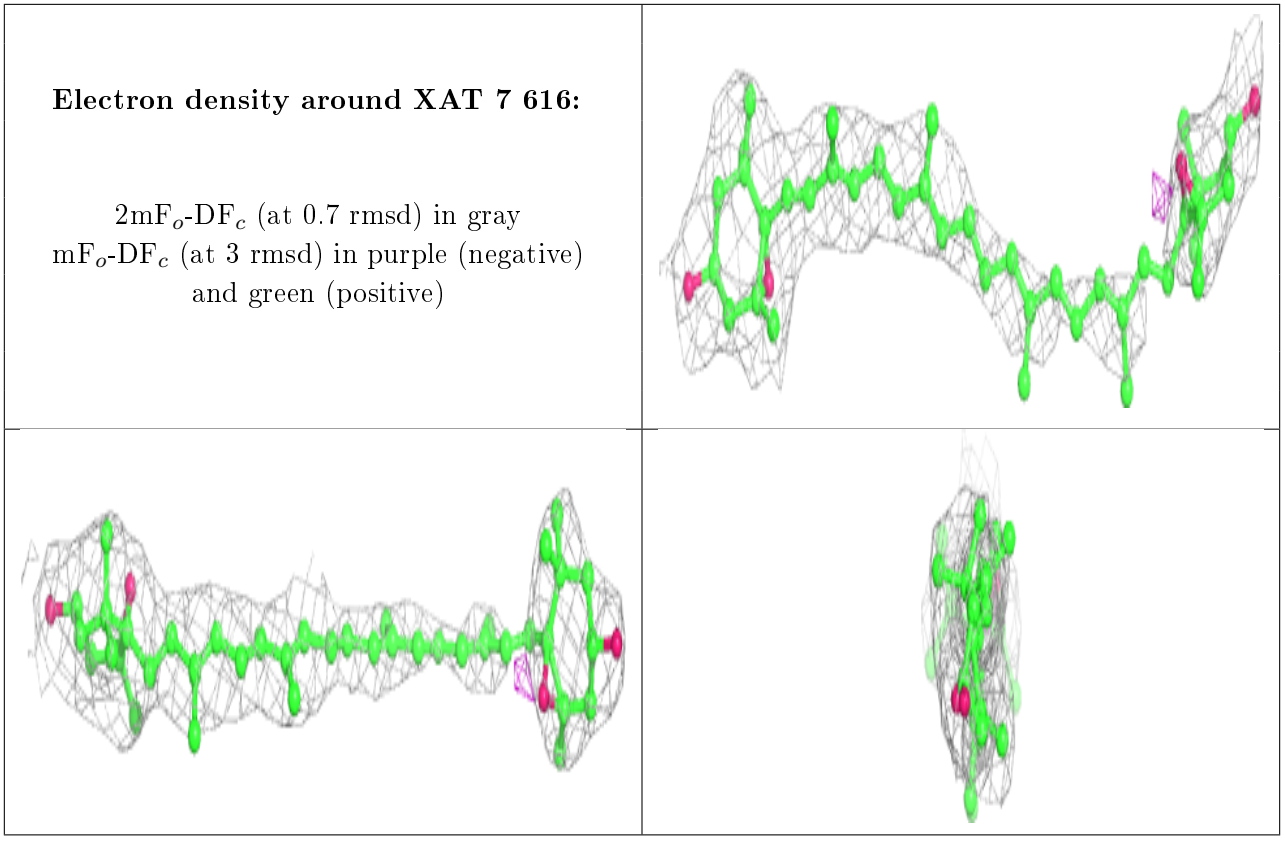
Electron density around BCR A 848:

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



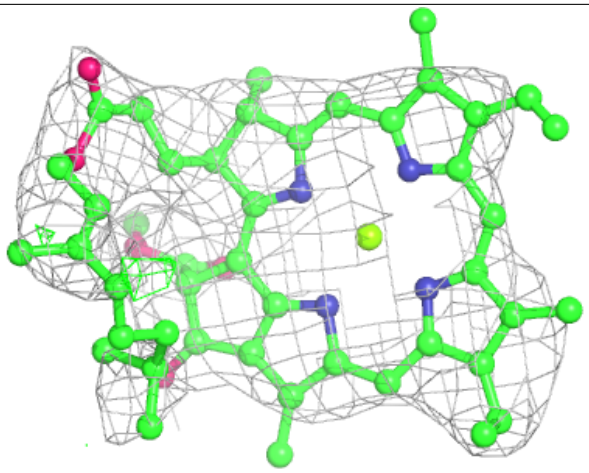
Electron density around XAT 7 616:

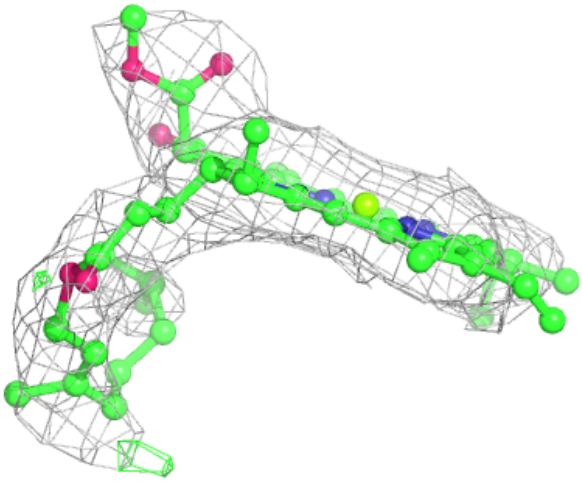
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

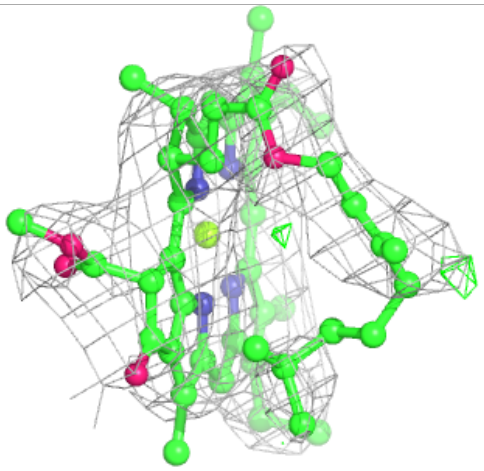


Electron density around CLA 1 314:

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

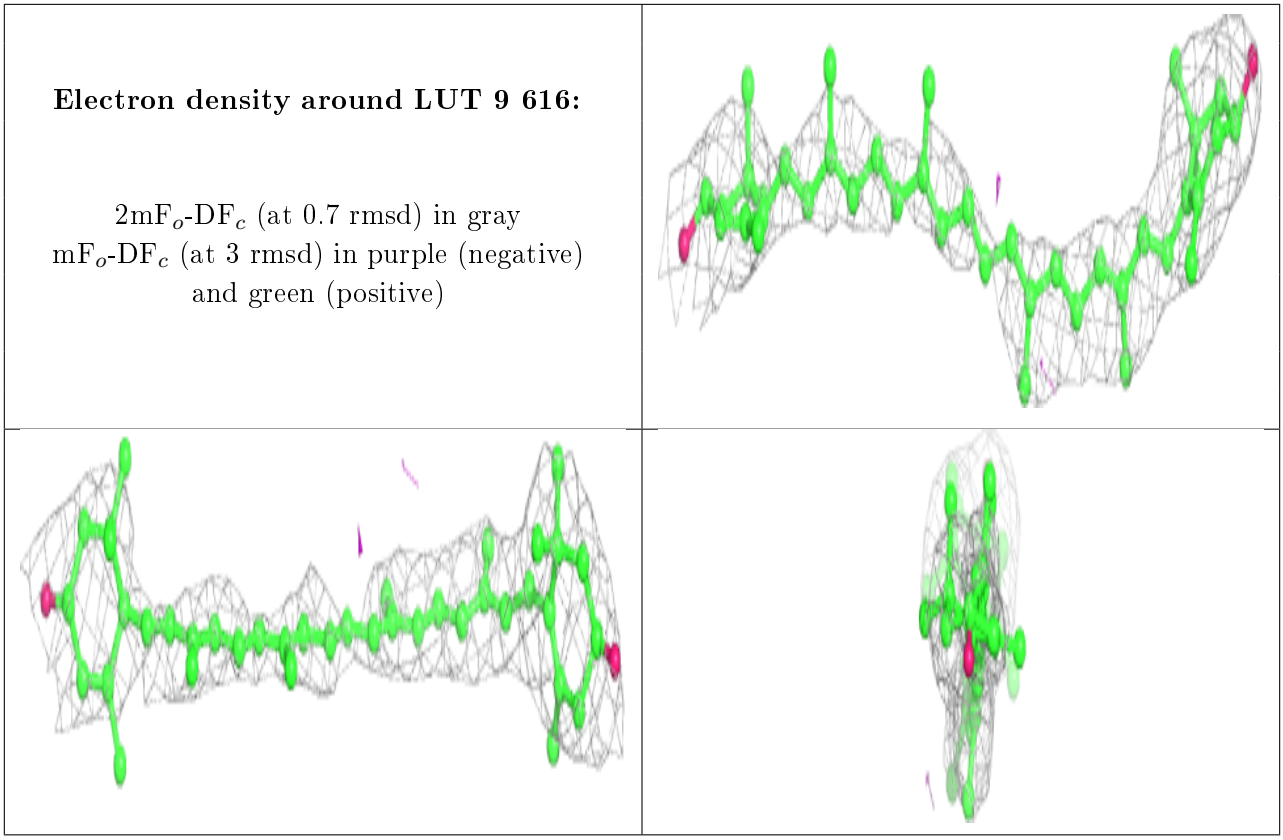






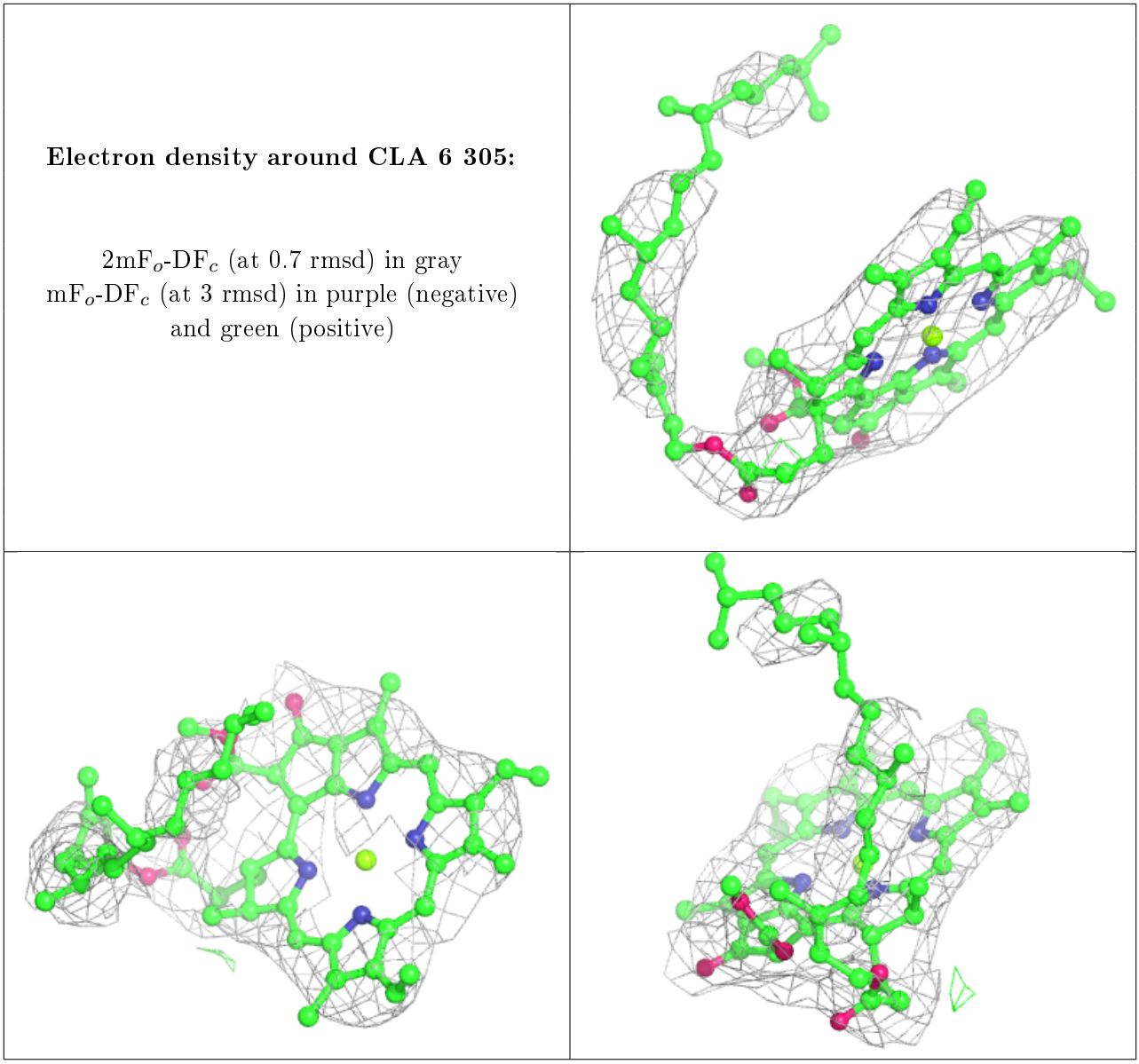
Electron density around LUT 9 616:

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



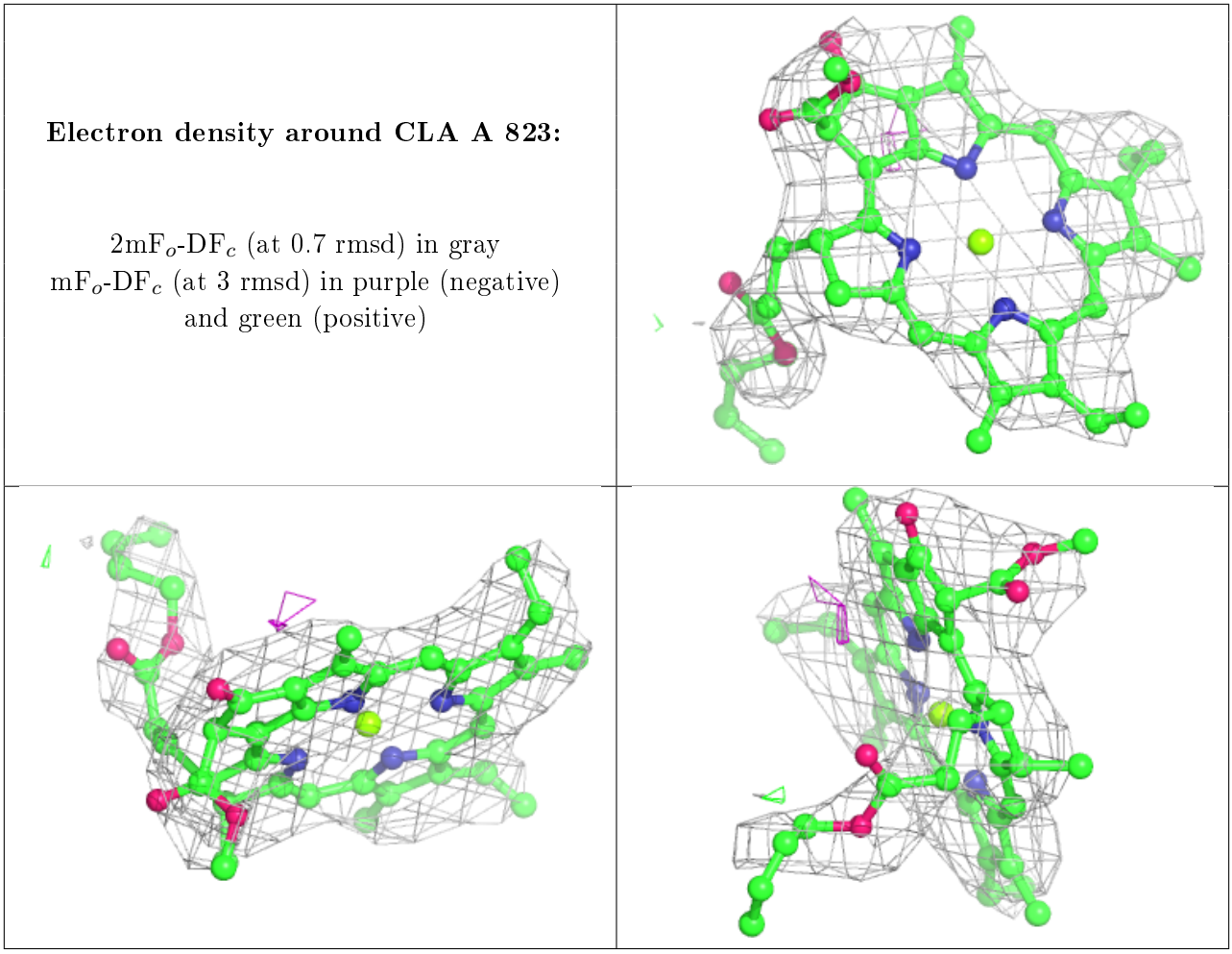
Electron density around CLA 6 305:

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



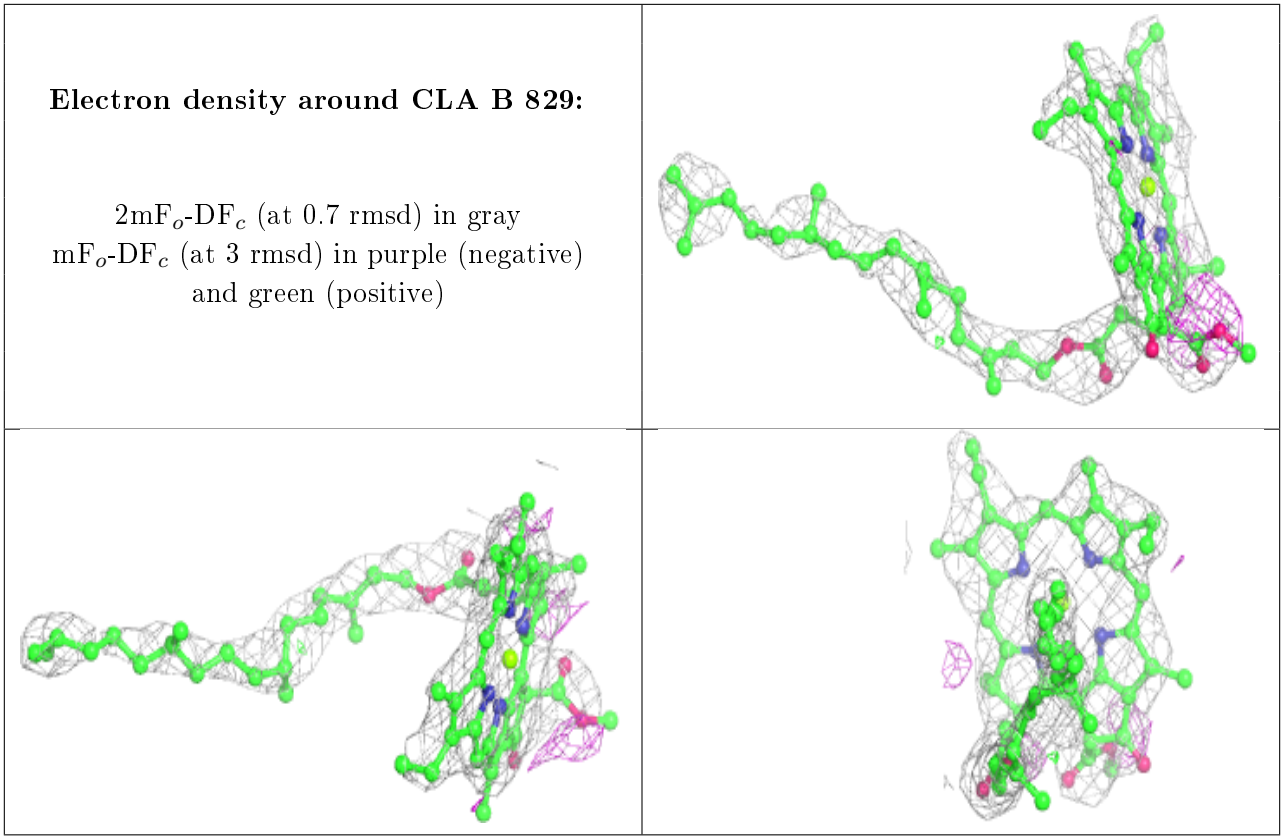
Electron density around CLA A 823:

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



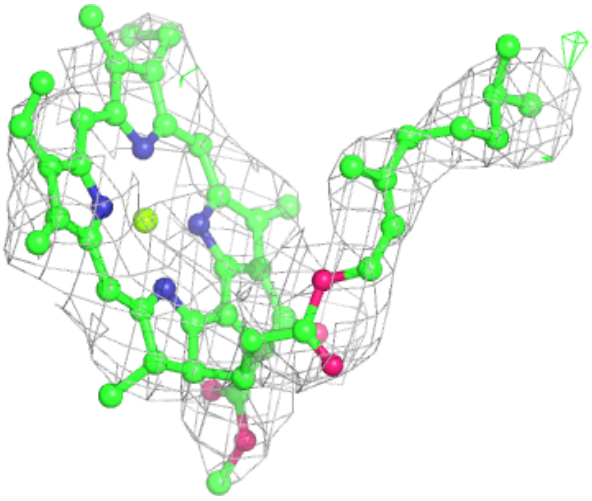
Electron density around CLA B 829:

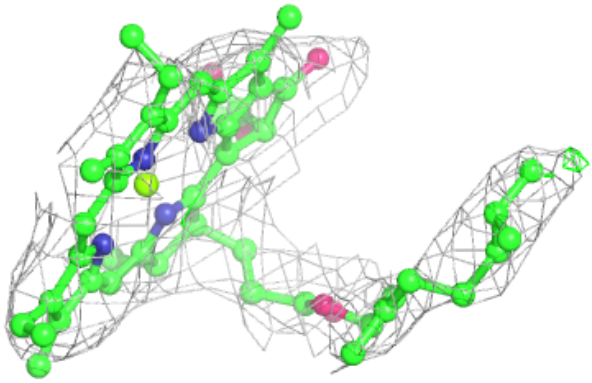
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

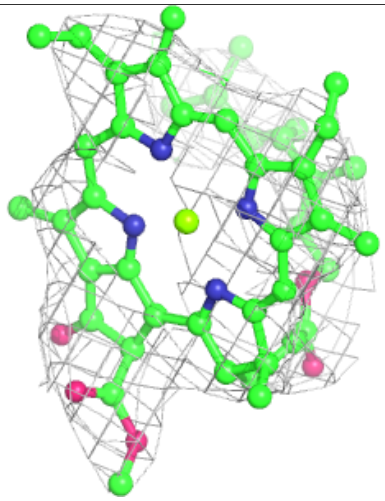


Electron density around CLA 4 610:

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

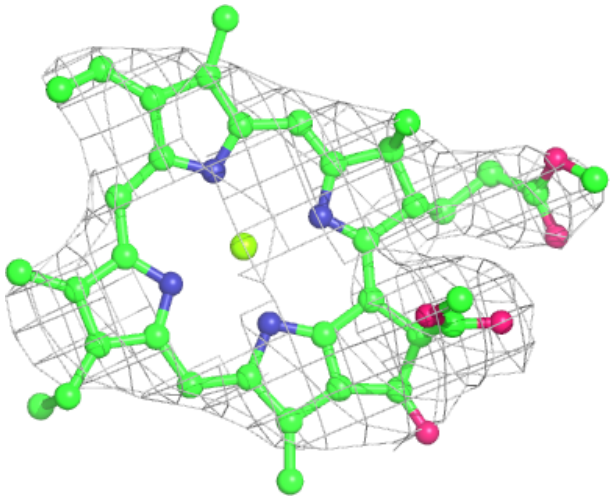


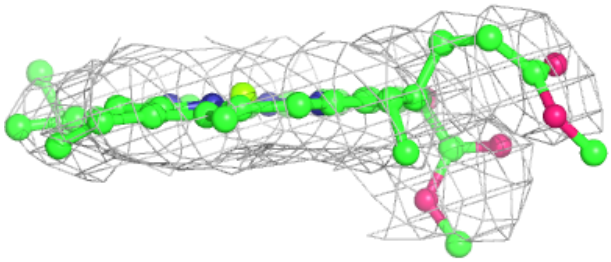


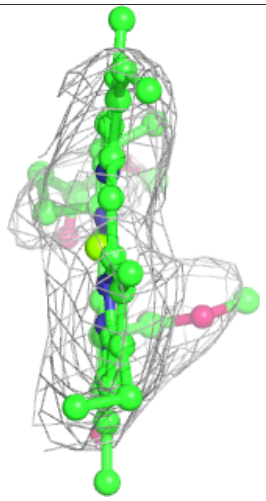


Electron density around CLA g 103:

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

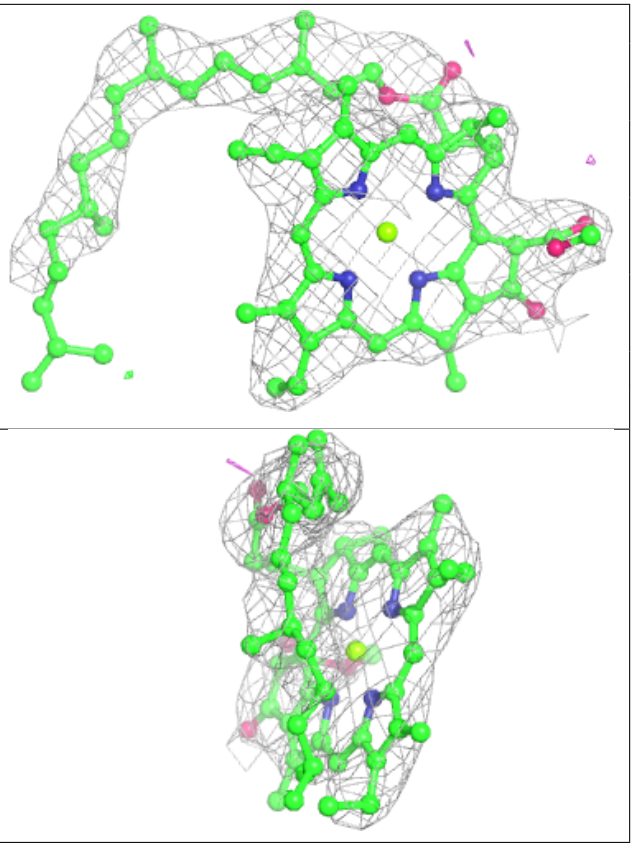


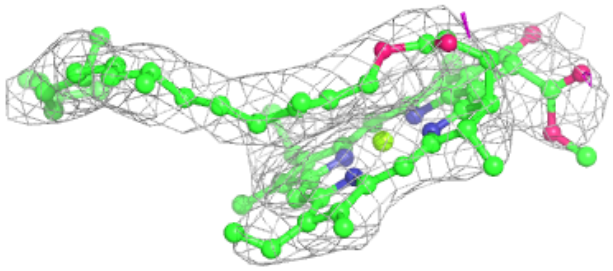




Electron density around CLA 1 303:

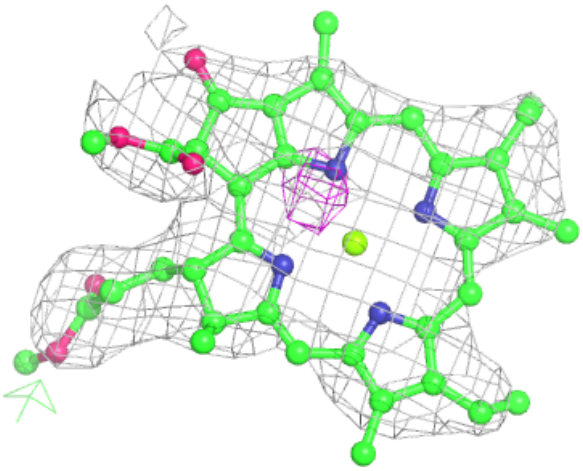
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

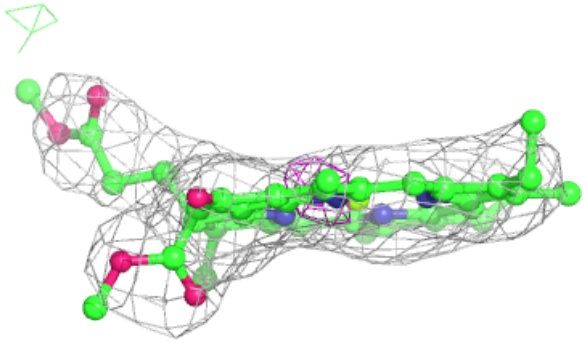


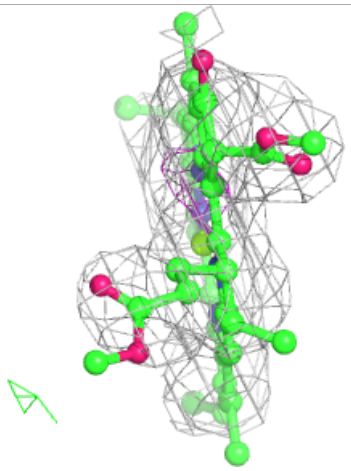


Electron density around CLA k 1402:

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

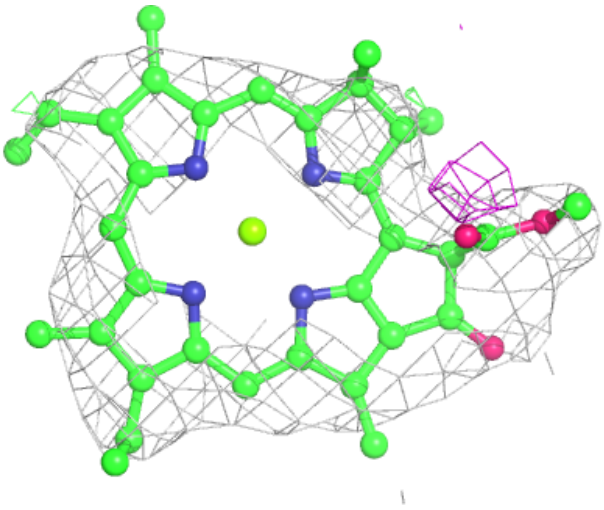


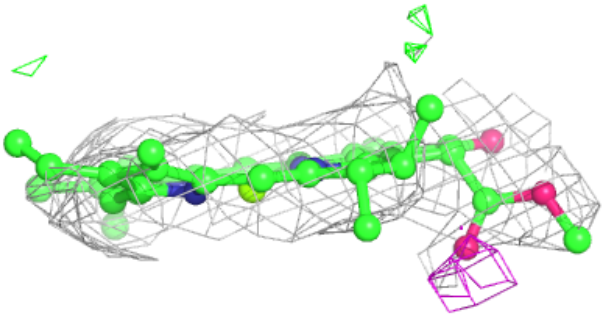


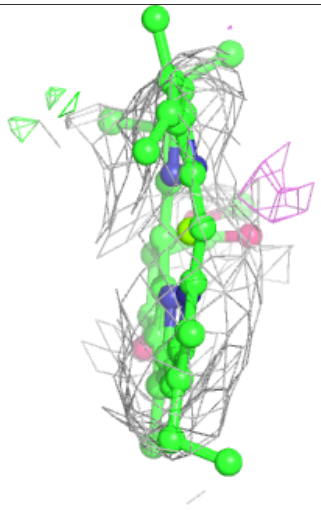


Electron density around CLA 2 610:

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

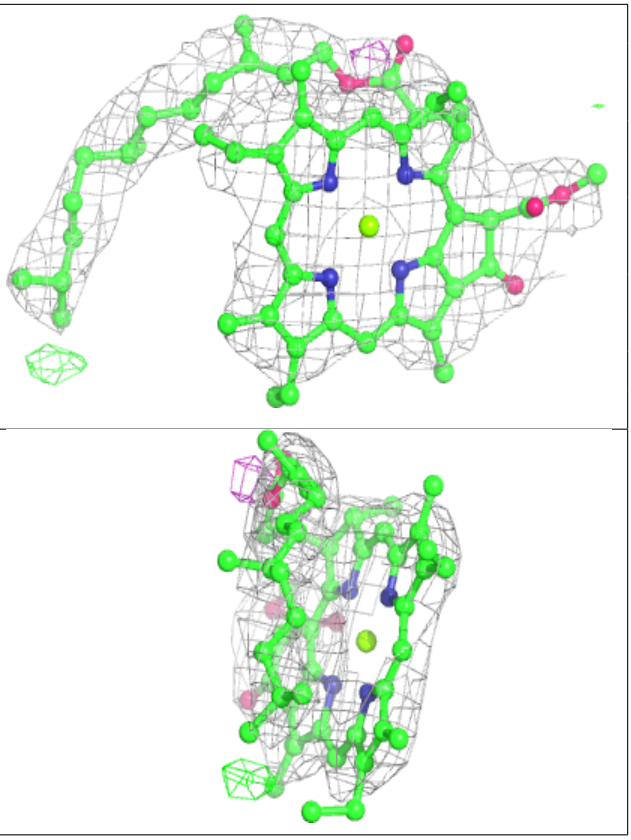


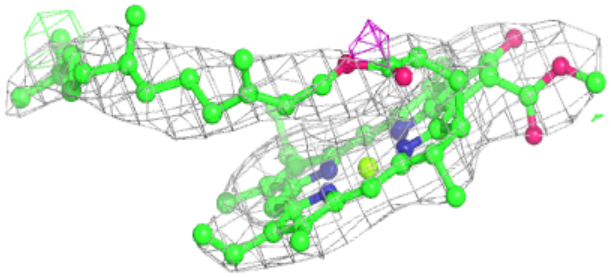




Electron density around CLA 1 310:

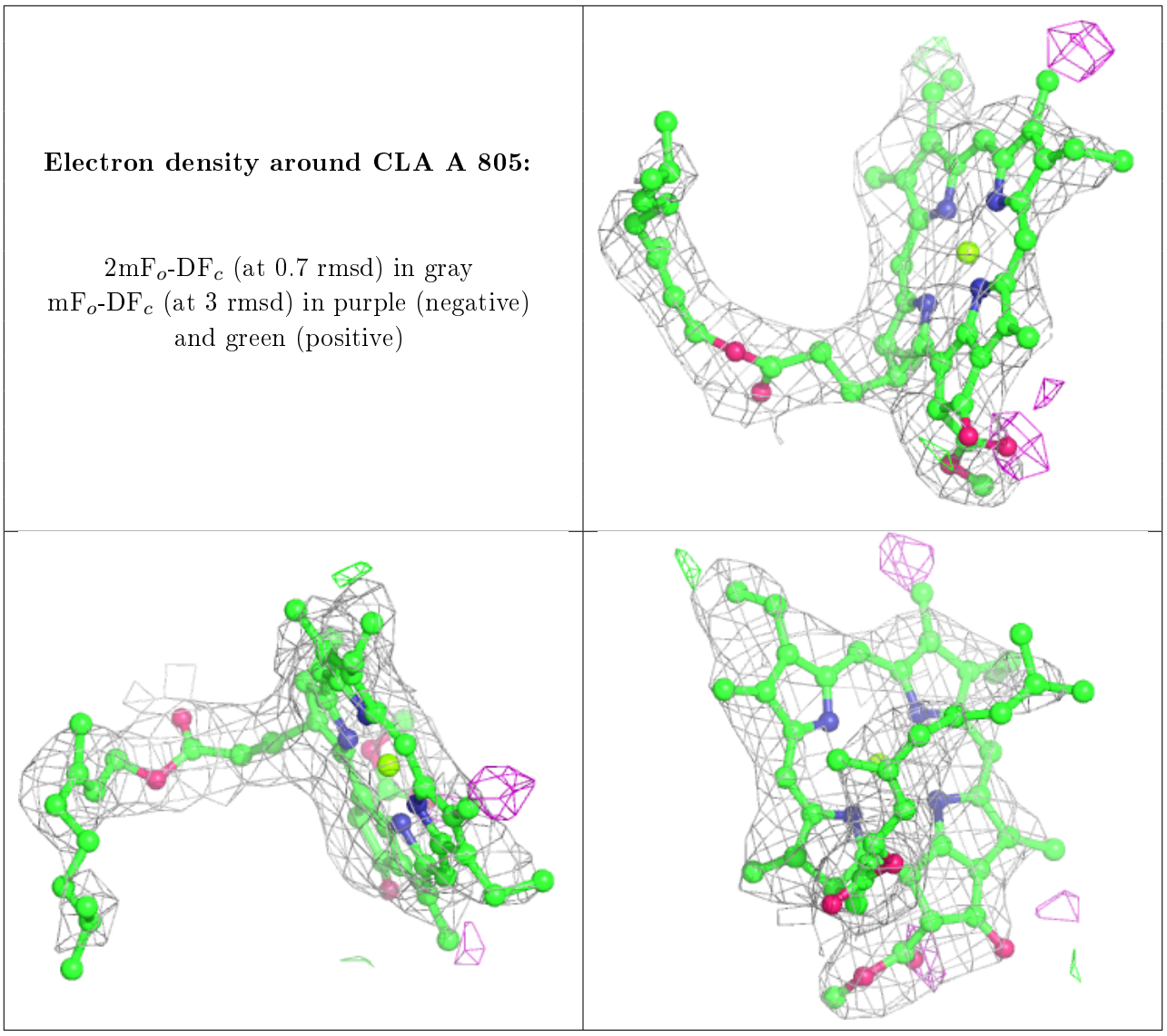
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)





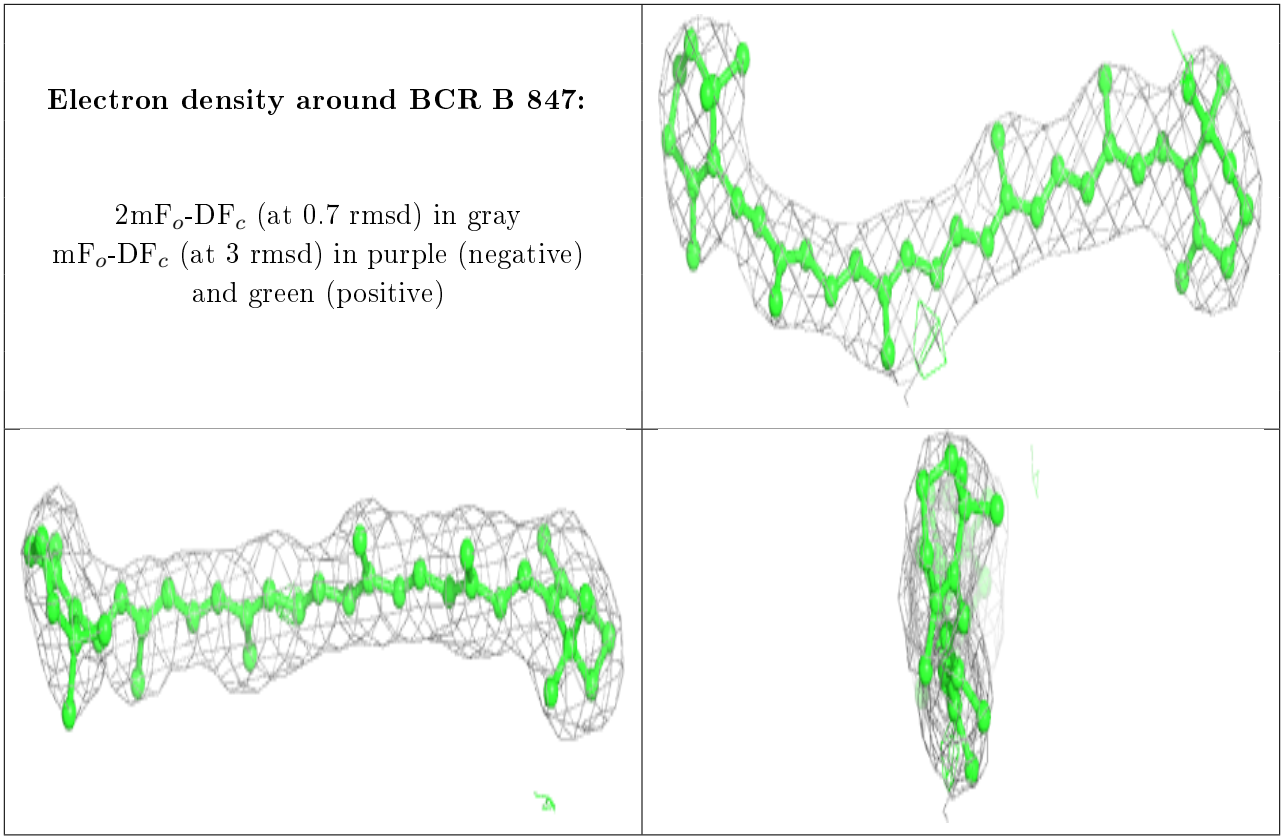
Electron density around CLA A 805:

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



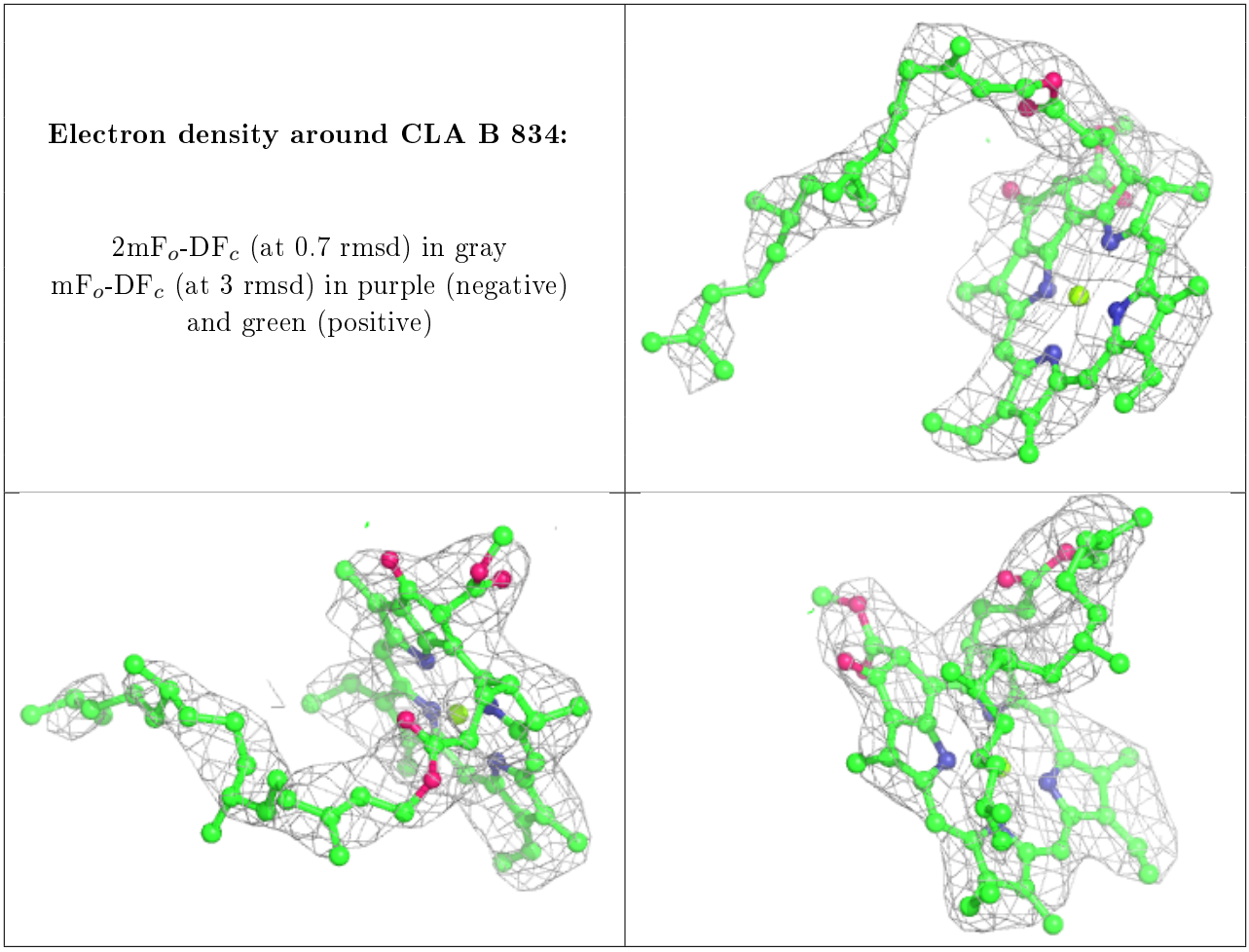
Electron density around BCR B 847:

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



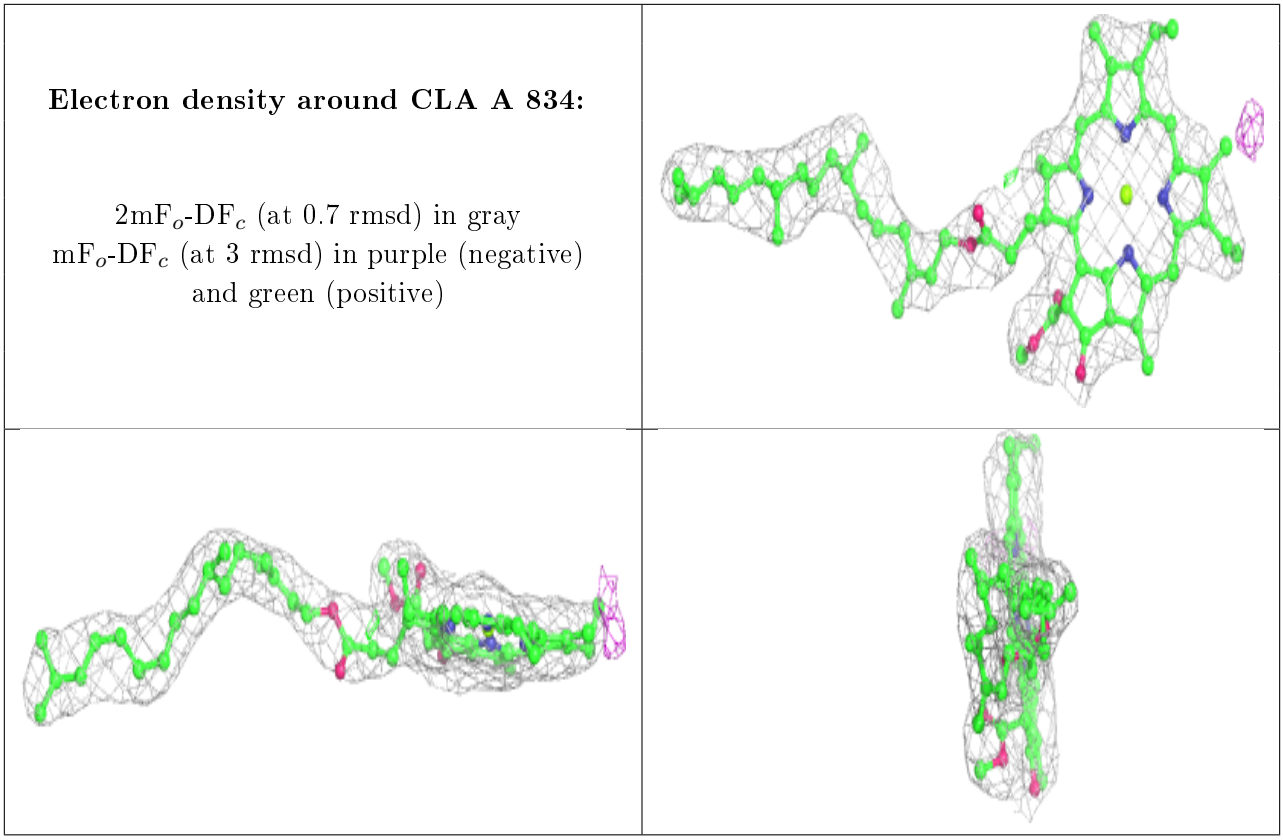
Electron density around CLA B 834:

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



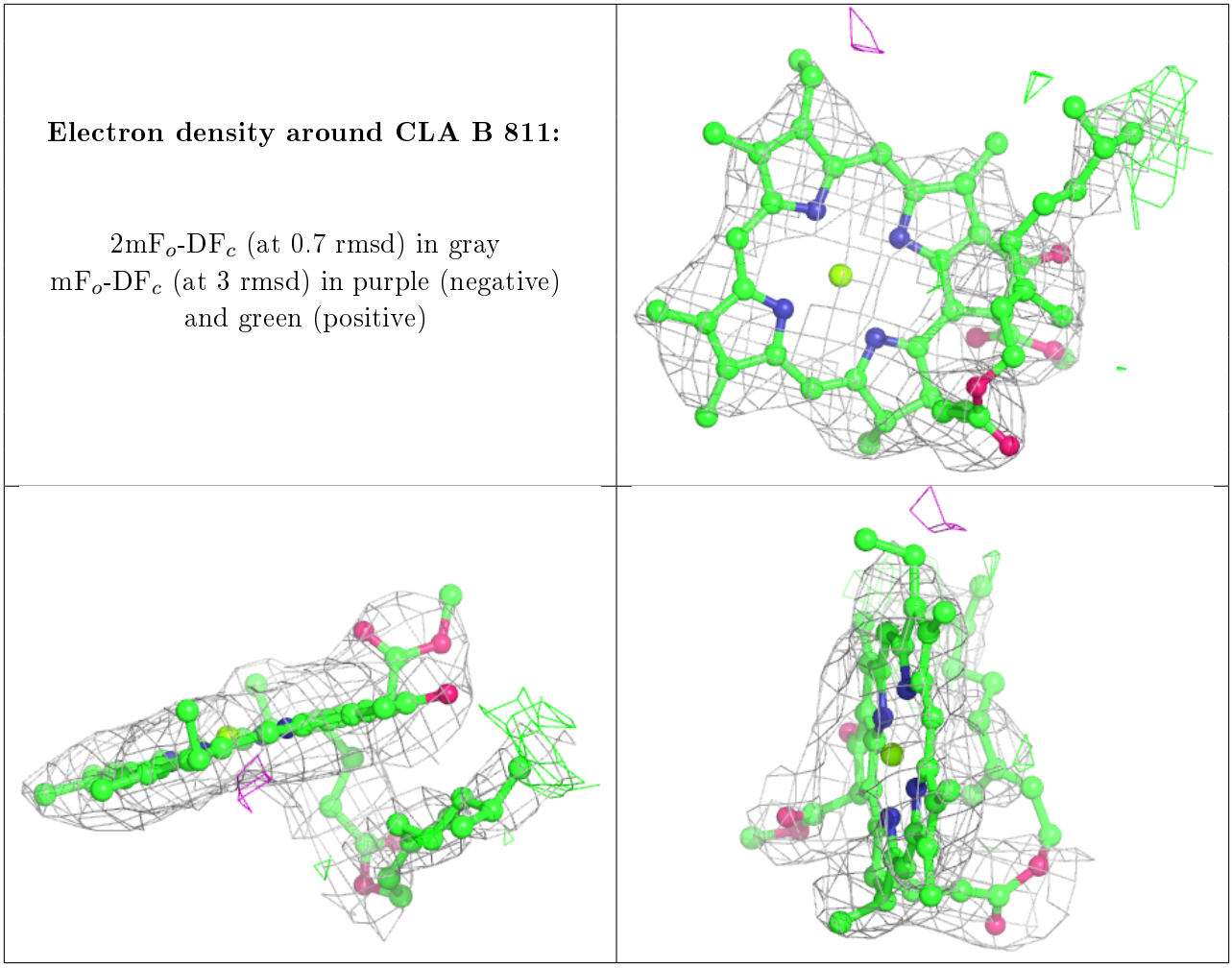
Electron density around CLA A 834:

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



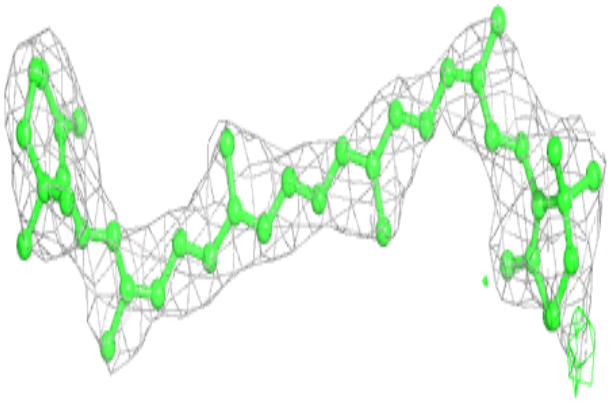
Electron density around CLA B 811:

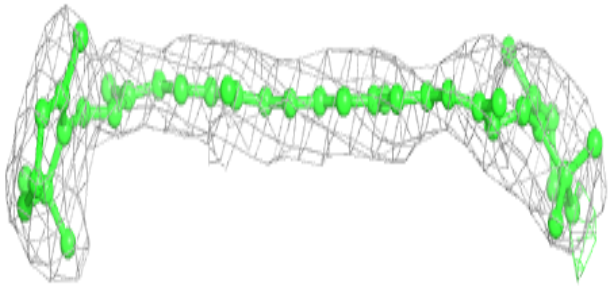
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

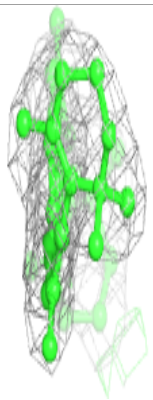


Electron density around BCR B 845:

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

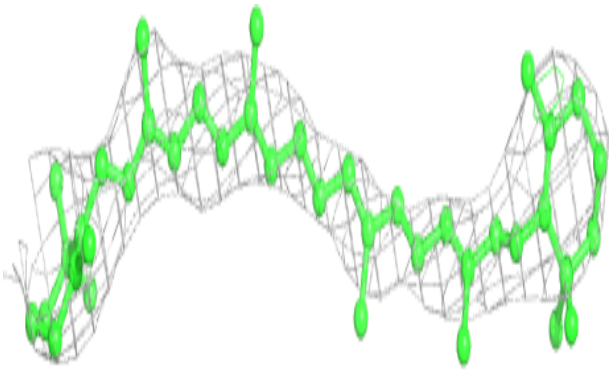


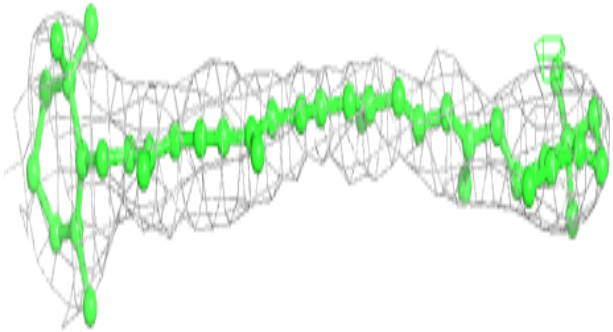


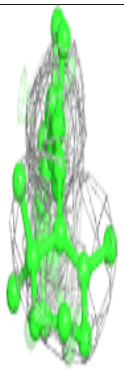


Electron density around BCR 9 618:

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

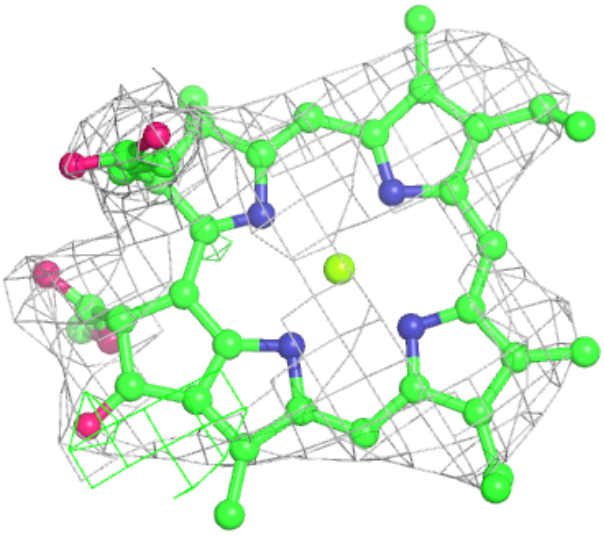


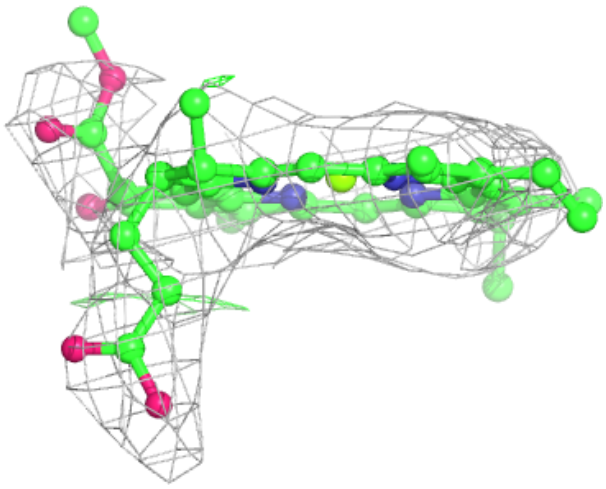


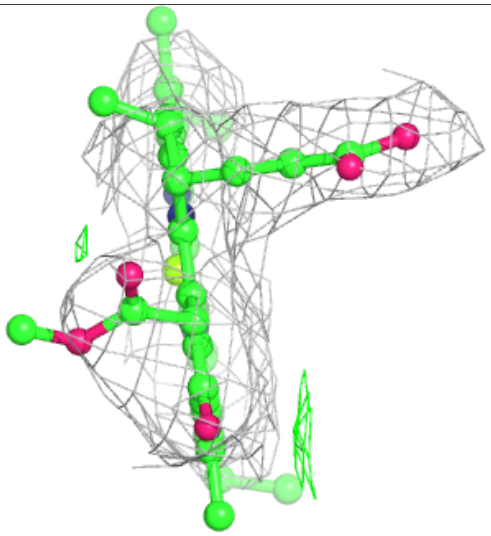


Electron density around CLA 3 304:

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

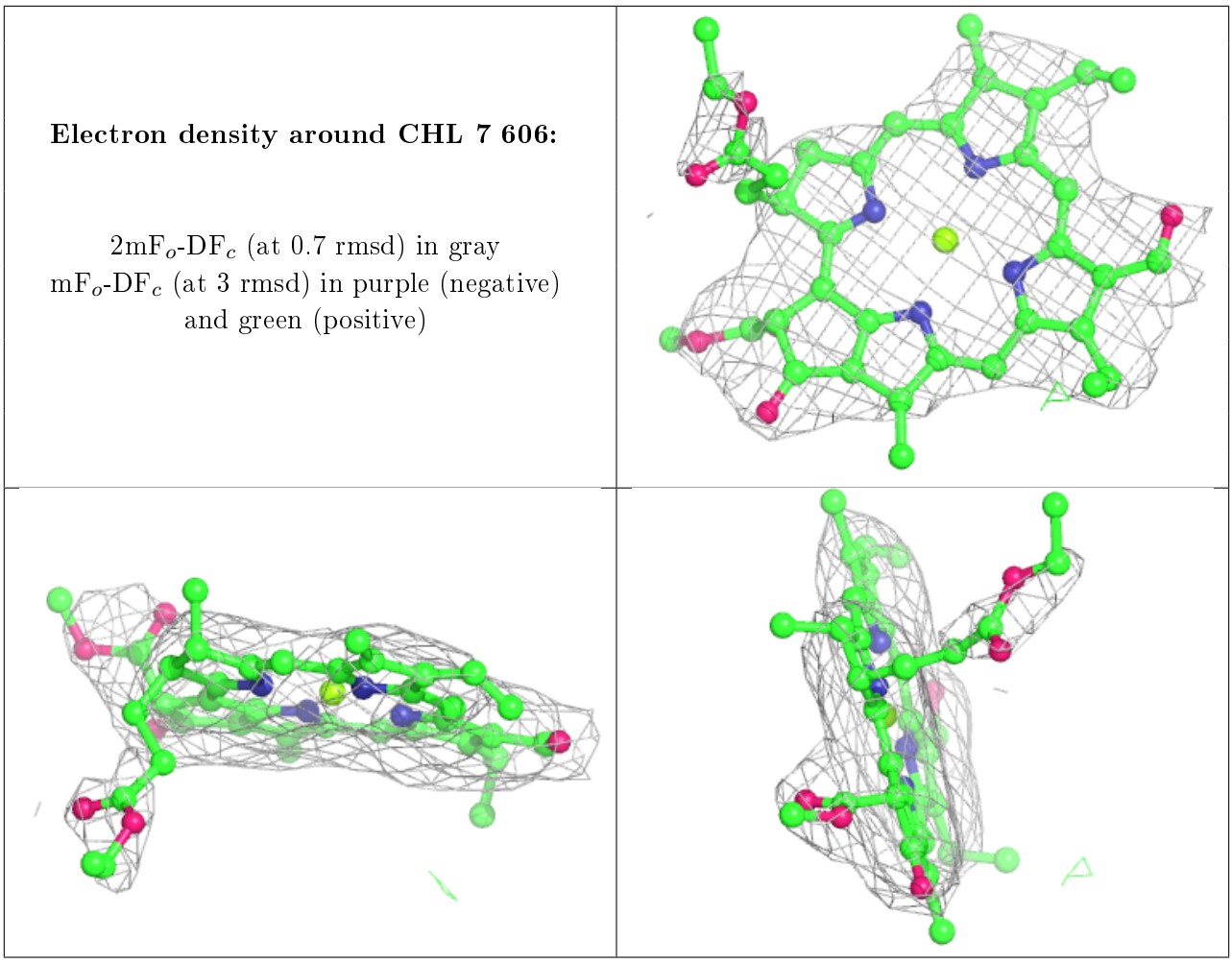






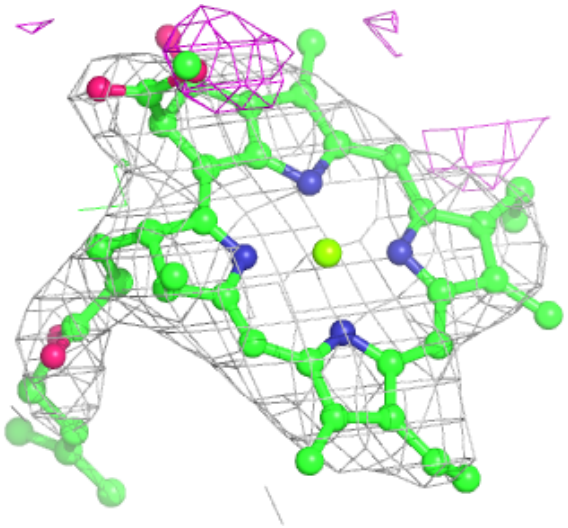
Electron density around CHL 7 606:

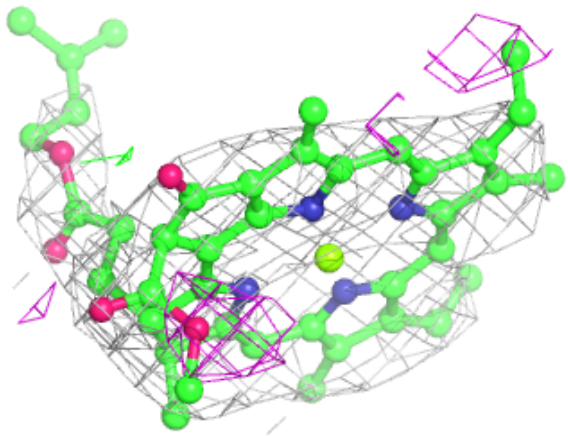
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

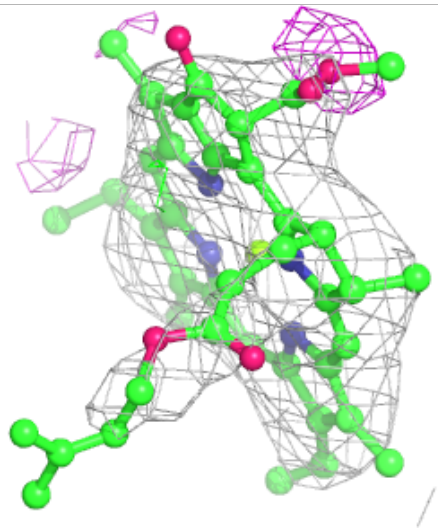


Electron density around CLA 4 604:

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

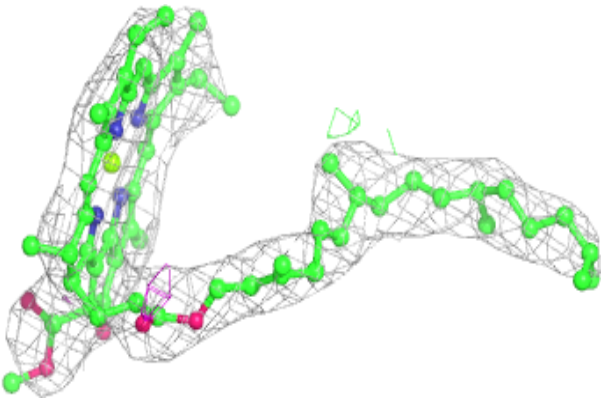


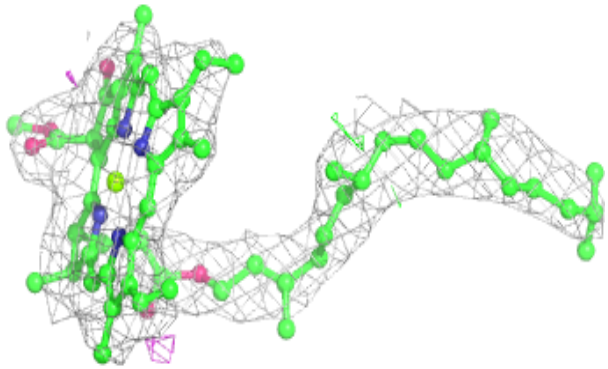


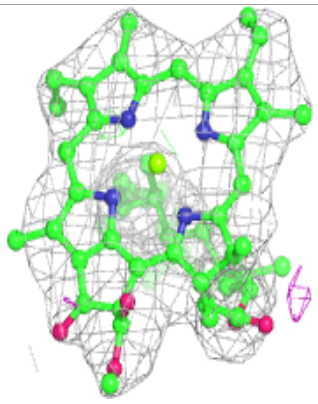


Electron density around CLA A 812:

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

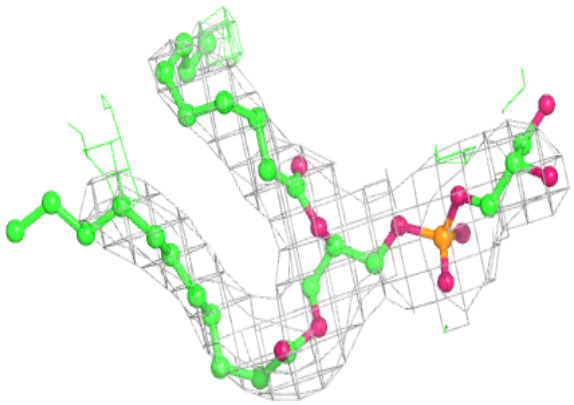


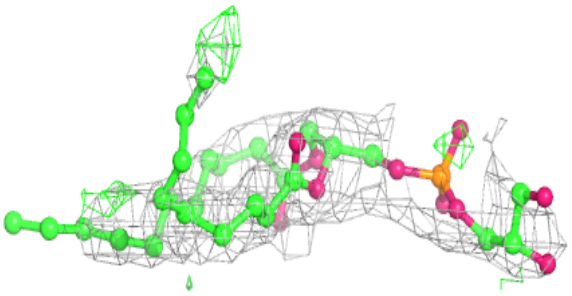


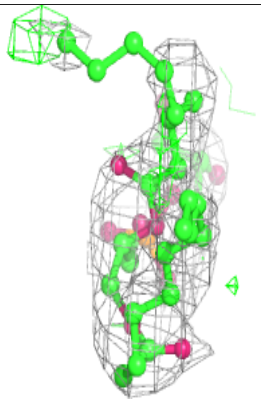


Electron density around LHG 7 618:

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

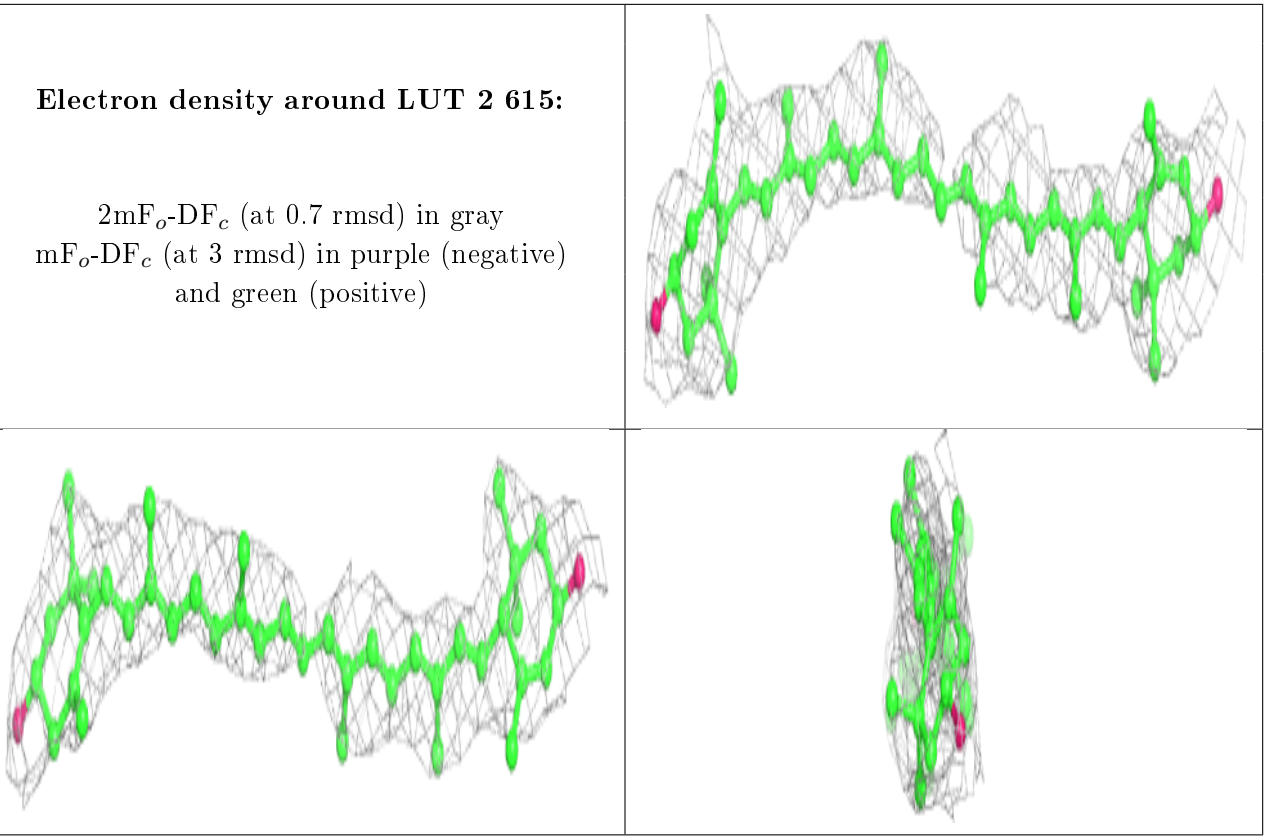






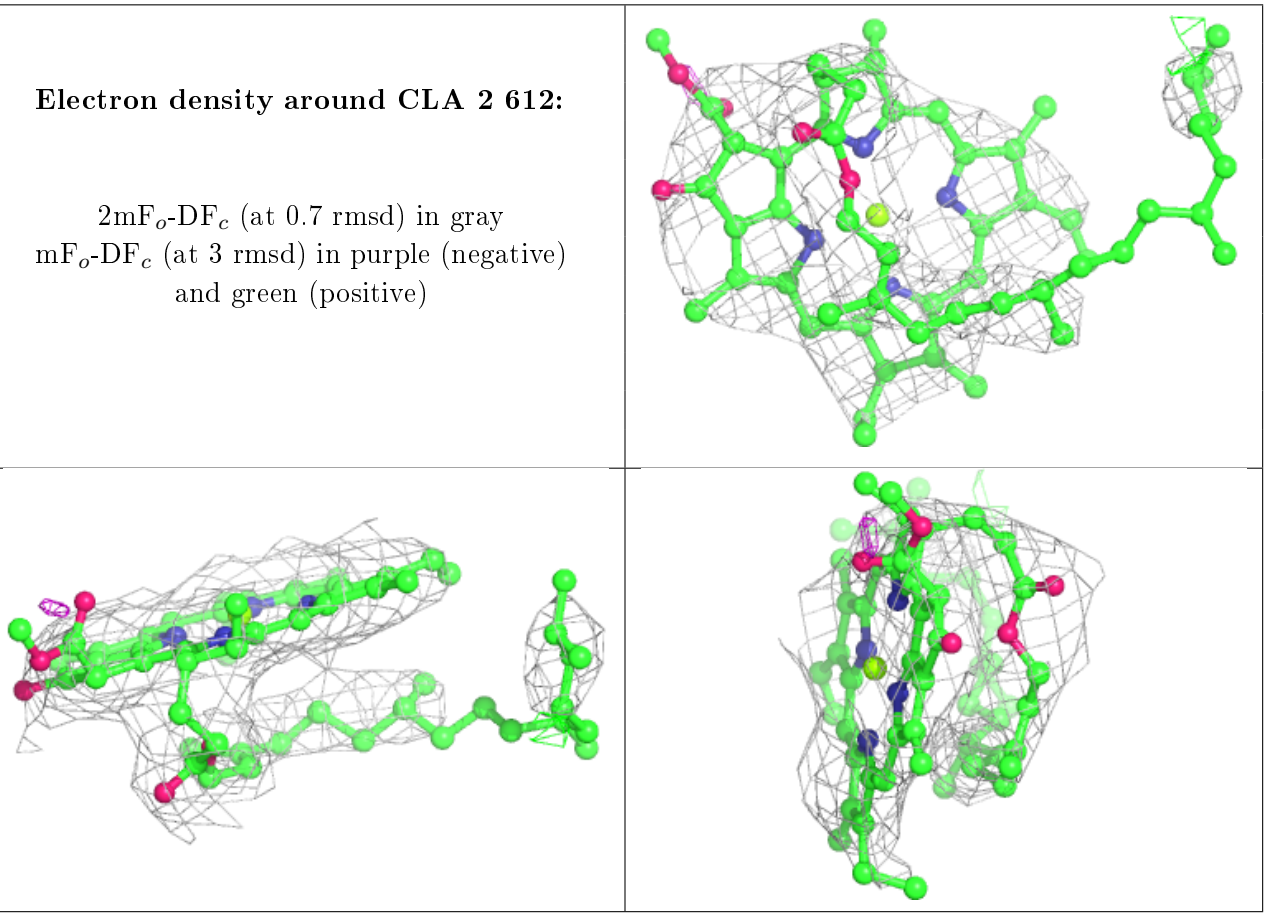
Electron density around LUT 2 615:

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



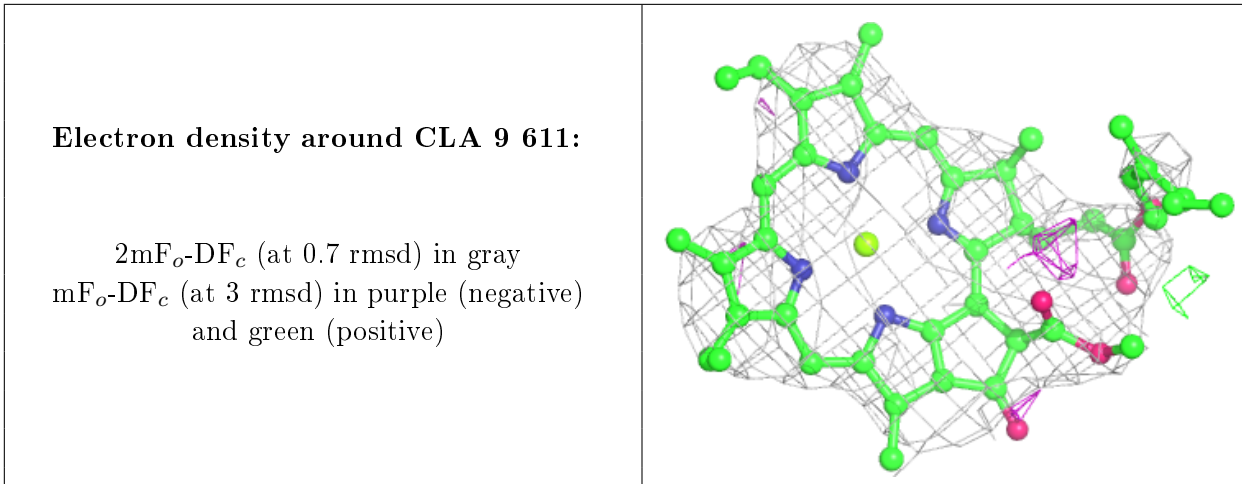
Electron density around CLA 2 612:

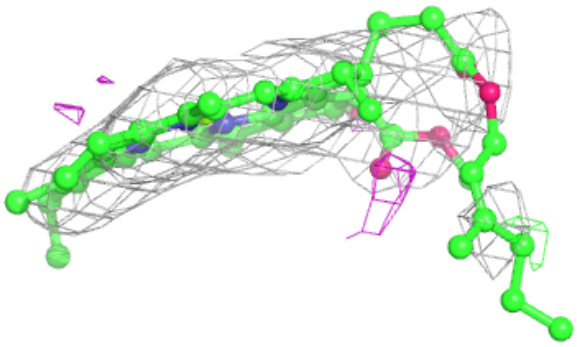
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

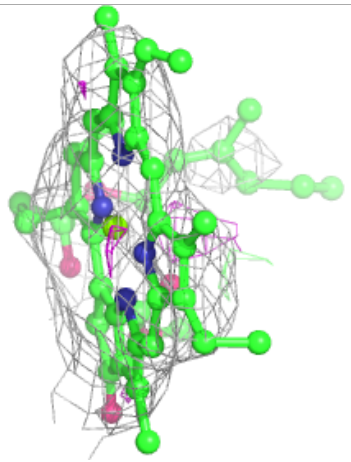


Electron density around CLA 9 611:

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

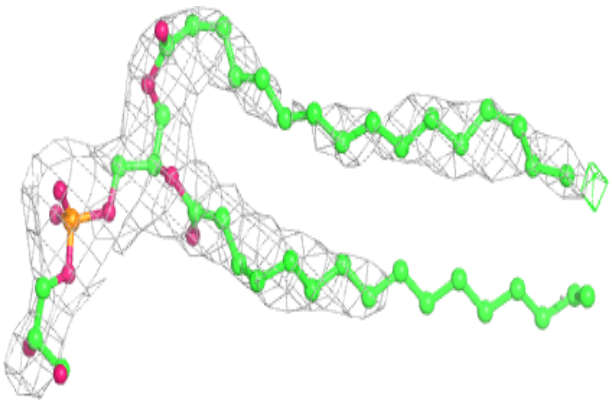


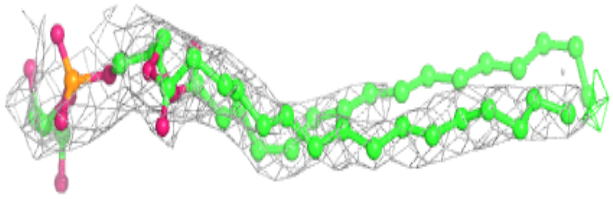




Electron density around LHG 1 319:

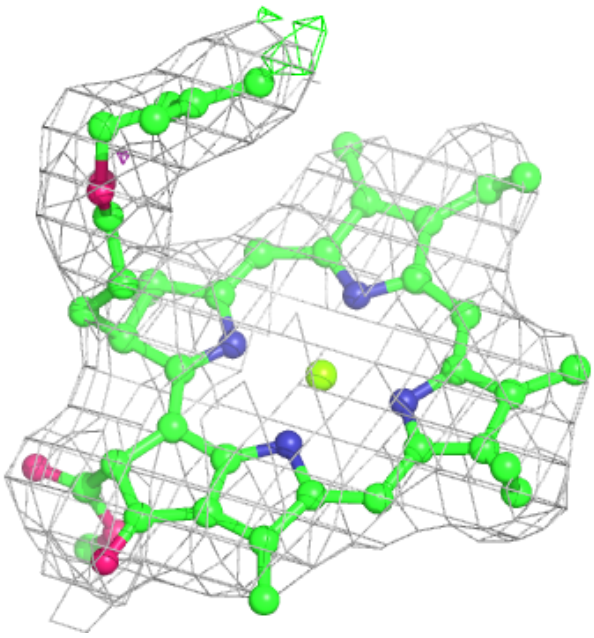
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

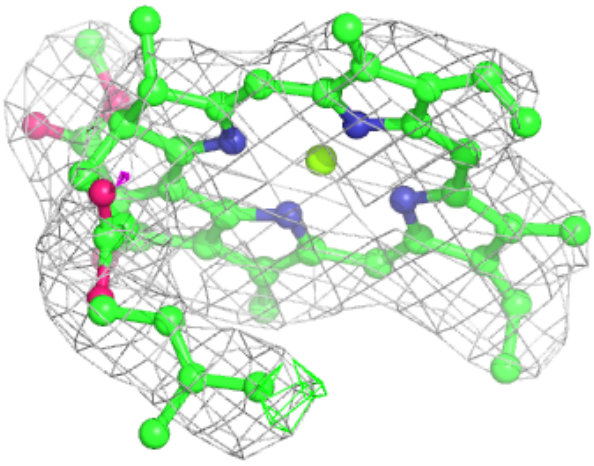


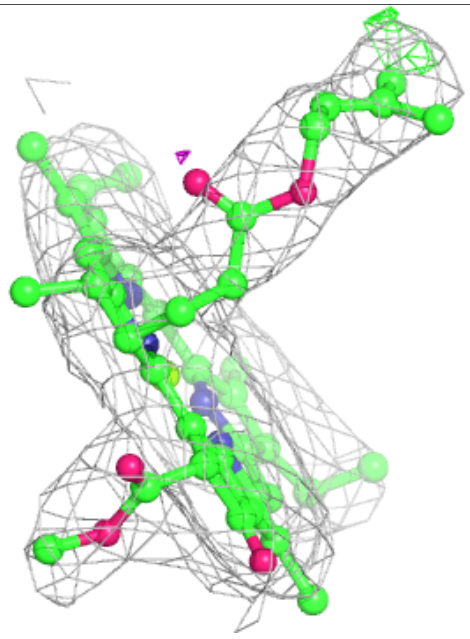


Electron density around CLA b 830:

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

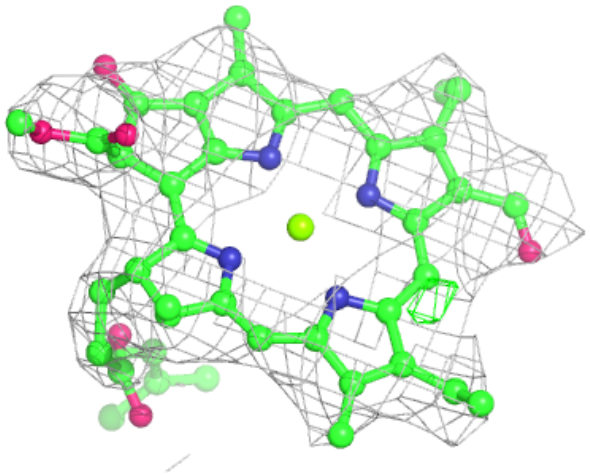


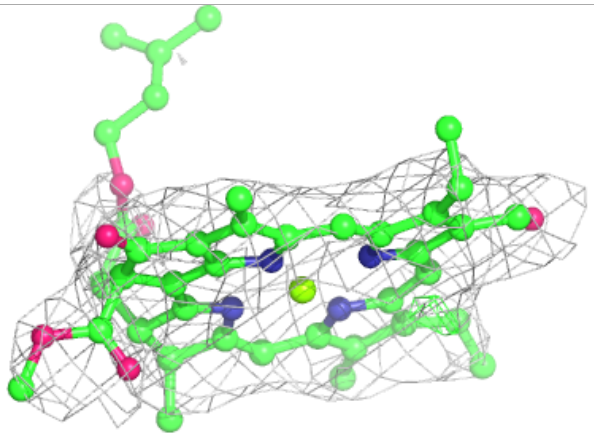


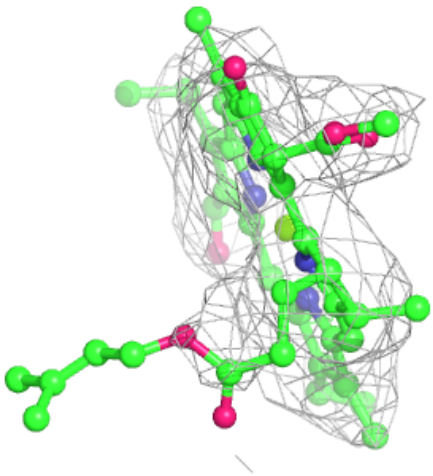


Electron density around CHL 4 606:

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

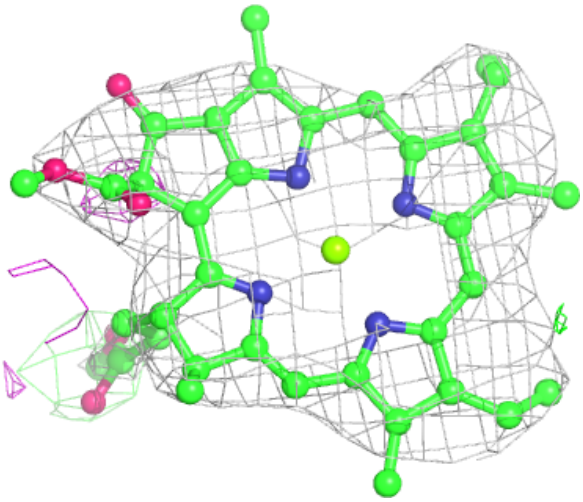


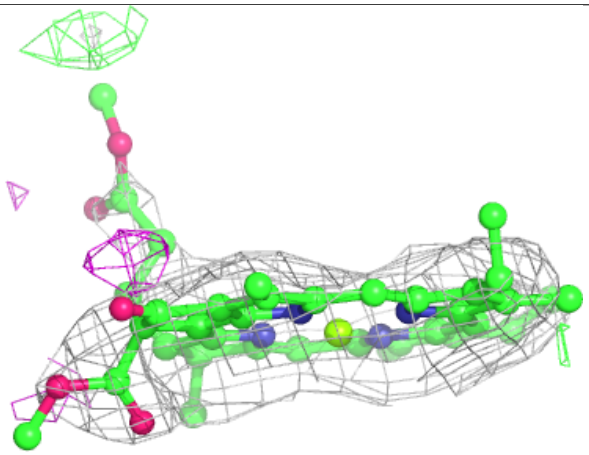


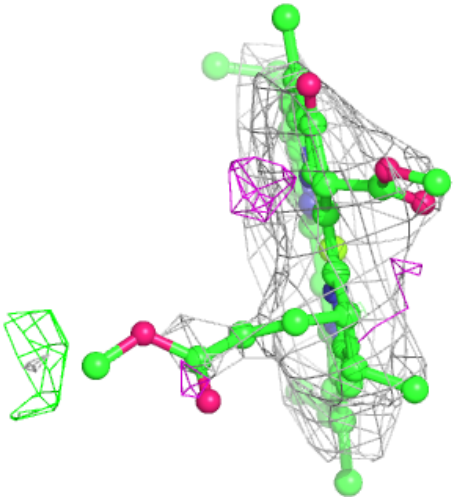


Electron density around CLA 6 309:

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

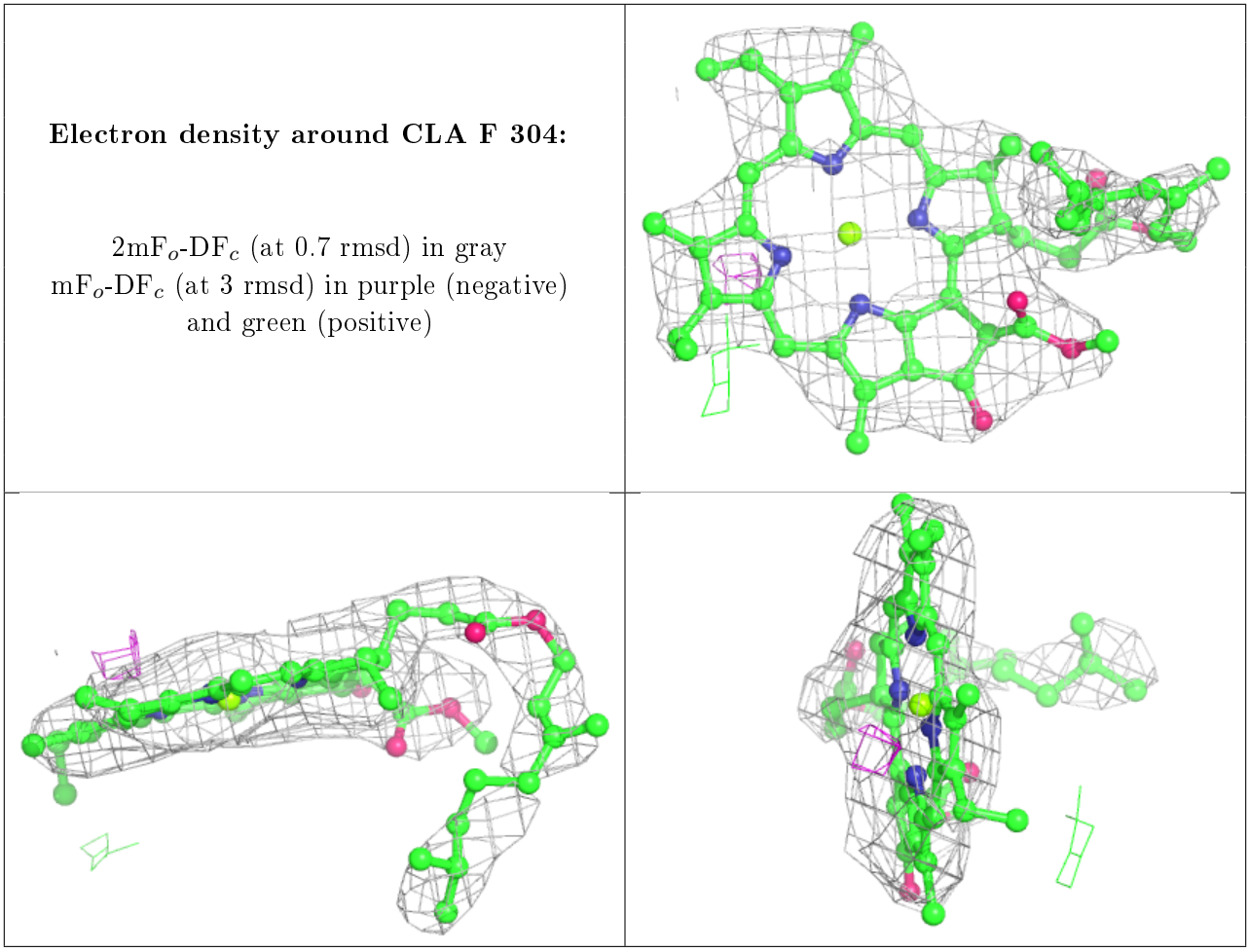






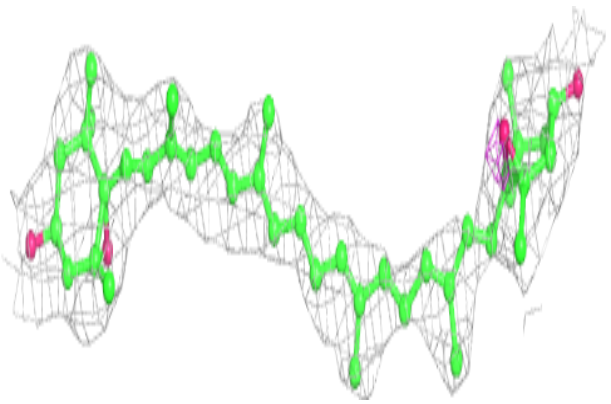
Electron density around CLA F 304:

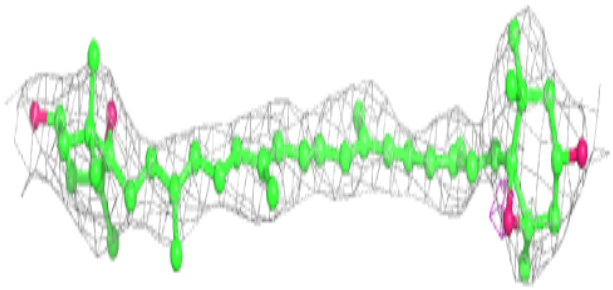
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

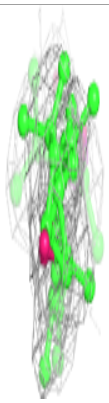


Electron density around XAT 8 315:

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

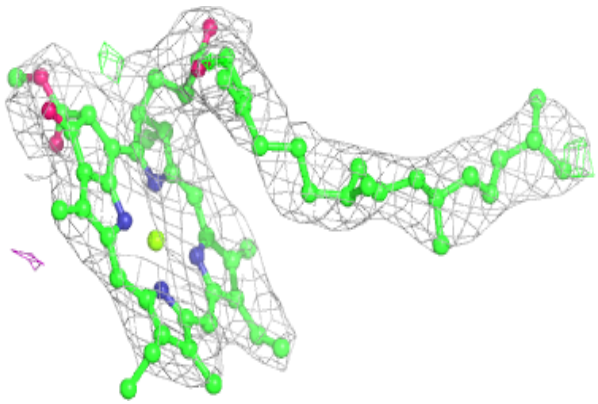


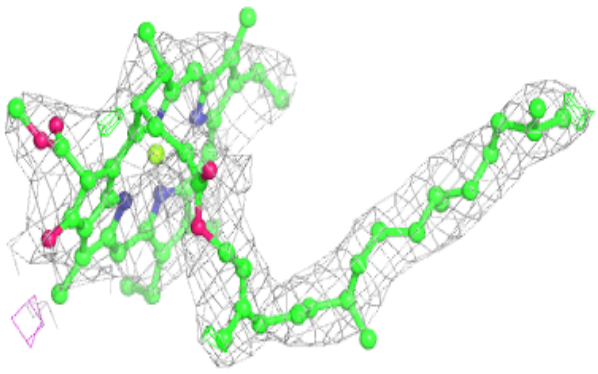


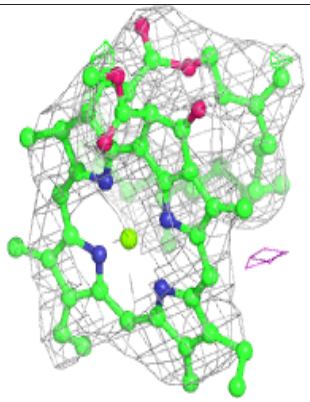


Electron density around CLA b 814:

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

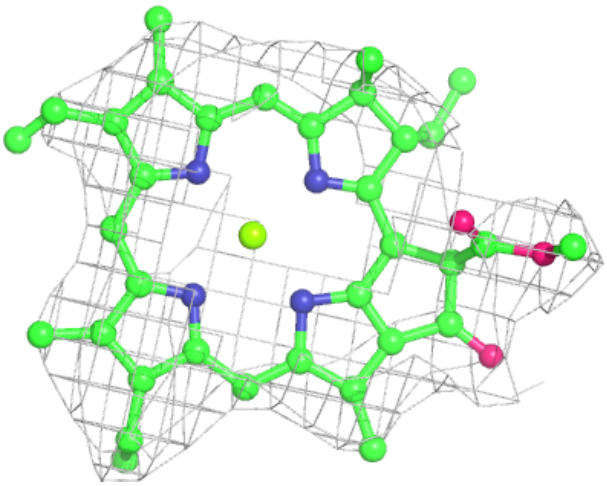


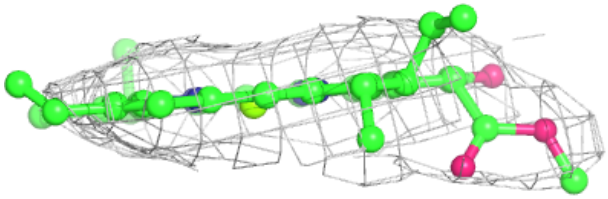


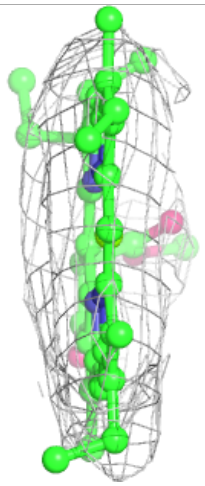


Electron density around CLA j 3002:

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

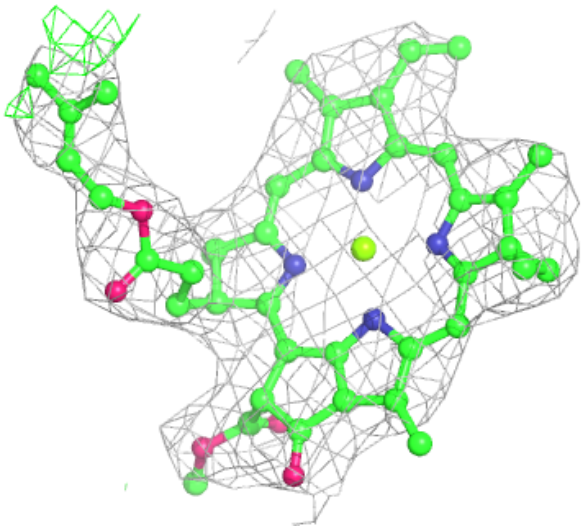


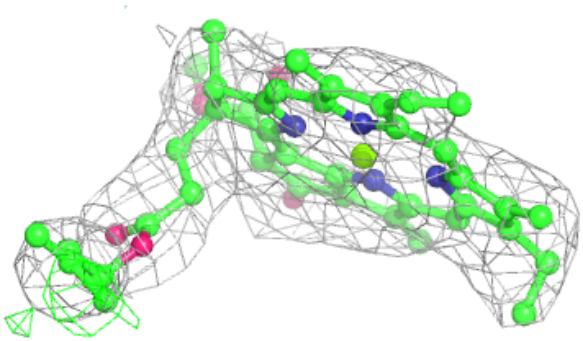


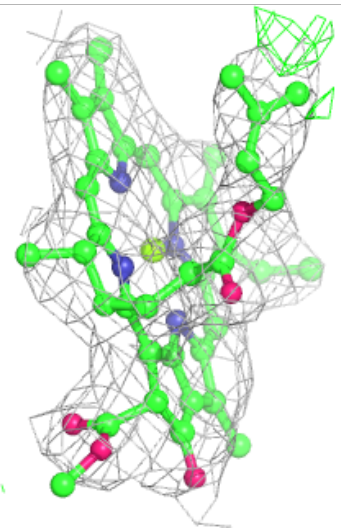


Electron density around CLA a 836:

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

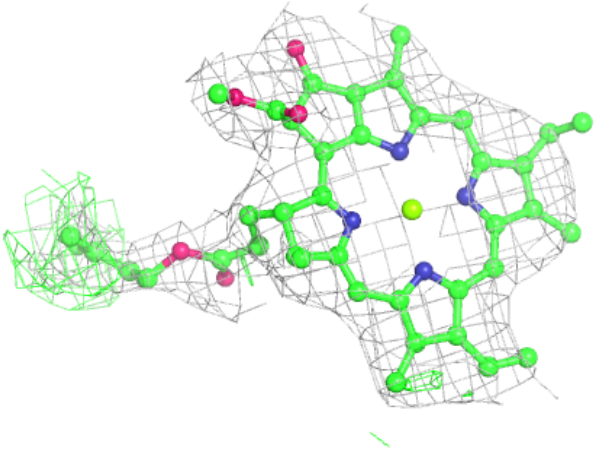


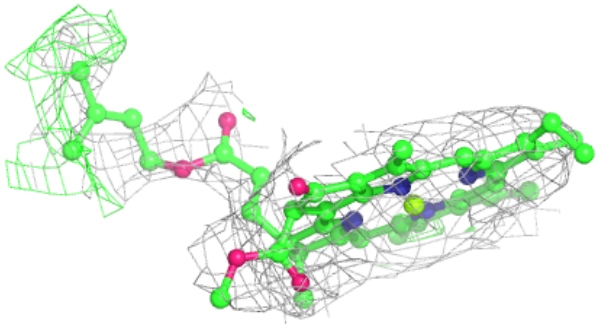


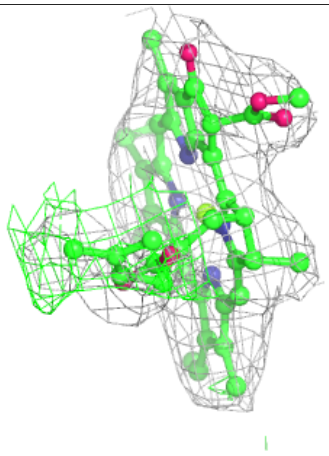


Electron density around CLA 2 608:

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

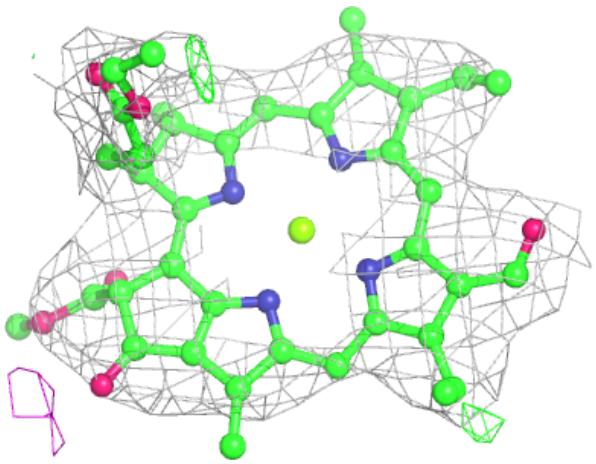


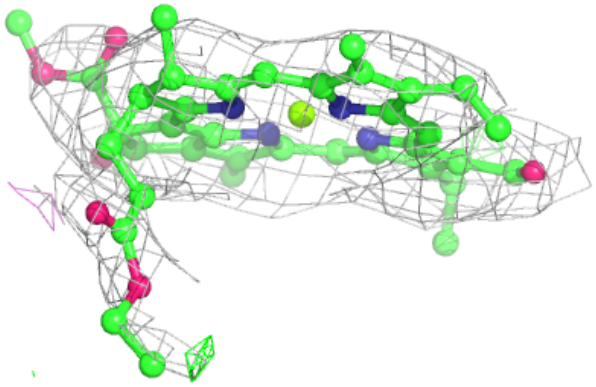


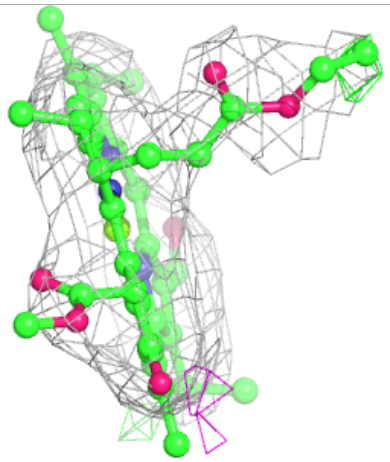


Electron density around CHL 1 307:

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

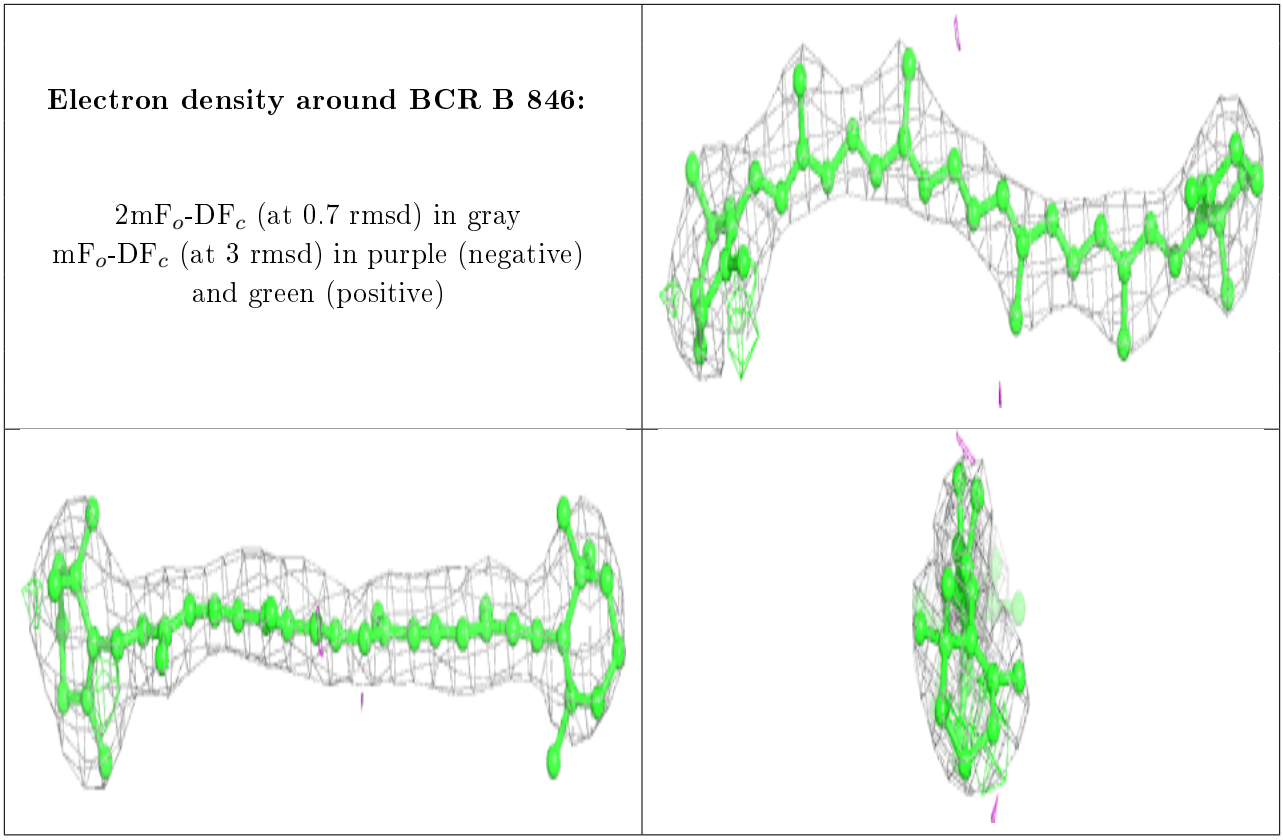






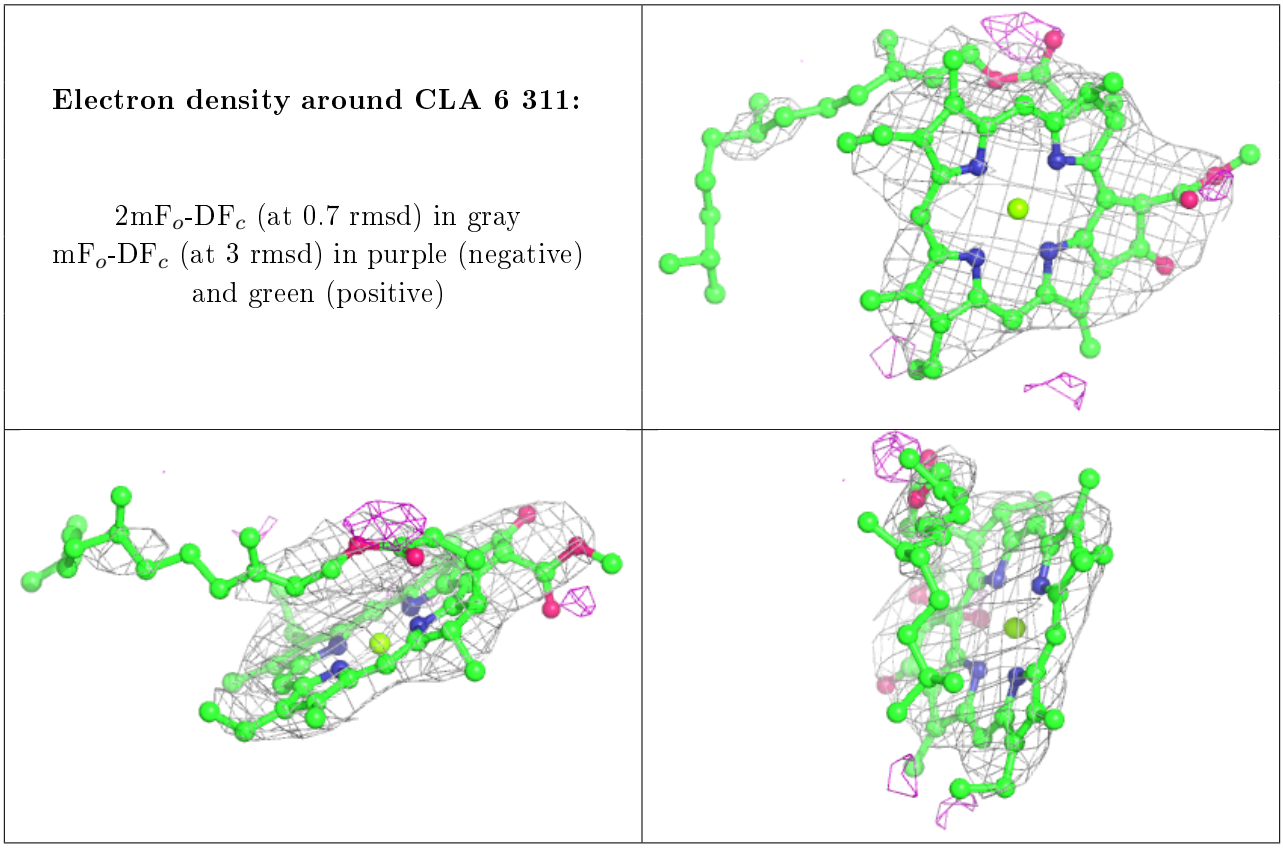
Electron density around BCR B 846:

