wwPDB X-ray Structure Validation Summary Report (i)

Oct 4, 2023 – 01:33 AM EDT

PDB ID	:	6PFY
Title	:	Membrane Protein Megahertz Crystallography at the European XFEL, Photosystem I at synchrotron to 2.9 A
Authors	:	Fromme, R.
Deposited on	:	2019-06-23
Resolution	:	2.90 Å(reported)

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

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

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references (i)) were used in the production of this report:

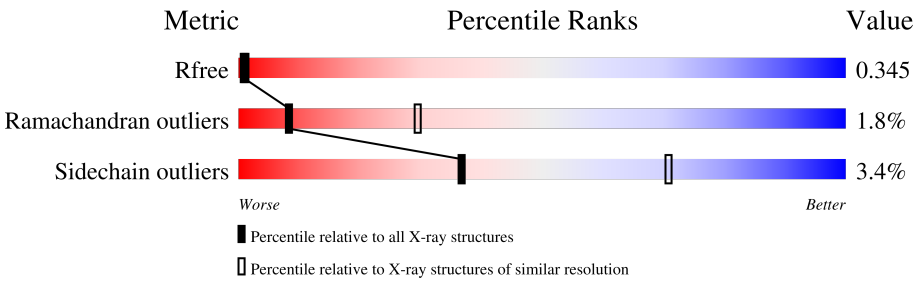
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

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 2.90 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	1957 (2.90-2.90)
Ramachandran outliers	138981	2115 (2.90-2.90)
Sidechain outliers	138945	2117 (2.90-2.90)

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

Mol	Chain	Length	Quality of chain
1	A	755	94%
1	G	755	95%
1	Y	755	93% 5%
2	B	741	95%
2	H	741	96%
2	Z	741	95%
3	C	81	96%
3	N	81	91% 7%

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Mol	Chain	Length	Quality of chain
3	a	81	93% 6%
4	D	139	96%
4	O	139	96%
4	b	139	91% 8%
5	E	76	86% 5% 9%
5	P	76	83% 8% 9%
5	c	76	86% 5% 9%
6	F	164	83% 14%
6	Q	164	83% 14%
6	d	164	79% 6% 14%
7	I	38	95% 5%
7	R	38	100%
7	e	38	97%
8	J	41	98%
8	S	41	98%
8	f	41	100%
9	K	83	47% 7% 45%
9	T	83	52% 45%
9	g	83	51% 5% 45%
10	L	155	94%
10	U	155	95%
10	h	155	93% 5%
11	M	31	94%
11	V	31	97%
11	i	31	97%

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Mol	Chain	Length	Quality of chain
12	W	39	67% 33%
12	X	39	64% • 33%
12	j	39	64% • 33%

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
13	CL0	A	801	X	-	-	-
13	CL0	G	801	X	-	-	-
13	CL0	Y	801	X	-	-	-
14	CLA	A	802	X	-	-	-
14	CLA	A	803	X	-	-	-
14	CLA	A	804	X	-	-	-
14	CLA	A	805	X	-	-	-
14	CLA	A	806	X	-	-	-
14	CLA	A	807	X	-	-	-
14	CLA	A	808	X	-	-	-
14	CLA	A	809	X	-	-	-
14	CLA	A	810	X	-	-	-
14	CLA	A	811	X	-	-	-
14	CLA	A	812	X	-	-	-
14	CLA	A	813	X	-	-	-
14	CLA	A	814	X	-	-	-
14	CLA	A	815	X	-	-	-
14	CLA	A	816	X	-	-	-
14	CLA	A	817	X	-	-	-
14	CLA	A	818	X	-	-	-
14	CLA	A	819	X	-	-	-
14	CLA	A	820	X	-	-	-
14	CLA	A	821	X	-	-	-
14	CLA	A	822	X	-	-	-
14	CLA	A	823	X	-	-	-
14	CLA	A	824	X	-	-	-
14	CLA	A	825	X	-	-	-
14	CLA	A	826	X	-	-	-
14	CLA	A	827	X	-	-	-
14	CLA	A	828	X	-	-	-
14	CLA	A	829	X	-	-	-
14	CLA	A	830	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
14	CLA	A	831	X	-	-	-
14	CLA	A	832	X	-	-	-
14	CLA	A	833	X	-	-	-
14	CLA	A	834	X	-	-	-
14	CLA	A	835	X	-	-	-
14	CLA	A	836	X	-	-	-
14	CLA	A	837	X	-	-	-
14	CLA	A	838	X	-	-	-
14	CLA	A	839	X	-	-	-
14	CLA	A	840	X	-	-	-
14	CLA	A	841	X	-	-	-
14	CLA	A	842	X	-	-	-
14	CLA	A	843	X	-	-	-
14	CLA	A	854	X	-	-	-
14	CLA	B	801	X	-	-	-
14	CLA	B	802	X	-	-	-
14	CLA	B	803	X	-	-	-
14	CLA	B	804	X	-	-	-
14	CLA	B	805	X	-	-	-
14	CLA	B	806	X	-	-	-
14	CLA	B	807	X	-	-	-
14	CLA	B	808	X	-	-	-
14	CLA	B	809	X	-	-	-
14	CLA	B	810	X	-	-	-
14	CLA	B	811	X	-	-	-
14	CLA	B	812	X	-	-	-
14	CLA	B	813	X	-	-	-
14	CLA	B	814	X	-	-	-
14	CLA	B	815	X	-	-	-
14	CLA	B	816	X	-	-	-
14	CLA	B	817	X	-	-	-
14	CLA	B	818	X	-	-	-
14	CLA	B	819	X	-	-	-
14	CLA	B	820	X	-	-	-
14	CLA	B	821	X	-	-	-
14	CLA	B	822	X	-	-	-
14	CLA	B	823	X	-	-	-
14	CLA	B	824	X	-	-	-
14	CLA	B	825	X	-	-	-
14	CLA	B	826	X	-	-	-
14	CLA	B	827	X	-	-	-
14	CLA	B	828	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
14	CLA	B	829	X	-	-	-
14	CLA	B	830	X	-	-	-
14	CLA	B	831	X	-	-	-
14	CLA	B	832	X	-	-	-
14	CLA	B	833	X	-	-	-
14	CLA	B	834	X	-	-	-
14	CLA	B	835	X	-	-	-
14	CLA	B	836	X	-	-	-
14	CLA	B	837	X	-	-	-
14	CLA	B	838	X	-	-	-
14	CLA	B	839	X	-	-	-
14	CLA	B	840	X	-	-	-
14	CLA	F	202	X	-	-	-
14	CLA	G	802	X	-	-	-
14	CLA	G	803	X	-	-	-
14	CLA	G	804	X	-	-	-
14	CLA	G	805	X	-	-	-
14	CLA	G	806	X	-	-	-
14	CLA	G	807	X	-	-	-
14	CLA	G	808	X	-	-	-
14	CLA	G	809	X	-	-	-
14	CLA	G	810	X	-	-	-
14	CLA	G	811	X	-	-	-
14	CLA	G	812	X	-	-	-
14	CLA	G	813	X	-	-	-
14	CLA	G	814	X	-	-	-
14	CLA	G	815	X	-	-	-
14	CLA	G	816	X	-	-	-
14	CLA	G	817	X	-	-	-
14	CLA	G	818	X	-	-	-
14	CLA	G	819	X	-	-	-
14	CLA	G	820	X	-	-	-
14	CLA	G	821	X	-	-	-
14	CLA	G	822	X	-	-	-
14	CLA	G	823	X	-	-	-
14	CLA	G	824	X	-	-	-
14	CLA	G	825	X	-	-	-
14	CLA	G	826	X	-	-	-
14	CLA	G	827	X	-	-	-
14	CLA	G	828	X	-	-	-
14	CLA	G	829	X	-	-	-
14	CLA	G	830	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
14	CLA	G	831	X	-	-	-
14	CLA	G	832	X	-	-	-
14	CLA	G	833	X	-	-	-
14	CLA	G	834	X	-	-	-
14	CLA	G	835	X	-	-	-
14	CLA	G	836	X	-	-	-
14	CLA	G	837	X	-	-	-
14	CLA	G	838	X	-	-	-
14	CLA	G	839	X	-	-	-
14	CLA	G	840	X	-	-	-
14	CLA	G	841	X	-	-	-
14	CLA	G	842	X	-	-	-
14	CLA	G	852	X	-	-	-
14	CLA	G	853	X	-	-	-
14	CLA	H	801	X	-	-	-
14	CLA	H	802	X	-	-	-
14	CLA	H	803	X	-	-	-
14	CLA	H	804	X	-	-	-
14	CLA	H	805	X	-	-	-
14	CLA	H	806	X	-	-	-
14	CLA	H	807	X	-	-	-
14	CLA	H	808	X	-	-	-
14	CLA	H	809	X	-	-	-
14	CLA	H	810	X	-	-	-
14	CLA	H	811	X	-	-	-
14	CLA	H	812	X	-	-	-
14	CLA	H	813	X	-	-	-
14	CLA	H	814	X	-	-	-
14	CLA	H	815	X	-	-	-
14	CLA	H	816	X	-	-	-
14	CLA	H	817	X	-	-	-
14	CLA	H	818	X	-	-	-
14	CLA	H	819	X	-	-	-
14	CLA	H	820	X	-	-	-
14	CLA	H	821	X	-	-	-
14	CLA	H	822	X	-	-	-
14	CLA	H	823	X	-	-	-
14	CLA	H	824	X	-	-	-
14	CLA	H	825	X	-	-	-
14	CLA	H	826	X	-	-	-
14	CLA	H	827	X	-	-	-
14	CLA	H	828	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
14	CLA	H	829	X	-	-	-
14	CLA	H	830	X	-	-	-
14	CLA	H	831	X	-	-	-
14	CLA	H	832	X	-	-	-
14	CLA	H	833	X	-	-	-
14	CLA	H	834	X	-	-	-
14	CLA	H	835	X	-	-	-
14	CLA	H	836	X	-	-	-
14	CLA	H	837	X	-	-	-
14	CLA	H	838	X	-	-	-
14	CLA	H	839	X	-	-	-
14	CLA	H	840	X	-	-	-
14	CLA	H	851	X	-	-	-
14	CLA	J	101	X	-	-	-
14	CLA	J	102	X	-	-	-
14	CLA	K	101	X	-	-	-
14	CLA	K	102	X	-	-	-
14	CLA	L	201	X	-	-	-
14	CLA	L	202	X	-	-	-
14	CLA	L	204	X	-	-	-
14	CLA	L	205	X	-	-	-
14	CLA	L	206	X	-	-	-
14	CLA	Q	202	X	-	-	-
14	CLA	S	1101	X	-	-	-
14	CLA	S	1102	X	-	-	-
14	CLA	S	1103	X	-	-	-
14	CLA	T	101	X	-	-	-
14	CLA	T	103	X	-	-	-
14	CLA	U	1002	X	-	-	-
14	CLA	U	1003	X	-	-	-
14	CLA	U	1004	X	-	-	-
14	CLA	U	1006	X	-	-	-
14	CLA	U	1007	X	-	-	-
14	CLA	W	1701	X	-	-	-
14	CLA	X	1701	X	-	-	-
14	CLA	Y	802	X	-	-	-
14	CLA	Y	803	X	-	-	-
14	CLA	Y	804	X	-	-	-
14	CLA	Y	805	X	-	-	-
14	CLA	Y	806	X	-	-	-
14	CLA	Y	807	X	-	-	-
14	CLA	Y	808	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
14	CLA	Y	809	X	-	-	-
14	CLA	Y	810	X	-	-	-
14	CLA	Y	811	X	-	-	-
14	CLA	Y	812	X	-	-	-
14	CLA	Y	813	X	-	-	-
14	CLA	Y	814	X	-	-	-
14	CLA	Y	815	X	-	-	-
14	CLA	Y	816	X	-	-	-
14	CLA	Y	817	X	-	-	-
14	CLA	Y	818	X	-	-	-
14	CLA	Y	819	X	-	-	-
14	CLA	Y	820	X	-	-	-
14	CLA	Y	821	X	-	-	-
14	CLA	Y	822	X	-	-	-
14	CLA	Y	823	X	-	-	-
14	CLA	Y	824	X	-	-	-
14	CLA	Y	825	X	-	-	-
14	CLA	Y	826	X	-	-	-
14	CLA	Y	827	X	-	-	-
14	CLA	Y	828	X	-	-	-
14	CLA	Y	829	X	-	-	-
14	CLA	Y	830	X	-	-	-
14	CLA	Y	831	X	-	-	-
14	CLA	Y	832	X	-	-	-
14	CLA	Y	833	X	-	-	-
14	CLA	Y	834	X	-	-	-
14	CLA	Y	835	X	-	-	-
14	CLA	Y	836	X	-	-	-
14	CLA	Y	837	X	-	-	-
14	CLA	Y	838	X	-	-	-
14	CLA	Y	839	X	-	-	-
14	CLA	Y	840	X	-	-	-
14	CLA	Y	841	X	-	-	-
14	CLA	Z	801	X	-	-	-
14	CLA	Z	802	X	-	-	-
14	CLA	Z	803	X	-	-	-
14	CLA	Z	804	X	-	-	-
14	CLA	Z	805	X	-	-	-
14	CLA	Z	806	X	-	-	-
14	CLA	Z	807	X	-	-	-
14	CLA	Z	808	X	-	-	-
14	CLA	Z	809	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
14	CLA	Z	810	X	-	-	-
14	CLA	Z	811	X	-	-	-
14	CLA	Z	812	X	-	-	-
14	CLA	Z	813	X	-	-	-
14	CLA	Z	814	X	-	-	-
14	CLA	Z	815	X	-	-	-
14	CLA	Z	816	X	-	-	-
14	CLA	Z	817	X	-	-	-
14	CLA	Z	818	X	-	-	-
14	CLA	Z	819	X	-	-	-
14	CLA	Z	820	X	-	-	-
14	CLA	Z	821	X	-	-	-
14	CLA	Z	822	X	-	-	-
14	CLA	Z	823	X	-	-	-
14	CLA	Z	824	X	-	-	-
14	CLA	Z	825	X	-	-	-
14	CLA	Z	826	X	-	-	-
14	CLA	Z	827	X	-	-	-
14	CLA	Z	828	X	-	-	-
14	CLA	Z	829	X	-	-	-
14	CLA	Z	830	X	-	-	-
14	CLA	Z	831	X	-	-	-
14	CLA	Z	832	X	-	-	-
14	CLA	Z	833	X	-	-	-
14	CLA	Z	834	X	-	-	-
14	CLA	Z	835	X	-	-	-
14	CLA	Z	836	X	-	-	-
14	CLA	Z	837	X	-	-	-
14	CLA	Z	838	X	-	-	-
14	CLA	Z	839	X	-	-	-
14	CLA	Z	840	X	-	-	-
14	CLA	Z	841	X	-	-	-
14	CLA	d	201	X	-	-	-
14	CLA	d	202	X	-	-	-
14	CLA	f	101	X	-	-	-
14	CLA	f	102	X	-	-	-
14	CLA	g	101	X	-	-	-
14	CLA	g	102	X	-	-	-
14	CLA	h	201	X	-	-	-
14	CLA	h	204	X	-	-	-
14	CLA	h	205	X	-	-	-
14	CLA	h	206	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
14	CLA	j	102	X	-	-	-

2 Entry composition (i)

There are 21 unique types of molecules in this entry. The entry contains 72737 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
			Total	C	N	O	S			
1	A	741	5791	3799	989	977	26	0	0	0
1	G	741	5791	3799	989	977	26	0	0	0
1	Y	741	5791	3799	989	977	26	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	739	5889	3876	987	1005	21	0	0	0
2	H	739	5889	3876	987	1005	21	0	0	0
2	Z	739	5889	3876	987	1005	21	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	C	80	598	367	103	117	11	0	0	0
3	N	80	598	367	103	117	11	0	0	0
3	a	80	598	367	103	117	11	0	0	0

- Molecule 4 is a protein called Photosystem I reaction center subunit II.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
4	D	138	1075	682	186	204	3	0	0	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
4	O	138	1075	682	186	204	3	0	0	0
			Total	C	N	O	S			
4	b	138	1075	682	186	204	3	0	0	0

- Molecule 5 is a protein called Photosystem I reaction center subunit IV.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
5	E	69	539	342	93	104	0	0	0
			Total	C	N	O			
5	P	69	539	342	93	104	0	0	0
			Total	C	N	O			
5	c	69	539	342	93	104	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
6	F	141	1065	680	184	197	4	0	0	0
			Total	C	N	O	S			
6	Q	141	1065	680	184	197	4	0	0	0
			Total	C	N	O	S			
6	d	141	1065	680	184	197	4	0	0	0

- Molecule 7 is a protein called Photosystem I reaction center subunit VIII.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
7	I	38	301	208	40	48	5	0	0	0
			Total	C	N	O	S			
7	R	38	301	208	40	48	5	0	0	0
			Total	C	N	O	S			
7	e	38	301	208	40	48	5	0	0	0

- Molecule 8 is a protein called Photosystem I reaction center subunit IX.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
8	J	41	338	231	51	54	2	0	0	0
			Total	C	N	O	S			
8	S	41	338	231	51	54	2	0	0	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
8	f	41	338	231	51	54	2	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
9	K	46	328	214	57	56	1	0	0	0
			Total	C	N	O	S			
9	T	46	328	214	57	56	1	0	0	0
			Total	C	N	O	S			
9	g	46	328	214	57	56	1	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
10	L	151	1119	735	179	201	4	0	0	0
			Total	C	N	O	S			
10	U	151	1119	735	179	201	4	0	0	0
			Total	C	N	O	S			
10	h	151	1119	735	179	201	4	0	0	0

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
L	143	LEU	SER	conflict	UNP Q8DGB4
U	143	LEU	SER	conflict	UNP Q8DGB4
h	143	LEU	SER	conflict	UNP Q8DGB4

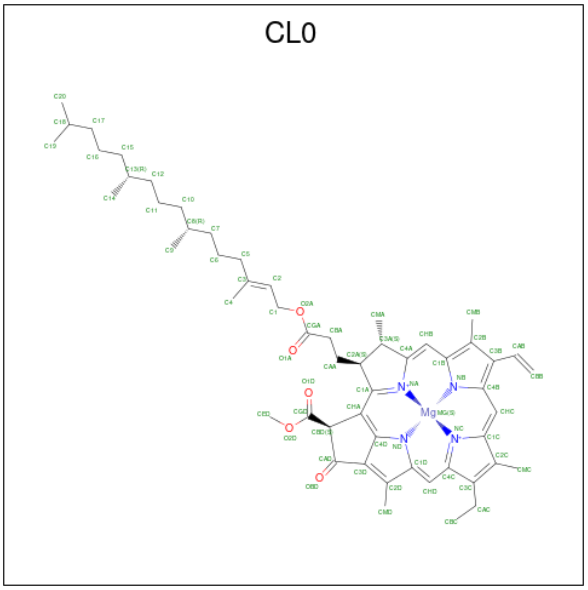
- Molecule 11 is a protein called Photosystem I reaction center subunit XII.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
11	M	30	233	156	35	42	0	0	0
			Total	C	N	O			
11	V	30	233	156	35	42	0	0	0
			Total	C	N	O			
11	i	30	233	156	35	42	0	0	0

- Molecule 12 is a protein called Photosystem I 4.8K protein.

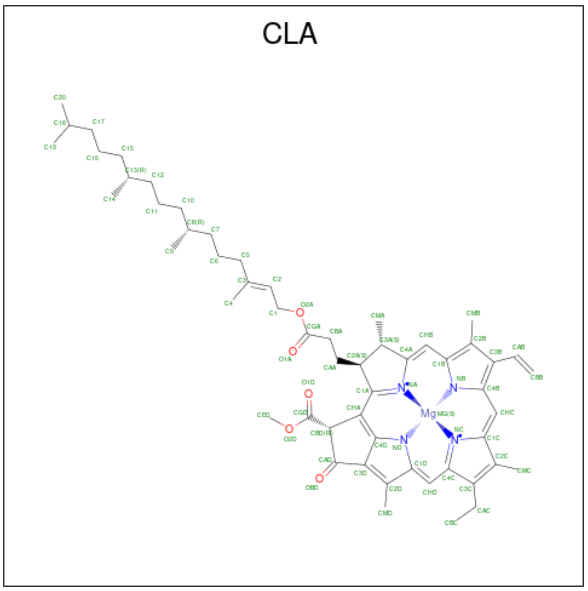
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
12	W	26	219	157	31	31	0	0	0
12	X	26	219	157	31	31	0	0	0
12	j	26	219	157	31	31	0	0	0

- Molecule 13 is CHLOROPHYLL A ISOMER (three-letter code: CL0) (formula: $C_{55}H_{72}MgN_4O_5$) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 14 is CHLOROPHYLL A (three-letter code: CLA) (formula: $C_{55}H_{72}MgN_4O_5$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	Mg	N	O		
14	A	1	65	55	1	4	5	0	0
			Total	C	Mg	N	O		
14	A	1	65	55	1	4	5	0	0
			Total	C	Mg	N	O		
14	A	1	65	55	1	4	5	0	0
			Total	C	Mg	N	O		
14	A	1	59	49	1	4	5	0	0
			Total	C	Mg	N	O		
14	A	1	65	55	1	4	5	0	0
			Total	C	Mg	N	O		
14	A	1	65	55	1	4	5	0	0
			Total	C	Mg	N	O		
14	A	1	51	41	1	4	5	0	0
			Total	C	Mg	N	O		
14	A	1	65	55	1	4	5	0	0
			Total	C	Mg	N	O		
14	A	1	65	55	1	4	5	0	0
			Total	C	Mg	N	O		
14	A	1	45	35	1	4	5	0	0
			Total	C	Mg	N	O		
14	A	1	65	55	1	4	5	0	0
			Total	C	Mg	N	O		
14	A	1	54	44	1	4	5	0	0
			Total	C	Mg	N	O		
14	A	1	60	50	1	4	5	0	0
			Total	C	Mg	N	O		
14	A	1	50	40	1	4	5	0	0

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

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	Mg	N	O		
14	A	1	65	55	1	4	5	0	0
			Total	C	Mg	N	O		
14	A	1	50	40	1	4	5	0	0
			Total	C	Mg	N	O		
14	A	1	65	55	1	4	5	0	0
			Total	C	Mg	N	O		
14	A	1	50	40	1	4	5	0	0
			Total	C	Mg	N	O		
14	A	1	65	55	1	4	5	0	0
			Total	C	Mg	N	O		
14	A	1	65	55	1	4	5	0	0
			Total	C	Mg	N	O		
14	A	1	50	40	1	4	5	0	0
			Total	C	Mg	N	O		
14	A	1	65	55	1	4	5	0	0
			Total	C	Mg	N	O		
14	B	1	65	55	1	4	5	0	0
			Total	C	Mg	N	O		
14	B	1	65	55	1	4	5	0	0
			Total	C	Mg	N	O		
14	B	1	54	44	1	4	5	0	0
			Total	C	Mg	N	O		
14	B	1	65	55	1	4	5	0	0
			Total	C	Mg	N	O		
14	B	1	65	55	1	4	5	0	0
			Total	C	Mg	N	O		
14	B	1	65	55	1	4	5	0	0
			Total	C	Mg	N	O		
14	B	1	65	55	1	4	5	0	0
			Total	C	Mg	N	O		
14	B	1	65	55	1	4	5	0	0
			Total	C	Mg	N	O		
14	B	1	55	45	1	4	5	0	0
			Total	C	Mg	N	O		
14	B	1	50	40	1	4	5	0	0
			Total	C	Mg	N	O		
14	B	1	65	55	1	4	5	0	0
			Total	C	Mg	N	O		
14	B	1	65	55	1	4	5	0	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	Mg	N	O		
14	B	1	45	35	1	4	5	0	0
			Total	C	Mg	N	O		
14	B	1	55	45	1	4	5	0	0
			Total	C	Mg	N	O		
14	B	1	65	55	1	4	5	0	0
			Total	C	Mg	N	O		
14	B	1	60	50	1	4	5	0	0
			Total	C	Mg	N	O		
14	B	1	60	50	1	4	5	0	0
			Total	C	Mg	N	O		
14	B	1	45	35	1	4	5	0	0
			Total	C	Mg	N	O		
14	B	1	45	35	1	4	5	0	0
			Total	C	Mg	N	O		
14	B	1	55	45	1	4	5	0	0
			Total	C	Mg	N	O		
14	B	1	60	50	1	4	5	0	0
			Total	C	Mg	N	O		
14	B	1	55	45	1	4	5	0	0
			Total	C	Mg	N	O		
14	B	1	65	55	1	4	5	0	0
			Total	C	Mg	N	O		
14	B	1	65	55	1	4	5	0	0
			Total	C	Mg	N	O		
14	B	1	65	55	1	4	5	0	0
			Total	C	Mg	N	O		
14	B	1	65	55	1	4	5	0	0
			Total	C	Mg	N	O		
14	B	1	65	55	1	4	5	0	0
			Total	C	Mg	N	O		
14	B	1	45	35	1	4	5	0	0
			Total	C	Mg	N	O		
14	B	1	45	35	1	4	5	0	0
			Total	C	Mg	N	O		
14	B	1	65	55	1	4	5	0	0
			Total	C	Mg	N	O		
14	B	1	55	45	1	4	5	0	0
			Total	C	Mg	N	O		
14	B	1	45	35	1	4	5	0	0
			Total	C	Mg	N	O		
14	B	1	45	35	1	4	5	0	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	Mg	N	O		
14	B	1	45	35	1	4	5	0	0
			Total	C	Mg	N	O		
14	B	1	60	50	1	4	5	0	0
			Total	C	Mg	N	O		
14	B	1	65	55	1	4	5	0	0
			Total	C	Mg	N	O		
14	B	1	45	35	1	4	5	0	0
			Total	C	Mg	N	O		
14	B	1	65	55	1	4	5	0	0
			Total	C	Mg	N	O		
14	B	1	65	55	1	4	5	0	0
			Total	C	Mg	N	O		
14	F	1	45	35	1	4	5	0	0
			Total	C	Mg	N	O		
14	G	1	65	55	1	4	5	0	0
			Total	C	Mg	N	O		
14	G	1	65	55	1	4	5	0	0
			Total	C	Mg	N	O		
14	G	1	59	49	1	4	5	0	0
			Total	C	Mg	N	O		
14	G	1	65	55	1	4	5	0	0
			Total	C	Mg	N	O		
14	G	1	65	55	1	4	5	0	0
			Total	C	Mg	N	O		
14	G	1	51	41	1	4	5	0	0
			Total	C	Mg	N	O		
14	G	1	65	55	1	4	5	0	0
			Total	C	Mg	N	O		
14	G	1	65	55	1	4	5	0	0
			Total	C	Mg	N	O		
14	G	1	45	35	1	4	5	0	0
			Total	C	Mg	N	O		
14	G	1	65	55	1	4	5	0	0
			Total	C	Mg	N	O		
14	G	1	54	44	1	4	5	0	0
			Total	C	Mg	N	O		
14	G	1	60	50	1	4	5	0	0
			Total	C	Mg	N	O		
14	G	1	50	40	1	4	5	0	0
			Total	C	Mg	N	O		
14	G	1	50	40	1	4	5	0	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	Mg	N	O		
14	G	1	50	40	1	4	5	0	0
			Total	C	Mg	N	O		
14	G	1	60	50	1	4	5	0	0
			Total	C	Mg	N	O		
14	G	1	65	55	1	4	5	0	0
			Total	C	Mg	N	O		
14	G	1	65	55	1	4	5	0	0
			Total	C	Mg	N	O		
14	G	1	60	50	1	4	5	0	0
			Total	C	Mg	N	O		
14	G	1	65	55	1	4	5	0	0
			Total	C	Mg	N	O		
14	G	1	65	55	1	4	5	0	0
			Total	C	Mg	N	O		
14	G	1	50	40	1	4	5	0	0
			Total	C	Mg	N	O		
14	G	1	60	50	1	4	5	0	0
			Total	C	Mg	N	O		
14	G	1	65	55	1	4	5	0	0
			Total	C	Mg	N	O		
14	G	1	60	50	1	4	5	0	0
			Total	C	Mg	N	O		
14	G	1	65	55	1	4	5	0	0
			Total	C	Mg	N	O		
14	G	1	65	55	1	4	5	0	0
			Total	C	Mg	N	O		
14	G	1	65	55	1	4	5	0	0
			Total	C	Mg	N	O		
14	G	1	65	55	1	4	5	0	0
			Total	C	Mg	N	O		
14	G	1	50	40	1	4	5	0	0
			Total	C	Mg	N	O		
14	G	1	65	55	1	4	5	0	0
			Total	C	Mg	N	O		
14	G	1	65	55	1	4	5	0	0
			Total	C	Mg	N	O		
14	G	1	55	45	1	4	5	0	0
			Total	C	Mg	N	O		
14	G	1	45	35	1	4	5	0	0
			Total	C	Mg	N	O		
14	G	1	50	40	1	4	5	0	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	Mg	N	O		
14	G	1	65	55	1	4	5	0	0
			Total	C	Mg	N	O		
14	G	1	50	40	1	4	5	0	0
			Total	C	Mg	N	O		
14	G	1	50	40	1	4	5	0	0
			Total	C	Mg	N	O		
14	G	1	65	55	1	4	5	0	0
			Total	C	Mg	N	O		
14	G	1	65	55	1	4	5	0	0
			Total	C	Mg	N	O		
14	G	1	50	40	1	4	5	0	0
			Total	C	Mg	N	O		
14	G	1	65	55	1	4	5	0	0
			Total	C	Mg	N	O		
14	G	1	45	35	1	4	5	0	0
			Total	C	Mg	N	O		
14	H	1	65	55	1	4	5	0	0
			Total	C	Mg	N	O		
14	H	1	65	55	1	4	5	0	0
			Total	C	Mg	N	O		
14	H	1	65	55	1	4	5	0	0
			Total	C	Mg	N	O		
14	H	1	54	44	1	4	5	0	0
			Total	C	Mg	N	O		
14	H	1	65	55	1	4	5	0	0
			Total	C	Mg	N	O		
14	H	1	65	55	1	4	5	0	0
			Total	C	Mg	N	O		
14	H	1	65	55	1	4	5	0	0
			Total	C	Mg	N	O		
14	H	1	65	55	1	4	5	0	0
			Total	C	Mg	N	O		
14	H	1	65	55	1	4	5	0	0
			Total	C	Mg	N	O		
14	H	1	55	45	1	4	5	0	0
			Total	C	Mg	N	O		
14	H	1	45	35	1	4	5	0	0
			Total	C	Mg	N	O		
14	H	1	65	55	1	4	5	0	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	Mg	N	O		
14	H	1	65	55	1	4	5	0	0
			Total	C	Mg	N	O		
14	H	1	45	35	1	4	5	0	0
			Total	C	Mg	N	O		
14	H	1	55	45	1	4	5	0	0
			Total	C	Mg	N	O		
14	H	1	65	55	1	4	5	0	0
			Total	C	Mg	N	O		
14	H	1	60	50	1	4	5	0	0
			Total	C	Mg	N	O		
14	H	1	60	50	1	4	5	0	0
			Total	C	Mg	N	O		
14	H	1	45	35	1	4	5	0	0
			Total	C	Mg	N	O		
14	H	1	45	35	1	4	5	0	0
			Total	C	Mg	N	O		
14	H	1	55	45	1	4	5	0	0
			Total	C	Mg	N	O		
14	H	1	60	50	1	4	5	0	0
			Total	C	Mg	N	O		
14	H	1	55	45	1	4	5	0	0
			Total	C	Mg	N	O		
14	H	1	65	55	1	4	5	0	0
			Total	C	Mg	N	O		
14	H	1	65	55	1	4	5	0	0
			Total	C	Mg	N	O		
14	H	1	65	55	1	4	5	0	0
			Total	C	Mg	N	O		
14	H	1	65	55	1	4	5	0	0
			Total	C	Mg	N	O		
14	H	1	65	55	1	4	5	0	0
			Total	C	Mg	N	O		
14	H	1	45	35	1	4	5	0	0
			Total	C	Mg	N	O		
14	H	1	65	55	1	4	5	0	0
			Total	C	Mg	N	O		
14	H	1	55	45	1	4	5	0	0
			Total	C	Mg	N	O		
14	H	1	45	35	1	4	5	0	0
			Total	C	Mg	N	O		
14	H	1	45	35	1	4	5	0	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	Mg	N	O		
14	H	1	45	35	1	4	5	0	0
			Total	C	Mg	N	O		
14	H	1	60	50	1	4	5	0	0
			Total	C	Mg	N	O		
14	H	1	65	55	1	4	5	0	0
			Total	C	Mg	N	O		
14	H	1	45	35	1	4	5	0	0
			Total	C	Mg	N	O		
14	H	1	65	55	1	4	5	0	0
			Total	C	Mg	N	O		
14	H	1	65	55	1	4	5	0	0
			Total	C	Mg	N	O		
14	H	1	50	40	1	4	5	0	0
			Total	C	Mg	N	O		
14	J	1	45	35	1	4	5	0	0
			Total	C	Mg	N	O		
14	J	1	55	45	1	4	5	0	0
			Total	C	Mg	N	O		
14	K	1	41	33	1	4	3	0	0
			Total	C	Mg	N	O		
14	K	1	45	35	1	4	5	0	0
			Total	C	Mg	N	O		
14	L	1	65	55	1	4	5	0	0
			Total	C	Mg	N	O		
14	L	1	65	55	1	4	5	0	0
			Total	C	Mg	N	O		
14	L	1	65	55	1	4	5	0	0
			Total	C	Mg	N	O		
14	L	1	65	55	1	4	5	0	0
			Total	C	Mg	N	O		
14	L	1	65	55	1	4	5	0	0
			Total	C	Mg	N	O		
14	Q	1	45	35	1	4	5	0	0
			Total	C	Mg	N	O		
14	S	1	65	55	1	4	5	0	0
			Total	C	Mg	N	O		
14	S	1	45	35	1	4	5	0	0
			Total	C	Mg	N	O		
14	S	1	55	45	1	4	5	0	0
			Total	C	Mg	N	O		
14	T	1	41	33	1	4	3	0	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	Mg	N	O		
14	T	1	45	35	1	4	5	0	0
			Total	C	Mg	N	O		
14	U	1	65	55	1	4	5	0	0
			Total	C	Mg	N	O		
14	U	1	65	55	1	4	5	0	0
			Total	C	Mg	N	O		
14	U	1	65	55	1	4	5	0	0
			Total	C	Mg	N	O		
14	U	1	65	55	1	4	5	0	0
			Total	C	Mg	N	O		
14	U	1	65	55	1	4	5	0	0
			Total	C	Mg	N	O		
14	W	1	45	35	1	4	5	0	0
			Total	C	Mg	N	O		
14	X	1	45	35	1	4	5	0	0
			Total	C	Mg	N	O		
14	Y	1	65	55	1	4	5	0	0
			Total	C	Mg	N	O		
14	Y	1	65	55	1	4	5	0	0
			Total	C	Mg	N	O		
14	Y	1	59	49	1	4	5	0	0
			Total	C	Mg	N	O		
14	Y	1	65	55	1	4	5	0	0
			Total	C	Mg	N	O		
14	Y	1	65	55	1	4	5	0	0
			Total	C	Mg	N	O		
14	Y	1	51	41	1	4	5	0	0
			Total	C	Mg	N	O		
14	Y	1	65	55	1	4	5	0	0
			Total	C	Mg	N	O		
14	Y	1	65	55	1	4	5	0	0
			Total	C	Mg	N	O		
14	Y	1	45	35	1	4	5	0	0
			Total	C	Mg	N	O		
14	Y	1	65	55	1	4	5	0	0
			Total	C	Mg	N	O		
14	Y	1	55	45	1	4	5	0	0
			Total	C	Mg	N	O		
14	Y	1	60	50	1	4	5	0	0
			Total	C	Mg	N	O		
14	Y	1	55	45	1	4	5	0	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	Mg	N	O		
14	Y	1	50	40	1	4	5	0	0
			Total	C	Mg	N	O		
14	Y	1	50	40	1	4	5	0	0
			Total	C	Mg	N	O		
14	Y	1	60	50	1	4	5	0	0
			Total	C	Mg	N	O		
14	Y	1	65	55	1	4	5	0	0
			Total	C	Mg	N	O		
14	Y	1	65	55	1	4	5	0	0
			Total	C	Mg	N	O		
14	Y	1	60	50	1	4	5	0	0
			Total	C	Mg	N	O		
14	Y	1	65	55	1	4	5	0	0
			Total	C	Mg	N	O		
14	Y	1	65	55	1	4	5	0	0
			Total	C	Mg	N	O		
14	Y	1	50	40	1	4	5	0	0
			Total	C	Mg	N	O		
14	Y	1	60	50	1	4	5	0	0
			Total	C	Mg	N	O		
14	Y	1	65	55	1	4	5	0	0
			Total	C	Mg	N	O		
14	Y	1	60	50	1	4	5	0	0
			Total	C	Mg	N	O		
14	Y	1	65	55	1	4	5	0	0
			Total	C	Mg	N	O		
14	Y	1	65	55	1	4	5	0	0
			Total	C	Mg	N	O		
14	Y	1	65	55	1	4	5	0	0
			Total	C	Mg	N	O		
14	Y	1	50	40	1	4	5	0	0
			Total	C	Mg	N	O		
14	Y	1	65	55	1	4	5	0	0
			Total	C	Mg	N	O		
14	Y	1	55	45	1	4	5	0	0
			Total	C	Mg	N	O		
14	Y	1	45	35	1	4	5	0	0
			Total	C	Mg	N	O		
14	Y	1	50	40	1	4	5	0	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	Mg	N	O		
14	Y	1	65	55	1	4	5	0	0
			Total	C	Mg	N	O		
14	Y	1	50	40	1	4	5	0	0
			Total	C	Mg	N	O		
14	Y	1	65	55	1	4	5	0	0
			Total	C	Mg	N	O		
14	Y	1	50	40	1	4	5	0	0
			Total	C	Mg	N	O		
14	Y	1	65	55	1	4	5	0	0
			Total	C	Mg	N	O		
14	Y	1	65	55	1	4	5	0	0
			Total	C	Mg	N	O		
14	Z	1	65	55	1	4	5	0	0
			Total	C	Mg	N	O		
14	Z	1	65	55	1	4	5	0	0
			Total	C	Mg	N	O		
14	Z	1	65	55	1	4	5	0	0
			Total	C	Mg	N	O		
14	Z	1	65	55	1	4	5	0	0
			Total	C	Mg	N	O		
14	Z	1	54	44	1	4	5	0	0
			Total	C	Mg	N	O		
14	Z	1	65	55	1	4	5	0	0
			Total	C	Mg	N	O		
14	Z	1	65	55	1	4	5	0	0
			Total	C	Mg	N	O		
14	Z	1	65	55	1	4	5	0	0
			Total	C	Mg	N	O		
14	Z	1	65	55	1	4	5	0	0
			Total	C	Mg	N	O		
14	Z	1	65	55	1	4	5	0	0
			Total	C	Mg	N	O		
14	Z	1	65	55	1	4	5	0	0
			Total	C	Mg	N	O		
14	Z	1	55	45	1	4	5	0	0
			Total	C	Mg	N	O		
14	Z	1	45	35	1	4	5	0	0
			Total	C	Mg	N	O		
14	Z	1	65	55	1	4	5	0	0
			Total	C	Mg	N	O		
14	Z	1	65	55	1	4	5	0	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	Mg	N	O		
14	Z	1	45	35	1	4	5	0	0
			Total	C	Mg	N	O		
14	Z	1	55	45	1	4	5	0	0
			Total	C	Mg	N	O		
14	Z	1	65	55	1	4	5	0	0
			Total	C	Mg	N	O		
14	Z	1	60	50	1	4	5	0	0
			Total	C	Mg	N	O		
14	Z	1	60	50	1	4	5	0	0
			Total	C	Mg	N	O		
14	Z	1	45	35	1	4	5	0	0
			Total	C	Mg	N	O		
14	Z	1	45	35	1	4	5	0	0
			Total	C	Mg	N	O		
14	Z	1	55	45	1	4	5	0	0
			Total	C	Mg	N	O		
14	Z	1	60	50	1	4	5	0	0
			Total	C	Mg	N	O		
14	Z	1	55	45	1	4	5	0	0
			Total	C	Mg	N	O		
14	Z	1	65	55	1	4	5	0	0
			Total	C	Mg	N	O		
14	Z	1	65	55	1	4	5	0	0
			Total	C	Mg	N	O		
14	Z	1	65	55	1	4	5	0	0
			Total	C	Mg	N	O		
14	Z	1	65	55	1	4	5	0	0
			Total	C	Mg	N	O		
14	Z	1	65	55	1	4	5	0	0
			Total	C	Mg	N	O		
14	Z	1	45	35	1	4	5	0	0
			Total	C	Mg	N	O		
14	Z	1	45	35	1	4	5	0	0
			Total	C	Mg	N	O		
14	Z	1	55	45	1	4	5	0	0
			Total	C	Mg	N	O		
14	Z	1	45	35	1	4	5	0	0
			Total	C	Mg	N	O		
14	Z	1	45	35	1	4	5	0	0
			Total	C	Mg	N	O		
14	Z	1	45	35	1	4	5	0	0

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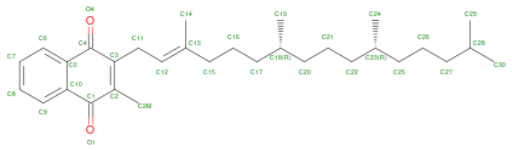
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	Mg	N	O		
14	Z	1	60	50	1	4	5	0	0
			Total	C	Mg	N	O		
14	Z	1	65	55	1	4	5	0	0
			Total	C	Mg	N	O		
14	Z	1	45	35	1	4	5	0	0
			Total	C	Mg	N	O		
14	Z	1	65	55	1	4	5	0	0
			Total	C	Mg	N	O		
14	Z	1	65	55	1	4	5	0	0
			Total	C	Mg	N	O		
14	d	1	65	55	1	4	5	0	0
			Total	C	Mg	N	O		
14	d	1	45	35	1	4	5	0	0
			Total	C	Mg	N	O		
14	f	1	45	35	1	4	5	0	0
			Total	C	Mg	N	O		
14	f	1	55	45	1	4	5	0	0
			Total	C	Mg	N	O		
14	g	1	41	33	1	4	3	0	0
			Total	C	Mg	N	O		
14	g	1	45	35	1	4	5	0	0
			Total	C	Mg	N	O		
14	h	1	65	55	1	4	5	0	0
			Total	C	Mg	N	O		
14	h	1	65	55	1	4	5	0	0
			Total	C	Mg	N	O		
14	h	1	65	55	1	4	5	0	0
			Total	C	Mg	N	O		
14	h	1	65	55	1	4	5	0	0
			Total	C	Mg	N	O		
14	j	1	45	35	1	4	5	0	0

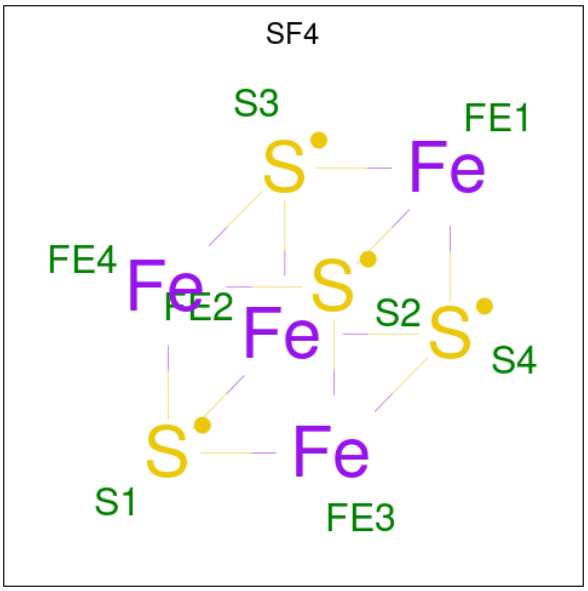
- Molecule 15 is PHYLLOQUINONE (three-letter code: PQN) (formula: $C_{31}H_{46}O_2$) (labeled as "Ligand of Interest" by depositor).

PQN



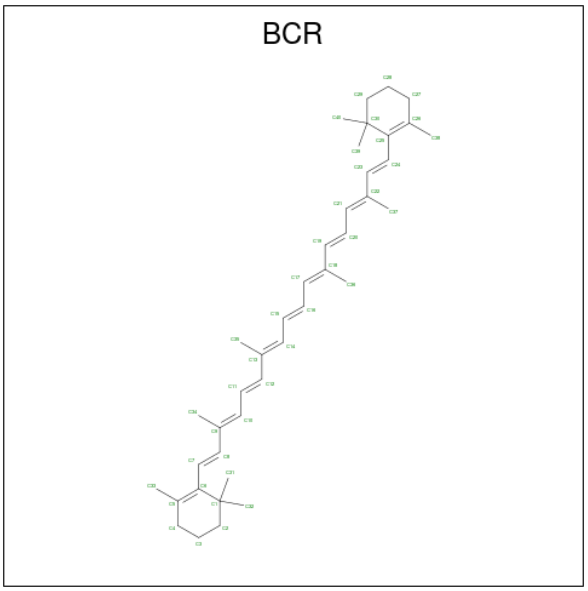
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
15	A	1	33	31	2	0	0
15	B	1	33	31	2	0	0
15	G	1	33	31	2	0	0
15	H	1	33	31	2	0	0
15	Y	1	33	31	2	0	0
15	Z	1	33	31	2	0	0

- Molecule 16 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe_4S_4) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	Fe	S		
16	A	1	8	4	4	0	0
16	C	1	8	4	4	0	0
16	C	1	8	4	4	0	0
16	G	1	8	4	4	0	0
16	N	1	8	4	4	0	0
16	N	1	8	4	4	0	0
16	Y	1	8	4	4	0	0
16	a	1	8	4	4	0	0
16	a	1	8	4	4	0	0

- Molecule 17 is BETA-CAROTENE (three-letter code: BCR) (formula: $C_{40}H_{56}$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	C		
17	A	1	40	40	0	0
			Total	C		
17	A	1	40	40	0	0
			Total	C		
17	A	1	40	40	0	0
			Total	C		
17	A	1	40	40	0	0
			Total	C		
17	A	1	40	40	0	0
			Total	C		
17	A	1	40	40	0	0
			Total	C		
17	B	1	30	30	0	0
			Total	C		
17	B	1	40	40	0	0
			Total	C		
17	B	1	40	40	0	0
			Total	C		
17	B	1	25	25	0	0
			Total	C		
17	B	1	40	40	0	0
			Total	C		
17	B	1	40	40	0	0
			Total	C		
17	B	1	40	40	0	0
			Total	C		
17	F	1	40	40	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	C		
17	F	1	40	40	0	0
			Total	C		
17	G	1	40	40	0	0
			Total	C		
17	G	1	40	40	0	0
			Total	C		
17	G	1	40	40	0	0
			Total	C		
17	G	1	40	40	0	0
			Total	C		
17	G	1	40	40	0	0
			Total	C		
17	H	1	40	40	0	0
			Total	C		
17	H	1	40	40	0	0
			Total	C		
17	H	1	40	40	0	0
			Total	C		
17	H	1	25	25	0	0
			Total	C		
17	H	1	40	40	0	0
			Total	C		
17	H	1	40	40	0	0
			Total	C		
17	H	1	40	40	0	0
			Total	C		
17	I	1	40	40	0	0
			Total	C		
17	I	1	40	40	0	0
			Total	C		
17	J	1	40	40	0	0
			Total	C		
17	J	1	40	40	0	0
			Total	C		
17	L	1	40	40	0	0
			Total	C		
17	L	1	40	40	0	0
			Total	C		
17	M	1	40	40	0	0
			Total	C		
17	Q	1	40	40	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	C		
17	Q	1	40	40	0	0
			Total	C		
17	R	1	40	40	0	0
			Total	C		
17	R	1	40	40	0	0
			Total	C		
17	S	1	40	40	0	0
			Total	C		
17	S	1	40	40	0	0
			Total	C		
17	T	1	40	40	0	0
			Total	C		
17	U	1	40	40	0	0
			Total	C		
17	U	1	40	40	0	0
			Total	C		
17	U	1	40	40	0	0
			Total	C		
17	V	1	40	40	0	0
			Total	C		
17	Y	1	40	40	0	0
			Total	C		
17	Y	1	40	40	0	0
			Total	C		
17	Y	1	40	40	0	0
			Total	C		
17	Y	1	40	40	0	0
			Total	C		
17	Y	1	40	40	0	0
			Total	C		
17	Y	1	40	40	0	0
			Total	C		
17	Y	1	40	40	0	0
			Total	C		
17	Y	1	40	40	0	0
			Total	C		
17	Z	1	40	40	0	0
			Total	C		
17	Z	1	40	40	0	0
			Total	C		
17	Z	1	40	40	0	0

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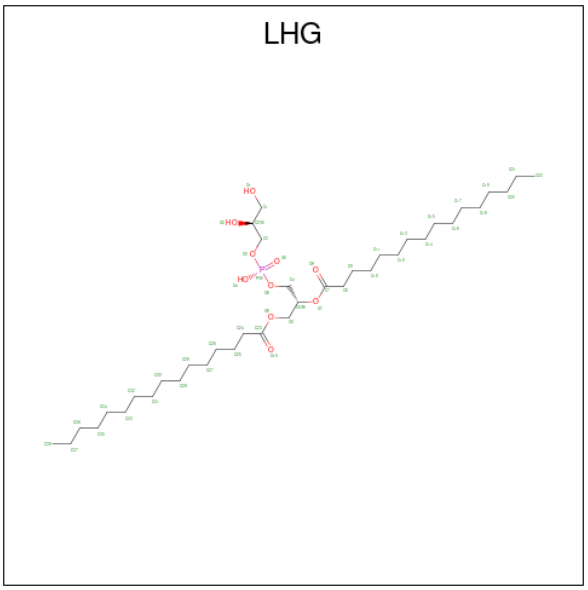
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	C		
17	Z	1	25	25	0	0
			Total	C		
17	Z	1	40	40	0	0
			Total	C		
17	Z	1	40	40	0	0
			Total	C		
17	Z	1	40	40	0	0
			Total	C		
17	d	1	40	40	0	0
			Total	C		
17	e	1	40	40	0	0
			Total	C		
17	f	1	40	40	0	0
			Total	C		
17	h	1	40	40	0	0
			Total	C		
17	h	1	40	40	0	0
			Total	C		
17	i	1	40	40	0	0

- Molecule 18 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (three-letter code: LHG) (formula: $C_{38}H_{75}O_{10}P$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	O	P		
18	A	1	49	38	10	1	0	0

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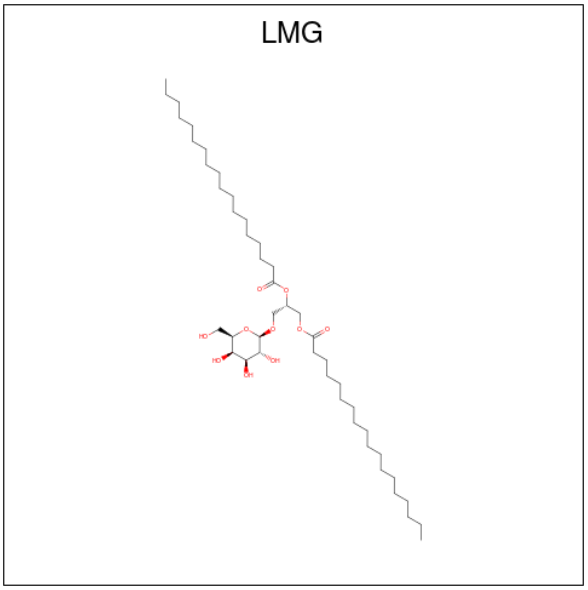
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	O	P		
18	A	1	32	21	10	1	0	0
18	B	1	39	28	10	1	0	0
18	G	1	49	38	10	1	0	0
18	G	1	32	21	10	1	0	0
18	H	1	37	26	10	1	0	0
18	Y	1	49	38	10	1	0	0
18	Y	1	25	14	10	1	0	0
18	j	1	28	17	10	1	0	0

- Molecule 19 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (three-letter code: LMG) (formula: $C_{45}H_{86}O_{10}$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
19	B	1	52	42	10	0	0
19	H	1	49	39	10	0	0
19	Z	1	49	39	10	0	0

- Molecule 20 is CALCIUM ION (three-letter code: CA) (formula: Ca) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Ca		
20	L	1	1	1	0	0
20	U	1	1	1	0	0
20	h	1	1	1	0	0

- Molecule 21 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
21	A	23	23	23	0	0
21	B	20	20	20	0	0
21	C	7	7	7	0	0
21	D	15	15	15	0	0
21	E	6	6	6	0	0
21	F	7	7	7	0	0
21	G	32	32	32	0	0
21	H	38	38	38	0	0
21	J	3	3	3	0	0
21	K	2	2	2	0	0
21	L	4	4	4	0	0
21	M	1	1	1	0	0
21	N	2	2	2	0	0
21	O	7	7	7	0	0
21	P	3	3	3	0	0

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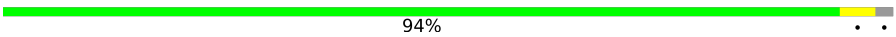
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
21	Q	7	Total O 7 7	0	0
21	S	2	Total O 2 2	0	0
21	T	1	Total O 1 1	0	0
21	U	9	Total O 9 9	0	0
21	V	2	Total O 2 2	0	0
21	W	3	Total O 3 3	0	0
21	X	2	Total O 2 2	0	0
21	Y	24	Total O 24 24	0	0
21	Z	21	Total O 21 21	0	0
21	a	4	Total O 4 4	0	0
21	b	6	Total O 6 6	0	0
21	c	4	Total O 4 4	0	0
21	d	7	Total O 7 7	0	0
21	f	5	Total O 5 5	0	0
21	g	2	Total O 2 2	0	0
21	h	4	Total O 4 4	0	0
21	i	1	Total O 1 1	0	0
21	j	2	Total O 2 2	0	0

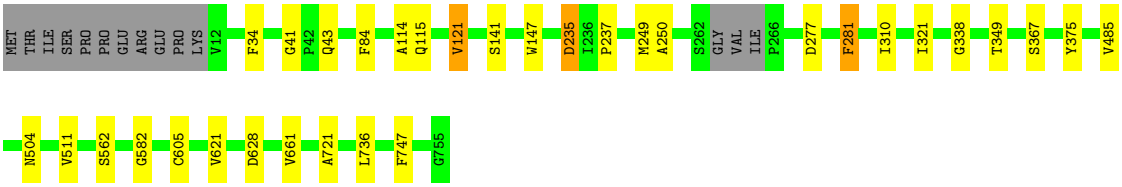
3 Residue-property plots (i)

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. 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. 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

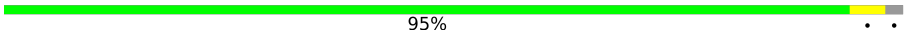
Chain A:

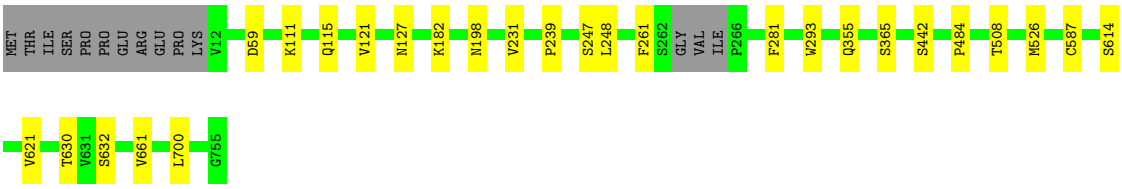




• Molecule 1: Photosystem I P700 chlorophyll a apoprotein A1

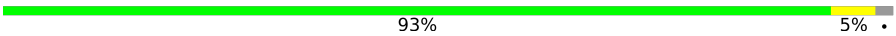
Chain G:

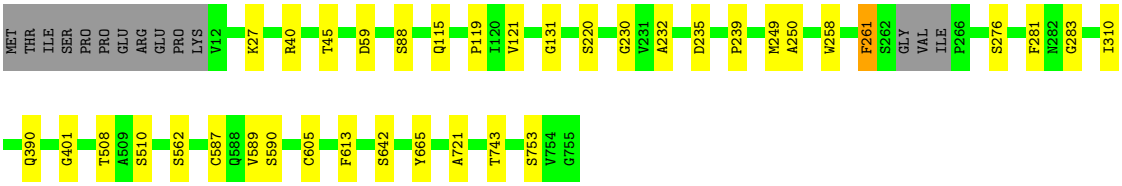




• Molecule 1: Photosystem I P700 chlorophyll a apoprotein A1

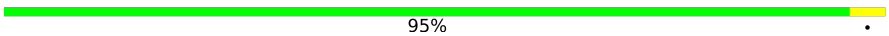
Chain Y:





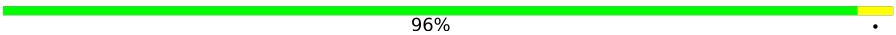
• Molecule 2: Photosystem I P700 chlorophyll a apoprotein A2

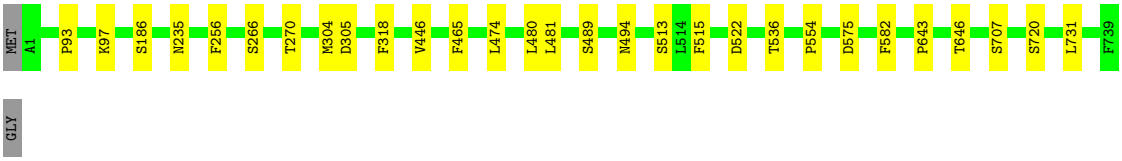
Chain B:



• Molecule 2: Photosystem I P700 chlorophyll a apoprotein A2

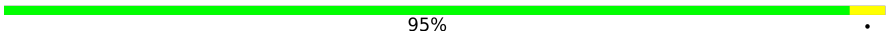
Chain H:

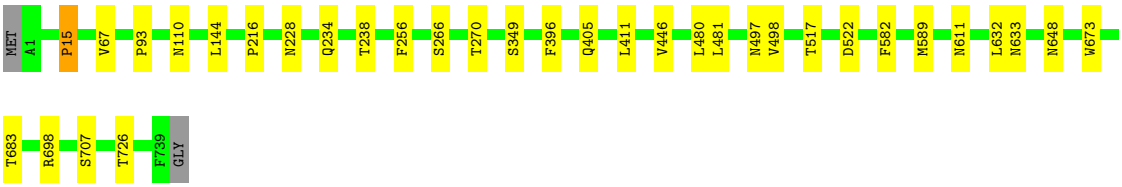




• Molecule 2: Photosystem I P700 chlorophyll a apoprotein A2

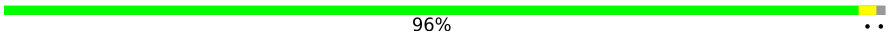
Chain Z:

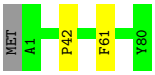




• Molecule 3: Photosystem I iron-sulfur center

Chain C:



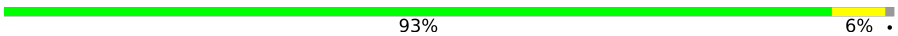


• Molecule 3: Photosystem I iron-sulfur center

Chain N:

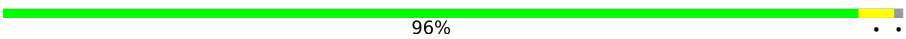
• Molecule 3: Photosystem I iron-sulfur center

Chain a:



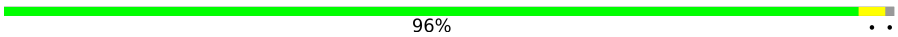
• Molecule 4: Photosystem I reaction center subunit II

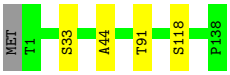
Chain D:



• Molecule 4: Photosystem I reaction center subunit II

Chain O:



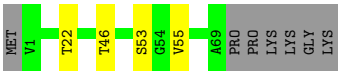


• Molecule 4: Photosystem I reaction center subunit II

Chain b:

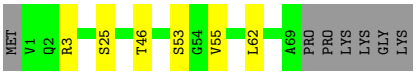
• Molecule 5: Photosystem I reaction center subunit IV

Chain E:



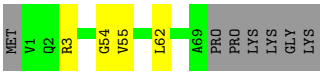
• Molecule 5: Photosystem I reaction center subunit IV

Chain P:



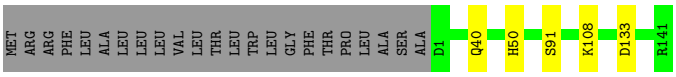
• Molecule 5: Photosystem I reaction center subunit IV

Chain c:



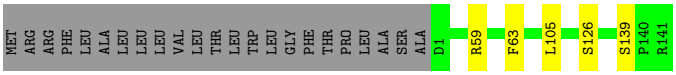
• Molecule 6: Photosystem I reaction center subunit III

Chain F:



• Molecule 6: Photosystem I reaction center subunit III

Chain Q:



• Molecule 6: Photosystem I reaction center subunit III

Chain d: 79% 6% 14%

MET ARG ARG PHE LEU ALA LEU LEU LEU VAL LEU THR LEU TRP LEU GLY PHE THR PRO LEU ALA SER ALA D1 P12 V52 V53 D54 F63 R89 E93 K97 L105 F114 K122 P140 R141

• Molecule 7: Photosystem I reaction center subunit VIII

Chain I: 95% 5%

M1 T24 E37 A38

• Molecule 7: Photosystem I reaction center subunit VIII

Chain R: 100%

There are no outlier residues recorded for this chain.

• Molecule 7: Photosystem I reaction center subunit VIII

Chain e: 97%

M1 M2 A38

• Molecule 8: Photosystem I reaction center subunit IX

Chain J: 98%

M1 M19 L41

• Molecule 8: Photosystem I reaction center subunit IX

Chain S: 98%

M1 L14 L41

• Molecule 8: Photosystem I reaction center subunit IX

Chain f: 100%

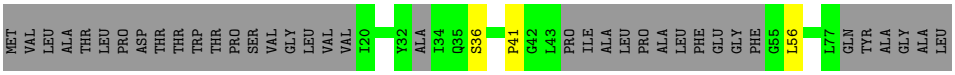
There are no outlier residues recorded for this chain.

• Molecule 9: Photosystem I reaction center subunit PsaK

Chain K: 47% 7% 45%

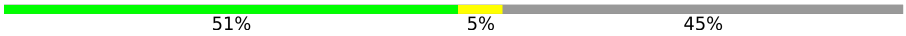
• Molecule 9: Photosystem I reaction center subunit PsaK

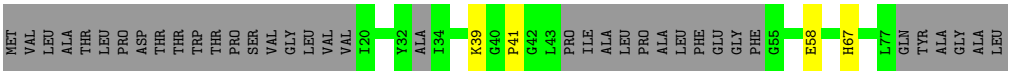
Chain T:



• Molecule 9: Photosystem I reaction center subunit PsaK

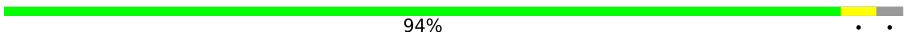
Chain g:

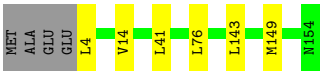




• Molecule 10: Photosystem I reaction center subunit XI

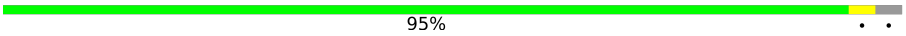
Chain L:





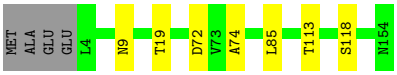
• Molecule 10: Photosystem I reaction center subunit XI

Chain U:



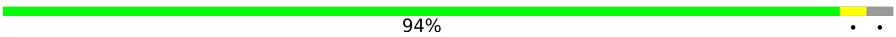
• Molecule 10: Photosystem I reaction center subunit XI

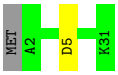
Chain h:



• Molecule 11: Photosystem I reaction center subunit XII

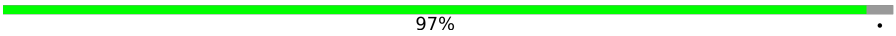
Chain M:





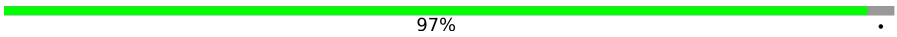
• Molecule 11: Photosystem I reaction center subunit XII

Chain V:



• Molecule 11: Photosystem I reaction center subunit XII

Chain i:



• Molecule 12: Photosystem I 4.8K protein

Chain W:

• Molecule 12: Photosystem I 4.8K protein

Chain X:

• Molecule 12: Photosystem I 4.8K protein

Chain j:

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	278.50Å 165.13Å 283.43Å 90.00° 119.42° 90.00°	Depositor
Resolution (Å)	48.87 – 2.90 48.87 – 2.90	Depositor EDS
% Data completeness (in resolution range)	99.6 (48.87-2.90) 93.9 (48.87-2.90)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.48 (at 2.91Å)	Xtriage
Refinement program	REFMAC 5.8.0238	Depositor
R, R_{free}	0.303 , 0.343 0.307 , 0.345	Depositor DCC
R_{free} test set	24873 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å^2)	56.7	Xtriage
Anisotropy	0.081	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.29 , 22.8	EDS
L-test for twinning[2]	$< \|L\| > = 0.31$, $< L^2 > = 0.14$	Xtriage
Estimated twinning fraction	0.247 for -h-l,k,h 0.247 for l,k,-h-l 0.177 for h,-k,-h-l 0.176 for -h-l,-k,l 0.176 for l,-k,h	Xtriage
F_o,F_c correlation	0.84	EDS
Total number of atoms	72737	wwPDB-VP
Average B, all atoms (Å^2)	46.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.45% 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 (i)

5.1 Standard geometry (i)

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

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	0.67	0/5990	0.77	0/8168
1	G	0.68	0/5990	0.76	0/8168
1	Y	0.68	0/5990	0.77	0/8168
2	B	0.66	0/6107	0.78	0/8345
2	H	0.67	0/6107	0.78	0/8345
2	Z	0.66	0/6107	0.74	0/8345
3	C	0.70	0/608	0.84	0/824
3	N	0.72	0/608	0.83	0/824
3	a	0.69	0/608	0.84	0/824
4	D	0.65	0/1101	0.79	0/1492
4	O	0.66	0/1101	0.79	0/1492
4	b	0.66	0/1101	0.82	0/1492
5	E	0.67	0/551	0.81	0/750
5	P	0.70	0/551	0.82	0/750
5	c	0.69	0/551	0.78	0/750
6	F	0.68	0/1087	0.79	0/1476
6	Q	0.69	0/1087	0.80	0/1476
6	d	0.68	0/1087	0.79	0/1476
7	I	0.66	0/312	0.75	0/425
7	R	0.69	0/312	0.77	0/425
7	e	0.66	0/312	0.74	0/425
8	J	0.64	0/350	0.69	0/477
8	S	0.65	0/350	0.70	0/477
8	f	0.67	0/350	0.73	0/477
9	K	0.70	0/331	0.81	0/444
9	T	0.75	0/331	0.84	0/444
9	g	0.73	0/331	0.81	0/444
10	L	0.71	0/1148	0.79	0/1558
10	U	0.71	0/1148	0.78	0/1558
10	h	0.70	0/1148	0.78	0/1558
11	M	0.68	0/236	0.75	0/322
11	V	0.69	0/236	0.80	0/322

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
11	i	0.71	0/236	0.76	0/322
12	W	0.69	0/227	0.71	0/310
12	X	0.66	0/227	0.72	0/310
12	j	0.63	0/227	0.63	0/310
All	All	0.67	0/54144	0.77	0/73773

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

Mol	Chain	#Chirality outliers	#Planarity outliers
2	Z	0	1
3	N	0	1
3	a	0	1
5	P	0	1
9	K	0	1
All	All	0	5

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
9	K	56	LEU	Peptide
3	N	60	ASP	Peptide
5	P	53	SER	Peptide
2	Z	673	TRP	Peptide
3	a	60	ASP	Peptide

5.2 Too-close contacts (i)

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

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	737/755 (98%)	644 (87%)	74 (10%)	19 (3%)	5	20
1	G	737/755 (98%)	654 (89%)	70 (10%)	13 (2%)	8	29
1	Y	737/755 (98%)	642 (87%)	77 (10%)	18 (2%)	6	22
2	B	737/741 (100%)	633 (86%)	95 (13%)	9 (1%)	13	40
2	H	737/741 (100%)	643 (87%)	87 (12%)	7 (1%)	17	48
2	Z	737/741 (100%)	649 (88%)	79 (11%)	9 (1%)	13	40
3	C	78/81 (96%)	70 (90%)	6 (8%)	2 (3%)	5	20
3	N	78/81 (96%)	67 (86%)	9 (12%)	2 (3%)	5	20
3	a	78/81 (96%)	70 (90%)	7 (9%)	1 (1%)	12	37
4	D	136/139 (98%)	119 (88%)	13 (10%)	4 (3%)	4	18
4	O	136/139 (98%)	123 (90%)	12 (9%)	1 (1%)	22	54
4	b	136/139 (98%)	123 (90%)	9 (7%)	4 (3%)	4	18
5	E	67/76 (88%)	56 (84%)	8 (12%)	3 (4%)	2	9
5	P	67/76 (88%)	56 (84%)	8 (12%)	3 (4%)	2	9
5	c	67/76 (88%)	57 (85%)	7 (10%)	3 (4%)	2	9
6	F	139/164 (85%)	115 (83%)	23 (16%)	1 (1%)	22	54
6	Q	139/164 (85%)	125 (90%)	13 (9%)	1 (1%)	22	54
6	d	139/164 (85%)	113 (81%)	19 (14%)	7 (5%)	2	7
7	I	36/38 (95%)	32 (89%)	3 (8%)	1 (3%)	5	19
7	R	36/38 (95%)	34 (94%)	2 (6%)	0	100	100
7	e	36/38 (95%)	31 (86%)	4 (11%)	1 (3%)	5	19
8	J	39/41 (95%)	36 (92%)	3 (8%)	0	100	100
8	S	39/41 (95%)	37 (95%)	2 (5%)	0	100	100
8	f	39/41 (95%)	36 (92%)	3 (8%)	0	100	100
9	K	40/83 (48%)	30 (75%)	8 (20%)	2 (5%)	2	7

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
9	T	40/83 (48%)	33 (82%)	5 (12%)	2 (5%)	2	7
9	g	40/83 (48%)	31 (78%)	7 (18%)	2 (5%)	2	7
10	L	149/155 (96%)	133 (89%)	16 (11%)	0	100	100
10	U	149/155 (96%)	130 (87%)	17 (11%)	2 (1%)	12	37
10	h	149/155 (96%)	133 (89%)	14 (9%)	2 (1%)	12	37
11	M	28/31 (90%)	25 (89%)	3 (11%)	0	100	100
11	V	28/31 (90%)	28 (100%)	0	0	100	100
11	i	28/31 (90%)	27 (96%)	1 (4%)	0	100	100
12	W	24/39 (62%)	23 (96%)	1 (4%)	0	100	100
12	X	24/39 (62%)	23 (96%)	0	1 (4%)	3	10
12	j	24/39 (62%)	24 (100%)	0	0	100	100
All	All	6630/7029 (94%)	5805 (88%)	705 (11%)	120 (2%)	8	29

5 of 120 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	121	VAL
1	A	250	ALA
3	C	61	PHE
4	D	95	HIS
5	E	55	VAL

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	590/603 (98%)	573 (97%)	17 (3%)	42	76
1	G	590/603 (98%)	576 (98%)	14 (2%)	49	79
1	Y	590/603 (98%)	570 (97%)	20 (3%)	37	71
2	B	597/598 (100%)	573 (96%)	24 (4%)	31	65
2	H	597/598 (100%)	575 (96%)	22 (4%)	34	68

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	Z	597/598 (100%)	572 (96%)	25 (4%)	30	63
3	C	67/68 (98%)	67 (100%)	0	100	100
3	N	67/68 (98%)	64 (96%)	3 (4%)	27	61
3	a	67/68 (98%)	64 (96%)	3 (4%)	27	61
4	D	115/116 (99%)	114 (99%)	1 (1%)	78	93
4	O	115/116 (99%)	112 (97%)	3 (3%)	46	77
4	b	115/116 (99%)	108 (94%)	7 (6%)	18	48
5	E	59/65 (91%)	58 (98%)	1 (2%)	60	86
5	P	59/65 (91%)	57 (97%)	2 (3%)	37	71
5	c	59/65 (91%)	58 (98%)	1 (2%)	60	86
6	F	109/128 (85%)	105 (96%)	4 (4%)	34	68
6	Q	109/128 (85%)	105 (96%)	4 (4%)	34	68
6	d	109/128 (85%)	104 (95%)	5 (5%)	27	60
7	I	32/32 (100%)	31 (97%)	1 (3%)	40	74
7	R	32/32 (100%)	32 (100%)	0	100	100
7	e	32/32 (100%)	31 (97%)	1 (3%)	40	74
8	J	36/36 (100%)	35 (97%)	1 (3%)	43	76
8	S	36/36 (100%)	35 (97%)	1 (3%)	43	76
8	f	36/36 (100%)	36 (100%)	0	100	100
9	K	33/61 (54%)	27 (82%)	6 (18%)	1	5
9	T	33/61 (54%)	32 (97%)	1 (3%)	41	75
9	g	33/61 (54%)	31 (94%)	2 (6%)	18	48
10	L	117/120 (98%)	111 (95%)	6 (5%)	24	56
10	U	117/120 (98%)	115 (98%)	2 (2%)	60	86
10	h	117/120 (98%)	112 (96%)	5 (4%)	29	62
11	M	25/26 (96%)	24 (96%)	1 (4%)	31	65
11	V	25/26 (96%)	25 (100%)	0	100	100
11	i	25/26 (96%)	25 (100%)	0	100	100
12	W	20/31 (64%)	20 (100%)	0	100	100
12	X	20/31 (64%)	20 (100%)	0	100	100
12	j	20/31 (64%)	19 (95%)	1 (5%)	24	57

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	5400/5652 (96%)	5216 (97%)	184 (3%)	37 71

5 of 184 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	Y	40	ARG
2	Z	396	PHE
1	Y	220	SER
1	Y	605	CYS
2	Z	589	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 120 such sidechains are listed below:

Mol	Chain	Res	Type
2	H	494	ASN
2	Z	688	HIS
4	O	54	ASN
2	Z	648	ASN
10	h	154	ASN

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)

Of 381 ligands modelled in this entry, 3 are monoatomic - leaving 378 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The

Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
14	CLA	H	836	-	60,68,73	2.29	18 (30%)	70,107,113	2.54	24 (34%)
14	CLA	H	838	-	45,53,73	2.58	20 (44%)	52,89,113	3.11	23 (44%)
17	BCR	Y	848	-	41,41,41	2.56	6 (14%)	56,56,56	7.16	26 (46%)
14	CLA	Z	823	-	55,63,73	2.51	20 (36%)	64,101,113	2.54	21 (32%)
14	CLA	Z	811	2	65,73,73	2.17	19 (29%)	76,113,113	2.78	32 (42%)
14	CLA	Z	813	-	45,53,73	2.64	20 (44%)	52,89,113	2.85	20 (38%)
14	CLA	G	807	-	51,59,73	2.57	19 (37%)	59,96,113	2.77	24 (40%)
14	CLA	G	810	-	45,53,73	2.70	21 (46%)	52,89,113	2.82	19 (36%)
14	CLA	A	809	1	65,73,73	2.22	21 (32%)	76,113,113	2.44	23 (30%)
14	CLA	A	837	-	65,73,73	2.20	17 (26%)	76,113,113	2.50	21 (27%)
17	BCR	R	102	-	41,41,41	2.89	6 (14%)	56,56,56	7.11	25 (44%)
17	BCR	U	1009	-	41,41,41	2.46	7 (17%)	56,56,56	7.38	31 (55%)
14	CLA	G	804	14	59,67,73	2.34	19 (32%)	68,105,113	2.83	21 (30%)
14	CLA	H	831	-	65,73,73	2.14	19 (29%)	76,113,113	2.86	27 (35%)
14	CLA	Z	828	-	65,73,73	2.30	21 (32%)	76,113,113	2.45	24 (31%)
14	CLA	Y	814	-	55,63,73	2.50	21 (38%)	64,101,113	2.68	23 (35%)
17	BCR	J	104	-	41,41,41	2.91	8 (19%)	56,56,56	7.06	27 (48%)
14	CLA	H	810	2	65,73,73	2.24	19 (29%)	76,113,113	2.83	31 (40%)
14	CLA	Z	819	-	60,68,73	2.32	19 (31%)	70,107,113	2.69	23 (32%)
14	CLA	Z	821	-	45,53,73	2.61	18 (40%)	52,89,113	2.87	23 (44%)
14	CLA	A	810	-	65,73,73	2.23	19 (29%)	76,113,113	2.43	23 (30%)
14	CLA	Z	825	2	55,63,73	2.53	20 (36%)	64,101,113	2.74	22 (34%)
17	BCR	B	843	-	41,41,41	2.72	6 (14%)	56,56,56	7.31	24 (42%)
17	BCR	G	846	-	41,41,41	2.90	6 (14%)	56,56,56	6.89	27 (48%)
14	CLA	H	813	-	65,73,73	2.34	20 (30%)	76,113,113	2.57	25 (32%)
14	CLA	Y	808	1	65,73,73	2.22	21 (32%)	76,113,113	2.65	27 (35%)
14	CLA	A	842	-	65,73,73	2.23	19 (29%)	76,113,113	2.57	25 (32%)
14	CLA	A	811	-	45,53,73	2.60	19 (42%)	52,89,113	2.95	23 (44%)
14	CLA	Y	827	-	65,73,73	2.30	20 (30%)	76,113,113	2.46	26 (34%)
14	CLA	Z	809	-	65,73,73	2.19	19 (29%)	76,113,113	2.72	30 (39%)
17	BCR	U	1005	-	41,41,41	2.86	6 (14%)	56,56,56	7.12	26 (46%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
14	CLA	H	806	-	65,73,73	2.27	20 (30%)	76,113,113	2.39	24 (31%)
14	CLA	G	828	-	65,73,73	2.23	20 (30%)	76,113,113	2.51	25 (32%)
14	CLA	H	828	-	65,73,73	2.20	22 (33%)	76,113,113	2.52	26 (34%)
16	SF4	G	844	1,2	0,12,12	-	-	-		
14	CLA	B	808	2	65,73,73	2.16	19 (29%)	76,113,113	2.75	31 (40%)
14	CLA	U	1006	-	65,73,73	2.30	20 (30%)	76,113,113	2.49	24 (31%)
14	CLA	Z	830	-	65,73,73	2.14	16 (24%)	76,113,113	2.67	22 (28%)
17	BCR	Y	849	-	41,41,41	3.03	6 (14%)	56,56,56	7.35	29 (51%)
17	BCR	L	207	-	41,41,41	2.80	7 (17%)	56,56,56	7.07	21 (37%)
14	CLA	G	808	1	65,73,73	2.24	19 (29%)	76,113,113	2.58	22 (28%)
14	CLA	H	824	2	55,63,73	2.57	20 (36%)	64,101,113	2.86	25 (39%)
14	CLA	T	103	-	45,53,73	2.62	19 (42%)	52,89,113	2.81	18 (34%)
14	CLA	B	832	-	55,63,73	2.42	20 (36%)	64,101,113	2.81	23 (35%)
14	CLA	H	803	-	65,73,73	2.24	20 (30%)	76,113,113	2.44	27 (35%)
16	SF4	N	102	3	0,12,12	-	-	-		
14	CLA	d	202	-	45,53,73	2.63	17 (37%)	52,89,113	2.79	19 (36%)
14	CLA	H	827	-	65,73,73	2.17	18 (27%)	76,113,113	2.44	22 (28%)
14	CLA	Y	815	-	50,58,73	2.61	20 (40%)	58,95,113	3.00	22 (37%)
14	CLA	A	828	-	65,73,73	2.19	20 (30%)	76,113,113	2.36	26 (34%)
14	CLA	G	809	-	65,73,73	2.26	20 (30%)	76,113,113	2.56	26 (34%)
17	BCR	T	102	-	41,41,41	2.57	6 (14%)	56,56,56	7.29	26 (46%)
16	SF4	a	102	3	0,12,12	-	-	-		
14	CLA	B	818	-	60,68,73	2.30	20 (33%)	70,107,113	2.61	23 (32%)
17	BCR	V	101	-	41,41,41	2.72	6 (14%)	56,56,56	7.26	30 (53%)
14	CLA	H	829	-	65,73,73	2.26	20 (30%)	76,113,113	2.67	26 (34%)
14	CLA	G	833	-	65,73,73	2.27	19 (29%)	76,113,113	2.61	24 (31%)
14	CLA	A	817	-	50,58,73	2.62	20 (40%)	58,95,113	2.97	23 (39%)
14	CLA	Y	841	-	65,73,73	2.14	17 (26%)	76,113,113	2.58	19 (25%)
17	BCR	I	101	-	41,41,41	2.85	7 (17%)	56,56,56	7.49	22 (39%)
14	CLA	J	102	-	55,63,73	2.51	21 (38%)	64,101,113	2.81	27 (42%)
14	CLA	Y	809	-	65,73,73	2.24	20 (30%)	76,113,113	2.42	24 (31%)
18	LHG	G	850	-	48,48,48	0.95	2 (4%)	51,54,54	1.16	5 (9%)
17	BCR	f	103	-	41,41,41	2.63	6 (14%)	56,56,56	7.10	24 (42%)
17	BCR	L	208	-	41,41,41	2.65	7 (17%)	56,56,56	7.07	31 (55%)
14	CLA	B	811	-	50,58,73	2.60	20 (40%)	58,95,113	2.82	23 (39%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
14	CLA	f	102	-	55,63,73	2.49	19 (34%)	64,101,113	2.79	25 (39%)
17	BCR	H	843	-	41,41,41	3.08	6 (14%)	56,56,56	6.96	29 (51%)
14	CLA	Y	837	-	50,58,73	2.65	21 (42%)	58,95,113	2.84	26 (44%)
14	CLA	G	836	-	50,58,73	2.69	20 (40%)	58,95,113	2.83	25 (43%)
14	CLA	G	838	-	50,58,73	2.64	19 (38%)	58,95,113	2.87	22 (37%)
14	CLA	Z	826	-	65,73,73	2.22	19 (29%)	76,113,113	2.79	27 (35%)
14	CLA	L	201	-	65,73,73	2.21	18 (27%)	76,113,113	2.59	25 (32%)
14	CLA	B	840	-	65,73,73	2.16	15 (23%)	76,113,113	2.67	32 (42%)
17	BCR	h	202	-	41,41,41	2.52	7 (17%)	56,56,56	7.11	29 (51%)
14	CLA	G	832	-	65,73,73	2.17	17 (26%)	76,113,113	2.57	22 (28%)
14	CLA	Z	829	-	65,73,73	2.30	21 (32%)	76,113,113	2.56	26 (34%)
17	BCR	B	842	-	30,30,41	3.31	6 (20%)	39,39,56	8.17	20 (51%)
14	CLA	G	819	-	65,73,73	2.26	19 (29%)	76,113,113	2.63	24 (31%)
14	CLA	A	830	-	65,73,73	2.31	22 (33%)	76,113,113	2.30	25 (32%)
14	CLA	G	824	-	60,68,73	2.43	20 (33%)	70,107,113	2.60	22 (31%)
14	CLA	A	804	-	65,73,73	2.38	21 (32%)	76,113,113	2.49	23 (30%)
14	CLA	H	822	-	55,63,73	2.39	20 (36%)	64,101,113	2.89	23 (35%)
14	CLA	G	825	-	65,73,73	2.26	20 (30%)	76,113,113	2.42	27 (35%)
14	CLA	A	803	-	65,73,73	2.18	18 (27%)	76,113,113	2.39	28 (36%)
17	BCR	Y	845	-	41,41,41	2.73	6 (14%)	56,56,56	7.17	28 (50%)
14	CLA	H	807	-	65,73,73	2.15	20 (30%)	76,113,113	2.71	23 (30%)
14	CLA	A	833	-	65,73,73	2.13	19 (29%)	76,113,113	2.51	23 (30%)
14	CLA	j	102	-	45,53,73	2.64	19 (42%)	52,89,113	2.91	19 (36%)
14	CLA	G	803	-	65,73,73	2.19	18 (27%)	76,113,113	2.54	27 (35%)
17	BCR	B	846	-	41,41,41	2.83	7 (17%)	56,56,56	7.13	28 (50%)
17	BCR	Z	844	-	41,41,41	2.66	6 (14%)	56,56,56	7.02	30 (53%)
14	CLA	Y	822	-	65,73,73	2.26	19 (29%)	76,113,113	2.62	22 (28%)
16	SF4	C	101	3	0,12,12	-	-	-		
17	BCR	H	845	-	25,25,41	2.19	2 (8%)	33,33,56	8.00	18 (54%)
14	CLA	A	835	1	45,53,73	2.62	18 (40%)	52,89,113	2.85	21 (40%)
14	CLA	B	826	-	65,73,73	2.19	19 (29%)	76,113,113	2.33	22 (28%)
14	CLA	Z	812	-	55,63,73	2.46	21 (38%)	64,101,113	2.64	23 (35%)
14	CLA	A	821	-	60,68,73	2.39	20 (33%)	70,107,113	2.67	25 (35%)
17	BCR	Z	848	-	41,41,41	2.82	7 (17%)	56,56,56	7.30	22 (39%)
14	CLA	d	201	-	65,73,73	2.16	19 (29%)	76,113,113	2.47	25 (32%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
14	CLA	B	812	-	65,73,73	2.28	19 (29%)	76,113,113	2.69	27 (35%)
14	CLA	A	808	-	51,59,73	2.53	20 (39%)	59,96,113	3.09	22 (37%)
14	CLA	G	811	14	65,73,73	2.29	19 (29%)	76,113,113	2.53	24 (31%)
14	CLA	A	805	14	59,67,73	2.37	21 (35%)	68,105,113	2.70	22 (32%)
14	CLA	Z	801	-	65,73,73	2.16	19 (29%)	76,113,113	2.66	23 (30%)
14	CLA	A	813	-	54,62,73	2.51	20 (37%)	62,99,113	2.62	20 (32%)
14	CLA	G	841	-	65,73,73	2.28	19 (29%)	76,113,113	2.43	24 (31%)
15	PQN	Z	842	-	34,34,34	1.82	2 (5%)	42,45,45	1.28	4 (9%)
14	CLA	Y	824	-	60,68,73	2.39	20 (33%)	70,107,113	2.72	25 (35%)
14	CLA	G	814	-	50,58,73	2.53	20 (40%)	58,95,113	3.12	30 (51%)
14	CLA	Z	837	-	60,68,73	2.31	20 (33%)	70,107,113	2.72	27 (38%)
17	BCR	Z	843	-	41,41,41	2.90	7 (17%)	56,56,56	6.88	26 (46%)
14	CLA	G	834	-	55,63,73	2.46	20 (36%)	64,101,113	2.54	27 (42%)
14	CLA	G	853	-	45,53,73	2.56	18 (40%)	52,89,113	2.71	22 (42%)
14	CLA	Z	833	-	55,63,73	2.46	18 (32%)	64,101,113	2.62	22 (34%)
14	CLA	G	830	-	65,73,73	2.21	18 (27%)	76,113,113	2.57	24 (31%)
14	CLA	A	802	-	65,73,73	2.21	18 (27%)	76,113,113	2.45	21 (27%)
14	CLA	Z	841	-	65,73,73	2.26	19 (29%)	76,113,113	2.66	26 (34%)
14	CLA	A	840	-	50,58,73	2.61	21 (42%)	58,95,113	2.94	23 (39%)
13	CL0	Y	801	-	65,73,73	2.37	19 (29%)	76,113,113	2.58	22 (28%)
19	LMG	H	848	-	49,49,55	1.37	6 (12%)	57,57,63	1.10	4 (7%)
14	CLA	B	831	-	65,73,73	2.20	19 (29%)	76,113,113	2.69	25 (32%)
14	CLA	H	832	-	55,63,73	2.50	18 (32%)	64,101,113	2.56	22 (34%)
14	CLA	Y	806	-	65,73,73	2.29	18 (27%)	76,113,113	2.56	24 (31%)
14	CLA	A	823	-	65,73,73	2.22	22 (33%)	76,113,113	2.79	25 (32%)
14	CLA	Y	820	-	60,68,73	2.34	19 (31%)	70,107,113	2.72	24 (34%)
17	BCR	H	842	-	41,41,41	2.94	7 (17%)	56,56,56	6.96	22 (39%)
17	BCR	Y	846	-	41,41,41	2.60	6 (14%)	56,56,56	7.42	28 (50%)
16	SF4	N	101	3	0,12,12	-	-	-		
14	CLA	B	820	-	45,53,73	2.70	20 (44%)	52,89,113	2.74	21 (40%)
14	CLA	H	801	-	65,73,73	2.24	20 (30%)	76,113,113	2.57	26 (34%)
14	CLA	A	820	-	65,73,73	2.33	21 (32%)	76,113,113	2.56	24 (31%)
14	CLA	H	833	-	45,53,73	2.52	20 (44%)	52,89,113	2.96	20 (38%)
14	CLA	h	206	-	65,73,73	2.21	20 (30%)	76,113,113	2.71	24 (31%)
17	BCR	G	849	-	41,41,41	2.77	7 (17%)	56,56,56	7.34	30 (53%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
14	CLA	B	823	2	55,63,73	2.51	18 (32%)	64,101,113	2.61	22 (34%)
14	CLA	U	1007	-	65,73,73	2.25	19 (29%)	76,113,113	2.46	28 (36%)
14	CLA	H	809	2	65,73,73	2.15	20 (30%)	76,113,113	2.66	29 (38%)
14	CLA	Z	815	-	65,73,73	2.30	21 (32%)	76,113,113	2.42	20 (26%)
17	BCR	H	844	-	41,41,41	2.96	8 (19%)	56,56,56	7.04	25 (44%)
14	CLA	Y	803	-	65,73,73	2.27	20 (30%)	76,113,113	2.77	24 (31%)
14	CLA	K	101	-	42,49,73	2.50	17 (40%)	48,83,113	3.02	20 (41%)
17	BCR	A	851	-	41,41,41	2.81	7 (17%)	56,56,56	7.25	28 (50%)
18	LHG	A	852	-	48,48,48	0.98	2 (4%)	51,54,54	1.23	5 (9%)
18	LHG	j	101	-	27,27,48	1.28	2 (7%)	30,33,54	1.19	2 (6%)
14	CLA	U	1002	10	65,73,73	2.24	19 (29%)	76,113,113	2.64	23 (30%)
16	SF4	Y	843	1,2	0,12,12	-	-	-		
14	CLA	Y	819	-	65,73,73	2.30	19 (29%)	76,113,113	2.74	24 (31%)
14	CLA	Y	818	-	65,73,73	2.27	18 (27%)	76,113,113	2.67	26 (34%)
14	CLA	Z	834	-	45,53,73	2.62	18 (40%)	52,89,113	3.06	24 (46%)
17	BCR	H	846	-	41,41,41	2.58	6 (14%)	56,56,56	7.13	27 (48%)
17	BCR	Y	853	-	41,41,41	2.88	6 (14%)	56,56,56	6.91	29 (51%)
17	BCR	B	850	-	41,41,41	2.78	6 (14%)	56,56,56	7.08	28 (50%)
14	CLA	Z	814	-	65,73,73	2.25	19 (29%)	76,113,113	2.47	24 (31%)
17	BCR	d	203	-	41,41,41	2.70	6 (14%)	56,56,56	6.90	29 (51%)
14	CLA	Z	840	-	65,73,73	2.24	19 (29%)	76,113,113	2.48	25 (32%)
14	CLA	B	816	-	65,73,73	2.24	20 (30%)	76,113,113	2.45	23 (30%)
18	LHG	G	851	14	31,31,48	1.27	2 (6%)	34,37,54	1.19	2 (5%)
14	CLA	B	803	-	54,62,73	2.47	21 (38%)	62,99,113	3.27	23 (37%)
14	CLA	A	818	-	60,68,73	2.34	20 (33%)	70,107,113	2.73	25 (35%)
14	CLA	Z	804	-	65,73,73	2.30	19 (29%)	76,113,113	2.27	25 (32%)
14	CLA	K	102	-	45,53,73	2.60	18 (40%)	52,89,113	2.92	20 (38%)
17	BCR	F	201	-	41,41,41	2.78	6 (14%)	56,56,56	7.11	24 (42%)
14	CLA	B	836	-	60,68,73	2.32	20 (33%)	70,107,113	2.69	27 (38%)
14	CLA	H	819	-	60,68,73	2.36	21 (35%)	70,107,113	2.48	26 (37%)
14	CLA	H	811	-	55,63,73	2.41	21 (38%)	64,101,113	2.71	30 (46%)
14	CLA	Y	840	-	65,73,73	2.22	19 (29%)	76,113,113	2.44	20 (26%)
17	BCR	A	847	-	41,41,41	2.51	7 (17%)	56,56,56	7.10	25 (44%)
14	CLA	B	819	-	45,53,73	2.62	19 (42%)	52,89,113	2.93	24 (46%)
18	LHG	H	849	-	36,36,48	1.12	2 (5%)	39,42,54	0.90	2 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
14	CLA	U	1004	-	65,73,73	2.21	20 (30%)	76,113,113	2.60	22 (28%)
14	CLA	B	806	-	65,73,73	2.20	21 (32%)	76,113,113	2.67	25 (32%)
14	CLA	Z	827	-	65,73,73	2.20	19 (29%)	76,113,113	2.58	24 (31%)
14	CLA	Y	832	-	65,73,73	2.22	20 (30%)	76,113,113	2.48	26 (34%)
14	CLA	W	1701	-	45,53,73	2.65	18 (40%)	52,89,113	3.04	19 (36%)
14	CLA	G	839	-	50,58,73	2.70	20 (40%)	58,95,113	2.92	27 (46%)
14	CLA	B	838	-	45,53,73	2.72	18 (40%)	52,89,113	2.58	19 (36%)
14	CLA	A	834	-	55,63,73	2.35	19 (34%)	64,101,113	2.80	23 (35%)
14	CLA	A	831	-	65,73,73	2.22	18 (27%)	76,113,113	2.44	26 (34%)
14	CLA	B	804	-	65,73,73	2.16	19 (29%)	76,113,113	2.63	25 (32%)
14	CLA	G	816	-	50,58,73	2.59	21 (42%)	58,95,113	2.90	23 (39%)
14	CLA	S	1103	-	55,63,73	2.46	19 (34%)	64,101,113	2.91	26 (40%)
14	CLA	H	837	-	65,73,73	2.36	19 (29%)	76,113,113	2.45	23 (30%)
14	CLA	H	840	-	65,73,73	2.19	19 (29%)	76,113,113	2.88	27 (35%)
14	CLA	G	817	-	60,68,73	2.41	20 (33%)	70,107,113	2.61	25 (35%)
14	CLA	A	814	-	60,68,73	2.35	21 (35%)	70,107,113	2.66	25 (35%)
14	CLA	Y	834	1	45,53,73	2.65	19 (42%)	52,89,113	2.77	20 (38%)
14	CLA	B	828	-	65,73,73	2.25	17 (26%)	76,113,113	2.64	25 (32%)
14	CLA	B	824	-	65,73,73	2.25	19 (29%)	76,113,113	2.65	27 (35%)
14	CLA	G	822	-	65,73,73	2.25	21 (32%)	76,113,113	2.73	23 (30%)
17	BCR	G	845	-	41,41,41	2.71	7 (17%)	56,56,56	7.15	27 (48%)
14	CLA	L	206	-	65,73,73	2.23	20 (30%)	76,113,113	2.49	23 (30%)
17	BCR	Z	847	-	41,41,41	2.60	6 (14%)	56,56,56	7.20	31 (55%)
18	LHG	B	849	-	38,38,48	1.09	2 (5%)	41,44,54	1.24	4 (9%)
14	CLA	U	1003	-	65,73,73	2.26	18 (27%)	76,113,113	2.49	22 (28%)
14	CLA	Z	807	-	65,73,73	2.33	17 (26%)	76,113,113	2.23	22 (28%)
14	CLA	G	805	-	65,73,73	2.20	20 (30%)	76,113,113	2.67	22 (28%)
14	CLA	T	101	-	42,49,73	2.54	17 (40%)	48,83,113	3.03	21 (43%)
14	CLA	G	812	-	54,62,73	2.49	19 (35%)	62,99,113	2.75	26 (41%)
14	CLA	B	813	-	65,73,73	2.22	18 (27%)	76,113,113	2.54	25 (32%)
16	SF4	C	102	21,3	0,12,12	-	-	-		
14	CLA	A	815	-	50,58,73	2.60	19 (38%)	58,95,113	3.00	28 (48%)
14	CLA	Y	807	-	51,59,73	2.56	20 (39%)	59,96,113	2.83	22 (37%)
14	CLA	Y	804	14	59,67,73	2.36	19 (32%)	68,105,113	2.88	21 (30%)
14	CLA	B	835	-	45,53,73	2.60	19 (42%)	52,89,113	2.92	21 (40%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
14	CLA	B	830	-	45,53,73	2.59	19 (42%)	52,89,113	2.65	22 (42%)
16	SF4	A	845	1,2	0,12,12	-	-	-		
14	CLA	f	101	8	45,53,73	2.64	21 (46%)	52,89,113	3.09	22 (42%)
14	CLA	A	841	-	65,73,73	2.24	18 (27%)	76,113,113	2.62	25 (32%)
14	CLA	B	834	-	45,53,73	2.61	20 (44%)	52,89,113	2.76	23 (44%)
14	CLA	G	837	-	65,73,73	2.23	20 (30%)	76,113,113	2.63	20 (26%)
14	CLA	Q	202	-	45,53,73	2.57	18 (40%)	52,89,113	2.85	20 (38%)
14	CLA	B	807	-	65,73,73	2.29	18 (27%)	76,113,113	2.60	22 (28%)
14	CLA	A	843	18	50,58,73	2.55	21 (42%)	58,95,113	3.15	25 (43%)
14	CLA	A	816	-	50,58,73	2.52	20 (40%)	58,95,113	3.13	25 (43%)
14	CLA	Y	823	-	50,58,73	2.65	19 (38%)	58,95,113	2.90	24 (41%)
14	CLA	Y	825	-	65,73,73	2.20	19 (29%)	76,113,113	2.48	25 (32%)
17	BCR	A	850	-	41,41,41	2.75	6 (14%)	56,56,56	7.15	24 (42%)
13	CL0	G	801	-	65,73,73	2.49	20 (30%)	76,113,113	2.79	26 (34%)
14	CLA	L	205	-	65,73,73	2.26	22 (33%)	76,113,113	2.63	26 (34%)
14	CLA	H	830	-	45,53,73	2.56	17 (37%)	52,89,113	3.12	25 (48%)
14	CLA	B	822	-	60,68,73	2.37	17 (28%)	70,107,113	2.51	25 (35%)
14	CLA	H	804	-	54,62,73	2.43	18 (33%)	62,99,113	3.01	22 (35%)
14	CLA	G	852	-	65,73,73	2.21	21 (32%)	76,113,113	2.26	24 (31%)
18	LHG	A	853	14	31,31,48	1.20	2 (6%)	34,37,54	1.15	2 (5%)
14	CLA	Z	802	-	65,73,73	2.17	19 (29%)	76,113,113	2.50	22 (28%)
15	PQN	A	844	-	34,34,34	1.60	2 (5%)	42,45,45	1.18	4 (9%)
14	CLA	Y	816	-	50,58,73	2.54	19 (38%)	58,95,113	2.88	23 (39%)
14	CLA	H	825	-	65,73,73	2.24	20 (30%)	76,113,113	2.78	26 (34%)
14	CLA	Z	822	-	45,53,73	2.67	18 (40%)	52,89,113	2.96	23 (44%)
17	BCR	e	101	-	41,41,41	2.64	7 (17%)	56,56,56	7.76	32 (57%)
14	CLA	Y	821	-	65,73,73	2.25	21 (32%)	76,113,113	2.36	24 (31%)
17	BCR	Q	203	-	41,41,41	2.59	6 (14%)	56,56,56	7.18	27 (48%)
14	CLA	Y	805	-	65,73,73	2.16	18 (27%)	76,113,113	2.69	27 (35%)
14	CLA	h	205	-	65,73,73	2.32	20 (30%)	76,113,113	2.89	24 (31%)
14	CLA	Y	826	-	60,68,73	2.29	18 (30%)	70,107,113	2.54	20 (28%)
14	CLA	B	829	-	45,53,73	2.53	19 (42%)	52,89,113	3.09	22 (42%)
14	CLA	H	835	-	45,53,73	2.59	17 (37%)	52,89,113	2.91	21 (40%)
14	CLA	Z	838	-	65,73,73	2.20	20 (30%)	76,113,113	2.56	22 (28%)
14	CLA	A	836	-	50,58,73	2.59	21 (42%)	58,95,113	2.98	26 (44%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
17	BCR	U	1008	-	41,41,41	2.72	6 (14%)	56,56,56	7.03	26 (46%)
14	CLA	G	815	-	50,58,73	2.62	19 (38%)	58,95,113	3.12	25 (43%)
17	BCR	J	103	-	41,41,41	2.70	6 (14%)	56,56,56	6.97	30 (53%)
14	CLA	Y	839	-	50,58,73	2.49	20 (40%)	58,95,113	3.02	25 (43%)
14	CLA	H	805	-	65,73,73	2.28	19 (29%)	76,113,113	2.52	23 (30%)
14	CLA	A	819	-	65,73,73	2.24	19 (29%)	76,113,113	2.59	27 (35%)
14	CLA	H	817	-	65,73,73	2.20	19 (29%)	76,113,113	2.83	27 (35%)
17	BCR	F	203	-	41,41,41	2.80	7 (17%)	56,56,56	7.00	28 (50%)
17	BCR	Y	852	-	41,41,41	2.63	7 (17%)	56,56,56	7.15	22 (39%)
14	CLA	B	827	-	65,73,73	2.27	19 (29%)	76,113,113	2.39	23 (30%)
14	CLA	A	806	-	65,73,73	2.14	17 (26%)	76,113,113	2.53	24 (31%)
15	PQN	H	841	-	34,34,34	1.67	2 (5%)	42,45,45	1.19	4 (9%)
17	BCR	Y	844	-	41,41,41	2.55	8 (19%)	56,56,56	7.33	23 (41%)
14	CLA	A	838	-	50,58,73	2.59	20 (40%)	58,95,113	2.97	28 (48%)
17	BCR	H	850	-	41,41,41	2.87	6 (14%)	56,56,56	7.05	28 (50%)
14	CLA	A	854	-	65,73,73	2.24	18 (27%)	76,113,113	2.67	24 (31%)
14	CLA	G	835	-	45,53,73	2.63	19 (42%)	52,89,113	3.15	21 (40%)
14	CLA	Y	811	14	65,73,73	2.31	20 (30%)	76,113,113	2.42	22 (28%)
18	LHG	Y	850	-	48,48,48	1.03	2 (4%)	51,54,54	1.30	5 (9%)
14	CLA	H	802	-	65,73,73	2.21	19 (29%)	76,113,113	2.63	23 (30%)
14	CLA	B	821	-	55,63,73	2.42	19 (34%)	64,101,113	2.53	19 (29%)
14	CLA	H	839	-	65,73,73	2.22	20 (30%)	76,113,113	2.65	24 (31%)
14	CLA	B	805	-	65,73,73	2.20	19 (29%)	76,113,113	2.45	22 (28%)
14	CLA	B	817	-	60,68,73	2.35	21 (35%)	70,107,113	2.45	20 (28%)
14	CLA	B	839	-	65,73,73	2.26	20 (30%)	76,113,113	2.48	23 (30%)
14	CLA	H	823	-	60,68,73	2.32	18 (30%)	70,107,113	2.70	26 (37%)
17	BCR	G	848	-	41,41,41	2.64	6 (14%)	56,56,56	7.17	24 (42%)
14	CLA	Y	812	-	55,63,73	2.44	21 (38%)	64,101,113	2.70	23 (35%)
17	BCR	B	847	-	41,41,41	2.59	6 (14%)	56,56,56	7.17	26 (46%)
14	CLA	B	801	-	65,73,73	2.20	18 (27%)	76,113,113	2.54	23 (30%)
14	CLA	H	820	-	45,53,73	2.50	17 (37%)	52,89,113	3.06	23 (44%)
14	CLA	Y	836	-	65,73,73	2.31	21 (32%)	76,113,113	2.49	26 (34%)
14	CLA	Y	838	-	65,73,73	2.34	20 (30%)	76,113,113	2.51	23 (30%)
15	PQN	G	843	-	34,34,34	1.68	2 (5%)	42,45,45	1.17	5 (11%)
17	BCR	A	848	-	41,41,41	2.63	6 (14%)	56,56,56	7.17	28 (50%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
14	CLA	Z	808	-	65,73,73	2.07	17 (26%)	76,113,113	2.50	22 (28%)
14	CLA	B	833	-	45,53,73	2.60	19 (42%)	52,89,113	3.10	23 (44%)
14	CLA	G	818	-	65,73,73	2.19	18 (27%)	76,113,113	2.69	26 (34%)
17	BCR	i	101	-	41,41,41	2.80	6 (14%)	56,56,56	7.58	28 (50%)
17	BCR	A	849	-	41,41,41	2.76	7 (17%)	56,56,56	6.98	29 (51%)
18	LHG	Y	851	14	24,24,48	1.56	2 (8%)	27,30,54	1.44	2 (7%)
17	BCR	G	847	-	41,41,41	2.70	6 (14%)	56,56,56	7.20	29 (51%)
19	LMG	Z	849	-	49,49,55	1.28	6 (12%)	57,57,63	1.27	5 (8%)
14	CLA	Z	806	-	65,73,73	2.30	21 (32%)	76,113,113	2.54	25 (32%)
14	CLA	L	204	-	65,73,73	2.22	19 (29%)	76,113,113	2.62	23 (30%)
14	CLA	Z	820	-	60,68,73	2.32	21 (35%)	70,107,113	2.46	22 (31%)
14	CLA	Y	813	-	60,68,73	2.34	20 (33%)	70,107,113	2.71	24 (34%)
19	LMG	B	848	-	52,52,55	1.42	7 (13%)	60,60,63	1.36	7 (11%)
14	CLA	h	201	-	65,73,73	2.22	18 (27%)	76,113,113	2.48	24 (31%)
14	CLA	g	102	-	45,53,73	2.66	18 (40%)	52,89,113	2.76	19 (36%)
14	CLA	H	815	-	45,53,73	2.60	20 (44%)	52,89,113	3.06	24 (46%)
17	BCR	B	844	-	41,41,41	2.71	6 (14%)	56,56,56	7.13	27 (48%)
14	CLA	H	814	-	65,73,73	2.31	20 (30%)	76,113,113	2.68	21 (27%)
14	CLA	H	818	-	60,68,73	2.33	18 (30%)	70,107,113	2.63	26 (37%)
14	CLA	A	807	-	65,73,73	2.25	20 (30%)	76,113,113	2.44	27 (35%)
14	CLA	B	837	-	65,73,73	2.17	18 (27%)	76,113,113	2.61	26 (34%)
14	CLA	G	826	-	60,68,73	2.34	20 (33%)	70,107,113	2.64	23 (32%)
14	CLA	B	802	-	65,73,73	2.26	20 (30%)	76,113,113	2.23	23 (30%)
14	CLA	G	827	-	65,73,73	2.28	19 (29%)	76,113,113	2.34	26 (34%)
17	BCR	H	847	-	41,41,41	2.51	7 (17%)	56,56,56	7.28	29 (51%)
14	CLA	A	824	-	50,58,73	2.66	21 (42%)	58,95,113	2.74	23 (39%)
17	BCR	S	1105	-	41,41,41	2.88	7 (17%)	56,56,56	7.33	29 (51%)
14	CLA	G	813	-	60,68,73	2.37	20 (33%)	70,107,113	2.75	25 (35%)
14	CLA	B	825	-	65,73,73	2.18	19 (29%)	76,113,113	2.64	24 (31%)
14	CLA	A	826	-	65,73,73	2.26	21 (32%)	76,113,113	2.54	25 (32%)
17	BCR	M	101	-	41,41,41	2.75	8 (19%)	56,56,56	7.14	28 (50%)
14	CLA	H	808	-	65,73,73	2.18	19 (29%)	76,113,113	2.46	28 (36%)
14	CLA	A	827	-	60,68,73	2.31	19 (31%)	70,107,113	2.69	26 (37%)
14	CLA	Z	810	2	65,73,73	2.13	19 (29%)	76,113,113	2.78	25 (32%)
14	CLA	A	812	14	65,73,73	2.17	18 (27%)	76,113,113	2.69	24 (31%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
14	CLA	H	834	-	45,53,73	2.57	18 (40%)	52,89,113	3.09	22 (42%)
14	CLA	Z	835	-	45,53,73	2.64	18 (40%)	52,89,113	2.73	20 (38%)
14	CLA	Y	828	-	65,73,73	2.27	21 (32%)	76,113,113	2.39	25 (32%)
17	BCR	Y	847	-	41,41,41	2.73	6 (14%)	56,56,56	7.17	26 (46%)
17	BCR	R	101	-	41,41,41	2.60	7 (17%)	56,56,56	7.50	23 (41%)
17	BCR	A	846	-	41,41,41	2.87	6 (14%)	56,56,56	7.35	28 (50%)
17	BCR	Z	846	-	25,25,41	2.13	2 (8%)	33,33,56	8.00	16 (48%)
14	CLA	A	829	-	65,73,73	2.16	19 (29%)	76,113,113	2.67	25 (32%)
16	SF4	a	101	3	0,12,12	-	-	-		
17	BCR	h	207	-	41,41,41	2.91	8 (19%)	56,56,56	7.00	18 (32%)
14	CLA	Y	830	-	65,73,73	2.30	19 (29%)	76,113,113	2.48	22 (28%)
14	CLA	S	1101	-	65,73,73	2.23	19 (29%)	76,113,113	2.58	23 (30%)
17	BCR	Z	845	-	41,41,41	2.55	6 (14%)	56,56,56	7.27	24 (42%)
14	CLA	F	202	-	45,53,73	2.52	20 (44%)	52,89,113	3.02	22 (42%)
14	CLA	A	825	-	60,68,73	2.35	20 (33%)	70,107,113	2.53	22 (31%)
14	CLA	B	809	-	65,73,73	2.28	19 (29%)	76,113,113	2.58	27 (35%)
14	CLA	Z	803	-	65,73,73	2.24	18 (27%)	76,113,113	2.58	26 (34%)
14	CLA	G	820	-	60,68,73	2.33	20 (33%)	70,107,113	2.65	25 (35%)
15	PQN	Y	842	-	34,34,34	1.77	2 (5%)	42,45,45	1.02	3 (7%)
17	BCR	I	102	-	41,41,41	2.90	6 (14%)	56,56,56	7.00	23 (41%)
14	CLA	X	1701	-	45,53,73	2.72	19 (42%)	52,89,113	2.69	23 (44%)
14	CLA	A	839	-	65,73,73	2.23	19 (29%)	76,113,113	2.50	22 (28%)
14	CLA	H	816	-	55,63,73	2.52	19 (34%)	64,101,113	2.93	26 (40%)
14	CLA	Y	810	-	45,53,73	2.63	20 (44%)	52,89,113	2.82	25 (48%)
14	CLA	H	821	-	45,53,73	2.75	18 (40%)	52,89,113	2.81	21 (40%)
14	CLA	h	204	10	65,73,73	2.26	18 (27%)	76,113,113	2.39	26 (34%)
17	BCR	B	845	-	25,25,41	2.14	2 (8%)	33,33,56	7.99	14 (42%)
14	CLA	Y	835	-	50,58,73	2.59	19 (38%)	58,95,113	2.94	24 (41%)
14	CLA	B	815	-	55,63,73	2.47	20 (36%)	64,101,113	2.65	19 (29%)
14	CLA	G	802	-	65,73,73	2.30	20 (30%)	76,113,113	2.51	22 (28%)
17	BCR	S	1104	-	41,41,41	2.96	6 (14%)	56,56,56	6.95	26 (46%)
13	CL0	A	801	-	65,73,73	2.32	17 (26%)	76,113,113	2.63	22 (28%)
14	CLA	Z	805	-	54,62,73	2.31	18 (33%)	62,99,113	3.03	26 (41%)
14	CLA	G	823	-	50,58,73	2.59	20 (40%)	58,95,113	2.91	23 (39%)
14	CLA	Z	817	-	55,63,73	2.43	20 (36%)	64,101,113	2.83	23 (35%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
14	CLA	S	1102	8	45,53,73	2.63	19 (42%)	52,89,113	2.85	18 (34%)
14	CLA	A	822	-	65,73,73	2.31	21 (32%)	76,113,113	2.50	21 (27%)
14	CLA	A	832	-	50,58,73	2.42	19 (38%)	58,95,113	2.75	25 (43%)
14	CLA	Z	832	-	45,53,73	2.50	19 (42%)	52,89,113	2.96	23 (44%)
14	CLA	Z	831	-	45,53,73	2.49	20 (44%)	52,89,113	3.12	23 (44%)
14	CLA	Y	817	-	60,68,73	2.40	21 (35%)	70,107,113	2.59	24 (34%)
17	BCR	Q	201	-	41,41,41	2.87	6 (14%)	56,56,56	7.00	27 (48%)
14	CLA	G	806	-	65,73,73	2.24	19 (29%)	76,113,113	2.63	24 (31%)
14	CLA	B	814	-	45,53,73	2.58	18 (40%)	52,89,113	3.02	23 (44%)
14	CLA	G	829	-	65,73,73	2.27	19 (29%)	76,113,113	2.30	27 (35%)
14	CLA	Z	836	-	45,53,73	2.56	19 (42%)	52,89,113	3.13	23 (44%)
14	CLA	Y	831	-	50,58,73	2.41	18 (36%)	58,95,113	2.93	21 (36%)
14	CLA	Z	839	-	45,53,73	2.57	19 (42%)	52,89,113	3.02	24 (46%)
14	CLA	H	851	18	50,58,73	2.57	20 (40%)	58,95,113	3.13	26 (44%)
14	CLA	G	840	-	65,73,73	2.27	20 (30%)	76,113,113	2.54	24 (31%)
17	BCR	Z	850	-	41,41,41	2.84	6 (14%)	56,56,56	7.07	24 (42%)
14	CLA	Y	833	-	55,63,73	2.56	21 (38%)	64,101,113	2.60	23 (35%)
14	CLA	Z	818	-	65,73,73	2.33	20 (30%)	76,113,113	2.58	23 (30%)
14	CLA	G	821	-	65,73,73	2.32	18 (27%)	76,113,113	2.54	22 (28%)
14	CLA	L	202	-	65,73,73	2.21	18 (27%)	76,113,113	2.61	30 (39%)
14	CLA	B	810	-	55,63,73	2.44	20 (36%)	64,101,113	2.71	25 (39%)
14	CLA	H	826	-	65,73,73	2.28	21 (32%)	76,113,113	2.41	22 (28%)
14	CLA	G	831	-	50,58,73	2.49	18 (36%)	58,95,113	2.89	26 (44%)
14	CLA	Y	829	-	65,73,73	2.34	20 (30%)	76,113,113	2.39	21 (27%)
14	CLA	G	842	18	50,58,73	2.52	20 (40%)	58,95,113	3.00	24 (41%)
14	CLA	g	101	-	42,49,73	2.57	15 (35%)	48,83,113	2.87	21 (43%)
14	CLA	Z	816	-	45,53,73	2.57	19 (42%)	52,89,113	3.02	19 (36%)
15	PQN	B	841	-	34,34,34	1.72	3 (8%)	42,45,45	1.09	4 (9%)
14	CLA	H	812	-	45,53,73	2.59	19 (42%)	52,89,113	2.76	21 (40%)
14	CLA	J	101	8	45,53,73	2.58	18 (40%)	52,89,113	2.94	22 (42%)
14	CLA	Z	824	-	60,68,73	2.42	20 (33%)	70,107,113	2.40	23 (32%)
14	CLA	Y	802	-	65,73,73	2.26	21 (32%)	76,113,113	2.42	30 (39%)

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
14	CLA	H	836	-	1/1/14/20	17/31/109/115	-
14	CLA	H	838	-	1/1/11/20	1/13/91/115	-
17	BCR	Y	848	-	-	3/29/63/63	0/2/2/2
14	CLA	Z	823	-	1/1/13/20	10/25/103/115	-
14	CLA	Z	811	2	1/1/15/20	18/37/115/115	-
14	CLA	Z	813	-	1/1/11/20	4/13/91/115	-
14	CLA	G	807	-	1/1/12/20	7/21/99/115	-
14	CLA	G	810	-	1/1/11/20	9/13/91/115	-
14	CLA	A	809	1	1/1/15/20	21/37/115/115	-
14	CLA	A	837	-	1/1/15/20	19/37/115/115	-
17	BCR	R	102	-	-	11/29/63/63	0/2/2/2
17	BCR	U	1009	-	-	8/29/63/63	0/2/2/2
14	CLA	G	804	14	1/1/13/20	11/30/108/115	-
14	CLA	H	831	-	1/1/15/20	17/37/115/115	-
14	CLA	Z	828	-	1/1/15/20	17/37/115/115	-
14	CLA	Y	814	-	1/1/13/20	12/25/103/115	-
17	BCR	J	104	-	-	9/29/63/63	0/2/2/2
14	CLA	H	810	2	1/1/15/20	16/37/115/115	-
14	CLA	Z	819	-	1/1/14/20	14/31/109/115	-
14	CLA	Z	821	-	1/1/11/20	8/13/91/115	-
14	CLA	A	810	-	1/1/15/20	13/37/115/115	-
14	CLA	Z	825	2	1/1/13/20	10/25/103/115	-
17	BCR	B	843	-	-	7/29/63/63	0/2/2/2
17	BCR	G	846	-	-	9/29/63/63	0/2/2/2
14	CLA	H	813	-	1/1/15/20	18/37/115/115	-
14	CLA	Y	808	1	1/1/15/20	22/37/115/115	-
14	CLA	A	842	-	1/1/15/20	15/37/115/115	-
14	CLA	A	811	-	1/1/11/20	6/13/91/115	-
14	CLA	Y	827	-	1/1/15/20	16/37/115/115	-
14	CLA	Z	809	-	1/1/15/20	15/37/115/115	-
17	BCR	U	1005	-	-	6/29/63/63	0/2/2/2
14	CLA	H	806	-	1/1/15/20	17/37/115/115	-
14	CLA	G	828	-	1/1/15/20	11/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
14	CLA	H	828	-	1/1/15/20	7/37/115/115	-
16	SF4	G	844	1,2	-	-	0/6/5/5
14	CLA	B	808	2	1/1/15/20	21/37/115/115	-
14	CLA	U	1006	-	1/1/15/20	15/37/115/115	-
14	CLA	Z	830	-	1/1/15/20	11/37/115/115	-
17	BCR	Y	849	-	-	8/29/63/63	0/2/2/2
17	BCR	L	207	-	-	11/29/63/63	0/2/2/2
14	CLA	G	808	1	1/1/15/20	16/37/115/115	-
14	CLA	H	824	2	1/1/13/20	13/25/103/115	-
14	CLA	T	103	-	1/1/11/20	4/13/91/115	-
14	CLA	B	832	-	1/1/13/20	10/25/103/115	-
14	CLA	H	803	-	1/1/15/20	20/37/115/115	-
16	SF4	N	102	3	-	-	0/6/5/5
14	CLA	d	202	-	1/1/11/20	3/13/91/115	-
14	CLA	H	827	-	1/1/15/20	16/37/115/115	-
14	CLA	Y	815	-	1/1/12/20	7/19/97/115	-
14	CLA	A	828	-	1/1/15/20	15/37/115/115	-
14	CLA	G	809	-	1/1/15/20	16/37/115/115	-
17	BCR	T	102	-	-	10/29/63/63	0/2/2/2
16	SF4	a	102	3	-	-	0/6/5/5
14	CLA	B	818	-	1/1/14/20	17/31/109/115	-
17	BCR	V	101	-	-	6/29/63/63	0/2/2/2
14	CLA	H	829	-	1/1/15/20	12/37/115/115	-
14	CLA	G	833	-	1/1/15/20	14/37/115/115	-
14	CLA	A	817	-	1/1/12/20	7/19/97/115	-
14	CLA	Y	841	-	1/1/15/20	14/37/115/115	-
17	BCR	I	101	-	-	5/29/63/63	0/2/2/2
14	CLA	J	102	-	1/1/13/20	13/25/103/115	-
14	CLA	Y	809	-	1/1/15/20	16/37/115/115	-
18	LHG	G	850	-	-	25/53/53/53	-
17	BCR	f	103	-	-	5/29/63/63	0/2/2/2
17	BCR	L	208	-	-	8/29/63/63	0/2/2/2
14	CLA	B	811	-	1/1/12/20	6/19/97/115	-
14	CLA	f	102	-	1/1/13/20	15/25/103/115	-
17	BCR	H	843	-	-	9/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
14	CLA	Y	837	-	1/1/12/20	5/19/97/115	-
14	CLA	G	836	-	1/1/12/20	5/19/97/115	-
14	CLA	G	838	-	1/1/12/20	4/19/97/115	-
14	CLA	Z	826	-	1/1/15/20	13/37/115/115	-
14	CLA	L	201	-	1/1/15/20	18/37/115/115	-
14	CLA	B	840	-	1/1/15/20	10/37/115/115	-
17	BCR	h	202	-	-	7/29/63/63	0/2/2/2
14	CLA	G	832	-	1/1/15/20	13/37/115/115	-
14	CLA	Z	829	-	1/1/15/20	15/37/115/115	-
17	BCR	B	842	-	-	3/24/41/63	0/1/1/2
14	CLA	G	819	-	1/1/15/20	19/37/115/115	-
14	CLA	A	830	-	1/1/15/20	17/37/115/115	-
14	CLA	G	824	-	1/1/14/20	17/31/109/115	-
14	CLA	A	804	-	1/1/15/20	16/37/115/115	-
14	CLA	H	822	-	1/1/13/20	9/25/103/115	-
14	CLA	G	825	-	1/1/15/20	11/37/115/115	-
14	CLA	A	803	-	1/1/15/20	7/37/115/115	-
17	BCR	Y	845	-	-	4/29/63/63	0/2/2/2
14	CLA	H	807	-	1/1/15/20	10/37/115/115	-
14	CLA	A	833	-	1/1/15/20	9/37/115/115	-
14	CLA	j	102	-	1/1/11/20	5/13/91/115	-
14	CLA	G	803	-	1/1/15/20	12/37/115/115	-
17	BCR	B	846	-	-	11/29/63/63	0/2/2/2
17	BCR	Z	844	-	-	8/29/63/63	0/2/2/2
14	CLA	Y	822	-	1/1/15/20	17/37/115/115	-
16	SF4	C	101	3	-	-	0/6/5/5
17	BCR	H	845	-	-	8/18/35/63	0/1/1/2
14	CLA	A	835	1	1/1/11/20	4/13/91/115	-
14	CLA	B	826	-	1/1/15/20	12/37/115/115	-
14	CLA	Z	812	-	1/1/13/20	13/25/103/115	-
14	CLA	A	821	-	1/1/14/20	14/31/109/115	-
17	BCR	Z	848	-	-	9/29/63/63	0/2/2/2
14	CLA	d	201	-	1/1/15/20	15/37/115/115	-
14	CLA	B	812	-	1/1/15/20	23/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
14	CLA	A	808	-	1/1/12/20	9/21/99/115	-
14	CLA	G	811	14	1/1/15/20	22/37/115/115	-
14	CLA	A	805	14	1/1/13/20	15/30/108/115	-
14	CLA	Z	801	-	1/1/15/20	17/37/115/115	-
14	CLA	A	813	-	1/1/12/20	9/24/102/115	-
14	CLA	G	841	-	1/1/15/20	15/37/115/115	-
15	PQN	Z	842	-	-	8/23/43/43	0/2/2/2
14	CLA	Y	824	-	1/1/14/20	17/31/109/115	-
14	CLA	G	814	-	1/1/12/20	5/19/97/115	-
14	CLA	Z	837	-	1/1/14/20	12/31/109/115	-
17	BCR	Z	843	-	-	12/29/63/63	0/2/2/2
14	CLA	G	834	-	1/1/13/20	5/25/103/115	-
14	CLA	G	853	-	1/1/11/20	6/13/91/115	-
14	CLA	Z	833	-	1/1/13/20	11/25/103/115	-
14	CLA	G	830	-	1/1/15/20	13/37/115/115	-
14	CLA	A	802	-	1/1/15/20	13/37/115/115	-
14	CLA	Z	841	-	1/1/15/20	10/37/115/115	-
14	CLA	A	840	-	1/1/12/20	5/19/97/115	-
13	CL0	Y	801	-	3/3/20/25	18/37/135/135	-
19	LMG	H	848	-	-	12/44/64/70	0/1/1/1
14	CLA	B	831	-	1/1/15/20	19/37/115/115	-
14	CLA	H	832	-	1/1/13/20	12/25/103/115	-
14	CLA	Y	806	-	1/1/15/20	17/37/115/115	-
14	CLA	A	823	-	1/1/15/20	18/37/115/115	-
14	CLA	Y	820	-	1/1/14/20	11/31/109/115	-
17	BCR	H	842	-	-	10/29/63/63	0/2/2/2
17	BCR	Y	846	-	-	18/29/63/63	0/2/2/2
16	SF4	N	101	3	-	-	0/6/5/5
14	CLA	B	820	-	1/1/11/20	8/13/91/115	-
14	CLA	H	801	-	1/1/15/20	15/37/115/115	-
14	CLA	A	820	-	1/1/15/20	18/37/115/115	-
14	CLA	H	833	-	1/1/11/20	6/13/91/115	-
14	CLA	h	206	-	1/1/15/20	17/37/115/115	-
17	BCR	G	849	-	-	9/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
14	CLA	B	823	2	1/1/13/20	12/25/103/115	-
14	CLA	U	1007	-	1/1/15/20	12/37/115/115	-
14	CLA	H	809	2	1/1/15/20	17/37/115/115	-
14	CLA	Z	815	-	1/1/15/20	9/37/115/115	-
17	BCR	H	844	-	-	10/29/63/63	0/2/2/2
14	CLA	Y	803	-	1/1/15/20	15/37/115/115	-
14	CLA	K	101	-	1/1/9/20	3/7/81/115	-
17	BCR	A	851	-	-	11/29/63/63	0/2/2/2
18	LHG	A	852	-	-	30/53/53/53	-
18	LHG	j	101	-	-	17/32/32/53	-
14	CLA	U	1002	10	1/1/15/20	21/37/115/115	-
16	SF4	Y	843	1,2	-	-	0/6/5/5
14	CLA	Y	819	-	1/1/15/20	20/37/115/115	-
14	CLA	Y	818	-	1/1/15/20	14/37/115/115	-
14	CLA	Z	834	-	1/1/11/20	5/13/91/115	-
17	BCR	H	846	-	-	14/29/63/63	0/2/2/2
17	BCR	Y	853	-	-	8/29/63/63	0/2/2/2
17	BCR	B	850	-	-	10/29/63/63	0/2/2/2
14	CLA	Z	814	-	1/1/15/20	19/37/115/115	-
17	BCR	d	203	-	-	5/29/63/63	0/2/2/2
14	CLA	Z	840	-	1/1/15/20	9/37/115/115	-
14	CLA	B	816	-	1/1/15/20	8/37/115/115	-
18	LHG	G	851	14	-	16/36/36/53	-
14	CLA	B	803	-	1/1/12/20	7/24/102/115	-
14	CLA	A	818	-	1/1/14/20	14/31/109/115	-
14	CLA	Z	804	-	1/1/15/20	14/37/115/115	-
14	CLA	K	102	-	1/1/11/20	4/13/91/115	-
17	BCR	F	201	-	-	10/29/63/63	0/2/2/2
14	CLA	B	836	-	1/1/14/20	8/31/109/115	-
14	CLA	H	819	-	1/1/14/20	14/31/109/115	-
14	CLA	H	811	-	1/1/13/20	9/25/103/115	-
14	CLA	Y	840	-	1/1/15/20	13/37/115/115	-
17	BCR	A	847	-	-	9/29/63/63	0/2/2/2
14	CLA	B	819	-	1/1/11/20	4/13/91/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
18	LHG	H	849	-	-	23/41/41/53	-
14	CLA	U	1004	-	1/1/15/20	15/37/115/115	-
14	CLA	B	806	-	1/1/15/20	11/37/115/115	-
14	CLA	Z	827	-	1/1/15/20	14/37/115/115	-
14	CLA	Y	832	-	1/1/15/20	20/37/115/115	-
14	CLA	W	1701	-	1/1/11/20	5/13/91/115	-
14	CLA	G	839	-	1/1/12/20	7/19/97/115	-
14	CLA	B	838	-	1/1/11/20	2/13/91/115	-
14	CLA	A	834	-	1/1/13/20	10/25/103/115	-
14	CLA	A	831	-	1/1/15/20	16/37/115/115	-
14	CLA	B	804	-	1/1/15/20	14/37/115/115	-
14	CLA	G	816	-	1/1/12/20	10/19/97/115	-
14	CLA	S	1103	-	1/1/13/20	14/25/103/115	-
14	CLA	H	837	-	1/1/15/20	13/37/115/115	-
14	CLA	H	840	-	1/1/15/20	9/37/115/115	-
14	CLA	G	817	-	1/1/14/20	13/31/109/115	-
14	CLA	A	814	-	1/1/14/20	12/31/109/115	-
14	CLA	Y	834	1	1/1/11/20	3/13/91/115	-
14	CLA	B	828	-	1/1/15/20	9/37/115/115	-
14	CLA	B	824	-	1/1/15/20	15/37/115/115	-
14	CLA	G	822	-	1/1/15/20	12/37/115/115	-
17	BCR	G	845	-	-	8/29/63/63	0/2/2/2
14	CLA	L	206	-	1/1/15/20	9/37/115/115	-
17	BCR	Z	847	-	-	10/29/63/63	0/2/2/2
18	LHG	B	849	-	-	28/43/43/53	-
14	CLA	U	1003	-	1/1/15/20	13/37/115/115	-
14	CLA	Z	807	-	1/1/15/20	16/37/115/115	-
14	CLA	G	805	-	1/1/15/20	20/37/115/115	-
14	CLA	T	101	-	1/1/9/20	5/7/81/115	-
14	CLA	G	812	-	1/1/12/20	8/24/102/115	-
14	CLA	B	813	-	1/1/15/20	19/37/115/115	-
16	SF4	C	102	21,3	-	-	0/6/5/5
14	CLA	A	815	-	1/1/12/20	9/19/97/115	-
14	CLA	Y	807	-	1/1/12/20	11/21/99/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
14	CLA	Y	804	14	1/1/13/20	13/30/108/115	-
14	CLA	B	835	-	1/1/11/20	4/13/91/115	-
14	CLA	B	830	-	1/1/11/20	5/13/91/115	-
16	SF4	A	845	1,2	-	-	0/6/5/5
14	CLA	f	101	8	1/1/11/20	5/13/91/115	-
14	CLA	A	841	-	1/1/15/20	16/37/115/115	-
14	CLA	B	834	-	1/1/11/20	4/13/91/115	-
14	CLA	G	837	-	1/1/15/20	21/37/115/115	-
14	CLA	Q	202	-	1/1/11/20	2/13/91/115	-
14	CLA	B	807	-	1/1/15/20	16/37/115/115	-
14	CLA	A	843	18	1/1/12/20	9/19/97/115	-
14	CLA	A	816	-	1/1/12/20	8/19/97/115	-
14	CLA	Y	823	-	1/1/12/20	8/19/97/115	-
14	CLA	Y	825	-	1/1/15/20	15/37/115/115	-
17	BCR	A	850	-	-	6/29/63/63	0/2/2/2
13	CL0	G	801	-	3/3/20/25	14/37/135/135	-
14	CLA	L	205	-	1/1/15/20	16/37/115/115	-
14	CLA	H	830	-	1/1/11/20	10/13/91/115	-
14	CLA	B	822	-	1/1/14/20	14/31/109/115	-
14	CLA	H	804	-	1/1/12/20	7/24/102/115	-
14	CLA	G	852	-	1/1/15/20	11/37/115/115	-
18	LHG	A	853	14	-	19/36/36/53	-
14	CLA	Z	802	-	1/1/15/20	19/37/115/115	-
15	PQN	A	844	-	-	4/23/43/43	0/2/2/2
14	CLA	Y	816	-	1/1/12/20	8/19/97/115	-
14	CLA	H	825	-	1/1/15/20	22/37/115/115	-
14	CLA	Z	822	-	1/1/11/20	5/13/91/115	-
17	BCR	e	101	-	-	18/29/63/63	0/2/2/2
14	CLA	Y	821	-	1/1/15/20	19/37/115/115	-
17	BCR	Q	203	-	-	6/29/63/63	0/2/2/2
14	CLA	Y	805	-	1/1/15/20	15/37/115/115	-
14	CLA	h	205	-	1/1/15/20	17/37/115/115	-
14	CLA	Y	826	-	1/1/14/20	8/31/109/115	-
14	CLA	B	829	-	1/1/11/20	4/13/91/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
14	CLA	H	835	-	1/1/11/20	4/13/91/115	-
14	CLA	Z	838	-	1/1/15/20	14/37/115/115	-
14	CLA	A	836	-	1/1/12/20	6/19/97/115	-
17	BCR	U	1008	-	-	16/29/63/63	0/2/2/2
14	CLA	G	815	-	1/1/12/20	7/19/97/115	-
17	BCR	J	103	-	-	6/29/63/63	0/2/2/2
14	CLA	Y	839	-	1/1/12/20	5/19/97/115	-
14	CLA	H	805	-	1/1/15/20	16/37/115/115	-
14	CLA	A	819	-	1/1/15/20	20/37/115/115	-
14	CLA	H	817	-	1/1/15/20	14/37/115/115	-
17	BCR	F	203	-	-	4/29/63/63	0/2/2/2
17	BCR	Y	852	-	-	12/29/63/63	0/2/2/2
14	CLA	B	827	-	1/1/15/20	21/37/115/115	-
14	CLA	A	806	-	1/1/15/20	22/37/115/115	-
15	PQN	H	841	-	-	5/23/43/43	0/2/2/2
17	BCR	Y	844	-	-	9/29/63/63	0/2/2/2
14	CLA	A	838	-	1/1/12/20	9/19/97/115	-
17	BCR	H	850	-	-	8/29/63/63	0/2/2/2
14	CLA	A	854	-	1/1/15/20	14/37/115/115	-
14	CLA	G	835	-	1/1/11/20	7/13/91/115	-
14	CLA	Y	811	14	1/1/15/20	18/37/115/115	-
18	LHG	Y	850	-	-	32/53/53/53	-
14	CLA	H	802	-	1/1/15/20	19/37/115/115	-
14	CLA	B	821	-	1/1/13/20	11/25/103/115	-
14	CLA	H	839	-	1/1/15/20	8/37/115/115	-
14	CLA	B	805	-	1/1/15/20	15/37/115/115	-
14	CLA	B	817	-	1/1/14/20	9/31/109/115	-
14	CLA	B	839	-	1/1/15/20	12/37/115/115	-
14	CLA	H	823	-	1/1/14/20	13/31/109/115	-
17	BCR	G	848	-	-	8/29/63/63	0/2/2/2
14	CLA	Y	812	-	1/1/13/20	8/25/103/115	-
17	BCR	B	847	-	-	6/29/63/63	0/2/2/2
14	CLA	B	801	-	1/1/15/20	19/37/115/115	-
14	CLA	H	820	-	1/1/11/20	9/13/91/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
14	CLA	Y	836	-	1/1/15/20	19/37/115/115	-
14	CLA	Y	838	-	1/1/15/20	11/37/115/115	-
15	PQN	G	843	-	-	11/23/43/43	0/2/2/2
17	BCR	A	848	-	-	11/29/63/63	0/2/2/2
14	CLA	Z	808	-	1/1/15/20	18/37/115/115	-
14	CLA	B	833	-	1/1/11/20	5/13/91/115	-
14	CLA	G	818	-	1/1/15/20	19/37/115/115	-
17	BCR	i	101	-	-	11/29/63/63	0/2/2/2
17	BCR	A	849	-	-	8/29/63/63	0/2/2/2
18	LHG	Y	851	14	-	17/28/28/53	-
17	BCR	G	847	-	-	8/29/63/63	0/2/2/2
19	LMG	Z	849	-	-	14/44/64/70	0/1/1/1
14	CLA	Z	806	-	1/1/15/20	13/37/115/115	-
14	CLA	L	204	-	1/1/15/20	20/37/115/115	-
14	CLA	Z	820	-	1/1/14/20	12/31/109/115	-
14	CLA	Y	813	-	1/1/14/20	10/31/109/115	-
19	LMG	B	848	-	-	13/47/67/70	0/1/1/1
14	CLA	h	201	-	1/1/15/20	12/37/115/115	-
14	CLA	g	102	-	1/1/11/20	3/13/91/115	-
14	CLA	H	815	-	1/1/11/20	7/13/91/115	-
17	BCR	B	844	-	-	12/29/63/63	0/2/2/2
14	CLA	H	814	-	1/1/15/20	17/37/115/115	-
14	CLA	H	818	-	1/1/14/20	15/31/109/115	-
14	CLA	A	807	-	1/1/15/20	20/37/115/115	-
14	CLA	B	837	-	1/1/15/20	13/37/115/115	-
14	CLA	G	826	-	1/1/14/20	6/31/109/115	-
14	CLA	B	802	-	1/1/15/20	10/37/115/115	-
14	CLA	G	827	-	1/1/15/20	15/37/115/115	-
17	BCR	H	847	-	-	8/29/63/63	0/2/2/2
14	CLA	A	824	-	1/1/12/20	8/19/97/115	-
17	BCR	S	1105	-	-	12/29/63/63	0/2/2/2
14	CLA	G	813	-	1/1/14/20	12/31/109/115	-
14	CLA	B	825	-	1/1/15/20	20/37/115/115	-
14	CLA	A	826	-	1/1/15/20	16/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
17	BCR	M	101	-	-	11/29/63/63	0/2/2/2
14	CLA	H	808	-	1/1/15/20	15/37/115/115	-
14	CLA	A	827	-	1/1/14/20	11/31/109/115	-
14	CLA	Z	810	2	1/1/15/20	16/37/115/115	-
14	CLA	A	812	14	1/1/15/20	12/37/115/115	-
14	CLA	H	834	-	1/1/11/20	6/13/91/115	-
14	CLA	Z	835	-	1/1/11/20	6/13/91/115	-
14	CLA	Y	828	-	1/1/15/20	15/37/115/115	-
17	BCR	Y	847	-	-	5/29/63/63	0/2/2/2
17	BCR	R	101	-	-	8/29/63/63	0/2/2/2
17	BCR	A	846	-	-	10/29/63/63	0/2/2/2
17	BCR	Z	846	-	-	8/18/35/63	0/1/1/2
14	CLA	A	829	-	1/1/15/20	13/37/115/115	-
16	SF4	a	101	3	-	-	0/6/5/5
17	BCR	h	207	-	-	10/29/63/63	0/2/2/2
14	CLA	Y	830	-	1/1/15/20	11/37/115/115	-
14	CLA	S	1101	-	1/1/15/20	19/37/115/115	-
17	BCR	Z	845	-	-	10/29/63/63	0/2/2/2
14	CLA	F	202	-	1/1/11/20	4/13/91/115	-
14	CLA	A	825	-	1/1/14/20	16/31/109/115	-
14	CLA	B	809	-	1/1/15/20	16/37/115/115	-
14	CLA	Z	803	-	1/1/15/20	19/37/115/115	-
14	CLA	G	820	-	1/1/14/20	13/31/109/115	-
15	PQN	Y	842	-	-	7/23/43/43	0/2/2/2
17	BCR	I	102	-	-	9/29/63/63	0/2/2/2
14	CLA	X	1701	-	1/1/11/20	5/13/91/115	-
14	CLA	A	839	-	1/1/15/20	13/37/115/115	-
14	CLA	H	816	-	1/1/13/20	12/25/103/115	-
14	CLA	Y	810	-	1/1/11/20	4/13/91/115	-
14	CLA	H	821	-	1/1/11/20	5/13/91/115	-
14	CLA	h	204	10	1/1/15/20	19/37/115/115	-
17	BCR	B	845	-	-	4/18/35/63	0/1/1/2
14	CLA	Y	835	-	1/1/12/20	8/19/97/115	-
14	CLA	B	815	-	1/1/13/20	8/25/103/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
14	CLA	G	802	-	1/1/15/20	17/37/115/115	-
17	BCR	S	1104	-	-	9/29/63/63	0/2/2/2
13	CL0	A	801	-	3/3/20/25	8/37/135/135	-
14	CLA	Z	805	-	1/1/12/20	4/24/102/115	-
14	CLA	G	823	-	1/1/12/20	6/19/97/115	-
14	CLA	Z	817	-	1/1/13/20	10/25/103/115	-
14	CLA	S	1102	8	1/1/11/20	8/13/91/115	-
14	CLA	A	822	-	1/1/15/20	16/37/115/115	-
14	CLA	A	832	-	1/1/12/20	3/19/97/115	-
14	CLA	Z	832	-	1/1/11/20	5/13/91/115	-
14	CLA	Z	831	-	1/1/11/20	4/13/91/115	-
14	CLA	Y	817	-	1/1/14/20	7/31/109/115	-
17	BCR	Q	201	-	-	11/29/63/63	0/2/2/2
14	CLA	G	806	-	1/1/15/20	22/37/115/115	-
14	CLA	B	814	-	1/1/11/20	3/13/91/115	-
14	CLA	G	829	-	1/1/15/20	16/37/115/115	-
14	CLA	Z	836	-	1/1/11/20	7/13/91/115	-
14	CLA	Y	831	-	1/1/12/20	6/19/97/115	-
14	CLA	Z	839	-	1/1/11/20	1/13/91/115	-
14	CLA	H	851	18	1/1/12/20	12/19/97/115	-
14	CLA	G	840	-	1/1/15/20	18/37/115/115	-
17	BCR	Z	850	-	-	4/29/63/63	0/2/2/2
14	CLA	Y	833	-	1/1/13/20	11/25/103/115	-
14	CLA	Z	818	-	1/1/15/20	13/37/115/115	-
14	CLA	G	821	-	1/1/15/20	20/37/115/115	-
14	CLA	L	202	-	1/1/15/20	13/37/115/115	-
14	CLA	B	810	-	1/1/13/20	12/25/103/115	-
14	CLA	H	826	-	1/1/15/20	9/37/115/115	-
14	CLA	G	831	-	1/1/12/20	10/19/97/115	-
14	CLA	Y	829	-	1/1/15/20	16/37/115/115	-
14	CLA	G	842	18	1/1/12/20	3/19/97/115	-
14	CLA	g	101	-	1/1/9/20	2/7/81/115	-
14	CLA	Z	816	-	1/1/11/20	5/13/91/115	-
15	PQN	B	841	-	-	8/23/43/43	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
14	CLA	H	812	-	1/1/11/20	6/13/91/115	-
14	CLA	J	101	8	1/1/11/20	7/13/91/115	-
14	CLA	Z	824	-	1/1/14/20	7/31/109/115	-
14	CLA	Y	802	-	1/1/15/20	8/37/115/115	-

The worst 5 of 5962 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	H	843	BCR	C10-C9	-9.34	1.23	1.35
17	S	1104	BCR	C10-C9	-9.19	1.23	1.35
13	G	801	CL0	MG-NA	9.08	2.27	2.06
13	A	801	CL0	MG-NA	9.06	2.27	2.06
13	Y	801	CL0	MG-NA	8.94	2.27	2.06

The worst 5 of 8569 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
17	Z	848	BCR	C16-C17-C18	33.23	174.73	127.31
17	i	101	BCR	C16-C17-C18	30.09	170.25	127.31
17	Y	846	BCR	C16-C17-C18	29.93	170.03	127.31
17	R	101	BCR	C16-C17-C18	29.41	169.28	127.31
17	Y	849	BCR	C16-C17-C18	28.25	167.63	127.31

5 of 291 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
13	A	801	CL0	ND
13	A	801	CL0	NC
13	A	801	CL0	NA
13	G	801	CL0	ND
13	G	801	CL0	NC

5 of 4236 torsion outliers are listed below:

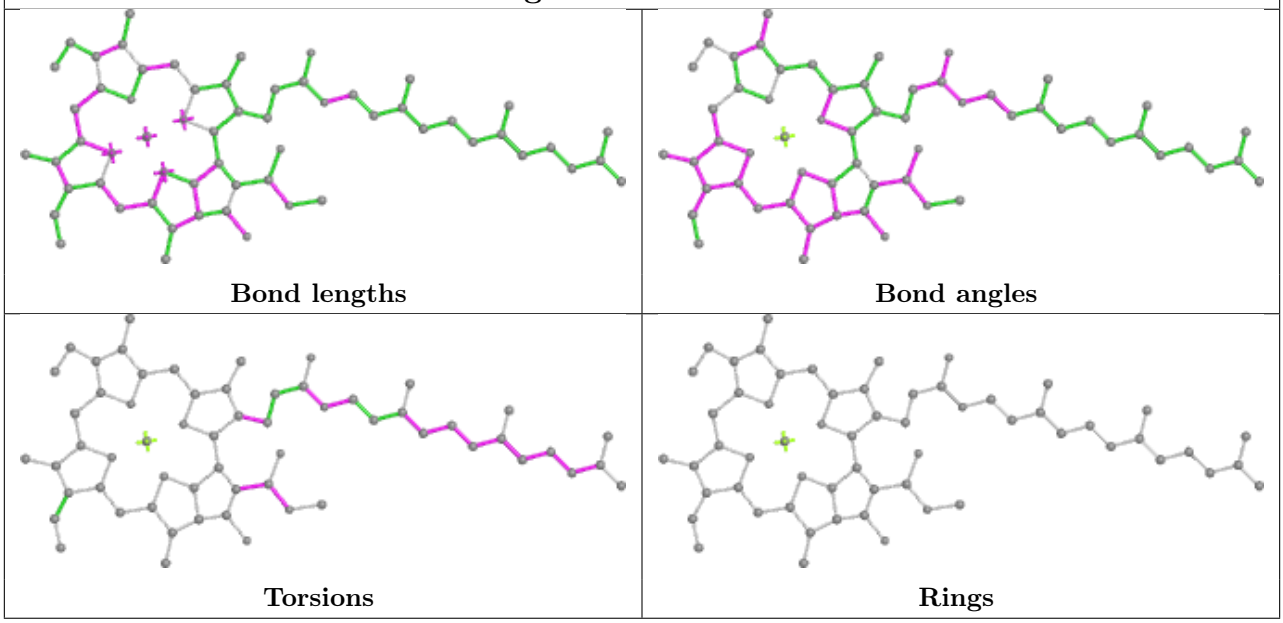
Mol	Chain	Res	Type	Atoms
13	G	801	CL0	C1A-C2A-CAA-CBA
13	G	801	CL0	C3A-C2A-CAA-CBA
13	G	801	CL0	CBD-CGD-O2D-CED
13	G	801	CL0	C2-C3-C5-C6
13	G	801	CL0	C4-C3-C5-C6

There are no ring outliers.

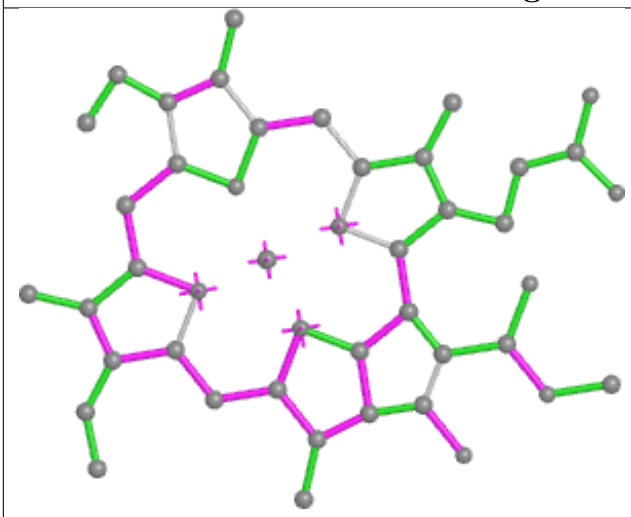
No monomer is involved in short contacts.

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.

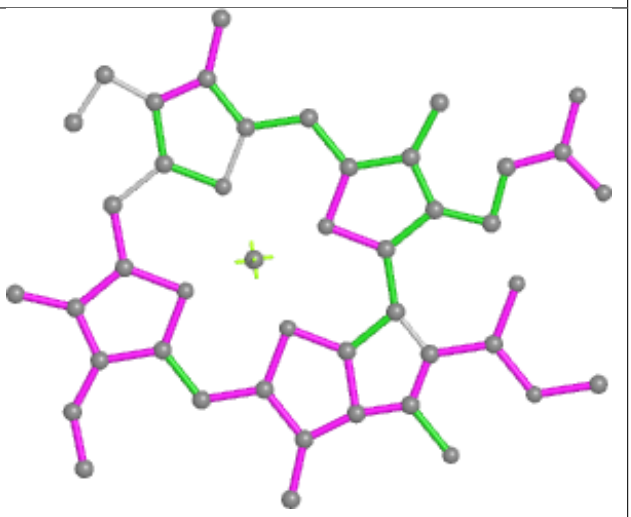
Ligand CLA H 836



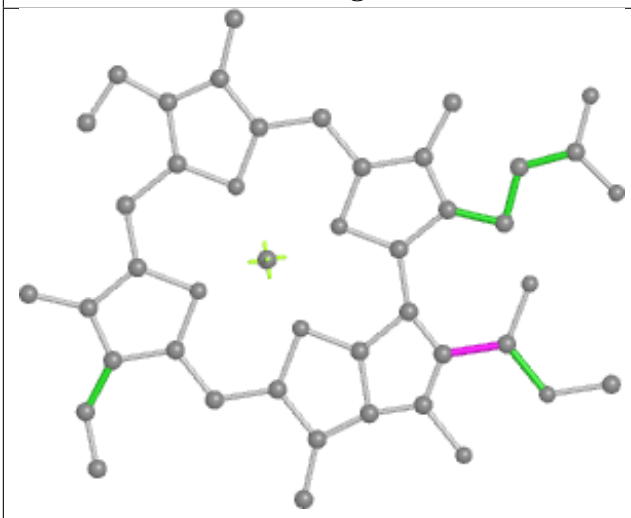
Ligand CLA H 838



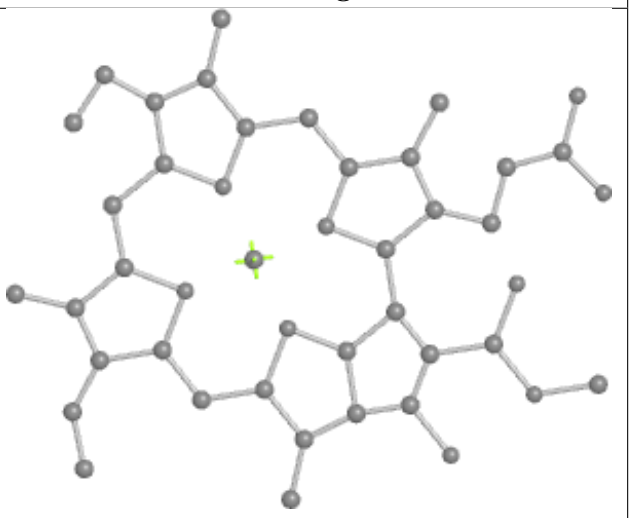
Bond lengths



Bond angles

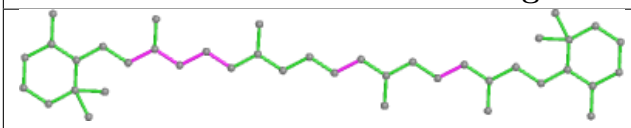


Torsions

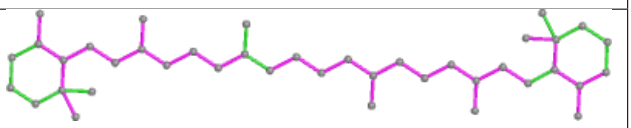


Rings

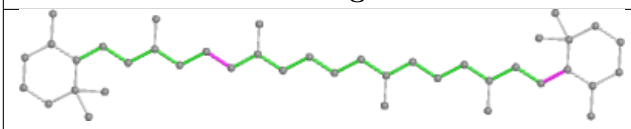
Ligand BCR Y 848



Bond lengths



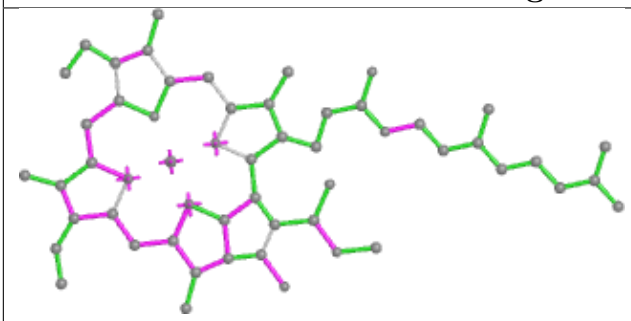
Bond angles



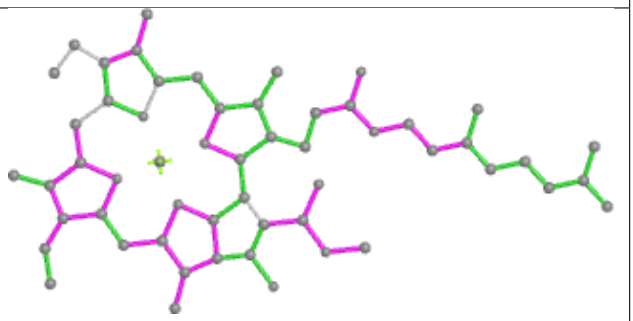
Torsions

Rings

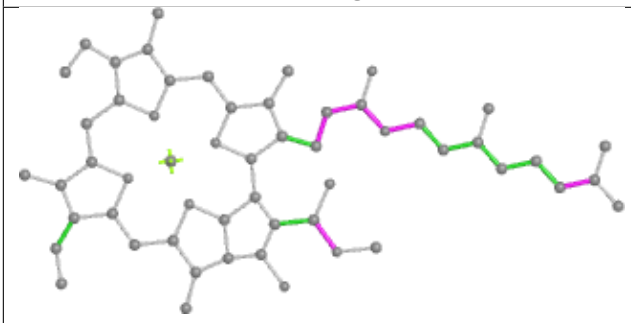
Ligand CLA Z 823



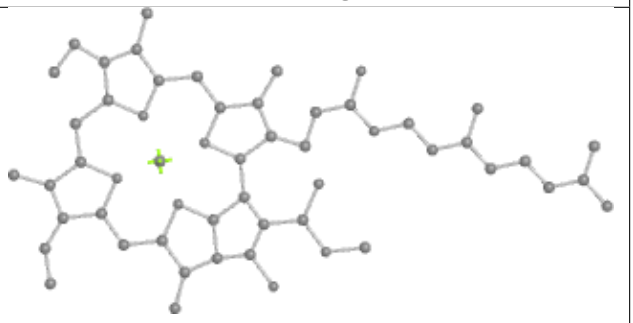
Bond lengths



Bond angles

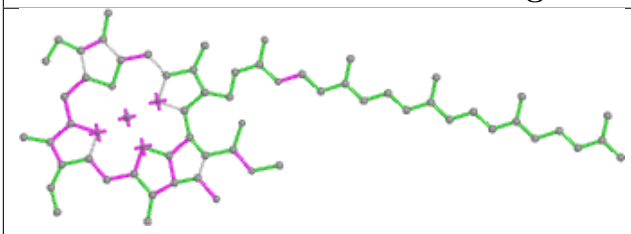


Torsions

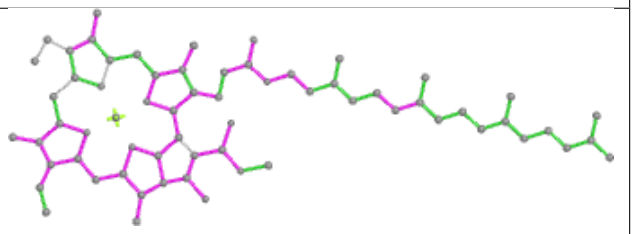


Rings

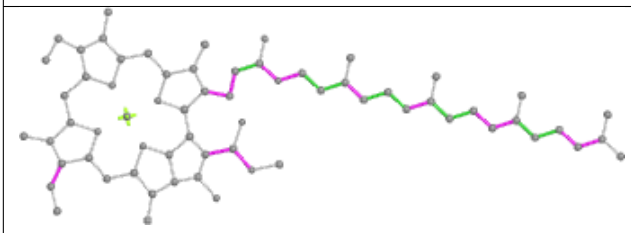
Ligand CLA Z 811



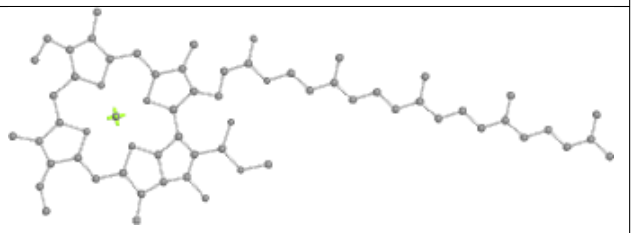
Bond lengths



Bond angles

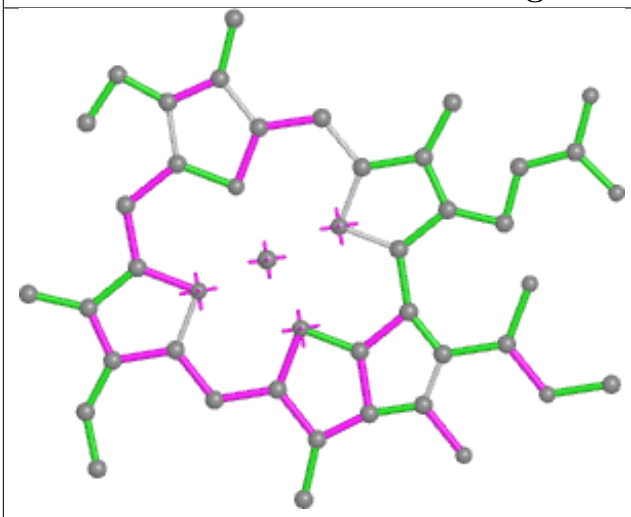


Torsions

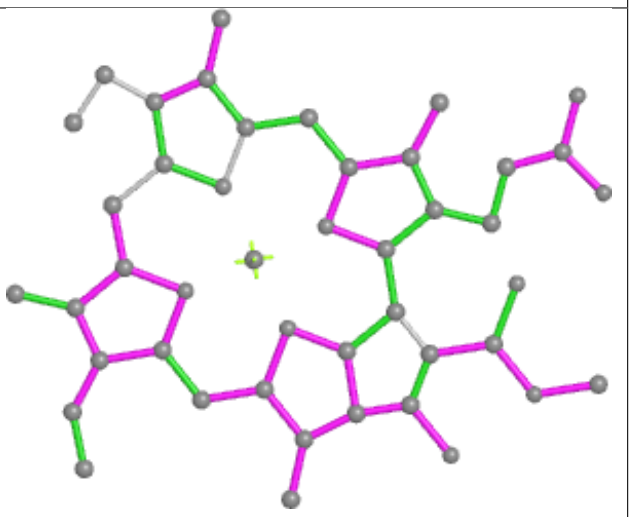


Rings

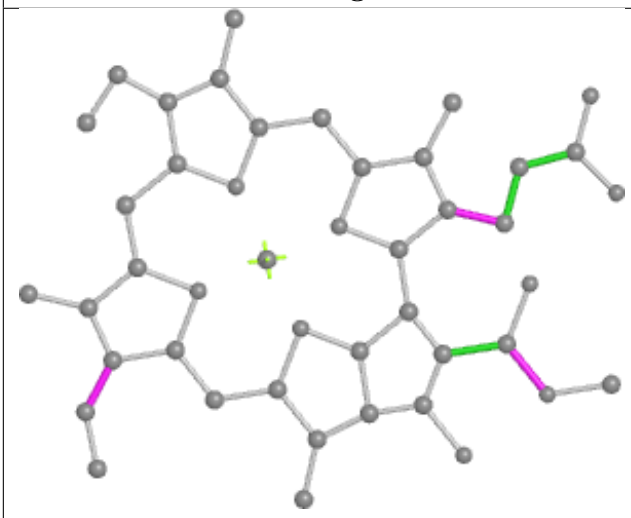
Ligand CLA Z 813



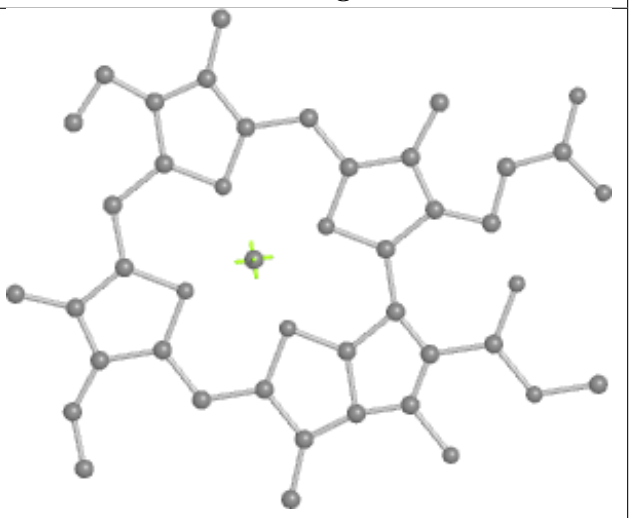
Bond lengths



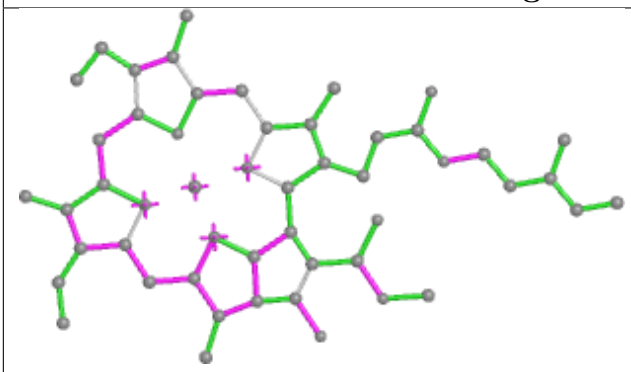
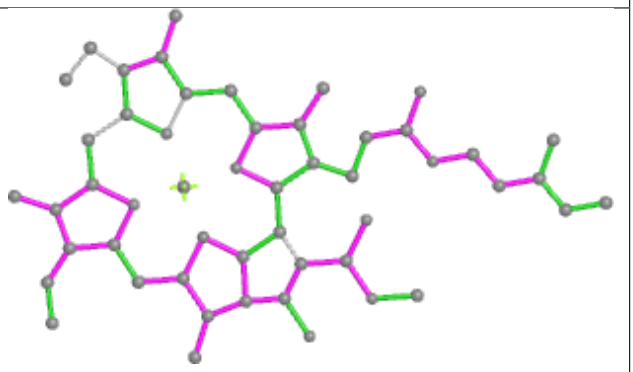
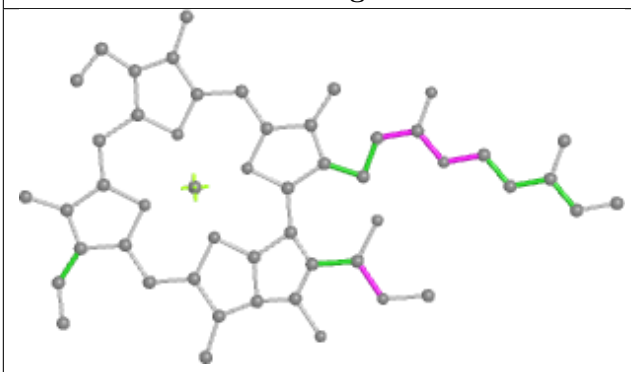
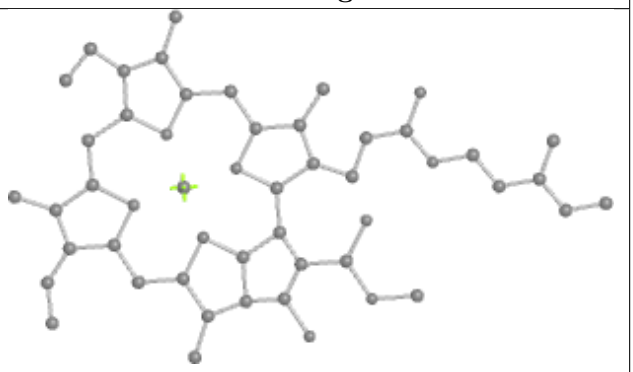
Bond angles



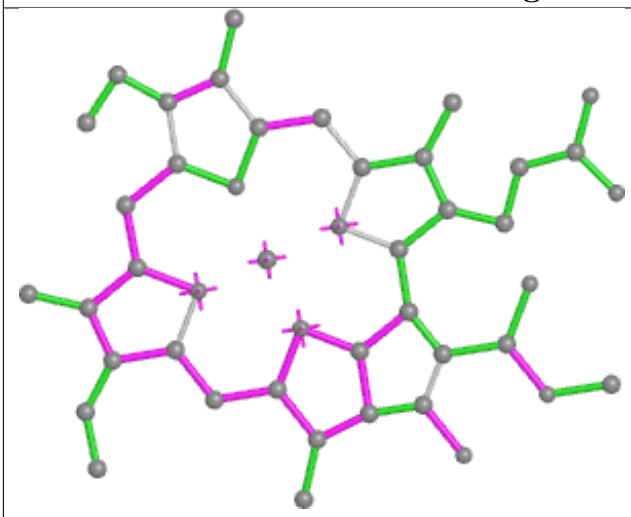
Torsions



Rings

Ligand CLA G 807	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA G 810



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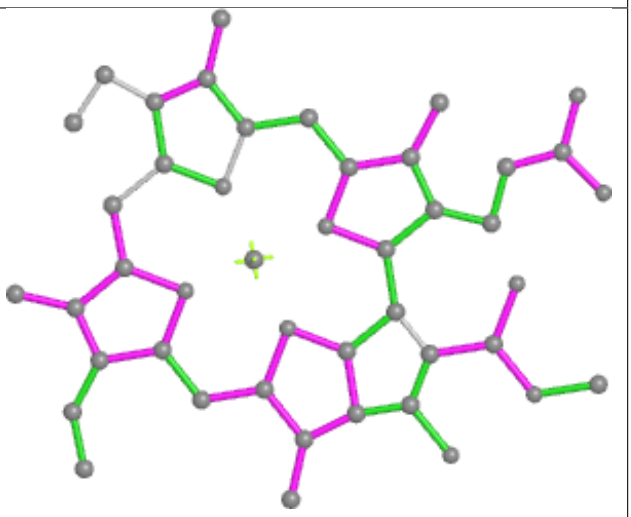
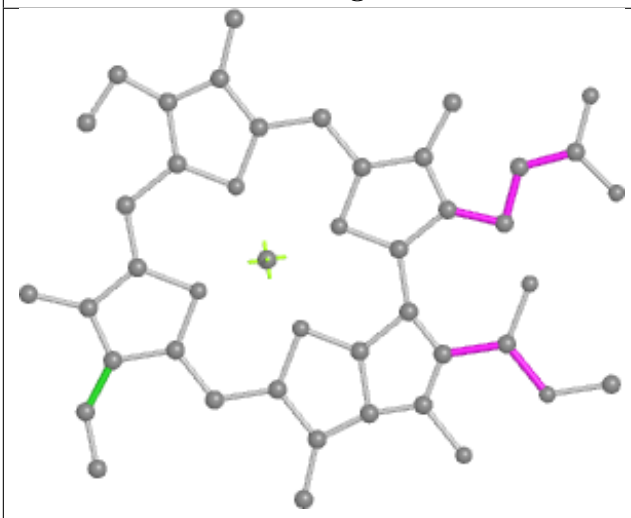


Bond angles



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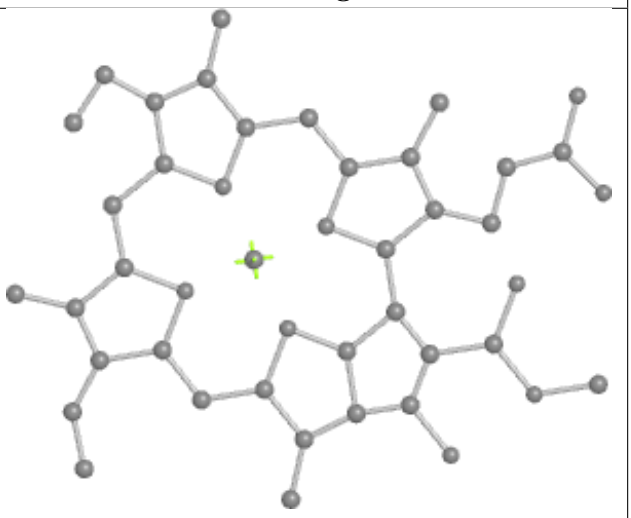
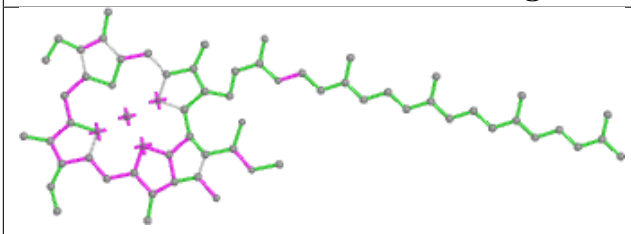


Rings

Ligand CLA A 809



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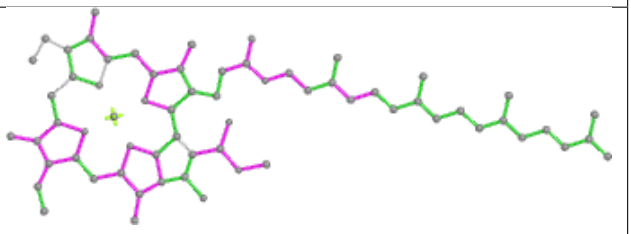
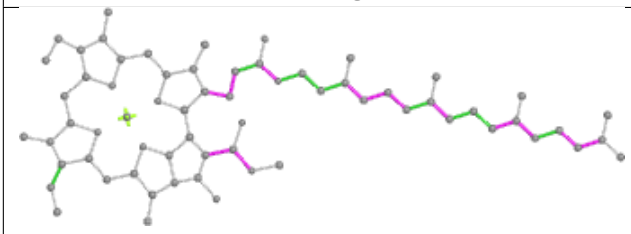


Bond angles



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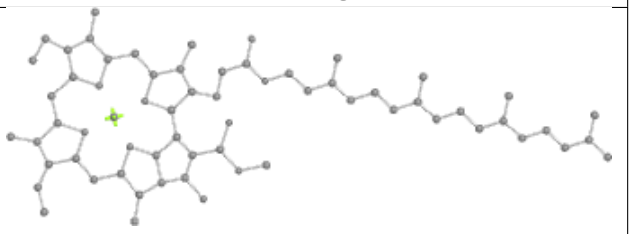
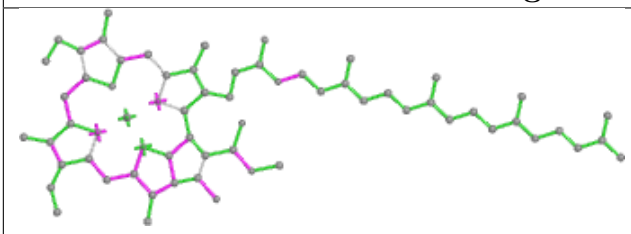


Rings

Ligand CLA A 837



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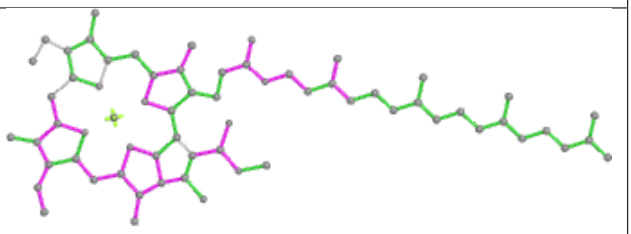
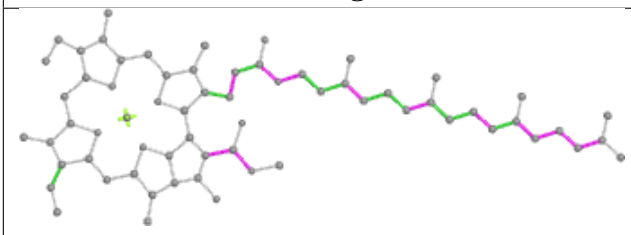


Bond angles



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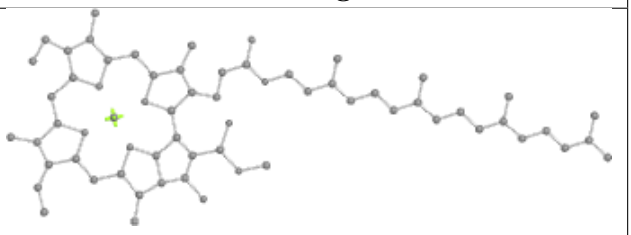
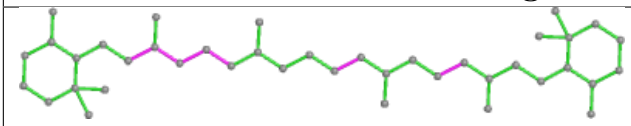


Rings

Ligand BCR R 102



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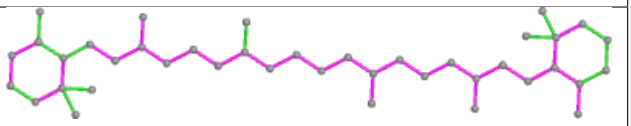
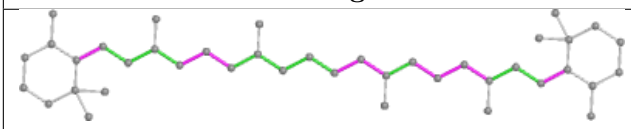


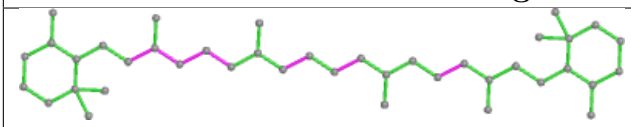
Bond angles



Torsions

Rings

Ligand BCR U 1009



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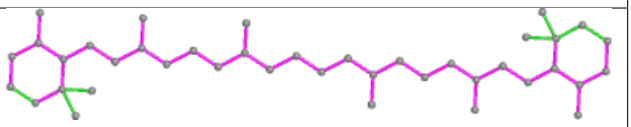
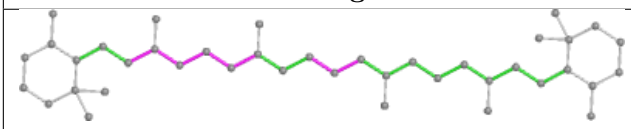
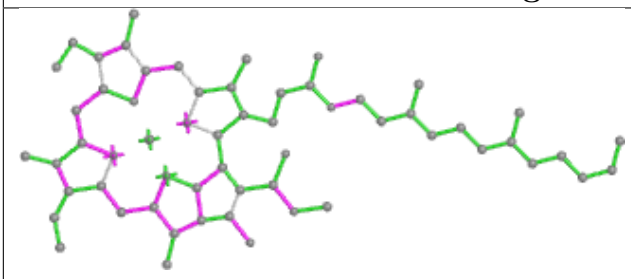
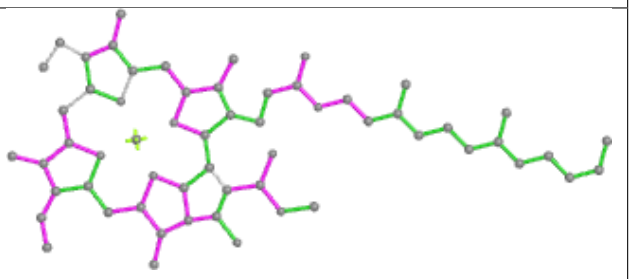
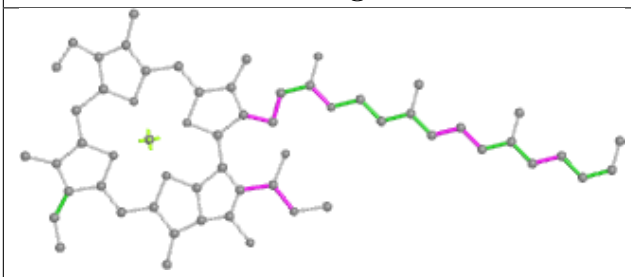
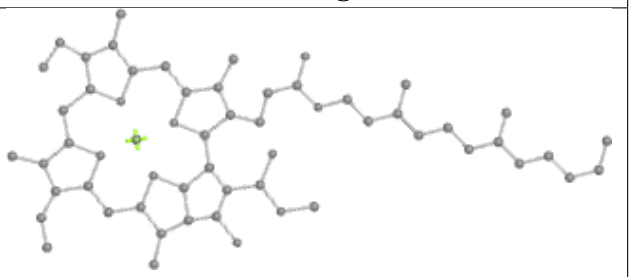


Bond angles



Torsions

Rings

Ligand CLA G 804	
 Bond lengths	 Bond angles
 Torsions	 Rings

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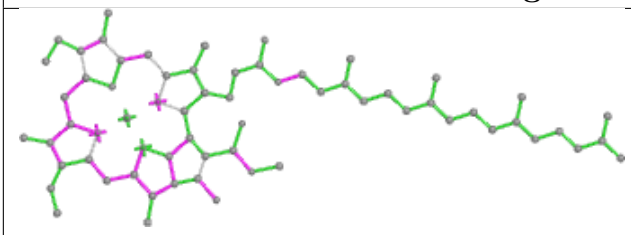
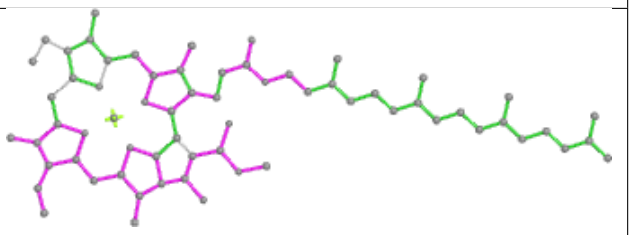
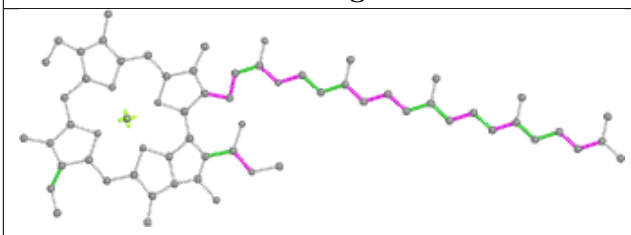
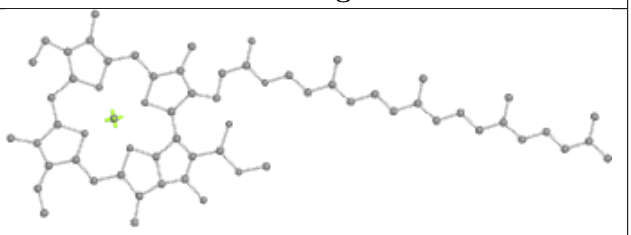
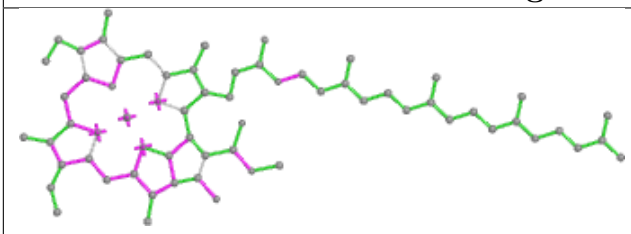
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA Z 828



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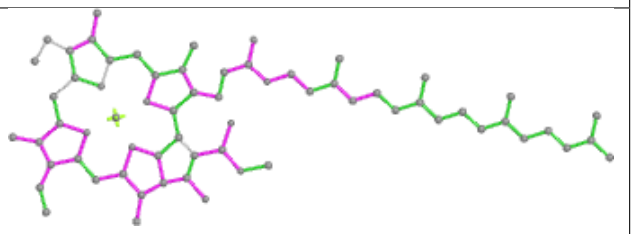
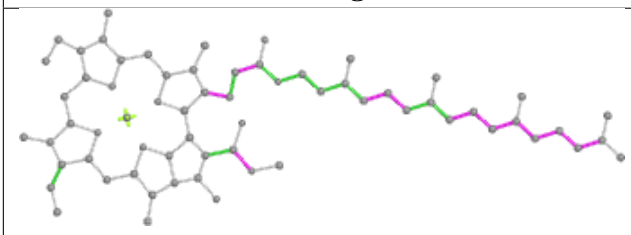


Bond angles



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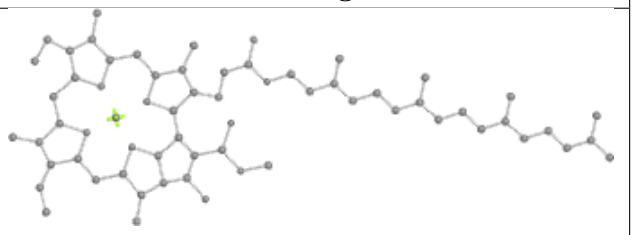
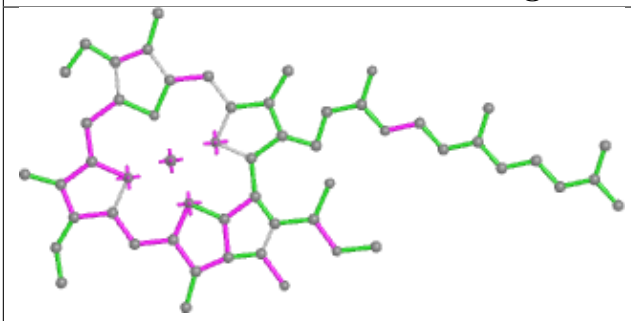


Rings

Ligand CLA Y 814



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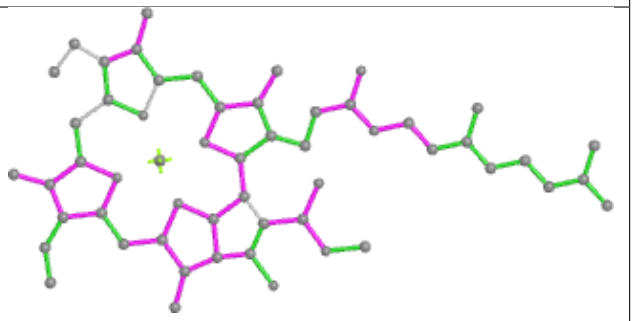
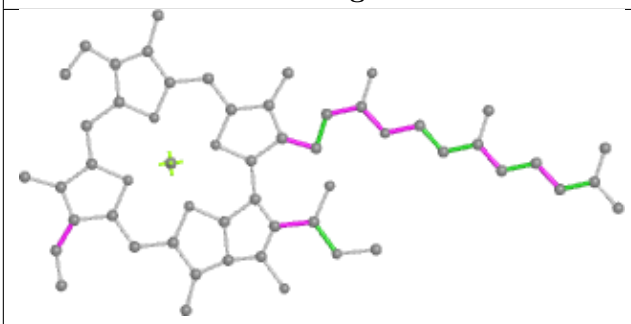


Bond angles



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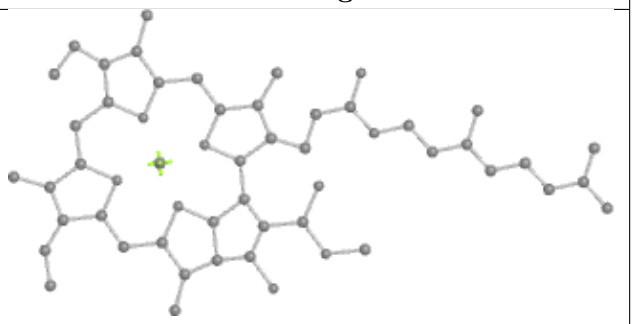
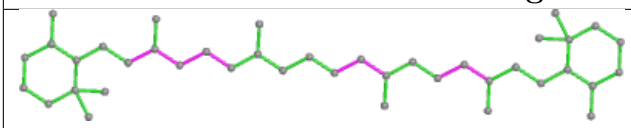


Rings

Ligand BCR J 104



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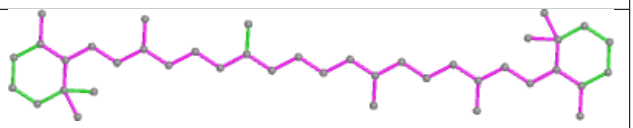

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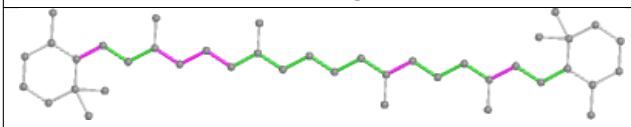

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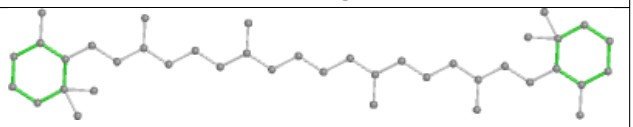
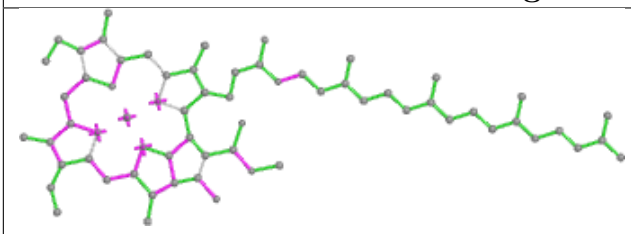
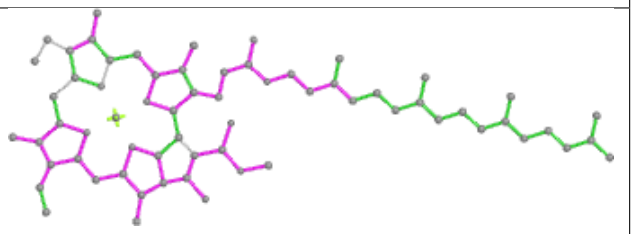
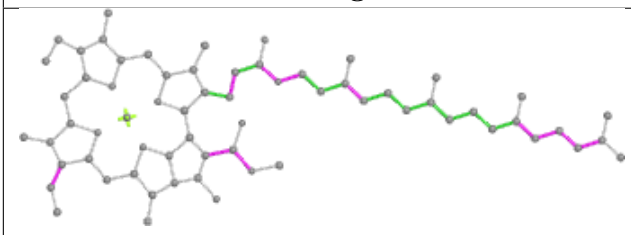
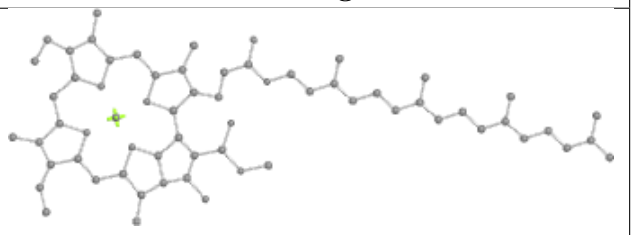


Rings

Ligand CLA H 810	
 Bond lengths	 Bond angles
 Torsions	 Rings

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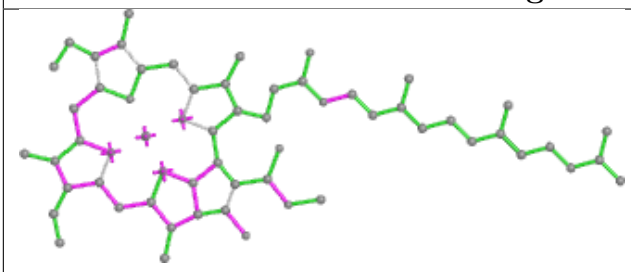
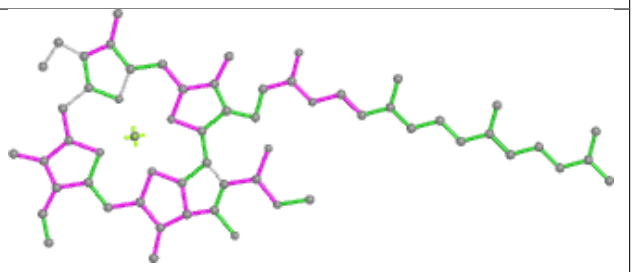
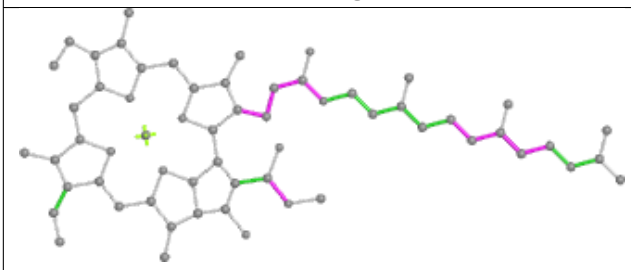
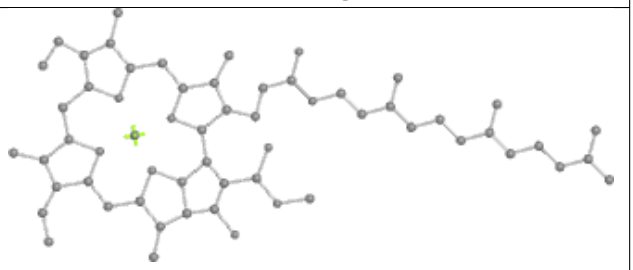
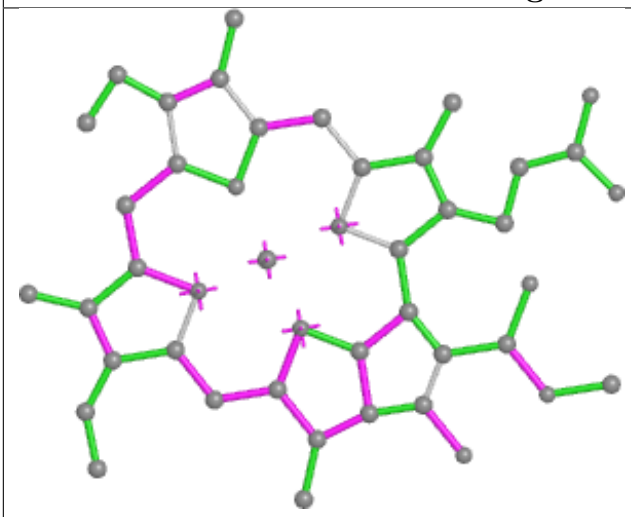
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA Z 821



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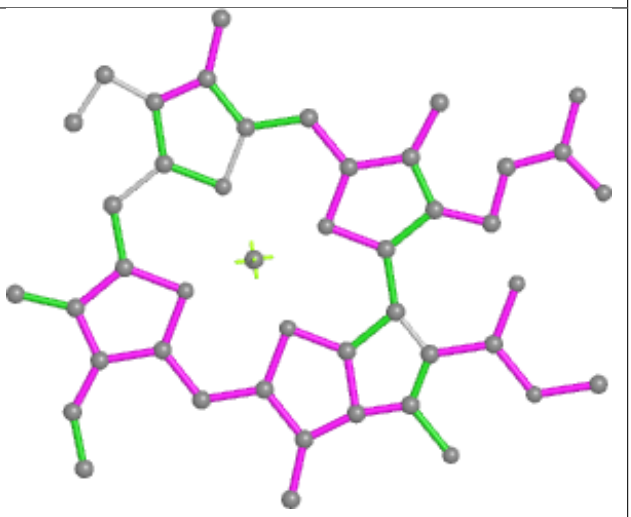

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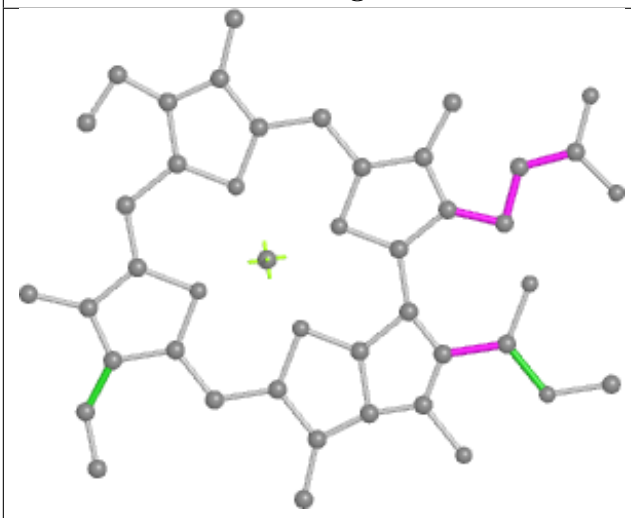

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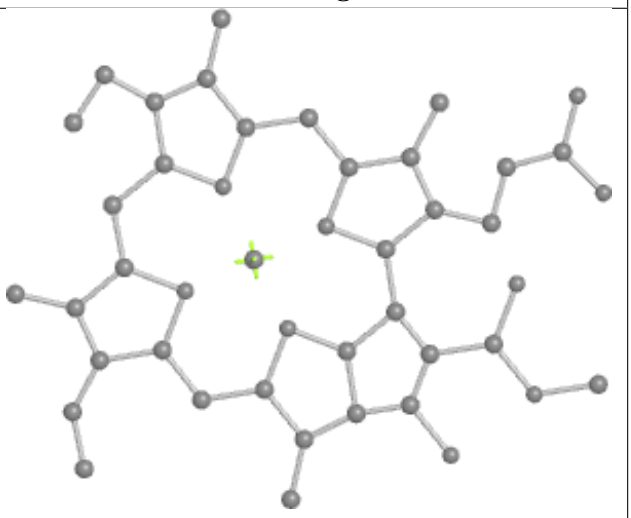
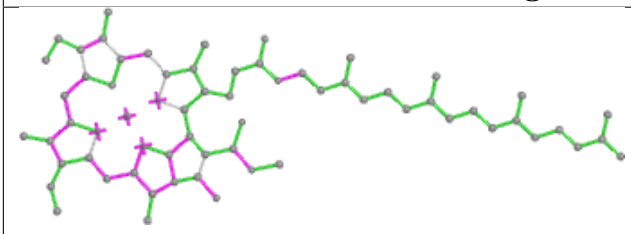


Rings

Ligand CLA A 810



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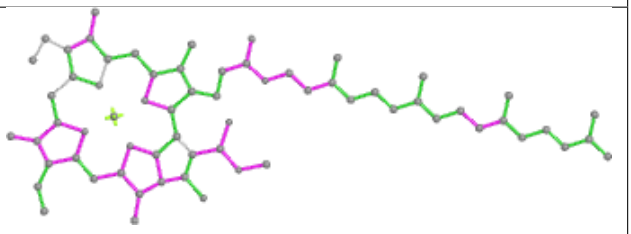

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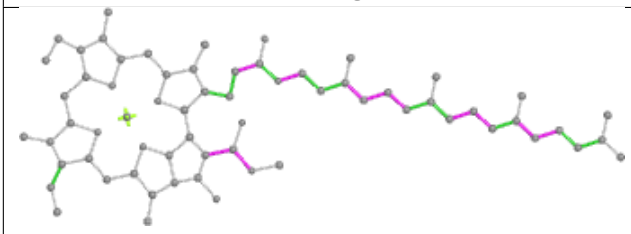

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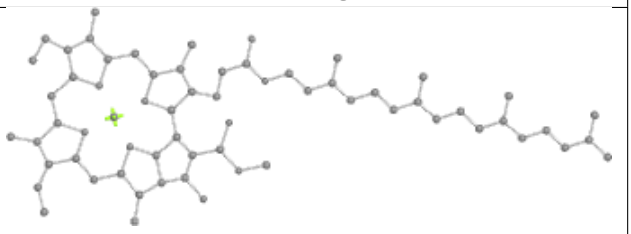
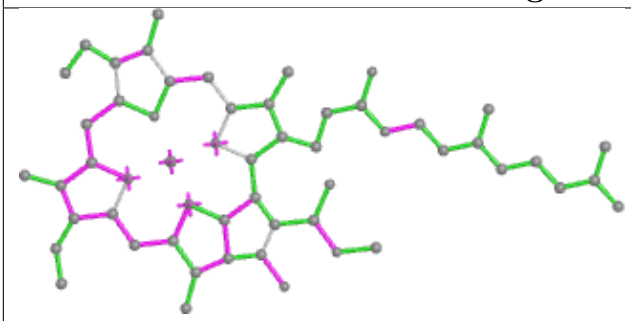


Rings

Ligand CLA Z 825



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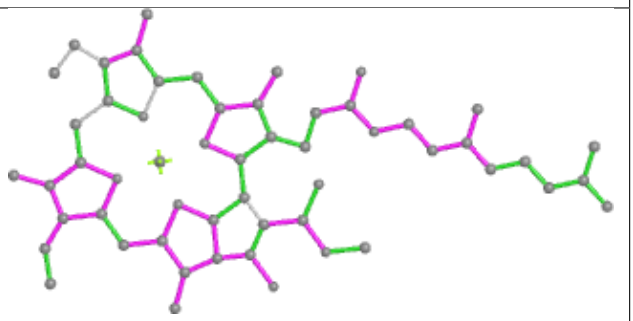

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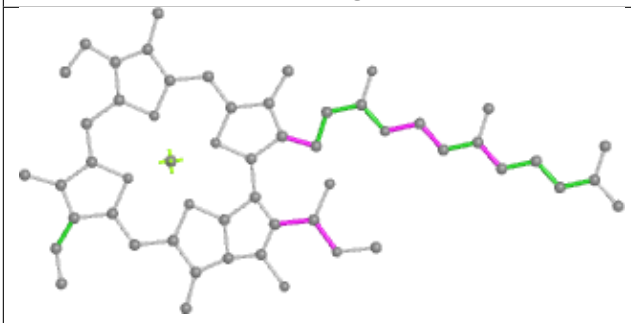

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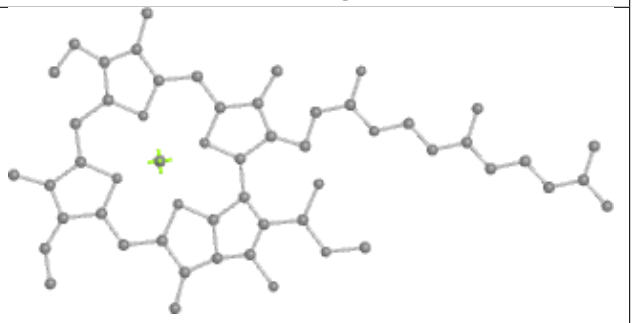
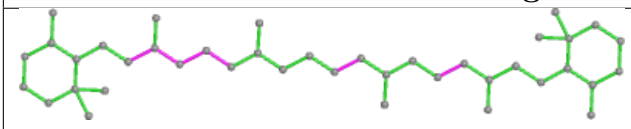


Rings

Ligand BCR B 843



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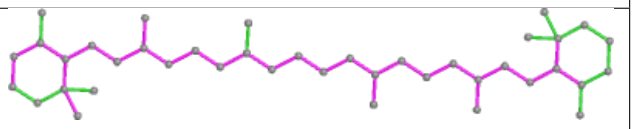

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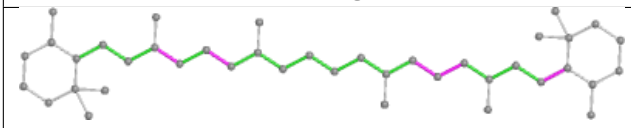
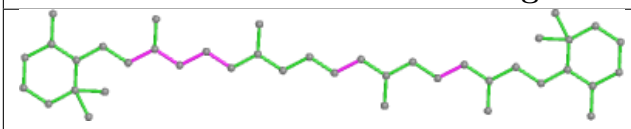


Torsions

Rings

Ligand BCR G 846



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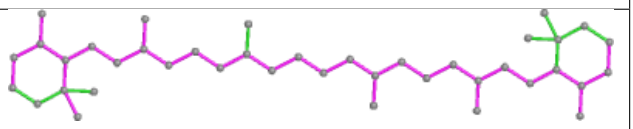

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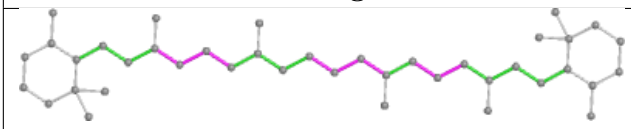
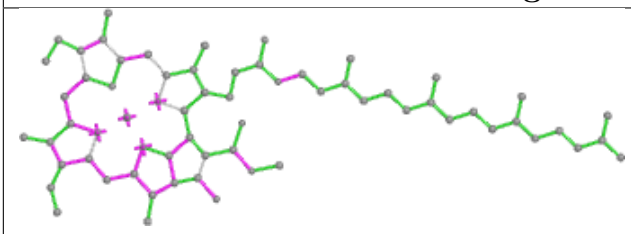


Torsions

Rings

Ligand CLA H 813



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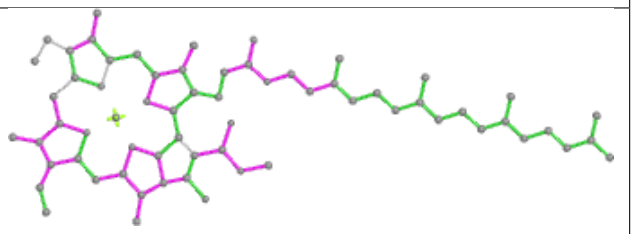

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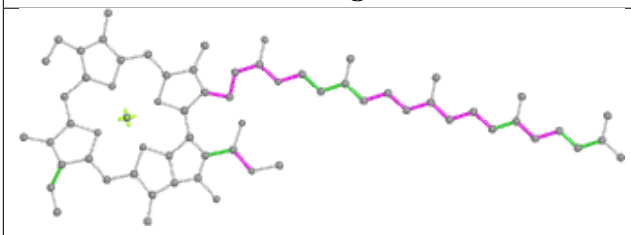

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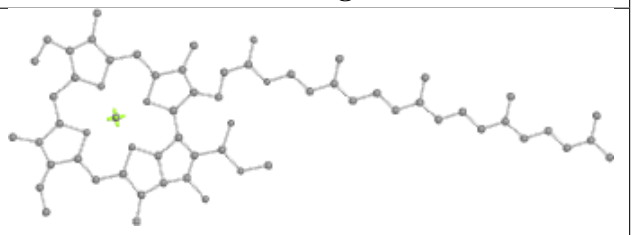
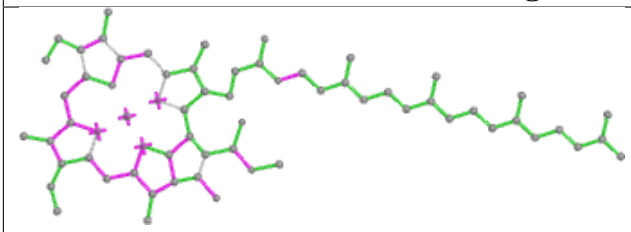


Rings

Ligand CLA Y 808



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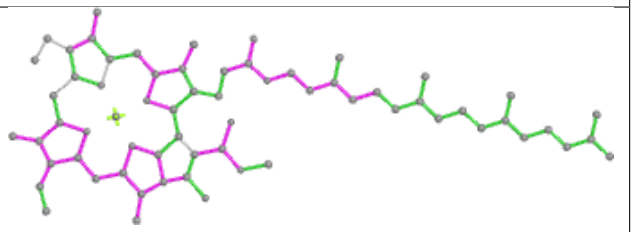

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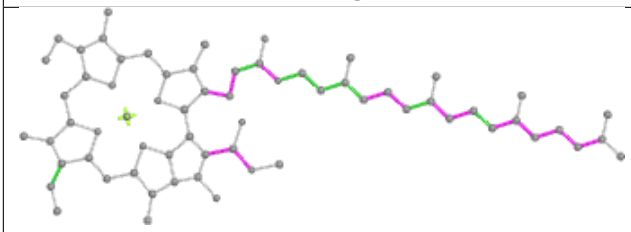

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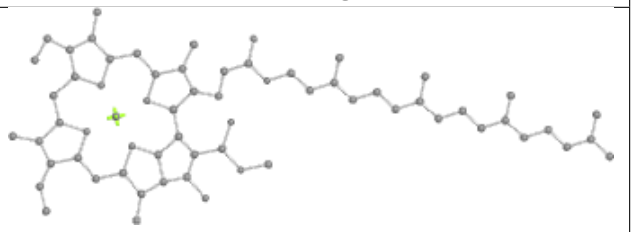
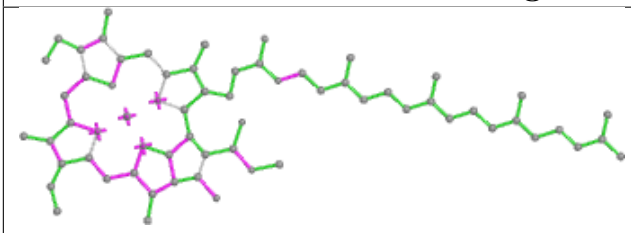


Rings

Ligand CLA A 842



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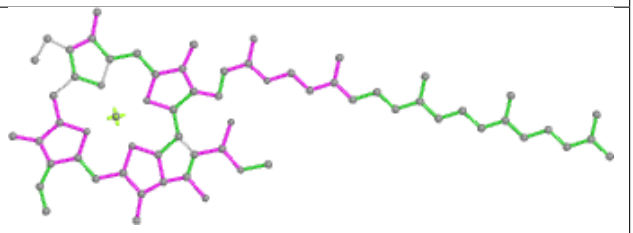

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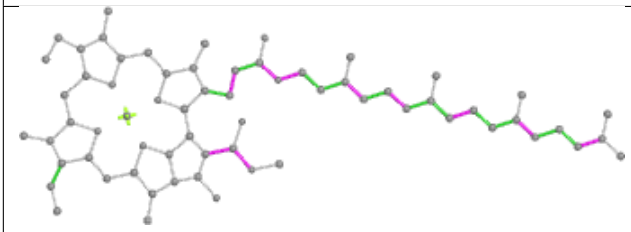

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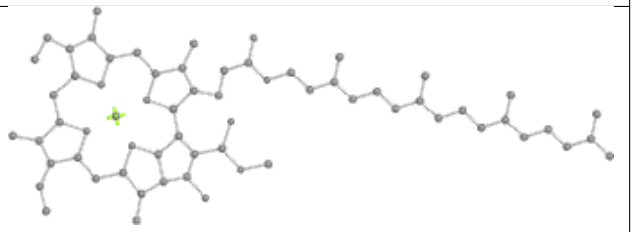
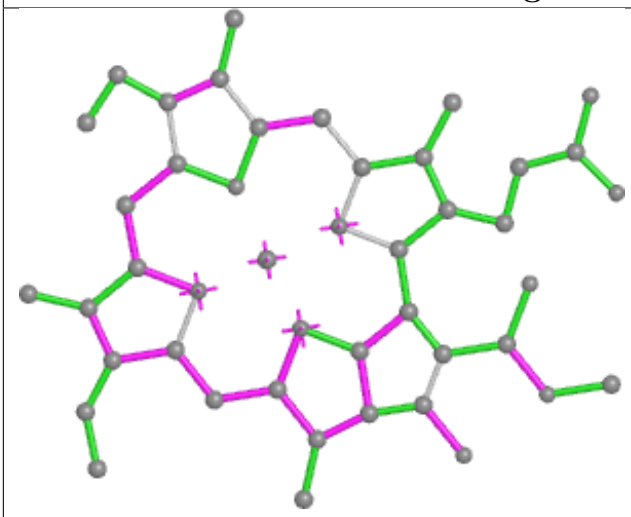


Rings

Ligand CLA A 811



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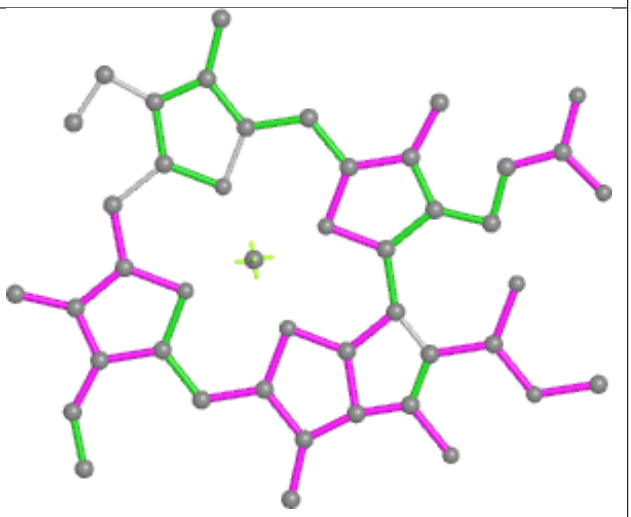

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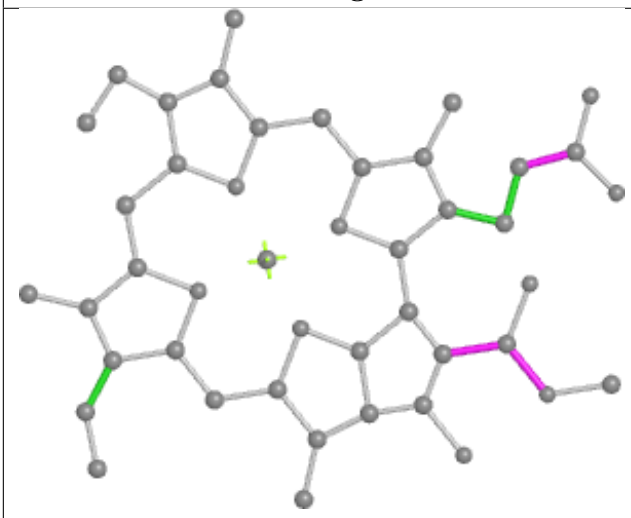

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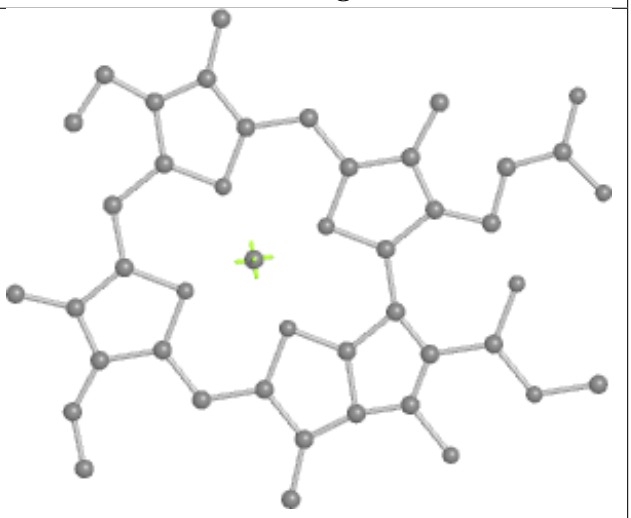
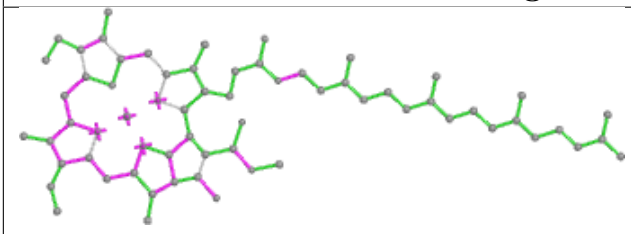


Rings

Ligand CLA Y 827



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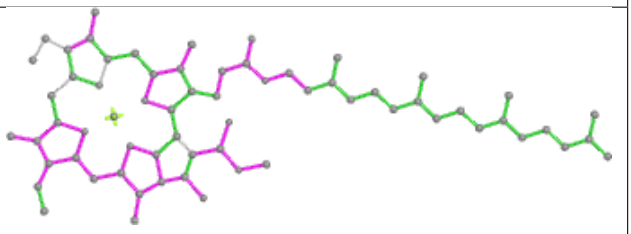

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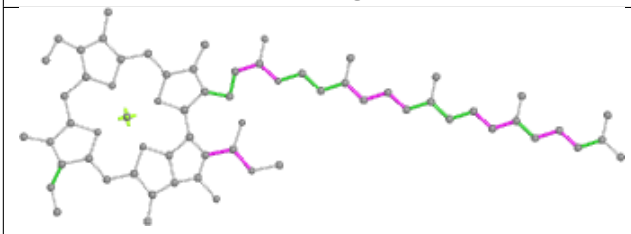

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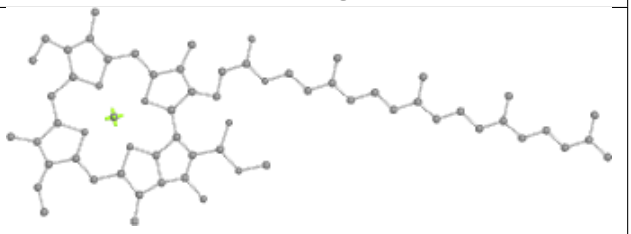
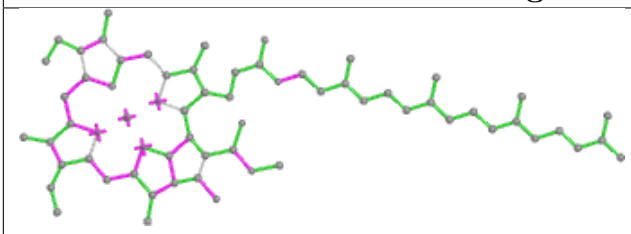


Rings

Ligand CLA Z 809



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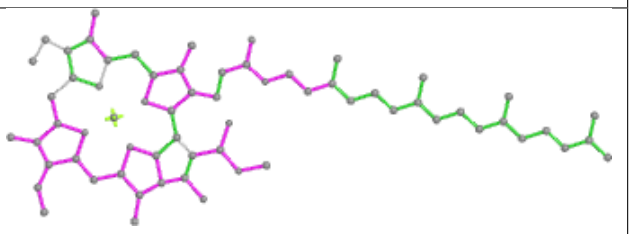
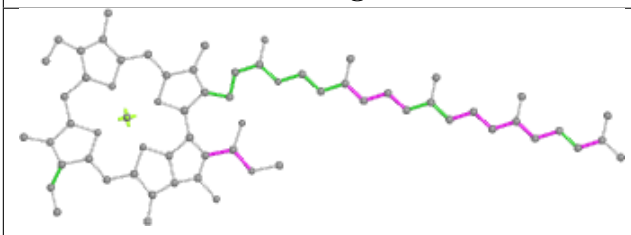
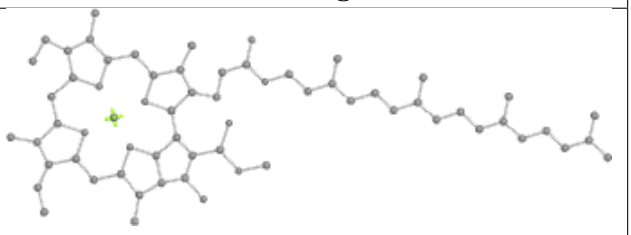


Bond angles

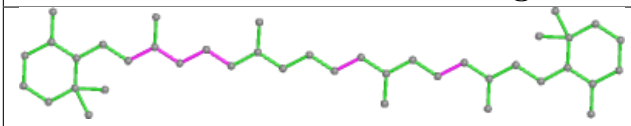


Torsions



Rings

Ligand BCR U 1005



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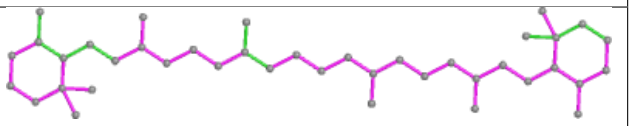
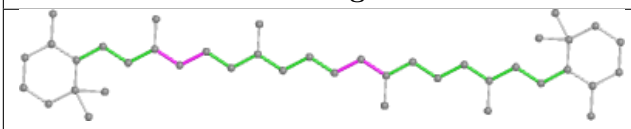


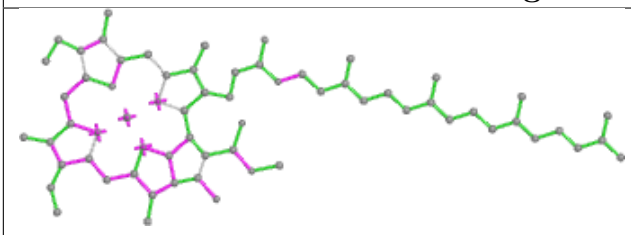
Bond angles



Torsions

Rings

Ligand CLA H 806



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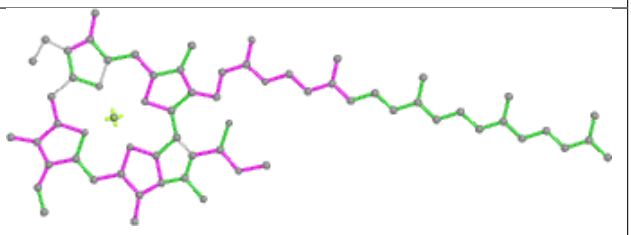

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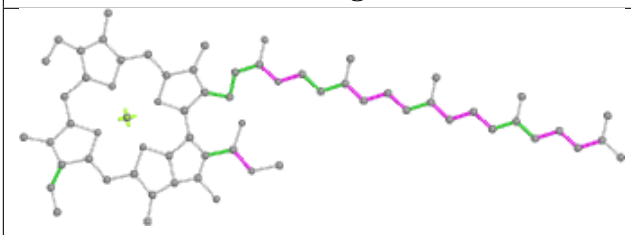
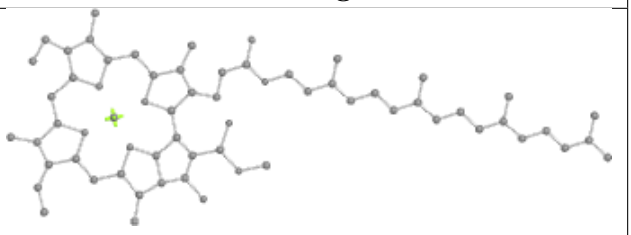
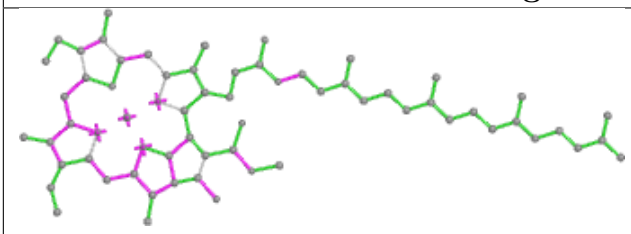
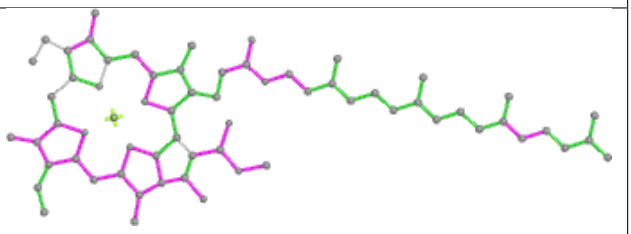
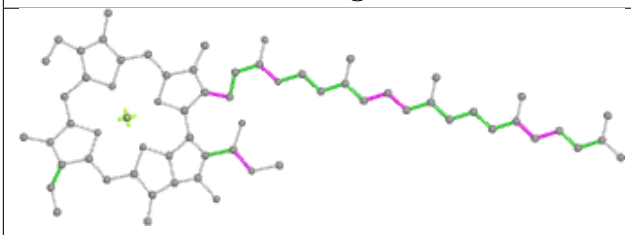
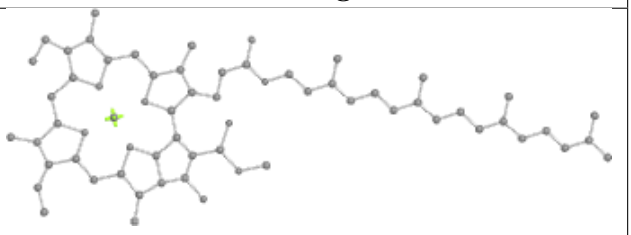
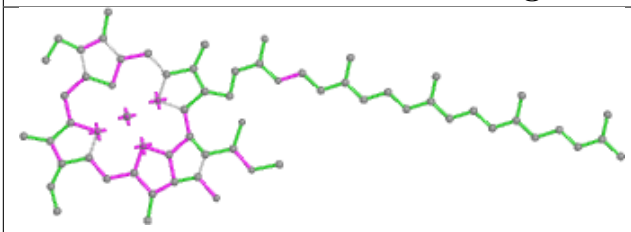
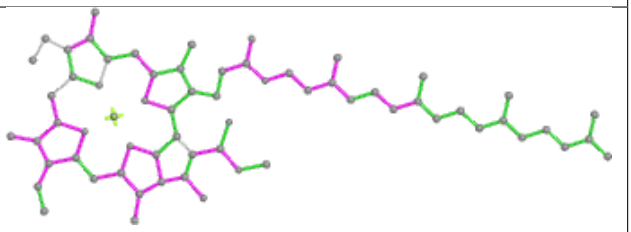
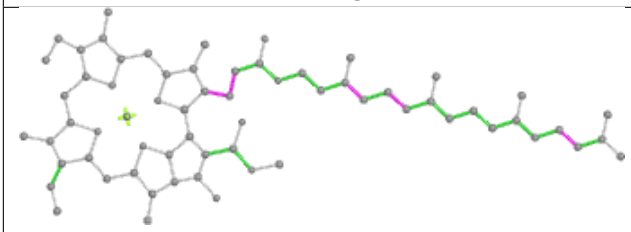
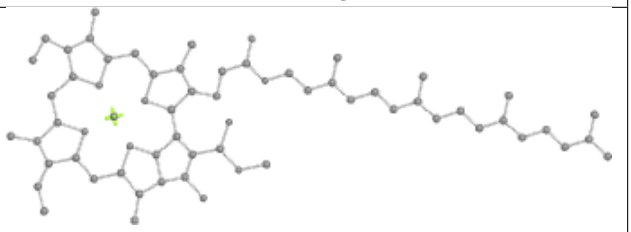


Torsions



Rings

Ligand CLA G 828	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA H 828	
 Bond lengths	 Bond angles
 Torsions	 Rings

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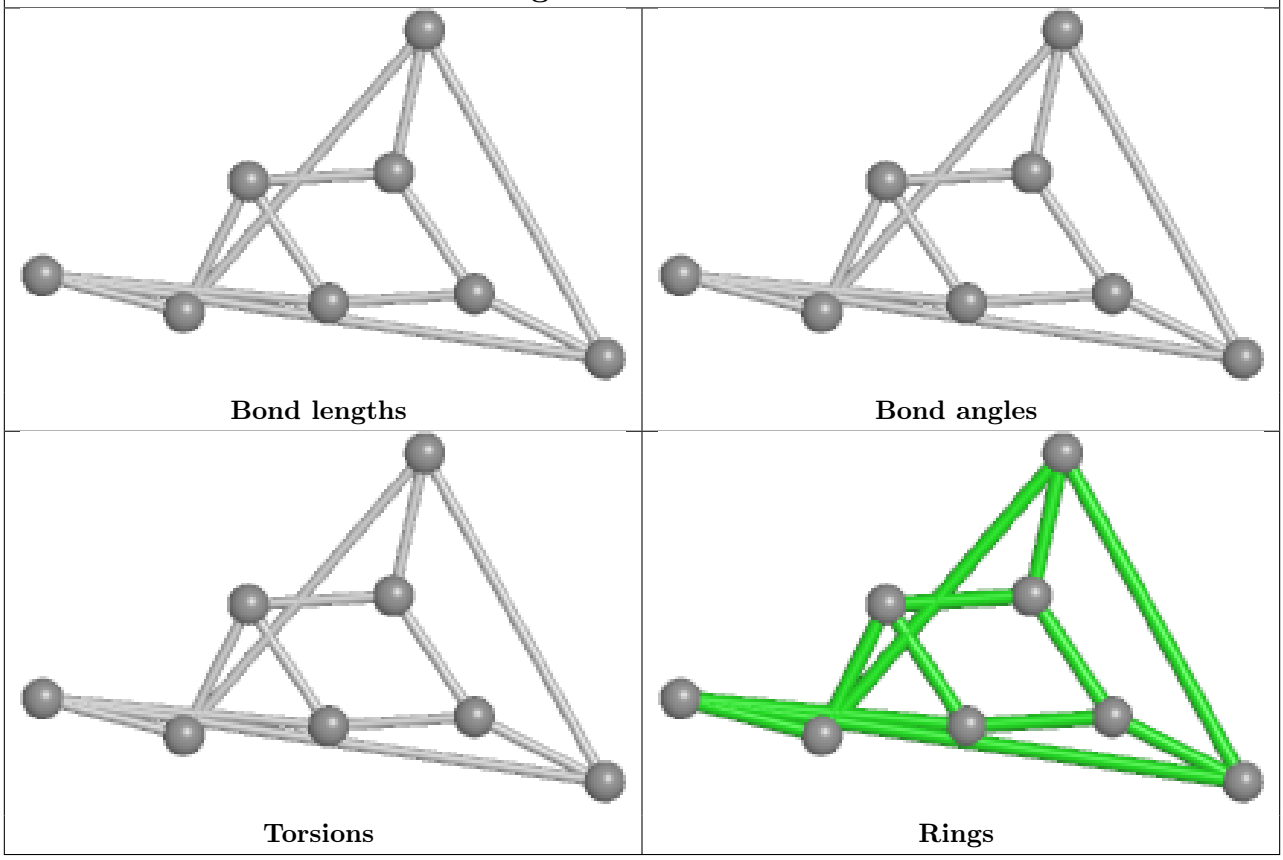
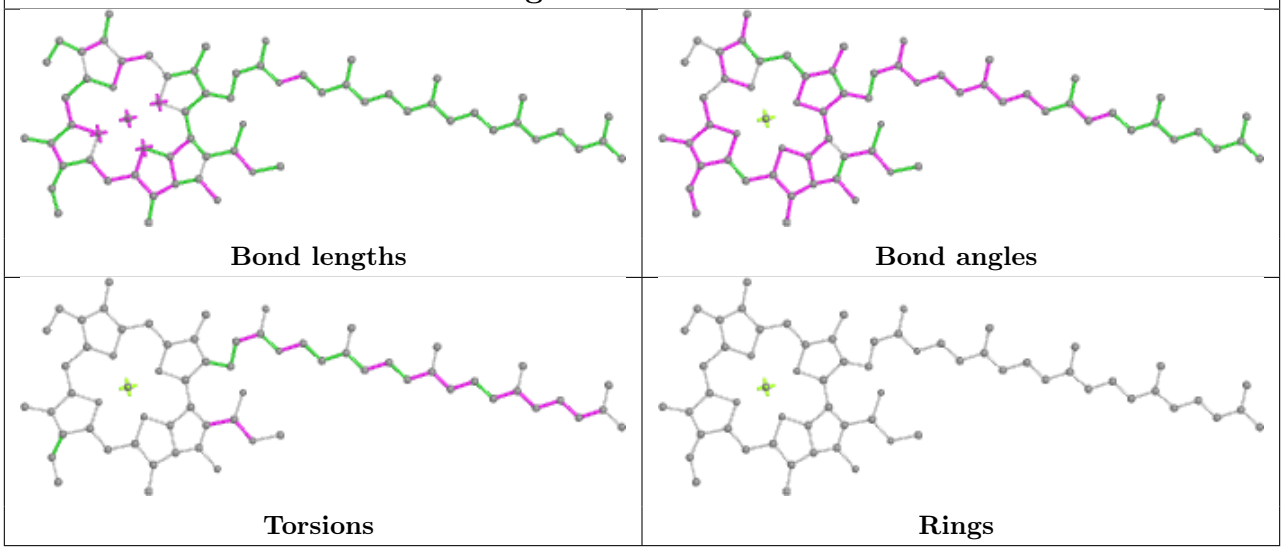
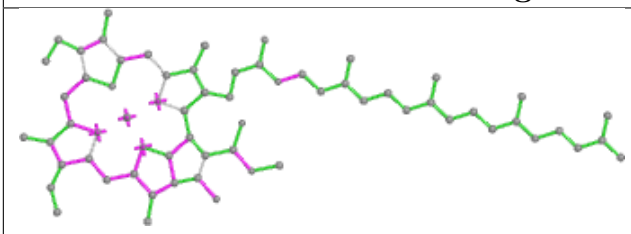


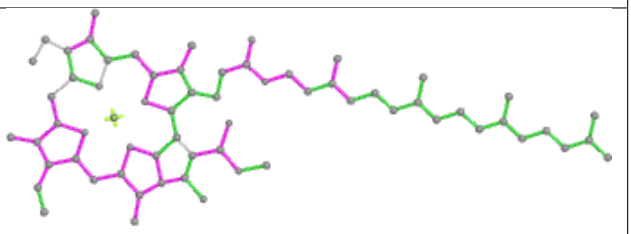
Ligand CLA B 808



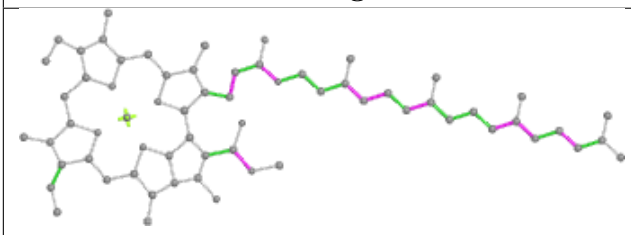
Ligand CLA U 1006



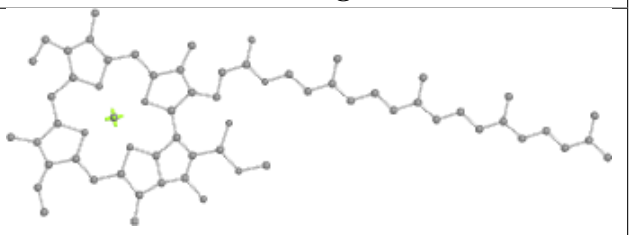
Bond lengths



Bond angles

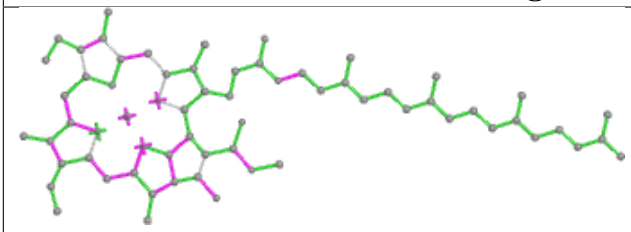


Torsions



Rings

Ligand CLA Z 830



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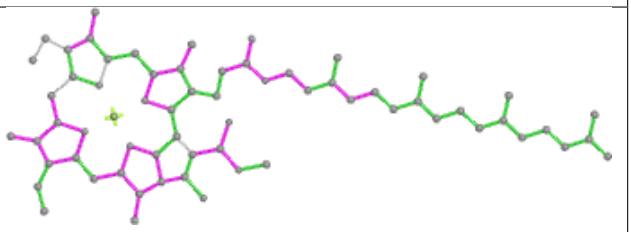
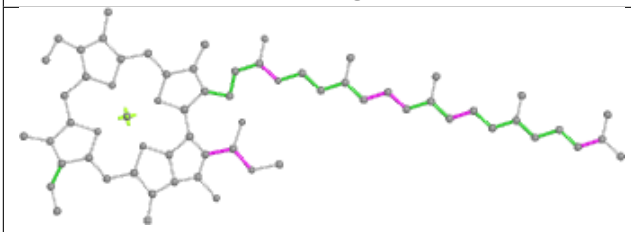


Bond angles



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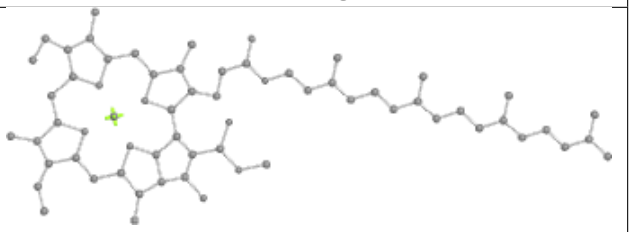
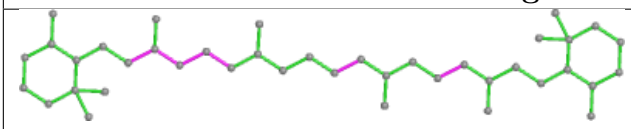


Rings

Ligand BCR Y 849



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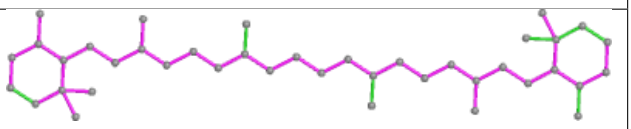

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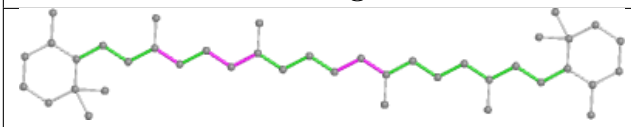
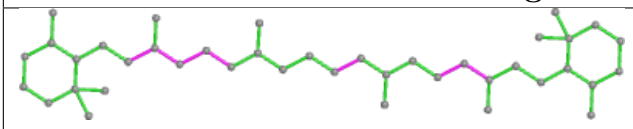


Torsions

Rings

Ligand BCR L 207



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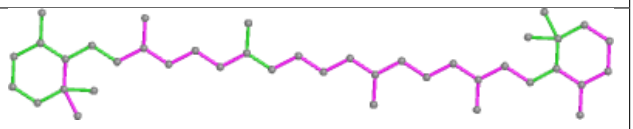

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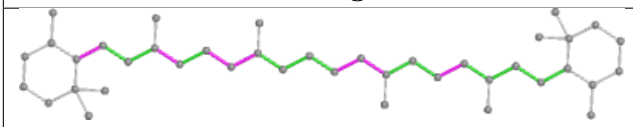

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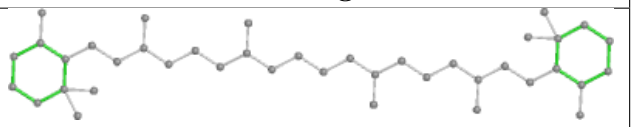
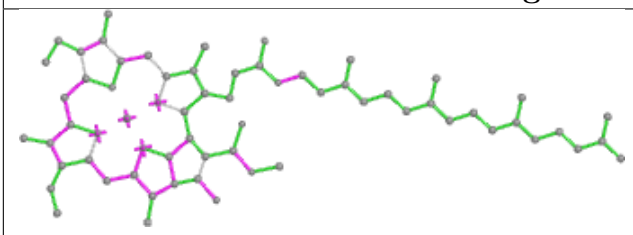