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



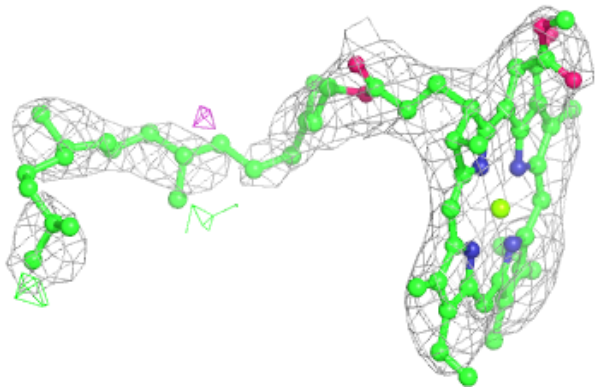
Electron density around CLA 6 311:

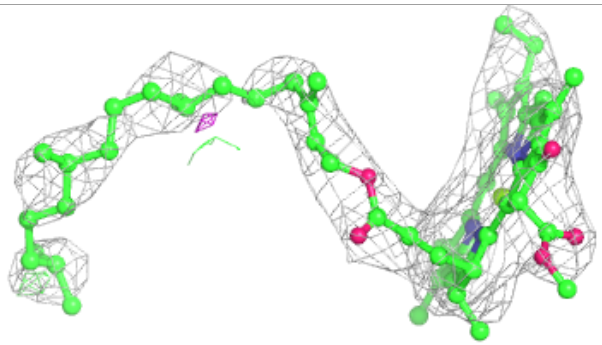
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

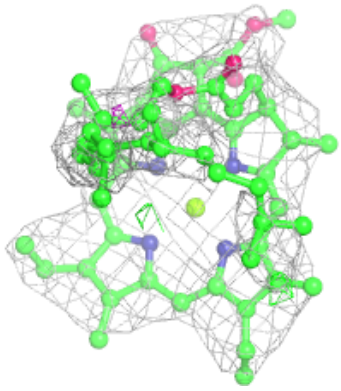


Electron density around CLA L 203:

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

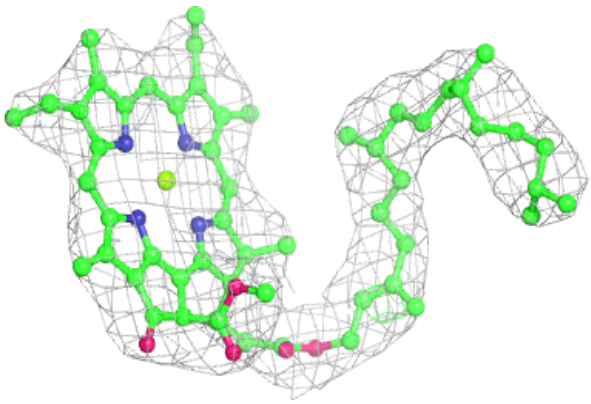


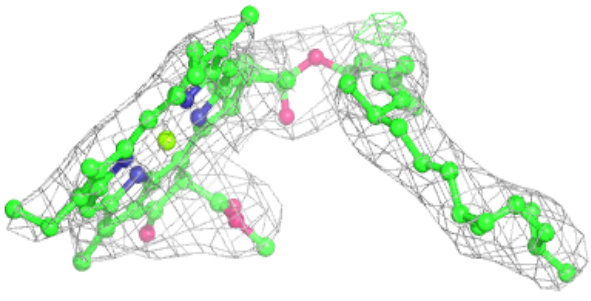


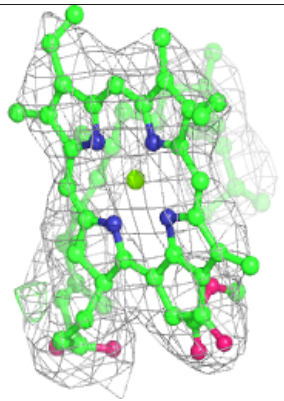


Electron density around CLA B 824:

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

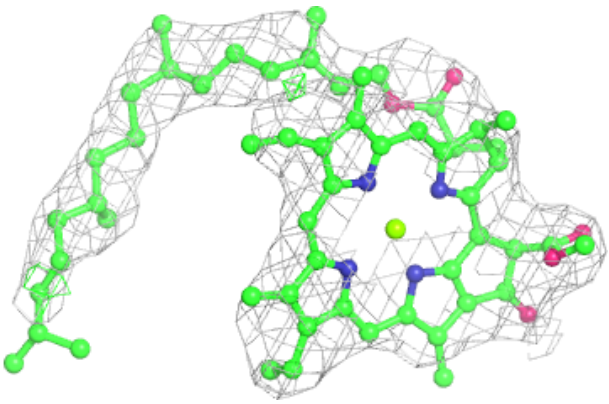


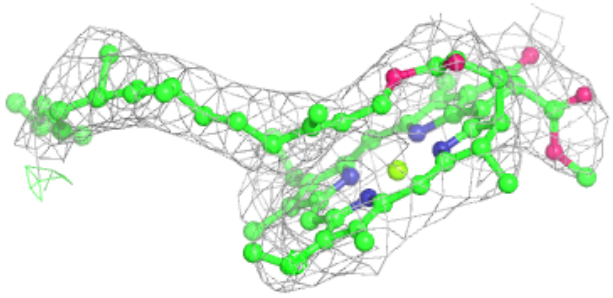


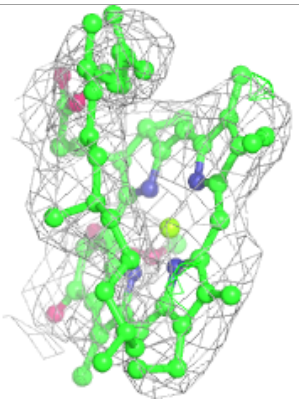


Electron density around CLA 7 602:

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

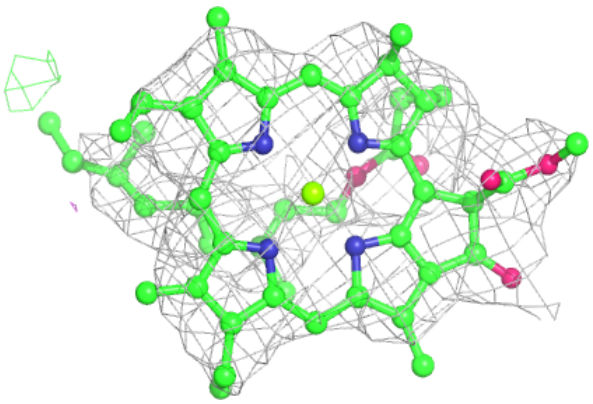


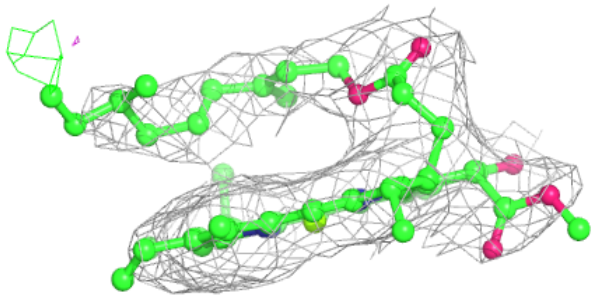


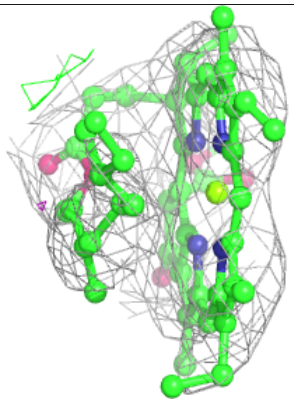


Electron density around CLA 9 612:

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

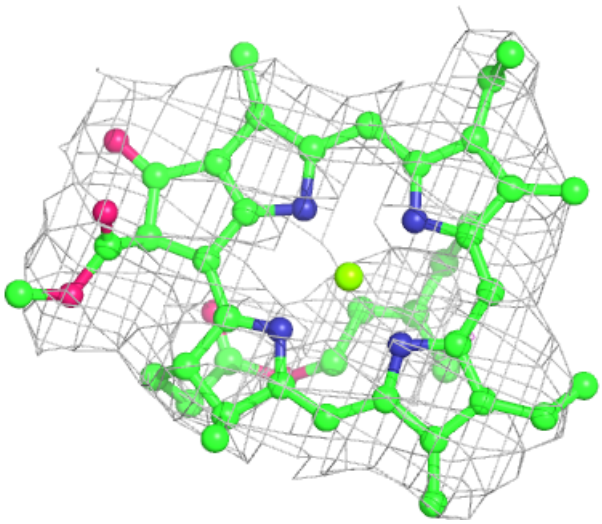


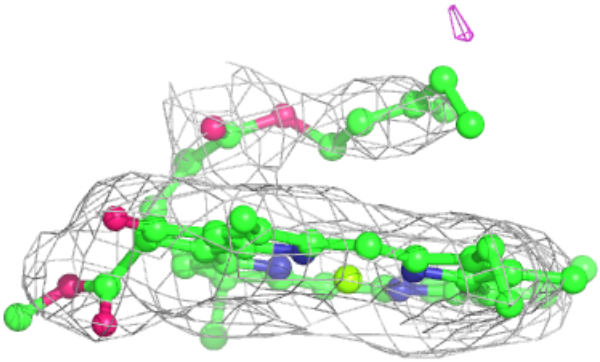


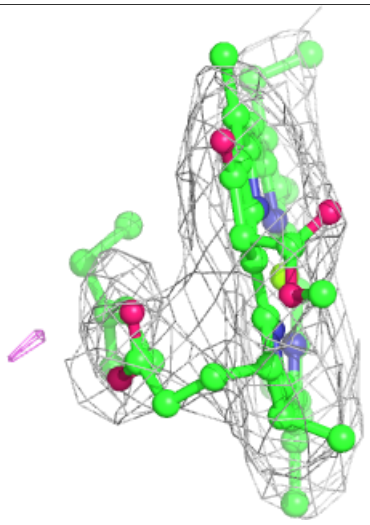


Electron density around CLA a 824:

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

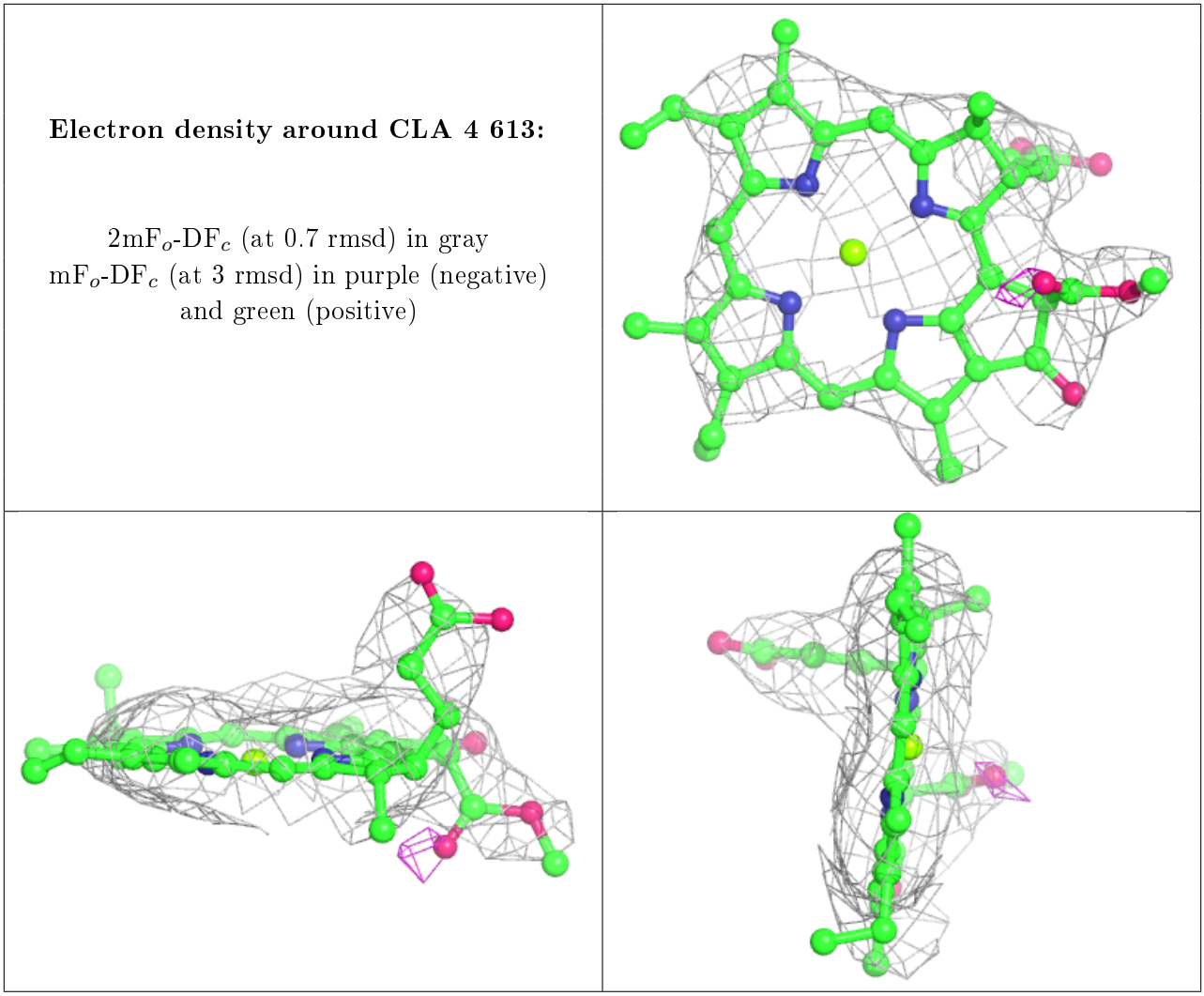






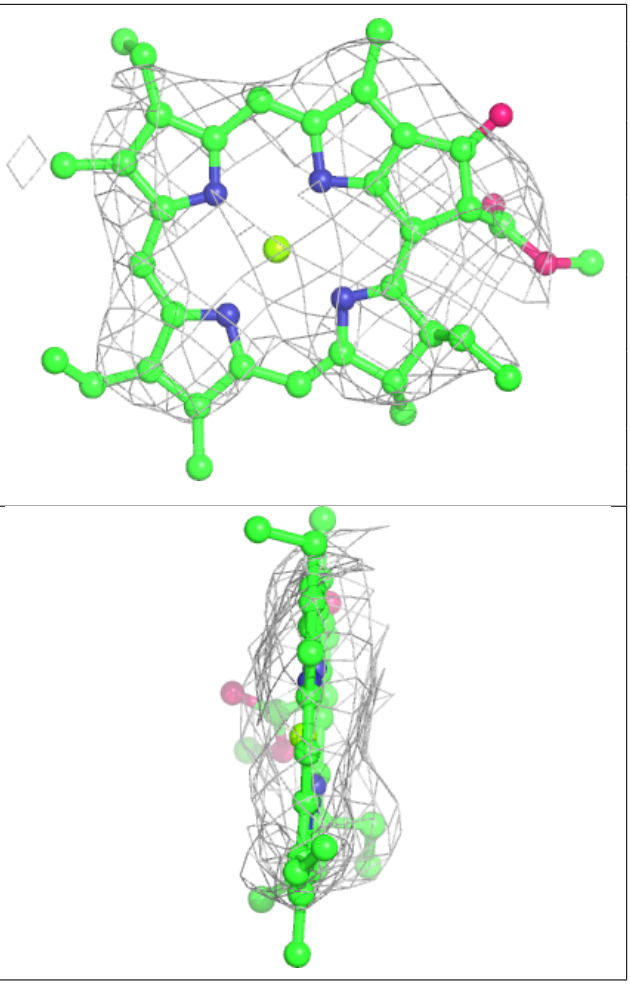
Electron density around CLA 4 613:

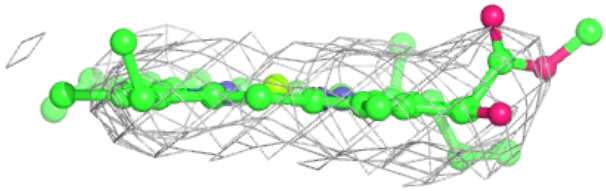
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



Electron density around CLA 6 307:

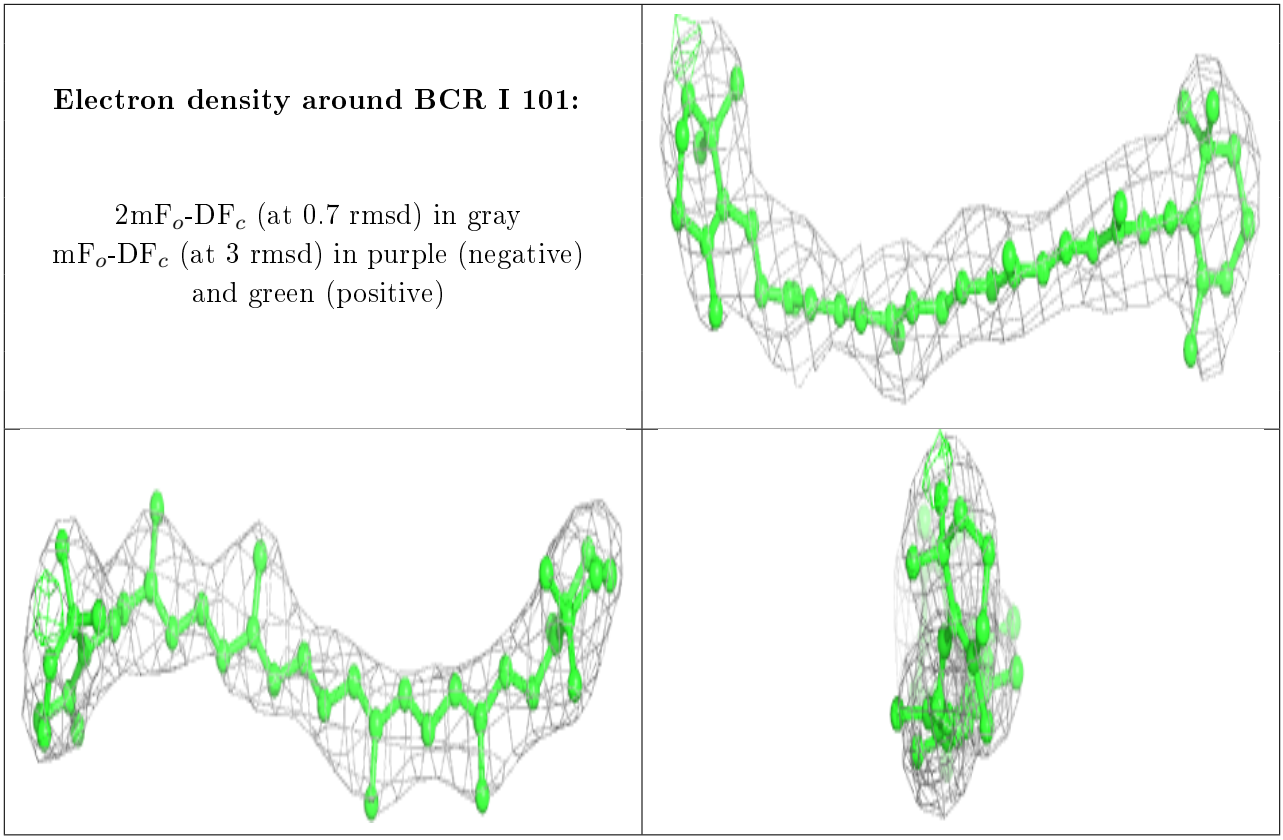
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)





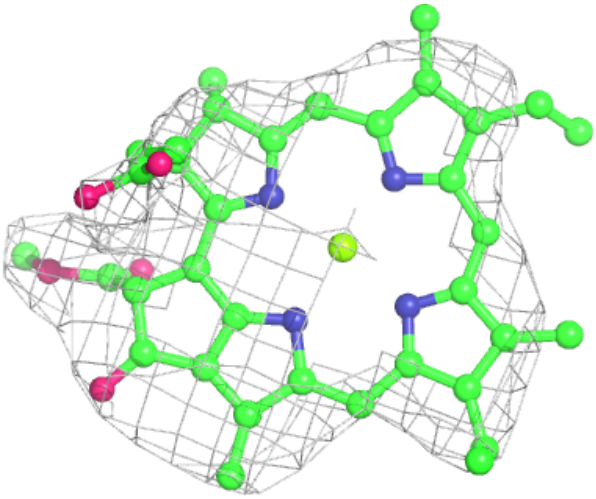
Electron density around BCR I 101:

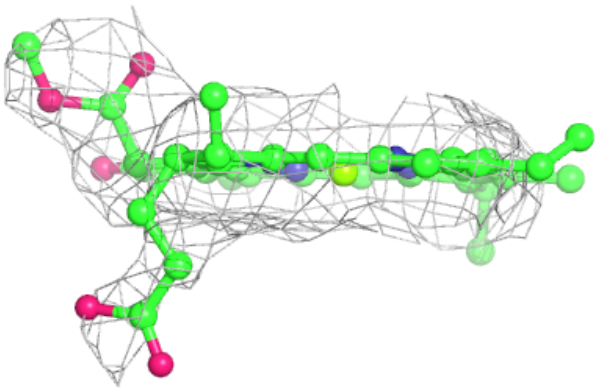
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

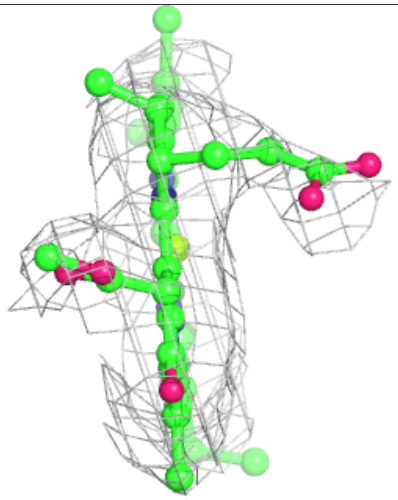


Electron density around CLA 9 613:

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

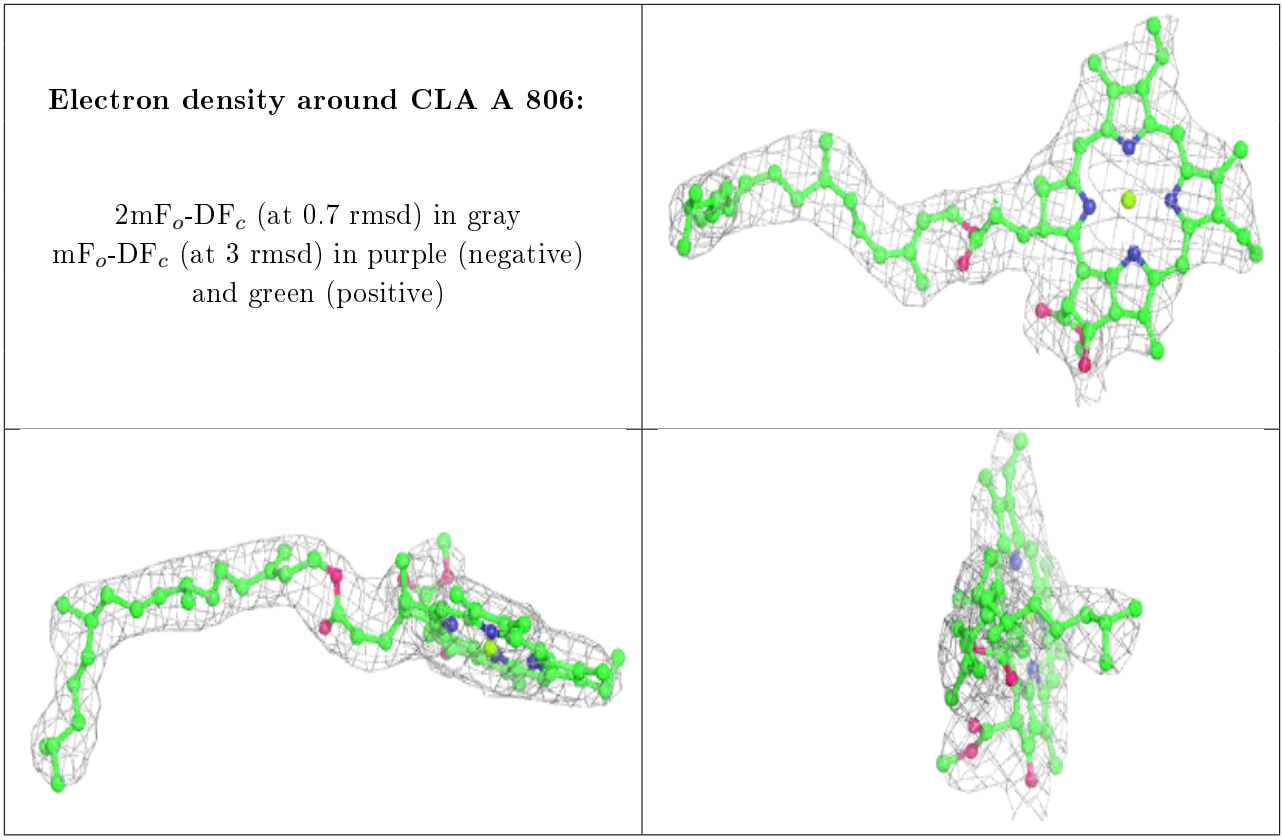






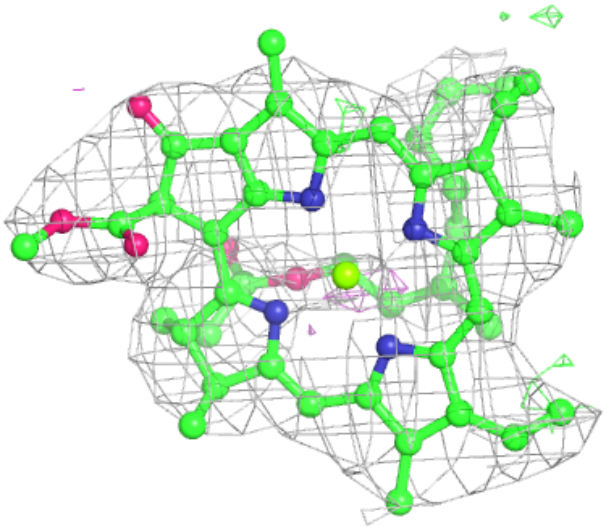
Electron density around CLA A 806:

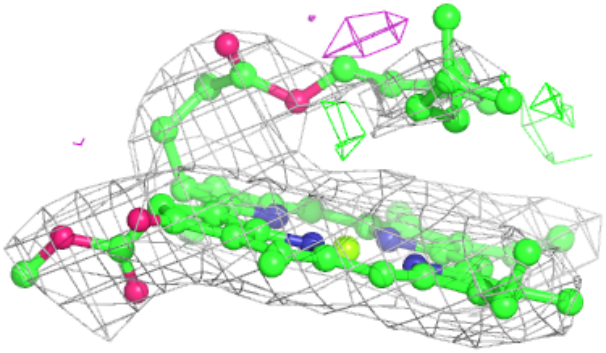
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

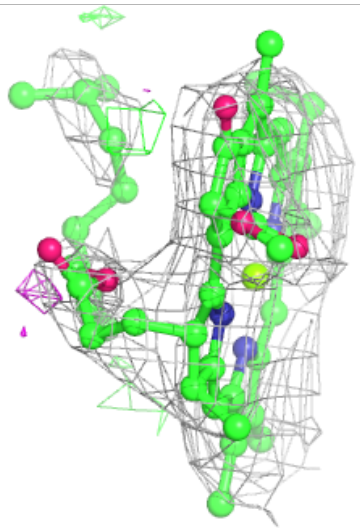


Electron density around CLA b 812:

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

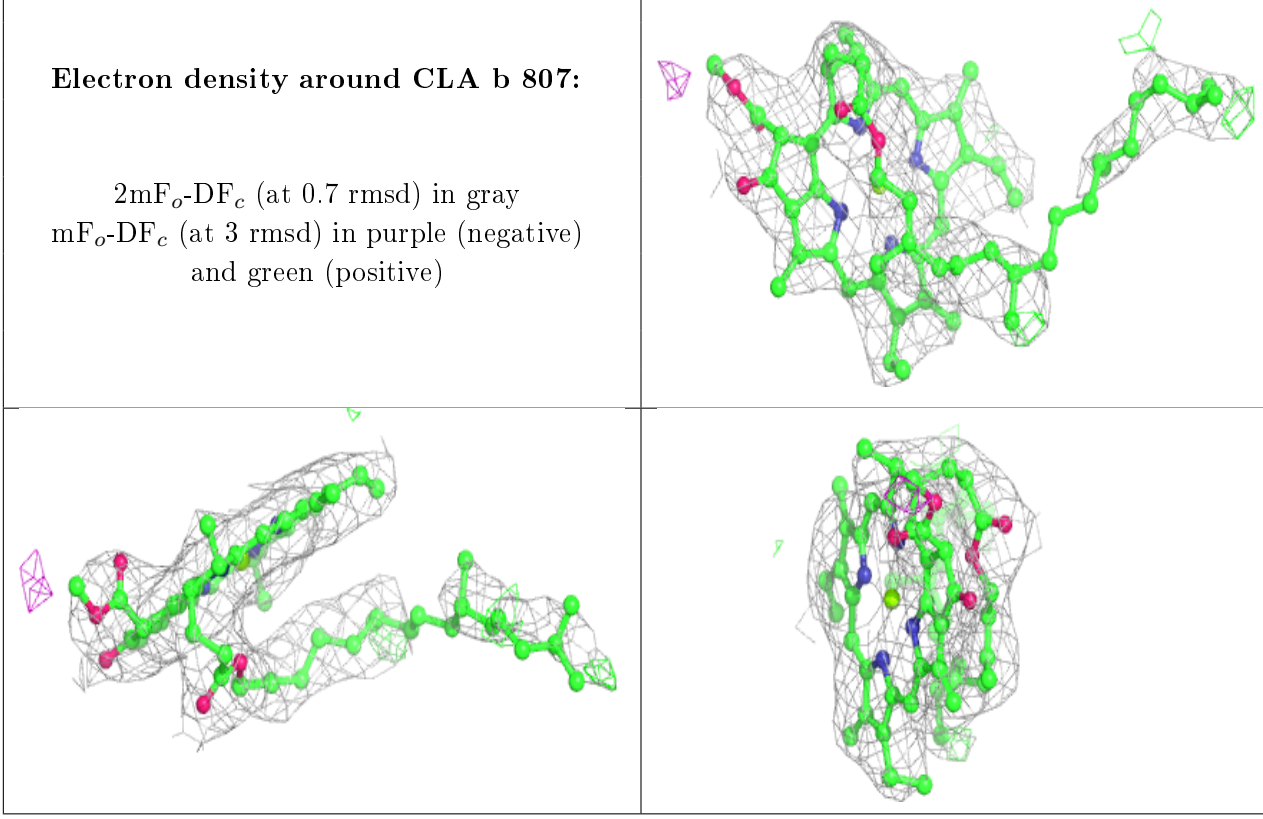






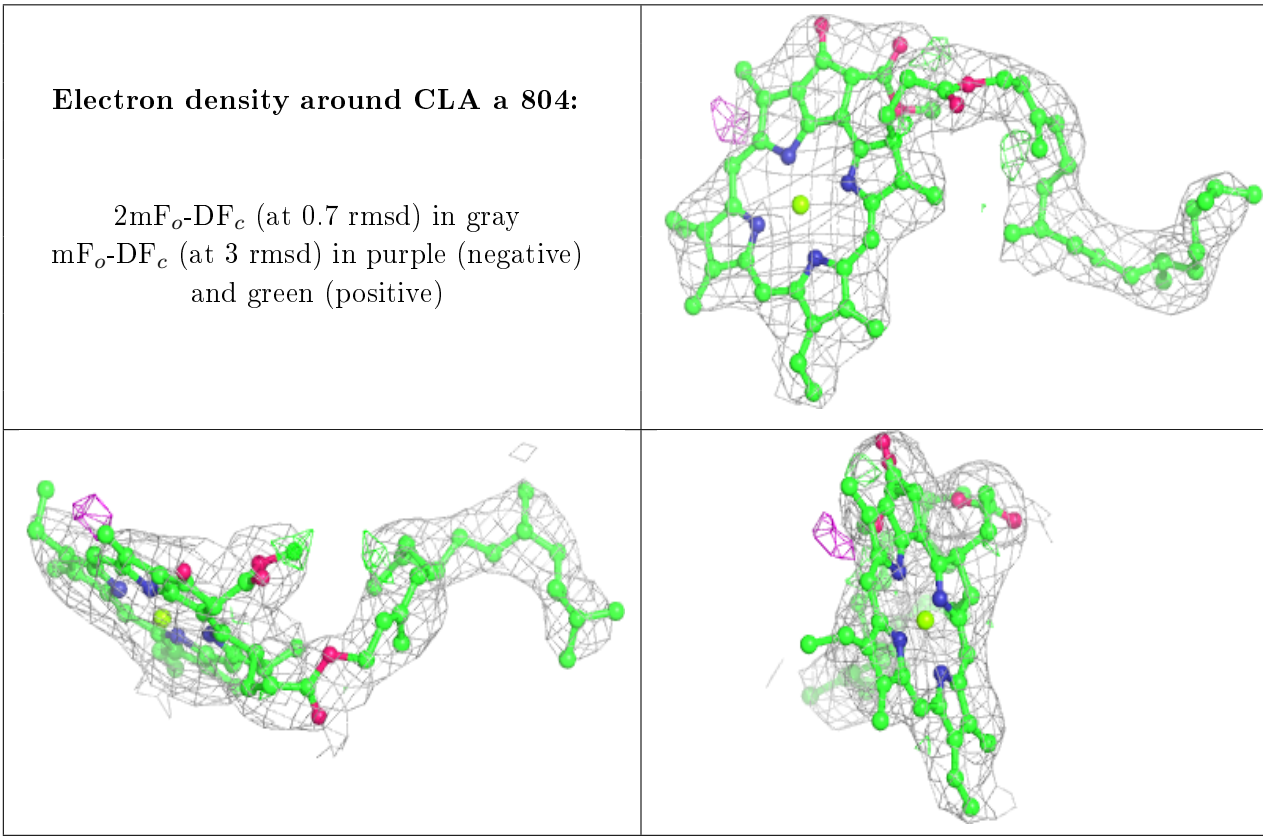
Electron density around CLA b 807:

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



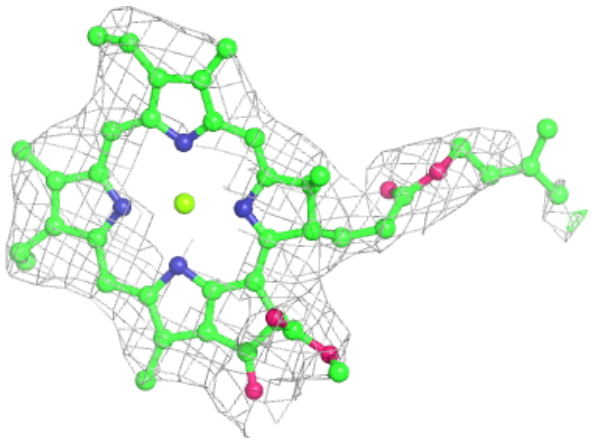
Electron density around CLA a 804:

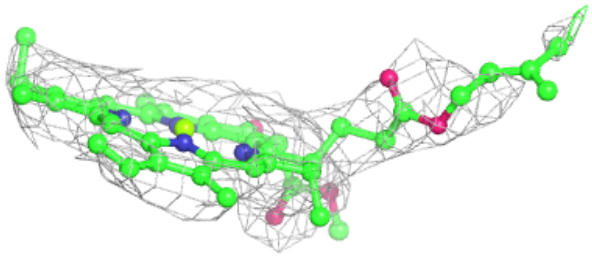
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

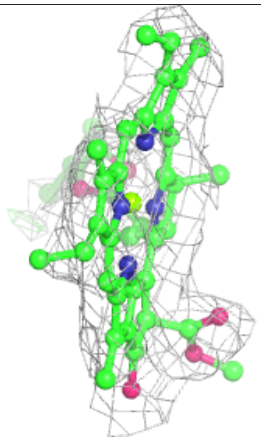


Electron density around CLA G 103:

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

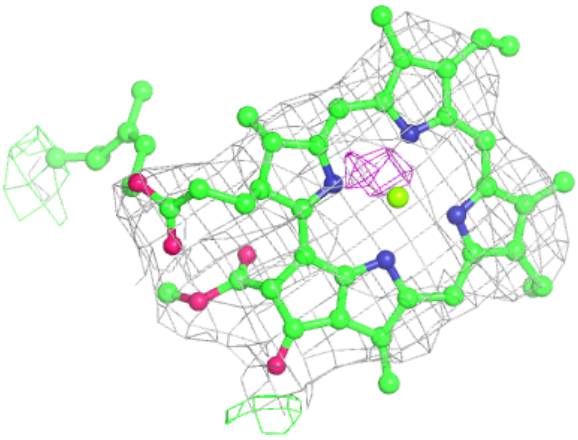


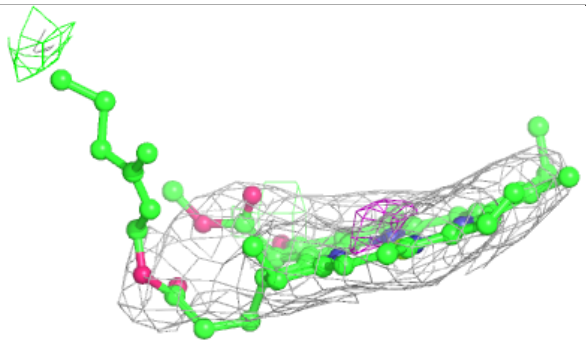


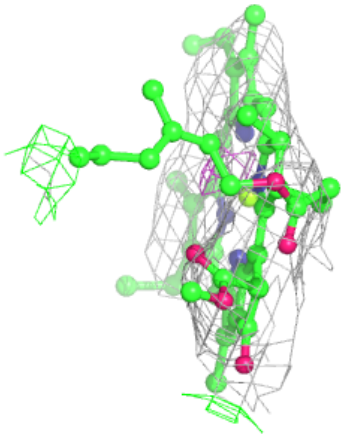


Electron density around CLA 7 611:

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

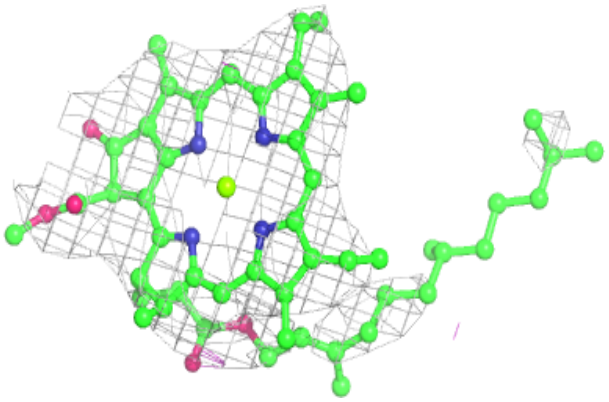


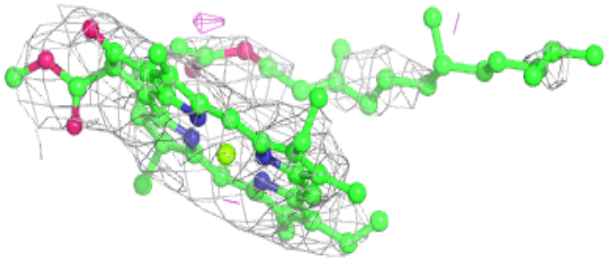


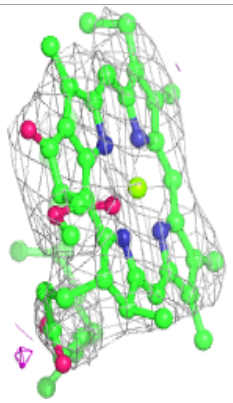


Electron density around CLA 9 609:

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

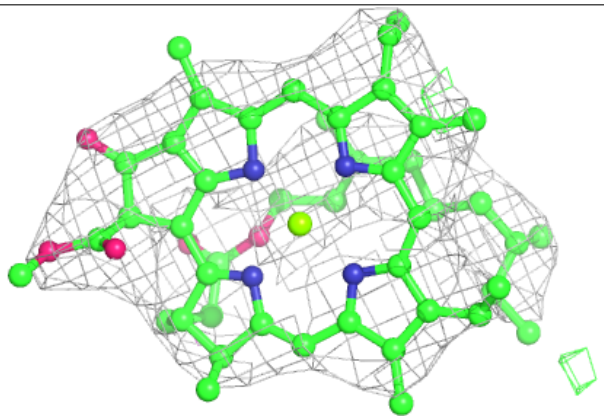


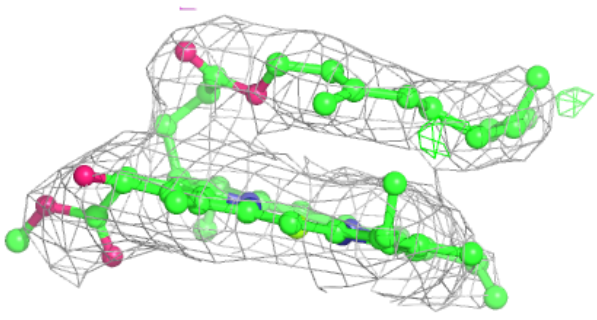


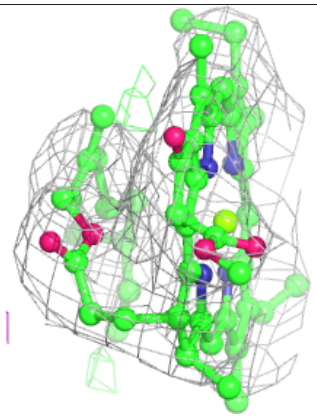


Electron density around CLA 4 612:

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

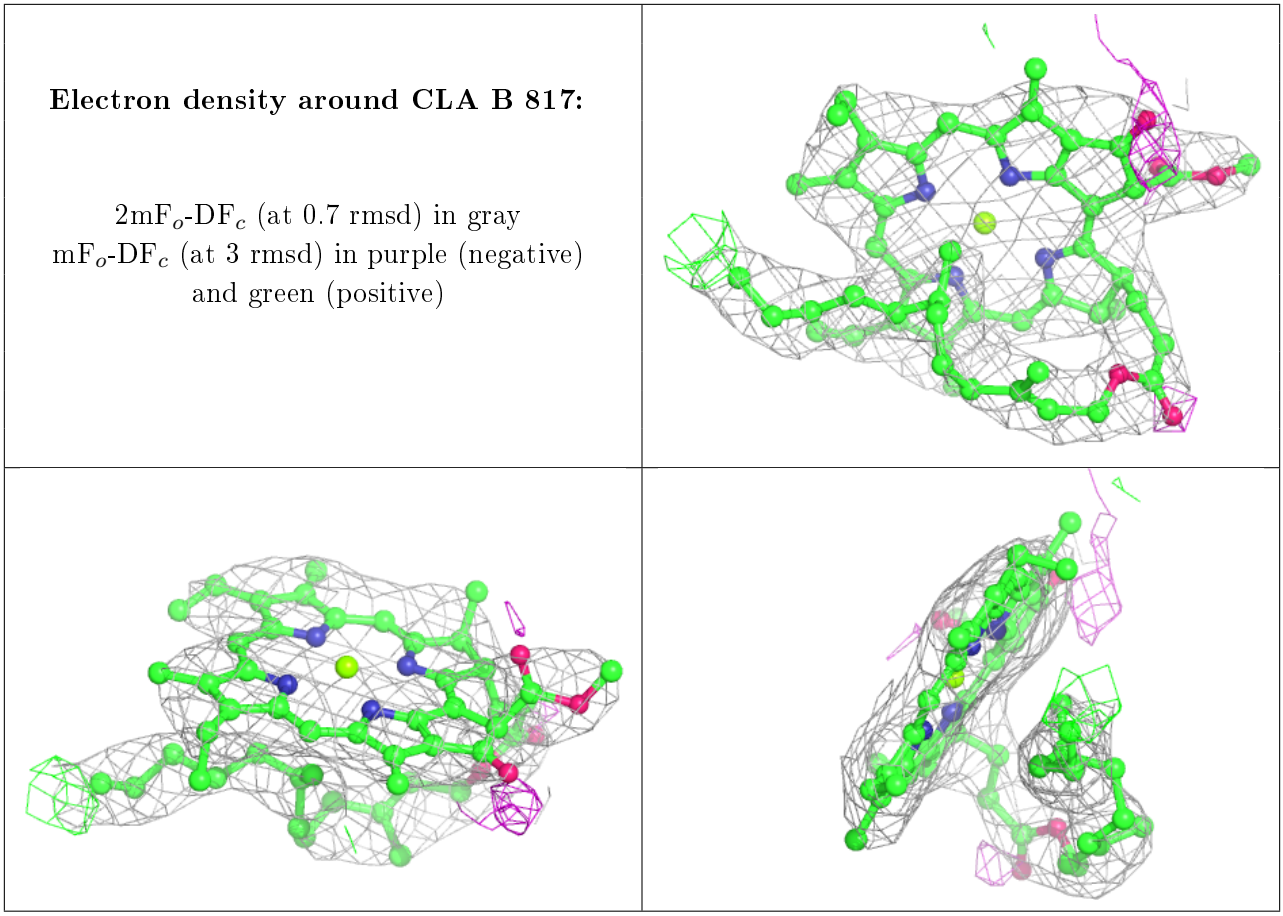






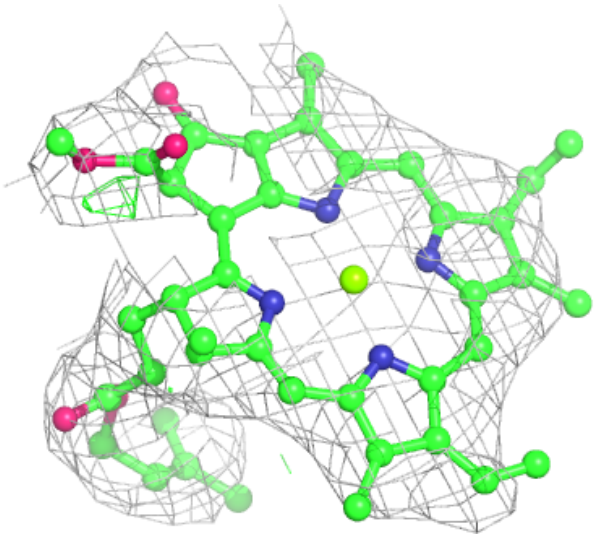
Electron density around CLA B 817:

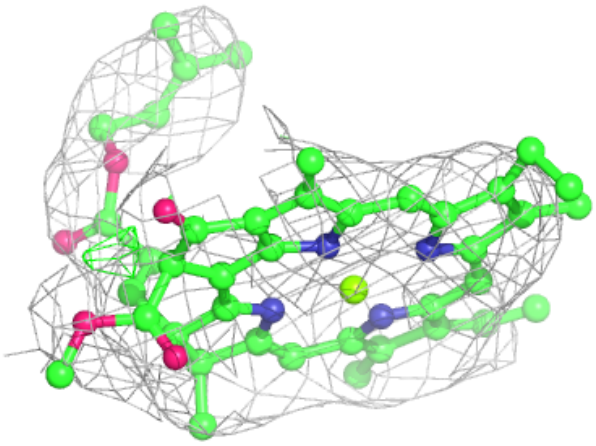
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

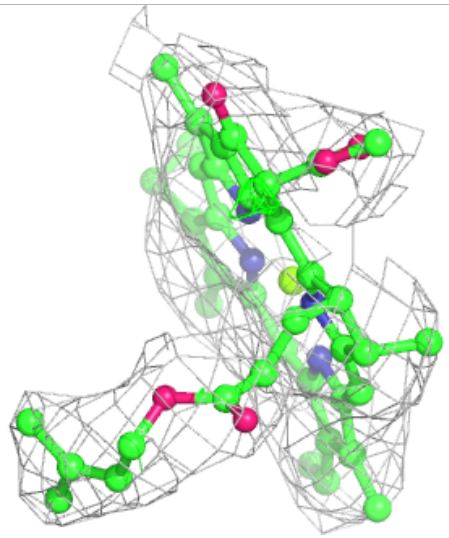


Electron density around CLA 7 608:

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

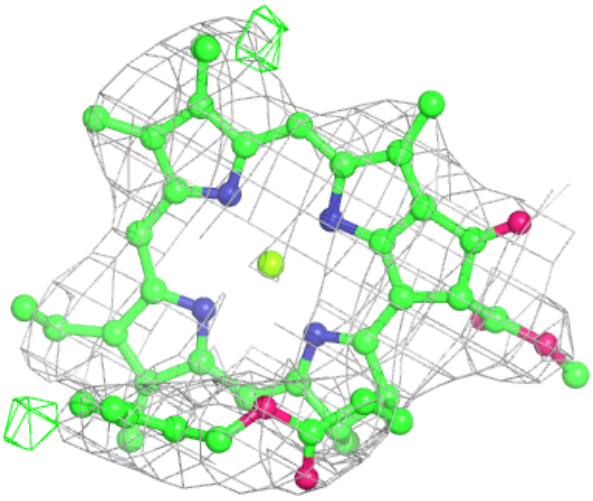


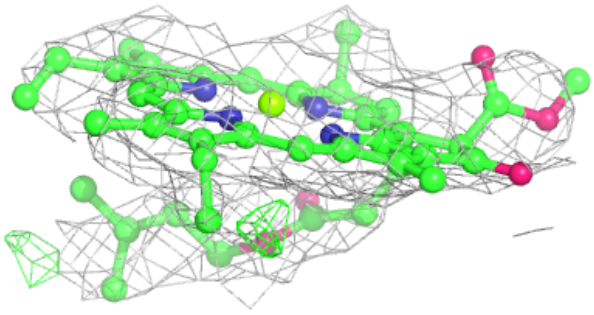


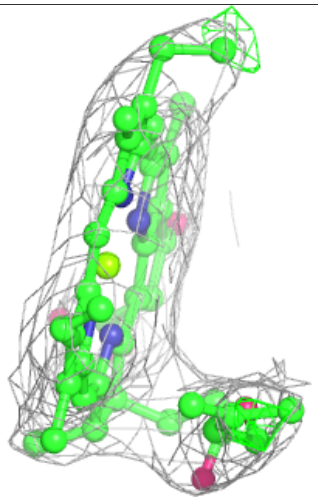


Electron density around CLA 3 309:

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

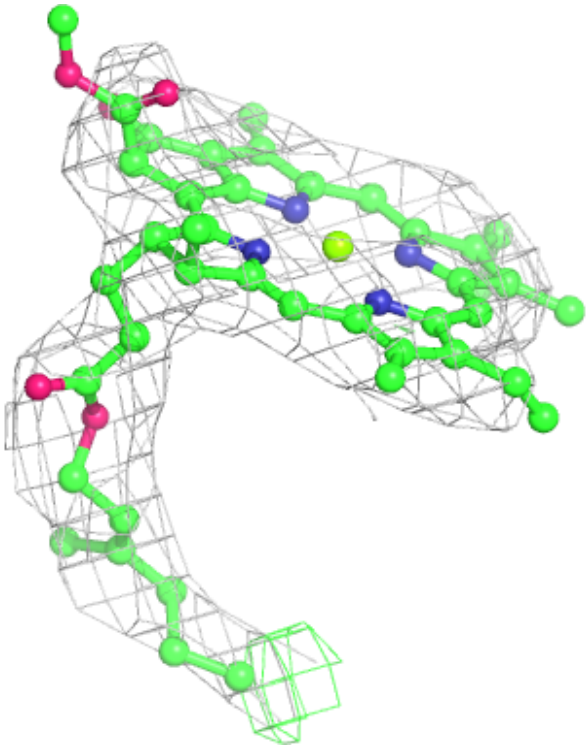


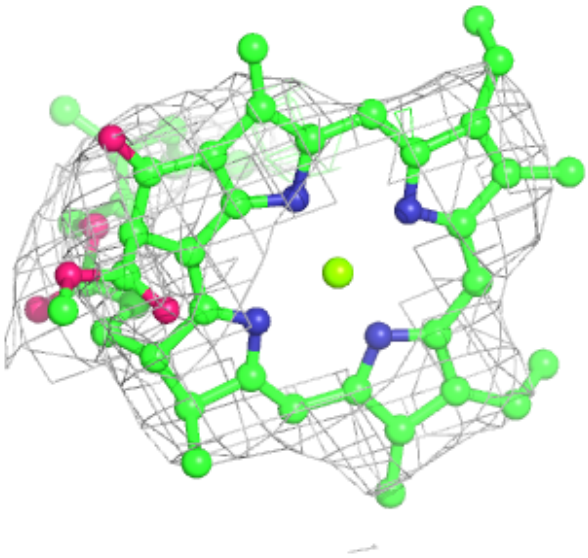


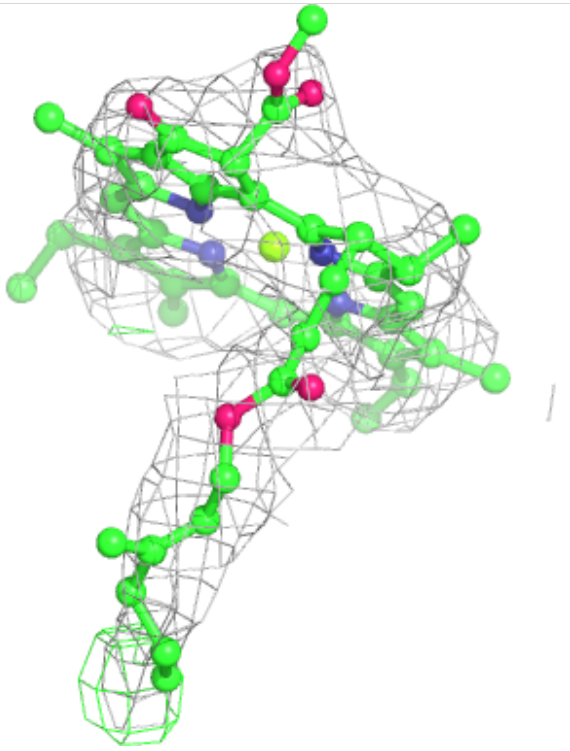


Electron density around CLA 1 305:

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

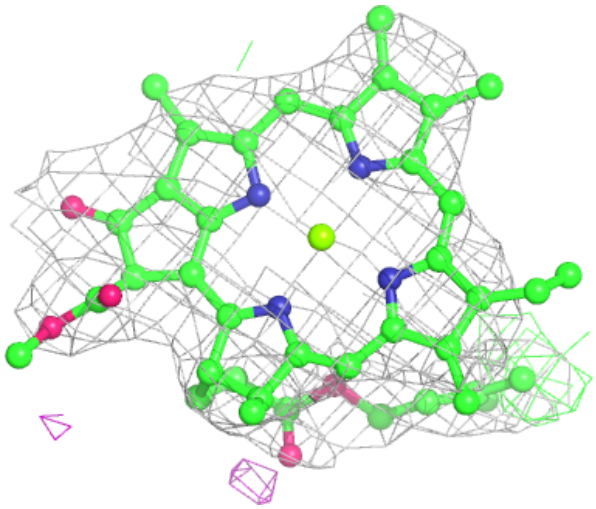


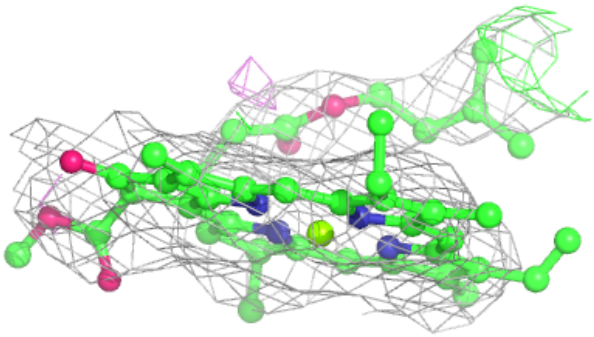


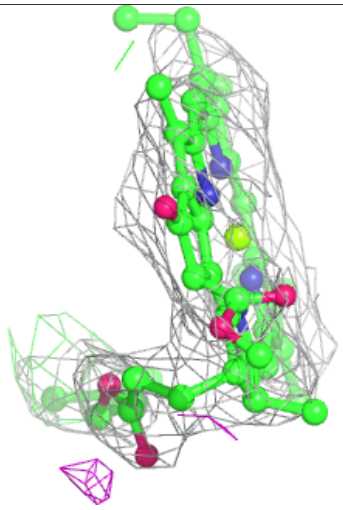


Electron density around CLA 8 308:

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

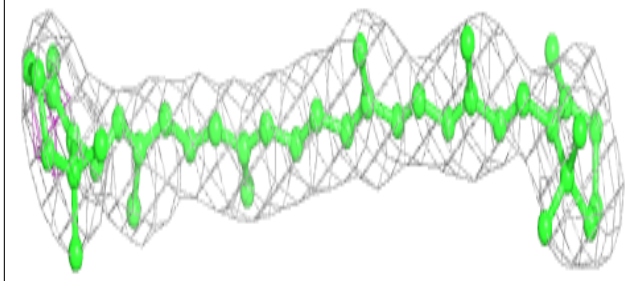


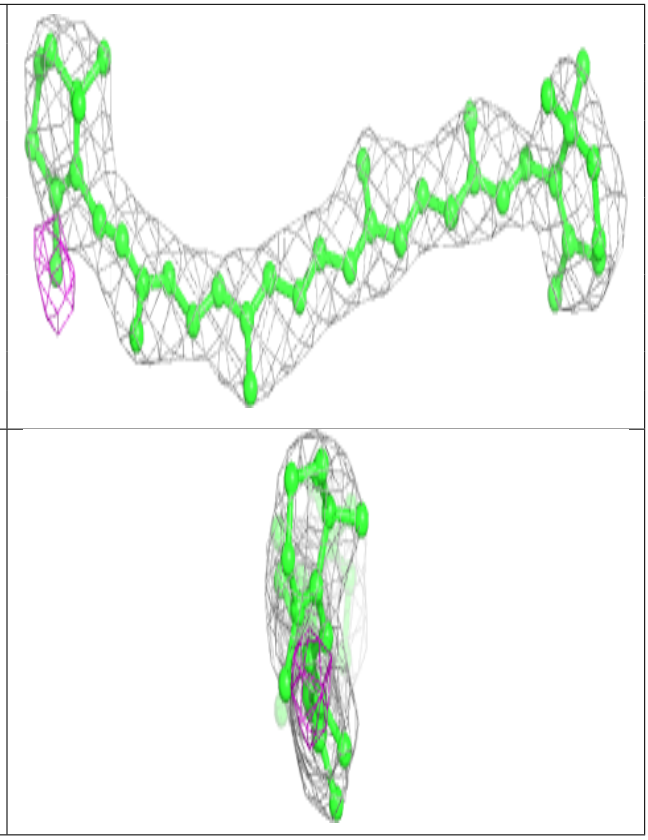




Electron density around BCR b 847:

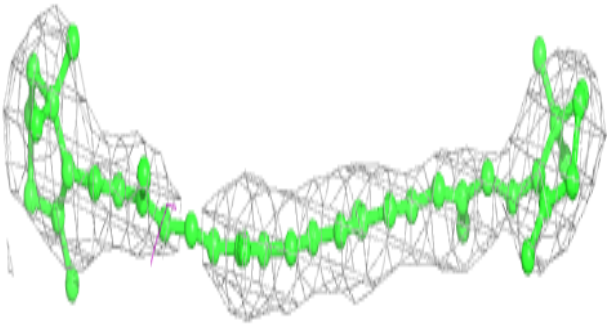
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

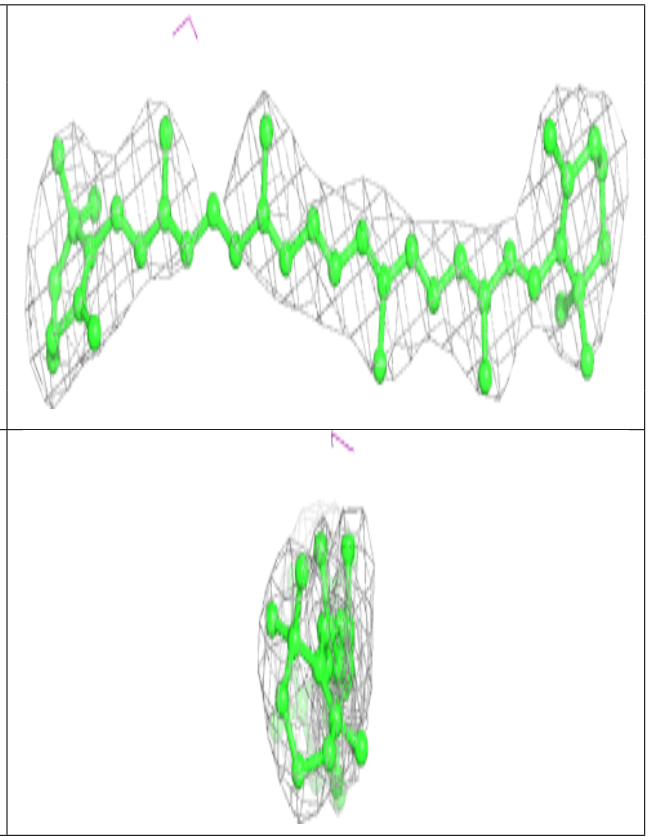




Electron density around BCR B 843:

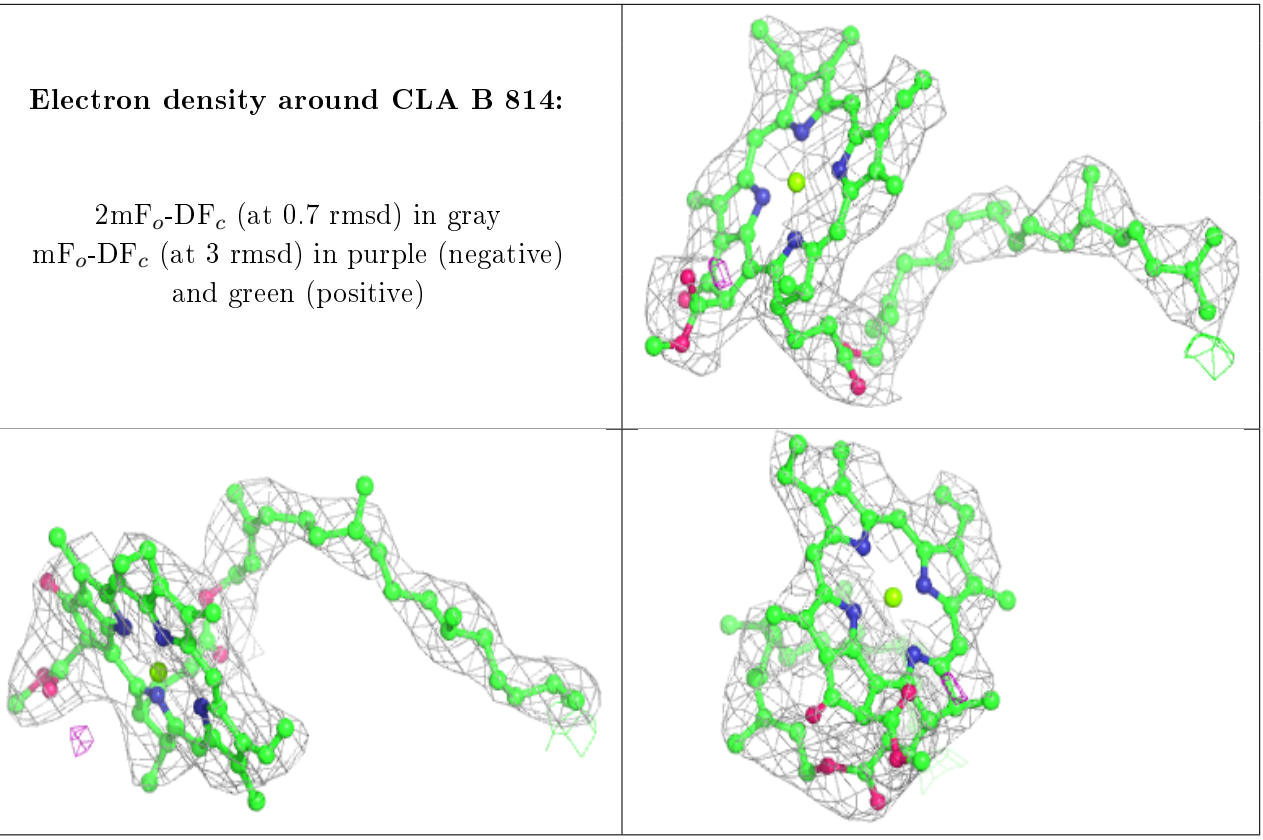
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)





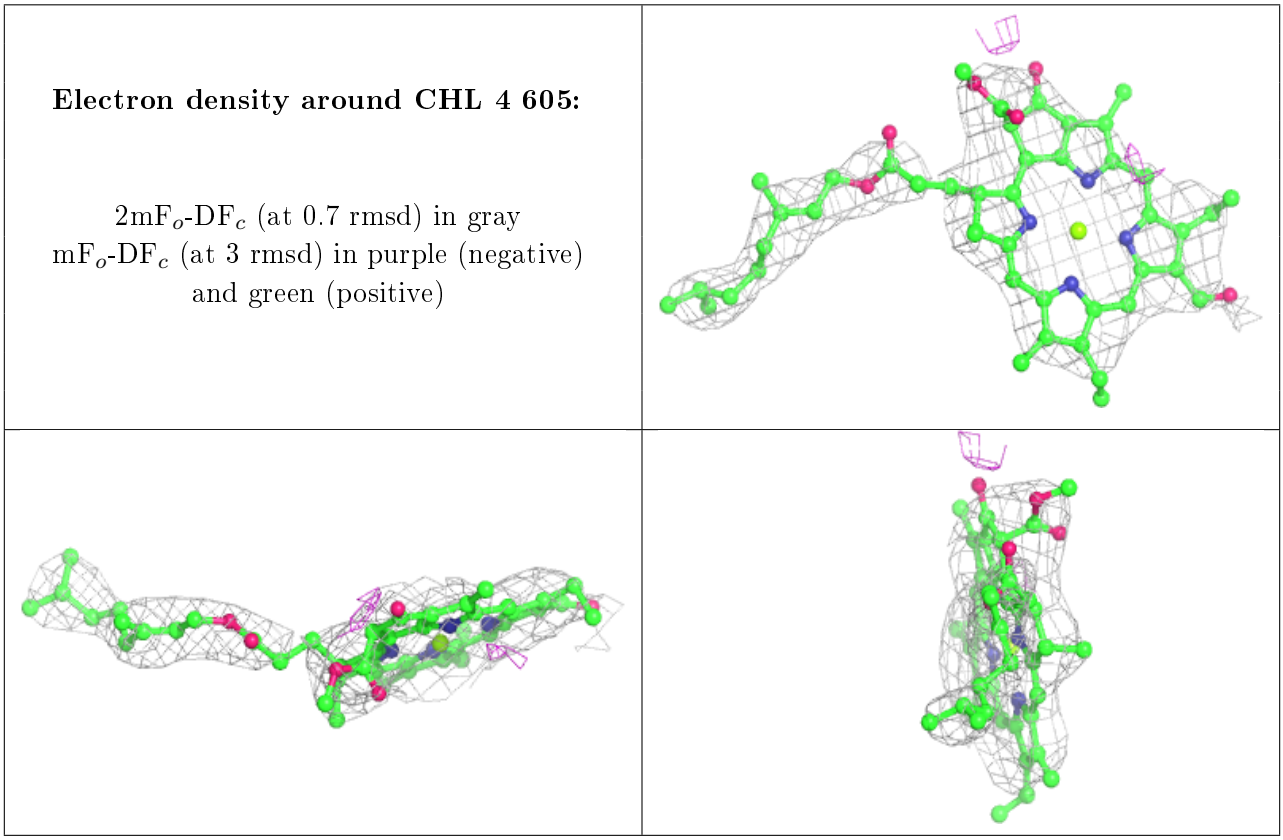
Electron density around CLA B 814:

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



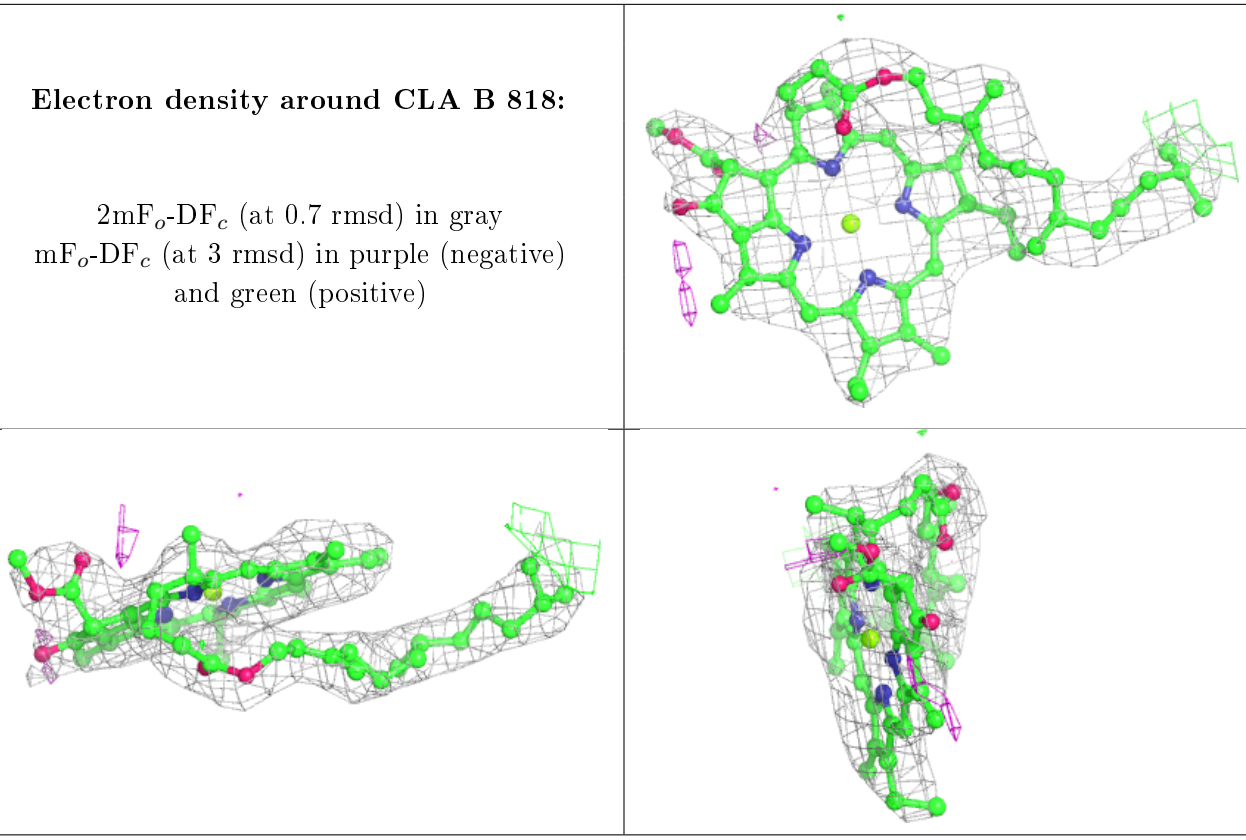
Electron density around CHL 4 605:

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



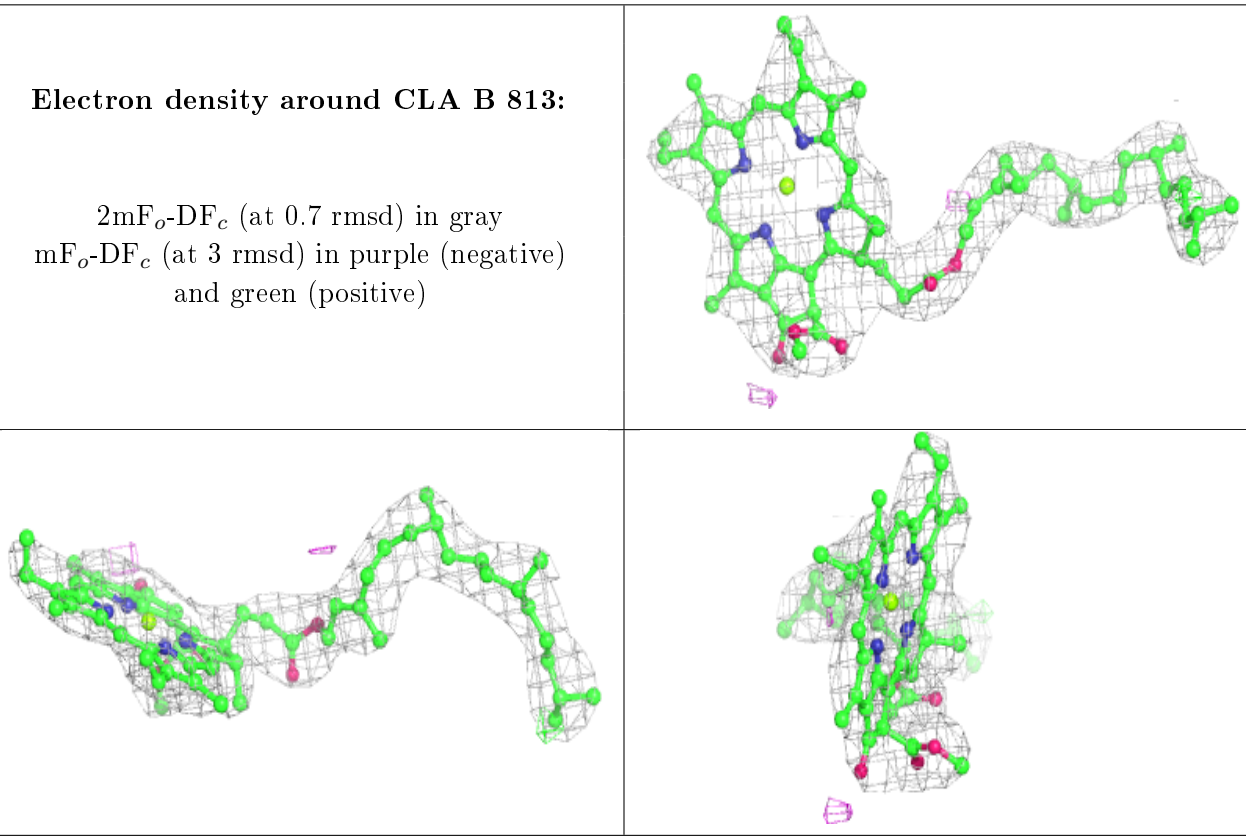
Electron density around CLA B 818:

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



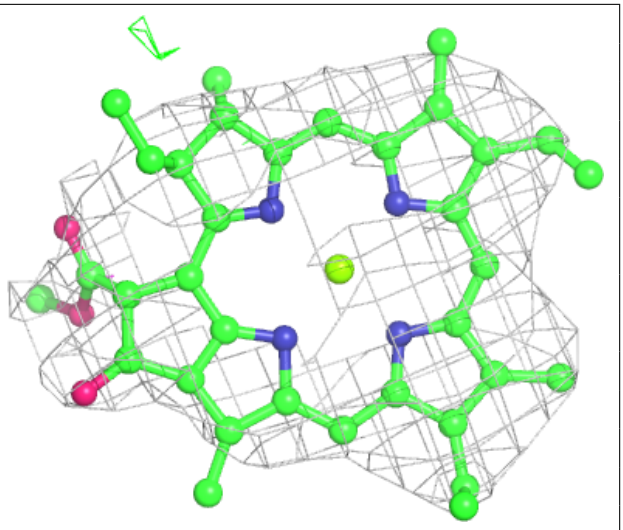
Electron density around CLA B 813:

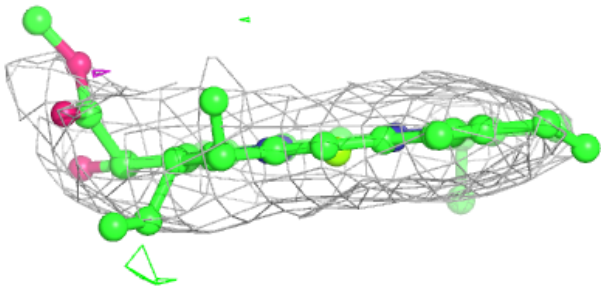
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

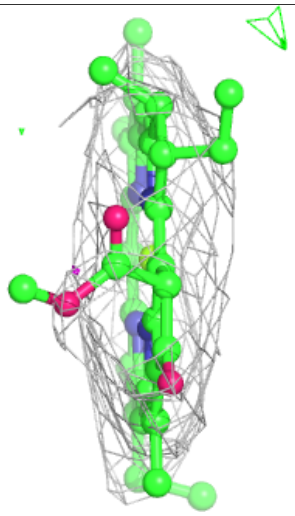


Electron density around CLA J 3002:

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

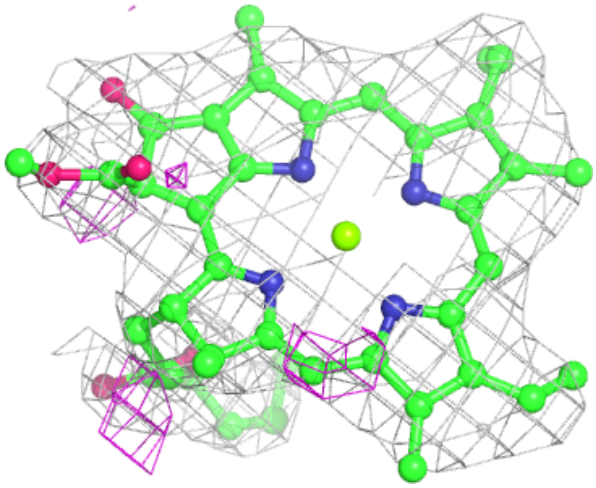


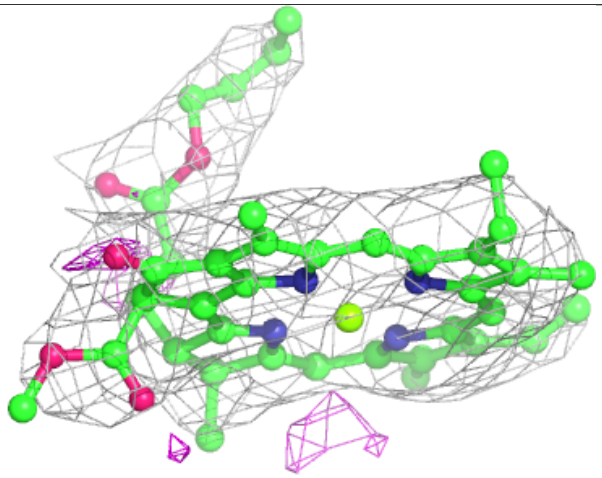


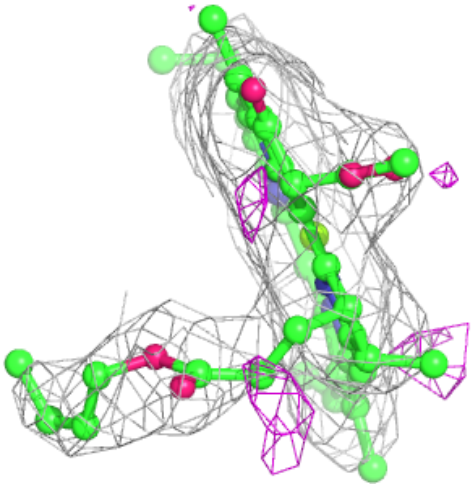


Electron density around CLA b 831:

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

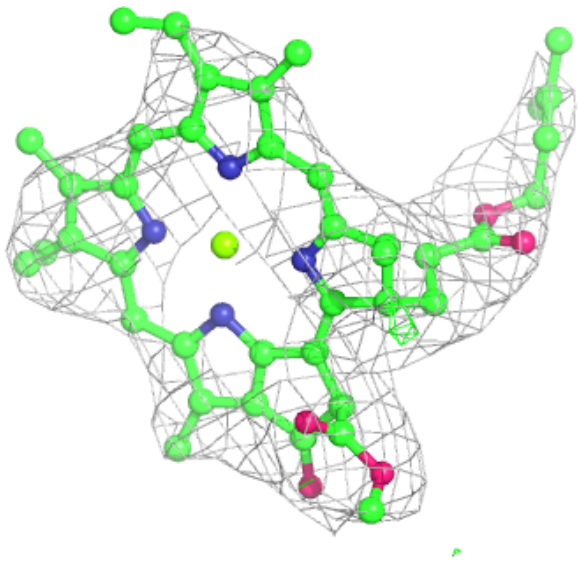


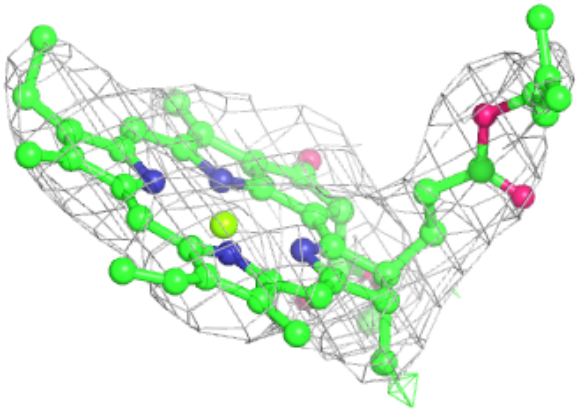


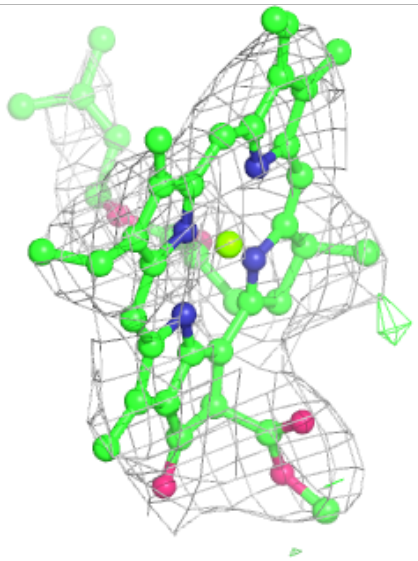


Electron density around CLA b 820:

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

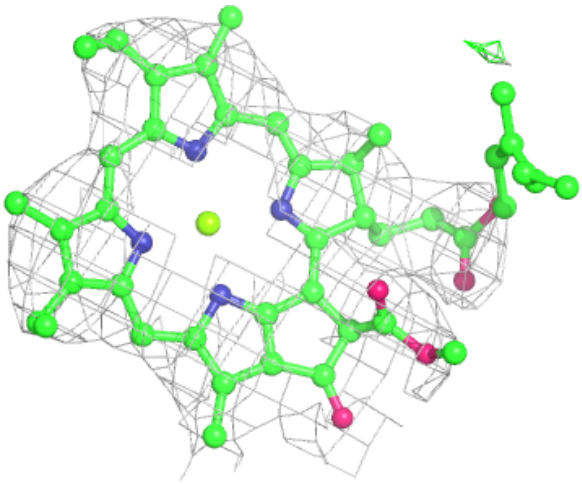


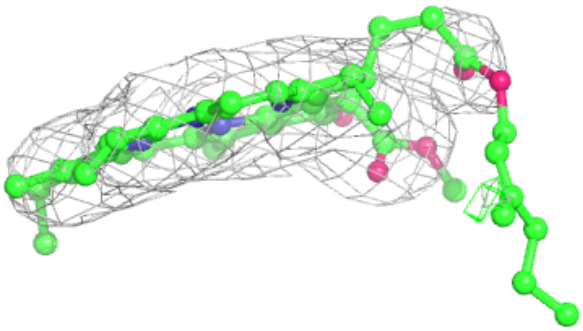


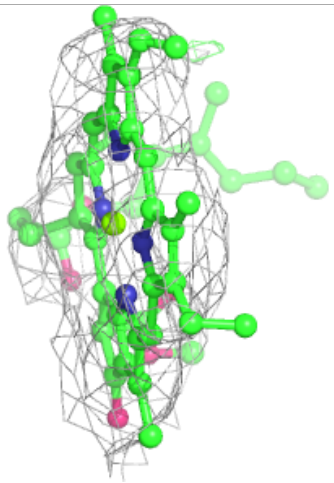


Electron density around CLA 4 611:

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

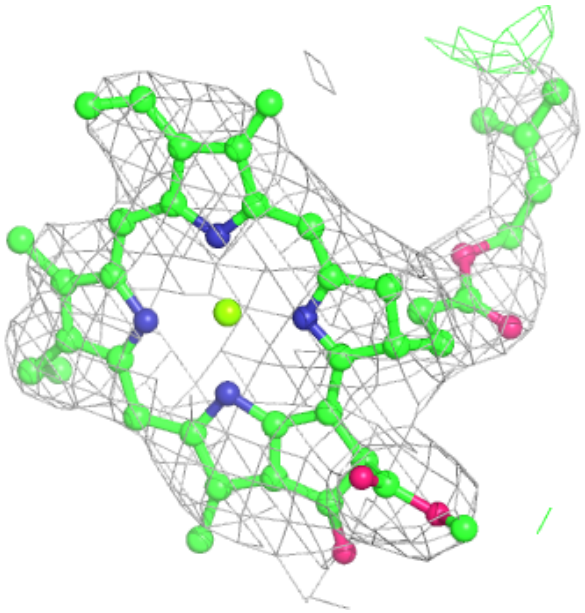


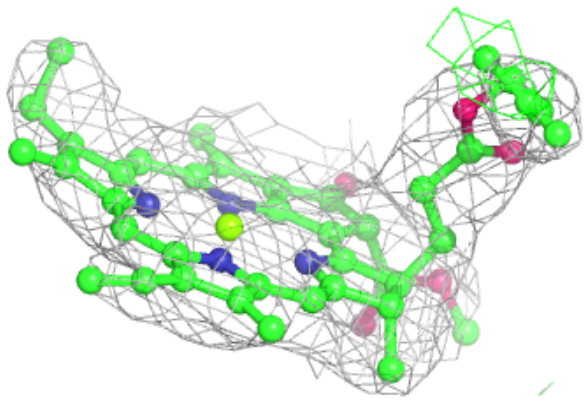


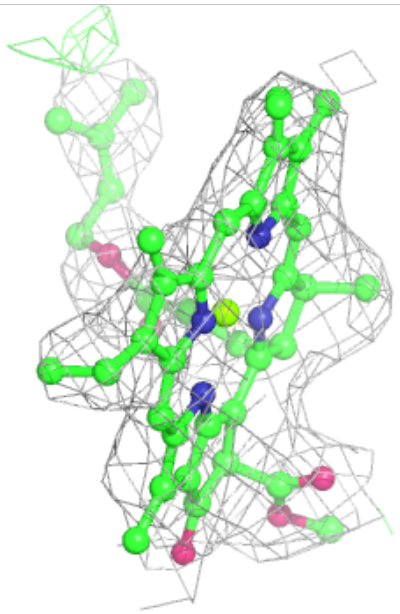


Electron density around CLA A 836:

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

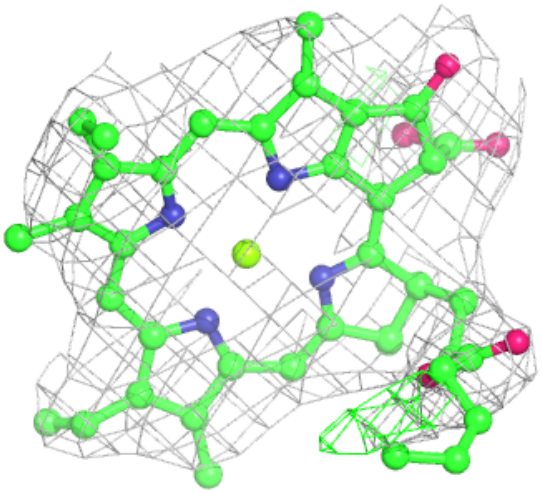


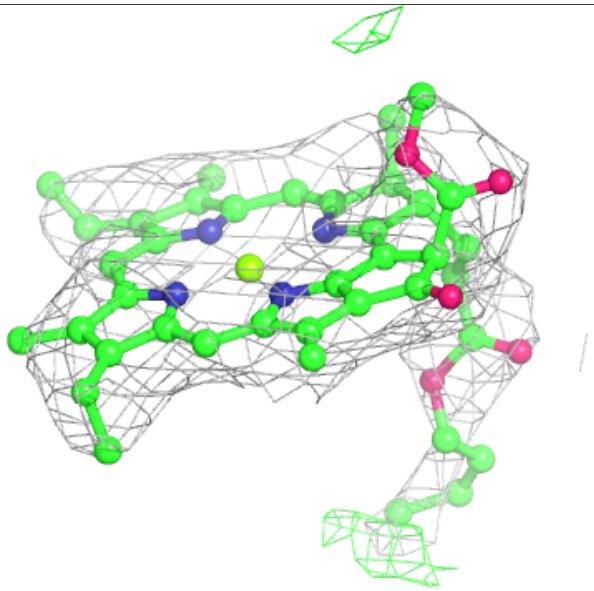


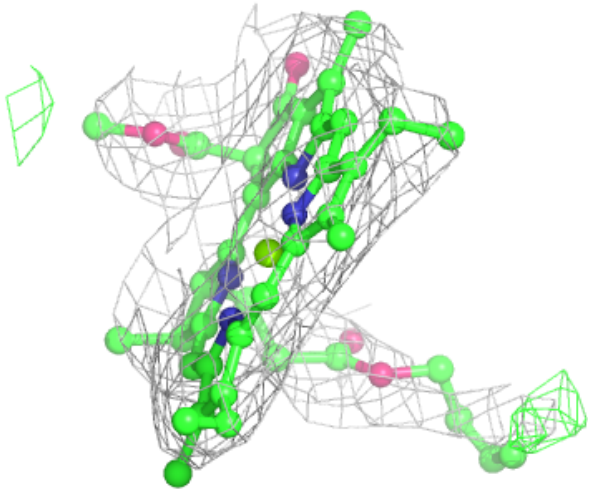


Electron density around CLA a 823:

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

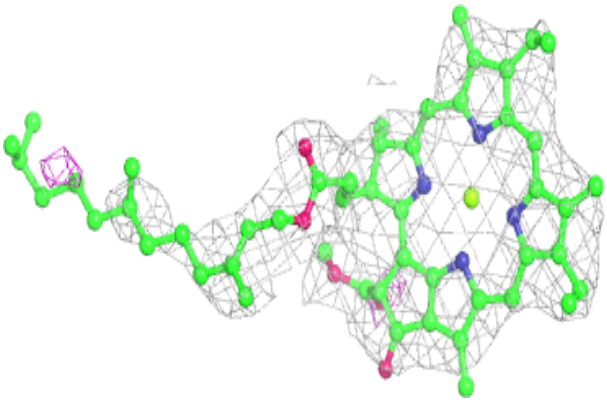


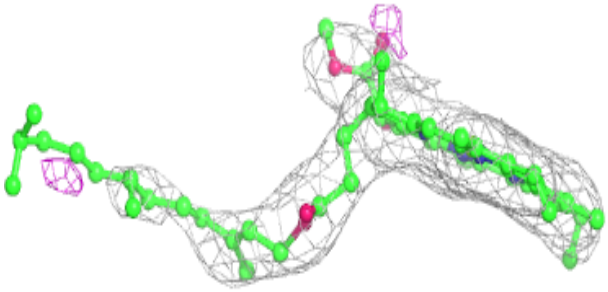


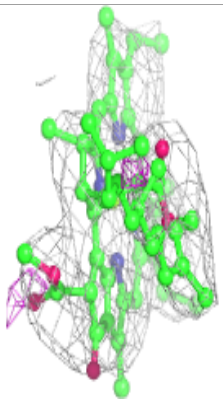


Electron density around CLA b 823:

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

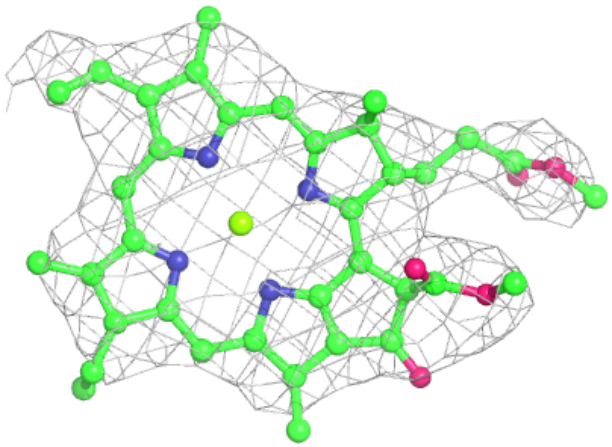


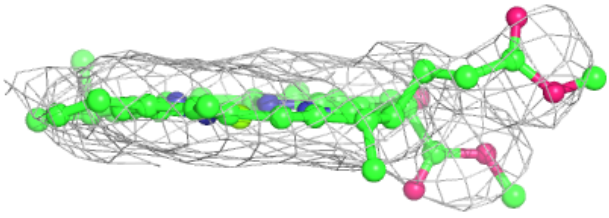


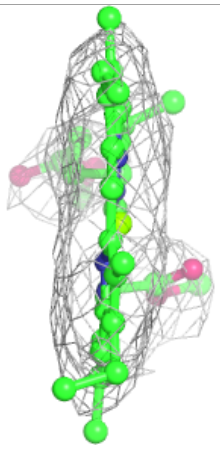


Electron density around CLA 3 314:

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

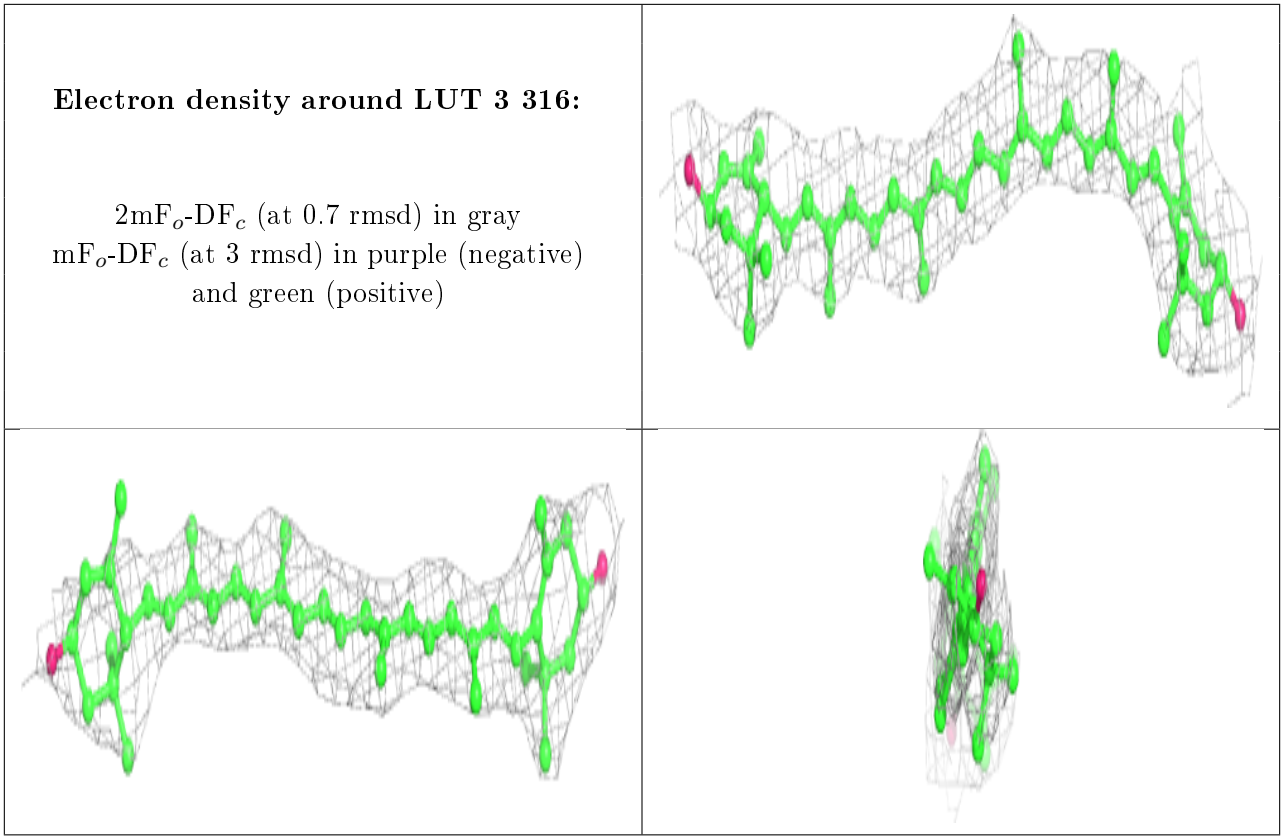






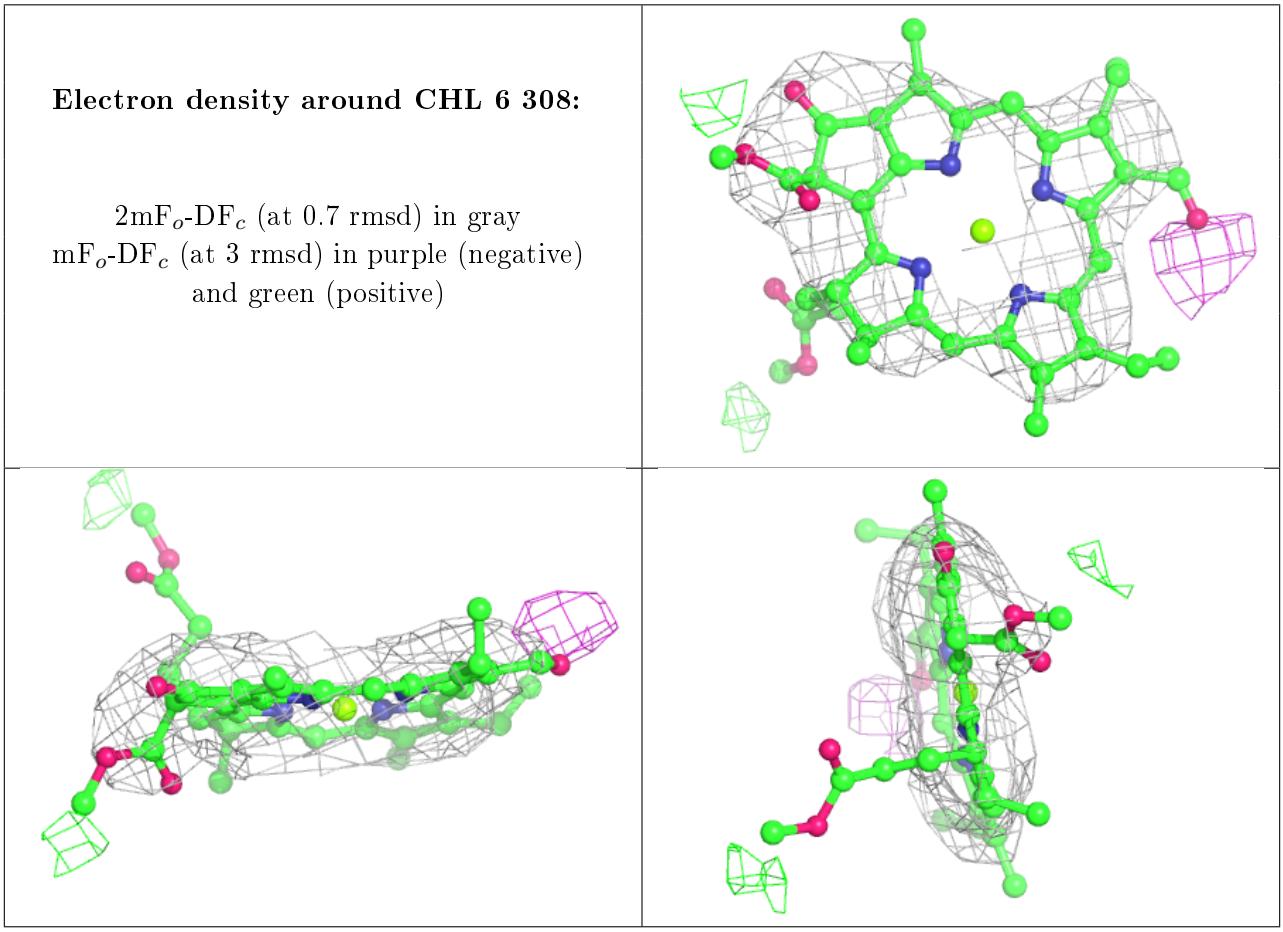
Electron density around LUT 3 316:

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



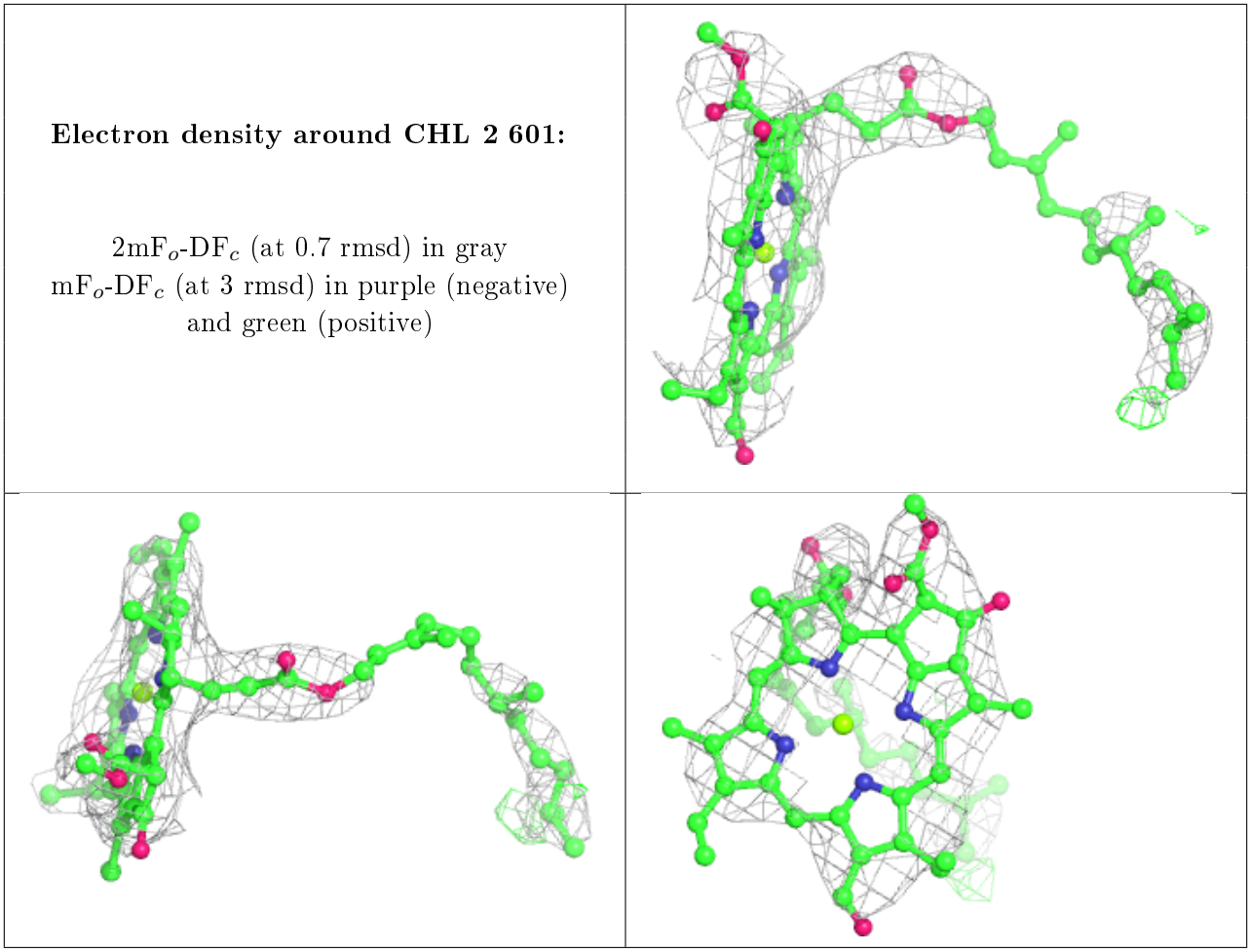
Electron density around CHL 6 308:

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



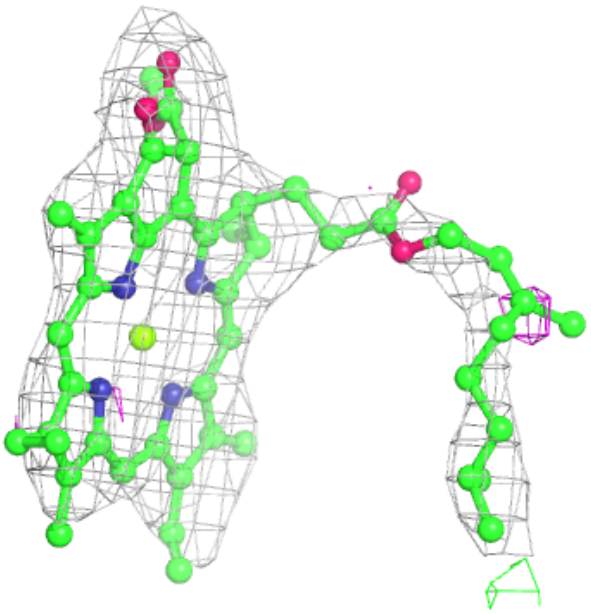
Electron density around CHL 2 601:

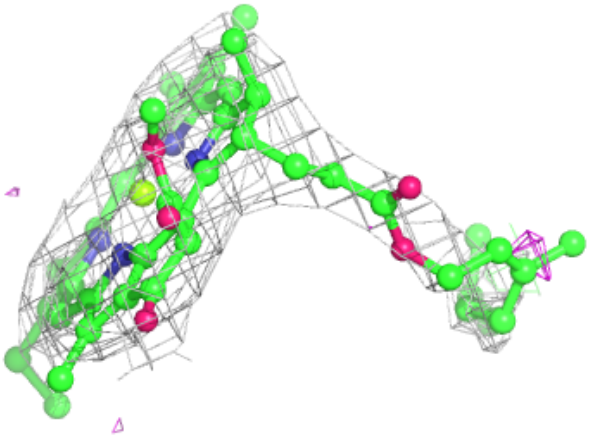
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

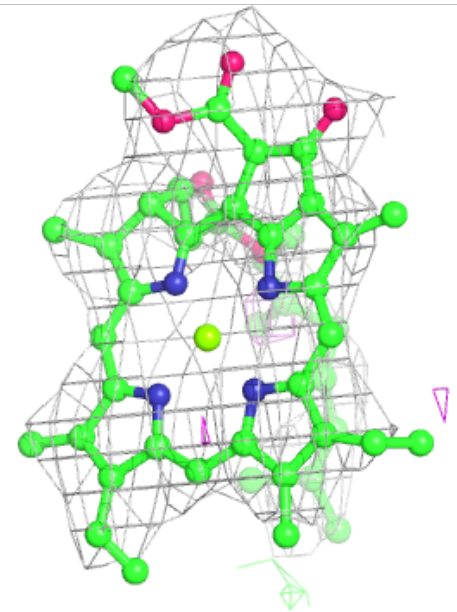


Electron density around CLA b 815:

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

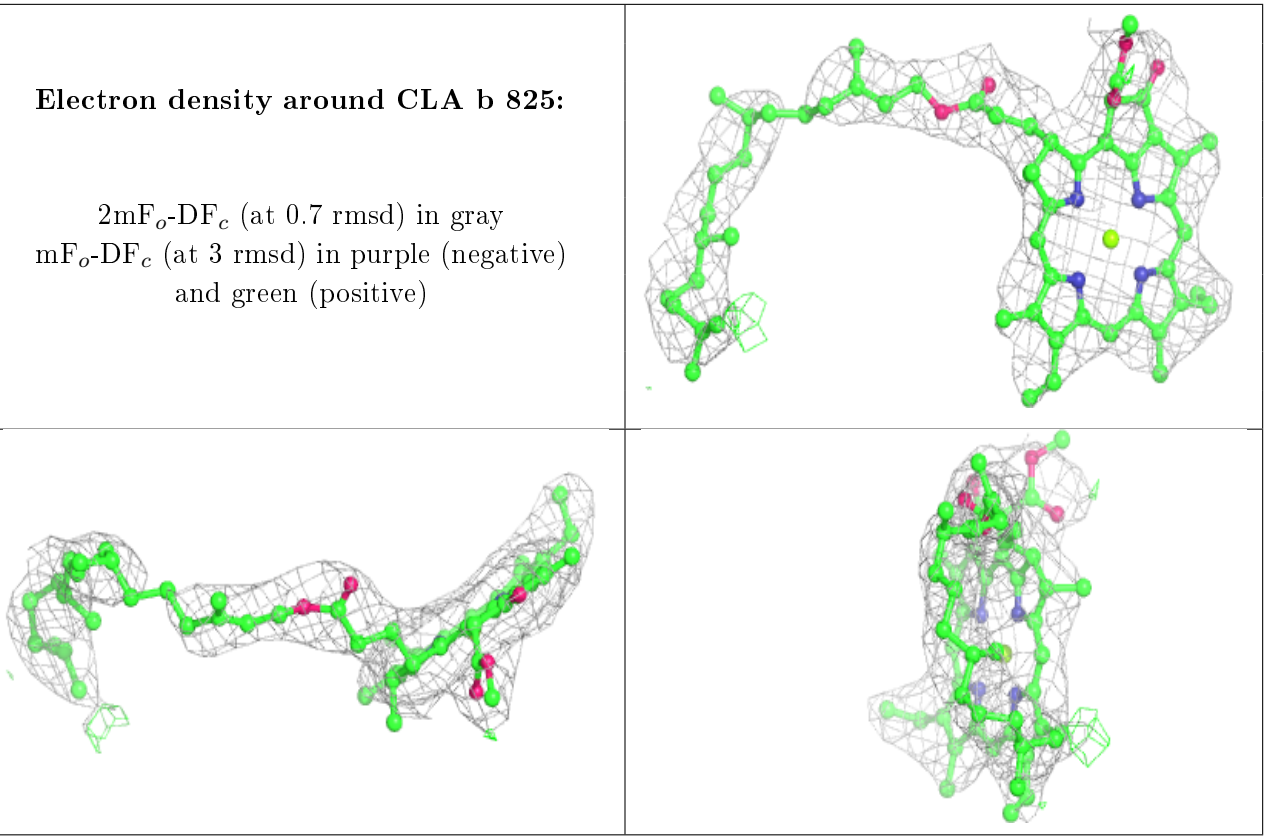






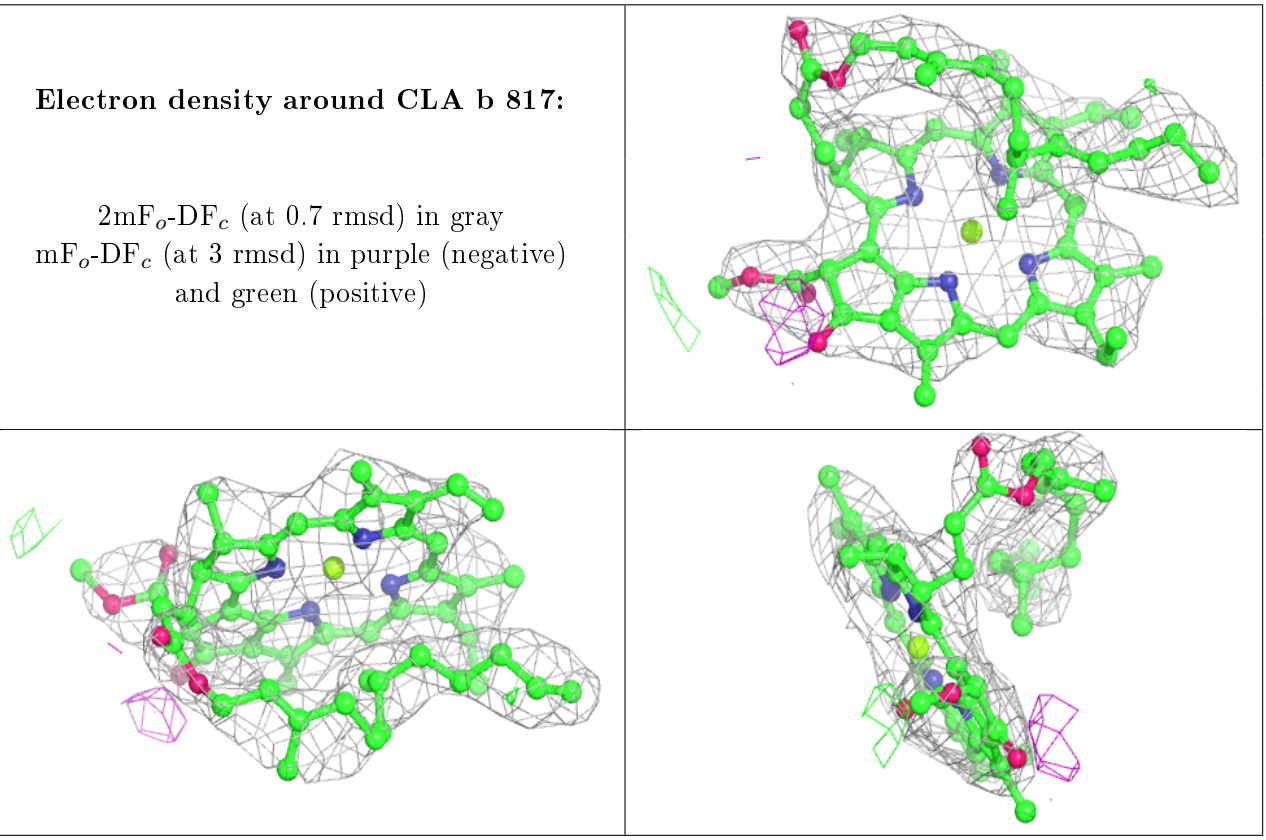
Electron density around CLA b 825:

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



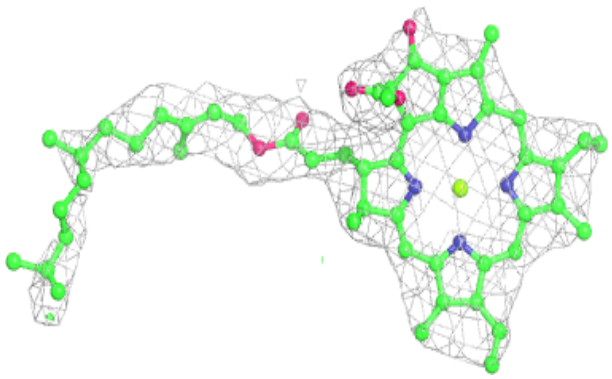
Electron density around CLA b 817:

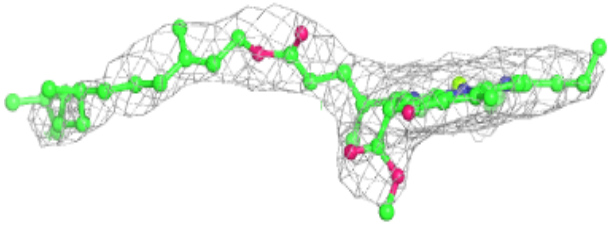
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

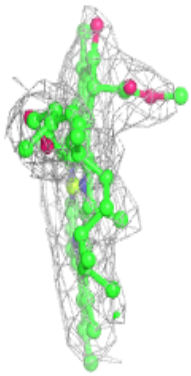


Electron density around CLA B 836:

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

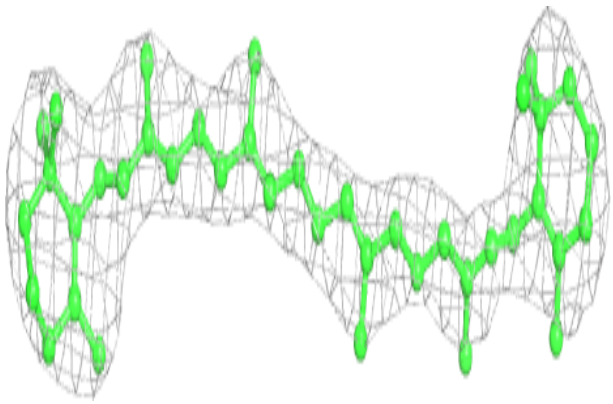


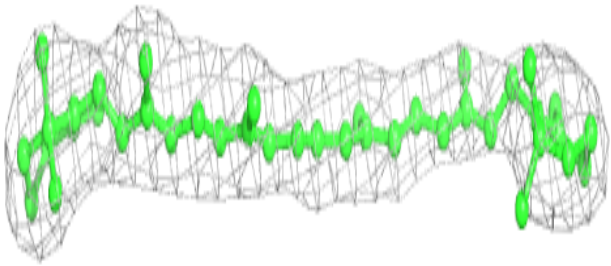


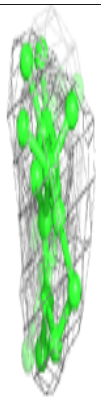


Electron density around BCR L 205:

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

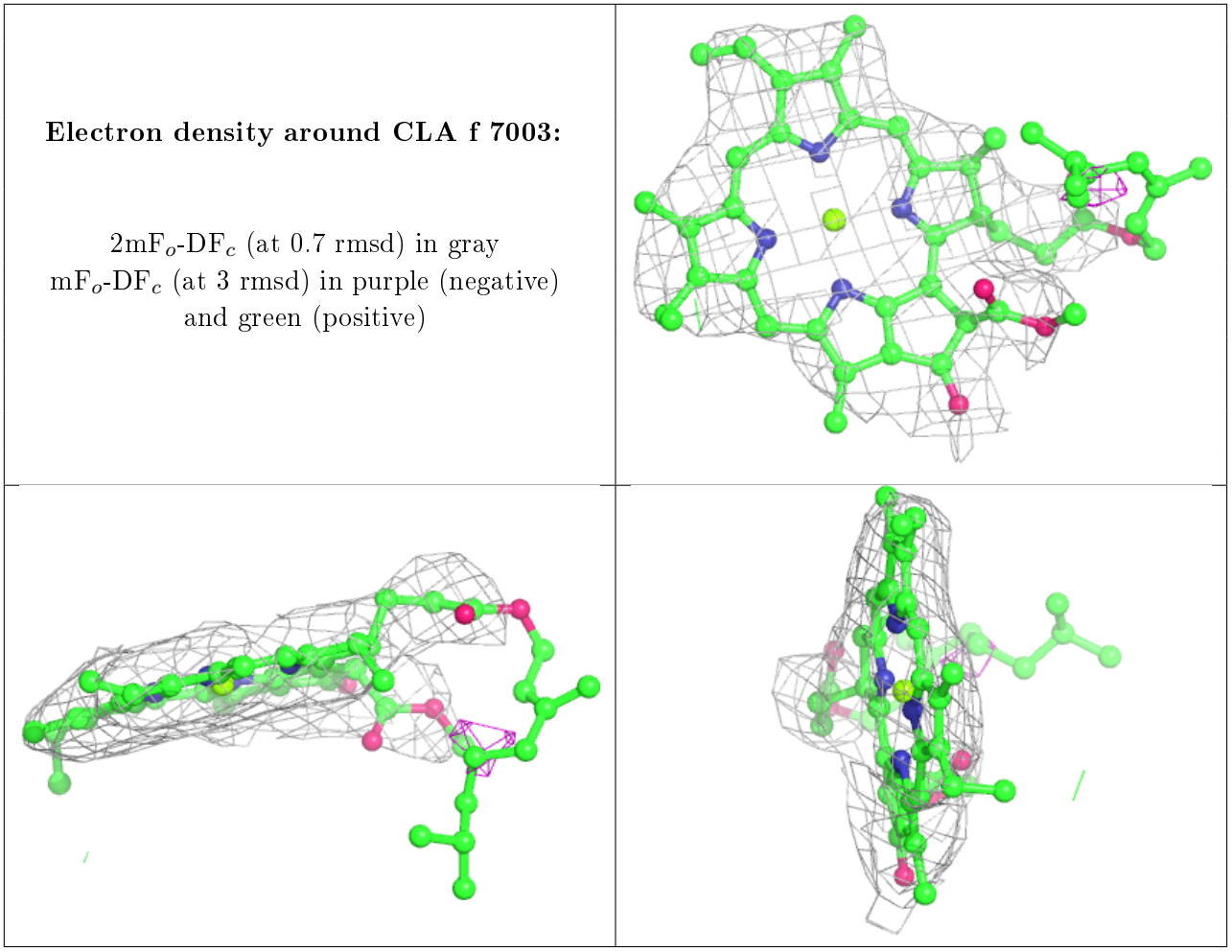






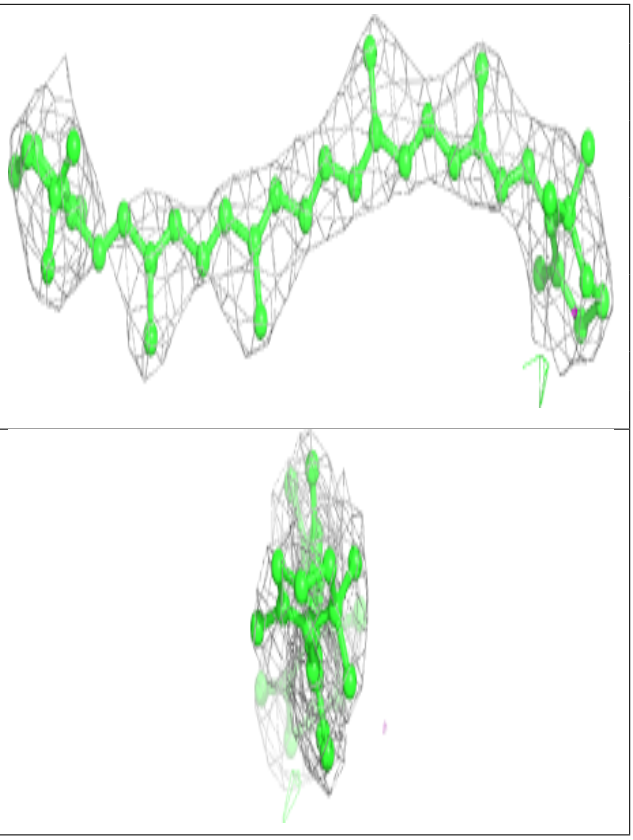
Electron density around CLA f 7003:

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



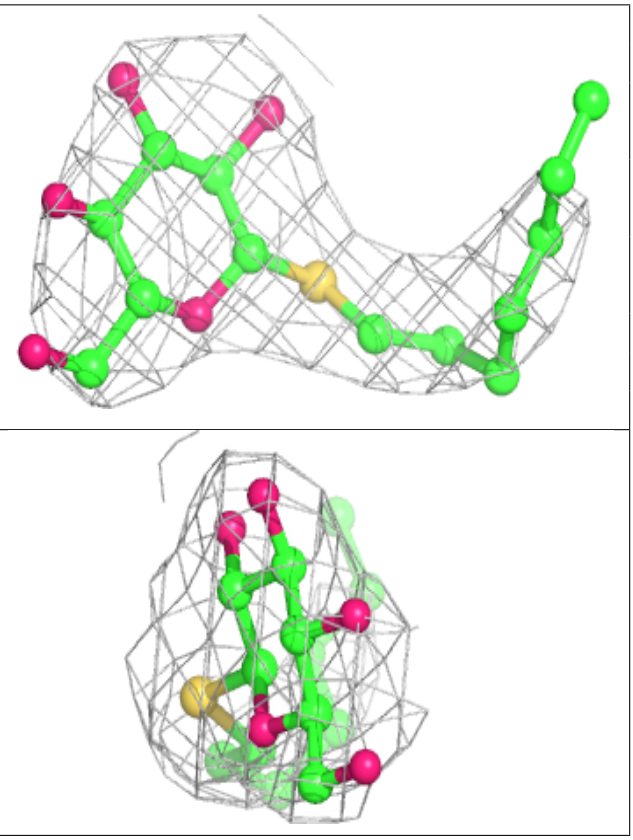
Electron density around BCR b 846:

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



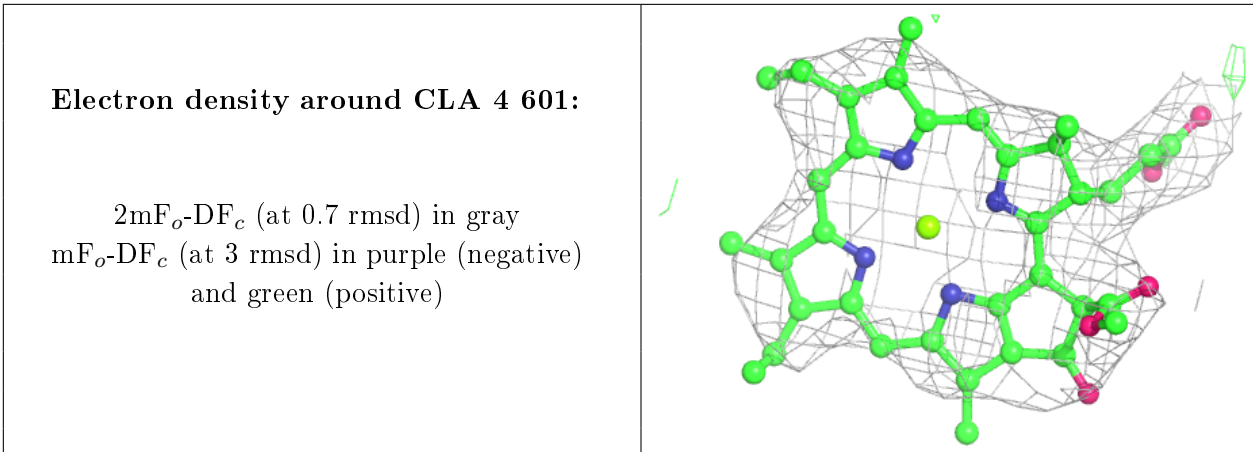
Electron density around HTG j 3001:

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



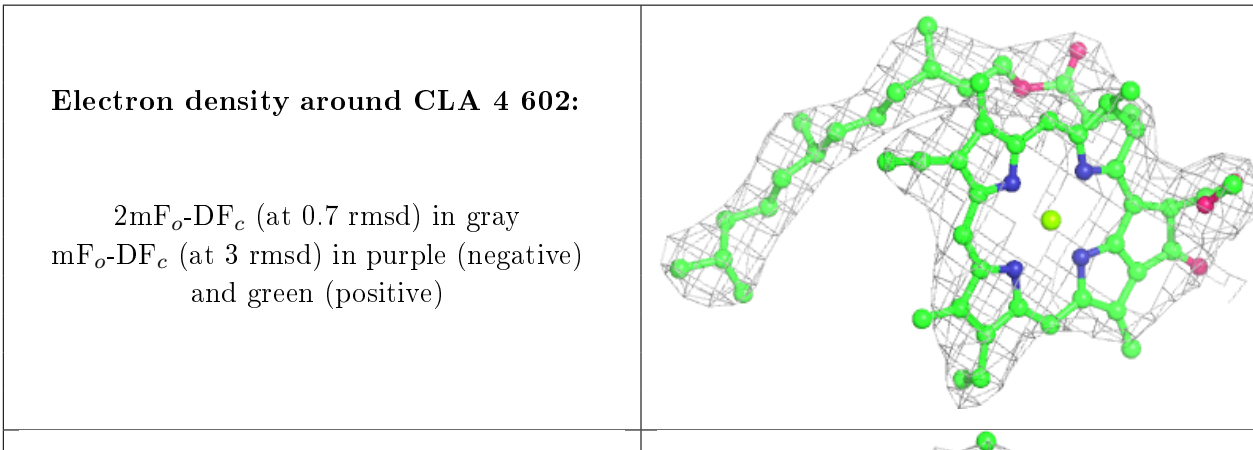
Electron density around CLA 4 601:

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



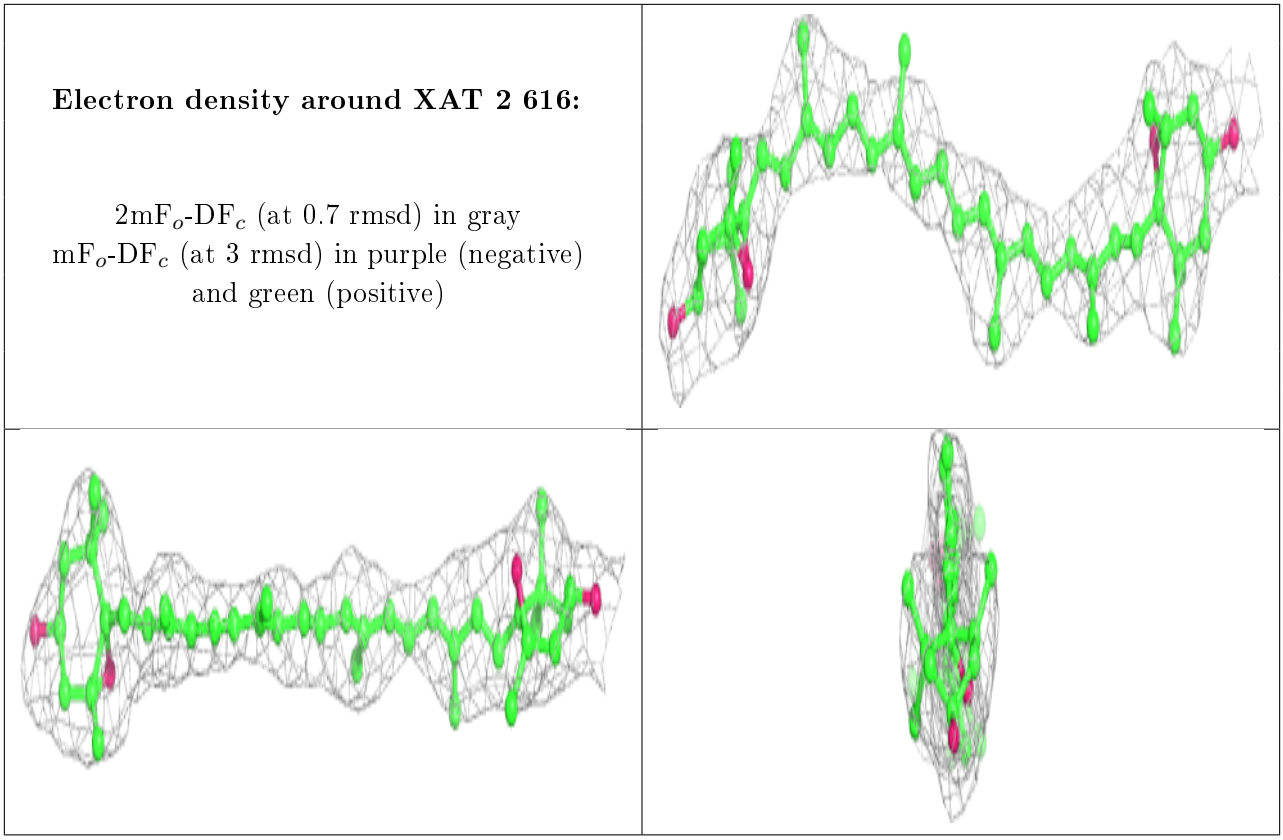
Electron density around CLA 4 602:

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



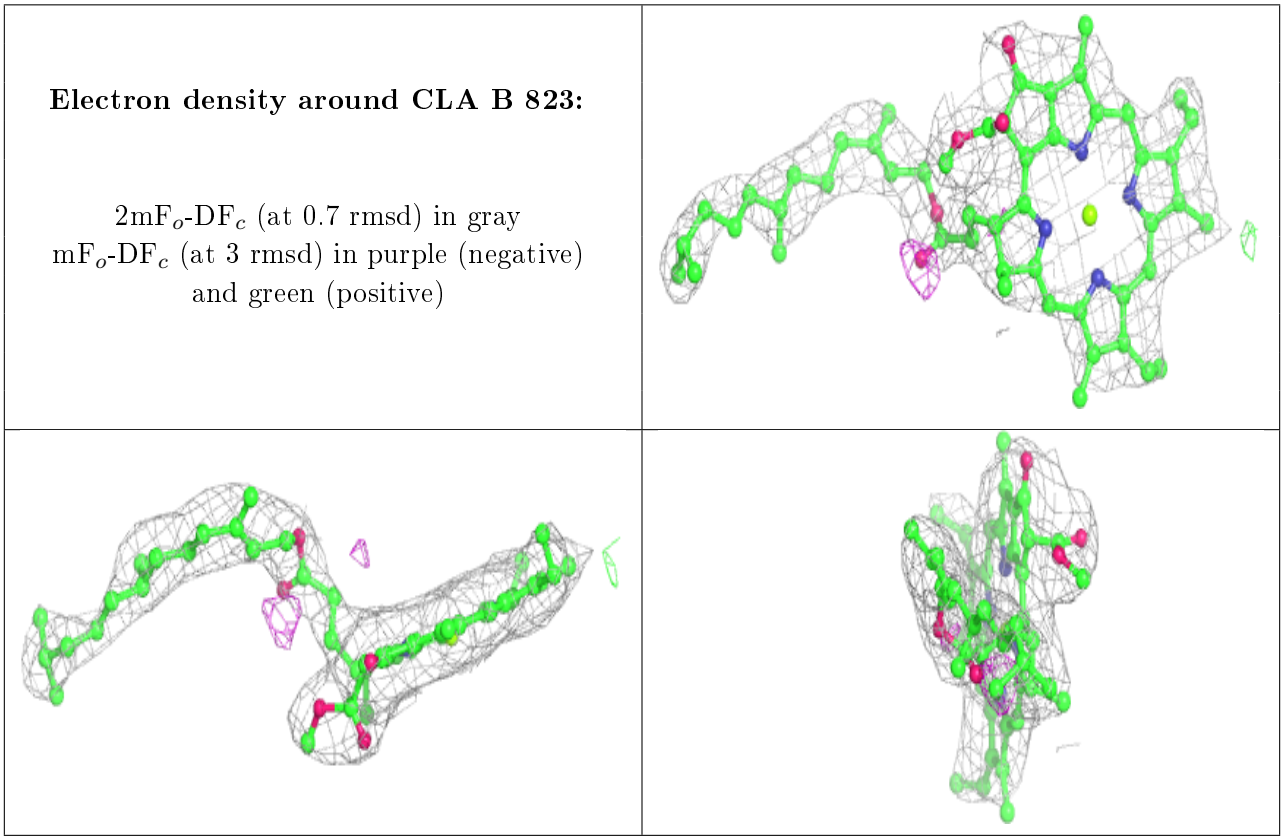
Electron density around XAT 2 616:

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



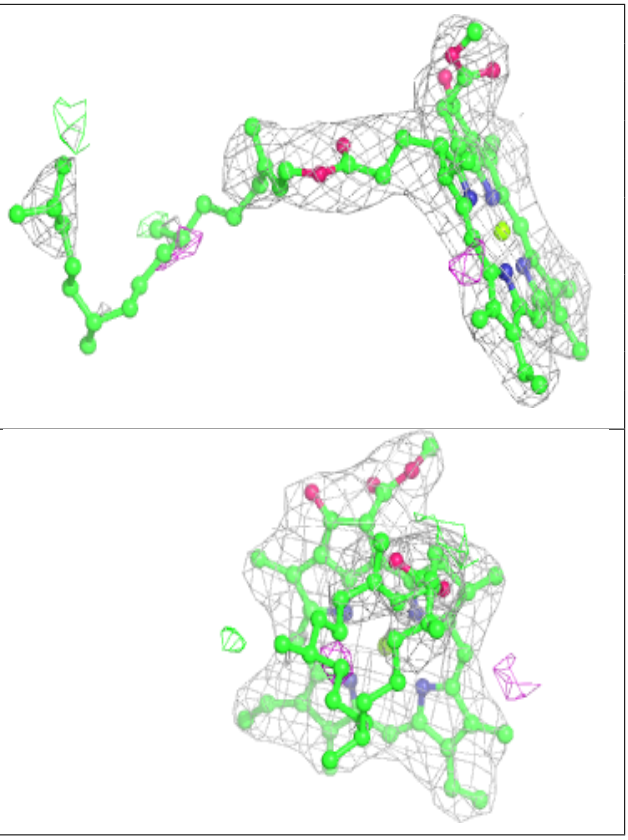
Electron density around CLA B 823:

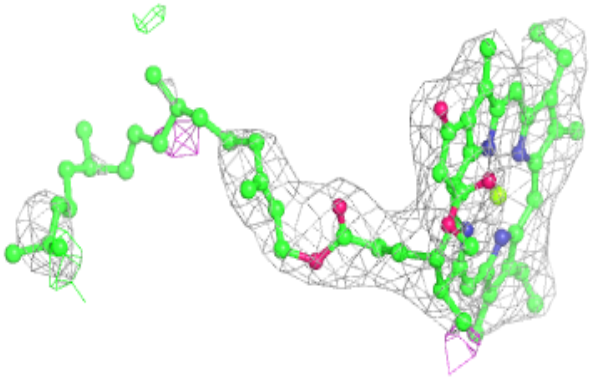
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



Electron density around CLA a 840:

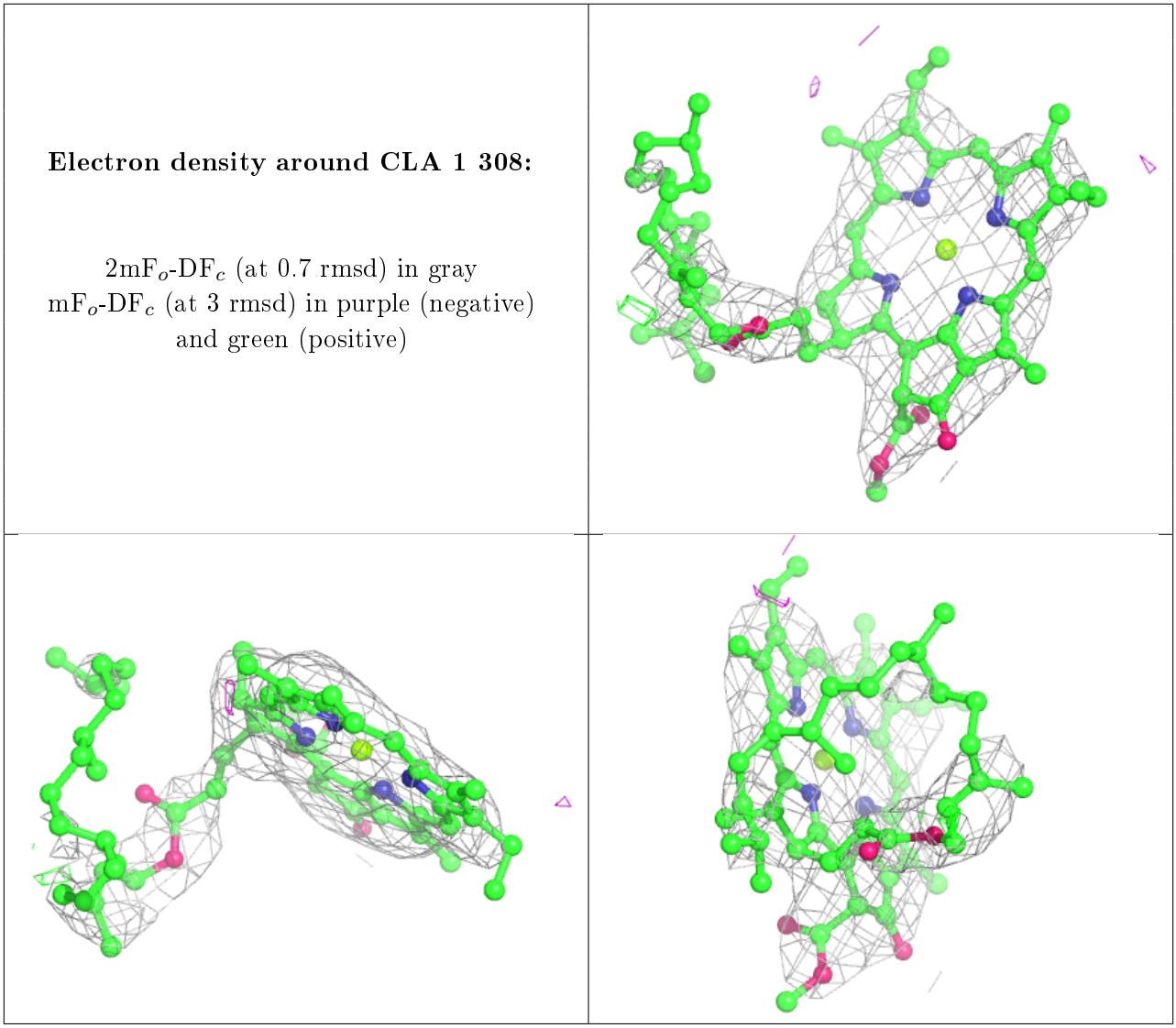
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)





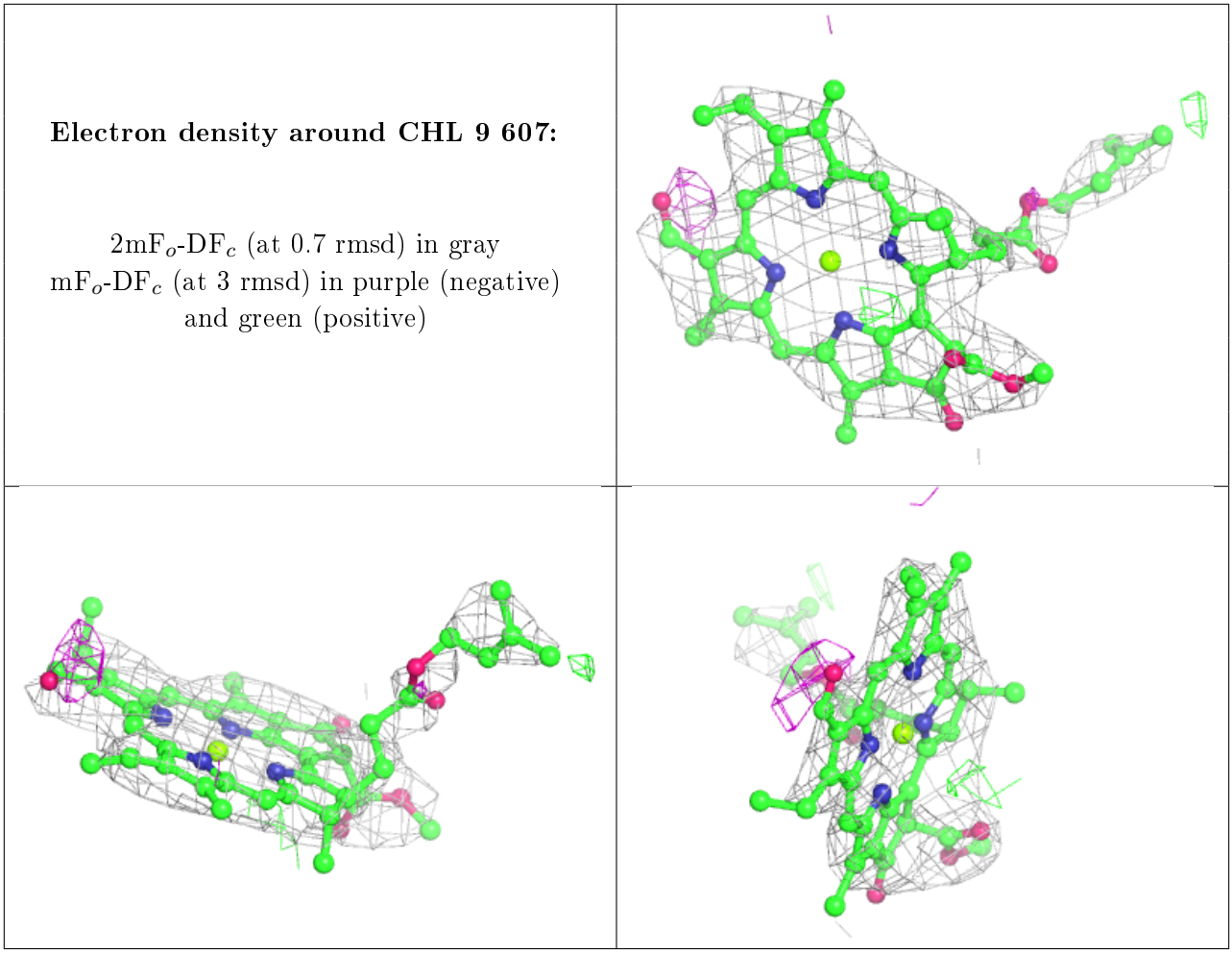
Electron density around CLA 1 308:

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



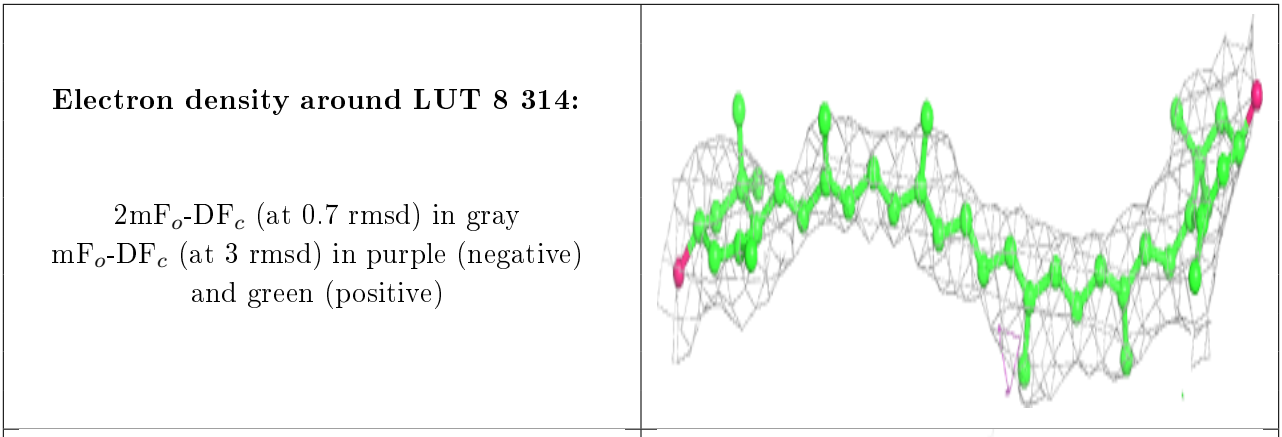
Electron density around CHL 9 607:

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



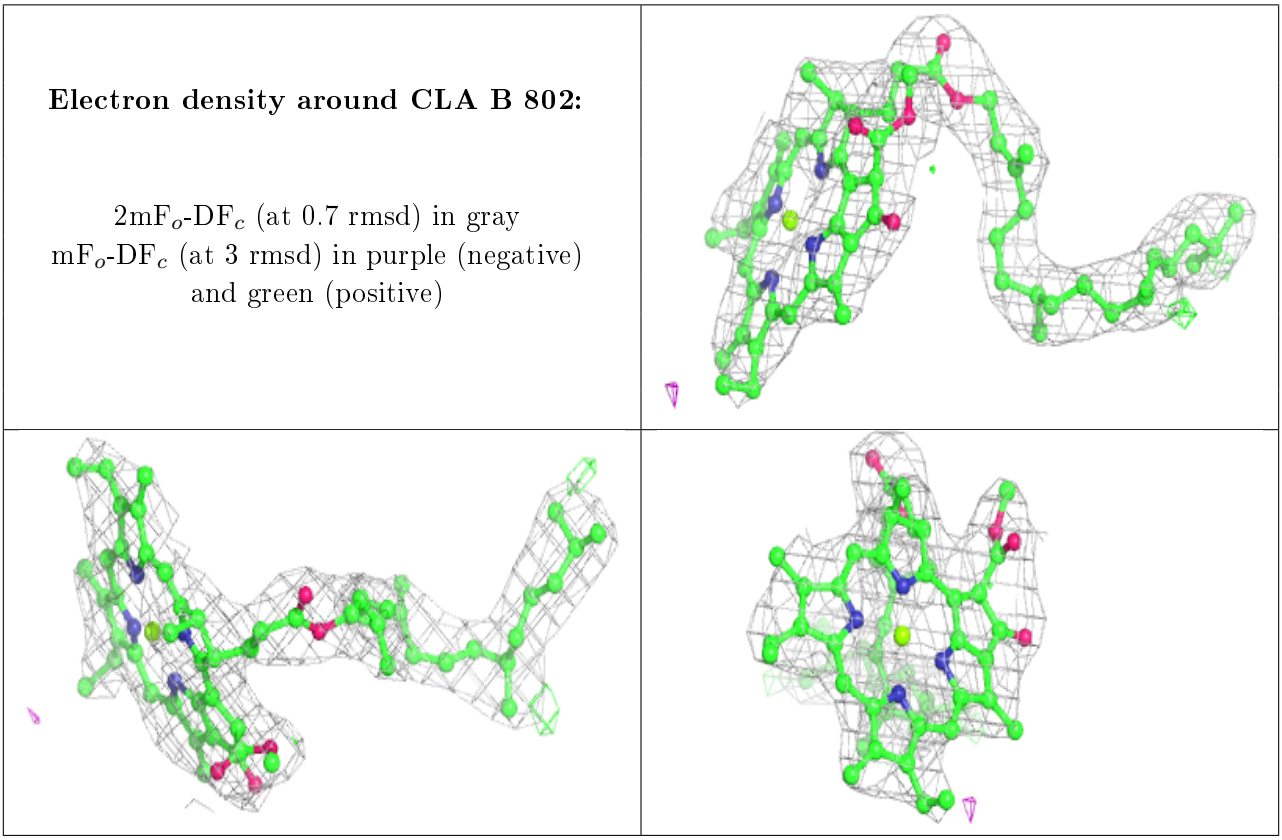
Electron density around LUT 8 314:

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



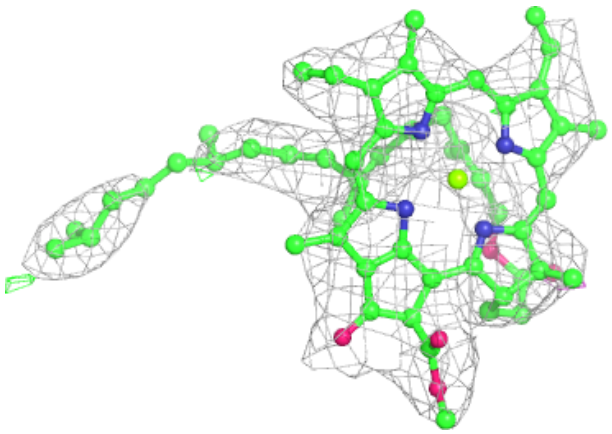
Electron density around CLA B 802:

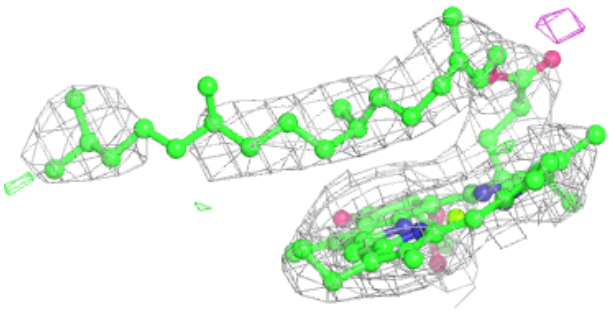
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

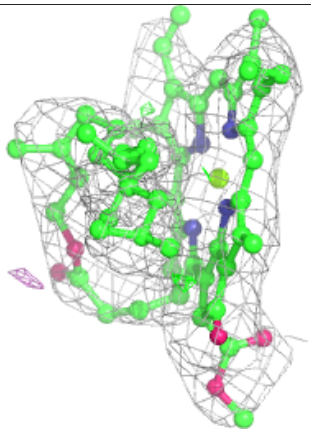


Electron density around CLA B 827:

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

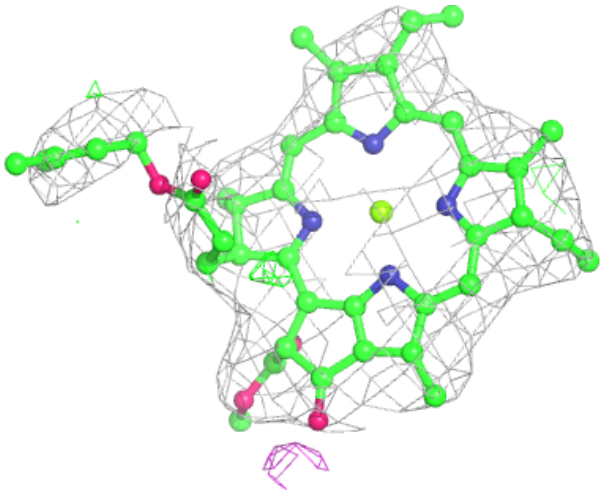


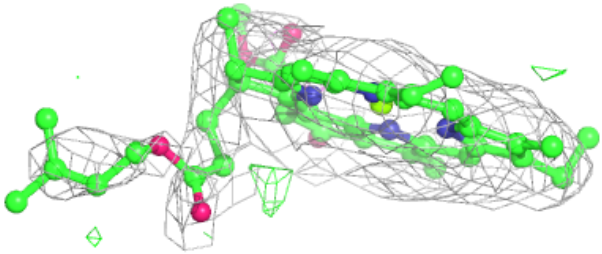


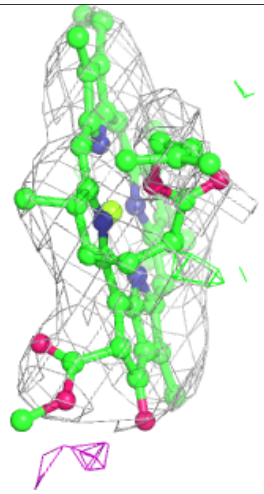


Electron density around CLA L 204:

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

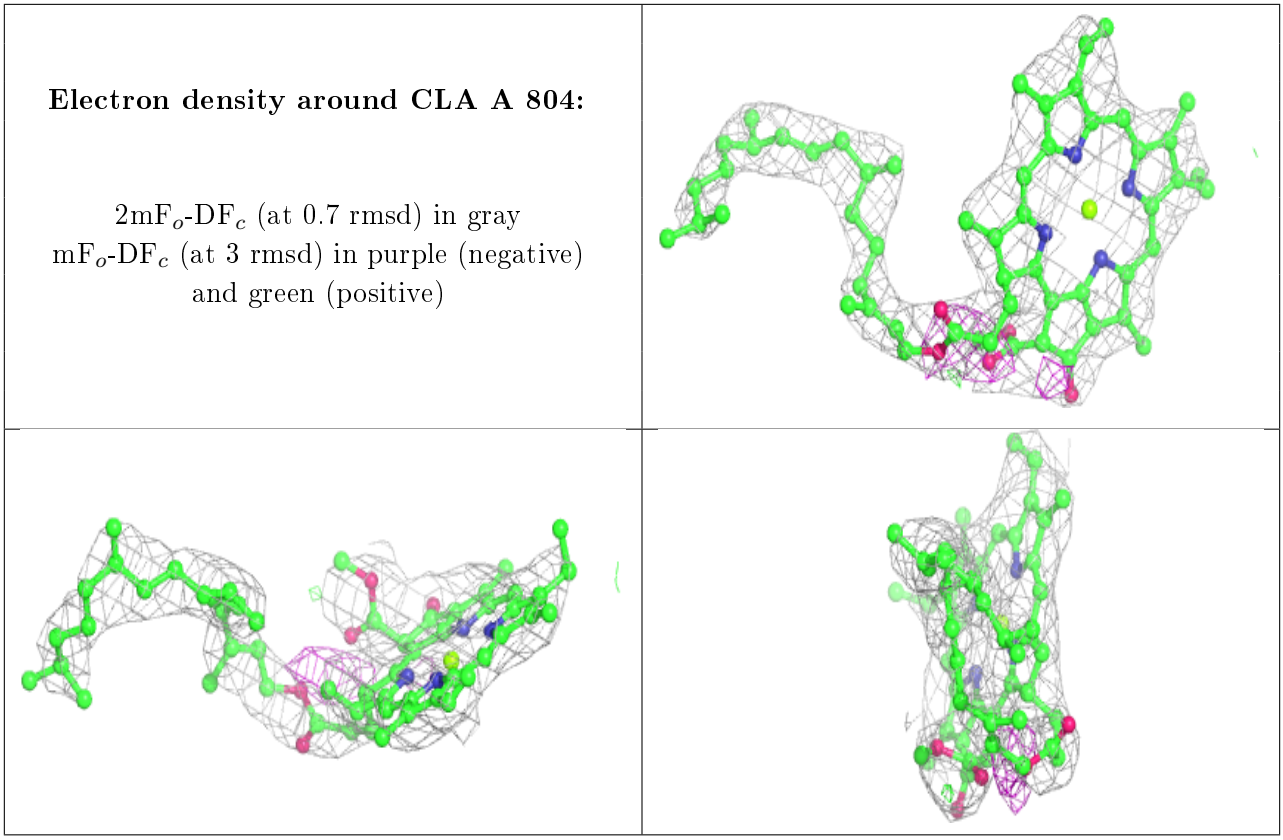






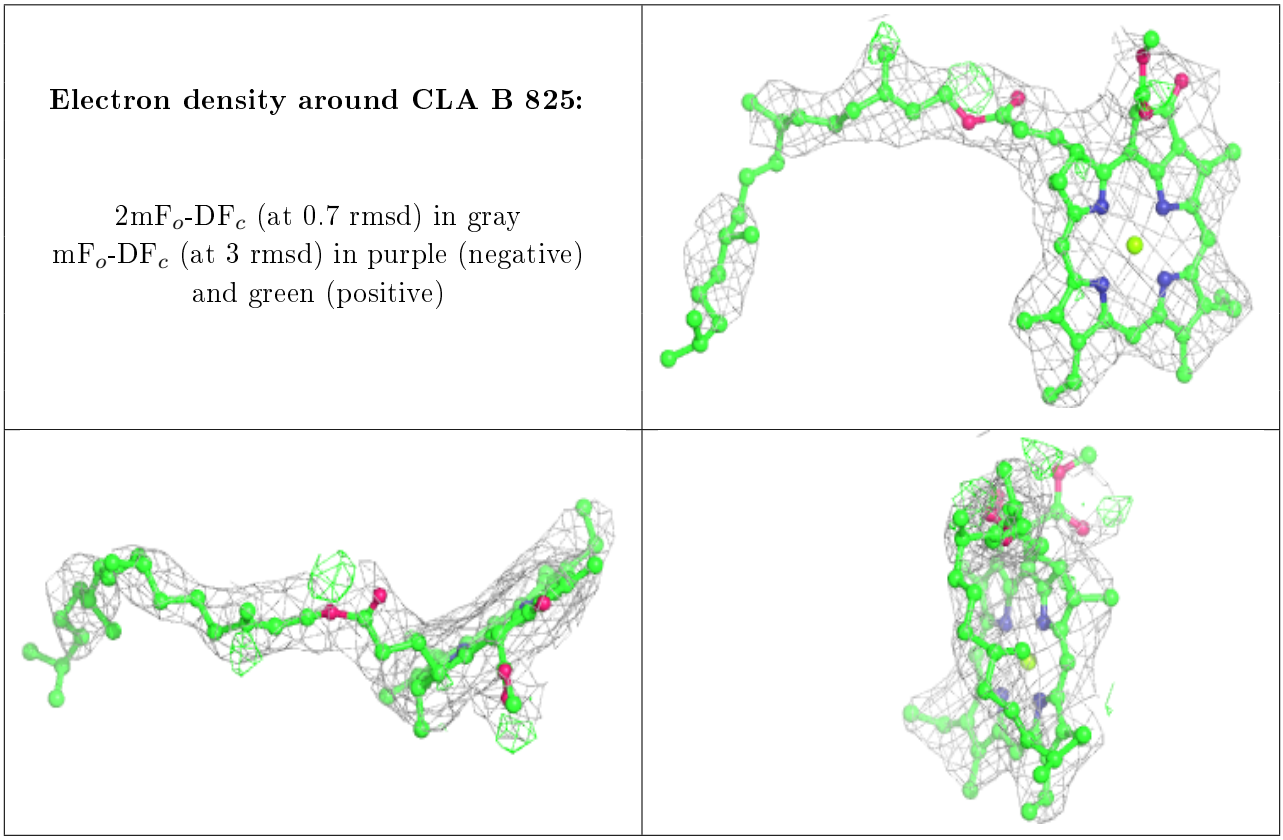
Electron density around CLA A 804:

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



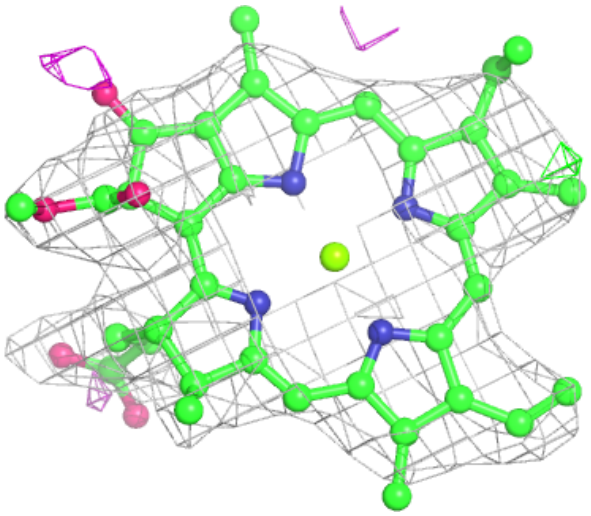
Electron density around CLA B 825:

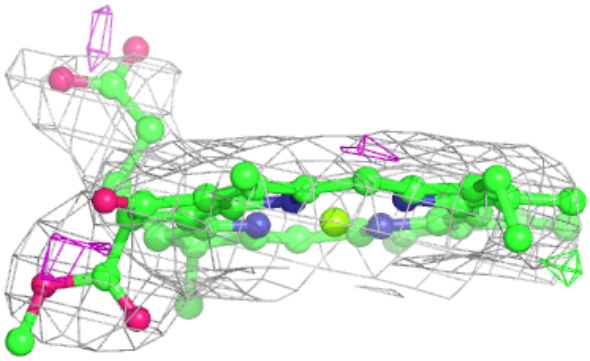
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

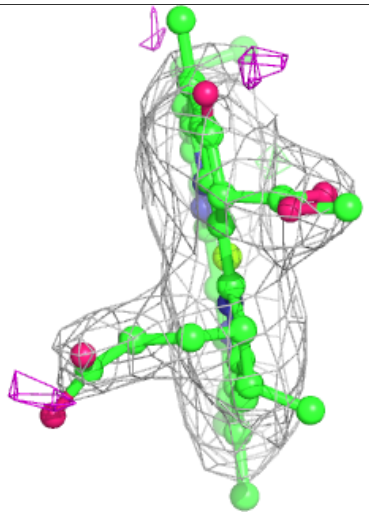


Electron density around CLA a 817:

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

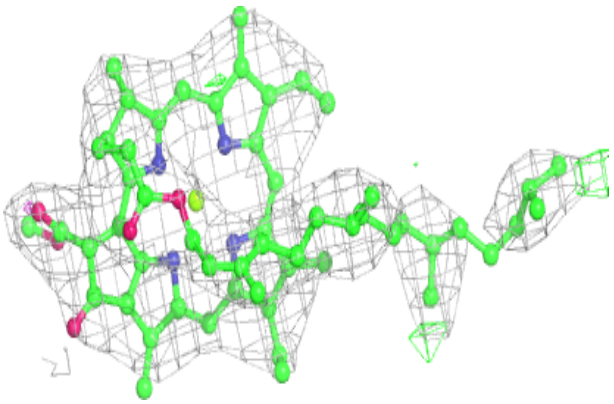


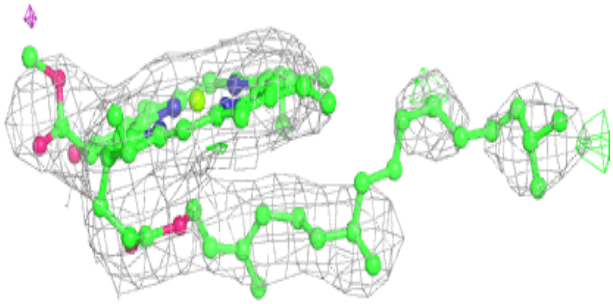


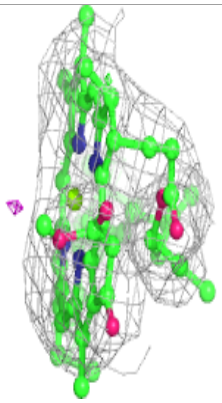


Electron density around CLA A 839:

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

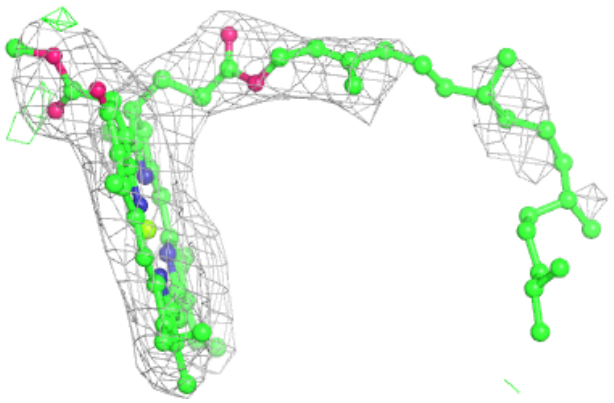


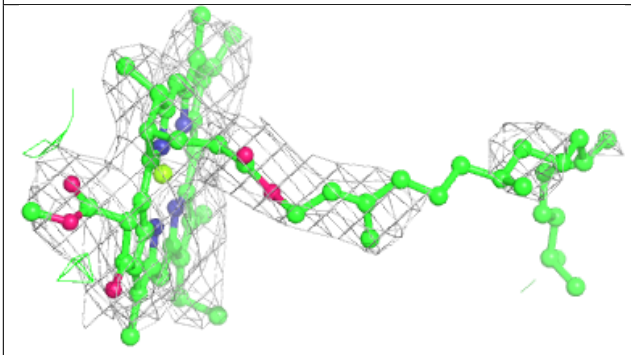


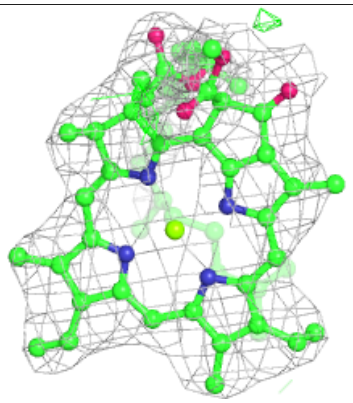


Electron density around CLA A 808:

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

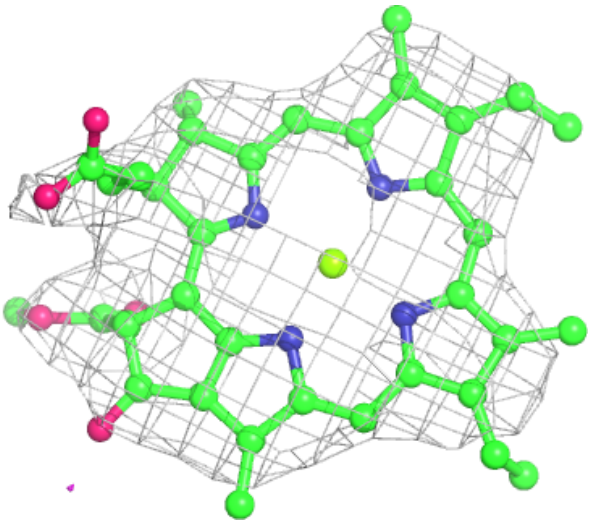


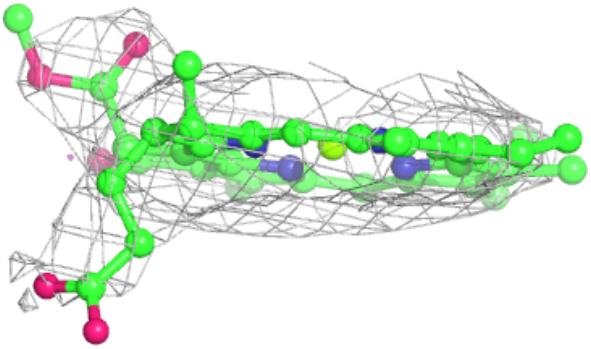


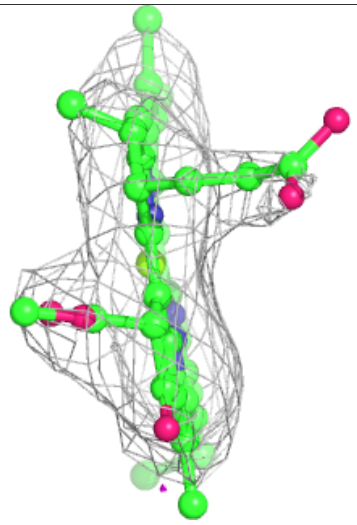


Electron density around CLA A 817:

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

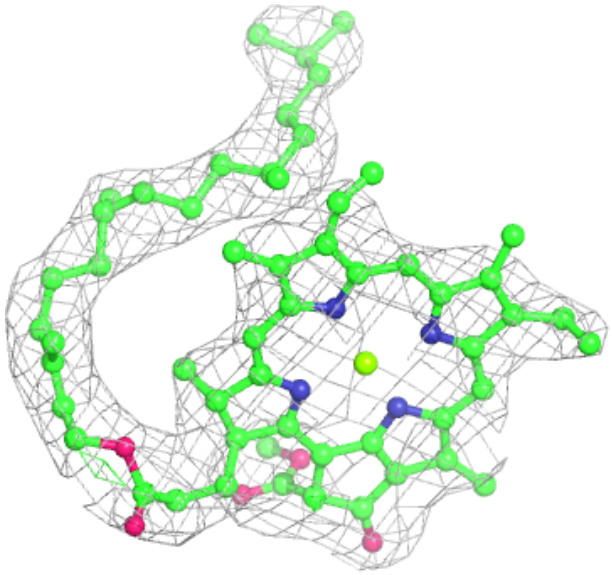


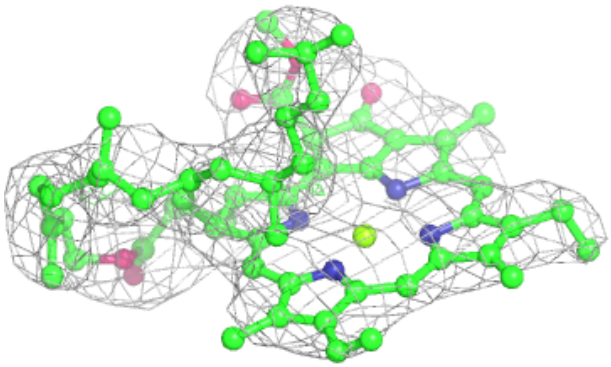


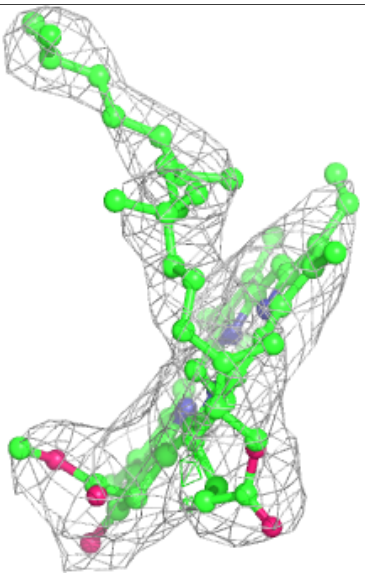


Electron density around CLA A 814:

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

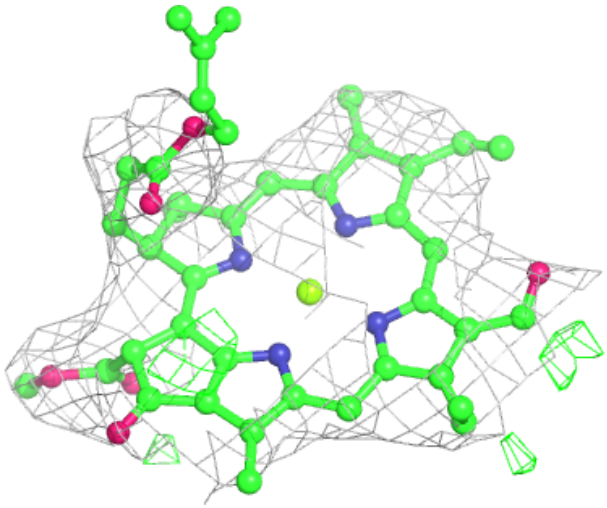


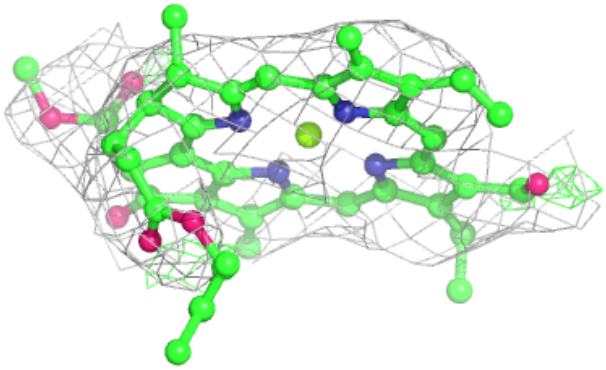


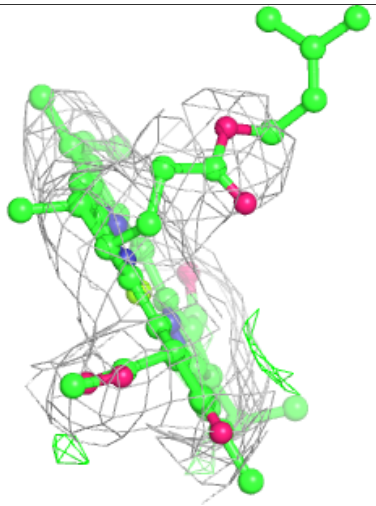


Electron density around CHL 9 606:

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

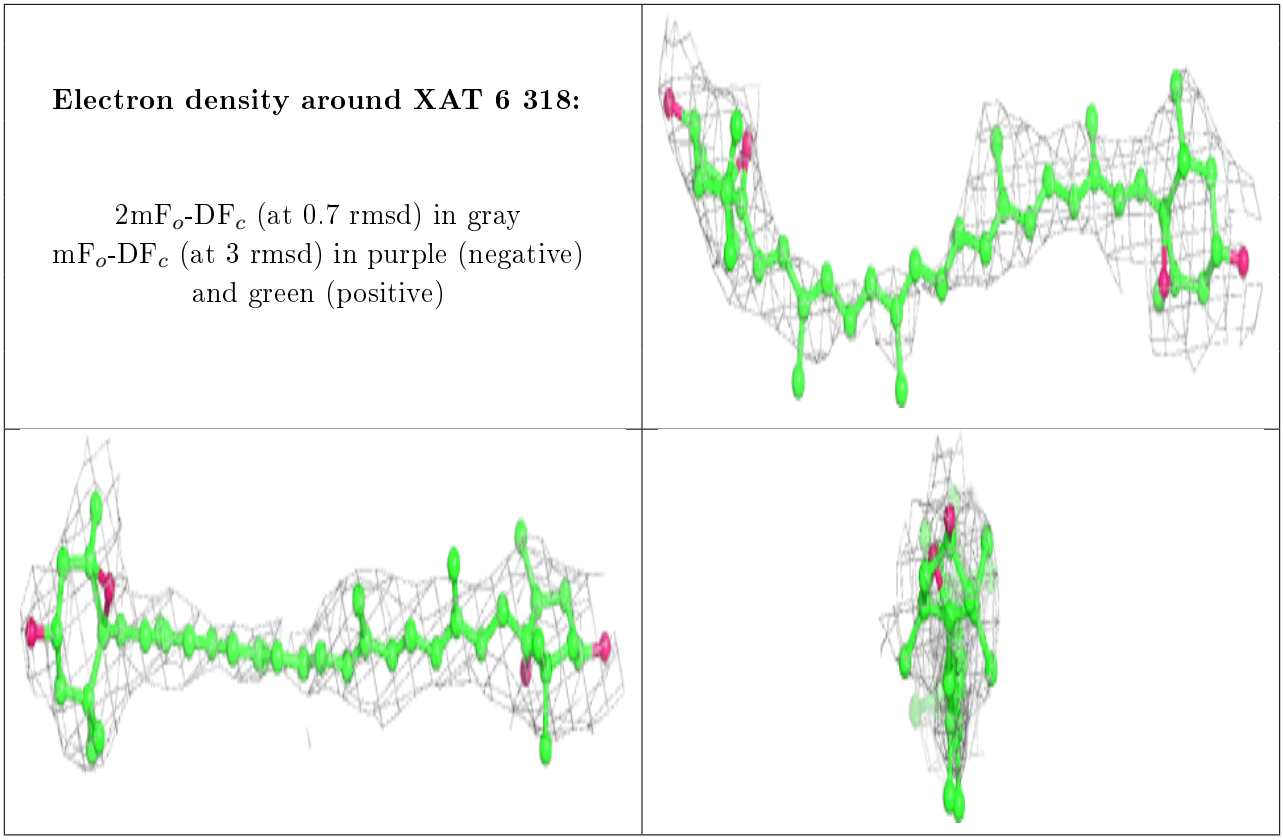






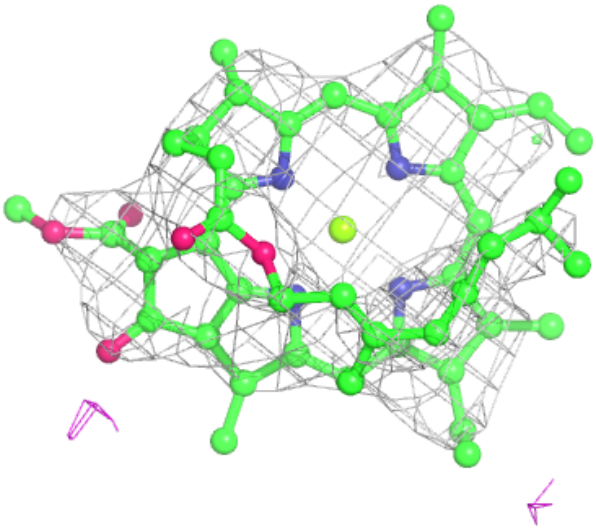
Electron density around XAT 6 318:

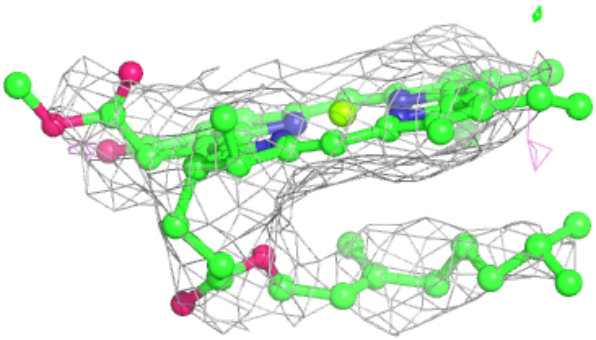
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

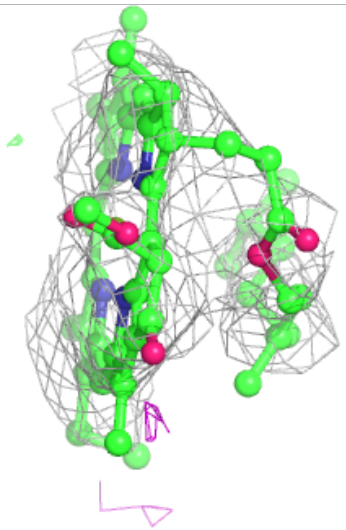


Electron density around CLA 8 310:

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

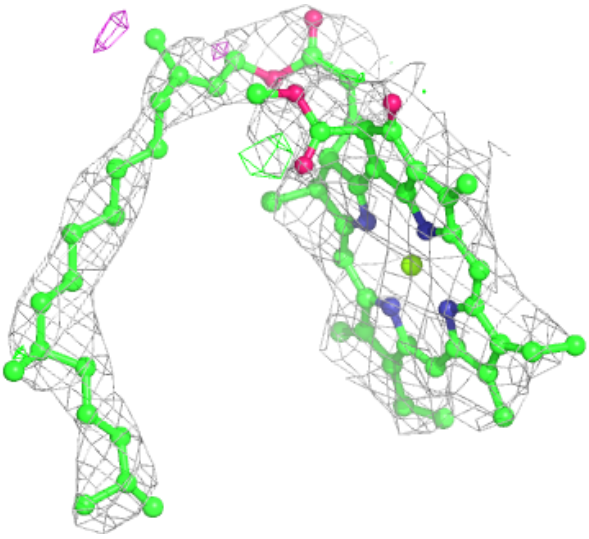


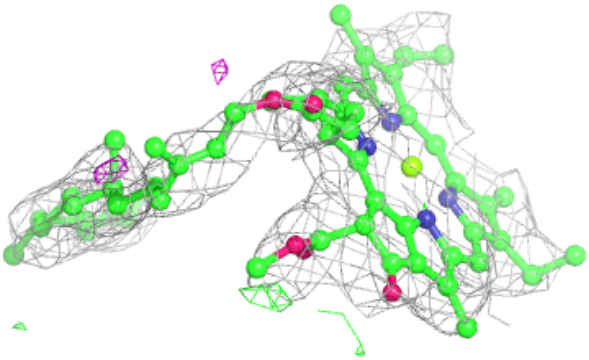


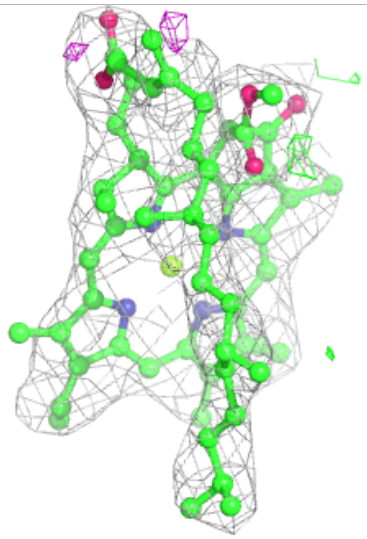


Electron density around CLA B 810:

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

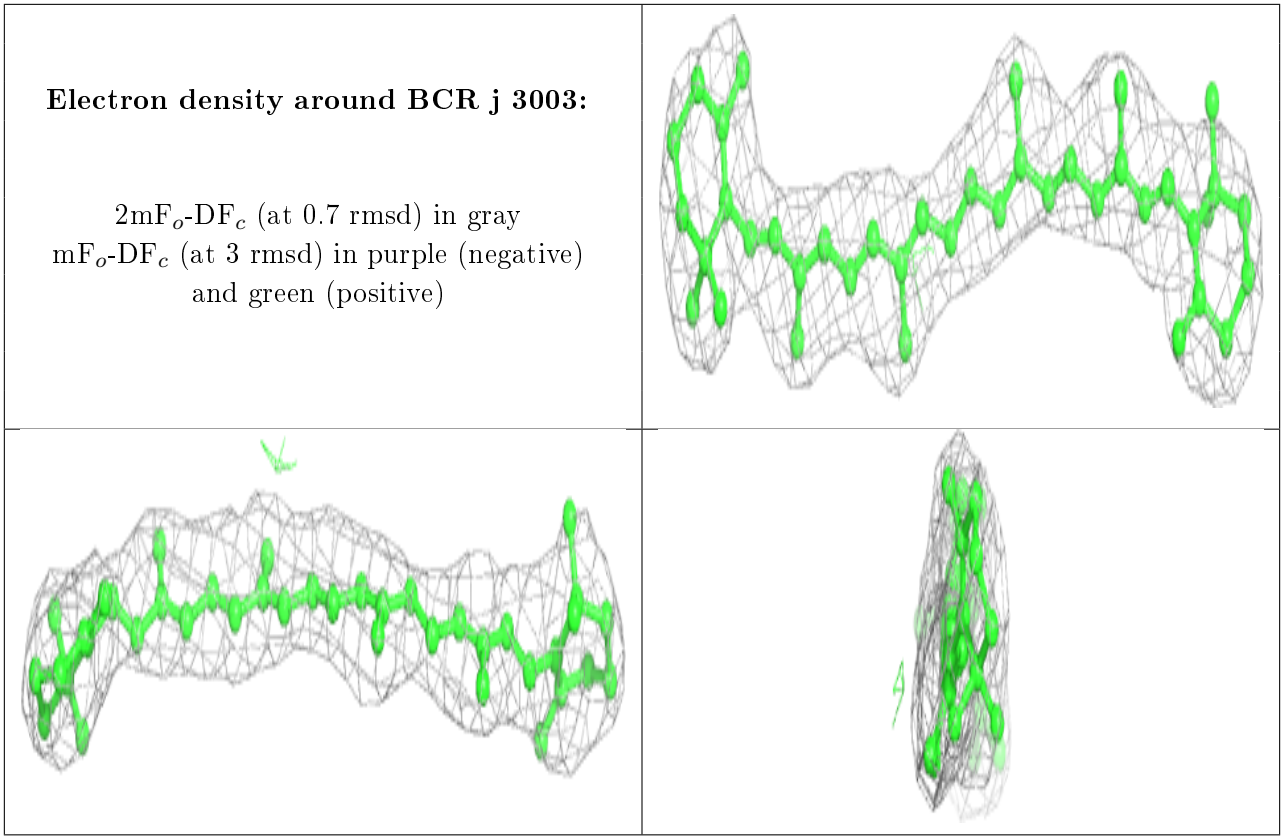






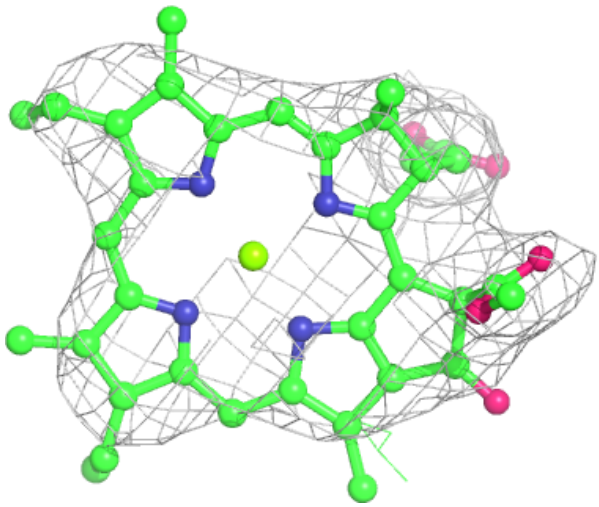
Electron density around BCR j 3003:

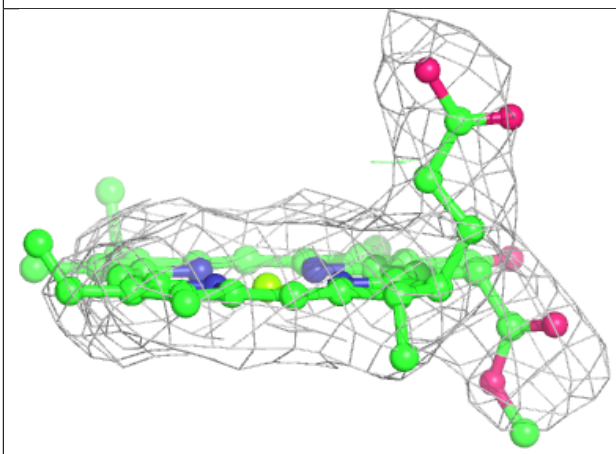
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

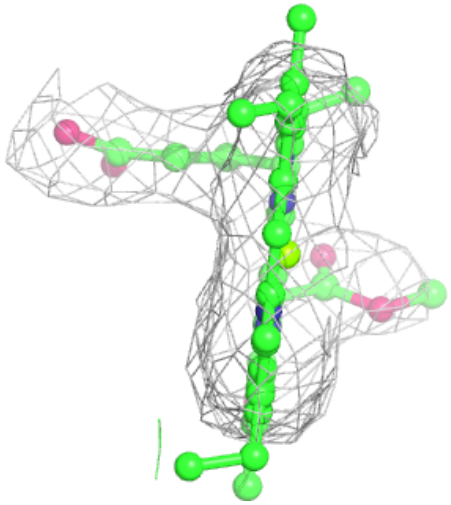


Electron density around CLA 8 303:

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

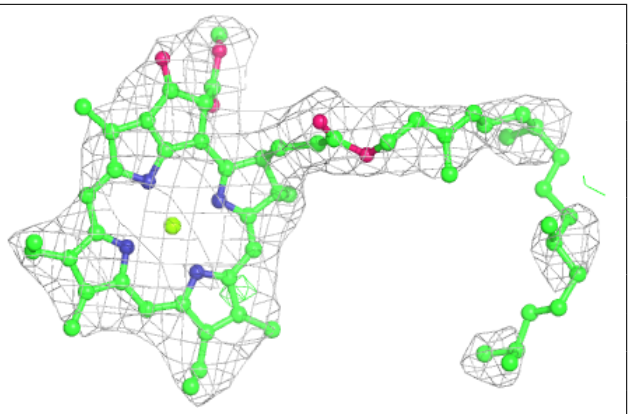


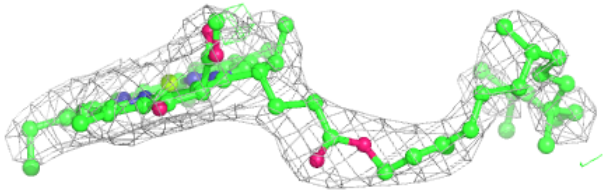


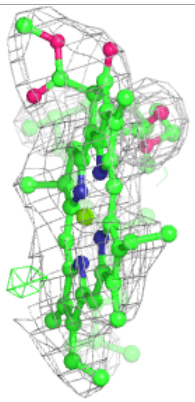


Electron density around CLA A 827:

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

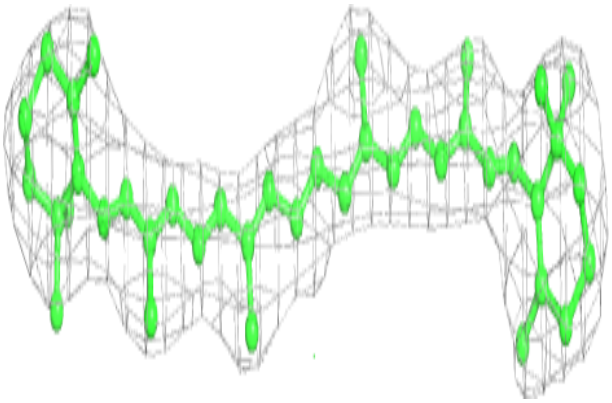


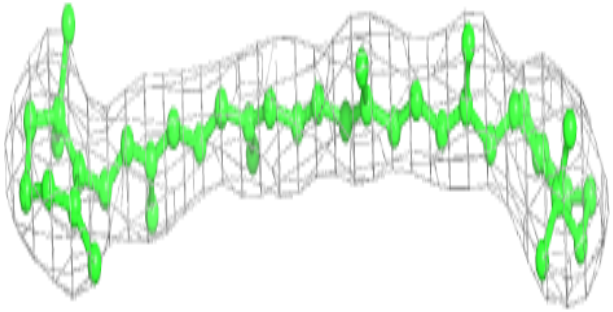


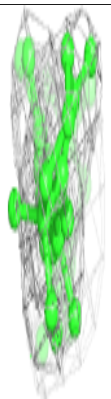


Electron density around BCR J 3003:

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

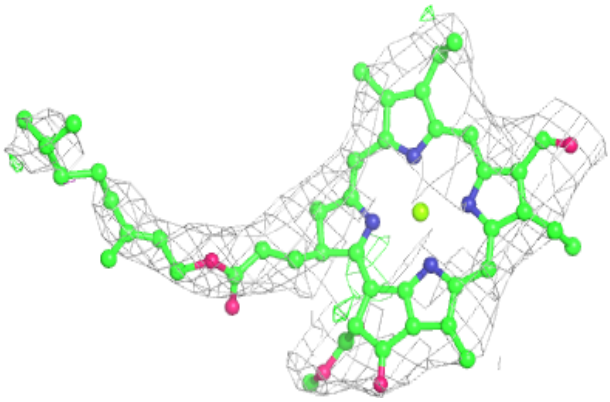


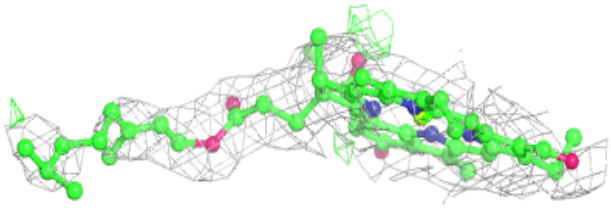


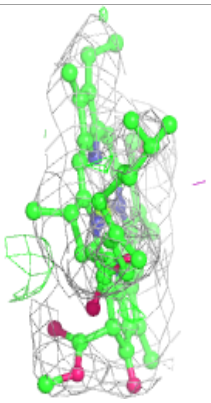


Electron density around CHL 9 605:

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

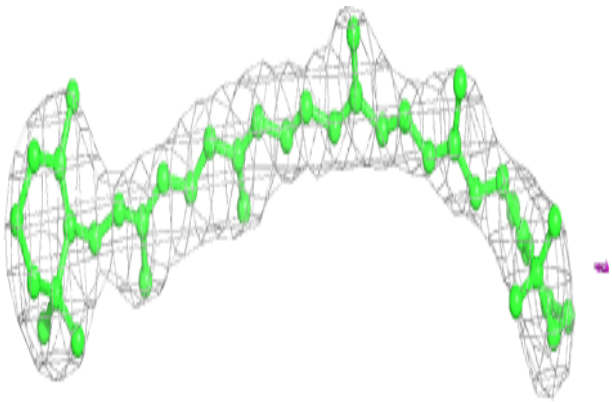


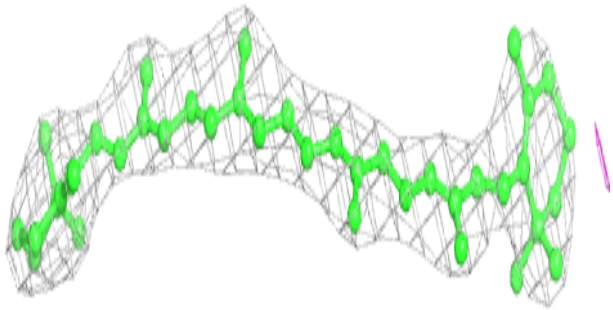


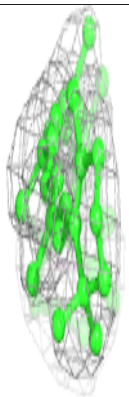


Electron density around BCR b 801:

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

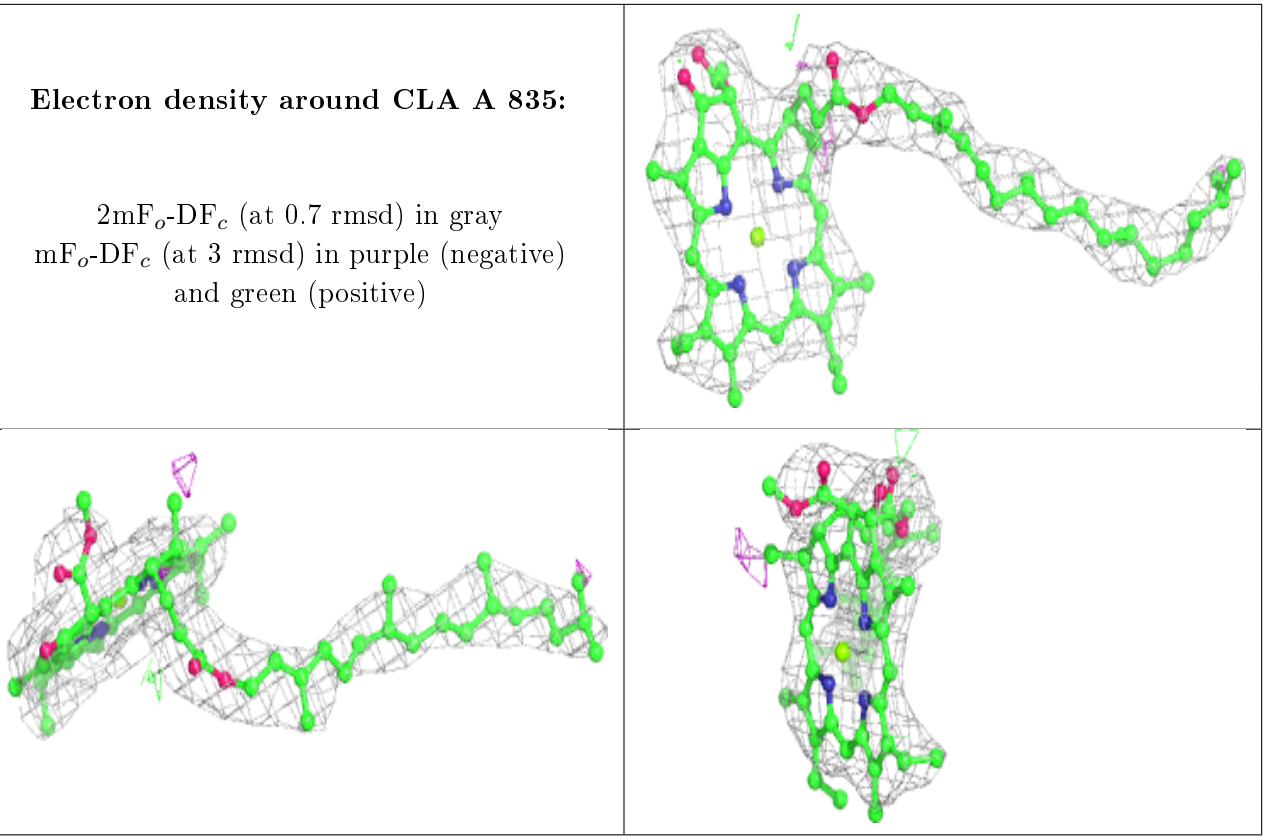






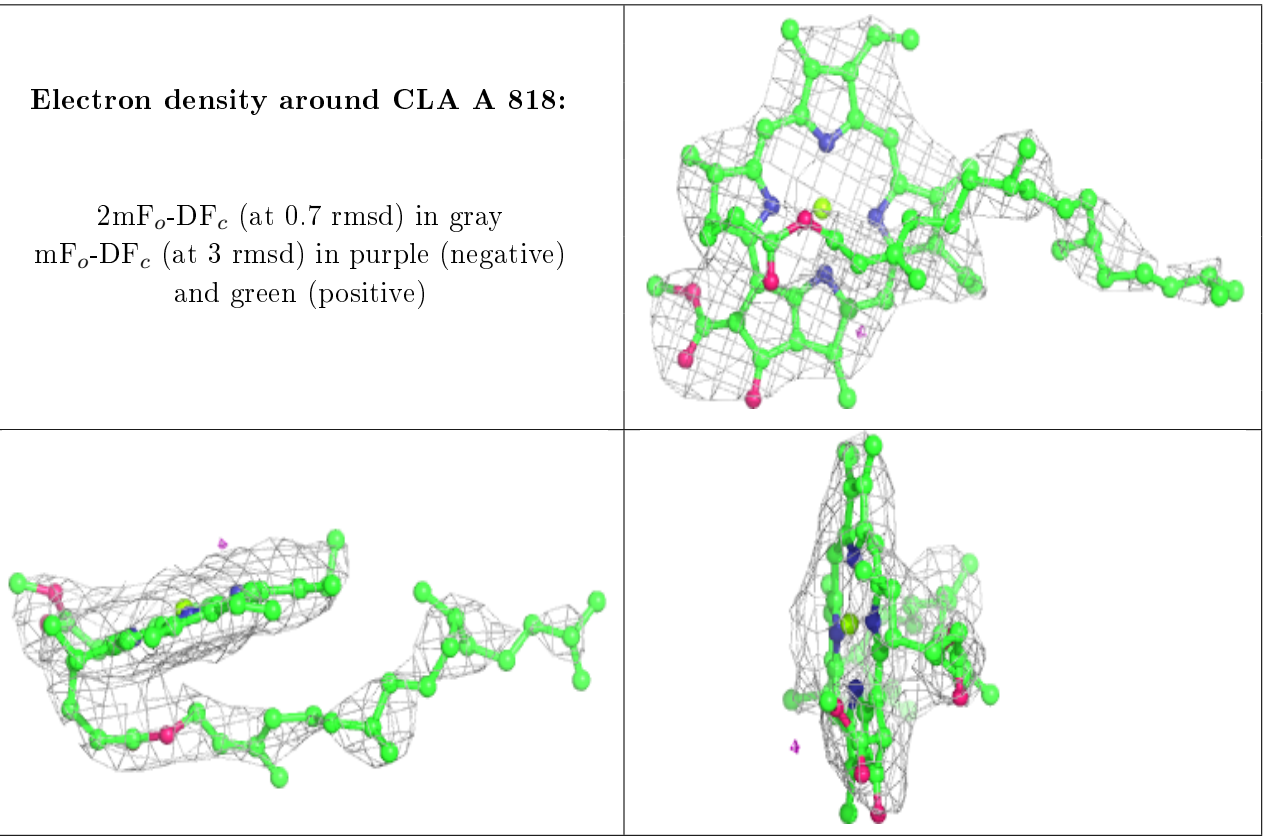
Electron density around CLA A 835:

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



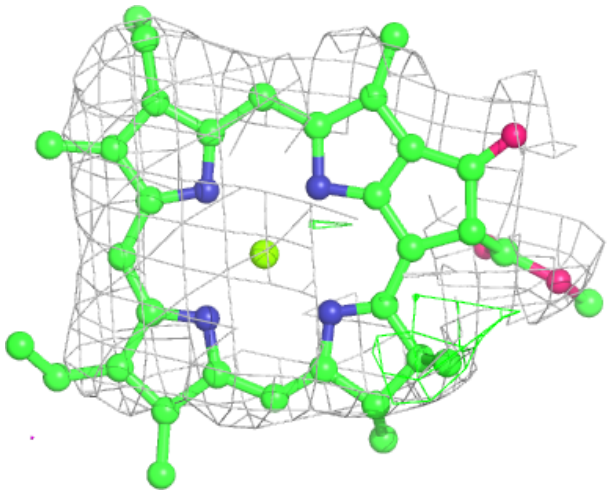
Electron density around CLA A 818:

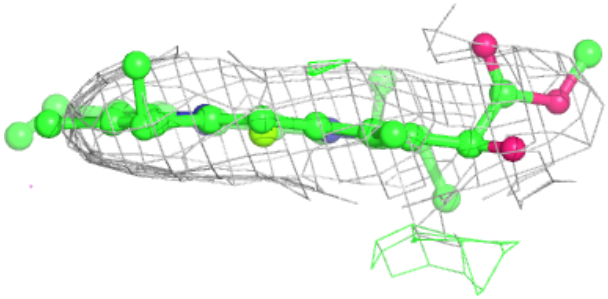
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

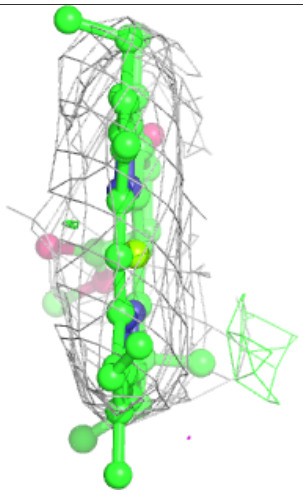


Electron density around CLA 6 312:

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

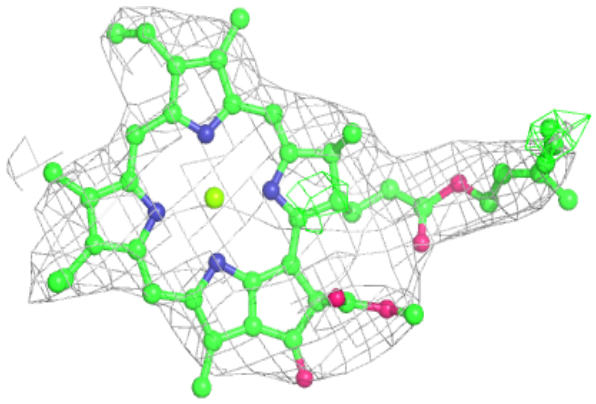


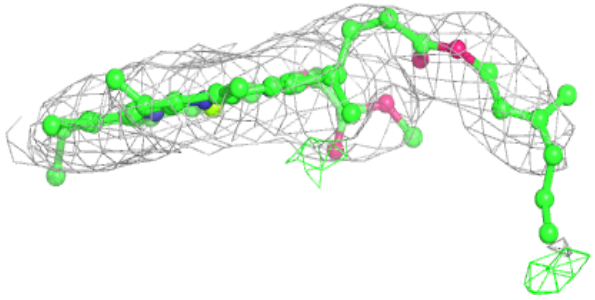


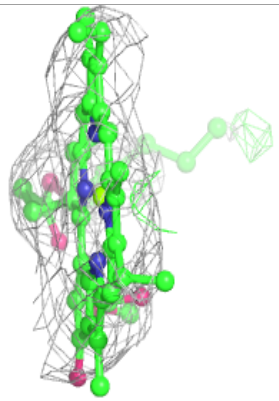


Electron density around CLA 1 306:

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

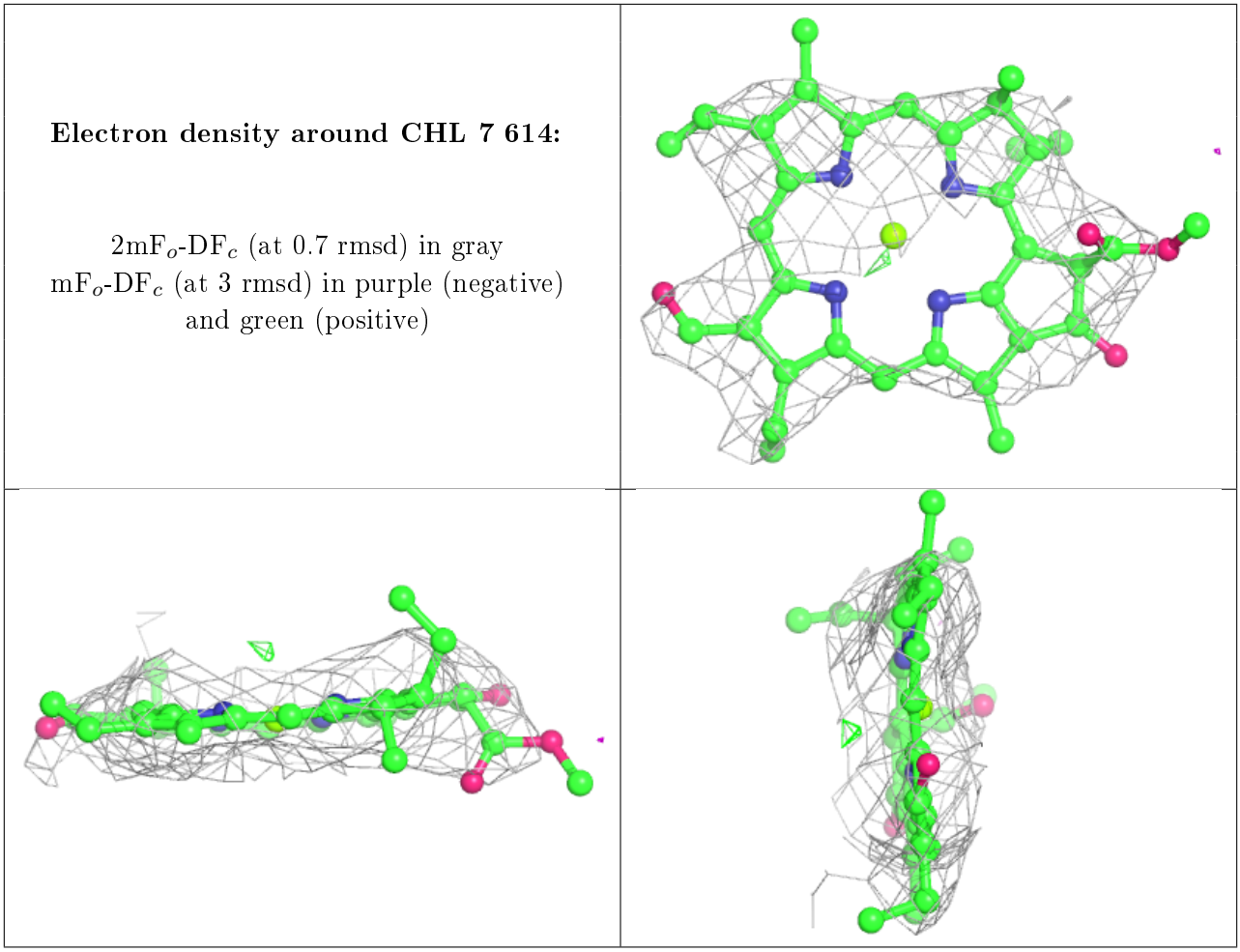






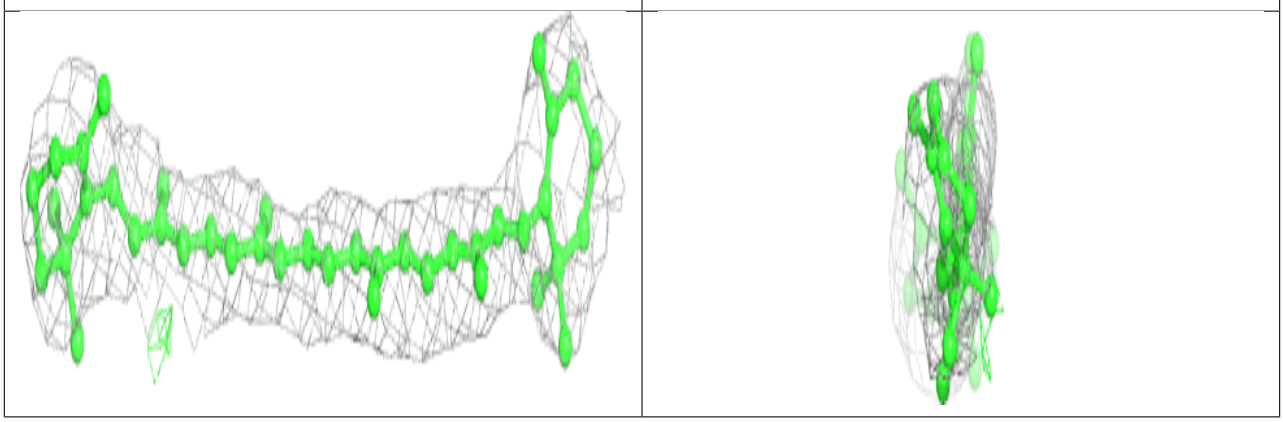
Electron density around CHL 7 614:

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



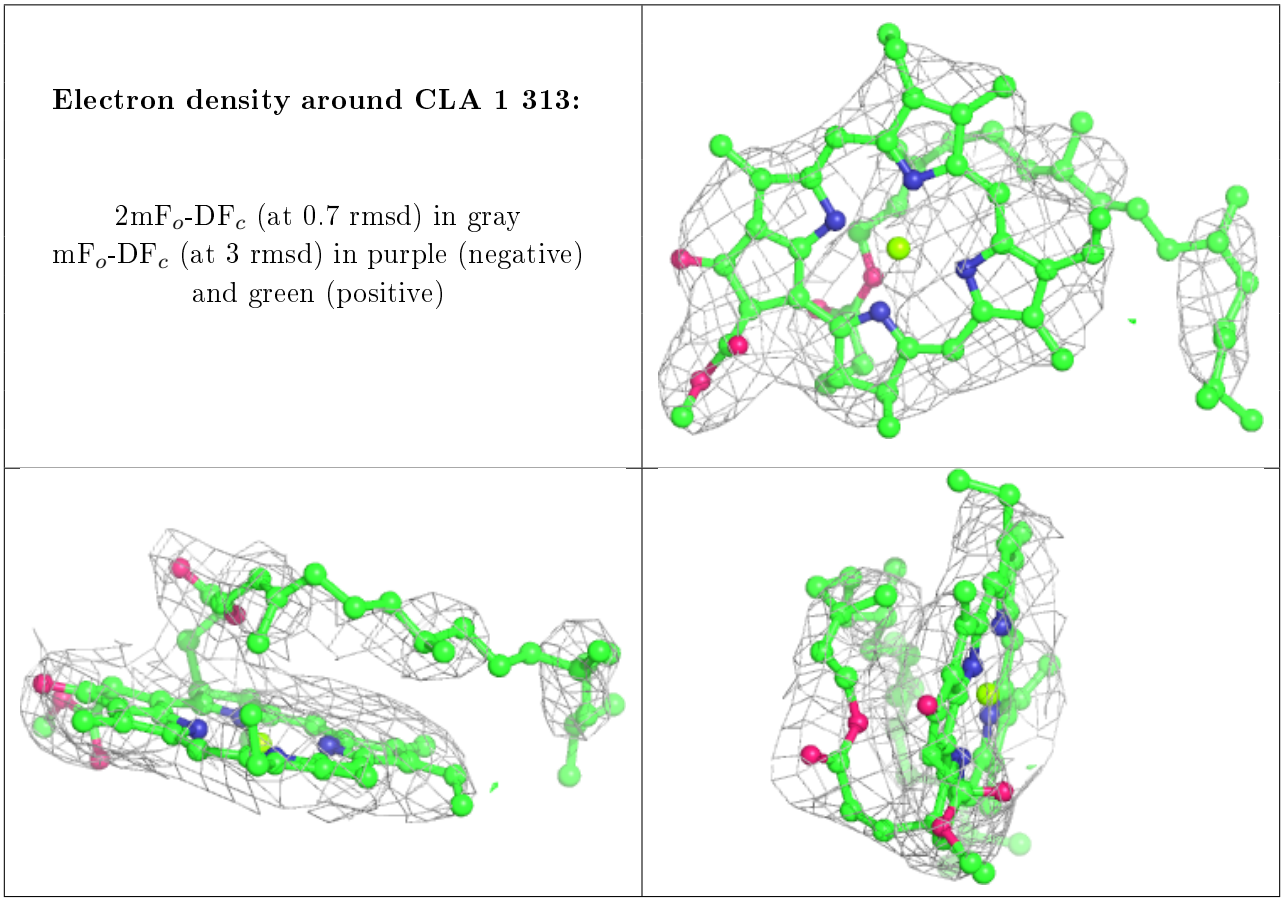
Electron density around BCR 3 318:

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



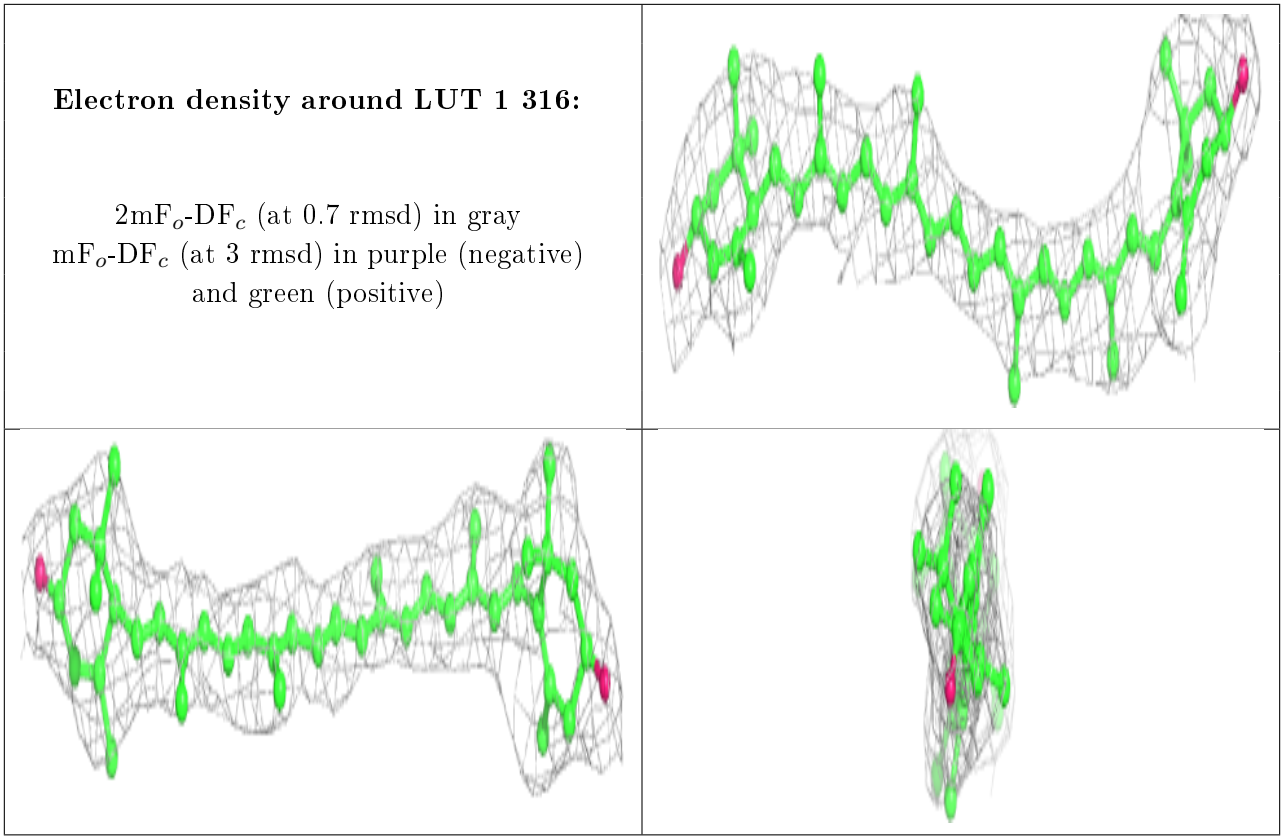
Electron density around CLA 1 313:

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



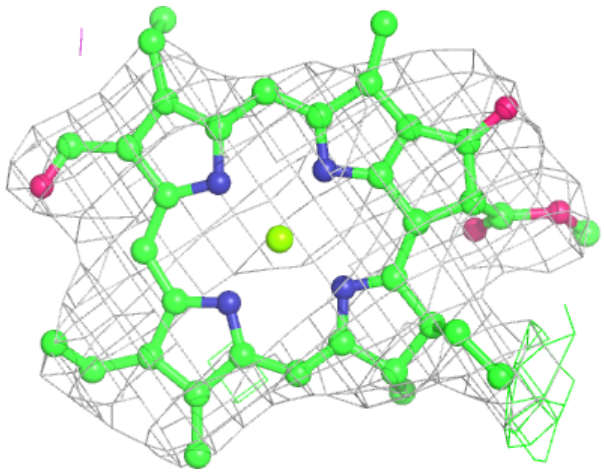
Electron density around LUT 1 316:

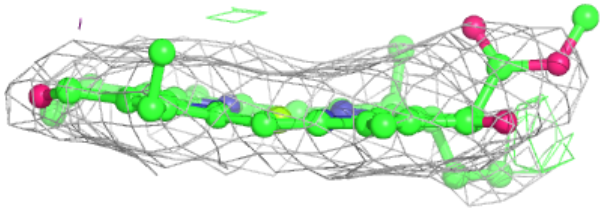
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

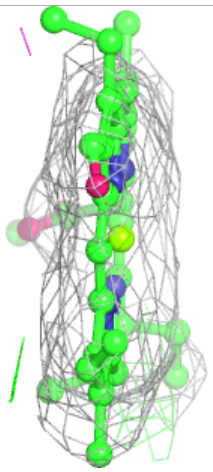


Electron density around CHL 4 615:

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

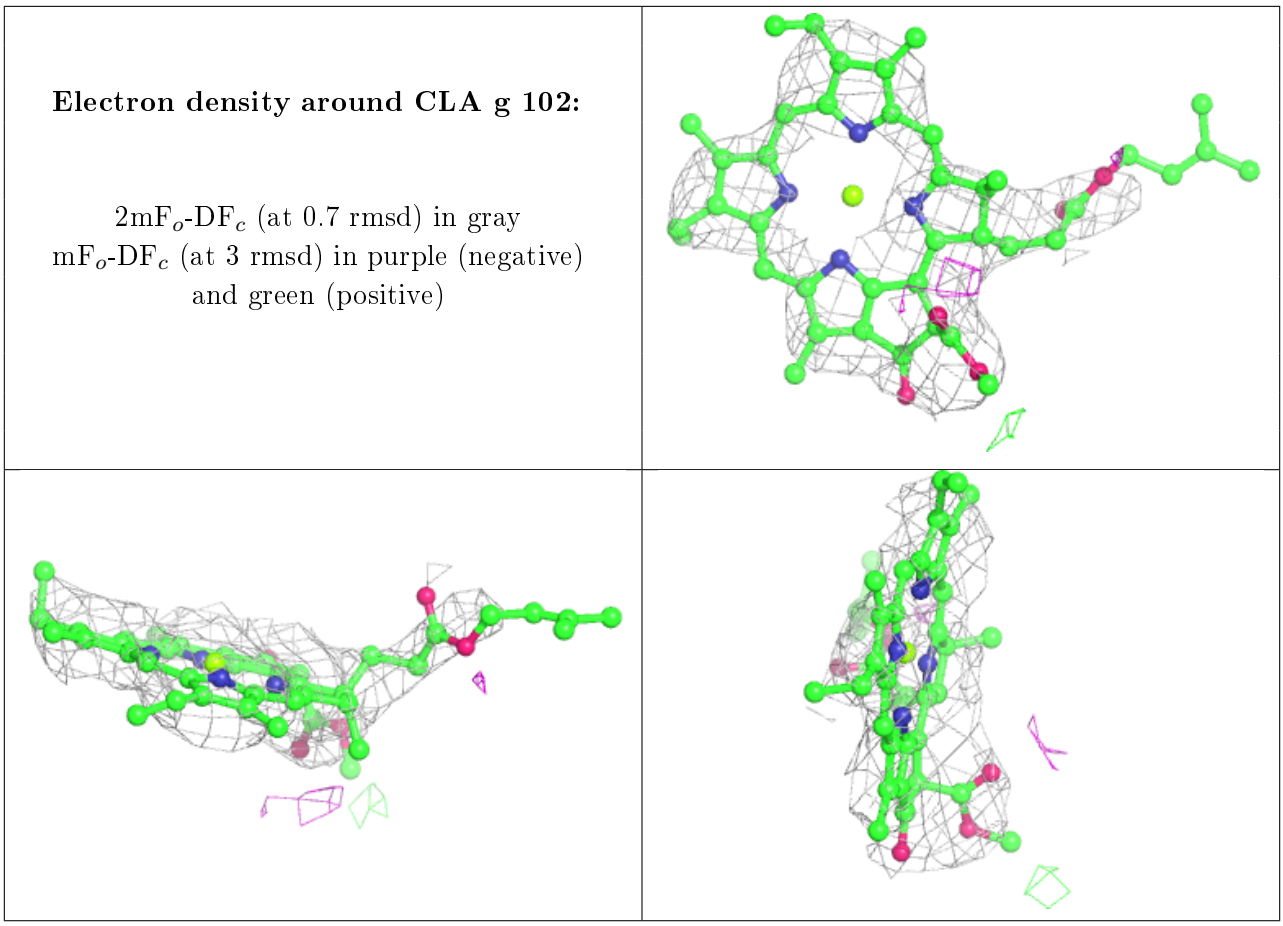






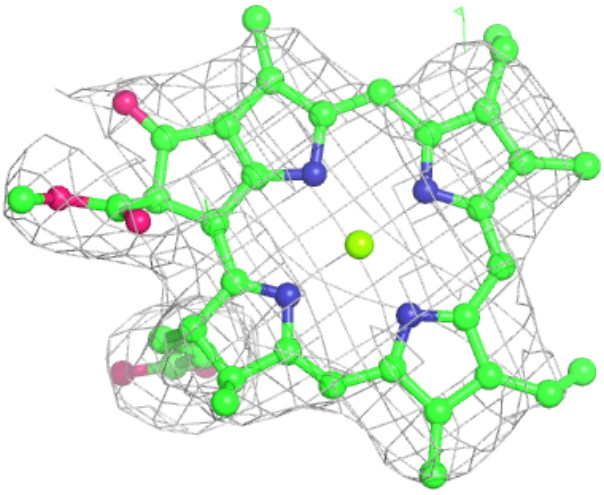
Electron density around CLA g 102:

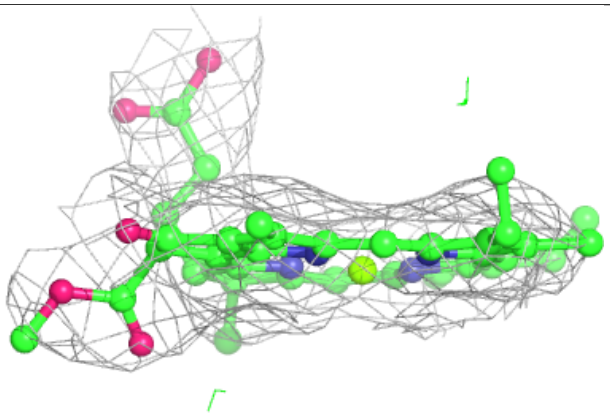
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

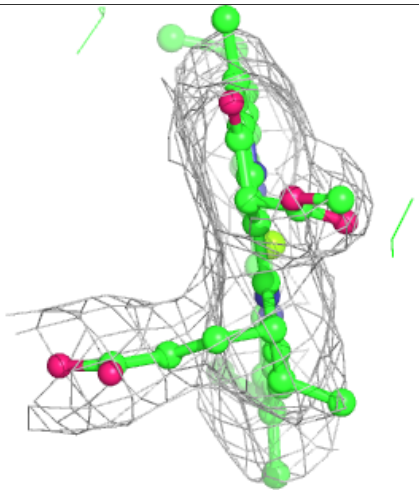


Electron density around CLA B 835:

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

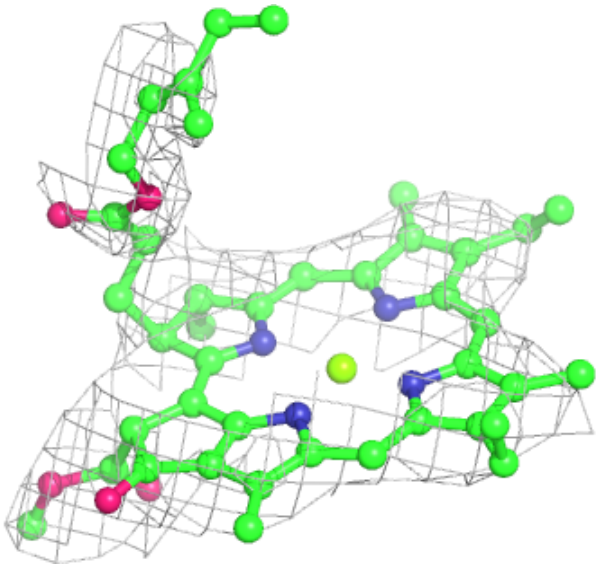


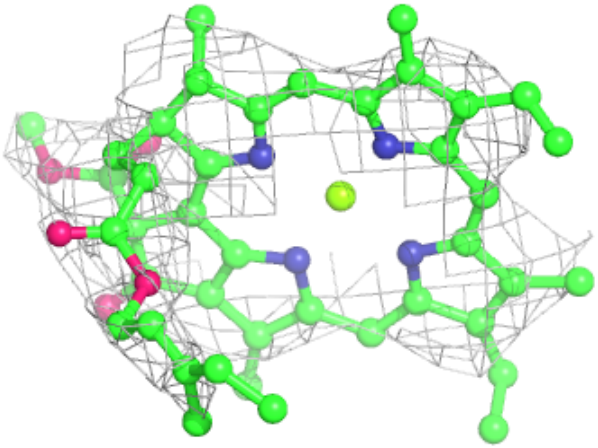


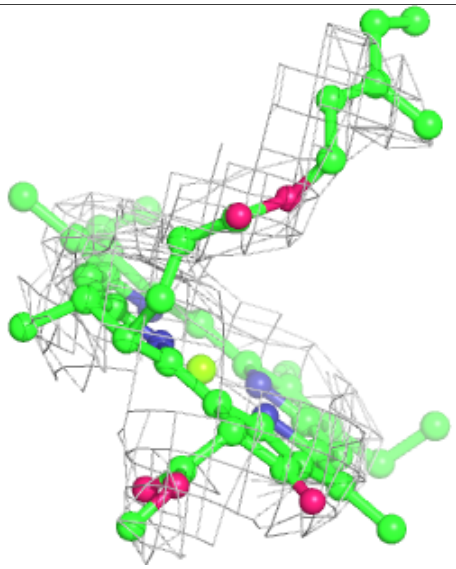


Electron density around CLA 6 306:

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

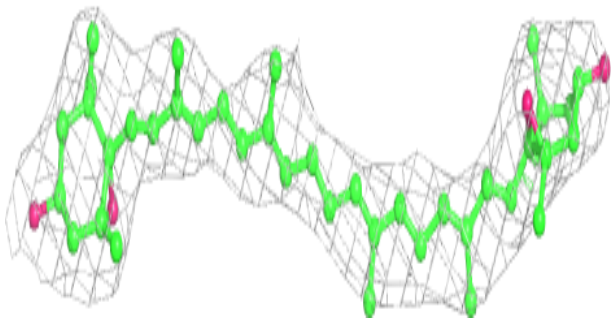


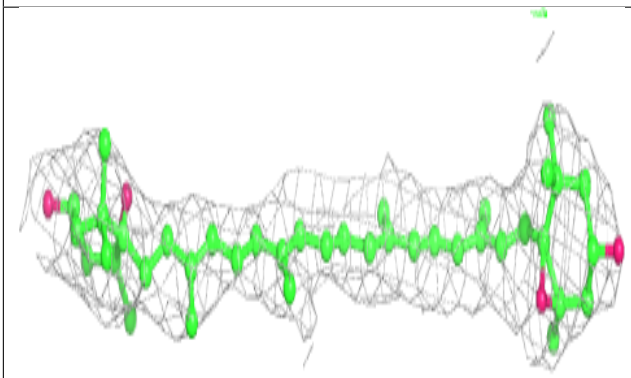


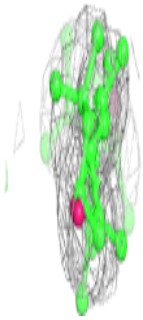


Electron density around XAT 4 617:

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

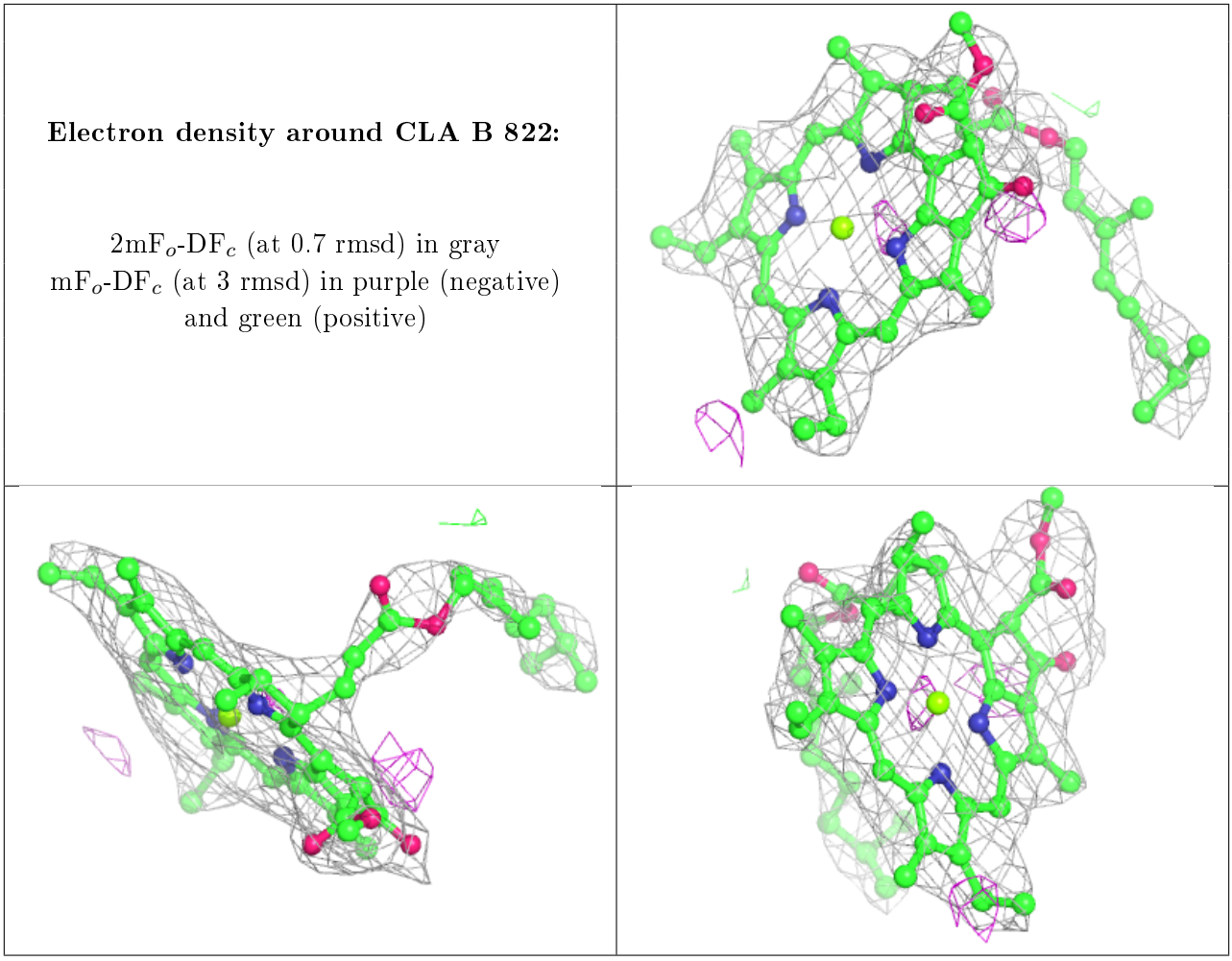






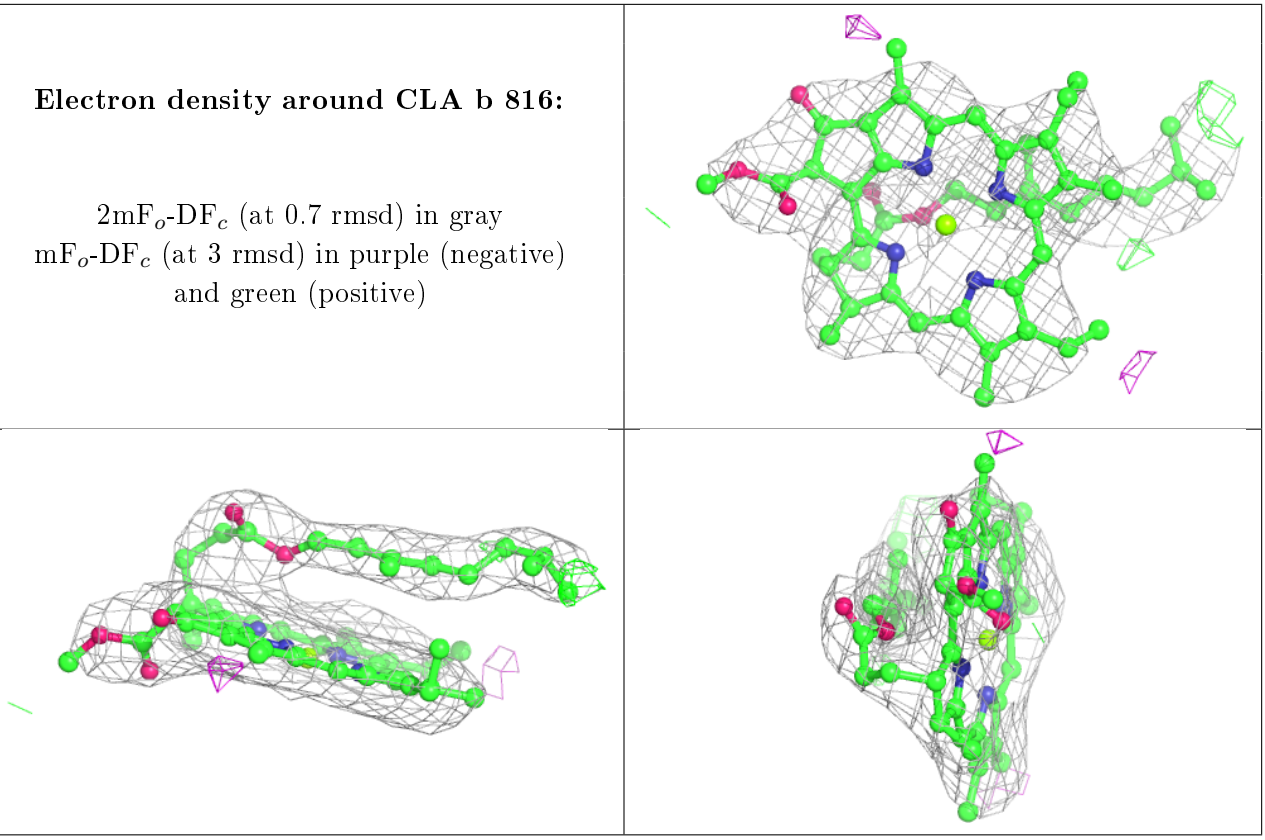
Electron density around CLA B 822:

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



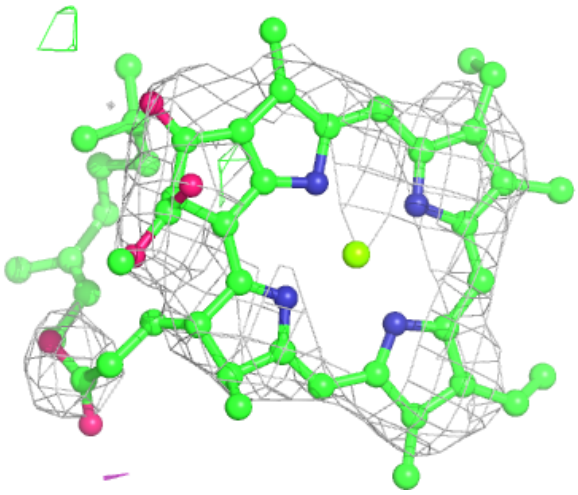
Electron density around CLA b 816:

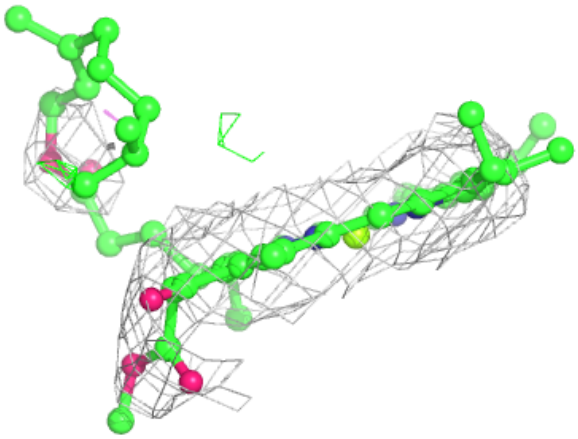
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

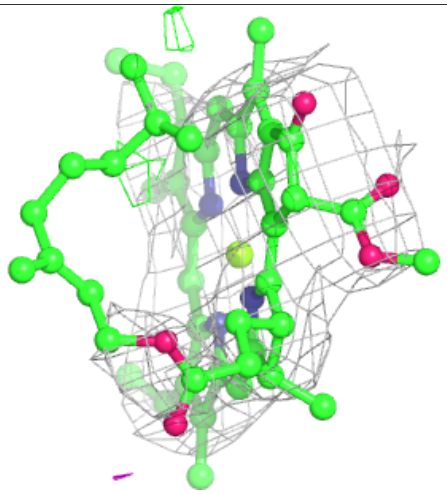


Electron density around CLA 6 315:

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

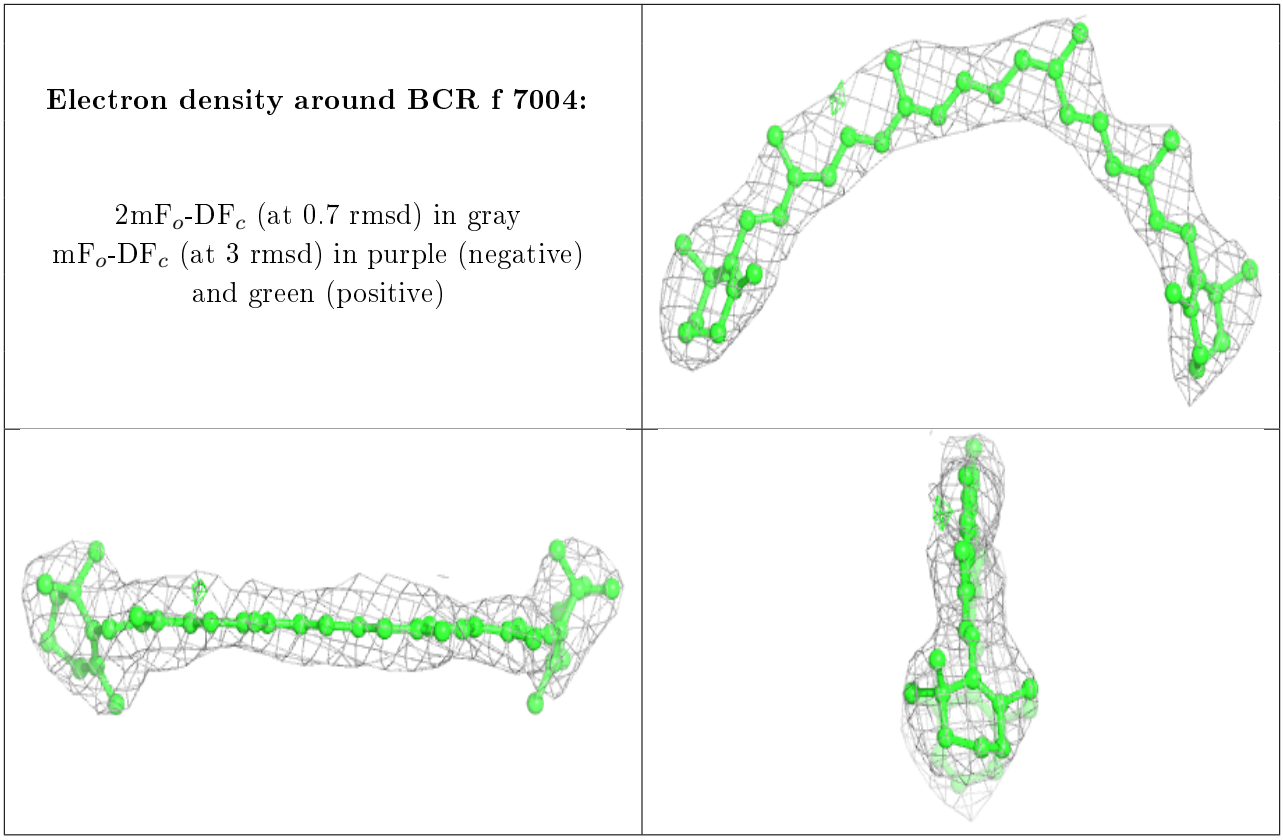






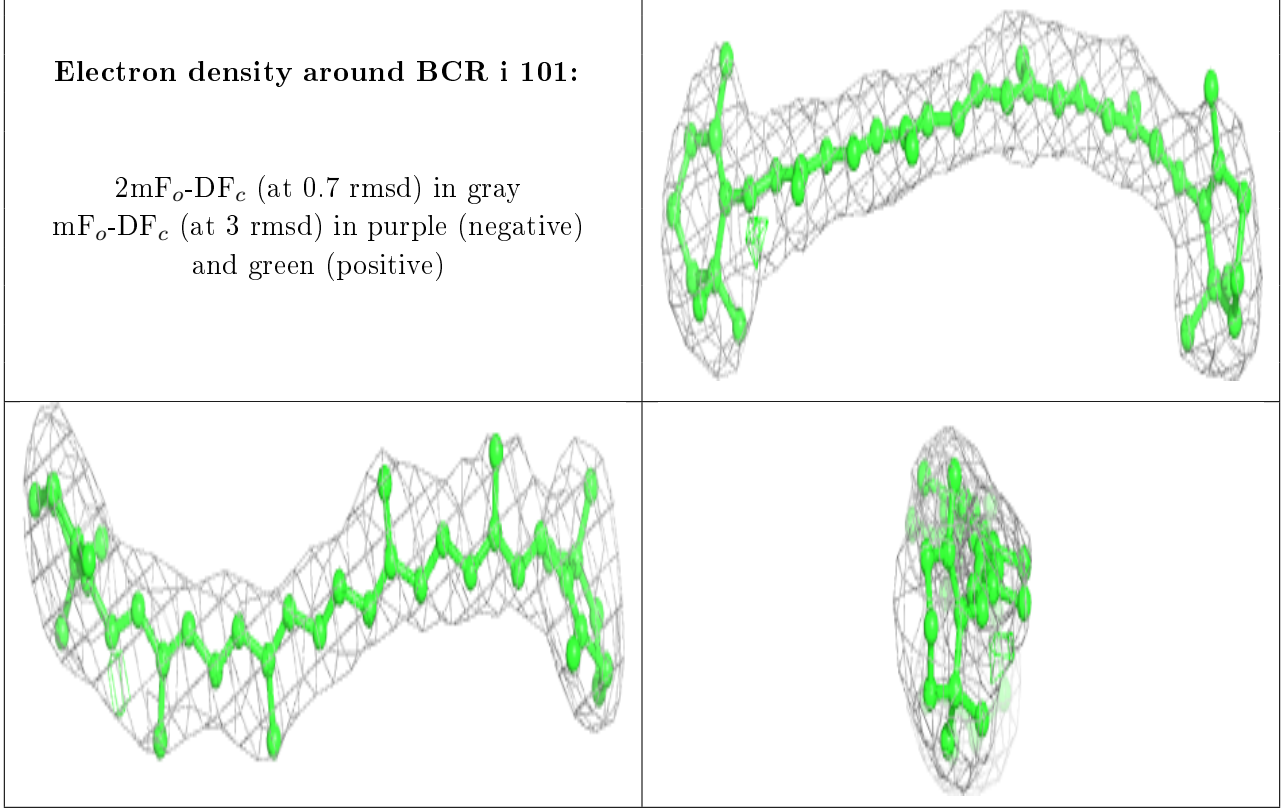
Electron density around BCR f 7004:

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



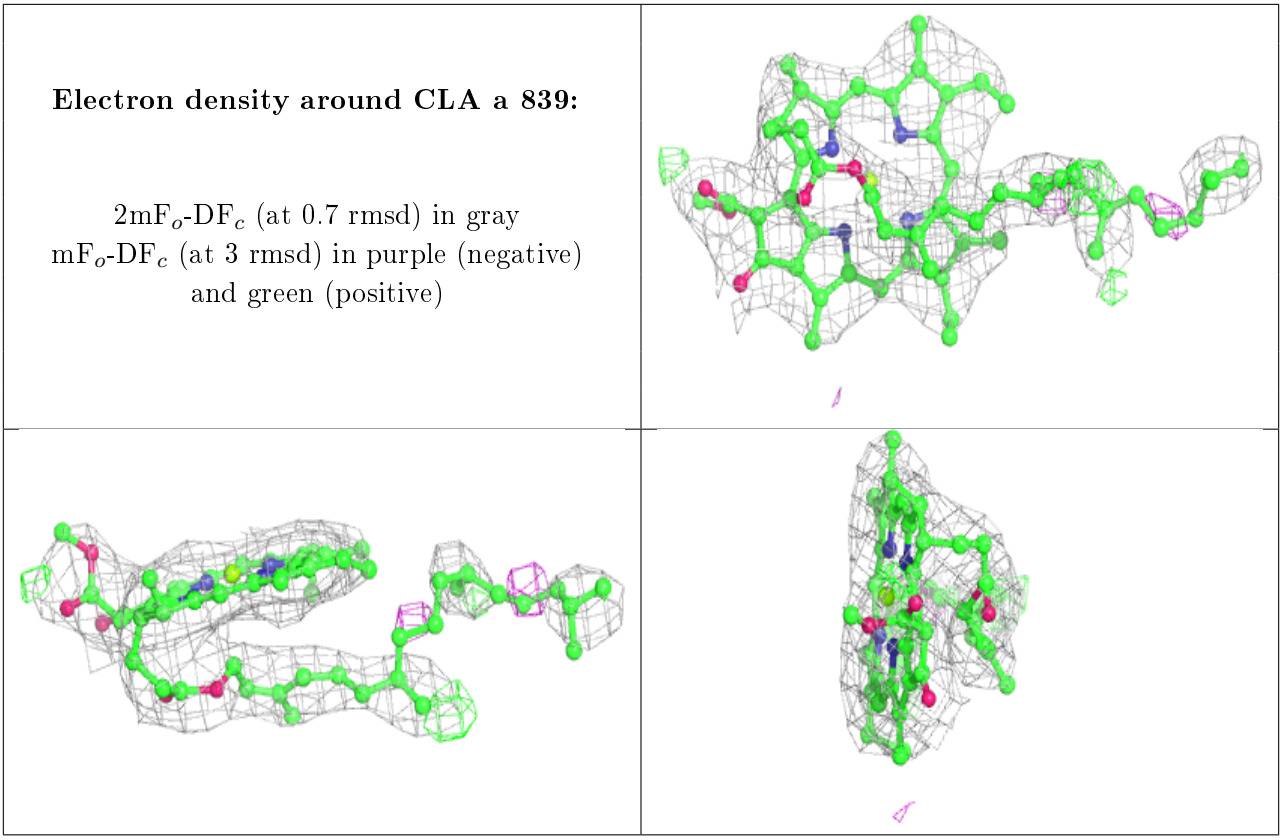
Electron density around BCR i 101:

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



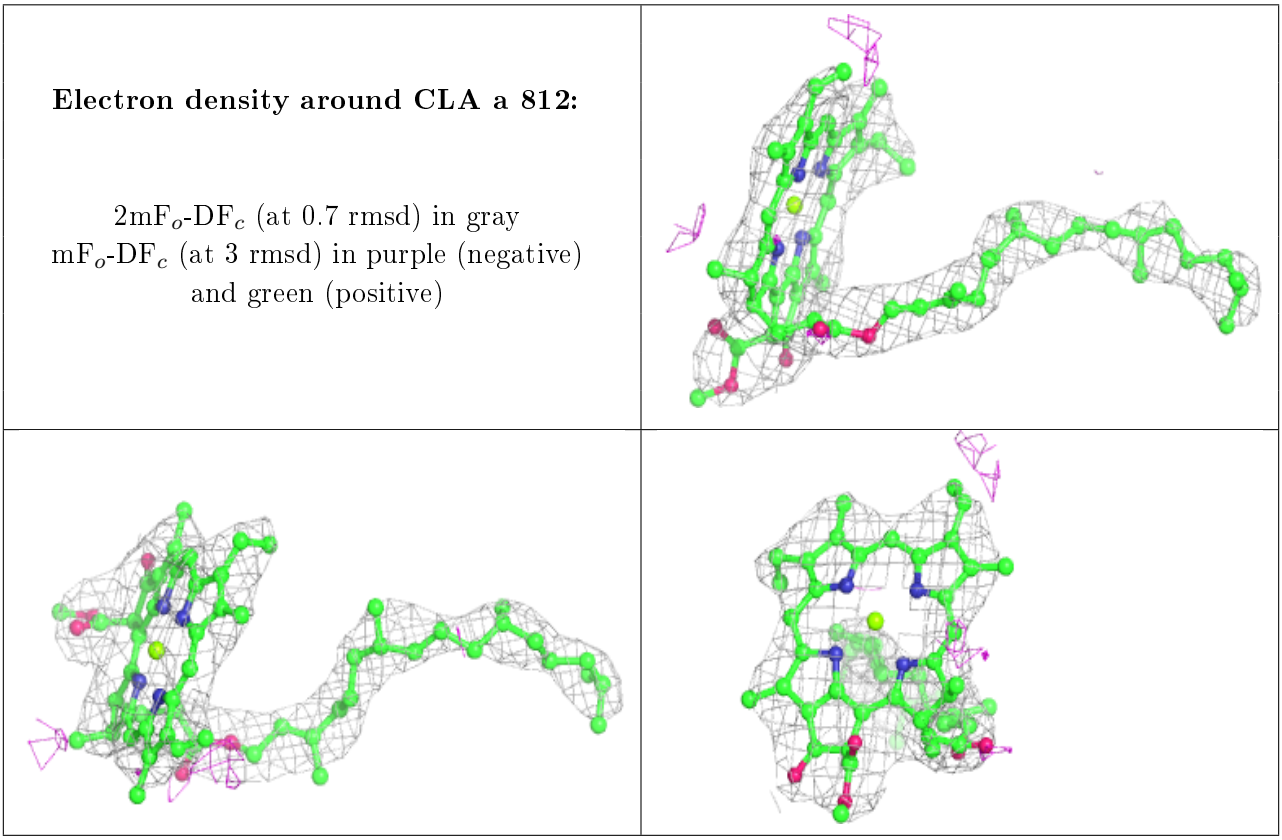
Electron density around CLA a 839:

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



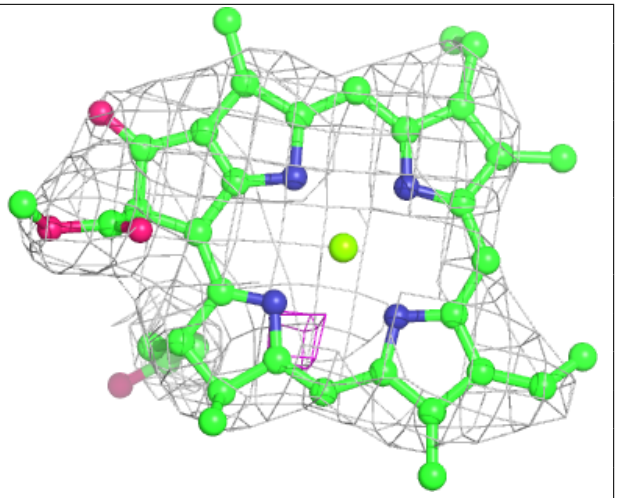
Electron density around CLA a 812:

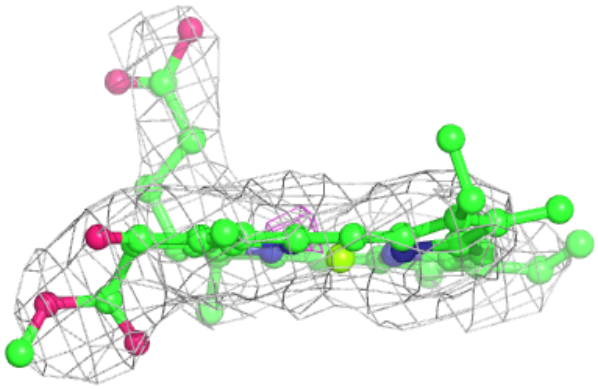
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

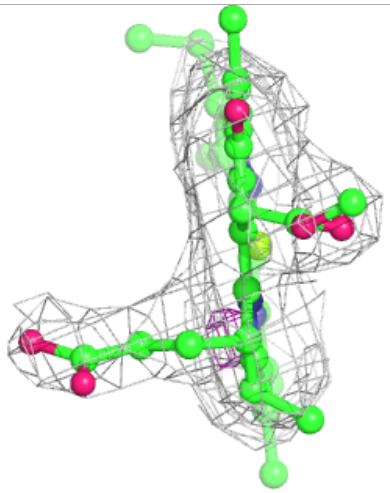


Electron density around CLA G 101:

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

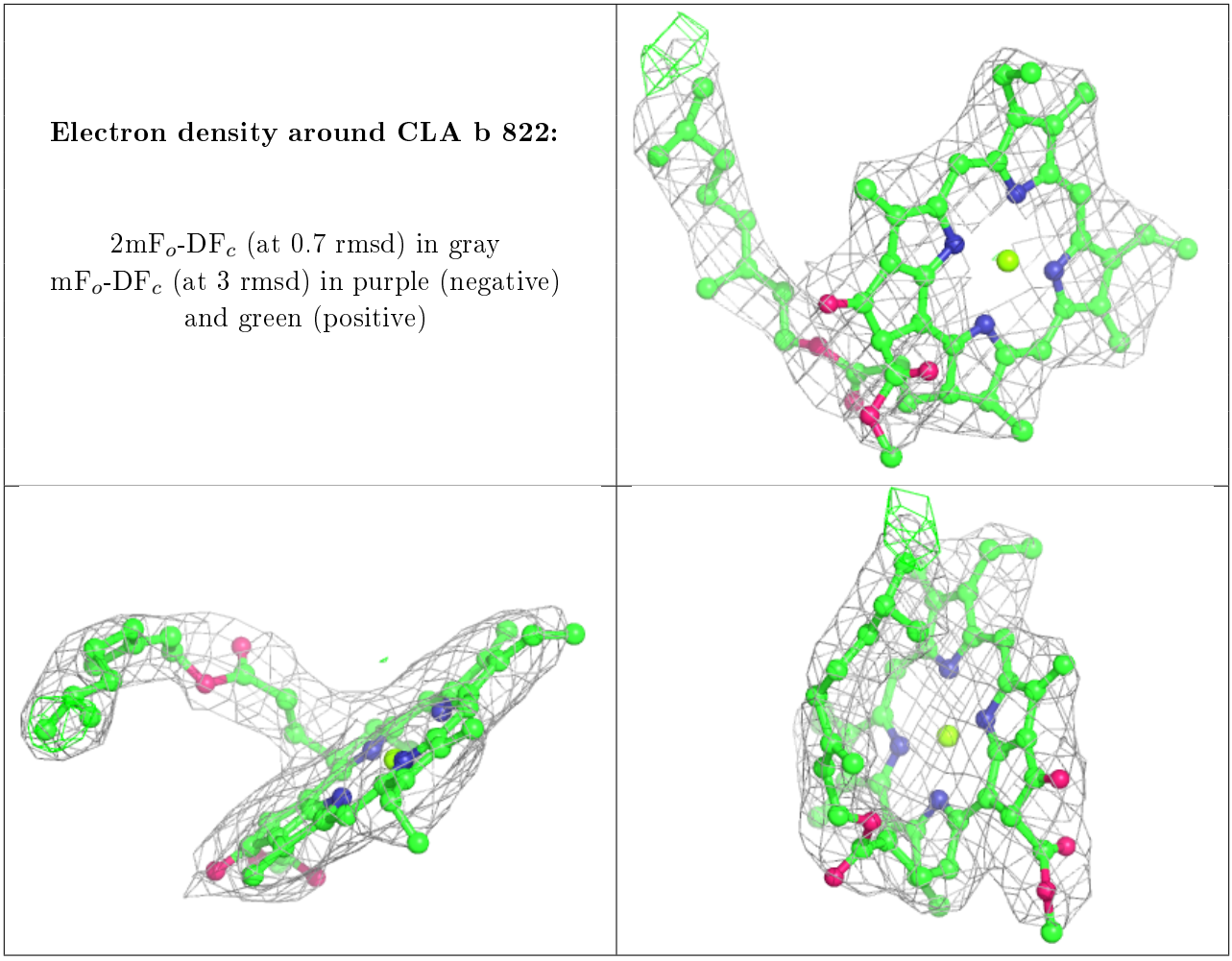






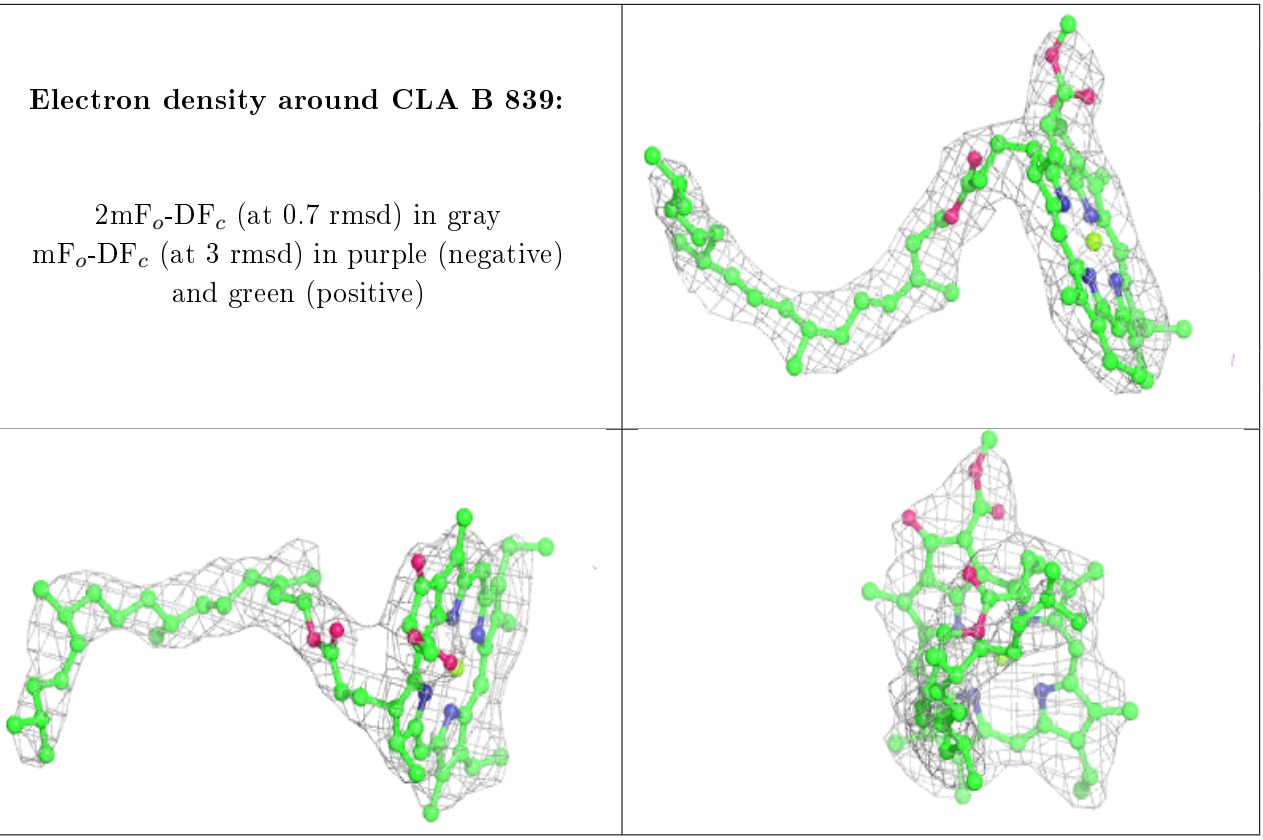
Electron density around CLA b 822:

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



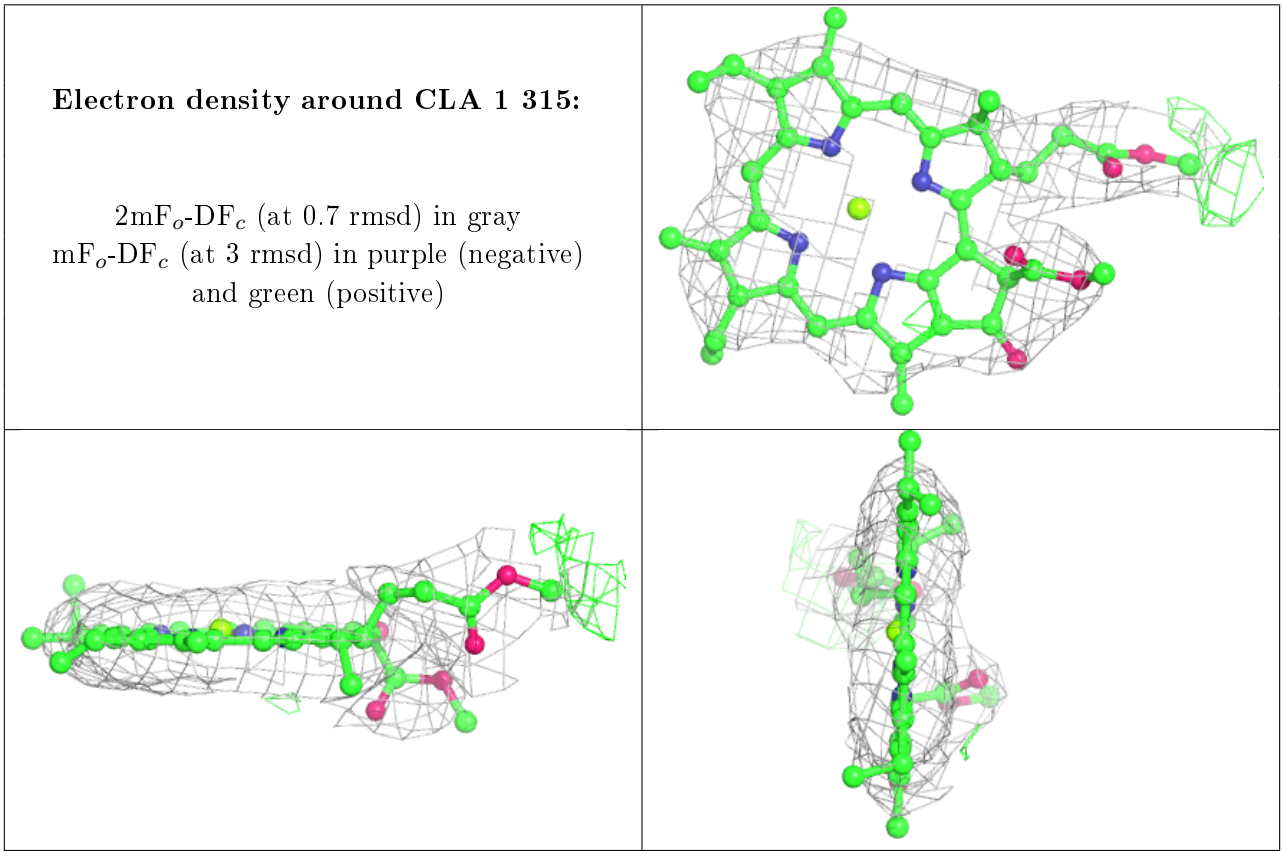
Electron density around CLA B 839:

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



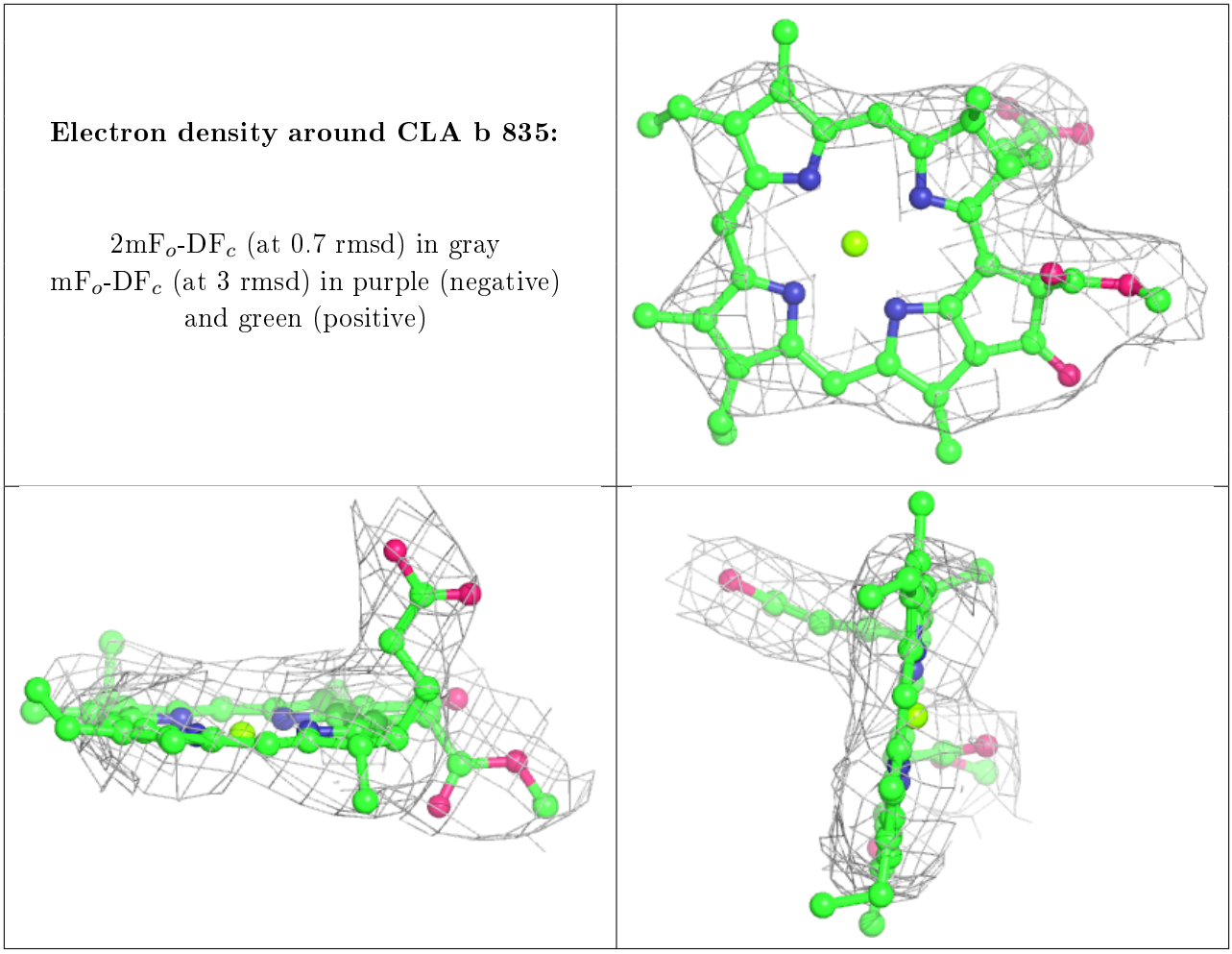
Electron density around CLA 1 315:

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



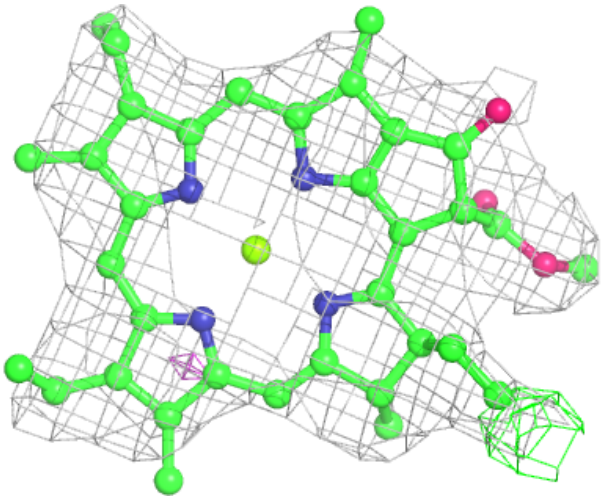
Electron density around CLA b 835:

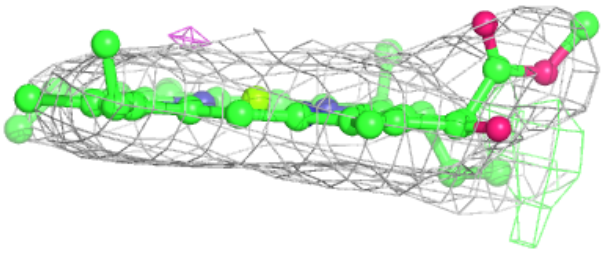
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

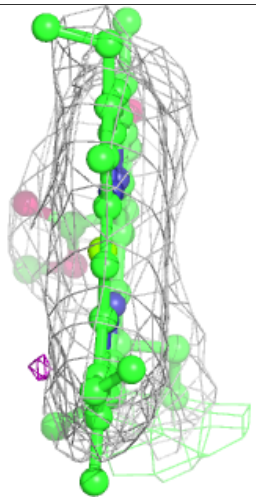


Electron density around CLA 3 305:

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

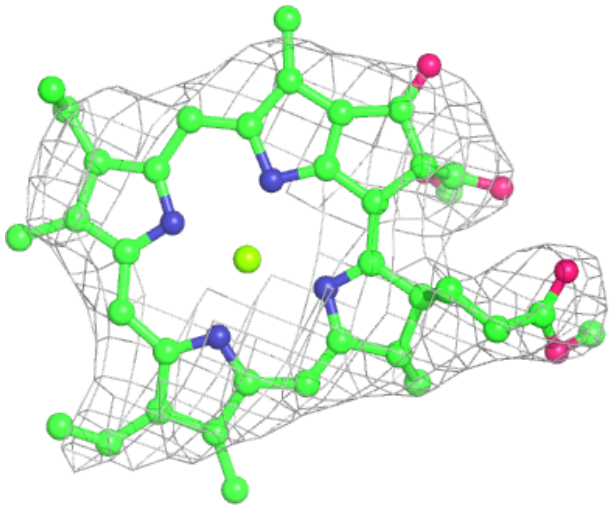


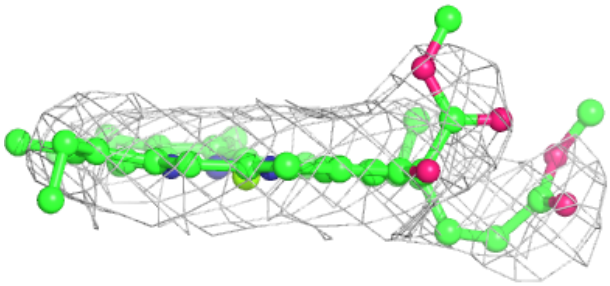


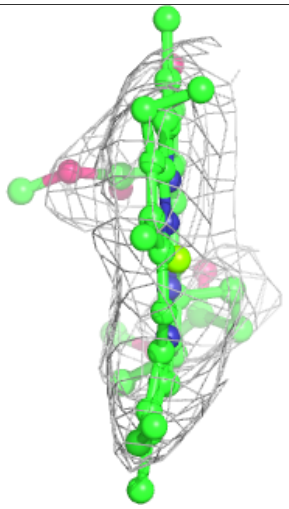


Electron density around CLA G 104:

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

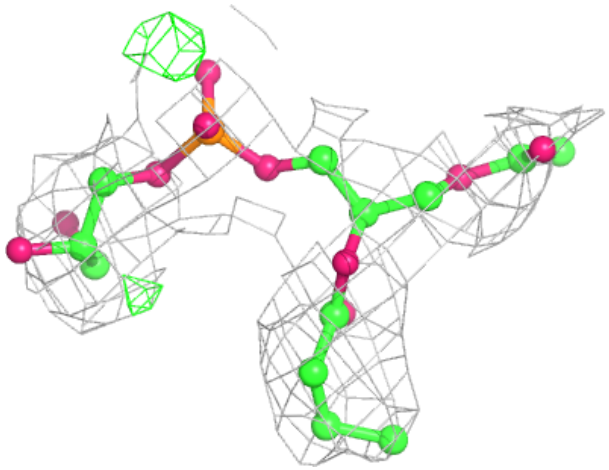


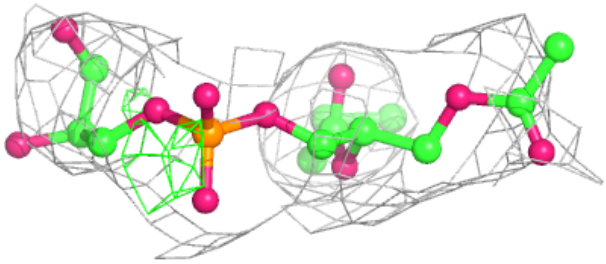


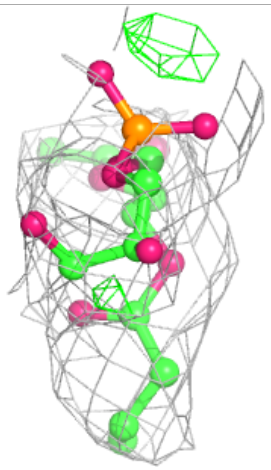


Electron density around LHG 6 301:

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

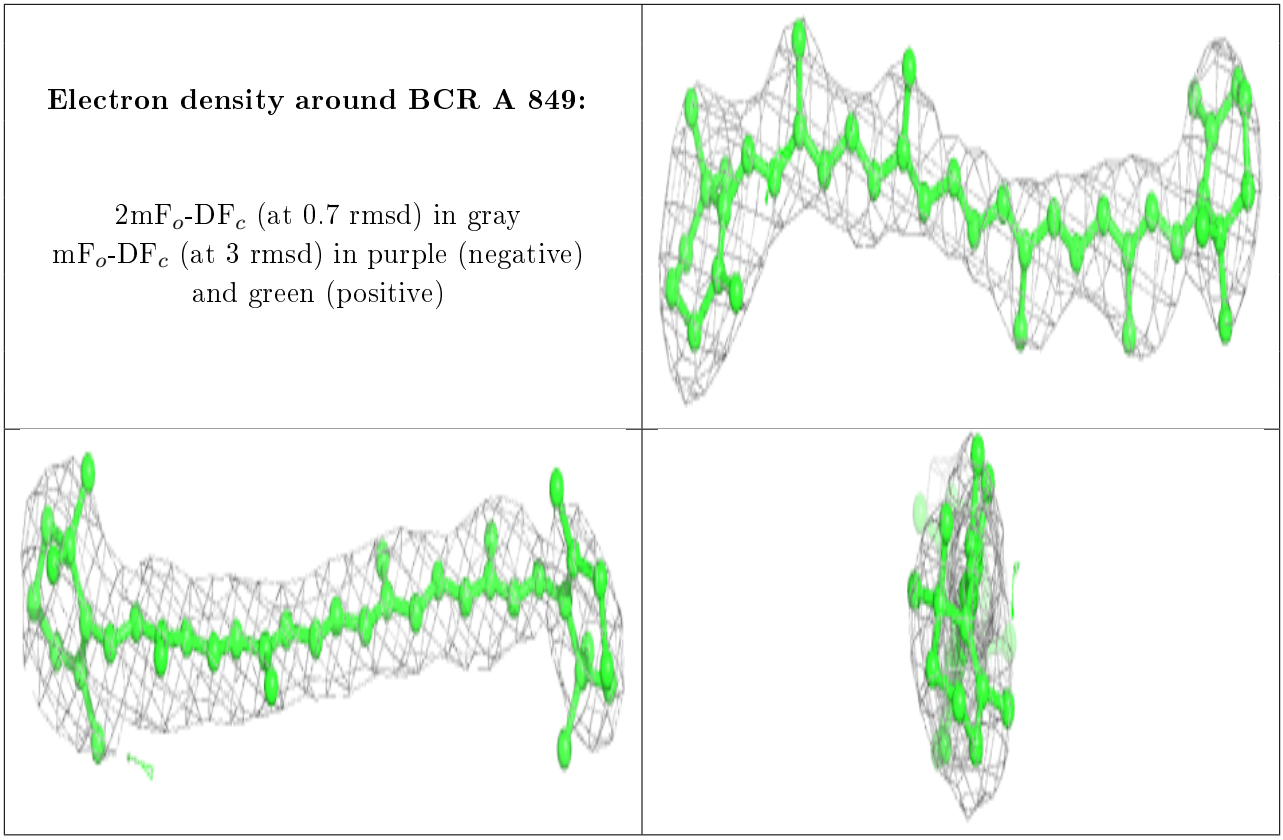






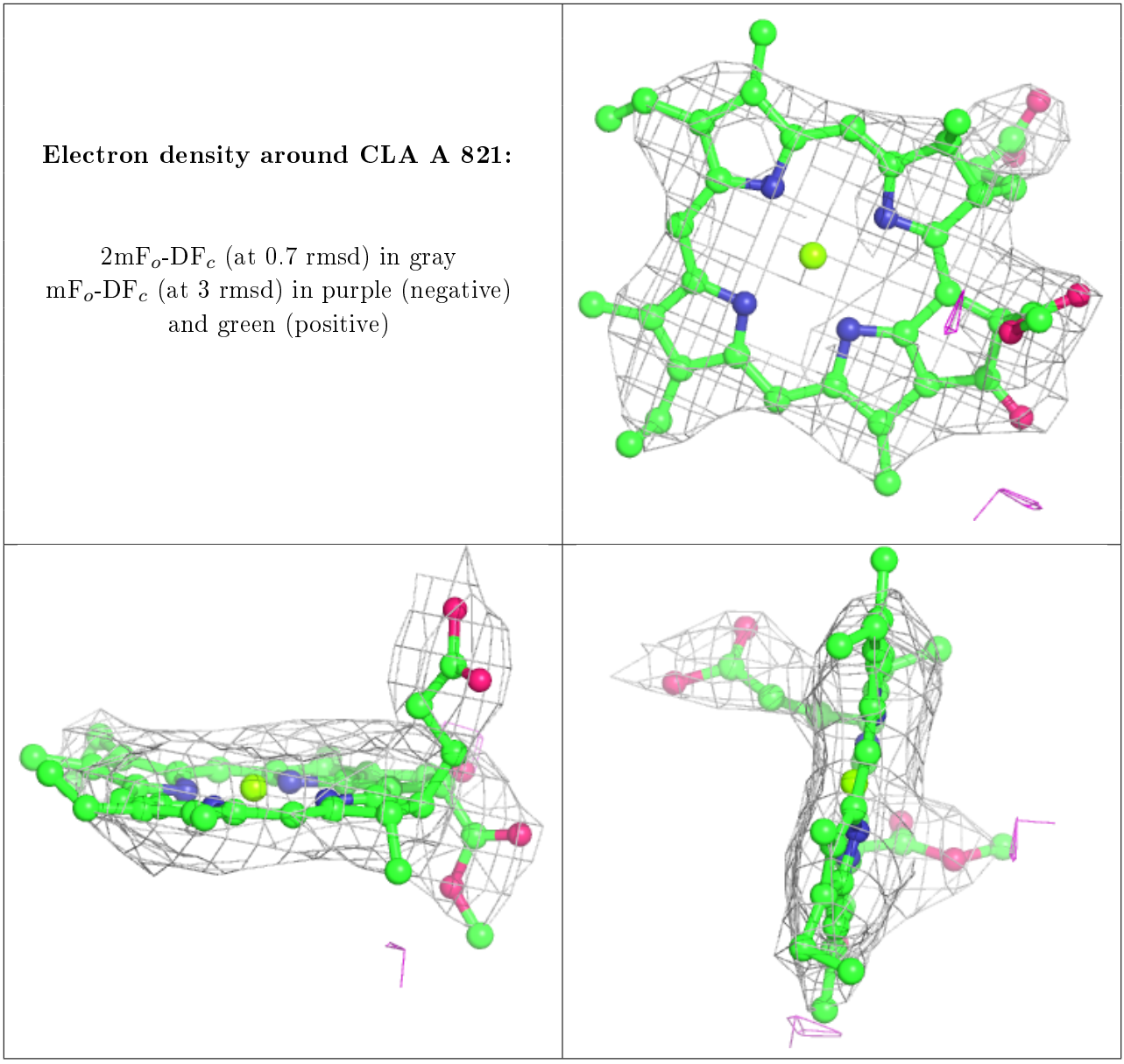
Electron density around BCR A 849:

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



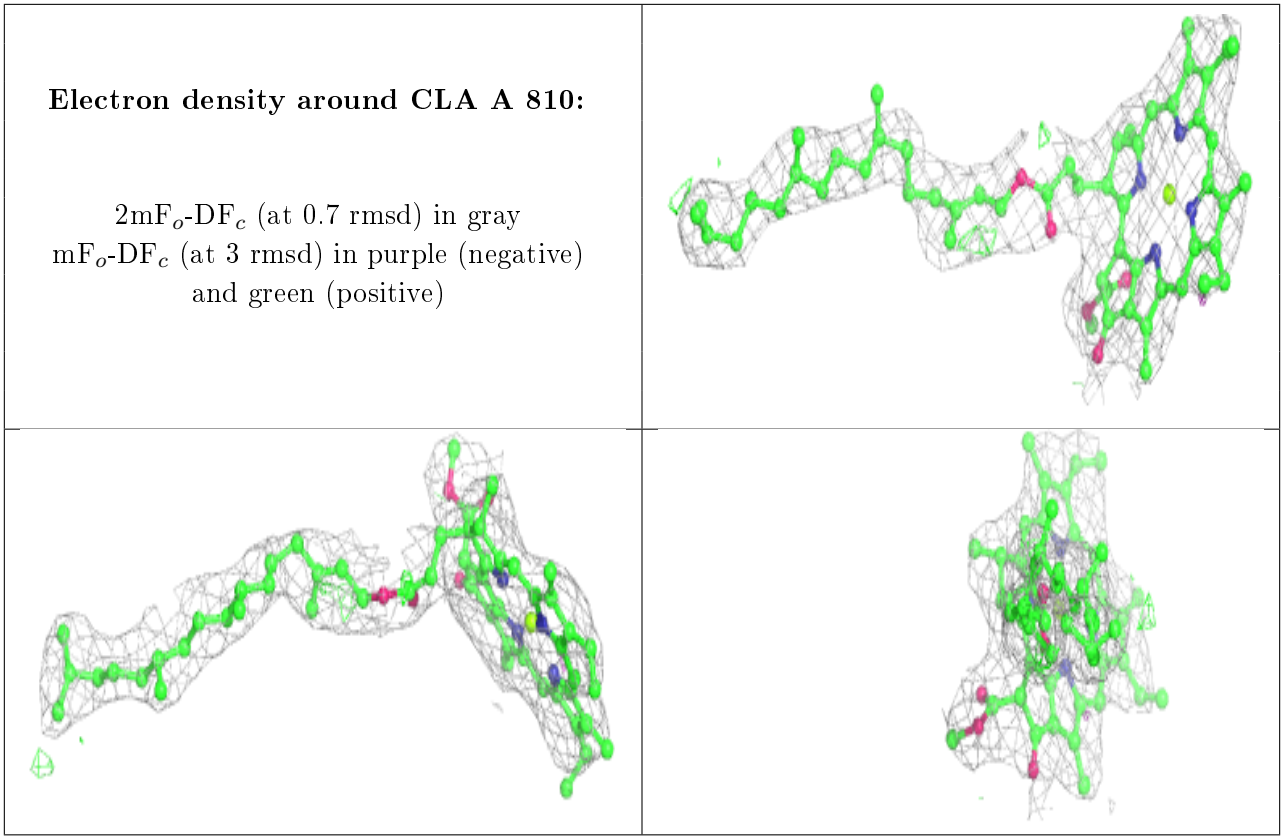
Electron density around CLA A 821:

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



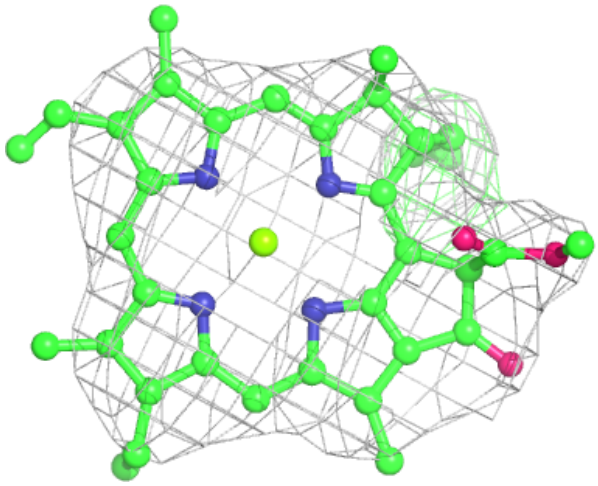
Electron density around CLA A 810:

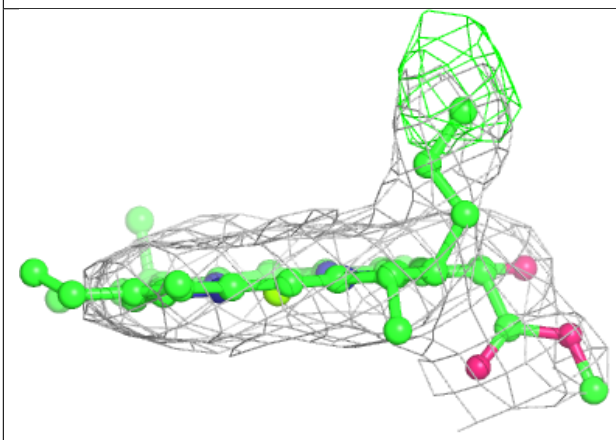
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

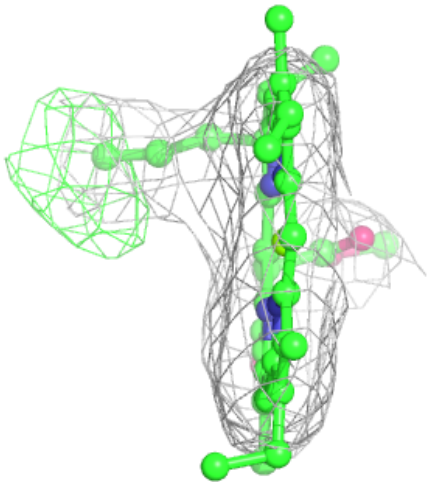


Electron density around CLA 7 613:

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

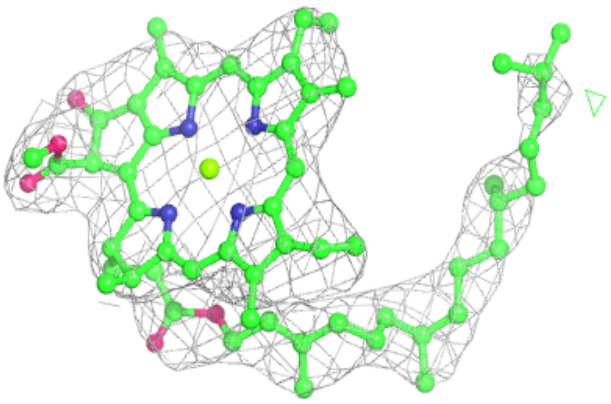


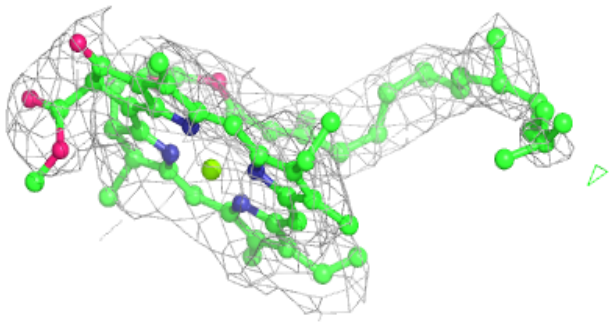


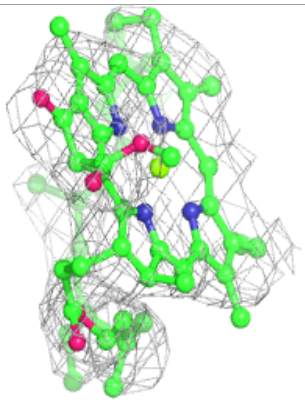


Electron density around CLA 2 602:

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

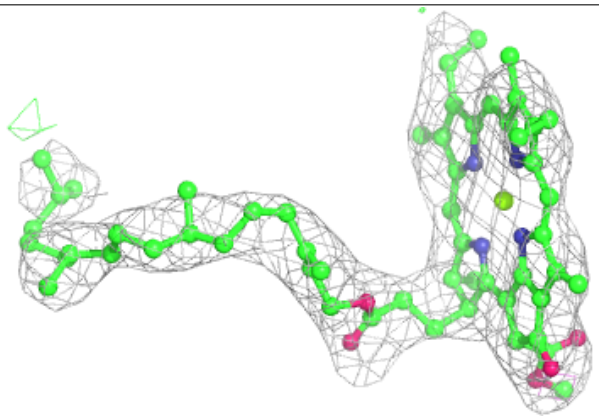


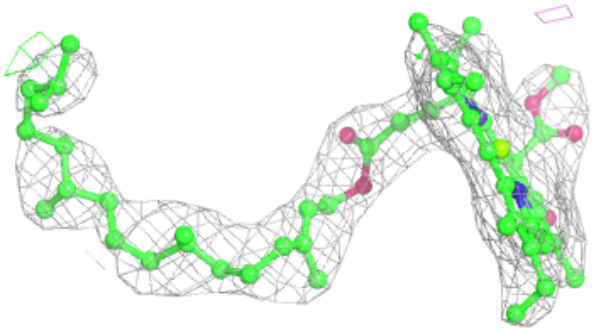


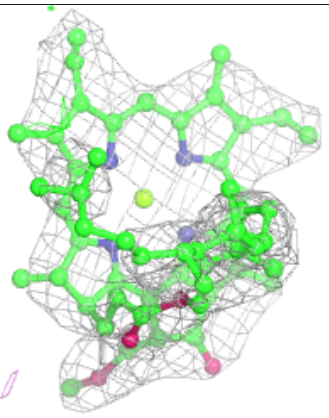


Electron density around CLA l 203:

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

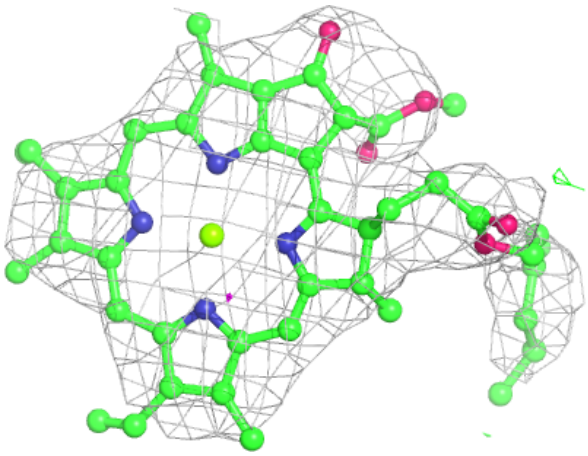


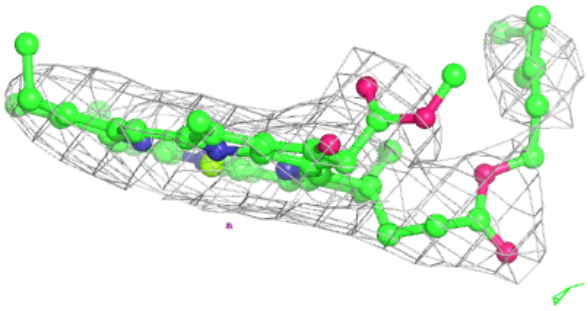


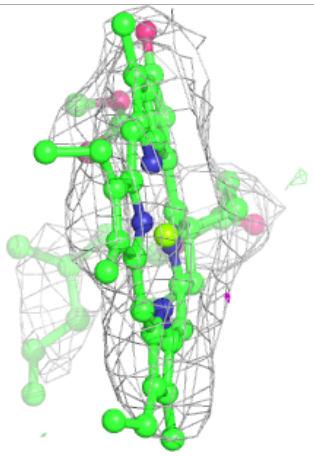


Electron density around CLA 1 312:

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

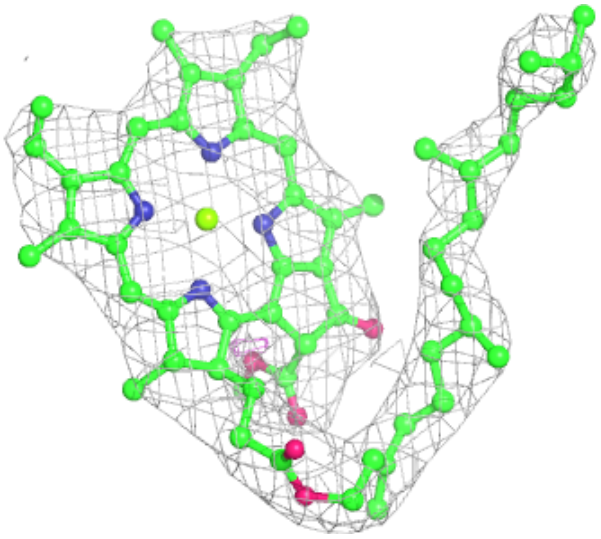


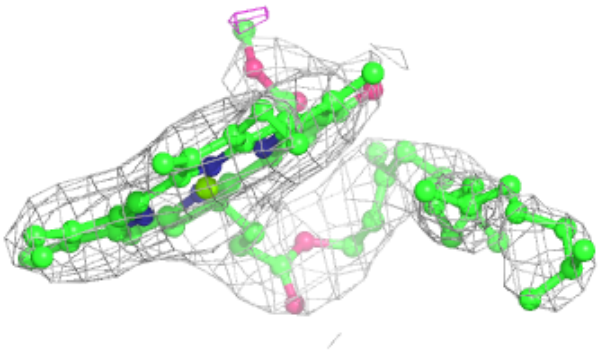


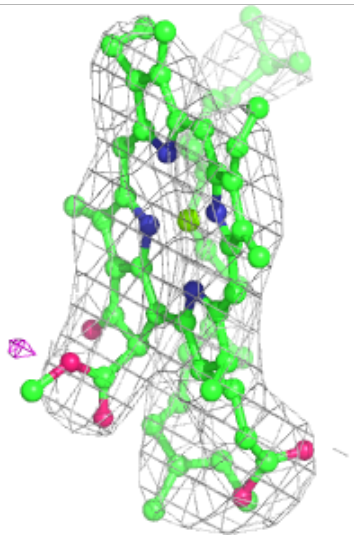


Electron density around CLA A 826:

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

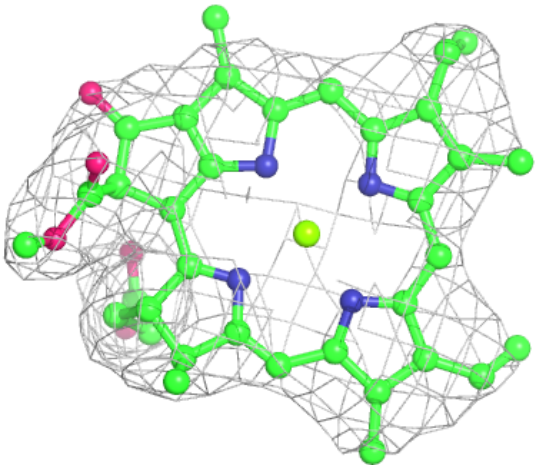


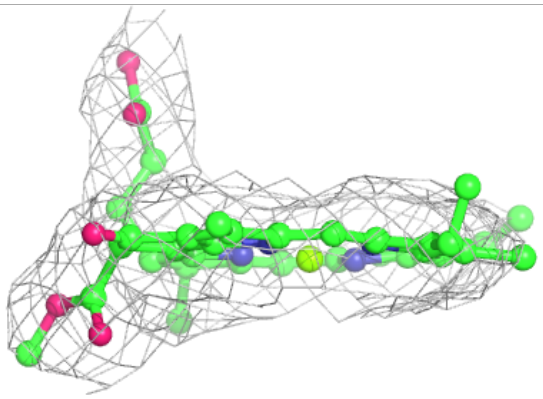


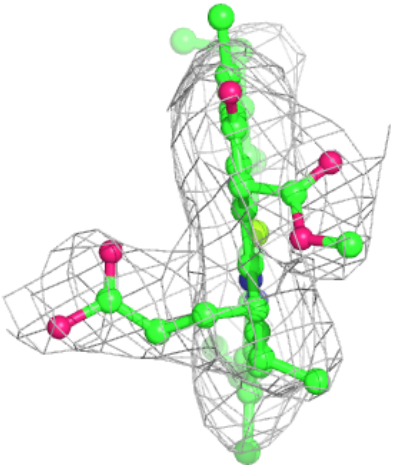


Electron density around CLA a 837:

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

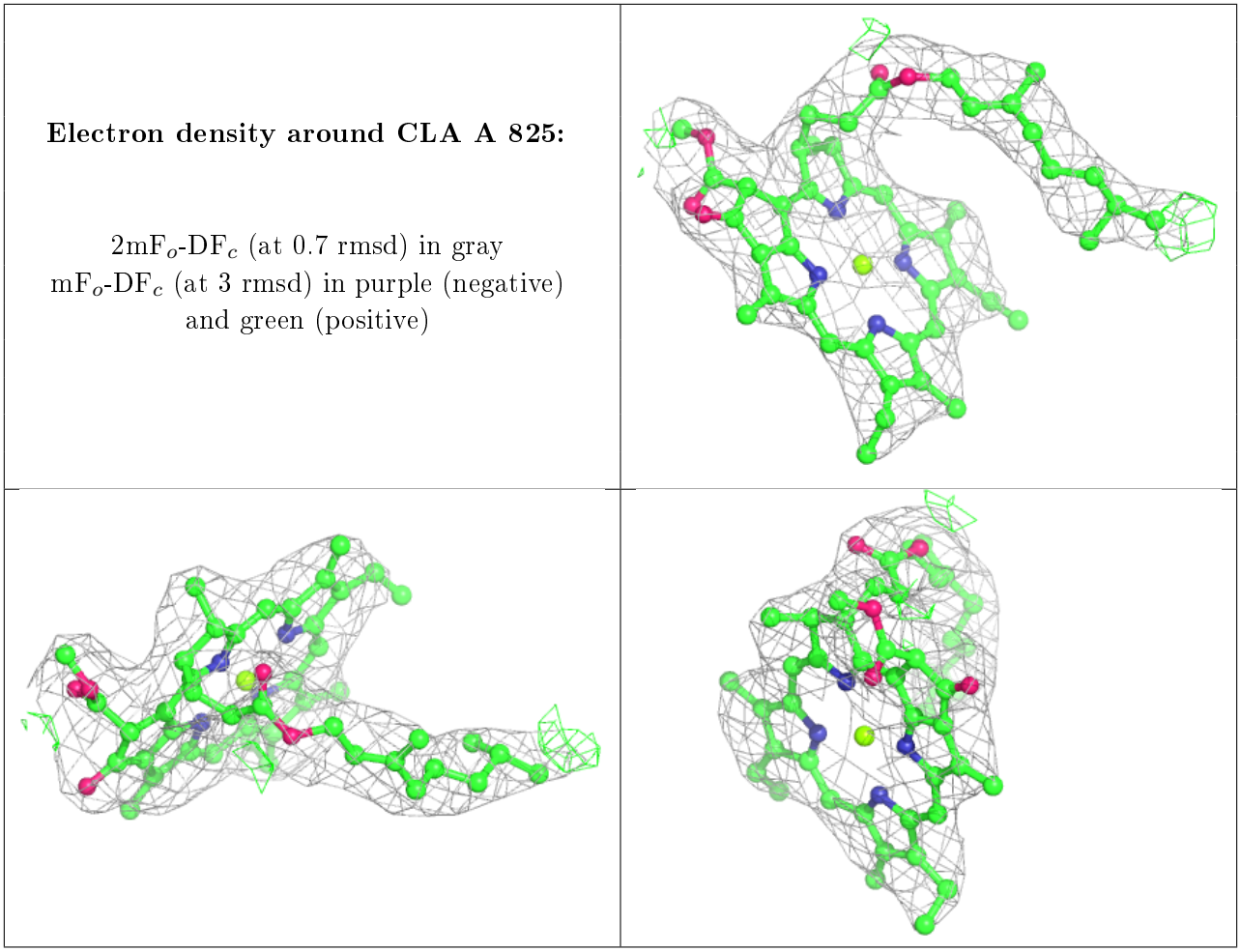






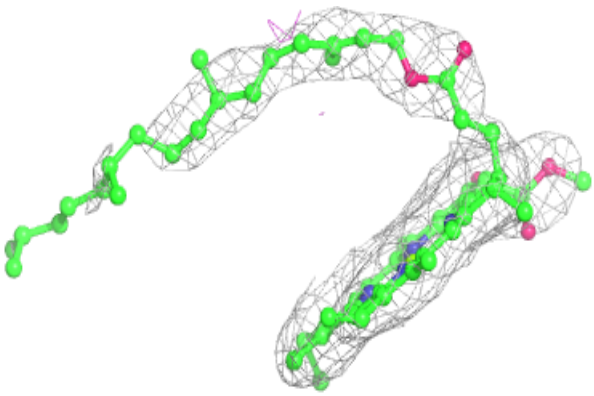
Electron density around CLA A 825:

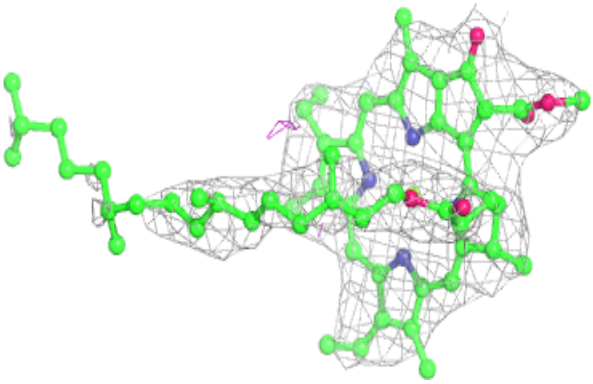
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

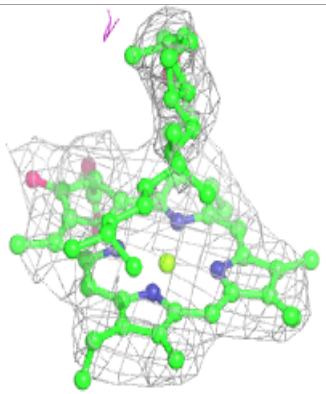


Electron density around CLA A 833:

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

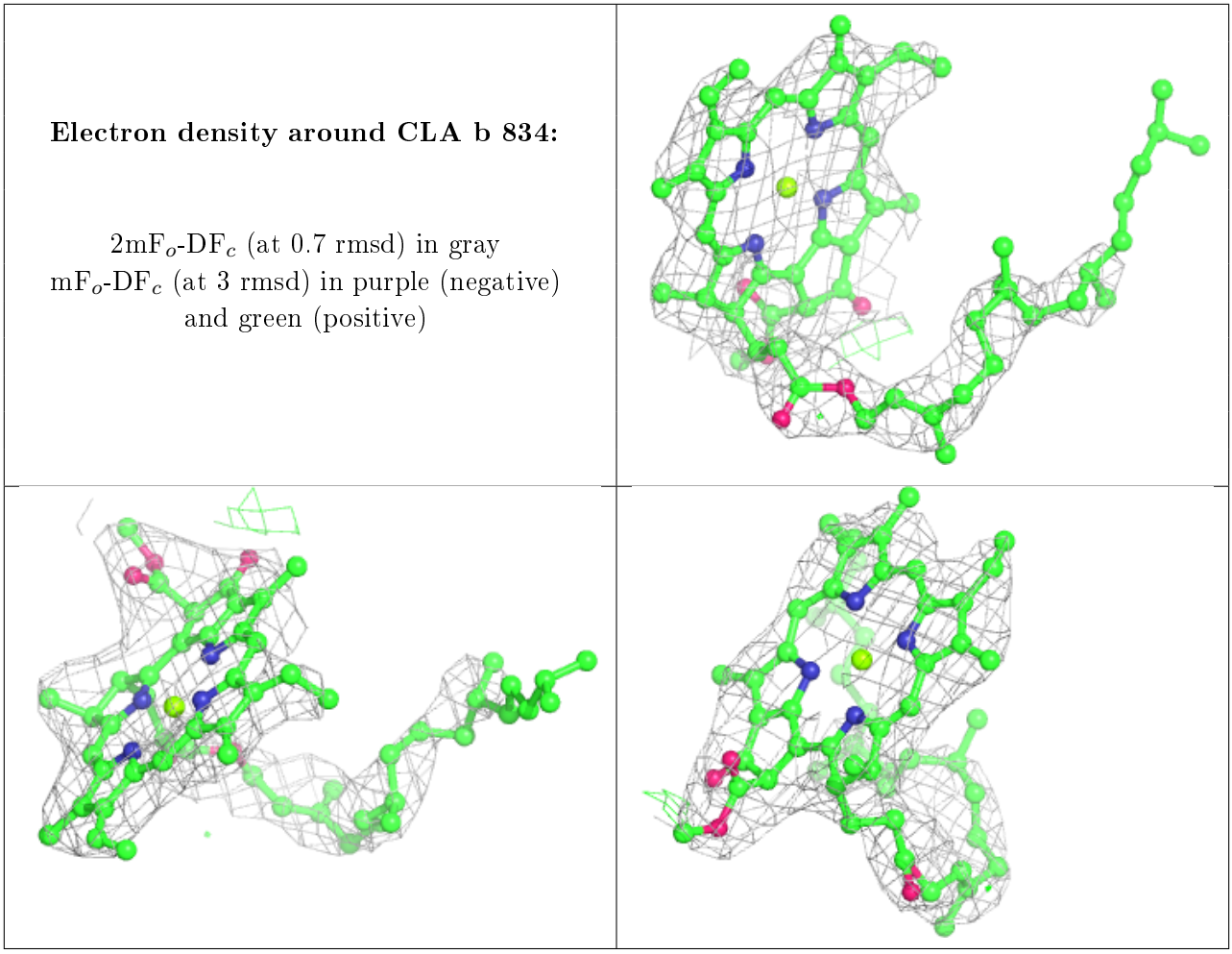






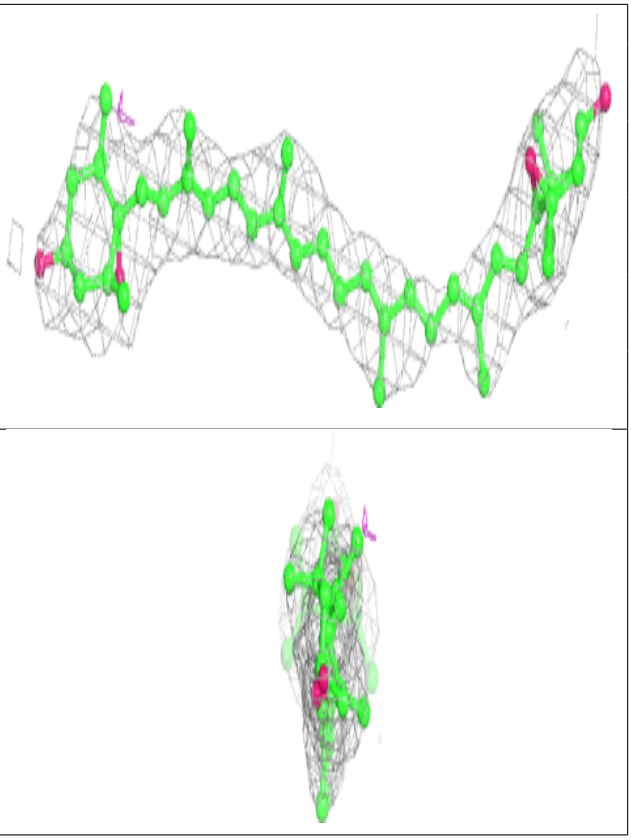
Electron density around CLA b 834:

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



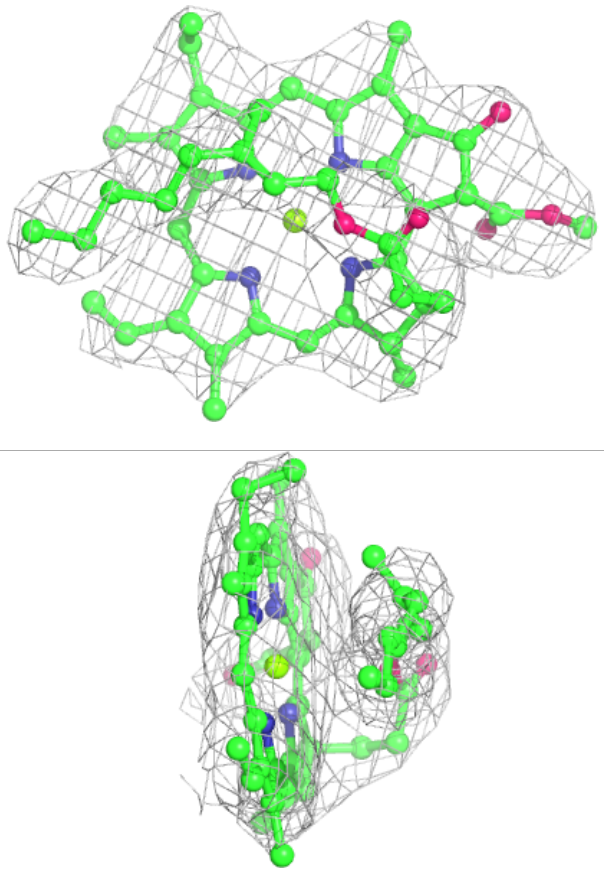
Electron density around XAT 1 317:

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



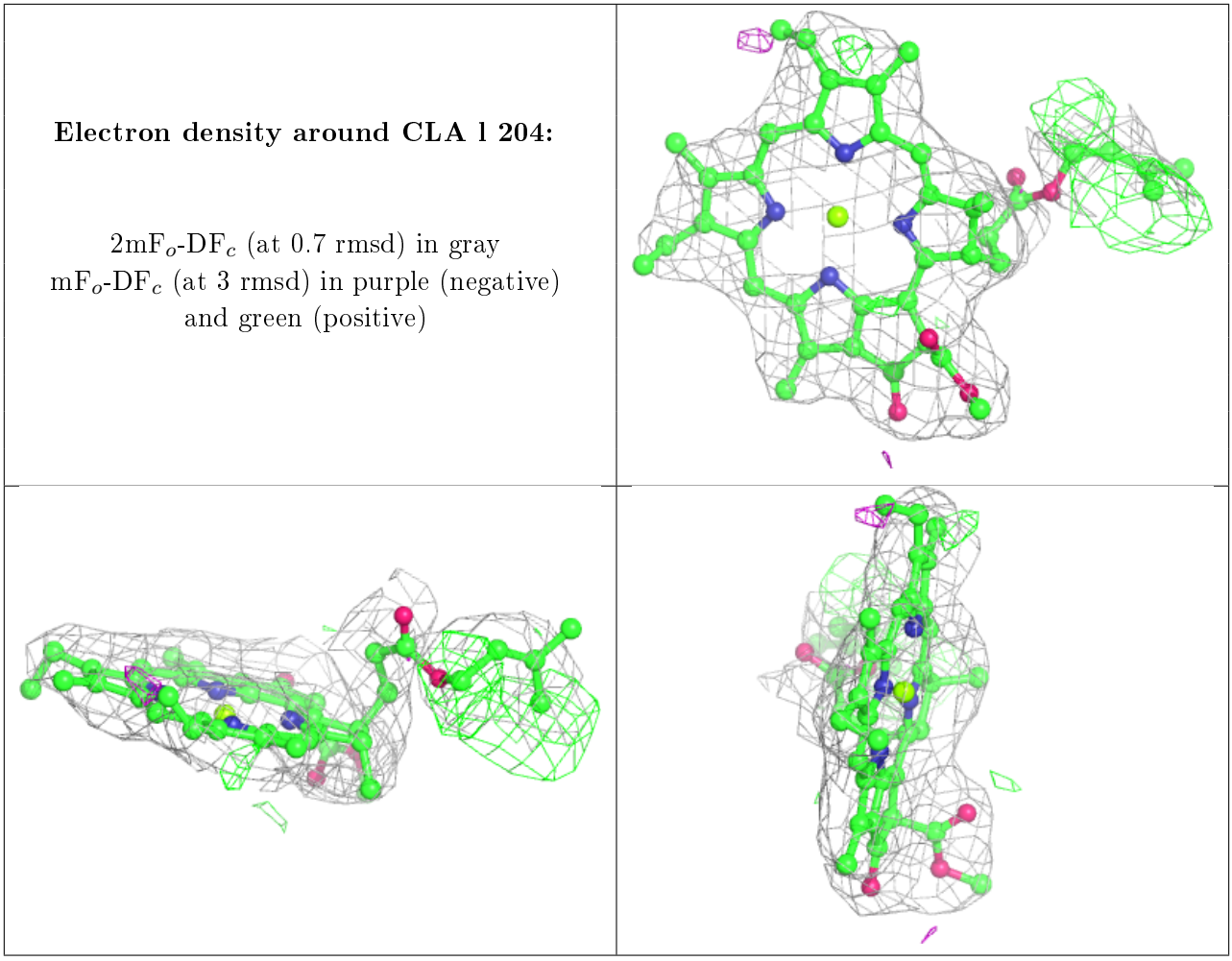
Electron density around CLA a 813:

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



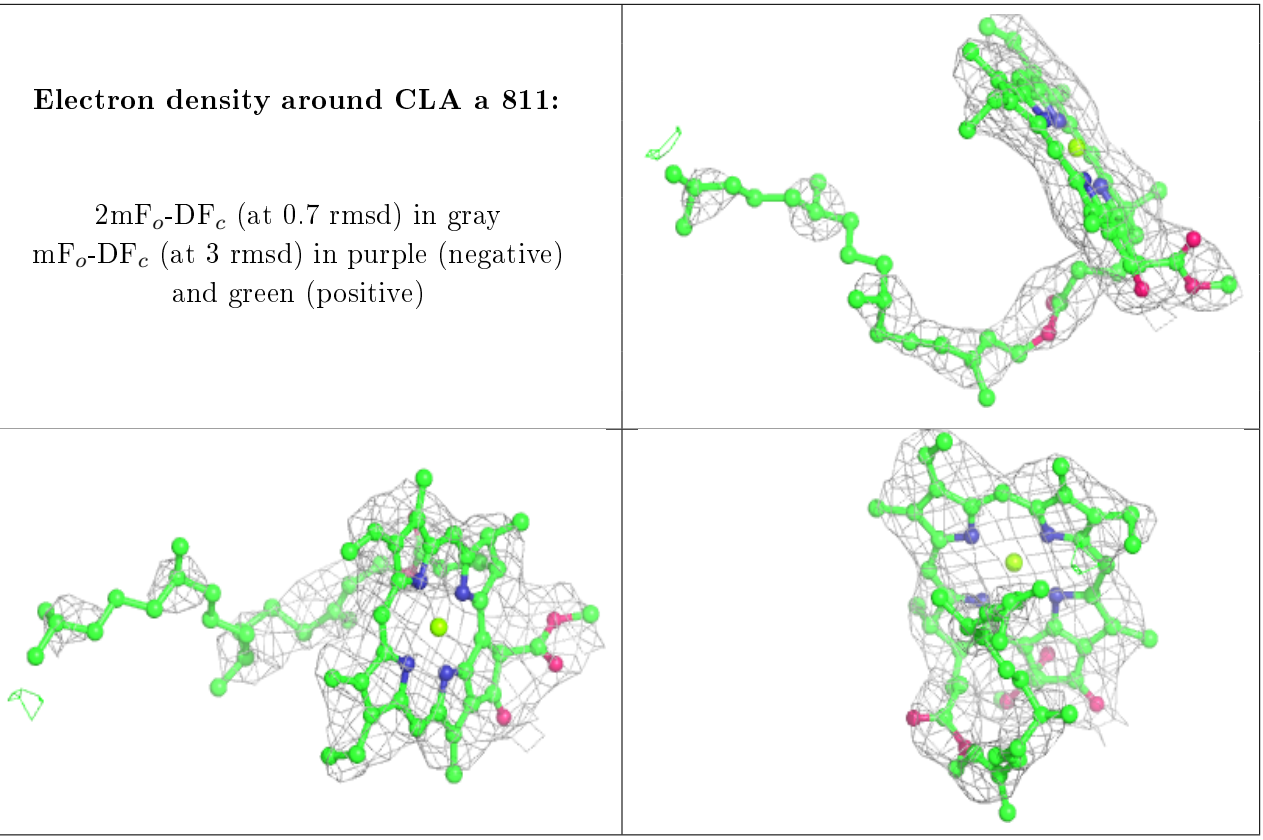
Electron density around CLA l 204:

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



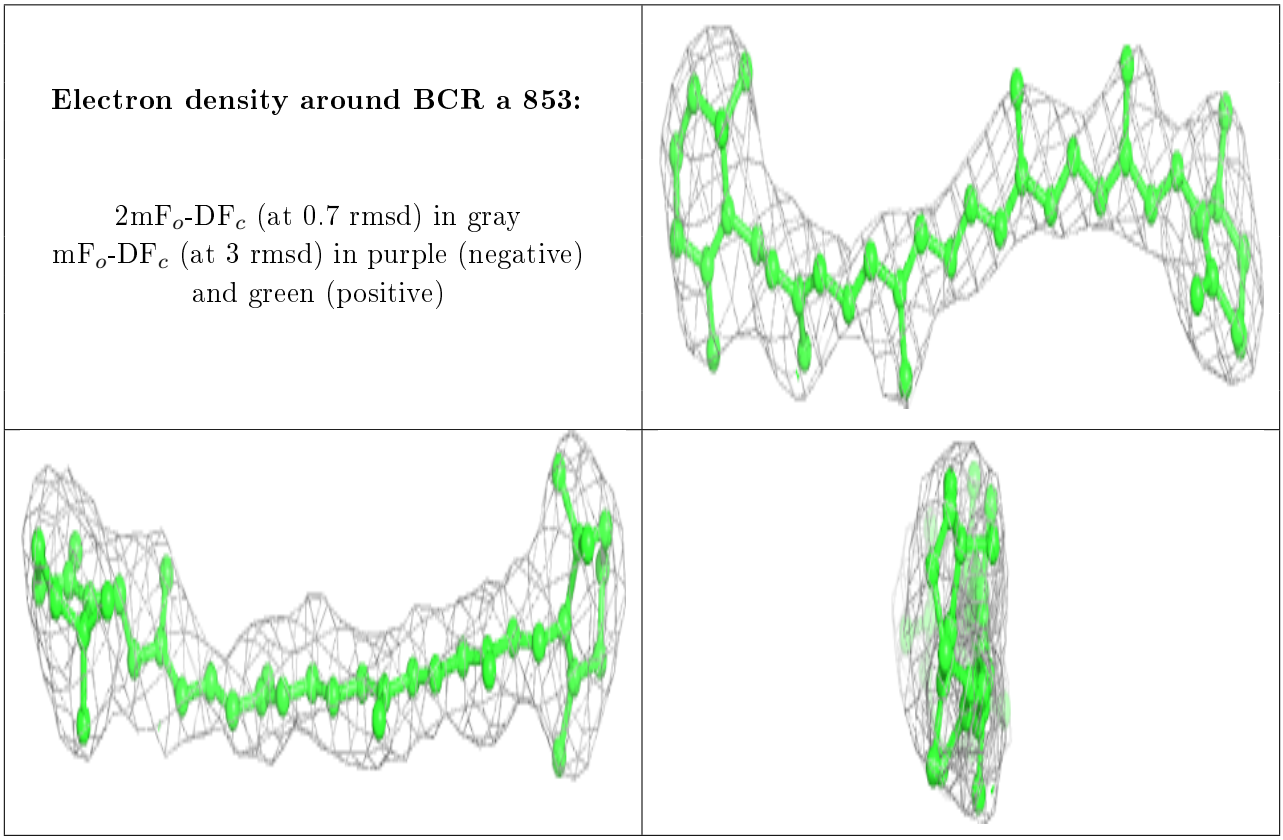
Electron density around CLA a 811:

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



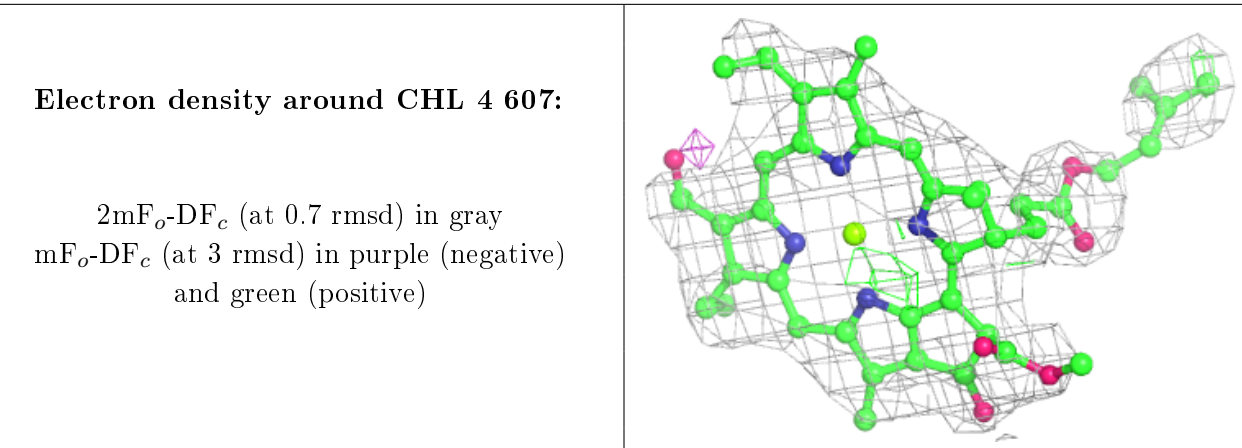
Electron density around BCR a 853:

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



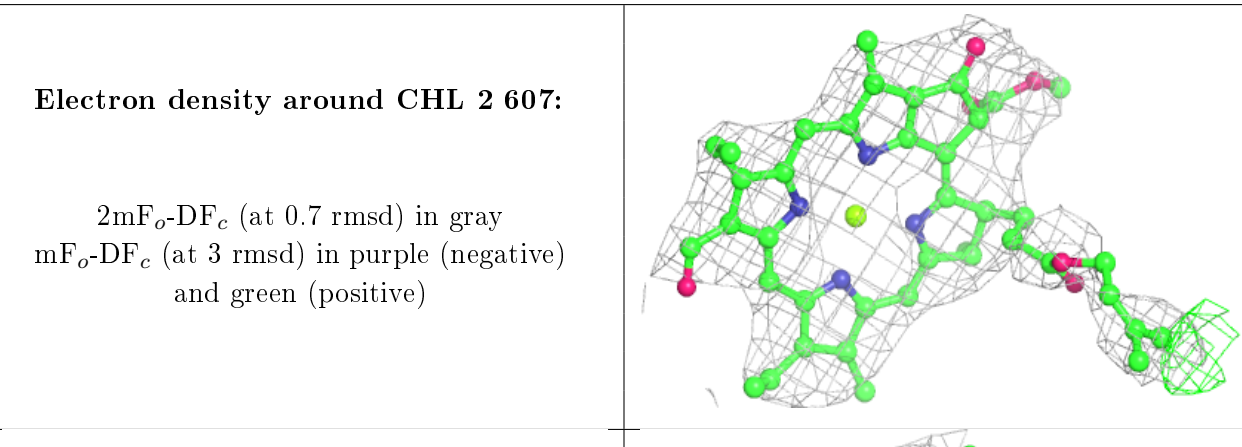
Electron density around CHL 4 607:

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



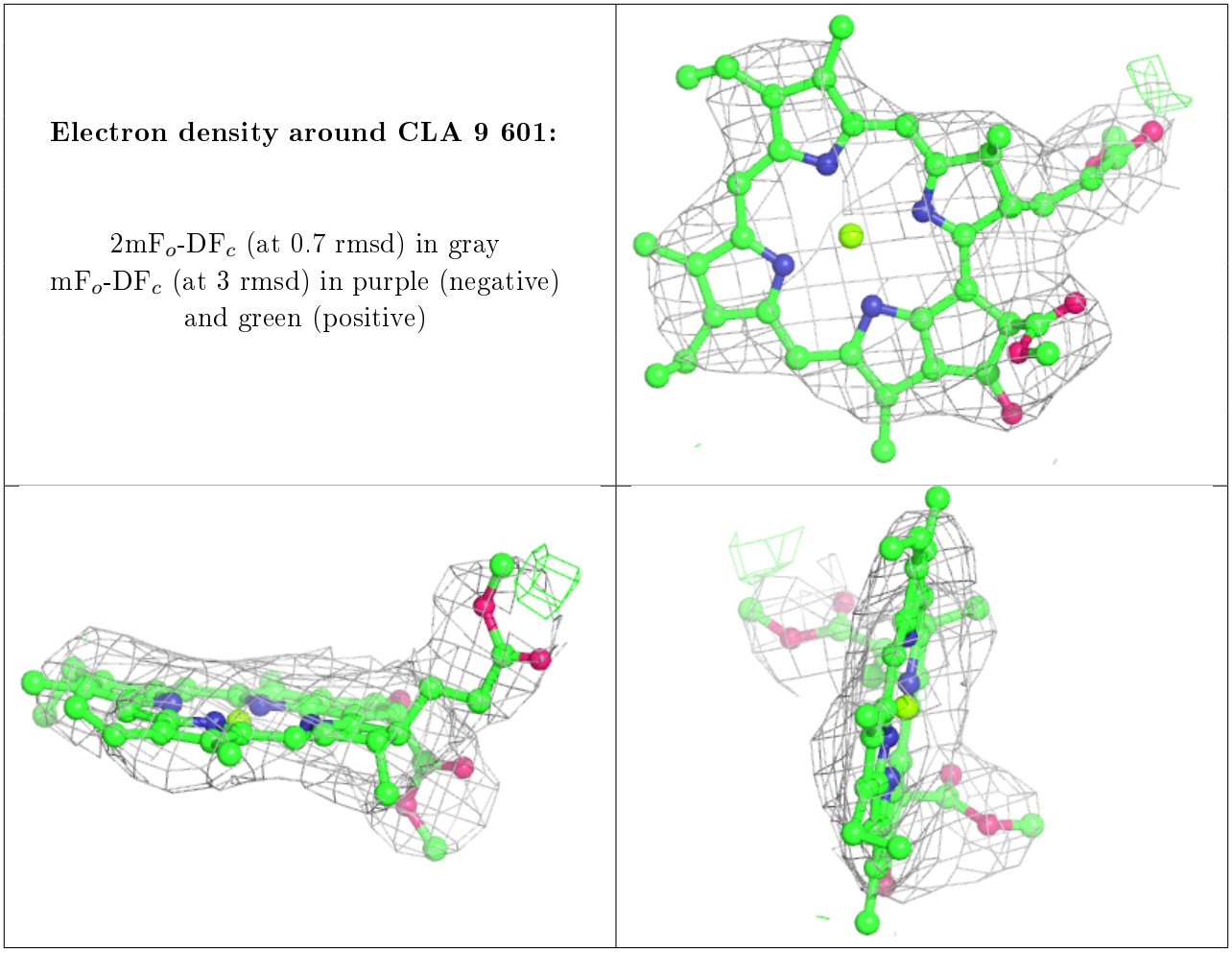
Electron density around CHL 2 607:

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



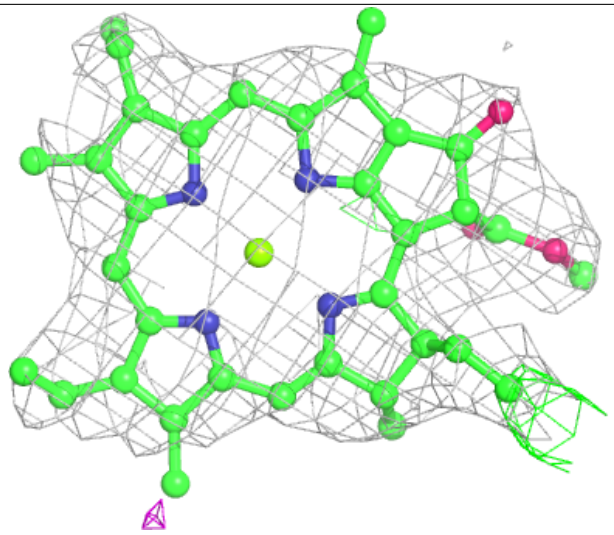
Electron density around CLA 9 601:

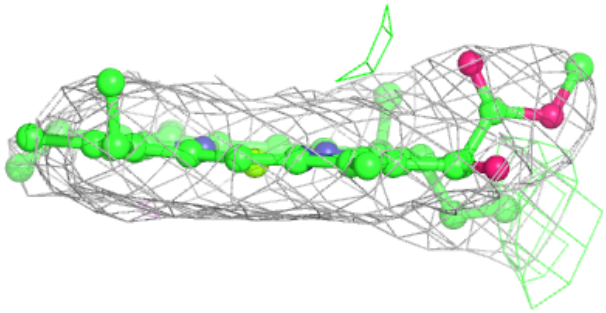
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

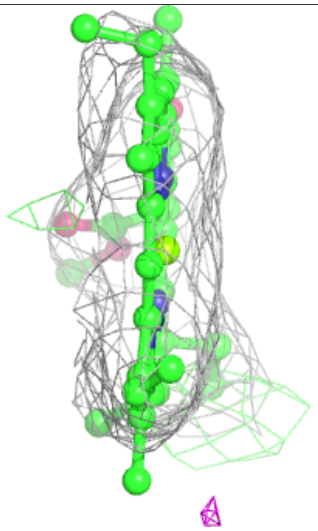


Electron density around CLA 8 304:

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

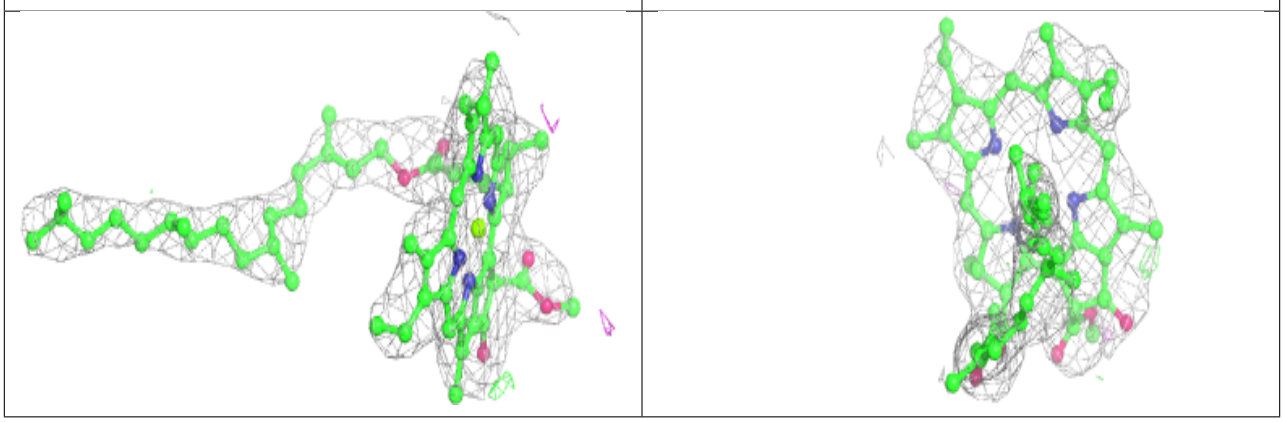






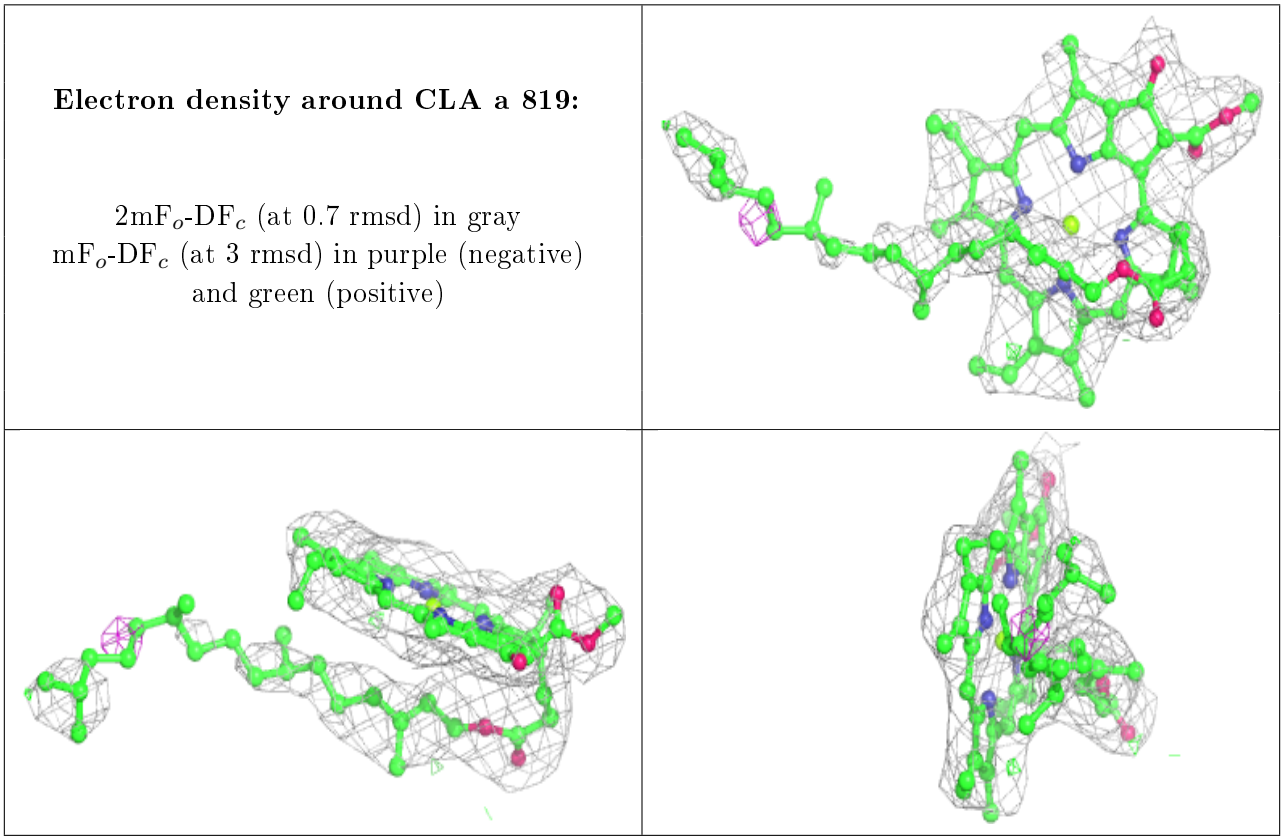
Electron density around CLA b 829:

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



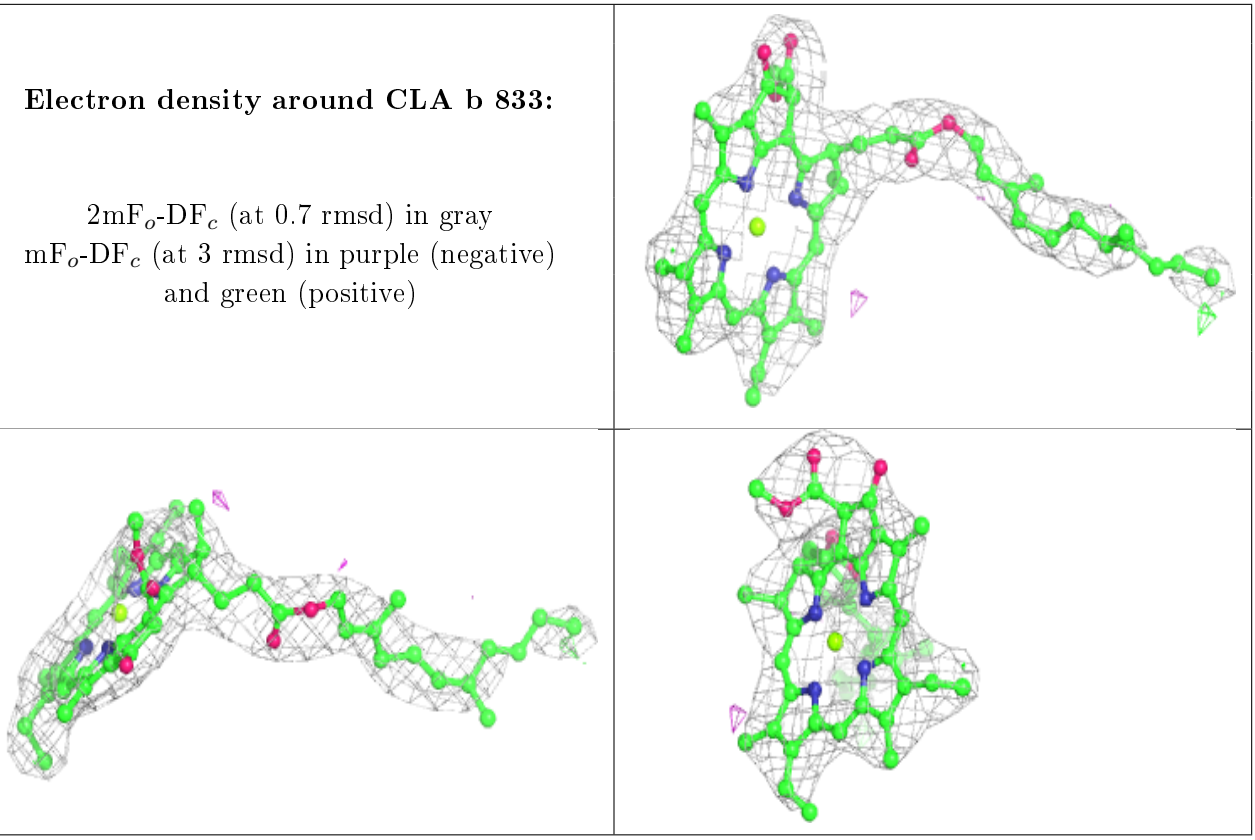
Electron density around CLA a 819:

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



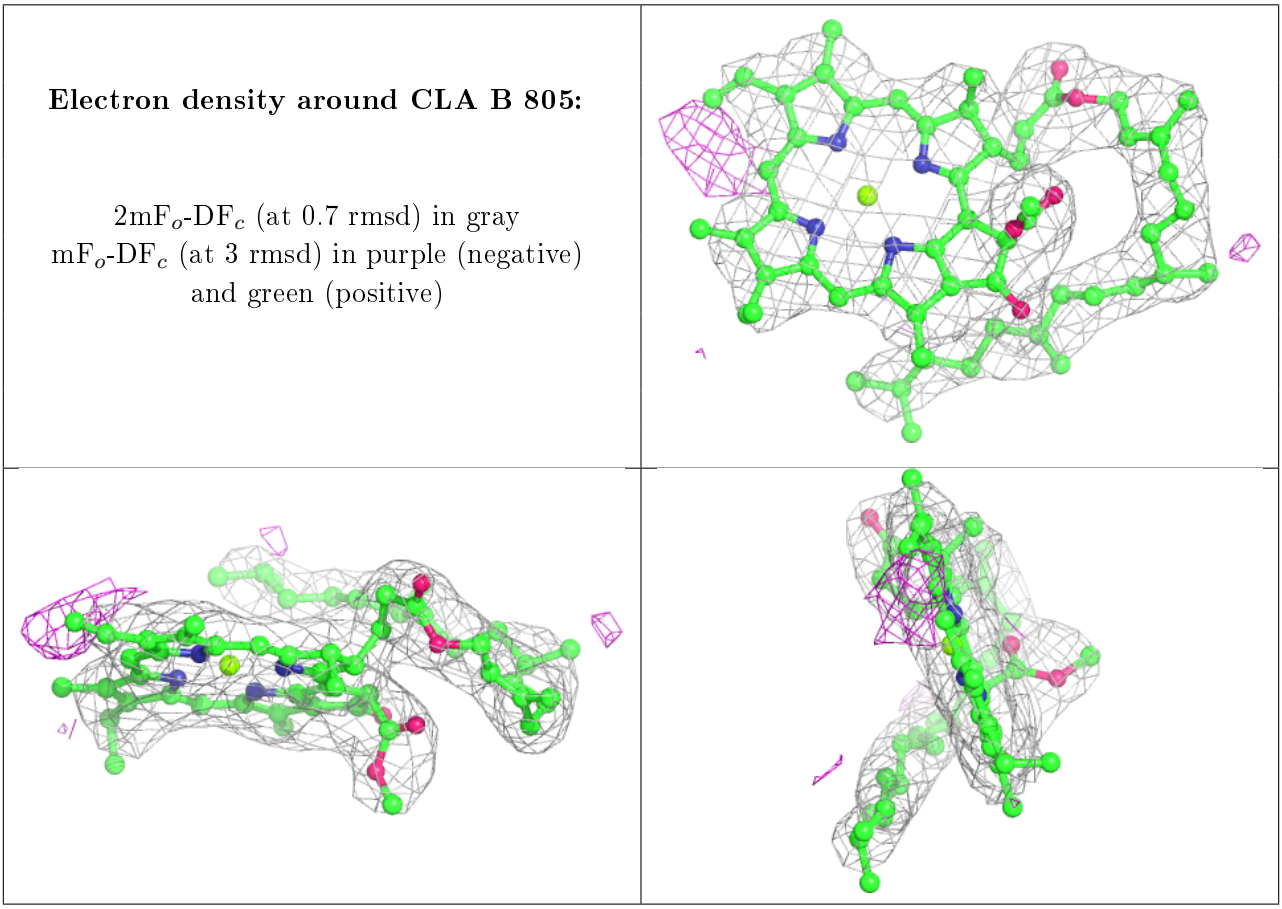
Electron density around CLA b 833:

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



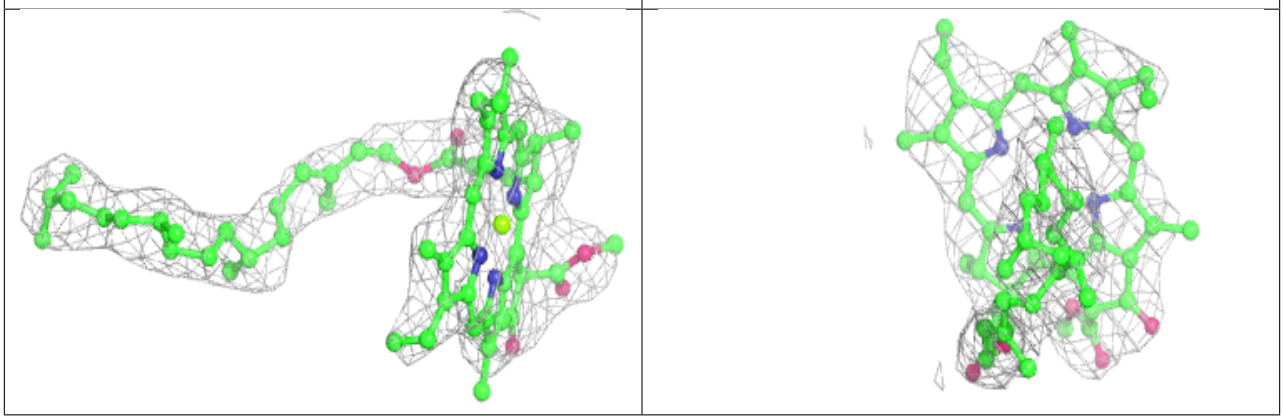
Electron density around CLA B 805:

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



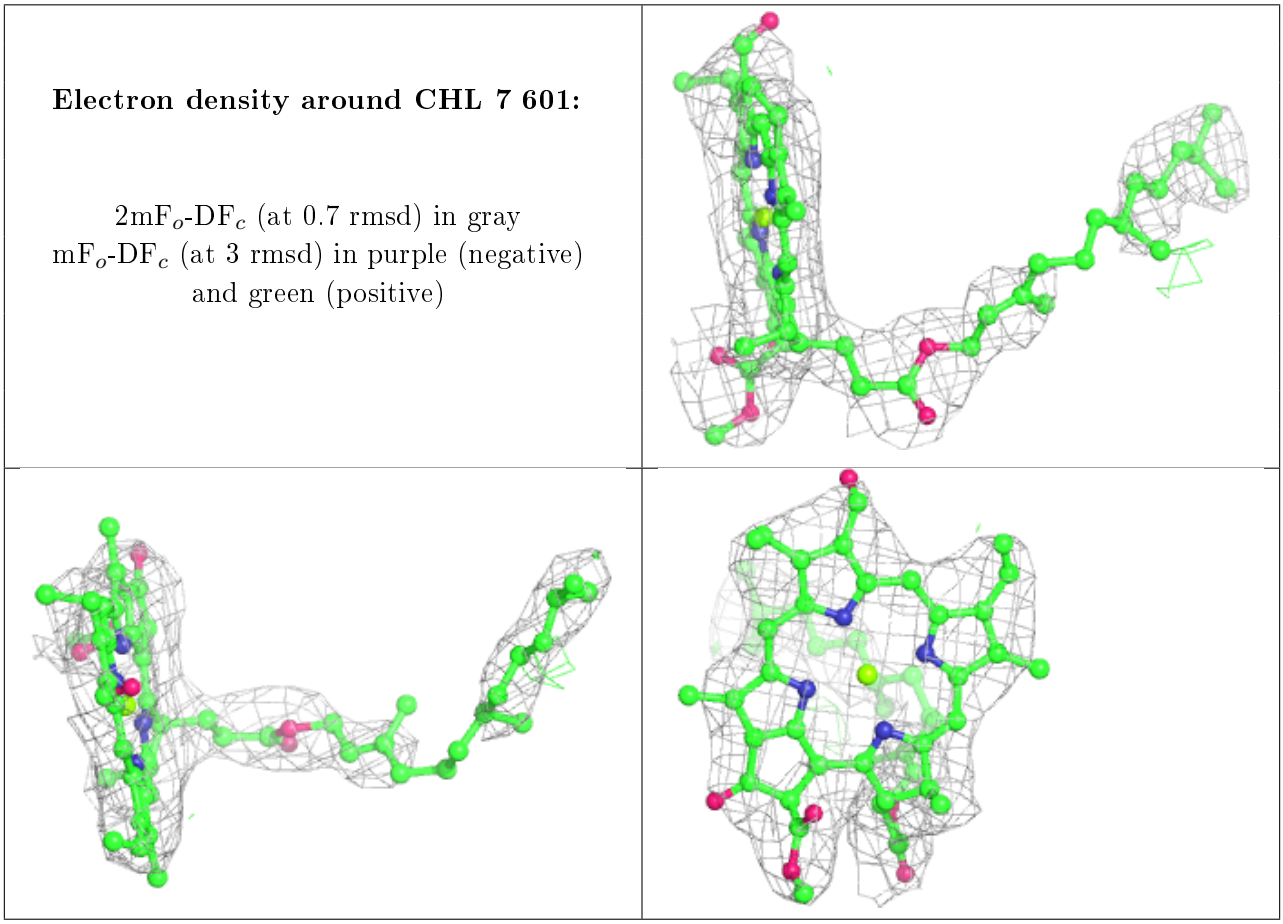
Electron density around CLA A 831:

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



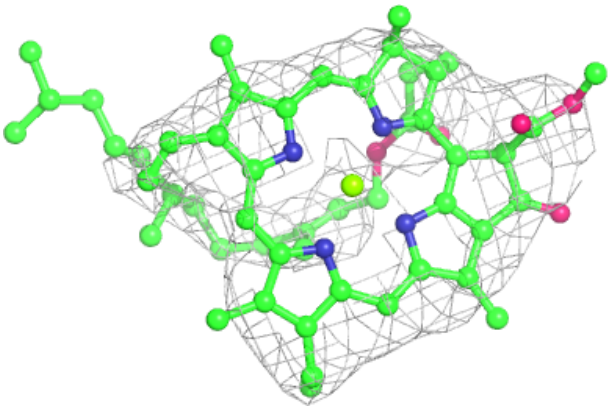
Electron density around CHL 7 601:

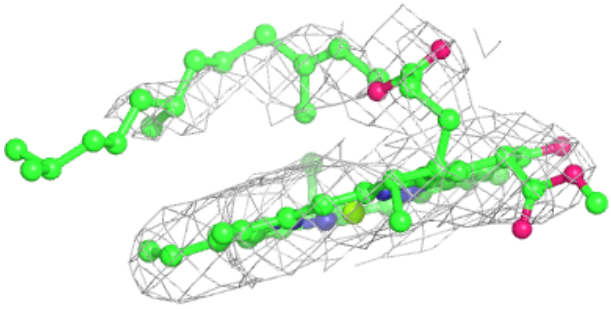
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

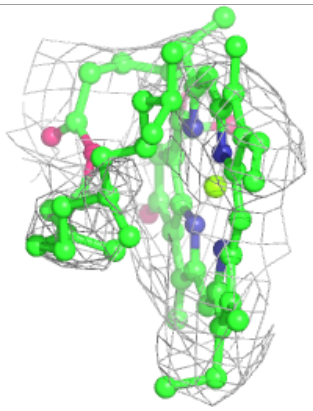


Electron density around CLA 6 314:

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

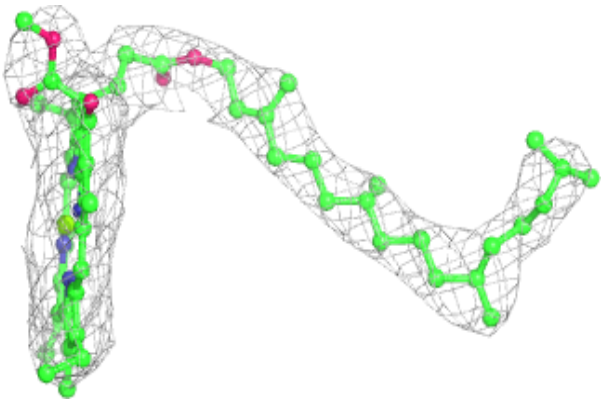


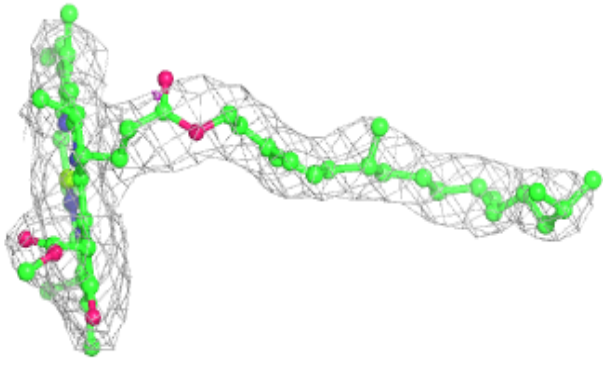


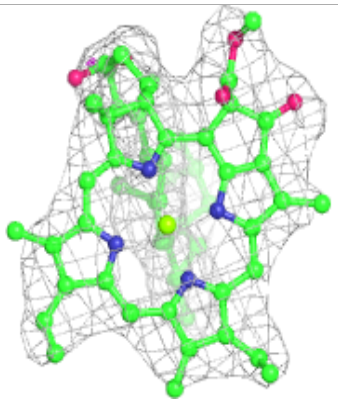


Electron density around CLA B 840:

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

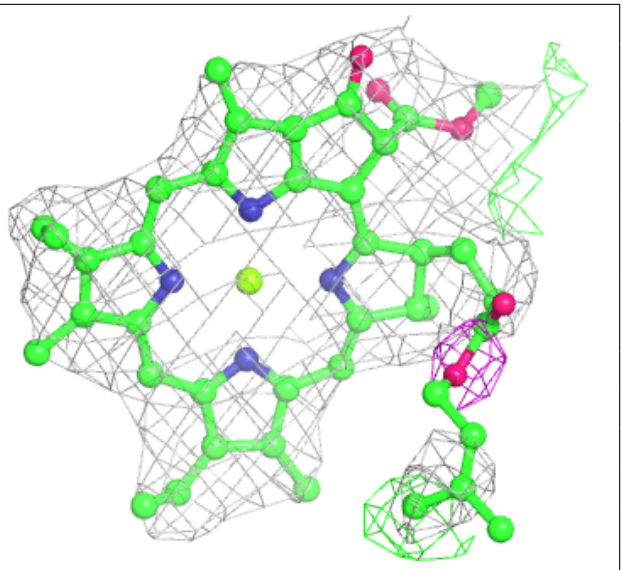


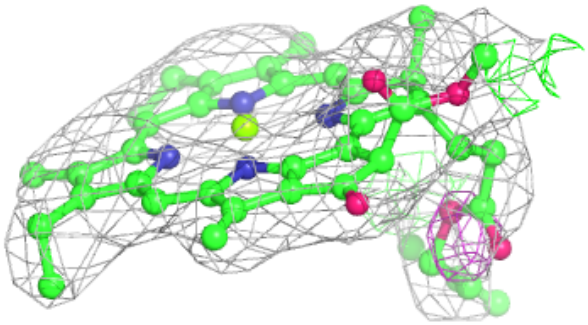


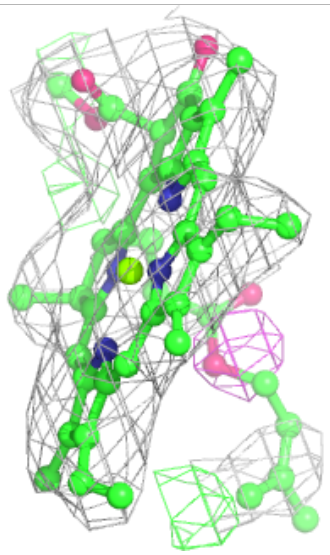


Electron density around CLA a 816:

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

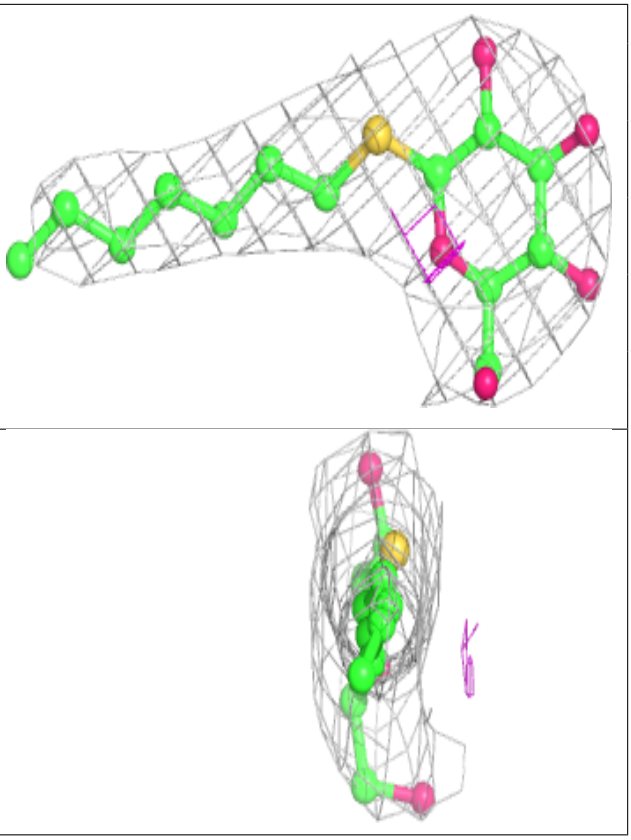






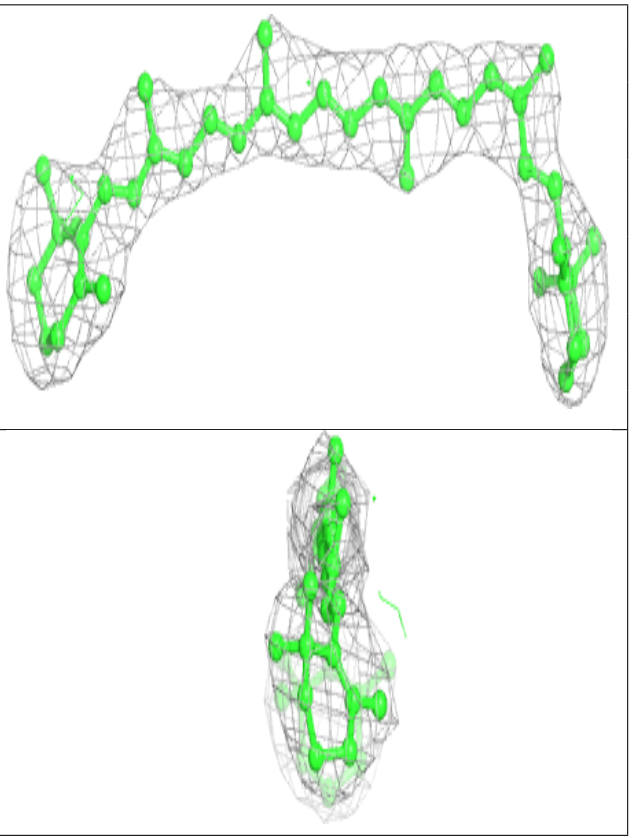
Electron density around HTG a 857:

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



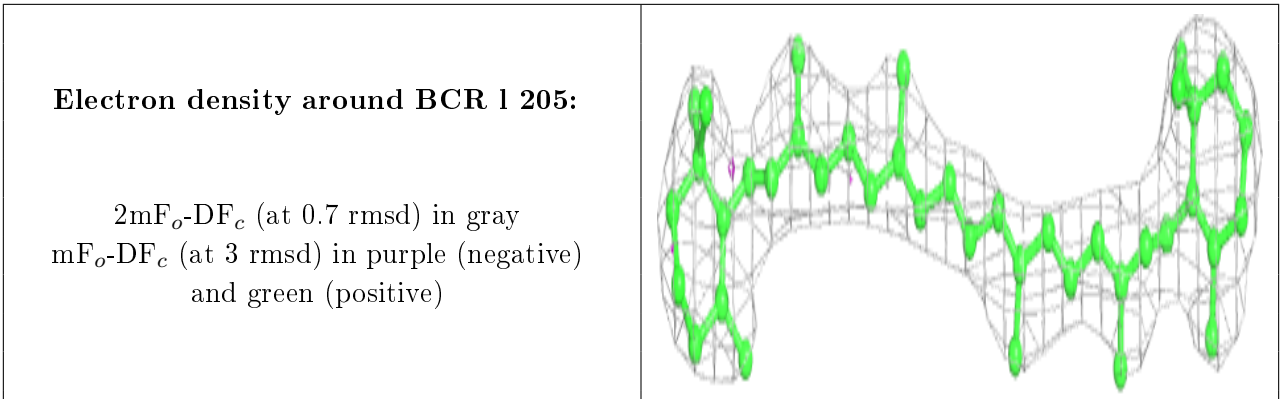
Electron density around BCR l 201:

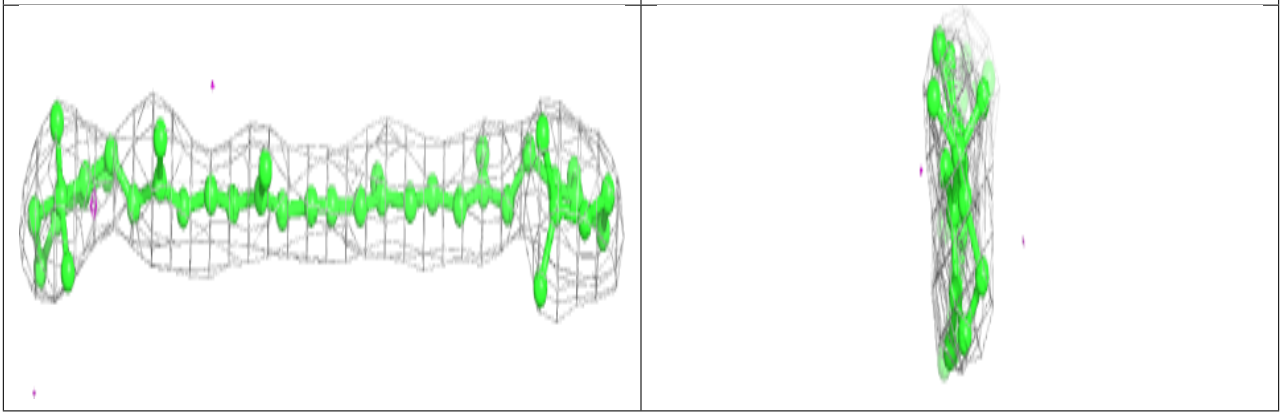
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



Electron density around BCR l 205:

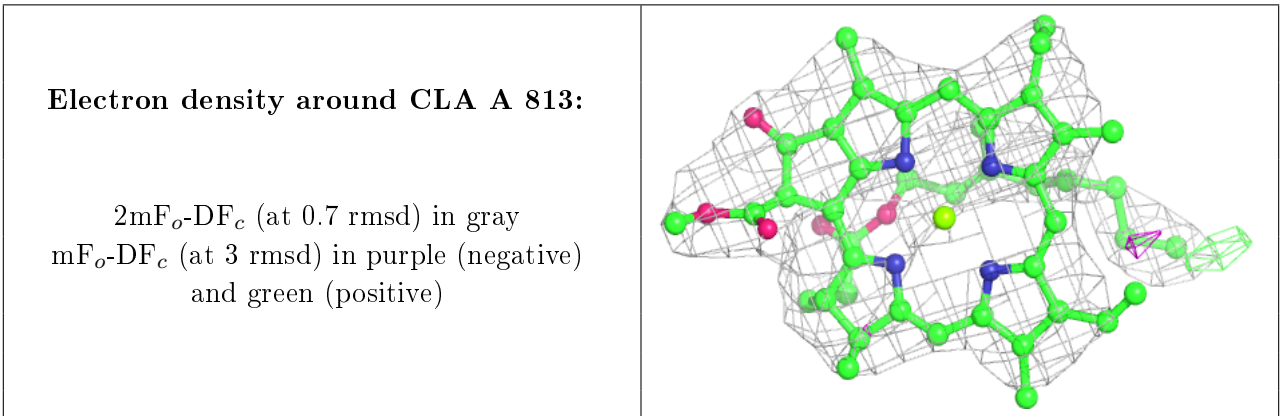
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

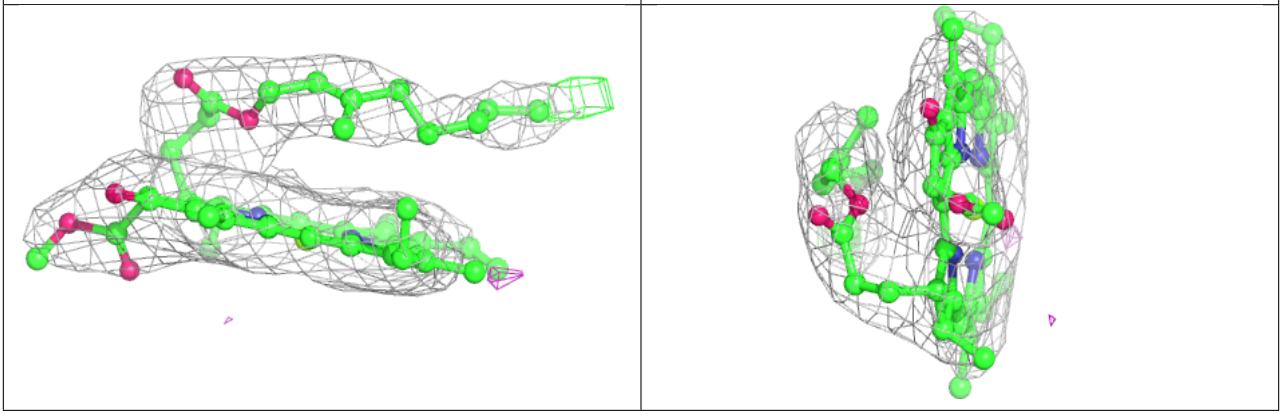




Electron density around CLA A 813:

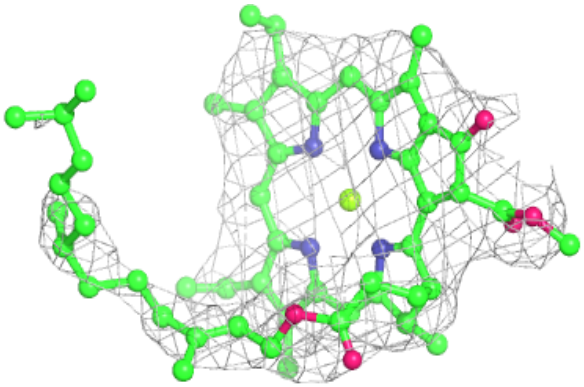
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

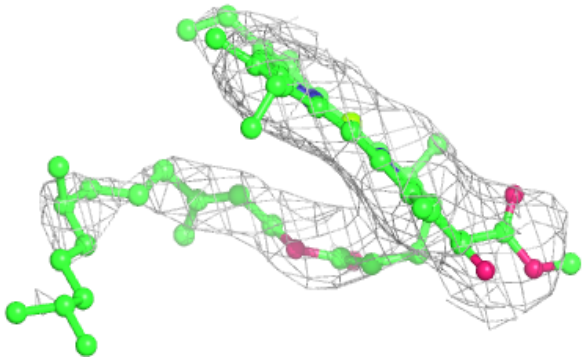


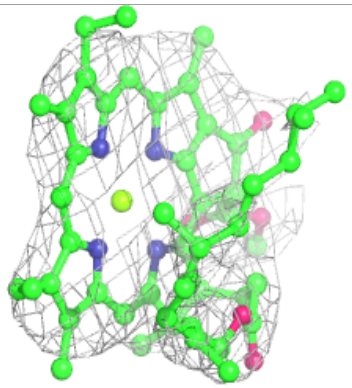


Electron density around CLA 7 609:

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

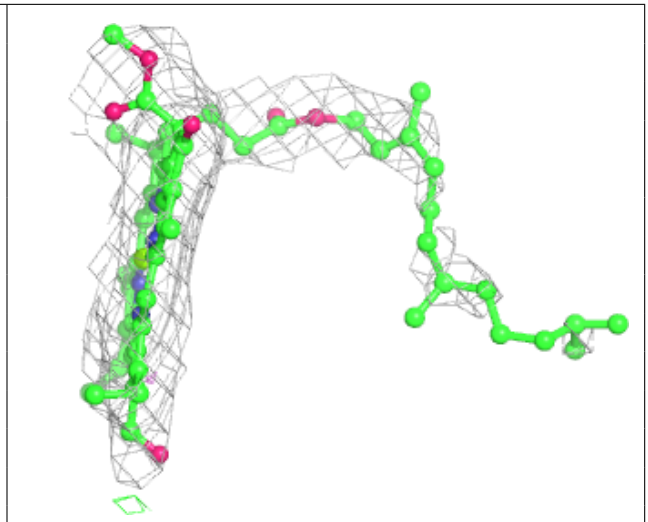


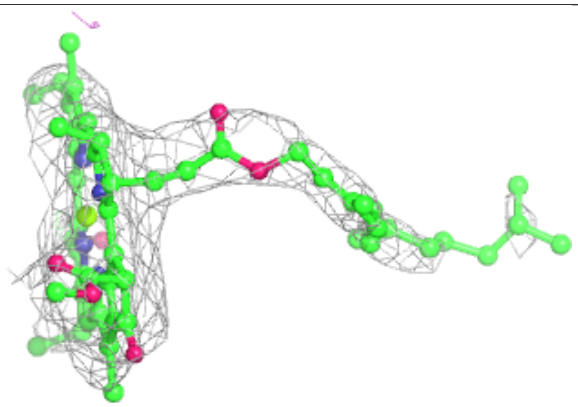


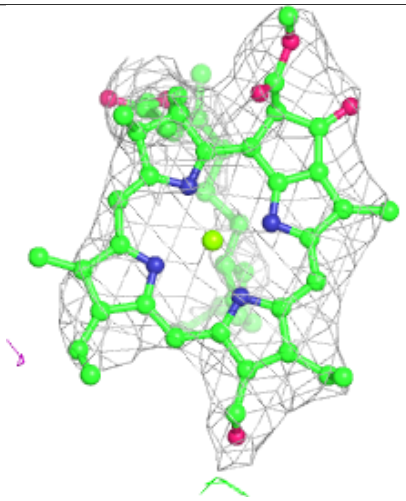


Electron density around CHL 6 303:

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

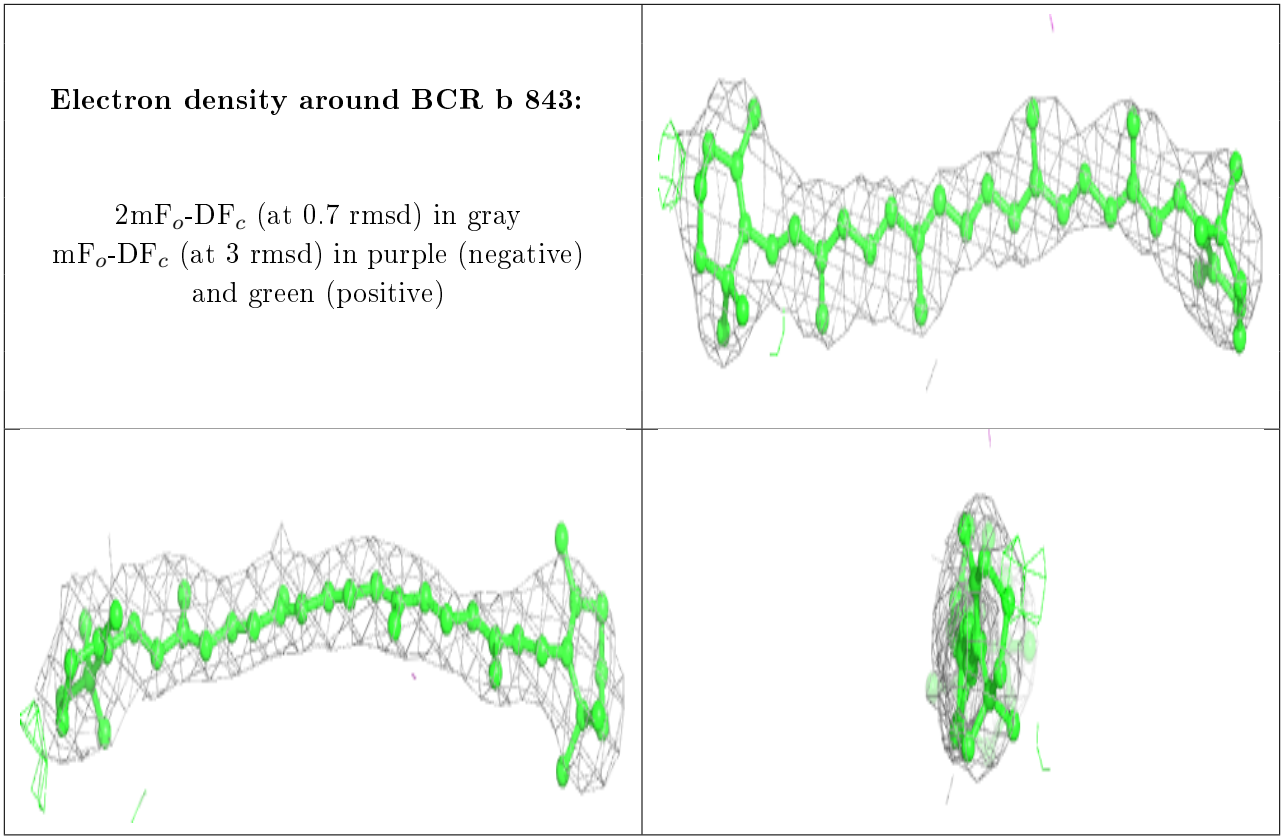






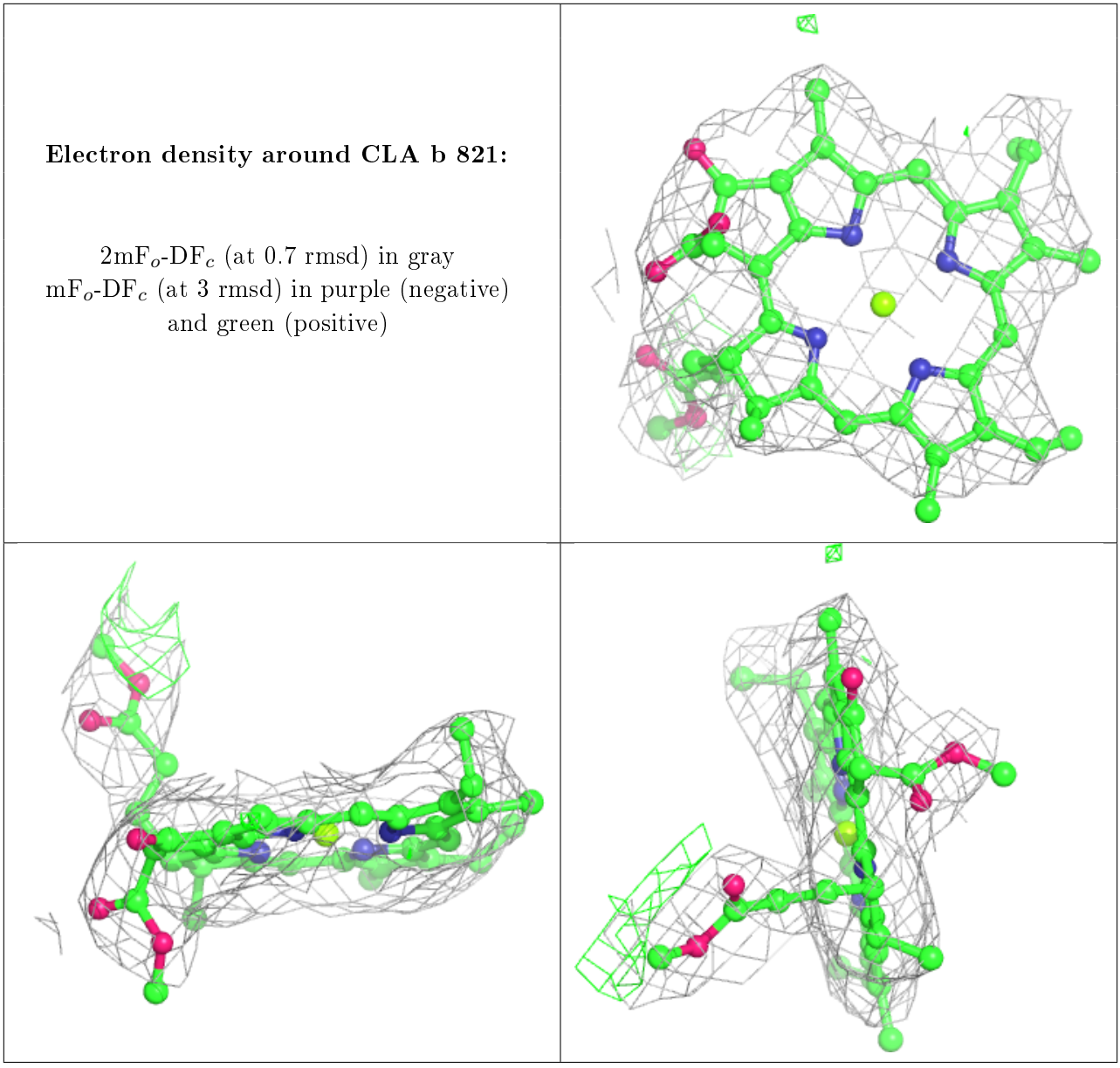
Electron density around BCR b 843:

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



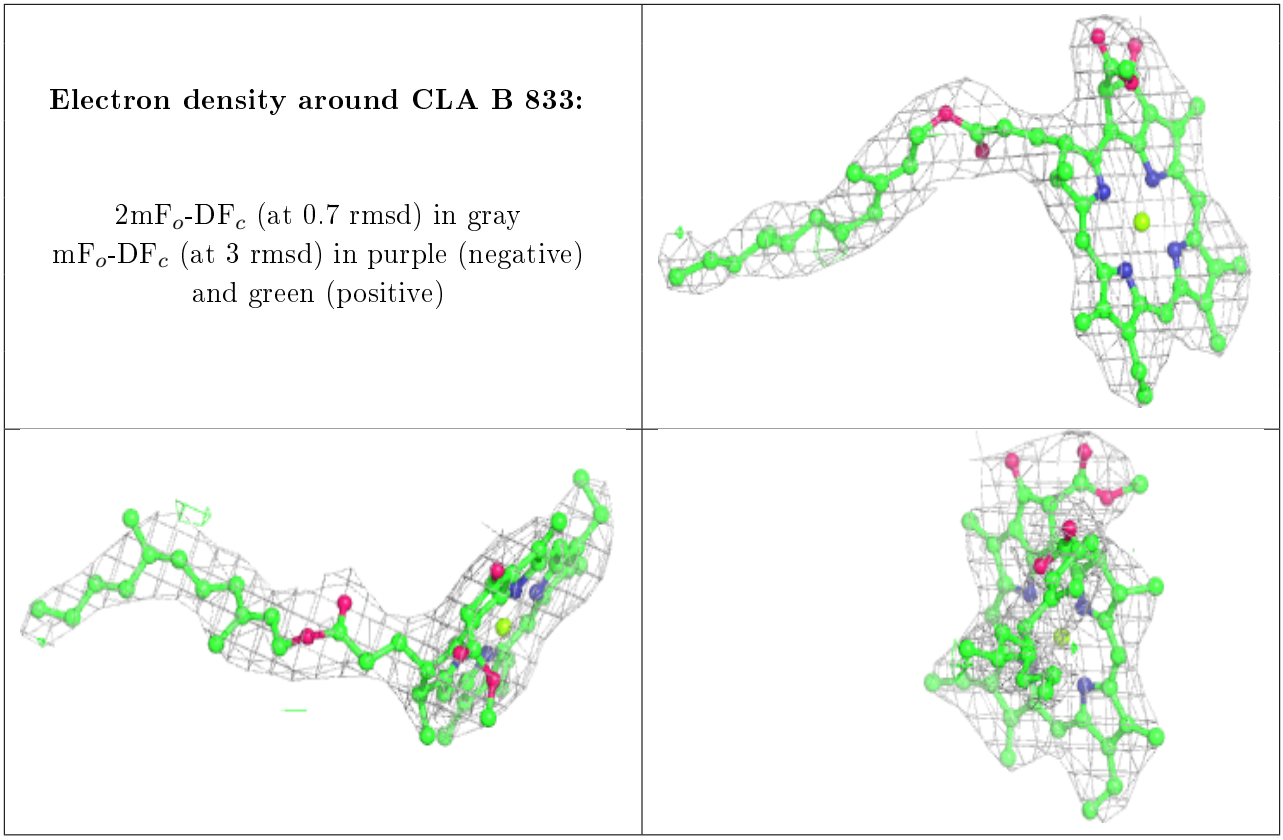
Electron density around CLA b 821:

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



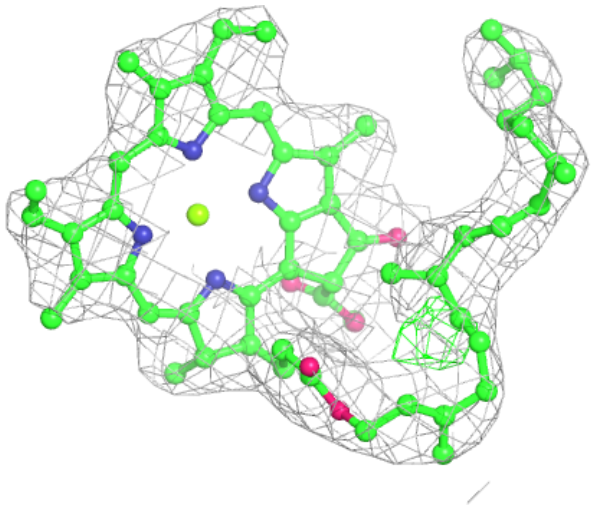
Electron density around CLA B 833:

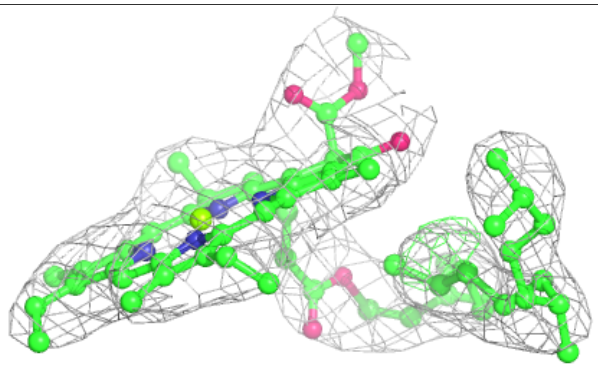
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

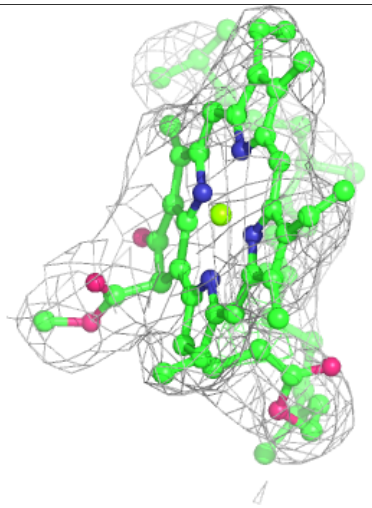


Electron density around CLA b 832:

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

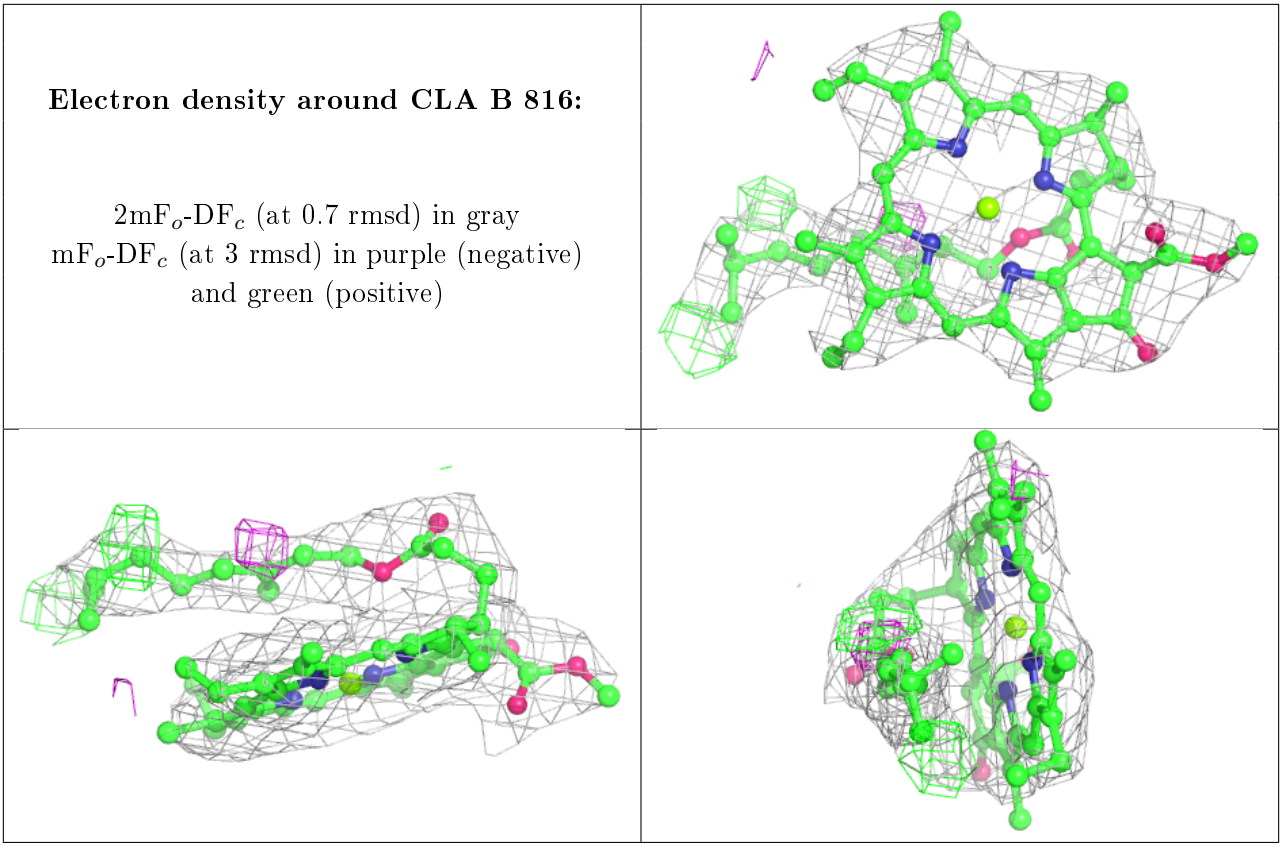






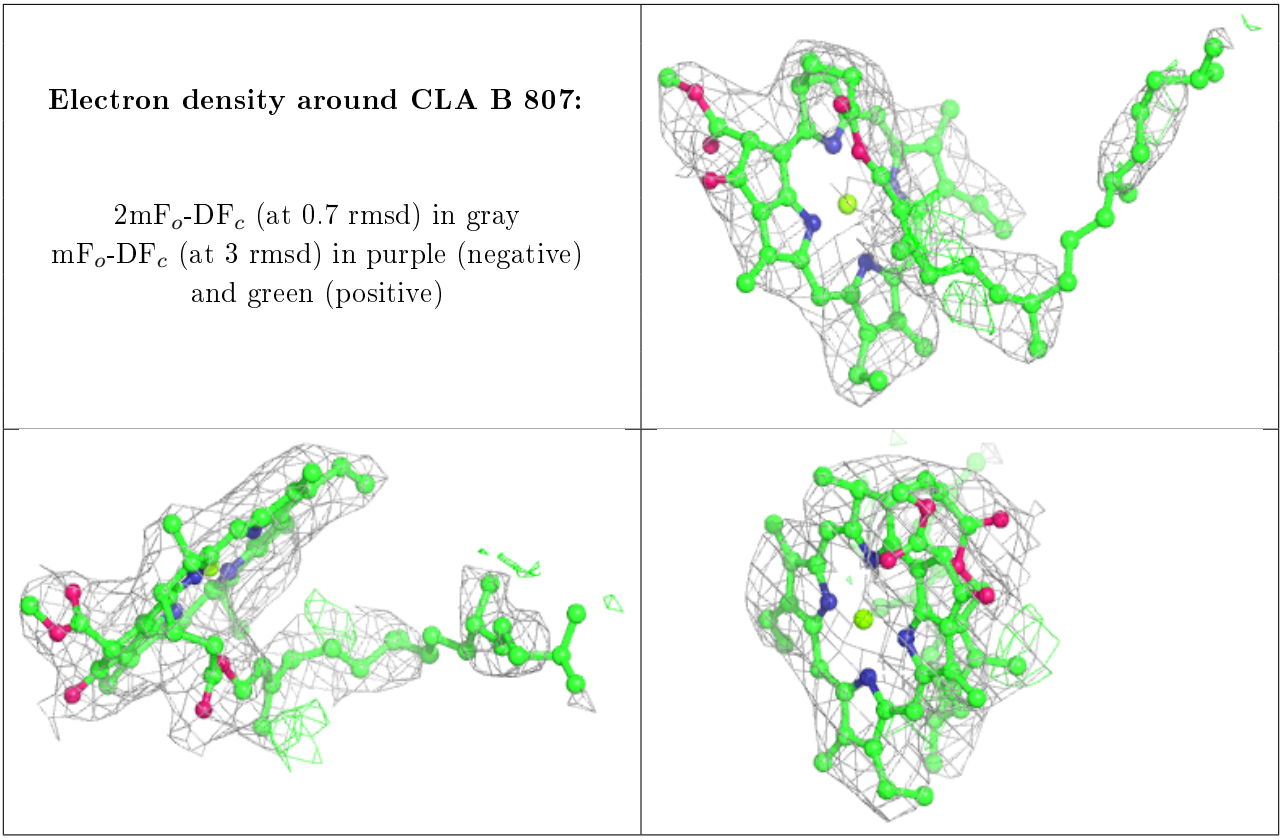
Electron density around CLA B 816:

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



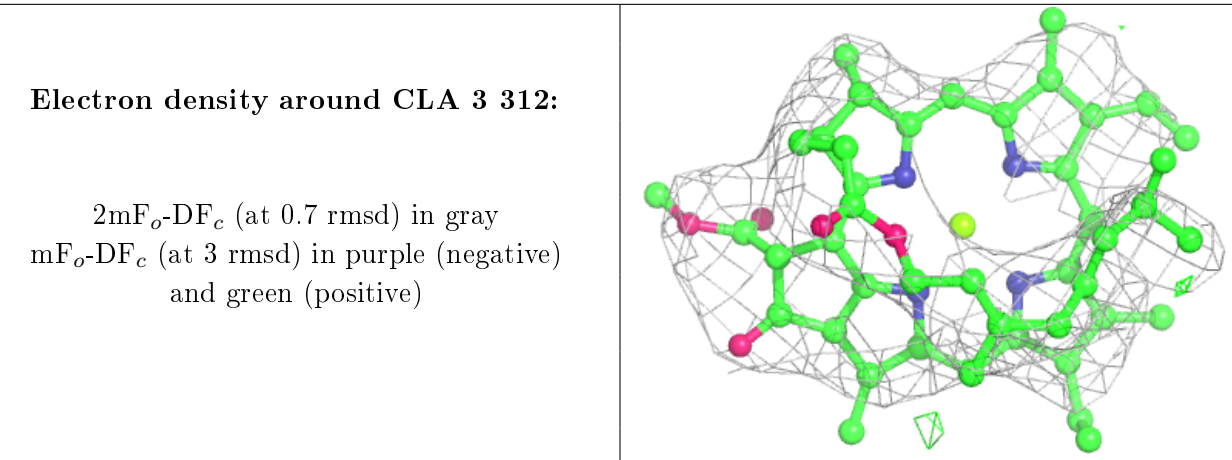
Electron density around CLA B 807:

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



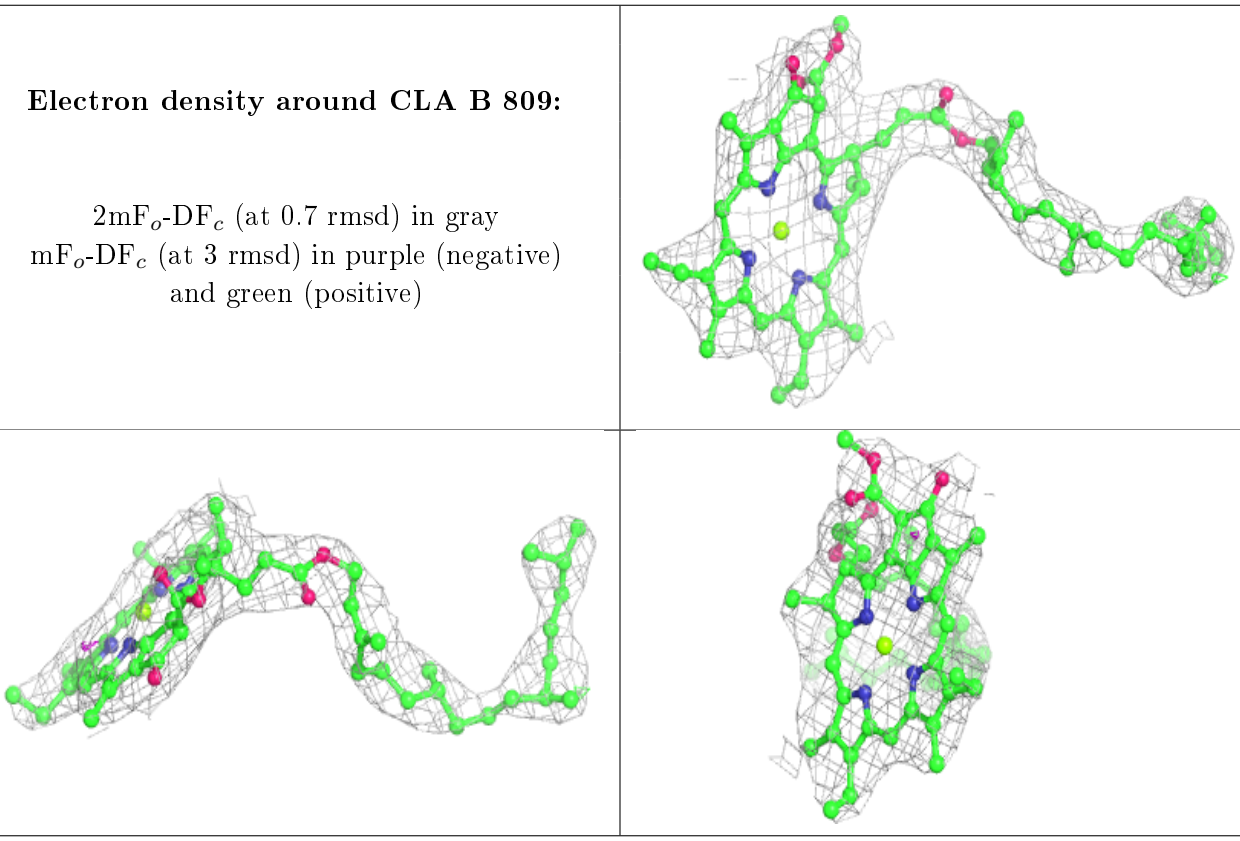
Electron density around CLA 3 312:

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



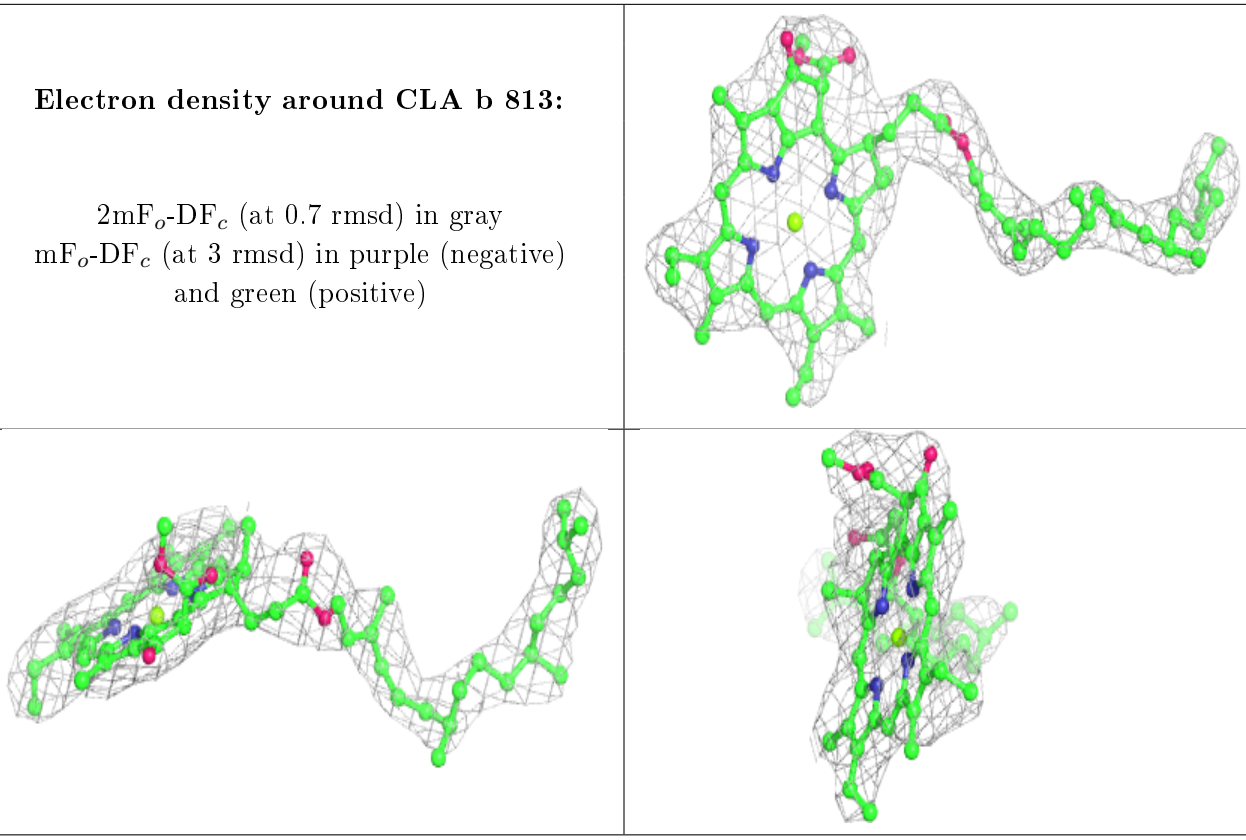
Electron density around CLA B 809:

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



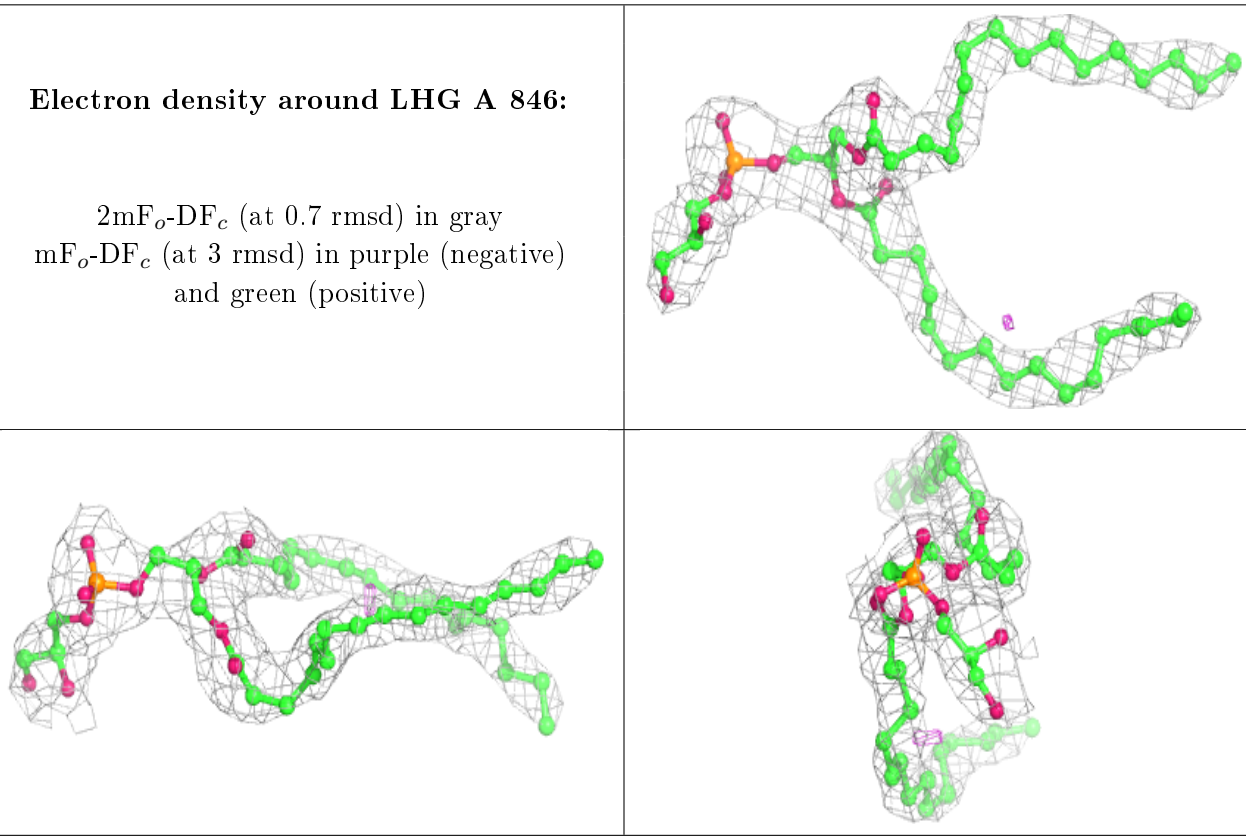
Electron density around CLA b 813:

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



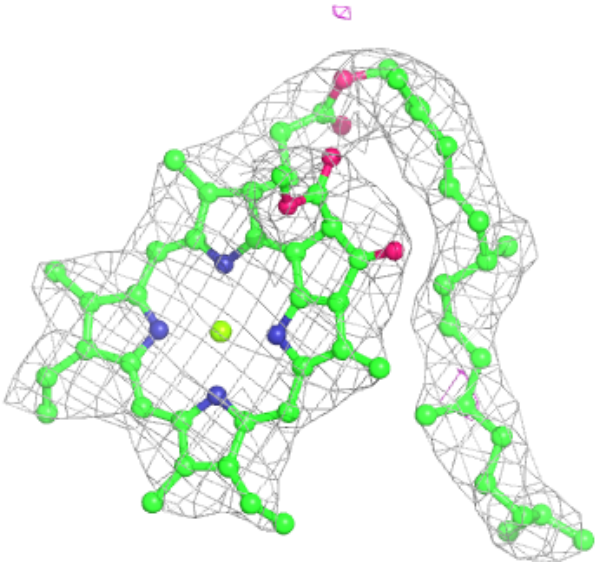
Electron density around LHG A 846:

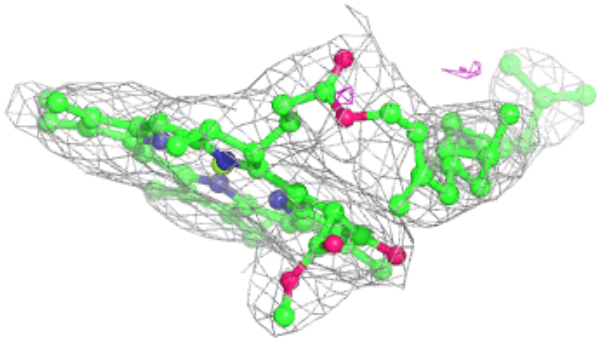
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

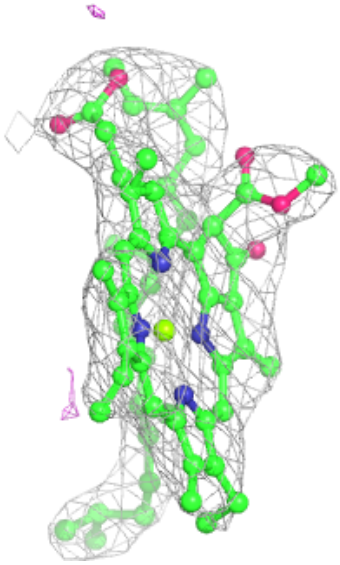


Electron density around CLA a 826:

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

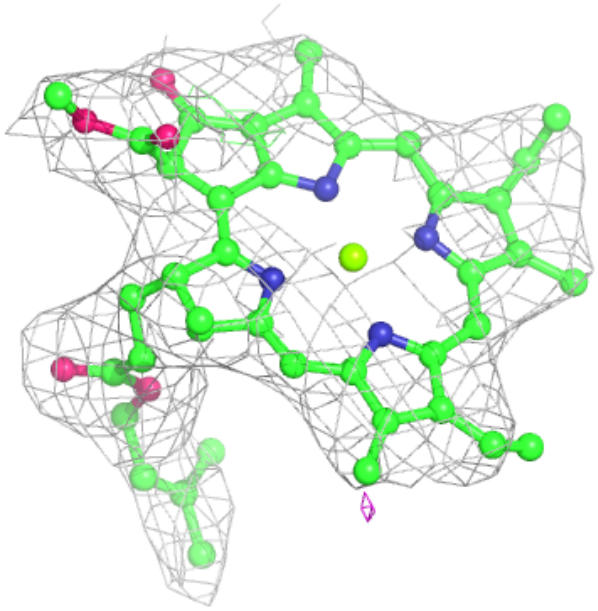


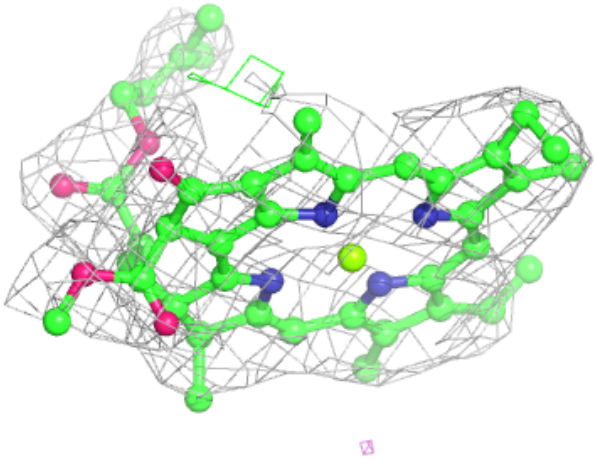


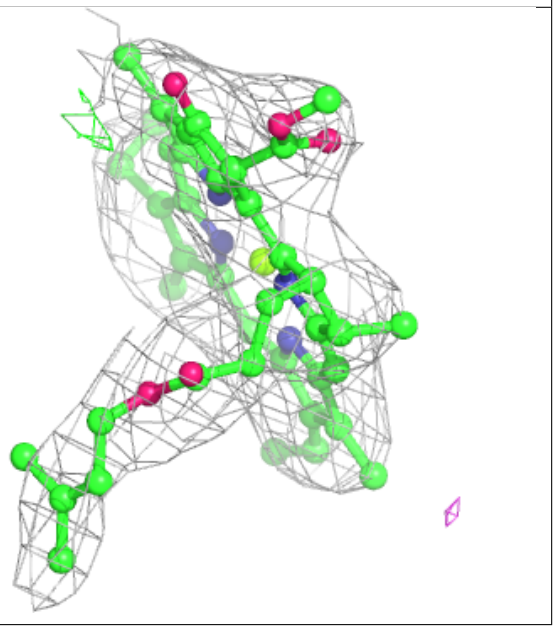


Electron density around CLA 4 608:

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

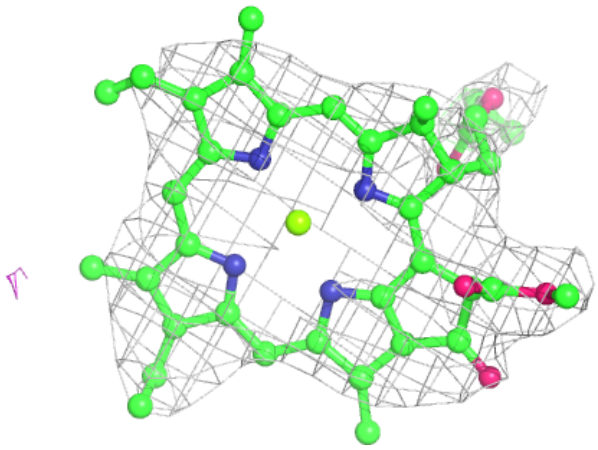


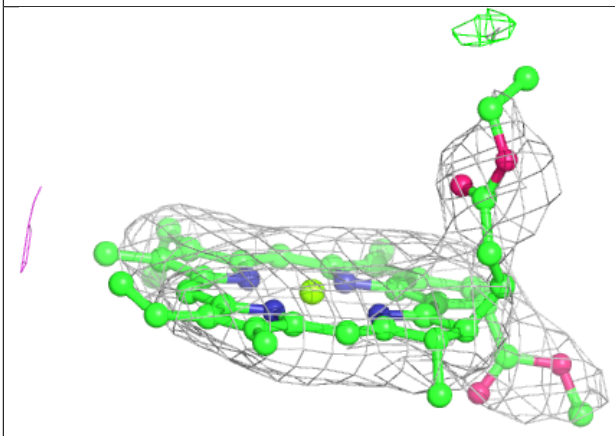


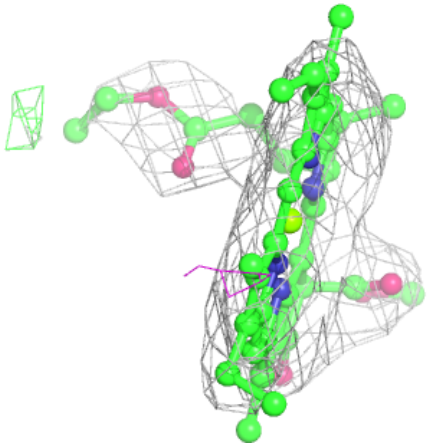


Electron density around CLA 3 306:

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

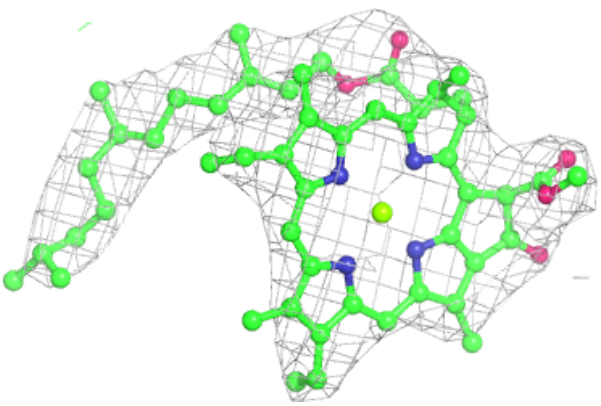


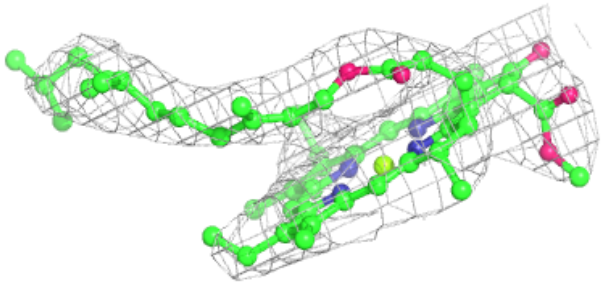


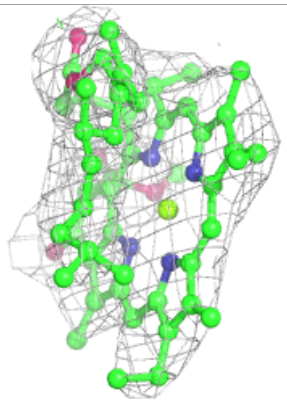


Electron density around CLA 9 602:

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

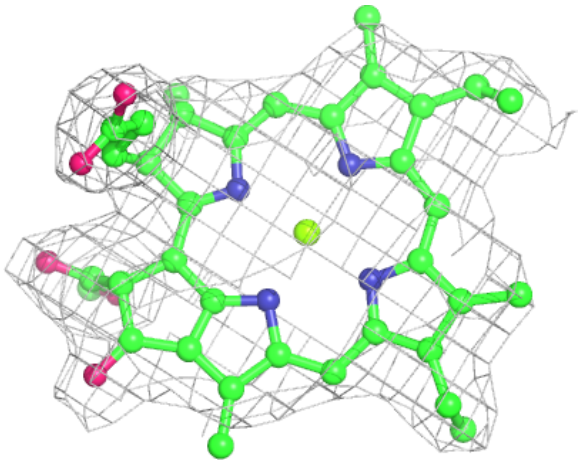


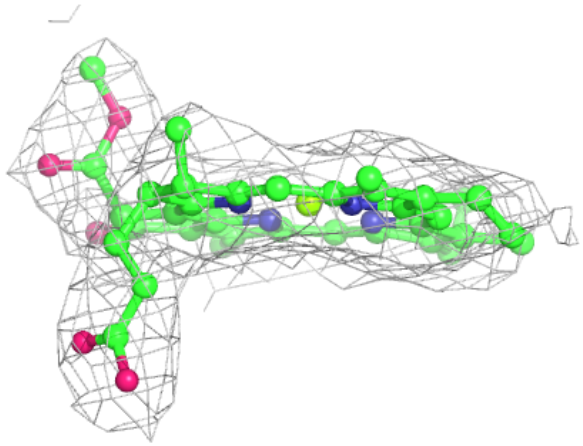


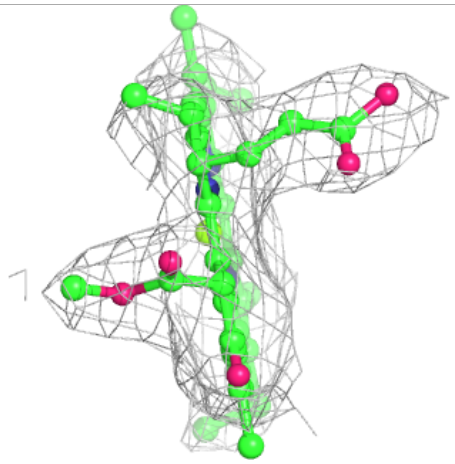


Electron density around CLA a 815:

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

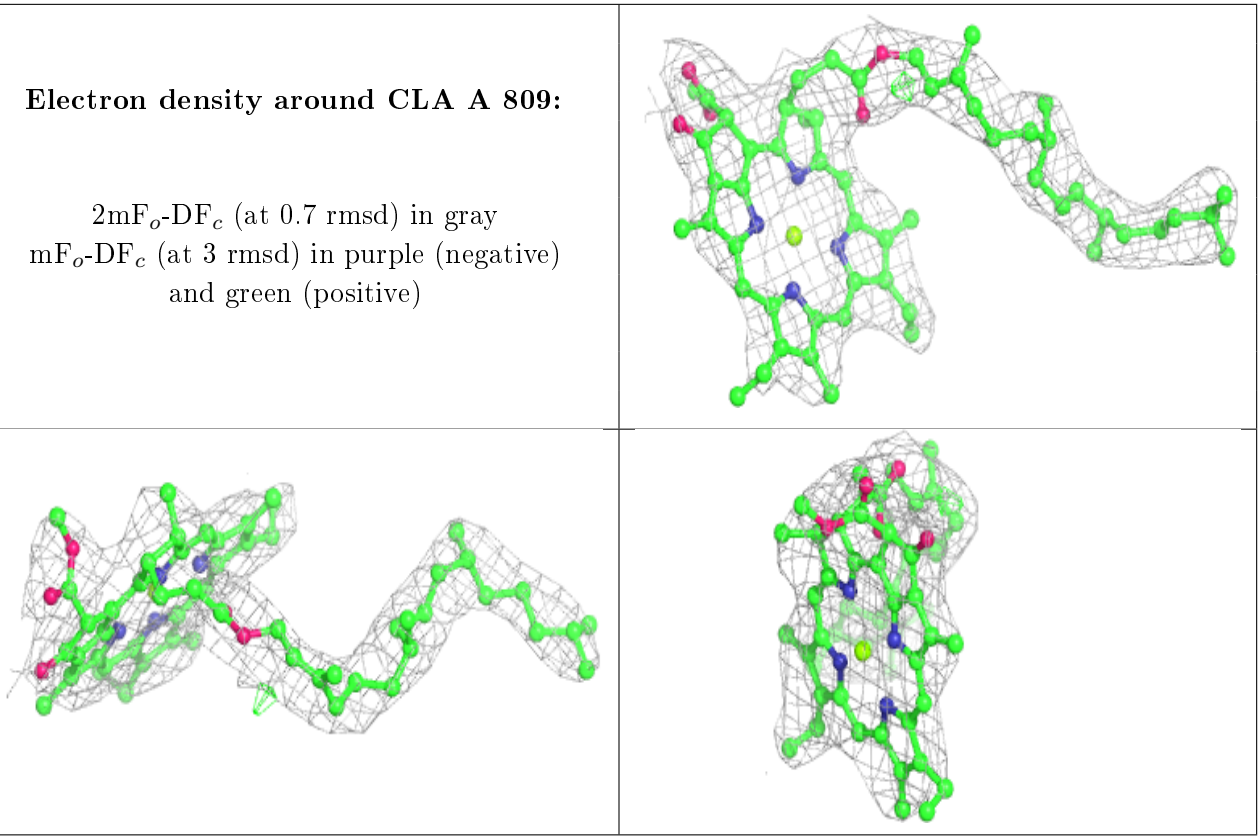






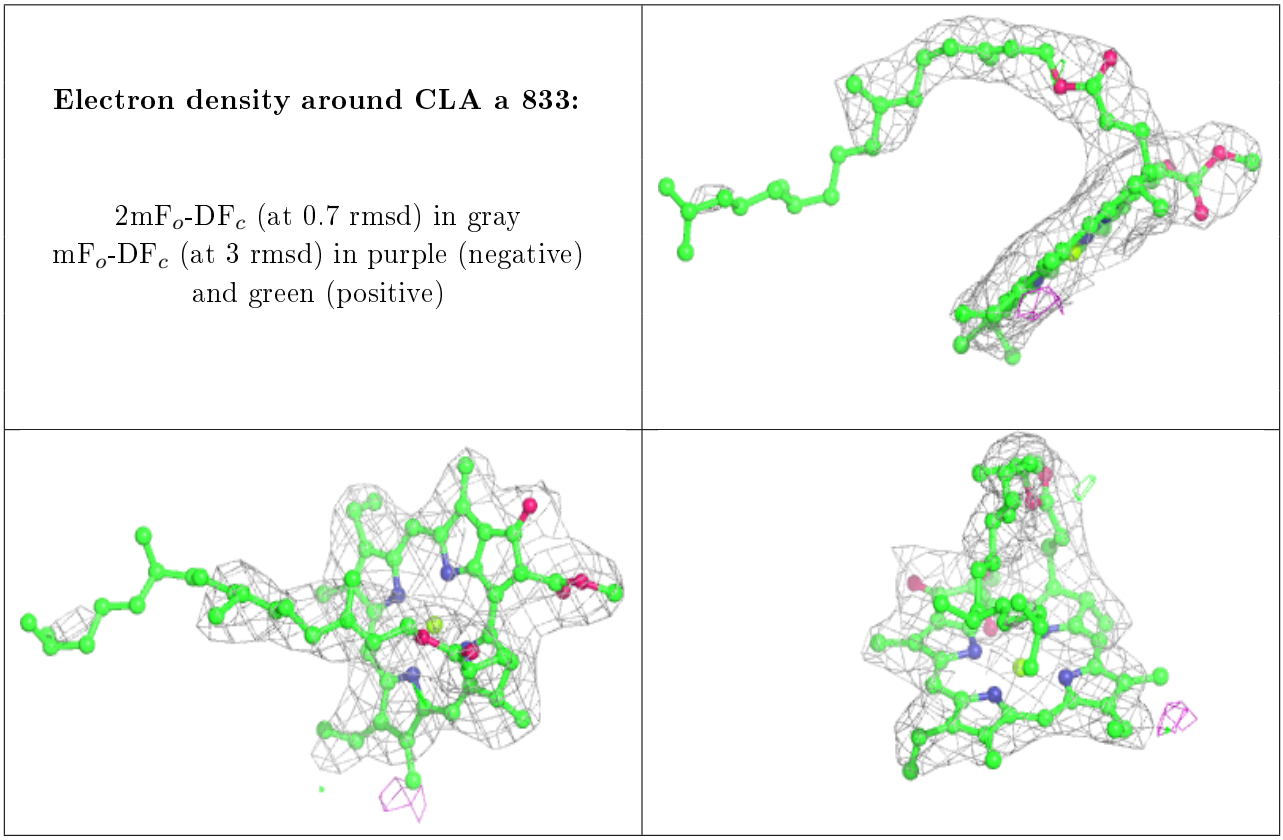
Electron density around CLA A 809:

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



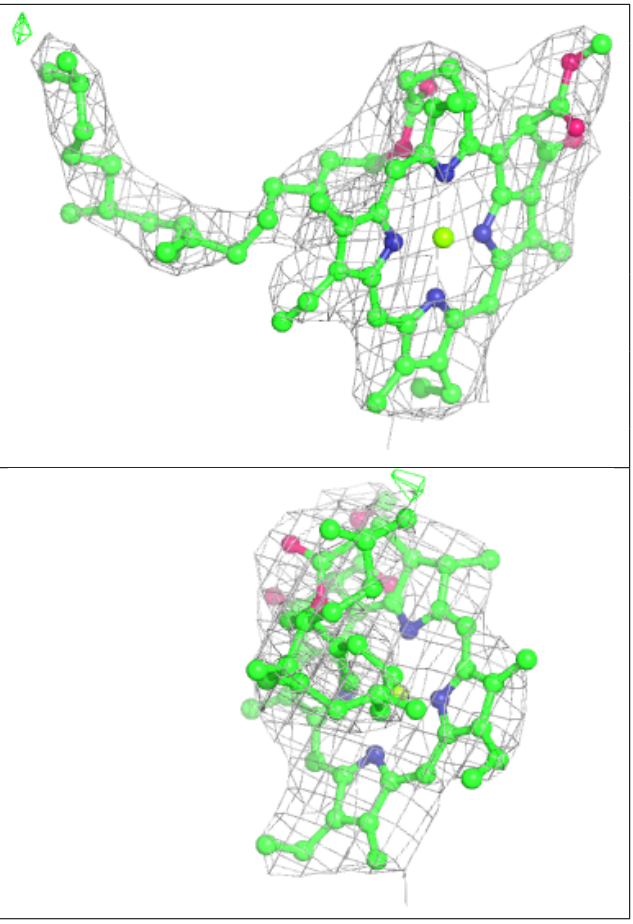
Electron density around CLA a 833:

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



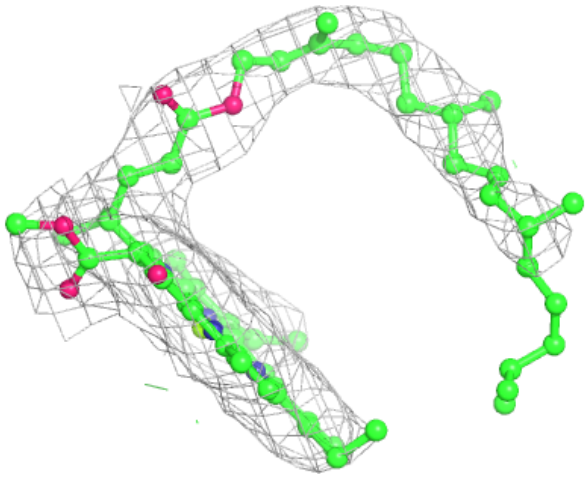
Electron density around CLA A 843:

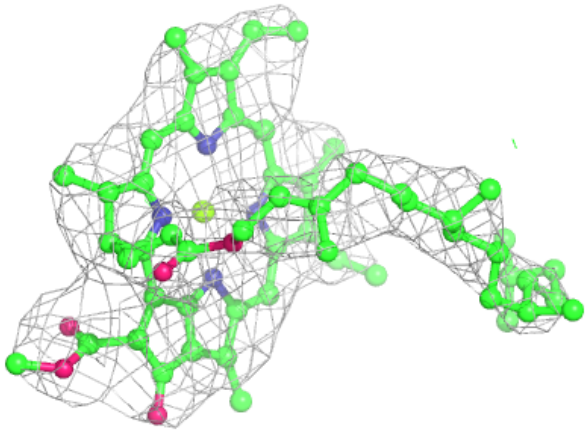
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

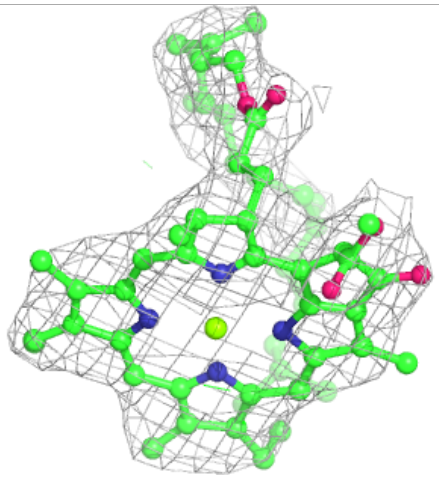


Electron density around CLA b 819:

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

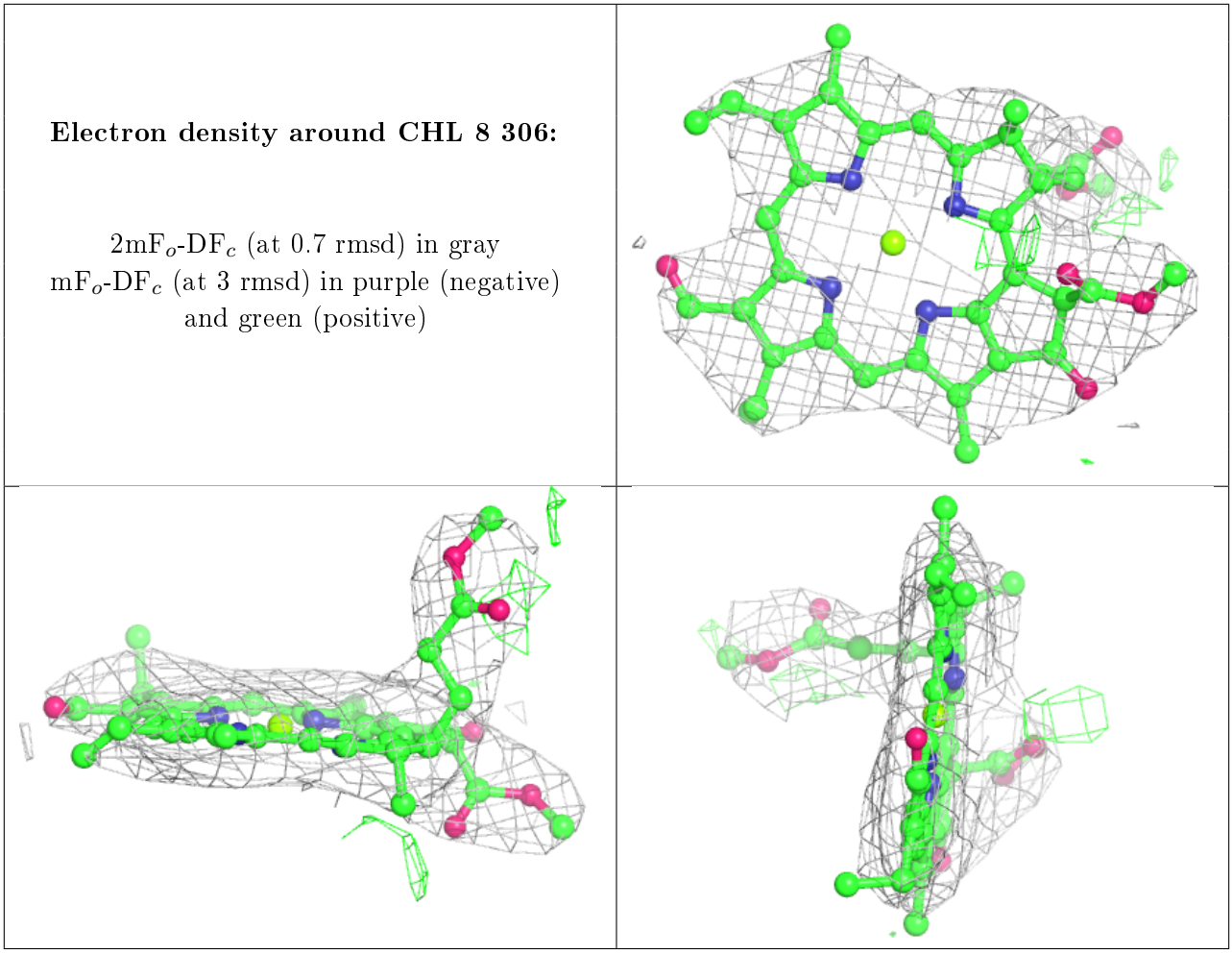






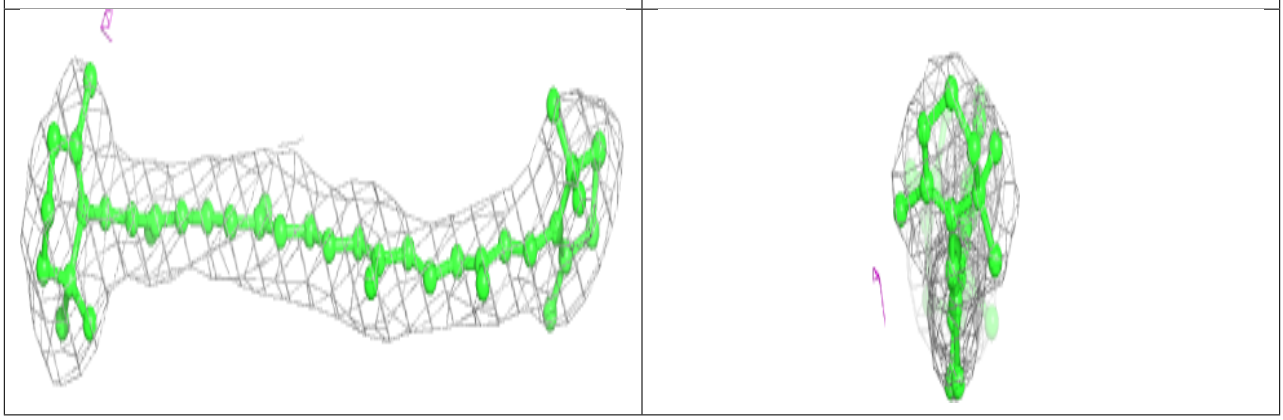
Electron density around CHL 8 306:

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



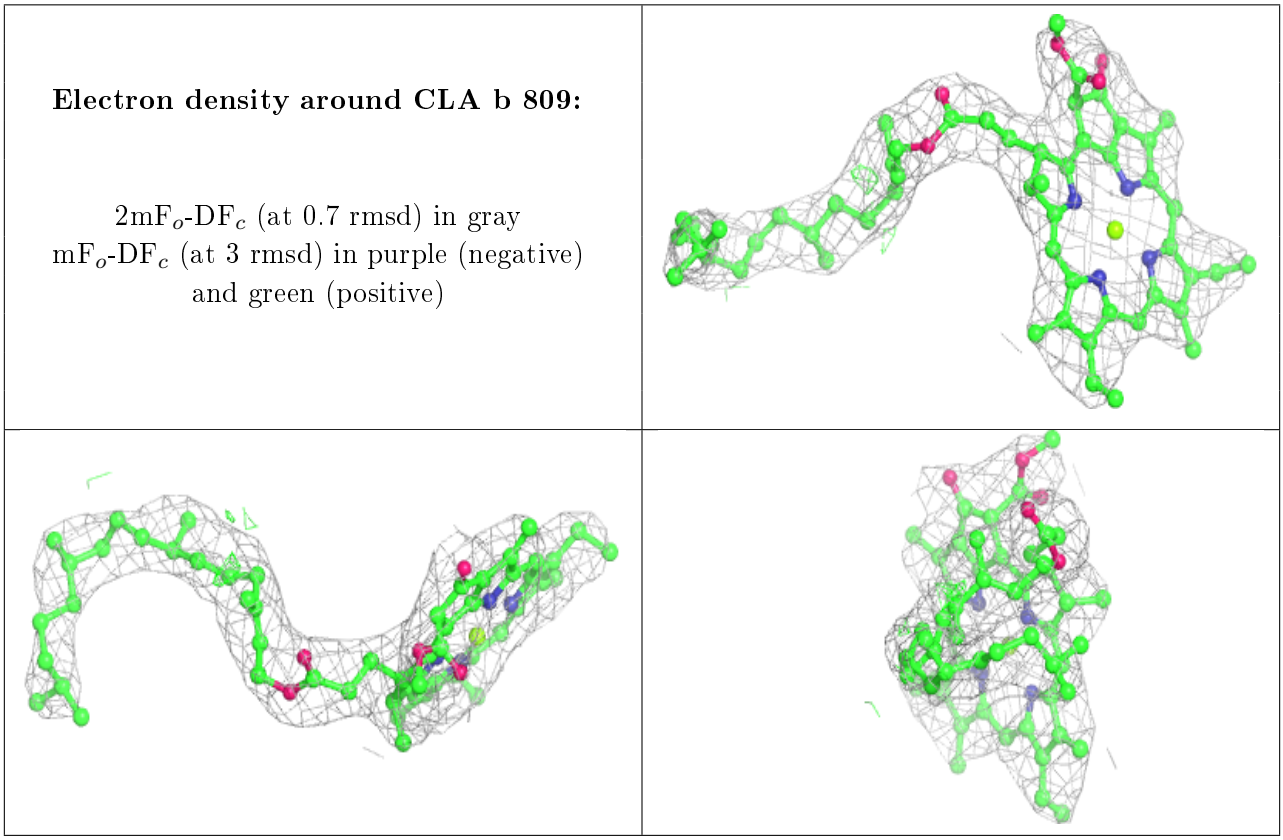
Electron density around BCR b 848:

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



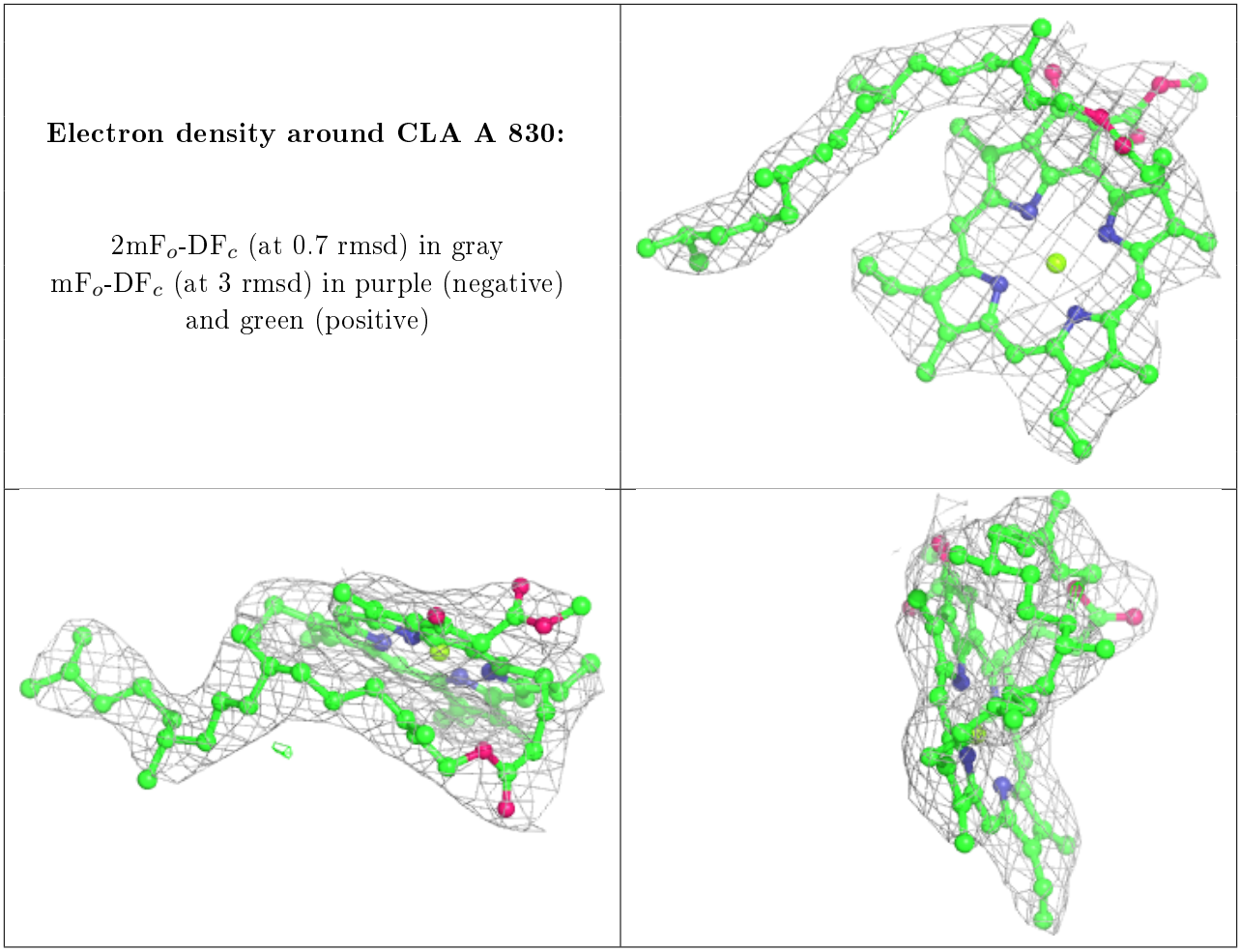
Electron density around CLA b 809:

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



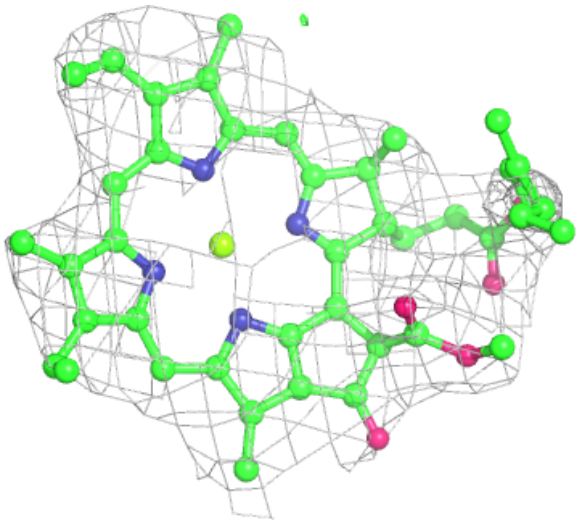
Electron density around CLA A 830:

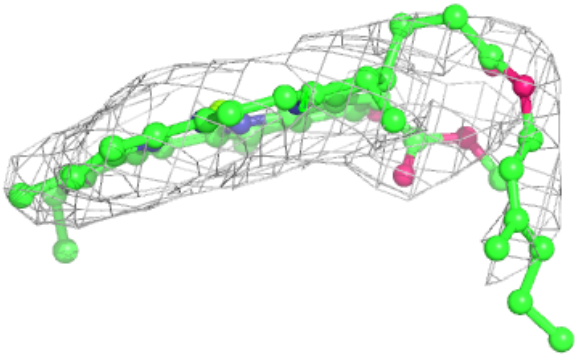
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

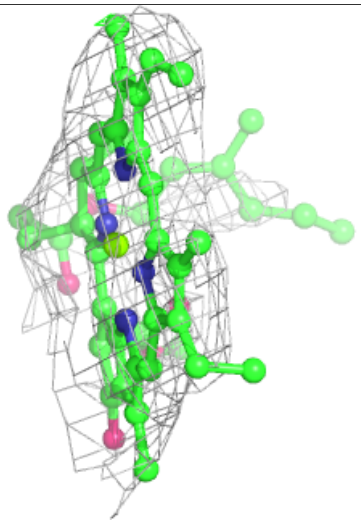


Electron density around CLA 2 611:

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

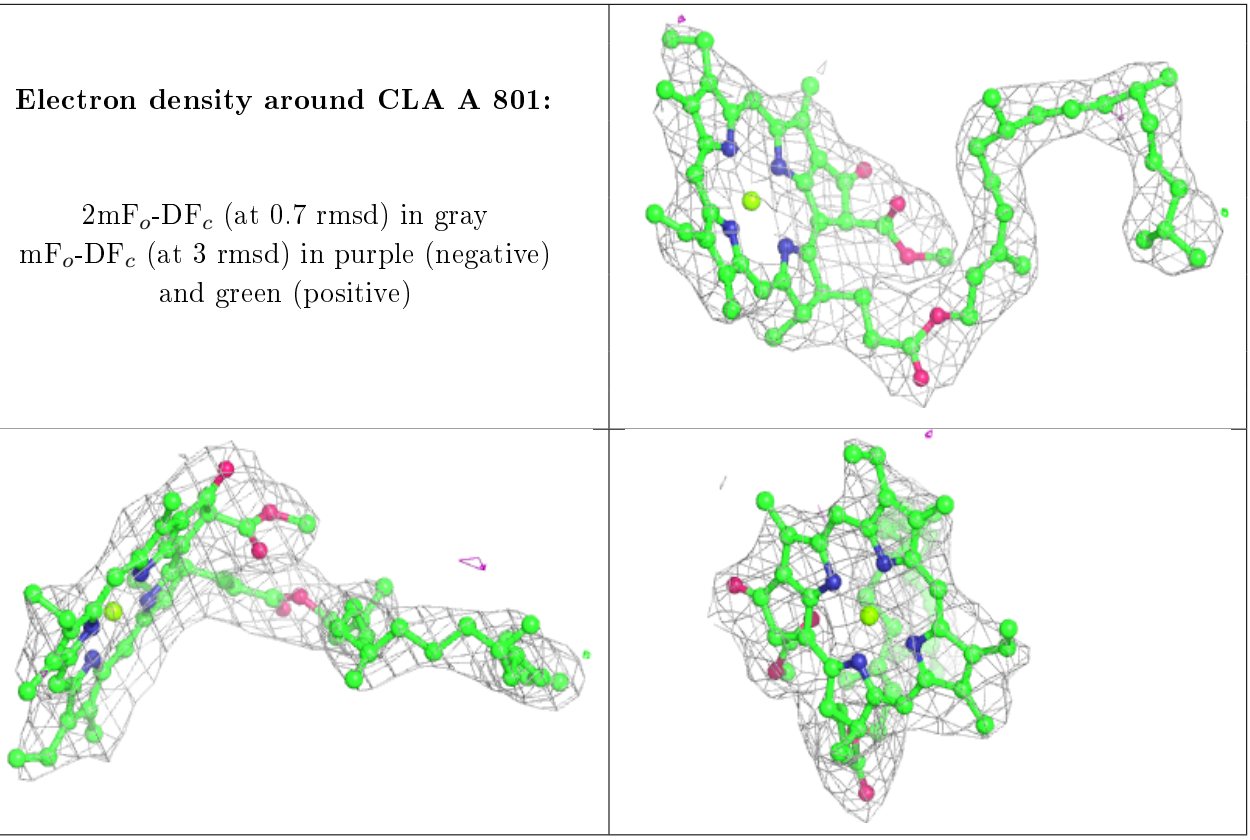






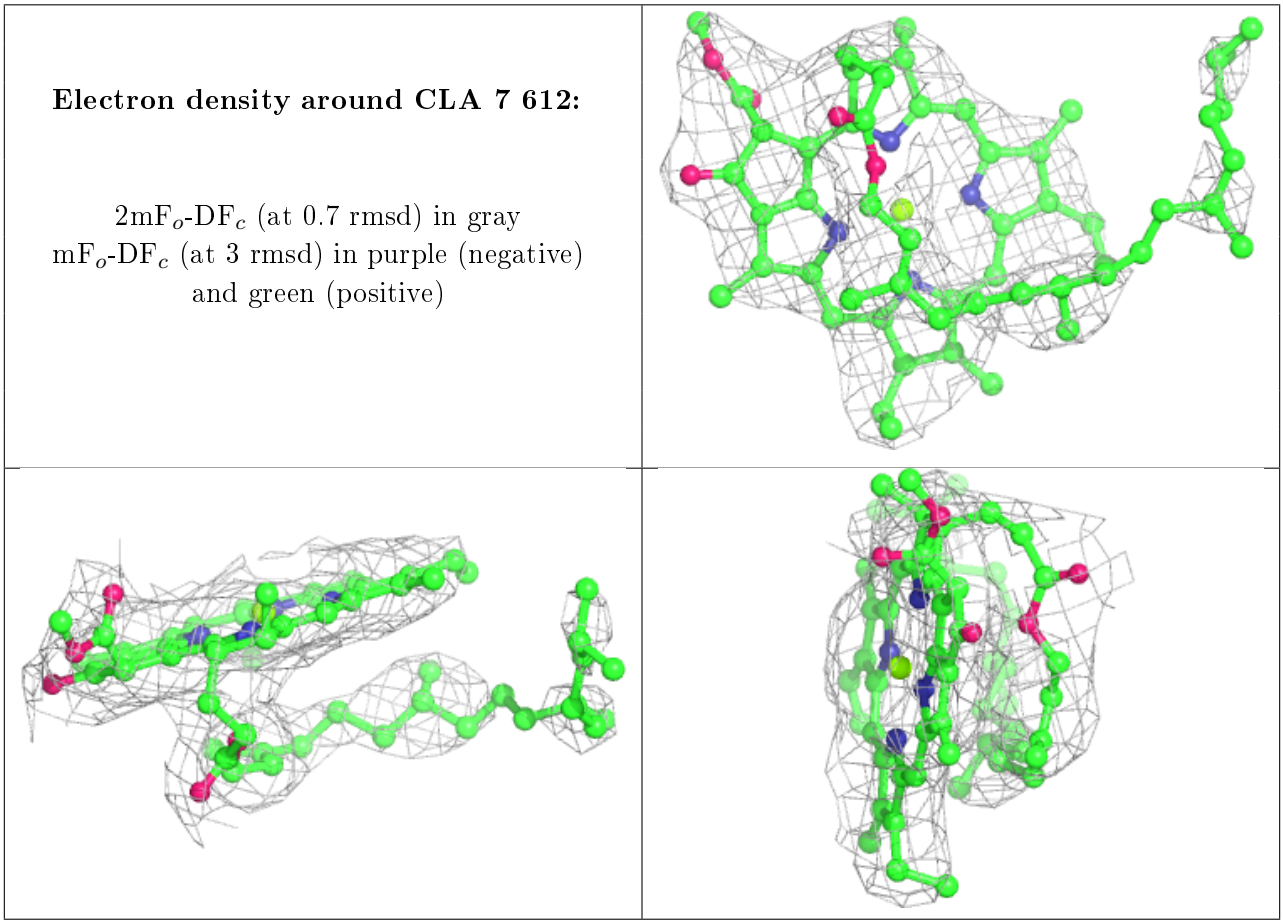
Electron density around CLA A 801:

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



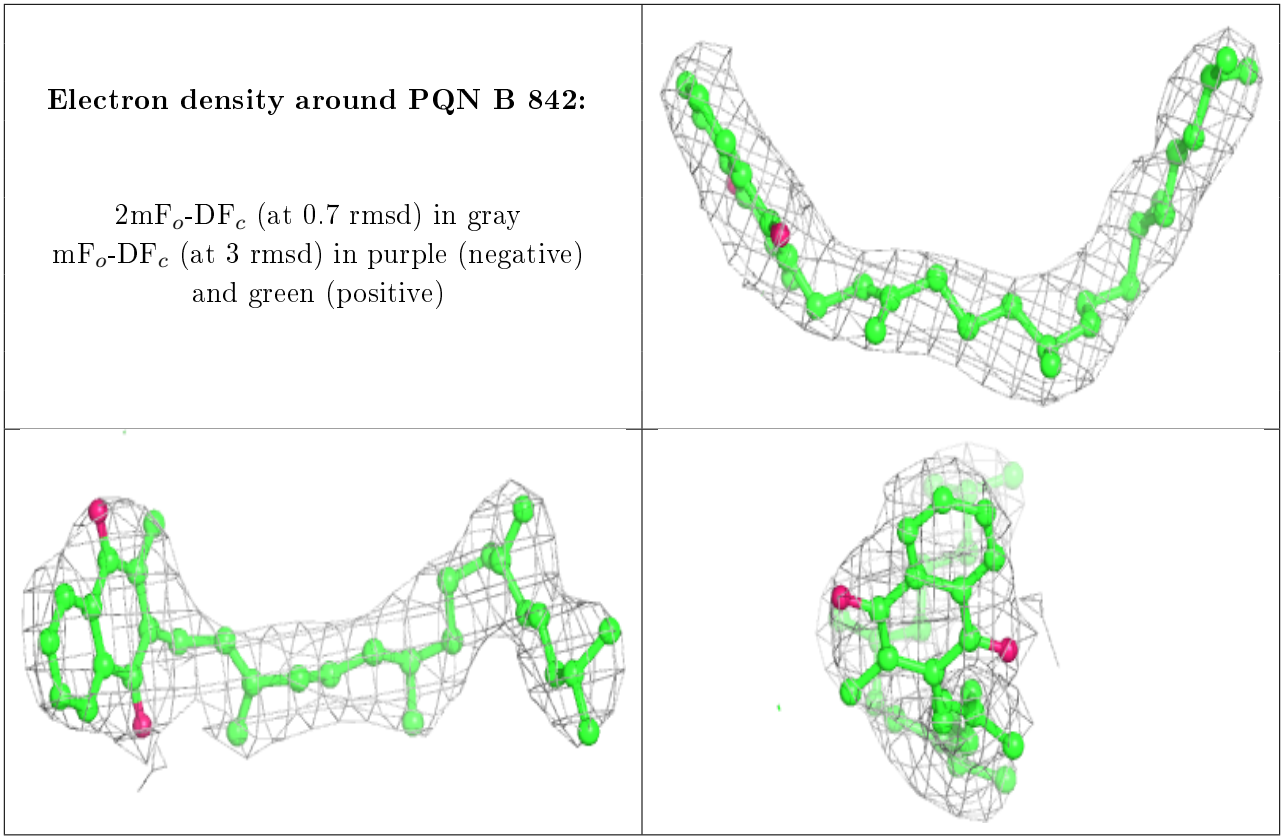
Electron density around CLA 7 612:

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



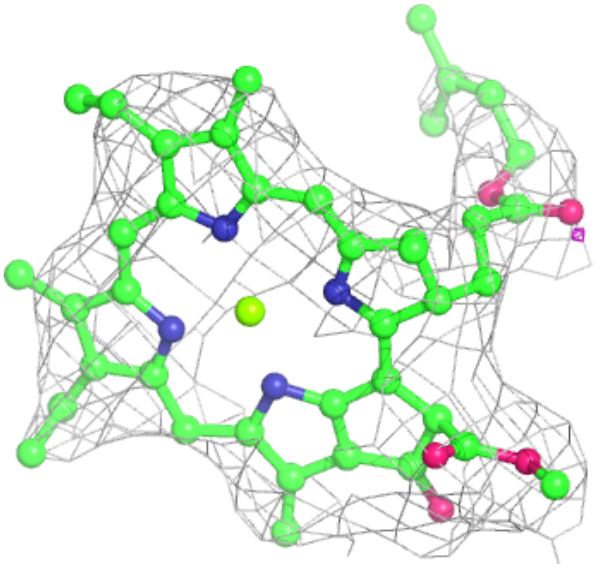
Electron density around PQN B 842:

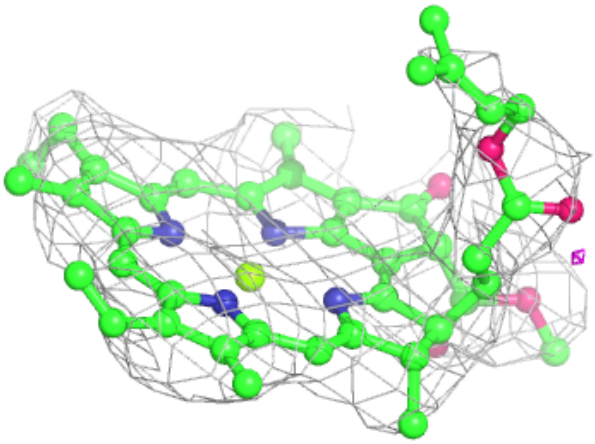
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

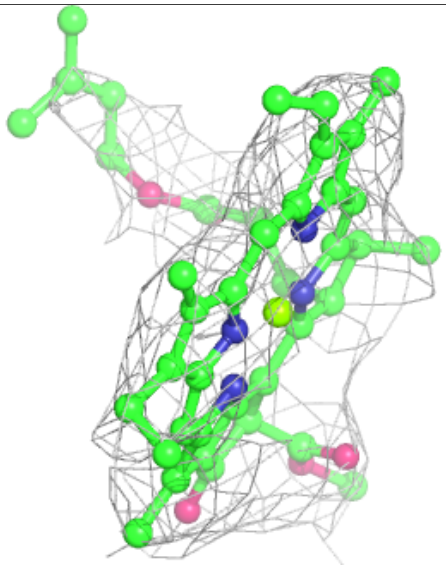


Electron density around CLA 9 608:

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

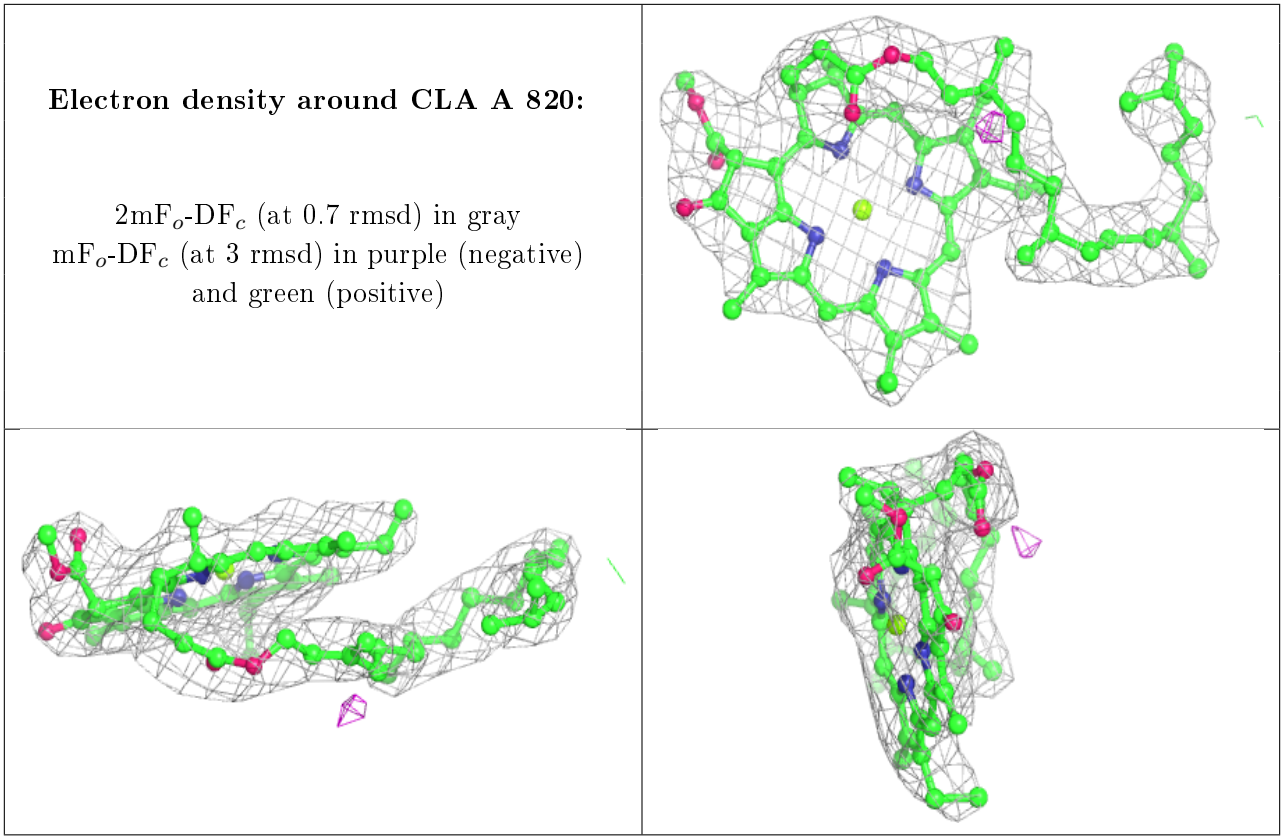






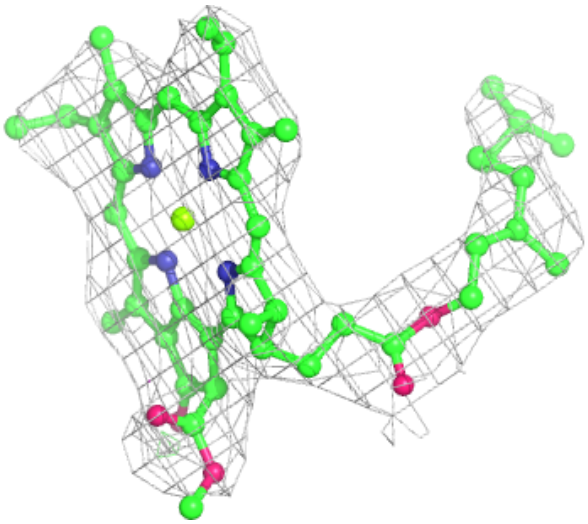
Electron density around CLA A 820:

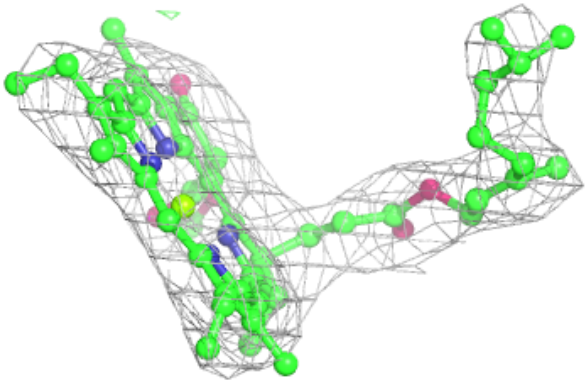
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

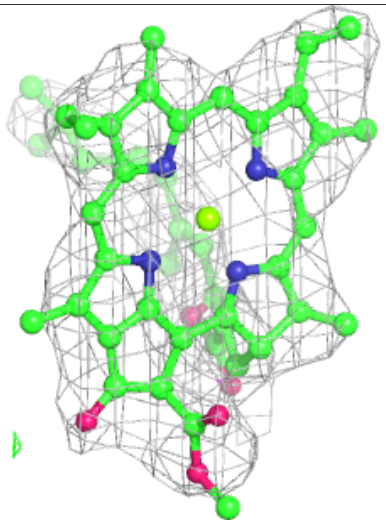


Electron density around CLA a 805:

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

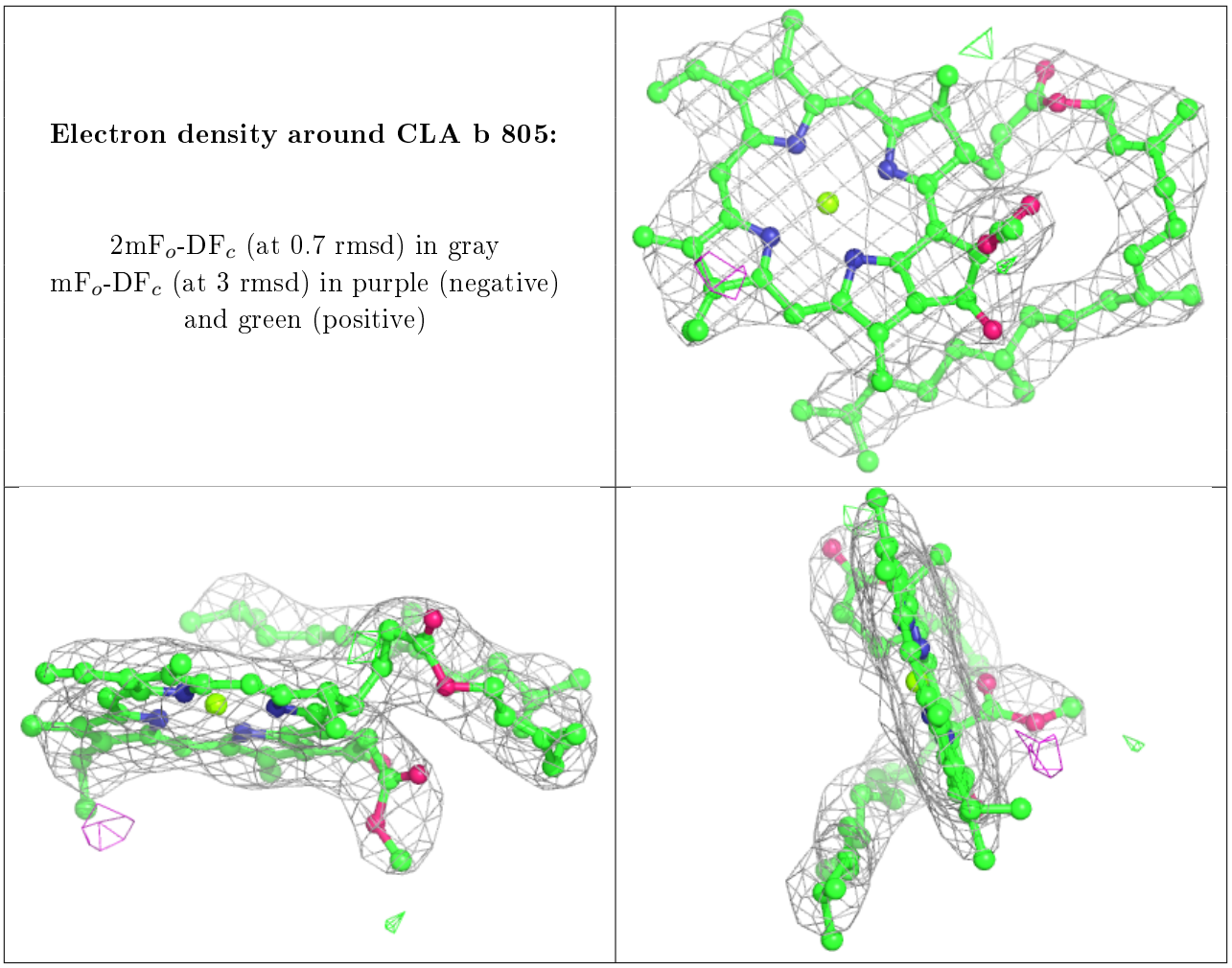






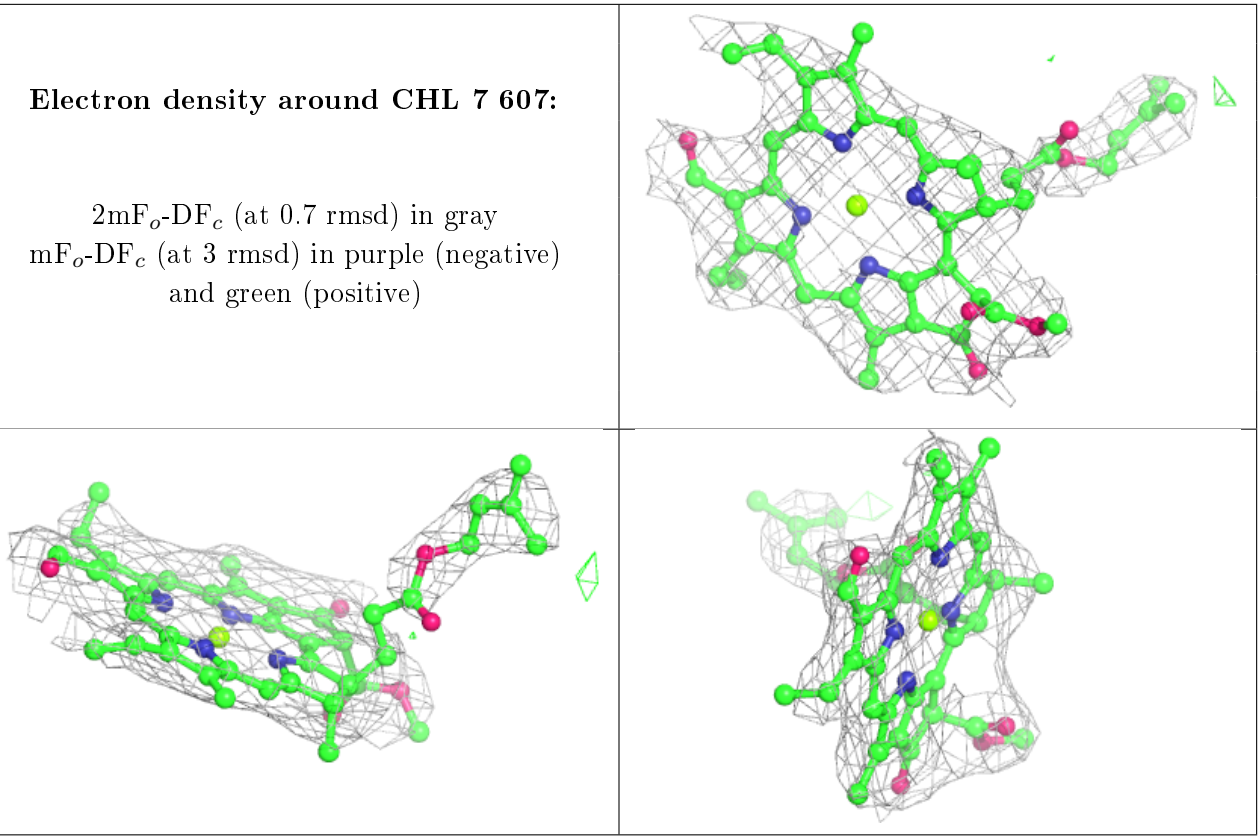
Electron density around CLA b 805:

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



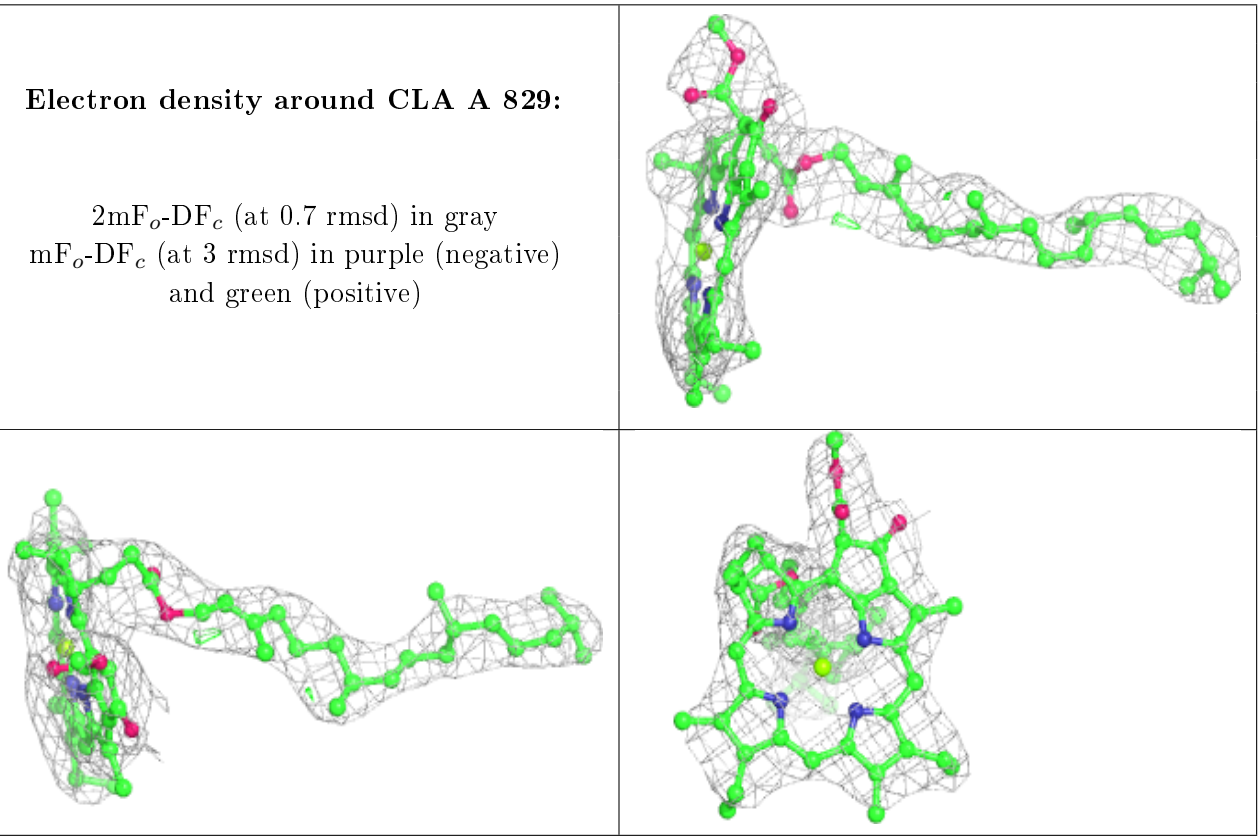
Electron density around CHL 7 607:

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



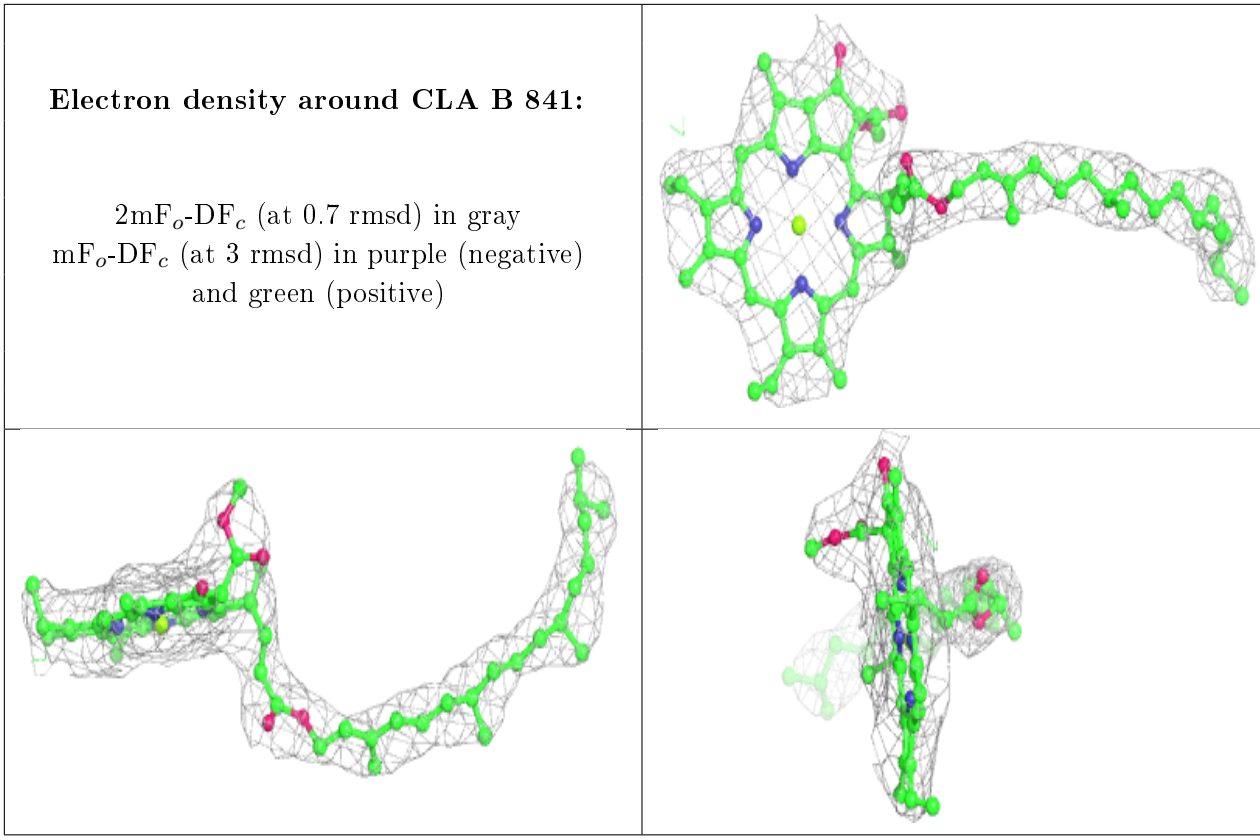
Electron density around CLA A 829:

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



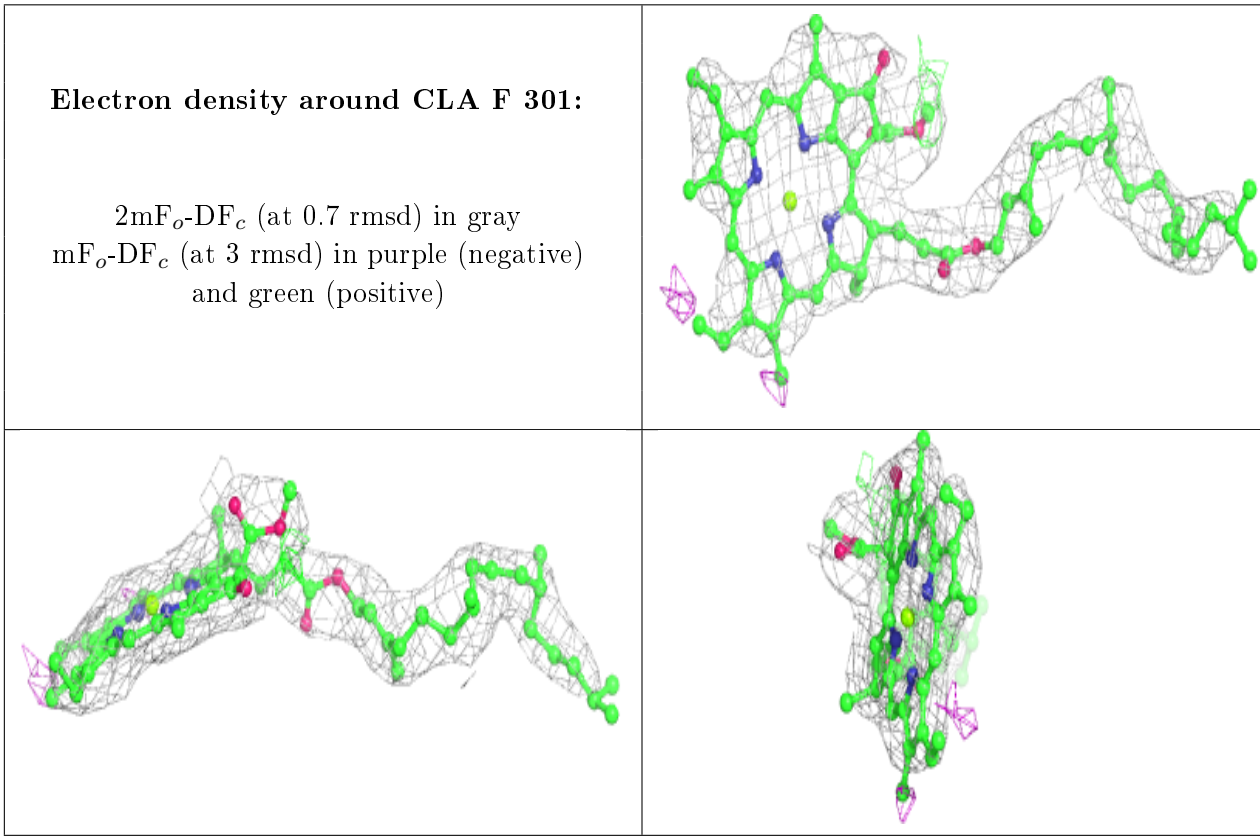
Electron density around CLA B 841:

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



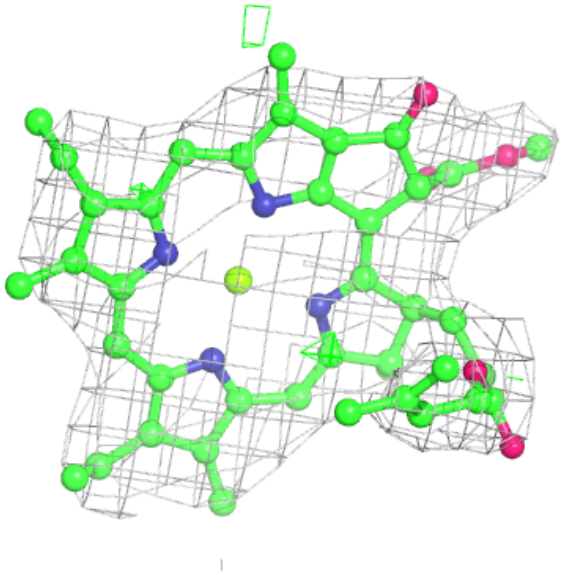
Electron density around CLA F 301:

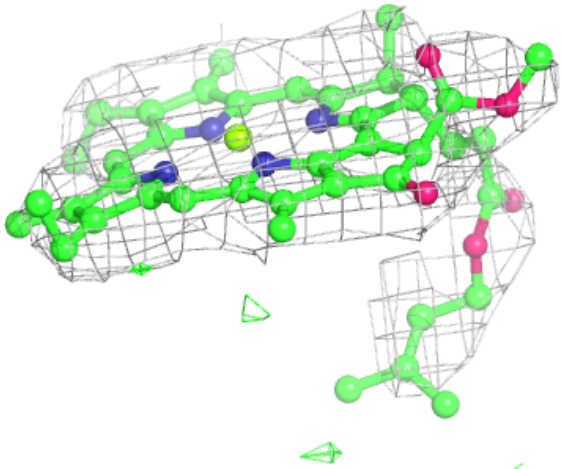
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

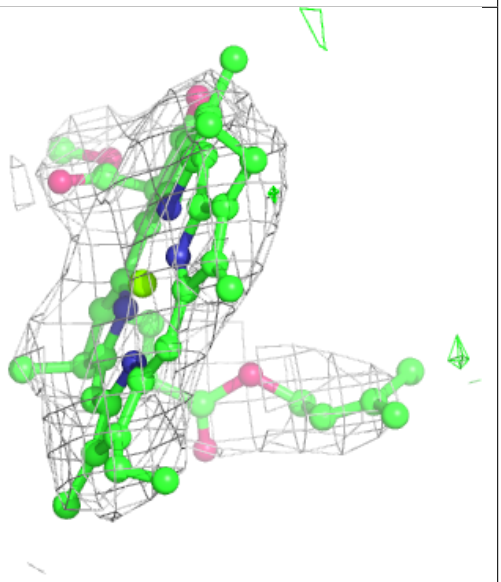


Electron density around CLA 3 308:

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

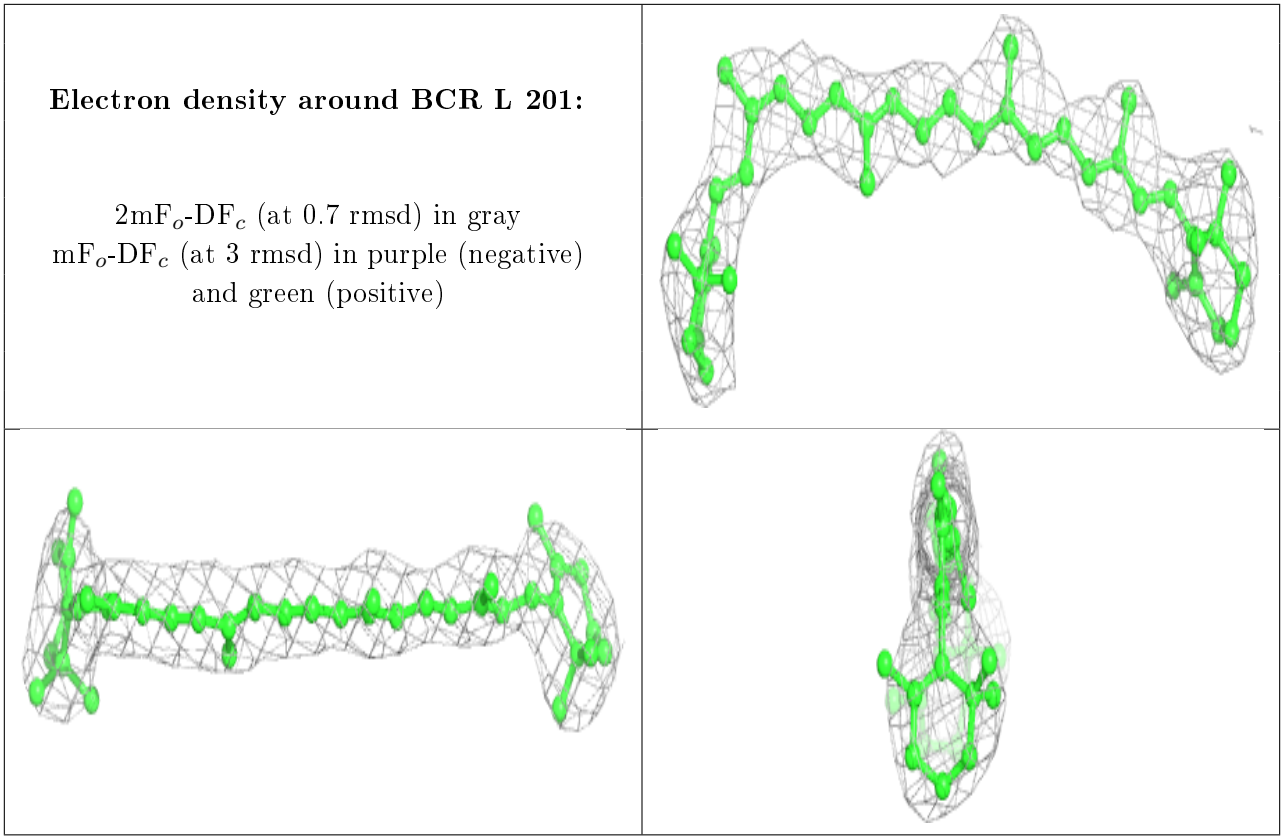






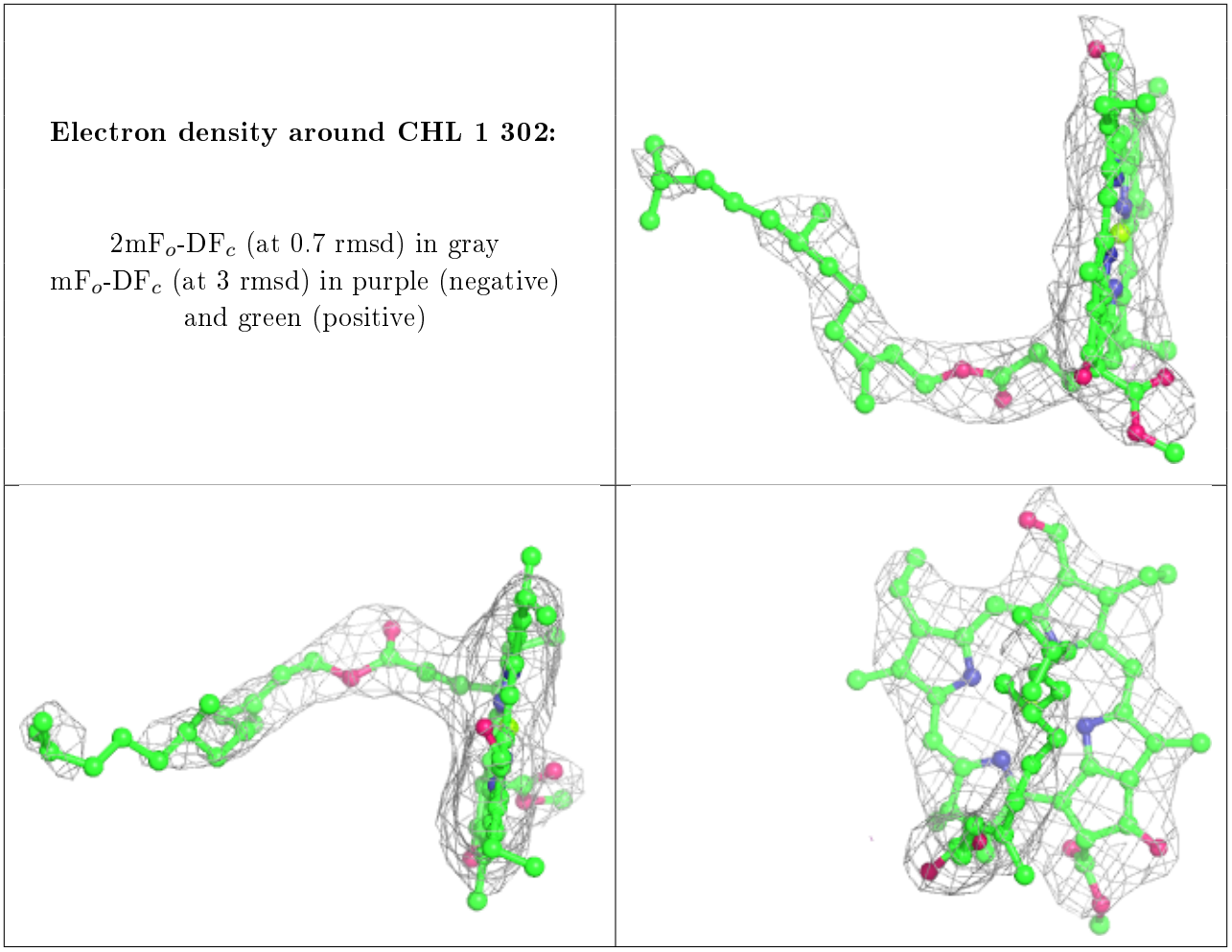
Electron density around BCR L 201:

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



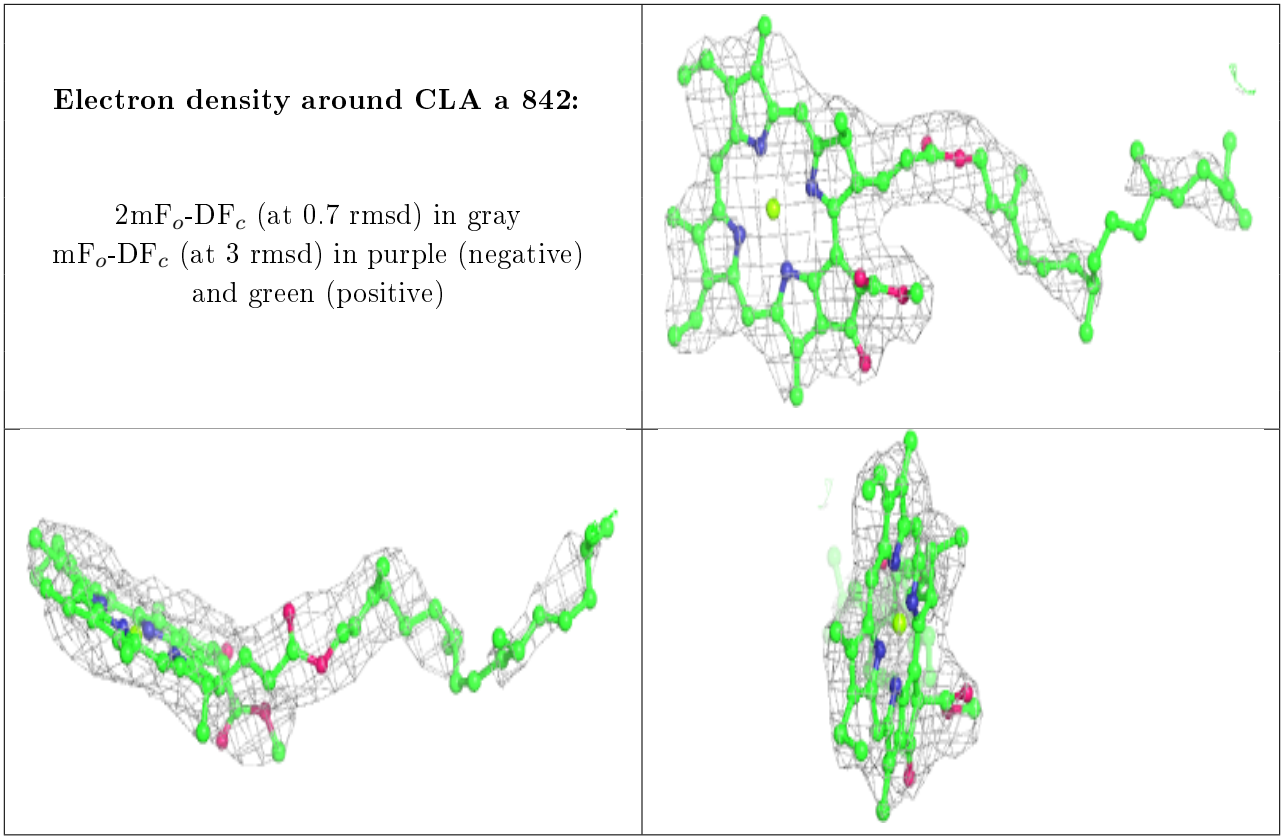
Electron density around CHL 1 302:

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



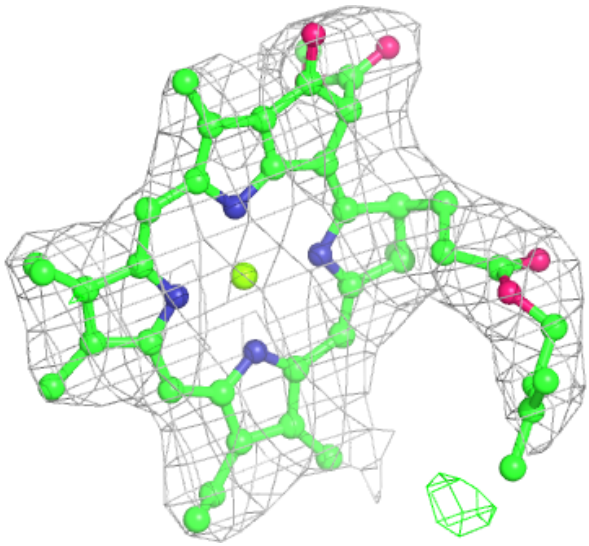
Electron density around CLA a 842:

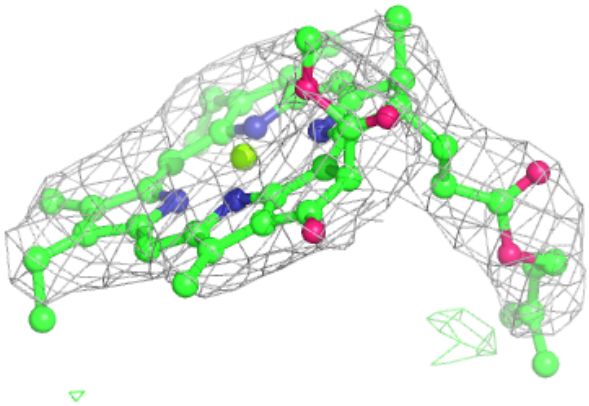
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

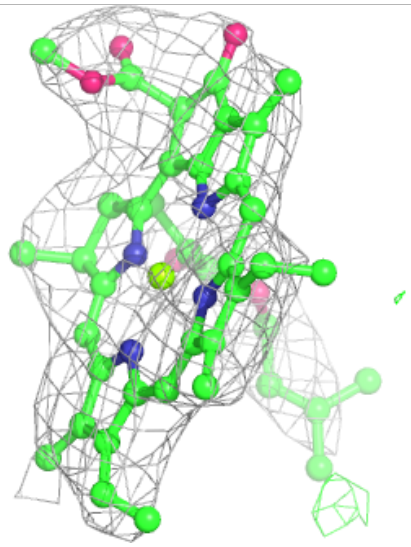


Electron density around CLA a 832:

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

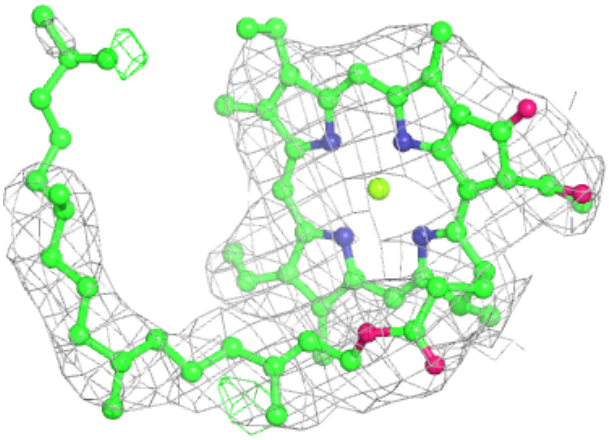


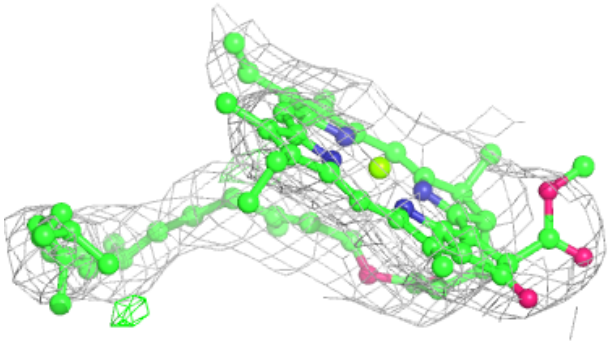


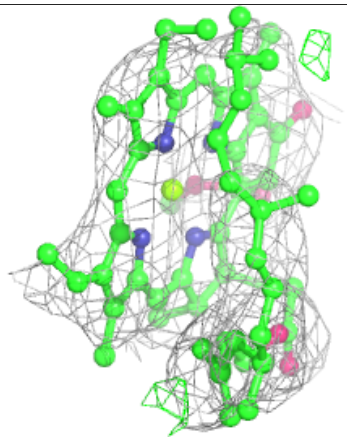


Electron density around CLA 6 304:

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

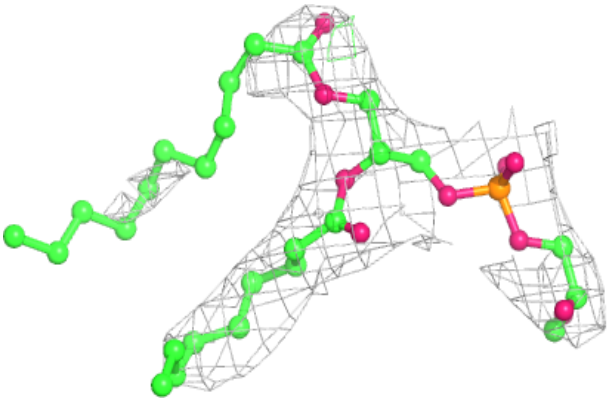


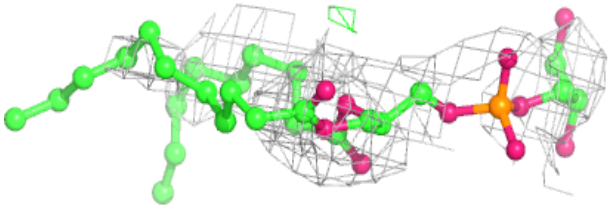




Electron density around LHG 2 618:

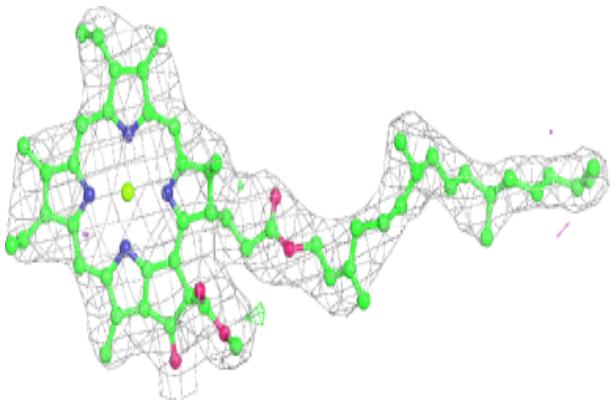
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

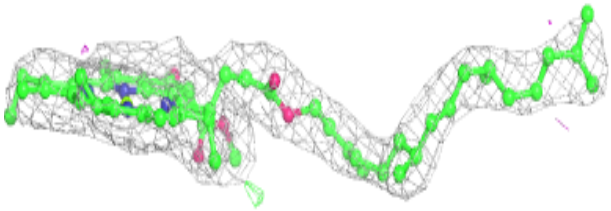


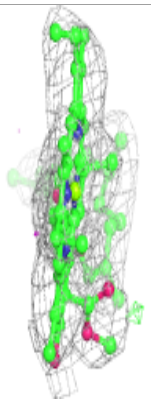


Electron density around CLA a 834:

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

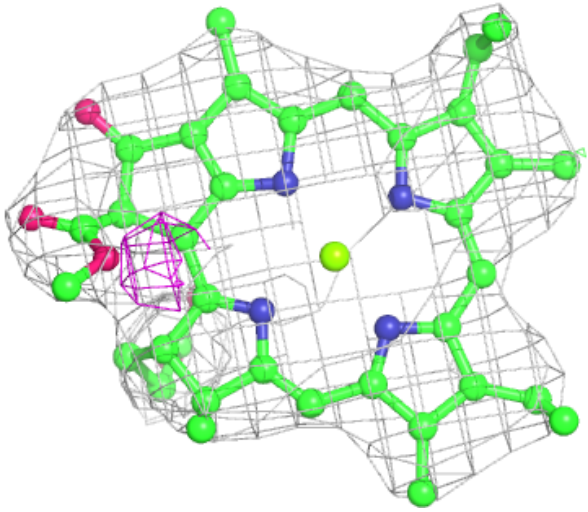


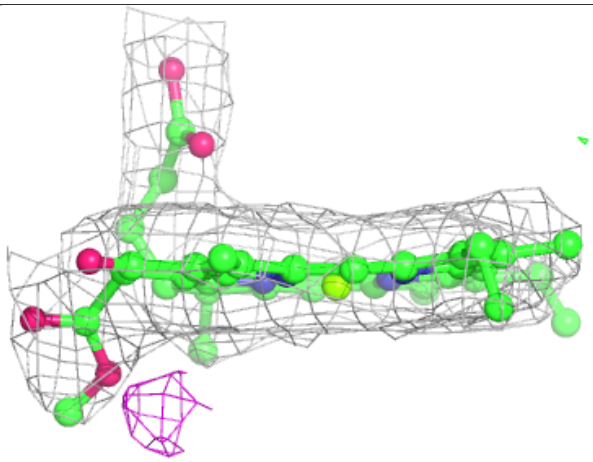


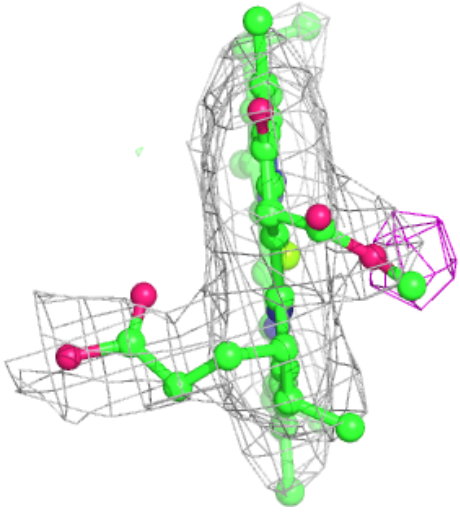


Electron density around CLA B 804:

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

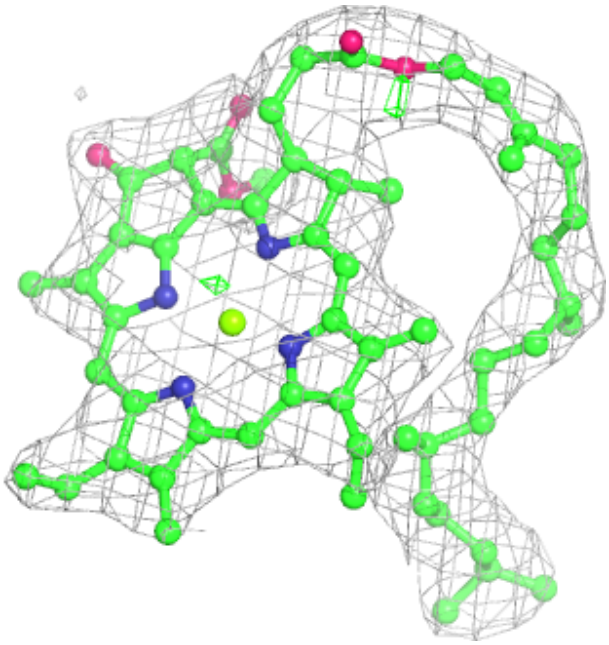


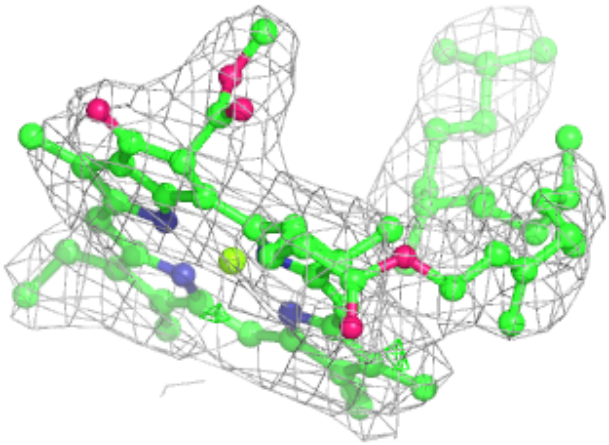




Electron density around CLA a 814:

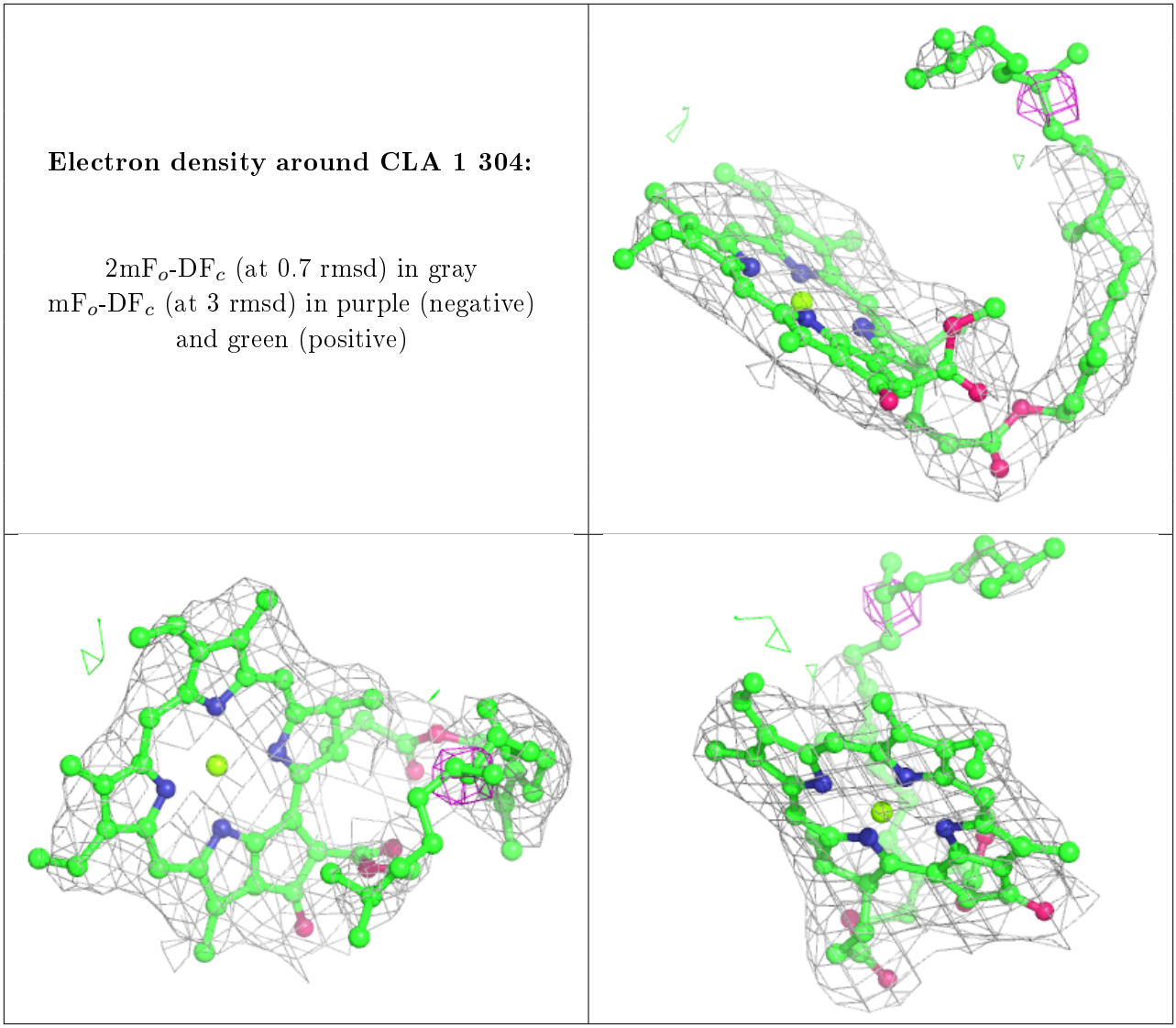
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)





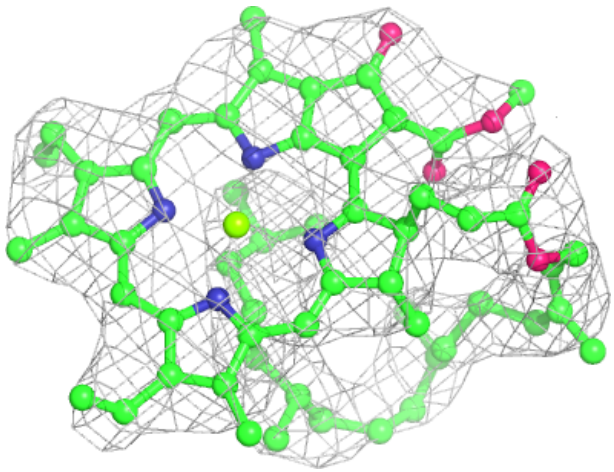
Electron density around CLA 1 304:

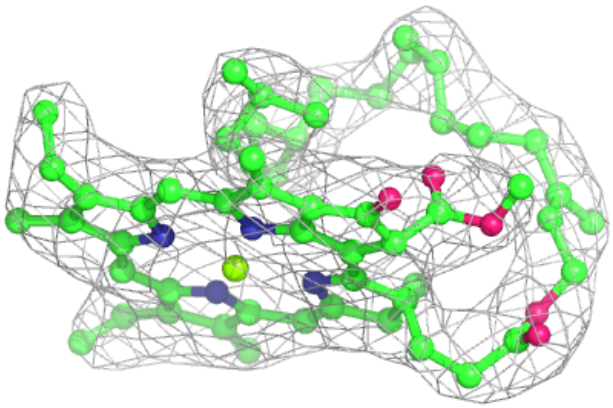
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

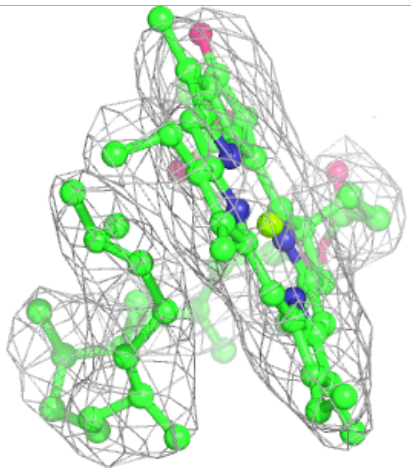


Electron density around CLA B 806:

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

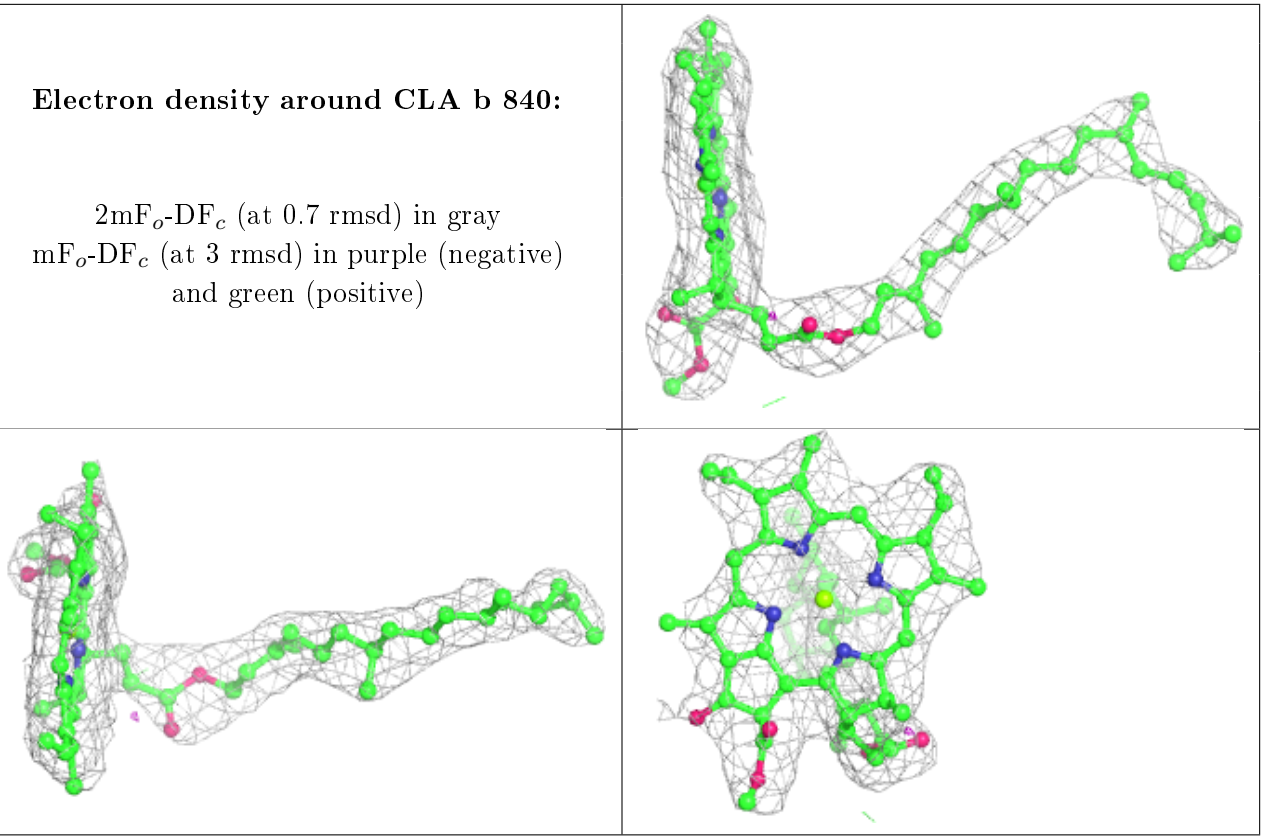






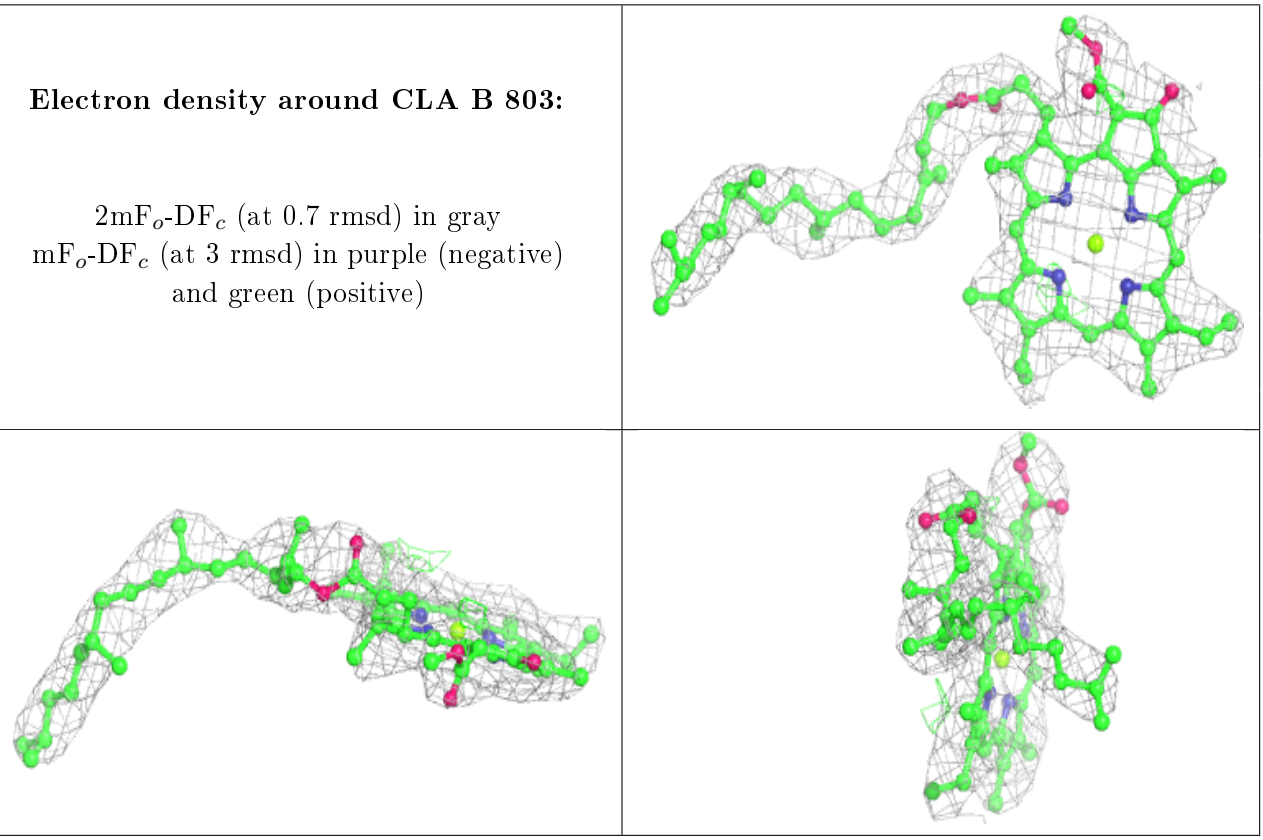
Electron density around CLA b 840:

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



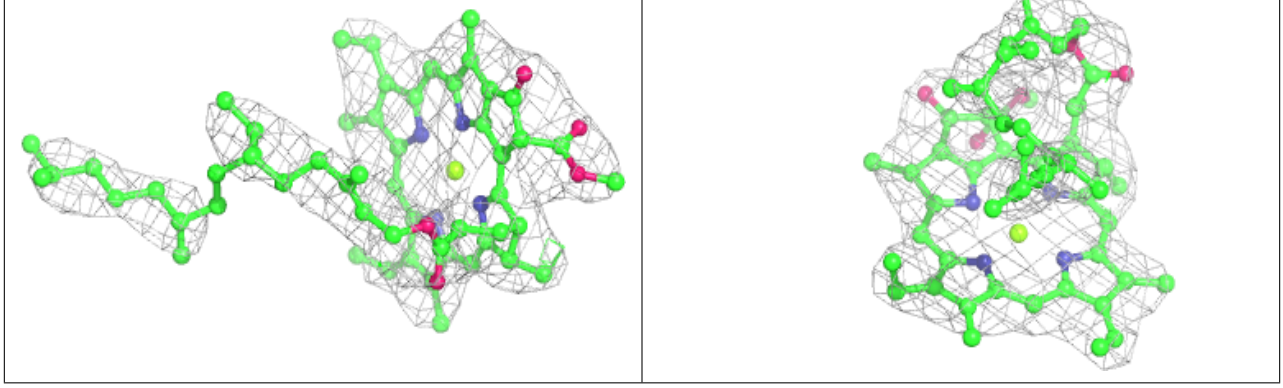
Electron density around CLA B 803:

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



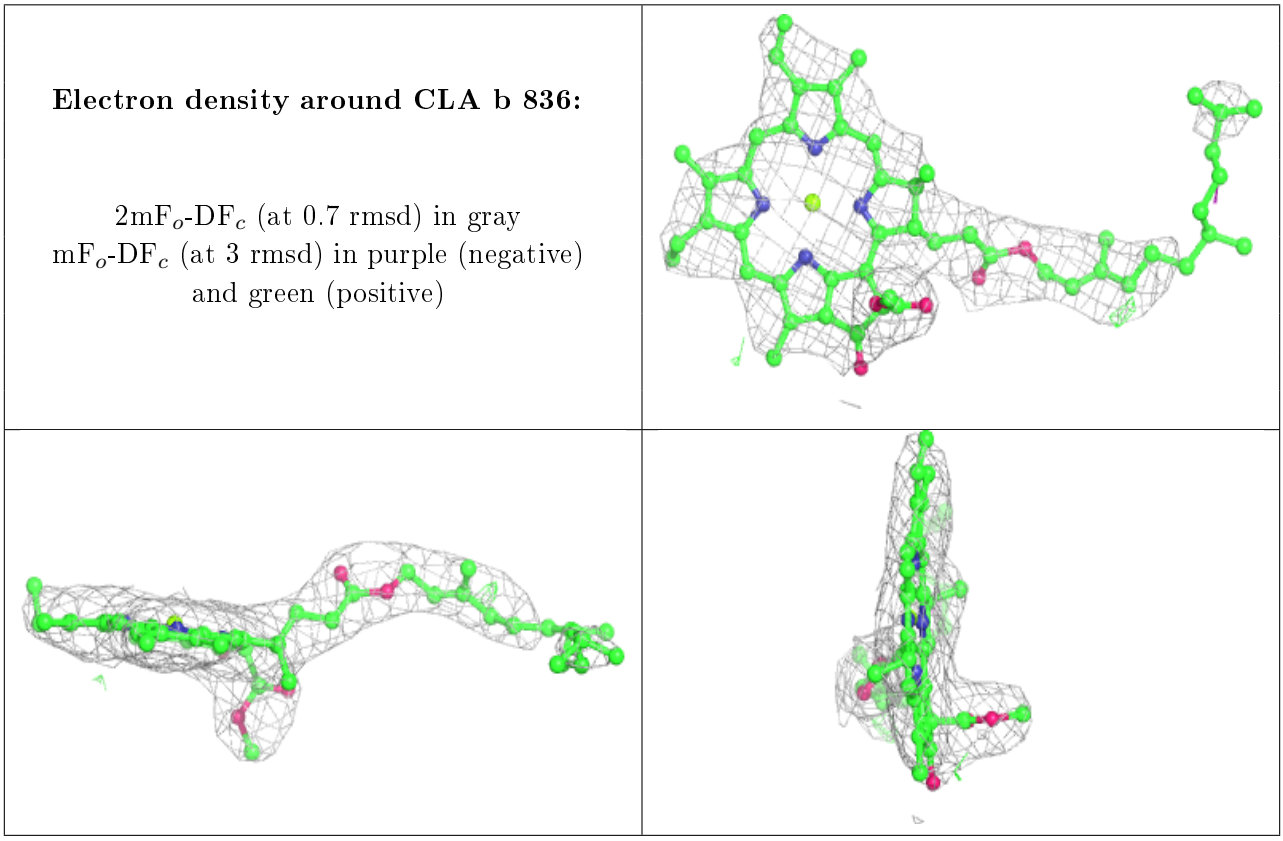
Electron density around CLA A 811:

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



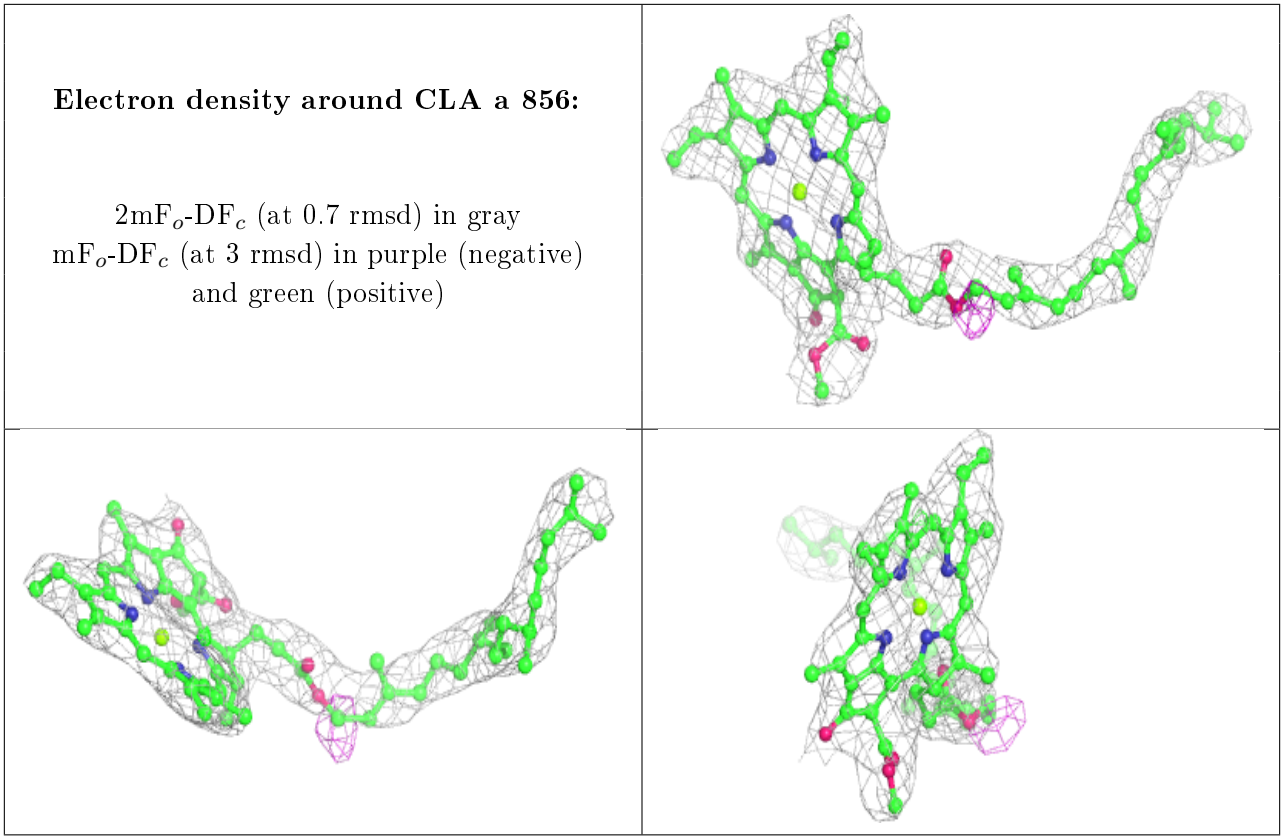
Electron density around CLA b 836:

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



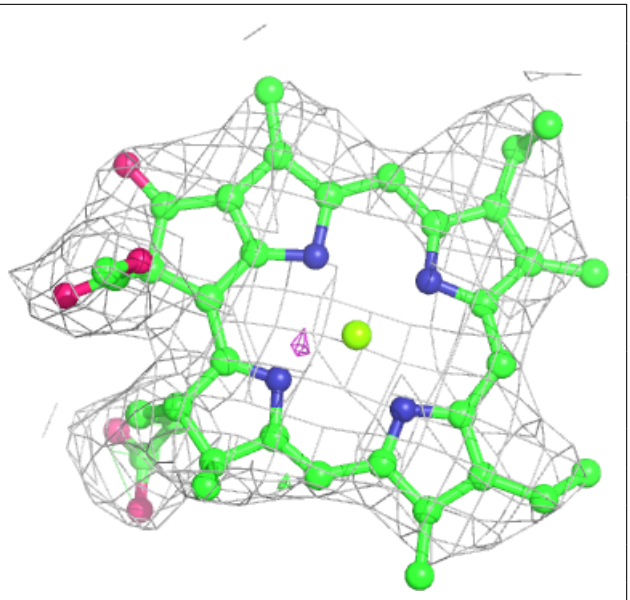
Electron density around CLA a 856:

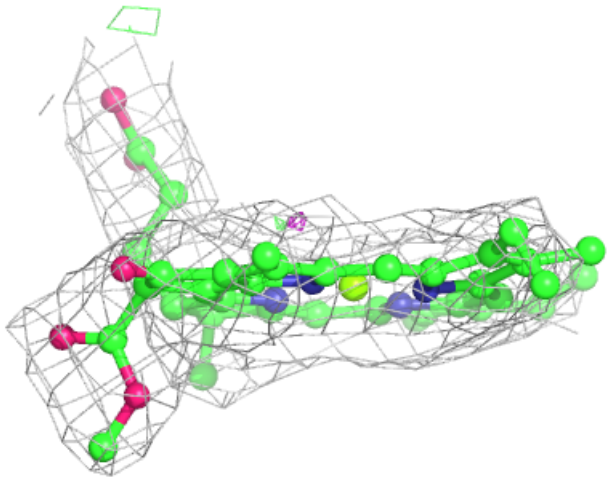
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



Electron density around CLA a 821:

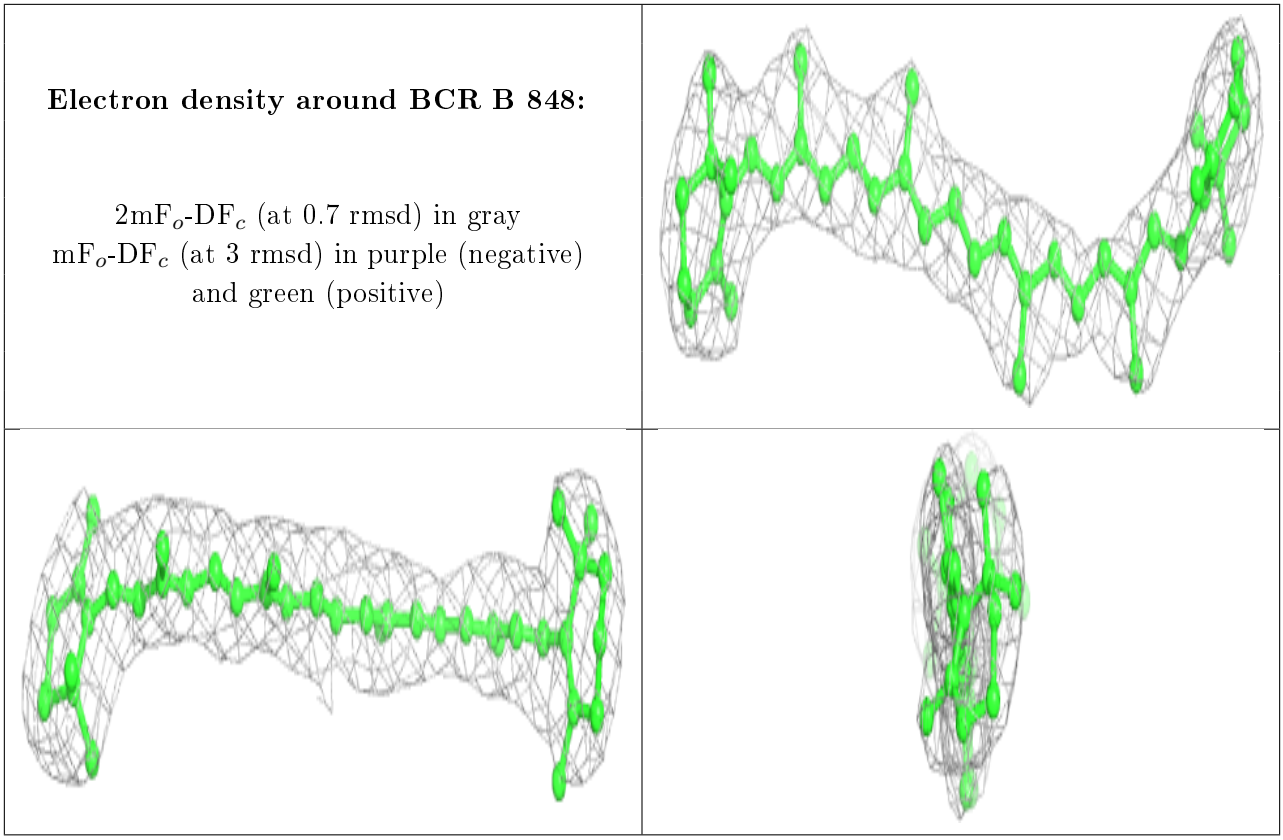
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)





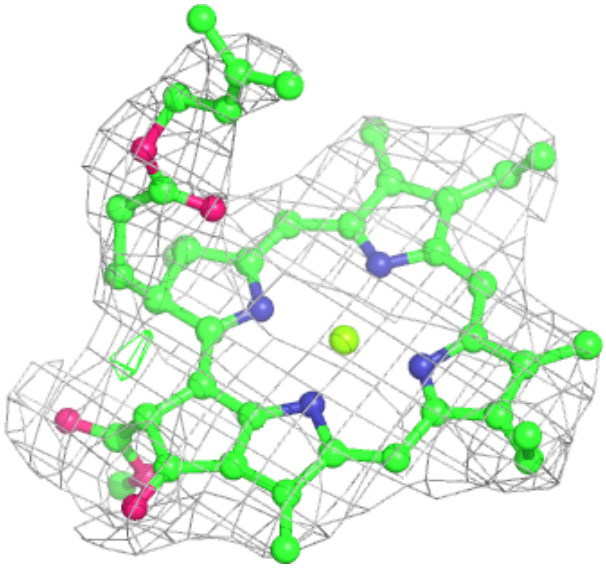
Electron density around BCR B 848:

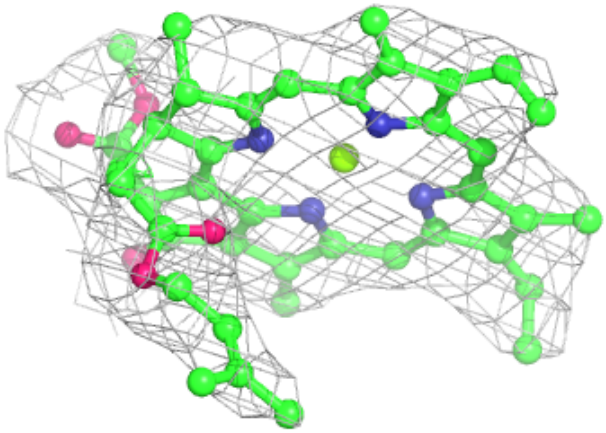
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

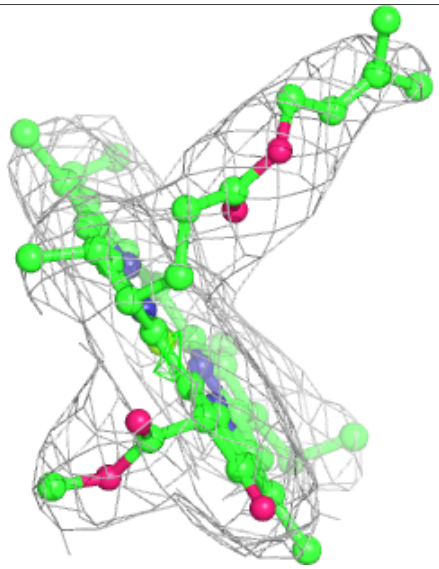


Electron density around CLA B 830:

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

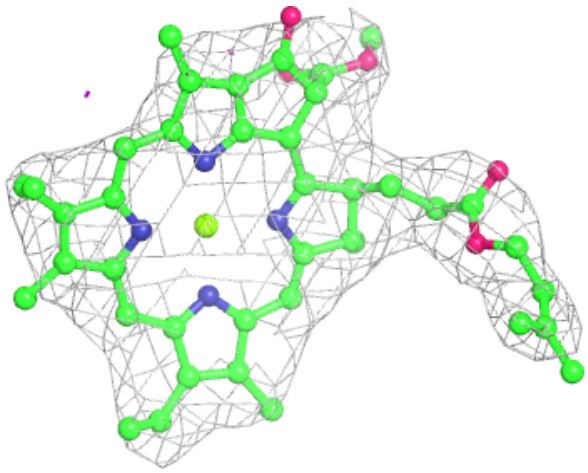


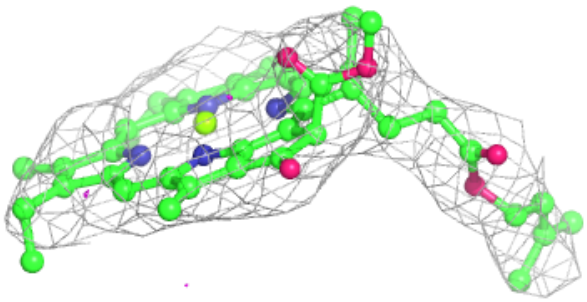


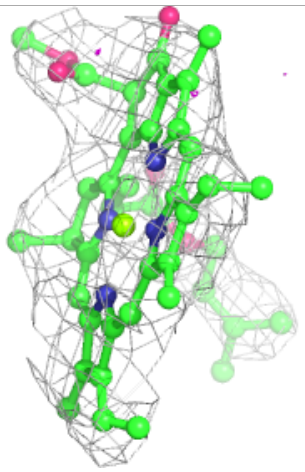


Electron density around CLA 4 614:

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

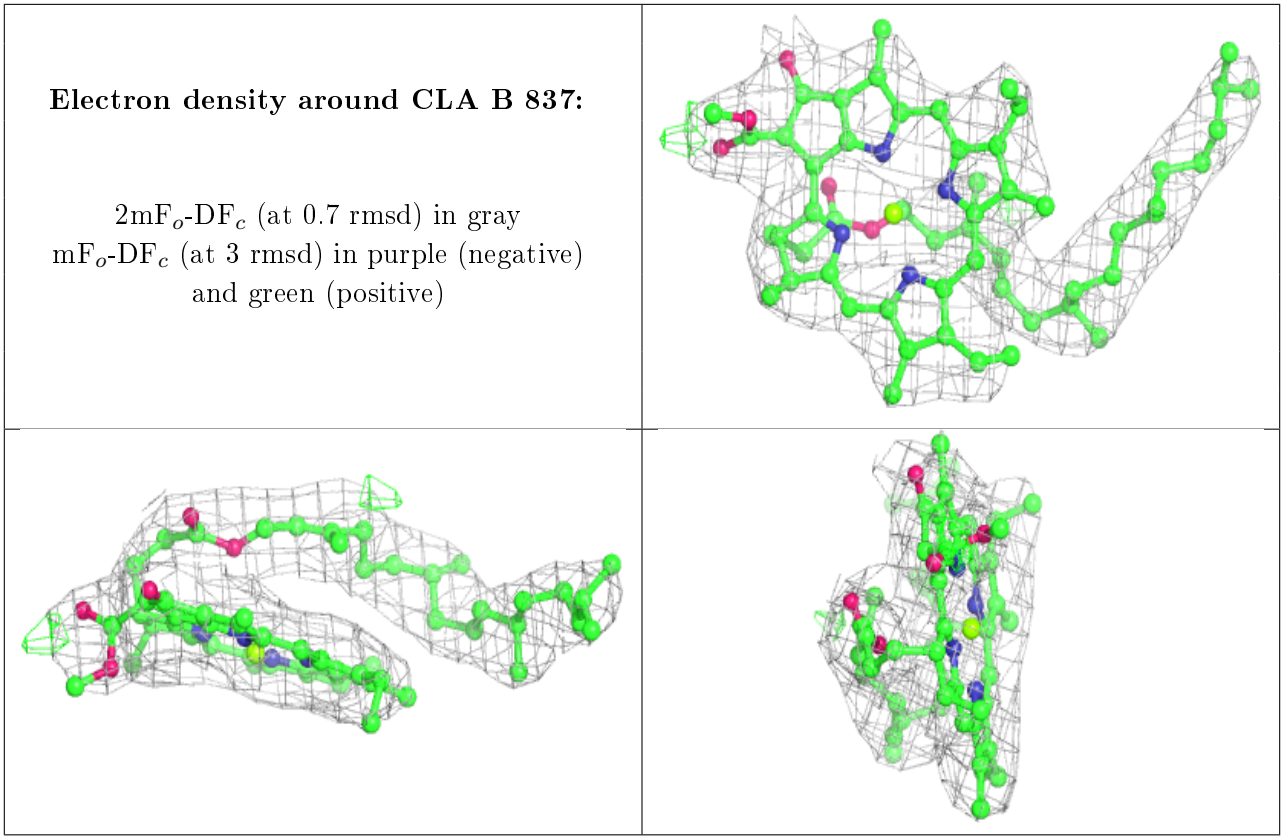






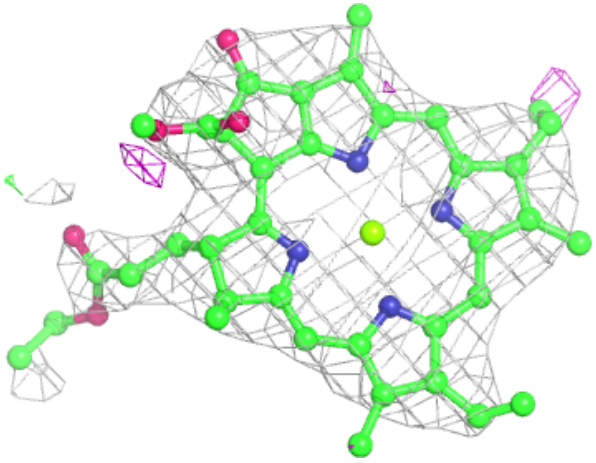
Electron density around CLA B 837:

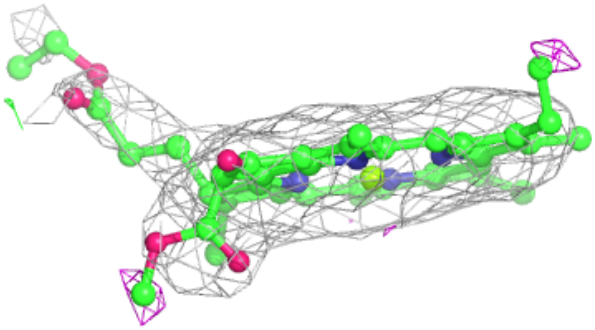
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

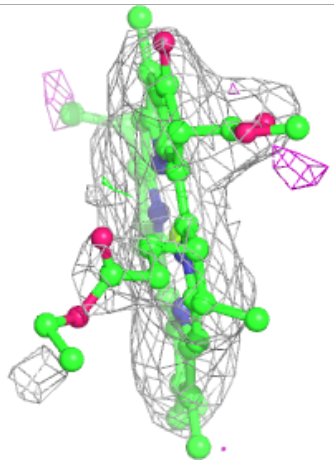


Electron density around CLA 9 614:

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

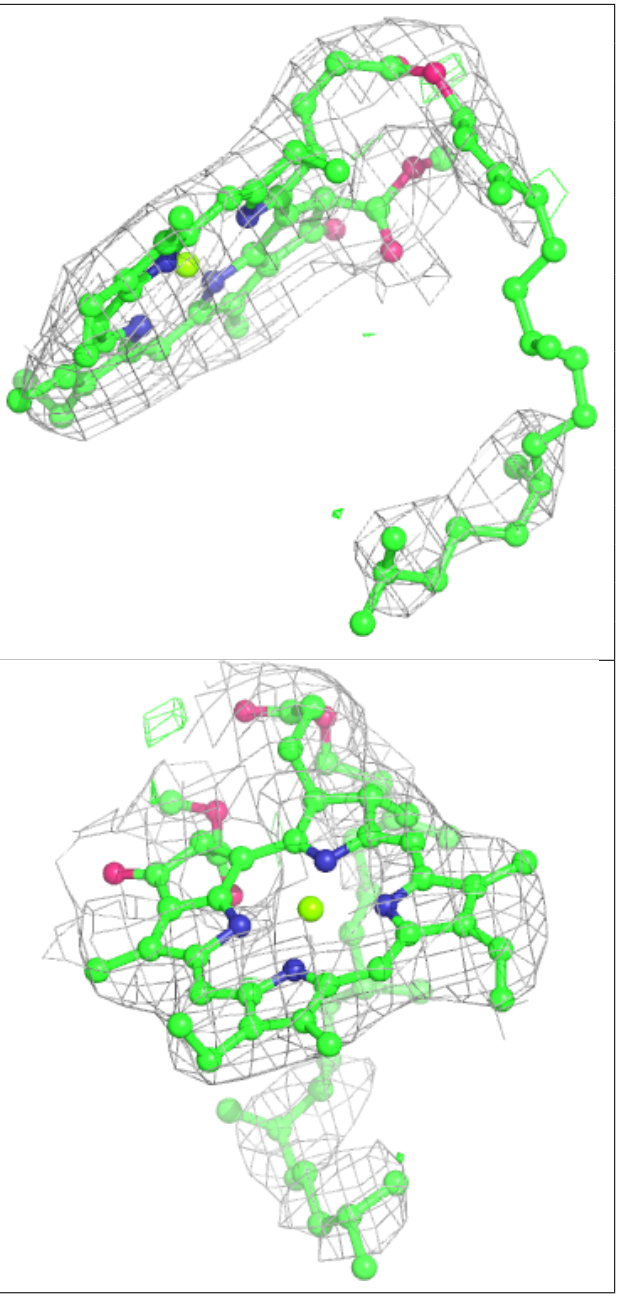


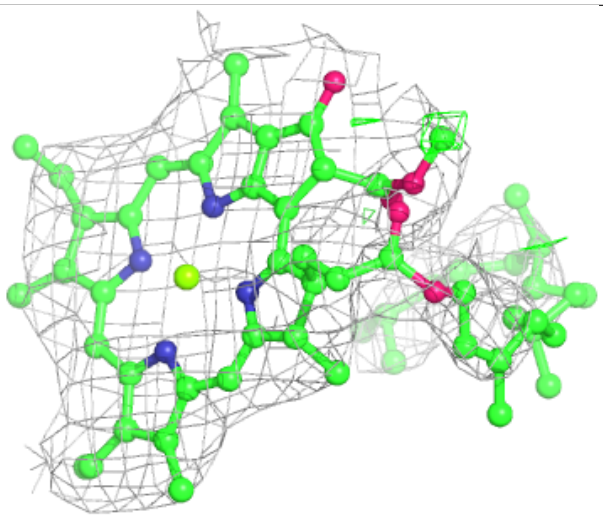




Electron density around CLA 2 603:

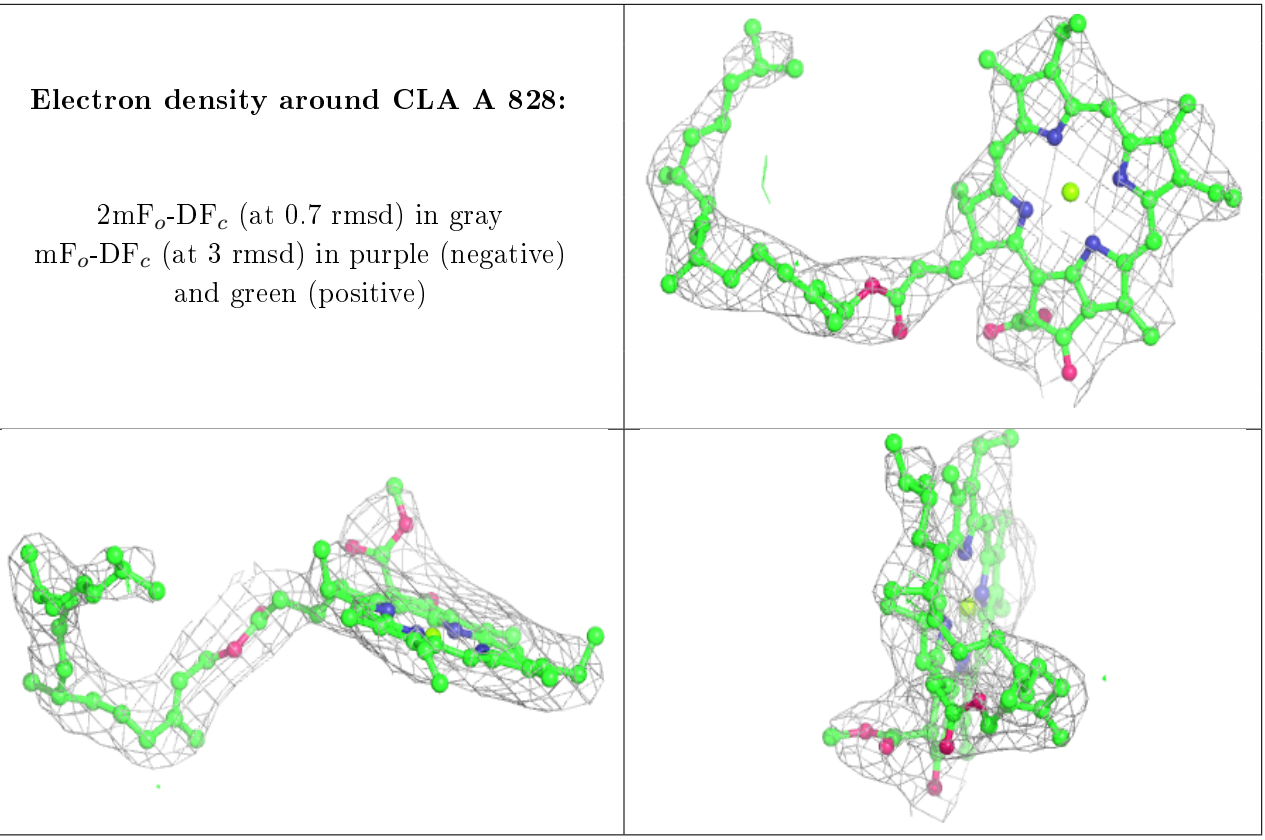
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)