Rings

Ligand CLA G 808



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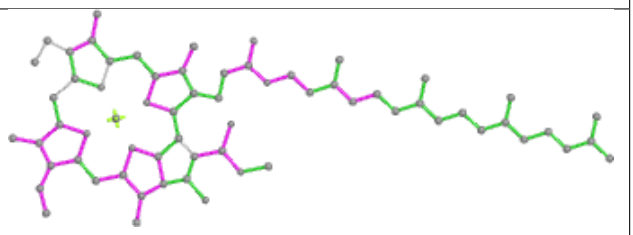

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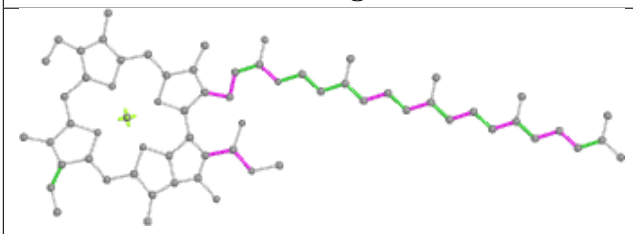

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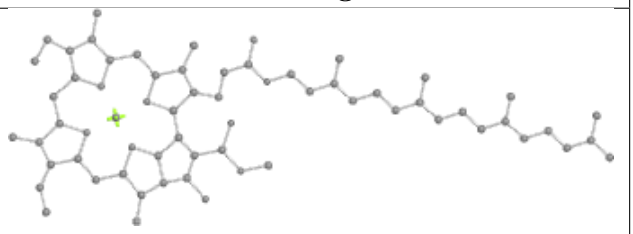
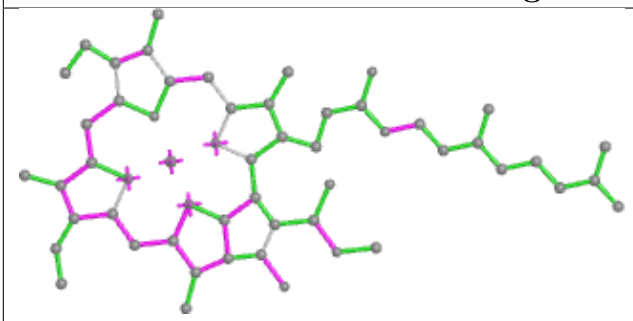


Rings

Ligand CLA H 824



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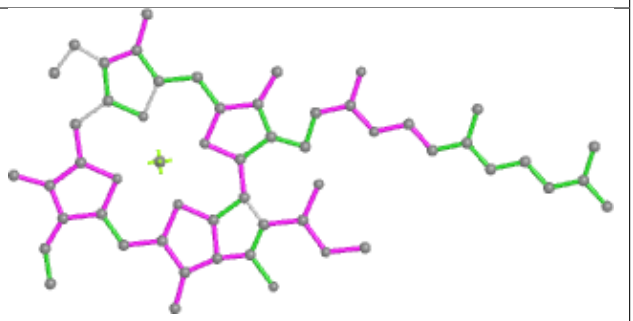

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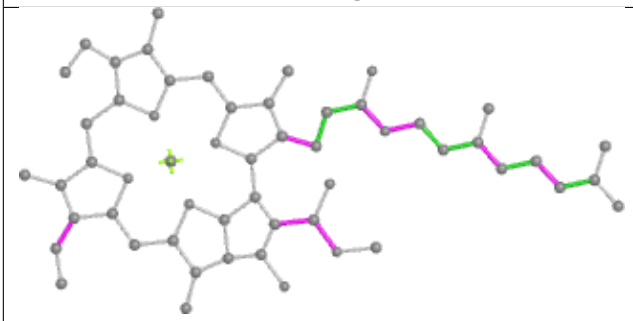

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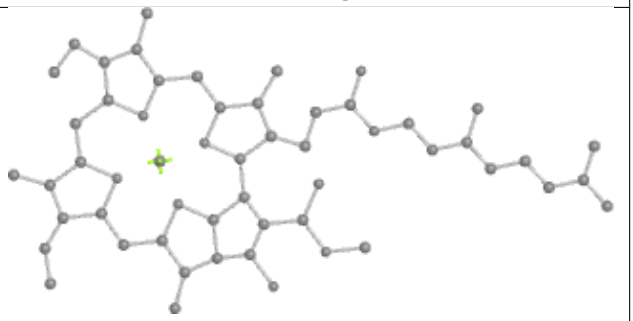
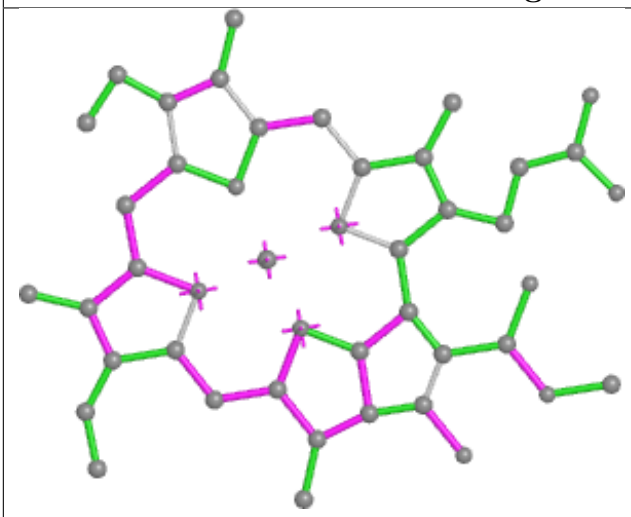


Rings

Ligand CLA T 103



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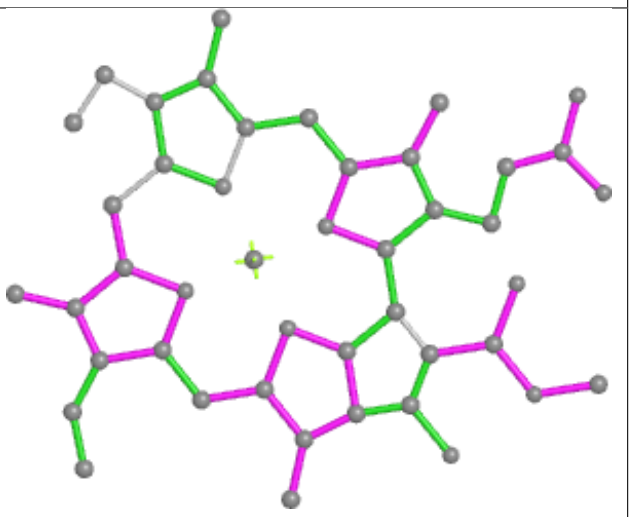

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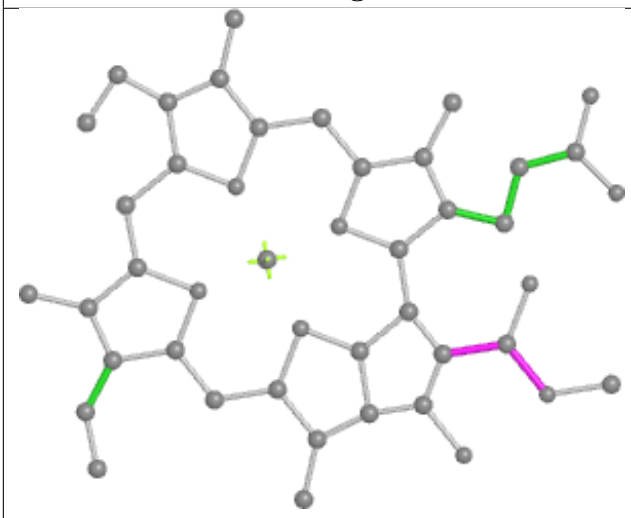

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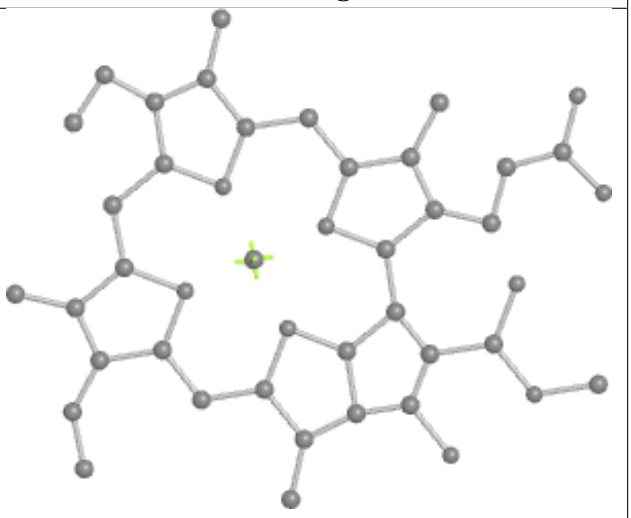
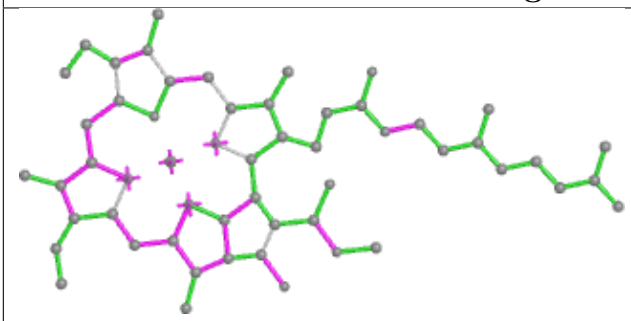


Rings

Ligand CLA B 832



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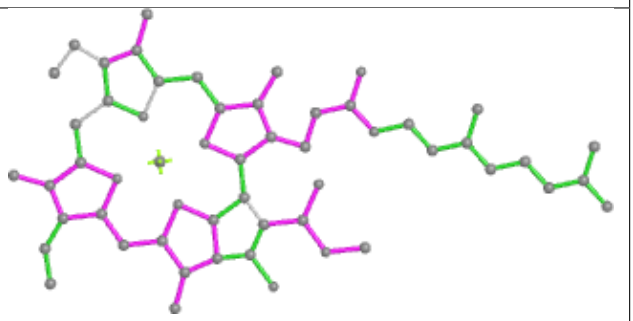

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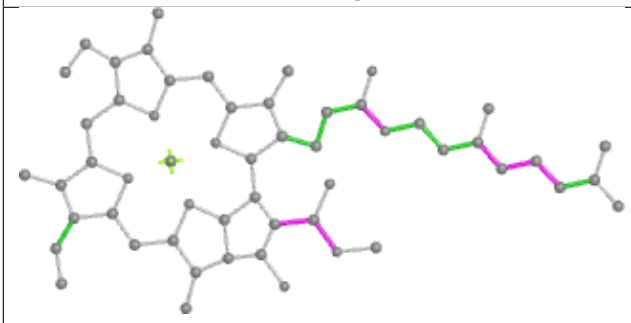

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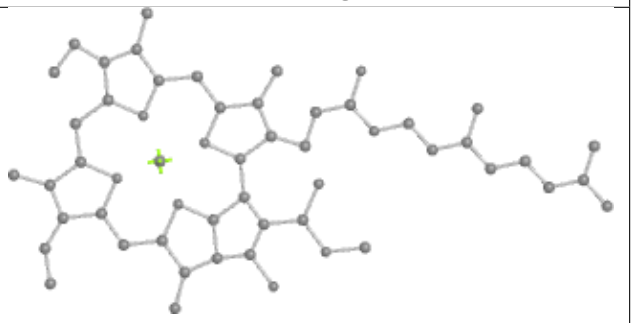
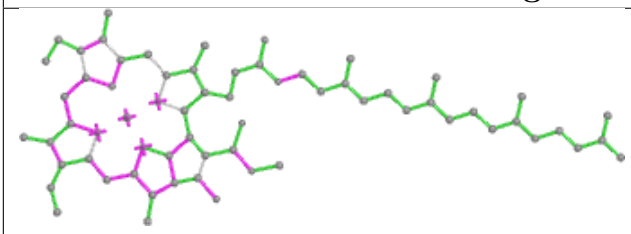


Rings

Ligand CLA H 803



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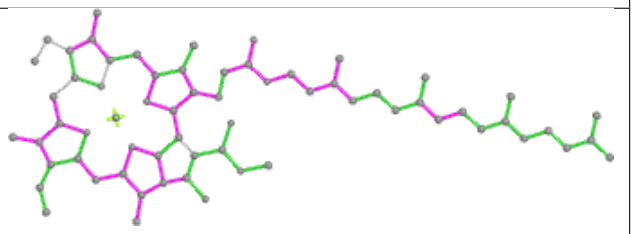

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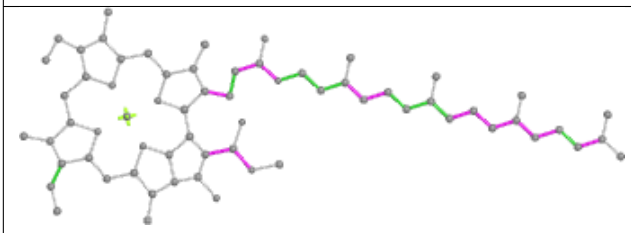

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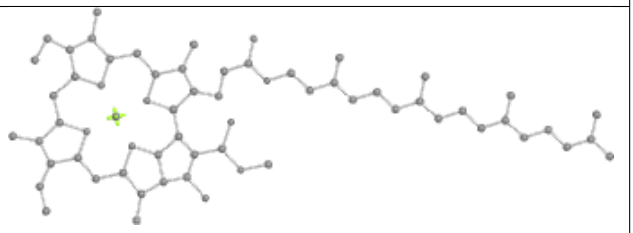
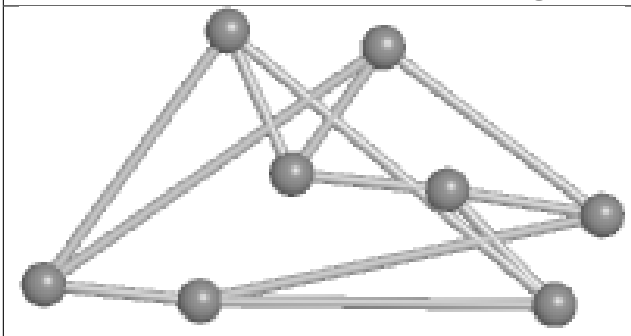


Rings

Ligand SF4 N 102



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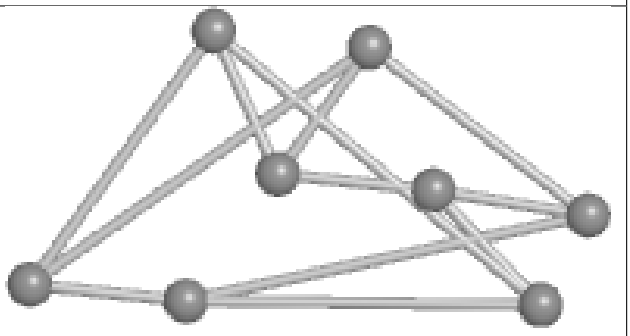
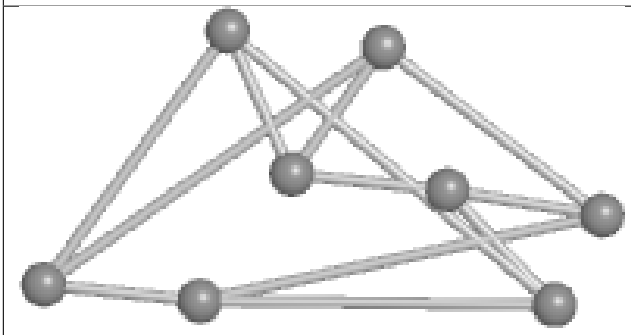


Bond angles



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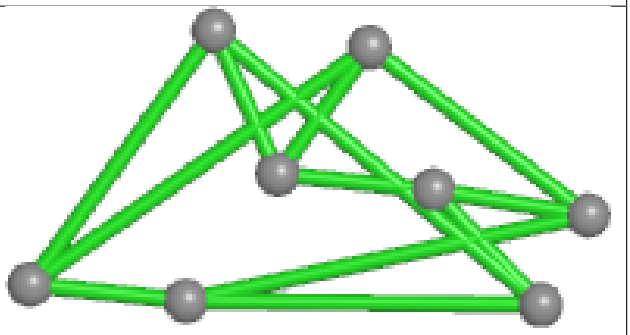
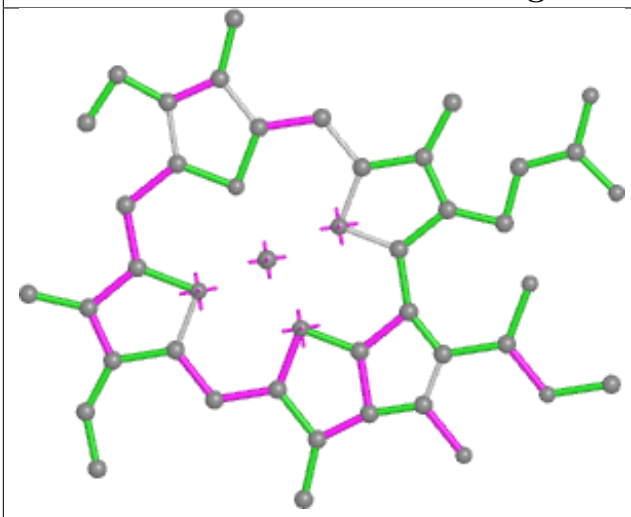


Rings

Ligand CLA d 202



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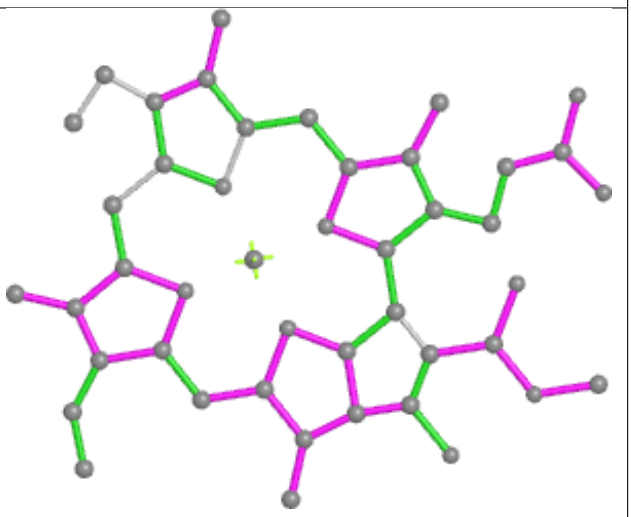
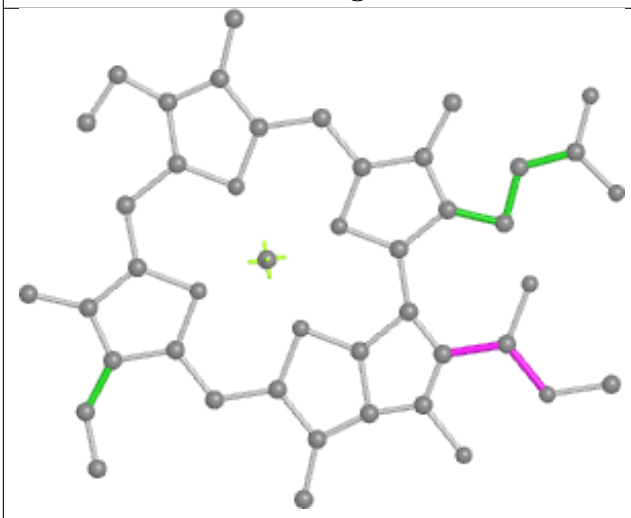


Bond angles



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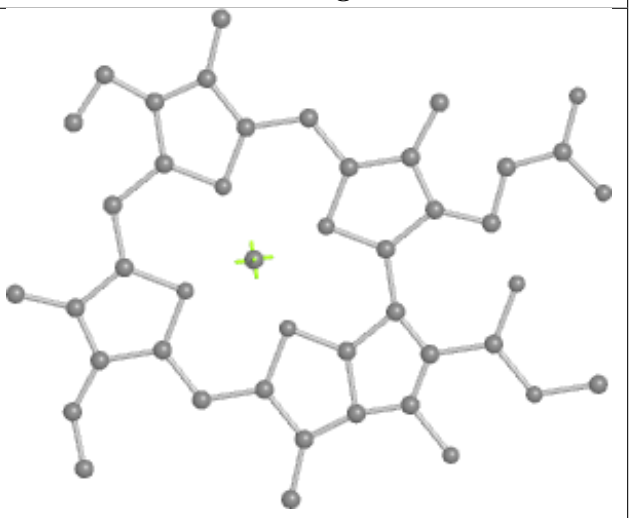
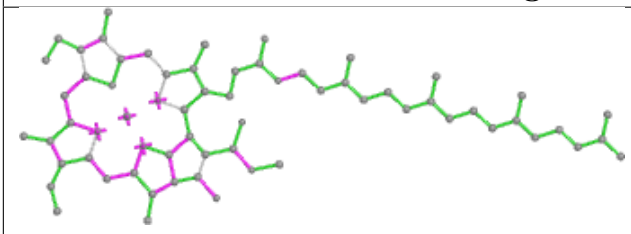
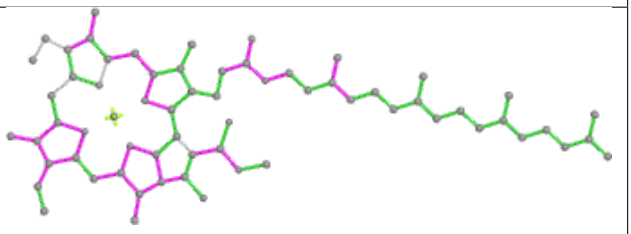


Rings

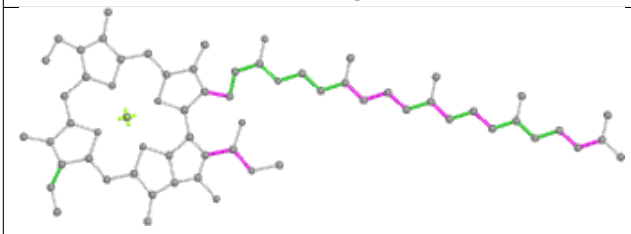
Ligand CLA H 827



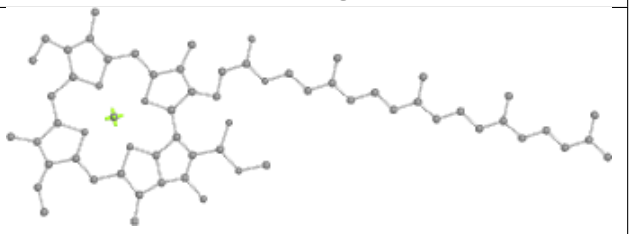
Bond lengths



Bond angles

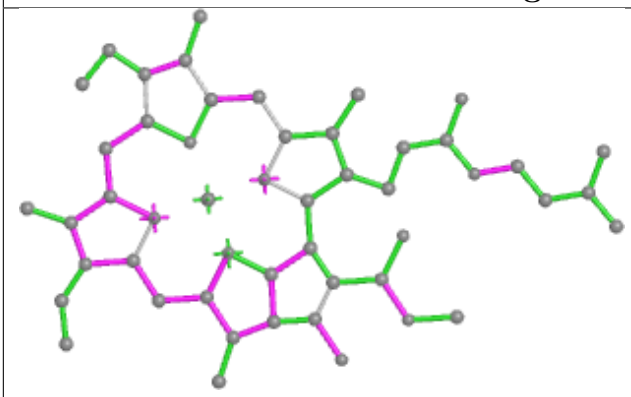


Torsions



Rings

Ligand CLA Y 815



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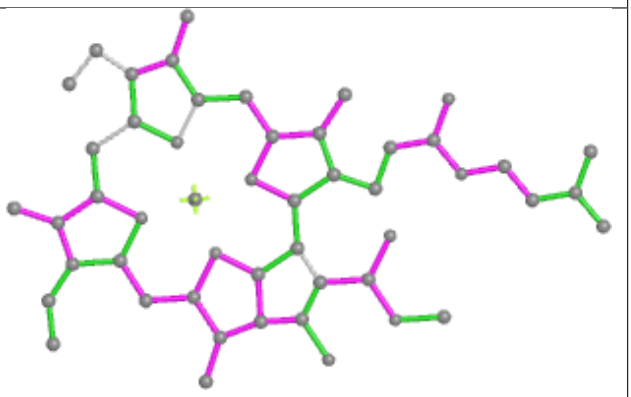

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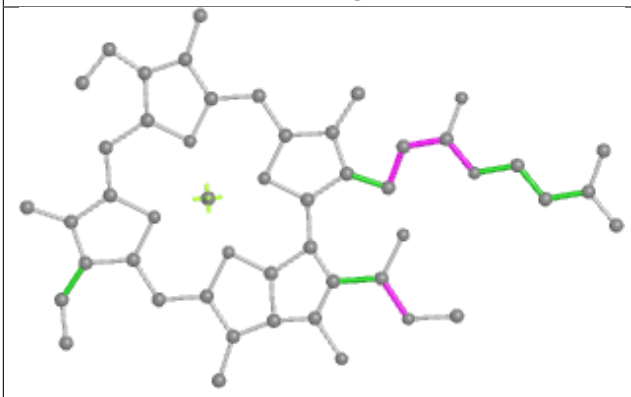

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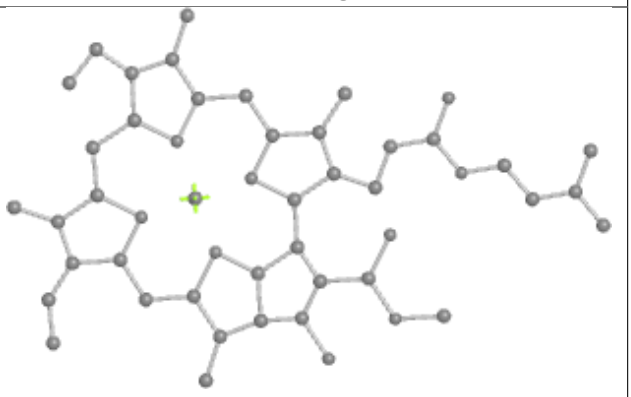
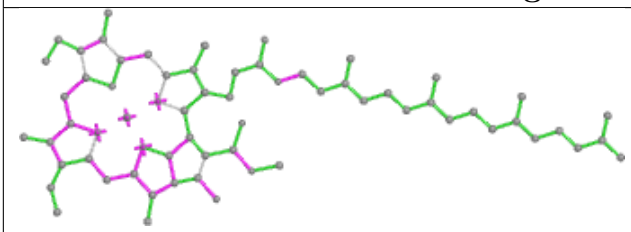


Rings

Ligand CLA A 828



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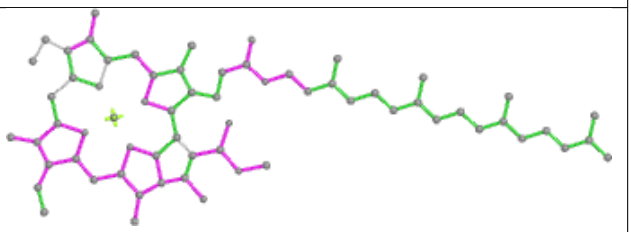
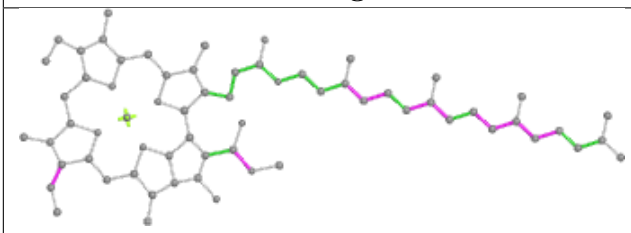


Bond angles



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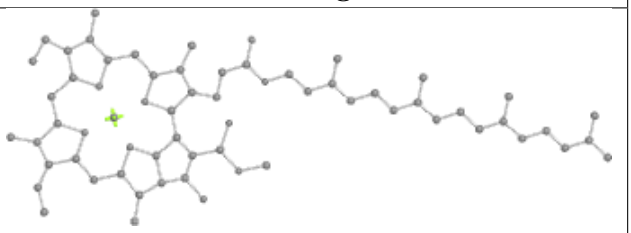
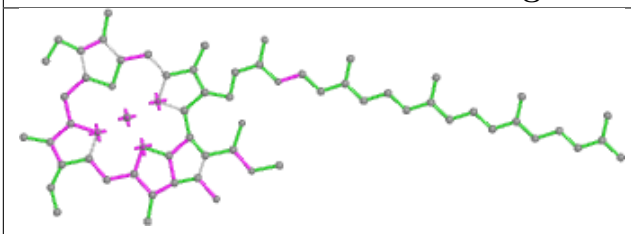


Rings

Ligand CLA G 809



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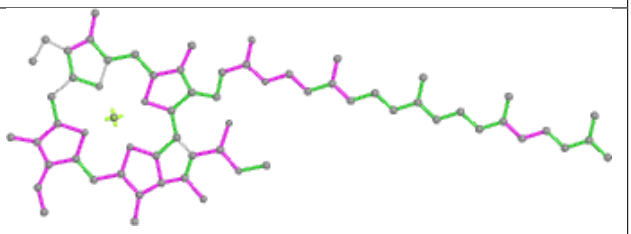
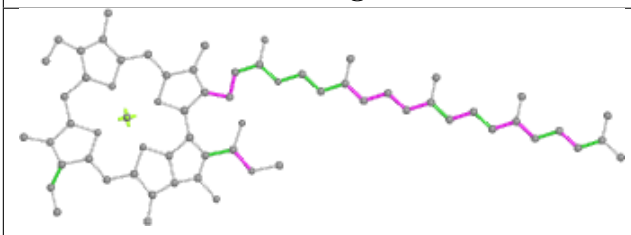


Bond angles



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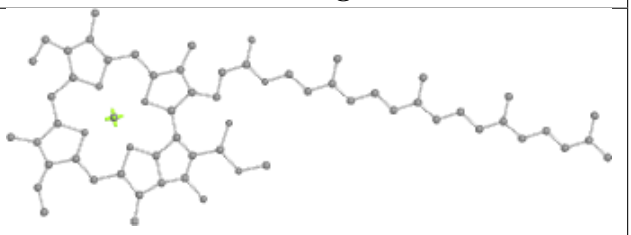
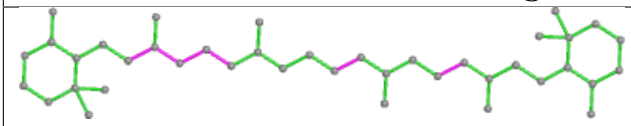


Rings

Ligand BCR T 102



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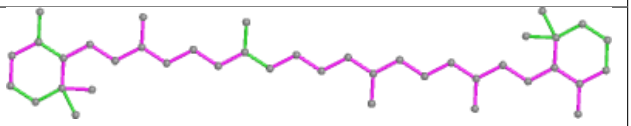
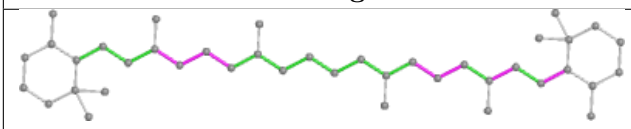


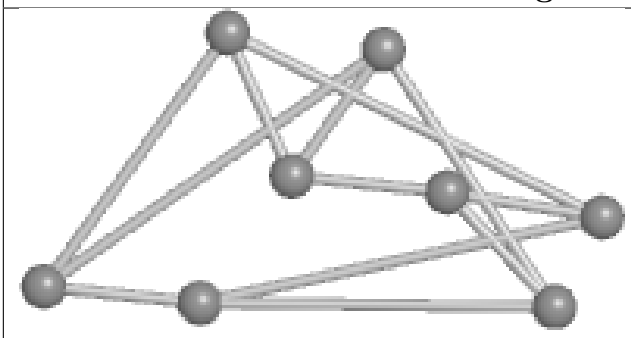
Bond angles



Torsions

Rings

Ligand SF4 a 102



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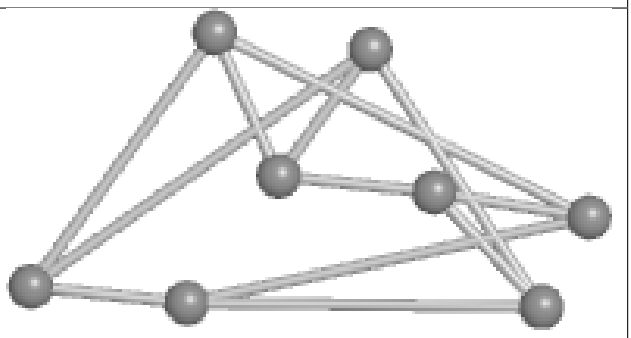
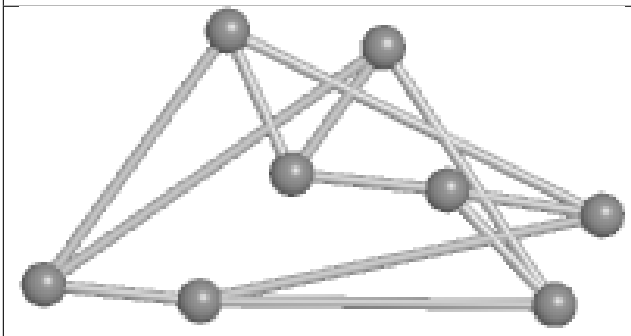
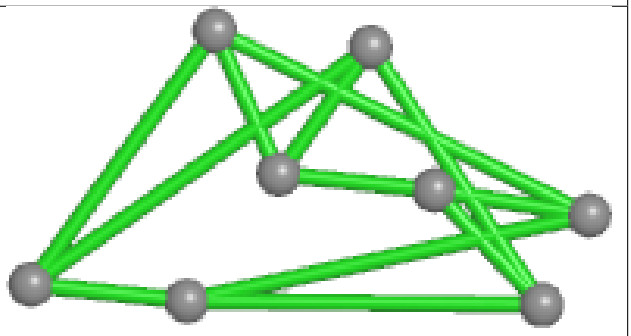


Bond angles

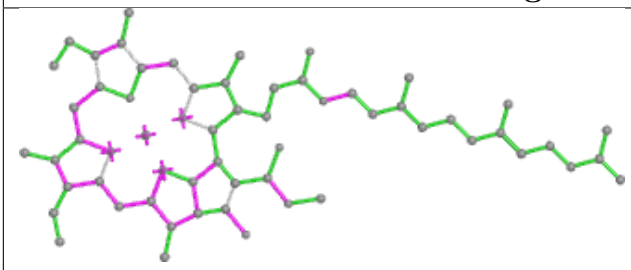


Torsions



Rings

Ligand CLA B 818



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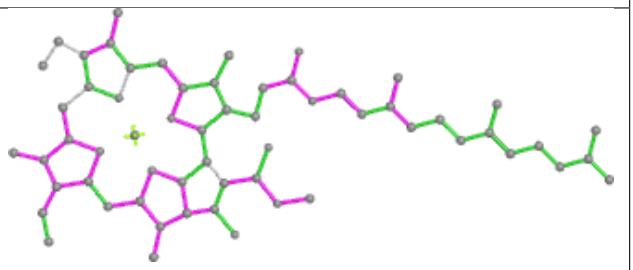
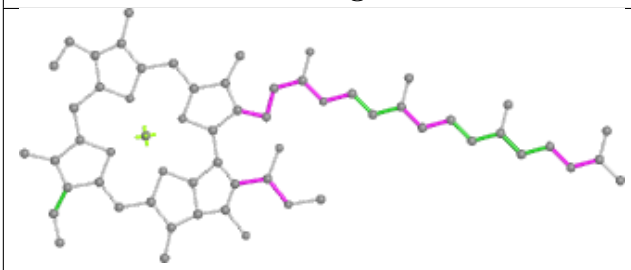
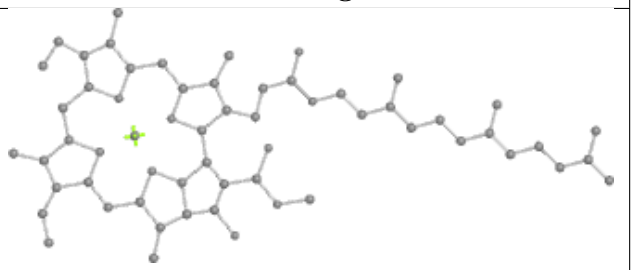


Bond angles

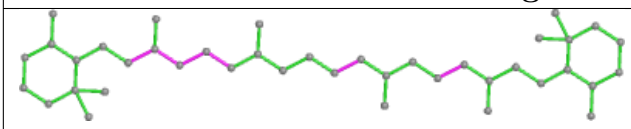


Torsions



Rings

Ligand BCR V 101



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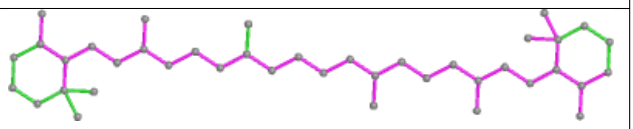
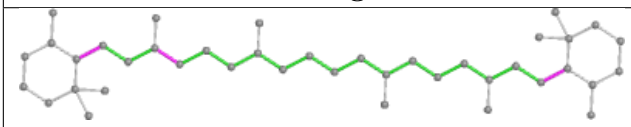


Bond angles



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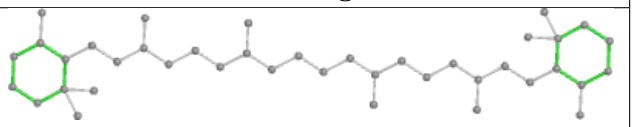
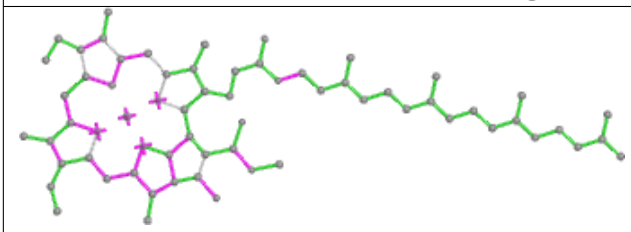


Rings

Ligand CLA H 829



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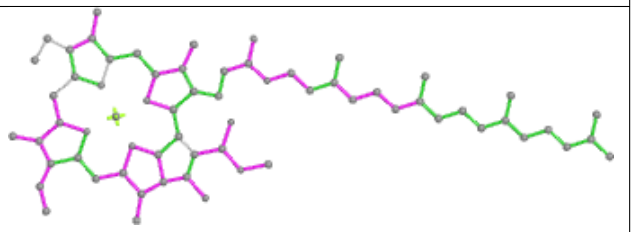
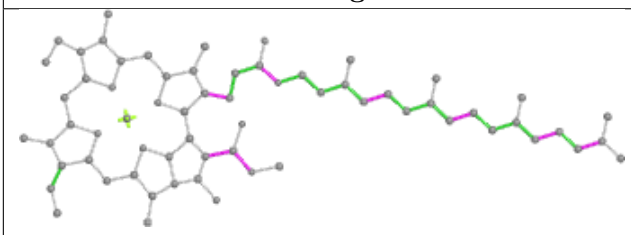


Bond angles



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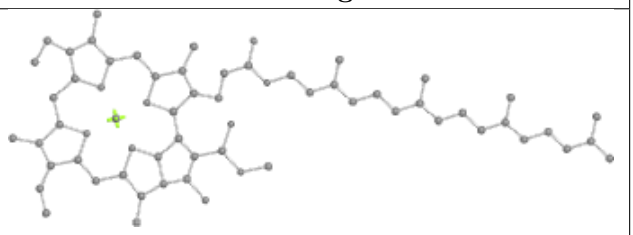
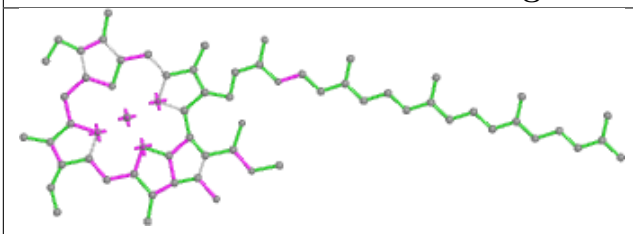


Rings

Ligand CLA G 833



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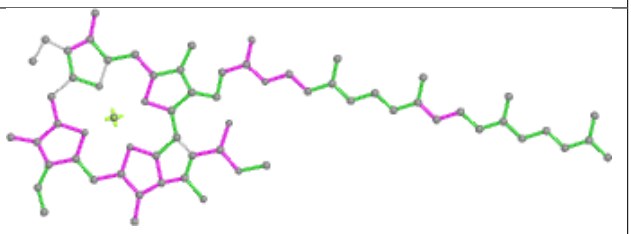
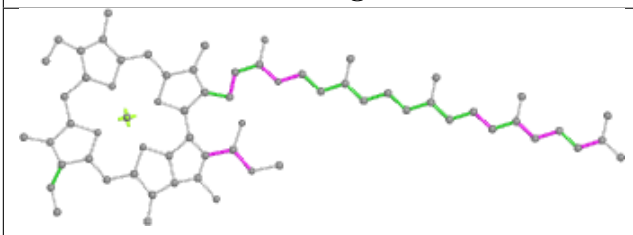


Bond angles



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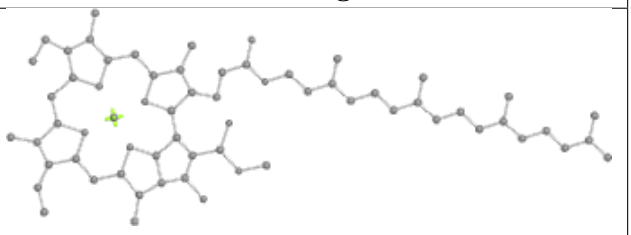
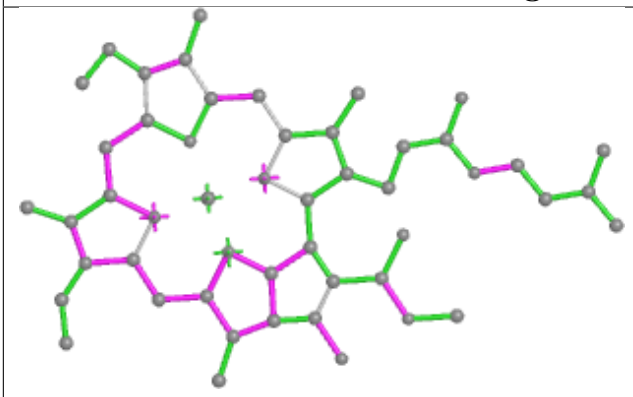


Rings

Ligand CLA A 817



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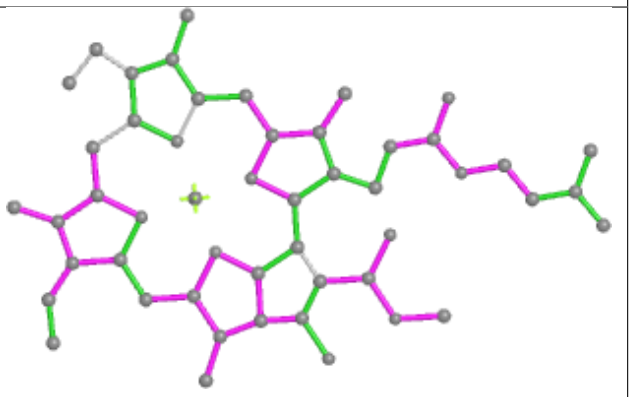
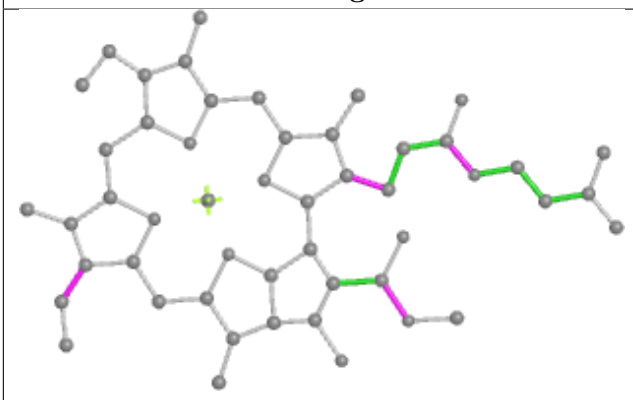


Bond angles



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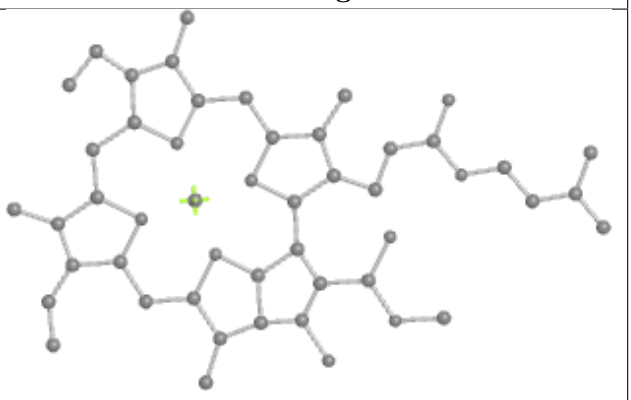
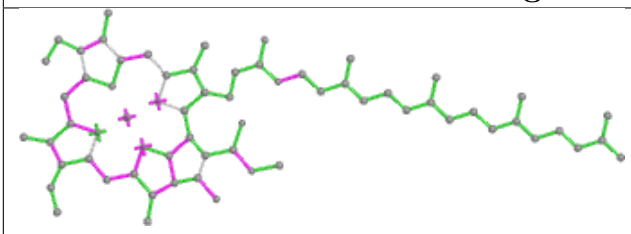


Rings

Ligand CLA Y 841



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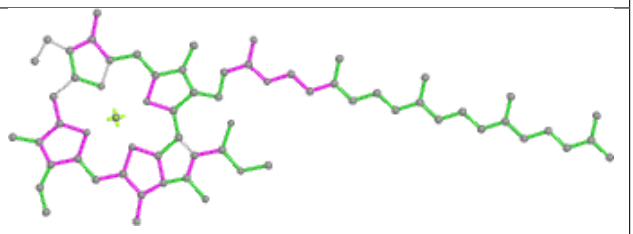
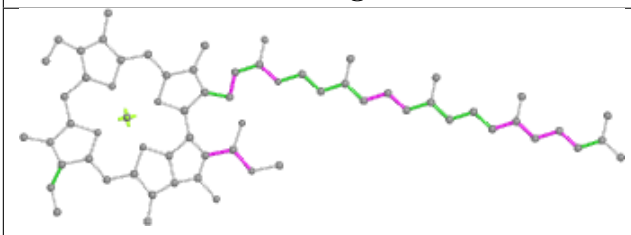


Bond angles



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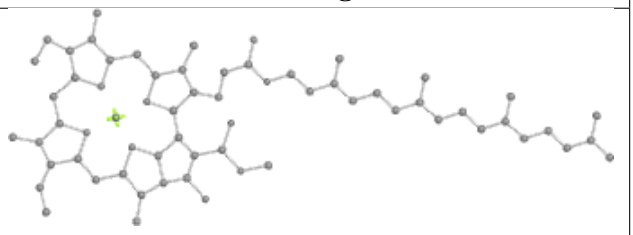
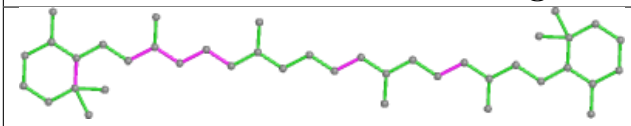


Rings

Ligand BCR I 101



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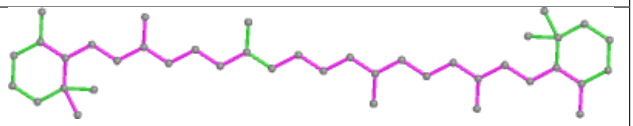
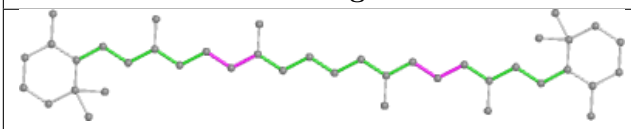


Bond angles



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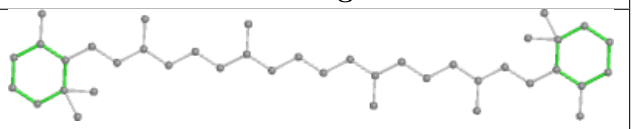
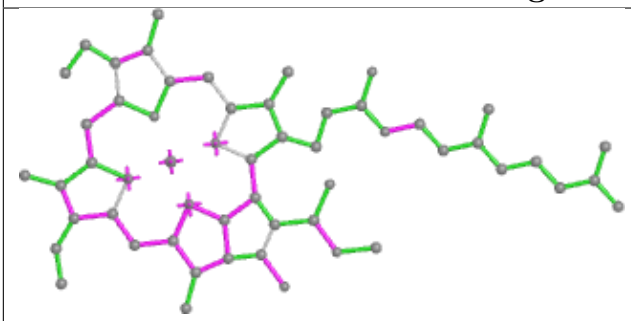


Rings

Ligand CLA J 102



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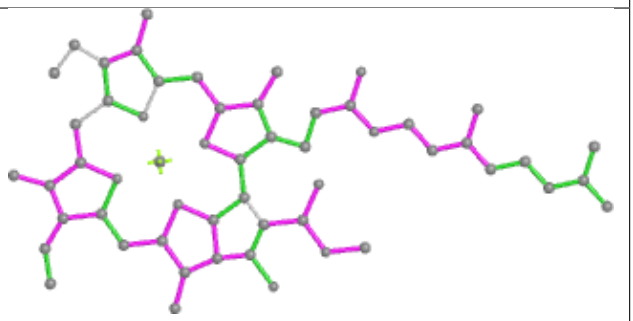
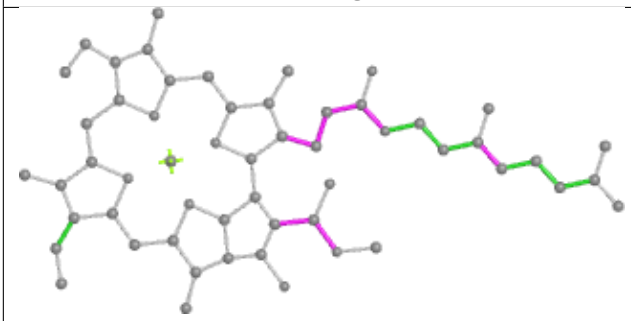
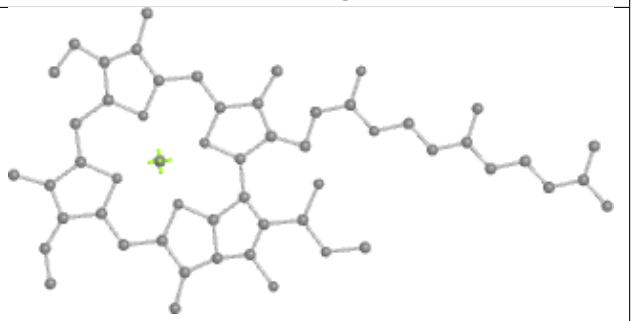


Bond angles

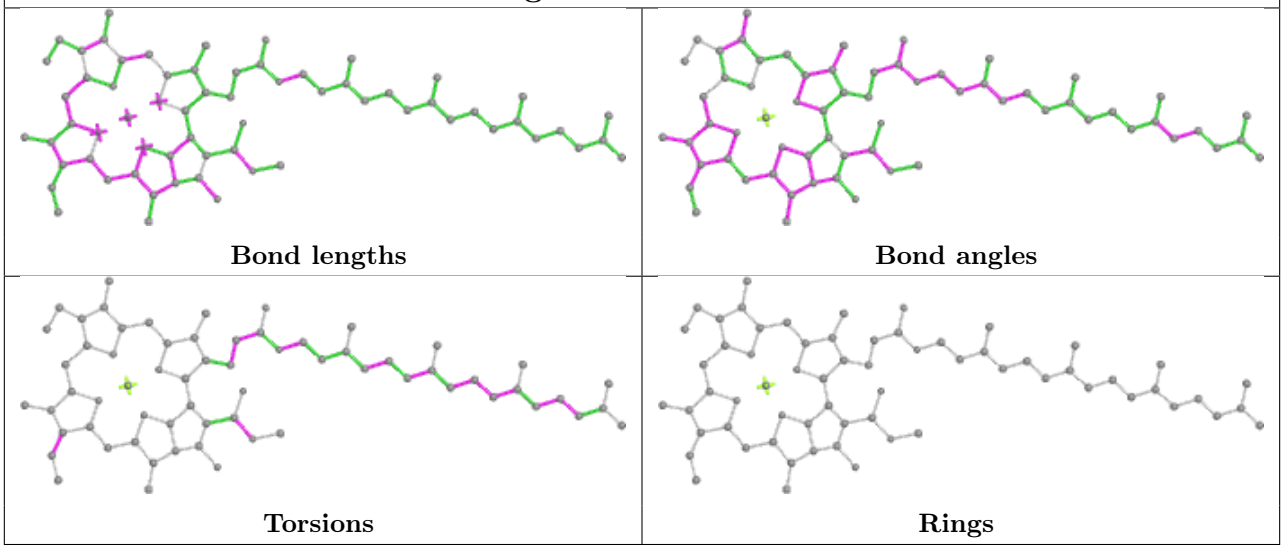


Torsions

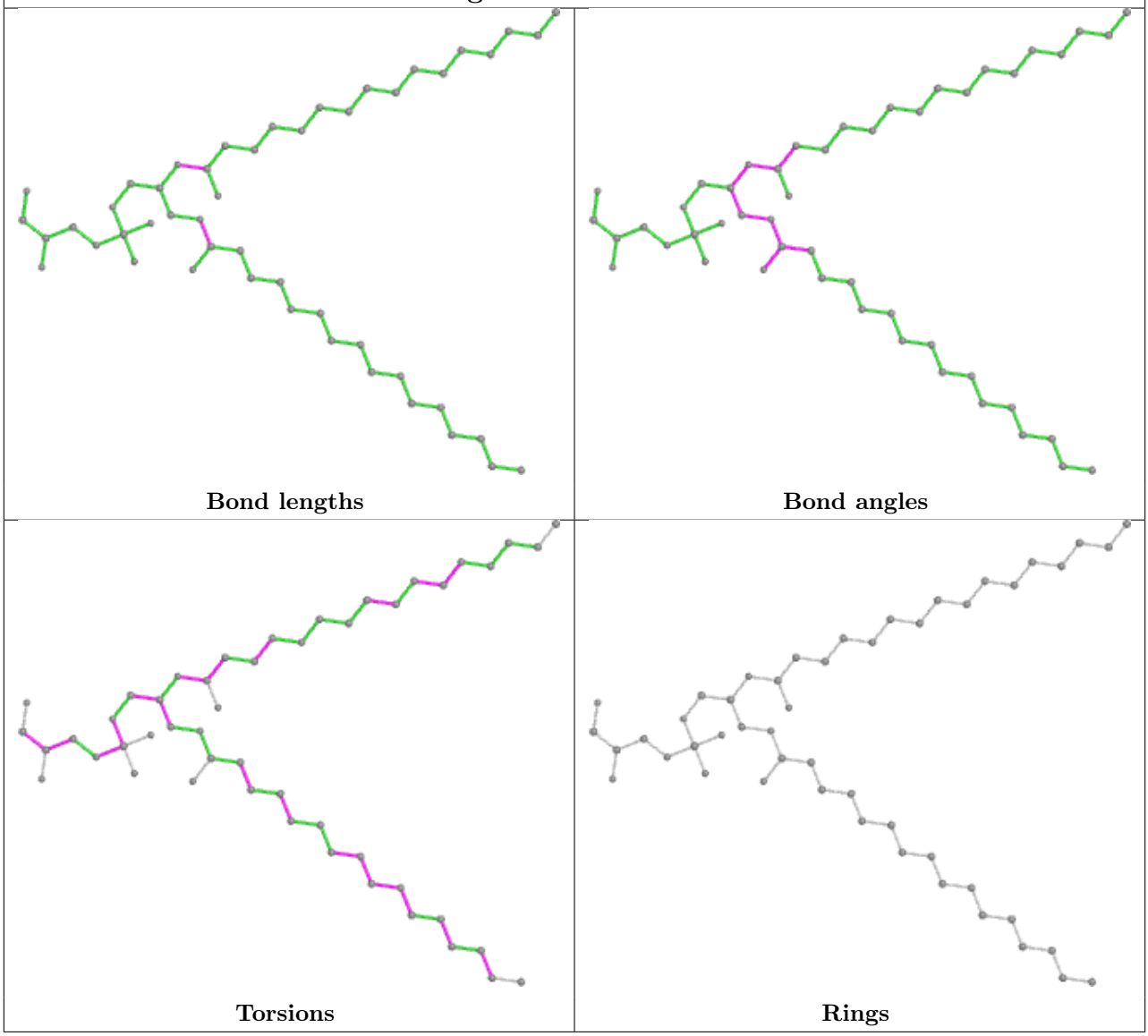


Rings

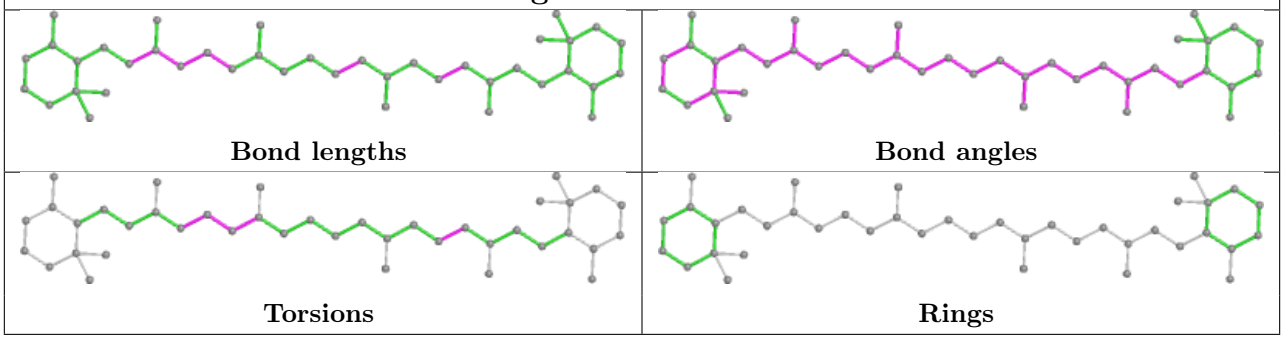
Ligand CLA Y 809



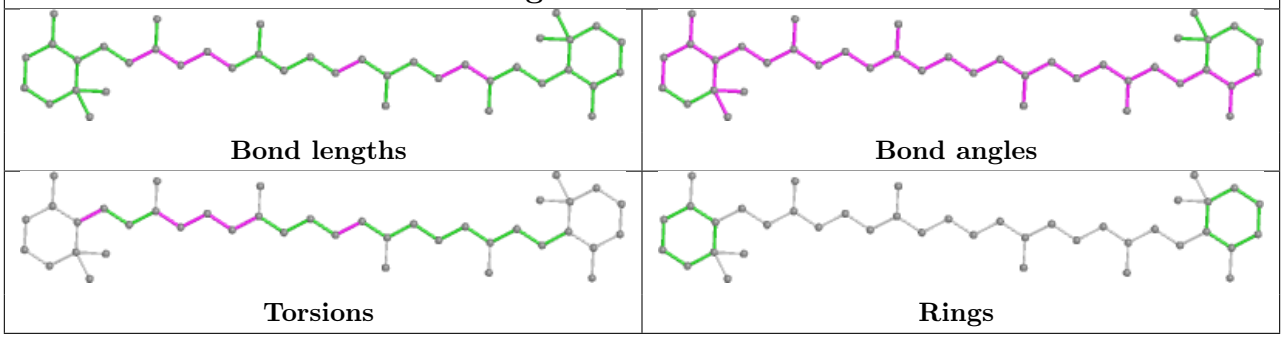
Ligand LHG G 850



Ligand BCR f 103



Ligand BCR L 208



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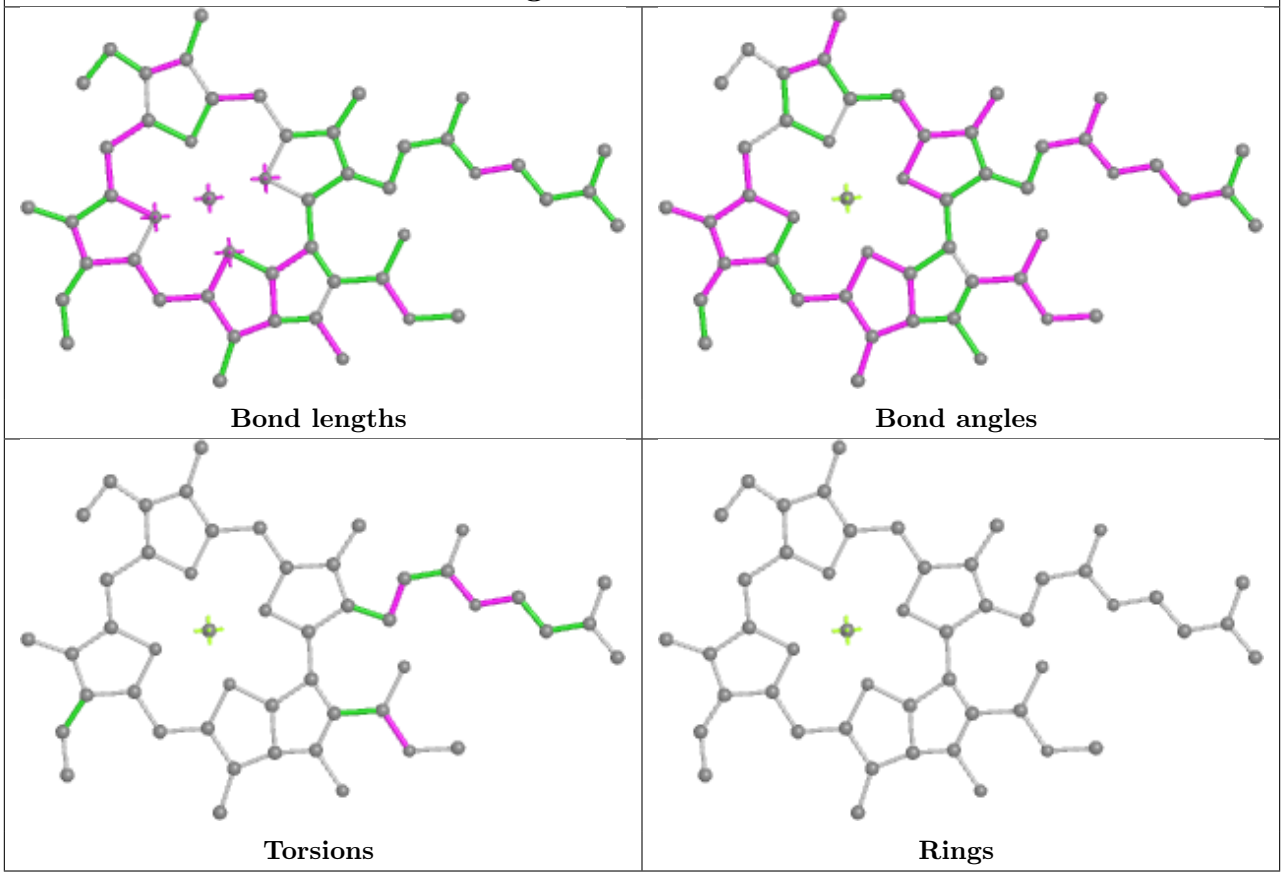
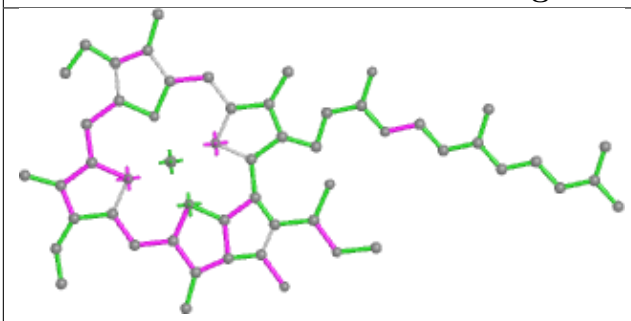
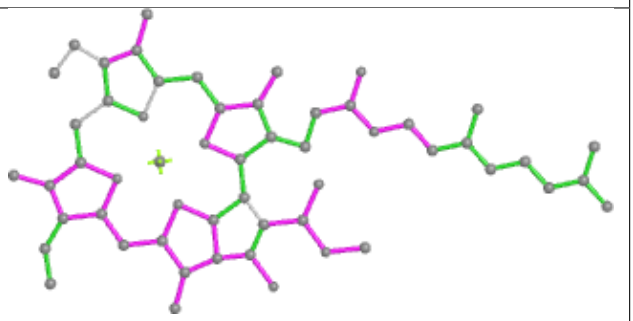


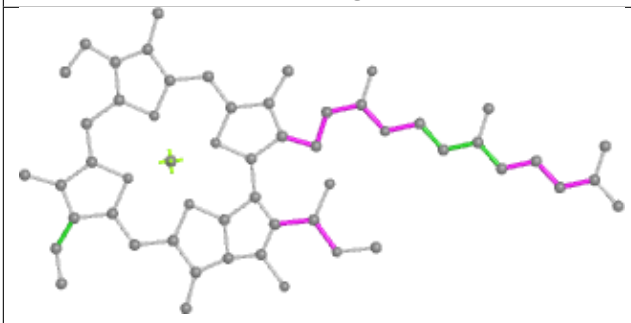
Ligand CLA f 102



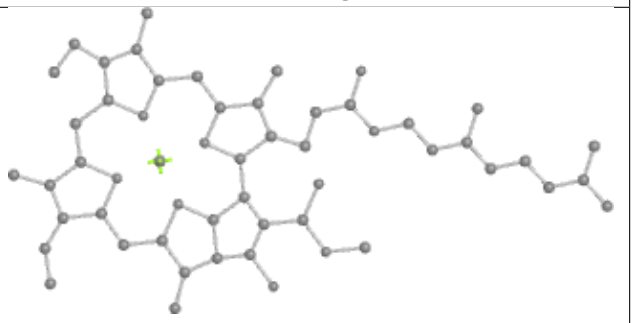
Bond lengths



Bond angles

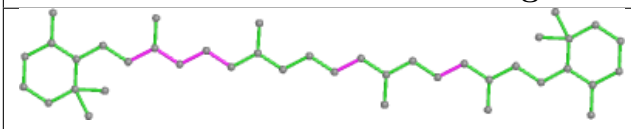


Torsions

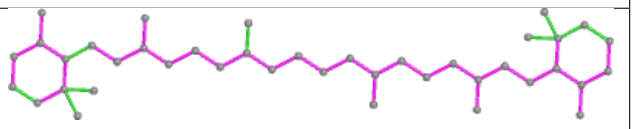


Rings

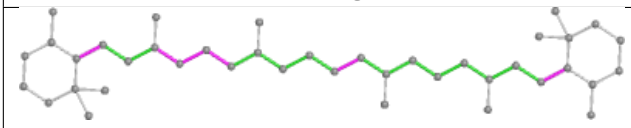
Ligand BCR H 843



Bond lengths

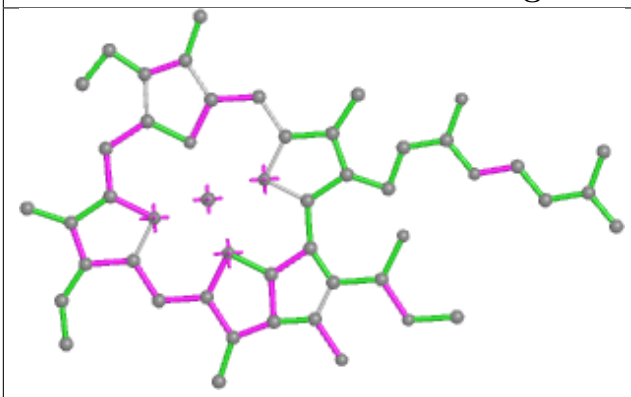
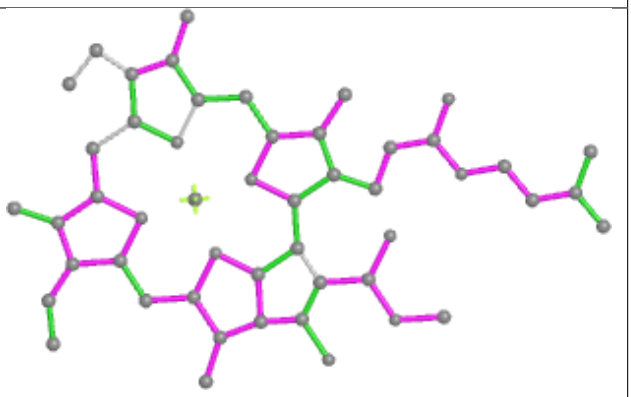
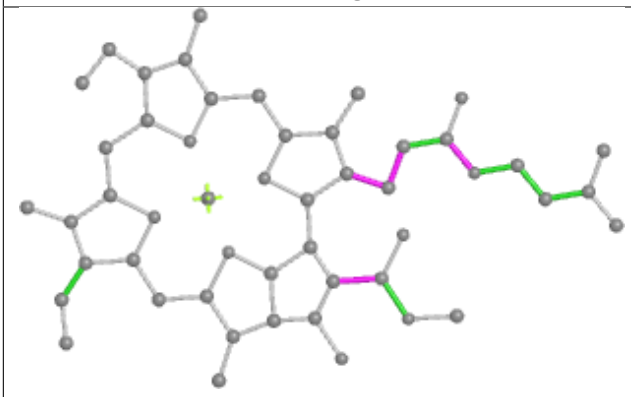
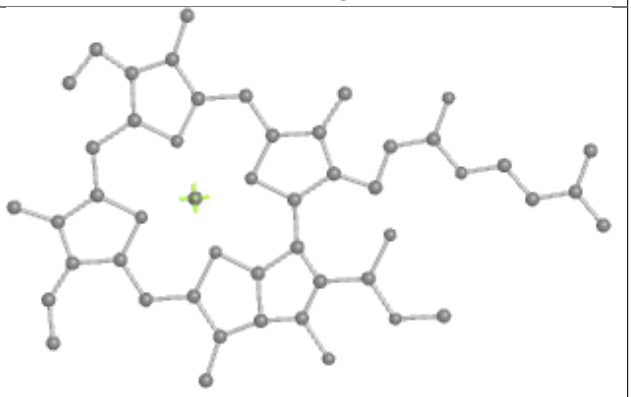


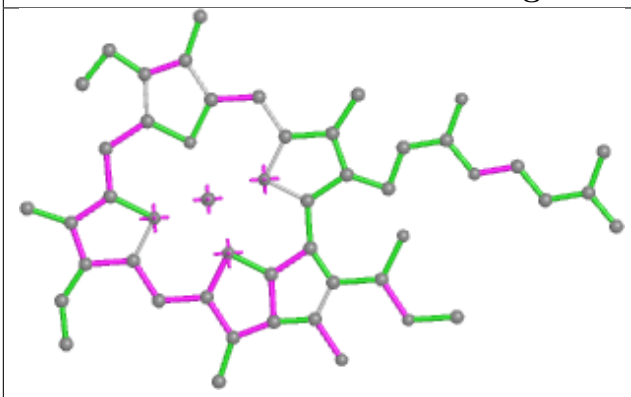
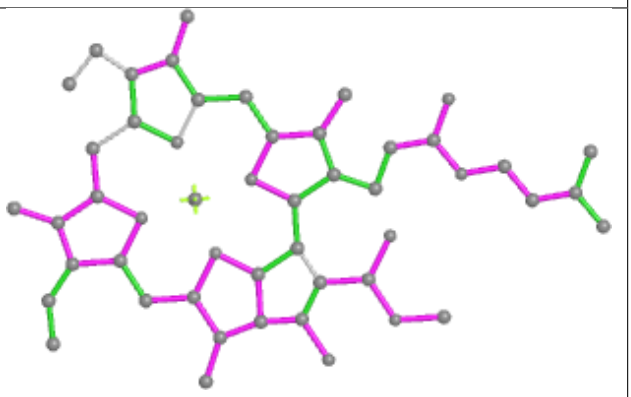
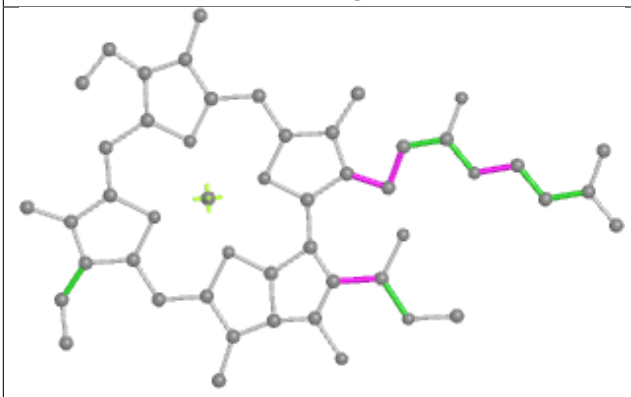
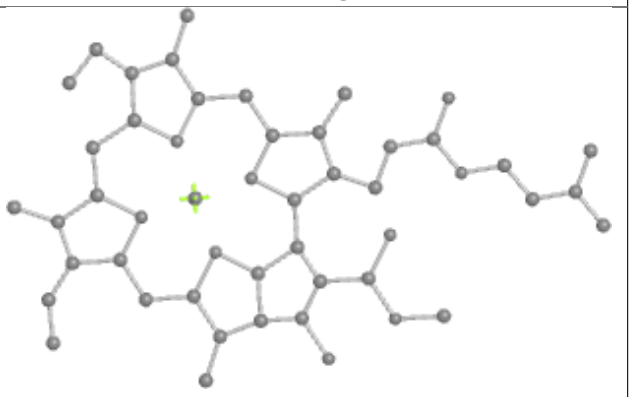
Bond angles



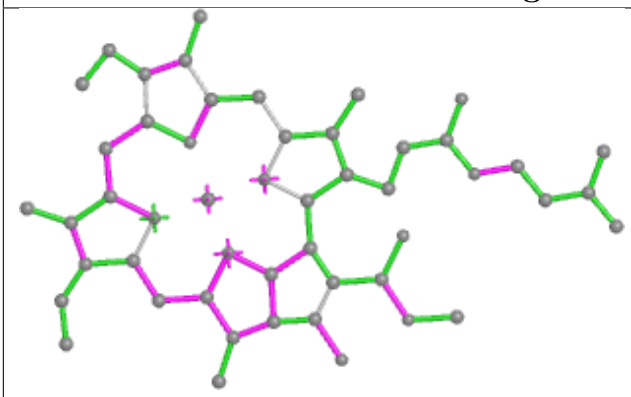
Torsions

Rings

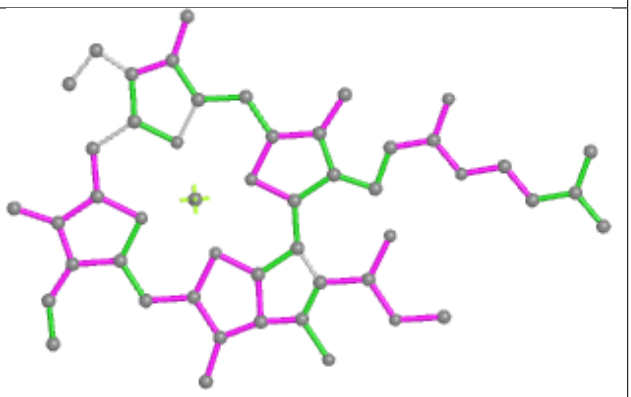
Ligand CLA Y 837	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA G 836	
 Bond lengths	 Bond angles
 Torsions	 Rings

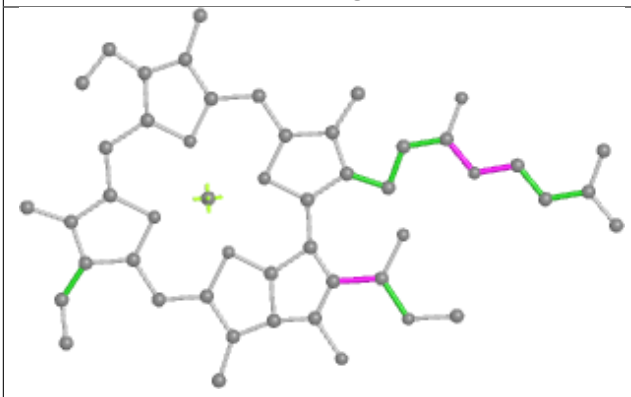
Ligand CLA G 838



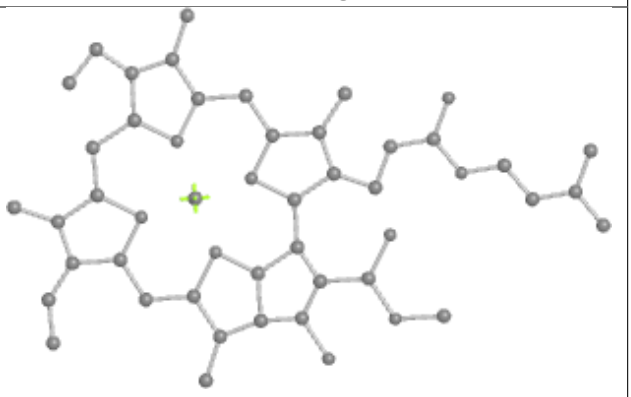
Bond lengths



Bond angles

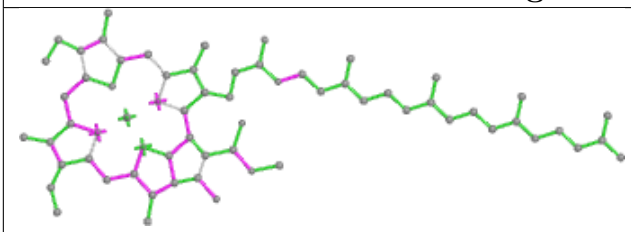


Torsions

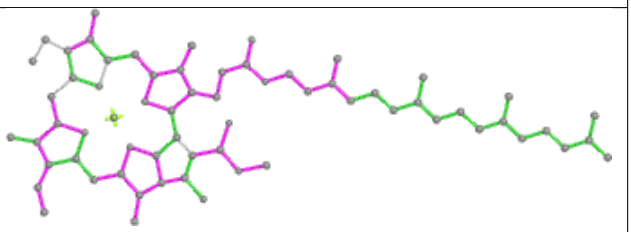


Rings

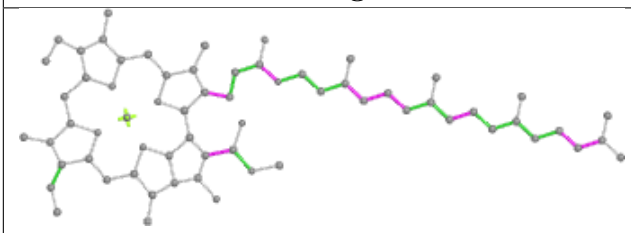
Ligand CLA Z 826



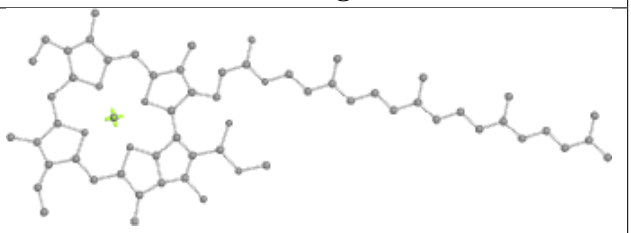
Bond lengths



Bond angles

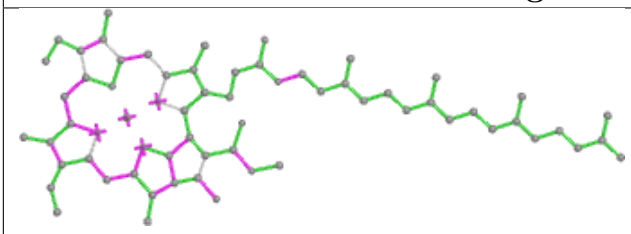


Torsions

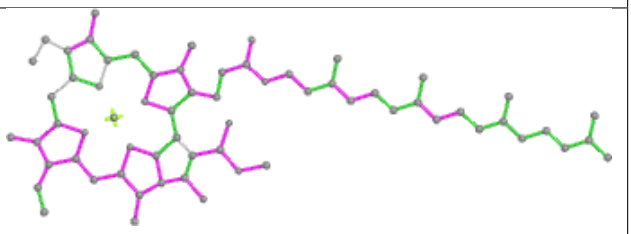


Rings

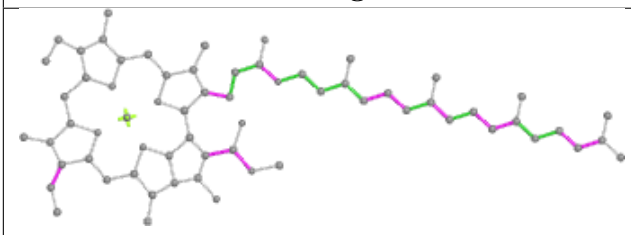
Ligand CLA L 201



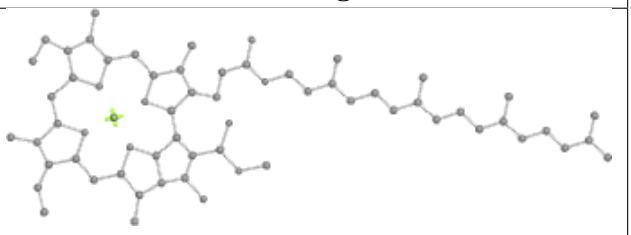
Bond lengths



Bond angles

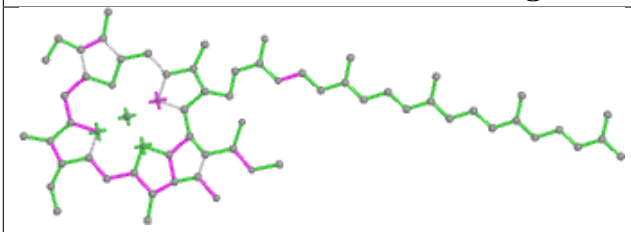


Torsions



Rings

Ligand CLA B 840



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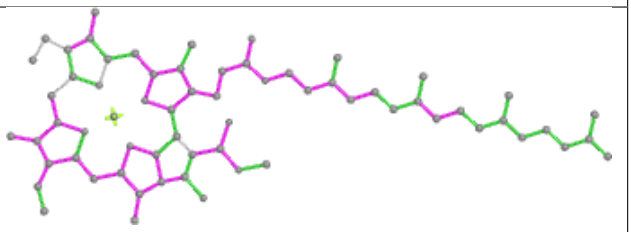
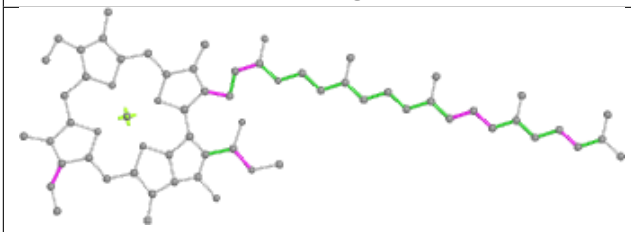


Bond angles



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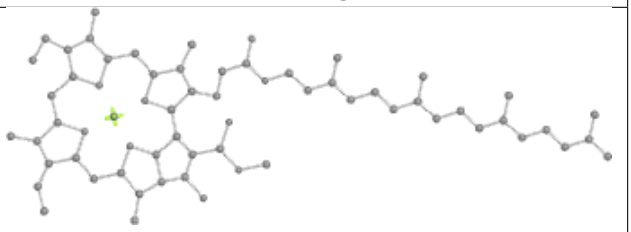
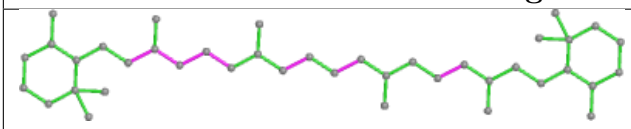
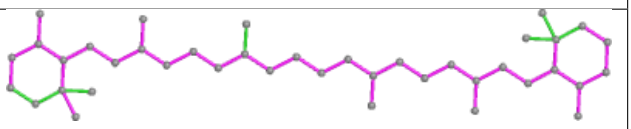


Rings

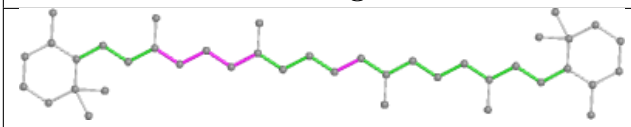
Ligand BCR h 202



Bond lengths



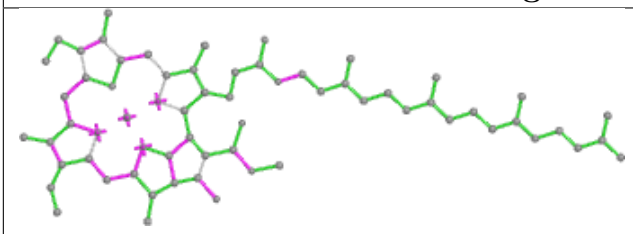
Bond angles



Torsions

Rings

Ligand CLA G 832



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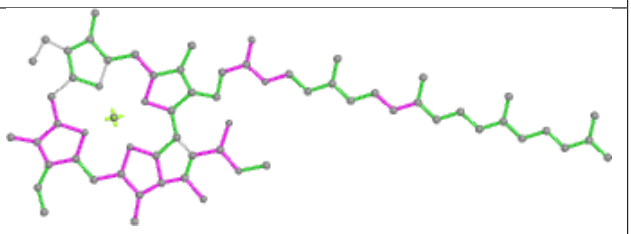
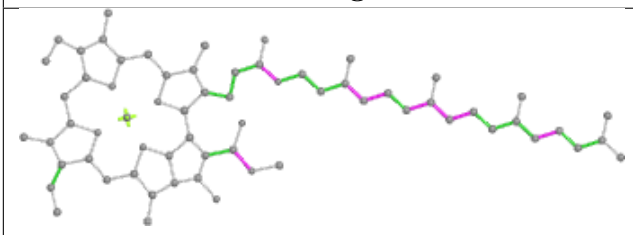
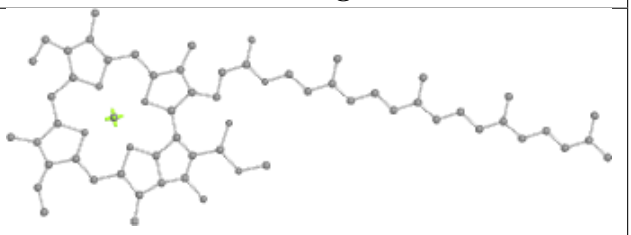


Bond angles

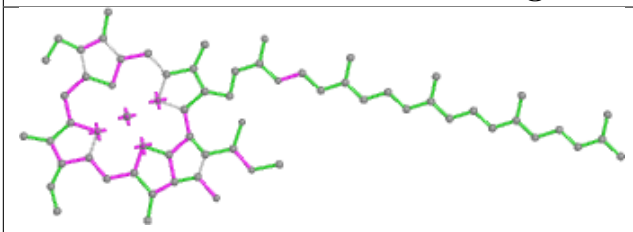


Torsions



Rings

Ligand CLA Z 829



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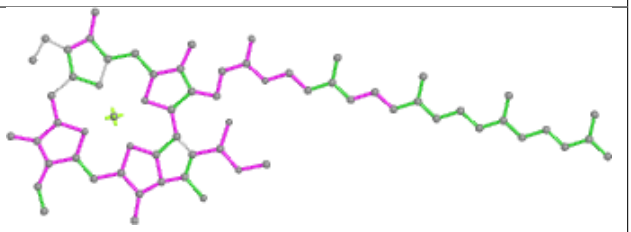
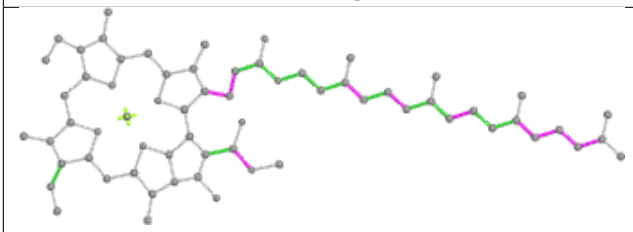


Bond angles



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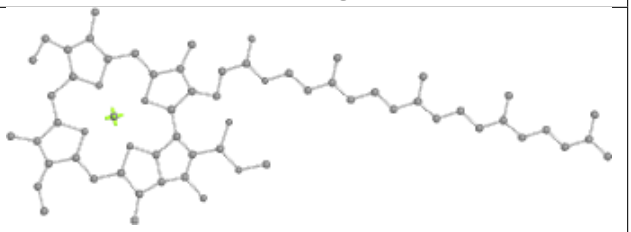
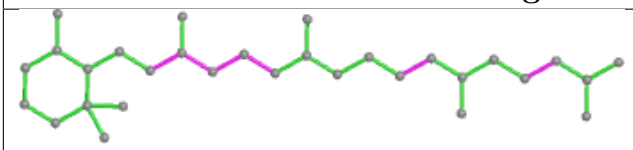


Rings

Ligand BCR B 842



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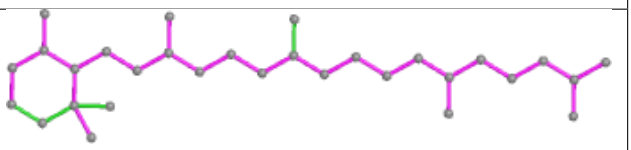
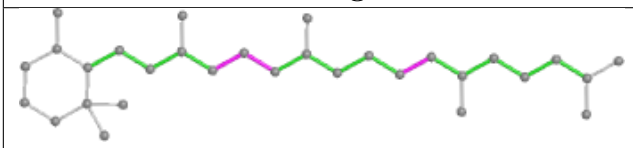
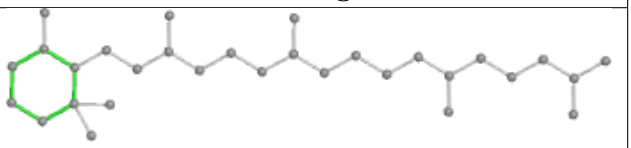


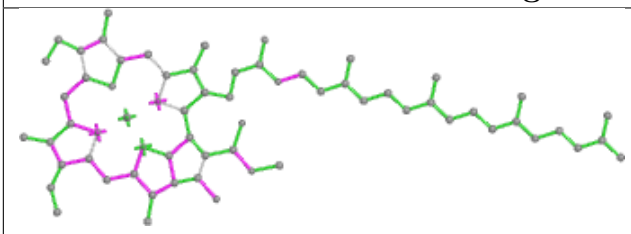
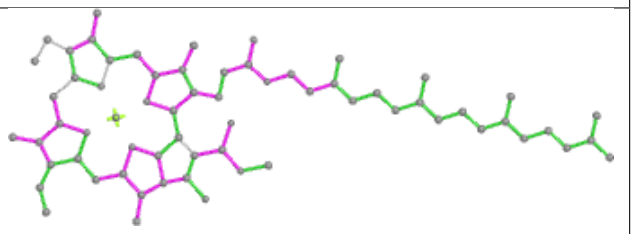
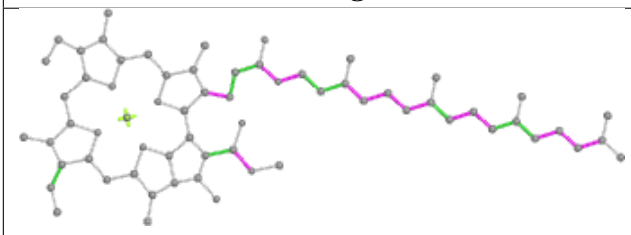
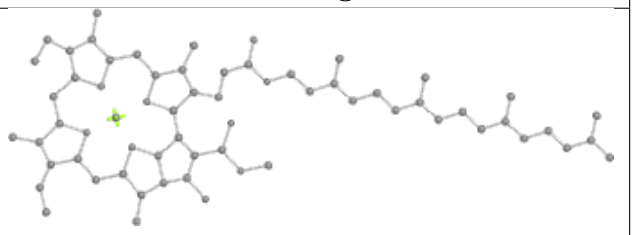
Bond angles

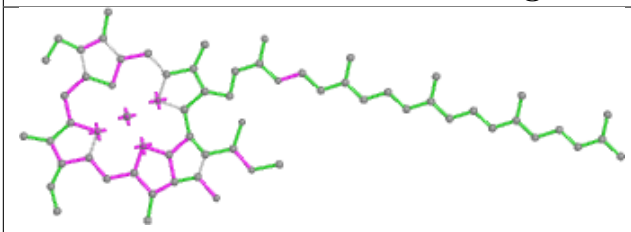
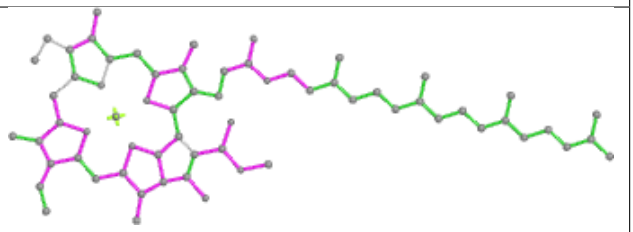
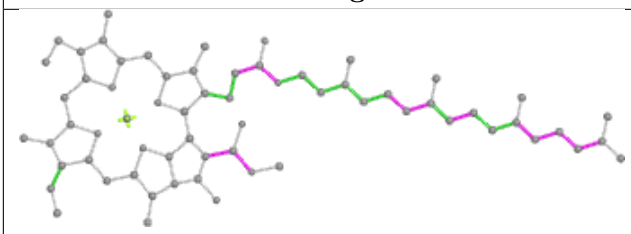
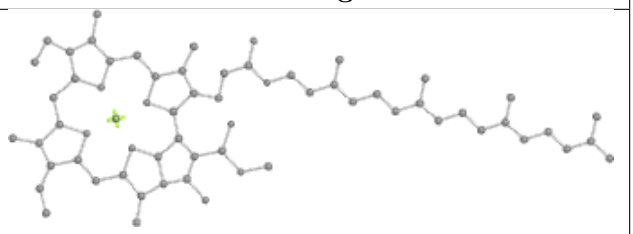


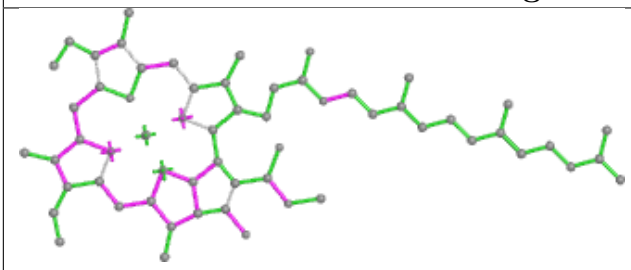
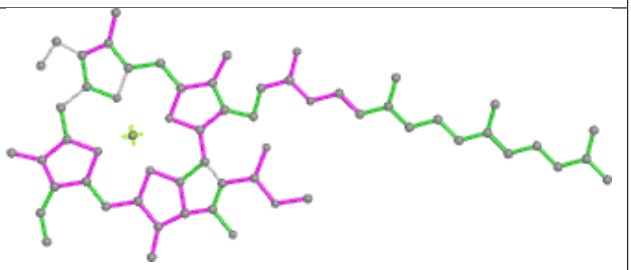
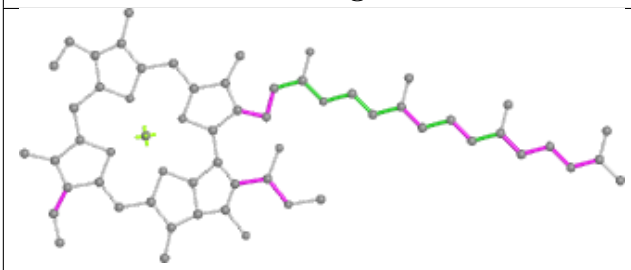
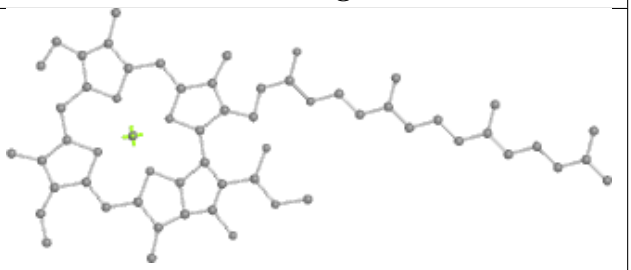
Torsions

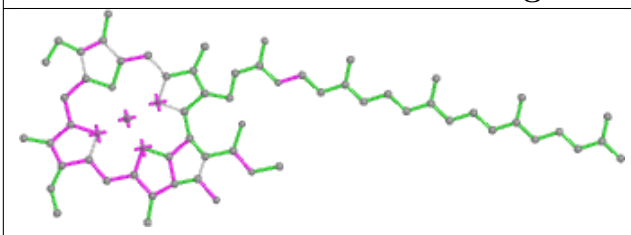
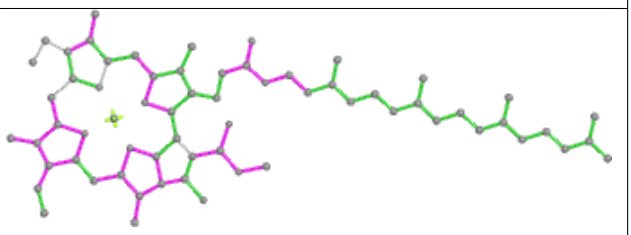
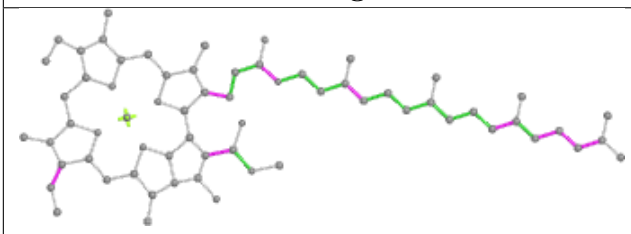
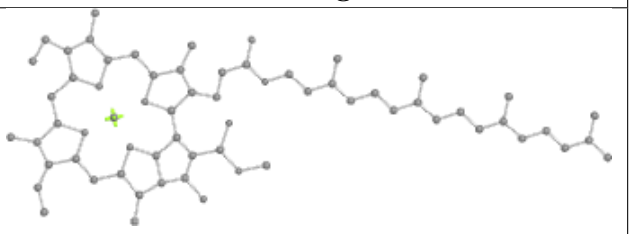


Rings

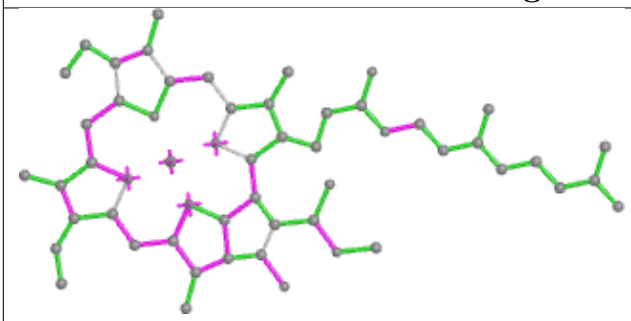
Ligand CLA G 819	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA A 830	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA G 824	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA A 804	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA H 822



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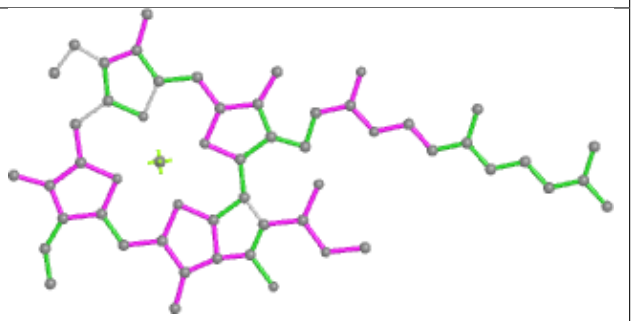
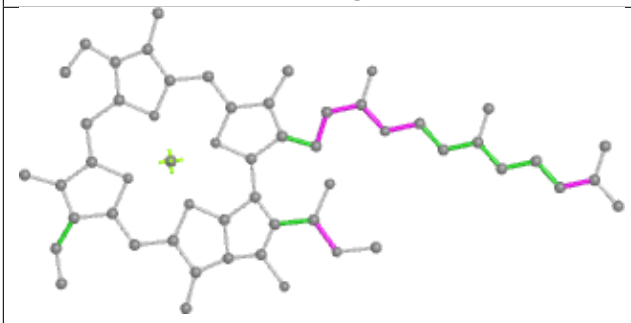


Bond angles



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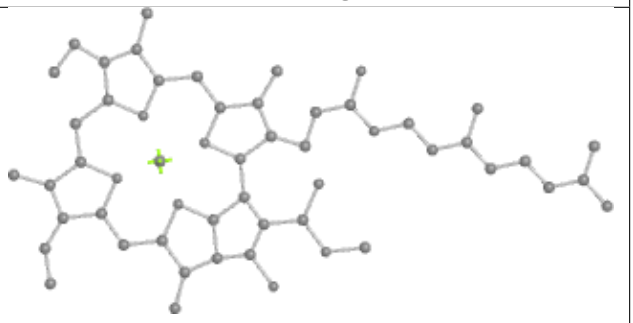
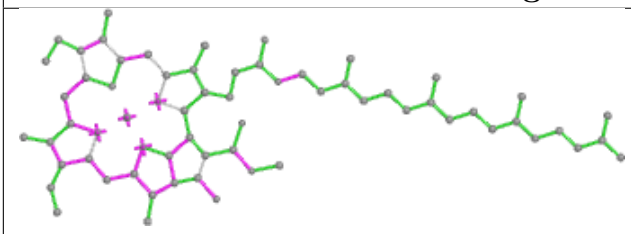


Rings

Ligand CLA G 825



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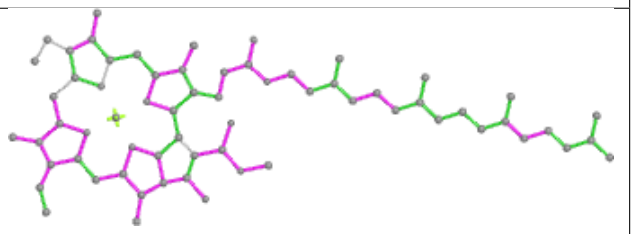
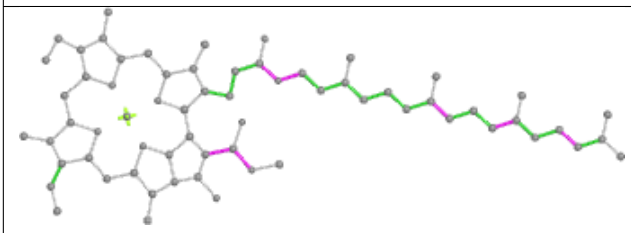


Bond angles



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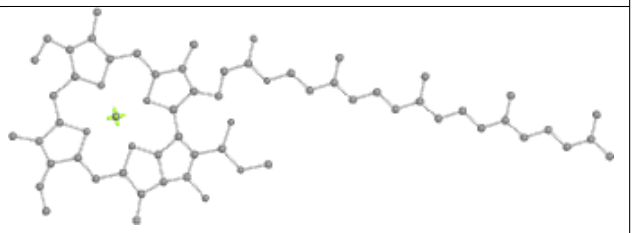
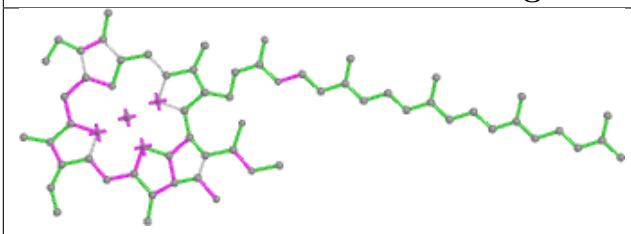


Rings

Ligand CLA A 803



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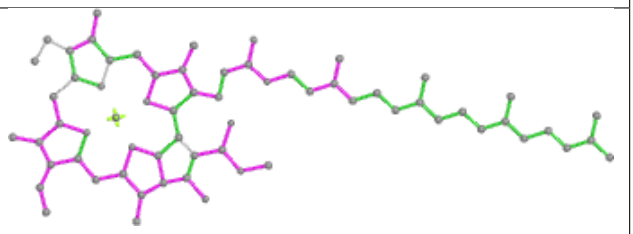
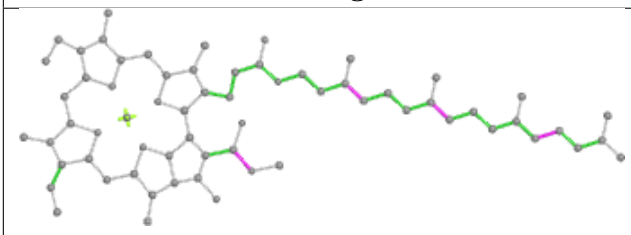


Bond angles



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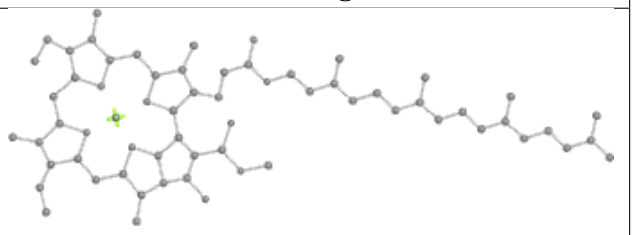
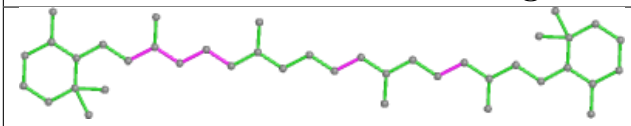


Rings

Ligand BCR Y 845



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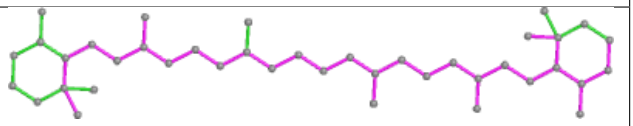
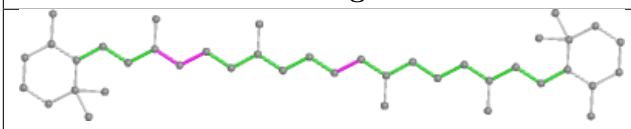


Bond angles



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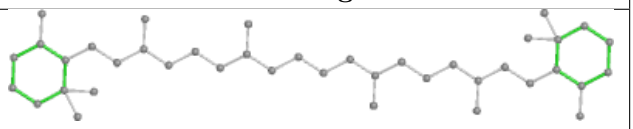
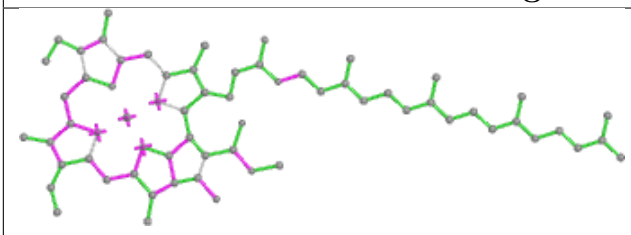


Rings

Ligand CLA H 807



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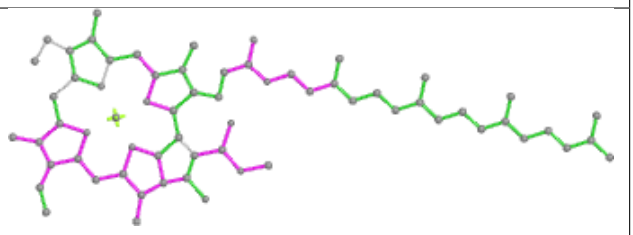
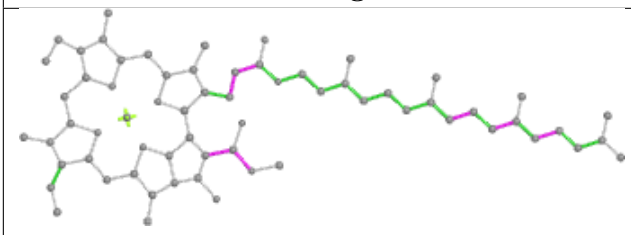


Bond angles



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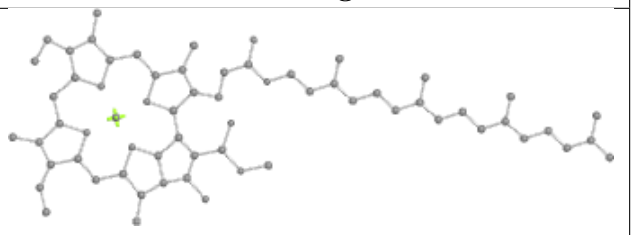
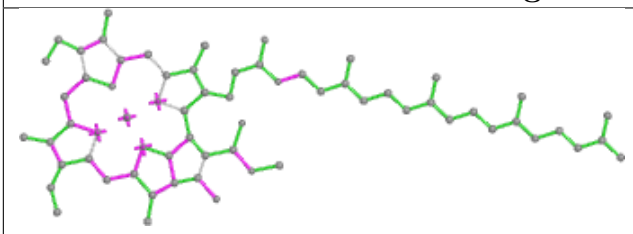


Rings

Ligand CLA A 833



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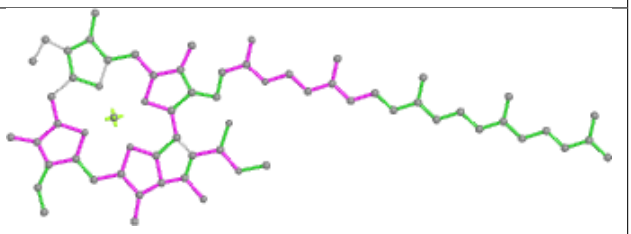

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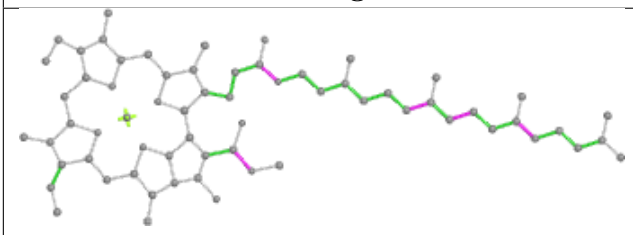

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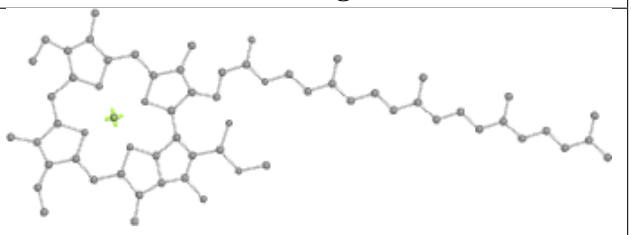
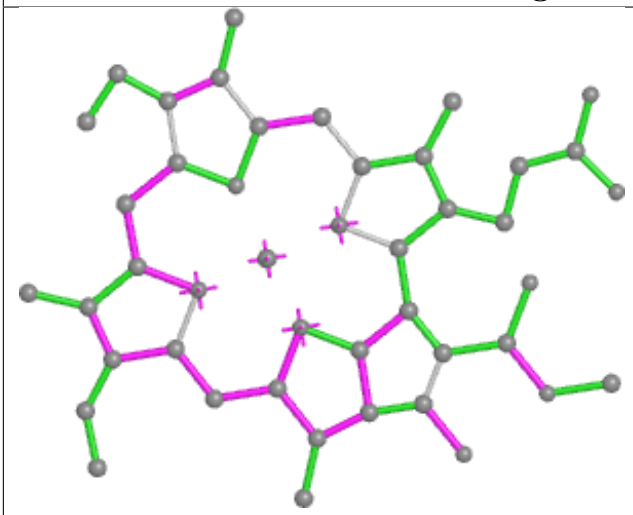


Rings

Ligand CLA j 102



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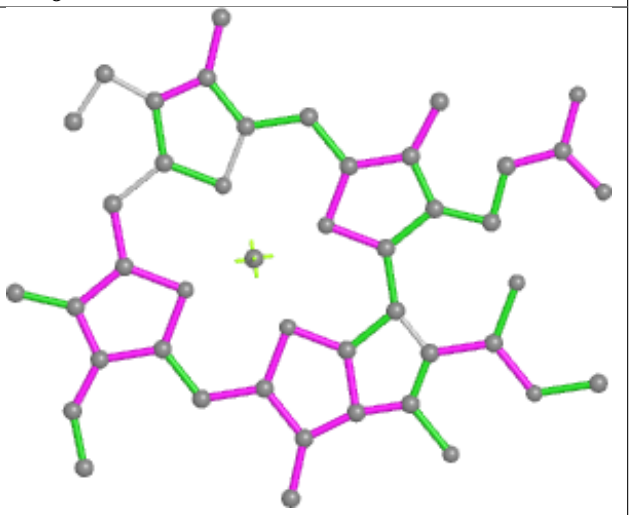

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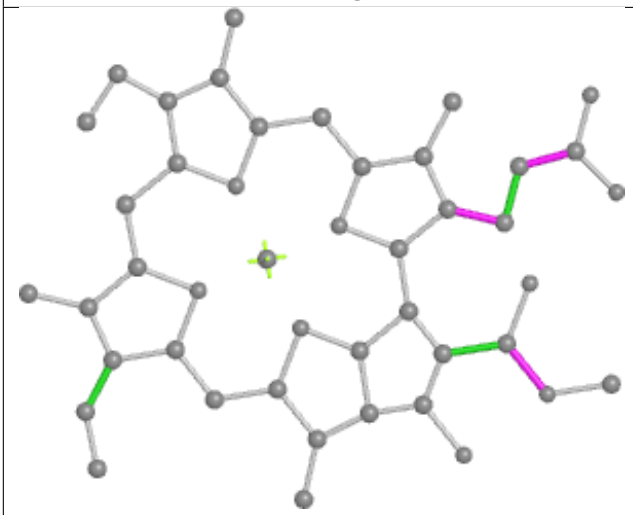

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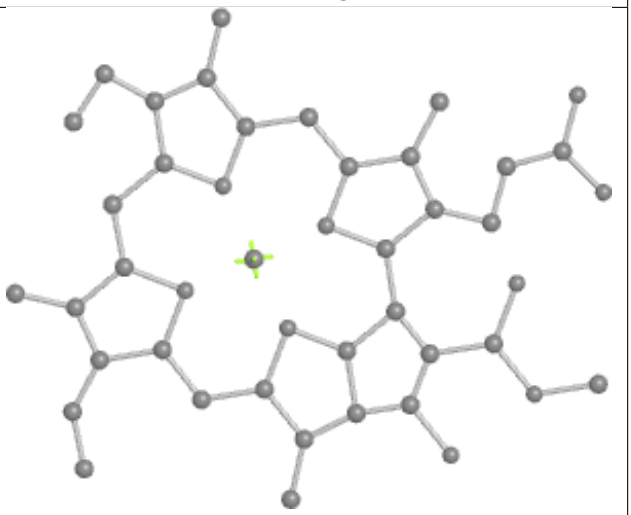
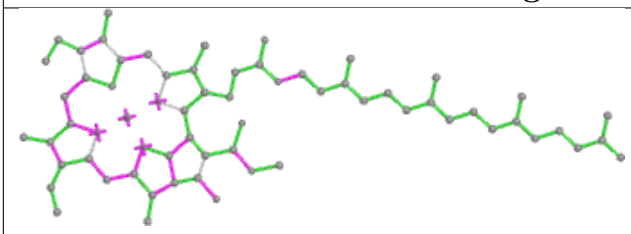


Rings

Ligand CLA G 803



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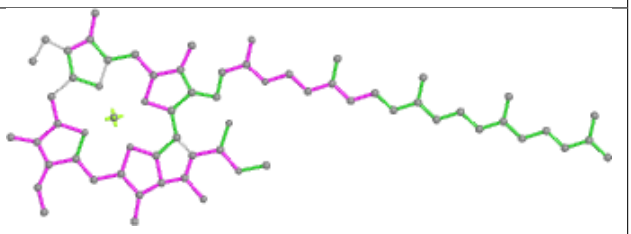

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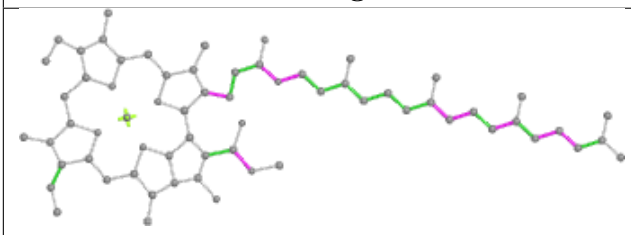

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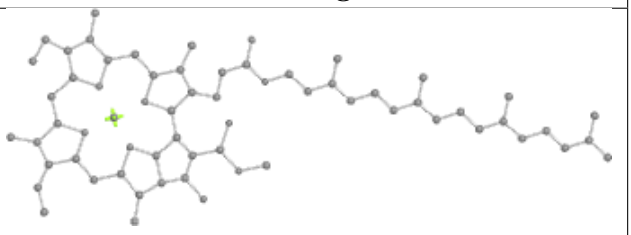
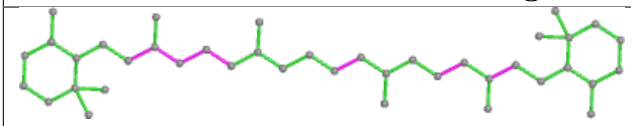


Rings

Ligand BCR B 846



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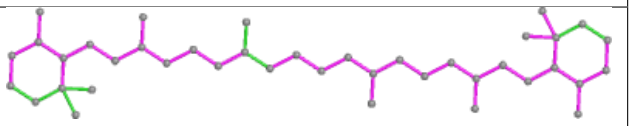
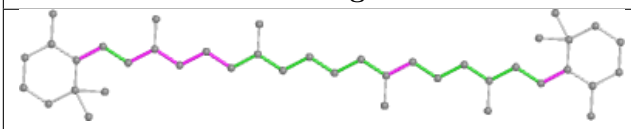


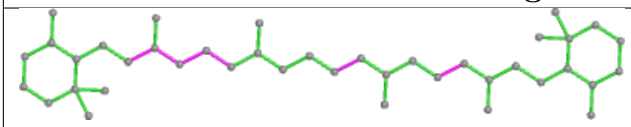
Bond angles



Torsions

Rings

Ligand BCR Z 844



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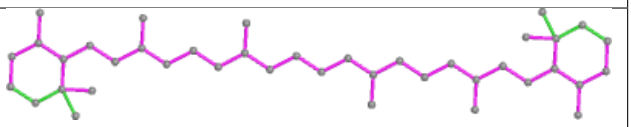
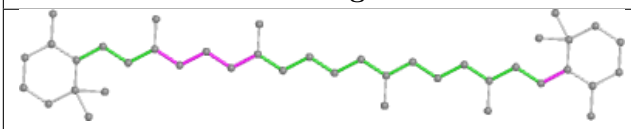


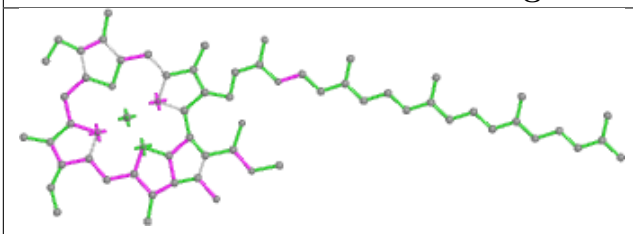
Bond angles



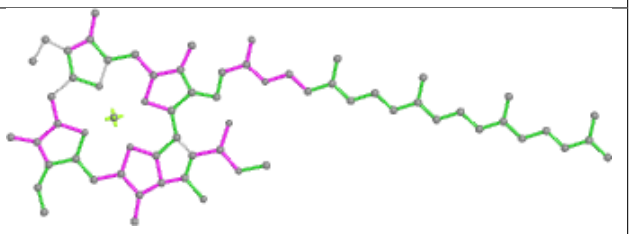
Torsions

Rings

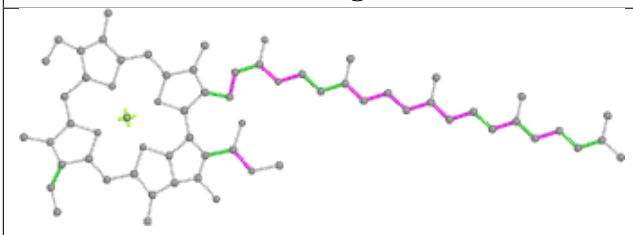
Ligand CLA Y 822



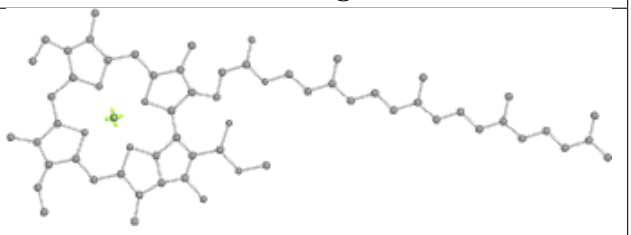
Bond lengths



Bond angles

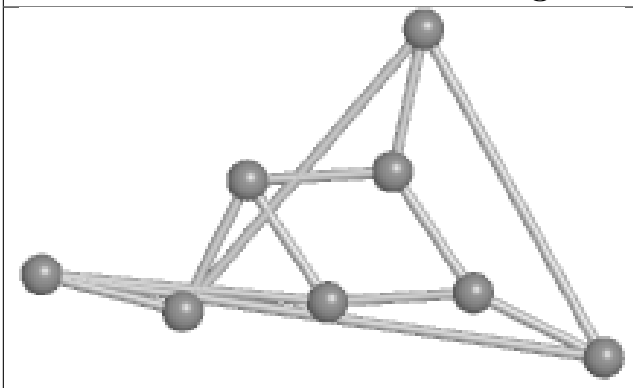


Torsions

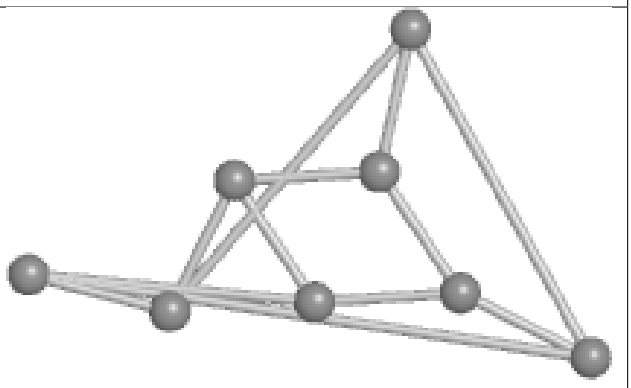


Rings

Ligand SF4 C 101



Bond lengths



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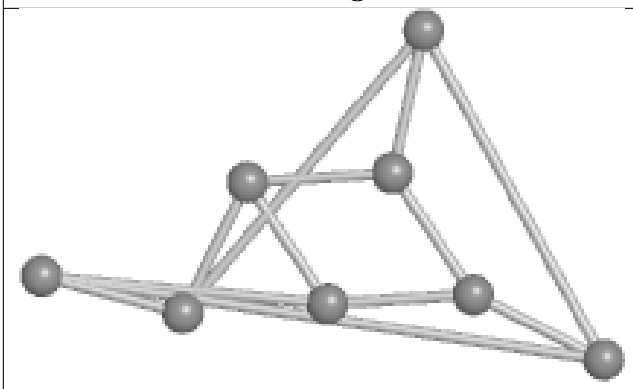

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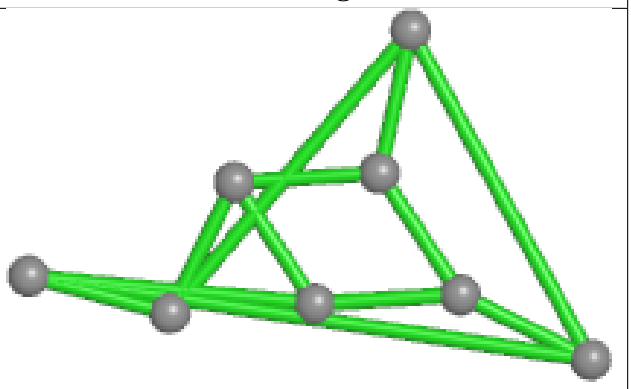
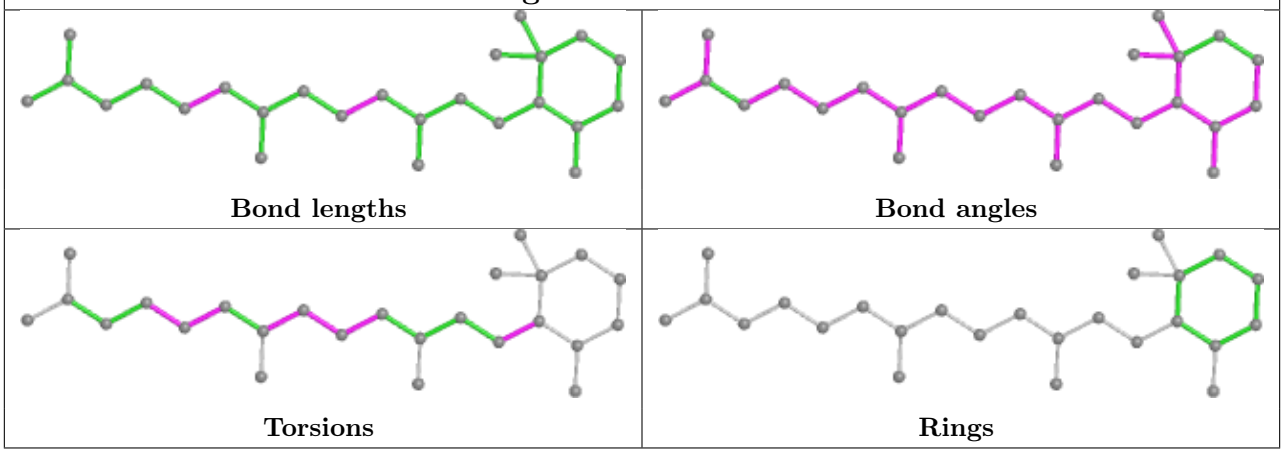
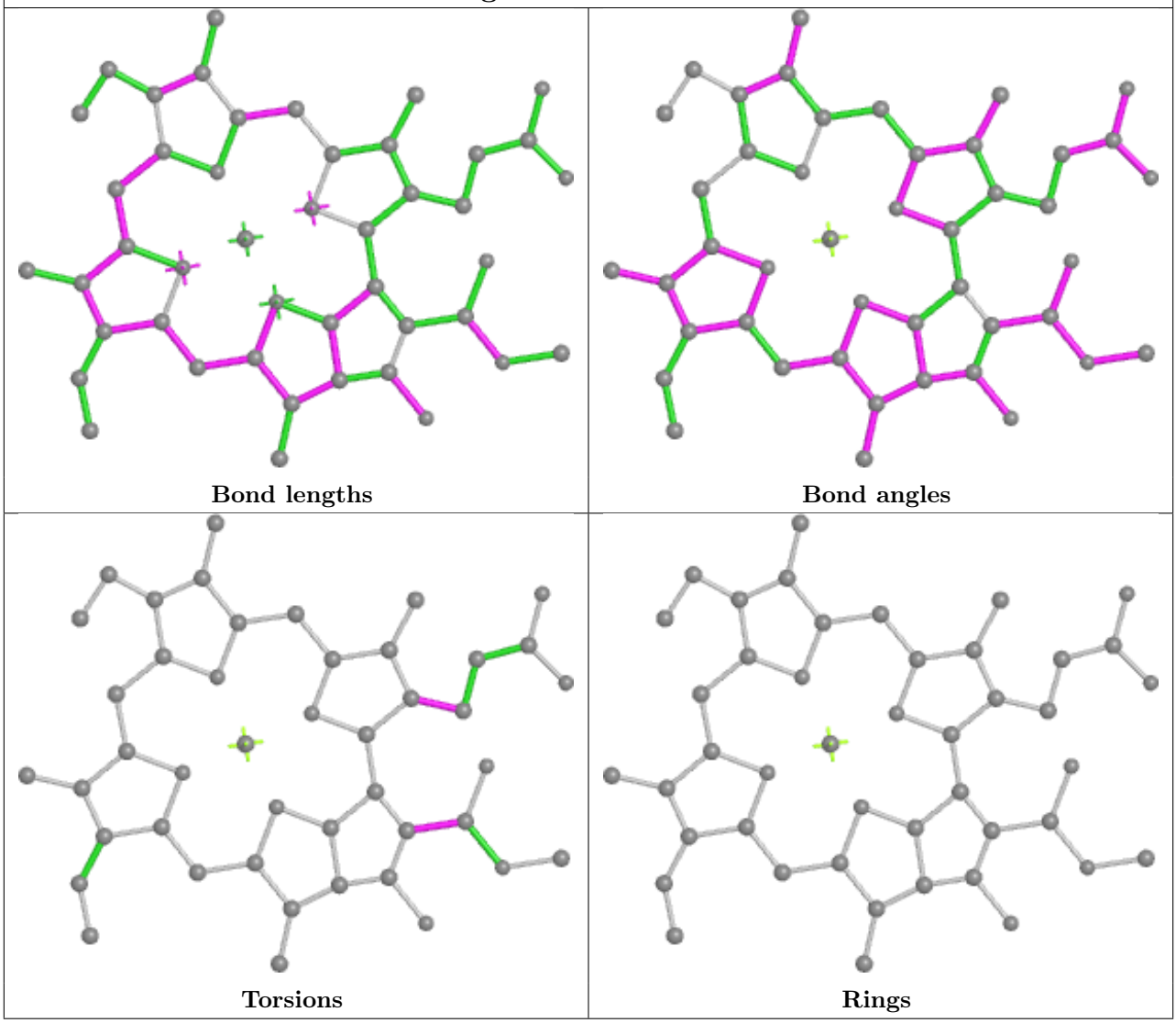


Rings

Ligand BCR H 845



Ligand CLA A 835



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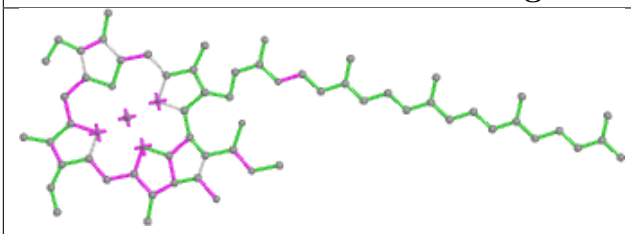
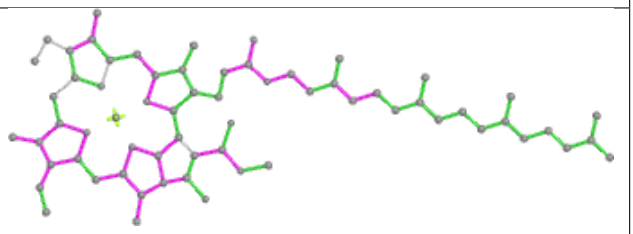
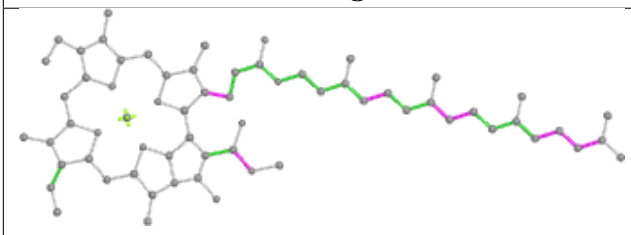
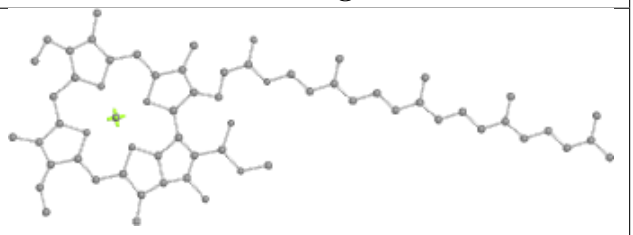
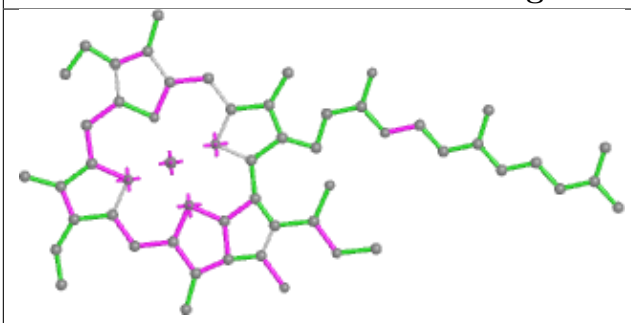
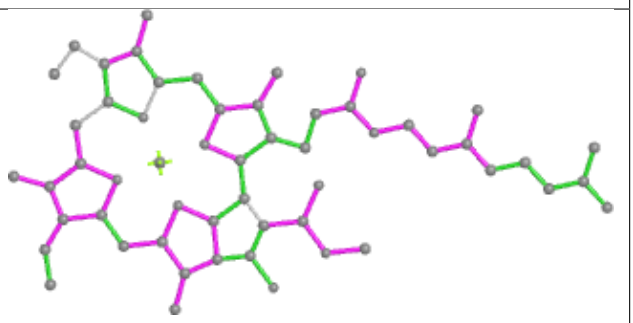
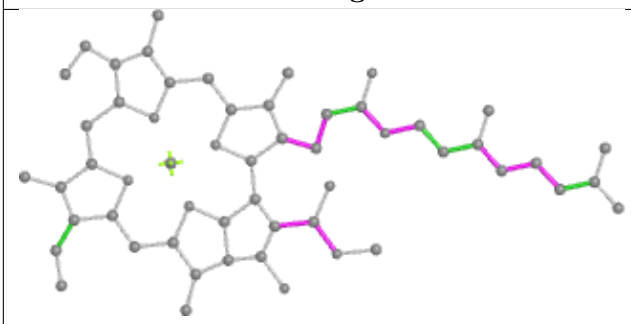
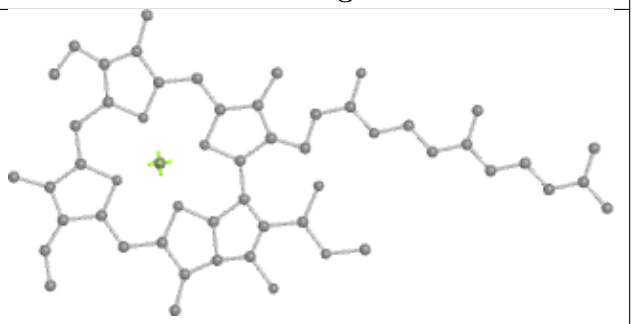
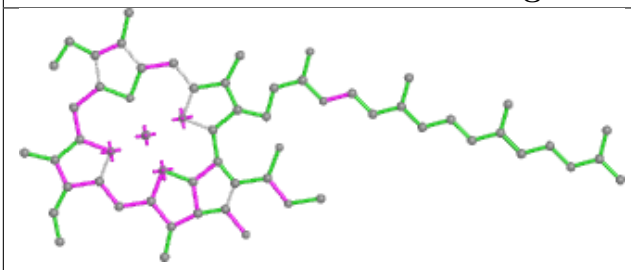
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA Z 812	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA A 821



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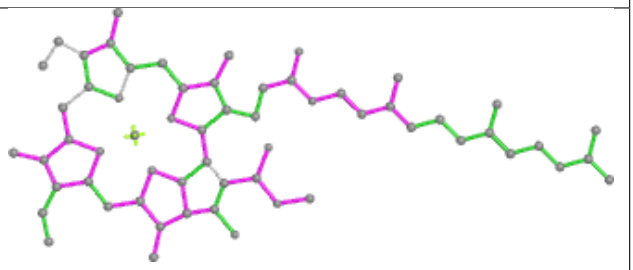

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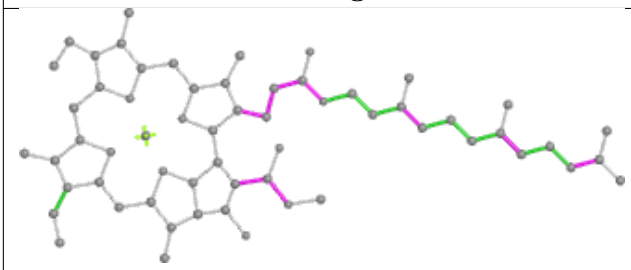

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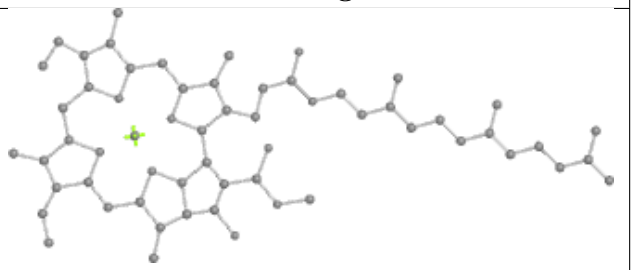
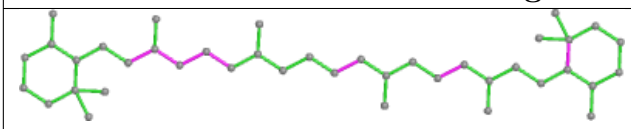


Rings

Ligand BCR Z 848



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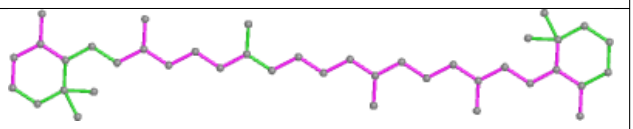

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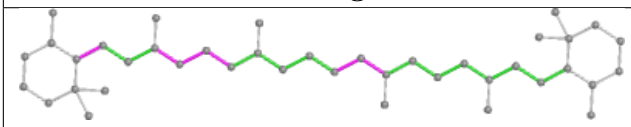

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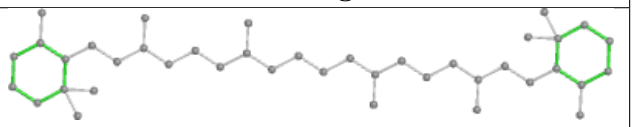
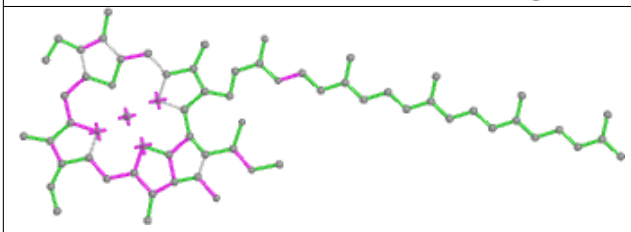


Rings

Ligand CLA d 201



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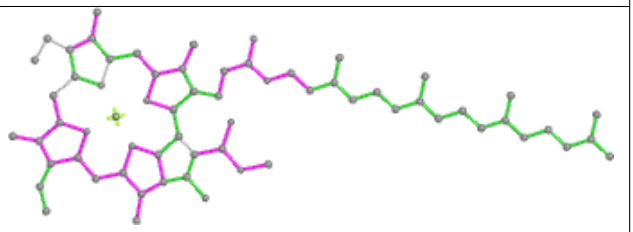
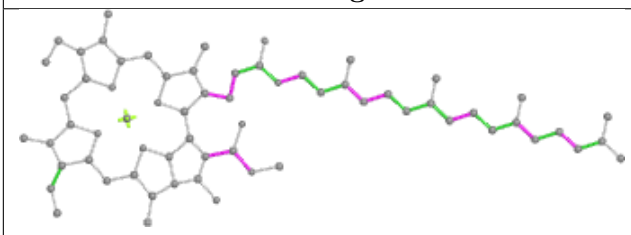


Bond angles



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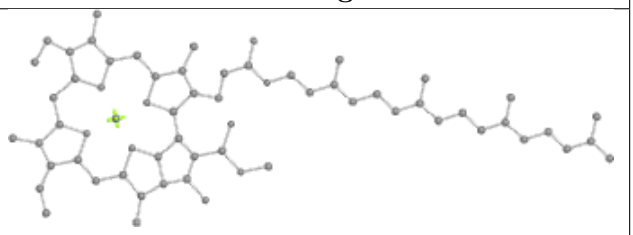
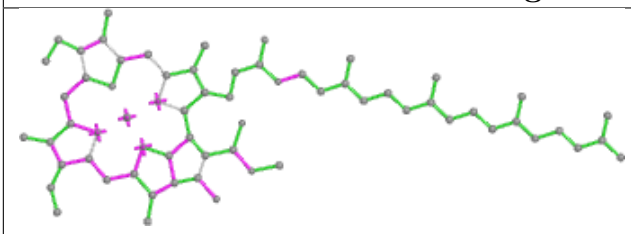


Rings

Ligand CLA B 812



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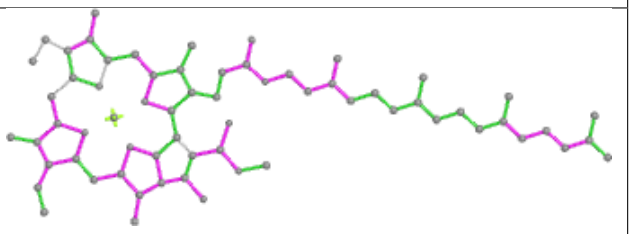

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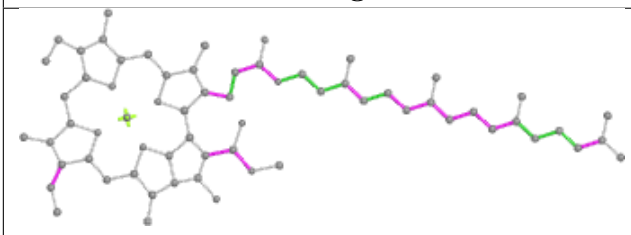

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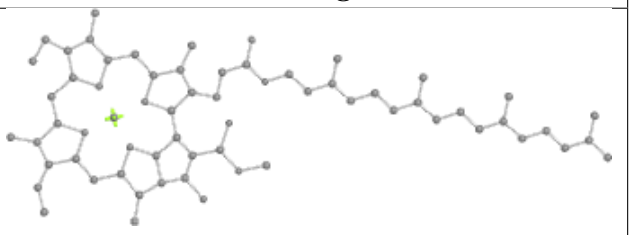
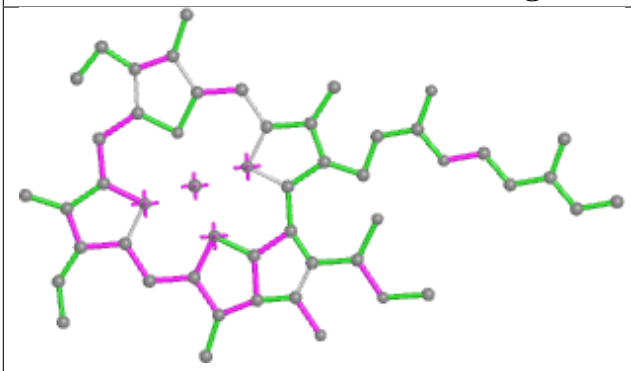


Rings

Ligand CLA A 808



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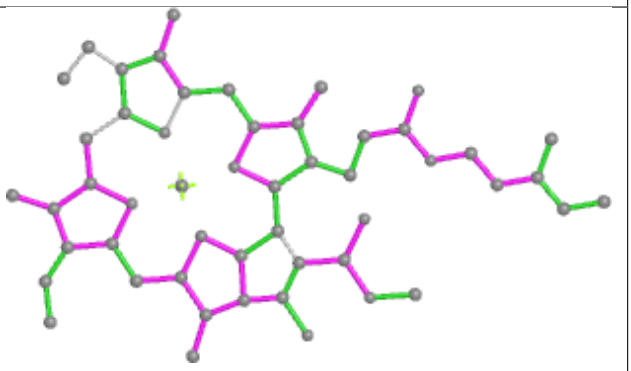

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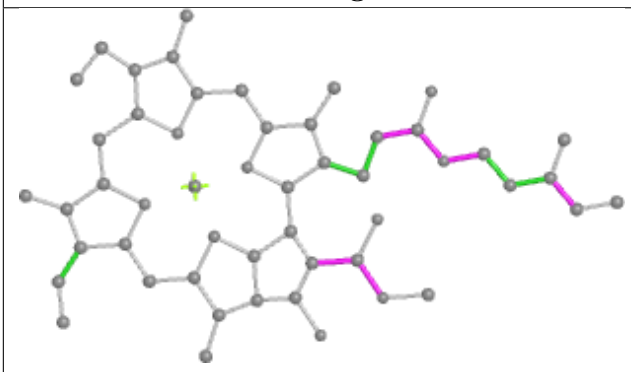

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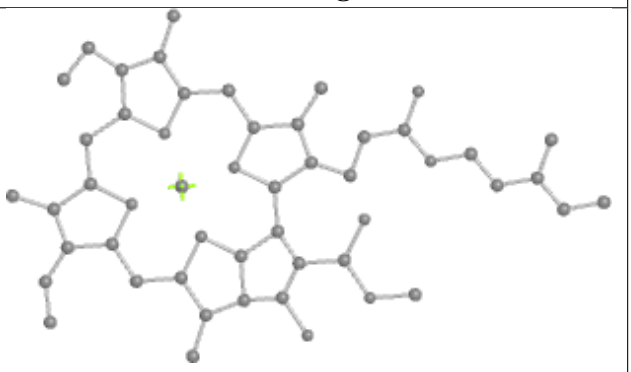
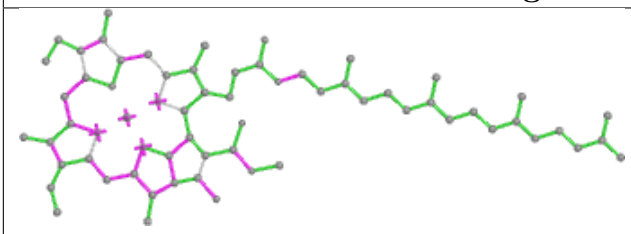
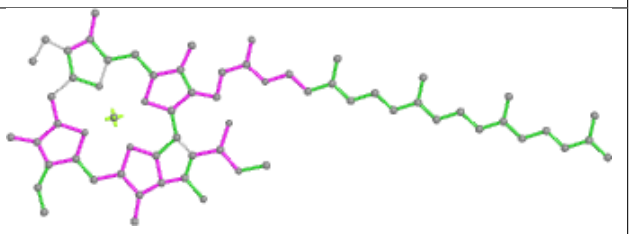
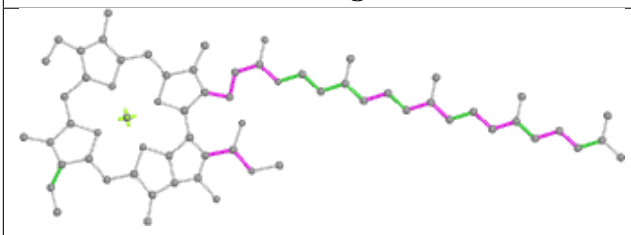
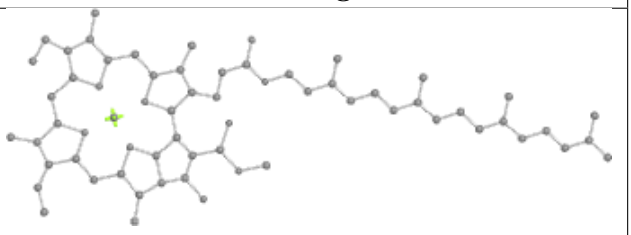
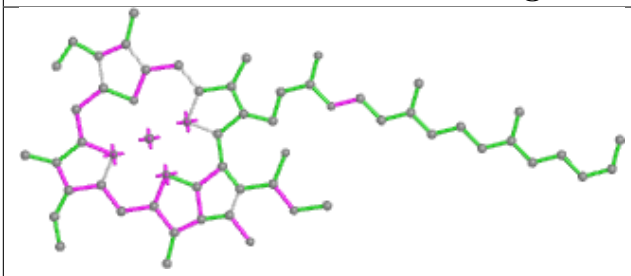
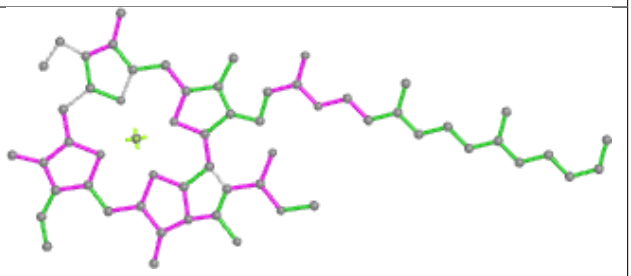
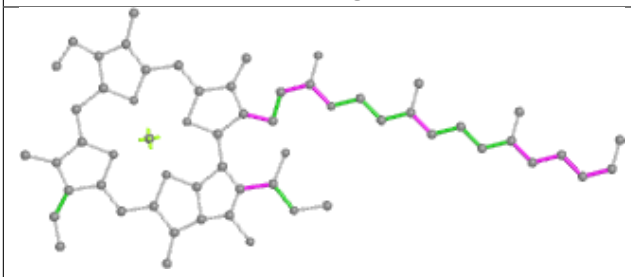
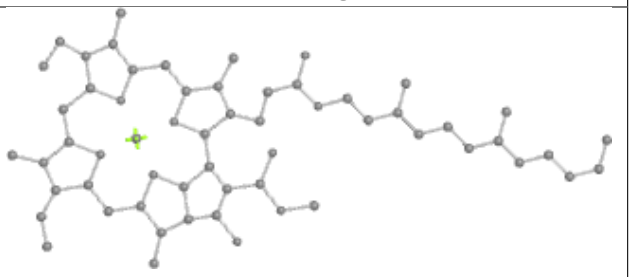


Rings

Ligand CLA G 811	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA A 805	
 Bond lengths	 Bond angles
 Torsions	 Rings

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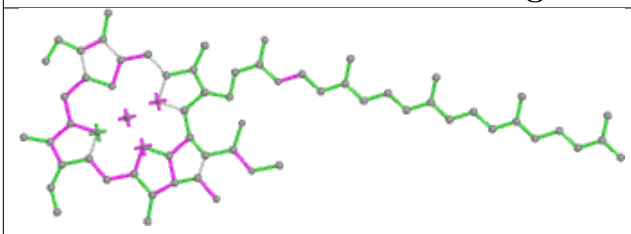
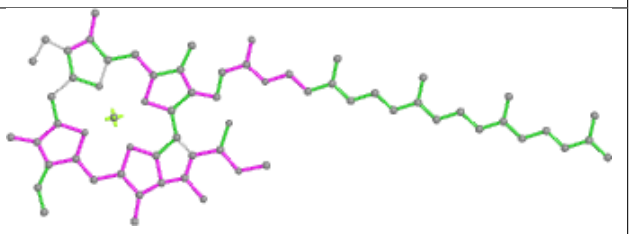
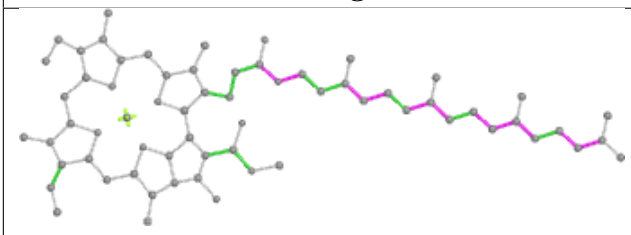
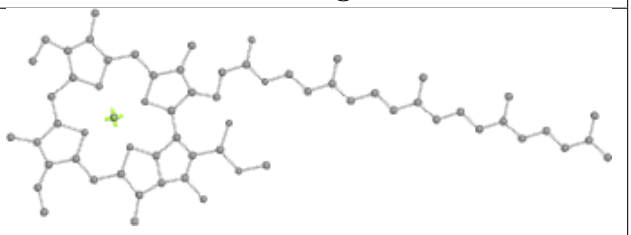
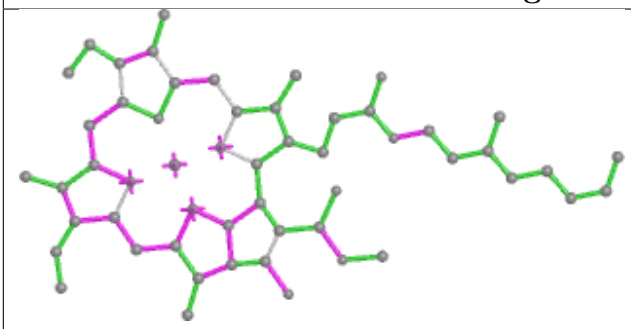
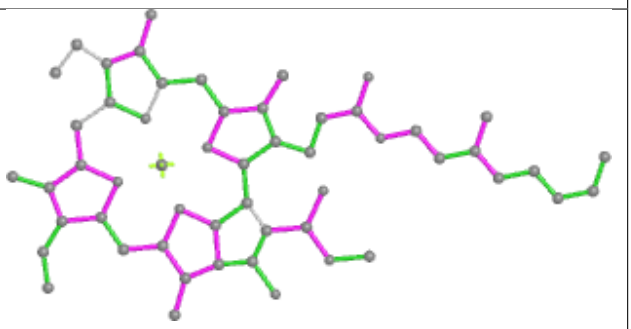
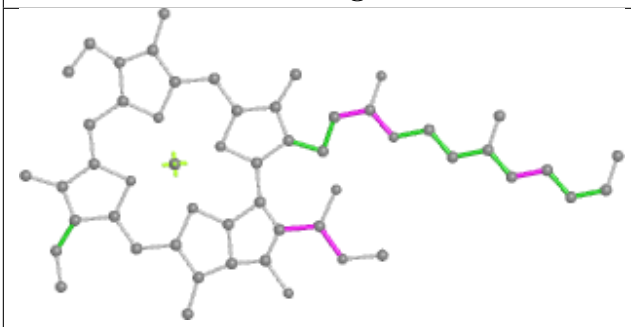
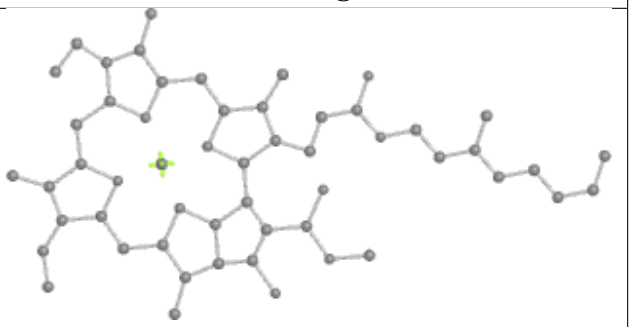
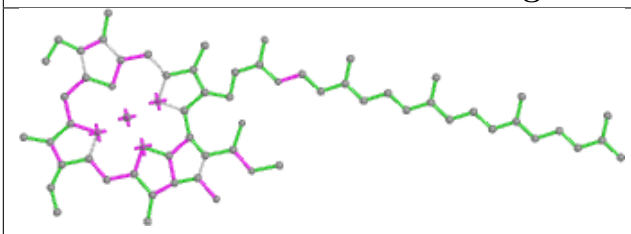
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA A 813	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA G 841



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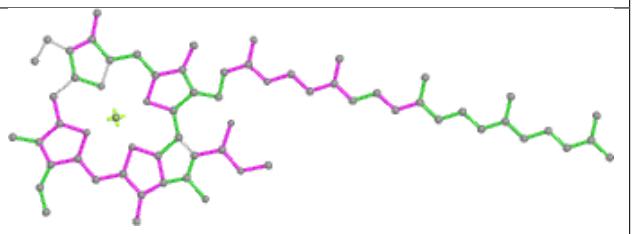
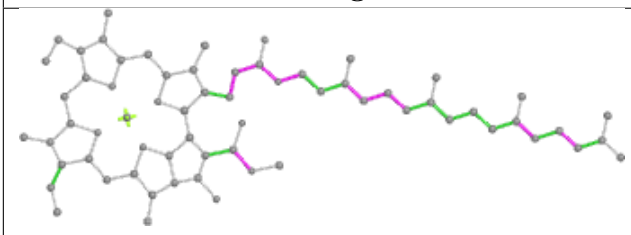


Bond angles



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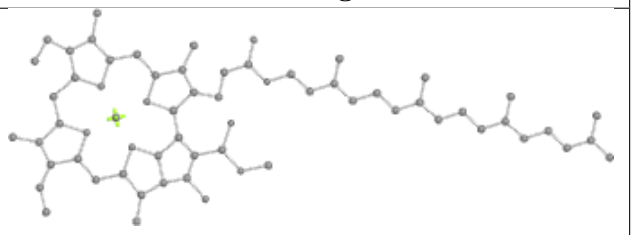
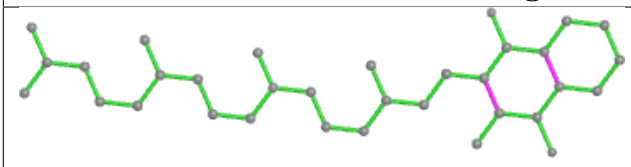


Rings

Ligand PQN Z 842



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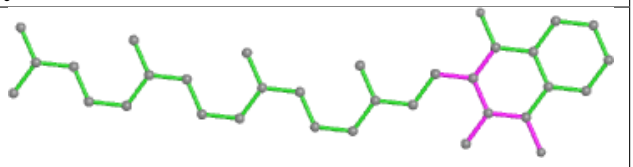

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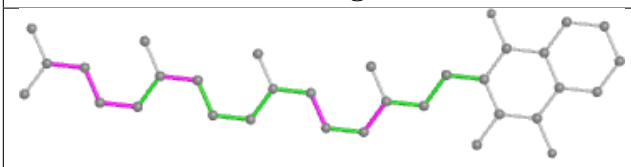

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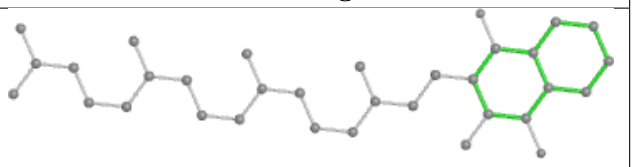
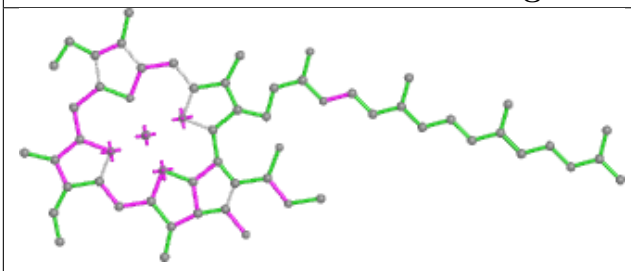


Rings

Ligand CLA Y 824



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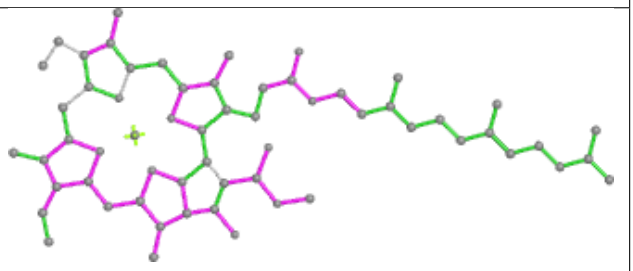

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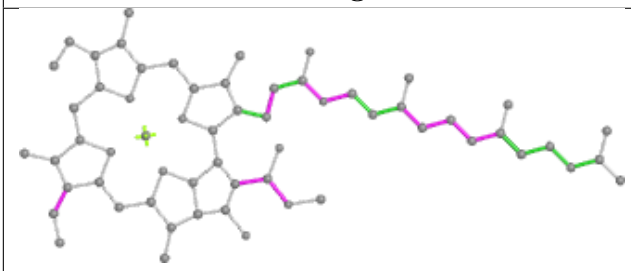

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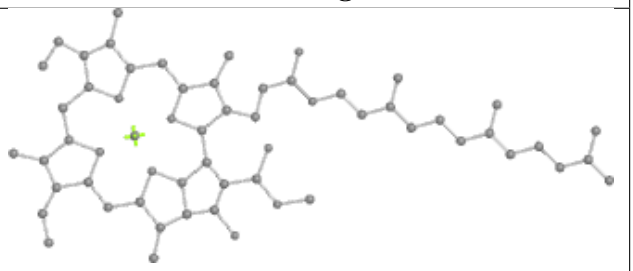
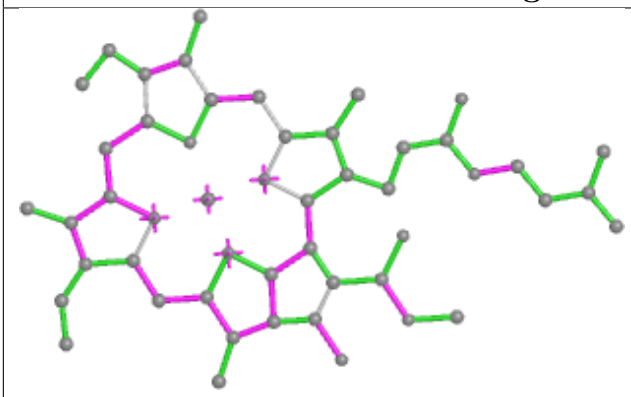


Rings

Ligand CLA G 814



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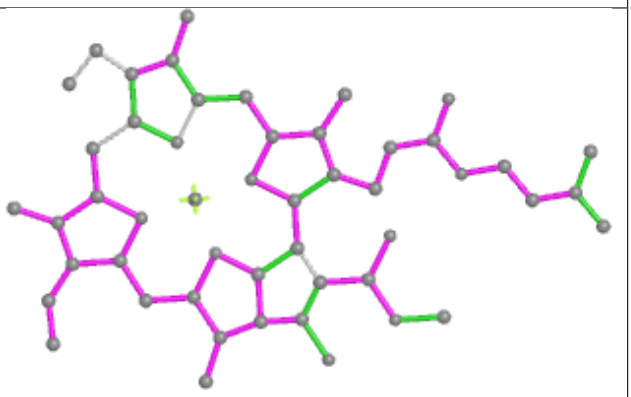

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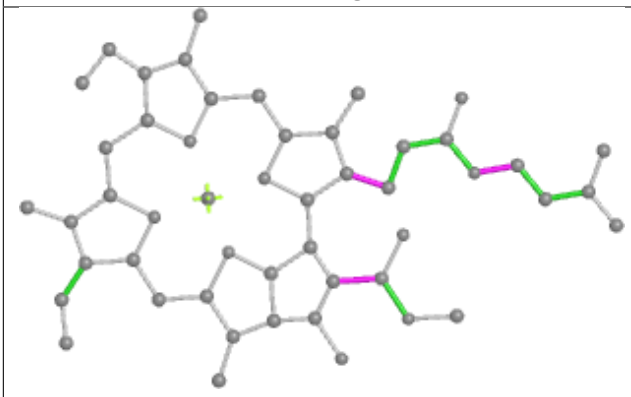

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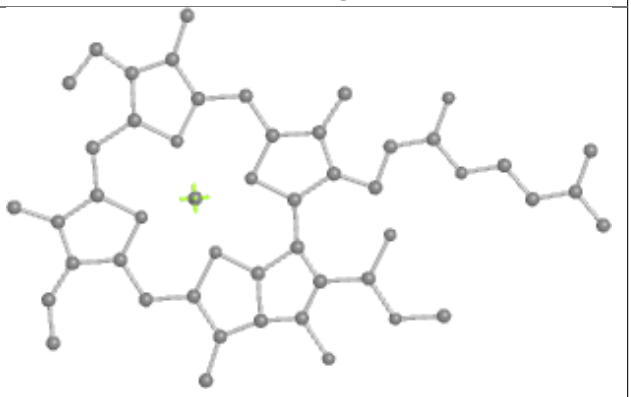
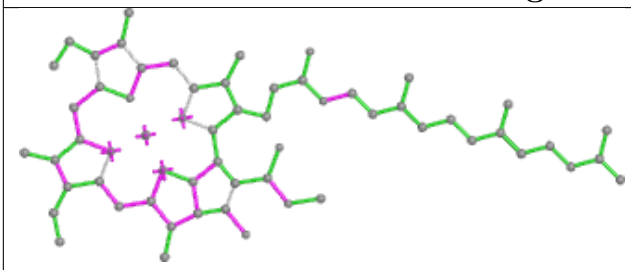


Rings

Ligand CLA Z 837



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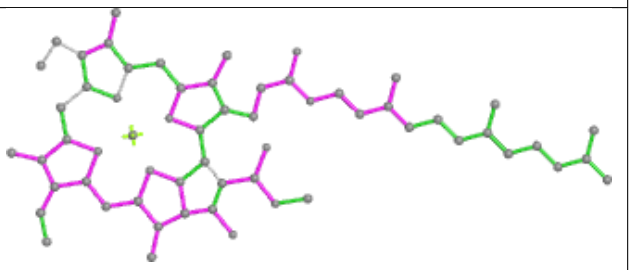

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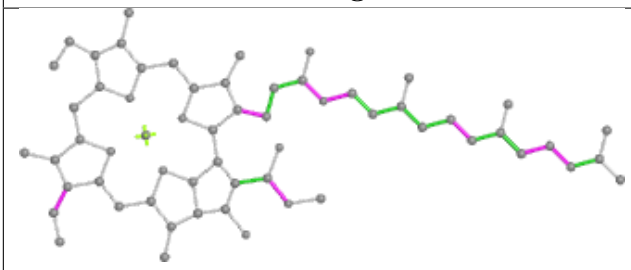

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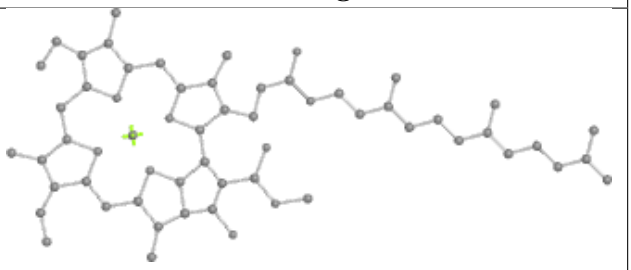
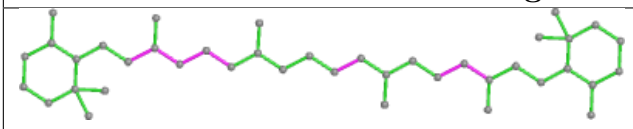


Rings

Ligand BCR Z 843



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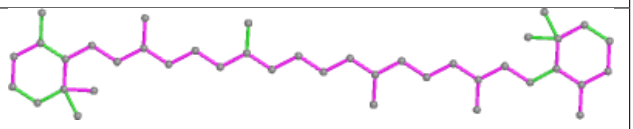

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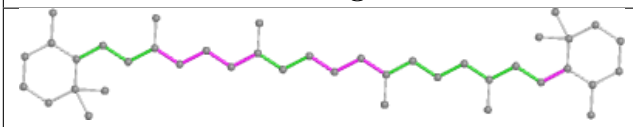

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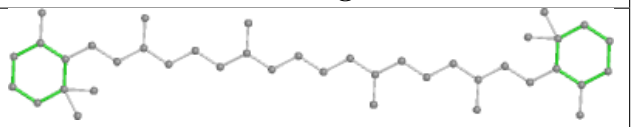
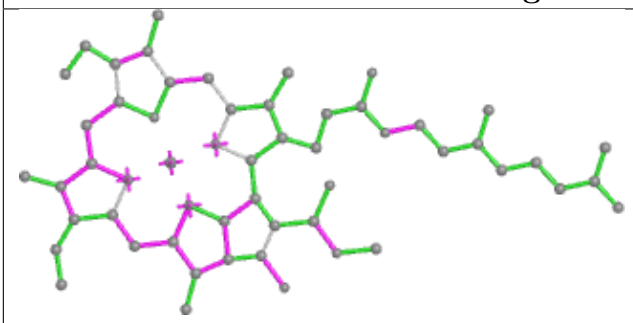


Rings

Ligand CLA G 834



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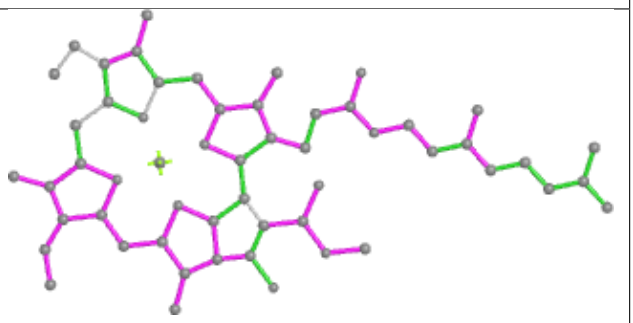

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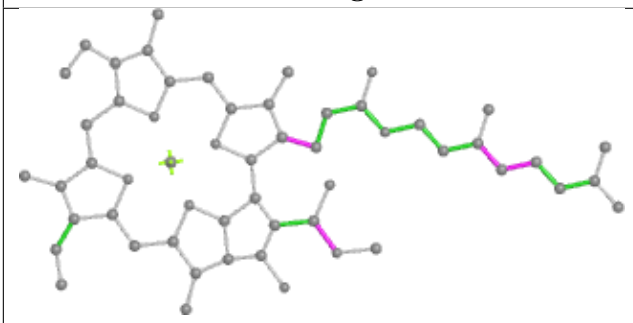

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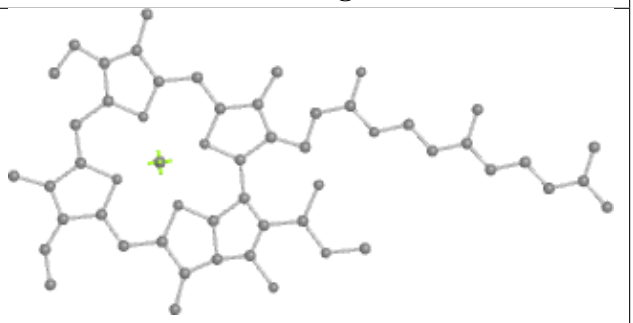

Rings

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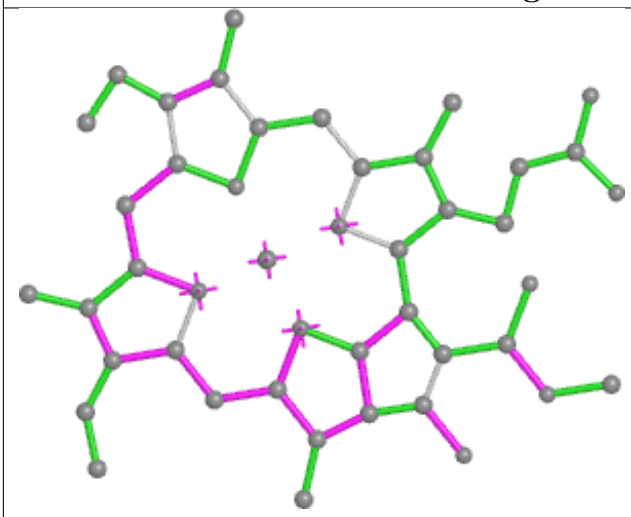

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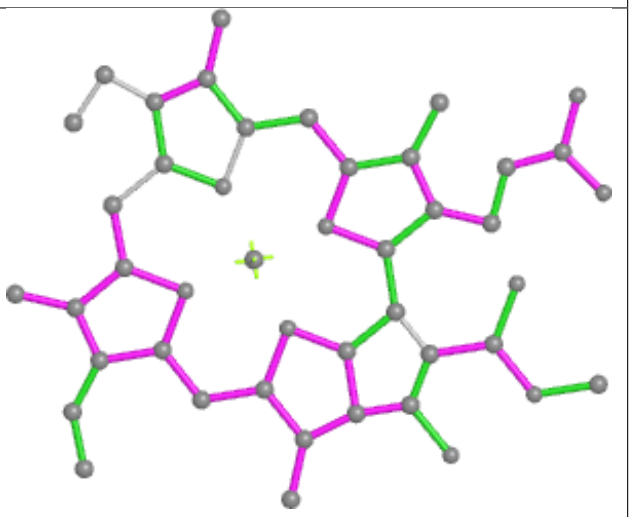

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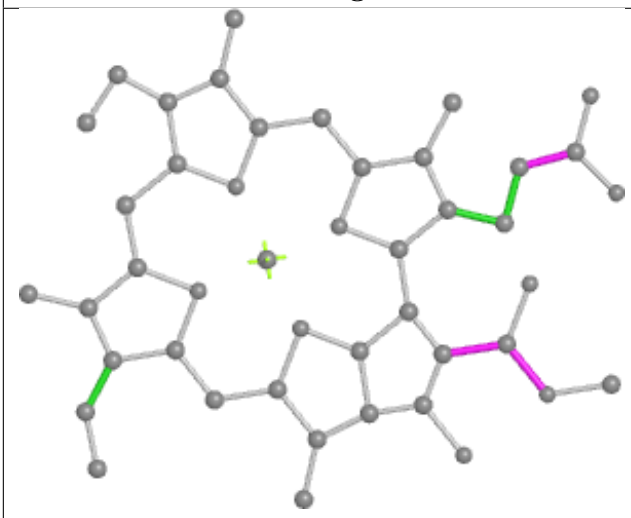

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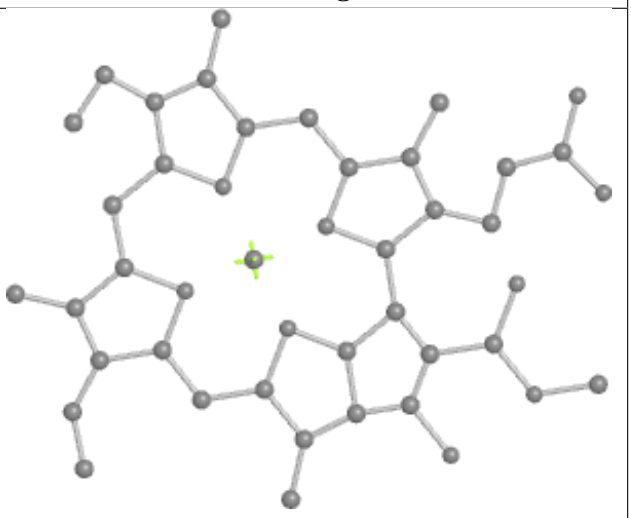

Rings

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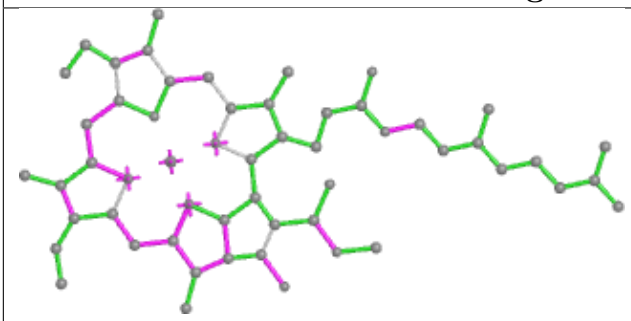

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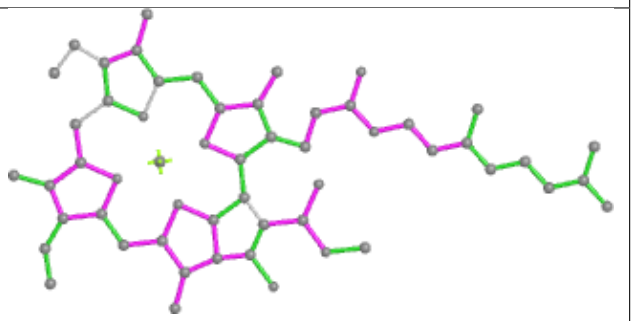

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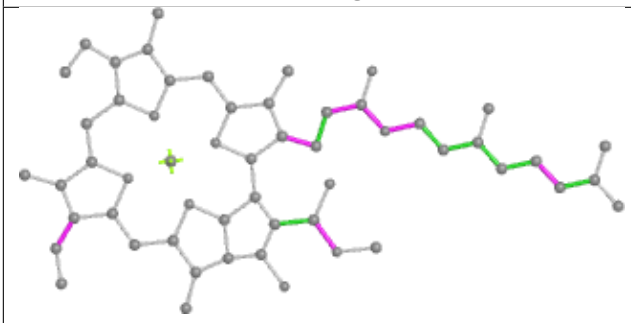

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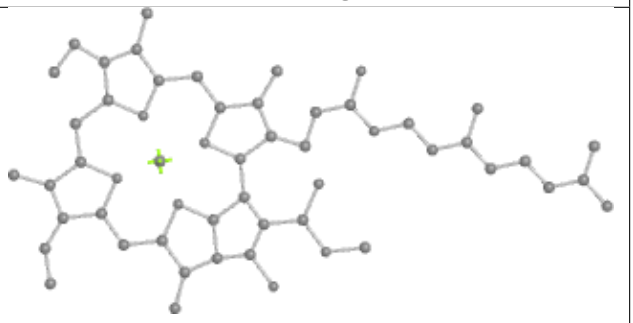

Rings

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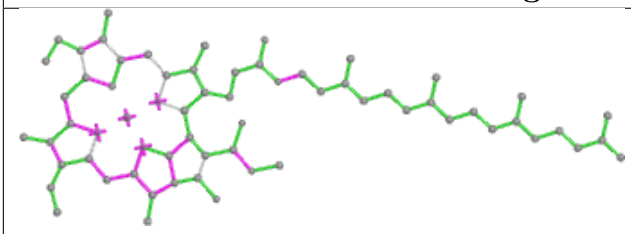

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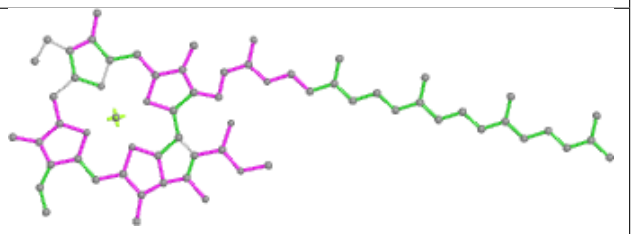

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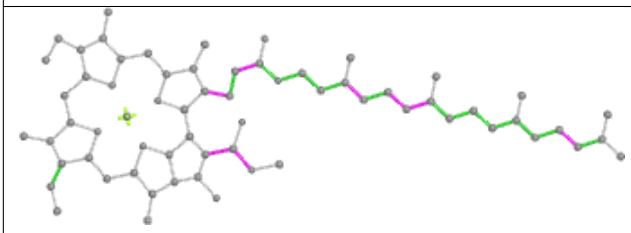

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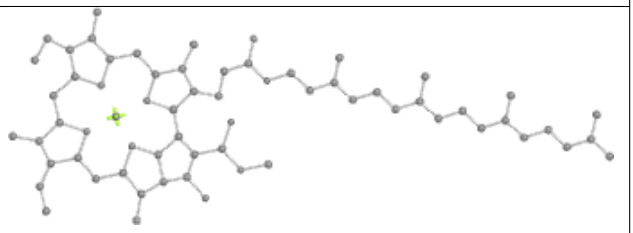
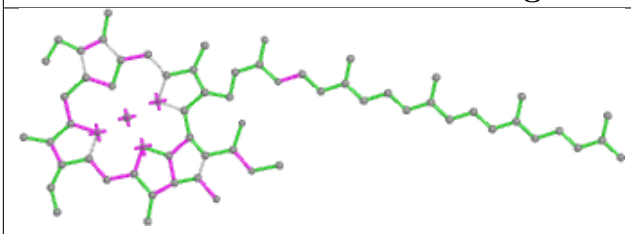
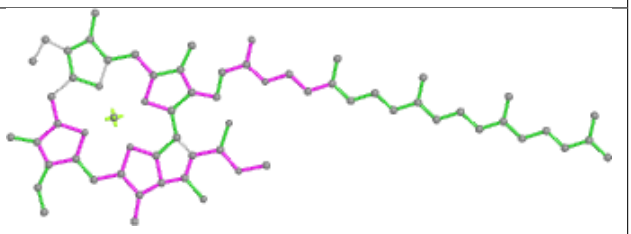
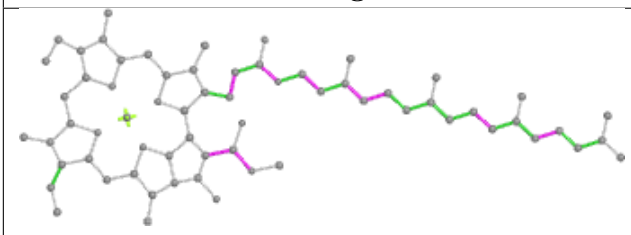
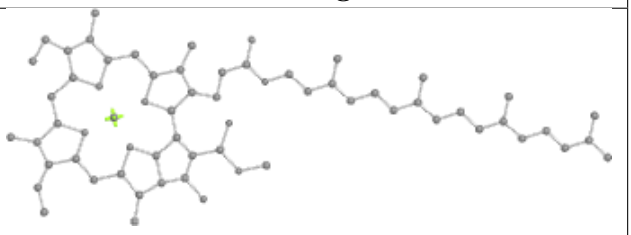


Rings

Ligand CLA A 802	
 Bond lengths	 Bond angles
 Torsions	 Rings

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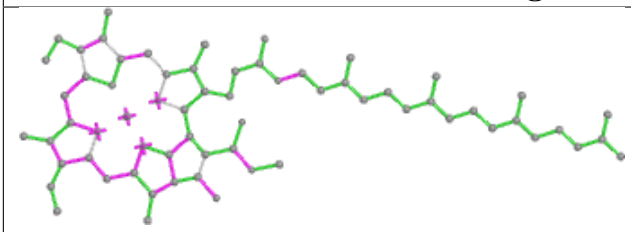
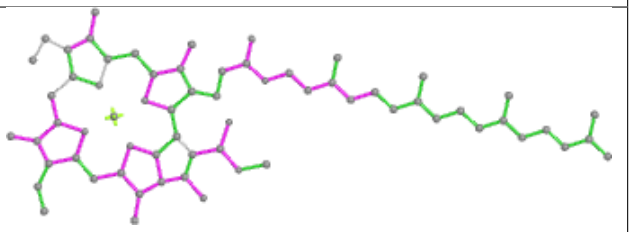
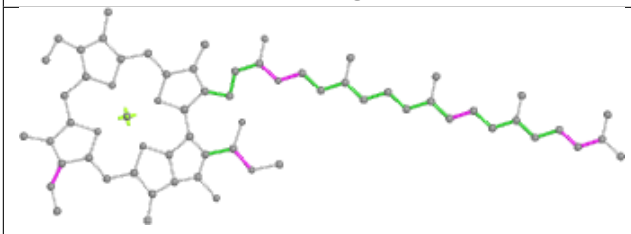
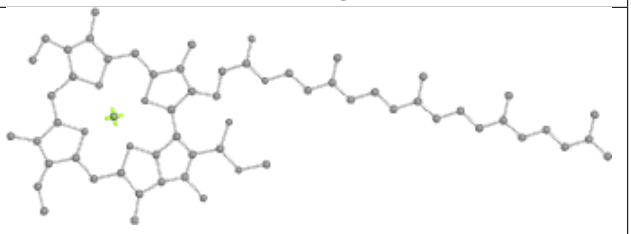
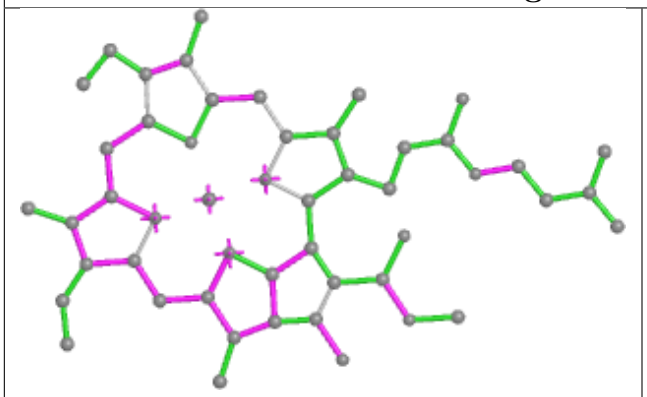
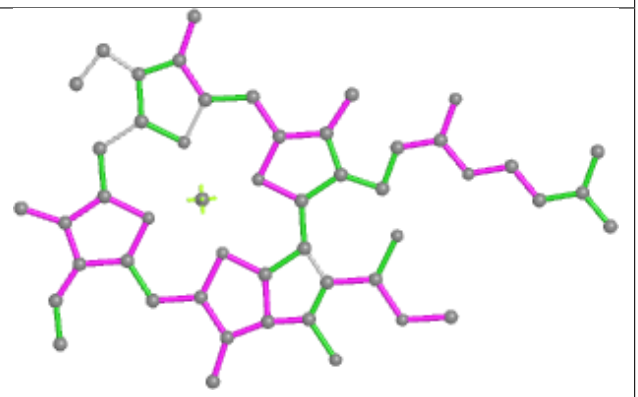
 Bond lengths	 Bond angles
 Torsions	 Rings

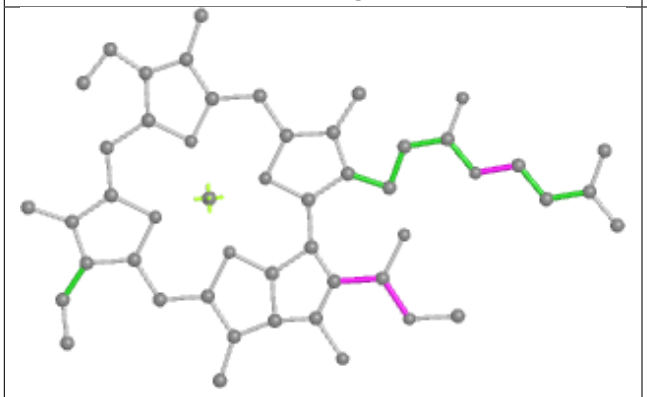
Ligand CLA A 840



Bond lengths



Bond angles



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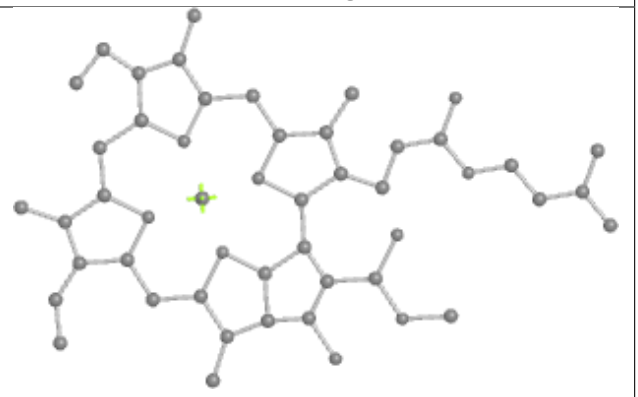
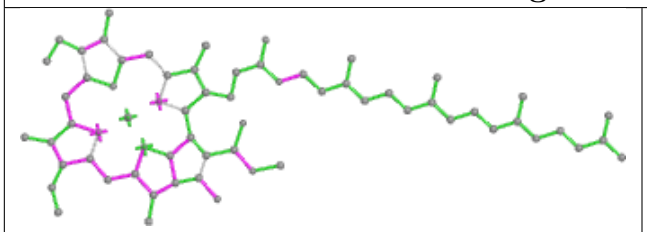
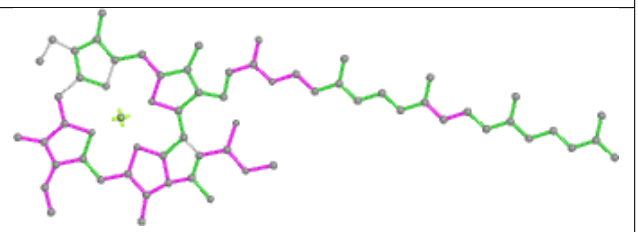


Rings

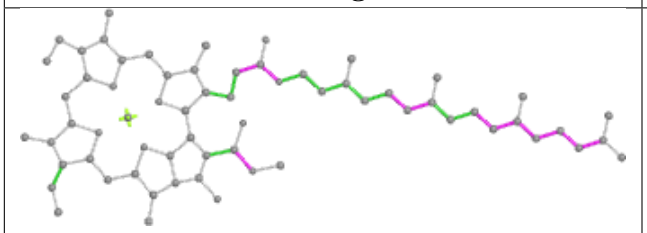
Ligand CL0 Y 801



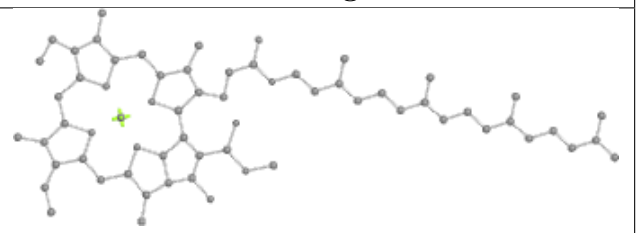
Bond lengths



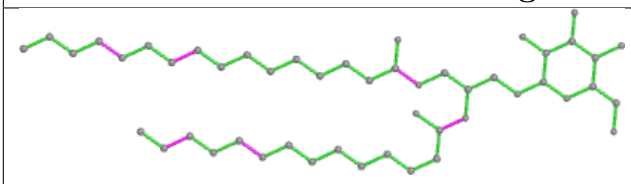
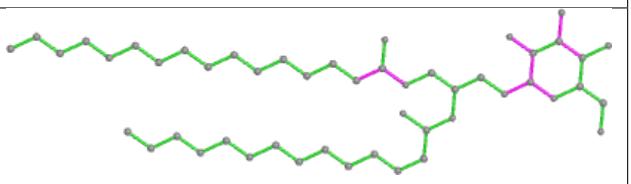
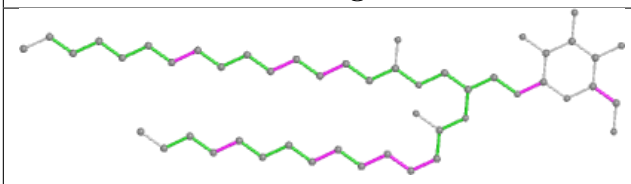
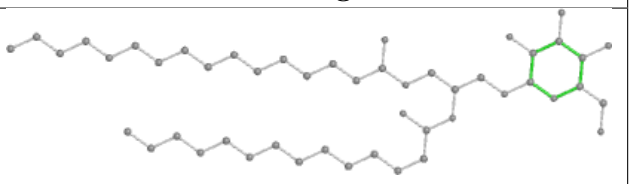
Bond angles

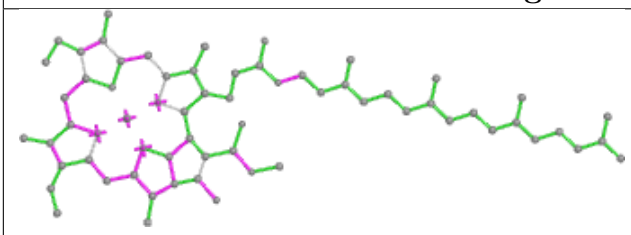
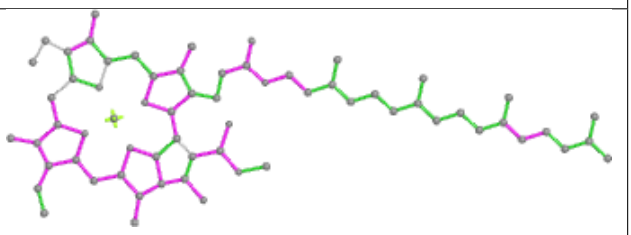
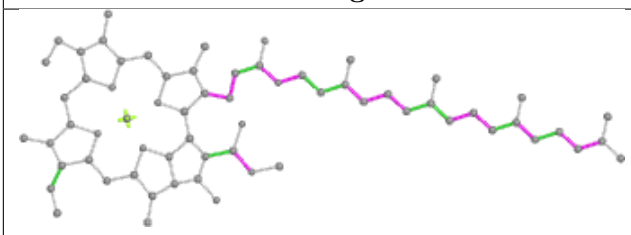
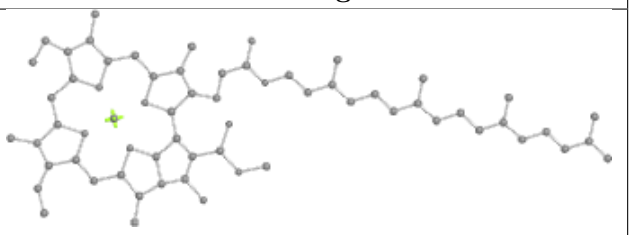


Torsions

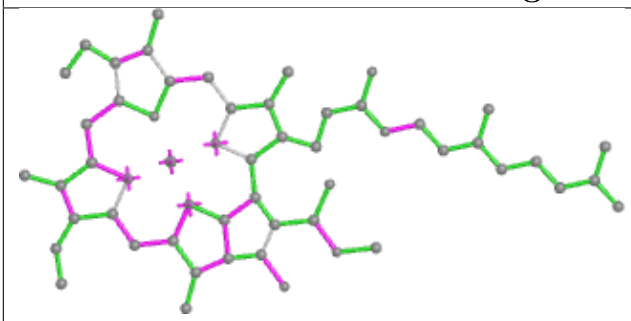


Rings

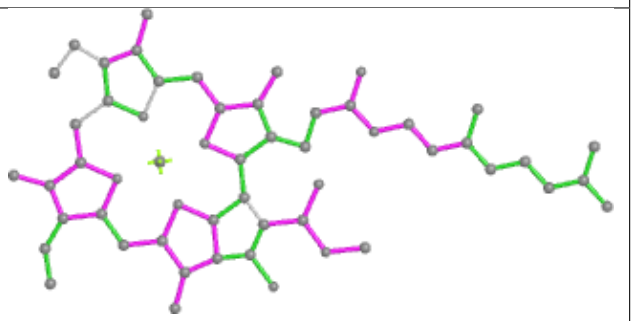
Ligand LMG H 848	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA B 831	
 Bond lengths	 Bond angles
 Torsions	 Rings

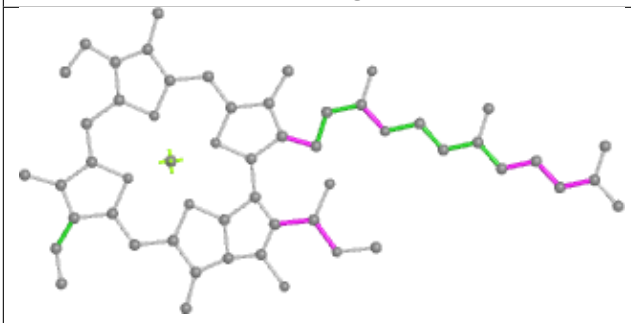
Ligand CLA H 832



Bond lengths



Bond angles



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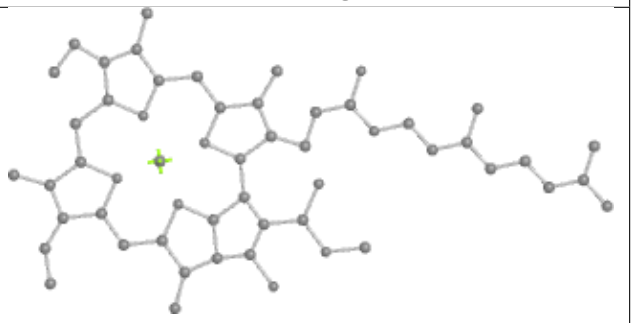
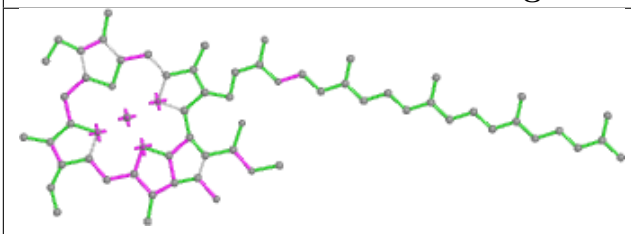


Rings

Ligand CLA Y 806



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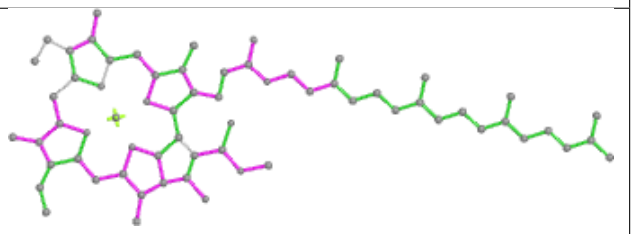

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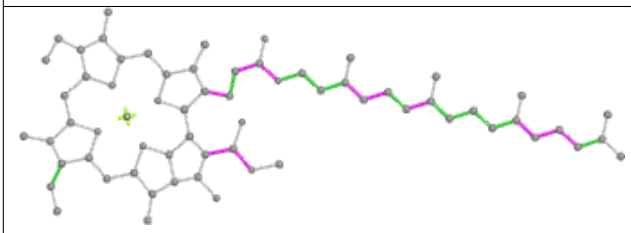

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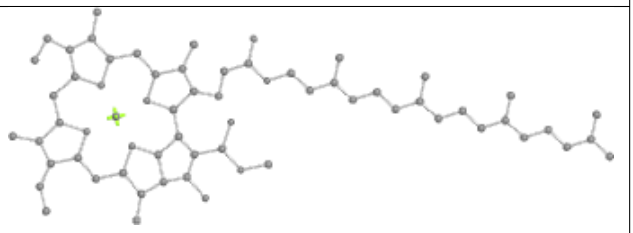

Rings

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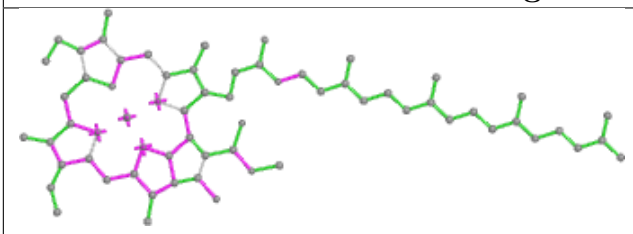

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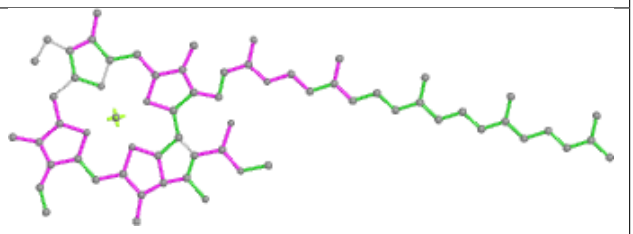
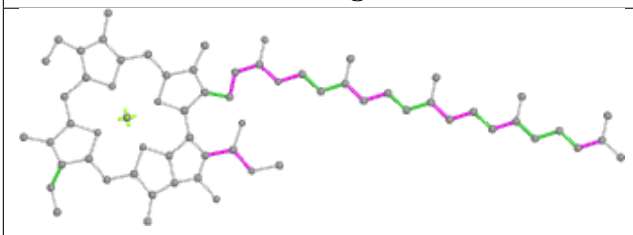


Bond angles



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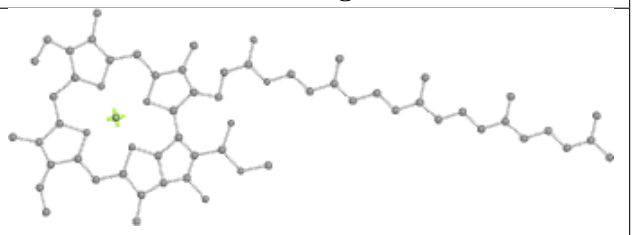
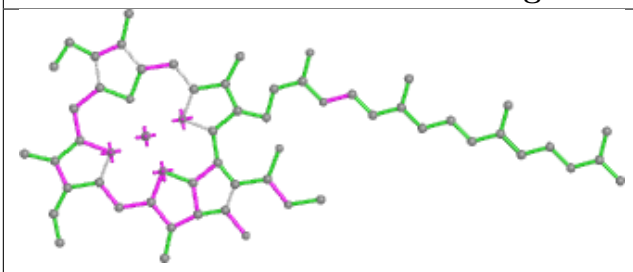


Rings

Ligand CLA Y 820



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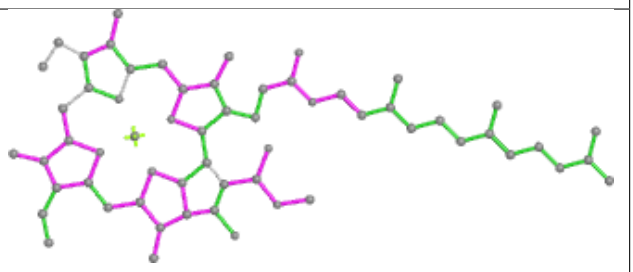
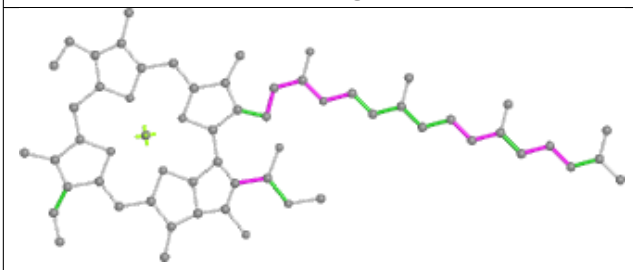


Bond angles



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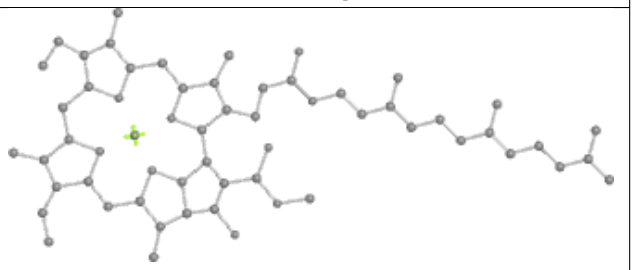
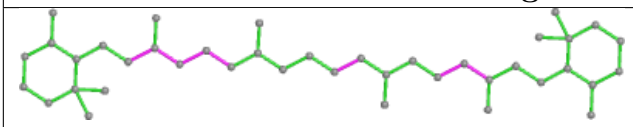


Rings

Ligand BCR H 842



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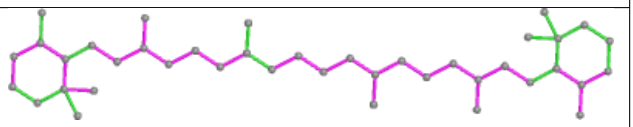
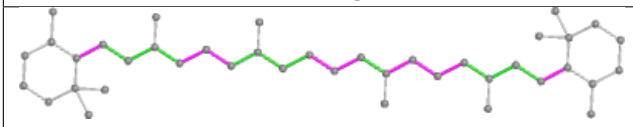
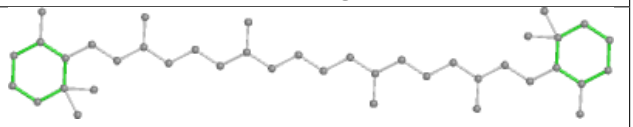


Bond angles

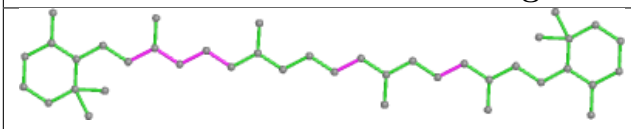


Torsions



Rings

Ligand BCR Y 846



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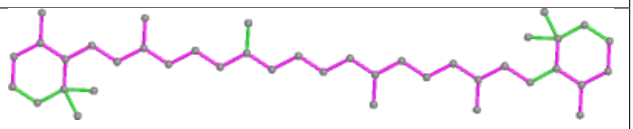
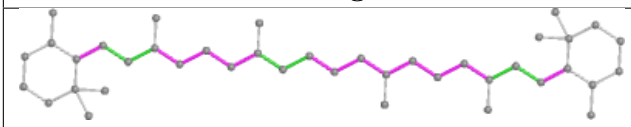


Bond angles



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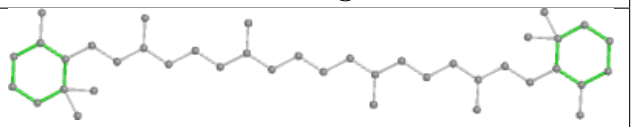
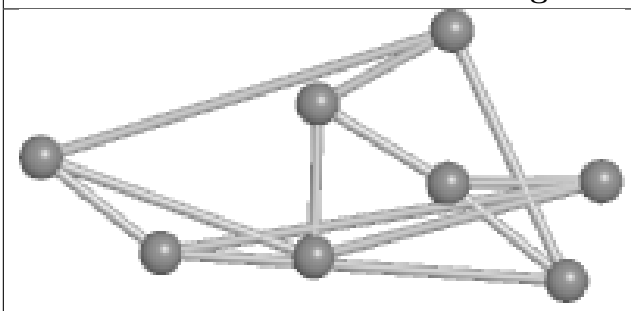


Rings

Ligand SF4 N 101



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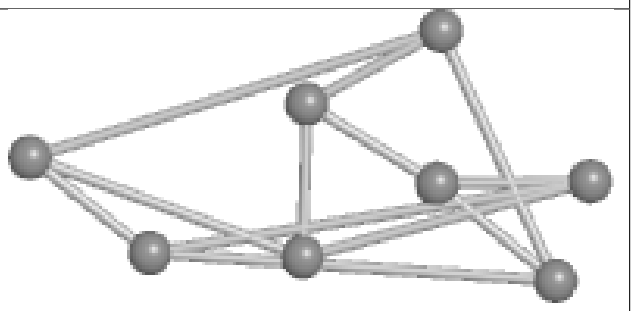
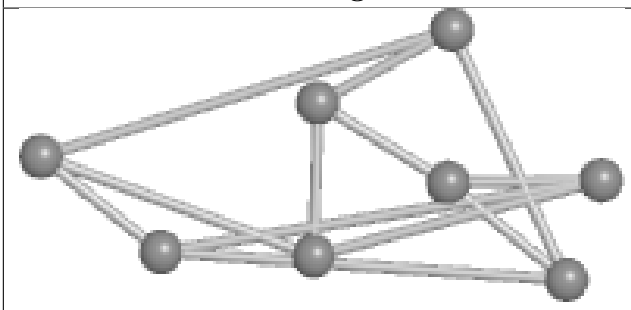


Bond angles



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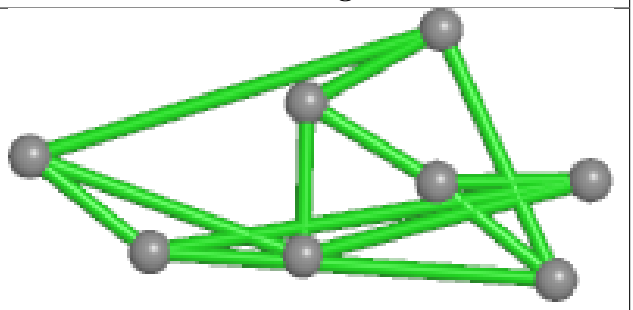
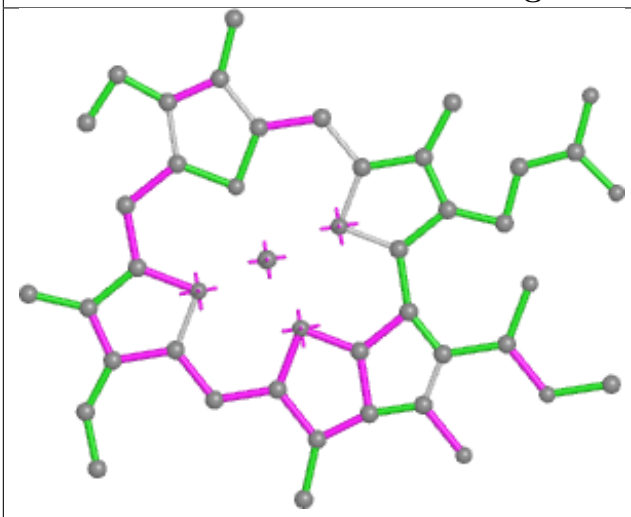


Rings

Ligand CLA B 820



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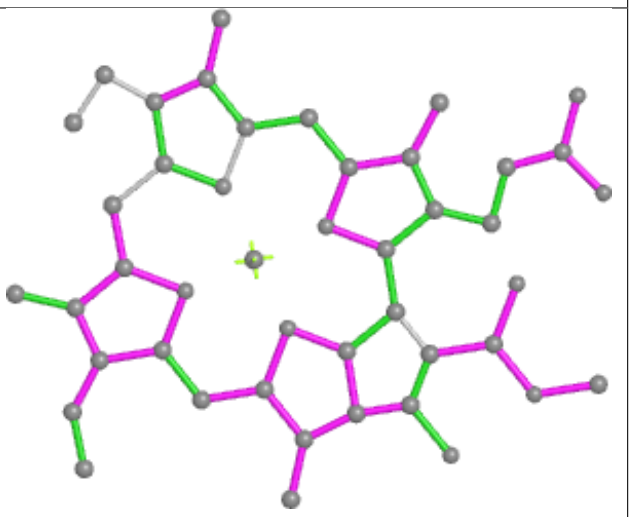
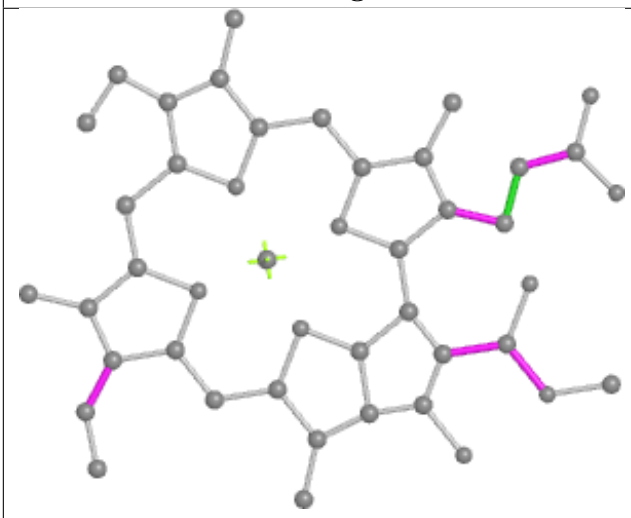


Bond angles



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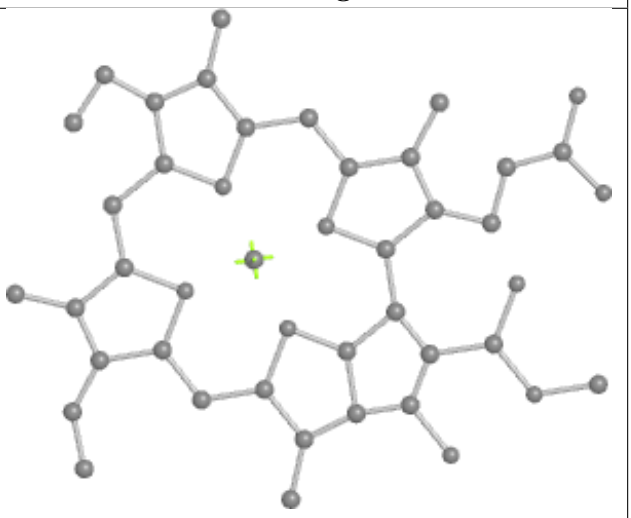
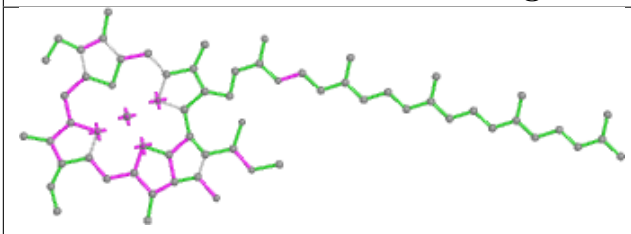


Rings

Ligand CLA H 801



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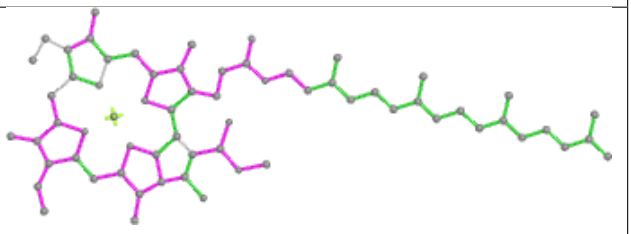
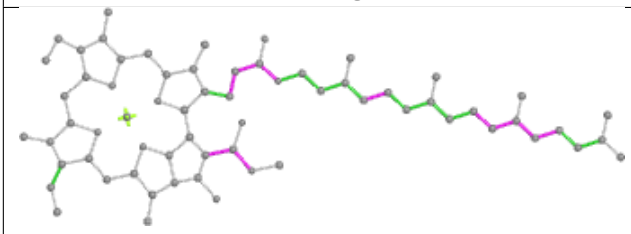


Bond angles



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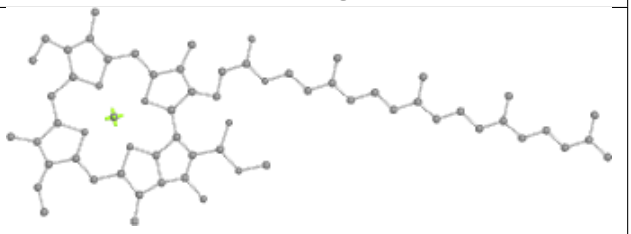
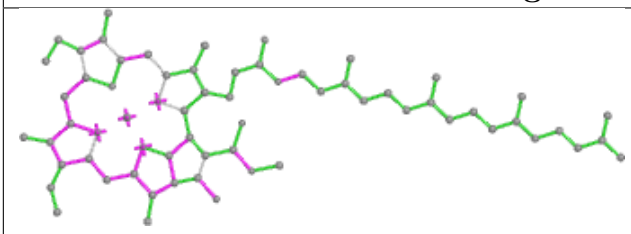


Rings

Ligand CLA A 820



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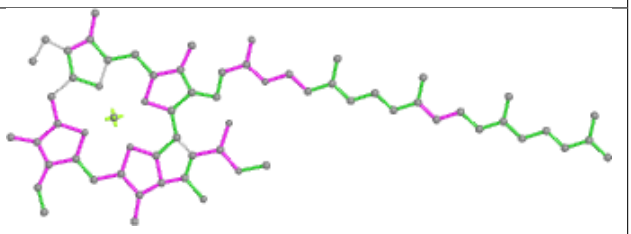
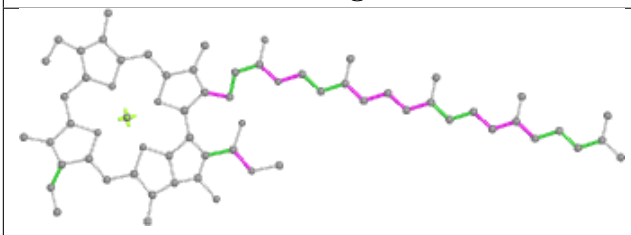


Bond angles



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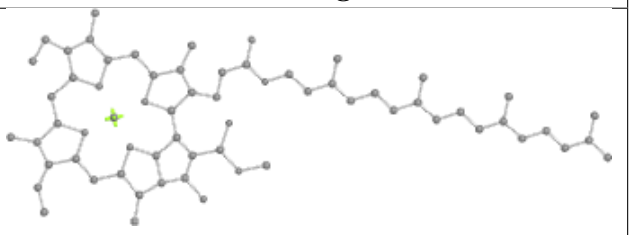
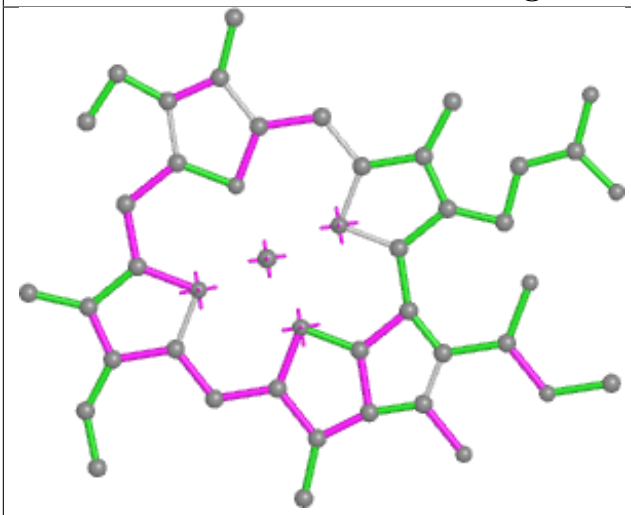
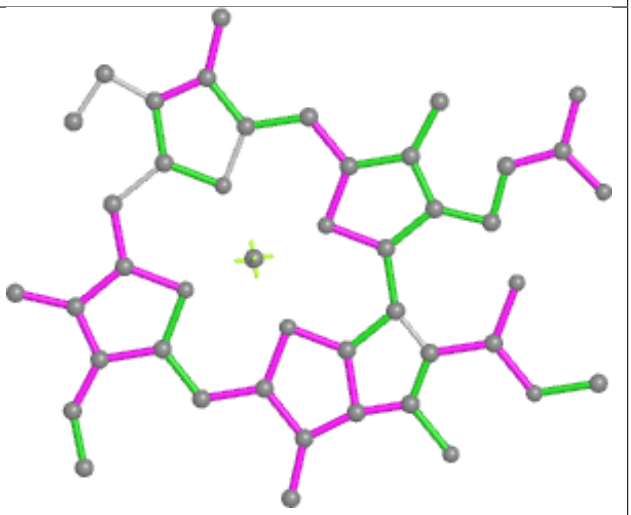


Rings

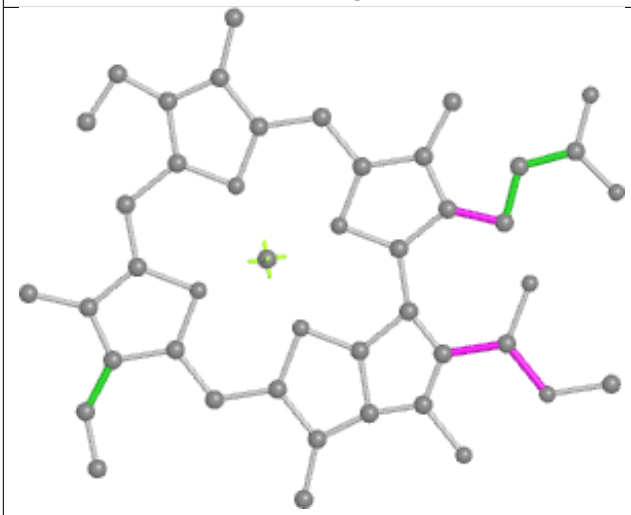
Ligand CLA H 833



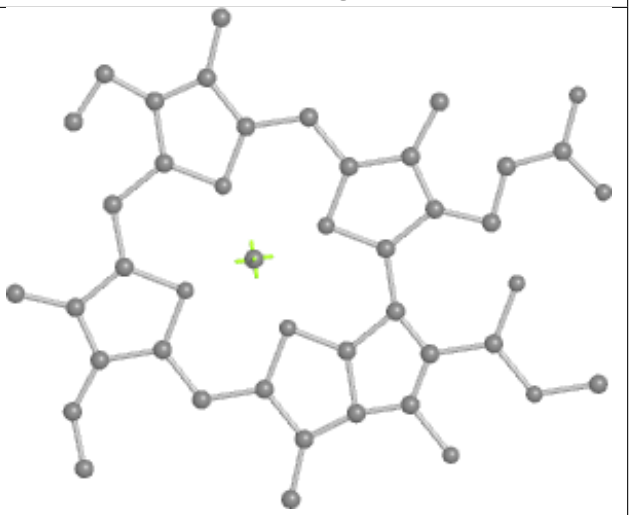
Bond lengths



Bond angles

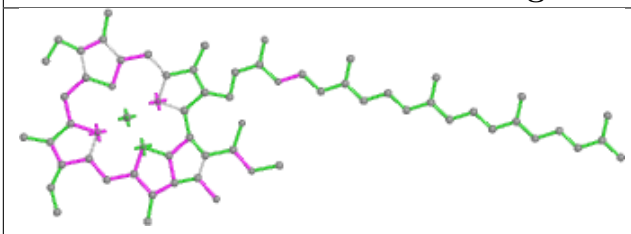


Torsions



Rings

Ligand CLA h 206



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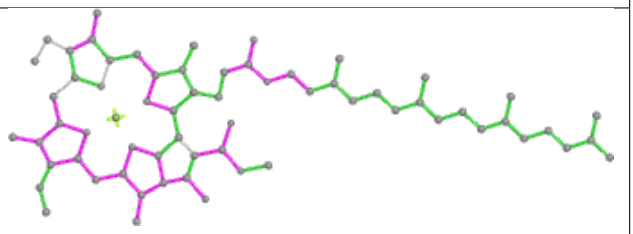
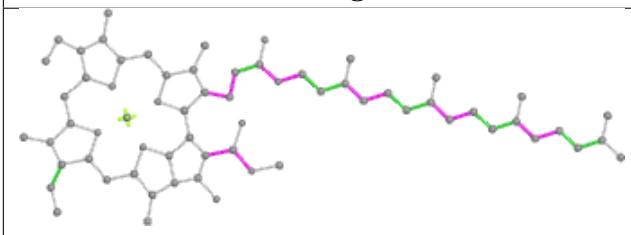


Bond angles



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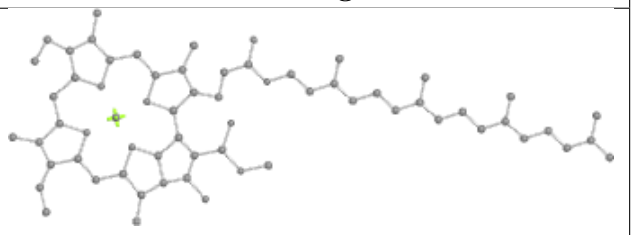
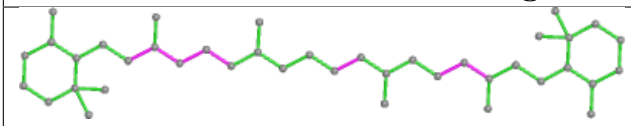


Rings

Ligand BCR G 849



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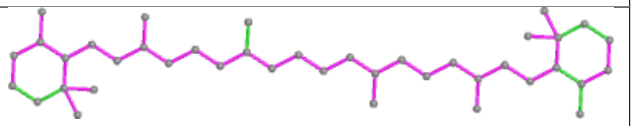
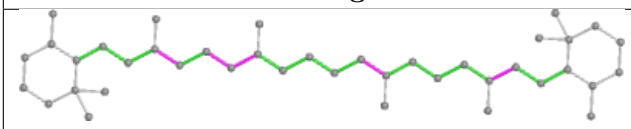


Bond angles



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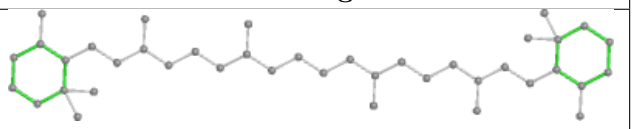
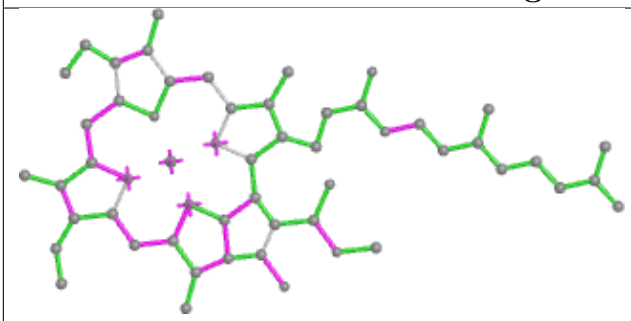


Rings

Ligand CLA B 823



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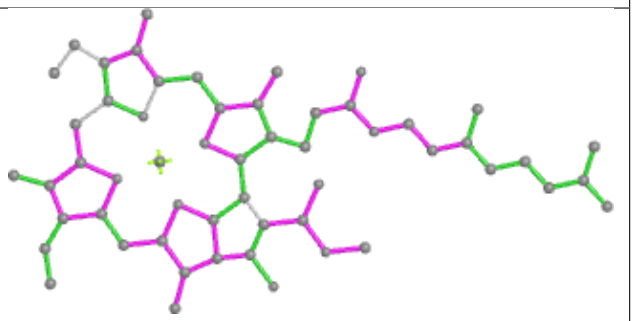
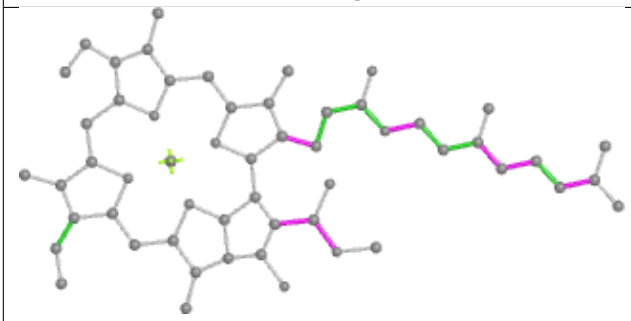


Bond angles



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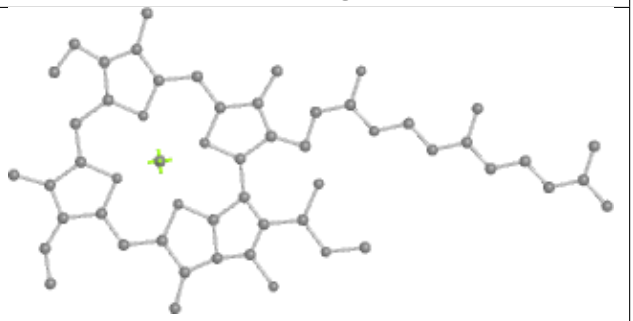
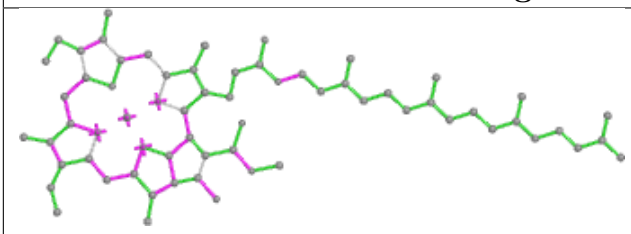


Rings

Ligand CLA U 1007



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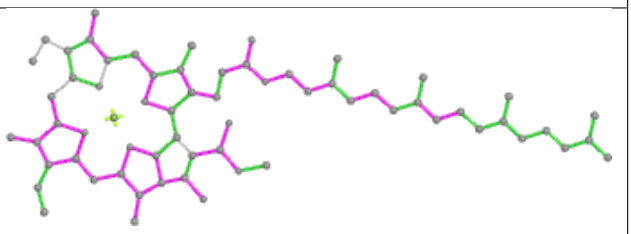
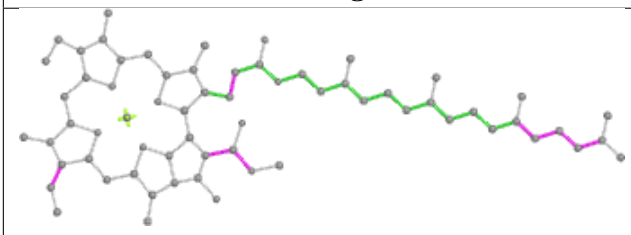


Bond angles



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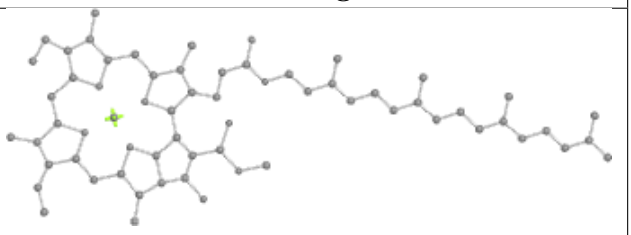
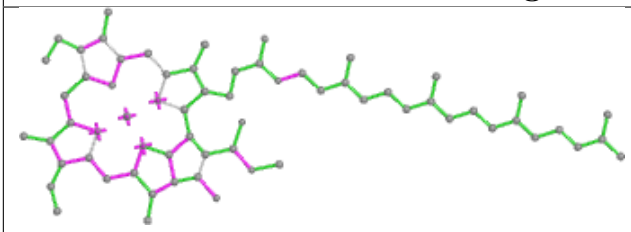


Rings

Ligand CLA H 809



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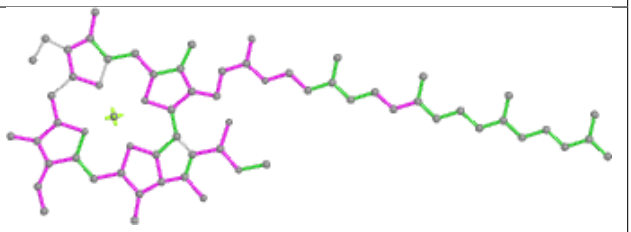
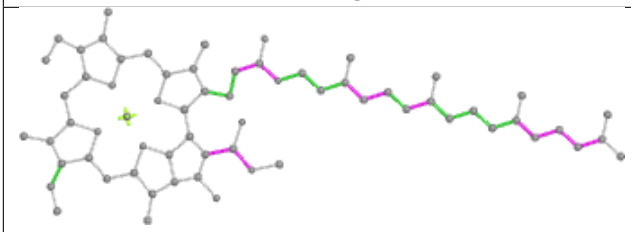


Bond angles



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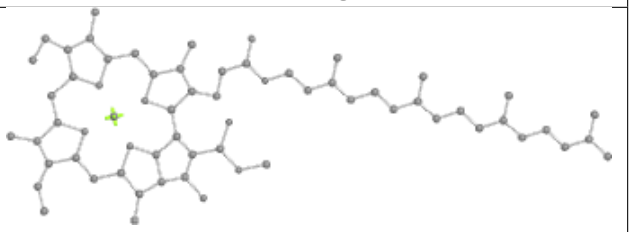
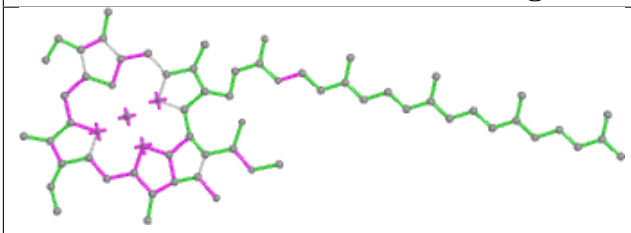


Rings

Ligand CLA Z 815



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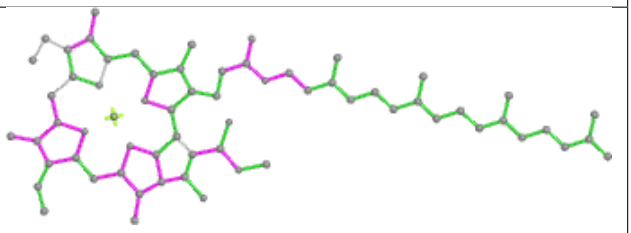
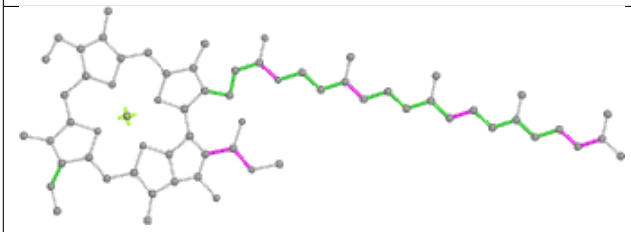
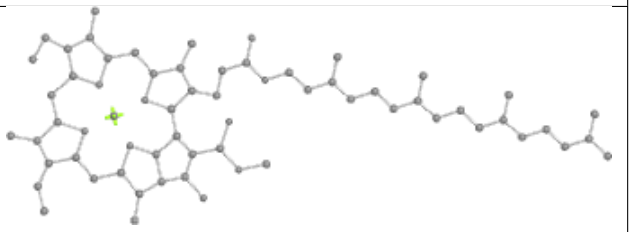


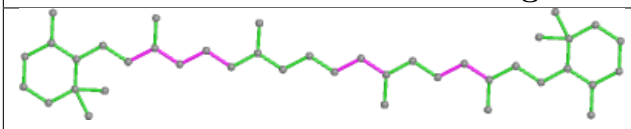
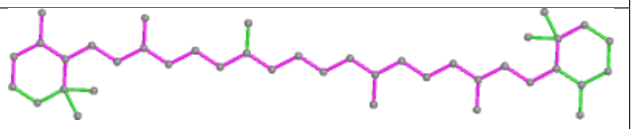
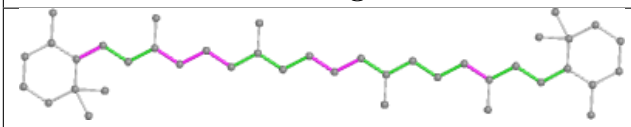
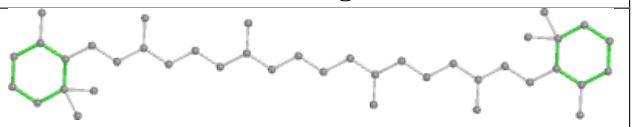
Bond angles



Torsions



Rings

Ligand BCR H 844	
 Bond lengths	 Bond angles
 Torsions	 Rings

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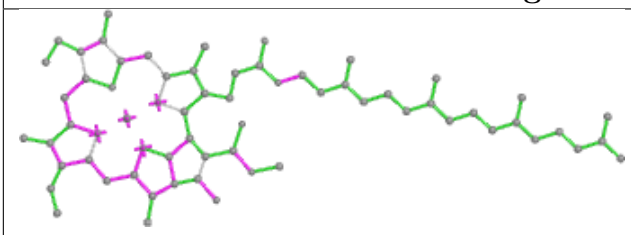
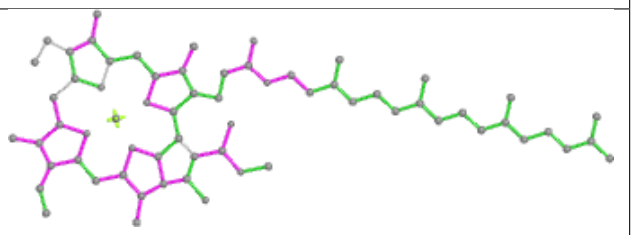
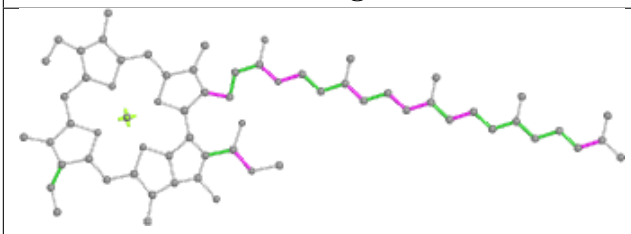
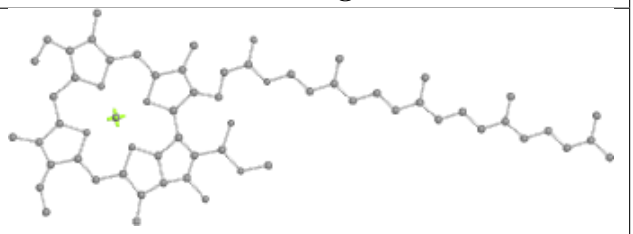
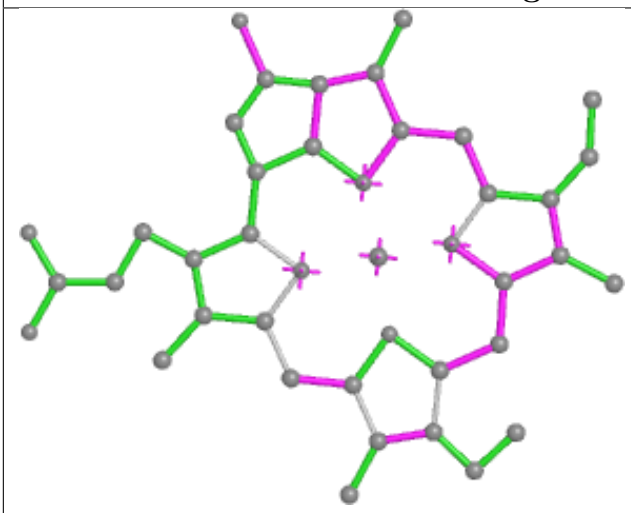
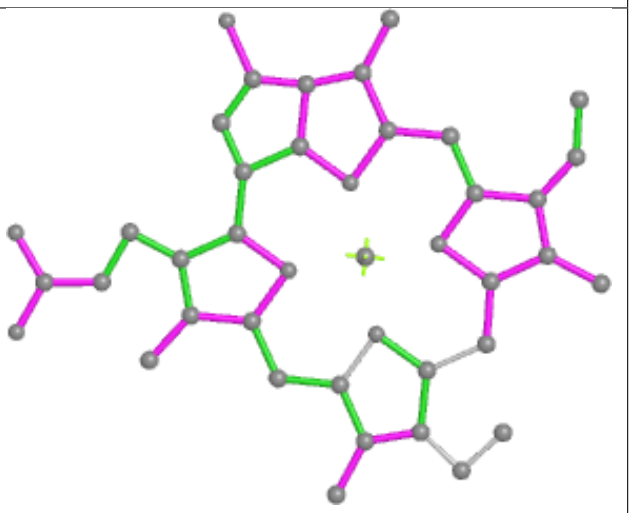
 Bond lengths	 Bond angles
 Torsions	 Rings

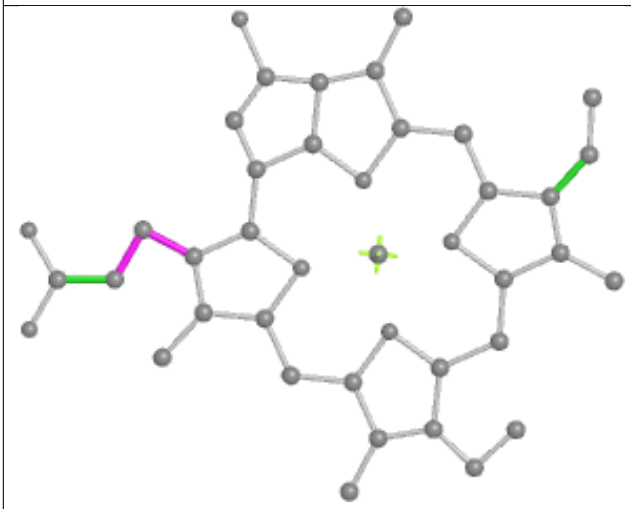
Ligand CLA K 101



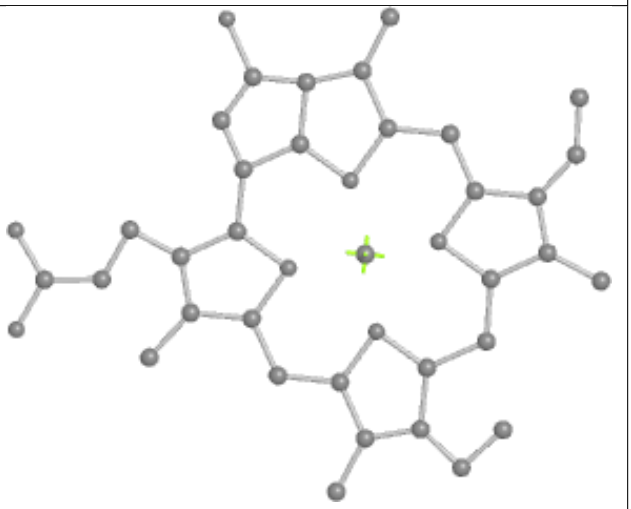
Bond lengths



Bond angles

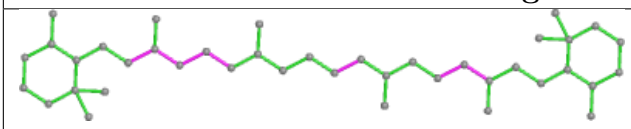


Torsions



Rings

Ligand BCR A 851



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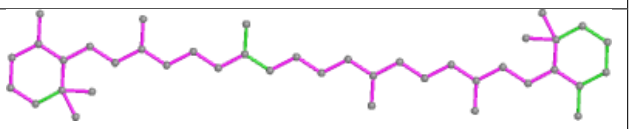
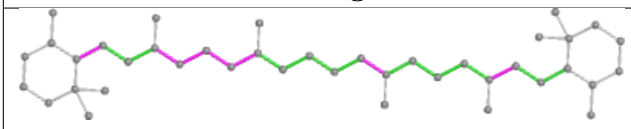


Bond angles



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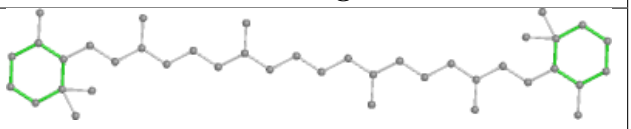
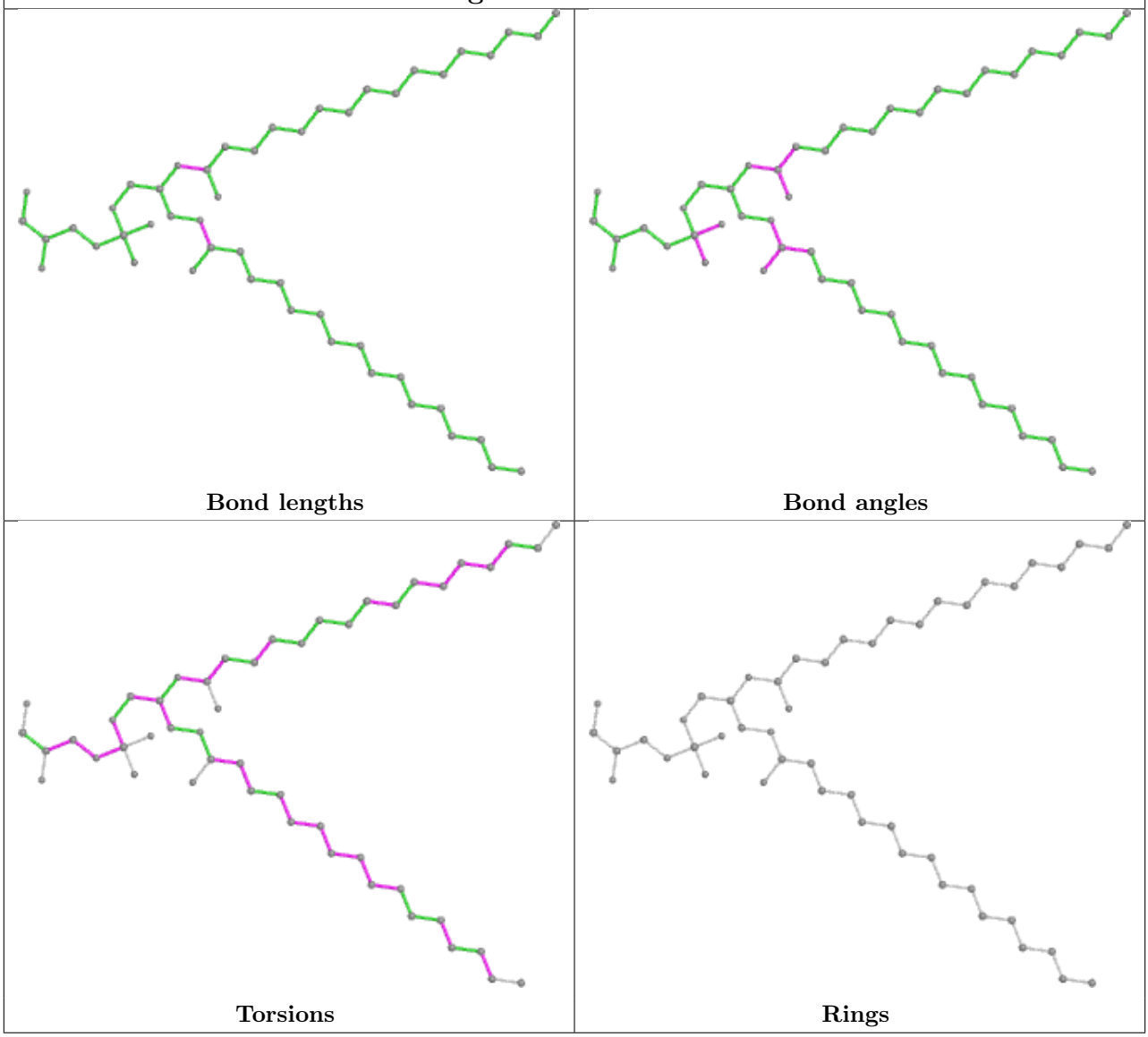
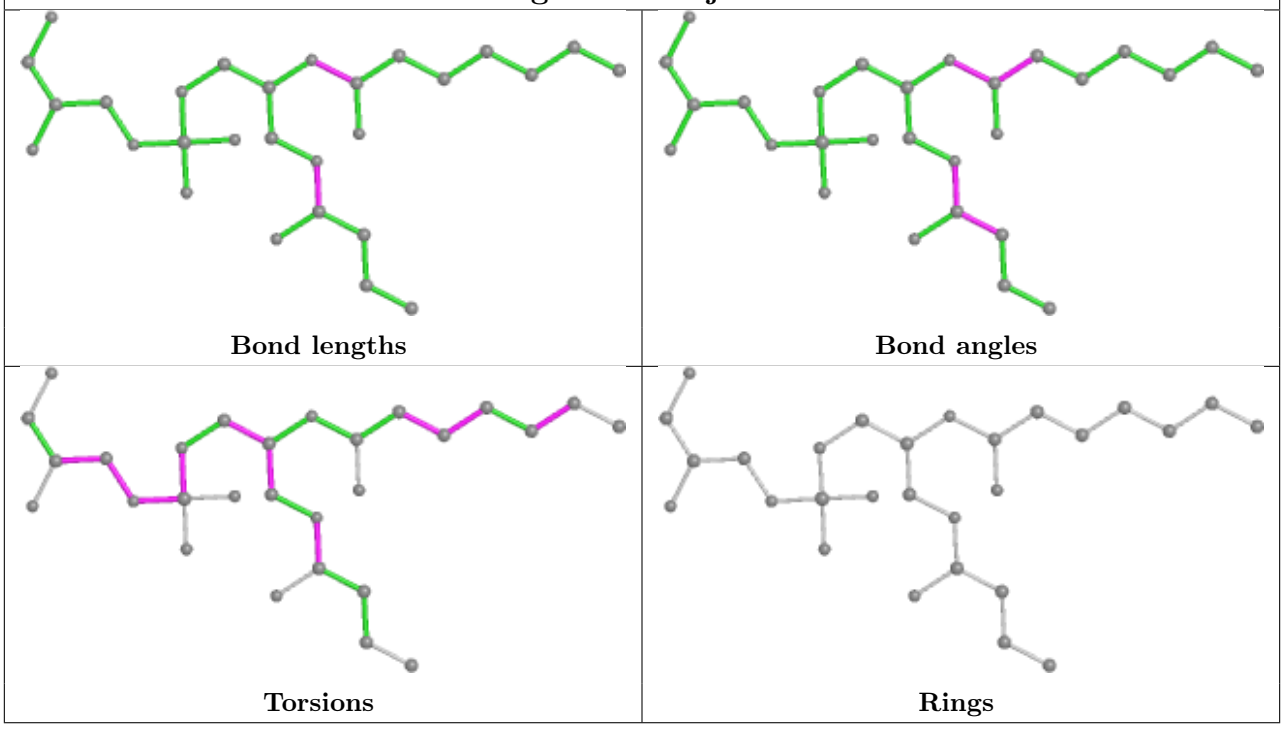


Rings

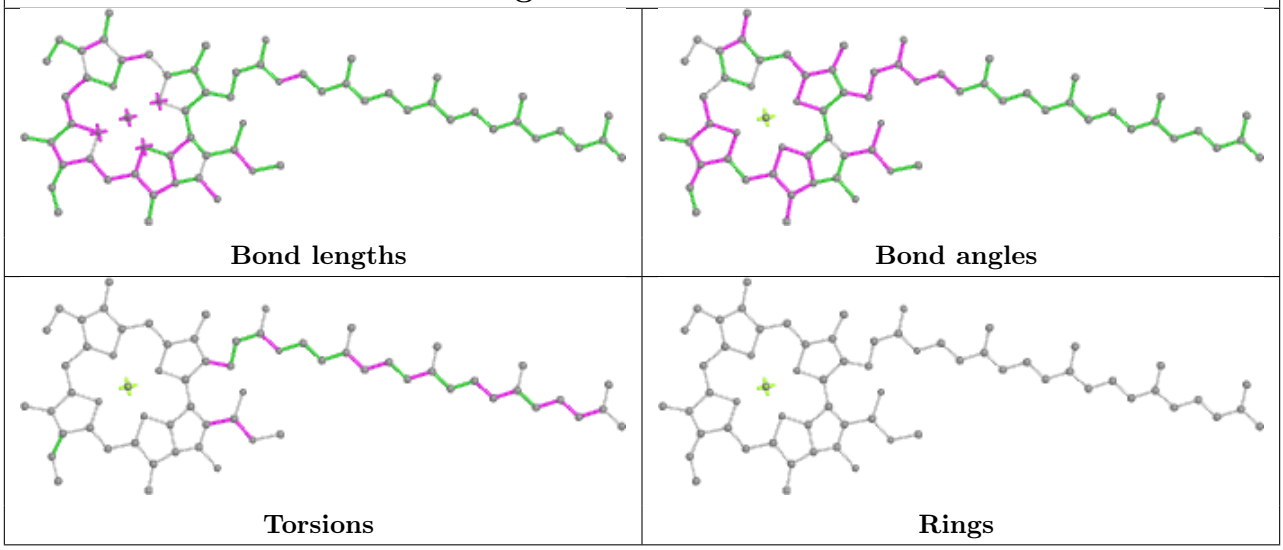
Ligand LHG A 852



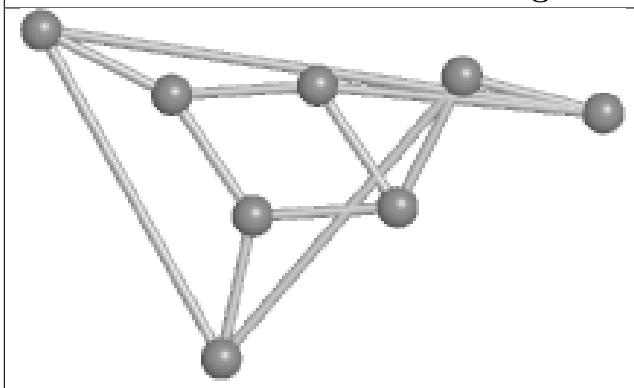
Ligand LHG j 101



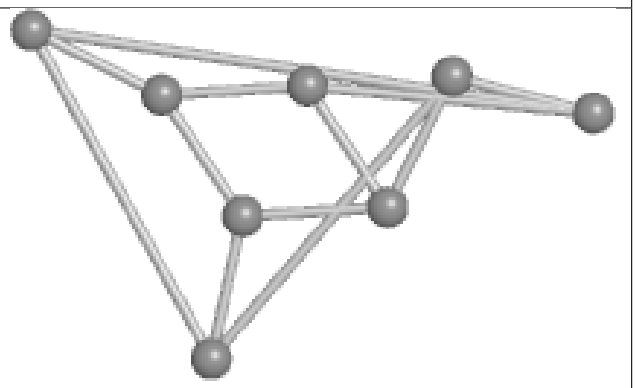
Ligand CLA U 1002



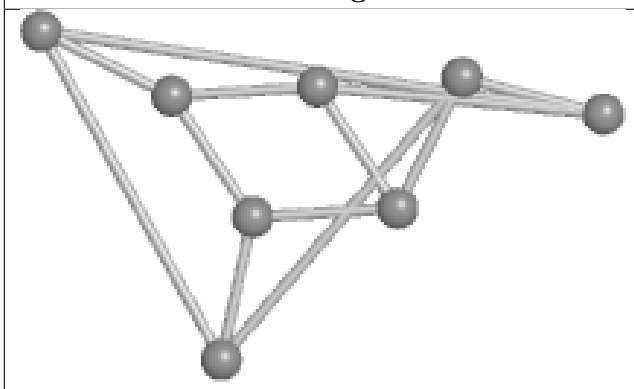
Ligand SF4 Y 843



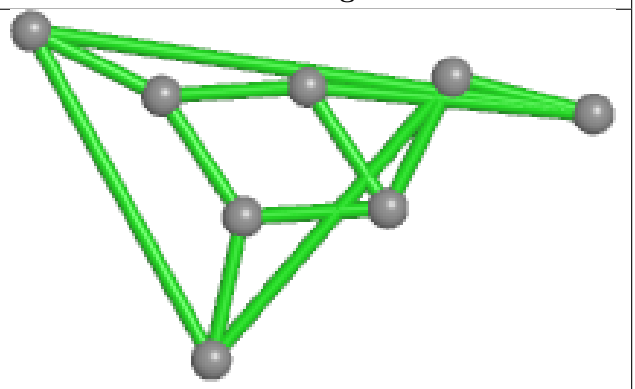
Bond lengths



Bond angles

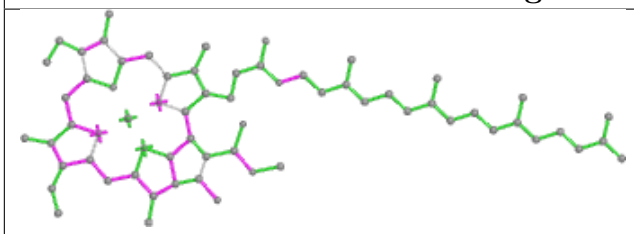


Torsions

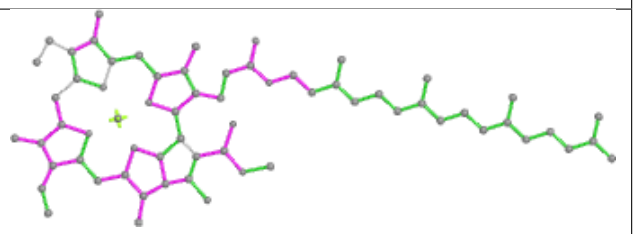


Rings

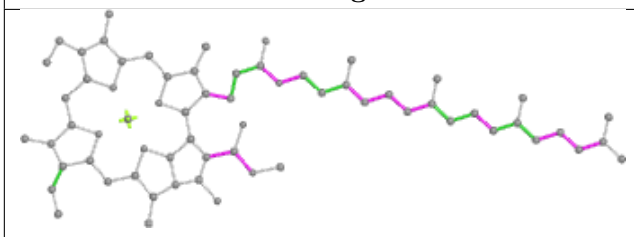
Ligand CLA Y 819



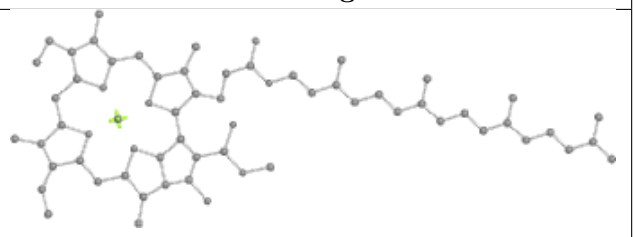
Bond lengths



Bond angles

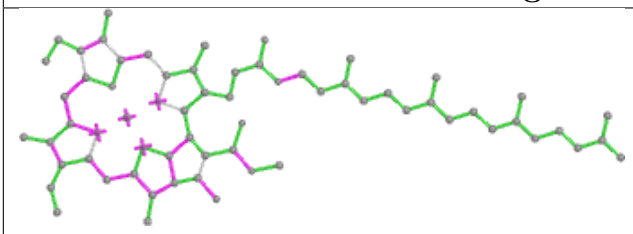


Torsions

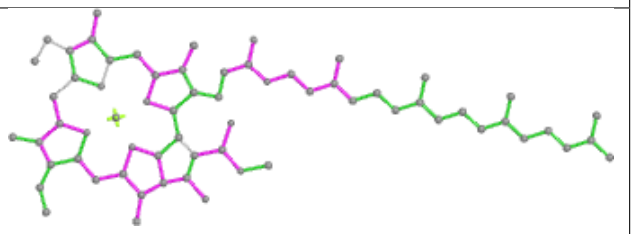


Rings

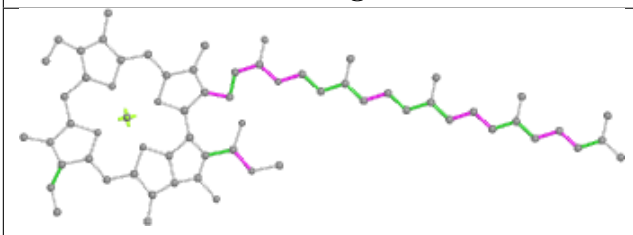
Ligand CLA Y 818



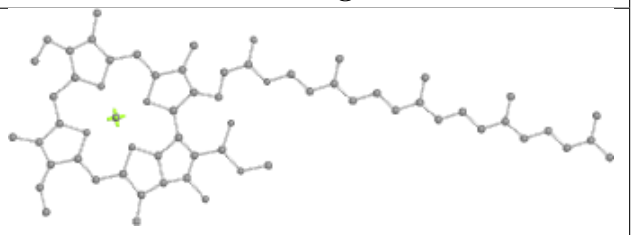
Bond lengths



Bond angles

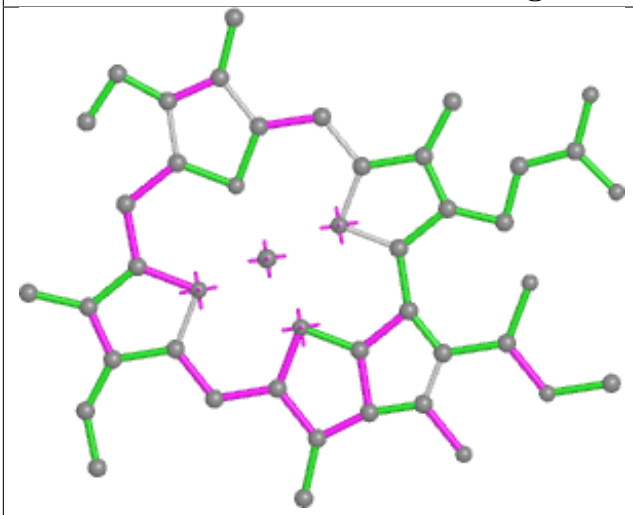


Torsions



Rings

Ligand CLA Z 834



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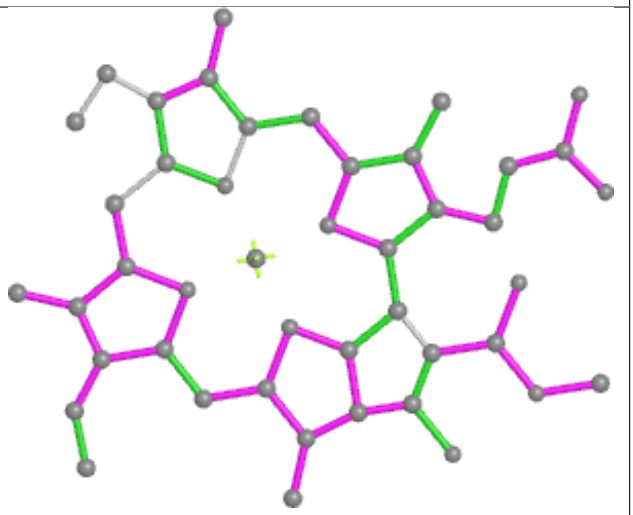
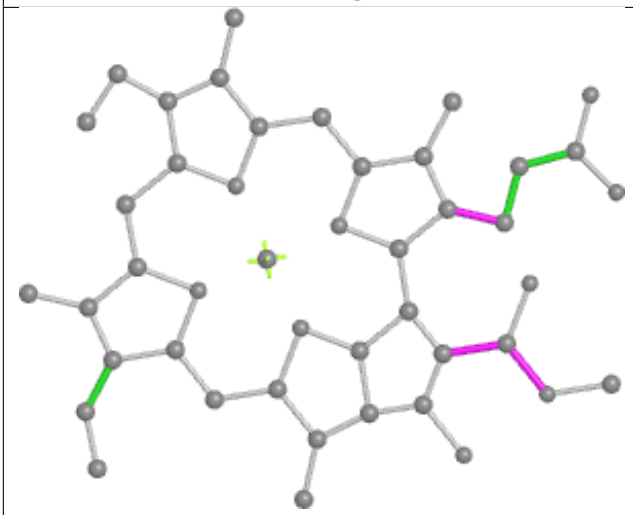
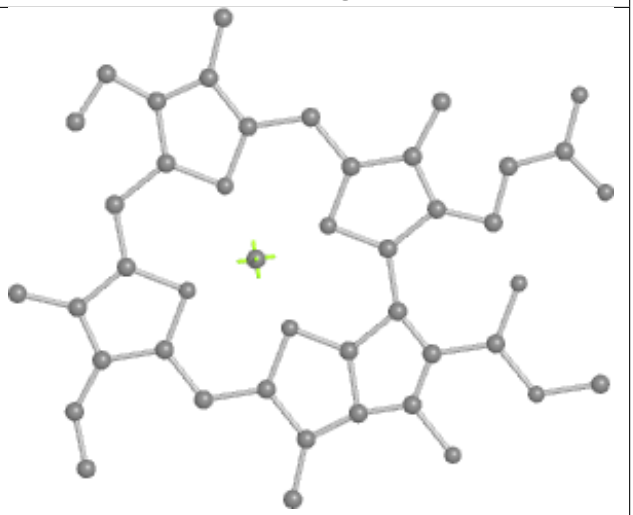


Bond angles

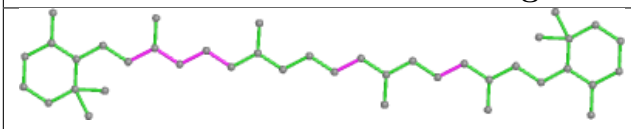


Torsions



Rings

Ligand BCR H 846



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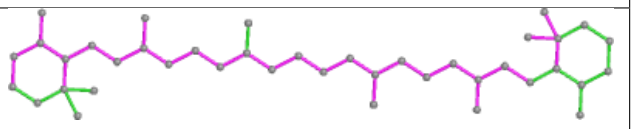
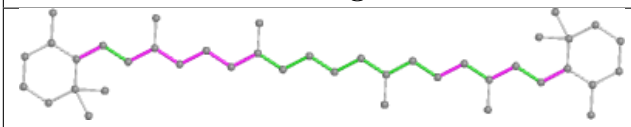


Bond angles



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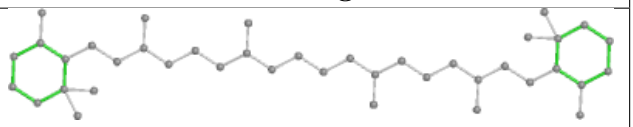
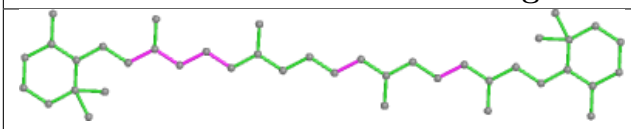


Rings

Ligand BCR Y 853



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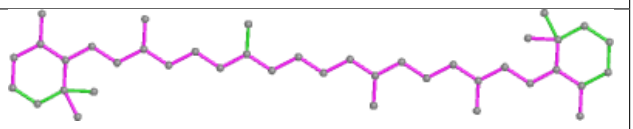
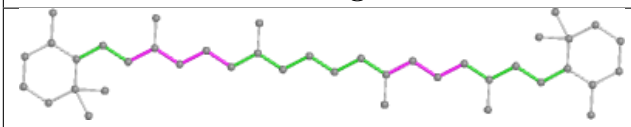
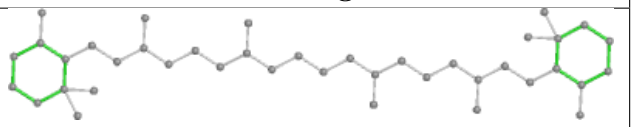


Bond angles

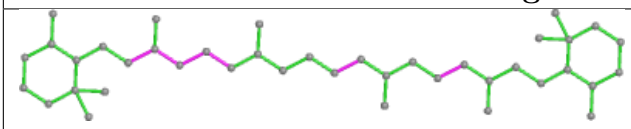


Torsions

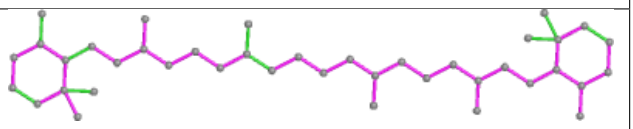


Rings

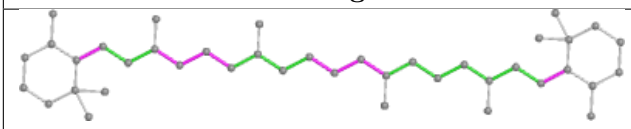
Ligand BCR B 850



Bond lengths



Bond angles



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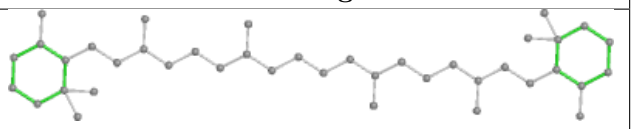
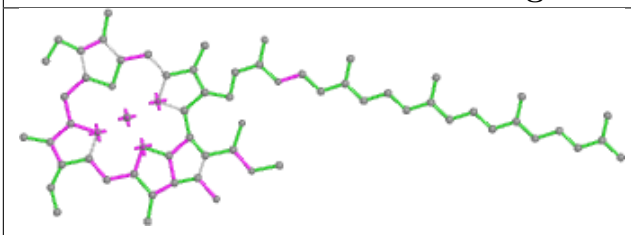


Rings

Ligand CLA Z 814



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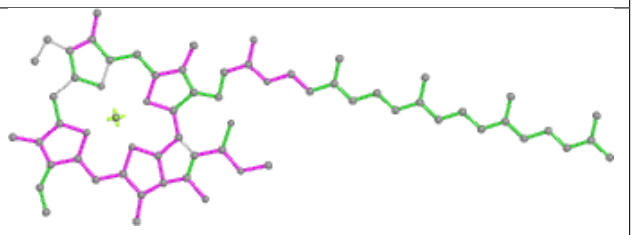
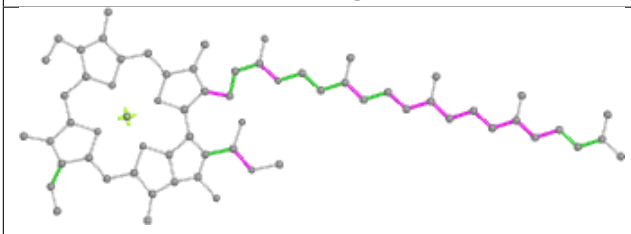


Bond angles



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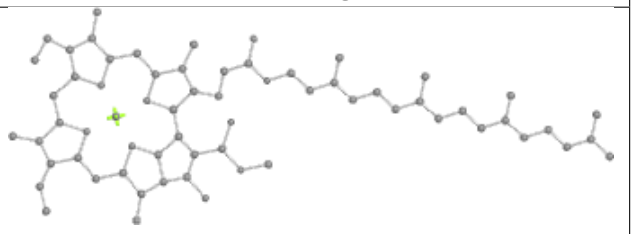
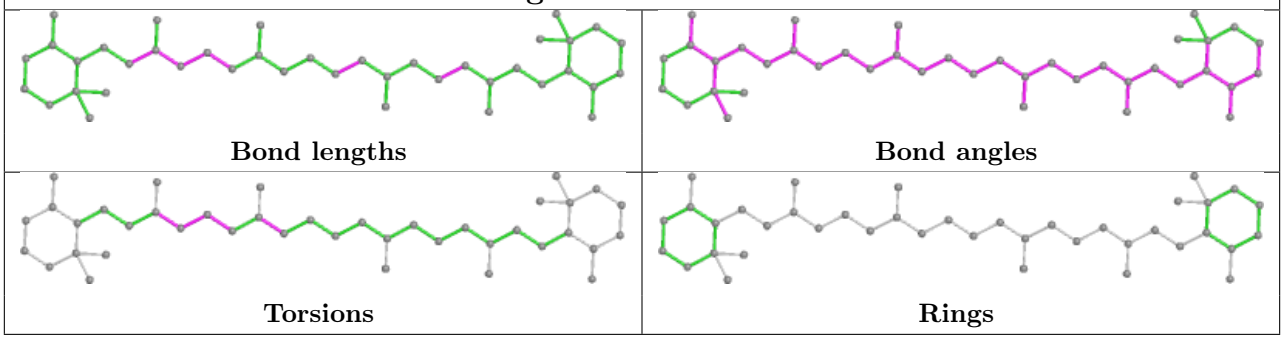


Rings

Ligand BCR d 203



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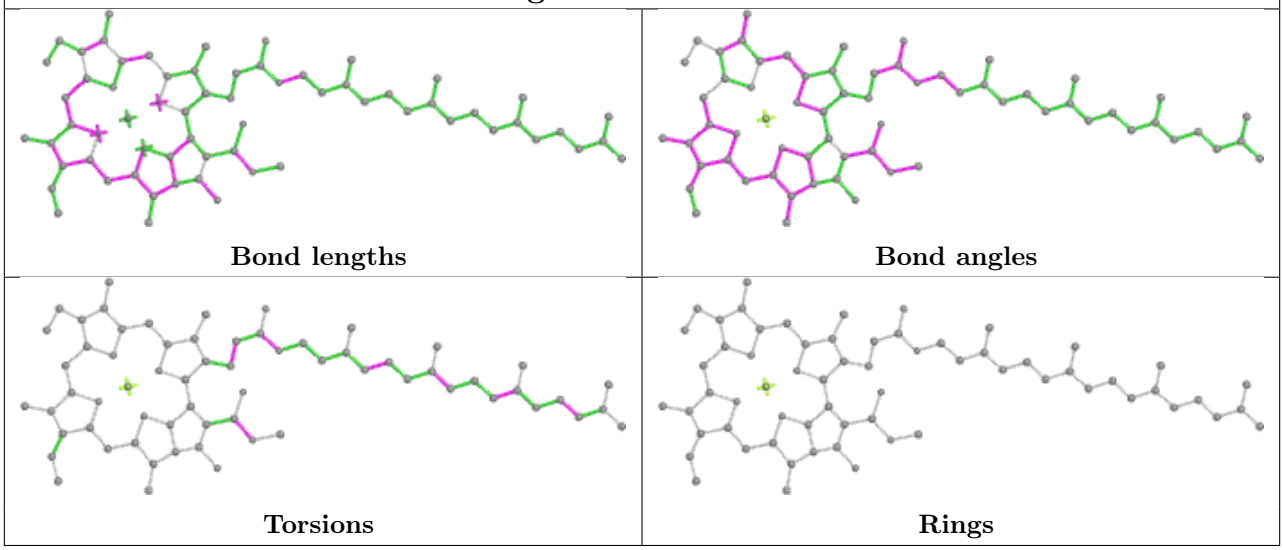

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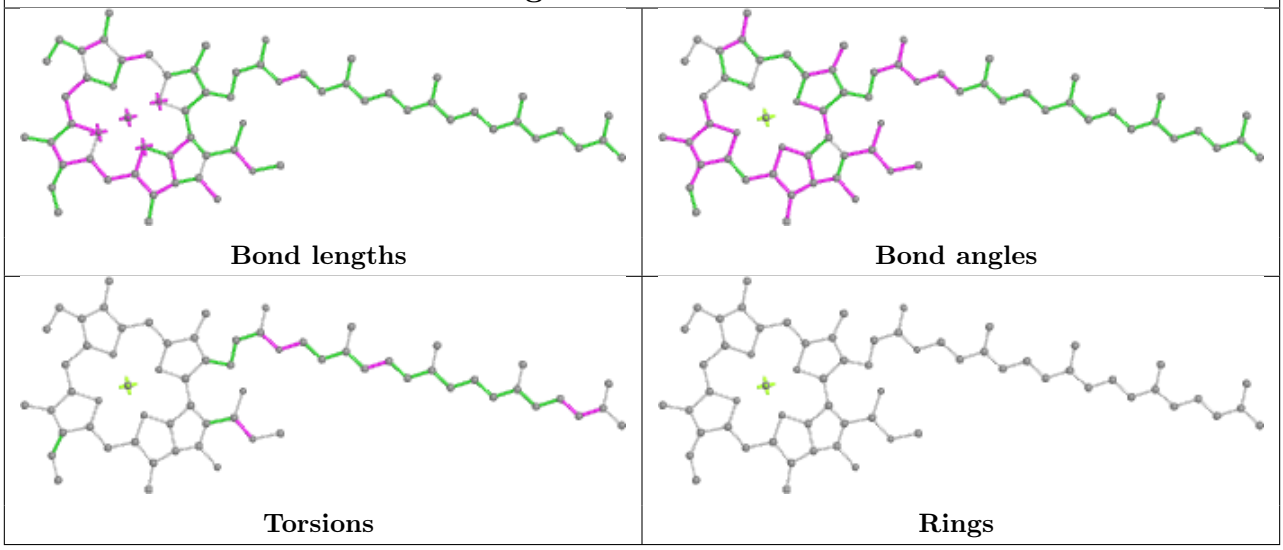

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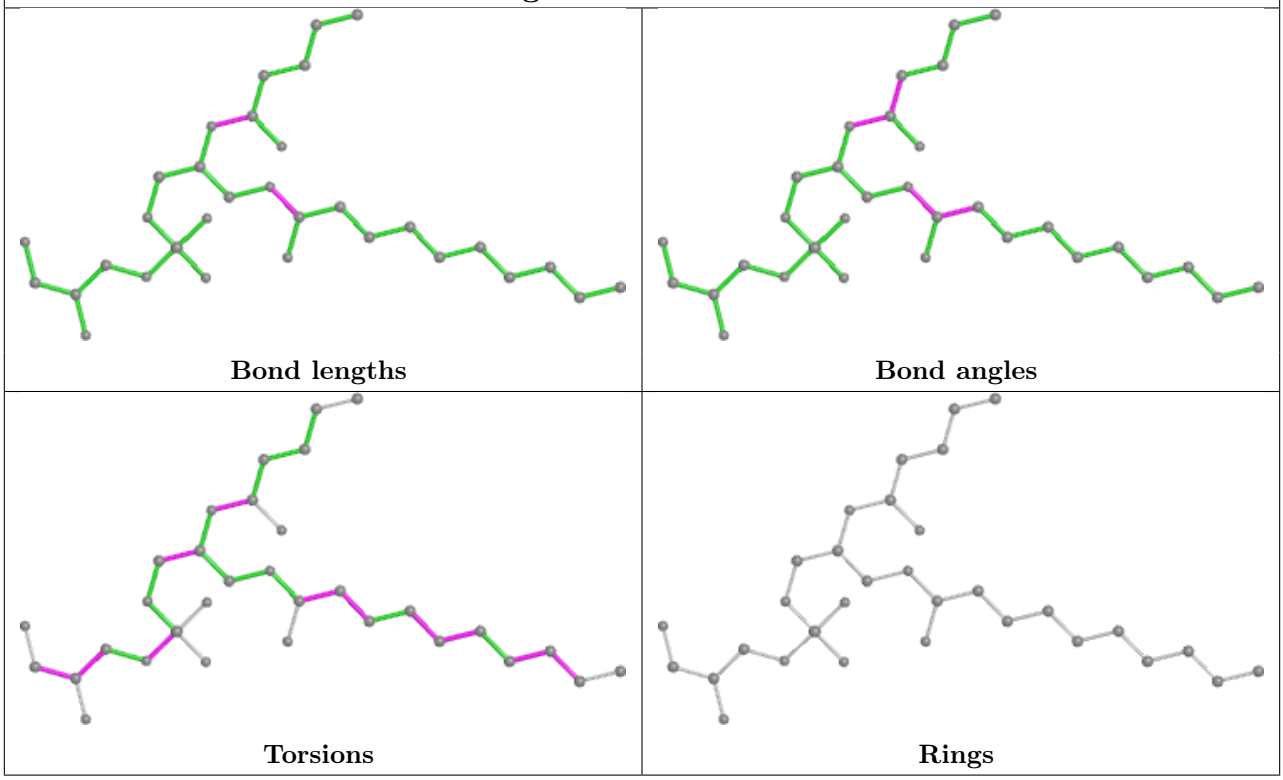

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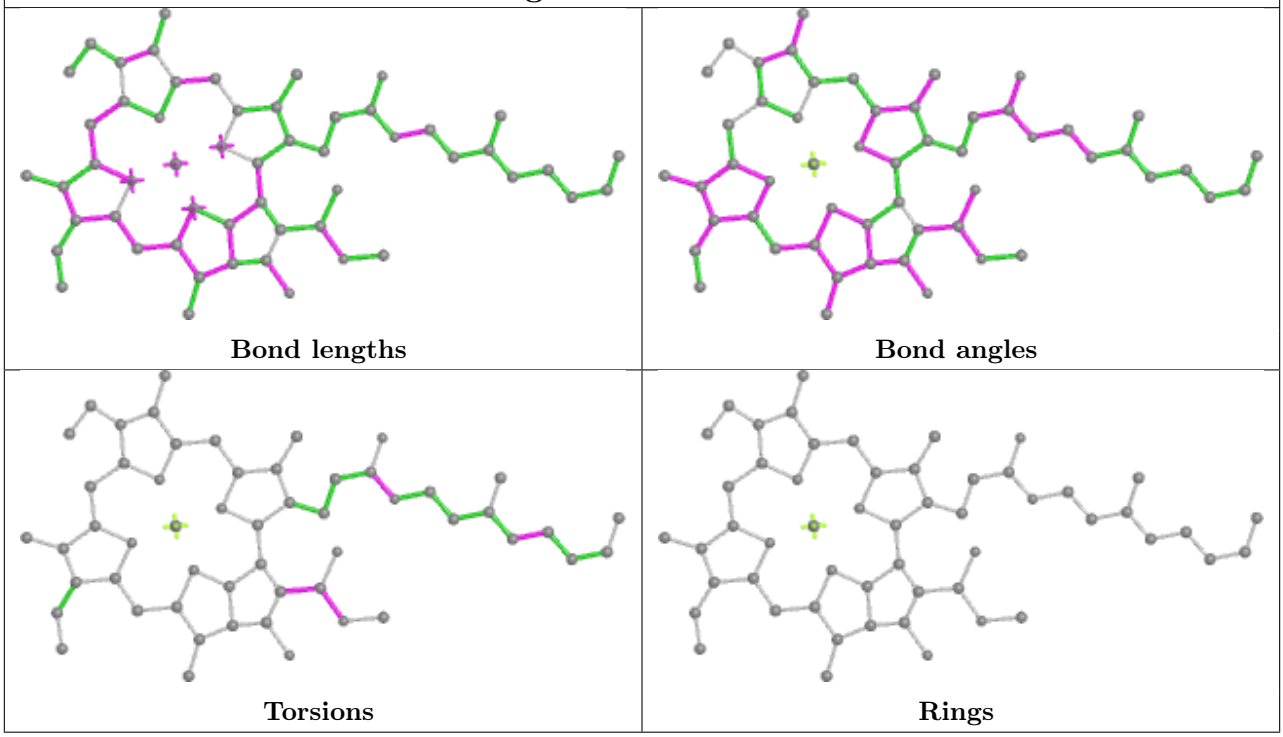
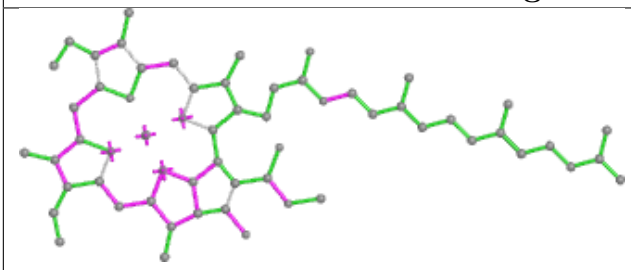
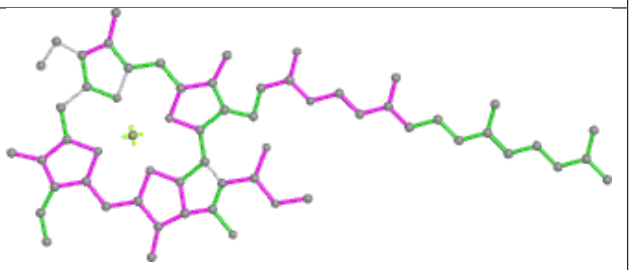
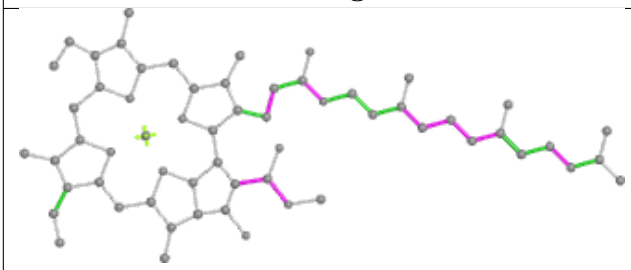
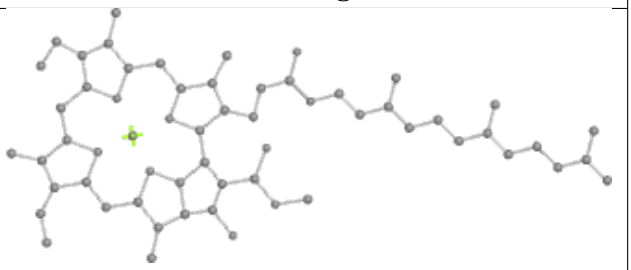


Ligand CLA A 818	
 Bond lengths	 Bond angles
 Torsions	 Rings

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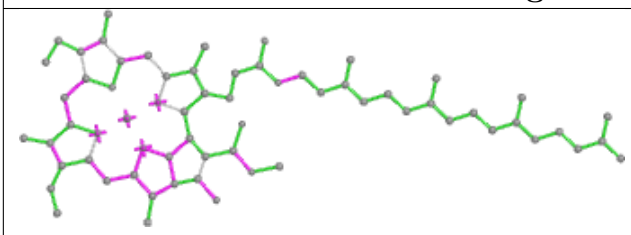
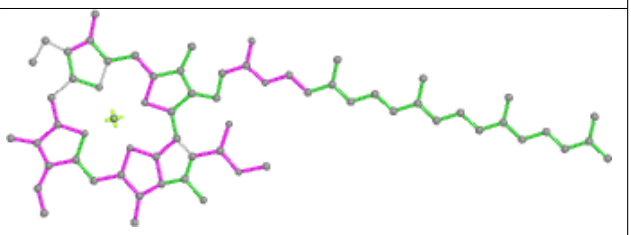
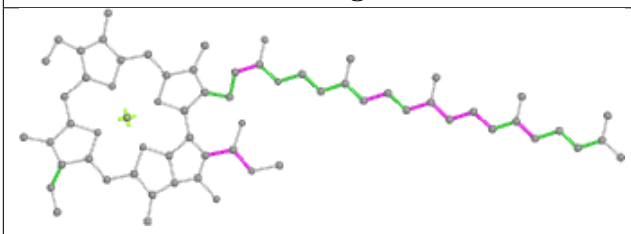
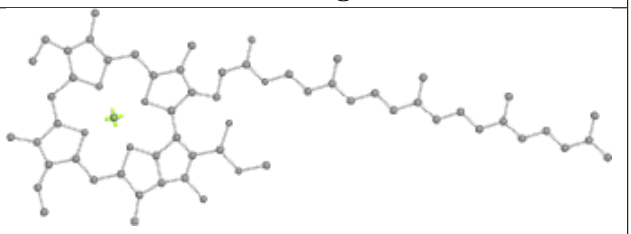
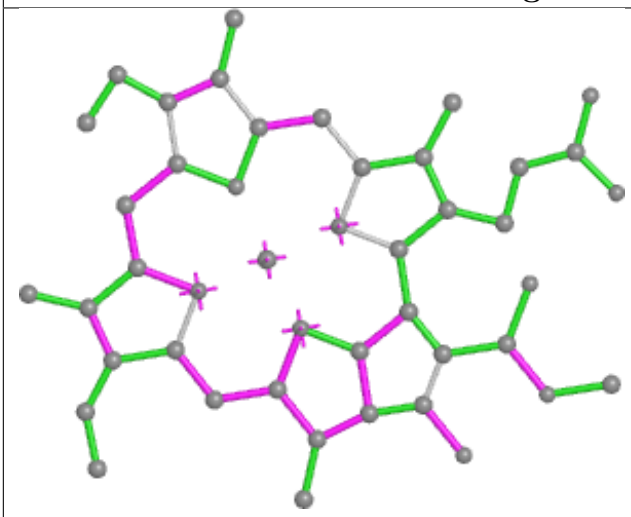
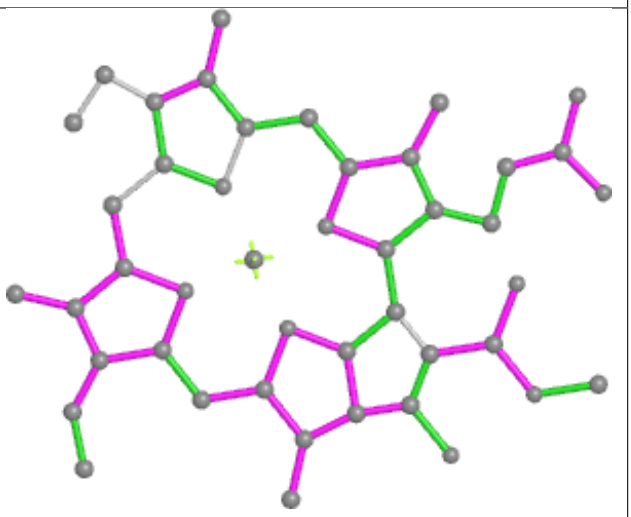
 Bond lengths	 Bond angles
 Torsions	 Rings

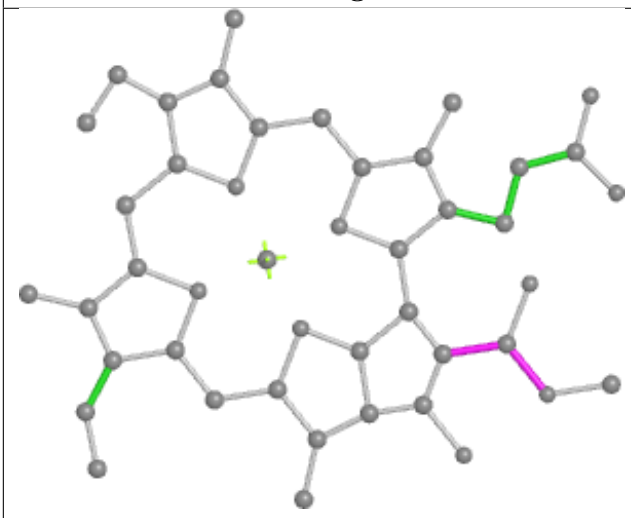
Ligand CLA K 102



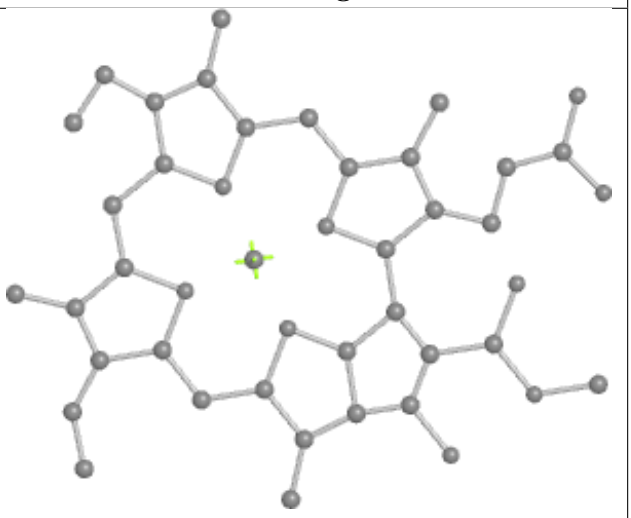
Bond lengths



Bond angles

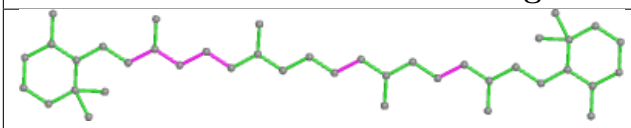


Torsions



Rings

Ligand BCR F 201



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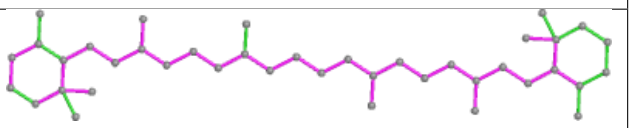
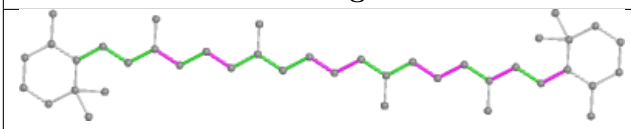
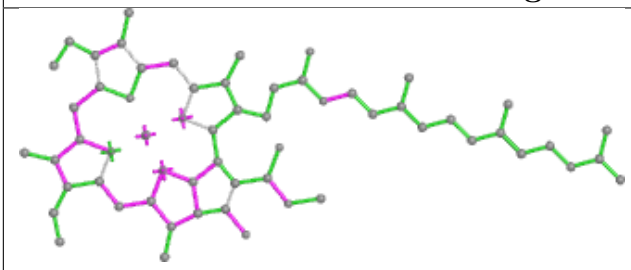
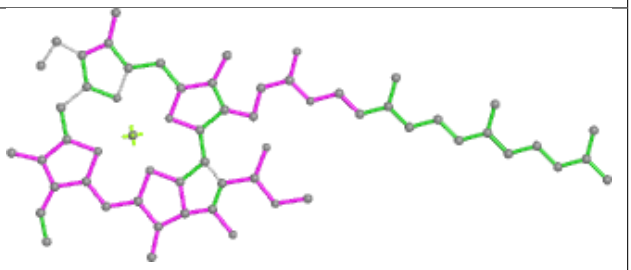
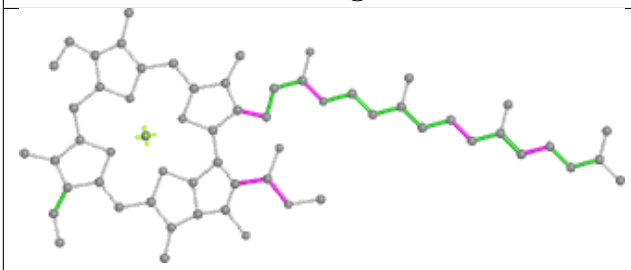
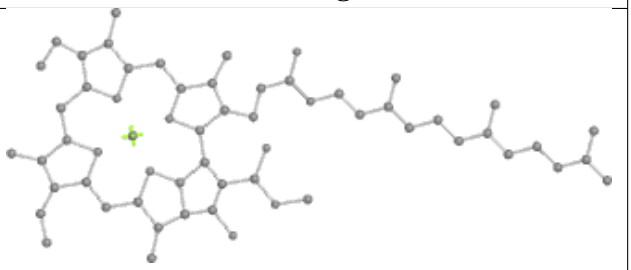


Bond angles



Torsions

Rings

Ligand CLA B 836	
 Bond lengths	 Bond angles
 Torsions	 Rings

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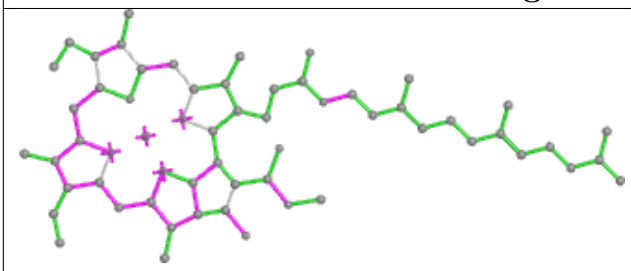
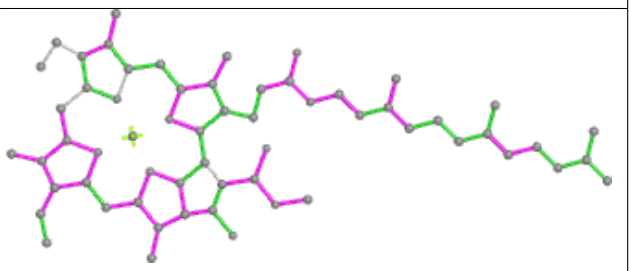
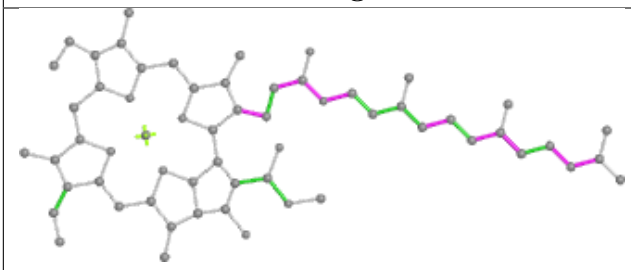
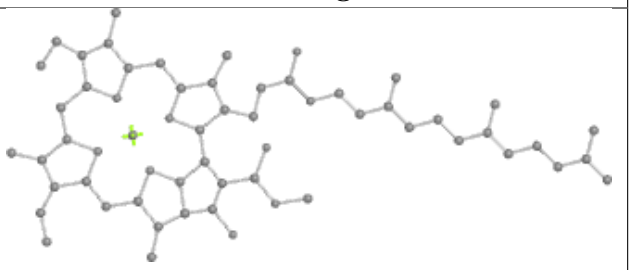
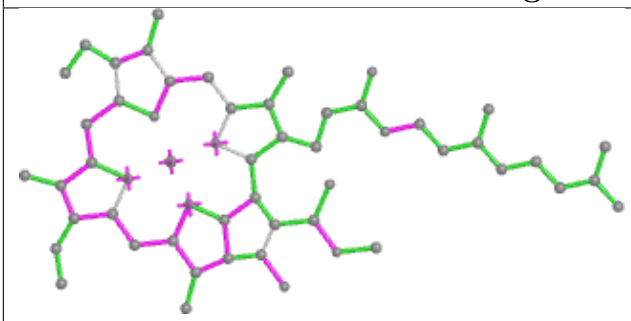
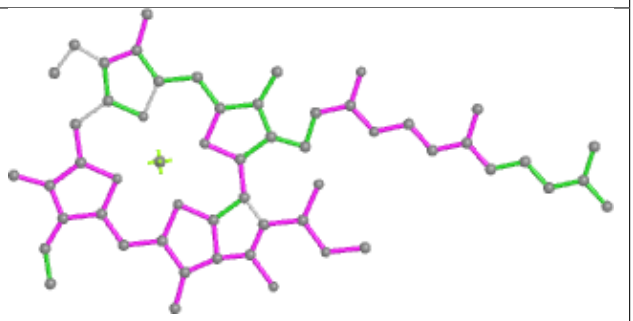
 Bond lengths	 Bond angles
 Torsions	 Rings

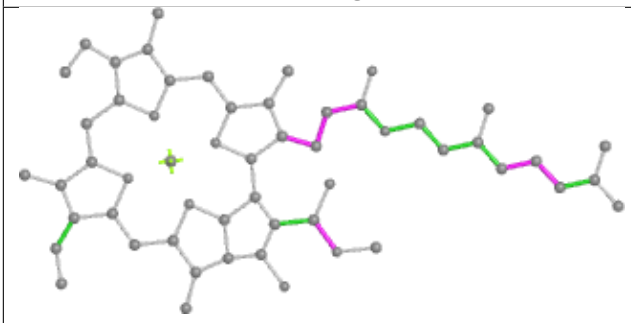
Ligand CLA H 811



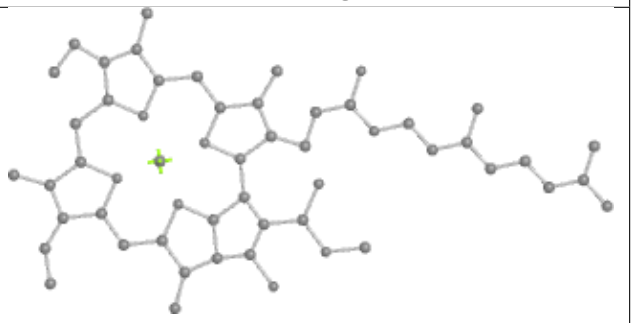
Bond lengths



Bond angles

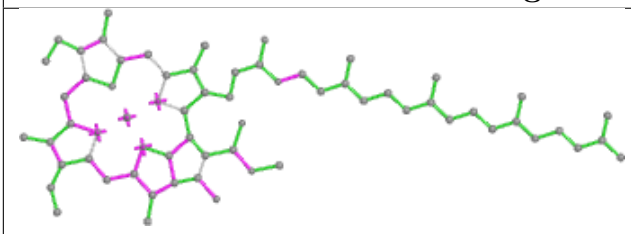


Torsions



Rings

Ligand CLA Y 840



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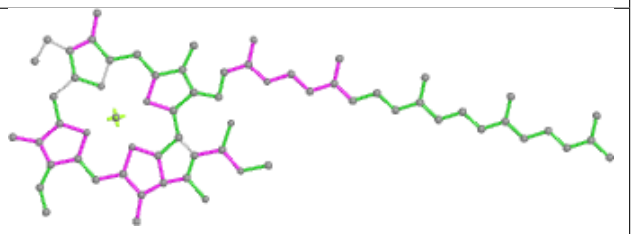

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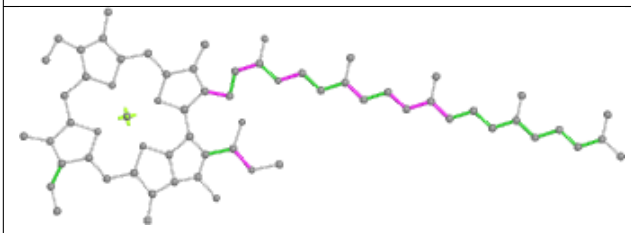

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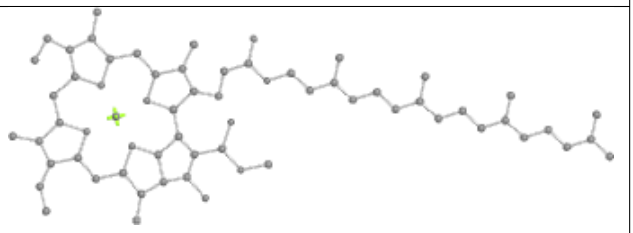
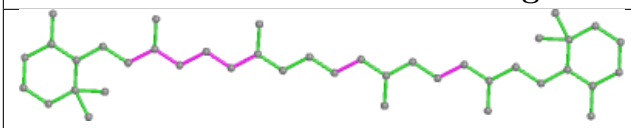


Rings

Ligand BCR A 847



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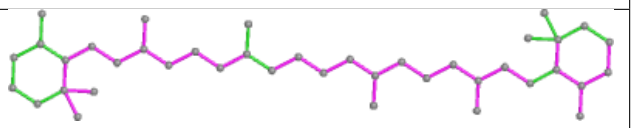
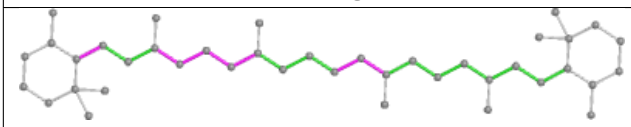


Bond angles



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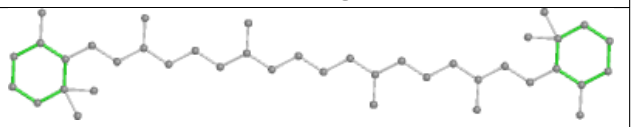
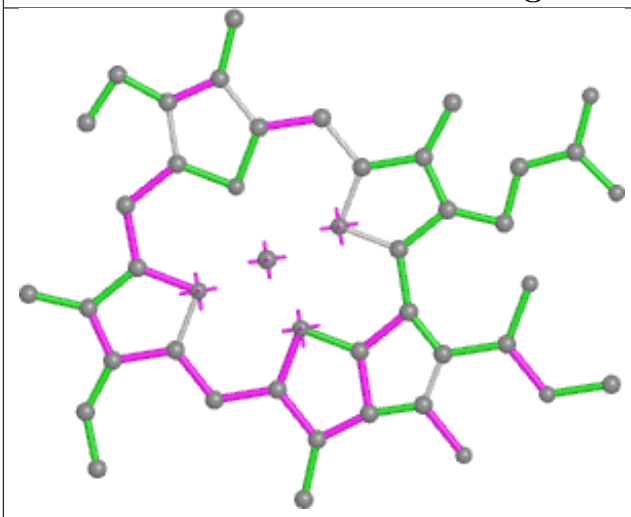


Rings

Ligand CLA B 819



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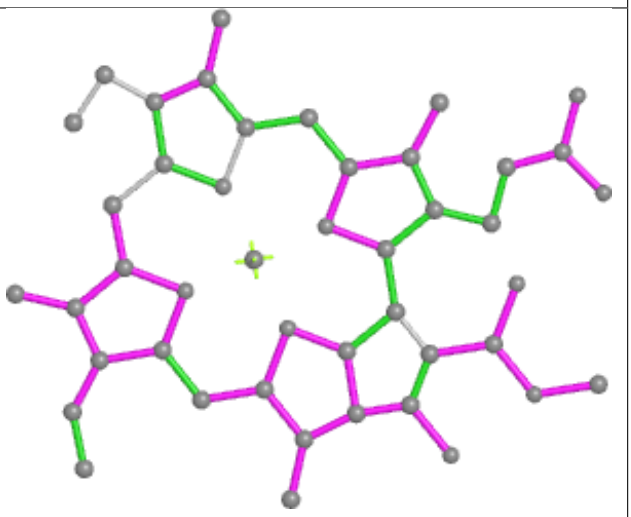
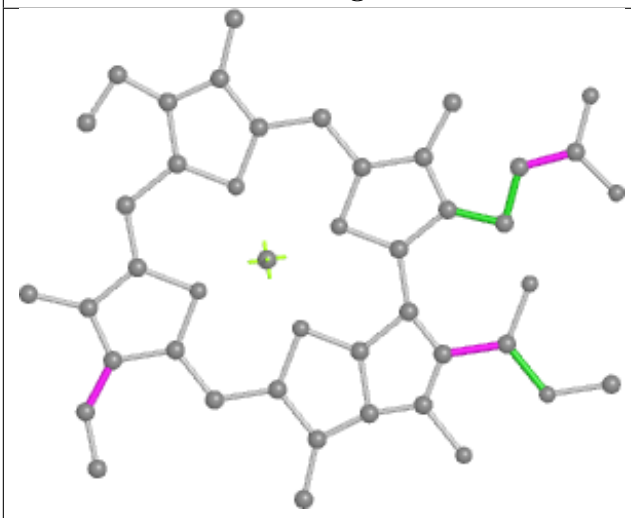


Bond angles



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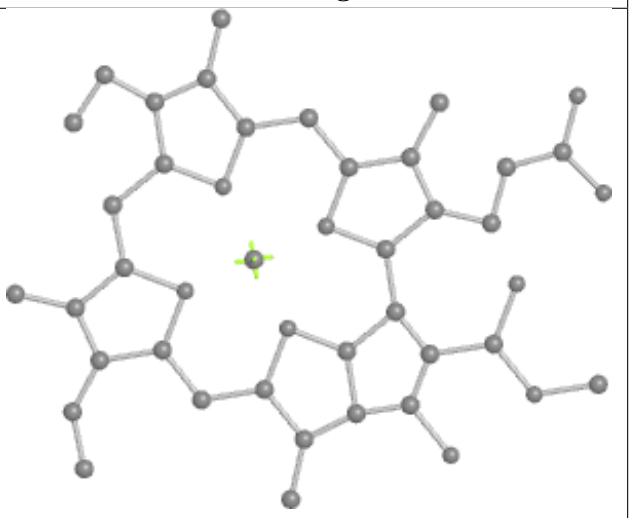
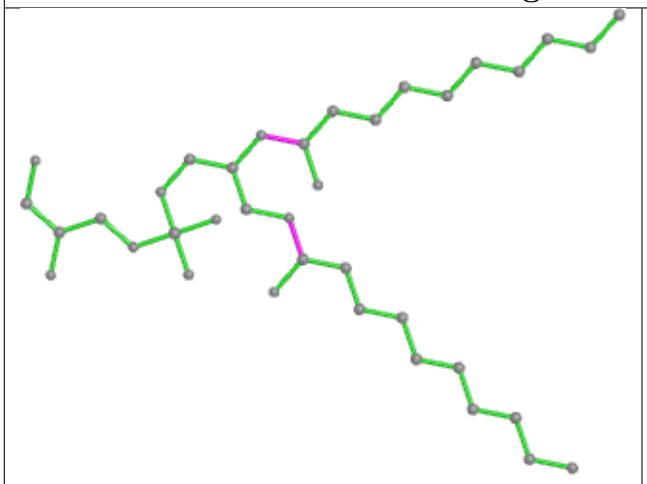


Rings

Ligand LHG H 849



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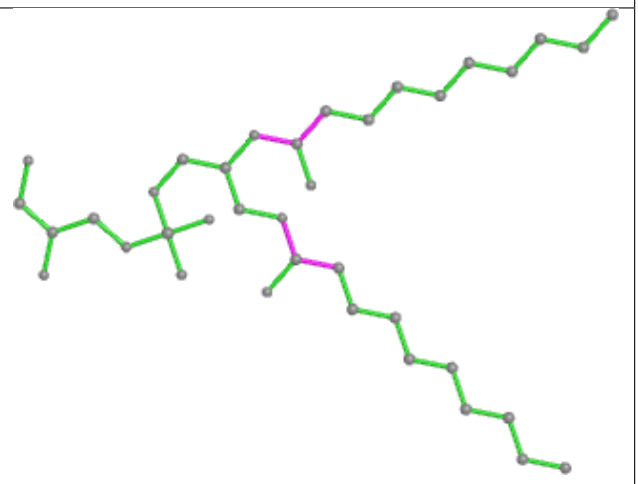
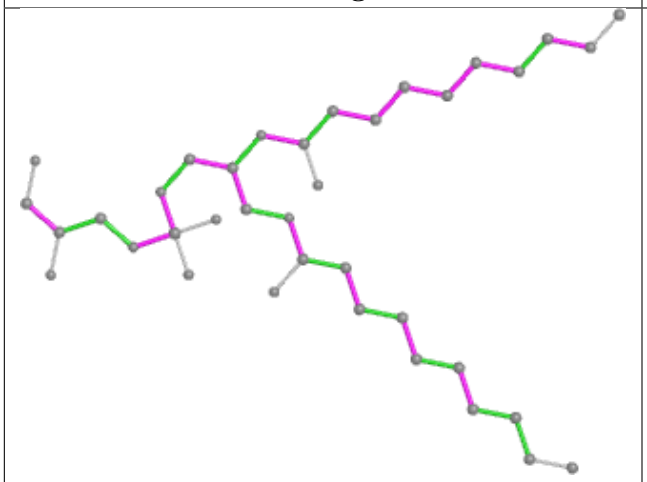


Bond angles



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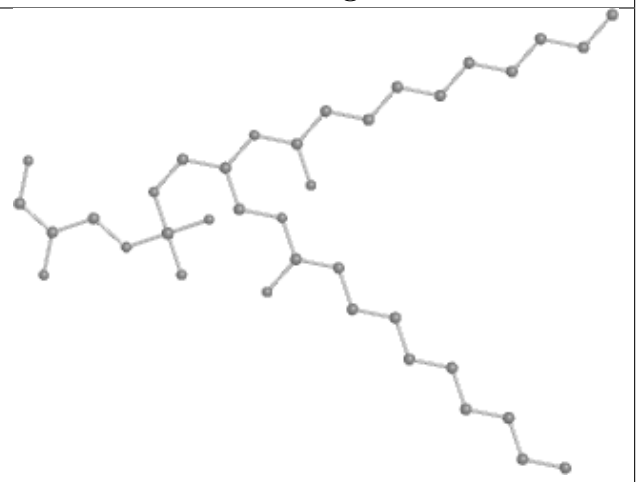
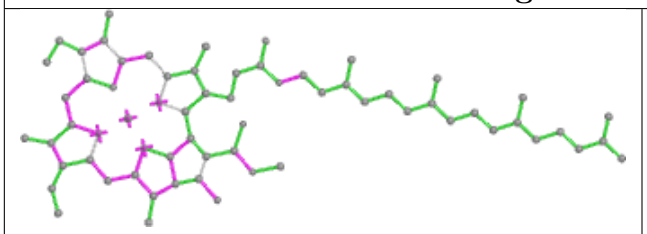


Rings

Ligand CLA U 1004



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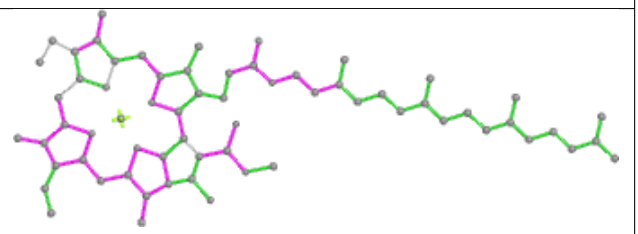
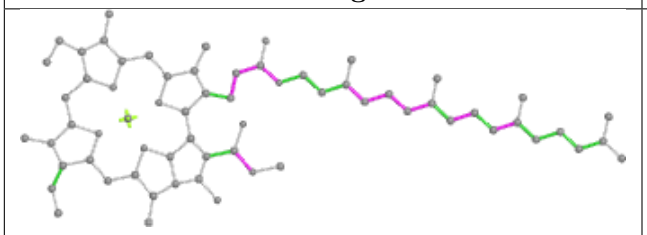


Bond angles



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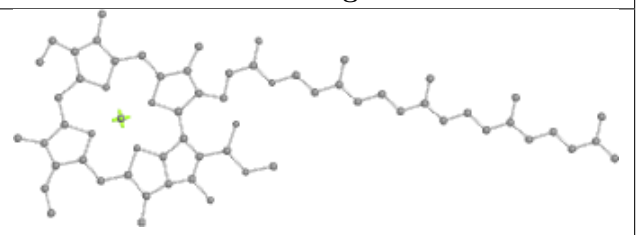
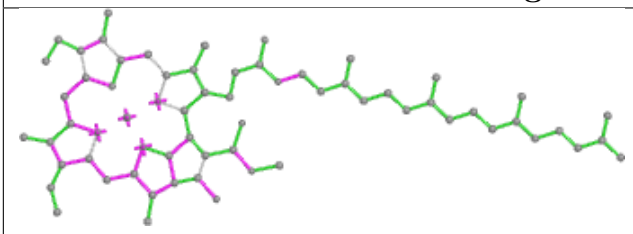


Rings

Ligand CLA B 806



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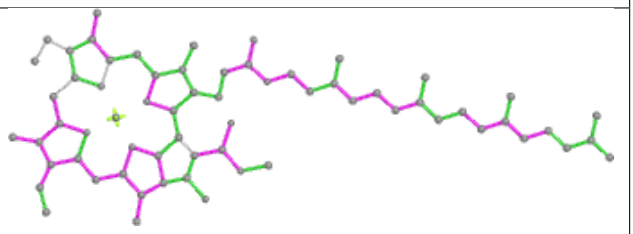
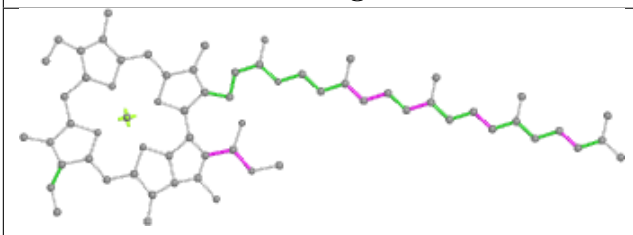


Bond angles



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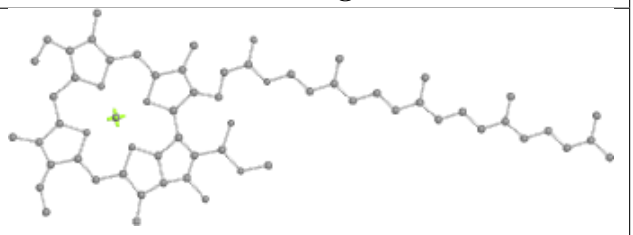

Rings

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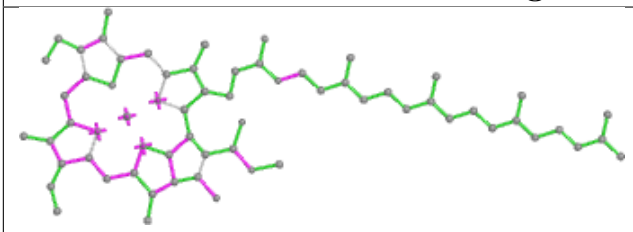

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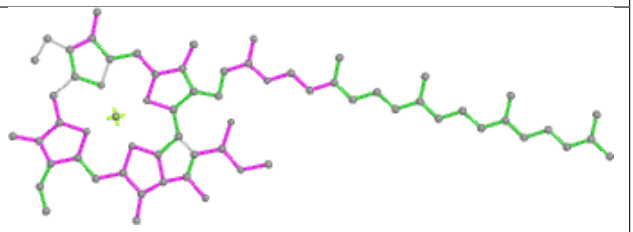

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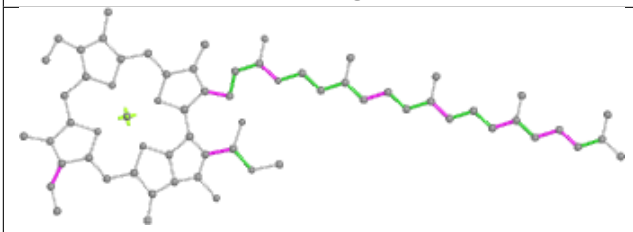

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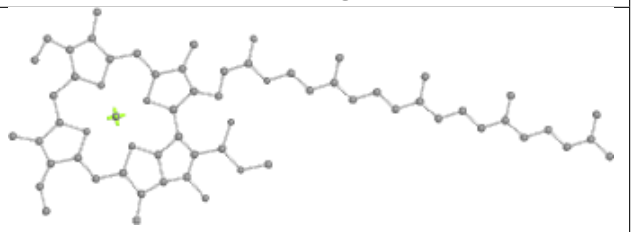
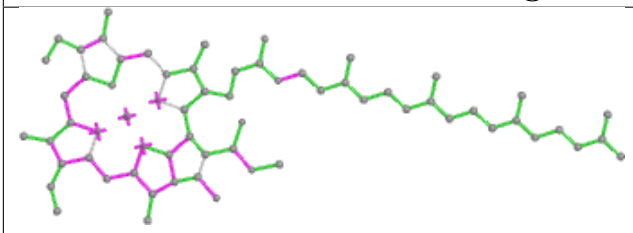


Rings

Ligand CLA Y 832



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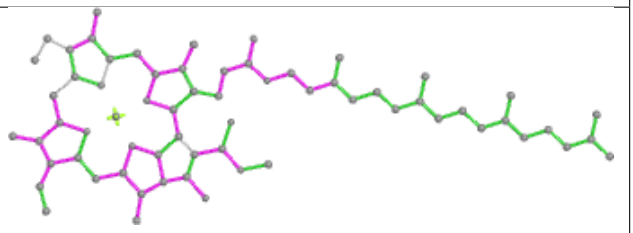
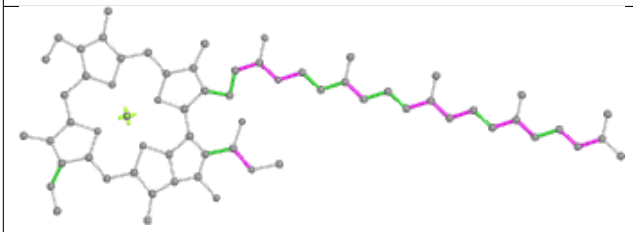


Bond angles



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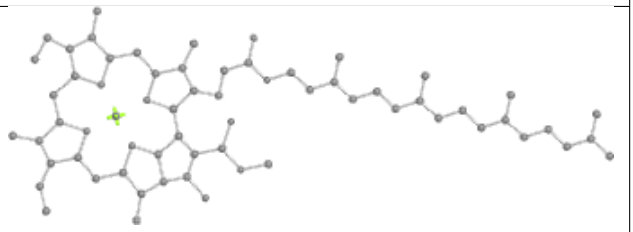
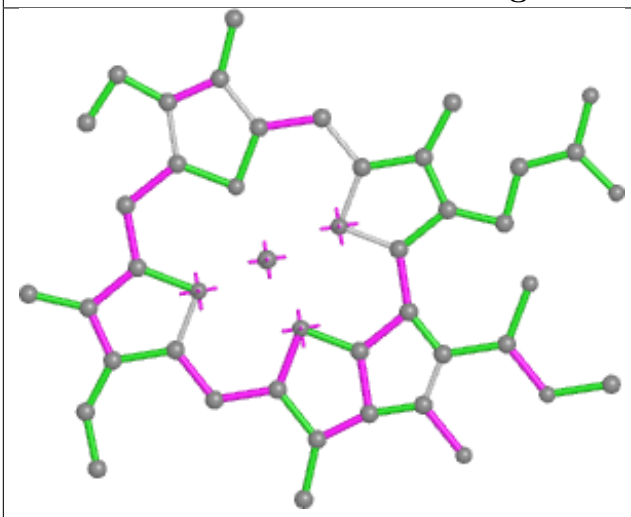


Rings

Ligand CLA W 1701



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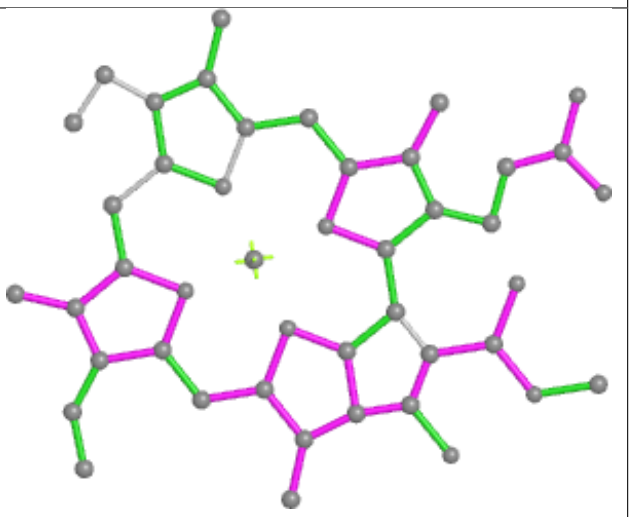

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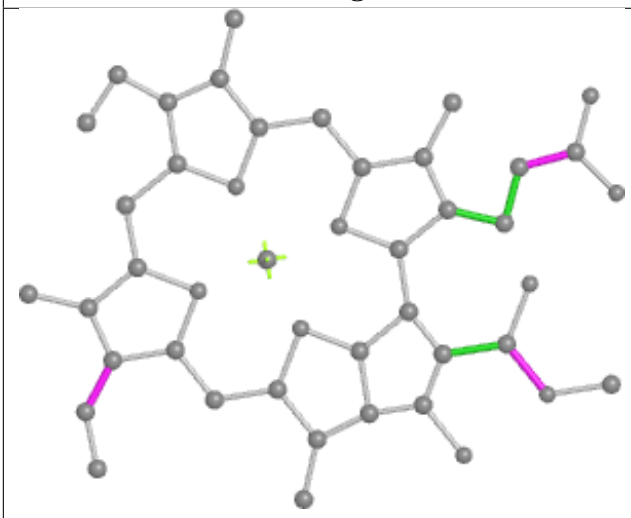

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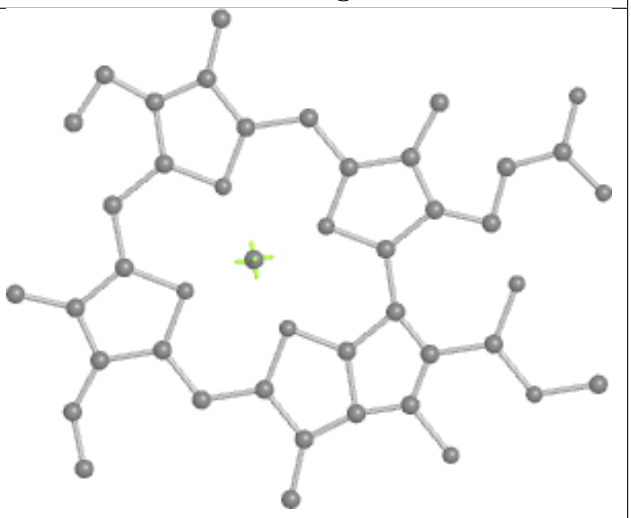
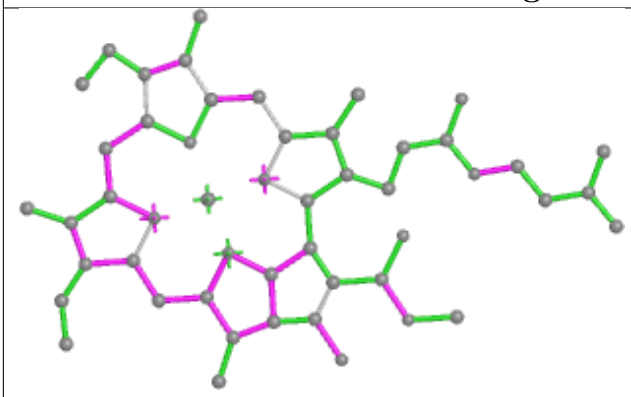
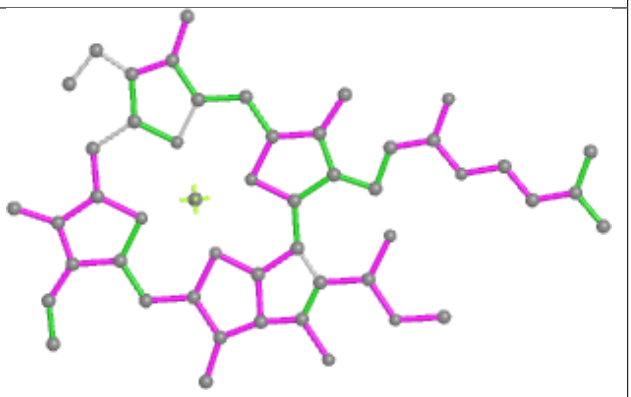
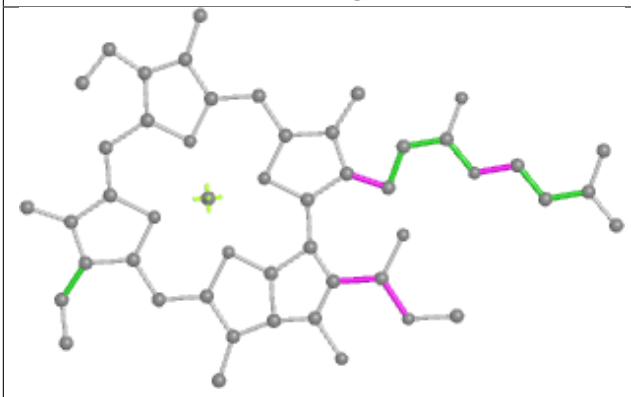
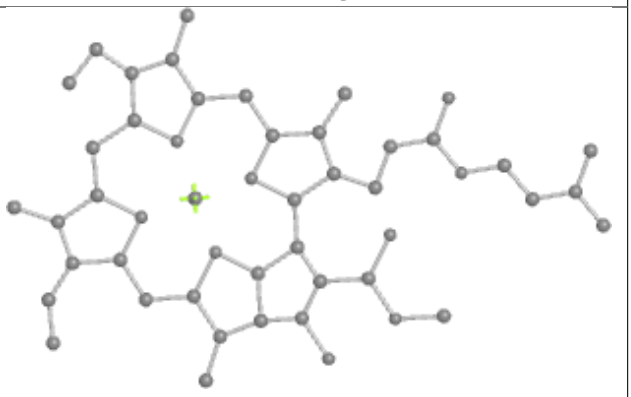
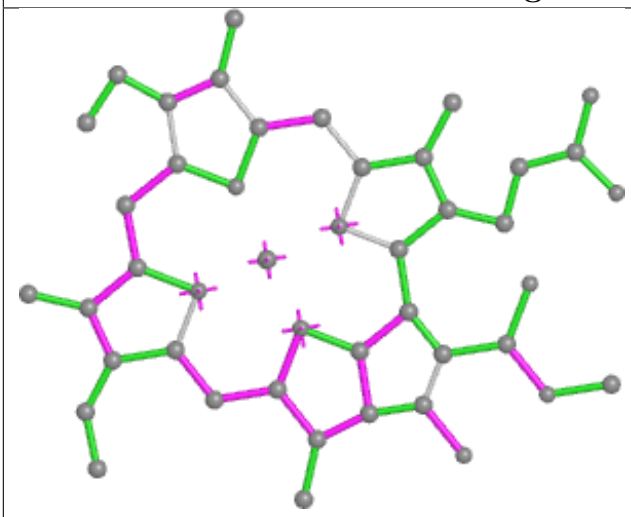


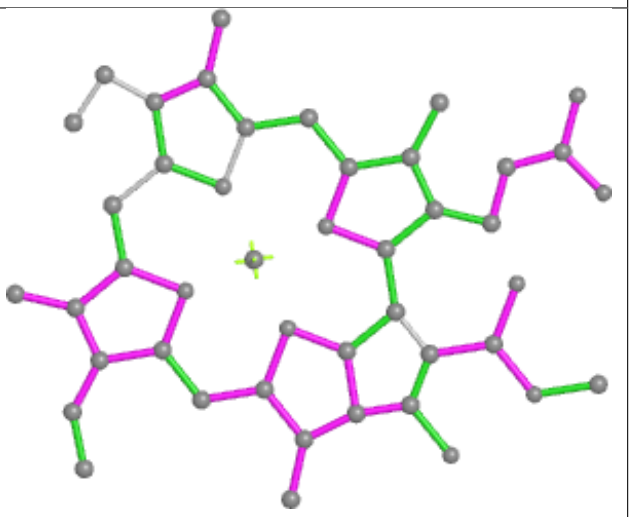
Rings

Ligand CLA G 839	
 Bond lengths	 Bond angles
 Torsions	 Rings

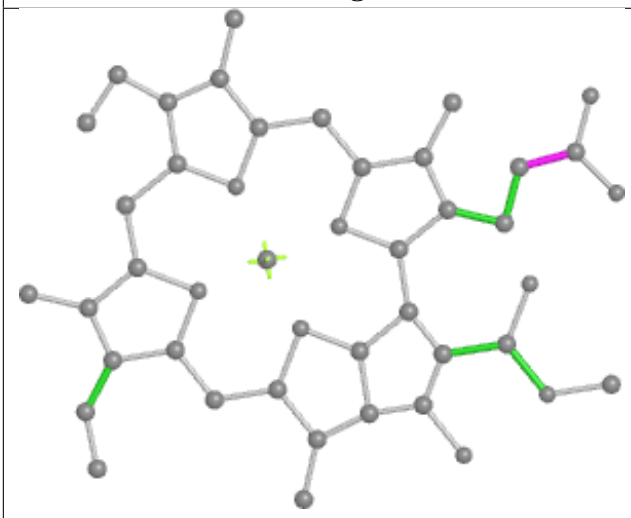
Ligand CLA B 838



Bond lengths



Bond angles



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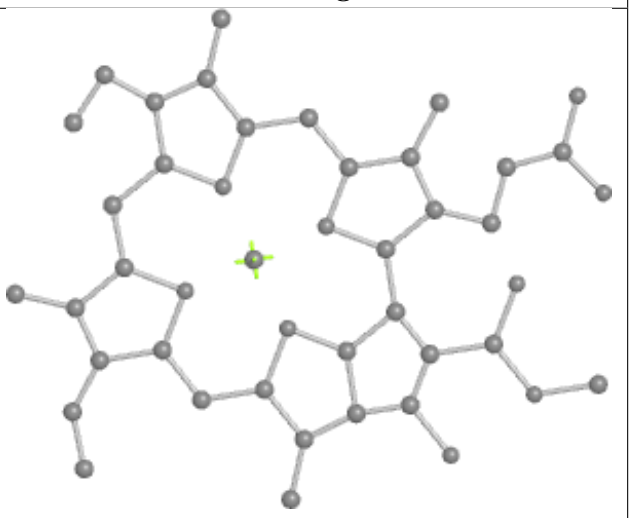
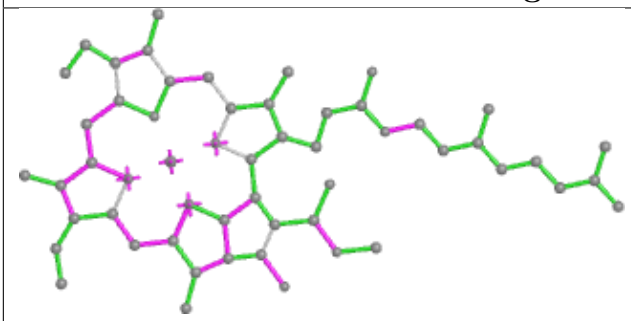


Rings

Ligand CLA A 834



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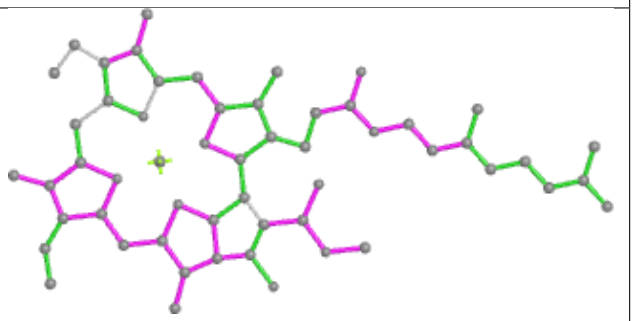

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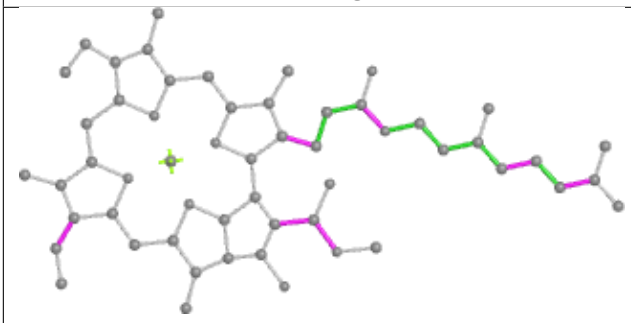

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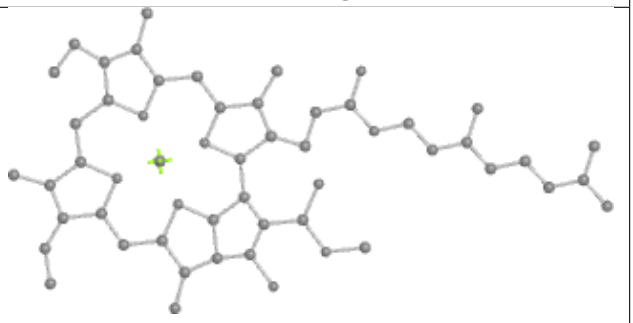
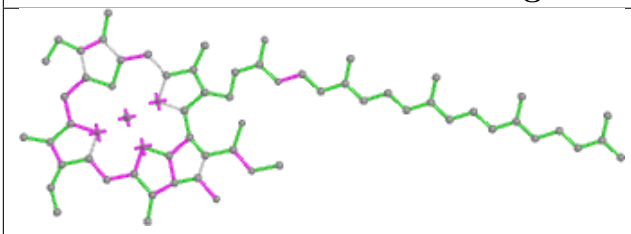


Rings

Ligand CLA A 831



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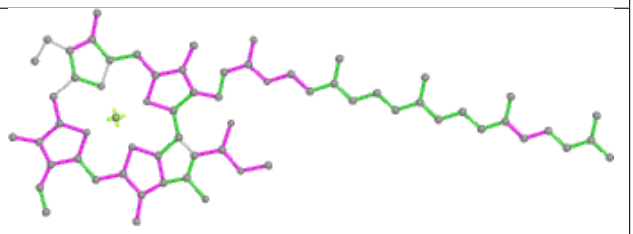
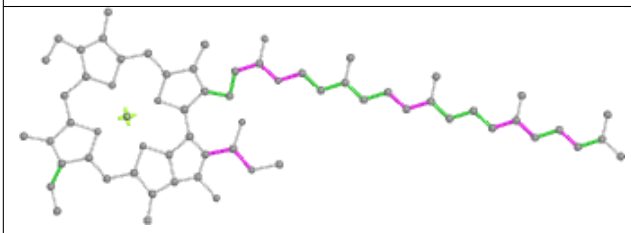
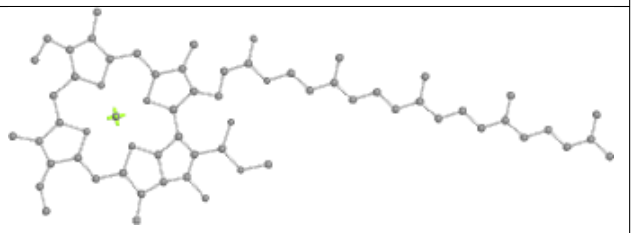


Bond angles

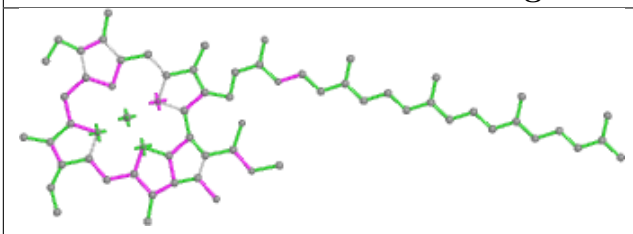


Torsions

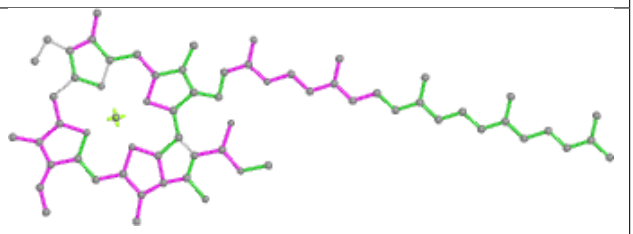


Rings

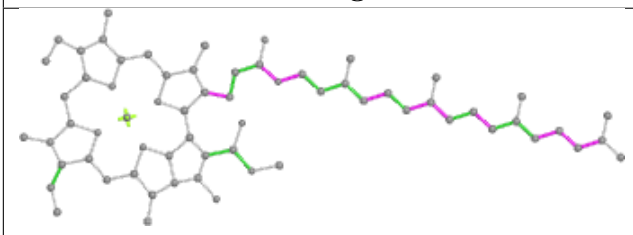
Ligand CLA B 804



Bond lengths



Bond angles



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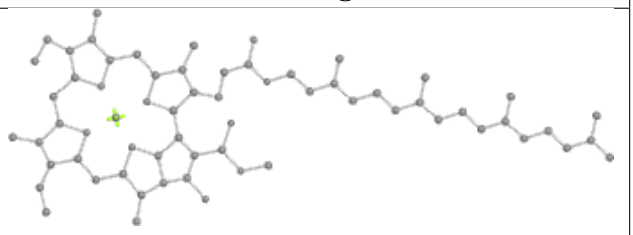
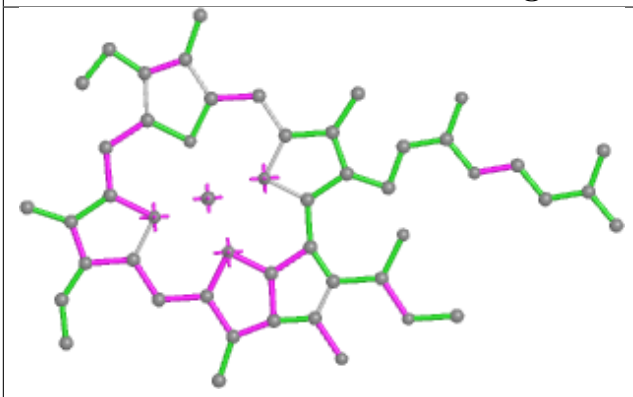


Rings

Ligand CLA G 816



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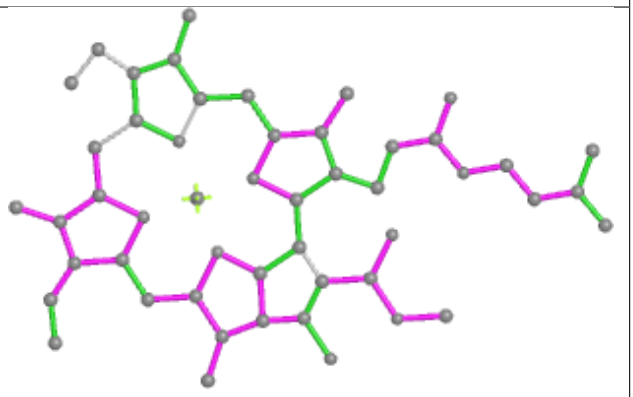
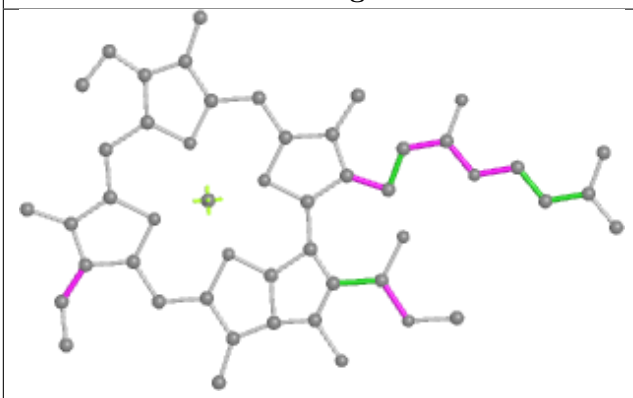


Bond angles



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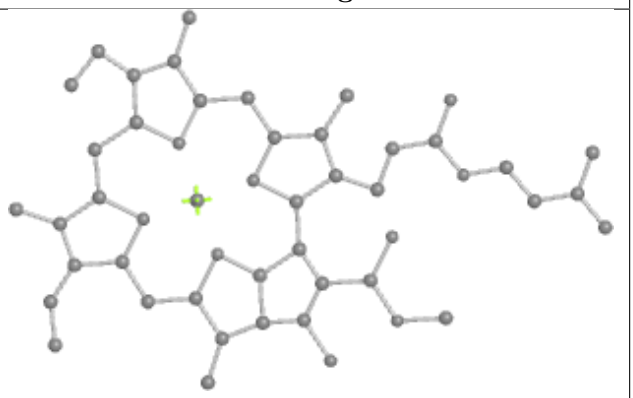
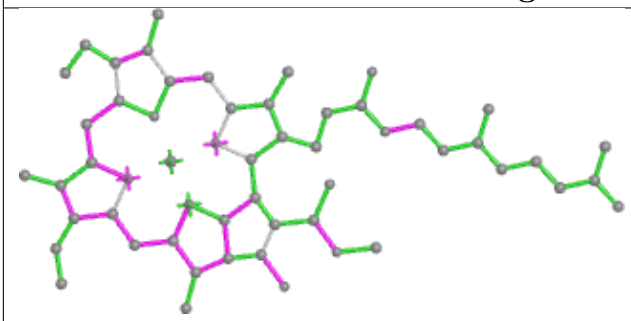


Rings

Ligand CLA S 1103



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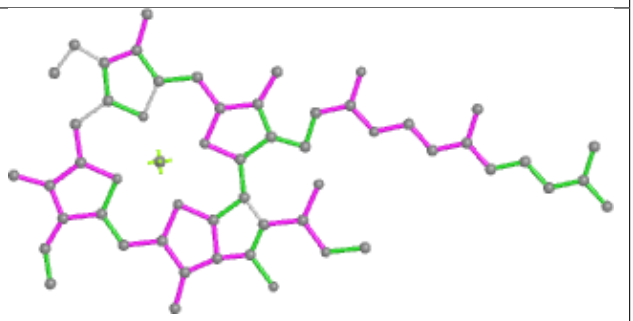
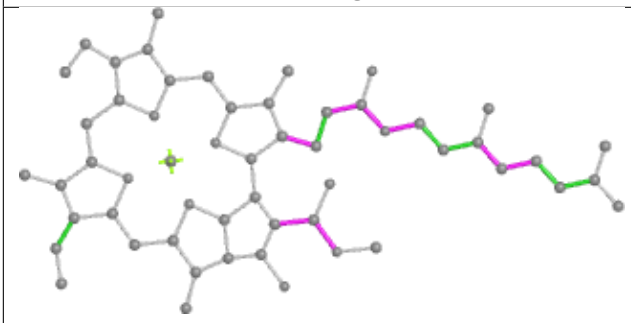


Bond angles



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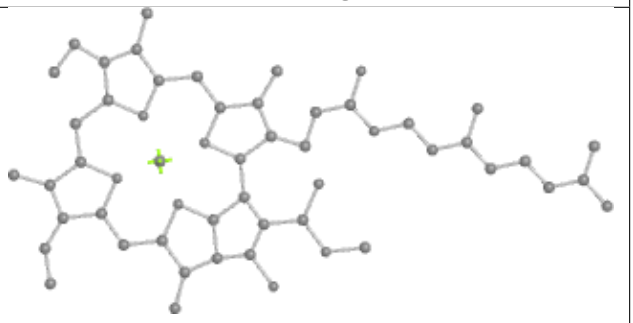
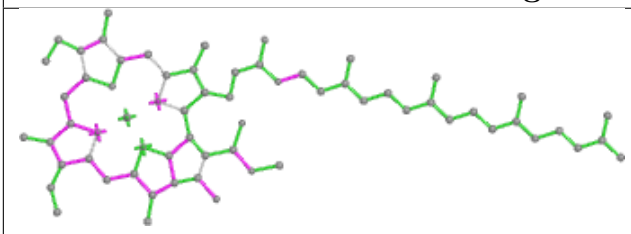


Rings

Ligand CLA H 837



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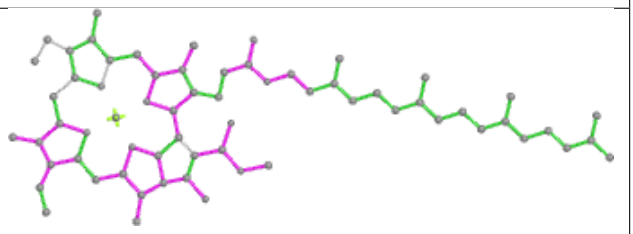

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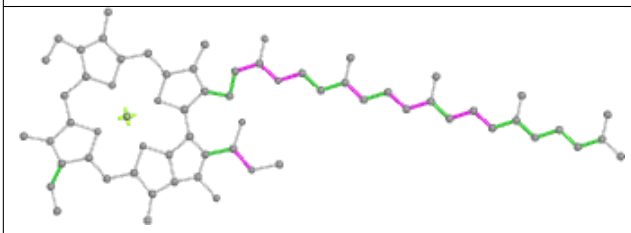

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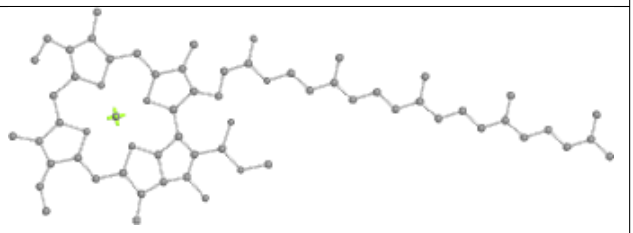

Rings

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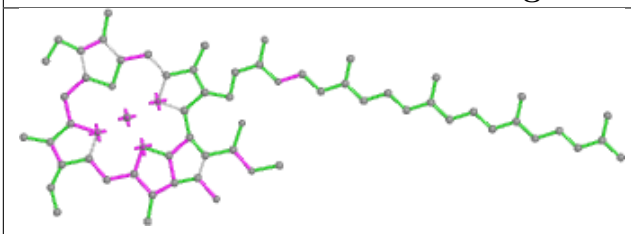
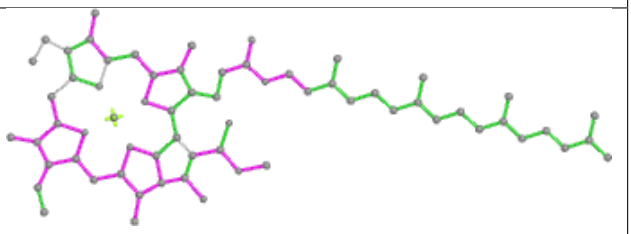
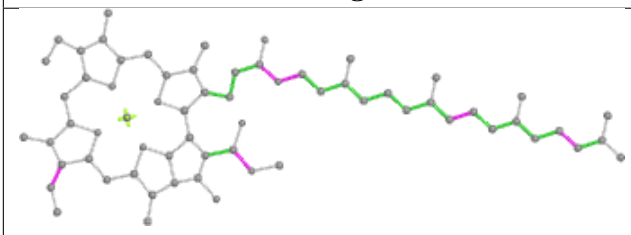
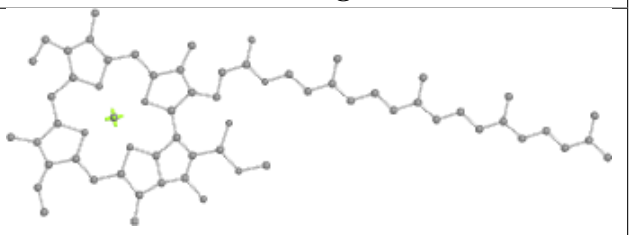
 Bond lengths	 Bond angles
 Torsions	 Rings

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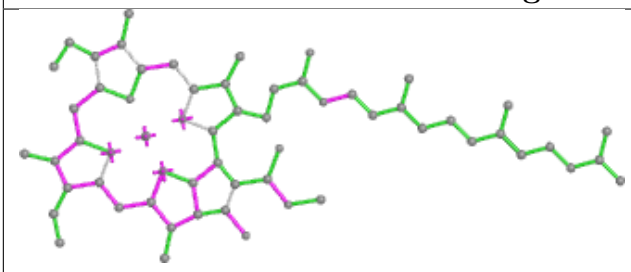
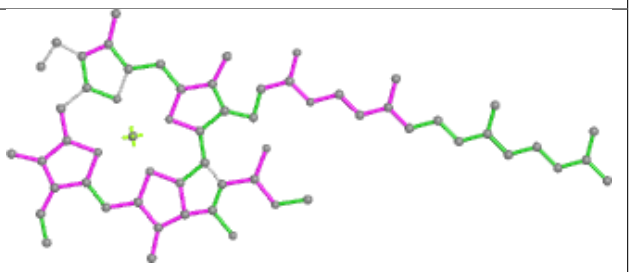
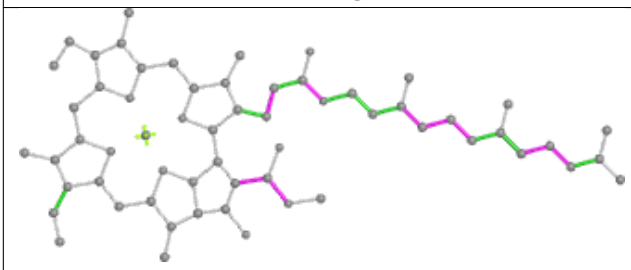
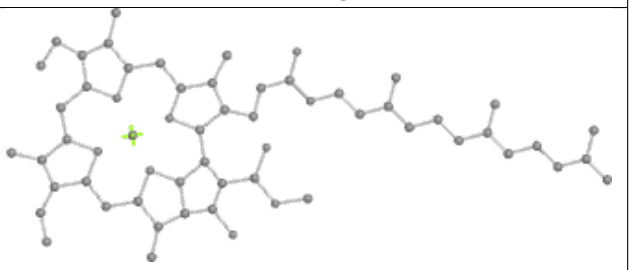
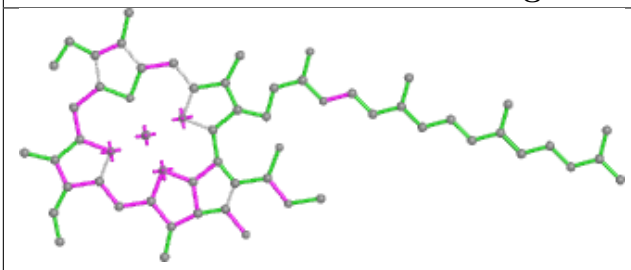
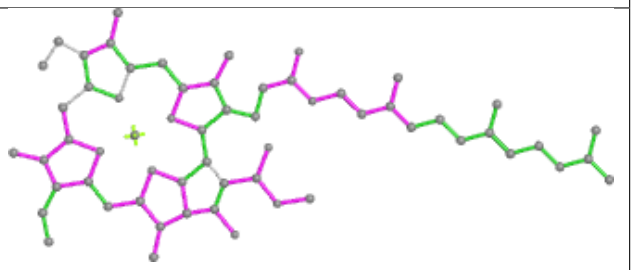
 Bond lengths	 Bond angles
 Torsions	 Rings

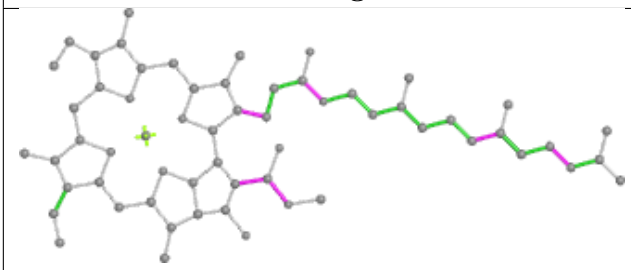
Ligand CLA A 814



Bond lengths



Bond angles



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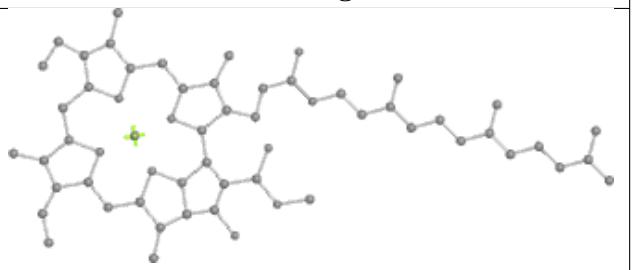
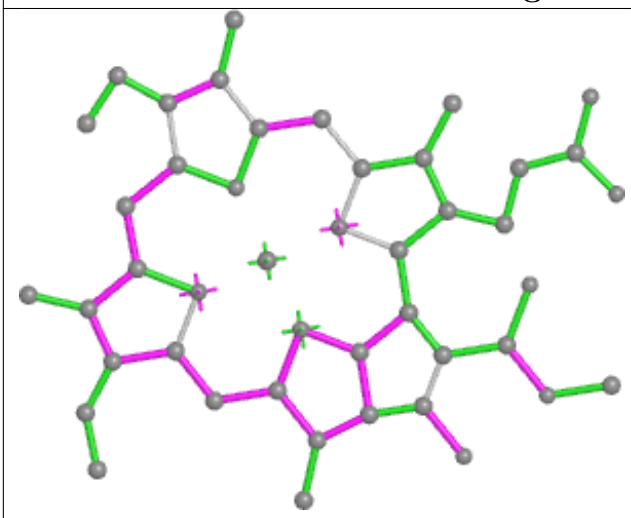


Rings

Ligand CLA Y 834



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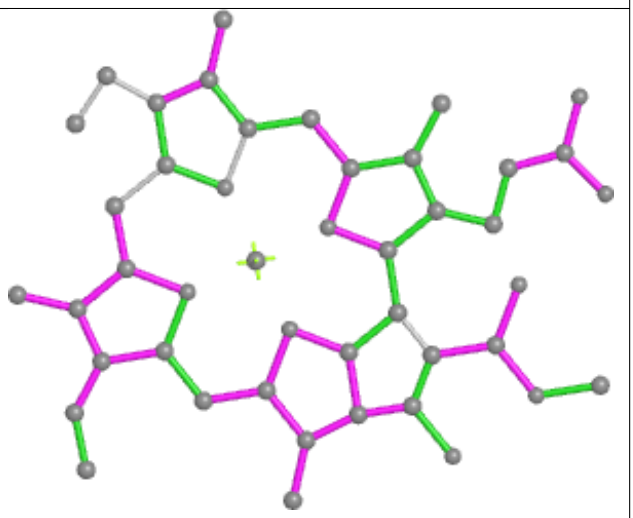
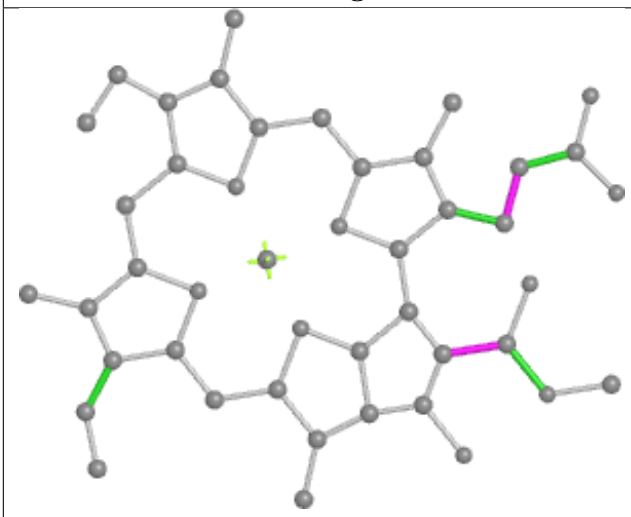


Bond angles



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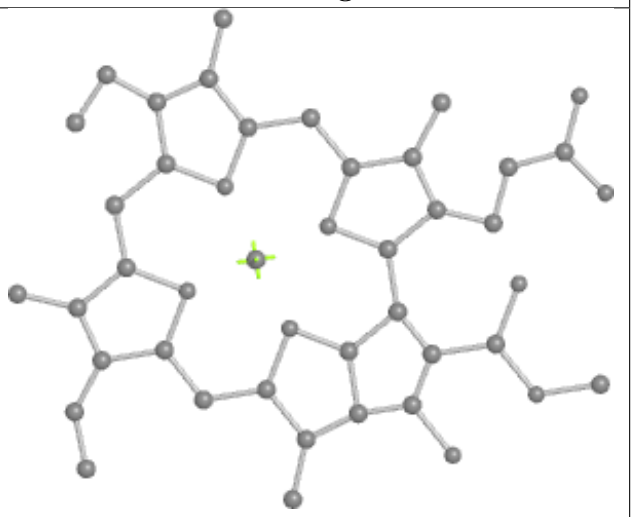
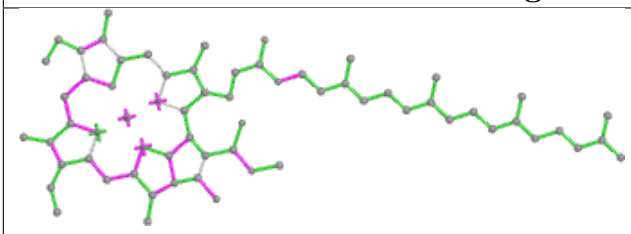


Rings

Ligand CLA B 828



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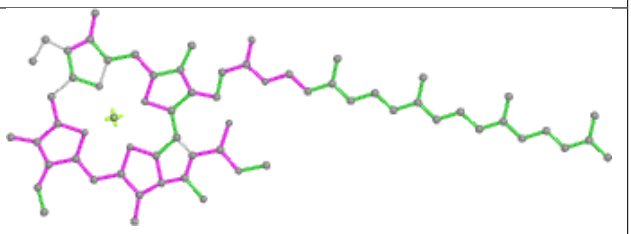

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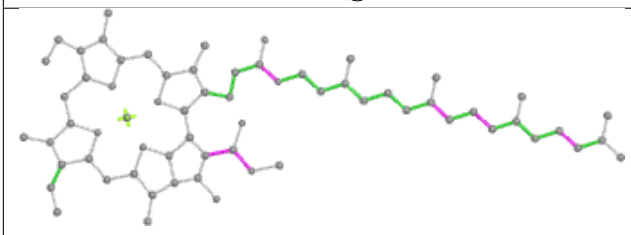

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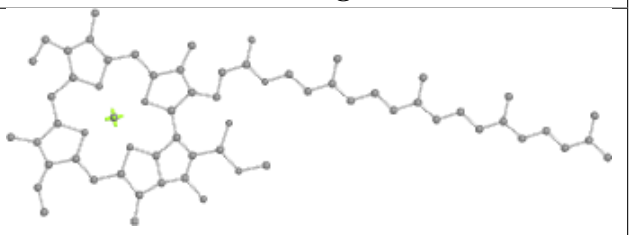
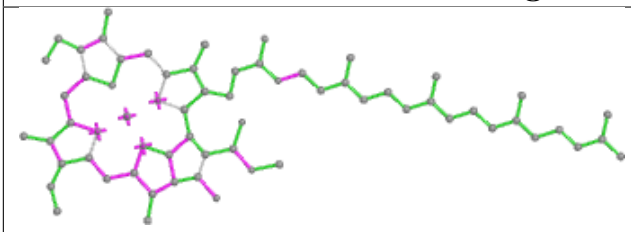


Rings

Ligand CLA B 824



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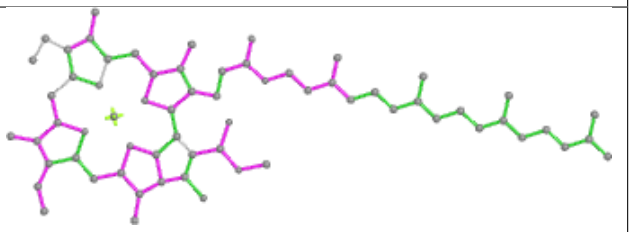

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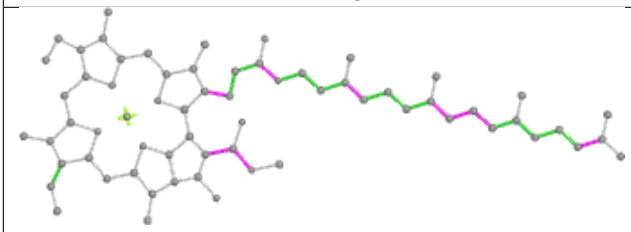

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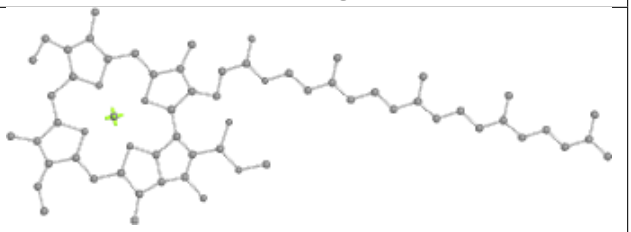
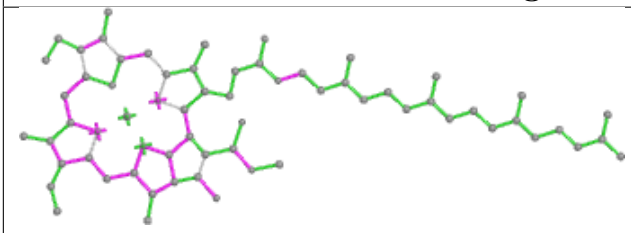


Rings

Ligand CLA G 822



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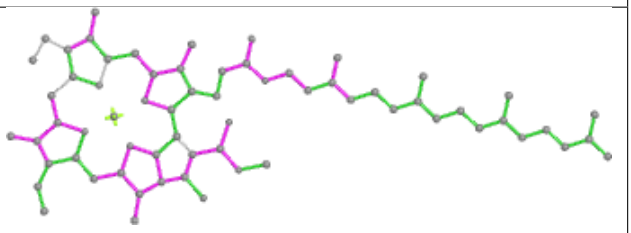
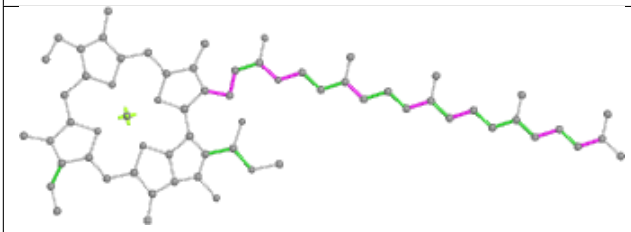


Bond angles



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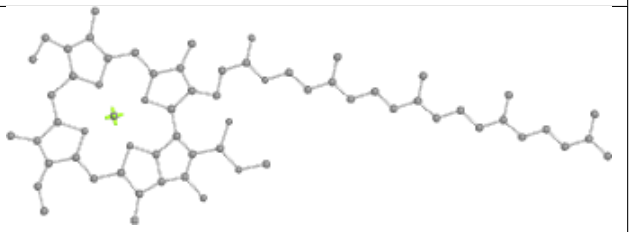
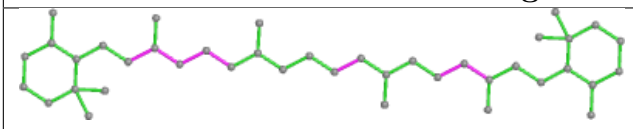


Rings

Ligand BCR G 845



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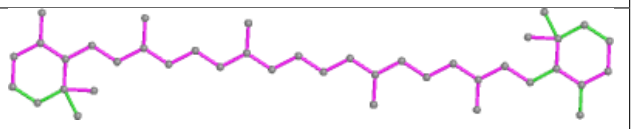
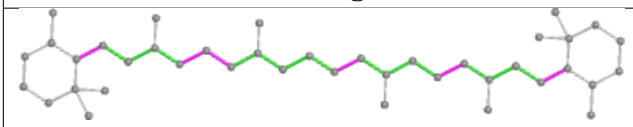


Bond angles



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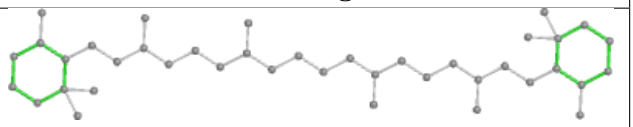
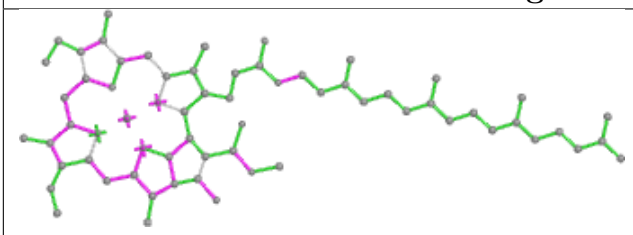


Rings

Ligand CLA L 206



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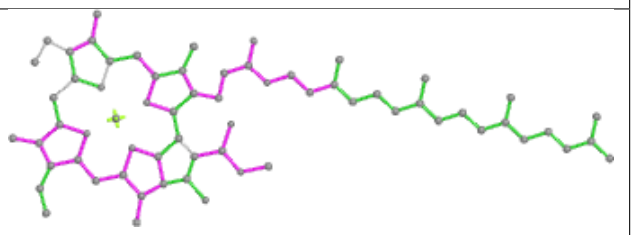
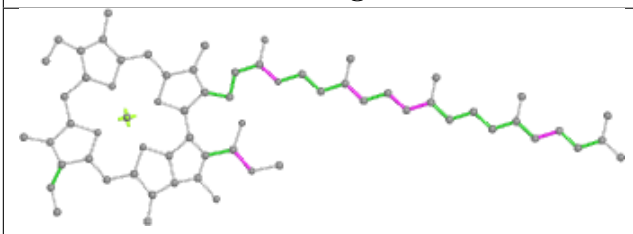


Bond angles



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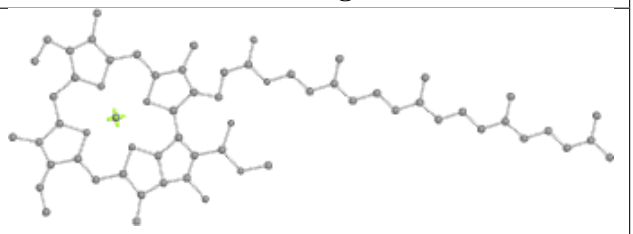
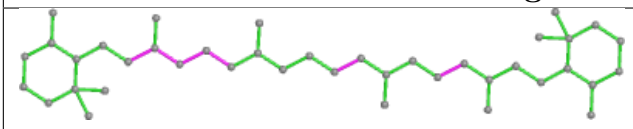
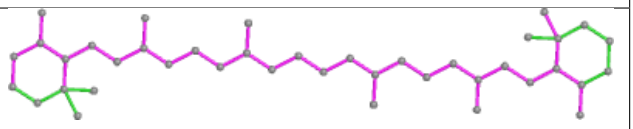


Rings

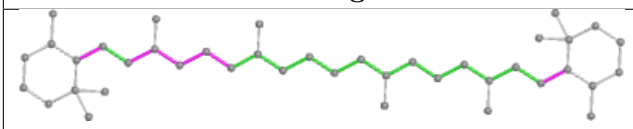
Ligand BCR Z 847



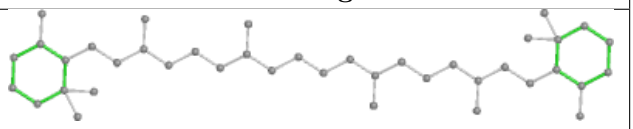
Bond lengths



Bond angles

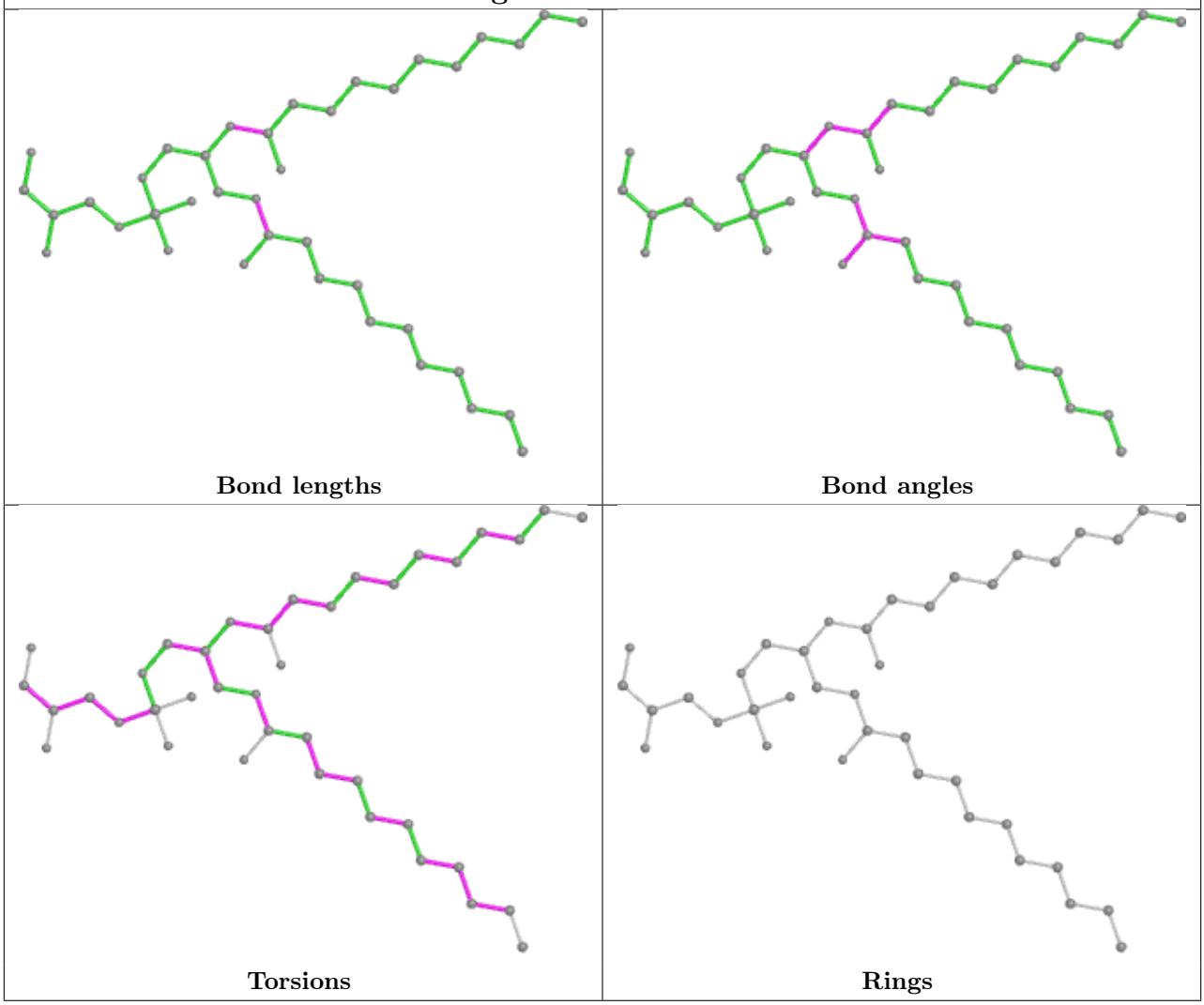


Torsions

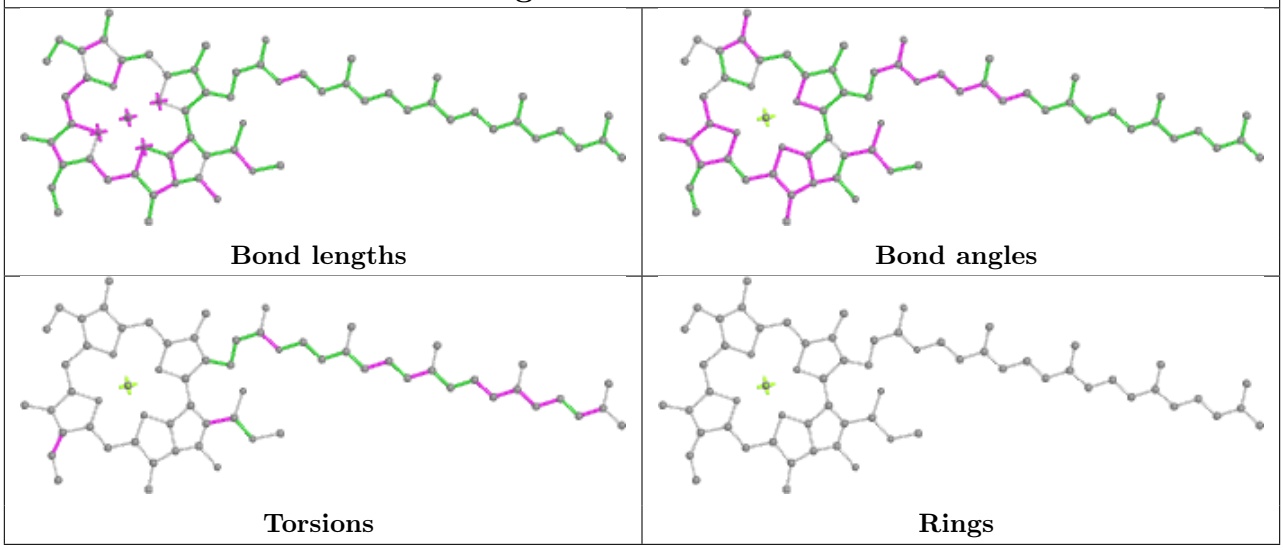


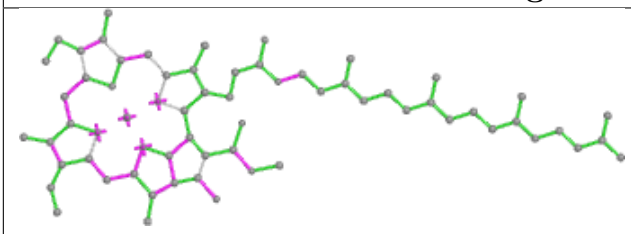
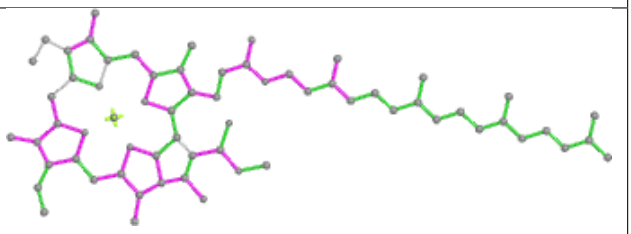
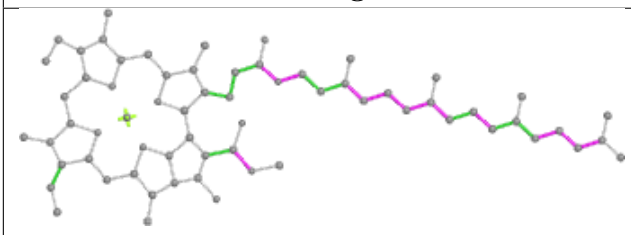
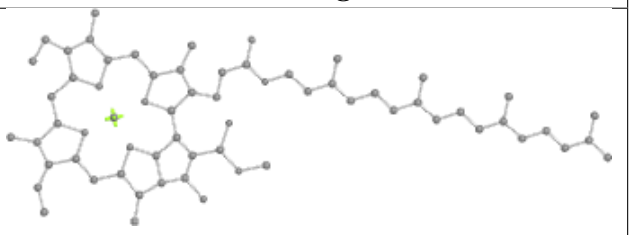
Rings

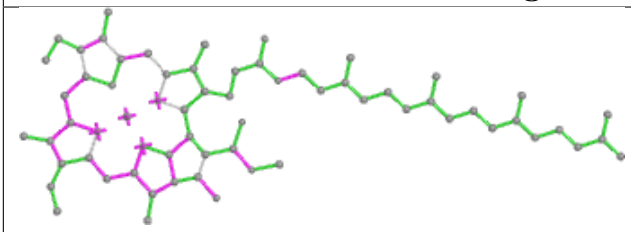
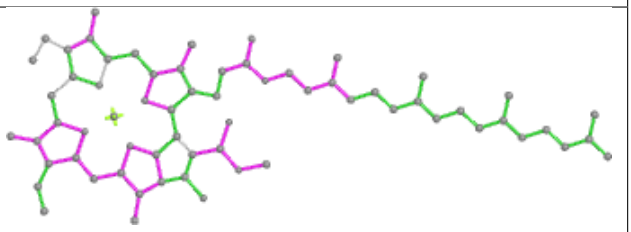
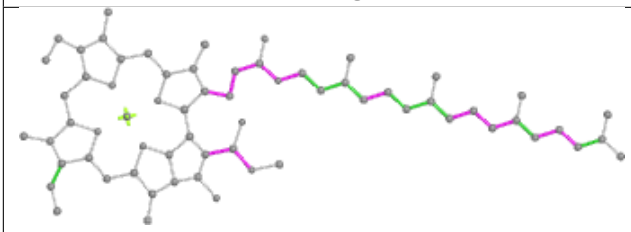
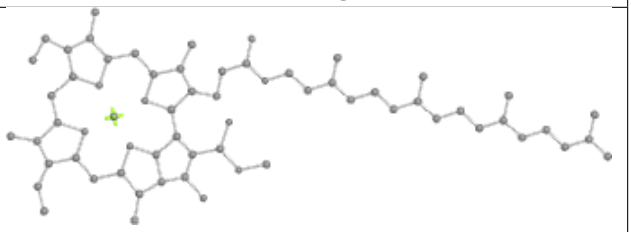
Ligand LHG B 849



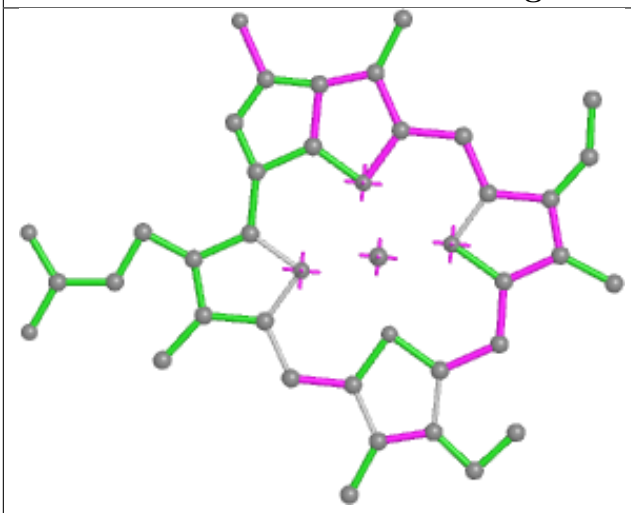
Ligand CLA U 1003



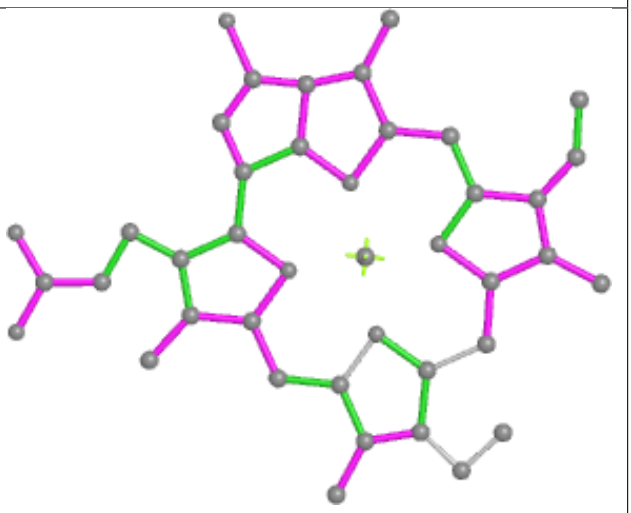
Ligand CLA Z 807	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA G 805	
 Bond lengths	 Bond angles
 Torsions	 Rings

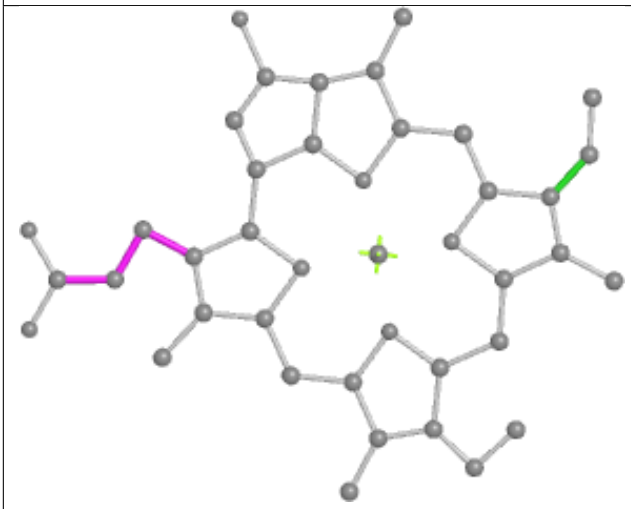
Ligand CLA T 101



Bond lengths



Bond angles



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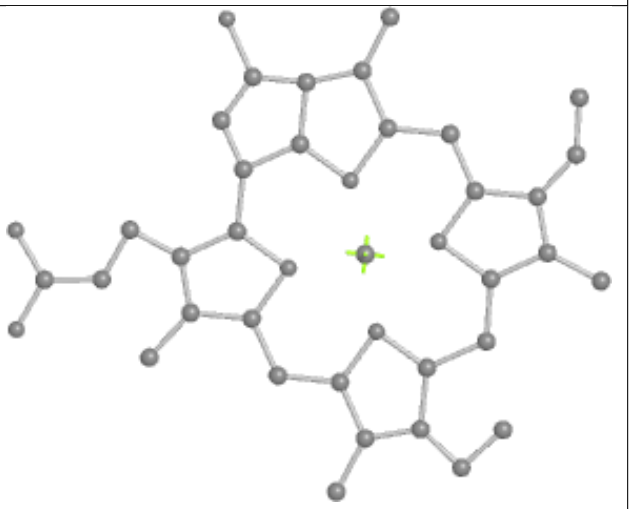
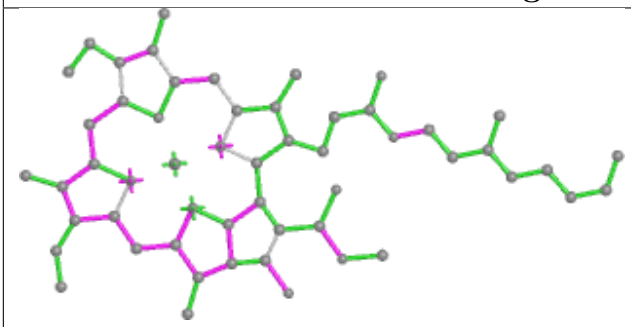


Rings

Ligand CLA G 812



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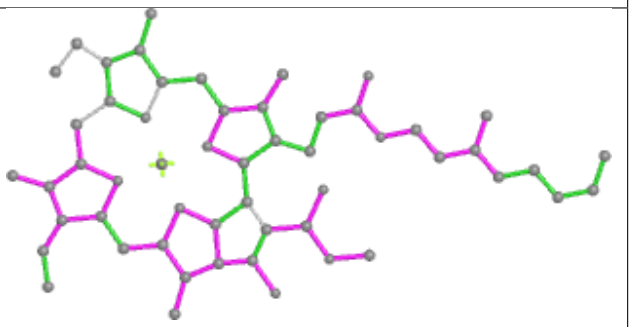

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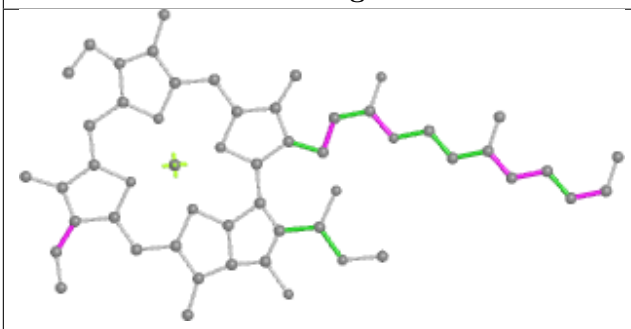

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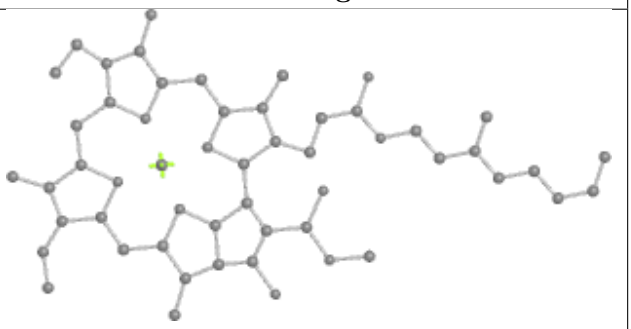
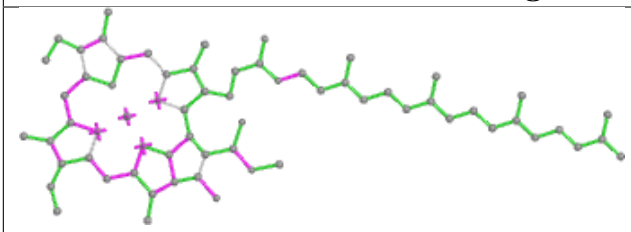


Rings

Ligand CLA B 813



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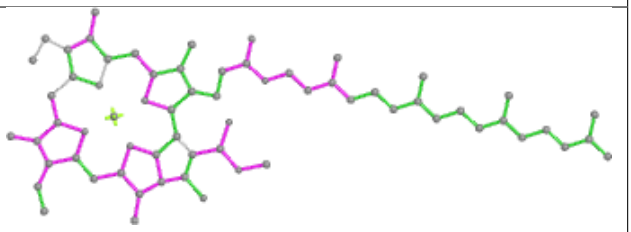

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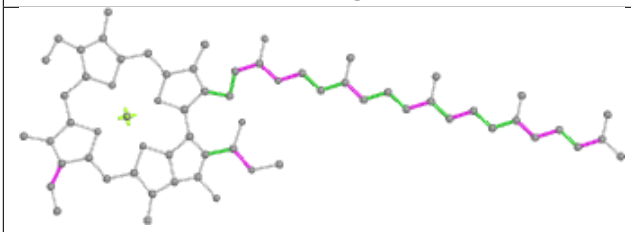

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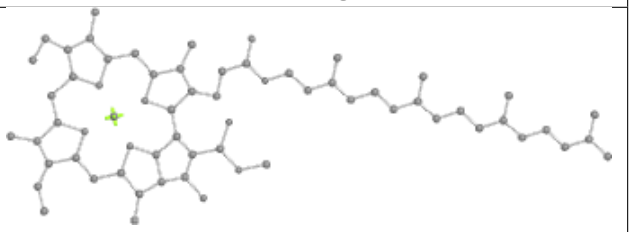
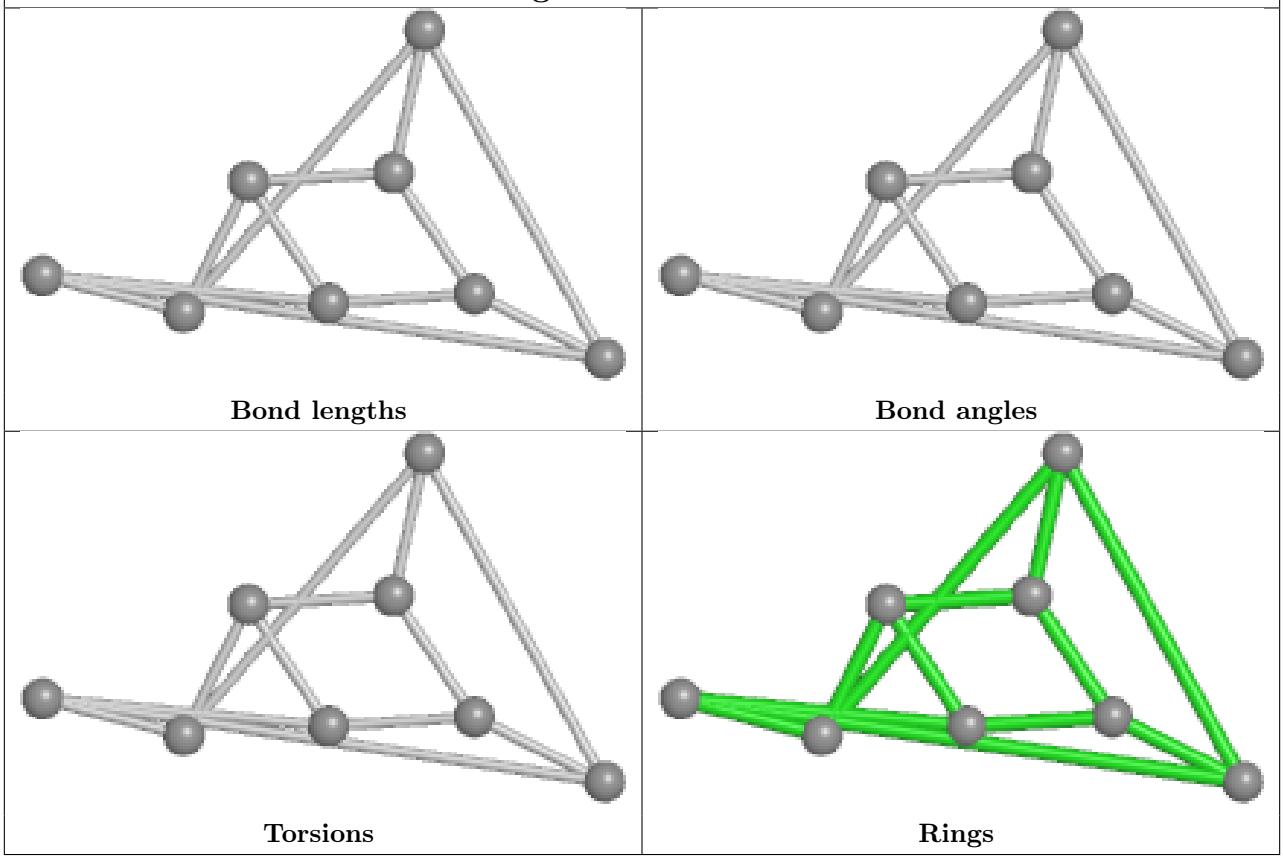
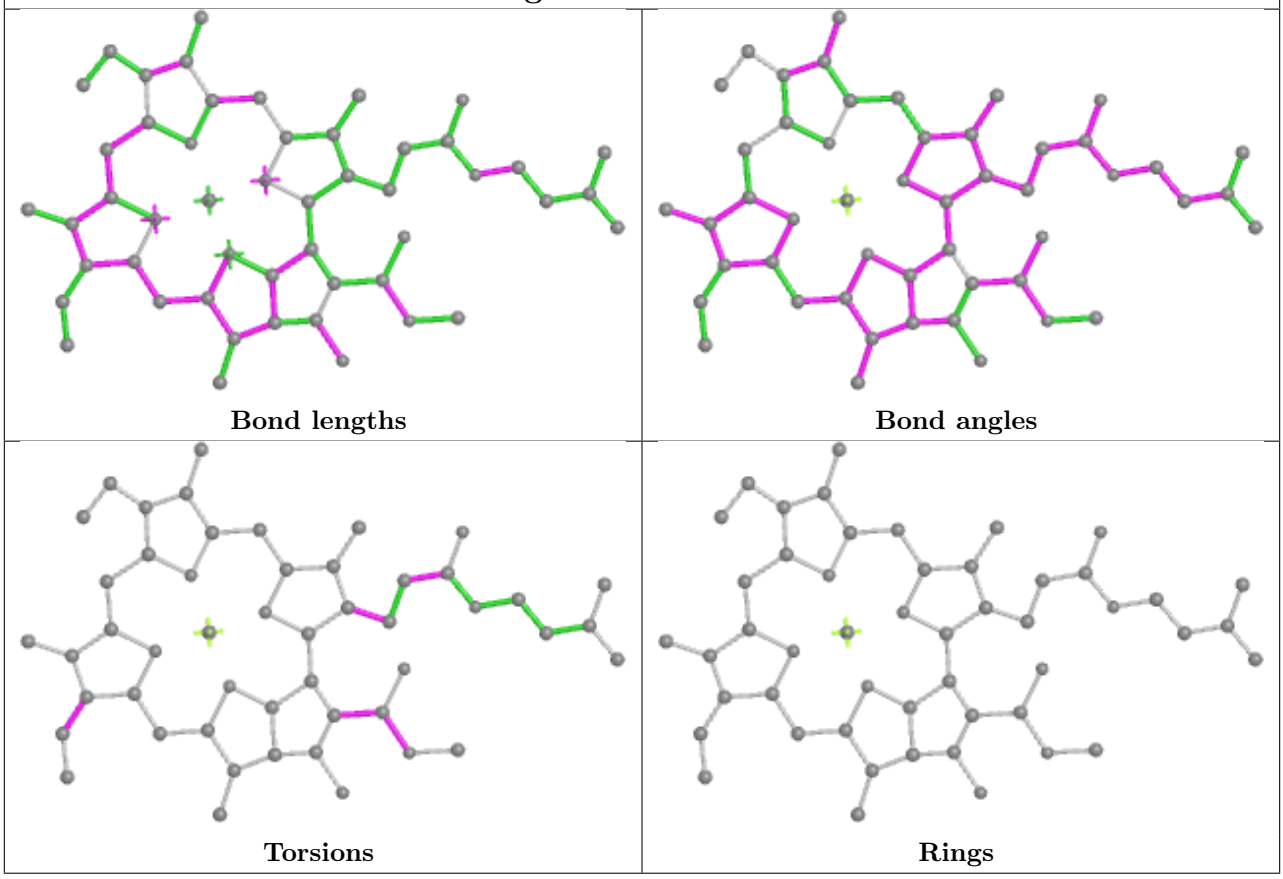


Rings

Ligand SF4 C 102



Ligand CLA A 815



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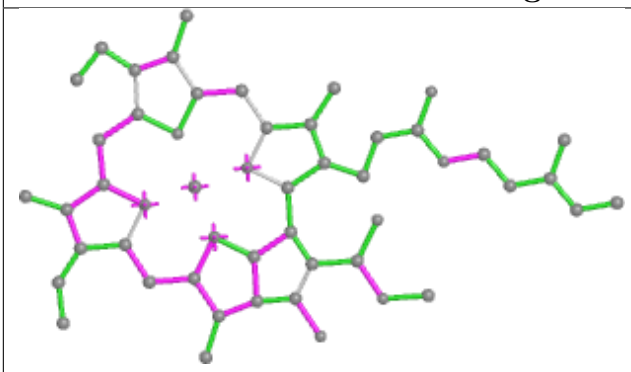
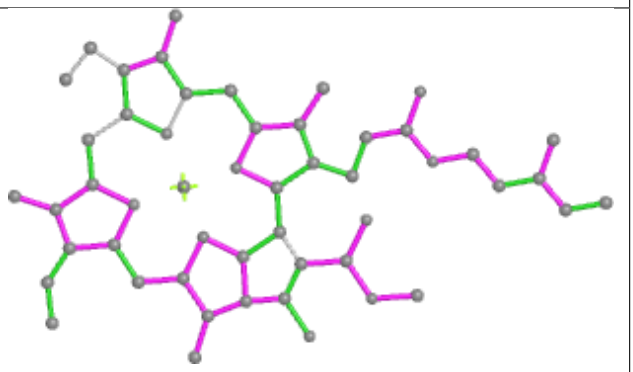
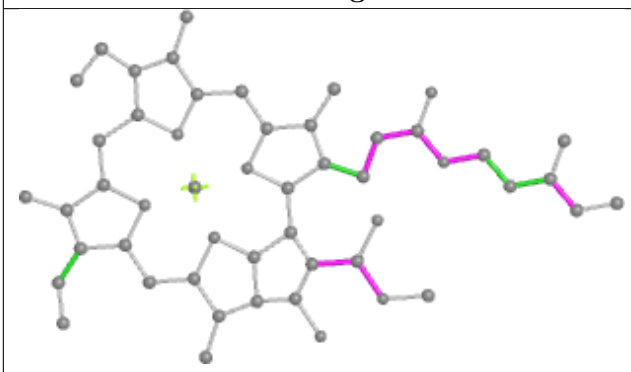


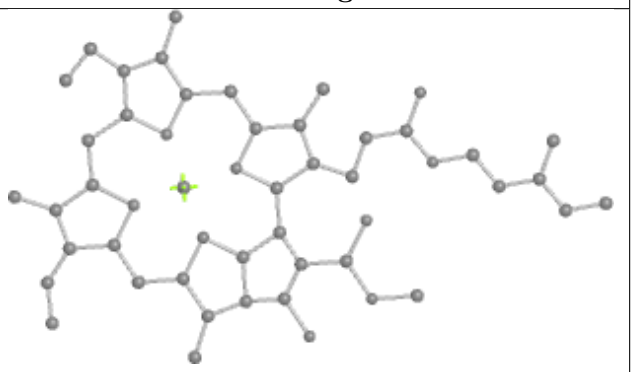
Bond lengths



Bond angles

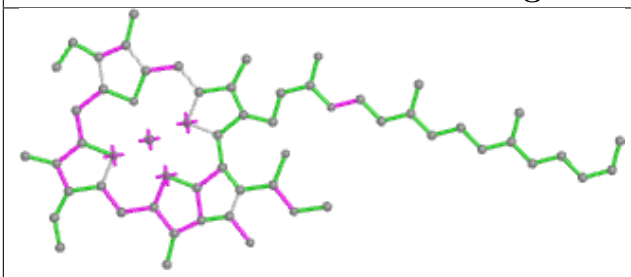


Torsions



Rings

Ligand CLA Y 804



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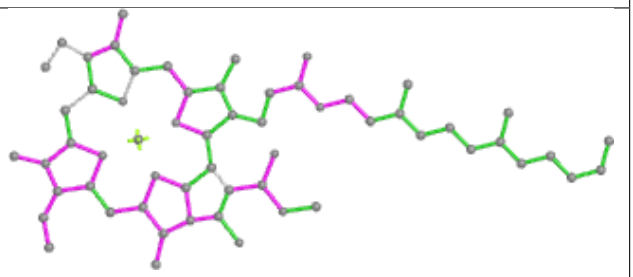
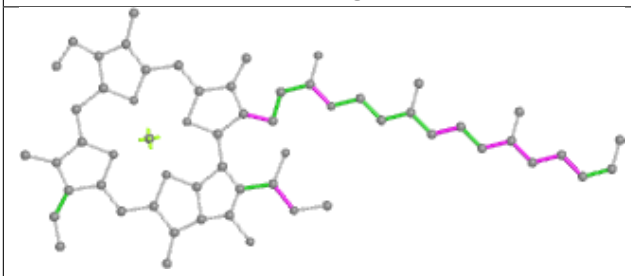


Bond angles



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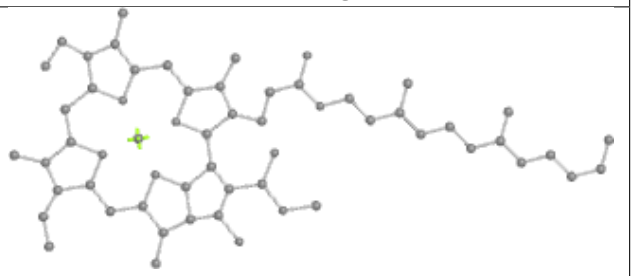
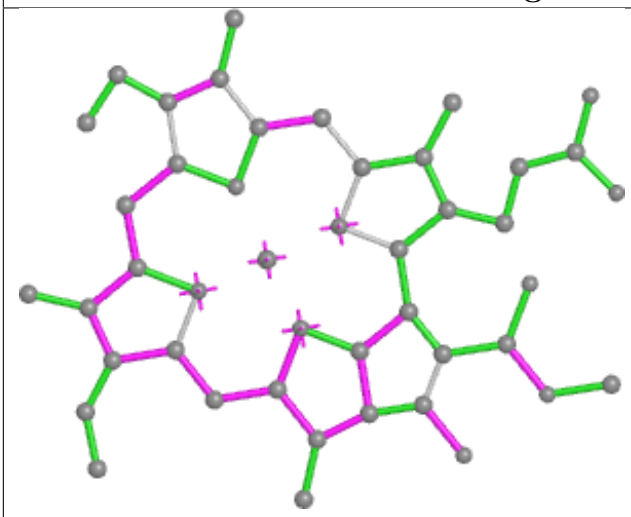


Rings

Ligand CLA B 835



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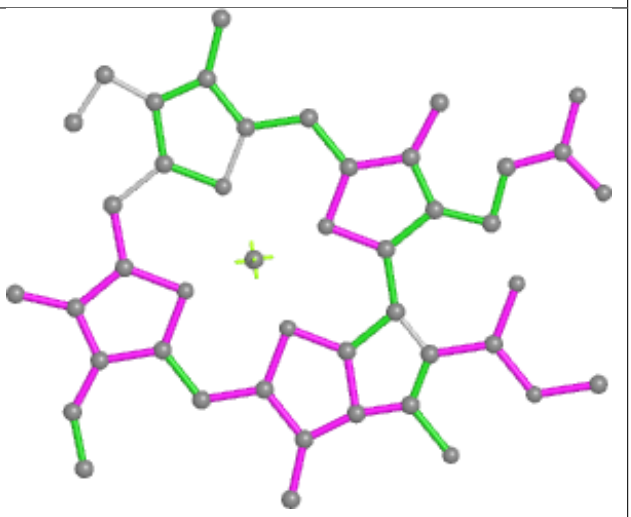

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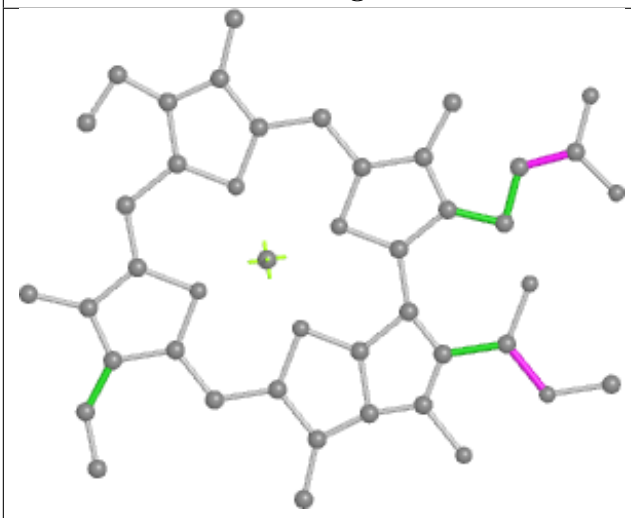

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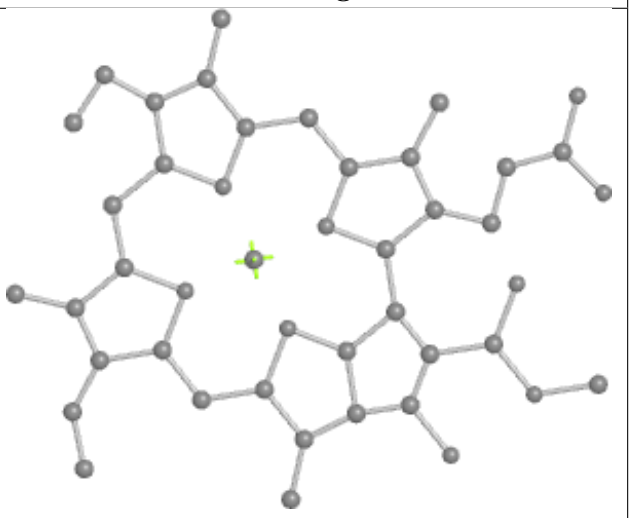
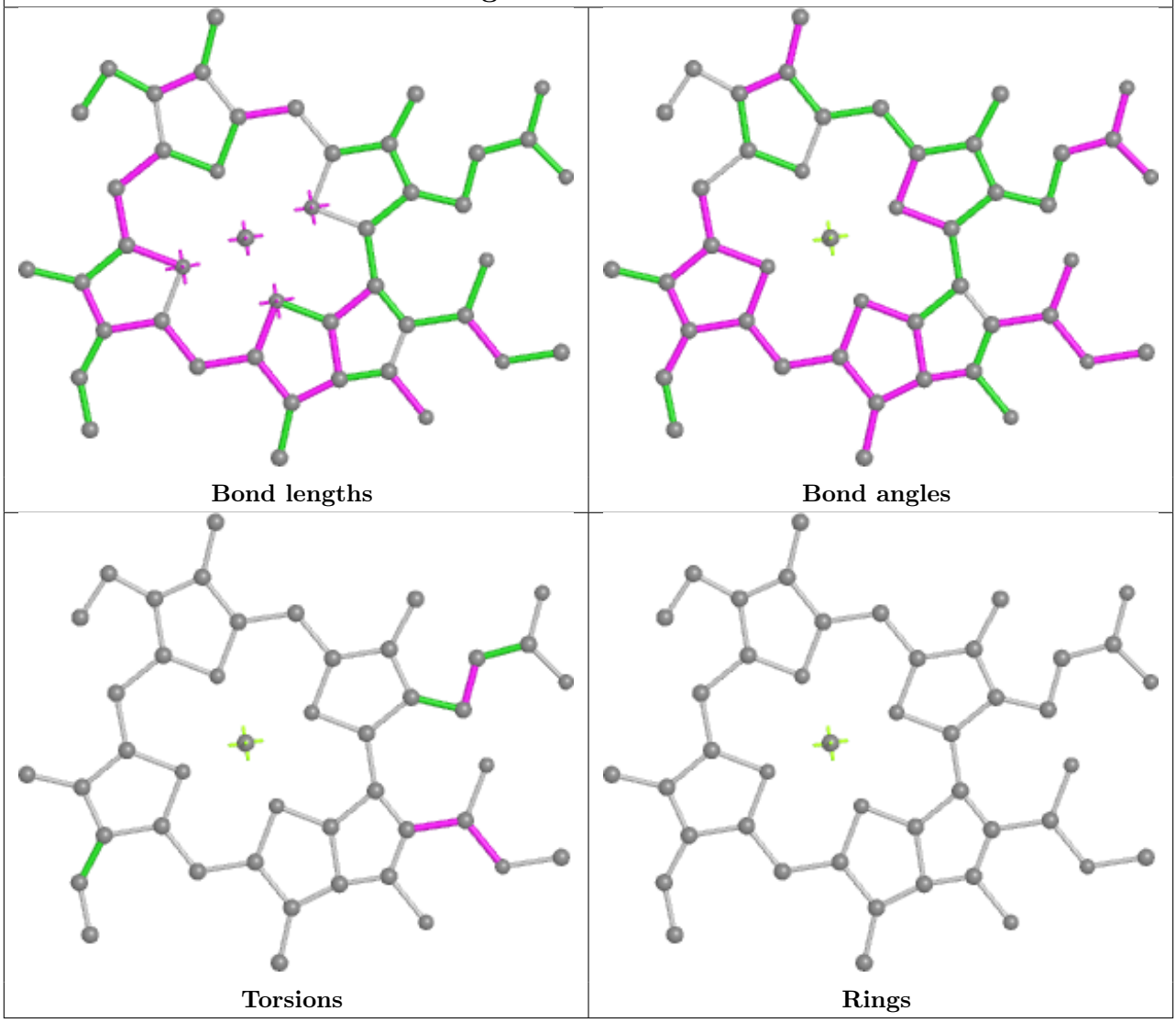
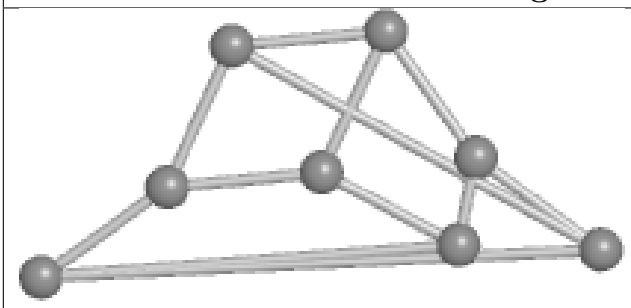


Rings

Ligand CLA B 830



Ligand SF4 A 845



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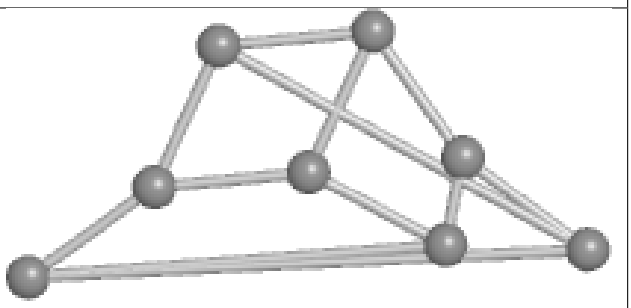
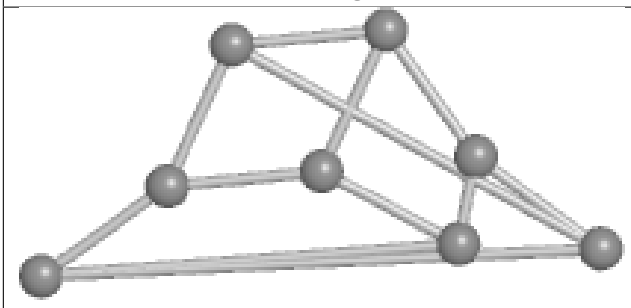


Bond angles



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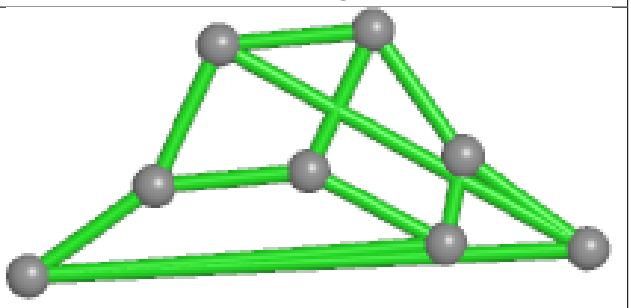
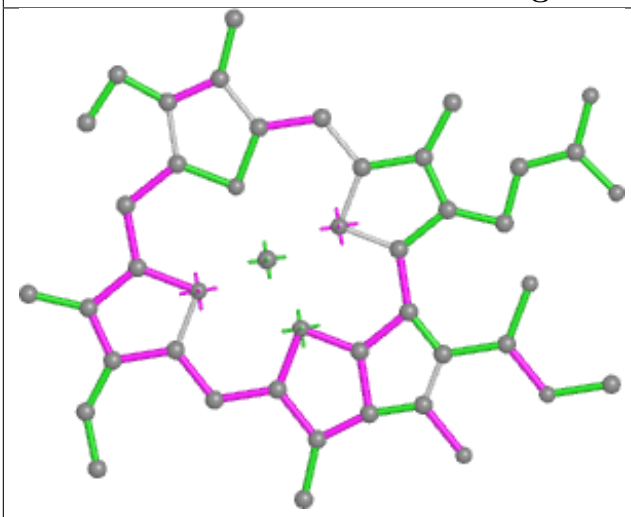


Rings

Ligand CLA f 101



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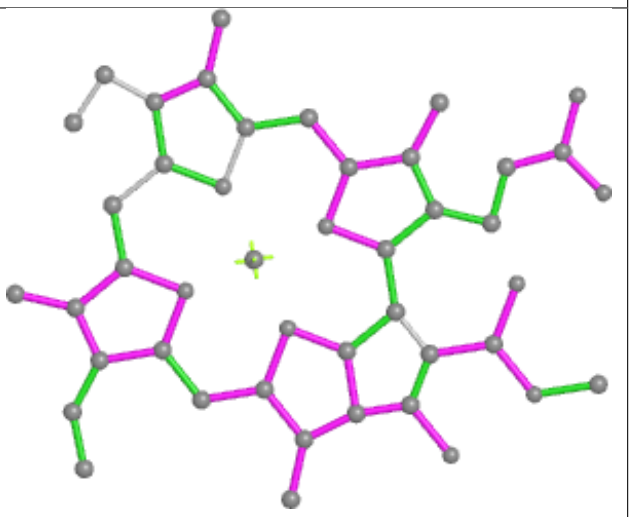
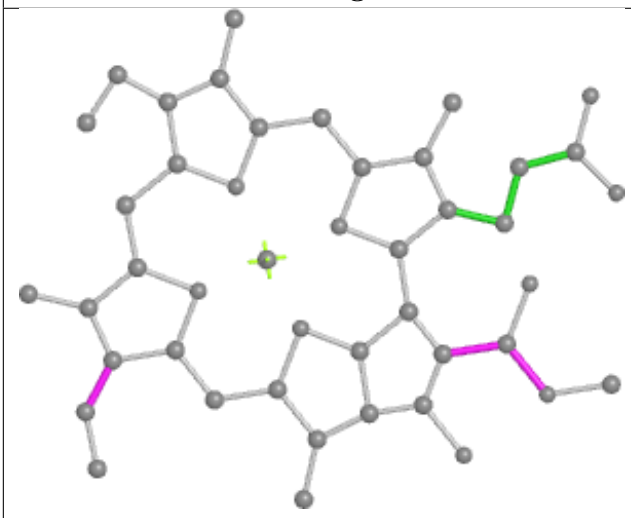


Bond angles



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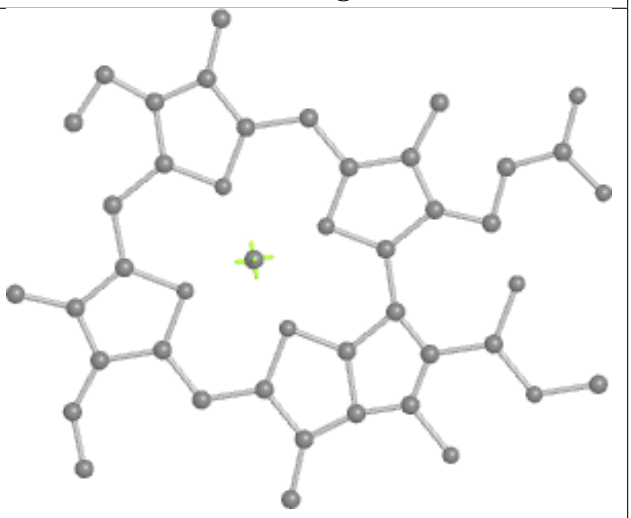
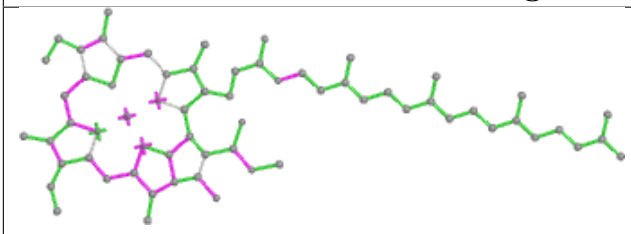


Rings

Ligand CLA A 841



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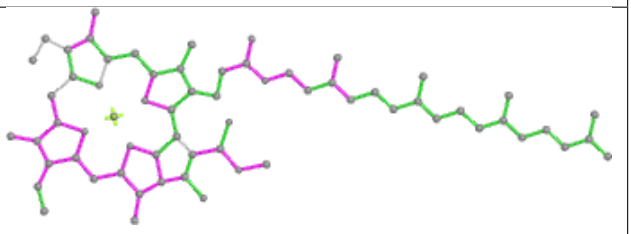
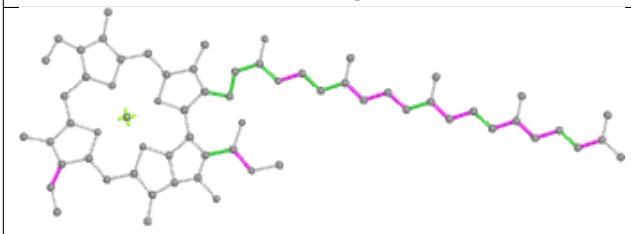
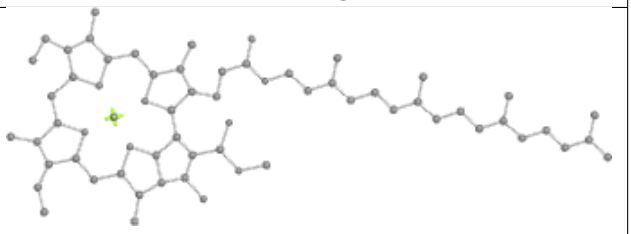


Bond angles

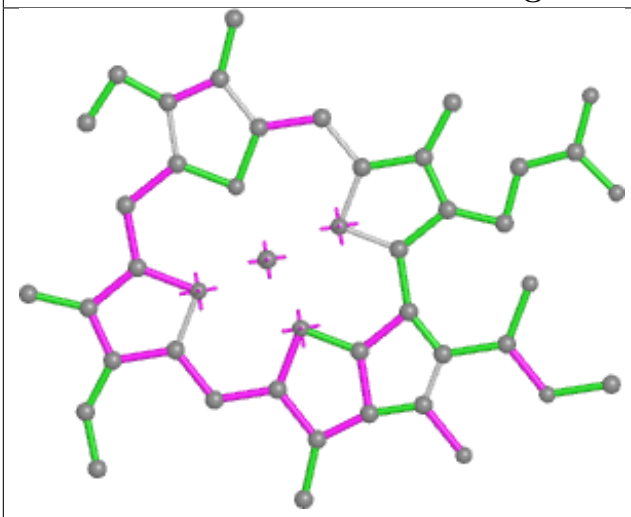


Torsions

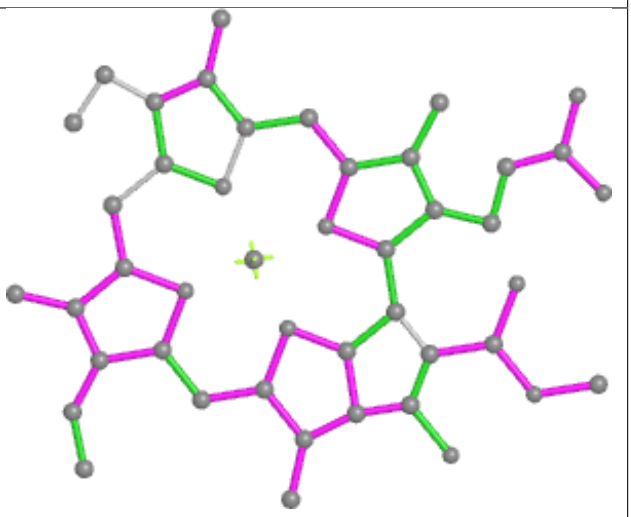


Rings

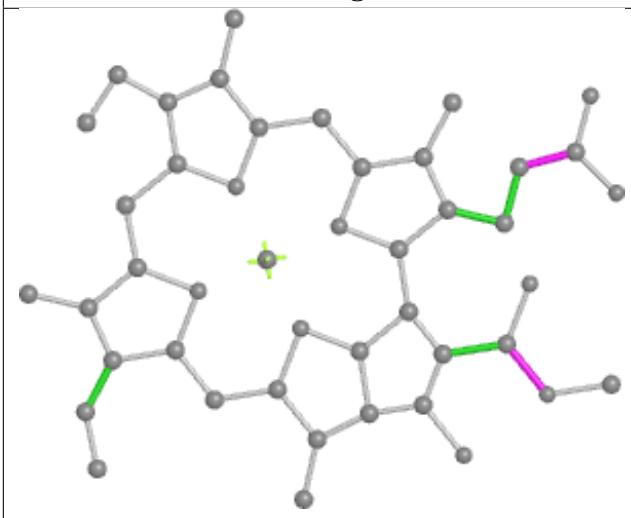
Ligand CLA B 834



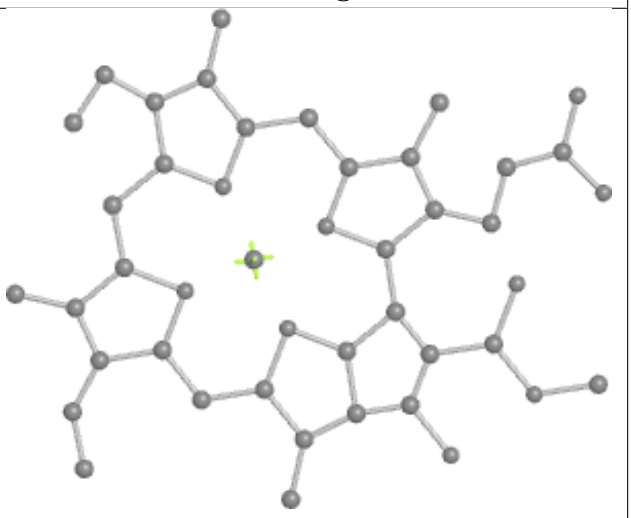
Bond lengths



Bond angles

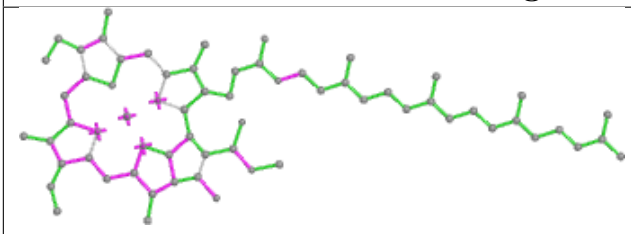


Torsions



Rings

Ligand CLA G 837



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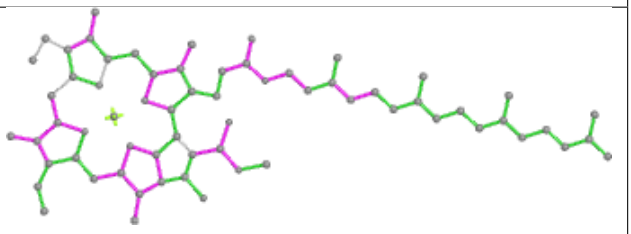

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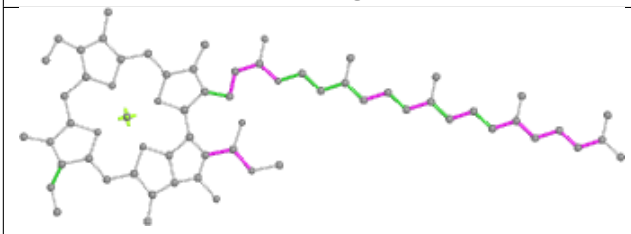

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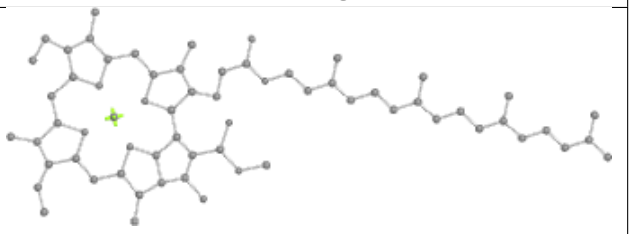
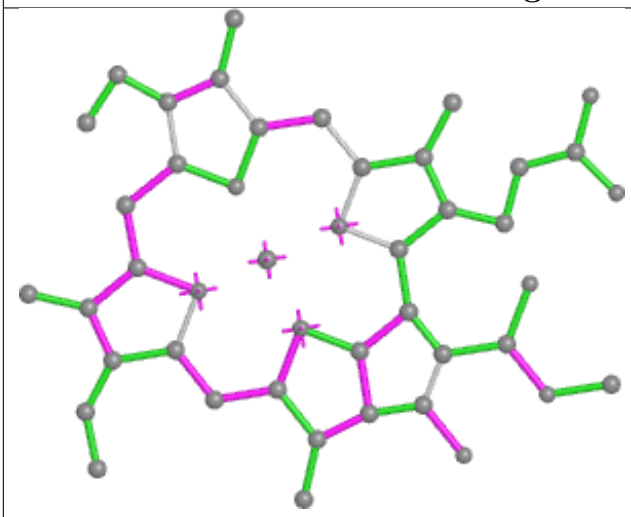


Rings

Ligand CLA Q 202



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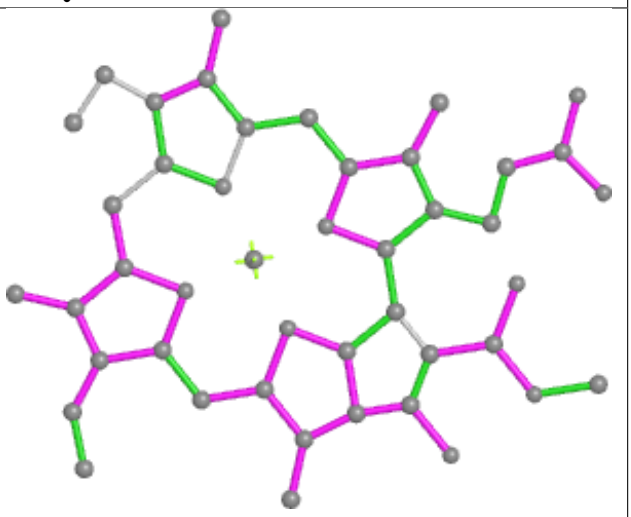
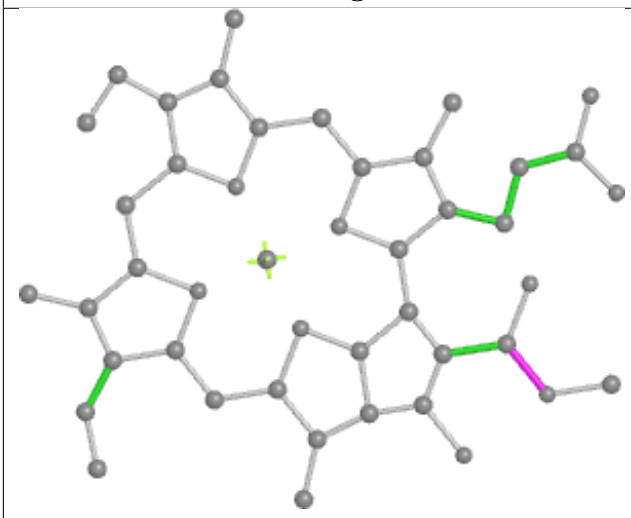
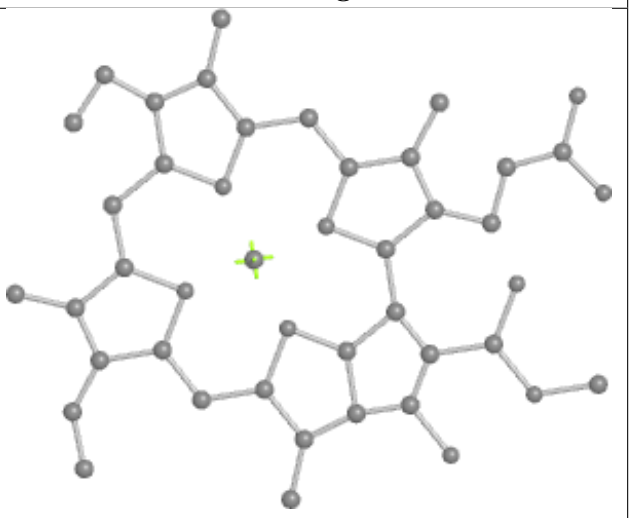


Bond angles

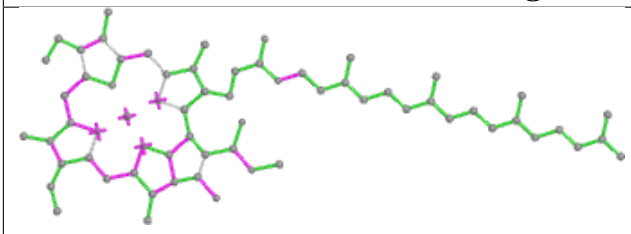


Torsions

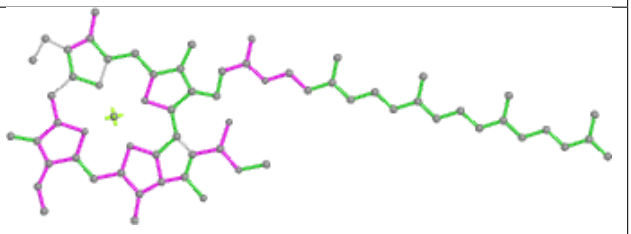


Rings

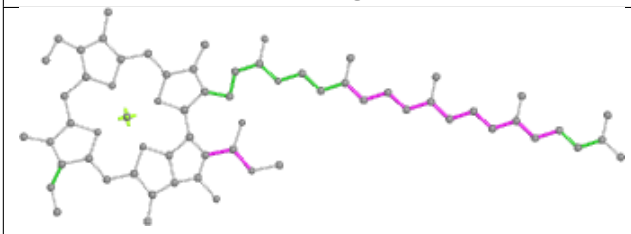
Ligand CLA B 807



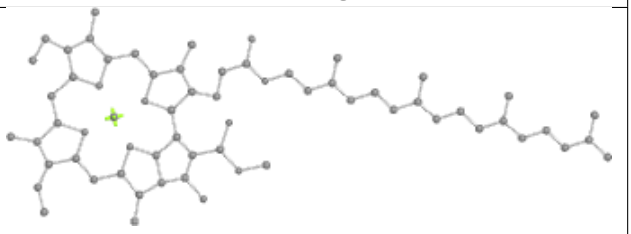
Bond lengths



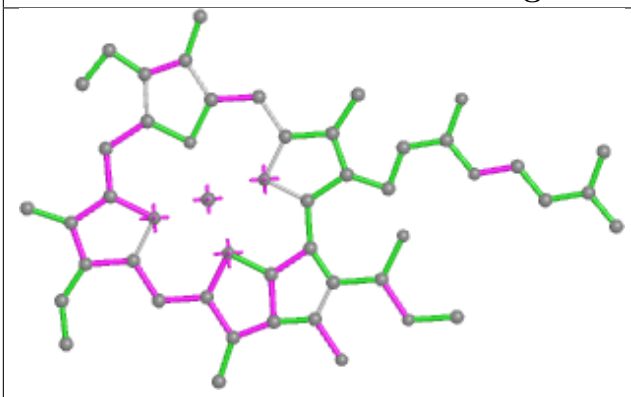
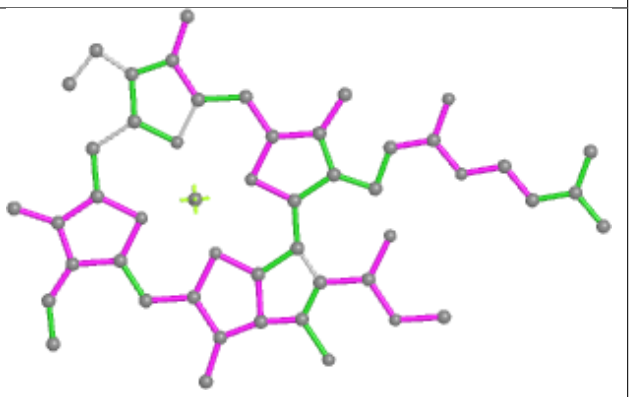
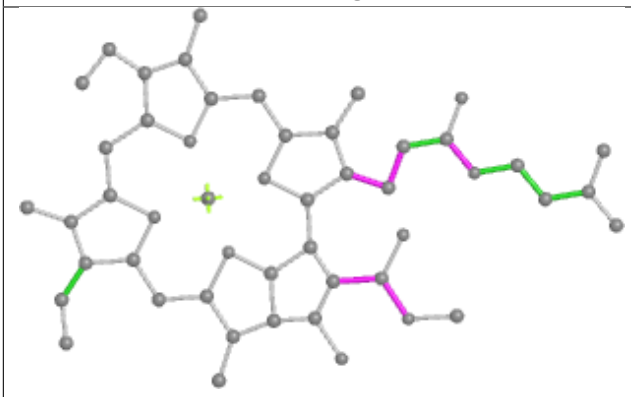
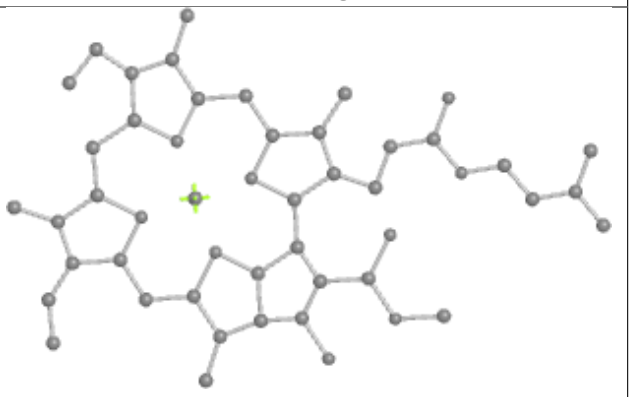
Bond angles



Torsions



Rings

Ligand CLA A 843	
 Bond lengths	 Bond angles
 Torsions	 Rings

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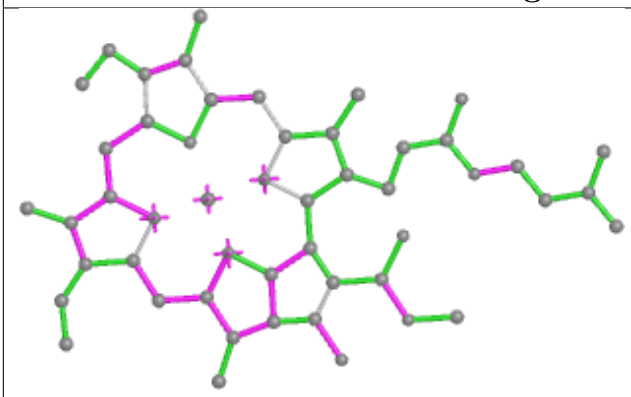
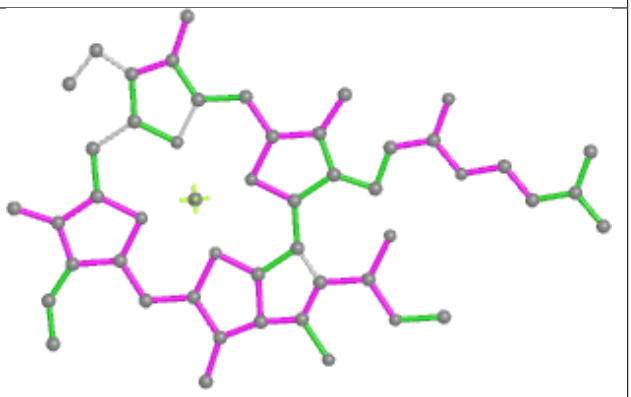
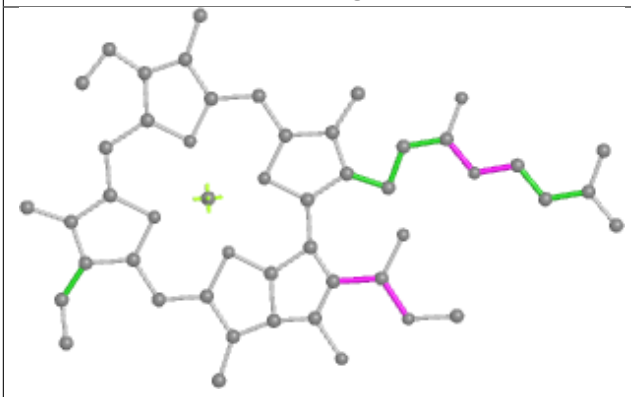
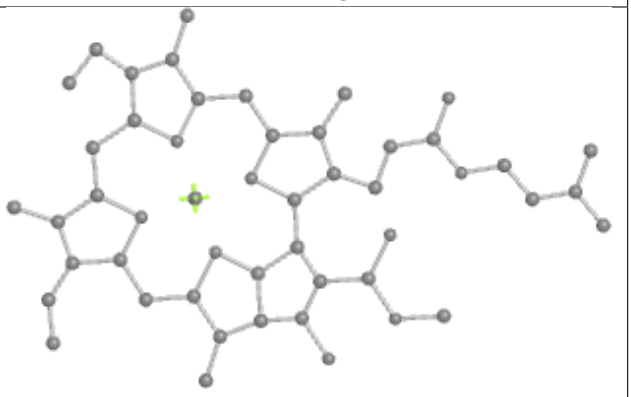
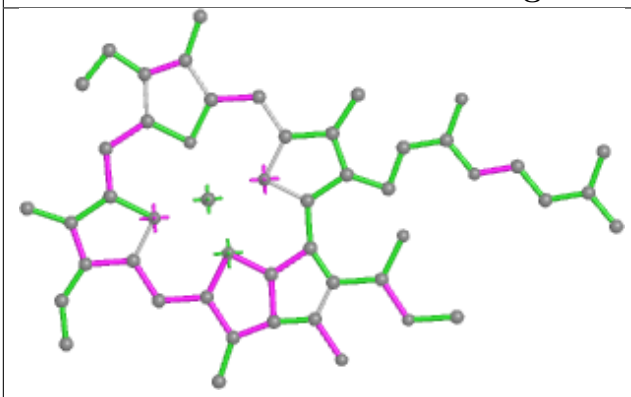
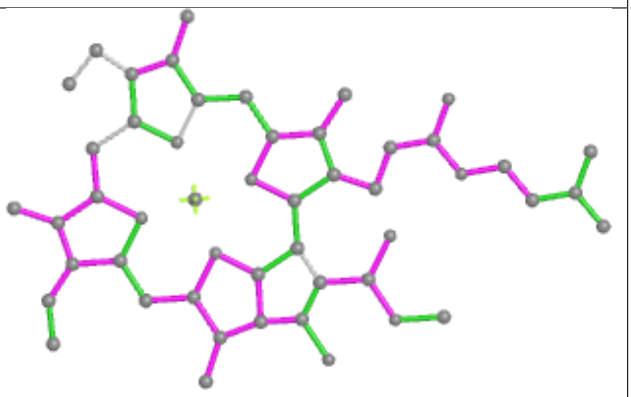
 Bond lengths	 Bond angles
 Torsions	 Rings

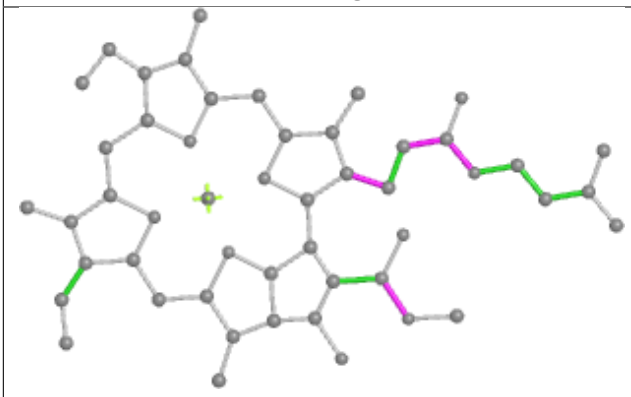
Ligand CLA Y 823



Bond lengths



Bond angles



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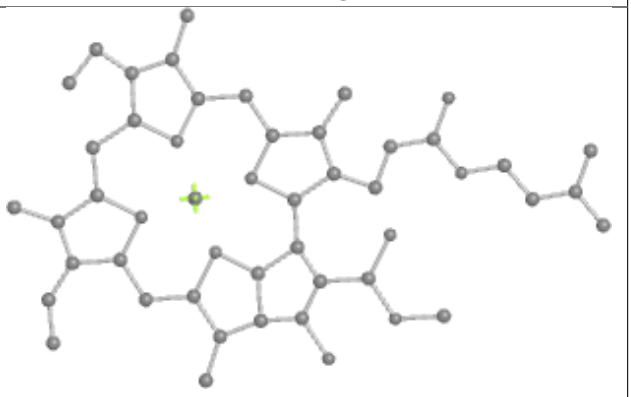

Rings

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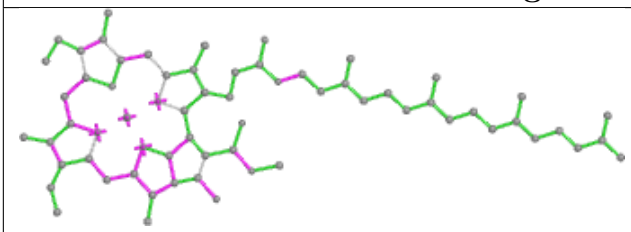

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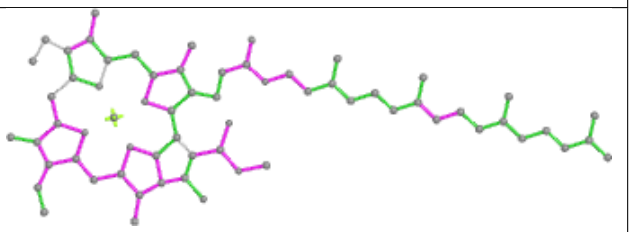
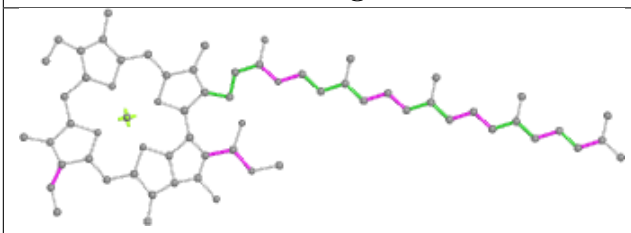


Bond angles



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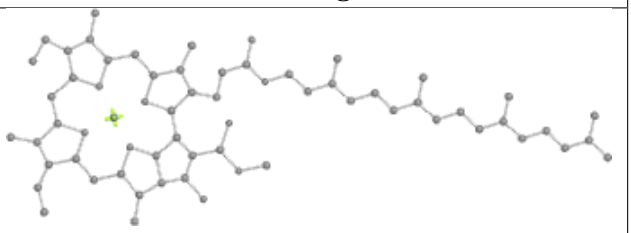

Rings

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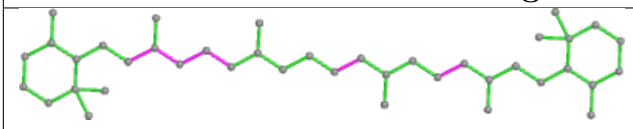

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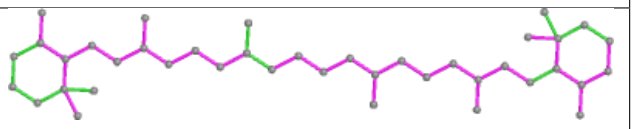
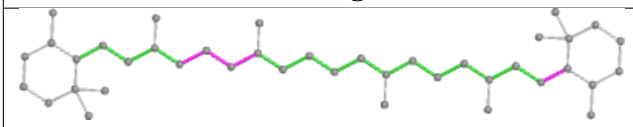


Bond angles



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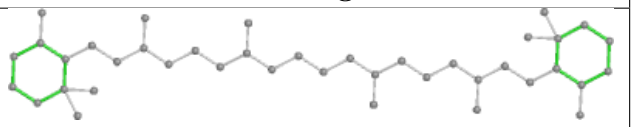
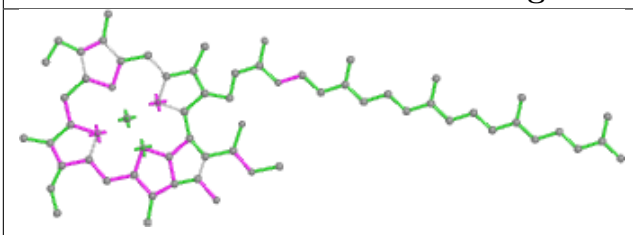


Rings

Ligand CL0 G 801



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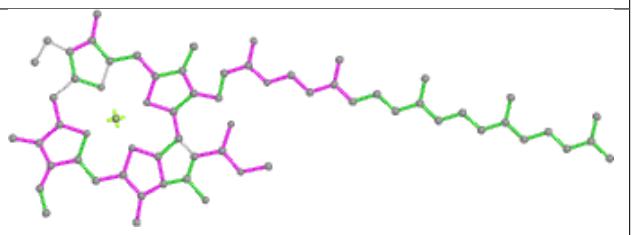
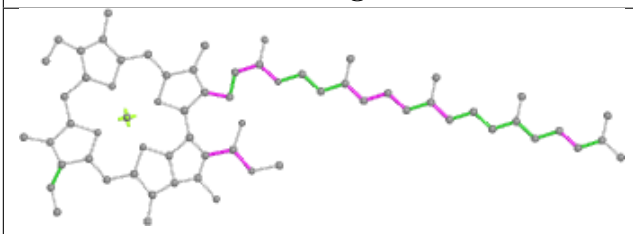


Bond angles



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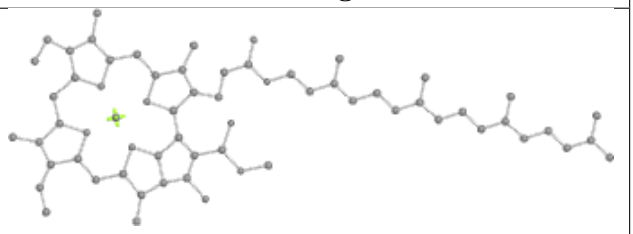
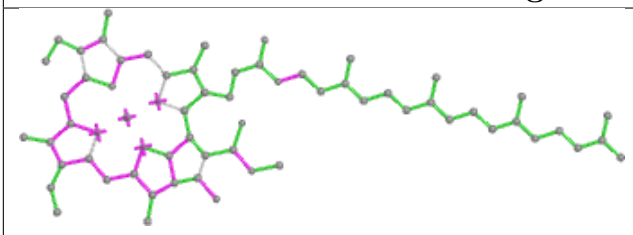


Rings

Ligand CLA L 205



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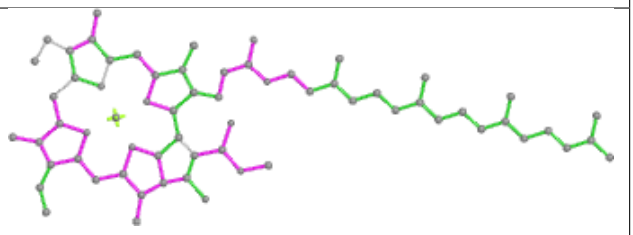
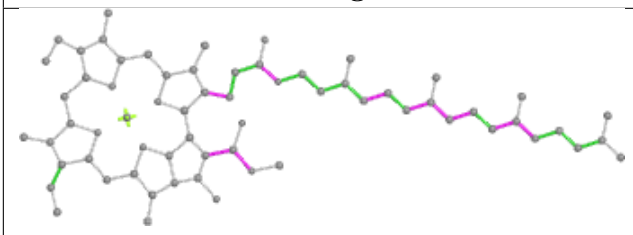


Bond angles



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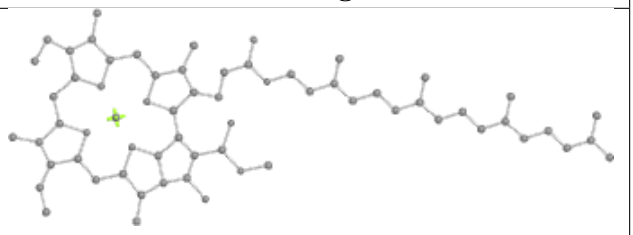
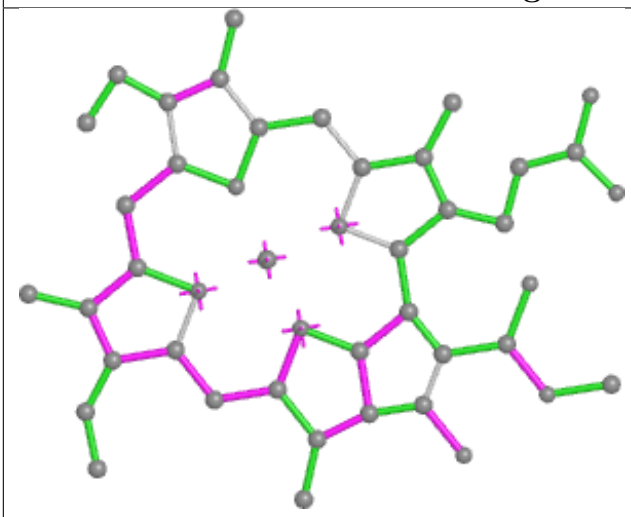


Rings

Ligand CLA H 830



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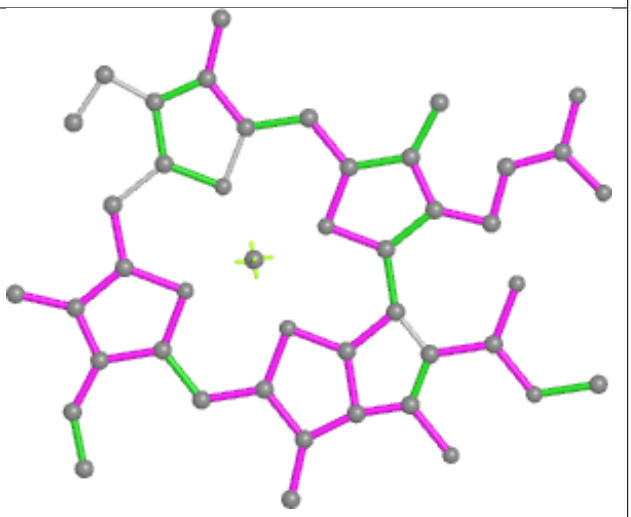
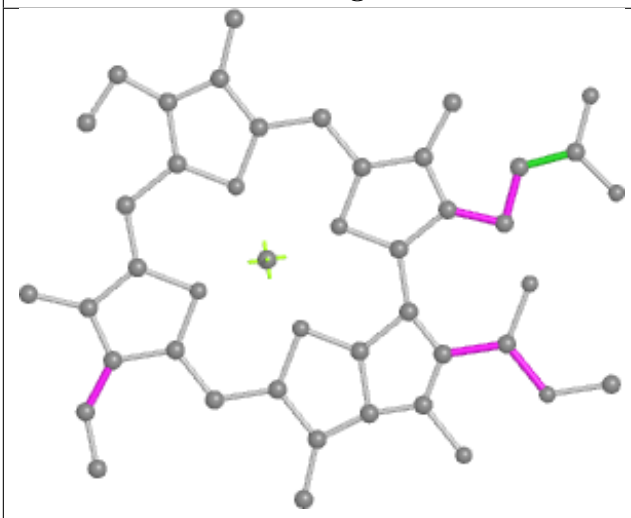


Bond angles



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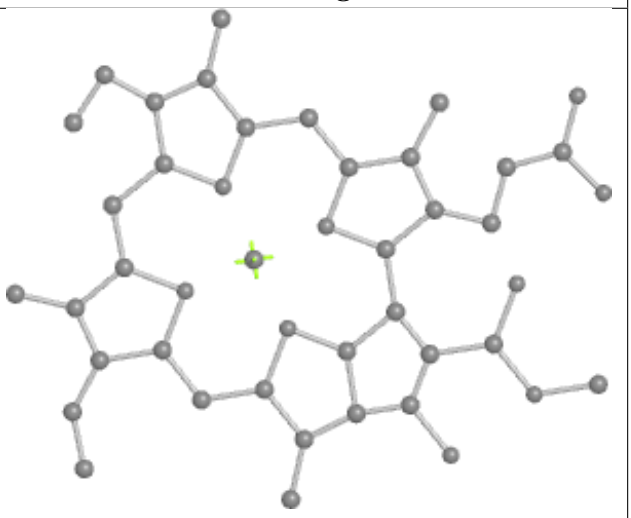
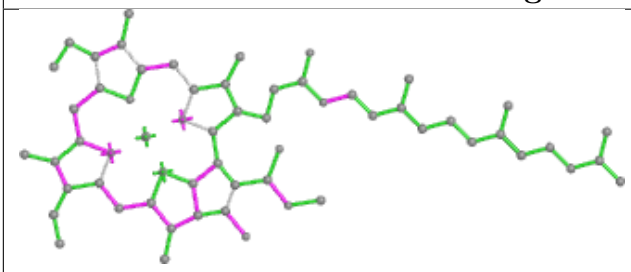


Rings

Ligand CLA B 822



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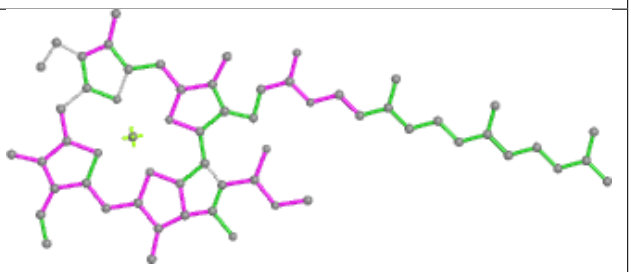
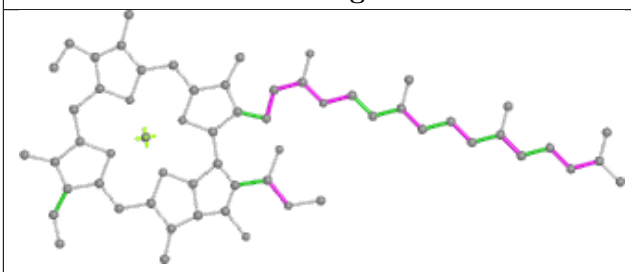


Bond angles



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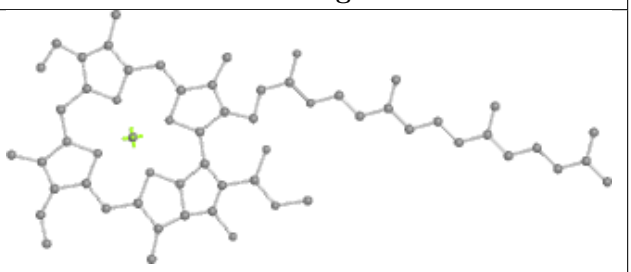

Rings

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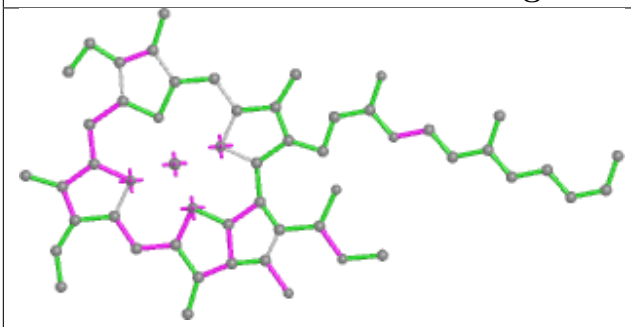

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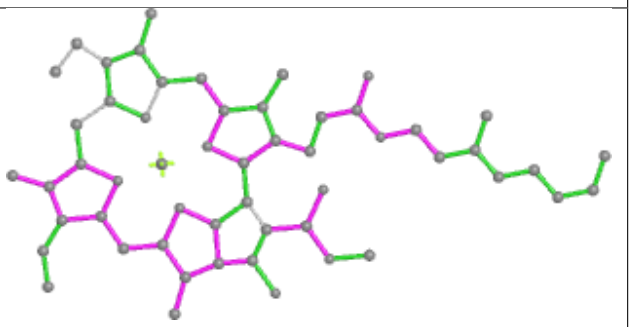
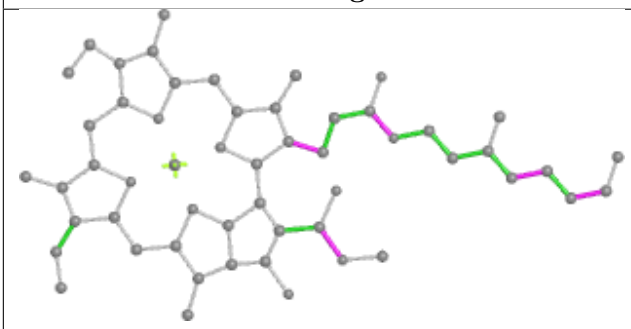
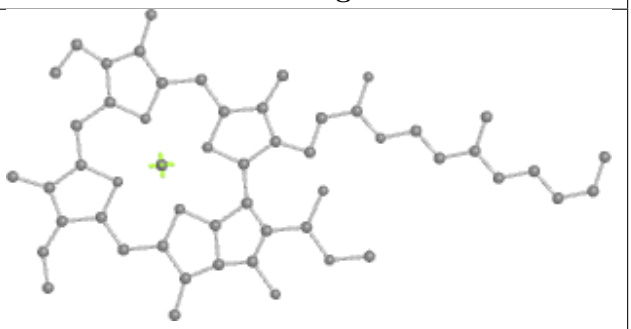


Bond angles

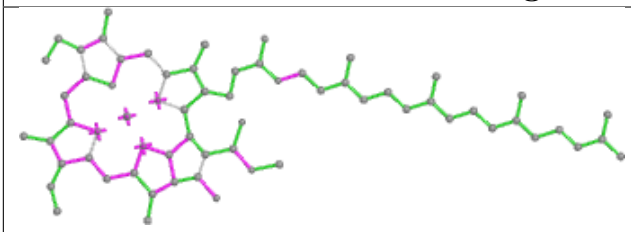


Torsions

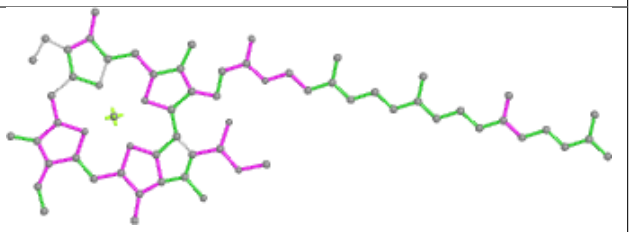


Rings

Ligand CLA G 852



Bond lengths



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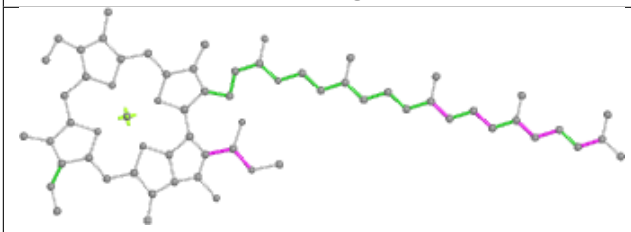

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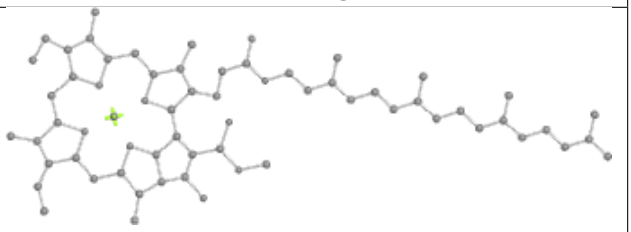
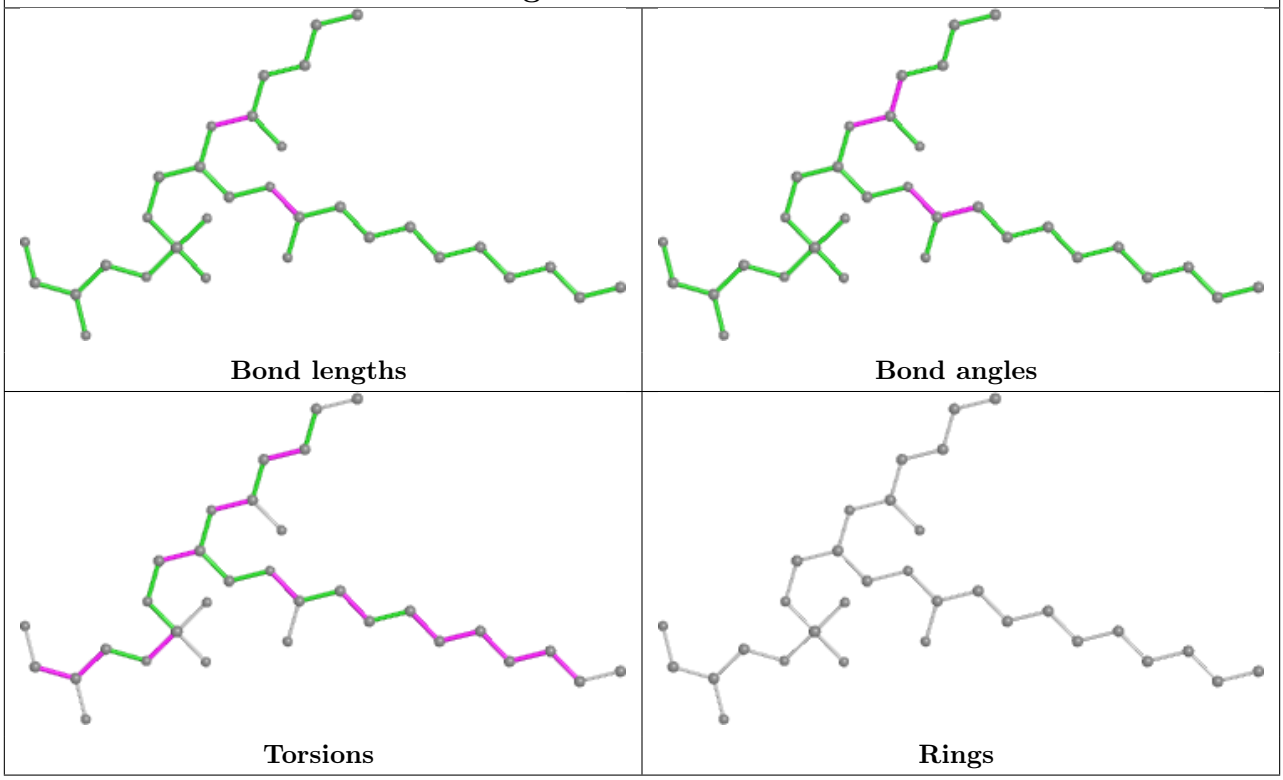
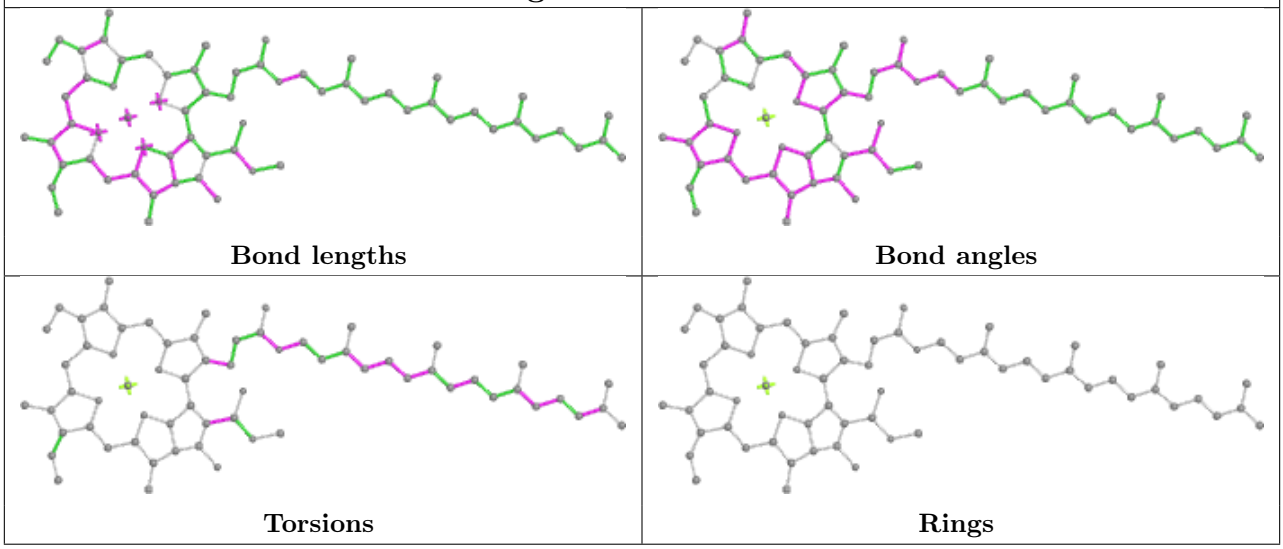


Rings

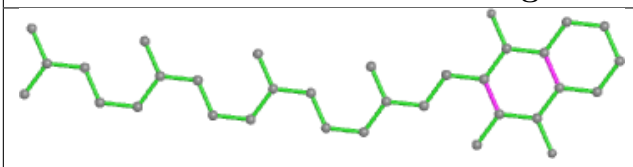
Ligand LHG A 853



Ligand CLA Z 802



Ligand PQN A 844



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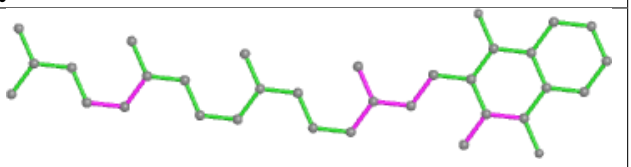
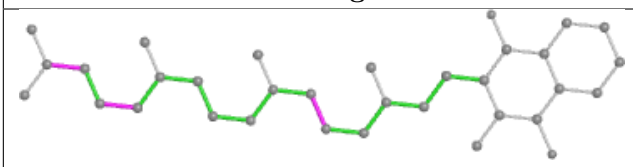
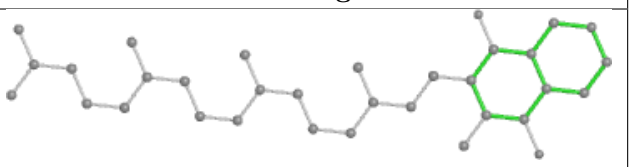


Bond angles

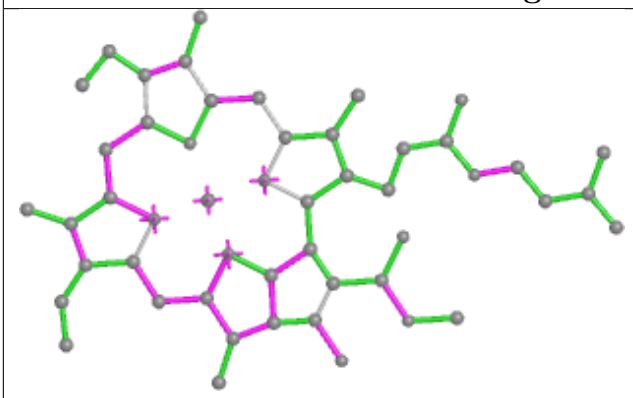


Torsions



Rings

Ligand CLA Y 816



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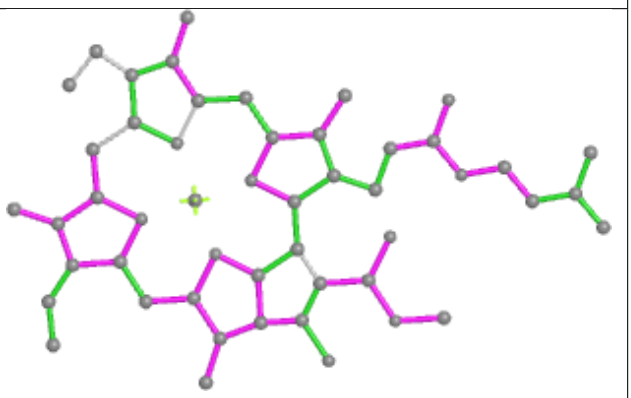
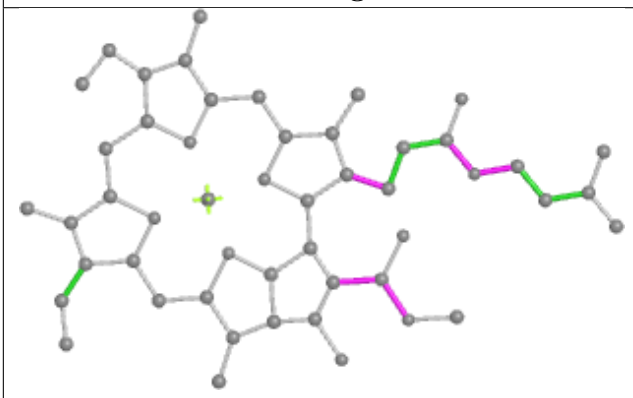


Bond angles



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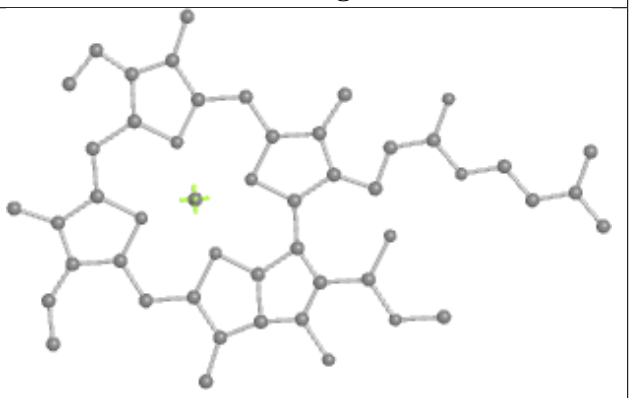
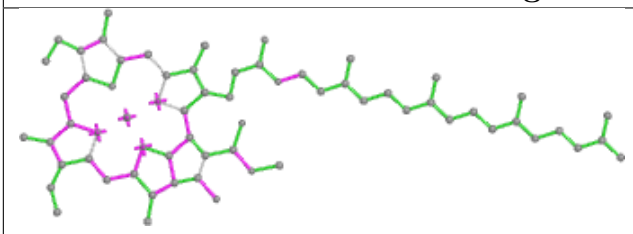


Rings

Ligand CLA H 825



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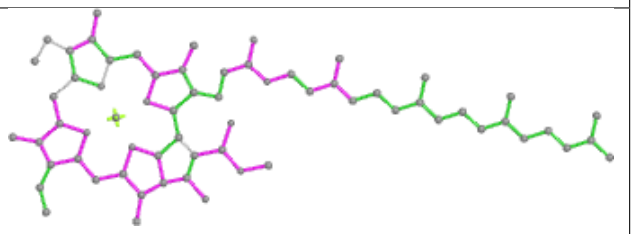

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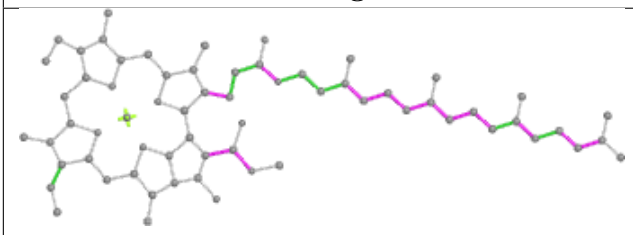

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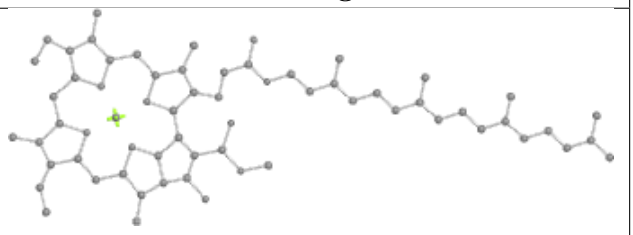
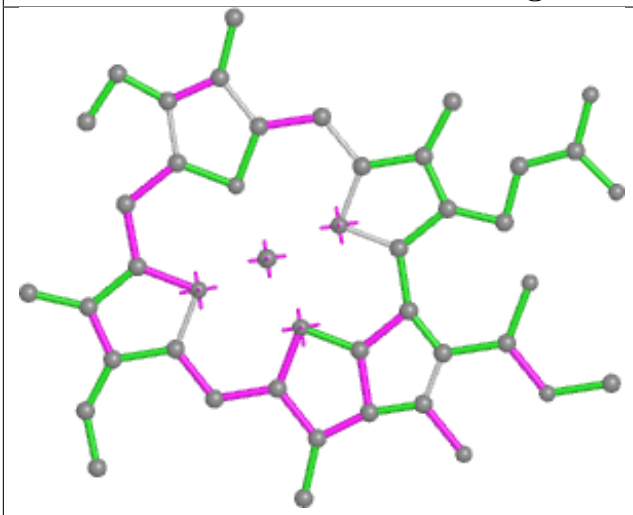


Rings

Ligand CLA Z 822



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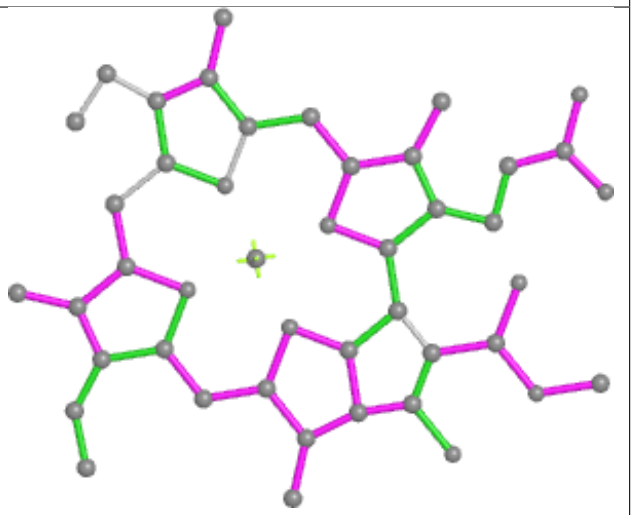