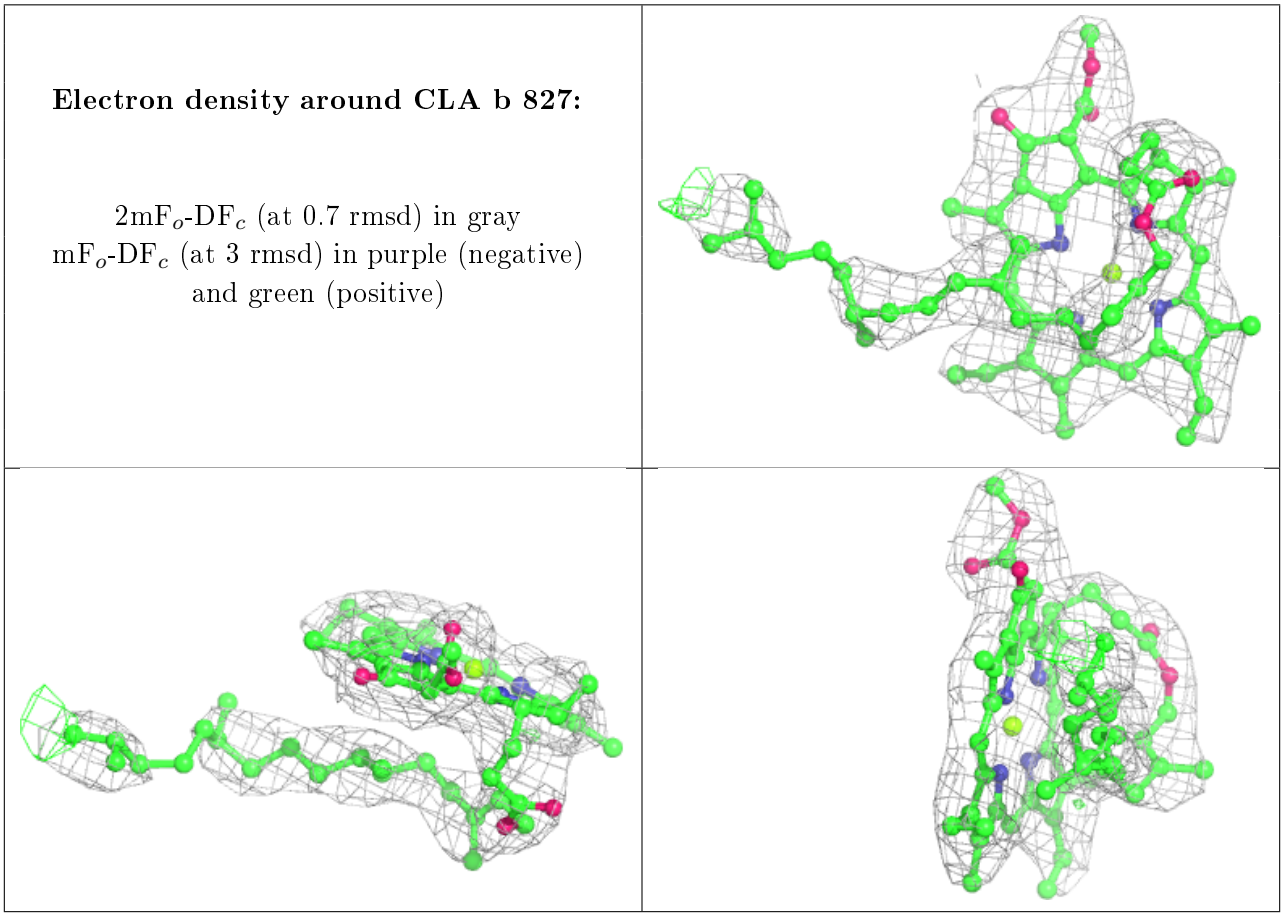
Electron density around CLA A 828:

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



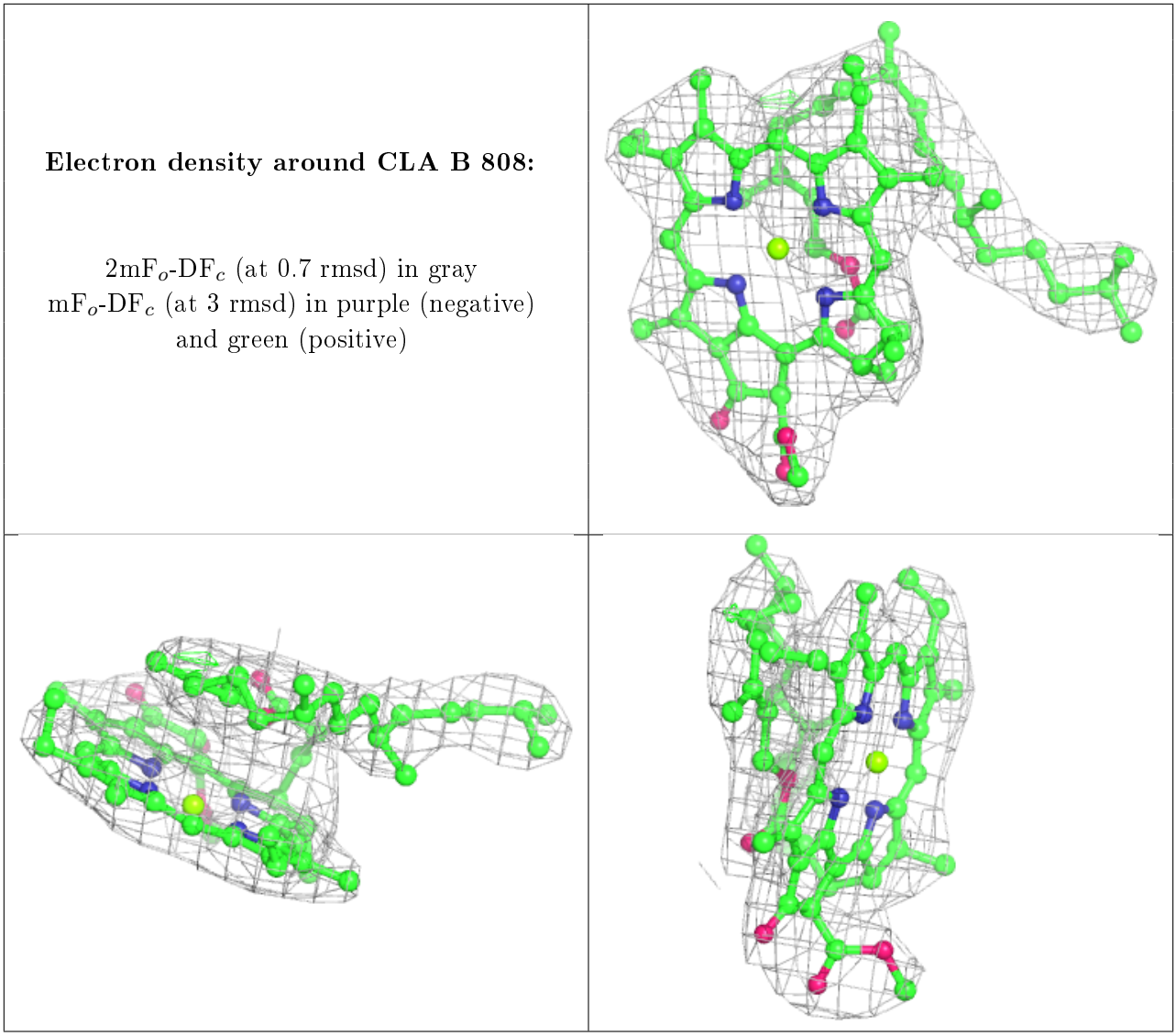
Electron density around CLA b 827:

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



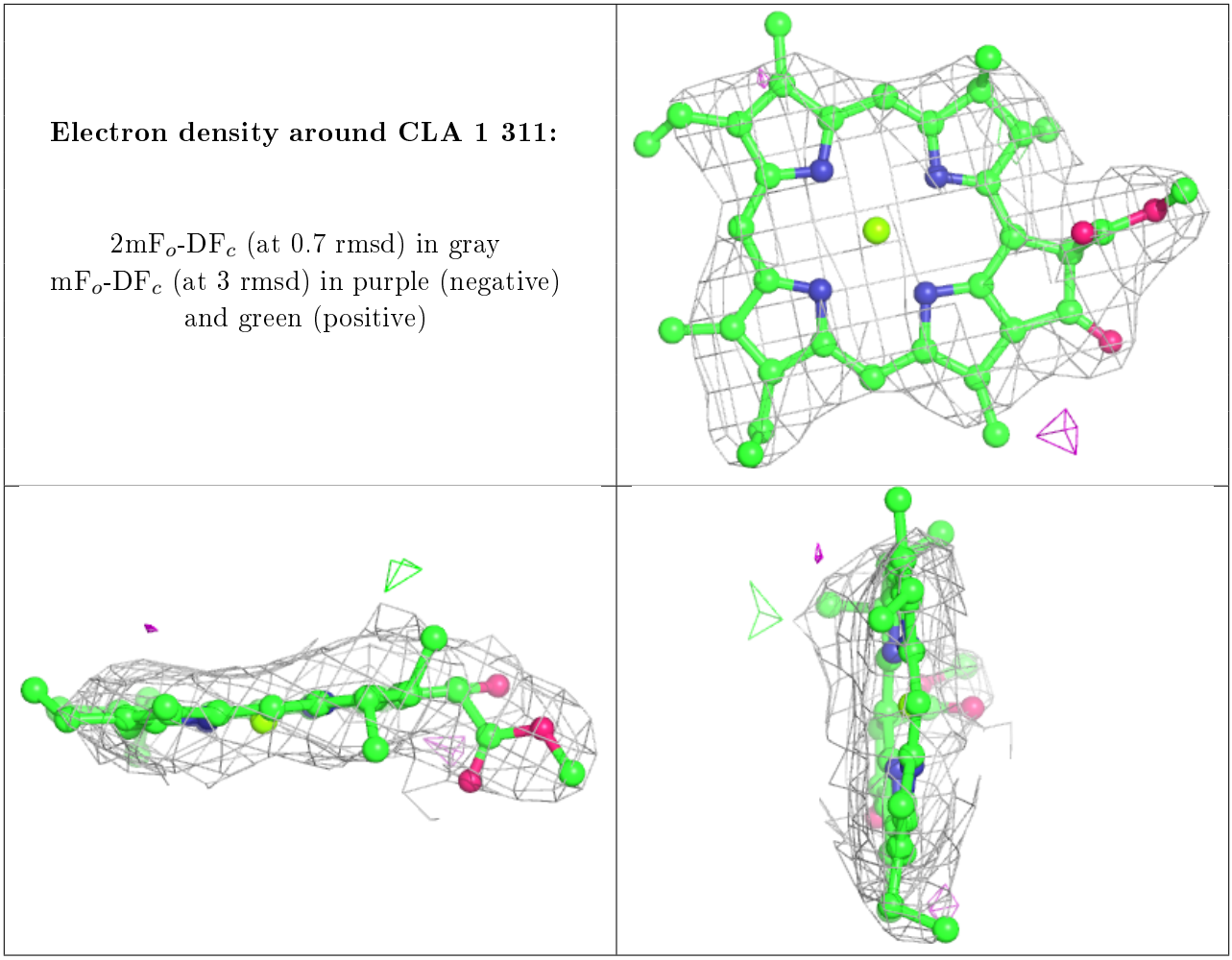
Electron density around CLA B 808:

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



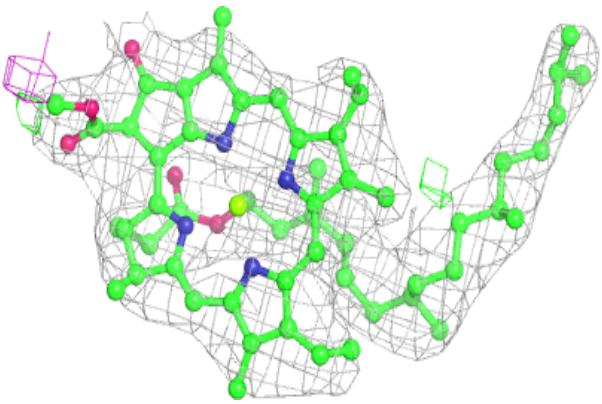
Electron density around CLA 1 311:

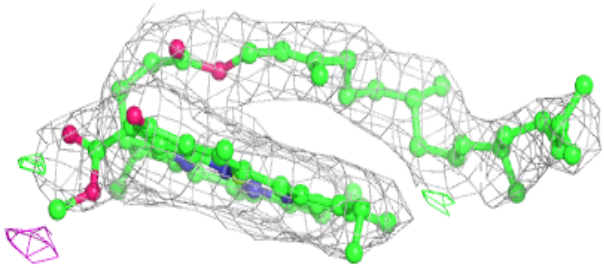
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

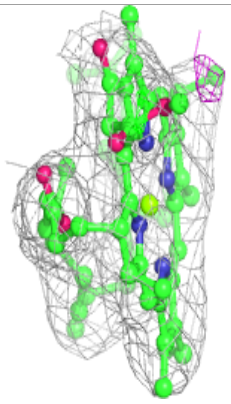


Electron density around CLA b 837:

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

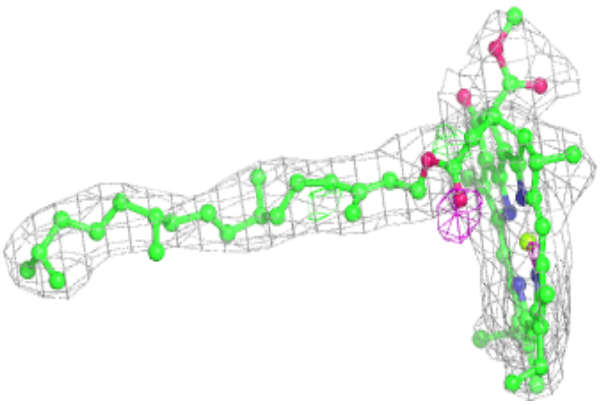


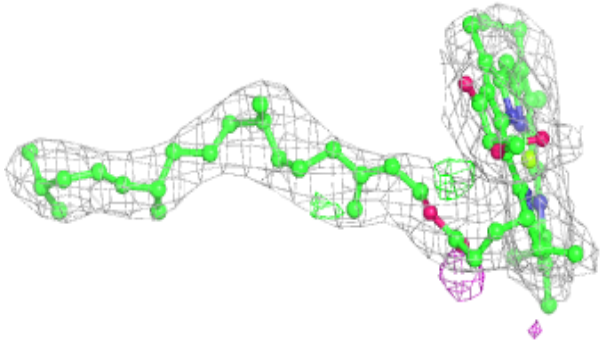


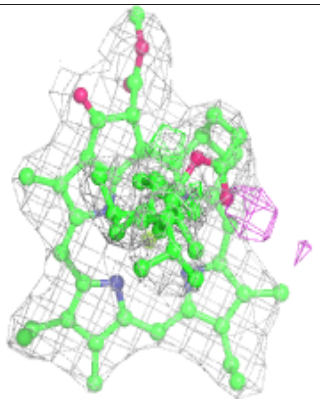


Electron density around CLA a 829:

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

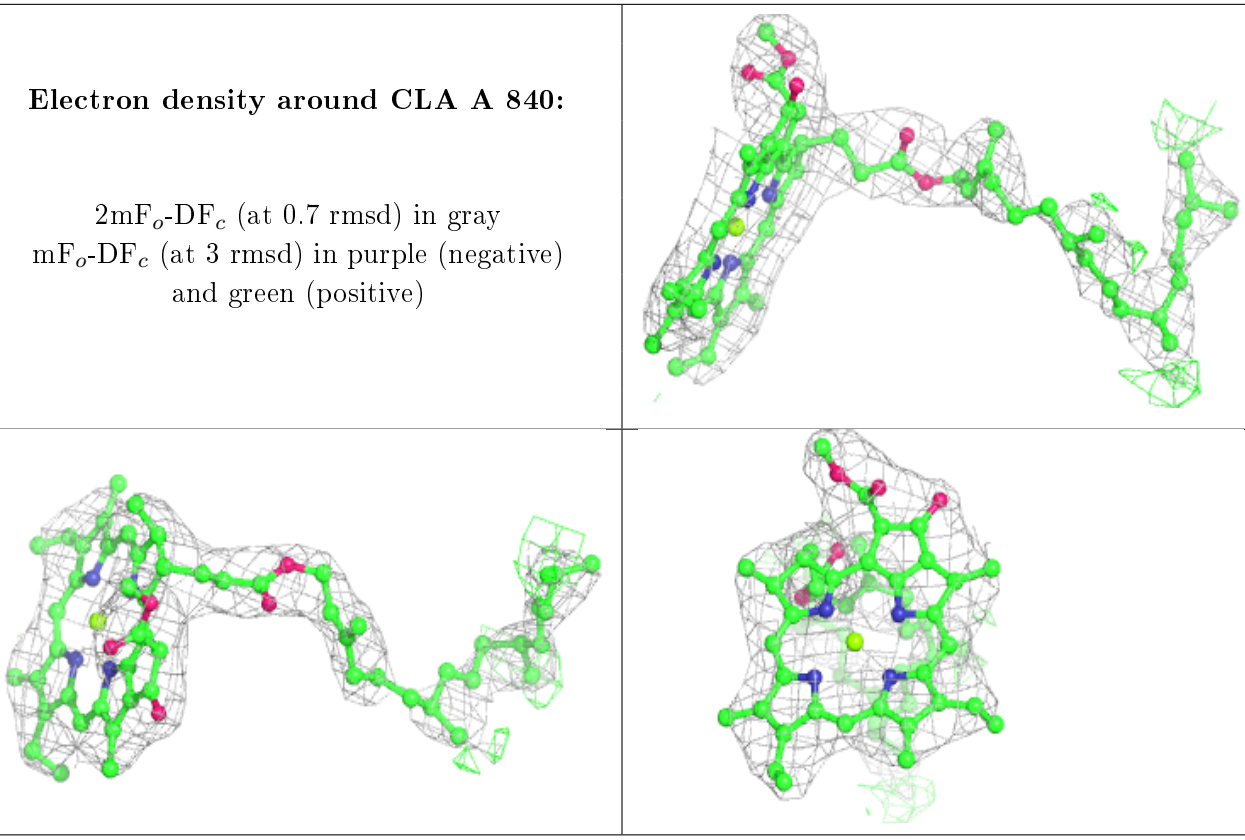






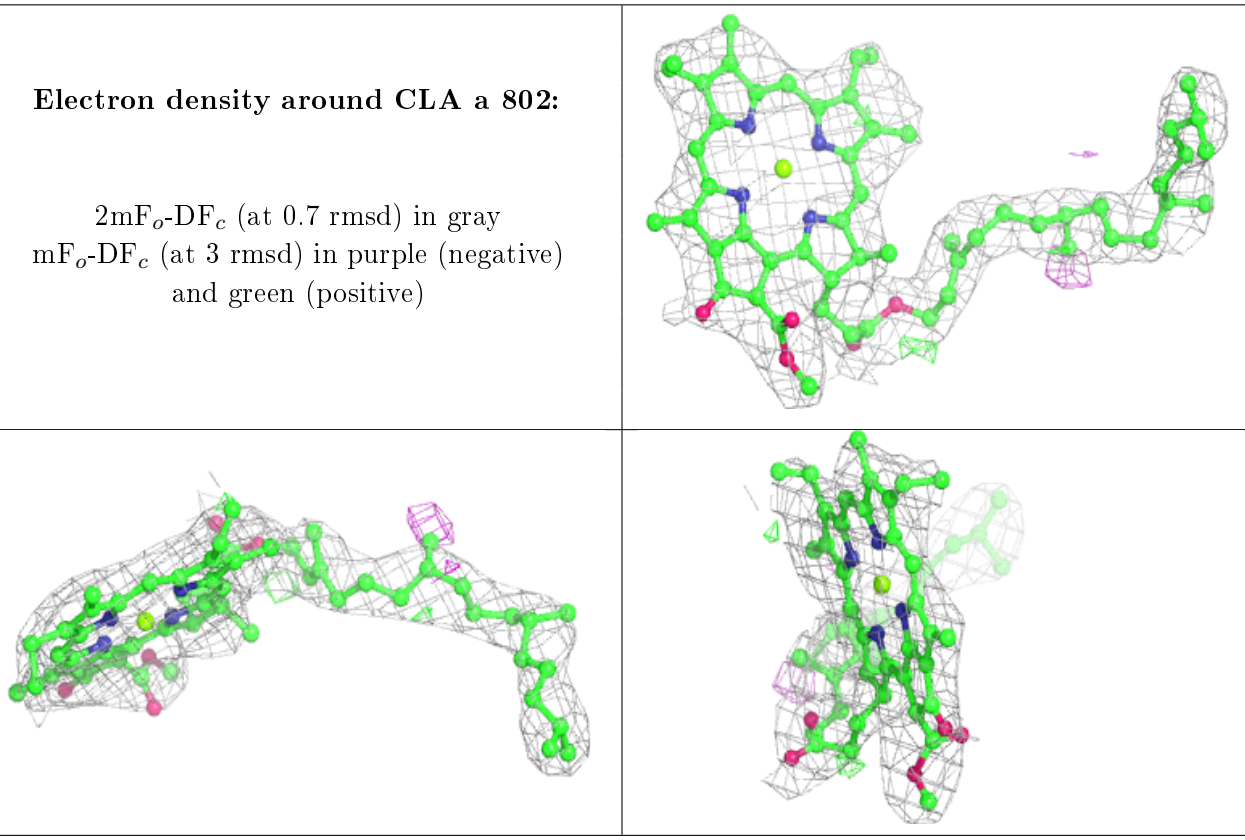
Electron density around CLA A 840:

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



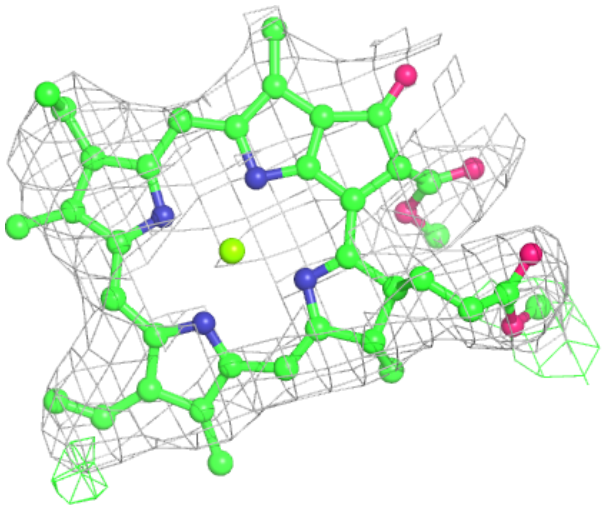
Electron density around CLA a 802:

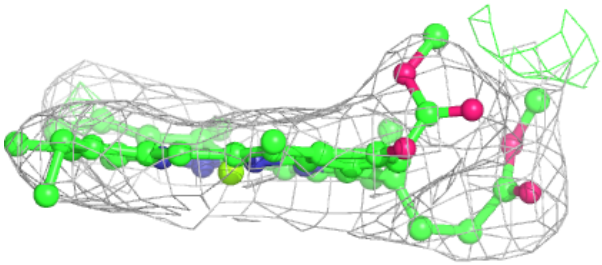
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

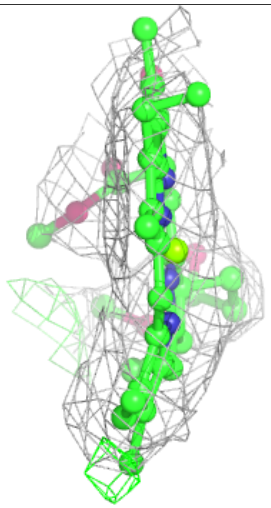


Electron density around CLA 9 603:

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

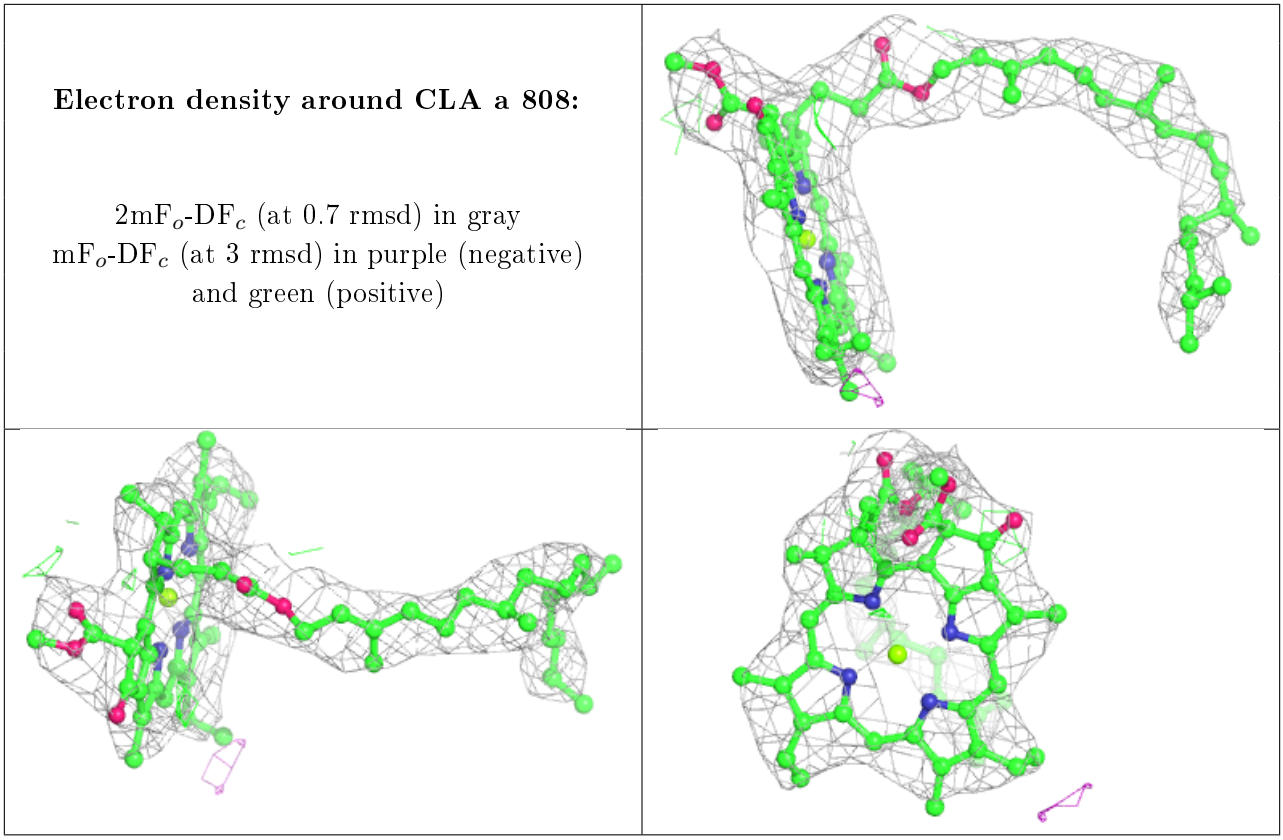






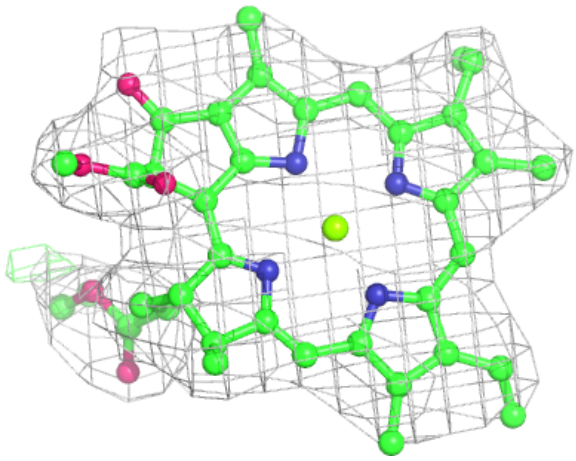
Electron density around CLA a 808:

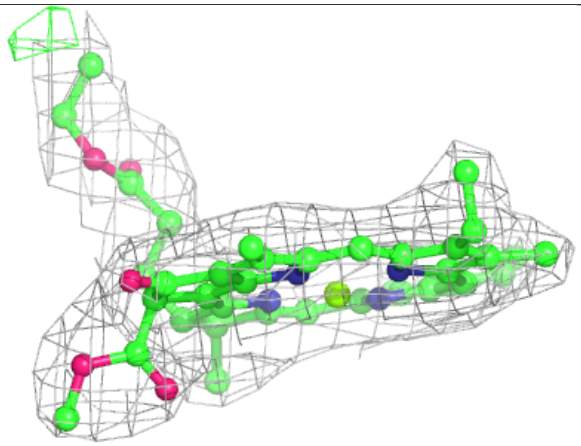
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

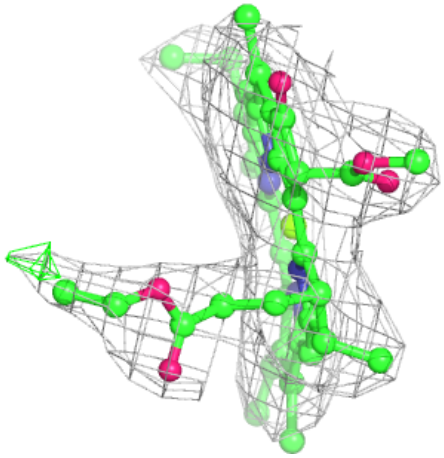


Electron density around CLA b 838:

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

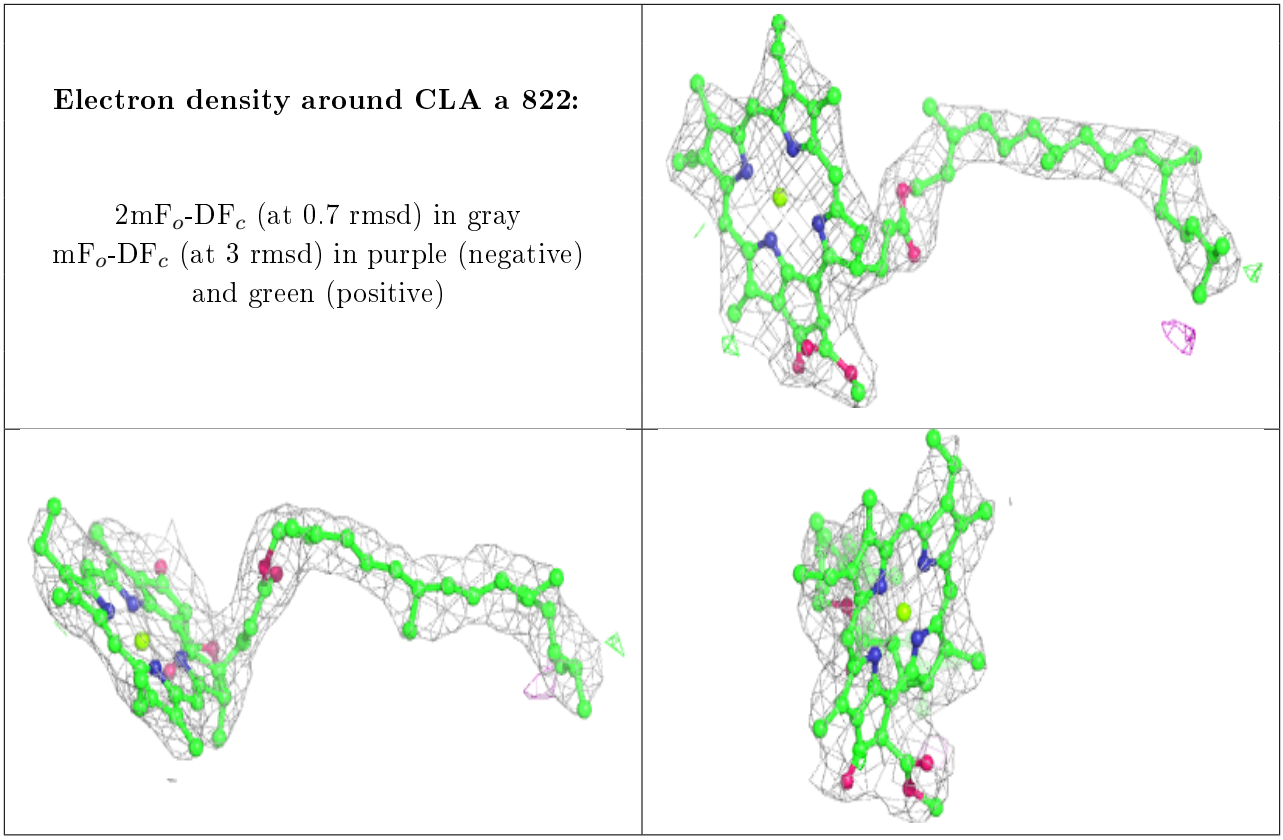






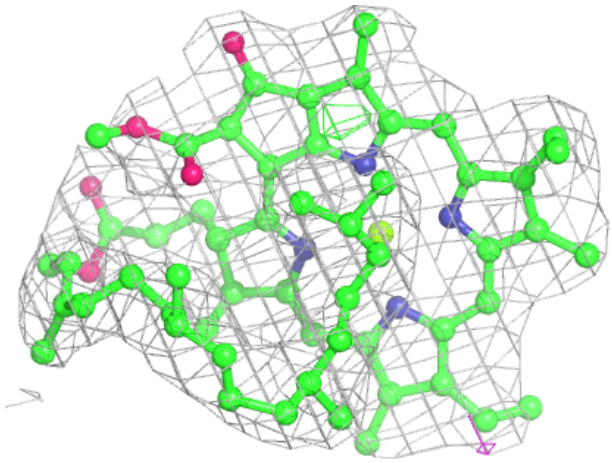
Electron density around CLA a 822:

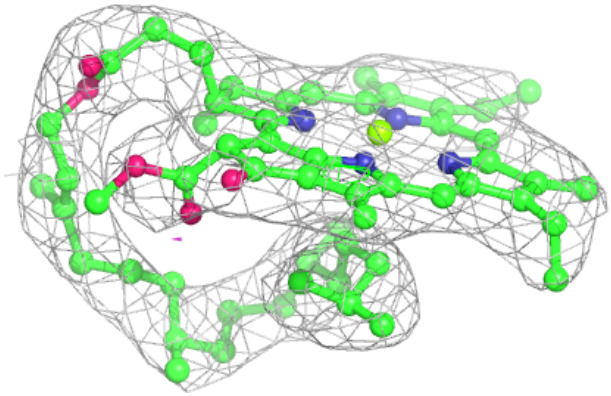
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

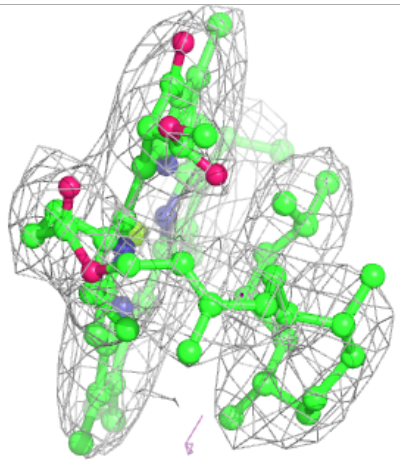


Electron density around CLA b 806:

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

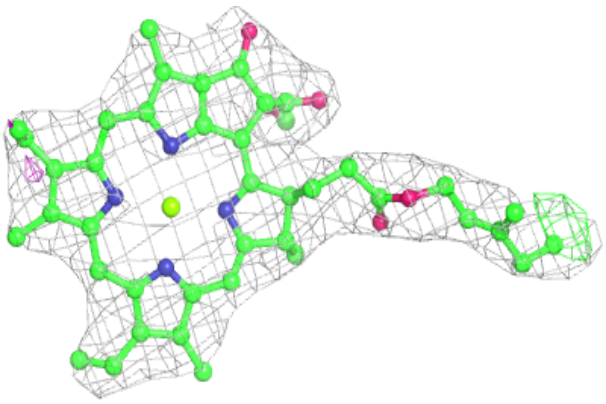


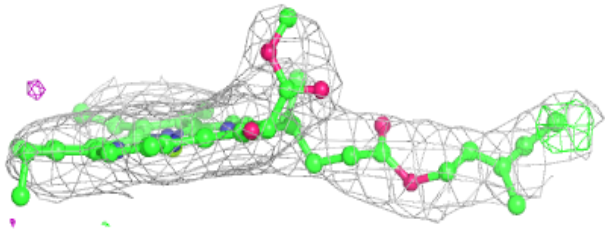


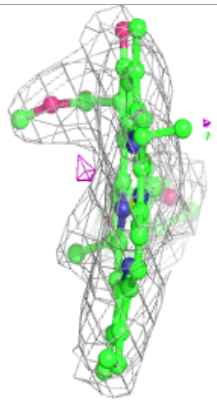


Electron density around CLA a 838:

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

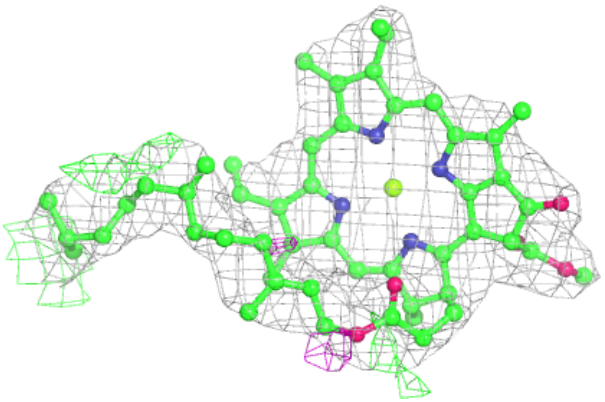


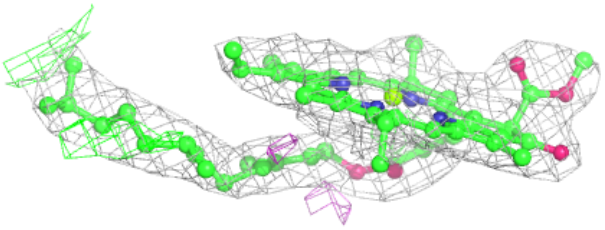


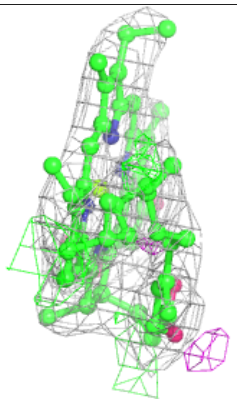


Electron density around CLA b 818:

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

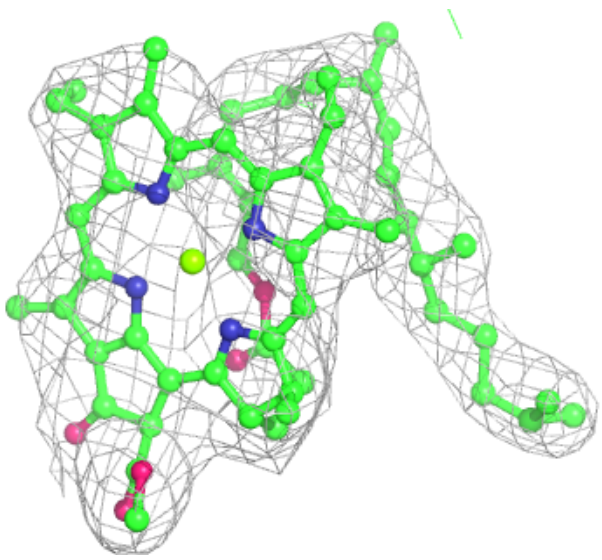


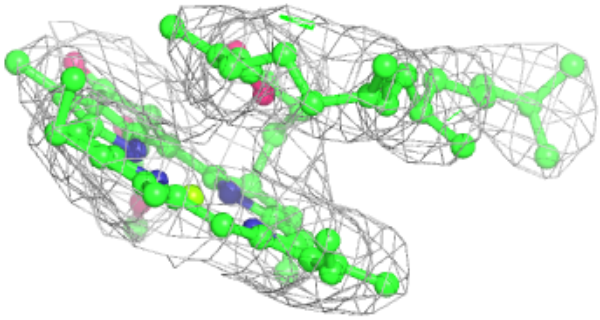


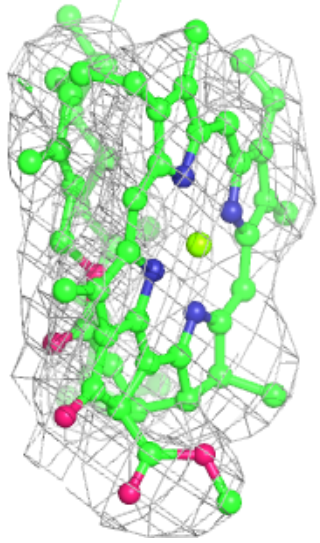


Electron density around CLA b 808:

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

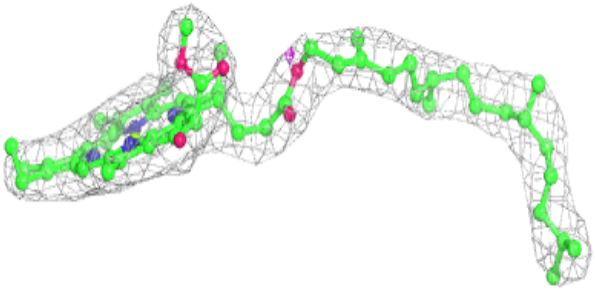


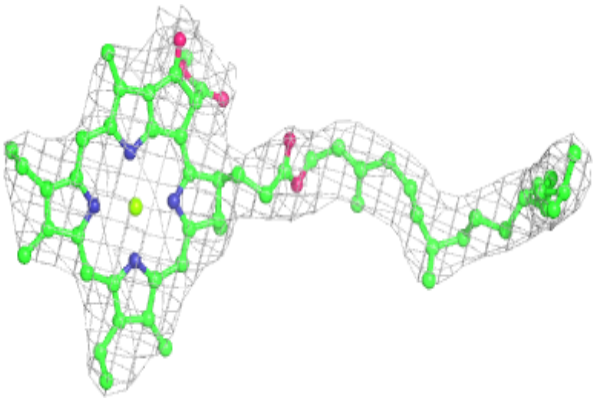


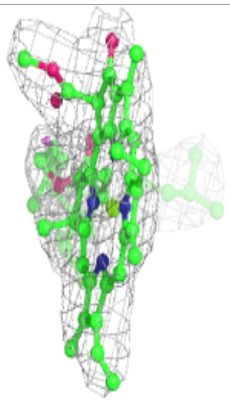


Electron density around CLA a 806:

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

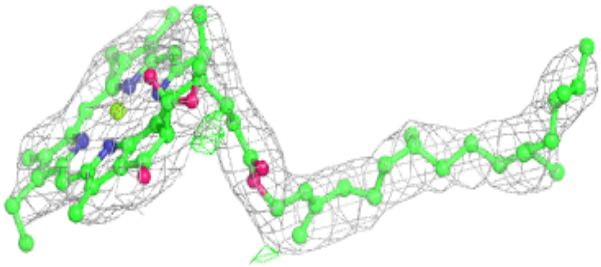


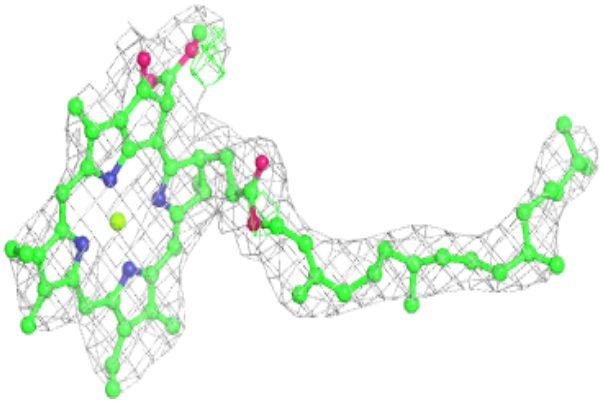


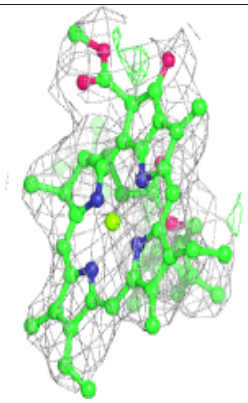


Electron density around CLA A 822:

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

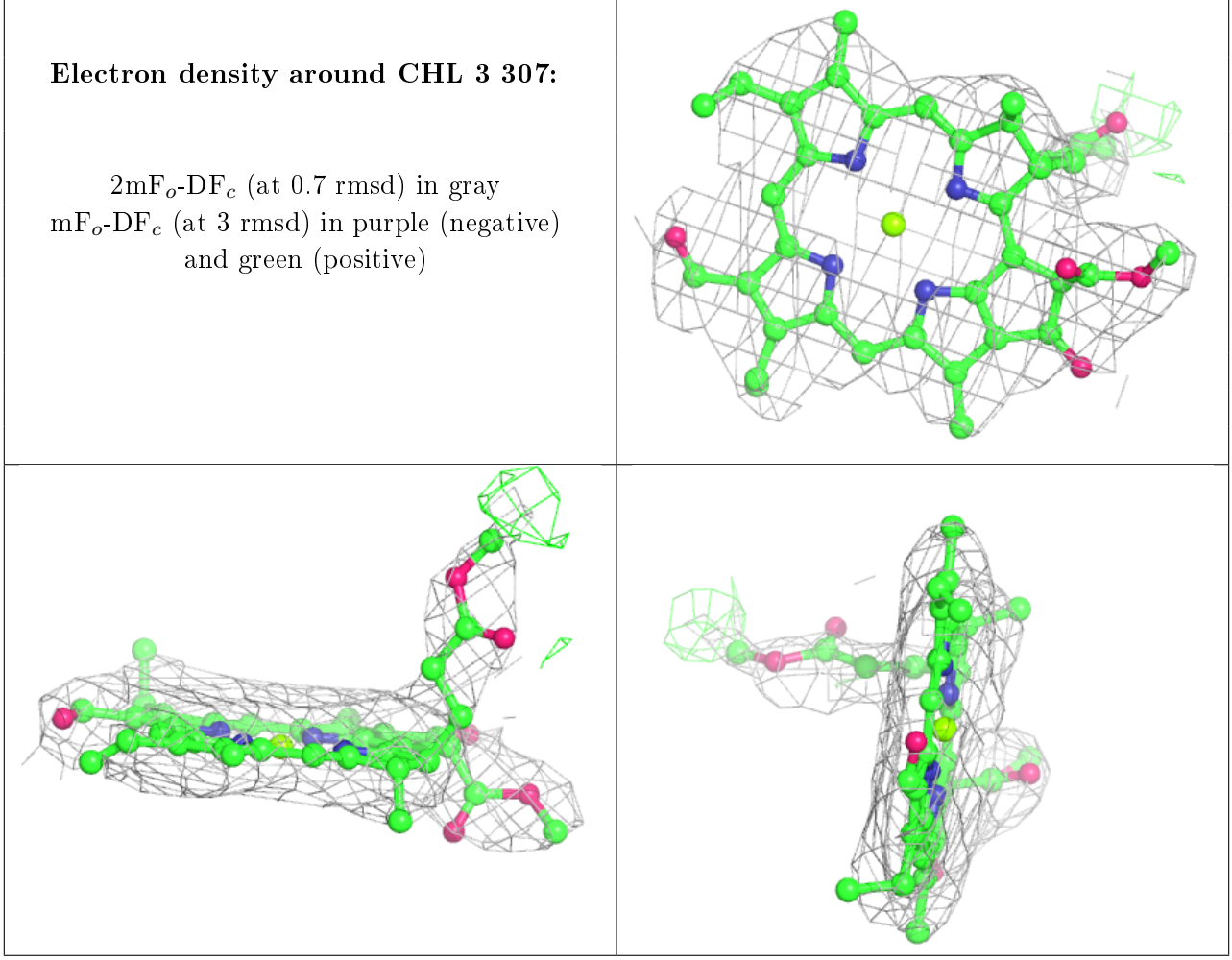






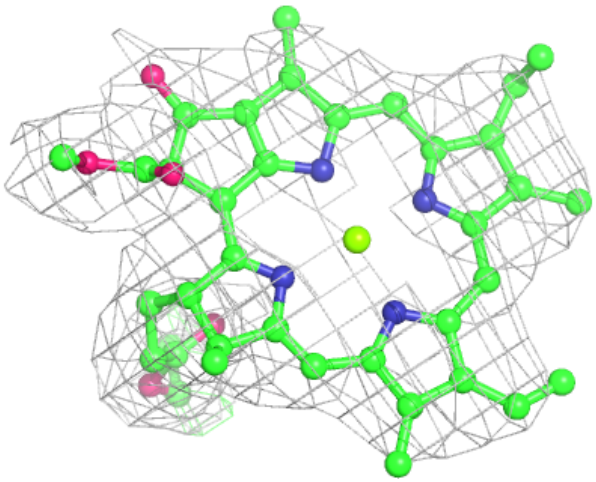
Electron density around CHL 3 307:

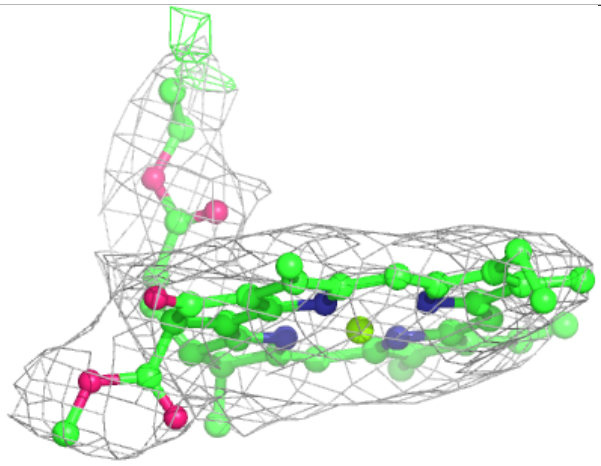
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

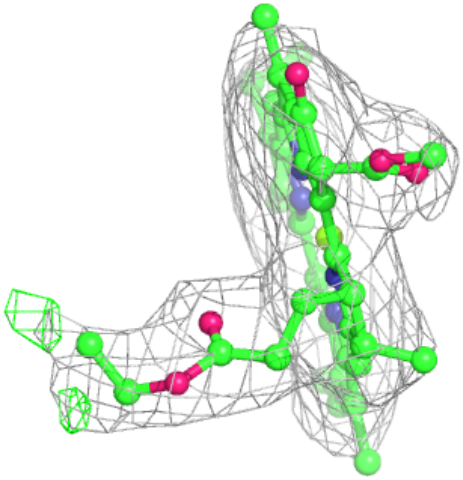


Electron density around CLA 8 305:

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

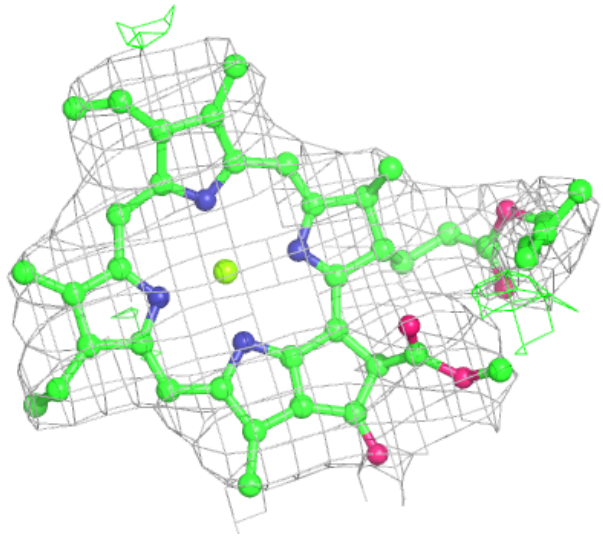


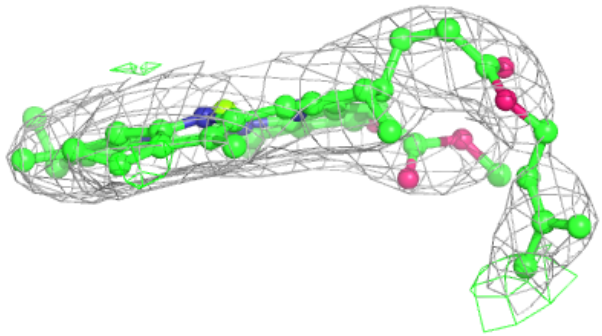


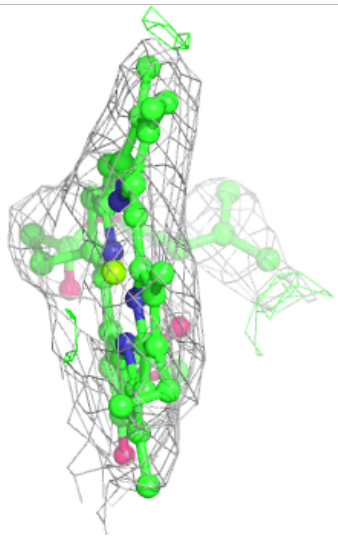


Electron density around CLA 3 303:

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

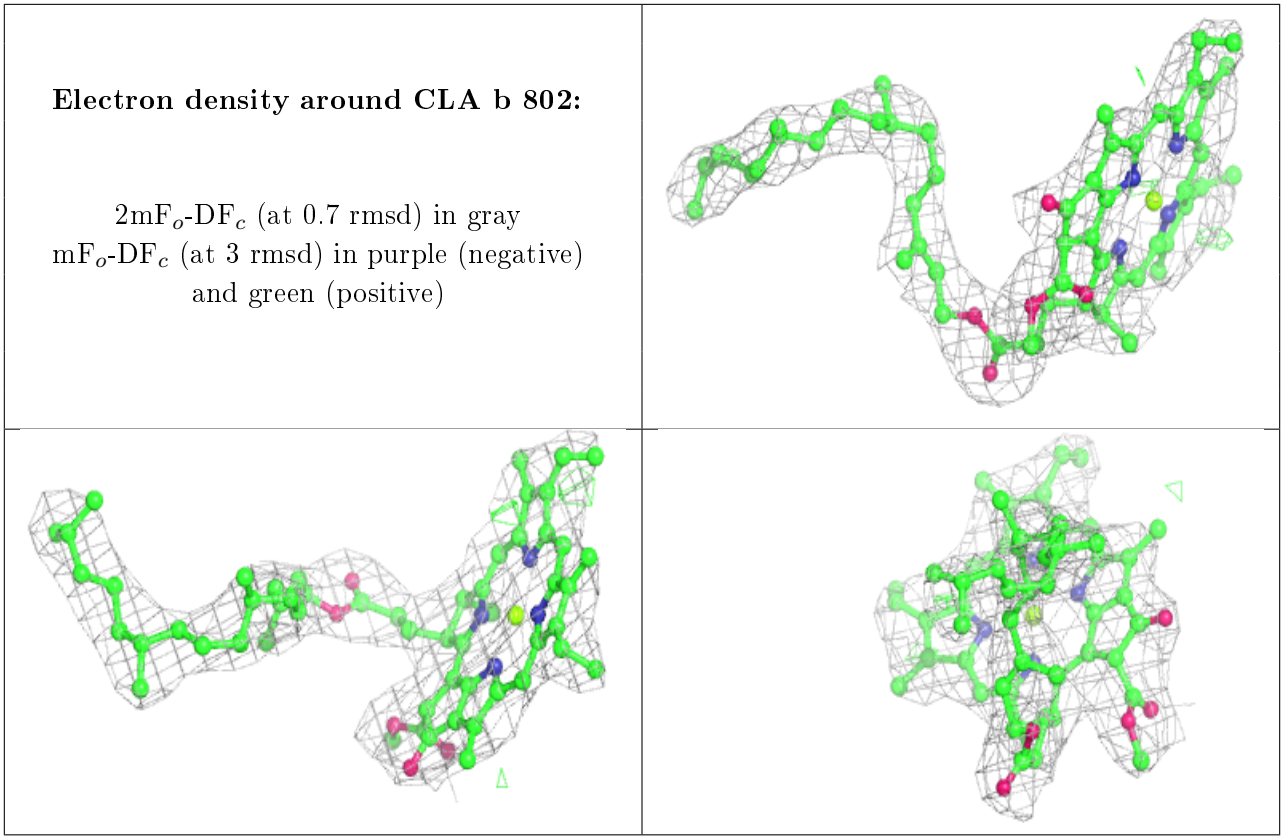






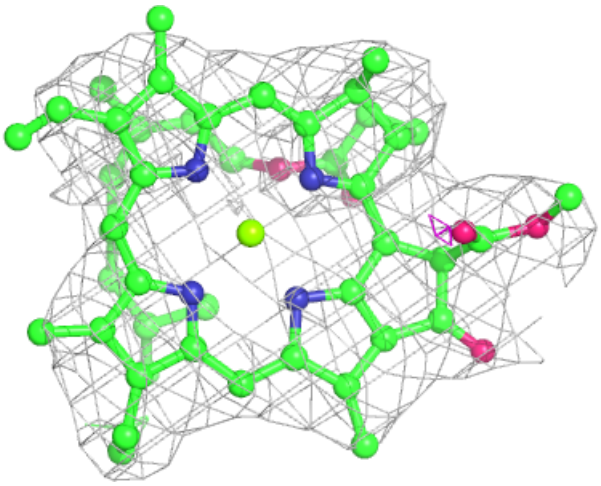
Electron density around CLA b 802:

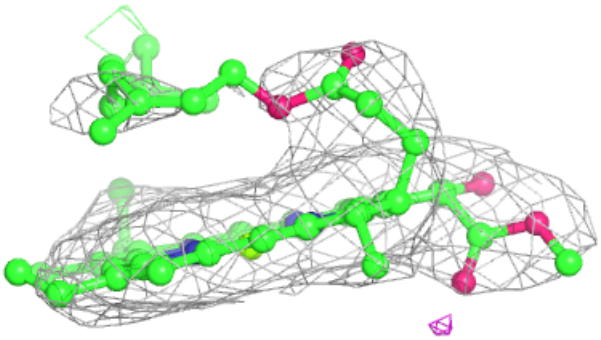
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

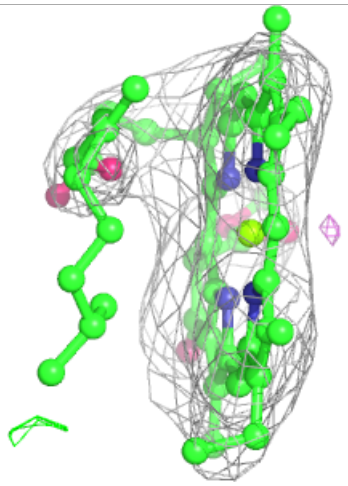


Electron density around CLA B 812:

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

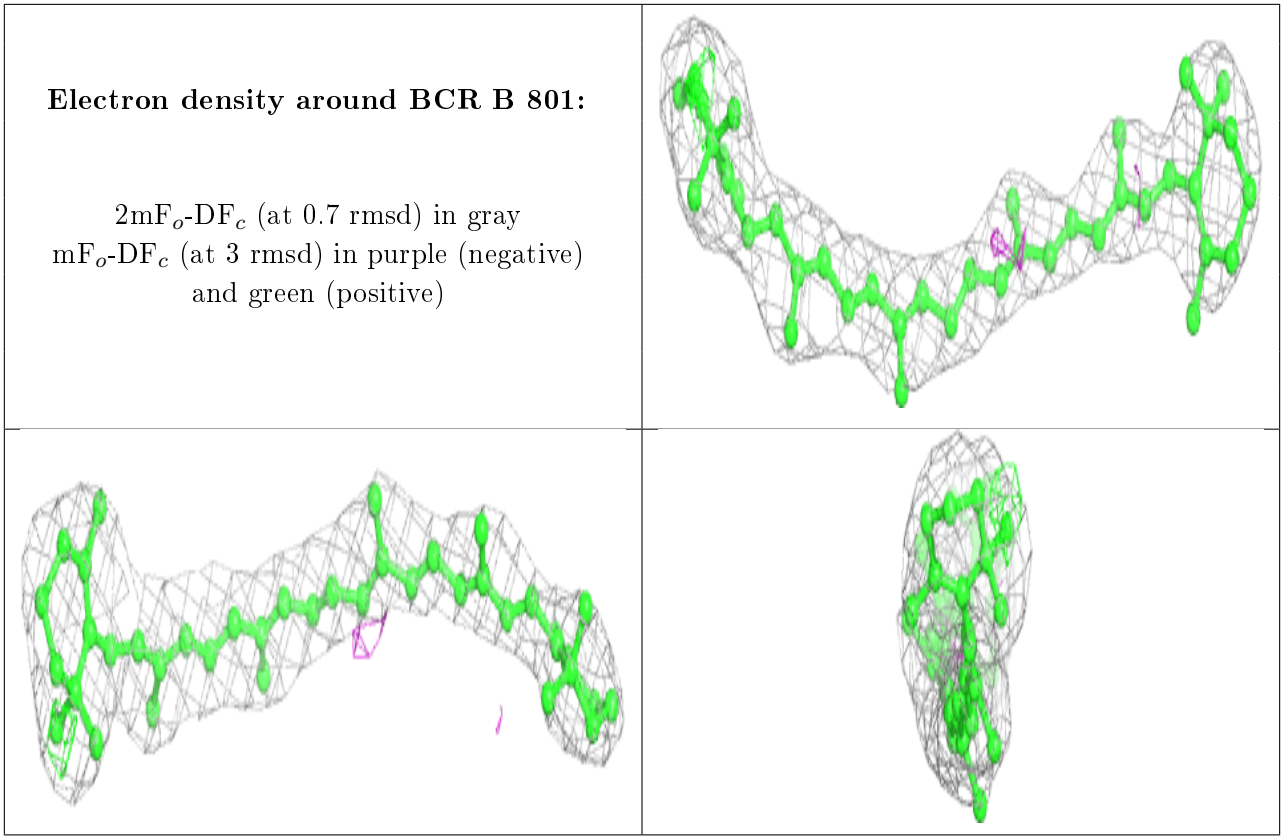






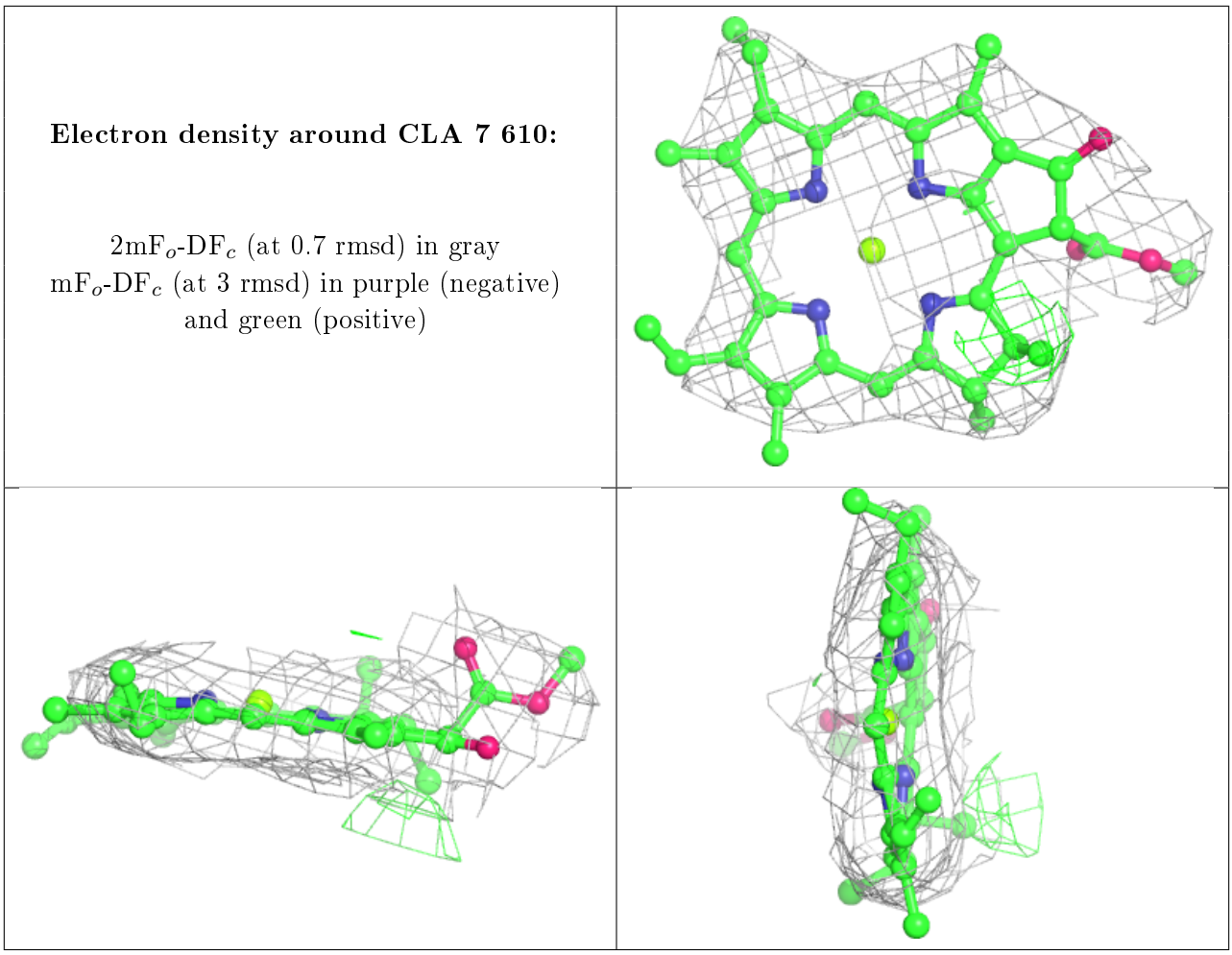
Electron density around BCR B 801:

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



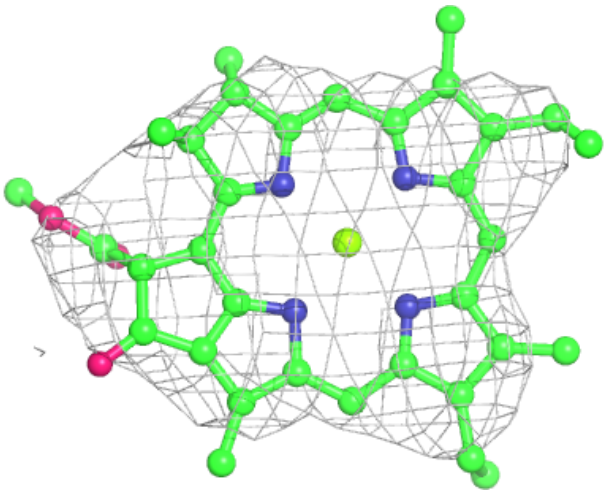
Electron density around CLA 7 610:

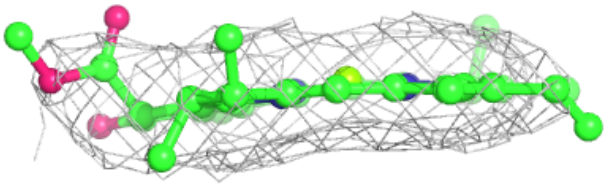
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

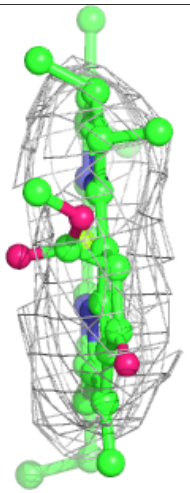


Electron density around CLA 9 610:

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

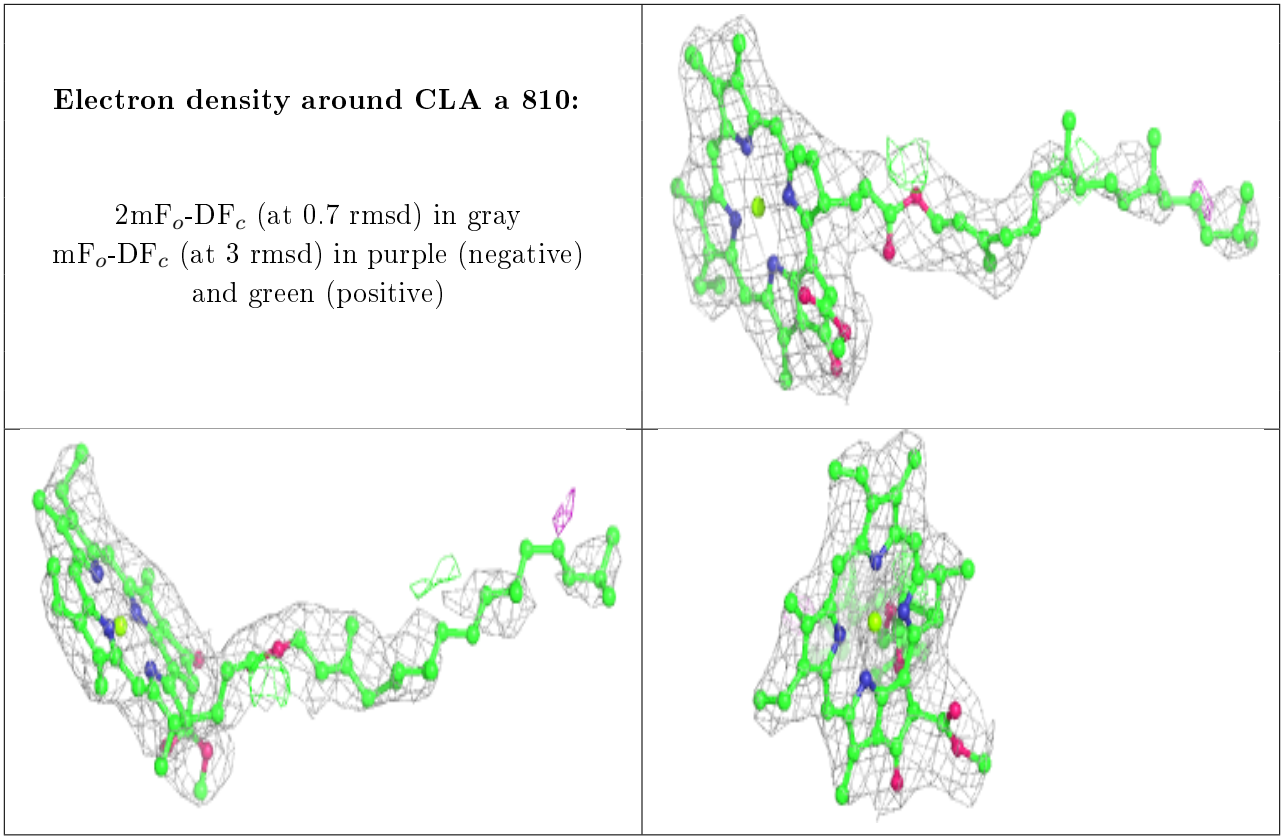






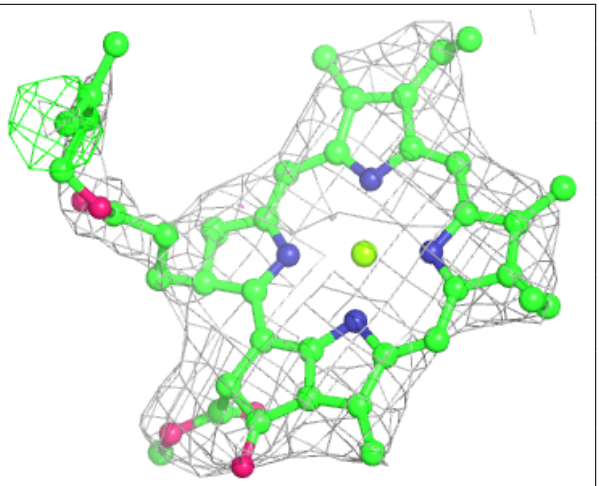
Electron density around CLA a 810:

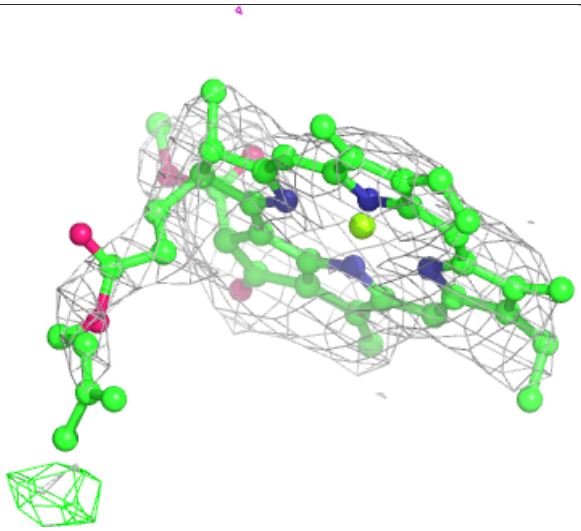
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

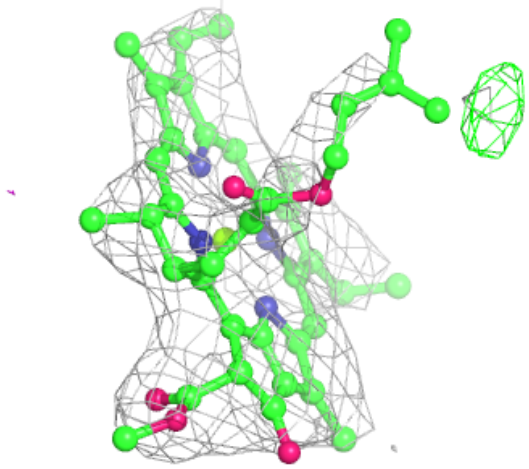


Electron density around CLA A 816:

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

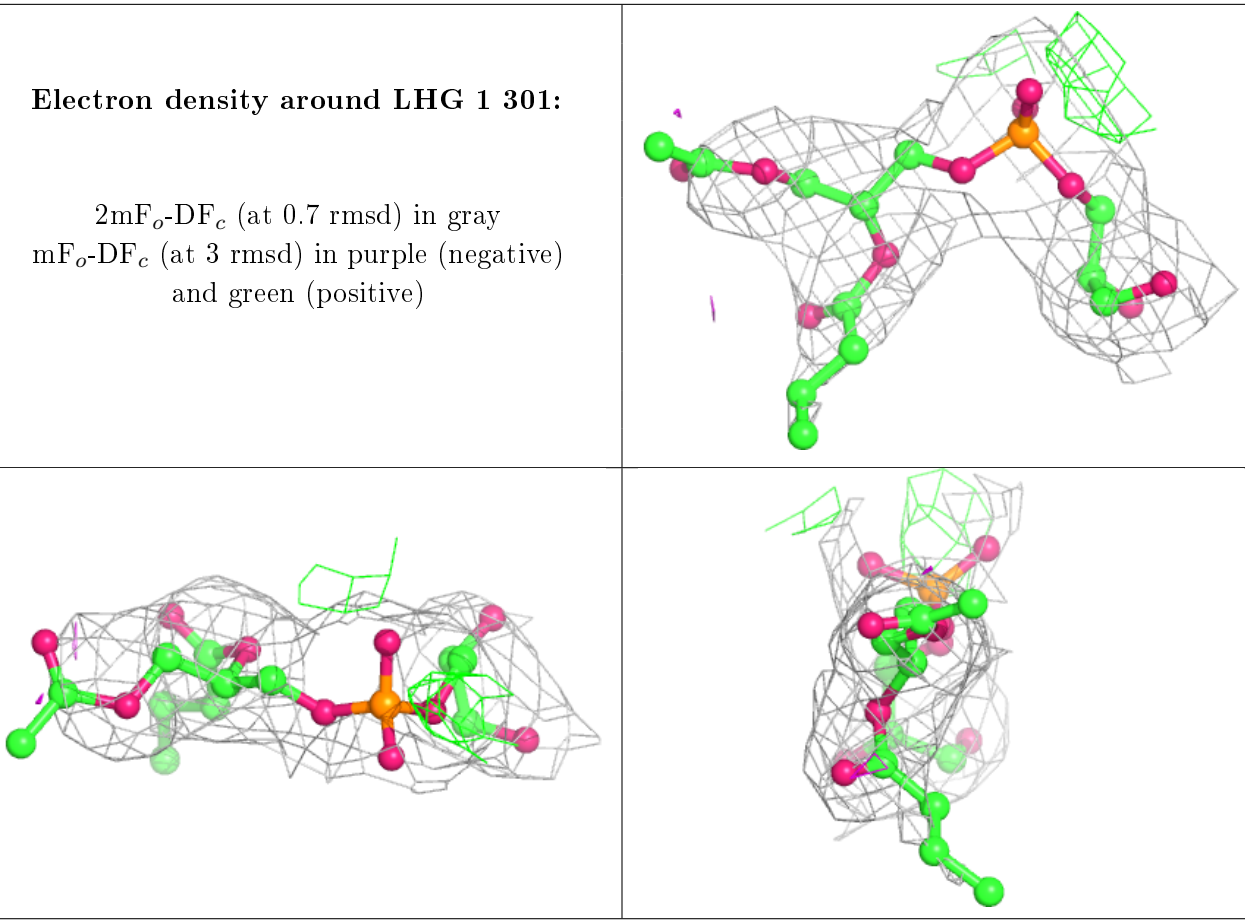






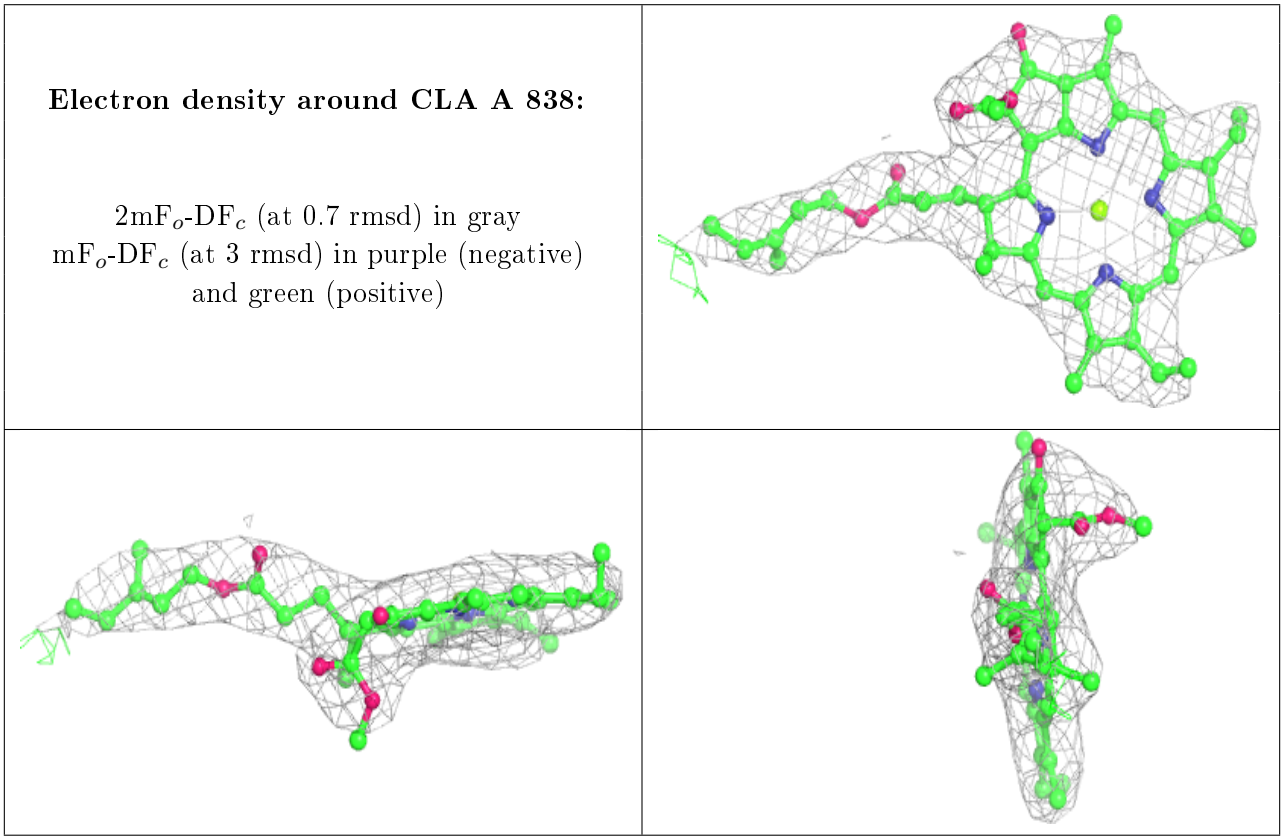
Electron density around LHG 1 301:

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



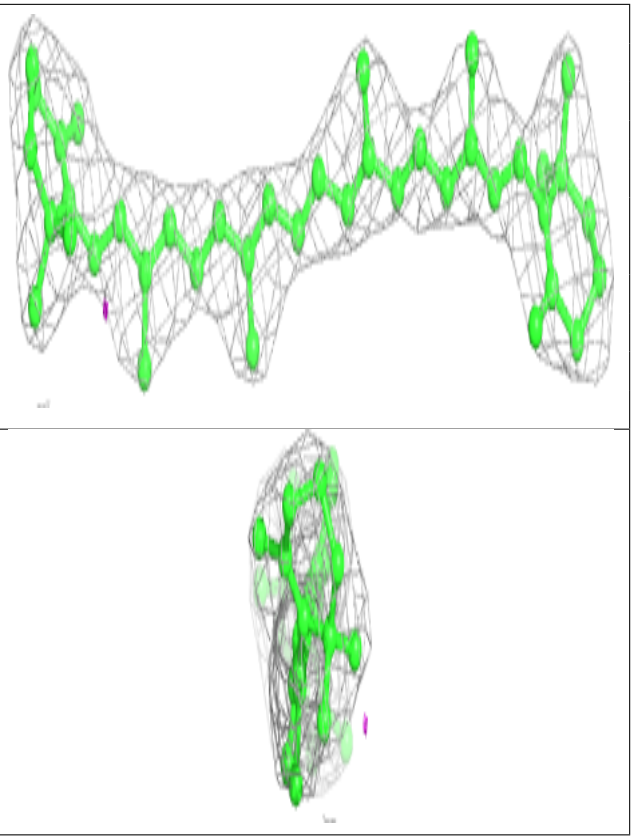
Electron density around CLA A 838:

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



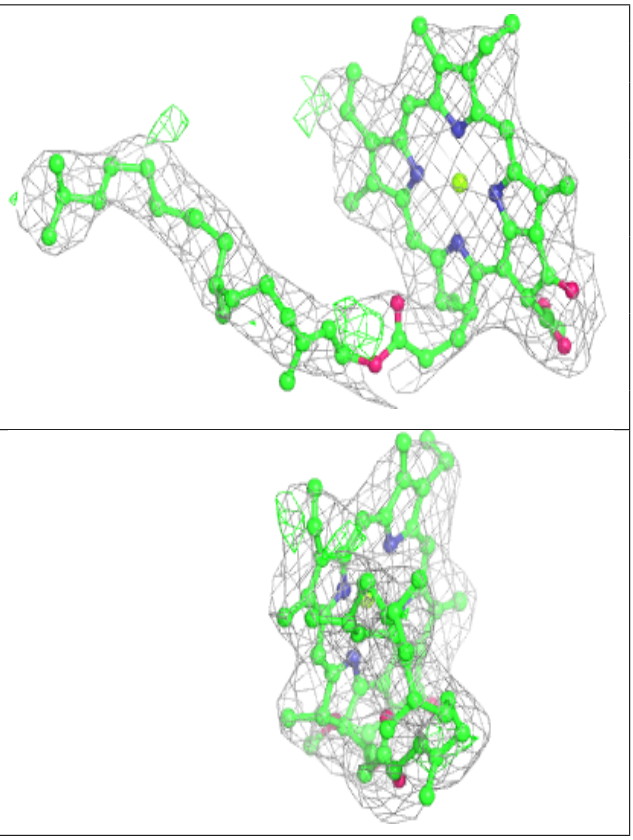
Electron density around BCR a 851:

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



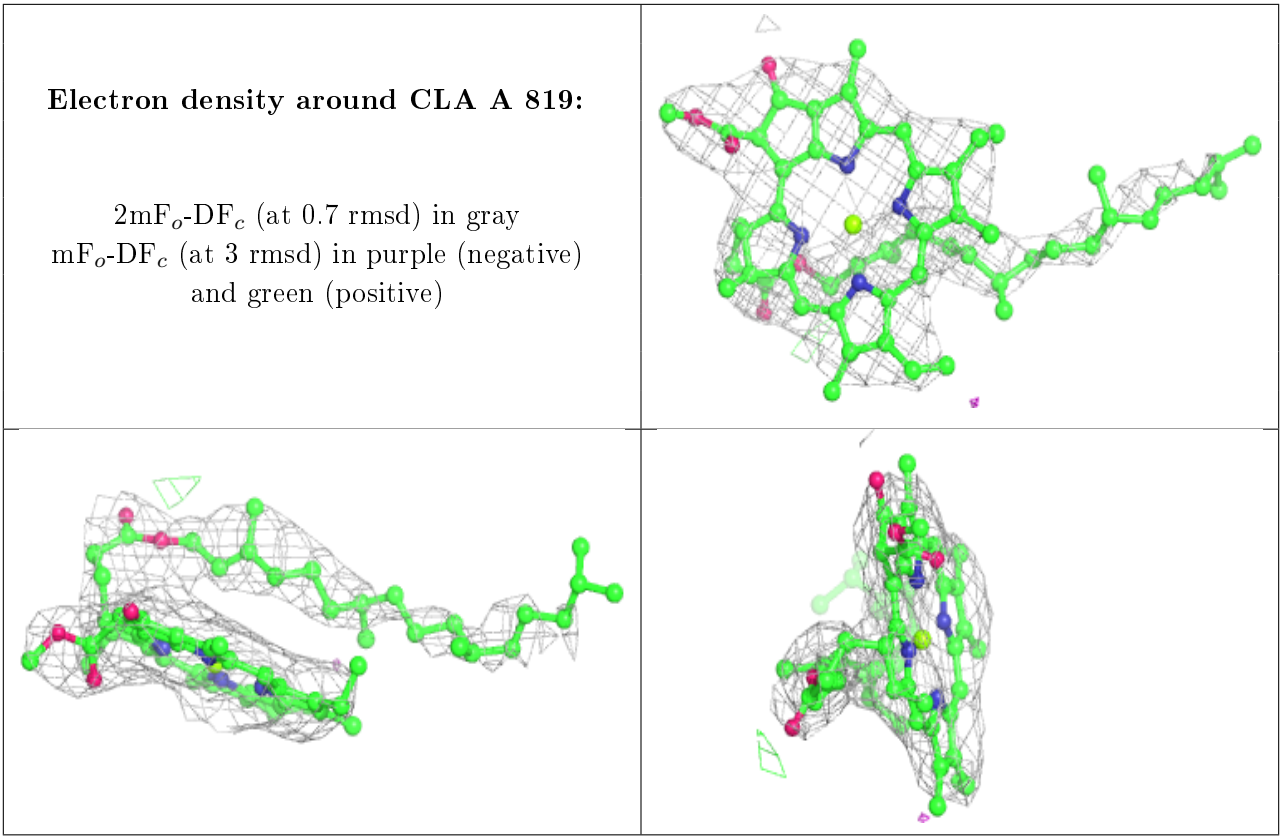
Electron density around CLA a 809:

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



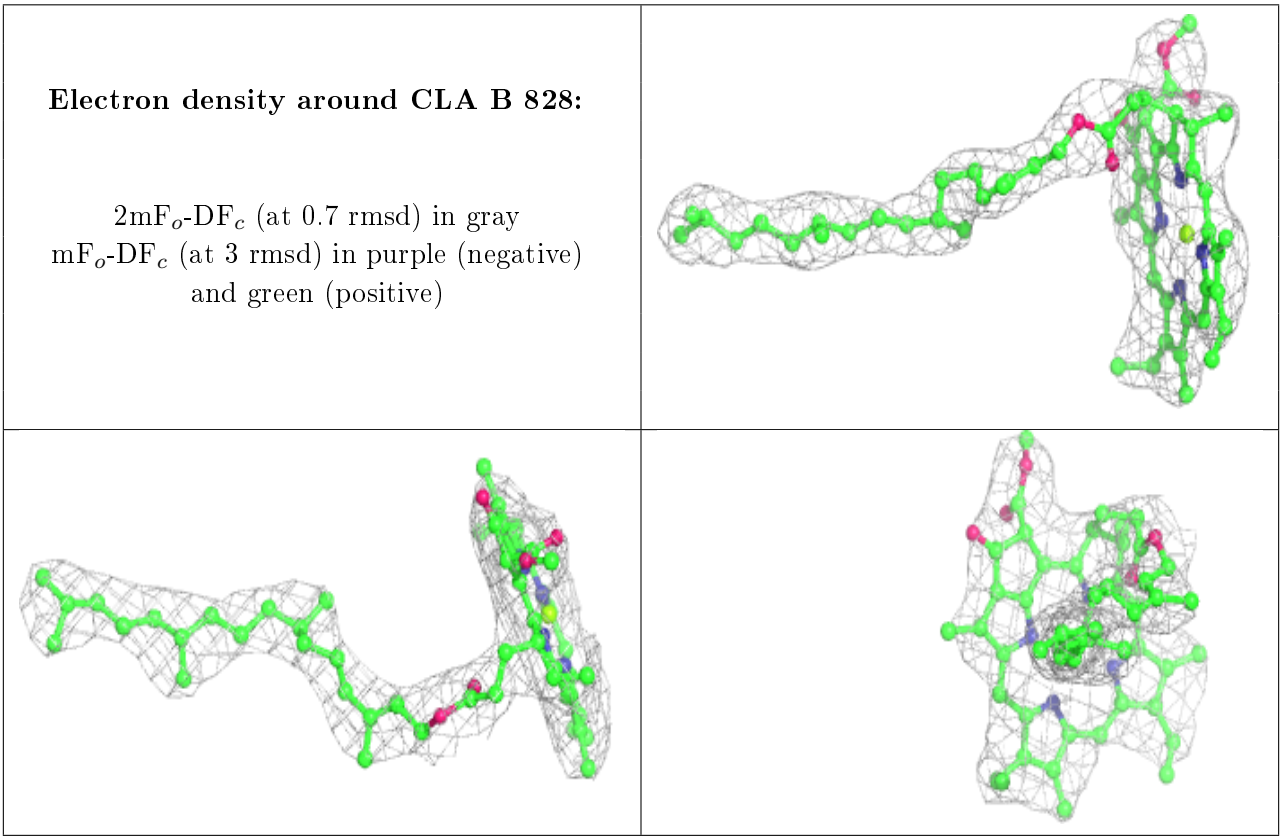
Electron density around CLA A 819:

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



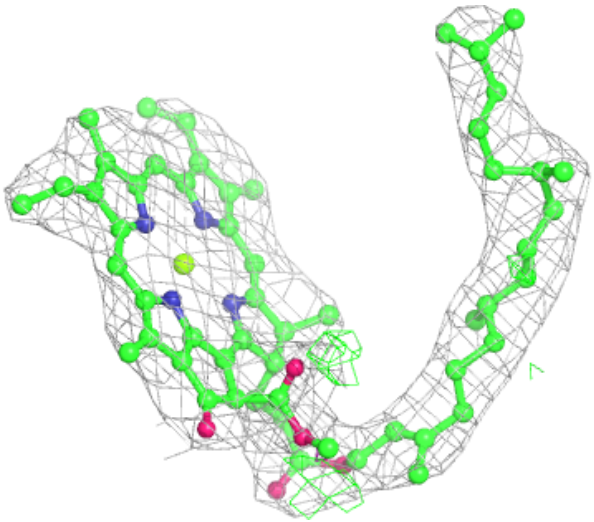
Electron density around CLA B 828:

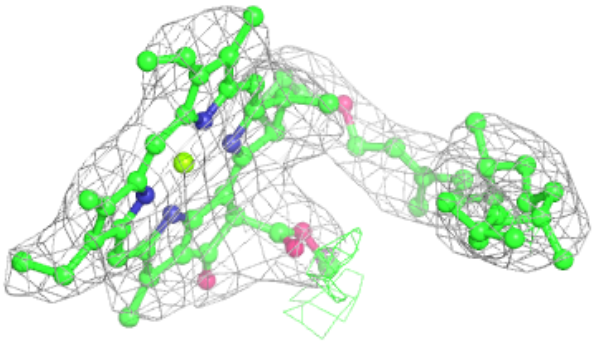
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

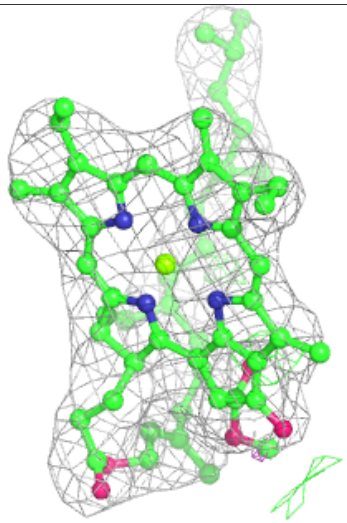


Electron density around CLA b 810:

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

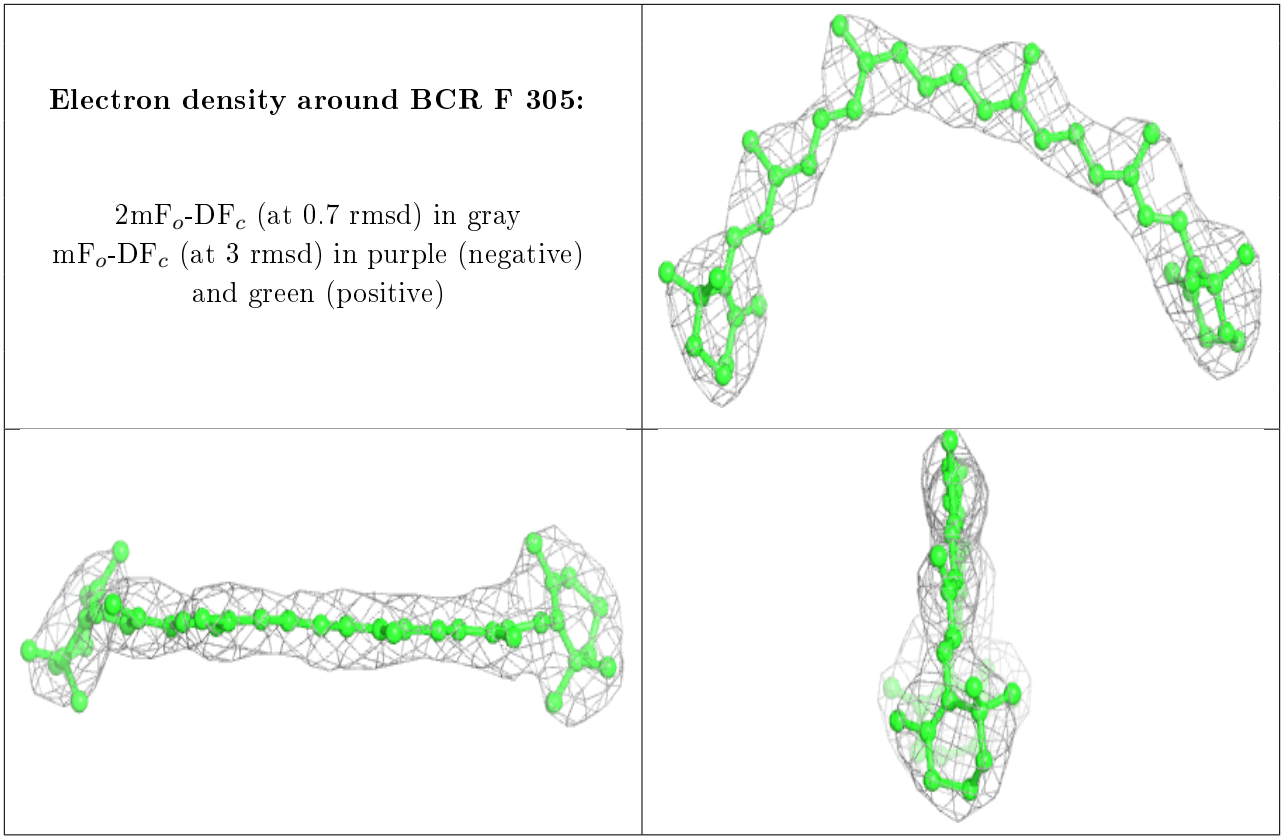






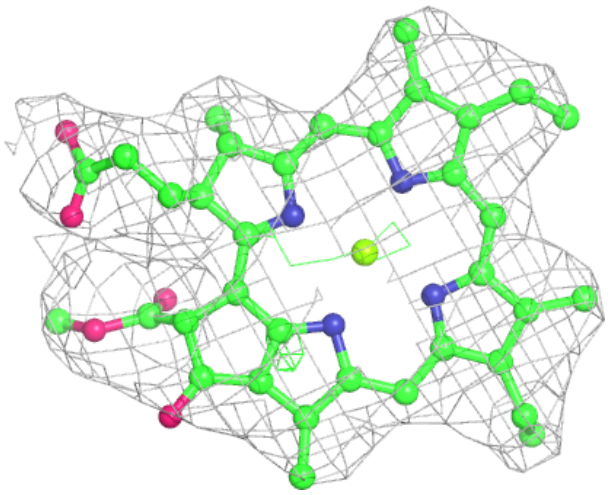
Electron density around BCR F 305:

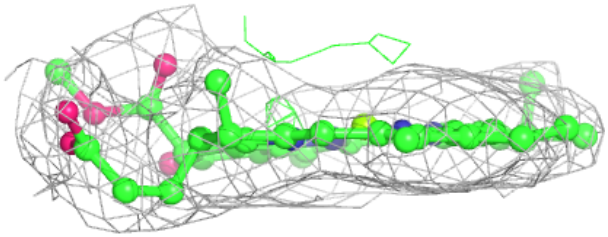
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

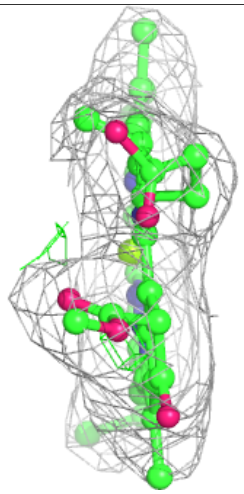


Electron density around CLA F 303:

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

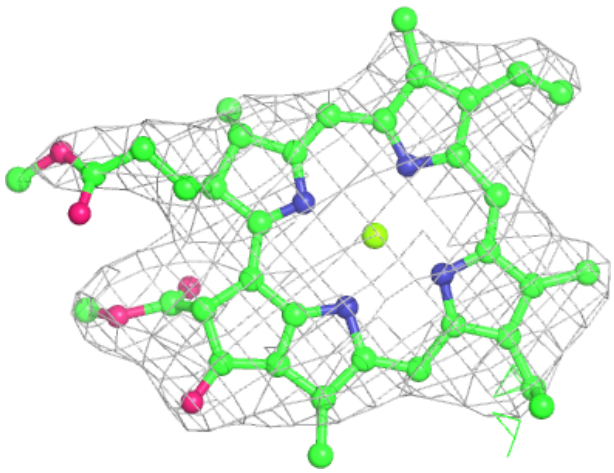


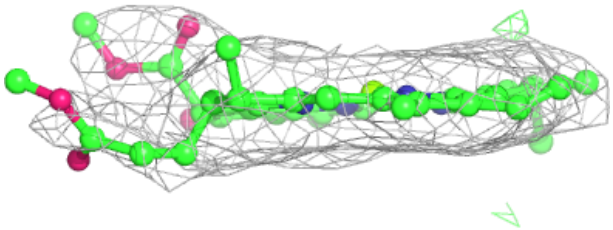


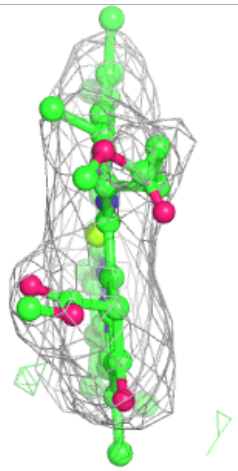


Electron density around CLA 8 312:

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

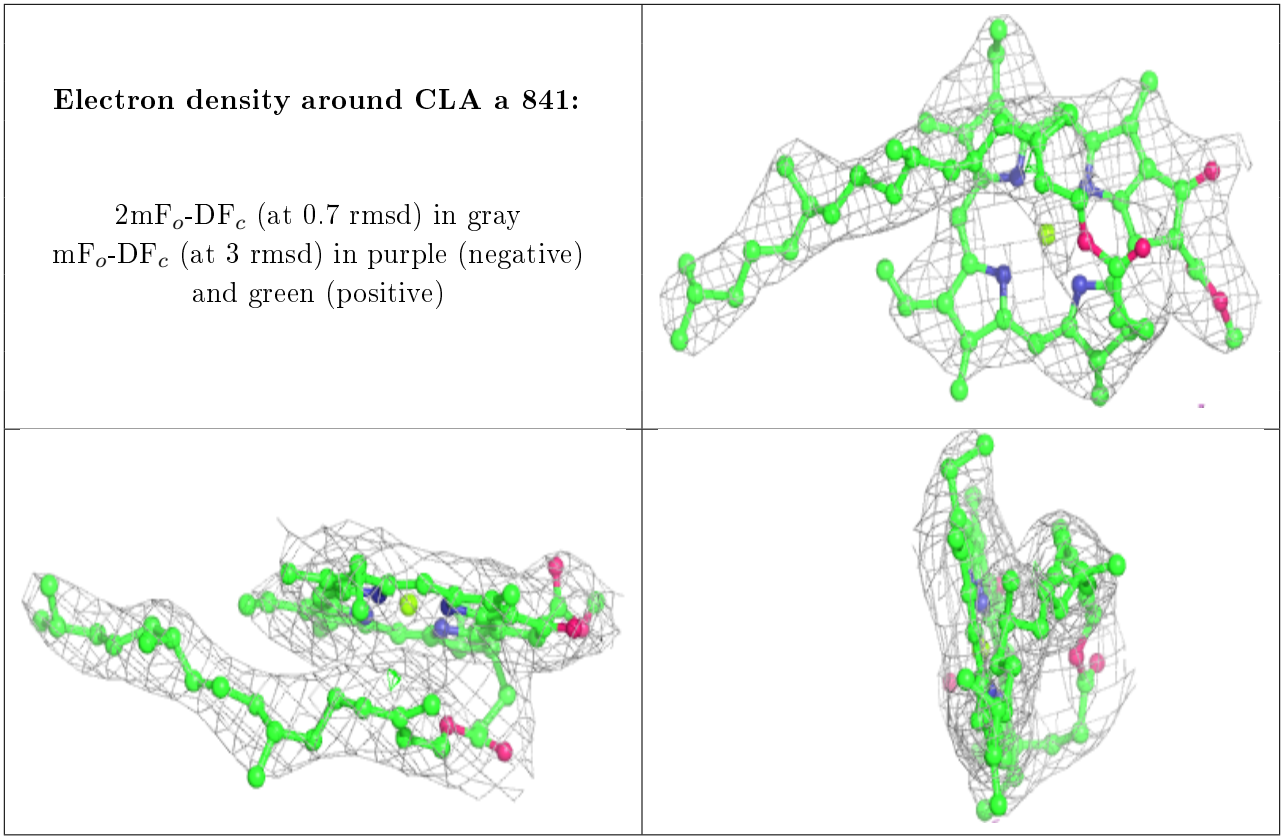






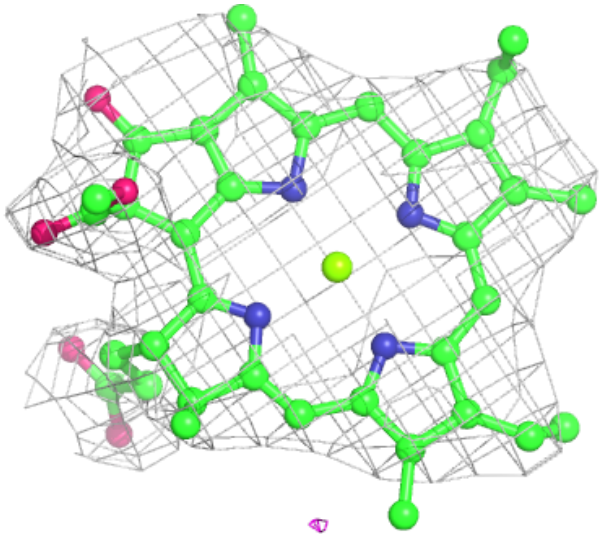
Electron density around CLA a 841:

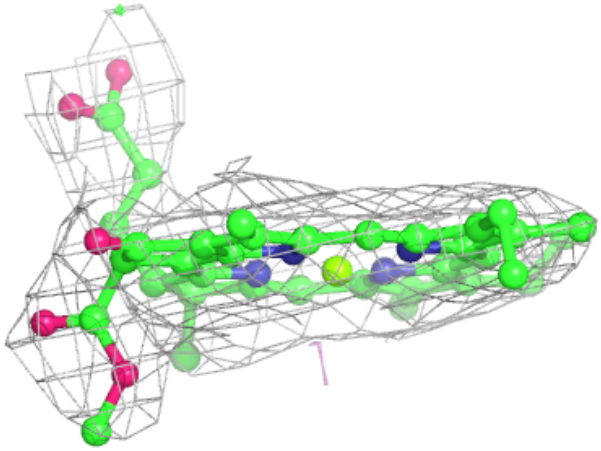
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

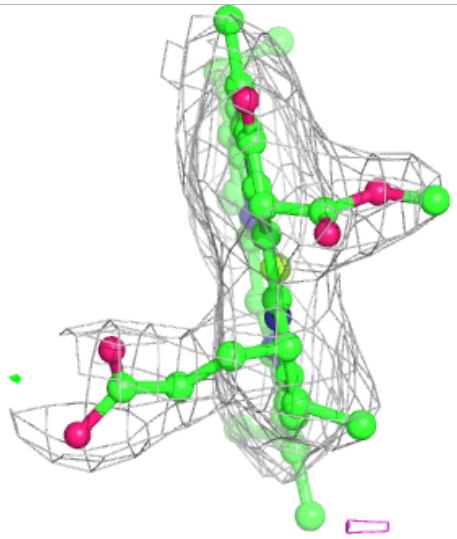


Electron density around CLA A 815:

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

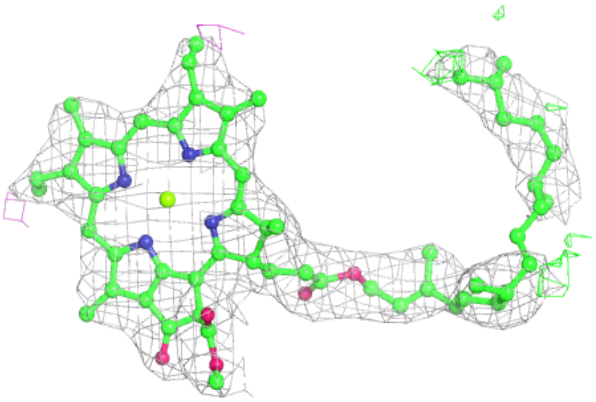


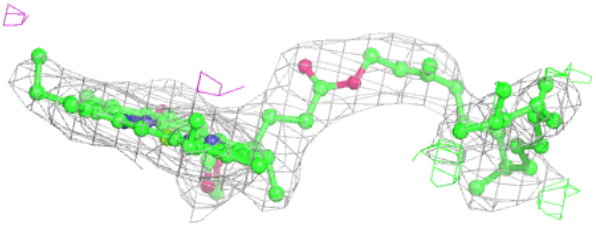


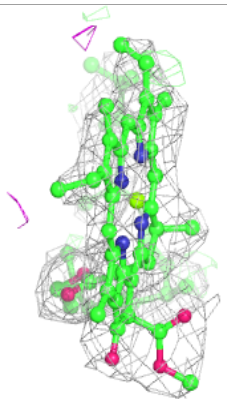


Electron density around CLA a 827:

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

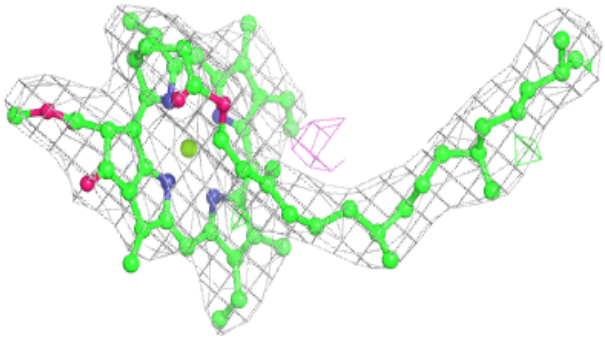


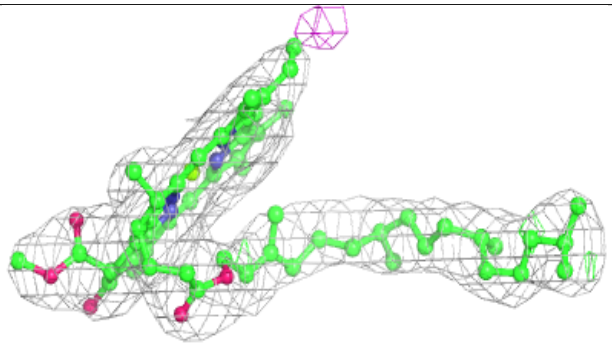


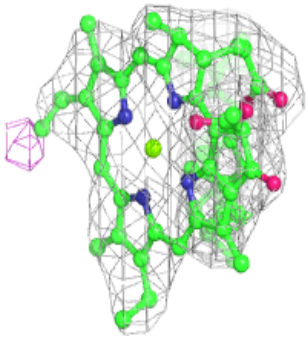


Electron density around CLA a 843:

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

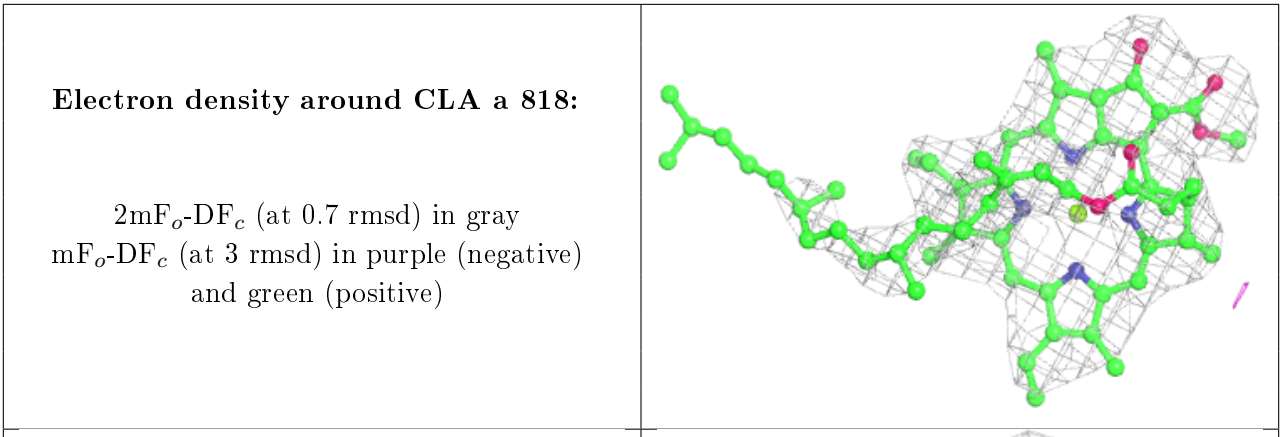






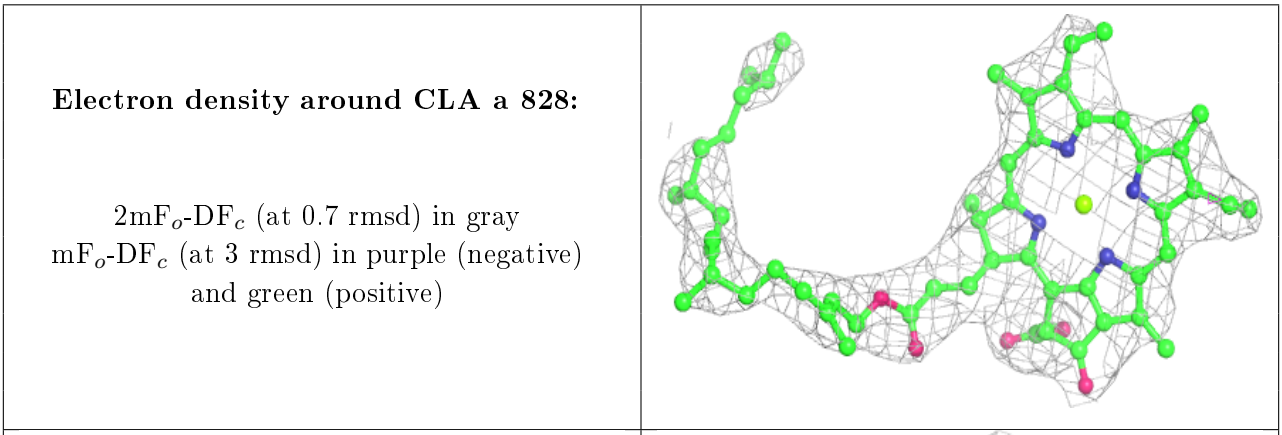
Electron density around CLA a 818:

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



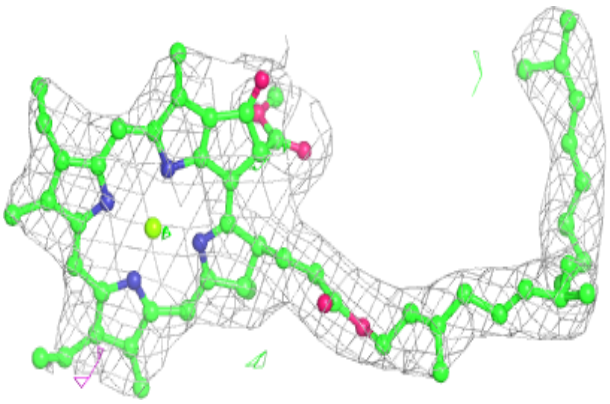
Electron density around CLA a 828:

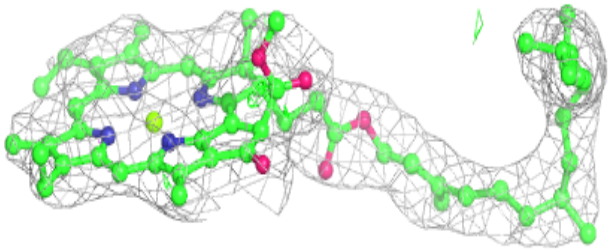
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

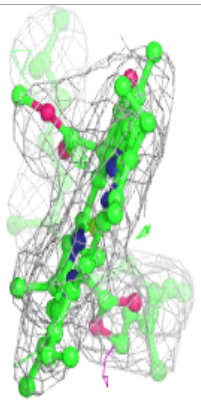


Electron density around CLA B 826:

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

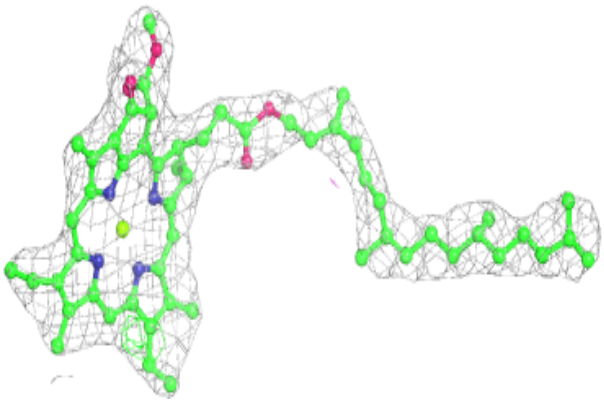


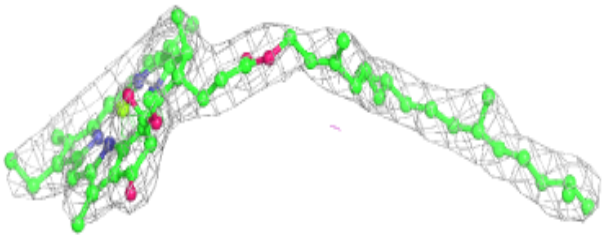


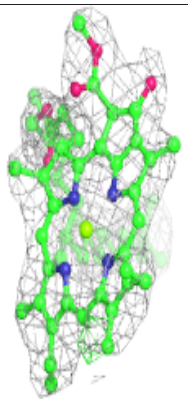


Electron density around CLA A 803:

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

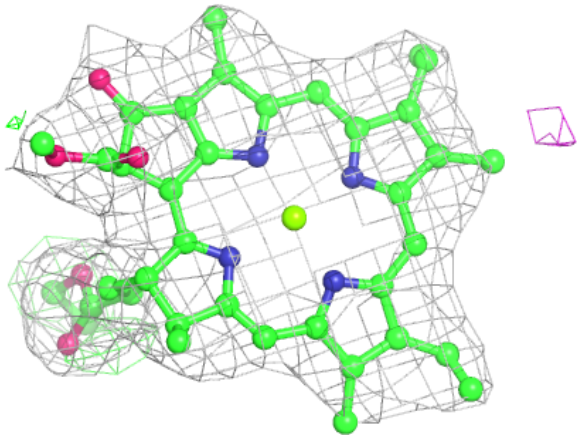


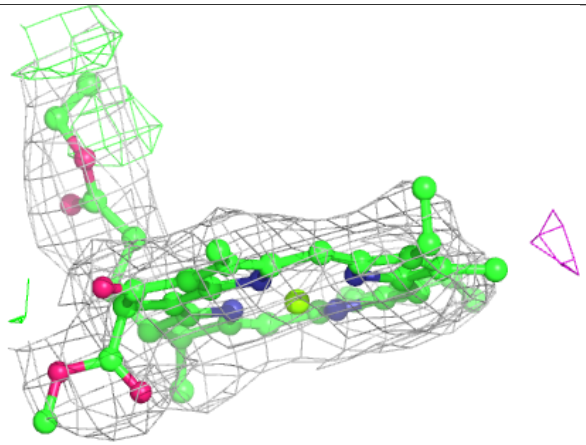


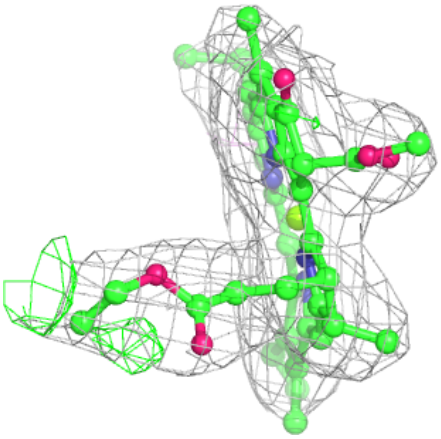


Electron density around CLA B 838:

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

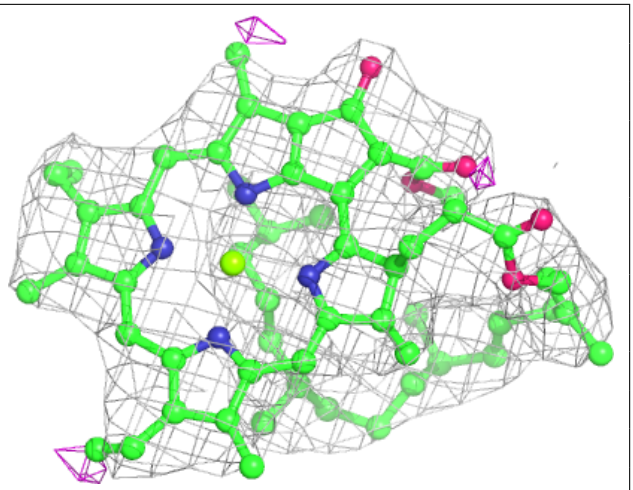


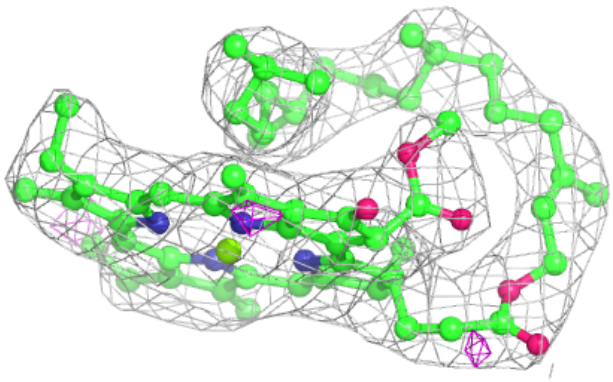


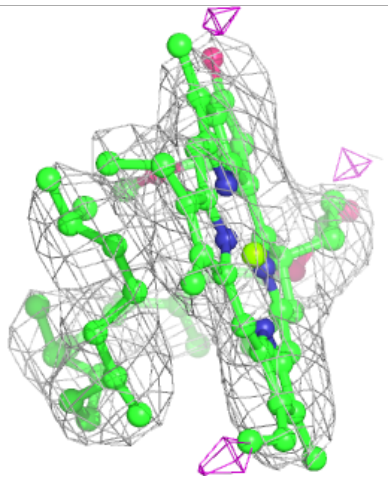


Electron density around CLA a 807:

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

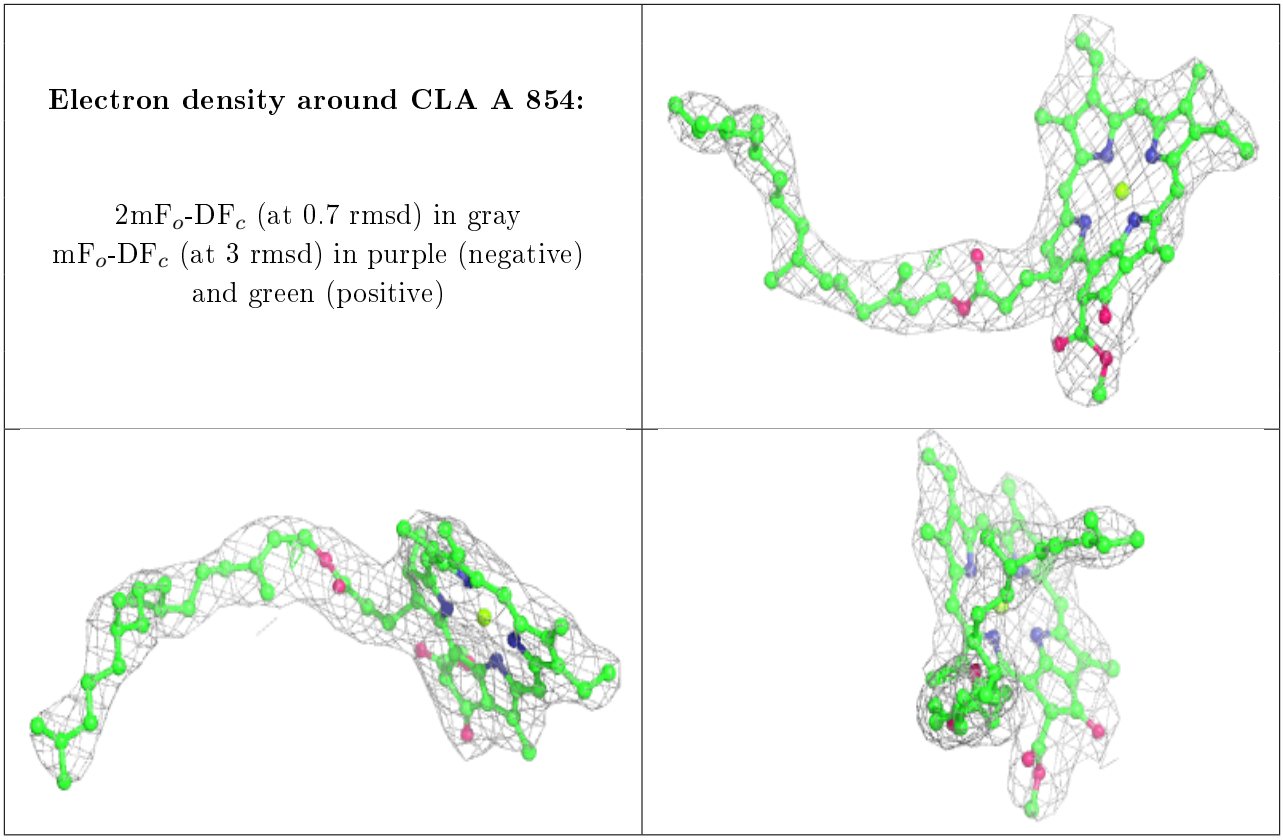






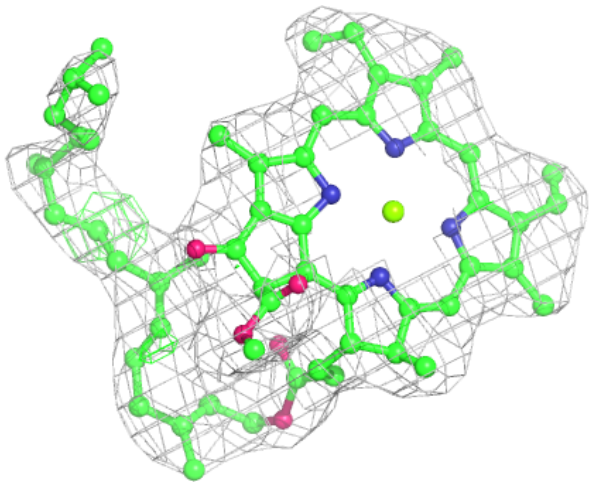
Electron density around CLA A 854:

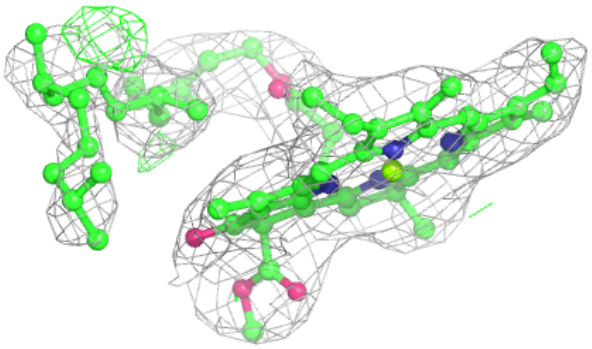
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

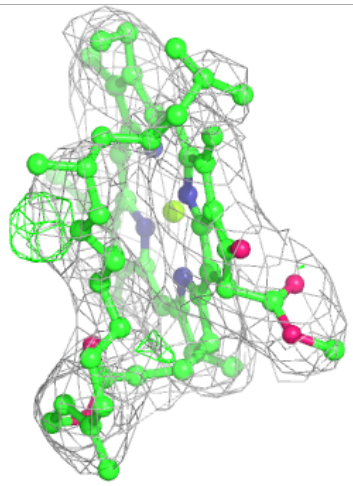


Electron density around CLA B 832:

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

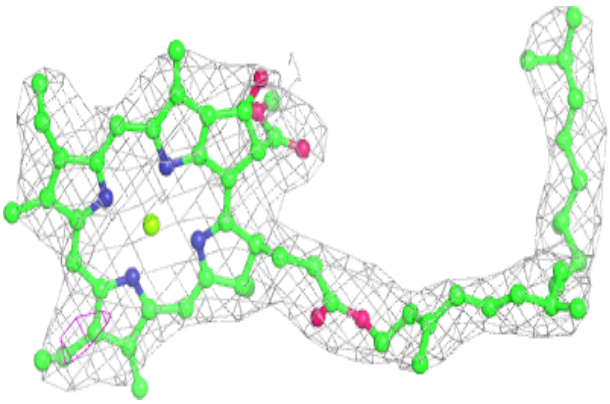


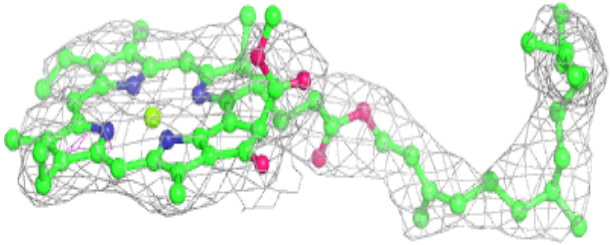


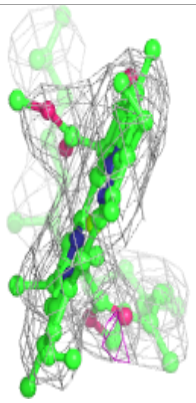


Electron density around CLA b 826:

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

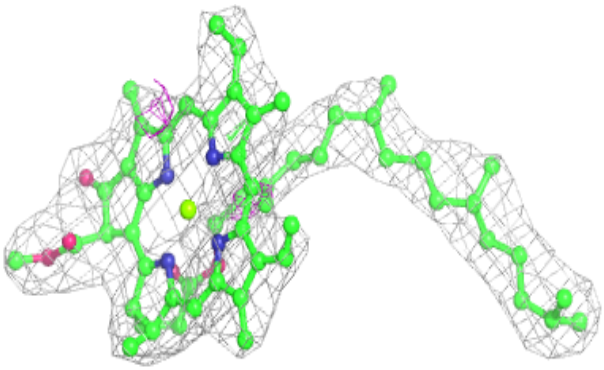


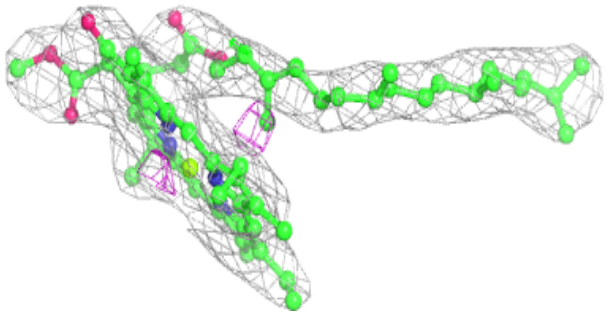


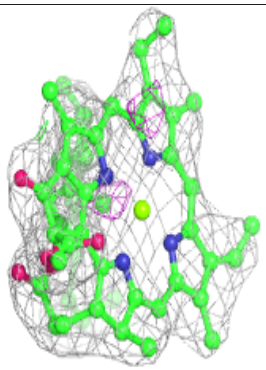


Electron density around CLA A 842:

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

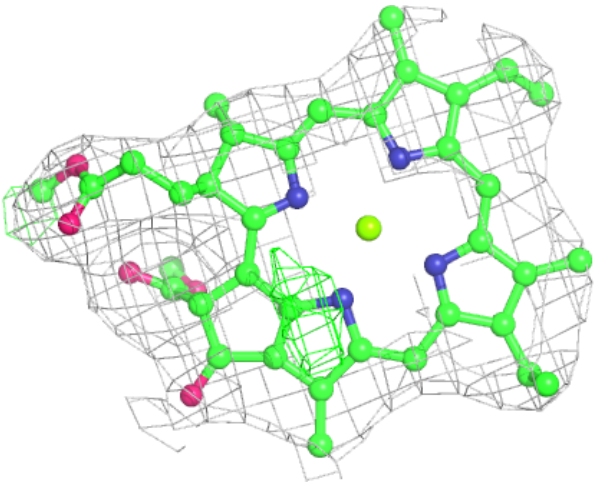


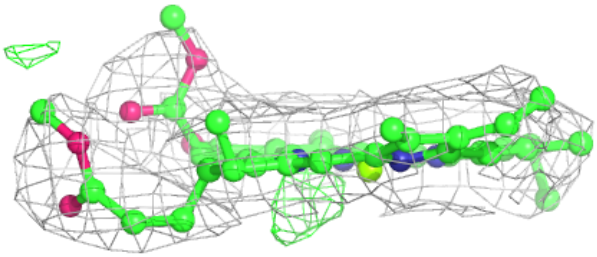


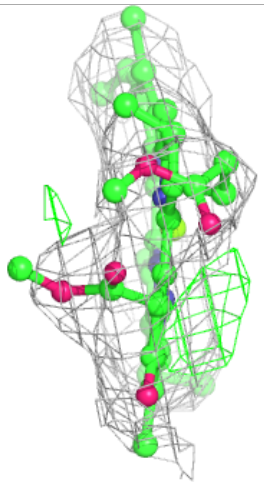


Electron density around CLA 4 603:

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

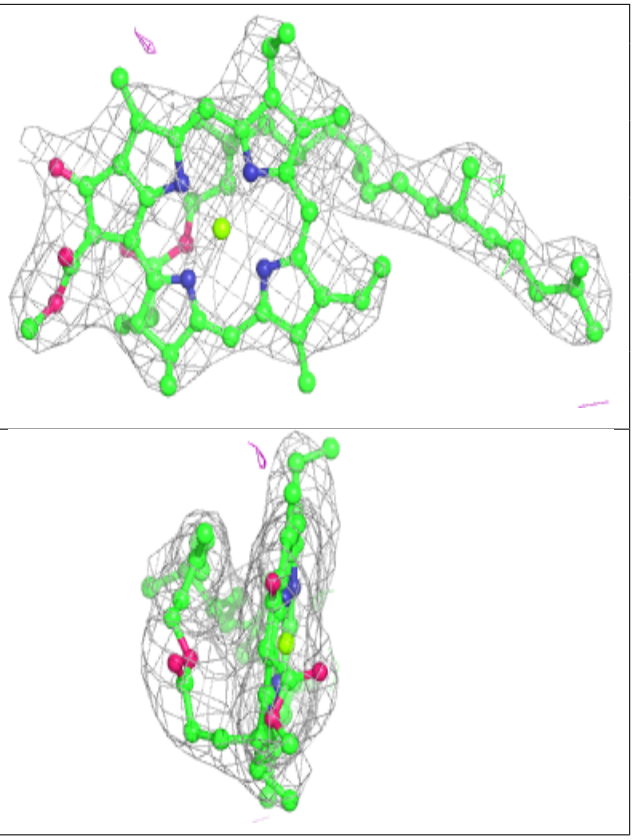






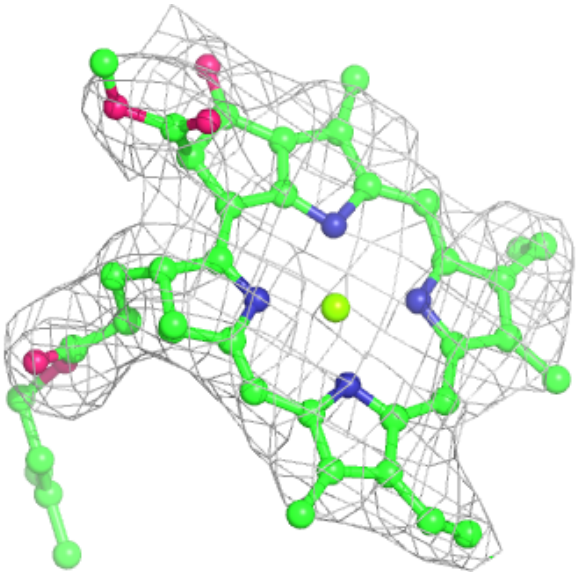
Electron density around CLA A 841:

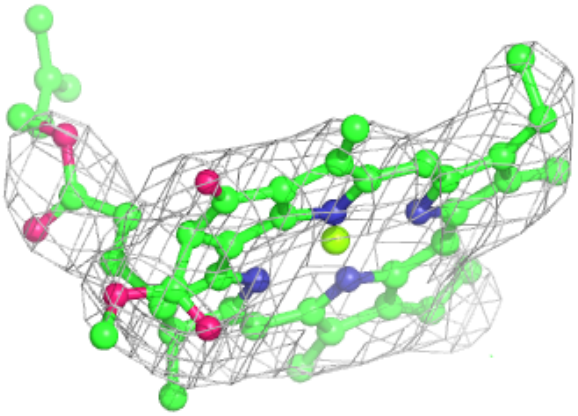
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

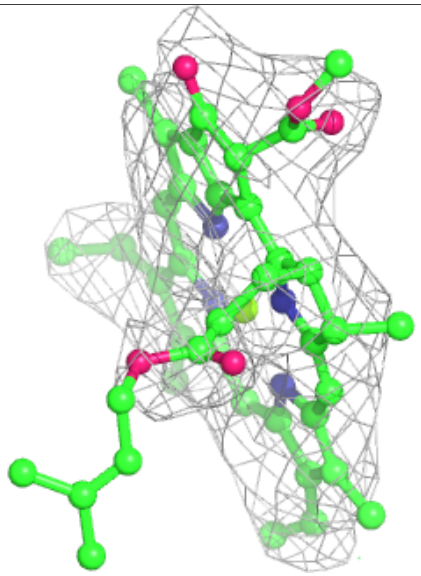


Electron density around CLA B 820:

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

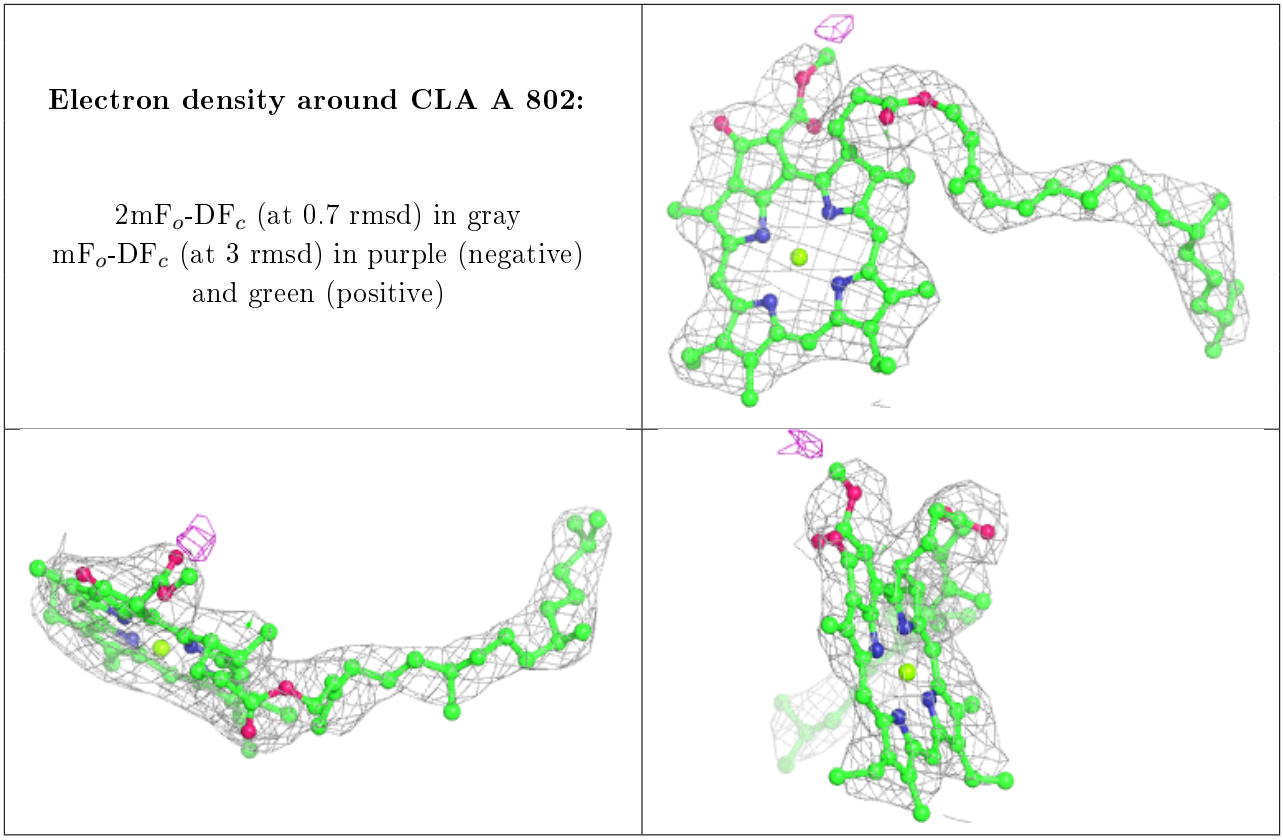






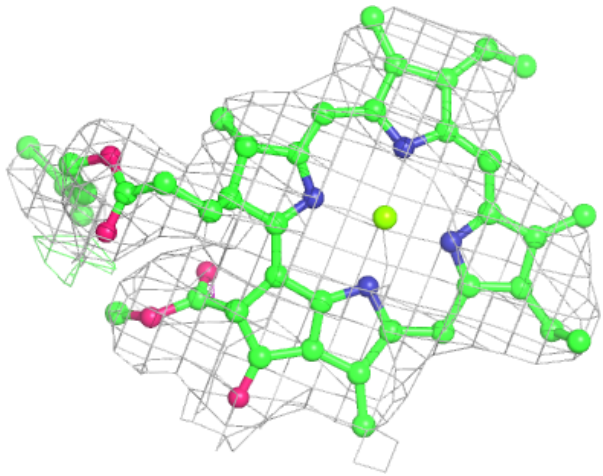
Electron density around CLA A 802:

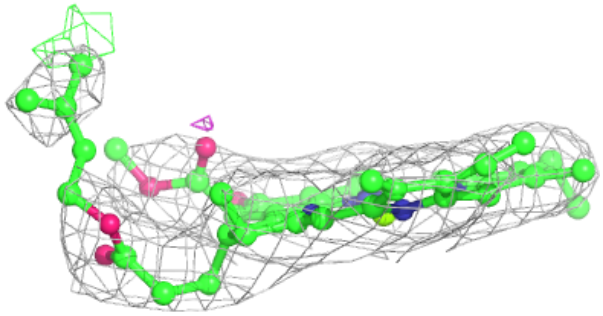
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

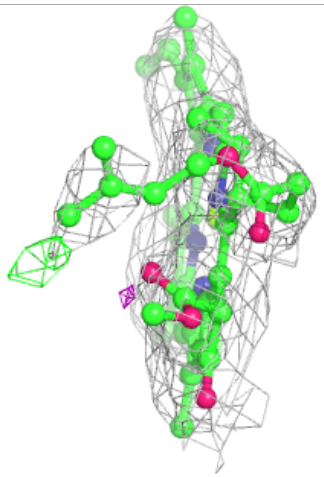


Electron density around CLA 8 302:

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

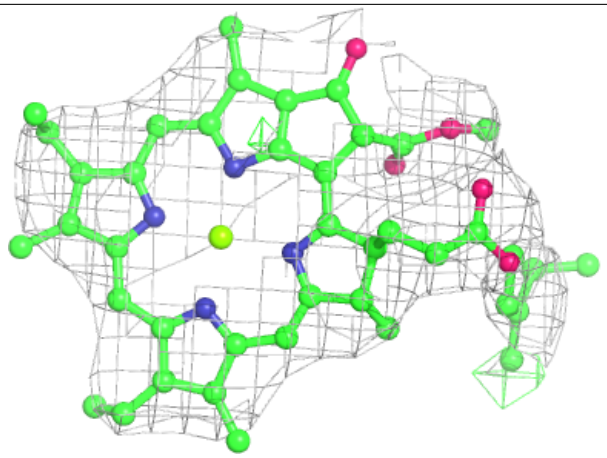


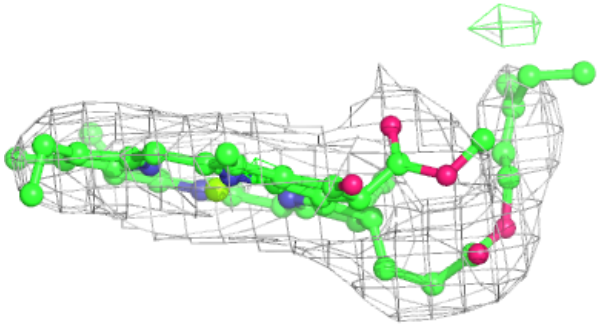


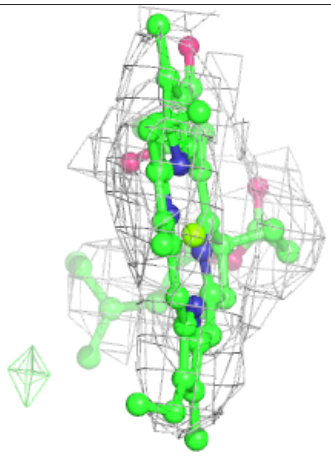


Electron density around CLA 7 603:

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

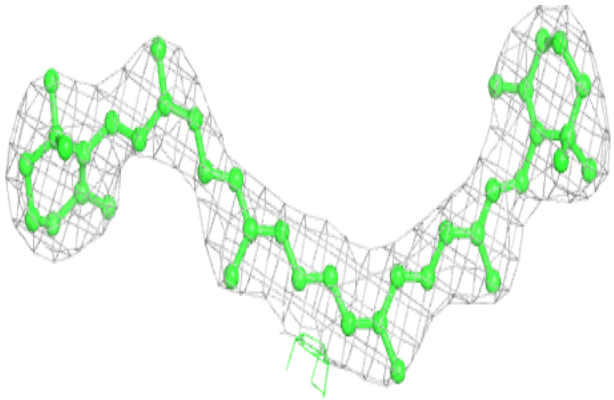


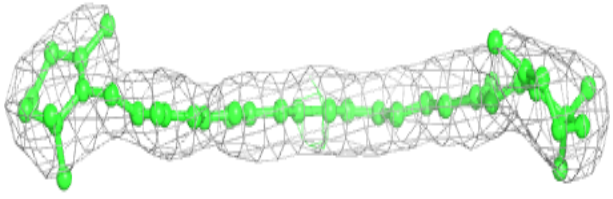




Electron density around BCR A 852:

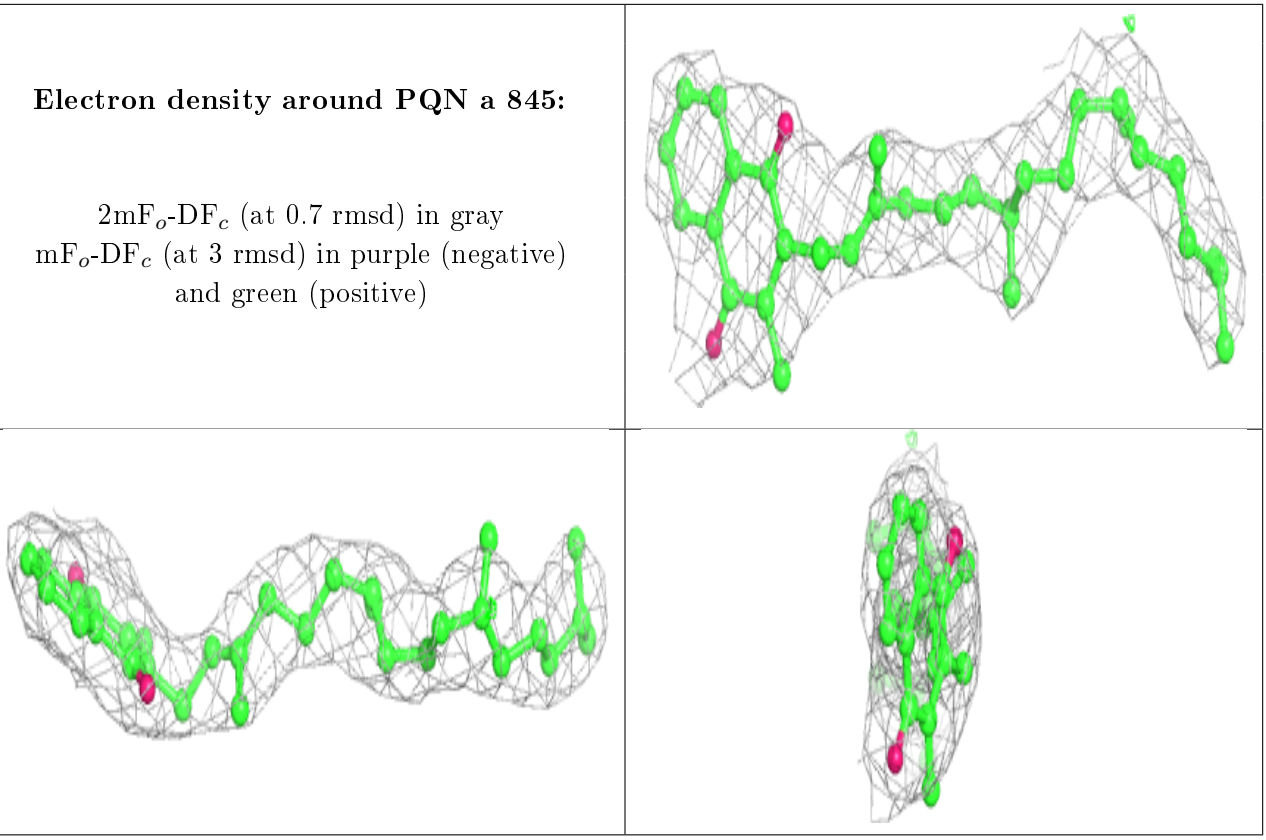
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)





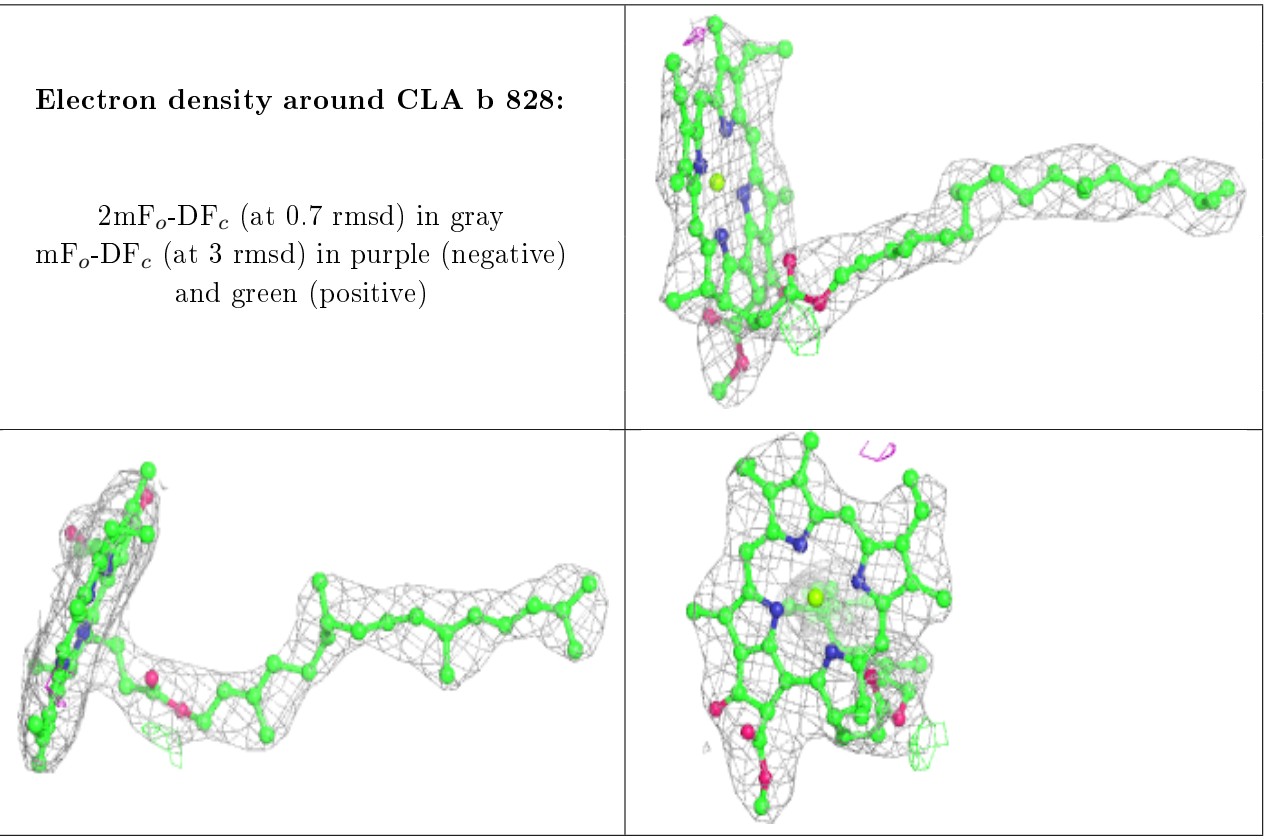
Electron density around PQN a 845:

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



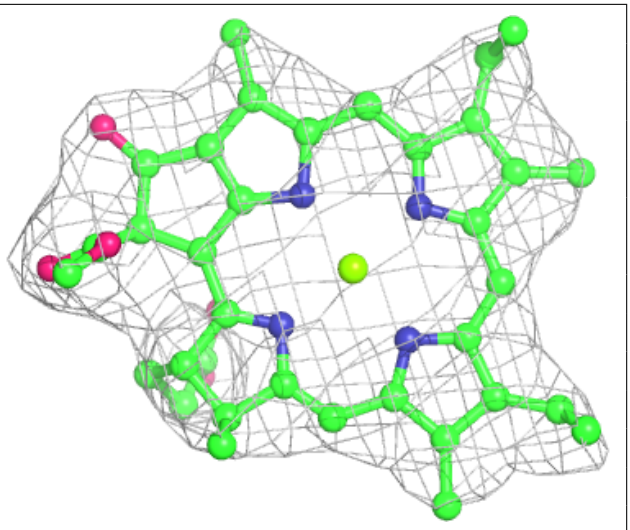
Electron density around CLA b 828:

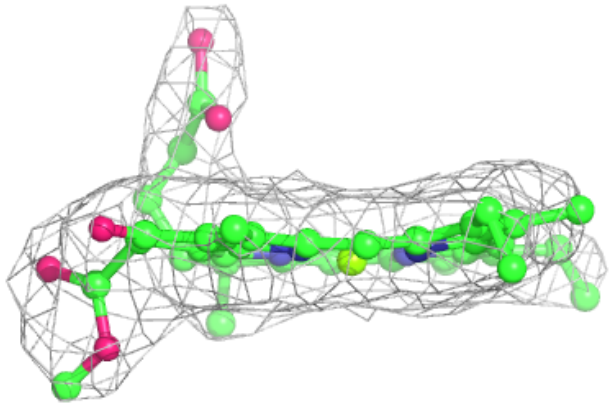
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

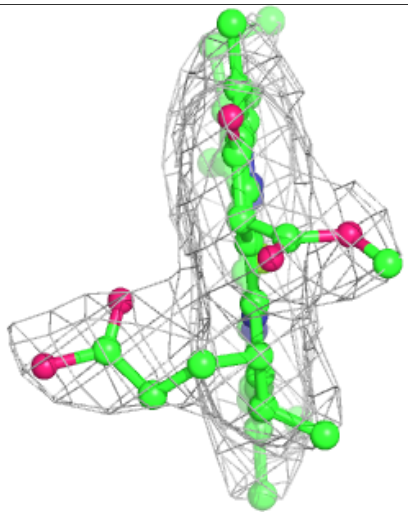


Electron density around CLA b 804:

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

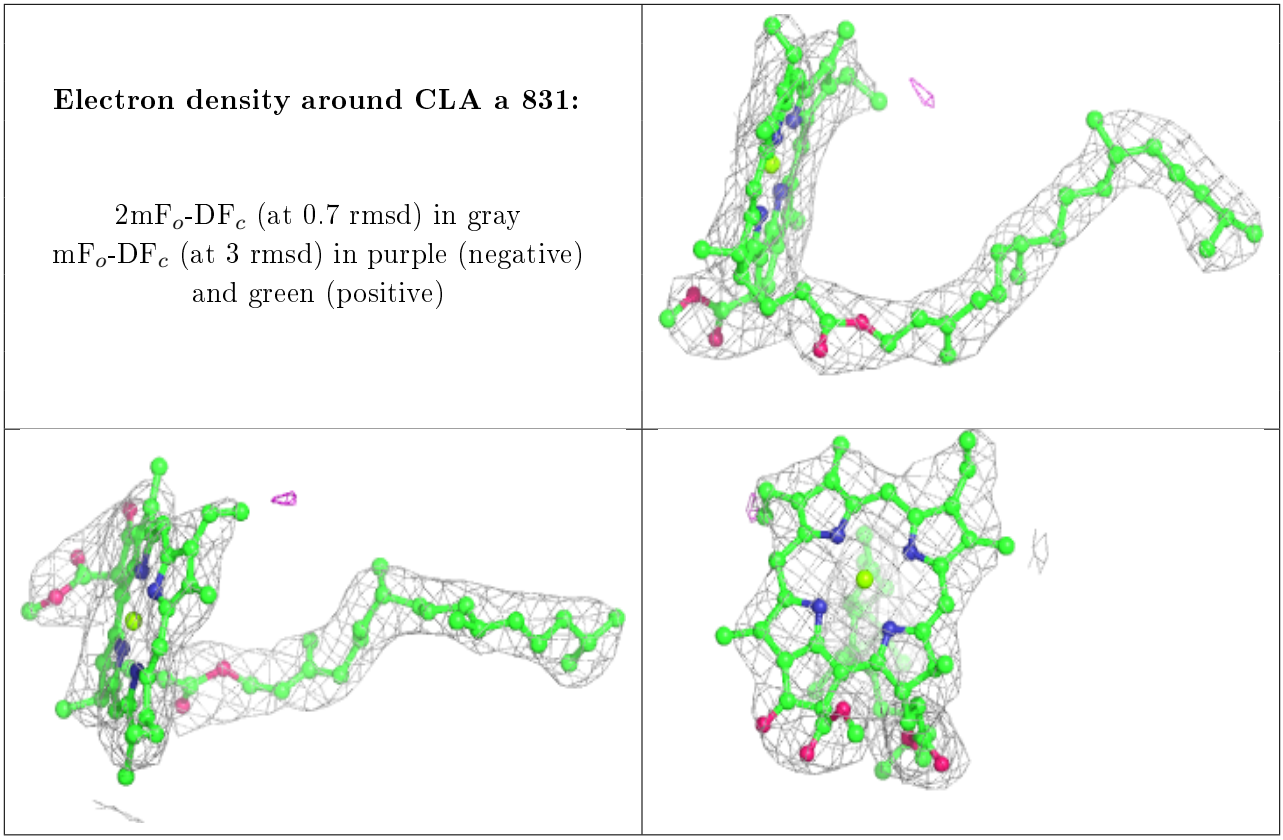






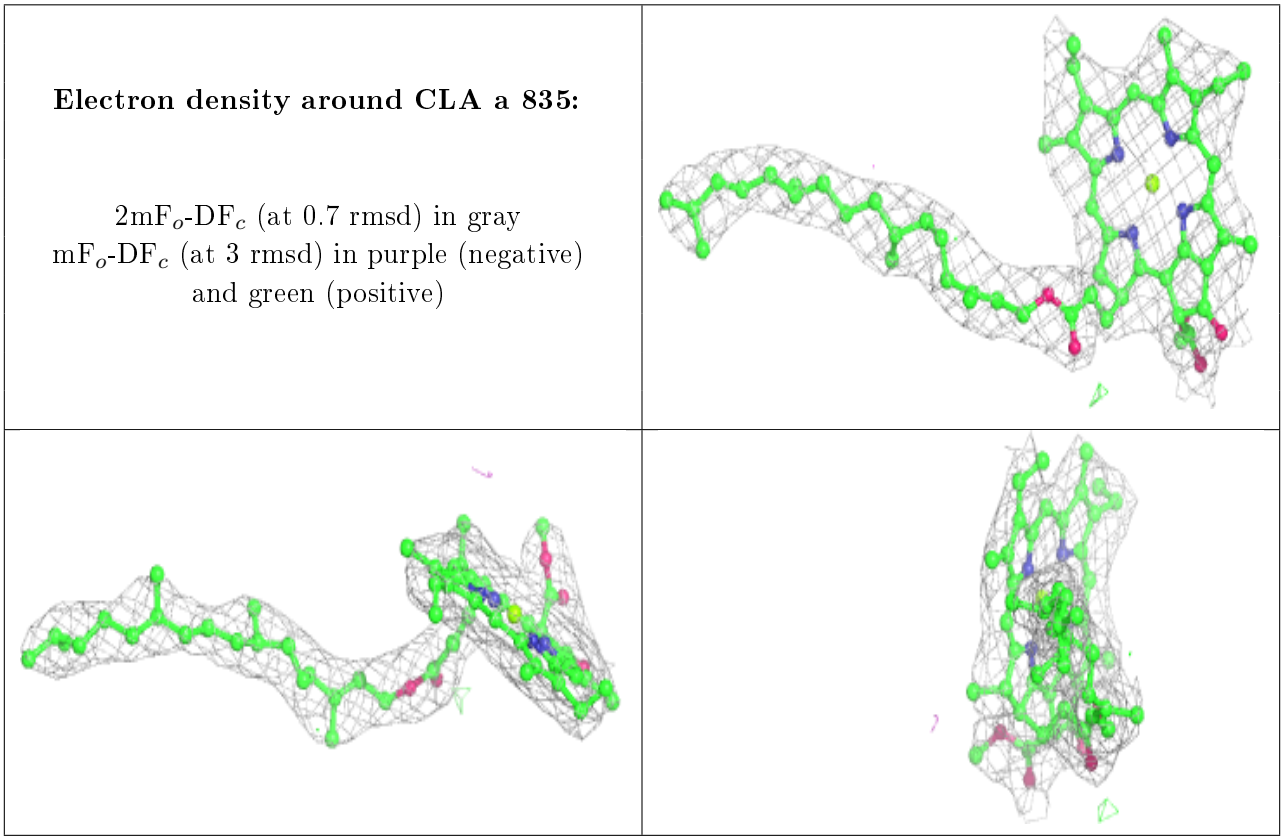
Electron density around CLA a 831:

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



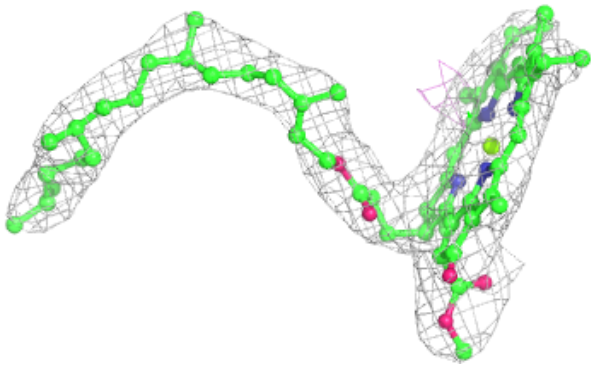
Electron density around CLA a 835:

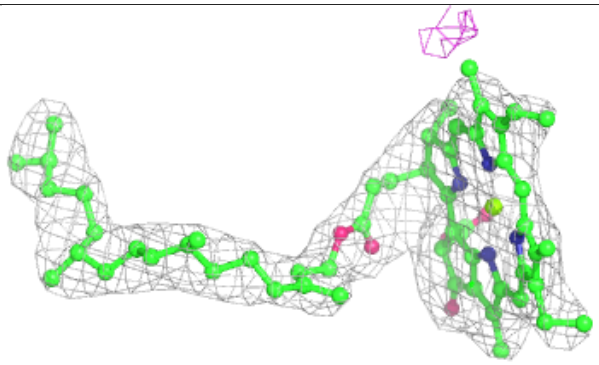
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

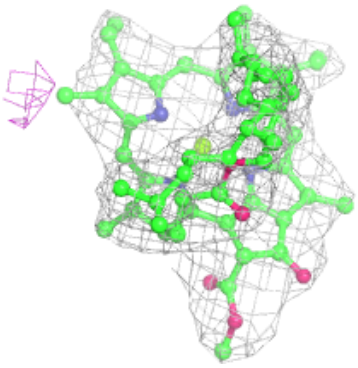


Electron density around CLA b 839:

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

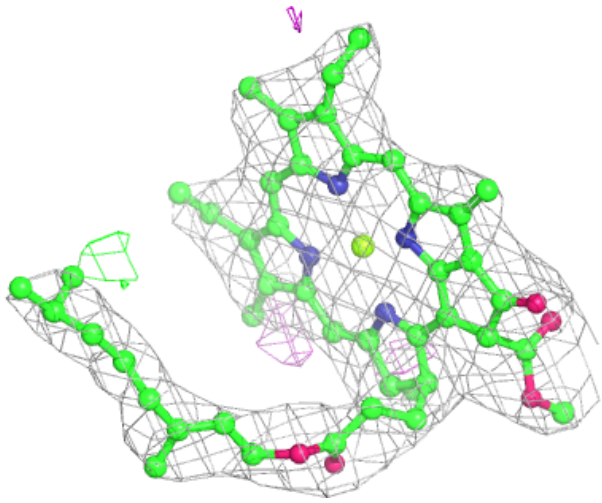


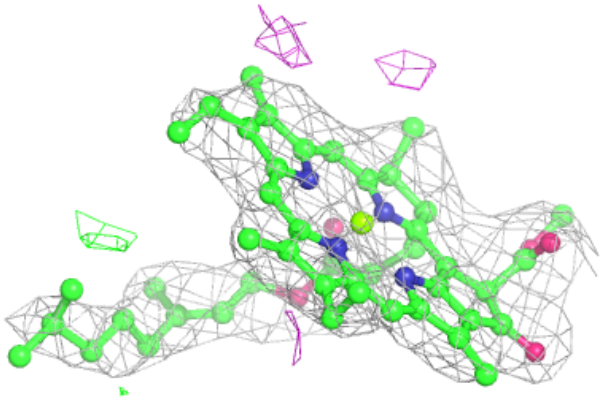


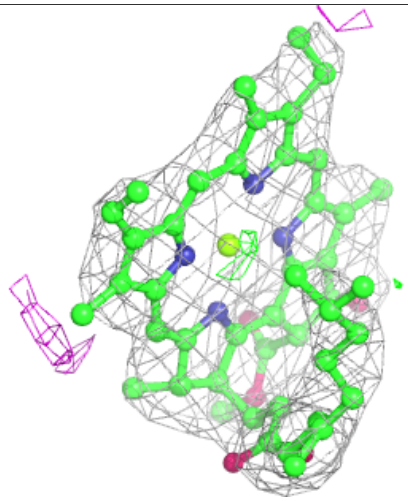


Electron density around CLA a 825:

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

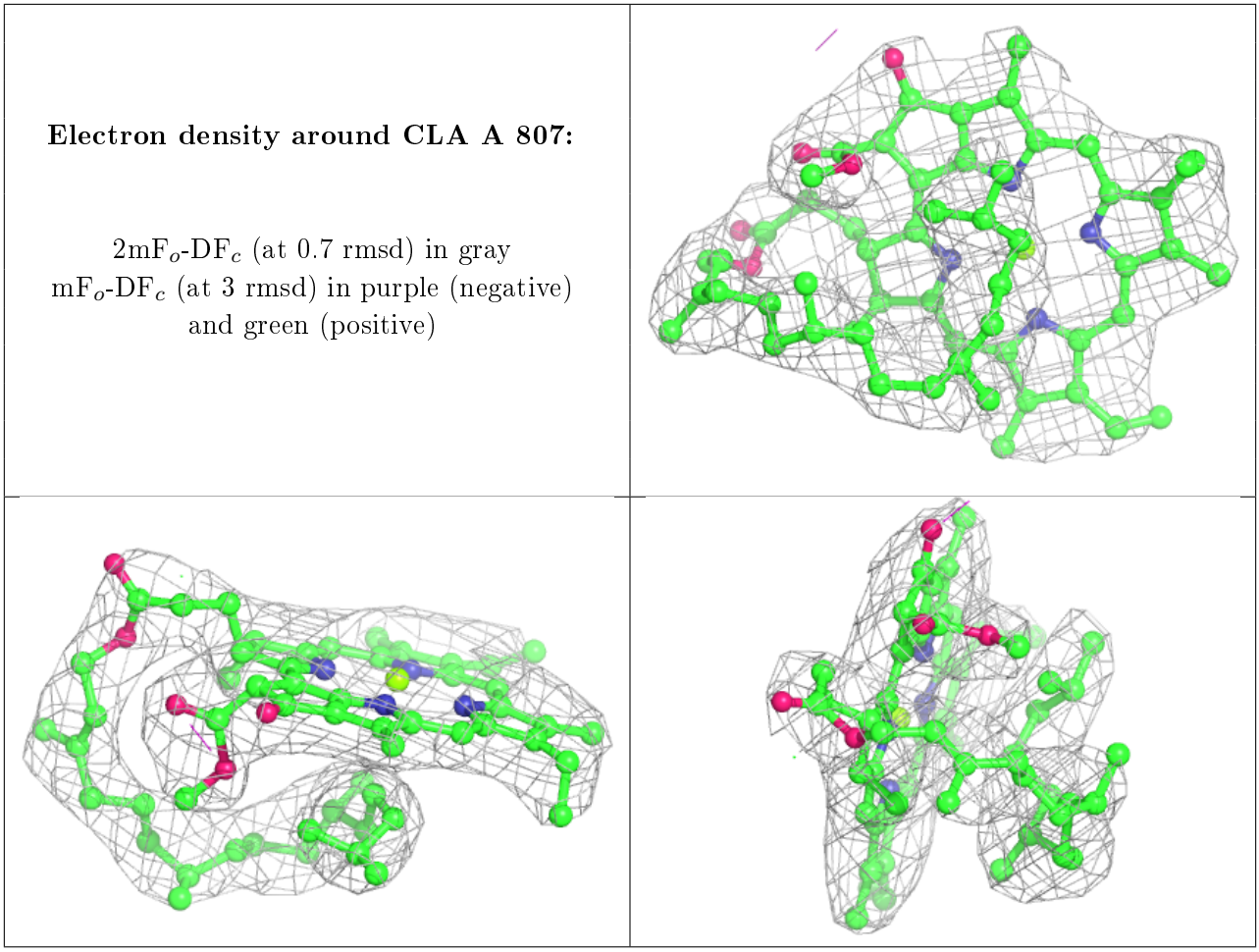






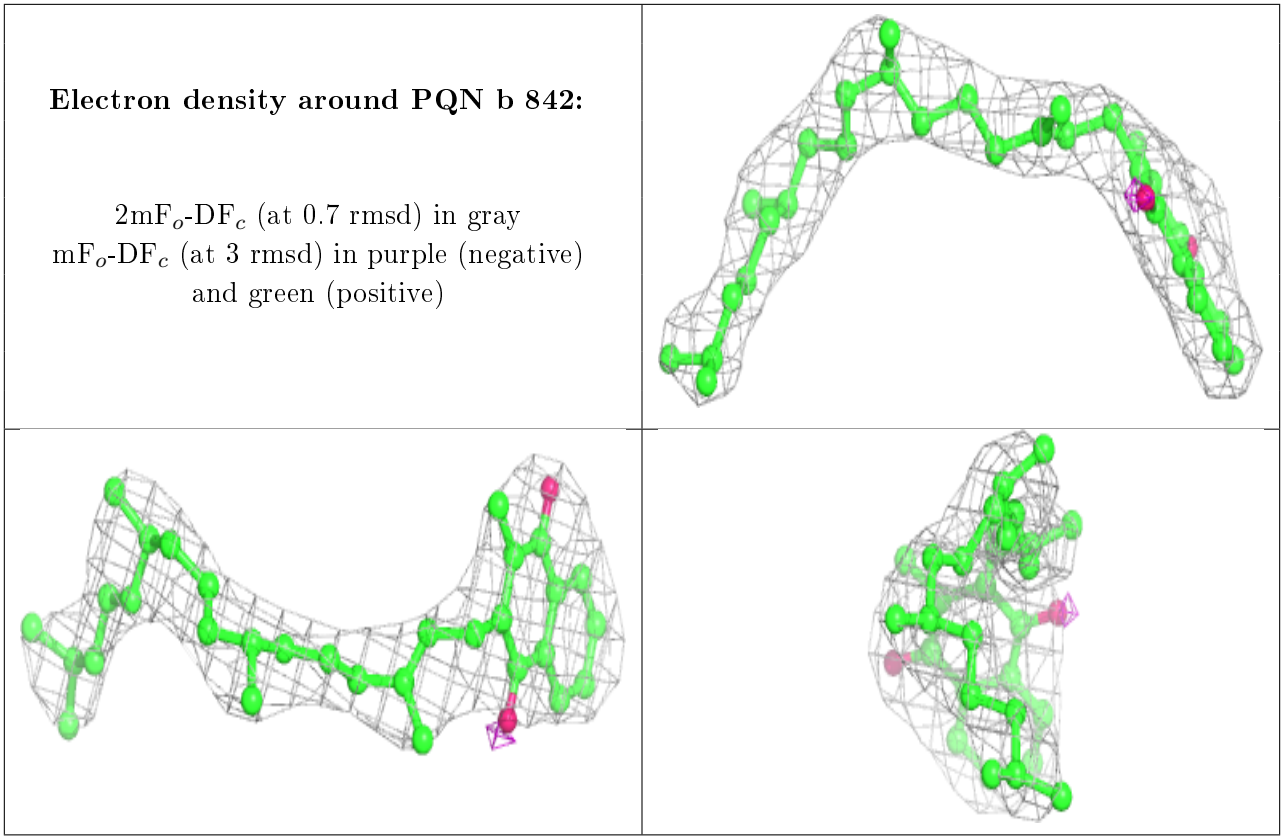
Electron density around CLA A 807:

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



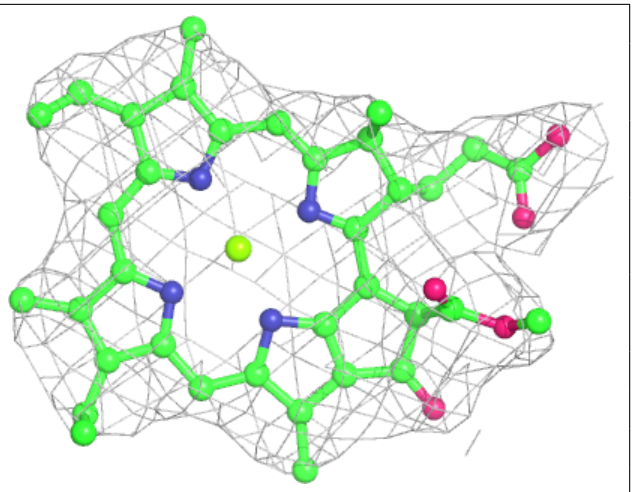
Electron density around PQN b 842:

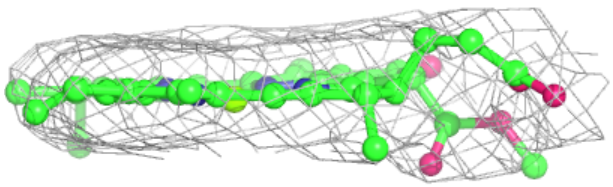
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

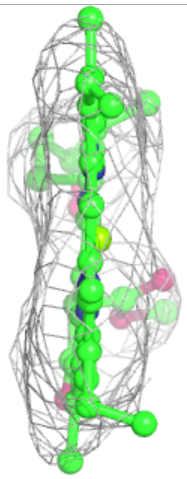


Electron density around CLA f 7002:

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

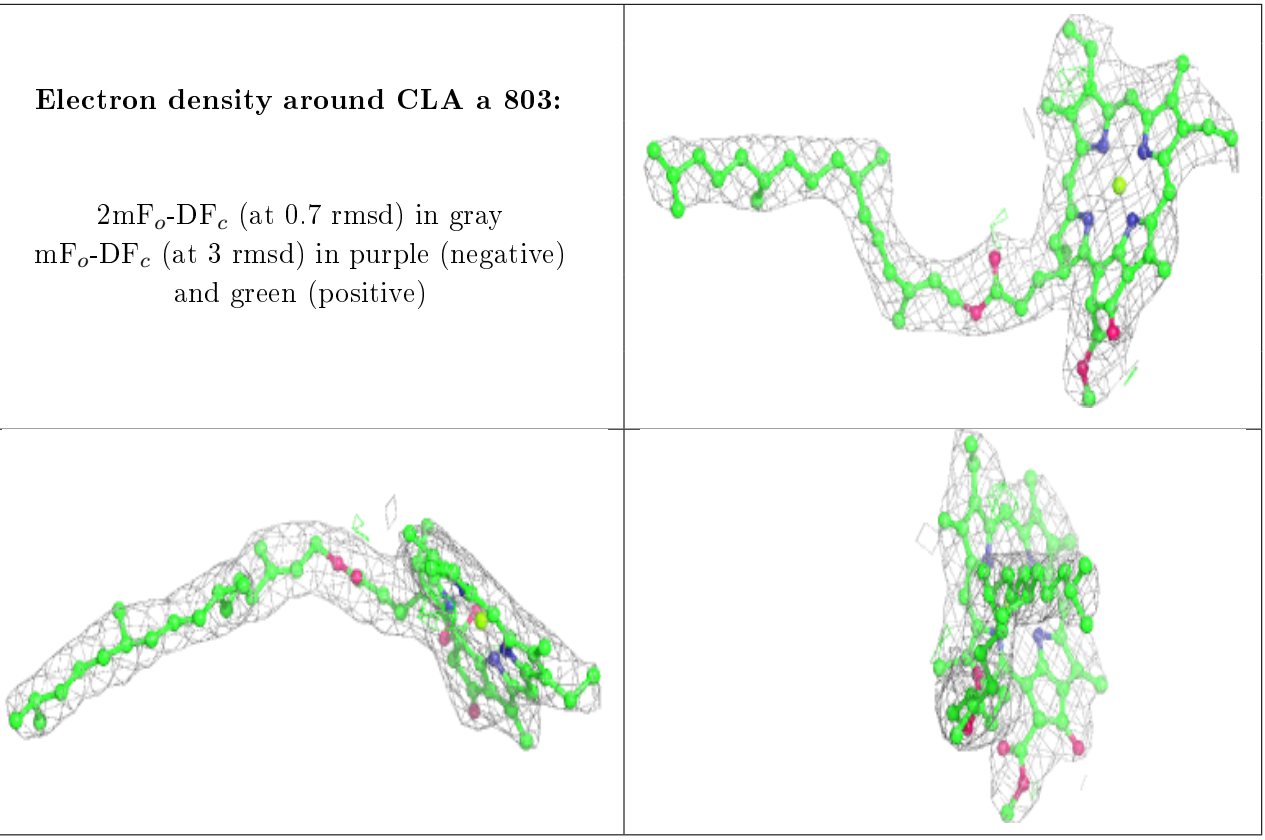






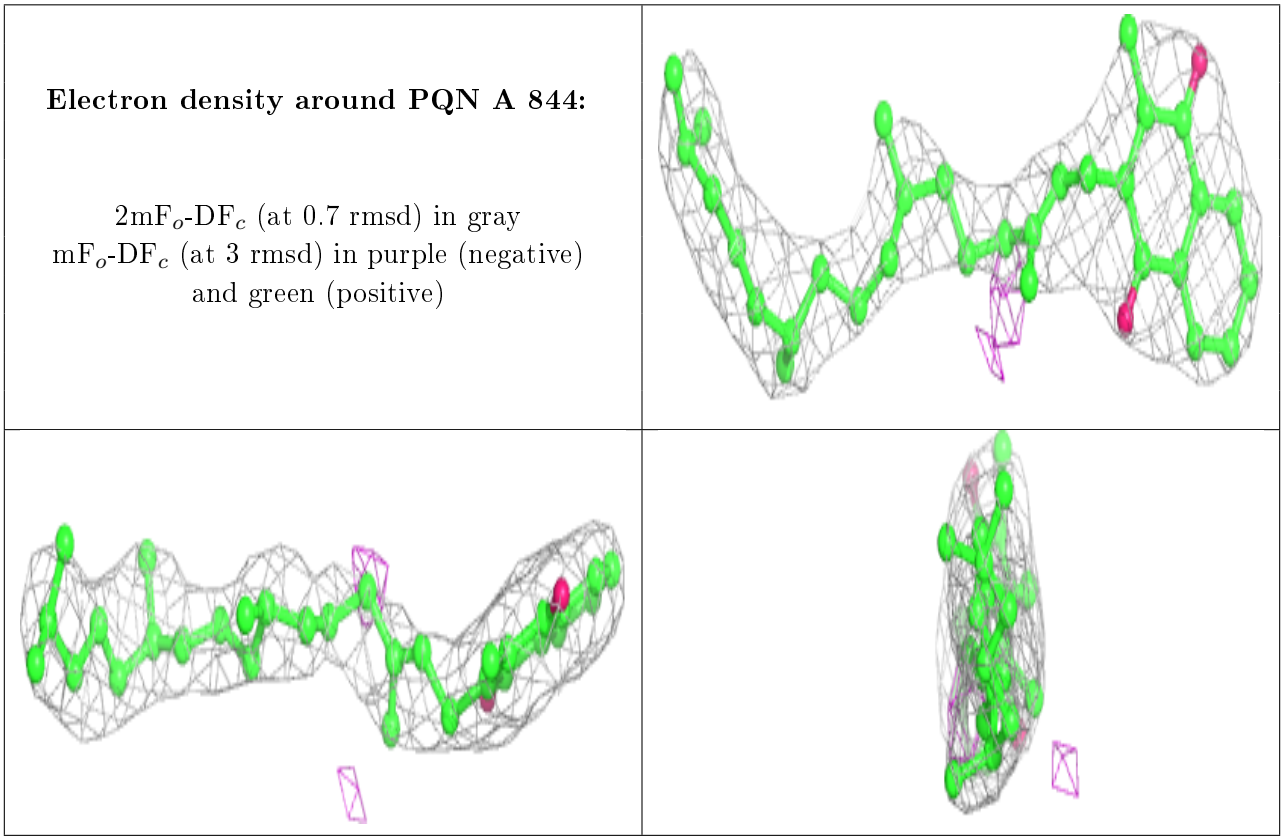
Electron density around CLA a 803:

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



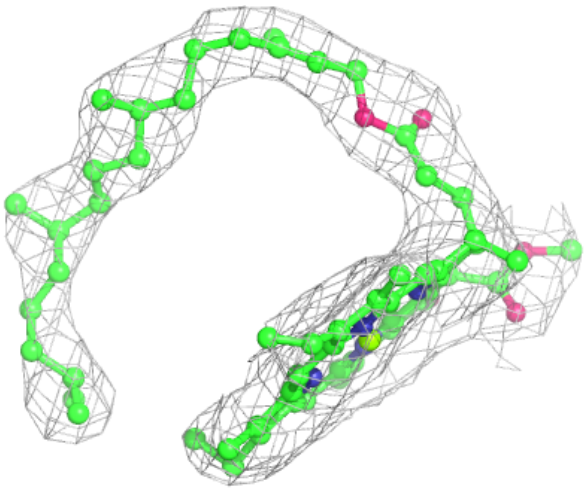
Electron density around PQN A 844:

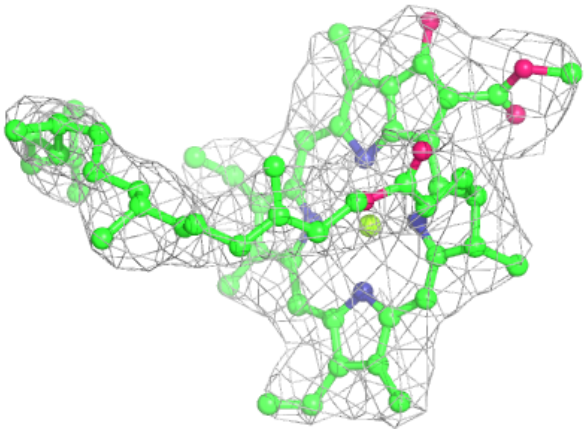
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

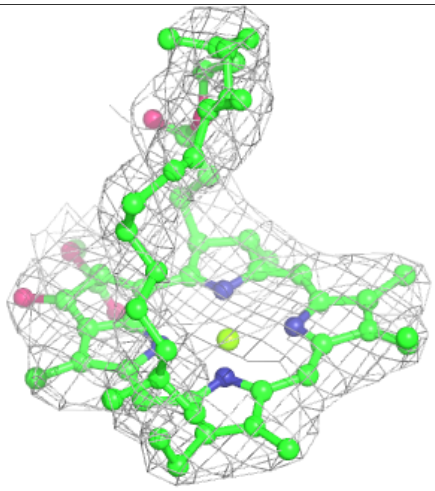


Electron density around CLA B 819:

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

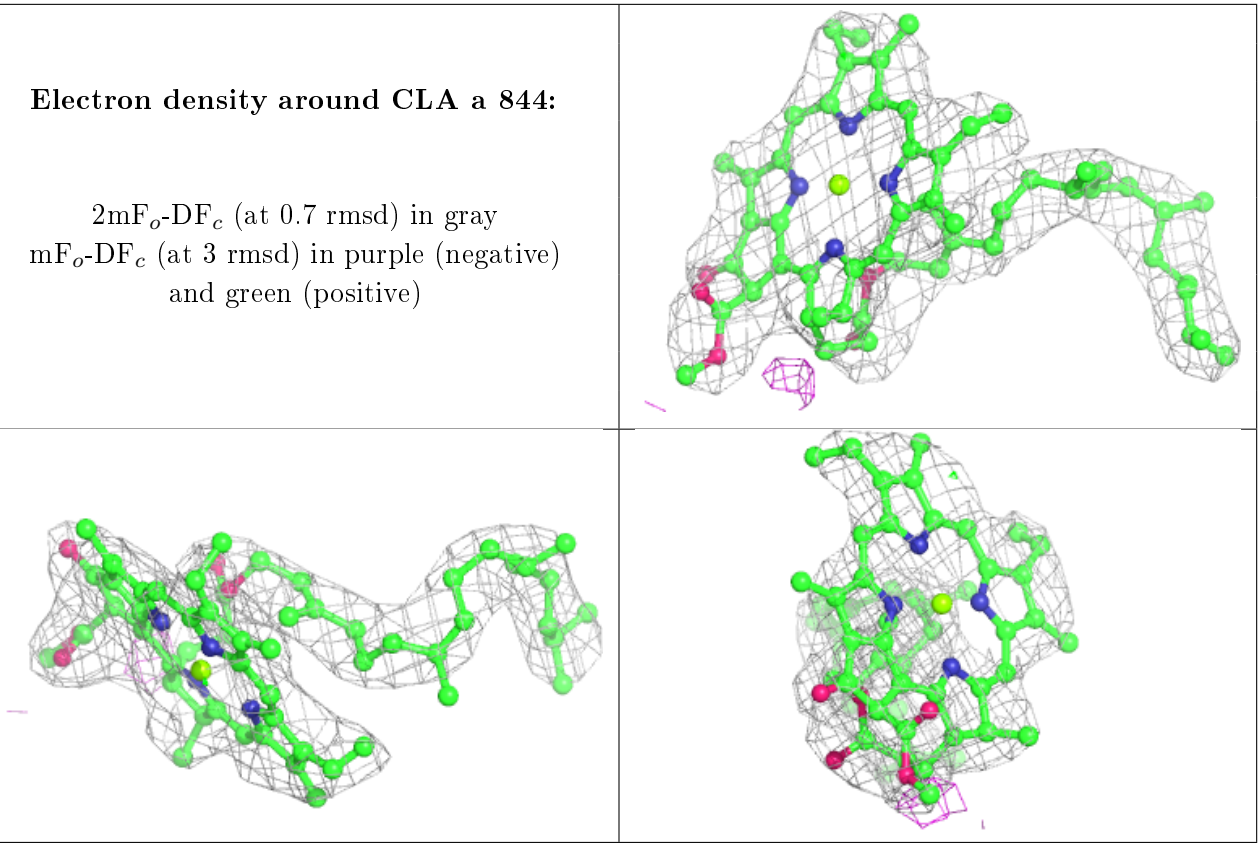






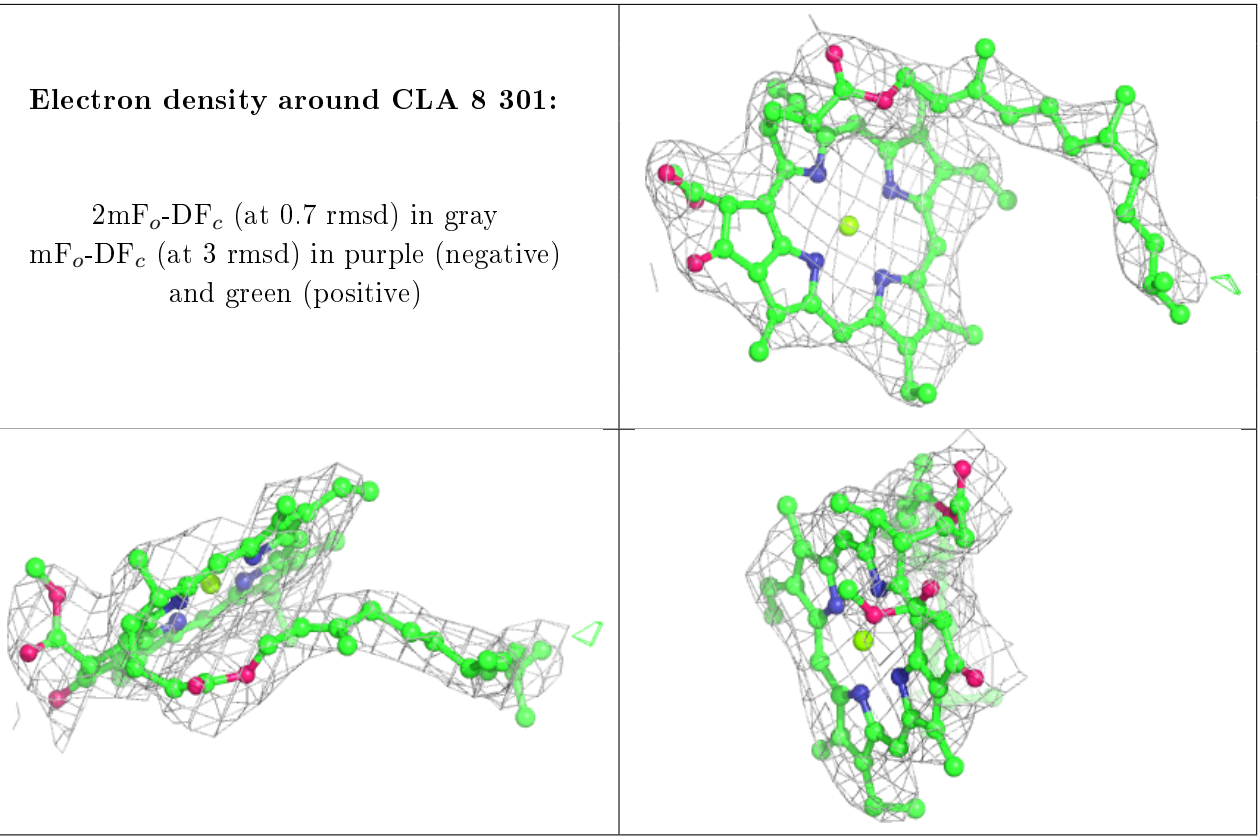
Electron density around CLA a 844:

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



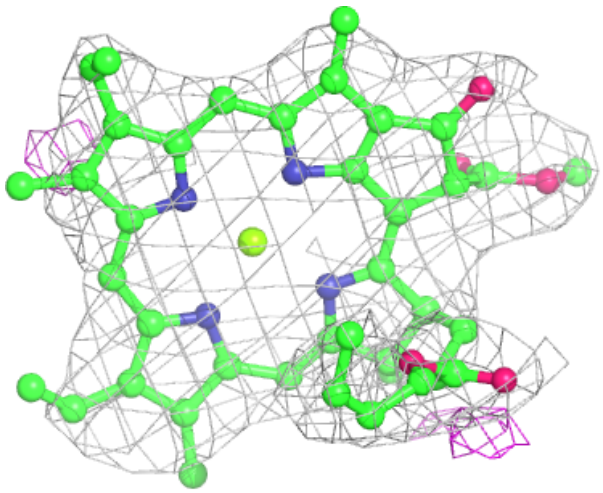
Electron density around CLA 8 301:

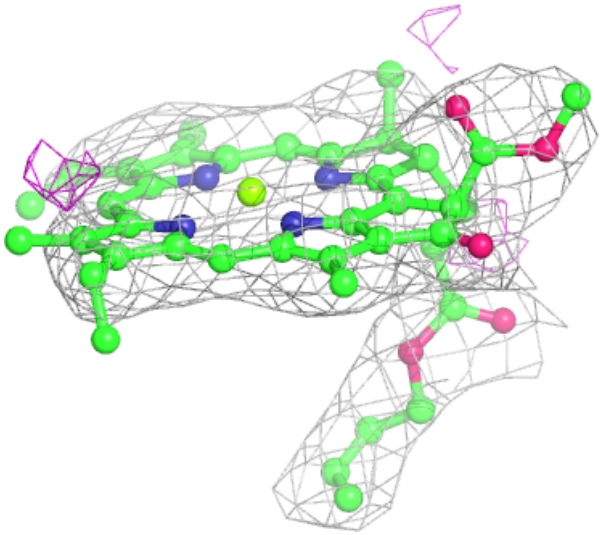
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

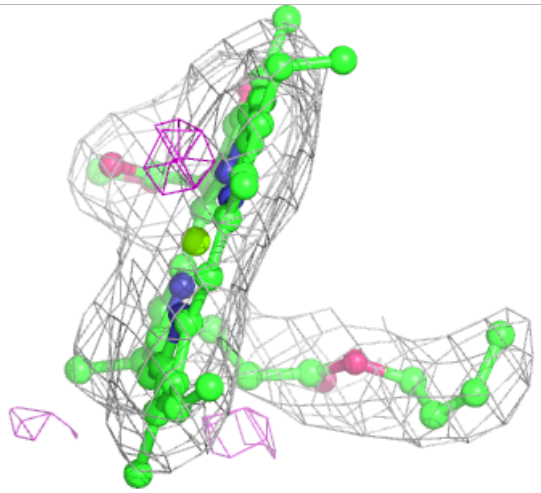


Electron density around CLA B 831:

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

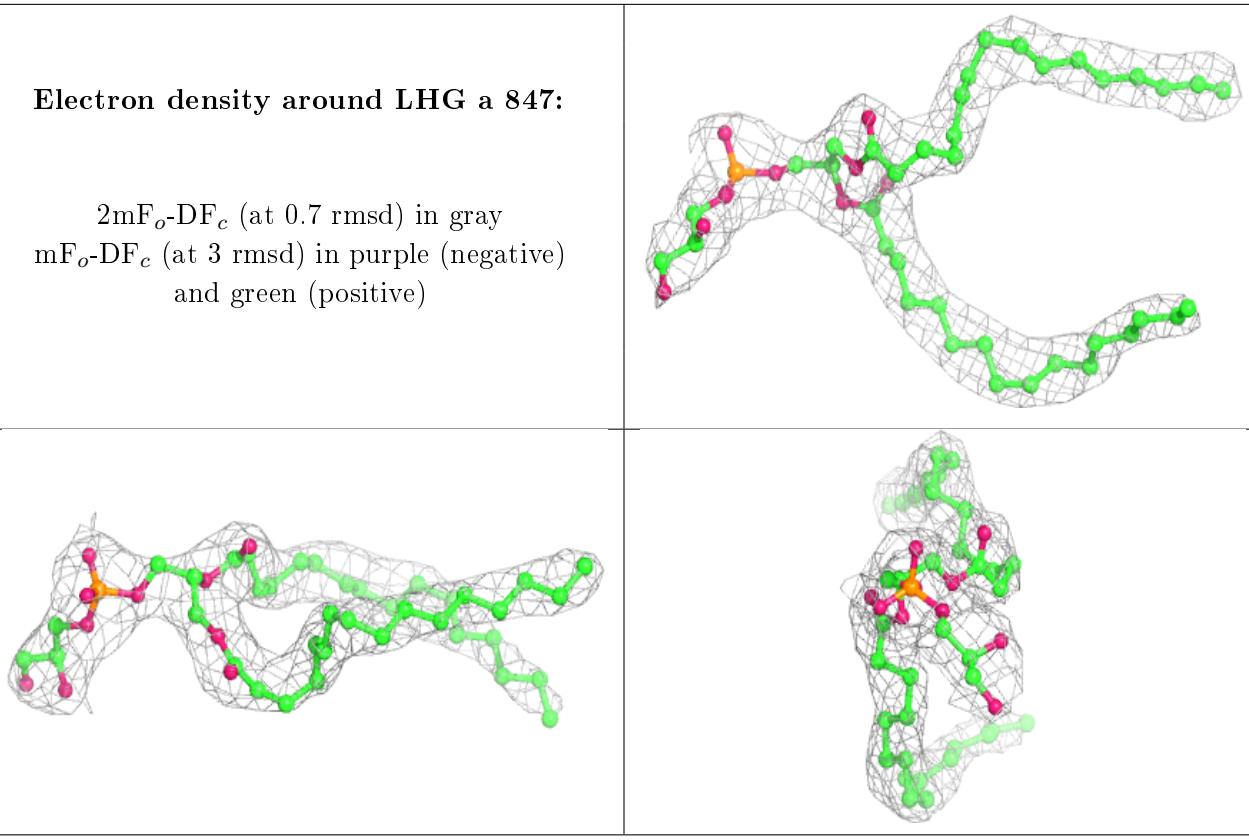






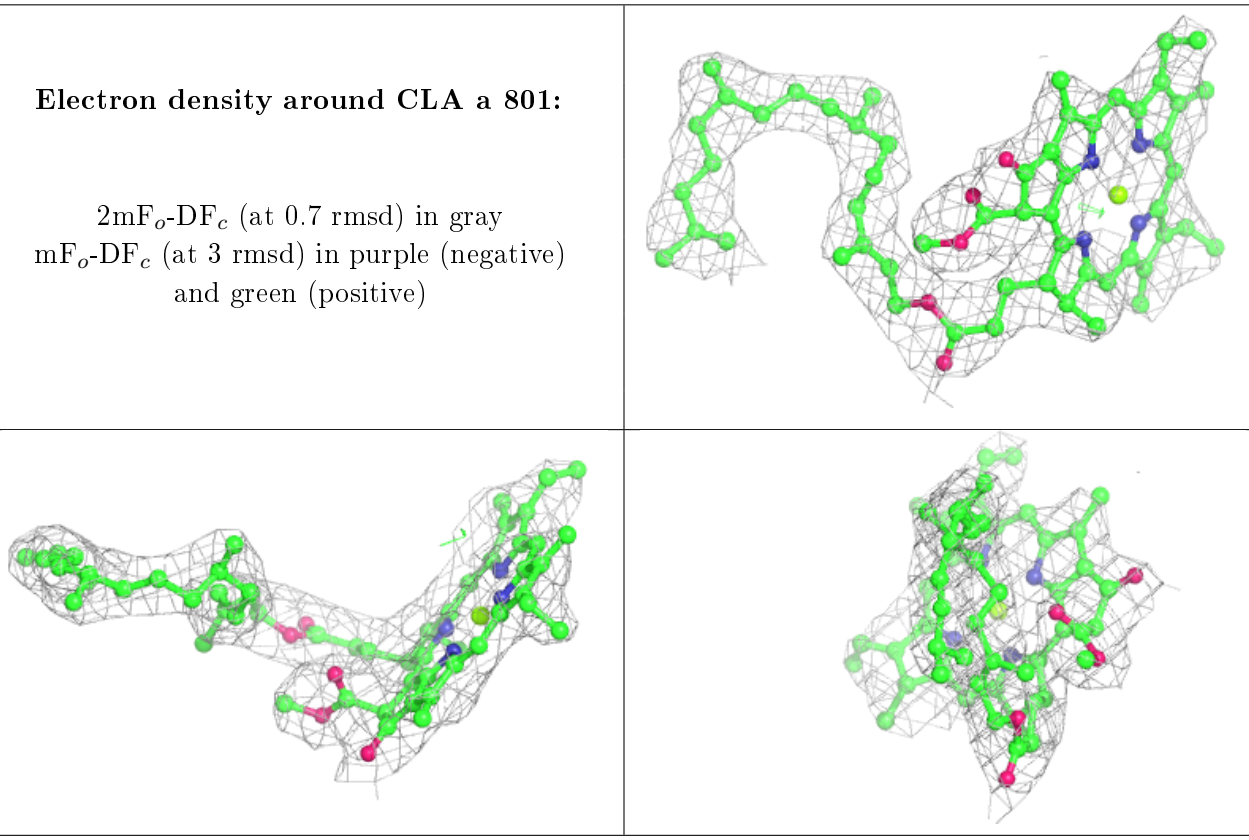
Electron density around LHG a 847:

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



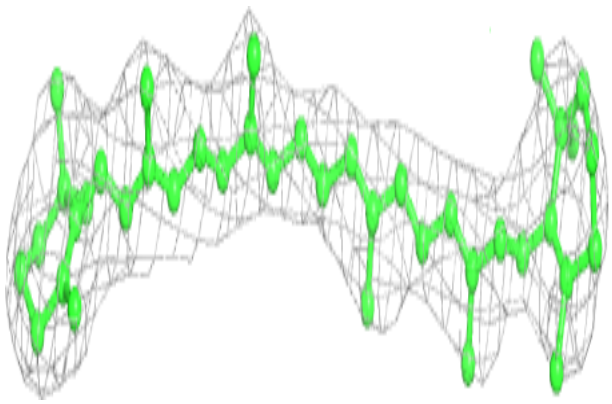
Electron density around CLA a 801:

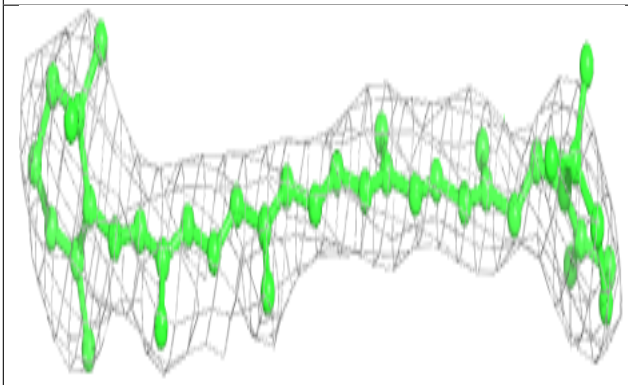
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

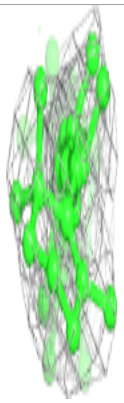


Electron density around BCR a 850:

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

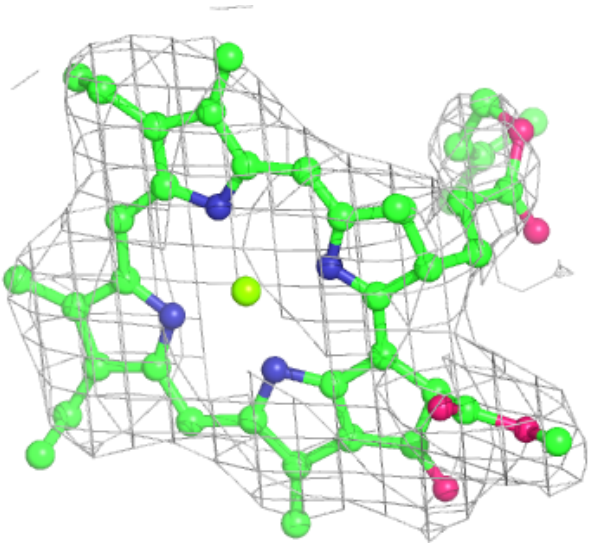


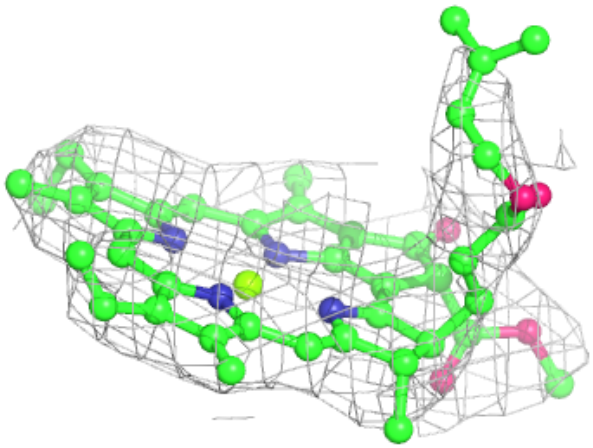




Electron density around CLA 8 307:

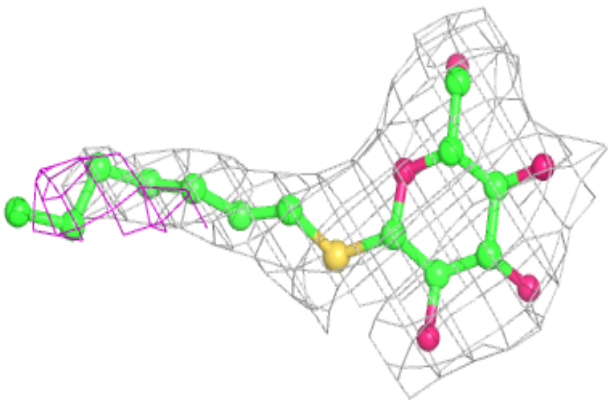
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

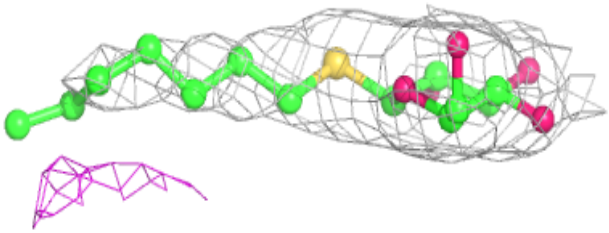


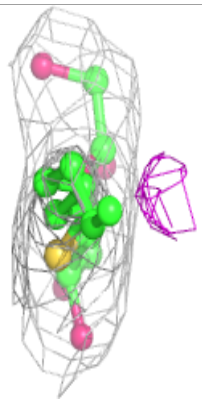


Electron density around HTG A 855:

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

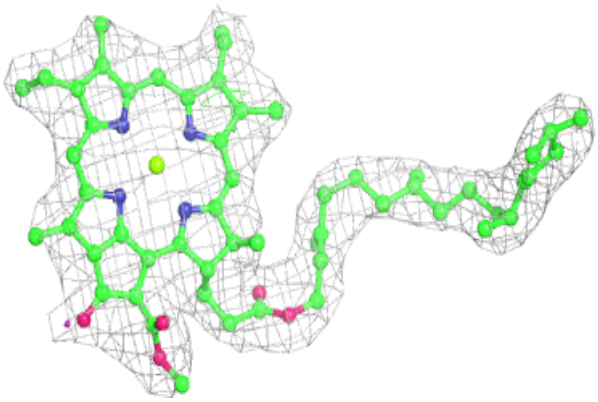


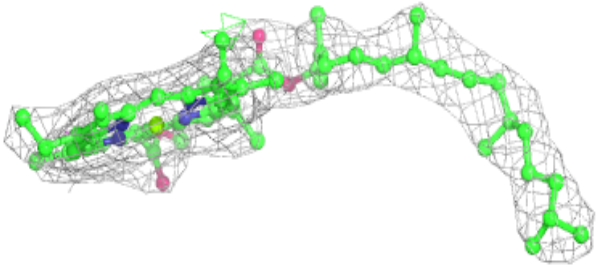


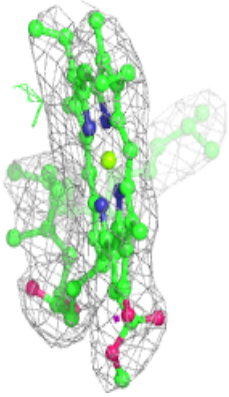


Electron density around CLA b 803:

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

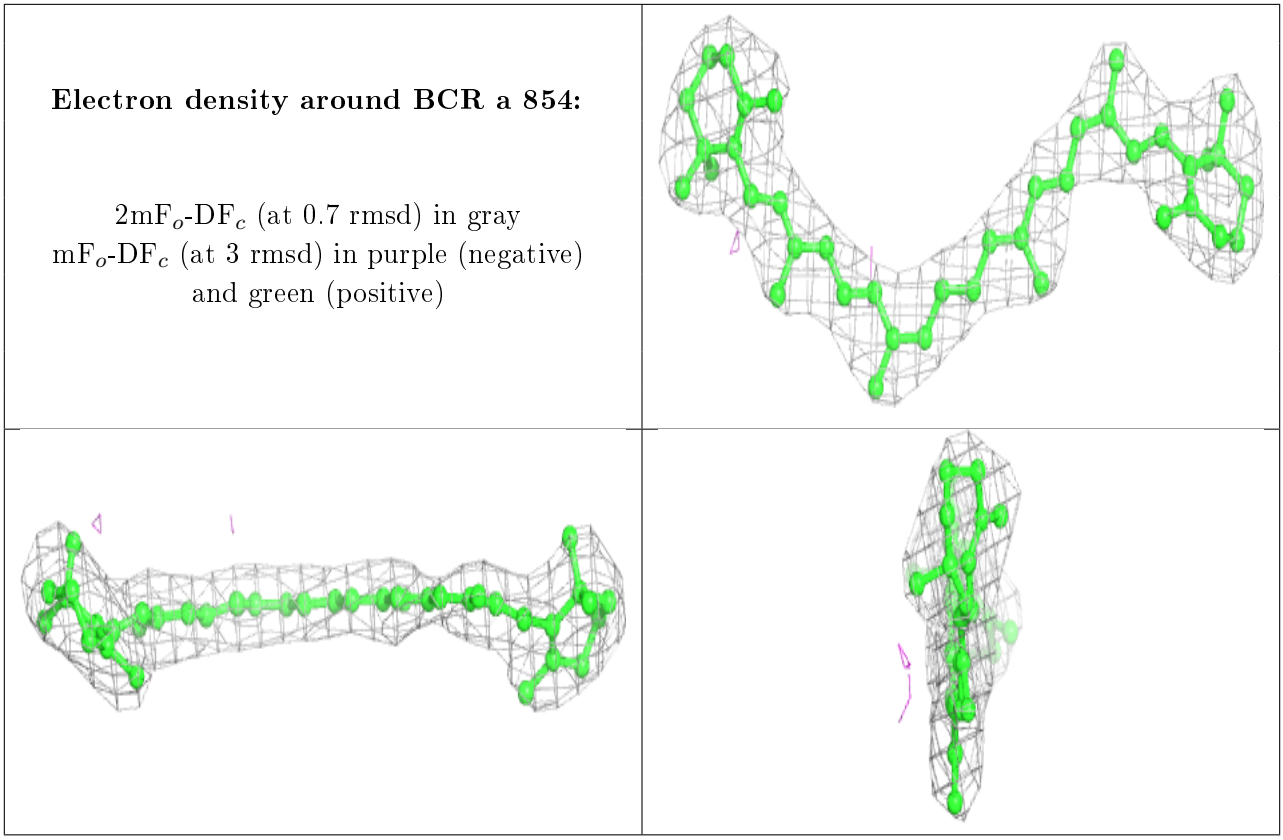






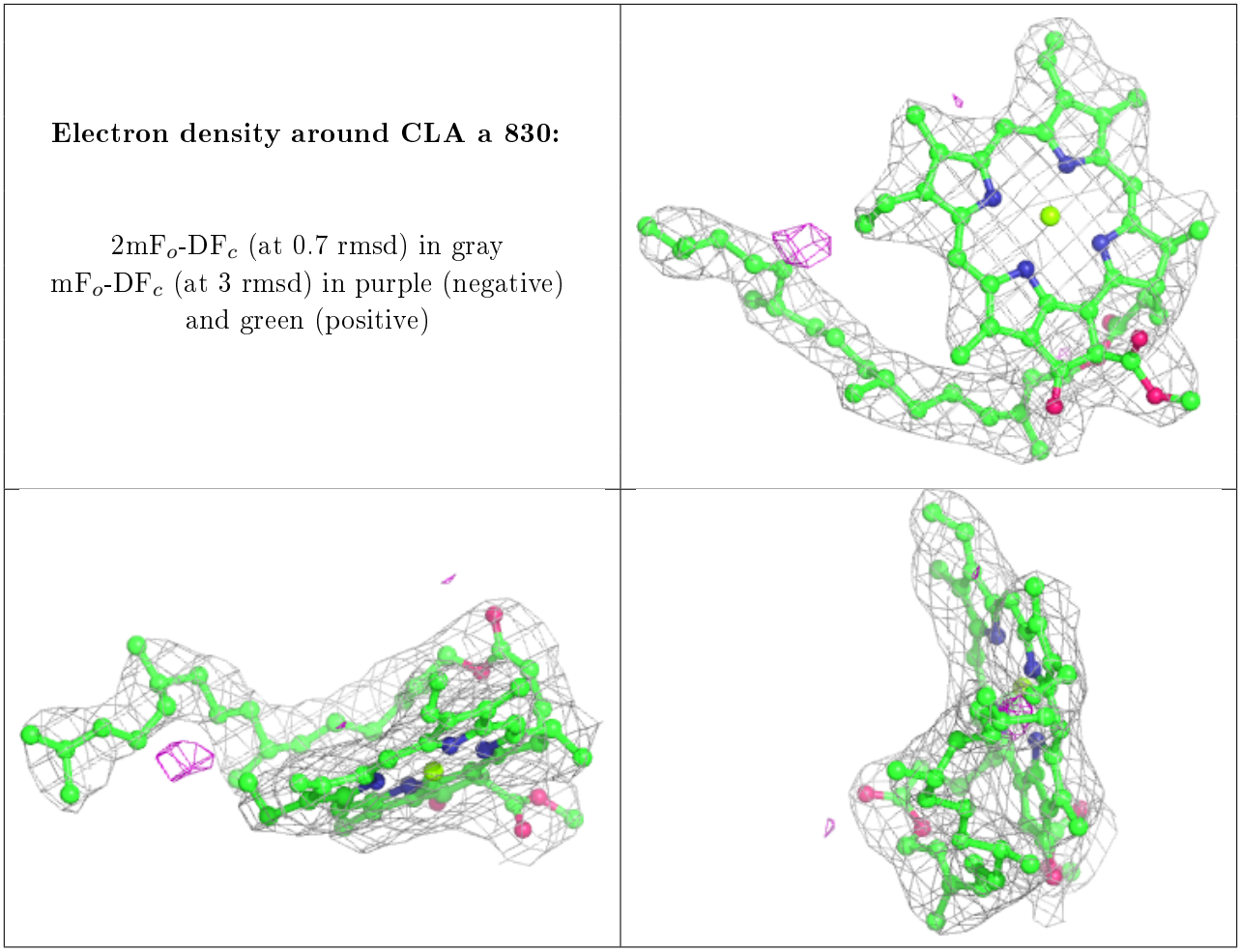
Electron density around BCR a 854:

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



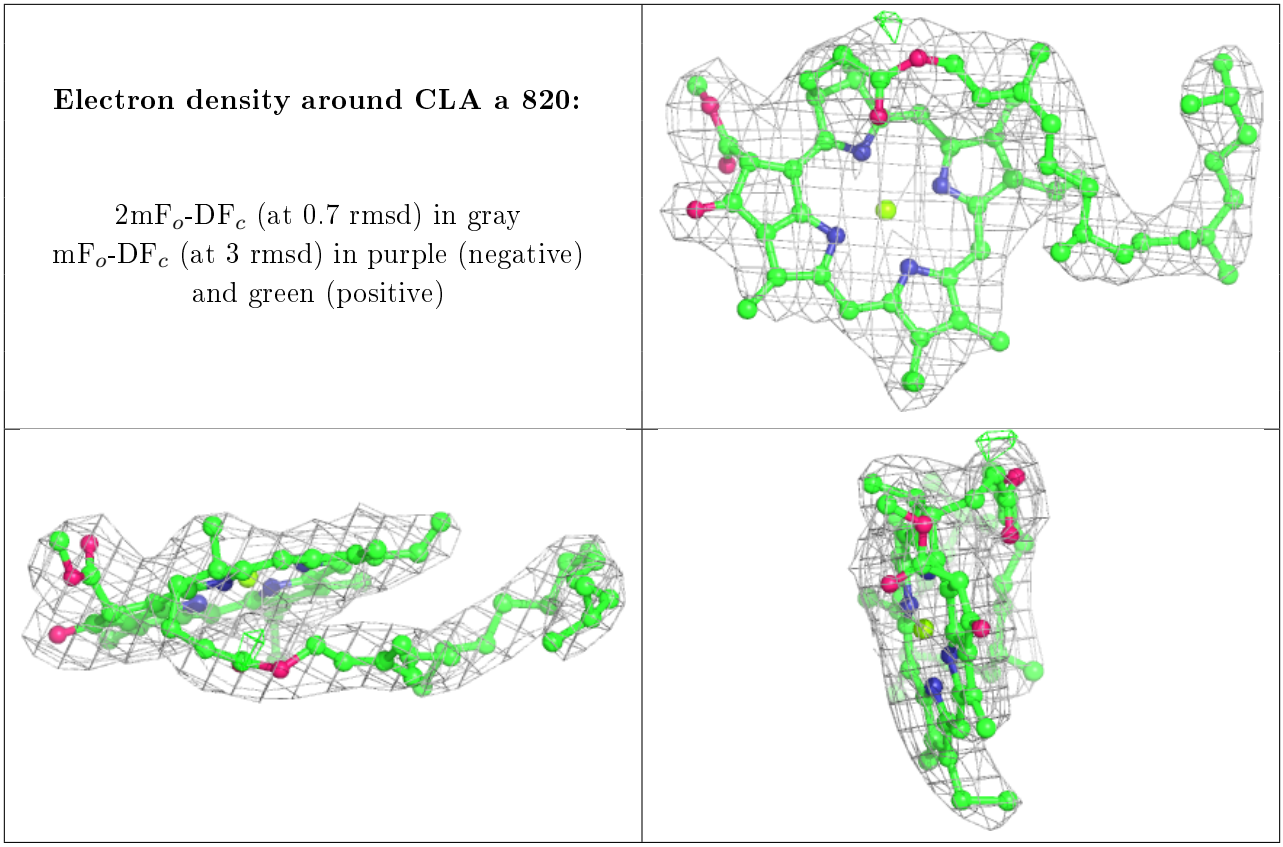
Electron density around CLA a 830:

$2mF_o$-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 820:

$2mF_o$-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

There are no such residues in this entry.