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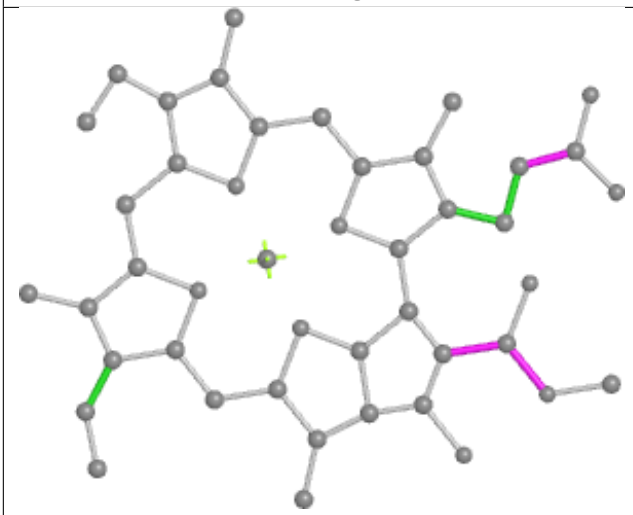

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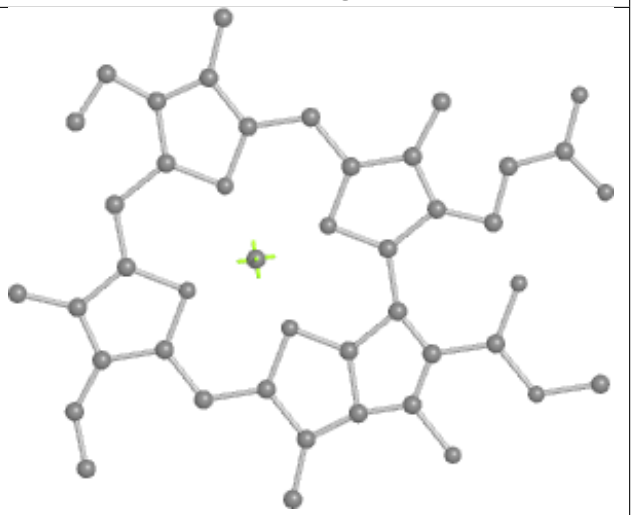
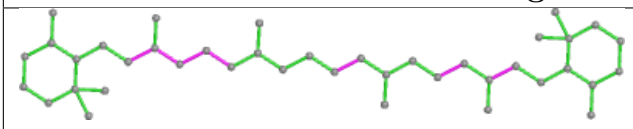


Rings

Ligand BCR e 101



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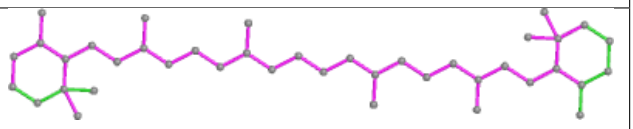

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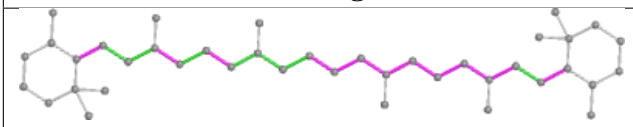

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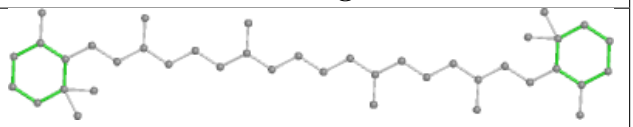
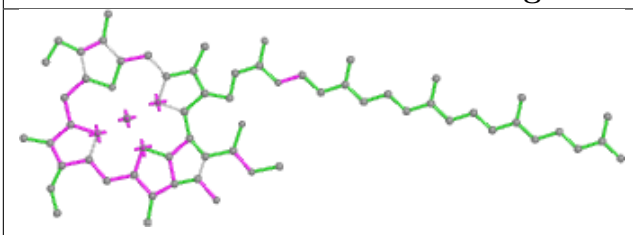


Rings

Ligand CLA Y 821



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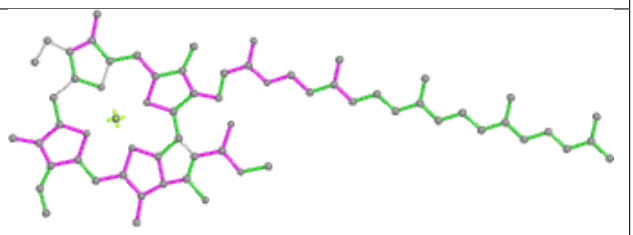
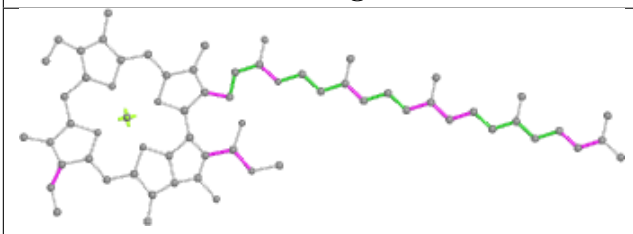


Bond angles



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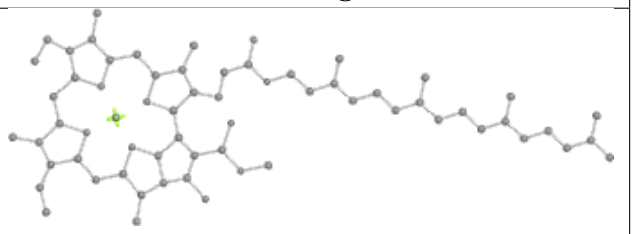
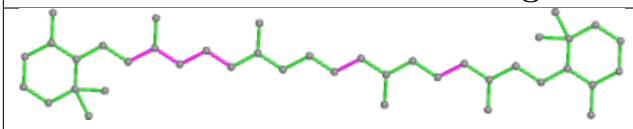


Rings

Ligand BCR Q 203



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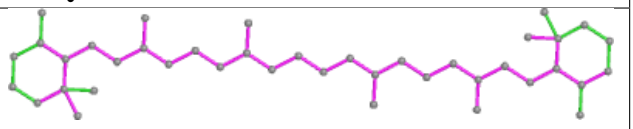
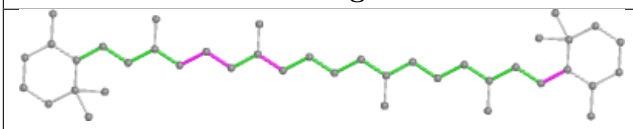


Bond angles



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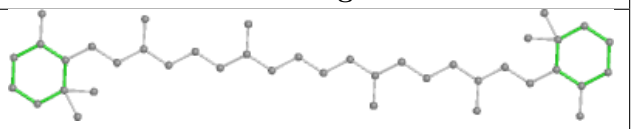

Rings

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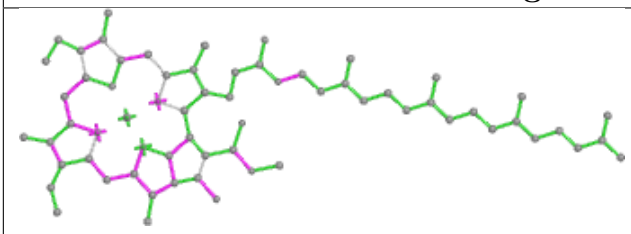
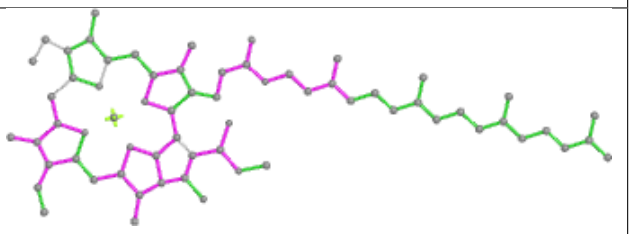
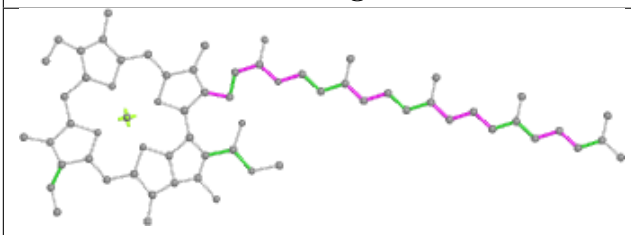
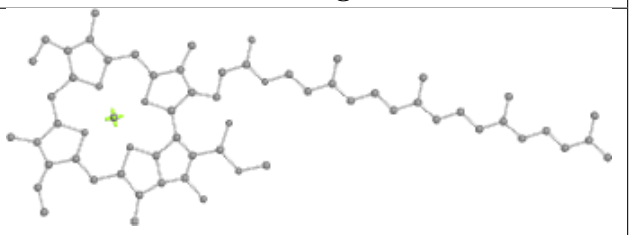
 Bond lengths	 Bond angles
 Torsions	 Rings

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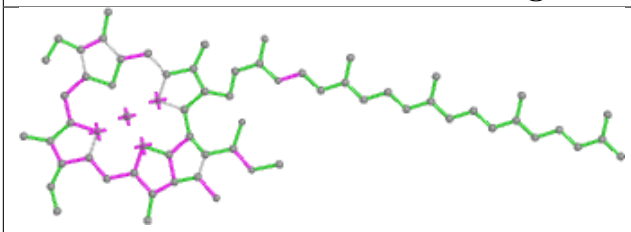
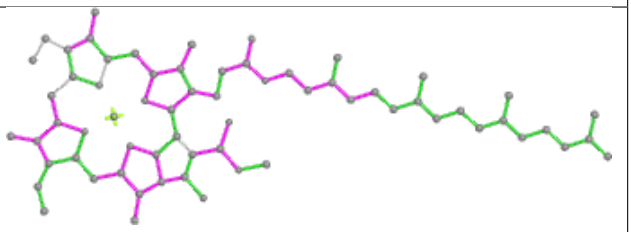
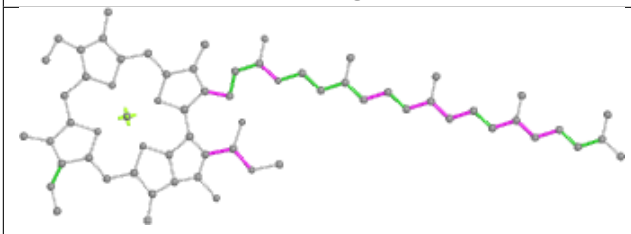
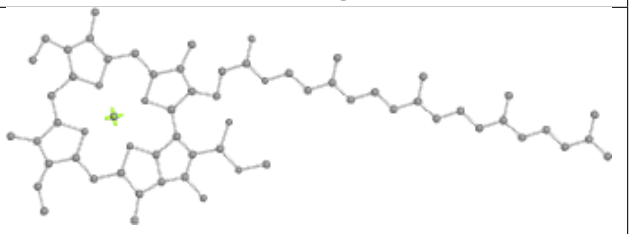
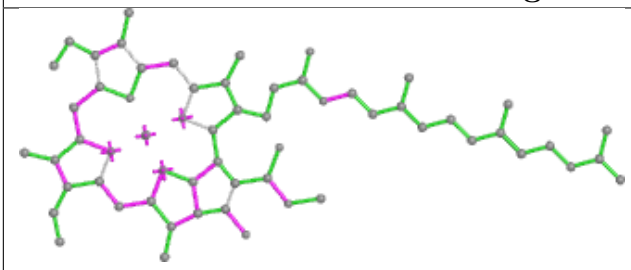
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA Y 826



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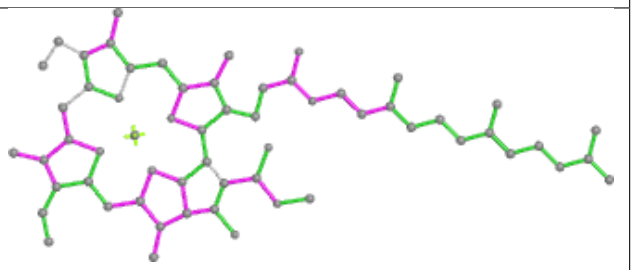
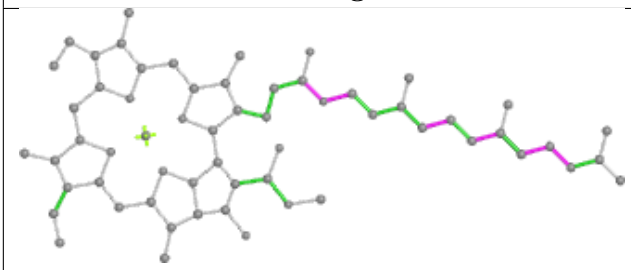
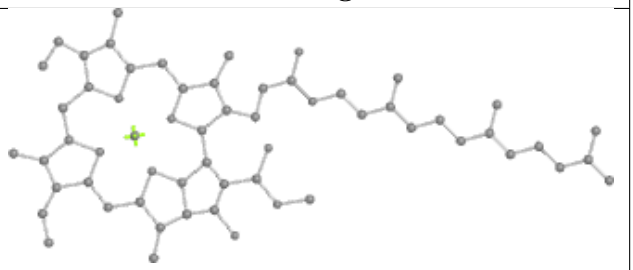


Bond angles

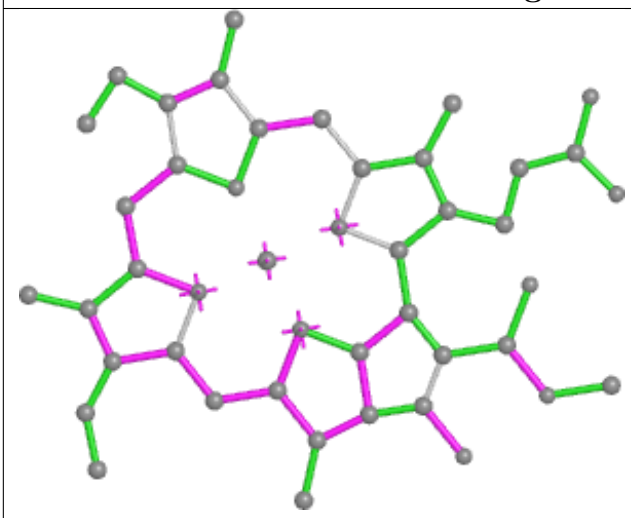


Torsions



Rings

Ligand CLA B 829



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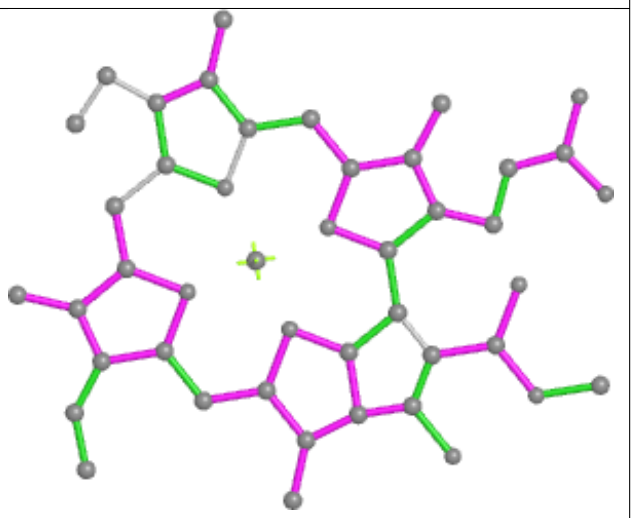
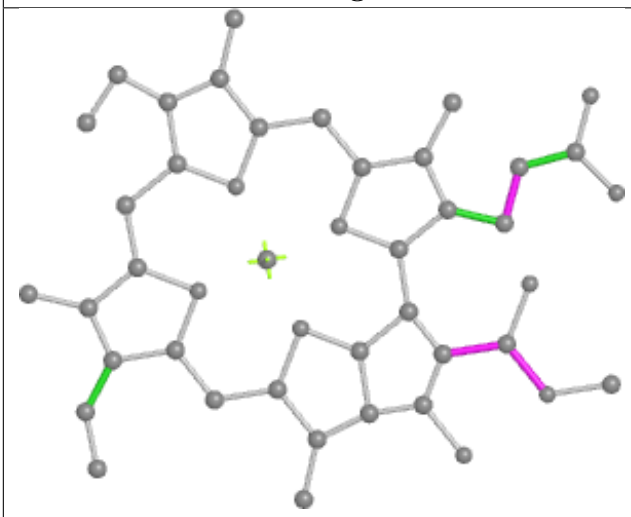


Bond angles



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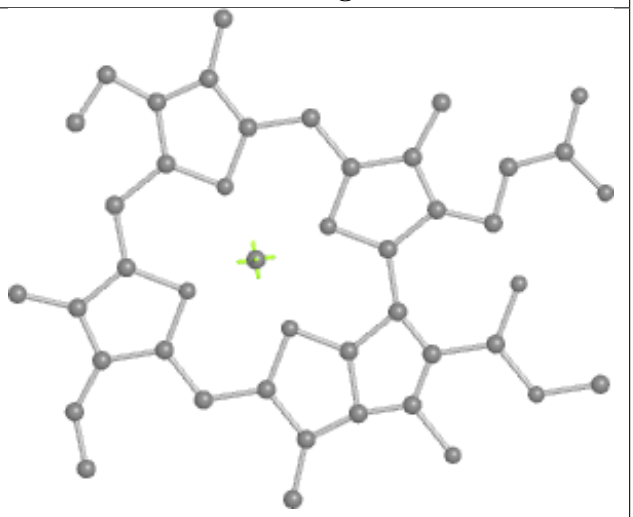
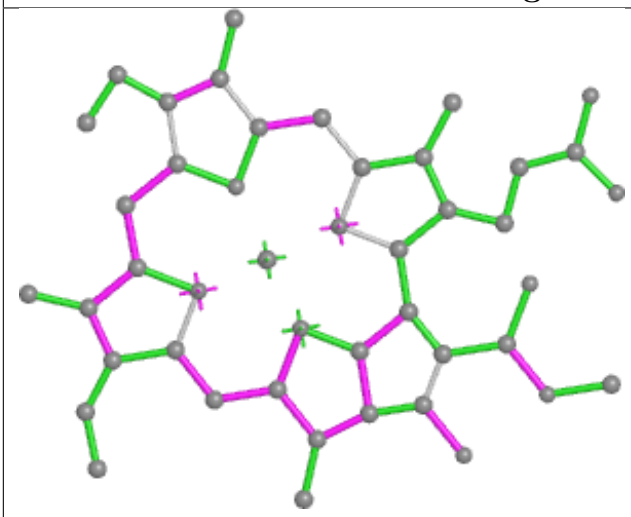
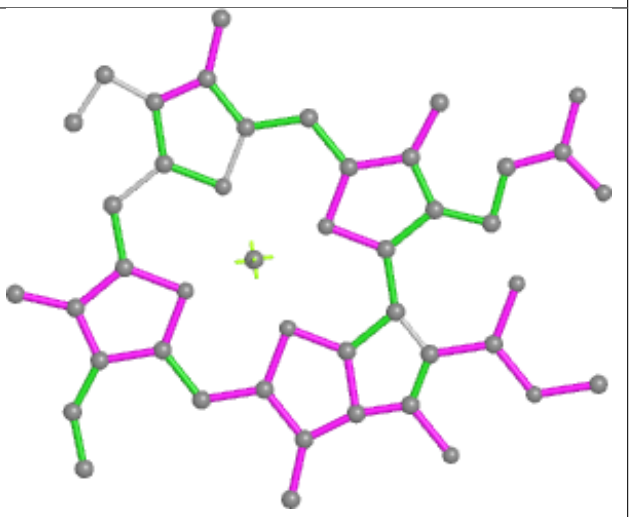


Rings

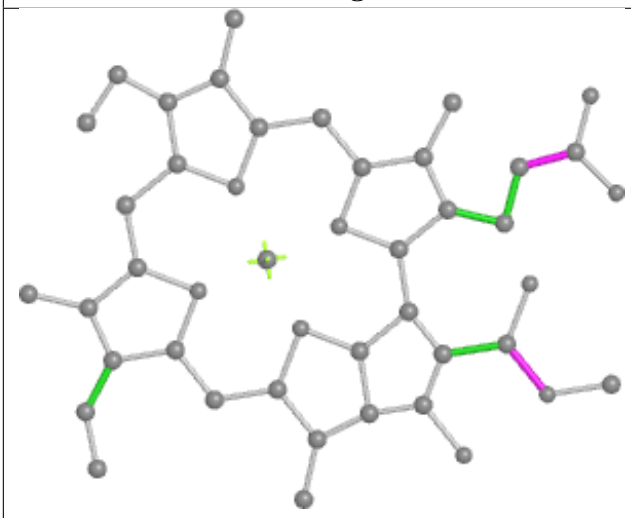
Ligand CLA H 835



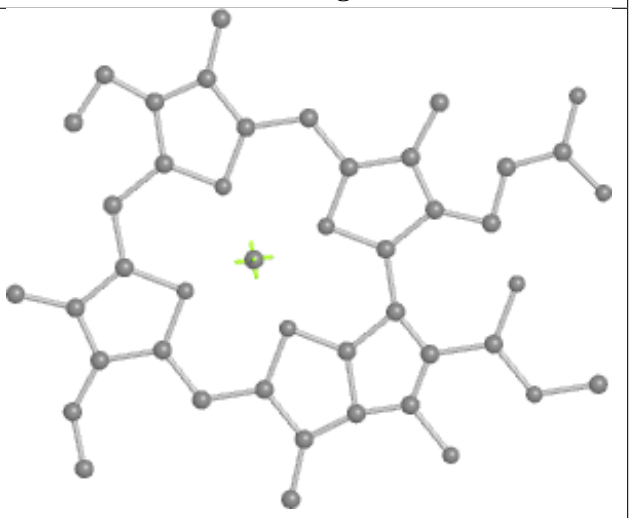
Bond lengths



Bond angles

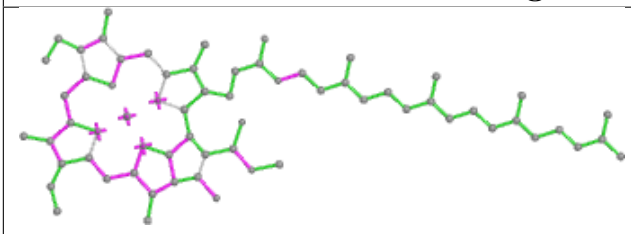


Torsions



Rings

Ligand CLA Z 838



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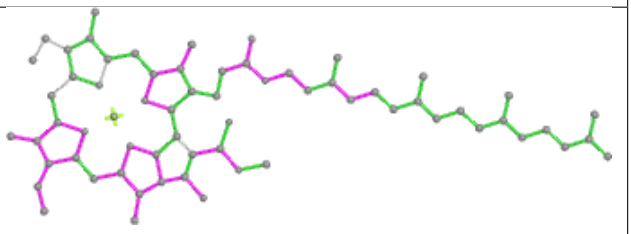
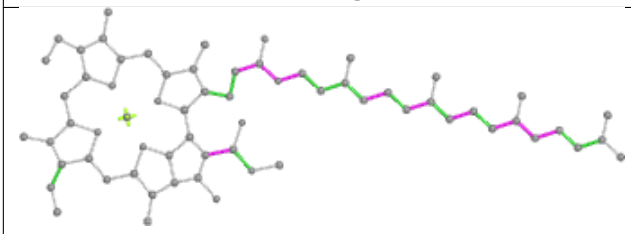


Bond angles



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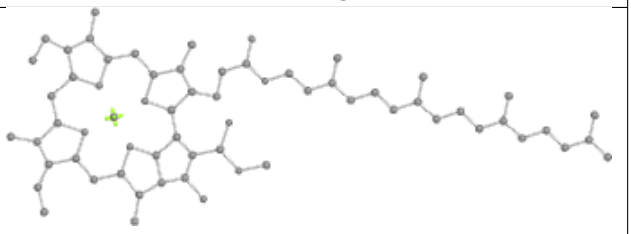
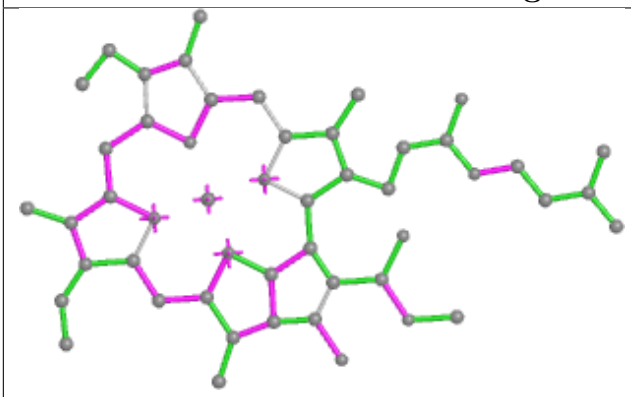


Rings

Ligand CLA A 836



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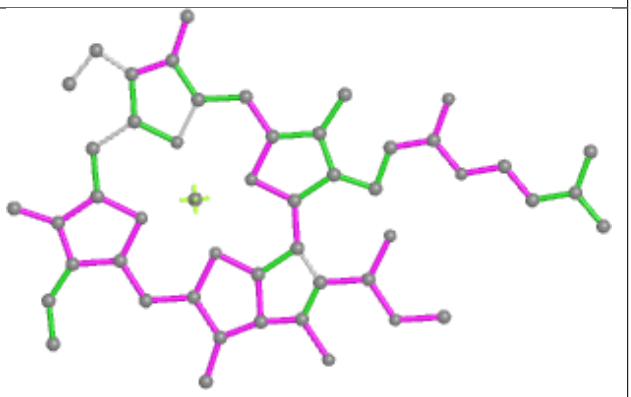
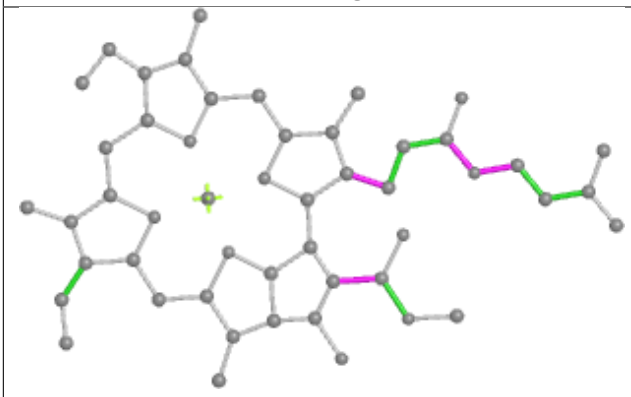
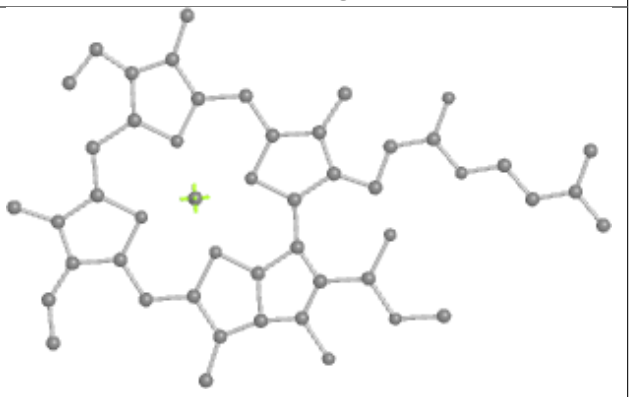


Bond angles

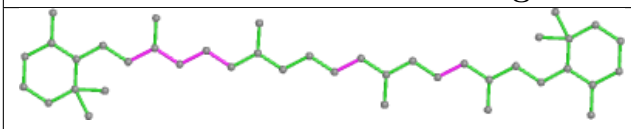


Torsions

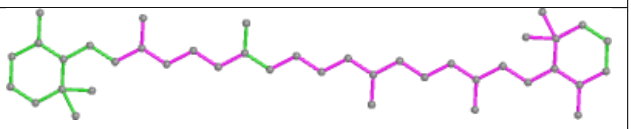


Rings

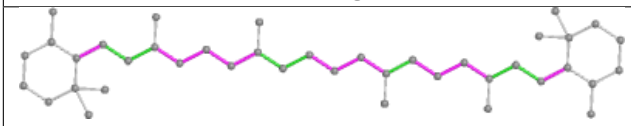
Ligand BCR U 1008



Bond lengths



Bond angles



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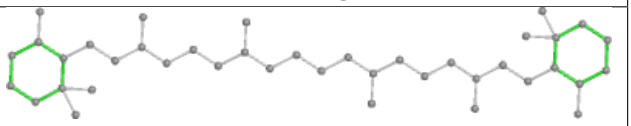
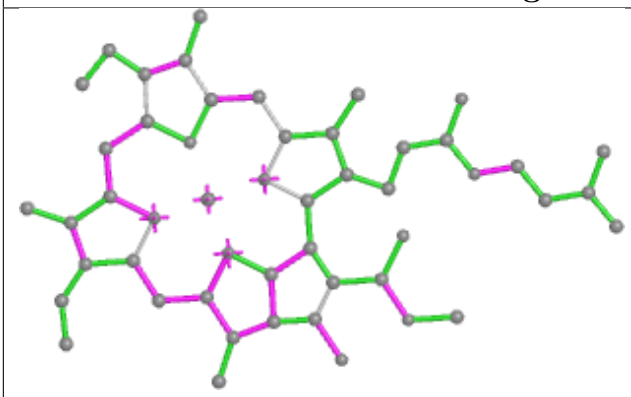


Rings

Ligand CLA G 815



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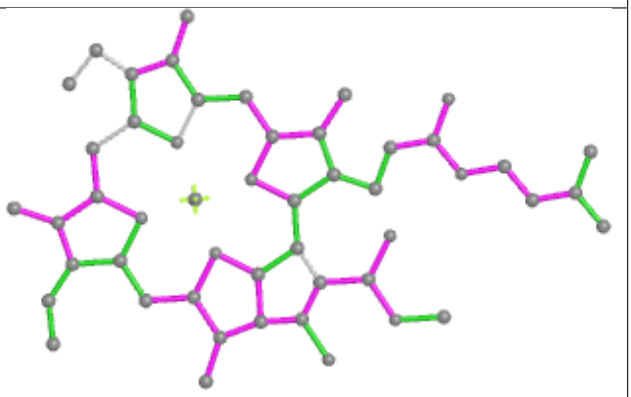
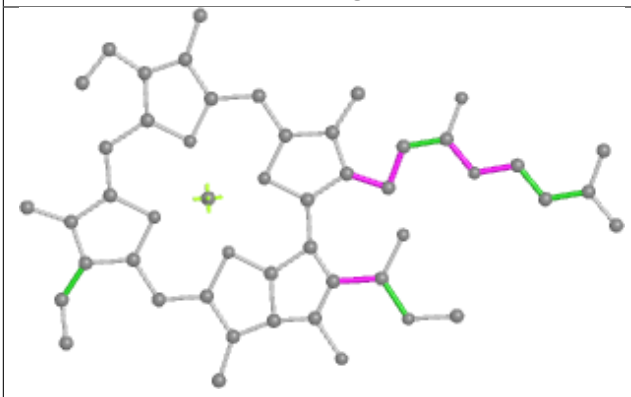


Bond angles



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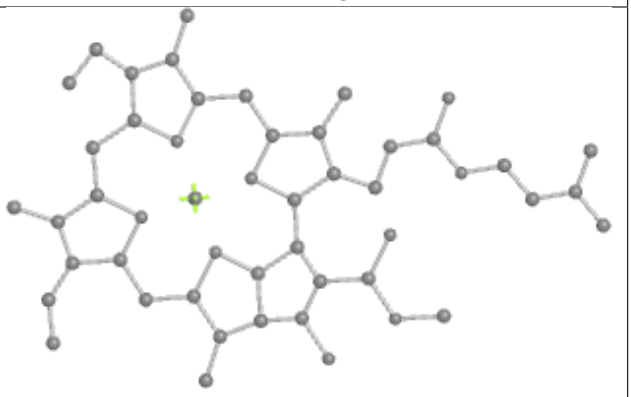
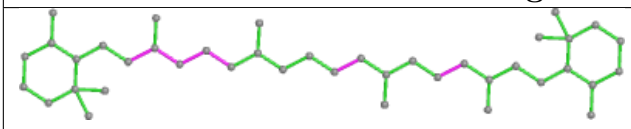


Rings

Ligand BCR J 103



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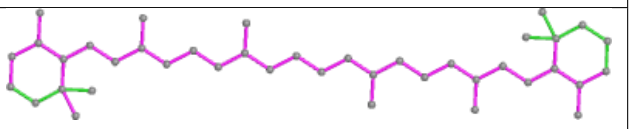
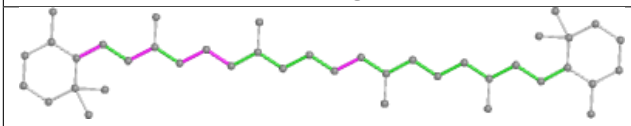
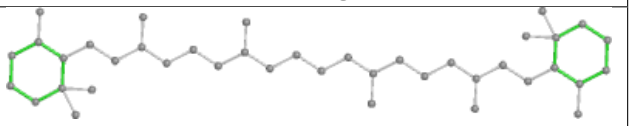


Bond angles

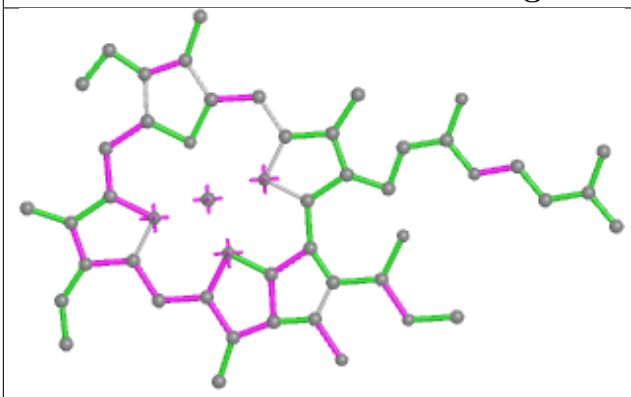


Torsions



Rings

Ligand CLA Y 839



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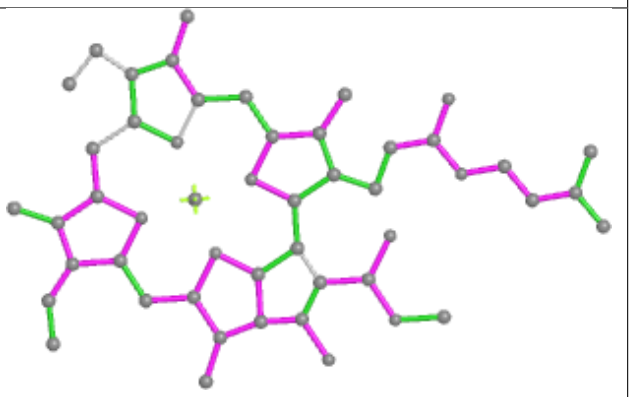
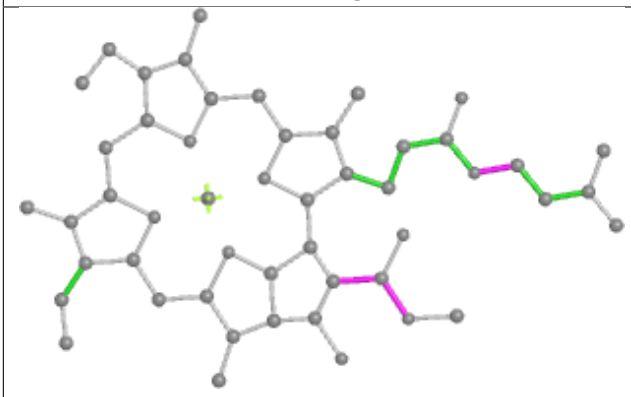


Bond angles



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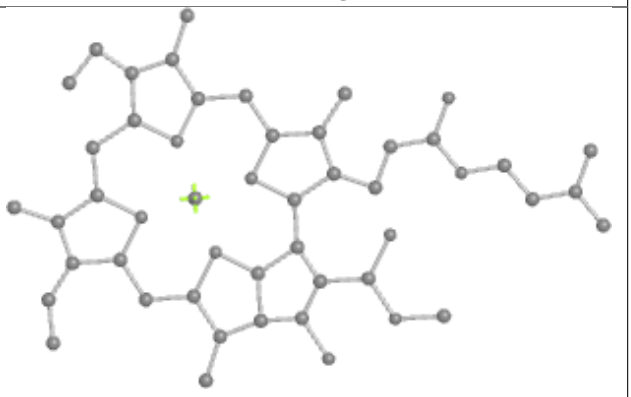
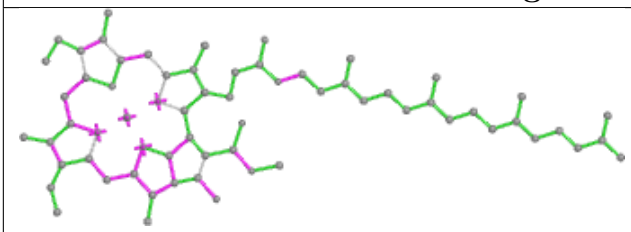


Rings

Ligand CLA H 805



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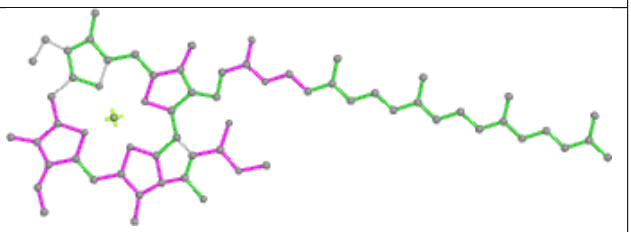
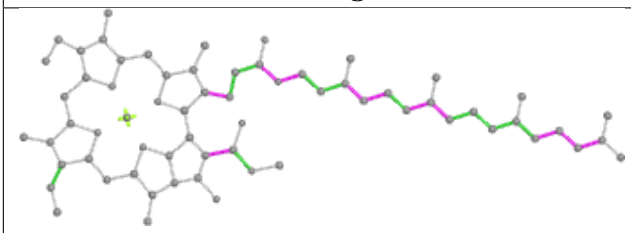


Bond angles



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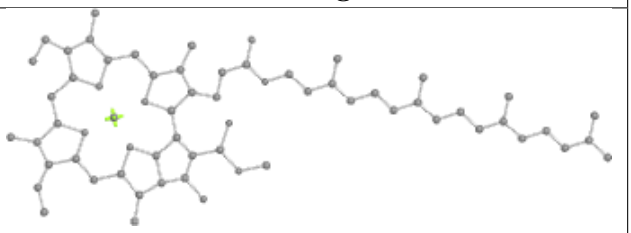
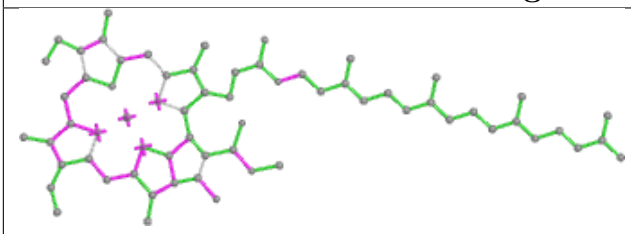


Rings

Ligand CLA A 819



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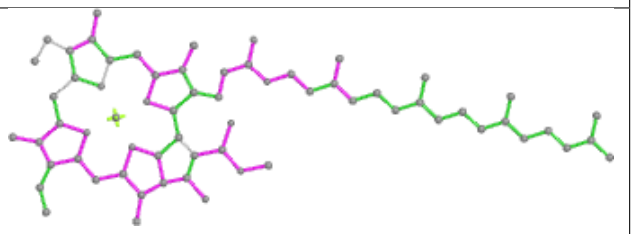
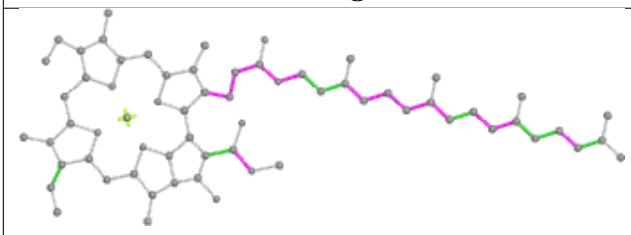


Bond angles



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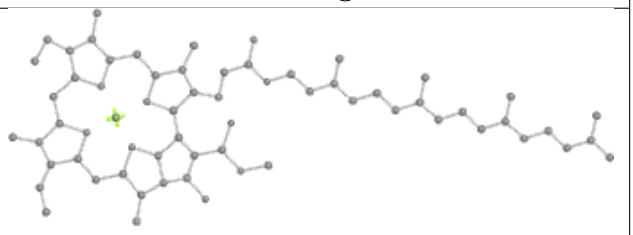
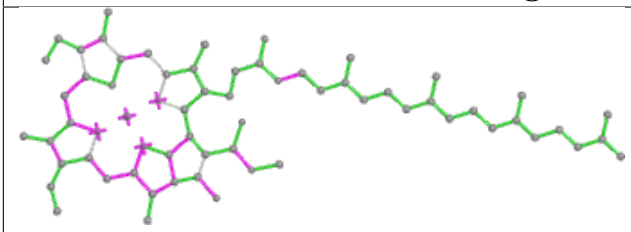


Rings

Ligand CLA H 817



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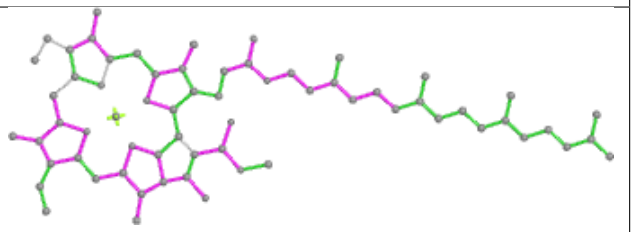
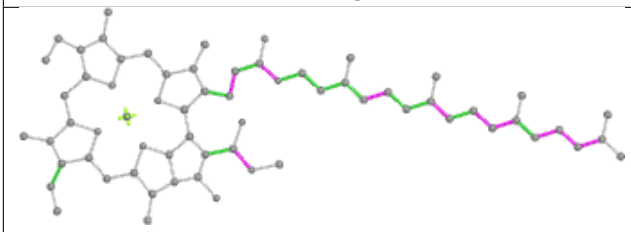


Bond angles



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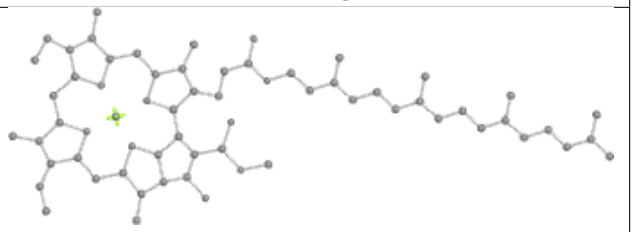
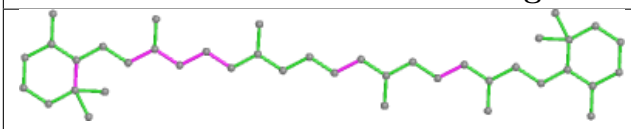


Rings

Ligand BCR F 203



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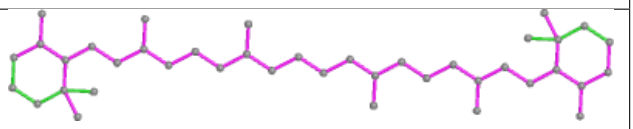
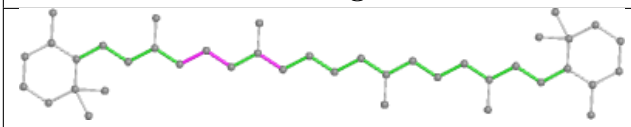


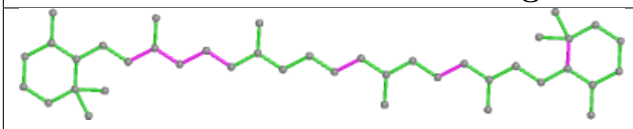
Bond angles



Torsions

Rings

Ligand BCR Y 852



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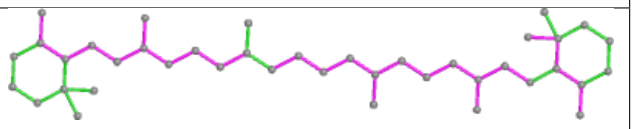
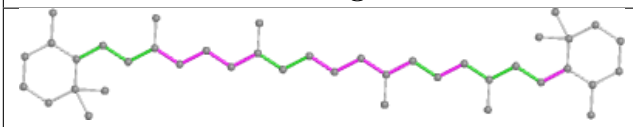
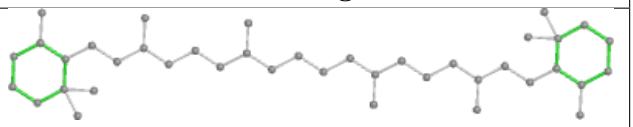


Bond angles

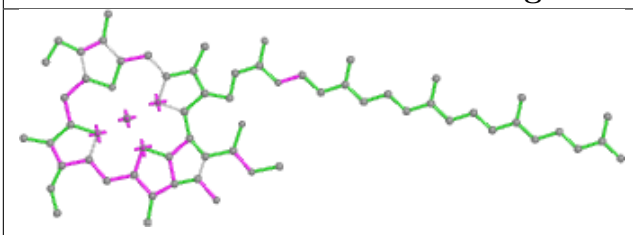


Torsions



Rings

Ligand CLA B 827



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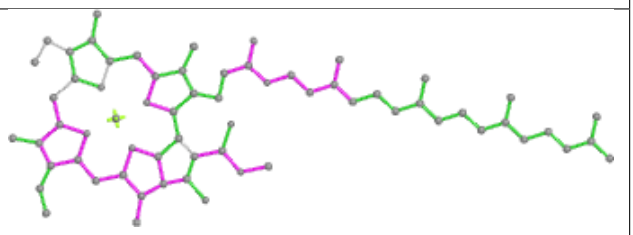
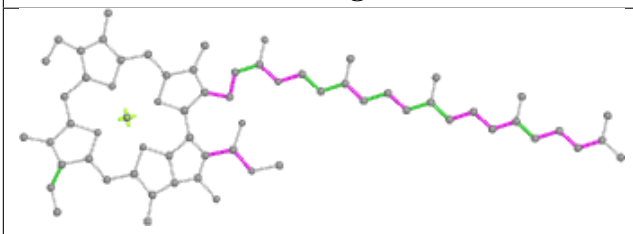


Bond angles



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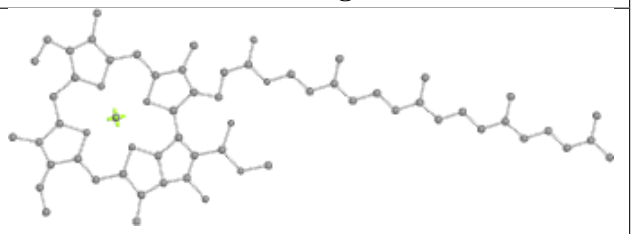
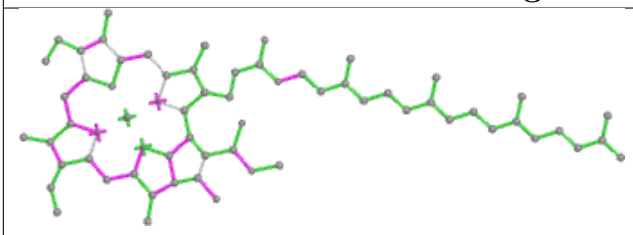


Rings

Ligand CLA A 806



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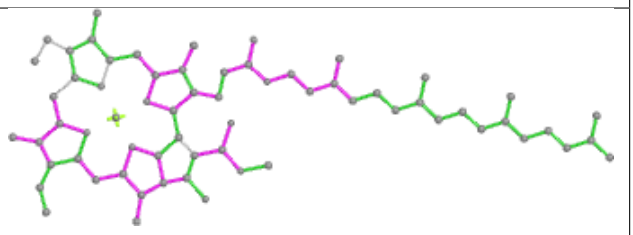
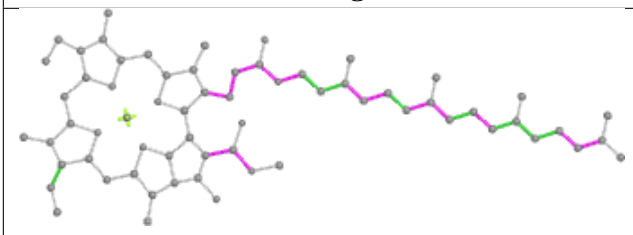
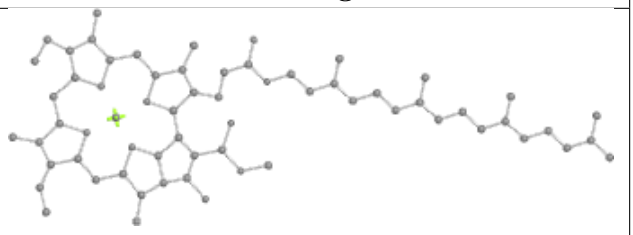


Bond angles

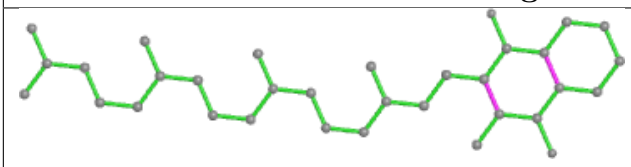


Torsions

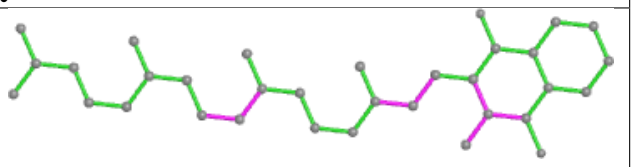


Rings

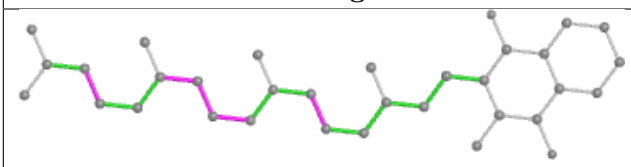
Ligand PQN H 841



Bond lengths



Bond angles



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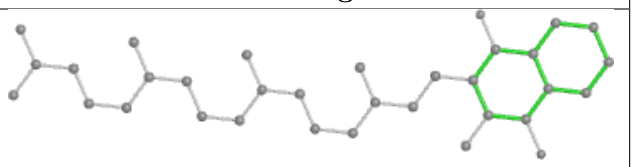
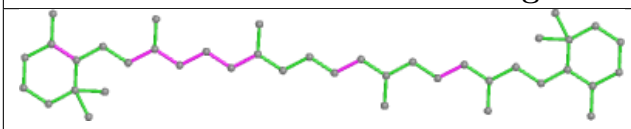


Rings

Ligand BCR Y 844



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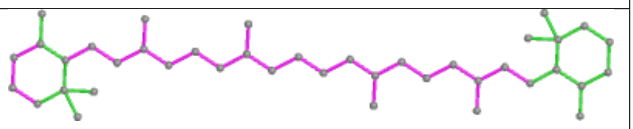
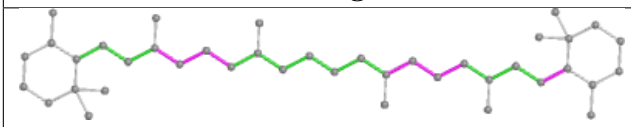


Bond angles



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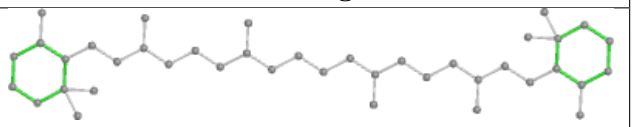
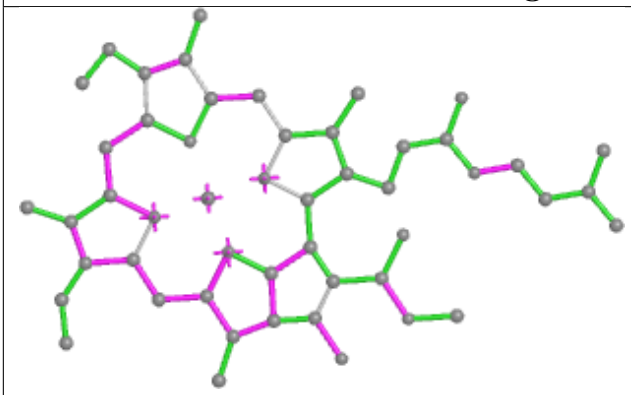


Rings

Ligand CLA A 838



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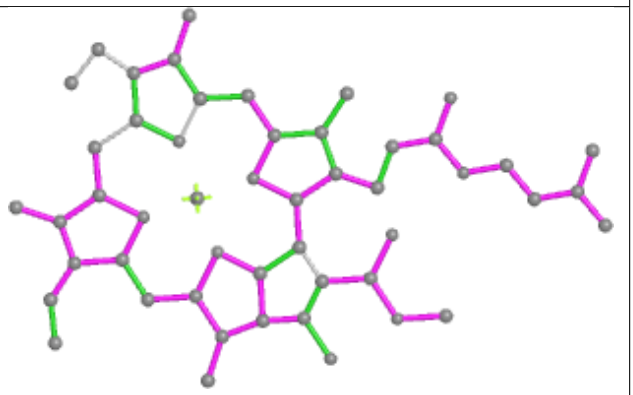
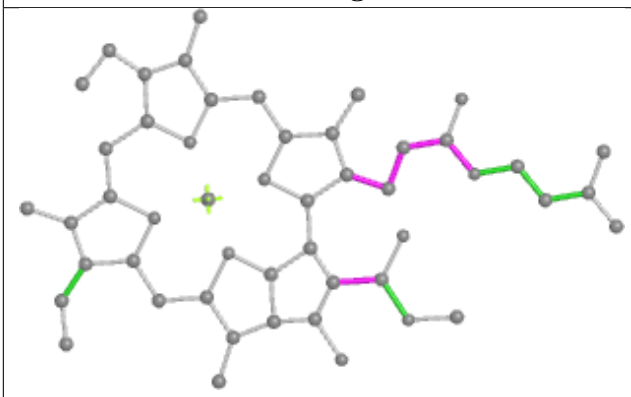


Bond angles



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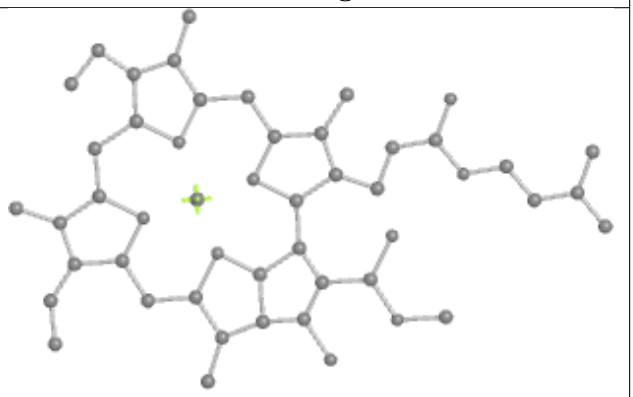
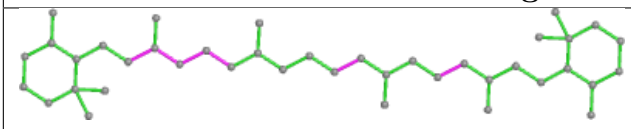
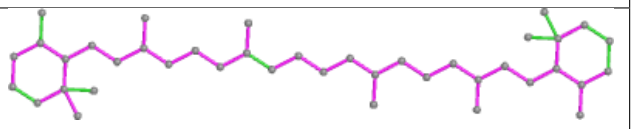
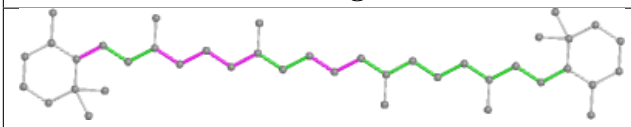
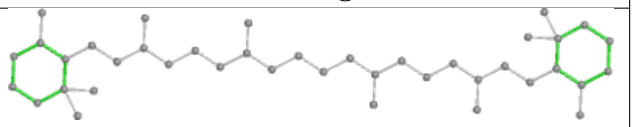
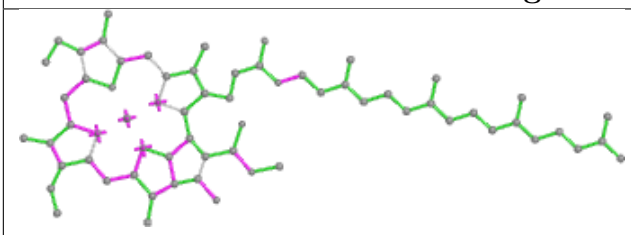
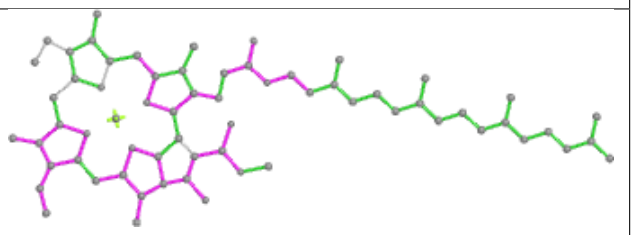
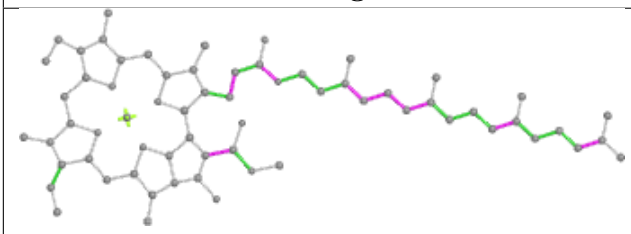
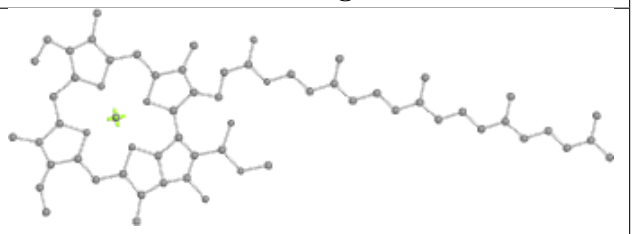
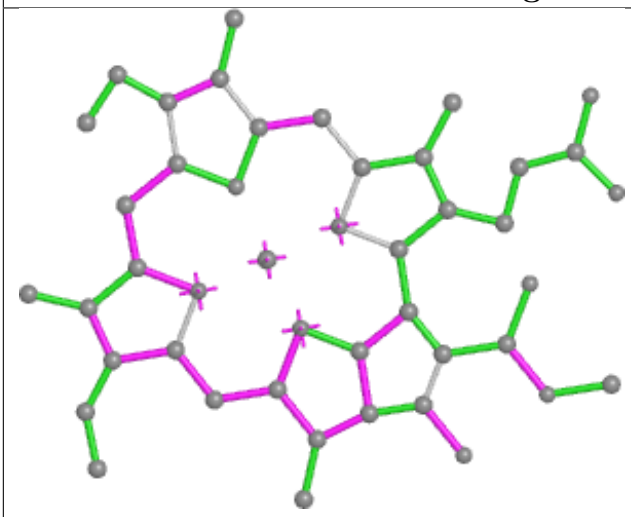


Rings

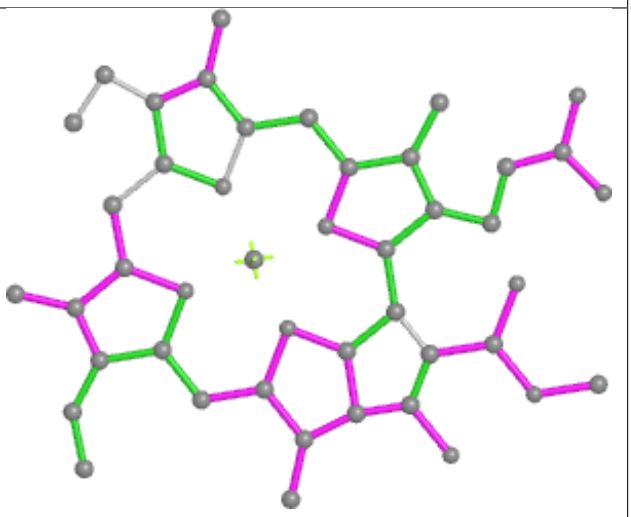
Ligand BCR H 850	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA A 854	
 Bond lengths	 Bond angles
 Torsions	 Rings

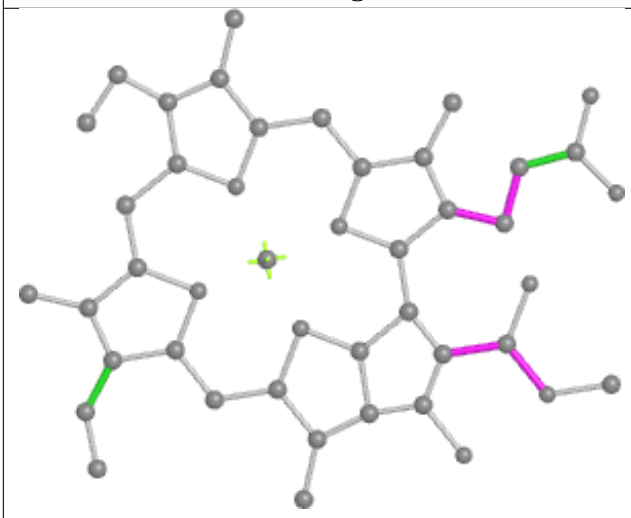
Ligand CLA G 835



Bond lengths



Bond angles



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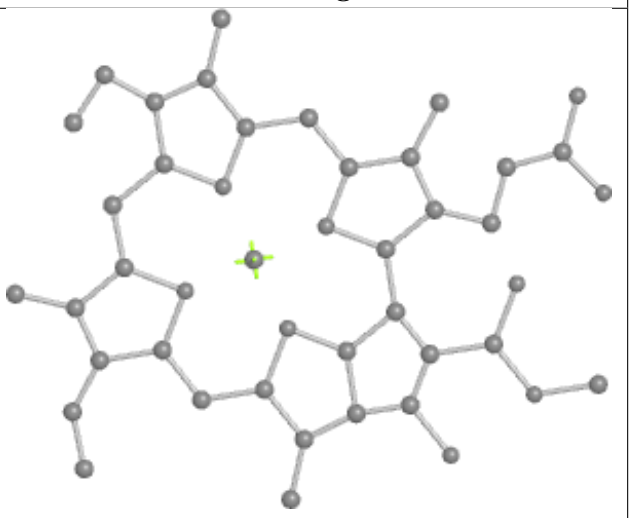
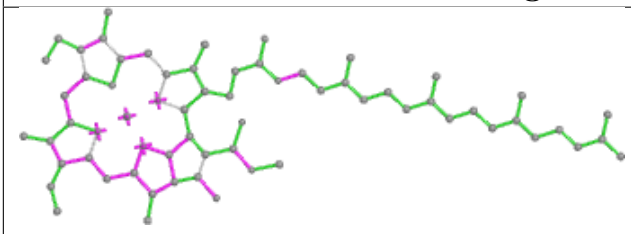


Rings

Ligand CLA Y 811



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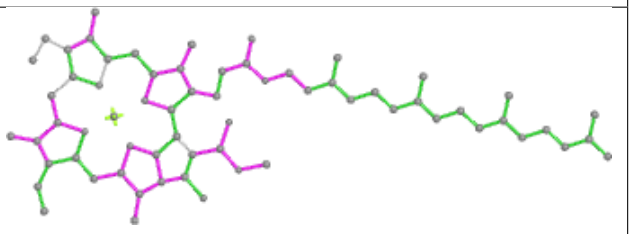
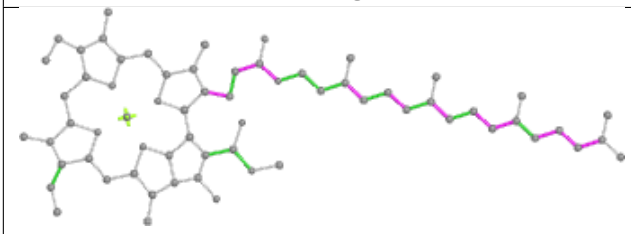


Bond angles



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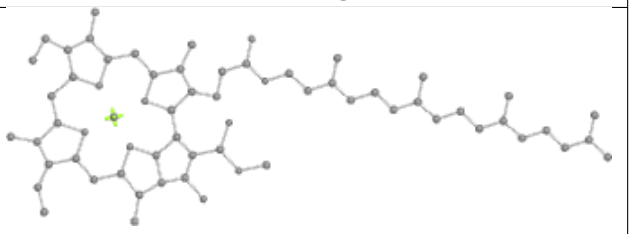
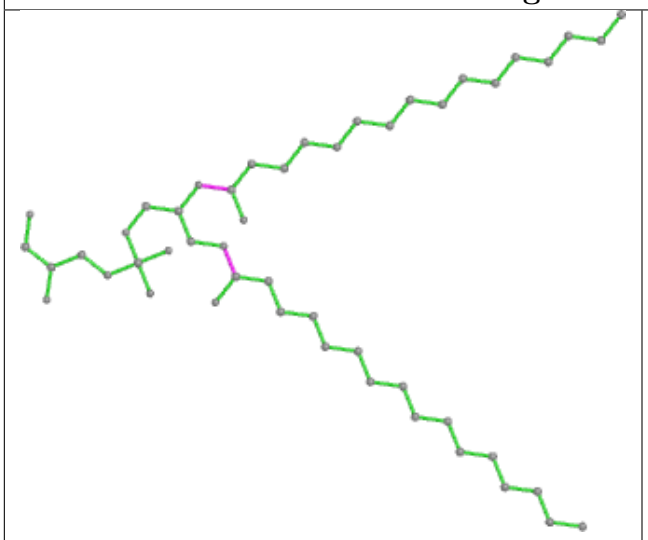


Rings

Ligand LHG Y 850



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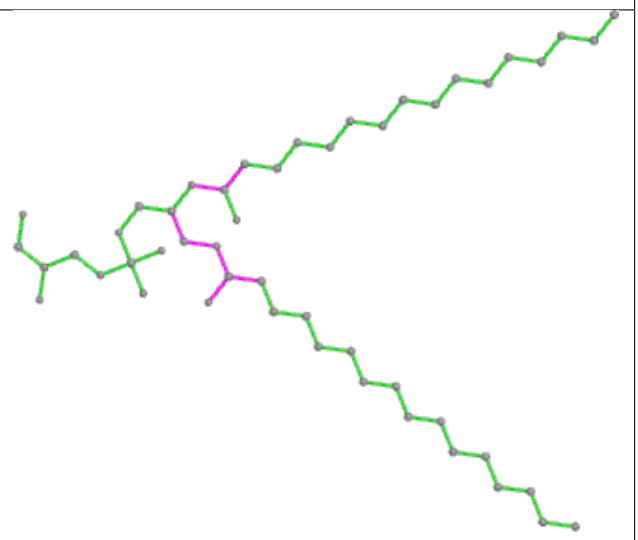
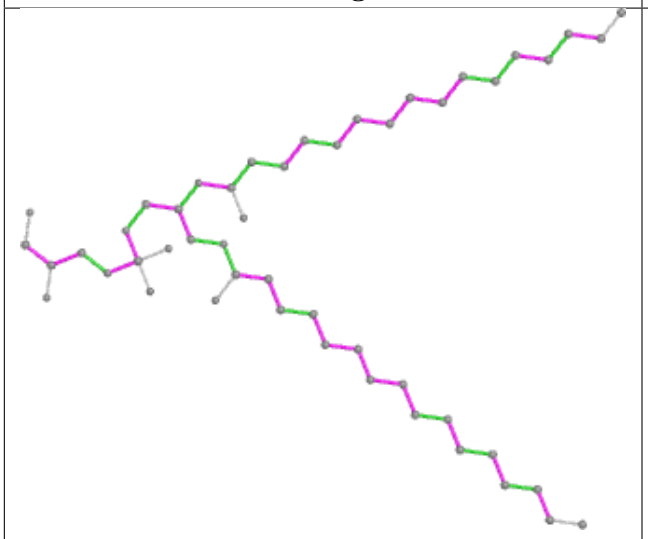


Bond angles



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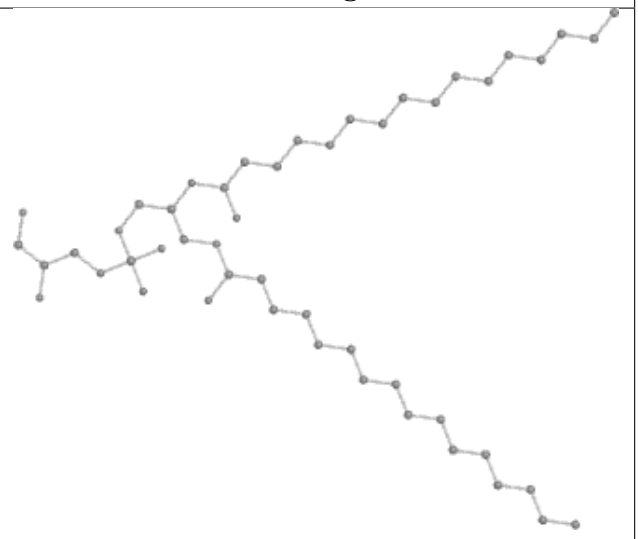
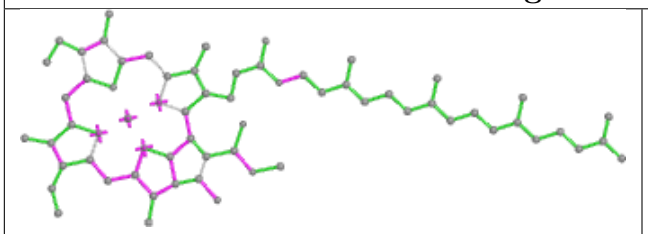


Rings

Ligand CLA H 802



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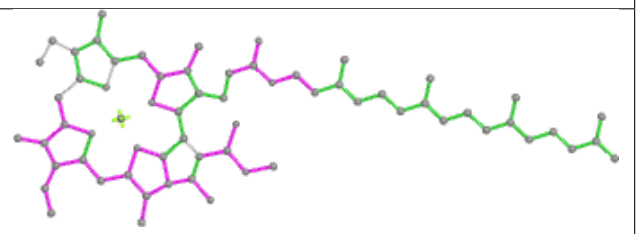

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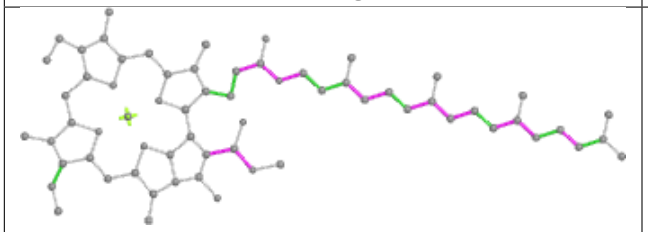

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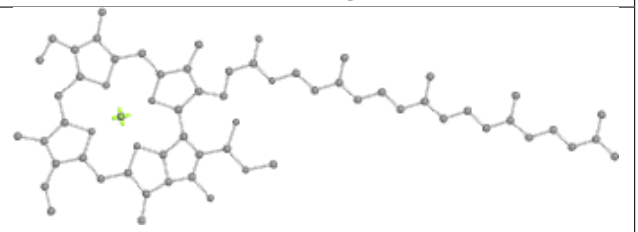
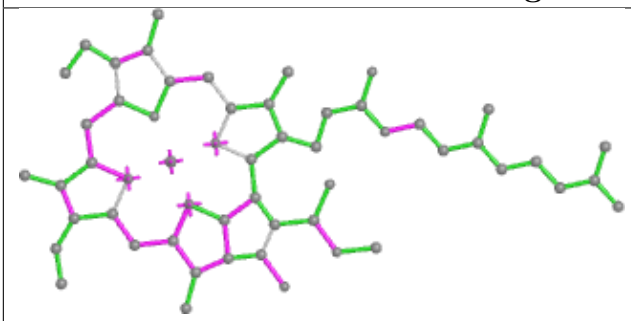


Rings

Ligand CLA B 821



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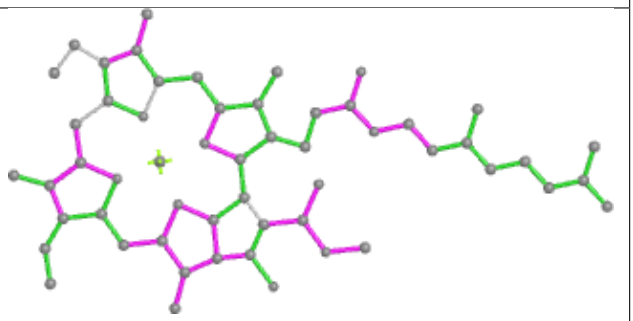
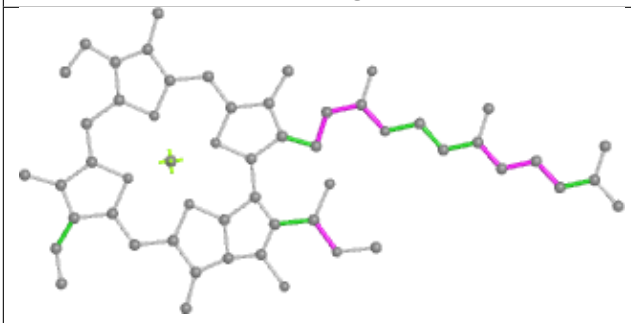


Bond angles



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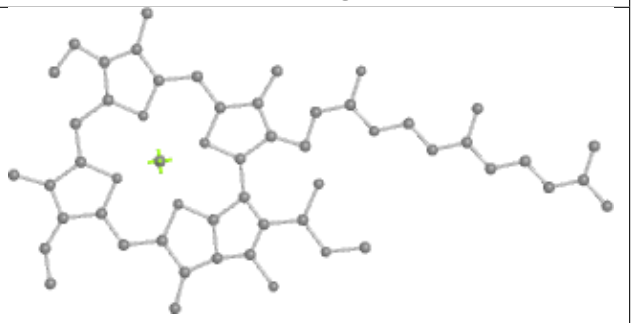
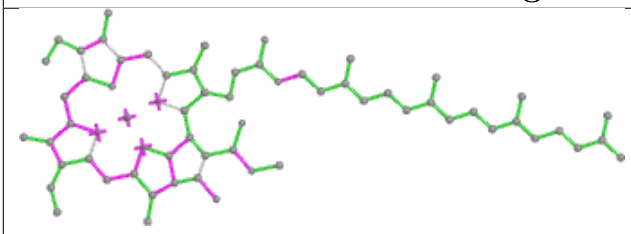


Rings

Ligand CLA H 839



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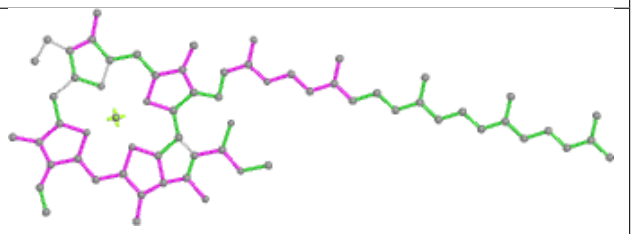
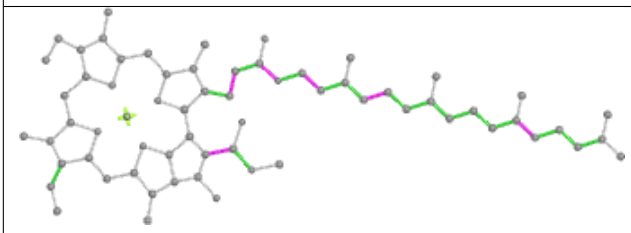


Bond angles



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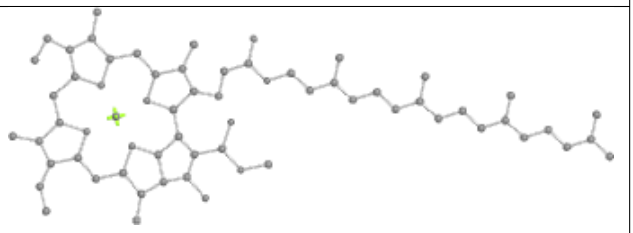
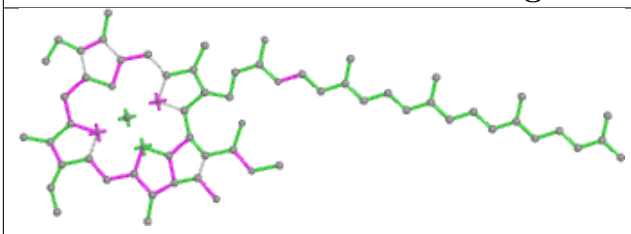
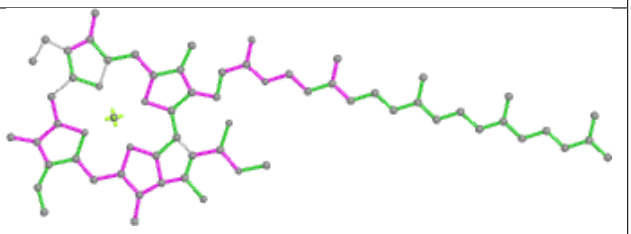
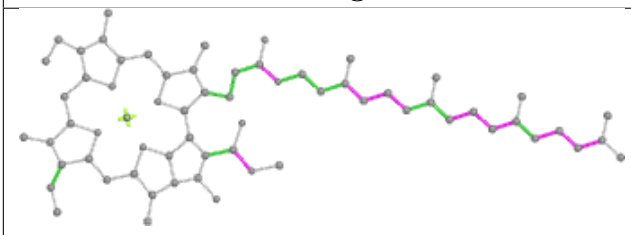
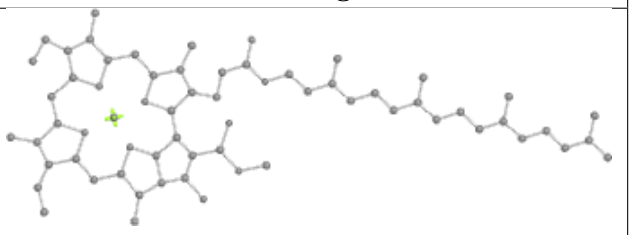


Rings

Ligand CLA B 805	
 Bond lengths	 Bond angles
 Torsions	 Rings

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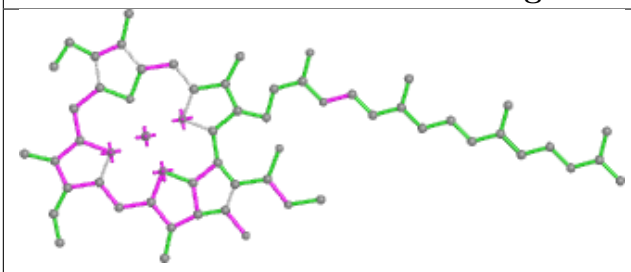
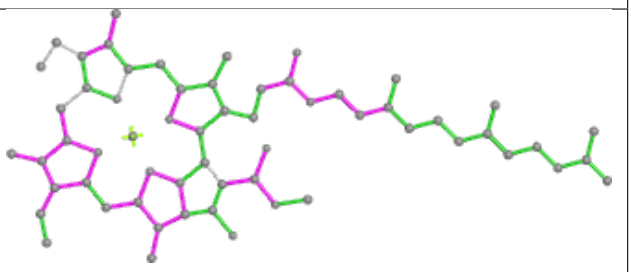
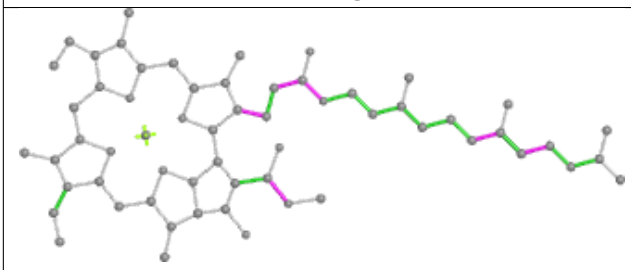
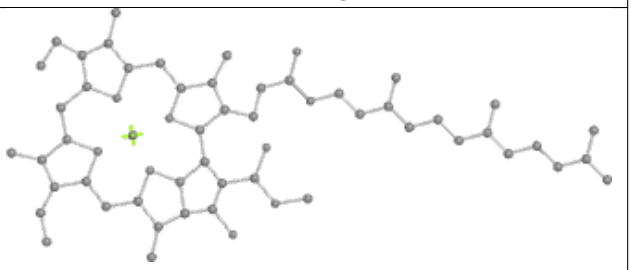
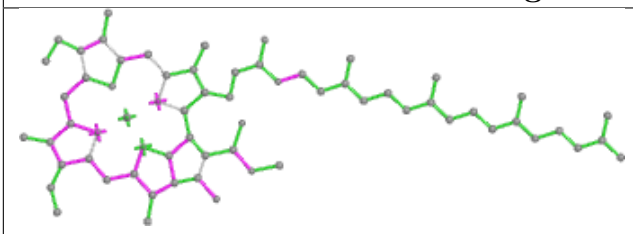
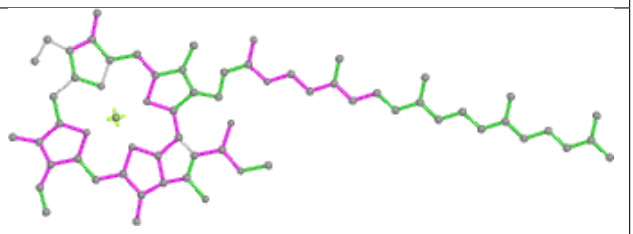
 Bond lengths	 Bond angles
 Torsions	 Rings

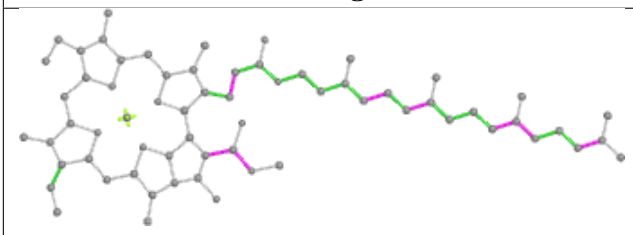
Ligand CLA B 839



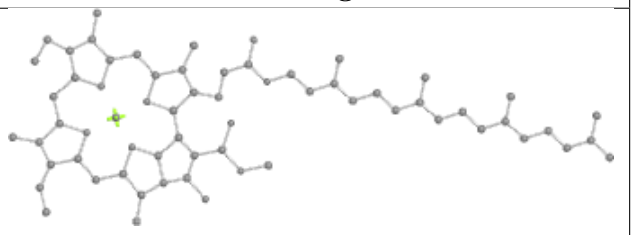
Bond lengths



Bond angles

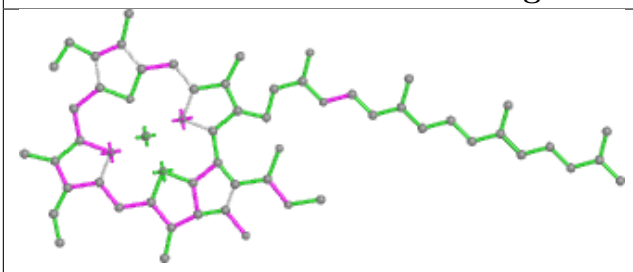


Torsions



Rings

Ligand CLA H 823



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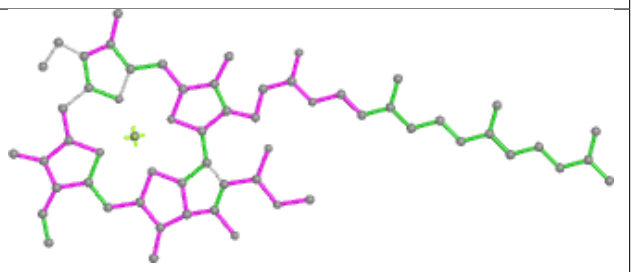

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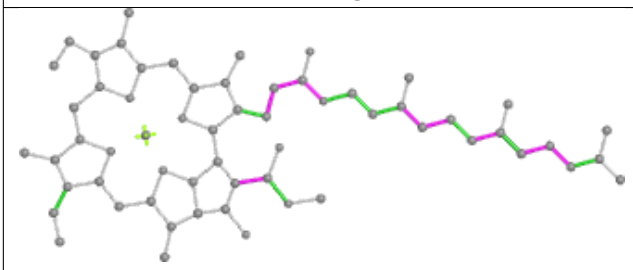

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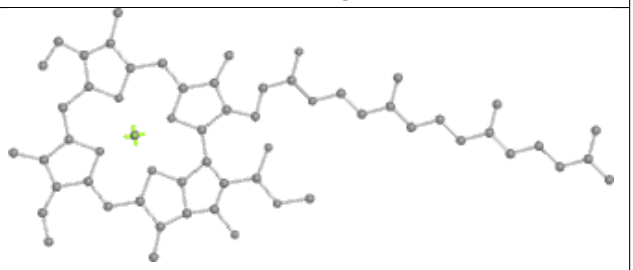
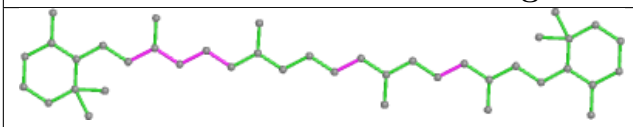


Rings

Ligand BCR G 848



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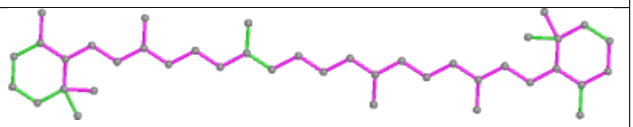
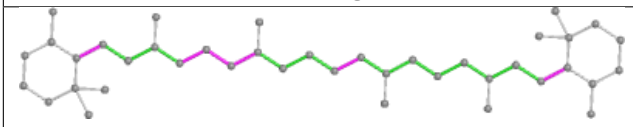


Bond angles



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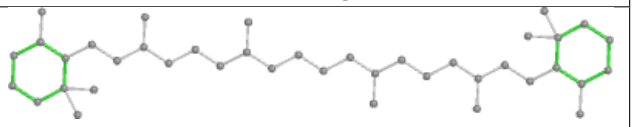
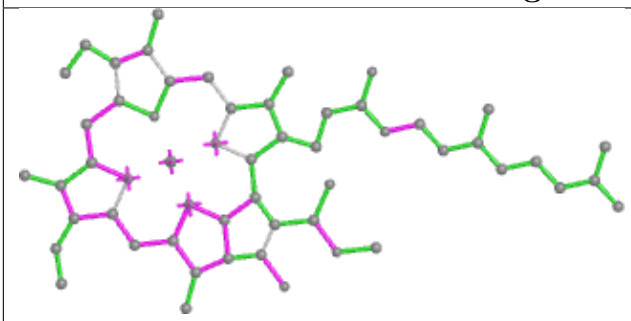


Rings

Ligand CLA Y 812



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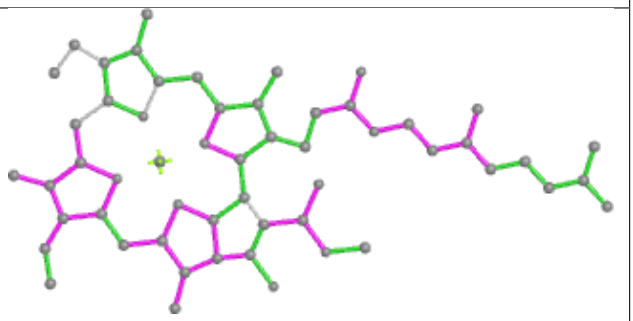
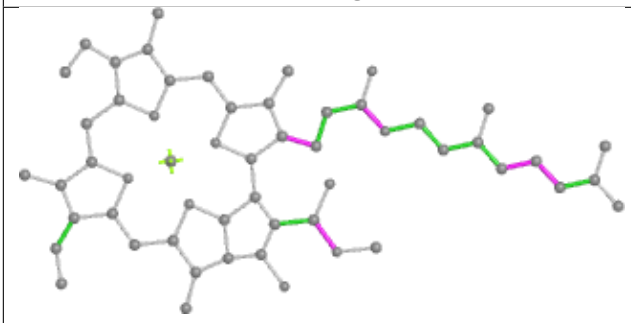


Bond angles



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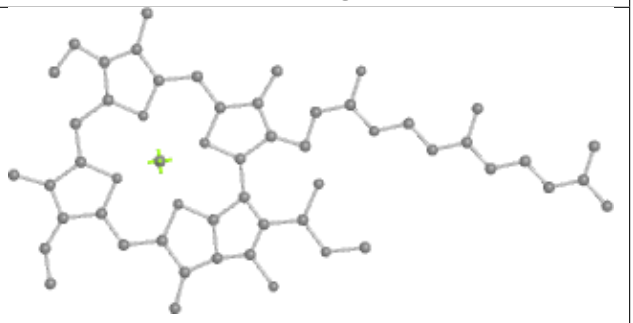
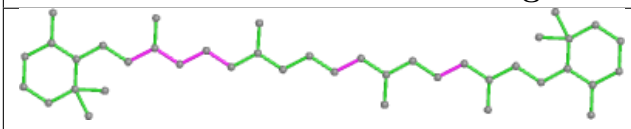


Rings

Ligand BCR B 847



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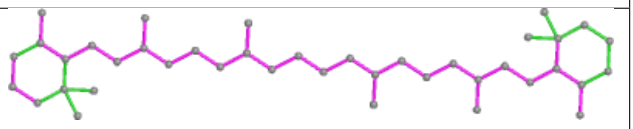

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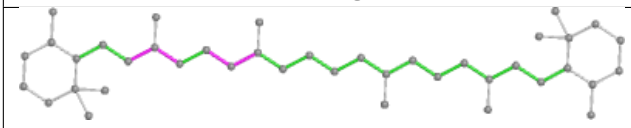
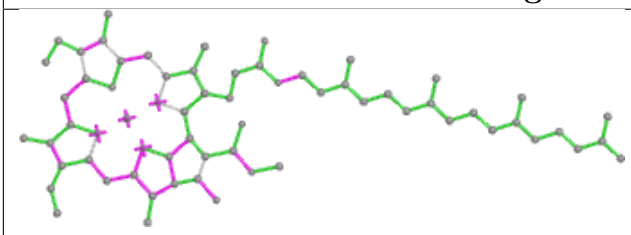


Torsions

Rings

Ligand CLA B 801



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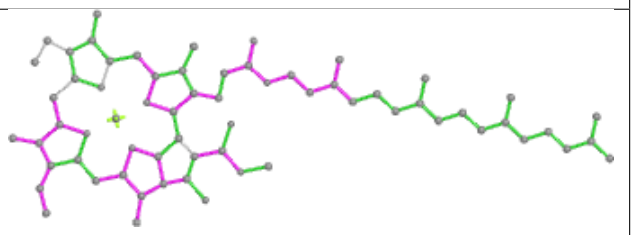
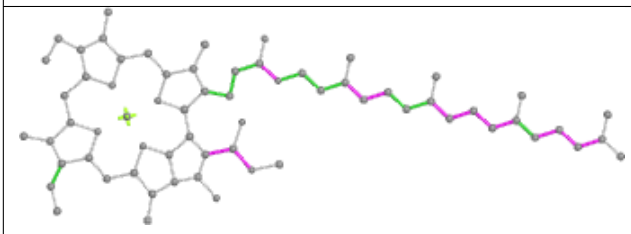


Bond angles



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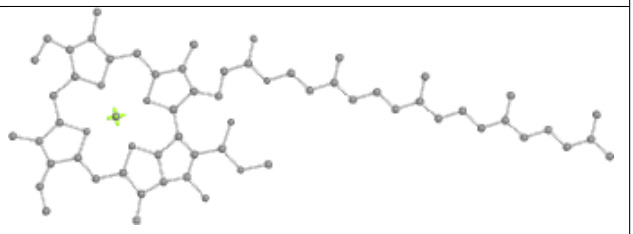
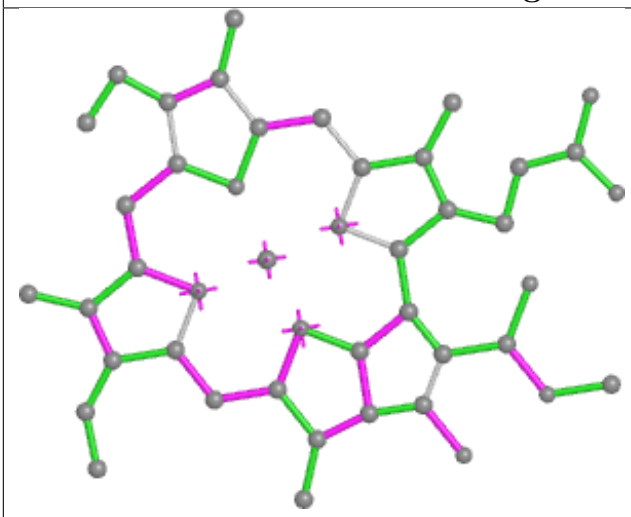


Rings

Ligand CLA H 820



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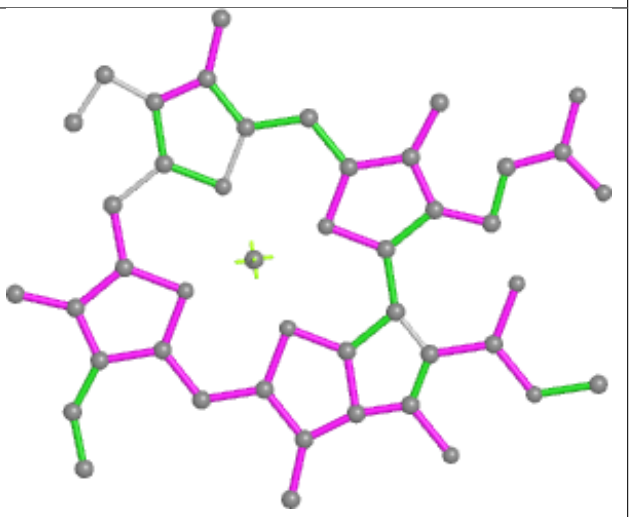

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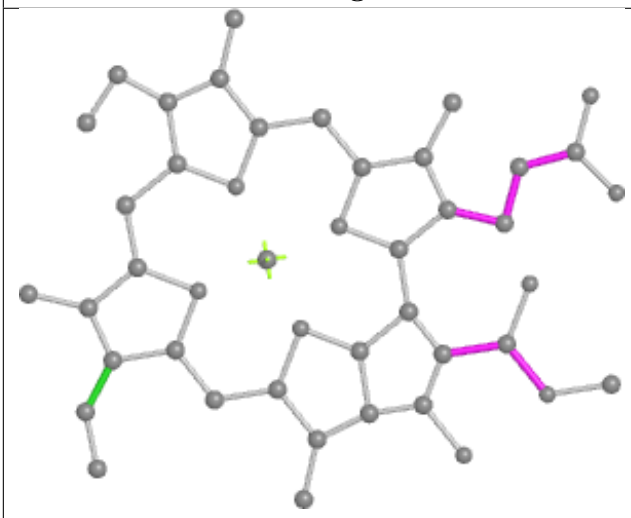

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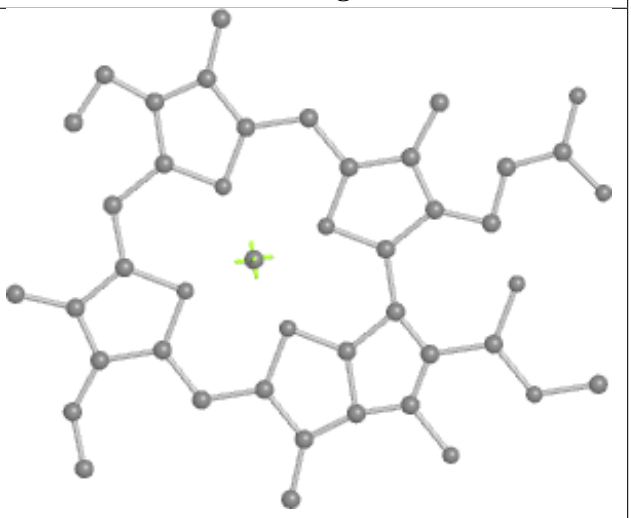

Rings

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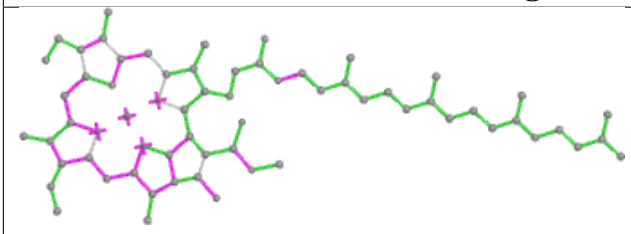

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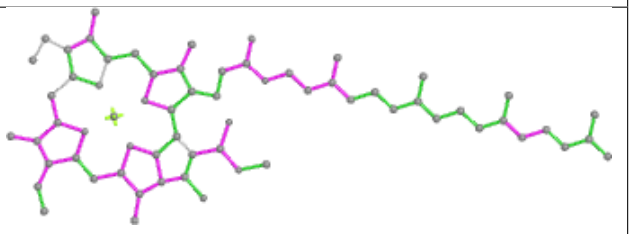
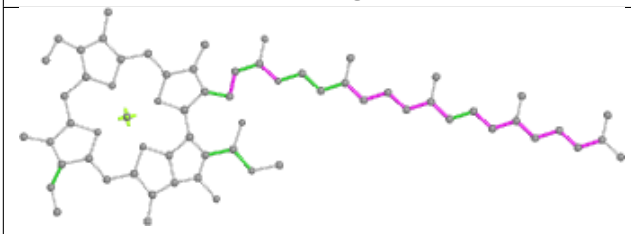


Bond angles



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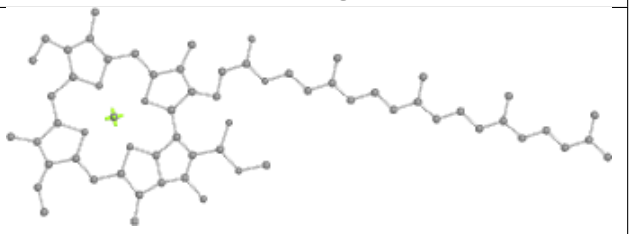
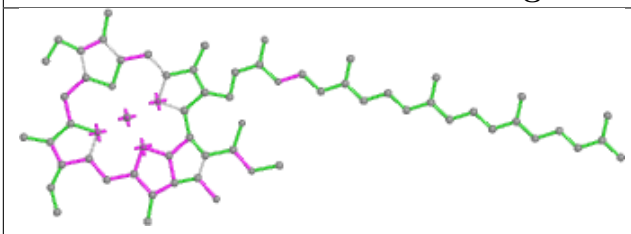


Rings

Ligand CLA Y 838



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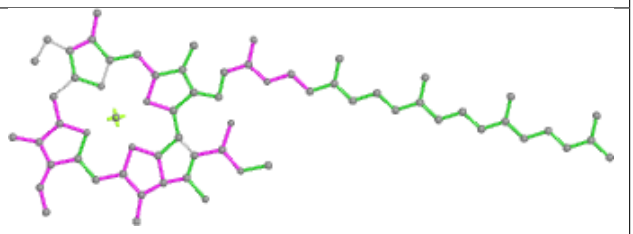

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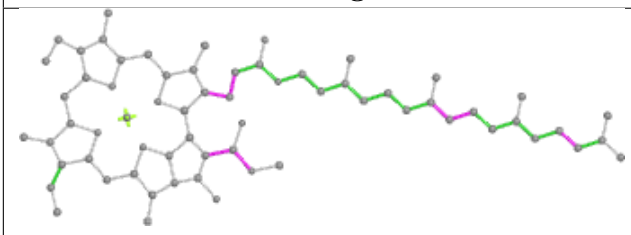

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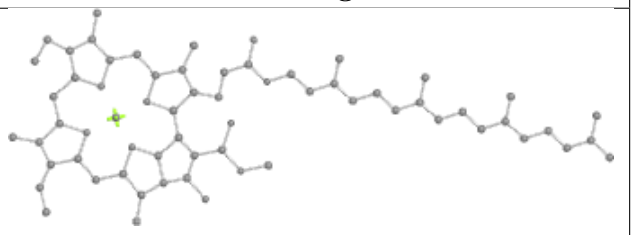
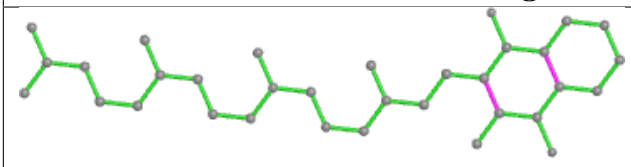


Rings

Ligand PQN G 843



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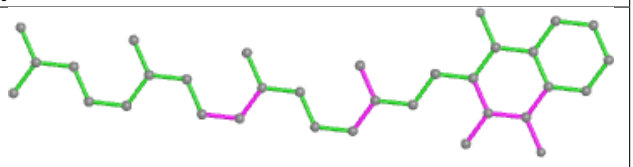

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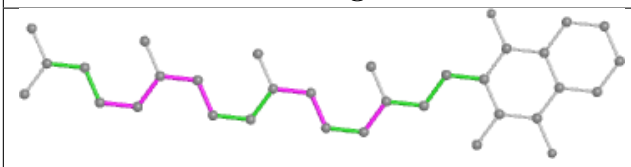

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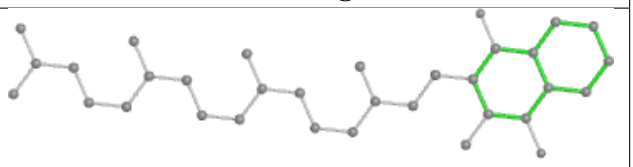
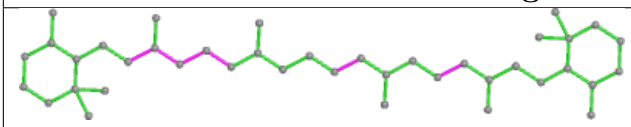


Rings

Ligand BCR A 848



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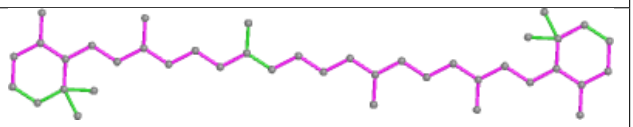
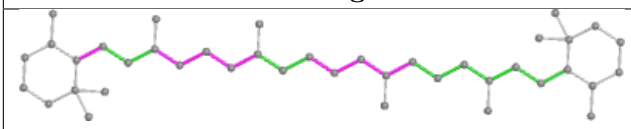


Bond angles



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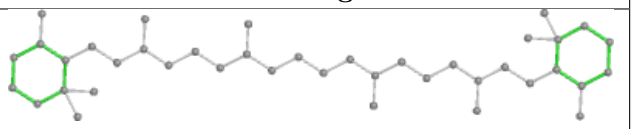
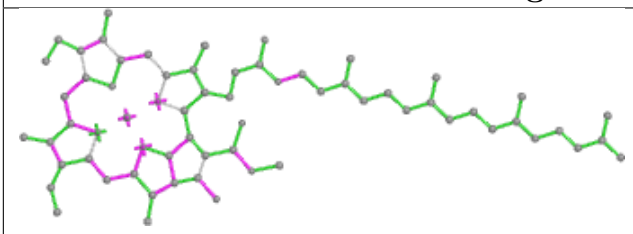


Rings

Ligand CLA Z 808



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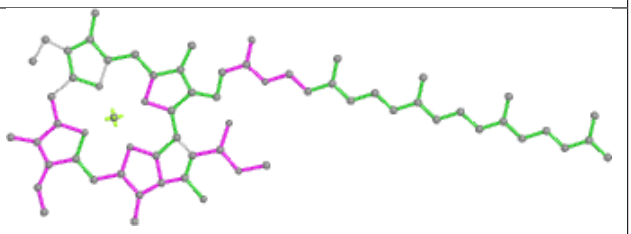
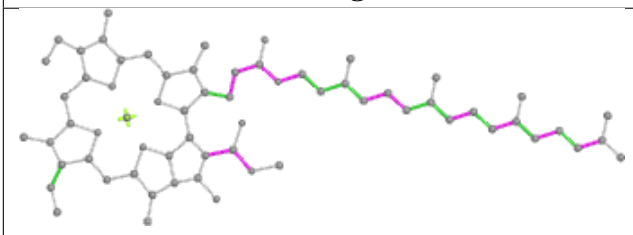


Bond angles



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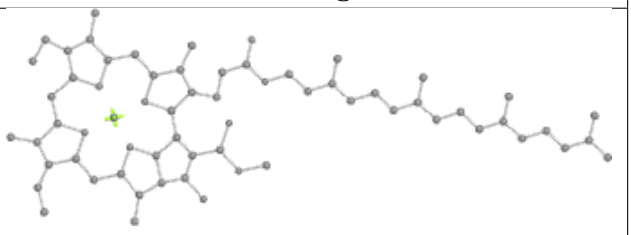
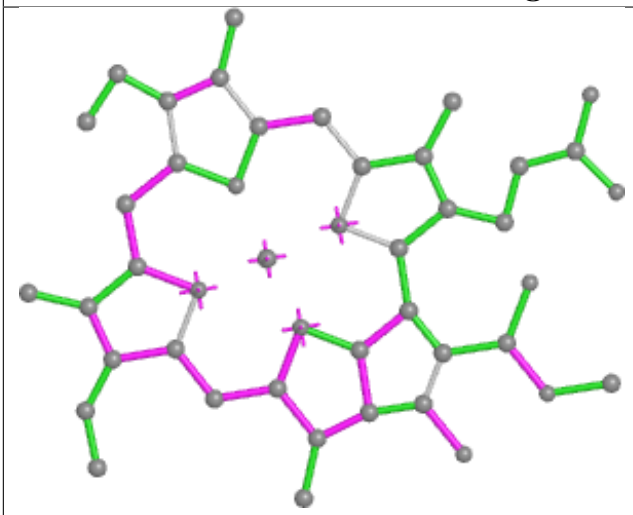


Rings

Ligand CLA B 833



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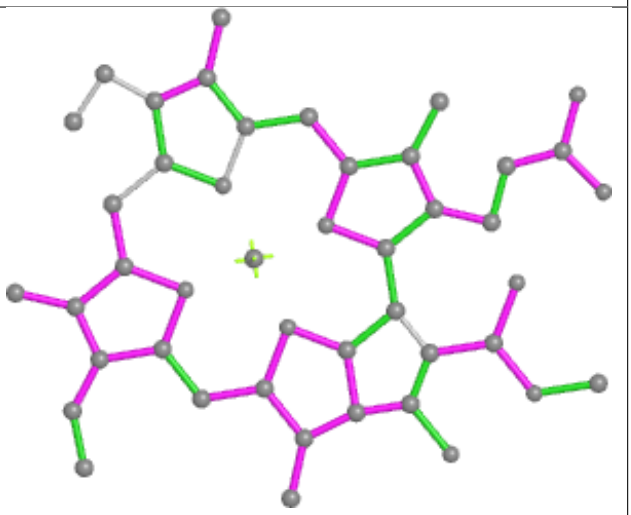
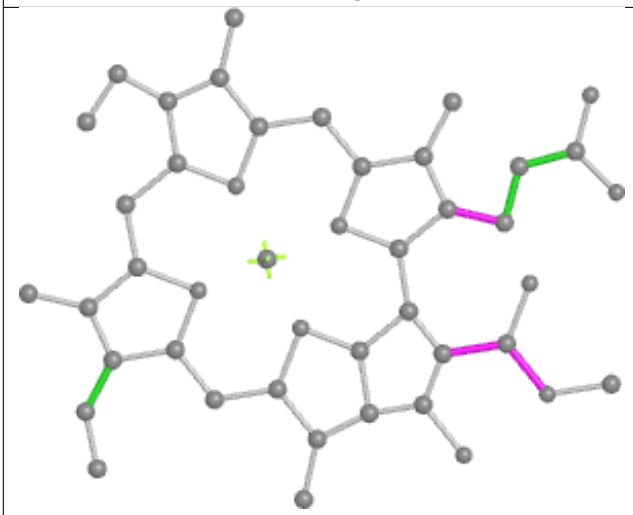


Bond angles



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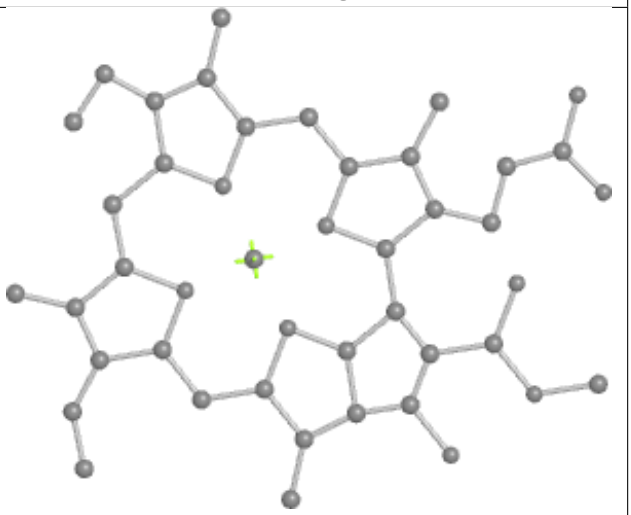
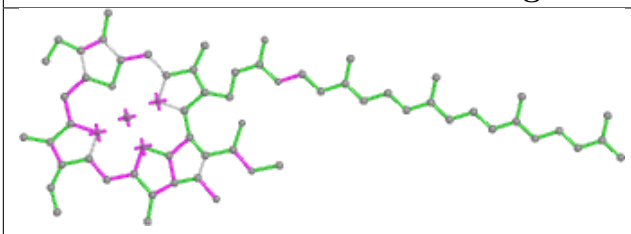
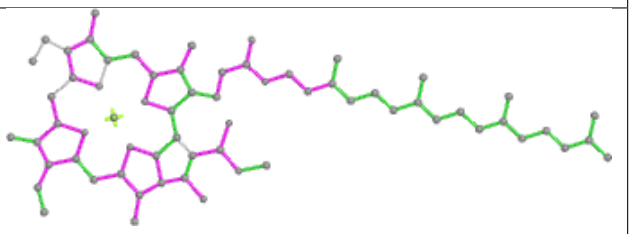


Rings

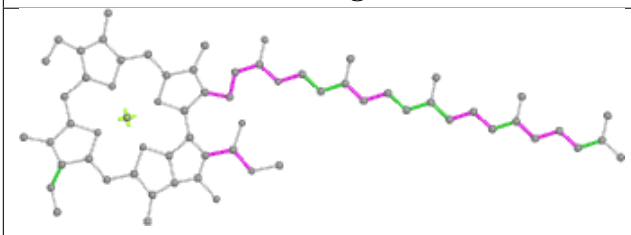
Ligand CLA G 818



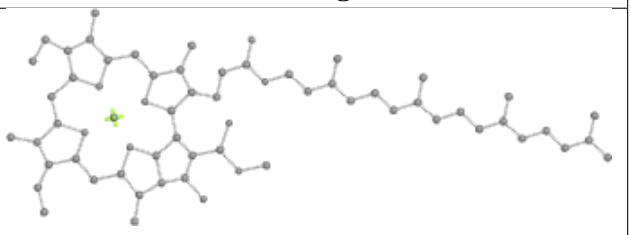
Bond lengths



Bond angles

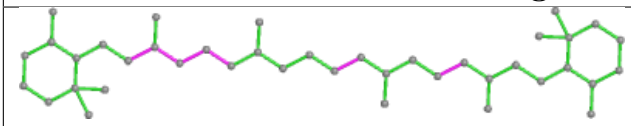


Torsions



Rings

Ligand BCR i 101



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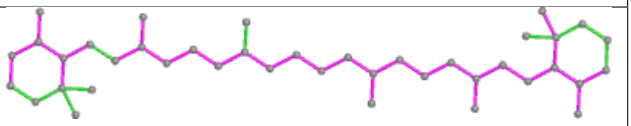
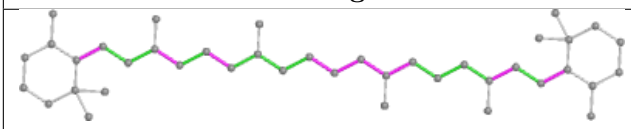


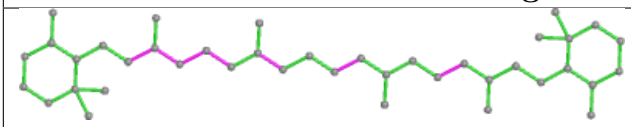
Bond angles



Torsions

Rings

Ligand BCR A 849



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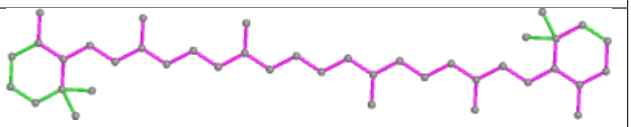
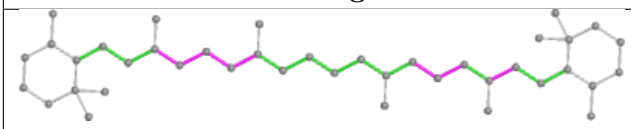


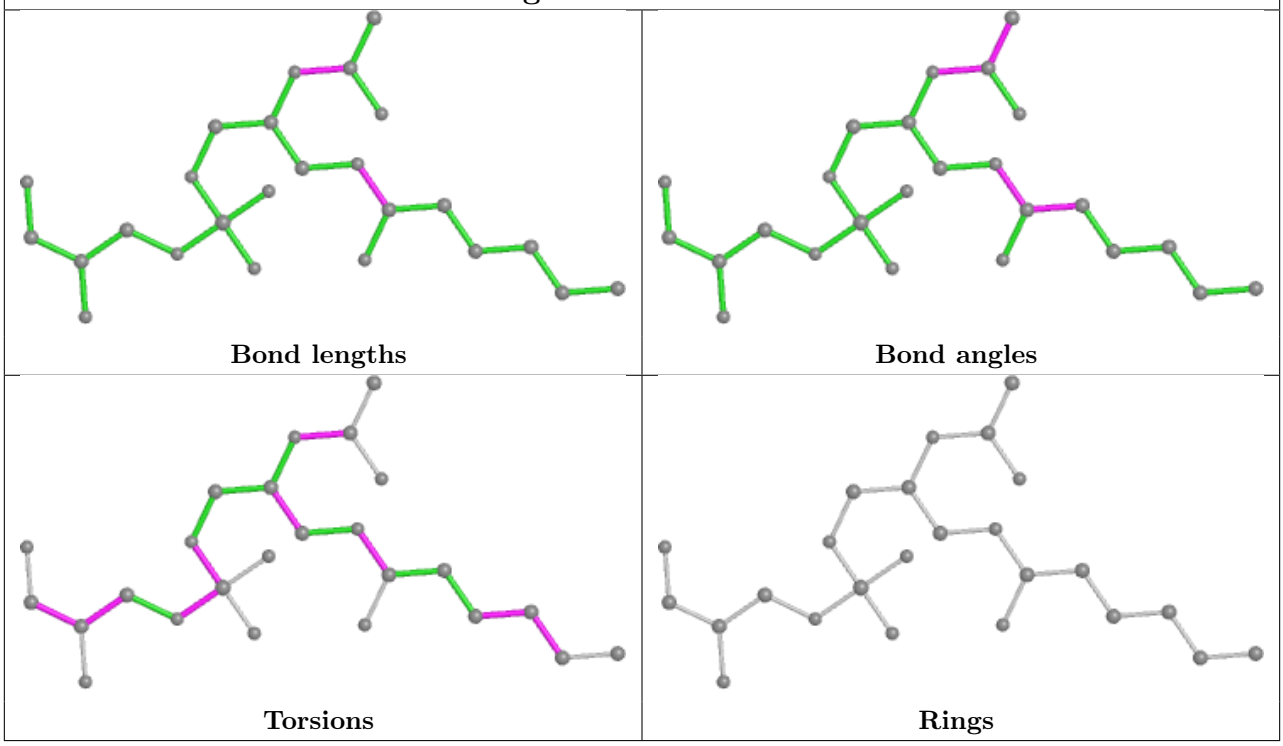
Bond angles



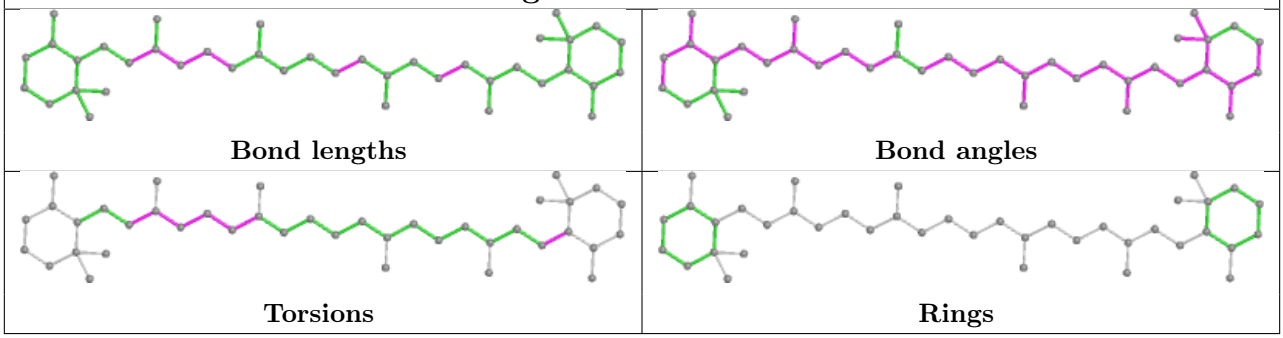
Torsions

Rings

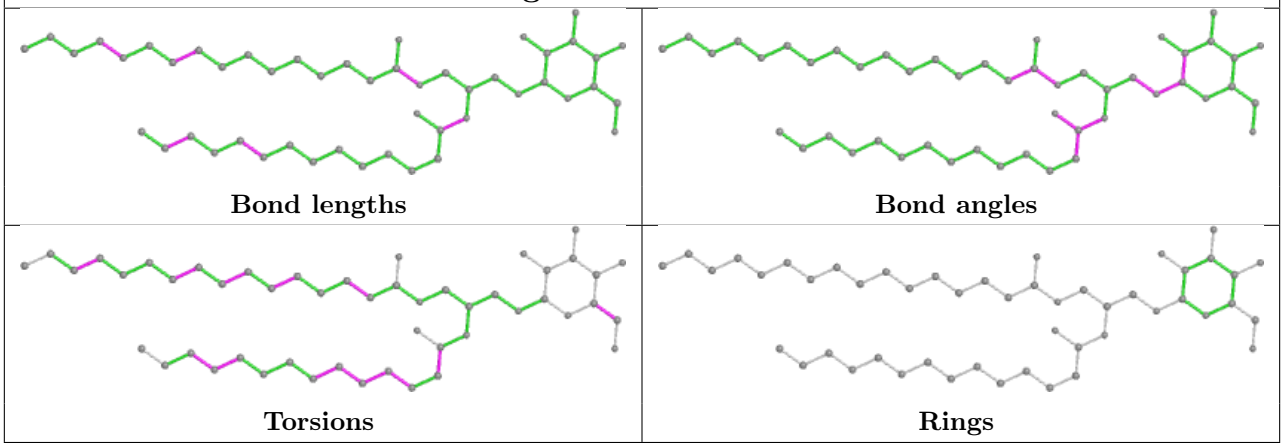
Ligand LHG Y 851

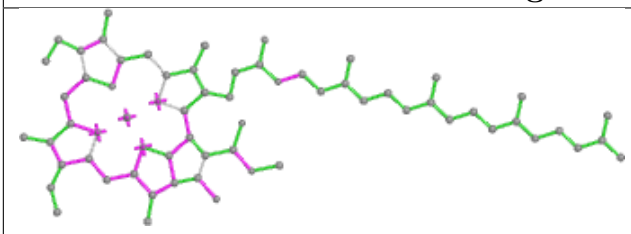
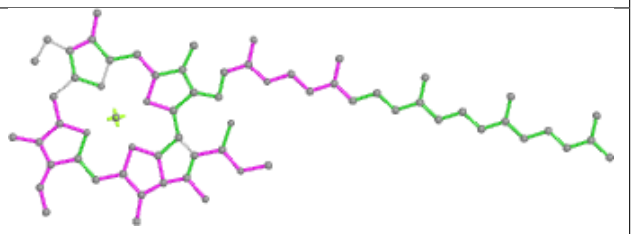
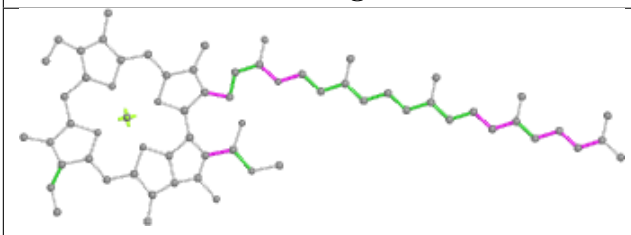
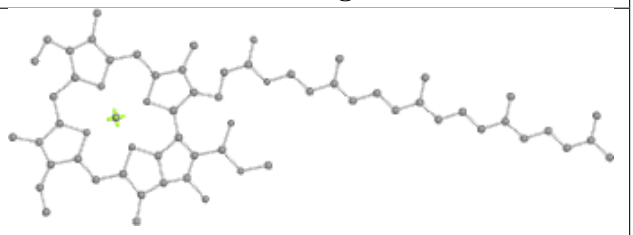


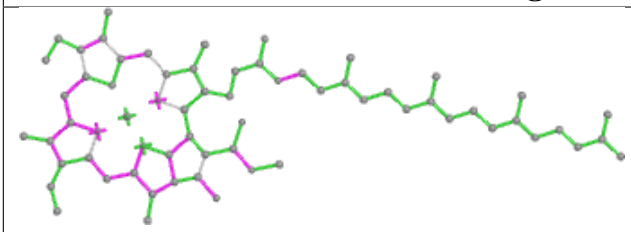
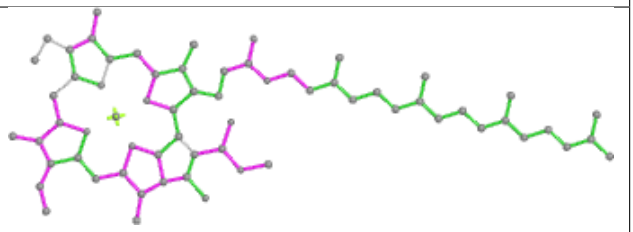
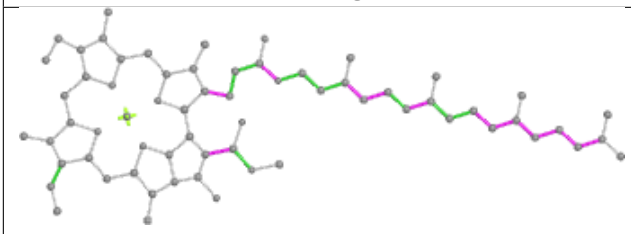
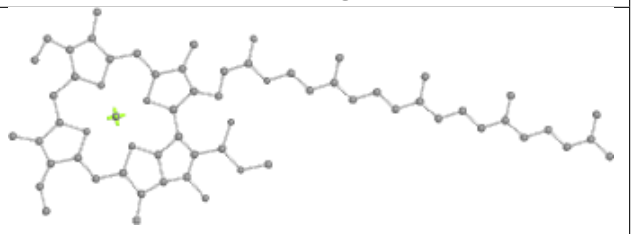
Ligand BCR G 847



Ligand LMG Z 849



Ligand CLA Z 806	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA L 204	
 Bond lengths	 Bond angles
 Torsions	 Rings

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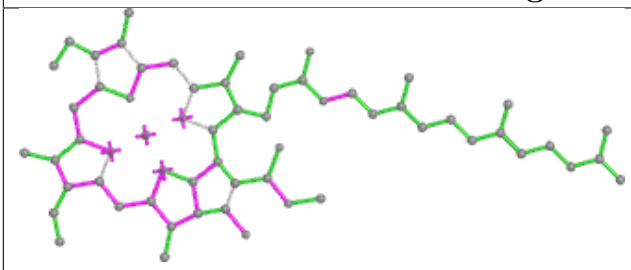

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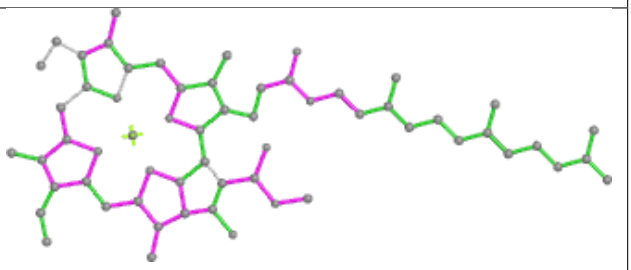
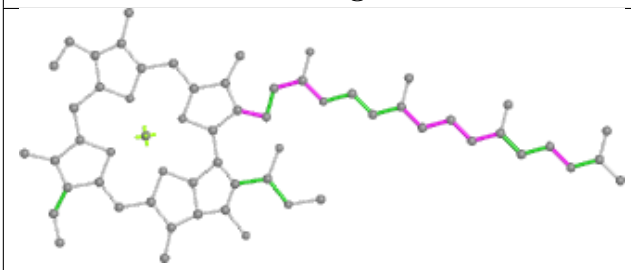


Bond angles



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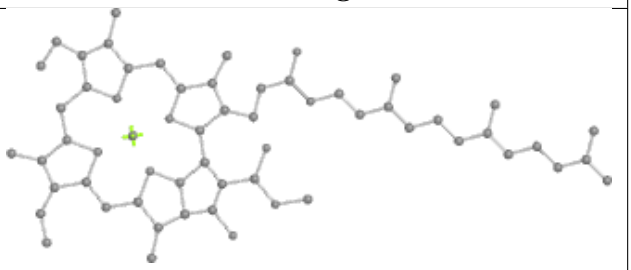
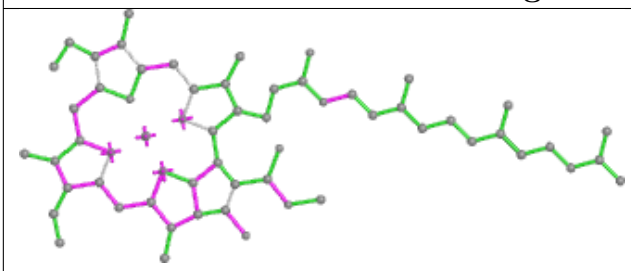


Rings

Ligand CLA Y 813



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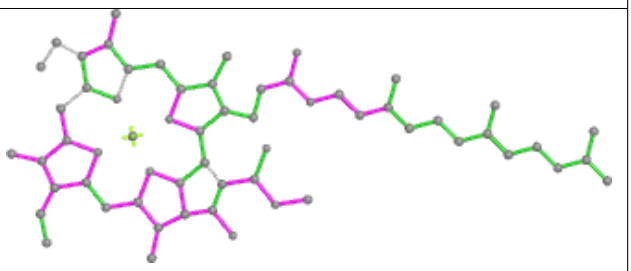
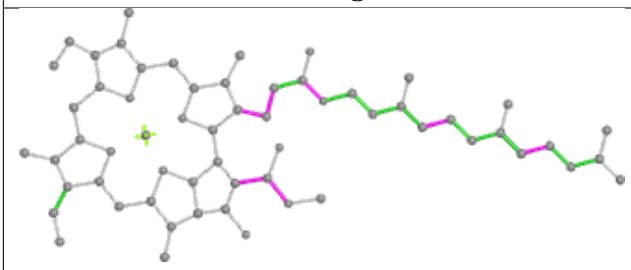


Bond angles



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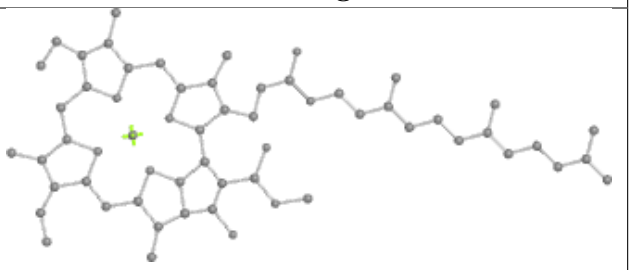
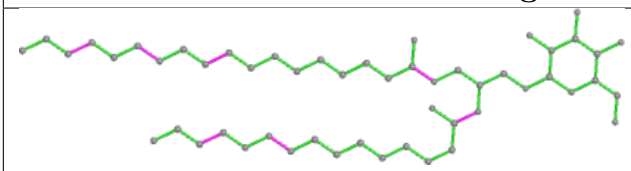


Rings

Ligand LMG B 848



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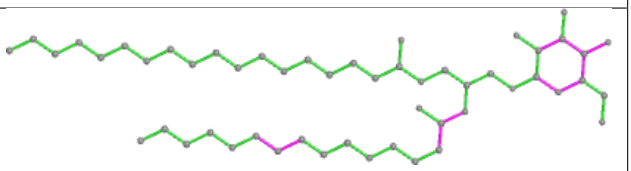
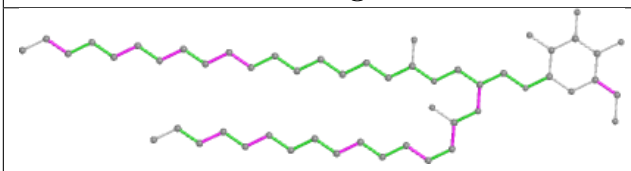


Bond angles



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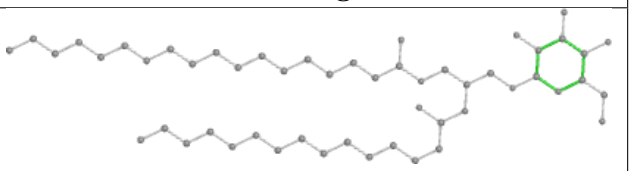
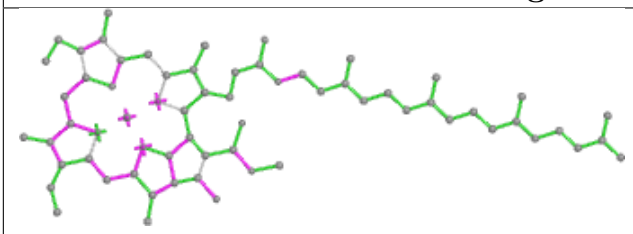


Rings

Ligand CLA h 201



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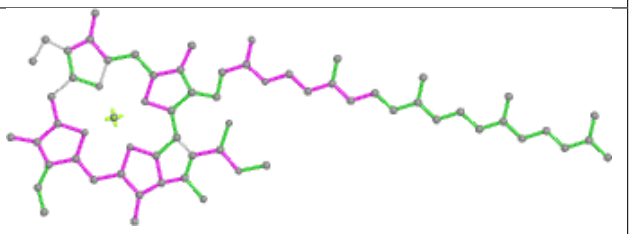
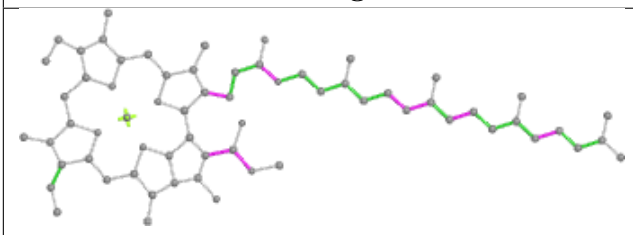


Bond angles



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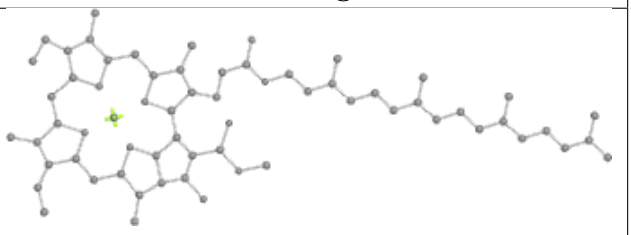
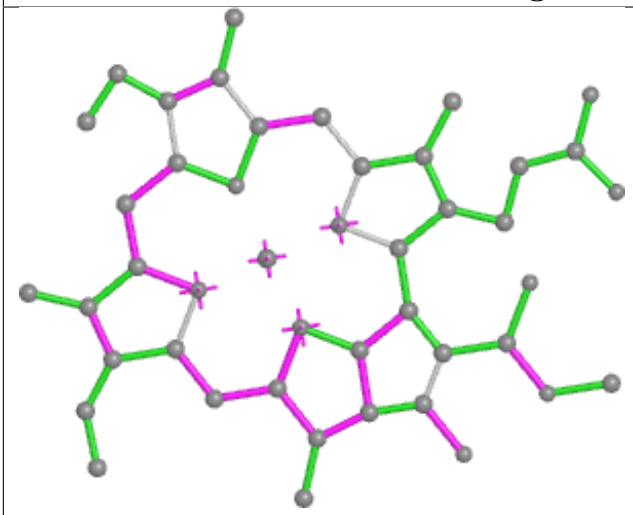


Rings

Ligand CLA g 102



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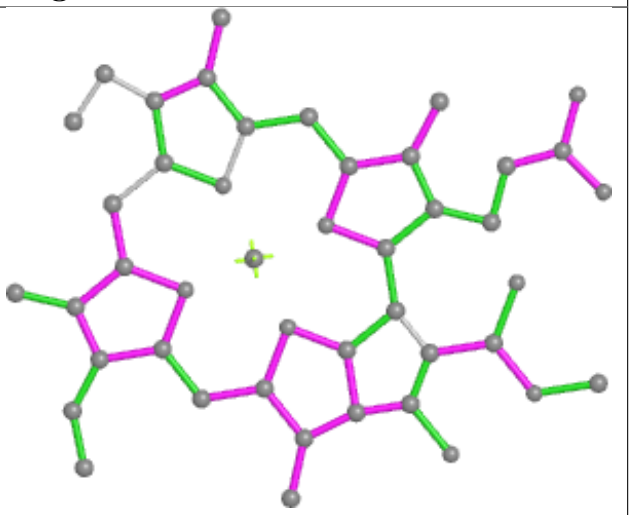
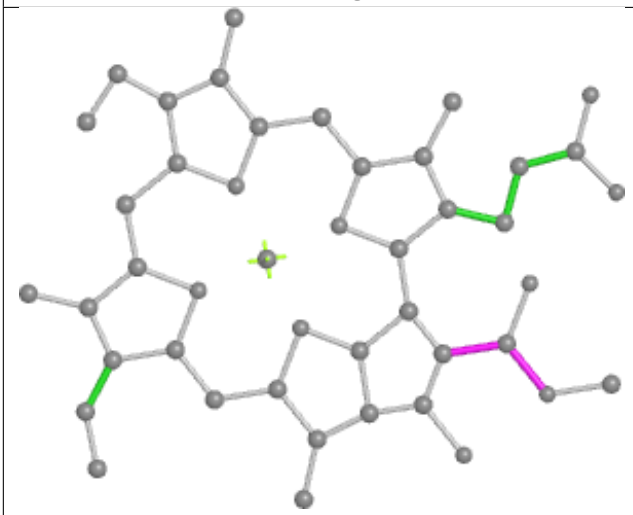


Bond angles



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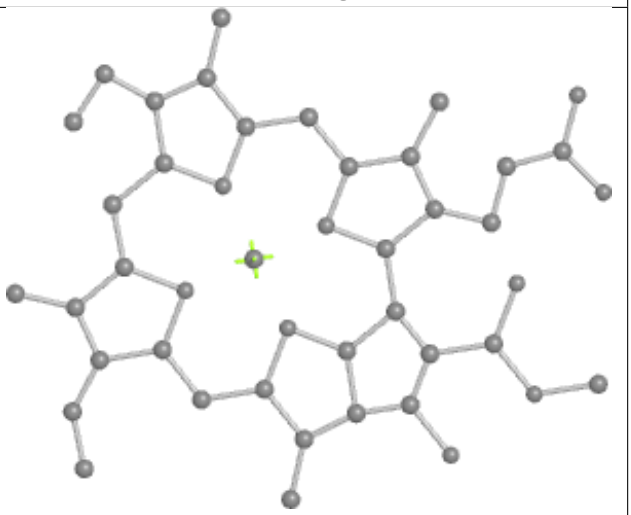
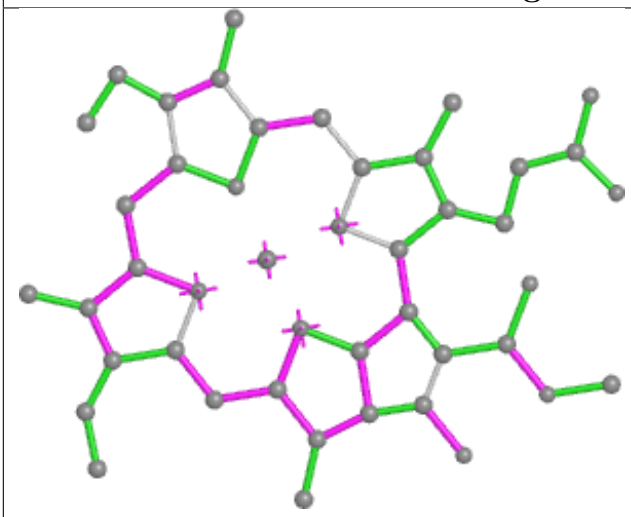


Rings

Ligand CLA H 815



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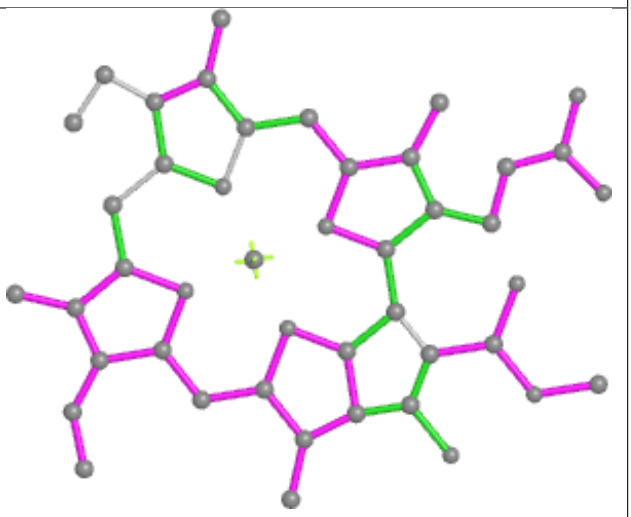
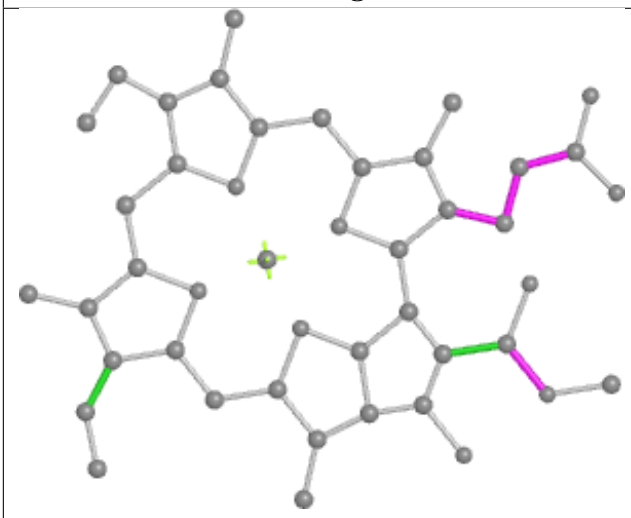


Bond angles



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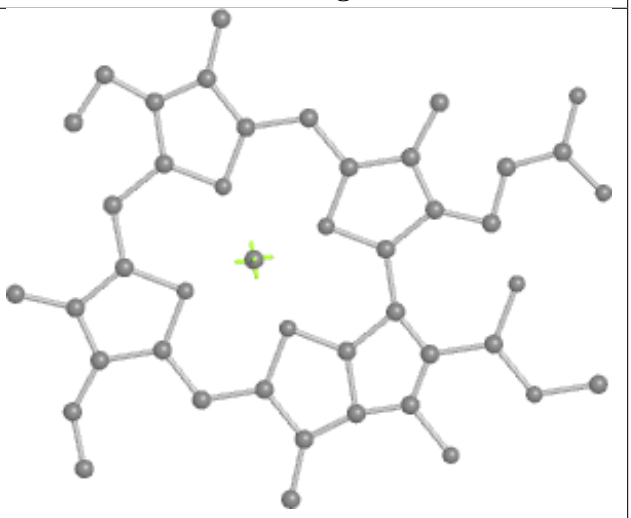
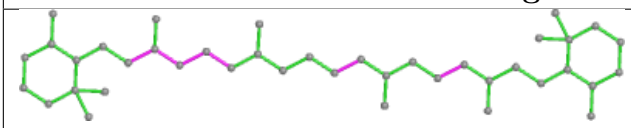


Rings

Ligand BCR B 844



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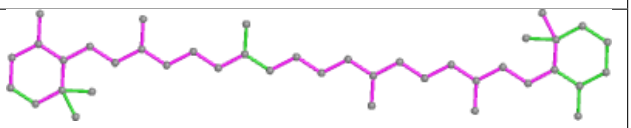
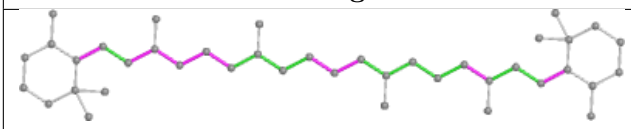
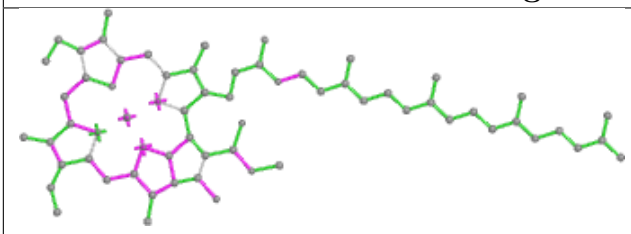
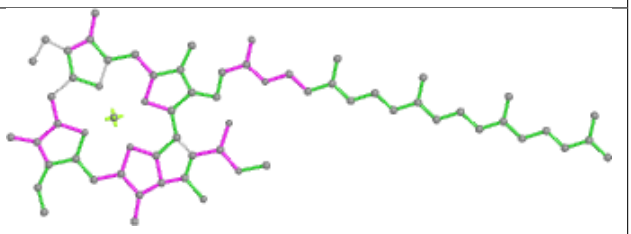
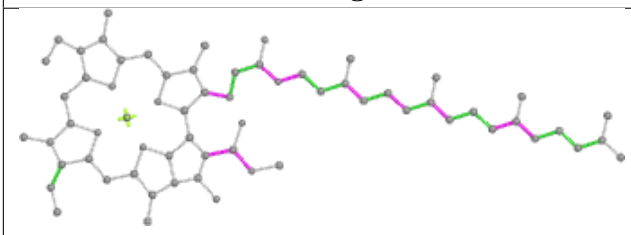
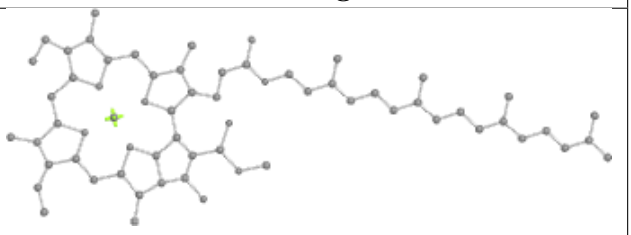


Bond angles



Torsions

Rings

Ligand CLA H 814	
 Bond lengths	 Bond angles
 Torsions	 Rings

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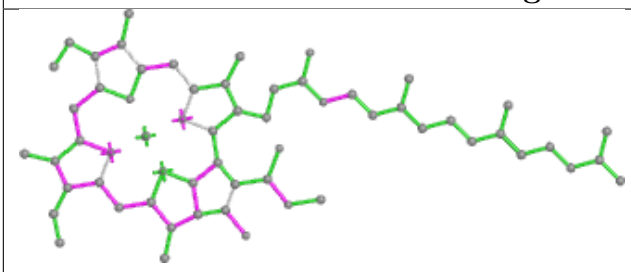
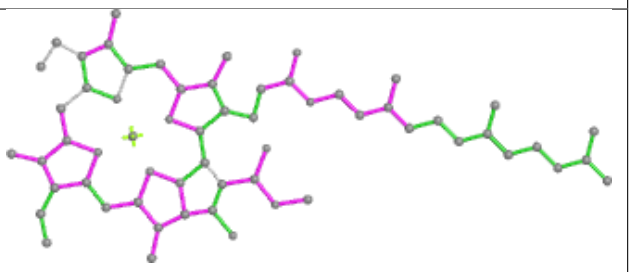
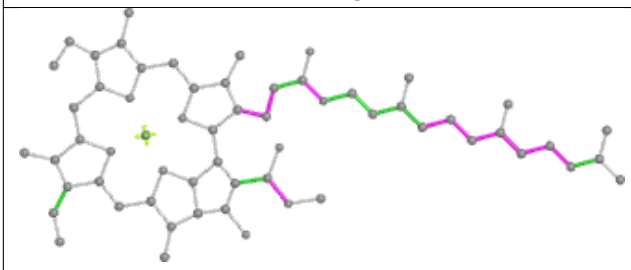
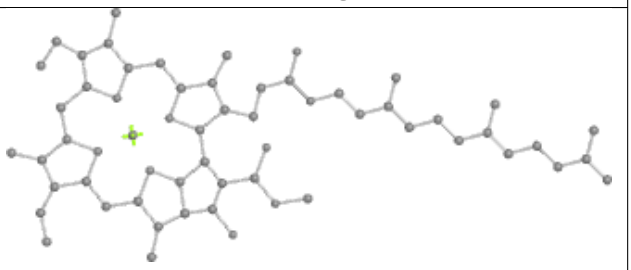
 Bond lengths	 Bond angles
 Torsions	 Rings

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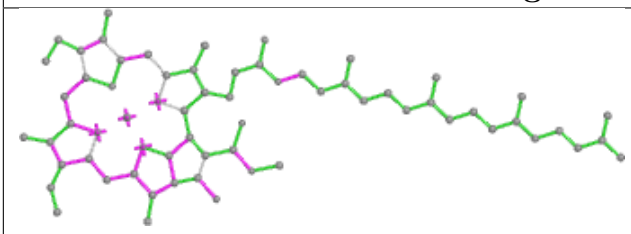
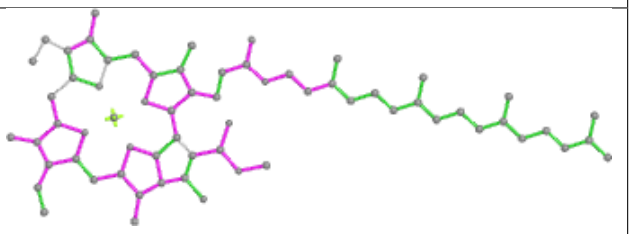
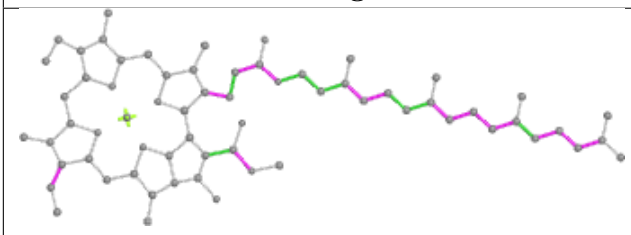
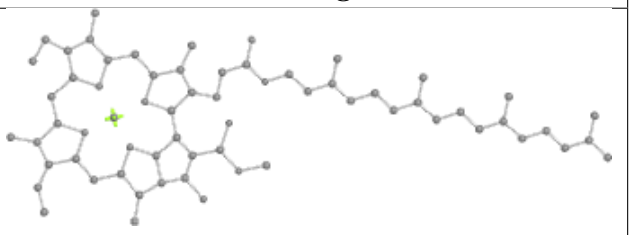
 Bond lengths	 Bond angles
 Torsions	 Rings

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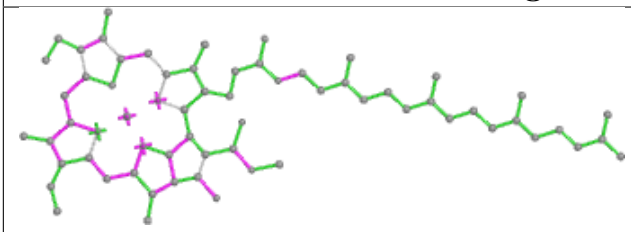
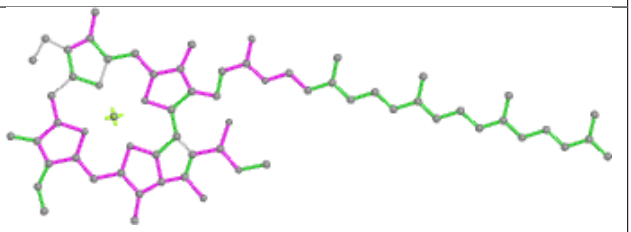
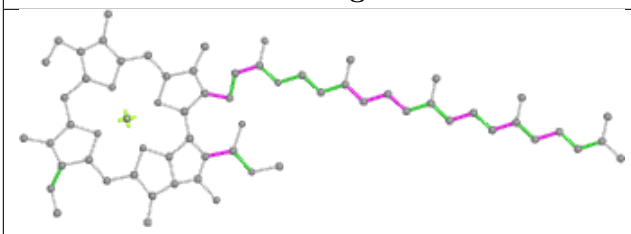
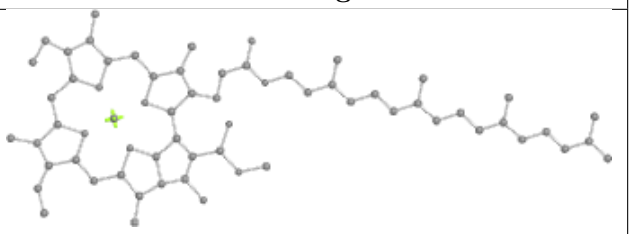
 Bond lengths	 Bond angles
 Torsions	 Rings

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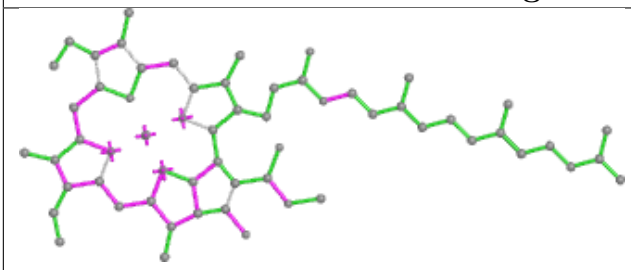
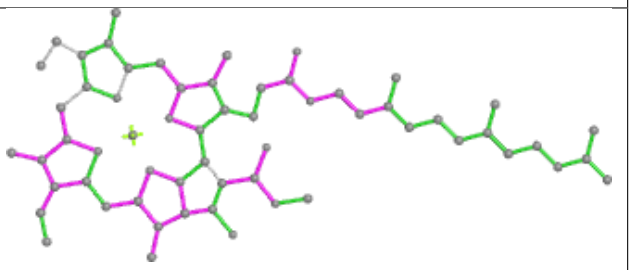
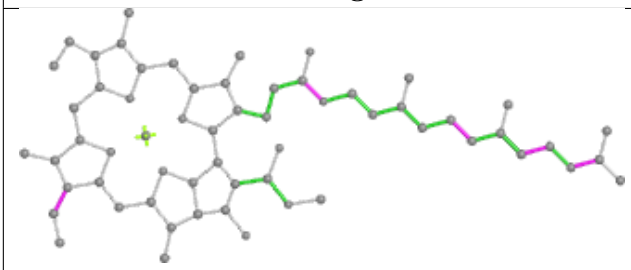
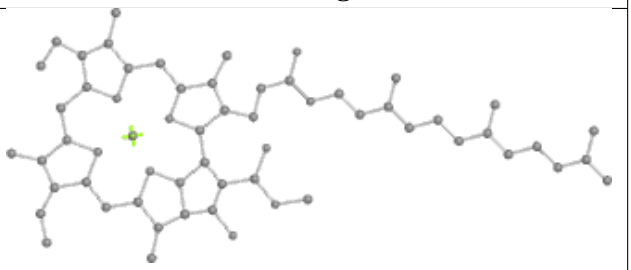
 Bond lengths	 Bond angles
 Torsions	 Rings

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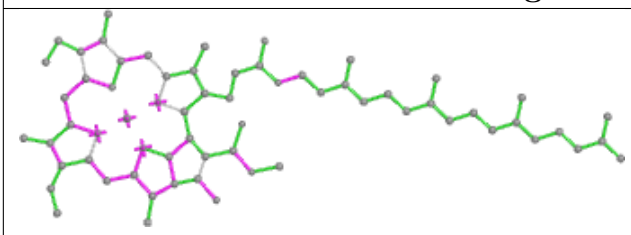
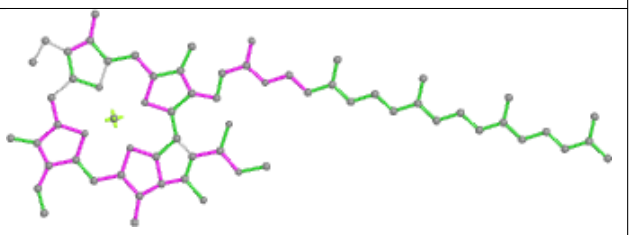
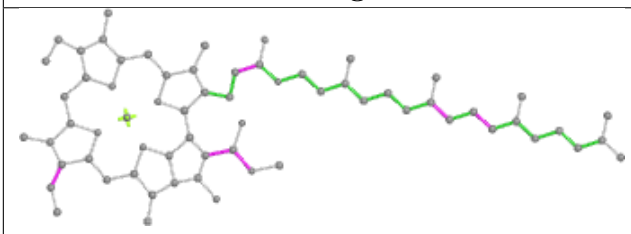
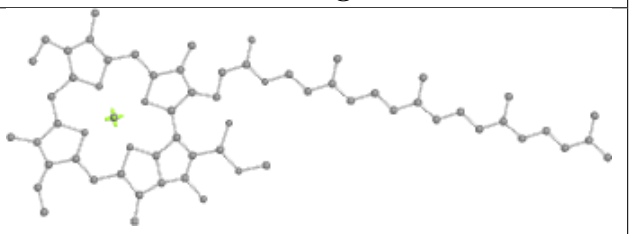
 Bond lengths	 Bond angles
 Torsions	 Rings

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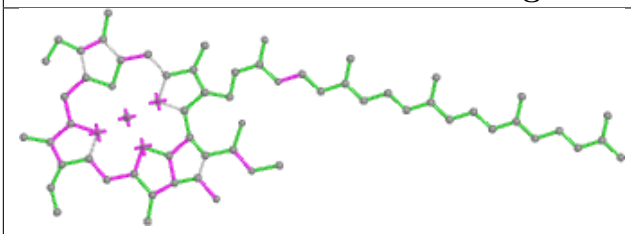
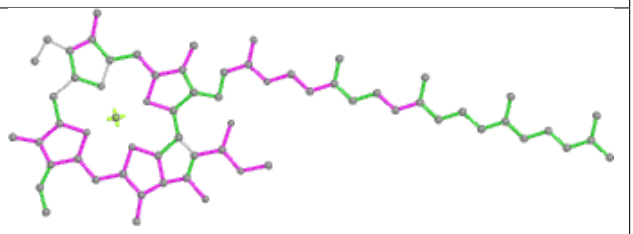
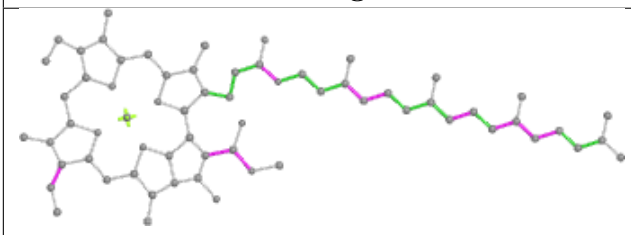
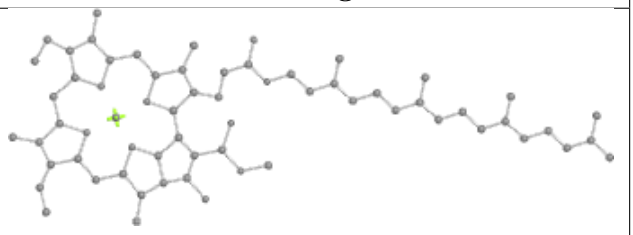
 Bond lengths	 Bond angles
 Torsions	 Rings

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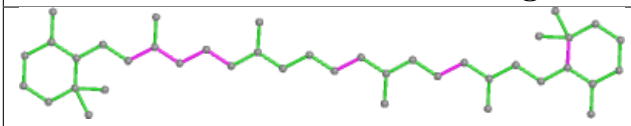
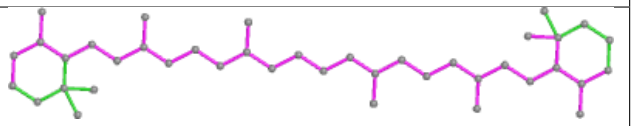
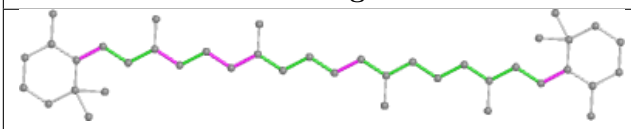
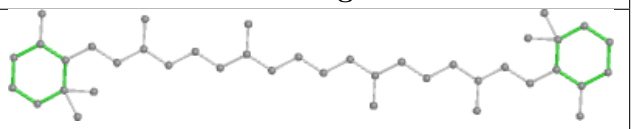
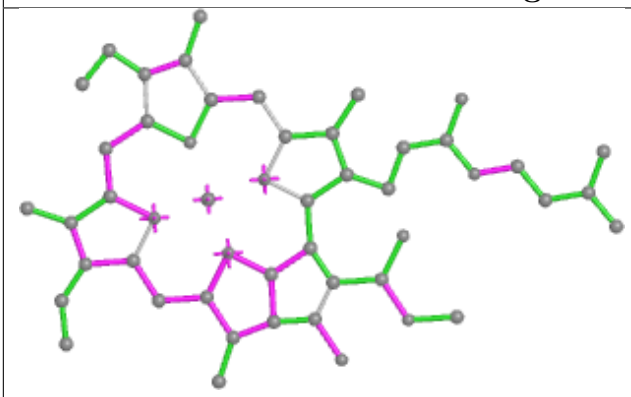
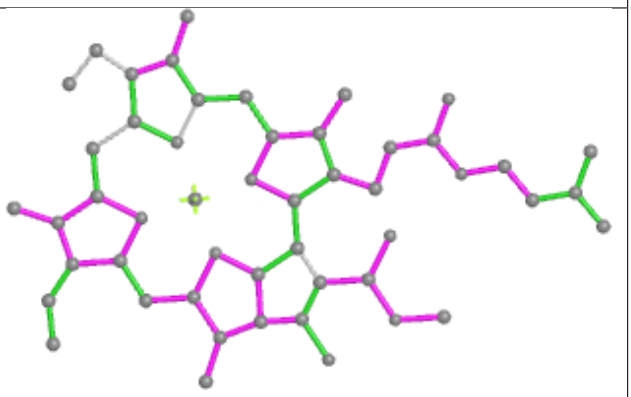
 Bond lengths	 Bond angles
 Torsions	 Rings

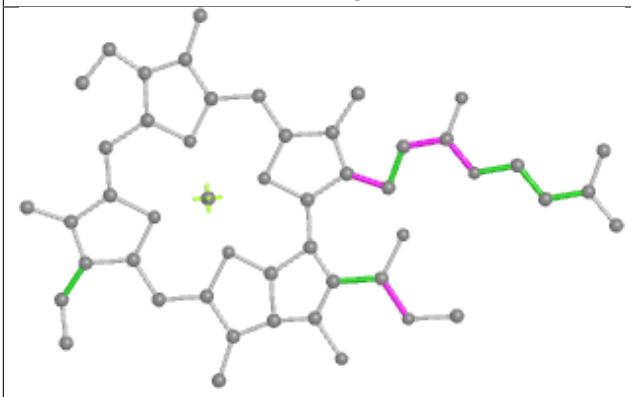
Ligand CLA A 824



Bond lengths



Bond angles



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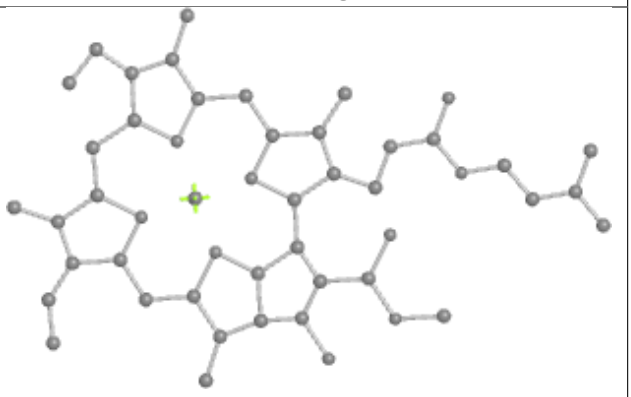
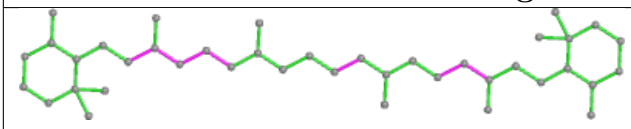


Rings

Ligand BCR S 1105



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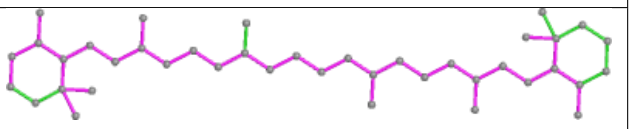
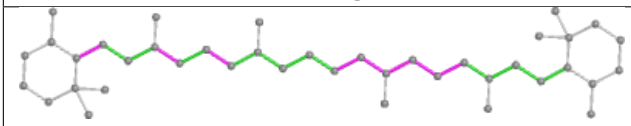


Bond angles



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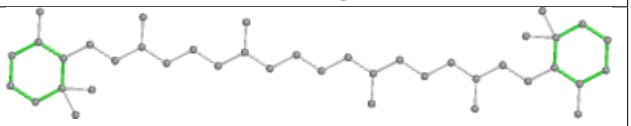
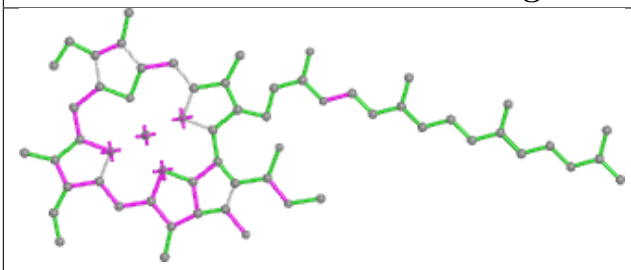
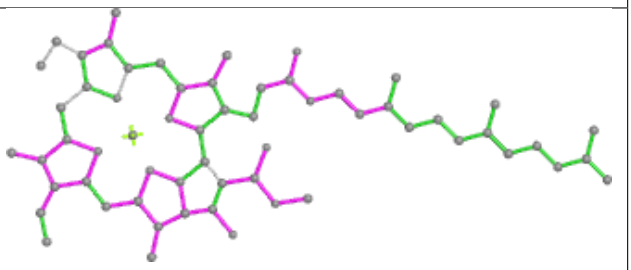
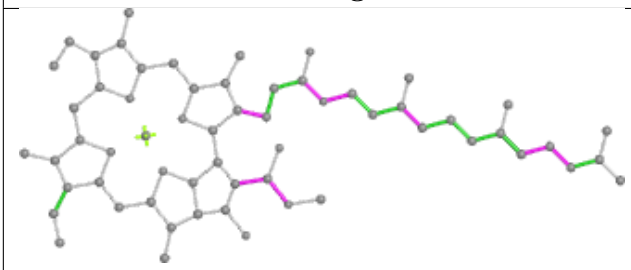
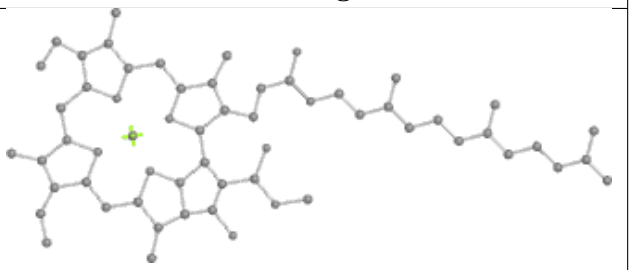


Rings

Ligand CLA G 813	
 Bond lengths	 Bond angles
 Torsions	 Rings

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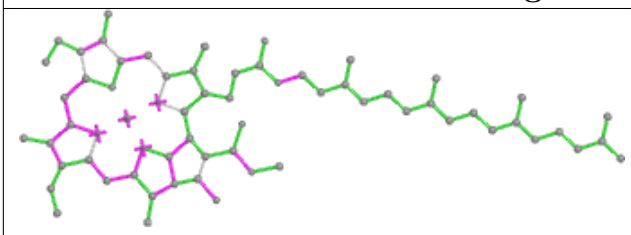
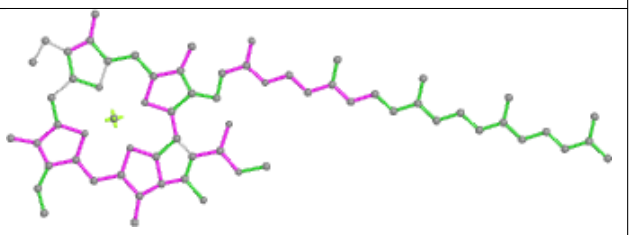
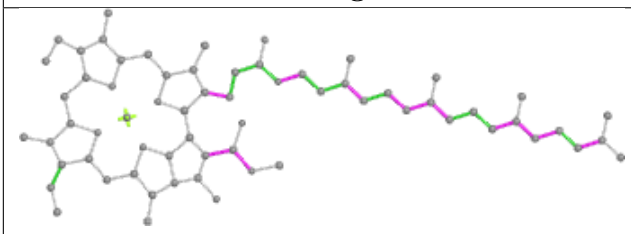
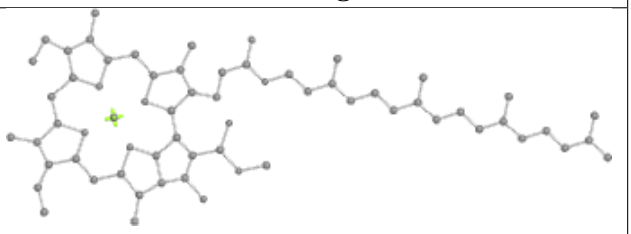
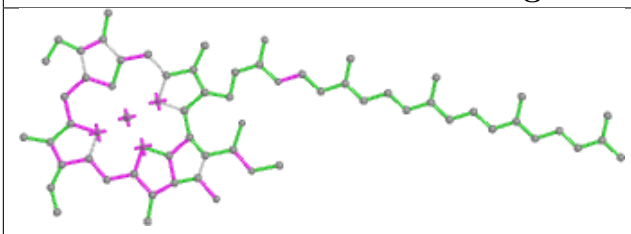
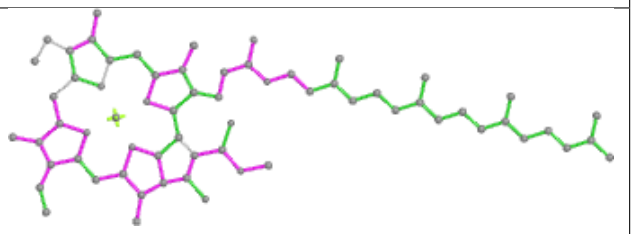
 Bond lengths	 Bond angles
 Torsions	 Rings

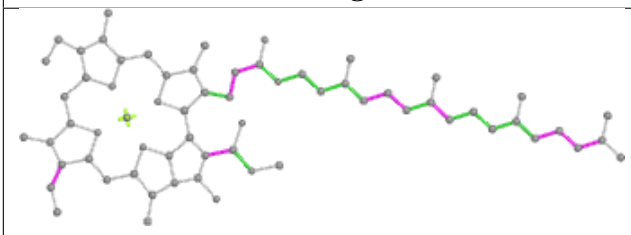
Ligand CLA A 826



Bond lengths



Bond angles



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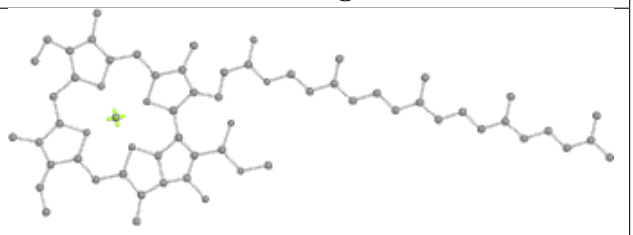
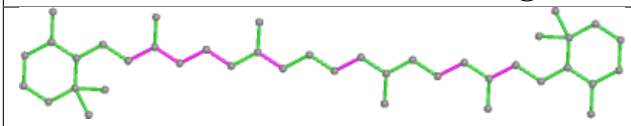


Rings

Ligand BCR M 101



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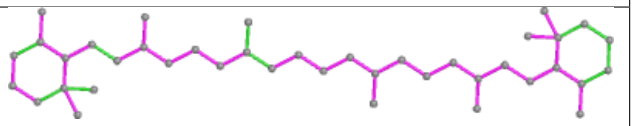
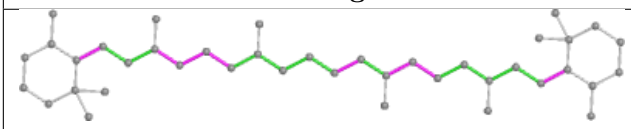


Bond angles



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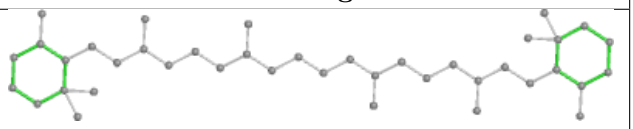
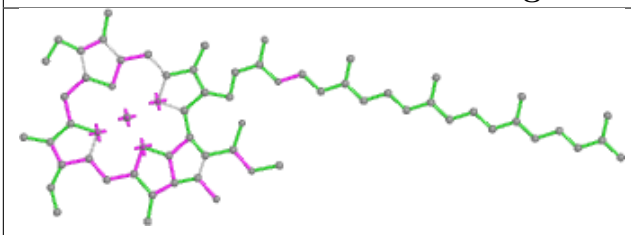
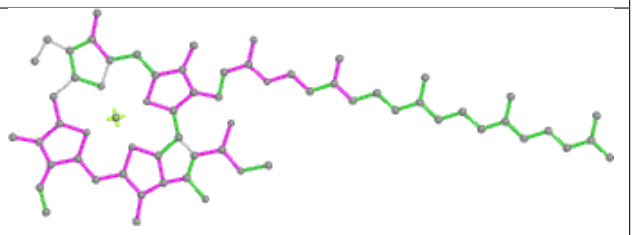


Rings

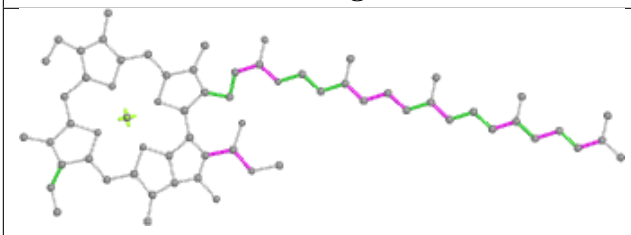
Ligand CLA H 808



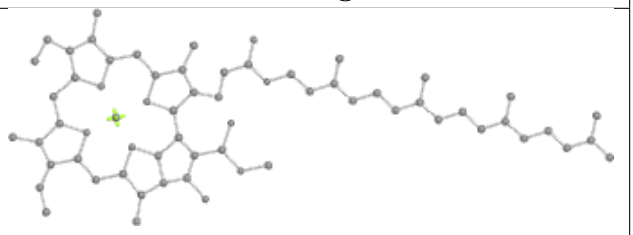
Bond lengths



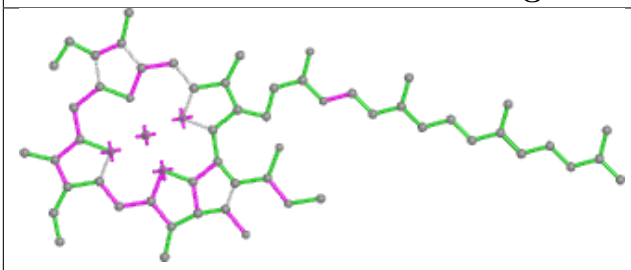
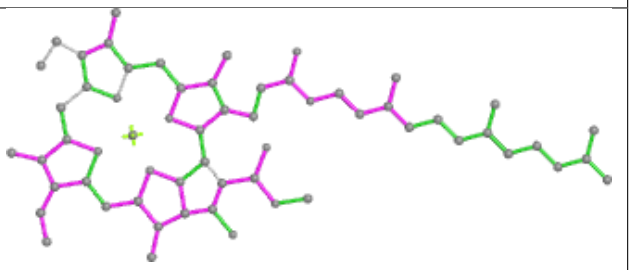
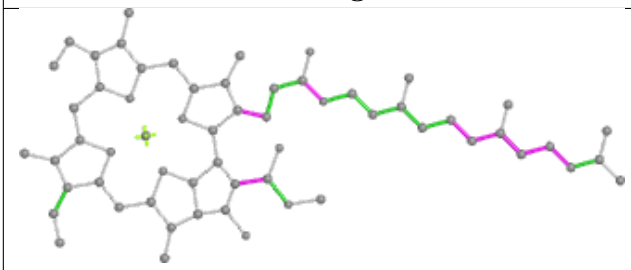
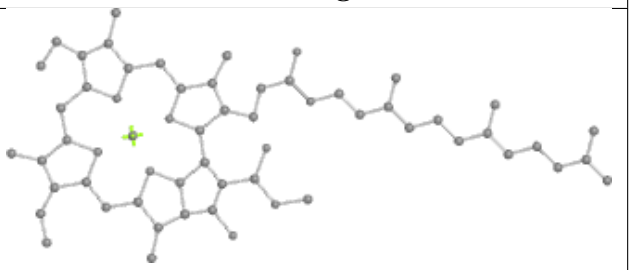
Bond angles

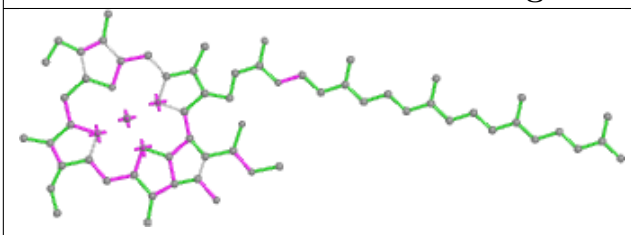
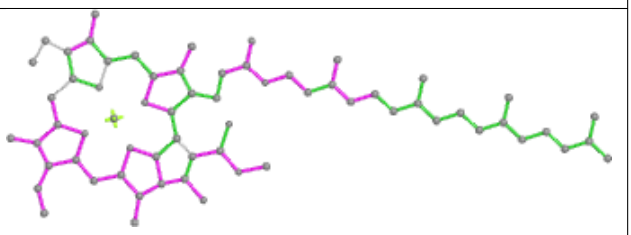
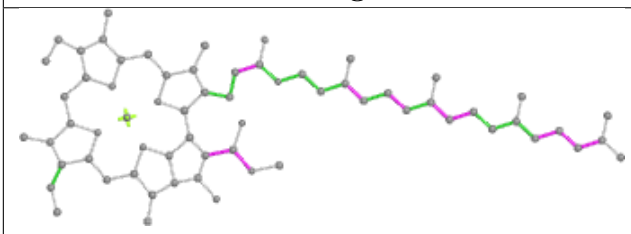
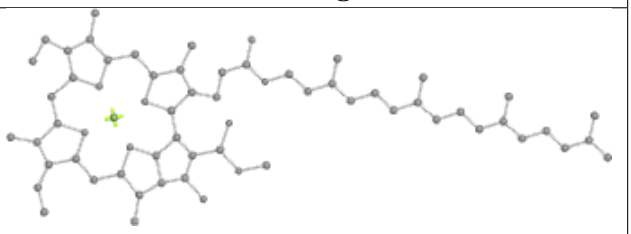


Torsions

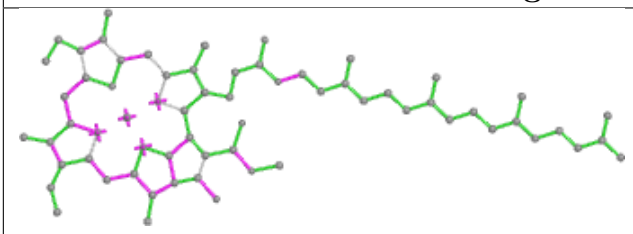


Rings

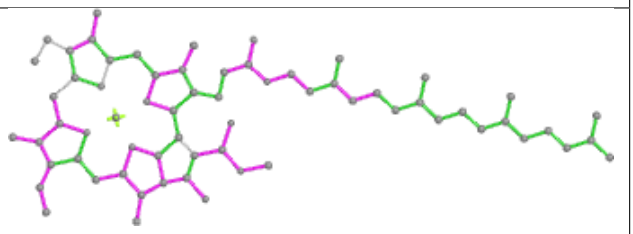
Ligand CLA A 827	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA Z 810	
 Bond lengths	 Bond angles
 Torsions	 Rings

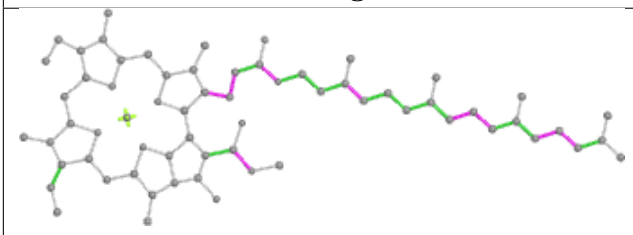
Ligand CLA A 812



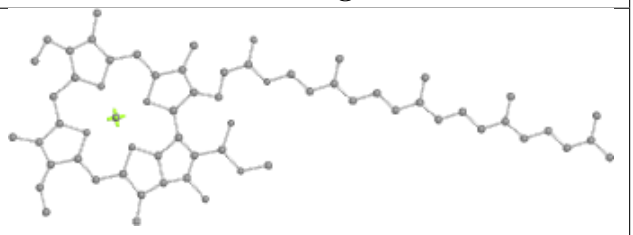
Bond lengths



Bond angles

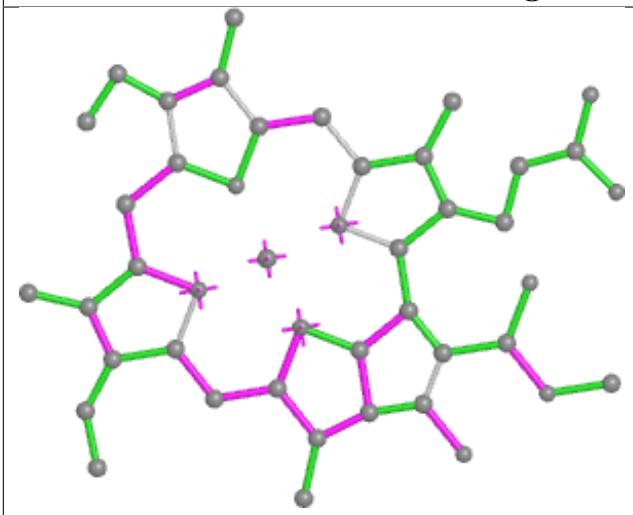


Torsions

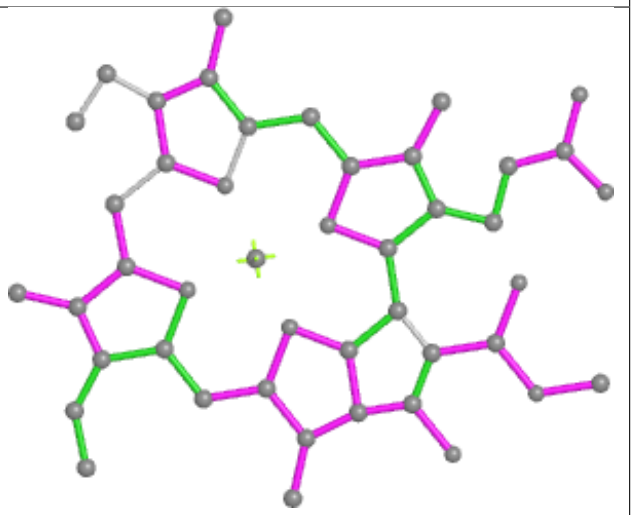


Rings

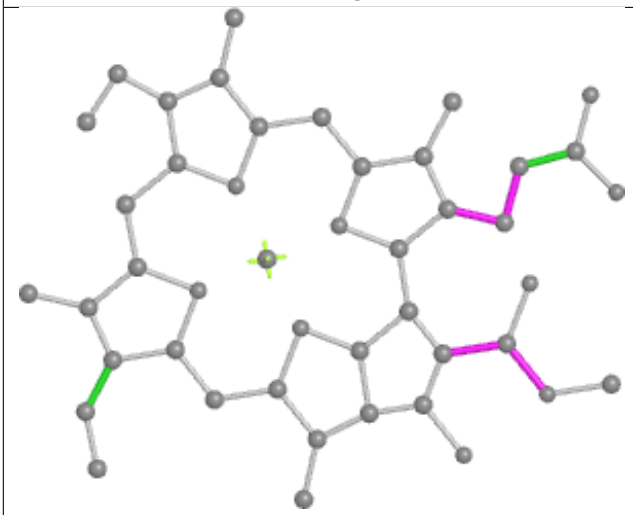
Ligand CLA H 834



Bond lengths



Bond angles



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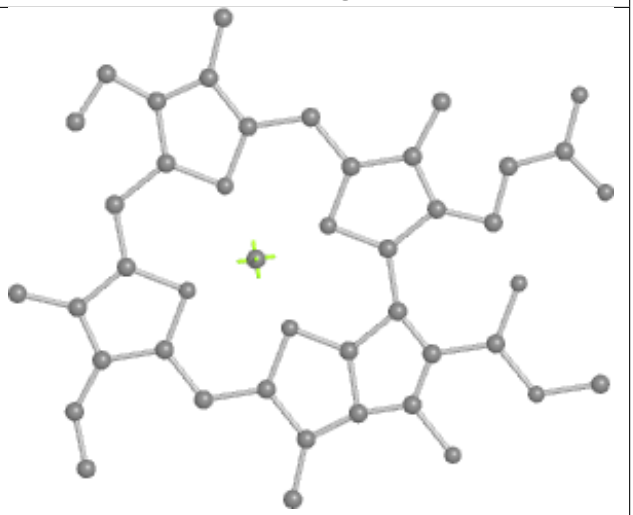
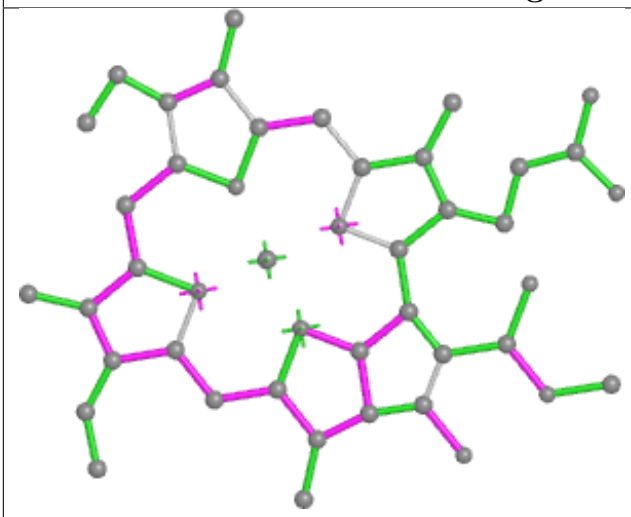


Rings

Ligand CLA Z 835



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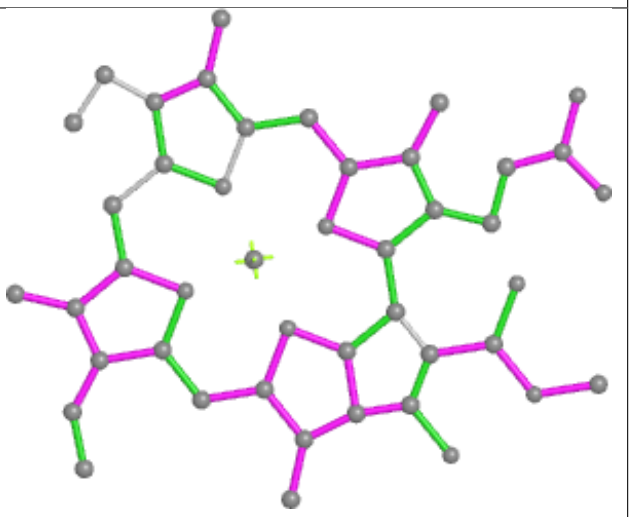
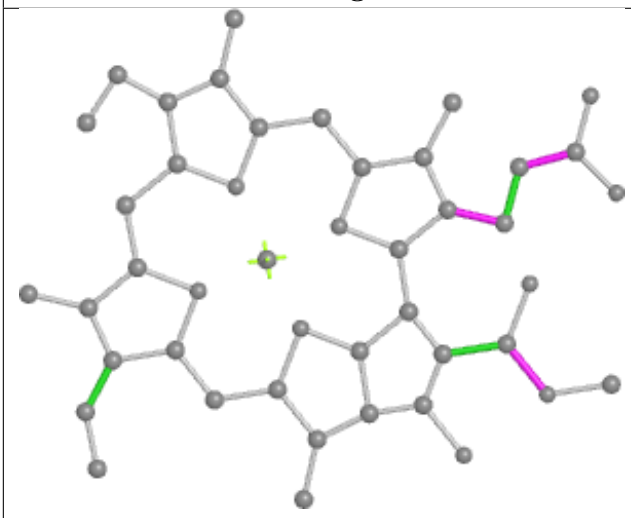


Bond angles



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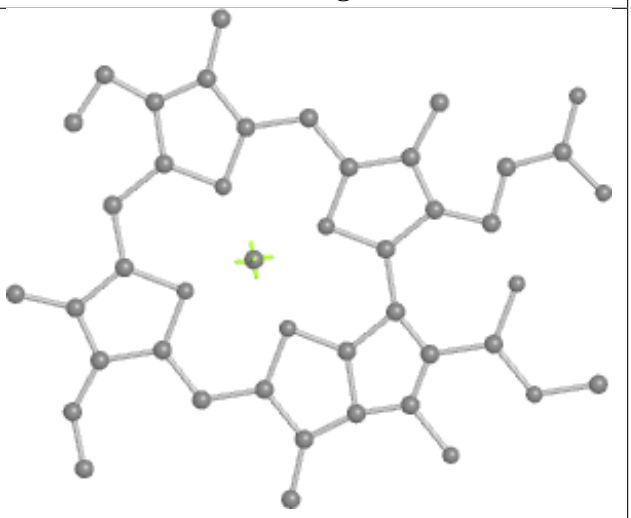
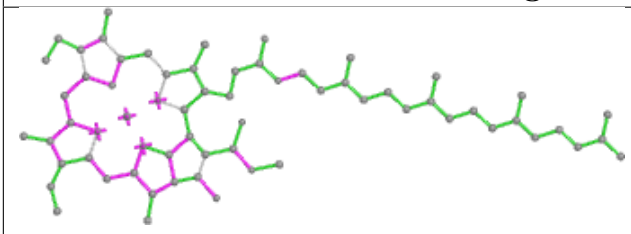


Rings

Ligand CLA Y 828



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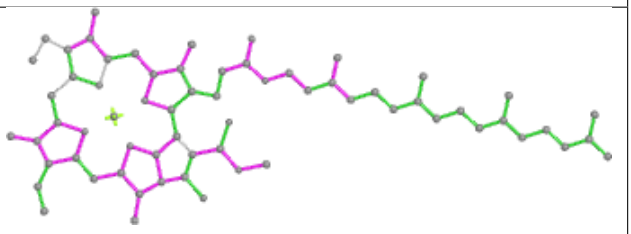
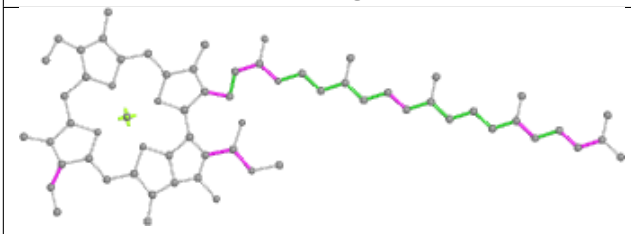


Bond angles



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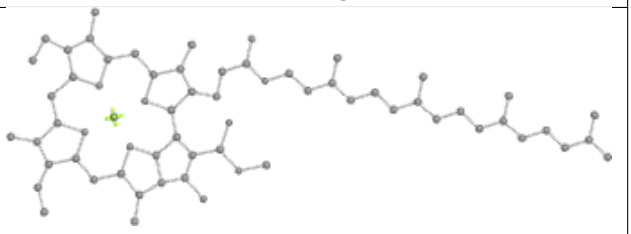
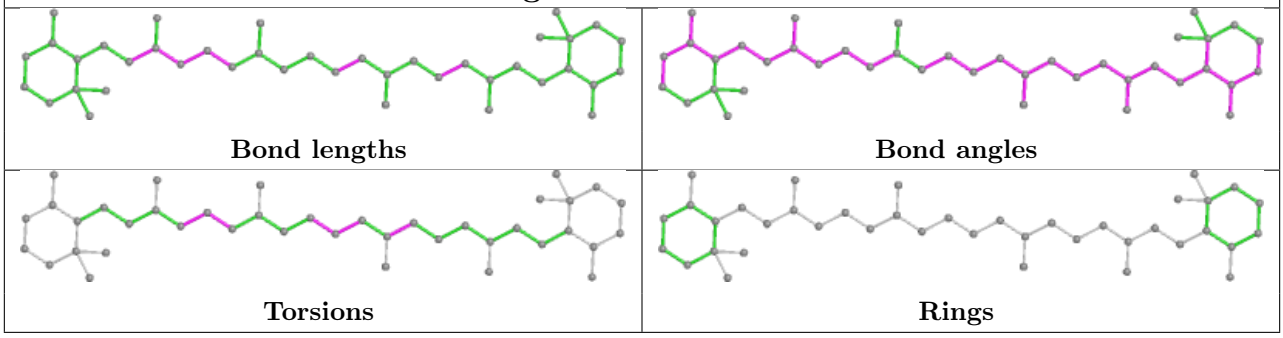
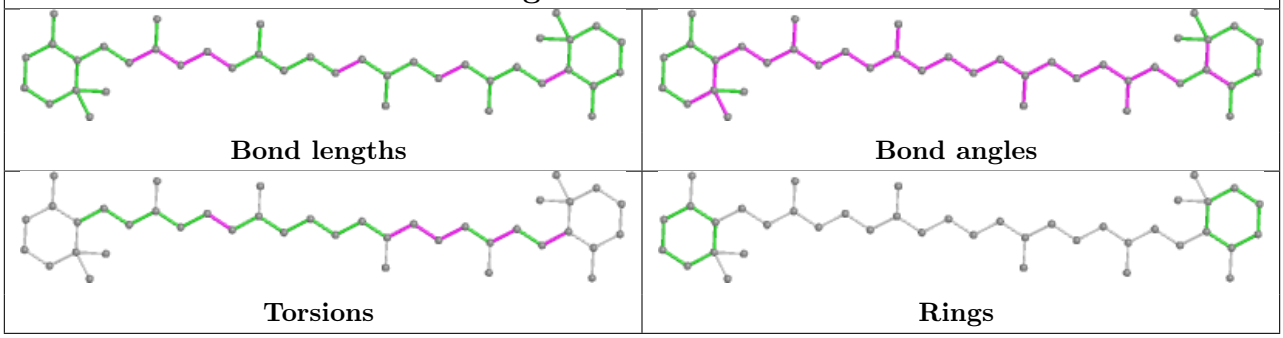


Rings

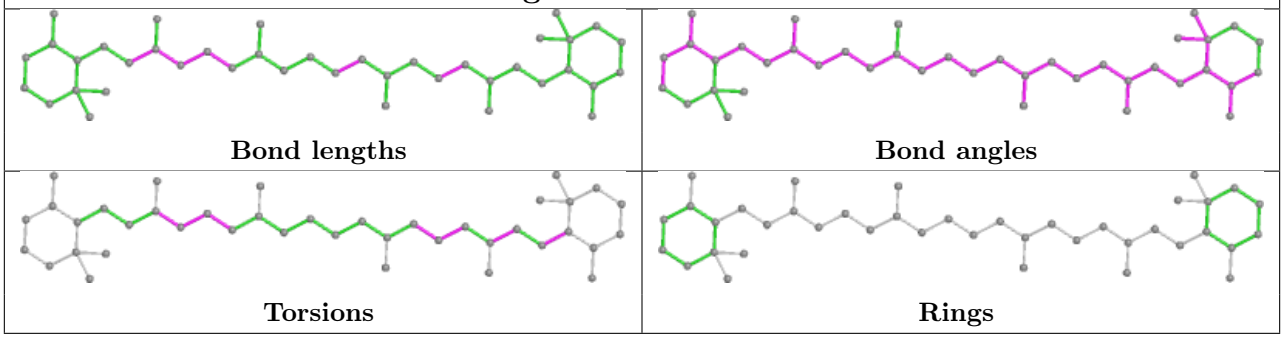
Ligand BCR Y 847



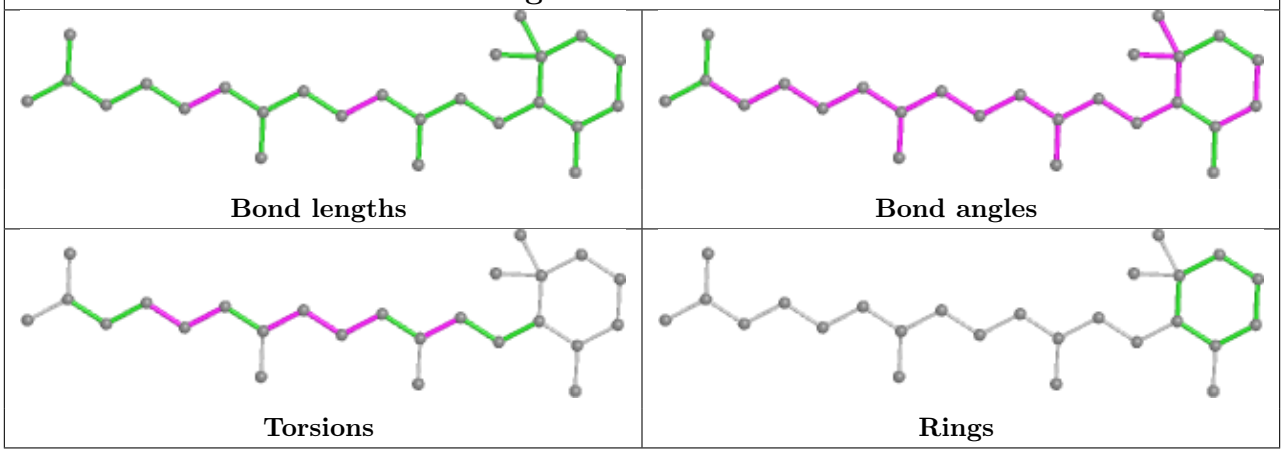
Ligand BCR R 101



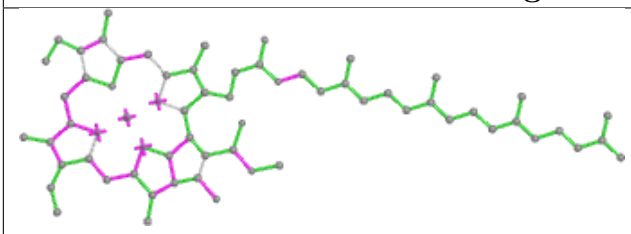
Ligand BCR A 846



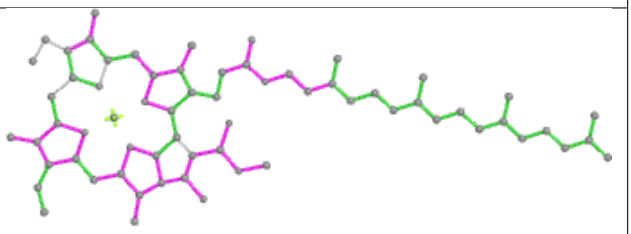
Ligand BCR Z 846



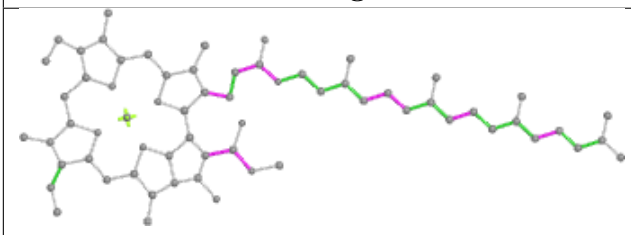
Ligand CLA A 829



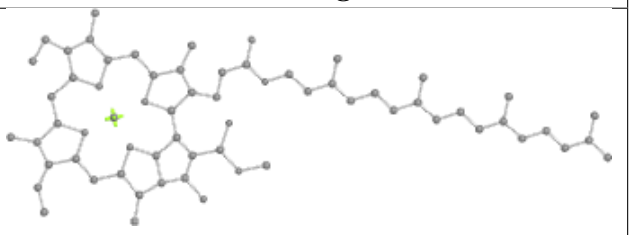
Bond lengths



Bond angles

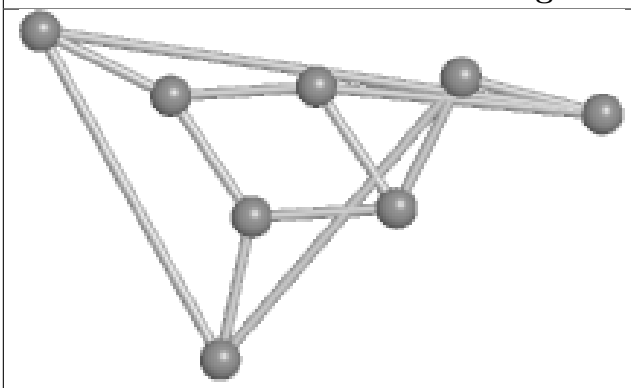


Torsions



Rings

Ligand SF4 a 101



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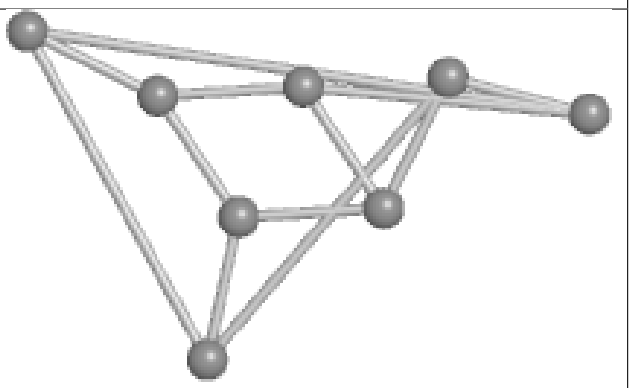
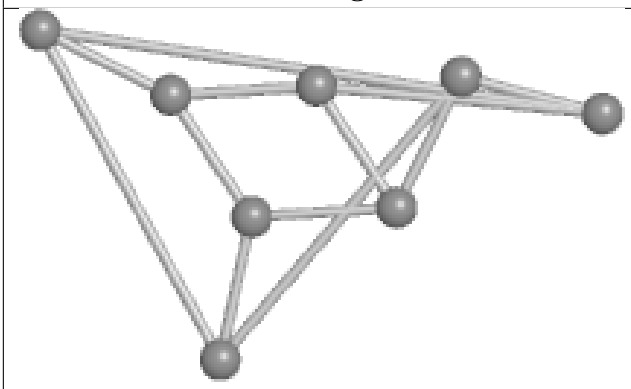


Bond angles



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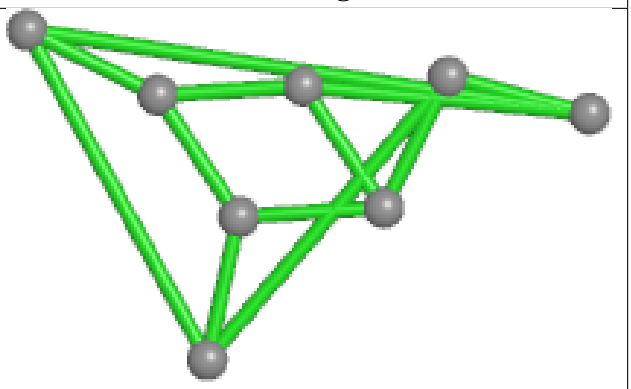
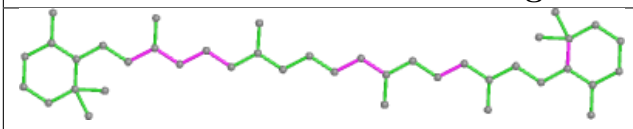


Rings

Ligand BCR h 207



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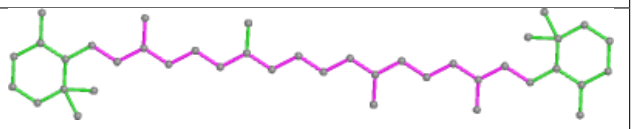
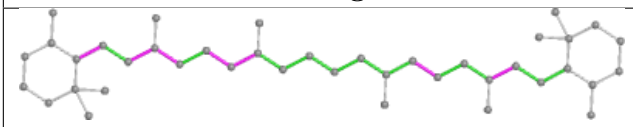


Bond angles



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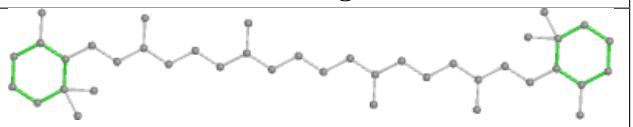
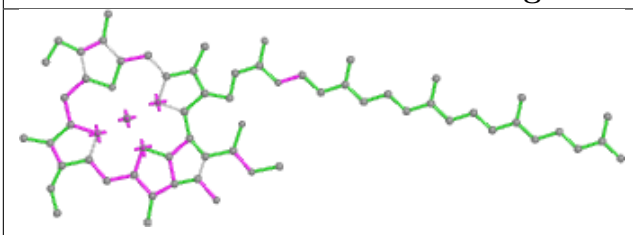


Rings

Ligand CLA Y 830



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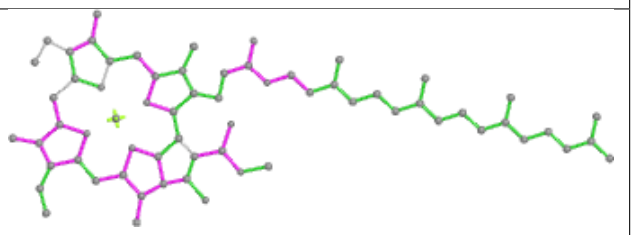
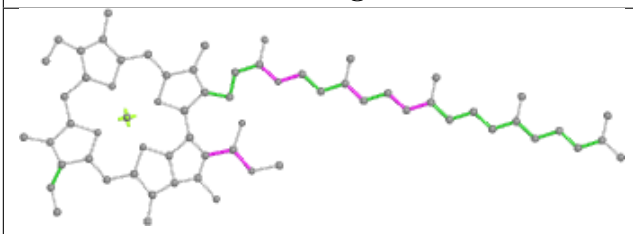
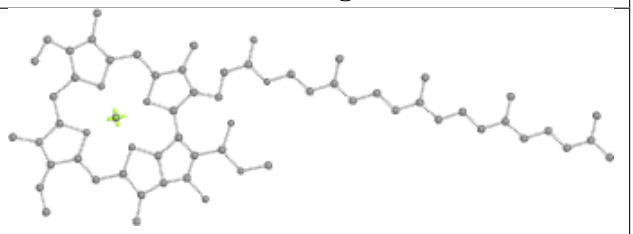


Bond angles

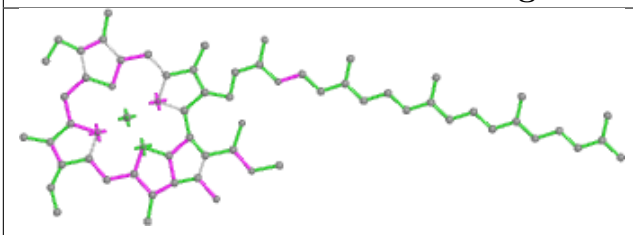


Torsions

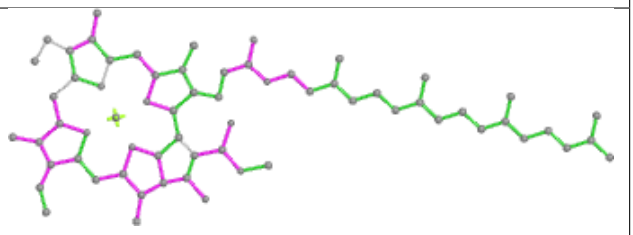


Rings

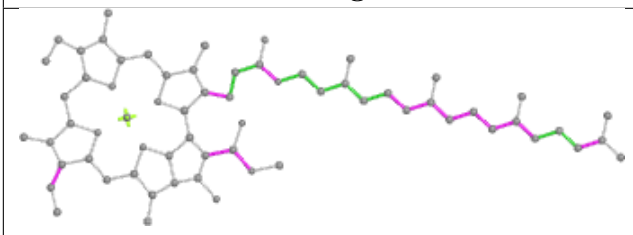
Ligand CLA S 1101



Bond lengths



Bond angles



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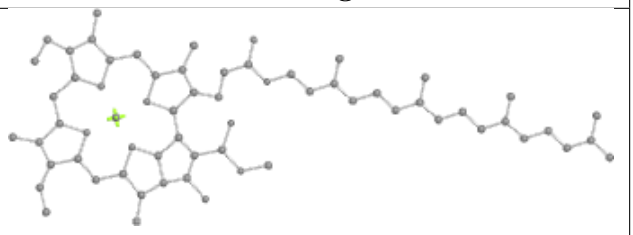
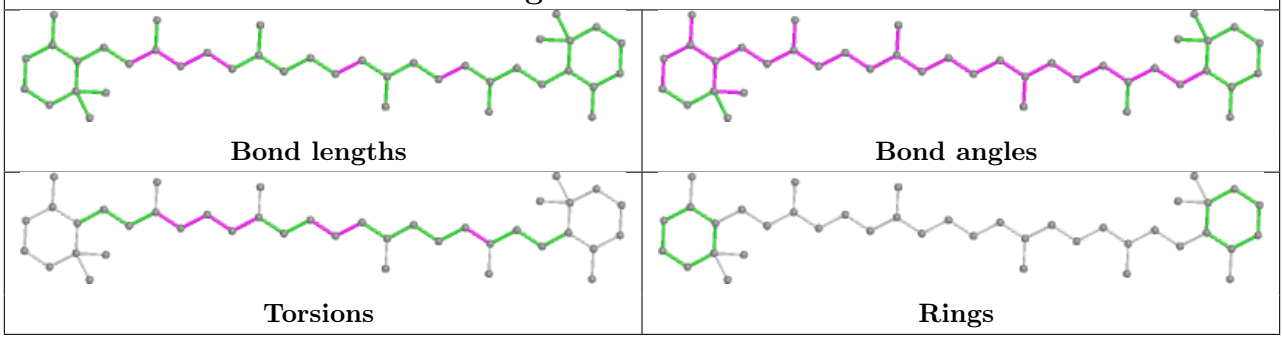
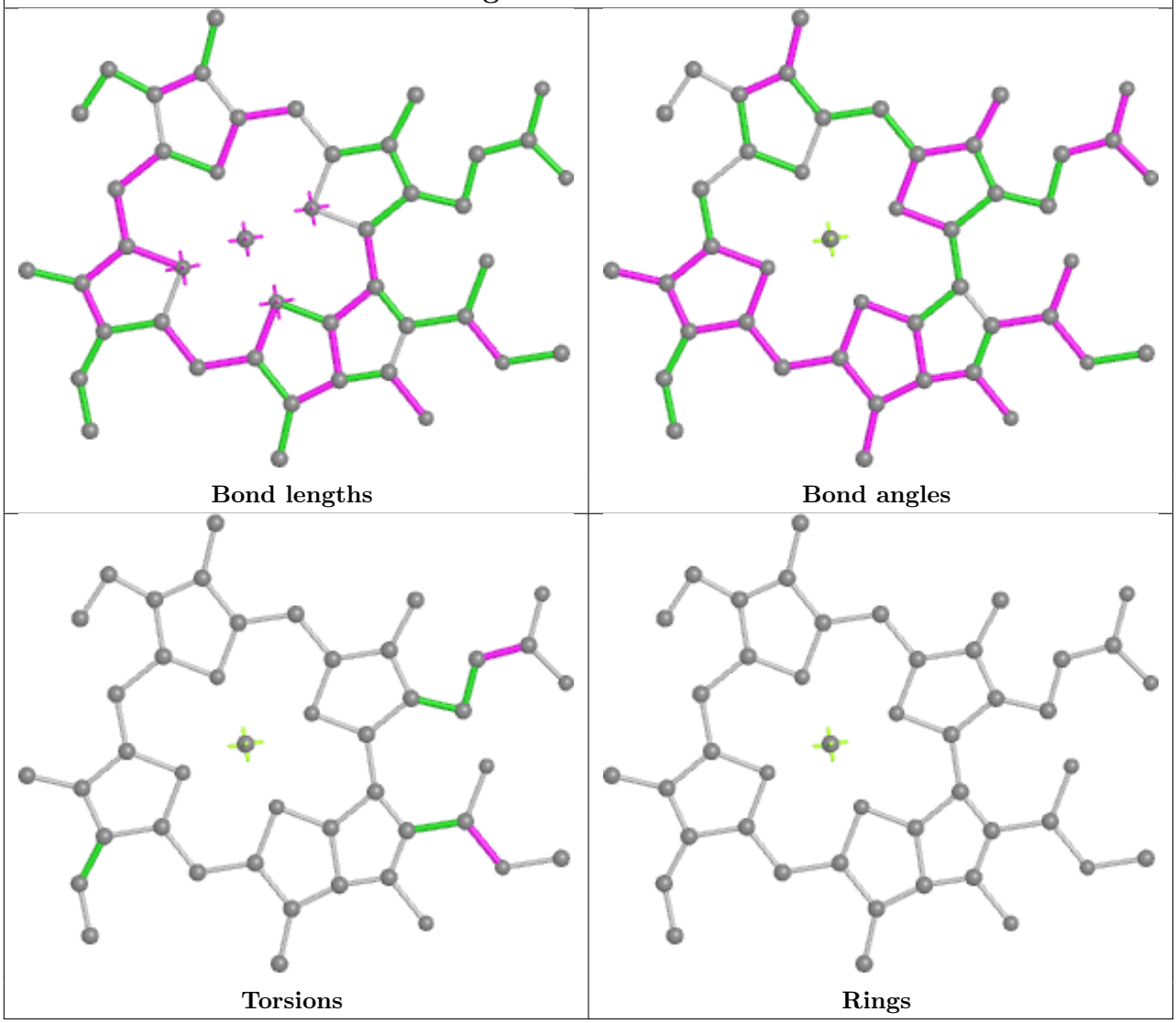


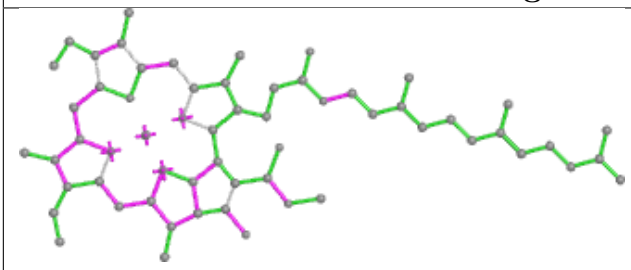
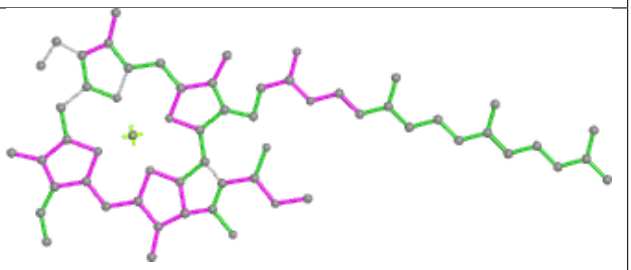
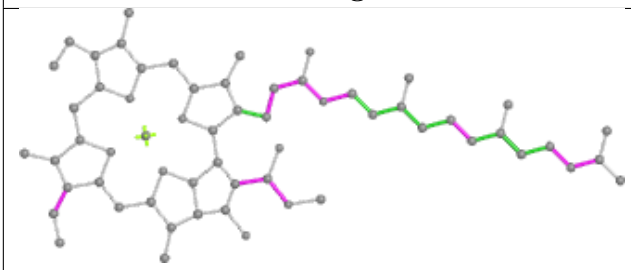
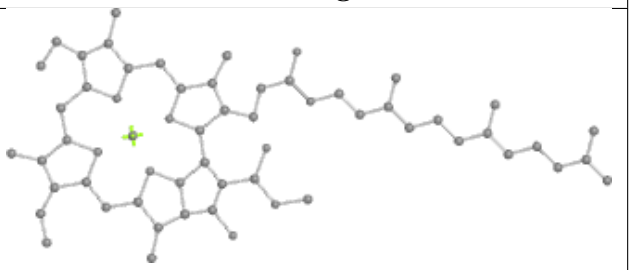
Rings

Ligand BCR Z 845



Ligand CLA F 202



Ligand CLA A 825	
 Bond lengths	 Bond angles
 Torsions	 Rings

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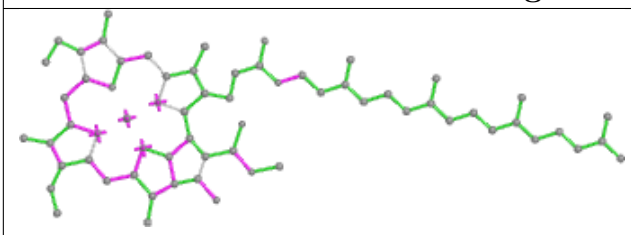
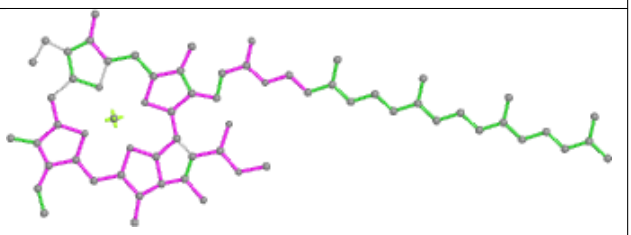
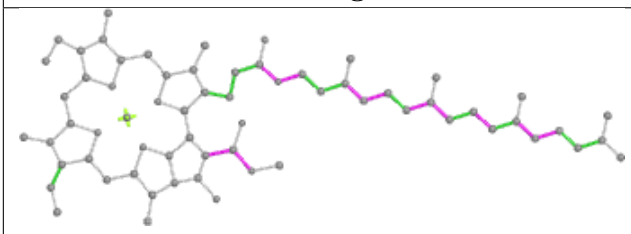
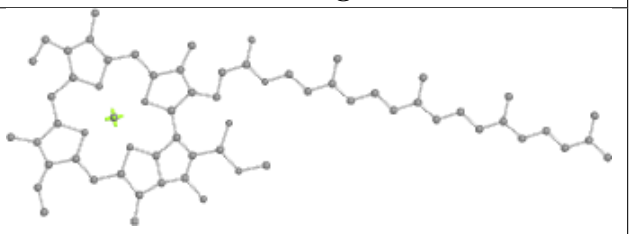
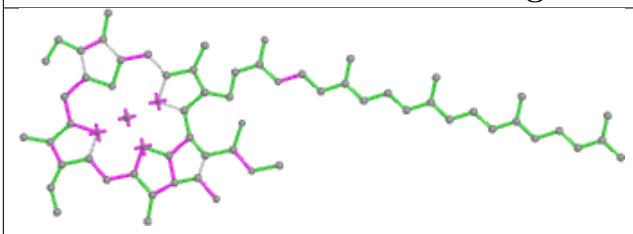
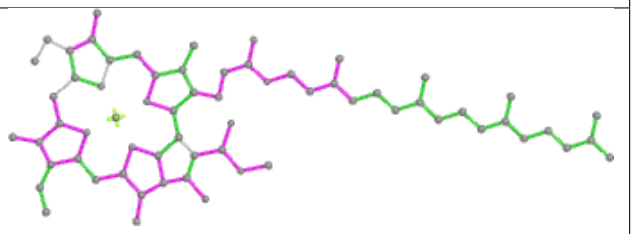
 Bond lengths	 Bond angles
 Torsions	 Rings

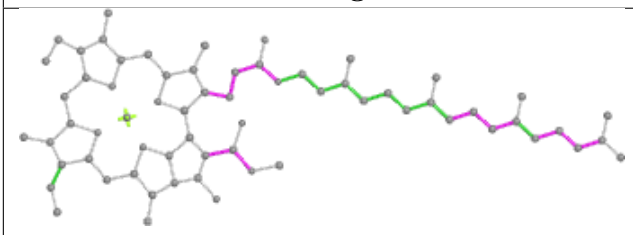
Ligand CLA Z 803



Bond lengths



Bond angles



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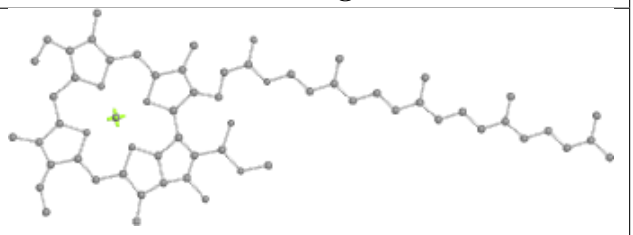
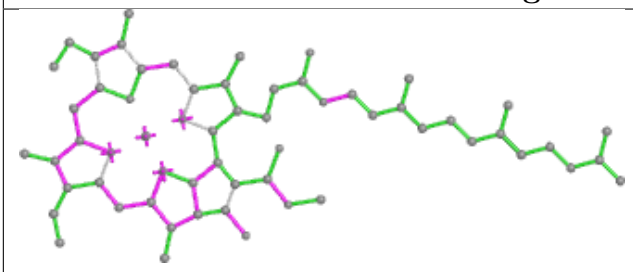


Rings

Ligand CLA G 820



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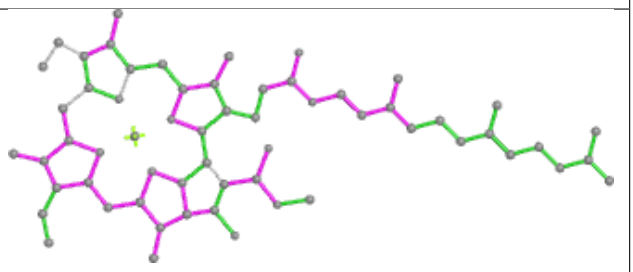
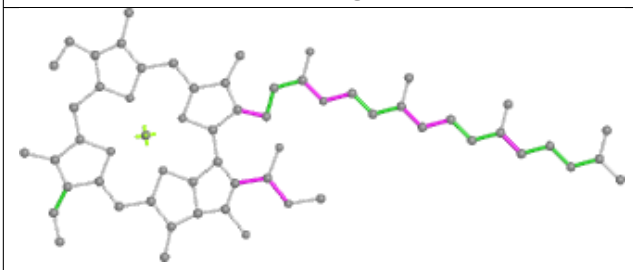


Bond angles



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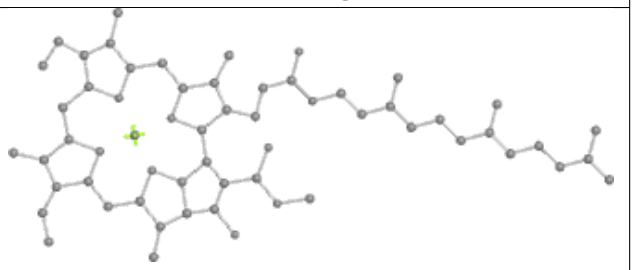
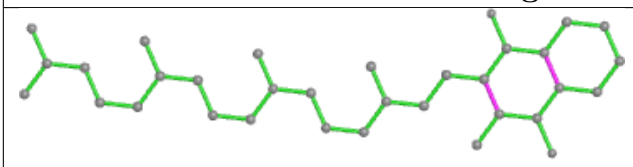


Rings

Ligand PQN Y 842



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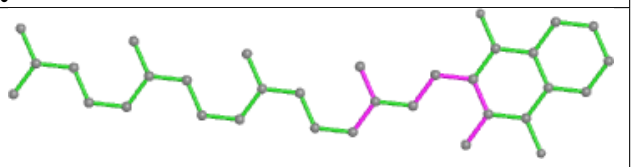
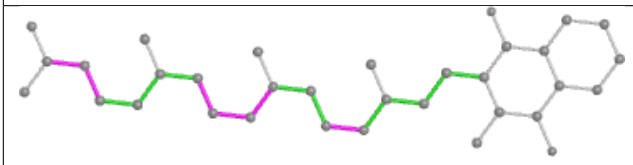


Bond angles



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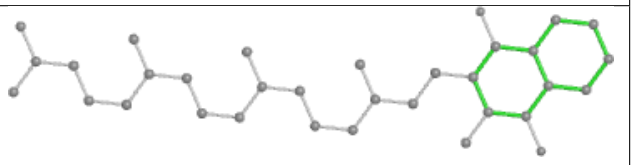
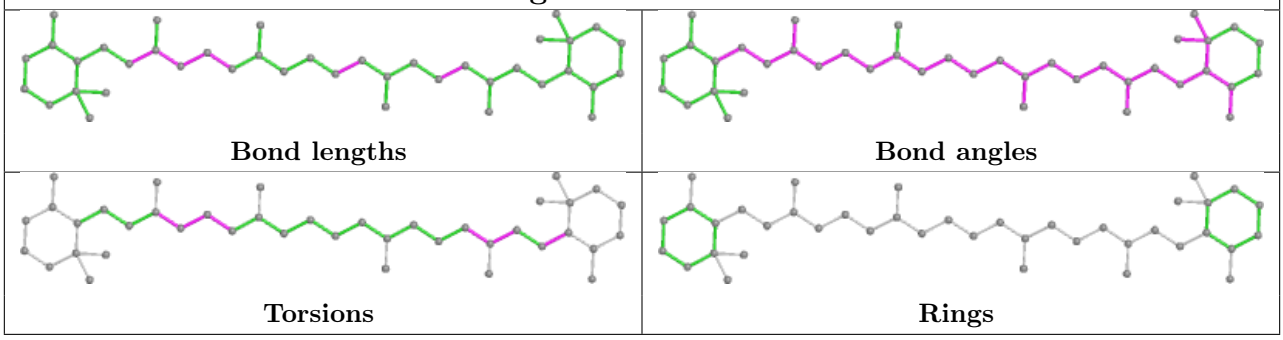
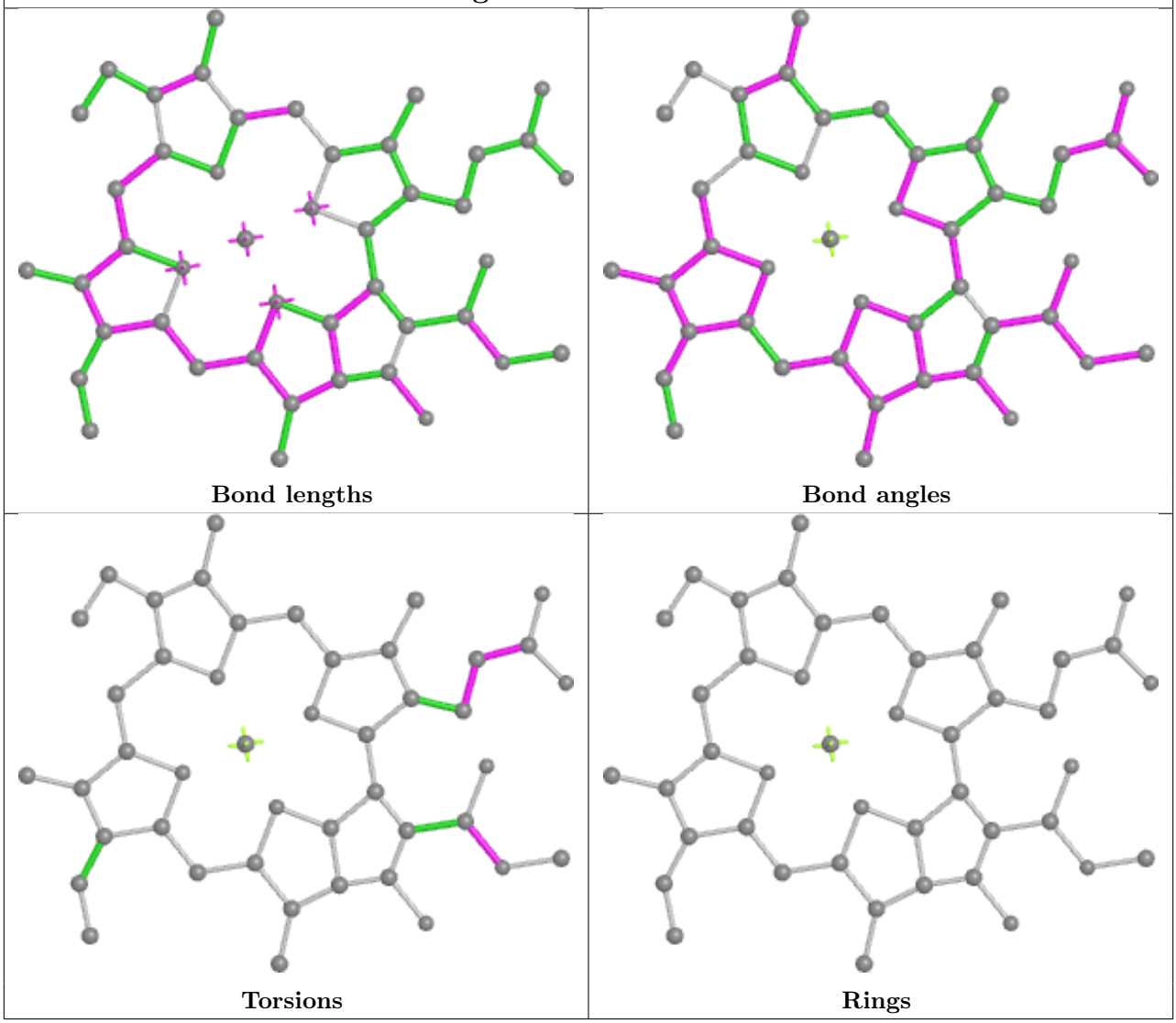


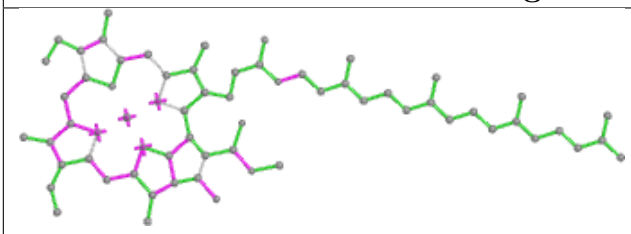
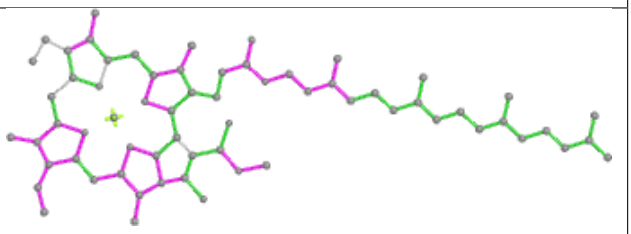
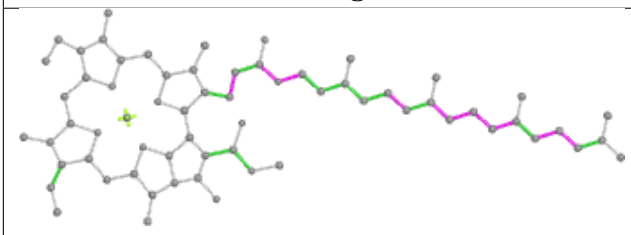
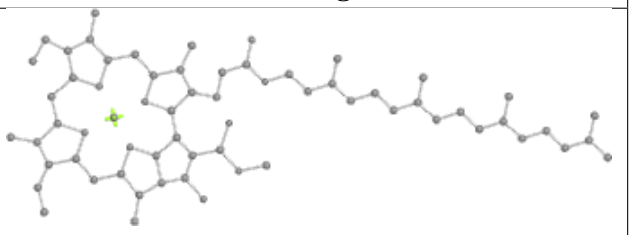
Rings

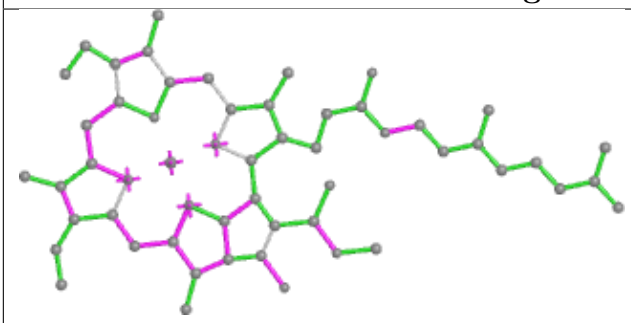
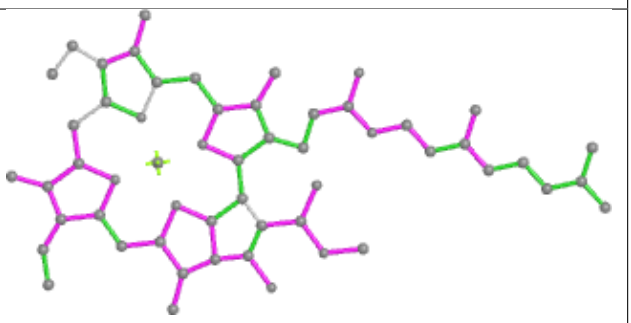
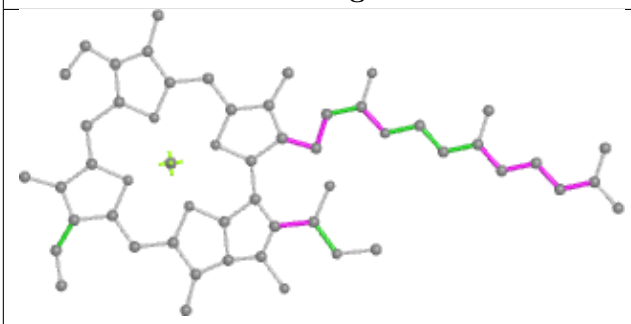
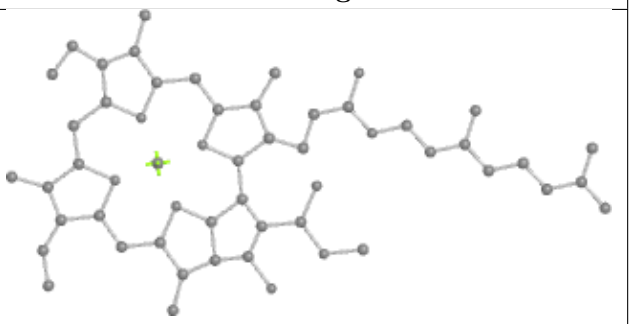
Ligand BCR I 102



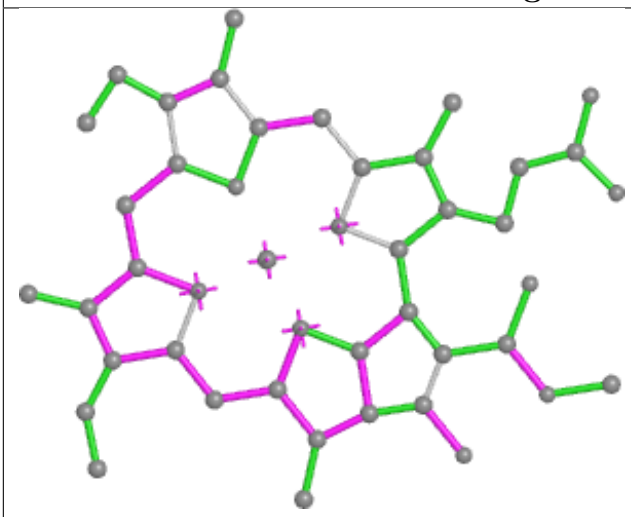
Ligand CLA X 1701



Ligand CLA A 839	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA H 816	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA Y 810



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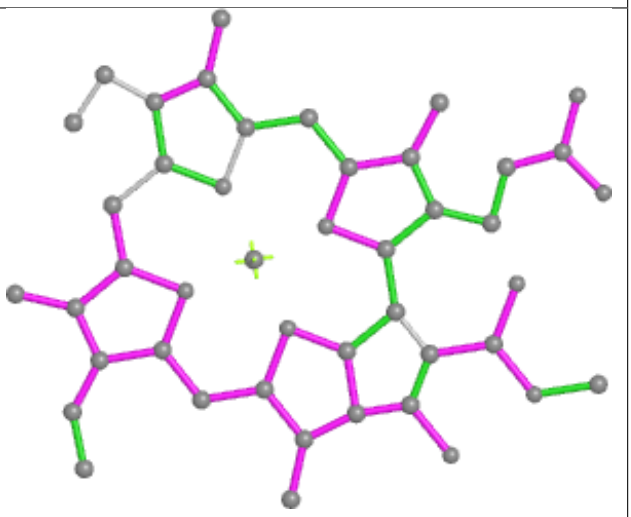
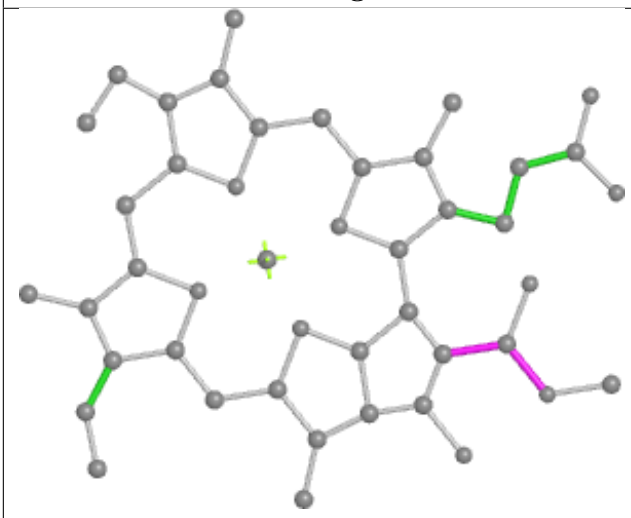
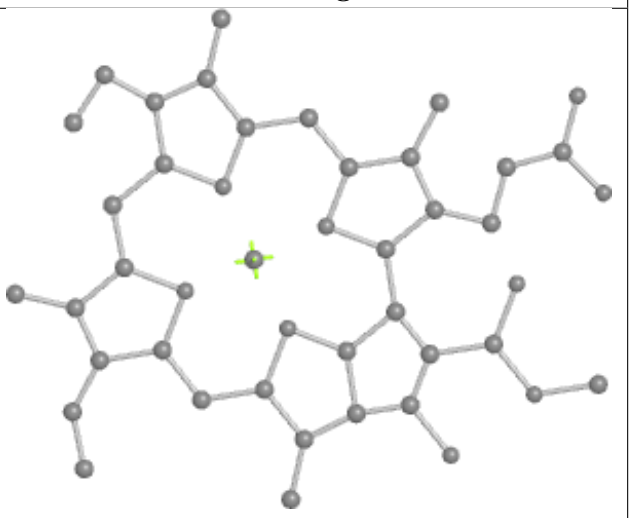


Bond angles

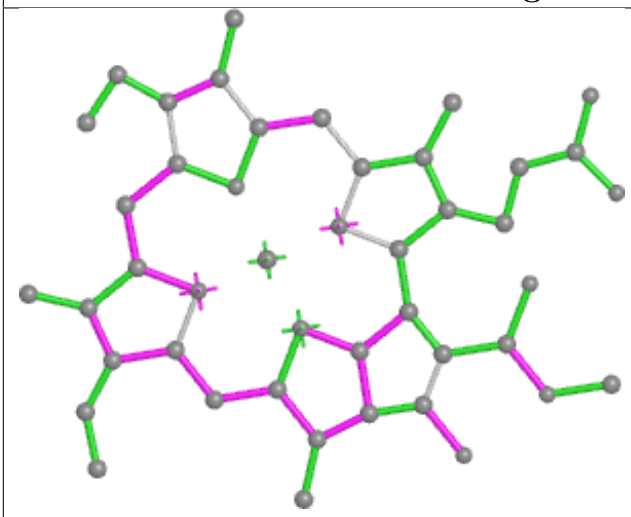


Torsions



Rings

Ligand CLA H 821



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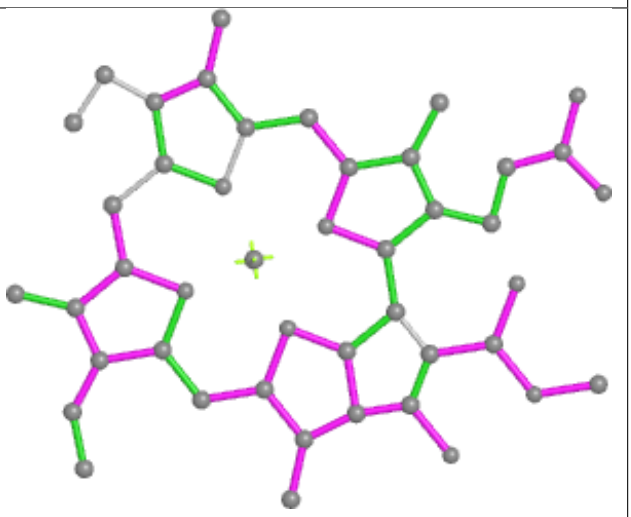

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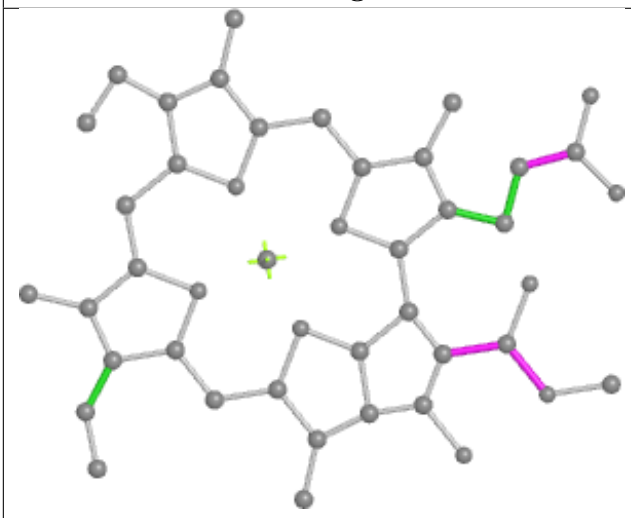

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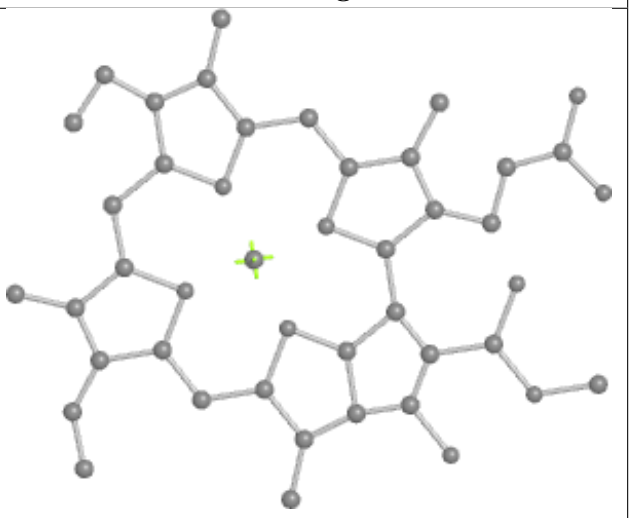
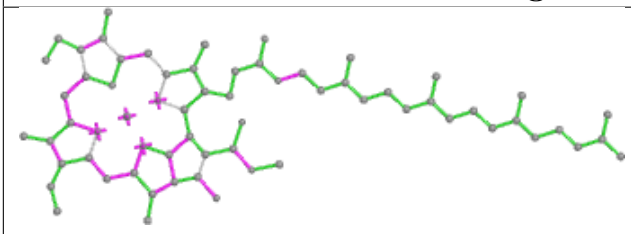


Rings

Ligand CLA h 204



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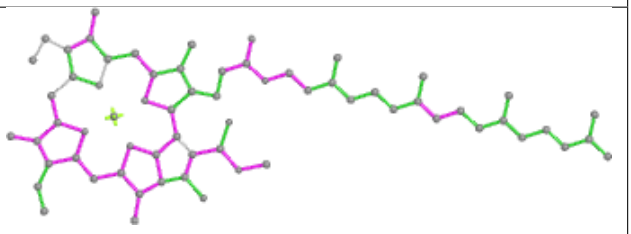

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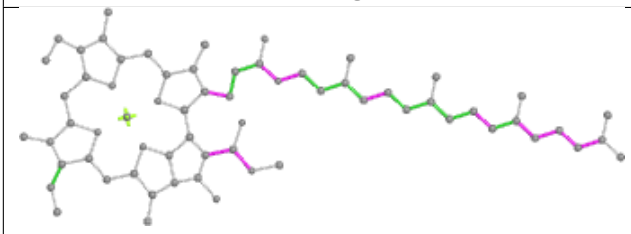

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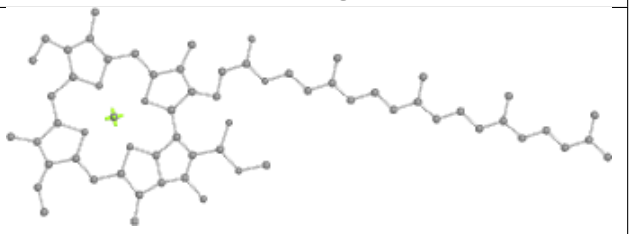
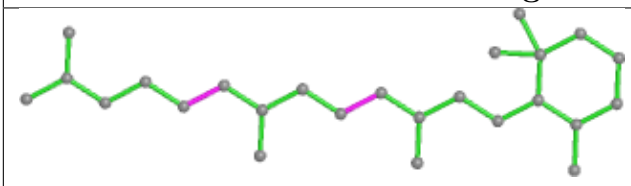


Rings

Ligand BCR B 845



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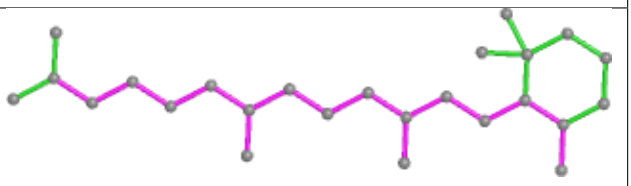
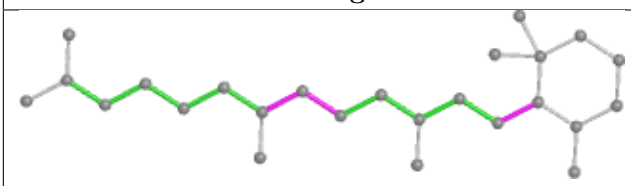


Bond angles



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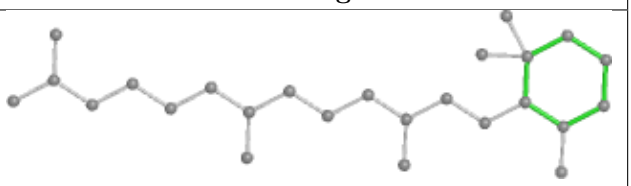
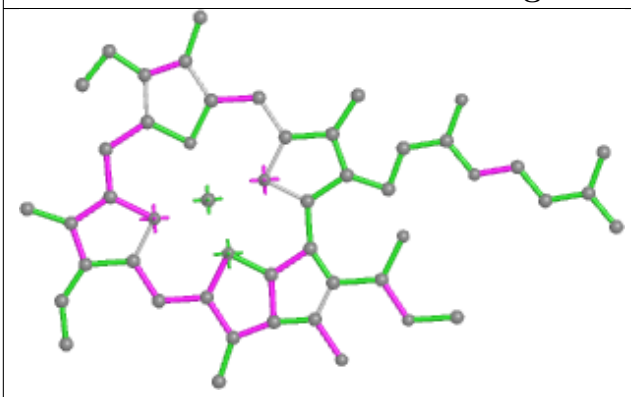


Rings

Ligand CLA Y 835



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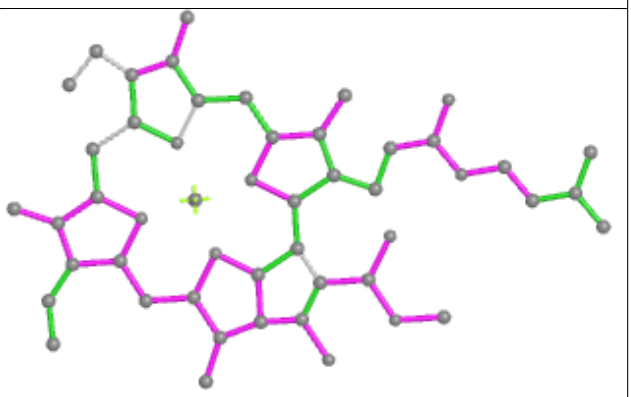
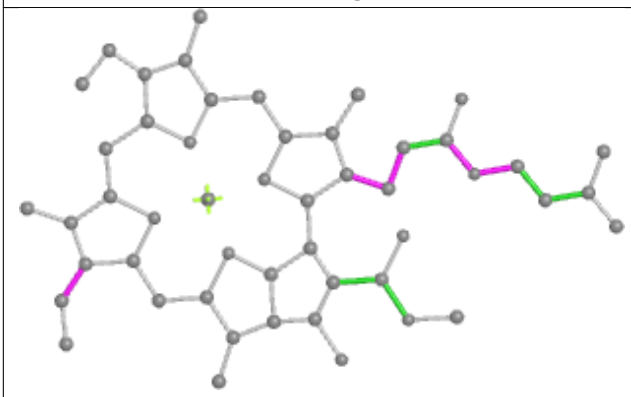


Bond angles



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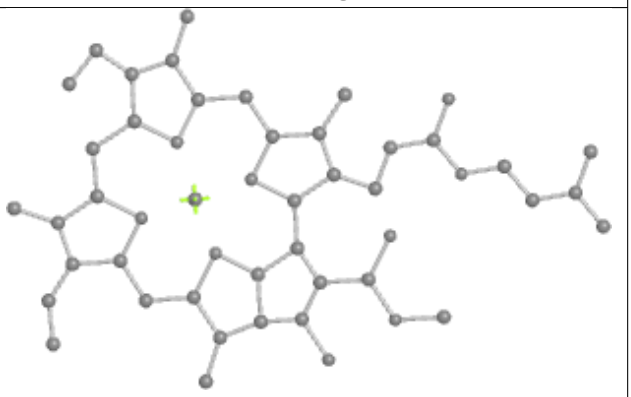
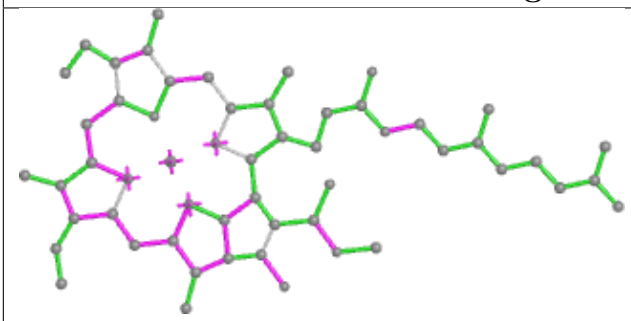


Rings

Ligand CLA B 815



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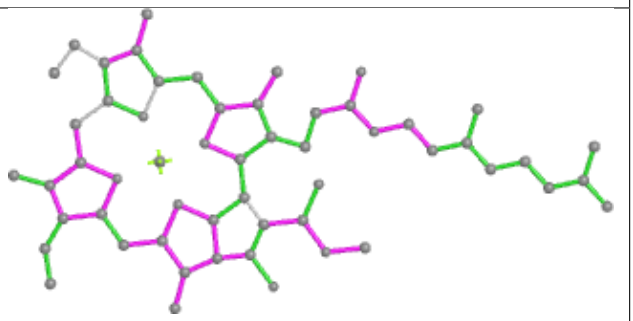
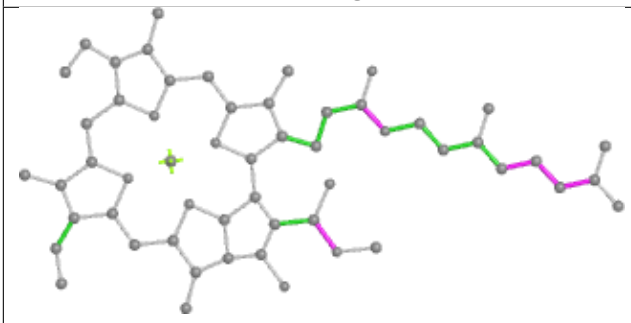
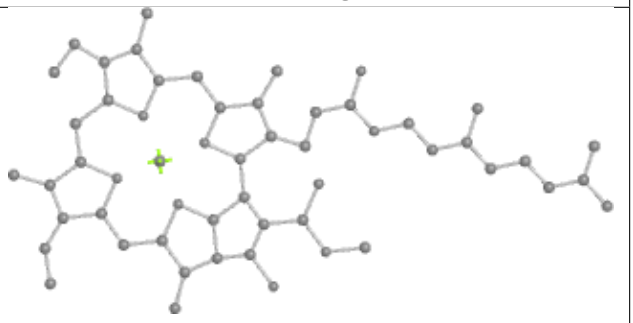


Bond angles

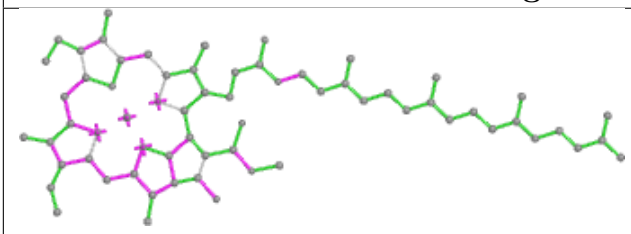


Torsions

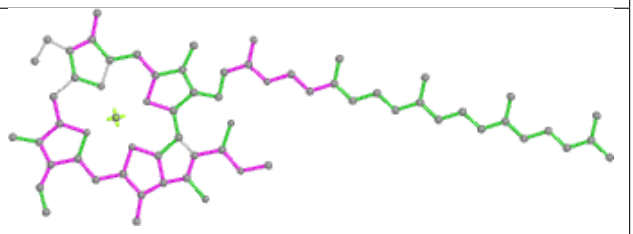


Rings

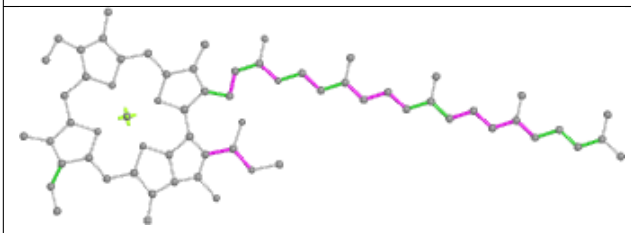
Ligand CLA G 802



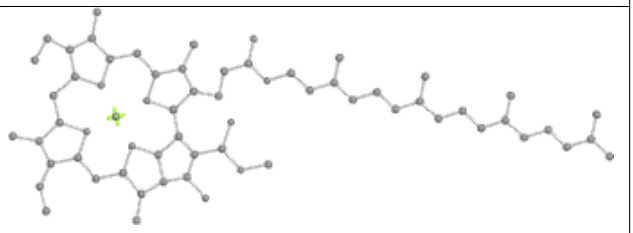
Bond lengths



Bond angles

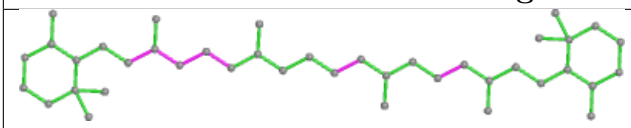


Torsions



Rings

Ligand BCR S 1104



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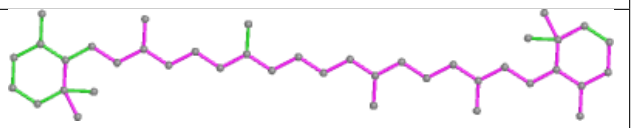
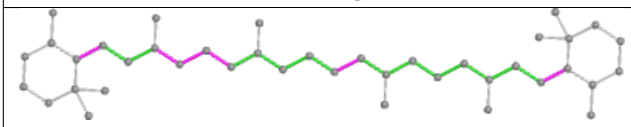
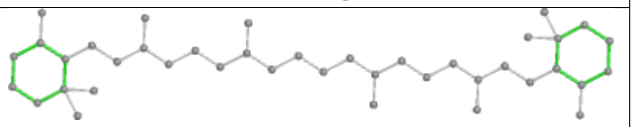


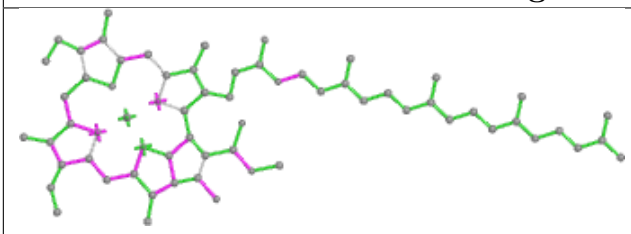
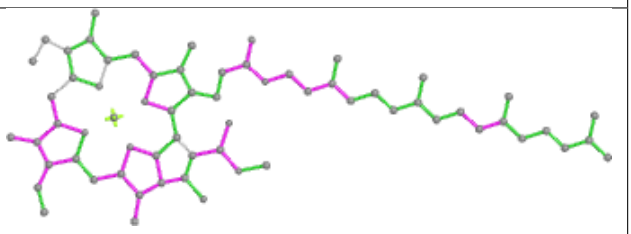
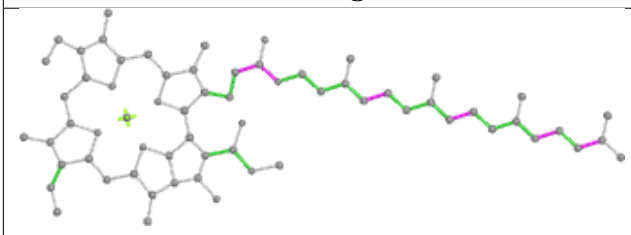
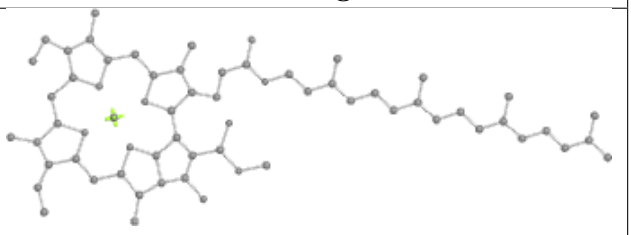
Bond angles

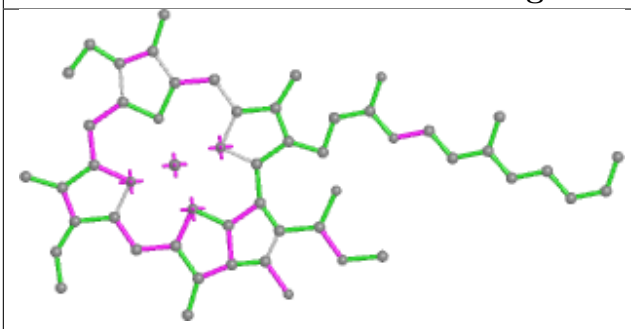
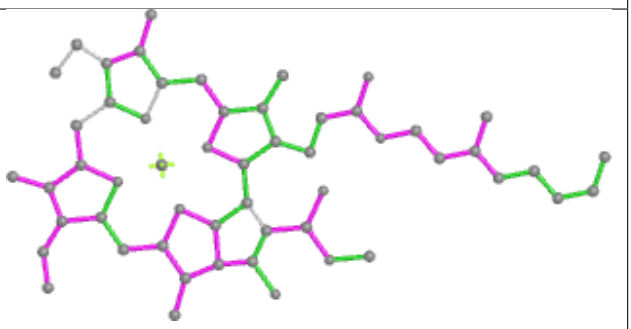
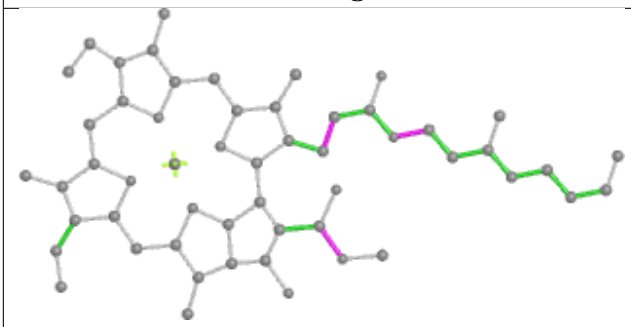
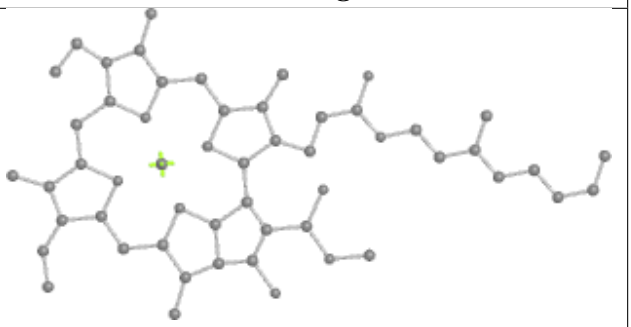


Torsions

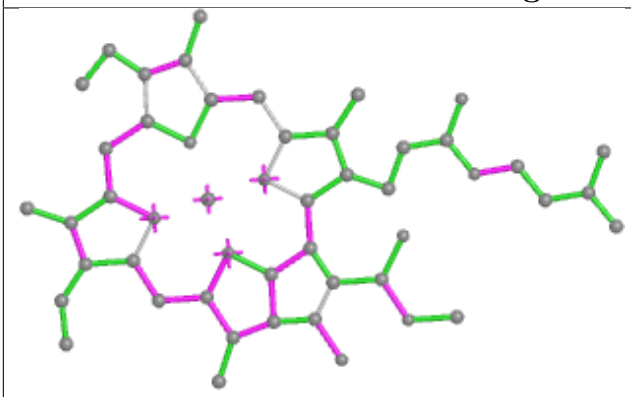


Rings

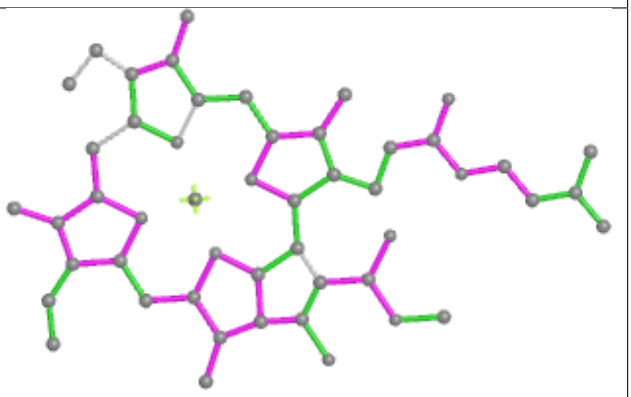
Ligand CL0 A 801	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA Z 805	
 Bond lengths	 Bond angles
 Torsions	 Rings

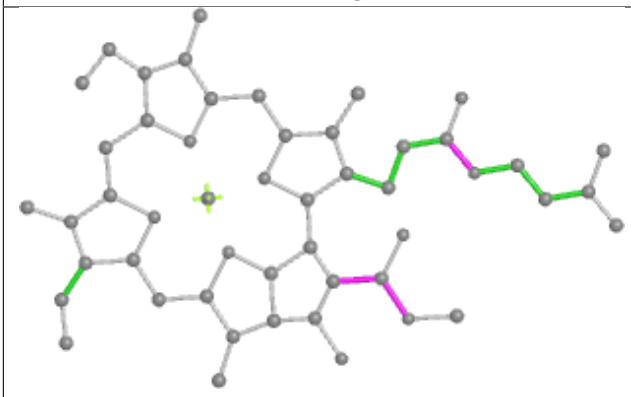
Ligand CLA G 823



Bond lengths



Bond angles



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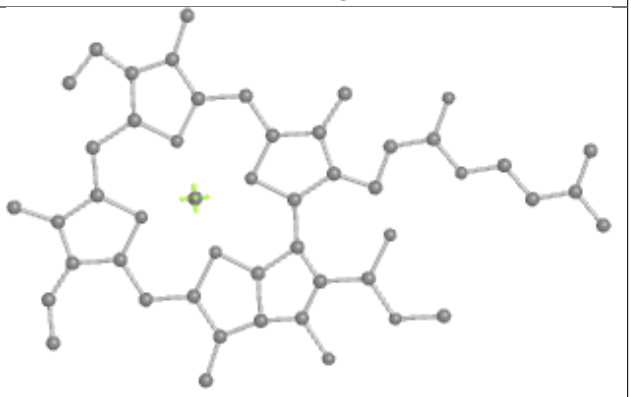
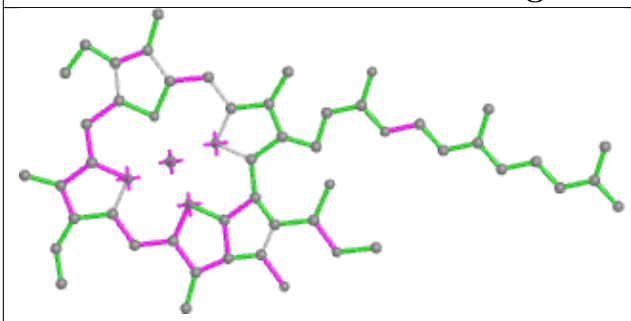


Rings

Ligand CLA Z 817



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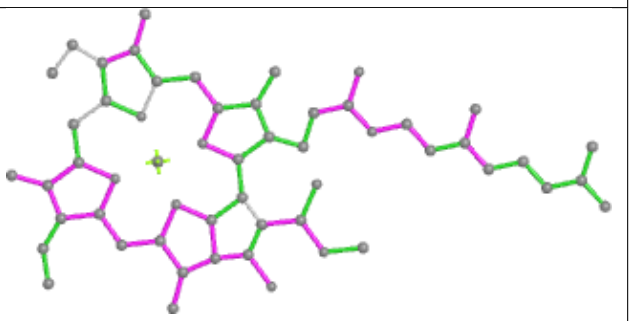
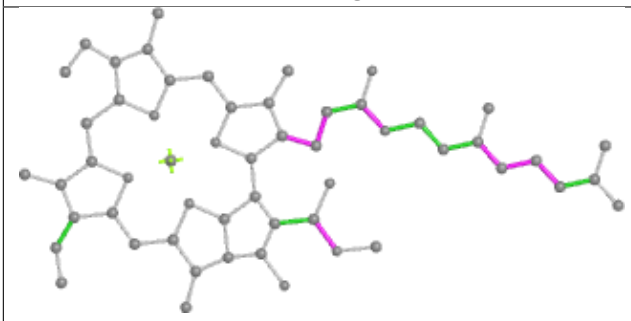


Bond angles



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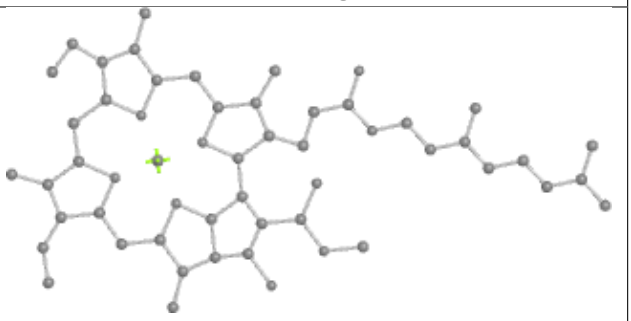
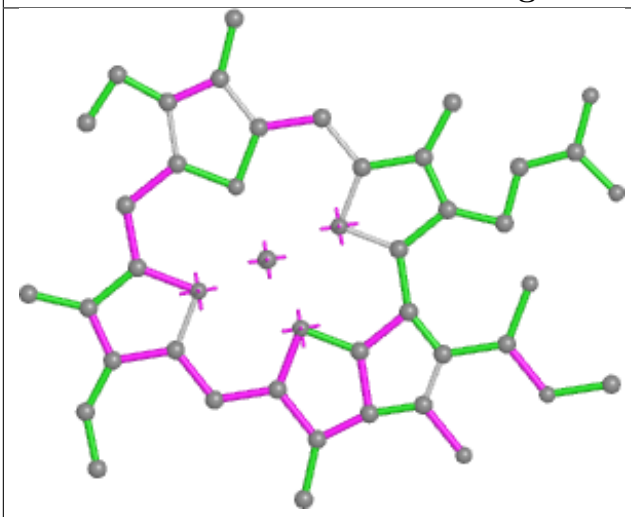
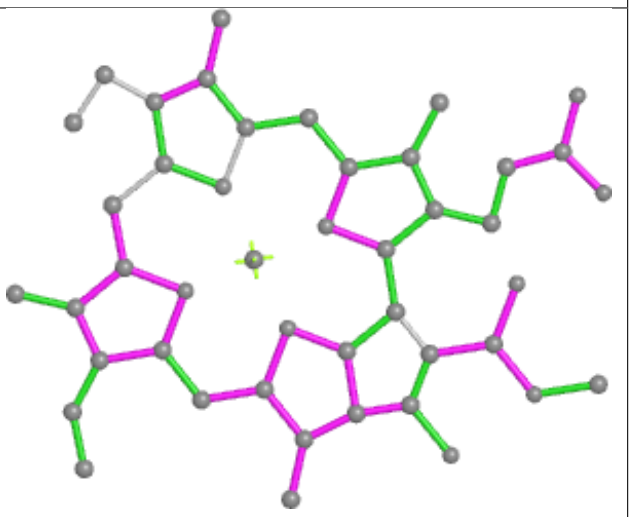


Rings

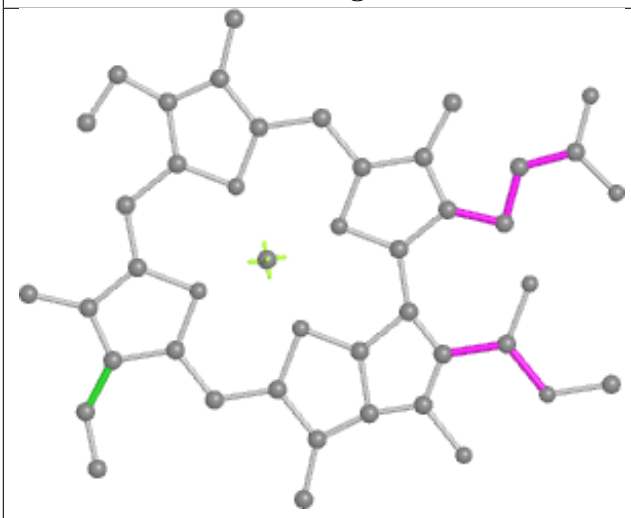
Ligand CLA S 1102



Bond lengths



Bond angles



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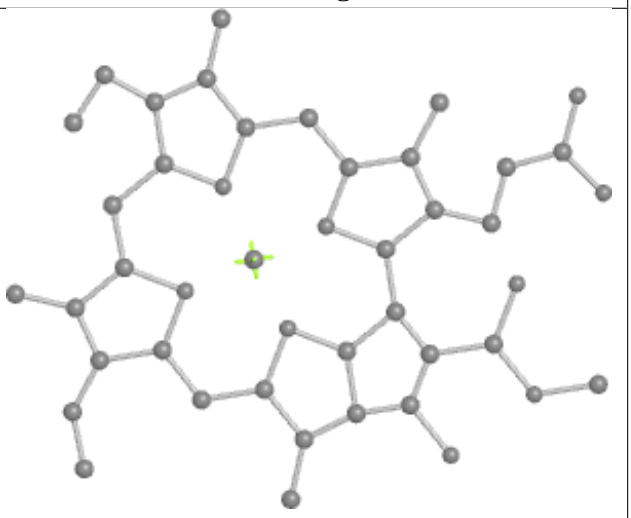
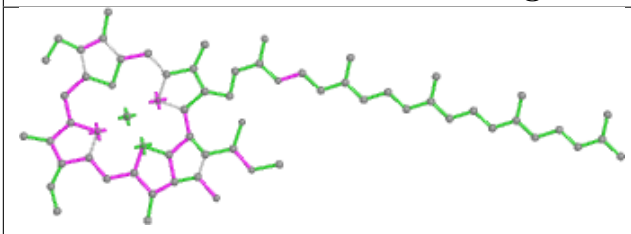


Rings

Ligand CLA A 822



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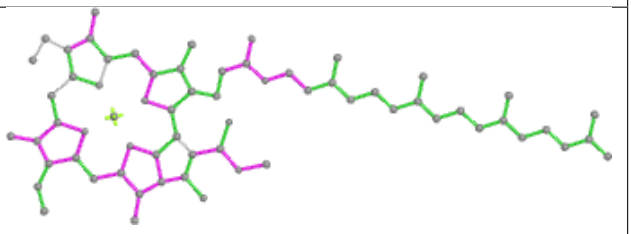
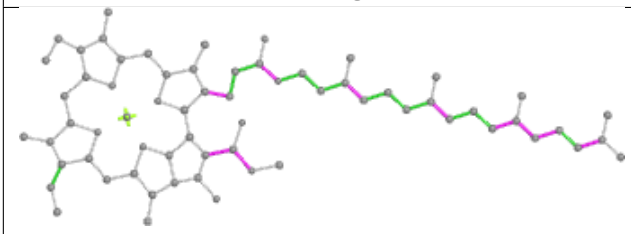


Bond angles



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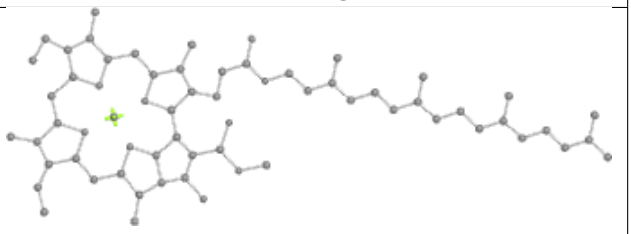
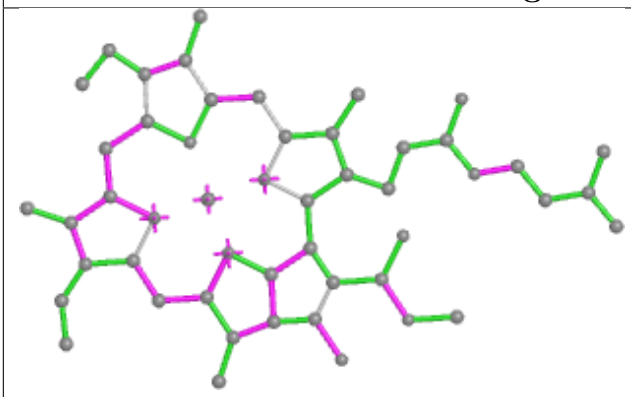
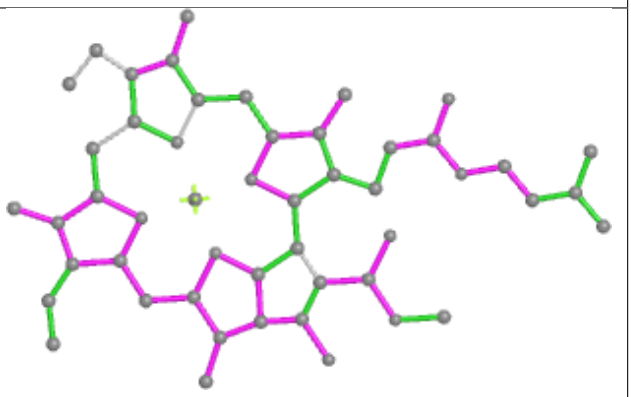
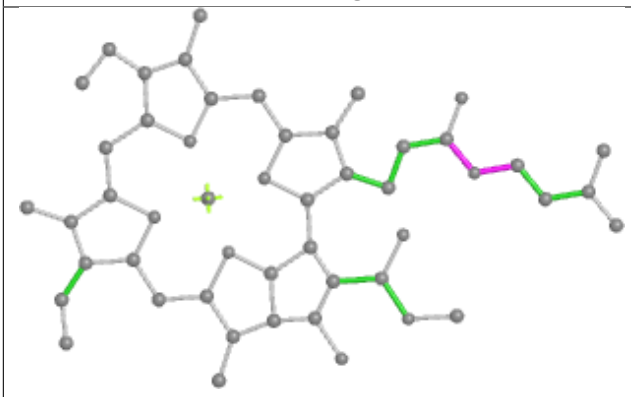
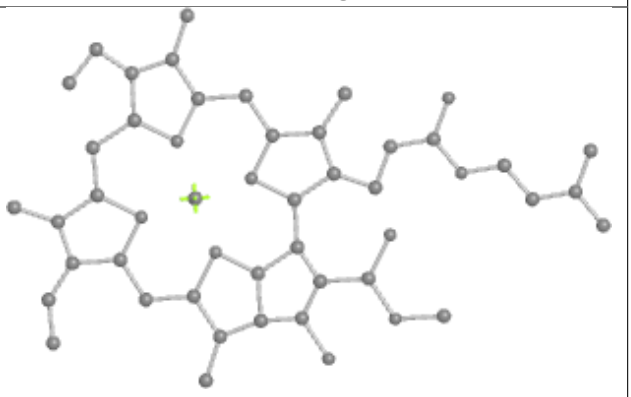
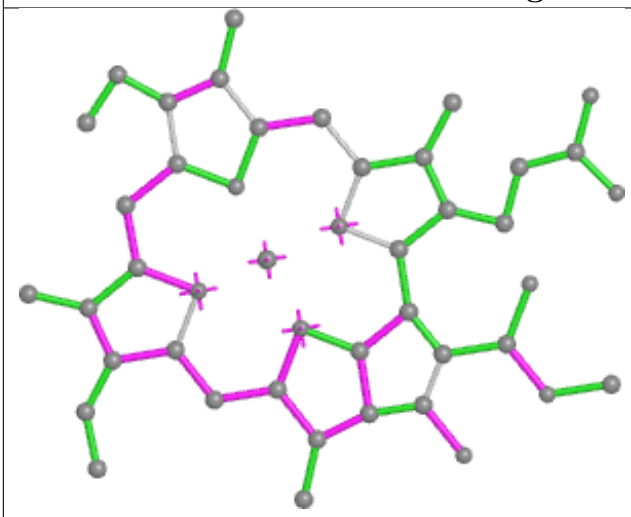


Rings

Ligand CLA A 832	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA Z 832



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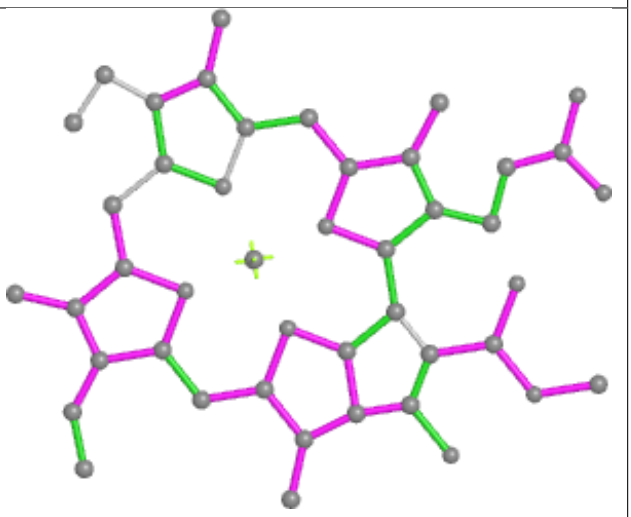
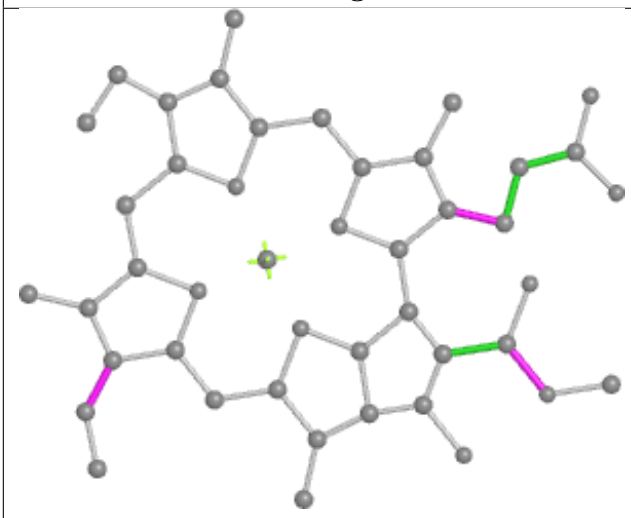


Bond angles



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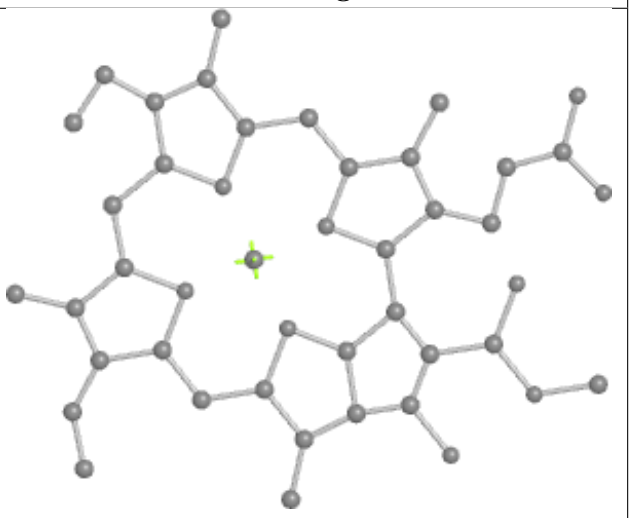
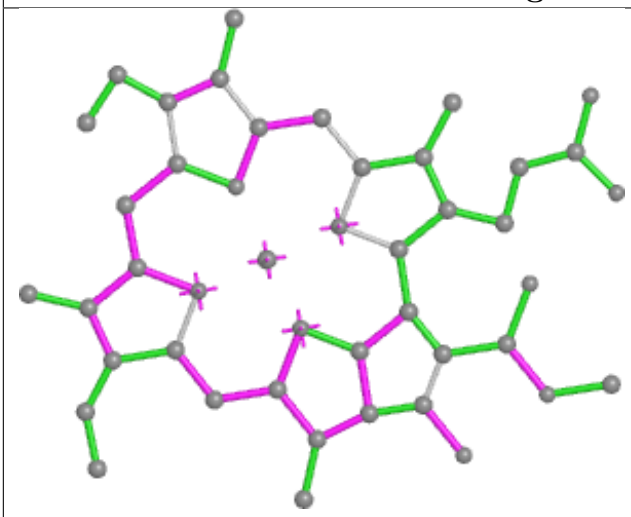


Rings

Ligand CLA Z 831



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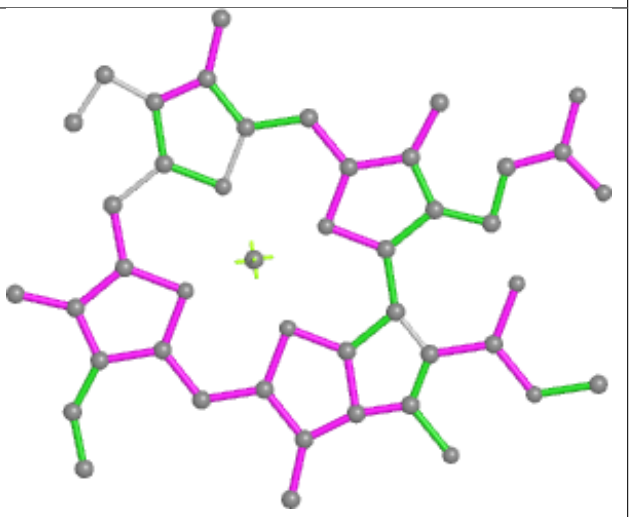
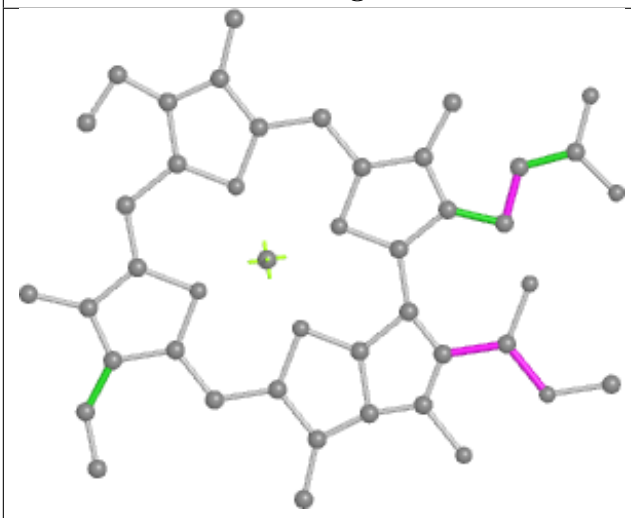


Bond angles



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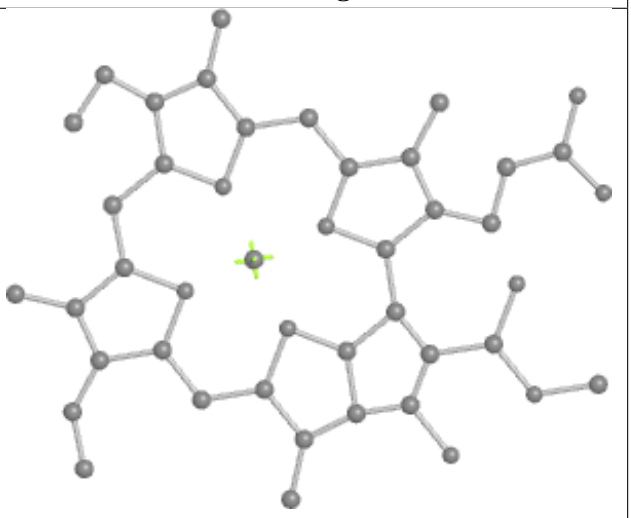
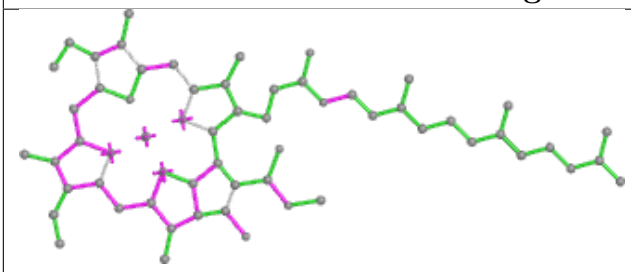
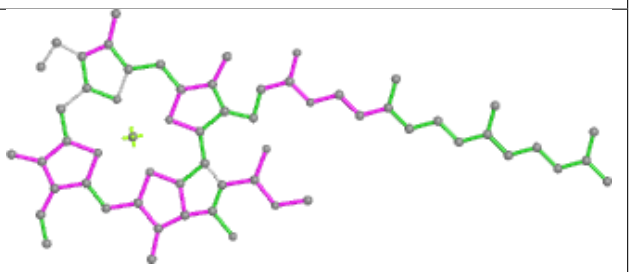


Rings

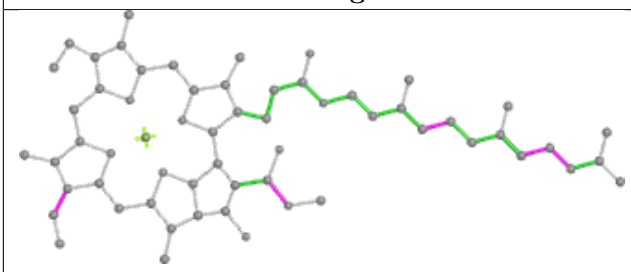
Ligand CLA Y 817



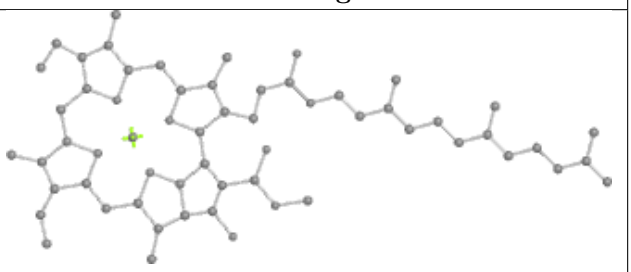
Bond lengths



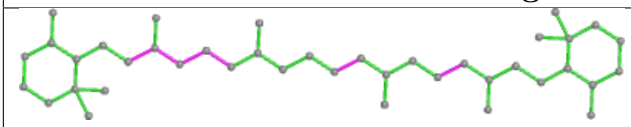
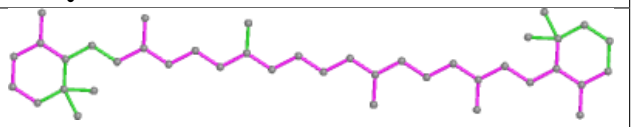
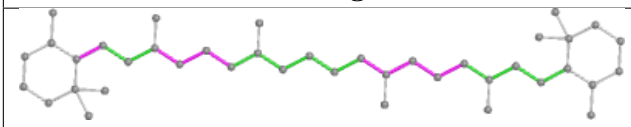
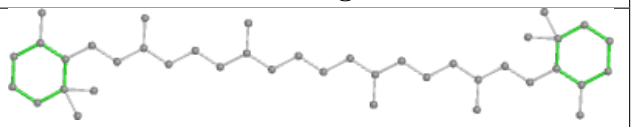
Bond angles

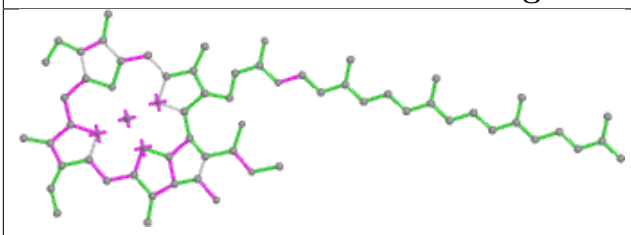
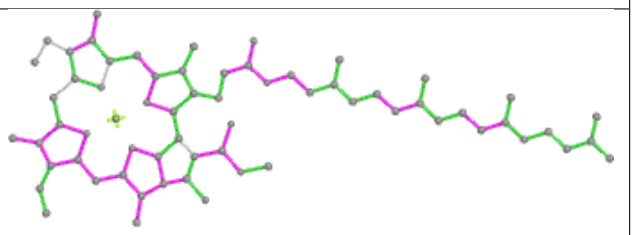
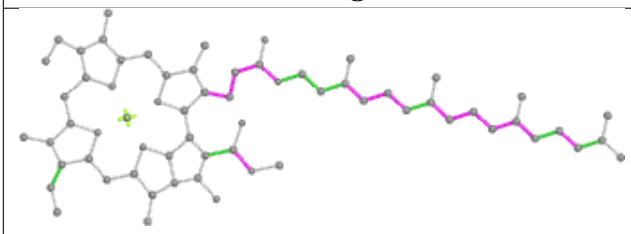
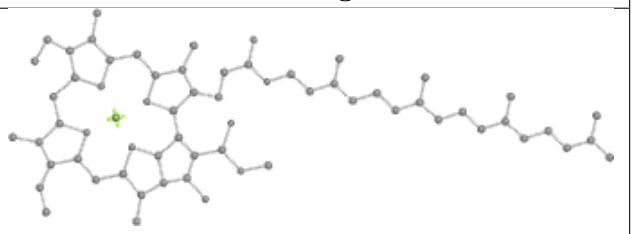


Torsions

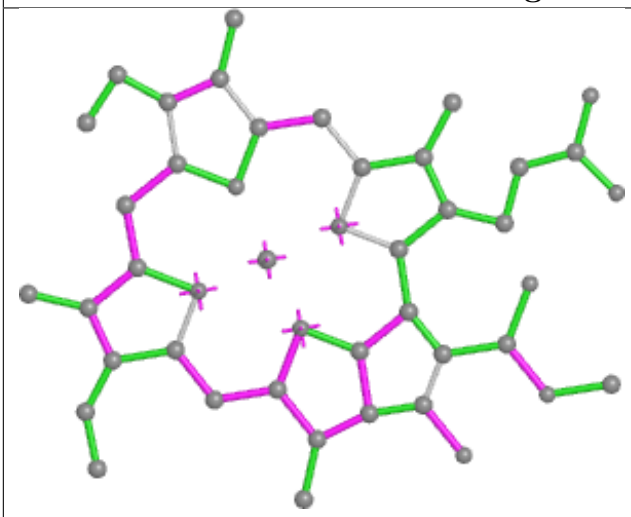


Rings

Ligand BCR Q 201	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA G 806	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA B 814



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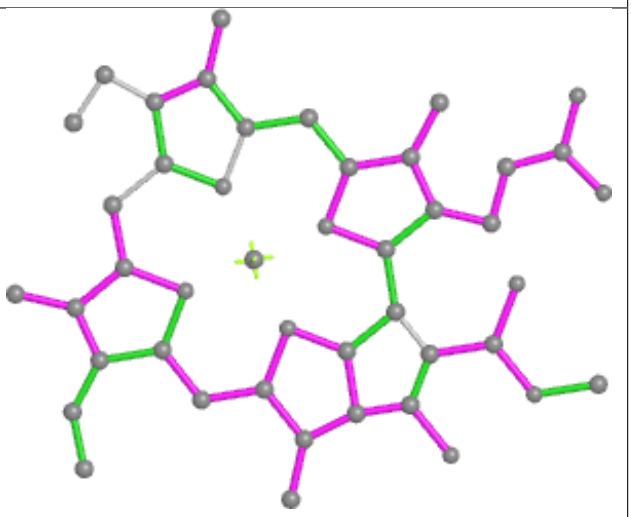
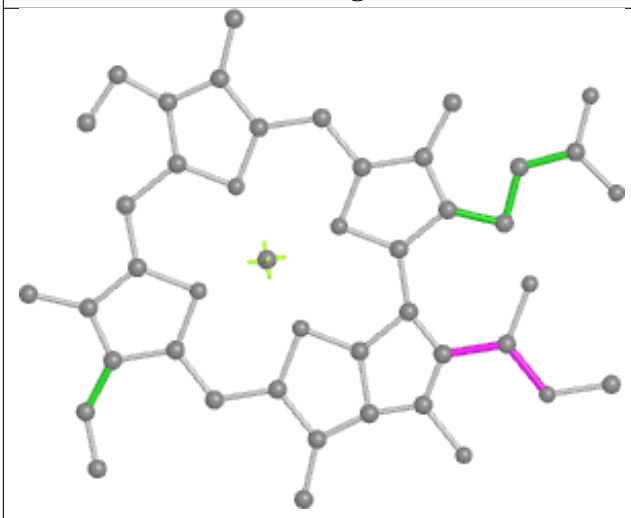


Bond angles



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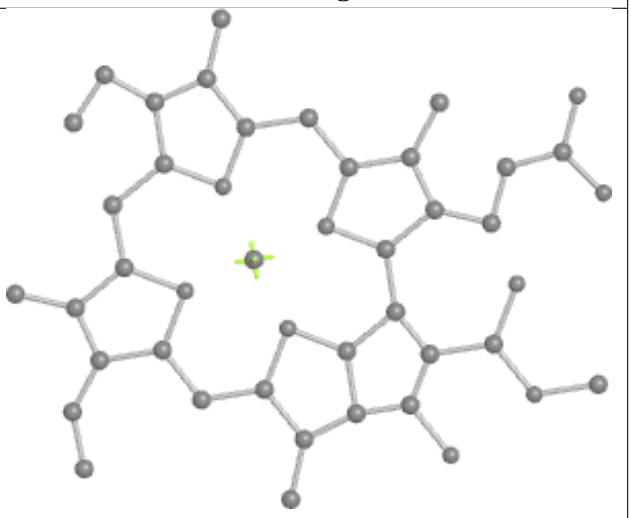

Rings

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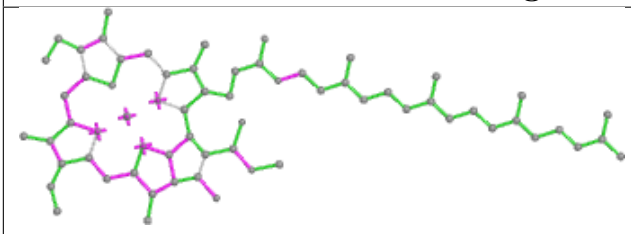

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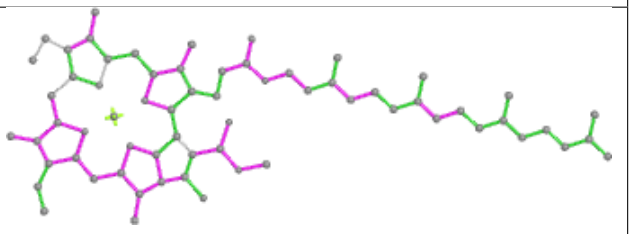
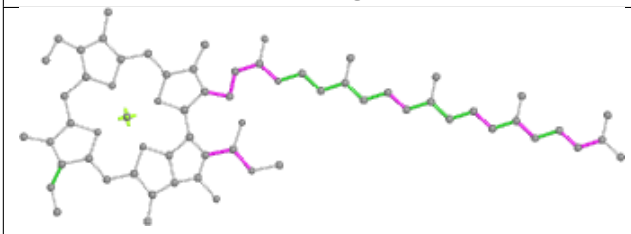


Bond angles



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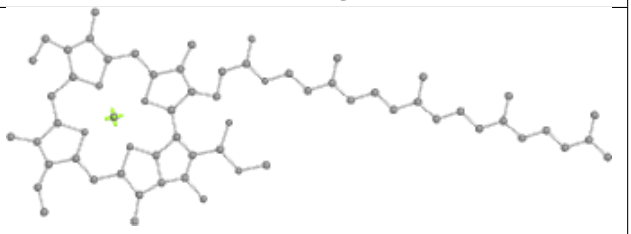
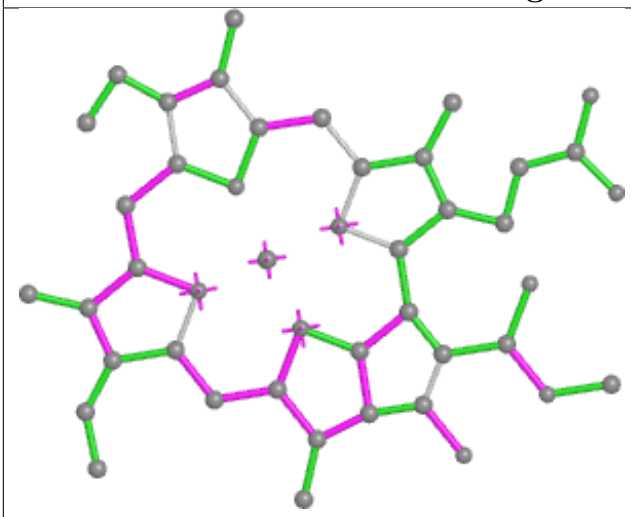


Rings

Ligand CLA Z 836



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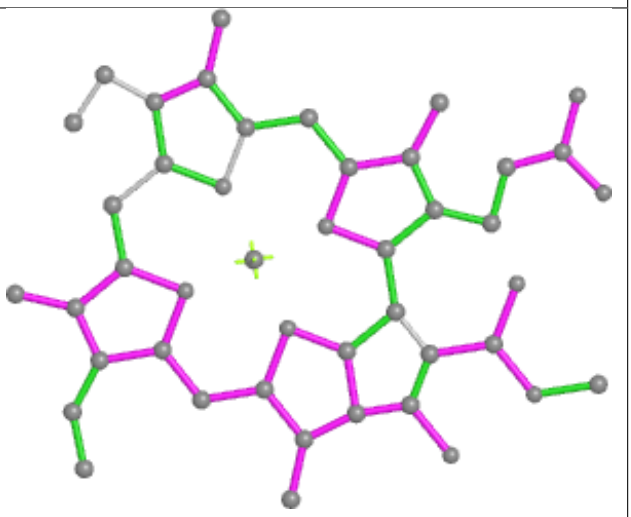
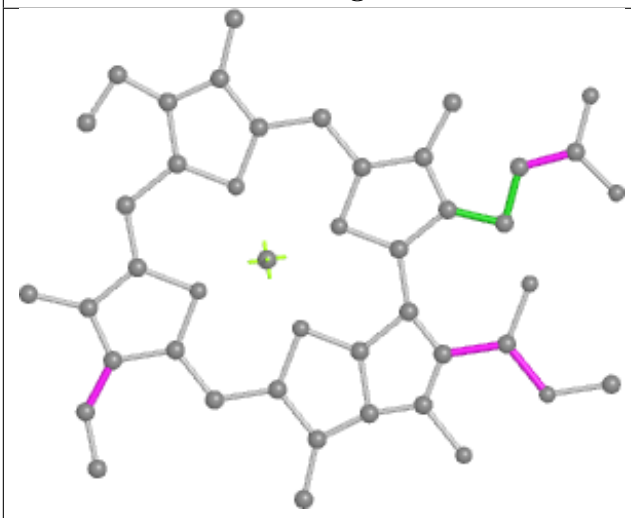


Bond angles



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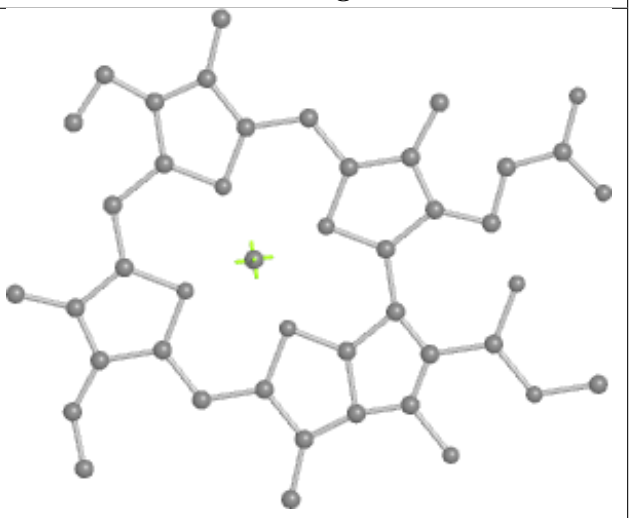

Rings

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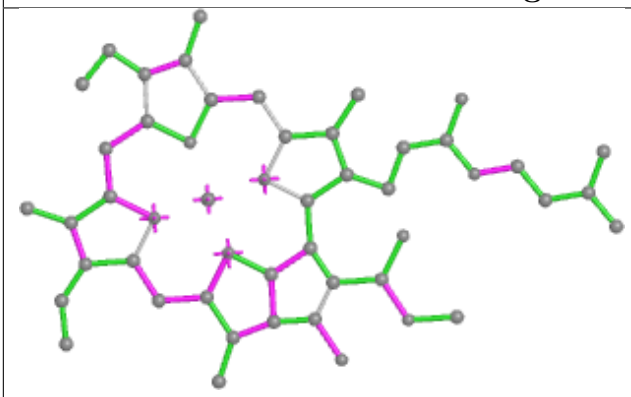
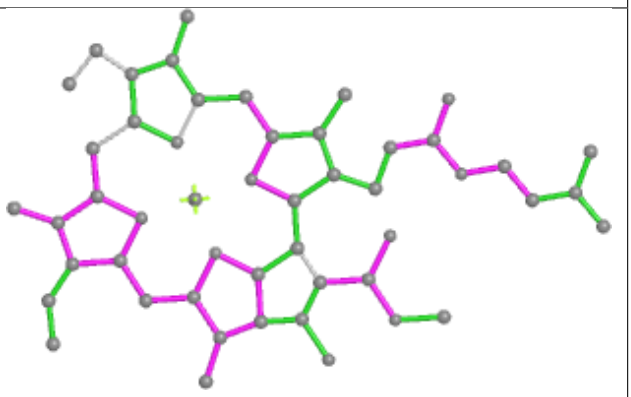
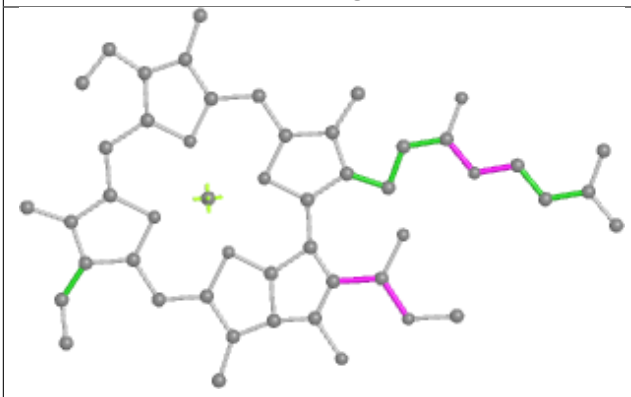
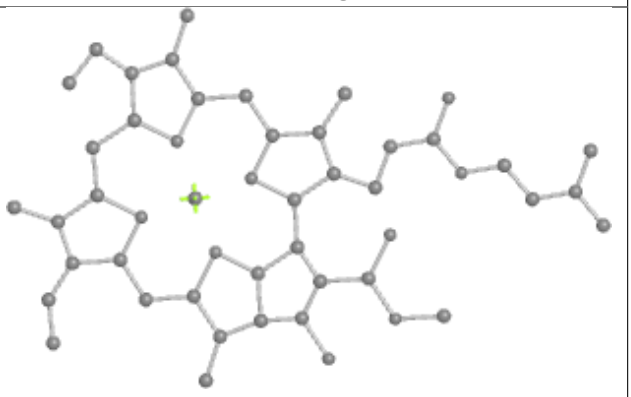
 Bond lengths	 Bond angles
 Torsions	 Rings

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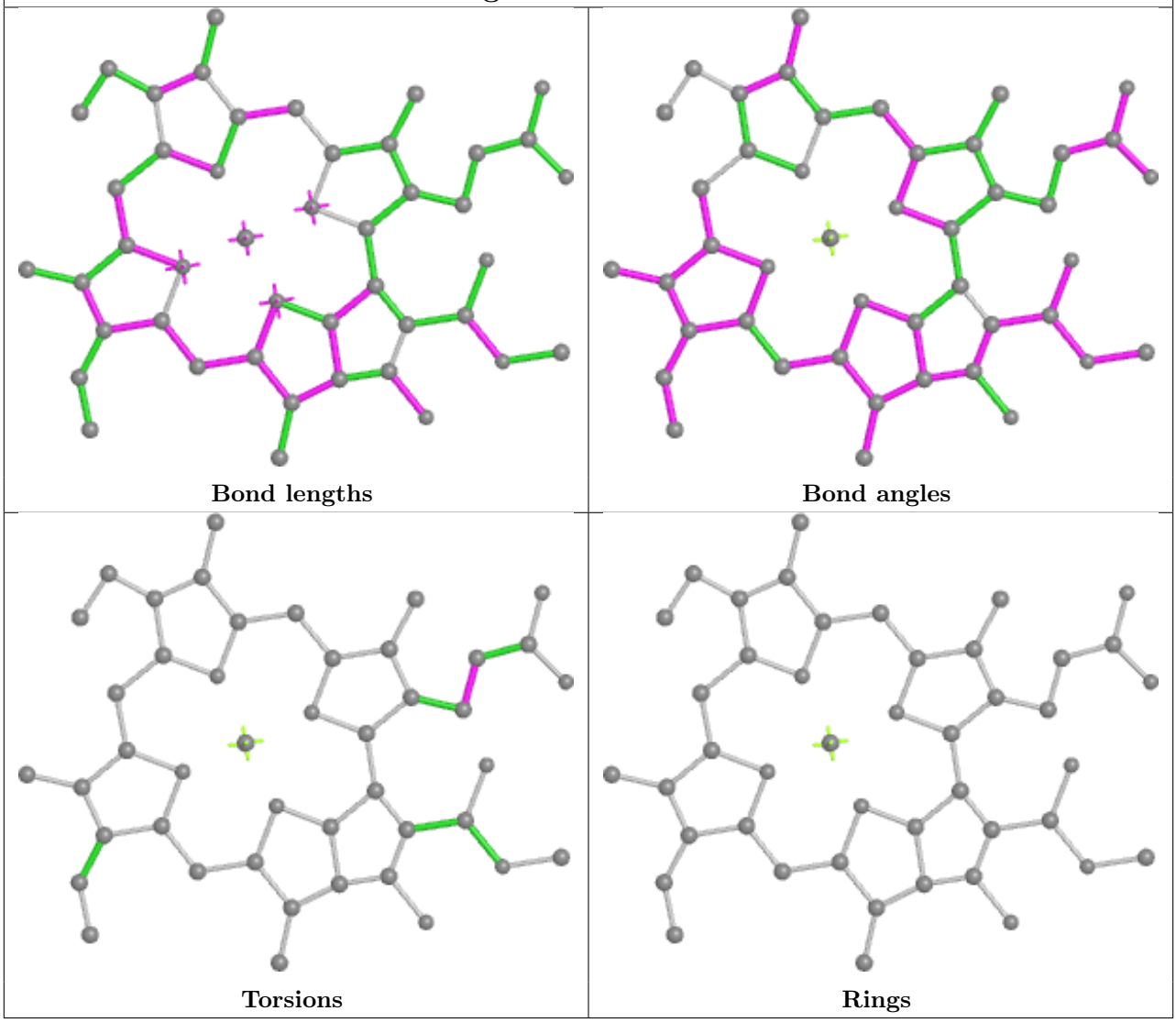
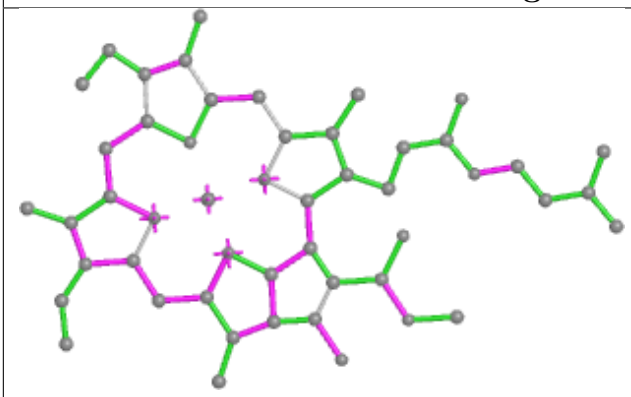
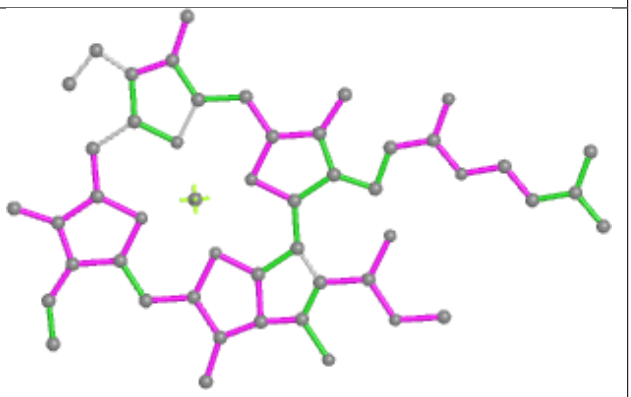


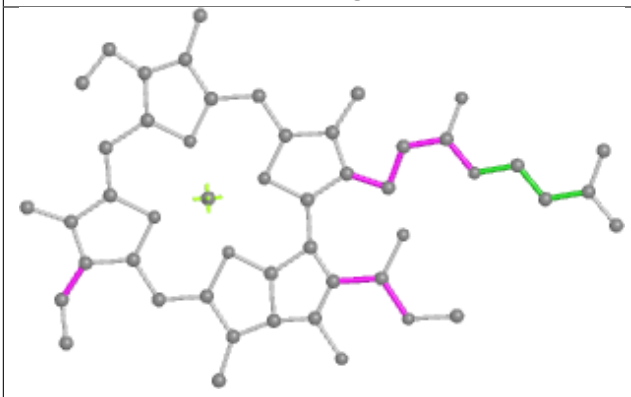
Ligand CLA H 851



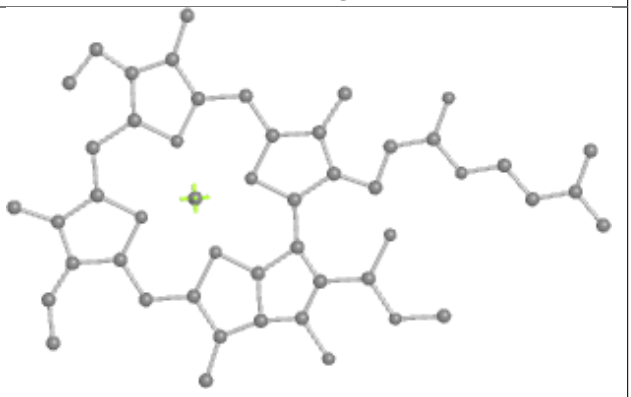
Bond lengths



Bond angles



Torsions



Rings

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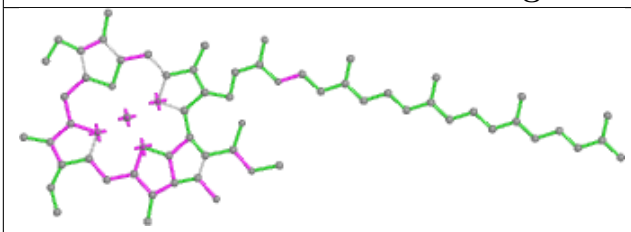

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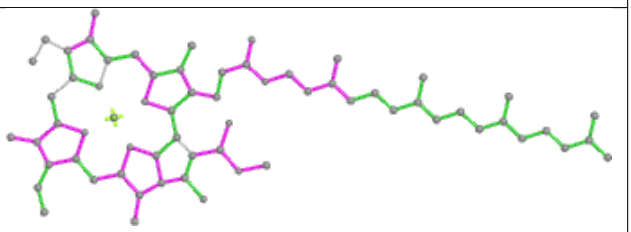

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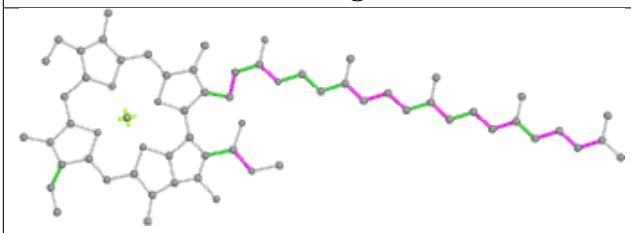

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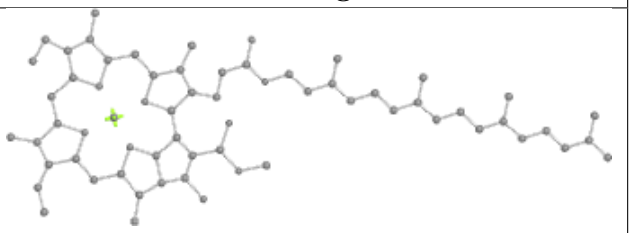
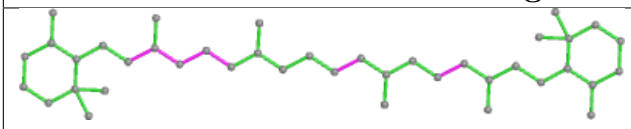


Rings

Ligand BCR Z 850



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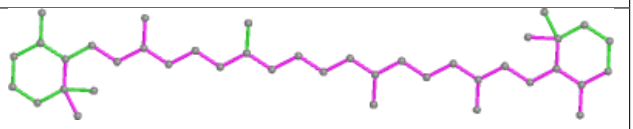

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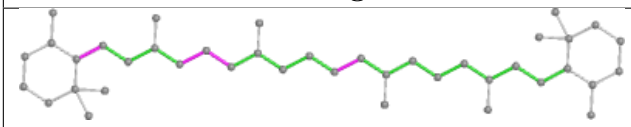

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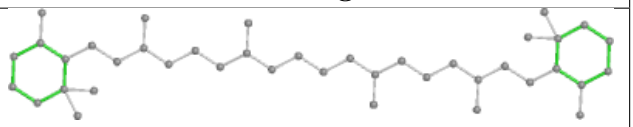

Rings

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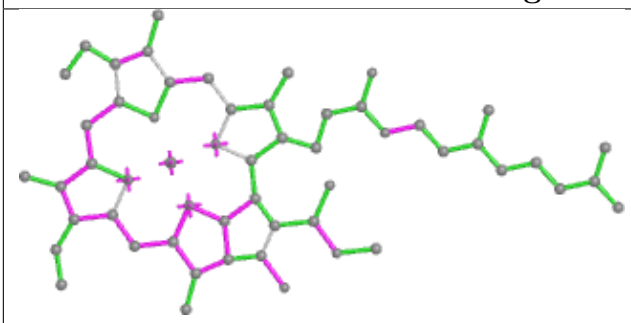

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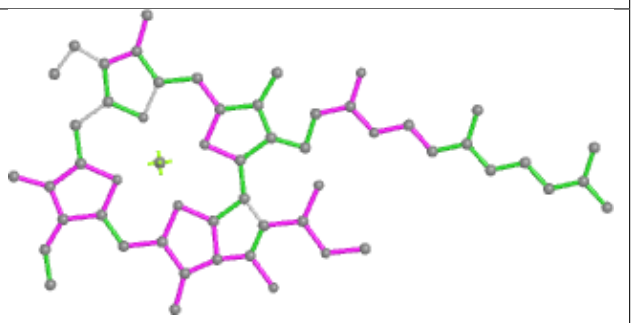

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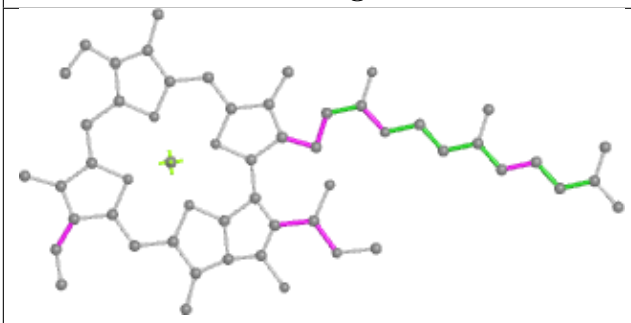

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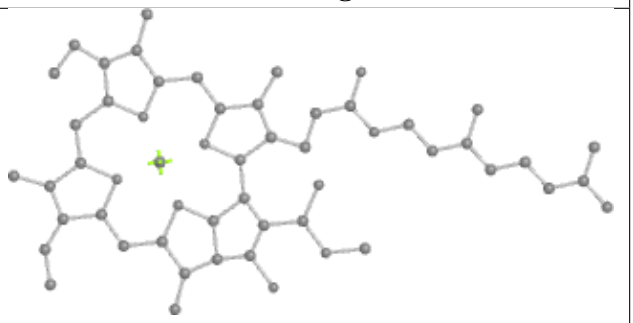
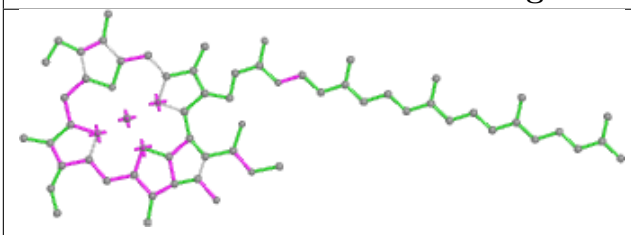


Rings

Ligand CLA Z 818



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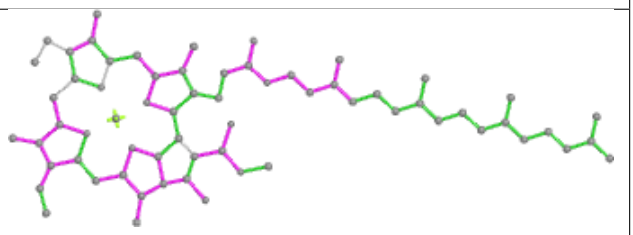

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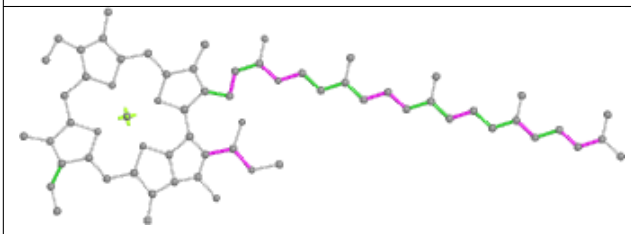

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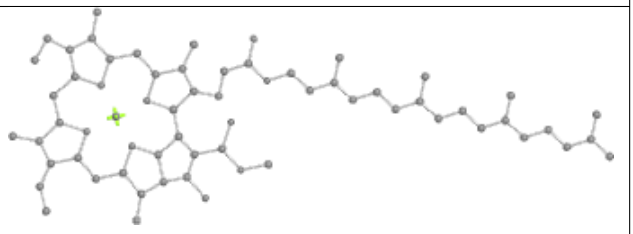
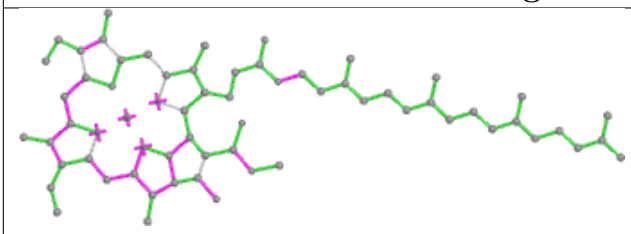
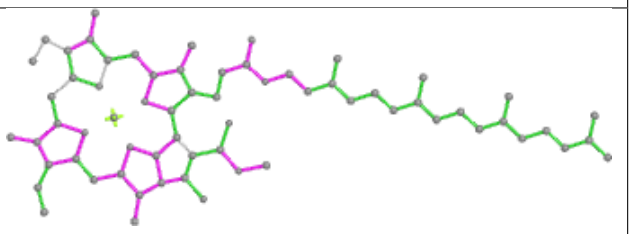
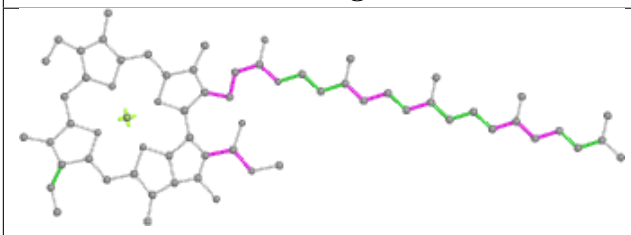
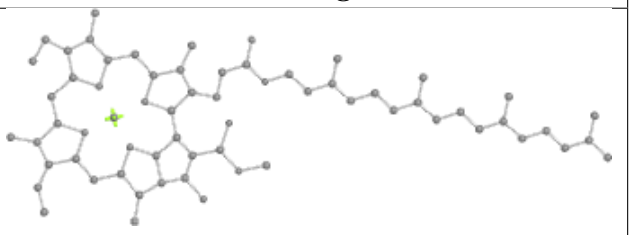


Rings

Ligand CLA G 821	
 Bond lengths	 Bond angles
 Torsions	 Rings

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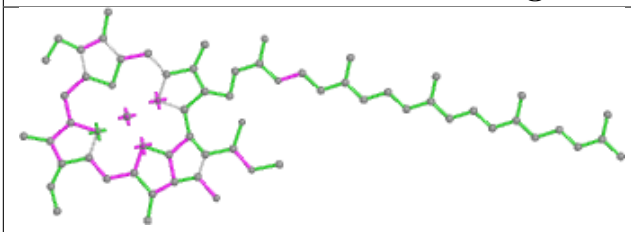
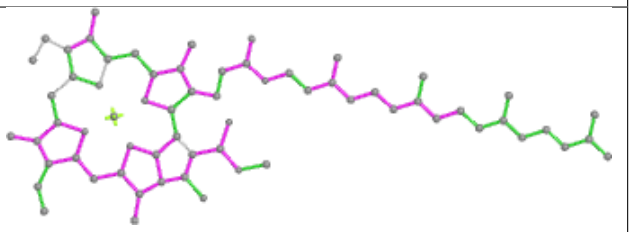
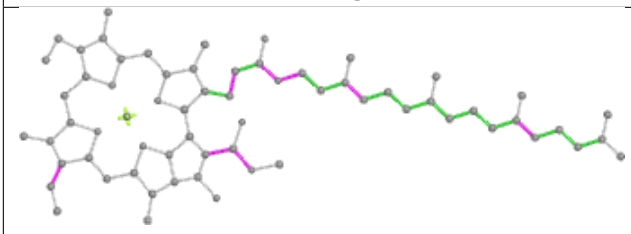
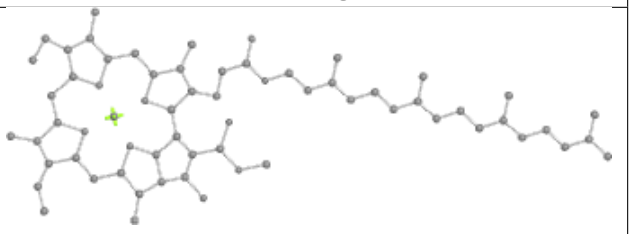
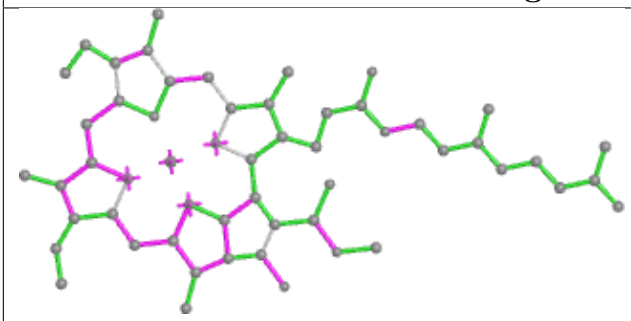
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA B 810



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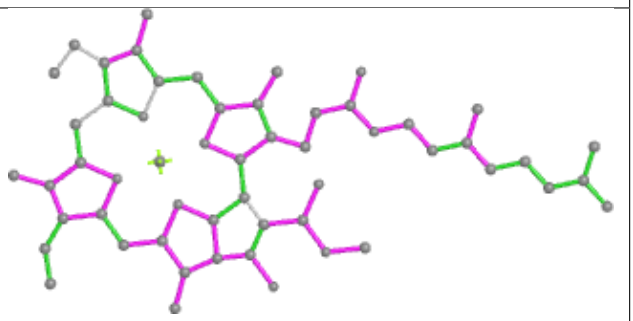
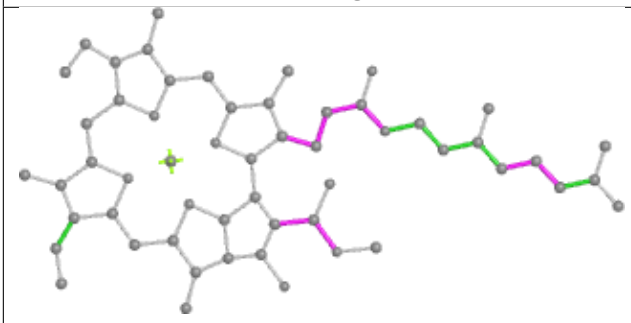
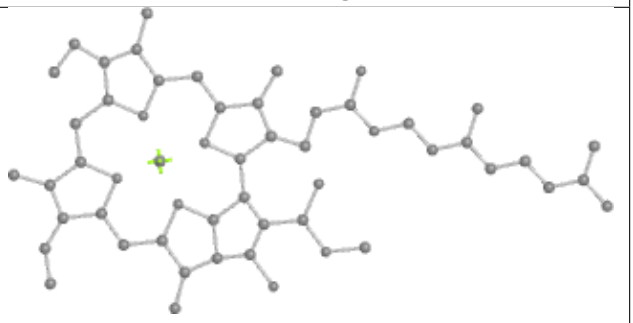


Bond angles

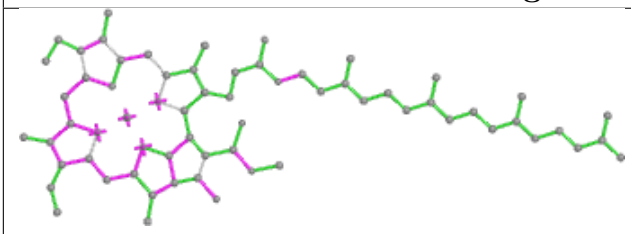


Torsions

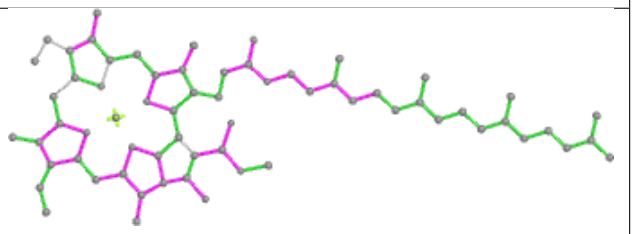


Rings

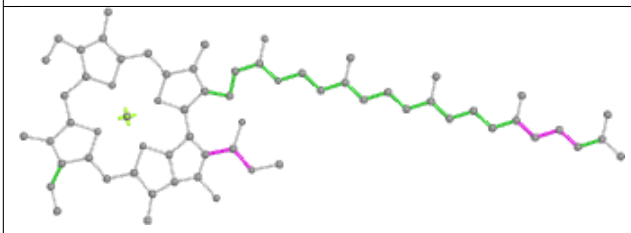
Ligand CLA H 826



Bond lengths



Bond angles



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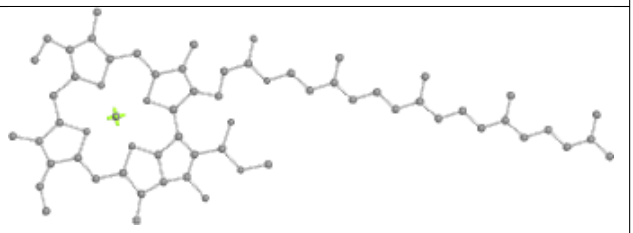
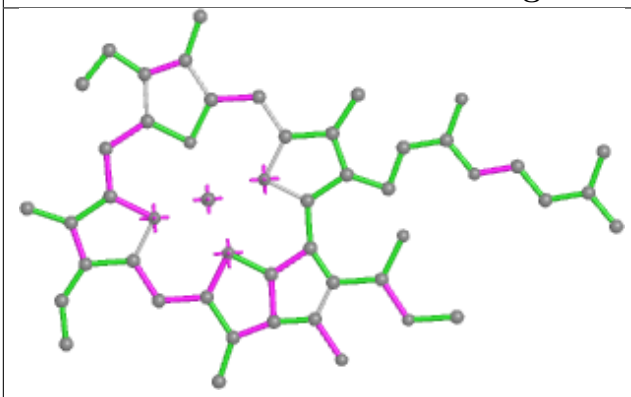


Rings

Ligand CLA G 831



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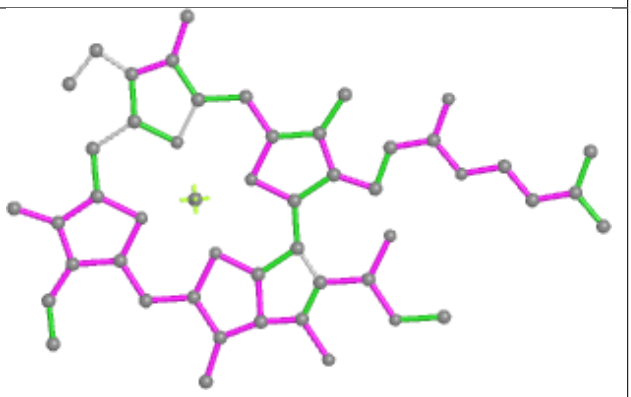
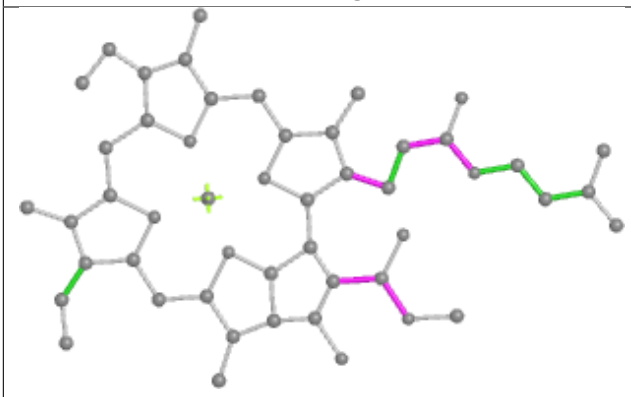
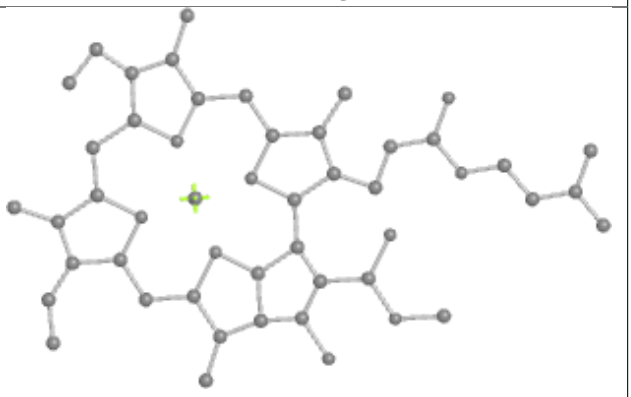


Bond angles

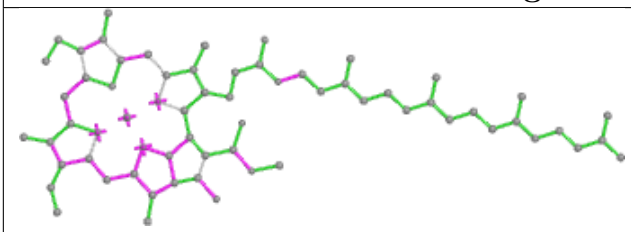


Torsions



Rings

Ligand CLA Y 829



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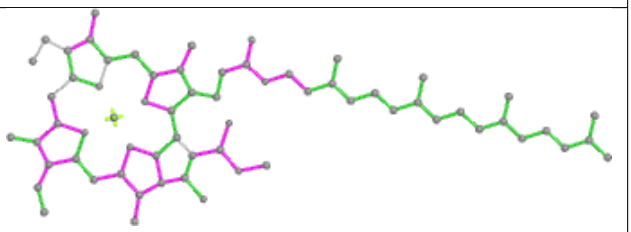
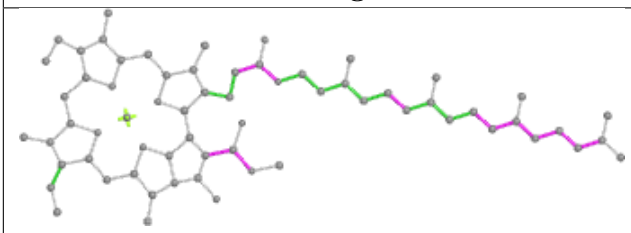


Bond angles



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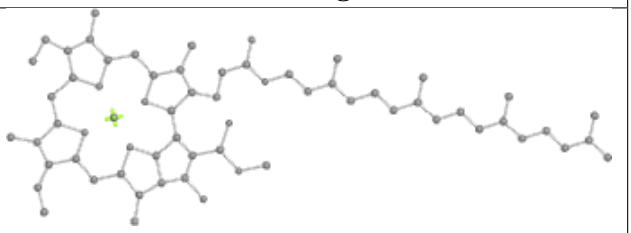
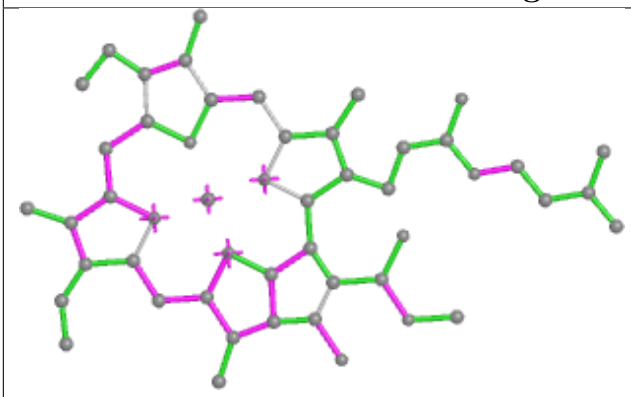
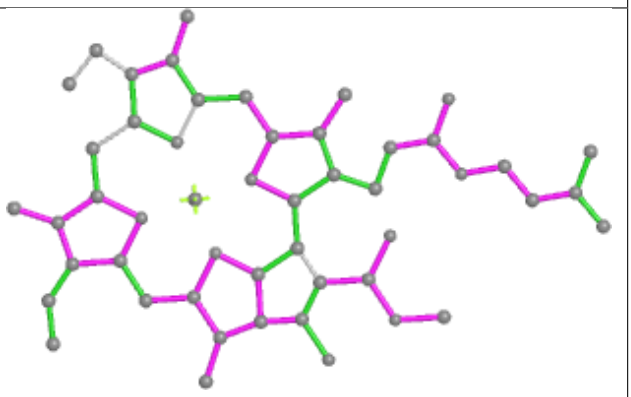
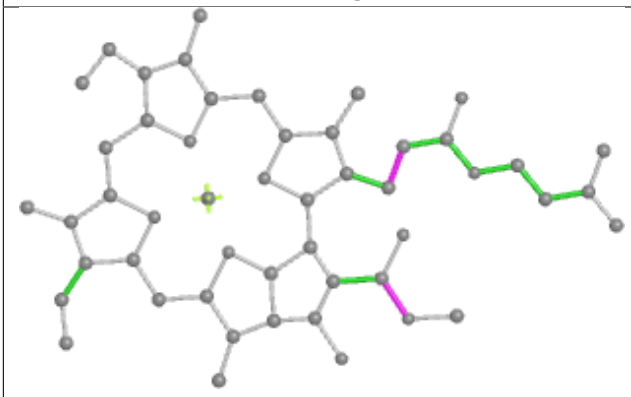
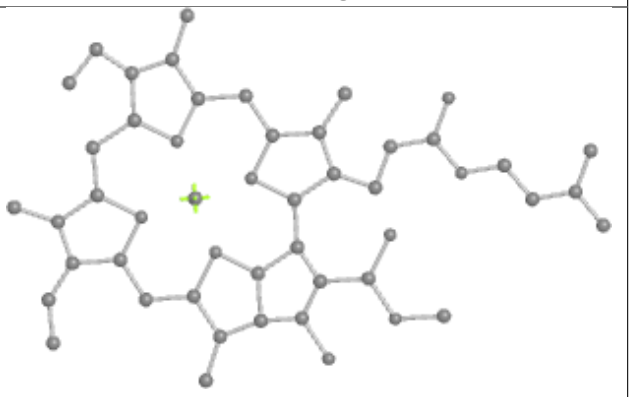
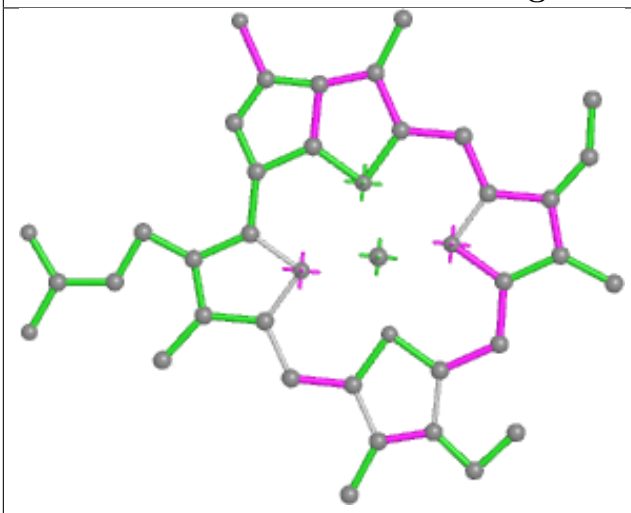


Rings

Ligand CLA G 842	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA g 101



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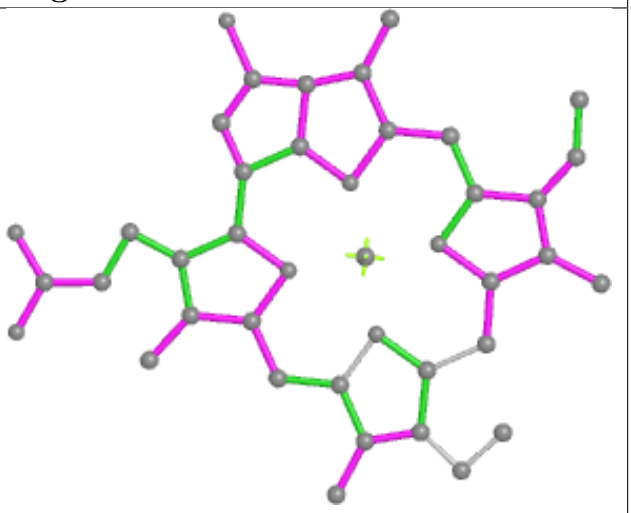
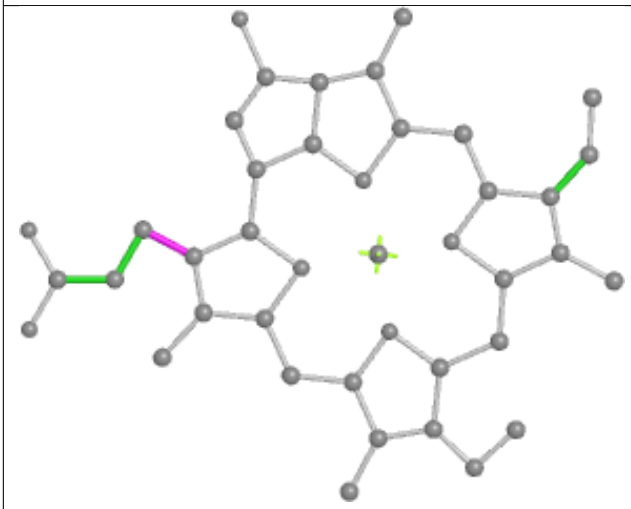


Bond angles



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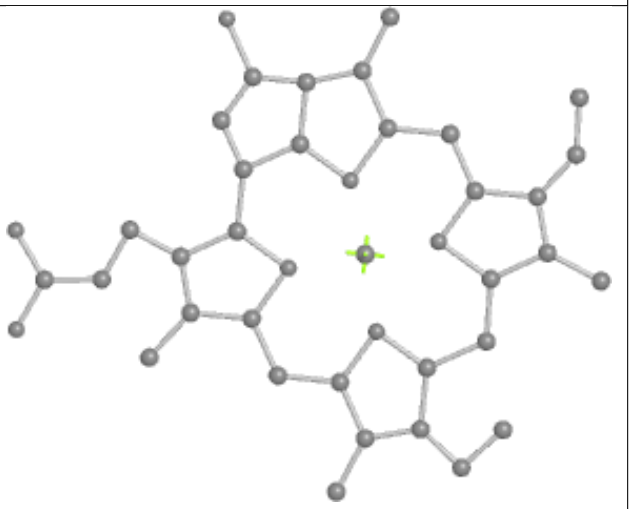
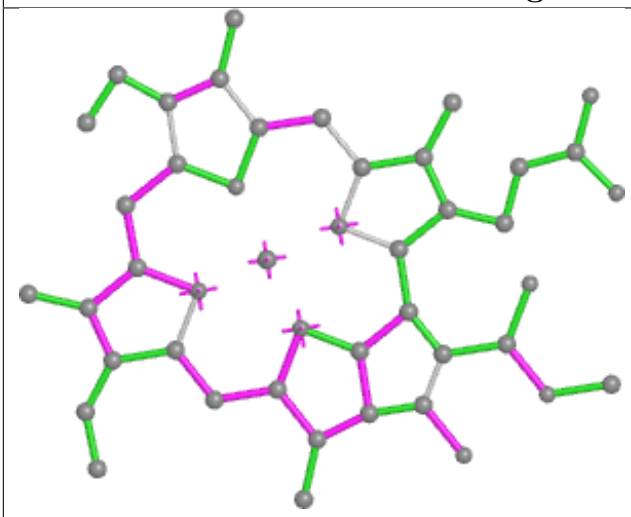


Rings

Ligand CLA Z 816



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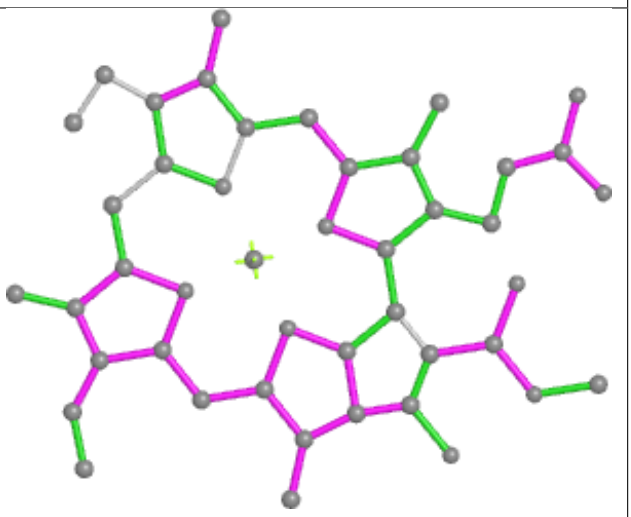
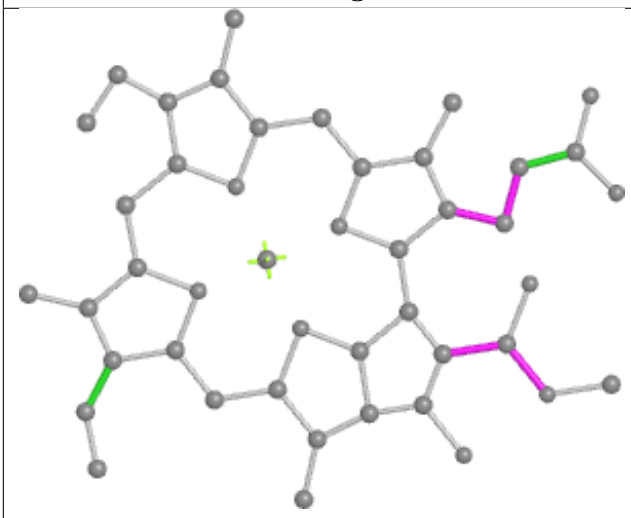


Bond angles



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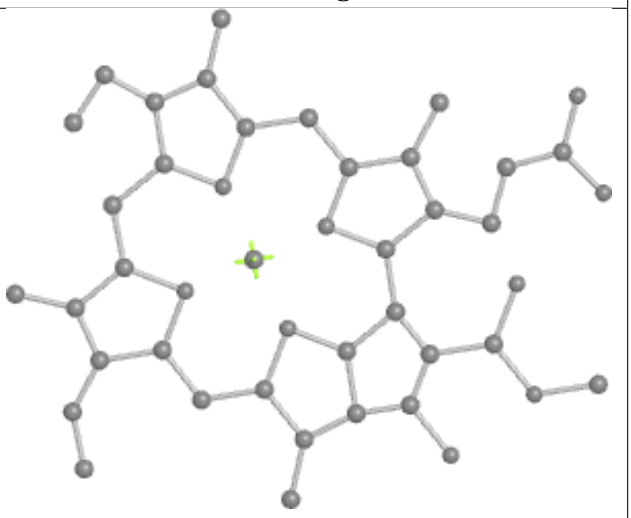
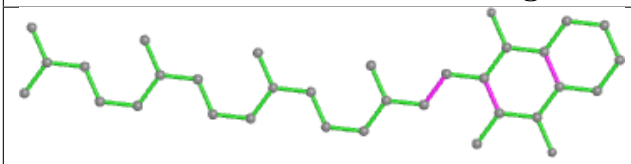


Rings

Ligand PQN B 841



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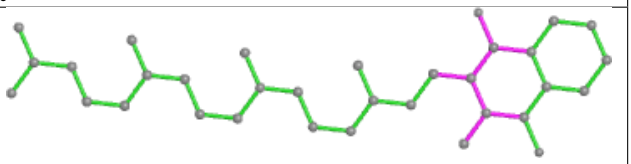
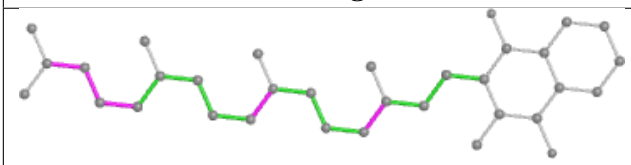


Bond angles



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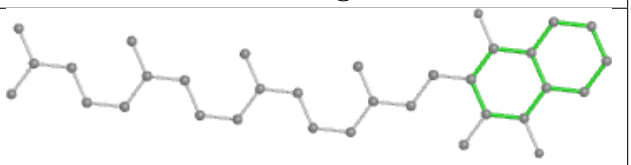
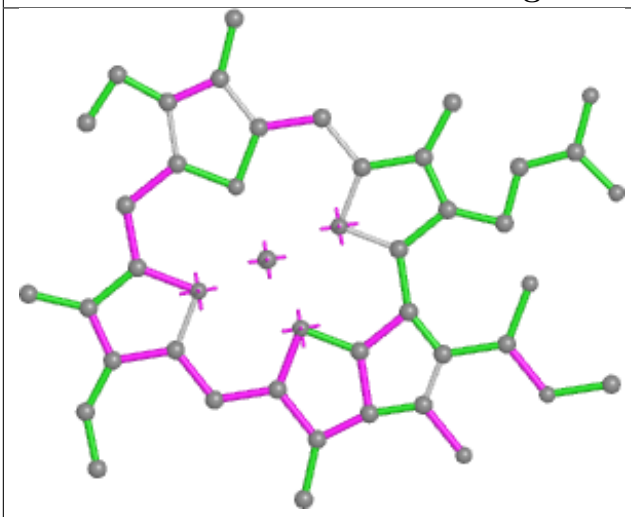


Rings

Ligand CLA H 812



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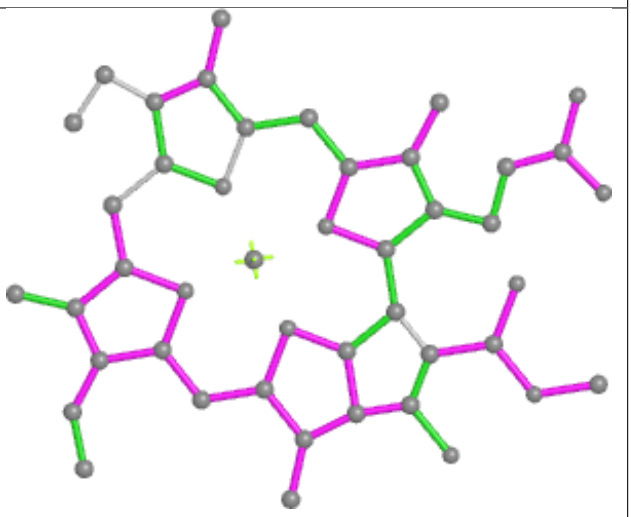
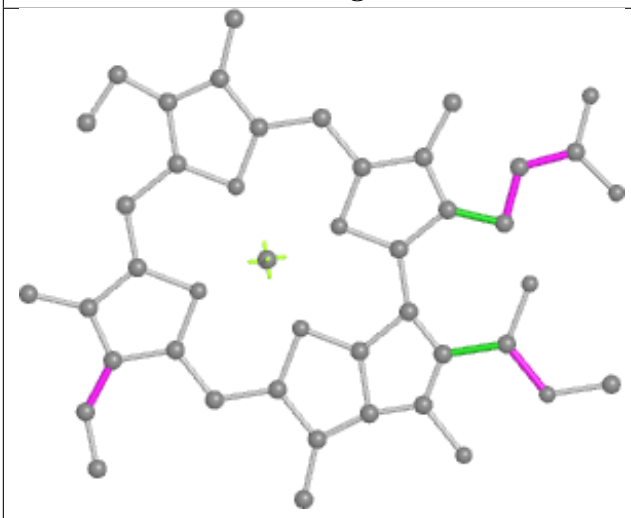


Bond angles



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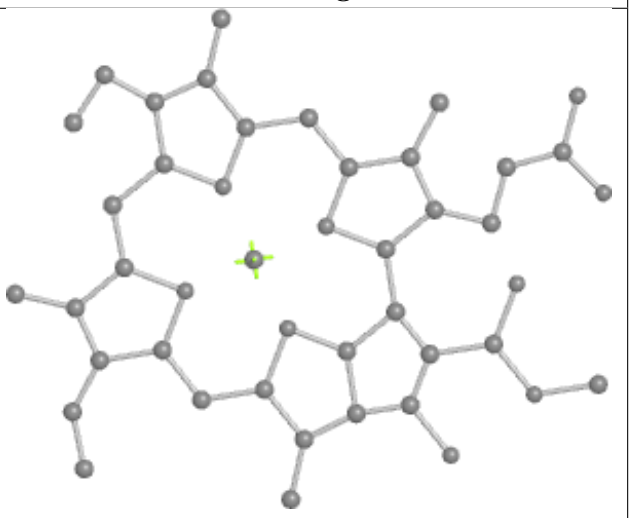
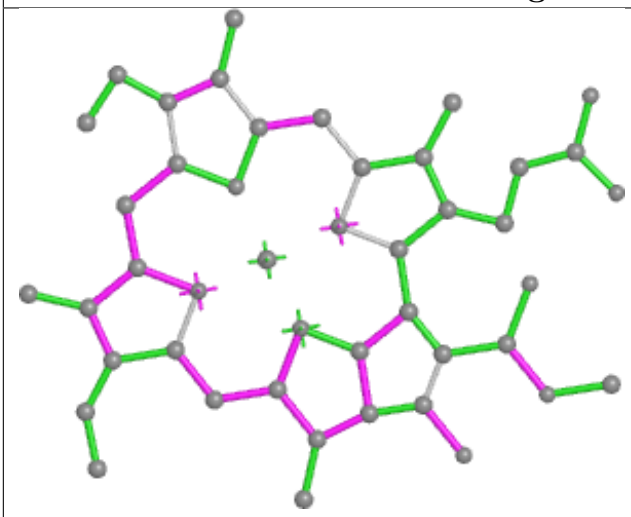


Rings

Ligand CLA J 101



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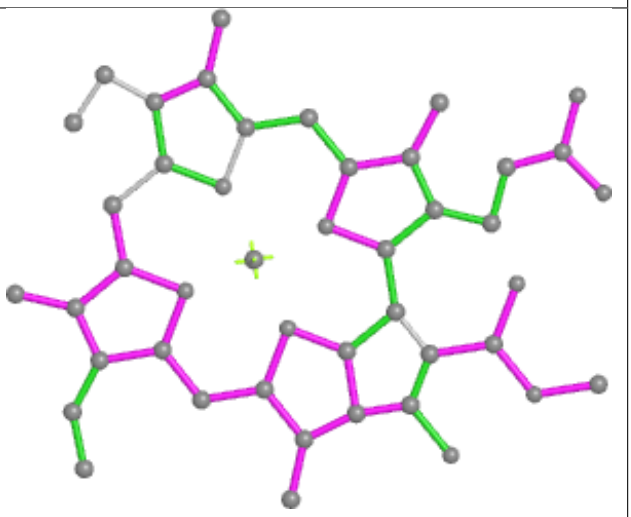
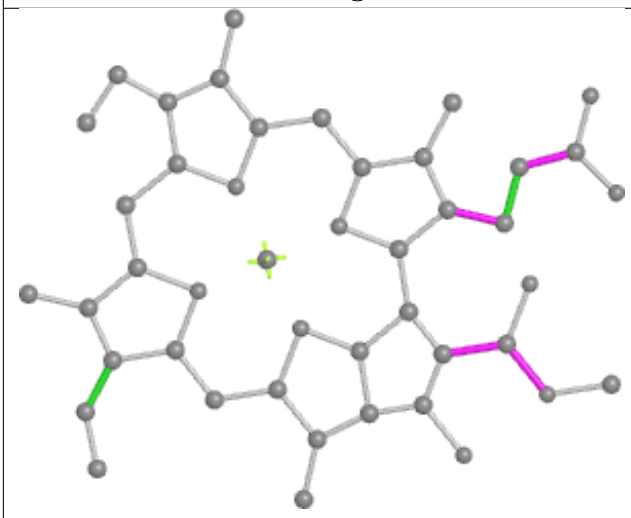


Bond angles



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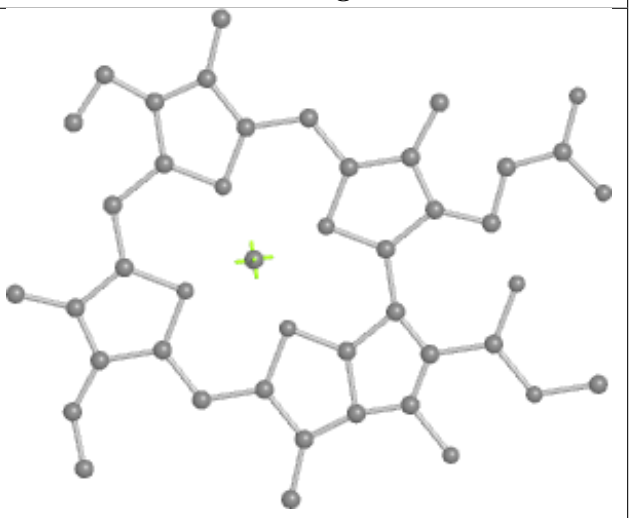
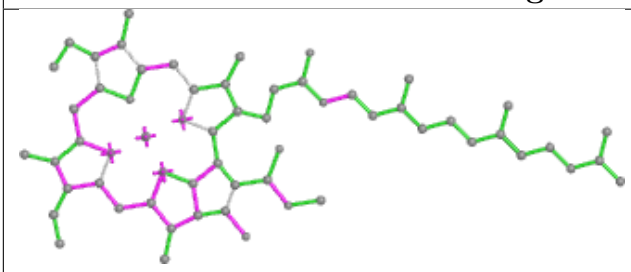


Rings

Ligand CLA Z 824



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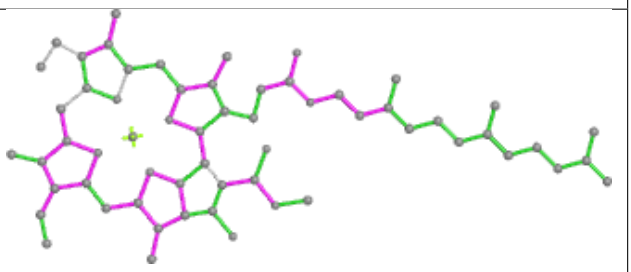
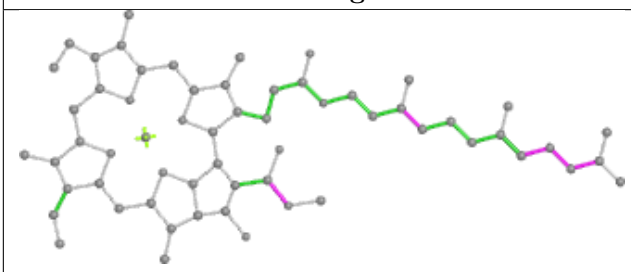


Bond angles



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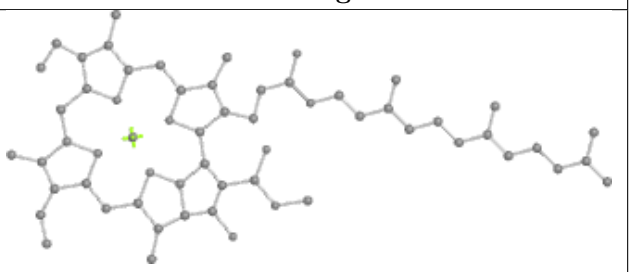
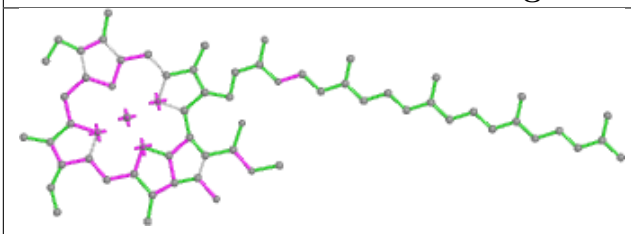
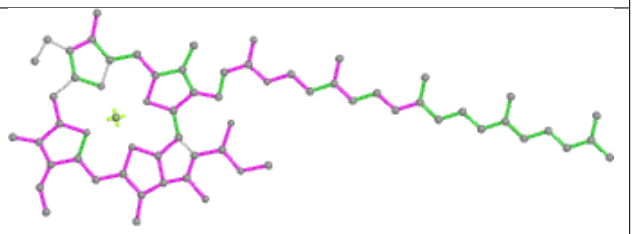
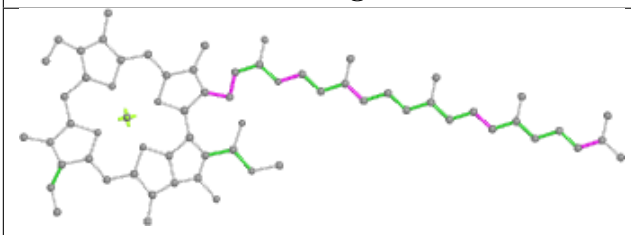
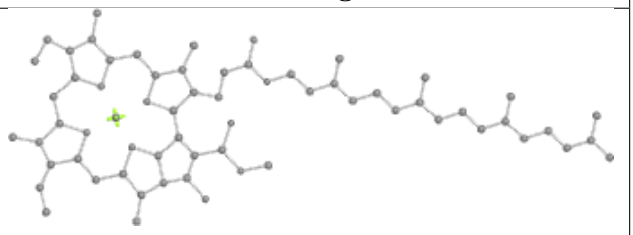


Rings

Ligand CLA Y 802	
 Bond lengths	 Bond angles
 Torsions	 Rings

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

Unable to reproduce the depositors R factor - this section is therefore empty.

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

Unable to reproduce the depositors R factor - this section is therefore empty.

6.3 Carbohydrates (i)

Unable to reproduce the depositors R factor - this section is therefore empty.

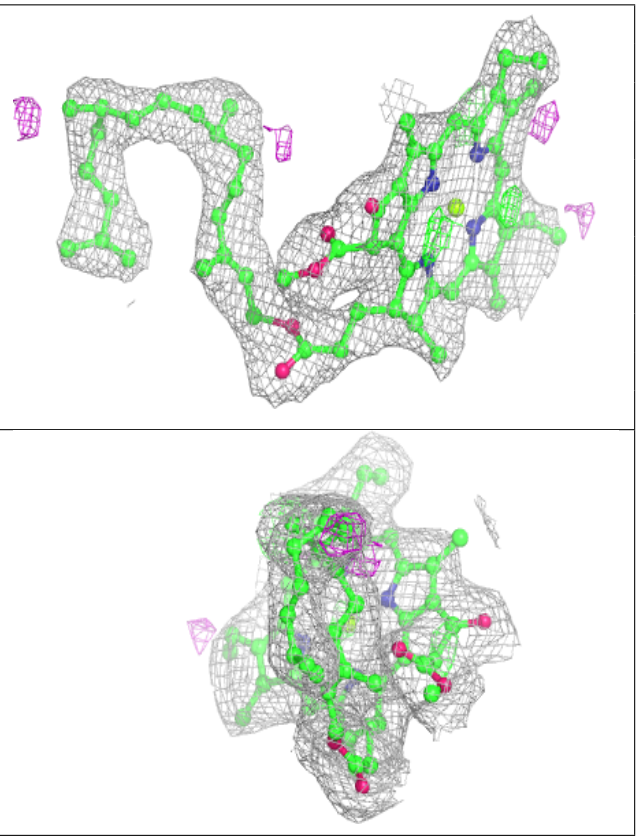
6.4 Ligands (i)

Unable to reproduce the depositors R factor - this section is therefore empty.

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.

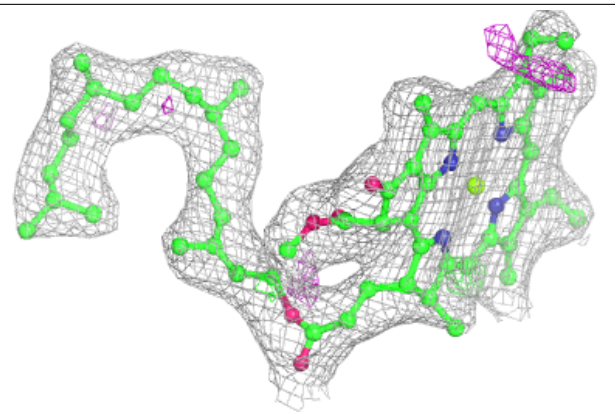
Electron density around CL0 A 801:

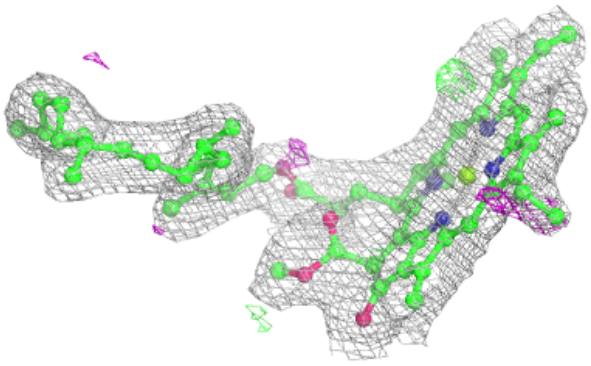
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

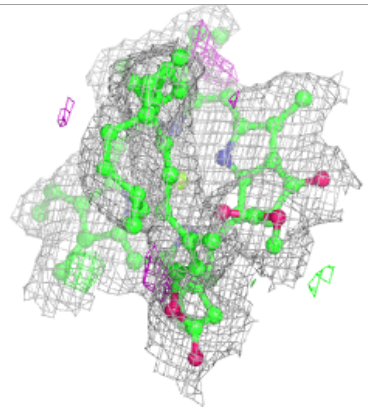


Electron density around CL0 G 801:

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

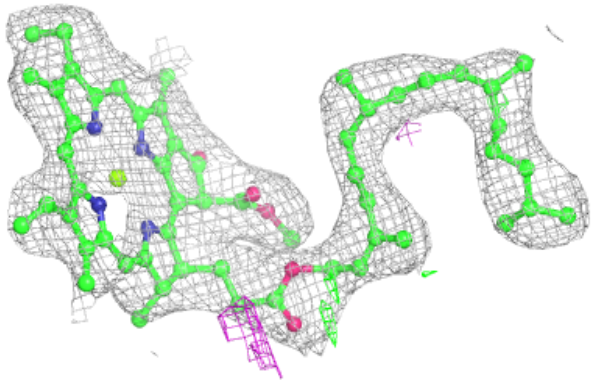


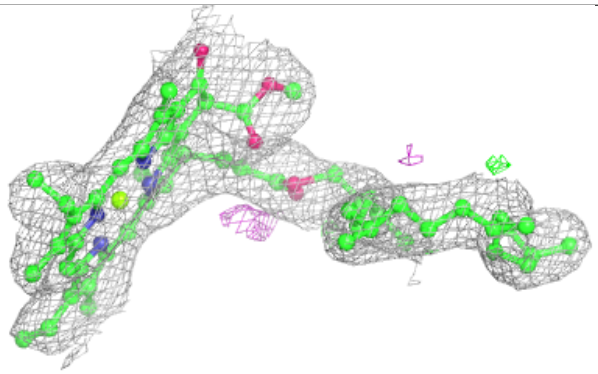


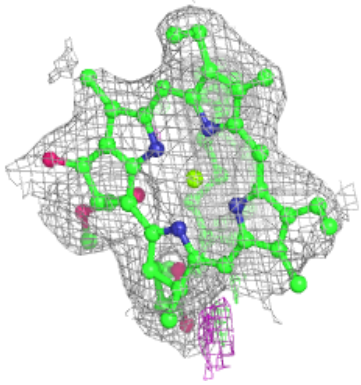


Electron density around CL0 Y 801:

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

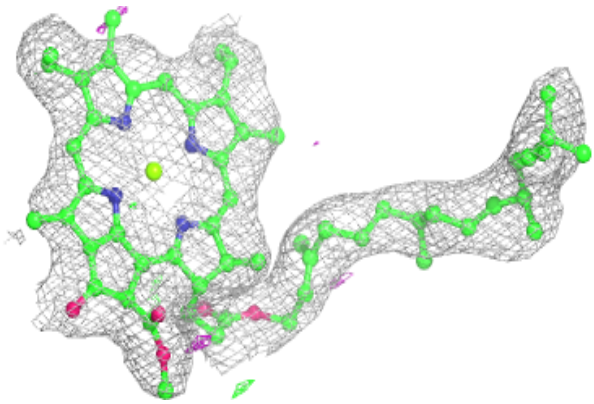


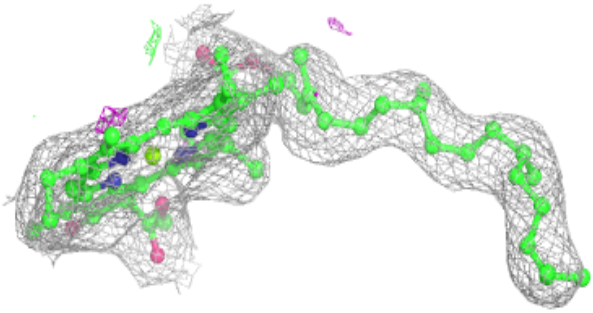


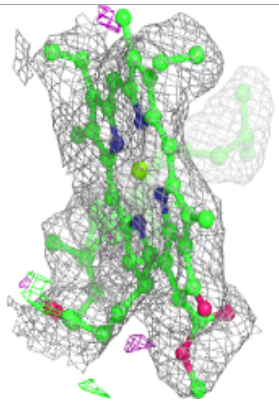


Electron density around CLA A 802:

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

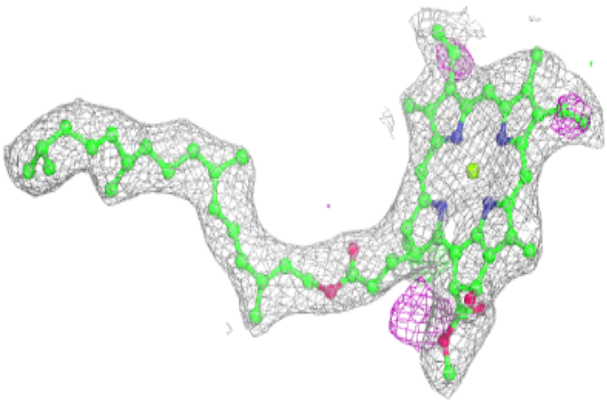


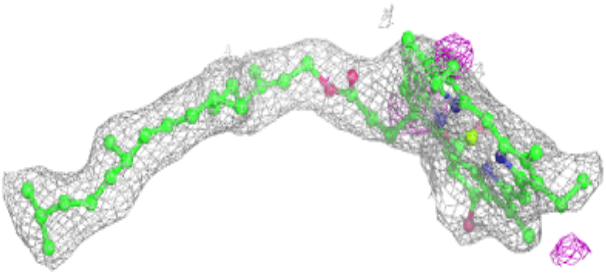


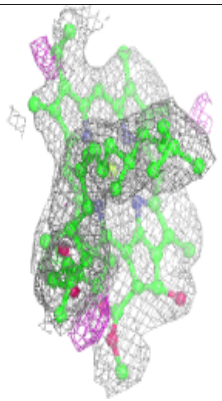


Electron density around CLA A 803:

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

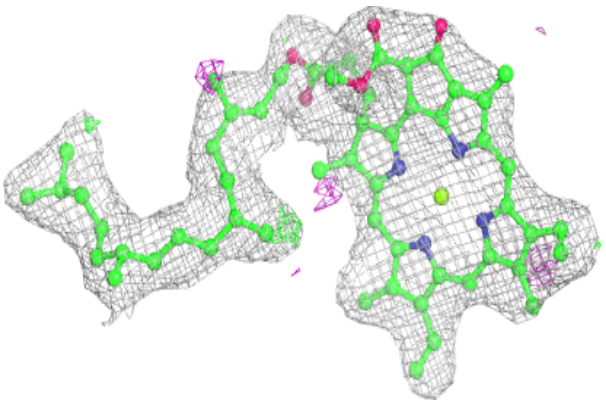


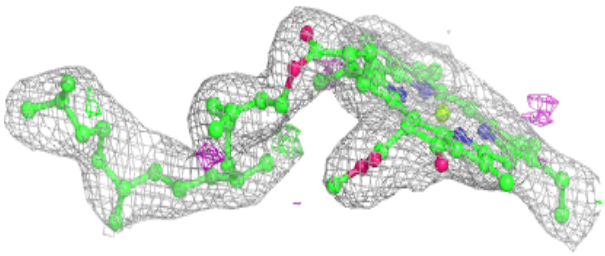


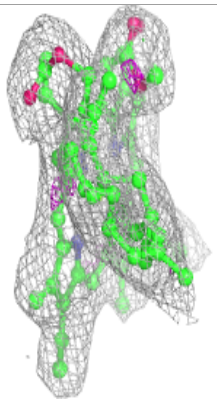


Electron density around CLA A 804:

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

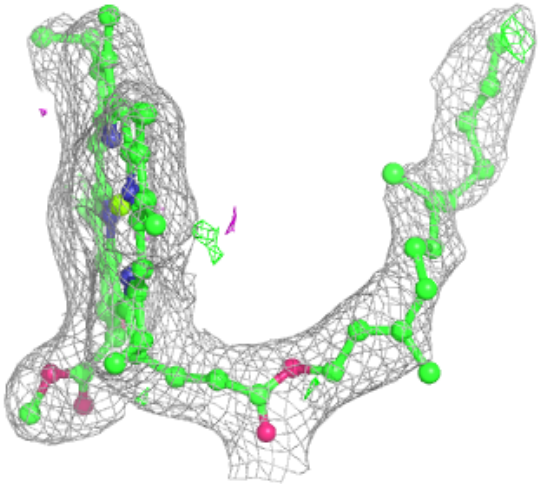


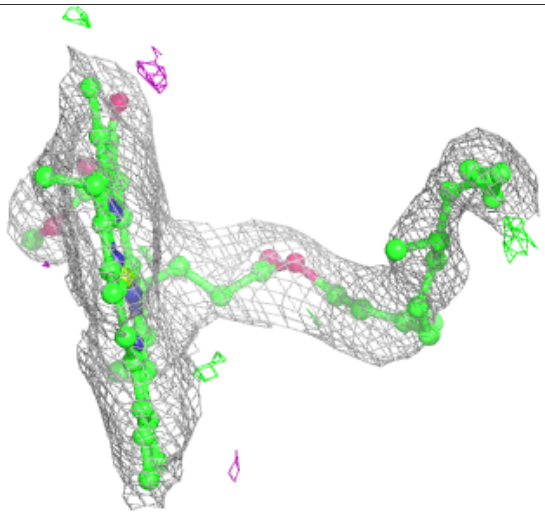


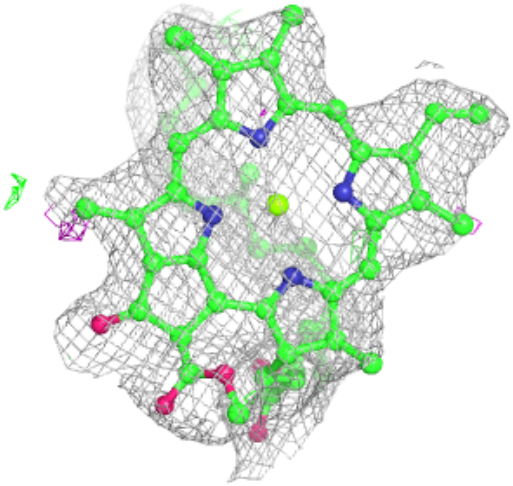


Electron density around CLA A 805:

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

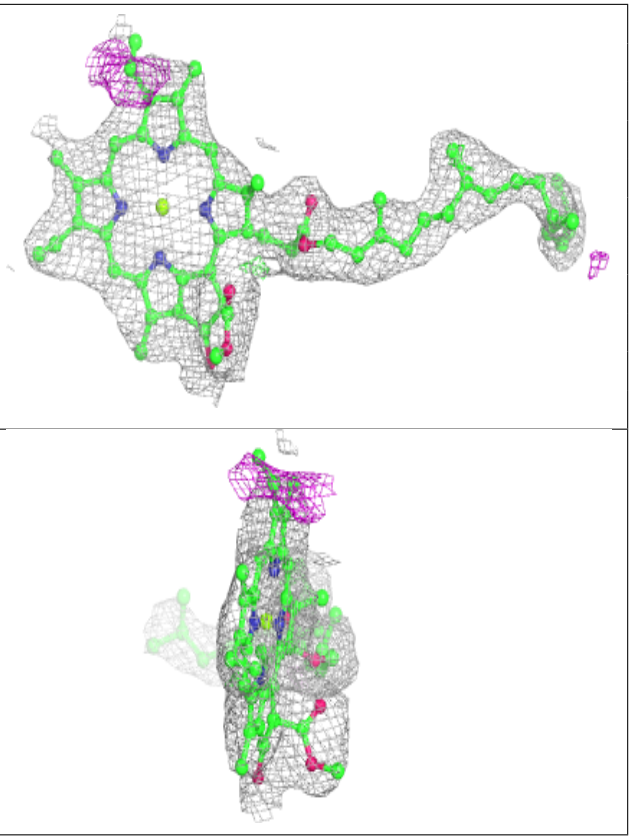






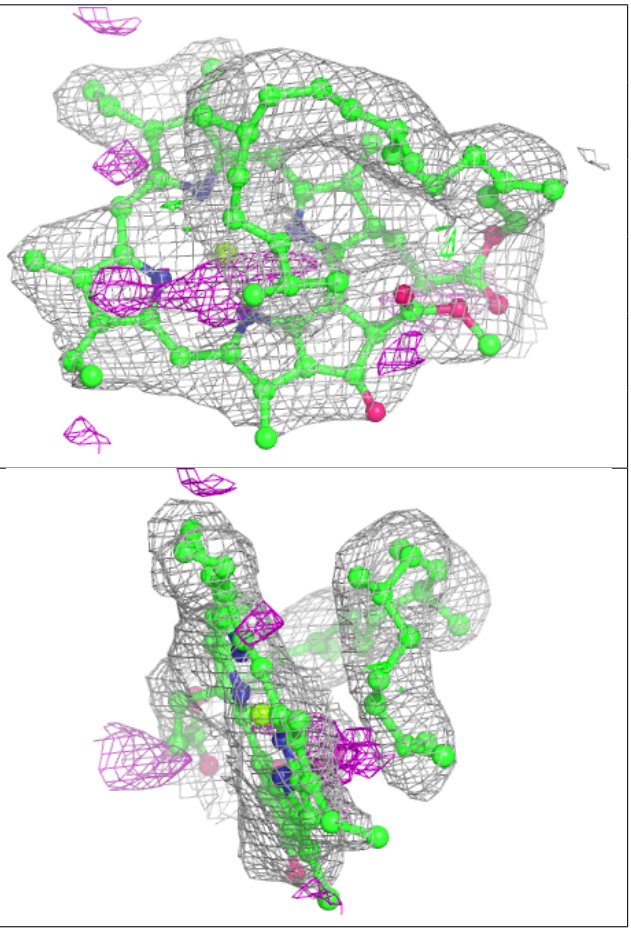
Electron density around CLA A 806:

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



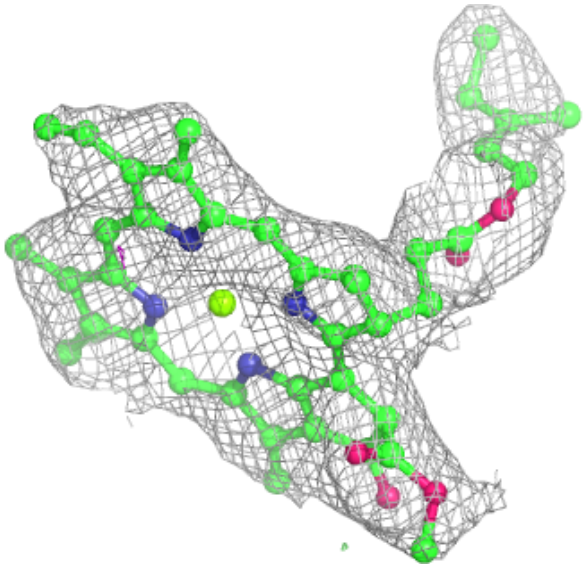
Electron density around CLA A 807:

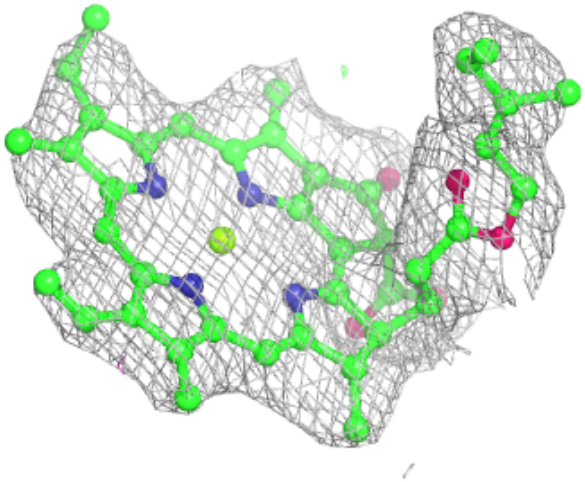
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

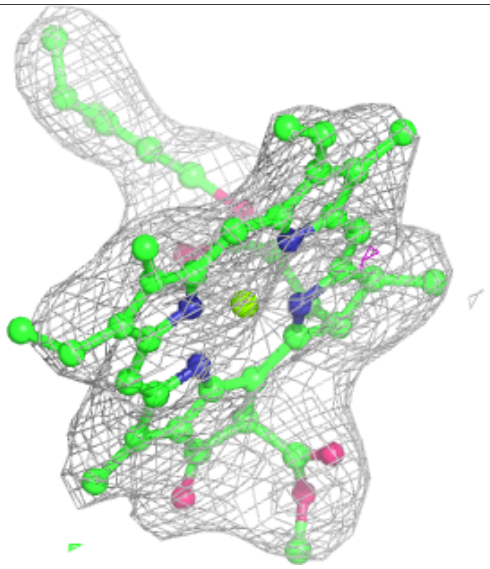


Electron density around CLA A 808:

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

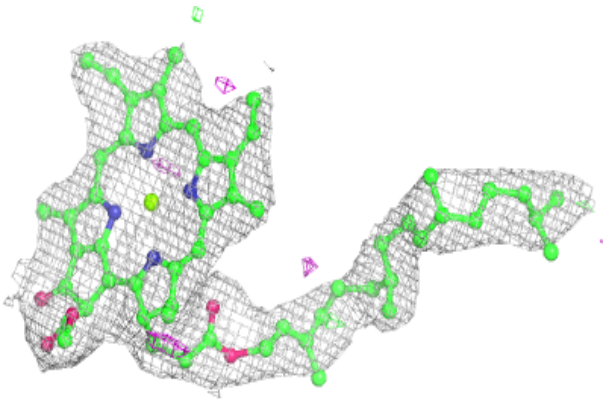


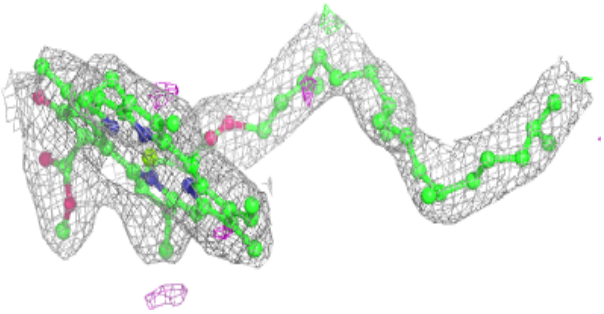


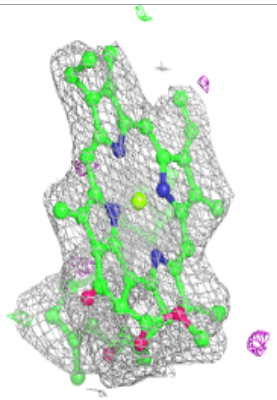


Electron density around CLA A 809:

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

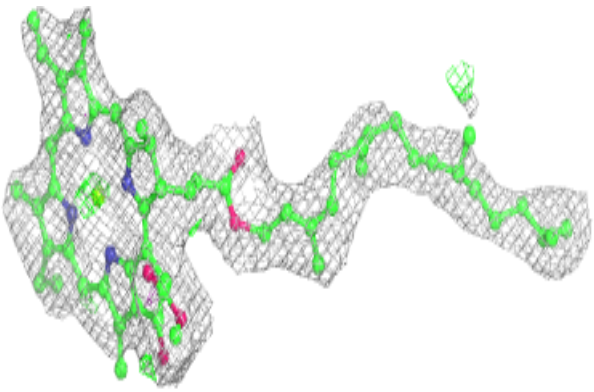


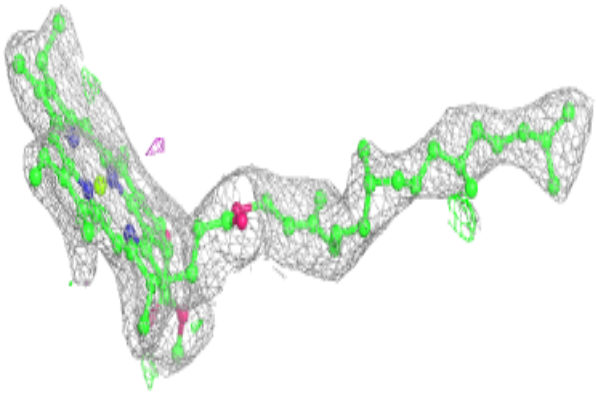


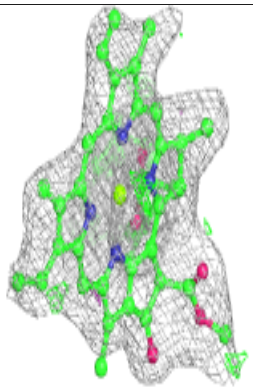


Electron density around CLA A 810:

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

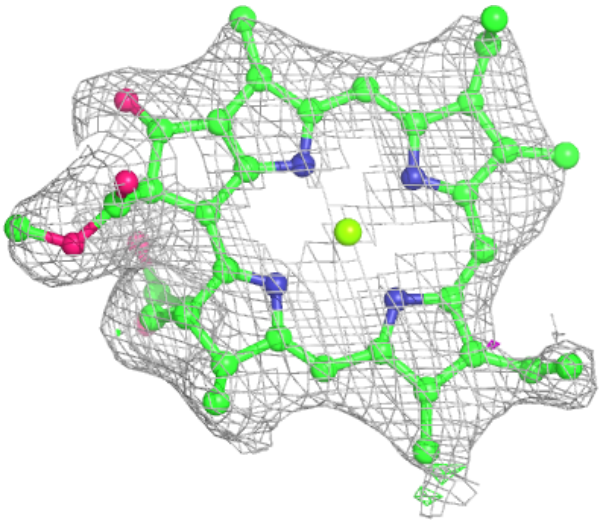


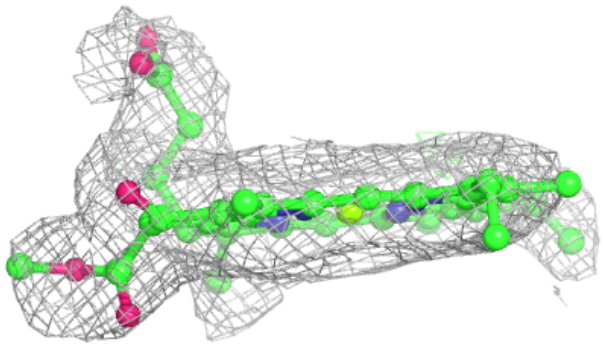


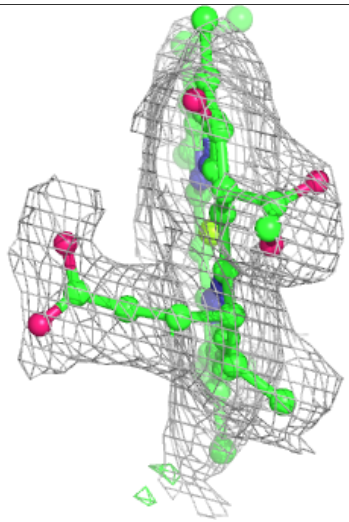


Electron density around CLA A 811:

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

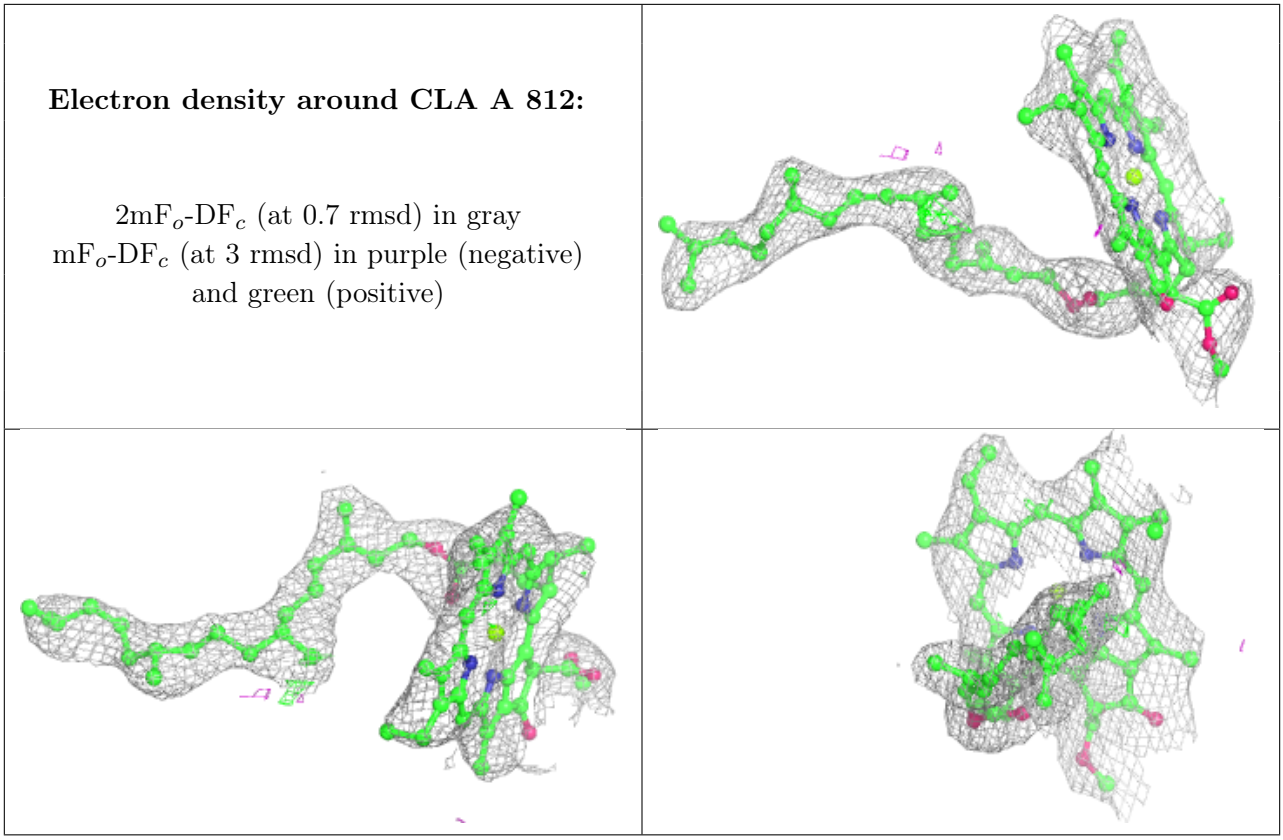






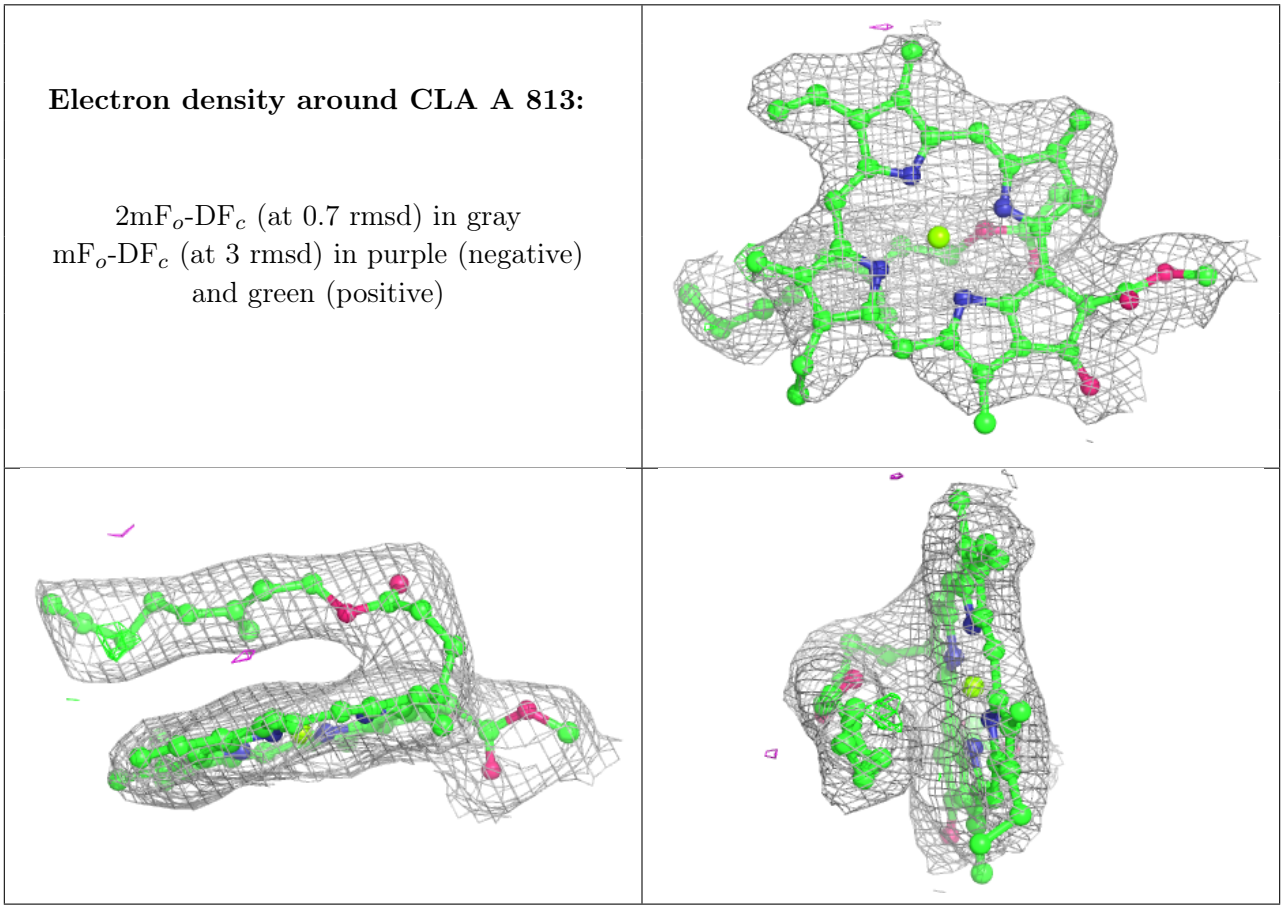
Electron density around CLA A 812:

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



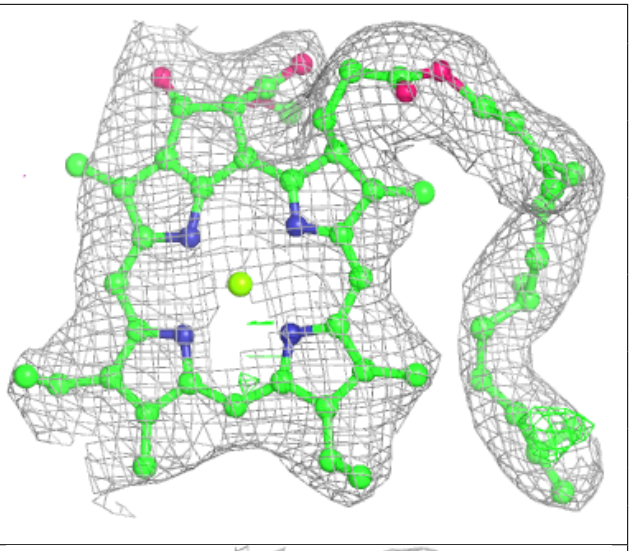
Electron density around CLA A 813:

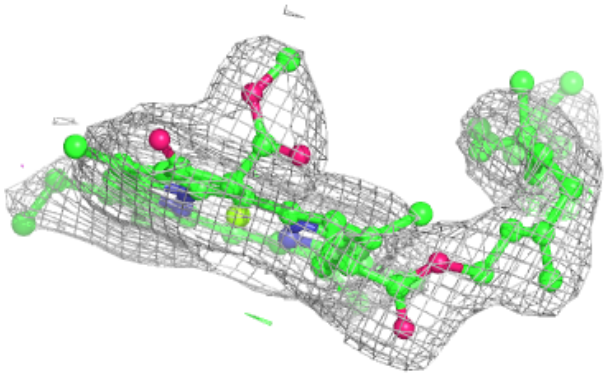
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

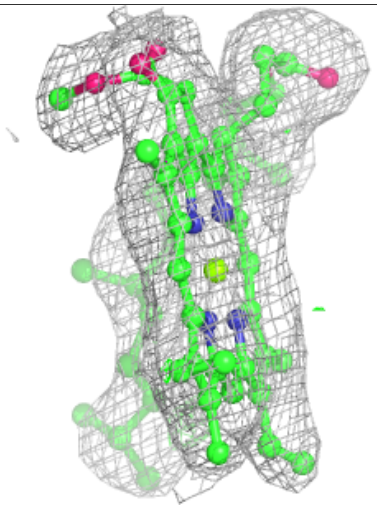


Electron density around CLA A 814:

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

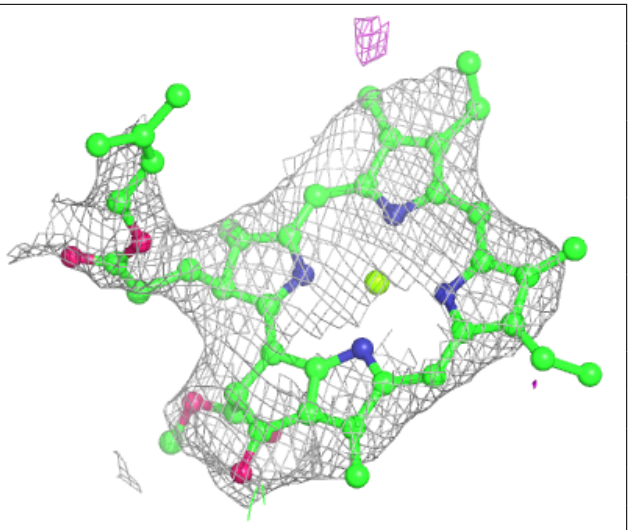


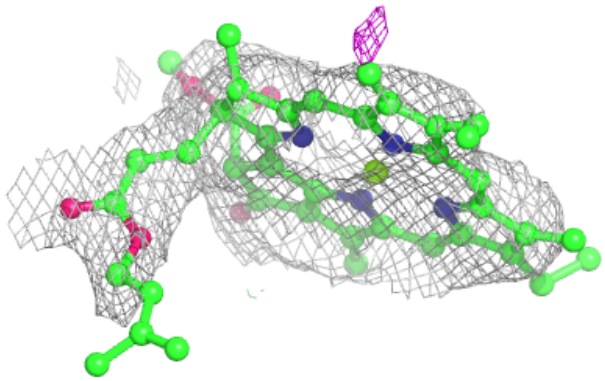


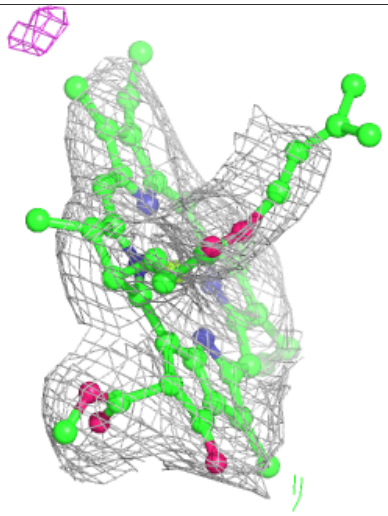


Electron density around CLA A 815:

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

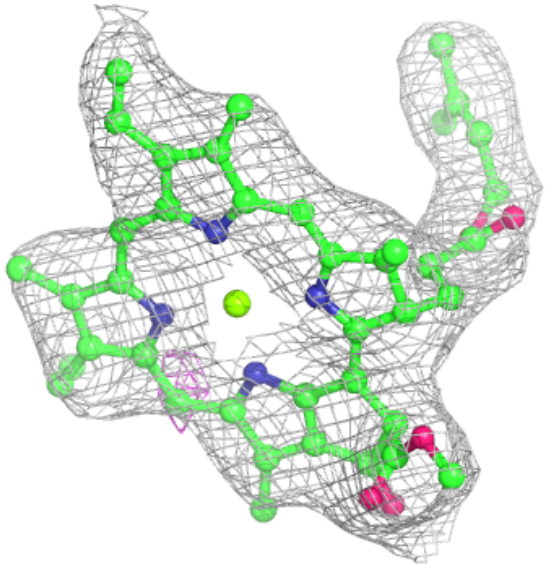


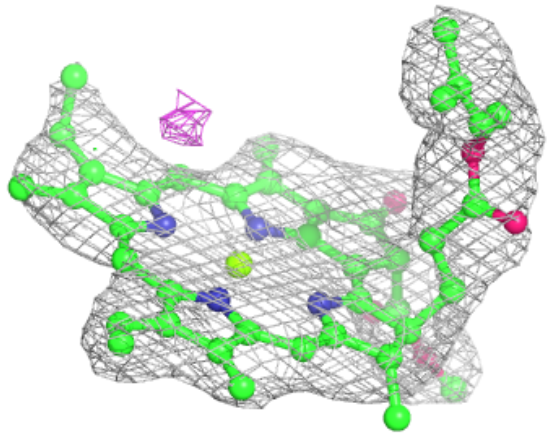


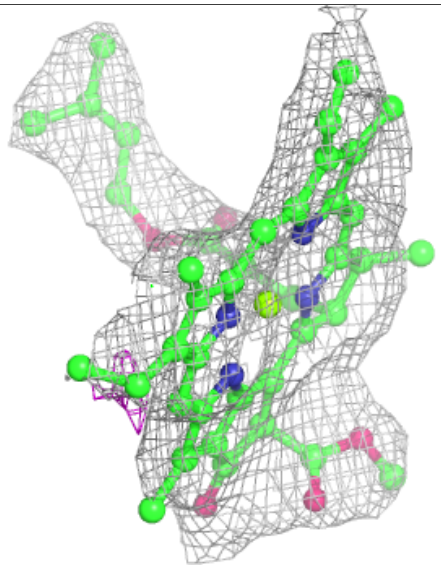


Electron density around CLA A 816:

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

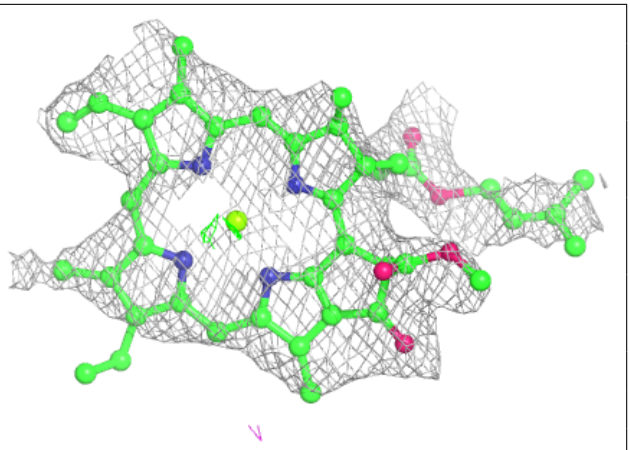


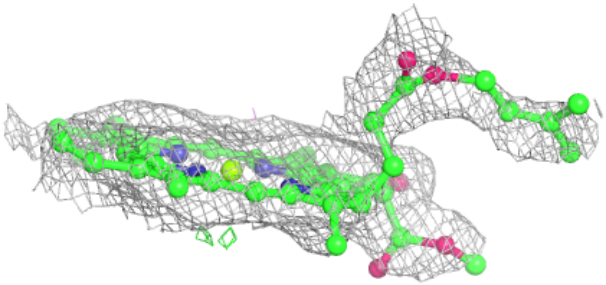


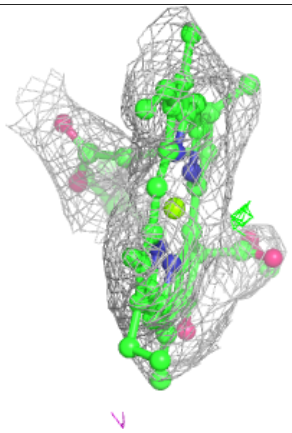


Electron density around CLA A 817:

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

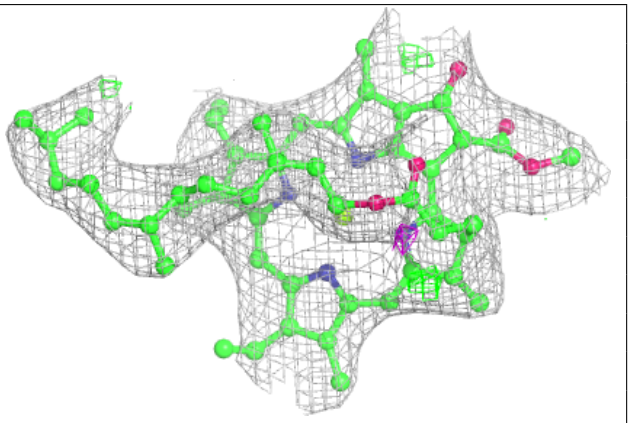


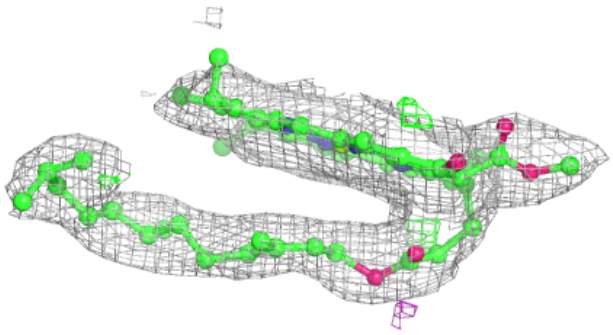


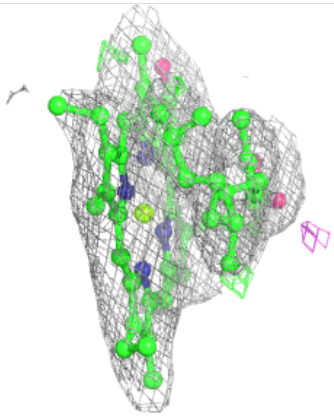


Electron density around CLA A 818:

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

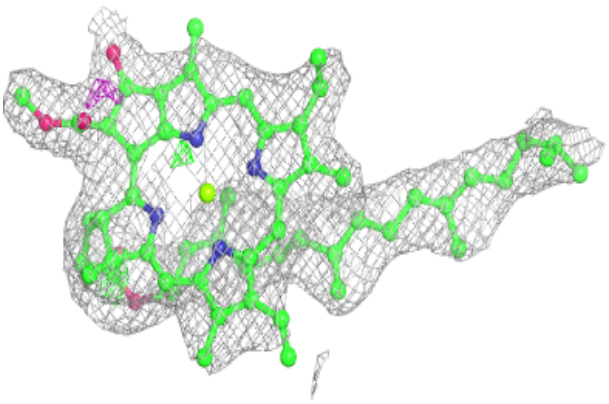


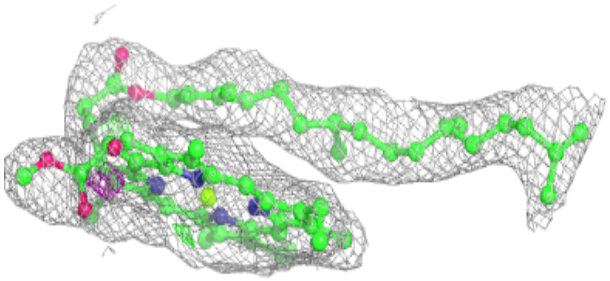


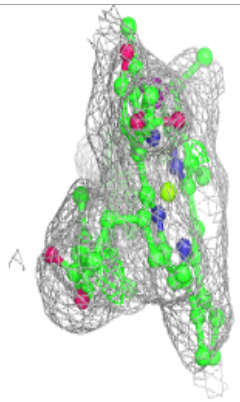


Electron density around CLA A 819:

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

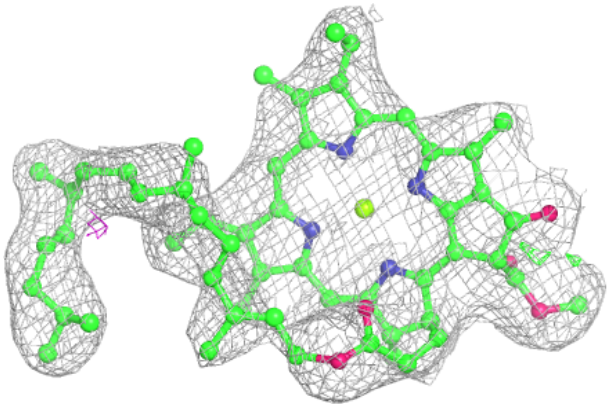


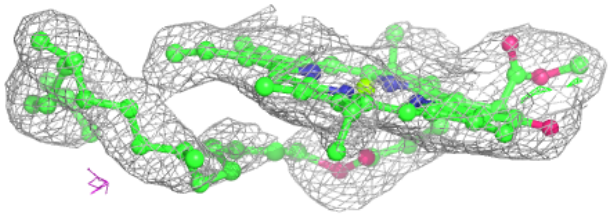


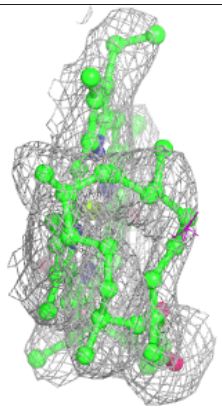


Electron density around CLA A 820:

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

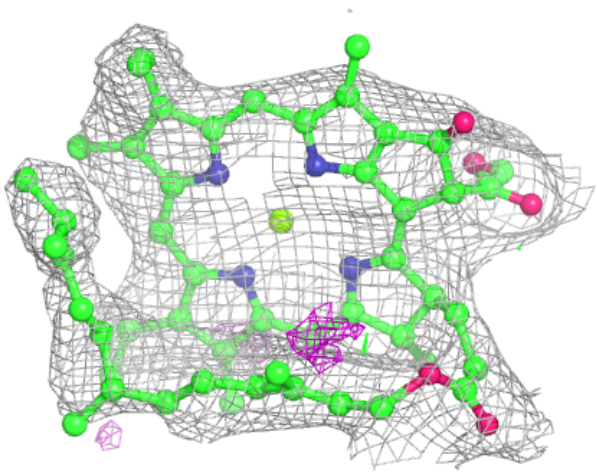


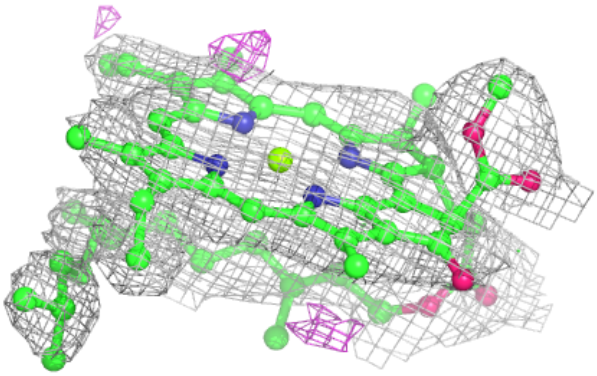


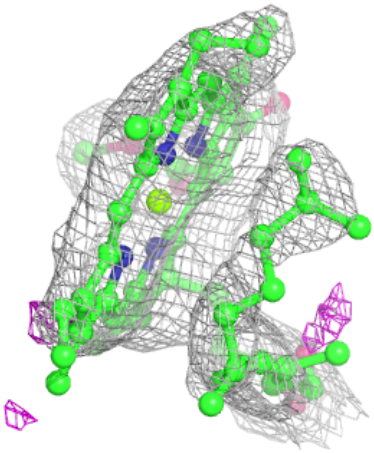


Electron density around CLA A 821:

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

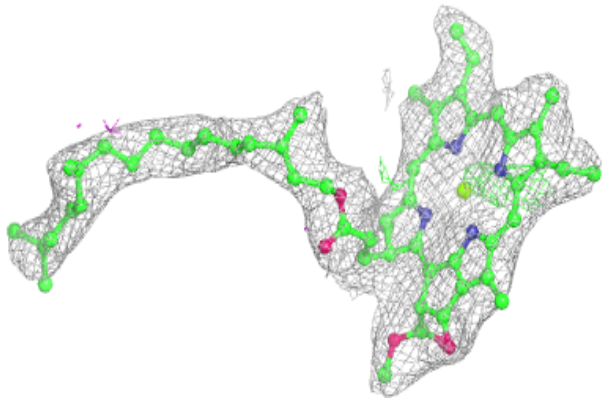


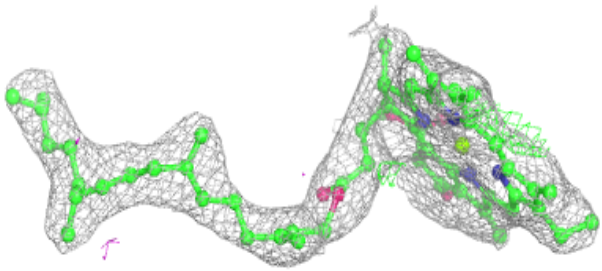


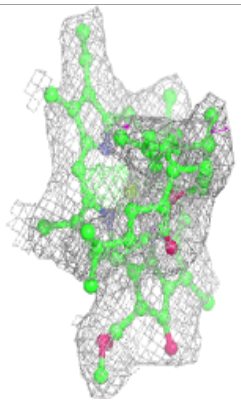


Electron density around CLA A 822:

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

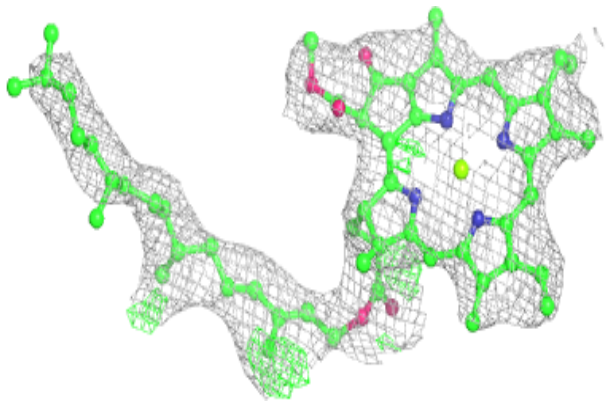


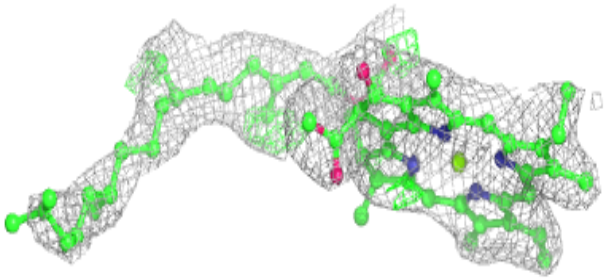


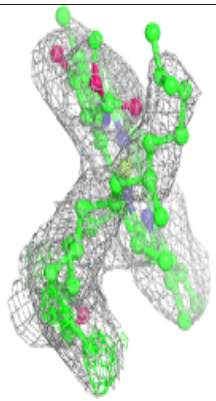


Electron density around CLA A 823:

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

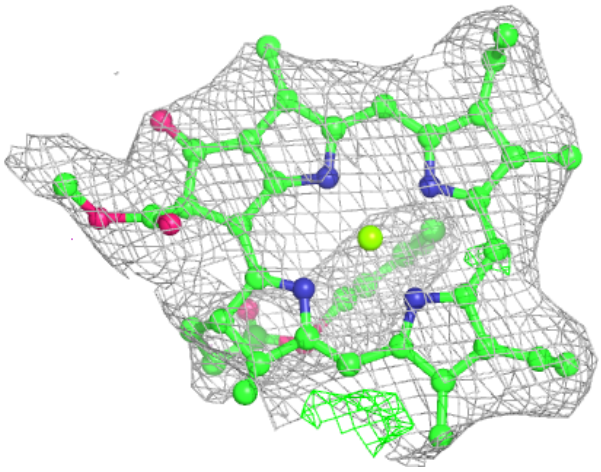


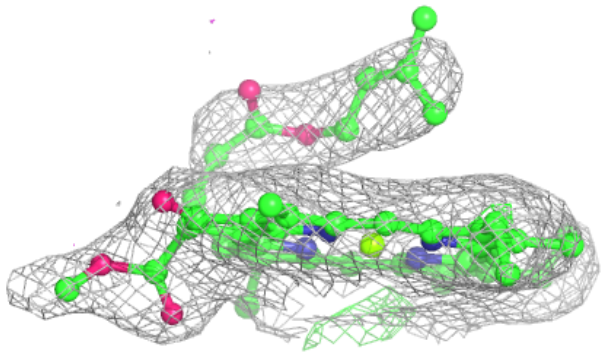


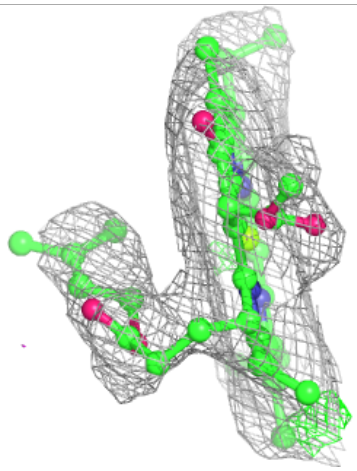


Electron density around CLA A 824:

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

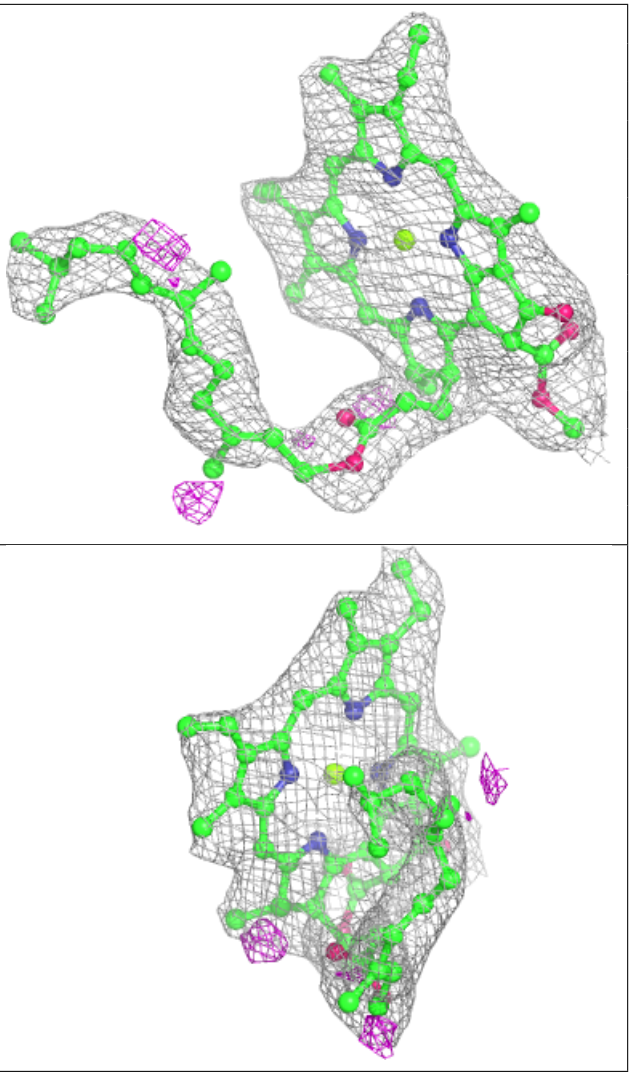






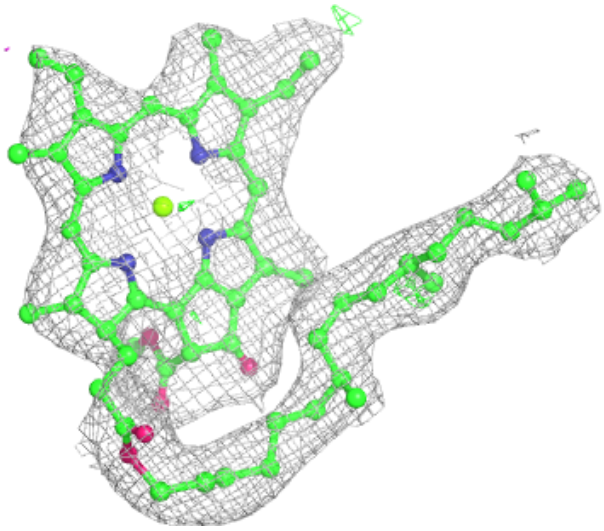
Electron density around CLA A 825:

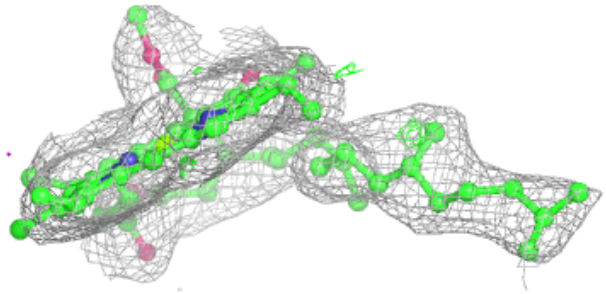
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

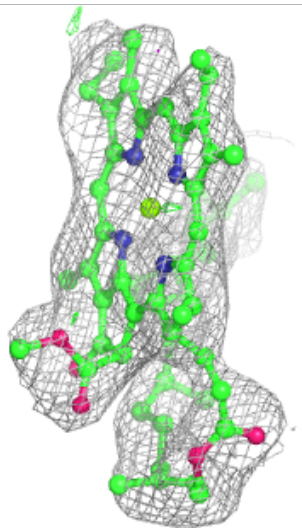


Electron density around CLA A 826:

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

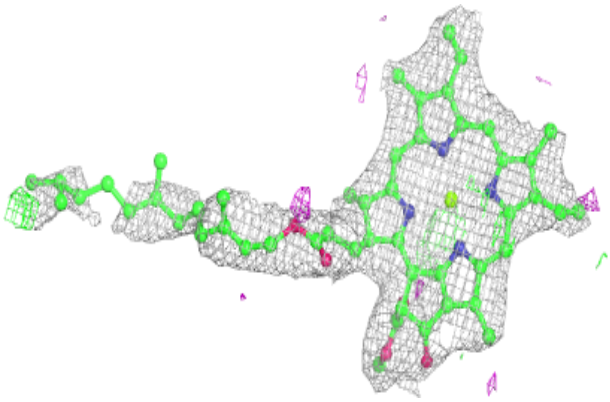


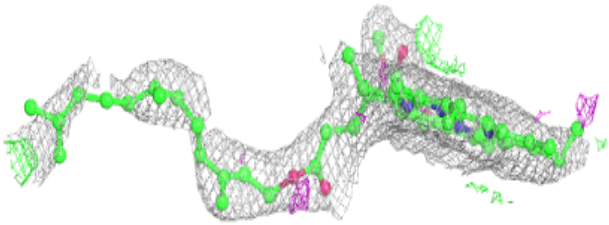


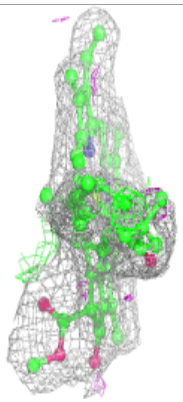


Electron density around CLA A 827:

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

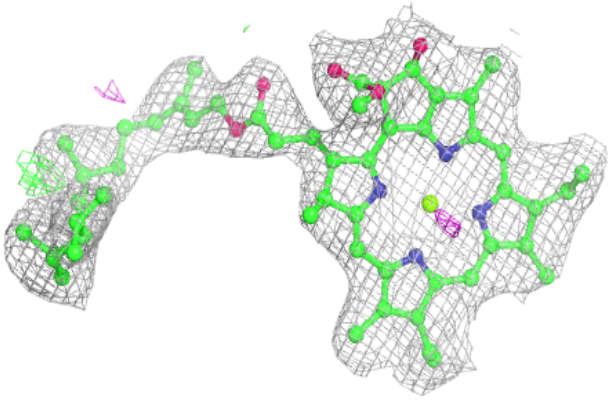


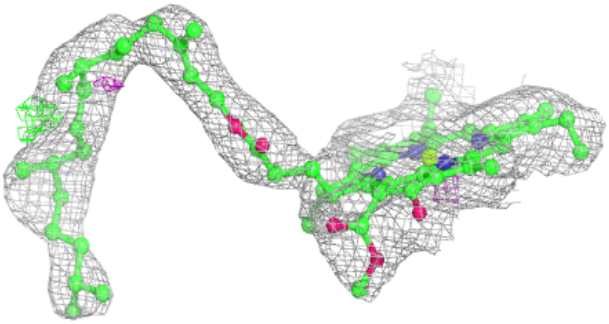


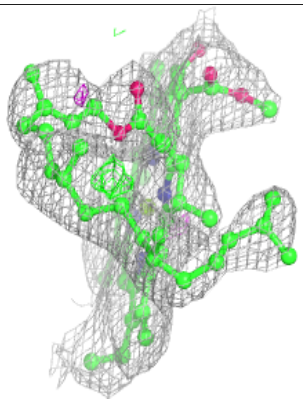


Electron density around CLA A 828:

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

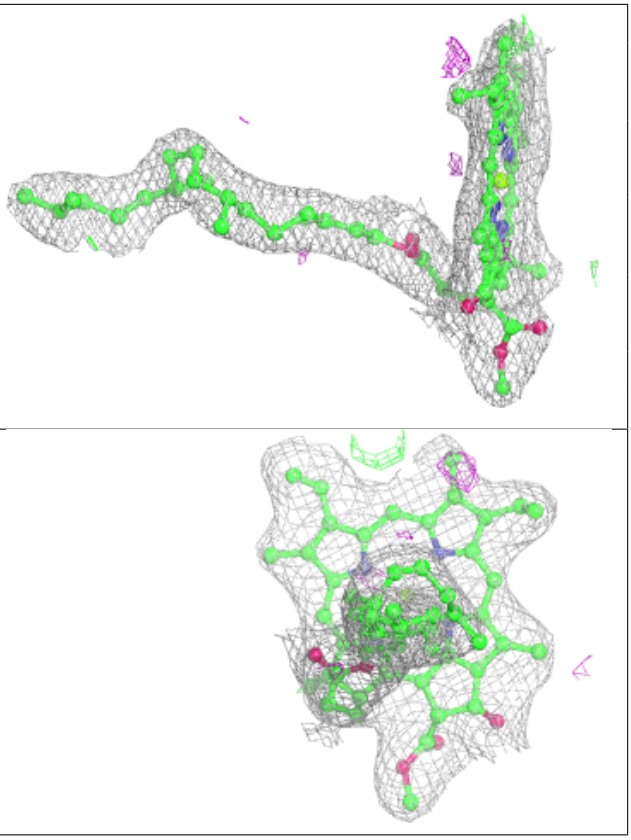






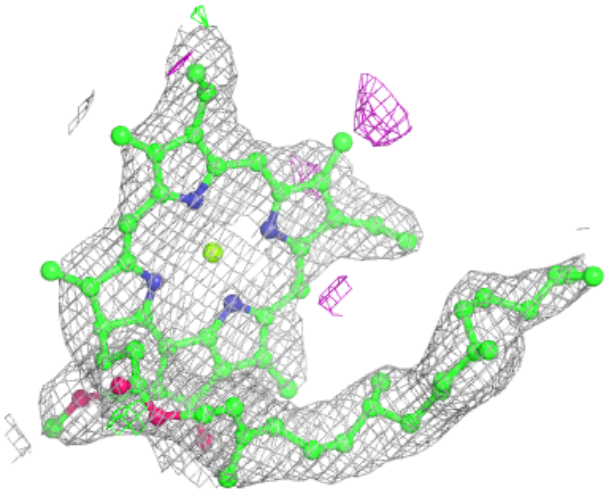
Electron density around CLA A 829:

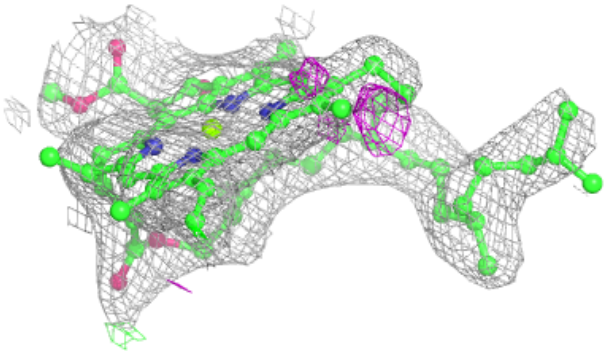
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

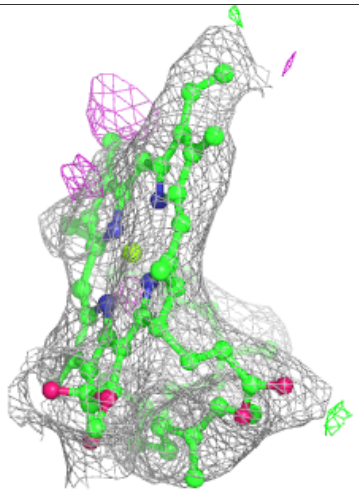


Electron density around CLA A 830:

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

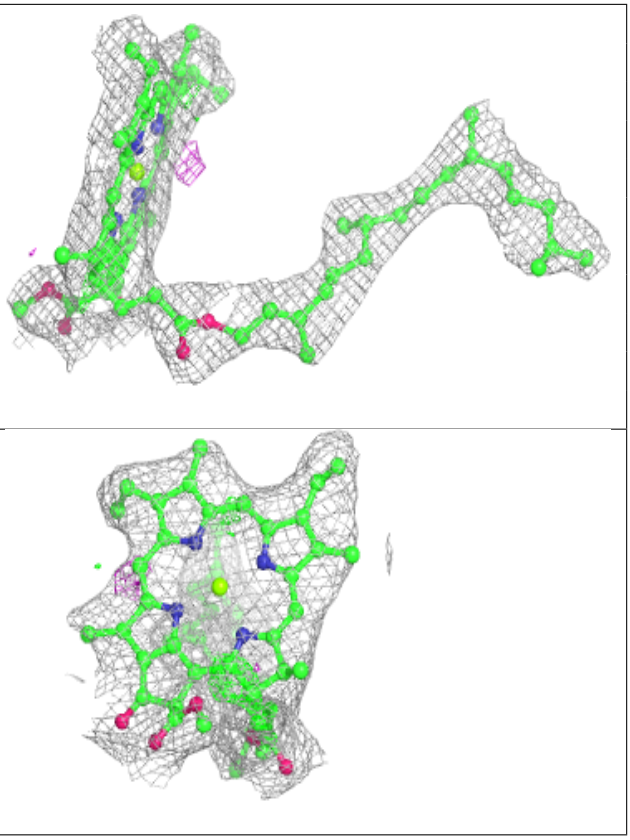






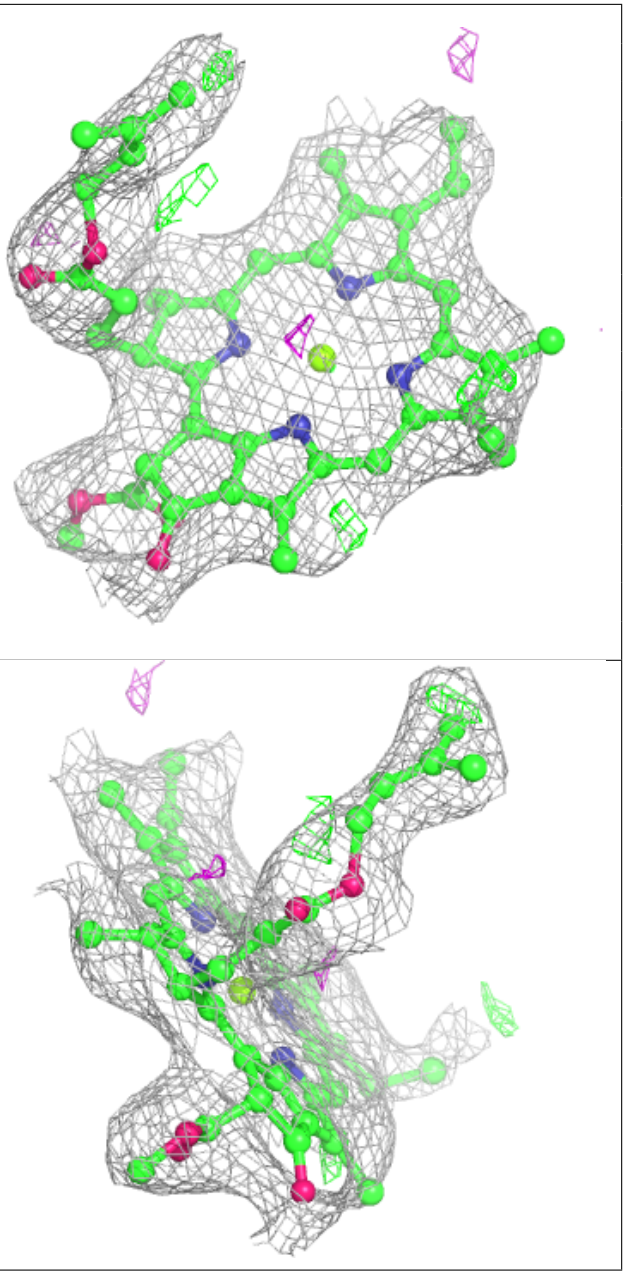
Electron density around CLA A 831:

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



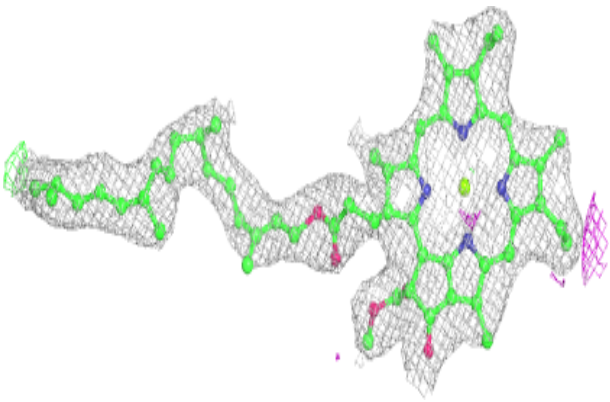
Electron density around CLA A 832:

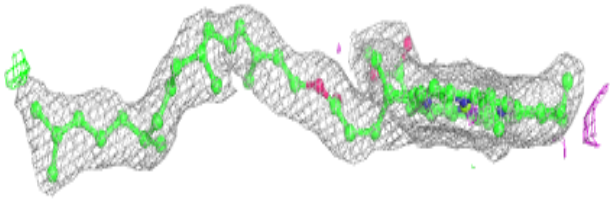
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

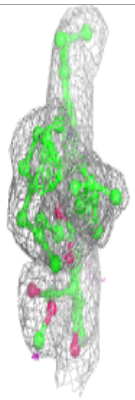


Electron density around CLA A 833:

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

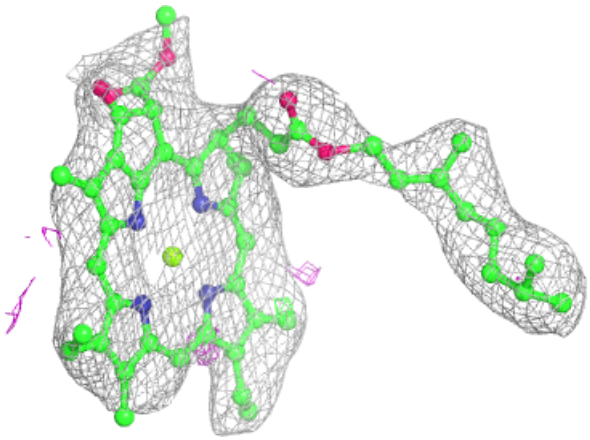


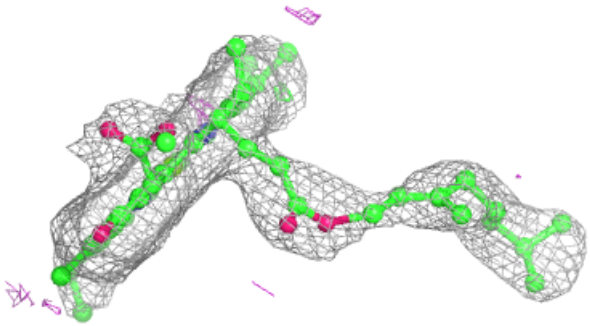


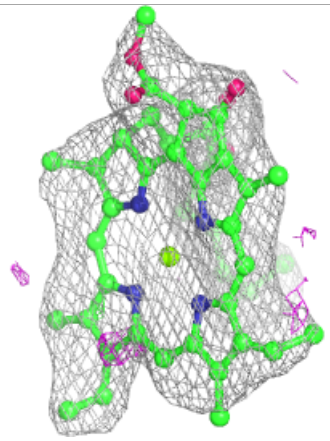


Electron density around CLA A 834:

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

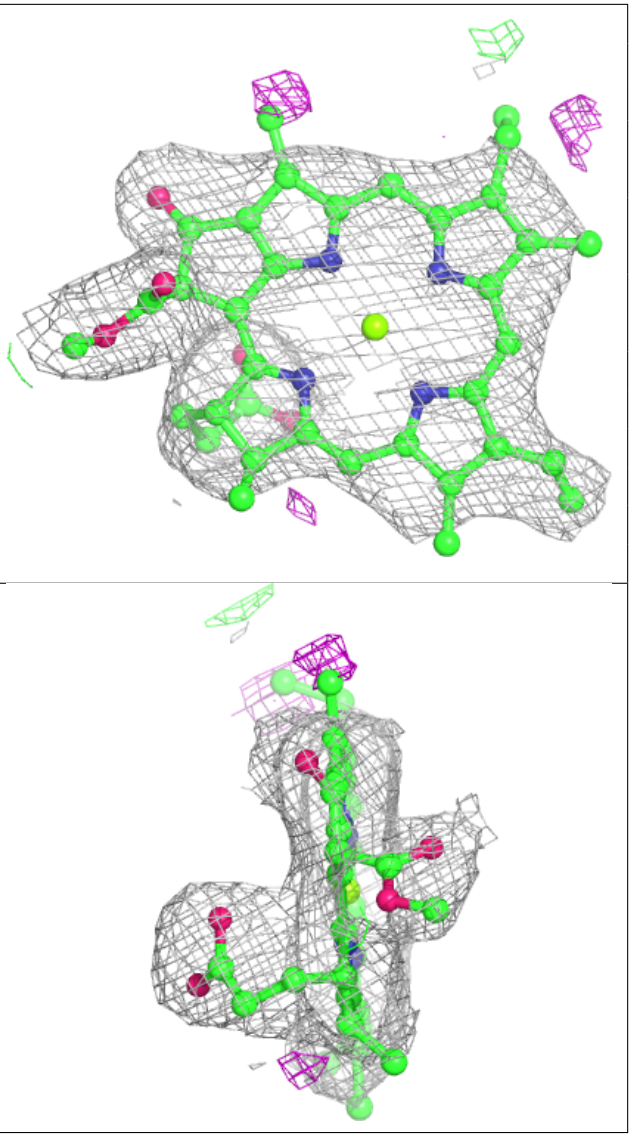






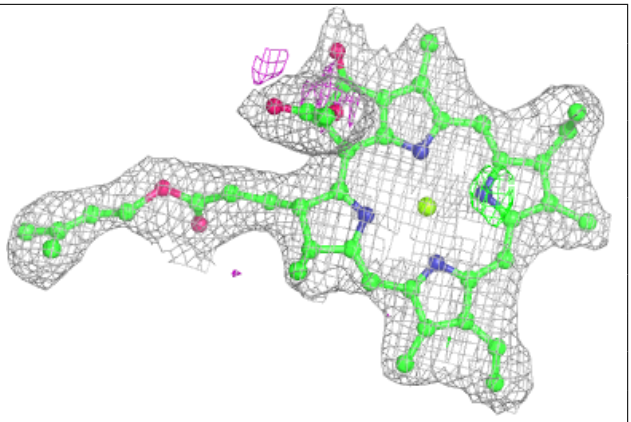
Electron density around CLA A 835:

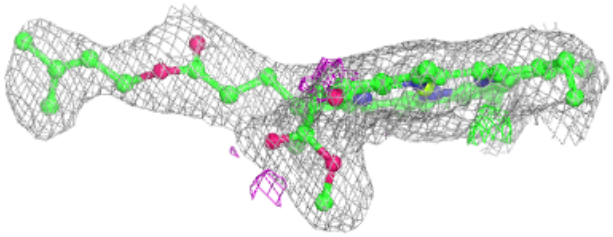
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

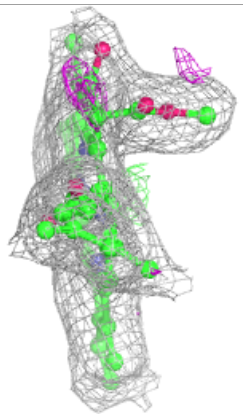


Electron density around CLA A 836:

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

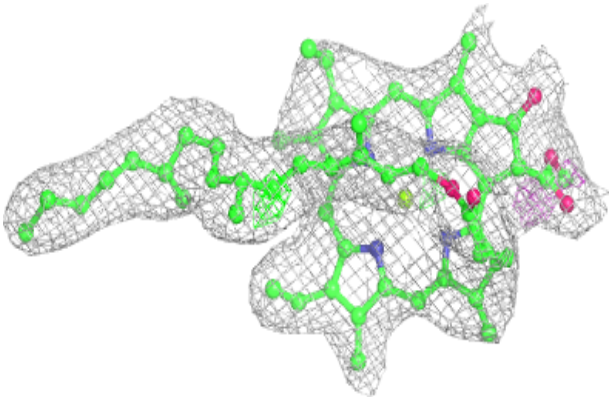


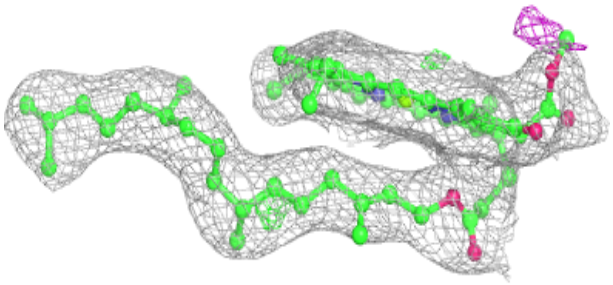


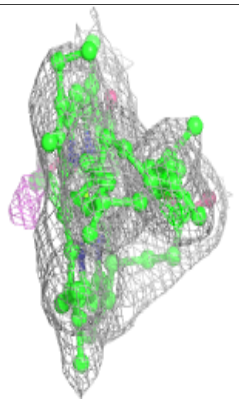


Electron density around CLA A 837:

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

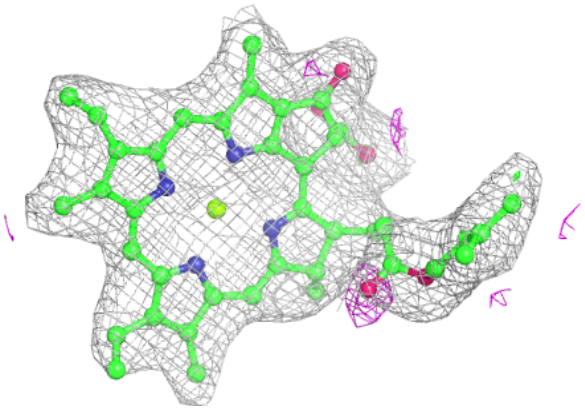


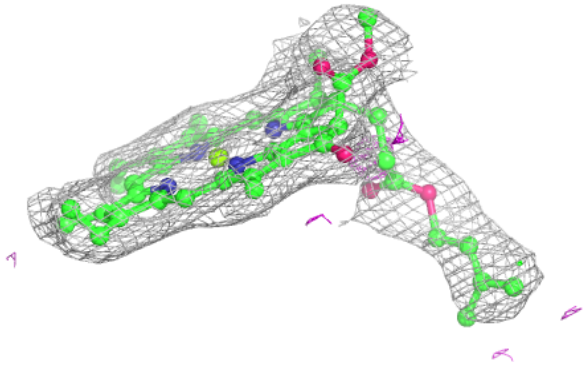


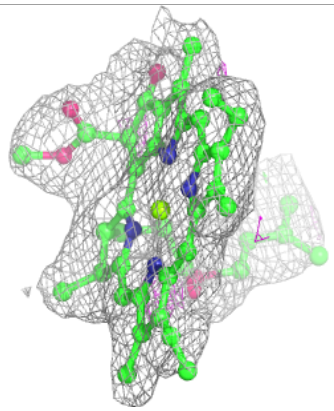


Electron density around CLA A 838:

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

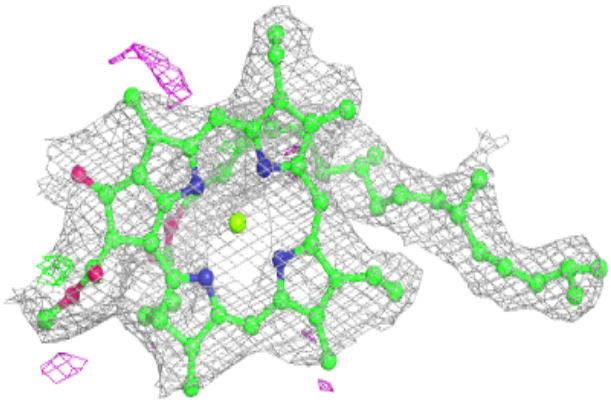


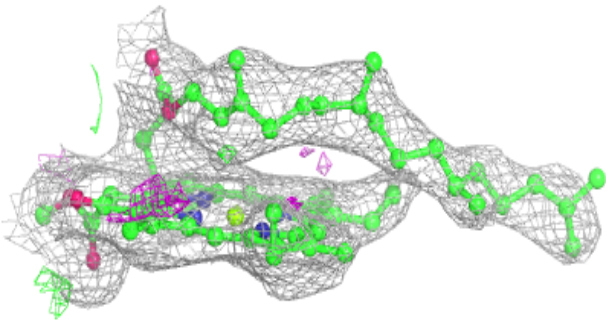


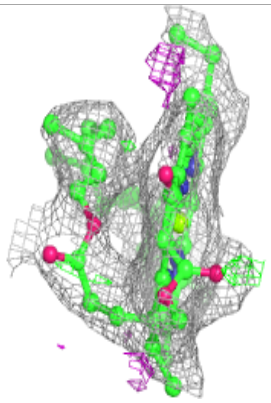


Electron density around CLA A 839:

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

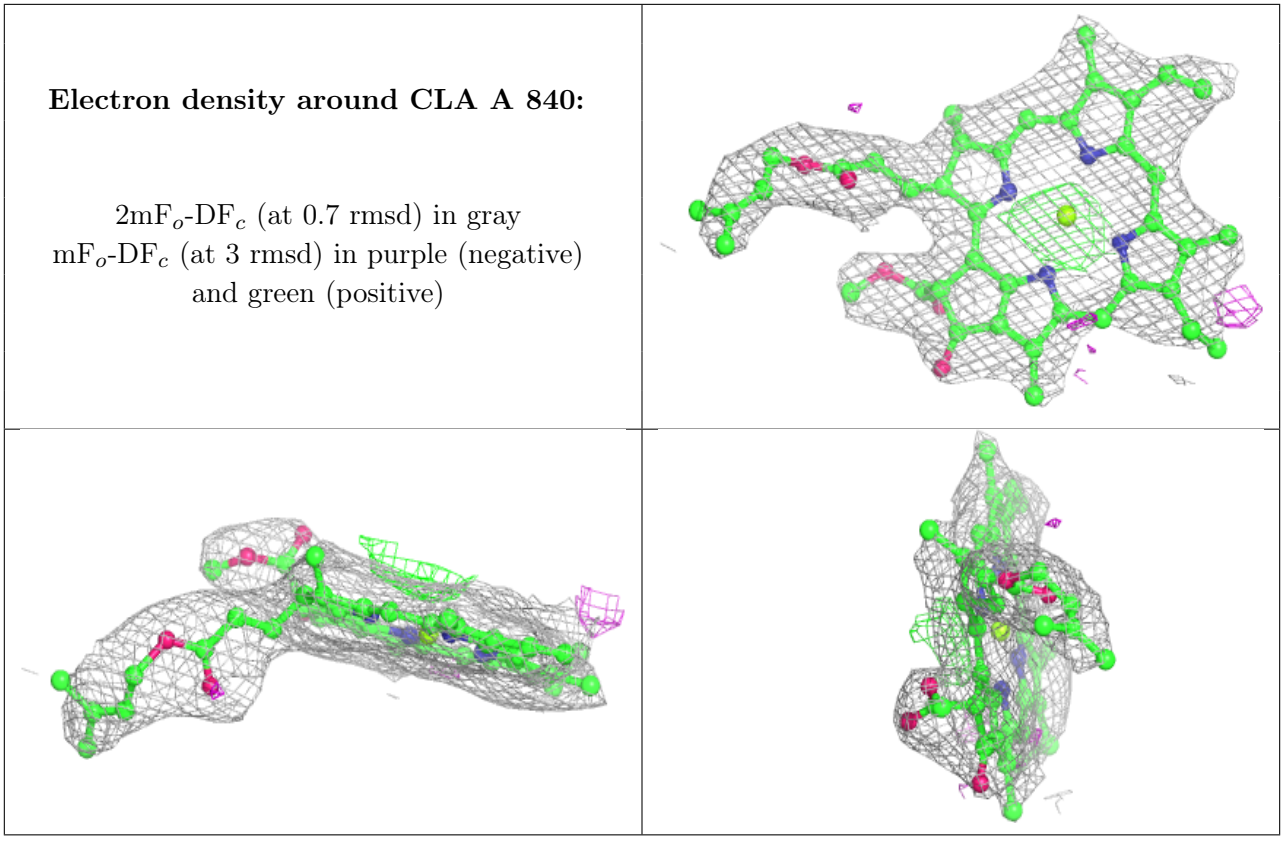






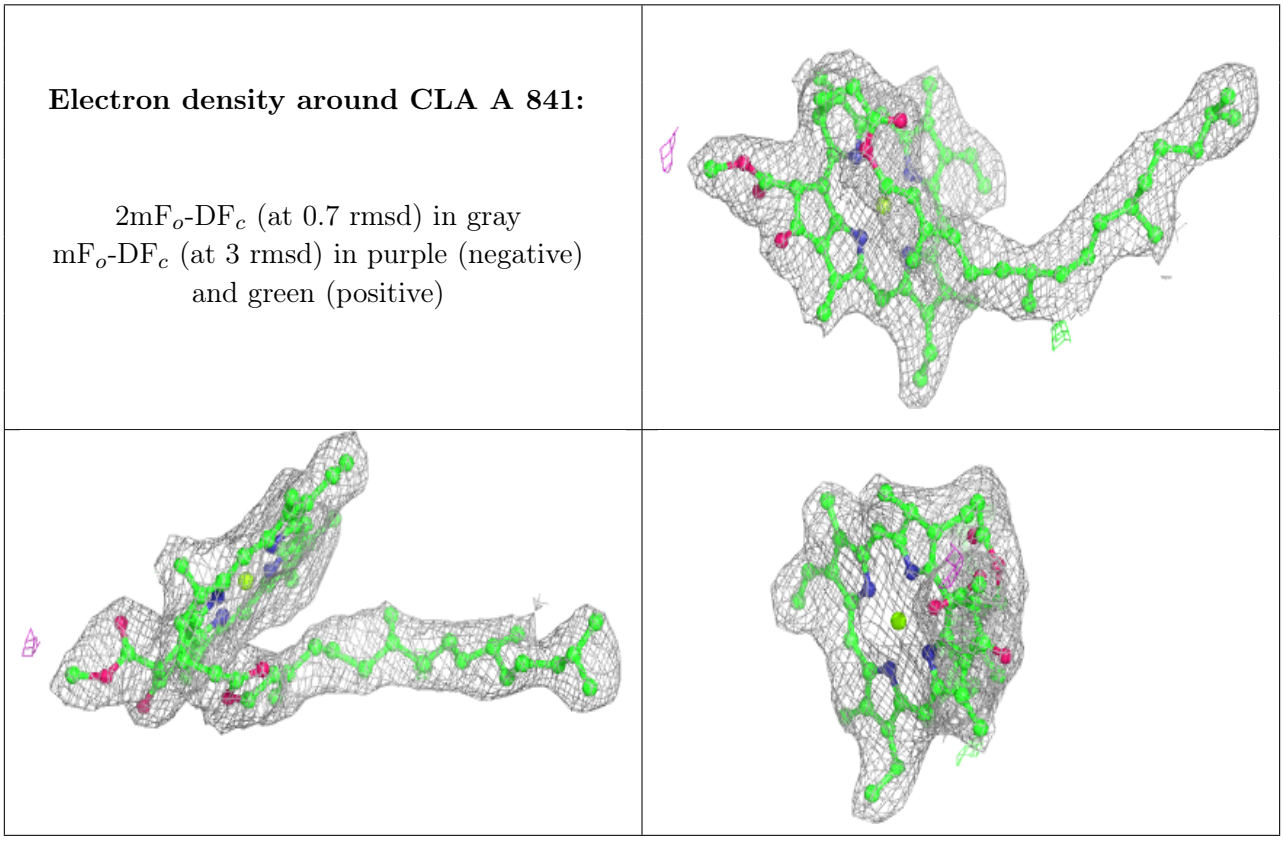
Electron density around CLA A 840:

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



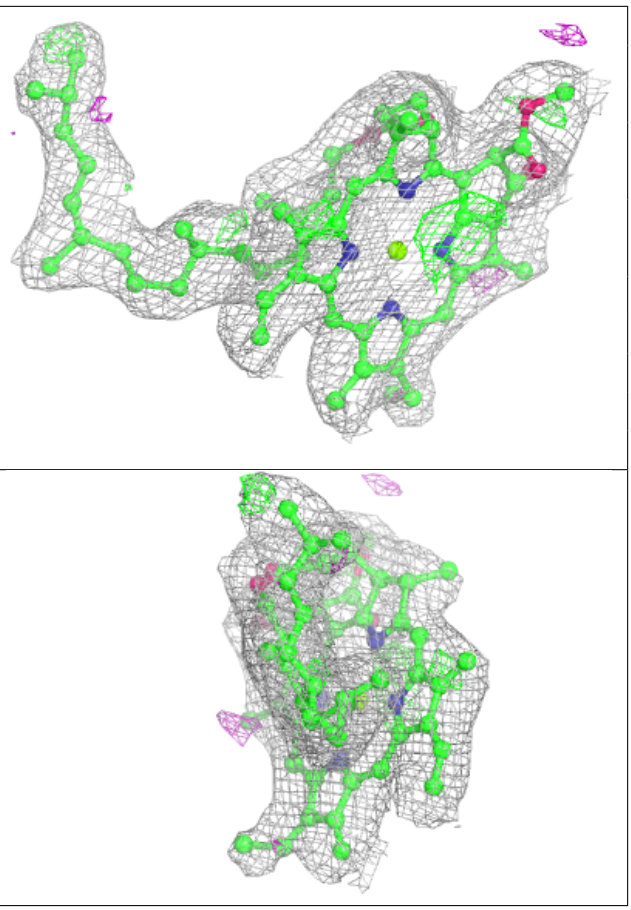
Electron density around CLA A 841:

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



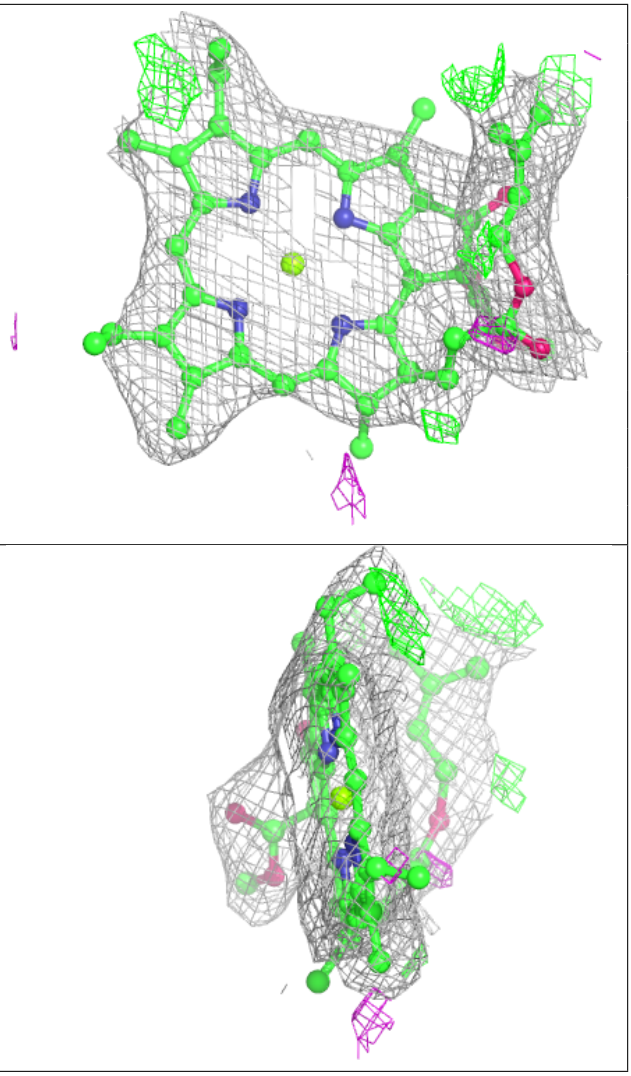
Electron density around CLA A 842:

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



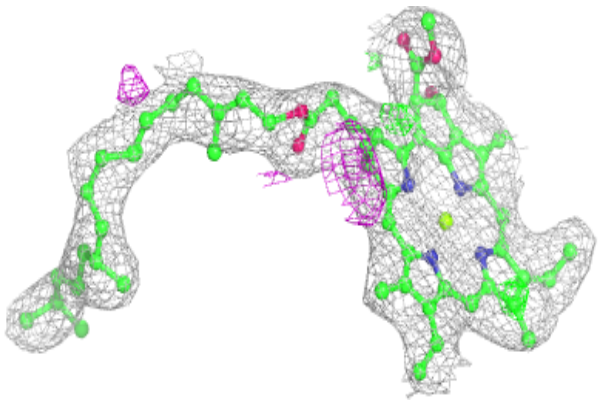
Electron density around CLA A 843:

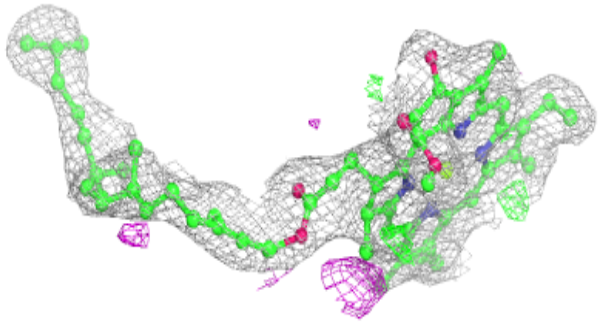
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

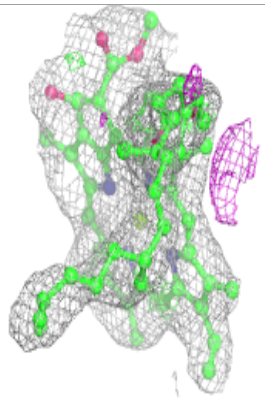


Electron density around CLA A 854:

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

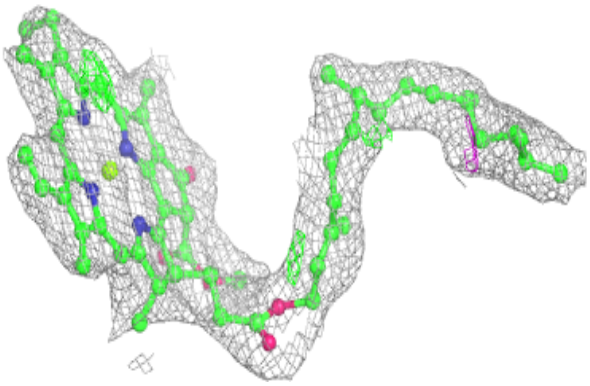


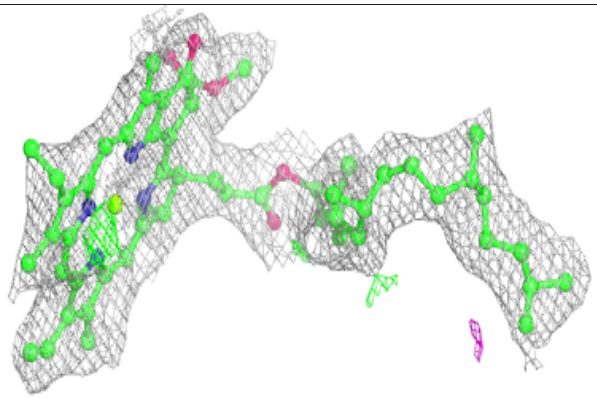


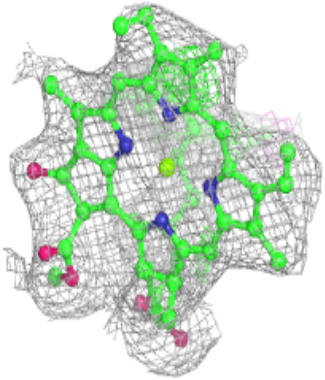


Electron density around CLA B 801:

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

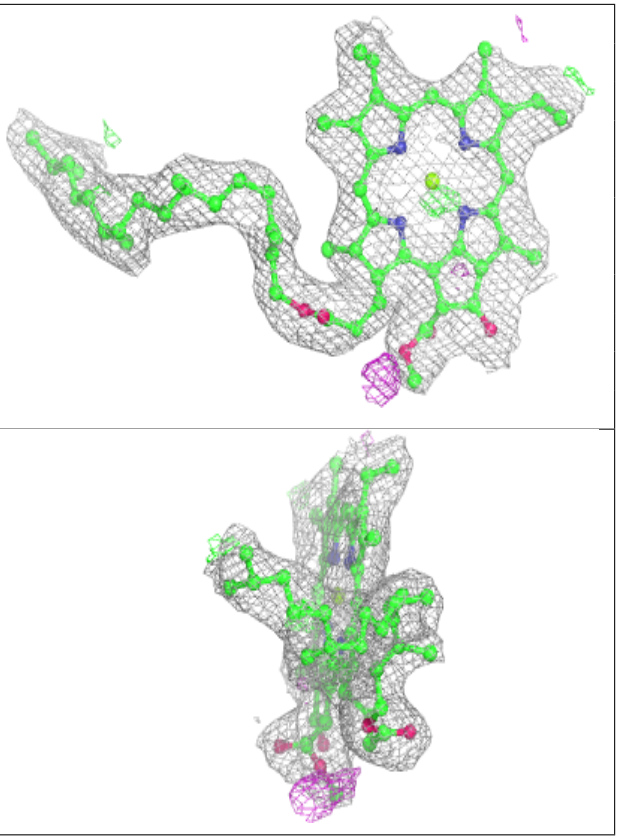


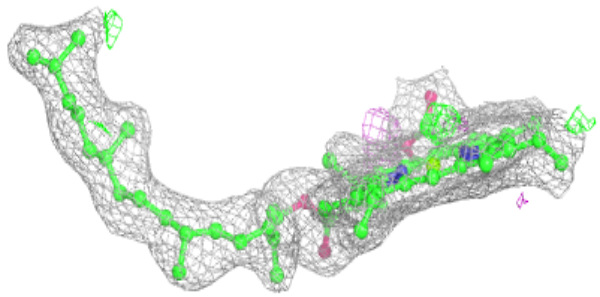




Electron density around CLA B 802:

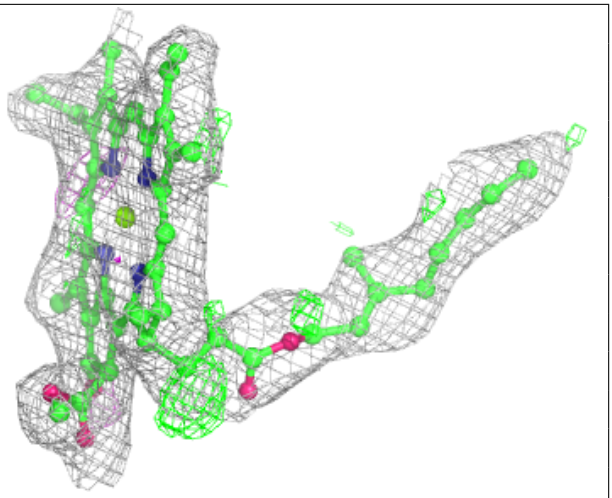
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

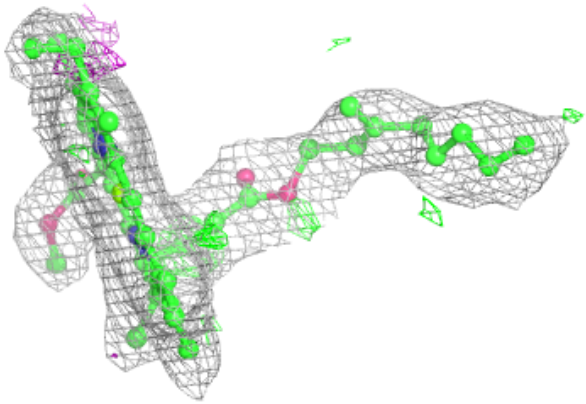


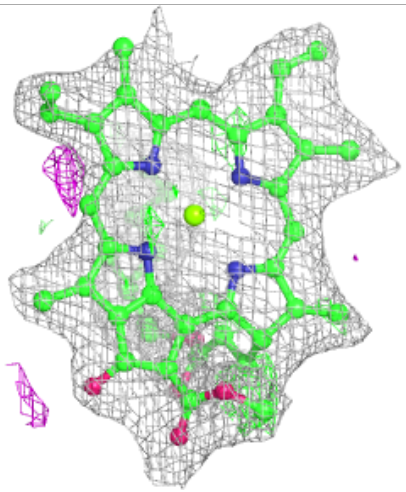


Electron density around CLA B 803:

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)

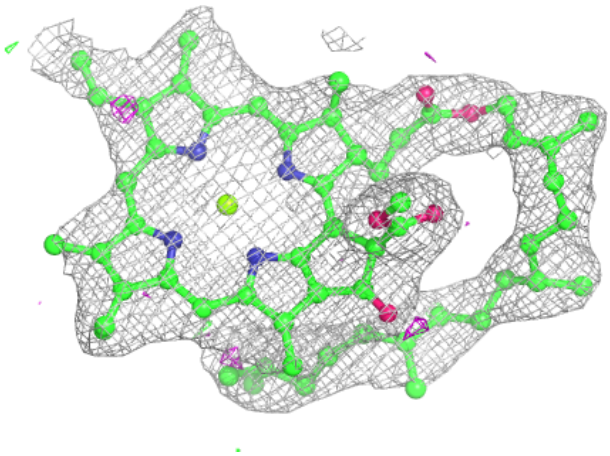


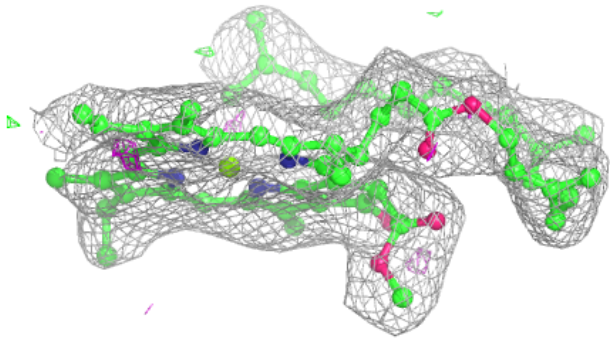


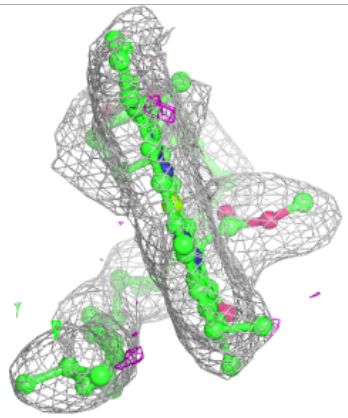


Electron density around CLA B 804:

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)

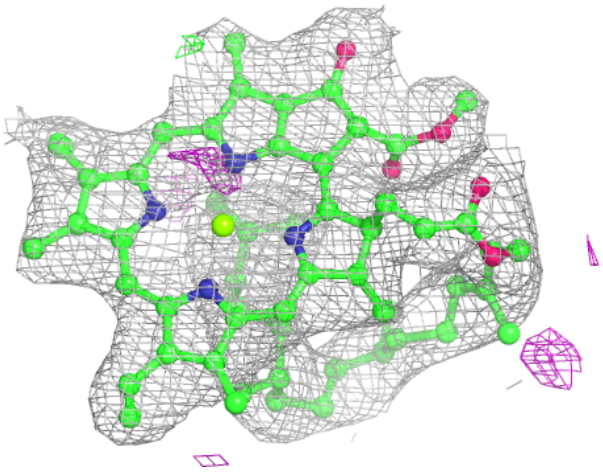


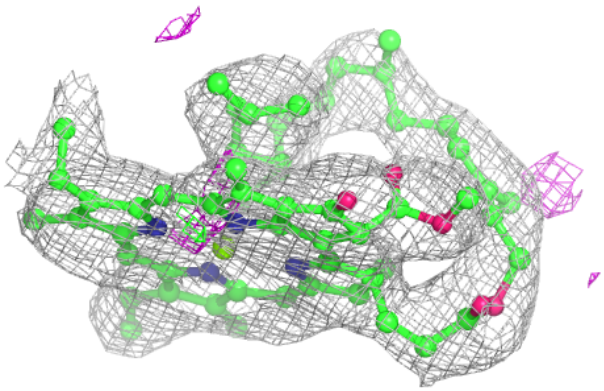


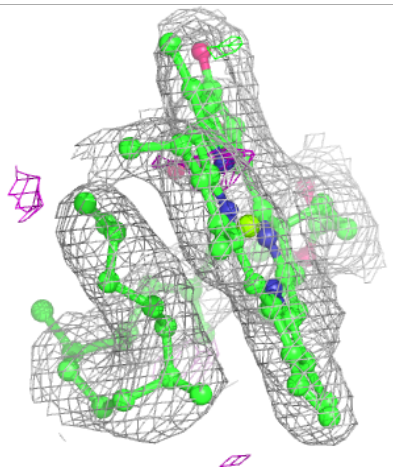


Electron density around CLA B 805:

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

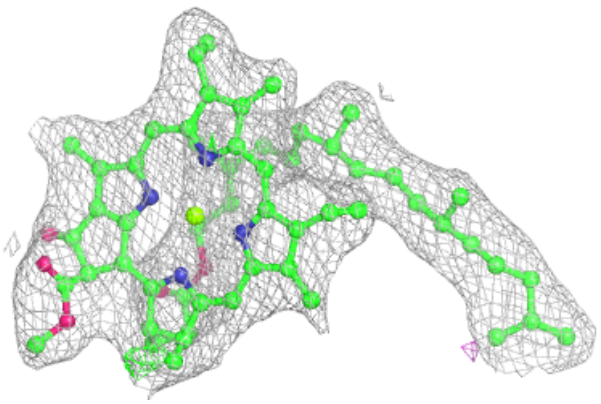


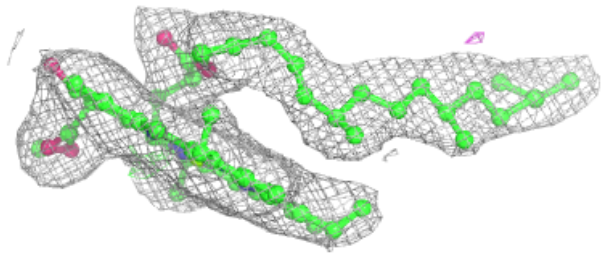


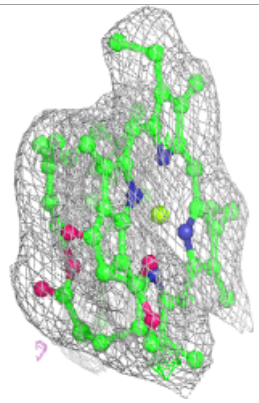


Electron density around CLA B 806:

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

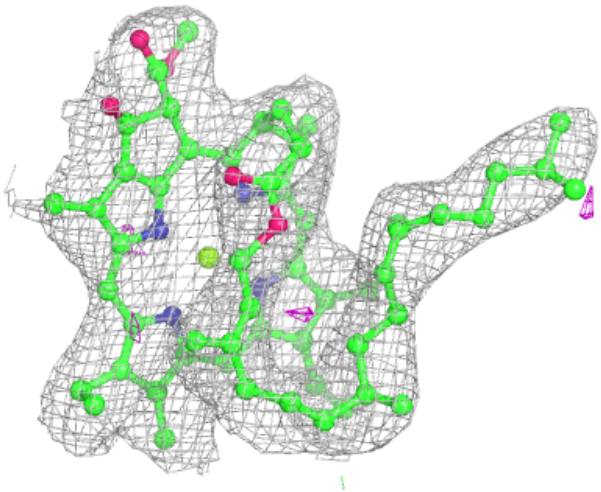


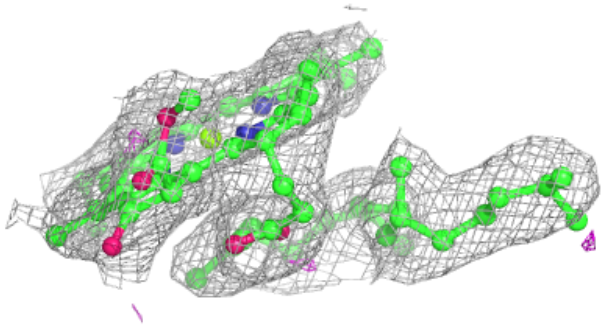


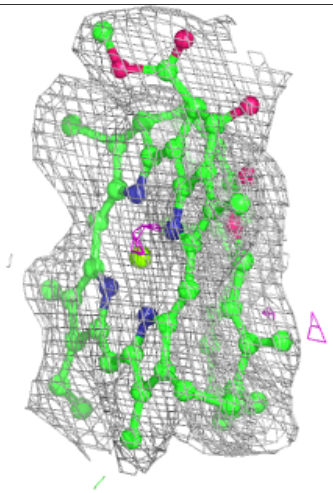


Electron density around CLA B 807:

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

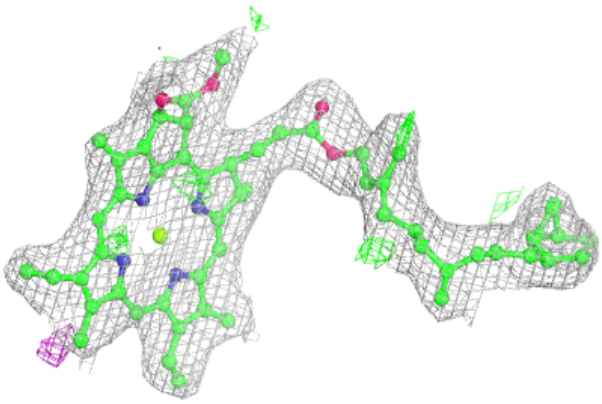


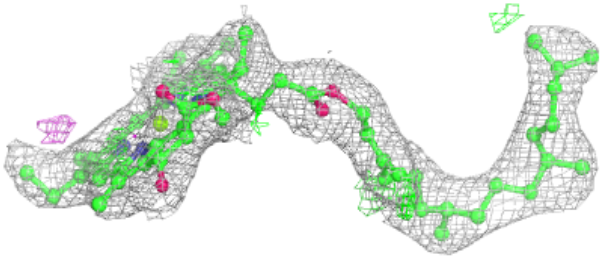


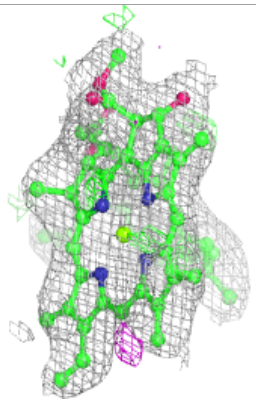


Electron density around CLA B 808:

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

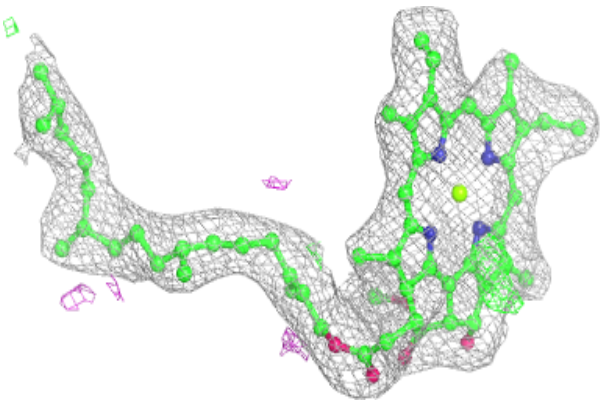


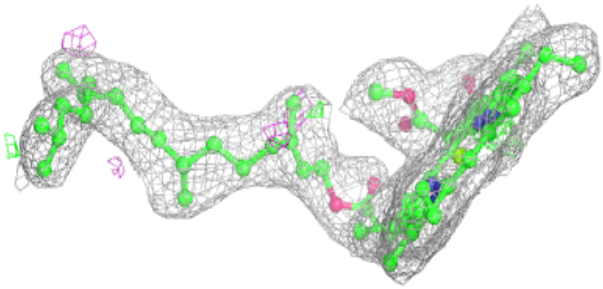


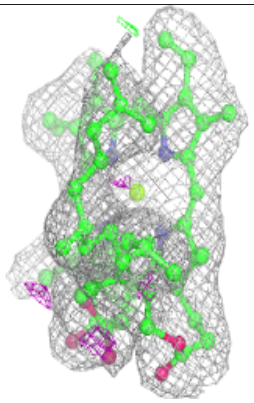


Electron density around CLA B 809:

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

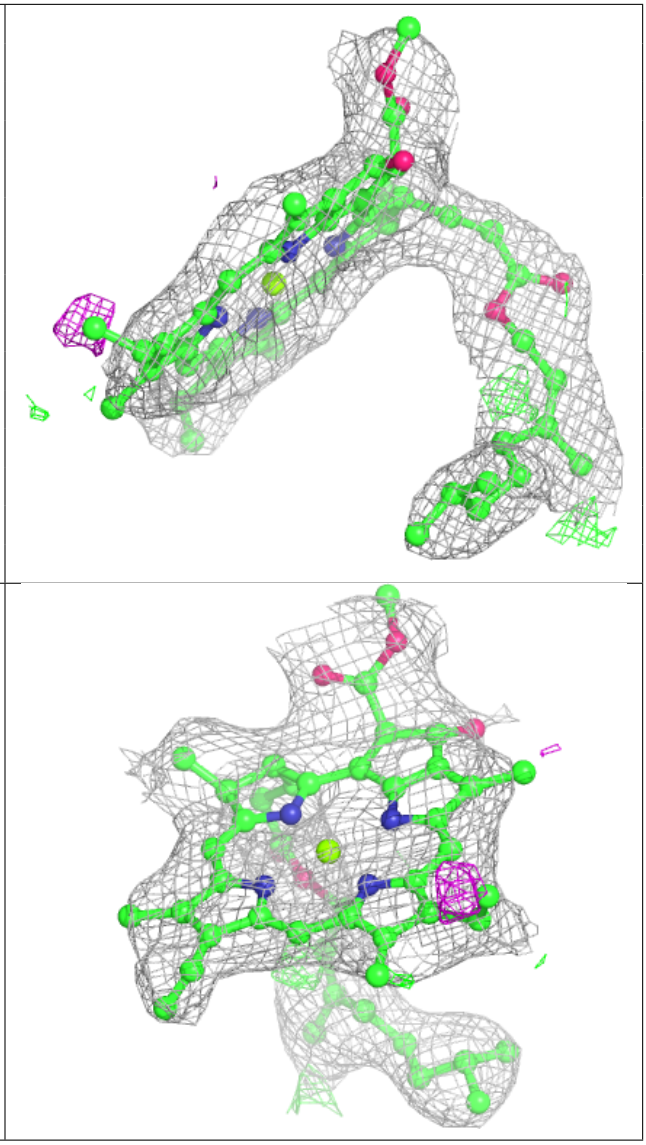






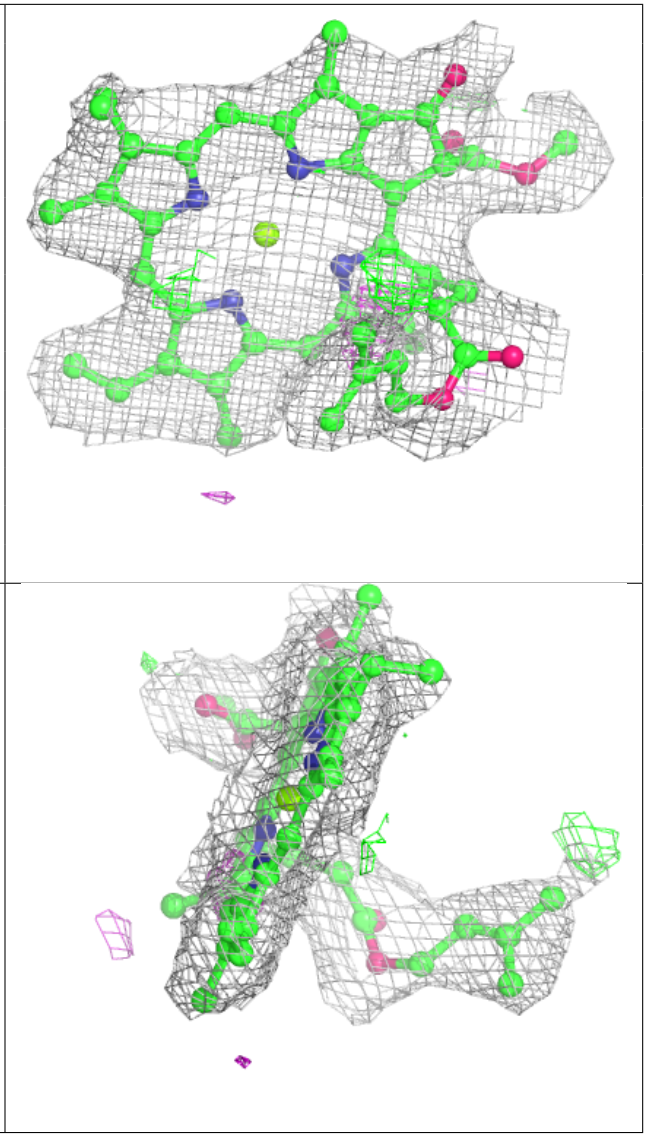
Electron density around CLA B 810:

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



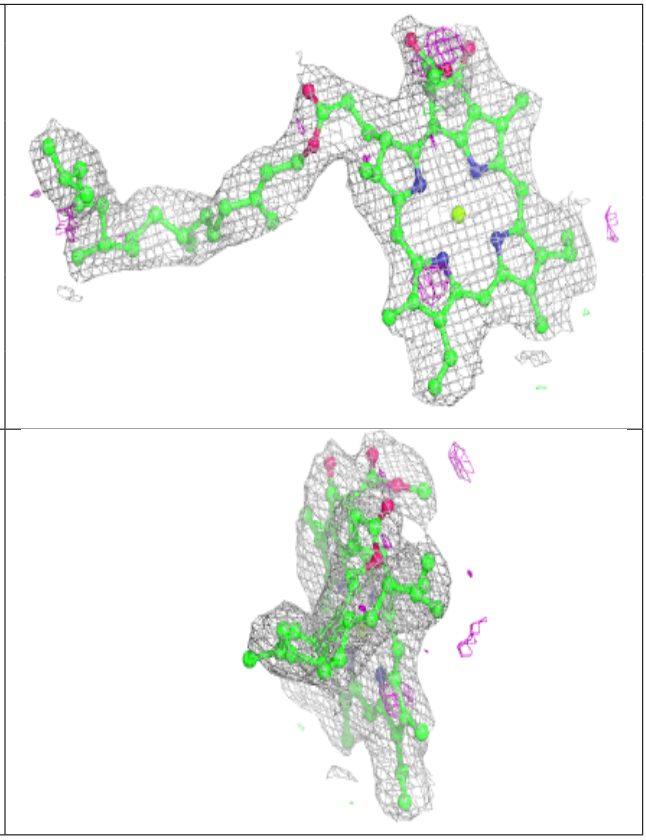
Electron density around CLA B 811:

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



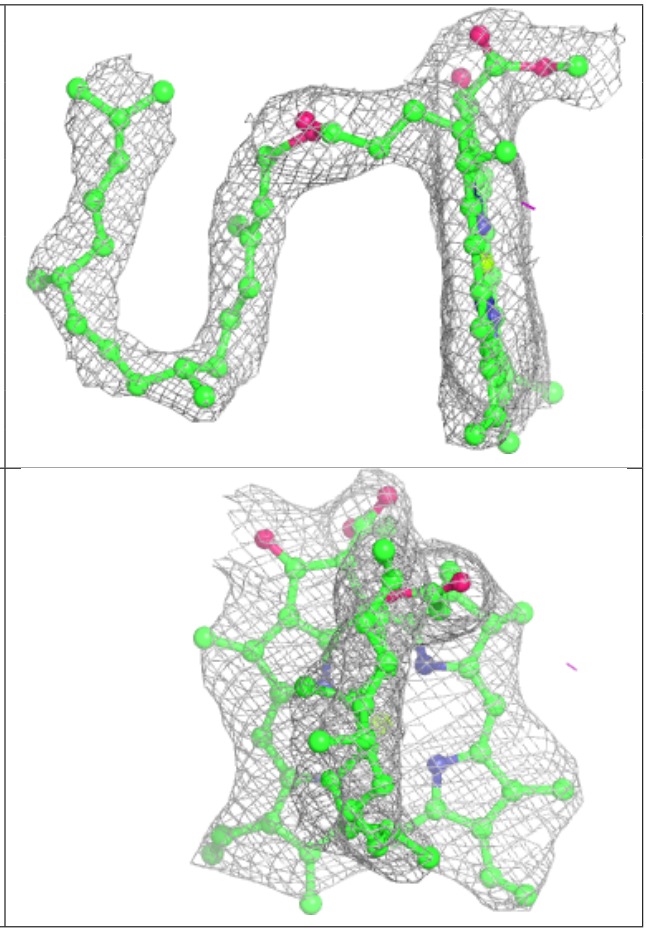
Electron density around CLA B 812:

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



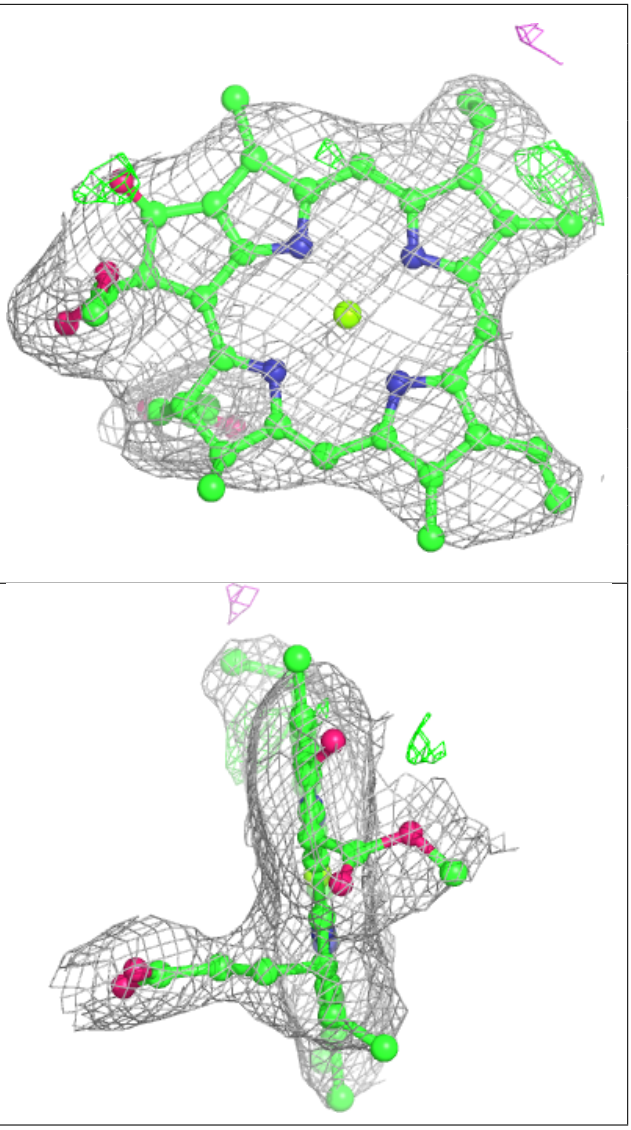
Electron density around CLA B 813:

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



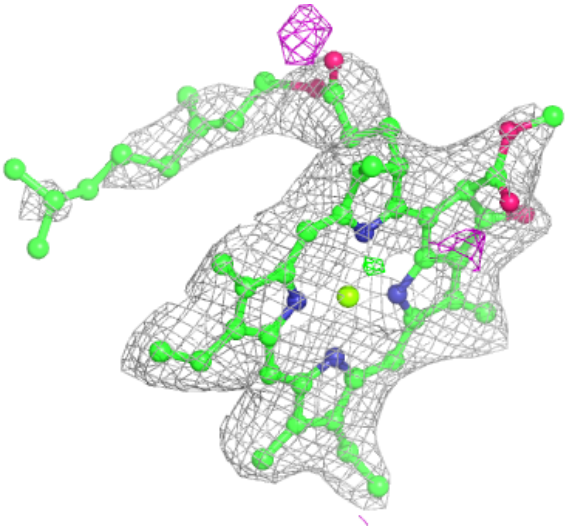
Electron density around CLA B 814:

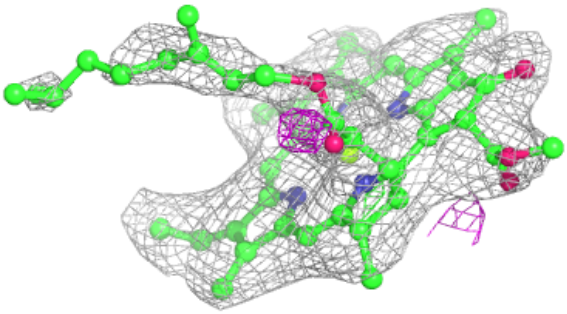
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

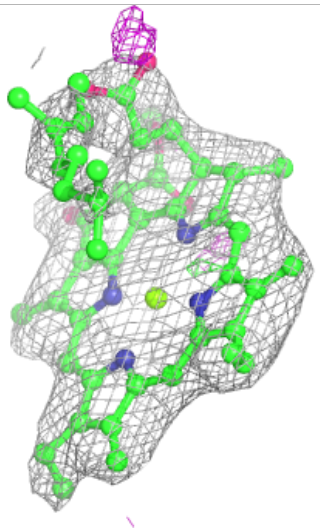


Electron density around CLA B 815:

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

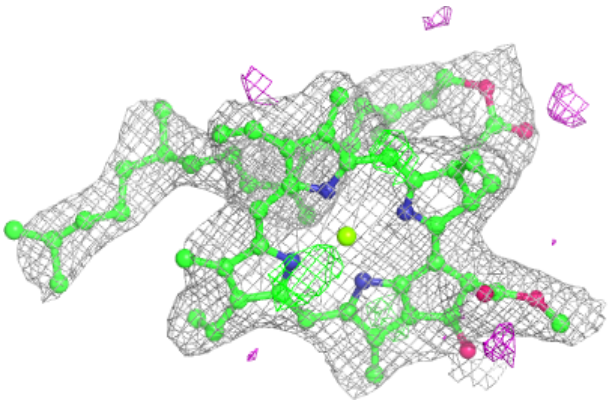


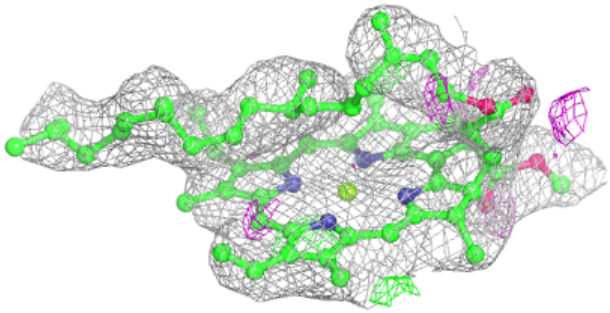


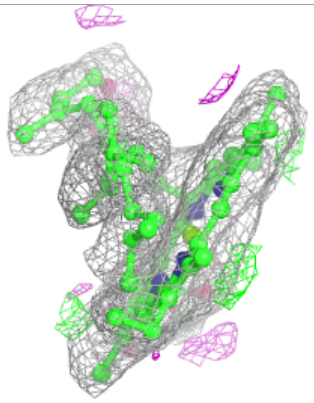


Electron density around CLA B 816:

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

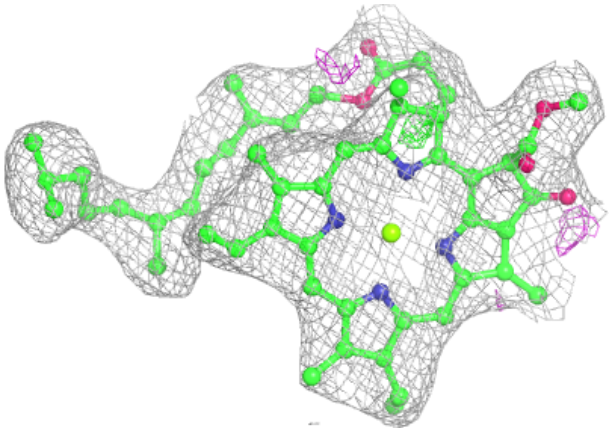


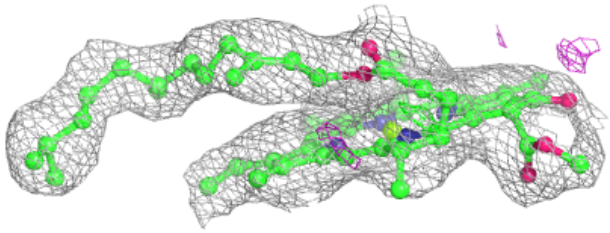


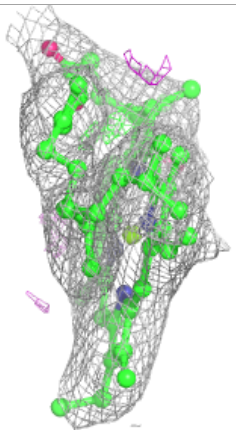


Electron density around CLA B 817:

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

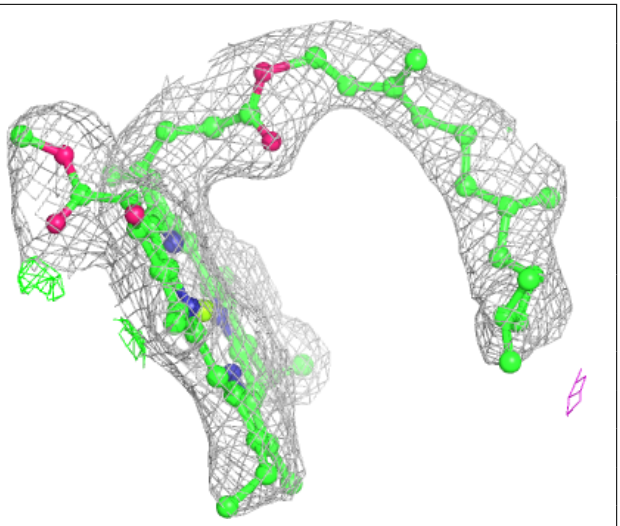


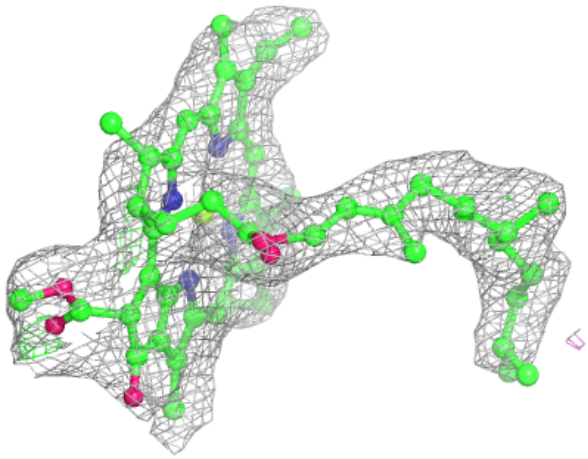


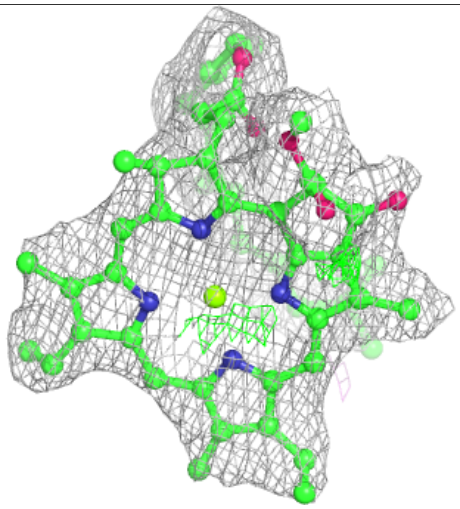


Electron density around CLA B 818:

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)

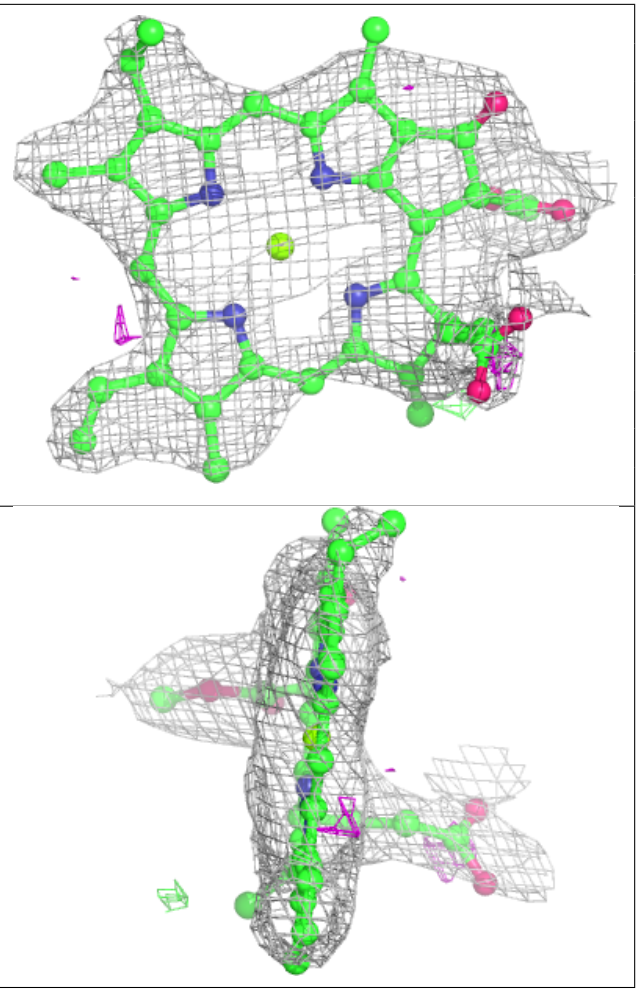






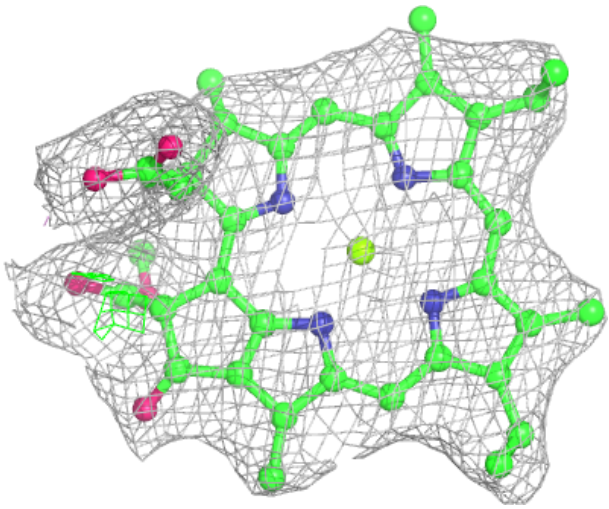
Electron density around CLA B 819:

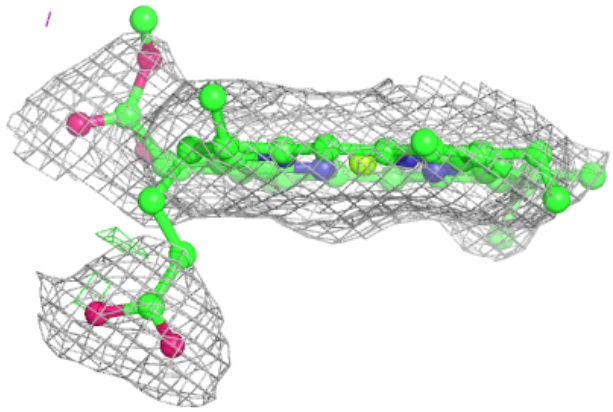
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

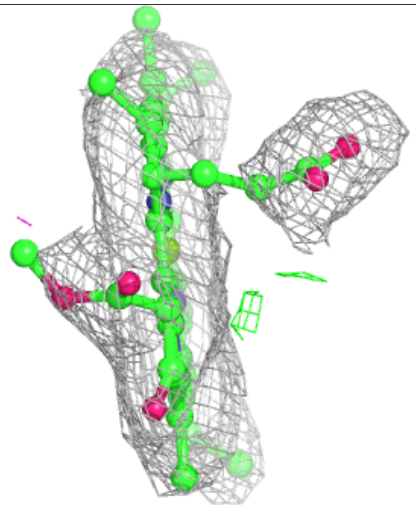


Electron density around CLA B 820:

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

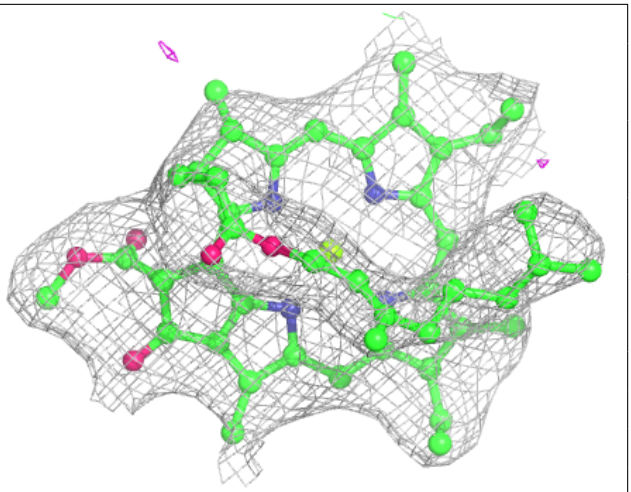


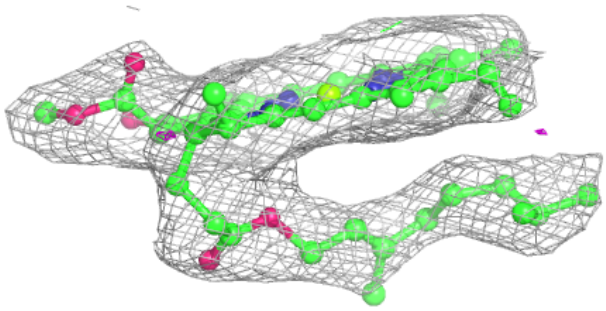


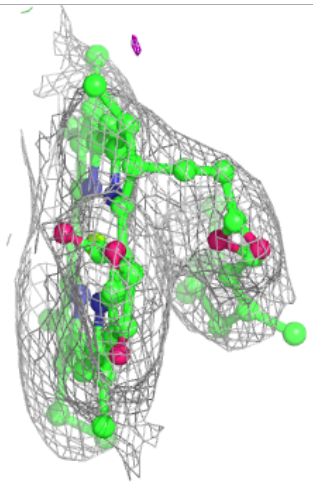


Electron density around CLA B 821:

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

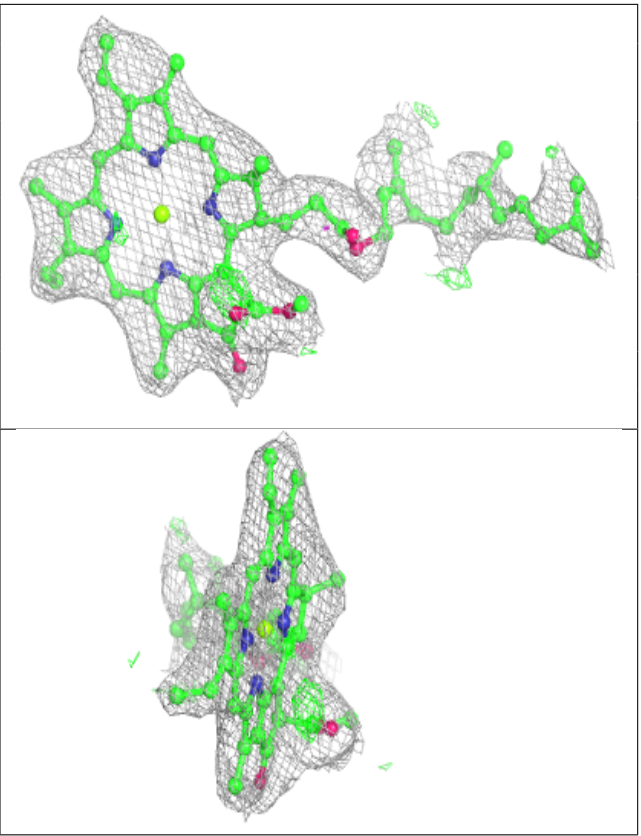


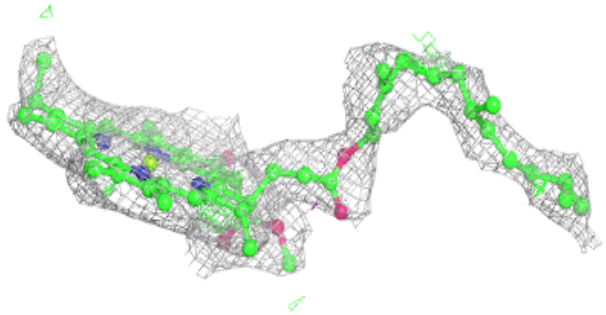




Electron density around CLA B 822:

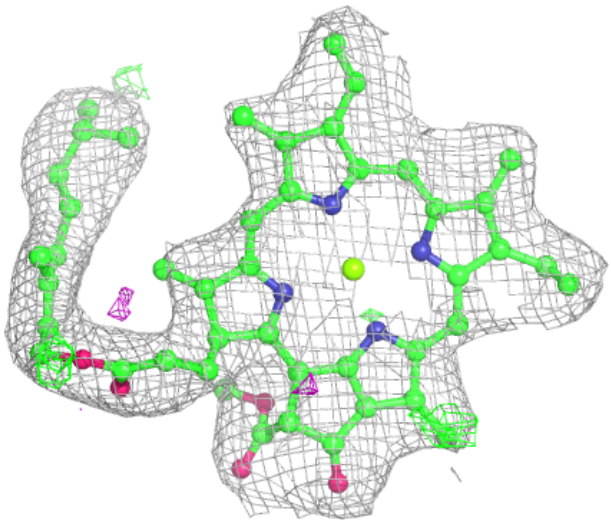
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

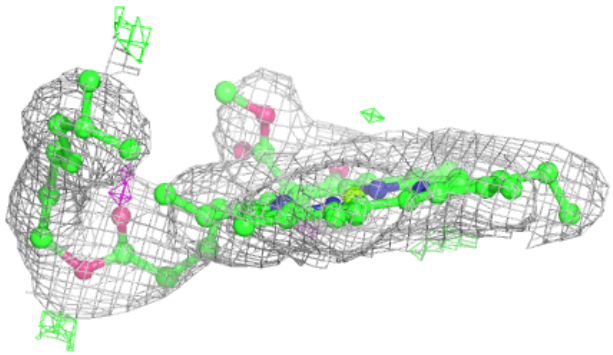


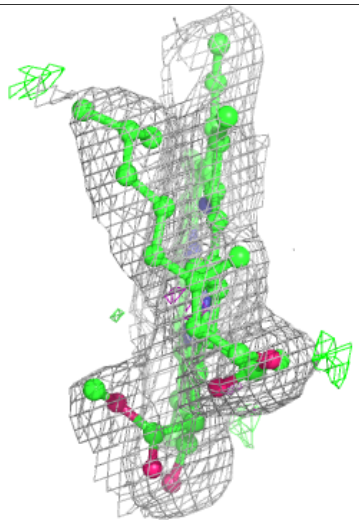


Electron density around CLA B 823:

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

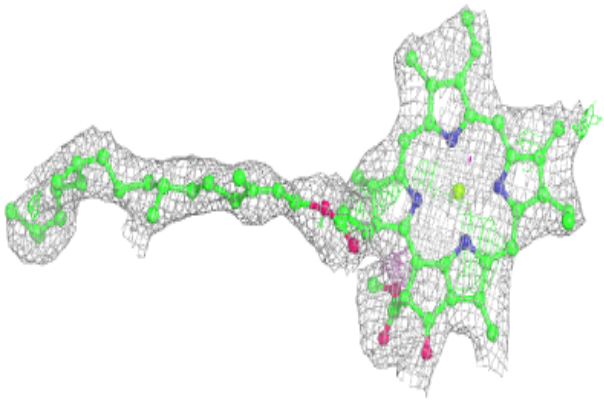


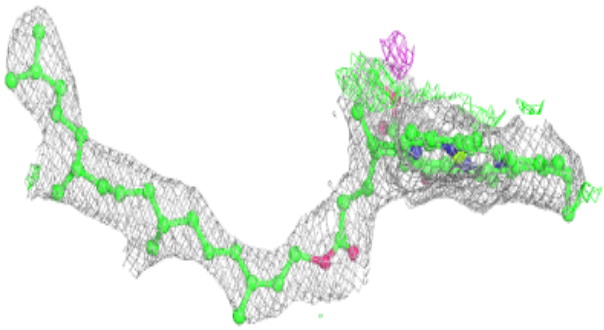


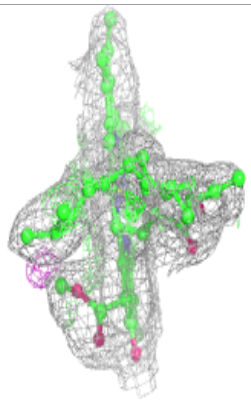


Electron density around CLA B 824:

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

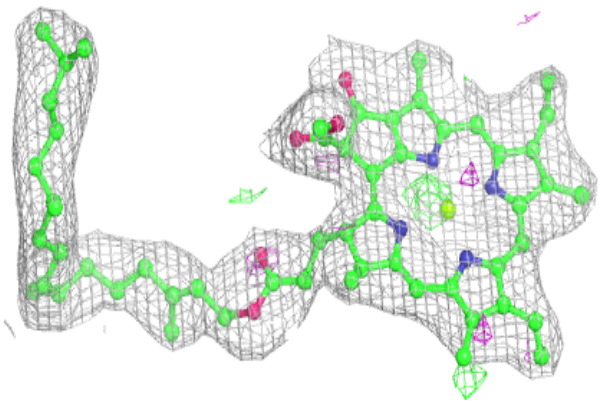


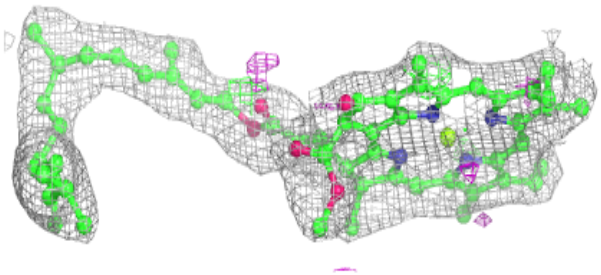


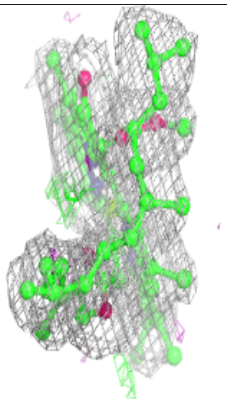


Electron density around CLA B 825:

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

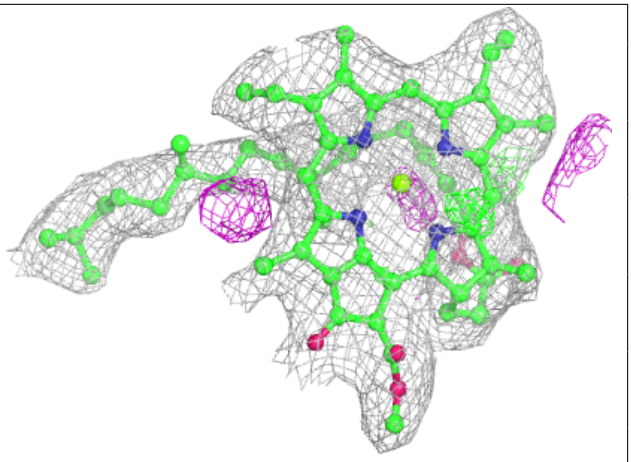


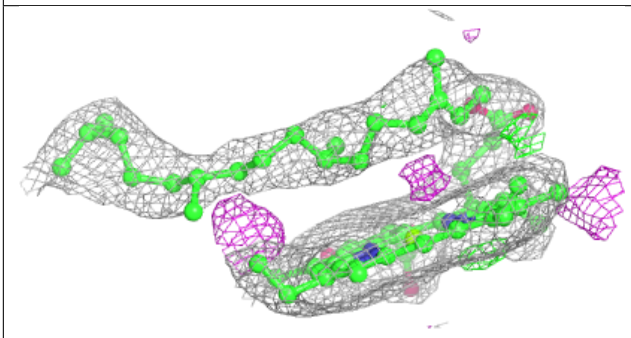


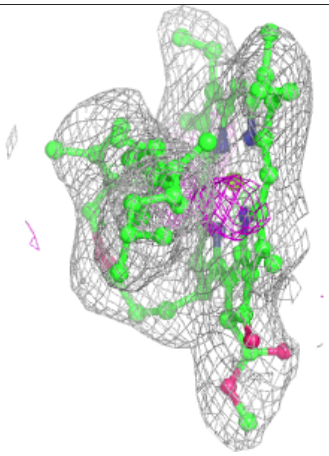


Electron density around CLA B 826:

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

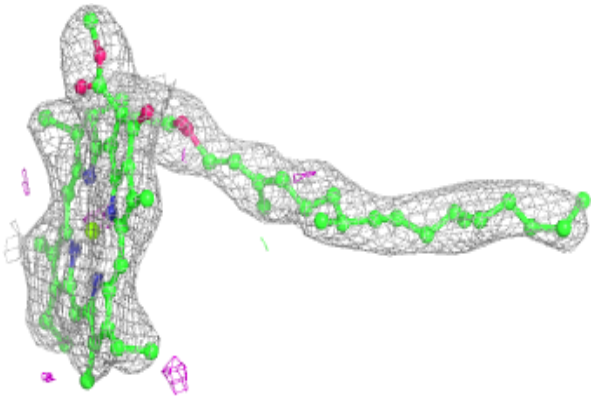


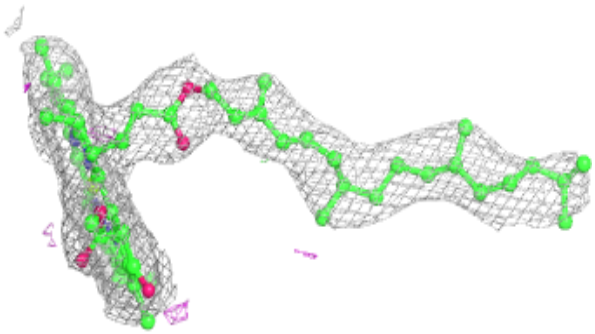


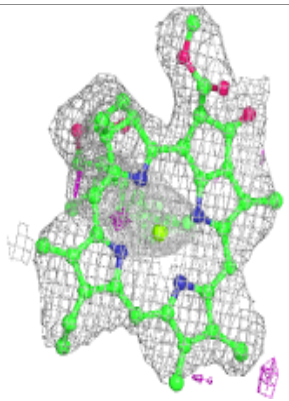


Electron density around CLA B 827:

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

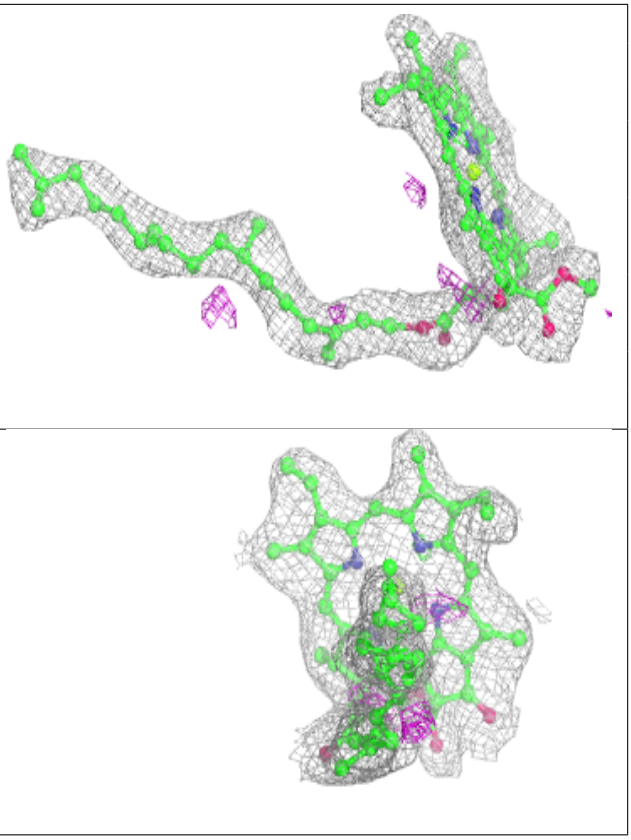






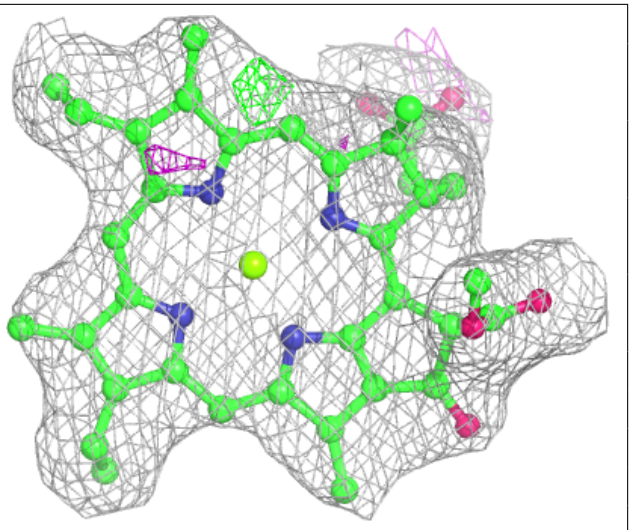
Electron density around CLA B 828:

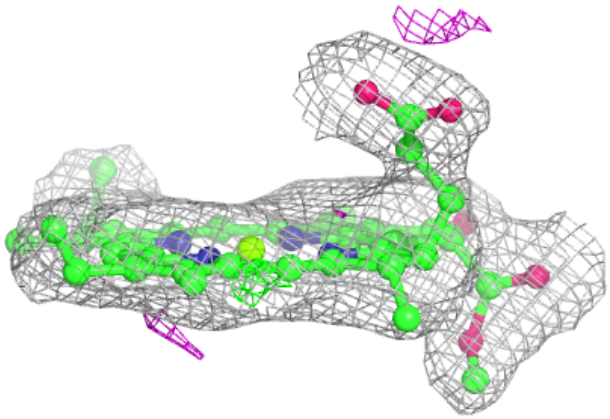
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

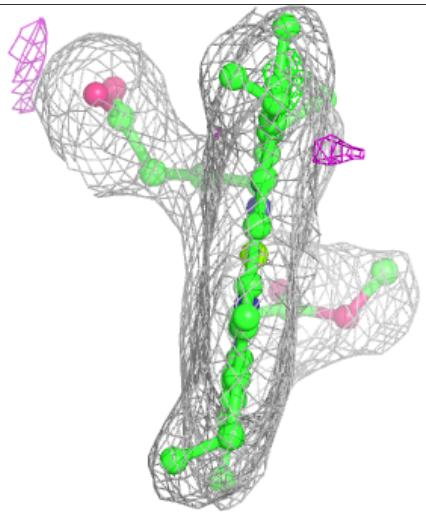


Electron density around CLA B 829:

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

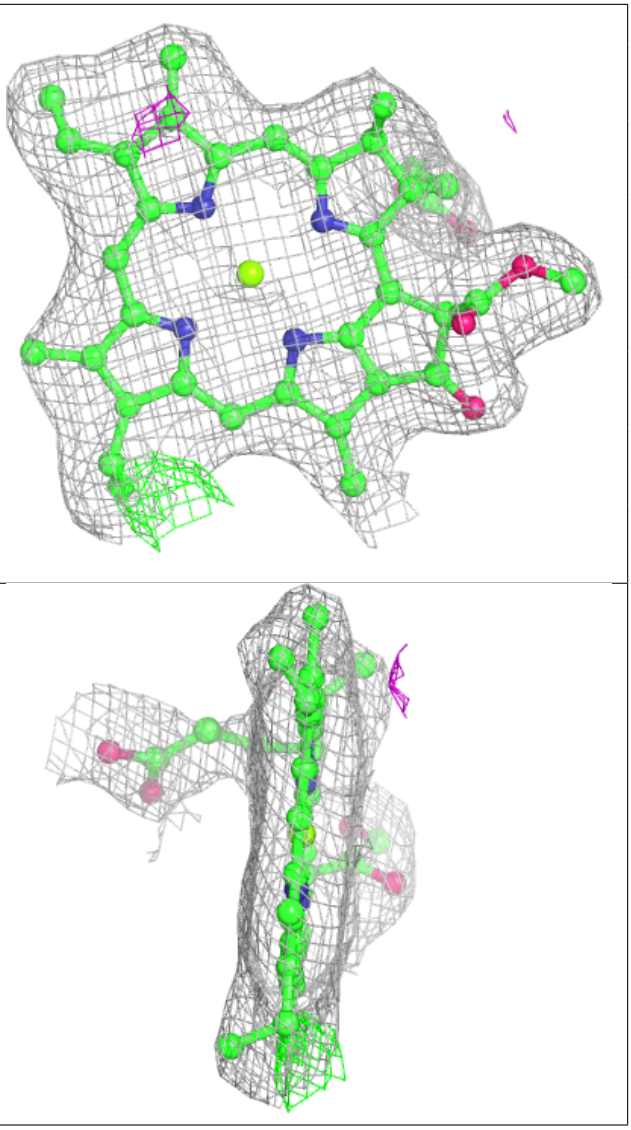






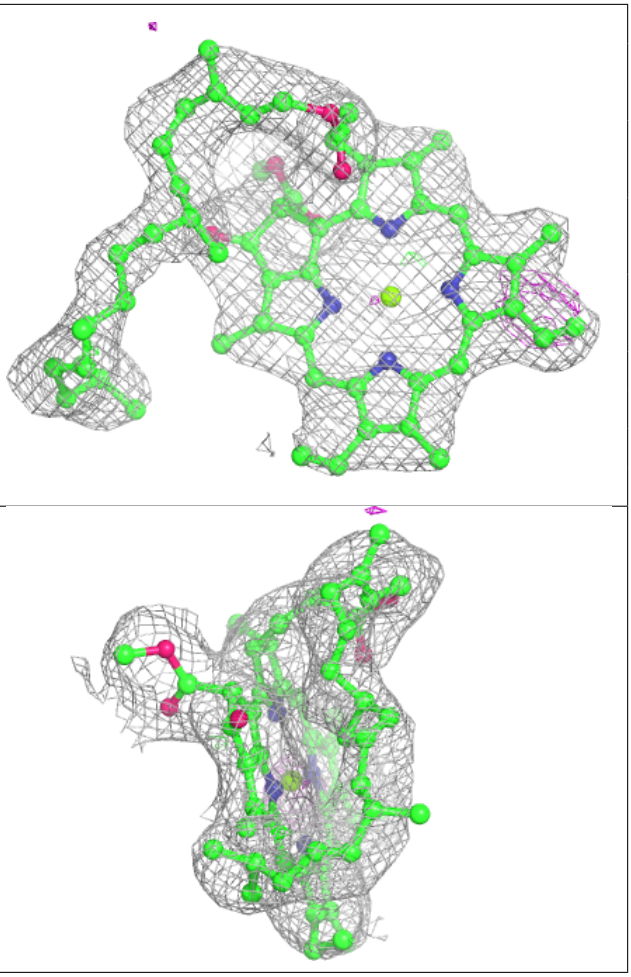
Electron density around CLA B 830:

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



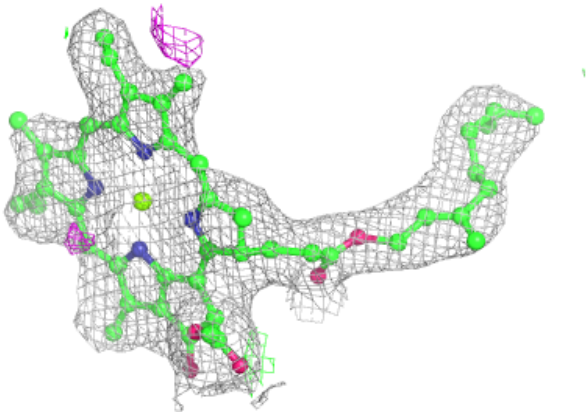
Electron density around CLA B 831:

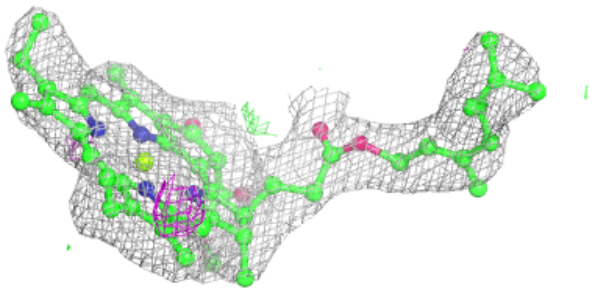
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

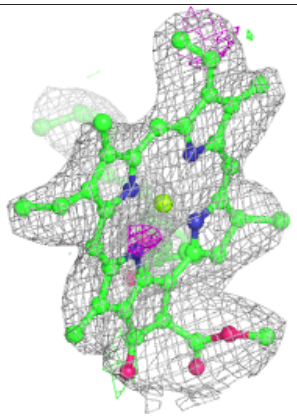


Electron density around CLA B 832:

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

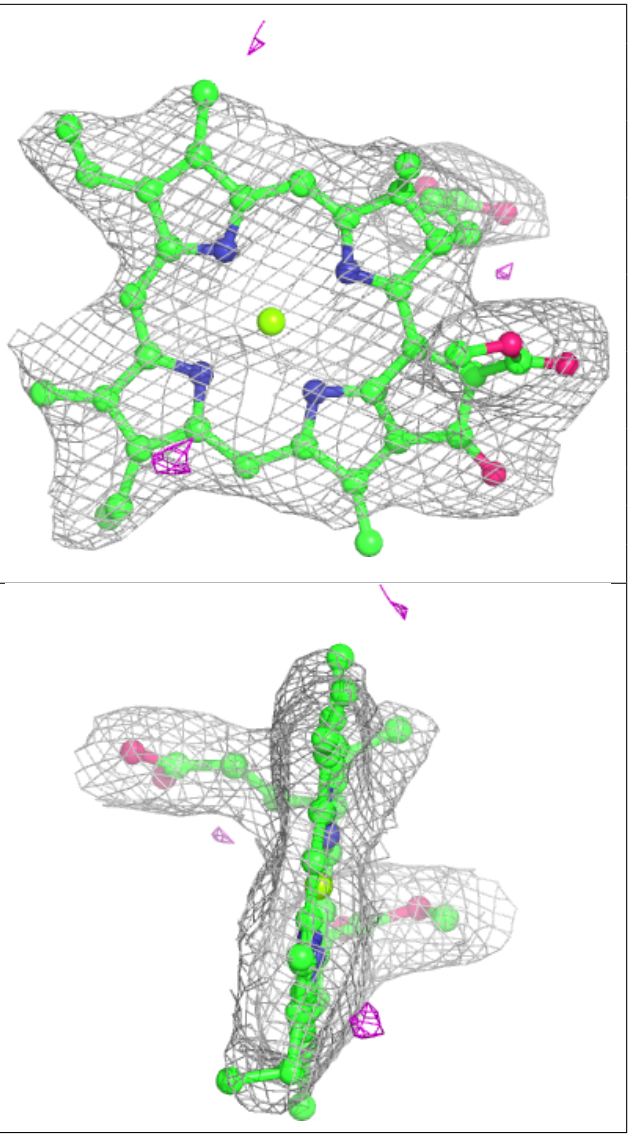






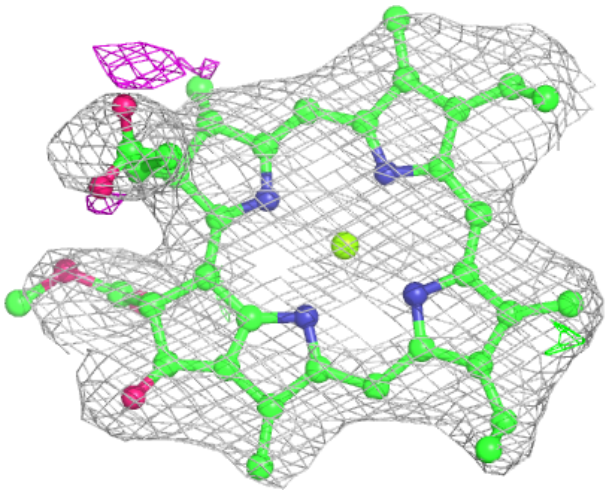
Electron density around CLA B 833:

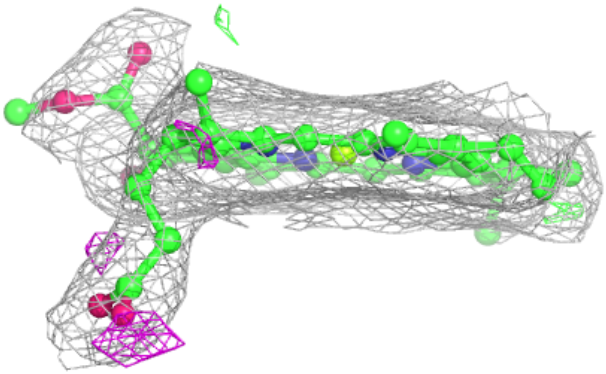
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

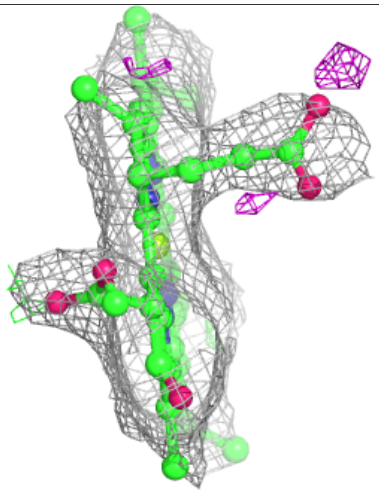


Electron density around CLA B 834:

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

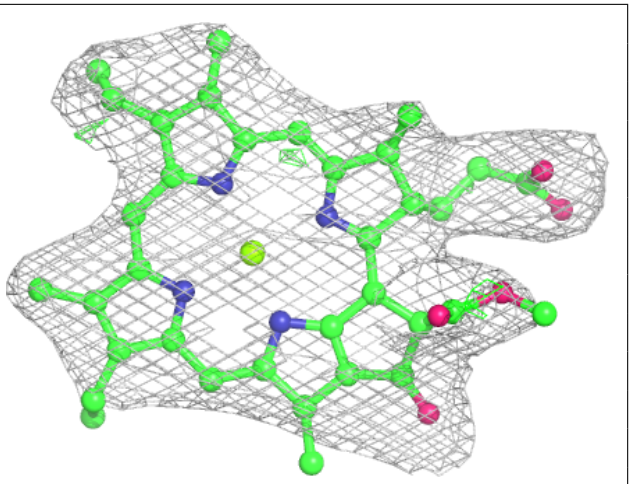


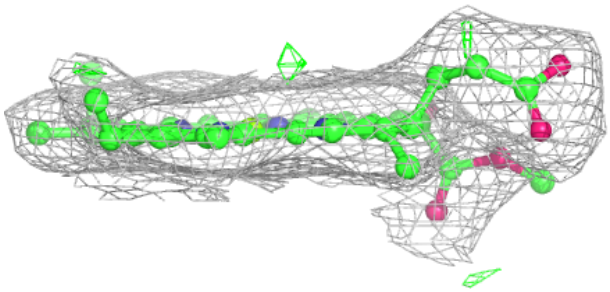


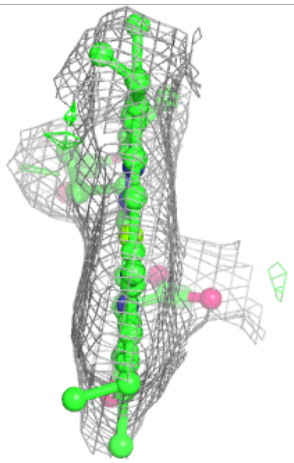


Electron density around CLA B 835:

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)

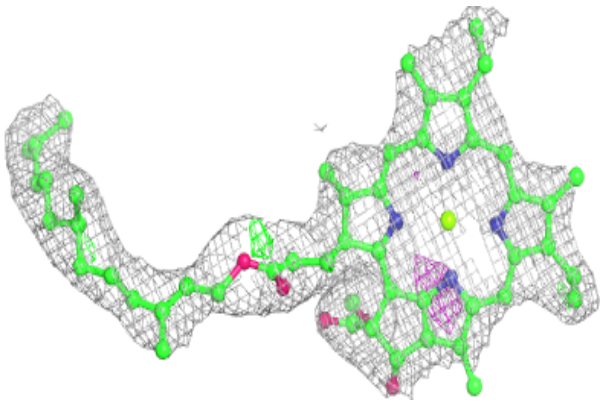


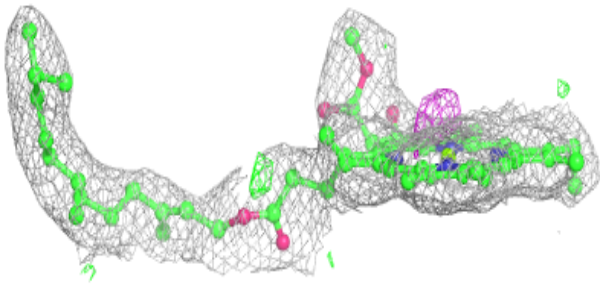


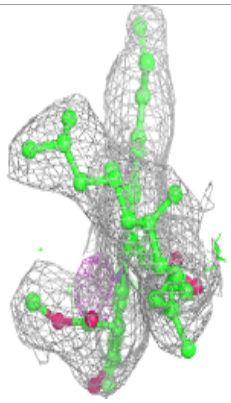


Electron density around CLA B 836:

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

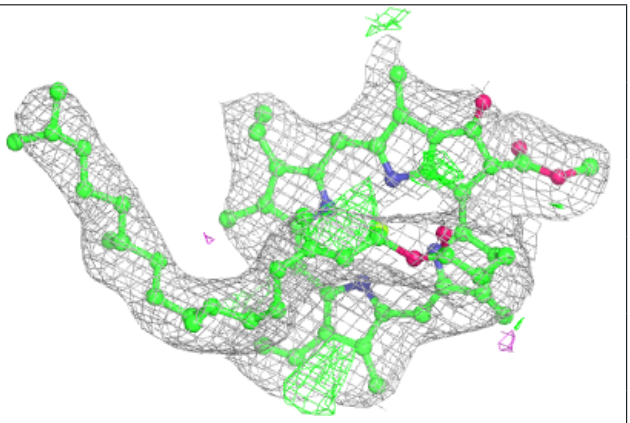


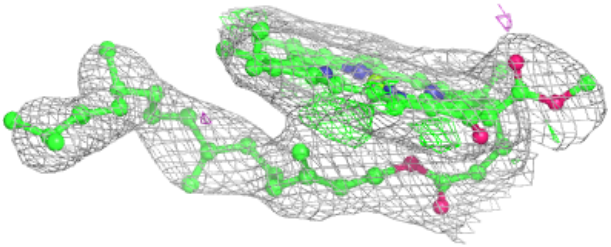


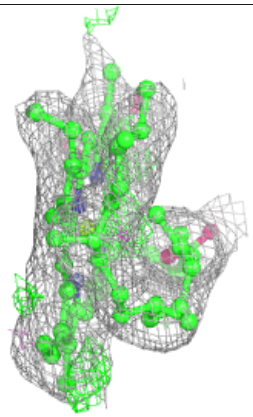


Electron density around CLA B 837:

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

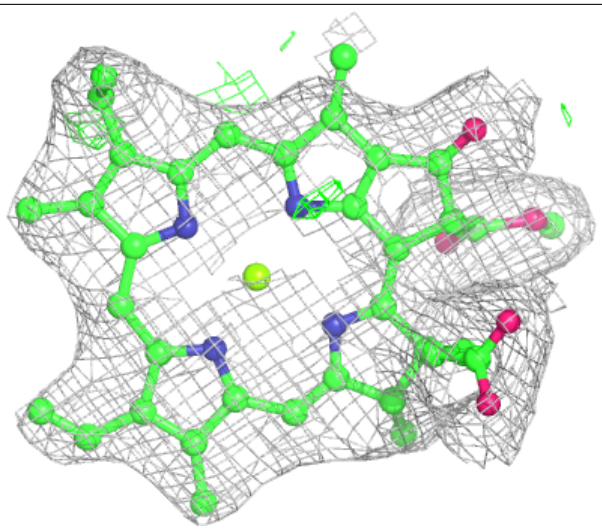


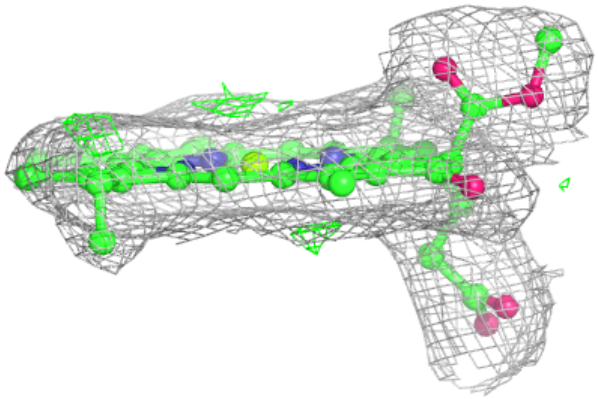


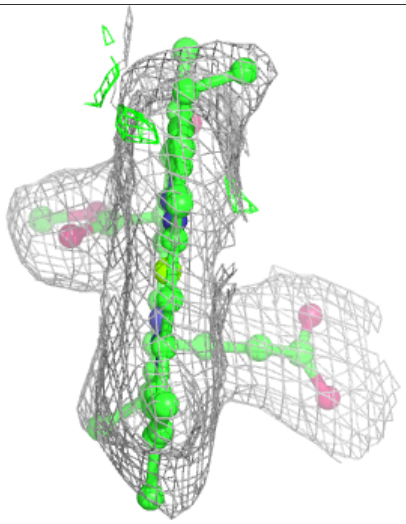


Electron density around CLA B 838:

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

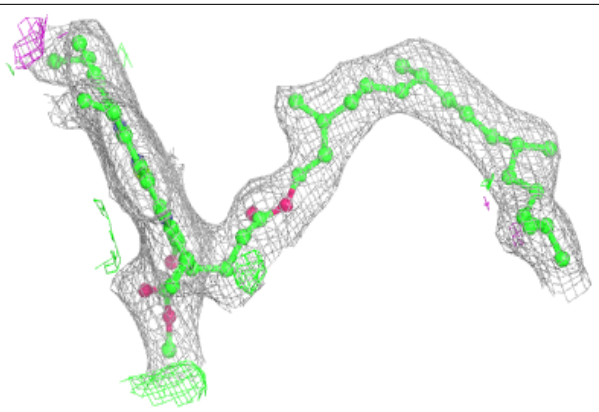


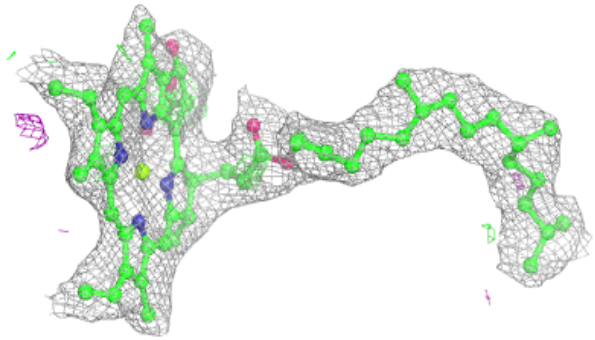


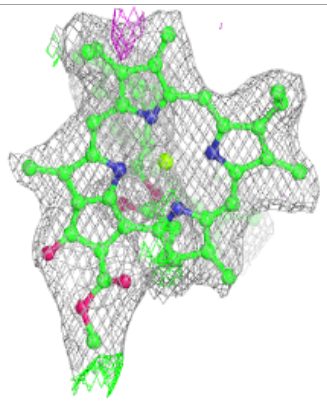


Electron density around CLA B 839:

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

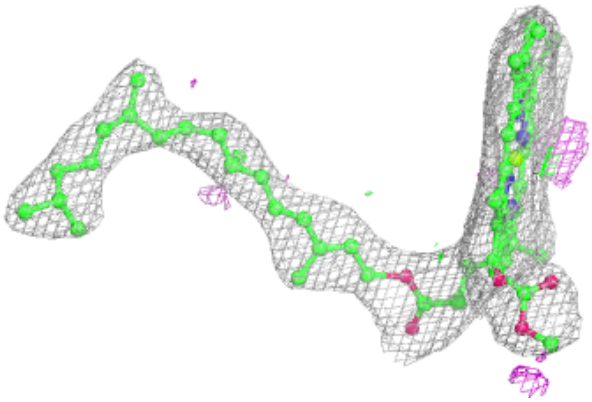


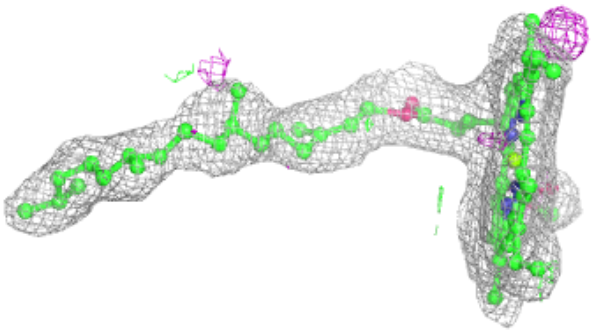


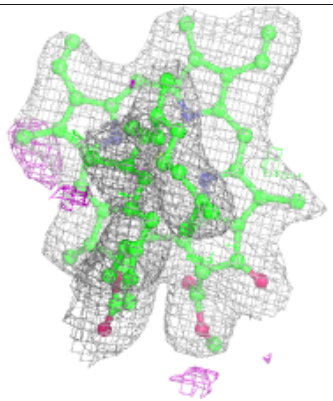


Electron density around CLA B 840:

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

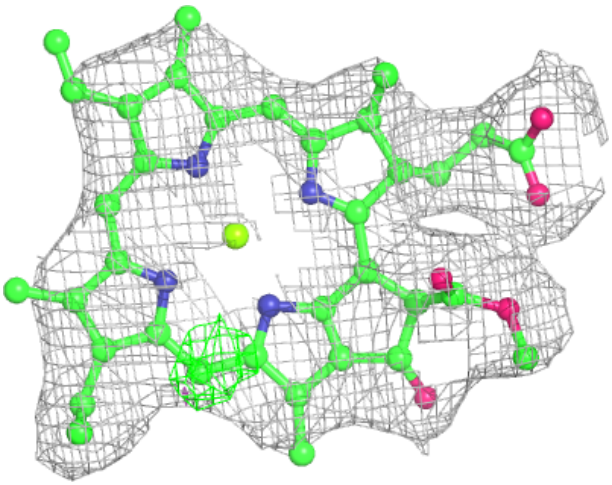


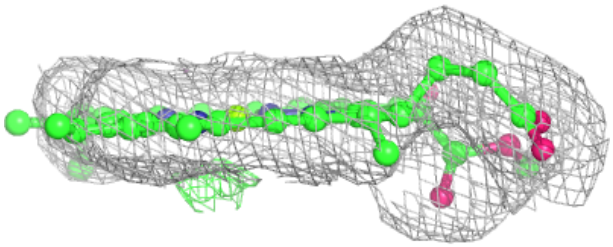


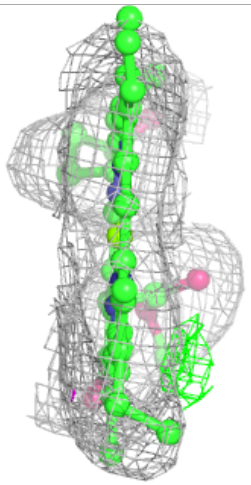


Electron density around CLA F 202:

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

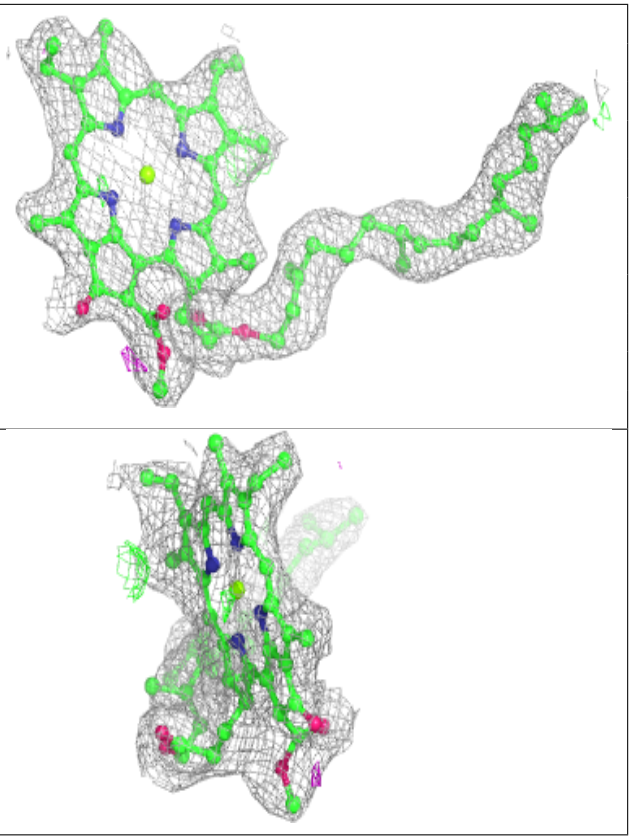






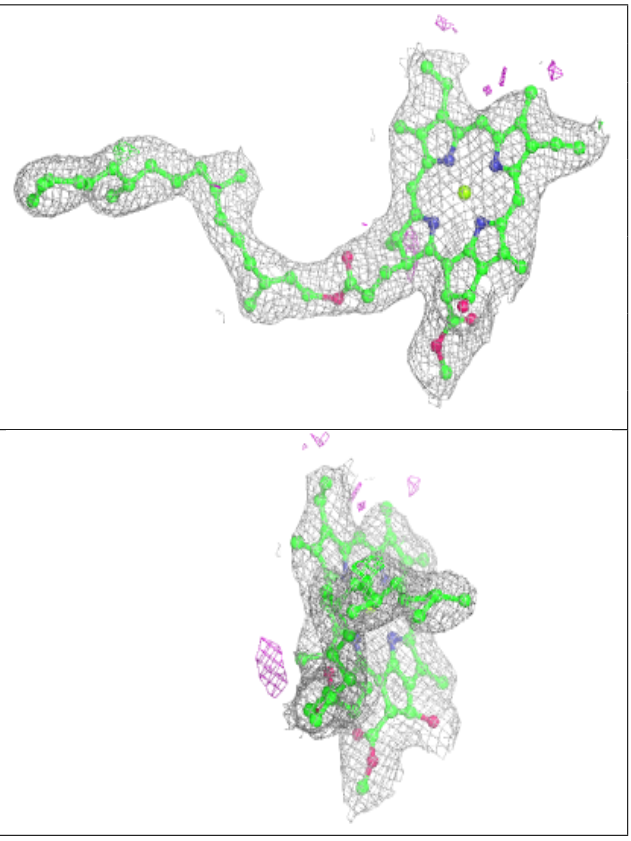
Electron density around CLA G 802:

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



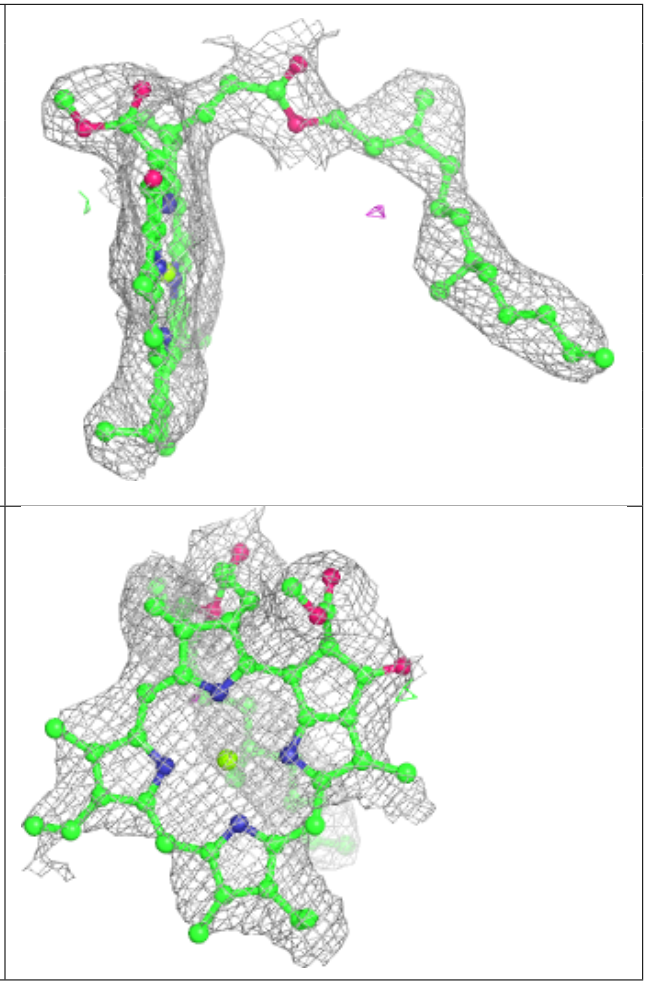
Electron density around CLA G 803:

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



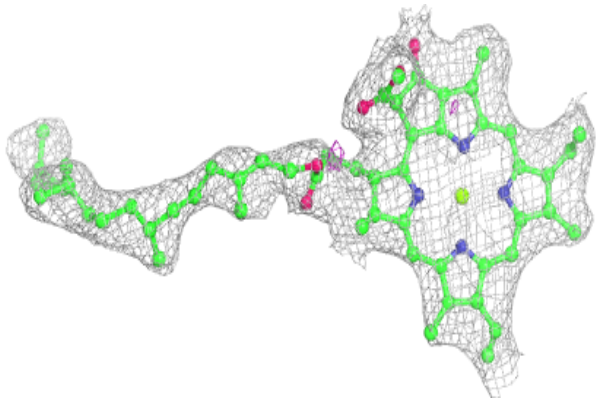
Electron density around CLA G 804:

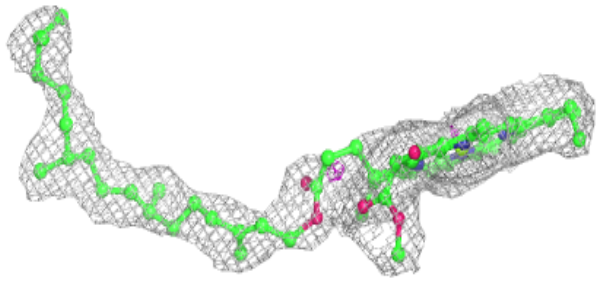
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

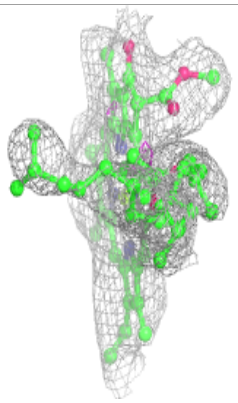


Electron density around CLA G 805:

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

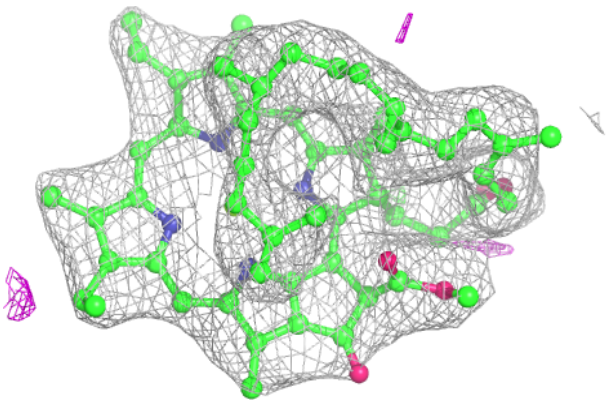


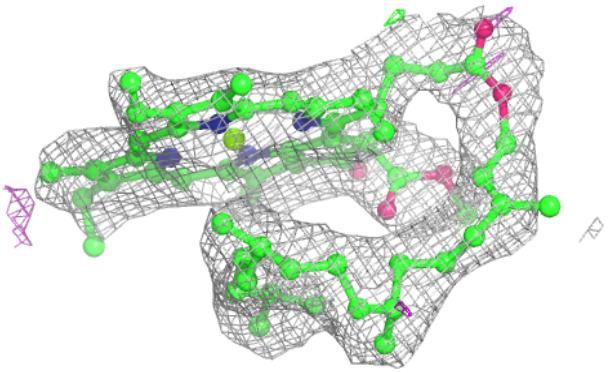


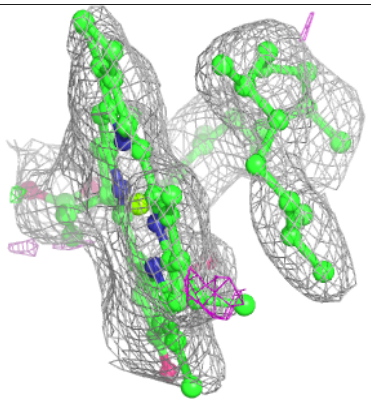


Electron density around CLA G 806:

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

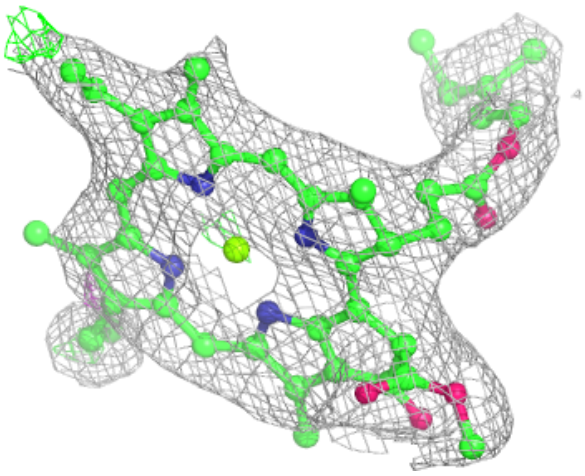


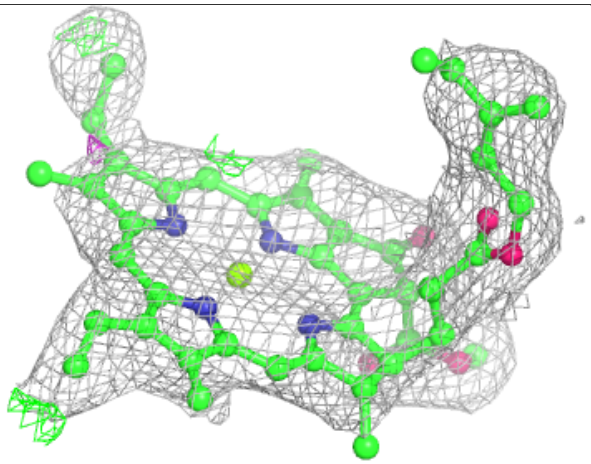


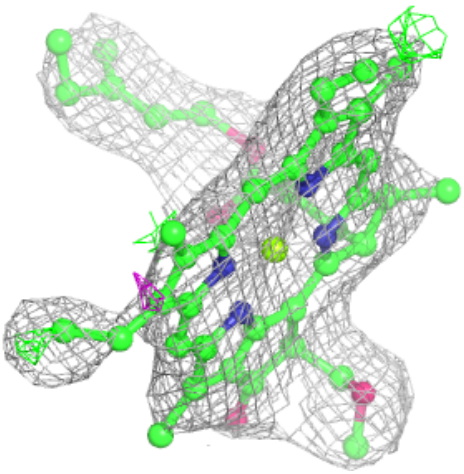


Electron density around CLA G 807:

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

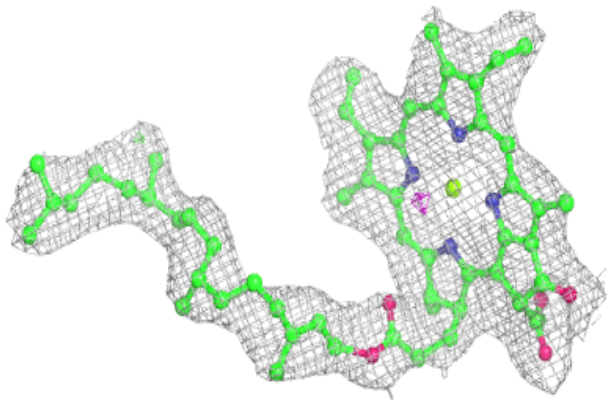


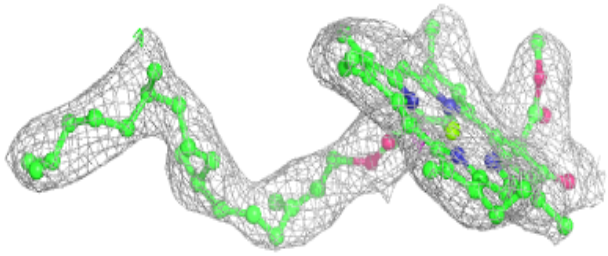


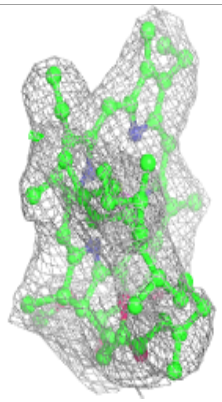


Electron density around CLA G 808:

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

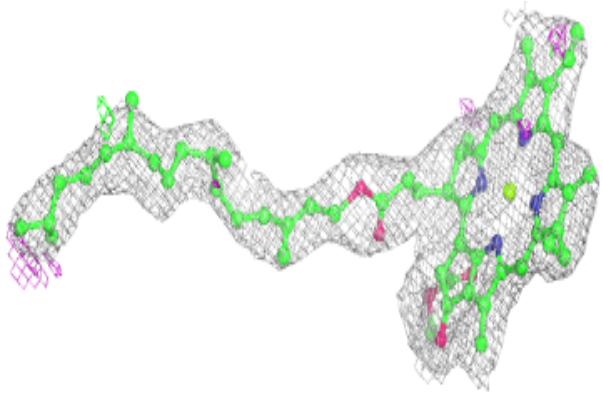


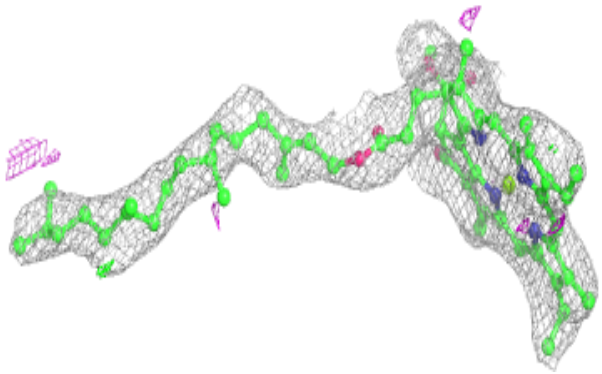


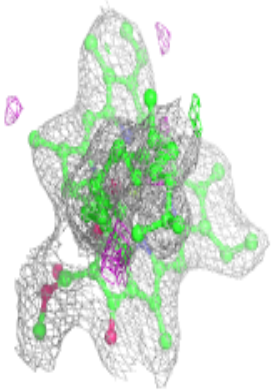


Electron density around CLA G 809:

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

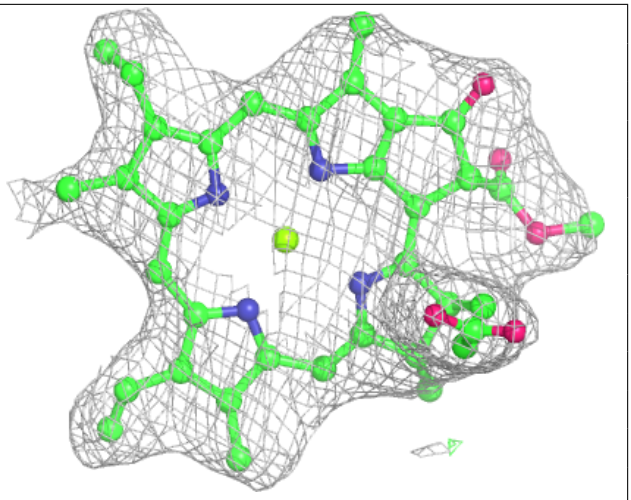


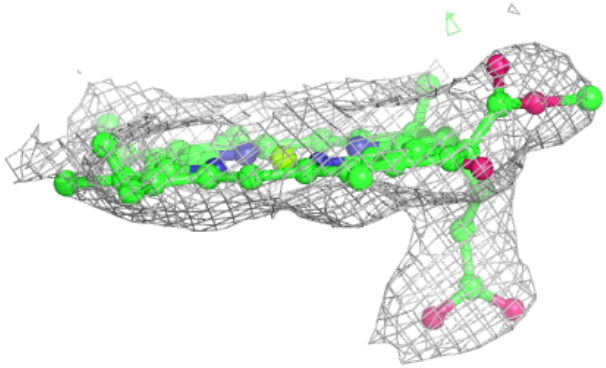


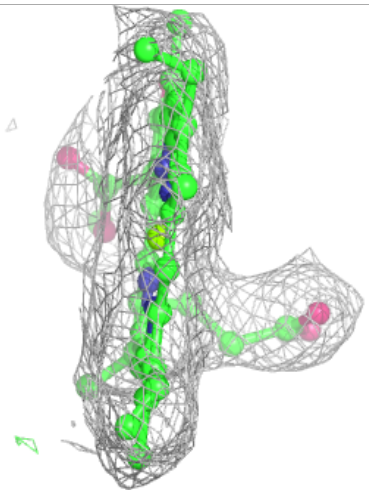


Electron density around CLA G 810:

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

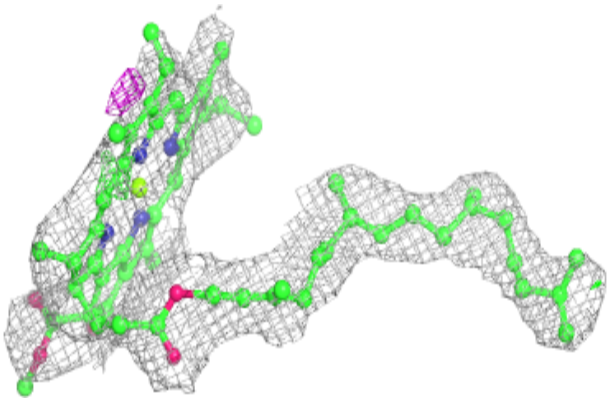


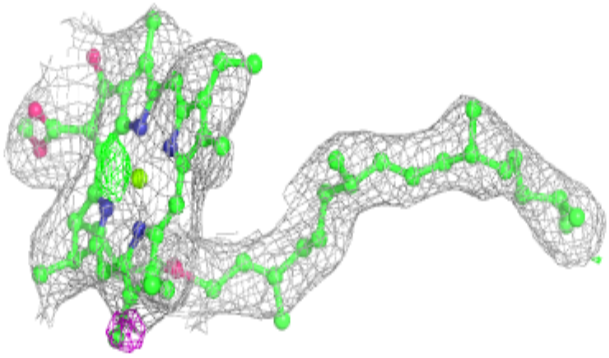


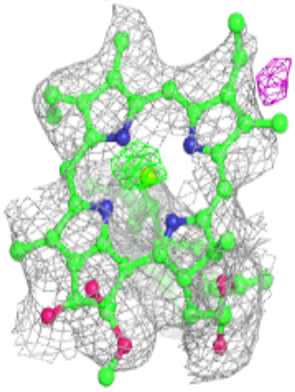


Electron density around CLA G 811:

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

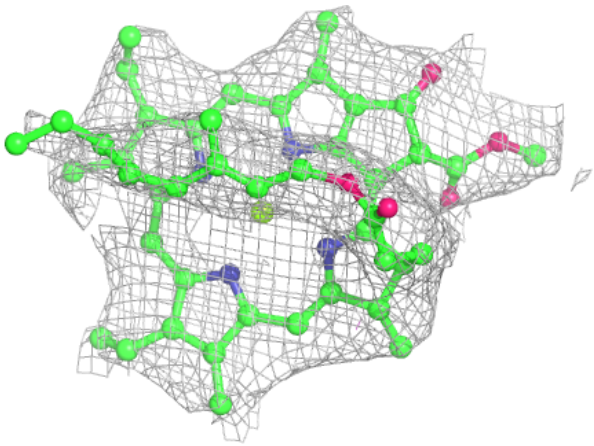


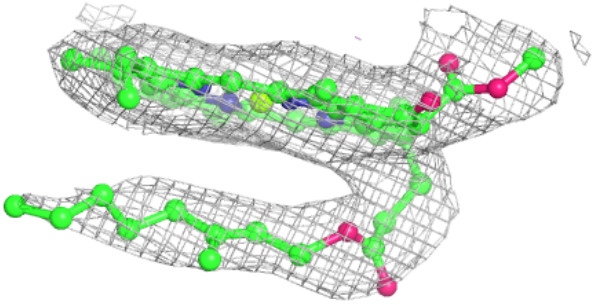


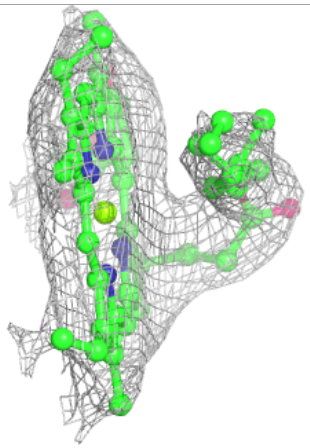


Electron density around CLA G 812:

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

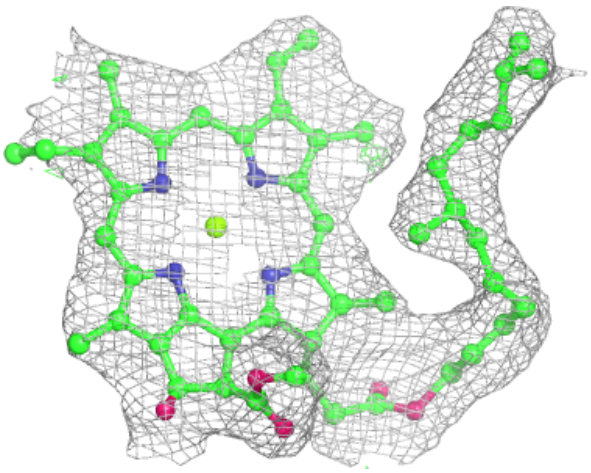


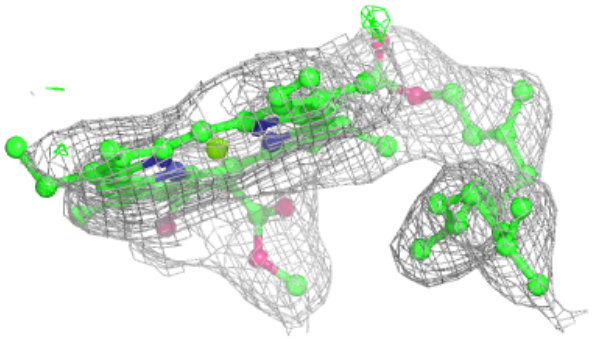


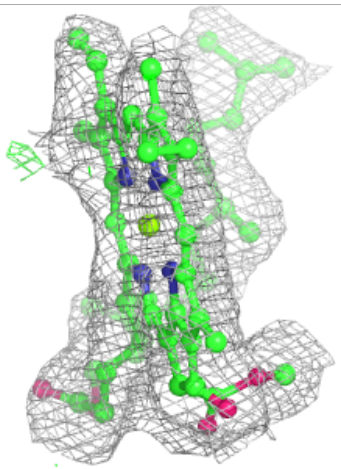


Electron density around CLA G 813:

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

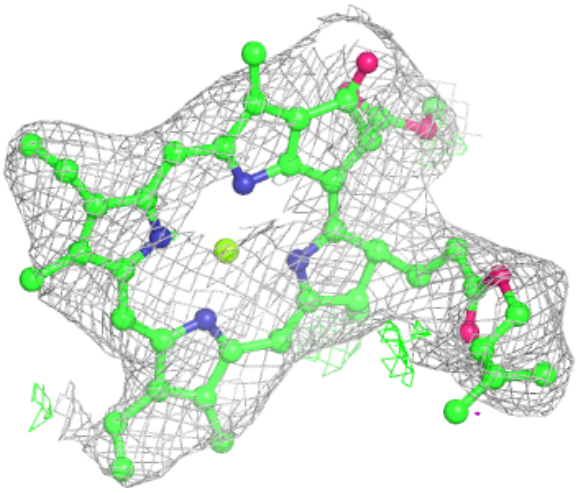


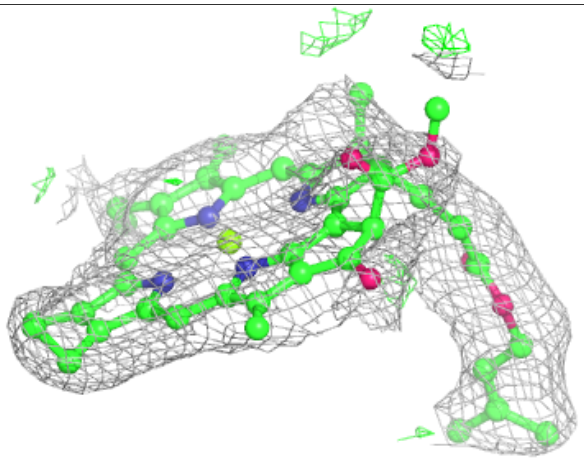


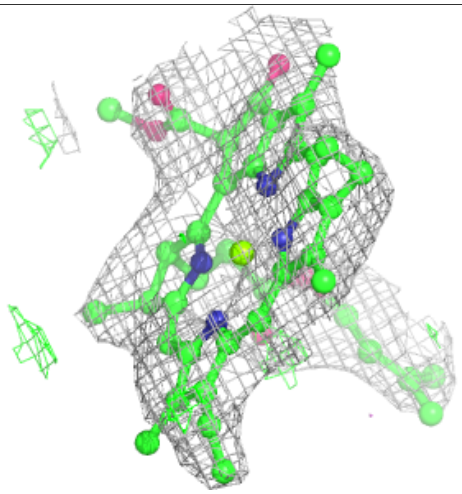


Electron density around CLA G 814:

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

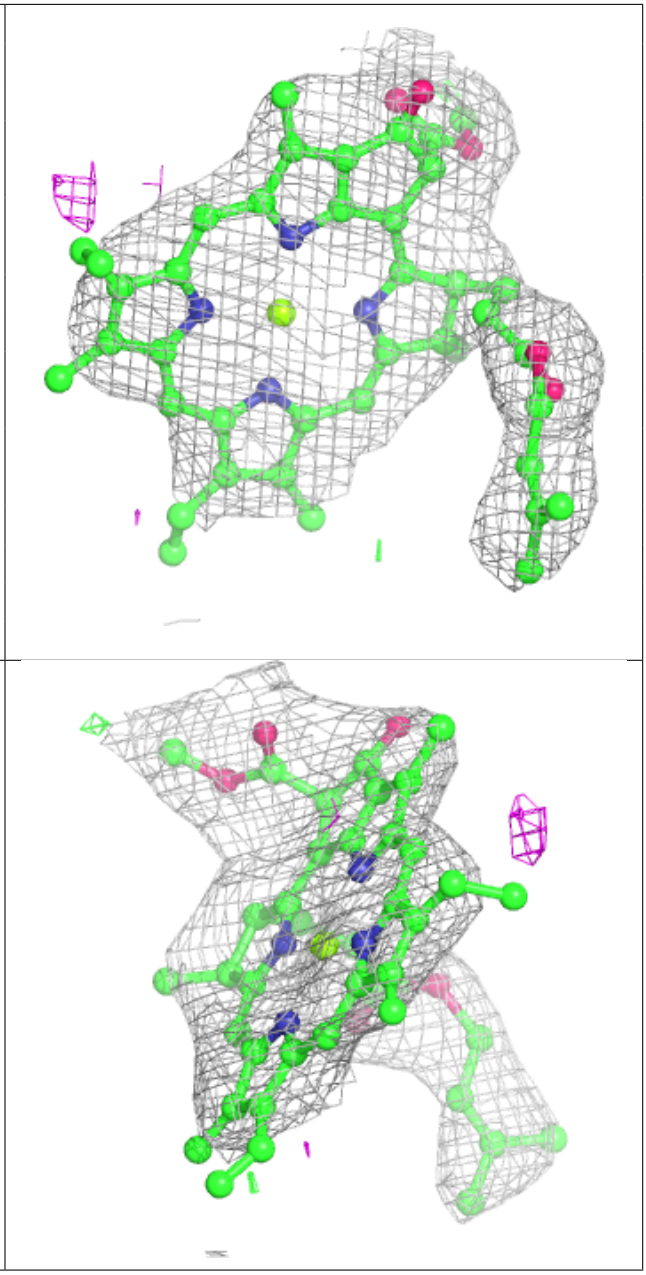






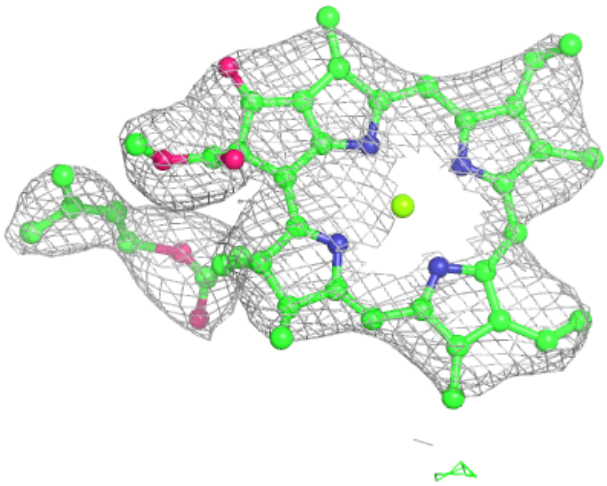
Electron density around CLA G 815:

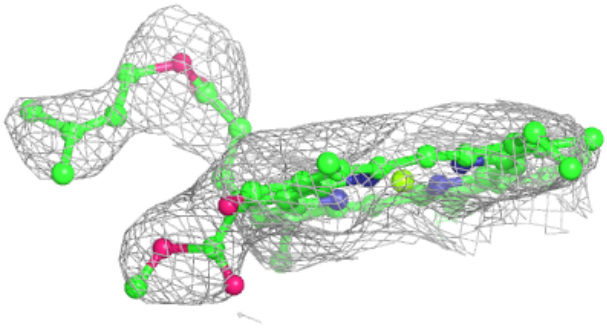
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

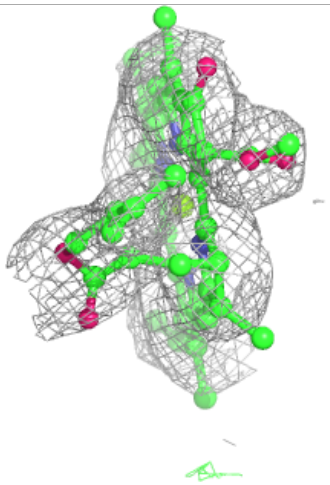


Electron density around CLA G 816:

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

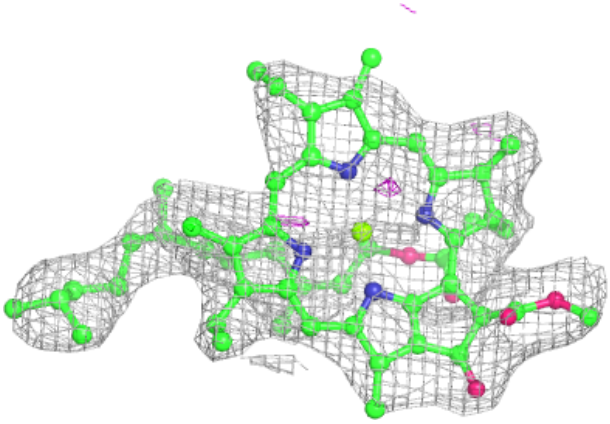


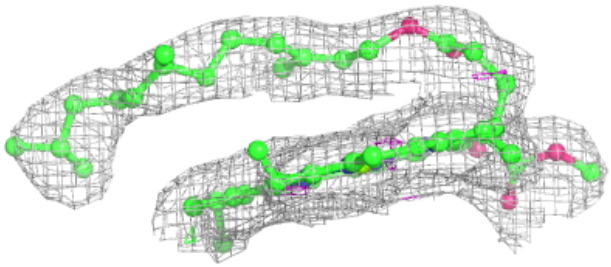


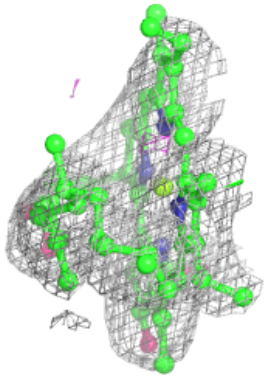


Electron density around CLA G 817:

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

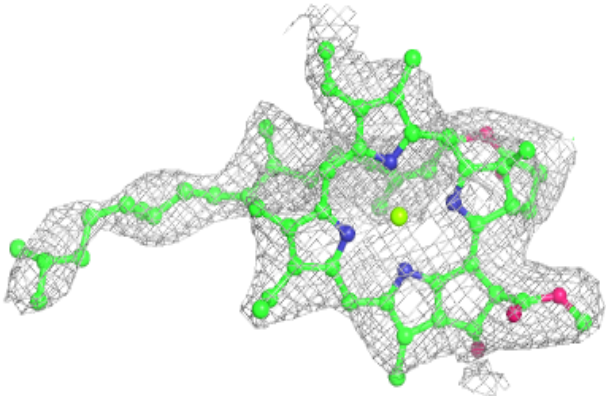


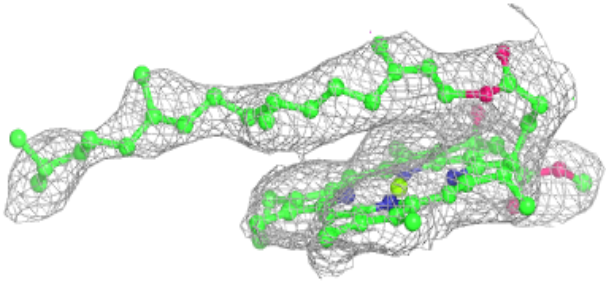


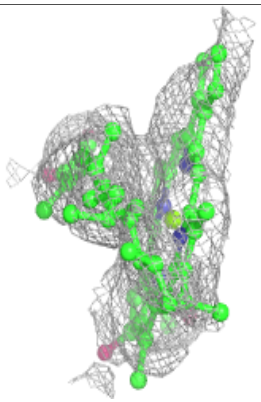


Electron density around CLA G 818:

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

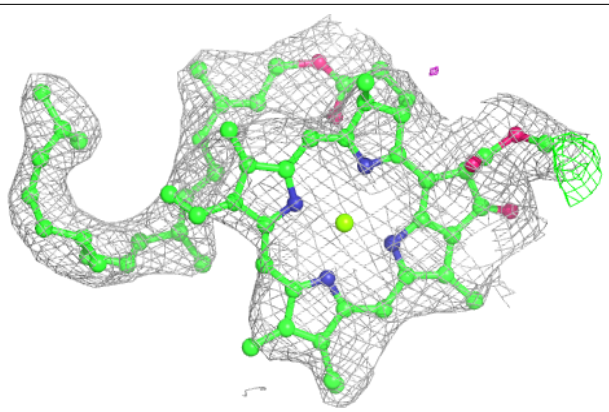


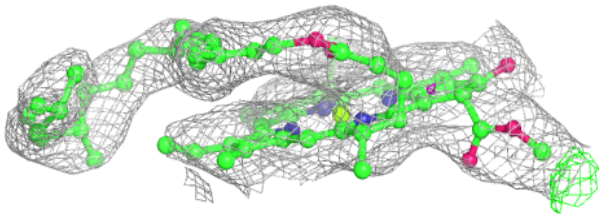


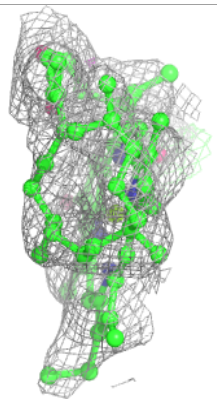


Electron density around CLA G 819:

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

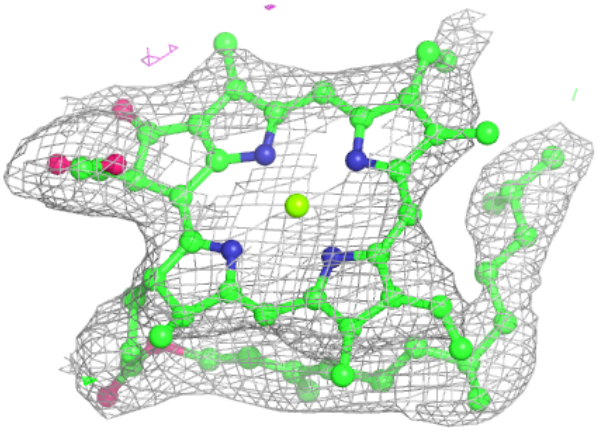


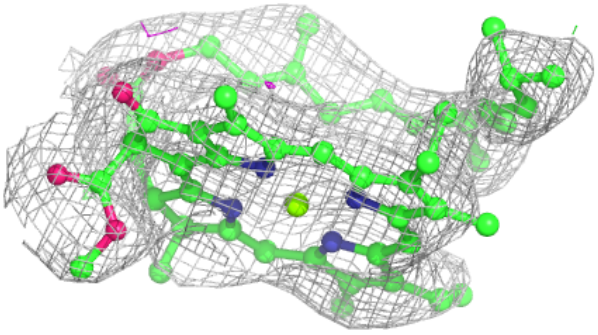


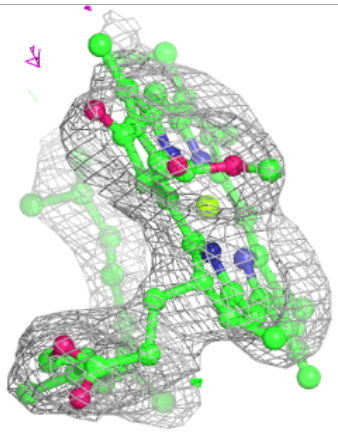


Electron density around CLA G 820:

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

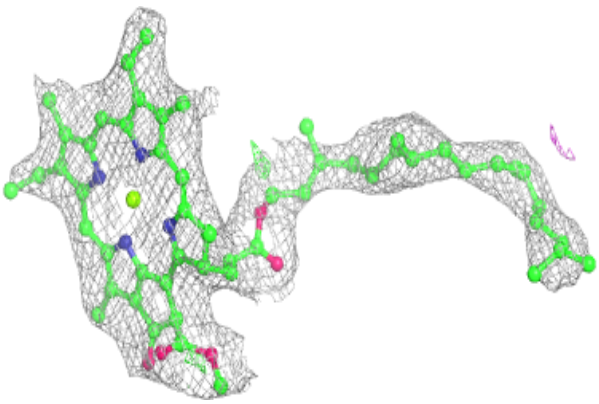


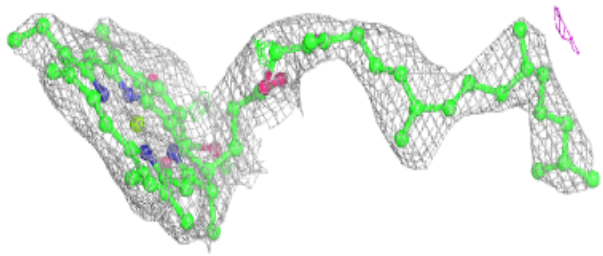


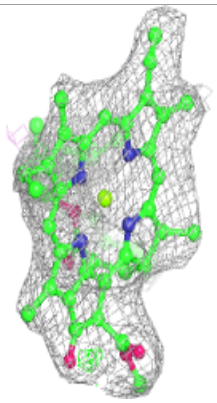


Electron density around CLA G 821:

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

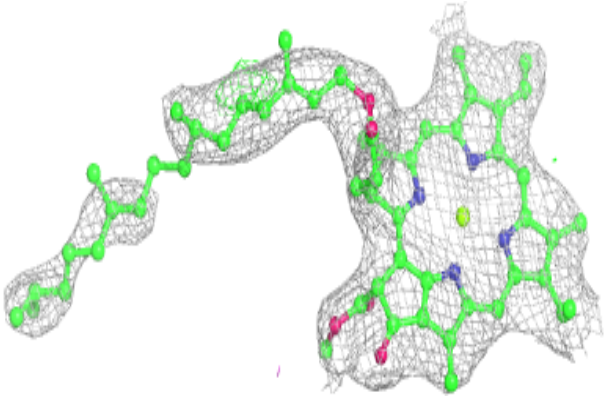


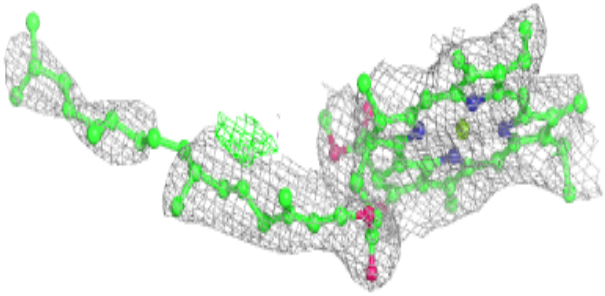


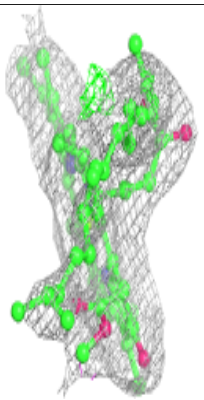


Electron density around CLA G 822:

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

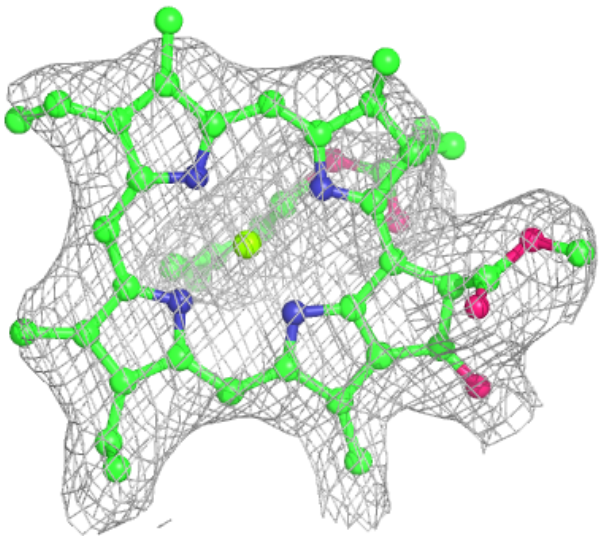


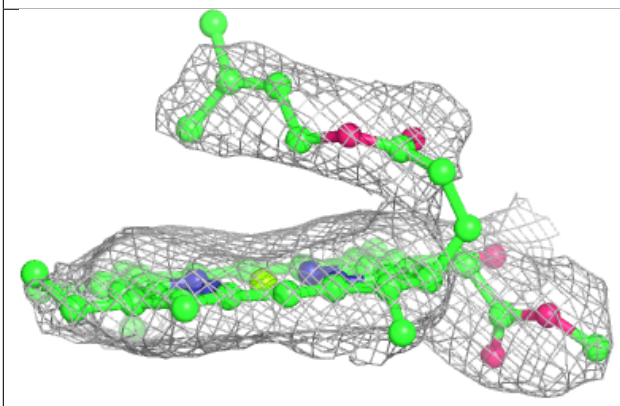


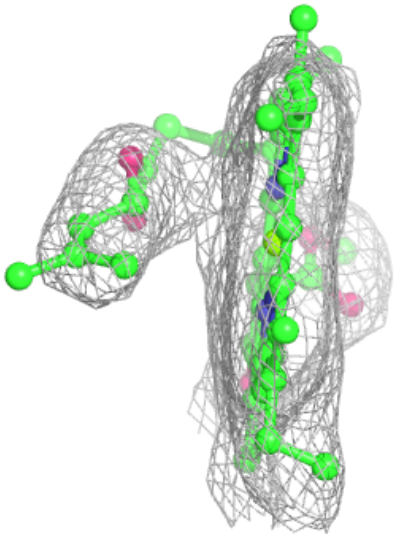


Electron density around CLA G 823:

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

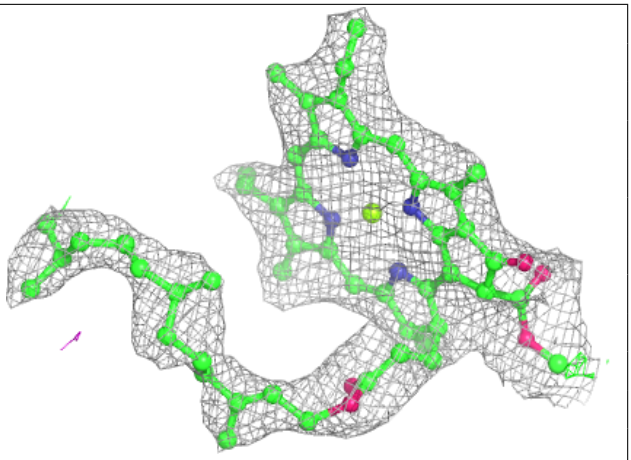


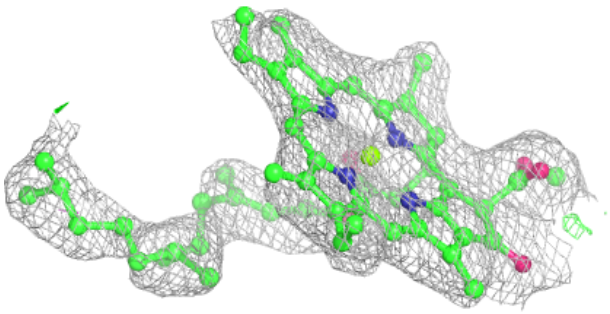


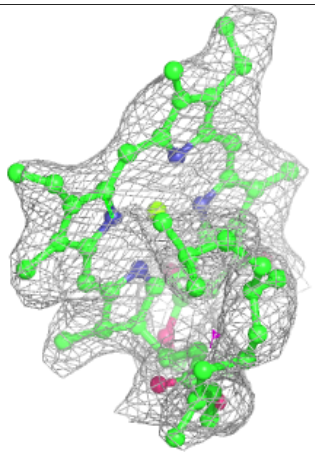


Electron density around CLA G 824:

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

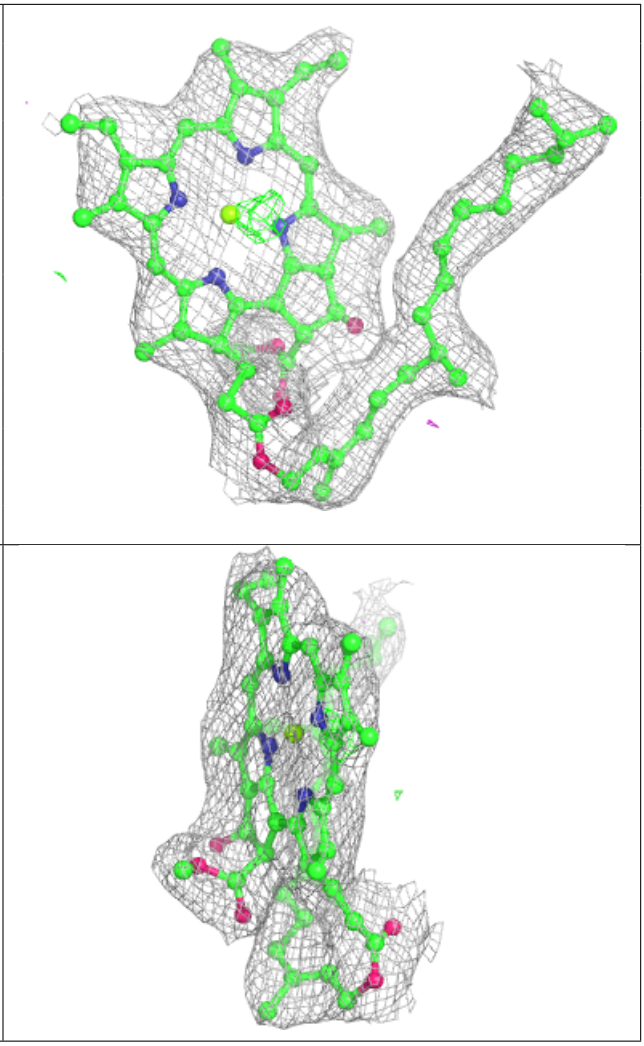






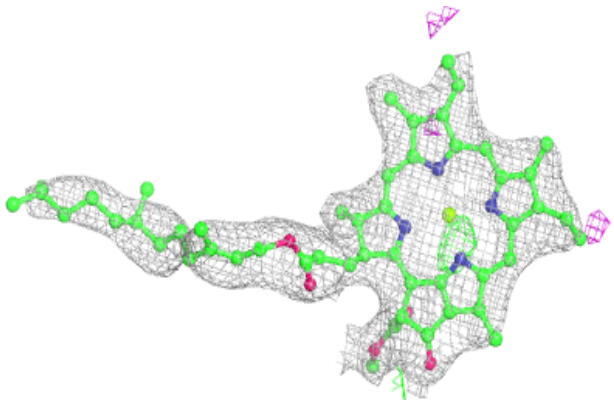
Electron density around CLA G 825:

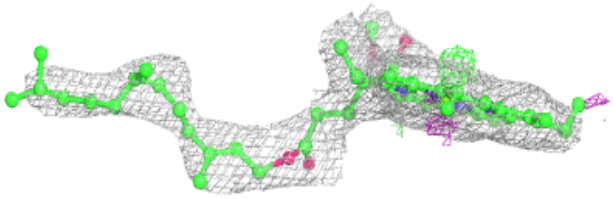
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

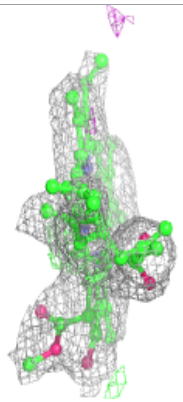


Electron density around CLA G 826:

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

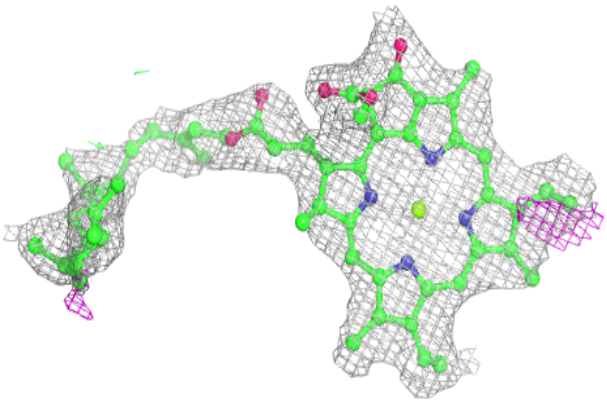


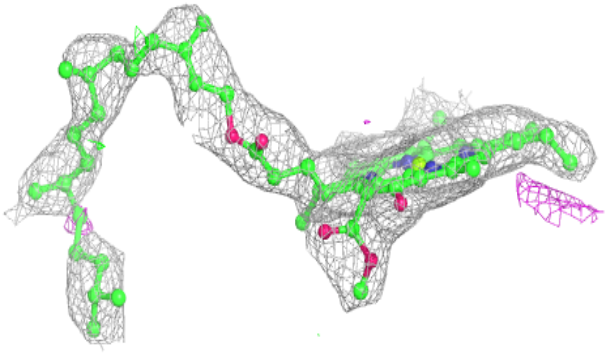


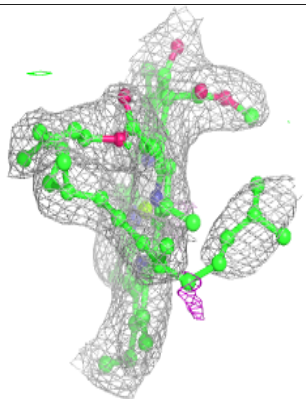


Electron density around CLA G 827:

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

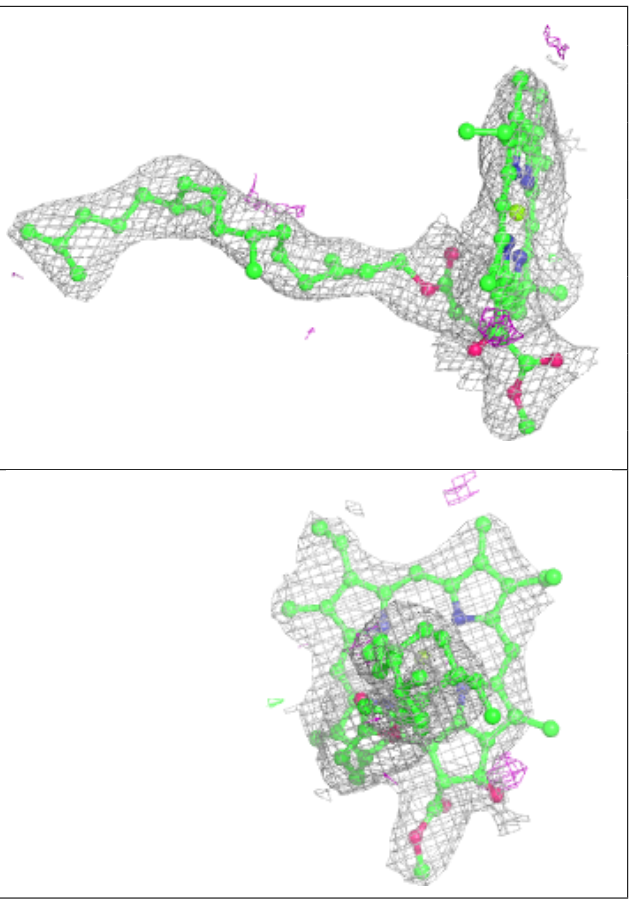


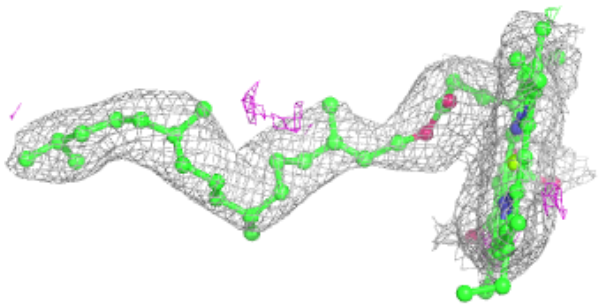




Electron density around CLA G 828:

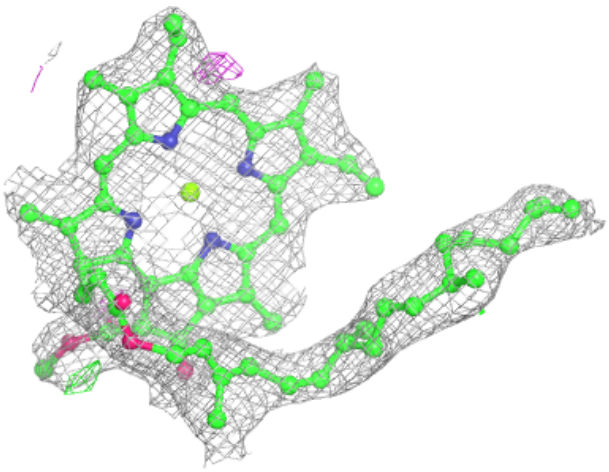
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

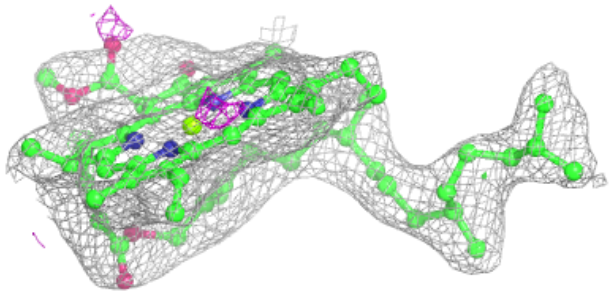


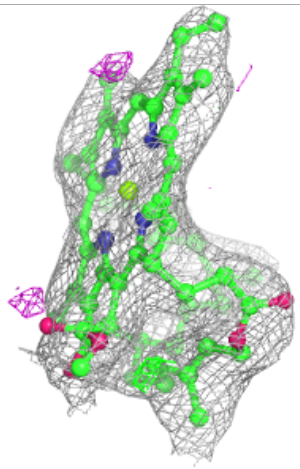


Electron density around CLA G 829:

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

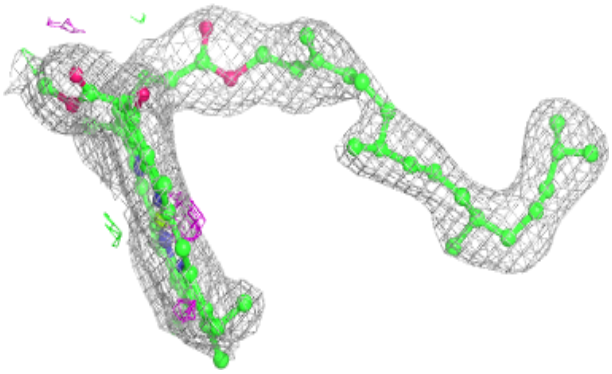


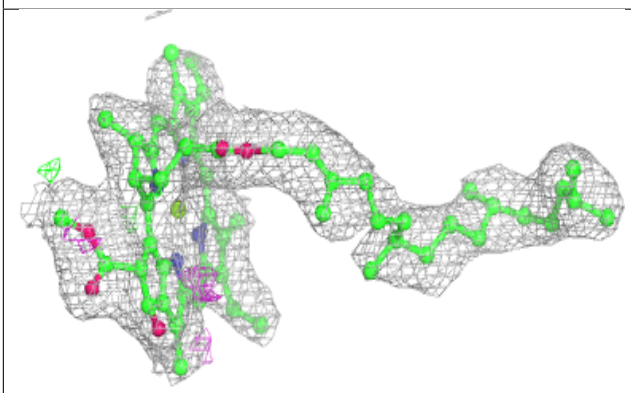


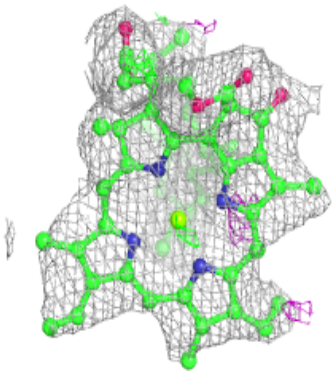


Electron density around CLA G 830:

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

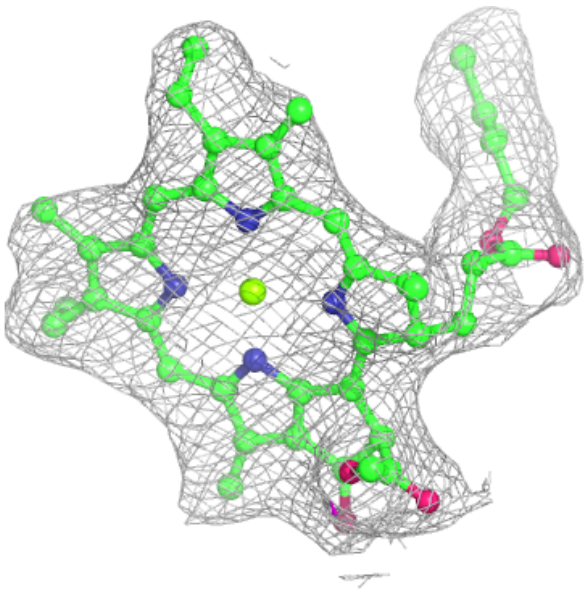


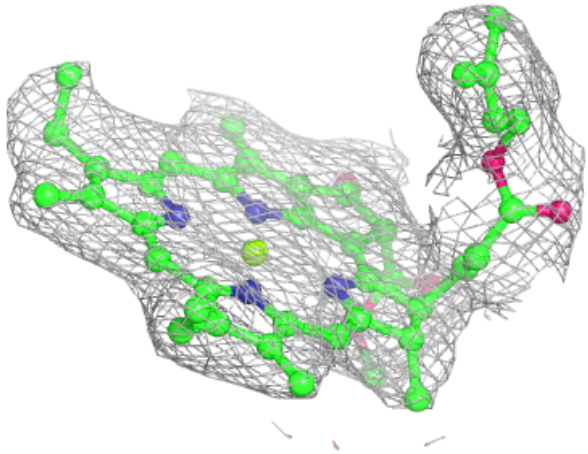


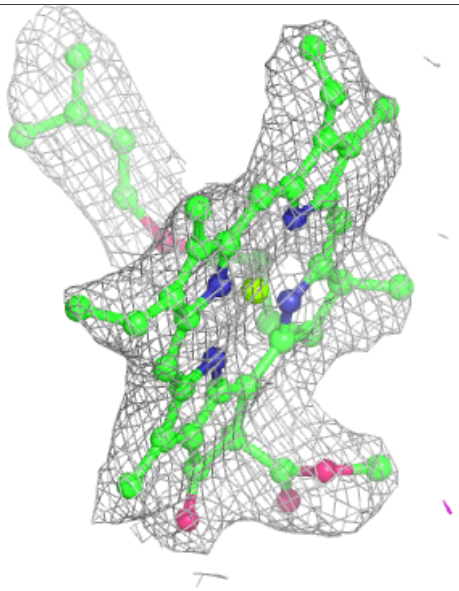


Electron density around CLA G 831:

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

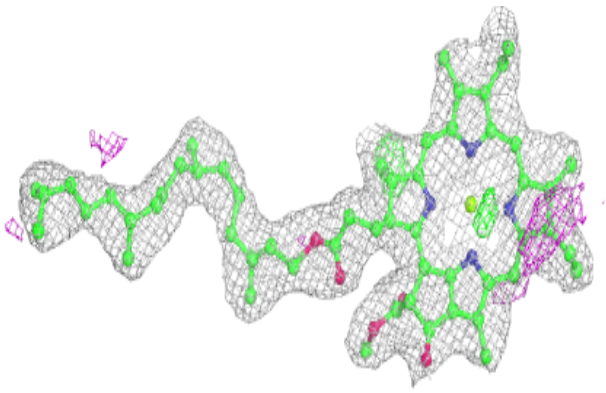


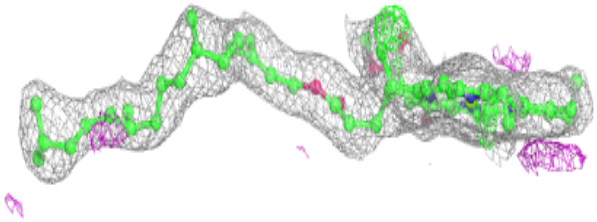


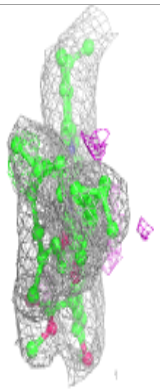


Electron density around CLA G 832:

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

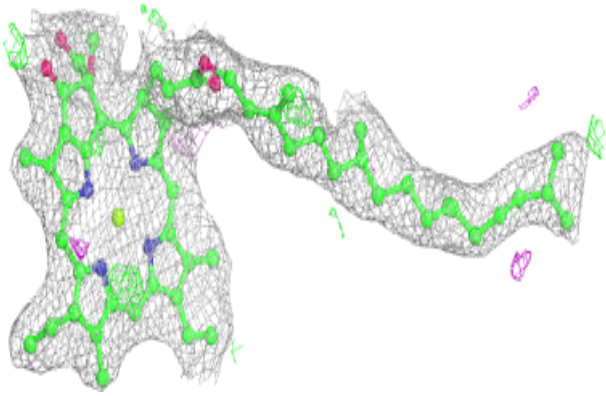


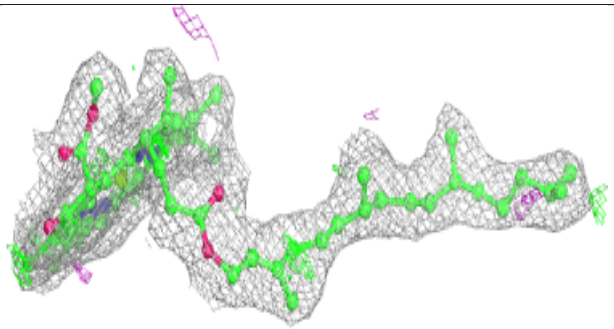


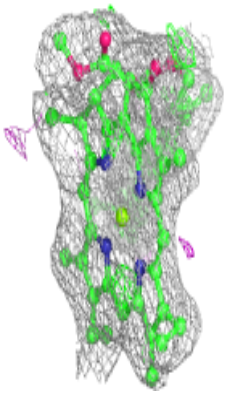


Electron density around CLA G 833:

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

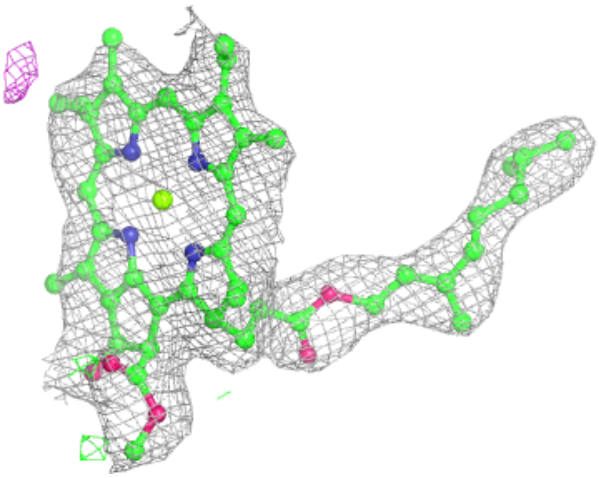


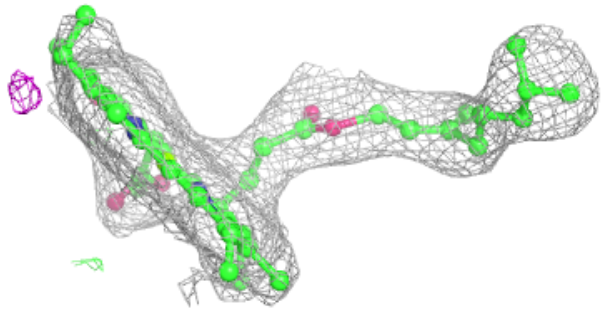


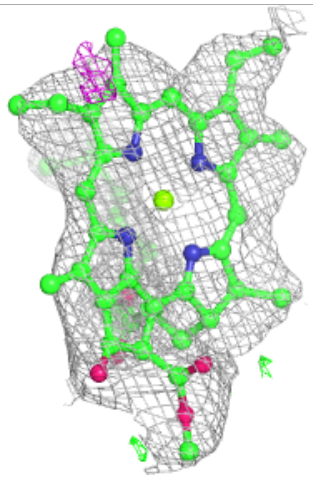


Electron density around CLA G 834:

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

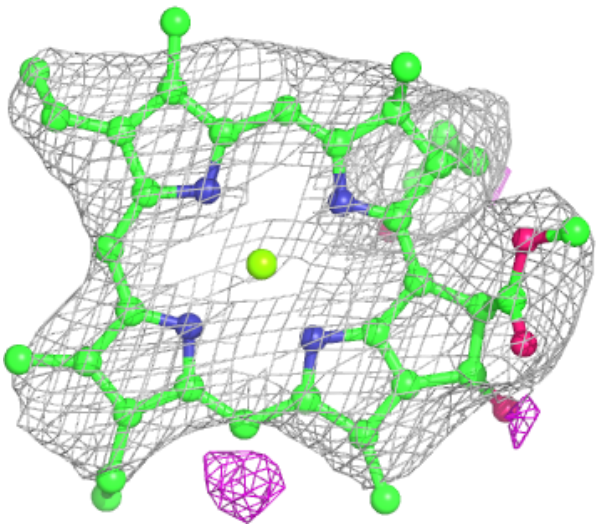


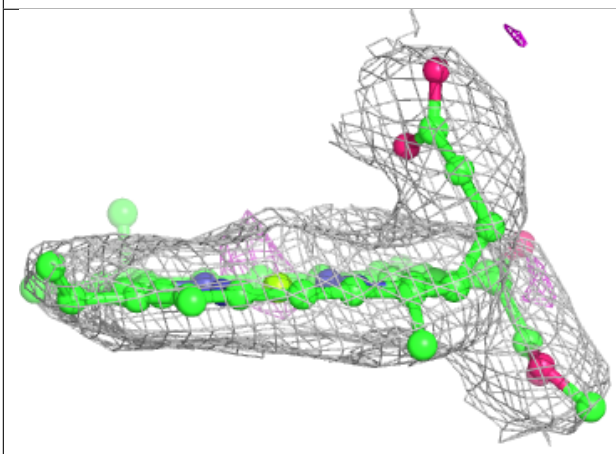


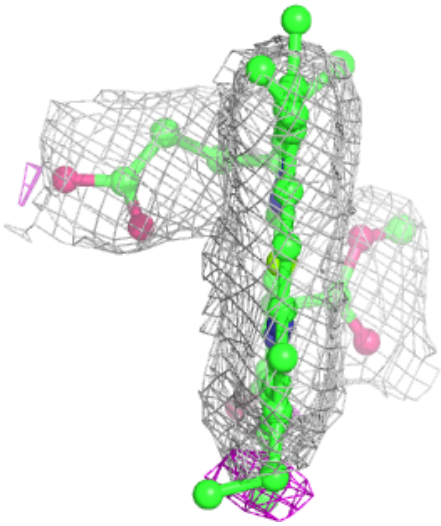


Electron density around CLA G 835:

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

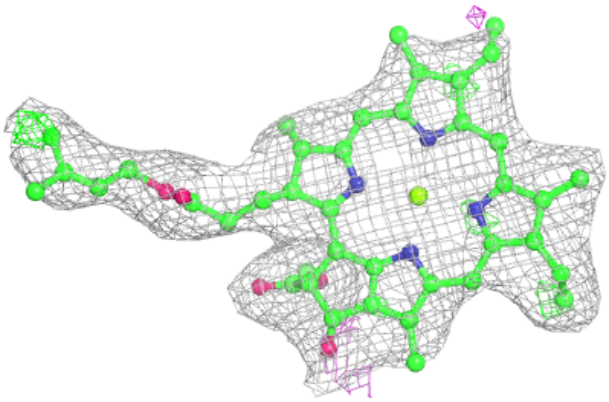


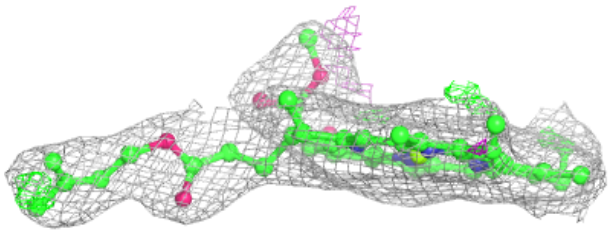


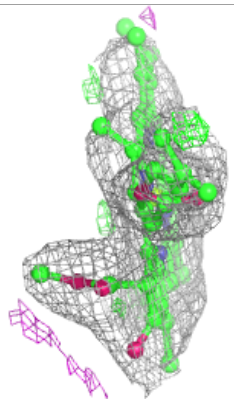


Electron density around CLA G 836:

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

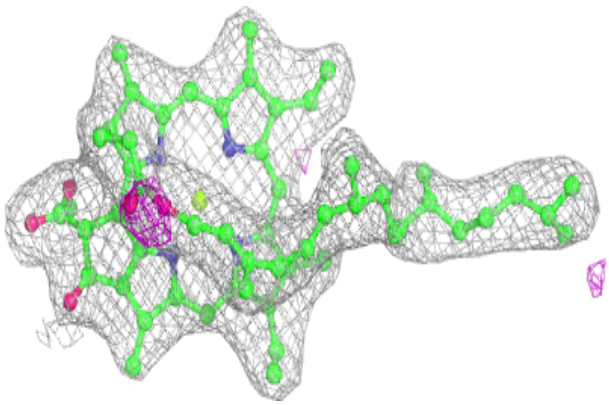


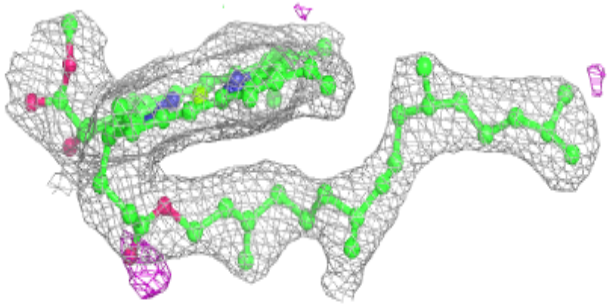


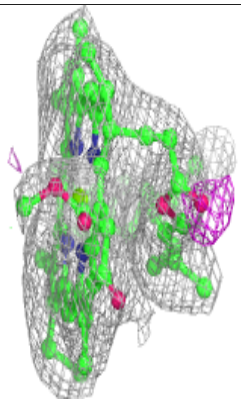


Electron density around CLA G 837:

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

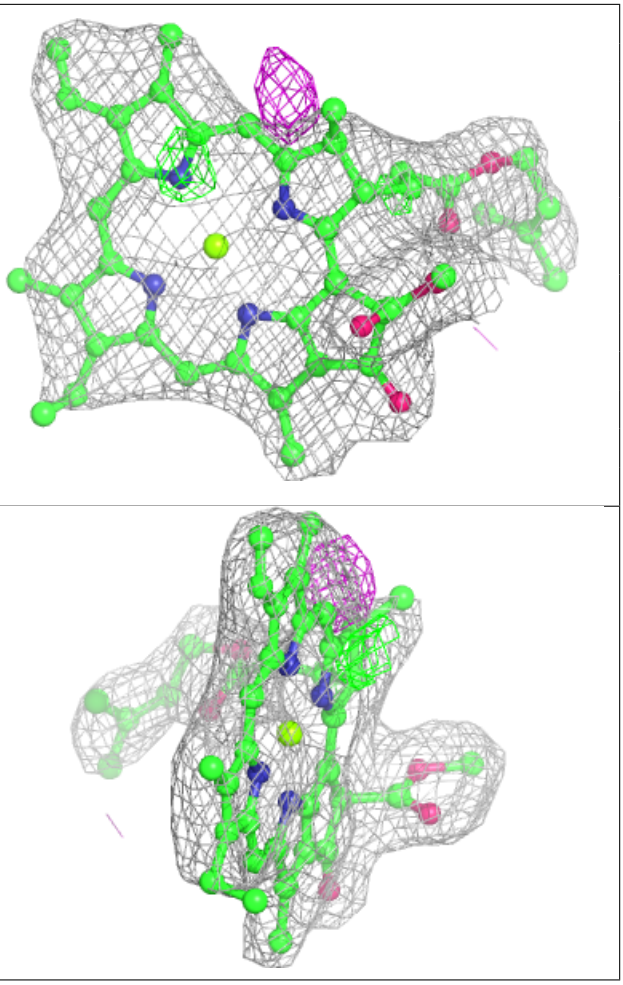






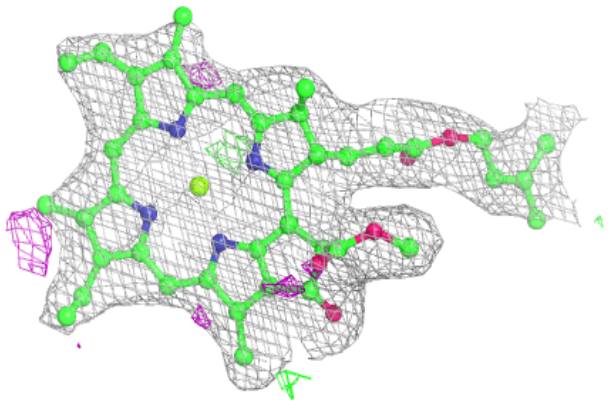
Electron density around CLA G 838:

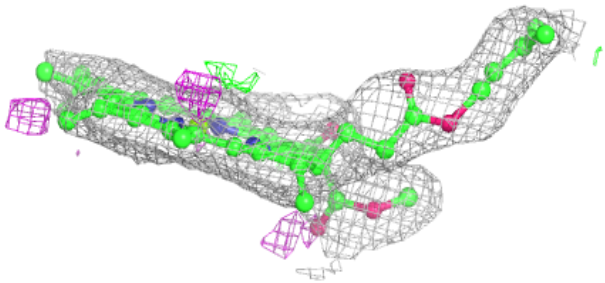
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

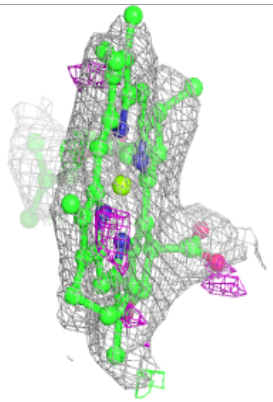


Electron density around CLA G 839:

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

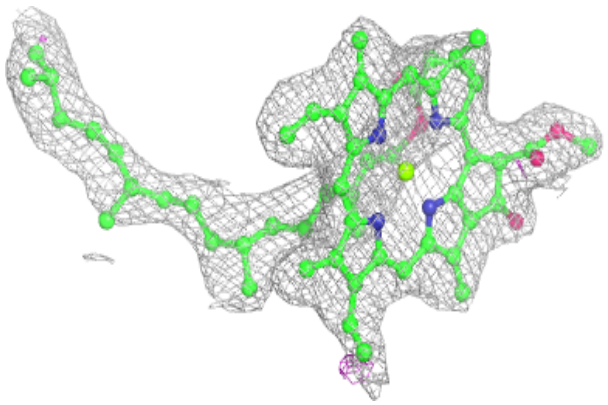


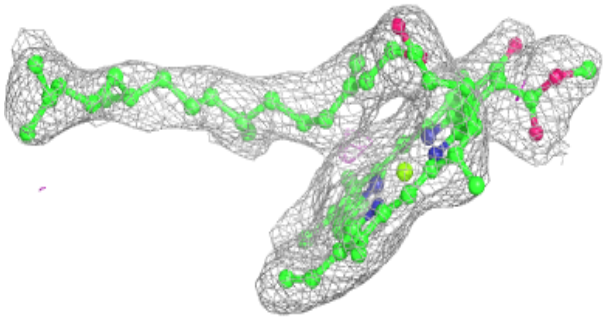


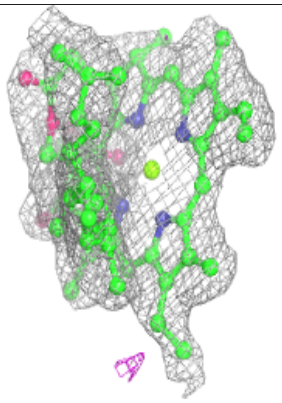


Electron density around CLA G 840:

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

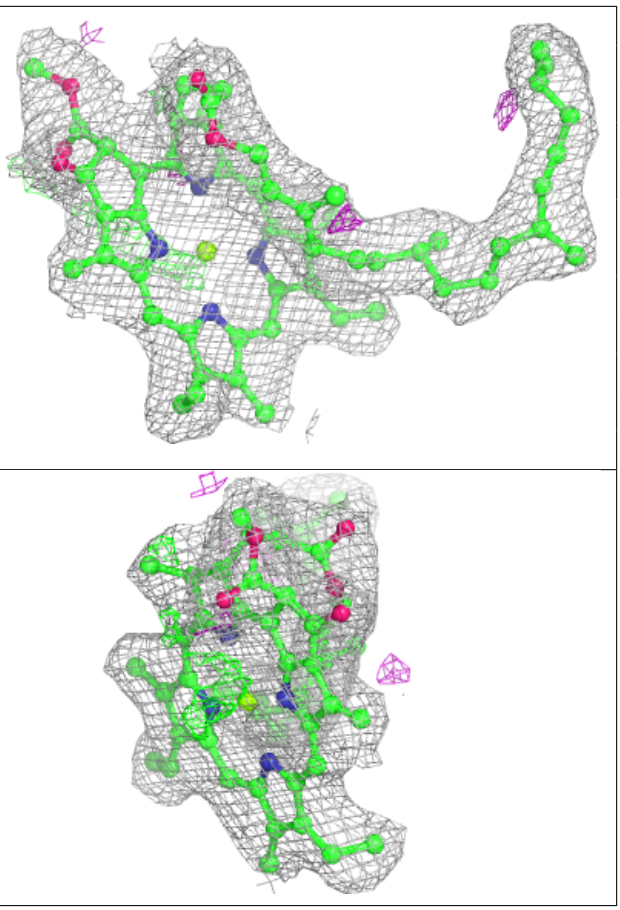


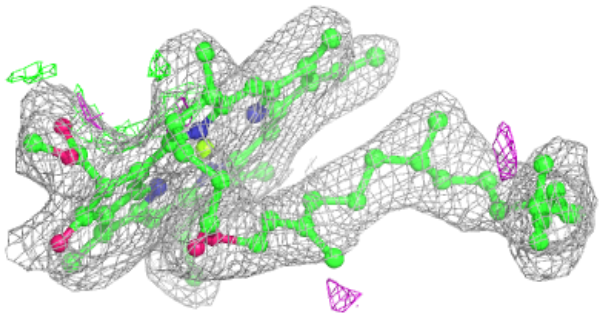




Electron density around CLA G 841:

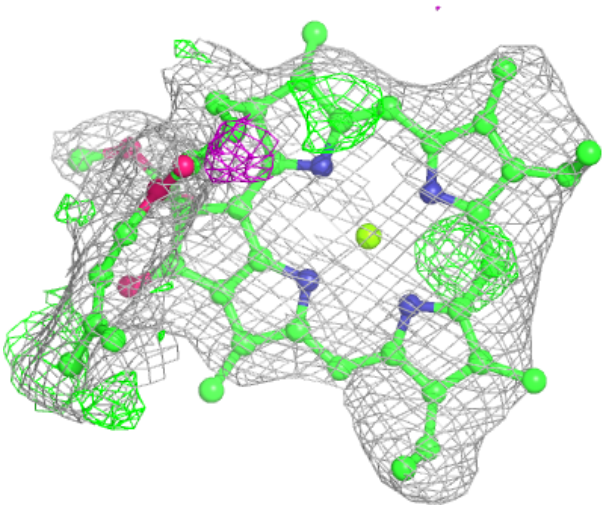
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

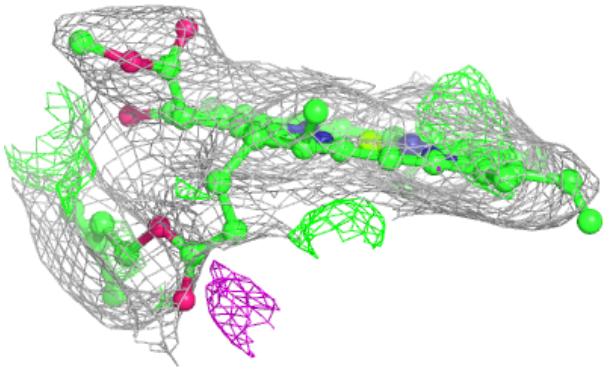


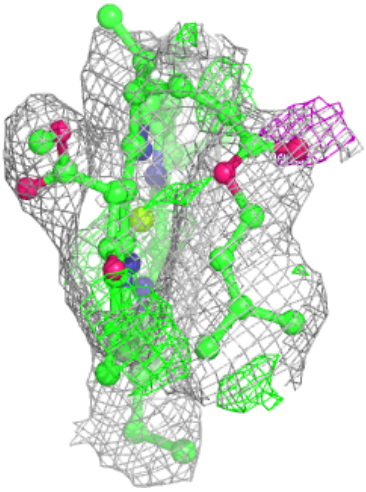


Electron density around CLA G 842:

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

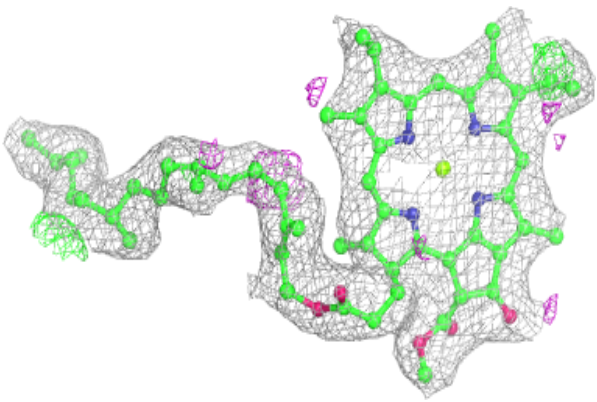


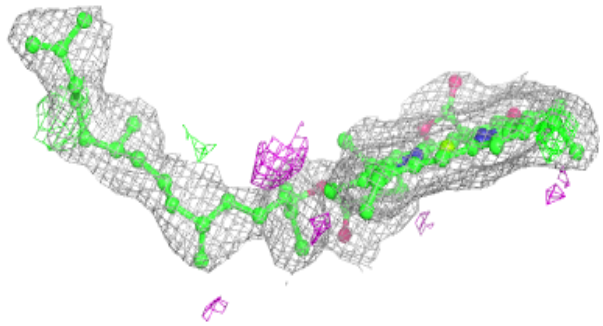


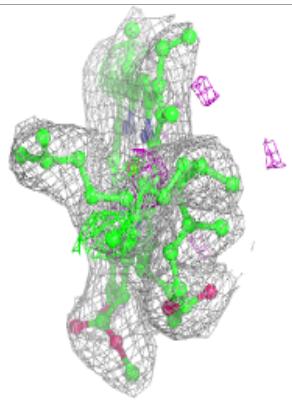


Electron density around CLA G 852:

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

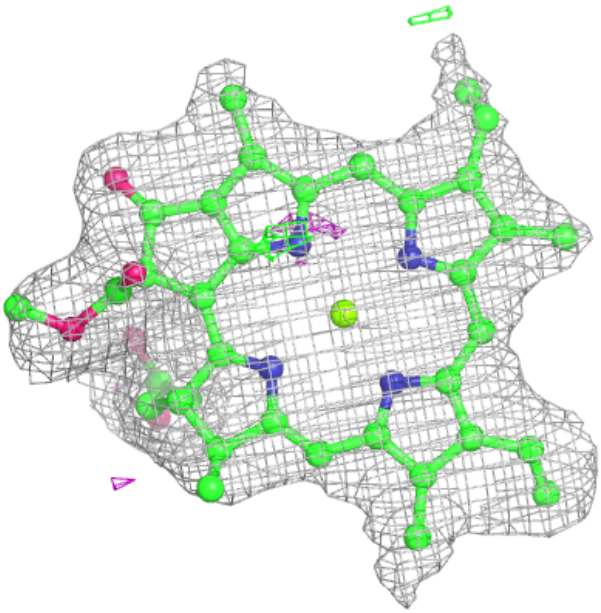


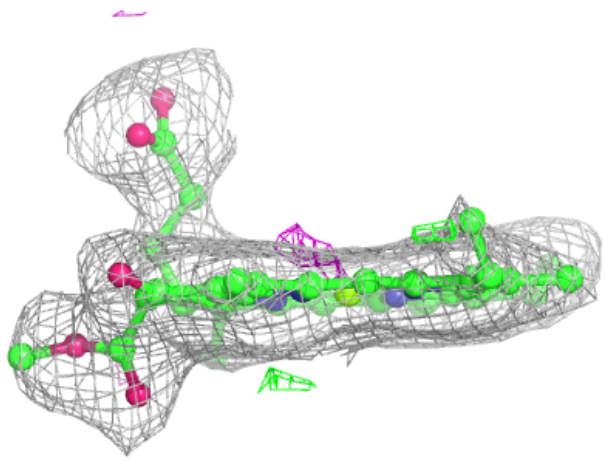


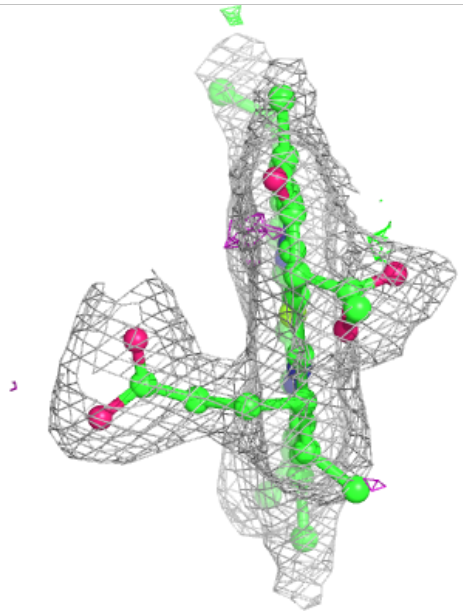


Electron density around CLA G 853:

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

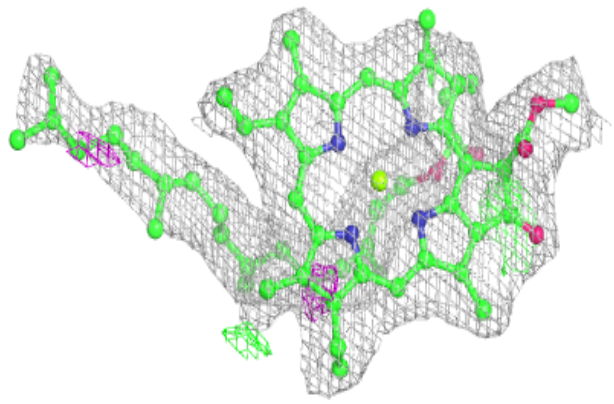


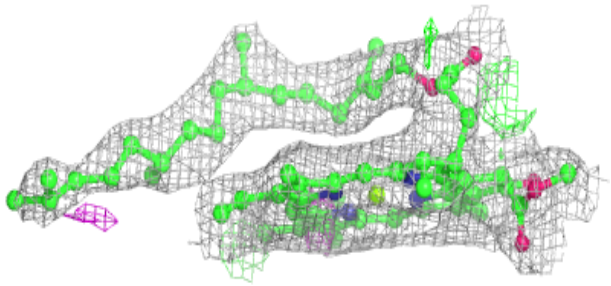




Electron density around CLA H 801:

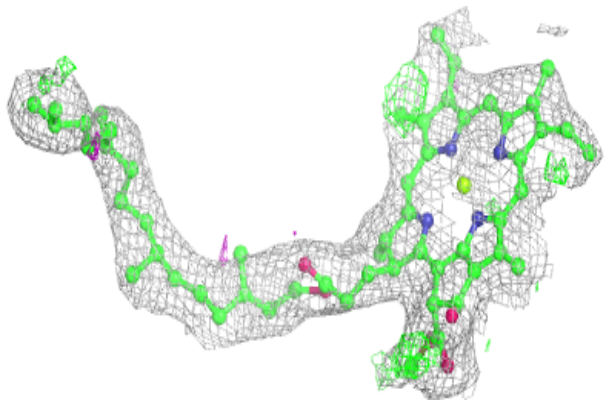
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

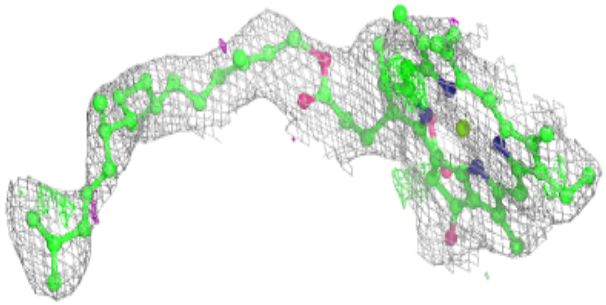


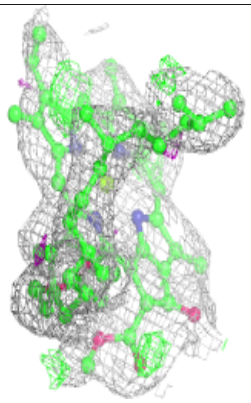


Electron density around CLA H 802:

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

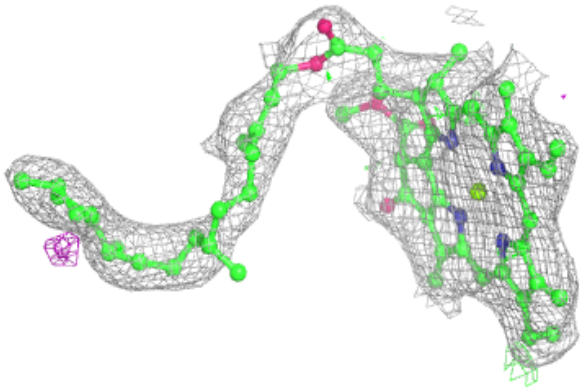


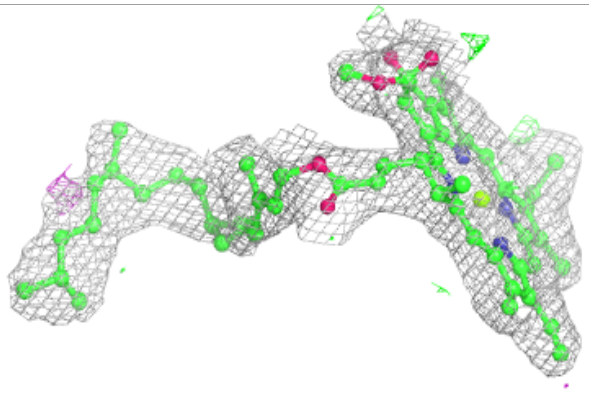


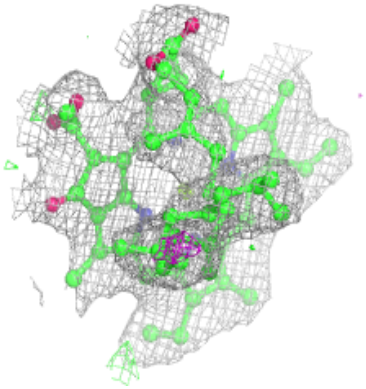


Electron density around CLA H 803:

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

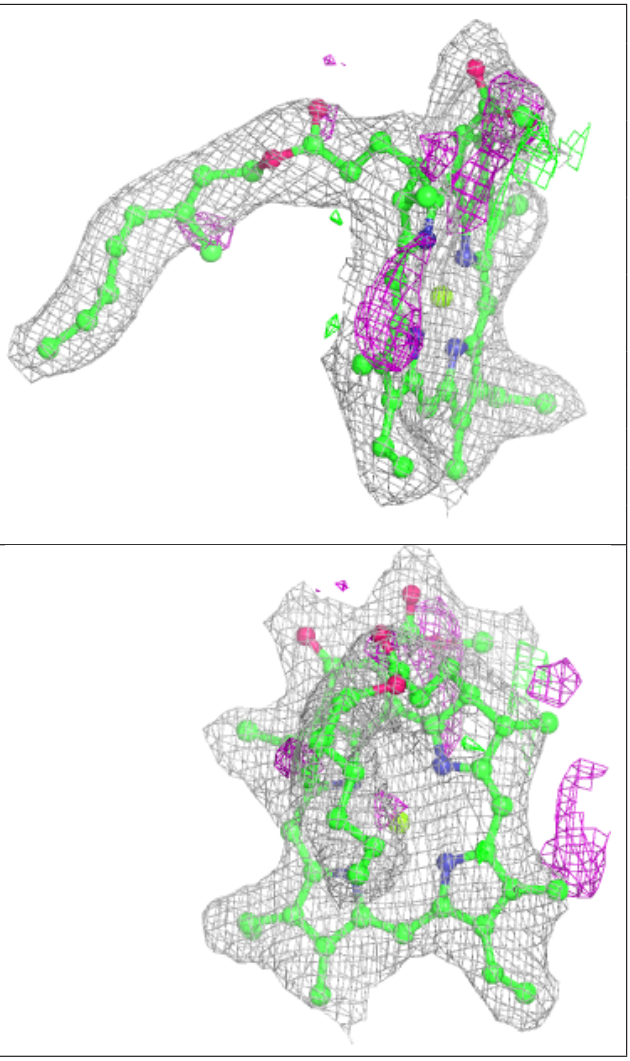


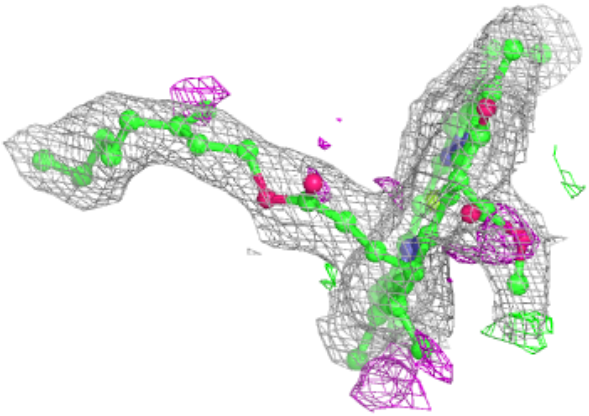




Electron density around CLA H 804:

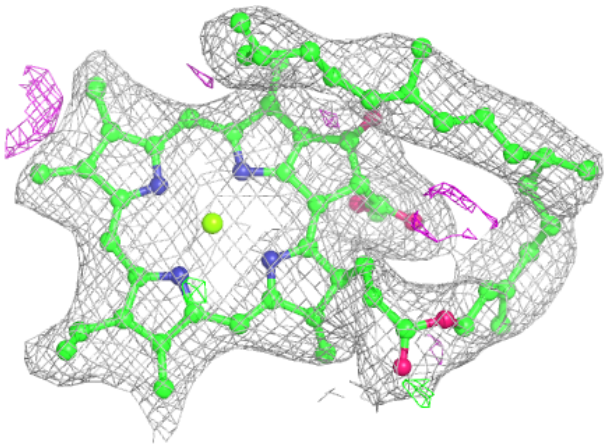
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

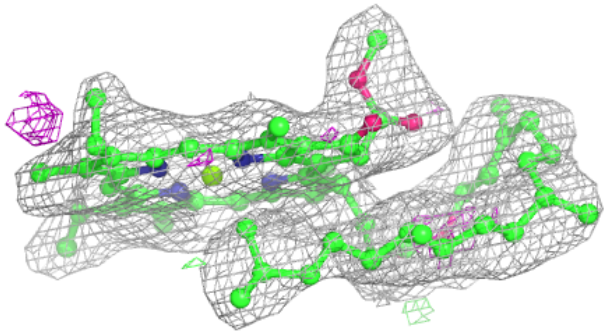


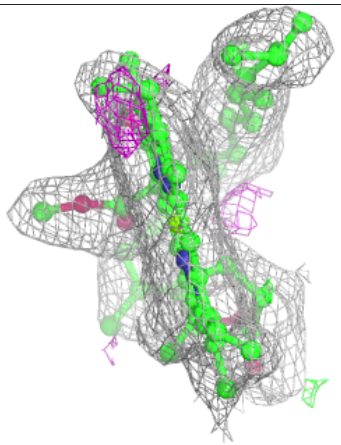


Electron density around CLA H 805:

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

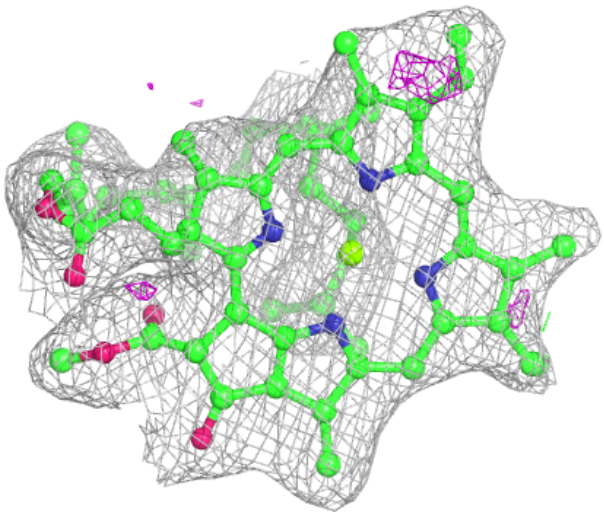


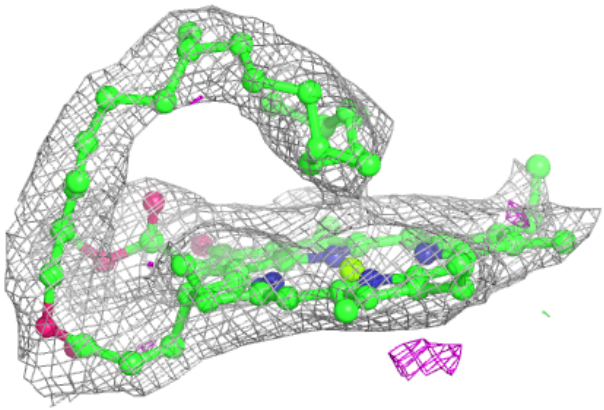


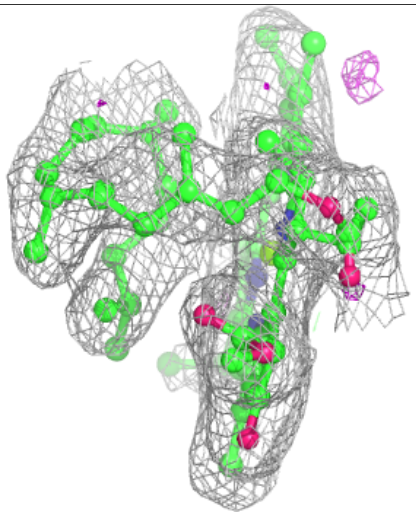


Electron density around CLA H 806:

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

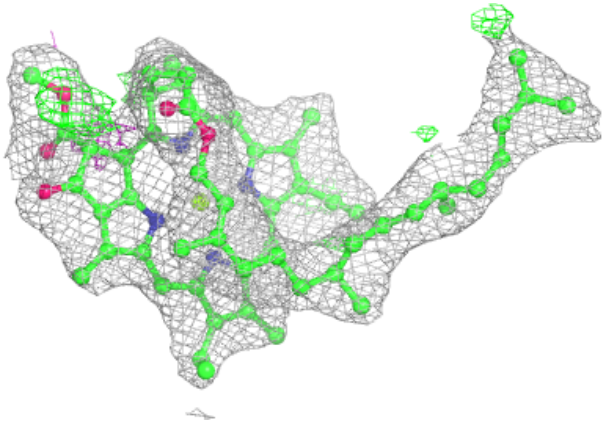


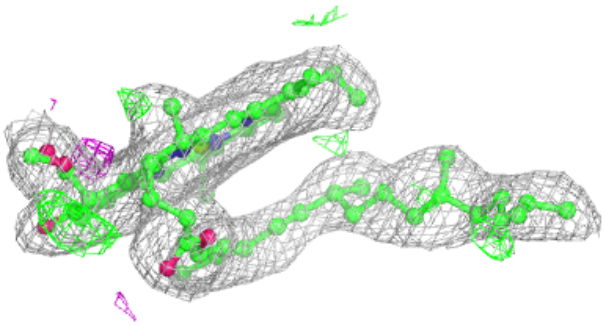


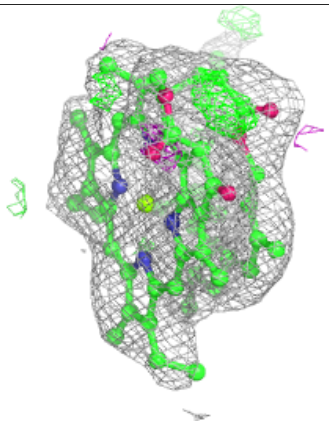


Electron density around CLA H 807:

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

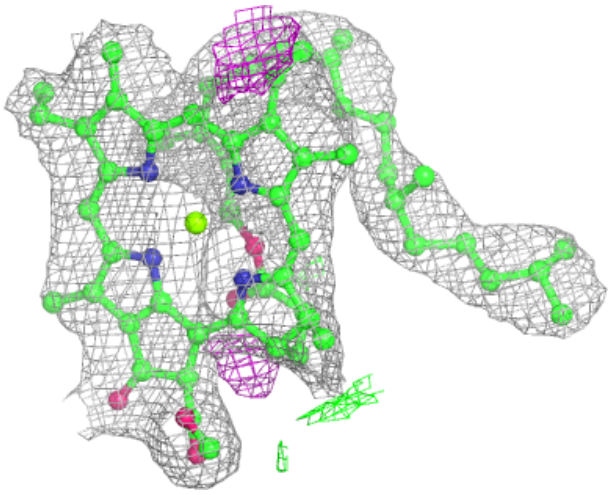


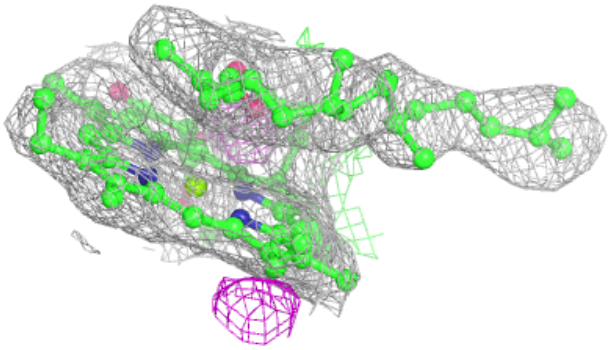


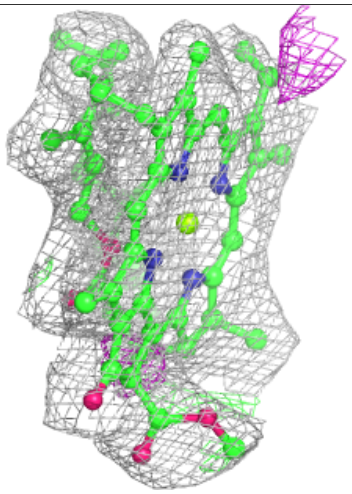


Electron density around CLA H 808:

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

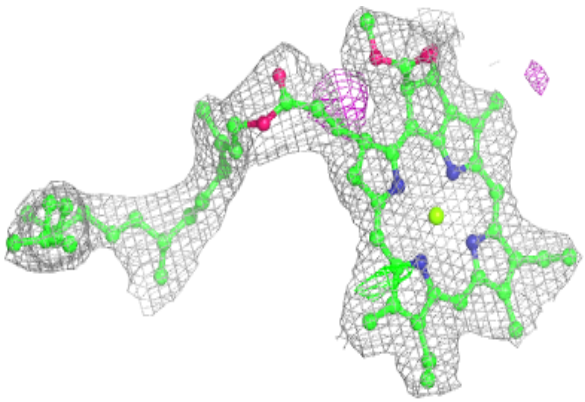


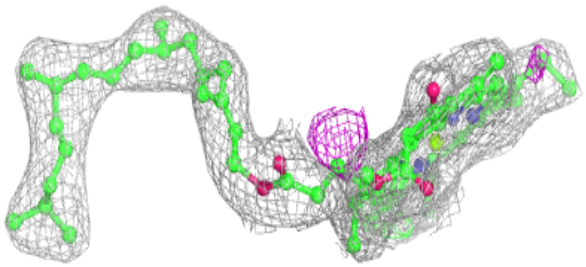


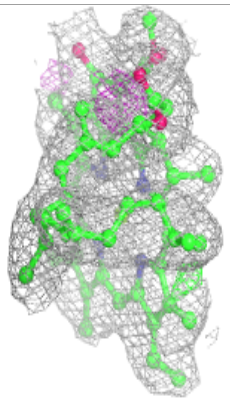


Electron density around CLA H 809:

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

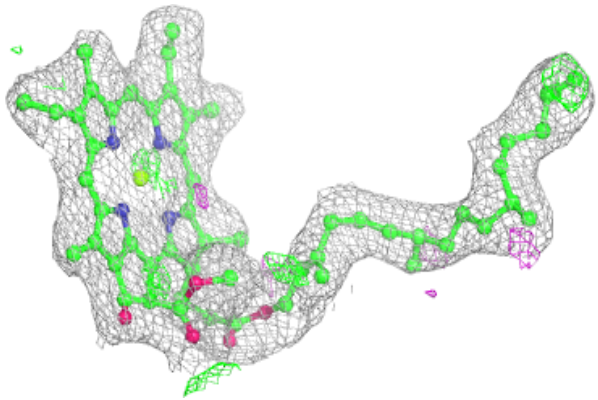


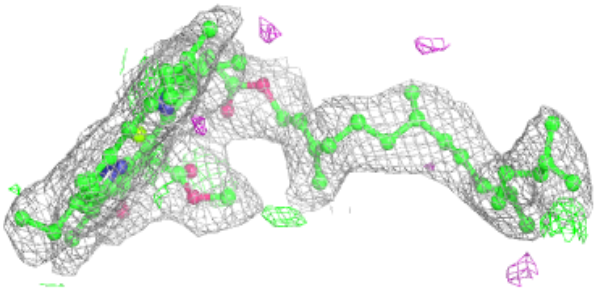


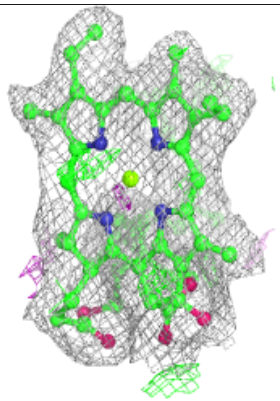


Electron density around CLA H 810:

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

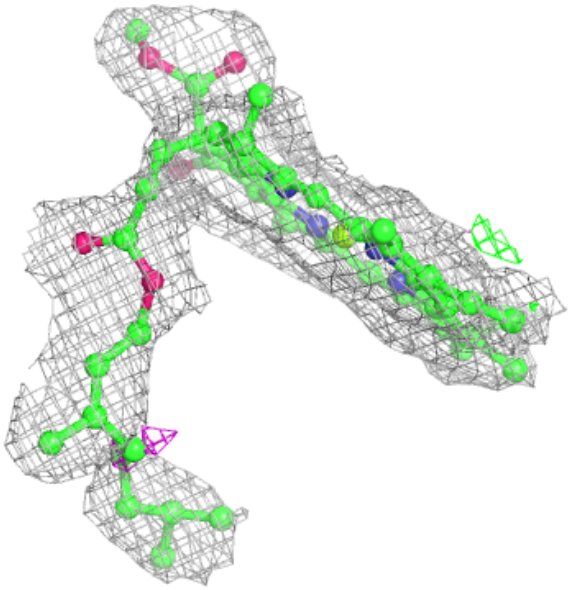


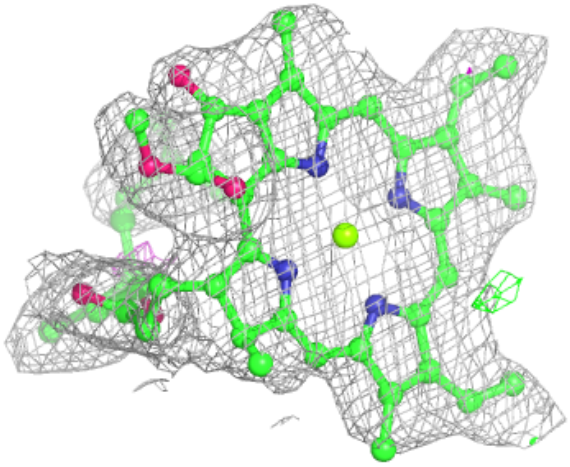


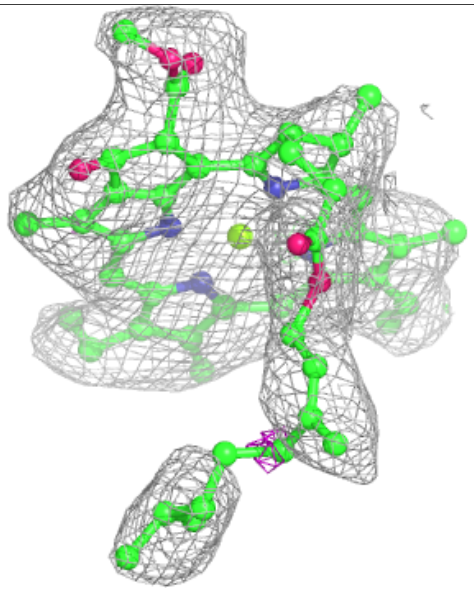


Electron density around CLA H 811:

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

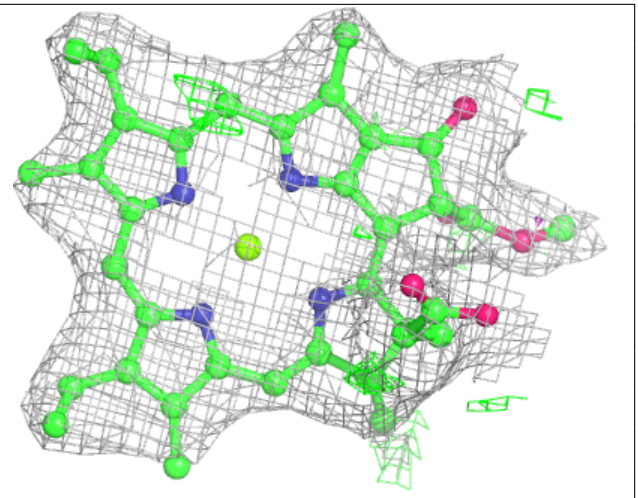


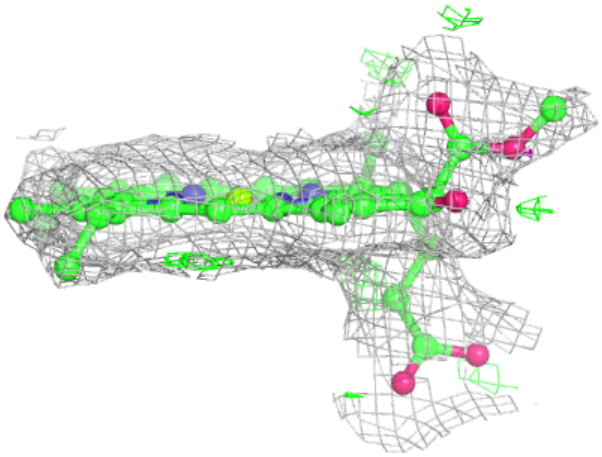


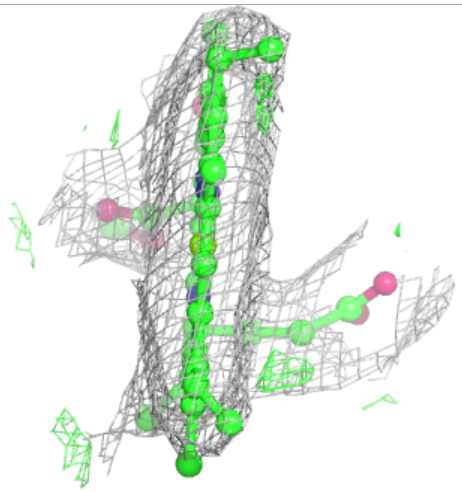


Electron density around CLA H 812:

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

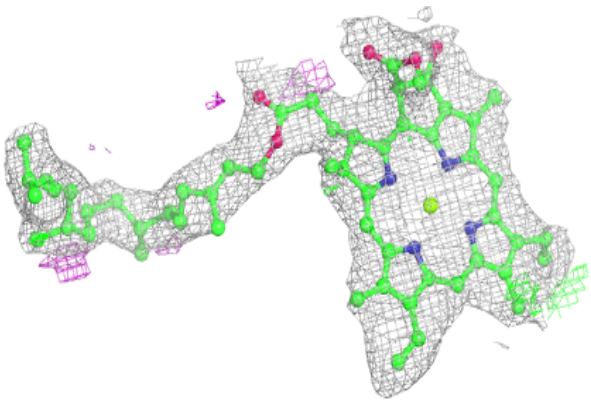


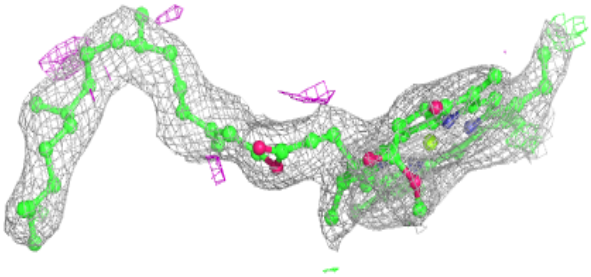




Electron density around CLA H 813:

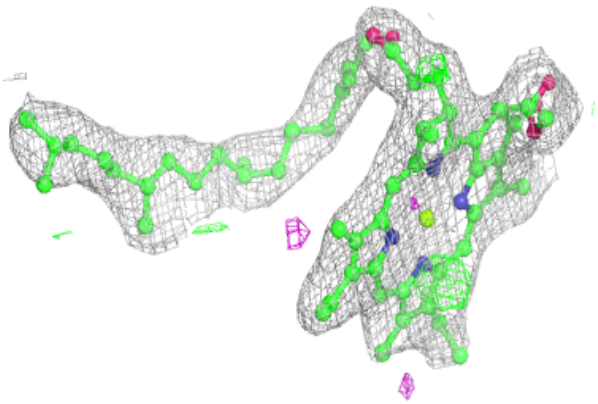
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

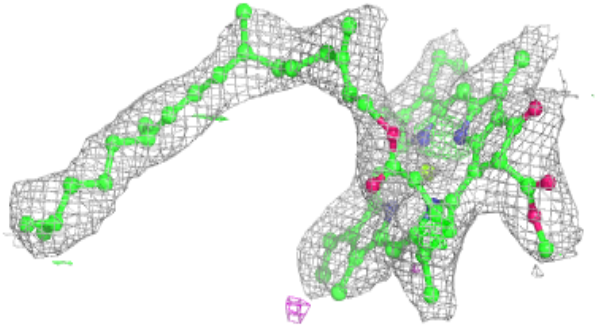


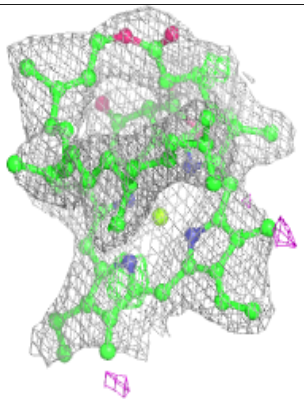


Electron density around CLA H 814:

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

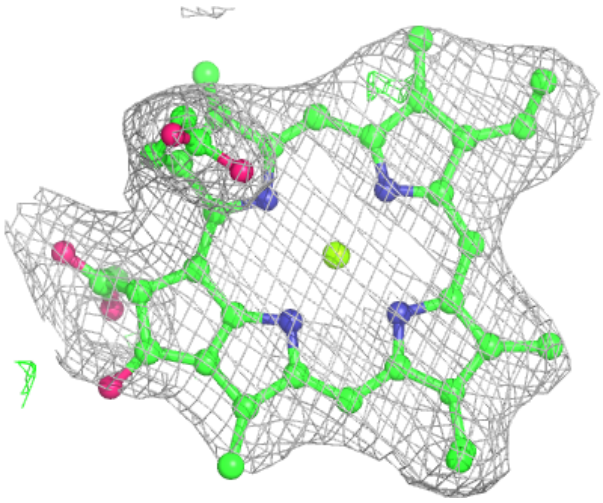


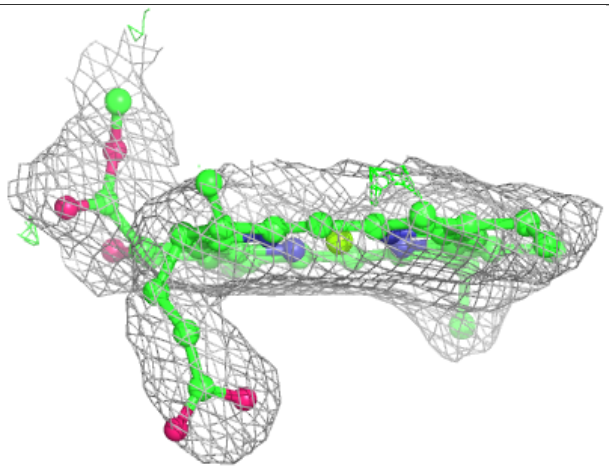


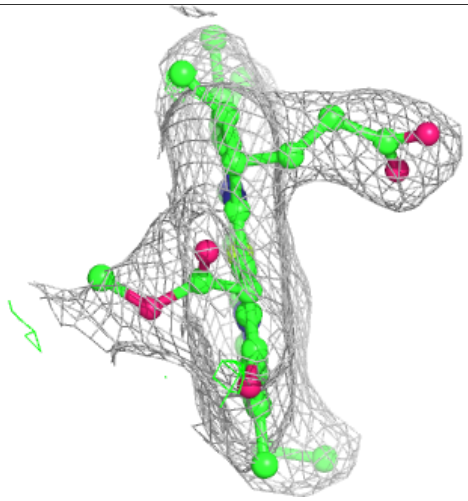


Electron density around CLA H 815:

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

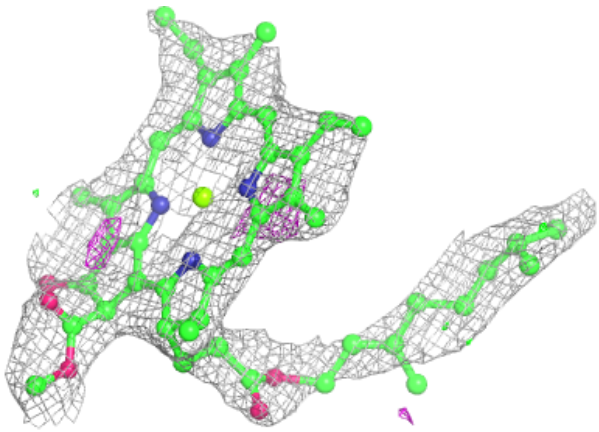


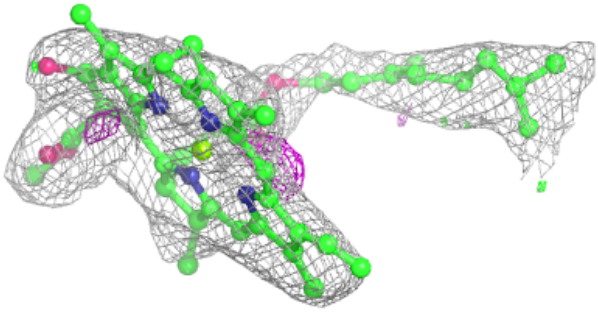


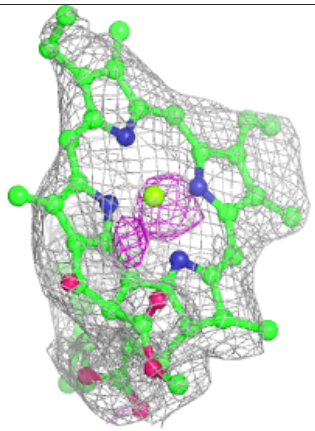


Electron density around CLA H 816:

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

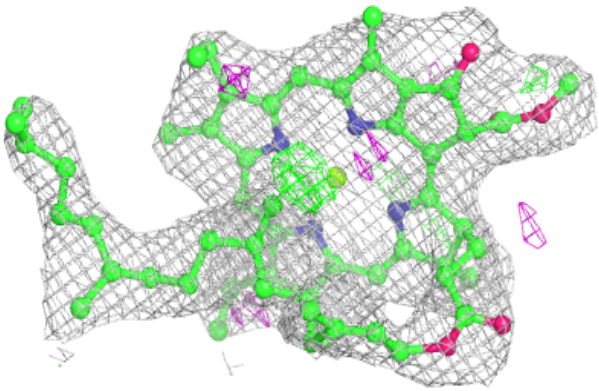


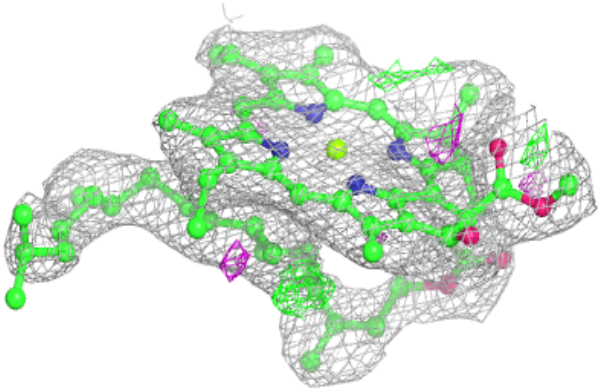


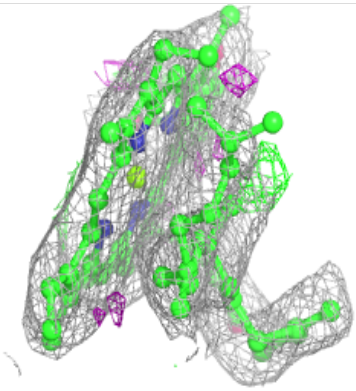


Electron density around CLA H 817:

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

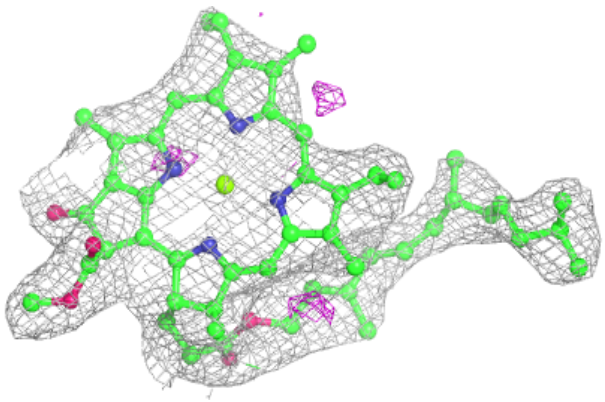


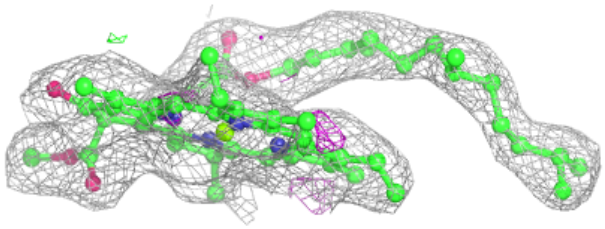


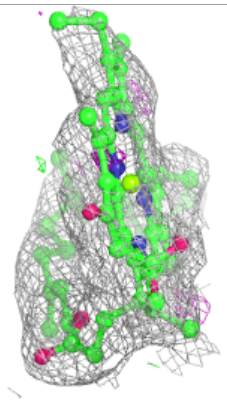


Electron density around CLA H 818:

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

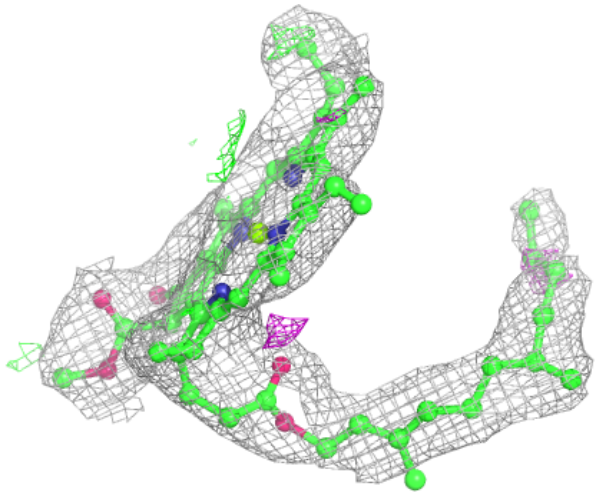


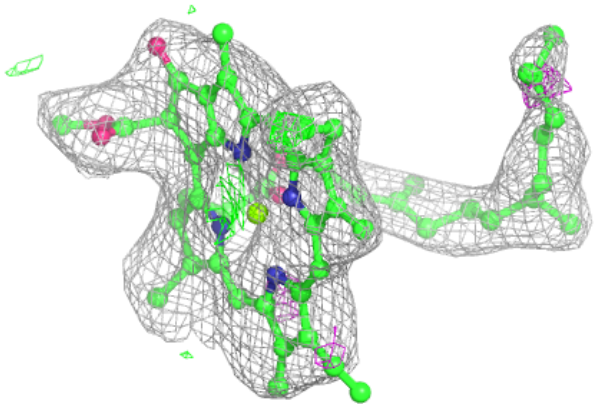


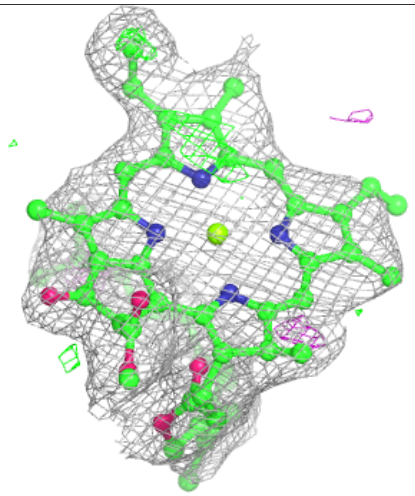


Electron density around CLA H 819:

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

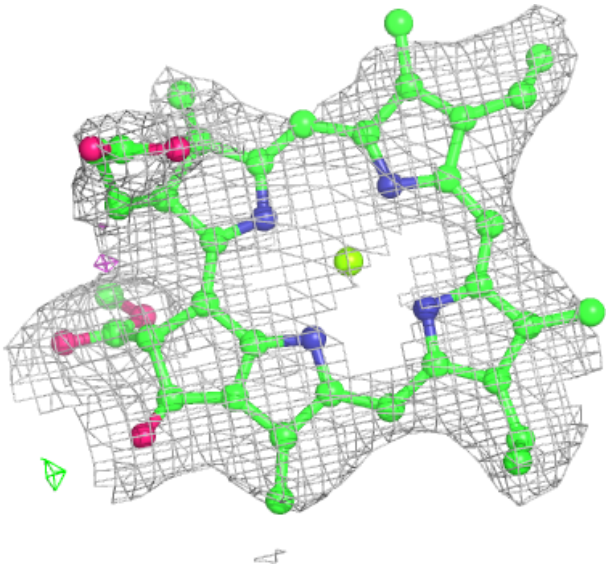


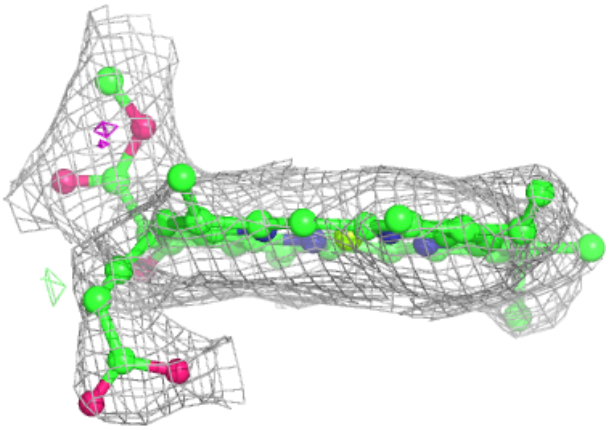


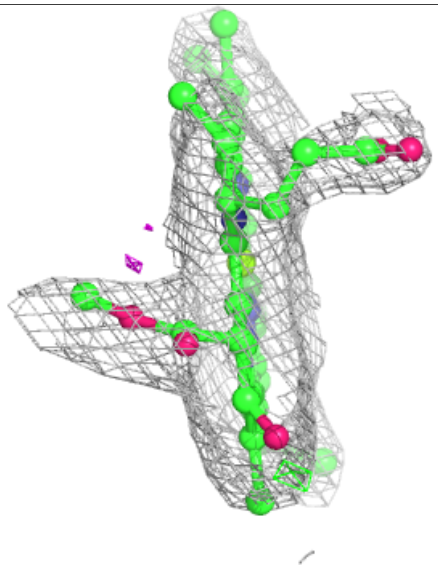


Electron density around CLA H 820:

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

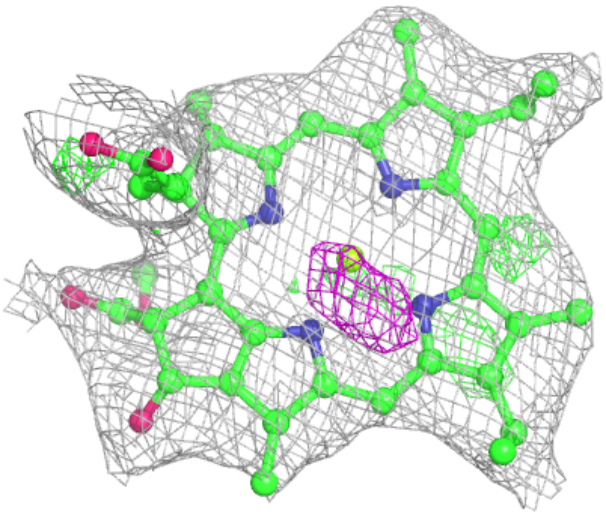


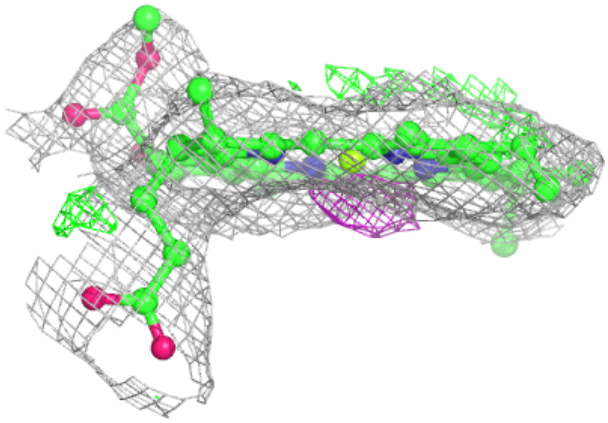


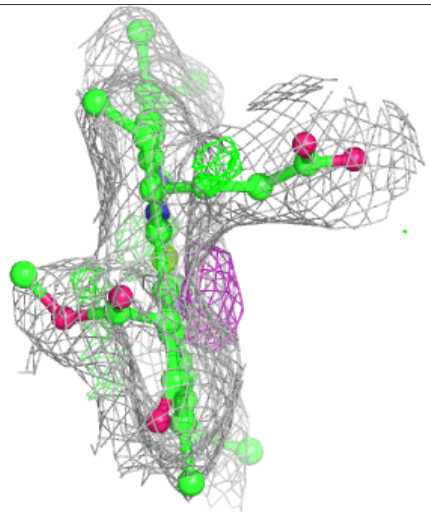


Electron density around CLA H 821:

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

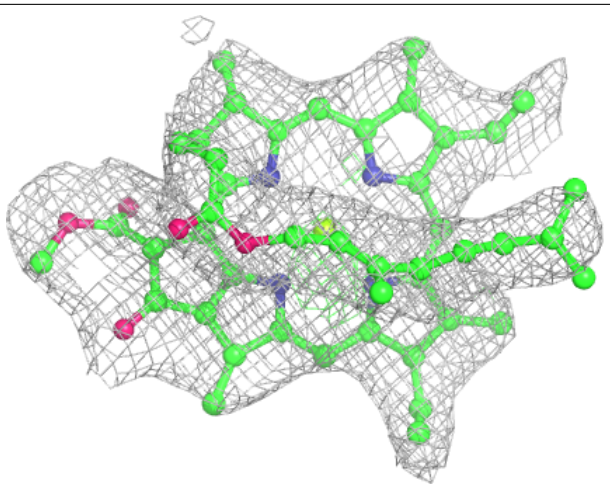


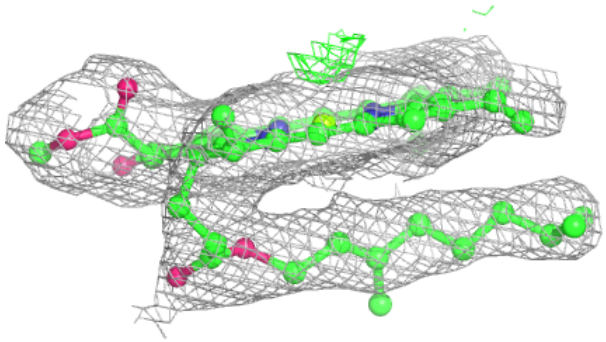


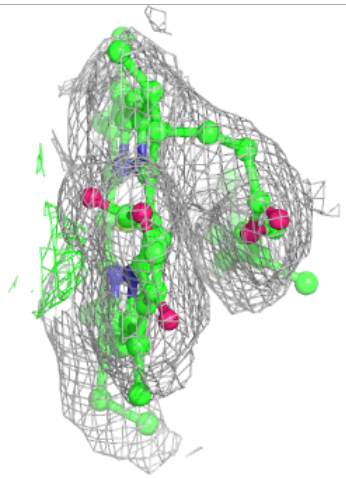


Electron density around CLA H 822:

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

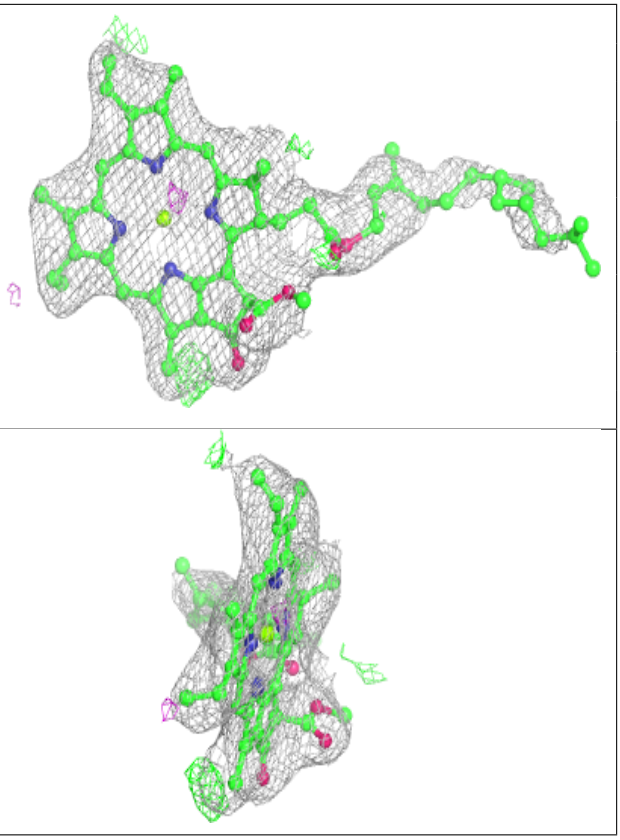


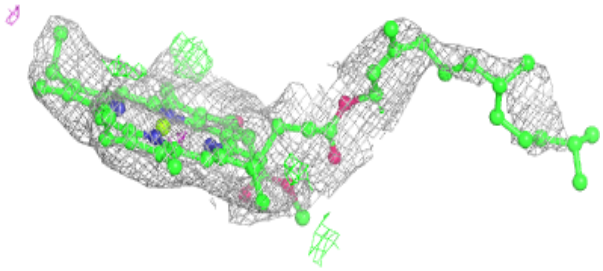




Electron density around CLA H 823:

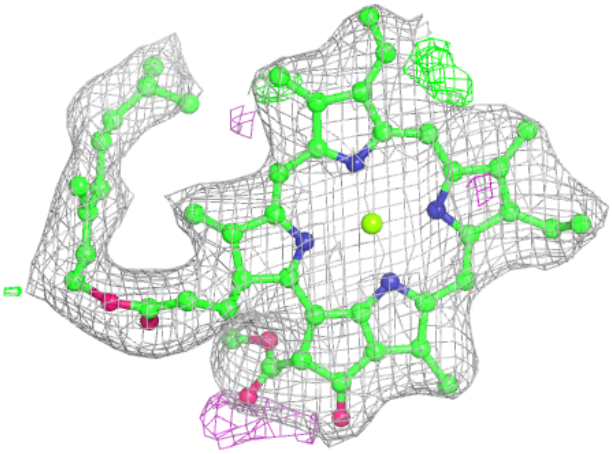
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

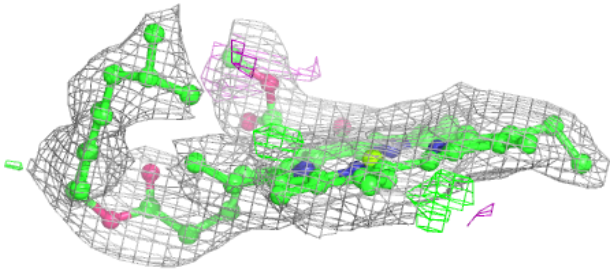


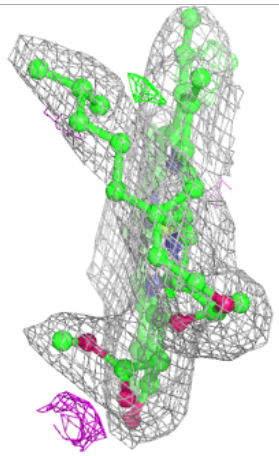


Electron density around CLA H 824:

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

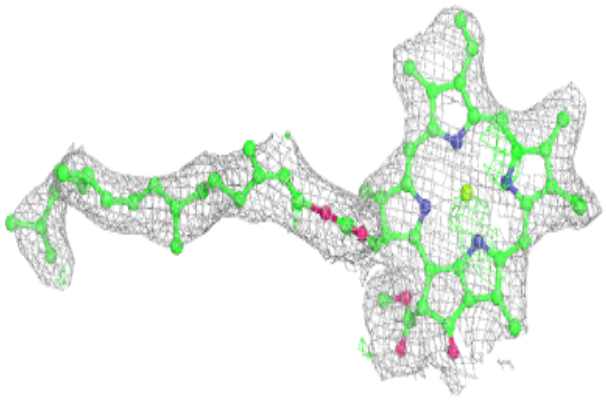


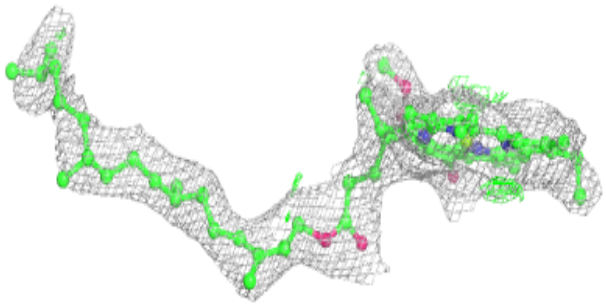


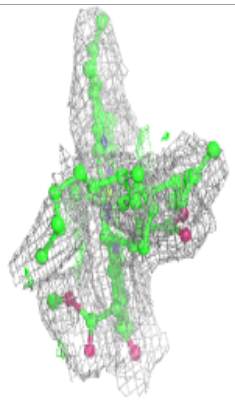


Electron density around CLA H 825:

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

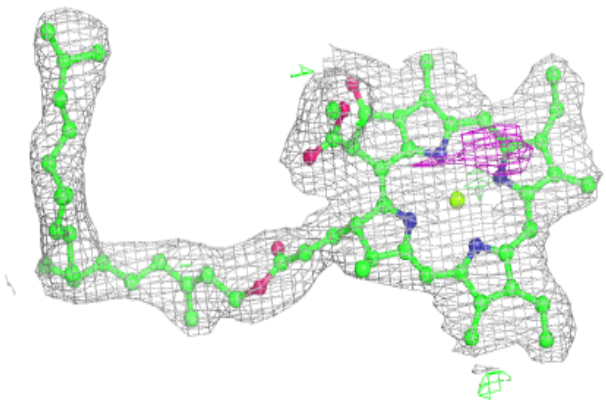


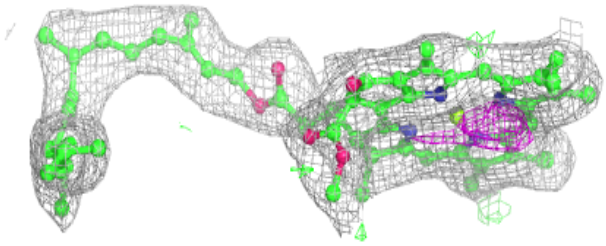


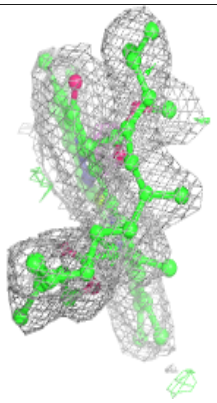


Electron density around CLA H 826:

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

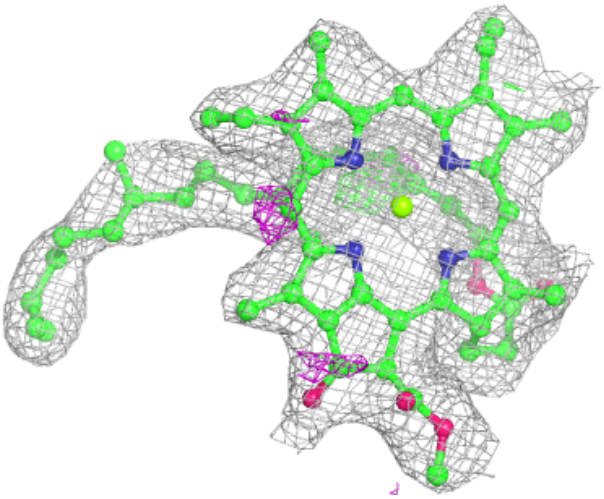


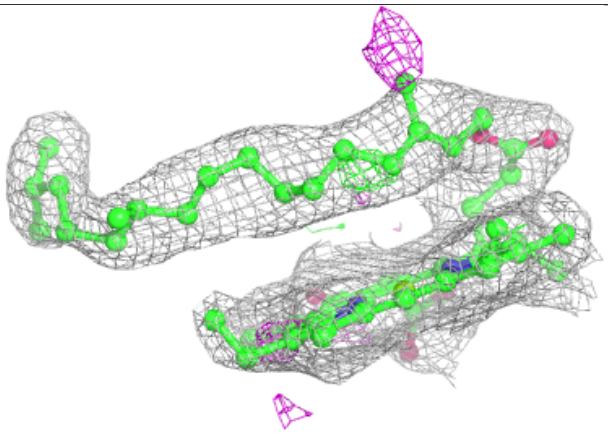


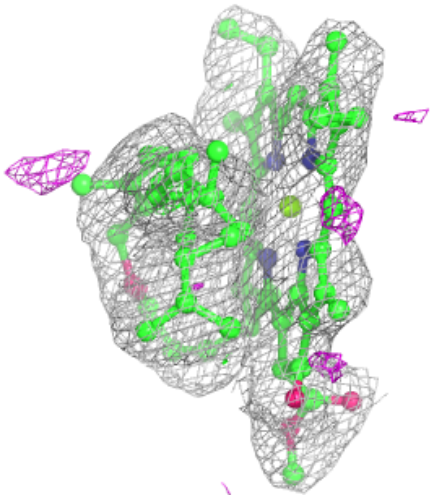


Electron density around CLA H 827:

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

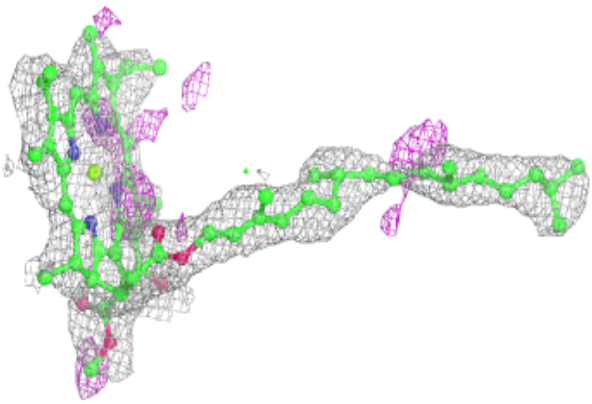


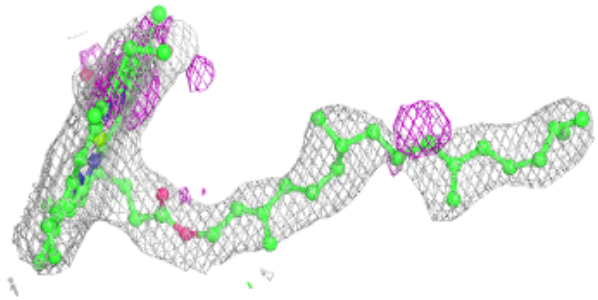


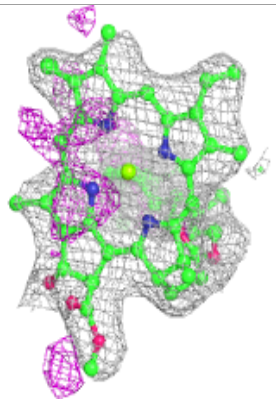


Electron density around CLA H 828:

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

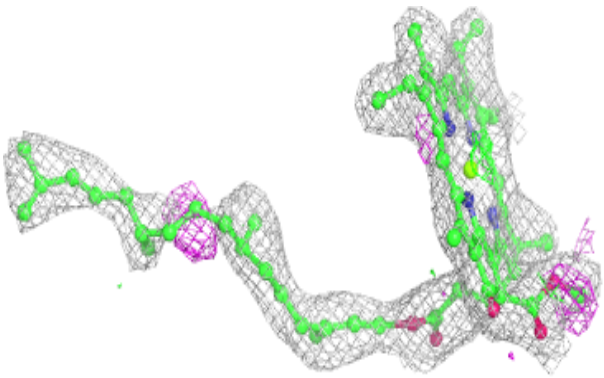


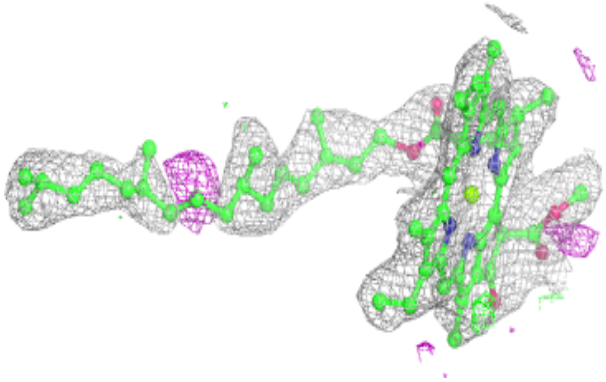


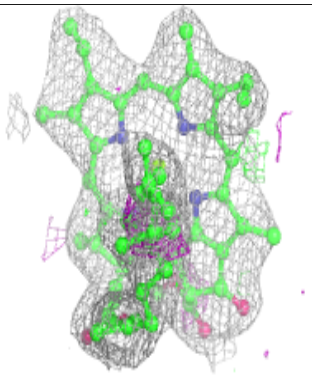


Electron density around CLA H 829:

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

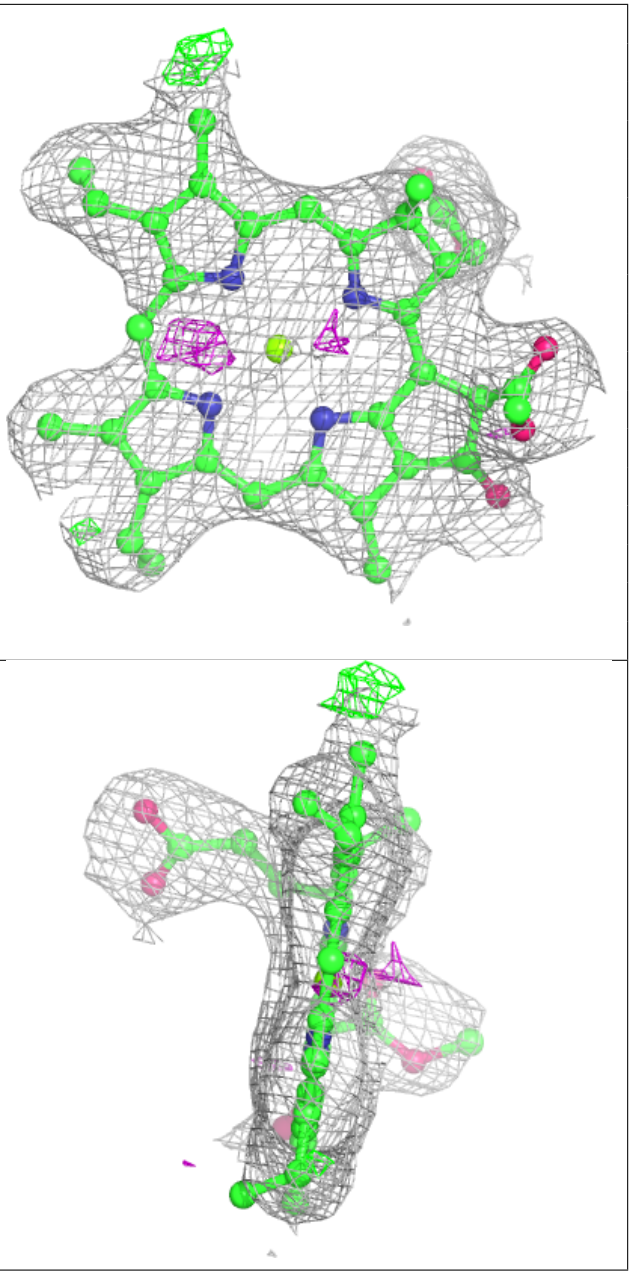






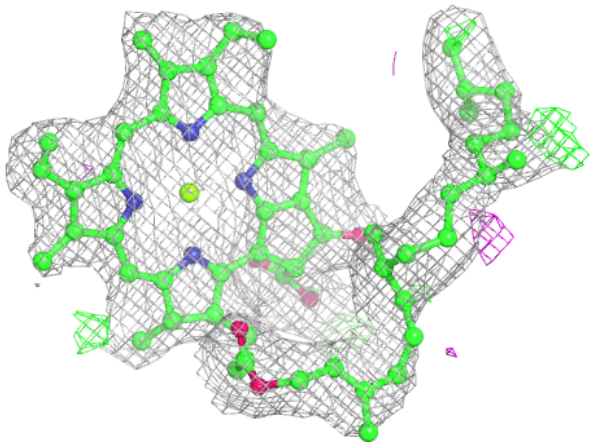
Electron density around CLA H 830:

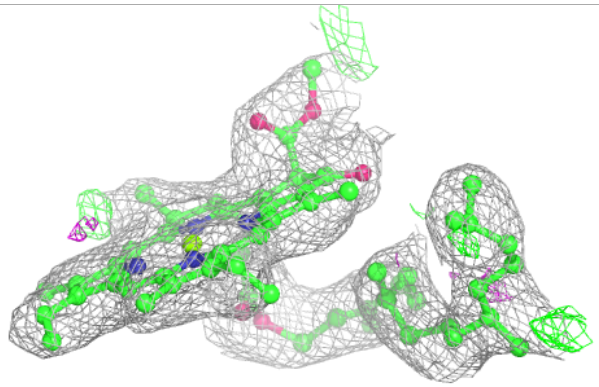
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

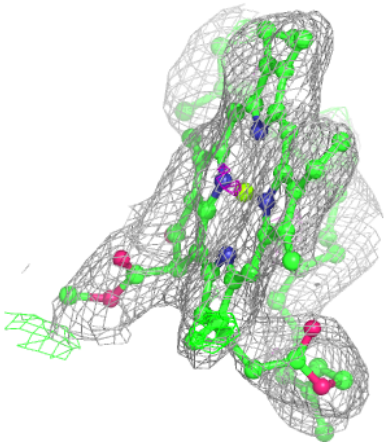


Electron density around CLA H 831:

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

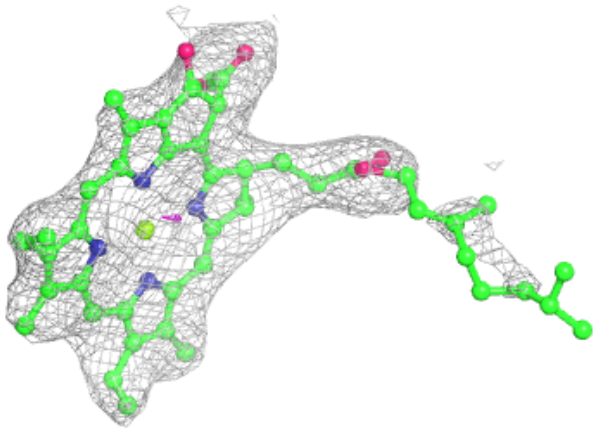


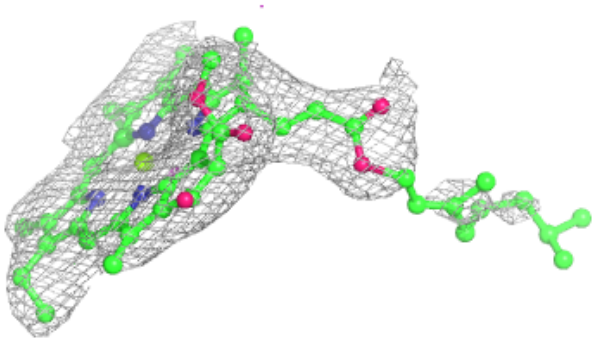


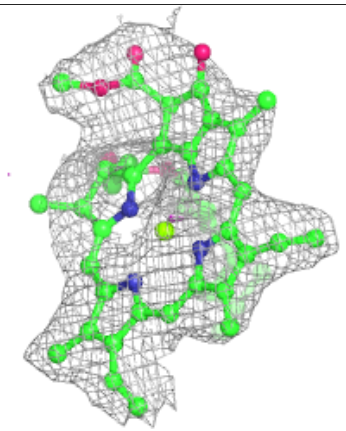


Electron density around CLA H 832:

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

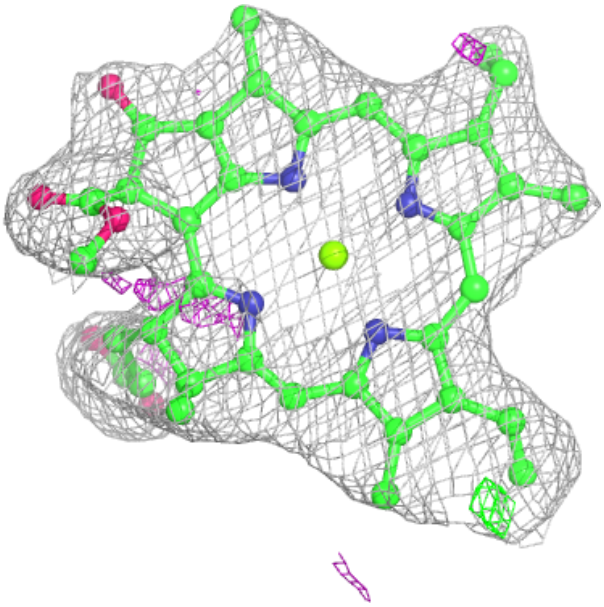


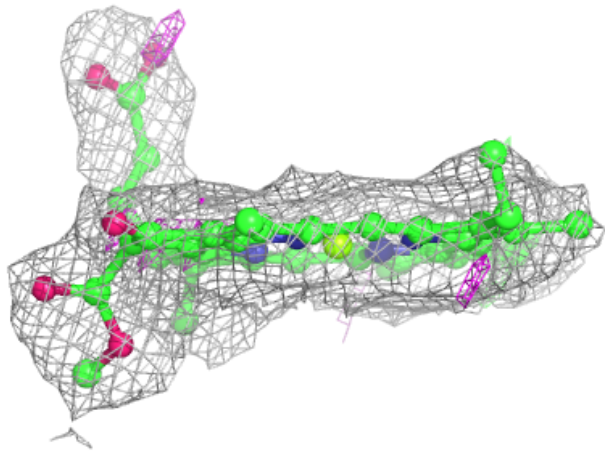




Electron density around CLA H 833:

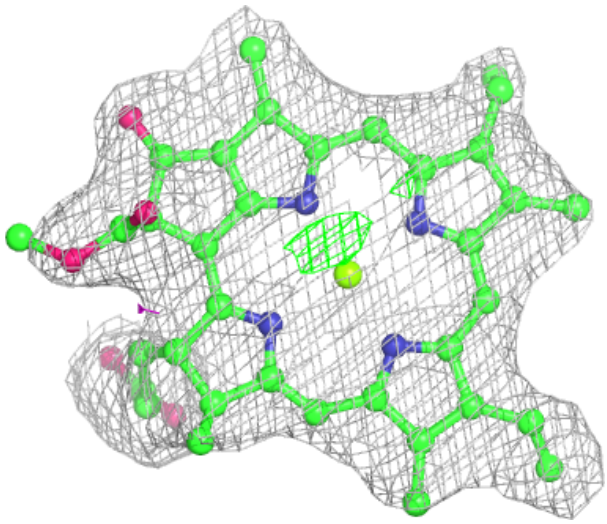
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

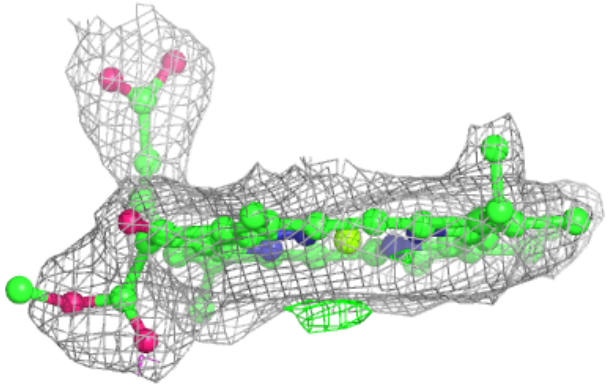


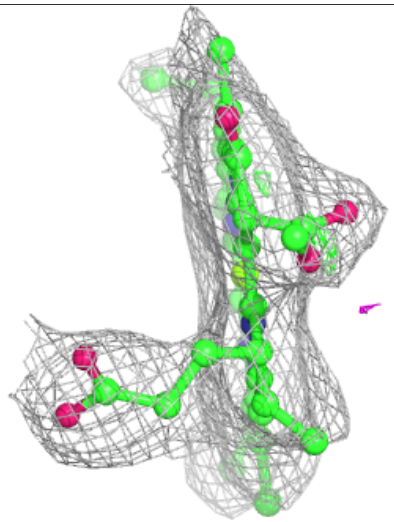


Electron density around CLA H 834:

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

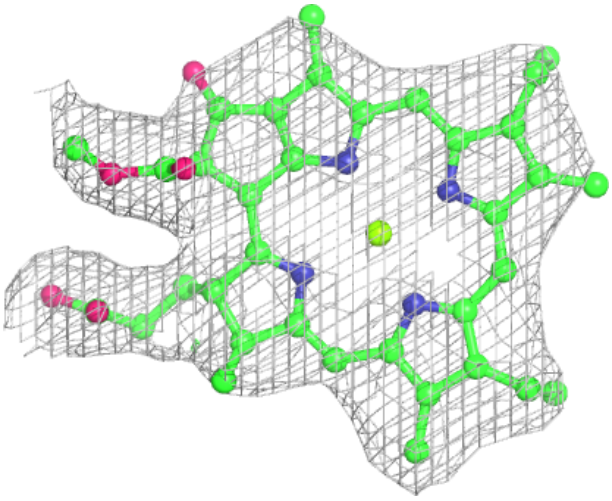


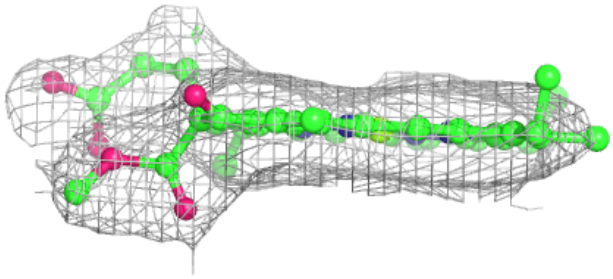


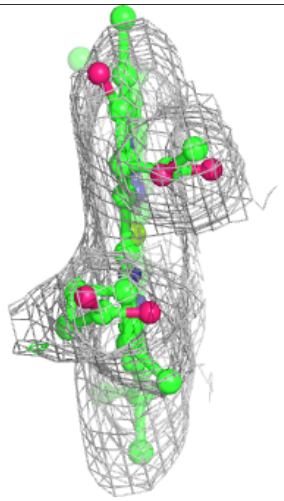


Electron density around CLA H 835:

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

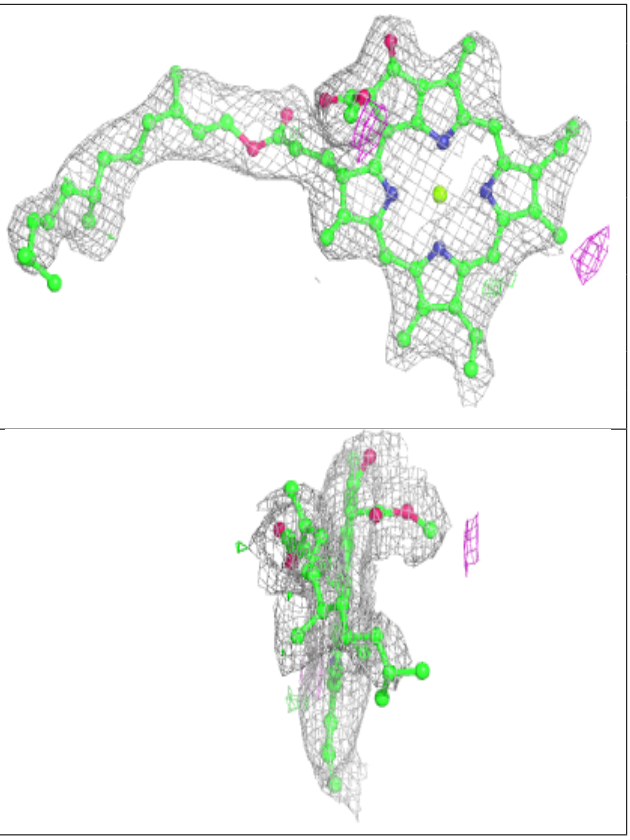






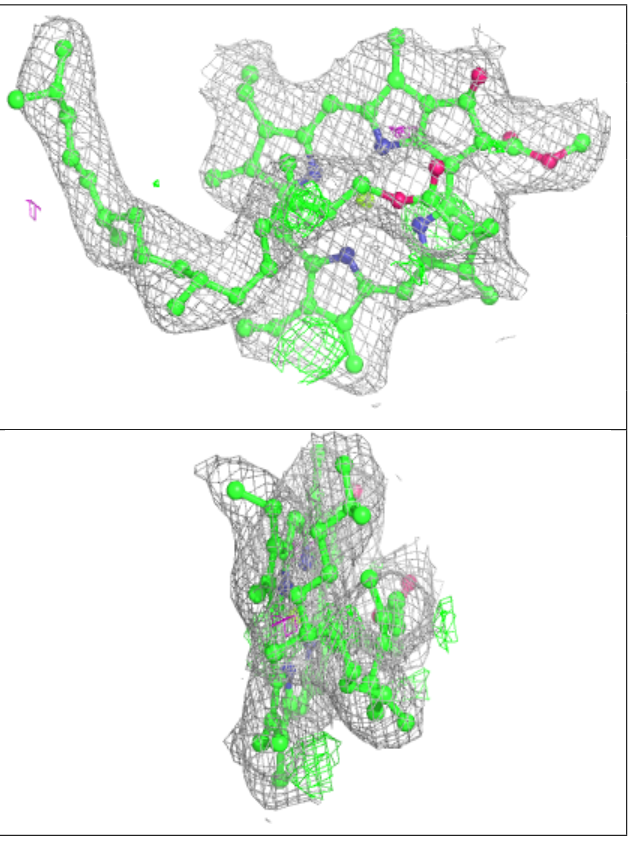
Electron density around CLA H 836:

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



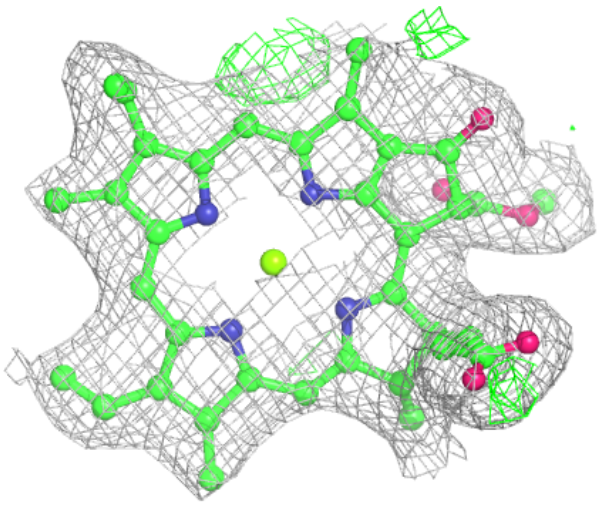
Electron density around CLA H 837:

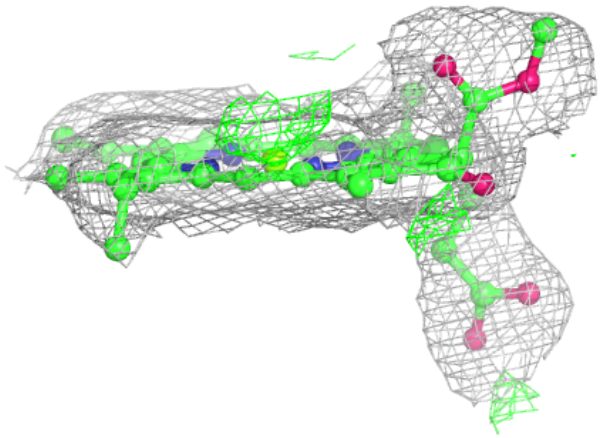
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

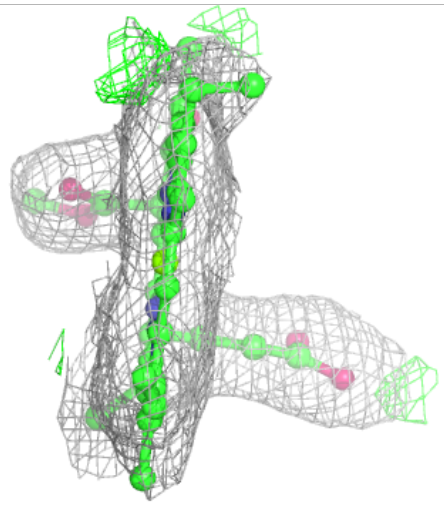


Electron density around CLA H 838:

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

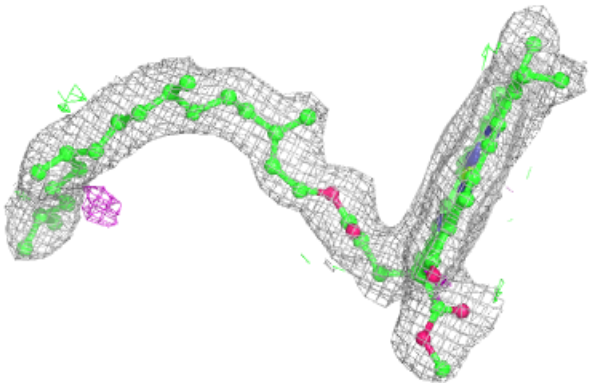


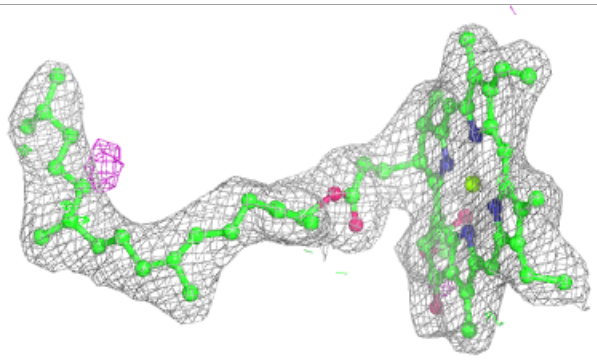


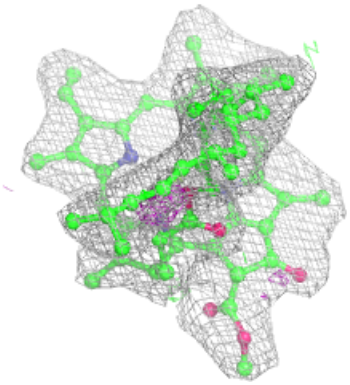


Electron density around CLA H 839:

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

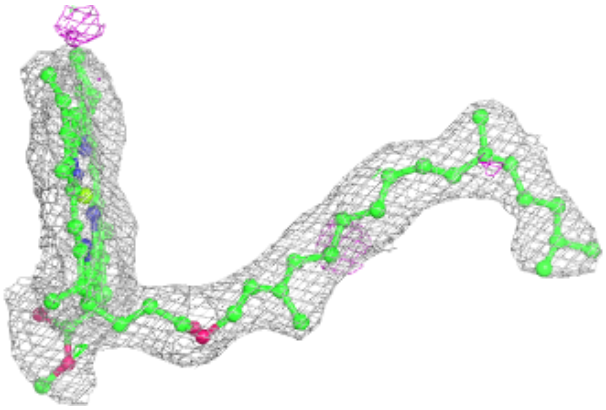


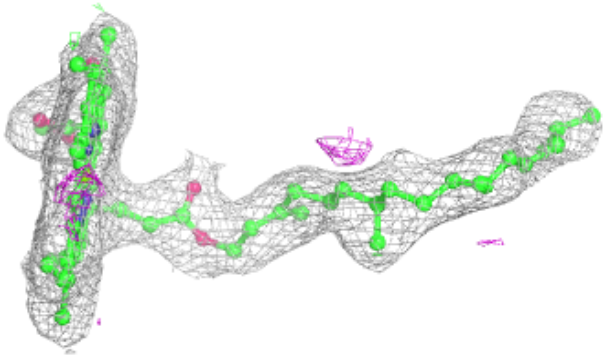


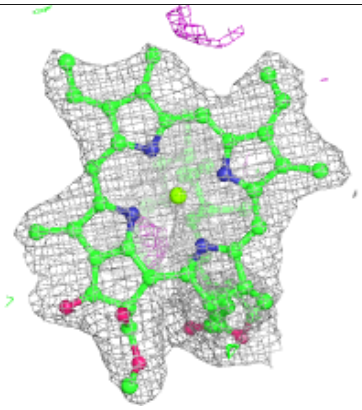


Electron density around CLA H 840:

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

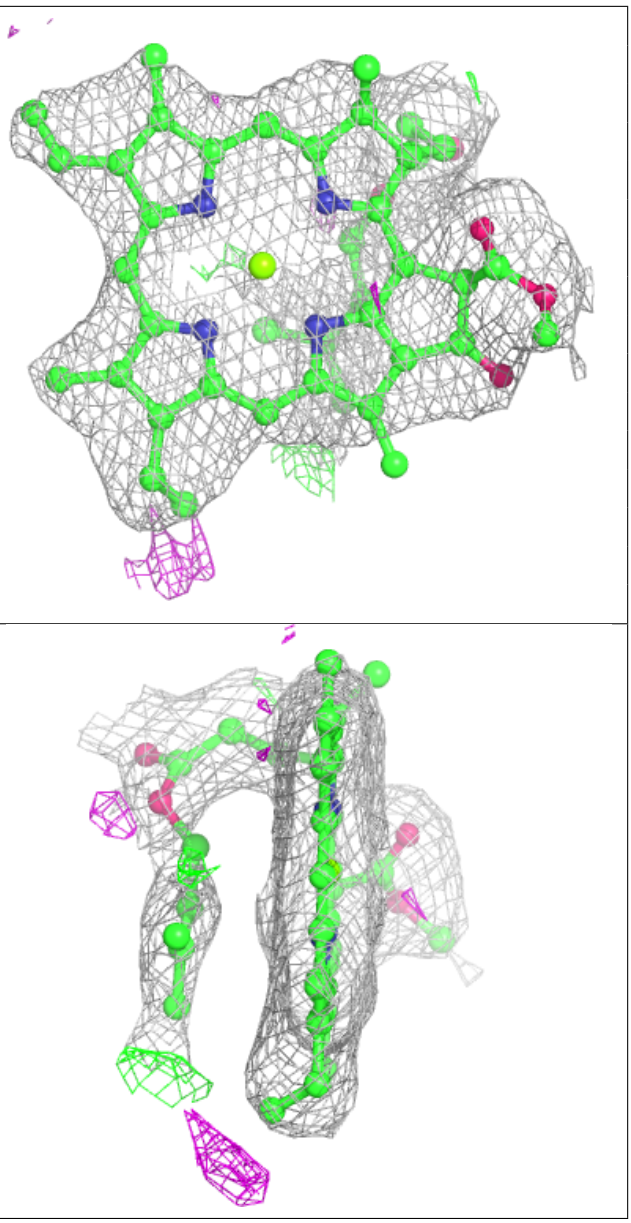






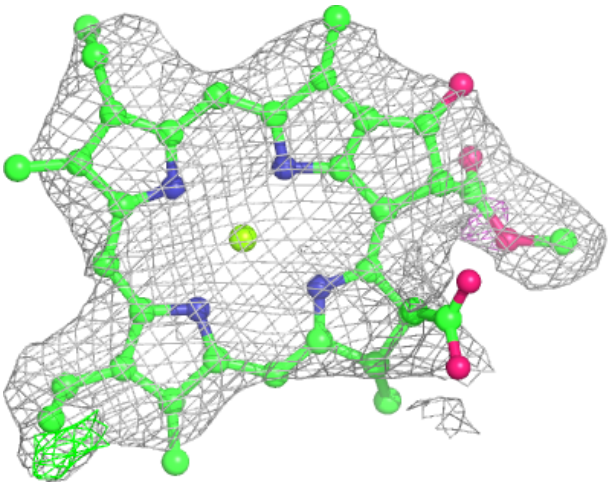
Electron density around CLA H 851:

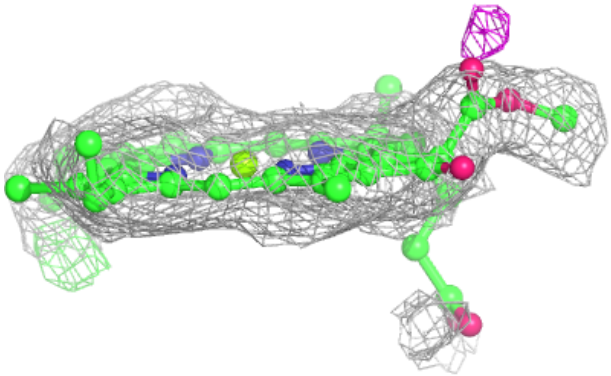
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

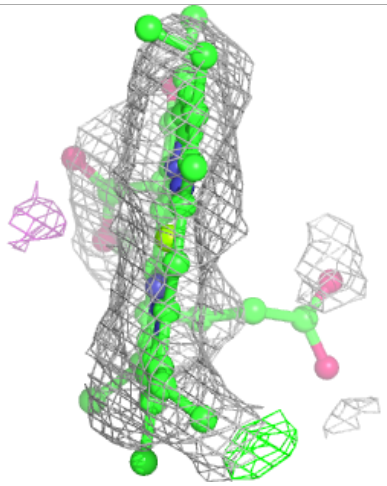


Electron density around CLA J 101:

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

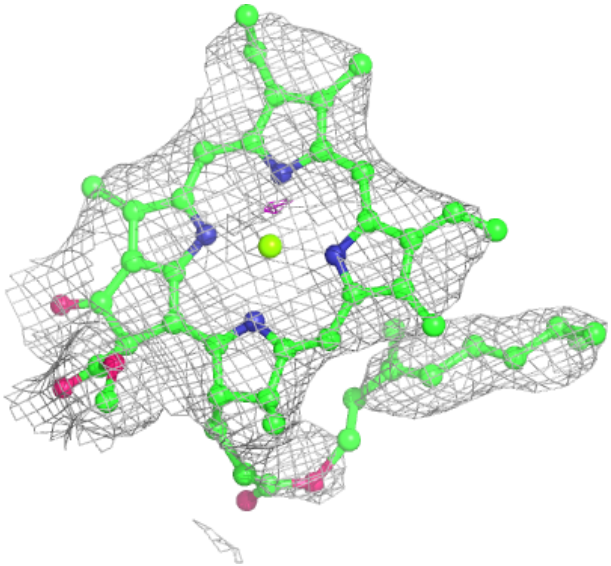


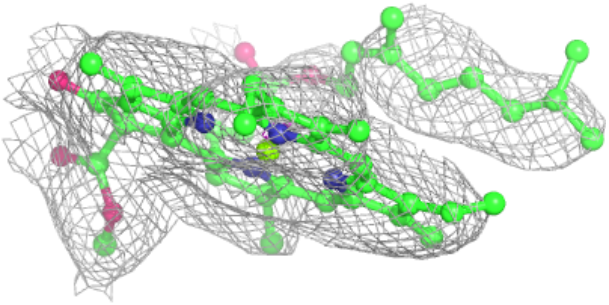


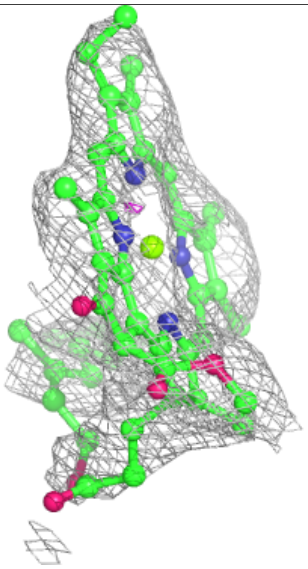


Electron density around CLA J 102:

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

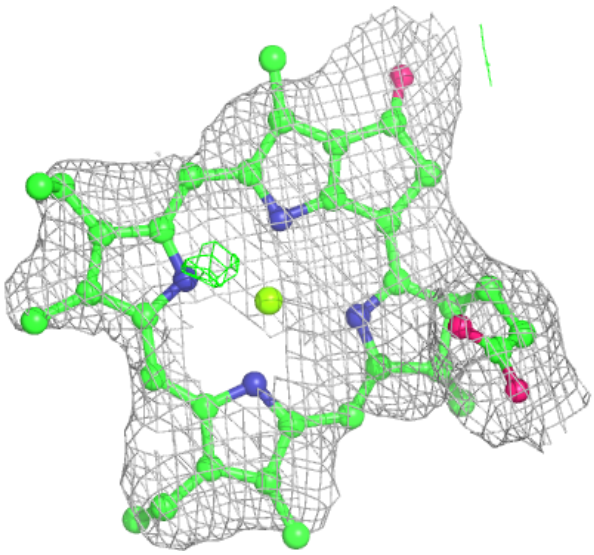


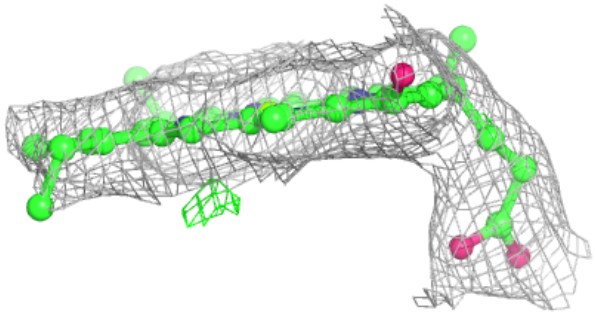


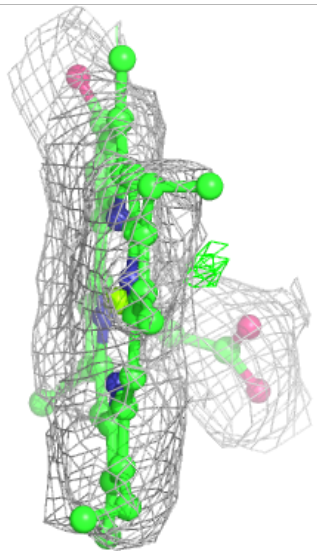


Electron density around CLA K 101:

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

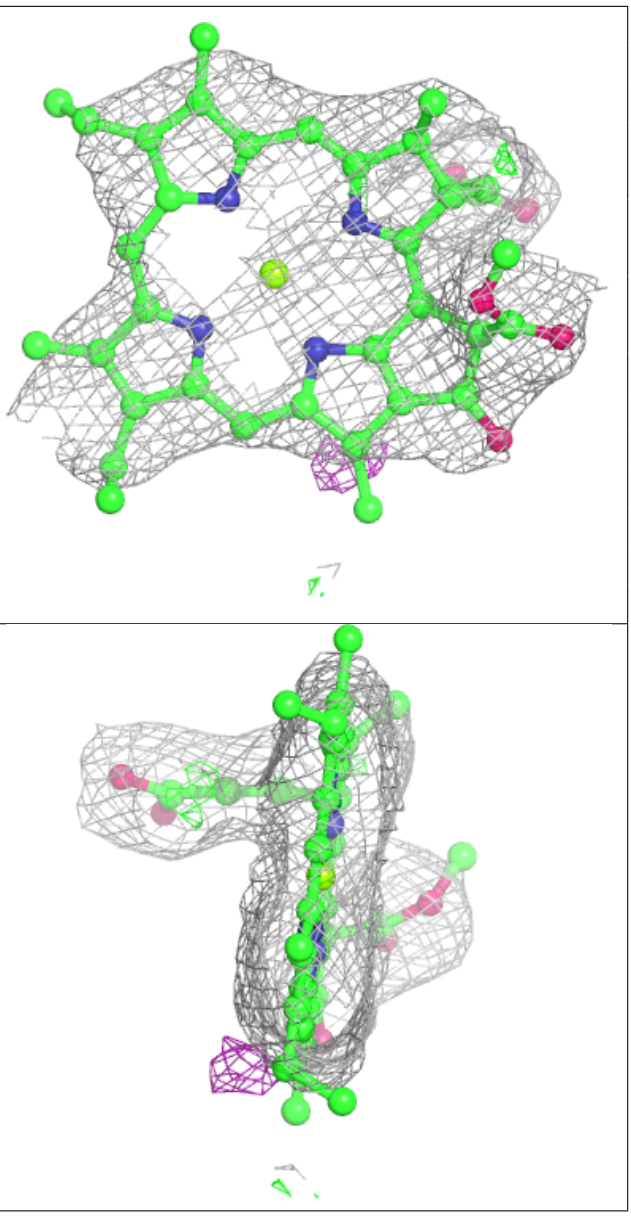






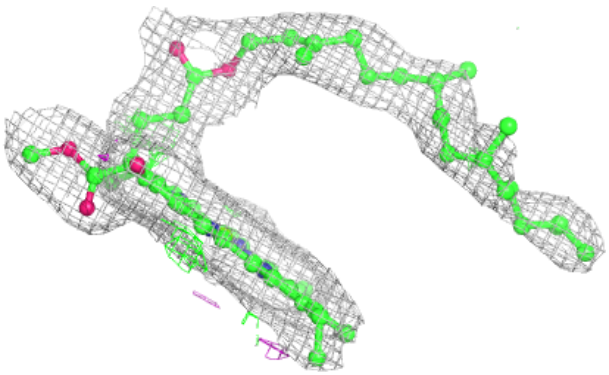
Electron density around CLA K 102:

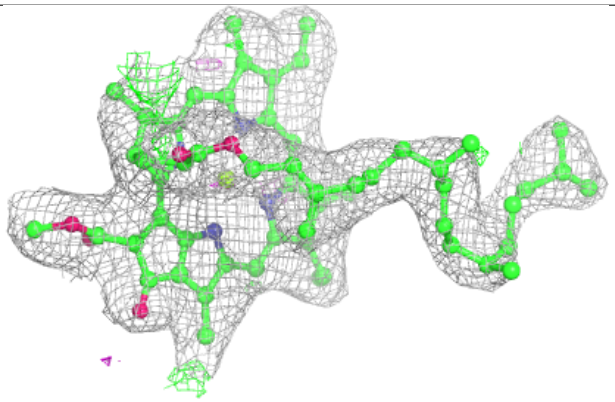
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

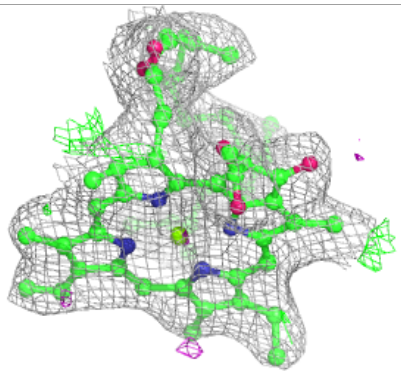


Electron density around CLA L 201:

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

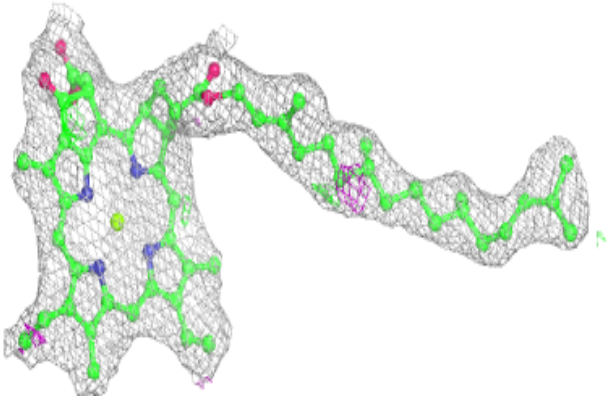


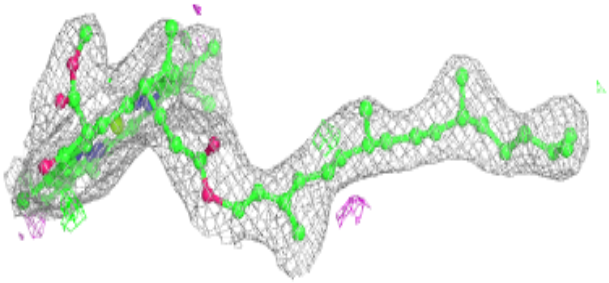


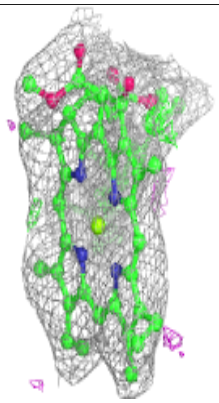


Electron density around CLA L 202:

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

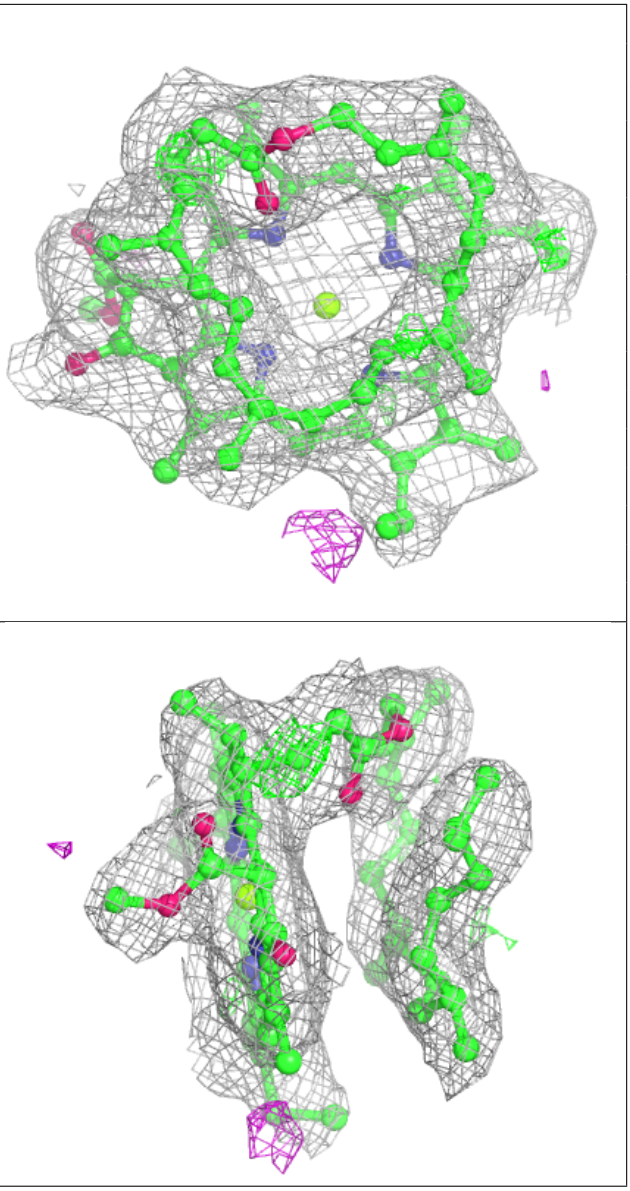






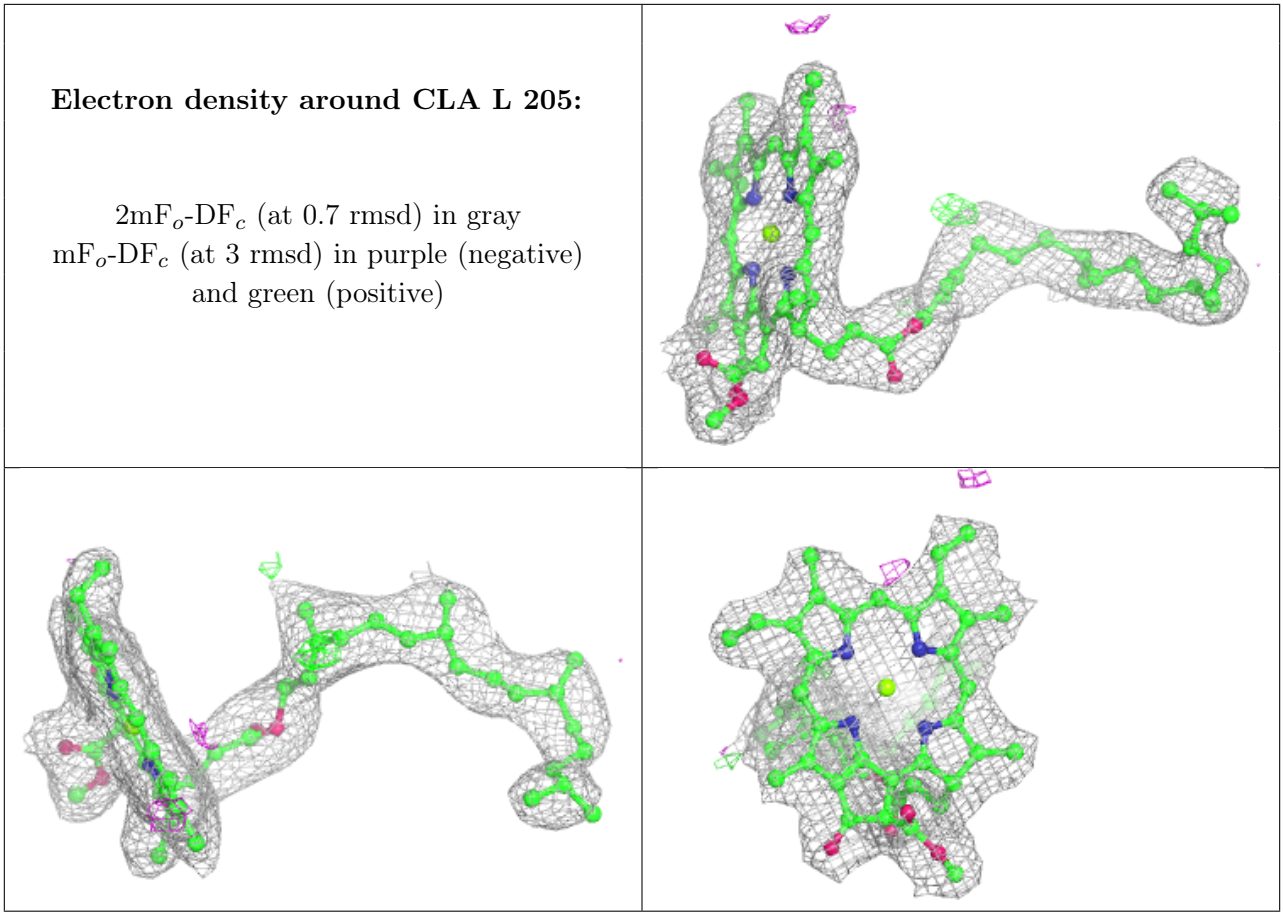
Electron density around CLA L 204:

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



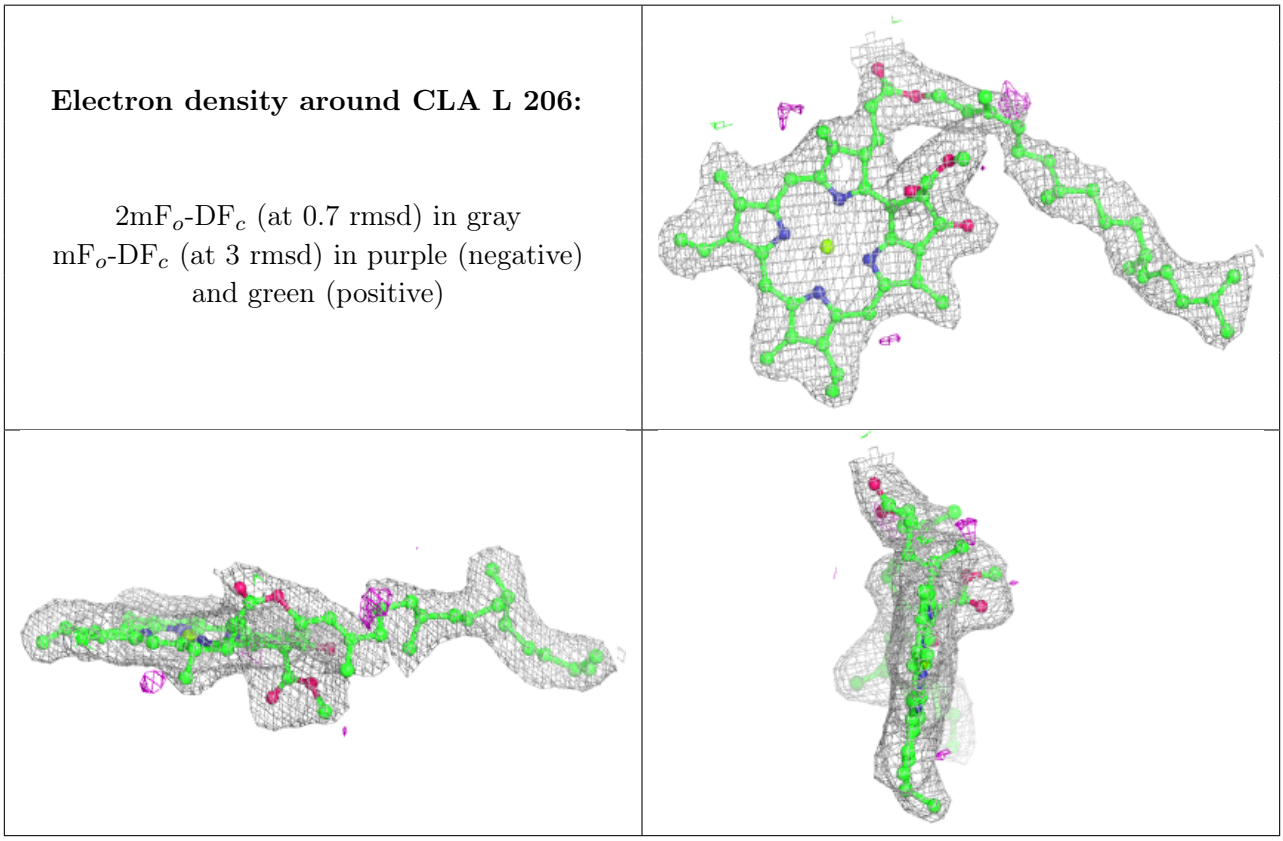
Electron density around CLA L 205:

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



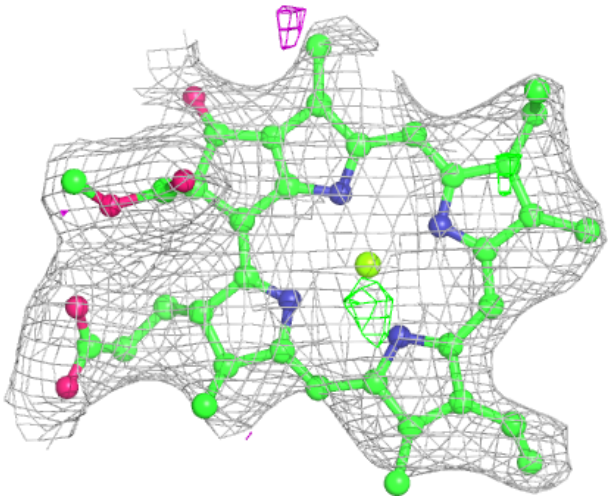
Electron density around CLA L 206:

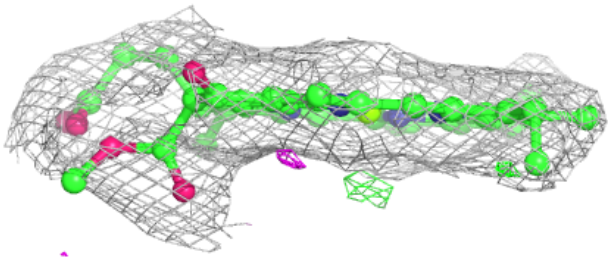
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

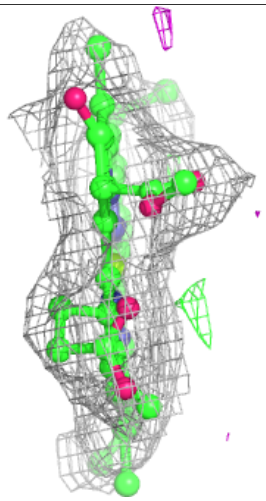


Electron density around CLA Q 202:

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

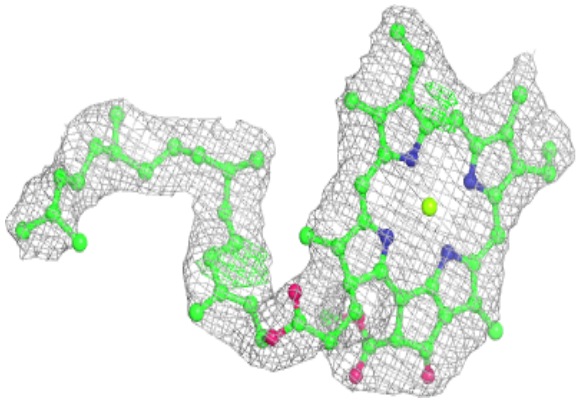


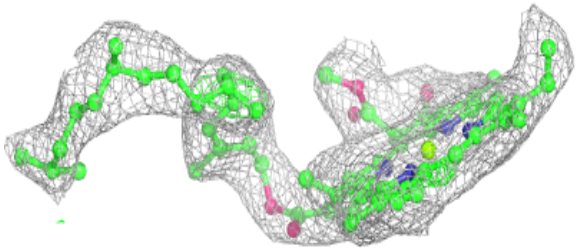


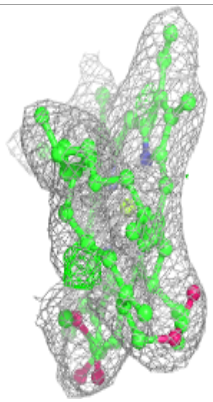


Electron density around CLA S 1101:

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

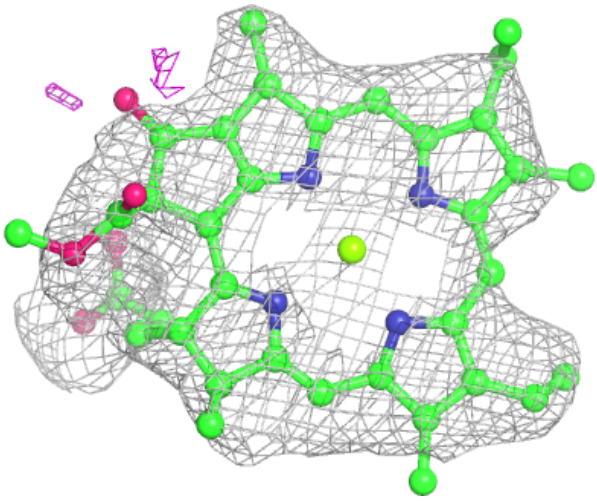


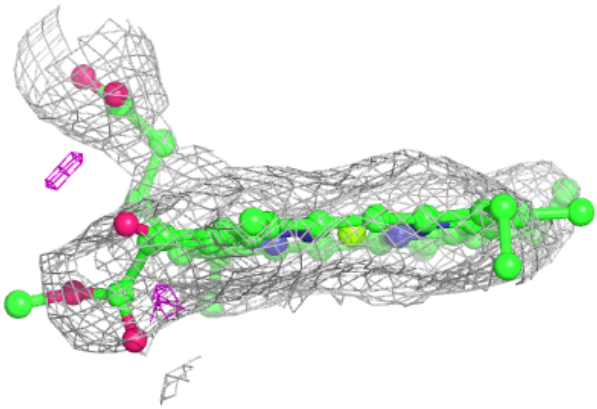


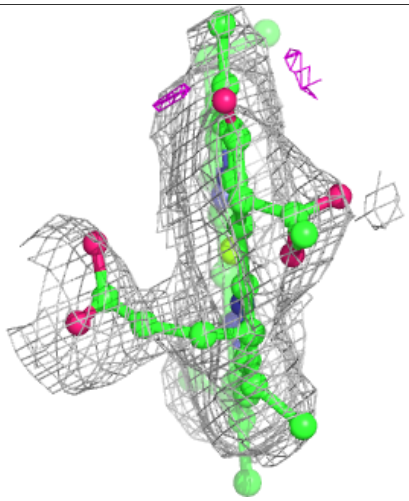


Electron density around CLA S 1102:

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

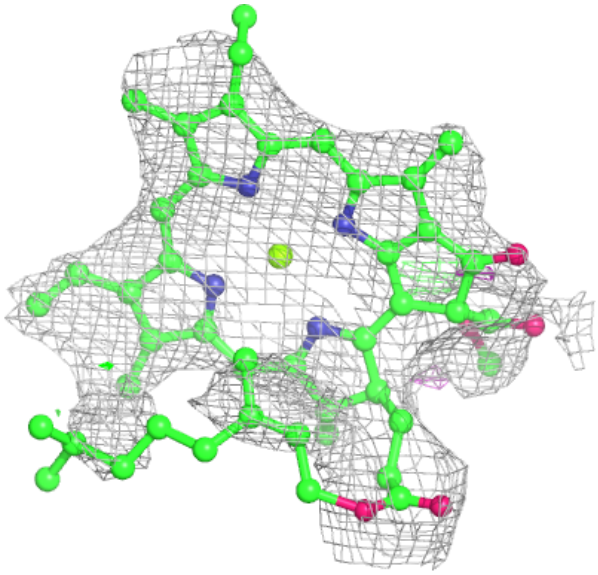


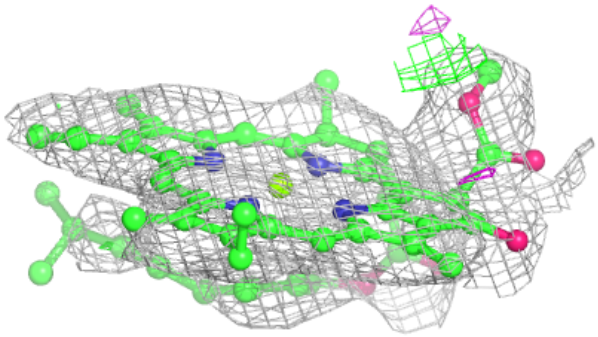


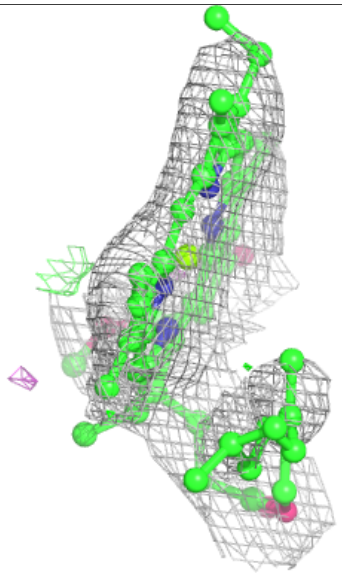


Electron density around CLA S 1103:

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

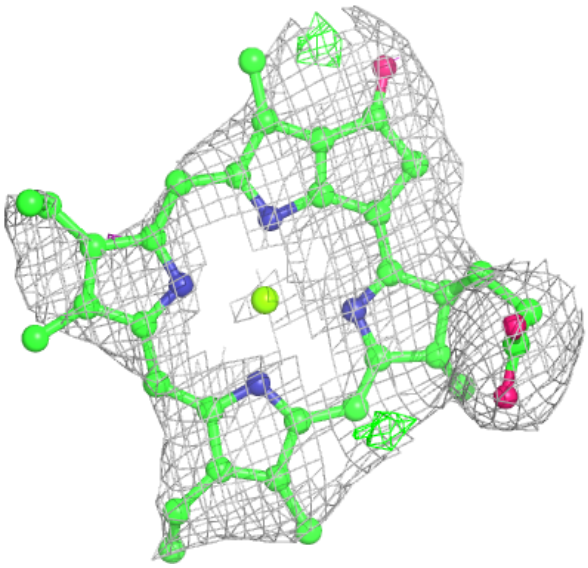


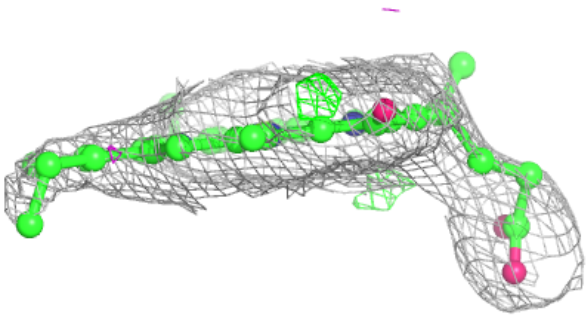


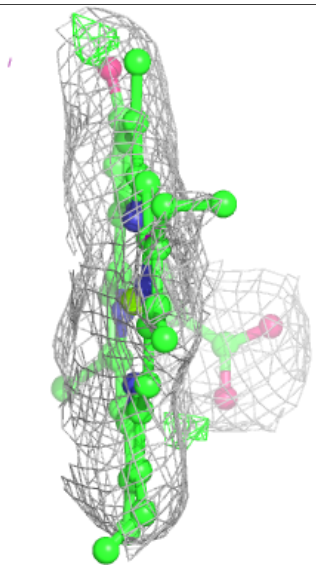


Electron density around CLA T 101:

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

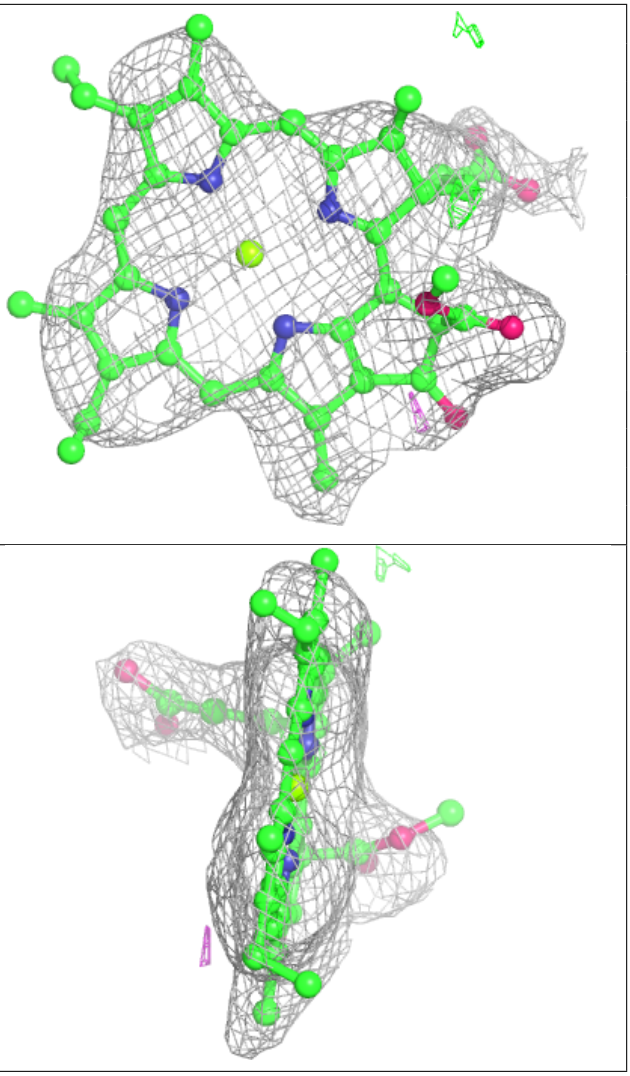






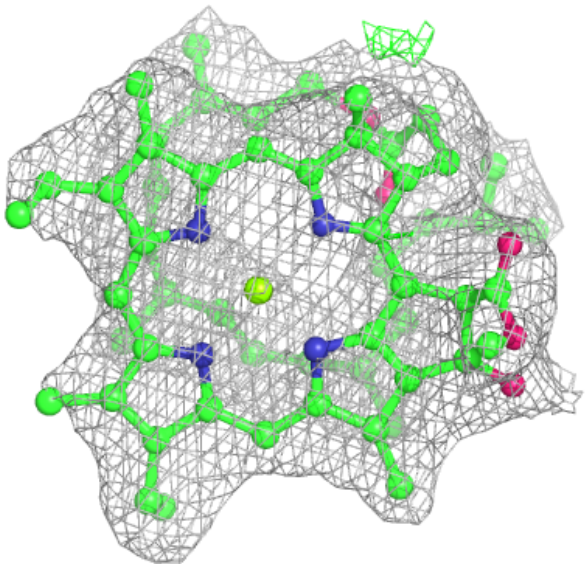
Electron density around CLA T 103:

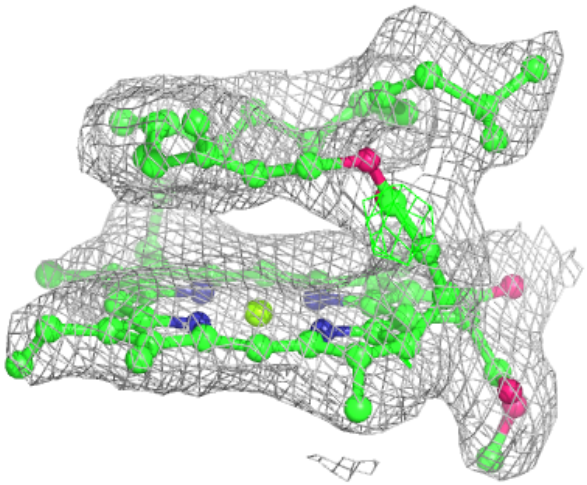
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around CLA U 1002:

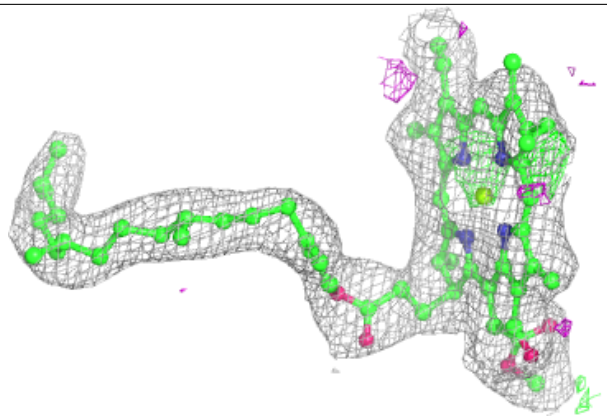
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

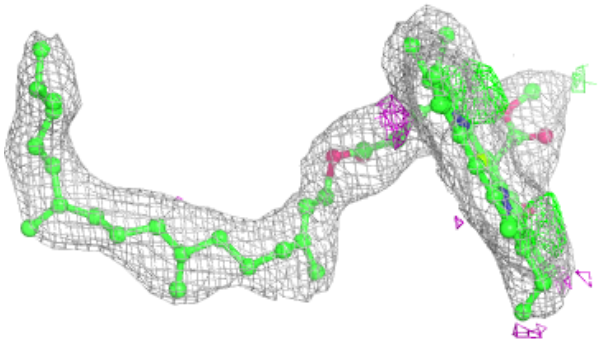


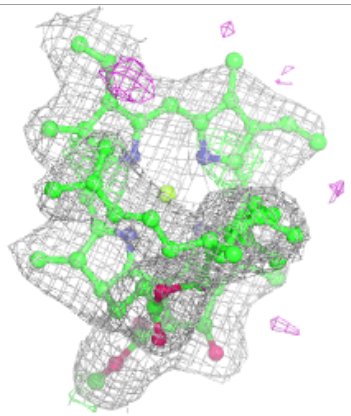


Electron density around CLA U 1003:

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

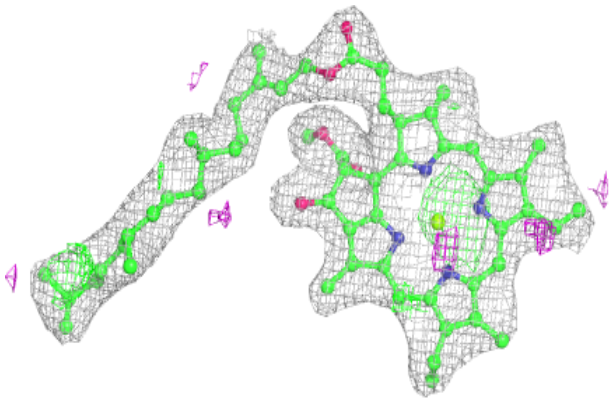


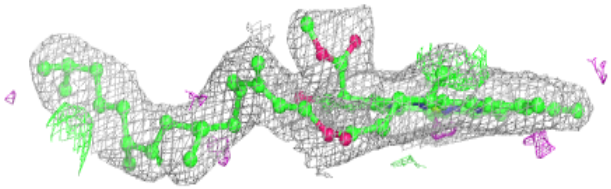


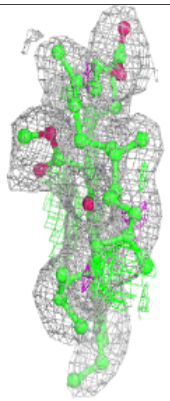


Electron density around CLA U 1004:

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

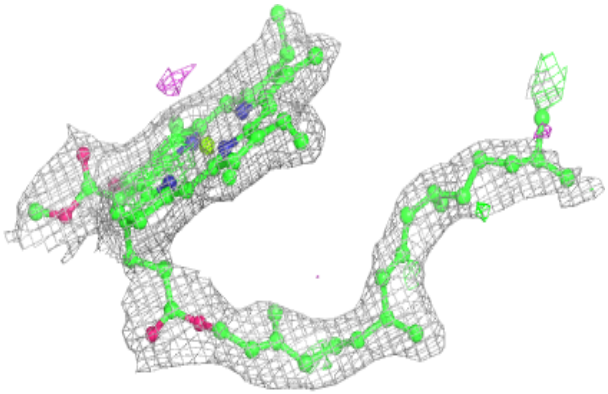


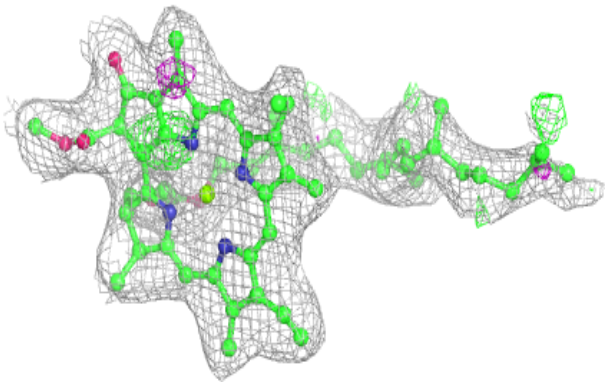


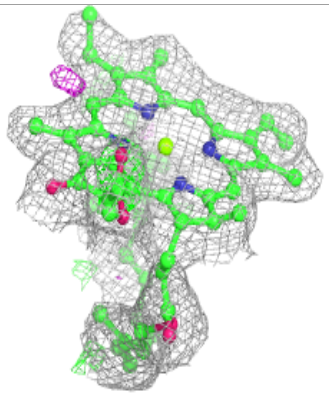


Electron density around CLA U 1006:

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

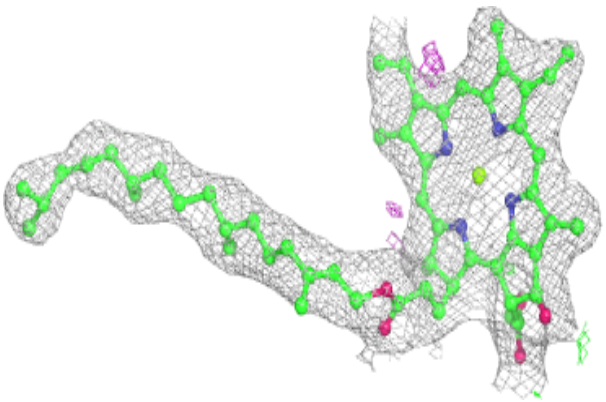


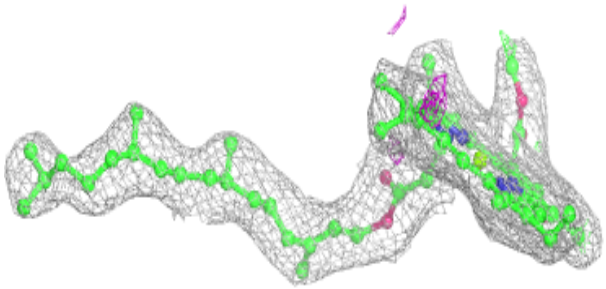


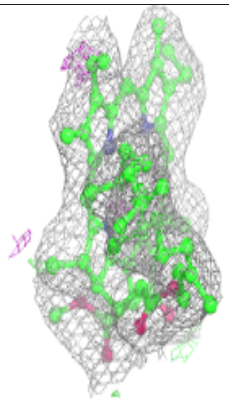


Electron density around CLA U 1007:

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

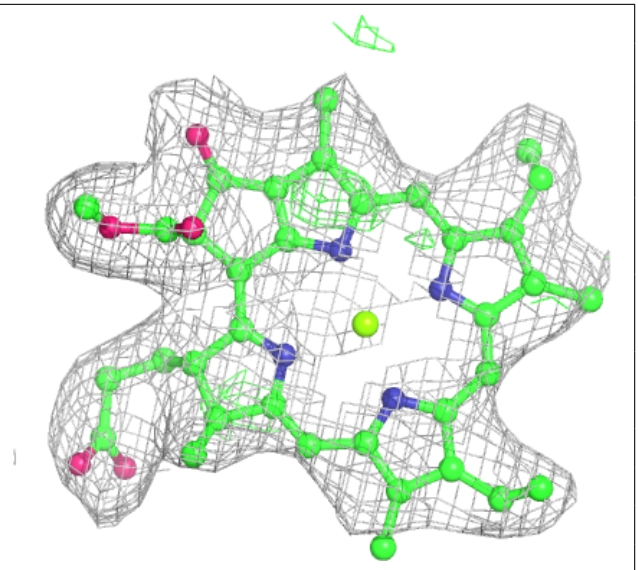


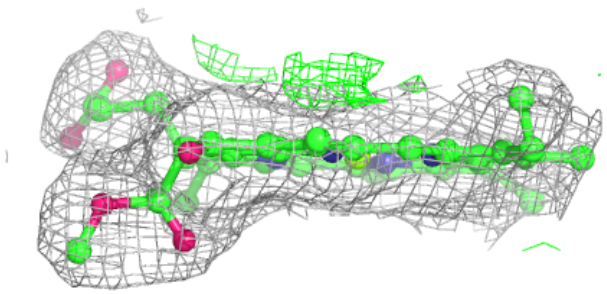


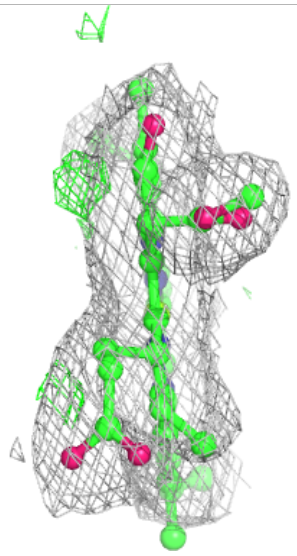


Electron density around CLA W 1701:

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

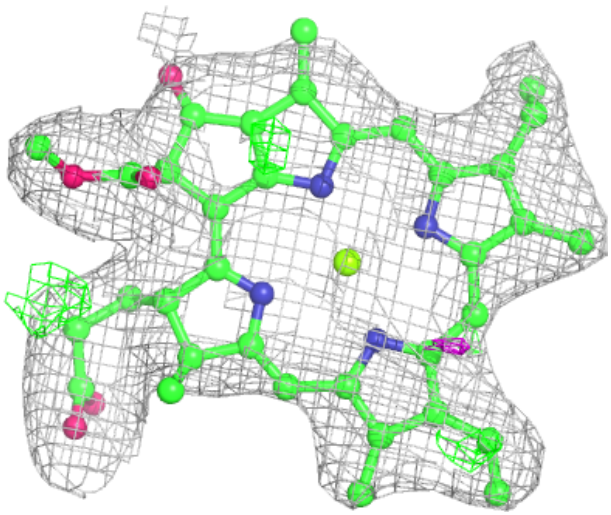


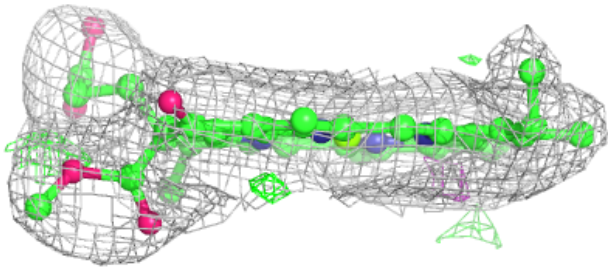


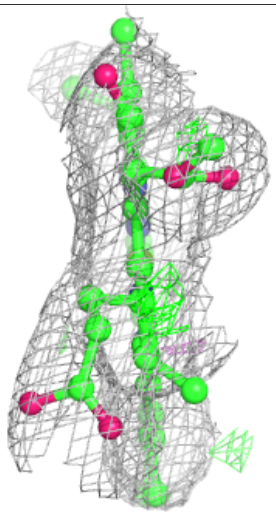


Electron density around CLA X 1701:

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

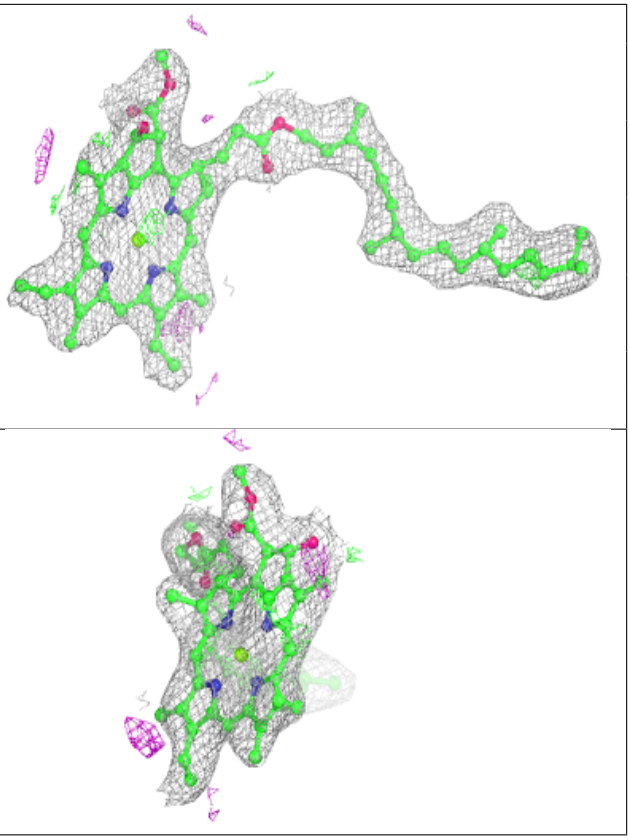


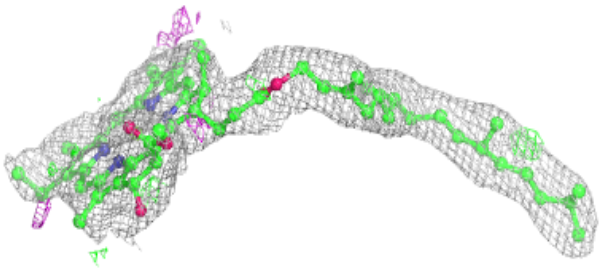




Electron density around CLA Y 802:

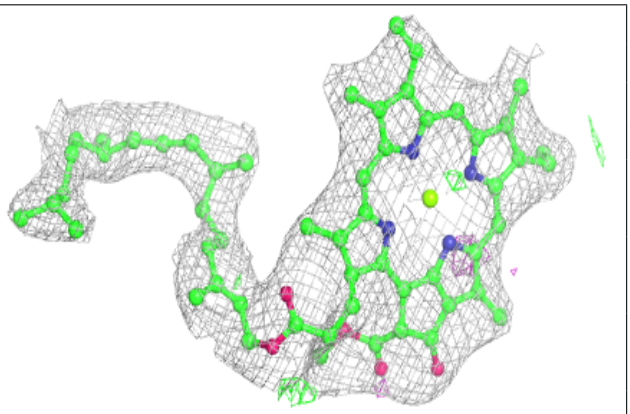
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

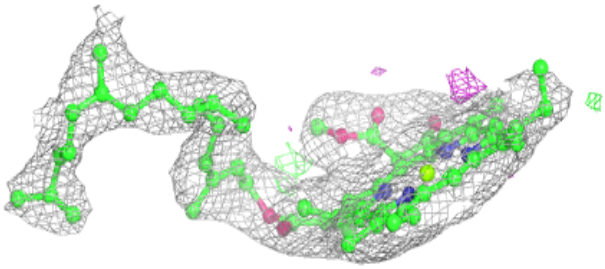


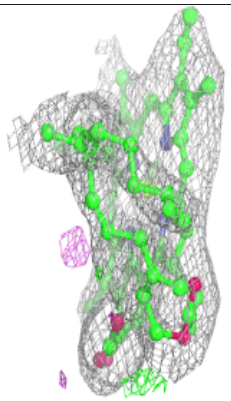


Electron density around CLA Y 803:

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

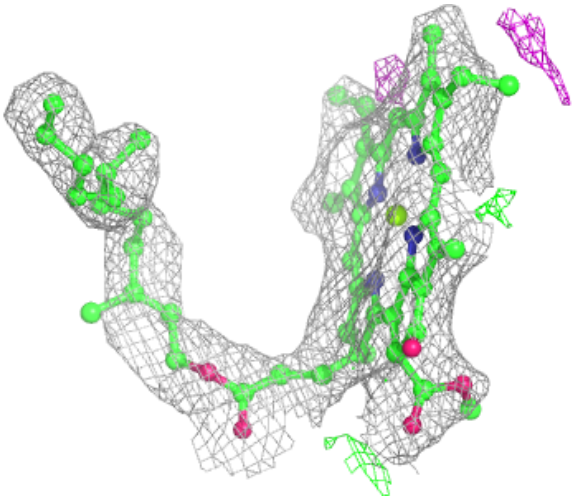


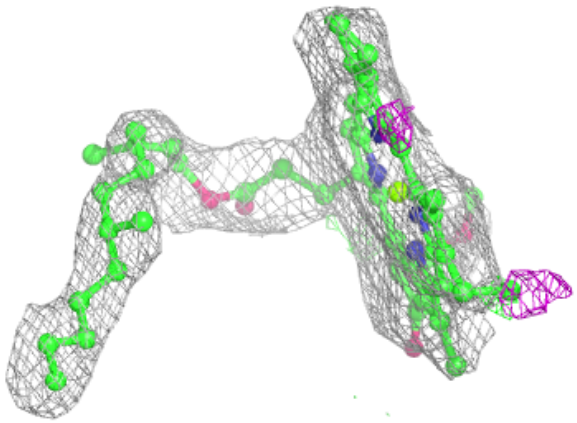


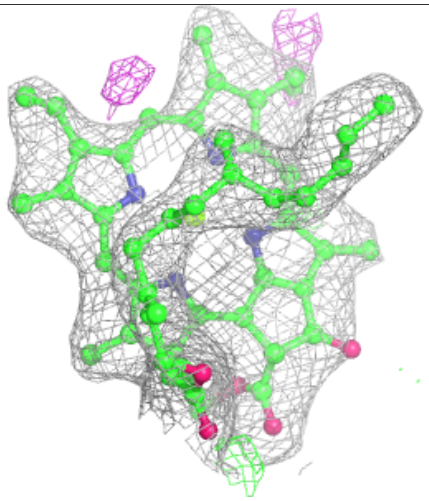


Electron density around CLA Y 804:

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

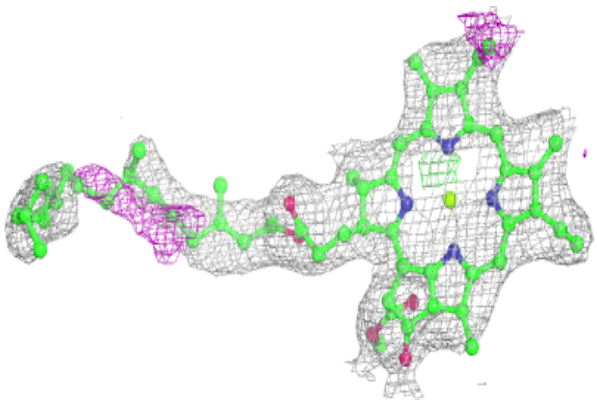


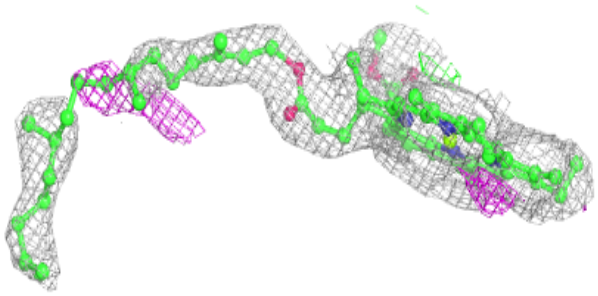


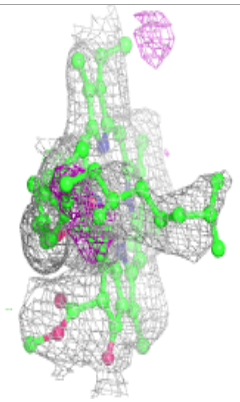


Electron density around CLA Y 805:

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

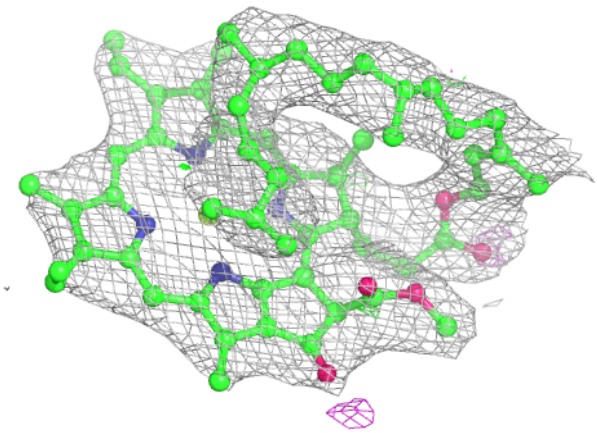


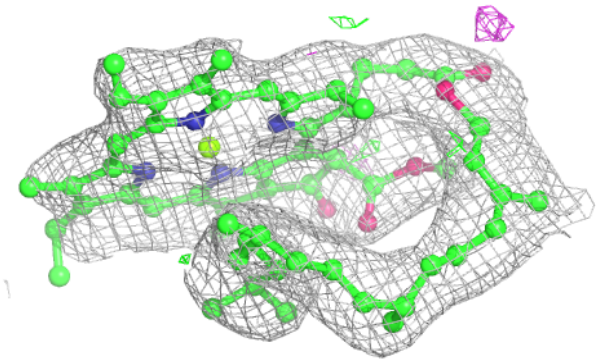


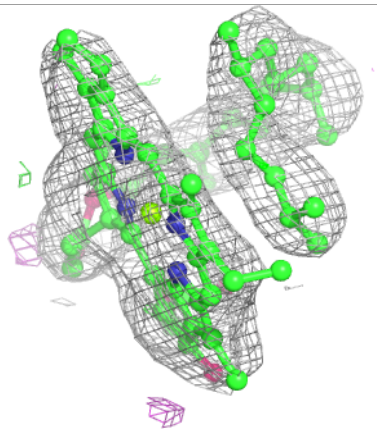


Electron density around CLA Y 806:

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

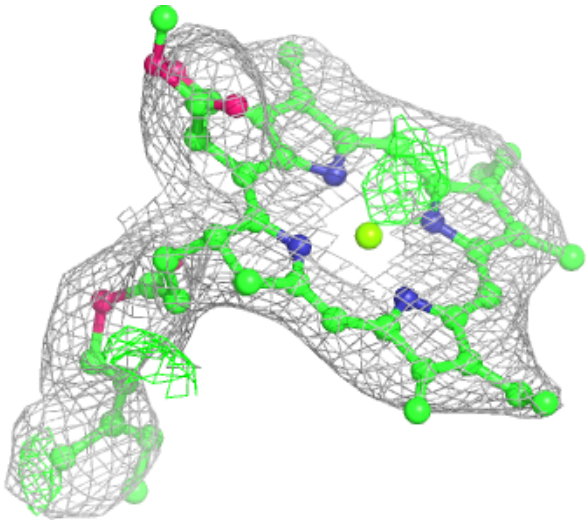


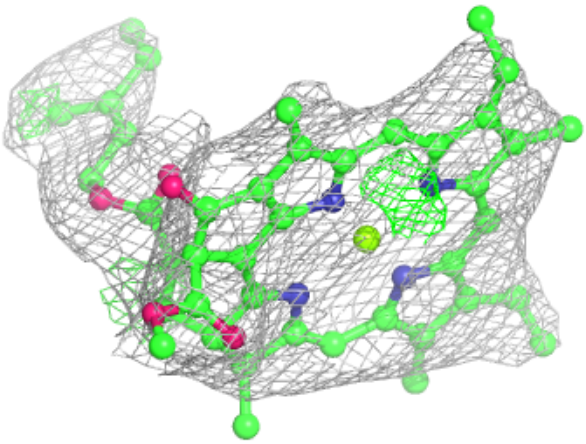


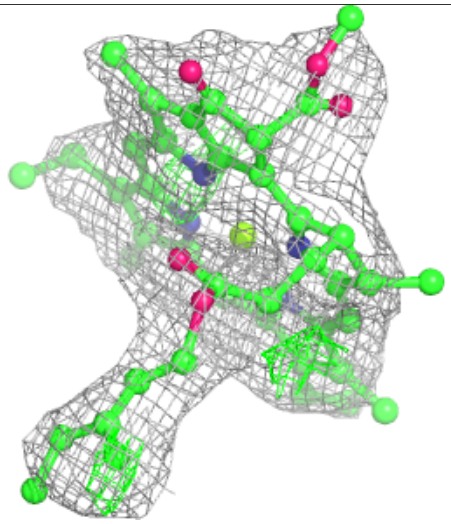


Electron density around CLA Y 807:

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

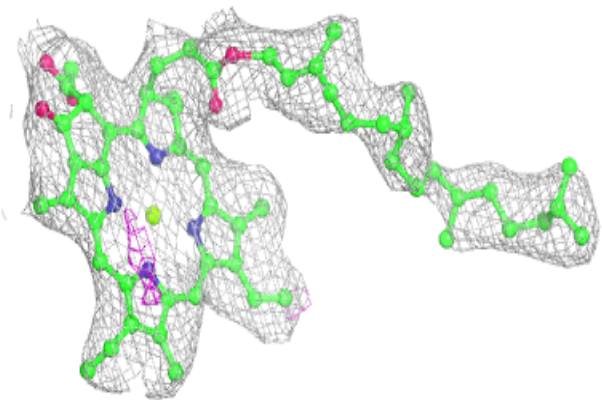


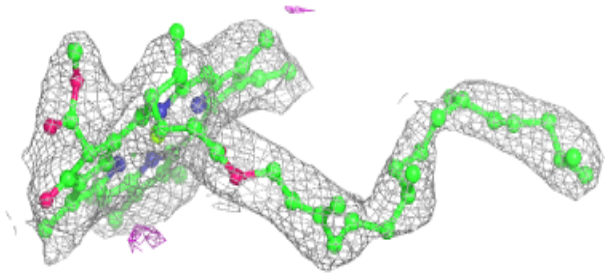


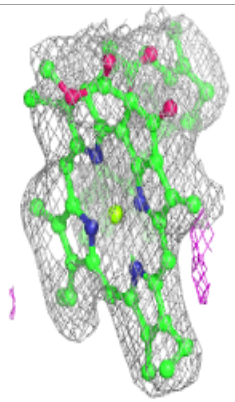


Electron density around CLA Y 808:

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

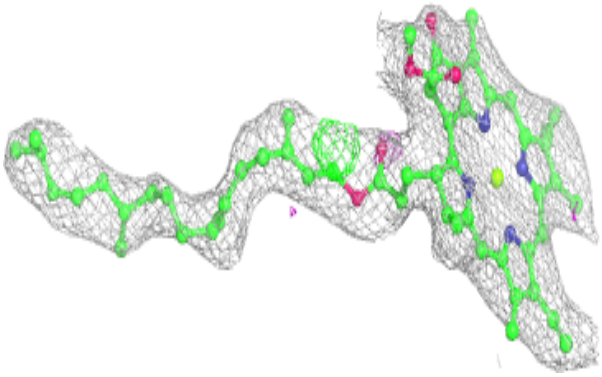


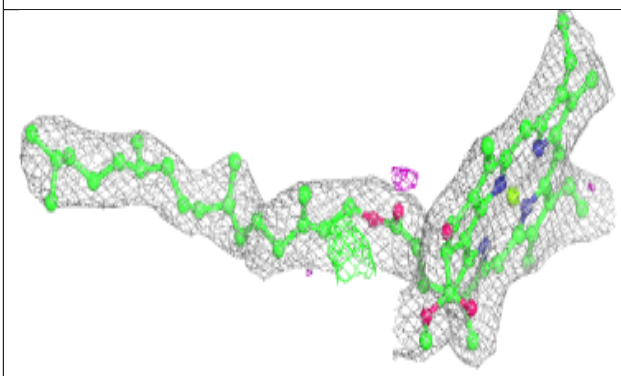


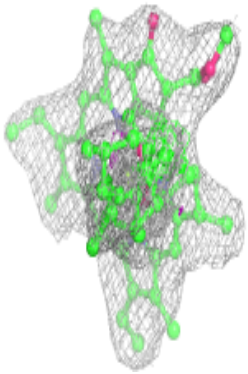


Electron density around CLA Y 809:

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

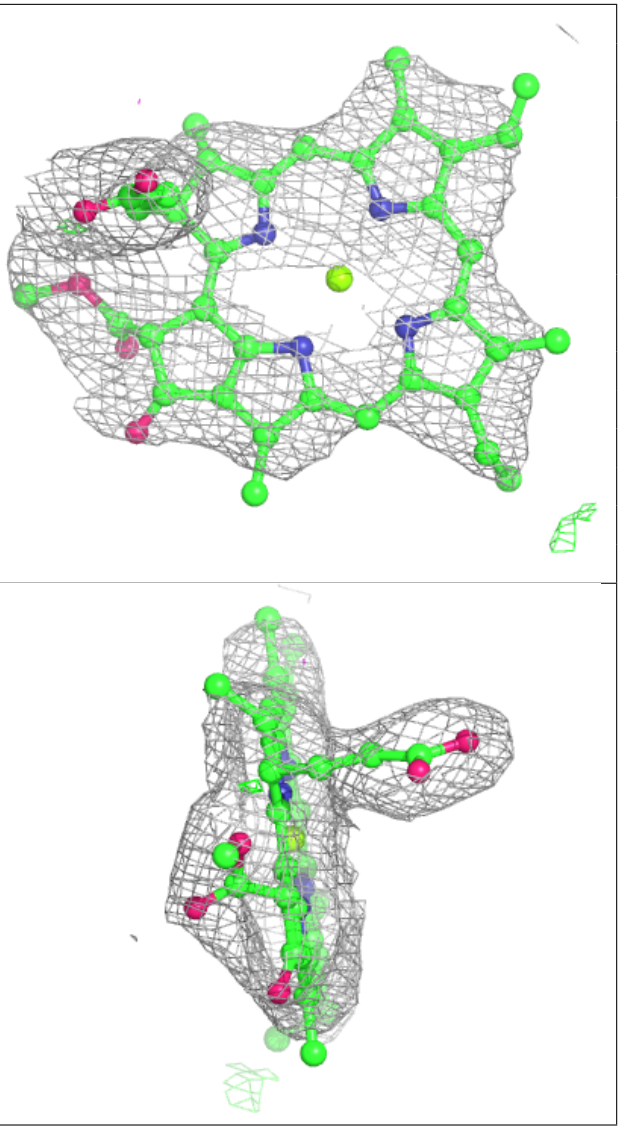






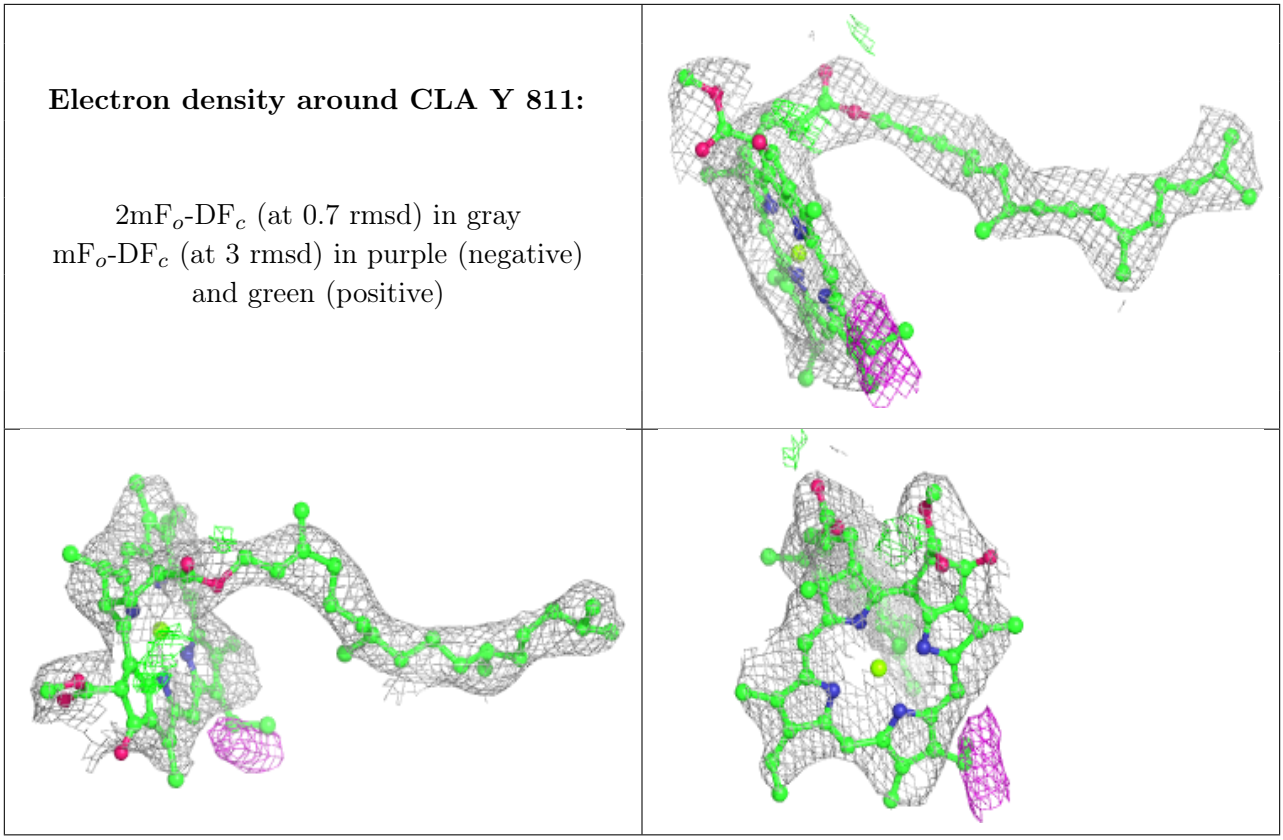
Electron density around CLA Y 810:

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



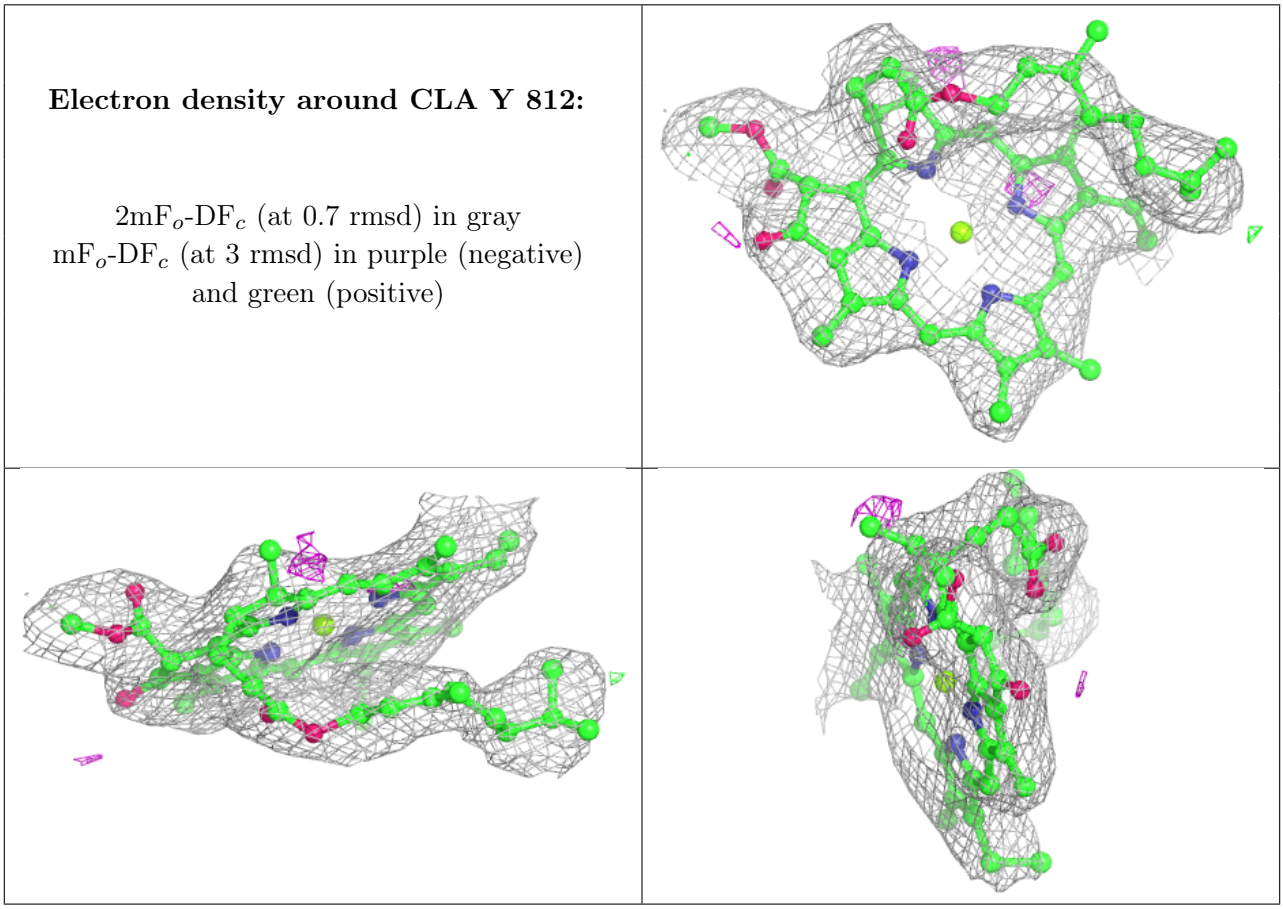
Electron density around CLA Y 811:

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



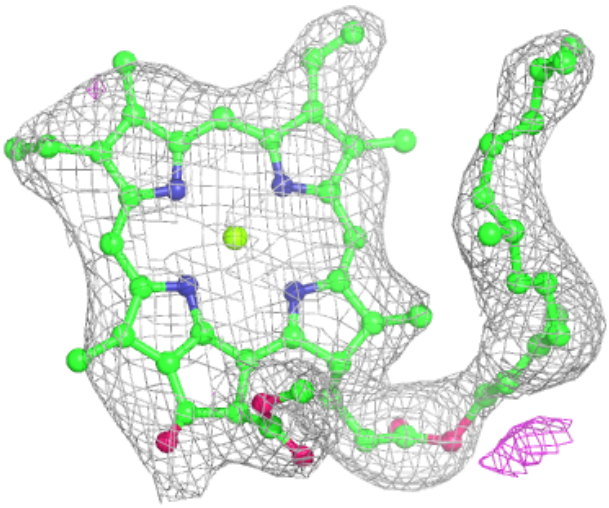
Electron density around CLA Y 812:

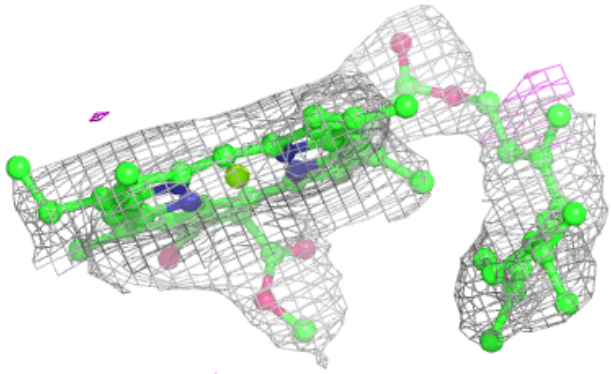
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

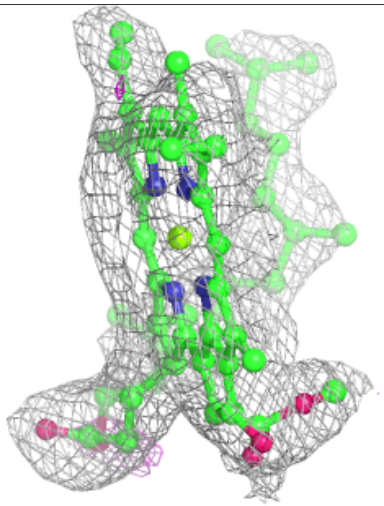


Electron density around CLA Y 813:

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

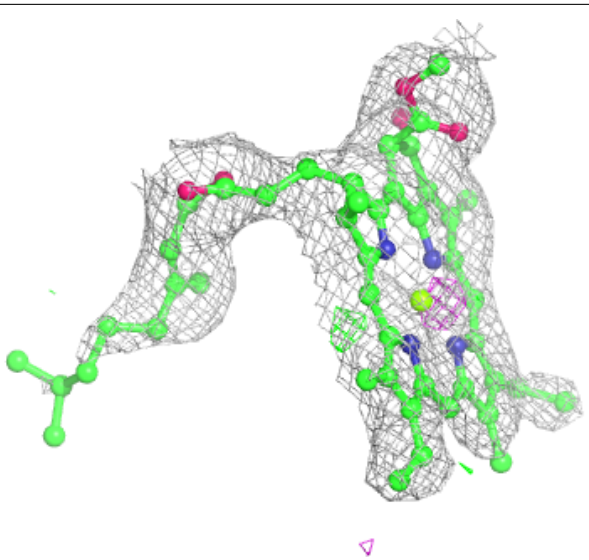


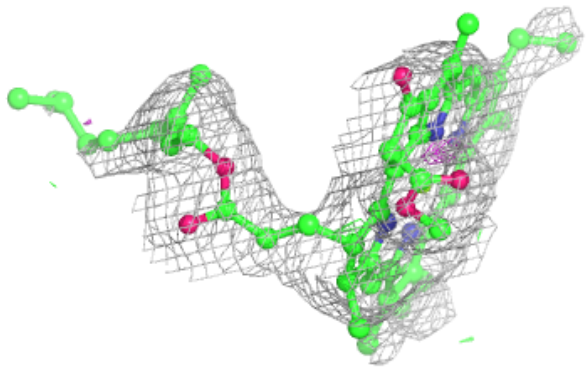


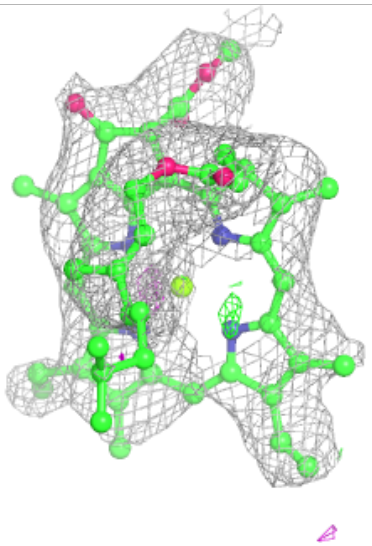


Electron density around CLA Y 814:

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

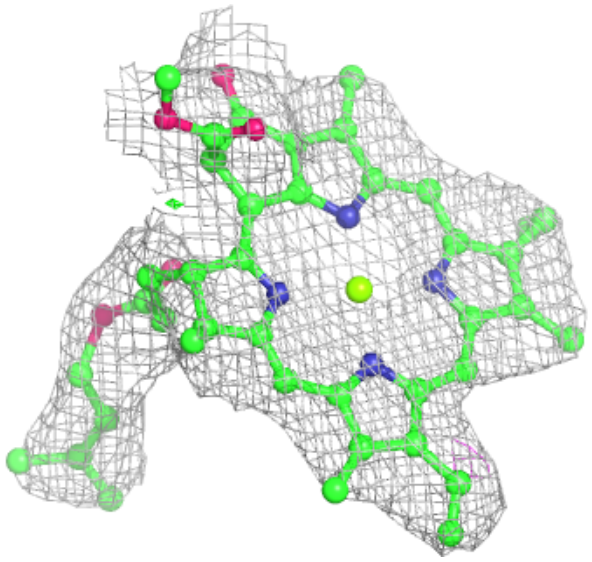


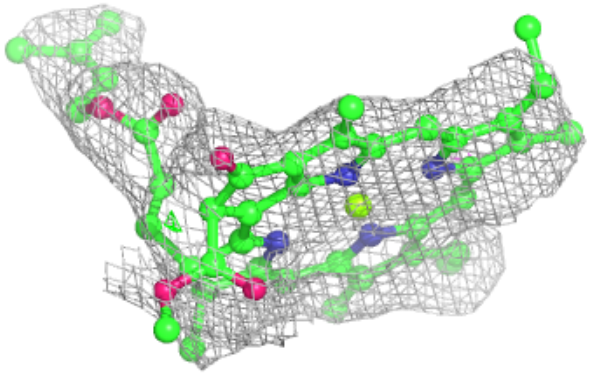


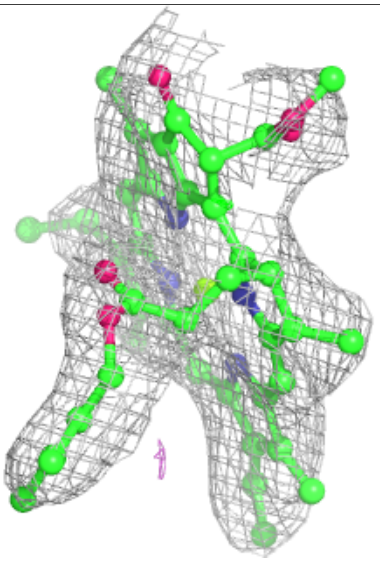


Electron density around CLA Y 815:

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

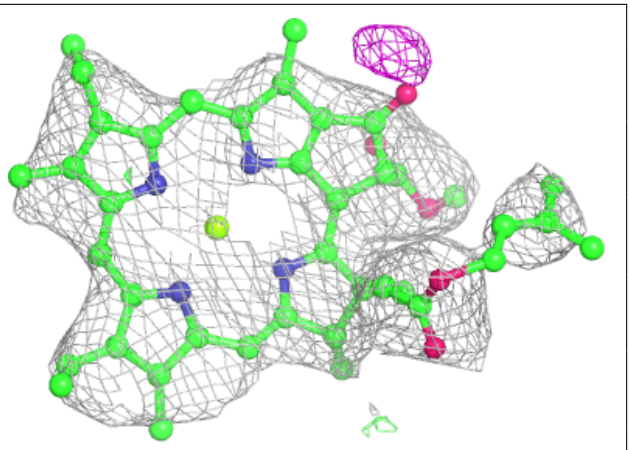


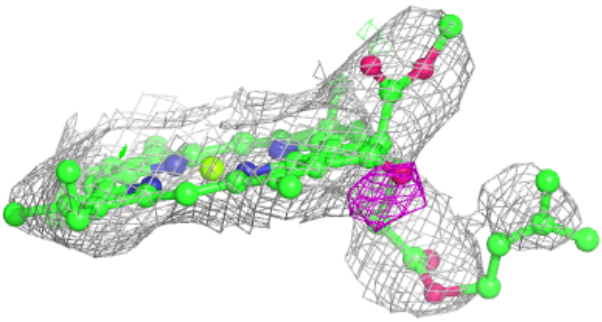


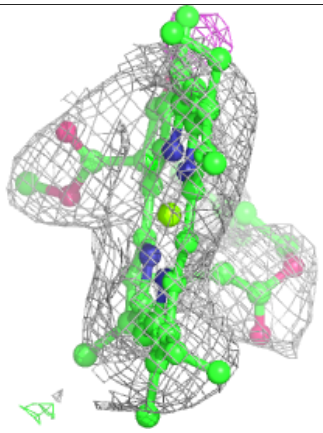


Electron density around CLA Y 816:

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

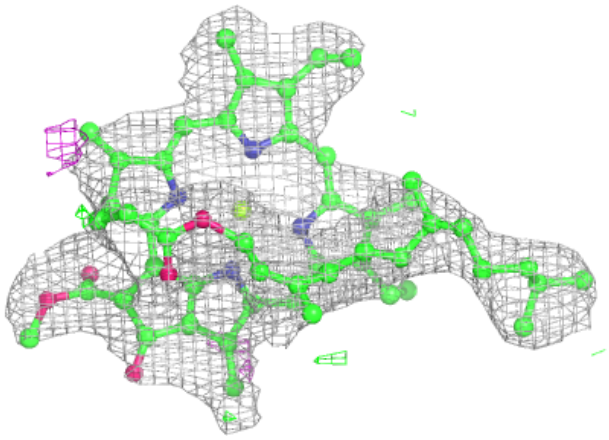


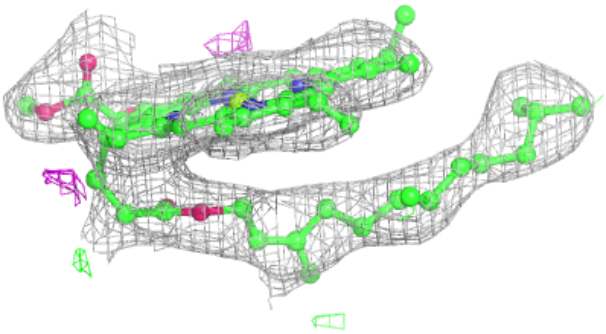


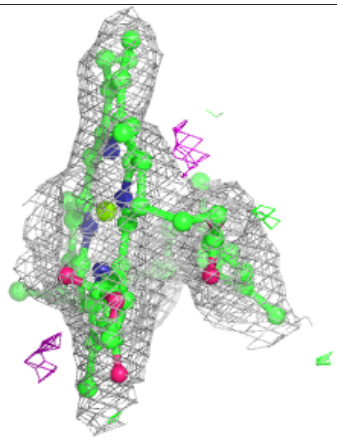


Electron density around CLA Y 817:

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

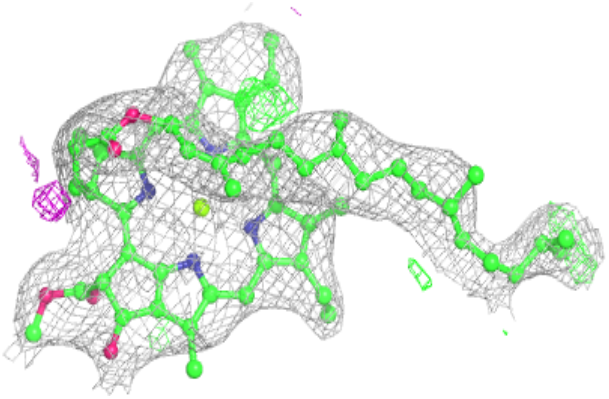


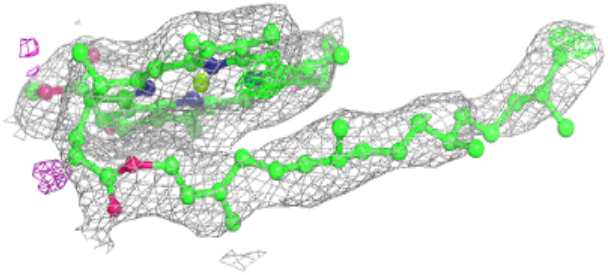


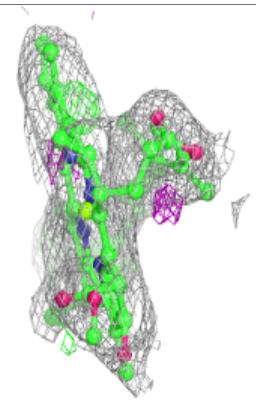


Electron density around CLA Y 818:

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

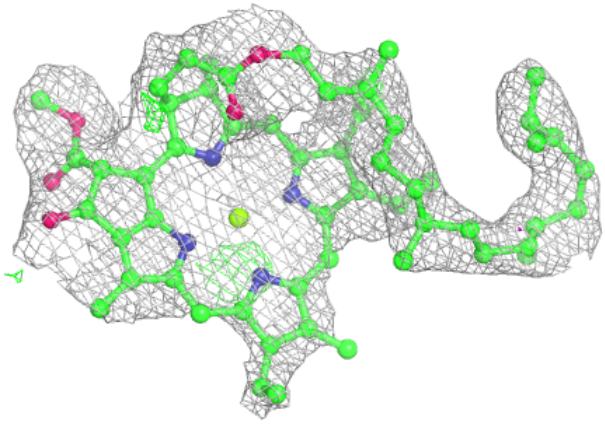


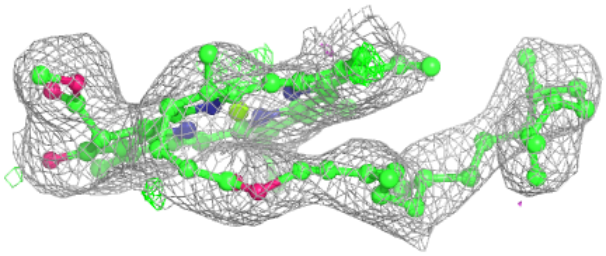


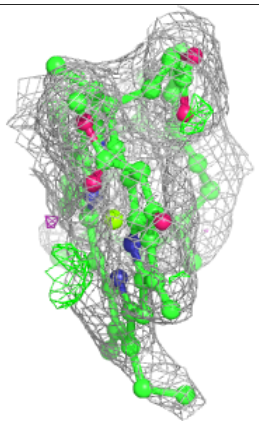


Electron density around CLA Y 819:

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

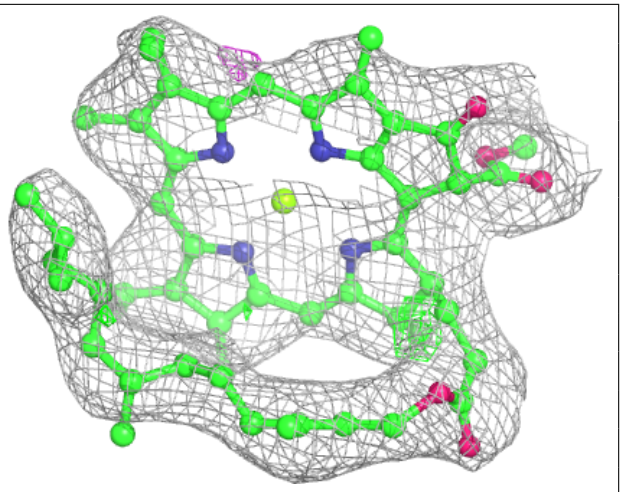


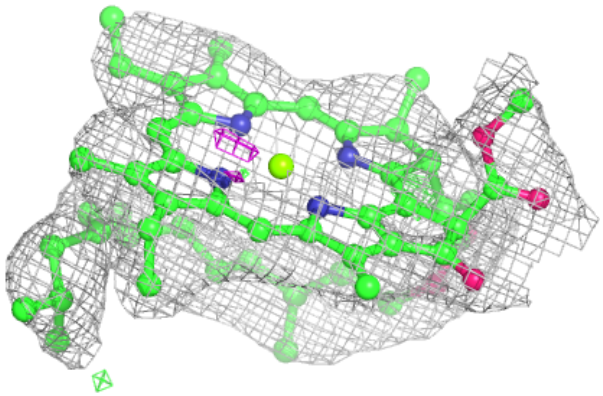


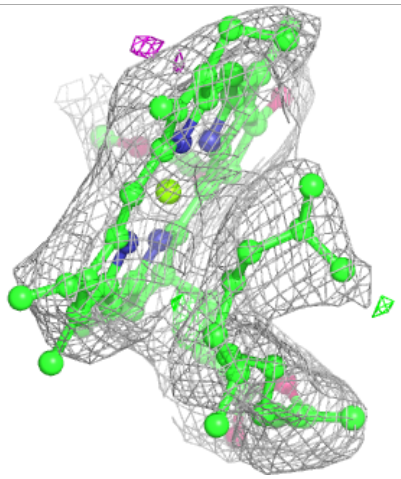


Electron density around CLA Y 820:

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

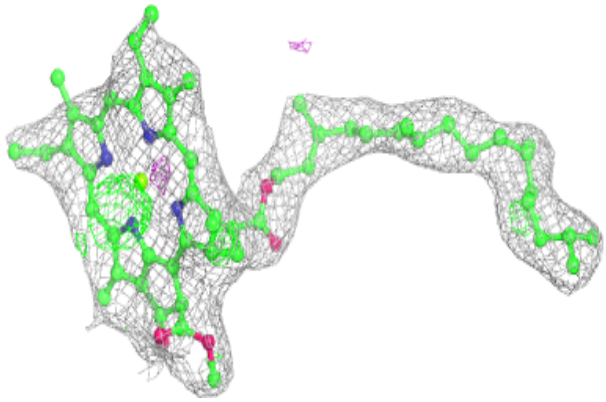


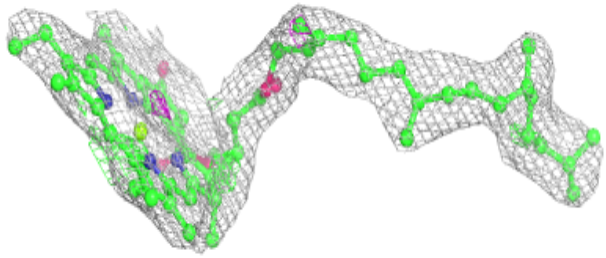


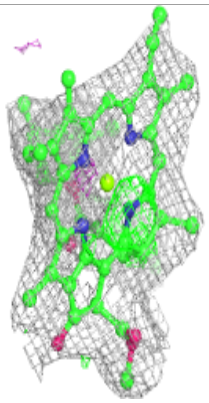


Electron density around CLA Y 821:

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

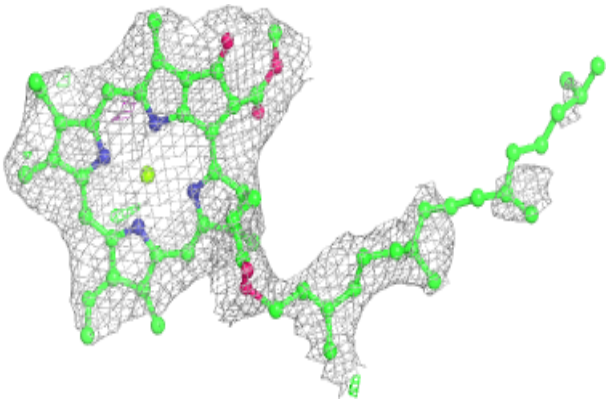


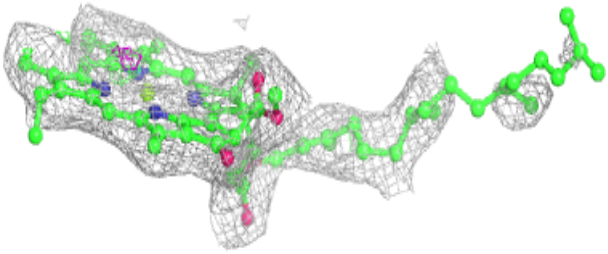


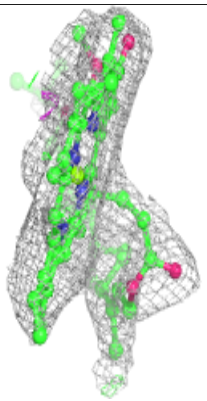


Electron density around CLA Y 822:

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

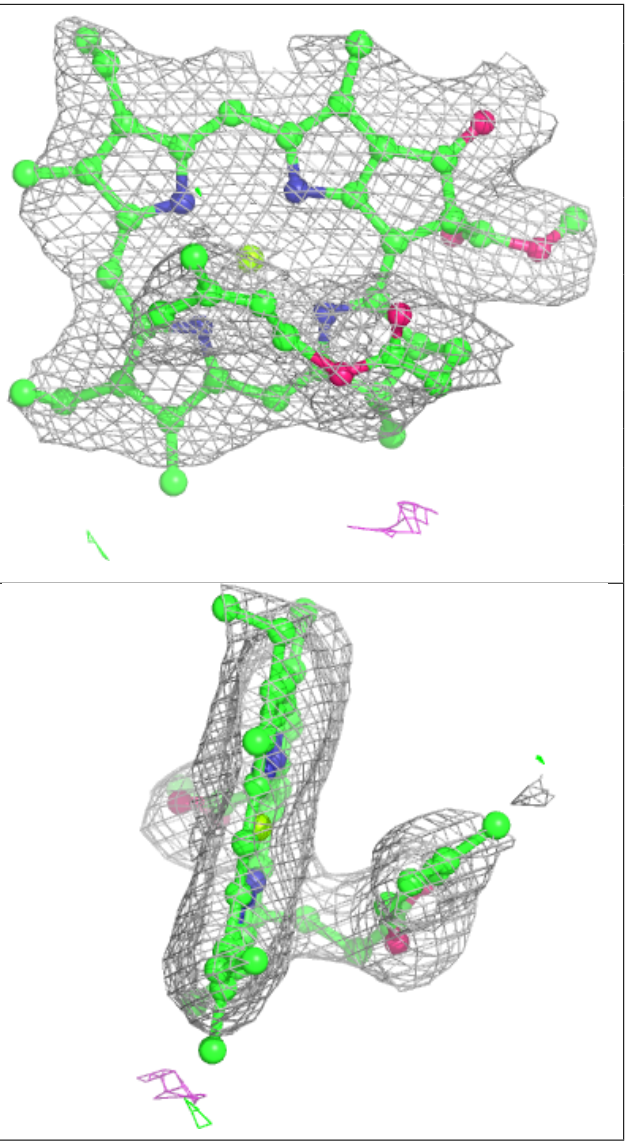






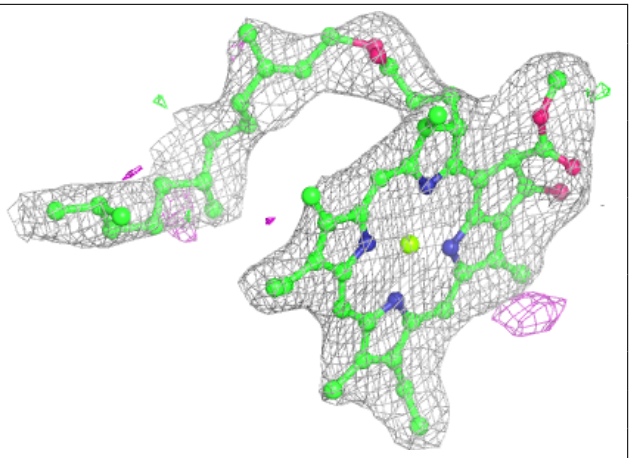
Electron density around CLA Y 823:

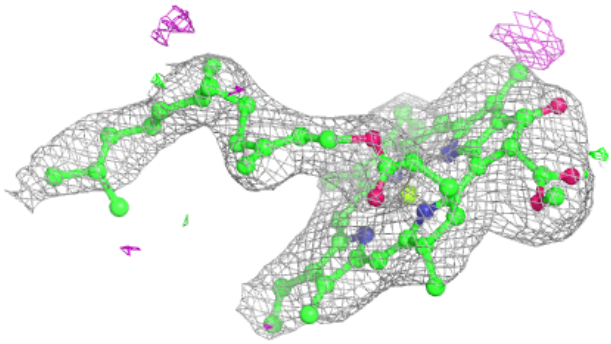
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

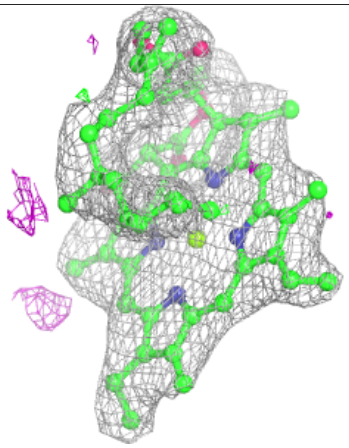


Electron density around CLA Y 824:

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

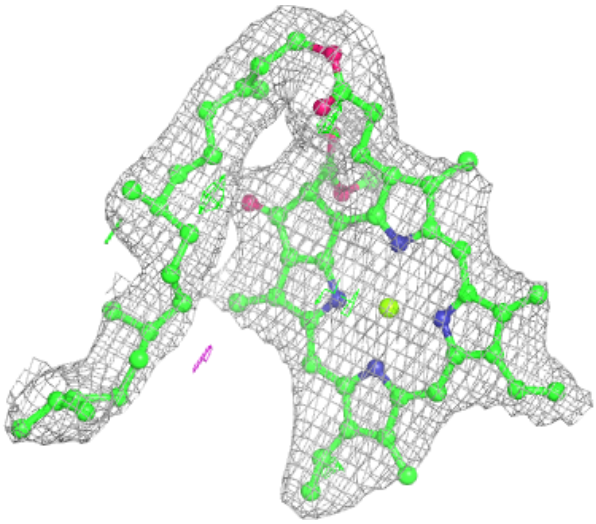


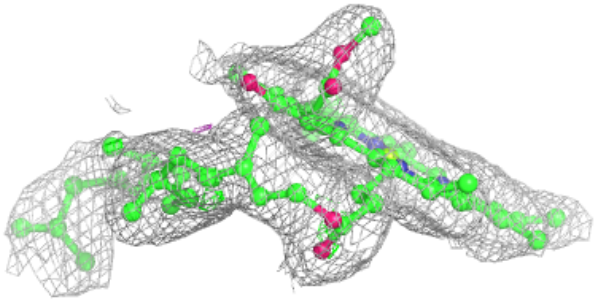


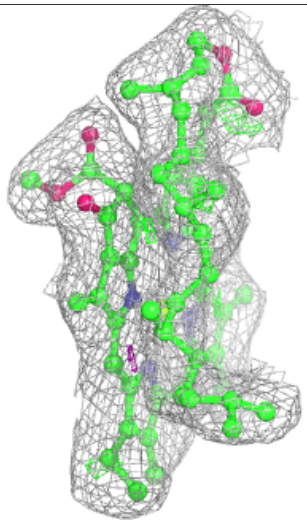


Electron density around CLA Y 825:

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

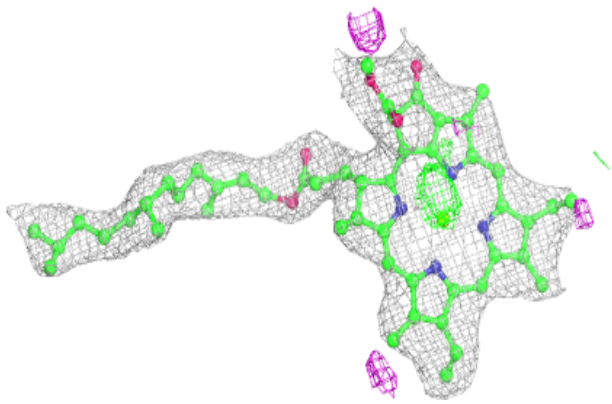


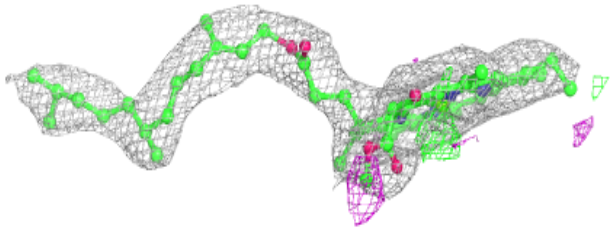


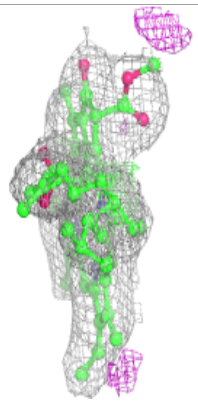


Electron density around CLA Y 826:

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

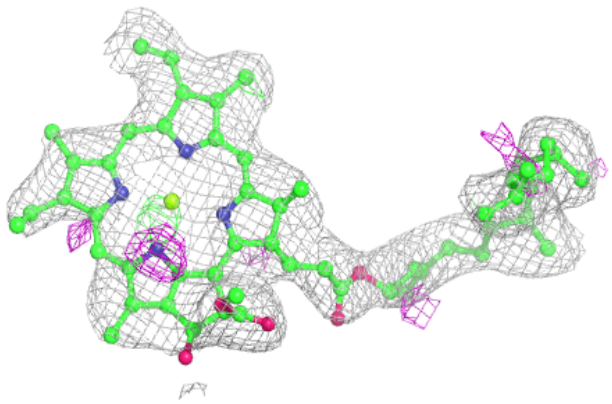


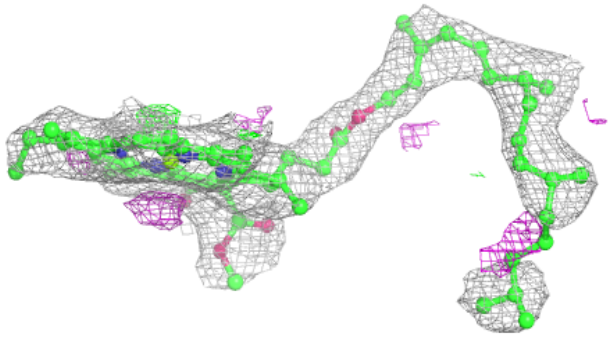


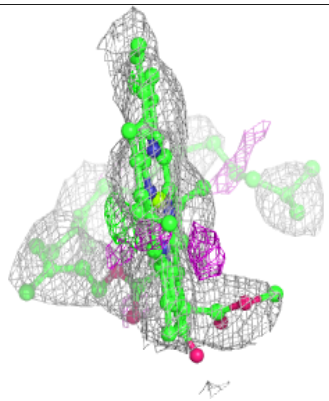


Electron density around CLA Y 827:

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

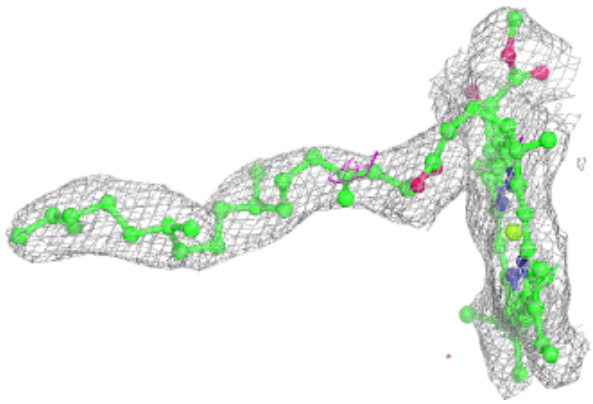


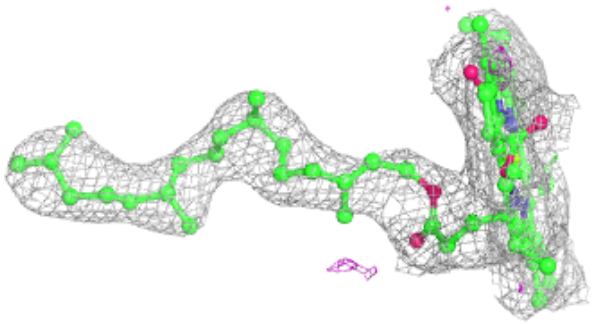


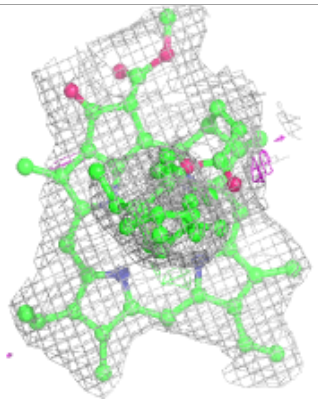


Electron density around CLA Y 828:

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

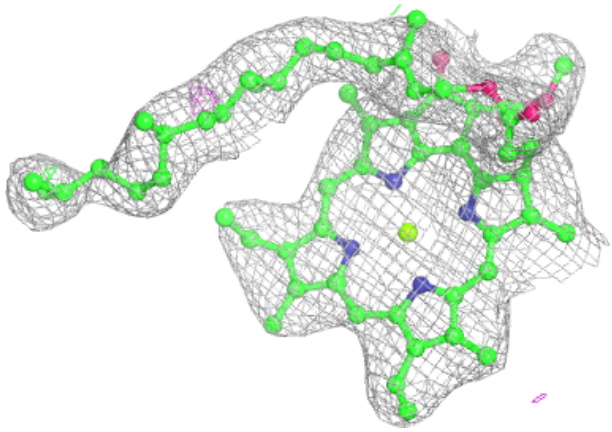


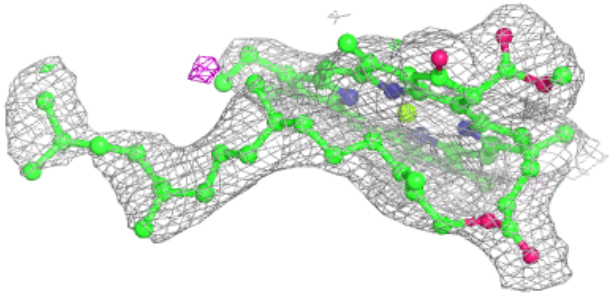


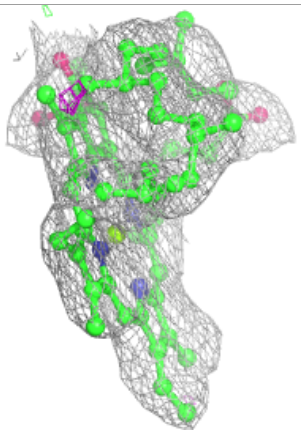


Electron density around CLA Y 829:

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

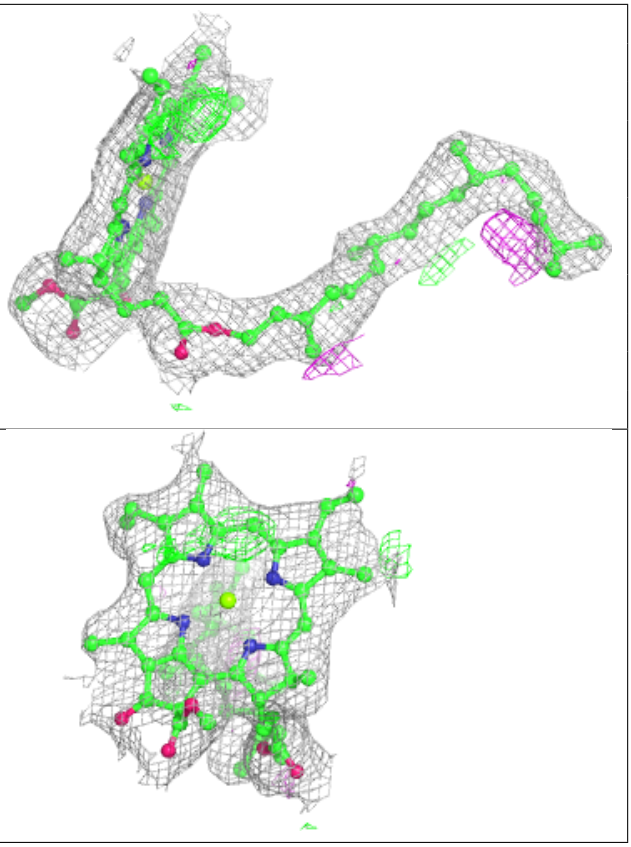


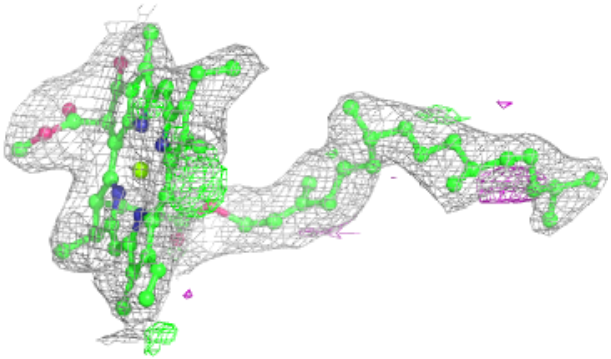




Electron density around CLA Y 830:

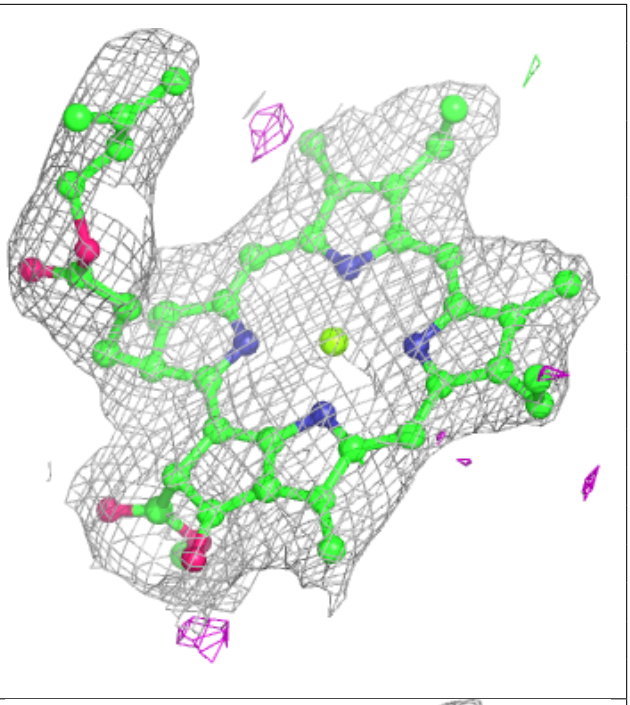
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

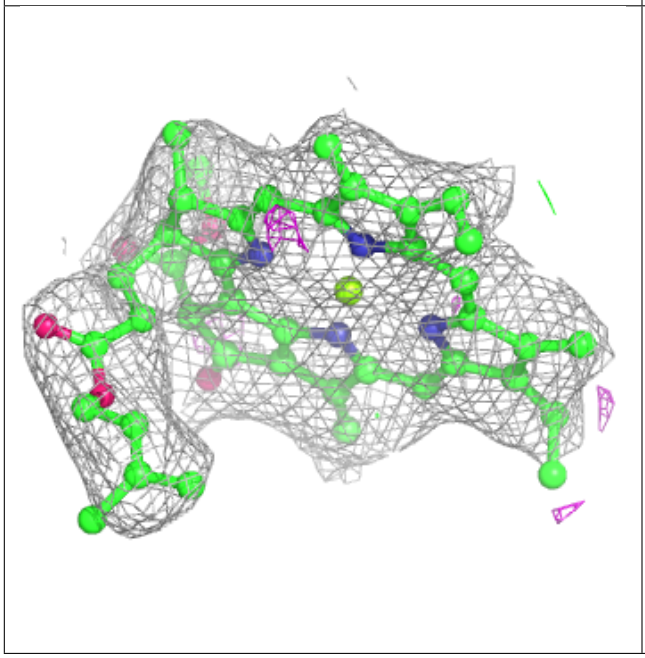


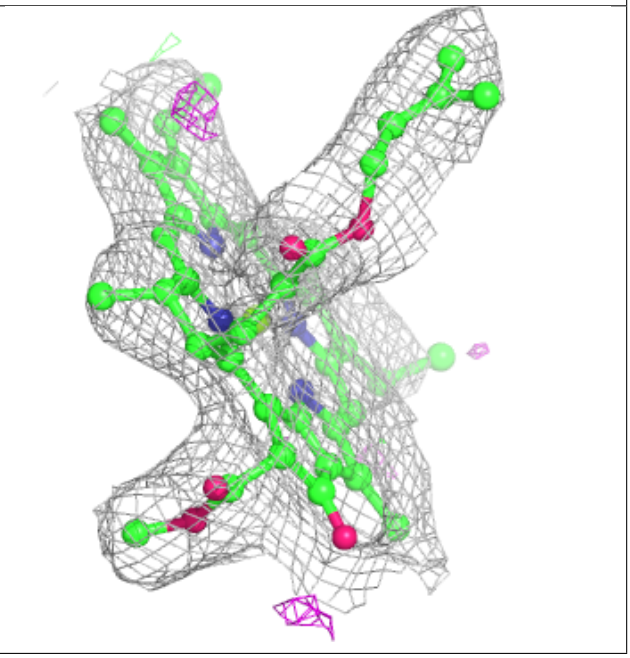


Electron density around CLA Y 831:

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

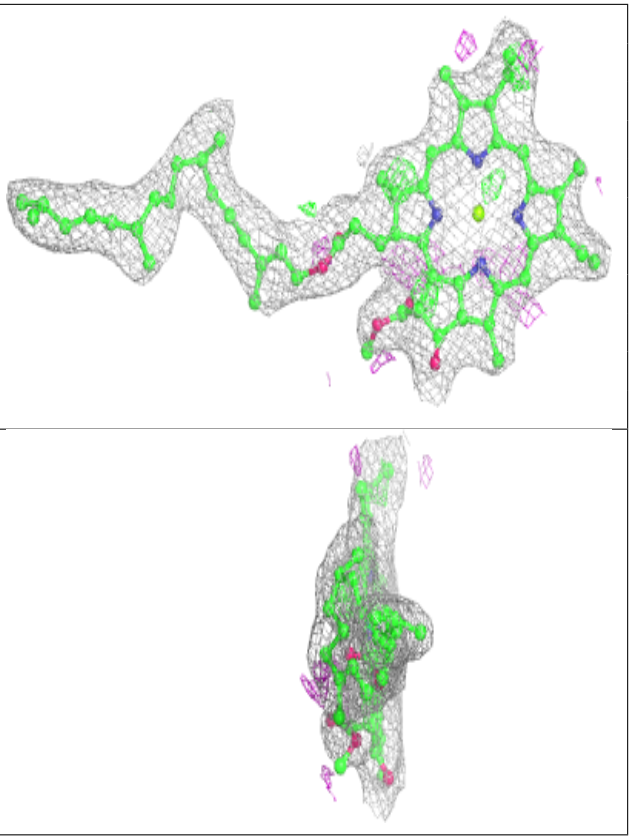


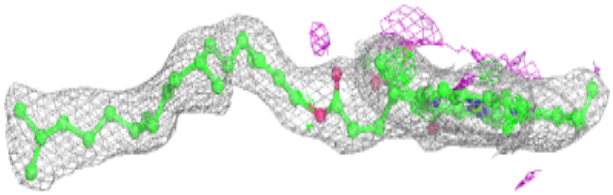




Electron density around CLA Y 832:

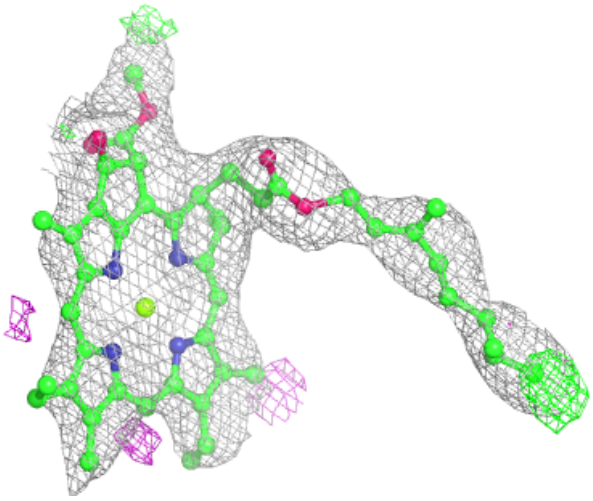
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

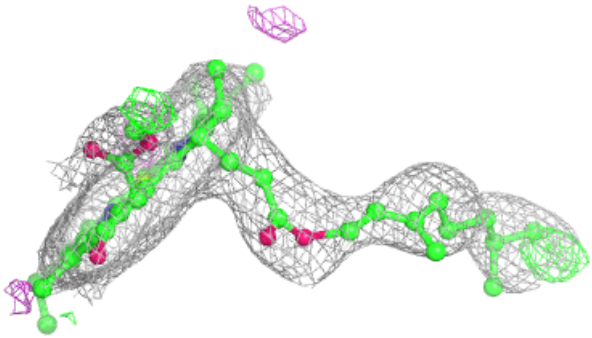


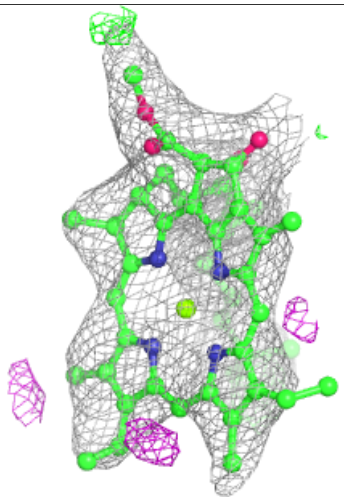


Electron density around CLA Y 833:

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

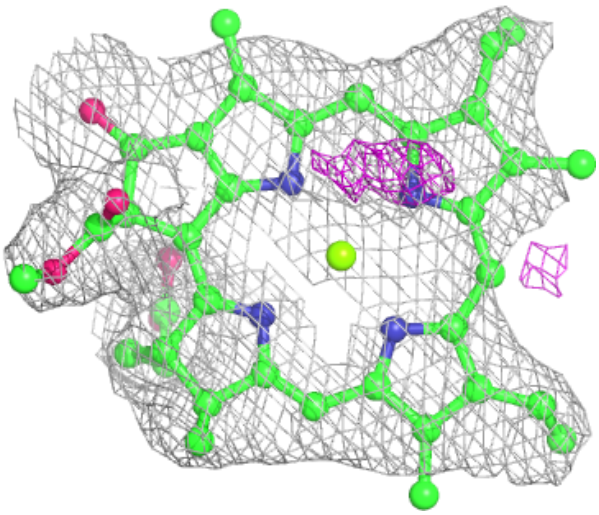


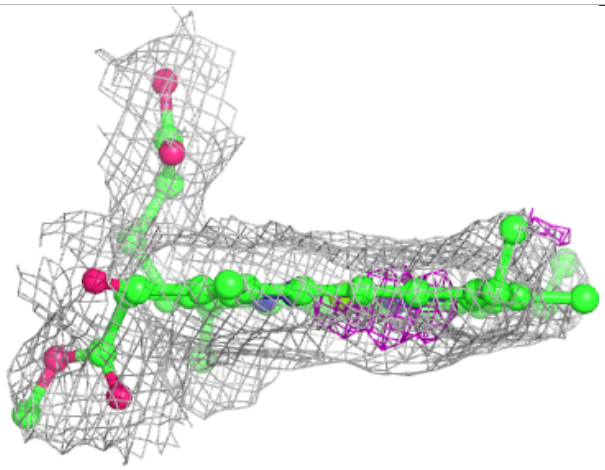




Electron density around CLA Y 834:

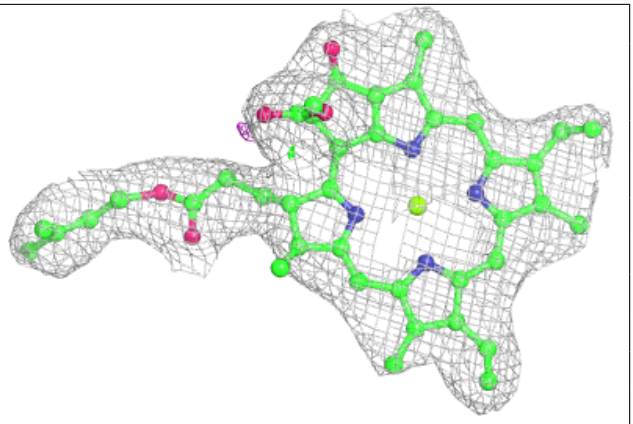
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

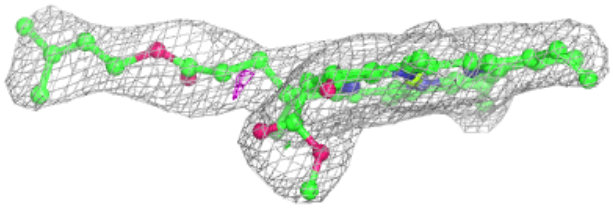


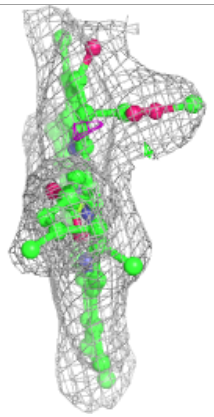


Electron density around CLA Y 835:

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

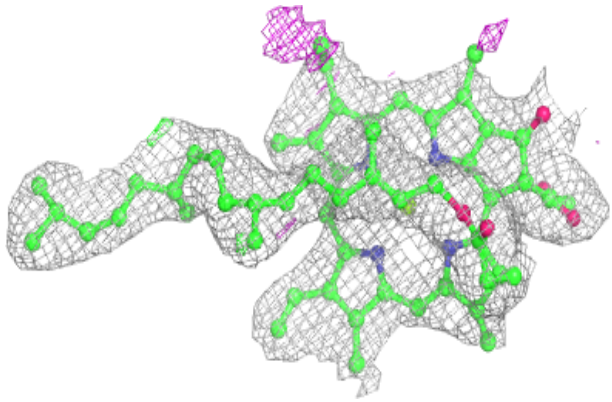


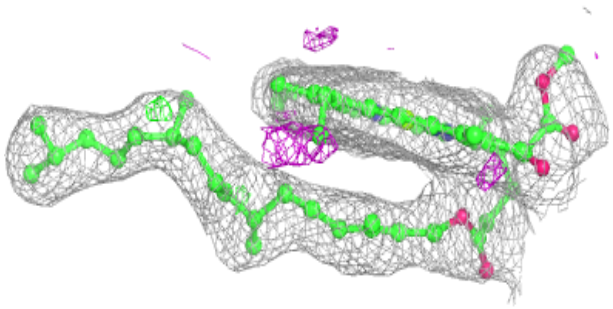


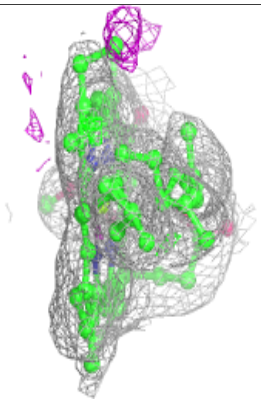


Electron density around CLA Y 836:

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

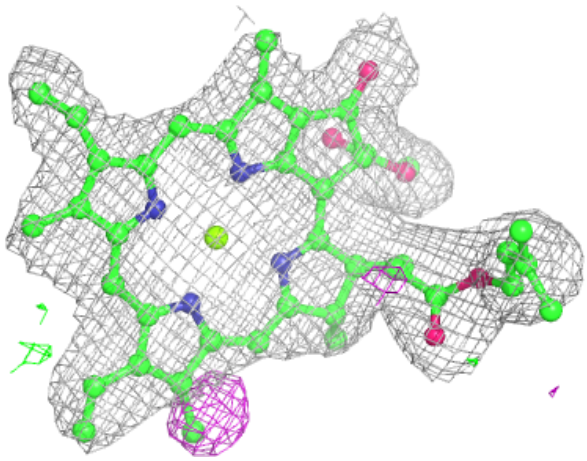


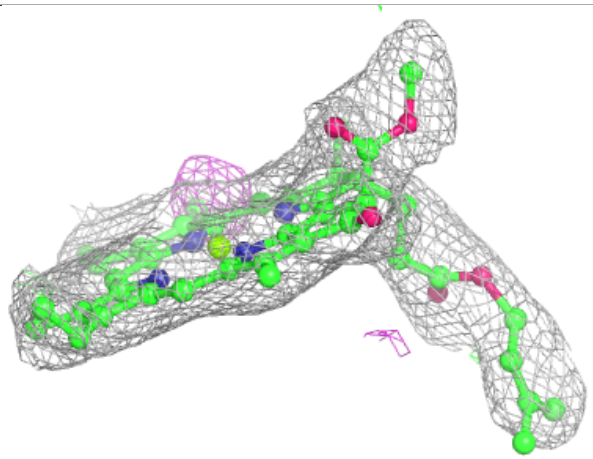


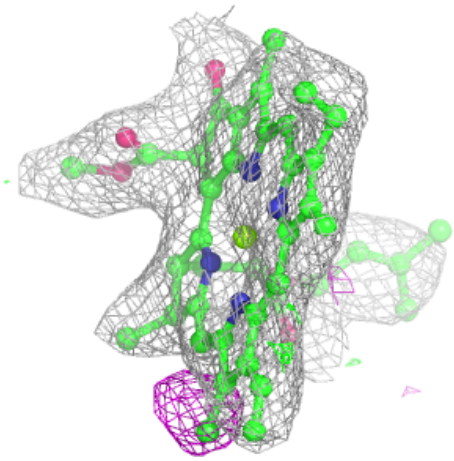


Electron density around CLA Y 837:

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

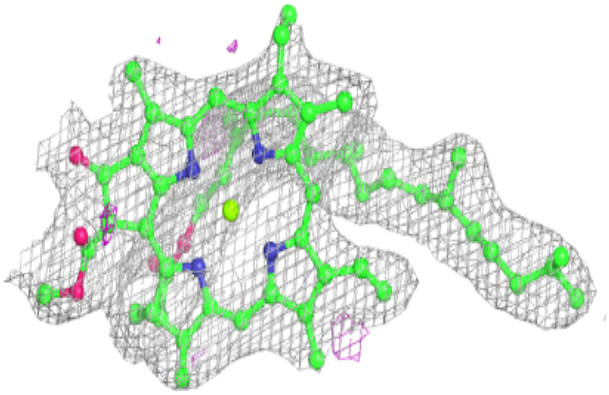


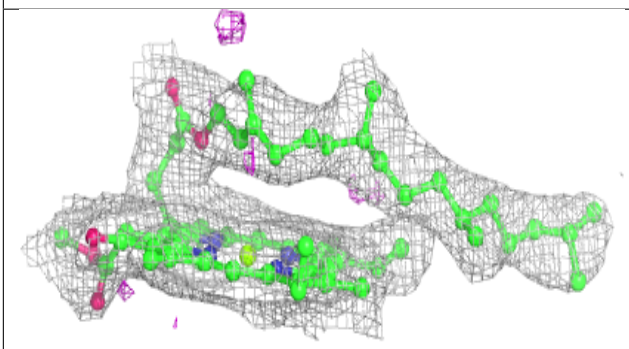


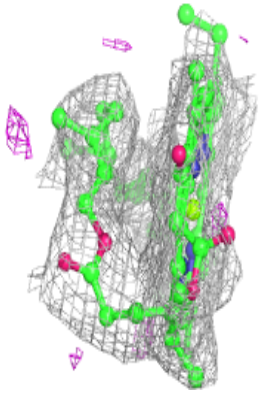


Electron density around CLA Y 838:

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

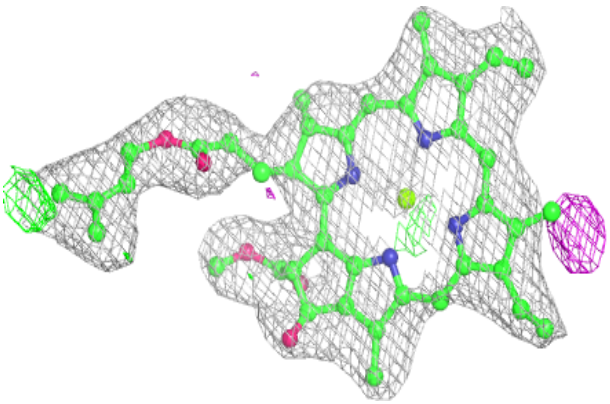


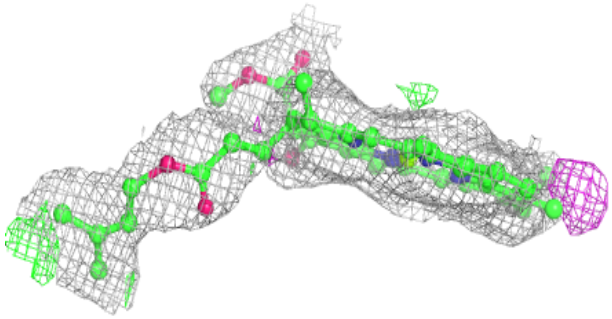


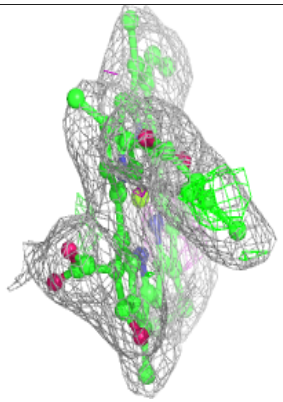


Electron density around CLA Y 839:

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

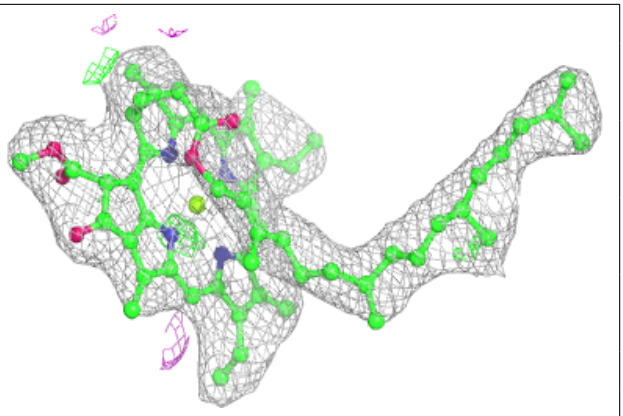


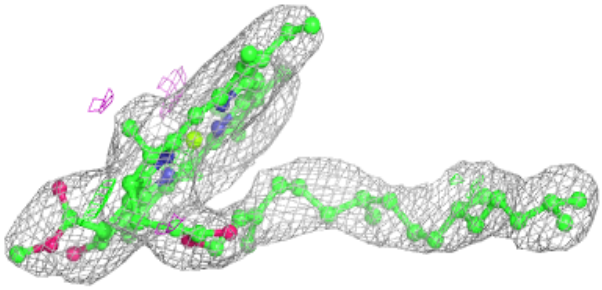


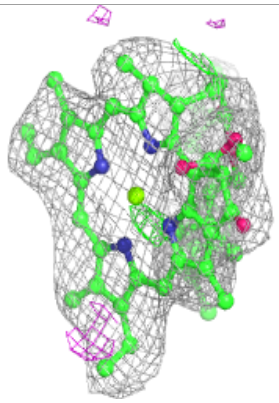


Electron density around CLA Y 840:

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

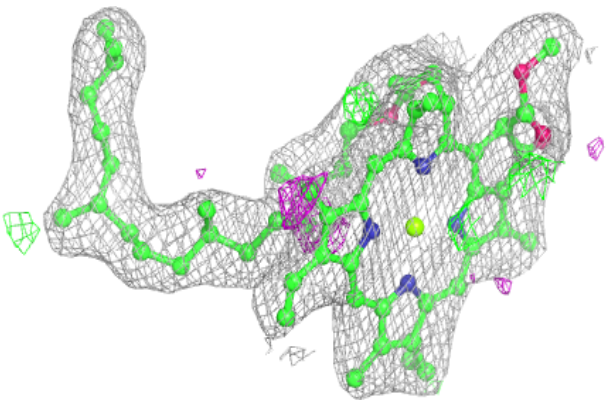


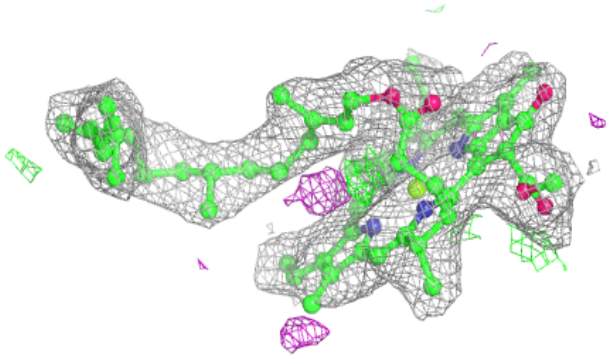


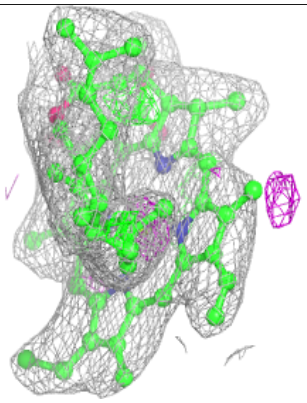


Electron density around CLA Y 841:

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

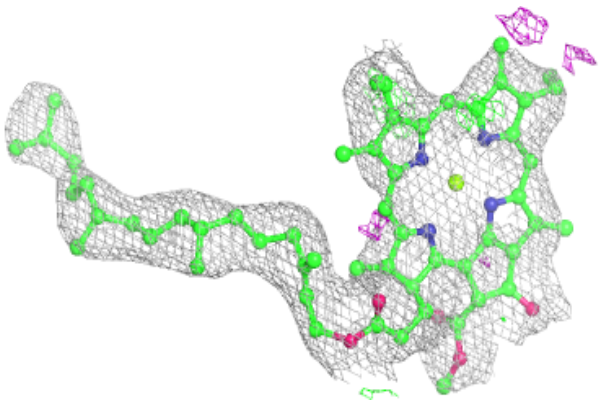


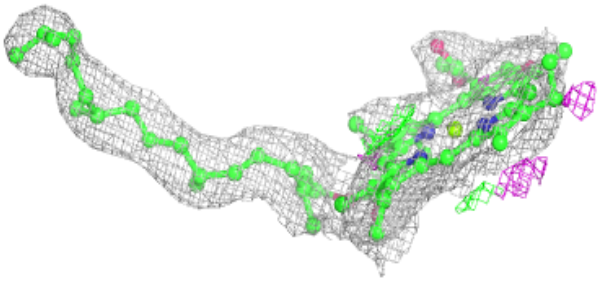


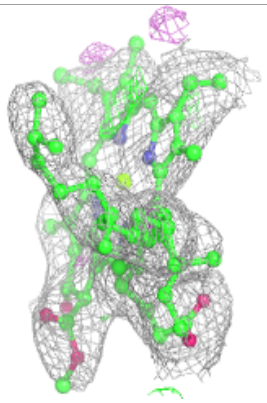


Electron density around CLA Z 801:

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

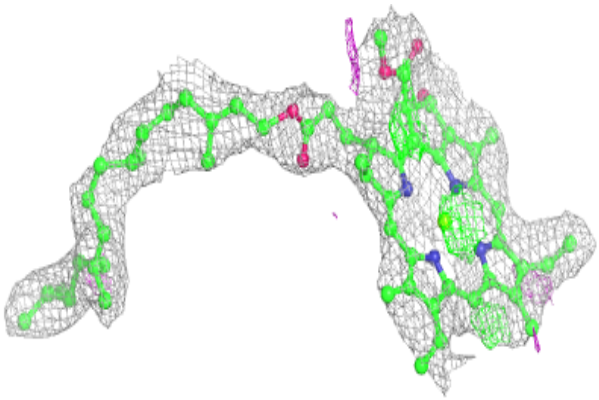


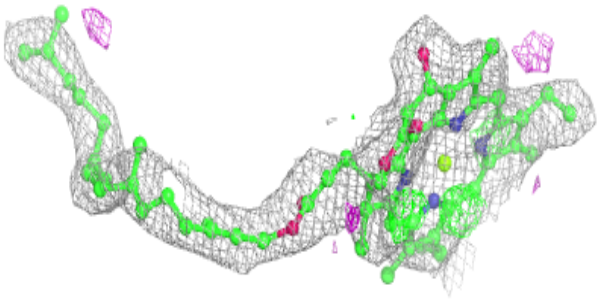


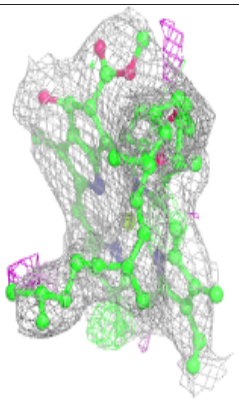


Electron density around CLA Z 802:

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

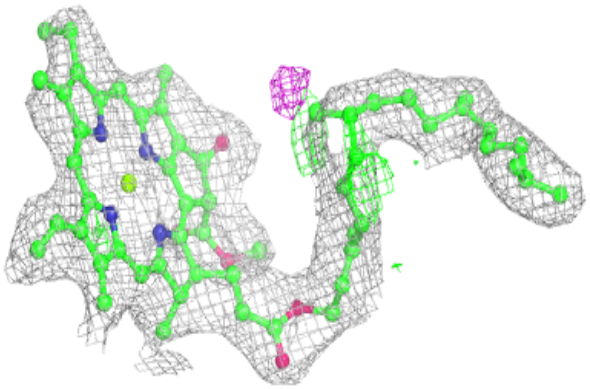


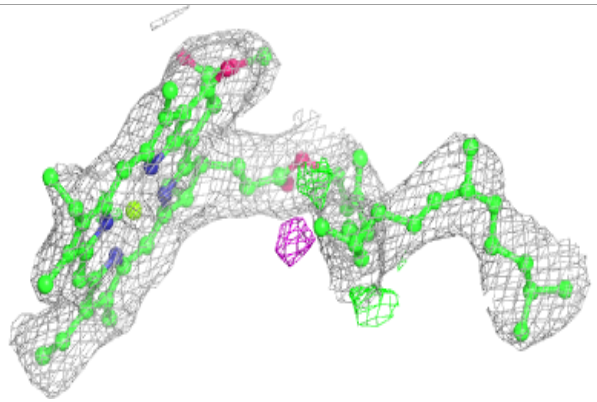


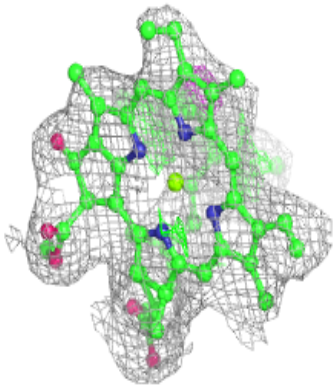


Electron density around CLA Z 803:

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

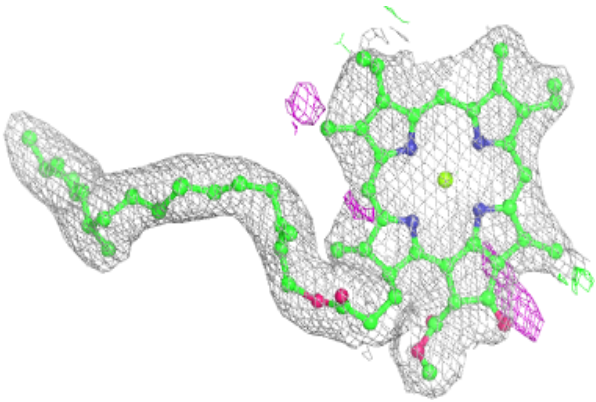


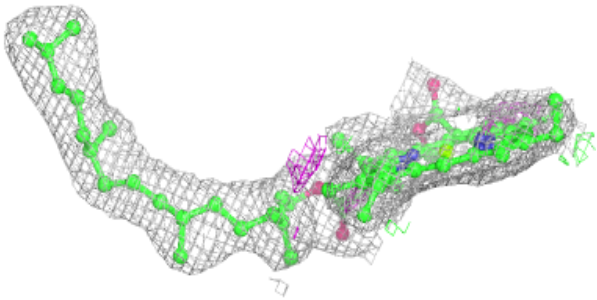


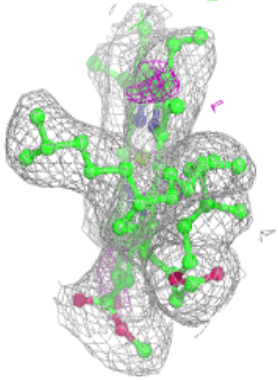


Electron density around CLA Z 804:

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

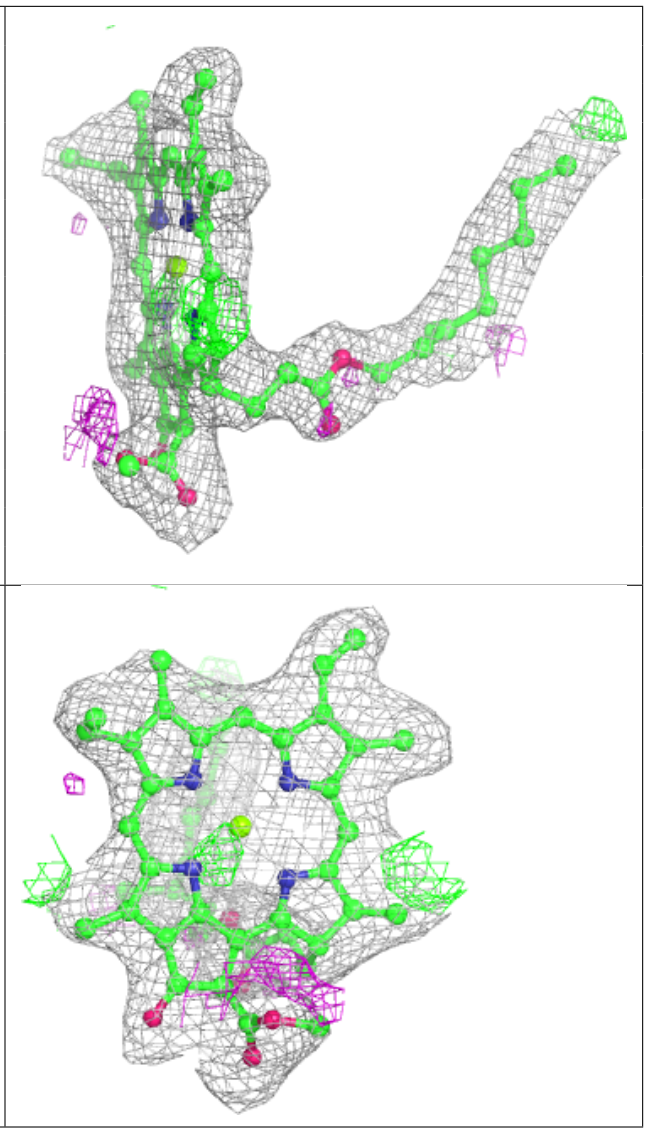






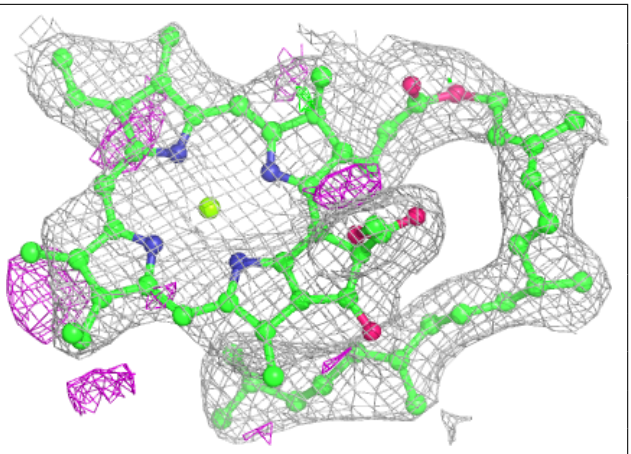
Electron density around CLA Z 805:

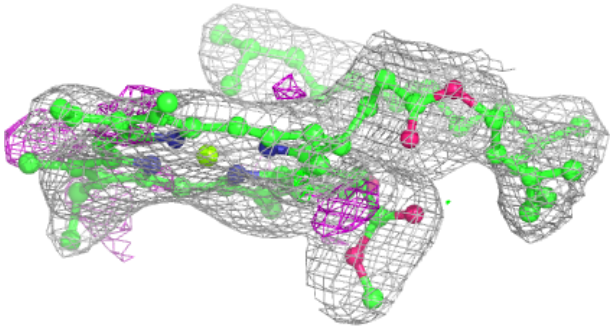
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

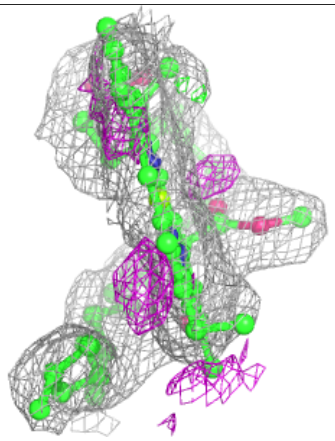


Electron density around CLA Z 806:

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

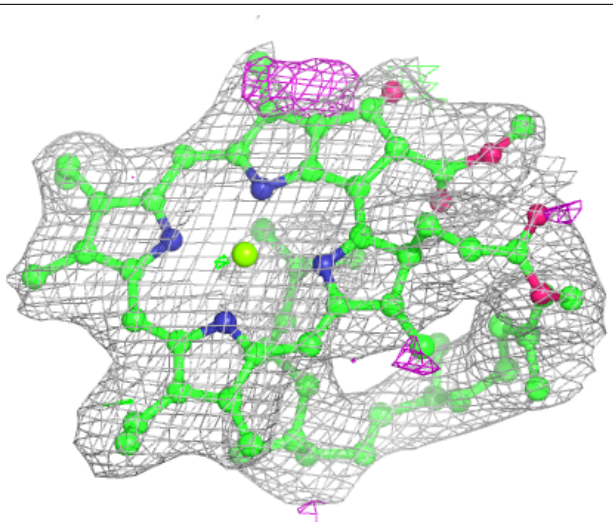


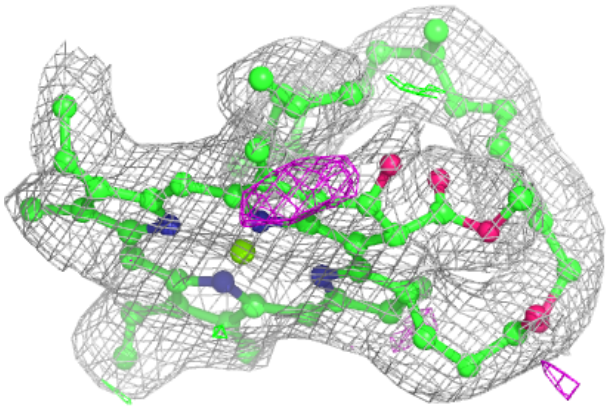


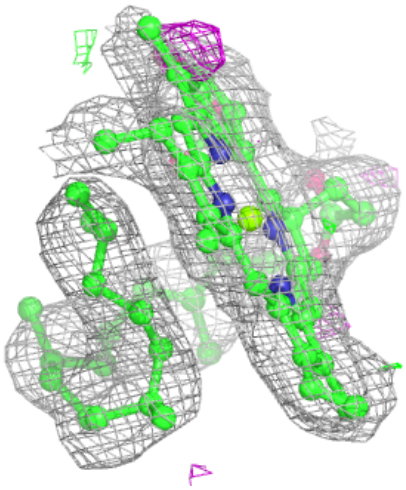


Electron density around CLA Z 807:

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

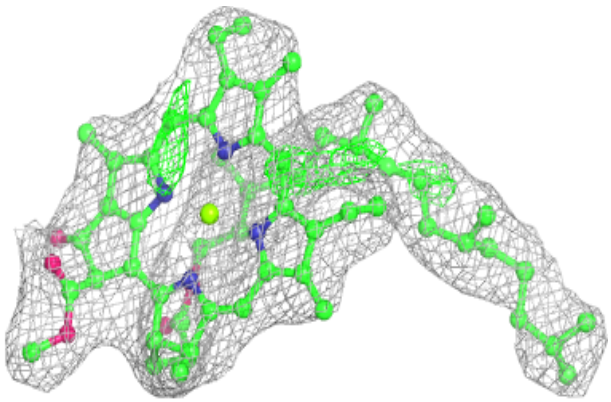


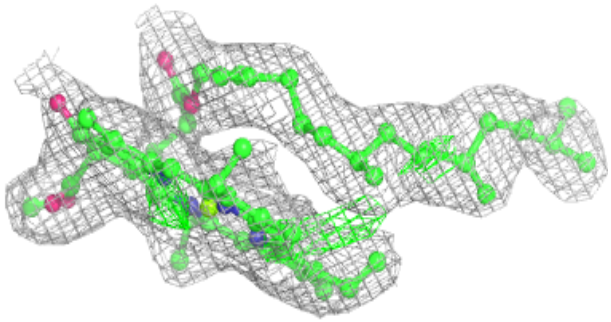


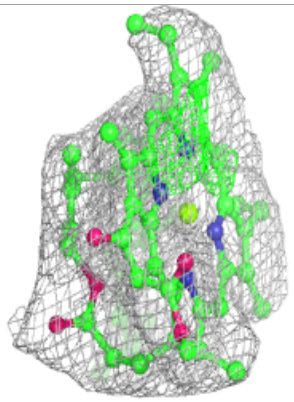


Electron density around CLA Z 808:

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

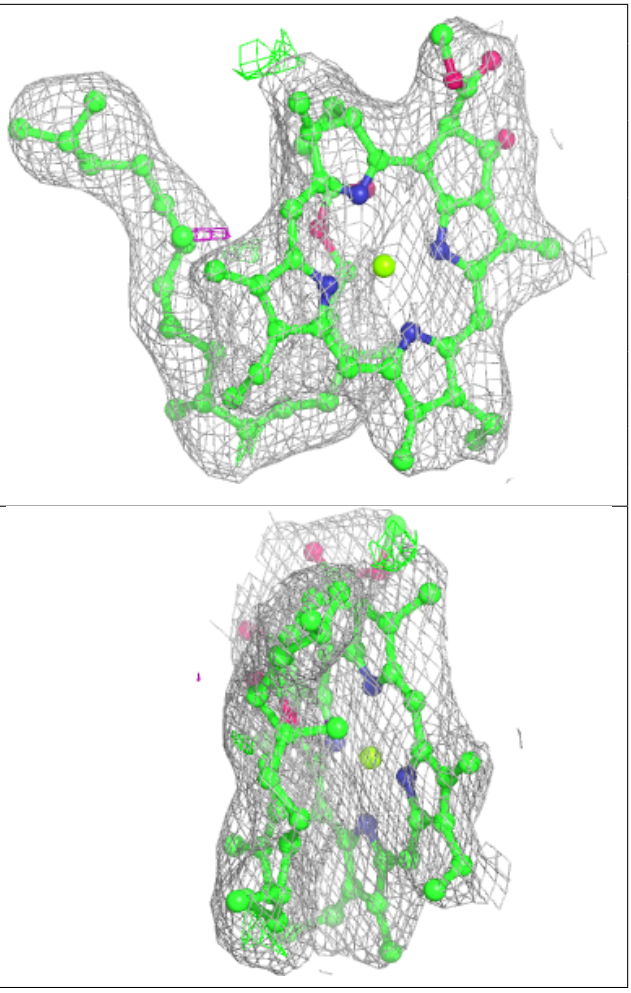






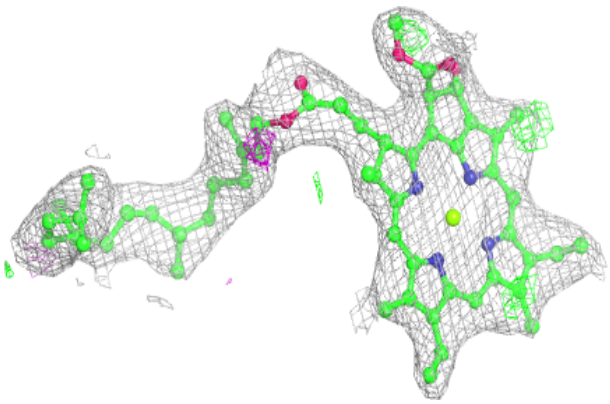
Electron density around CLA Z 809:

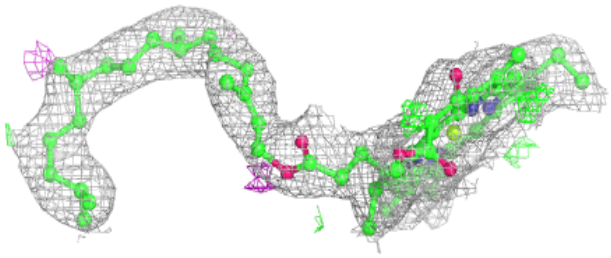
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

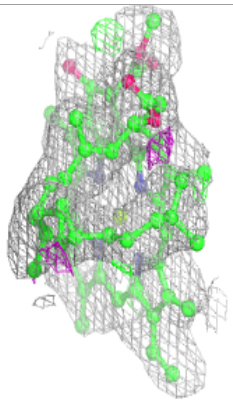


Electron density around CLA Z 810:

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

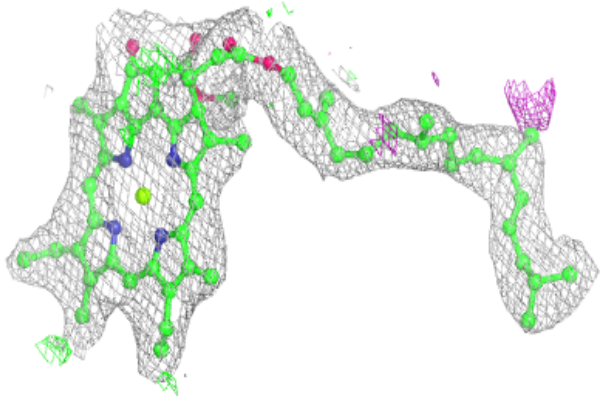


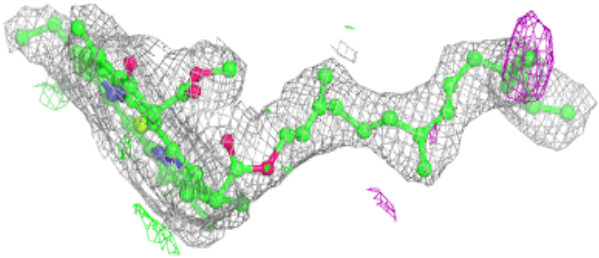


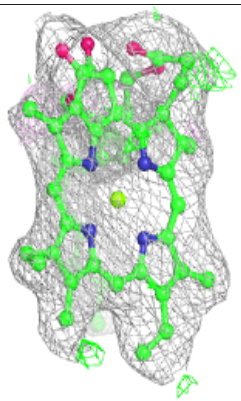


Electron density around CLA Z 811:

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

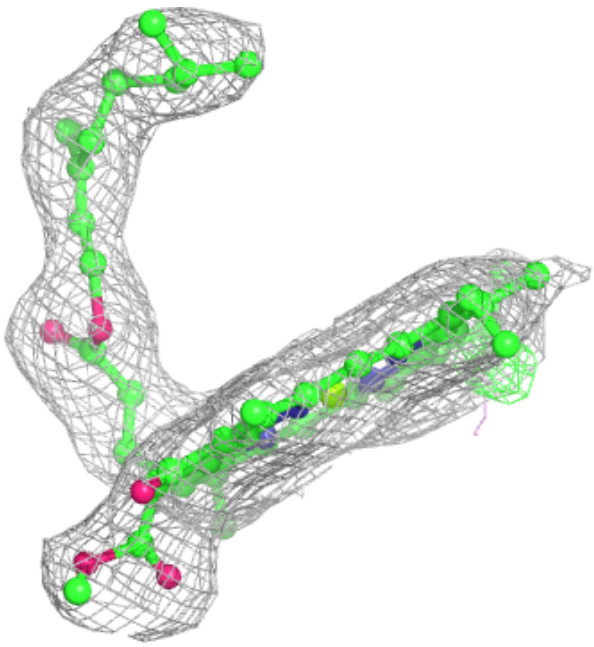


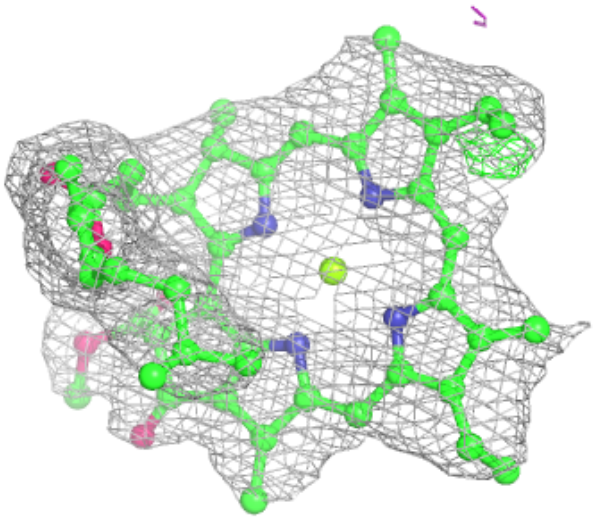


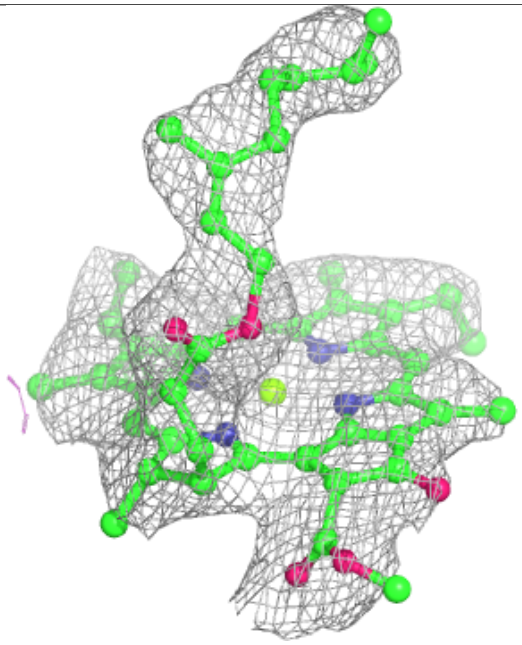


Electron density around CLA Z 812:

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

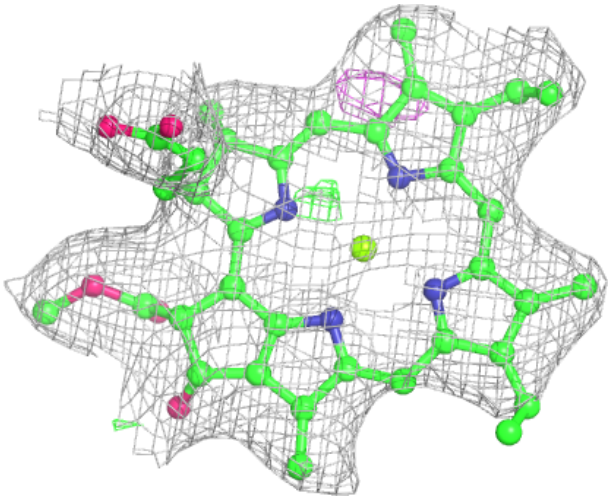


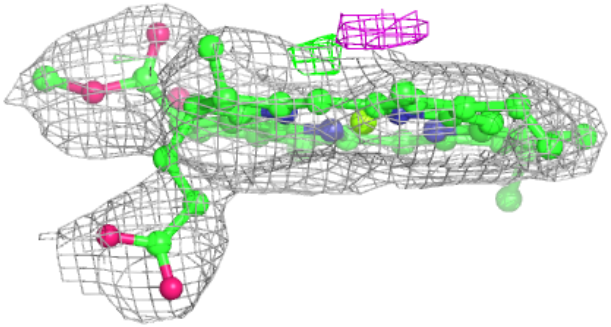


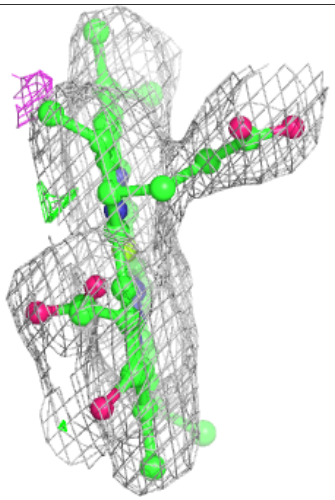


Electron density around CLA Z 813:

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

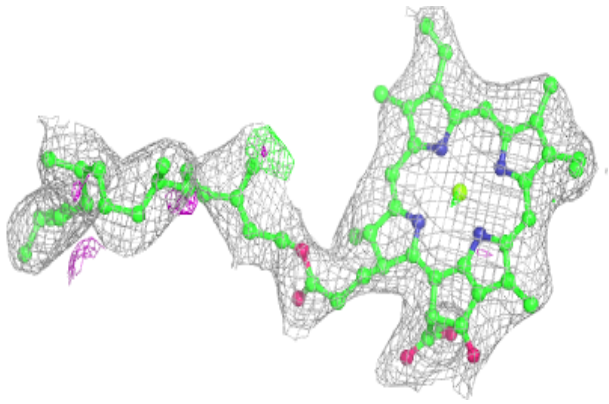


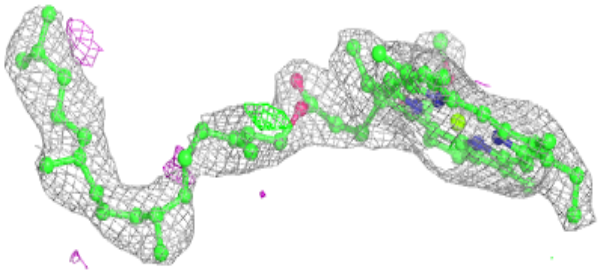


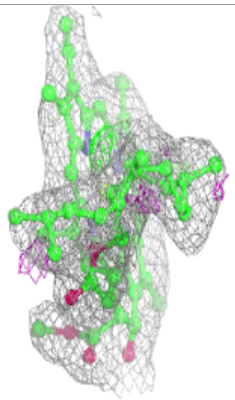


Electron density around CLA Z 814:

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

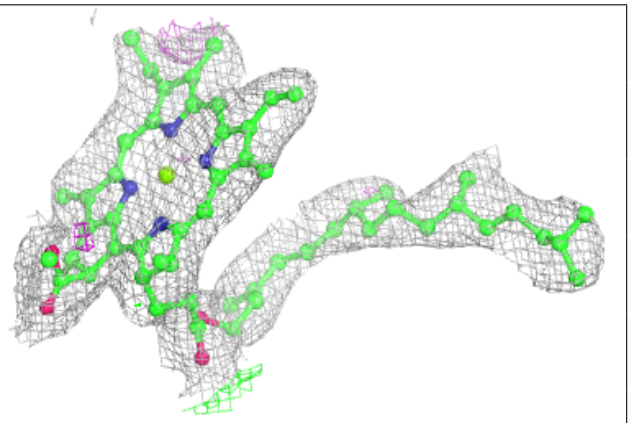


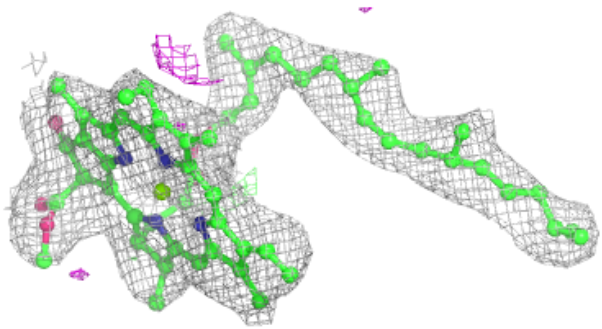


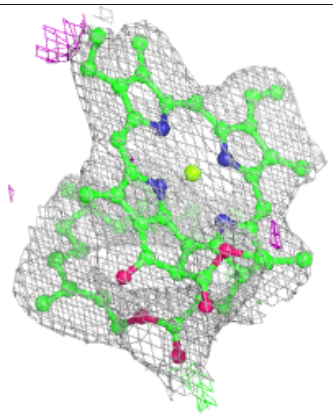


Electron density around CLA Z 815:

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

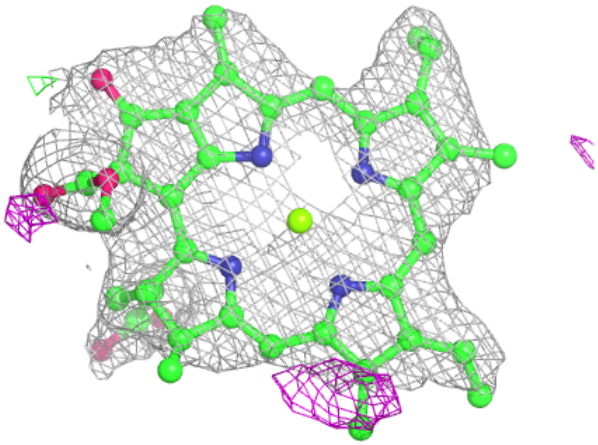


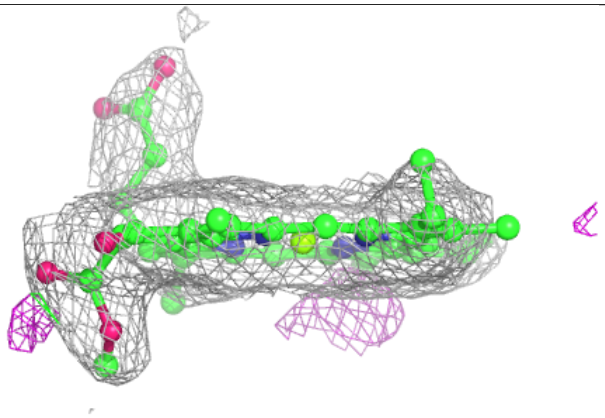


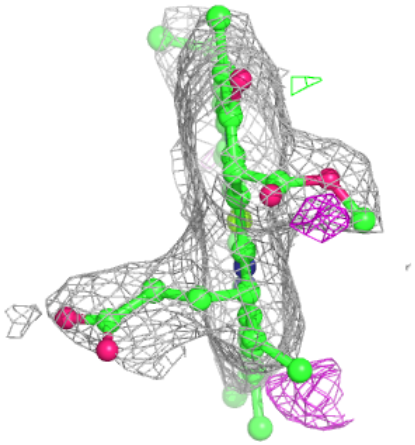


Electron density around CLA Z 816:

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

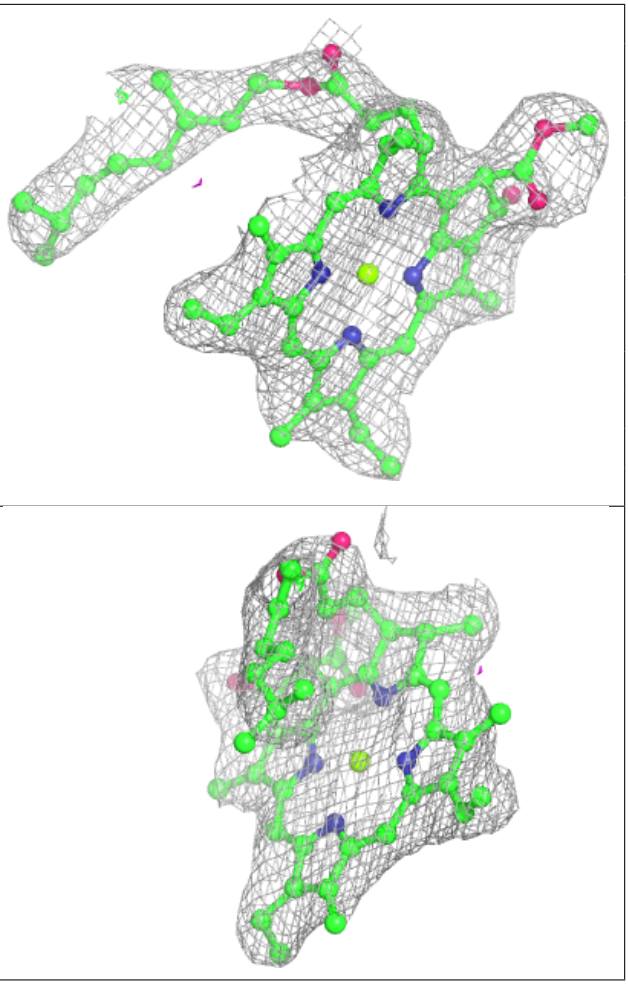






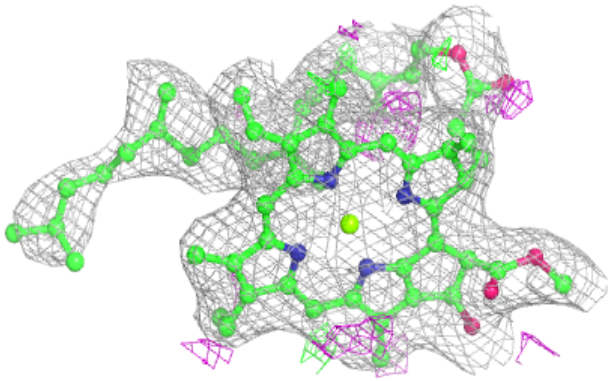
Electron density around CLA Z 817:

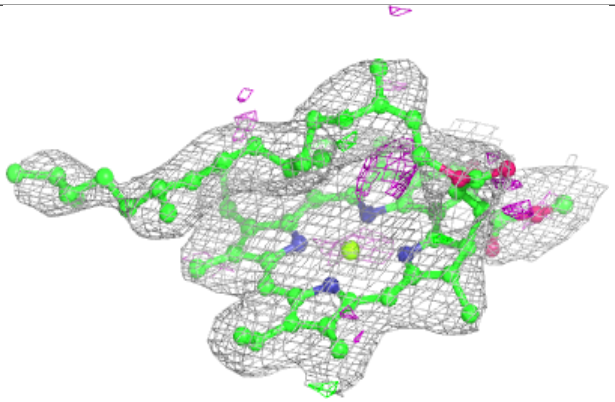
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

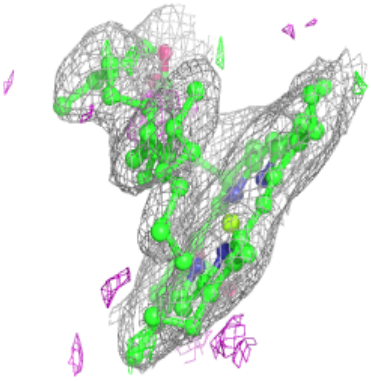


Electron density around CLA Z 818:

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

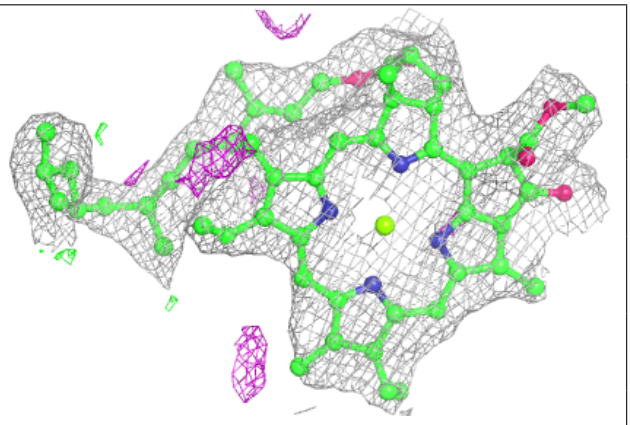


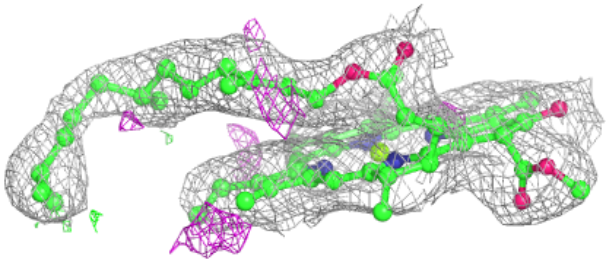


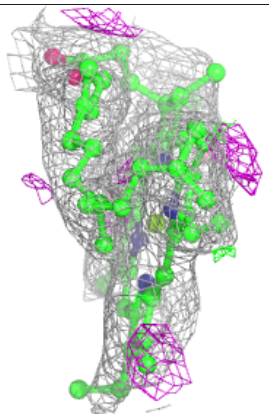


Electron density around CLA Z 819:

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

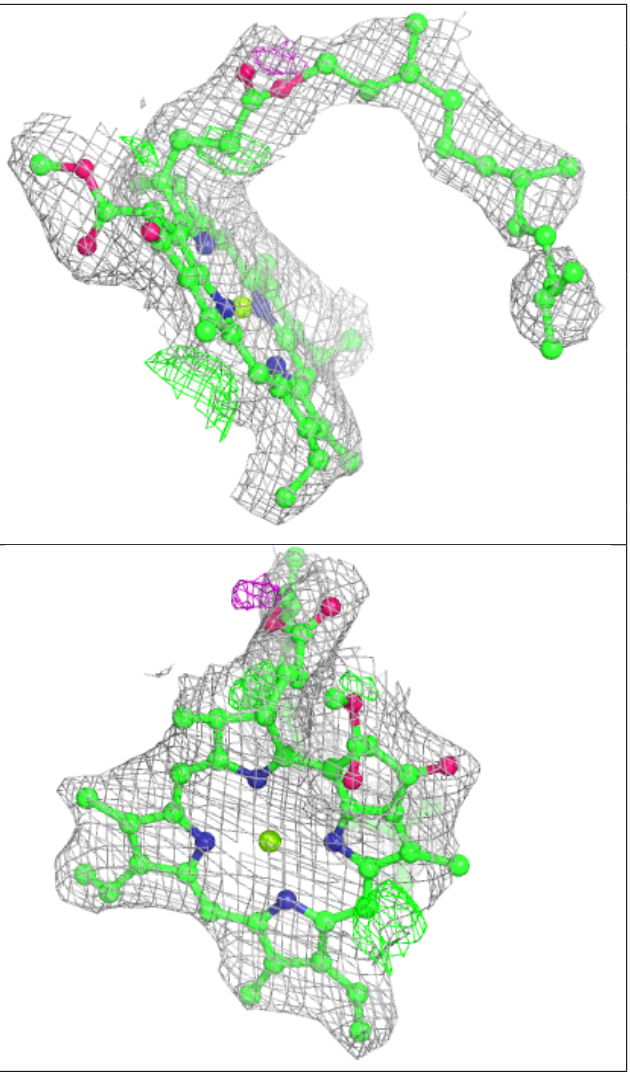






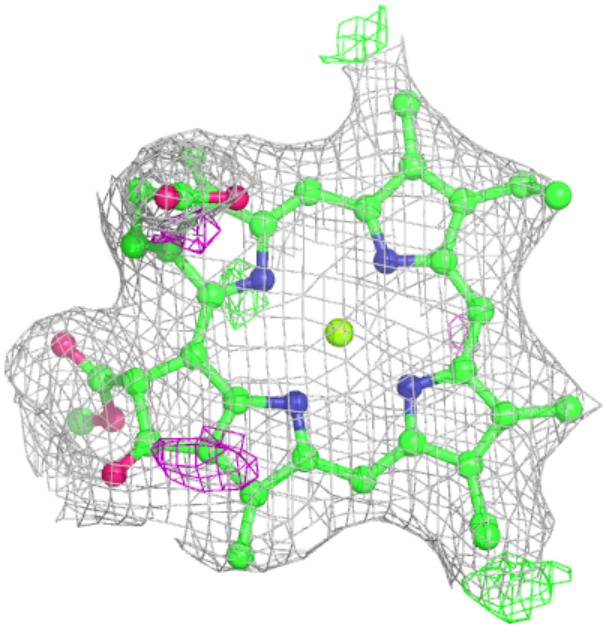
Electron density around CLA Z 820:

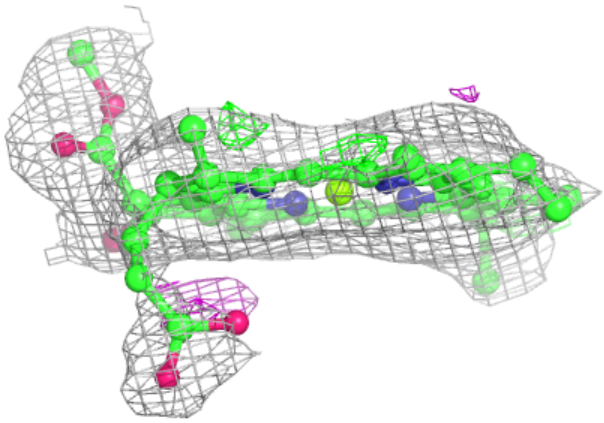
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

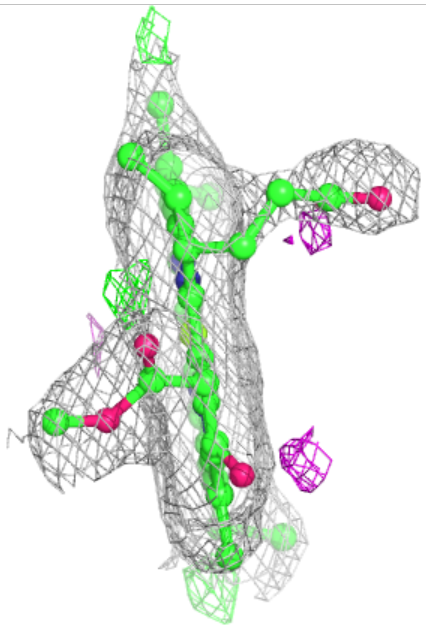


Electron density around CLA Z 821:

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

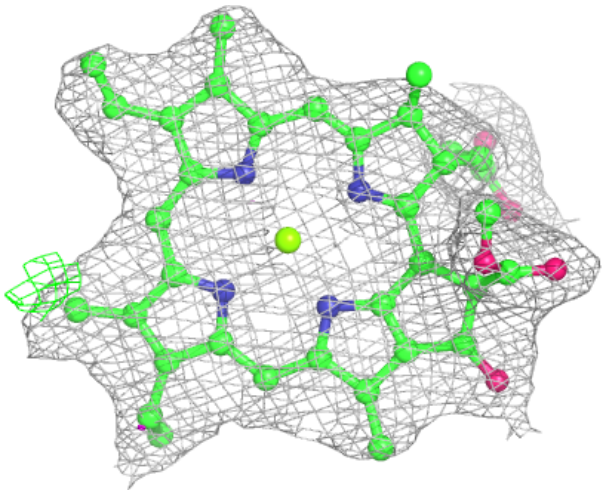


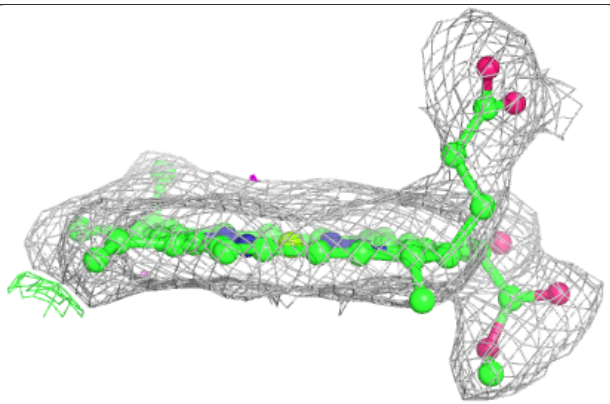


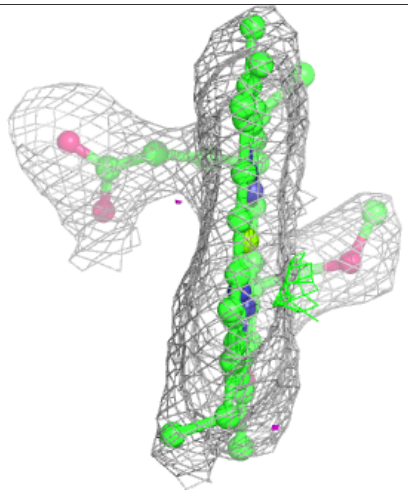


Electron density around CLA Z 822:

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

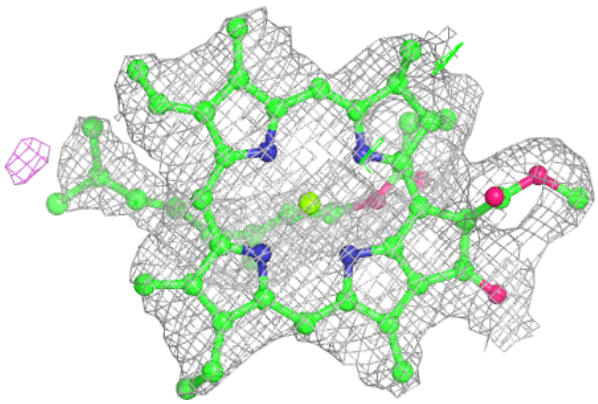


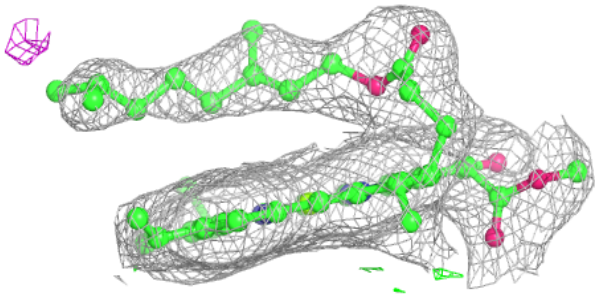


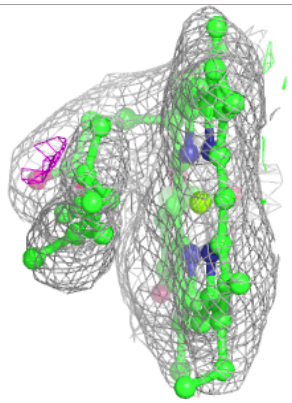


Electron density around CLA Z 823:

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

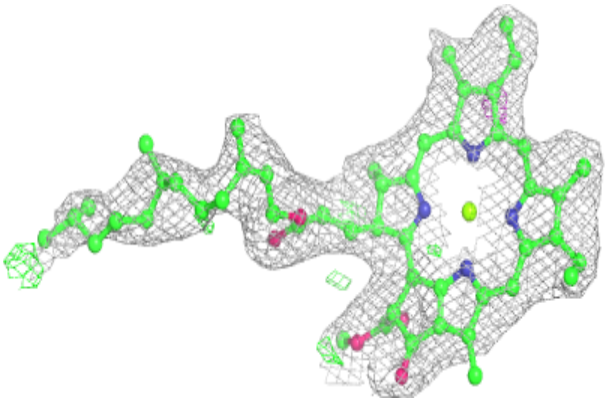


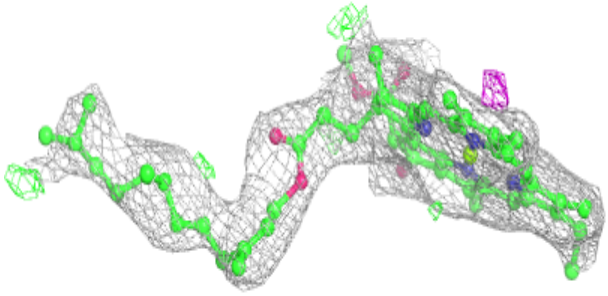


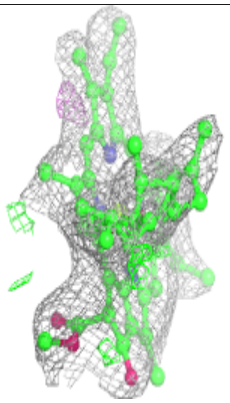


Electron density around CLA Z 824:

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

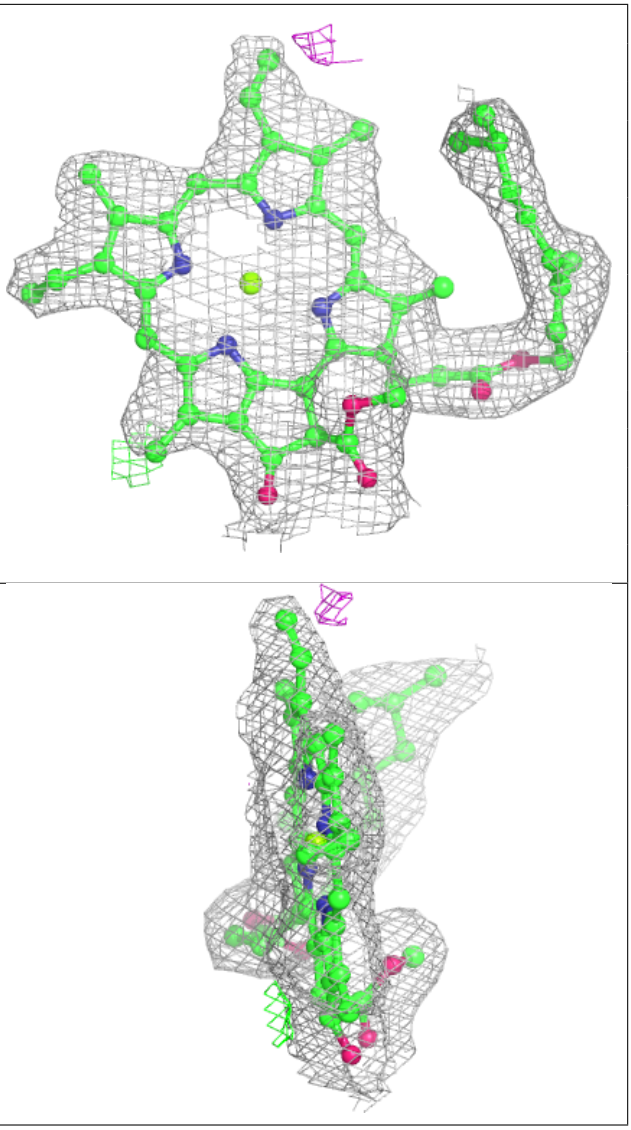






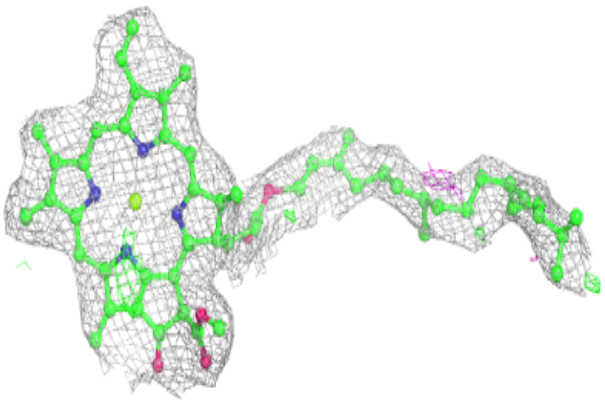
Electron density around CLA Z 825:

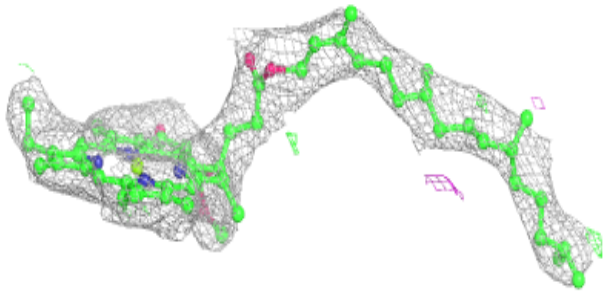
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

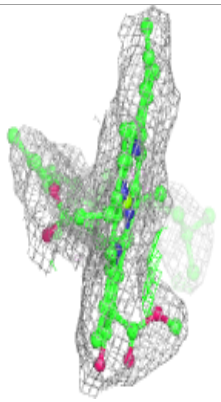


Electron density around CLA Z 826:

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

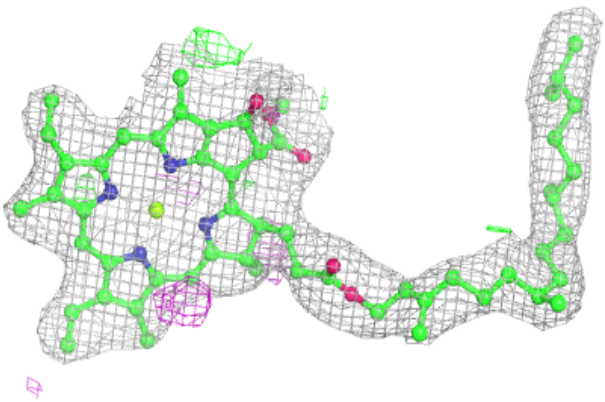


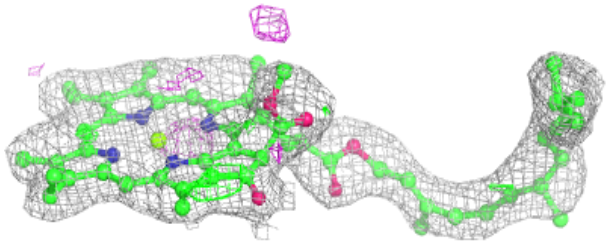


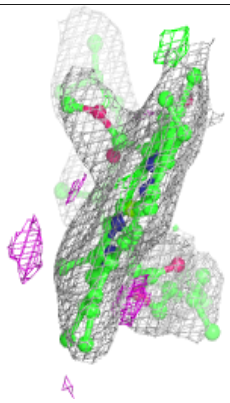


Electron density around CLA Z 827:

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

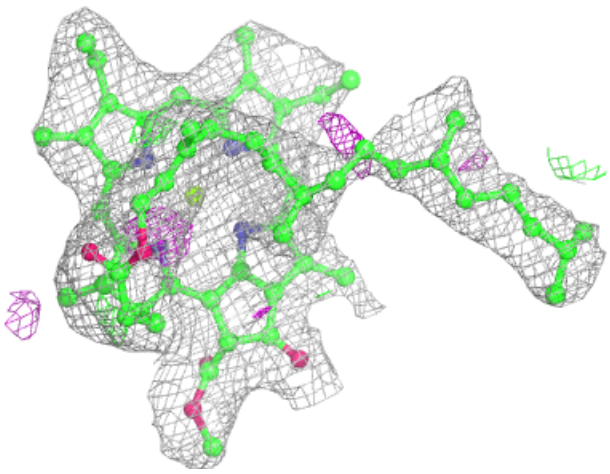


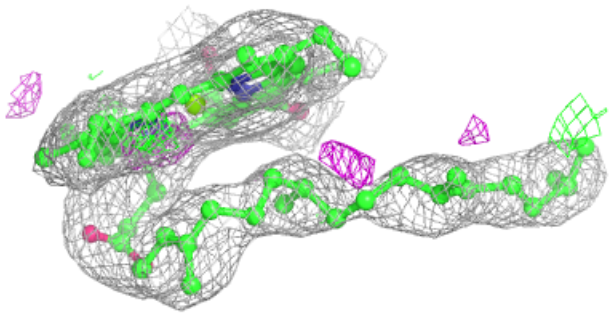


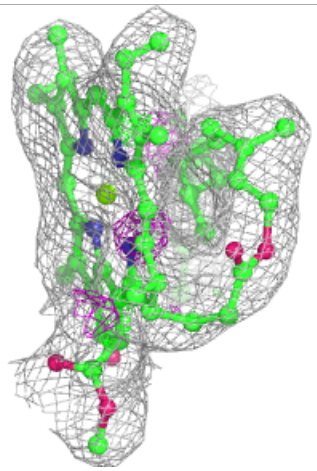


Electron density around CLA Z 828:

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

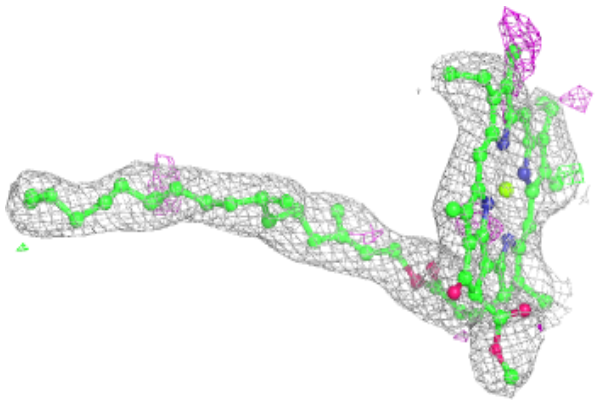


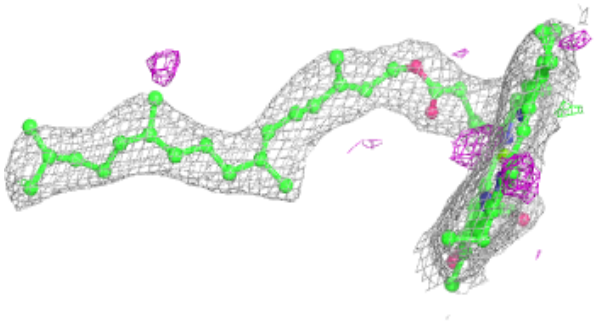


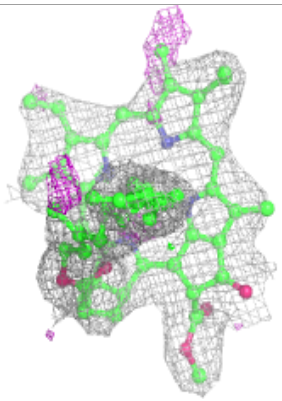


Electron density around CLA Z 829:

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

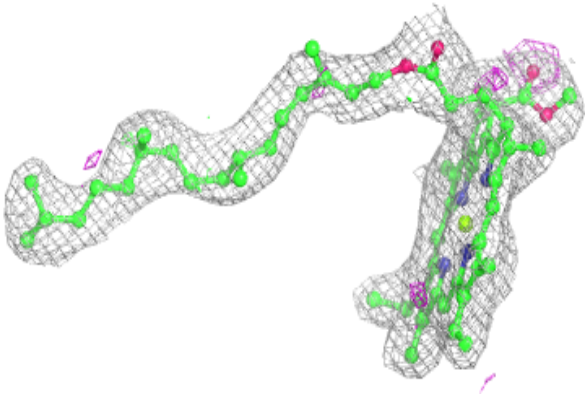


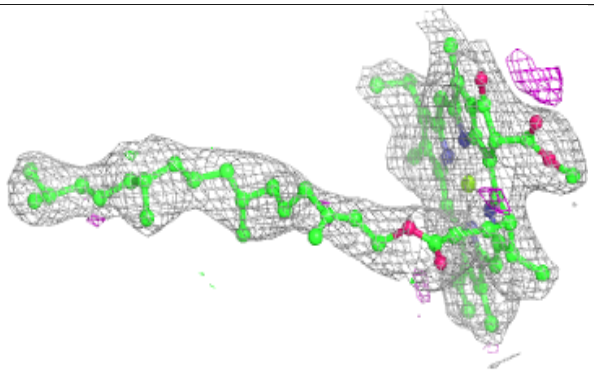


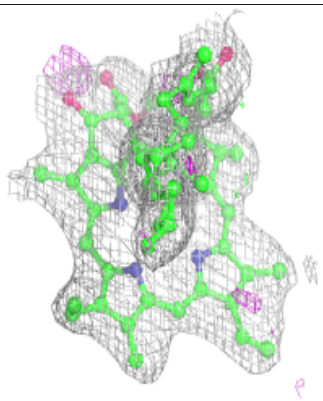


Electron density around CLA Z 830:

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

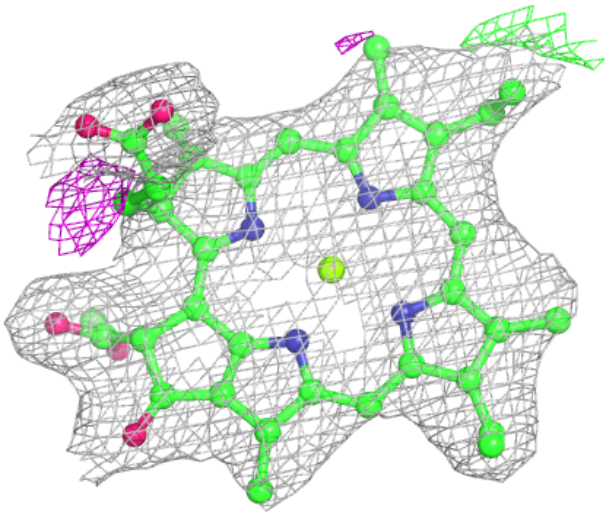


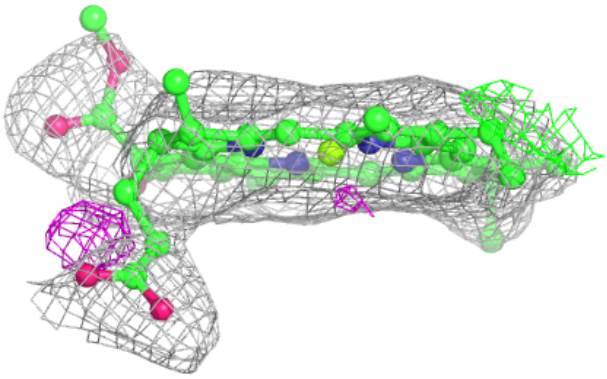


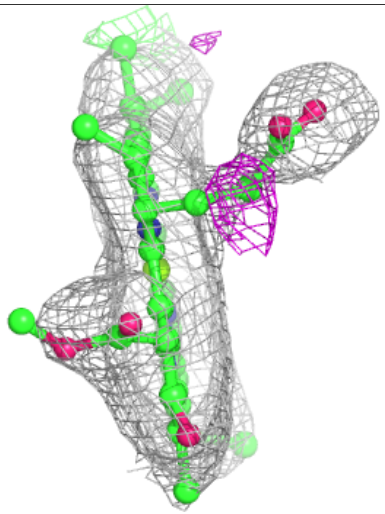


Electron density around CLA Z 831:

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

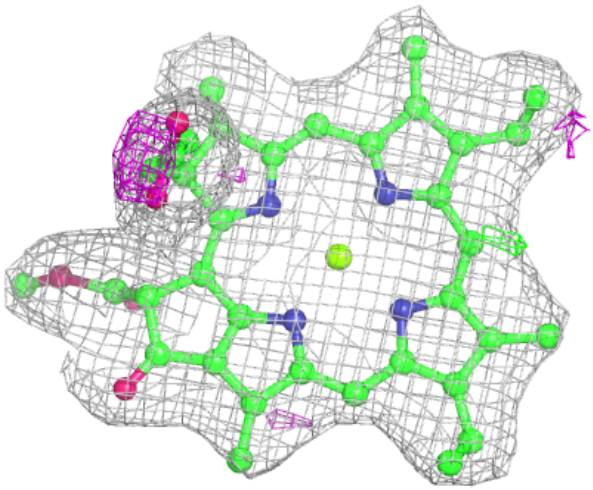


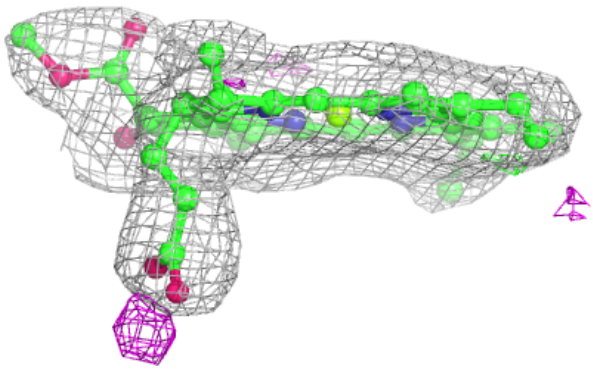


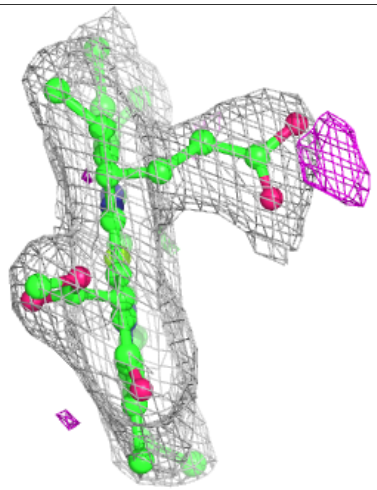


Electron density around CLA Z 832:

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

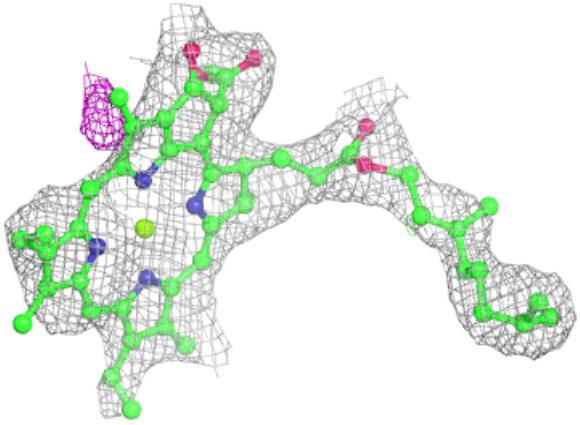


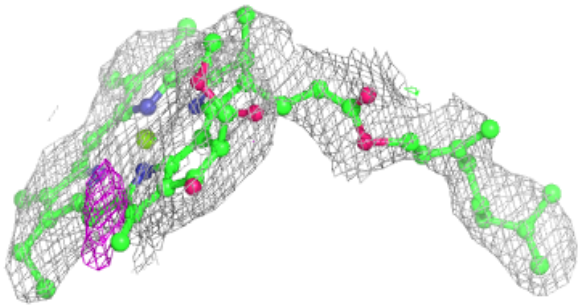


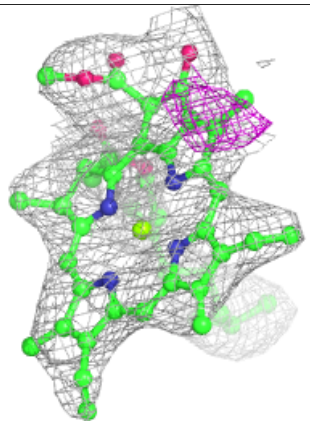


Electron density around CLA Z 833:

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

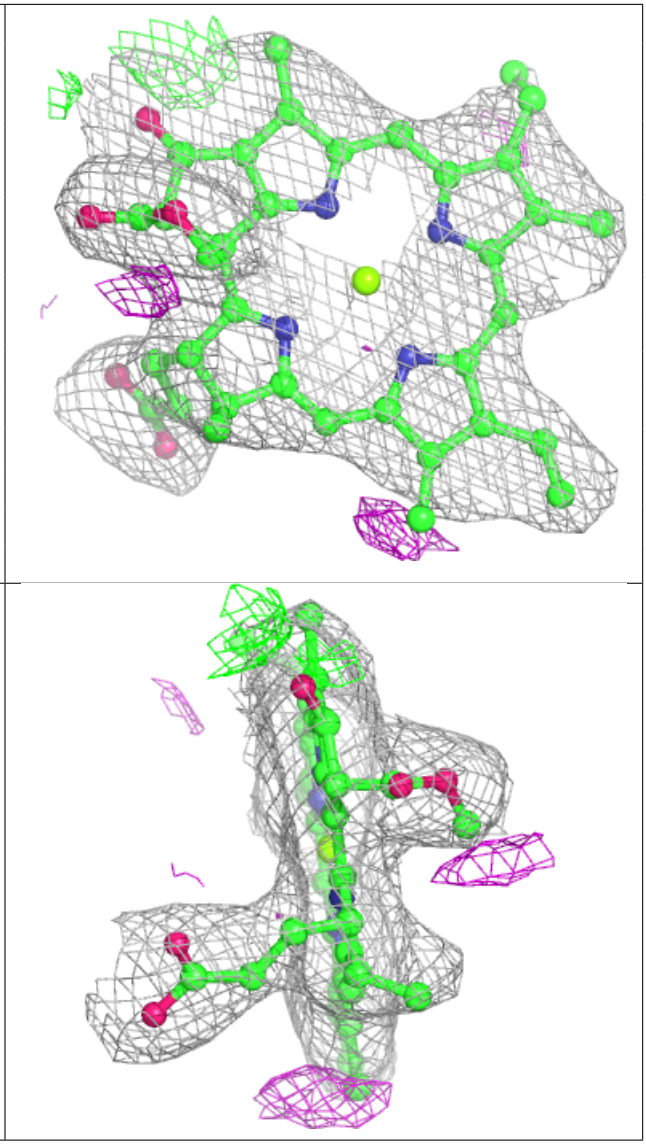






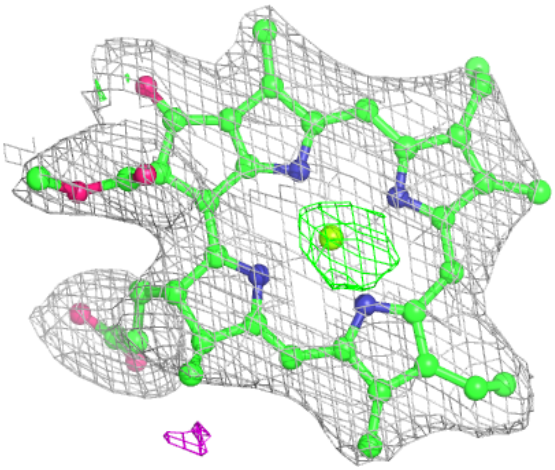
Electron density around CLA Z 834:

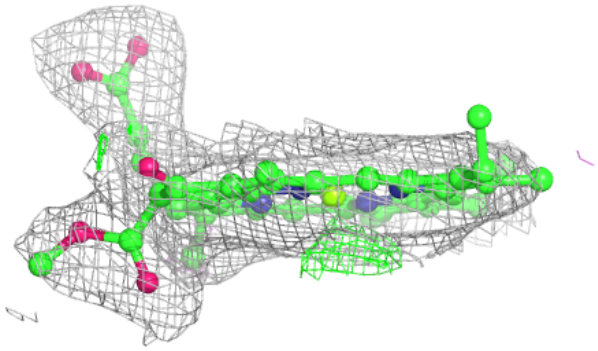
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

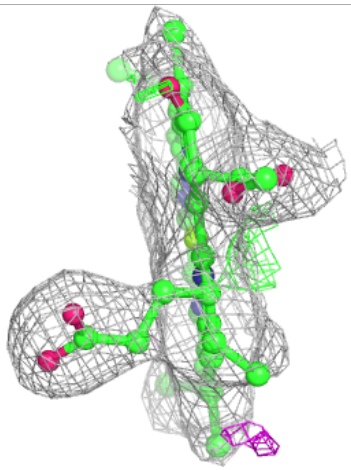


Electron density around CLA Z 835:

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)

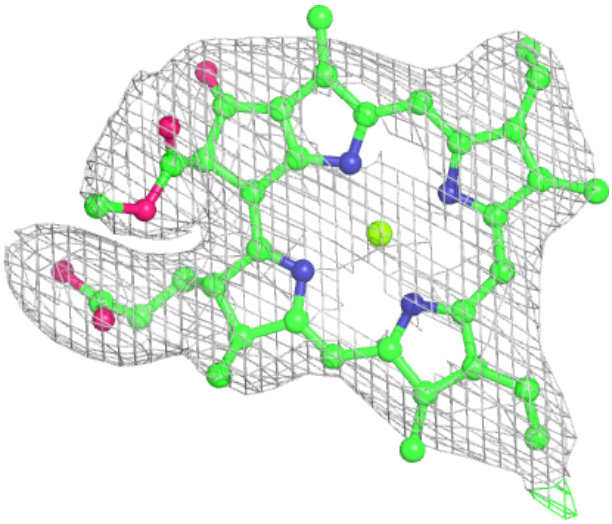


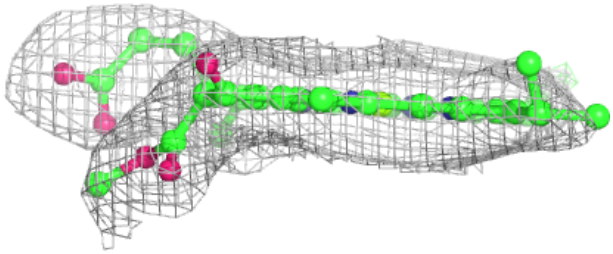


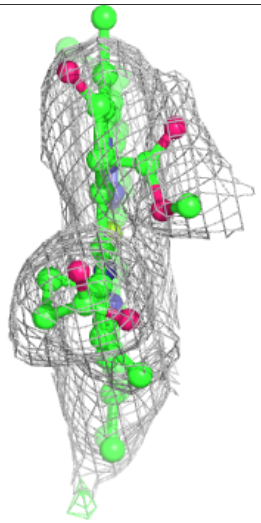


Electron density around CLA Z 836:

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

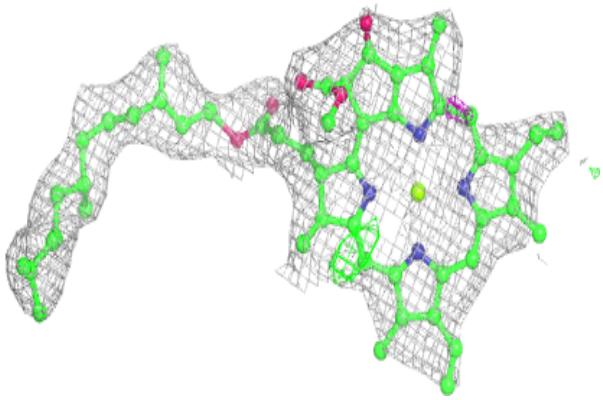


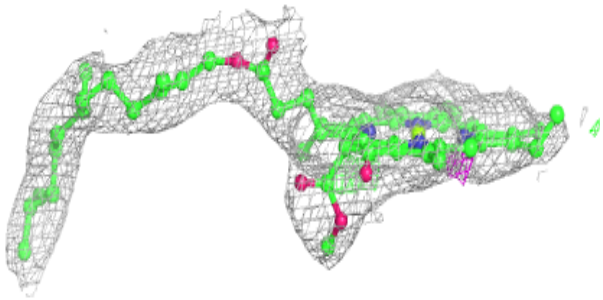




Electron density around CLA Z 837:

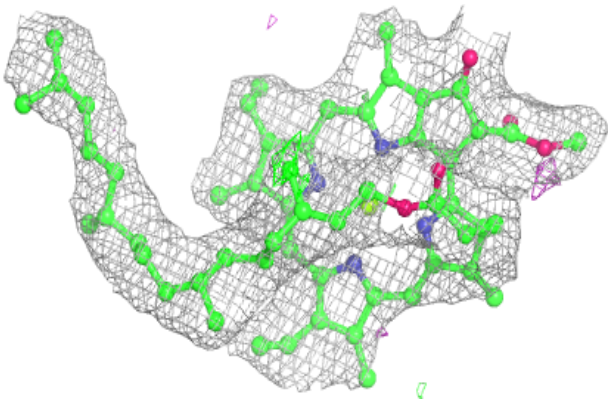
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

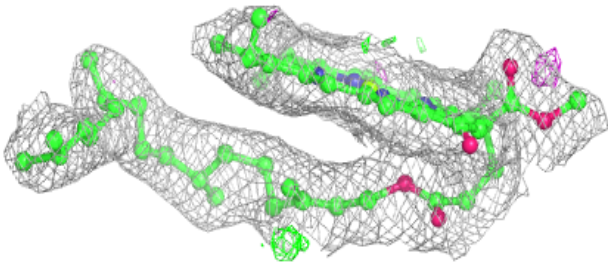


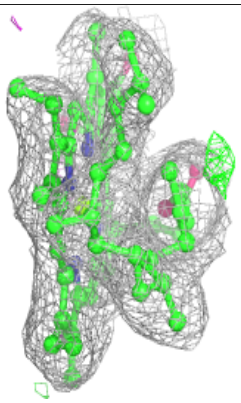


Electron density around CLA Z 838:

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

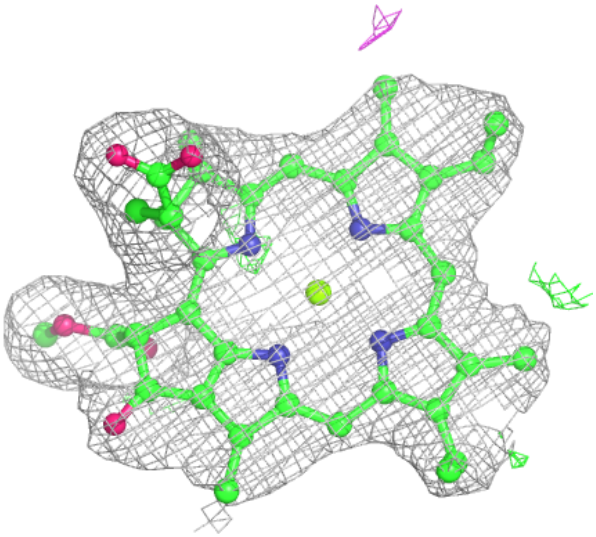


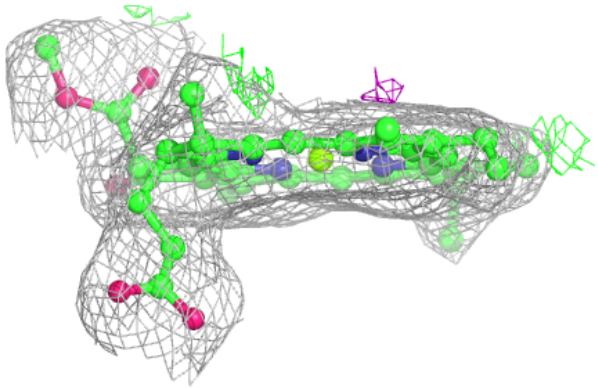


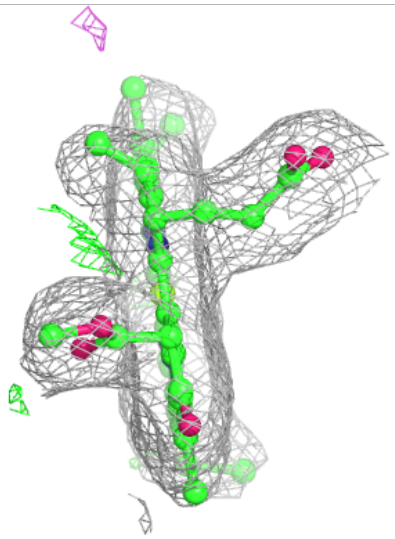


Electron density around CLA Z 839:

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

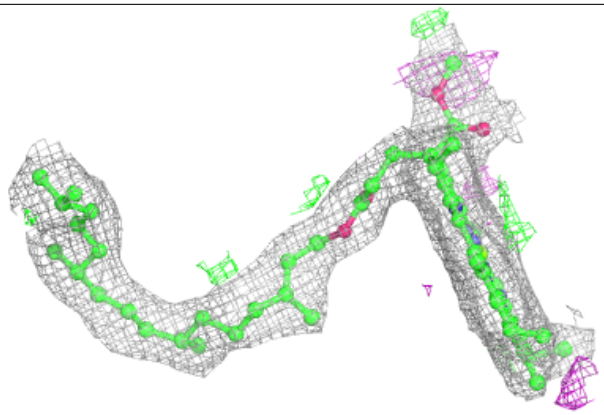


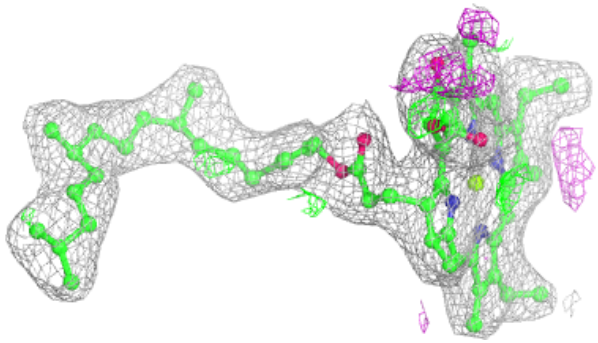


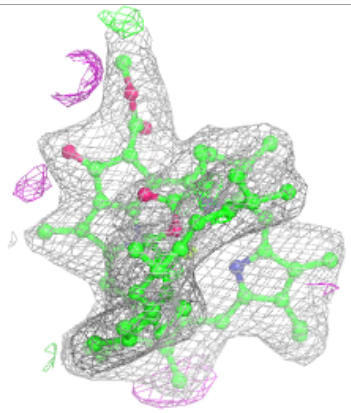


Electron density around CLA Z 840:

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

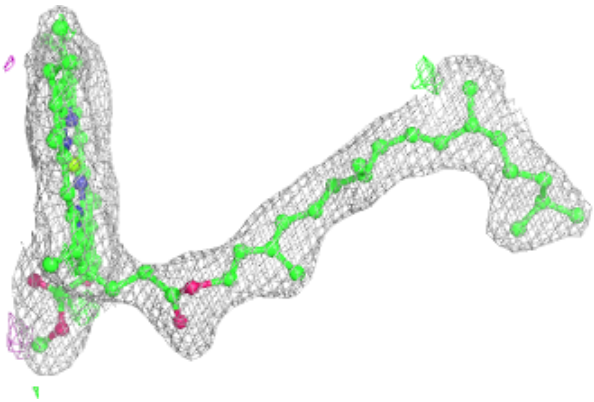


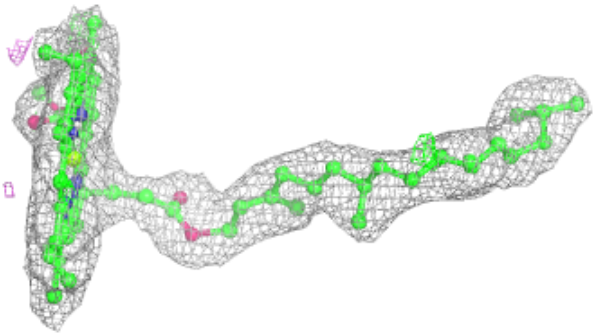


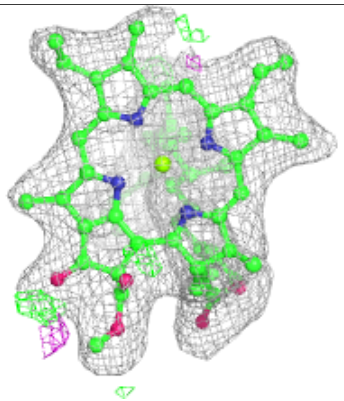


Electron density around CLA Z 841:

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

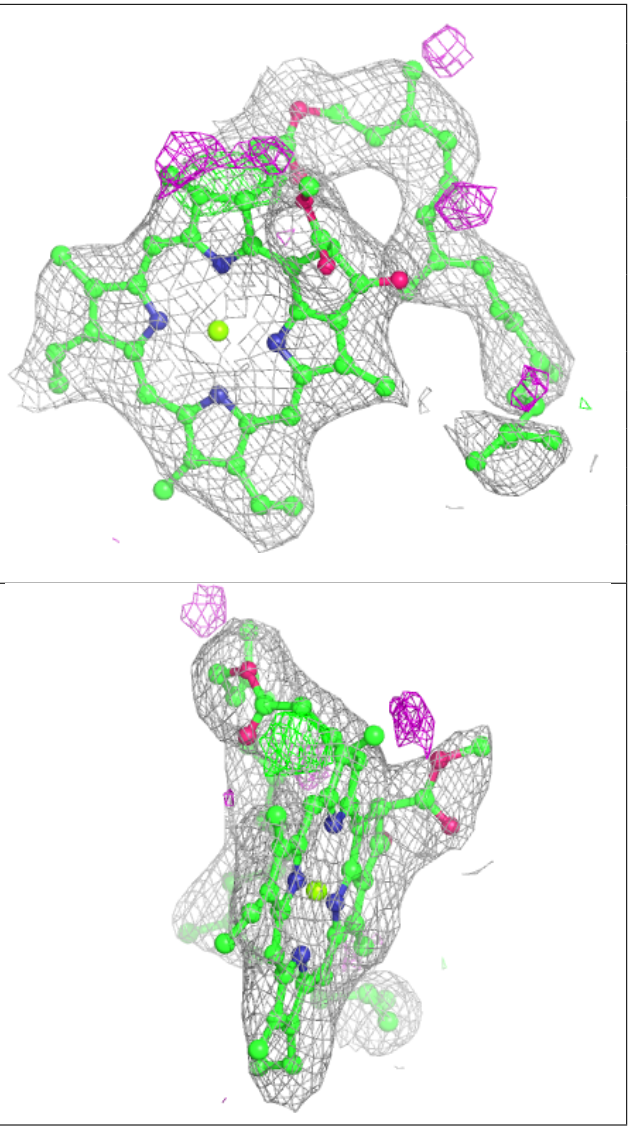






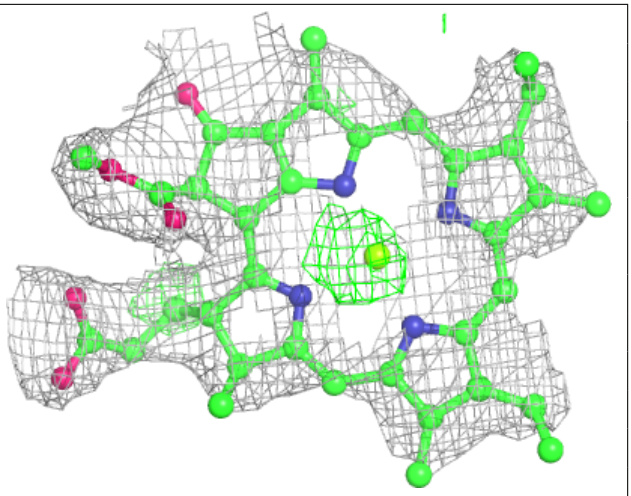
Electron density around CLA d 201:

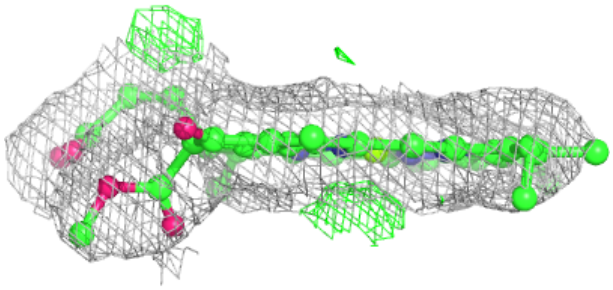
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

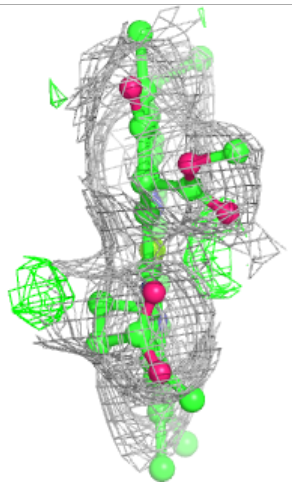


Electron density around CLA d 202:

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

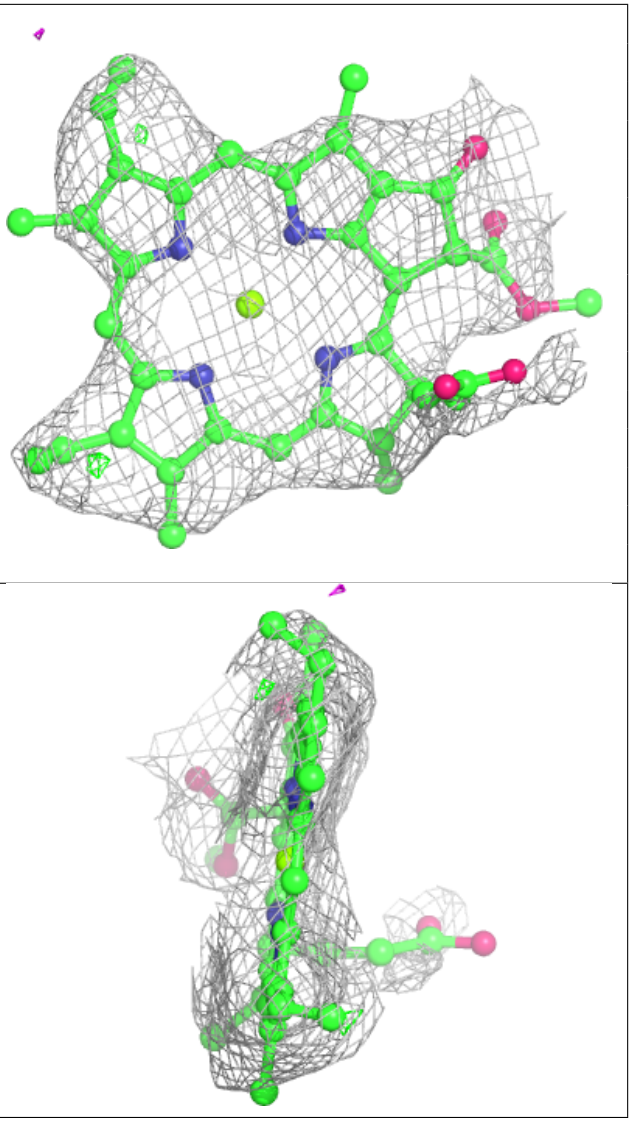






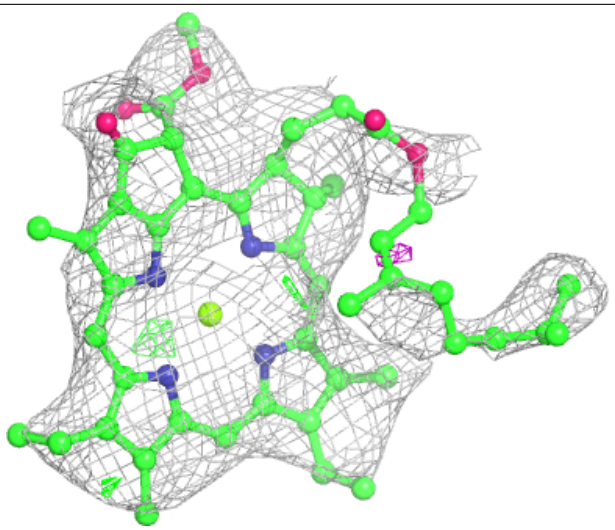
Electron density around CLA f 101:

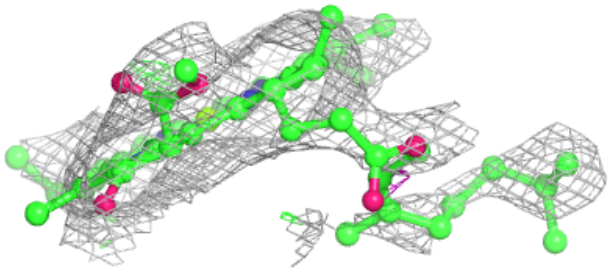
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

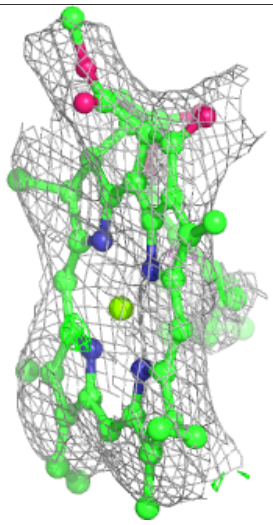


Electron density around CLA f 102:

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

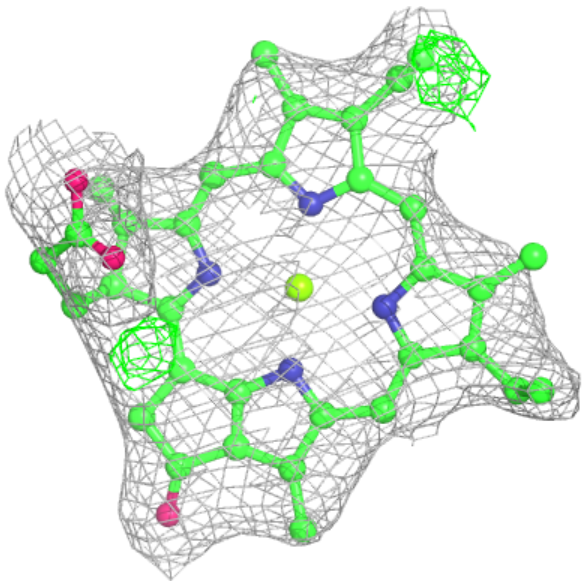


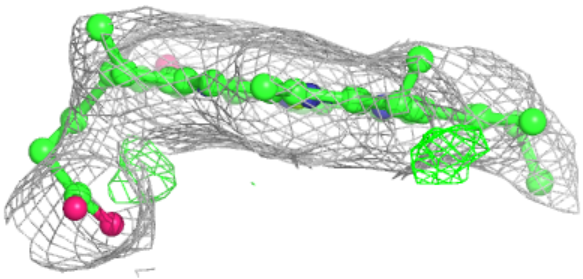


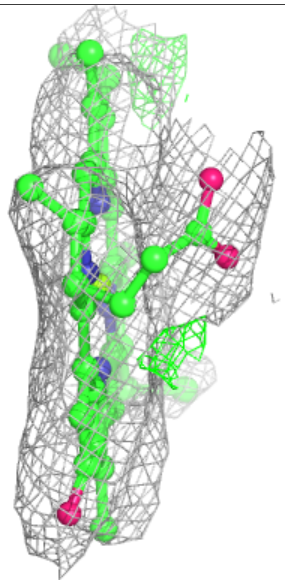


Electron density around CLA g 101:

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

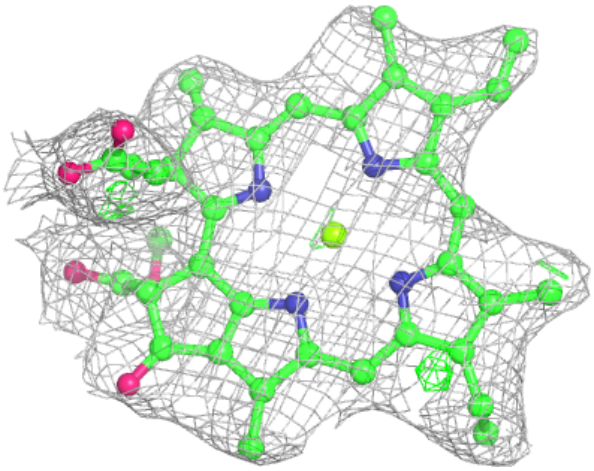


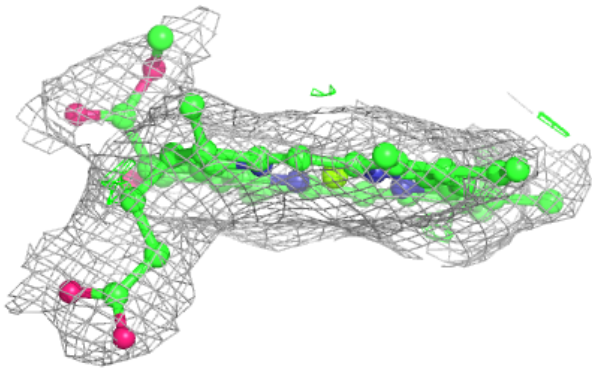


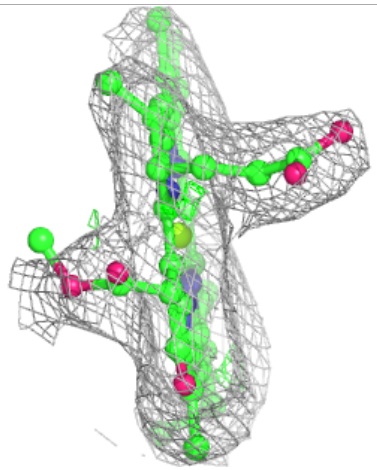


Electron density around CLA g 102:

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

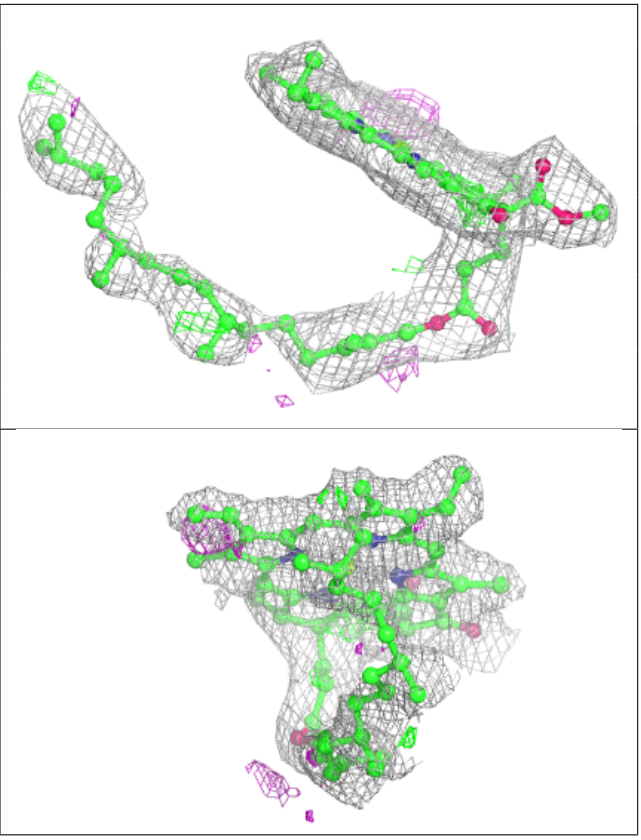






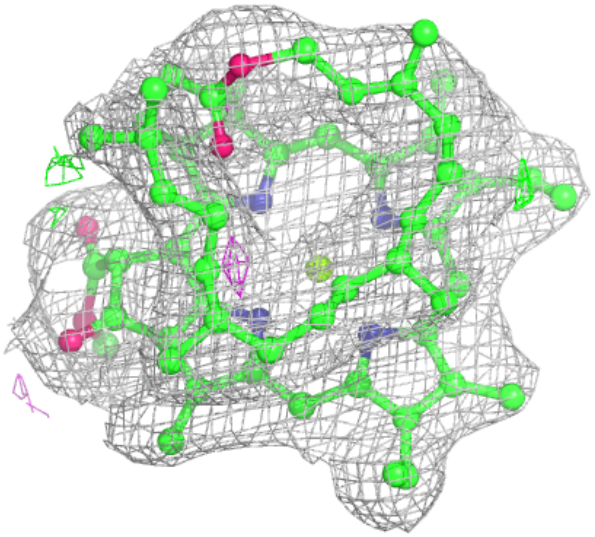
Electron density around CLA h 201:

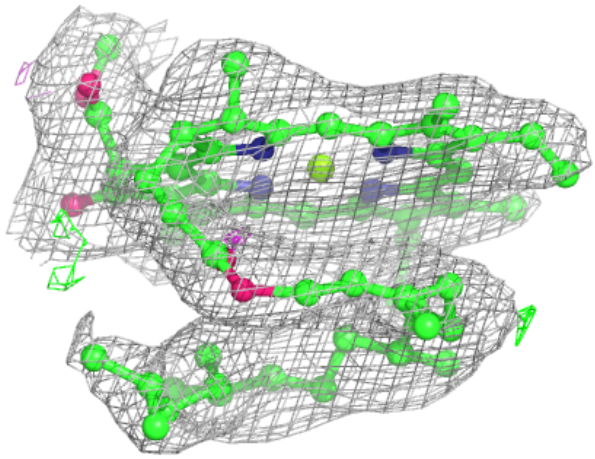
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

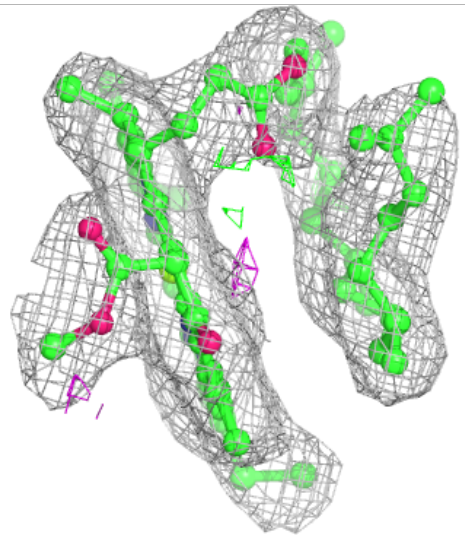


Electron density around CLA h 204:

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

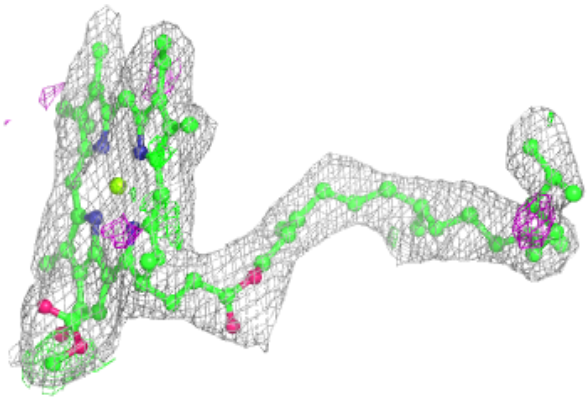


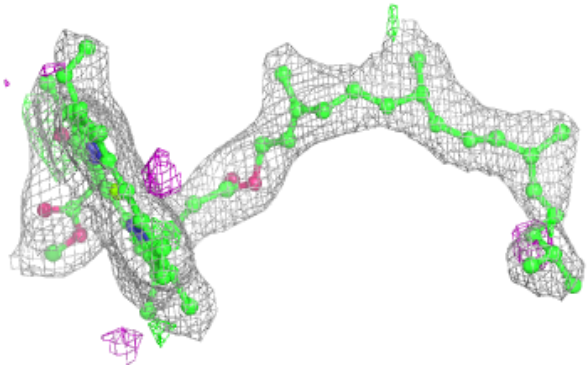


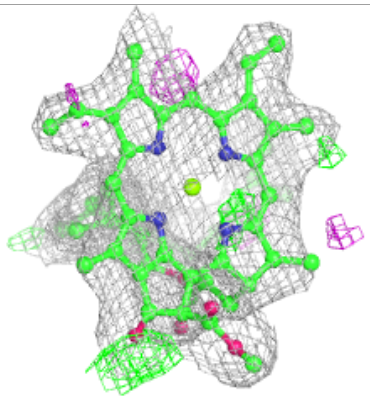


Electron density around CLA h 205:

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

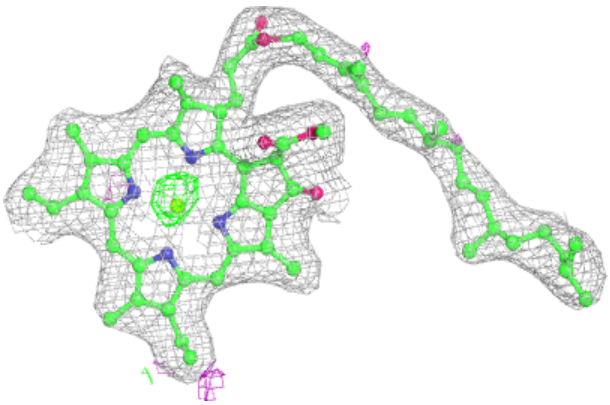


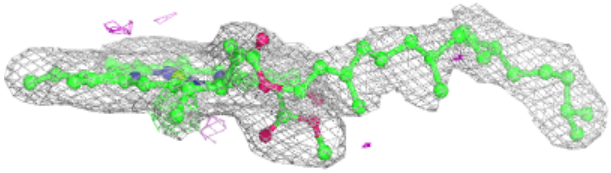


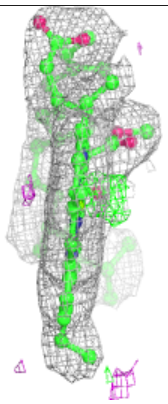


Electron density around CLA h 206:

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

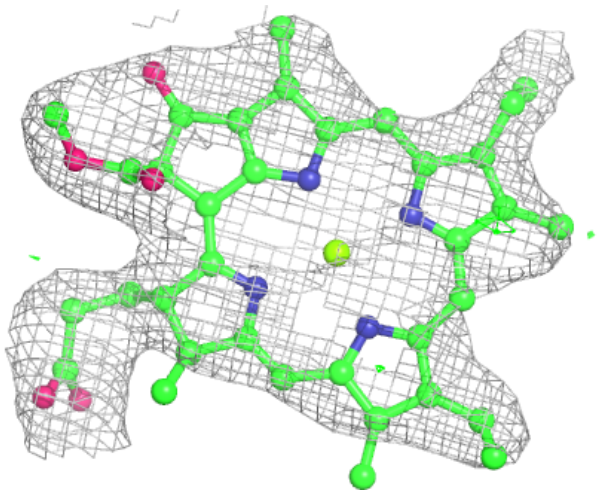


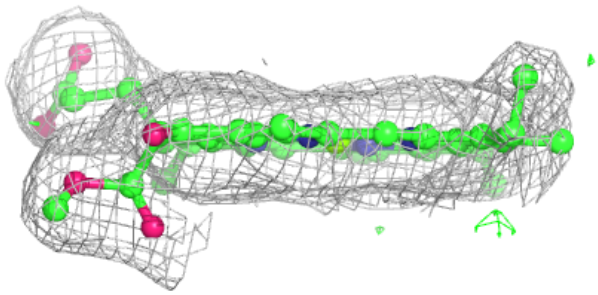




Electron density around CLA j 102:

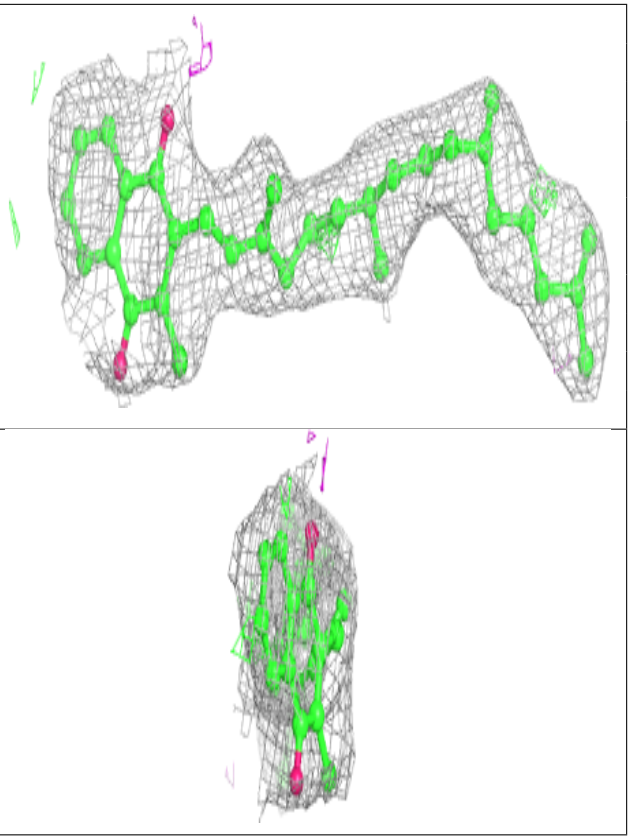
2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)





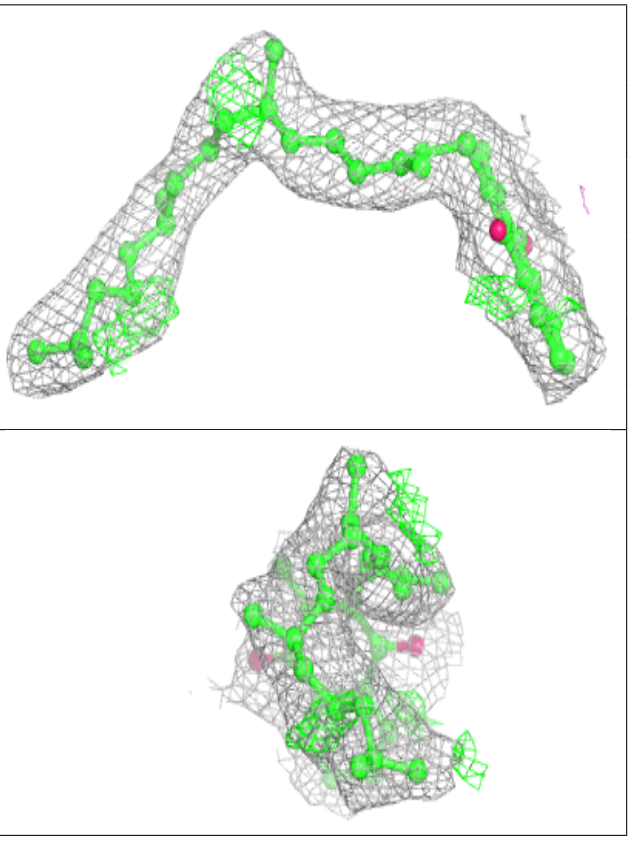
Electron density around PQN A 844:

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



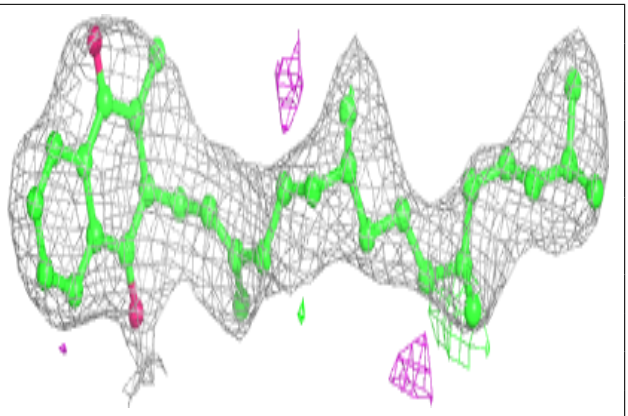
Electron density around PQN B 841:

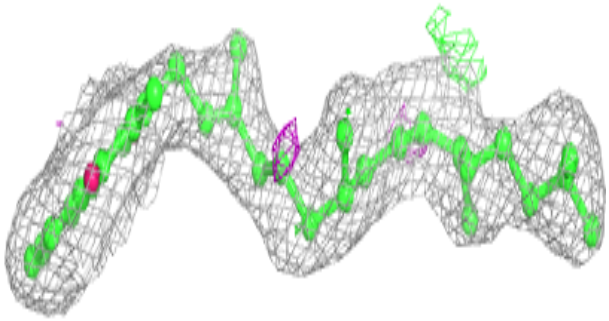
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

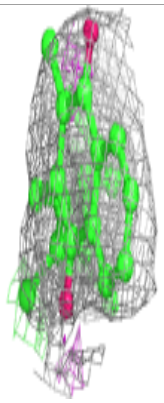


Electron density around PQN G 843:

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

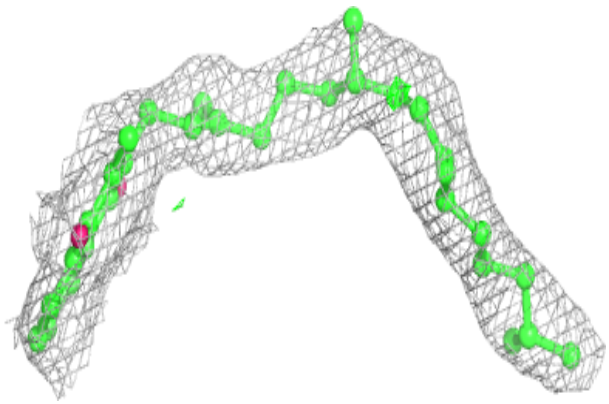


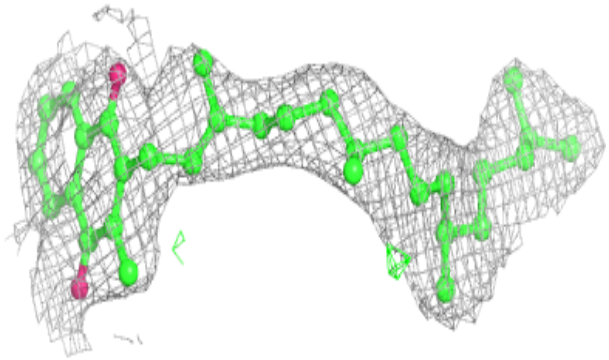


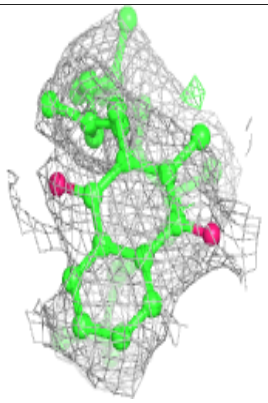


Electron density around PQN H 841:

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

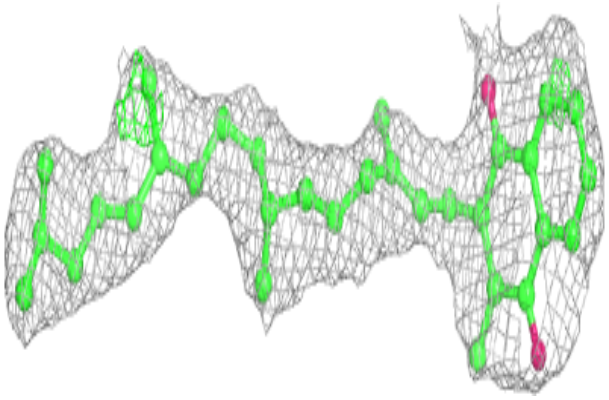


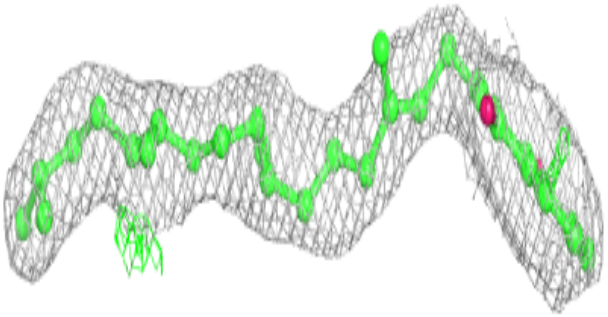


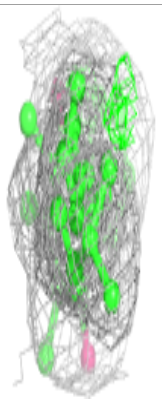


Electron density around PQN Y 842:

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

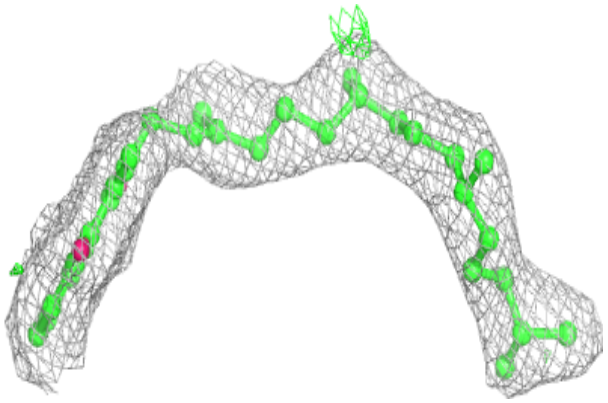


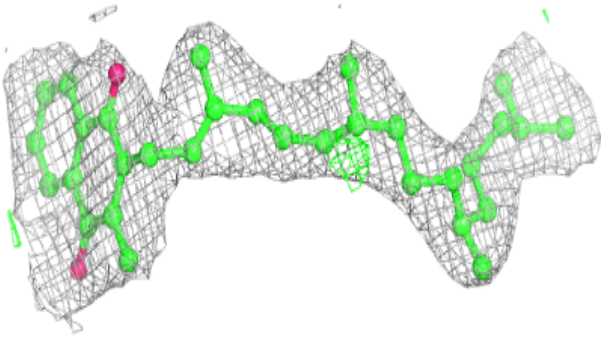


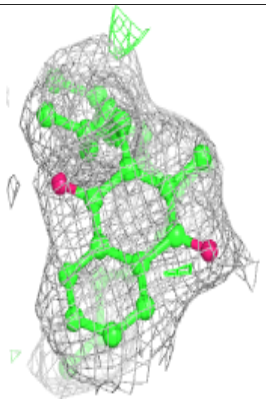


Electron density around PQN Z 842:

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

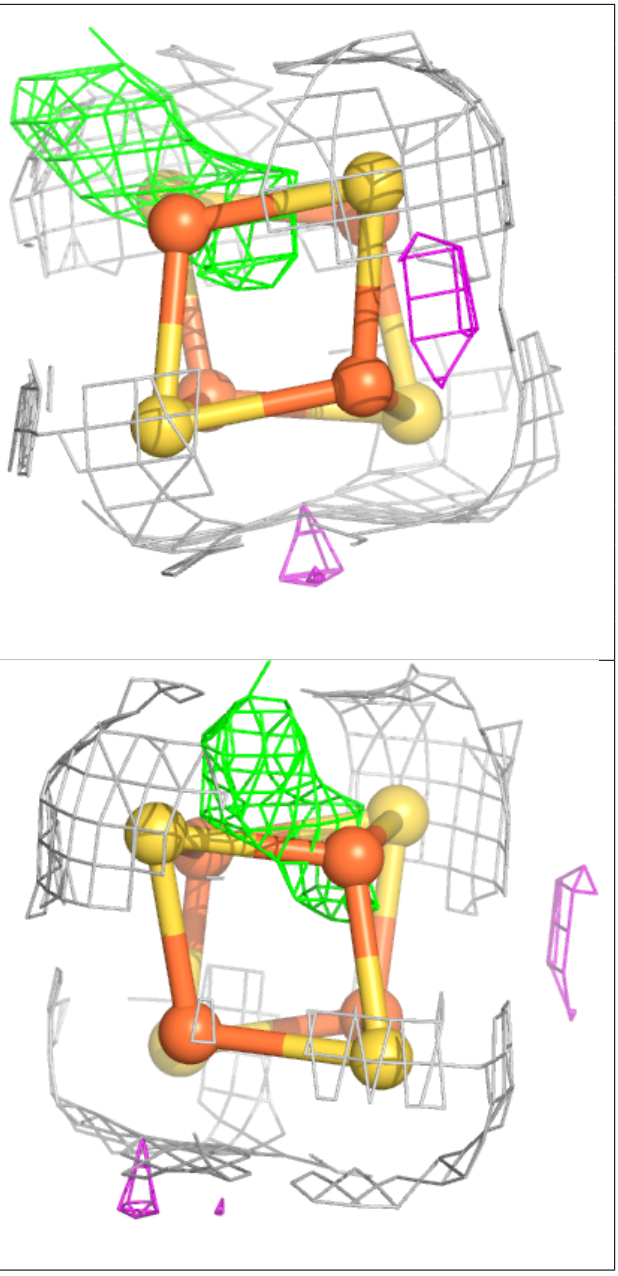






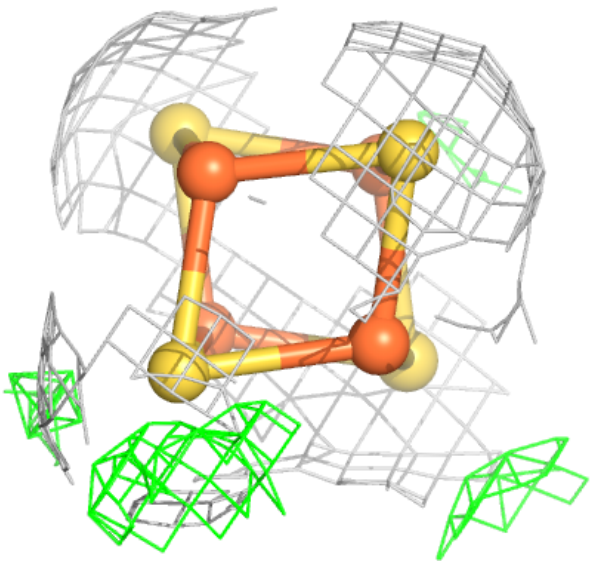
Electron density around SF4 A 845:

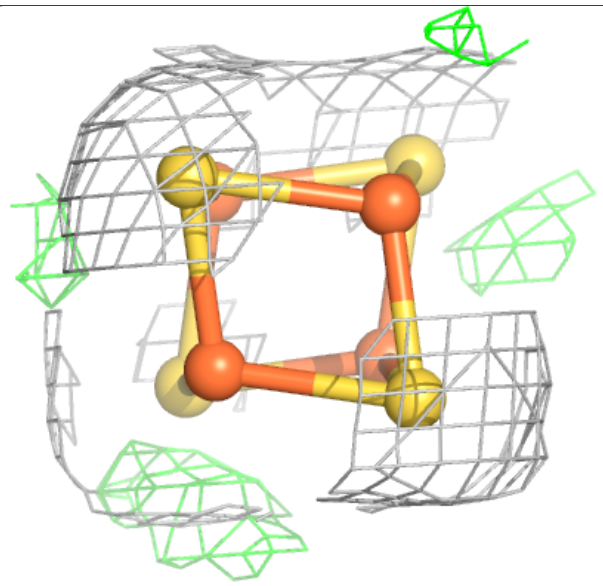
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

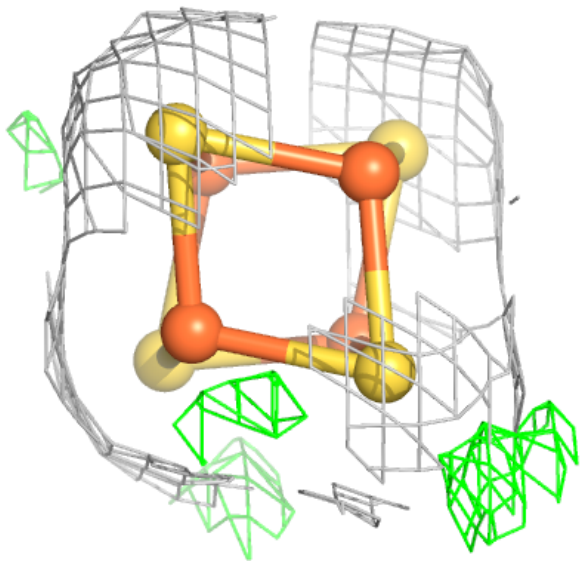


Electron density around SF4 C 101:

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

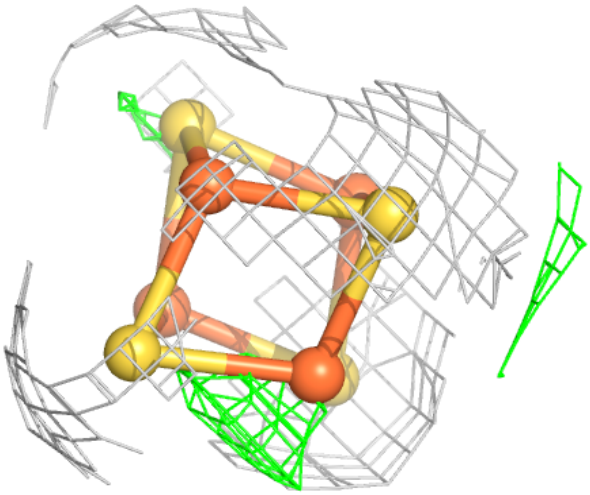


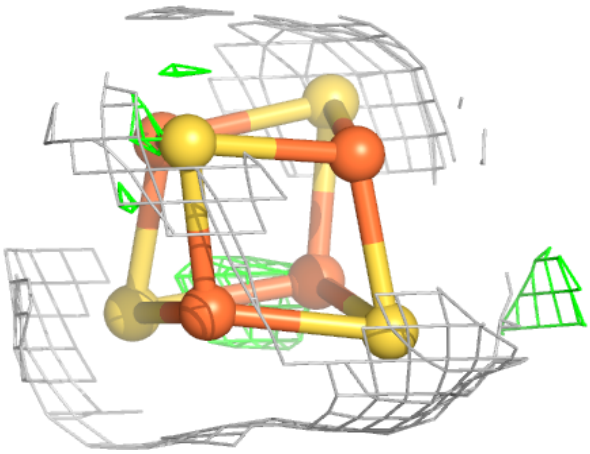


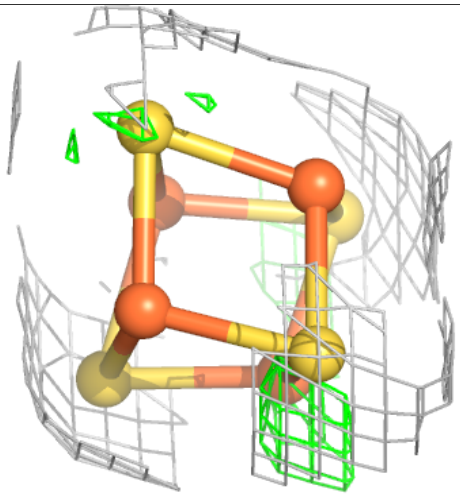


Electron density around SF4 C 102:

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

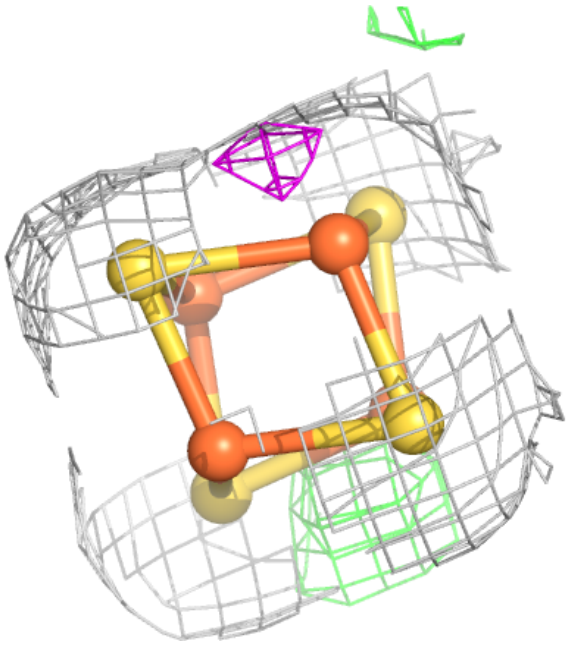


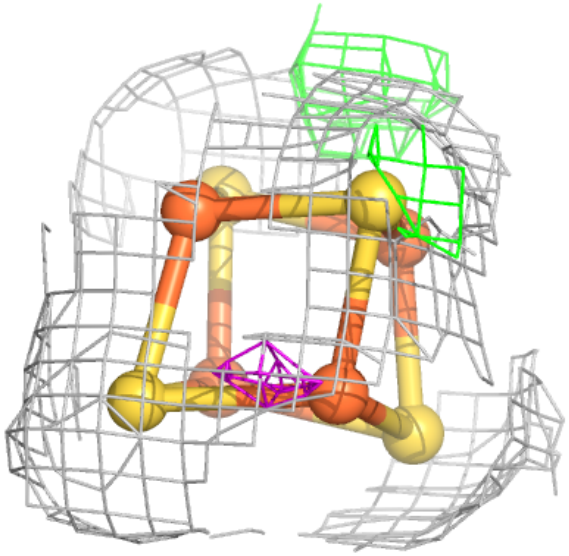


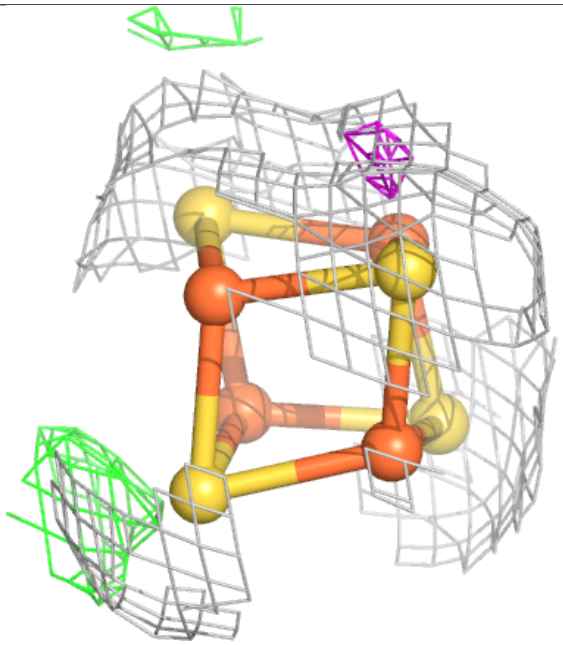


Electron density around SF4 G 844:

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

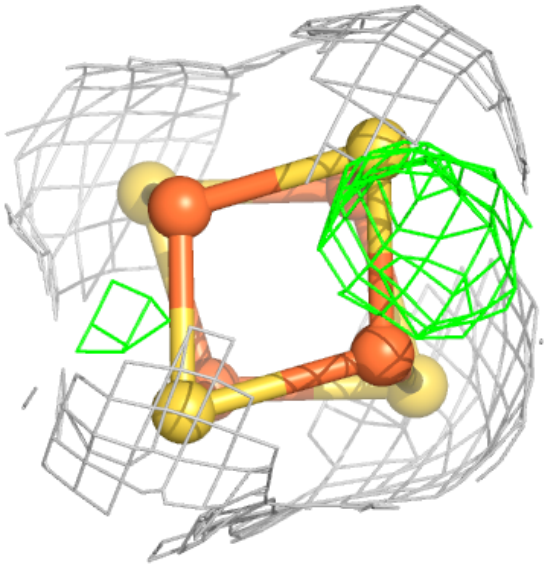


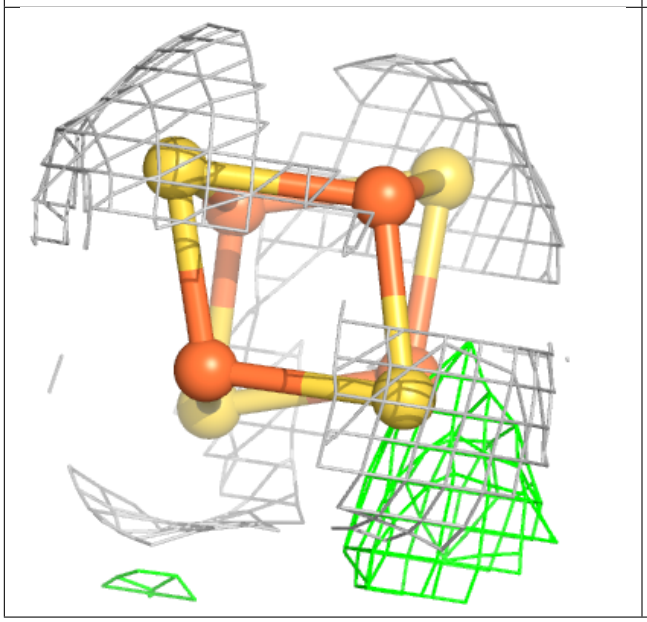


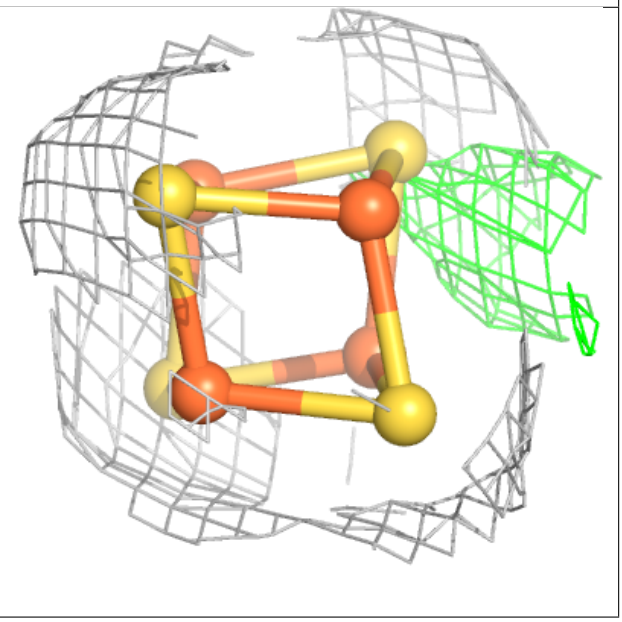


Electron density around SF4 N 101:

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

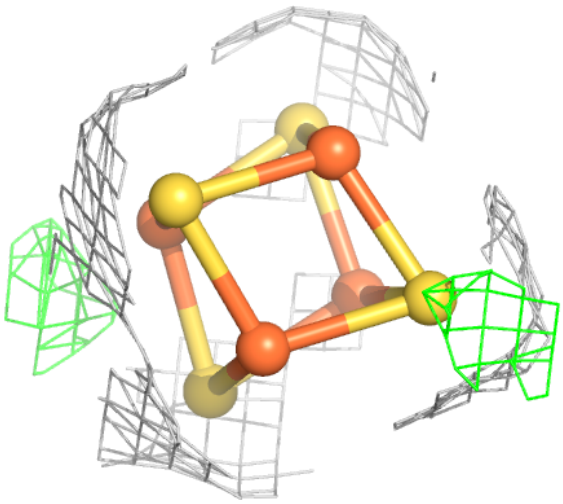


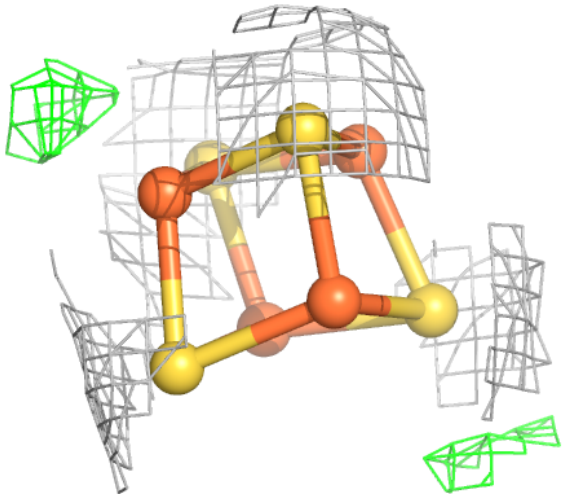


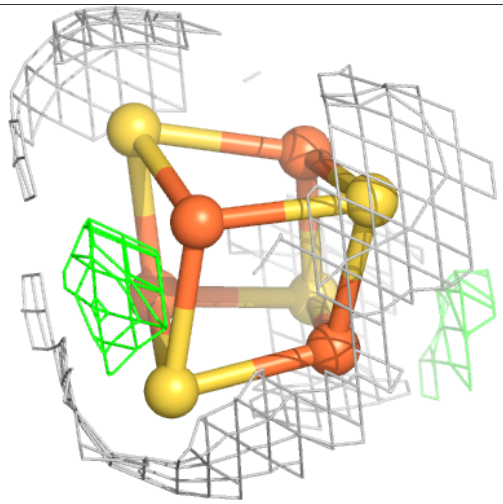


Electron density around SF4 N 102:

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

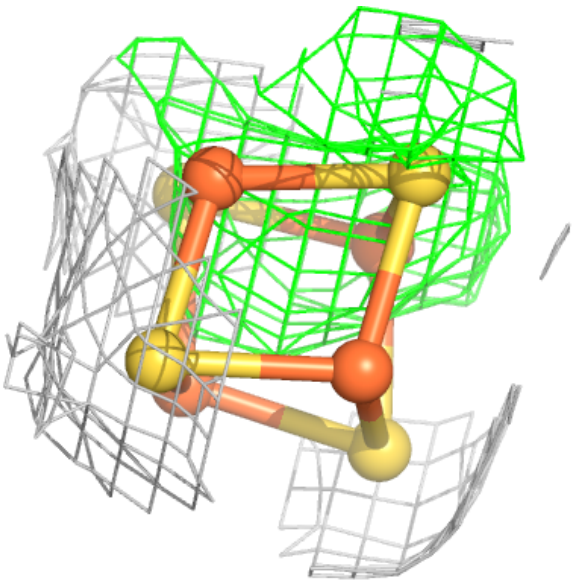


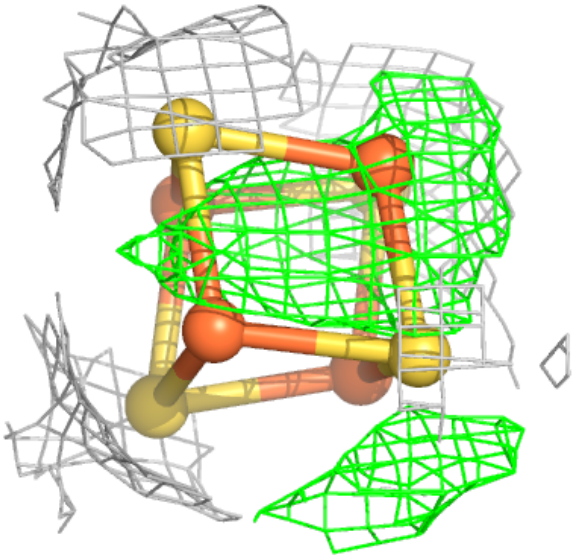


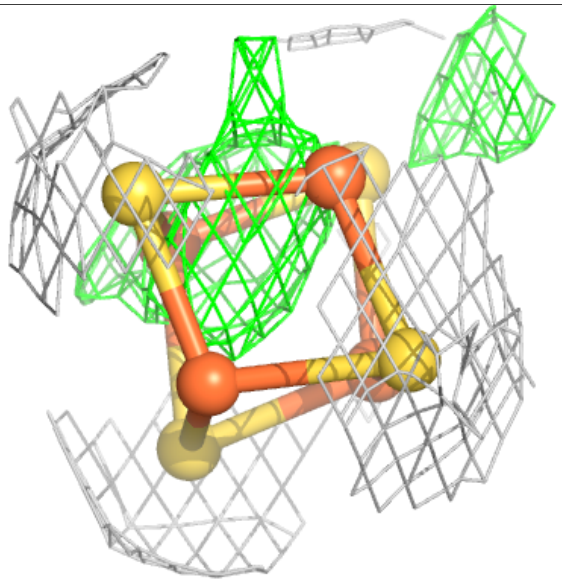


Electron density around SF4 Y 843:

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

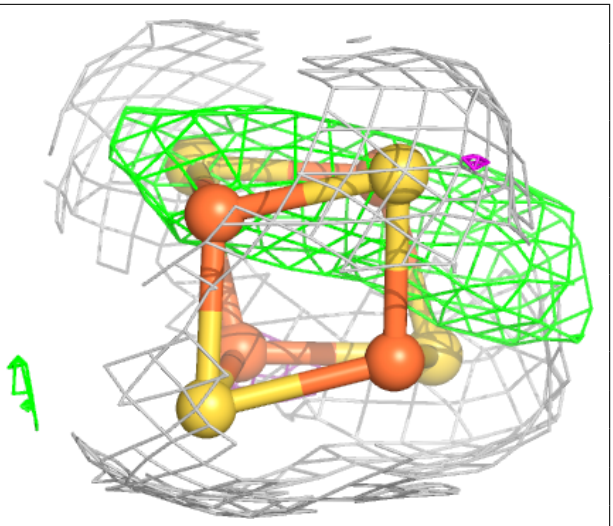


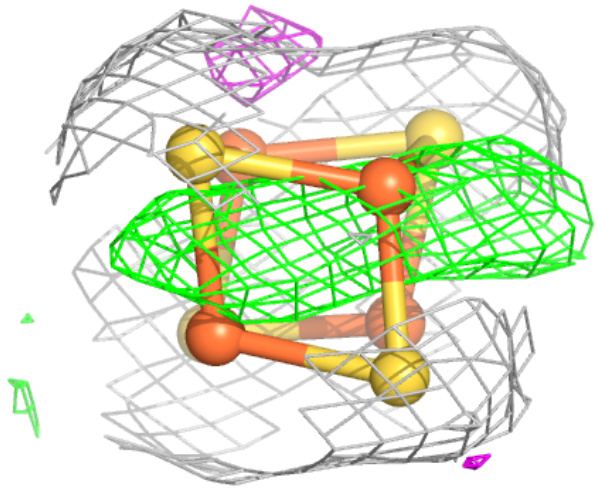


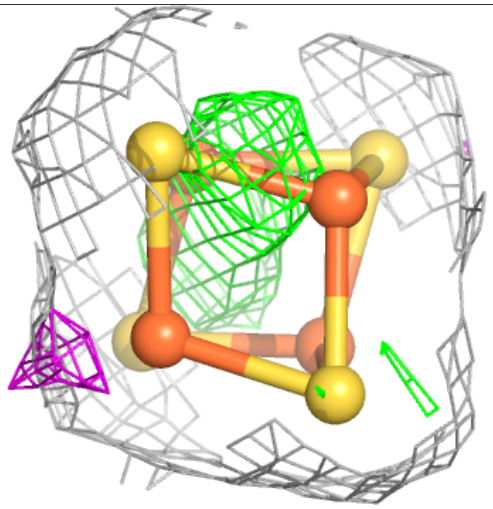


Electron density around SF4 a 101:

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

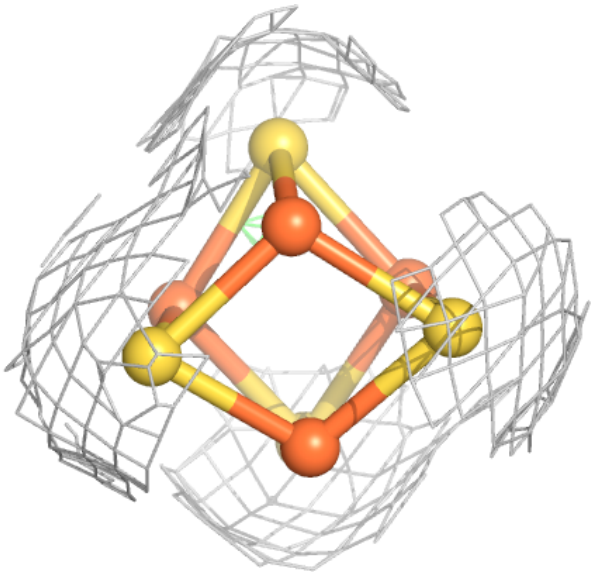


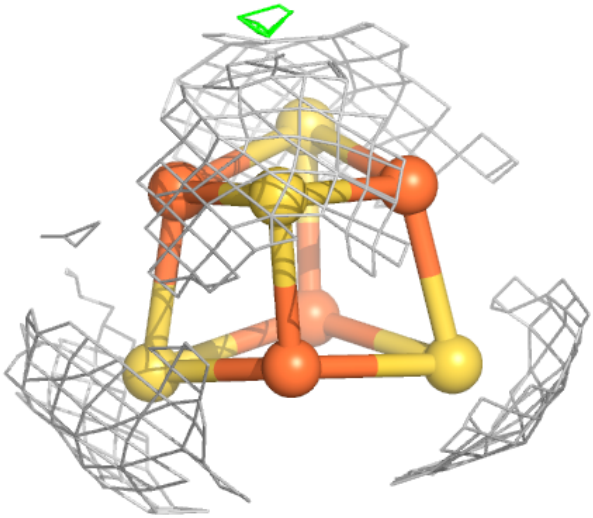


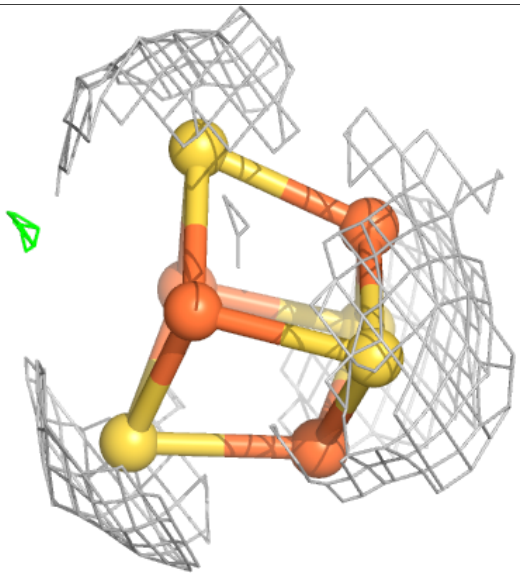


Electron density around SF4 a 102:

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

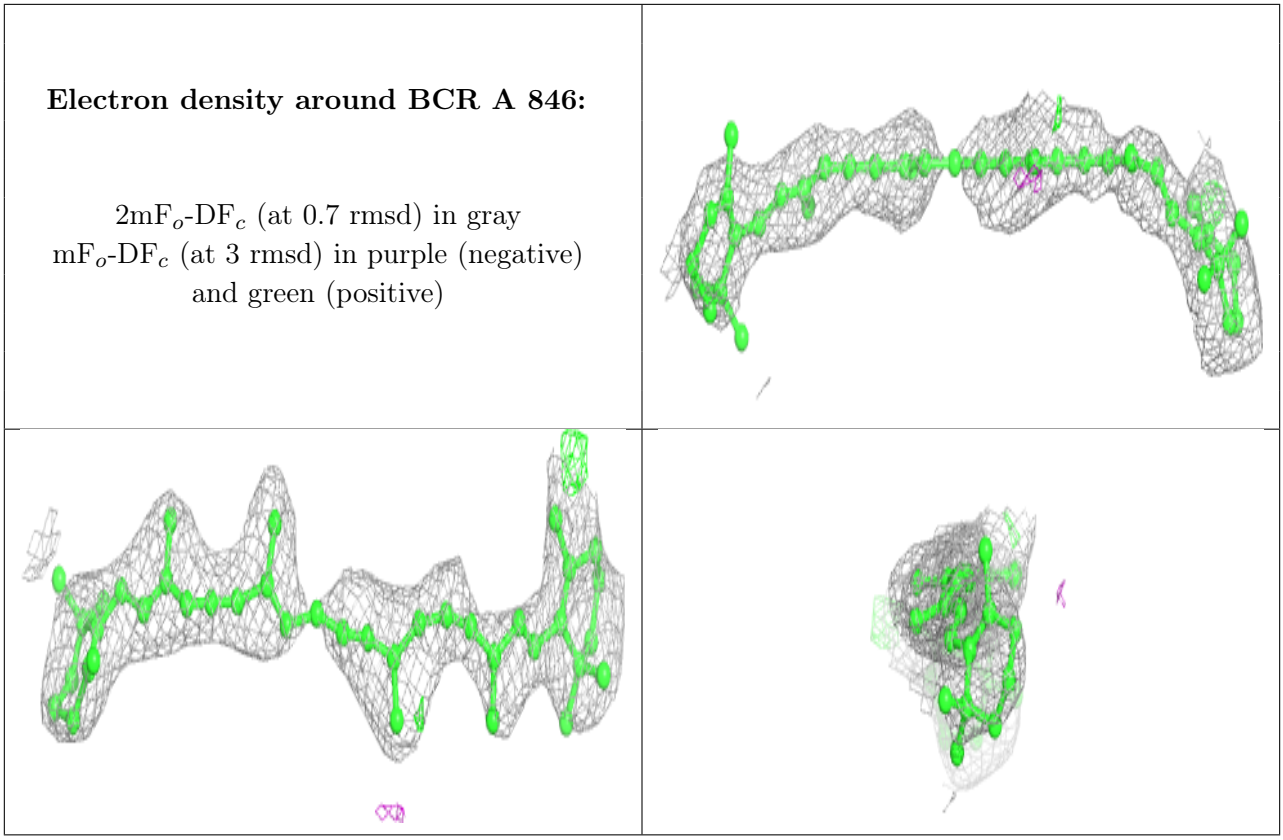






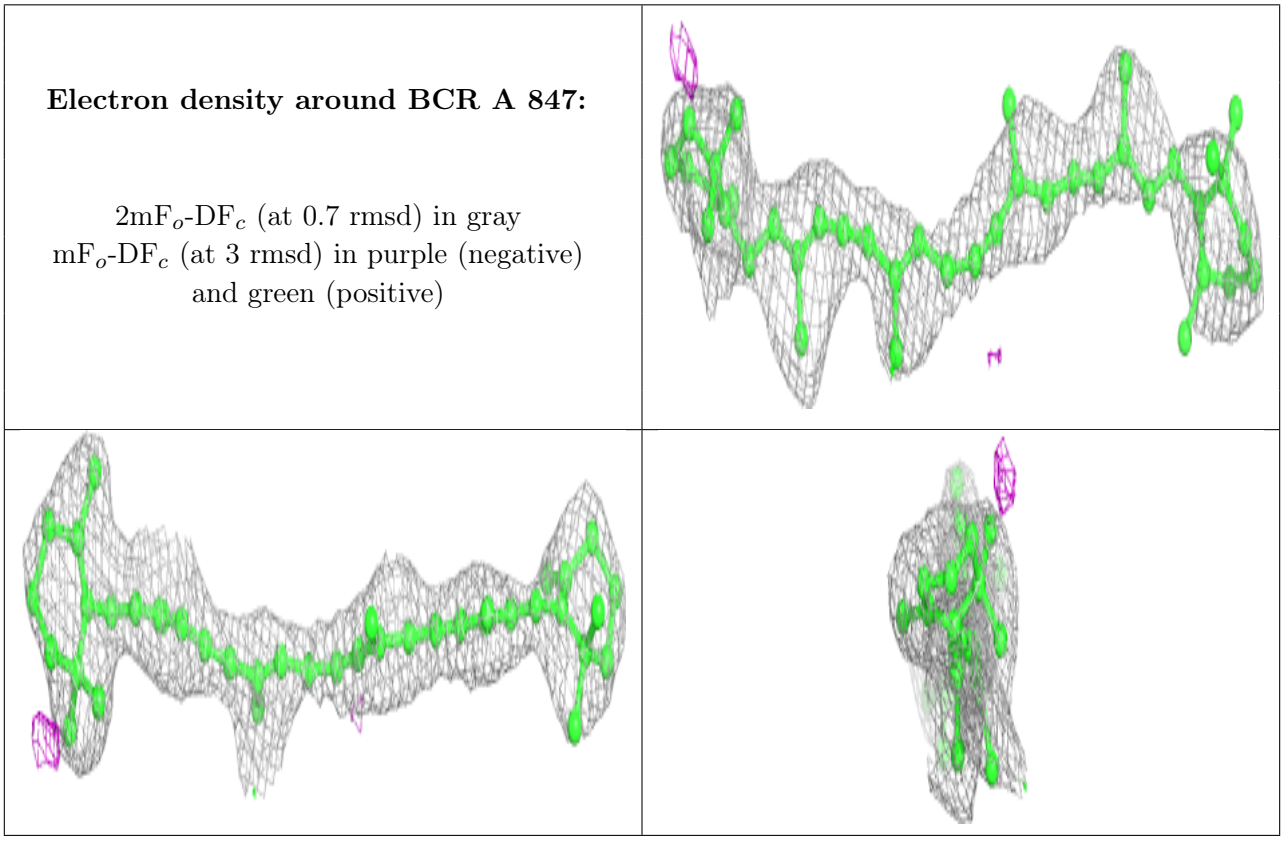
Electron density around BCR A 846:

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



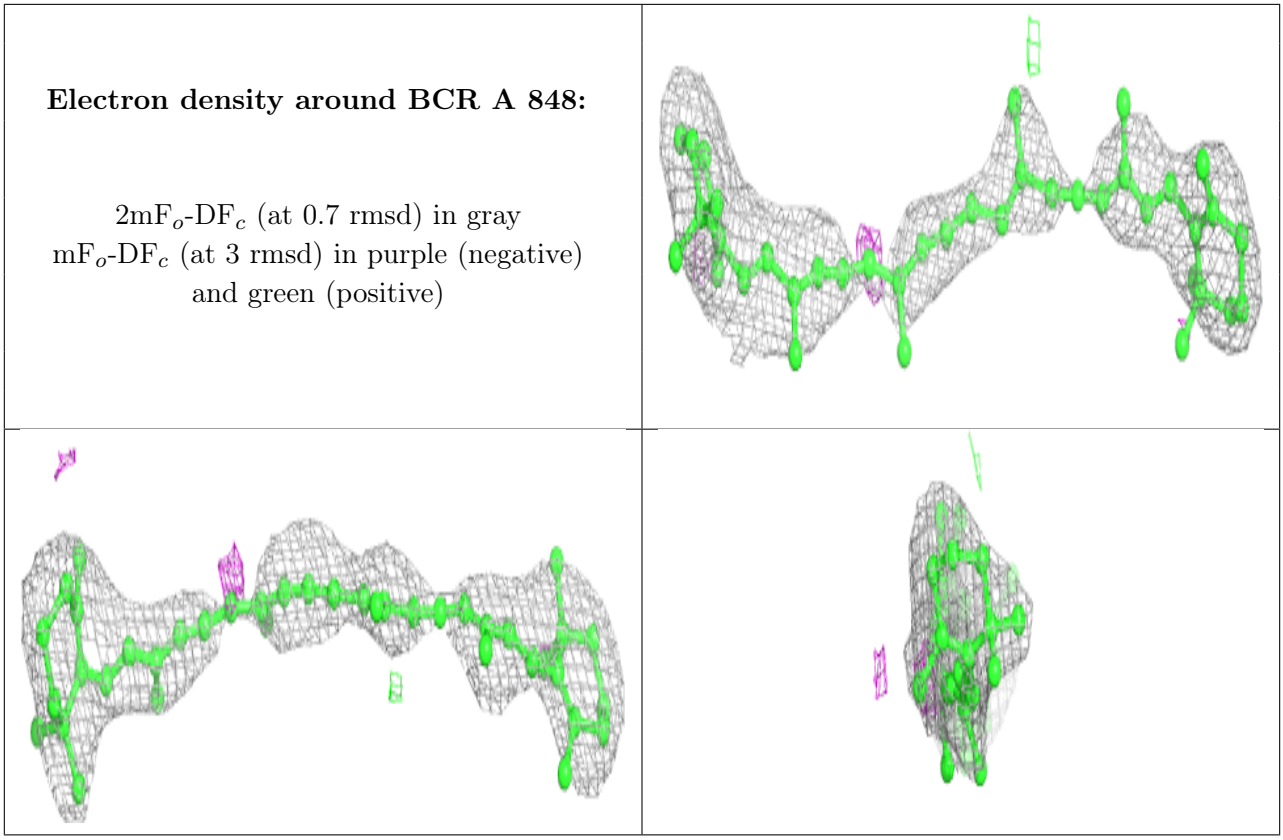
Electron density around BCR A 847:

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



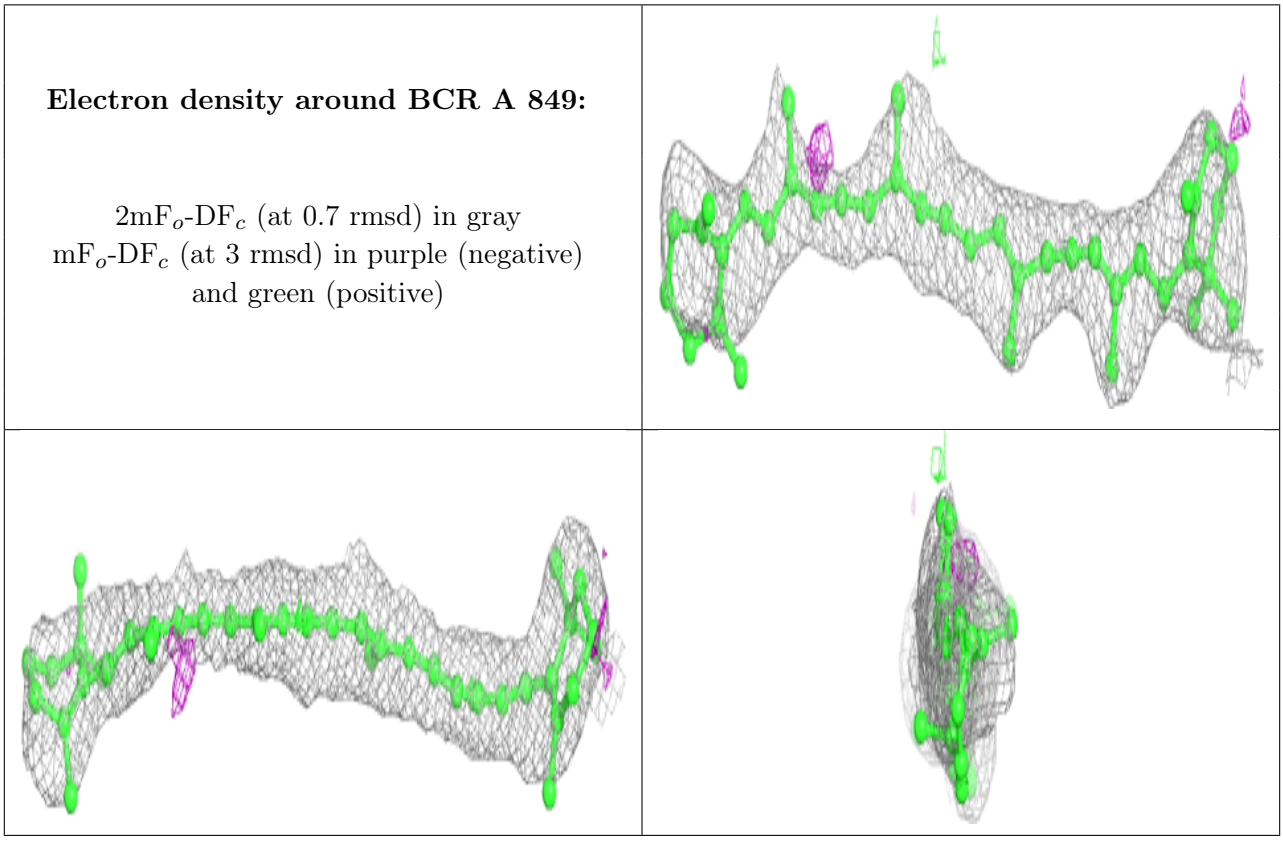
Electron density around BCR A 848:

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



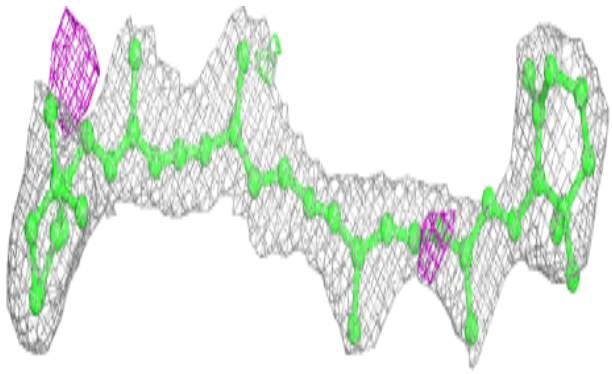
Electron density around BCR A 849:

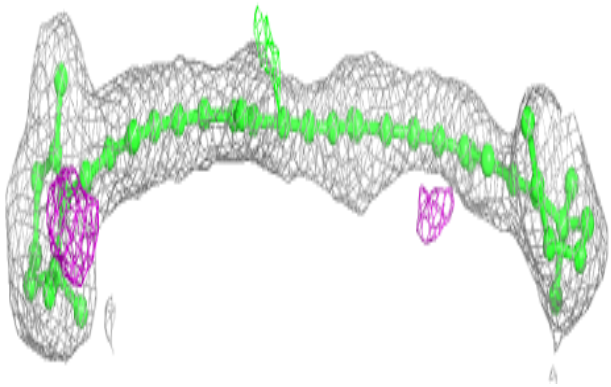
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

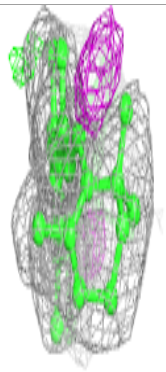


Electron density around BCR A 850:

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

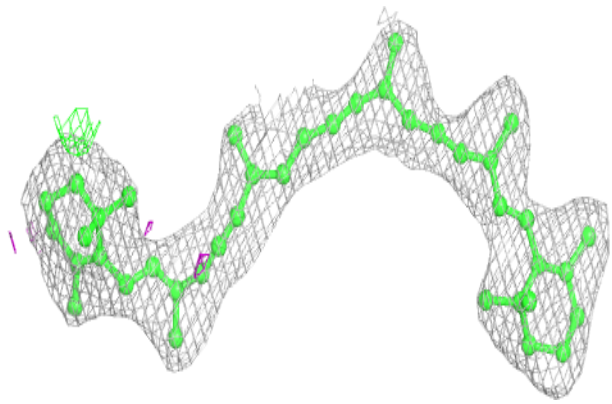


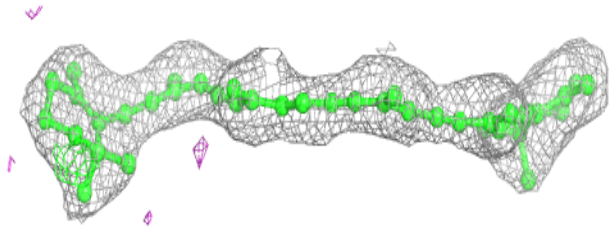


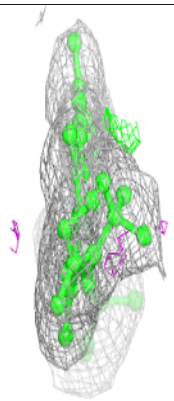


Electron density around BCR A 851:

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

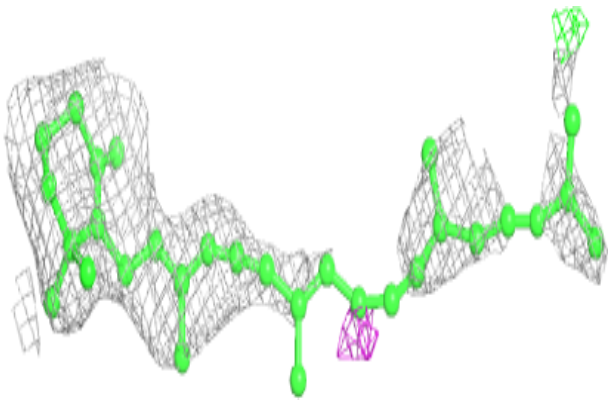


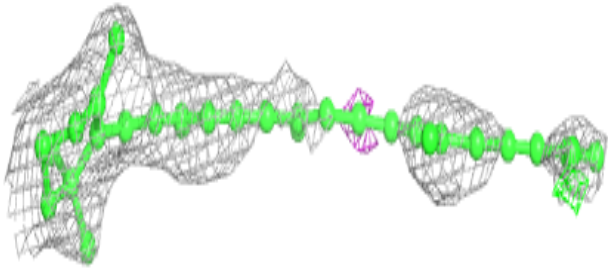


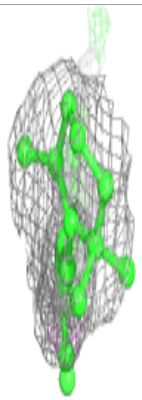


Electron density around BCR B 842:

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

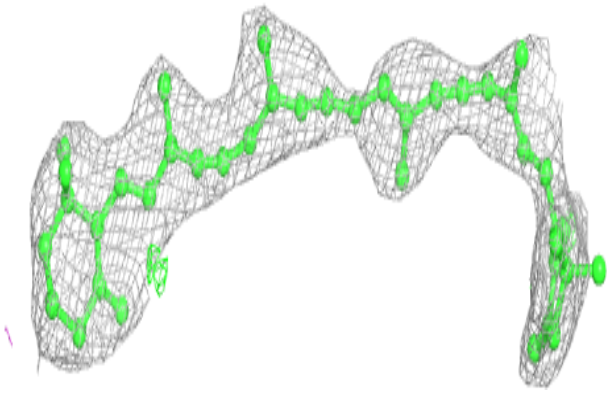


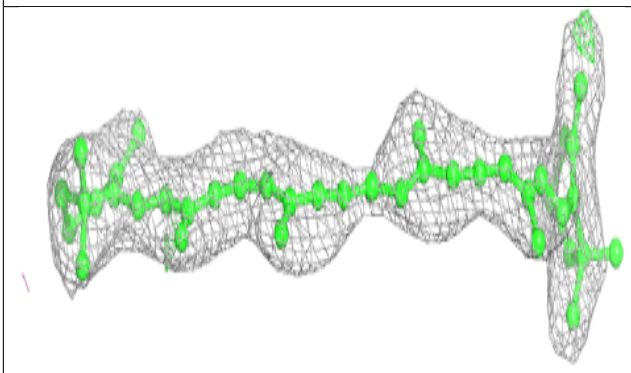


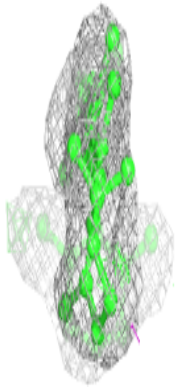


Electron density around BCR B 843:

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

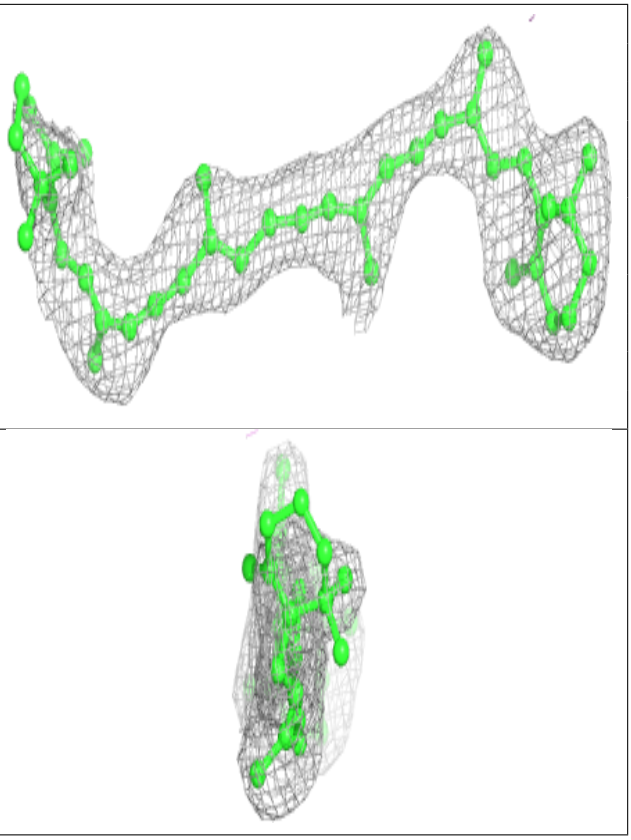


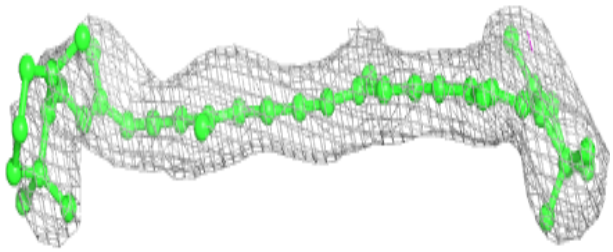




Electron density around BCR B 844:

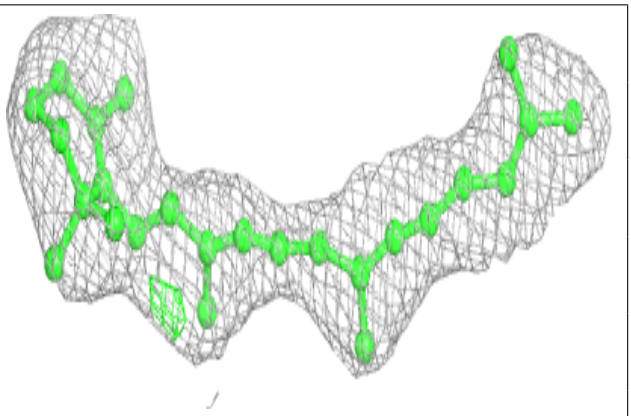
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

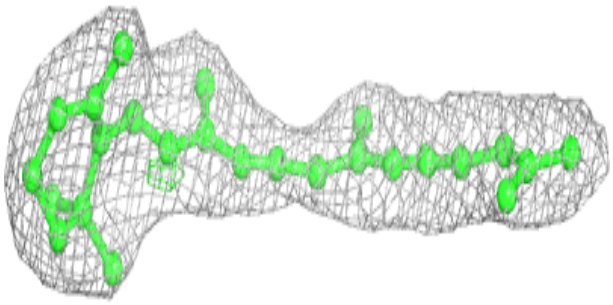


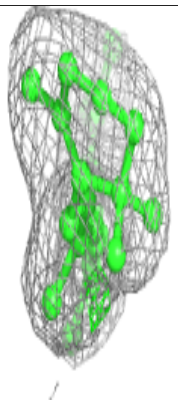


Electron density around BCR B 845:

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

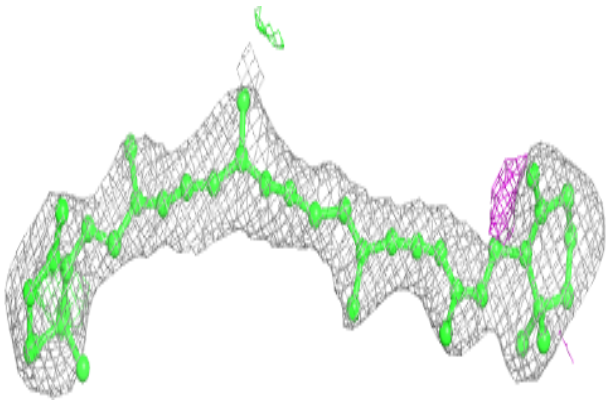


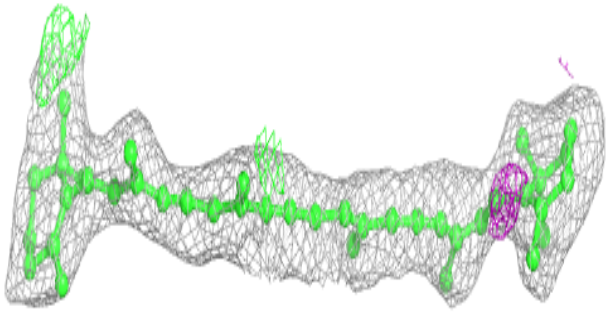


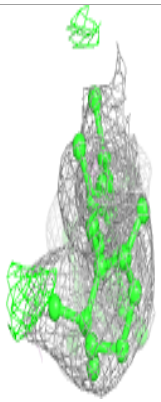


Electron density around BCR B 846:

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

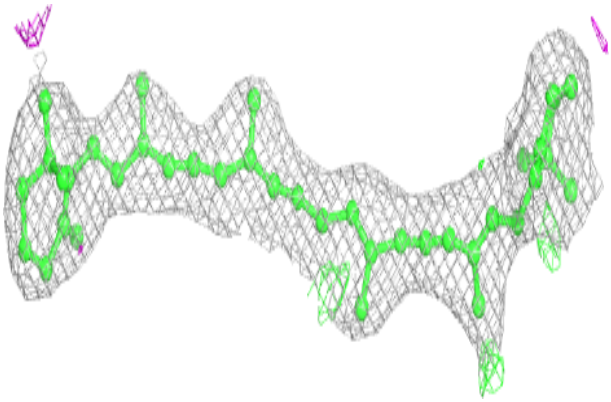


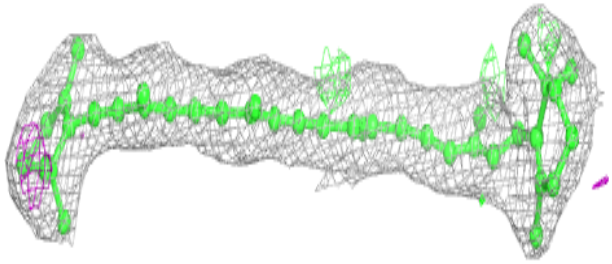


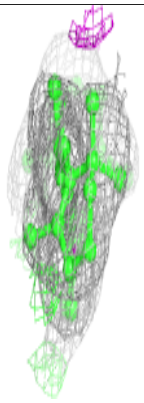


Electron density around BCR B 847:

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

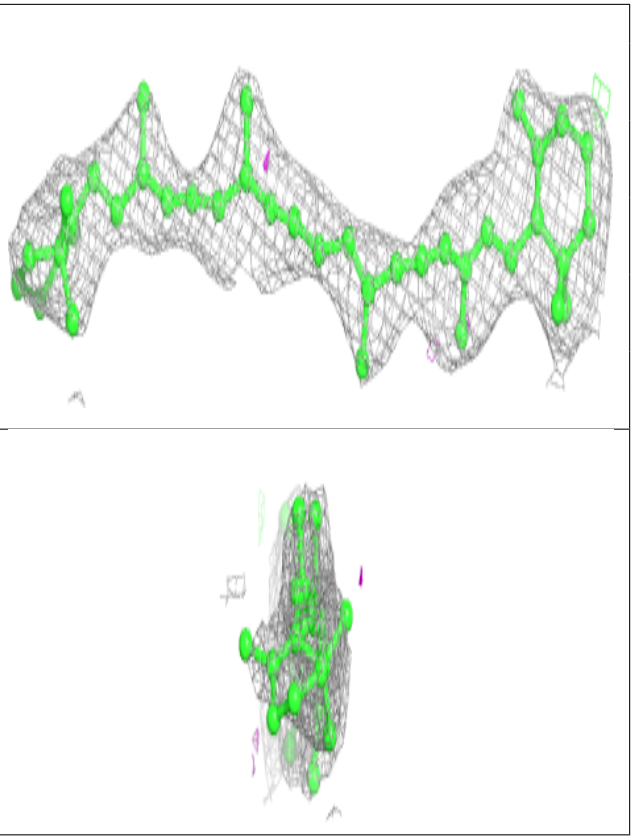






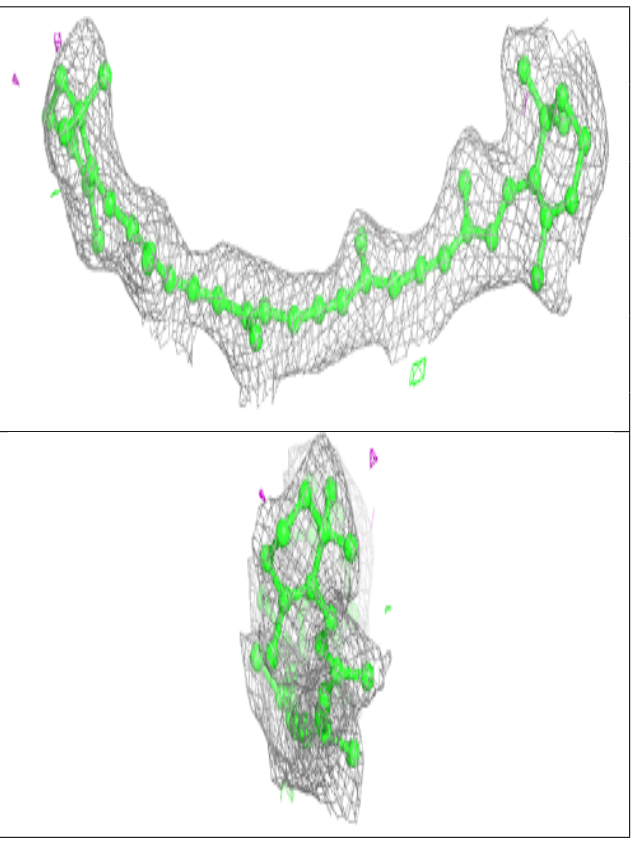
Electron density around BCR B 850:

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



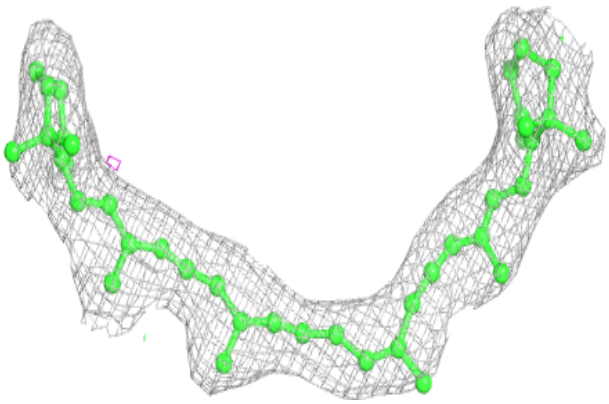
Electron density around BCR F 201:

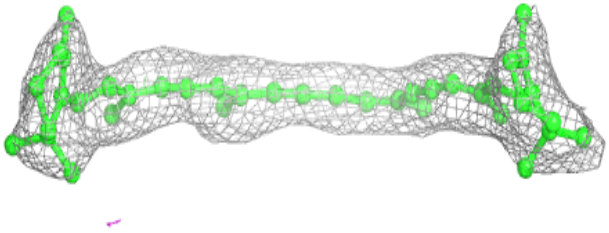
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

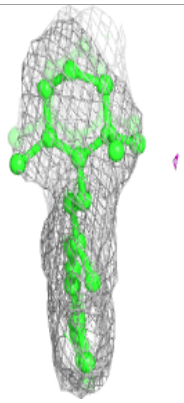


Electron density around BCR F 203:

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

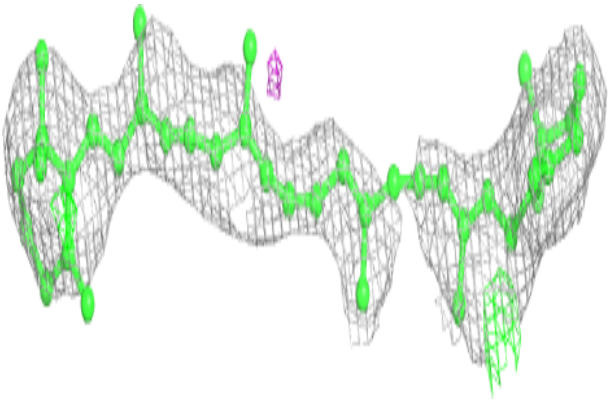


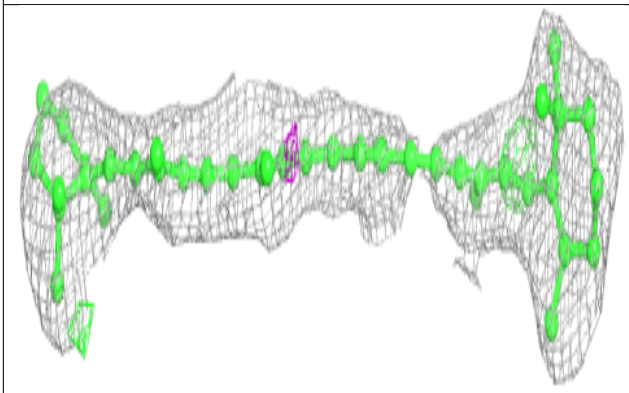


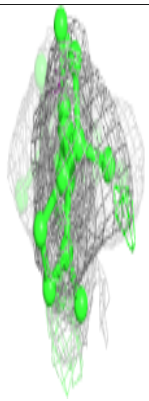


Electron density around BCR G 845:

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

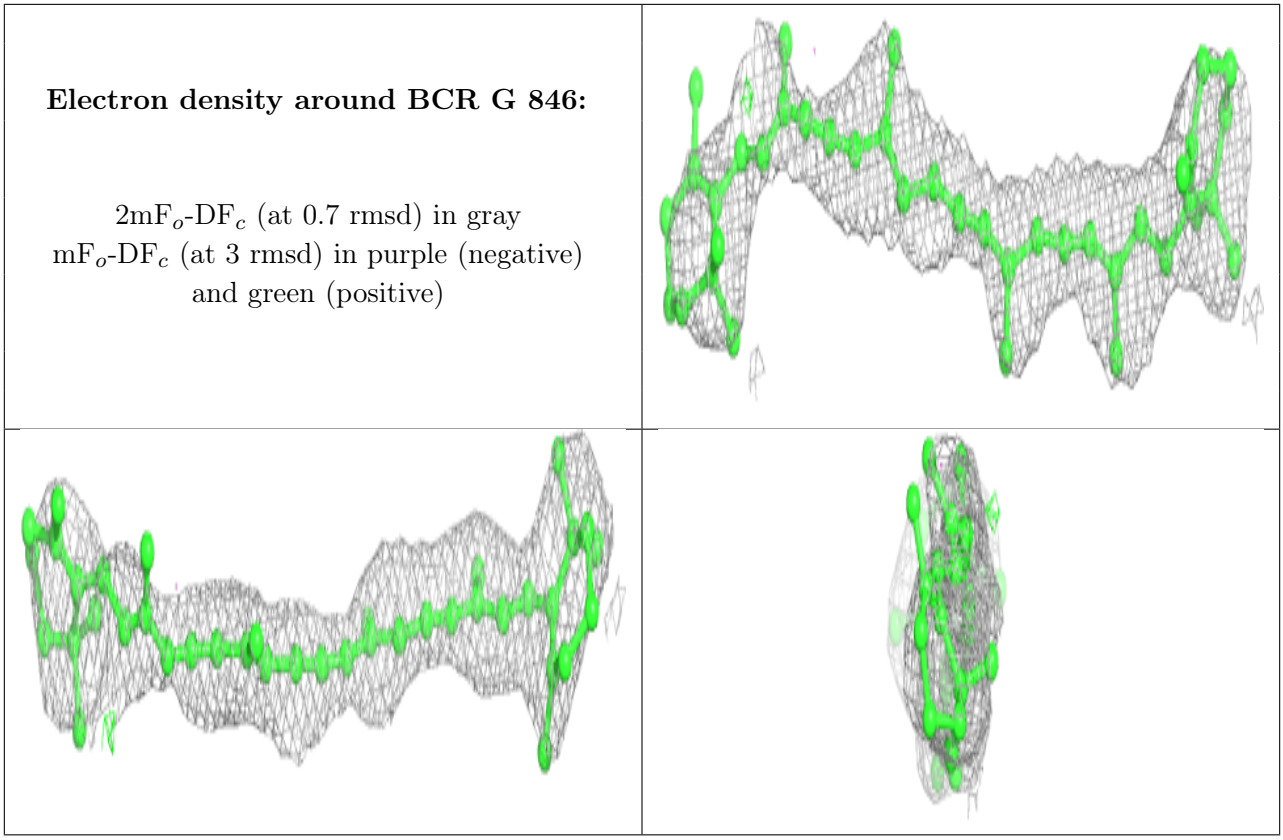






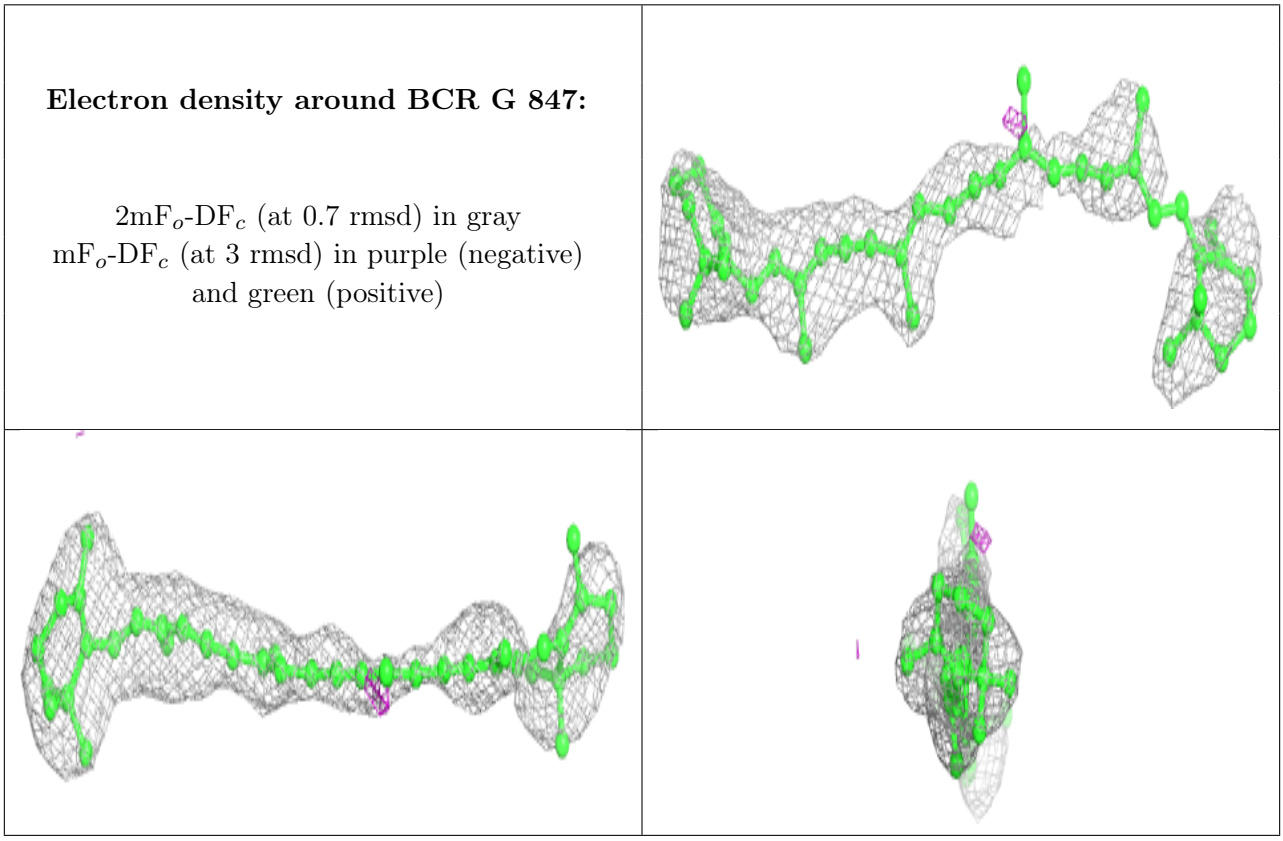
Electron density around BCR G 846:

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



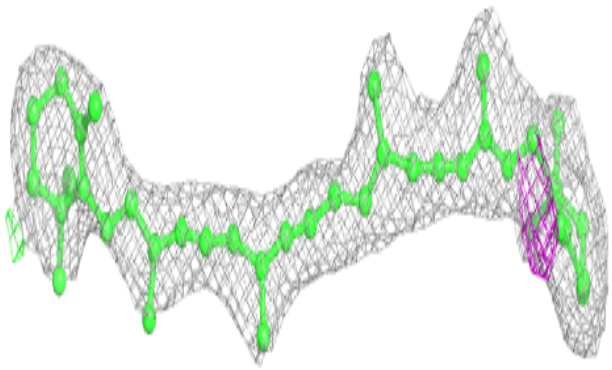
Electron density around BCR G 847:

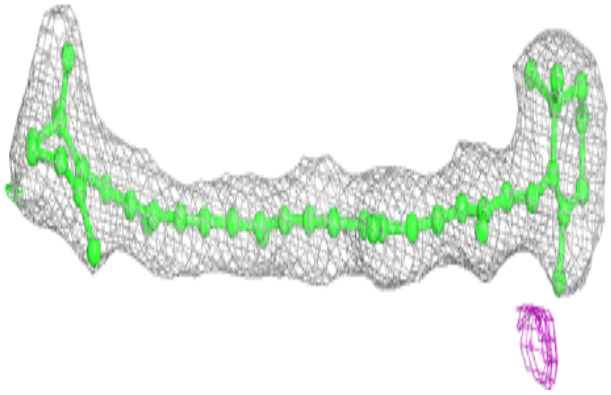
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

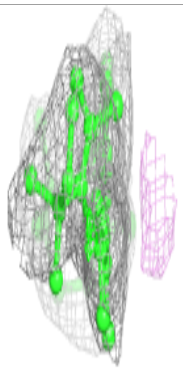


Electron density around BCR G 848:

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

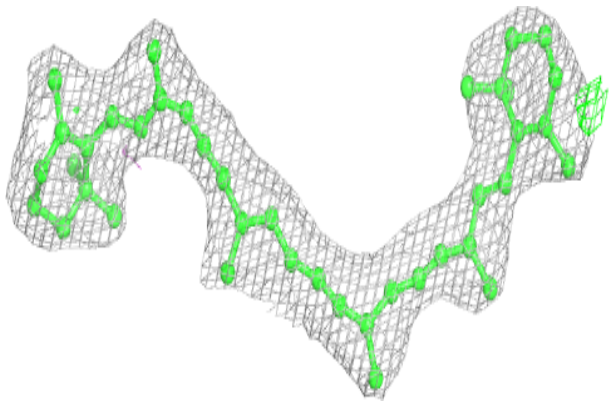


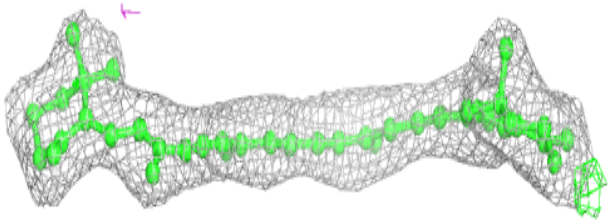


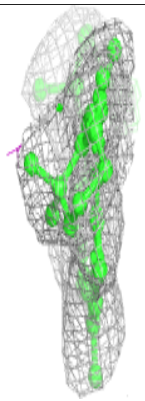


Electron density around BCR G 849:

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

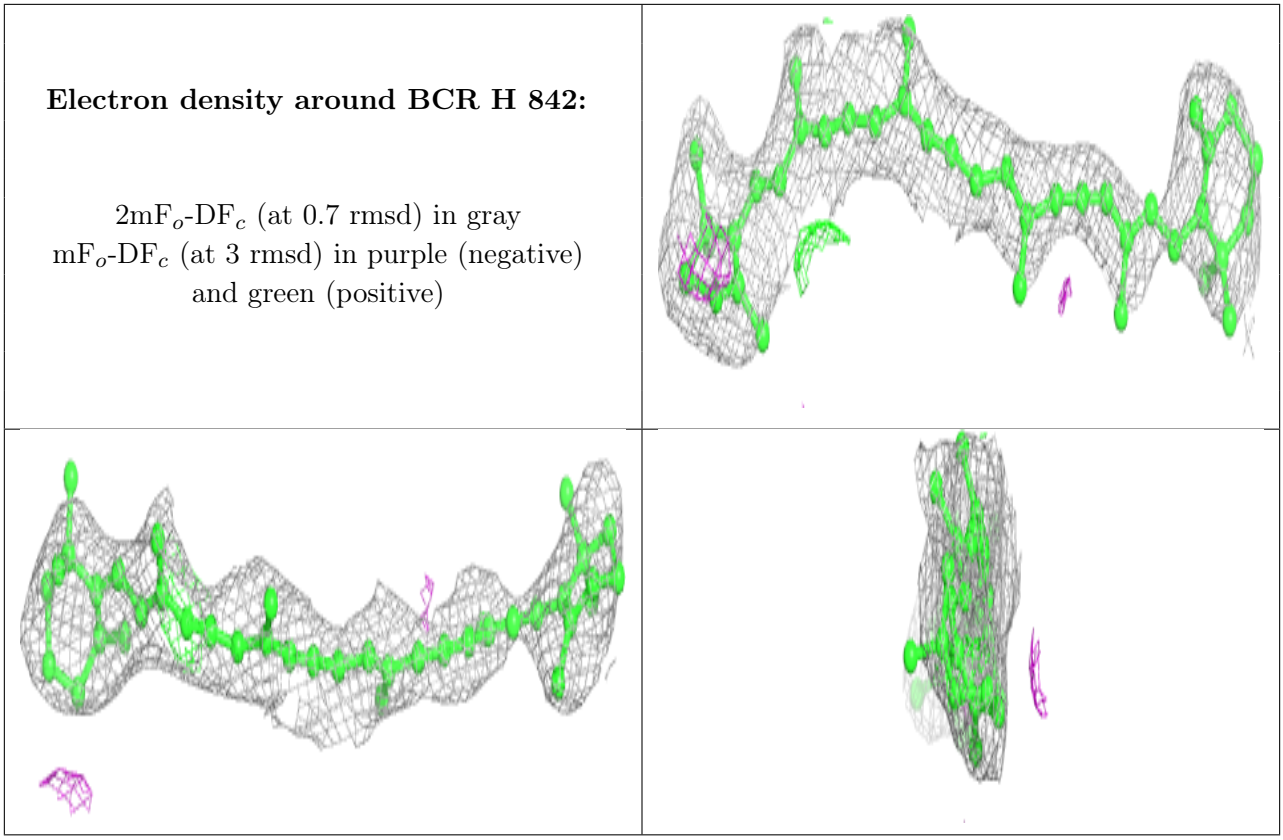






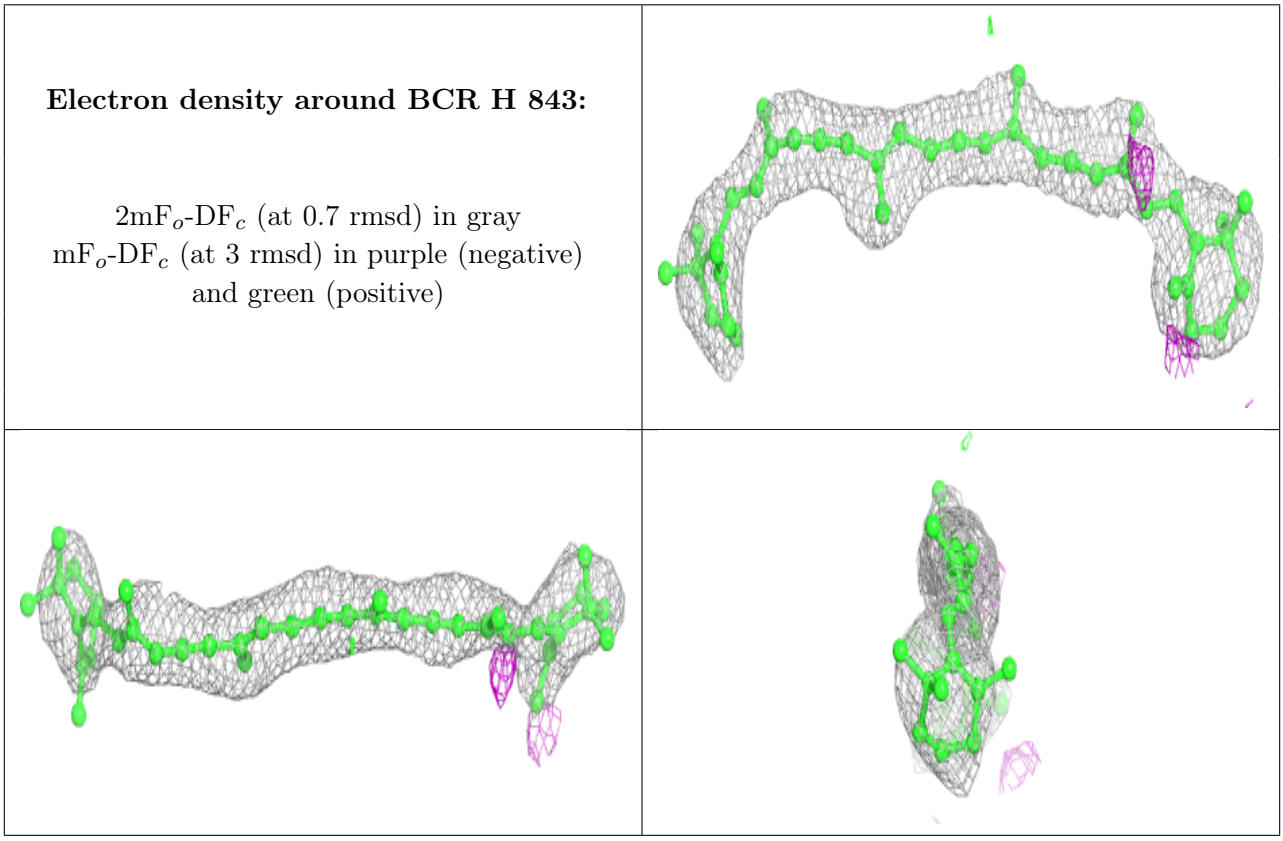
Electron density around BCR H 842:

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



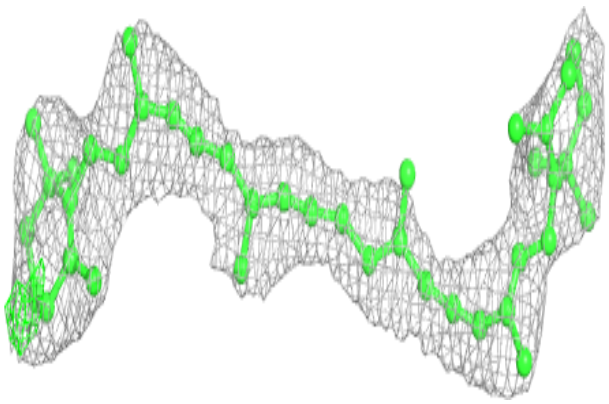
Electron density around BCR H 843:

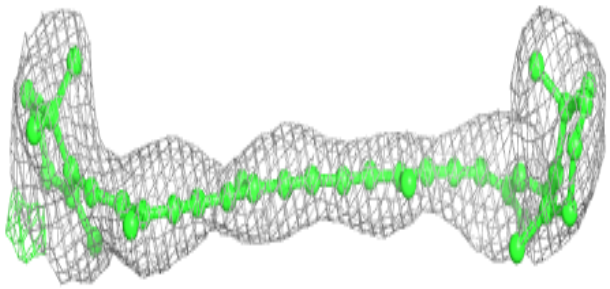
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

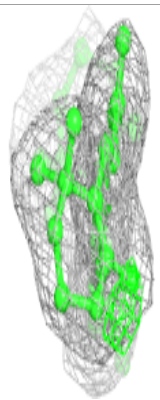


Electron density around BCR H 844:

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

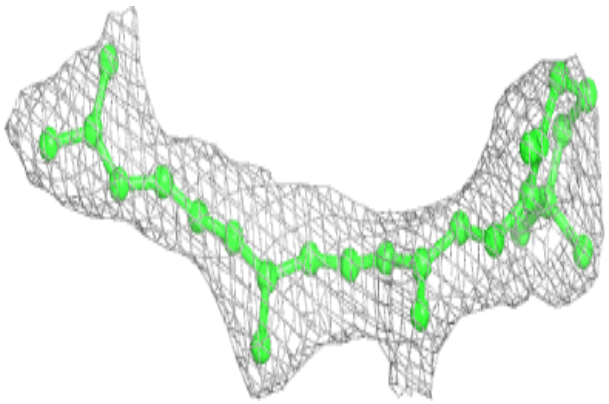


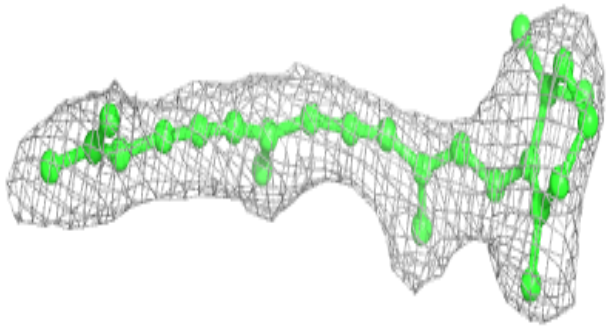


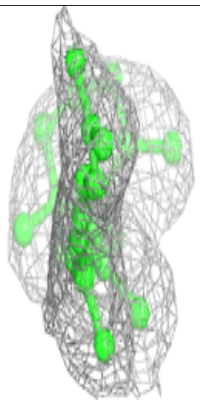


Electron density around BCR H 845:

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

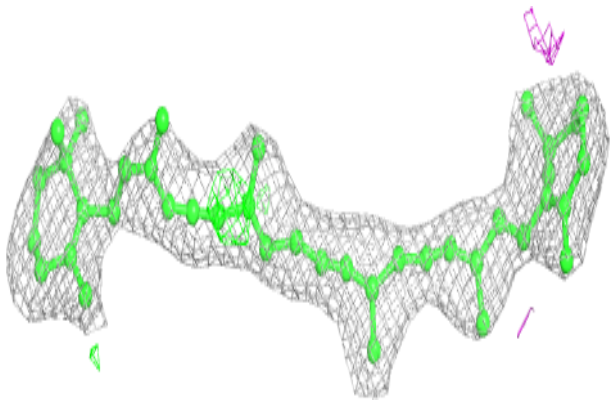


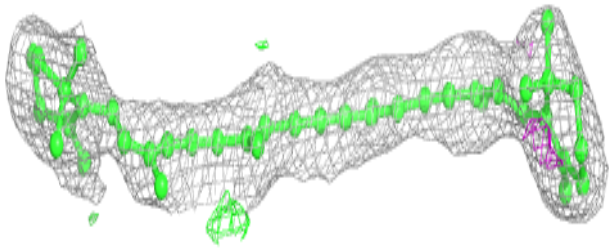


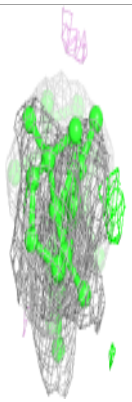


Electron density around BCR H 846:

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

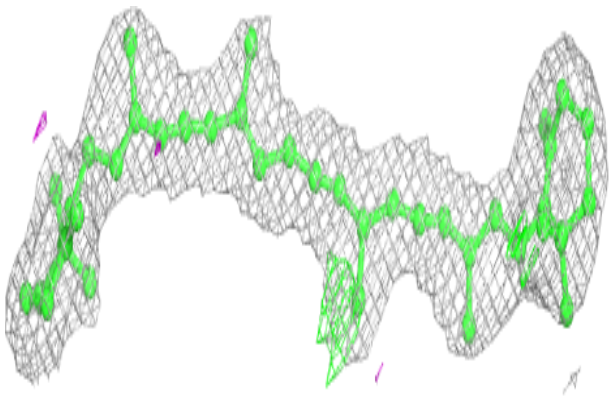


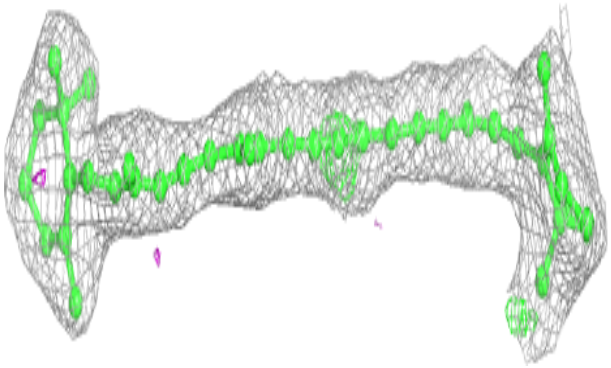


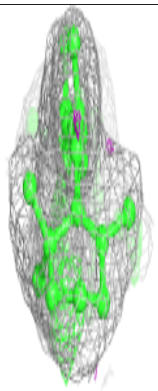


Electron density around BCR H 847:

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

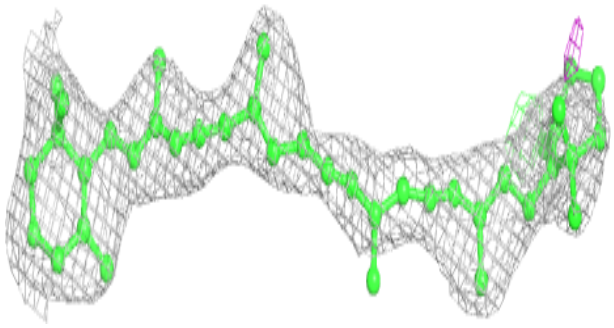


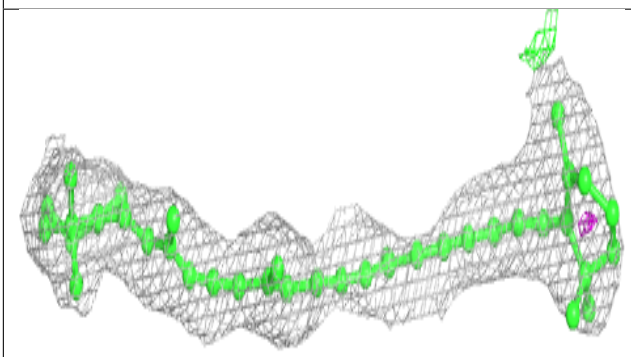


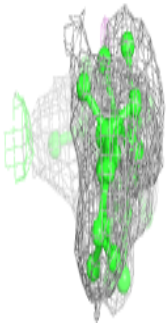


Electron density around BCR H 850:

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

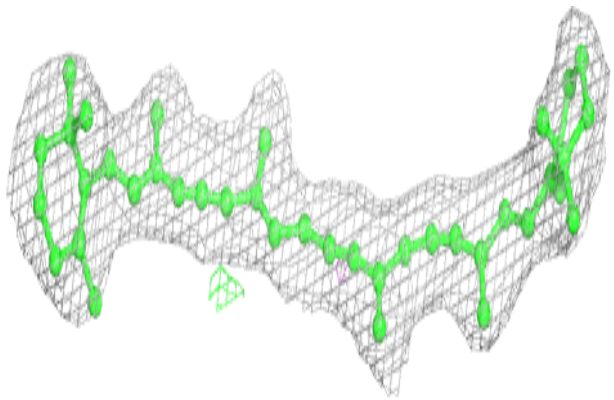


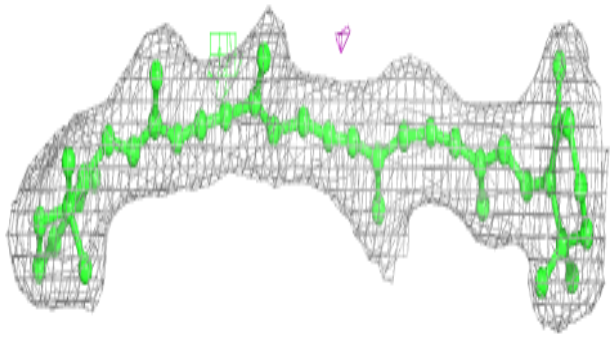


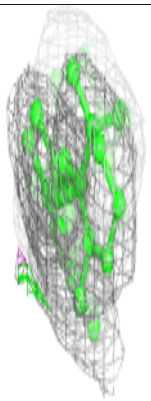


Electron density around BCR I 101:

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

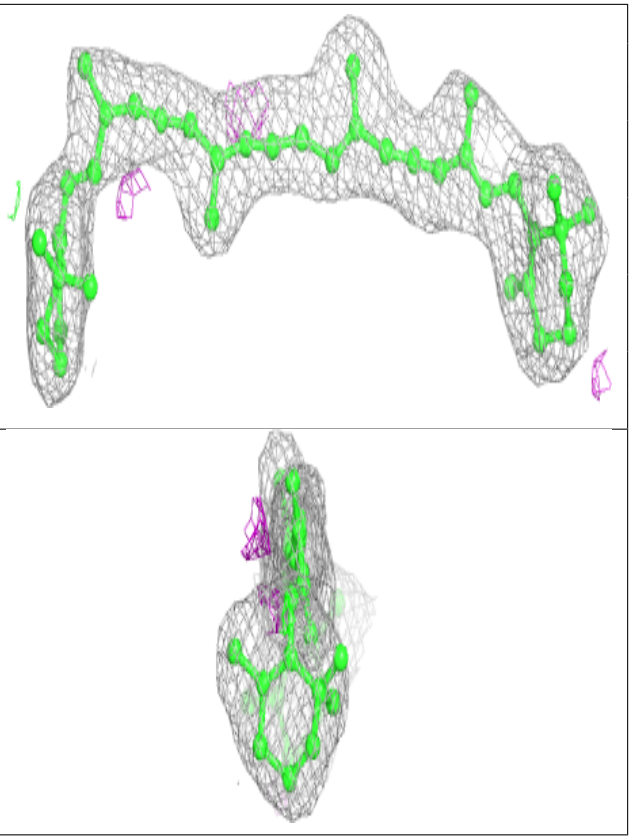






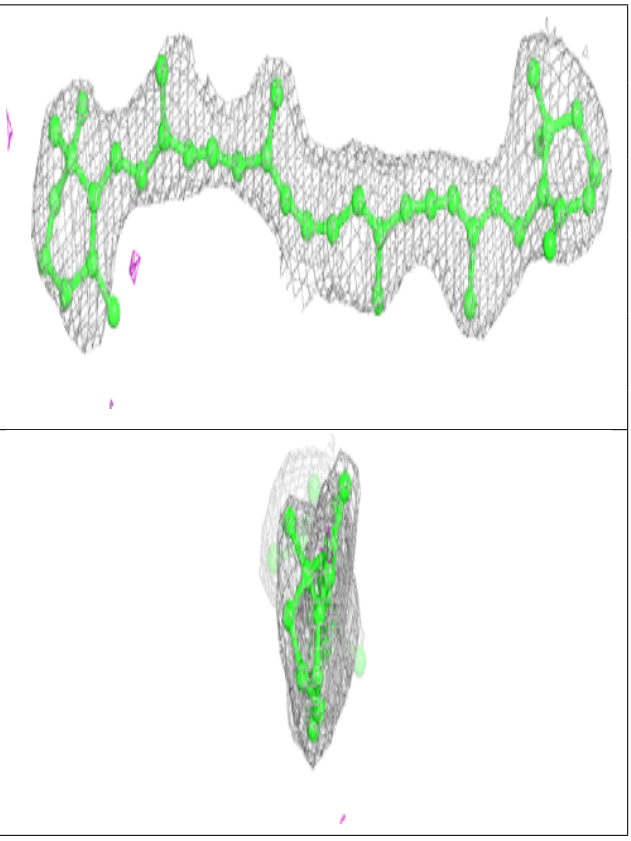
Electron density around BCR I 102:

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



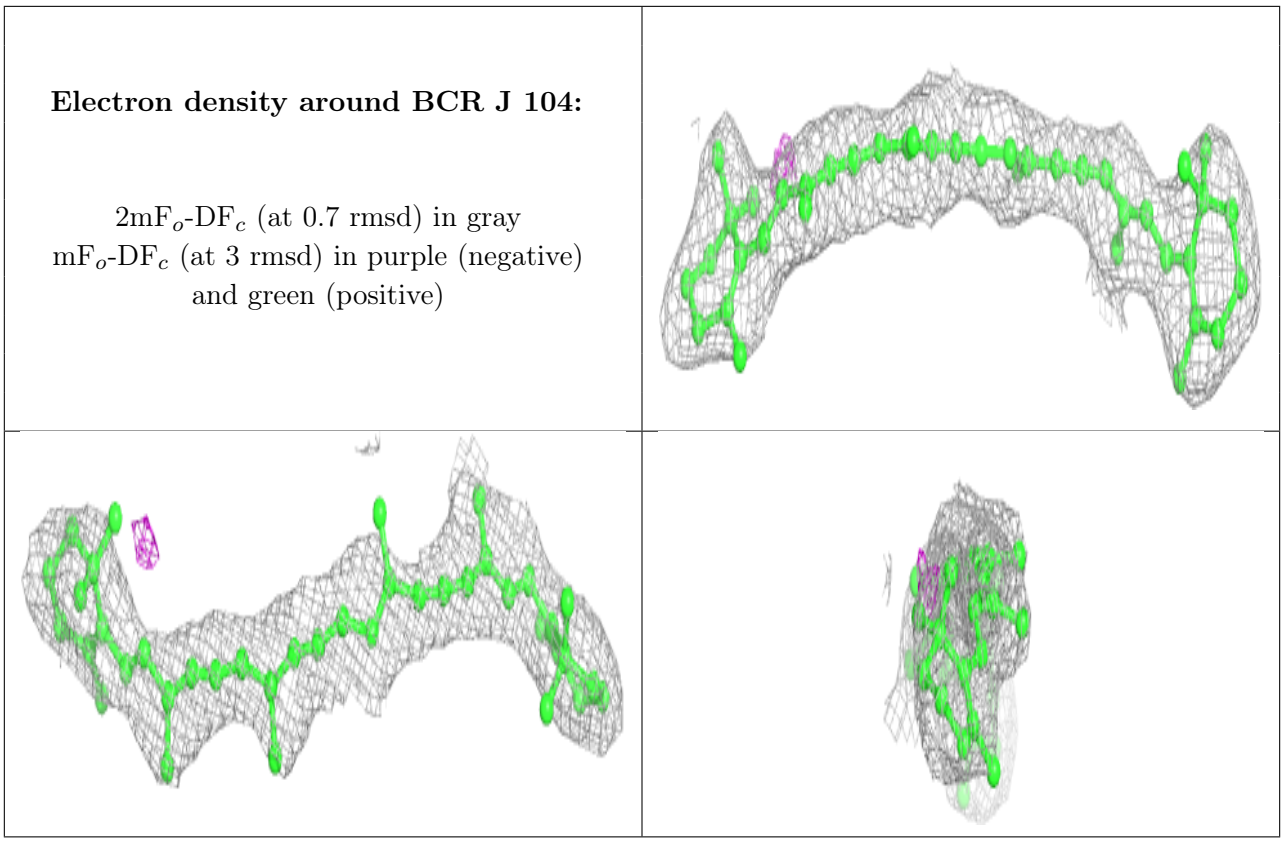
Electron density around BCR J 103:

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



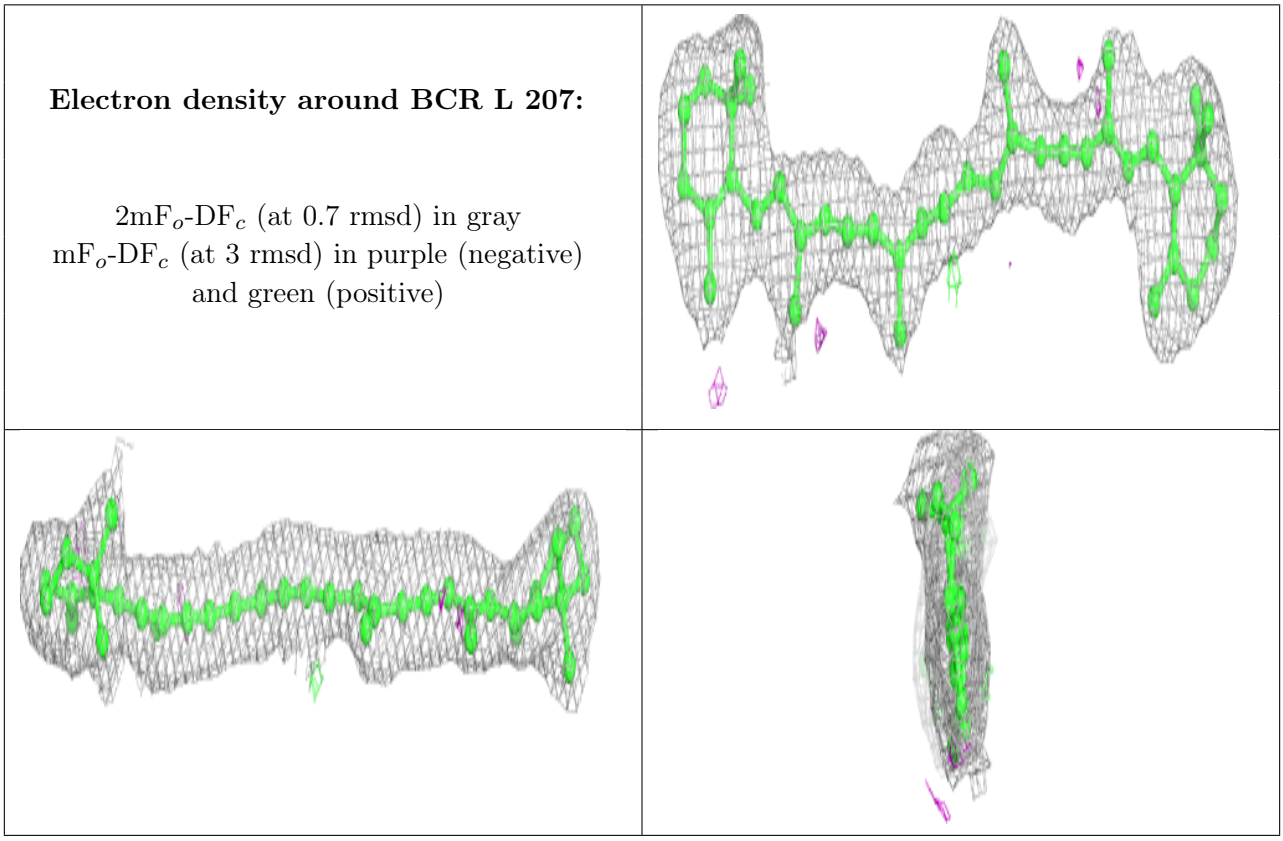
Electron density around BCR J 104:

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



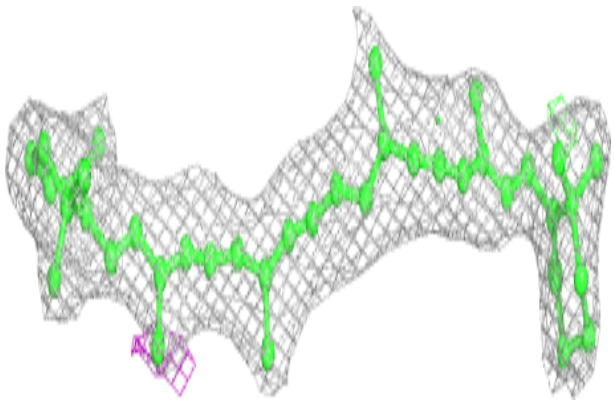
Electron density around BCR L 207:

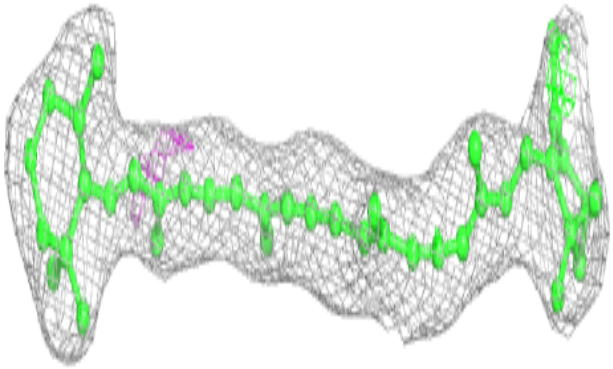
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

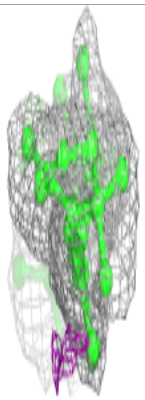


Electron density around BCR L 208:

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

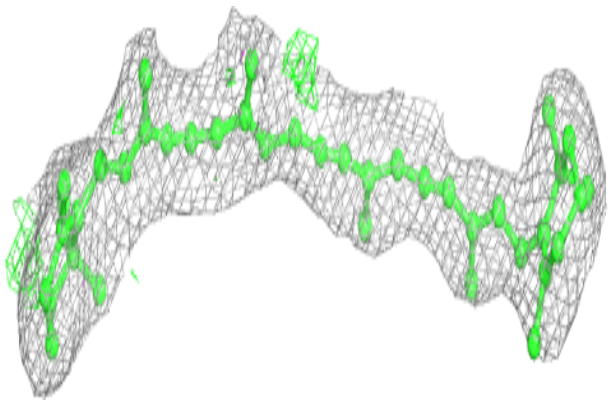


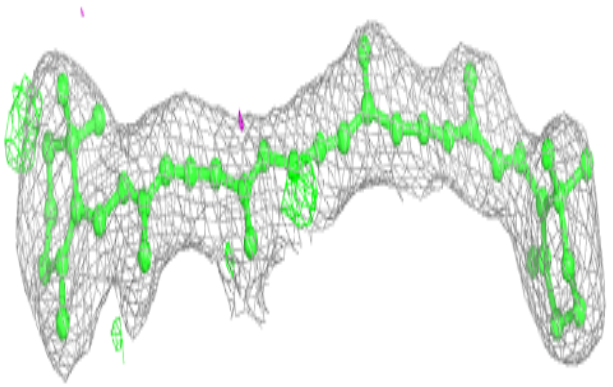


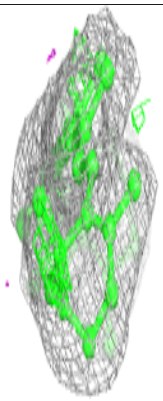


Electron density around BCR M 101:

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

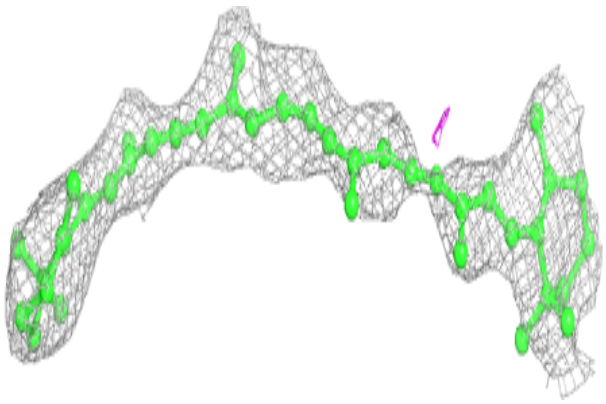


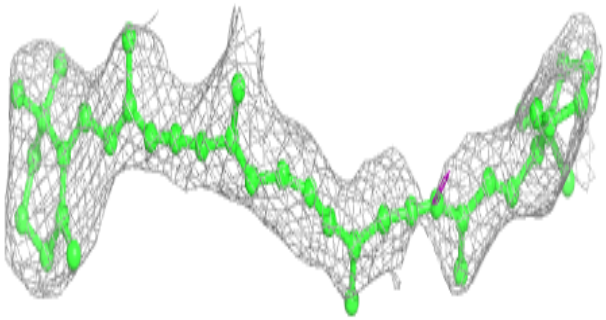


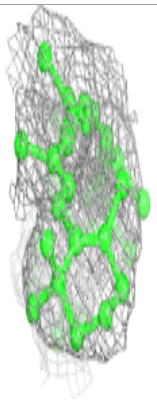


Electron density around BCR Q 201:

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

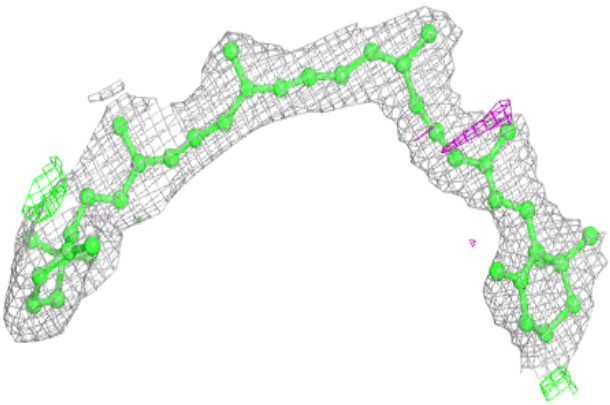


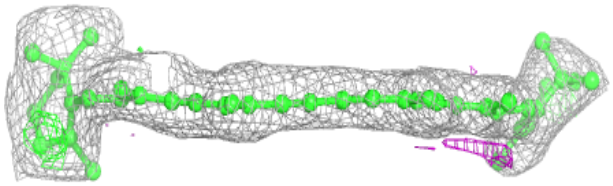


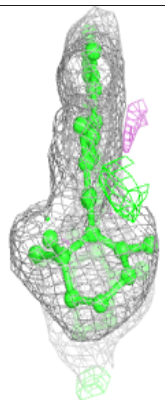


Electron density around BCR Q 203:

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

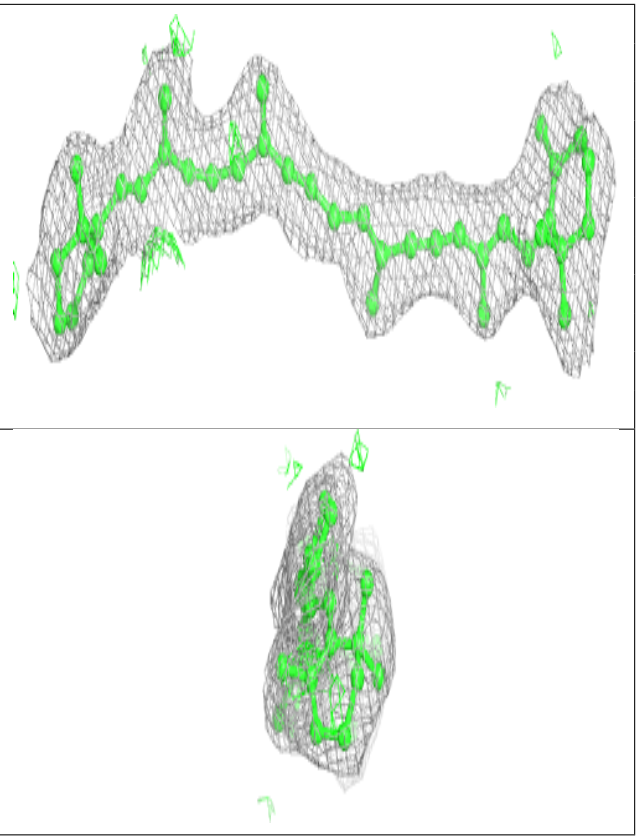






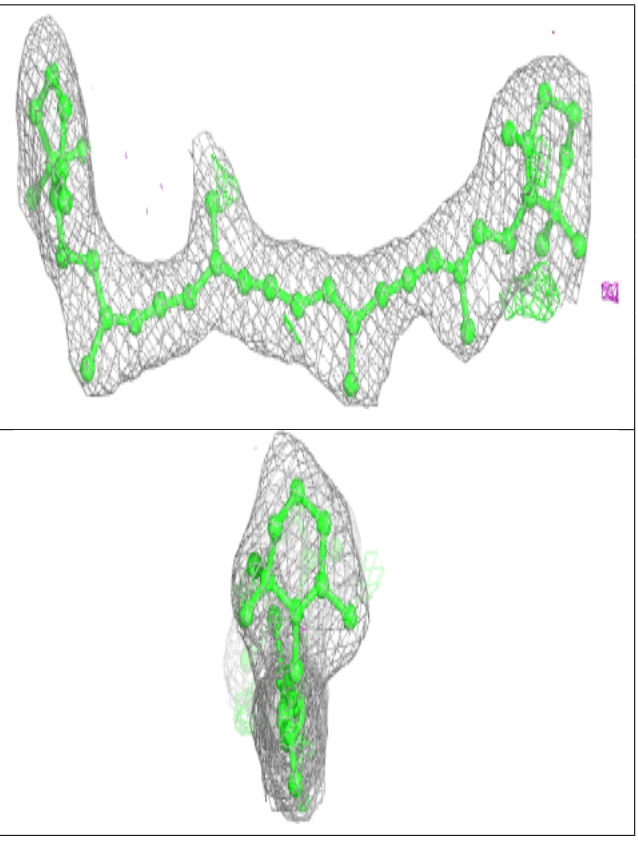
Electron density around BCR R 101:

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



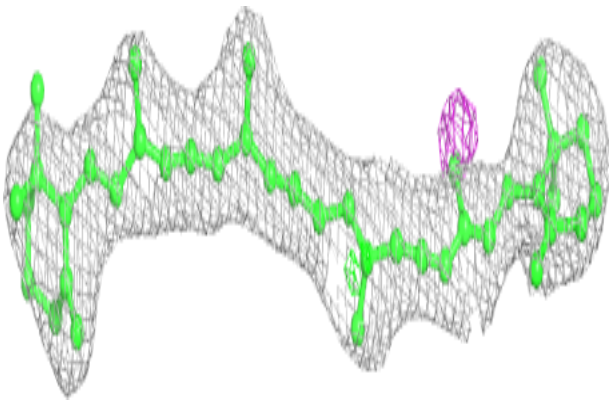
Electron density around BCR R 102:

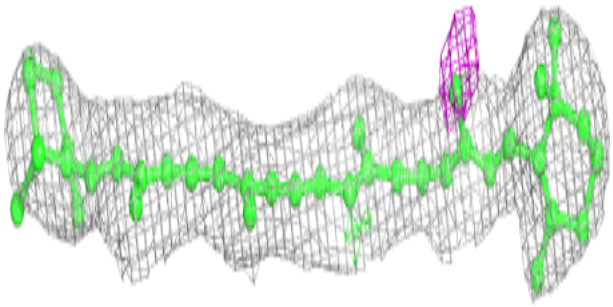
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

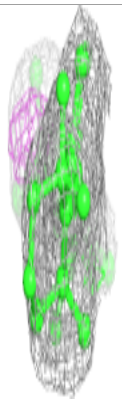


Electron density around BCR S 1104:

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

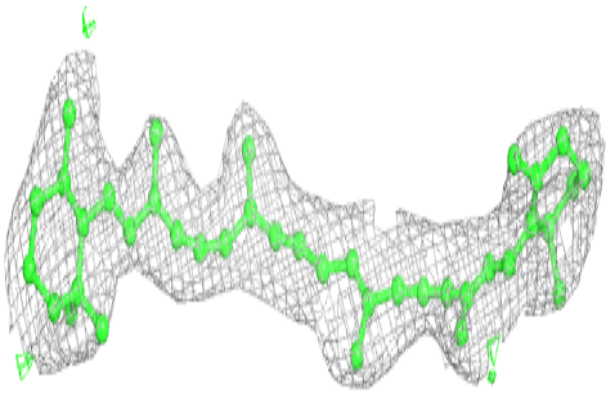


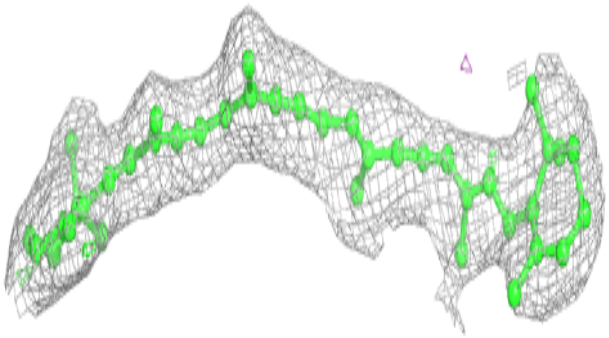


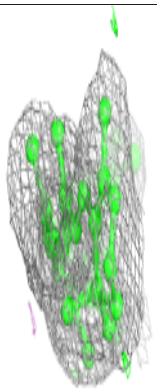


Electron density around BCR S 1105:

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

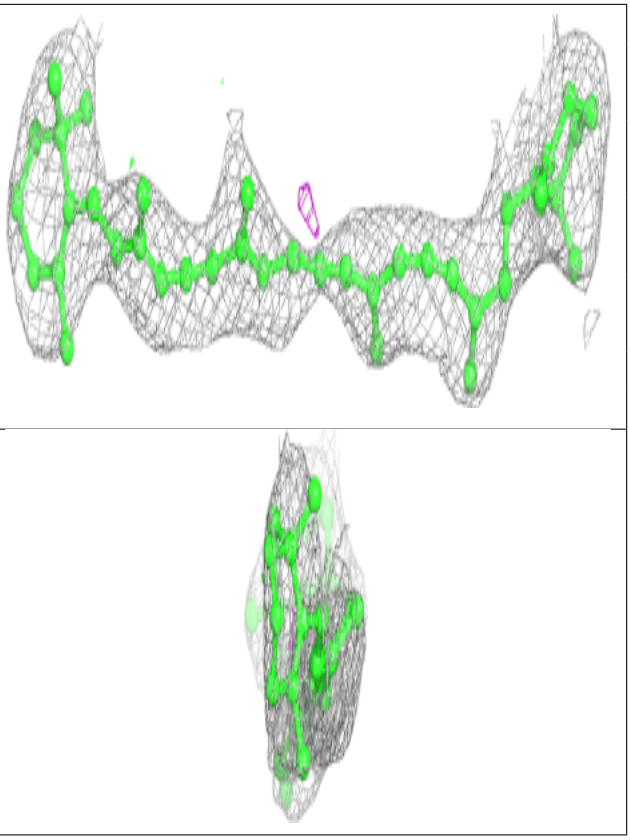






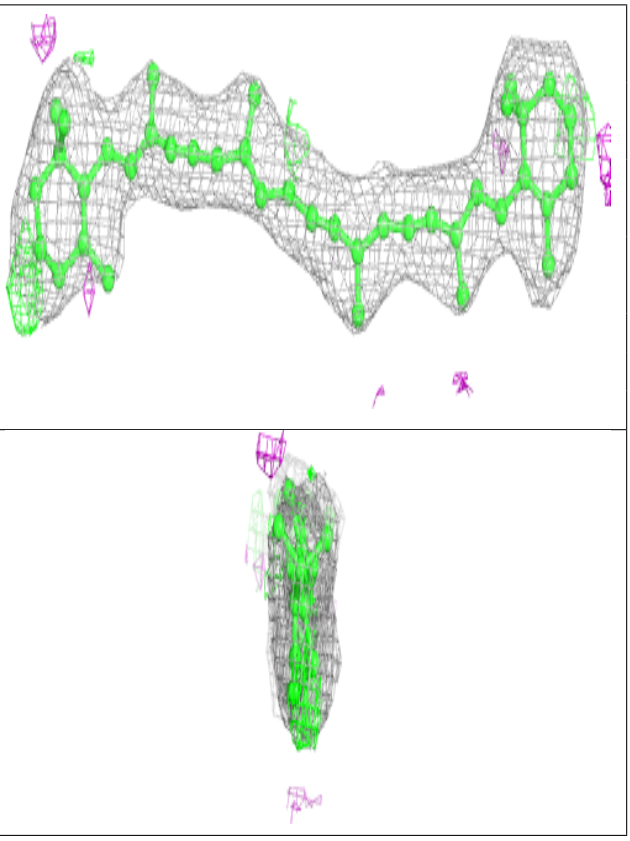
Electron density around BCR T 102:

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



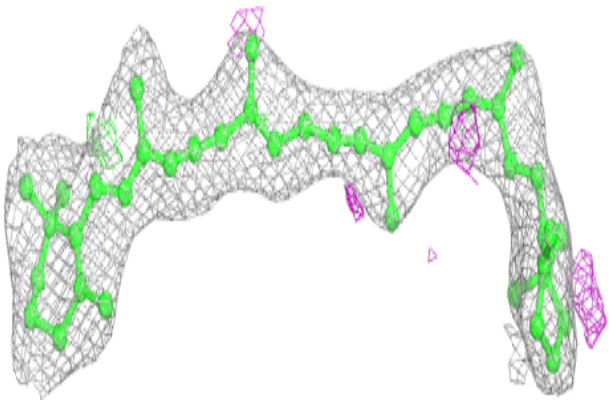
Electron density around BCR U 1005:

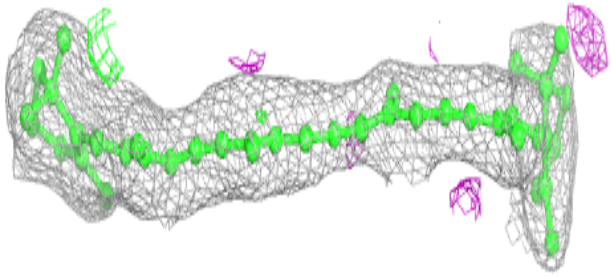
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

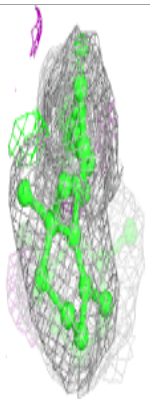


Electron density around BCR U 1008:

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

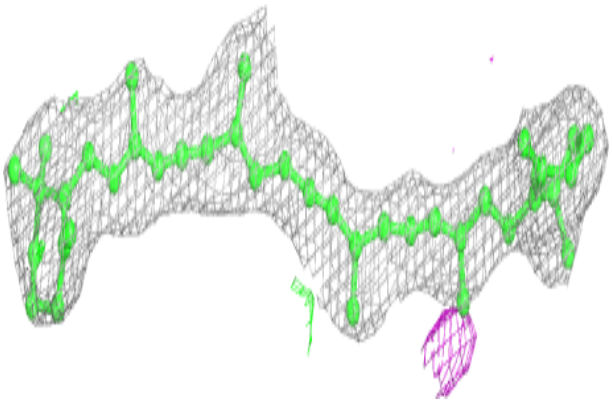


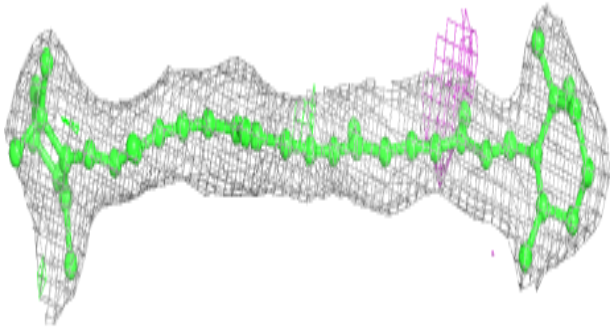


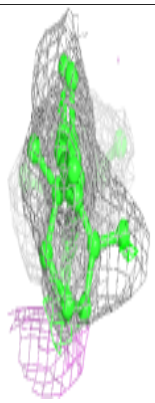


Electron density around BCR U 1009:

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

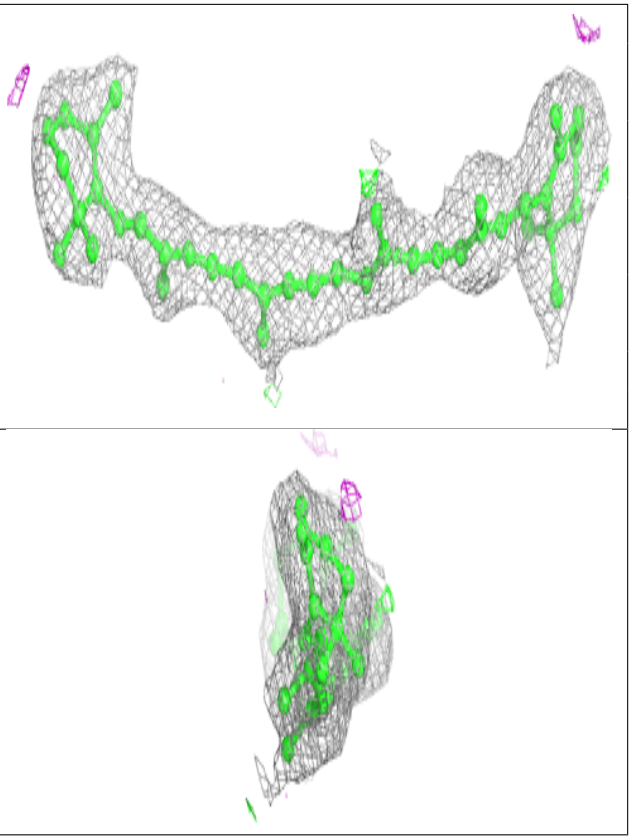






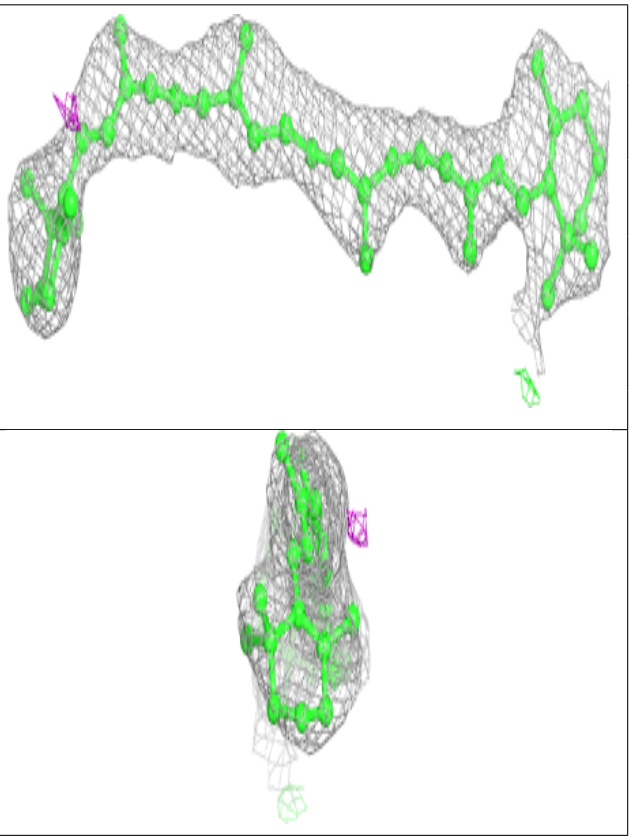
Electron density around BCR V 101:

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



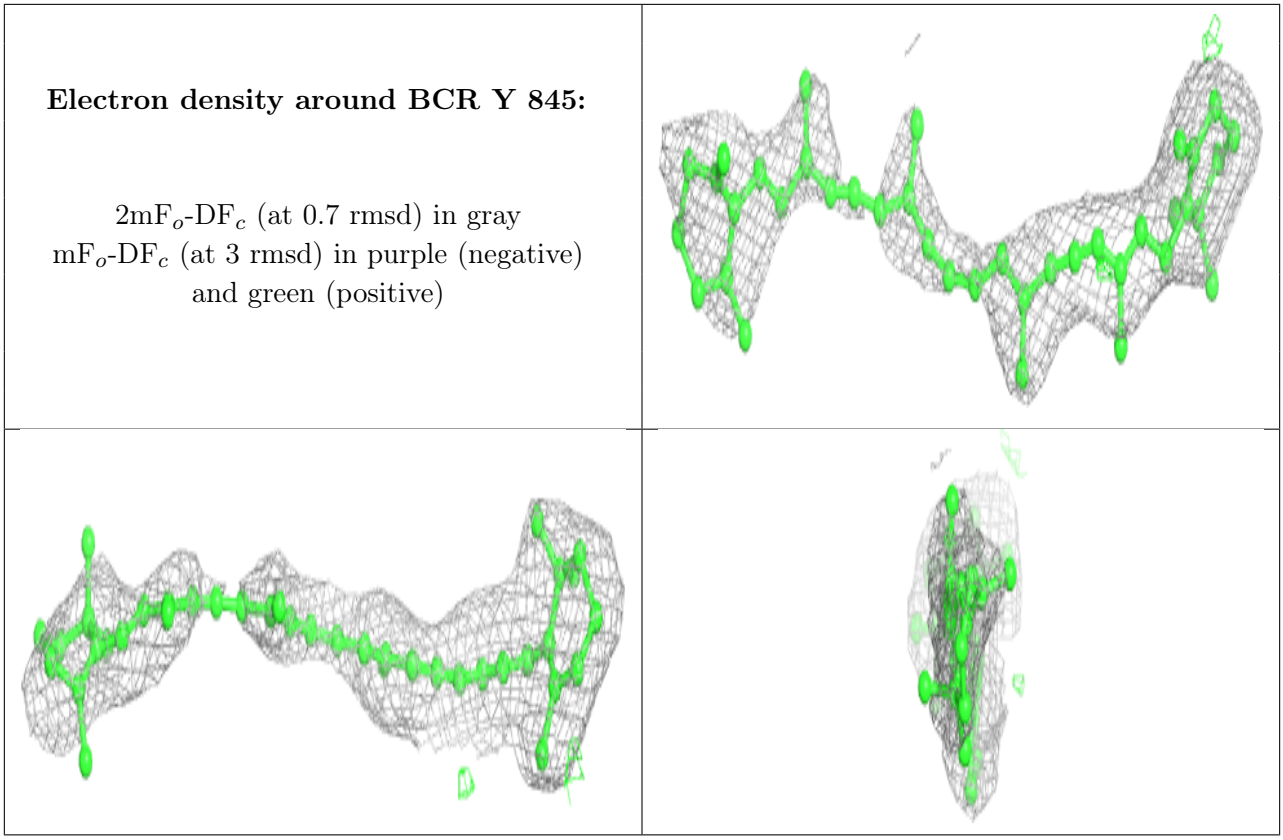
Electron density around BCR Y 844:

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



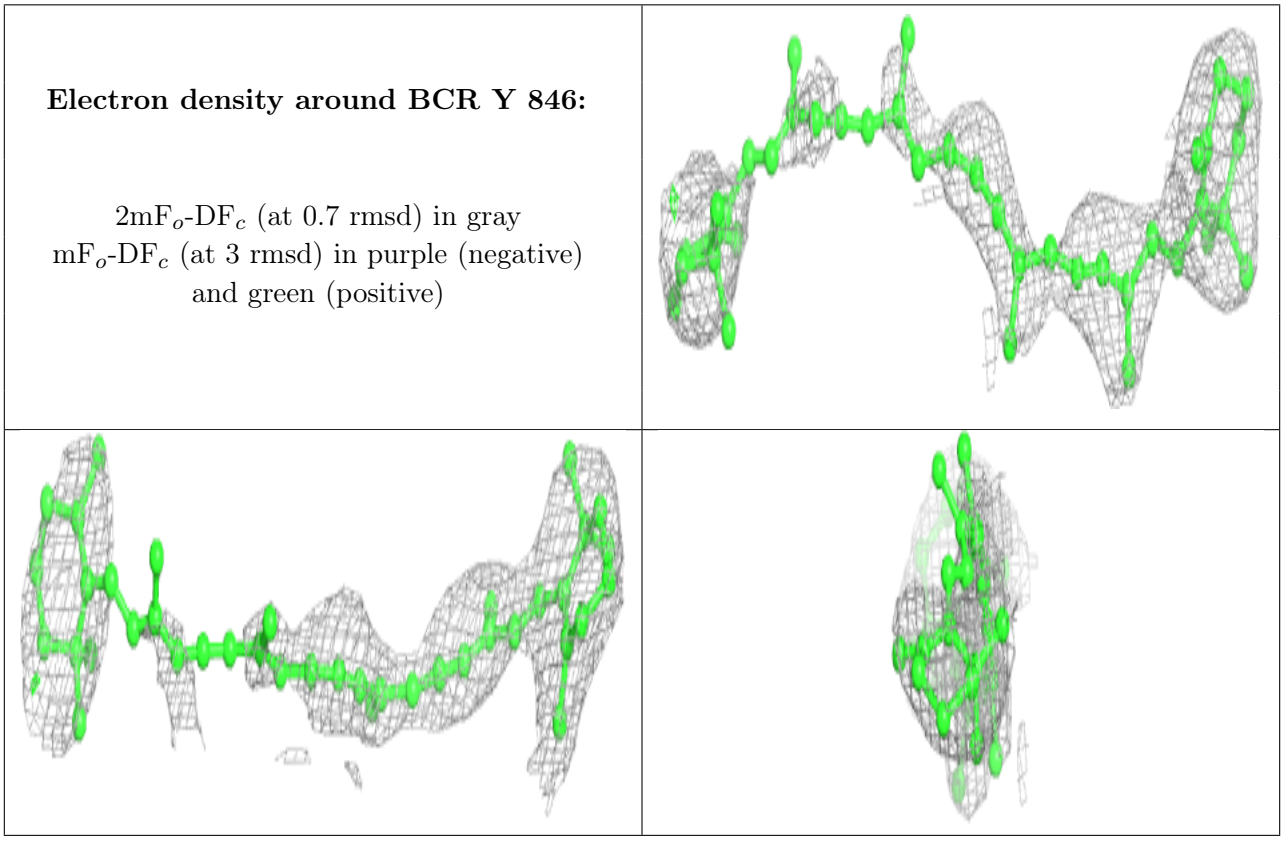
Electron density around BCR Y 845:

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



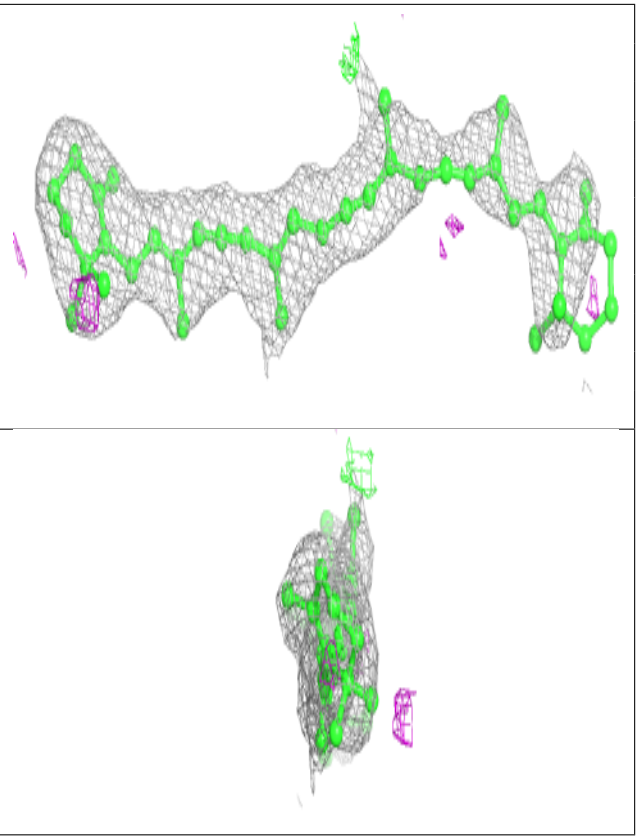
Electron density around BCR Y 846:

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



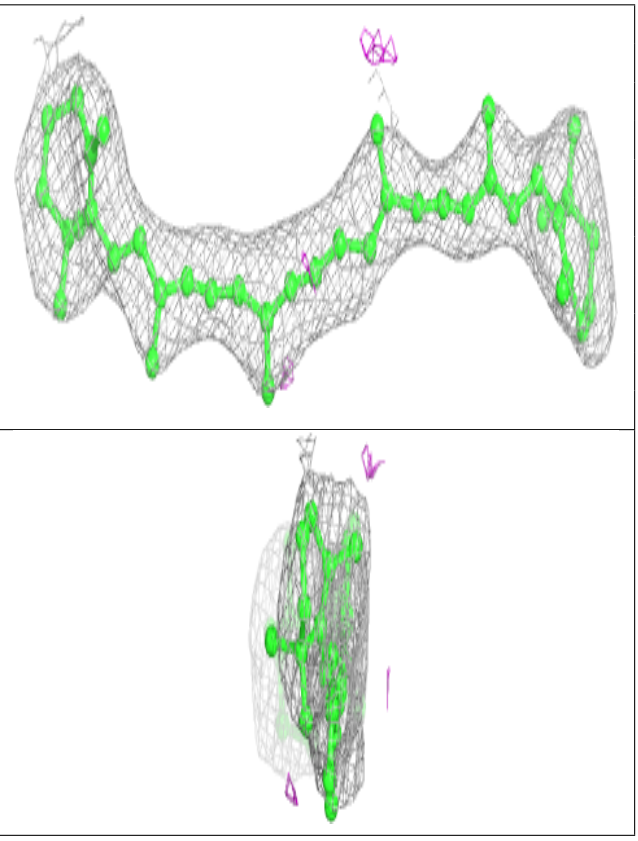
Electron density around BCR Y 847:

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



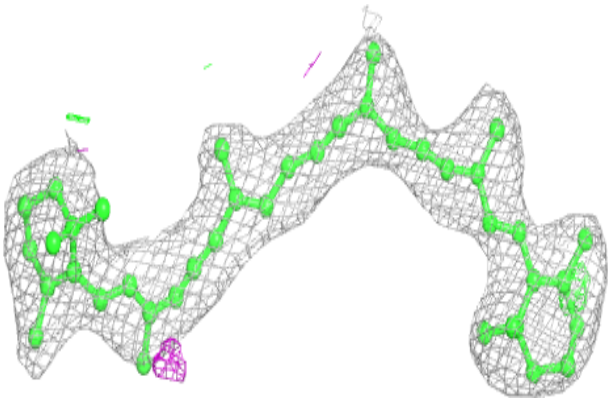
Electron density around BCR Y 848:

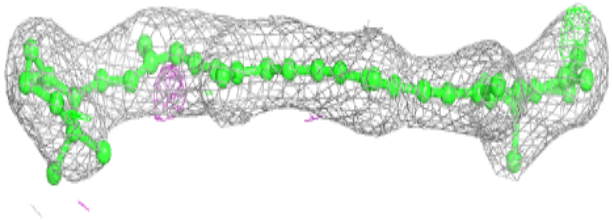
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

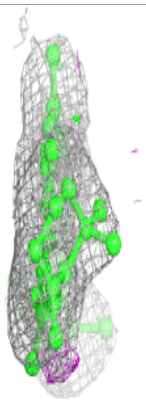


Electron density around BCR Y 849:

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

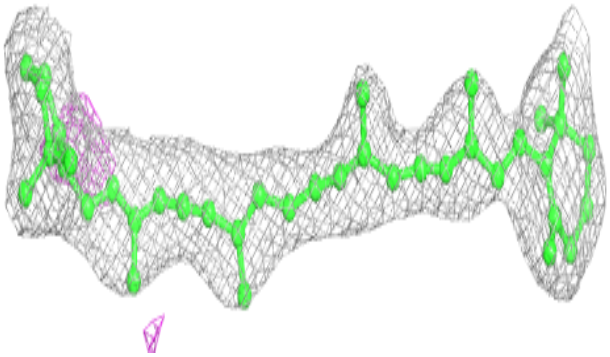


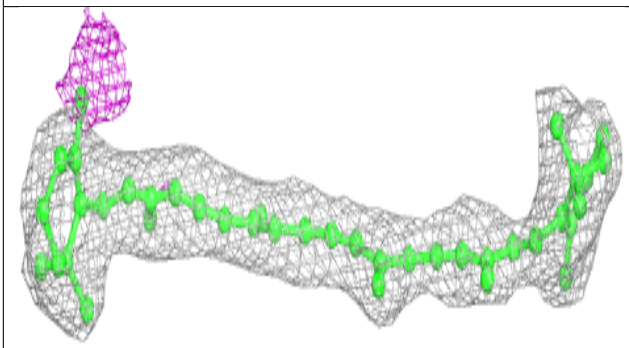


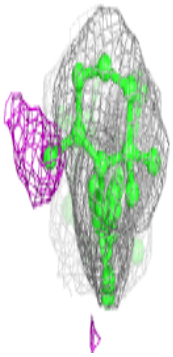


Electron density around BCR Y 852:

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

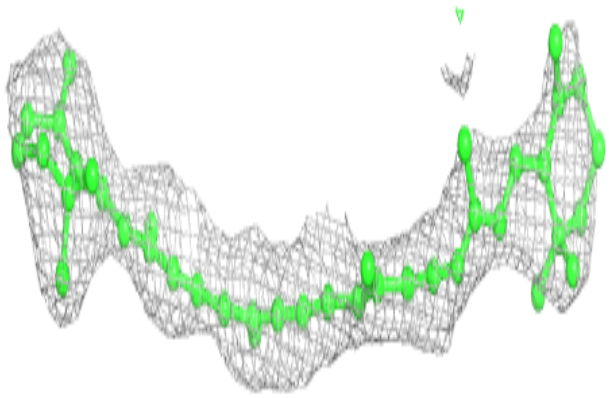


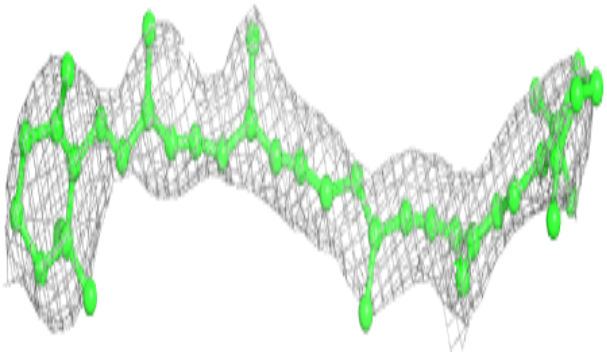


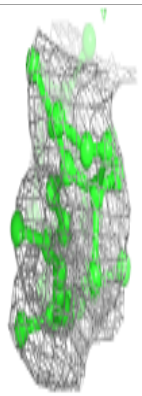


Electron density around BCR Y 853:

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

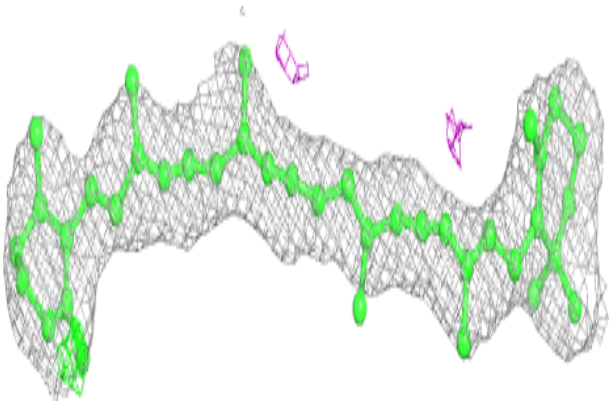


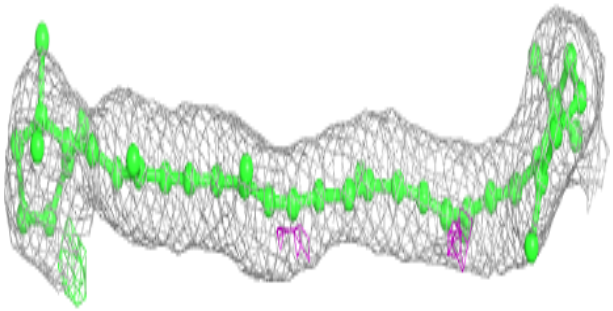


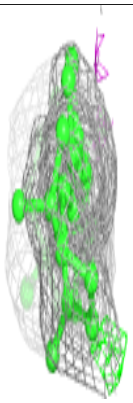


Electron density around BCR Z 843:

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

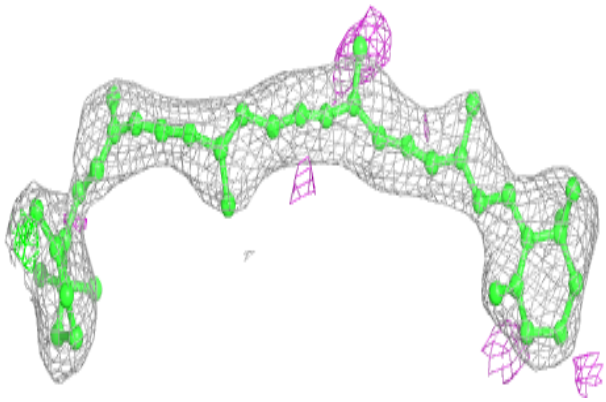


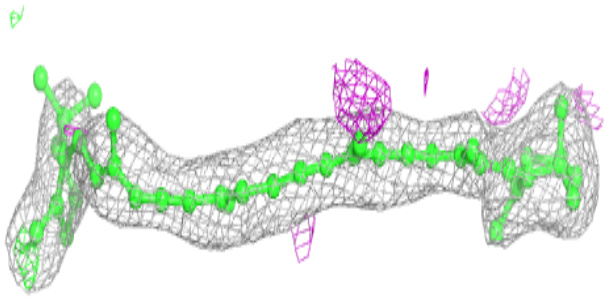


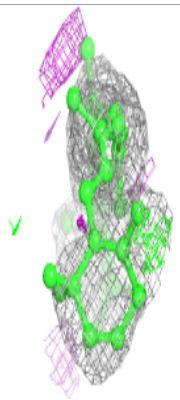


Electron density around BCR Z 844:

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

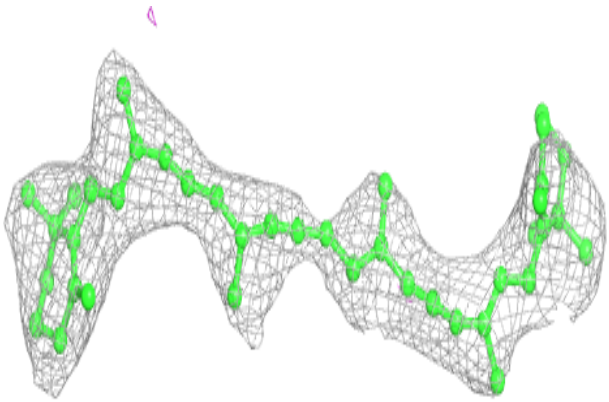


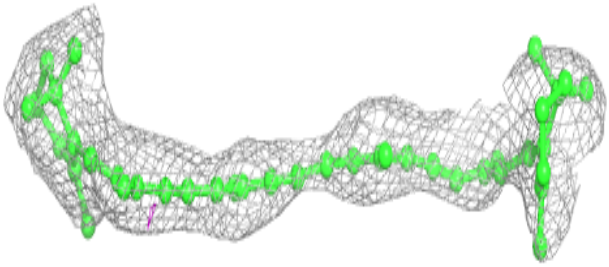


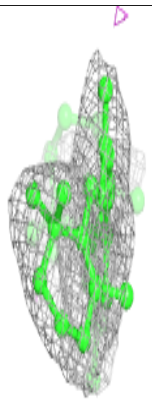


Electron density around BCR Z 845:

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

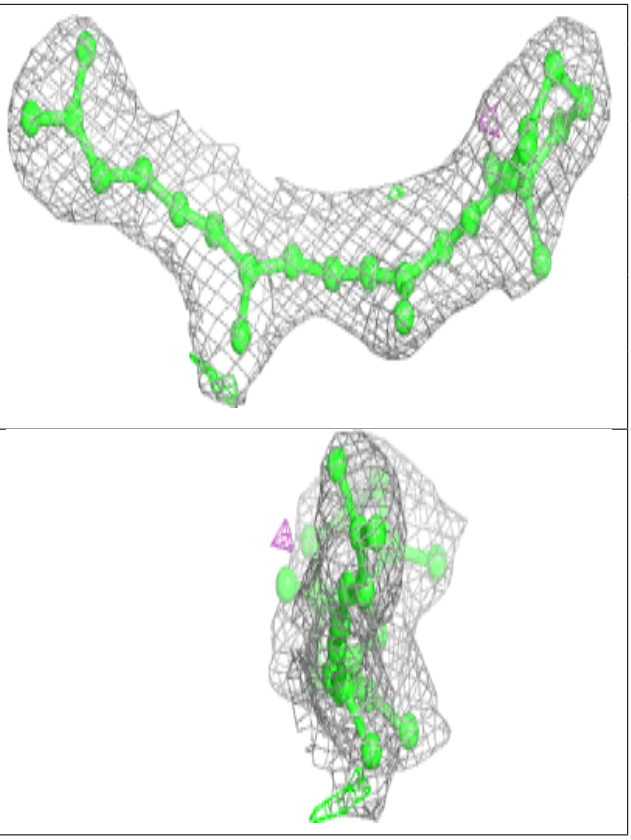


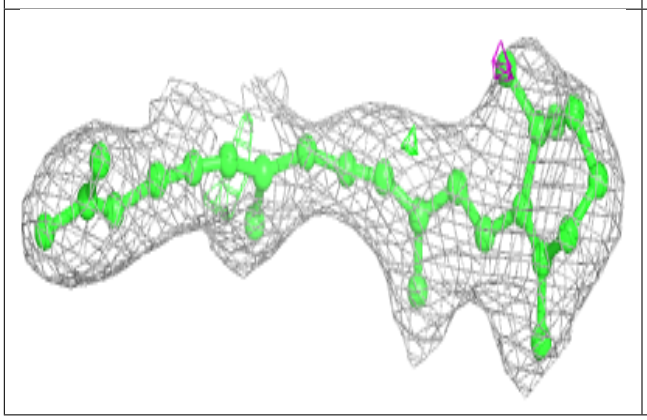




Electron density around BCR Z 846:

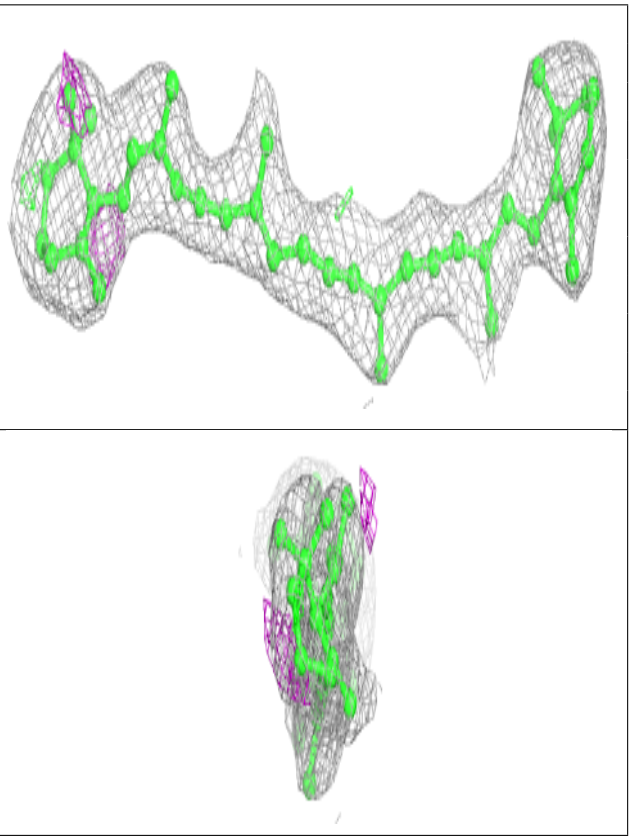
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

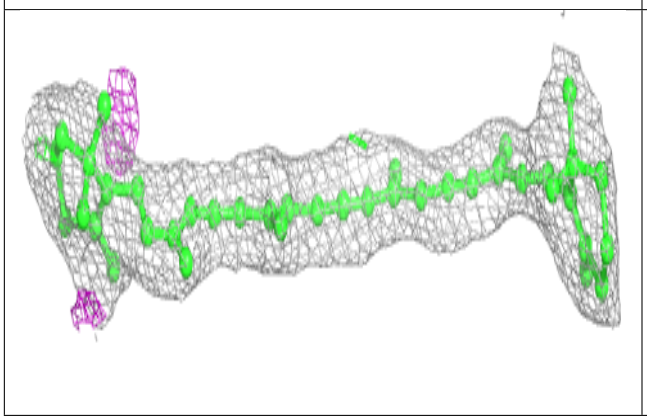




Electron density around BCR Z 847:

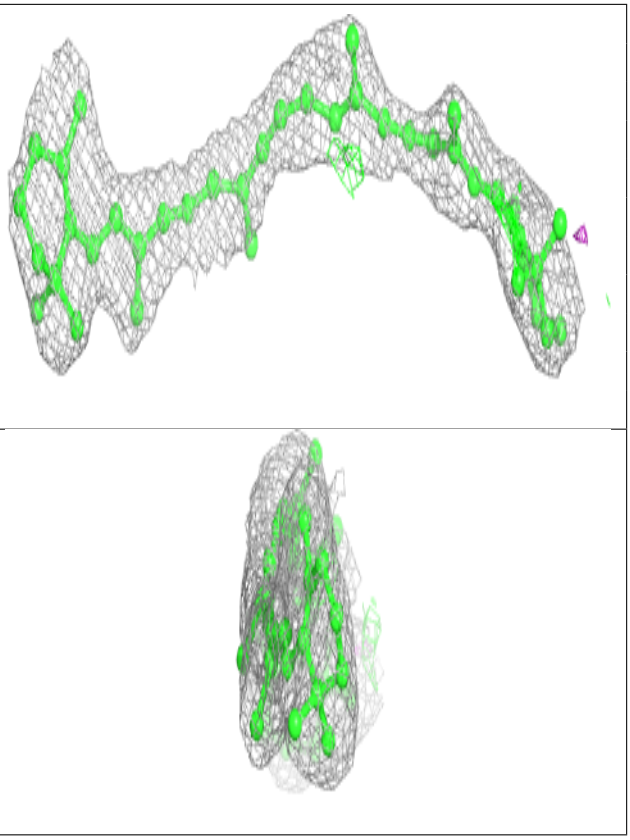
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





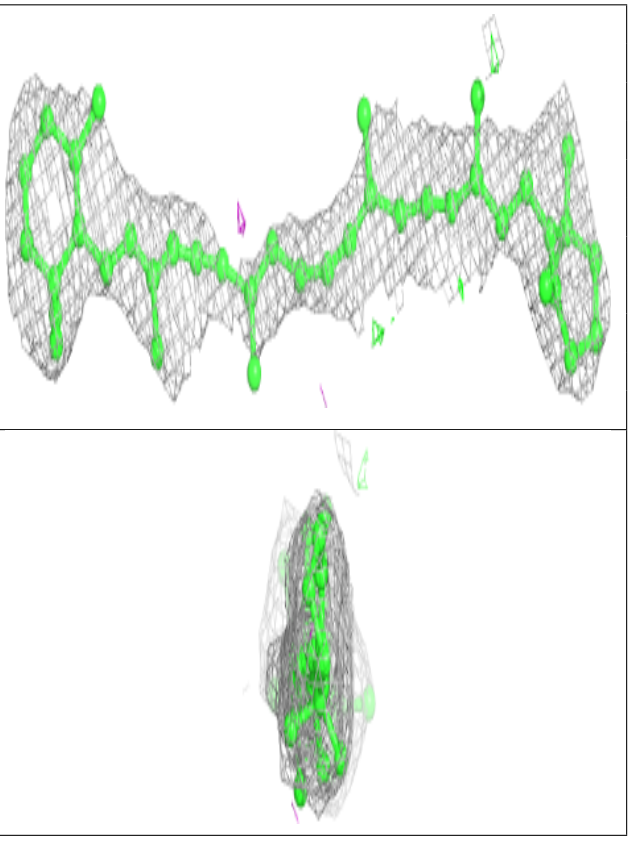
Electron density around BCR Z 848:

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



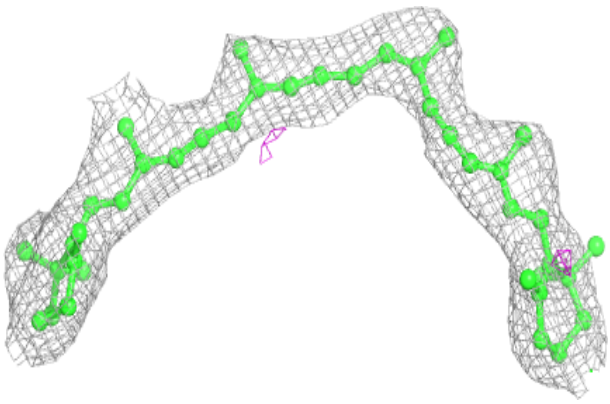
Electron density around BCR Z 850:

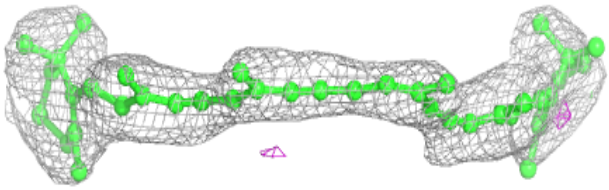
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

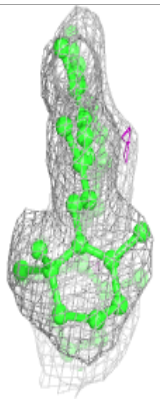


Electron density around BCR d 203:

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

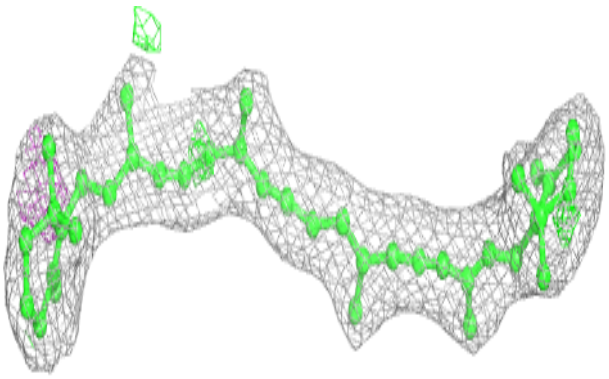


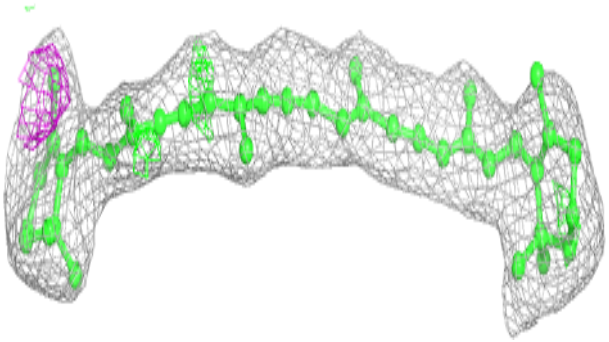


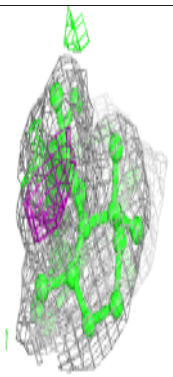


Electron density around BCR e 101:

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

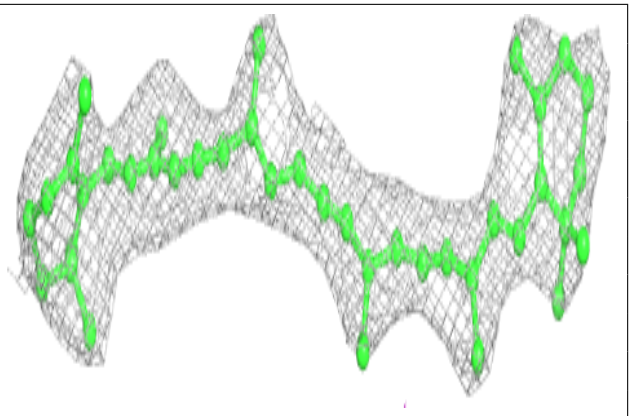


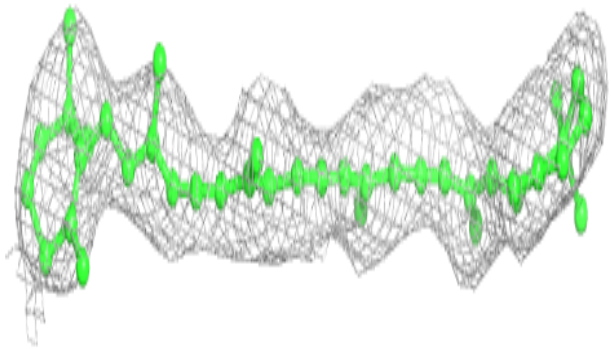


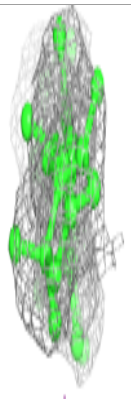


Electron density around BCR f 103:

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

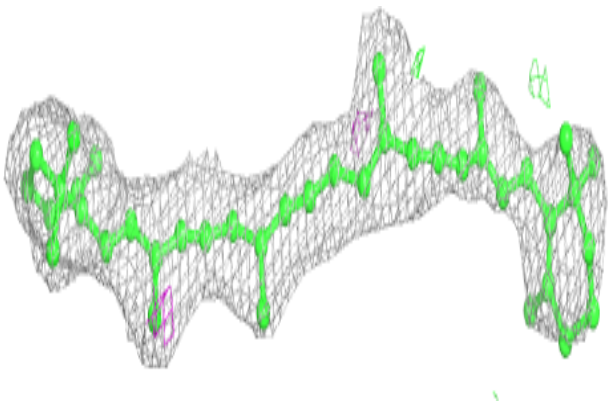


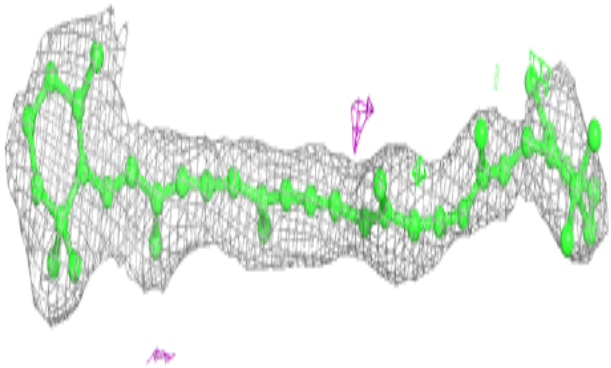


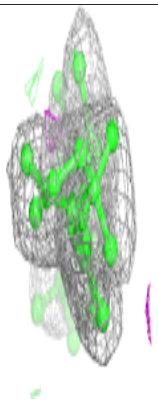


Electron density around BCR h 202:

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

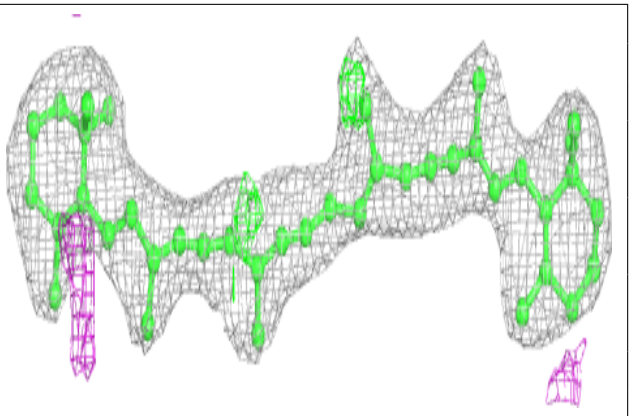


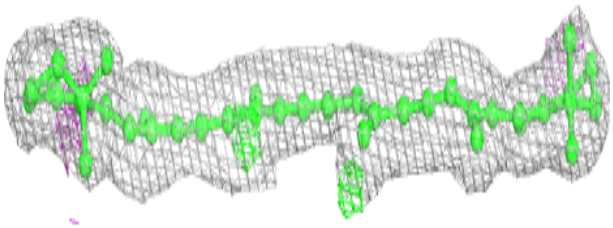


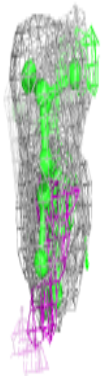


Electron density around BCR h 207:

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

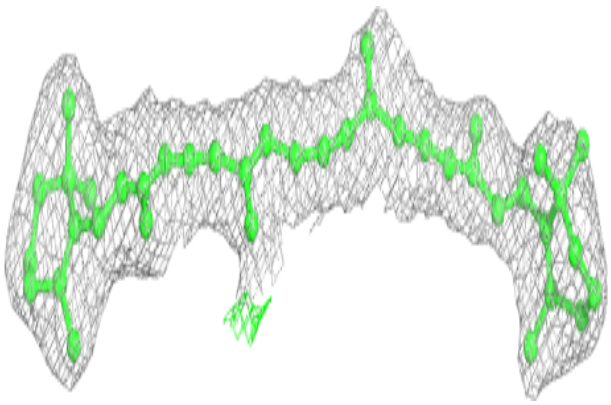


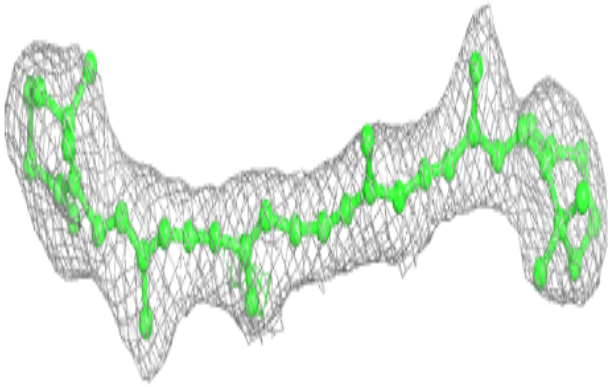


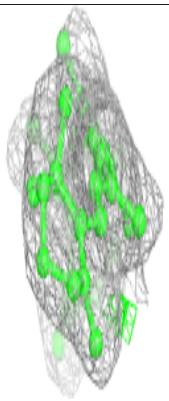


Electron density around BCR i 101:

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

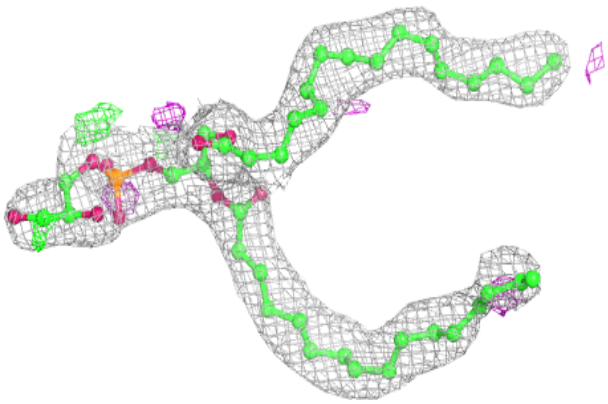


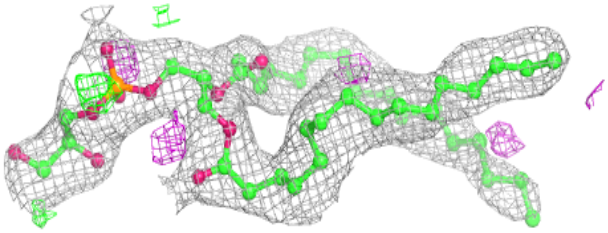


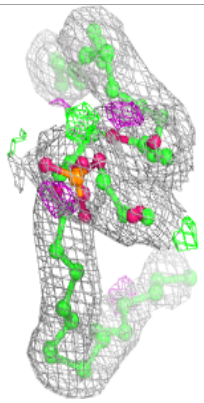


Electron density around LHG A 852:

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

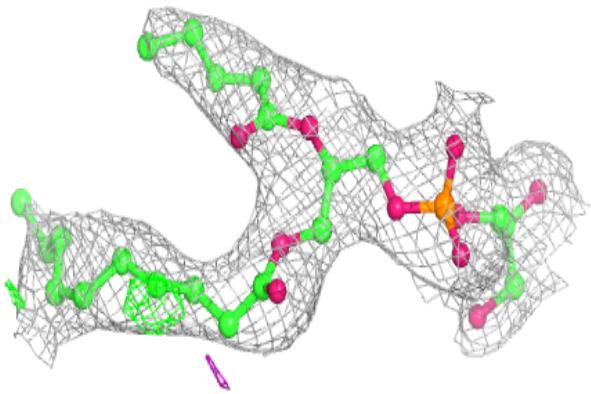


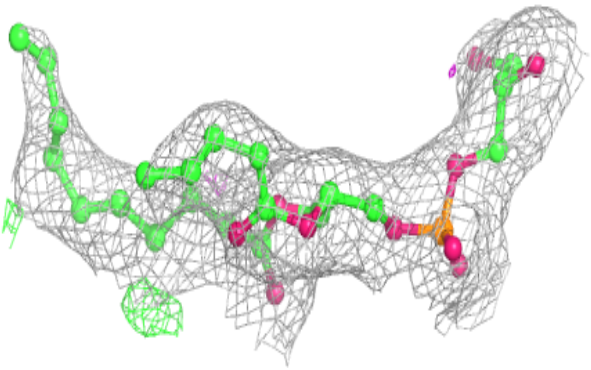


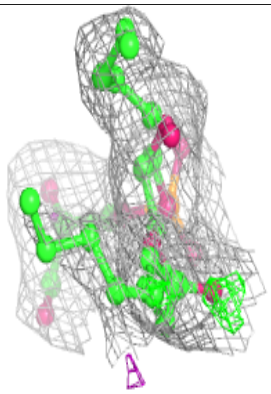


Electron density around LHG A 853:

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

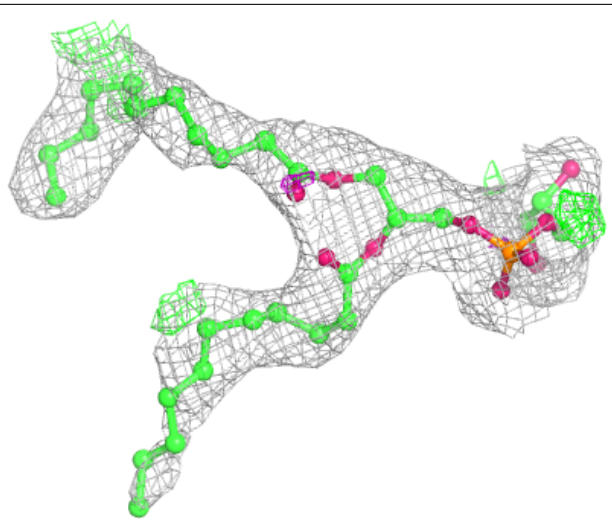


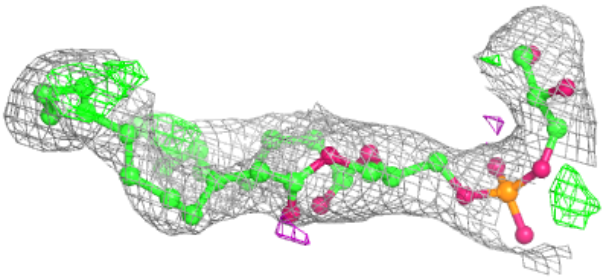


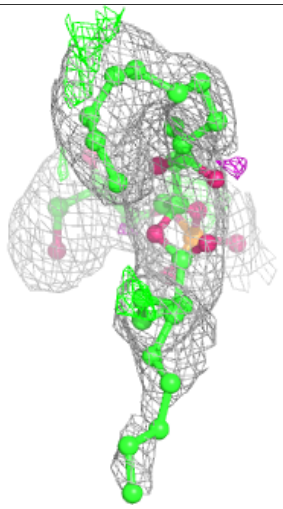


Electron density around LHG B 849:

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

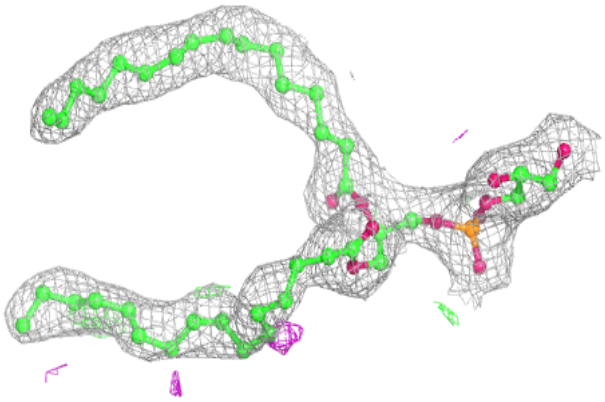


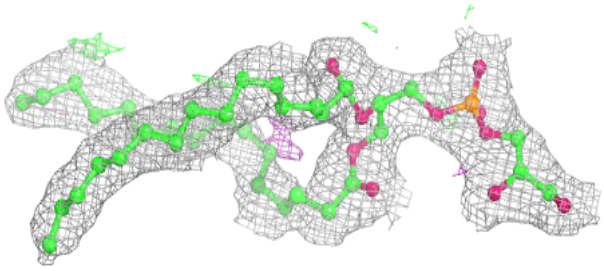


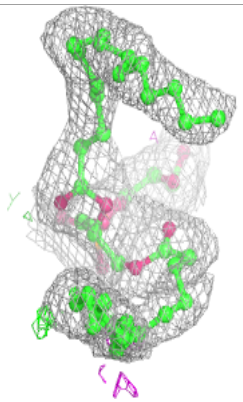


Electron density around LHG G 850:

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

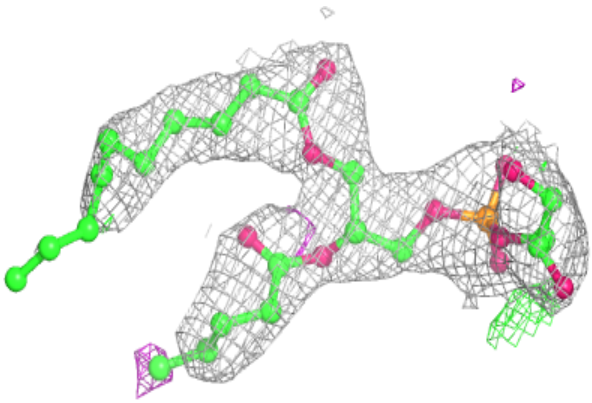


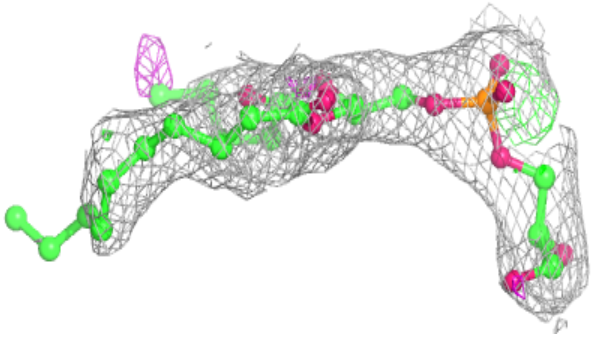


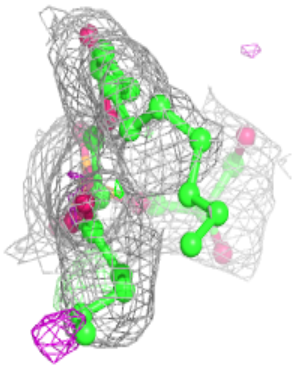


Electron density around LHG G 851:

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

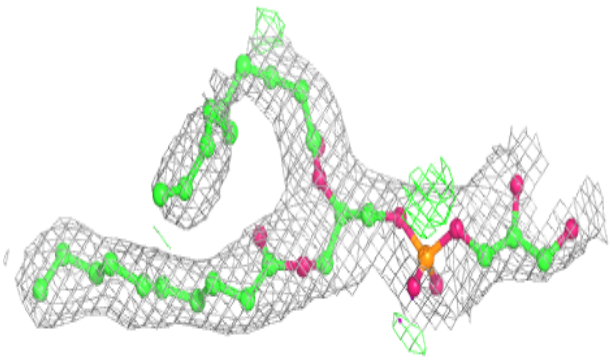


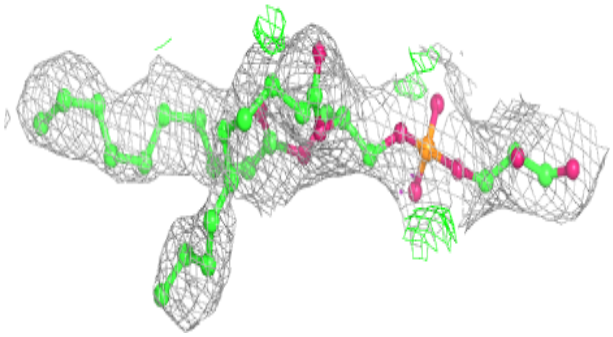


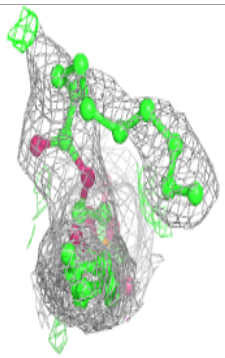


Electron density around LHG H 849:

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

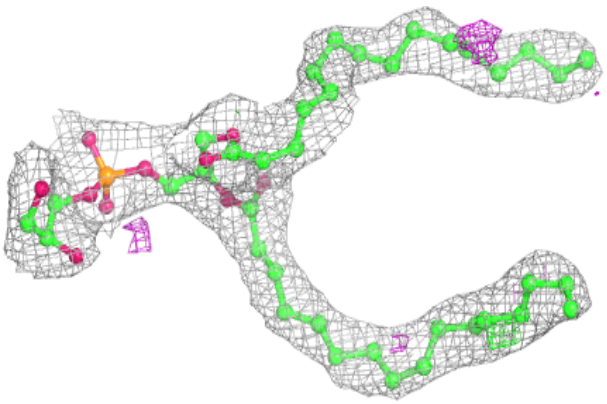


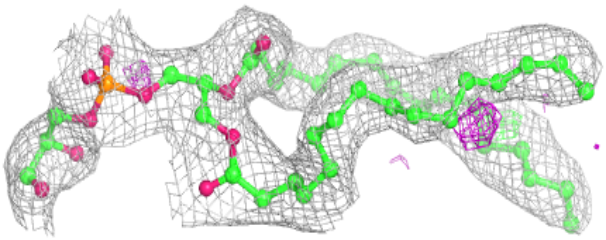


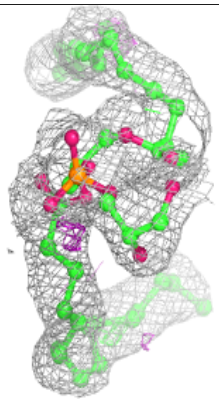


Electron density around LHG Y 850:

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

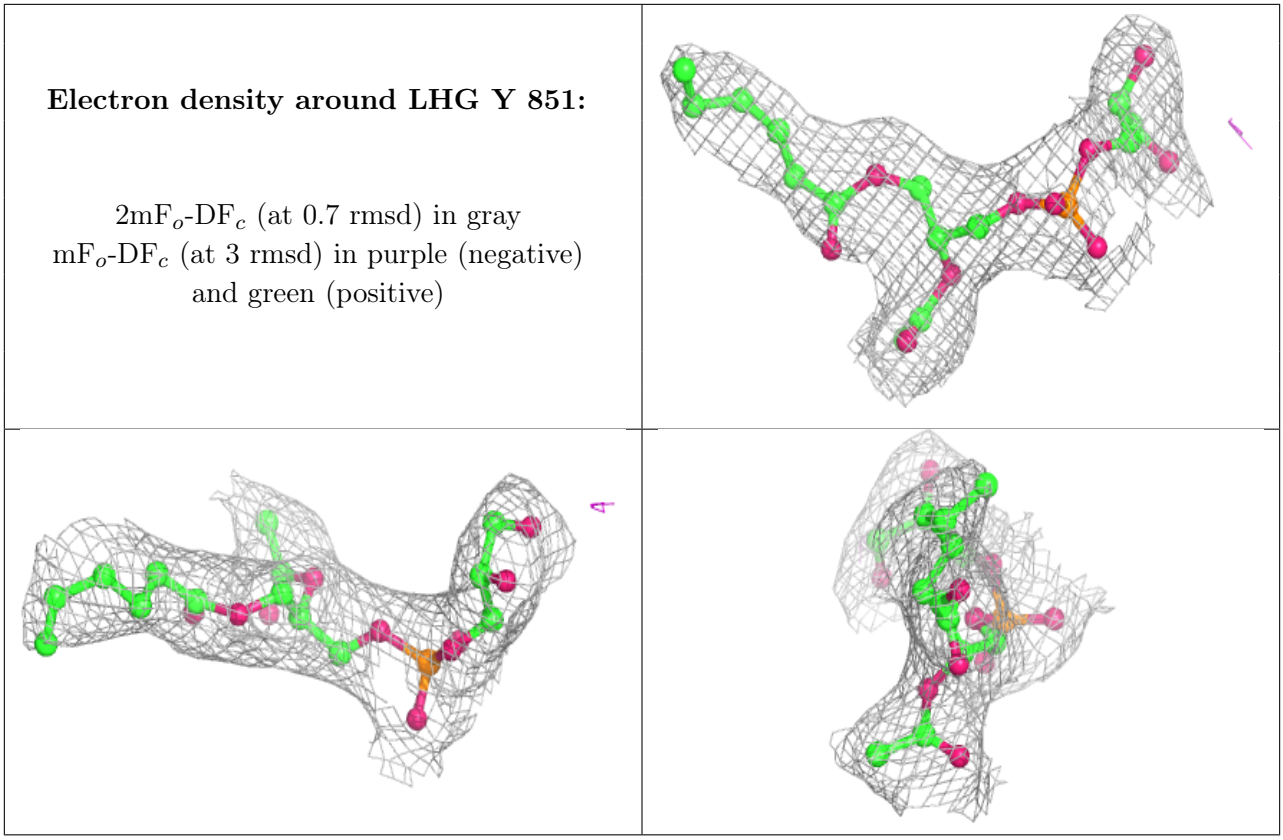






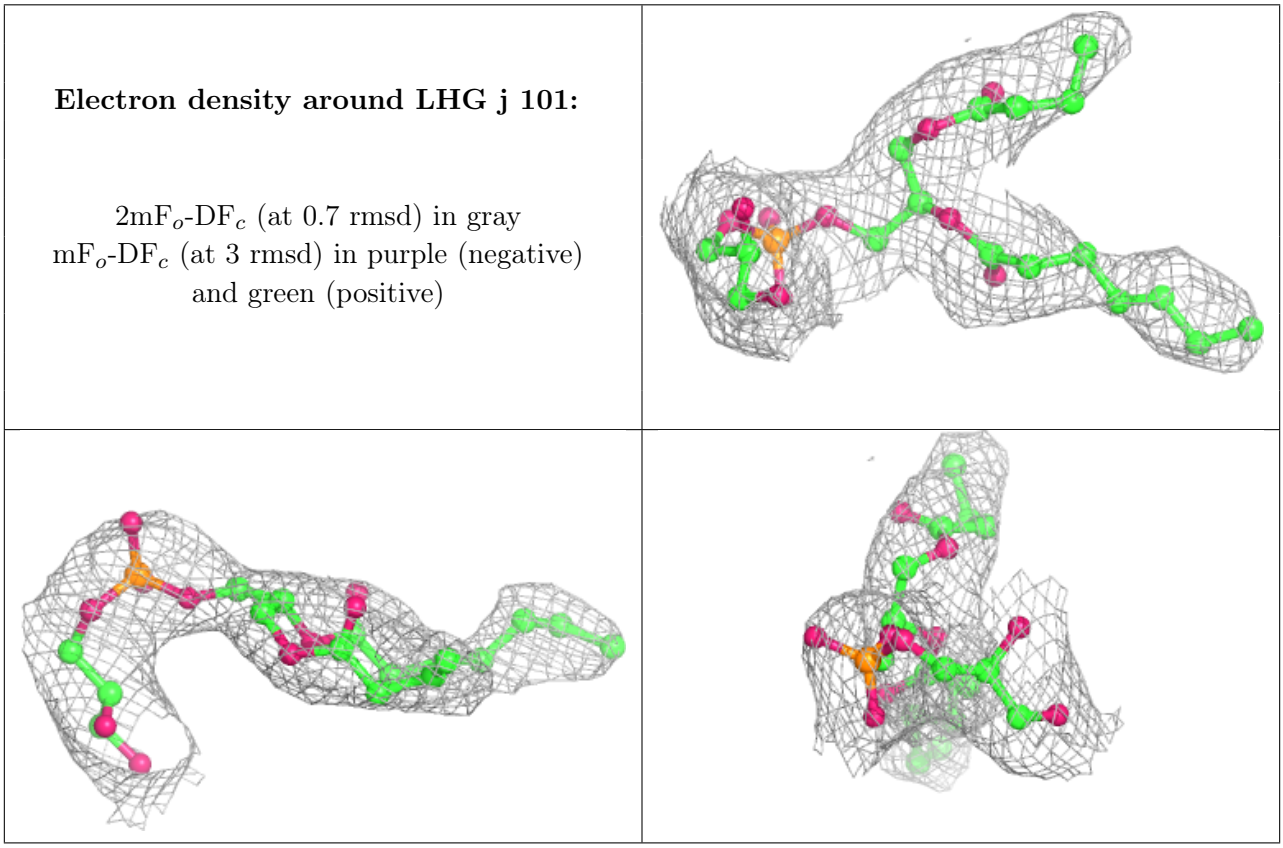
Electron density around LHG Y 851:

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



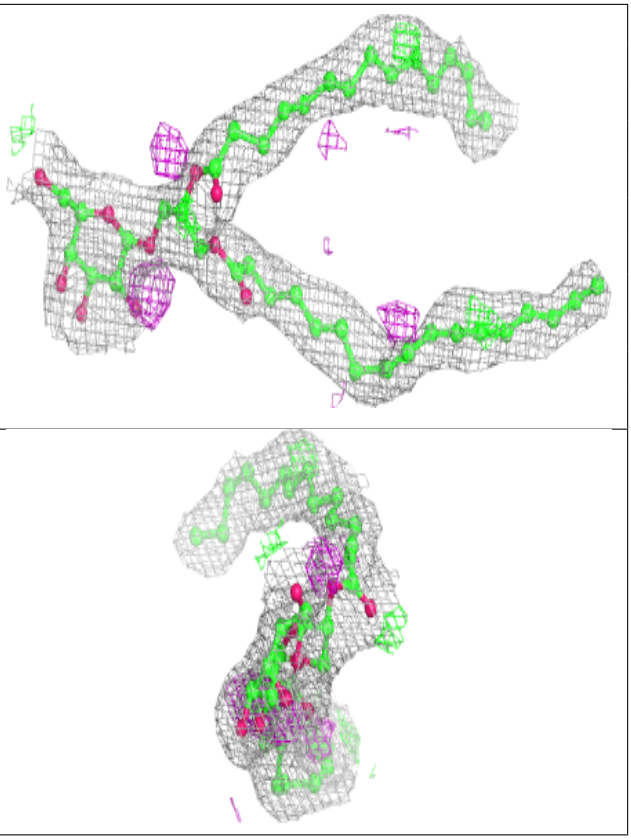
Electron density around LHG j 101:

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



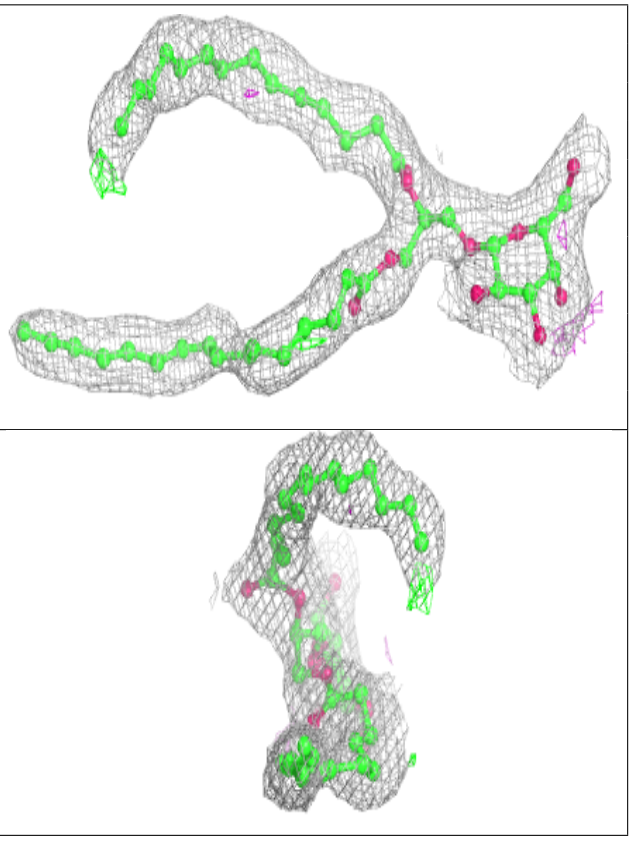
Electron density around LMG B 848:

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



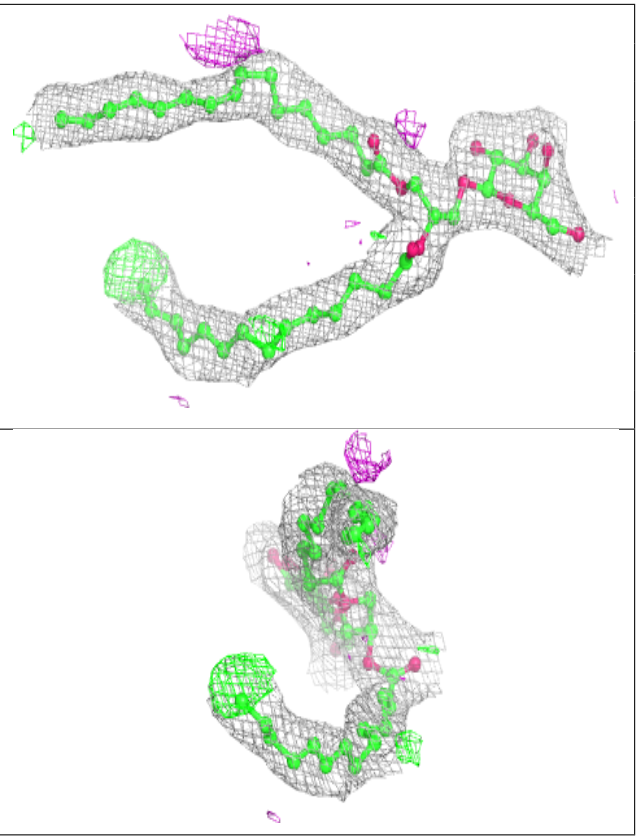
Electron density around LMG H 848:

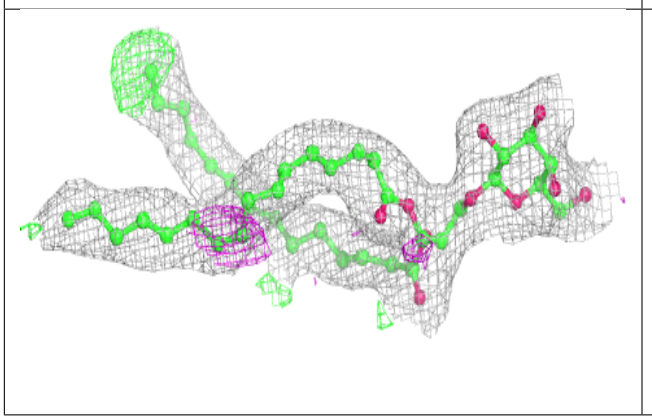
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around LMG Z 849:

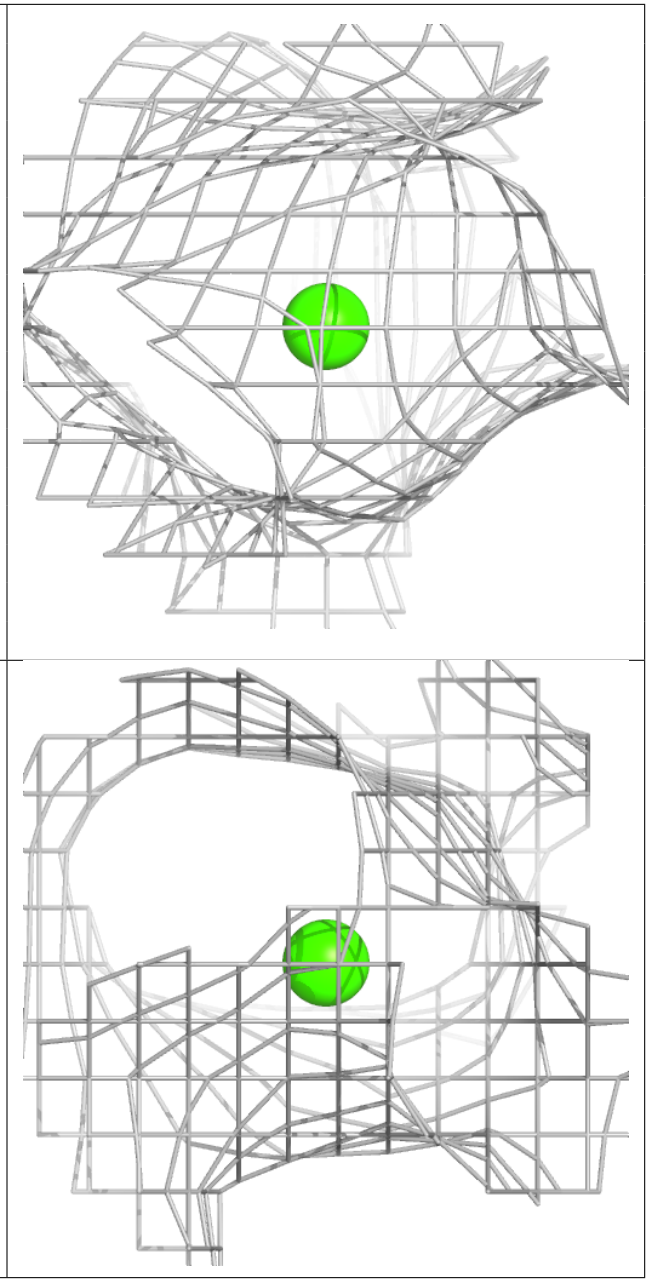
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





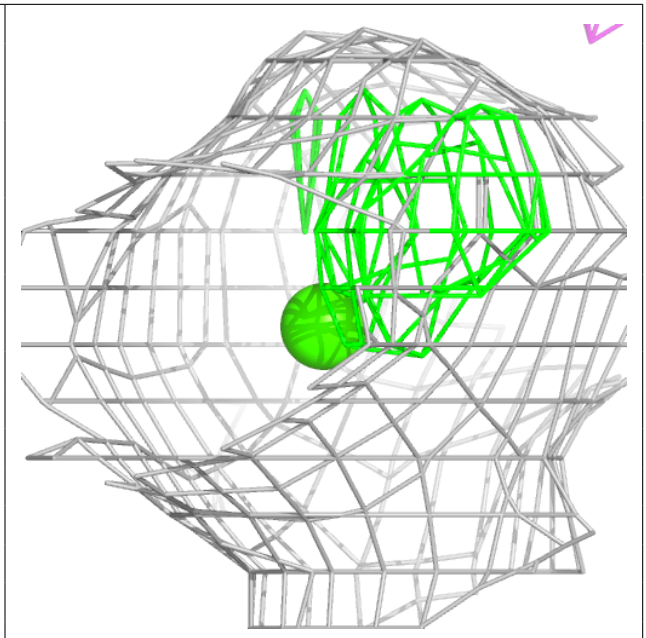
Electron density around CA L 203:

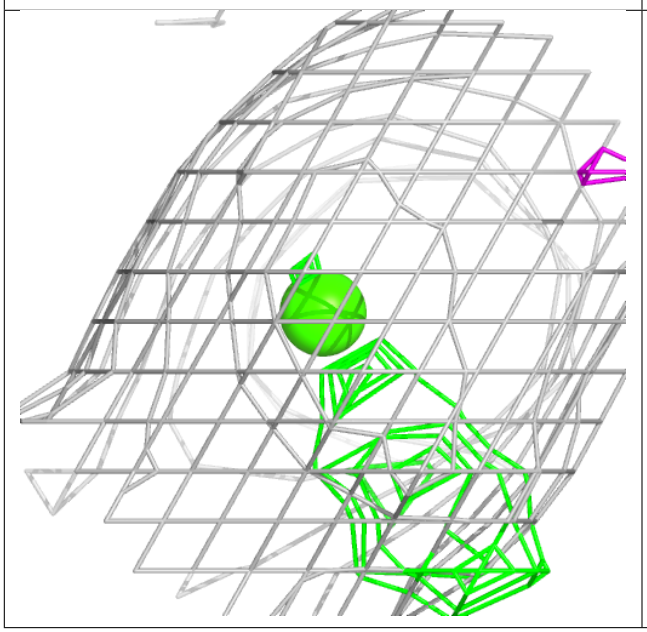
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

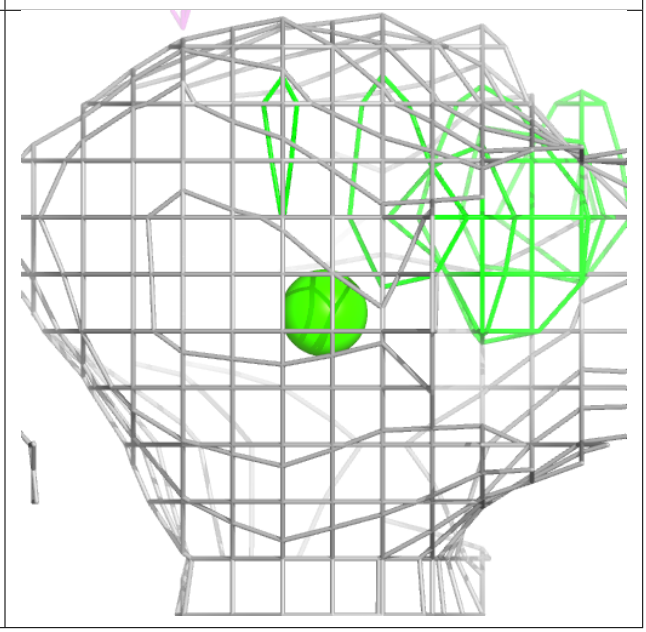


Electron density around CA U 1001:

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

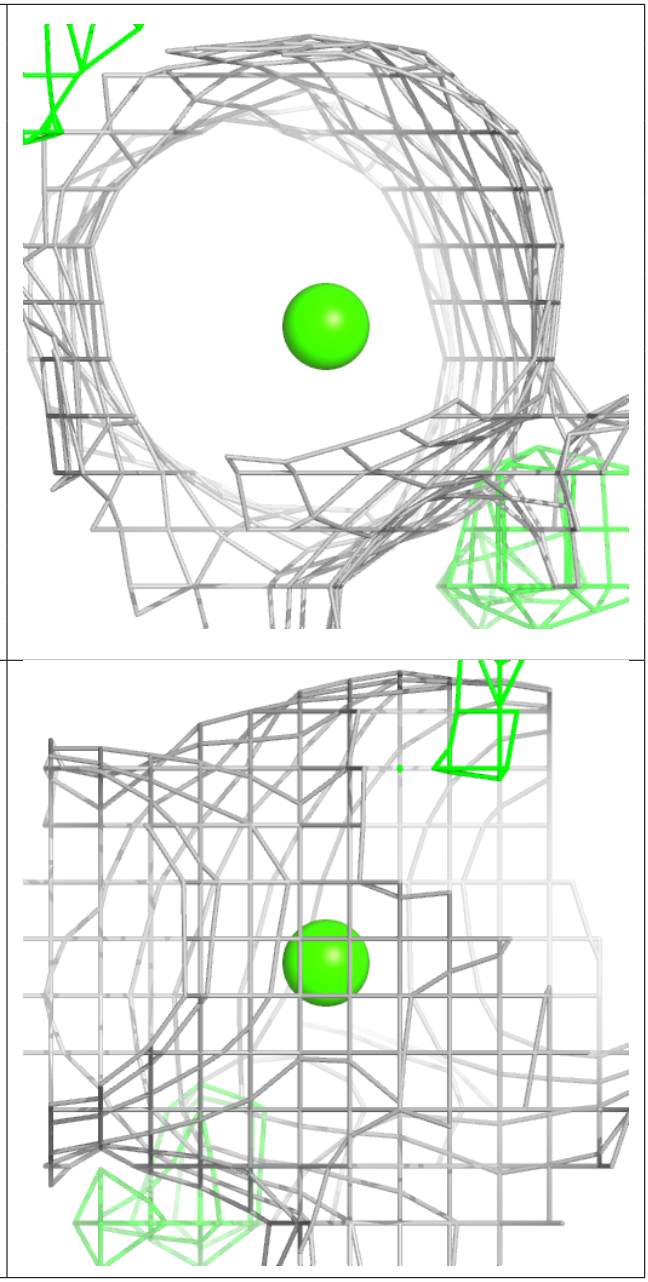






Electron density around CA h 203:

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



6.5 Other polymers (i)

Unable to reproduce the depositors R factor - this section is therefore empty.